


Supplementary Table S1: Target protein receptor (PDB) results of studied bacteria receptors

Target Bacteria	Target protein receptor (PDB)
<i>Klebsiella pneumoniae</i>	<p>5HFT</p> <p>Crystal structure of HpxW</p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb5HFT/pdb • Classification: TRANSFERASE • Organism(s): <i>Klebsiella pneumoniae</i> subsp. <i>pneumoniae</i> MGH 78578 • Expression System: <i>Escherichia coli</i> • Mutation(s): No • Deposited: 2016-01-07 Released: 2016-06-29 • Deposition Author(s): Ealick, S.E., Hicks, K.A. • Funding Organization(s): National Institutes of Health/National Institute of General Medical Sciences (NIH/NIGMS) <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.65 Å • R-Value Free: 0.298 • R-Value Work: 0.254 • R-Value Observed: 0.257 <p>Biochemical and structural characterization of <i>Klebsiella pneumoniae</i> oxamate amidohydrolase in the uric acid degradation pathway. Hicks, K.A., Ealick, S.E.</p> <p>(2016) <i>Acta Crystallogr D Struct Biol</i> 72: 808-816</p> <ul style="list-style-type: none"> • PubMed: 27303801 Search on PubMedSearch on PubMed Central • DOI: https://doi.org/10.1107/S2059798316007099 

4HWM

Crystal structure of a lipoprotein YedD (KPN_02420) from *Klebsiella pneumoniae* subsp. *pneumoniae* MGH 78578 at 1.38 Å resolution

- **PDB DOI:** <https://doi.org/10.2210/pdb4HWM/pdb>
- **Classification:** **STRUCTURAL GENOMICS, UNKNOWN FUNCTION**
- **Organism(s):** *Klebsiella pneumoniae* subsp. *pneumoniae* MGH 78578
- **Expression System:** *Escherichia coli*
- **Mutation(s):** No
- **Deposited:** 2012-11-08 **Released:** 2013-01-02
- **Deposition Author(s):** Joint Center for Structural Genomics (JCSG)

Experimental Data Snapshot


- **Method:** X-RAY DIFFRACTION
- **Resolution:** 1.38 Å
- **R-Value Free:** 0.179
- **R-Value Work:** 0.149
- **R-Value Observed:** 0.151

Crystal structure of a lipoprotein YedD (KPN_02420) from *Klebsiella pneumoniae* subsp. *pneumoniae* MGH 78578 at 1.38 Å resolution

Joint Center for Structural Genomics (JCSG)

To be published.



<i>Pseudomonas aeruginos</i>	<p>4F1R</p> <p>Structure analysis of the global metabolic regulator Crc from <i>Pseudomonas aeruginos</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb4F1R/pdb • Classification: TRANSCRIPTION REGULATOR • Organism(s): <i>Pseudomonas aeruginosa</i> • Expression System: <i>Escherichia coli</i> • Mutation(s): No • Deposited: 2012-05-07 Released: 2013-02-06 • Deposition Author(s): Zhang, H., Wei, Y., Gao, Z.Q., Dong, Y.H. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.20 Å • R-Value Free: 0.246 • R-Value Work: 0.202 • R-Value Observed: 0.204 <p>Structure analysis of the global metabolic regulator Crc from <i>Pseudomonas aeruginosa</i>.</p> <p>Wei, Y., Zhang, H., Gao, Z.Q., Xu, J.H., Liu, Q.S., Dong, Y.H.</p> <p>(2013) <i>IUBMB Life</i> 65: 50-57</p> <ul style="list-style-type: none"> • PubMed: 23281037 Search on PubMed • DOI: https://doi.org/10.1002/iub.1103 
<i>Staphylococcus aureus</i>	<p>1DUA</p> <p>CRYSTAL STRUCTURE OF EXFOLIATIVE TOXIN A</p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1DUA/pdb • Classification: TOXIN, HYDROLASE • Organism(s): <i>Staphylococcus aureus</i> • Expression System: <i>Escherichia coli</i> • Mutation(s): No • Deposited: 2000-01-17 Released: 2003-01-21 • Deposition Author(s): Papageorgiou, A.C., Plano, L.R.W., Collins, C.M., Acharya, K.R. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.00 Å • R-Value Free: 0.252

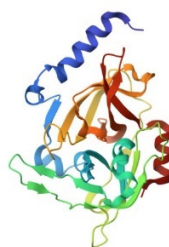
- **R-Value Work:** 0.214
- **R-Value Observed:** 0.214

Structural similarities and differences in Staphylococcus aureus exfoliative toxins A and B as revealed by their crystal structures.

Papageorgiou, A.C., Plano, L.R., Collins, C.M., Acharya, K.R.

(2000) Protein Sci **9**: 610-618

- **PubMed:** **10752623** Search on PubMedSearch on PubMed Central
- **DOI:** <https://doi.org/10.1110/ps.9.3.610>



1DUE

CRYSTAL STRUCTURE OF EXFOLIATIVE TOXIN A S195A MUTANT

- **PDB DOI:** <https://doi.org/10.2210/pdb1DUE/pdb>
- **Classification:** **TOXIN, HYDROLASE**
- **Organism(s):** Staphylococcus aureus
- **Expression System:** Escherichia coli
- **Mutation(s):** Yes
- **Deposited:** 2000-01-17 **Released:** 2003-01-21
- **Deposition Author(s):** Papageorgiou, A.C., Plano, L.R.W., Collins, C.M., Acharya, K.R.

Experimental Data Snapshot

- **Method:** X-RAY DIFFRACTION
- **Resolution:** 2.00 Å
- **R-Value Free:** 0.238
- **R-Value Work:** 0.214
- **R-Value Observed:** 0.214

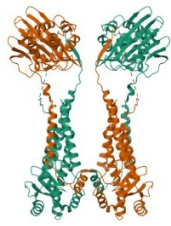
Structural similarities and differences in Staphylococcus aureus exfoliative Toxins A and B as revealed by their crystal structures

Papageorgiou, A.C., Plano, L.R., Collins, C.M., Acharya, K.R.

(2000) Protein Sci **9**: 610-618

- **PubMed:** **10752623** Search on PubMedSearch on PubMed Central
- **DOI:** <https://doi.org/10.1110/ps.9.3.610>



	<p>8EXP</p> <p>Cryo-EM structure of <i>S. aureus</i> BlaR1 with C2 symmetry</p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb8EXP/pdb • EM Map EMD-28658: EMDB EMDataResource <ol style="list-style-type: none"> 1. Classification: SIGNALING PROTEIN 2. Organism(s): <i>Staphylococcus aureus</i> 3. Expression System: <i>Lactobacillus delbrueckii</i> subsp. <i>lactis</i> 4. Mutation(s): No 5. Membrane Protein: Yes OPMPDBTM 6. Deposited: 2022-10-25 Released: 2023-01-11 7. Deposition Author(s): Worrall, L.J., Alexander, J.A.N., Vuckovic, M., Strynadka, N.C.J. 8. Funding Organization(s): Canadian Institutes of Health Research (CIHR) <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: ELECTRON MICROSCOPY • Resolution: 4.20 Å • Aggregation State: PARTICLE • Reconstruction Method: SINGLE PARTICLE <p>Structural basis of broad-spectrum beta-lactam resistance in <i>Staphylococcus aureus</i>. Alexander, J.A.N., Worrall, L.J., Hu, J., Vuckovic, M., Satishkumar, N., Poon, R., Sobhanifar, S., Rosell, F.I., Jenkins, J., Chiang, D., Mosimann, W.A., Chambers, H.F., Paetzel, M., Chatterjee, S.S., Strynadka, N.C.J.</p> <p>(2023) <i>Nature</i> 613: 375-382</p> <ul style="list-style-type: none"> • PubMed: 36599987 Search on PubMedSearch on PubMed Central • DOI: https://doi.org/10.1038/s41586-022-05583-3 
<p><i>30S prokaryotic ribosoma (binding unit of antibiotic)</i></p>	<p>3OS3</p> <p>Mitogen-activated protein kinase kinase 1 (MEK1) in complex with CH4858061 and MgATP</p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb3OS3/pdb • Classification: TRANSFERASE/TRANSFERASE INHIBITOR • Organism(s): <i>Homo sapiens</i> • Expression System: <i>Escherichia coli</i> • Mutation(s): No • Deposited: 2010-09-08 Released: 2011-07-27

- **Deposition Author(s):** Lukacs, C.M., Janson, C., Schuck, V., Belunis, C.

Experimental Data Snapshot

- **Method:** X-RAY DIFFRACTION
- **Resolution:** 2.80 Å
- **R-Value Free:** 0.356
- **R-Value Work:** 0.268

Design and synthesis of novel allosteric MEK inhibitor CH4987655 as an orally available anticancer agent.

Isshiki, Y., Kohchi, Y., Iikura, H., Matsubara, Y., Asoh, K., Murata, T., Kohchi, M., Mizuguchi, E., Tsujii, S., Hattori, K., Miura, T., Yoshimura, Y., Aida, S., Miwa, M., Saitoh, R., Murao, N., Okabe, H., Belunis, C., Janson, C., Lukacs, C., Schuck, V., Shimma, N.

(2011) Bioorg Med Chem Lett **21**: 1795-1801

- **PubMed:** **21316218** Search on PubMed
- **DOI:** <https://doi.org/10.1016/j.bmcl.2011.01.062>



Supplementary Table S2: The chemical structure from PubChem CID results of GSE Components.

	Name	The chemical structure from PubChem CID:
1.	Stigmastan-3,5-diene	<p>Compound CID: 525918</p> <p>MF: C₂₉H₄₈</p> <p>MW: 396.7g/mol</p> <p>IUPAC Name: 17-(5-ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,7,8,9,11,12,14,15,16,17-decahydro-1H-cyclopenta[a]phenanthrene</p> <p>Isomeric</p> <p>SMILES: <chem>CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC=C4)C)C(C)C</chem></p> <p>InChIKey: ICCTZARHLGPHMT-UHFFFAOYSA-N</p> <p>InChI: InChI=1S/C29H48/c1-7-22(20(2)3)12-11-21(4)25-15-16-26-24-14-13-23-10-8-9-18-28(23,5)27(24)17-19-29(25,26)6/h8,10,13,20-22,24-27H,7,9,11-12,14-19H2,1-6H3</p> <p>Create Date: 2005-03-27</p>
2.	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	<p>Compound CID: 5284421</p> <p>MF: C₁₉H₃₄O₂</p> <p>MW: 294.5g/mol</p> <p>IUPAC Name: methyl (9Z,12Z)-octadeca-9,12-dienoate</p> <p>Isomeric SMILES: <chem>CCCC/C=C\C/C=C\CCCCCCCC(=O)OC</chem></p> <p>InChIKey: WTTJVINHCBCLGX-NQLNTRKDSA-N</p> <p>InChI: InChI=1S/C19H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h7-8,10-11H,3-6,9,12-18H2,1-2H3/b8-7-,11-10-</p> <p>Create Date: 2005-03-27</p>
3.	Oleamide	<p>Compound CID: 5283387</p> <p>MF: C₁₈H₃₅NO</p> <p>MW: 281.5g/mol</p> <p>IUPAC Name: (Z)-octadec-9-enamide</p> <p>Isomeric SMILES: <chem>CCCCCCCC/C=C\CCCCCCCC(=O)N</chem></p> <p>InChIKey: FATBGEAMYMYZAF-KTKRTIGZSA-N</p> <p>InChI: InChI=1S/C18H35NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h9-10H,2-8,11-17H2,1H3,(H2,19,20)/b10-9-</p> <p>Create Date: 2005-03-27</p>
4.	Hexadecanamide	<p>Compound CID: 69421</p> <p>MF: C₁₆H₃₃NO</p> <p>MW: 255.44g/mol</p> <p>IUPAC Name: hexadecanamide</p> <p>Isomeric SMILES: <chem>CCCCCCCCCCCCCCCC(=O)N</chem></p> <p>InChIKey: HSEMFIZWXHQJAE-UHFFFAOYSA-N</p> <p>InChI: InChI=1S/C16H33NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h2-15H2,1H3,(H2,17,18)</p> <p>Create Date: 2005-03-26</p>
5.	Phosphoric acid, trimethyl ester	<p>Compound CID: 10541</p> <p>MF: C₃H₉O₄P</p> <p>MW: 140.07g/mol</p> <p>IUPAC Name: trimethyl phosphate</p> <p>Isomeric SMILES: <chem>COP(=O)(OC)OC</chem></p> <p>InChIKey: WVLBCYQITXONBZ-UHFFFAOYSA-N</p>

		InChI: InChI=1S/C3H9O4P/c1-5-8(4,6-2)7-3/h1-3H3 Create Date: 2005-03-26
6.	Dodecyl acrylate	Compound CID: 75084 MF: C ₁₅ H ₂₈ O ₂ MW: 240.38g/mol IUPAC Name: dodecyl prop-2-enoate Isomeric SMILES: CCCCCCCCCCCCCOC(=O)C=C InChIKey: PBOSTUDLECTMNL-UHFFFAOYSA-N InChI: InChI=1S/C15H28O2/c1-3-5-6-7-8-9-10-11-12-13-14-17-15(16)4-2/h4H,2-3,5-14H2,1H3 Create Date: 2005-03-26
7.	Pentanoic acid, 5-hydroxy-, 2,4-di- <i>t</i> -butylphenyl esters	Substance SID: 250069723 Compound CID: 605777 Data Source: NIST Mass Spectrometry Data Center External ID: ZUJLXOZKNAZSJ-UHFFFAOYSA-N Data Source Category: Governmental Organizations; Legacy Depositors Deposit Date: 2015-04-28 Last Modified Date: 2015-04-28
8.	Methyl stearate	Compound CID: 8201 MF: C ₁₉ H ₃₈ O ₂ MW: 298.5g/mol IUPAC Name: methyl octadecanoate Isomeric SMILES: CCCCCCCCCCCCCCCCCC(=O)OC InChIKey: HPEUJPOZXNMSJ-UHFFFAOYSA-N InChI: InChI=1S/C19H38O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h3-18H2,1-2H3 Create Date: 2005-03-26
9.	1-Pentadecyne	Compound CID: 69825 MF: C ₁₅ H ₂₈ MW: 208.38g/mol IUPAC Name: pentadec-1-yne Isomeric SMILES: CCCCCCCCCCCCCC#C InChIKey: DONJGKADZJEXRJ-UHFFFAOYSA-N InChI: InChI=1S/C15H28/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h1H,4-15H2,2H3 Create Date: 2005-03-27
10.	11,13-Dimethyl-12-tetradecen-1-ol acetate	Compound CID: 549821 MF: C ₁₈ H ₃₄ O ₂ MW: 282.5g/mol IUPAC Name: 11,13-dimethyltetradec-12-enyl acetate Isomeric SMILES: CC(CCCCCCCCCCOC(=O)C)C=C(C)C InChIKey: MNUWBCKALSZWEW-UHFFFAOYSA-N InChI: InChI=1S/C18H34O2/c1-16(2)15-17(3)13-11-9-7-5-6-8-10-12-14-20-18(4)19/h15,17H,5-14H2,1-4H3 Create Date: 2005-03-27

11.	4-Methyl-2,4-bis(4'-trimethylsilyloxyphenyl)pentene-1	<p>Compound CID: 610040</p> <p>MF: C₂₄H₃₆O₂Si₂</p> <p>MW: 412.7g/mol</p> <p>IUPAC Name: trimethyl-[4-[2-methyl-4-(4-trimethylsilyloxyphenyl)pent-4-en-2-yl]phenoxy]silane</p> <p>Isomeric</p> <p>SMILES: CC(C)(CC(=C)C1=CC=C(C=C1)O[Si](C)(C)C)C2=CC=C(C=C2)O[Si](C)(C)C</p> <p>InChIKey: YCRIXHKHAODKFH-UHFFFAOYSA-N</p> <p>InChI: InChI=1S/C24H36O2Si2/c1-19(20-10-14-22(15-11-20)25-27(4,5)6)18-24(2,3)21-12-16-23(17-13-21)26-28(7,8)9/h10-17H,1,18H2,2-9H3</p> <p>Create Date: 2005-03-27</p>
12.	1,3-Benzenediol, o-(4-methylbenzoyl)-o'-(2-methoxybenzoyl)-	<p>Compound CID: 91715040</p> <p>MF: C₂₂H₁₈O₅</p> <p>MW: 362.4g/mol</p> <p>IUPAC Name: [3-(4-methylbenzoyl)oxyphenyl] 2-methoxybenzoate</p> <p>Isomeric</p> <p>SMILES: CC1=CC=C(C=C1)C(=O)OC2=CC(=CC=C2)OC(=O)C3=CC=CC=C3OC</p> <p>InChIKey: YKAUQBZMUPNUKE-UHFFFAOYSA-N</p> <p>InChI: InChI=1S/C22H18O5/c1-15-10-12-16(13-11-15)21(23)26-17-6-5-7-18(14-17)27-22(24)19-8-3-4-9-20(19)25-2/h3-14H,1-2H3</p> <p>Create Date: 2015-04-28</p>
13.	Cyclotrisiloxane, hexamethyl-	<p>Compound CID: 10914</p> <p>MF: C₆H₁₈O₃Si₃</p> <p>MW: 222.46g/mol</p> <p>IUPAC Name: 2,2,4,4,6,6-hexamethyl-1,3,5,2,4,6-trioxatrisilinane</p> <p>Isomeric SMILES: C[Si]1(O[Si](O[Si](O1)(C)C)(C)C)C</p> <p>InChIKey: HTDJPCNNEPUOOQ-UHFFFAOYSA-N</p> <p>InChI: InChI=1S/C6H18O3Si3/c1-10(2)7-11(3,4)9-12(5,6)8-10/h1-6H3</p> <p>Create Date: 2005-03-27</p>
14.	Isooctyl 3-mercaptopropionate	<p>Compound CID: 104386</p> <p>MF: C₁₁H₂₂O₂S</p> <p>MW: 218.36g/mol</p> <p>IUPAC Name: 6-methylheptyl 3-sulfanylpropanoate</p> <p>Isomeric SMILES: CC(C)CCCCCOC(=O)CCS</p> <p>InChIKey: ZHUWXKIPGGZJNW-UHFFFAOYSA-N</p> <p>InChI: InChI=1S/C11H22O2S/c1-10(2)6-4-3-5-8-13-11(12)7-9-14/h10,14H,3-9H2,1-2H3</p> <p>Create Date: 2005-03-26</p>
15.	Standard antibiotic (Doxycycline)	<p>Compound CID: 54671203</p> <p>MF: C₂₂H₂₄N₂O₈</p> <p>MW: 444.4g/mol</p> <p>IUPAC Name: (4S,4aR,5S,5aR,6R,12aR)-4-(dimethylamino)-1,5,10,11,12a-pentahydroxy-6-methyl-3,12-dioxo-4a,5,5a,6-tetrahydro-4H-tetracene-2-carboxamide</p>

	<p>Isomeric</p> <p>SMILES: <chem>C[C@@H]1[C@H]2[C@@H]([C@H]3[C@@H](C(=O)C(=C([C@]3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)C(=O)N)N(C)C)O</chem></p> <p>InChIKey: SGKRLCUIYIXIAHR-AKNGSSGZSA-N</p> <p>InChI: InChI=1S/C22H24N2O8/c1-7-8-5-4-6-9(25)11(8)16(26)12-10(7)17(27)14-15(24(2)3)18(28)13(21(23)31)20(30)22(14,32)19(12)29/h4-7,10,14-15,17,25-27,30,32H,1-3H3,(H2,23,31)/t7-,10+,14+,15-,17-,22-/m0/s1</p> <p>Create Date: 2011-12-26</p>
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Supplementary Table S3: Analysis of Phytochemical content and Metals in Grape seed extract using ICP-MS.

Components	Concentrations
Phytochemical	
Tannins (mg/100g TAE)	Not detected
Polyphenols (mg/100g GAE)	125.1
Flavonoids (mg/100g CE)	57.0
Alkaloid (mg/g AE)	22.5
Metals	
Na (µg/g)	21.0
Cr (µg/g)	Not detected
Zn (µg/g)	9.1
K (µg/g)	172.0
Cd (µg/g)	Not detected
Pb (µg/g)	Not detected
Al (µg/g)	Not detected
Ca (µg/g)	27.2
Fe (µg/g)	29.1

Supplementary Table S4. Urine Analysis (Metals).

	N= 100 (Mean±SD)
Na (µg/L)	0.007±0.001
Cr (µg/L)	Not detected
Zn (µg/L)	0.0032±0.002
K (µg/L)	0.0045±0.021
Cd (µg/L)	Not detected
Pb (µg/L)	0.0023±0.031
Al (µg/L)	0.0012±0.021
Ca (µg/L)	0.0029±0.011

Fe (µg/L)	Not detected
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Supplementary Table S5. Urine Analysis (Bacteria) N= 100.

	Positive results	Negative results
<i>Klebsiella pneumoniae</i>	97%	3%
<i>Staphylococcus epidermidis</i>	52%	48%
<i>Pseudomonas aeruginos</i>	23%	77%
<i>Staphylococcus aureus</i>	10%	90%