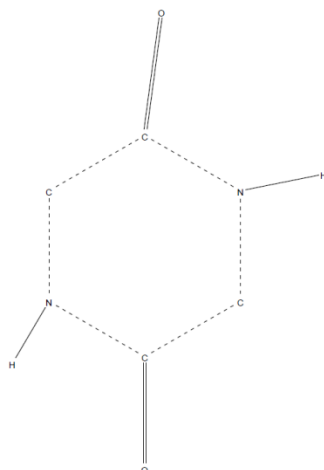


RESULTS OF SURVEY OF THE CSD:



DUBSIF

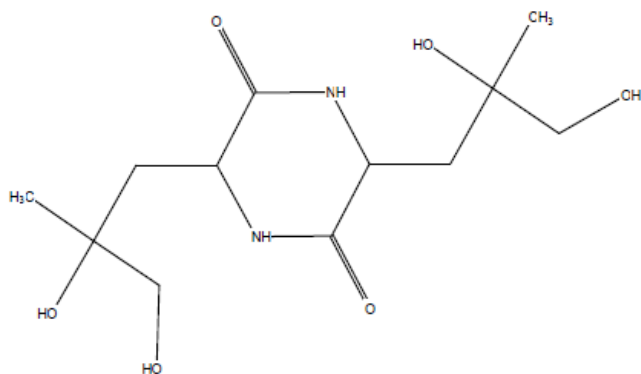
Reference: B.Edagwa, C.M.Taylor, F.R.Fronczek (2019)
CSD Communication(Private Communication) ,

Formula: C₁₂ H₂₂ N₂ O₆

Compound Name: 3,6-bis(2,3-dihydroxy-2-methylpropyl)piperazine-2,5-dione

Space Group: P212121 **Cell:** a 7.440(0) b 6.027(0) c 30.328(3)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.75 **Temperature(K):** 100 **Density(g/cm³):** 1.418



GESXOT02

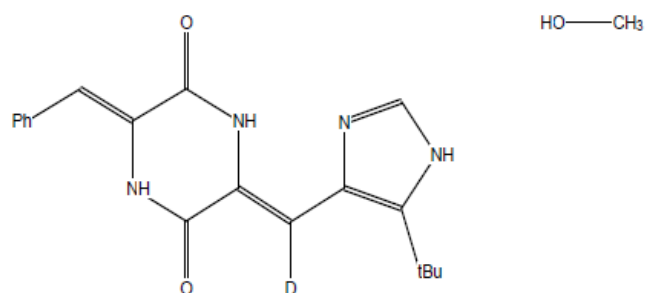
Reference: Mingxu Ma, Zhongpeng Ding, Shixiao Wang, Lingling Ma,
Yuxi Wang, Lili Zhong, Zhongping Li, Jinliang Yang, Wenbao Li (2019)
Bioorg.Med.Chem. ,27,1836

Formula: C₁₉ H₁₉ D₁ N₄ O₂,C₁ H₄ O₁

Compound Name: 3-benzylidene-6-((5-*t*-butyl-1H-imidazol-4-yl)deuteromethylene)
piperazine-2,5-dione methanol solvate

Space Group: P21/n **Cell:** a 14.619(0) b 17.039(0) c 16.071(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 103.56(0) γ 90.00

R-Factor (%): 5.76 **Temperature(K):** 293 **Density(g/cm³):** 1.258



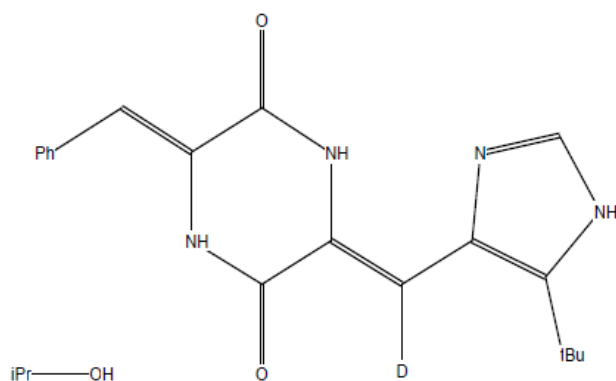
LOXJEQ

Reference: Mingxu Ma, Zhongpeng Ding, Shixiao Wang, Lingling Ma, Yuxi Wang, Lili Zhong, Zhongping Li, Jinliang Yang, Wenbao Li (2019) *Bioorg.Med.Chem.* ,**27**,1836

Formula: C₁₉ H₁₉ D₁ N₄ O₂ C₃ H₈ O₁

Compound Name: 3-benzylidene-6-[(5-t-butyl-1H-imidazol-4-yl)(deutero)methylidene]piperazine-2,5-dione propan-2-ol solvate

Space Group: P21/c **Cell:** **a** 11.784(1) **b** 8.365(0) **c** 22.778(2)
Space Group No.: 14 **Cell:** **(Å,°)** **α** 90.00 **β** 101.18(0) **γ** 90.00
R-Factor (%): 6.46 **Temperature(K):** 293 **Density(g/cm³):** 1.196



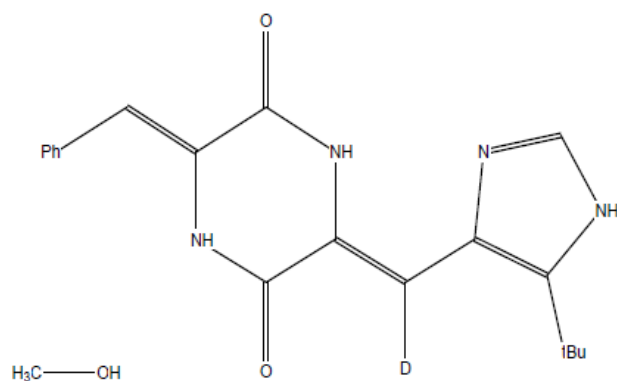
LOXJIU

Reference: Mingxu Ma, Zhongpeng Ding, Shixiao Wang, Lingling Ma, Yuxi Wang, Lili Zhong, Zhongping Li, Jinliang Yang, Wenbao Li (2019) *Bioorg.Med.Chem.* ,**27**,1836

Formula: C₁₉ H₁₉ D₁ N₄ O₂·2(C₁ H₄ O₁)

Compound Name: 3-benzylidene-6-[(5-t-butyl-1H-imidazol-4-yl)(deutero)methylidene]piperazine-2,5-dione methanol solvate

Space Group: P1 **Cell:** **a** 9.449(0) **b** 10.115(1) **c** 12.126(1)
Space Group No.: 1 **Cell:** **(Å,°)** **α** 101.77(0) **β** 96.73(0) **γ** 105.60(0)
R-Factor (%): 5.70 **Temperature(K):** 293 **Density(g/cm³):** 1.238



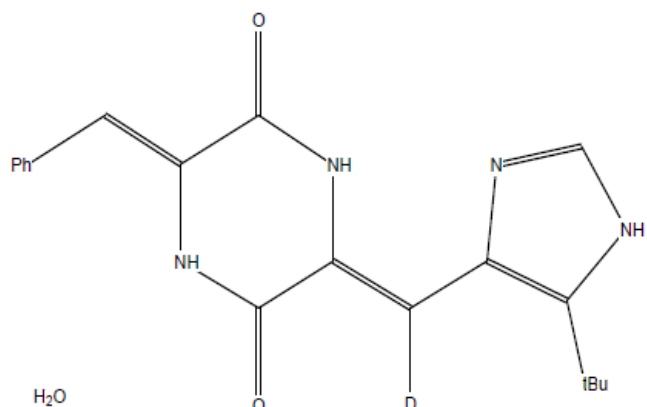
LOXJOA

Reference: Mingxu Ma, Zhongpeng Ding, Shixiao Wang, Lingling Ma, Yuxi Wang, Lili Zhong, Zhongping Li, Jinliang Yang, Wenbao Li (2019) *Bioorg.Med.Chem.* ,**27**,1836

Formula: C₁₉ H₁₉ D₁ N₄ O₂·H₂ O₁

Compound Name: 3-benzylidene-6-[(5-t-butyl-1H-imidazol-4-yl)(deutero)methylidene]piperazine-2,5-dione monohydrate

Space Group: P21/c **Cell:** **a** 9.705(0) **b** 8.525(0) **c** 22.007(1)
Space Group No.: 14 **Cell:** **(Å,°)** **α** 90.00 **β** 97.65(0) **γ** 90.00
R-Factor (%): 4.83 **Temperature(K):** 293 **Density(g/cm³):** 1.305



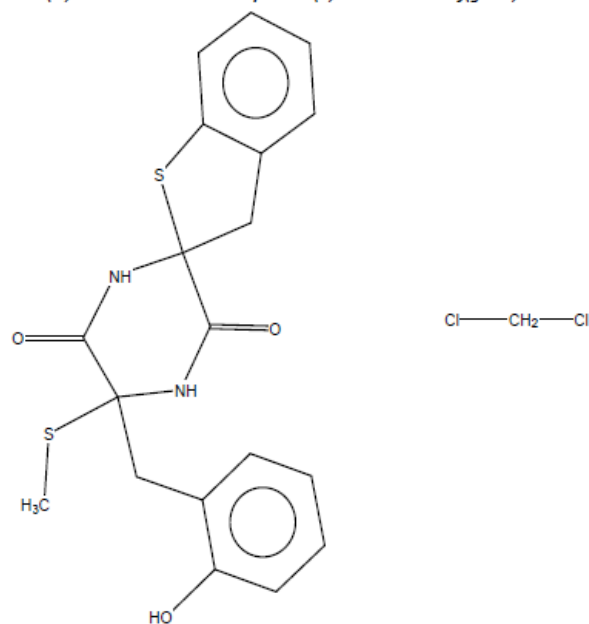
SUFXID

Reference: Xiao-Lu Li, Lu-Ping Chi, A.Navarro-Vazquez, Songhwan Hwang, P.Schmieder, Xiao-Ming Li, Xin Li, Sui-Qun Yang, Xinxiang Lei, Bin-Gui Wang, Han Sun (2020) *J.Am.Chem.Soc.* ,**142**, 2301

Formula: C₁₉ H₁₈ N₂ O₃ S₂·0.5(C₁ H₂ Cl₂)

Compound Name: 5'-[(2-hydroxyphenyl)methyl]-5'-(methylsulfanyl)-3H-spiro[[1]benzothiophene-2,2'-piperazine]-3',6'-dione dichloromethane solvate

Space Group: C2 **Cell:** **a** 23.324(1) **b** 6.769(0) **c** 13.915(0)
Space Group No.: 5 **Cell:** **(Å,°)** **α** 90.00 **β** 116.16(0) **γ** 90.00
R-Factor (%): 6.49 **Temperature(K):** 293 **Density(g/cm³):** 1.445



ABOTOB

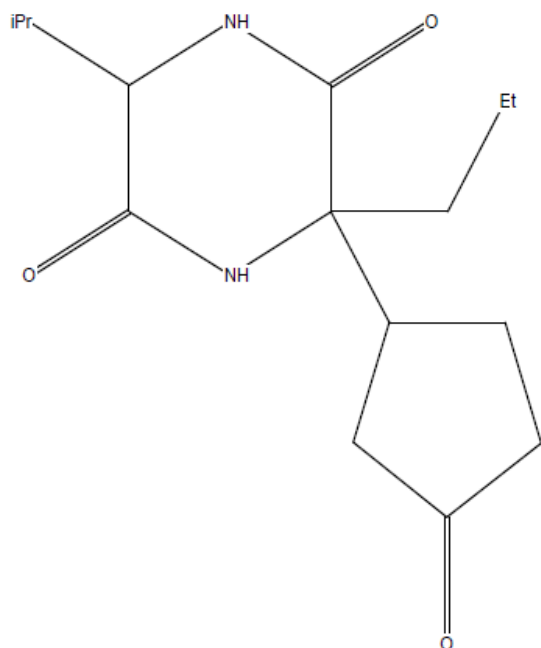
Reference: M.Andrei, C.Romming, K.Undheim (2004) *Tetrahedron:Asymm.* ,**15**,2711

Formula: C₁₅ H₂₄ N₂ O₃

Compound Name: (3R,6R)-6-Isopropyl-3-((1S)-3-oxocyclopentyl)-3-n-propylpiperazine-2,5-dione

Synonym: Cyclic peptide (2 residues): GLY*-VAL-

Space Group:	P21	Cell:	a 6.147(0)	b 14.671(1)	c 8.650(0)
Space Group No.:	4	(Å,°)	α 90.00	β 97.90(0)	γ 90.00
R-Factor (%):	3.03	Temperature(K):	105	Density(g/cm³):	1.205



AGETUE

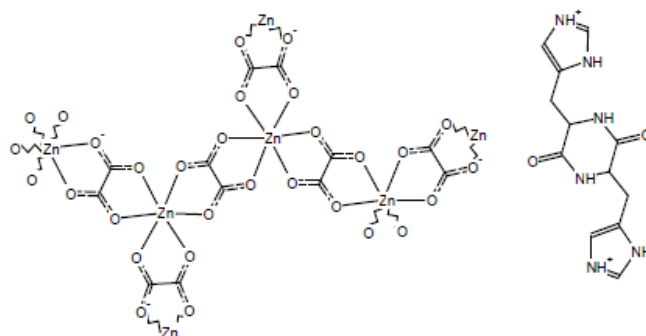
Reference: Jingyu Shi, Jing Li, Hongmei Zeng, Guohong Zou, Qinghua Zhang, Zhien Lin (2018) *Dalton Trans.* ,**47**,15288

Formula: (C₁₂ O₂₄ Zn₄⁴⁺)_n·2(C₁₂ H₁₆ N₆ O₂²⁺)

Compound Name: catena-(bis(5,5'-[(3,6-dioxopiperazine-2,5-diyf)]bis(methylene))bis(1H-imidazol-3-ium)) hexakis(μ-oxalato)-tetra-zinc(ii)

Synonym: SCU-63

Space Group:	P-1	Cell:	a 8.418(0)	b 9.148(0)	c 16.421(0)
Space Group No.:	2	(Å,°)	α 84.69(0)	β 84.26(0)	γ 71.50(0)
R-Factor (%):	3.20	Temperature(K):	292	Density(g/cm³):	1.872



AGEVAM

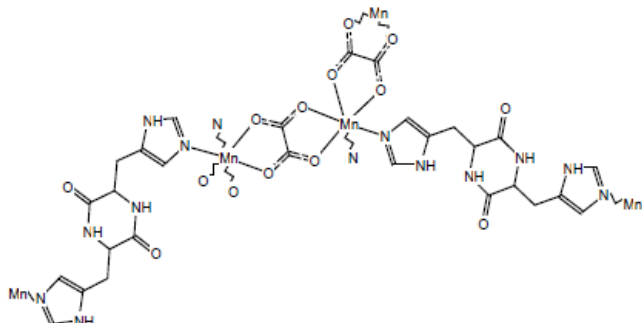
Reference: Jingyu Shi, Jing Li, Hongmei Zeng, Guohong Zou, Qinghua Zhang, Zhien Lin (2018) *Dalton Trans.* ,**47**,15288

Formula: (C₂₈ H₂₈ Mn₂ N₁₂ O₁₂)_n

Compound Name: catena-(bis(μ-3,6-bis((1H-imidazol-5-yl)methyl)piperazine-2,5-dione)-bis(μ-oxalato)-di-manganese(ii))

Synonym: SCU-66

Space Group:	P21/c	Cell:	a 9.782(0)	b 11.574(0)	c 14.918(0)
Space Group No.:	14	(Å,°)	α 90.00	β 95.66(0)	γ 90.00
R-Factor (%):	4.56	Temperature(K):	293	Density(g/cm³):	1.649



AJAGEX

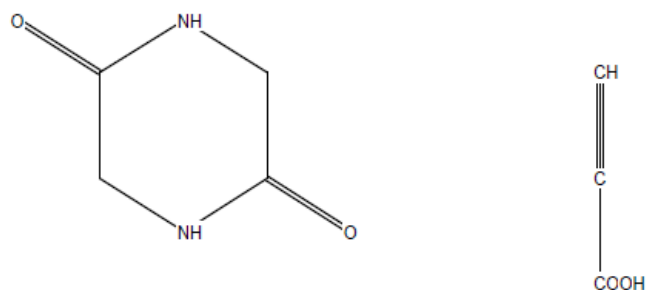
Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.* ,**2**,337

Formula: C₄ H₈ N₂ O₂·2(C₃ H₂ O₂)

Compound Name: Piperazine-2,5-dione bis(propionic acid)

Synonym: Cyclo(glycyl-glycyl) bis(propionic acid); Cyclic peptide (2 residues): GLY-GLY-

Space Group:	P21/c	Cell:	a 9.374(0)	b 29.318(2)	c 12.588(0)
Space Group No.:	14	(Å,°)	α 90.00	β 102.96(0)	γ 90.00
R-Factor (%):	4.16	Temperature(K):	90	Density(g/cm³):	1.502



AJAGIB

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

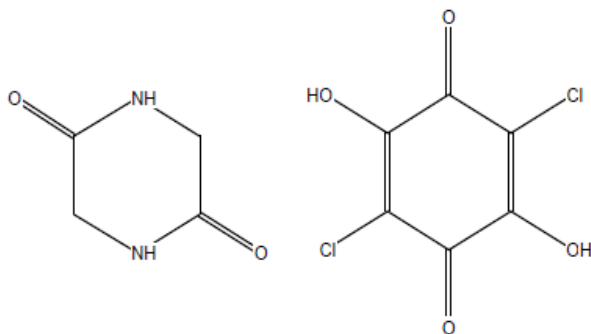
Formula: C₄ H₈ N₂ O₂, C₈ H₂ Cl₂ O₄

Compound Name: Piperazine-2,5-dione chloranilic acid

Synonym: Cyclo(glycyl-glycyl) chloranilic acid;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P21/c **Cell:** a 9.828(1) b 6.194(0) c 10.646(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 106.62(0) γ 90.00

R-Factor (%): 3.83 **Temperature(K):** 90 **Density(g/cm³):** 1.728



AJAGOH

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

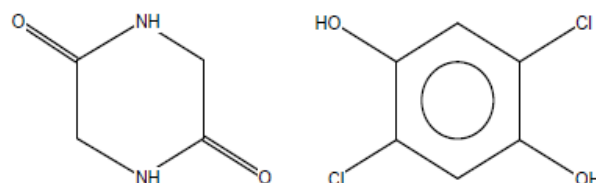
Formula: C₄ H₈ N₂ O₂, C₈ H₄ Cl₂ O₂

Compound Name: Piperazine-2,5-dione 2,5-dichloro-1,4-hydroquinone

Synonym: Cyclo(glycyl-glycyl) 2,5-dichloro-1,4-hydroquinone;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P21/n **Cell:** a 8.895(2) b 5.118(1) c 12.390(3)
Space Group No.: 14 **(Å,°)** α 90.00 β 107.17(0) γ 90.00

R-Factor (%): 3.68 **Temperature(K):** 90 **Density(g/cm³):** 1.806



AJAGUN

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

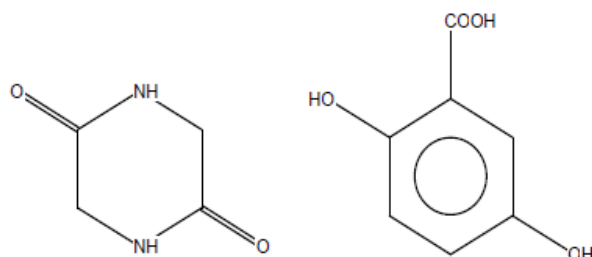
Formula: C₄ H₈ N₂ O₂, C₇ H₆ O₄

Compound Name: Piperazine-2,5-dione 2,5-dihydroxybenzoic acid

Synonym: Cyclo(glycyl-glycyl) 2,5-dihydroxybenzoic acid;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: Pna21 **Cell:** a 26.332(1) b 6.355(0) c 12.914(0)
Space Group No.: 33 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.04 **Temperature(K):** 90 **Density(g/cm³):** 1.649



AJAHAU

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

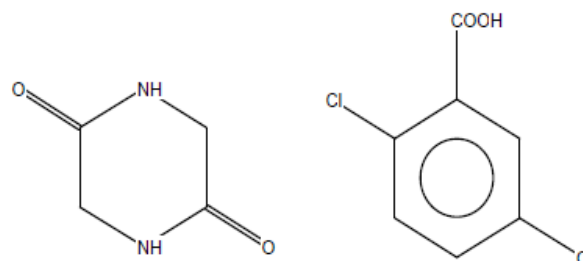
Formula: C₄ H₈ N₂ O₂, 2(C₇ H₄ Cl₂ O₂)

Compound Name: Piperazine-2,5-dione bis(2,5-dichlorobenzoic acid)

Synonym: Cyclo(glycyl-glycyl) bis(2,5-dichlorobenzoic acid);
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P21/n **Cell:** a 3.847(0) b 6.173(0) c 40.630(3)
Space Group No.: 14 **(Å,°)** α 90.00 β 90.78(0) γ 90.00

R-Factor (%): 4.64 **Temperature(K):** 90 **Density(g/cm³):** 1.708



AJAHEY

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

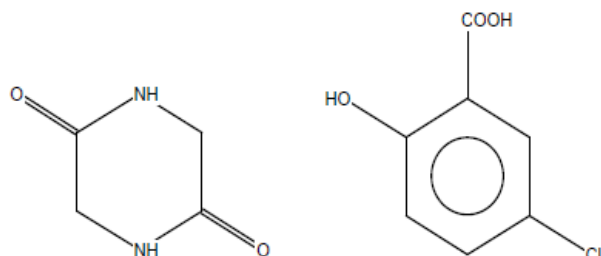
Formula: C₄ H₈ N₂ O₂, 2(C₇ H₅ Cl₁ O₃)

Compound Name: Piperazine-2,5-dione bis(5-chloro-2-hydroxybenzoic acid)

Synonym: Cyclo(glycyl-glycyl) bis(5-chloro-2-hydroxybenzoic acid);
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P21/n **Cell:** a 11.816(2) b 5.455(1) c 14.331(3)
Space Group No.: 14 **(Å,°)** α 90.00 β 98.25(0) γ 90.00

R-Factor (%): 3.82 **Temperature(K):** 90 **Density(g/cm³):** 1.668



AJAHIC

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

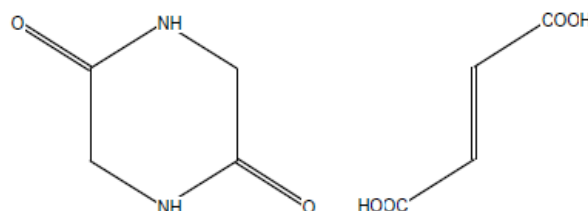
Formula: C₄ H₈ N₂ O₂, C₄ H₄ O₄

Compound Name: Piperazine-2,5-dione fumaric acid

Synonym: Cyclo(glycyl-glycyl) fumaric acid;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P-1 **Cell:** a 5.936(0) b 6.594(0) c 7.304(1)
Space Group No.: 2 **(Å,°)** α 109.26(0) β 90.76(0) γ 116.53(0)

R-Factor (%): 4.10 **Temperature(K):** 90 **Density(g/cm³):** 1.612



AJAHOI

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

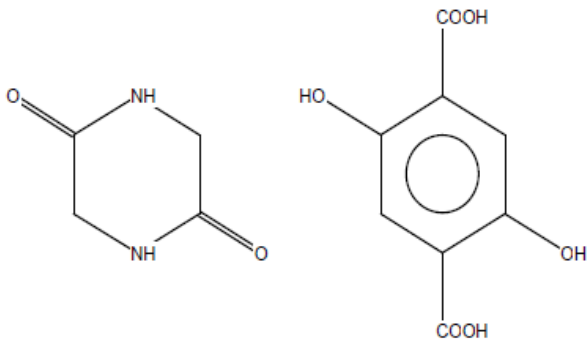
Formula: C₄ H₈ N₂ O₂, C₈ H₈ O₈

Compound Name: Piperazine-2,5-dione 2,5-dihydroxyterephthalic acid

Synonym: Cyclo(glycyl-glycyl) 2,5-dihydroxyterephthalic acid;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P-1 **Cell:** **a** 6.570(0) **b** 6.686(1) **c** 6.961(1)
Space Group No.: 2 **(Å,°)** α 97.89(0) β 93.11(0) γ 93.43(0)

R-Factor (%): 3.96 **Temperature(K):** 90 **Density(g/cm³):** 1.718



AJAHUO

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

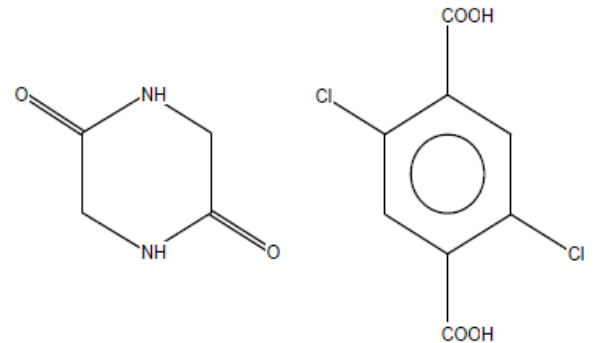
Formula: C₄ H₈ N₂ O₂, C₈ H₄ Cl₂ O₄

Compound Name: Piperazine-2,5-dione 2,5-dichloroterephthalic acid

Synonym: Cyclo(glycyl-glycyl) 2,5-dichloroterephthalic acid;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P-1 **Cell:** **a** 6.639(1) **b** 6.991(1) **c** 7.063(1)
Space Group No.: 2 **(Å,°)** α 100.37(0) β 97.43(0) γ 92.84(0)

R-Factor (%): 4.18 **Temperature(K):** 90 **Density(g/cm³):** 1.818



AJAJEA

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

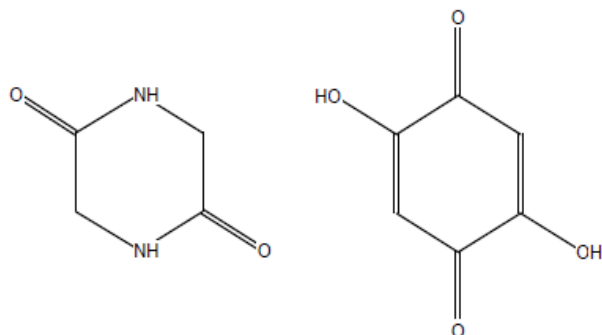
Formula: C₄ H₈ N₂ O₂, C₈ H₄ O₄

Compound Name: Piperazine-2,5-dione 2,5-dihydroxy-p-benzoquinone

Synonym: Cyclo(glycyl-glycyl) 2,5-dihydroxy-p-benzoquinone;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P-1 **Cell:** **a** 5.322(1) **b** 7.831(3) **c** 12.080(4)
Space Group No.: 2 **(Å,°)** α 99.81(0) β 91.11(0) γ 91.28(0)

R-Factor (%): 9.27 **Temperature(K):** 90 **Density(g/cm³):** 1.703



AJAJEA01

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, 2,337

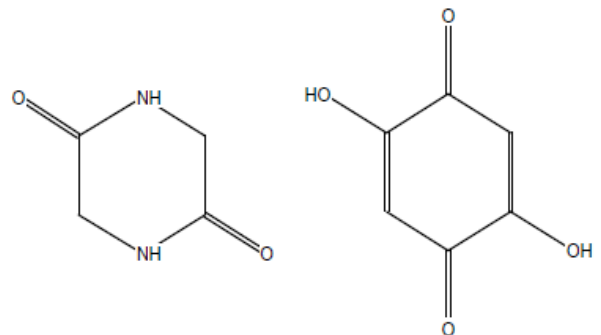
Formula: C₄ H₈ N₂ O₂, C₈ H₄ O₄

Compound Name: Piperazine-2,5-dione 2,5-dihydroxy-p-benzoquinone

Synonym: Cyclo(glycyl-glycyl) 2,5-dihydroxy-p-benzoquinone;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P21/c **Cell:** **a** 12.080(4) **b** 6.278(2) **c** 6.788(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 95.02(0) γ 90.00

R-Factor (%): 12.01 **Temperature(K):** 90 **Density(g/cm³):** 1.646



AJAJIE

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore (2002) *Cryst. Growth Des.*, **2**,337

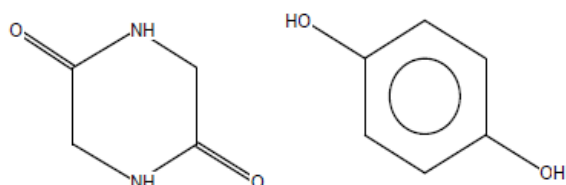
Formula: C₄ H₈ N₂ O₂, C₈ H₈ O₂

Compound Name: Piperazine-2,5-dione 1,4-hydroquinone

Synonym: Cyclo(glycyl-glycyl) 1,4-hydroquinone;
Cyclic peptide (2 residues): GLY-GLY-

Space Group: P1 **Cell:** **a** 5.477(0) **b** 6.463(0) **c** 7.526(1)
Space Group No.: 1 **(Å, °)** **α** 94.20(0) **β** 95.27(0) **γ** 114.94(0)

R-Factor (%): 3.80 **Temperature(K)**: 90 **Density(g/cm³)**: 1.560



ANTSUL10

Reference: R.B. Von Dreele (1981)
Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem., **37**,93

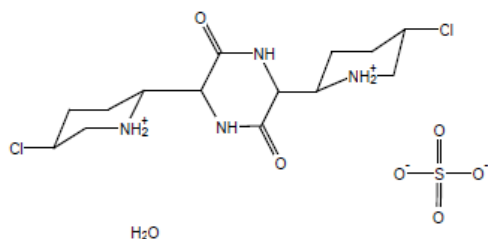
Formula: C₁₄ H₂₄ Cl₂ N₄ O₂²⁺, O₄ S₁²⁻, 5(H₂O)

Compound Name: (3S,6S)-3,6-bis((2R,5S)-5-Chloro-2-piperidinio)-piperazine-2,5-dione sulfate pentahydrate

Synonym: Cyclo(H-streptolutyl-H-streptolutyl) sulfate pentahydrate

Space Group: P2₁2₁2₁ **Cell:** **a** 26.570(14) **b** 14.913(8) **c** 6.006(3)
Space Group No.: 19 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 8.66 **Temperature(K)**: 295 **Density(g/cm³)**: 1.500



ANTSUL

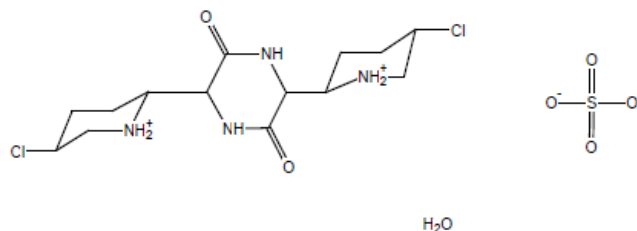
Reference: G.R.Pettit, R.B. Von Dreele, D.L.Herald, M.T.Edgar,
H.B.Wood Junior (1976) *J. Am. Chem. Soc.*, **98**,6742

Formula: C₁₄ H₂₄ Cl₂ N₄ O₂²⁺, O₄ S₁²⁻, 5(H₂O)

Compound Name: Antibiotic 593A sulfate pentahydrate

Space Group: P2₁2₁2₁ **Cell:** **a** 26.570(14) **b** 14.913(8) **c** 6.006(3)
Space Group No.: 19 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 8.72 **Temperature(K)**: 295 **Density(g/cm³)**: 1.500



BAGYOX

Reference: T.Shiba, H.Uratani, I.Kubota, Y.Sumii (1981) *Biopolymers*, **20**,1985

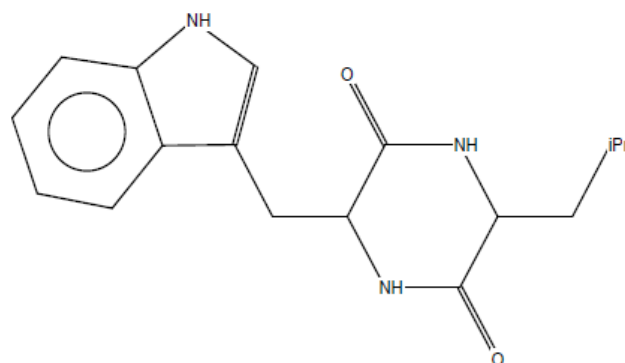
Formula: C₁₇ H₂₁ N₃ O₂

Compound Name: Cyclo(L-leucyl-L-tryptophyl)

Synonym: Cyclic peptide (2 residues): LEU-TRP-

Space Group: 0 **Cell:** **a** 0.000 **b** 0.000 **c** 0.000
Space Group No.: 0 **(Å, °)** **α** 0.00 **β** 0.00 **γ** 0.00

R-Factor (%): 0.00 **Temperature(K)**: 295 **Density(g/cm³)**: 0.000



BCYMYC

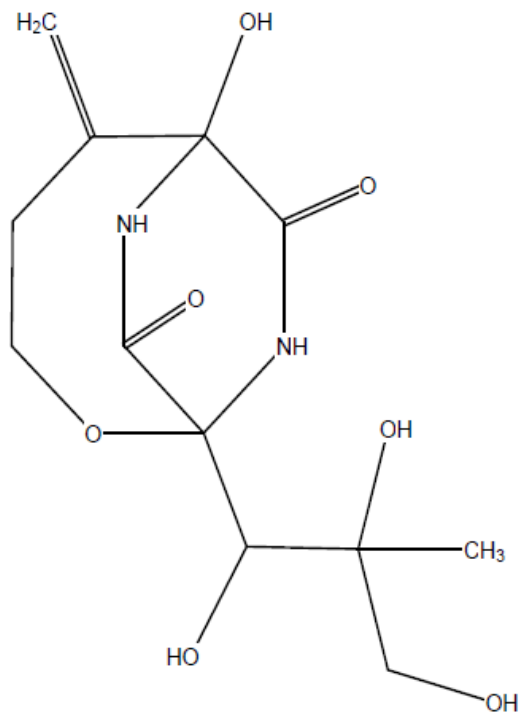
Reference: Y.Tokuma, S.Koda, T.Miyoshi, Y.Morimoto (1974)
Bull.Chem.Soc.Jpn., **47**,18

Formula: C₁₂ H₁₈ N₂ O₇

Compound Name: Bicyclomycin

Space Group: P212121 **Cell:** **a** 11.720(10) **b** 12.720(10) **c** 8.800(10)
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 7.00 **Temperature(K)**: 295 **Density(g/cm³)**: 1.530



BEMYEY

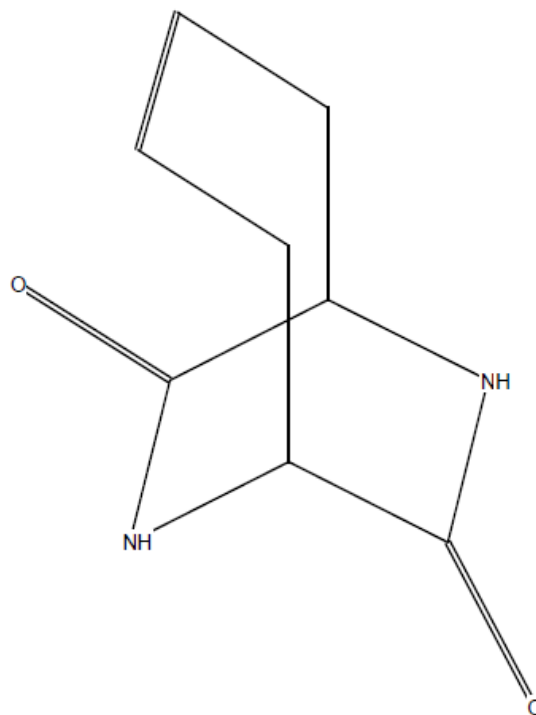
Reference: Yanming Du, C.J.Creighton, B.A.Tounge, A.B.Reitz (2004)
Org.Lett., **6**,309

Formula: C₈ H₁₀ N₂ O₂

Compound Name: 7,9-Diaza-bicyclo(4.2.2)dec-3-ene-8,10-dione

Space Group: P212121 **Cell:** **a** 6.099(0) **b** 9.948(1) **c** 13.123(1)
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 4.15 **Temperature(K)**: 193 **Density(g/cm³)**: 1.386



BEMYIC

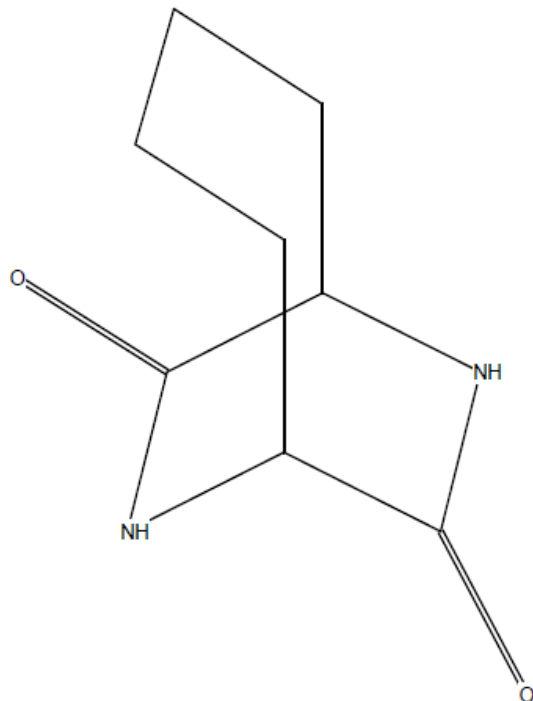
Reference: Yanming Du, C.J.Creighton, B.A.Toung, A.B.Reitz (2004)
Org.Lett. ,6,309

Formula: C₈ H₁₂ N₂ O₂

Compound Name: 7,9-Diaza-bicyclo(4.2.2)decane-8,10-dione

Space Group: P21 **Cell:** a 7.528(1) b 9.814(1) c 11.777(1)
Space Group No.: 4 **(Å,°)** α 90.00 β 96.54(0) γ 90.00

R-Factor (%): 5.21 **Temperature(K):** 193 **Density(g/cm³):** 1.292



BIMGEJ

Reference: G.Valle (1982) *Eur.Cryst.Meeting* ,7,190

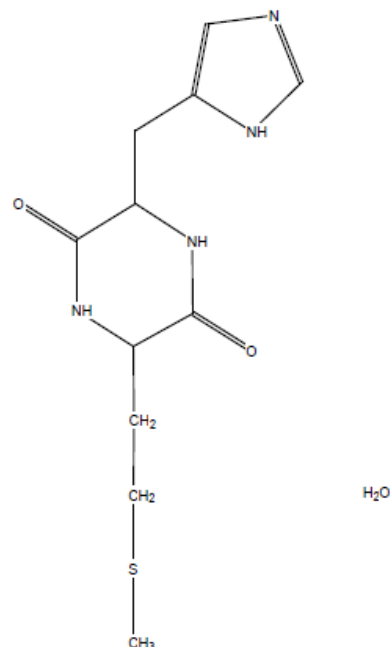
Formula: C₁₁ H₁₆ N₄ O₂ S₁·H₂ O₁

Compound Name: Cyclo-(L-methionyl-L-histidine) monohydrate

Synonym: Cyclic peptide (2 residues): MET-HIS-

Space Group: P212121 **Cell:** a 29.445(7) b 7.898(4) c 6.047(4)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 10.50 **Temperature(K):** 295 **Density(g/cm³):** 1.352



BIMGEJ10

Reference: M.Bressan, F.Marchiori, G.Valle (1984)
Int.J.Pept.Protein Res. ,23,104

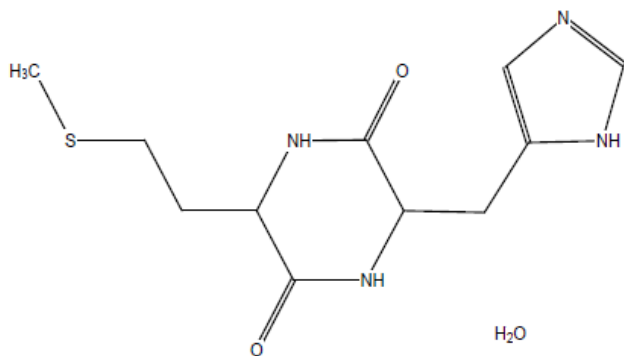
Formula: C₁₁ H₁₆ N₄ O₂ S₁·H₂ O₁

Compound Name: Cyclo-(L-histidyl-L-methionine) monohydrate

Synonym: Cyclic peptide (2 residues): MET-HIS-

Space Group: P212121 **Cell:** a 29.445(7) b 7.898(4) c 6.047(4)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.34 **Temperature(K):** 295 **Density(g/cm³):** 1.353



BIMGIN

Reference: G.Valle (1982) *Eur.Cryst.Meeting* ,7,190

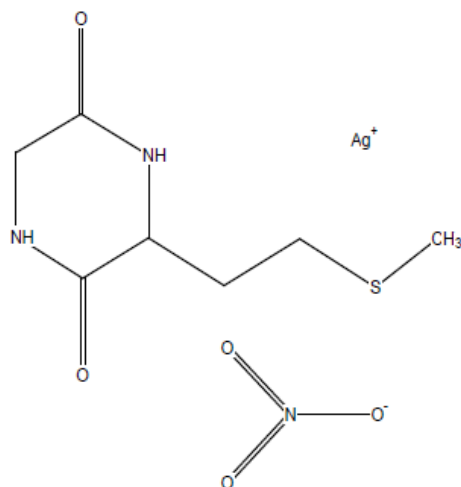
Formula: C₇ H₁₂ N₂ O₂ S₁·N₁ O₃¹⁻·Ag₁¹⁺

Compound Name: Cyclo-L-methionyl-glycine silver nitrate

Synonym: Cyclic peptide (2 residues): MET-GLY-

Space Group: P21 **Cell:** a 13.634(5) b 6.225(3) c 6.784(4)
Space Group No.: 4 **(Å,°)** α 90.00 β 104.84 γ 90.00

R-Factor (%): 5.50 **Temperature(K):** 295 **Density(g/cm³):** 2.136



BIMGIN10

Reference: G.Valle, R.Ettore (1983) *J.Chem.Soc.,Dalton Trans.* ,453

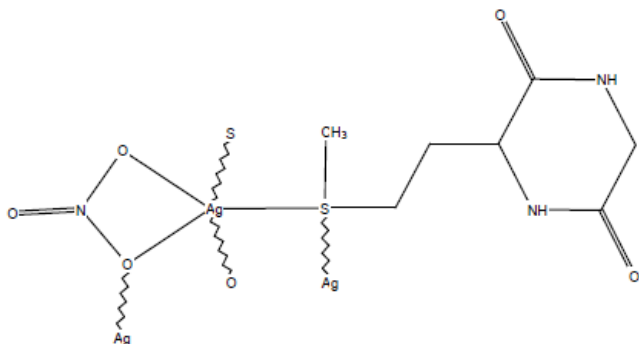
Formula: (C₇ H₁₂ Ag₁ N₃ O₅ S₁)ⁿ

Compound Name: catena((Cyclo-L-methionyl-glycine)-(nitrate-O,O')-silver(ii))

Synonym: catena-(μ₂-3-(2'-Methylthioethyl)-piperazine-2,5-dione-S)-(μ₂-nitrate-O, O':O',O')-silver(i)

Space Group: P21 **Cell:** a 13.634(6) b 6.225(4) c 6.784(4)
Space Group No.: 4 **(Å,°)** α 90.00 β 104.80(70) γ 90.00

R-Factor (%): 5.20 **Temperature(K):** 295 **Density(g/cm³):** 2.137



BIVMUO

Reference: M.Bressan, R.Ettore, F.Marchiori, G.Valle (1982) *Int.J.Pept.Protein Res.* ,19,402

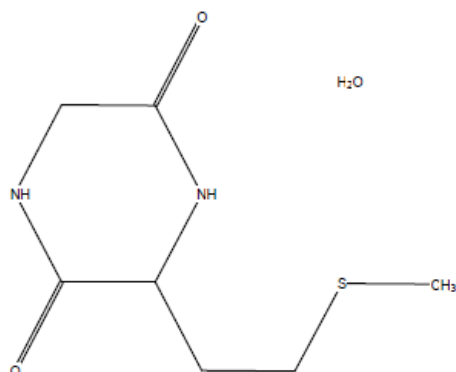
Formula: C₇ H₁₂ N₂ O₂ S₁·3(H₂ O₁)

Compound Name: Cyclo-L-methionyl-glycine trihydrate

Synonym: Cyclic peptide (2 residues): MET-GLY-

Space Group: P212121 **Cell:** a 28.915(6) b 6.698(3) c 6.186(3)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.34 **Temperature(K):** 295 **Density(g/cm³):** 1.343



BOCSIV

Reference: K.Suguna, S.Ramakumar, N.Shamala, B.V.V.Prasad, P.Balaram (1982) *Biopolymers* ,21,1847

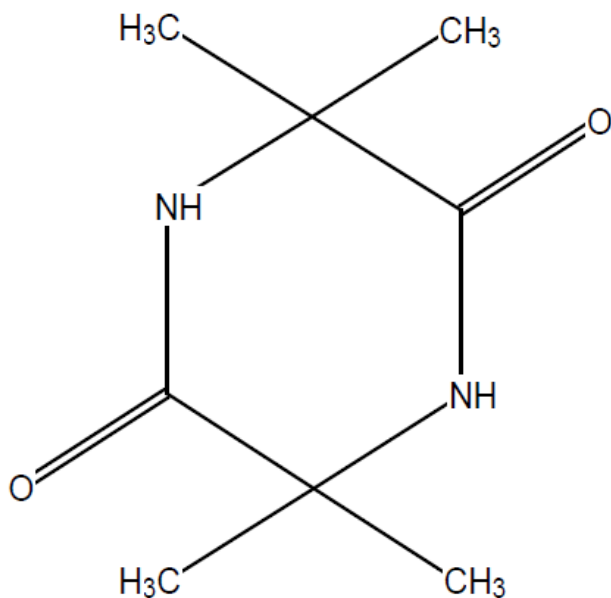
Formula: C₈ H₁₄ N₂ O₂

Compound Name: Cyclo-bis(α-aminoisobutyryl)

Synonym: Cyclic peptide (2 residues): AIB-AIB-

Space Group: P-1 **Cell:** a 5.649(3) b 5.865(2) c 8.363(1)
Space Group No.: 2 **(Å,°)** α 69.89(6) β 113.04(8) γ 116.00(30)

R-Factor (%): 8.50 **Temperature(K):** 295 **Density(g/cm³):** 1.261



BOCSIV01

Reference: S.W.Gordon-Wylie, E.Teplin, J.C.Morris, M.I.Trombley, S.M.McCarthy, W.M.Cleaver, G.R.Clark (2004) *Cryst.Growth Des.* ,4, 789

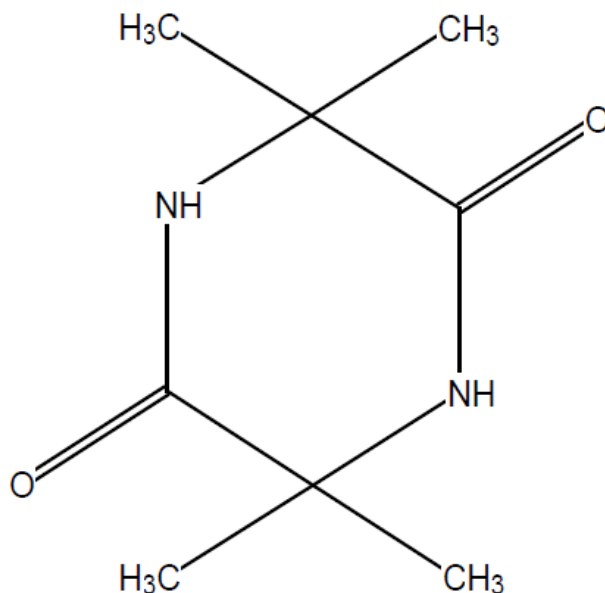
Formula: C₈ H₁₄ N₂ O₂

Compound Name: Cyclo-bis(α-aminoisobutyryl)

Synonym: 3,3,6,6-Tetramethylpiperazine-2,5-dione;
Cyclic peptide (2 residues): AIB-AIB-

Space Group: P-1 **Cell:** a 5.653(1) b 5.876(1) c 8.049(2)
Space Group No.: 2 **(Å,°)** α 92.91(1) β 106.97(1) γ 116.02(1)

R-Factor (%): 4.61 **Temperature(K):** 296 **Density(g/cm³):** 1.258



BOCSOB

Reference: K.Suguna, S.Ramakumar, N.Shamala, B.V.V.Prasad, P.Balaram (1982) *Biopolymers*, **21**,1847

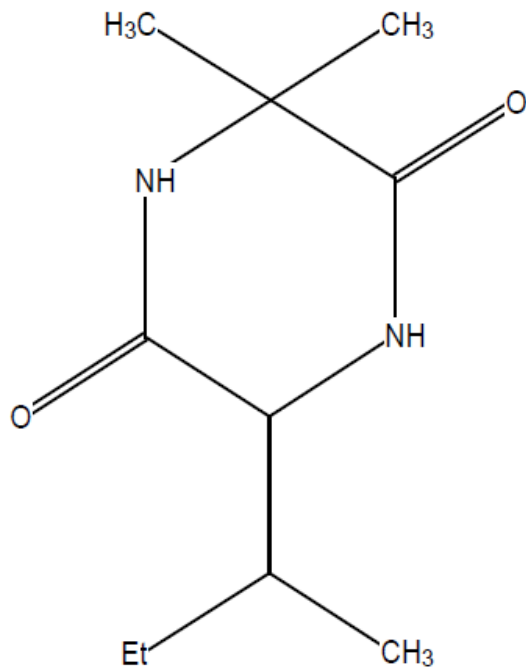
Formula: C₁₀ H₁₈ N₂ O₂

Compound Name: Cyclo(α -aminoisobutyryl-isoleucyl)

Synonym: Cyclic peptide (2 residues): AIB-Ile-

Space Group: P212121 **Cell:** **a** 6.177(1) **b** 10.791(1) **c** 16.676(1)
Space Group No.: 19 **($\text{\AA},^\circ$)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.60 **Temperature(K)**: 295 **Density(g/cm³)**: 1.185



BUPZOB

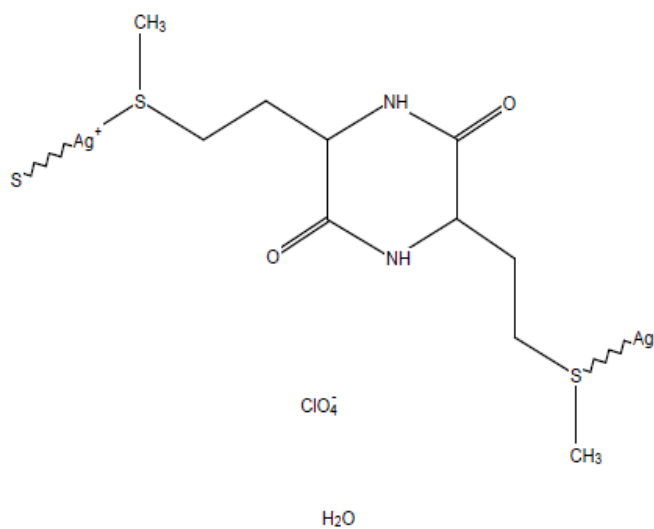
Reference: Y.Kojima, T.Yamashita, Y.Ishino, T.Hirashima, K.Hirotsu (1983) *Chem.Lett.*, 453

Formula: (C₁₀ H₁₈ Ag₁ N₂ O₂ S₂¹⁺)_n(Cl₁ O₄¹⁻)_{2n}(H₂ O₁)

Compound Name: catena-(μ_2 -Cyclo(L-methionyl-L-methionyl)-S,S')-silver(i) perchlorate dihydrate

Space Group: P212121 **Cell:** **a** 29.380(7) **b** 10.429(2) **c** 6.026(2)
Space Group No.: 19 **($\text{\AA},^\circ$)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.819



BUVKEJ

Reference: A.P.Mendham, R.A.Palmer, B.S.Potter, T.J.Dines, M.J.Snowden, R.Withnalland, B.Z.Chowdhry (2010) *J.Raman Spectrosc.* ,41,288

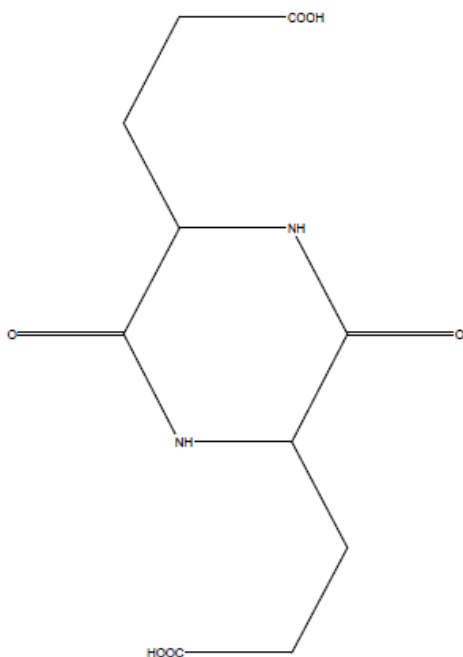
Formula: C₁₀ H₁₄ N₂ O₆

Compound Name: Cyclo(L-glutamyl-L-glutamyl)

Synonym: Cyclic peptide (2 residues): GLU-GLU-

Space Group: P21 **Cell:** **a** 6.744(0) **b** 10.859(1) **c** 7.840(0)
Space Group No.: 4 **(Å,°)** **α** 90.00 **β** 94.50(0) **γ** 90.00

R-Factor (%): 4.33 **Temperature(K):** 293 **Density(g/cm³):** 1.498



BUVKEJ01

Reference: A.P.Mendham, R.A.Palmer, B.S.Potter, T.J.Dines, M.J.Snowden, R.Withnalland, B.Z.Chowdhry (2010) *J.Raman Spectrosc.* ,41,288

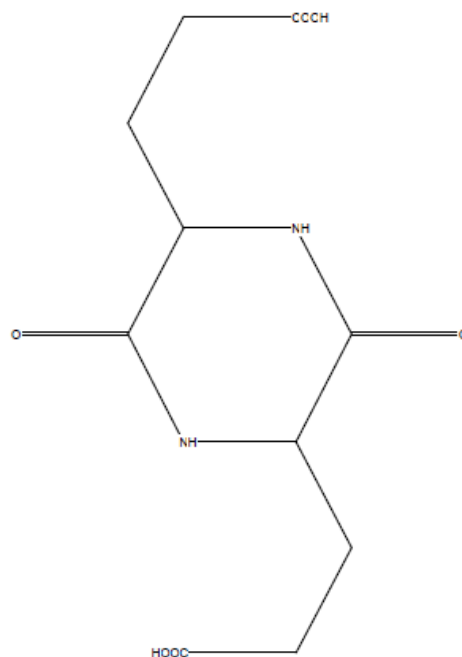
Formula: C₁₀ H₁₄ N₂ O₆

Compound Name: Cyclo(L-glutamyl-L-glutamyl)

Synonym: Cyclic peptide (2 residues): GLU-GLU-

Space Group: C2 **Cell:** **a** 13.954(1) **b** 6.664(1) **c** 6.148(1)
Space Group No.: 5 **(Å,°)** **α** 90.00 **β** 100.08(1) **γ** 90.00

R-Factor (%): 3.38 **Temperature(K):** 293 **Density(g/cm³):** 1.524



CANKEH

Reference: C.Howes, N.W.Alcock, B.T.Golding, R.W.McCabe (1983) *J.Chem.Soc.,Perkin Trans.1* ,2287

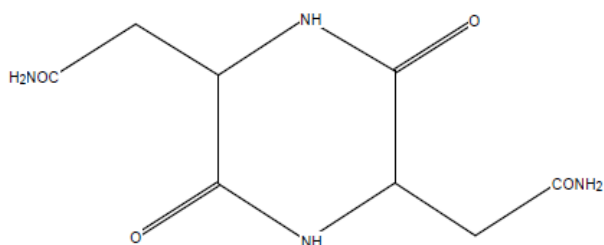
Formula: C₈ H₁₂ N₄ O₄

Compound Name: (3S,6S)-3,6-bis(Carbamoylmethyl)-piperazine-2,5-dione

Synonym: Cyclo-(l-asparagyl-L-asparagyl); Cyclic peptide (2 residues): ASN-ASN-

Space Group: P212121 **Cell:** **a** 5.400(3) **b** 5.732(3) **c** 31.831(18)
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 7.50 **Temperature(K):** 295 **Density(g/cm³):** 1.538



CATZUS

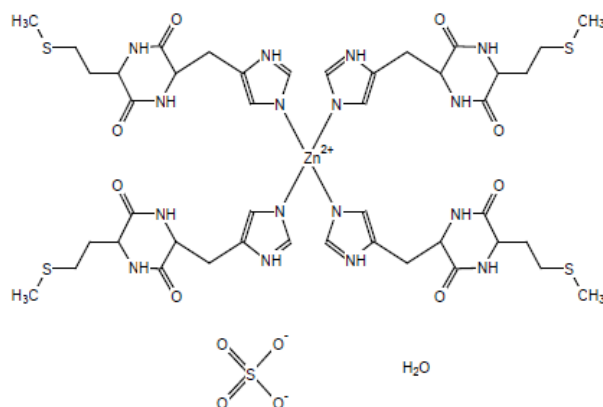
Reference: Y.Kojima, N.Ishio, T.Yamashita, K.Hirotsu (1983) *Chem.Lett.* ,1365

Formula: C₄₄ H₆₄ N₁₆ O₈ S₄ Zn₁²⁺,O₄ S₁²⁻,10(H₂O)

Compound Name: tetrakis(Cyclo-L-methionyl-L-histidyl-N)-zinc(ii) sulfate decahydrate

Space Group: P21 **Cell:** **a** 15.143(2) **b** 20.586(4) **c** 11.007(2)
Space Group No.: 4 **(Å,°)** **α** 90.00 **β** 97.89(1) **γ** 90.00

R-Factor (%): 7.50 **Temperature(K):** 295 **Density(g/cm³):** 1.383



CATZUS10

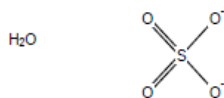
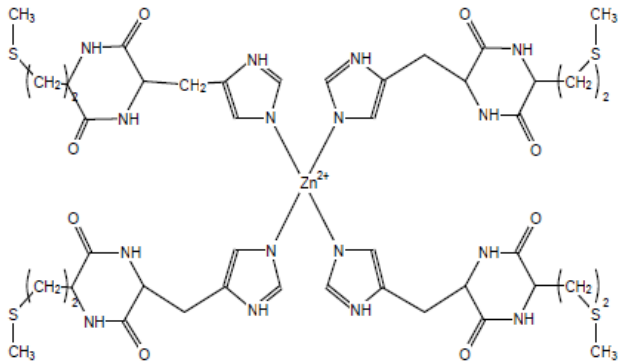
Reference: Y.Kojima, K.Hirotsu, T.Yamashita, T.Miwa (1985)
Bull.Chem.Soc.Jpn., **58**,1894

Formula: C₄₄ H₆₄ N₁₆ O₈ S₄ Zn₁²⁺·O₄ S₁²⁻·10(H₂O)₁

Compound Name: tetrakis(Cyclo(L-methionyl-L-histidyl))-zinc(II) sulfate decahydrate

Space Group: P21 **Cell:** **a** 15.143(2) **b** 20.586(4) **c** 11.007(2)
Space Group No.: 4 **(Å,°)** **α** 90.00 **β** 97.89(1) **γ** 90.00

R-Factor (%): 6.20 **Temperature(K):** 295 **Density(g/cm³):** 1.383



CEWFIV

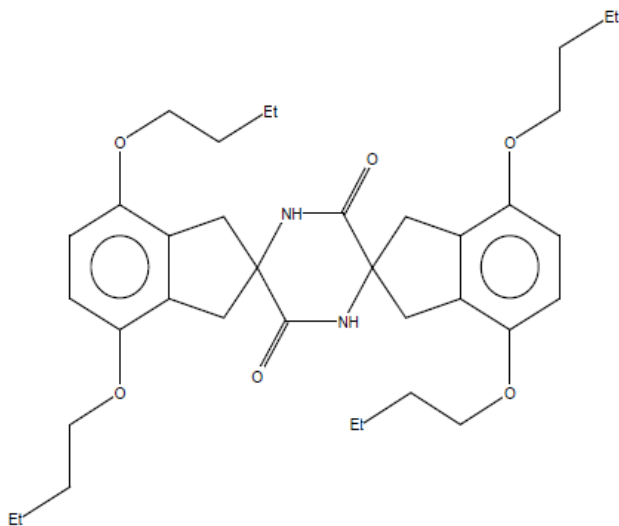
Reference: K.E.Wells, R.A.Weatherhead, F.N.Murigi, G.S.Nichol,
M.D.Carducci, H.D.Selby, E.A.Mash (2012) *Cryst.Growth Des.*, **12**,
5056

Formula: C₃₆ H₅₀ N₂ O₆

Compound Name: 4,4',7,7'-Tetrabutoxy-1,1',3,3'-tetrahydro-3H,6H-dispiro[indene-2,2'-piperazine-5',2''-indene]-3',6'-dione

Space Group: P21/n **Cell:** **a** 14.617(1) **b** 6.038(0) **c** 19.251(3)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 92.89(0) **γ** 90.00

R-Factor (%): 5.03 **Temperature(K):** 170 **Density(g/cm³):** 1.188



CEWFER

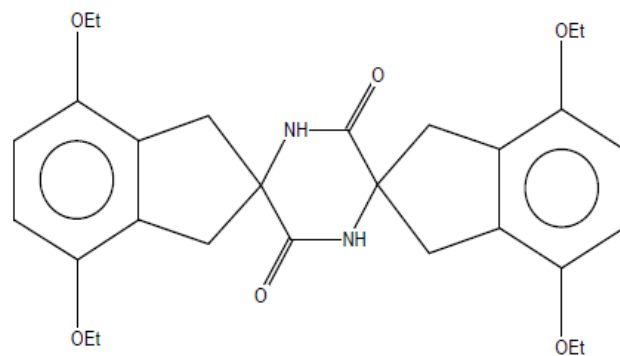
Reference: K.E.Wells, R.A.Weatherhead, F.N.Murigi, G.S.Nichol,
M.D.Carducci, H.D.Selby, E.A.Mash (2012) *Cryst.Growth Des.*, **12**,
5056

Formula: C₂₈ H₃₄ N₂ O₆

Compound Name: 4,4',7,7'-Tetraethoxy-1,1',3,3'-tetrahydro-3H,6H-dispiro[indene-2,2'-piperazine-5',2''-indene]-3',6'-dione

Space Group: P21/n **Cell:** **a** 9.843(1) **b** 6.119(0) **c** 21.635(3)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 91.33(0) **γ** 90.00

R-Factor (%): 4.23 **Temperature(K):** 170 **Density(g/cm³):** 1.261



CGLYTP

Reference: A.J.Morris, A.J.Geddes, B.Sheldrick (1974)
Cryst.Struct.Comm., **3**,345

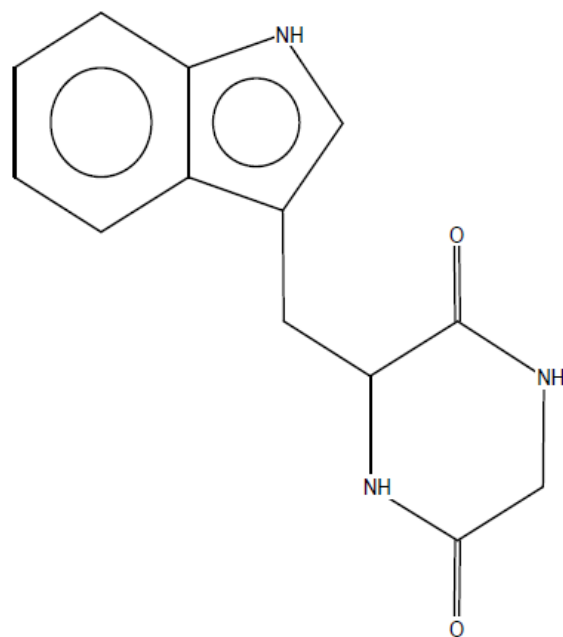
Formula: C₁₃ H₁₃ N₃ O₂

Compound Name: Cyclo(glycyl-tryptophyl)

Synonym: Cyclic peptide (2 residues): GLY-TRP-

Space Group: P21 **Cell:** **a** 7.600(4) **b** 6.167(3) **c** 12.232(7)
Space Group No.: 4 **(Å,°)** **α** 90.00 **β** 91.98(7) **γ** 90.00

R-Factor (%): 5.40 **Temperature(K):** 295 **Density(g/cm³):** 1.409



CHISCU

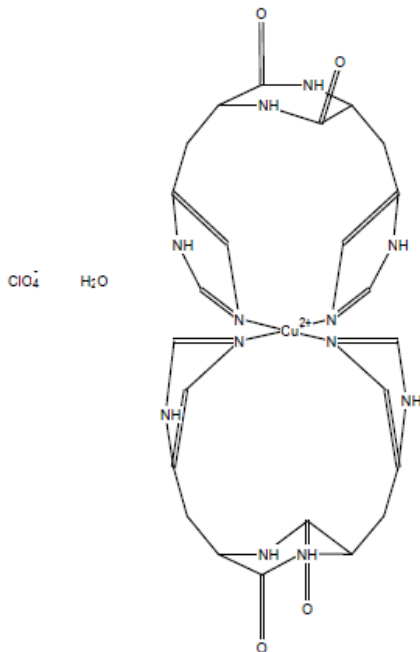
Reference: F.Hori, Y.Kojima, K.Matsumoto, S.Ooi, H.Kuroya (1979)
Bull.Chem.Soc.Jpn., **52**,1076

Formula: C₂₄ H₂₈ Cu₁ N₁₂ O₄²⁺·2(Cl₁ O₄¹⁻)·4(H₂ O₁)

Compound Name: bis(Cyclo-L-histidyl-L-histidyl)-copper(II) perchlorate tetrahydrate

Space Group: P3221 **Cell:** **a** 8.450(3) **b** 8.450(3) **c** 42.000(600)
Space Group No.: 154 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 120.00

R-Factor (%): 10.30 **Temperature(K):** 295 **Density(g/cm³):** 1.694



CLCYST

Reference: C.T.Lu, G.Kartha (1973) *ACS,Abstr.Papers(Summer)*, 188

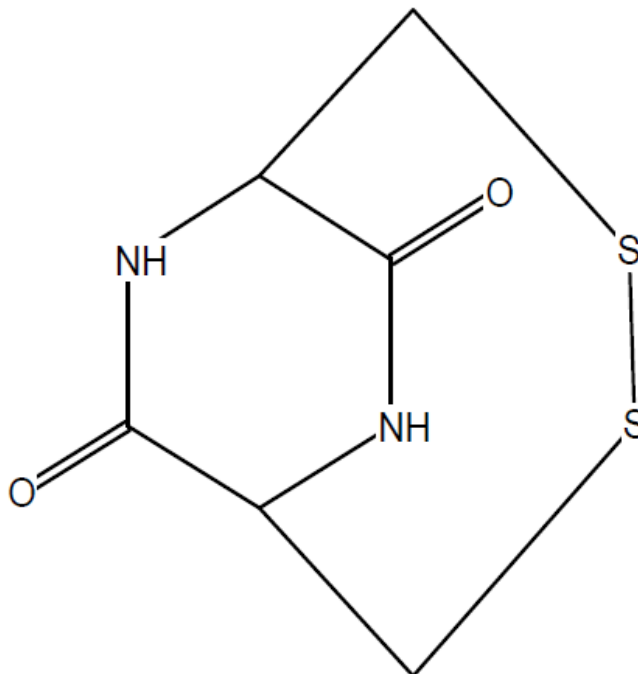
Formula: C₈ H₈ N₂ O₂ S₂

Compound Name: Cyclo-L-cystine

Synonym: Cyclic peptide (2 residues): CYS-CYS-

Space Group: P212121 **Cell:** **a** 11.220 **b** 12.870 **c** 5.980
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 8.20 **Temperature(K):** 295 **Density(g/cm³):** 1.571



CLCYST10

Reference: K.I.Varughese, C.T.Lu, G.Kartha (1981)
Int.J.Pept.Protein Res., **18**,88

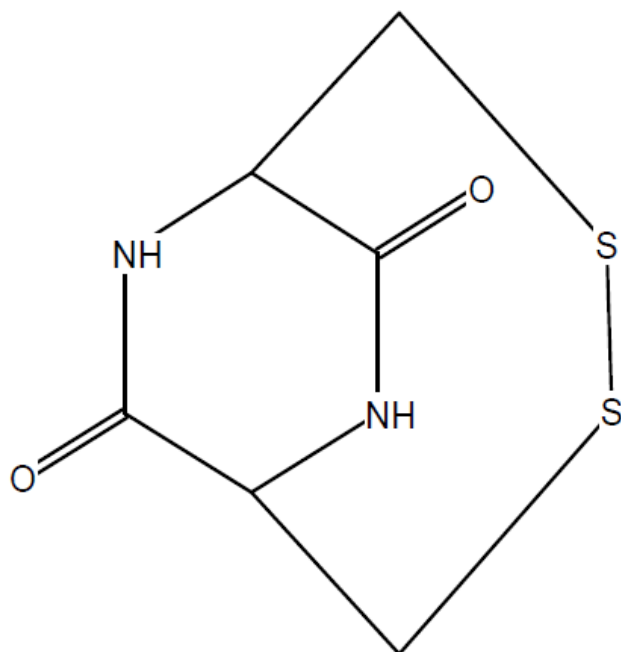
Formula: C₈ H₈ N₂ O₂ S₂

Compound Name: Cyclo-L-cystine

Synonym: Cyclic peptide (2 residues): CYS-CYS-

Space Group: P212121 **Cell:** **a** 11.216(4) **b** 12.874(4) **c** 5.978(3)
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 6.50 **Temperature(K):** 295 **Density(g/cm³):** 1.572



CLDVAL

Reference: E.Benedetti (1976)
Izv.Jug.Cent.Krist.,Ser.A(Bull.Yugoslav.Cryst.Centre,Sect.A), **11**,151

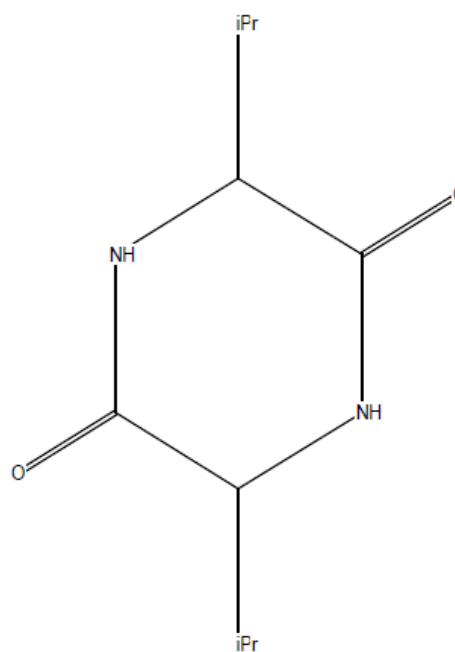
Formula: C₁₀ H₁₈ N₂ O₂

Compound Name: cyclo(L-Valyl-D-valyl)

Synonym: Cyclic peptide (2 residues): VAL-VAL-

Space Group: P-1 **Cell:** **a** 9.318(2) **b** 10.143(2) **c** 6.190(1)
Space Group No.: 2 **(Å,°)** **α** 99.40(30) **β** 99.20(30) **γ** 99.20(30)

R-Factor (%): 6.90 **Temperature(K):** 295 **Density(g/cm³):** 1.177



CLEUHS

Reference: I.Tanaka, T.Iwata, N.Takahashi, T.Ashida, M.Tanihara (1977) *Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem.*, **33**,3902

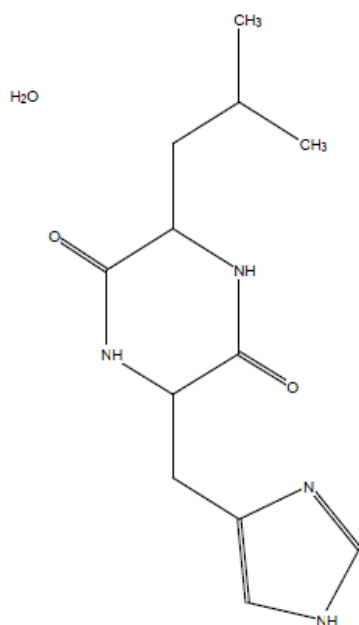
Formula: C₁₂ H₁₈ N₄ O₂·H₂O₁

Compound Name: Cyclo(L-leucyl-L-histidyl) monohydrate

Synonym: Cyclic peptide (2 residues): LEU-HIS-

Space Group: P212121 **Cell:** *a* 29.074(1) *b* 6.017(1) *c* 8.306(1)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.90 **Temperature(K):** 295 **Density(g/cm³):** 1.227



CLHISP10

Reference: R.Ramani, K.Venkatesan, R.E.Marsh (1978) *J.Am.Chem.Soc.*, **100**,949

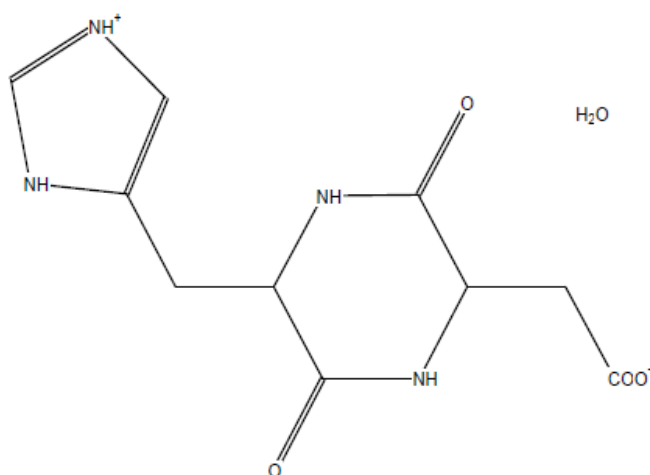
Formula: C₁₀ H₁₂ N₄ O₄·3(H₂O₁)

Compound Name: Cyclo(L-histidyl-L-aspartyl) trihydrate

Synonym: Cyclic peptide (2 residues): HIS-ASP-

Space Group: P212121 **Cell:** *a* 16.771(2) *b* 13.792(1) *c* 6.143(1)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.60 **Temperature(K):** 295 **Density(g/cm³):** 1.432



CLTRHS

Reference: M.Cotrait, M.Ptak, B.Busetta, A.Heitz (1976) *J.Am.Chem.Soc.*, **98**,1073

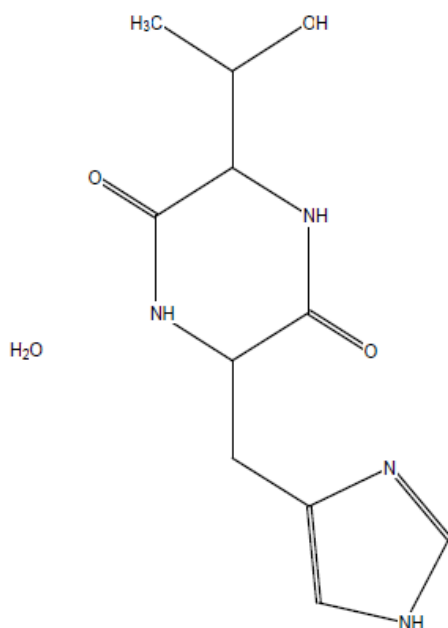
Formula: C₁₀ H₁₄ N₄ O₃·2(H₂O₁)

Compound Name: Cyclo(L-threonyl-L-histidyl) dihydrate

Synonym: Cyclic peptide (2 residues): THR-HIS-

Space Group: P212121 **Cell:** *a* 8.649(3) *b* 25.557(9) *c* 6.212(5)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.40 **Temperature(K):** 295 **Density(g/cm³):** 1.327



COBXIA

Reference: G.D.Grant, A.L.Hunt, P.J.Milne, H.M.Roos, J.A.Joubert (1999) *J.Chem.Cryst.*, **29**,435

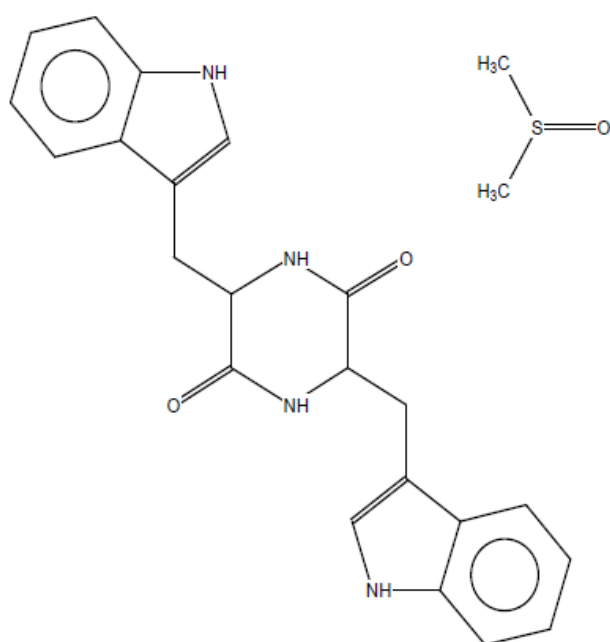
Formula: C₂₂ H₂₀ N₄ O₂·C₂ H₆ O₁ S₁

Compound Name: Cyclo(L-tryptophanyl-L-tryptophanyl) dimethylsulfoxide solvate

Synonym: Cyclic peptide (2 residues): TRP-TRP-

Space Group: P212121 **Cell:** *a* 6.193(2) *b* 11.545(3) *c* 31.117(4)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.44 **Temperature(K):** 291 **Density(g/cm³):** 1.345



COFDIK

Reference: D.van der Helm, M.B.Hossain, M.A.F.Jalal, B.Benson, C.L.Barnes (1984) *Acta Crystallogr., Sect.A:Found Crystallogr.*, **40**,C92

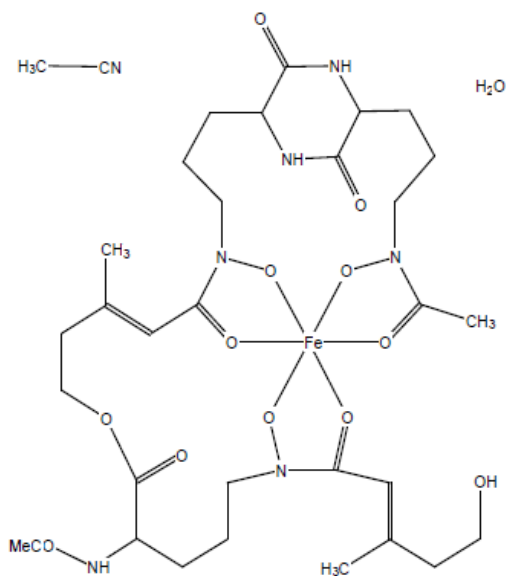
Formula: C₃₁ H₄₇ Fe₁ N₉ O₁₂.0.75(C₂ H₃ N₁),5(H₂ O₁)

Compound Name: Neocoprogen I acetonitrile solvate pentahydrate

Synonym: (5-[(hydroxy)3-[5-(3-[(hydroxy)[1-(oxo)ethylamino]propyl)-3,6-dioxopiperazin-2-yl]propyl]amino]-3-methyl-5-(oxo)pent-3-en-1-yl N²-acetyl-N⁵-hydroxy-N⁵-[5-hydroxy-3-methyl-1-(oxo)pent-2-en-1-yl]ornithinato)-iron acetonitrile solvate pentahydrate

Space Group: P22121 **Cell:** **a** 8.683(12) **b** 28.334(39) **c** 36.835(40)
Space Group No.: 18 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 12.50 **Temperature(K):** 138 **Density(g/cm³):** 1.279



COFDIK10

Reference: M.B.Hossain, M.A.F.Jalal, B.A.Benson, C.L.Barnes, D.van der Helm (1987) *J.Am.Chem.Soc.*, **109**,4948

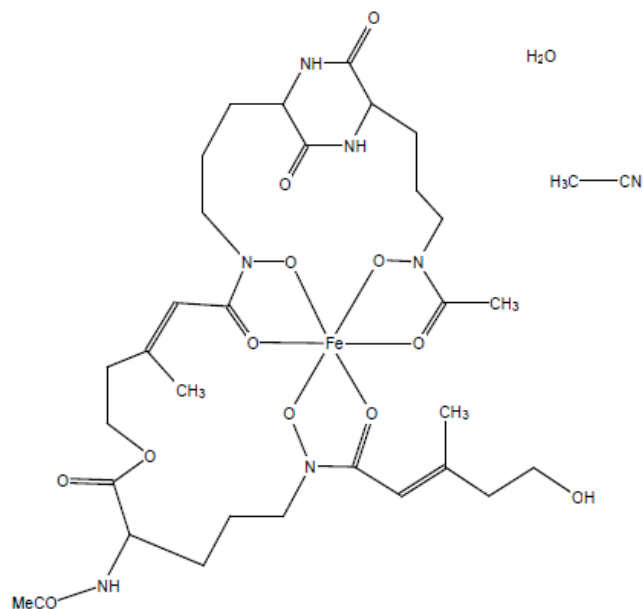
Formula: C₃₁ H₄₇ Fe₁ N₉ O₁₂.0.75(C₂ H₃ N₁),7(H₂ O₁)

Compound Name: Neocoprogen I acetonitrile solvate heptahydrate

Synonym: Ferric isotriomycin acetonitrile solvate heptahydrate

Space Group: P22121 **Cell:** **a** 8.683(12) **b** 28.330(40) **c** 36.840(40)
Space Group No.: 18 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 10.90 **Temperature(K):** 138 **Density(g/cm³):** 1.332



COPHOE

Reference: K.Suguna, S.Ramakumar, K.D.Kopple (1984) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, **40**,2053

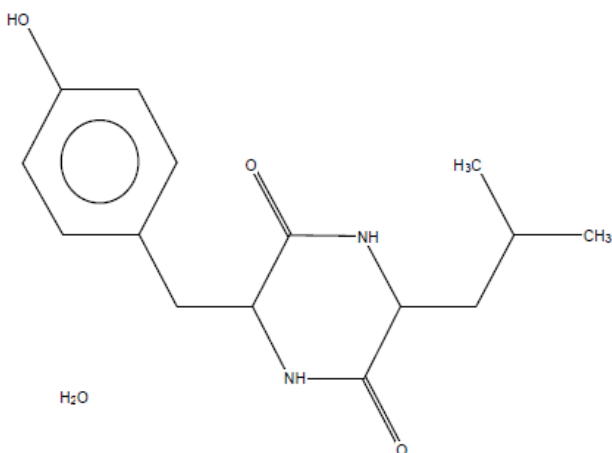
Formula: C₁₅ H₂₀ N₂ O₃.H₂ O₁

Compound Name: Cyclo-(L-leucyl-L-tyrosyl) monohydrate

Synonym: Cyclic peptide (2 residues): LEU-TYR-

Space Group: P21 **Cell:** **a** 8.883(5) **b** 6.105(3) **c** 14.582(5)
Space Group No.: 4 **(Å,°)** α 90.00 β 99.53(4) γ 90.00

R-Factor (%): 7.50 **Temperature(K):** 295 **Density(g/cm³):** 1.253



COYRIR

Reference: K.Suguna, S.Ramakumar, R.Nagaraj, P.Balaran (1985) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, **41**,284

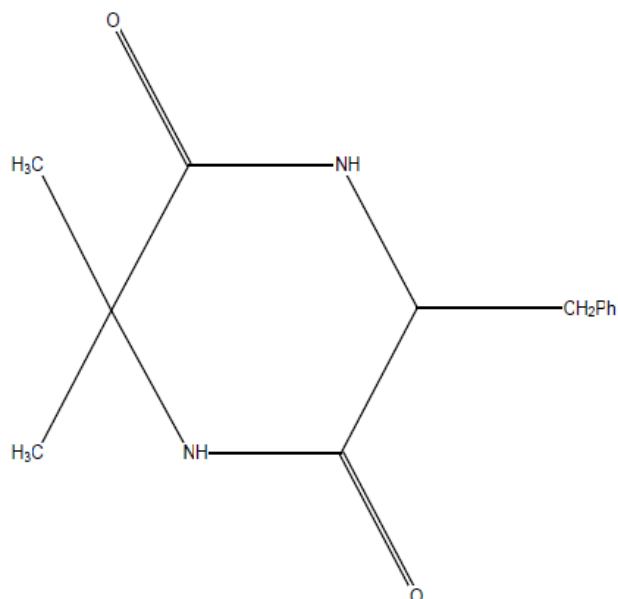
Formula: C₁₃ H₁₆ N₂ O₂

Compound Name: Cyclo(α-amino-isobutyryl-L-phenylalanyl)

Synonym: Cyclic peptide (2 residues): AIB-PHE-

Space Group: P21 **Cell:** **a** 9.646(4) **b** 6.133(3) **c** 10.757(6)
Space Group No.: 4 **(Å,°)** α 90.00 β 101.97(4) γ 90.00

R-Factor (%): 6.50 **Temperature(K):** 295 **Density(g/cm³):** 1.239



CSEHSM

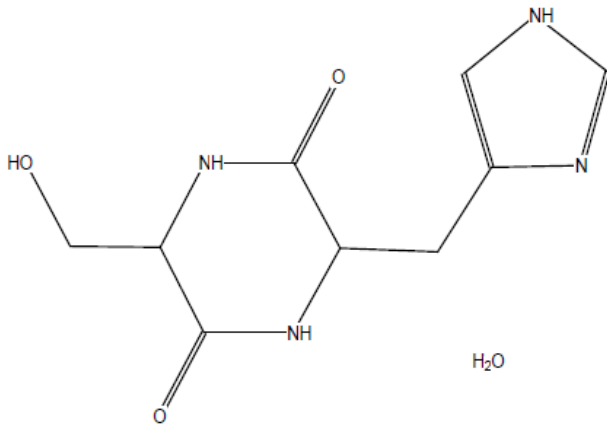
Reference: M.Cotrait, M.Ptak (1978)
Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem., **34**,528

Formula: C₉ H₁₂ N₄ O₃ H₂ O₁

Compound Name: Cyclo(L-seryl-L-histidyl) monohydrate

Synonym: Cyclic peptide (2 residues): SER-HIS-

Space Group: P212121 **Cell:** **a** 8.162(3) **b** 23.191(7) **c** 5.756(4)
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 3.60 **Temperature(K)**: 295 **Density(g/cm³)**: 1.477



CYLCYS

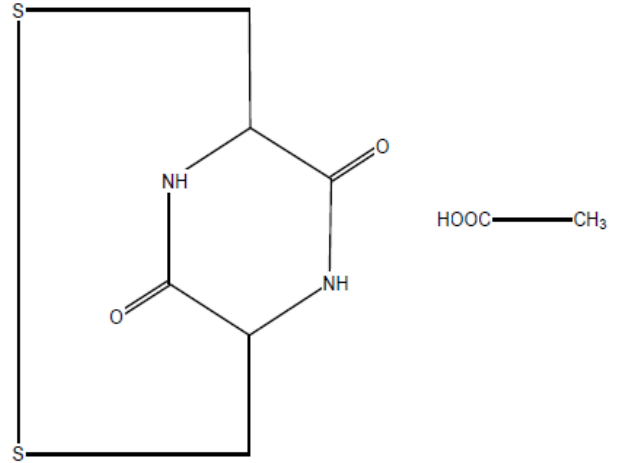
Reference: H.-C.Mez (1974) *Cryst. Struct. Commun.*, **3**,657

Formula: C₈ H₈ N₂ O₂ S₂ C₂ H₄ O₂

Compound Name: Cyclo-L-cystine acetic acid solvate

Synonym: Cyclic peptide (2 residues): CYS-CYS-

Space Group: P212121 **Cell:** **a** 9.387 **b** 6.149 **c** 20.263
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 13.00 **Temperature(K)**: 295 **Density(g/cm³)**: 1.501



CYSESE

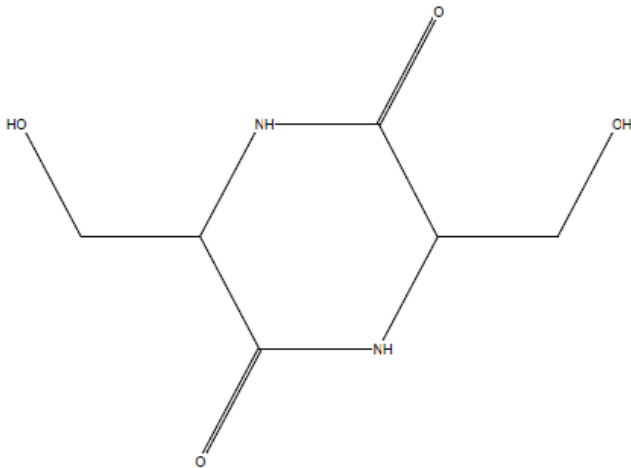
Reference: G.G.Fava, M.F.Belicchi, R.Marchelli, A.Dossena (1981)
Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem., **37**,625

Formula: C₈ H₁₀ N₂ O₄

Compound Name: Cyclo(L-seryl-L-seryl)

Synonym: Cyclic peptide (2 residues): SER-SER-

Space Group: P212121 **Cell:** **a** 11.096(2) **b** 7.787(1) **c** 8.538(1)
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 5.30 **Temperature(K)**: 295 **Density(g/cm³)**: 1.568



CYSESE01

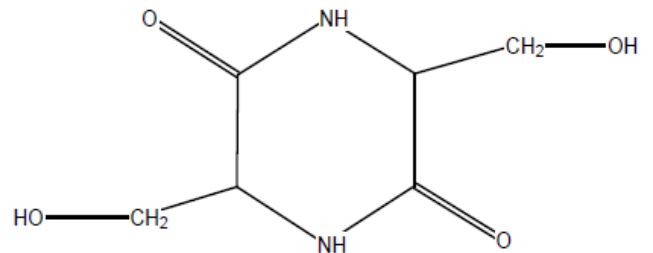
Reference: K.I.Varughese, G.Kartha (1979) *ACA, Ser.2*, **7**,25a

Formula: C₈ H₁₀ N₂ O₄

Compound Name: Cyclo(L-seryl-L-seryl)

Synonym: Cyclic peptide (2 residues): SER-SER-

Space Group: P212121 **Cell:** **a** 7.776 **b** 8.531 **c** 11.076
Space Group No.: 19 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 4.40 **Temperature(K)**: 295 **Density(g/cm³)**: 1.574



DAJJED

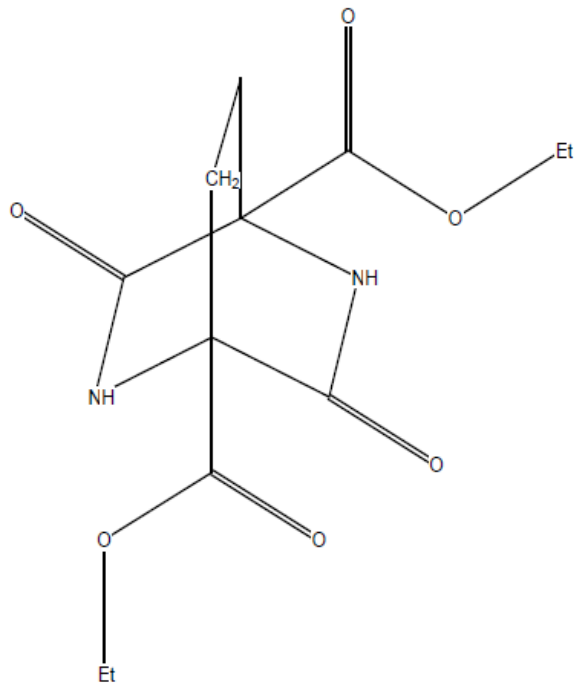
Reference: R.G.Kostyanovsky, Y.I.El'natanov, O.N.Krutijs, I.I.Chervin, K.A.Lyssenko (1998) *Mendeleev Commun.*, 228

Formula: C₁₂ H₁₆ N₂ O₆

Compound Name: (+)-Diethyl 2,5-diaza-3,6-dioxobicyclo(2.2.2)octane-1,4-dicarboxylate

Space Group: P21/n **Cell:** a 10.189(2) b 5.567(1) c 24.114(5)
Space Group No.: 14 **(Å,°)** α 90.00 β 95.39(2) γ 90.00

R-Factor (%): 5.45 **Temperature(K):** 295 **Density(g/cm³):** 1.386



DAJJED01

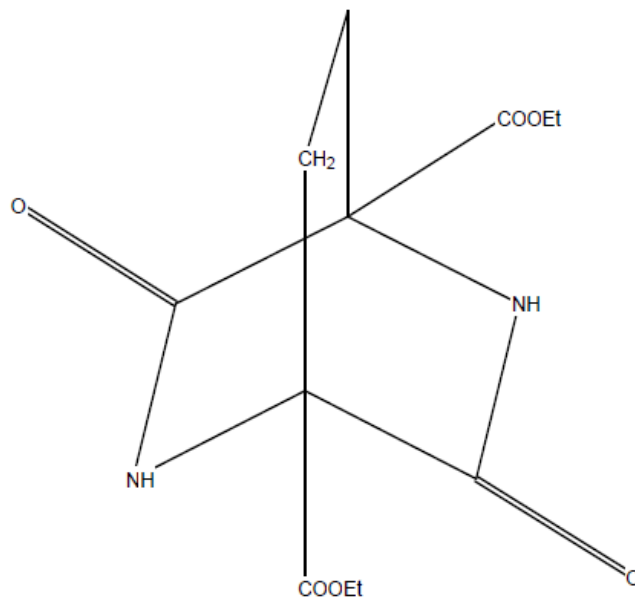
Reference: K.A.Lyssenko, D.A.Lenev, R.G.Kostyanovsky (2002) *Tetrahedron*, 58,8525

Formula: C₁₂ H₁₆ N₂ O₆

Compound Name: (+)-Diethyl 2,5-diazabicyclo(2.2.2)octane-3,6-dione-1,4-dicarboxylate

Space Group: P21/n **Cell:** a 10.189(2) b 5.567(1) c 24.114(5)
Space Group No.: 14 **(Å,°)** α 90.00 β 95.39(2) γ 90.00

R-Factor (%): 5.45 **Temperature(K):** 293 **Density(g/cm³):** 1.386



DAWSUP

Reference: K.H.Ongania, G.Granozzi, V.Buseti, M.Casarin, D.Ajo (1985) *Tetrahedron*, **41**,2015

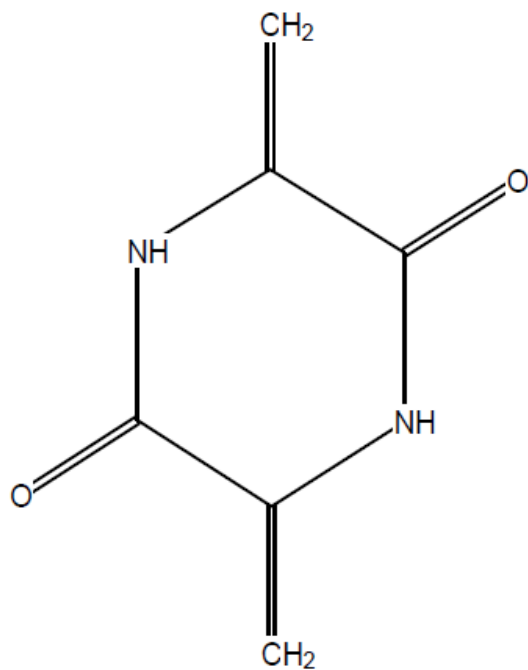
Formula: C₈ H₈ N₂ O₂

Compound Name: 3,6-Dimethylene-piperazine-2,5-dione

Synonym: Cyclo-bis(dehydro-alanyl); Cyclic peptide (2 residues): ALA*-ALA*.

Space Group: P21 **Cell:** *a* 5.261(3) *b* 13.617(4) *c* 4.570(3)
Space Group No.: 4 **(Å,°)** *α* 90.00 *β* 104.58(5) *γ* 90.00

R-Factor (%): 7.10 **Temperature(K):** 295 **Density(g/cm³):** 1.448



DAWSUP01

Reference: D.A.Clemente (2003) *Tetrahedron*, **59**,8445

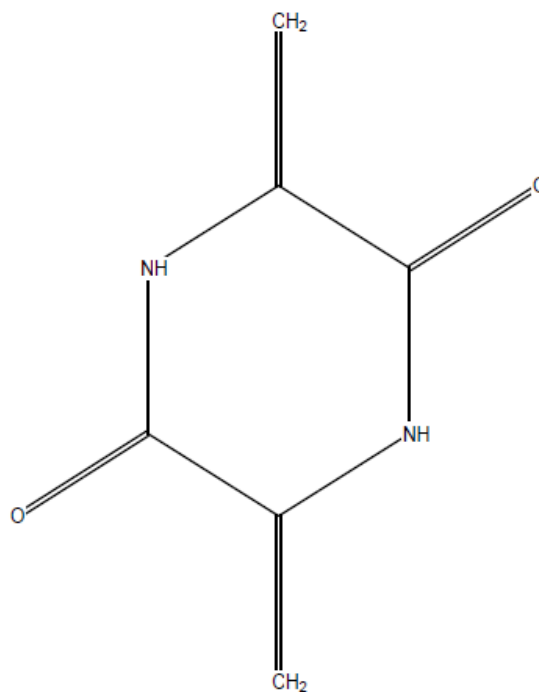
Formula: C₈ H₈ N₂ O₂

Compound Name: 3,6-Dimethylene-piperazine-2,5-dione

Synonym: Cyclo-bis(dehydro-alanyl); Cyclic peptide (2 residues): ALA*-ALA*.

Space Group: P21/c **Cell:** *a* 4.570(3) *b* 13.617(4) *c* 5.261(3)
Space Group No.: 14 **(Å,°)** *α* 90.00 *β* 104.58(5) *γ* 90.00

R-Factor (%): 7.81 **Temperature(K):** 293 **Density(g/cm³):** 1.448



DESXOO

Reference: D.Ajo, M.Casarin, R.Bertoncello, V.Busetti,
H.C.J.Ottenheijm, R.Plata (1965) *Tetrahedron* ,**41**,5543

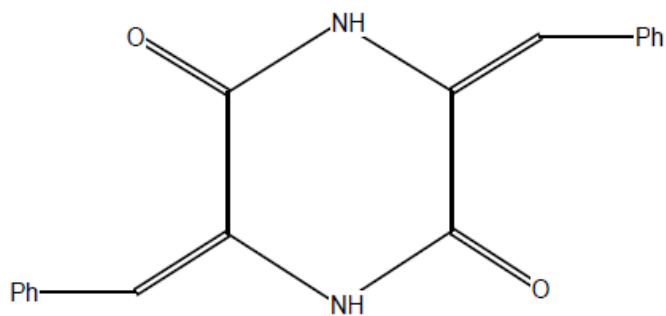
Formula: C₁₈ H₁₄ N₂ O₂

Compound Name: 3,6-bis(Phenylmethylene)-piperazine-2,5-dione

Synonym: Cyclo-bis(dehydrophenylalanine);
Cyclic peptide (2 residues): PHE*-PHE*-

Space Group: C2/c **Cell:** **a** 40.774(0) **b** 6.237(2) **c** 17.731(3)
Space Group No.: 15 **(Å,°)** **α** 90.00 **β** 107.76(5) **γ** 90.00

R-Factor (%): 6.10 **Temperature(K)**: 295 **Density(g/cm³)**: 1.347



DIKPIP

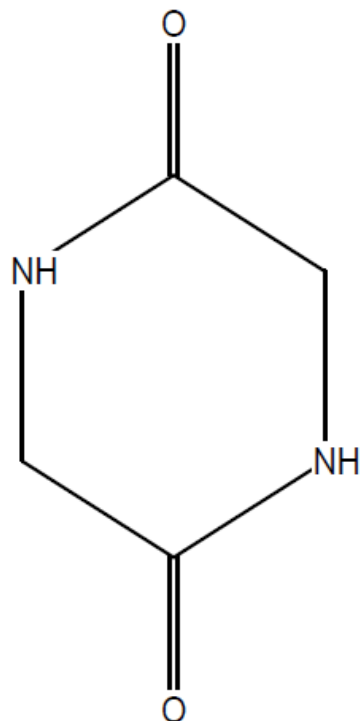
Reference: K.Lonsdale (1961) *Acta Crystallogr.* ,**14**,37

Formula: C₄ H₆ N₂ O₂

Compound Name: Diketopiperazine

Space Group: P21/a **Cell:** **a** 5.228 **b** 11.554 **c** 3.980
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 97.93 **γ** 90.00

R-Factor (%): 0.00 **Temperature(K)**: 295 **Density(g/cm³)**: 1.591



DIKPIP01

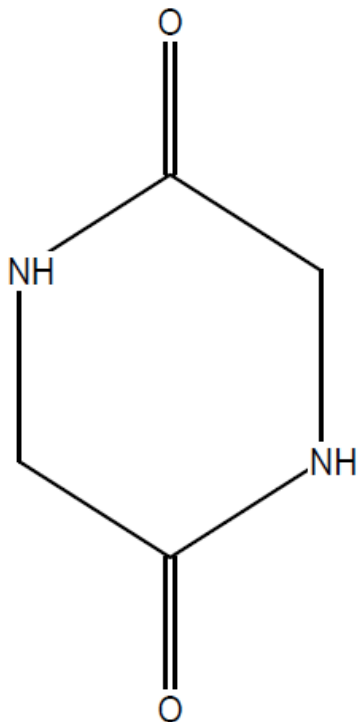
Reference: R.Degeilh, R.E.Marsh (1959) *Acta Crystallogr.*, **12**,1007

Formula: C₄ H₈ N₂ O₂

Compound Name: Diketopiperazine

Space Group: P21/a **Cell:** **a** 5.228(2) **b** 11.554(2) **c** 3.980(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 97.98(2) γ 90.00

R-Factor (%): 7.20 **Temperature(K):** 295 **Density(g/cm³):** 1.592



DIKPIP02

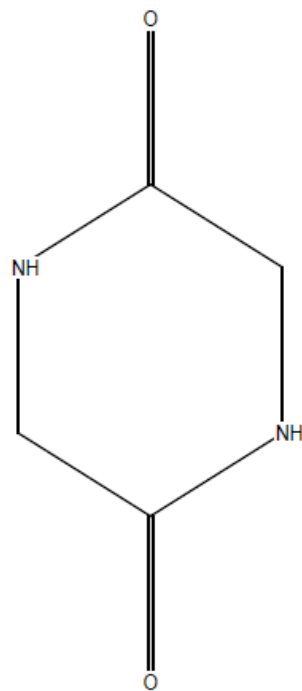
Reference: T.R.Sarangarajan, K.Panchanatheswaran, J.N.Low, C.Glidewell (2005) *Acta Crystallogr., Sect.C: Cryst. Struct. Commun.*, **61**, o118

Formula: C₄ H₈ N₂ O₂

Compound Name: 2,5-Piperazinedione

Space Group: P21/c **Cell:** **a** 3.897(1) **b** 11.527(3) **c** 5.159(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 96.46(2) γ 90.00

R-Factor (%): 6.70 **Temperature(K):** 120 **Density(g/cm³):** 1.646



DIKPIP03

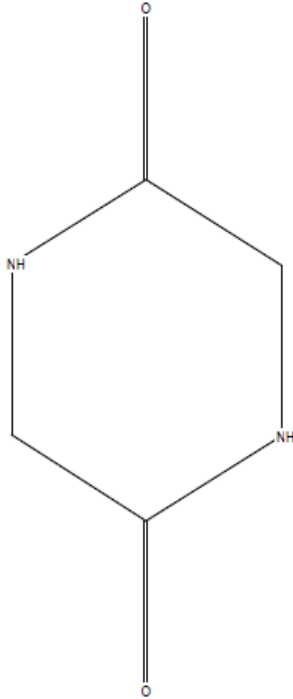
Reference: Nonappa, K.Ahonen, M.Lahtinen, E.Kolehmainen (2011)
Green Chemistry, **13**,1203

Formula: C₄ H₈ N₂ O₂

Compound Name: Piperazine-2,5-dione

Space Group: P21/c **Cell:** **a** 3.905(0) **b** 11.565(1) **c** 5.168(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.46(0) γ 90.00

R-Factor (%): 3.67 **Temperature(K):** 123 **Density(g/cm³):** 1.634



DIKSIZ

Reference: Y.Kojima, T.Yamashita, S.Nishide, K.Hirotsu, T.Higuchi
(1985) *Bull.Chem.Soc.Jpn.*, **58**,409

Formula: C₁₂ H₁₄ N₈ O₂·2.5(H₂O)

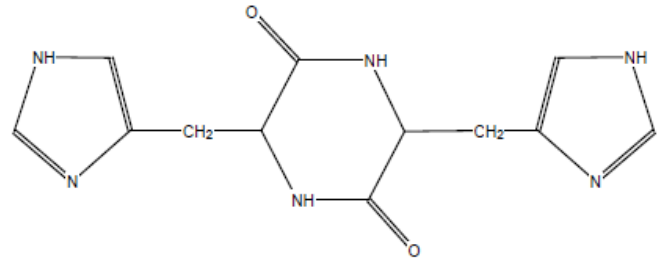
Compound Name: Cyclo-(L-histidyl-L-histidyl) hydrate

Synonym: Cyclic peptide (2 residues): HIS-HIS-

Space Group: P21212 **Cell:** **a** 19.910(10) **b** 12.660(10) **c** 6.163(3)
Space Group No.: 18 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.40 **Temperature(K):** 295 **Density(g/cm³):** 1.365

H₂O



DITBAM

Reference: War War May Zin, S. Buttachon, T. Dethoup, J.A. Pereira, L. Gales, Angela Inacio, P.M. Costa, M. Lee, N. Sekeroglu, A.M.S. Silva, M.M.M. Pinto, A. Kijjoa (2017) *Phytochemistry*, **141**, 86

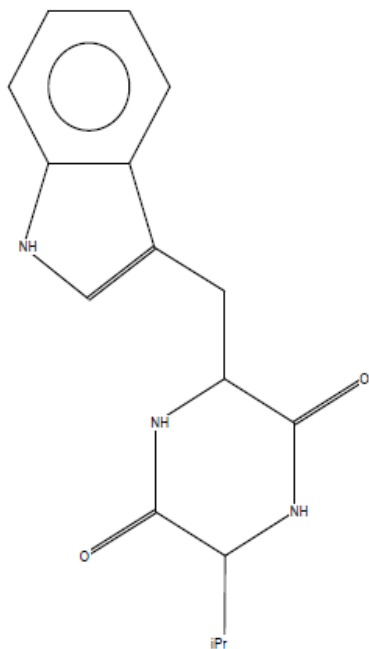
Formula: C₁₈ H₁₉ N₃ O₂

Compound Name: 3-[(1H-indol-3-yl)methyl]-6-isopropylpiperazine-2,5-dione

Synonym: (11S,14R)-cyclo(tryptophylvalyl); Cyclic peptide (2 residues): TRP-VAL-

Space Group: P21 **Cell:** **a** 6.103(0) **b** 13.427(0) **c** 9.477(0)
Space Group No.: 4 **(Å, °)** α 90.00 β 105.46(0) γ 90.00

R-Factor (%): 3.14 **Temperature(K):** 293 **Density(g/cm³):** 1.266



DKPSAL

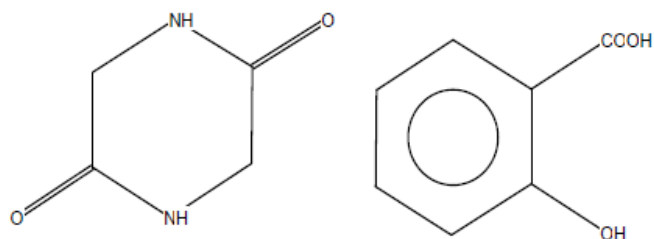
Reference: G. Kartha, K.I. Varughese (1978) *Acta Crystallogr., Sect. A: Cryst. Phys., Diffr., Theor. Crystallogr.*, **34**, S90

Formula: C₄ H₆ N₂ O₂ · 2(C₇ H₆ O₃)

Compound Name: Piperazine-2,5-dione bis(salicylic acid)

Space Group: P21/a **Cell:** **a** 18.550 **b** 5.480 **c** 8.790
Space Group No.: 14 **(Å, °)** α 90.00 β 104.30 γ 90.00

R-Factor (%): 0.00 **Temperature(K):** 295 **Density(g/cm³):** 1.497



DKPSAL10

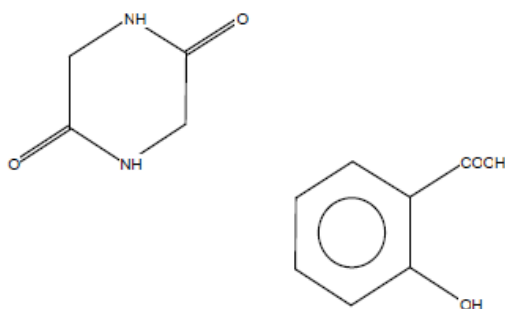
Reference: K.I.Varughese, G.Kartha (1982)
Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem., **38**,301

Formula: C₄ H₈ N₂ O₂·2(C₇ H₆ O₃)

Compound Name: Piperazine-2,5-dione bis(salicylic acid)

Space Group: P21/a **Cell:** a 18.520(10) b 5.455(5) c 8.787(8)
Space Group No.: 14 **(Å,°)** α 90.00 β 104.28(4) γ 90.00

R-Factor (%): 4.10 **Temperature(K):** 295 **Density(g/cm³):** 1.507



DLALGL

Reference: T.Srikrishnan, P.K.S.Gupta, R.Parthasarathy (1977)
ACA, Ser.2, **5**,34a

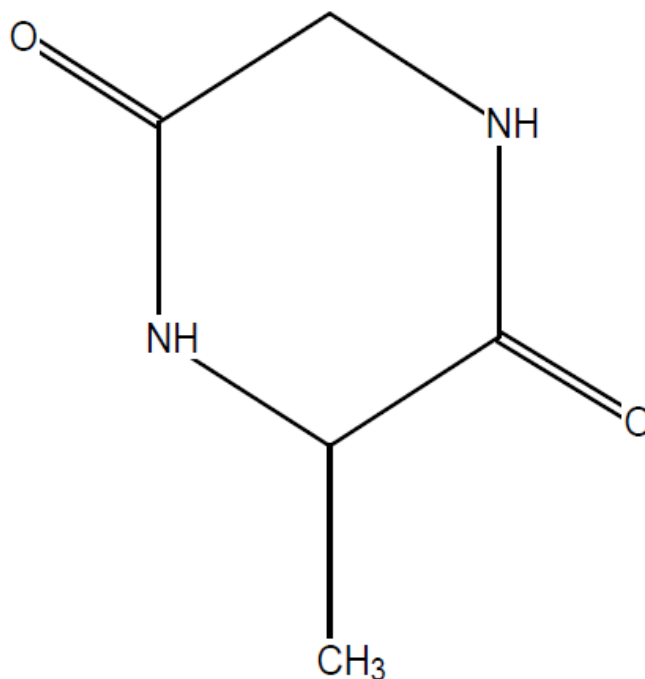
Formula: C₅ H₈ N₂ O₂

Compound Name: Cyclo(DL-alanyl-glycyl)

Synonym: Cyclic peptide (2 residues): ALA-GLY-

Space Group: Pc **Cell:** a 11.460(3) b 6.126(2) c 11.577(4)
Space Group No.: 7 **(Å,°)** α 90.00 β 132.52(2) γ 90.00

R-Factor (%): 7.60 **Temperature(K):** 295 **Density(g/cm³):** 1.421



DOGQEV

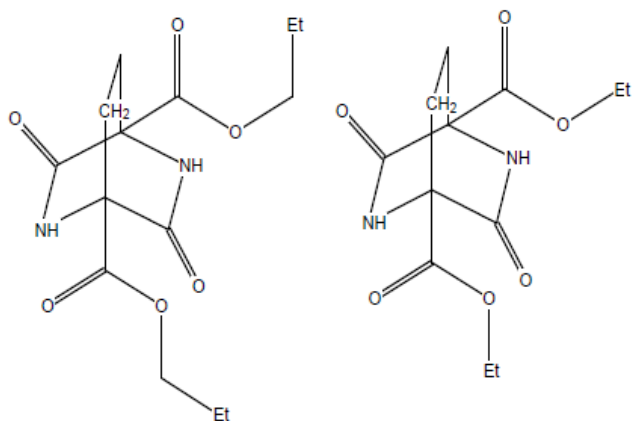
Reference: R.G.Kostyanovsky, K.A.Lyssenko, D.A.Lenev (1999)
Mendeleev Commun., **154**

Formula: C₁₄ H₂₀ N₂ O₆·C₁₂ H₁₈ N₂ O₆

Compound Name: Diethyl 2,5-diazabicyclo(2.2.2)octane-3,6-dione-1,4-carboxylate dipropyl 2,5-diazabicyclo(2.2.2)octane-3,6-dione-1,4-carboxylate

Space Group: P21 **Cell:** a 10.199(7) b 5.597(3) c 25.107(15)
Space Group No.: 4 **(Å,°)** α 90.00 β 95.96(5) γ 90.00

R-Factor (%): 7.61 **Temperature(K):** 153 **Density(g/cm³):** 1.390



DOGQEV01

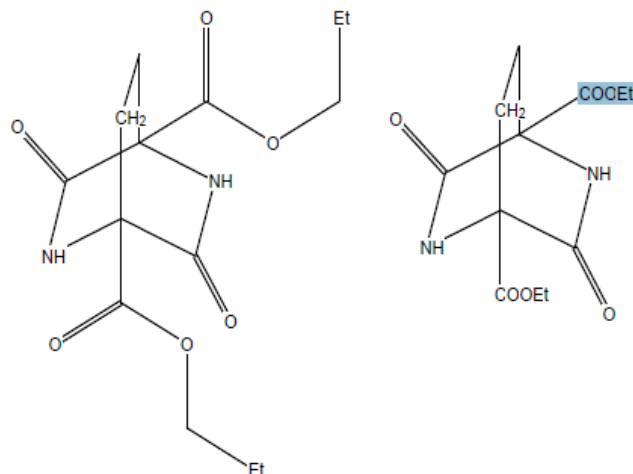
Reference: K.A.Lyssenko, D.A.Lenev, R.G.Kostyanovsky (2002)
Tetrahedron, **58**,8525

Formula: C₁₄ H₂₀ N₂ O₆·C₁₂ H₁₈ N₂ O₆

Compound Name: (+)-Diethyl 2,5-diazabicyclo(2.2.2)octane-3,6-dione-1,4-carboxylate (-)-di-n-propyl 2,5-diazabicyclo(2.2.2)octane-3,6-dione-1,4-carboxylate

Space Group: P21 **Cell:** a 10.199(7) b 5.597(3) c 25.107(15)
Space Group No.: 4 **(Å,°)** α 90.00 β 95.96(5) γ 90.00

R-Factor (%): 7.61 **Temperature(K):** 153 **Density(g/cm³):** 1.390



DOGQIZ

Reference: R.G.Kostyanovsky, K.A.Lyssenko, D.A.Lenev (1999) *Mendeleev Commun.*, 154

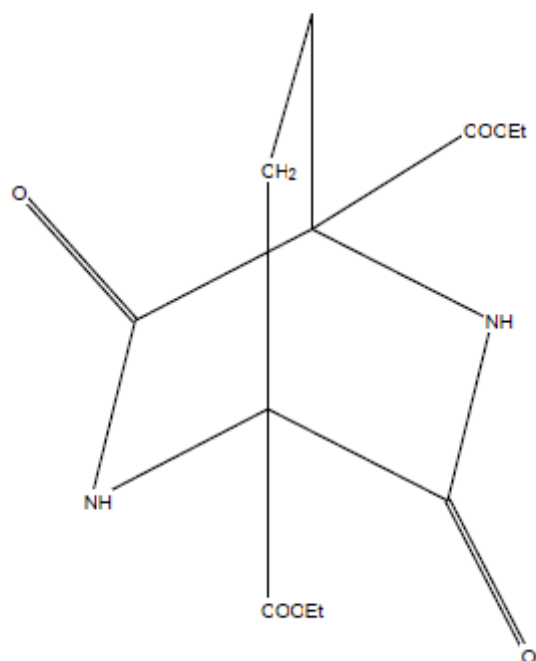
Formula: C₁₂H₁₆N₂O₆

Compound Name: (1*R*,4*R*)-(-)-Diethyl 2,5-diazabicyclo(2.2.2)octane-3,6-dione-1,4-carboxylate

Space Group: P2₁12₁1
Space Group No.: 19

Cell: (Å,°)
a 5.534(3) b 9.908(4) c 25.773(10)
α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.15 **Temperature(K)**: 153 **Density(g/cm³)**: 1.336



DOGQIZ01

Reference: K.A.Lyssenko, D.A.Lenev, R.G.Kostyanovsky (2002) *Tetrahedron*, 58,8525

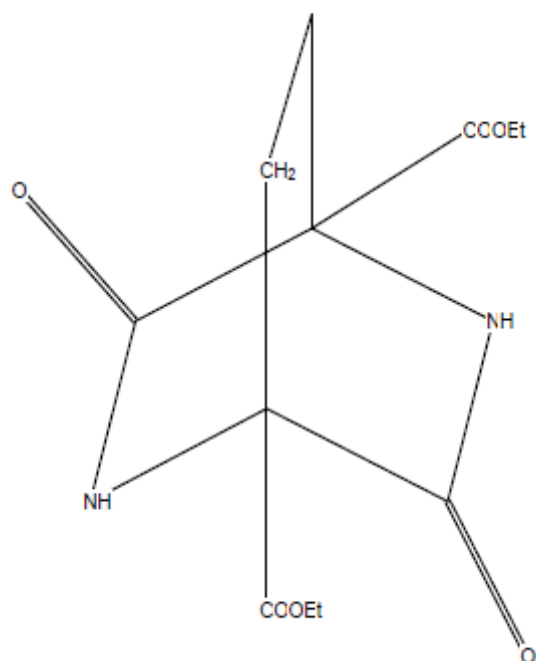
Formula: C₁₂H₁₆N₂O₆

Compound Name: (1*R*,4*R*)-(-)-Diethyl 2,5-diazabicyclo(2.2.2)octane-3,6-dione-1,4-carboxylate

Space Group: P2₁12₁1
Space Group No.: 19

Cell: (Å,°)
a 5.534(3) b 9.908(4) c 25.773(10)
α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.15 **Temperature(K)**: 153 **Density(g/cm³)**: 1.336



DOGQUL

Reference: R.G.Kostyanovsky, Yu.I.El'matanov, O.N.Krutius, K.A.Lyssenko, I.I.Chervin, D.A.Lenev (1999) *Mendeleev Commun.*, 109

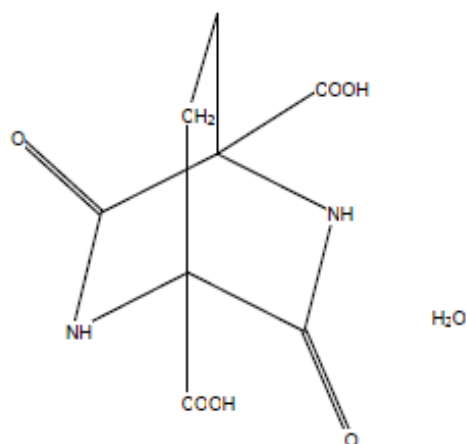
Formula: C₈H₈N₂O₆·2(H₂O)₁

Compound Name: (1*R*,4*R*)-(-)-2,5-Diazabicyclo(2.2.2)octane-3,6-dione-1,4-dicarboxylic acid dihydrate

Space Group: P2₁
Space Group No.: 4

Cell: (Å,°)
a 6.871(3) b 11.260(3) c 7.162(2)
α 90.00 β 93.98(3) γ 90.00

R-Factor (%): 3.19 **Temperature(K)**: 295 **Density(g/cm³)**: 1.587



DOGQUL01

Reference: K.A.Lyssenko, D.A.Lenev, R.G.Kostyanovsky (2002) *Tetrahedron*, 58,8525

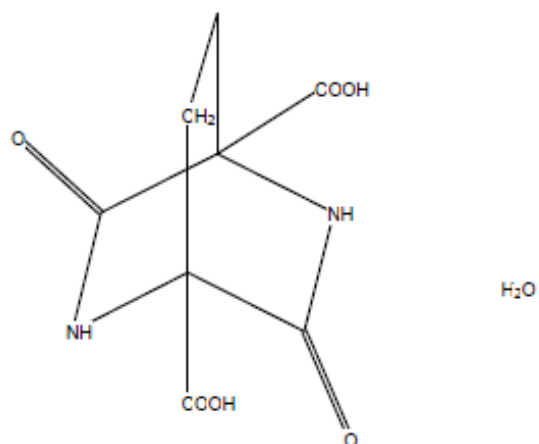
Formula: C₈H₈N₂O₆·2(H₂O)₁

Compound Name: (1*R*,4*R*)-(-)-2,5-Diazabicyclo(2.2.2)octane-3,6-dione-1,4-dicarboxylic acid dihydrate

Space Group: P2₁
Space Group No.: 4

Cell: (Å,°)
a 6.871(3) b 11.260(3) c 7.162(2)
α 90.00 β 93.98(3) γ 90.00

R-Factor (%): 3.19 **Temperature(K)**: 293 **Density(g/cm³)**: 1.587



DOGSIB

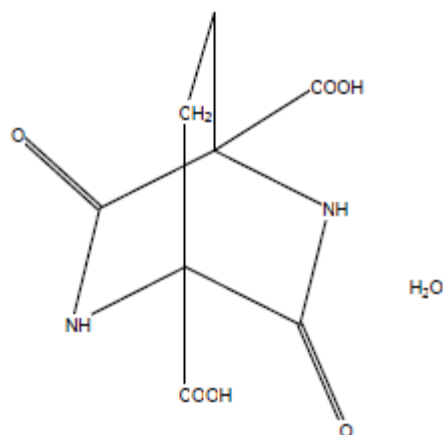
Reference: R.G.Kostyanovsky, Yu.I.El'matanov, O.N.Krutius, K.A.Lyssenko, I.I.Chervin, D.A.Lenev (1999) *Mendeleev Commun.*, 109

Formula: C₈H₈N₂O₆·2(H₂O)₁

Compound Name: (+)-2,5-Diazabicyclo[2.2.2]octane-3,6-dione-1,4-dicarboxylic acid dihydrate

Space Group: P2₁/n **Cell:** a 8.900(4) b 11.590(3) c 10.401(2)
Space Group No.: 14 **Cell:** (Å,°) α 90.00 β 92.93(3) γ 90.00

R-Factor (%): 4.19 **Temperature(K):** 295 **Density(g/cm³):** 1.638



DOGSIB01

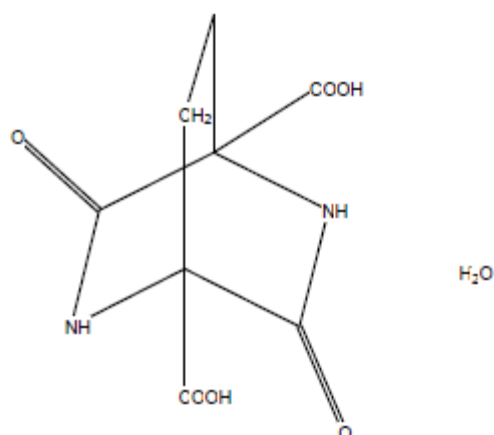
Reference: K.A.Lyssenko, D.A.Lenev, R.G.Kostyanovsky (2002) *Tetrahedron*, 58,8525

Formula: C₈H₈N₂O₆·2(H₂O)₁

Compound Name: (+)-2,5-Diazabicyclo[2.2.2]octane-3,6-dione-1,4-dicarboxylic acid dihydrate

Space Group: P2₁/n **Cell:** a 8.900(4) b 11.590(3) c 10.401(2)
Space Group No.: 14 **Cell:** (Å,°) α 90.00 β 92.93(3) γ 90.00

R-Factor (%): 4.19 **Temperature(K):** 293 **Density(g/cm³):** 1.638



DONQOO

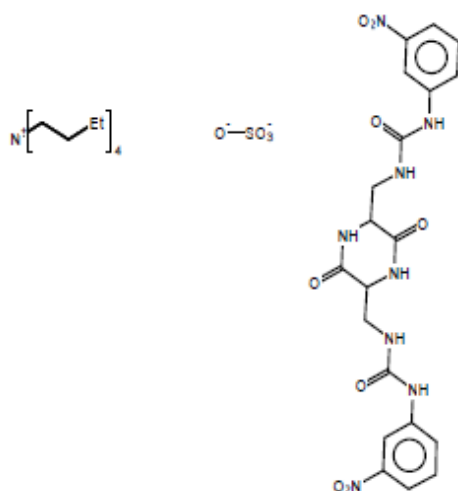
Reference: S.R.Naini, R.A.Lalancette, O.Gorlova, K.V.S.Ramakrishna, Jhiliu Singh Yadav, Subramania Ranganathan (2014) *Eur.J.Org.Chem.*, 7015

Formula: C₂₀H₂₀N₈O₈S₄·2(C₁₆H₃₆N₄¹⁺)

Compound Name: Tetra-n-butylammonium sulfate 1,1'-[(3,6-dioxoperazine-2,5-diy)] bis(methylene)bis(3-(3-nitrophenyl)urea)

Space Group: P2₁ **Cell:** a 10.049(0) b 16.348(0) c 18.182(0)
Space Group No.: 4 **Cell:** (Å,°) α 90.00 β 105.30(0) γ 90.00

R-Factor (%): 7.50 **Temperature(K):** 100 **Density(g/cm³):** 1.247



DONQUU

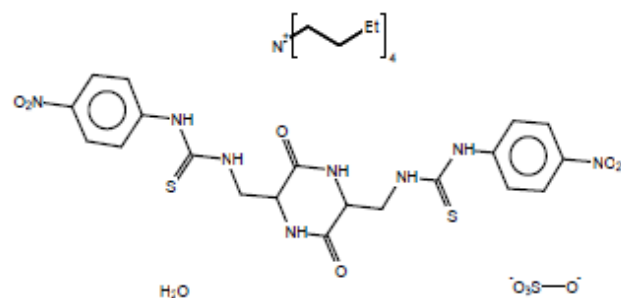
Reference: S.R.Naini, R.A.Lalancette, O.Gorlova, K.V.S.Ramakrishna, Jhiliu Singh Yadav, Subramania Ranganathan (2014) *Eur.J.Org.Chem.*, 7015

Formula: C₂₀H₂₀N₈O₈S₄·0.25(H₂O)₁·2(C₁₆H₃₆N₄¹⁺)

Compound Name: bis(tetra-n-butylammonium) 1,1'-[(3,6-dioxoperazine-2,5-diy)] bis(methylene)bis(3-(4-nitrophenyl)thiourea) sulfate hydrate

Space Group: P2₁ **Cell:** a 10.241(0) b 19.861(0) c 58.509(0)
Space Group No.: 4 **Cell:** (Å,°) α 90.00 β 93.86(0) γ 90.00

R-Factor (%): 7.60 **Temperature(K):** 100 **Density(g/cm³):** 1.251



DUZDUX

Reference: M.Gdaniec, B.Liberek (1986)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **42**,1343

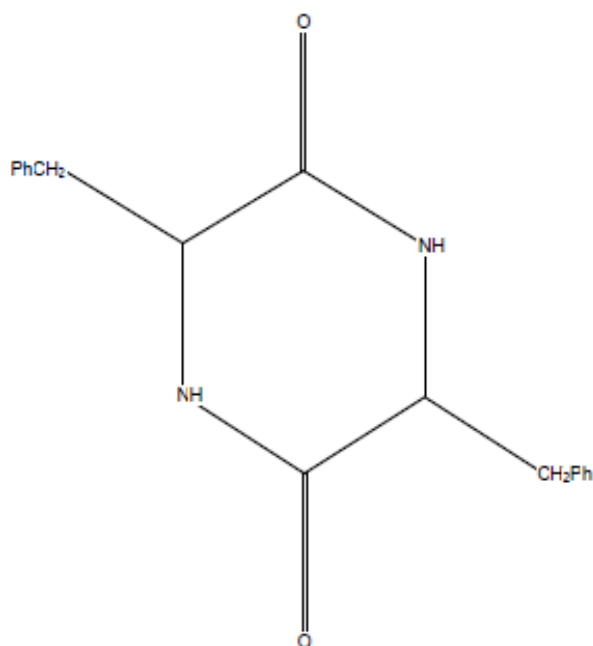
Formula: C₁₈H₁₈N₂O₂

Compound Name: Cyclo-(L-phenylalanyl-L-phenylalanyl)

Synonym: 3,6-Dibenzyl-2,5-piperazinedione;
Cyclic peptide (2 residues): PHE-PHE-

Space Group: P22121 **Cell:** a 6.181(1) b 10.380(3) c 23.795(4)
Space Group No.: 18 **Cell:** (Å,°) α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.281



DUZDUX01

Reference: M.Kurbasic, S.Semeraro, Ana Garcia, S.Kraj, E.Parisi, C.Deganutti, R.De Zorzi, S.Marchesan (2019) *Synthesis*, **51**,2829

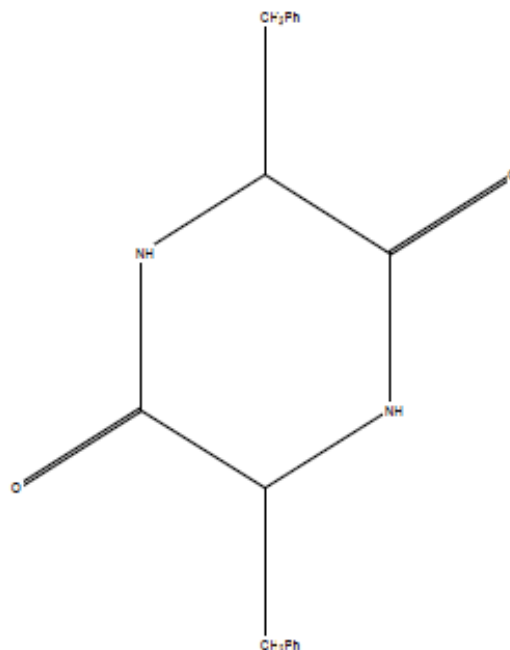
Formula: C₁₈H₁₈N₂O₂

Compound Name: 3,6-dibenzylpiperazine-2,5-dione

Synonym: Cyclo-(L-phenylalanyl-L-phenylalanyl);
Cyclic peptide (2 residues): PHE-PHE-

Space Group: P21212 **Cell:** a 10.370(2) b 23.340(5) c 6.150(1)
Space Group No.: 18 **Cell:** (Å,°) α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.80 **Temperature(K)**: 100 **Density(g/cm³)**: 1.313



EBEQOU

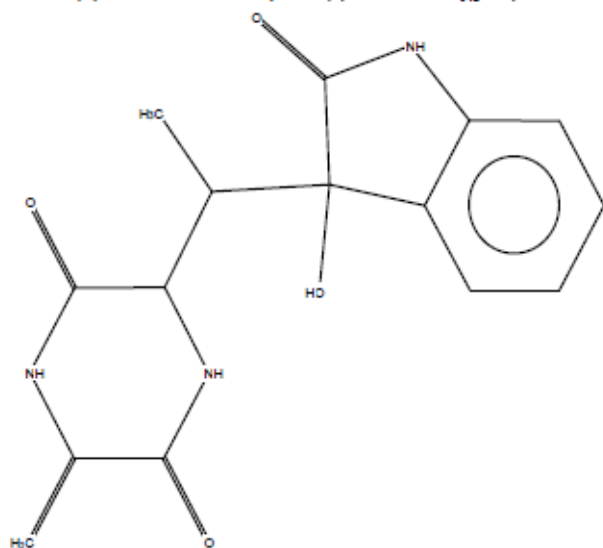
Reference: Yingxia Lan, Yi Zou, Tingting Huang, Xiaozheng Wang, N.L.Brock, Zixin Deng, Shuangjun Lin (2016) *Sci.China.Chem.*, **59**, 1224

Formula: C₁₅H₁₅N₃O₄

Compound Name: 3-(1-(3-hydroxy-2-oxo-2,3-dihydro-1H-indol-3-yl)ethyl)-6-methylenepiperazine-2,5-dione

Space Group: P212121 **Cell:** a 5.444(0) b 12.275(0) c 21.022(0)
Space Group No.: 19 **Cell:** (Å,°) α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.50 **Temperature(K)**: 100 **Density(g/cm³)**: 1.425



EBEQUA

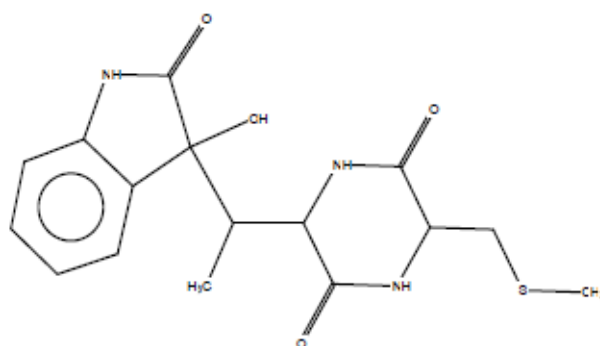
Reference: Yingxia Lan, Yi Zou, Tingting Huang, Xiaozheng Wang, N.L.Brock, Zixin Deng, Shuangjun Lin (2016) *Sci.China.Chem.*, **59**, 1224

Formula: C₁₆H₁₅N₃O₄S₁

Compound Name: 3-(1-(3-hydroxy-2-oxo-2,3-dihydro-1H-indol-3-yl)ethyl)-6-((methylsulfanyl)methyl)piperazine-2,5-dione

Space Group: P21 **Cell:** a 8.131(0) b 10.443(0) c 10.230(0)
Space Group No.: 4 **Cell:** (Å,°) α 90.00 β 106.58(0) γ 90.00

R-Factor (%): 7.26 **Temperature(K)**: 298 **Density(g/cm³)**: 1.394



EBIZUK

Reference: L.J.Williams, B.Jagadish, M.G.Lansdown, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14301

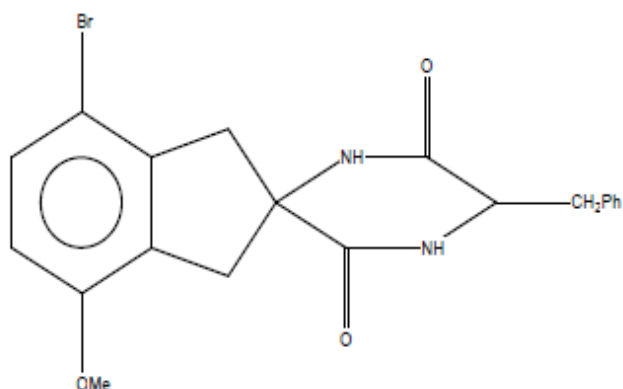
Formula: C₂₀H₁₉Br₁N₂O₃

Compound Name: (R,S)-Cyclo(phenylalanyl-(2-amino-4-bromo-7-methoxyindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): PHE-GLY⁻

Space Group: P21 **Cell:** a 11.065(0) b 6.086(0) c 13.735(0)
Space Group No.: 4 **(Å,°)** α 90.00 β 94.42(0) γ 90.00

R-Factor (%): 4.85 **Temperature(K):** 295 **Density(g/cm³):** 1.496



EBOBAY

Reference: L.J.Williams, B.Jagadish, M.G.Lansdown, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14301

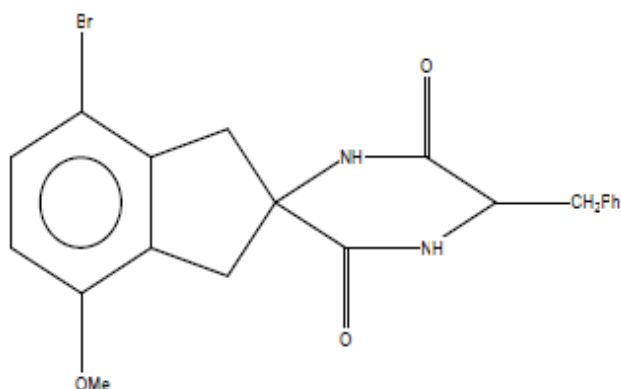
Formula: C₂₀H₁₉Br₁N₂O₃

Compound Name: (S,S)-Cyclo(phenylalanyl-(2-amino-4-bromo-7-methoxyindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): PHE-GLY⁻

Space Group: P21 **Cell:** a 11.410(1) b 6.095(1) c 13.475(2)
Space Group No.: 4 **(Å,°)** α 90.00 β 98.93(0) γ 90.00

R-Factor (%): 5.38 **Temperature(K):** 295 **Density(g/cm³):** 1.490



EBOBEC

Reference: L.J.Williams, B.Jagadish, M.G.Lansdown, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14301

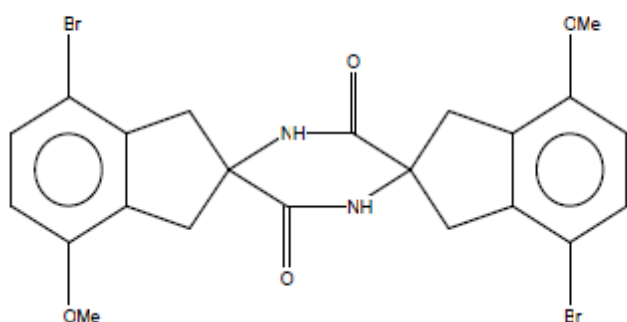
Formula: C₂₂H₂₀Br₂N₂O₄

Compound Name: meso-Cyclo(bis(2-amino-4-bromo-7-methoxyindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P21/n **Cell:** a 8.282(1) b 6.103(1) c 21.736(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 97.25(0) γ 90.00

R-Factor (%): 5.13 **Temperature(K):** 295 **Density(g/cm³):** 1.634



EBOBIG

Reference: L.J.Williams, B.Jagadish, M.G.Lansdown, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14301

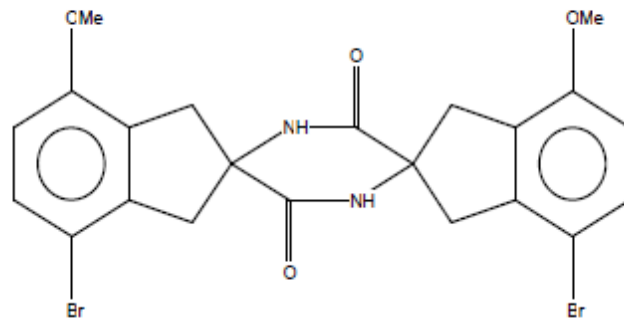
Formula: C₂₂H₂₀Br₂N₂O₄

Compound Name: rac-Cyclo(bis(2-amino-4-bromo-7-methoxyindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P21/n **Cell:** a 8.296(0) b 6.118(0) c 21.771(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 97.27(0) γ 90.00

R-Factor (%): 5.66 **Temperature(K):** 295 **Density(g/cm³):** 1.625



EBOBOM

Reference: L.J.Williams, B.Jagadish, M.G.Lansdown, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14301

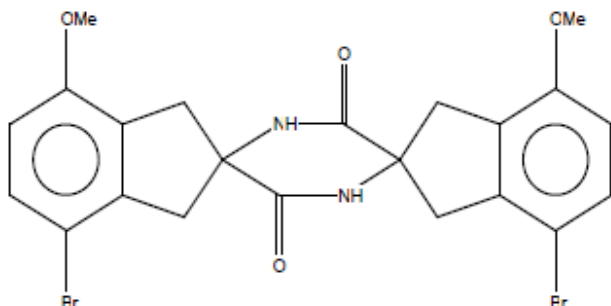
Formula: C₂₂H₂₀Br₂N₂O₄

Compound Name: (S,S)-Cyclo(bis(2-amino-4-bromo-7-methoxyindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: C2 **Cell:** a 31.259(0) b 6.101(0) c 24.268(0)
Space Group No.: 5 **(Å,°)** α 90.00 β 108.93(0) γ 90.00

R-Factor (%): 7.08 **Temperature(K):** 295 **Density(g/cm³):** 1.627



EBOCAZ

Reference: L.J.Williams, B.Jagadish, S.R.Lyon, R.A.Kloster, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14281

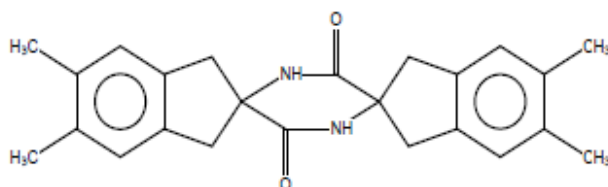
Formula: C₂₄H₂₆N₂O₂

Compound Name: Cyclo(bis(2-amino-5,6-dimethylindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: C2/c **Cell:** a 29.941(2) b 6.029(1) c 11.620(1)
Space Group No.: 15 **(Å,°)** α 90.00 β 110.35(6) γ 90.00

R-Factor (%): 5.20 **Temperature(K):** 293 **Density(g/cm³):** 1.265



EBOCED

Reference: L.J.Williams, B.Jagadish, S.R.Lyon, R.A.Kloster, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14281

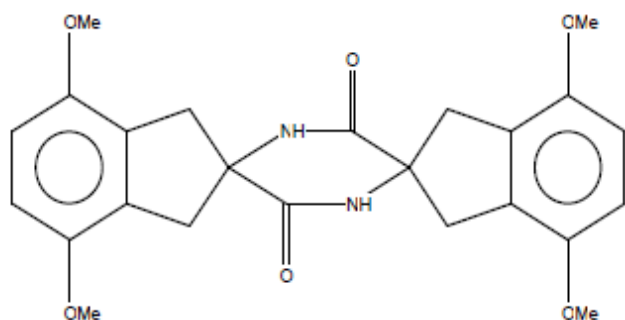
Formula: C₂₄H₂₆N₂O₆

Compound Name: Cyclo(bis(2-amino-4,7-dimethoxyindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: C2 **Cell:** a 23.940(2) b 6.163(1) c 15.725(1)
Space Group No.: 5 **(Å,°)** α 90.00 β 106.98(1) γ 90.00

R-Factor (%): 4.00 **Temperature(K):** 293 **Density(g/cm³):** 1.313



EBOCIH

Reference: L.J.Williams, B.Jagadish, S.R.Lyon, R.A.Kloster, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14281

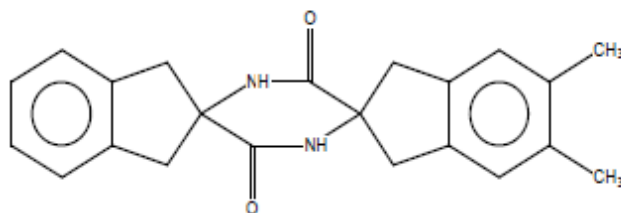
Formula: C₂₂H₂₂N₂O₂

Compound Name: Cyclo((2-amino-5,6-dimethylindan-2-carboxylic acid)-(2-aminoindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P21/c **Cell:** a 10.564(1) b 11.008(1) c 31.039(3)
Space Group No.: 14 **(Å,°)** α 90.00 β 97.92(0) γ 90.00

R-Factor (%): 6.99 **Temperature(K):** 295 **Density(g/cm³):** 1.287



EBOCON

Reference: L.J.Williams, B.Jagadish, S.R.Lyon, R.A.Kloster, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14281

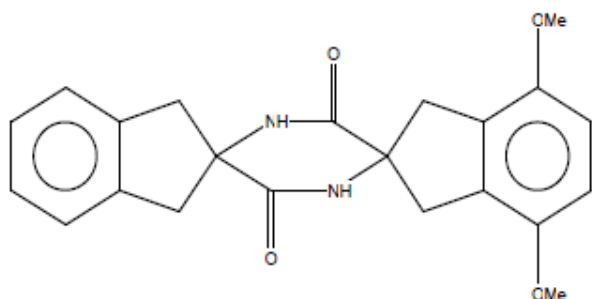
Formula: C₂₂H₂₂N₂O₄

Compound Name: Cyclo((2-amino-4,7-dimethoxyindan-2-carboxylic acid)(2-aminoindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P21 **Cell:** a 8.421(0) b 6.154(0) c 17.624(2)
Space Group No.: 4 **(Å,°)** α 90.00 β 96.48(0) γ 90.00

R-Factor (%): 7.33 **Temperature(K):** 295 **Density(g/cm³):** 1.385



EBOCUT

Reference: L.J.Williams, B.Jagadish, S.R.Lyon, R.A.Kloster, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**,14281

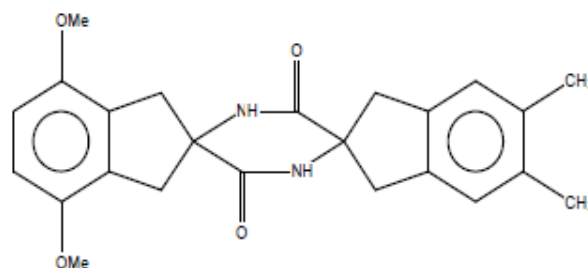
Formula: C₂₄H₂₆N₂O₄

Compound Name: Cyclo((2-amino-4,7-dimethoxyindan-2-carboxylic acid)(2-amino-5,6-dimethylindan-2-carboxylic acid))

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P21/n **Cell:** a 17.377(1) b 6.060(0) c 19.332(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 101.45(0) γ 90.00

R-Factor (%): 5.59 **Temperature(K):** 295 **Density(g/cm³):** 1.353



FECVUF

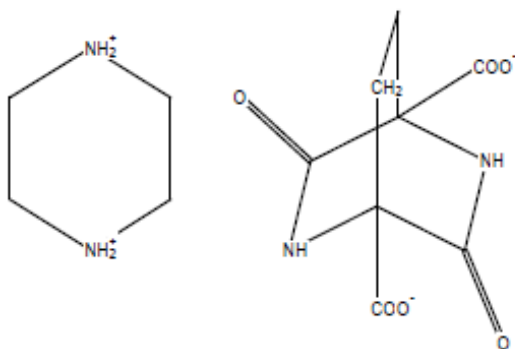
Reference: D.A.Lenev, K.A.Lyssenko, R.G.Kostyanovsky (2004)
Mendeleev Commun., 312

Formula: $C_4H_{12}N_2^{2+} \cdot C_8H_8N_2O_6^{2-}$

Compound Name: Piperidinedi-lum (1S,4S)-(+)-2,5-diaza-3,6-dioxobicyclo(2.2.2)octane-1,4-dicarboxylate

Space Group: P212121 **Cell:** a 6.812(1) b 10.891(2) c 18.519(4)
Space Group No.: 19 **(Å³):** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.01 **Temperature(K):** 293 **Density(g/cm³):** 1.520



FECWAM

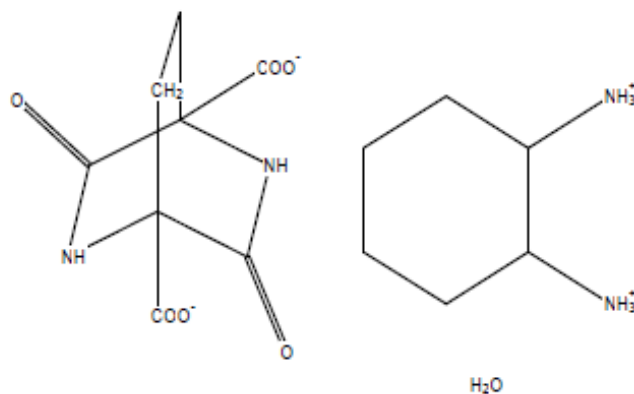
Reference: D.A.Lenev, K.A.Lyssenko, R.G.Kostyanovskya (2004)
Mendeleev Commun., 312

Formula: $C_8H_{16}N_2^{2+} \cdot C_8H_8N_2O_6^{2-} \cdot H_2O$

Compound Name: (1R,2R)-(-)-Diammoniocyclohexane (1R,4R)-(-)-2,5-diaza-3,6-dioxobicyclo(2.2.2)octane-1,4-dicarboxylate monohydrate

Space Group: P212121 **Cell:** a 10.380(0) b 12.110(1) c 12.998(1)
Space Group No.: 19 **(Å³):** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.44 **Temperature(K):** 120 **Density(g/cm³):** 1.465



FEFNIO

Reference: A.Bagarla, S.Ramakumar, M.Gupta, V.S.Chauhan (2005)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., 61, o174

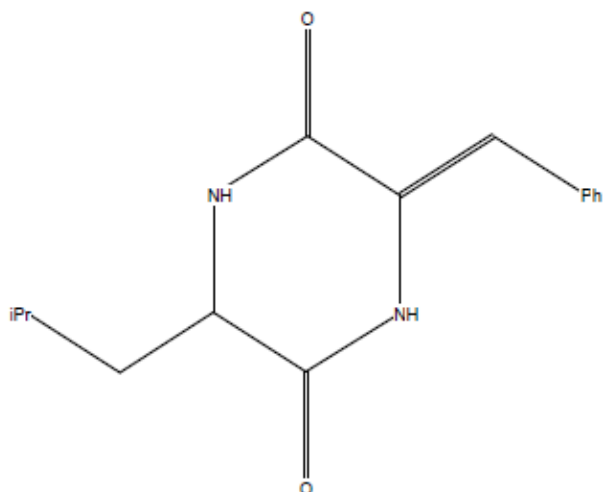
Formula: $C_{15}H_{18}N_2O_2$

Compound Name: 3-benzylidene-6-isobutylpiperazine-2,5-dione

Synonym: cyclo(L-leucyl-α,β-dehydrophenylalanyl);
Cyclic peptide (2 residues): LEU-PHE¹⁻

Space Group: P1 **Cell:** a 6.238(0) b 9.825(0) c 12.543(0)
Space Group No.: 1 **(Å³):** α 69.34(0) β 78.05(0) γ 79.40(0)

R-Factor (%): 4.50 **Temperature(K):** 293 **Density(g/cm³):** 1.228



FEFQOX

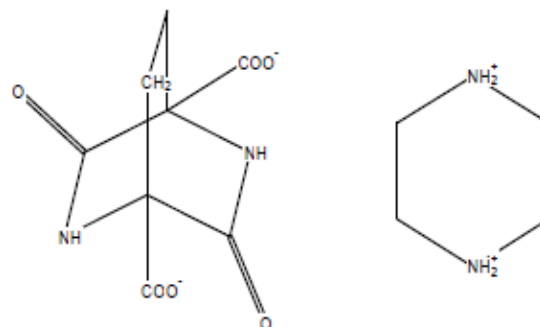
Reference: D.A.Lenev, K.A.Lyssenko, R.G.Kostyanovsky (2004)
Mendeleev Commun., 312

Formula: $C_4H_{12}N_2^{2+} \cdot C_8H_8N_2O_6^{2-}$

Compound Name: Piperidinedi-lum rac-(+)-2,5-diaza-3,6-dioxobicyclo(2.2.2)octane-1,4-dicarboxylate

Space Group: C2/c **Cell:** a 7.037(1) b 10.558(1) c 18.365(3)
Space Group No.: 15 **(Å³):** α 90.00 β 91.72(0) γ 90.00

R-Factor (%): 5.59 **Temperature(K):** 120 **Density(g/cm³):** 1.531



FEPFOV

Reference: J.Symersky, K.Blaha, V.Langer (1987)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **43**,303

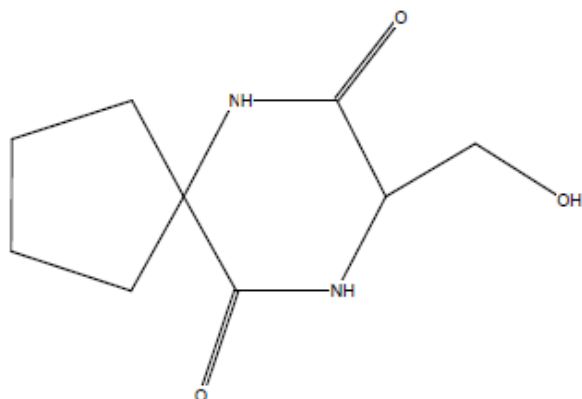
Formula: C₉H₁₄N₂O₃

Compound Name: (8S)-8-Hydroxymethyl-6,9-diazaspiro[4.5]decane-7,10-dione

Synonym: Cyclic peptide (2 residues): GLY⁻SER⁻

Space Group: P212121 **Cell:** a 7.437(6) b 20.187(15) c 6.241(4)
Space Group No.: 19 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.31 **Temperature(K)**: 295 **Density(g/cm³)**: 1.405



FICLOV

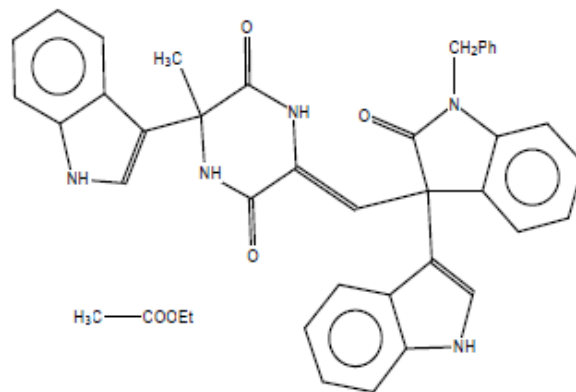
Reference: T.R.Hodges, N.M.Benjamin, S.F.Martin (2018)
Tetrahedron, **74**,3329

Formula: C₃₇H₂₉N₅O₃C₄H₅O₂

Compound Name: 6-[(1'-benzyl-2'-oxo[1',2'-dihydro-1H,3'H-(3,3'-bimole)]-3'-yl)methylidene]-3-(1H-indol-3-yl)-3-methylpiperazine-2,5-dione ethyl acetate solvate

Space Group: P-1 **Cell:** a 10.742(1) b 12.479(2) c 12.837(1)
Space Group No.: 2 **(Å³)** α 86.81(0) β 79.62(0) γ 87.36(0)

R-Factor (%): 8.08 **Temperature(K)**: 223 **Density(g/cm³)**: 1.337



FOHDIS

Reference: M.Kurbasic, S.Semeraro, Ana Garcia, S.Kraj, E.Parisi, C.Deganutti, R.De Zorzi, S.Marchesan (2019) *Synthesis*, **51**,2829

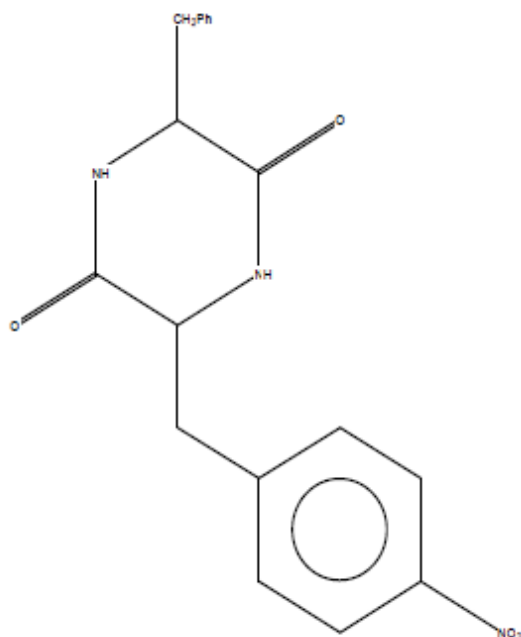
Formula: C₁₈H₁₇N₃O₄

Compound Name: 3-benzyl-5-[(4-nitrophenyl)methyl]piperazine-2,5-dione

Synonym: Cyclic peptide (2 residues): PHE-PHE⁻

Space Group: P21 **Cell:** a 16.630(3) b 6.200(1) c 30.410(6)
Space Group No.: 4 **(Å³)** α 90.00 β 90.02(3) γ 90.00

R-Factor (%): 13.23 **Temperature(K)**: 100 **Density(g/cm³)**: 1.438



FUPDUP

Reference: C.H.Gorbitz (1987) *Acta Chem.Scand.*, **41**,83

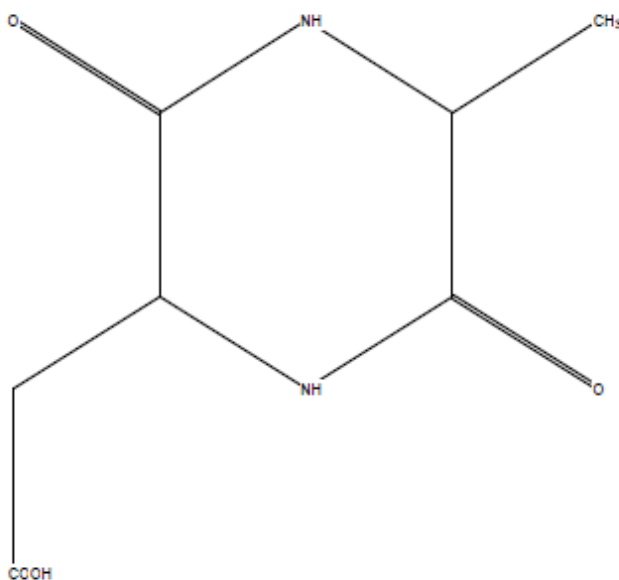
Formula: C₇H₁₀N₂O₄

Compound Name: cyclo-L-Aspartyl-L-alanyl

Synonym: (3,6-Dioxo-5-methyl-2-piperazinyl)acetic acid;
Cyclic peptide (2 residues): ASP-ALA⁻

Space Group: P21 **Cell:** a 7.573(3) b 8.650(2) c 6.151(1)
Space Group No.: 4 **(Å³)** α 90.00 β 95.88(3) γ 90.00

R-Factor (%): 3.20 **Temperature(K)**: 120 **Density(g/cm³)**: 1.543



GANJIQ

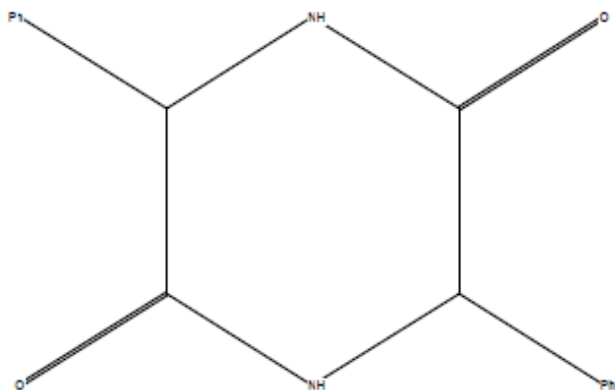
Reference: T.Govindaraju, M.Pandeeswar, K.Jayaramulu, G.Jaipuria, H.S.Atreya (2011) *Supramol.Chem.*, **23**,487

Formula: C₁₆H₁₄N₂O₂

Compound Name: 3,6-Diphenylpiperazine-2,5-dione

Space Group: Pbc_a **Cell:** **a** 10.128(0) **b** 8.205(0) **c** 15.578(1)
Space Group No.: 61 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.83 **Temperature(K):** 293 **Density(g/cm³):** 1.366



GEBVEQ

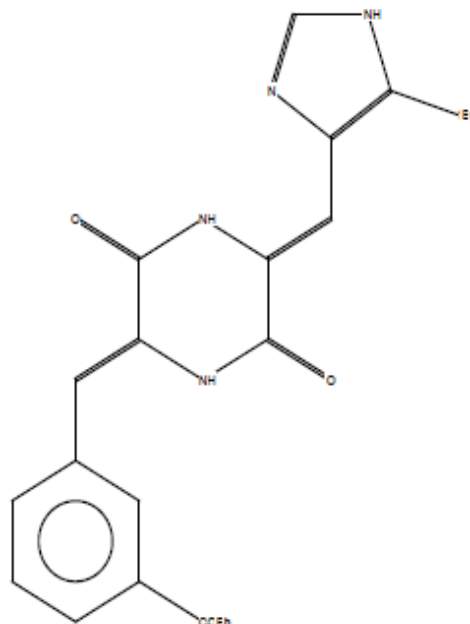
Reference: Y.Yamazaki, M.Sumikura, Y.Masuda, Y.Hayashi H.Yasui, Y.Kiso, T.Chinen, T.Usui, F.Yakushiji, B.Potts, S.Neuteboom, M.Palladino, G.K.Lloyd, Y.Hayashi (2012) *Bioorg.Med.Chem.*, **20**,4279

Formula: C₂₆H₂₄N₄O₃

Compound Name: 3-(3-Benzoylbenzylidene)-6-((5-t-butyl-1H-imidazol-4-yl)methylene)piperazine-2,5-dione

Space Group: P21/c **Cell:** **a** 7.799(0) **b** 10.570(0) **c** 26.715(2)
Space Group No.: 14 **(Å³)** α 90.00 β 94.15(0) γ 90.00

R-Factor (%): 3.29 **Temperature(K):** 90 **Density(g/cm³):** 1.332



GEJCOO

Reference: C.H.Gorbitz, L.M.Hartviksen (2006) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, **62**,o2358

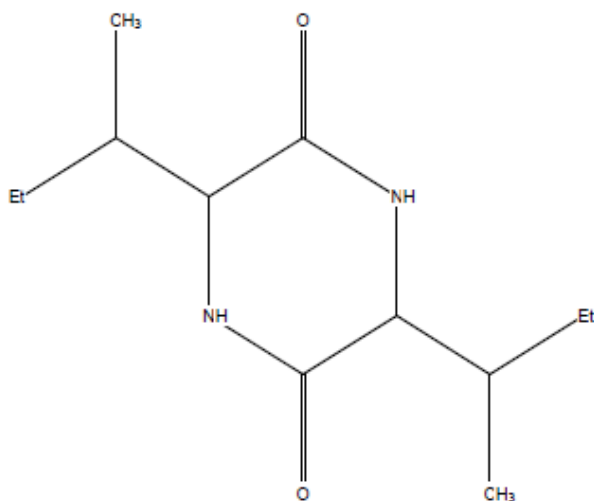
Formula: C₁₂H₂₂N₂O₂

Compound Name: (3*S*,6*S*)-3,6-bis((*S*)-*Sec*-butyl)piperazine-2,5-dione

Synonym: cyclo(L-Isoleucyl-L-Isoleucyl); Cyclic peptide (2 residues): ILE-ILE-

Space Group: P212121 **Cell:** **a** 6.242(9) **b** 10.814(15) **c** 19.790(30)
Space Group No.: 19 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.61 **Temperature(K):** 105 **Density(g/cm³):** 1.125



GESXOT

Reference: Y.Yamazaki, K.Tanaka, B.Nicholson, G.Deyanat-Yazdi, B.Potts, T.Yoshida, A.Oda, T.Kitagawa, S.Önkasa, Y.Kiso, H.Yasui, M.Akamatsu, T.Chinen, T.Usui, Y.Shinozaki, F.Yakushiji, B.R.Miller, S.Neuteboom, M.Palladino, K.Kanoh, G.K.Lloyd, Y.Hayashi (2012) *J.Med.Chem.*, **55**,1056

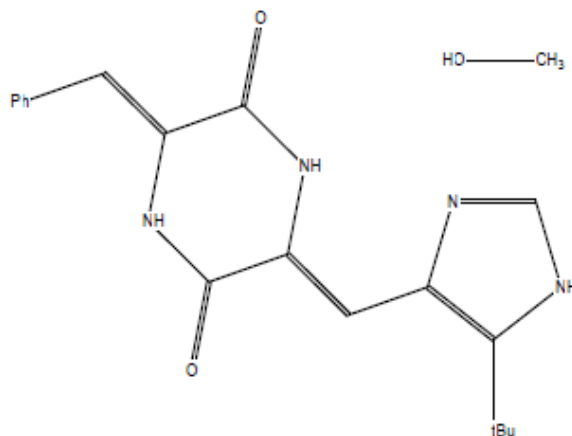
Formula: C₁₉H₂₀N₄O₂·C₁H₄O₁

Compound Name: 3-Benzylidene-6-((5-t-butyl-1H-imidazol-4-yl)methylene)piperazine-2,5-dione methanol solvate

Synonym: PDB Chemical Component code: PN6

Space Group: P21/c **Cell:** **a** 14.615(2) **b** 16.871(3) **c** 18.851(1)
Space Group No.: 14 **(Å³)** α 90.00 β 125.95(0) γ 90.00

R-Factor (%): 6.46 **Temperature(K):** 90 **Density(g/cm³):** 1.301



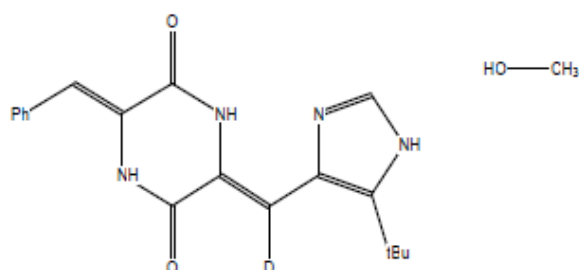
GESXOT01

Reference: Zhongpeng Ding, Hejuan Cheng, Shixiao Wang, Yingwei Hou, Jianchun Zhao, Huashi Guan, Wenbao Li (2017) *Bloog.Med.Chem.Lett.* ,27,1416

Formula: C₁₅ H₁₃ D₁ N₄ O₂ C₁ H₄ O₁

Compound Name: 3-benzylidene-5-((5-*t*-butyl-1H-imidazol-4-yl)deuteromethylene) piperazine-2,5-dione methanol solvate

Space Group: P21/n
Space Group No.: 14
Cell: (Å³)
 α 90.00
 β 103.56(0)
 γ 90.00
R-Factor (%): 5.76
Temperature(K): 293
Density(g/cm³): 1.258



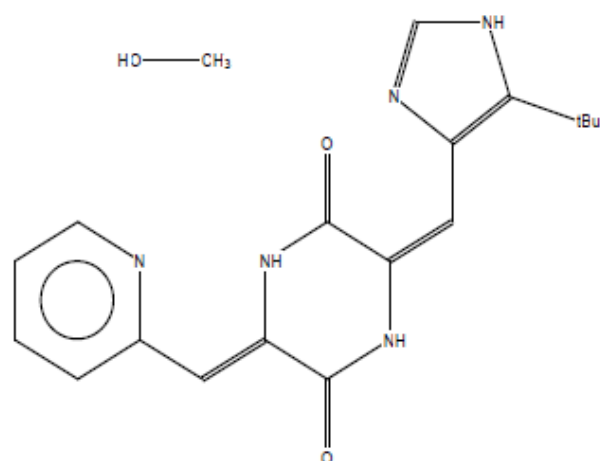
GESXUZ

Reference: Y.Yamazaki, K.Tanaka, B.Nicholson, G.Deyanat-Yazdi, B.Potts, T.Yoshida, A.Oda, T.Kitagawa, S.Orikasa, Y.Kiso, H.Yasui, M.Akamatsu, T.Chinen, T.Usui, Y.Shinozaki, F.Yakushi, B.R.Miller, S.Neuteboom, M.Paladino, K.Kanoh, G.K.Lloyd, Y.Hayashi (2012) *J.Med.Chem.* ,55,1056

Formula: C₁₈ H₁₉ N₅ O₂ 0.5(C₁ H₄ O₁)

Compound Name: 3-((5-*t*-Butyl-1H-imidazol-4-yl)methylene)-6-(pyridin-2-ylmethylene) piperazine-2,5-dione methanol solvate

Space Group: P-1
Space Group No.: 2
Cell: (Å³)
 α 88.98(0)
 β 83.69(0)
 γ 78.49(0)
R-Factor (%): 5.49
Temperature(K): 90
Density(g/cm³): 1.345



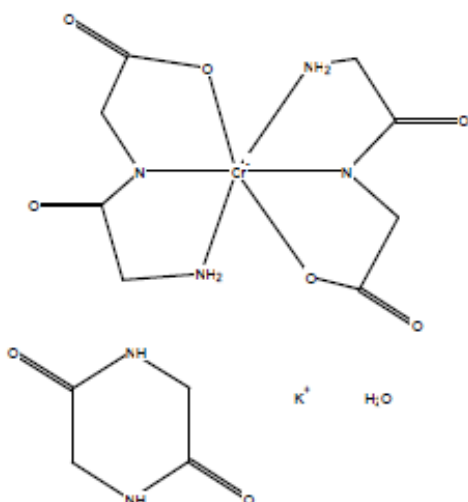
GEWYEM

Reference: V.Subramaniam, Kyu-Wang Lee, R.G.Garvey, P.E.Hoggard (1988) *Polyhedron* ,7,523

Formula: C₈ H₁₂ Cr₁ N₄ O₆ 1·C₄ H₆ N₂ O₂ K₁ 1·2(H₂ O₁)

Compound Name: Potassium bis(glycylglycinato-N,N',O)-chromium(III) piperazine-2,5-dione dihydrate

Space Group: P21/c
Space Group No.: 14
Cell: (Å³)
 α 90.00
 β 107.39(4)
 γ 90.00
R-Factor (%): 6.20
Temperature(K): 295
Density(g/cm³): 1.702



GLYTYR10

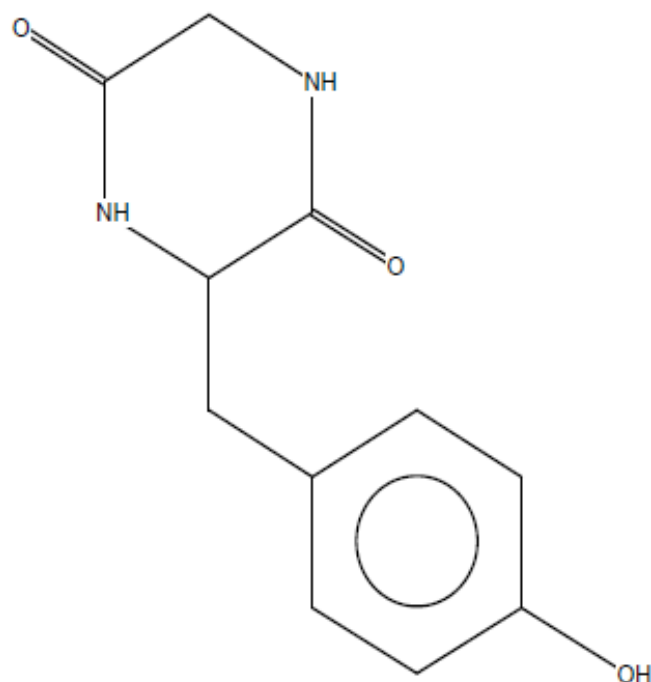
Reference: C.-F.Lin, L.E.Webb (1973) *J.Am.Chem.Soc.* ,95,6803

Formula: C₁₁ H₁₂ N₂ O₃

Compound Name: Cyclo(glycyl-L-tyrosyl)

Synonym: Cyclic peptide (2 residues); GLY-TYR-

Space Group: P212121
Space Group No.: 19
Cell: (Å³)
 α 90.00
 β 90.00
 γ 90.00
R-Factor (%): 9.90
Temperature(K): 295
Density(g/cm³): 1.420



GUTQOD

Reference: A.Jeziomska, K.Stopczyk, E.Skorupska, K.Luberda-Dumas, M.Osajca, W.Lasocha, M.Gorecki, J.Frelek, M.J.Potrzebowski (2015) *Cryst.Growth Des.*, 15,5138

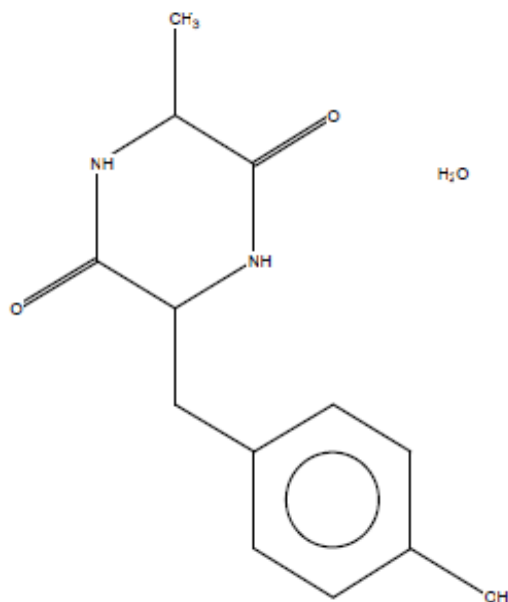
Formula: C₁₂H₁₄N₂O₃·H₂O

Compound Name: 3-(4-hydroxybenzyl)-6-methylpiperazine-2,5-dione monohydrate

Synonym: cyclo(L-Tyrosine-L-Alanine) monohydrate;
Cyclic peptide (2 residues): TYR-ALA-

Space Group: P21 **Cell:** a 11.124(0) b 6.192(0) c 8.915(0)
Space Group No.: 4 **(Å³)** α 90.00 β 100.56(0) γ 90.00

R-Factor (%): 9.73 **Temperature(K):** 293 **Density(g/cm³):** 1.388



GUTQOD01

Reference: A.Jeziomska, K.Stopczyk, E.Skorupska, K.Luberda-Dumas, M.Osajca, W.Lasocha, M.Gorecki, J.Frelek, M.J.Potrzebowski (2015) *Cryst.Growth Des.*, 15,5138

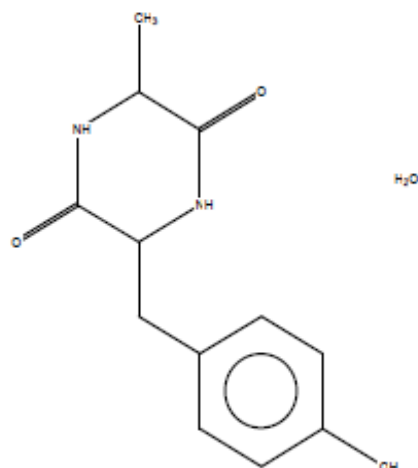
Formula: C₁₂H₁₄N₂O₃·H₂O

Compound Name: 3-(4-hydroxybenzyl)-6-methylpiperazine-2,5-dione monohydrate

Synonym: cyclo(L-Tyrosine-L-Alanine) monohydrate

Space Group: P21 **Cell:** a 11.124(0) b 6.192(0) c 8.915(0)
Space Group No.: 4 **(Å³)** α 90.00 β 100.56(0) γ 90.00

R-Factor (%): 6.43 **Temperature(K):** 293 **Density(g/cm³):** 1.388



HIFPOB

Reference: D.C.Swenson, S.M.Habermann, K.P.Murphy (1996) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, 52,383

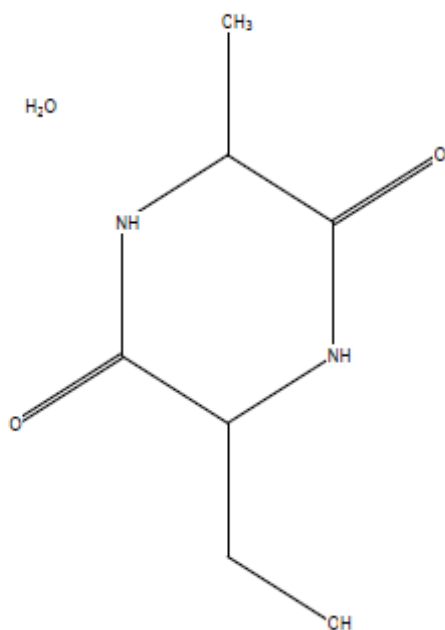
Formula: C₆H₁₀N₂O₃·H₂O

Compound Name: cis-6-Hydroxymethyl-3-methyl-2,5-piperazinedione monohydrate

Synonym: Cyclo-(L-alanyl-L-seryl) monohydrate;
Cyclic peptide (2 residues): ALA-SER-

Space Group: P1 **Cell:** a 5.222(2) b 8.389(2) c 4.759(1)
Space Group No.: 1 **(Å³)** α 93.04(3) β 102.59(2) γ 92.57(2)

R-Factor (%): 4.63 **Temperature(K):** 295 **Density(g/cm³):** 1.442



HIFPUH

Reference: D.C.Swenson, S.M.Habermann, K.P.Murphy (1996) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, 52,383

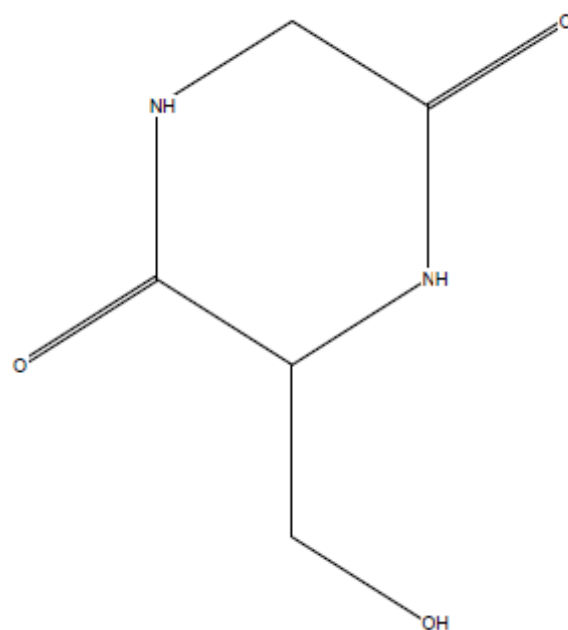
Formula: C₅H₈N₂O₃

Compound Name: Cyclo(glycyl-L-seryl)

Synonym: 3-Hydroxymethyl-2,5-piperazinedione;
Cyclic peptide (2 residues): GLY-SER-

Space Group: P21 **Cell:** a 4.896(2) b 6.550(3) c 9.737(4)
Space Group No.: 4 **(Å³)** α 90.00 β 90.80(4) γ 90.00

R-Factor (%): 3.00 **Temperature(K):** 295 **Density(g/cm³):** 1.533



HIVXIU

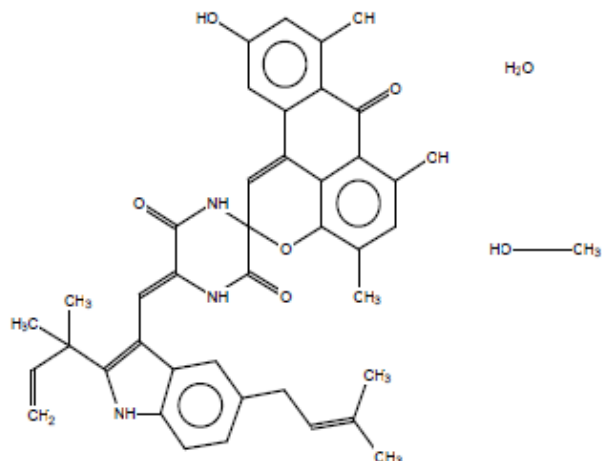
Reference: Wen-Liang Wang, Tian-Jiao Zhu, Hong-Wen Tao, Zhen-Yu Lu, Yu-Chun Fang, Qian-Qun Gu, Wei-Ming Zhu (2007) *Chem.Biodiversity* ,4,2913

Formula: C₃₃H₃₅N₃O₇·C₁H₄O₁·H₂O

Compound Name: Varilecolotide A methanol solvate monohydrate

Space Group: P-1 **Cell:** a 10.095(12) b 12.676(15) c 14.898(19)
Space Group No.: 2 **(Å³)** α 70.64(2) β 87.14(2) γ 83.84(2)

R-Factor (%): 7.64 **Temperature(K):** 298 **Density(g/cm³):** 1.315



HMOZST

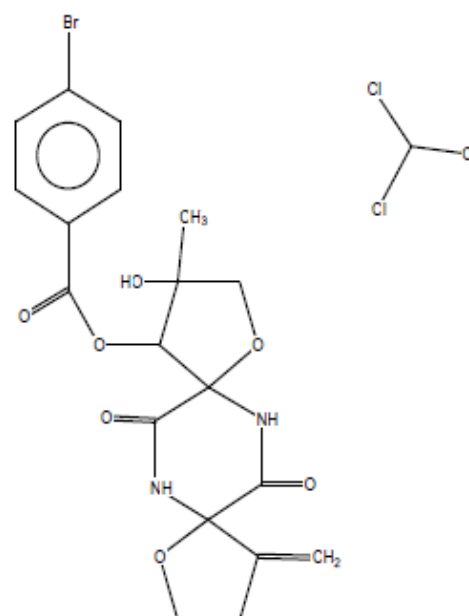
Reference: H.Magg, J.F.Blount, D.L.Coffen, T.V.Steppe, F.Wong (1978) *J.Am.Chem.Soc.* ,100,6786

Formula: C₁₉H₁₉Br₁N₂O₇·C₁H₁Cl₃

Compound Name: 3-Hydroxy-3-methyl-12-methylene-4-(p-bromobenzoyloxy)-trans-1,9-dioxo-5,13-diazadispiro[4.2.4.2]tetradeca-7,14-dione chloroform solvate

Space Group: P1 **Cell:** a 6.090 b 10.102 c 11.437
Space Group No.: 1 **(Å³)** α 113.49 β 97.56 γ 102.37

R-Factor (%): 4.20 **Temperature(K):** 295 **Density(g/cm³):** 1.593



HMOZST01

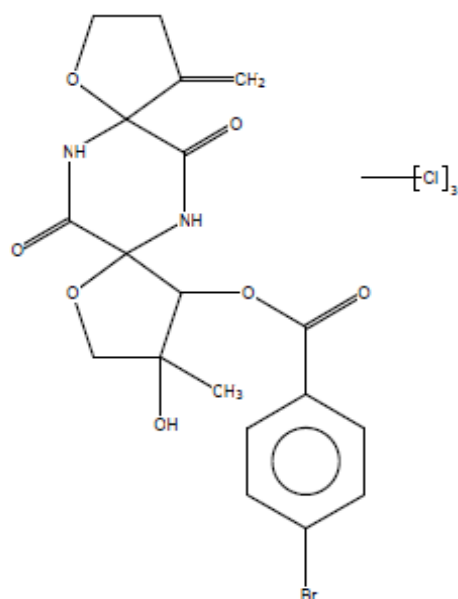
Reference: A.Santilian Junior, Xiangdong Zhang, J.Hardesty, W.R.Widger, H.Kohn (1998) *J.Med.Chem.* ,41,1185

Formula: C₁₉H₁₉Br₁N₂O₇·C₁H₁Cl₃

Compound Name: 3-Hydroxy-3-methyl-12-methylene-4-(p-bromobenzoyloxy)-trans-1,9-dioxo-5,13-diazadispiro[4.2.4.2]tetradeca-7,14-dione chloroform solvate

Space Group: P1 **Cell:** a 6.077(1) b 10.039(2) c 11.403(2)
Space Group No.: 1 **(Å³)** α 114.62(1) β 97.05(1) γ 102.22(1)

R-Factor (%): 2.50 **Temperature(K):** 223 **Density(g/cm³):** 1.622



HOQRUD

Reference: A.V.Churakov, D.A.Grishanov, A.G.Medvedev, A.A.Mikhaylov, T.A.Tripol'skaya, M.V.Vener, M.A.Navasardyan, O.Lev, P.V.Prikhodchenko (2019) *CrystEngComm* ,21,4961

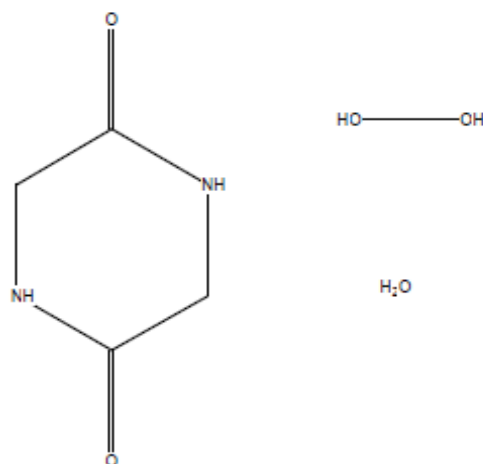
Formula: C₄H₈N₂O₂·1.786(H₂O)₂·0.214(H₂O)₁

Compound Name: cyclo-diglycine hydrogen peroxide hydrate

Synonym: Cyclic peptide (2 residues): GLY-GLY-

Space Group: P-1 **Cell:** a 5.501(0) b 5.826(0) c 6.561(0)
Space Group No.: 2 **(Å³)** α 76.39(0) β 67.82(0) γ 79.14(0)

R-Factor (%): 3.85 **Temperature(K):** 150 **Density(g/cm³):** 1.578



HOQSAK

Reference: A.V.Churakov, D.A.Grishanov, A.G.Medvedev, A.A.Mikhailov, T.A.Tripol'skaya, M.V.Vener, M.A.Navasardyan, O.Lev, P.V.Prkhodchenko (2019) *CrystEngComm*, 21,4961

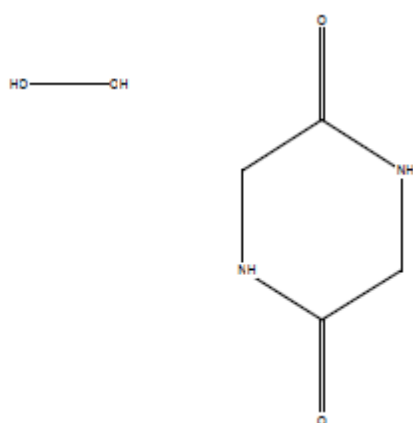
Formula: C₄H₈N₂O₂·2(H₂O₂)

Compound Name: cyclo-diglycine hydrogen peroxide

Synonym: Cyclic peptide (2 residues): GLY-GLY-

Space Group: P-1 **Cell:** a 5.654(3) b 5.802(3) c 6.648(3)
Space Group No.: 2 **(Å³)** α 76.50(0) β 66.44(0) γ 79.98(0)

R-Factor (%): 4.17 **Temperature(K):** 230 **Density(g/cm³):** 1.562



HOQSIG

Reference: A.V.Churakov, D.A.Grishanov, A.G.Medvedev, A.A.Mikhailov, T.A.Tripol'skaya, M.V.Vener, M.A.Navasardyan, O.Lev, P.V.Prkhodchenko (2019) *CrystEngComm*, 21,4961

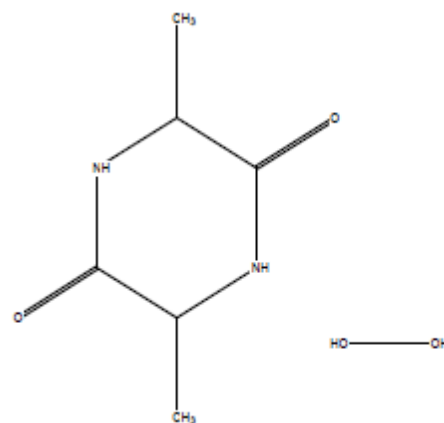
Formula: C₆H₁₀N₂O₂·2(H₂O₂)

Compound Name: cyclo-dialanine bis(hydrogen peroxide)

Synonym: Cyclic peptide (2 residues): ALA-ALA-

Space Group: P-1 **Cell:** a 7.439(2) b 8.215(2) c 8.298(2)
Space Group No.: 2 **(Å³)** α 97.33(0) β 104.58(0) γ 104.05(0)

R-Factor (%): 5.55 **Temperature(K):** 150 **Density(g/cm³):** 1.497



HUVKEQ

Reference: A.Jeziomska, K.Stopczyk, E.Skorupska, K.Luberda-Dumas, M.Oszajca, W.Lasocha, M.Gorecki, J.Frelek, M.J.Potrzebowski (2015) *Cryst.Growth Des.*, 15,5138

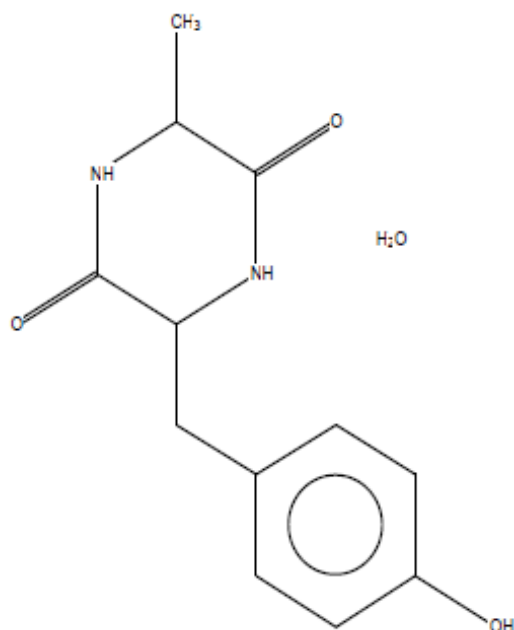
Formula: C₁₂H₁₄N₂O₃·H₂O₁

Compound Name: 3-(4-hydroxybenzyl)-6-methylpiperazine-2,5-dione monohydrate

Synonym: cyclo(L-Tyrosine-D-Alanine) monohydrate

Space Group: P21 **Cell:** a 11.689(1) b 6.160(0) c 8.874(1)
Space Group No.: 4 **(Å³)** α 90.00 β 106.42(0) γ 90.00

R-Factor (%): 10.94 **Temperature(K):** 293 **Density(g/cm³):** 1.367



HUVKEQ01

Reference: A.Jeziomska, K.Stopczyk, E.Skorupska, K.Luberda-Dumas, M.Oszajca, W.Lasocha, M.Gorecki, J.Frelek, M.J.Potrzebowski (2015) *Cryst.Growth Des.*, 15,5138

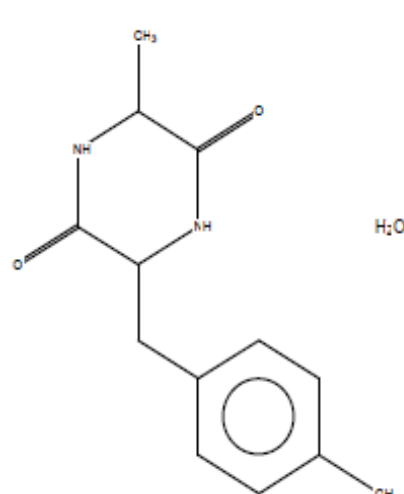
Formula: C₁₂H₁₄N₂O₃·H₂O₁

Compound Name: 3-(4-hydroxybenzyl)-6-methylpiperazine-2,5-dione monohydrate

Synonym: cyclo(L-Tyrosine-D-Alanine) monohydrate

Space Group: P21 **Cell:** a 11.689(1) b 6.160(0) c 8.873(1)
Space Group No.: 4 **(Å³)** α 90.00 β 106.42(0) γ 90.00

R-Factor (%): 8.71 **Temperature(K):** 293 **Density(g/cm³):** 1.367



IJABEC

Reference: Ling-Hong Meng, Feng-Yu Du, Xiao-Ming Li, P. Pedradab, Gang-Ming Xu, Bin-Gui Wang (2015) *J.Nat.Prod.* ,78,909

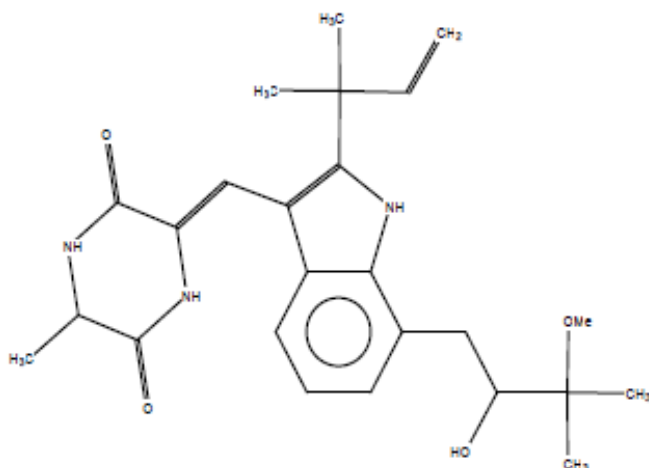
Formula: C₂₅H₃₃N₃O₄

Compound Name: 3-((7-(2-Hydroxy-3-methoxy-3-methylbutyl)-2-(2-methylbut-3-en-2-yl)-1H-Indol-3-yl)methylene)-6-methylpiperazine-2,5-dione

Synonym: Rubrumazine A

Space Group: P2₁2₁2₁ **Cell:** a 6.037(0) b 19.126(1) c 20.503(1)
Space Group No.: 19 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 10.21 **Temperature(K):** 293 **Density(g/cm³):** 1.233



IKOLOJ

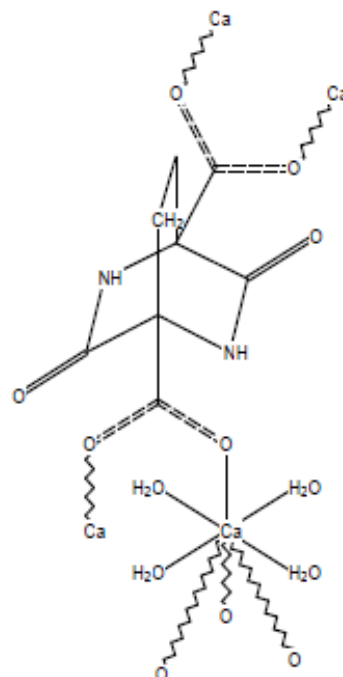
Reference: D.A.Lenev, K.A.Lyssenkov, R.G.Kostyanovsky (2003) *Eur.J.Inorg.Chem.* ,2979

Formula: (C₉H₁₄Ca₁N₂O₁₀)_n

Compound Name: catena-((+)-(μ₄-3,6-Dioxo-2,5-diazabicyclo(2.2.2)octane-1,4-dicarboxylato)-tetraaqua-calcium)

Space Group: P2₁/c **Cell:** a 10.851(2) b 5.987(1) c 9.980(2)
Space Group No.: 13 **(Å³)** α 90.00 β 112.39(0) γ 90.00

R-Factor (%): 4.65 **Temperature(K):** 110 **Density(g/cm³):** 1.874



IKOLUP

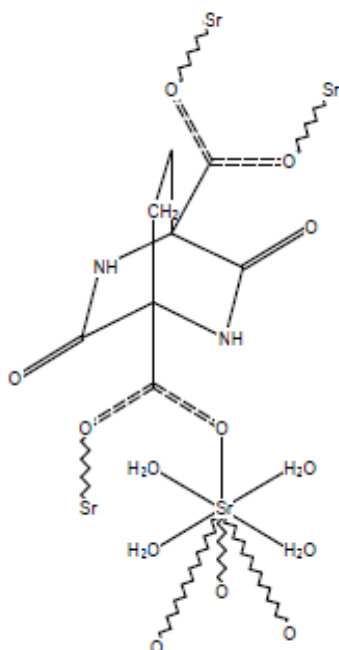
Reference: D.A.Lenev, K.A.Lyssenkov, R.G.Kostyanovsky (2003) *Eur.J.Inorg.Chem.* ,2979

Formula: (C₉H₁₄N₂O₁₀Sr₁)_n

Compound Name: catena-((+)-(μ₄-3,6-Dioxo-2,5-diazabicyclo(2.2.2)octane-1,4-dicarboxylato)-tetraaqua-strontium)

Space Group: Pc **Cell:** a 11.027(2) b 6.117(1) c 10.191(2)
Space Group No.: 7 **(Å³)** α 90.00 β 112.88(3) γ 90.00

R-Factor (%): 2.03 **Temperature(K):** 293 **Density(g/cm³):** 2.023



IKOMAW

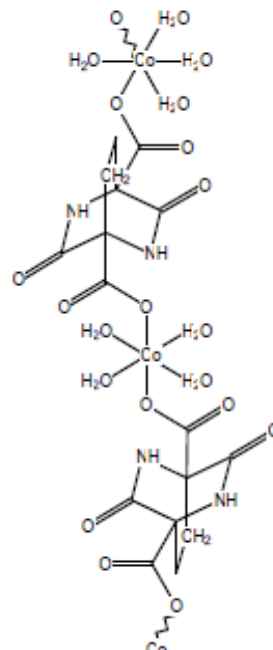
Reference: D.A.Lenev, K.A.Lyssenkov, R.G.Kostyanovsky (2003) *Eur.J.Inorg.Chem.* ,2979

Formula: (C₁₆H₂₈Co₂N₄O₂₀)_n

Compound Name: catena-((+)-bis(μ₂-3,6-Dioxo-2,5-diazabicyclo(2.2.2)octane-1,4-dicarboxylato)-octaqua-di-cobalt(II))

Space Group: P-1 **Cell:** a 5.804(1) b 10.261(2) c 11.449(3)
Space Group No.: 2 **(Å³)** α 77.58(0) β 79.04(0) γ 75.16(0)

R-Factor (%): 4.67 **Temperature(K):** 110 **Density(g/cm³):** 1.862



IKOMEA

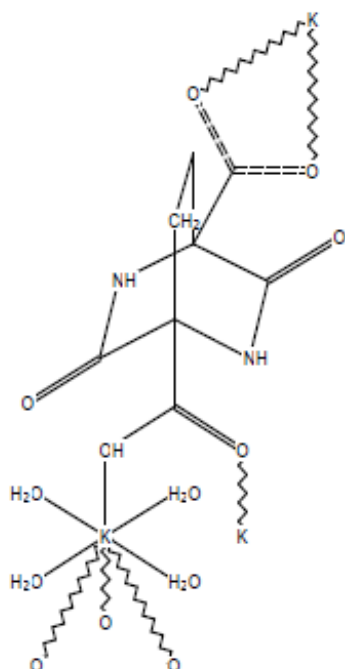
Reference: D.A.Lenev, K.A.Lyssenko, R.G.Kostyanovsky (2003) *Eur.J.Inorg.Chem.*, 2979

Formula: $(C_8 H_{15} K_1 N_2 O_{10})_n$

Compound Name: catena-[(+)-(μ_2 -4-carboxy-3,6-dioxo-2,5-diazabicyclo(2.2.2)octane-1-carboxylic acid)-tetraaqua-potassium]

Space Group: Pca21
Space Group No.: 29
Cell: a 11.429(2) Å, b 5.493(1) Å, c 20.021(4) Å
 α 90.00°, β 90.00°, γ 90.00°

R-Factor (%): 4.35
Temperature(K): 293
Density(g/cm³): 1.788



IKOMIE

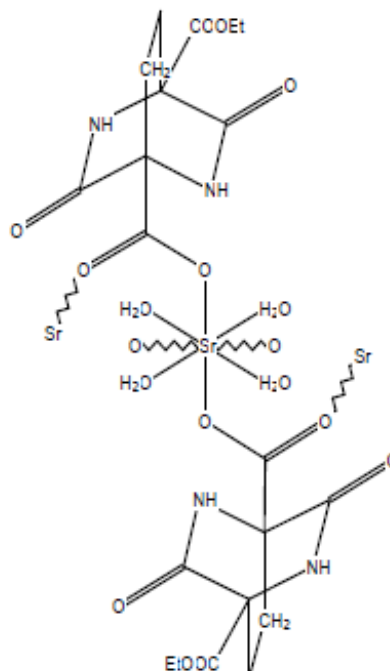
Reference: D.A.Lenev, K.A.Lyssenko, R.G.Kostyanovsky (2003) *Eur.J.Inorg.Chem.*, 2979

Formula: $(C_{20} H_{30} N_4 O_{16} Sr_1)_n$

Compound Name: catena-[(+)-bis(μ_2 -4-(Ethoxycarbonyl)-3,6-dioxo-2,5-diazabicyclo(2.2.2)octane-1-carboxylato)-tetraaqua-strontium]

Space Group: C2/c
Space Group No.: 15
Cell: a 43.554(5) Å, b 5.957(0) Å, c 10.371(1) Å
 α 90.00°, β 99.05(0)°, γ 90.00°

R-Factor (%): 5.24
Temperature(K): 110
Density(g/cm³): 1.675



IKOMOK

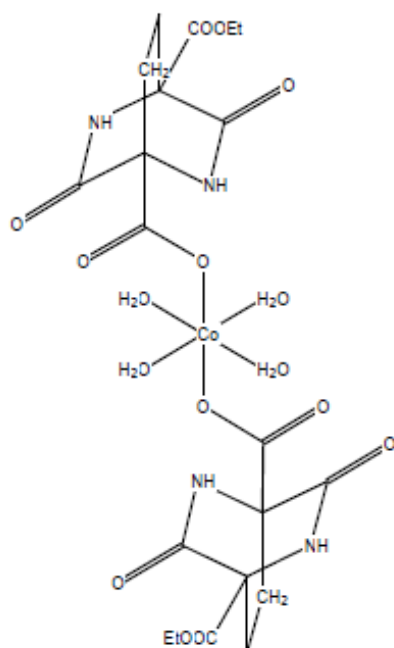
Reference: D.A.Lenev, K.A.Lyssenko, R.G.Kostyanovsky (2003) *Eur.J.Inorg.Chem.*, 2979

Formula: $C_{20} H_{30} Co_1 N_4 O_{16}$

Compound Name: (+)-bis(4-(Ethoxycarbonyl)-3,6-dioxo-2,5-diazabicyclo(2.2.2)octane-1-carboxylato)-tetraaqua-cobalt(II)

Space Group: Pca21
Space Group No.: 29
Cell: a 10.326(2) Å, b 5.586(1) Å, c 44.179(9) Å
 α 90.00°, β 90.00°, γ 90.00°

R-Factor (%): 4.96
Temperature(K): 110
Density(g/cm³): 1.672



IMUWES

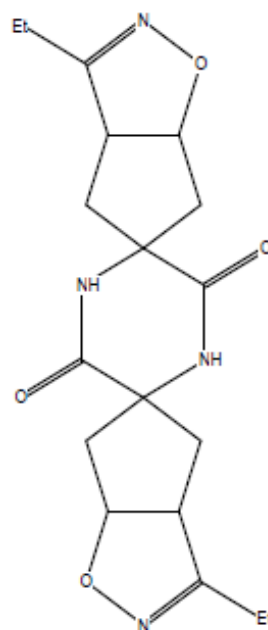
Reference: Kyung-Ho Park, M.M.Olmstead, M.J.Kurth (2003) *Synlett*, 2003,1267

Formula: $C_{18} H_{24} N_4 O_4$

Compound Name: 3,3'-Diethyl-3a,3a'',4,4'',6,6'',6a,6a''-octahydro-3H,6H-dispiro(cyclopenta(d)isoxazole-5,2'-piperazine-5',5'-cyclopenta(d)isoxazole)-3',6'-dione

Space Group: P-1
Space Group No.: 2
Cell: a 6.007(0) Å, b 6.010(0) Å, c 14.110(2) Å
 α 87.88(0)°, β 86.76(1)°, γ 60.96(0)°

R-Factor (%): 5.69
Temperature(K): 130
Density(g/cm³): 1.346



IMUWIW

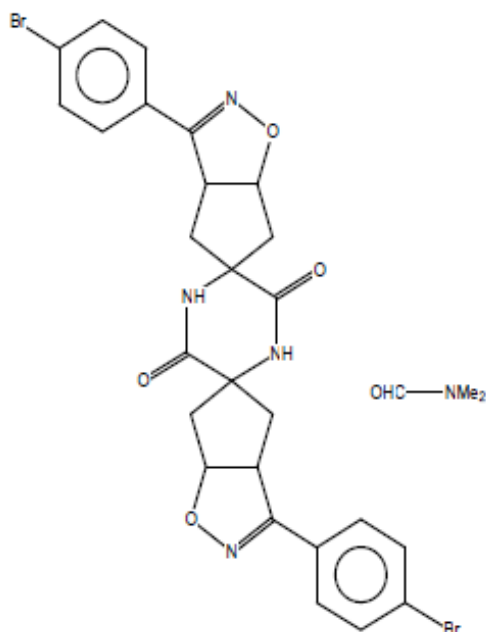
Reference: Kyung-Ho Park, M.M.Olmstead, M.J.Kurth (2003) *Synlett*, 2003,1267

Formula: C₂₆H₂₂Br₂N₄O₄·2(C₃H₇N₁O₁)

Compound Name: 3,3'-bis(4-Bromophenyl)-3a,3a',4,4',6,6',6a,6a'-octahydro-3'H,6'H-dispiro(cyclopenta(d)isoxazole-5,2'-piperazine-5,5'-cyclopenta(d)isoxazole)-3',6'-dione dimethylformamide solvate

Space Group: P2₁/c **Cell:** a 14.891(2) b 5.828(1) c 18.276(3)
Space Group No.: 14 **(Å³)** α 90.00 β 90.95(1) γ 90.00

R-Factor (%): 4.62 **Temperature(K):** 130 **Density(g/cm³):** 1.593



IMUWOC

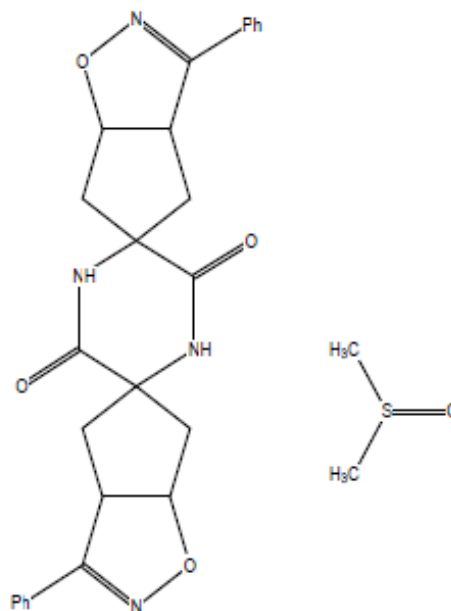
Reference: Kyung-Ho Park, M.M.Olmstead, M.J.Kurth (2003) *Synlett*, 2003,1267

Formula: C₂₆H₂₄N₄O₄·2(C₂H₆O₁S₁)

Compound Name: 3,3'-Diphenyl-3a,3a',4,4',6,6',6a,6a'-octahydro-3'H,6'H-dispiro(cyclopenta(d)isoxazole-5,2'-piperazine-5,5'-cyclopenta(d)isoxazole)-3',6'-dione dimethylsulfoxide solvate

Space Group: P-1 **Cell:** a 10.560(3) b 11.492(3) c 13.927(3)
Space Group No.: 2 **(Å³)** α 104.60(1) β 91.87(2) γ 106.57(2)

R-Factor (%): 5.03 **Temperature(K):** 130 **Density(g/cm³):** 1.306



IMUWUI

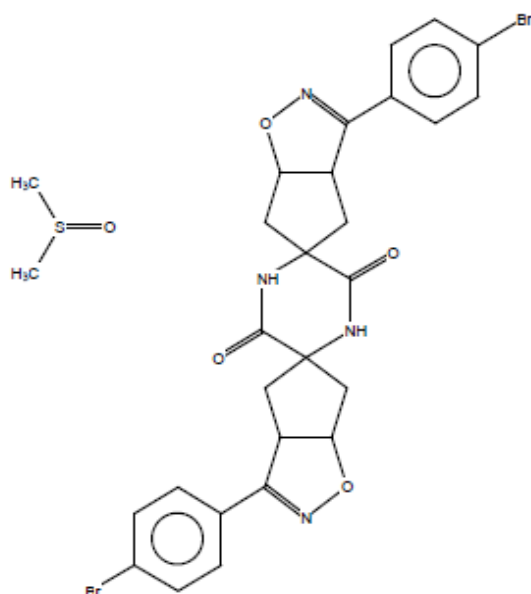
Reference: Kyung-Ho Park, M.M.Olmstead, M.J.Kurth (2003) *Synlett*, 2003,1267

Formula: C₂₆H₂₂Br₂N₄O₄·2.25(C₂H₆O₁S₁)

Compound Name: 3,3'-bis(4-Bromophenyl)-3a,3a',4,4',6,6',6a,6a'-octahydro-3'H,6'H-dispiro(cyclopenta(d)isoxazole-5,2'-piperazine-5,5'-cyclopenta(d)isoxazole)-3',6'-dione dimethylsulfoxide solvate

Space Group: C2/c **Cell:** a 18.034(4) b 13.184(3) c 30.183(5)
Space Group No.: 15 **(Å³)** α 90.00 β 91.16(1) γ 90.00

R-Factor (%): 8.04 **Temperature(K):** 130 **Density(g/cm³):** 1.463



JAGFOM

Reference: E.Benedetti, A.Bavoso, B.Di Blasio, V.Pavone, C.Pedone, L.Paolillo, M.D'Alagni (1988) *Int.J.Pept.Protein Res.*, 31,220

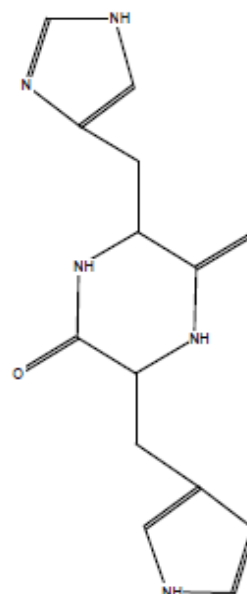
Formula: C₁₂H₁₄N₆O₂

Compound Name: cyclo(L-Histidyl-D-histidyl)

Synonym: Cyclic peptide (2 residues): HIS-HIS-

Space Group: P2₁/a **Cell:** a 7.726(1) b 9.677(1) c 8.430(1)
Space Group No.: 14 **(Å³)** α 90.00 β 106.88(5) γ 90.00

R-Factor (%): 4.70 **Temperature(K):** 295 **Density(g/cm³):** 1.480



JODGIT

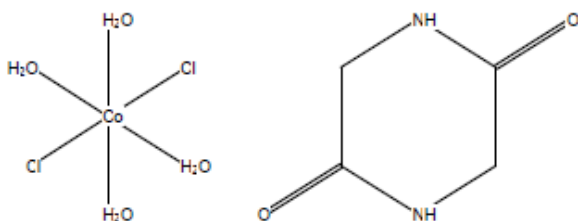
Reference: T.R.Sarangarajan, B.S.Krishnamoorthy, K.Panchanatheswaran, J.N.Low, C.Gildewell (2008) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **64**, m286

Formula: $H_3 Cl_2 Co_1 O_4 C_4 H_6 N_2 O_2$

Compound Name: trans-Tetraaqua-dichloro-cobalt(II) piperazine-2,5-dione

Space Group: P21/n **Cell:** a 9.533(0) b 6.660(0) c 10.017(0)
Space Group No.: 14 **(Å³)** α 90.00 β 114.17(0) γ 90.00

R-Factor (%): 2.05 **Temperature(K)**: 120 **Density(g/cm³)**: 1.809



JODGOZ

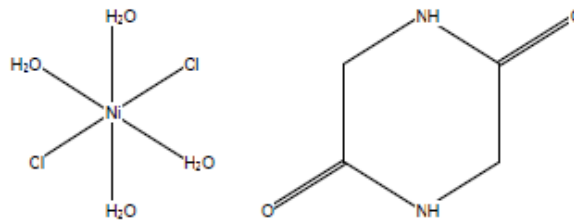
Reference: T.R.Sarangarajan, B.S.Krishnamoorthy, K.Panchanatheswaran, J.N.Low, C.Gildewell (2008) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **64**, m286

Formula: $H_3 Cl_2 Ni_1 O_4 C_4 H_6 N_2 O_2$

Compound Name: trans-Tetraaqua-dichloro-nickel(II) piperazine-2,5-dione

Space Group: P21/n **Cell:** a 9.484(0) b 6.662(0) c 9.998(0)
Space Group No.: 14 **(Å³)** α 90.00 β 114.63(0) γ 90.00

R-Factor (%): 1.89 **Temperature(K)**: 120 **Density(g/cm³)**: 1.826



JODGUF

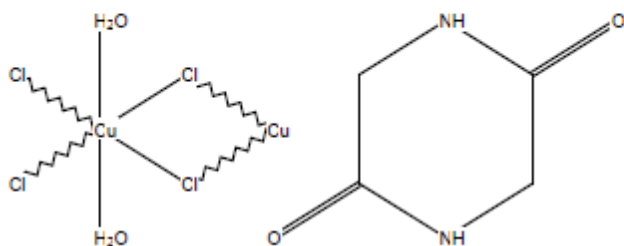
Reference: T.R.Sarangarajan, B.S.Krishnamoorthy, K.Panchanatheswaran, J.N.Low, C.Gildewell (2008) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **64**, m286

Formula: $(H_4 Cl_2 Cu_1 O_2)n.n(C_4 H_6 N_2 O_2)$

Compound Name: catena-[bis(μ₂-chloro)-trans-diaqua-copper(II) piperazine-2,5-dione solvate]

Space Group: I2/a **Cell:** a 15.224(3) b 3.969(0) c 15.444(4)
Space Group No.: 15 **(Å³)** α 90.00 β 94.73(3) γ 90.00

R-Factor (%): 5.83 **Temperature(K)**: 120 **Density(g/cm³)**: 2.032



JODHAM

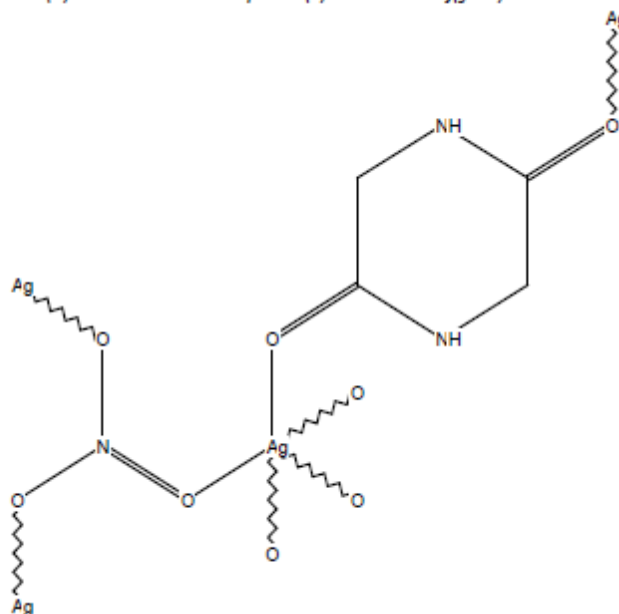
Reference: T.R.Sarangarajan, B.S.Krishnamoorthy, K.Panchanatheswaran, J.N.Low, C.Gildewell (2008) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **64**, m286

Formula: $(C_4 H_6 Ag_1 N_3 O_5)n$

Compound Name: catena-[(μ₂-Nitrate)-(μ₂-piperazine-2,5-dione)-silver(I)]

Space Group: Pnma **Cell:** a 9.628(0) b 14.718(0) c 5.247(0)
Space Group No.: 62 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 1.70 **Temperature(K)**: 120 **Density(g/cm³)**: 2.537



JODKAP

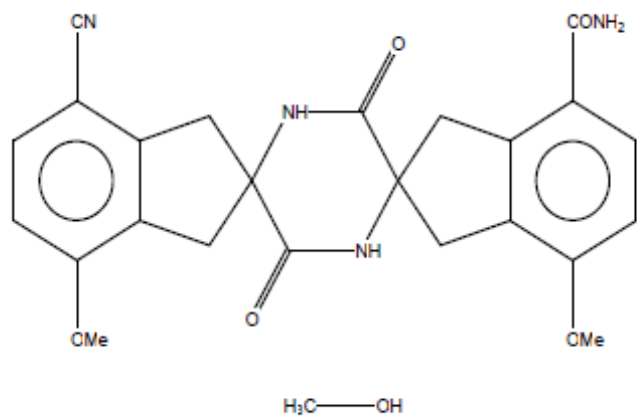
Reference: B.Jagadish, M.D.Carduoli, A.Dawson, G.S.Nichol, E.A.Mash (2008) *Acta Crystallogr., Sect.C:Cryst. Struct. Commun.* , **64**, 0431

Formula: C₂₄H₂₂N₄O₅·C₁H₄O₁

Compound Name: 4'-cyano-7,7'-dimethoxy-3',6'-dioxodispiro[indane-2,2'-piperazine-5',2''-indane]-4-carboxamide methanol solvate

Space Group: P212121 **Cell:** a 9.641(0) b 10.463(0) c 25.559(1)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.92 **Temperature(K):** 170 **Density(g/cm³):** 1.233



JOXMIS

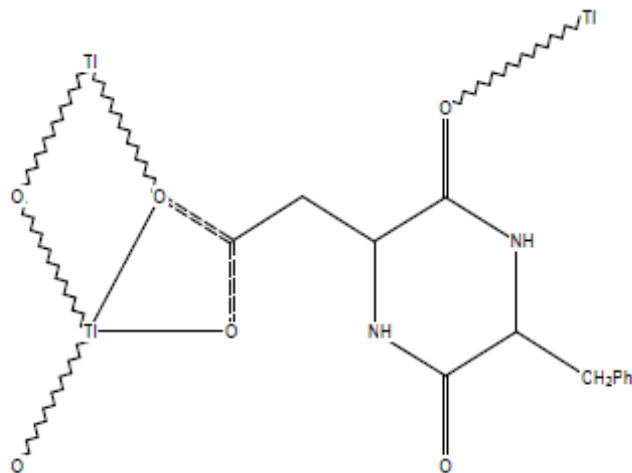
Reference: P.Mikulcik, P.Bissinger, J.Riede, H.Schmidbaur (1992) *Z.Naturforsch.,B:Chem. Sci.* , **47**,952

Formula: (C₁₃H₁₃N₂O₄Tl)_n

Compound Name: catena(μ₂-3-Benzyl-6-carboxylatomethyl-2,5-diketopiperazinato)-thallium(I)

Space Group: P-1 **Cell:** a 6.117(1) b 7.866(1) c 14.329(2)
Space Group No.: 2 **(Å,°)** α 101.13 β 99.66 γ 98.39

R-Factor (%): 1.90 **Temperature(K):** 295 **Density(g/cm³):** 2.359



KOCJUH

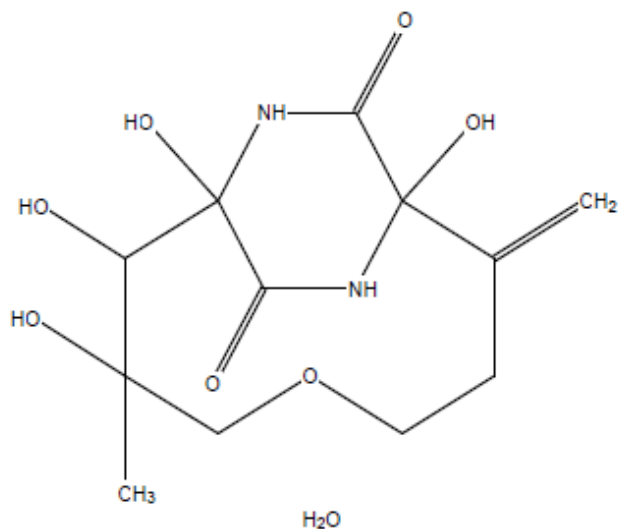
Reference: M.A.Veila, H.Kohn (1991) *J.Org.Chem.* , **56**,5462

Formula: C₁₂H₁₈N₂O₇·H₂O₁

Compound Name: (1R,2S,3S,9R)-1,2,3,9-Tetrahydroxy-3-methyl-8-methylene-5-oxa-10,12-diazabicyclo(7.2.2)tridecane-11,13-dione monohydrate

Space Group: P1 **Cell:** a 6.151(3) b 6.938(4) c 9.111(5)
Space Group No.: 1 **(Å,°)** α 90.12(4) β 95.29(4) γ 111.85(4)

R-Factor (%): 3.10 **Temperature(K):** 295 **Density(g/cm³):** 1.481



KPIPFA

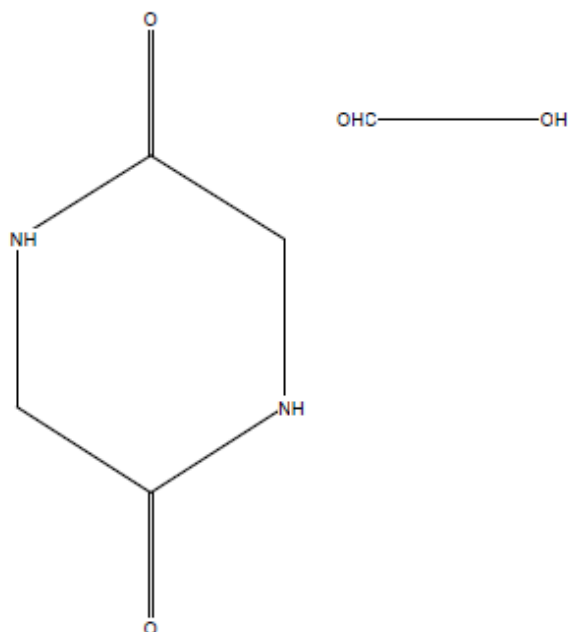
Reference: K.I.Varughese, G.Kartha, C.T.Lu (1978) *ACA,Ser.2* , **6**,27

Formula: C₄H₈N₂O₂·2(C₁H₂O₂)

Compound Name: 2,5-Diketopiperazine formic acid

Space Group: P-1 **Cell:** a 6.852(2) b 7.078(2) c 6.253(2)
Space Group No.: 2 **(Å,°)** α 109.76(2) β 122.12(2) γ 95.28(3)

R-Factor (%): 5.70 **Temperature(K):** 295 **Density(g/cm³):** 1.506



KPIPFA10

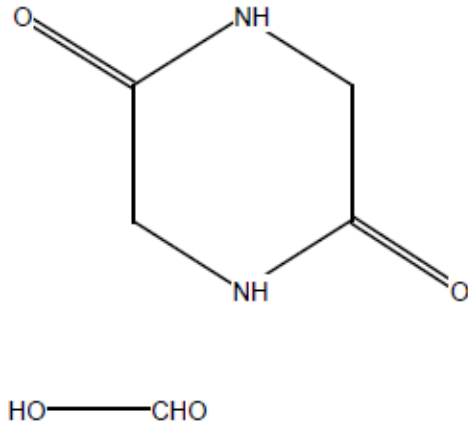
Reference: G.Kartha, K.I.Varughese, C.T.Lu (1981)
Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem., **37**, 1798

Formula: C₄ H₆ N₂ O₂·2(C₁ H₂ O₂)

Compound Name: 2,5-Piperazinedione bis(formic acid)

Space Group: P-1 **Cell:** a 6.852(2) b 7.078(2) c 6.253(2)
Space Group No.: 2 (Å³) α 109.76(2) β 122.12(2) γ 95.28(3)

R-Factor (%): 5.70 **Temperature(K):** 295 **Density(g/cm³):** 1.507



KUTBEH

Reference: J.Rohilcek, J.Malmer, R.Pazout, M.Husak, J.Cibulkova, B.Kralochvil (2010) *Acta Crystallogr., Sect.E: Struct. Rep. Online*, **66**, o821

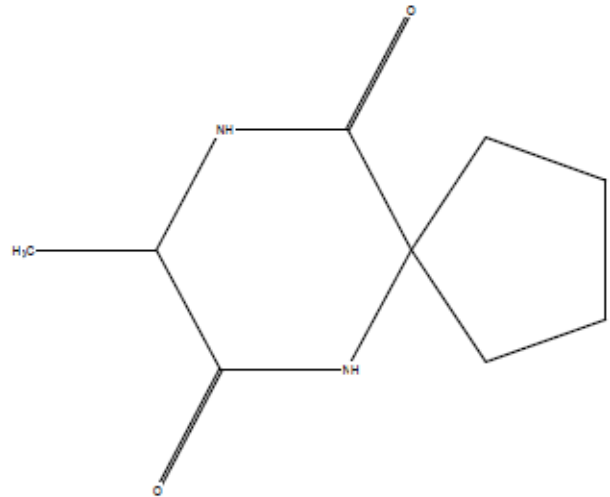
Formula: C₉ H₁₄ N₂ O₂

Compound Name: (8S)-8-methyl-6,9-diazaspiro[4.5]decane-7,10-dione

Synonym: alaptide

Space Group: P212121 **Cell:** a 21.141(0) b 7.222(0) c 6.146(0)
Space Group No.: 19 (Å³) α 90.00 β 90.00 γ 90.00

R-Factor (%): 10.20 **Temperature(K):** 293 **Density(g/cm³):** 1.290



LCDMPP01

Reference: E.Sletten (1970) *J.Am. Chem. Soc.*, **92**, 172

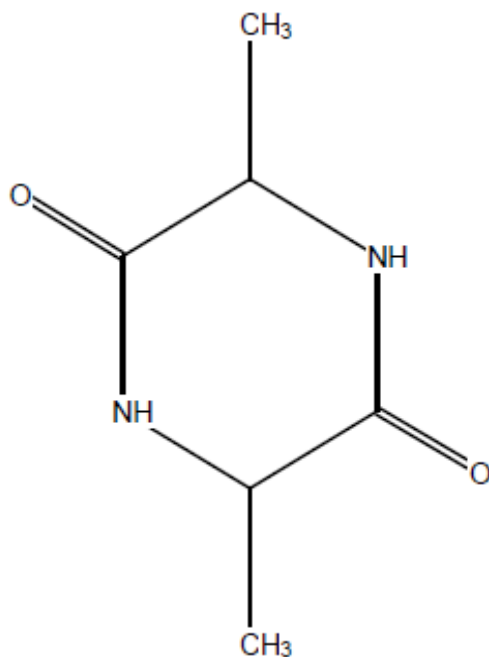
Formula: C₆ H₁₀ N₂ O₂

Compound Name: cis-3,6-Dimethylpiperazine-2,5-dione

Synonym: Cyclo-L-alanyl-L-alanyl; Cyclic peptide (2 residues): ALA-ALA-

Space Group: P1 **Cell:** a 5.155(0) b 8.060(0) c 4.670(0)
Space Group No.: 1 (Å³) α 103.16 β 103.68 γ 97.59

R-Factor (%): 3.00 **Temperature(K):** 295 **Density(g/cm³):** 1.312



LCDMPP10

Reference: E.Benedetti, P.Corradini, C.Pedone (1969) *Biopolymers*, **7**, 751

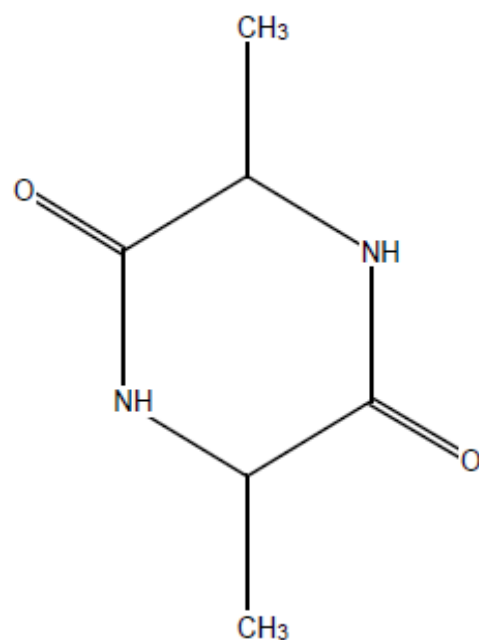
Formula: C₆ H₁₀ N₂ O₂

Compound Name: cis-3,6-Dimethylpiperazine-2,5-dione

Synonym: Cyclo-L-alanyl-L-alanyl; Cyclic peptide (2 residues): ALA-ALA-

Space Group: P1 **Cell:** a 6.067(4) b 6.082(4) c 5.155(4)
Space Group No.: 1 (Å³) α 131.70(17) β 82.40(25) γ 106.60(25)

R-Factor (%): 4.60 **Temperature(K):** 295 **Density(g/cm³):** 1.309



LEKJUG

Reference: M.B.Szkaradzinska, M.Kubicki, P.W.Codding (1994)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **50**,565

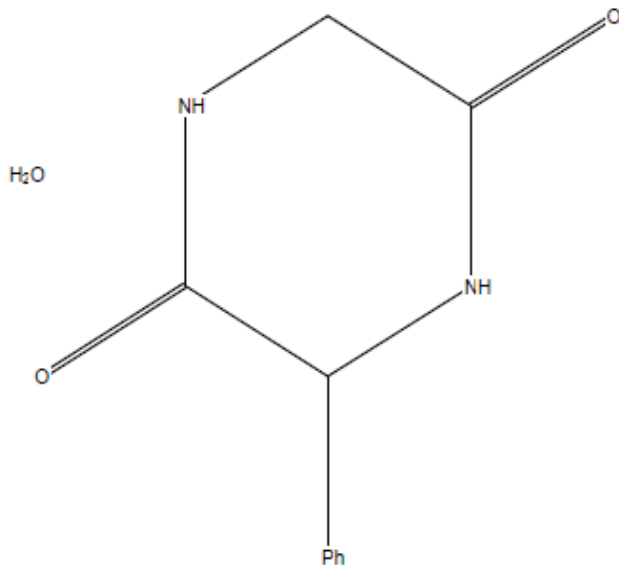
Formula: C₁₀H₁₀N₂O₂·0.25(H₂O)₁

Compound Name: Cyclo-glycyl-L-phenylglycine hydrate

Synonym: Cyclic peptide (2 residues): GLY-GLY⁻

Space Group: C2
Space Group No.: 5
Cell: (Å,°)
a 37.462(2) b 6.202(0) c 8.184(0)
α 90.00 β 98.89(0) γ 90.00

R-Factor (%): 4.44 **Temperature(K)**: 295 **Density(g/cm³)**: 1.377



LEKKAN

Reference: M.B.Szkaradzinska, M.Kubicki, P.W.Codding (1994)
Acta Crystallogr., Sect. C: Cryst. Struct. Commun., **50**,565

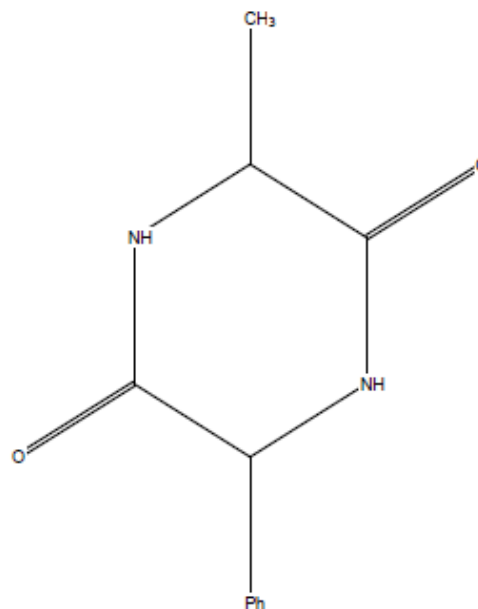
Formula: C₁₁H₁₂N₂O₂

Compound Name: Cyclo-(L-alanyl-D-phenylglycine)

Synonym: Cyclic peptide (2 residues): ALA-GLY⁻

Space Group: P21
Space Group No.: 4
Cell: (Å,°)
a 5.008(0) b 20.367(3) c 5.206(0)
α 90.00 β 105.20(0) γ 90.00

R-Factor (%): 4.62 **Temperature(K)**: 295 **Density(g/cm³)**: 1.324



LURJOY

Reference: R.S.Glass, G.L.Hug, C.Shoneich, G.S.Wilson,
L.Kuznetsova, Tang-man Lee, M.Ammam, E.Lorance, T.Nauser,
G.S.Nichol, T.Yamamoto (2009) *J.Am.Chem.Soc.*, **131**,13791

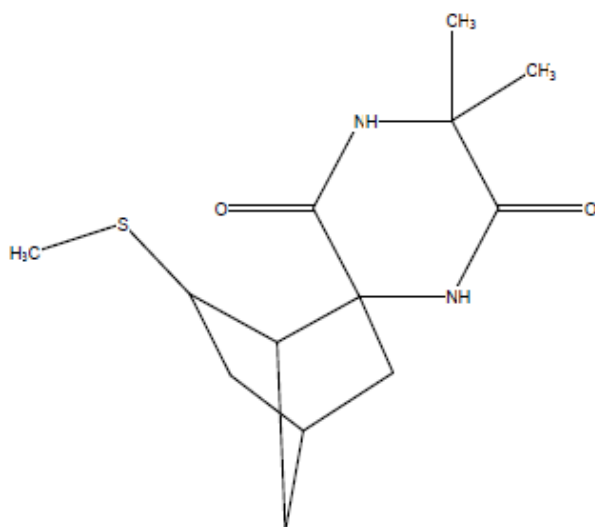
Formula: C₁₃H₂₀N₂O₂S₁

Compound Name: (1R,2R,4S)-Spiro[[6-endo-methylthio]bicyclo[2.2.1]heptane-2,2'-piperazine]-5',5'-dimethyl-3',6'-dione

Synonym: 5',5'-Dimethyl-6-(methylsulfanyl)-3H,6H-spiro[bicyclo[2.2.1]heptane-2,2'-piperazine]-3',6'-dione

Space Group: C2/c
Space Group No.: 15
Cell: (Å,°)
a 22.211(2) b 7.992(0) c 16.819(1)
α 90.00 β 110.41(0) γ 90.00

R-Factor (%): 4.65 **Temperature(K)**: 150 **Density(g/cm³)**: 1.274



MIKDUF

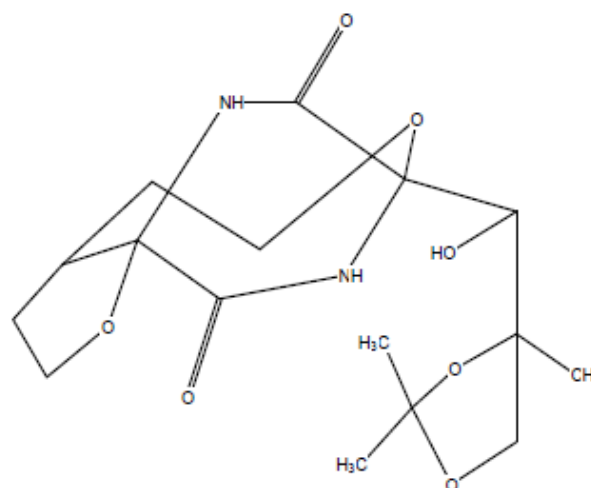
Reference: F.Vincent, J.Srinivasan, A.Santillan Junior, W.R.Widger,
H.Kohn (2001) *J.Org.Chem.*, **66**,2251

Formula: C₁₆H₂₄N₂O₇

Compound Name: 3-[hydroxy(2,2,4-trimethyl-1,3-dioxolan-4-yl)methyl]-tetrahydro-1H,5H-3,9a-(epiminomethano)furo[2,3-e][1,4]oxazocine-2,10-dione

Space Group: P212121
Space Group No.: 19
Cell: (Å,°)
a 6.610(1) b 10.120(1) c 24.963(3)
α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.00 **Temperature(K)**: 223 **Density(g/cm³)**: 1.418



MIKFAN

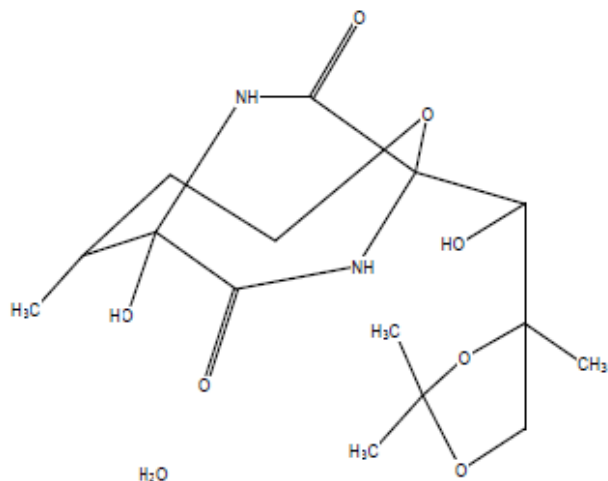
Reference: F.Vincent, J.Srinivasan, A.Santilian Junior, W.R.Widger, H.Kohn (2001) *J.Org.Chem.*, **66**,2251

Formula: C₁₅H₂₄N₂O₇·H₂O₁

Compound Name: 6-hydroxy-1-[hydroxy(2,2,4-trimethyl-1,3-dioxolan-4-yl)methyl]-5-methyl-2-oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione monohydrate

Space Group: P21 **Cell:** a 10.935(1) b 7.296(1) c 11.372(1)
Space Group No.: 4 **(Å³)** α 90.00 β 108.74(1) γ 90.00

R-Factor (%): 4.70 **Temperature(K):** 223 **Density(g/cm³):** 1.401



MOKDOG

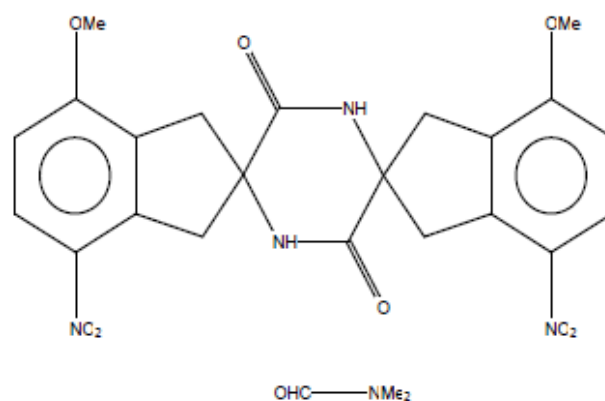
Reference: D.Nitrampebura, B.Jagadish, G.S.Nichol, M.D.Carduoli, A.Dawson, A.Rajapakshe, A.G.Oliver, W.Clegg, R.W.Harrington, L.Layne Junior, J.I.Margolis, E.A.Mash (2008) *Cryst.Growth Des.*, **8**, 3257

Formula: C₂₂H₂₀N₄O₉·C₃H₇N₁O₁

Compound Name: (S,S)-4,4'-Dimethoxy-7,7'-dinitro-1,1',3,3'-tetrahydro-3H,6'H-dispiro[indene-2,2'-piperazine-5',2''-indene]-3',6'-dione dimethylformamide solvate

Space Group: P212121 **Cell:** a 6.341(3) b 19.275(10) c 20.483(10)
Space Group No.: 19 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 10.63 **Temperature(K):** 150 **Density(g/cm³):** 1.437



MOKDUM

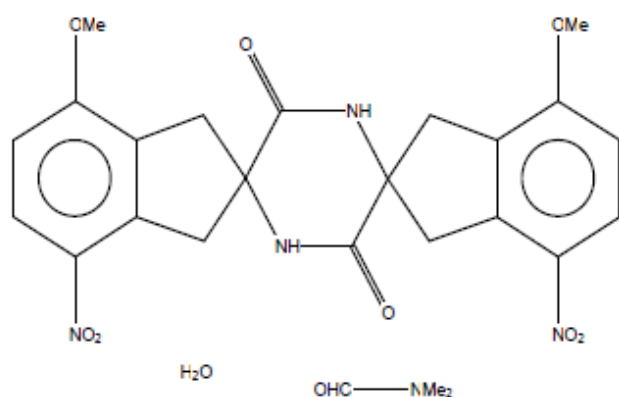
Reference: D.Nitrampebura, B.Jagadish, G.S.Nichol, M.D.Carduoli, A.Dawson, A.Rajapakshe, A.G.Oliver, W.Clegg, R.W.Harrington, L.Layne Junior, J.I.Margolis, E.A.Mash (2008) *Cryst.Growth Des.*, **8**, 3257

Formula: C₂₂H₂₀N₄O₉·2(C₃H₇N₁O₁)·0.67(H₂O₁)

Compound Name: rac-4,4'-Dimethoxy-7,7'-dinitro-1,1',3,3'-tetrahydro-3H,6'H-dispiro[indene-2,2'-piperazine-5',2''-indene]-3',6'-dione dimethylformamide solvate hydrate

Space Group: P-1 **Cell:** a 14.721(4) b 15.416(5) c 20.197(4)
Space Group No.: 2 **(Å³)** α 93.42(2) β 100.89(1) γ 94.46(2)

R-Factor (%): 6.24 **Temperature(K):** 150 **Density(g/cm³):** 1.395



MOKFAU

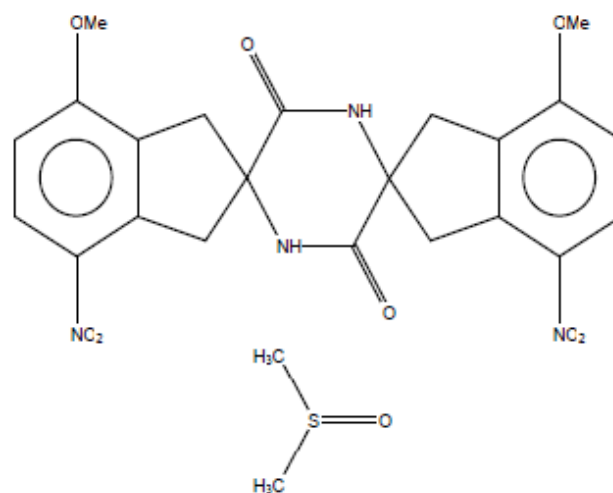
Reference: D.Nitrampebura, B.Jagadish, G.S.Nichol, M.D.Carduoli, A.Dawson, A.Rajapakshe, A.G.Oliver, W.Clegg, R.W.Harrington, L.Layne Junior, J.I.Margolis, E.A.Mash (2008) *Cryst.Growth Des.*, **8**, 3257

Formula: C₂₂H₂₀N₄O₉·2.5(C₂H₆O₁S₁)

Compound Name: rac-4,4'-Dimethoxy-7,7'-dinitro-1,1',3,3'-tetrahydro-3H,6'H-dispiro[indene-2,2'-piperazine-5',2''-indene]-3',6'-dione dimethylsulfoxide solvate

Space Group: P-1 **Cell:** a 9.603(2) b 11.614(3) c 14.295(3)
Space Group No.: 2 **(Å³)** α 82.50(0) β 79.19(0) γ 82.97(0)

R-Factor (%): 5.96 **Temperature(K):** 170 **Density(g/cm³):** 1.427



MOKFEY

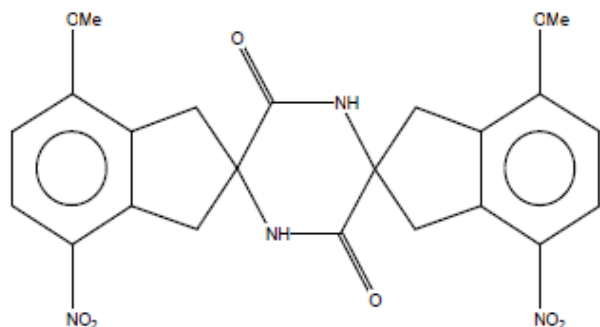
Reference: D.Nitrampebura, B.Jagadish, G.S.Nichol, M.D.Carducci, A.Dawson, A.Rajapakshe, A.G.Oliver, W.Clegg, R.W.Harrington, L.Layne Junior, J.I.Margolis, E.A.Mash (2008) *Cryst.Growth Des.*, **8**, 3257

Formula: C₂₂H₂₀N₄O₈

Compound Name: meso-4,4'-Dimethoxy-7,7'-dinitro-1,1',3,3'-tetrahydro-3'H,6'H-dispiro[indene-2,2'-piperazine-5',2'-indene]-3',6'-dione

Space Group: C2/m **Cell:** a 17.149(7) b 6.368(3) c 9.310(4)
Space Group No.: 12 **(Å,°)** α 90.00 β 106.21(0) γ 90.00

R-Factor (%): 5.98 **Temperature(K):** 120 **Density(g/cm³):** 1.593



MOKFIC

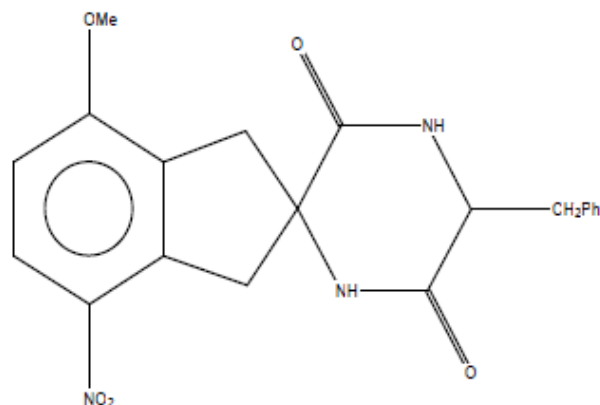
Reference: D.Nitrampebura, B.Jagadish, G.S.Nichol, M.D.Carducci, A.Dawson, A.Rajapakshe, A.G.Oliver, W.Clegg, R.W.Harrington, L.Layne Junior, J.I.Margolis, E.A.Mash (2008) *Cryst.Growth Des.*, **8**, 3257

Formula: C₂₀H₁₉N₃O₅

Compound Name: (R,S)-5-Benzyl-4-methoxy-7-nitro-1,3-dihydro-3'H,6'H-spiro[indene-2,2'-piperazine]-3',6'-dione

Space Group: P21 **Cell:** a 11.872(5) b 6.262(3) c 12.819(6)
Space Group No.: 4 **(Å,°)** α 90.00 β 111.22(1) γ 90.00

R-Factor (%): 5.37 **Temperature(K):** 173 **Density(g/cm³):** 1.426



MOLJUT

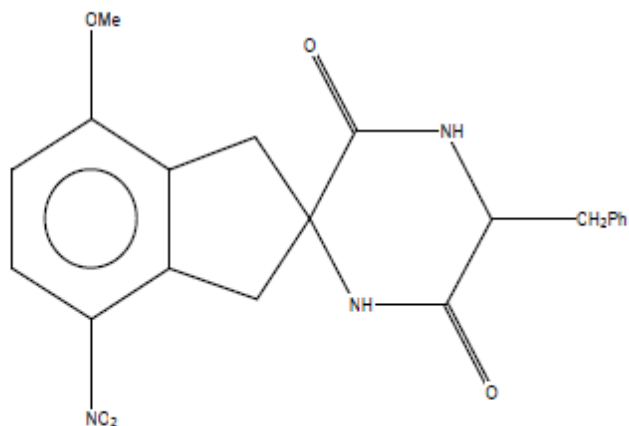
Reference: D.Nitrampebura, B.Jagadish, G.S.Nichol, M.D.Carducci, A.Dawson, A.Rajapakshe, A.G.Oliver, W.Clegg, R.W.Harrington, L.Layne Junior, J.I.Margolis, E.A.Mash (2008) *Cryst.Growth Des.*, **8**, 3257

Formula: C₂₀H₁₉N₃O₅

Compound Name: (S,S)-5-Benzyl-4-methoxy-7-nitro-1,3-dihydro-3'H,6'H-spiro[indene-2,2'-piperazine]-3',6'-dione

Space Group: P21 **Cell:** a 10.655(1) b 6.048(0) c 13.991(1)
Space Group No.: 4 **(Å,°)** α 90.00 β 91.17(0) γ 90.00

R-Factor (%): 5.79 **Temperature(K):** 170 **Density(g/cm³):** 1.405



MULREQ

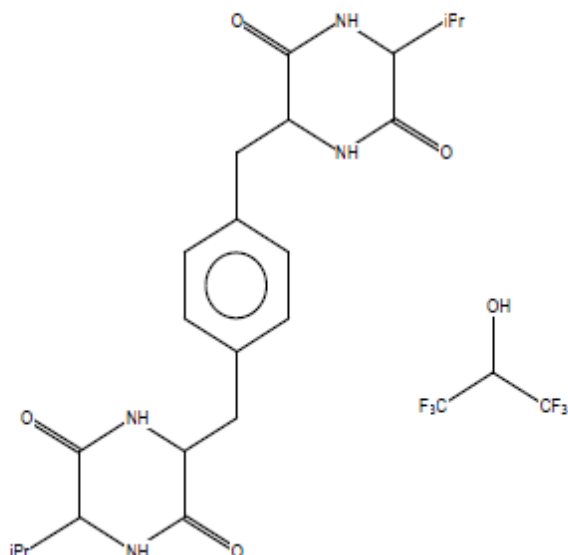
Reference: Y.Ishida, T.Aida (2002) *J.Am.Chem.Soc.*, **124**,14017

Formula: C₂₂H₃₀N₄O₄·2(C₃H₂F₆O)₁

Compound Name: 1,4-bis((3-(6-Isopropyl)piperazine-2,5-dione)methyl)benzene 1,1,1,3,3,3-hexafluoro-2-propanol solvate

Space Group: P21212 **Cell:** a 18.860(80) b 18.550(30) c 6.244(9)
Space Group No.: 18 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 13.60 **Temperature(K):** 123 **Density(g/cm³):** 1.141



MULRIU

Reference: Y.Ishida, T.Aida (2002) *J.Am.Chem.Soc.*, **124**,14017

Formula: C₂₂H₃₀N₄O₄(C₂H₅F₃O₂)

Compound Name: 1,4-bis((5-Isopropylpiperazine-2,5-dione-3-yl)methyl)benzene trifluoroacetic acid solvate

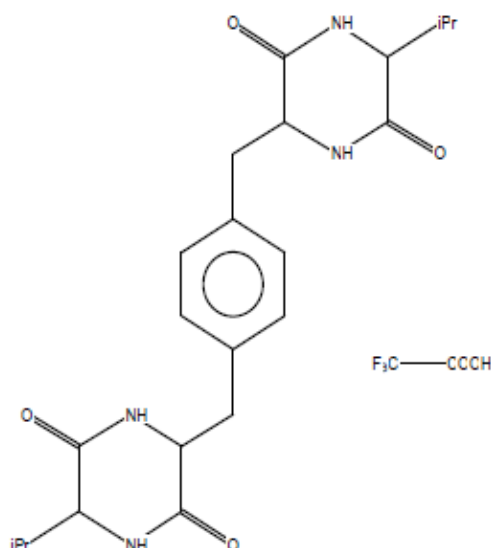
Space Group: P-1

Space Group No.: 2

R-Factor (%): 7.80

Cell: a 6.235(2) b 11.743(5) c 14.210(7)
α 105.67(2) β 95.62(0) γ 96.00(0)

Temperature(K): 123 **Density(g/cm³):** 1.454



MUSJUF

Reference: R.G.Kostyanovsky, K.A.Lyssenko, D.A.Lenev, I.A.Bronzova (2002) *Tetrahedron:Asymm.*, **13**,2697

Formula: C₈H₁₀N₄O₄·2(H₂O)

Compound Name: 2,5-Diazabicyclo[2.2.2]octane-3,6-dione-1,4-dicarboxamide dihydrate

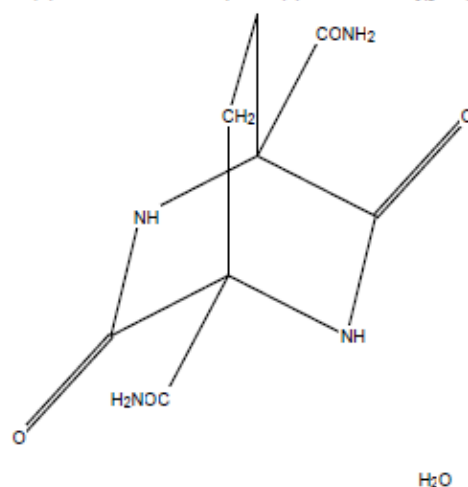
Space Group: C2/c

Space Group No.: 15

R-Factor (%): 3.45

Cell: a 21.950(4) b 5.609(1) c 28.430(6)
α 90.00 β 105.33(3) γ 90.00

Temperature(K): 153 **Density(g/cm³):** 1.548



NELFAO

Reference: Ling-Hong Meng, Xiao-Ming Li, Yang Liu, Gang-Ming Xu, Bin-Gui Wang (2017) *RSC Advances*, **7**,55026

Formula: C₁₉H₁₈N₂O₃S₁·C₁H₄O₁

Compound Name: 3-benzyl-6-[(2-hydroxyphenyl)methylidene]-3-(methylsulfonyl)piperazine-2,5-dione methanol solvate

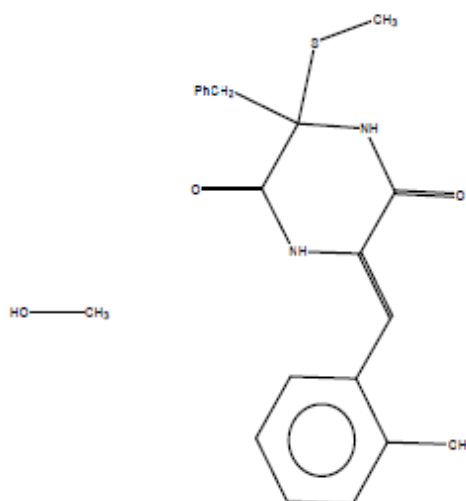
Space Group: P21

Space Group No.: 4

R-Factor (%): 5.77

Cell: a 8.369(0) b 6.172(0) c 18.270(1)
α 90.00 β 95.73(0) γ 90.00

Temperature(K): 293 **Density(g/cm³):** 1.367



NEZTIV

Reference: J.M.Wolff, W.S.Sheldrick (1997) *J.Organomet.Chem.*, **531**, 141

Formula: C₃₈H₄₈N₂O₂Ru₂·4(C₁F₃O₃S₁)⁻¹

Compound Name: (μ₂-η⁵,η⁶-Cyclophenylalanyl-phenylalanyl)-bis(η⁶-p-cymene)-diruthenium(II) tetrakis(trifluoromethanesulfonate)

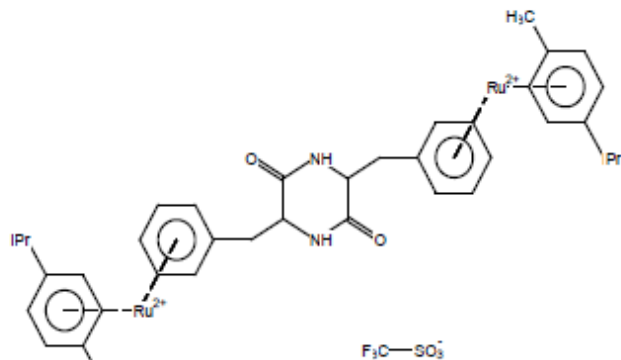
Space Group: C2

Space Group No.: 5

R-Factor (%): 6.98

Cell: a 26.640(5) b 19.136(4) c 10.026(2)
α 90.00 β 96.04(3) γ 90.00

Temperature(K): 295 **Density(g/cm³):** 1.779



NISTIS

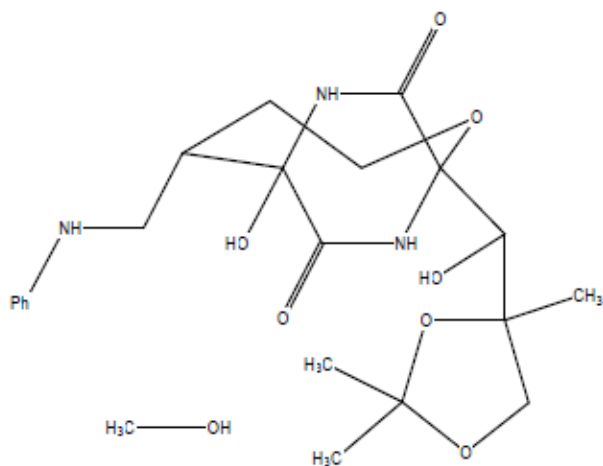
Reference: H.Park, Z.Zhang, X.Zhang, W.R.Widger, H.Kohn (1996)
J.Org.Chem., **61**,7764

Formula: C₂₁H₂₉N₃O₇·C₁H₄O₁

Compound Name: C(5a)-Anilnodihydrocycloimycin C(2'),C(3')-acetone methanol solvate

Space Group: P212121 **Cell:** a 6.921(1) b 10.979(2) c 29.915(7)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.90 **Temperature(K):** 295 **Density(g/cm³):** 1.366



NIWPUF

Reference: C.H.Gorbitz, L.M.Hartviksen (2008)
Acta Crystallogr., Sect.E:Struct.Rep.Online, **64**,0436

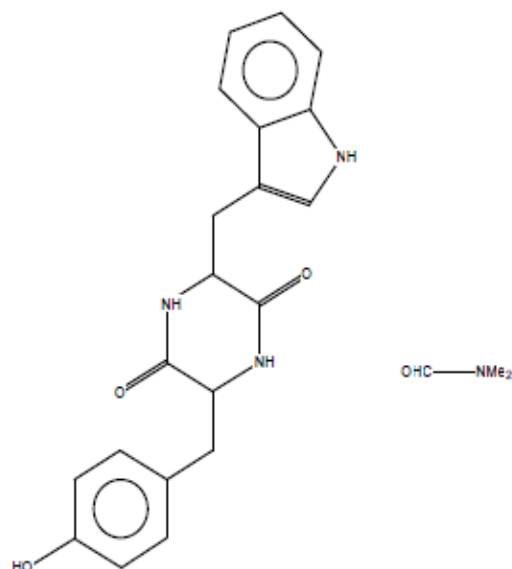
Formula: C₂₀H₁₉N₃O₃·C₃H₇N₁O₁

Compound Name: (3S,6S)-3-(4-Hydroxybenzyl)-6-(1H-indol-3-ylmethyl)piperazine-2,5-dione dimethylformamide solvate

Synonym: Cyclo-(L-tyrosyl-L-tryptophanyl) dimethylformamide solvate; PDB Chemical Component code: 1GB; Cyclic peptide (2 residues): TYR-TRP-

Space Group: P21 **Cell:** a 6.192(0) b 15.387(0) c 11.378(0)
Space Group No.: 4 **(Å,°)** α 90.00 β 96.66(0) γ 90.00

R-Factor (%): 4.53 **Temperature(K):** 105 **Density(g/cm³):** 1.303



NUVYEI

Reference: S.Palaich, D.N.Chin, E.E.Simanek, J.C.MacDonald, G.M.Whiteides, M.T.McBride, G.T.R.Palmore (1997)
J.Am.Chem.Soc., **119**,11807

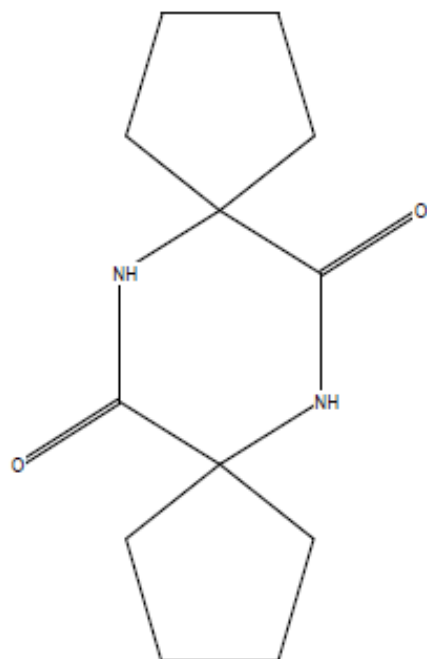
Formula: C₁₂H₁₈N₂O₂

Compound Name: 3,6-bis(Cycloletramethylene)-2,5-piperazinedione

Synonym: Cyclic peptide (2 residues): GLY⁺-GLY⁻

Space Group: P-1 **Cell:** a 6.208(0) b 8.931(2) c 5.786(1)
Space Group No.: 2 **(Å,°)** α 104.97(2) β 116.84(2) γ 78.18(2)

R-Factor (%): 4.23 **Temperature(K):** 295 **Density(g/cm³):** 1.342



NUVYIM

Reference: S.Palaich, D.N.Chin, E.E.Simanek, J.C.MacDonald, G.M.Whiteides, M.T.McBride, G.T.R.Palmore (1997)
J.Am.Chem.Soc., **119**,11807

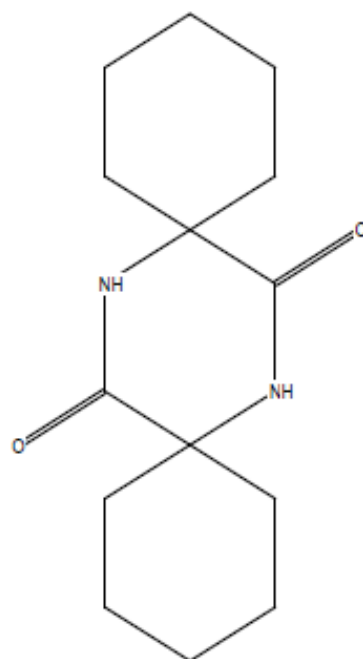
Formula: C₁₄H₂₂N₂O₂

Compound Name: 3,6-bis(Cycloleptamethylene)-2,5-piperazinedione

Synonym: Cyclic peptide (2 residues): GLY⁺-GLY⁻

Space Group: P-1 **Cell:** a 5.928(1) b 6.264(1) c 9.820(1)
Space Group No.: 2 **(Å,°)** α 87.38 β 80.52 γ 66.27

R-Factor (%): 5.73 **Temperature(K):** 295 **Density(g/cm³):** 1.263



NUVYOS

Reference: S.Palacin, D.N.Chin, E.E.Simaneck, J.C.MacDonald, G.M.Whiteides, M.T.McBride, G.T.R.Palmore (1997) *J.Am.Chem.Soc.*, 119,11807

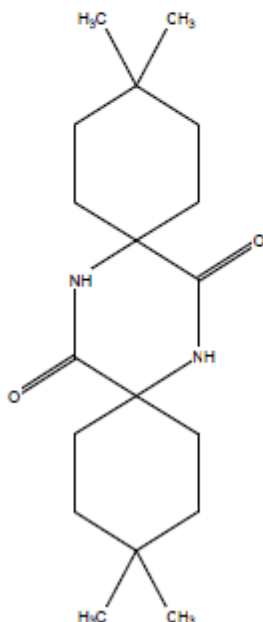
Formula: C₁₈H₃₀N₂O₂

Compound Name: 3,6-bis-Cyclo(4,4-dimethyl)pentamethylene-2,5-piperazinedione

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P-1 **Cell:** a 6.086(1) b 6.321(1) c 11.573(1)
Space Group No.: 2 **(Å³)** α 90.09 β 101.15 γ 109.83

R-Factor (%): 3.31 **Temperature(K):** 130 **Density(g/cm³):** 1.242



NUVYUY

Reference: S.Palacin, D.N.Chin, E.E.Simaneck, J.C.MacDonald, G.M.Whiteides, M.T.McBride, G.T.R.Palmore (1997) *J.Am.Chem.Soc.*, 119,11807

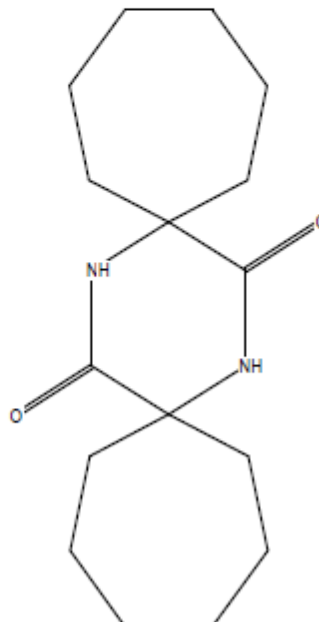
Formula: C₁₆H₂₆N₂O₂

Compound Name: 3,6-bis(Cyclohexamethylene)-2,5-piperazinedione

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P-1 **Cell:** a 5.962(1) b 6.127(2) c 11.156(2)
Space Group No.: 2 **(Å³)** α 85.98 β 82.68 γ 68.48

R-Factor (%): 4.57 **Temperature(K):** 223 **Density(g/cm³):** 1.230



NUVZAF

Reference: S.Palacin, D.N.Chin, E.E.Simaneck, J.C.MacDonald, G.M.Whiteides, M.T.McBride, G.T.R.Palmore (1997) *J.Am.Chem.Soc.*, 119,11807

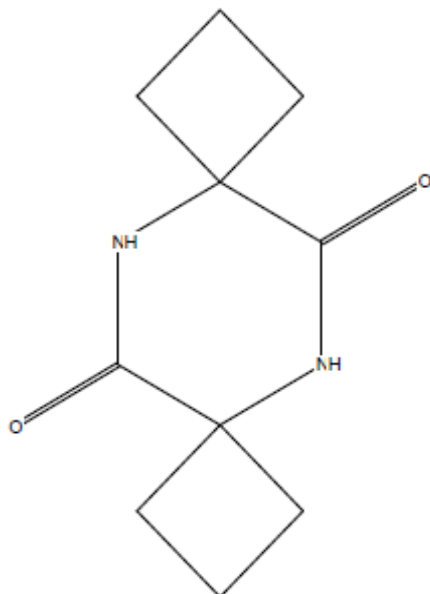
Formula: C₁₀H₁₄N₂O₂

Compound Name: 3,6-bis(Cyclo(trimethylene)-2,5-piperazinedione

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P21/c **Cell:** a 6.076(1) b 17.232(2) c 8.971(1)
Space Group No.: 14 **(Å³)** α 90.00 β 95.66 γ 90.00

R-Factor (%): 4.54 **Temperature(K):** 295 **Density(g/cm³):** 1.380



NUVZEJ

Reference: S.Palacin, D.N.Chin, E.E.Simaneck, J.C.MacDonald, G.M.Whiteides, M.T.McBride, G.T.R.Palmore (1997) *J.Am.Chem.Soc.*, 119,11807

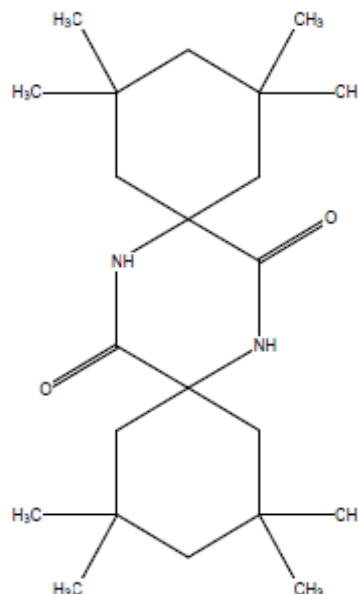
Formula: C₂₂H₃₈N₂O₂

Compound Name: 3,6-bis(Cyclo(3,3,5,5-tetramethyl)pentamethylene)-2,5-piperazinedione

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P-1 **Cell:** a 6.098(3) b 7.884(3) c 23.070(12)
Space Group No.: 2 **(Å³)** α 94.48(4) β 94.73(4) γ 107.09(3)

R-Factor (%): 5.92 **Temperature(K):** 130 **Density(g/cm³):** 1.146



NUVZIN

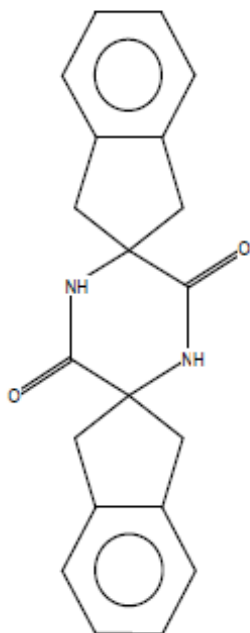
Reference: S.Palacin, D.N.Chin, E.E.Simonek, J.C.MacDonald, G.M.Whitelesides, M.T.McBride, G.T.R.Palmore (1997) *J.Am. Chem. Soc.*, **119**, 11807

Formula: C₂₀H₁₈N₂O₂

Compound Name: Dispiro[indan-2,3'-piperazine-6',2''-indan]-2,8-dione

Synonym: Cyclic peptide (2 residues): GLY'-GLY'-

Space Group: C2/c
Space Group No.: 15
Cell: a 9.772(2) b 14.046(3) c 11.822(3)
(Å³)
α 90.00 β 95.93 γ 90.00
R-Factor (%): 3.79
Temperature(K): 295
Density(g/cm³): 1.310



NUVZIN01

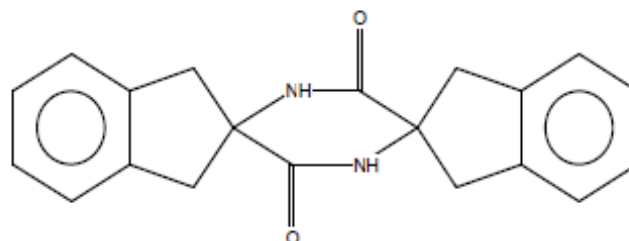
Reference: L.J.Williams, B.Jagadish, S.R.Lyon, R.A.Kloster, M.D.Carducci, E.A.Mash (1999) *Tetrahedron*, **55**, 14281

Formula: C₂₀H₁₈N₂O₂

Compound Name: Cyclo[bis(2-aminoindan-2-carboxylic acid)]

Synonym: Cyclic peptide (2 residues): GLY'-GLY'-

Space Group: C2/c
Space Group No.: 15
Cell: a 9.757(2) b 14.014(3) c 11.840(1)
(Å³)
α 90.00 β 95.96(1) γ 90.00
R-Factor (%): 4.20
Temperature(K): 295
Density(g/cm³): 1.313



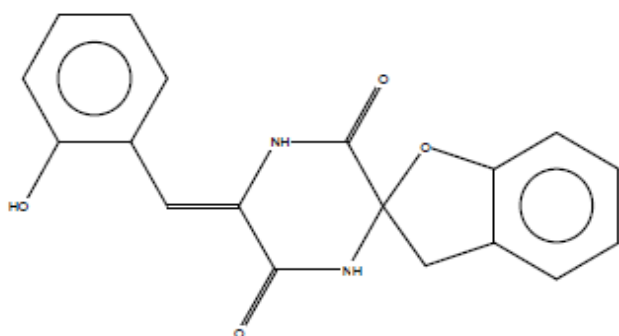
OBIPOH

Reference: Ling-Hong Meng, Chen-Yin Wang, A.Mandi, Xiao-Ming Li, Xue-Yi Hu, M.U.Kassack, T.Kurtan, Bin-Gui Wang (2016) *Org.Lett.*, **18**, 5304

Formula: C₁₈H₁₄N₂O₄

Compound Name: 5'-(2-hydroxybenzylidene)-3H,3H,6'H-spiro[1-benzofuran-2,2'-piperazine]-3',6'-dione

Space Group: Cc
Space Group No.: 9
Cell: a 5.554(0) b 22.348(1) c 25.462(3)
(Å³)
α 90.00 β 94.48(0) γ 90.00
R-Factor (%): 7.37
Temperature(K): 293
Density(g/cm³): 1.359



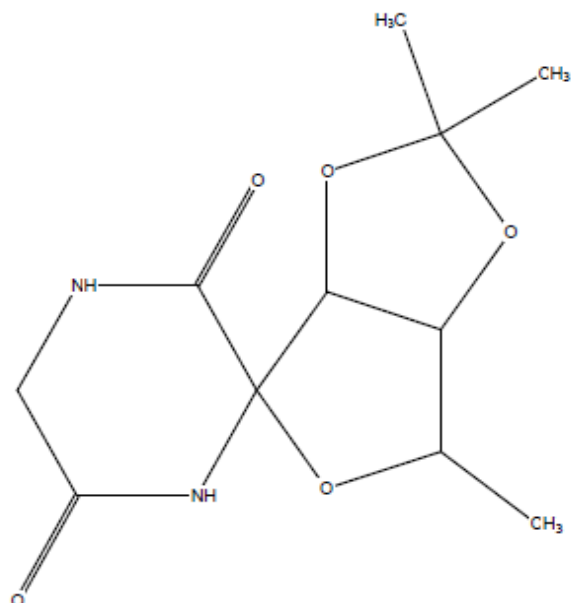
OCAGEF

Reference: D.J.Walton, M.Muier, Y.Bierot, M.I.Simone, G.W.J.Fleet (2004) *Acta Crystallogr., Sect.E: Struct. Rep. Online*, **60**, o1820

Formula: C₁₁H₁₆N₂O₅

Compound Name: (2S,3R,4R,5S)-3,4-O-isopropylidene-2-methyl-6,9-diaza-1-oxaspiro(4.5)decane-7,10-dione

Space Group: P21
Space Group No.: 4
Cell: a 11.100(2) b 7.994(2) c 13.895(2)
(Å³)
α 90.00 β 93.00(2) γ 90.00
R-Factor (%): 7.33
Temperature(K): 293
Density(g/cm³): 1.382



OHEXOO

Reference: M.Belohradsky, I.Cisarova, P.Holy, J.Pastor, J.Zavada (2002) *Tetrahedron*, **58**,8811

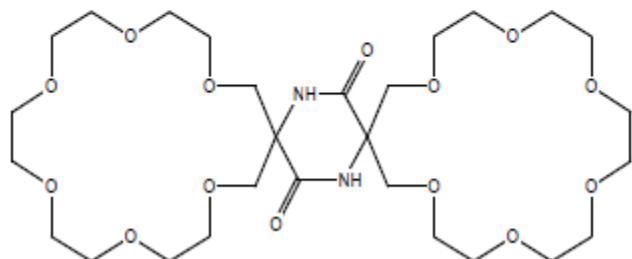
Formula: $C_{28}H_{50}N_2O_{14} \cdot 2(H_2O)$

Compound Name: 2,5,8,11,14,17,24,27,30,33,36,39-Dodecaoxa-20,41-diazadispiro(18.2.18.2)dodecacontane-21,42-dione dihydrate

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P-1 **Cell:** a 8.095(0) b 10.764(0) c 11.278(0)
Space Group No.: 2 **(Å³)** α 115.70(0) β 105.86(0) γ 91.41(0)

R-Factor (%): 3.13 **Temperature(K)**: 150 **Density(g/cm³)**: 1.334



H₂O

OHEYOP

Reference: M.Belohradsky, I.Cisarova, P.Holy, J.Pastor, J.Zavada (2002) *Tetrahedron*, **58**,8811

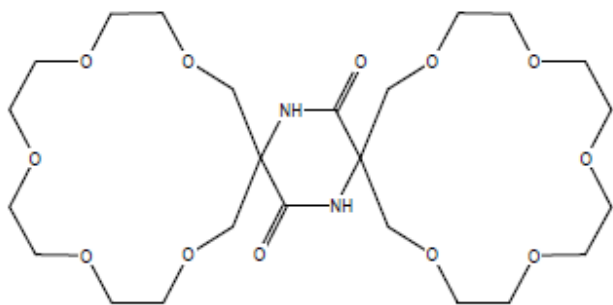
Formula: $C_{24}H_{42}N_2O_{12}$

Compound Name: 2,5,8,11,14,21,24,27,30,33-Decaoxa-17,35-diazadispiro(15.2.15.2)hexatriacontane-18,36-dione

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P2₁/c **Cell:** a 7.930(0) b 21.678(0) c 8.229(0)
Space Group No.: 14 **(Å³)** α 90.00 β 104.55(0) γ 90.00

R-Factor (%): 3.62 **Temperature(K)**: 150 **Density(g/cm³)**: 1.335



OHEYIJ

Reference: M.Belohradsky, I.Cisarova, P.Holy, J.Pastor, J.Zavada (2002) *Tetrahedron*, **58**,8811

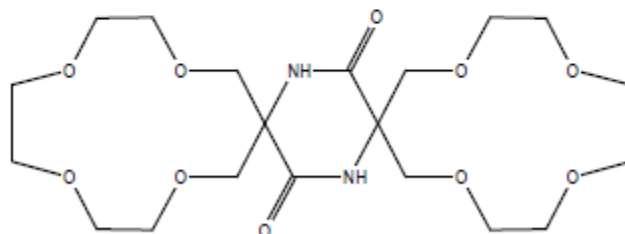
Formula: $C_{20}H_{34}N_2O_{10}$

Compound Name: 2,5,8,11,18,21,24,27-Octaoxa-14,29-diazadispiro(12.2.12.2)triacontane-15,30-dione

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: P-1 **Cell:** a 8.199(0) b 8.600(0) c 8.656(0)
Space Group No.: 2 **(Å³)** α 70.92(0) β 75.53(0) γ 86.12(0)

R-Factor (%): 3.44 **Temperature(K)**: 150 **Density(g/cm³)**: 1.375



OHEYUV

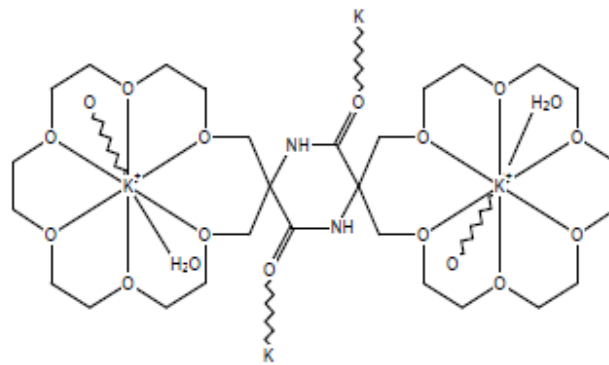
Reference: M.Belohradsky, I.Cisarova, P.Holy, J.Pastor, J.Zavada (2002) *Tetrahedron*, **58**,8811

Formula: $(C_{28}H_{54}K_2N_2O_{16} \cdot 2^n \cdot n(C_1N_1S_1 \cdot)^{-1}) \cdot n(C_1H_4O_1)$

Compound Name: catena-((μ₄-2,5,8,11,14,17,24,27,30,33,36,39-Dodecaoxa-20,41-diazadispiro(18.2.18.2)dodecacontane-21,42-dione)-diaqua-di-potassium dithiocyanate methanol solvate)

Space Group: P2₁/c **Cell:** a 8.243(0) b 19.073(0) c 14.601(0)
Space Group No.: 14 **(Å³)** α 90.00 β 97.28(0) γ 90.00

R-Factor (%): 4.06 **Temperature(K)**: 150 **Density(g/cm³)**: 1.314



H₃C—OH

N=C=S

OHIVUW

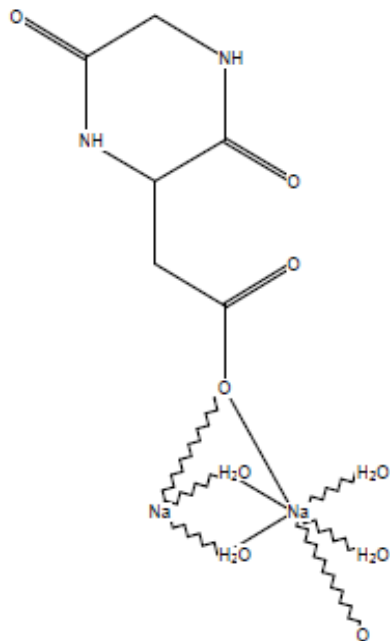
Reference: P.Mayer, J.Schapp, W.Beck (2003)
Z.Kristallogr.-New Cryst.Struct. ,218,113

Formula: (C₉ H₁₁ N₂ Na₁ O₆)_n

Compound Name: catena-(bis(μ₂-Aqua)-μ₂-(3,6-dioxopiperazine-2-yl)acetato-O,O)-sodium)

Space Group: P21/c **Cell:** a 13.955(0) b 10.737(0) c 6.216(0)
Space Group No.: 14 (Å,°) α 90.00 β 93.98(0) γ 90.00

R-Factor (%): 4.50 **Temperature(K):** 200 **Density(g/cm³):** 1.645



OPUFIP

Reference: B.S.Antia, T.Aree, C.Kasettrathat, S.Wiyakrutta,
O.D.Ekpa, U.J.Ekpe, C.Mahdol, S.Ruchirawat, P.Kittakoop (2011)
Phytochemistry ,72,816

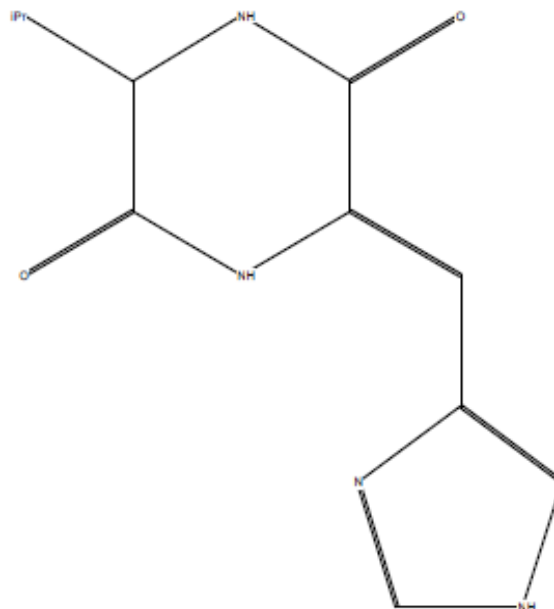
Formula: C₁₁ H₁₄ N₄ O₂

Compound Name: (Z)-3-[(1H-imidazol-4-yl)methylene]-6-isopropylpiperazine-2,5-dione

Synonym: pre-aurantamine

Space Group: P32 **Cell:** a 9.053(0) b 9.053(0) c 12.277(0)
Space Group No.: 145 (Å,°) α 90.00 β 90.00 γ 120.00

R-Factor (%): 5.80 **Temperature(K):** 298 **Density(g/cm³):** 1.339



OWADUM

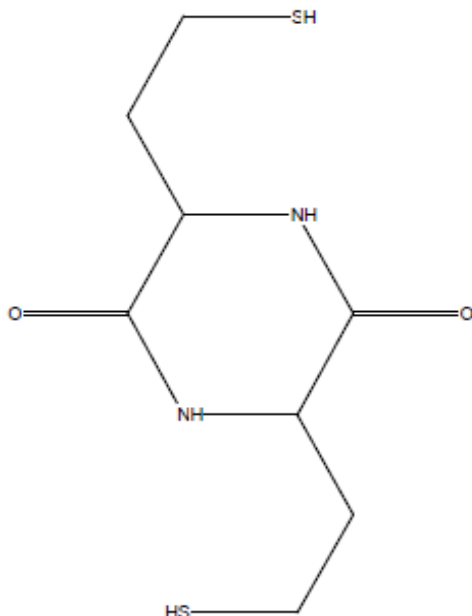
Reference: A.P.Mendham, J.Spencer, B.Z.Chowdhry, T.J.Dines,
M.Mujahid, R.A.Palmer, G.J.Tizzard, S.J.Coles (2011) *J.Chem.Cryst.* ,
41,1328

Formula: C₈ H₁₄ N₂ O₂ S₂

Compound Name: (3S,6S)-3,6-bis(2-sulfanylethyl)piperazine-2,5-dione

Space Group: P212121 **Cell:** a 6.151(0) b 18.022(0) c 29.617(1)
Space Group No.: 19 (Å,°) α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.46 **Temperature(K):** 120 **Density(g/cm³):** 1.422



PAXNIL

Reference: G.Tayhas, R.Palmore, M.T.McBride (1998)
Chem.Commun. ,145

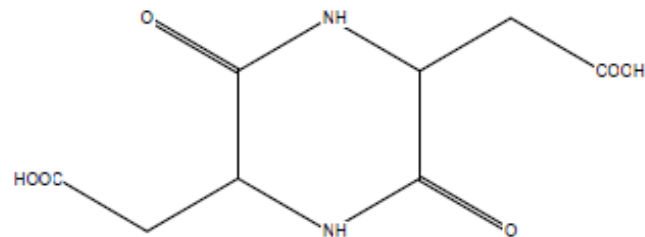
Formula: C₈ H₁₀ N₂ O₆

Compound Name: (S,S)-3,6-bis(Carboxymethyl)-2,5-diketopiperazine

Synonym: Cyclo-diaspartic acid; Cyclic peptide (2 residues): ASP-ASP-

Space Group: P1 **Cell:** a 4.985(1) b 5.039(1) c 18.853(4)
Space Group No.: 1 (Å,°) α 82.50(3) β 88.47(3) γ 75.33(3)

R-Factor (%): 3.44 **Temperature(K):** 130 **Density(g/cm³):** 1.683



PAXNIL01

Reference: G.T.R.Palmore, T.-J.M.Luo, M.T.McBride-Wieser, E.A.Picciotto, C.M.Reynoso-Paz (1999) *Chem.Mater.*, 11,3315

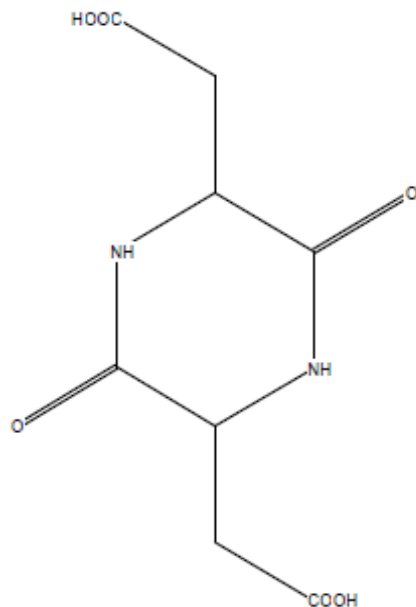
Formula: C₈H₁₀N₂O₆

Compound Name: (S,S)-3,6-bis(Carboxymethyl)-2,5-diketopiperazine

Synonym: Cyclic peptide (2 residues): ASP-ASP-

Space Group: P1 **Cell:** a 4.985(1) b 5.039(1) c 18.853(4)
Space Group No.: 1 **(Å,°)** α 82.50(3) β 88.47(3) γ 75.33(3)

R-Factor (%): 3.44 **Temperature(K):** 130 **Density(g/cm³):** 1.683



PAXNIL02

Reference: R.A.Palmer, B.S.Potter, A.P.Mendham, T.J.Dines, B.Z.Chowdhry (2010) *J.Chem.Cryst.*, 40,608

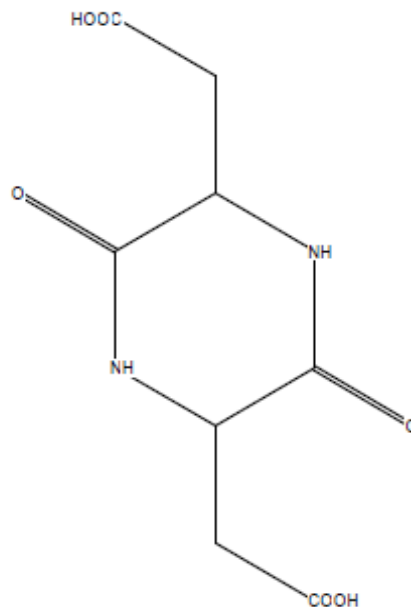
Formula: C₈H₁₀N₂O₆

Compound Name: 2,2'-(3,6-Dioxopiperazine-2,5-diyli)diacetic acid

Synonym: Cyclo-(L-Aspartyl-L-Aspartyl)

Space Group: P1 **Cell:** a 5.083(0) b 5.029(0) c 18.877(1)
Space Group No.: 1 **(Å,°)** α 88.95(2) β 83.72(2) γ 74.79(2)

R-Factor (%): 4.92 **Temperature(K):** 293 **Density(g/cm³):** 1.652



PAXNOR

Reference: G.Tayhas, R.Palmore, M.T.McBride (1998) *Chem.Commun.*, 145

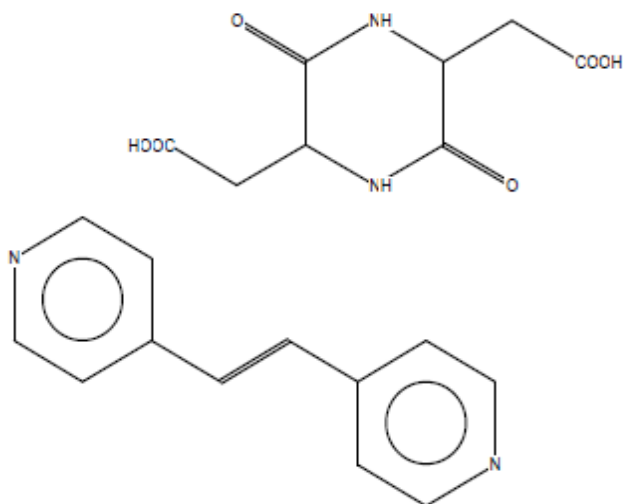
Formula: C₈H₁₀N₂O₆·C₁₂H₁₀N₂

Compound Name: (S,S)-3,6-bis(Carboxymethyl)-2,5-diketopiperazine trans-1,2-bis(4-pyridyl)ethene dihydrate

Synonym: Cyclo-diaspartic acid (E)-1,2-bis(4-pyridyl)ethene dihydrate;
Cyclic peptide (2 residues): ASP-ASP-

Space Group: P1 **Cell:** a 6.178(1) b 6.187(2) c 13.404(3)
Space Group No.: 1 **(Å,°)** α 82.63(2) β 83.92(2) γ 68.23(2)

R-Factor (%): 8.60 **Temperature(K):** 130 **Density(g/cm³):** 1.454



PAXNOR01

Reference: G.T.R.Palmore, T.-J.M.Luo, M.T.McBride-Wieser, E.A.Picciotto, C.M.Reynoso-Paz (1999) *Chem.Mater.*, 11,3315

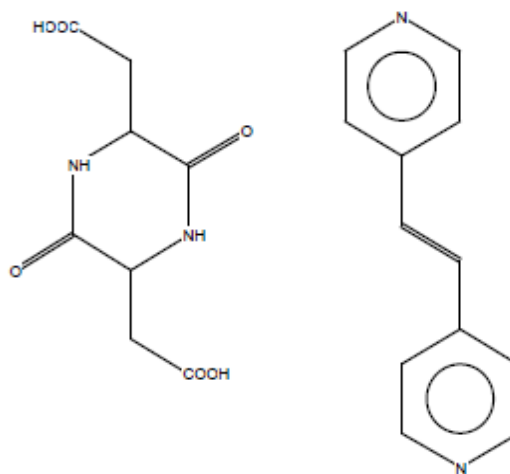
Formula: C₈H₁₀N₂O₆·C₁₂H₁₀N₂

Compound Name: (S,S)-3,6-bis(Carboxymethyl)-2,5-diketopiperazine trans-1,2-bis(4-pyridyl)ethene dihydrate

Synonym: Cyclic peptide (2 residues): ASP-ASP-

Space Group: P1 **Cell:** a 6.178(1) b 6.187(2) c 13.404(3)
Space Group No.: 1 **(Å,°)** α 82.63(2) β 83.92(2) γ 68.23(2)

R-Factor (%): 8.60 **Temperature(K):** 130 **Density(g/cm³):** 1.454



QANMEY

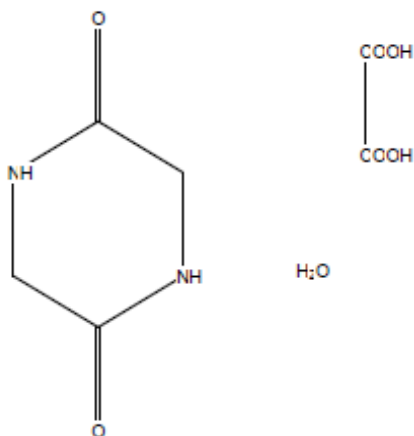
Reference: T.R.Sarangarajan, K.Panchanatheswaran, J.N.Low, C.Gildewell (2005) *Acta Crystallogr., Sect.C: Cryst. Struct. Commun.* , 61, 0118

Formula: $C_4H_6N_2O_2 \cdot C_2H_2O_4 \cdot 2(H_2O)$

Compound Name: 2,5-Piperazinedione oxalic acid dihydrate

Space Group: P-1
Space Group No.: 2
Cell: a 6.149(0) b 6.198(0) c 7.364(0)
 α 83.49(0) β 82.58(0) γ 65.07(0)

R-Factor (%): 4.24 **Temperature(K):** 120 **Density(g/cm³):** 1.583



QAPCIW

Reference: Chang-An Geng, Xiao-Yan Huang, Yun-Bao Ma, Bo Hou, Tian-Ze Li, Xue-Mei Zhang, Ji-Jun Chen (2017) *J.Nat.Prod.* , 80,959

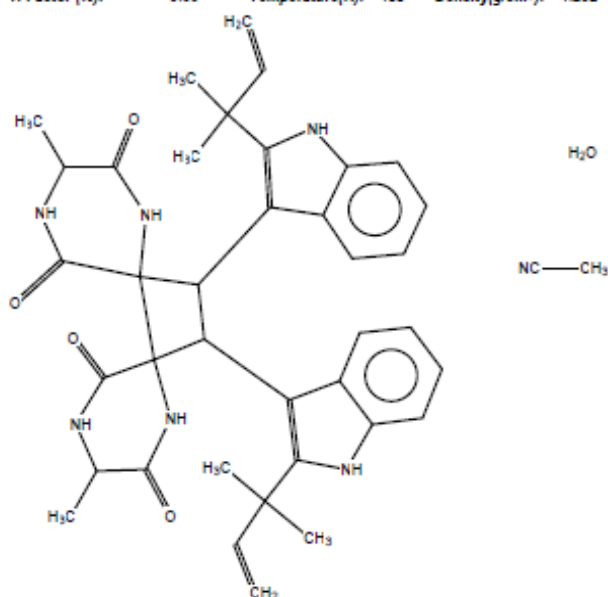
Formula: $C_{38}H_{42}N_6O_4 \cdot 0.5(C_2H_3N_1) \cdot 0.5(H_2O)$

Compound Name: 3,10-dimethyl-13,14-bis(2-(2-methylbut-3-en-2-yl)-1H-indol-3-yl)-1,4,8,11-tetraazadispiro[5.0.57.2⁶]tetradecane-2,5,9,12-tetrone acetonitrile solvate hemihydrate

Synonym: uncarlin A acetonitrile solvate hemihydrate

Space Group: P-1
Space Group No.: 2
Cell: a 10.727(0) b 15.336(0) c 22.605(0)
 α 77.61(0) β 80.47(0) γ 76.42(0)

R-Factor (%): 8.35 **Temperature(K):** 100 **Density(g/cm³):** 1.282



QAPCOC

Reference: Chang-An Geng, Xiao-Yan Huang, Yun-Bao Ma, Bo Hou, Tian-Ze Li, Xue-Mei Zhang, Ji-Jun Chen (2017) *J.Nat.Prod.* , 80,959

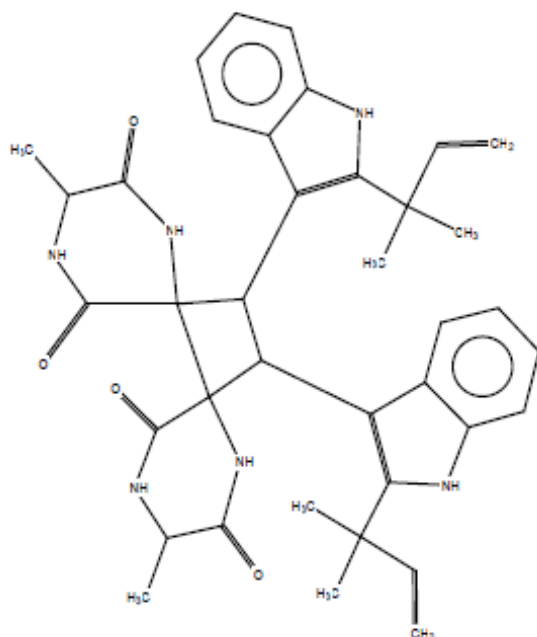
Formula: $C_{38}H_{42}N_6O_4$

Compound Name: 3,10-dimethyl-13,14-bis(2-(2-methylbut-3-en-2-yl)-1H-indol-3-yl)-1,4,8,11-tetraazadispiro[5.0.57.2⁶]tetradecane-2,5,9,12-tetrone

Synonym: uncarlin B

Space Group: C2/c
Space Group No.: 15
Cell: a 22.160(0) b 15.599(0) c 11.411(0)
 α 90.00 β 120.94(0) γ 90.00

R-Factor (%): 4.59 **Temperature(K):** 100 **Density(g/cm³):** 1.270



QQGLV

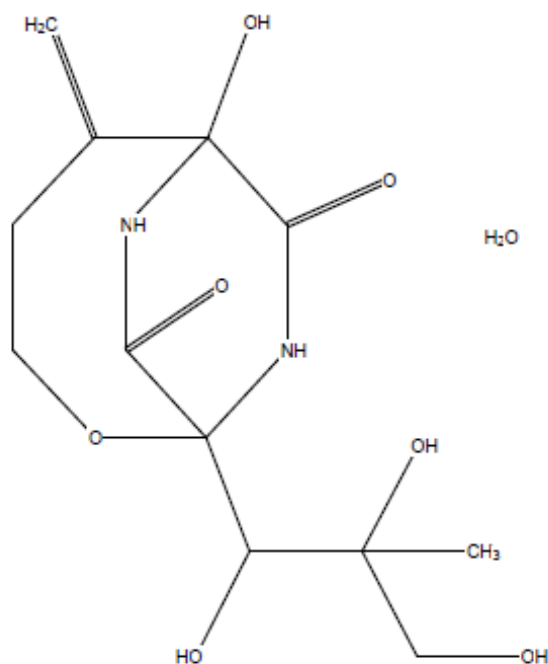
Reference: Y.Tokuma, S.Koda, T.Miyoshi, Y.Morimoto (1974) *Bull.Chem.Soc.Jpn.* , 47,18

Formula: $C_{12}H_{18}N_2O_7 \cdot H_2O$

Compound Name: Bicyclomycin monohydrate

Space Group: P21
Space Group No.: 4
Cell: a 10.270(10) b 10.910(10) c 6.670(10)
 α 90.00 β 101.40(10) γ 90.00

R-Factor (%): 0.00 **Temperature(K):** 295 **Density(g/cm³):** 1.452



RACKAH

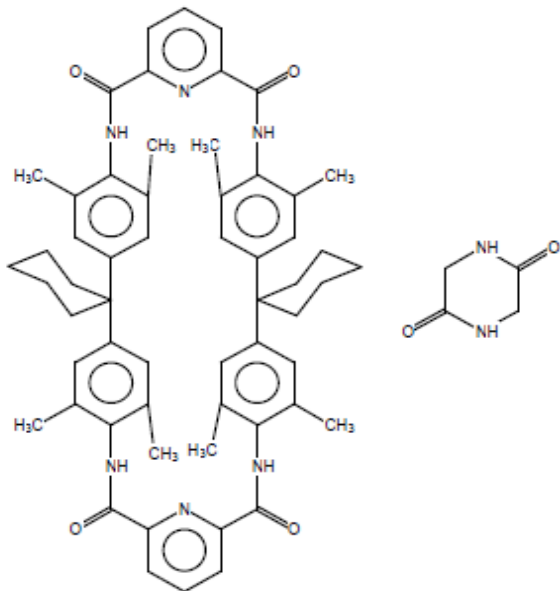
Reference: H.Adams, F.J.Carver, C.A.Hunter, N.J.Osborne (1996) Chem. Commun. ,2529

Formula: $C_{58}H_{62}N_6O_4 \cdot C_4H_6N_2O_2$

Compound Name: bis(Pyridine-2,6-diy)-N,N'-bis(cyclohexane-1,1-diy)bis(3,5-dimethyl-p-phenylene)carbamoyl(pyridine) piperazine-2,5-dione dihydrate

Space Group: R3r **Cell:** a 28.042(3) b 28.042(3) c 28.042(3)
Space Group No.: 146 **Cell:** (Å,°) α 118.64(2) β 118.64(2) γ 118.64(2)

R-Factor (%): 9.54 **Temperature(K)**: 295 **Density(g/cm³)**: 1.533



RACKAH01

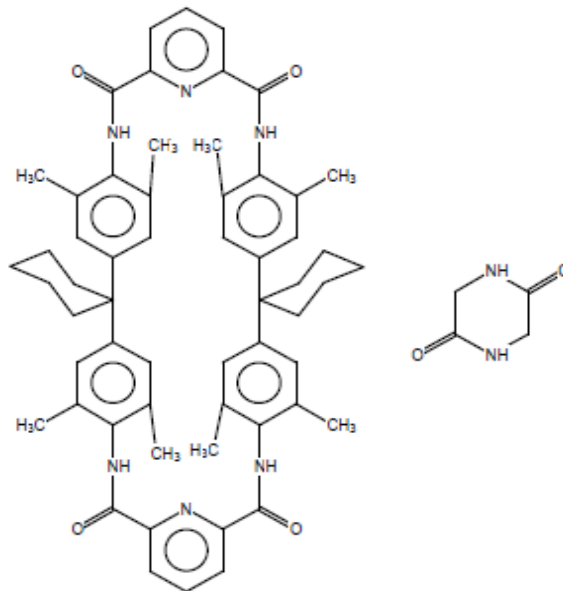
Reference: R.E.Marsh (2002) Acta Crystallogr.,Sect.B:Struct.Sci. ,58, 893

Formula: $C_{58}H_{62}N_6O_4 \cdot C_4H_6N_2O_2$

Compound Name: bis(Pyridine-2,6-diy)-N,N'-bis(cyclohexane-1,1-diy)bis(3,5-dimethyl-p-phenylene)carbamoyl(pyridine) piperazine-2,5-dione dihydrate

Space Group: R-3r **Cell:** a 28.042 b 28.042 c 28.042
Space Group No.: 148 **Cell:** (Å,°) α 118.64 β 118.64 γ 118.64

R-Factor (%): 0.00 **Temperature(K)**: 295 **Density(g/cm³)**: 0.767



RAPKAV

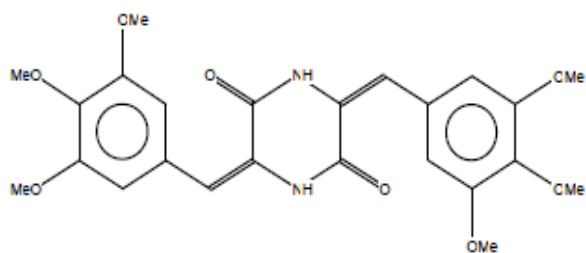
Reference: W.A.Loughlin, R.L.Marshall, K.E.Fairfull-Smith, P.C.Healy (2005) Acta Crystallogr.,Sect.E:Struct.Rep.Online ,61,01443

Formula: $C_{24}H_{26}N_2O_8$

Compound Name: (Z,Z)-3,6-bis((3,4,5-Trimethoxyphenyl)methylene)piperazine-2,5-dione

Space Group: C2/c **Cell:** a 35.204(3) b 5.282(6) c 12.738(4)
Space Group No.: 15 **Cell:** (Å,°) α 90.00 β 97.50(1) γ 90.00

R-Factor (%): 5.17 **Temperature(K)**: 295 **Density(g/cm³)**: 1.331



RAWNEK

Reference: J.R.Cochrane, J.M.White, U.Wille, C.A.Hutton (2012) Org.Lett. ,14,2402

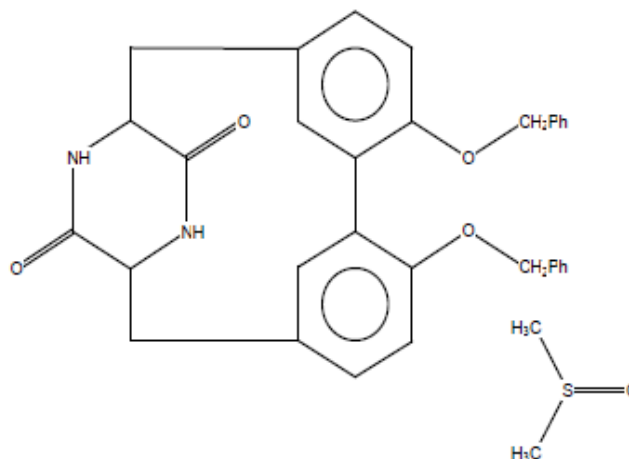
Formula: $C_{32}H_{28}N_2O_4 \cdot 2(C_2H_6O_1S_1)$

Compound Name: 6,9-bis(Benzyloxy)-15,17-diazatetracyclo[12.2.2.1^{3,7}.1^{8,12}]cosa-3(20),4,6,8(19),9,11-hexaene-16,18-dione dimethylsulfoxide solvate

Synonym: bis(O-Benzyl)mycocyclosin dimethylsulfoxide solvate

Space Group: P212121 **Cell:** a 9.444(0) b 9.642(0) c 36.127(3)
Space Group No.: 19 **Cell:** (Å,°) α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.43 **Temperature(K)**: 130 **Density(g/cm³)**: 1.334



REFTUR

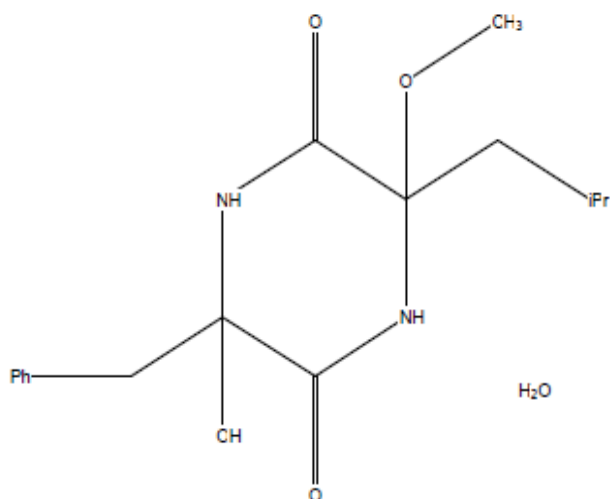
Reference: A.Amone, S.Capelli, G.Nasini, S.V.Melle, O.V.de Pava (1996) *Liebigs Ann.*, 1875

Formula: C₁₆H₂₂N₂O₄·H₂O₁

Compound Name: Dlatreol monohydrate

Synonym: 6-Benzyl-6-hydroxy-3-isobutyl-3-methoxy-piperazine-2,5-dione monohydrate

Space Group:	P21	Cell:	a 6.103(0)	b 16.460(1)	c 9.256(1)
Space Group No.:	4	(Å³)	α 90.00	β 108.06(1)	γ 90.00
R-Factor (%):	6.89	Temperature(K):	295	Density(g/cm³):	1.219



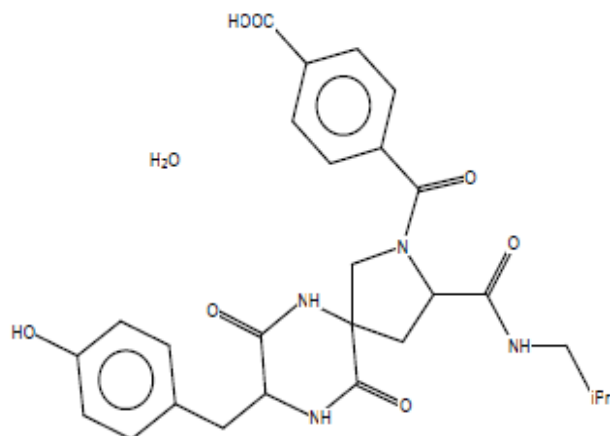
ROBCUI

Reference: M.F.L.Parker, S.Osuna, G.Bollot, S.Vaddypally, M.J.Zdilla, K.N.Houk, C.E.Schatmeister (2014) *J.Am.Chem.Soc.*, 136,3817

Formula: C₂₇H₃₀N₄O₇·2(H₂O₄)

Compound Name: 4-((8-(4-Hydroxybenzyl)-3-(isobutylcarbamoyl)-7,10-dioxo-2,6,9-triazaspiro[4.5]deco-2-yl)carbonyl)benzoic acid dihydrate

Space Group:	P212121	Cell:	a 6.166(0)	b 15.042(0)	c 29.201(1)
Space Group No.:	19	(Å³)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	3.64	Temperature(K):	100	Density(g/cm³):	1.370



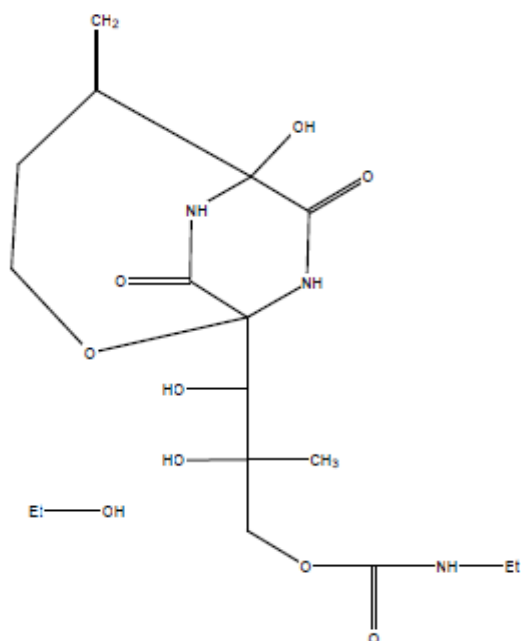
SADCOP

Reference: H.Kohn, S.Abuzar, J.D.Korp, A.S.Zekizer, G.E.Martin (1988) *J.Heterocycl.Chem.*, 25,1511

Formula: C₁₅H₂₃N₃O₉·C₂H₆O₁

Compound Name: Bicyclomycin-3'-ethyl carbamate ethanol solvate

Space Group:	P212121	Cell:	a 7.931(2)	b 10.834(4)	c 24.468(7)
Space Group No.:	19	(Å³)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	4.90	Temperature(K):	295	Density(g/cm³):	1.325



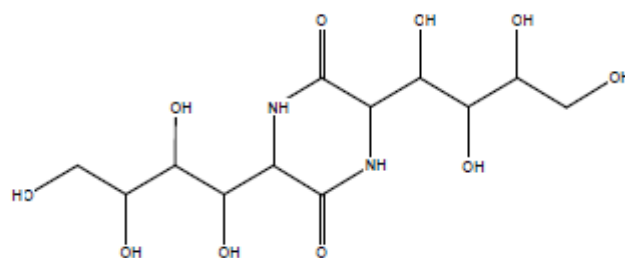
SEGZAF

Reference: A.Perczel, M.Holloi, J.Csaszar, V.Fulop, A.Kalman, G.D.Fasman (1989) *Carbohydr.Res.*, 187, 187

Formula: C₁₂H₂₂N₂O₁₀

Compound Name: (3R,6R)-bis((1R,2S,3R)-1,2,3,4-Tetrahydroxybutyl)-2,5-dioxopiperazine

Space Group:	C2221	Cell:	a 6.542(1)	b 7.308(1)	c 30.571(3)
Space Group No.:	20	(Å³)	α 90.00	β 90.00	γ 90.00
R-Factor (%):	4.10	Temperature(K):	295	Density(g/cm³):	1.610



SEQKII

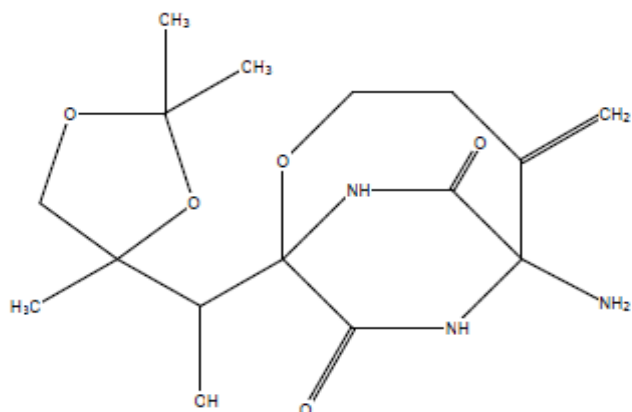
Reference: A.Santilian Junior, Xiangdong Zhang, J.Hardesty, W.R.Widger, H.Kohn (1998) *J.Med.Chem.* ,**41**,1185

Formula: C₁₅ H₂₃ N₃ O₆

Compound Name: C(6)-Aminobicyclomycolin C(2'),C(3')-acetoneid

Space Group: P212121 **Cell:** a 7.155(1) b 9.104(3) c 25.169(7)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.80 **Temperature(K):** 223 **Density(g/cm³):** 1.383



SERTYR10

Reference: C.-F.Lin, L.E.Webb (1973) *J.Am.Chem.Soc.* ,**95**,6803

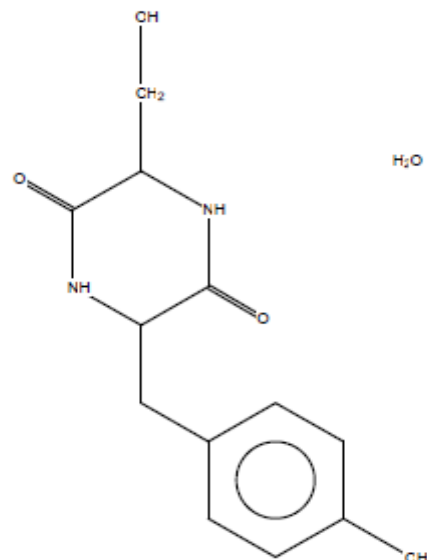
Formula: C₁₂ H₁₄ N₂ O₄·H₂O

Compound Name: Cyclo(L-seryl-L-tyrosyl) monohydrate

Synonym: Cyclic peptide (2 residues): SER-TYR-

Space Group: P21 **Cell:** a 11.445(2) b 6.191(1) c 8.828(1)
Space Group No.: 4 **(Å,°)** α 90.00 β 99.10(1) γ 90.00

R-Factor (%): 5.30 **Temperature(K):** 295 **Density(g/cm³):** 1.442



SIHVAG

Reference: G.Valle, M.Crisma, C.Toniolo, E.M.Holt, M.Tamura, J.Bland, C.H.Stammer (1989) *Int.J.Pept.Protein Res.* ,**34**,56

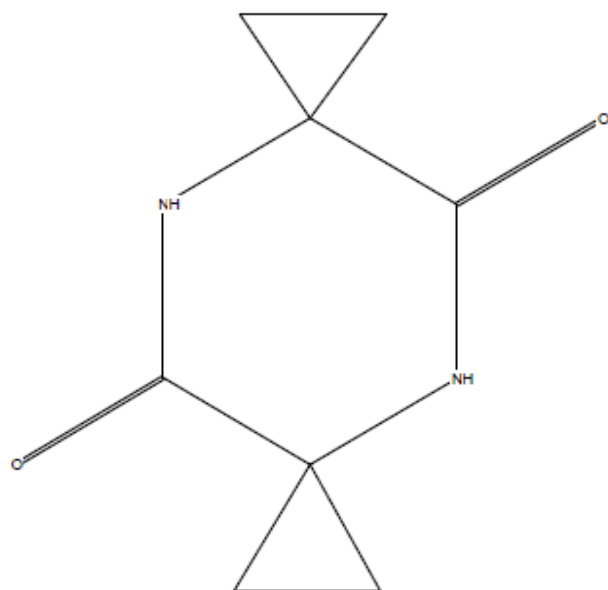
Formula: C₉ H₁₀ N₂ O₂

Compound Name: cyclo-bis(1-Aminocyclopropanecarboxylic acid)

Synonym: Cyclic peptide (2 residues): GLY⁻-GLY⁻

Space Group: C2/c **Cell:** a 9.051(2) b 7.956(1) c 11.370(2)
Space Group No.: 15 **(Å,°)** α 90.00 β 97.70(20) γ 90.00

R-Factor (%): 3.80 **Temperature(K):** 295 **Density(g/cm³):** 1.360



SIJZOC

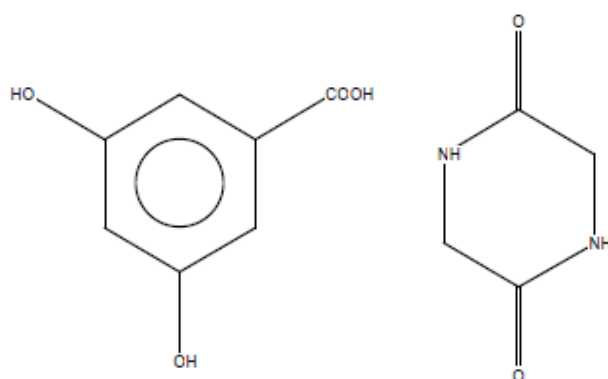
Reference: Lei Wang, Lei Zhao, WeiMing Liu, RuiXin Chen, YuanXiang Gu, Yu Yang (2012) *Sci.China.Chem.* ,**55**,2381

Formula: C₇ H₅ O₄·0.5(C₄ H₈ N₂ O₂)

Compound Name: 3,5-Dihydroxybenzoic acid piperazine-2,5-dione

Space Group: P-1 **Cell:** a 6.634(0) b 7.286(0) c 10.194(0)
Space Group No.: 2 **(Å,°)** α 84.87(0) β 79.55(0) γ 65.69(0)

R-Factor (%): 4.00 **Temperature(K):** 293 **Density(g/cm³):** 1.589



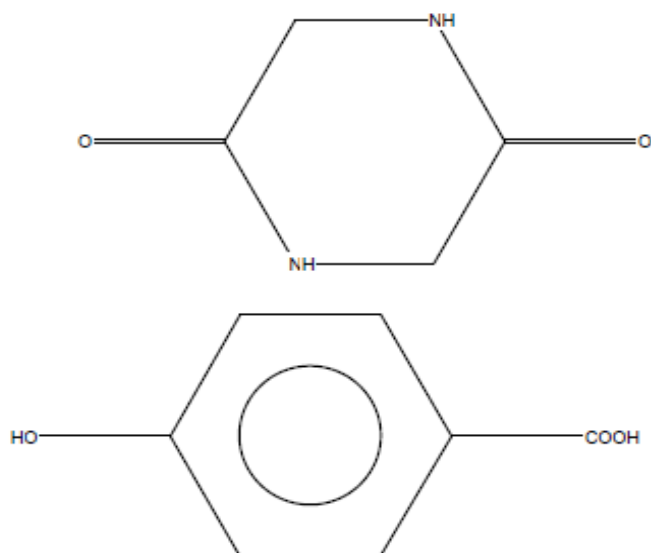
SIJZUI

Reference: Lei Wang, Lei Zhao, Weiming Liu, Ruixin Chen, Yuanxiang Gu, Yu Yang (2012) *Sci.China.Chem.* ,55,2381

Formula: C₇H₅O₃·0.5(C₄H₈N₂O₂)

Compound Name: 4-Hydroxybenzoic acid piperazine-2,5-dione

Space Group: P21/c **Cell:** a 7.490(0) b 6.234(0) c 18.837(2)
Space Group No.: 14 **(Å³):** α 90.00 β 96.02(0) γ 90.00
R-Factor (%): 4.78 **Temperature(K):** 293 **Density(g/cm³):** 1.482



SIKWEO

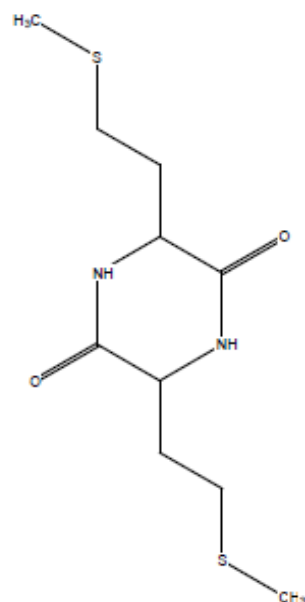
Reference: G.Valle, V.Guantieri, A.M.Tamburro (1990) *J.Mol.Struct.* , 220,19

Formula: C₁₀H₁₈N₂O₂S₂

Compound Name: cyclo(L-Methionyl-L-methionyl)

Synonym: Cyclic peptide (2 residues): MET-MET-

Space Group: P1 **Cell:** a 13.469(2) b 5.304(1) c 4.885(1)
Space Group No.: 1 **(Å³):** α 105.80(10) β 99.70(10) γ 79.40(10)
R-Factor (%): 9.06 **Temperature(K):** 295 **Density(g/cm³):** 1.331



SIKWEO01

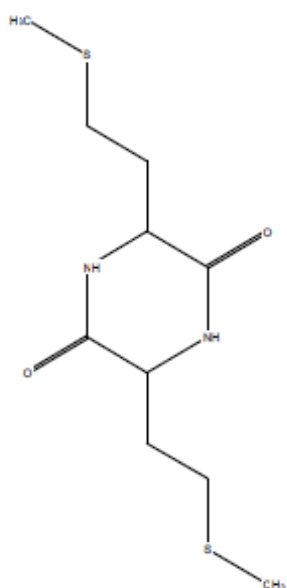
Reference: A.P.Mendham, B.S.Potter, R.A.Palmer, T.J.Dines, J.C.Mitchell, R.Withnall, B.Z.Chowdhry (2010) *J.Raman Spectrosc.* ,41, 148

Formula: C₁₀H₁₈N₂O₂S₂

Compound Name: Cyclo(L-methionyl-L-methionyl)

Synonym: Cyclic peptide (2 residues): MET-MET-

Space Group: P1 **Cell:** a 4.903(1) b 5.252(1) c 13.231(3)
Space Group No.: 1 **(Å³):** α 101.35(3) β 93.36(3) γ 105.76(3)
R-Factor (%): 4.46 **Temperature(K):** 100 **Density(g/cm³):** 1.365



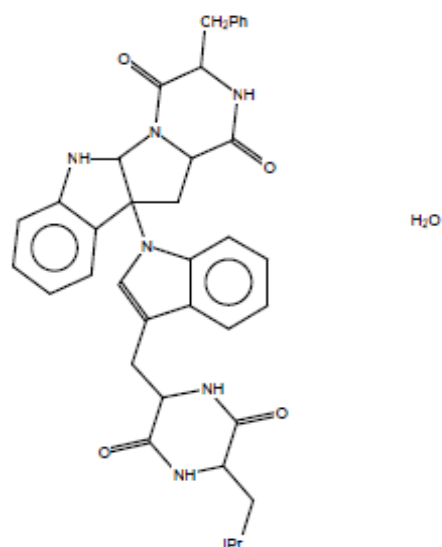
TADNOD

Reference: C.Perez-Balado, A.R.de Lera (2010) *Org.Biomol.Chem.* , 8, 5179

Formula: C₃₇H₃₈N₆O₄·3(H₂O)₄

Compound Name: 3-Benzyl-10b-(3-((5-isobutyl-3,6-dioxopiperazin-2-yl)methyl)-1H-indol-1-yl)-6,10b,11,11a-tetrahydro-2H-pyrazino[1',2':1,5]pyrrolo[2,3-b]indole-1,4(3H,5aH)-dione trihydrate

Space Group: P43 **Cell:** a 12.021(0) b 12.021(0) c 25.881(3)
Space Group No.: 78 **(Å³):** α 90.00 β 90.00 γ 90.00
R-Factor (%): 6.13 **Temperature(K):** 293 **Density(g/cm³):** 1.216



TAZZOM

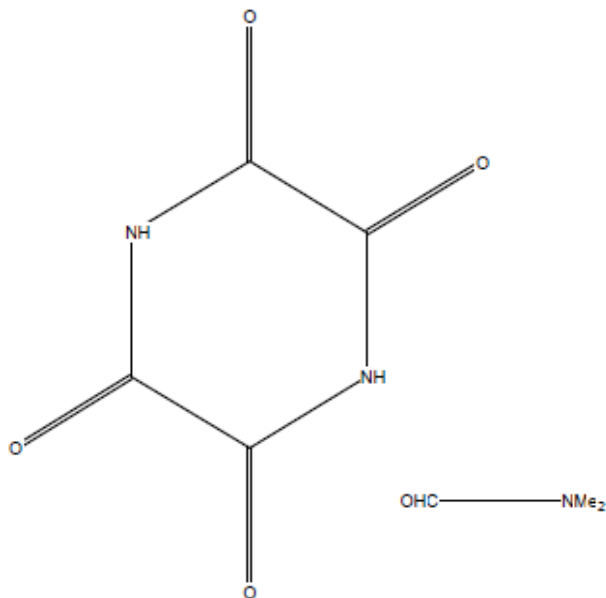
Reference: C.J.Kingsbury, B.F.Abrahams, R.Robson (2017)
CSD Communication(Private Communication),

Formula: C₄ H₂ N₂ O₄·2(C₃ H₇ N₁ O₁)

Compound Name: piperazine-2,3,5,6-tetrone N,N-dimethylformamide solvate

Space Group: P21/c **Cell:** a 5.152(0) b 14.668(0) c 9.856(0)
Space Group No.: 14 **(Å³)** α 90.00 β 104.62(0) γ 90.00

R-Factor (%): 7.12 **Temperature(K)**: 130 **Density(g/cm³)**: 1.328



TOTVAB

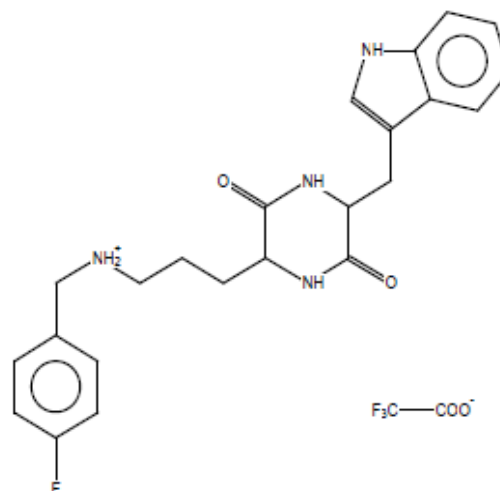
Reference: Halyang Sun, Jayli Wang, Gonghua Song (2014)
CSD Communication(Private Communication),

Formula: C₂₃ H₂₆ F₁ N₄ O₂ 1⁺·C₂ F₃ O₂ 1⁻

Compound Name: N-(4-fluorobenzyl)-3-[5-(1H-indol-3-yl)methyl]-3,6-dioxopiperazin-2-yl) propan-1-aminium trifluoroacetate

Space Group: P21 **Cell:** a 6.116(1) b 12.416(2) c 16.534(3)
Space Group No.: 4 **(Å³)** α 90.00 β 92.45(0) γ 90.00

R-Factor (%): 6.04 **Temperature(K)**: 293 **Density(g/cm³)**: 1.383



TOTVAB01

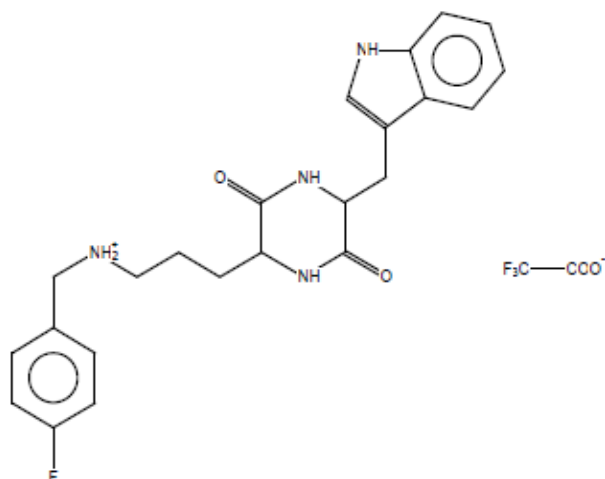
Reference: Halyang Sun, Hui Li, Jayli Wang, Gonghua Song (2018)
Chin.Chem.Lett., 29,977

Formula: C₂₃ H₂₆ F₁ N₄ O₂ 1⁺·C₂ F₃ O₂ 1⁻

Compound Name: N-(4-fluorobenzyl)-3-[5-(1H-indol-3-yl)methyl]-3,6-dioxopiperazin-2-yl) propan-1-aminium trifluoroacetate

Space Group: P21 **Cell:** a 6.116(1) b 12.416(2) c 16.534(3)
Space Group No.: 4 **(Å³)** α 90.00 β 92.45(0) γ 90.00

R-Factor (%): 6.04 **Temperature(K)**: 293 **Density(g/cm³)**: 1.383



TRDMPP01

Reference: E.Sletten (1970) J.Am.Chem.Soc., 92,172

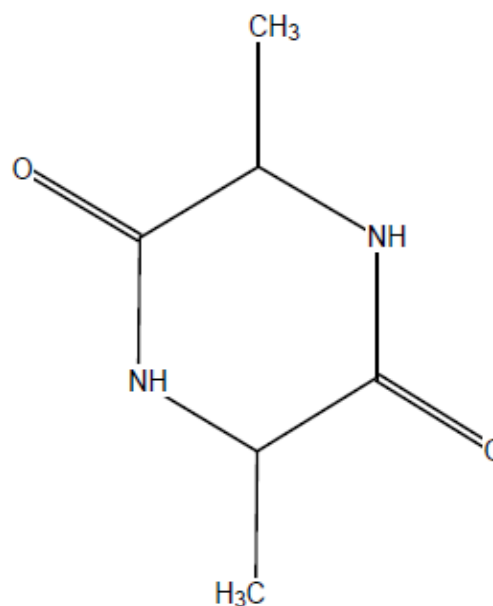
Formula: C₆ H₁₀ N₂ O₂

Compound Name: trans-3,6-Dimethylpiperazine-2,5-dione

Synonym: Cyclo-D-alanyl-L-alanyl; Cyclic peptide (2 residues); ALA-ALA-

Space Group: P21/n **Cell:** a 6.350(0) b 6.220(0) c 9.044(0)
Space Group No.: 14 **(Å³)** α 90.00 β 95.81(1) γ 90.00

R-Factor (%): 3.70 **Temperature(K)**: 295 **Density(g/cm³)**: 1.329



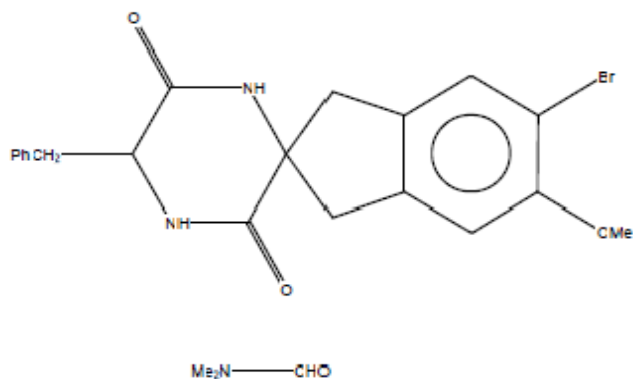
TUWDIZ

Reference: G.S.Nichol, F.N.Murigi, E.A.Mash (2010) *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **66**, 0302

Formula: C₂₀H₁₉Br₁N₂O₃C₃H₇N₁O₁

Compound Name: (2*R*,5*S*)-5'-benzyl-5-bromo-6-methoxyspiro[indane-2,2'-piperazine]-3',6'-dione N,N-dimethylformamide solvate

Space Group: P212121 **Cell:** a 6.074(0) b 13.834(1) c 26.076(3)
Space Group No.: 19 **(Å³):** α 90.00 β 90.00 γ 90.00
R-Factor (%): 3.36 **Temperature(K):** 100 **Density(g/cm³):** 1.481



UCEWUU

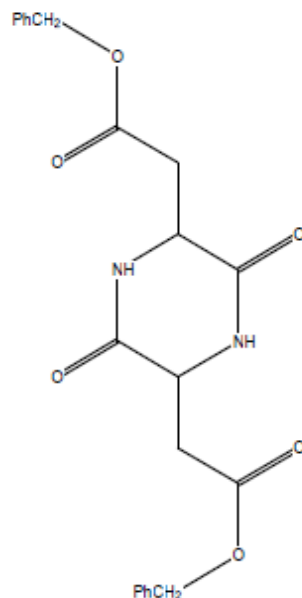
Reference: G.T.R.Palmore, T.-J.M.Luo, M.T.McBride-Wieser, E.A.Picciotto, C.M.Reynoso-Paz (1999) *Chem.Mater.*, **11**, 3315

Formula: C₂₂H₂₂N₂O₆

Compound Name: (S,S)-3,6-bis(Benzoyloxycarbonylmethyl)-2,5-diketopiperazine

Synonym: Cyclic peptide (2 residues): ASP⁻-ASP⁻

Space Group: C2 **Cell:** a 43.900(30) b 7.172(3) c 6.176(3)
Space Group No.: 5 **(Å³):** α 90.00 β 96.00(4) γ 90.00
R-Factor (%): 4.85 **Temperature(K):** 130 **Density(g/cm³):** 1.410



UCEXAB

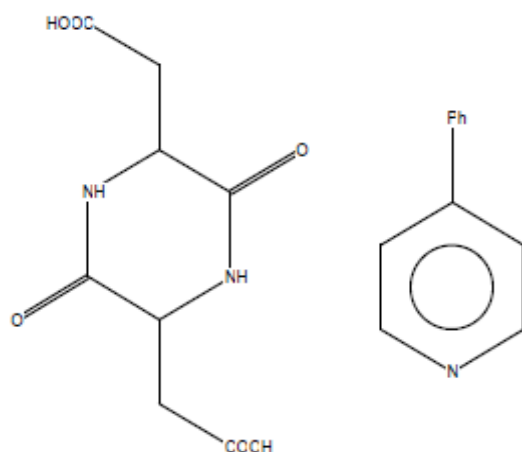
Reference: G.T.R.Palmore, T.-J.M.Luo, M.T.McBride-Wieser, E.A.Picciotto, C.M.Reynoso-Paz (1999) *Chem.Mater.*, **11**, 3315

Formula: C₉H₁₀N₂O₆·2(C₁₁H₉N₁)

Compound Name: (S,S)-3,6-bis(Carboxymethyl)-2,5-diketopiperazine bis(4-phenylpyridine) clathrate

Synonym: Cyclic peptide (2 residues): ASP-ASP-

Space Group: P1 **Cell:** a 6.256(1) b 14.645(4) c 15.660(3)
Space Group No.: 1 **(Å³):** α 111.14(2) β 94.60(2) γ 95.27(2)
R-Factor (%): 5.68 **Temperature(K):** 130 **Density(g/cm³):** 1.357



UCEXIJ

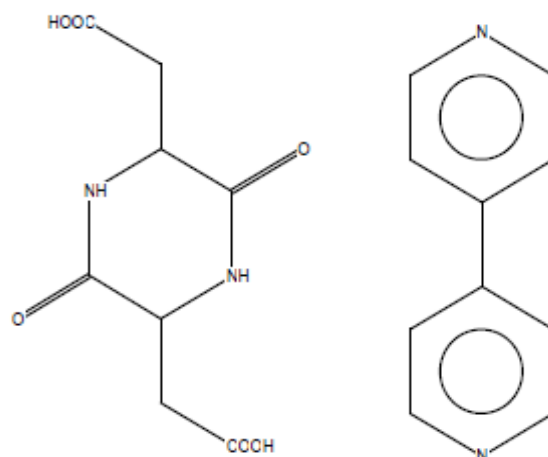
Reference: G.T.R.Palmore, T.-J.M.Luo, M.T.McBride-Wieser, E.A.Picciotto, C.M.Reynoso-Paz (1999) *Chem.Mater.*, **11**, 3315

Formula: C₉H₁₀N₂O₆·C₁₀H₈N₂

Compound Name: (S,S)-3,6-bis(Carboxymethyl)-2,5-diketopiperazine 4,4'-bipyridine clathrate

Synonym: Cyclic peptide (2 residues): ASP-ASP-

Space Group: P21 **Cell:** a 5.544(0) b 27.073(3) c 6.045(0)
Space Group No.: 4 **(Å³):** α 90.00 β 99.81(0) γ 90.00
R-Factor (%): 3.37 **Temperature(K):** 130 **Density(g/cm³):** 1.435



UCEXUV

Reference: G.T.R.Palmore, T.-J.M.Luo, M.T.McBride-Wieser, E.A.Picciotto, C.M.Reynoso-Paz (1999) *Chem.Mater.* ,11,3315

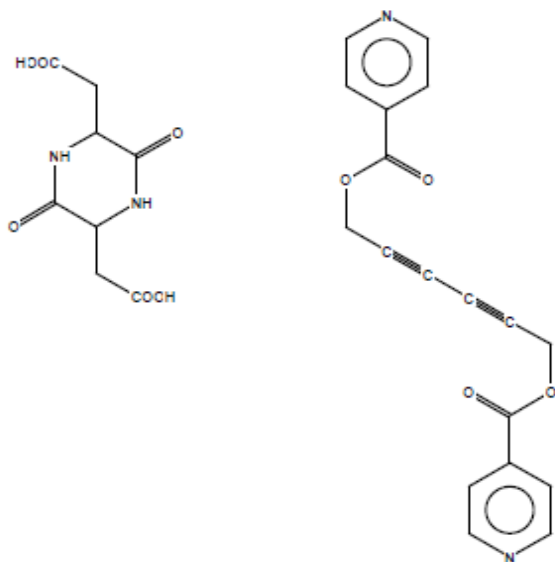
Formula: $C_8 H_{10} N_2 O_6 C_{18} H_{12} N_2 O_4$

Compound Name: (S,S)-3,6-Dicarboxymethyl-2,5-diketopiperazine hexa-2,4-diyne-1,6-dioldidnicotinate clathrate

Synonym: Cyclic peptide (2 residues): ASP-ASP-

Space Group: C2 **Cell:** a 28.616(5) b 14.284(2) c 6.043(1)
Space Group No.: 5 **(Å³)** α 90.00 β 90.76(1) γ 90.00

R-Factor (%): 5.05 **Temperature(K):** 130 **Density(g/cm³):** 1.480



UCEYAC

Reference: G.T.R.Palmore, T.-J.M.Luo, M.T.McBride-Wieser, E.A.Picciotto, C.M.Reynoso-Paz (1999) *Chem.Mater.* ,11,3315

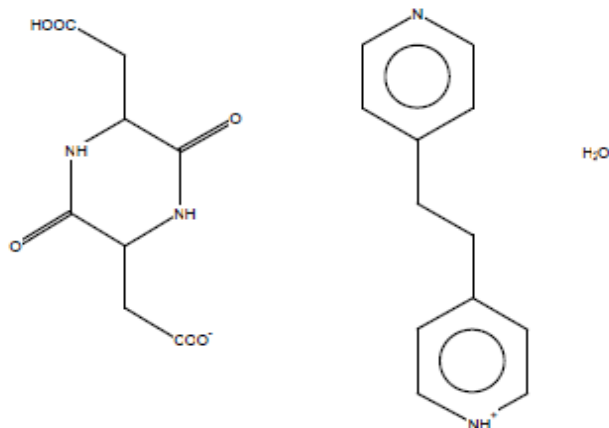
Formula: $C_8 H_5 N_2 O_6 \cdot C_{12} H_{13} N_2 \cdot H_2 O_1$

Compound Name: (S,S)-3,6-bis(Carboxymethyl)-2,5-diketopiperazine 1,2-bis(4-pyridyl) ethane clathrate monohydrate

Synonym: Cyclic peptide (2 residues): ASP-ASP-

Space Group: P212121 **Cell:** a 4.913(1) b 10.636(2) c 37.446(8)
Space Group No.: 19 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.82 **Temperature(K):** 130 **Density(g/cm³):** 1.468



UCEYEG

Reference: G.T.R.Palmore, T.-J.M.Luo, M.T.McBride-Wieser, E.A.Picciotto, C.M.Reynoso-Paz (1999) *Chem.Mater.* ,11,3315

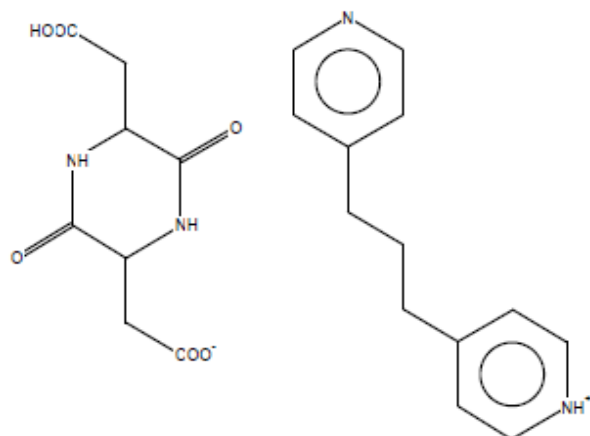
Formula: $C_8 H_5 N_2 O_6 \cdot C_{13} H_{15} N_2 \cdot H_2 O_1$

Compound Name: (S,S)-3,6-bis(Carboxymethyl)-2,5-diketopiperazine 1,3-bis(4-pyridyl) propane clathrate

Synonym: Cyclic peptide (2 residues): ASP-ASP-

Space Group: P21 **Cell:** a 4.852(1) b 19.800(4) c 10.554(2)
Space Group No.: 4 **(Å³)** α 90.00 β 94.95(3) γ 90.00

R-Factor (%): 13.50 **Temperature(K):** 130 **Density(g/cm³):** 1.409



ULEJIE

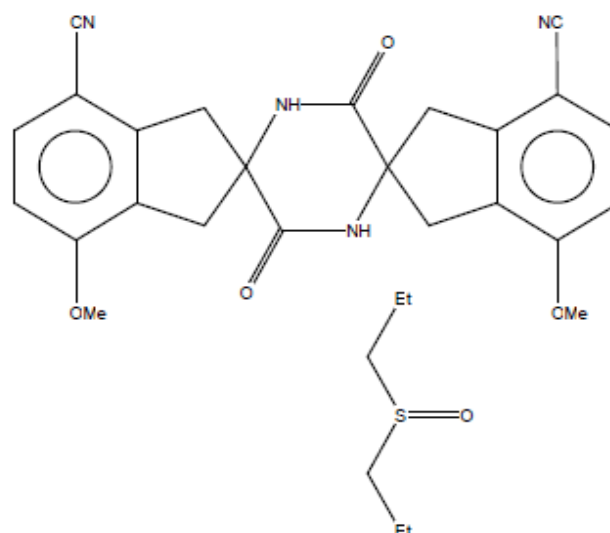
Reference: B.Jagadish, M.D.Carducci, C.Bosshard, P.Gunter, J.I.Margolis, L.J.Williams, E.A.Mash (2003) *Cryst.Growth Des.* ,3,811

Formula: $C_{24} H_{20} N_4 O_4 \cdot 2(C_6 H_{14} O_1 S_1)$

Compound Name: (S,S)-Cyclo-bis(2-amino-7-cyano-4-methoxyindan-2-carboxylic acid) bis(di-n-propylsulfoxide)

Space Group: P1 **Cell:** a 10.059(0) b 13.158(0) c 15.774(1)
Space Group No.: 1 **(Å³)** α 70.13(0) β 76.42(0) γ 78.16(0)

R-Factor (%): 6.83 **Temperature(K):** 170 **Density(g/cm³):** 1.224



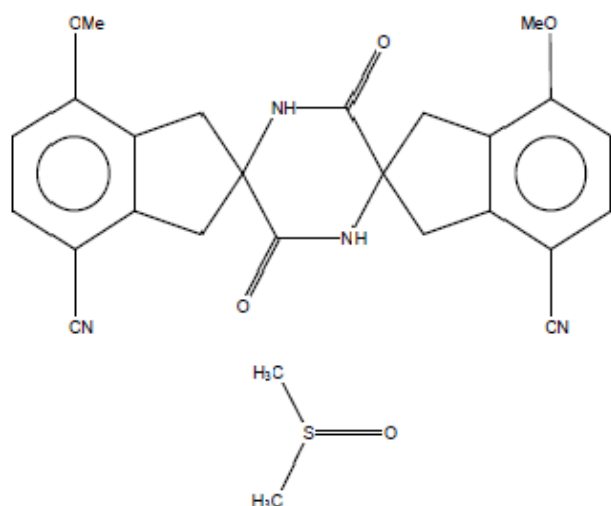
ULEJOK

Reference: B.Jagadish, M.D.Carducci, C.Bosshard, P.Gunter, J.J.Margolis, L.J.Williams, E.A.Mash (2003) *Cryst. Growth Des.*, 3,811

Formula: $C_{24}H_{20}N_4O_4 \cdot 3(C_2H_6O_1S_1)$

Compound Name: (R,R)-Cyclo-bis(2-amino-7-cyano-4-methoxyindan-2-carboxylic acid) tris(dimethylsulfoxide)

Space Group: C2 Cell: a 16.526(2) b 10.384(1) c 12.326(1)
Space Group No.: 5 (Å³) α 90.00 β 130.40(0) γ 90.00
R-Factor (%): 3.60 Temperature(K): 200 Density(g/cm³): 1.367



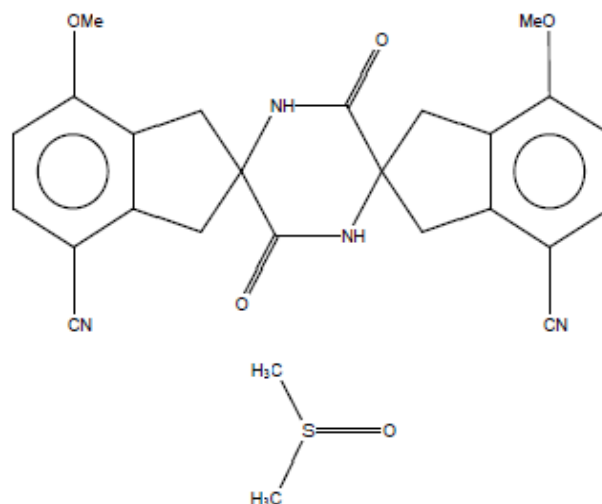
ULEJUQ

Reference: B.Jagadish, M.D.Carducci, C.Bosshard, P.Gunter, J.J.Margolis, L.J.Williams, E.A.Mash (2003) *Cryst. Growth Des.*, 3,811

Formula: $C_{24}H_{20}N_4O_4 \cdot 3(C_2H_6O_1S_1)$

Compound Name: rac-Cyclo-bis(2-amino-7-cyano-4-methoxyindan-2-carboxylic acid) tris(dimethylsulfoxide)

Space Group: P21/n Cell: a 19.919(3) b 11.992(1) c 28.951(5)
Space Group No.: 14 (Å³) α 90.00 β 108.56(0) γ 90.00
R-Factor (%): 6.75 Temperature(K): 170 Density(g/cm³): 1.343



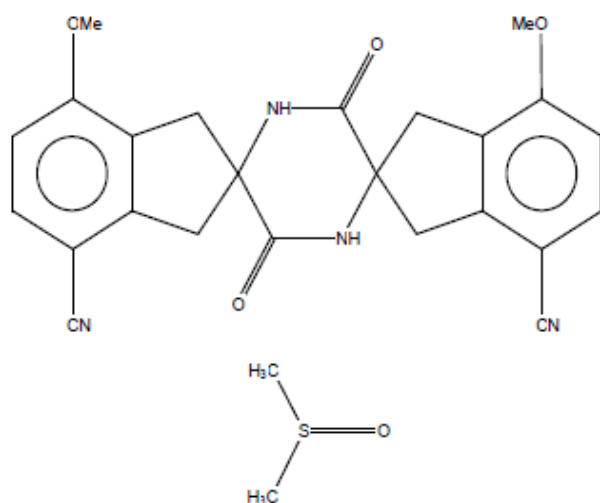
ULEKAX

Reference: B.Jagadish, M.D.Carducci, C.Bosshard, P.Gunter, J.J.Margolis, L.J.Williams, E.A.Mash (2003) *Cryst. Growth Des.*, 3,811

Formula: $C_{24}H_{20}N_4O_4 \cdot 3(C_2H_6O_1S_1)$

Compound Name: meso-(R,S)-Cyclo-bis(2-amino-7-cyano-4-methoxyindan-2-carboxylic acid) tris(dimethylsulfoxide)

Space Group: C2/c Cell: a 21.156(3) b 8.864(1) c 18.640(2)
Space Group No.: 15 (Å³) α 90.00 β 110.29(0) γ 90.00
R-Factor (%): 4.49 Temperature(K): 170 Density(g/cm³): 1.343



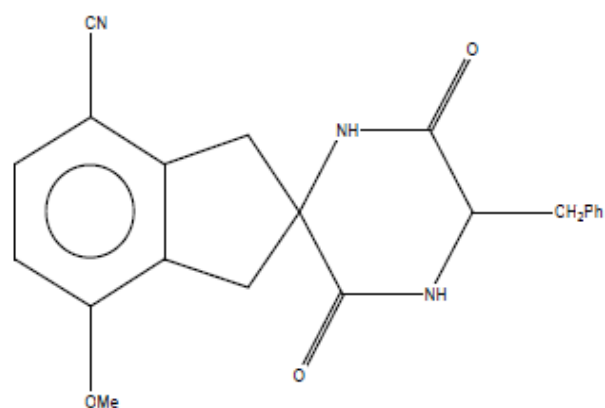
ULEKEB

Reference: B.Jagadish, M.D.Carducci, C.Bosshard, P.Gunter, J.J.Margolis, L.J.Williams, E.A.Mash (2003) *Cryst. Growth Des.*, 3,811

Formula: $C_{21}H_{19}N_3O_3$

Compound Name: (R,S)-Cyclo((2-amino-7-cyano-4-methoxyindan-2-carboxylic acid)(2-amino-3-phenylpropanoic acid))

Space Group: P21 Cell: a 11.042(4) b 6.121(2) c 13.549(5)
Space Group No.: 4 (Å³) α 90.00 β 104.81(0) γ 90.00
R-Factor (%): 4.71 Temperature(K): 170 Density(g/cm³): 1.356



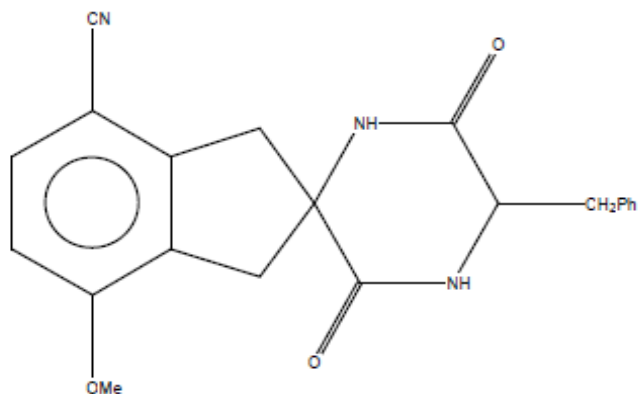
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Reference: B.Jagadish, M.D.Carducci, C.Bosshard, P.Gunter, J.J.Margolis, L.J.Williams, E.A.Mash (2003) *Cryst. Growth Des.* , 3,811

Formula: C₂₁H₁₉N₃O₃

Compound Name: (S,S)-Cyclo[(2-amino-7-cyano-4-methoxyindan-2-carboxylic acid)(2-amino-3-phenylpropanoic acid)]

Space Group: P21 **Cell:** a 10.913(1) b 6.077(0) c 13.753(1)
Space Group No.: 4 **(Å³)** α 90.00 β 94.08(0) γ 90.00
R-Factor (%): 4.78 **Temperature(K):** 170 **Density(g/cm³):** 1.319



VAHXIM

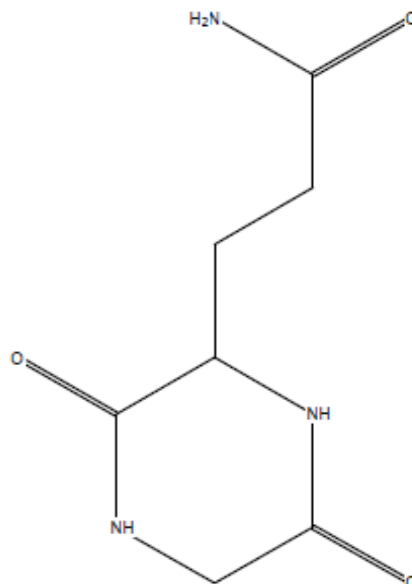
Reference: M.R.Caira, E.Buyukbingol, A.Adejare, W.R.Millington (2002) *Anal.Sci.* ,18,1175

Formula: C₇H₁₁N₃O₃

Compound Name: Cyclo[glycyl-L-glutamyl]

Synonym: Cyclic peptide (2 residues): GLY-GLN-

Space Group: P21 **Cell:** a 4.510(1) b 18.919(2) c 5.087(1)
Space Group No.: 4 **(Å³)** α 90.00 β 99.38(0) γ 90.00
R-Factor (%): 3.90 **Temperature(K):** 295 **Density(g/cm³):** 1.436



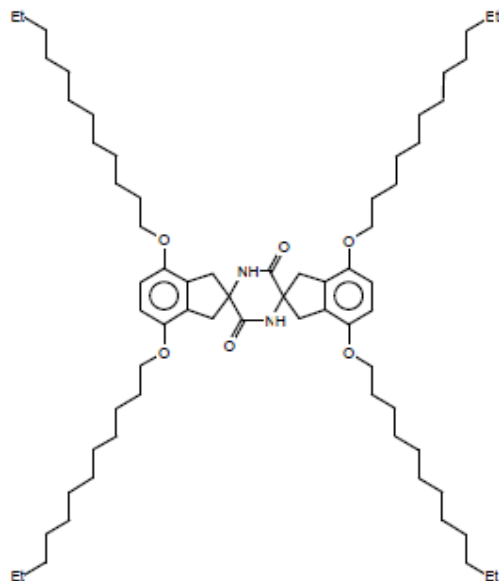
VARPOU

Reference: R.A.Kloster, M.D.Carducci, E.A.Mash (2003) *Org.Lett.* ,5, 3683

Formula: C₆₈H₁₁₄N₂O₆

Compound Name: Dispiro[[4,7-bis(dodecyloxy)indan]-2,2'-(3',6'-dioxo-1',4'-diazacyclohexane)-5',2''-(4'',7''-bis(dodecyloxy)indan)]

Space Group: P21/c **Cell:** a 21.981(4) b 18.298(4) c 24.801(5)
Space Group No.: 14 **(Å³)** α 90.00 β 108.72(3) γ 90.00
R-Factor (%): 9.92 **Temperature(K):** 100 **Density(g/cm³):** 1.113



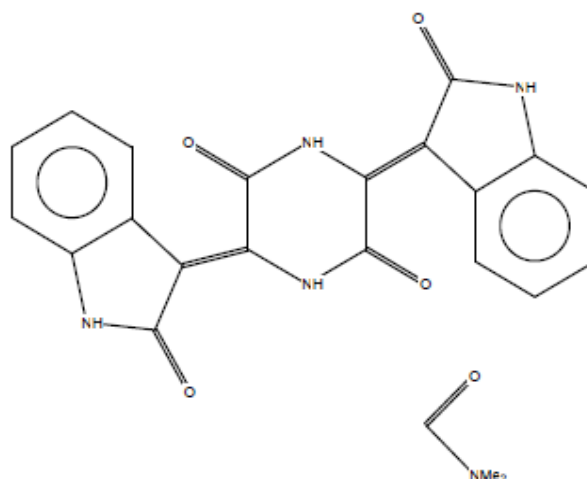
VECTAY

Reference: A.R.Katritzky, Wei-Qiang Fan, A.E.Kozlowski, G.J.Palenik (1989) *J.Heterocycl.Chem.* ,26,821

Formula: C₂₀H₁₂N₄O₄·2(C₃H₇N₁O₁)

Compound Name: 3,6-bis(2-Oxo-3-Indolylidene)piperazine-2,5-dione dimethylformamide solvate

Space Group: P21/n **Cell:** a 12.483(2) b 5.869(1) c 17.328(3)
Space Group No.: 14 **(Å³)** α 90.00 β 96.19(1) γ 90.00
R-Factor (%): 4.40 **Temperature(K):** 295 **Density(g/cm³):** 1.364



VOPKAM

Reference: P.Mikulcik, J.Riede, H.Schmidbauer (1991) *Chem.Ber.*, **124**, 2743

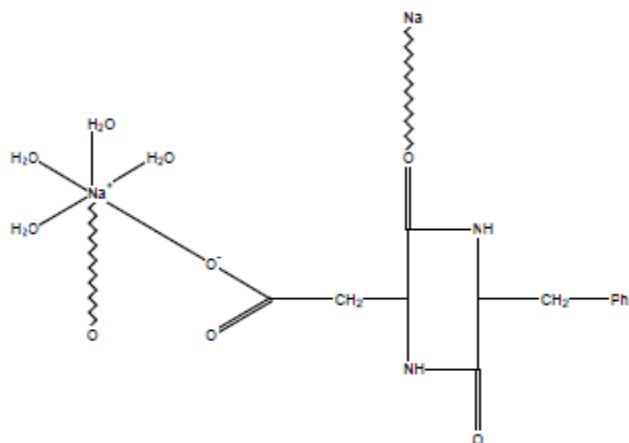
Formula: $(C_{13}H_{21}N_2Na_4O_3)_n$

Compound Name: catena-(Tetra-aqua-(μ_2 -cyclo(L- α -aspartyl-L-phenylalanyl)-O,O')-sodium)

Synonym: catena-(Tetra-aqua-(μ_2 -3-benzyl-5-(carboxylatomethyl)-2,5-dioxopiperazine-O,O')-sodium)

Space Group: P212121 **Cell:** a 6.062(1) b 8.267(1) c 33.175(3)
Space Group No.: 19 **Cell:** (\AA , $^\circ$) α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.70 **Temperature(K):** 295 **Density(g/cm 3):** 1.424



WAFHAO

Reference: Jing-Jing Jia, Xiu-Jin Meng, Shi-Zhang Liang, Shu-Hua Zhang, Yi-Min Jiang (2010) *Acta Crystallogr., Sect.E:Struct.Rep. Online*, **66**,o3315

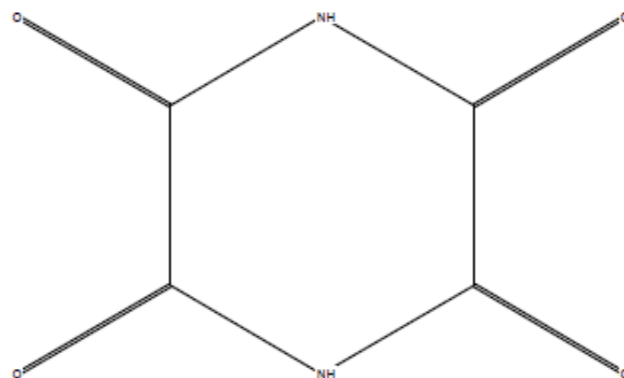
Formula: $C_4H_2N_2O_4$

Compound Name: Piperazine-2,3,5,6-tetraone

Synonym: Piperazine-2,3,5,6-tetrone

Space Group: P21/m **Cell:** a 5.163(1) b 8.622(1) c 5.654(1)
Space Group No.: 14 **Cell:** (\AA , $^\circ$) α 90.00 β 105.25(3) γ 90.00

R-Factor (%): 4.77 **Temperature(K):** 293 **Density(g/cm 3):** 1.943



WAFHAO01

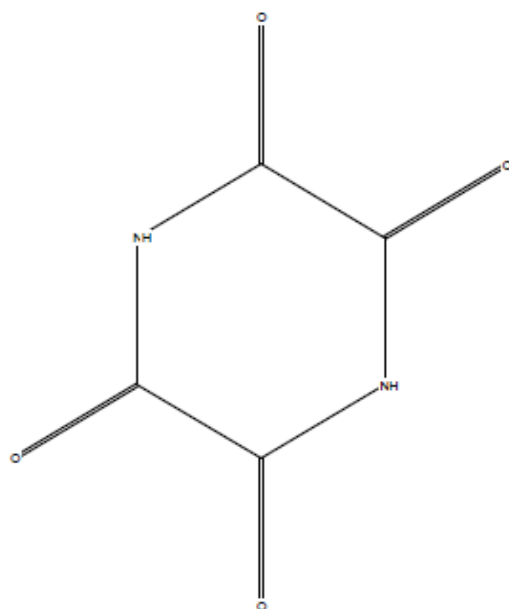
Reference: O.V.Kovalchikova, N.D.Do, A.I.Stash, S.B.Strashnova, B.E.Zaitsev (2014) *Kristallografiya(Russ.)(Crystallogr.Rep.)*, **59**,65

Formula: $C_4H_2N_2O_4$

Compound Name: piperazine-2,3,5,6-tetraone

Space Group: P21/m **Cell:** a 5.177(1) b 8.625(2) c 5.662(1)
Space Group No.: 14 **Cell:** (\AA , $^\circ$) α 90.00 β 105.22(3) γ 90.00

R-Factor (%): 3.08 **Temperature(K):** 293 **Density(g/cm 3):** 1.934



WANZOB

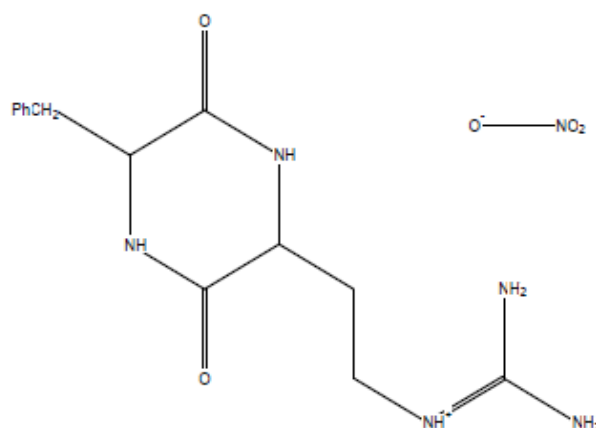
Reference: C.Becker, C.Hoben, D.Schollmeyer, G.Schem, H.Kunz (2005) *Eur.J.Org.Chem.*, 1497

Formula: $C_{14}H_{20}N_5O_2 \cdot 1^+ \cdot N_3O_3 \cdot 1^-$

Compound Name: 2-(5-Benzyl-2,5-dioxopiperazin-3-yl)-N-(diaminomethylene)ethanaminium nitrate

Space Group: P1 **Cell:** a 9.241(3) b 9.502(4) c 11.449(4)
Space Group No.: 1 **Cell:** (\AA , $^\circ$) α 112.66(2) β 104.91(3) γ 98.91(3)

R-Factor (%): 6.57 **Temperature(K):** 143 **Density(g/cm 3):** 1.362



WAPPOT

Reference: M.Crisma, J.R.Deschamps, C.George, J.L.Flippen-Anderson, B.Kaptein, Q.B.Broxterman, A.Moretto, S.Oancea, M.Jost, F.Fornagallo, C.Toniolo (2005) *J.Pept.Res.*, **65**,564

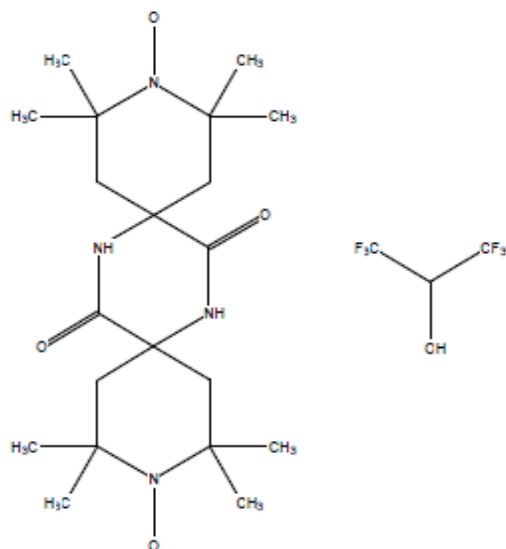
Formula: C₂₀H₂₄N₄O₄·2(C₃H₂F₅O₁)

Compound Name: 2,2,4,4,11,11,13,13-Octamethyl-8,16-dioxo-3,12-dioxo-3,7,12,15-tetra-azadspiro[5.2.5.2]hexadecane 1,1,1,3,3,3-hexafluoroisopropanol solvate

Synonym: Cyclic peptide (2 residues): GLY⁺-GLY⁻

Space Group: A2/n **Cell:** a 12.193(3) b 18.254(4) c 14.623(3)
Space Group No.: 15 **(Å³)** α 90.00 β 92.08(8) γ 90.00

R-Factor (%): 7.07 **Temperature(K):** 293 **Density(g/cm³):** 1.492



WEQSUG

Reference: K.Kanoh, S.Kohno, J.Katada, J.Takahashi, I.Uno, Y.Hayashi (1999) *Bioorg.Med.Chem.*, **7**,1451

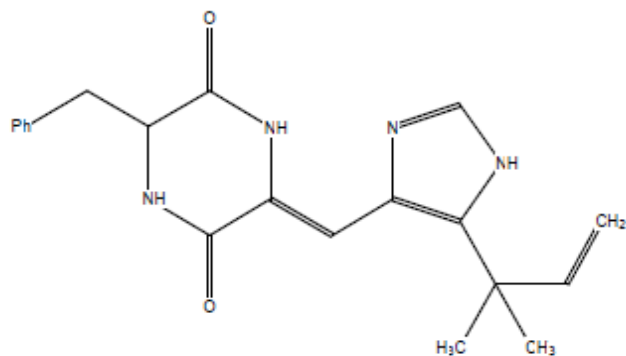
Formula: C₂₀H₂₂N₄O₂

Compound Name: (+)-Cyclo(5-(1,1-dimethylprop-2-enyl)dehydrohistidinyl-L-phenylalanine)

Synonym: (+)-Phenylahistin; Cyclic peptide (2 residues): HIS⁺-PHE⁻

Space Group: P42 **Cell:** a 15.351(0) b 15.351(0) c 8.309(2)
Space Group No.: 77 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.70 **Temperature(K):** 295 **Density(g/cm³):** 1.189



WOBWUF

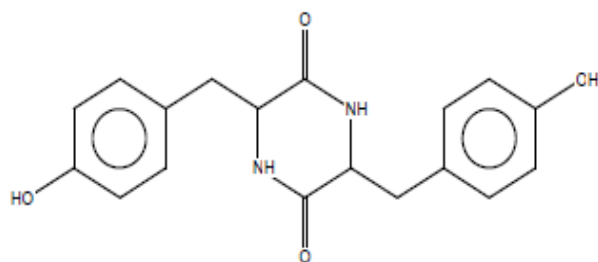
Reference: I.A.Razak, S.S.S.Raj, Hoong-Kun Fun, Zheng-Feng Chen, JingZhang, Ren-Gen Xiong, Xiao-Zeng You (2000) *Acta Crystallogr., Sect. C:Cryst.Struct.Commun.*, **56**,e341

Formula: C₁₈H₁₈N₂O₄

Compound Name: 3,6-bis(4-Hydroxybenzyl)piperazine-2,5-dione

Space Group: C2/c **Cell:** a 16.259(0) b 8.058(0) c 14.779(0)
Space Group No.: 15 **(Å³)** α 90.00 β 121.97(0) γ 90.00

R-Factor (%): 5.50 **Temperature(K):** 295 **Density(g/cm³):** 1.320



WOBWUF01

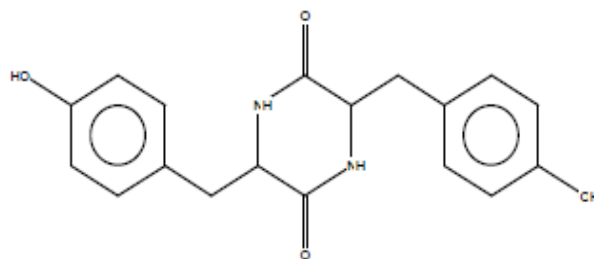
Reference: A.V.Churakov, P.V.Prikhodchenko, M.A.Navasardyan, D.A.Grishanov (2015) *CSD Communication(Private Communication)*,

Formula: C₁₈H₁₈N₂O₄

Compound Name: 3,6-bis(4-hydroxybenzyl)piperazine-2,5-dione

Space Group: C2/c **Cell:** a 16.010(1) b 8.030(0) c 15.034(1)
Space Group No.: 15 **(Å³)** α 90.00 β 123.88(0) γ 90.00

R-Factor (%): 3.78 **Temperature(K):** 150 **Density(g/cm³):** 1.351



XABMIX

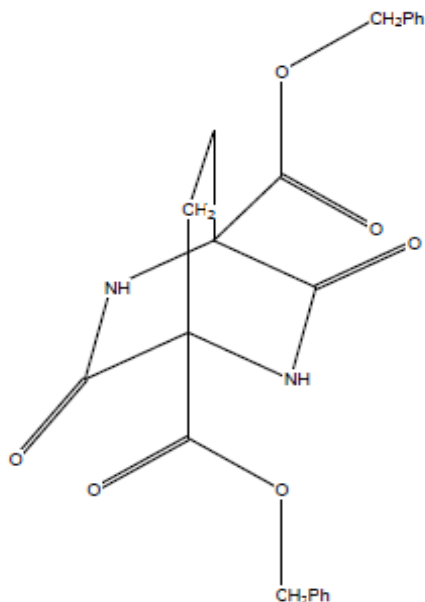
Reference: K.A.Lyssenkov, D.A.Lenev, R.G.Kostyanovsky (2002) *Tetrahedron*, **58**,8525

Formula: C₂₂H₂₀N₂O₆

Compound Name: (+)-Dibenzyl 2,5-diazabicyclo[2.2.2]octane-3,6-dione-1,4-dicarboxylate

Space Group: P-1 **Cell:** a 5.583(4) b 9.765(7) c 17.760(11)
Space Group No.: 2 **(Å,°)** α 93.45(5) β 92.14(5) γ 90.18(5)

R-Factor (%): 6.42 **Temperature(K):** 293 **Density(g/cm³):** 1.404



XABMOD

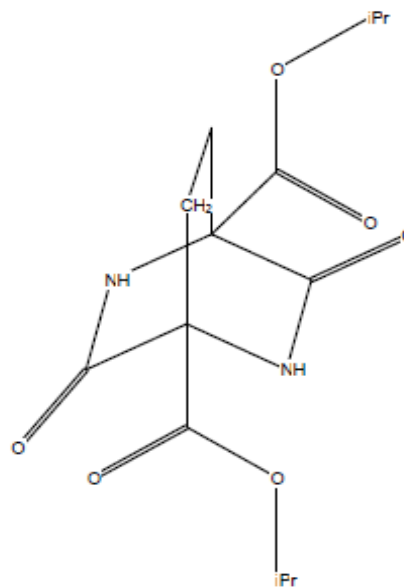
Reference: K.A.Lyssenkov, D.A.Lenev, R.G.Kostyanovsky (2002) *Tetrahedron*, **58**,8525

Formula: C₁₄H₂₀N₂O₆

Compound Name: (+)-Diisopropyl 2,5-diazabicyclo[2.2.2]octane-3,6-dione-1,4-dicarboxylate

Space Group: P-1 **Cell:** a 5.931(3) b 10.381(6) c 13.596(8)
Space Group No.: 2 **(Å,°)** α 73.43(4) β 77.89(4) γ 89.45(5)

R-Factor (%): 7.36 **Temperature(K):** 293 **Density(g/cm³):** 1.324



XAZHIQ

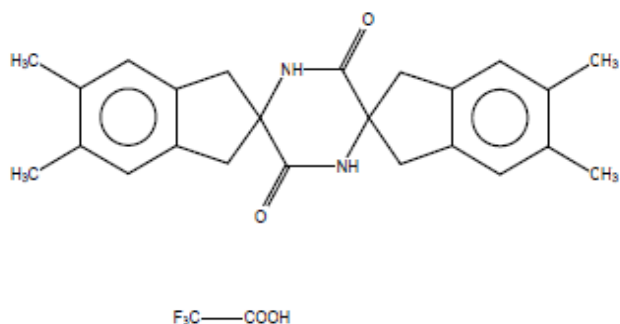
Reference: R.A.Weatherhead-Kloster, H.D.Selby, W.B.Miller III, E.A.Mash (2005) *J.Org.Chem.*, **70**,8693

Formula: C₂₄H₂₆N₂O₂·2(C₂H₃F₃O₂)

Compound Name: 5,6,5',6'-Tetramethyl-2',4'-dioxidospiro[indan-2,3'-piperazine-6',2''-indan] trifluoroacetic acid solvent

Space Group: C2/c **Cell:** a 28.566(5) b 5.956(4) c 17.494(10)
Space Group No.: 15 **(Å,°)** α 90.00 β 97.17(5) γ 90.00

R-Factor (%): 10.10 **Temperature(K):** 294 **Density(g/cm³):** 1.355



XEHIDAS

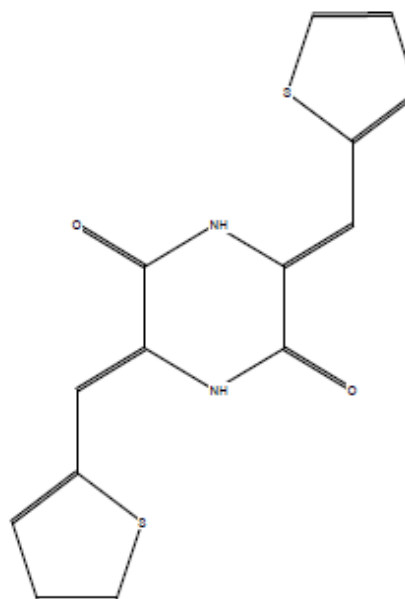
Reference: Xuncheng Liu, Bo He, C.L.Anderson, Jun Kang, T.Chen, Jinxiang Chen, Shizhen Feng, Lianjie Zhang, M.A.Kolaczowski, S.J.Teat, M.A.Brady, Chenhui Zhu, Lin-Wang Wang, Junwu Chen, Yi Liu (2017) *J.Am.Chem.Soc.*, **139**,8355

Formula: C₁₄H₁₀N₂O₂S₂

Compound Name: 3,6-bis[(thiophen-2-yl)methylidene]piperazine-2,5-dione

Space Group: P-1 **Cell:** a 3.814(0) b 5.585(0) c 14.344(1)
Space Group No.: 2 **(Å,°)** α 95.39(0) β 96.17(0) γ 94.84(0)

R-Factor (%): 5.25 **Temperature(K):** 100 **Density(g/cm³):** 1.668



XELGAW

Reference: B.Jagadish, L.J.Williams, M.D.Carducci, C.Bosshard, E.A.Mash (2000) *Tetrahedron Lett.* ,41,9483

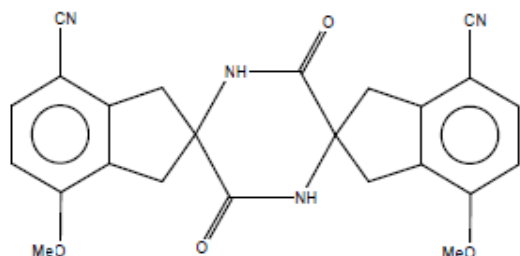
Formula: $C_{24}H_{20}N_4O_4 \cdot 3(C_2H_6O_1S_1)$

Compound Name: (S,S)-Cyclo-bis(2-amino-4-methoxy-7-cyanoindan-2-carboxylic acid) dimethylsulfoxide solvate

Space Group: C2
Space Group No.: 5
R-Factor (%): 3.39

Cell: a 16.432(1) Å, b 10.370(0) Å, c 12.268(0) Å
 α 90.00°, β 130.24(0)°, γ 90.00°

Temperature(K): 170
Density(g/cm³): 1.379



XELGAW01

Reference: B.Jagadish, M.D.Carducci, C.Bosshard, P.Gunter, J.I.Margolis, L.J.Williams, E.A.Mash (2003) *Cryst.Growth Des.* ,3,811

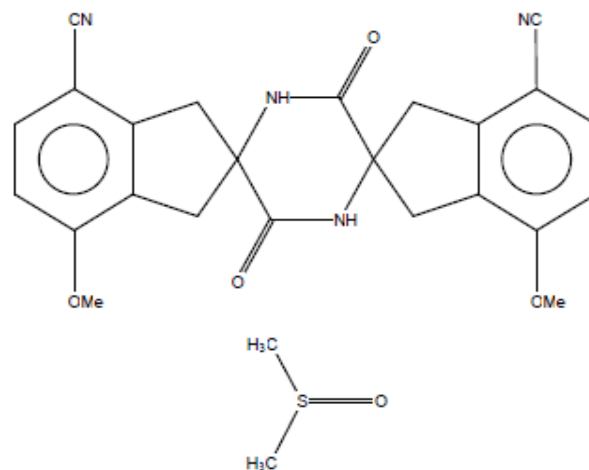
Formula: $C_{24}H_{20}N_4O_4 \cdot 3(C_2H_6O_1S_1)$

Compound Name: (S,S)-Cyclo-bis(2-amino-7-cyano-4-methoxyindan-2-carboxylic acid) tris(dimethylsulfoxide)

Space Group: C2
Space Group No.: 5
R-Factor (%): 3.39

Cell: a 16.432(1) Å, b 10.370(0) Å, c 12.268(0) Å
 α 90.00°, β 130.24(0)°, γ 90.00°

Temperature(K): 170
Density(g/cm³): 1.379



YAHJUO

Reference: Ping Li, Chun Zhang, Wei Xu (2011) *Acta Crystallogr., Sect.E: Struct.Rep. Online* ,67,03041

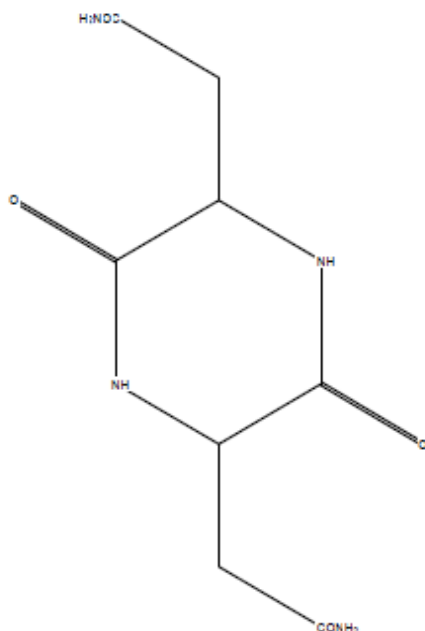
Formula: $C_8H_{12}N_4O_4$

Compound Name: meso-3,6-Dioxopiperazine-2,5-diacetamide

Space Group: P21/c
Space Group No.: 14
R-Factor (%): 3.57

Cell: a 5.041(1) Å, b 8.318(1) Å, c 12.900(3) Å
 α 90.00°, β 109.76(3)°, γ 90.00°

Temperature(K): 293
Density(g/cm³): 1.489



YEKGAW

Reference: Zhuming Zhang, H.Kohn (1994) *J.Am.Chem.Soc.* ,116, 9815

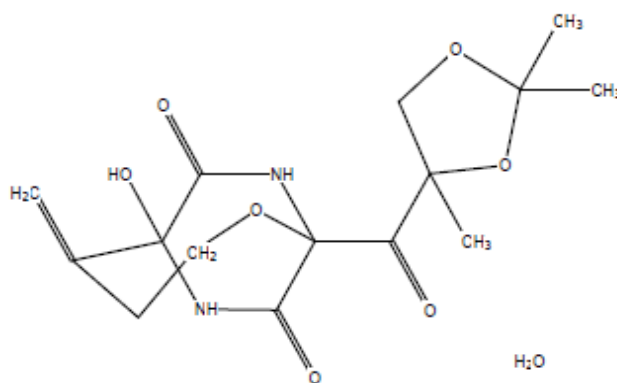
Formula: $C_{15}H_{20}N_2O_7 \cdot H_2O_1$

Compound Name: 6-Hydroxy-5-methylene-1-((2,2,4-trimethyl)-1,3-dioxolan-4-yl-carbonyl)-2-oxa-7,9-diazabicyclo[4.2.2]decan-8,10-dione monohydrate

Space Group: P21
Space Group No.: 4
R-Factor (%): 3.50

Cell: a 6.497(3) Å, b 10.908(5) Å, c 12.294(7) Å
 α 90.00°, β 90.73(4)°, γ 90.00°

Temperature(K): 295
Density(g/cm³): 1.366



YEKGEA

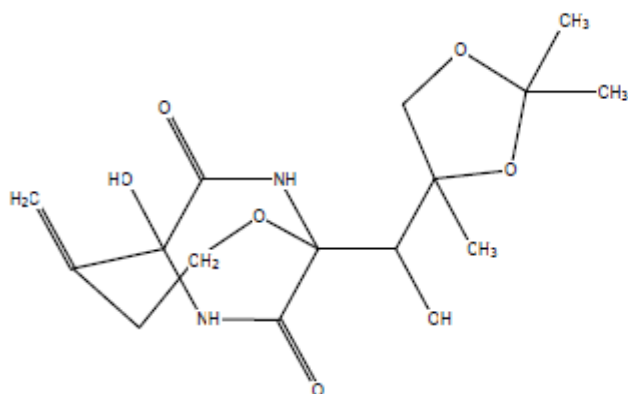
Reference: Zhuming Zhang, H.Kohn (1994) *J.Am.Chem.Soc.*, **116**, 9815

Formula: $C_{15}H_{22}N_2O_7$

Compound Name: 6-Hydroxy-5-methylene-1-(((2,2,4-trimethyl)-1,3-dioxolan-4-yl)(hydroxymethyl)-2-oxa-7,9-diazabicyclo(4.2.2)decan-8,10-dione

Space Group: P21
Space Group No.: 4
Cell: a 7.579(2) b 10.355(2) c 11.266(2) (\AA , $^\circ$)
 α 90.00 β 108.80(2) γ 90.00

R-Factor (%): 3.10 **Temperature(K):** 223 **Density(g/cm 3):** 1.358



YEKGOK

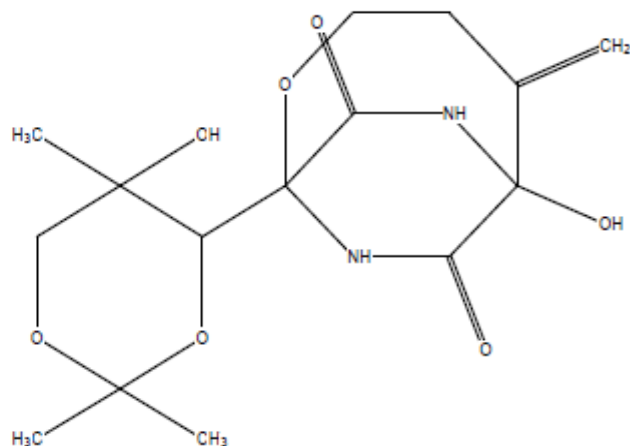
Reference: Zhuming Zhang, H.Kohn (1994) *J.Am.Chem.Soc.*, **116**, 9815

Formula: $C_{15}H_{22}N_2O_7$

Compound Name: 6-Hydroxy-5-methylene-1-(5-hydroxy-2,2,5-trimethyl-1,3-dioxacyclohexan-4-yl)-2-oxa-7,9-diazabicyclo(4.2.2)decan-8,10-dione

Space Group: P21
Space Group No.: 4
Cell: a 10.468(5) b 10.889(4) c 14.416(5) (\AA , $^\circ$)
 α 90.00 β 102.70(3) γ 90.00

R-Factor (%): 3.40 **Temperature(K):** 223 **Density(g/cm 3):** 1.419



YERJIO

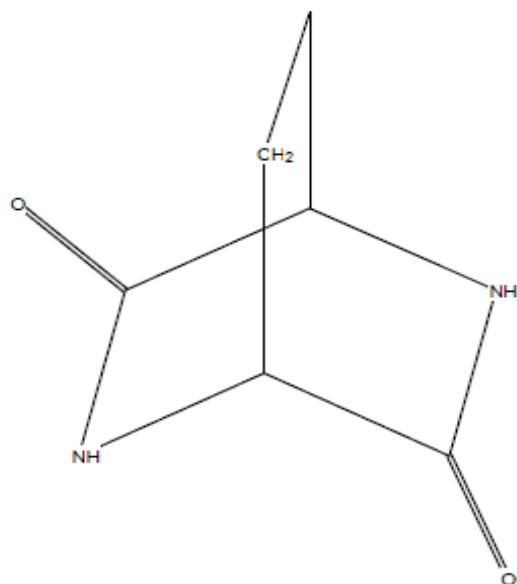
Reference: M.-J.Brienne, J.Gabard, M.Leclercq, J.-M.Lehn, M.Cesario, C.Pascard, M.Cheve, G.Dutruc-Rosset (1994) *Tetrahedron Lett.*, **35**,8157

Formula: $C_8H_8N_2O_2$

Compound Name: (+)-2,5-Diazabicyclo(2.2.2)octane-3,6-dione

Space Group: Pccn
Space Group No.: 56
Cell: a 6.793(3) b 8.362(6) c 11.156(9) (\AA , $^\circ$)
 α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.81 **Temperature(K):** 295 **Density(g/cm 3):** 1.469



YERJOU

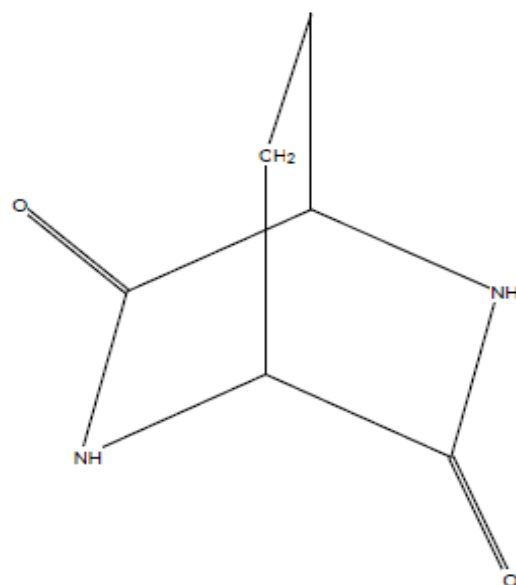
Reference: M.-J.Brienne, J.Gabard, M.Leclercq, J.-M.Lehn, M.Cesario, C.Pascard, M.Cheve, G.Dutruc-Rosset (1994) *Tetrahedron Lett.*, **35**,8157

Formula: $C_8H_8N_2O_2$

Compound Name: (-)-2,5-Diazabicyclo(2.2.2)octane-3,6-dione

Space Group: P21212
Space Group No.: 16
Cell: a 8.314(2) b 6.864(2) c 5.556 (\AA , $^\circ$)
 α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.12 **Temperature(K):** 295 **Density(g/cm 3):** 1.458



YUSBIX

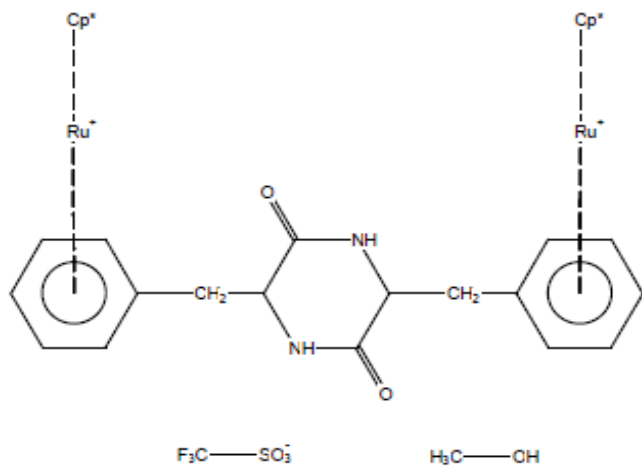
Reference: A.J.Gleichmann, J.M.Wolff, W.S.Sheldrick (1995) *J.Chem.Soc.,Dalton Trans.*, 1549

Formula: $C_{38}H_{48}N_2O_2Ru_2 \cdot 2(C_1F_3O_3S_1^{-}) \cdot 1.5(C_1H_4O_1)$

Compound Name: $(\mu_2-\eta^6, \eta^6\text{-Cyclobis(phenylalanyl)})\text{-bis}(\eta^5\text{-pentamethyl-cyclopentadienyl})\text{-d-iruthenium(II) bis(trifluoromethanesulfonate) methanol solvate}$

Space Group: P212121 **Cell:** a 11.896(5) b 16.996(6) c 22.694(5)
Space Group No.: 19 **(Å³)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.90 **Temperature(K):** 173 **Density(g/cm³):** 1.611



YUZPUG

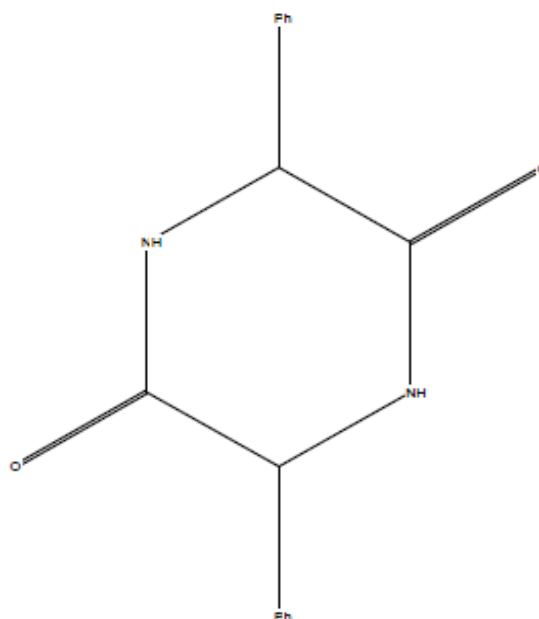
Reference: M.B.Avinash, D.Raut, M.K.Mishra, U.Ramamurty, T.Govindaraju (2015) *Scientific Reports*, 5,16070

Formula: $C_{16}H_{14}N_2O_2$

Compound Name: 3,6-diphenylpiperazine-2,5-dione

Space Group: P-1 **Cell:** a 6.221(2) b 10.109(3) c 10.929(5)
Space Group No.: 2 **(Å³)** α 81.20(6) β 86.78(7) γ 77.74(5)

R-Factor (%): 6.52 **Temperature(K):** 150 **Density(g/cm³):** 1.333



ZICLAY

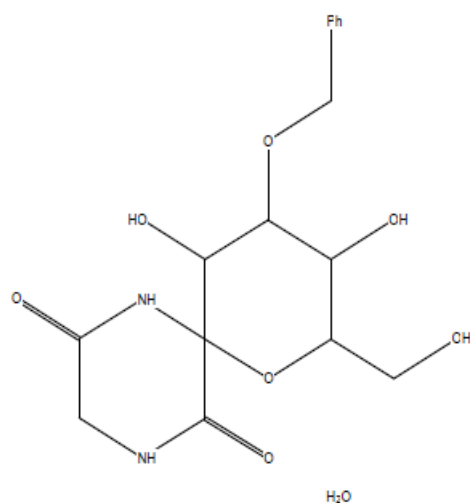
Reference: T.M.Krulle, K.A.Watson, M.Gregoriou, L.N.Johnson, S.Crook, D.J.Watkin, R.C.Griffiths, R.J.Nash, K.E.Tsitsanou, S.E.Zographos, N.G.Oikonomakos, G.W.J.Fleet (1995) *Tetrahedron Lett.*, 36,8291

Formula: $C_{16}H_{20}N_2O_7 \cdot H_2O_1$

Compound Name: (2R,3S,4S,5R,6S)-4-Benzoyloxy-3,5-dihydroxy-2-hydroxymethyl-7,10-diaza-1-oxaspiro[5.5]undecan-8,11-dione monohydrate

Space Group: P1 **Cell:** a 6.142(4) b 7.469(3) c 10.075(4)
Space Group No.: 1 **(Å³)** α 83.61(4) β 87.12(4) γ 70.39(4)

R-Factor (%): 4.79 **Temperature(K):** 295 **Density(g/cm³):** 1.422



ZUSDAU

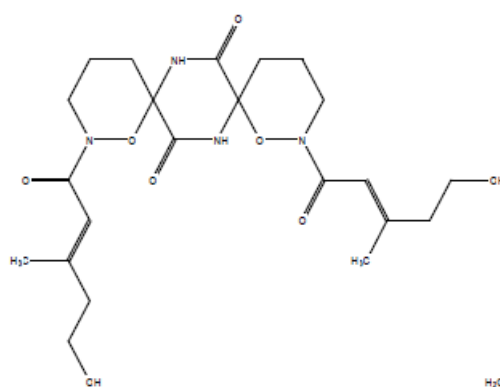
Reference: Yan-Lai Jia, Mei-Yan Wei, Hai-Yan Chen, Fei-Fei Guan, Chang-Yun Wang, Chang-Lun Shao (2015) *Org.Lett.*, 17,4216

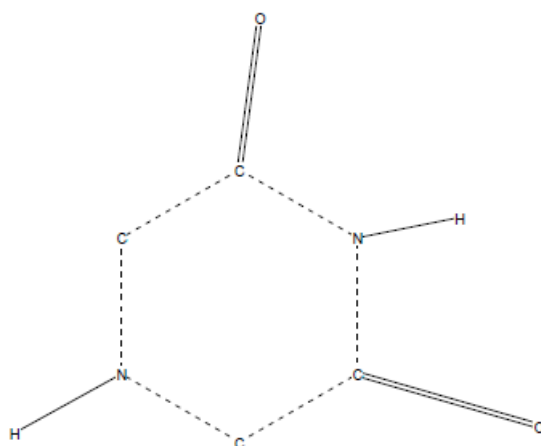
Formula: $C_{22}H_{32}N_4O_9 \cdot H_2O_1$

Compound Name: 2,11-bis(5-hydroxy-3-methylpent-2-enyl)-1,10-dioxo-2,7,11,15-tetraazadispiro[5.2.5.2]hexadecane-8,16-dione monohydrate

Space Group: P-1 **Cell:** a 9.749(1) b 10.793(2) c 12.316(3)
Space Group No.: 2 **(Å³)** α 106.75(3) β 97.22(3) γ 95.45(3)

R-Factor (%): 4.73 **Temperature(K):** 293 **Density(g/cm³):** 1.355





TAZZOM

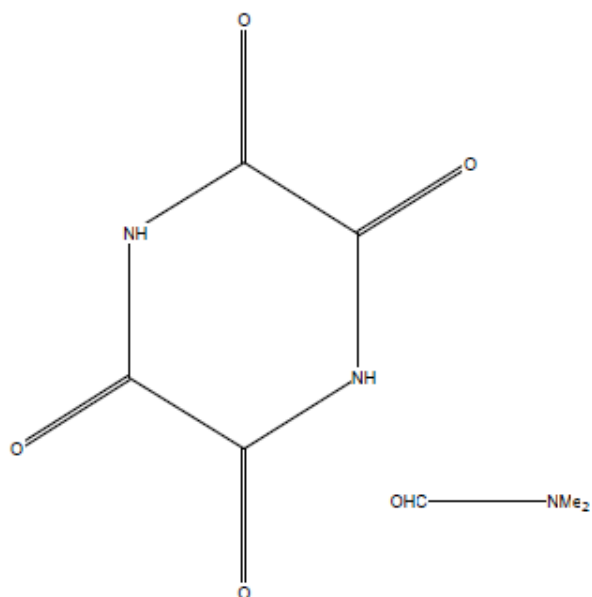
Reference: C.J.Kingsbury, B.F.Abrahams, R.Robson (2017)
CSD Communication(Private Communication),

Formula: $C_4H_2N_2O_4 \cdot 2(C_2H_7N_1O_1)$

Compound Name: piperazine-2,3,5,6-tetrone N,N-dimethylformamide solvate

Space Group: P21/c **Cell:** a 5.152(0) b 14.668(0) c 9.856(0)
Space Group No.: 14 (\AA^3) α 90.00 β 104.62(0) γ 90.00

R-Factor (%): 7.12 **Temperature(K):** 130 **Density(g/cm³):** 1.328



WAFHAO

Reference: Jing-Jing Jia, Xiu-Jin Meng, Shi-Zhang Liang,
Shu-Hua Zhang, Yi-Min Jiang (2010)
Acta Crystallogr., Sect.E: Struct.Rep. Online ,66,o3315

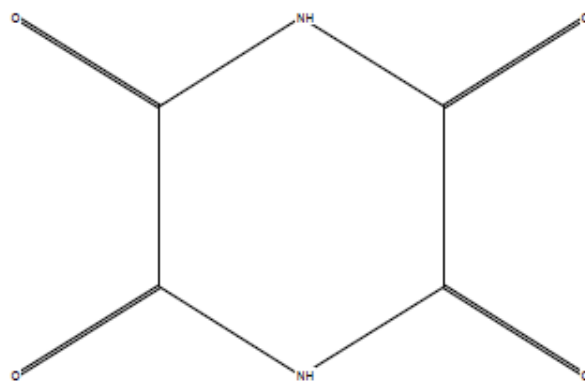
Formula: $C_4H_2N_2O_4$

Compound Name: Piperazine-2,3,5,6-tetraone

Synonym: Piperazine-2,3,5,6-tetrone

Space Group: P21/n **Cell:** a 5.163(1) b 8.622(1) c 5.654(1)
Space Group No.: 14 (\AA^3) α 90.00 β 105.25(3) γ 90.00

R-Factor (%): 4.77 **Temperature(K):** 293 **Density(g/cm³):** 1.943



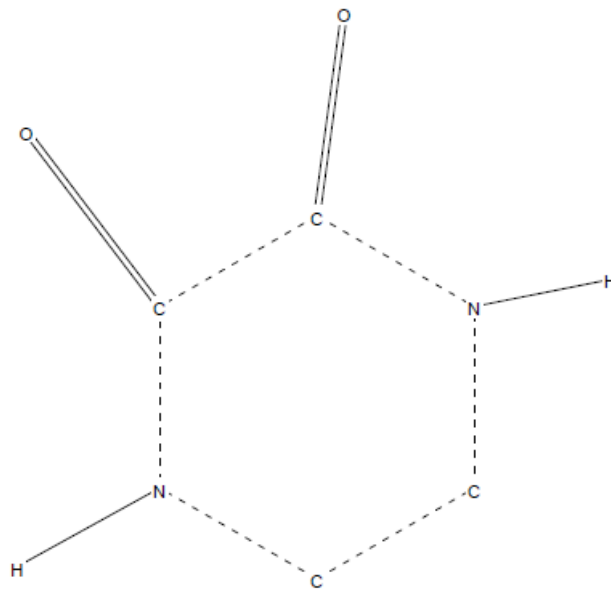
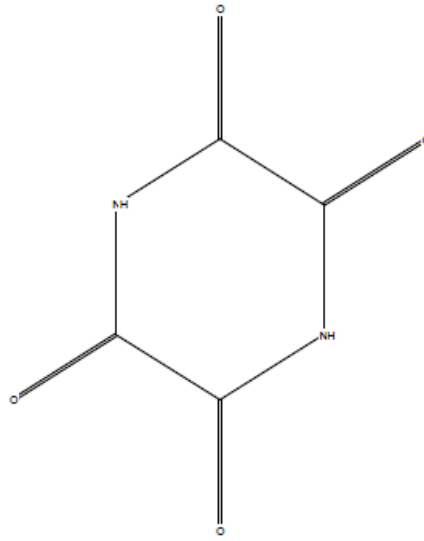
WAFHA001

Reference: O.V.Kovalchikova, N.D.Do, A.I.Stash, S.B.Strashnova, B.E.Zaitsev (2014) Kristallografiya(Russ.)(Crystallogr.Rep.), 59,65

Formula: $C_4H_2N_2O_4$

Compound Name: piperazine-2,3,5,6-tetraone

Space Group: P21/n Cell: a 5.177(1) b 8.625(2) c 5.662(1)
Space Group No.: 14 (\AA^3) α 90.00 β 105.22(3) γ 90.00
R-Factor (%): 3.08 Temperature(K): 293 Density(g/cm^3): 1.934



BAKGOJ

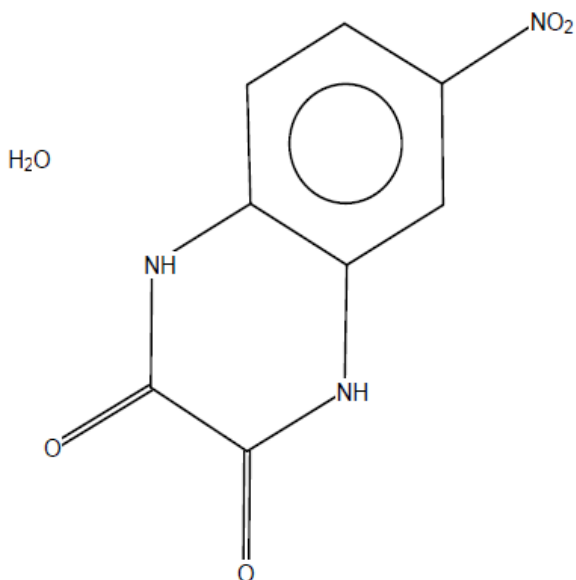
Reference: A.Stepien (1981)
Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem., **37**,2087

Formula: C₈ H₅ N₃ O₄·H₂O

Compound Name: 6-Nitro-2,3-dihydroquinoxaline monohydrate

Synonym: 6-Nitro-2,3-(1H,4H)-quinoxalinedione monohydrate

Space Group: P21/c **Cell:** **a** 7.489(1) **b** 11.949(2) **c** 12.066(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 120.43(2) γ 90.00
R-Factor (%): 5.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.606



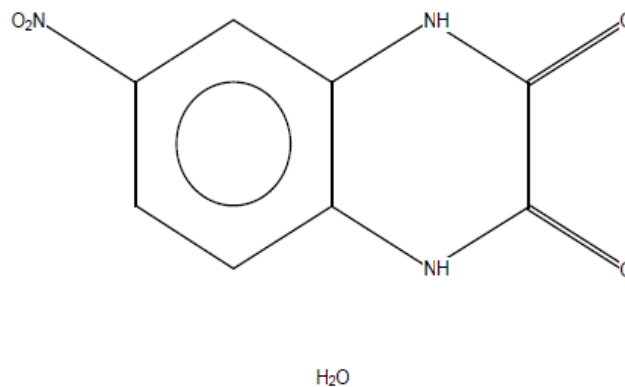
BAKGOJ01

Reference: M.Kubicki, T.W.Kindopp, M.V.Cappareli, P.W.Codding (1996) *Acta Crystallogr., Sect.B: Struct. Sci.*, **52**,487

Formula: C₈ H₅ N₃ O₄·H₂O

Compound Name: 6-Nitro-1,4-dihydro-2,3-quinoxalinedione monohydrate

Space Group: P21/n **Cell:** **a** 7.474(0) **b** 11.927(0) **c** 10.491(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 97.51(0) γ 90.00
R-Factor (%): 5.06 **Temperature(K)**: 295 **Density(g/cm³)**: 1.613



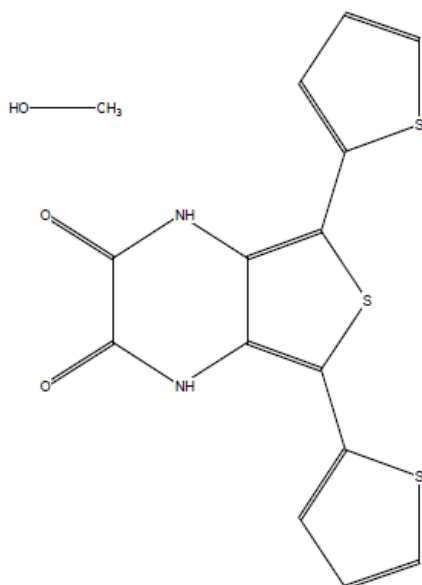
BIFREP

Reference: R.L.Schwiderski, S.C.Rasmussen (2013) *J.Org.Chem.*, **78**, 5453

Formula: C₁₄ H₈ N₂ O₂ S₃·C₁ H₄ O₁

Compound Name: 5,7-bis(2-thienyl)thieno[3,4-b]pyrazine-2,3(1H,4H)-dione methanol solvate

Space Group: P21/c **Cell:** **a** 11.982(0) **b** 13.202(0) **c** 10.906(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 115.49(0) γ 90.00
R-Factor (%): 4.27 **Temperature(K)**: 100 **Density(g/cm³)**: 1.555



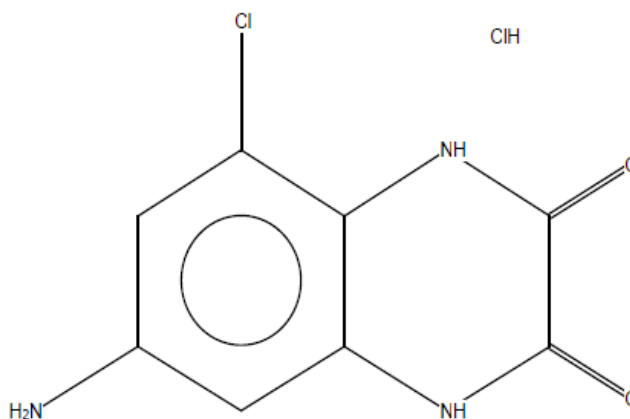
CAHXQX

Reference: A.Stepien (1977)
Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem., **33**,2854

Formula: C₈ H₆ Cl₁ N₃ O₂·0.52(H₁ Cl₁)

Compound Name: 5-Chloro-7-amino-2,3-dihydroquinoxaline hydrochloride

Space Group: Pbc_a **Cell:** **a** 8.554(2) **b** 16.639(3) **c** 13.402(3)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 4.00 **Temperature(K)**: 295 **Density(g/cm³)**: 1.606



CNIXQX

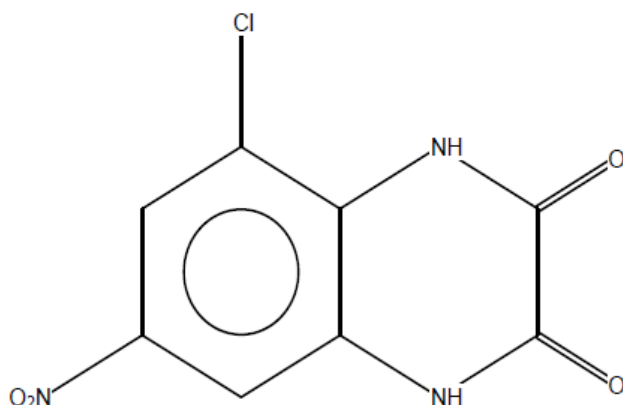
Reference: M.J.Grabowski, A.Stepien, M.Cyglar, E.Wajsman (1977)
Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem., **33**,2851

Formula: C₈ H₄ Cl₁ N₃ O₄

Compound Name: 5-Chloro-7-nitro-2,3-dihydroquinoxaline

Space Group: P-1 **Cell:** a 9.280(2) b 12.870(3) c 8.503(2)
Space Group No.: 2 **(Å,°)** α 90.95(2) β 97.08(2) γ 118.48(2)

R-Factor (%): 4.60 **Temperature(K):** 295 **Density(g/cm³):** 1.818



DULFUM

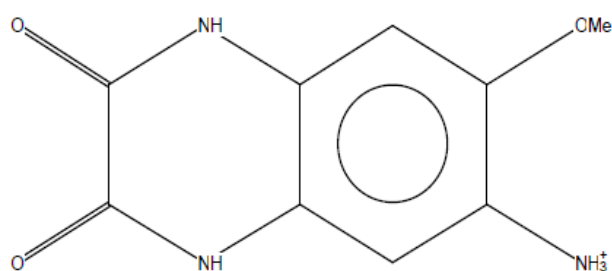
Reference: J.Bruning, A.Peters, J.W.Bats, M.U.Schmidt (2010)
Acta Crystallogr., Sect.C:Cryst.Struct.Commun., **66**,o1

Formula: C₉ H₁₀ N₃ O₃¹⁺·H₂ O₁·Cl₁¹⁻

Compound Name: 7-Methoxy-2,3-dioxo-1,4-dihydroquinoxalin-6-aminium chloride monohydrate

Space Group: Pbc_a **Cell:** a 6.734(1) b 15.469(4) c 21.327(4)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.38 **Temperature(K):** 168 **Density(g/cm³):** 1.565



H₂O Cl⁻

DECLOP

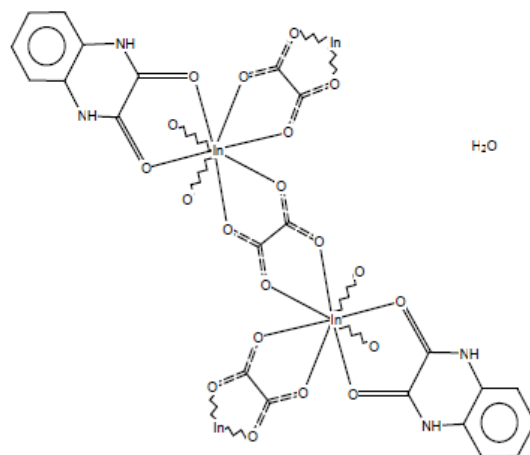
Reference: Yeshuang Zhong, Cheng Chen, Chunchun Zhang,
Dingguo Xu, Zhien Lin (2017) *Inorg.Chem.Commun.*, **84**,186

Formula: (C₂₂ H₁₂ In₂ N₄ O₁₈)_n·3(H₂ O₁)

Compound Name: catena-[tris(μ-oxalato)-bis(1,4-dihydroquinoxaline-2,3-dione)-di-indium(III) trihydrate]

Space Group: P2₁/c **Cell:** a 9.810(0) b 10.986(0) c 12.949(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 91.65(0) γ 90.00

R-Factor (%): 2.80 **Temperature(K):** 293 **Density(g/cm³):** 2.076



EVAFIR

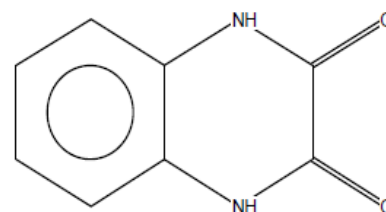
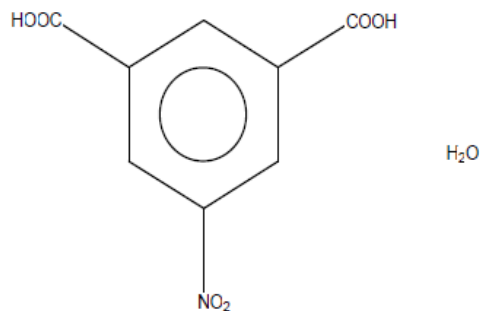
Reference: Ming-Feng Wang (2011)
Acta Crystallogr., Sect.E:Struct.Rep.Online, **67**,o1581

Formula: C₈ H₅ N₁ O₆·C₈ H₆ N₂ O₂·H₂ O₁

Compound Name: 5-Nitroisophthalic acid 1,4-dihydroquinoxaline-2,3-dione monohydrate

Space Group: P-1 **Cell:** a 7.245(2) b 8.686(3) c 13.142(4)
Space Group No.: 2 **(Å,°)** α 93.94(0) β 95.62(0) γ 95.79(0)

R-Factor (%): 3.33 **Temperature(K):** 295 **Density(g/cm³):** 1.592



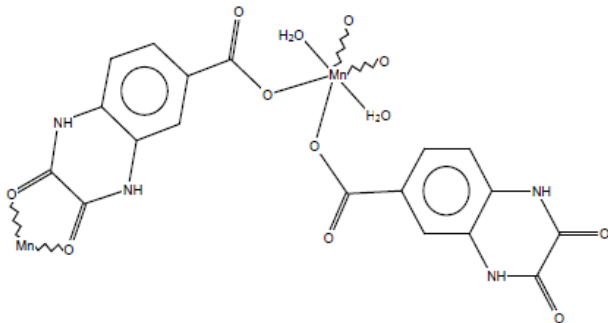
HAPGOX

Reference: Gang Yuan, Chao Zhang, Kui-Zhan Shao, Xiang-Rong Hao, Zhong-Min Su (2017) *Z. Anorg. Allg. Chem.*, **643**,531

Formula: (C₁₈ H₁₄ Mn₁ N₄ O₁₀)_n

Compound Name: catena-[bis(μ-2,3-dioxo-1,2,3,4-tetrahydroquinoxaline-6-carboxylato)-diaqua-manganese(II)]

Space Group: P-1
Space Group No.: 2
Cell: **a** 5.083(5) **b** 11.583(4) **c** 15.374(4)
(Å,°) **α** 88.07(0) **β** 88.31(0) **γ** 84.82(0)
R-Factor (%): 4.03 **Temperature(K)**: 293 **Density(g/cm³)**: 1.848



HIHZUT

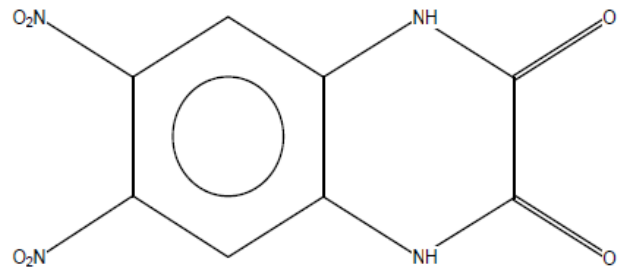
Reference: M.Kubicki, T.W.Kindopp, M.V.Capparelli, P.W.Codding (1996) *Acta Crystallogr., Sect.B:Struct.Sci.*, **52**,487

Formula: C₈ H₄ N₄ O₈

Compound Name: 6,7-Dinitro-1,4-dihydro-2,3-quinoxalinedione

Synonym: DrugBank: DB03759

Space Group: P21/c
Space Group No.: 14
Cell: **a** 8.467(0) **b** 8.553(0) **c** 12.466(0)
(Å,°) **α** 90.00 **β** 90.34(0) **γ** 90.00
R-Factor (%): 3.14 **Temperature(K)**: 295 **Density(g/cm³)**: 1.855



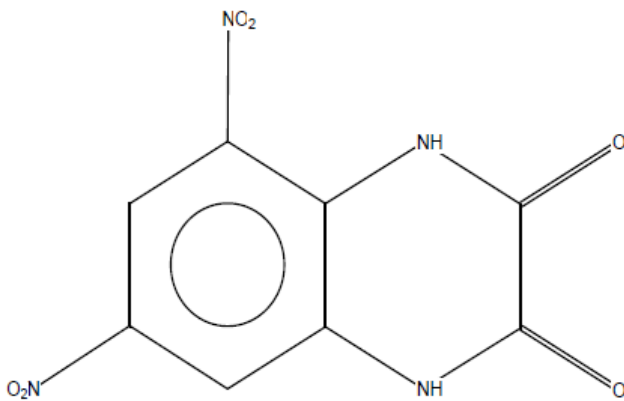
HIJBAD

Reference: M.Kubicki, T.W.Kindopp, M.V.Capparelli, P.W.Codding (1996) *Acta Crystallogr., Sect.B:Struct.Sci.*, **52**,487

Formula: C₈ H₄ N₄ O₈

Compound Name: 5,7-Dinitro-1,4-dihydro-2,3-quinoxalinedione

Space Group: P212121
Space Group No.: 19
Cell: **a** 6.977(0) **b** 13.083(1) **c** 20.401(1)
(Å,°) **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 3.50 **Temperature(K)**: 295 **Density(g/cm³)**: 1.799



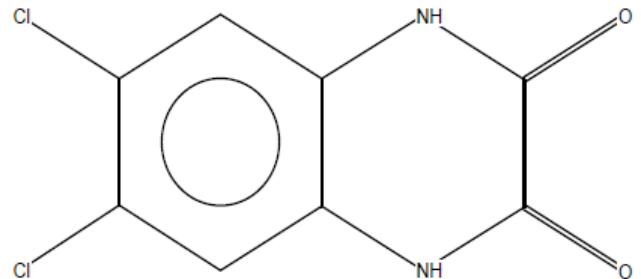
HIJBIL

Reference: M.Kubicki, T.W.Kindopp, M.V.Capparelli, P.W.Codding (1996) *Acta Crystallogr., Sect.B:Struct.Sci.*, **52**,487

Formula: C₈ H₄ Cl₂ N₂ O₂

Compound Name: 6,7-Dichloro-1,4-dihydro-2,3-quinoxalinedione

Space Group: P21/n
Space Group No.: 14
Cell: **a** 7.207(0) **b** 8.450(0) **c** 14.471(0)
(Å,°) **α** 90.00 **β** 99.71(0) **γ** 90.00
R-Factor (%): 2.80 **Temperature(K)**: 295 **Density(g/cm³)**: 1.767



HIJBOR

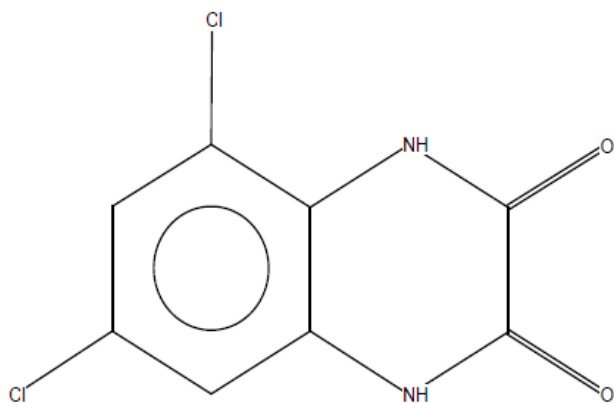
Reference: M.Kubiicki, T.W.Kindopp, M.V.Capparelli, P.W.Codding (1996) *Acta Crystallogr., Sect.B: Struct. Sci.* , **52**,487

Formula: C₈ H₄ Cl₂ N₂ O₂ · C₃ H₇ N₁ O₁

Compound Name: 5,7-Dichloro-1,4-dihydro-2,3-quinoxalinedione

Space Group: P-1 **Cell:** a 6.150(0) b 8.379(0) c 13.736(1)
Space Group No.: 2 **(Å,°)** α 107.41(0) β 99.30(0) γ 95.03(0)

R-Factor (%): 4.25 **Temperature(K):** 295 **Density(g/cm³):** 1.532



Me₂N—CHO

HOYVEX

Reference: M.U.Schmidt, S.Bruhne, A.K.Wolf, A.Rech, J.Bruning, E.Alig, L.Fink, C.Buchsbaum, J.Glinnemann, J.van de Streek, F.Gozzo, M.Brunelli, F.Stowasser, T.Gorelik, E.Mugnaioli, U.Kolb (2009) *Acta Crystallogr., Sect.B: Struct. Sci.* , **65**,189

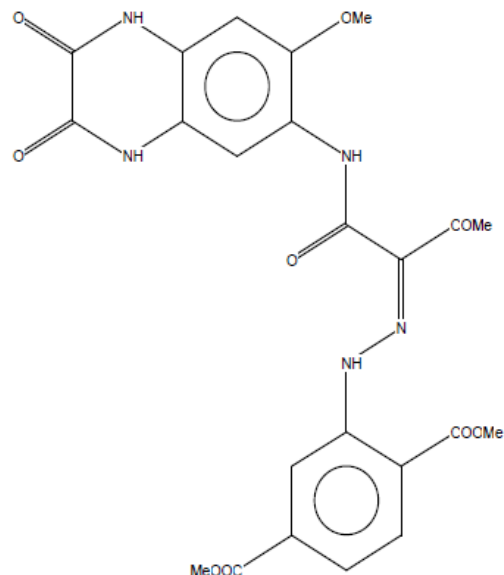
Formula: C₂₃ H₂₁ N₅ O₉

Compound Name: Pigment yellow 213

Synonym: Dimethyl 2-(2-(1-((7-methoxy-2,3-dioxo-1,2,3,4-tetrahydro-6-quinoxaliny)amino)-1,3-dioxo-2-butanylidene)hydrazino)terephthalate

Space Group: P-1 **Cell:** a 6.901(0) b 11.835(0) c 14.059(0)
Space Group No.: 2 **(Å,°)** α 81.81(0) β 81.03(0) γ 87.54(1)

R-Factor (%): 26.10 **Temperature(K):** 293 **Density(g/cm³):** 1.513



HQOXDO

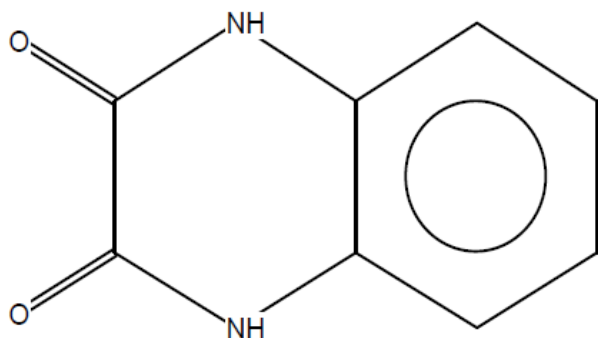
Reference: C.Svensson (1976) *Acta Chem.Scand.* , **30**,581

Formula: C₈ H₈ N₂ O₂

Compound Name: 1,4-Dihydro-2,3-quinoxalinedione

Space Group: P21/n **Cell:** a 8.068(1) b 4.275(1) c 20.911(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 100.42(1) γ 90.00

R-Factor (%): 4.30 **Temperature(K):** 295 **Density(g/cm³):** 1.518



HQOXDO01

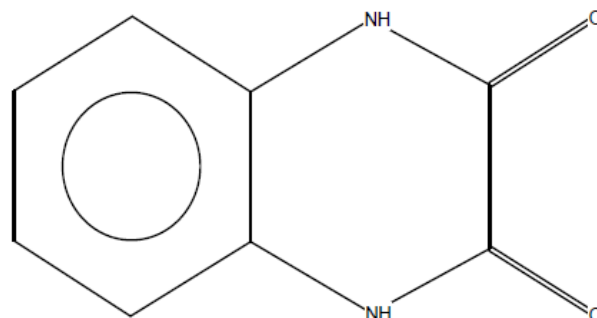
Reference: M.C.Munoz, R.Ruiz, M.Triannidis, A.Aukauloo, Y.Jourmaux, I.Fernandez, J.R.Pedro (1999) *CSD Communication(Private Communication)* ,

Formula: C₈ H₈ N₂ O₂

Compound Name: 1,4-Dihydro-2,3-quinoxalinedione

Space Group: P21/n **Cell:** a 8.072(1) b 4.280(2) c 20.920(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 100.39(1) γ 90.00

R-Factor (%): 4.50 **Temperature(K):** 295 **Density(g/cm³):** 1.515



HQOXD002

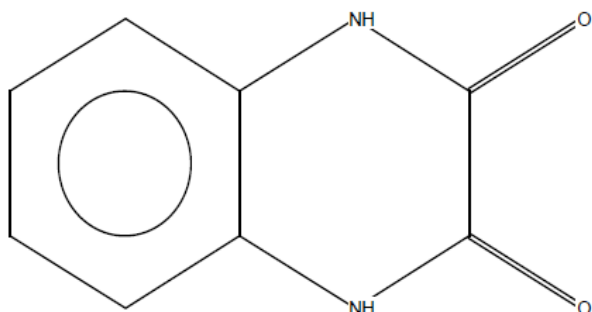
Reference: Fang-Fang Jian, Pu-Su Zhao (2004) *J.Mol.Struct.* ,705,133

Formula: C₈ H₈ N₂ O₂

Compound Name: 1,4-Dihydro-2,3-quinoxalinedione

Synonym: 2,3-Diketobenzopiperazine

Space Group: P2₁/c **Cell:** **a** 8.050(1) **b** 4.286(0) **c** 20.995(6)
Space Group No.: 14 **(Å,°)** α 90.00 β 102.14(3) γ 90.00
R-Factor (%): 6.23 **Temperature(K):** 293 **Density(g/cm³):** 1.521



HQOXD003

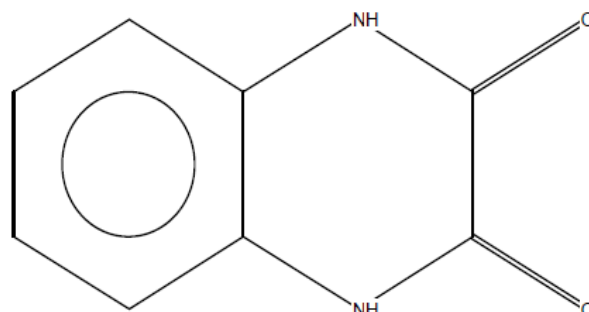
Reference: P.S.Zhao, F.F.Jian, H.L.Xiao, P.P.Sun (2004) *Pol.J.Chem.* ,78,1935

Formula: C₈ H₈ N₂ O₂

Compound Name: 1,4-Dihydro-2,3-quinoxalinedione

Synonym: 2,3-Diketobenzopiperazine

Space Group: P2₁/c **Cell:** **a** 8.050(1) **b** 4.286(0) **c** 20.995(6)
Space Group No.: 14 **(Å,°)** α 90.00 β 102.14(3) γ 90.00
R-Factor (%): 6.23 **Temperature(K):** 293 **Density(g/cm³):** 1.521



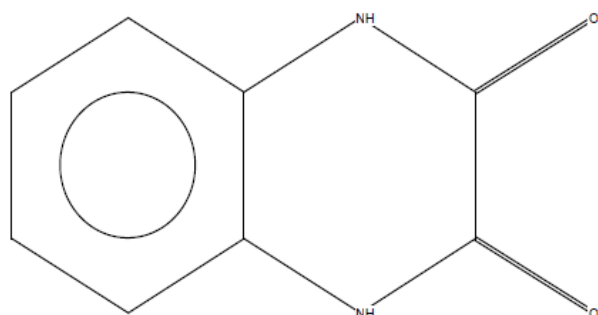
HQOXD004

Reference: S.M.Soliman, J.Albering, M.A.M.Abu-Youssef (2013) *J.Mol.Struct.* ,1053,48

Formula: C₈ H₈ N₂ O₂

Compound Name: 1,4-Dihydroquinoxaline-2,3-dione

Space Group: P2₁/n **Cell:** **a** 8.062(0) **b** 4.217(0) **c** 20.789(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 100.36(0) γ 90.00
R-Factor (%): 3.48 **Temperature(K):** 100 **Density(g/cm³):** 1.549



KIZKOU

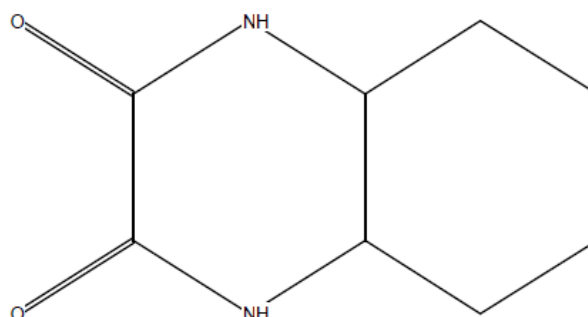
Reference: B.Piotrkowska, M.Myslinska, M.Gdaniec, A.Herman, T.Polonski (2008) *J.Org.Chem.* ,73,2852

Formula: C₈ H₁₂ N₂ O₂

Compound Name: (R,R)-2,3-Decahydrobenzopyrazinodione

Synonym: (R,R)-Octahydroquinoxaline-2,3-dione

Space Group: P4₃2₁2 **Cell:** **a** 6.609(0) **b** 6.609(0) **c** 18.834(1)
Space Group No.: 96 **(Å,°)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 3.67 **Temperature(K):** 293 **Density(g/cm³):** 1.358



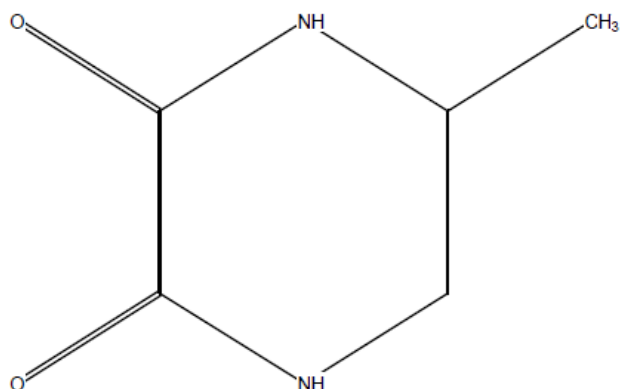
KIZKUA

Reference: B.Piotrkowska, M.Myslinska, M.Gdaniec, A.Herman, T.Polonski (2008) *J.Org.Chem.*, **73**,2852

Formula: C₅ H₈ N₂ O₂

Compound Name: (R)-5-Methylpiperazine-2,3-dione

Space Group: P43212 **Cell:** **a** 6.981(0) **b** 6.981(0) **c** 24.202(0)
Space Group No.: 96 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 2.82 **Temperature(K)**: 293 **Density(g/cm³)**: 1.443



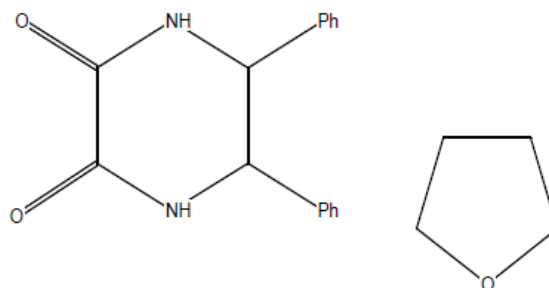
KIZLIP

Reference: B.Piotrkowska, M.Myslinska, M.Gdaniec, A.Herman, T.Polonski (2008) *J.Org.Chem.*, **73**,2852

Formula: C₁₈ H₁₄ N₂ O₂·C₄ H₈ O₁

Compound Name: (5S,6S)-5,6-Diphenylpiperazine-2,3-dione tetrahydrofuran solvate

Space Group: P2221 **Cell:** **a** 12.405(2) **b** 6.906(1) **c** 11.003(1)
Space Group No.: 17 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 5.90 **Temperature(K)**: 200 **Density(g/cm³)**: 1.192



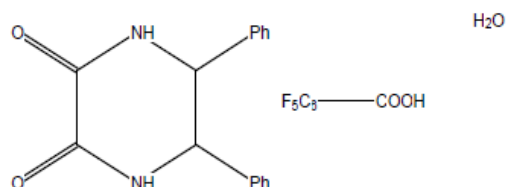
KIZLOV

Reference: B.Piotrkowska, M.Myslinska, M.Gdaniec, A.Herman, T.Polonski (2008) *J.Org.Chem.*, **73**,2852

Formula: C₁₈ H₁₄ N₂ O₂·2(C₇ H₅ F₅ O₂)·H₂ O₁

Compound Name: (5S,6S)-5,6-Diphenylpiperazine-2,3-dione bis(pentafluorobenzoic acid) monohydrate

Space Group: P21 **Cell:** **a** 14.500(1) **b** 5.948(0) **c** 16.791(1)
Space Group No.: 4 **(Å,°)** **α** 90.00 **β** 94.63(0) **γ** 90.00
R-Factor (%): 2.97 **Temperature(K)**: 100 **Density(g/cm³)**: 1.630



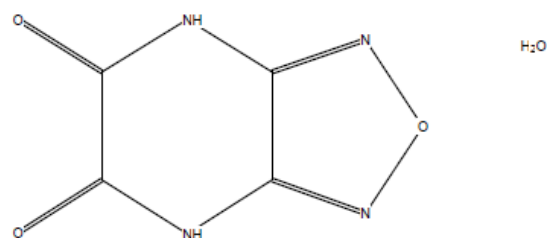
LIPWEP

Reference: Qi Sun, Xin Li, Qiuhan Lin, Ming Lu (2018) *Org.Biomol.Chem.*, **16**,8034

Formula: 3(C₄ H₂ N₄ O₃)·2(H₂ O₁)

Compound Name: [1,2,5]oxadiazolo[3,4-b]pyrazine-5,6(4H,7H)-dione dihydrate

Space Group: P21/c **Cell:** **a** 19.279(1) **b** 5.473(0) **c** 19.468(1)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 111.92(0) **γ** 90.00
R-Factor (%): 4.68 **Temperature(K)**: 173 **Density(g/cm³)**: 1.737



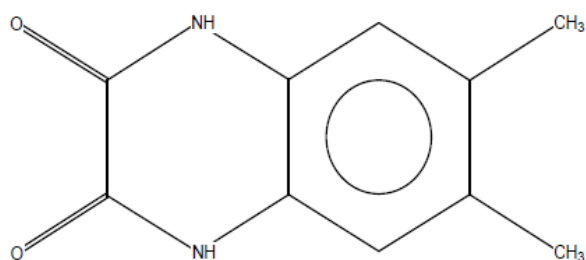
OCUSOU

Reference: R.T.Stibrany, J.A.Potenza, H.J.Schugar (2001) *CSD Communication(Private Communication)*,

Formula: C₁₀ H₁₀ N₂ O₂

Compound Name: 6,7-Dimethyl-1,4-dihydro-2,3-quinoxalinedione

Space Group: P21/c **Cell:** **a** 8.914(1) **b** 8.588(1) **c** 12.349(1)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 92.39(0) **γ** 90.00
R-Factor (%): 3.44 **Temperature(K)**: 294 **Density(g/cm³)**: 1.338



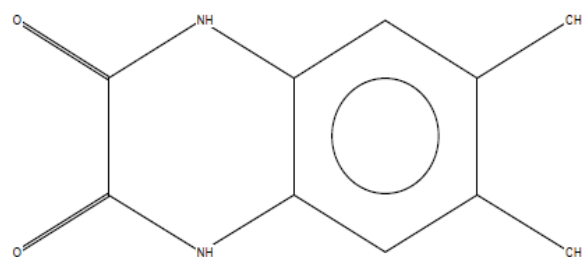
OCUSOU01

Reference: C.Mukhopadhyay, S.Ghosh, R.J.Butcher (2010) *ARKIVOC*, **11**,75-9

Formula: C₁₀ H₁₀ N₂ O₂

Compound Name: 6,7-Dimethyl-1,4-dihydroquinoxaline-2,3-dione

Space Group: P21/c **Cell:** **a** 8.814(0) **b** 8.737(0) **c** 12.099(0)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 93.77(0) **γ** 90.00
R-Factor (%): 4.33 **Temperature(K)**: 110 **Density(g/cm³)**: 1.359



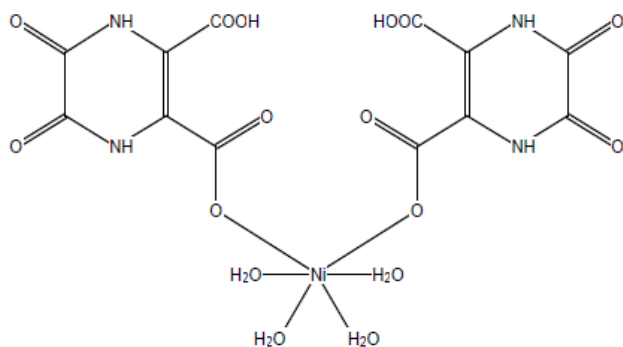
OGERUN

Reference: Cai-Ming Liu, De-Qing Zhang, An-Jun Qin, Chen Ye, Huai-Ming Hu, Dao-Ben Zhu (2002) *Eur.J.Inorg.Chem.* ,1595

Formula: C₁₂ H₁₄ N₄ Ni₁ O₁₈

Compound Name: bis(2,3-Dioxo-1,4-dihydropyrazine-5,6-dicarboxylato)-tetra-aqua-nickel(ii)

Space Group: C2/c **Cell:** a 17.858(4) b 11.098(2) c 9.869(2)
Space Group No.: 15 **(Å,°)** α 90.00 β 119.87(3) γ 90.00
R-Factor (%): 4.41 **Temperature(K):** 293 **Density(g/cm³):** 2.072



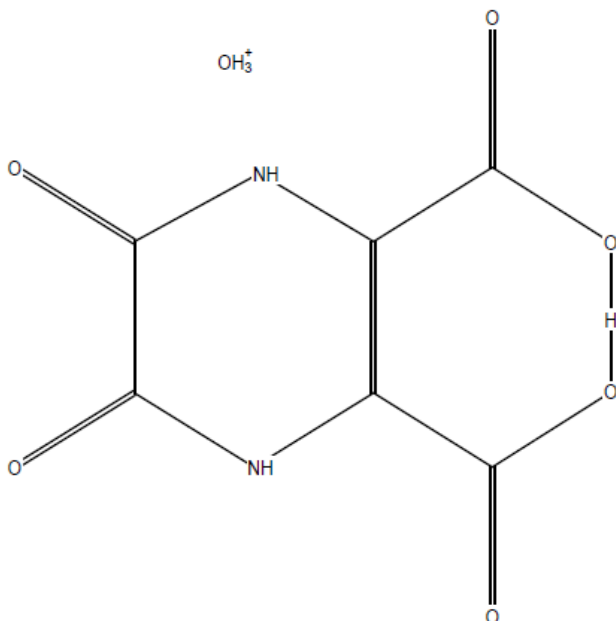
OGESAU

Reference: Cai-Ming Liu, De-Qing Zhang, An-Jun Qin, Chen Ye, Huai-Ming Hu, Dao-Ben Zhu (2002) *Eur.J.Inorg.Chem.* ,1595

Formula: C₈ H₃ N₂ O₈¹⁻ · H₃ O₁¹⁺

Compound Name: oxonium 2,3-dioxo-1,4-dihydropyrazine-5-carboxylate-6-carboxylic acid

Space Group: C2/m **Cell:** a 8.893(1) b 18.176(4) c 5.035(1)
Space Group No.: 12 **(Å,°)** α 90.00 β 96.65(3) γ 90.00
R-Factor (%): 5.10 **Temperature(K):** 293 **Density(g/cm³):** 1.792



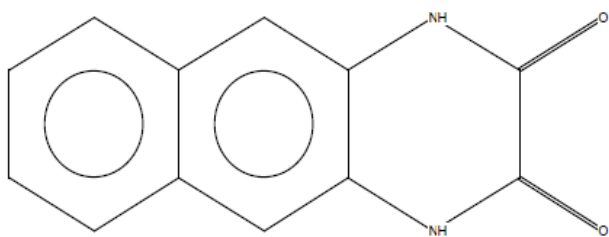
PECYON

Reference: F.Eya'ane Meva, D.Schaarschmidt, M.A.Abdulmalic, T.Ruffer (2012) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,68,o3460

Formula: C₁₂ H₈ N₂ O₂

Compound Name: 1,4-Dihydrobenzo[g]quinoxaline-2,3-dione

Space Group: P21/n **Cell:** a 7.133(1) b 8.423(1) c 15.292(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 99.79(1) γ 90.00
R-Factor (%): 9.38 **Temperature(K):** 293 **Density(g/cm³):** 1.557



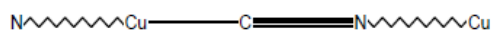
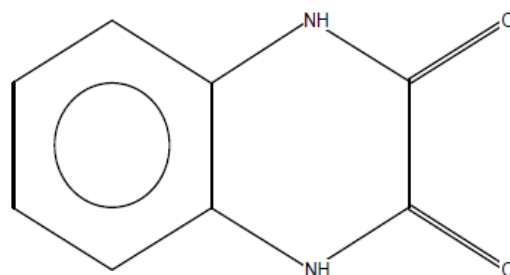
QERCOF

Reference: M.Heller, W.S.Sheldrick (2001) *Z.Anorg.Allg.Chem.* ,627, 569

Formula: (C₈ H₆ N₂ O₂)_n · n(C₁ Cu₁ N₁)

Compound Name: catena-[(μ₂-Cyano-C,N)-copper(i) 1,2,3,4-tetrahydroquinoxaline-2,3-dione]

Space Group: P21/n **Cell:** a 12.447(3) b 4.843(1) c 15.820(3)
Space Group No.: 14 **(Å,°)** α 90.00 β 97.94(3) γ 90.00
R-Factor (%): 5.61 **Temperature(K):** 295 **Density(g/cm³):** 1.770



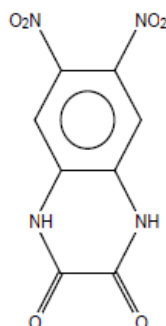
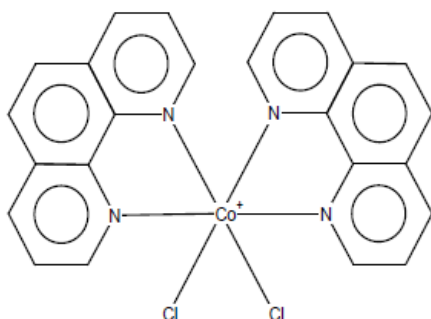
QODCAO

Reference: Ming Yu, Hai Lin, Huakuan Lin (2008) *Supramol. Chem.*, **20**,309

Formula: $C_{24}H_{16}Cl_2Co_1N_4^{1+}, C_8H_4N_4O_6, Cl_1^{-1}, H_2O_1$

Compound Name: Dichloro-bis(1,10-phenanthroline)-cobalt(III) 6,7-dinitroquinoxaline-2,3-dione chloride monohydrate

Space Group: P-1 **Cell:** **a** 8.126(3) **b** 10.093(4) **c** 19.651(7)
Space Group No.: 2 **(Å,°)** α 93.67(0) β 99.23(0) γ 92.24(0)
R-Factor (%): 7.44 **Temperature(K):** 294 **Density(g/cm³):** 1.667



Cl⁻

H₂O

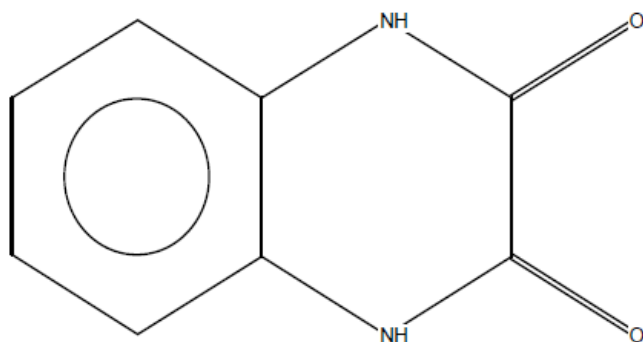
RAVFEA

Reference: N.S.Oxtoby, A.J.Blake, N.R.Champness, C.Wilson (2005) *Chem.-Eur.J.*, **11**,4643

Formula: $C_8H_8N_2O_2, 2(H_2O_1)$

Compound Name: 1,4-Dihydroquinoxaline-2,3-dione dihydrate

Space Group: P-1 **Cell:** **a** 7.024(0) **b** 7.728(0) **c** 8.805(0)
Space Group No.: 2 **(Å,°)** α 85.62(0) β 78.44(0) γ 76.03(0)
R-Factor (%): 4.76 **Temperature(K):** 150 **Density(g/cm³):** 1.449



H₂O

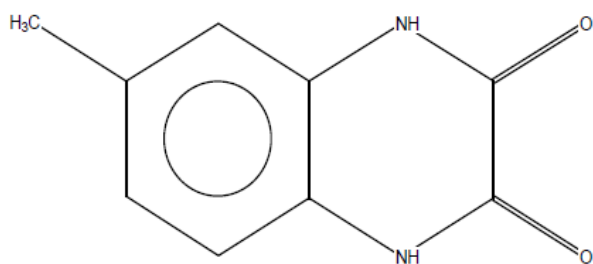
RAVFIE

Reference: N.S.Oxtoby, A.J.Blake, N.R.Champness, C.Wilson (2005) *Chem.-Eur.J.*, **11**,4643

Formula: $C_9H_8N_2O_2, 0.5(H_2O_1)$

Compound Name: 6-Methyl-1,4-dihydroquinoxaline-2,3-dione hemihydrate

Space Group: P-1 **Cell:** **a** 4.362(3) **b** 12.833(10) **c** 16.034(12)
Space Group No.: 2 **(Å,°)** α 70.39(1) β 88.89(1) γ 87.70(1)
R-Factor (%): 8.31 **Temperature(K):** 150 **Density(g/cm³):** 1.456



H₂O

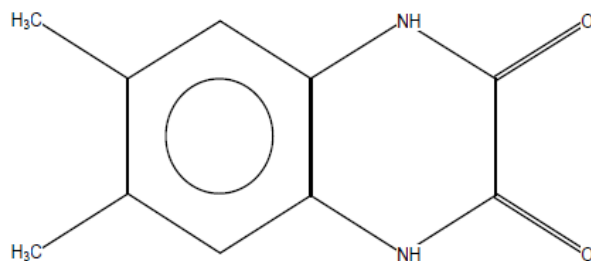
RAVFOK

Reference: N.S.Oxtoby, A.J.Blake, N.R.Champness, C.Wilson (2005) *Chem.-Eur.J.*, **11**,4643

Formula: $C_{10}H_{10}N_2O_2, 6(H_2O_1)$

Compound Name: 6,7-Dimethyl-1,4-dihydroquinoxaline-2,3-dione hexahydrate

Space Group: P21/n **Cell:** **a** 6.810(0) **b** 19.604(2) **c** 11.761(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 104.47(0) γ 90.00
R-Factor (%): 4.19 **Temperature(K):** 150 **Density(g/cm³):** 1.303



H₂O

RAVFOK01

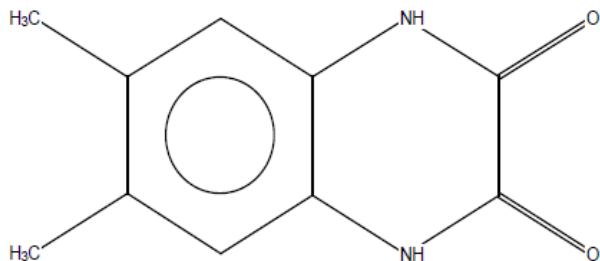
Reference: N.S.Oxtoby, A.J.Blake, N.R.Champness, C.Wilson (2005)
Chem.-Eur.J., **11**,4643

Formula: C₁₀ H₁₀ N₂ O₂·6(H₂ O)₁

Compound Name: 6,7-Dimethyl-1,4-dihydroquinoxaline-2,3-dione hexahydrate

Space Group: P2₁/n **Cell:** *a* 6.789(0) *b* 19.617(2) *c* 11.739(1)
Space Group No.: 14 **Cell:** (*A*,°) *α* 90.00 *β* 104.30(0) *γ* 90.00

R-Factor (%): 3.56 **Temperature(K):** 90 **Density(g/cm³):** 1.308



H₂O

RAVFUQ

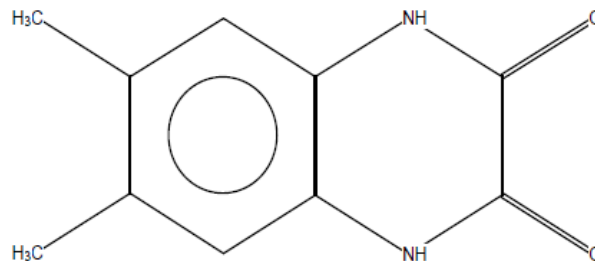
Reference: N.S.Oxtoby, A.J.Blake, N.R.Champness, C.Wilson (2005)
Chem.-Eur.J., **11**,4643

Formula: 3(C₁₀ H₁₀ N₂ O₂)·H₂ O₁

Compound Name: 6,7-Dimethyl-1,4-dihydroquinoxaline-2,3-dione monohydrate

Space Group: P-1 **Cell:** *a* 9.359(2) *b* 10.049(2) *c* 16.360(3)
Space Group No.: 2 **Cell:** (*A*,°) *α* 99.27(0) *β* 98.17(0) *γ* 110.01(0)

R-Factor (%): 8.53 **Temperature(K):** 150 **Density(g/cm³):** 1.402



H₂O

RAVGAX

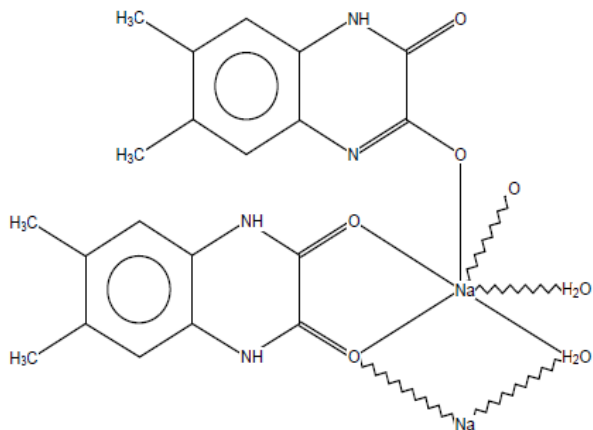
Reference: N.S.Oxtoby, A.J.Blake, N.R.Champness, C.Wilson (2005)
Chem.-Eur.J., **11**,4643

Formula: (C₂₀ H₂₁ N₄ Na₁ O₅)_n

Compound Name: catena-((μ₂-6,7-Dimethyl-1,4-dihydroquinoxaline-2,3-dione)-(μ₂-aqua)-(6,7-dimethyl-4H-quinoxaline-3-one-2-onato)-sodium)

Space Group: R-3 **Cell:** *a* 34.530(6) *b* 34.530(6) *c* 8.600(3)
Space Group No.: 148 **Cell:** (*A*,°) *α* 90.00 *β* 90.00 *γ* 120.00

R-Factor (%): 4.21 **Temperature(K):** 150 **Density(g/cm³):** 1.415



RAVGAX01

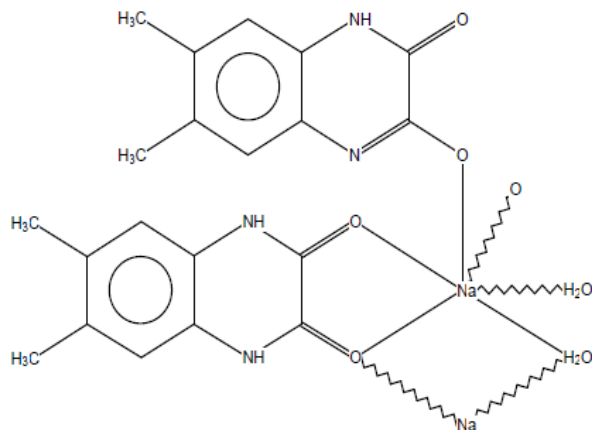
Reference: N.S.Oxtoby, A.J.Blake, N.R.Champness, C.Wilson (2005)
Chem.-Eur.J., **11**,4643

Formula: (C₂₀ H₂₁ N₄ Na₁ O₅)_n

Compound Name: catena-((μ₂-6,7-Dimethyl-1,4-dihydroquinoxaline-2,3-dione)-(μ₂-aqua)-(6,7-dimethyl-4H-quinoxaline-3-one-2-onato)-sodium)

Space Group: R-3 **Cell:** *a* 34.631(3) *b* 34.631(3) *c* 8.629(0)
Space Group No.: 148 **Cell:** (*A*,°) *α* 90.00 *β* 90.00 *γ* 120.00

R-Factor (%): 4.27 **Temperature(K):** 298 **Density(g/cm³):** 1.402



RAVGEB

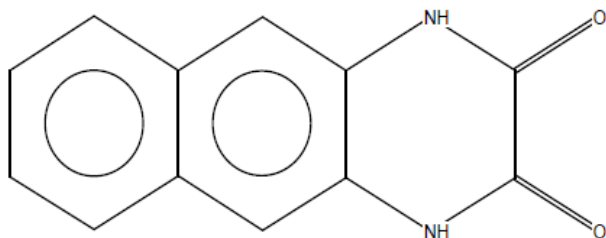
Reference: N.S.Oxtoby, A.J.Blake, N.R.Champness, C.Wilson (2005) *Chem.-Eur.J.*, **11**,4643

Formula: C₁₂H₈N₂O₂·2(H₂O)

Compound Name: 1,4-Dihydrobenzo(g)quinoxaline-2,3-dione trihydrate

Space Group: P2₁/c **Cell:** *a* 7.164(1) *b* 20.084(3) *c* 8.516(1)
Space Group No.: 14 **Cell:** *α* 90.00 *β* 92.34(0) *γ* 90.00

R-Factor (%): 4.34 **Temperature(K):** 150 **Density(g/cm³):** 1.445



H₂O

SAJWOP

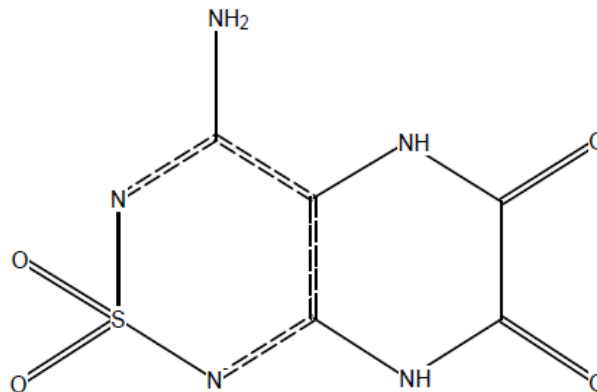
Reference: J.Elguero, P.Goya, J.A.Paez, C.Foces-Foces, F.H.Cano, M.Martinez-Ripoll (1988) *J.Mol.Struct.*, **172**,423

Formula: C₅H₄N₅O₄S₁¹⁻·H₃O₁¹⁺·2(H₂O)

Compound Name: Oxonium 4-amino-6,7-dioxo-5,6,7,8-tetrahydropyrazino(2,3-c)-1,2,6-thiadiazine-2,2-dioxide dihydrate

Space Group: P-1 **Cell:** *a* 9.342(0) *b* 9.407(0) *c* 7.334(0)
Space Group No.: 2 **Cell:** *α* 115.73(0) *β* 78.81(0) *γ* 110.41(0)

R-Factor (%): 4.50 **Temperature(K):** 295 **Density(g/cm³):** 1.743



OH₃⁺ H₂O

SATCUL

Reference: A.T.H.Lenstra, B.Bracke, B.van Dijk, S.Maes, C.Vanhulle, H.O.Desseyn (1998) *Acta Crystallogr., Sect.B: Struct.Sci.*, **54**,851

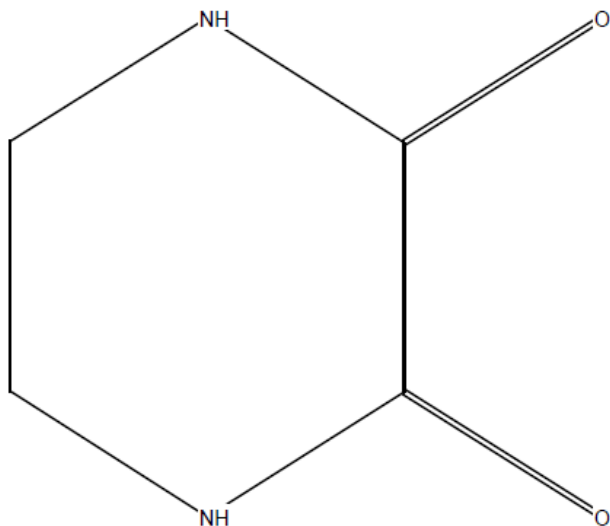
Formula: C₄H₈N₂O₂

Compound Name: 2,3-Piperazinedione

Synonym: 2,3-Diketopiperazine

Space Group: P2₁/c **Cell:** *a* 5.941(3) *b* 10.080(3) *c* 8.282(2)
Space Group No.: 14 **Cell:** *α* 90.00 *β* 95.87(3) *γ* 90.00

R-Factor (%): 3.40 **Temperature(K):** 295 **Density(g/cm³):** 1.536



SUHHEI

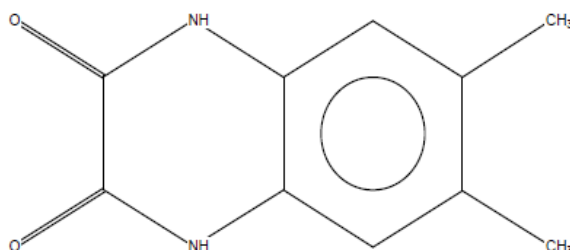
Reference: M.Kubicki, P.W.Codding (1993) *Can.J.Chem.*, **71**,68

Formula: C₁₀H₁₀N₂O₂·2(H₂O)

Compound Name: 6,7-Dimethyl-1,4-dihydro-2,3-quinoxalinedione dihydrate

Space Group: P-1 **Cell:** *a* 7.011(0) *b* 8.590(0) *c* 10.789(0)
Space Group No.: 2 **Cell:** *α* 112.70(0) *β* 96.05(0) *γ* 107.59(0)

R-Factor (%): 4.30 **Temperature(K):** 295 **Density(g/cm³):** 1.359



H₂O

SUHHIM

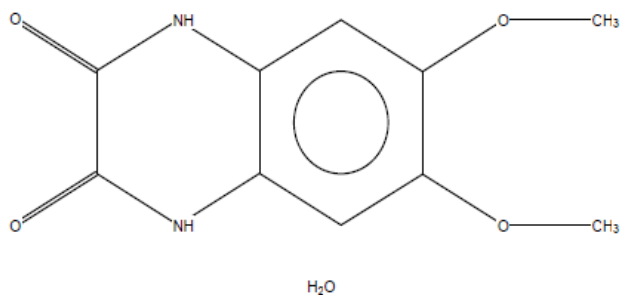
Reference: M.Kubicki, P.W.Codding (1993) *Can.J.Chem.* ,71,68

Formula: C₁₀ H₁₀ N₂ O₄ H₂ O₁

Compound Name: 6,7-Dimethoxy-1,4-dihydro-2,3-quinoxalinedione monohydrate

Space Group: Pbc_a **Cell:** **a** 12.277(0) **b** 6.929(0) **c** 25.864(0)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.60 **Temperature(K):** 295 **Density(g/cm³):** 1.450



TAZZOM

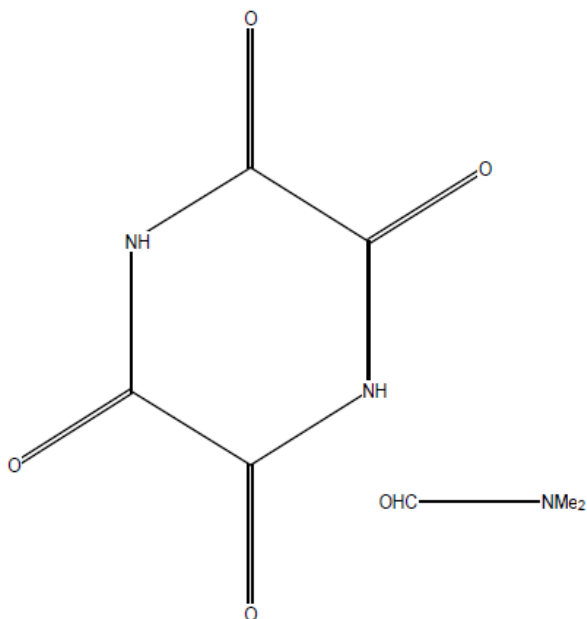
Reference: C.J.Kingsbury, B.F.Abrahams, R.Robson (2017) *CSD Communication(Private Communication)* ,

Formula: C₄ H₂ N₂ O₄ · 2(C₃ H₇ N₁ O₁)

Compound Name: piperazine-2,3,5,6-tetrone N,N-dimethylformamide solvate

Space Group: P2₁/c **Cell:** **a** 5.152(0) **b** 14.668(0) **c** 9.856(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 104.62(0) γ 90.00

R-Factor (%): 7.12 **Temperature(K):** 130 **Density(g/cm³):** 1.328



TASWAL

Reference: J.Ohmori, H.Kubota, M.Shimizu-Sasamata, M.Okada, S.Sakamoto (1996) *J.Med.Chem.* ,39,1331

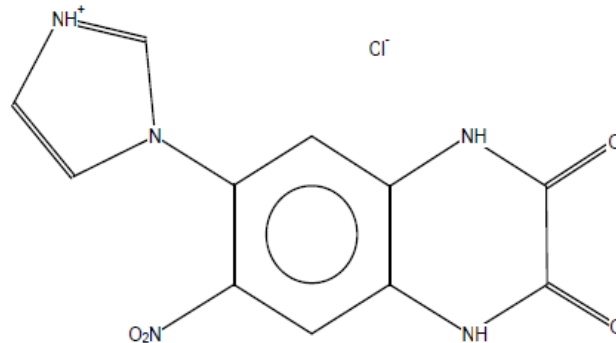
Formula: C₁₁ H₈ N₅ O₄ 1⁺, Cl₁ 1⁻

Compound Name: 6-(1H-Imidazol-1-yl)-7-nitro-2,3-(1H,4H)-quinoxalinedione hydrochloride

Synonym: YMS90K hydrochloride

Space Group: P2₁/n **Cell:** **a** 9.613(1) **b** 9.093(1) **c** 14.154(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 90.20(1) γ 90.00

R-Factor (%): 3.90 **Temperature(K):** 295 **Density(g/cm³):** 1.663



UQUCOZ

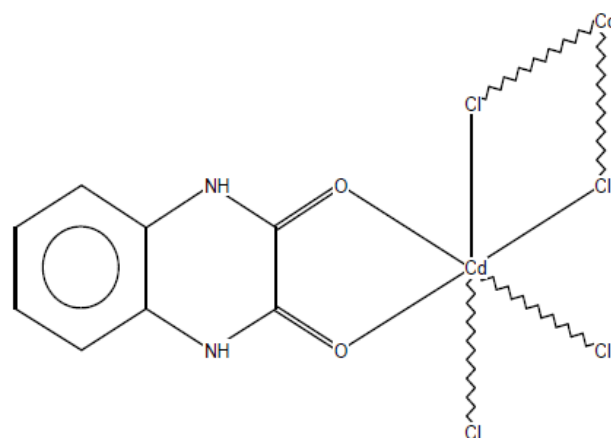
Reference: Ling Shi, Bin Cai, Guang Huang, Jian-Zhong Wu, Ying Yu (2011) *Z.Anorg.Allg.Chem.* ,637,306

Formula: (C₈ H₈ Cd₁ Cl₂ N₂ O₂)_n

Compound Name: catena-(bis(μ₂-Chloro)-(1,4-dihydro-2,3-quinoxalinedione)-cadmium(ii))

Space Group: C2/c **Cell:** **a** 13.079(2) **b** 12.793(2) **c** 7.064(1)
Space Group No.: 15 **(Å,°)** α 90.00 β 119.77(0) γ 90.00

R-Factor (%): 2.40 **Temperature(K):** 293 **Density(g/cm³):** 2.237



WAFHAO

Reference: Jing-Jing Jia, Xiu-Jin Meng, Shi-Zhang Liang, Shu-Hua Zhang, Yi-Min Jiang (2010) *Acta Crystallogr., Sect.E: Struct.Rep. Online* ,66,o3315

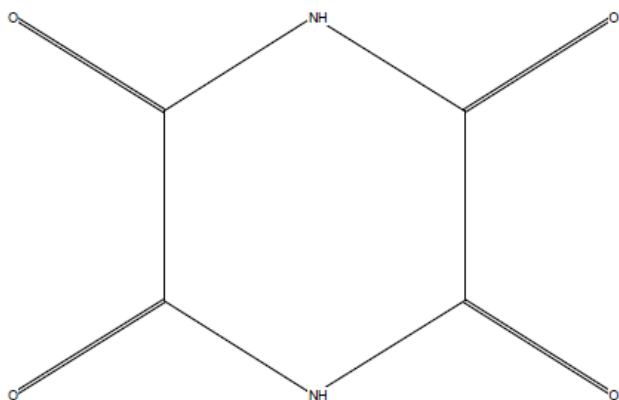
Formula: C₄ H₂ N₂ O₄

Compound Name: Piperazine-2,3,5,6-tetraone

Synonym: Piperazine-2,3,5,6-tetrone

Space Group: P21/n **Cell:** **a** 5.163(1) **b** 8.622(1) **c** 5.654(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 105.25(3) **γ** 90.00

R-Factor (%): 4.77 **Temperature(K):** 293 **Density(g/cm³):** 1.943



WAFHAO01

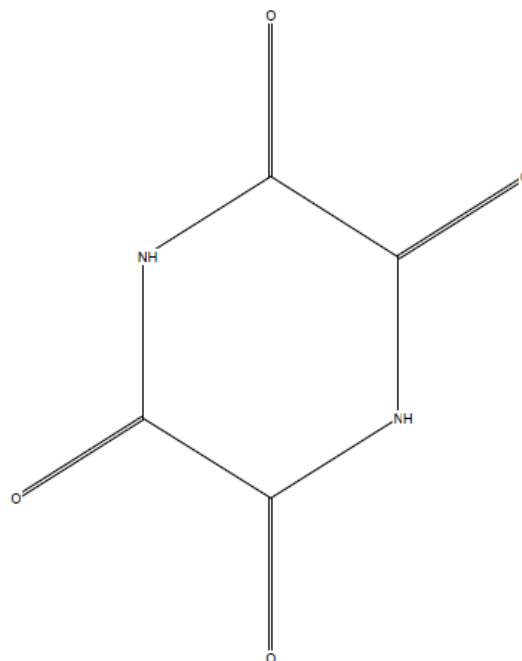
Reference: O.V.Kovalchikova, N.D.Do, A.I.Stash, S.B.Strashnova, B.E.Zaitsev (2014) *Kristallografiya(Russ.)(Crystallogr.Rep.)* ,59,65

Formula: C₄ H₂ N₂ O₄

Compound Name: piperazine-2,3,5,6-tetraone

Space Group: P21/n **Cell:** **a** 5.177(1) **b** 8.625(2) **c** 5.662(1)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 105.22(3) **γ** 90.00

R-Factor (%): 3.08 **Temperature(K):** 293 **Density(g/cm³):** 1.934



ZASGUY

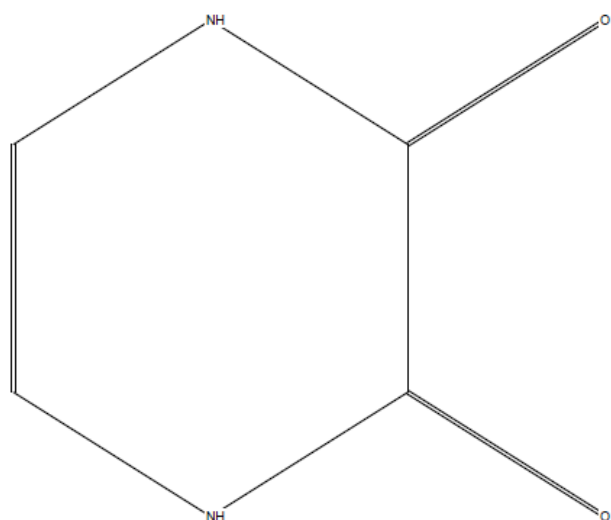
Reference: L.H.Finger, A.Venker, F.G.Schroder, J.Sundermeyer (2017) *Dalton Trans.* ,46,3014

Formula: C₄ H₄ N₂ O₂

Compound Name: 1,4-dihydropyrazine-2,3-dione

Space Group: P21/c **Cell:** **a** 6.111(0) **b** 10.226(0) **c** 6.967(0)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 93.97(0) **γ** 90.00

R-Factor (%): 3.14 **Temperature(K):** 100 **Density(g/cm³):** 1.714



ZILROB

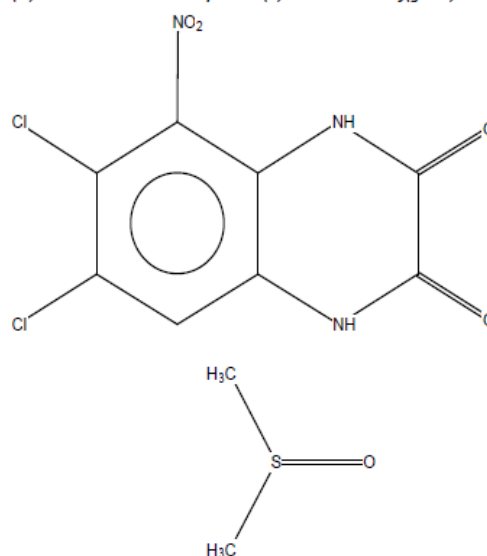
Reference: J.F.W.Keana, S.M.Kher, Sui Xiong Cai, C.M.Dinsmore, A.G.Glenn, J.Guastella, Jin-Cheng Huang, V.Jlyin, Yixin Lu, P.L.Mouser, R.L.Woodward, E.Weber (1995) *J.Med.Chem.* ,38,4367

Formula: C₈ H₃ Cl₂ N₃ O₄ · C₂ H₆ O₁ S₁

Compound Name: 6,7-Dichloro-1,4-dihydro-5-nitroquinoxaline-2,3-dione dimethylsulfoxide solvate

Space Group: P21/n **Cell:** **a** 10.349(3) **b** 6.504(1) **c** 21.131(4)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 99.89(2) **γ** 90.00

R-Factor (%): 4.20 **Temperature(K):** 295 **Density(g/cm³):** 1.679



ZILRUH

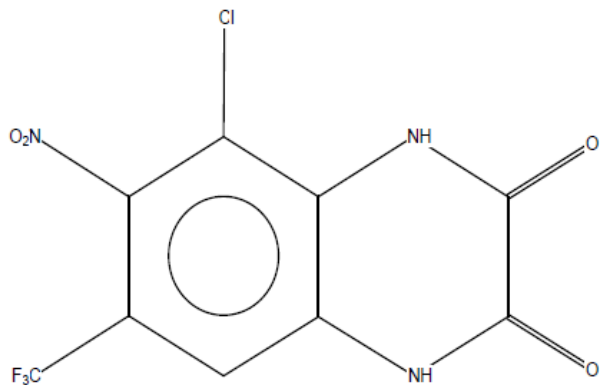
Reference: J.F.W.Keana, S.M.Kher, Sui Xiong Cai, C.M.Dinsmore, A.G.Glenn, J.Guastella, Jin-Cheng Huang, V.Ilyin, Yixin Lu, P.L.Mouser, R.L.Woodward, E.Weber (1995) *J.Med.Chem.*, **38**,4367

Formula: C₉H₃Cl₁F₃N₃O₄H₂O₁

Compound Name: 5-Chloro-1,4-dihydro-6-nitro-7-trifluoromethylquinoxaline-2,3-dione monohydrate

Space Group: P21/c **Cell:** **a** 7.832(2) **b** 11.686(2) **c** 13.315(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 100.26(2) γ 90.00

R-Factor (%): 4.90 **Temperature(K):** 295 **Density(g/cm³):** 1.815



H₂O

ZILSAO

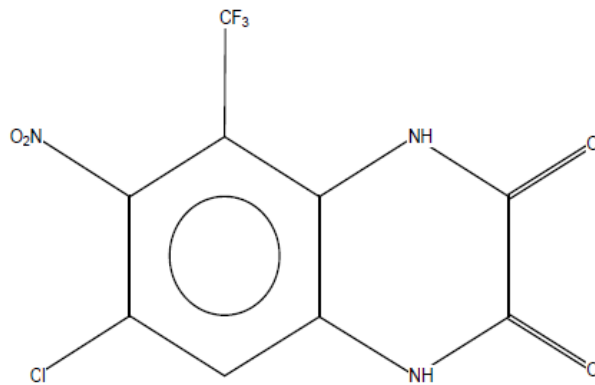
Reference: J.F.W.Keana, S.M.Kher, Sui Xiong Cai, C.M.Dinsmore, A.G.Glenn, J.Guastella, Jin-Cheng Huang, V.Ilyin, Yixin Lu, P.L.Mouser, R.L.Woodward, E.Weber (1995) *J.Med.Chem.*, **38**,4367

Formula: C₉H₃Cl₁F₃N₃O₄H₂O₁

Compound Name: 7-Chloro-1,4-dihydro-6-nitro-5-trifluoromethylquinoxaline-2,3-dione monohydrate

Space Group: P21/n **Cell:** **a** 7.032(2) **b** 19.603(4) **c** 8.719(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.77(2) γ 90.00

R-Factor (%): 5.40 **Temperature(K):** 295 **Density(g/cm³):** 1.823



H₂O