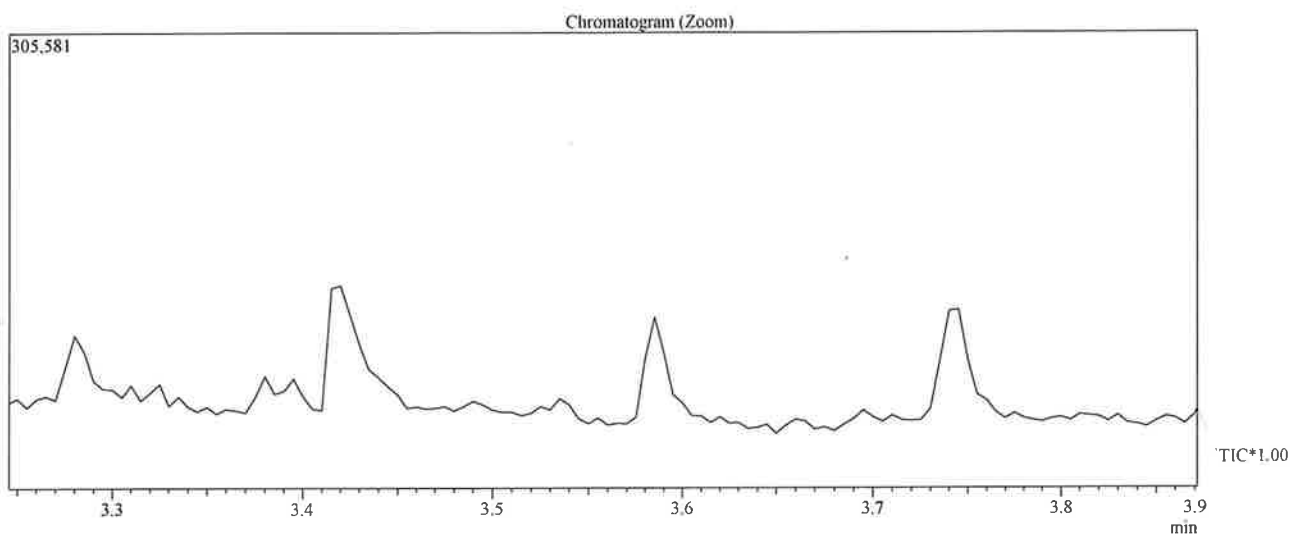
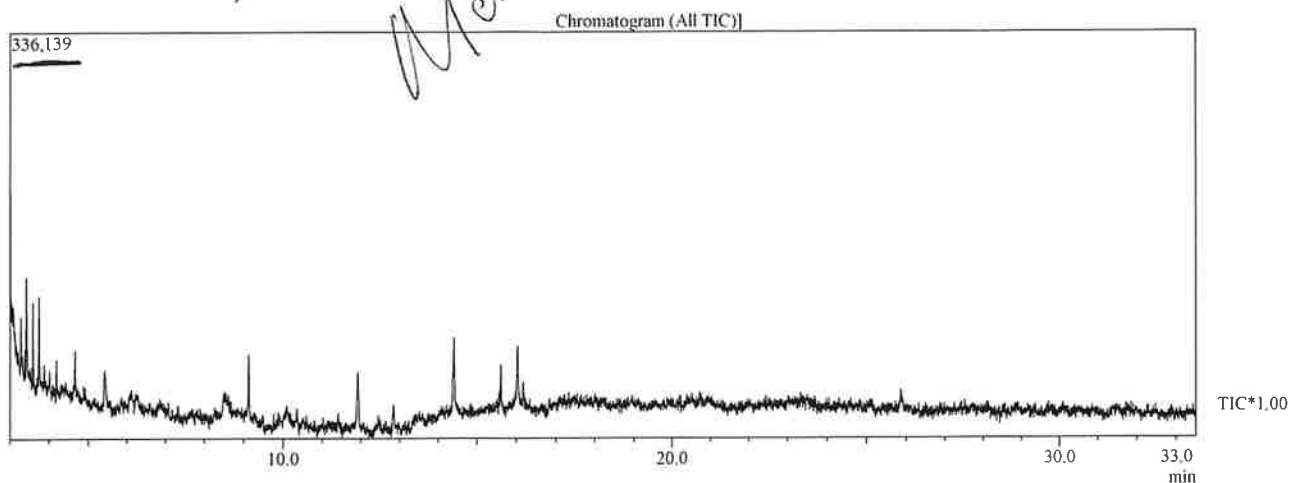


C:\GCMSsolution\Data\Project1\MS Math\SAMPLE 3_UNKNOWN_20221130_3.qgd



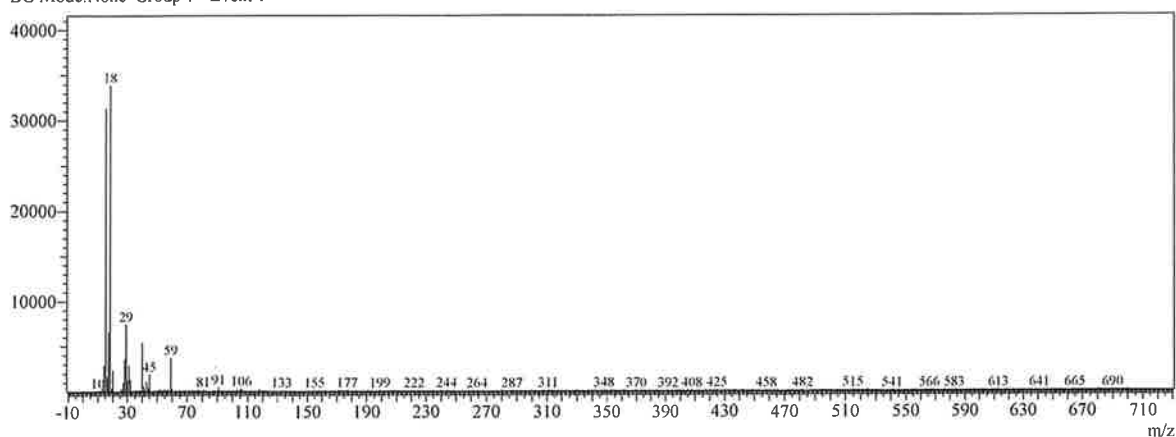
Spectrum

Line#:1 R Time:3.280(Scan#:57)

MassPeaks:598

RawMode:Single 3.280(57) BasePeak:18.10(33884)

BG Mode:None Group 1 - Event 1

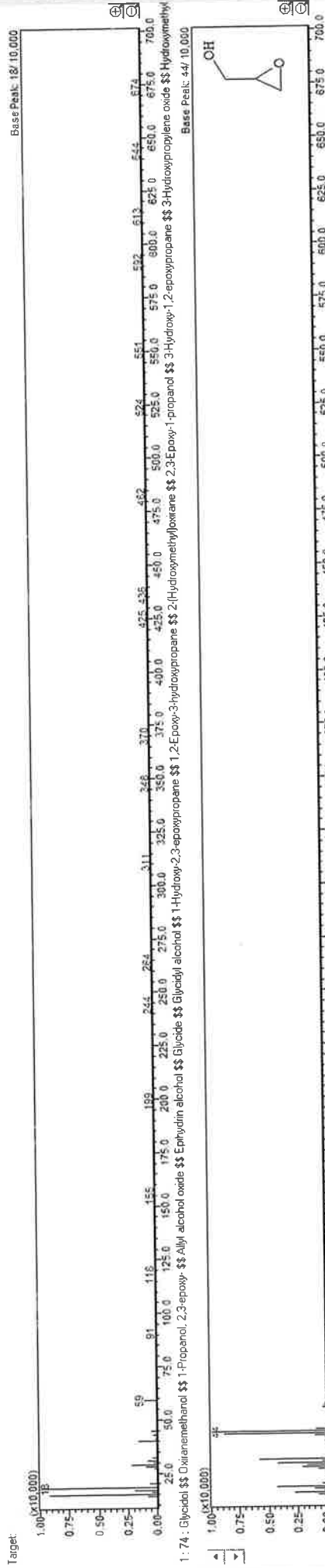


Similarity Search Results

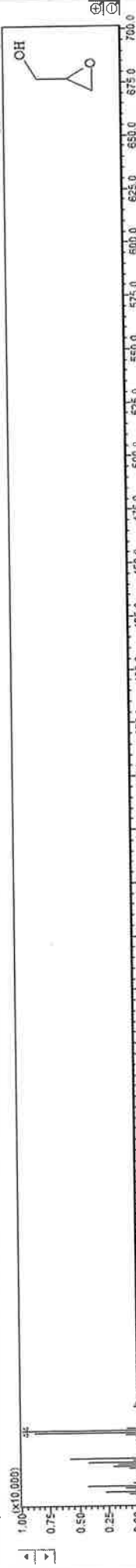
Report View Compound Info Process Help

Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library
1	69	✓	Glycidol SS Oxiranemethanol SS 1-Propanol 2-	74	C3H6O2	NIST08.LIB
2	65		Ethanedioic acid, dimethyl ester SS Oxalic acid	118	C4H6O4	NIST08.LIB
3	67		Carbonic acid, dimethyl ester SS Dimethyl carb	90	C3H6O3	NIST08.LIB
4	67		Ethene, methoxy- SS Ether, methyl vinyl SS Me	58	C3H6O	NIST08.LIB
5	66		Acetonitrile, hydroxy- SS Glycolonitrile SS Cyan	57	C2H3NO	NIST08.LIB
6	66		Ethylene oxide SS Oxirane SS Dioxolane	44	C2H4O	NIST08.LIB
7	65		Ethane, methoxy- SS Ether, ethyl methyl SS Et	60	C3H8O	NIST08.LIB
8	65		Butanoic acid, 4-(2,4,5-trichlorophenoxymethyl)- met	296	C11H11Cl3O3	NIST08.LIB
9	65		Hydrazine, 1,1-dimethyl- SS aS-Dimethylhydraz	60	C2H8N2	NIST08.LIB
10	64		Acetaldoxime SS [E]-CH3CH=NOH SS Acetald	59	C2H5NO	NIST08.LIB
11	64		2-Propanone 1,3-dihydrimov- SS Dihydrimovacet	90	C3H6O3	NIST08.LIB

Target:



1: 74: Glycidol SS Oxiranemethanol SS 1-Propanol, 2,3-epoxy- SS Allyl alcohol oxide SS Epithydrin alcohol SS Glycidol SS Glycidol alcohol SS 1-Hydroxy-2,3-epoxypropane SS 1,2-Epoxy-3-hydroxypropane SS 2-(Hydroxymethyl)oxirane SS 2,3-Epoxy-1-propanol SS 3-Hydroxypropylene oxide SS Hydroxymethyl



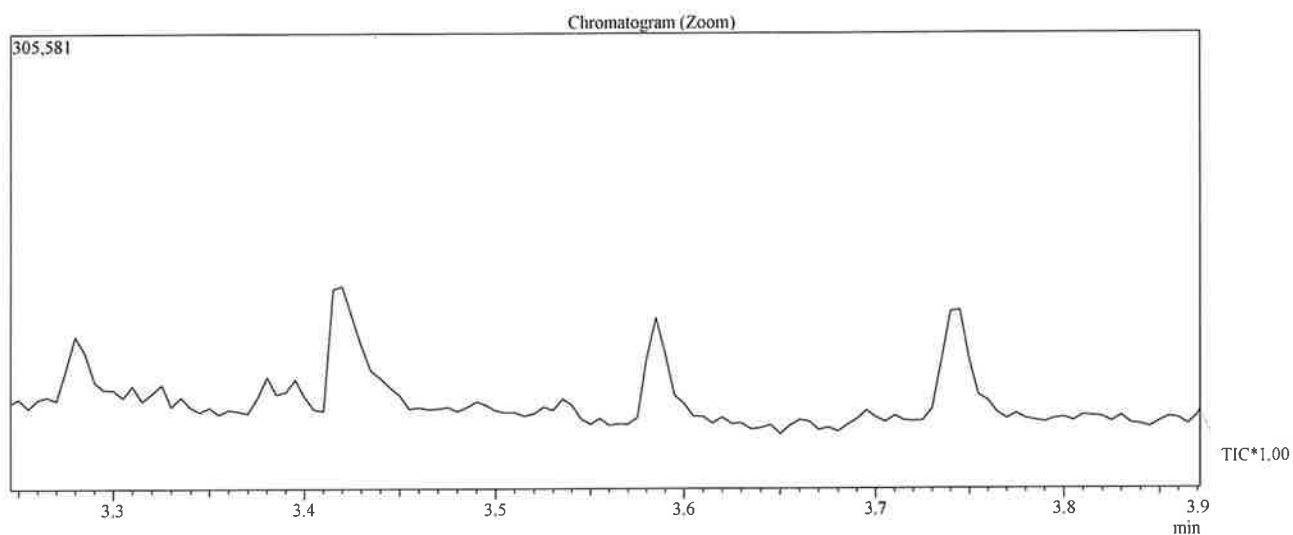
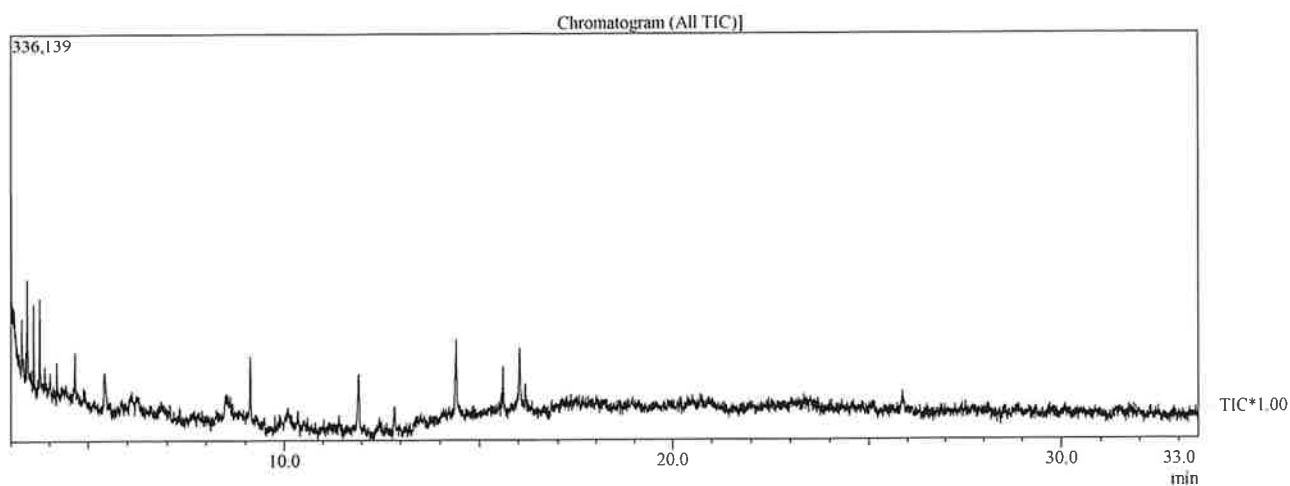
CAS#: 556-52-5 Mol Wt: 74 Serial#: 375

Empd Name: Glycidol SS Oxiranemethanol SS 1-Propanol, 2,3-epoxy- SS Allyl alcohol oxide SS Epithydrin alcohol SS Glycidol SS Glycidol alcohol SS 1-Hydroxy-2,3-epoxypropane SS 1,2-Epoxy-3-hydroxypropane SS 2-(Hydroxymethyl)oxirane SS 2,3-Epoxy-1-propanol SS 3-Hydroxypropylene oxide SS Hydric

Formula: C3H6O2 Class Flag: No Class Flags

Ref Index: 853

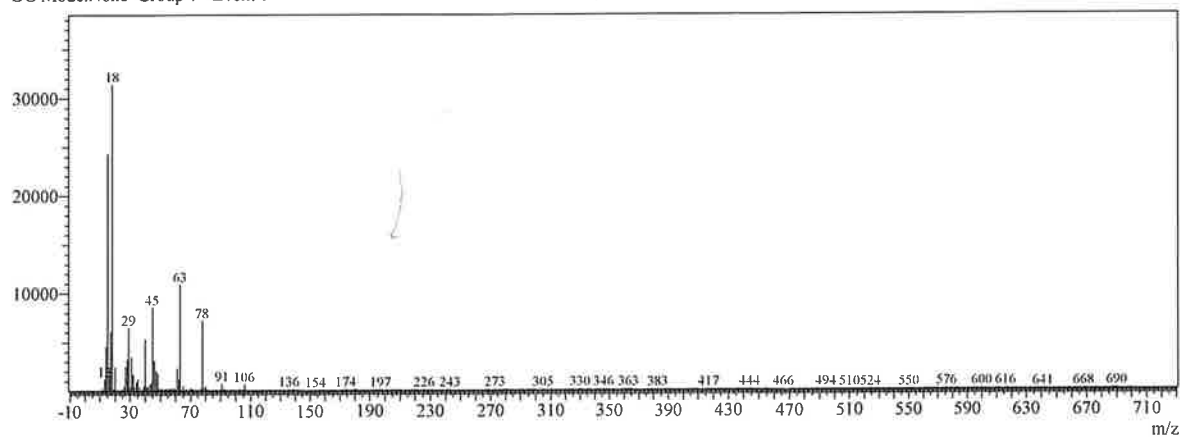
C:\GCMSSolution\Data\Project1\Ms Mathe\SAMPLE 3_UNKNOWN_20221130_3.qgd



Spectrum

Line#:1 R.Time:3.420(Scan#:85)
MassPeaks:579
RawMode:Single 3.420(85) BasePeak:18.10(31369)
BG Mode:None Group 1 - Event 1

91332

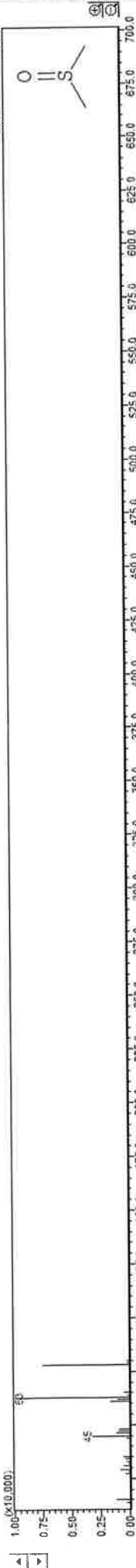
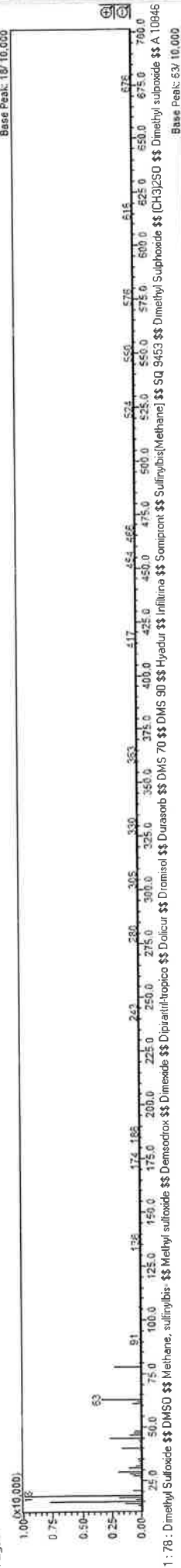


Similarity Search Results

Report View Compound Info Process Help

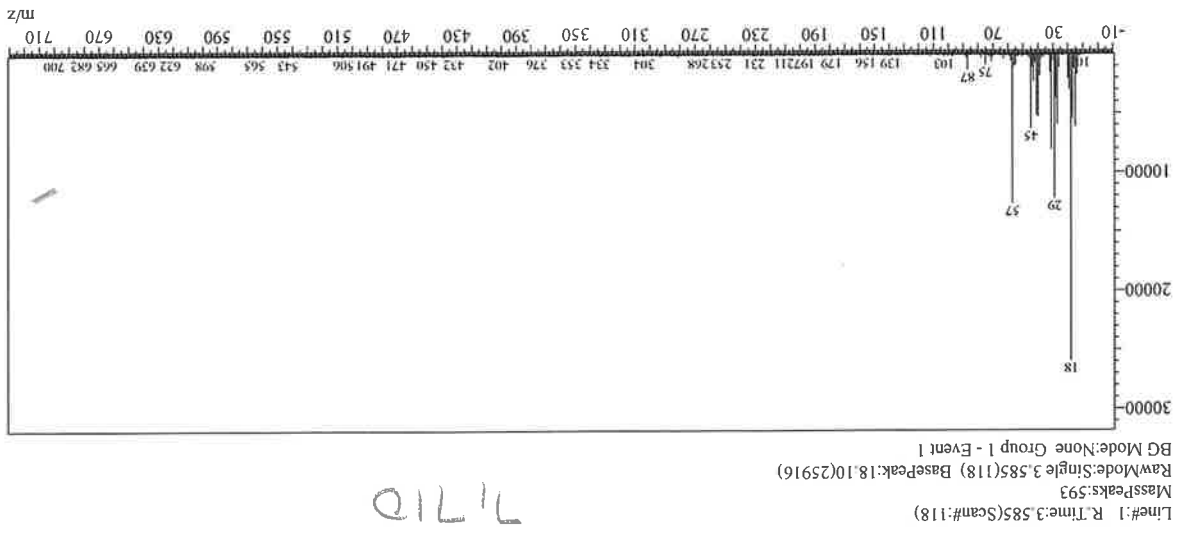
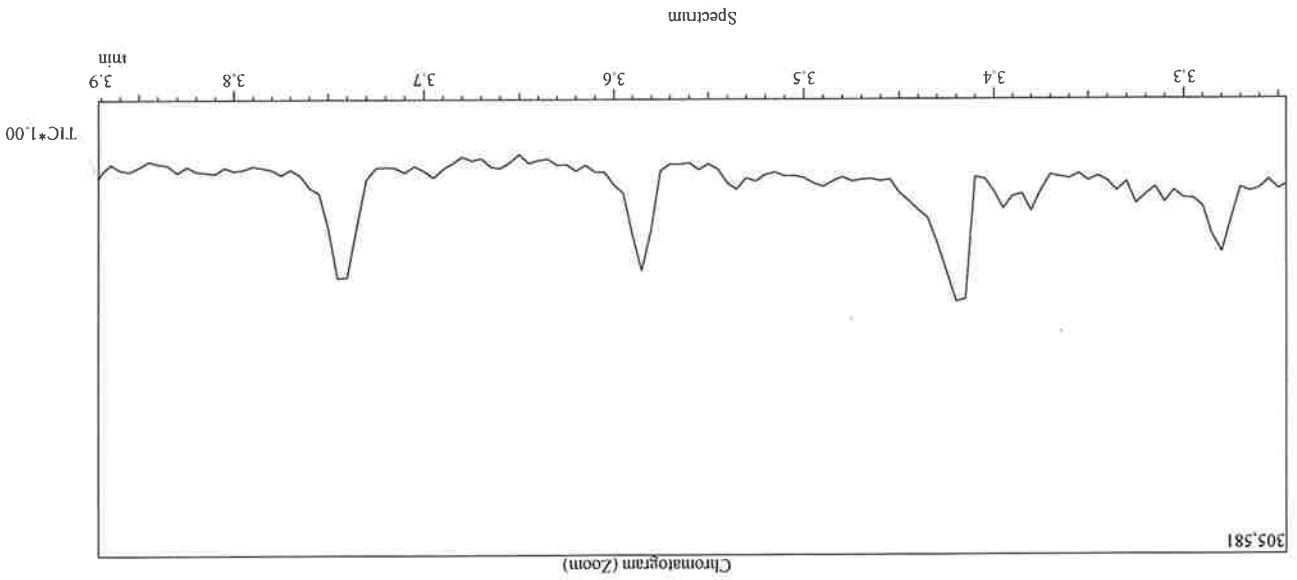
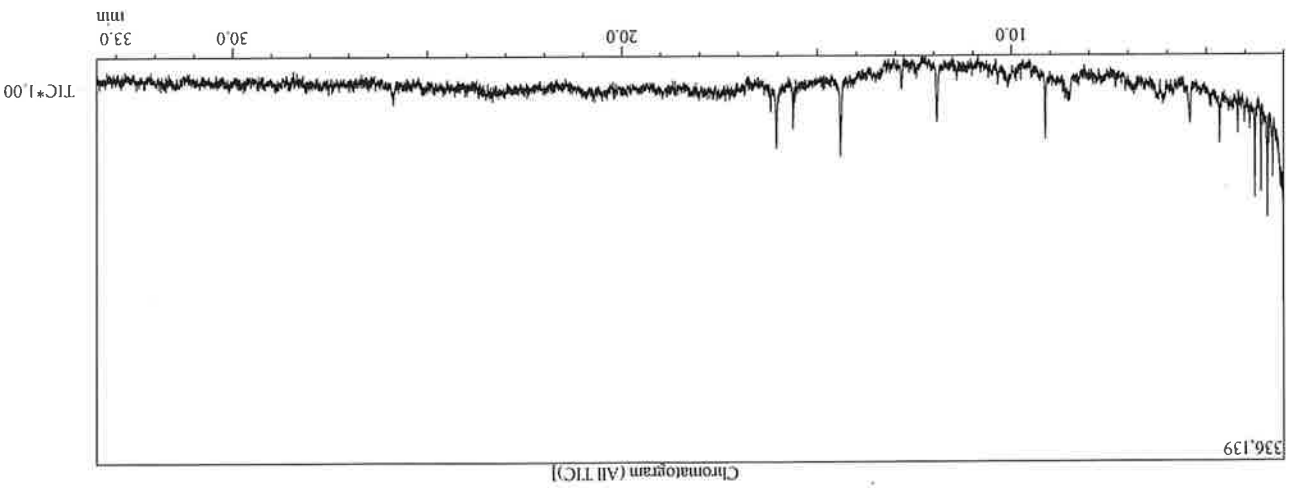
Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library
1	70	✓	Dimethyl Sulfoxide SS DMSO SS Methane sulf	78	C2H6OS	NIST08.LIB
2	66		Carbonic acid, dimethyl ester SS Dimethyl carb	90	C3H8O3	NIST08.LIB
3	66		Dimethoxyamine SS N-Methoxy-O-methylhydro	77	C2H7NO2	NIST08.LIB
4	64		Peroxide, diethyl SS Ethyl peroxide SS Diethyl	90	C4H10O2	NIST08.LIB
5	63		Glycol SS Oxiranemethanol SS 1-Propanol, 2-	74	C3H8O2	NIST08.LIB
6	63		Acetyl chloride SS Ethanol chloride SS Acetic	78	C2H3ClO	NIST08.LIB
7	63		Maltene, chloromethoxy- SS Ether, chloromet	80	C2H5ClO	NIST08.LIB
8	62		Fluoroacetic acid SS Acetic acid, fluoro- SS Cy	78	C2H3FO2	NIST08.LIB
9	62		2-Butanol, 3-chloro-, (R)-, R-7- SS 2-Butanol, 3-c	108	C4H9ClO	NIST08.LIB
10	62		Carbonic acid, ethyl-, methyl ester SS Ethoxy	104	C4H8O3	NIST08.LIB
11	62		2-Methanesulfonamethanol SS 2-Hydroxyethan	124	C2H6O3S	NIST08.LIB

Target:



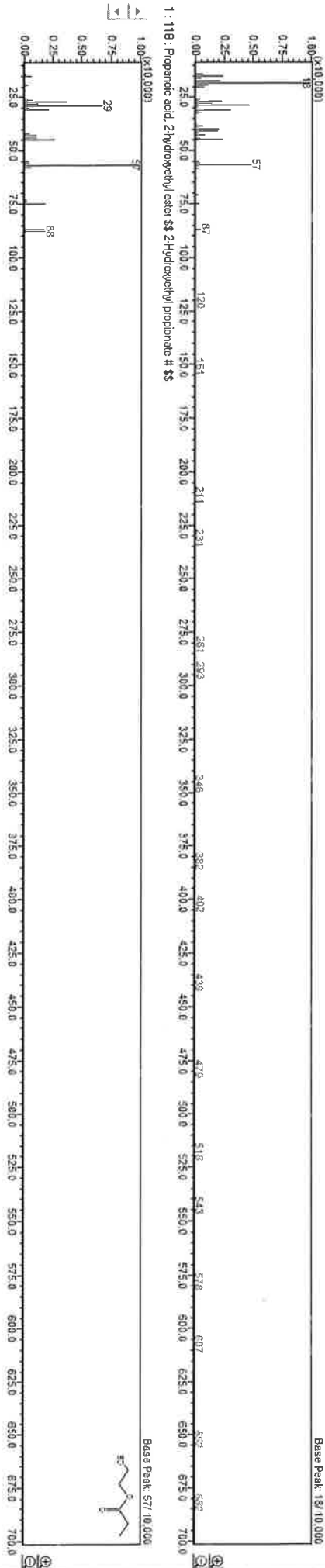
CAS#: 67-68-5 MolWt: 78 Serial#: 468
 Cmpd Name: Dimethyl Sulfoxide SS DMSO SS Methane, sulfinylbis- SS Methyl sulfoxide SS DMSO SS Dimethyl Sulfoxide SS (CH3)2SO SS Dimethyl sulfoxide SS
 Formula: C2H6OS Class Flag: No Class Flags

RefIndex: 691



Hit	Similar	Ref	Compound Name	Mol Wt	Formula	Library
1	76	76	Propenoic acid, 2-hydroxyethyl ester, SS 2-Hydroxyethyl ester SS 2-Hydroxyethyl ester SS 2-Hydroxyethyl ester	118	C5H10O3	NIST08.LIB
2	75	75	Glycidol SS Oxazepam SS 1-Propanol, 2-	74	C3H8O2	NIST08.LIB
3	74	74	Formic acid, 1-methylpropyl ester SS Formic acid	102	C5H10O2	NIST08.LIB
4	74	74	2-Hydroxy-3-pentanone SS 3-Pentanone, 2-hy	102	C5H10O2	NIST08.LIB
5	74	74	Propenoic acid, 2-methylpropyl ester SS Propic	130	C7H14O2	NIST08.LIB
6	74	74	Oxazone, (ethoxymethyl)- SS Ethyl glycidyl ether	102	C5H10O2	NIST08.LIB
7	74	74	Butane, 2,2-dimethyl- SS 2,2-Dimethylbutane	100	C6H14	NIST08.LIB
8	73	73	1,3-Propanediol, 2-hydroxyethyl-2-nitro- SS 1	151	C4H9NO5	NIST08.LIB
9	73	73	Butyl glyoxylate SS Acetic acid, oxo-, butyl est	130	C6H12O3	NIST08.LIB
10	73	73	1,3-Butanediol SS Buta-2-Butylene glycol SS M	98	C4H10O2	NIST08.LIB
11	73	73	1-Hydroxy-2-hydroxy-2-hydroxy-2-hydroxy-1-hydroxy	88	C4H8O7	NIST08.LIB

Target:

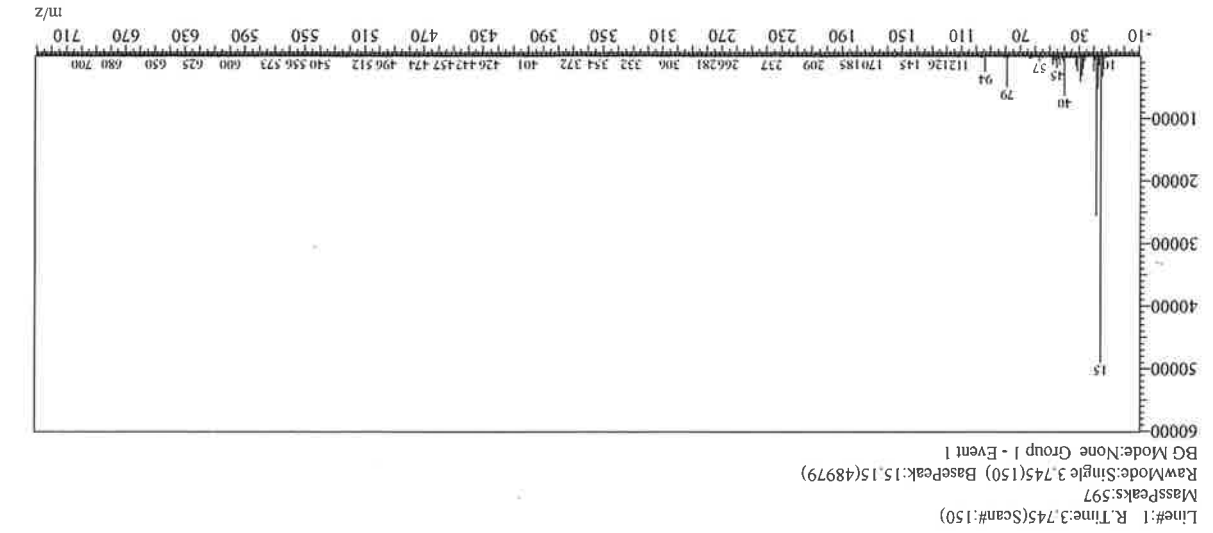
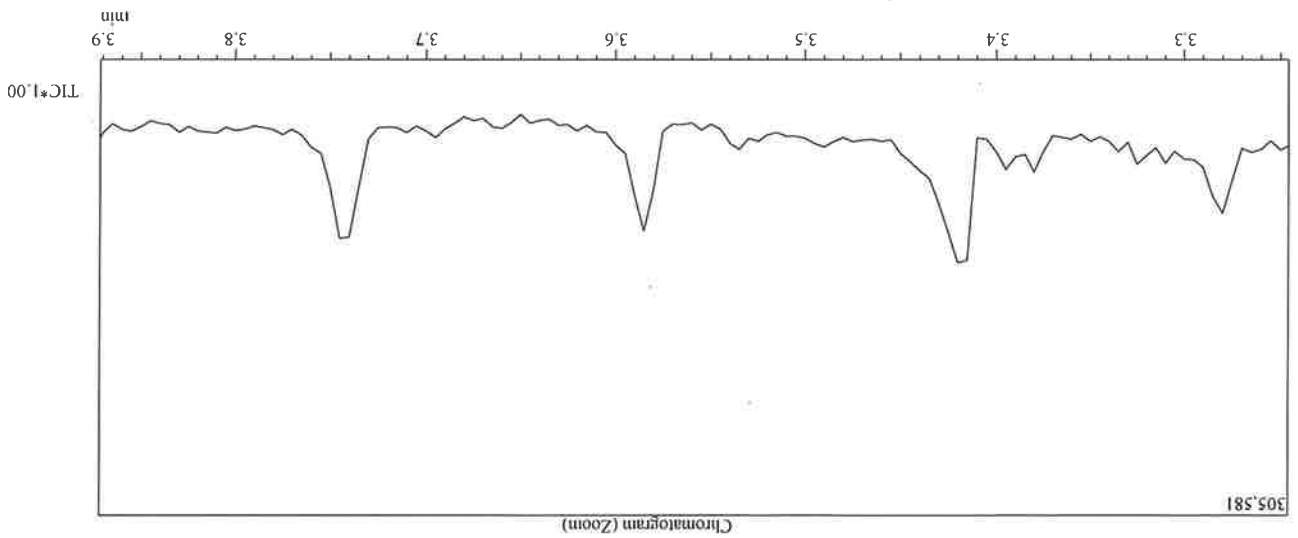
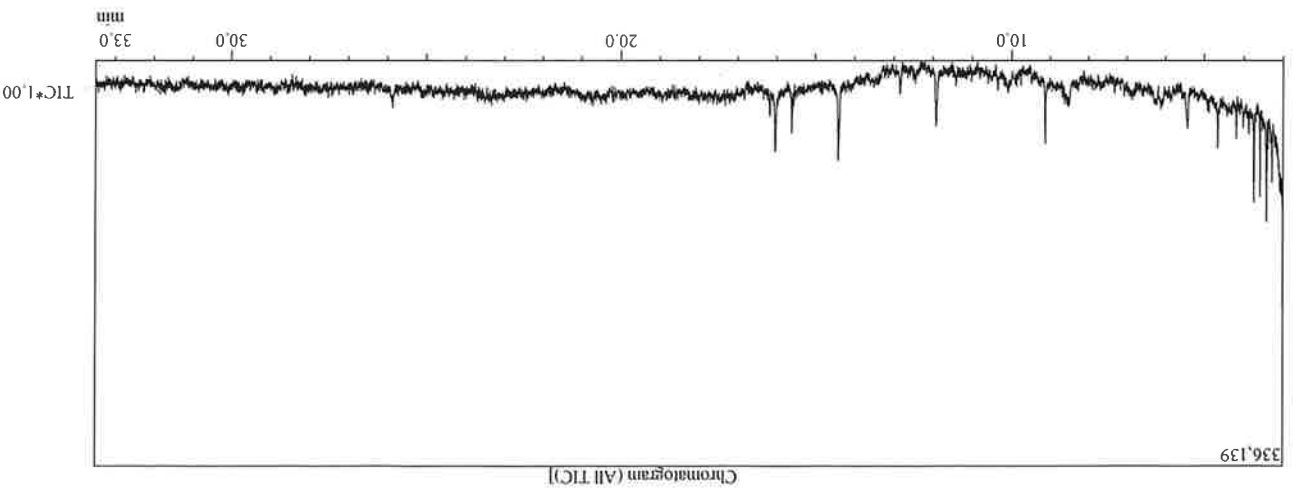


CAS#: 24567-27-9 Mol Wt: 118 Serial#: 4913

Compound Name: Propenoic acid, 2-hydroxyethyl ester SS 2-Hydroxyethyl propionate # 33

Formula: C5H10O3 Class Flag: No Class Flags

RetIndex: 928

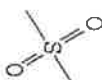
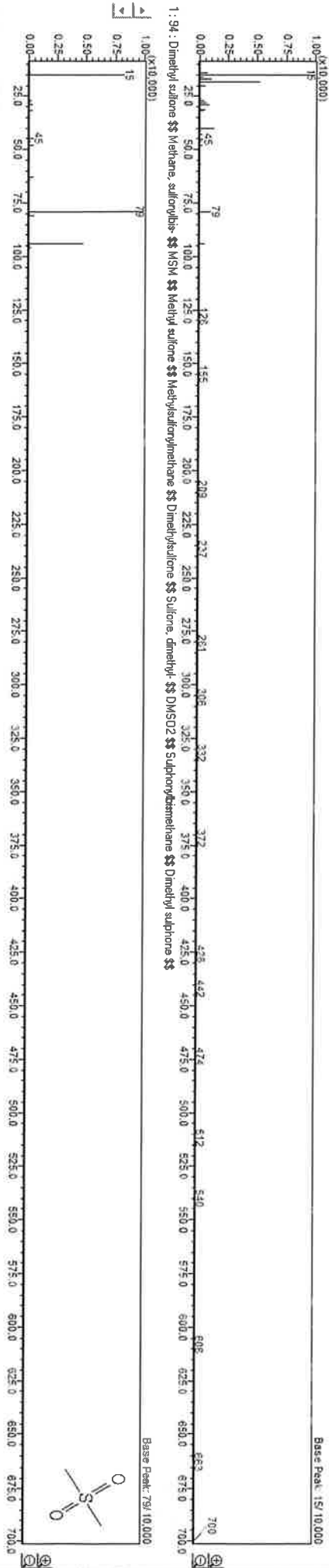


Similarity Search Results

Report View Compound Info Process Help

Hit	Similar	Reg	Compound Name	Mol Wt	Formula	Library
1	70	62	Dimethyl sulfone, sulfolene, sulfolene, \$S\$	94	C2H6O2S	NIST08.LIB
2	66	62	Glycidol \$S\$ Oxiranemethanol \$S\$ 1-Propanol, 2,	74	C3H6O2	NIST08.LIB
3	64	62	Ethylene oxide \$S\$ Oxirane \$S\$ Dioxirane	44	C2H4O	NIST08.LIB
4	63	62	anti-2-Acetoxyacetaldehyde \$S\$ (2E)-2-Hydroxy	117	C4H7NO3	NIST08.LIB
5	63	62	Acetone, 1-methyl- \$S\$ N-Methylaziridine \$S\$ N-	57	C3H7N	NIST08.LIB
6	62	62	Acetyl bromide \$S\$ CH3COBr \$S\$ UN 1716 \$S\$	122	C2H3BrO	NIST08.LIB
7	62	62	Acetonitrile, hydroxy- \$S\$ Glycolonitrile \$S\$ Cyan	57	C2H3NO	NIST08.LIB
8	62	62	Methane, nitro- \$S\$ Nitromethane \$S\$ Nitrocarbo	61	CH3NO2	NIST08.LIB
9	62	62	Carbonic acid, dimethyl ester \$S\$ Dimethyl carb	90	C3H6O3	NIST08.LIB
10	62	62	Dimethylfluoroamine \$S\$ N-Fluoro-N-methylmeth	63	C2H5FN	NIST08.LIB
11	62	62	2-Hydroxypropanoic acid, methyl est	145	C5H7NO4	NIST08.LIB

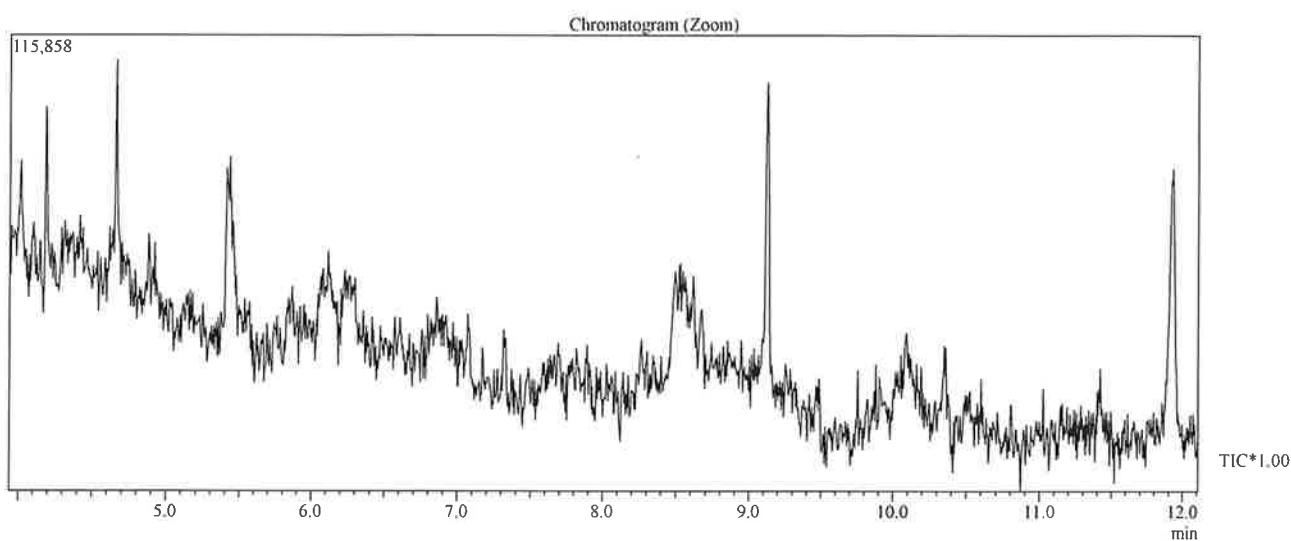
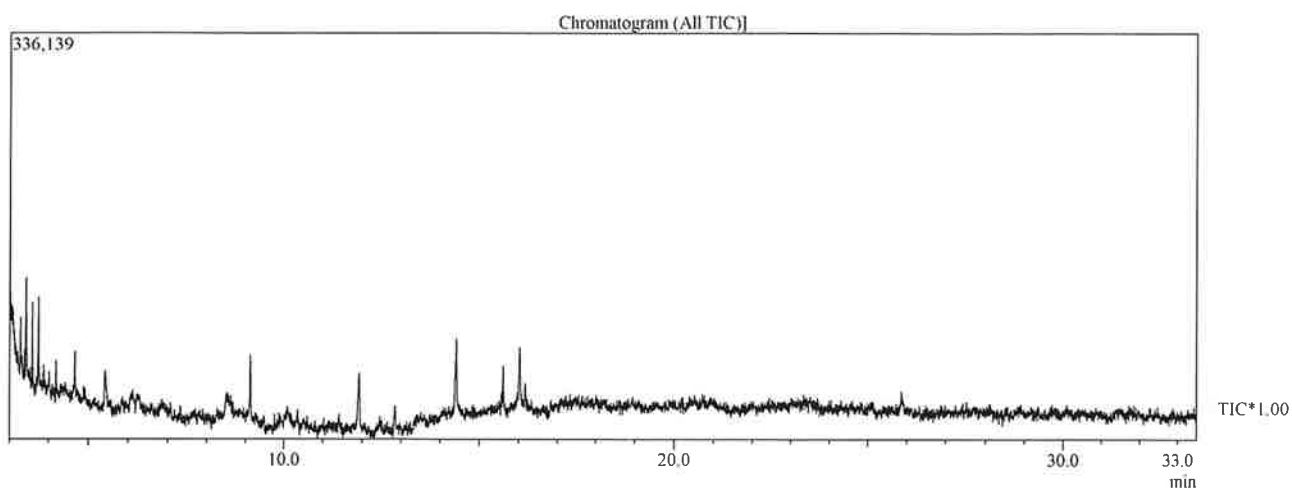
Target:



DAS# 67-71-0 Mol Wt 94 Serial# 1234
 Cpnd Name Dimethyl sulfone, sulfolene, \$S\$ MSM \$S\$ Methyl sulfone \$S\$ Methylsulfonylmethane \$S\$ Dimethylsulfone \$S\$ Sulfone, dimethyl- \$S\$ DMSO2 \$S\$ Sulphonylbis(methane) \$S\$ Dimethyl sulphone \$S\$
 Formula C2H6O2S Class Flag No Class Flags

RefIndex 727

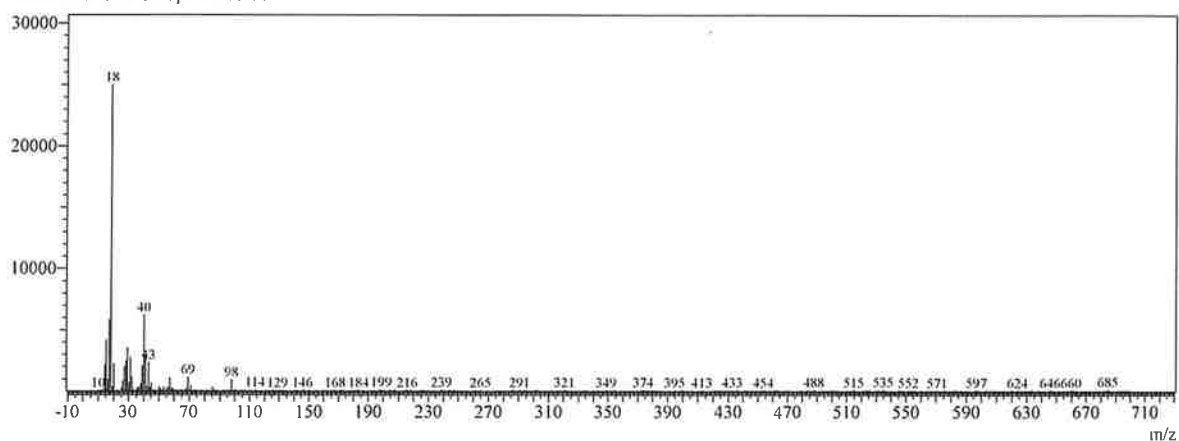
C:\GCMSsolution\Data\Project\1\Ms Mathe\SAMPLE 3_UNKNOWN_20221130_3.qgd



Spectrum

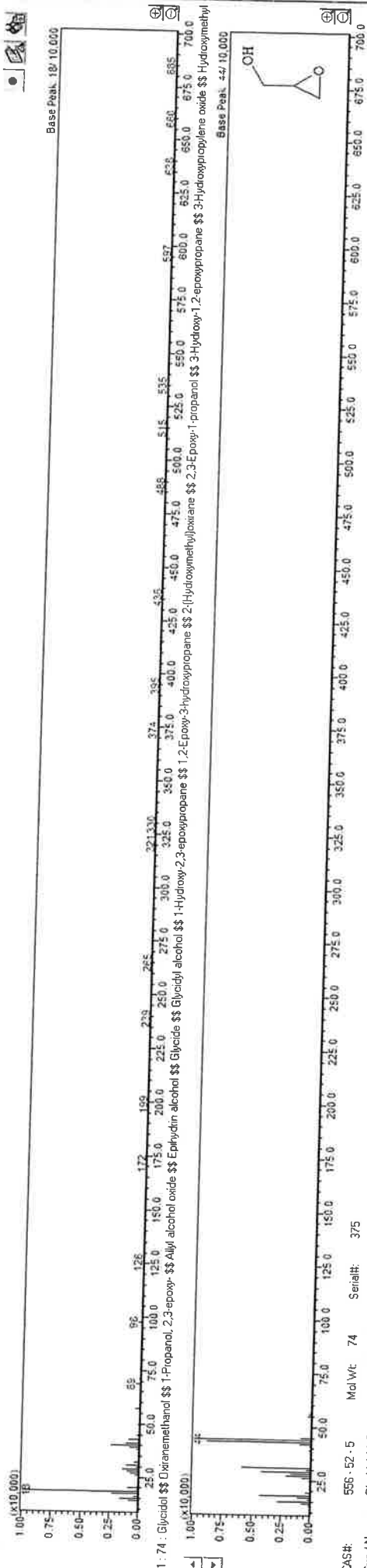
Line#:1 R.Time:4.015(Scan#:204)
MassPeaks:583
RawMode:Single 4.015(204) BasePeak:18.10(24991)
BG Mode:None Group 1 - Event 1

7,435



Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library
1	65	✓	Glycidol \$\$ Oxiranemethanol \$\$ 1-Propanol, 2	74	C3H6O2	NIST08 LIB
2	69		Acetonitrile hydroxy-\$\$ Glycolnitrite \$\$ Cyan	57	C2H3NO	NIST08 LIB
3	68		1-Hydroxy-2-pentanone \$\$ 2-Pentanone, 1-Hy	102	C5H10O2	NIST08 LIB
4	68		Glycyl-D-asparagine	189	C5H11N3O4	NIST08 LIB
5	66		2-Butenedioic acid, 2-methyl-, (Z)-\$\$ Citraconil	130	C5H6O4	NIST08 LIB
6	66		2-Propanone, 1,3-dihydroxy-\$\$ Dihydroxyacet	90	C3H6O3	NIST08 LIB
7	66		1-Propanol, 2-amino-, (-)-\$\$ 1-Propanol, 2-	75	C3H9NO	NIST08 LIB
8	66		Ethanol, 2-(2-propyloxy)-\$\$ Ethylene glycol	100	C5H10O2	NIST08 LIB
9	65		2-Nitro-1-propanol \$\$ 2-Nitropropanol-1 \$\$ 1-P	105	C3H7NO3	NIST08 LIB
10	65		Azelidene, 1,3-dimethyl-\$\$ 1,3-Dimethylazetid	85	C5H11N	NIST08 LIB
11	65		Propanone, 2-methoxy-\$\$ Ether isomethyl methy	74	C4H10O	NIST08 LIB

Target:



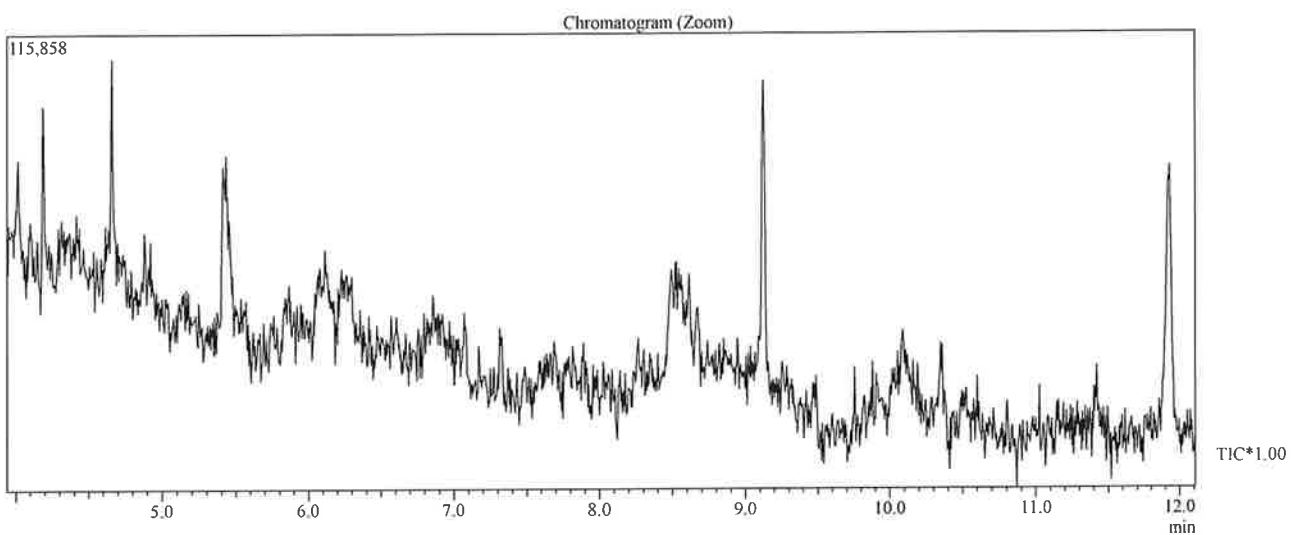
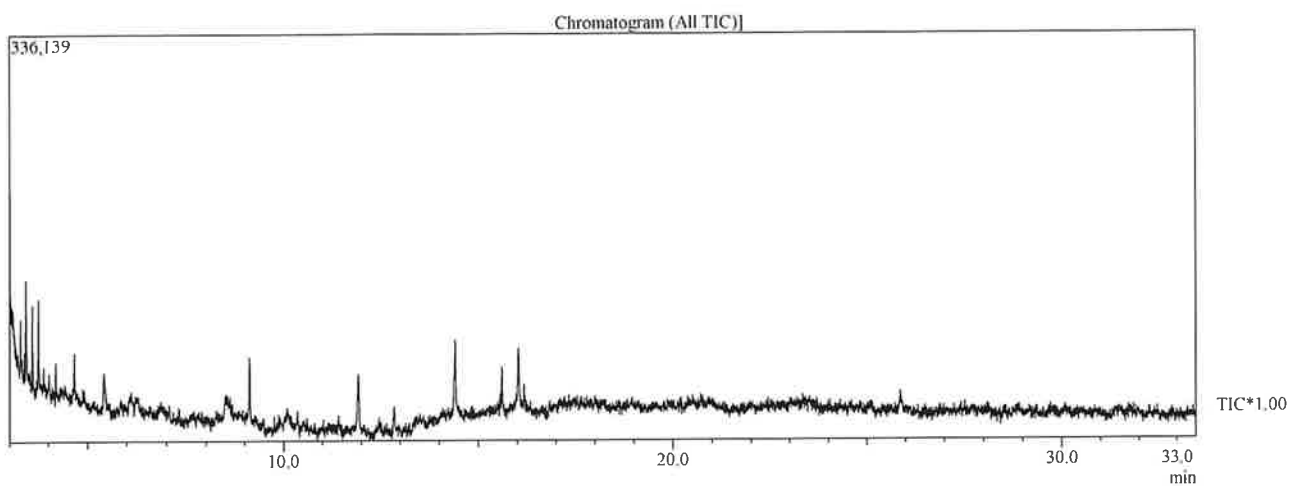
CAS#: 555-52-5 Mol Wt: 74 Serial#: 375

Compound Name: Glycidol \$\$ Oxiranemethanol \$\$ 1-Propanol, 2,3-epoxy-\$\$ Allyl alcohol oxide \$\$ Epichlorohydrin alcohol oxide \$\$ Glycidol alcohol oxide \$\$ Glycidol alcohol oxide

Formula: C3H6O2 Class Flag: No Class Flags

Ref Index: 653

C:\GCMSsolution\Data\Project1\Ms Mathel\SAMPLE 3_UNKNOWN_20221130_3.qgd

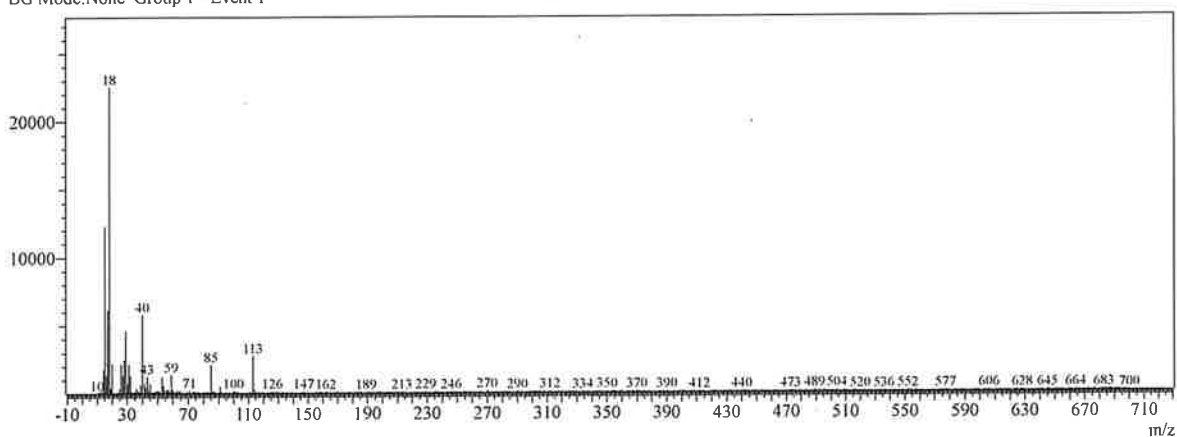


Spectrum

Line#:1 R.Time:4.190(Scan#:239)
MassPeaks:579
RawMode:Single 4.190(239) BasePeak:18.10(22530)
BG Mode:None Group 1 - Event 1

②

6,703

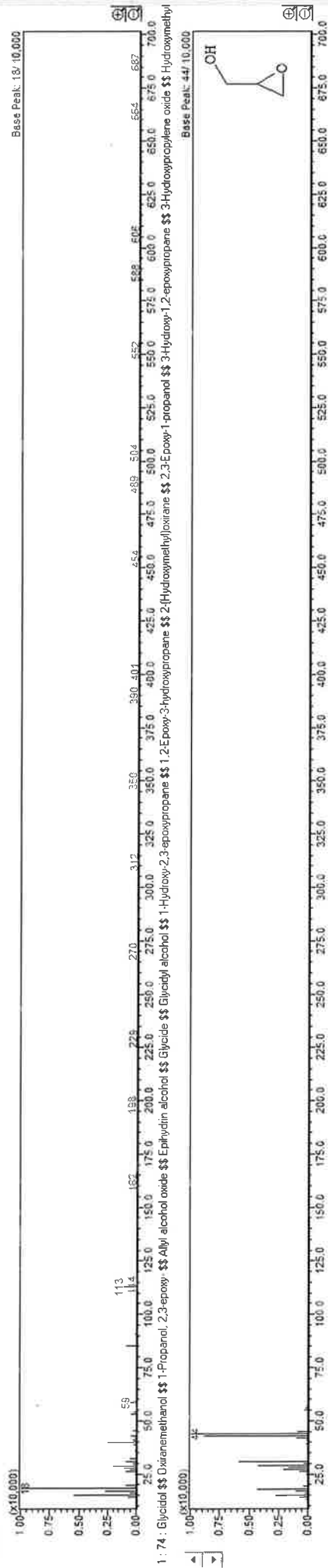


Similarity Search Results

Report View Compound Info Process Help

Idx	Similar	Regd	Compound Name	Mol Wt	Formula	Library
1	63	67	Glycidol SS Oxazironeal SS 1-Propanol 2	74	C ₃ H ₆ O ₂	NIST08.LIB
2	67	67	Glycidol SS Oxazironeal SS 1-Propanol 2	74	C ₃ H ₆ O ₂	NIST08.LIB
3	67	67	Acetonitrile, hydroxy- SS Glycolonitrile SS Cyan	57	C ₂ H ₃ NO	NIST08.LIB
4	65	65	Azidine, 1-methyl- SS N-Methylaziridine SS N-	57	C ₃ H ₇ N	NIST08.LIB
5	65	65	DL-Arabinose SS Pentopyranose # SS	150	C ₅ H ₁₀ O ₅	NIST08.LIB
6	64	64	2-Hydroxyimino-3-oxo-butanolic acid, methyl es	145	C ₅ H ₇ NO ₄	NIST08.LIB
7	64	64	2-Propanone, 1,3-dihydroxy- SS Dihydroxyacet	90	C ₃ H ₆ O ₃	NIST08.LIB
8	64	64	Acetaldehyde SS (E)-CH ₃ CH=NOH SS Acetal	59	C ₂ H ₄ NO	NIST08.LIB
9	63	63	N-Ethoxy-2-carbaminoaziridine SS 1-Ethoxy-2-a	130	C ₅ H ₁₀ N ₂ O ₂	NIST08.LIB
10	63	63	Ethene, methoxy- SS Ether, methyl vinyl SS Me	58	C ₃ H ₆ O	NIST08.LIB
11	63	63	1,3-Dihydroxypropanone, dimer	148	C ₆ H ₁₂ O ₆	NIST08.LIB

Target:

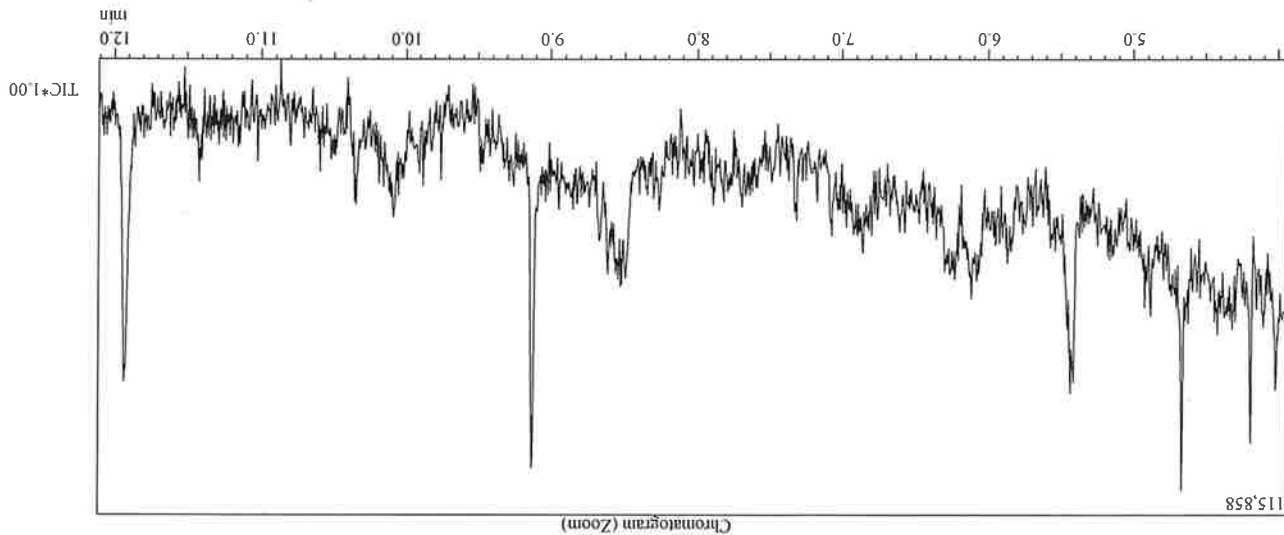
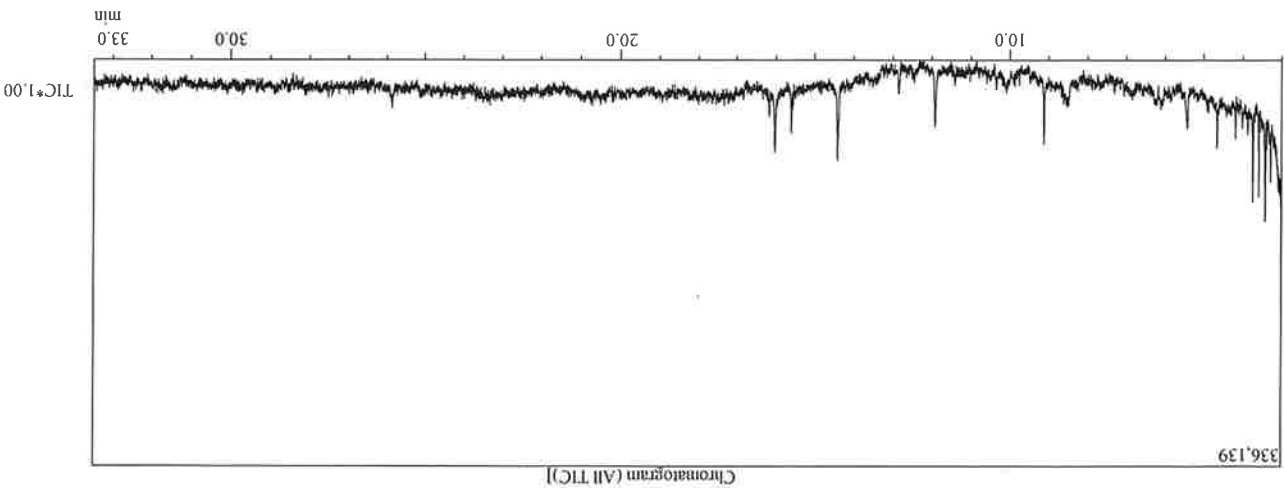


CAS#: 556-52-5 Mol Wt: 74 Serial#: 375

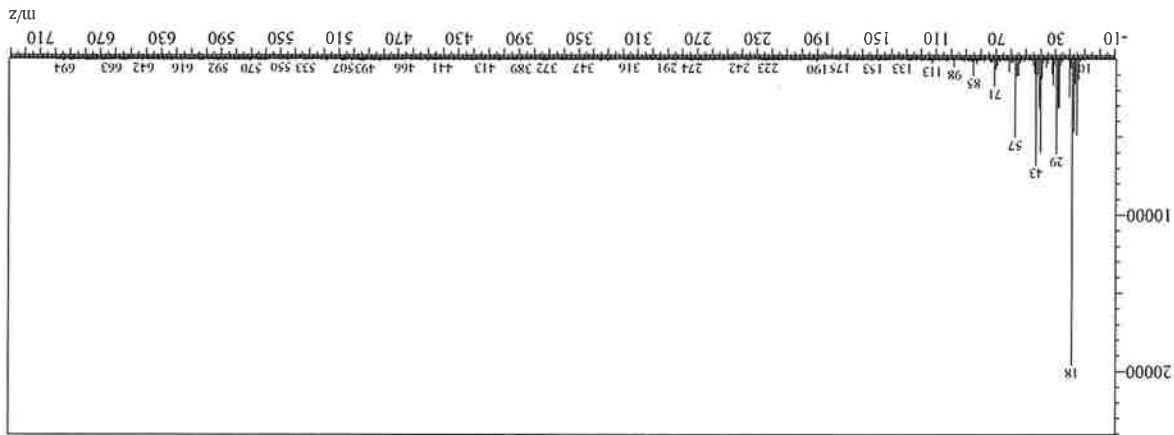
Cmpd Name: Glycidol SS Oxazironeal SS 1-Propanol 2,3-epoxy- SS Allyl alcohol oxide SS Epithym alcohol SS Glycidol SS Glycidol SS 1-Hydroxy-2,3-epoxypropane SS 2,3-Epoxy-1-propanol SS 3-Hydroxypropylene oxide SS Hydr

Formula: C₃H₆O₂ Class Flag: No Class Flags

Ref Index: 653



Spectrum

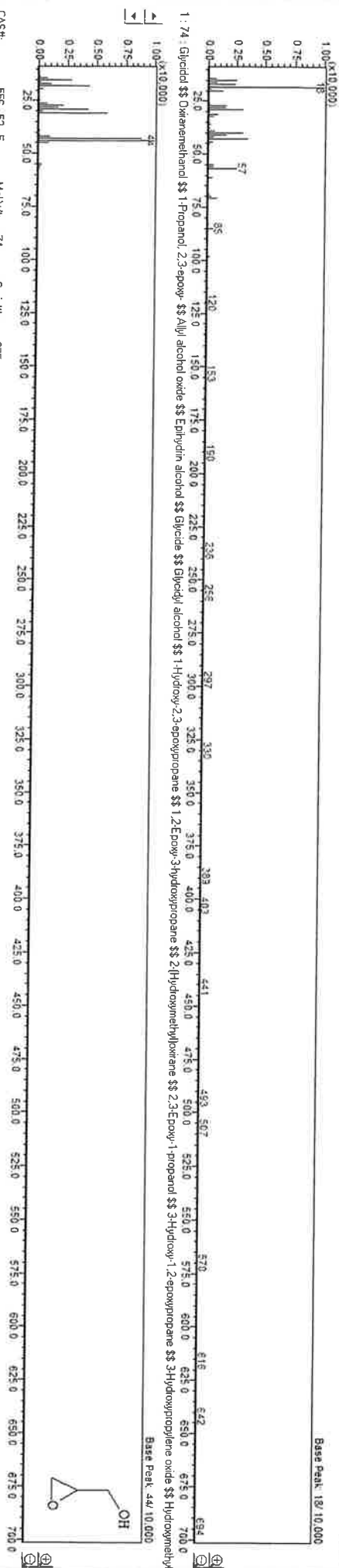


Line#: 1 R.Time: 4.660 (Scan#: 333)
MassPeaks: 609
RawMode: Single 4.660 (333) BasePeak: 18.10 (19593)
BG Mode: None Group 1 - Event 1

③ 5.829

Hit	Similarity	Ref	Compound Name	Mol Wt	Formula	Library
1	72		Glycidol \$\$ Oxiranemethanol \$\$ 1-Propanol, 2	74	C3H6O2	NIST09.LIB
2	71		DL-Xarabiose \$\$ Parityranose # 55	150	C5H10O5	NIST08.LIB
3	71		Glycol-D-asparagine	189	C6H11N3O4	NIST08.LIB
4	71		3,3-Dimethyl-2-pentanone \$\$ 3,3-Dimethyl-2p	114	C7H14O	NIST08.LIB
5	71		1-Hydroxy-2-pentanone \$\$ 2-Pentanone, 1-Hy	102	C5H10O2	NIST08.LIB
6	70		Hexane, 1-phenyloxy- \$\$ Ether, heavy vinyl s	128	C8H16O	NIST08.LIB
7	70		Propane, 2-methoxy- \$\$ Ether, isopropyl methyl	74	C4H10O	NIST08.LIB
8	70		(2S,3S)-3-Propyloxiranemethanol \$\$ (2-Prop	116	C6H12O2	NIST08.LIB
9	70		Pecozide, bis(1-methylglycidyl) \$\$ Isopropyl perox	102	C5H10O2	NIST08.LIB
10	70		Hydroxamine, 1-methylhexyl \$\$ n-C3H17Cl, Hf	118	C8H14O2	NIST08.LIB
11	70			132	C7H16O2	NIST08.LIB

Target:

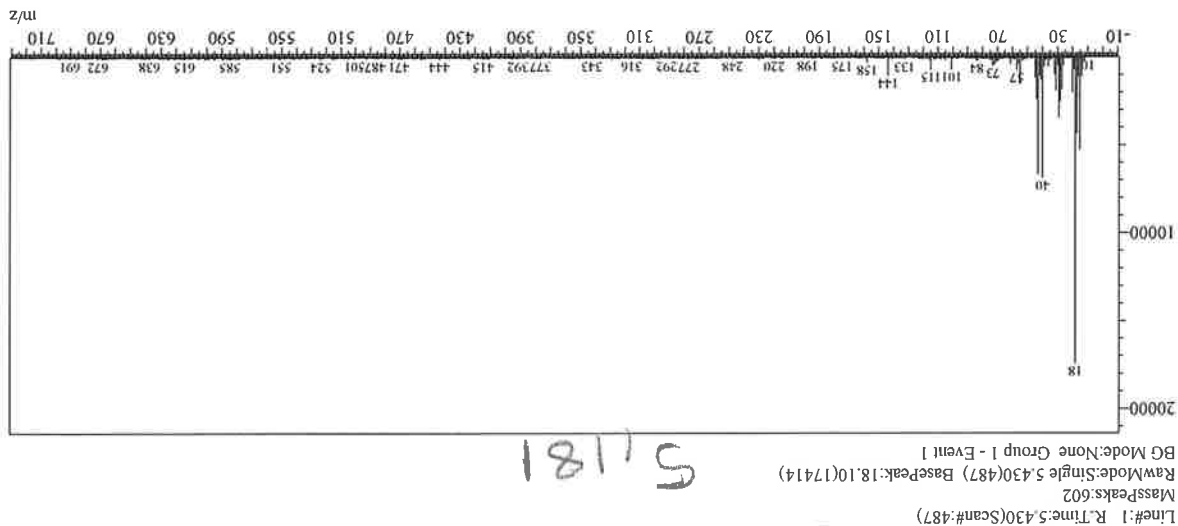
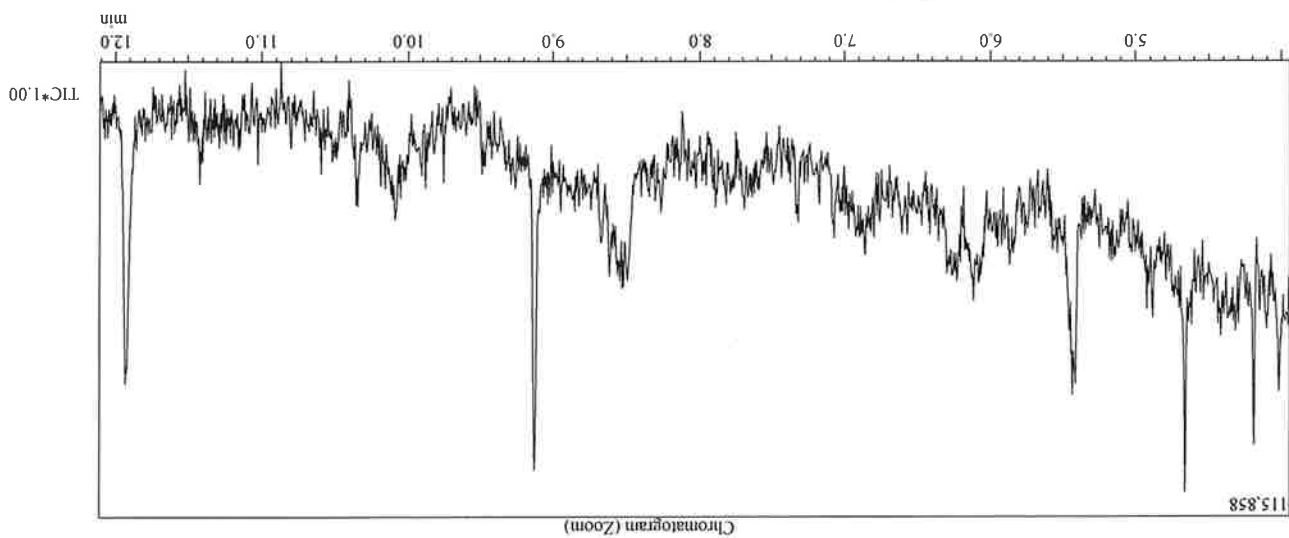
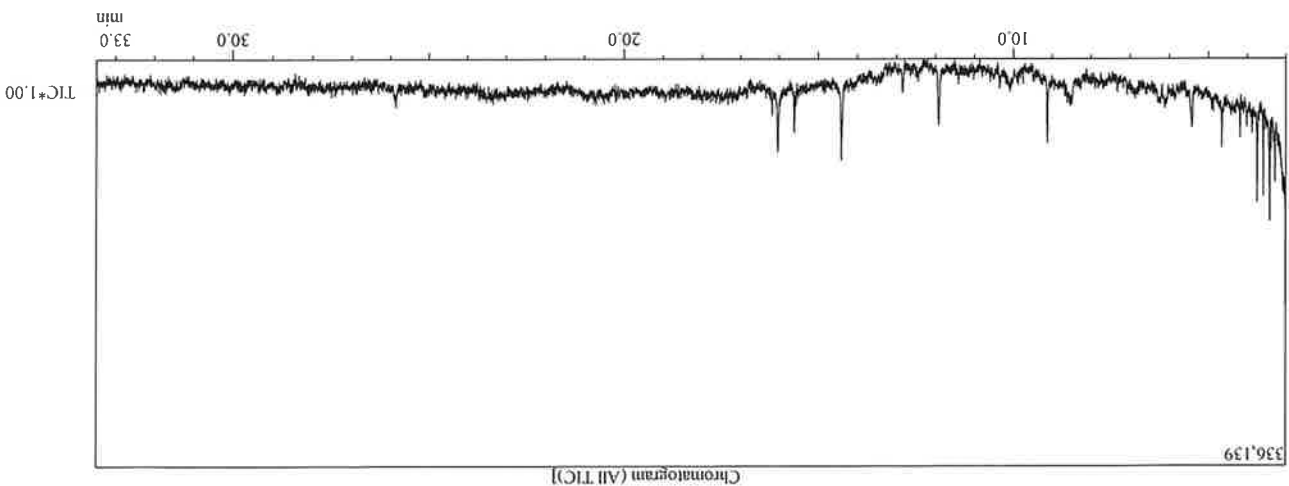


CAS#: 556-52-5 Mol Wt: 74 Serial#: 375

Compound Name: Glycidol \$\$ Oxiranemethanol \$\$ 1-Propanol, 2,3-epoxy- \$\$ Allyl alcohol oxide \$\$ Epichlorhydrin alcohol \$\$ Glycidol alcohol \$\$ 1-Hydroxy-2,3-epoxypropane \$\$ 1,2-Epoxy-3-hydroxypropane \$\$ 2-(Hydroxymethyl)oxirane \$\$ 2,3-Epoxy-1-propanol \$\$ 3-Hydroxy-1,2-epoxypropane \$\$ 3-Hydroxypropylene oxide \$\$ Hydr

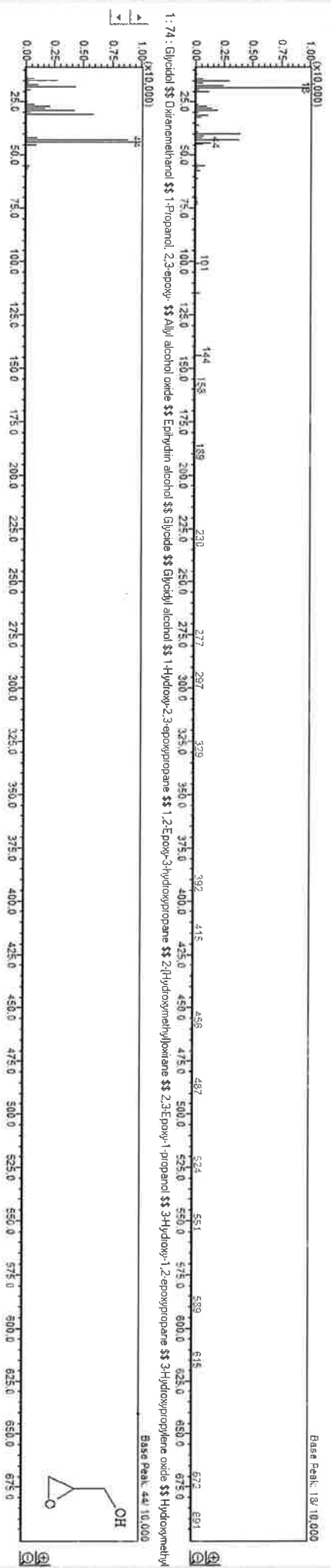
Formula: C3H6O2 Class Flag: No Class Flags

RelIndex: 653



Hit	Similarity	Regd	Compound Name	Mol Wt	Formula	Library
1	74	74	Glycidol SS Oxiranemethanol SS 1-Propanol 2	74	C3H6O2	NIST08.LIB
2	70	70	1-Hydroxy-2-propanone SS 2-Pentanone, 1-Hy	102	C5H10O2	NIST08.LIB
3	69	69	DL-Malbinose SS Pentopyranose # SS	150	C5H10O5	NIST08.LIB
4	69	69	Ethanamine, 2,2'-oxybis- SS 2-(2-Aminoethoxy)	104	C4H12N2O	NIST08.LIB
5	68	68	Glycid-D-asparagine	189	C6H11N3O4	NIST08.LIB
6	68	68	Oxirane, 2,3-dimethyl-, trans- SS Butane, 2,3-e	72	C4H8O	NIST08.LIB
7	68	68	2-Propanone, 1,3-dihydroxy- SS Dihydroxyacet	90	C3H6O3	NIST08.LIB
8	68	68	Oxiranemethanol, (S)- SS (S)-Glycidol SS 2-O	74	C3H6O2	NIST08.LIB
9	68	68	2-Heptanol, 3-methyl-, SS 3-Methyl-2-heptanol	130	C8H18O	NIST08.LIB
10	68	68	1,3-Bis(oxirane) SS beta-Buryle glycol SS M	90	C4H8O2	NIST08.LIB
11	68	68	n-Dioxane, methylene- SS 2-Methylen-1,4-di	108	C5H8O2	NIST08.LIB

Target:

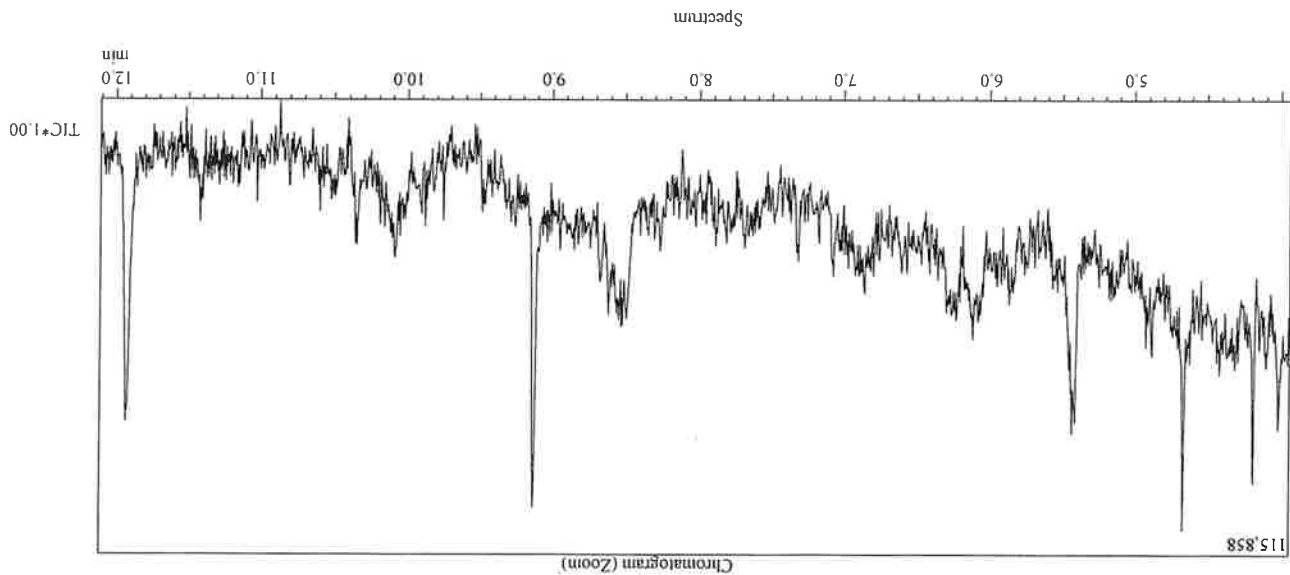
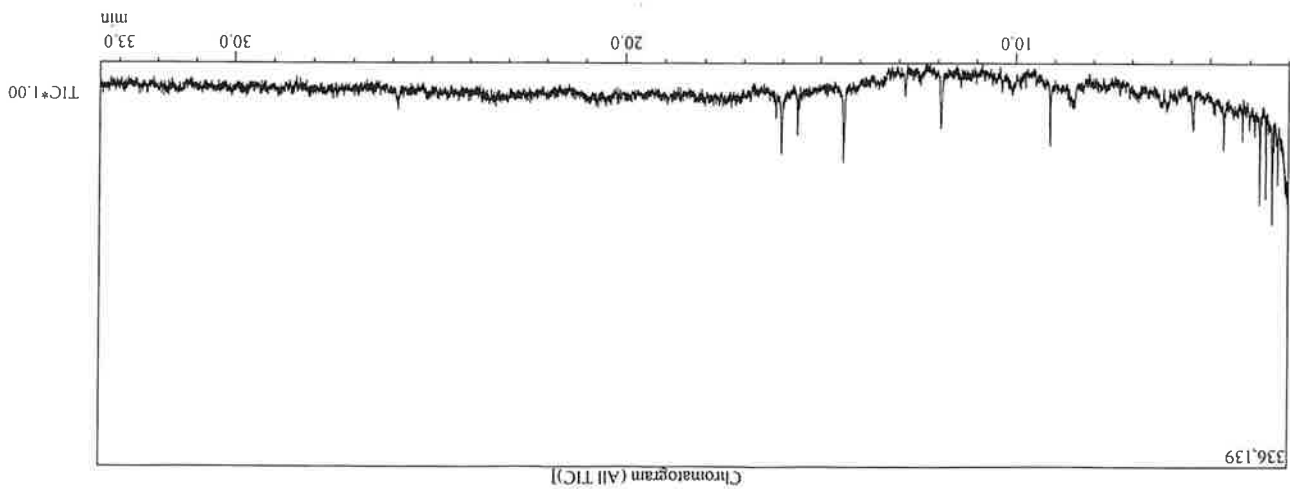


CAS#: 558-52-5 Mol Wt: 74 Serial#: 375

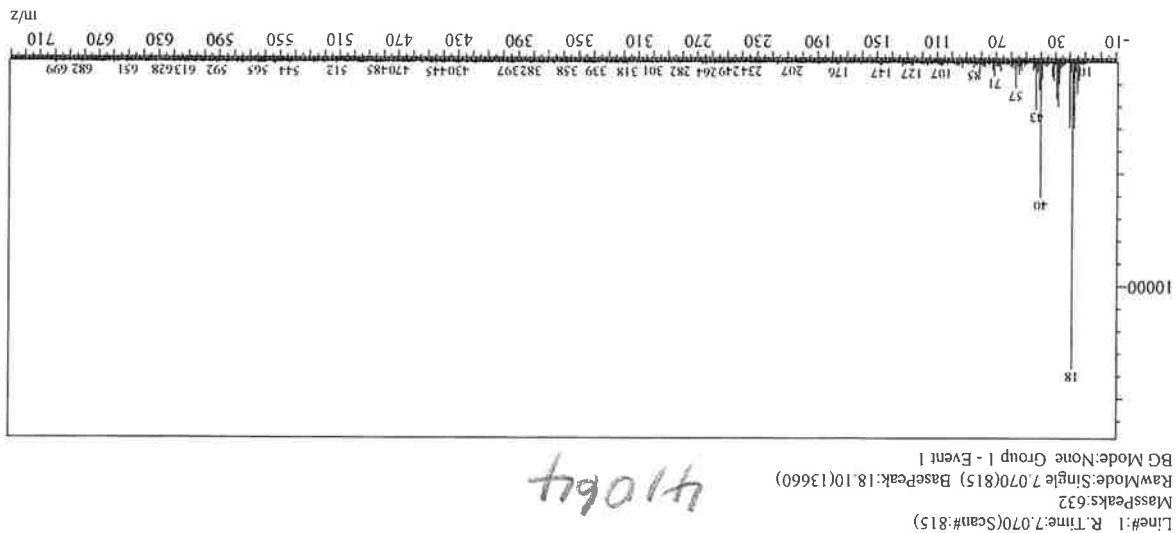
Compd Name: Glycidol SS Oxiranemethanol SS 1-Propanol 2, 3-epoxy- SS Allyl alcohol oxide SS Epilysin alcohol SS Glycidol alcohol SS 1-Hydroxy-2,3-epoxypropane SS 1,2-Epoxy-3-hydroxypropane SS 2-(1-Hydroxymethyl)oxirane SS 2,3-Epoxy-1-propanol SS 3-Hydroxy-1,2-epoxypropane SS 3-Hydroxypropylene oxide SS Hydroxymethyl

Formula: C3H6O2 Class Flag: No Class Flags

RelIndex: 663



Spectrum

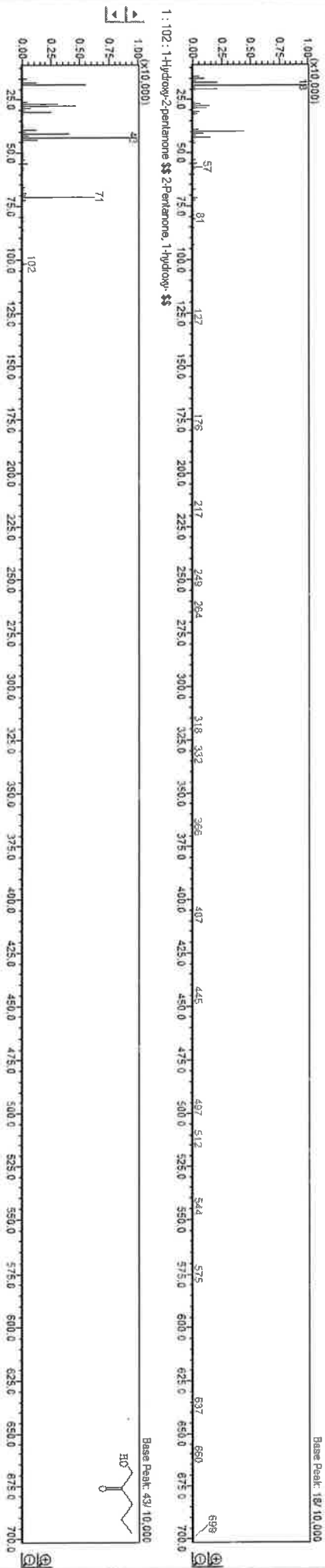


Similarity Search Results

Report View Compound Info Process Help

Hit	Similar	Peak	Compound Name	Mol Wt	Formula	Library
1	57	18	1-Hydroxy-2-pentanone SS 2-Pentanone, 1-Hy	102	C5H10O2	NIST08.LIB
2	66	18	Glycyl-D-asparagine	189	C8H17N3O4	NIST08.LIB
3	66	18	Glycidyl SS Octanemethanol SS 1-Propanol, 2-	74	C3H6O2	NIST08.LIB
4	65	18	2-Butenedioic acid, 2-methyl-, (Z)- SS Citracon	130	C5H6O4	NIST08.LIB
5	64	18	2-Propanone, 1,3-dihydroxy- SS Dihydroxyacet	90	C3H6O3	NIST08.LIB
6	64	18	3,3-Dimethyl-2-pentanone SS 3,3-Dimethyl-2-p	114	C7H16O	NIST08.LIB
7	64	18	anti-2-Acetoxyacetaldoxime SS (2E)-2-(4-Hydroxy	117	C4H7NO3	NIST08.LIB
8	63	18	2-Hexanone, 5-methyl-, SS isoamyl methyl keto	114	C7H14O	NIST08.LIB
9	63	18	1-Hydroxy-3-methyl-2-butanone SS 2-Butanone	102	C5H10O2	NIST08.LIB
10	63	18	3,4-Dimethyl-2-pentanone	114	C7H16O	NIST08.LIB
11	63	18	4,4-Dimethyl-2-pentanone SS 2-Acetyltrimine, 4-6	129	C5H7NO3	NIST08.LIB

Target:

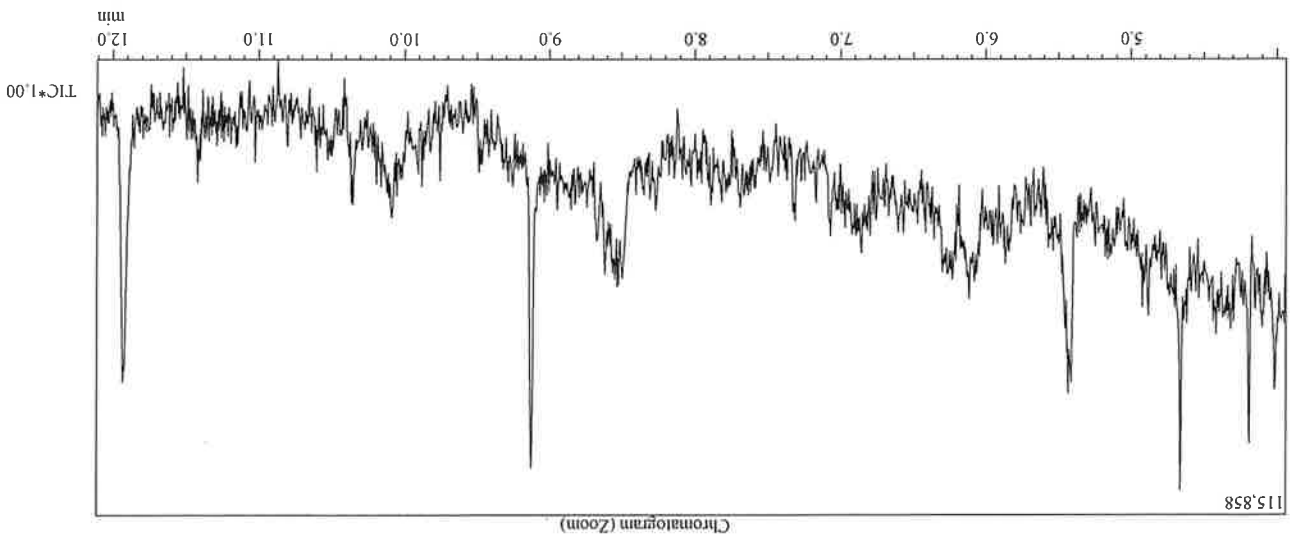
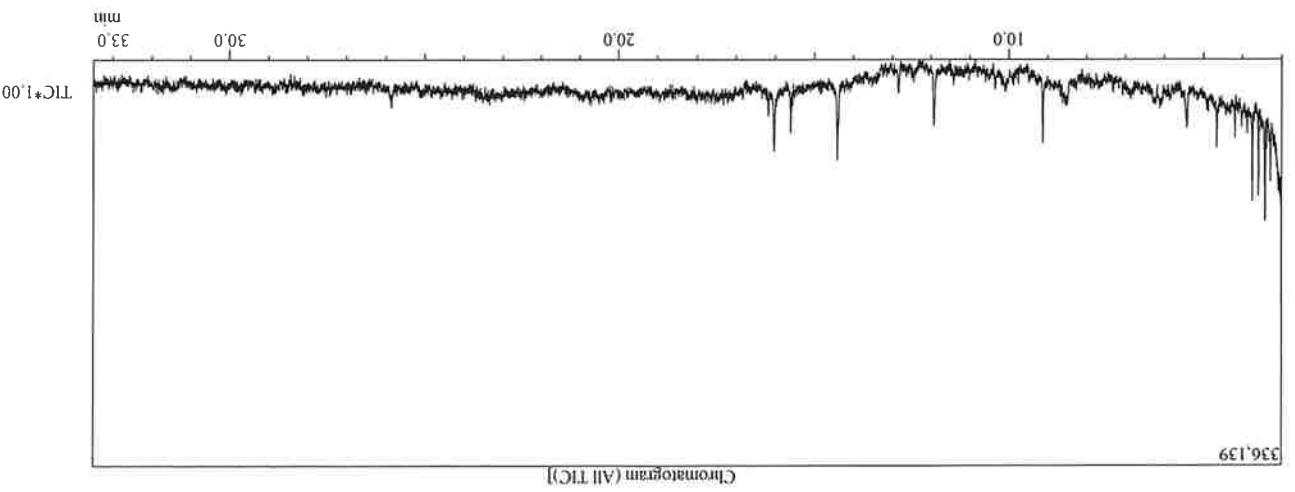


CAS#: 64502-89-2 Mol Wt: 102 Serial#: 2241

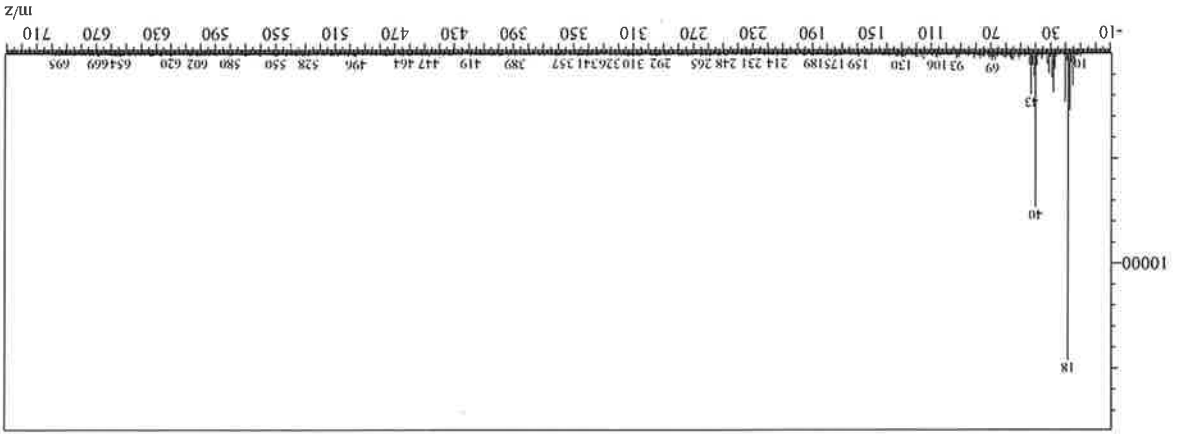
Compd Name: 1-Hydroxy-2-pentanone SS 2-Pentanone, 1-Hydroxy- SS

Formula: C5H10O2 Class Flag: No Class Flags

RelIndex: 897



Spectrum



Line#: 1 R.Time: 7.325 (Scan#: 866)
Raw Mode: Single 7.325 (866) Base Peak: 18.10 (14594)
Mass Peaks: 611

BG Mode: None Group 1 - Event 1

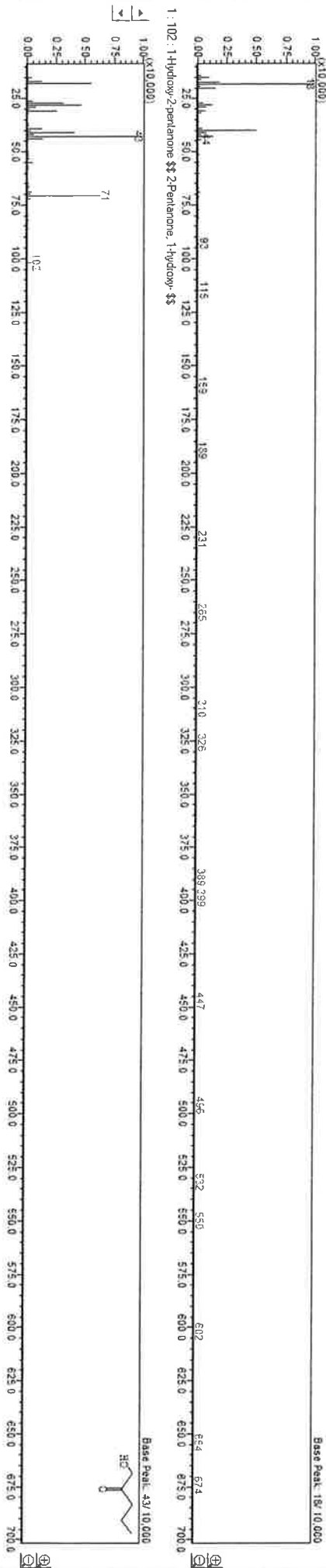
② 41342

Similarity Search Results

Report View Compound Info Process Help

Hit	Similar	Rank	Compound Name	Mol Wt	Formula	Library
1	65	1	1-Hydroxy-2-pentanone SS 2-Pentanone, 1-Hy	102	C5H10O2	NIST08.LIB
2	65	2	Acetamide, hydroxy- SS Glycolamide SS Cyn	57	C2H3NO	NIST08.LIB
3	65	3	3-Amino-1,2-propanediol SS 1-Aminopropan-1-ol	91	C3H9NO2	NIST08.LIB
4	65	4	Glycidol SS Oxiranemethanol SS 1-Propanol, 2-	74	C3H6O2	NIST08.LIB
5	65	5	Glycidol SS Oxiranemethanol SS 1-Propanol, 2-	189	C3H7NO3	NIST08.LIB
6	64	6	anti-2-Acetoxyacetaldehyde SS (2E)-2-Hydroxy	117	C4H7NO3	NIST08.LIB
7	63	7	1-Propanol, 2-amino-, (-)-, SS 1-Propanol, 2-	75	C3H9NO	NIST08.LIB
8	63	8	2-Butoxyacetic acid, 2-methyl-, (Z)- SS Citraconic	130	C5H8O4	NIST08.LIB
9	62	9	2-Propanone, 1,3-dihydroxy- SS Dihydroxyacetone	90	C3H6O3	NIST08.LIB
10	62	10	3-Butyn-1-ol SS 1-Butyn-4-ol SS 2-Hydroxyethyl	70	C4H6O	NIST08.LIB
11	62	11	Oxazoline SS 1,3-Oxazoline SS	69	C3H5NO	NIST08.LIB

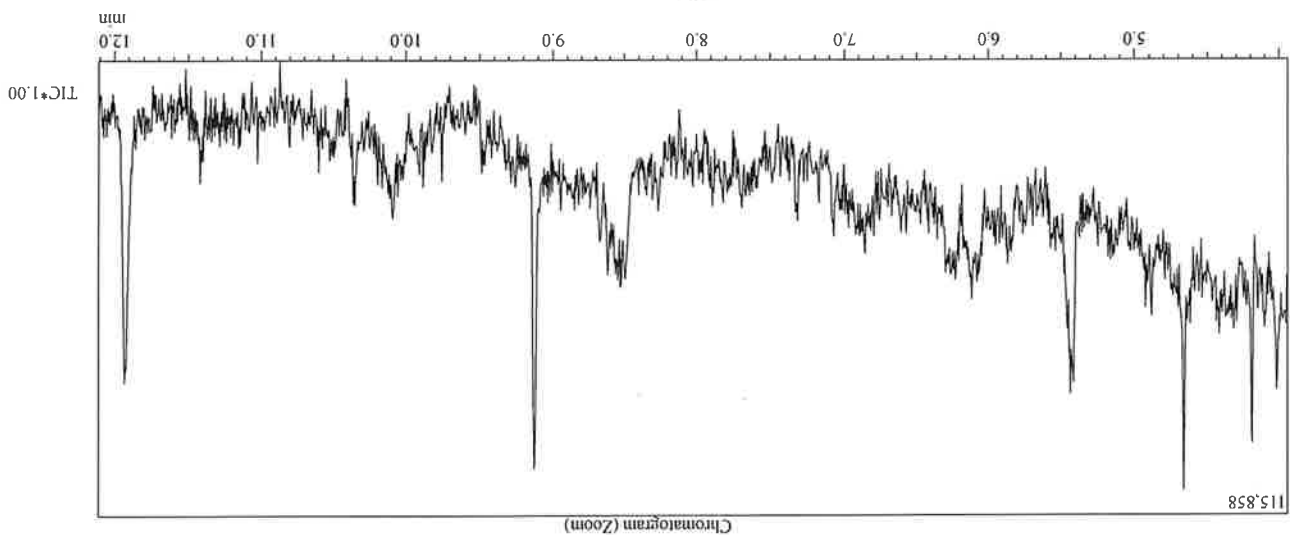
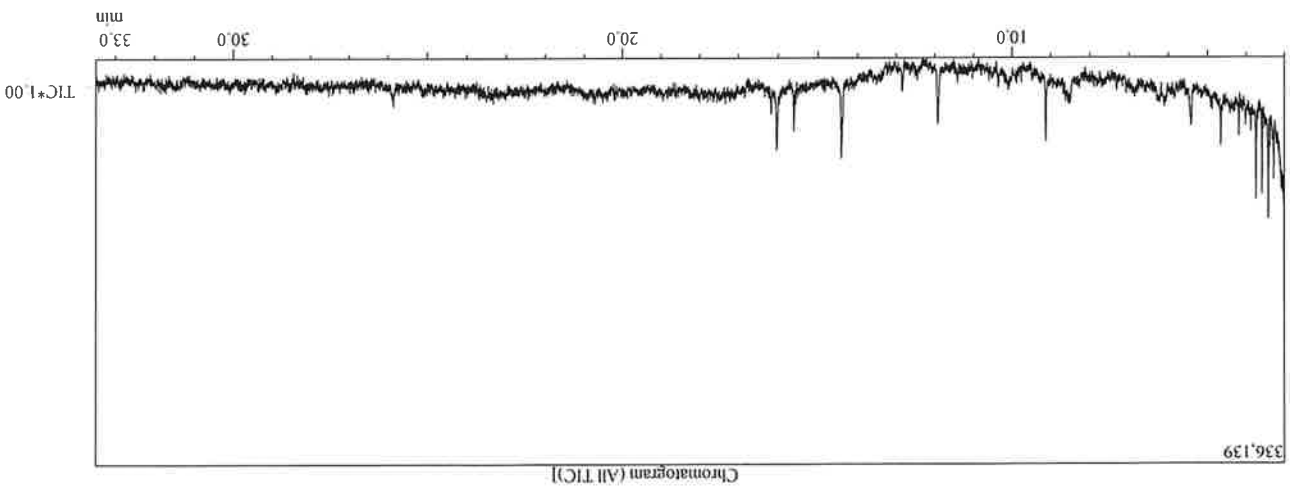
Target:



1 : 102: 1-Hydroxy-2-pentanone SS 2-Pentanone, 1-Hydroxy, SS

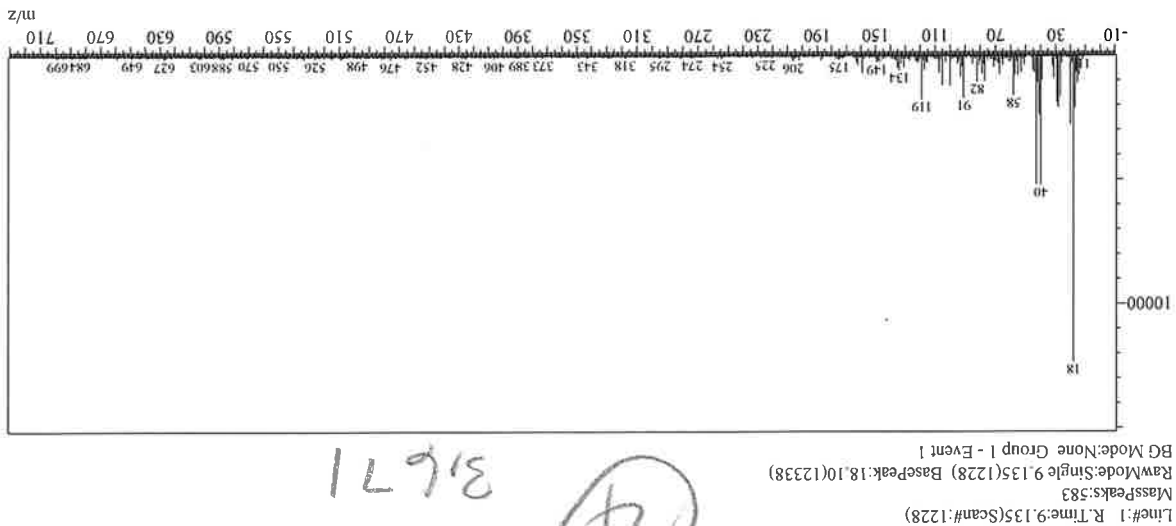
CAS#: 64502-89-2 Mol Wt: 102 Serial#: 2241
 Compd Name: 1-Hydroxy-2-pentanone SS 2-Pentanone, 1-Hydroxy, SS
 Formula: C5H10O2 Class Flag: No Class Flags

RefIndex: 897



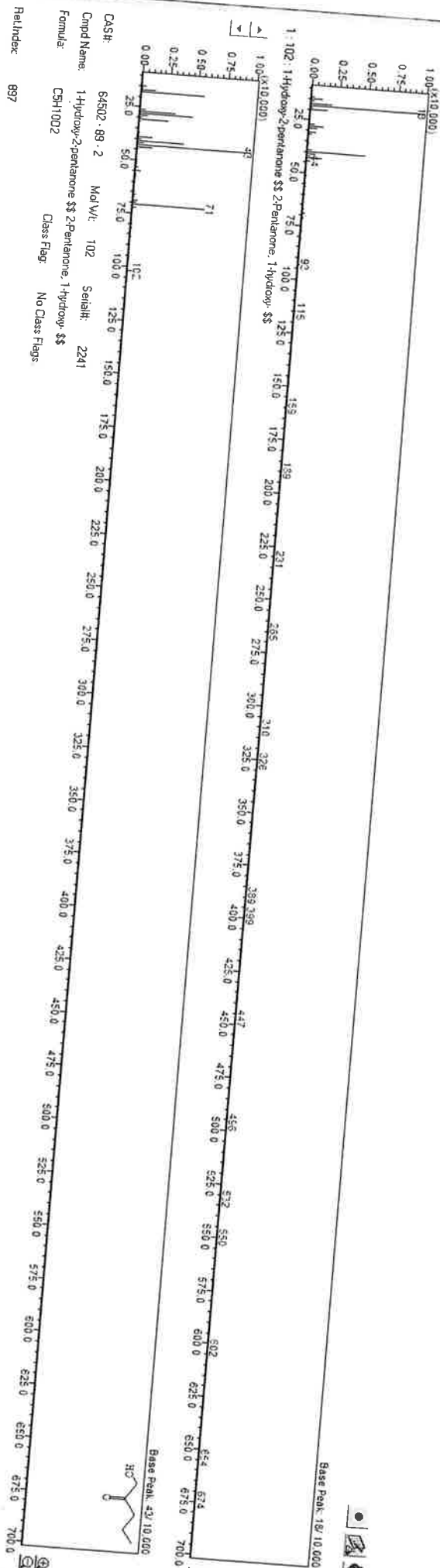
Spectrum

3.671



[illegible]

... ..

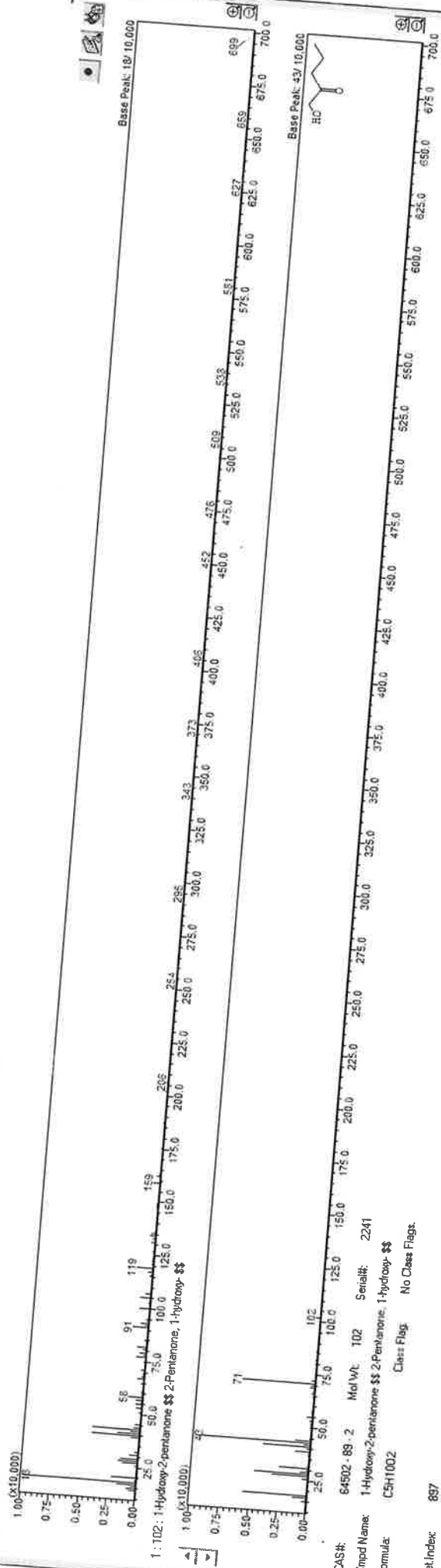


CAS#:	64502-89-2	MolWt:	102	Selfish:	224
Cmpd Name:	1-Hydroxy-2-pentanone \$ 2-Pentanone, 1-Hydroxy- \$				
Formula:	C5H10O2				
		Class Flag:	No Class Flags		
RefIndex:	897				

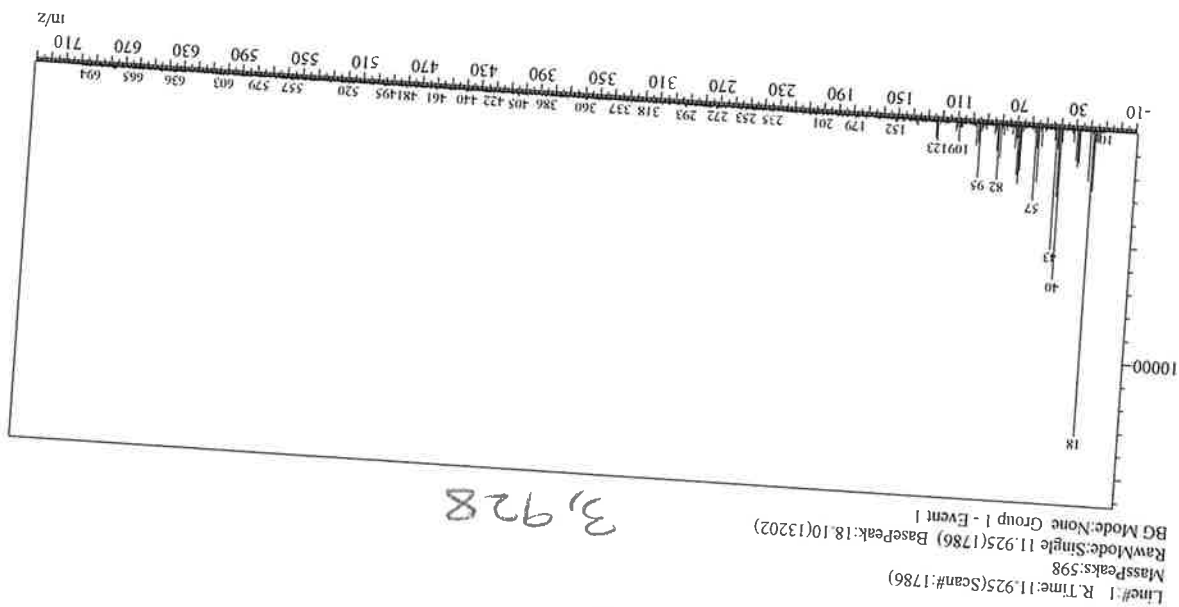
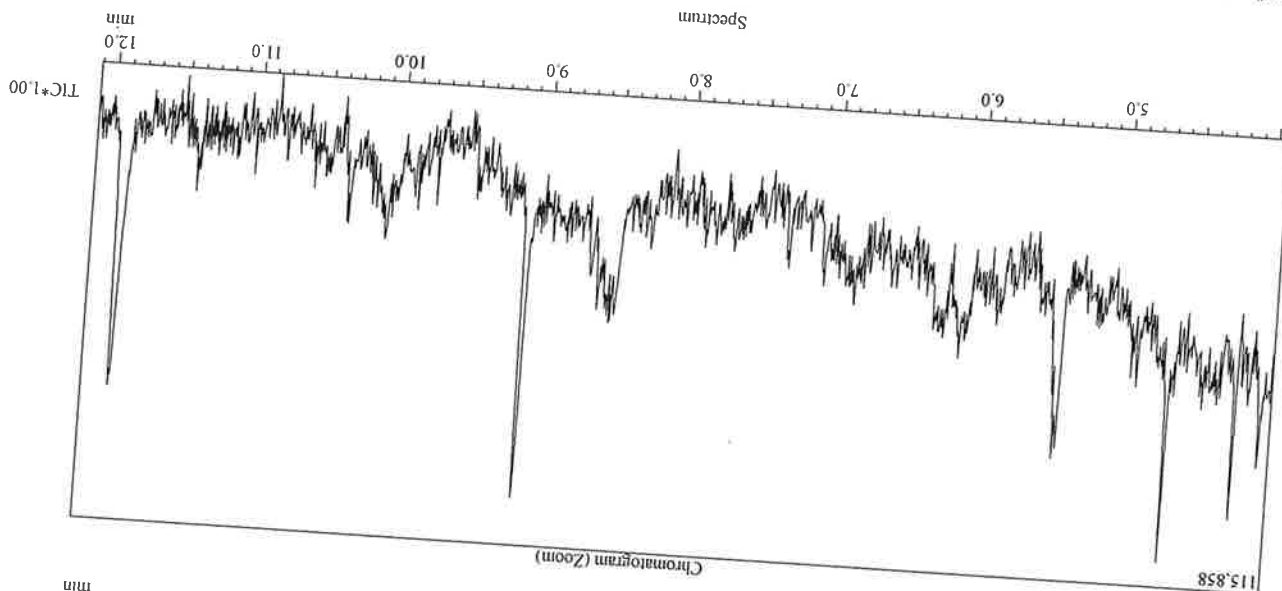
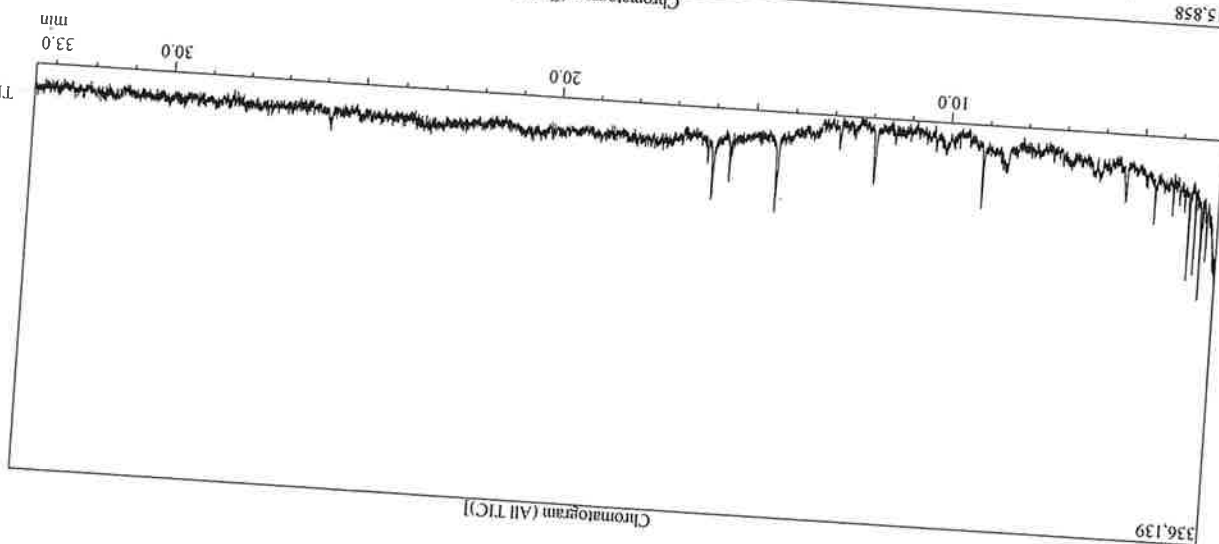
HelIndex: 897

Hit	Similarity	Compound Name	Mol Wt	Formula	Library
1	64	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
2	64	Triazolo(1,2,3,4,5-pentamethyl)cyclopenta-2,4-	335	C ₁₀ H ₁₅ GeN	NIST08.LIB
3	63	2-(N-Benzoyloxycarbonylamino)propanol	209	C ₁₁ H ₁₅ NO ₃	NIST08.LIB
4	63	3-Cyclohexen-1-ol, 1-methyl-	112	C ₇ H ₁₂ O	NIST08.LIB
5	62	Glycidol	74	C ₃ H ₆ O ₂	NIST08.LIB
6	62	1,3,4,5-Tetrahydro-2H-pyran-2-one	528	C ₅ H ₈ O ₂	NIST08.LIB
7	61	7-Methyloctene-2,4-dione, enol form	156	C ₉ H ₁₆ O ₄	NIST08.LIB
8	60	4,4,6-Trimethyltetrahydro-1,3-oxazine-2-thione	159	C ₇ H ₁₃ NO ₃	NIST08.LIB
9	60	3,3-Dimethyl-2-pentanone	114	C ₇ H ₁₄ O	NIST08.LIB
10	60	2,4,6,8,10-Tetradecapentanoic acid, S-isomer	606	C ₃₅ H ₇₀ O ₂	NIST08.LIB
11	60	1,3-Dimethyl-2-pentanol	114	C ₇ H ₁₄ O	NIST08.LIB

Target:



DAS# 64502-88-2 Mol Wt: 102 Serial#: 2241
 Cmpd Name: 1-Hydroxy-2-pentanone
 Formula: C₅H₁₀O₂
 Class Flag: No Class Flags
 Ret.Index: 887

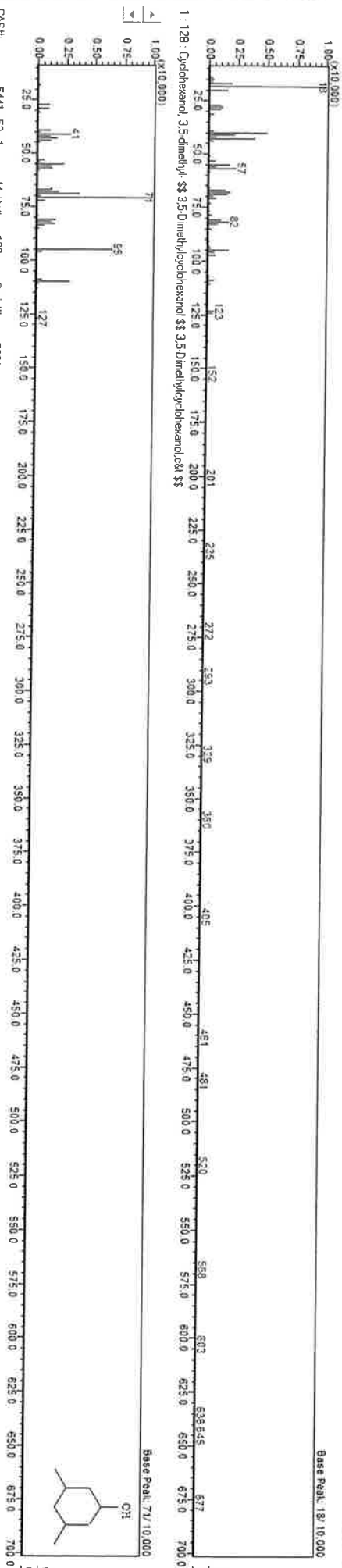


Similarity Search Results

Report View Compound Info Process Help

Hit	Similar	Peak	Compound Name	Mol Wt	Formula	Library
1	71	128	Cyclohexanol, 3,5-dimethyl- Cyclohexanol, 3,5-dimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	128	C8H16O	NIST08.LIB
2	70	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	142	C9H18O	NIST08.LIB
3	69	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	128	C8H16O	NIST08.LIB
4	69	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	240	C16H32O	NIST08.LIB
5	69	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	184	C12H24O	NIST08.LIB
6	69	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	128	C8H16O	NIST08.LIB
7	69	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	156	C10H20O	NIST08.LIB
8	69	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	134	C10H18O3	NIST08.LIB
9	68	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	144	C8H16O2	NIST08.LIB
10	68	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	194	C12H24O	NIST08.LIB
11	68	128	Cyclohexanol, 3,3,5-trimethyl- 3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS 11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen- Hexanol-1, 5-epidihexyl SS Cyclohexanethiol 2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS 2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2- Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS 7-Octene-1,2-diol trans-2-Dodecen-1-ol 1-Pentadecanecarboximide SS 1-Pentadecanecarboximide	124	C7H12N2	NIST08.LIB

Target

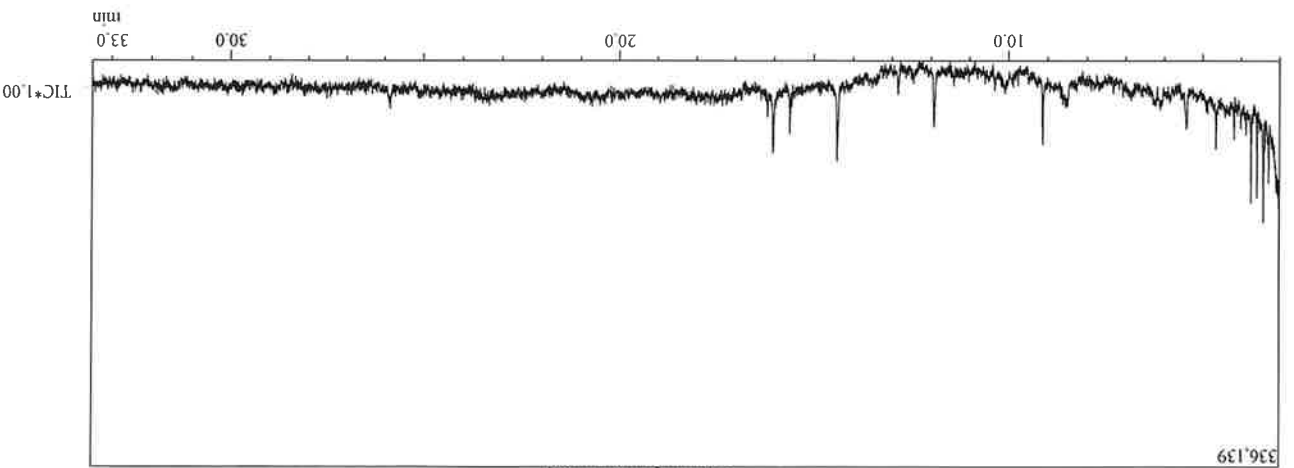


1: 128: Cyclohexanol, 3,5-dimethyl-
Cyclohexanol, 3,5-dimethyl-
3-Octen-1-ol SS (2E)-3-Octen-1-ol # SS
11-Hexadecen-1-ol (Z)-SS (Z)-11-Hexadecen-
Hexanol-1, 5-epidihexyl SS Cyclohexanethiol
2-Octen-1-ol SS Oct-2-en-1-ol SS 2-Octenol SS
2-Decen-1-ol SS trans-2-Decen-1-ol SS (2E)-2-
Bicyclo[2.2.2]octane-1,4-diol, monoacetate SS
7-Octene-1,2-diol
trans-2-Dodecen-1-ol
1-Pentadecanecarboximide SS 1-Pentadecanecarboximide

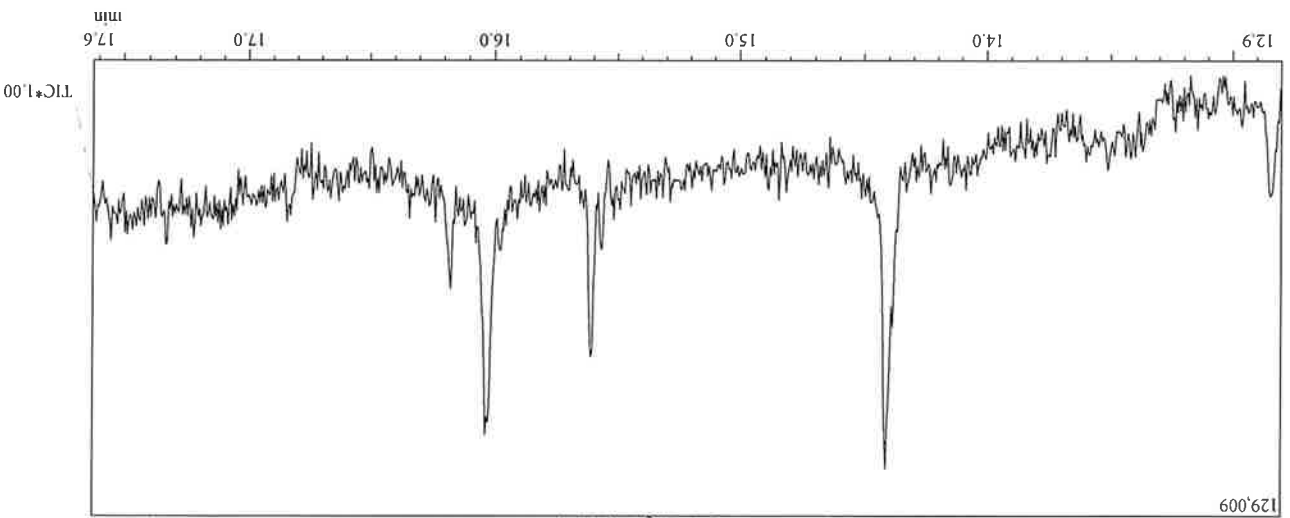
CAS#: 5441-52-1 Mol Wt: 128 Serial#: 7351
Cmpd Name: Cyclohexanol, 3,5-dimethyl-
Formula: C8H16O Class Flag: No Class Flags

Rel Index: 1030

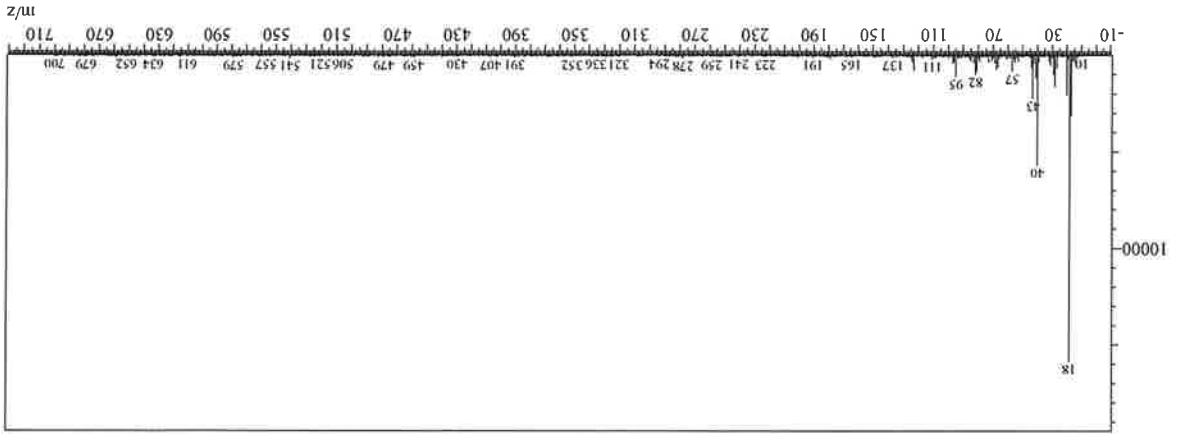
Chromatogram (All TIC)



Chromatogram (Zoom)



Spectrum

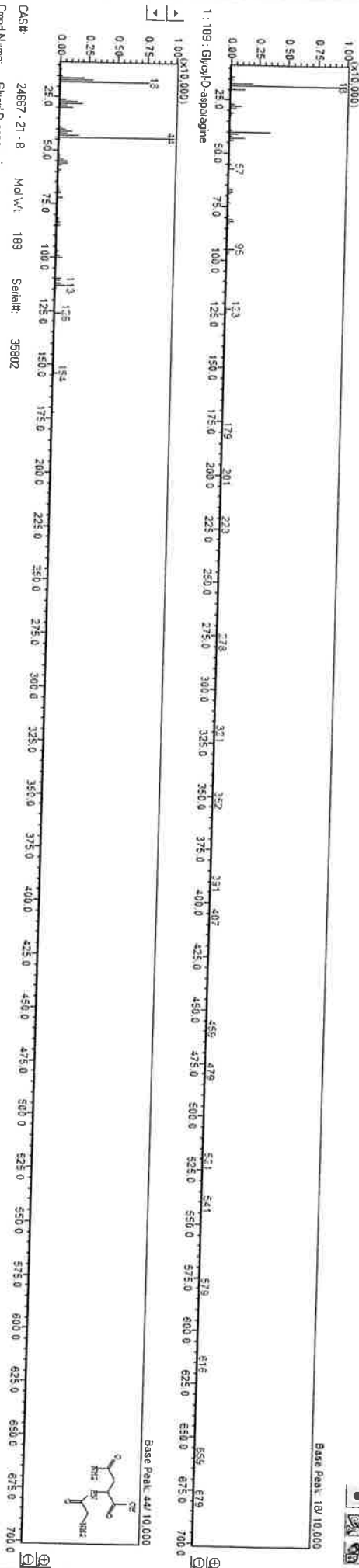


Line#: 1 R.Time: 12.850 (Scan#: 1971)
MassPeaks: 589
RawMode: Single 12.850 (1971) BasePeak: 18.10 (15865)
BG Mode: None Group 1 - Event 1

41720

Hit	Similar Key	Compound Name	Mol Wt	Formula	Library
1	53	Glycyl-D-asparagine	189	C ₈ H ₁₁ N ₃ O ₄	NIST08.LIB
2	54	trans-1,4-Cyclohexanediene S5 1,4-Diamino	114	C ₆ H ₁₄ N ₂	NIST08.LIB
3	53	1-Hydroxy-2-pentanone S5 2-Pentanone, 1-Hy	102	C ₅ H ₁₀ O ₂	NIST08.LIB
4	63	7-Hydroxyamino-1,3,5-hexadecanediene	170	C ₁₆ H ₃₄ N ₂ O	NIST08.LIB
5	62	4-(4-Chlorophenyl)-3-methylpiperidine-2-carboxyl	320	C ₁₆ H ₁₇ ClN ₂	NIST08.LIB
6	62	3-Amino-1,2-propanediol S5 1-Aminopropan-2-ol	91	C ₃ H ₉ N ₂ O ₂	NIST08.LIB
7	62	2-Butenediol acid, 2-methyl-, (2Z)-S5 Citraconic	130	C ₆ H ₈ O ₄	NIST08.LIB
8	62	Acetonitrile, hydroxy-, S5 Glycolonitrile S5 Cyan	57	C ₂ H ₃ NO	NIST08.LIB
9	62	Cyclohexanone S5 4,4'-trimethyl-2-oxazoli	181	C ₁₁ H ₁₉ NO	NIST08.LIB
10	61	Heptanoic acid, 2-oxoethyl-, methyl ester S5	202	C ₁₀ H ₁₉ O ₄	NIST08.LIB
11	51	11-Aminocyclohexanone S5 11-Aminocyclohexan-1-one	150	C ₆ H ₁₁ N ₂ O	NIST08.LIB

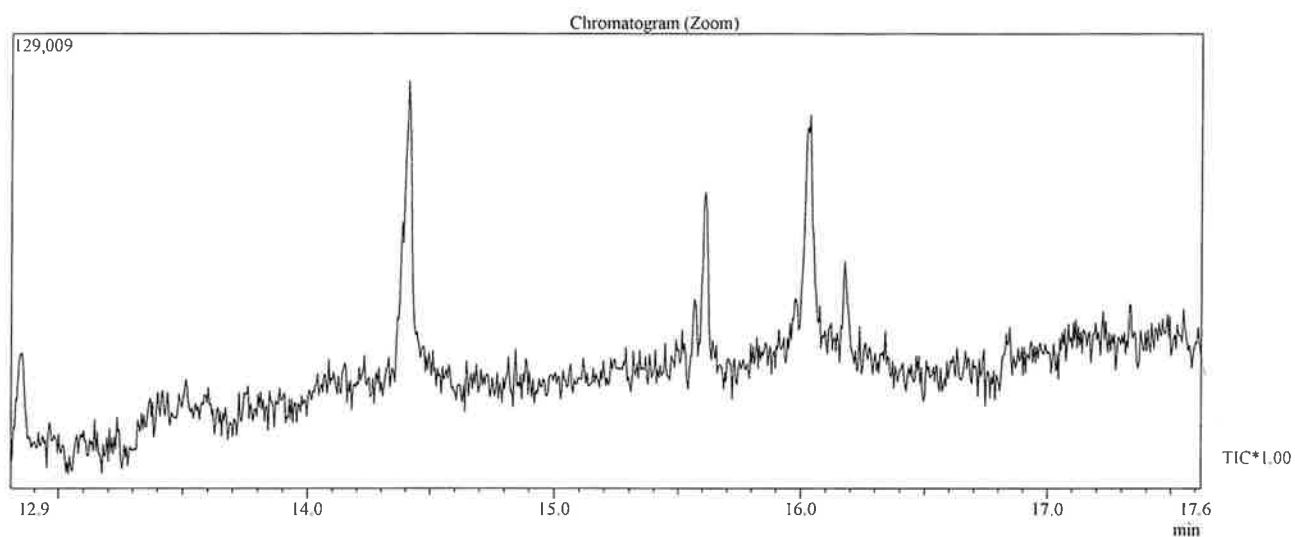
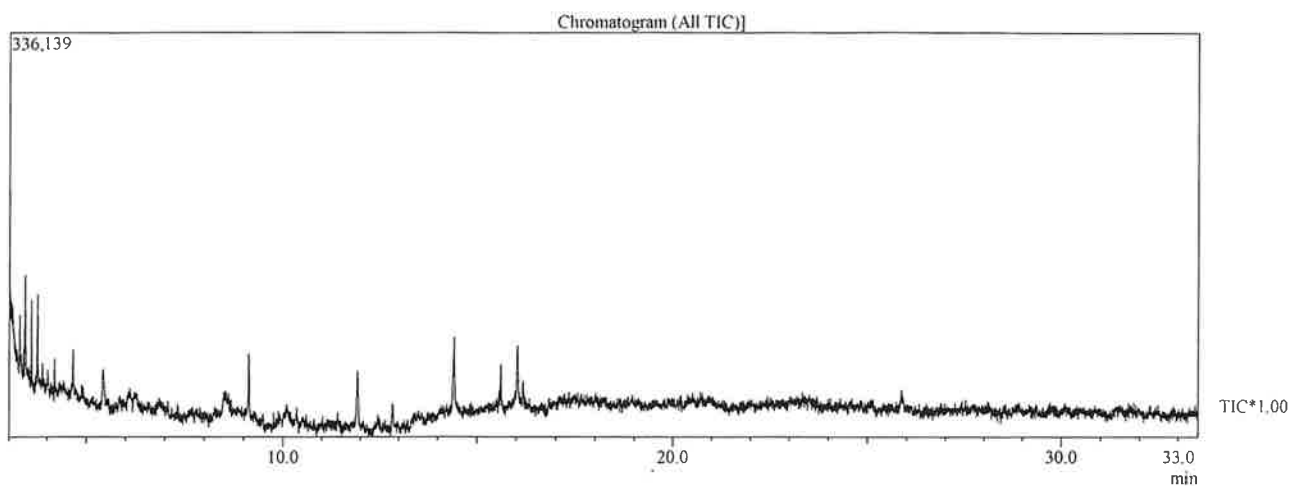
Target:



CAS#: 24667-21-8 Mol Wt: 189 Serial#: 36802
 Compd Name: Glycyl-D-asparagine
 Formula: C₈H₁₁N₃O₄ Class Flag: No Class Page

RelIndex: 1963

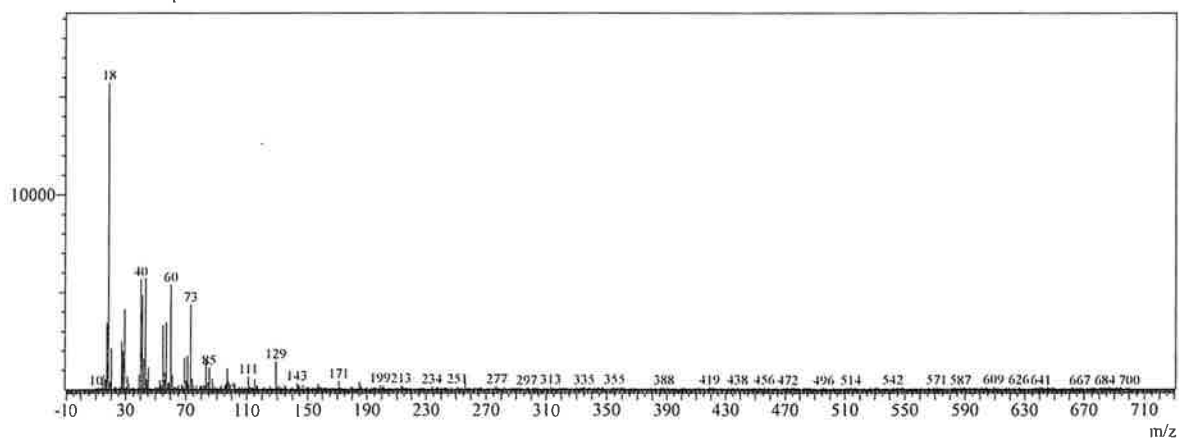
C:\MSsolution\Data\Project\1\MS Mathe\SAMPLE 3_UNKNOWN_20221130_3.qgd



Spectrum

Line#:1 R.Time:14.410(Scan#:2283)
MassPeaks:640
RawMode:Single 14.410(2283) BasePeak:18.10(15721)
BG Mode:None Group 1 - Event 1

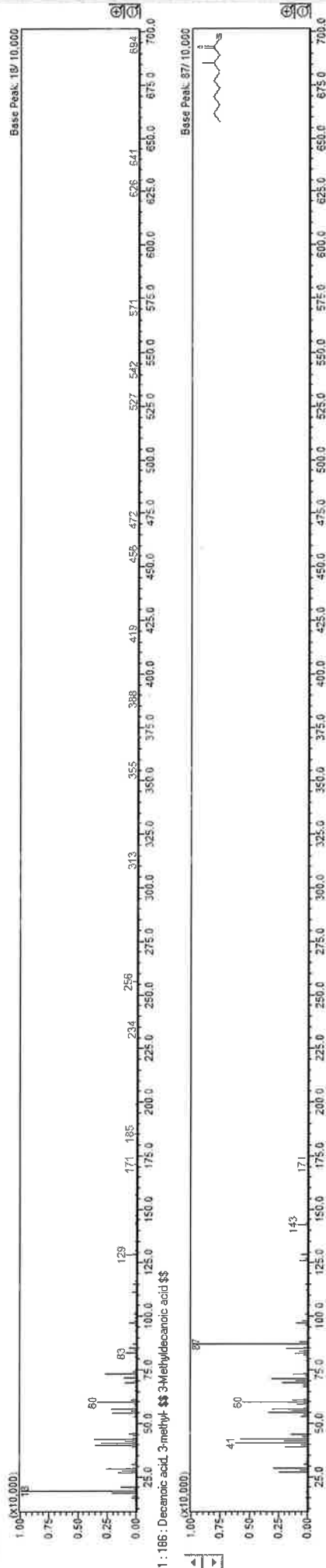
41677



Similarity Search Results

H#	Similar	Flags	Compound Name	Mol Wt	Formula	Library
1	73	✓	Pentanoic acid, 4-methyl-, \$S\$-Methyldecanoic	186	C ₁₁ H ₂₂ O ₂	NIST08.LIB
2	72		Pentanoic acid, 4-methyl-, \$S\$-valeric acid, 4-m	115	C ₆ H ₁₂ O ₂	NIST08.LIB
3	72		Octane, 1-methoxy-, \$S\$-Ethyl, octyl propyl, \$S\$-n-	172	C ₁₁ H ₂₄ O	NIST08.LIB
3	72		3-Heptanol, 2,4-dimethyl-, \$S\$-2,4-Dimethyl-3-he	144	C ₉ H ₂₀ O	NIST08.LIB
4	71		Nonanedioic acid, dihexyl ester, \$S\$-Aulalic aci	356	C ₂₁ H ₄₄ O ₄	NIST08.LIB
5	71		3-Octanol, 3,6-dimethyl-, \$S\$-AR 1, \$S\$-3,6-Dimet	158	C ₁₀ H ₂₂ O	NIST08.LIB
6	71		DL-Arabinose, \$S\$-Pentoprenase # \$S\$	150	C ₅ H ₁₀ O ₅	NIST08.LIB
7	71		beta-D-Glucopyranose \$S\$ Hexoprenase # \$	180	C ₆ H ₁₂ O ₆	NIST08.LIB
8	70		L-Galactose, 6-deoxy-, \$S\$-6-Deoxyhexose # \$S\$	164	C ₆ H ₁₂ O ₅	NIST08.LIB
9	70		3-Hexanol, 3-methyl-, \$S\$-2-Ethyl-2-pentanol \$S\$	115	C ₇ H ₁₆ O	NIST08.LIB
10	70		DL-Glucosamine iminic acid, \$S\$-Glucosamine iminic	194	C ₆ H ₁₂ N ₂ O ₄	NIST08.LIB
11	70					

Target:



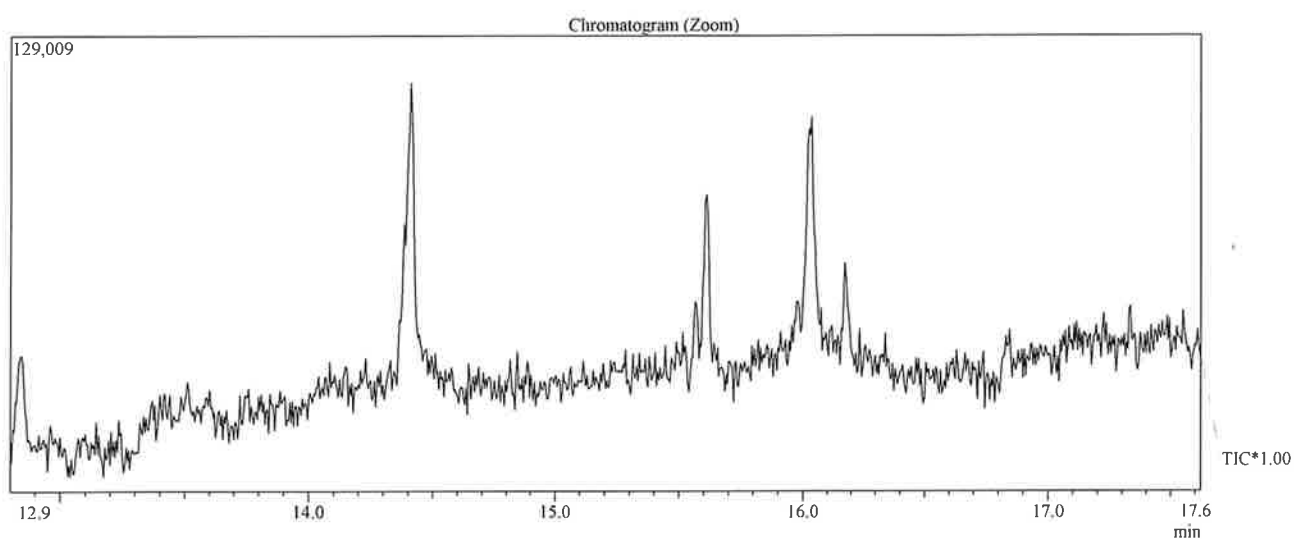
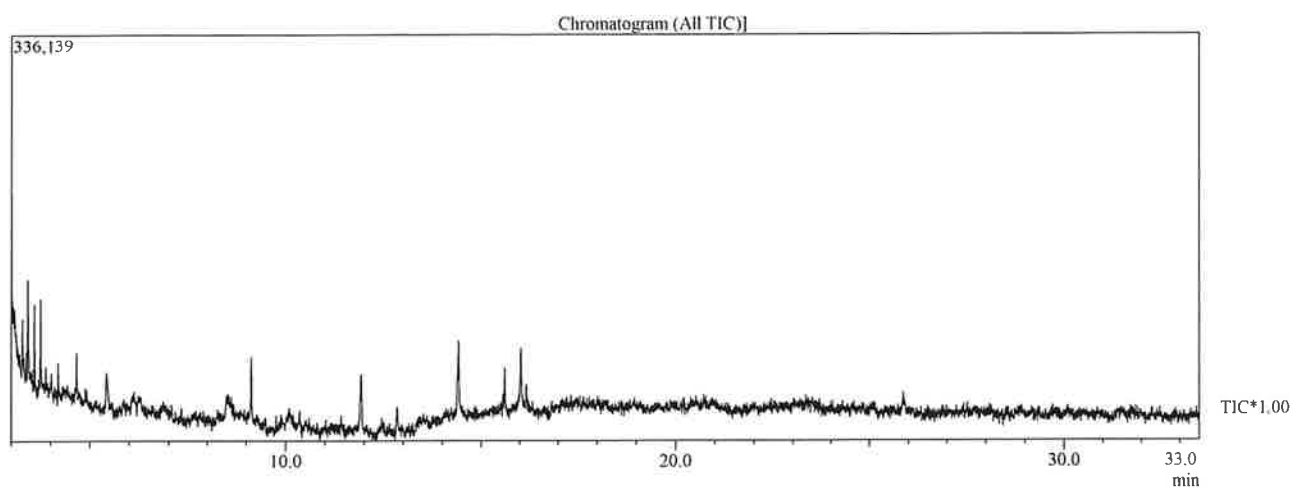
CAS#:	60308-82-9	Mol Wt:	186	Serial#:	34564
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Decanoic acid, 3-methyl- \$3-Methyldecanoic acid \$ \$

Formula:	C11H22O2	Class Flag:	No Class Flags:

Ret. Index: 1407

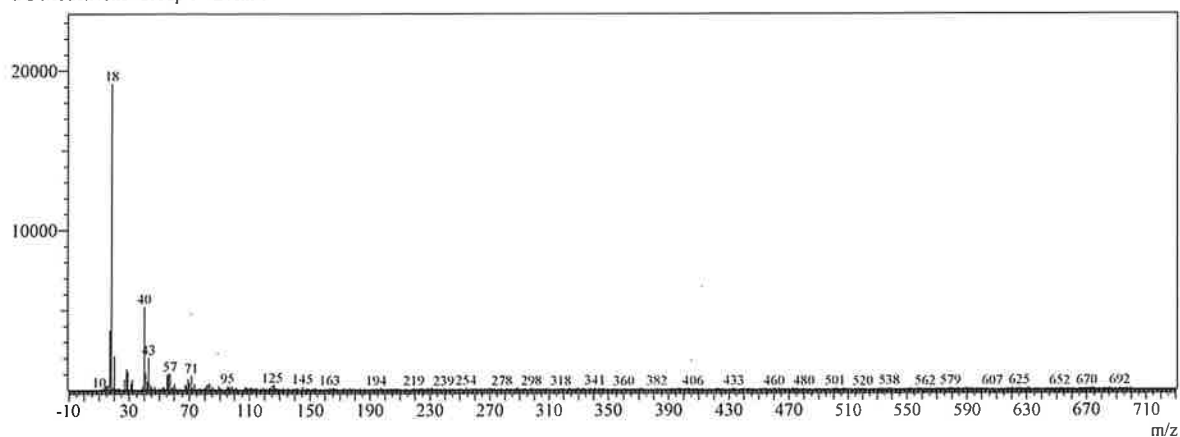
C:\GCMSsolution\Data\Project\1\Ms Mathe\SAMPLE 3_UNKNOWN_20221130_3.qgd



Spectrum

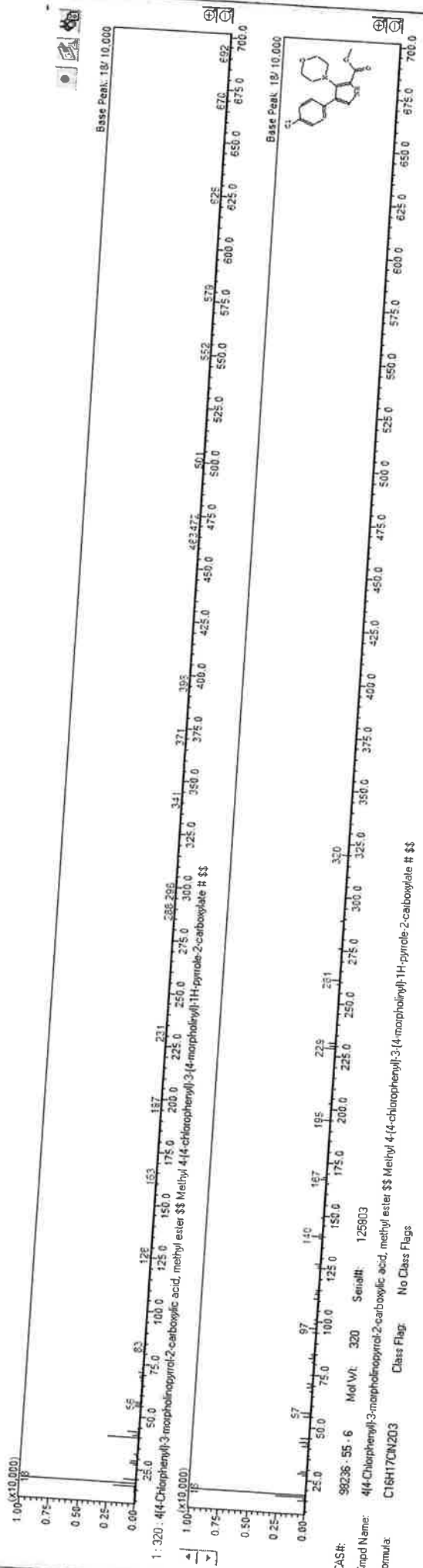
Line#:1 R.Time:15.575(Scan#:2516)
MassPeaks:631
RawMode:Single 15.575(2516) BasePeak:18.10(19174)
BG Mode:None Group 1 - Event 1

5.704



Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library
1	83		4-(4-chlorophenyl)-3-morpholinopropyl-2-carboxylate	320	C16H17ClN2O4	NIST08.LIB
2	67		Glycyl-D-asparagine	189	C8H11N3O4	NIST08.LIB
3	64		Water	18	H2O	NIST08.LIB
4	64		1-Hydroxy-2-pentanone	102	C5H10O2	NIST08.LIB
5	63		Heptenoic acid, 2-(acetyloxy)-, methyl ester	202	C10H18O4	NIST08.LIB
6	62		Guandine	99	CH5N3	NIST08.LIB
7	61		Glycidol	74	C3H6O2	NIST08.LIB
8	61		2-Azetidinone	99	C3H5NO	NIST08.LIB
9	61		3,4,4,6-Tetramethyltetrahydro-1,3-oxazin-2-one	157	C8H15NO2	NIST08.LIB
10	60		2-Butenedioic acid, 2-methyl-, (Z)-, SS Crystalline	130	C5H6O4	NIST08.LIB
11	60		pent-2-en-1-ol	117	C4H7NO3	NIST08.LIB

Target:



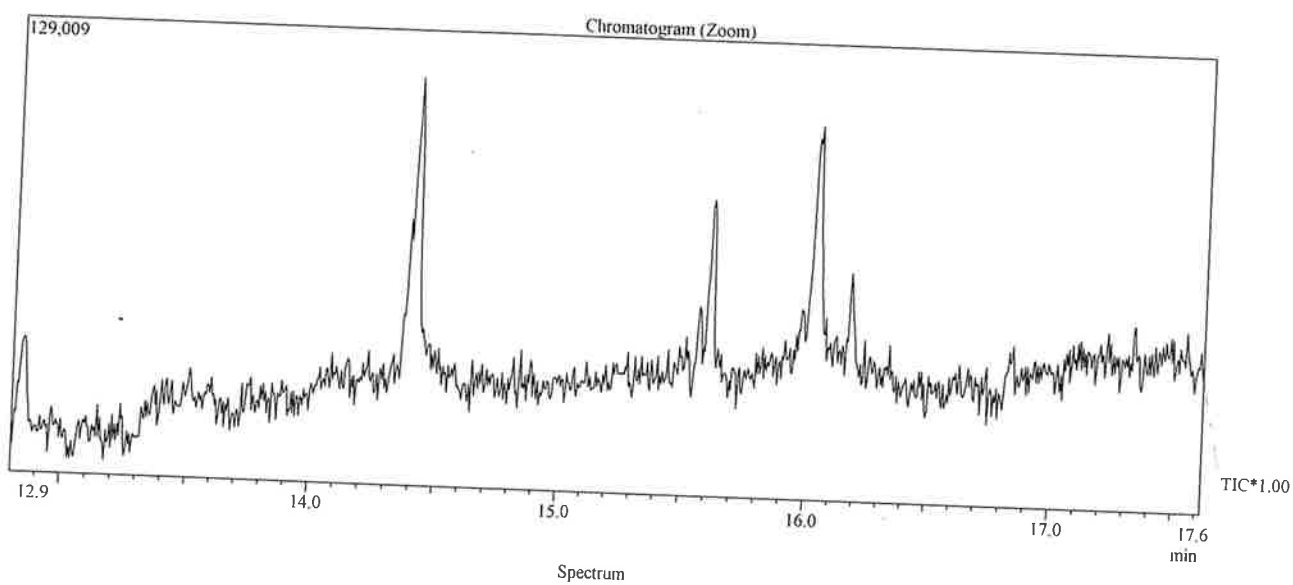
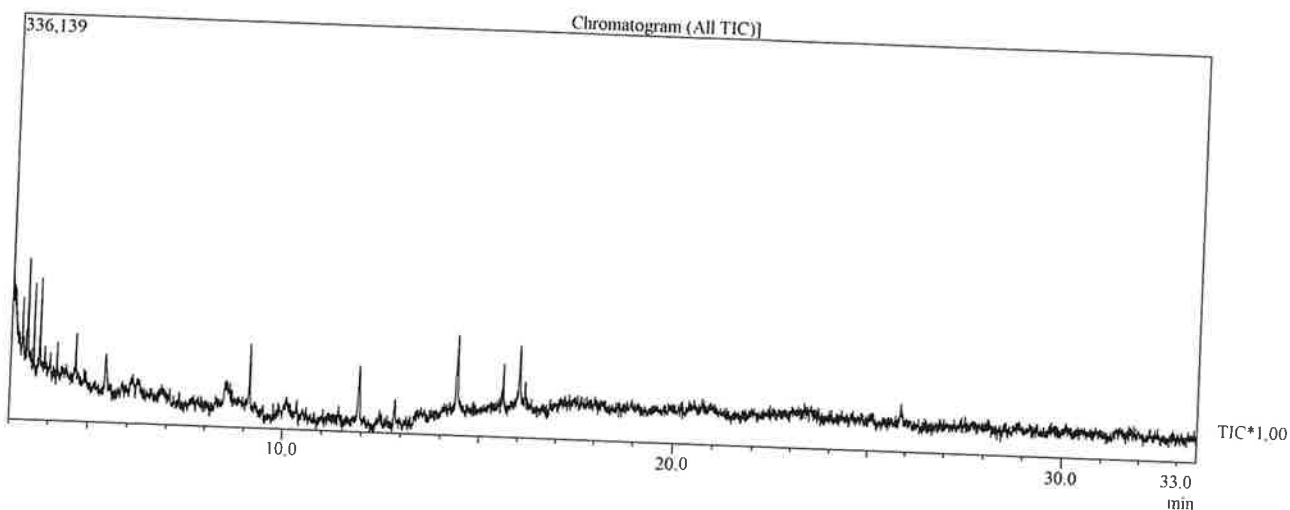
CAS# 98238-55-6 Mol Wt 320 Serial# 125803

Compound Name 4-(4-chlorophenyl)-3-morpholinopropyl-2-carboxylic acid, methyl ester

Formula C16H17ClN2O4 Class Flag No Class Flags

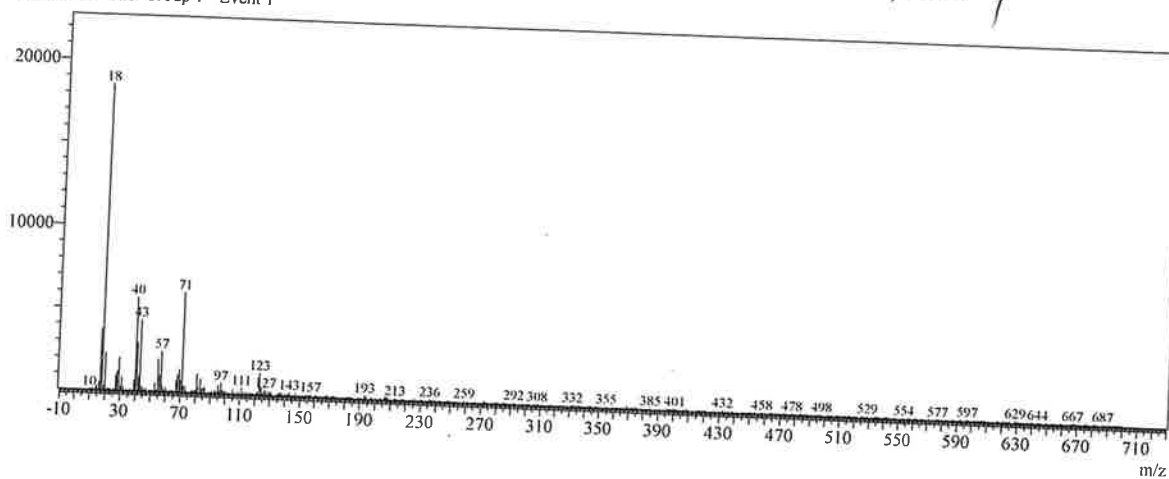
Ref Index 2600

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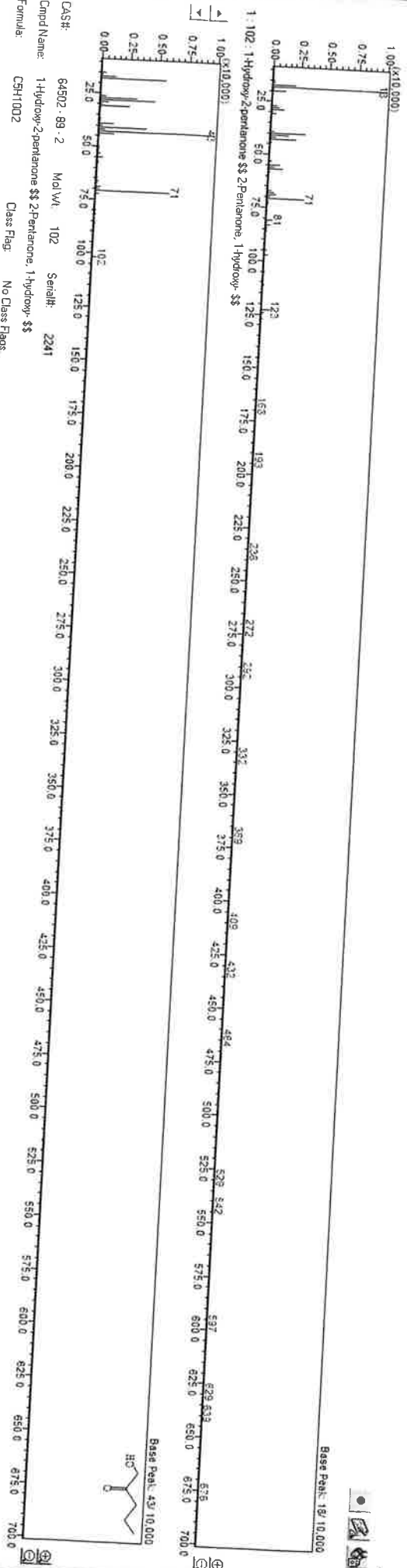
Line#:1 R.Time:15.610(Scan#:2523)
MassPeaks:627
RawMode:Single 15.610(2523) BasePeak:18,10(18518)
BG Mode:None Group 1 - Event 1

5,589



Hit	Similarity	Compound Name	Mol Wt	Formula	Library
1	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
2	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
3	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
4	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
5	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
6	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
7	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
8	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
9	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
10	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB
11	53	1-Hydroxy-2-pentanone	102	C ₅ H ₁₀ O ₂	NIST08.LIB

Target:

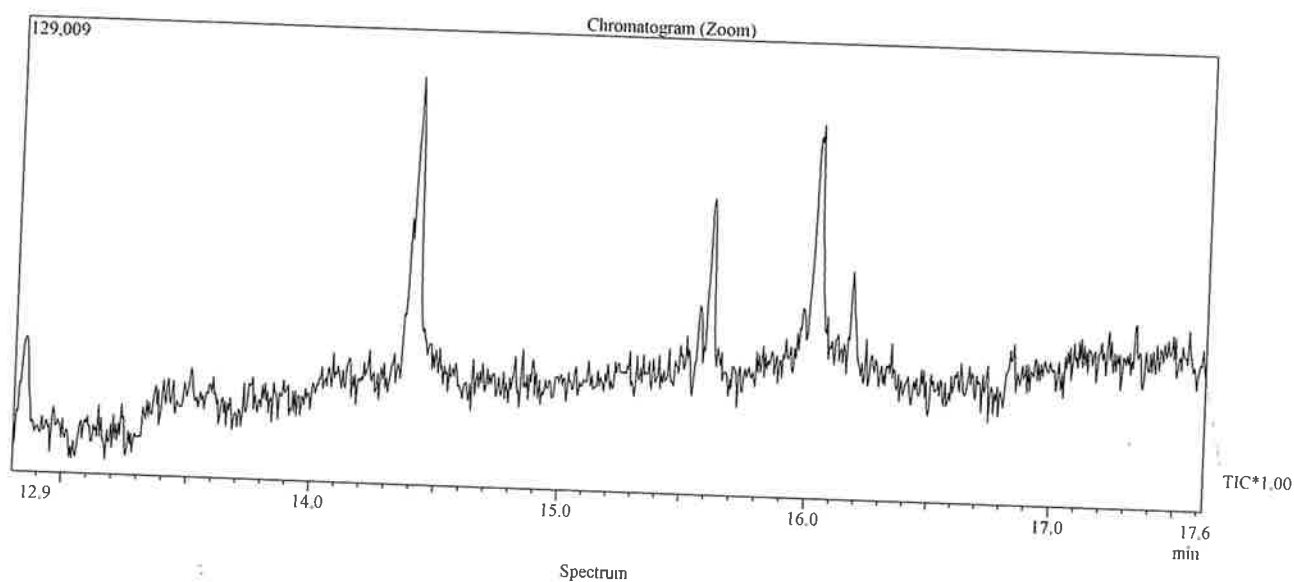
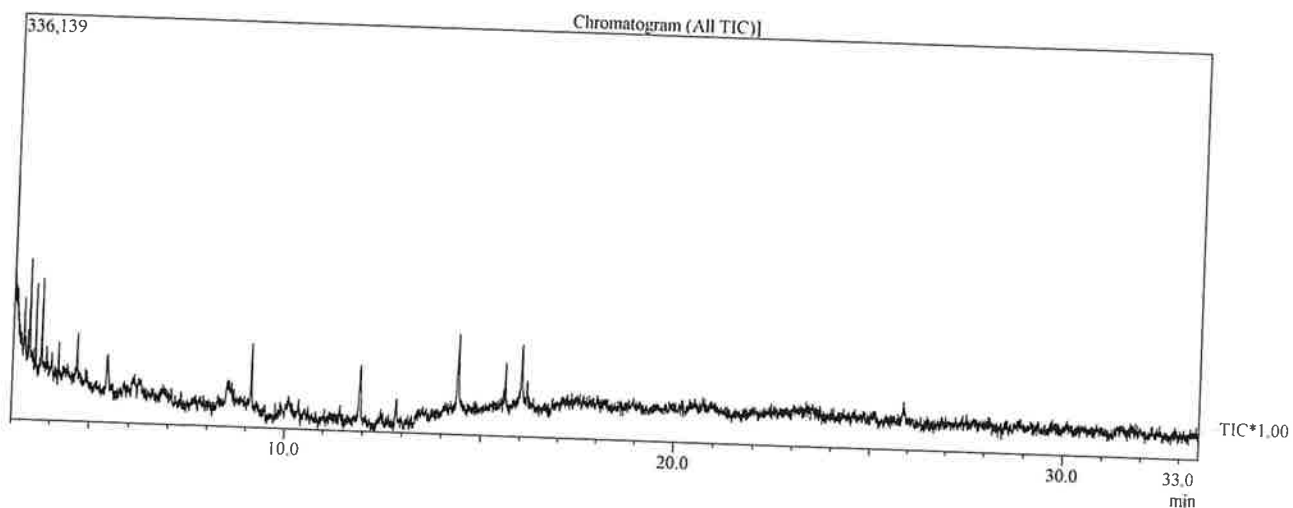


RelIndex: 897

CAS#: 64502-89-2 Mol Wt: 102 Serial#: 2241
 Compound Name: 1-Hydroxy-2-pentanone
 Formula: C₅H₁₀O₂ Class Flag: No Class Flags

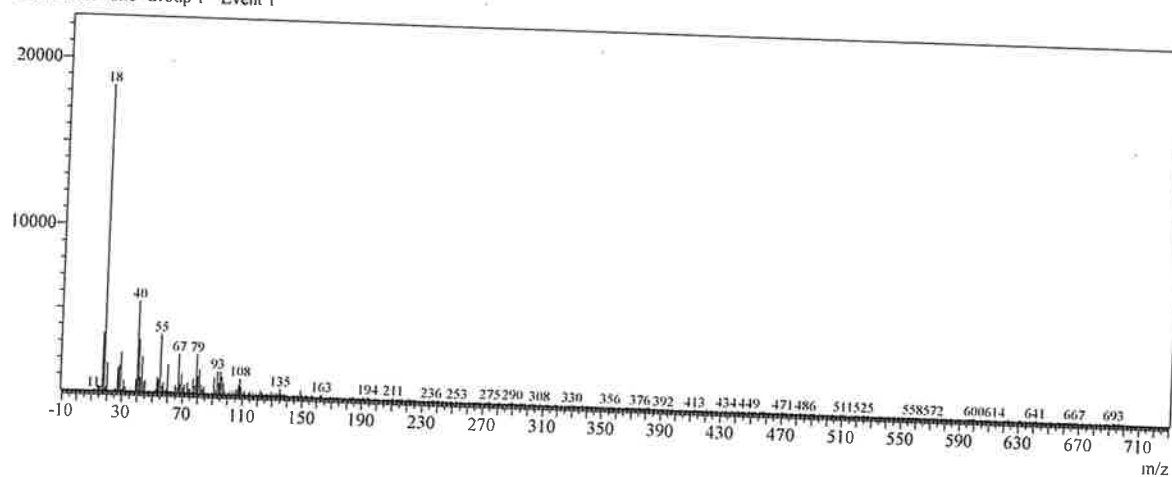


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Line#:1 R.Time:16.040(Scan#:2609)
MassPeaks:624
RawMode:Single 16.040(2609) BasePeak:18.15(18369)
BG Mode:None Group 1 - Event 1

5.465

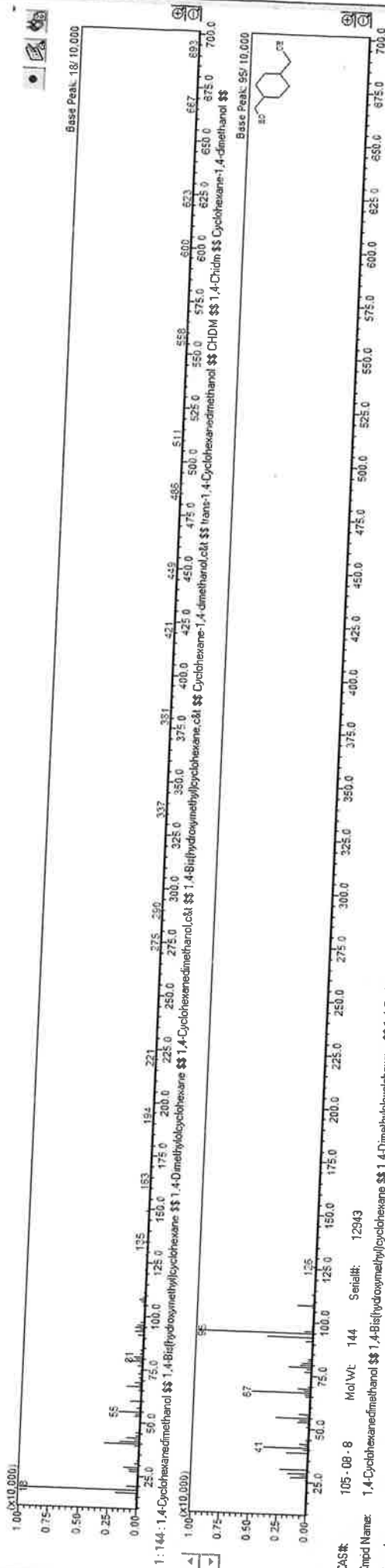


Similarity Search Results

Report View Compound Info Process Help

Hit	Similar	Regi	Compound Name	Mol Wt	Formula	Library
1	55	✓	1,4-Cyclohexanedimethanol SS 1,4-Bis(hydroxy	144	C8H16O2	NIST08.LIB
2	66	✓	7-Octene-1,2-diol	144	C8H16O2	NIST08.LIB
3	65	✓	2,4,6,8,10-Tetradecapentaenoic acid, Saffor	606	C36H60O8	NIST08.LIB
4	64	✓	2,7-Octadien-1-ol SS 1-Octa-2,7-dienol SS (2E)	126	C8H14O	NIST08.LIB
5	64	✓	1-(5-Oxopentylidene-2-ylamino)adamantane	234	C14H22N2O	NIST08.LIB
6	64	✓	Bicyclo[2.2.1]heptan-2-ol, endo- SS 2-Norborn	112	C7H12O	NIST08.LIB
7	64	✓	2,4-Heptadien-1-ol, (E,E)- SS (E,E)-2,4-Heptadi	112	C7H12O	NIST08.LIB
8	64	✓	Cycloheptanemethanol SS Cycloheptylmethan	128	C8H16O	NIST08.LIB
9	64	✓	3-Heptyn-1-ol	112	C7H12O	NIST08.LIB
10	64	✓	cis-Hexenyl octyne carbonate SS 2-Nonylnol	236	C15H24O2	NIST08.LIB
11	64	✓	2,4-Norbornadien-1-ol SS Norbornen-1-ol SS (7E) 4F	140	C7H10O	NIST08.LIB

Target:



CAS# 105-08-8 Mol Wt: 144 Serial#: 12943

Compd Name: 1,4-Cyclohexanedimethanol SS 1,4-Bis(hydroxymethyl)cyclohexane SS 1,4-Dimethylcyclohexane SS 1,4-Cyclohexanedimethanol.c&t

Formula: C8H16O2 Class Flag: No Class Flags.

Rel. Index 1327