LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.416	212	218	222	rBV	41102	66966	3.74%	0.537%
2	2.459	222	225	234	rVB	19160	31713	1.77%	0.254%
3	2.569	234	243	251	rBV2	21135	45706	2.55%	0.366%
4	4.635	574	582	595	rBV	12463	35319	1.97%	0.283%
5	5.464	705	718	730	rBV	139074	394742	22.03%	3.164%
6	5.629	734	745	760	rVB	237909	668786	37.32%	5.361%
7	6.031	799	811	823	rBV	141635	379390	21.17%	3.041%
8	6.830	931	942	954	rBV	357872	856684	47.81%	6.867%
9	7.184	993	1000	1010	rBV4	14749	48978	2.73%	0.393%
10	8.622	1229	1236	1241	rBV	28901	46995	2.62%	0.377%
11	8.696	1241	1248	1254	rVV	773735	1207661	67.39%	9.680%
12	8.763	1254	1259	1271	rVB	353903	573700	32.02%	4.598%
13	9.074	1304	1310	1315	rBV	12826	21031	1.17%	0.169%
14	10.098	1468	1478	1484	rBV	813890	1114763	62.21%	8.935%
15	11.122	1636	1646	1657	rBV	748192	941419	52.54%	7.546%
16	11.610	1720	1726	1730	rBV	19498	26276	1.47%	0.211%
17	11.878	1764	1770	1774	rBV4	11428	18928	1.06%	0.152%
18	12.061	1795	1800	1807	rVB	975035	1180977	65.90%	9.466%
19	12.256	1826	1832	1859	rBV	1312990	1791952	100.00%	14.363%
20	13.006	1950	1955	1967	rBV	128143	196706	10.98%	1.577%
21	13.109	1967	1972	1973	rBV	159782	187574	10.47%	1.503%
22	13.134	1973	1976	1993	rVB	582413	904072	50.45%	7.246%
23	13.378	2012	2016	2020	rVB	70343	87007	4.86%	0.697%
24	13.457	2023	2029	2037	rBV	265732	377636	21.07%	3.027%
25	13.548	2041	2044	2049	rBV4	14239	22156	1.24%	0.178%
26	13.628	2053	2057	2060	rBV	56251	64545	3.60%	0.517%
27	13.731	2071	2074	2076	rBV2	23555	27990	1.56%	0.224%
28	13.768	2076	2080	2081	rVV2	55608	70340	3.93%	0.564%
29	13.786	2081	2083	2089	rVB2	93343	117894	6.58%	0.945%
30	13.871	2094	2097	2098	rVV2	36655	48163	2.69%	0.386%
31	13.896	2098	2101	2103	rVV	116342	153969	8.59%	1.234%
32	13.926	2103	2106	2128	rVB	263901	509797	28.45%	4.086%
33	14.231	2152	2156	2171	rVB4	29806	54314	3.03%	0.435%
34	14.524	2201	2204	2209	rVB7	12574	18200	1.02%	0.146%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Title : SW846 8260

35	14.603	2213	2217	2220	rBV3	17629	24260	1.35%	0.194%
36	14.664	2224	2227	2233	rVB6	16610	27700	1.55%	0.222%
37	15.609	2377	2382	2388	rBV	85978	131753	7.35%	1.056%

Sum of corrected areas: 12476062

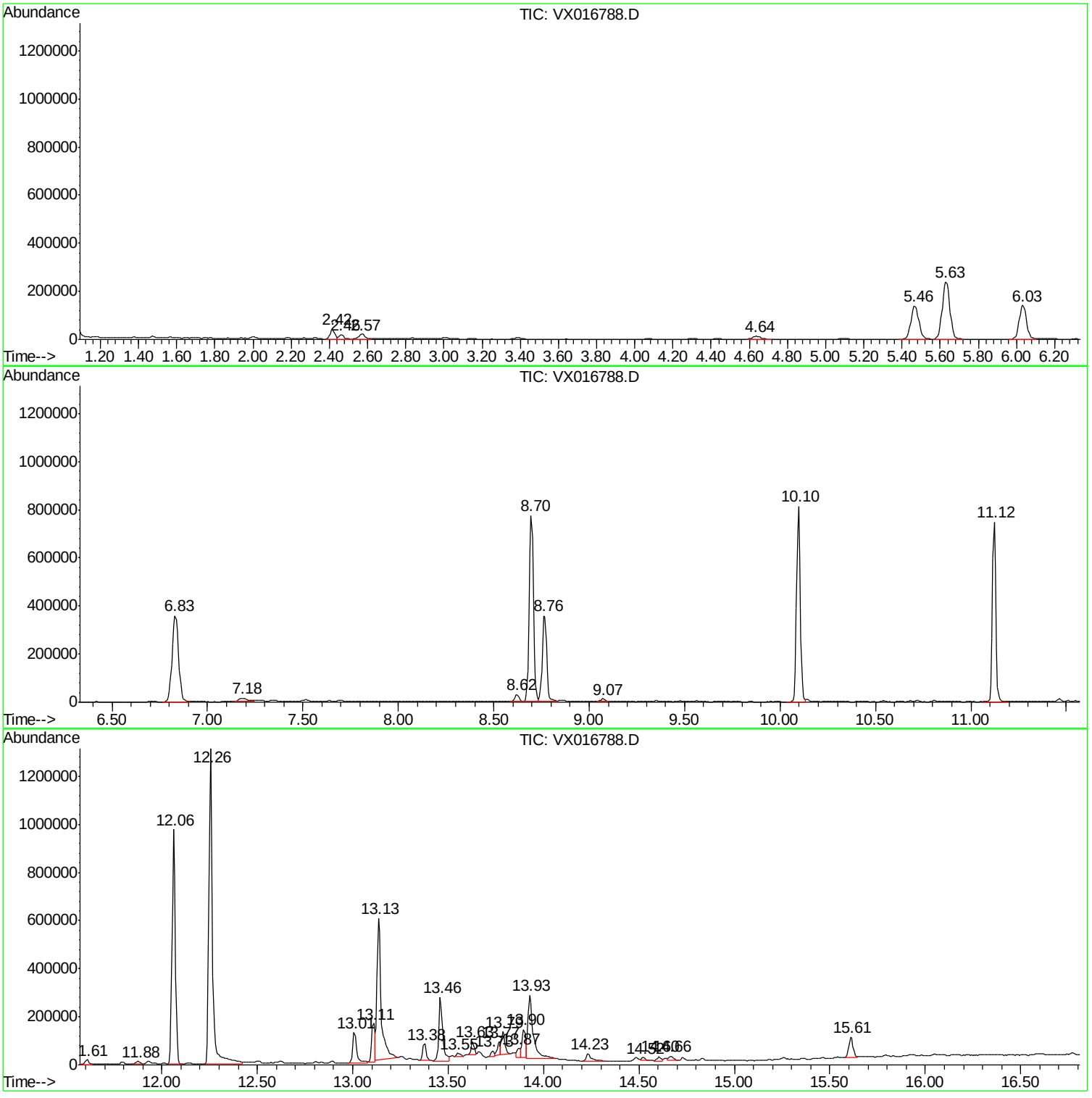
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

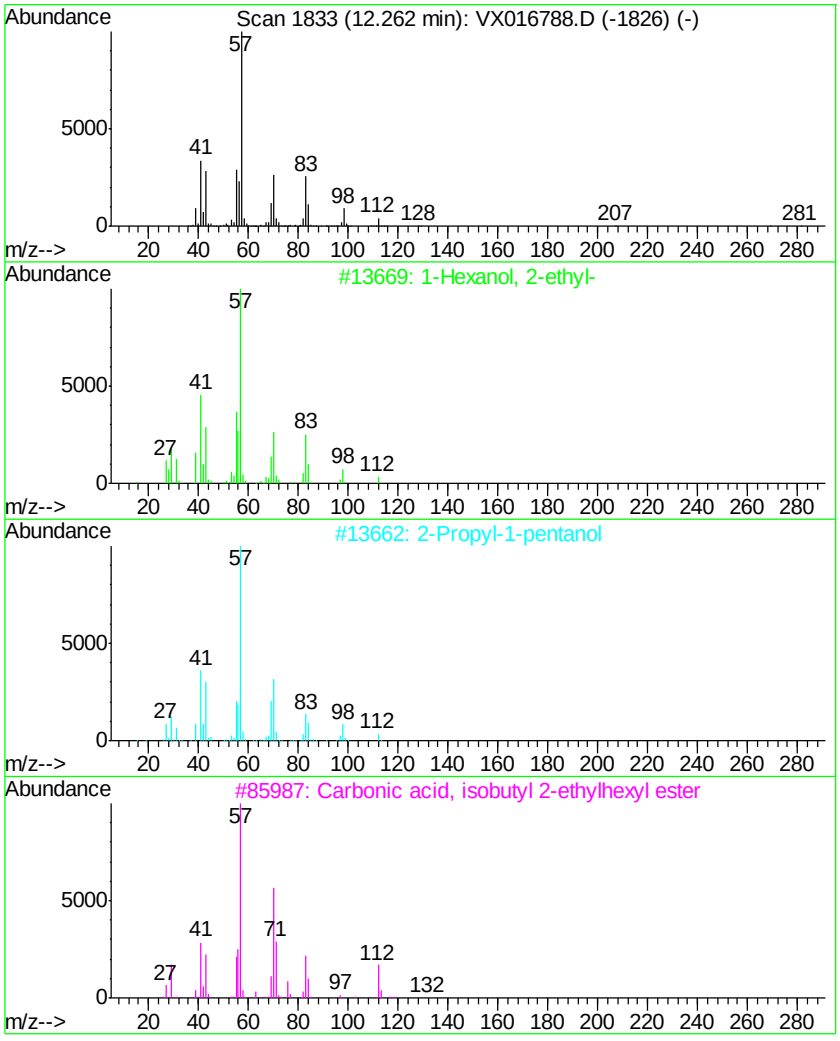
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

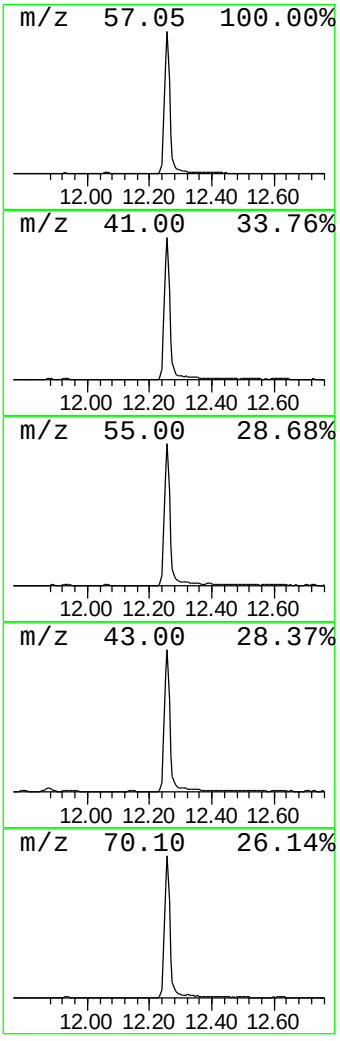
****

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	75.87 ug/l	1791950	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

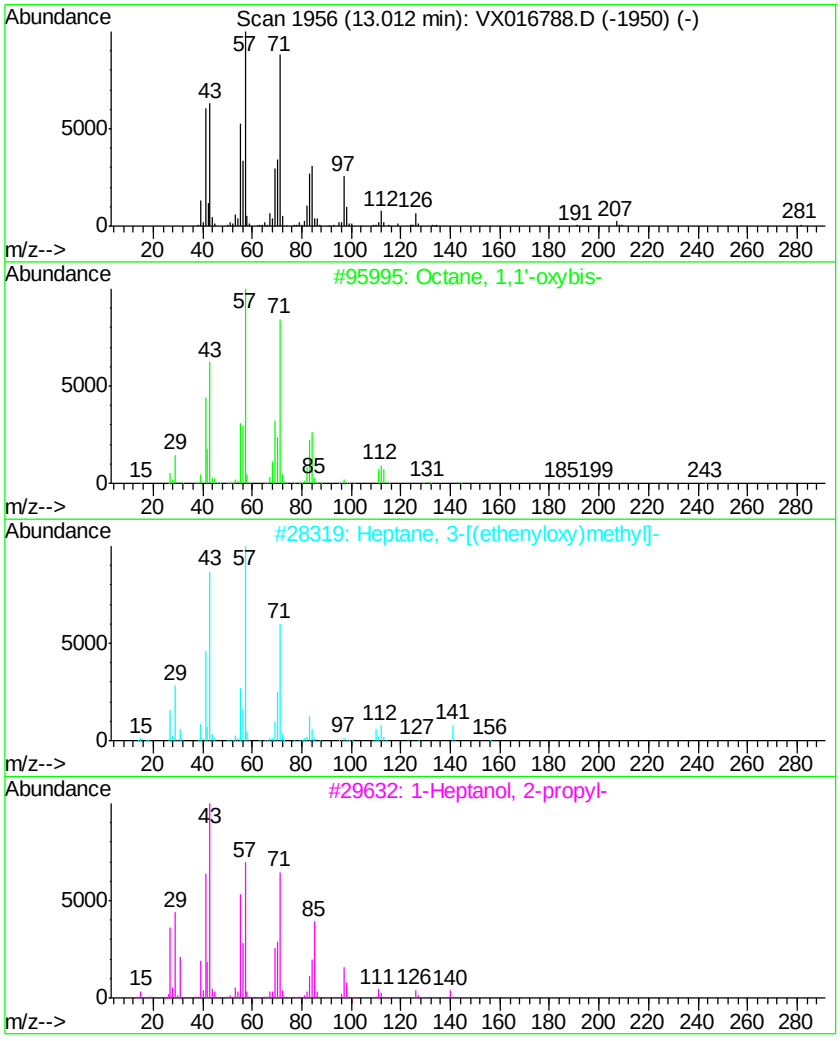
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

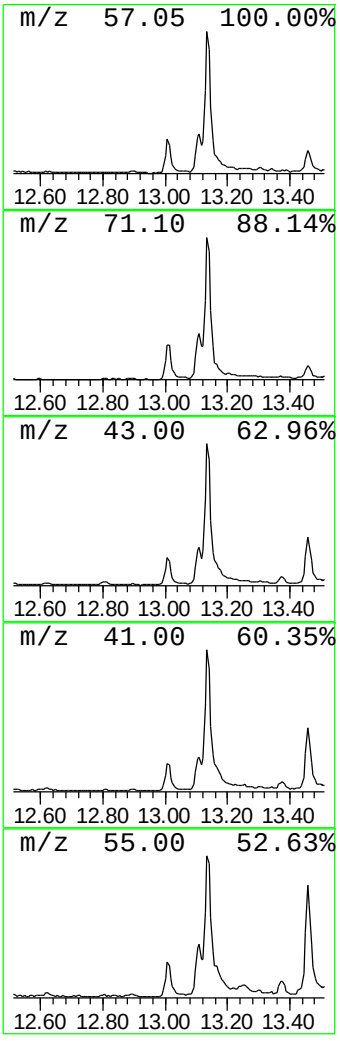
****

Peak Number 2 Octane, 1,1'-oxybis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	8.33 ug/l	196706	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
2	Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	50
3	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	50
4	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	47
5	Octane, 3-ethyl-	142	C10H22	005881-17-4	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

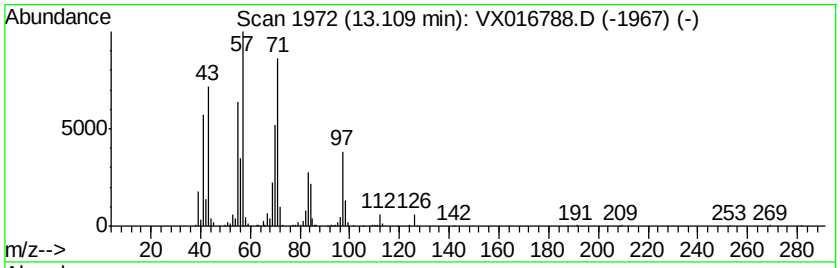
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

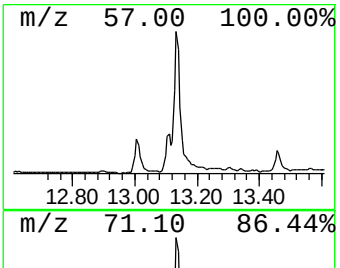
****

Peak Number 3 Oxalic acid, decyl 2-ethylh... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	7.94 ug/l	187574	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, decyl 2-ethylhexyl ...	342	C20H38O4	1000309-39-3	59
2	Octane, 3-ethyl-	142	C10H22	005881-17-4	43
3	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	38
4	Oxalic acid, octyl propyl ester	244	C13H24O4	1000309-26-1	38
5	1-Octene, 3-methyl-	126	C9H18	013151-08-1	30





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

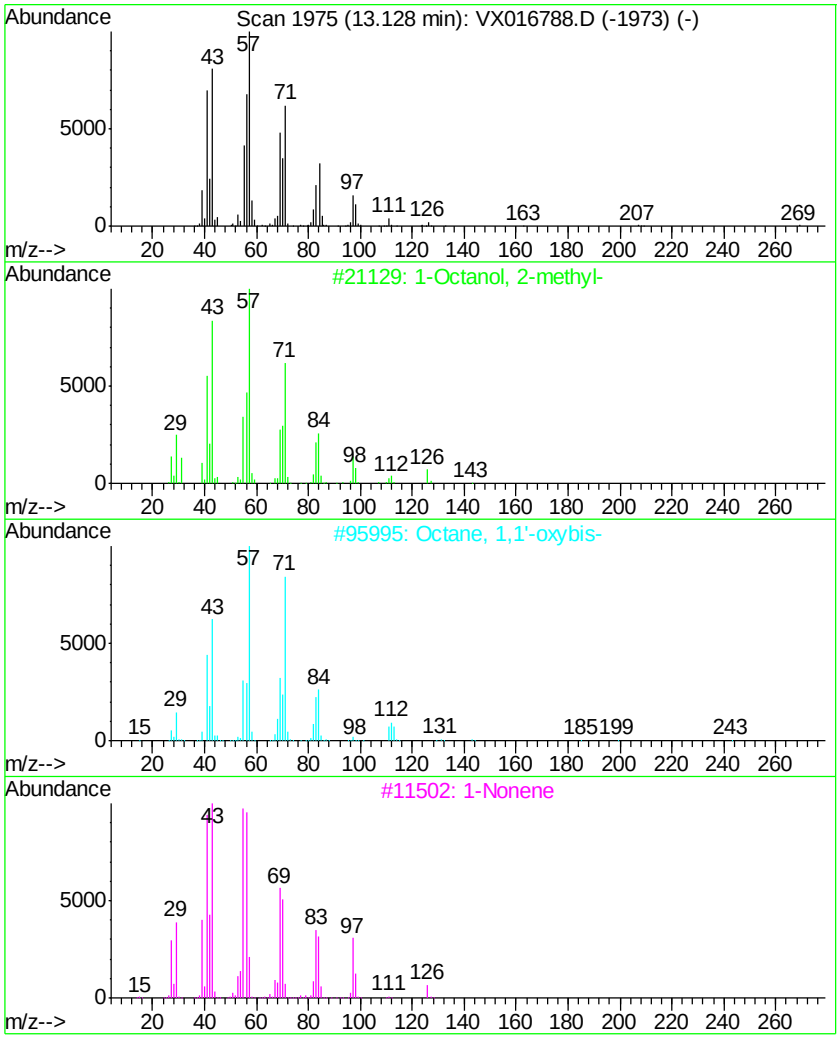
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

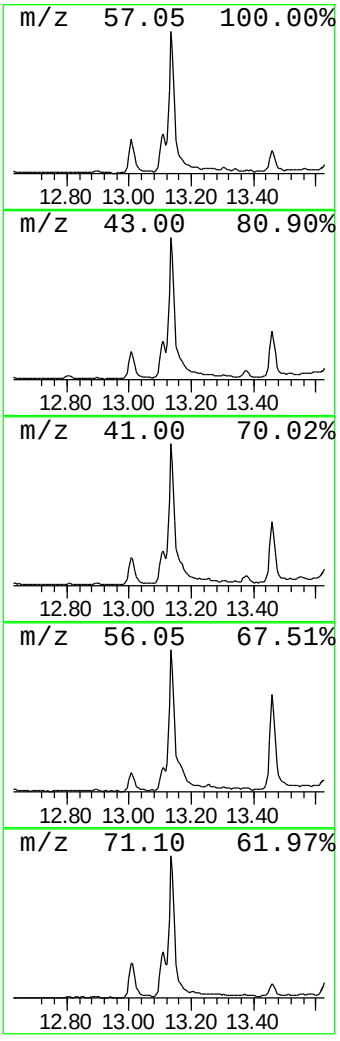
****

Peak Number 4 1-Octanol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	38.28 ug/l	904072	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	78
2	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	59
3	1-Nonene	126	C9H18	000124-11-8	58
4	Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	49
5	1-Heptene, 6-methyl-	112	C8H16	005026-76-6	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

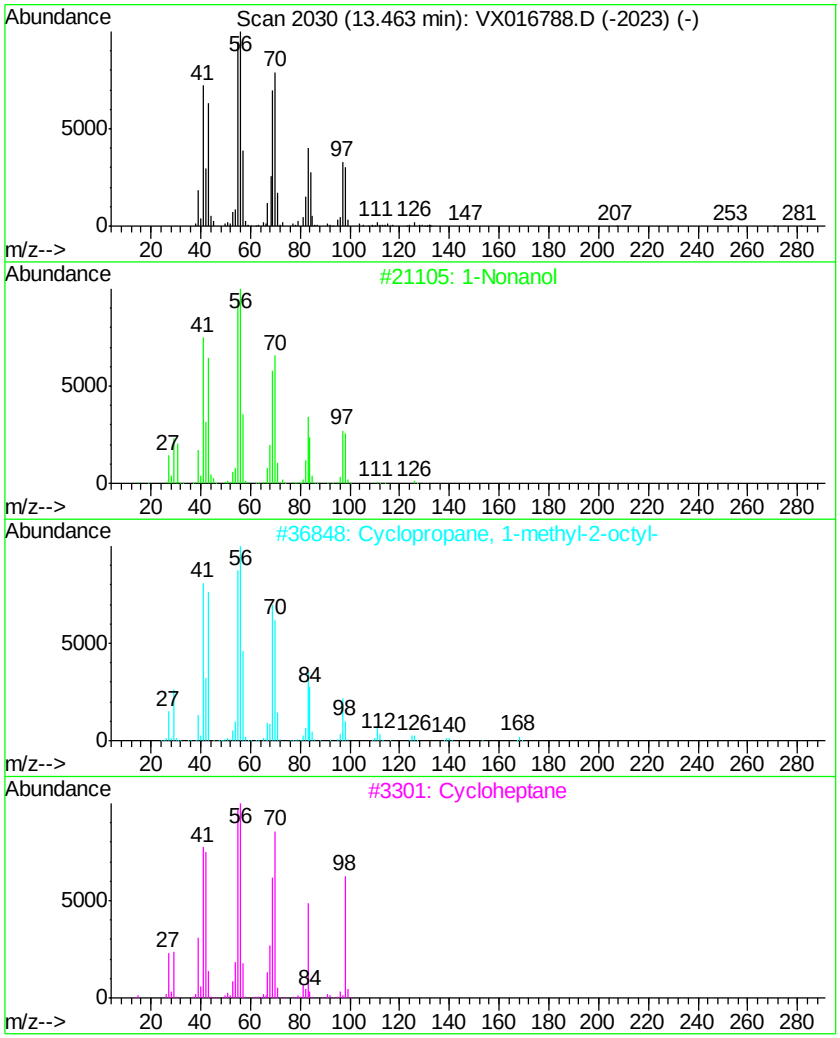
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

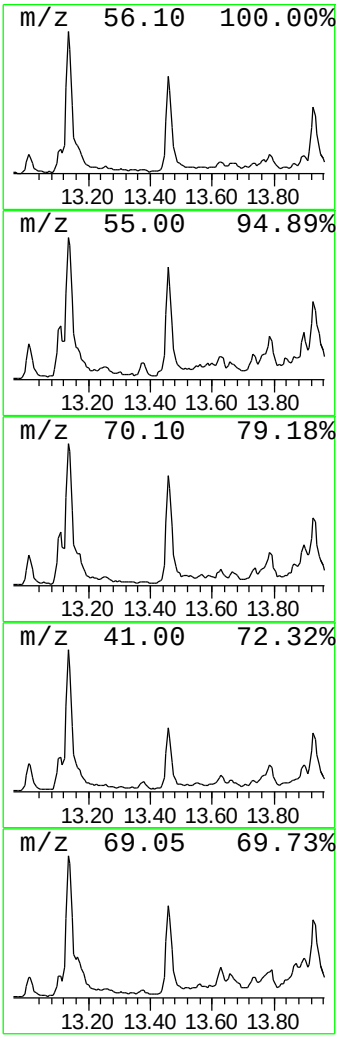
****

Peak Number 5 1-Nonanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	15.99 ug/l	377636	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	86
3	Cycloheptane	98	C7H14	000291-64-5	74
4	Cyclopropane, octyl-	154	C11H22	001472-09-9	72
5	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

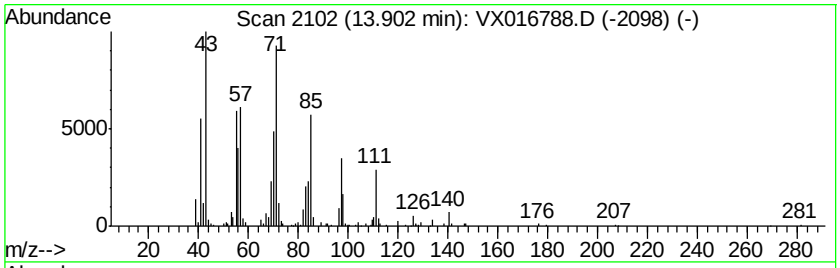
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

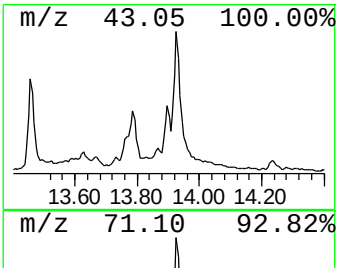
****

Peak Number 6 L-Homoserine lactone, N,N-d... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	6.52 ug/l	153969	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Homoserine lactone, N,N-dimethyl-	129	C6H11NO2	1000374-45-7	76
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50
3	Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	47
4	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	38
5	Acetic acid, trifluoro-, nonyl e...	240	C11H19F3O2	030767-14-7	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

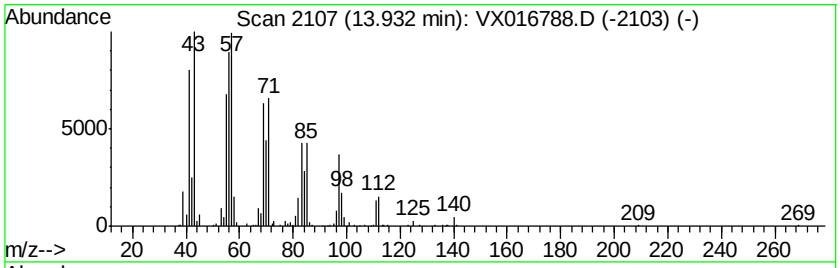
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

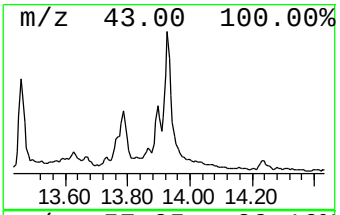
****

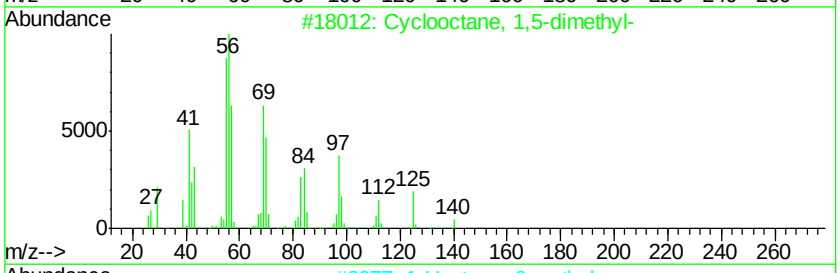
Peak Number 7 Cyclooctane, 1,5-dimethyl- Concentration Rank 3

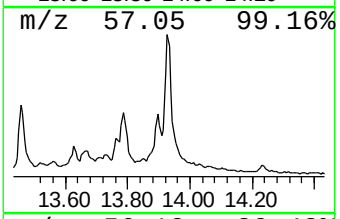
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	21.58 ug/l	509797	1,4-Dichlorobenzene-d4	12.06

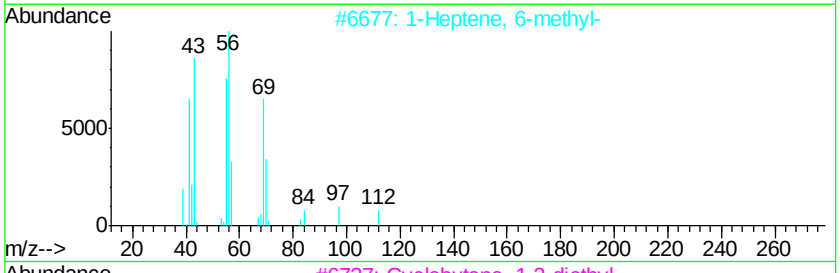
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	78
2	1-Heptene, 6-methyl-	112	C8H16	005026-76-6	46
3	Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	46
4	3-Tetradecene, (E)-	196	C14H28	041446-68-8	43
5	1-Dodecene	168	C12H24	000112-41-4	43

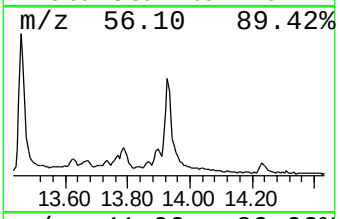


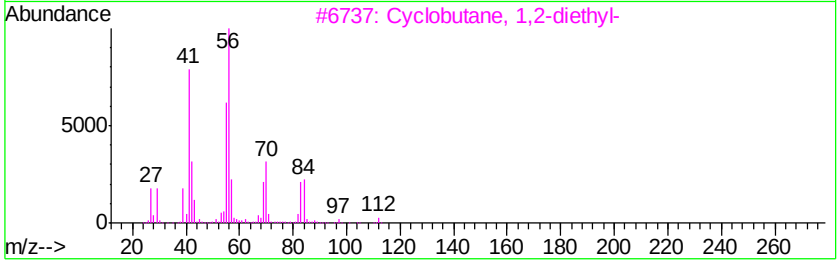


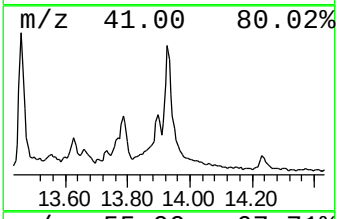


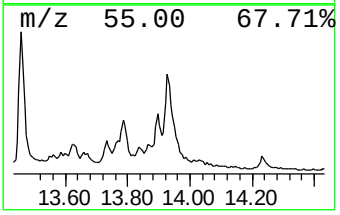












Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

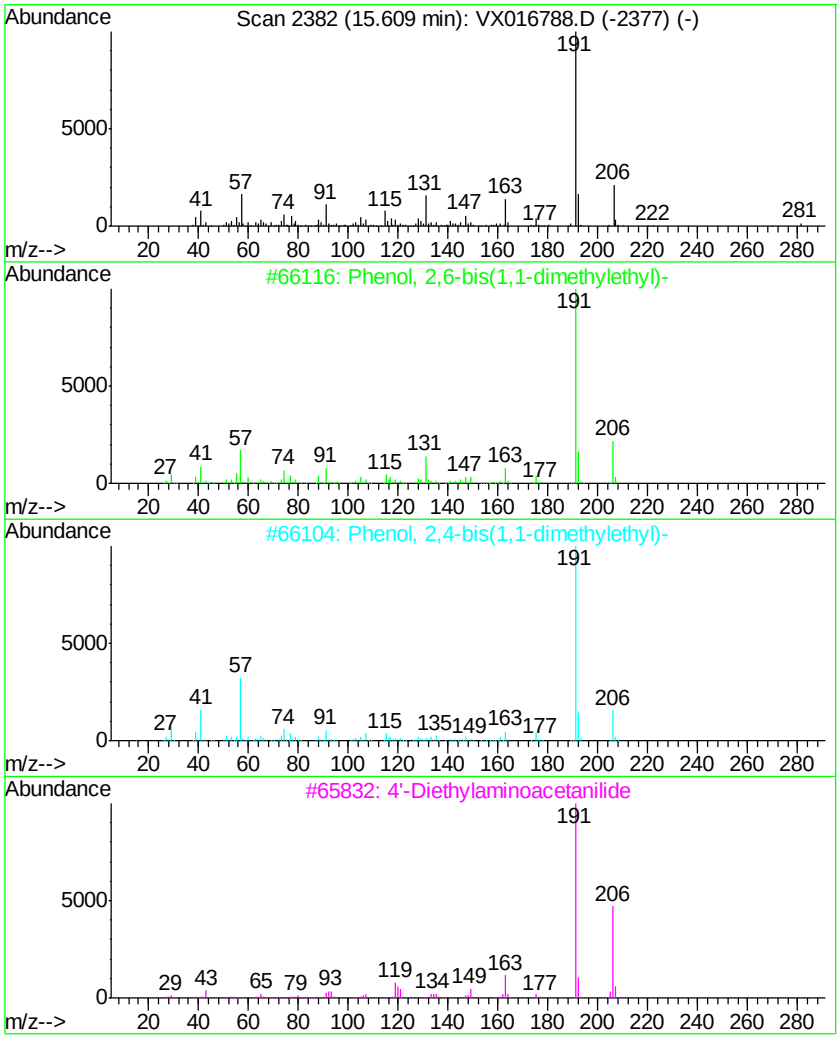
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

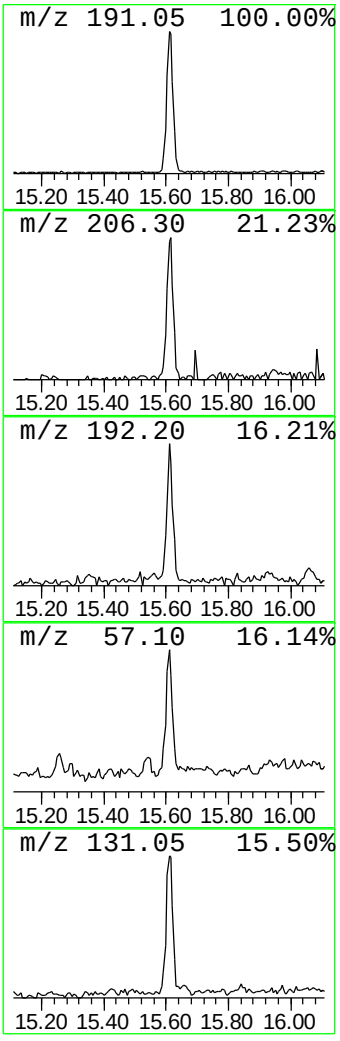
****

Peak Number 8 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	5.58 ug/l	131753	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	97
2	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	86
3	4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	83
4	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	83
5	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061620\
Data File : VX016788.D
Acq On : 16 Jun 2020 18:31
Operator : JC/SP
Sample : L2986-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16-20-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061520W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-ethyl-	12.26	75.9	ug/l	1791950	4	12.06	1180980	50.0
Octane, 1,1'-oxybis-	13.01	8.3	ug/l	196706	4	12.06	1180980	50.0
Oxalic acid, decy...	13.11	7.9	ug/l	187574	4	12.06	1180980	50.0
1-Octanol, 2-methyl-	13.13	38.3	ug/l	904072	4	12.06	1180980	50.0
1-Nonanol	13.46	16.0	ug/l	377636	4	12.06	1180980	50.0
L-Homoserine lact...	13.90	6.5	ug/l	153969	4	12.06	1180980	50.0
Cyclooctane, 1,5-...	13.93	21.6	ug/l	509797	4	12.06	1180980	50.0
Phenol, 2,6-bis(1...	15.61	5.6	ug/l	131753	4	12.06	1180980	50.0