LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

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\82X110718W.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	5.507	702	714	728	rBV	76986	223553	3.37%	0.329%
2	5.653	728	738	755	rVB2	137271	399808	6.03%	0.589%
3	6.068	794	806	820	rBV	81965	222468	3.36%	0.328%
4	6.860	924	936	955	rBV	211160	494952	7.47%	0.729%
5	8.714	1234	1240	1254	rVB	371863	602750	9.10%	0.887%
6	10.116	1464	1470	1486	rVB	369973	526559	7.95%	0.775%
7	10.945	1603	1606	1611	rVB	52560	74752	1.13%	0.110%
8	11.140	1632	1638	1642	rBV	335147	445873	6.73%	0.656%
9	11.274	1652	1660	1664	rBV	111467	183124	2.76%	0.270%
10	11.396	1675	1680	1683	rBV2	47797	76549	1.16%	0.113%
11	11.536	1699	1703	1707	rBV4	85417	121235	1.83%	0.179%
12	11.689	1724	1728	1731	rBV2	74784	92546	1.40%	0.136%
13	11.737	1732	1736	1738	rBV4	102291	136703	2.06%	0.201%
14	11.768	1738	1741	1744	rVV	214606	225672	3.41%	0.332%
15	11.798	1744	1746	1749	rVV2	111319	123124	1.86%	0.181%
16	11.896	1758	1762	1763	rBV2	111090	141137	2.13%	0.208%
17	11.945	1767	1770	1774	rVB3	196992	274458	4.14%	0.404%
18	11.987	1774	1777	1780	rBV3	115990	149028	2.25%	0.219%
19	12.030	1780	1784	1788	rVB3	128457	177104	2.67%	0.261%
20	12.079	1788	1792	1798	rBV	444793	638140	9.63%	0.940%
21	12.182	1802	1809	1811	rBV7	119719	248096	3.74%	0.365%
22	12.213	1811	1814	1818	rVB3	237586	319035	4.82%	0.470%
23	12.256	1818	1821	1824	rVB	120875	149773	2.26%	0.221%
24	12.317	1824	1831	1834	rBV4	215871	450688	6.80%	0.664%
25	12.371	1836	1840	1841	rBV2	235755	310046	4.68%	0.457%
26	12.426	1846	1849	1854	rVB5	203872	344038	5.19%	0.507%
27	12.536	1855	1867	1871	rBV6	474497	1420767	21.44%	2.092%
28	12.597	1874	1877	1878	rVV2	140960	179043	2.70%	0.264%
29	12.640	1880	1884	1889	rVB3	565038	1094284	16.52%	1.611%
30	12.695	1889	1893	1895	rBV	207697	264975	4.00%	0.390%
31	12.737	1896	1900	1904	rBV3	692660	894171	13.50%	1.317%
32	12.877	1918	1923	1928	rVB	975062	1503563	22.69%	2.214%
33	12.975	1929	1939	1947	rBV5	628230	2308014	34.83%	3.398%
34	13.042	1947	1950	1956	rVV2	796417	1400783	21.14%	2.062%

LSC Area Percent Report

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Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

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\82X110718W.M
Title : SW846 8260

35	13.097	1956	1959	1963	rVB4	408539	527110	7.96%	0.776%
36	13.146	1963	1967	1973	rBV5	397687	993927	15.00%	1.463%
37	13.268	1981	1987	1990	rBV	873971	1465880	22.12%	2.158%
38	13.353	1997	2001	2007	rVB3	1155206	1755282	26.49%	2.584%
39	13.408	2007	2010	2012	rBV	407768	480807	7.26%	0.708%
40	13.444	2012	2016	2019	rBV	2415801	3318047	50.08%	4.885%
41	13.475	2019	2021	2024	rVB4	712955	828777	12.51%	1.220%
42	13.615	2041	2044	2047	rBV	419374	417762	6.31%	0.615%
43	13.768	2065	2069	2072	rBV	1379770	1533333	23.14%	2.258%
44	13.829	2077	2079	2081	rBV3	466526	464092	7.00%	0.683%
45	13.865	2081	2085	2088	rBV2	1490852	1675565	25.29%	2.467%
46	13.908	2088	2092	2097	rBV	5701380	6625824	100.00%	9.756%
47	13.969	2098	2102	2109	rVB4	1402575	2703966	40.81%	3.981%
48	14.054	2113	2116	2118	rBV2	865854	1063189	16.05%	1.565%
49	14.127	2124	2128	2131	rBV3	1239768	2004061	30.25%	2.951%
50	14.164	2132	2134	2137	rVV	924854	1046422	15.79%	1.541%
51	14.200	2137	2140	2143	rVV3	1166131	1415462	21.36%	2.084%
52	14.676	2215	2218	2225	rVB	3929703	4776083	72.08%	7.032%
53	14.822	2238	2242	2245	rBV2	1454313	1825336	27.55%	2.688%
54	14.914	2254	2257	2268	rVB5	1266457	2691948	40.63%	3.964%
55	15.005	2268	2272	2273	rBV2	1128230	1392765	21.02%	2.051%
56	15.036	2273	2277	2285	rVB	2451060	3984141	60.13%	5.866%
57	15.499	2348	2353	2358	rVB	2779309	4206639	63.49%	6.194%
58	15.767	2392	2397	2402	rBV3	591552	1268813	19.15%	1.868%
59	15.828	2403	2407	2414	rVB	1140214	1901137	28.69%	2.799%
60	15.901	2416	2419	2423	rVV3	191359	296909	4.48%	0.437%
61	15.950	2423	2427	2439	rVB	463558	1037338	15.66%	1.527%

Sum of corrected areas: 67917426

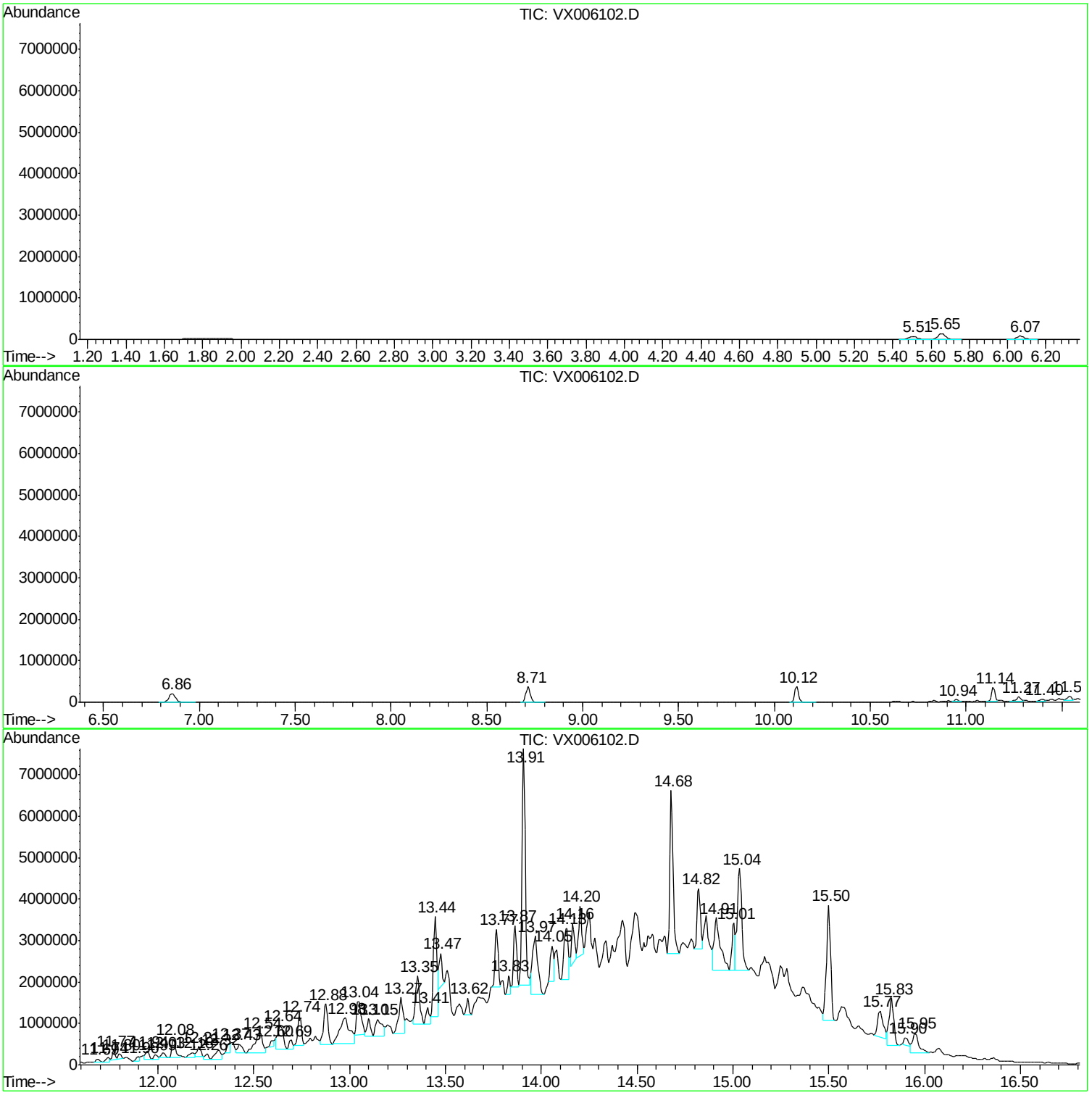
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

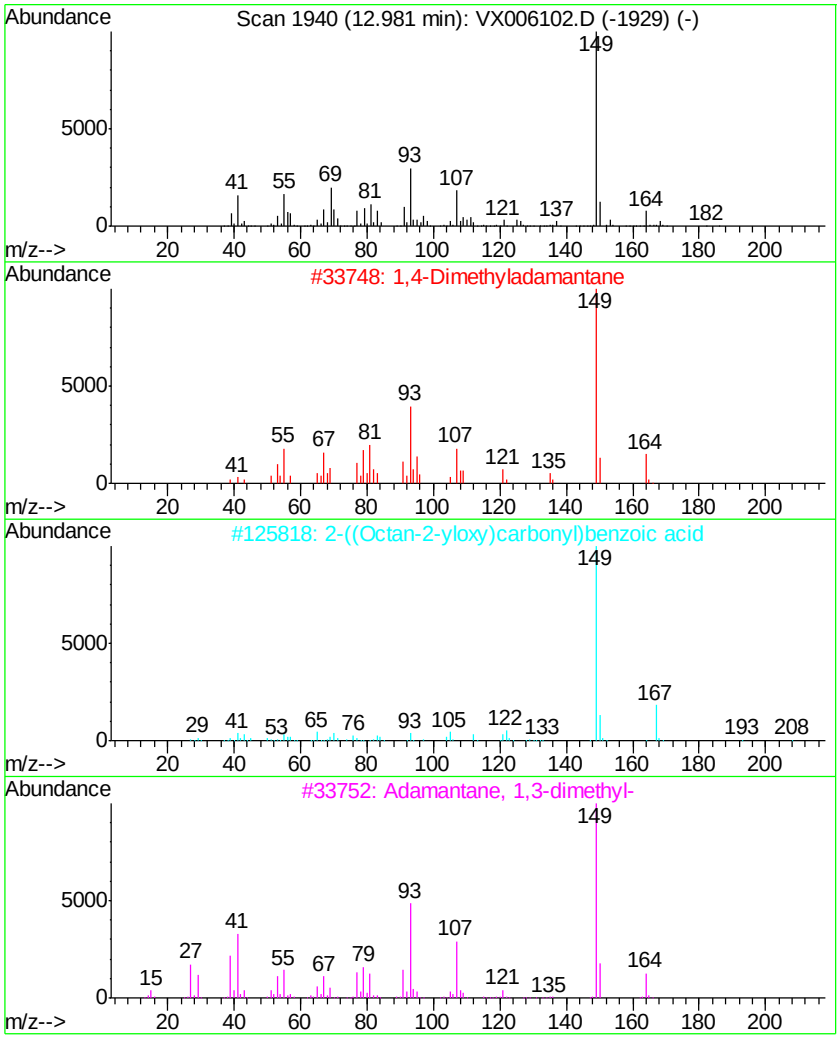
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

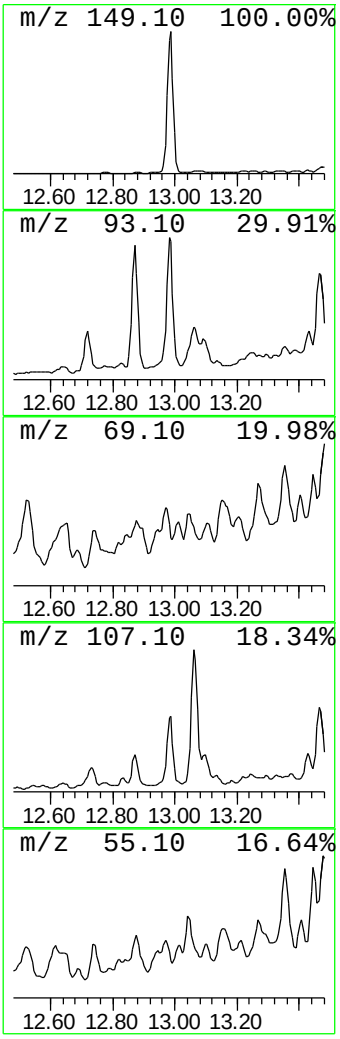
****

Peak Number 1 1,4-Dimethyladamantane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	180.84 ug/l	2308010	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane	164	C12H20	024145-88-8	62
2	2-((Octan-2-yloxy)carbonyl)benzo...	278	C16H22O4	1000373-83-2	47
3	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	46
4	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	43
5	Didodecyl phthalate	502	C32H54O4	002432-90-8	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

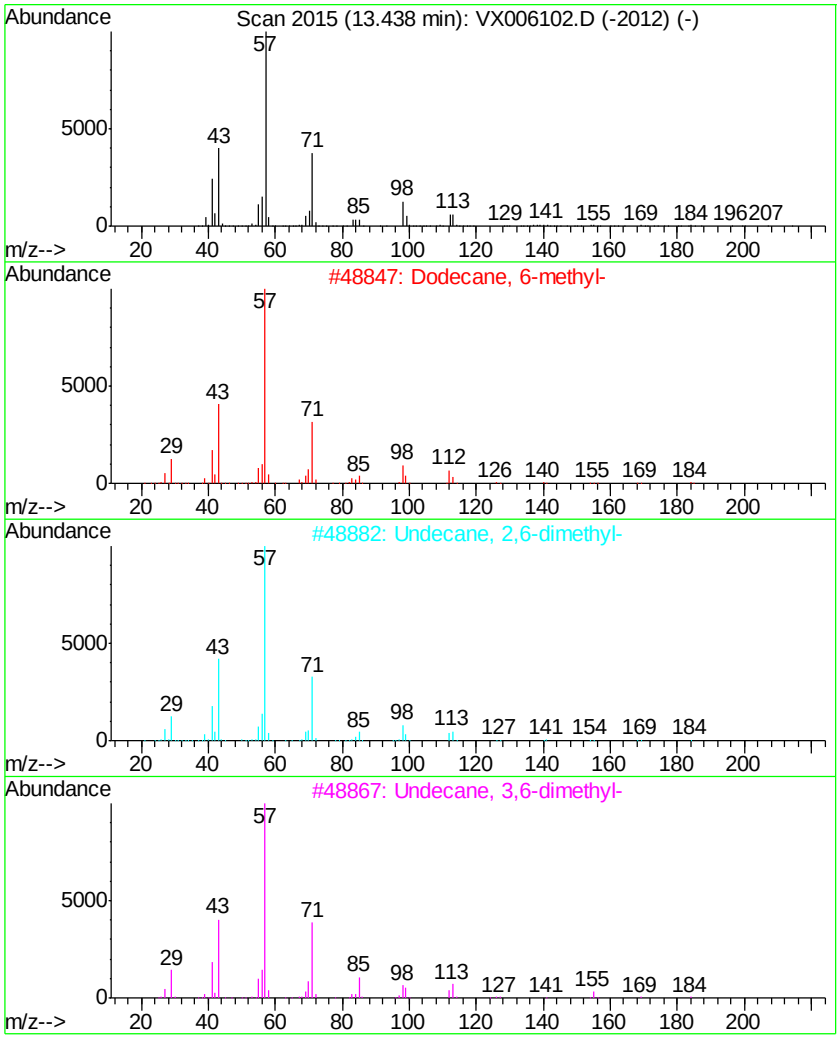
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

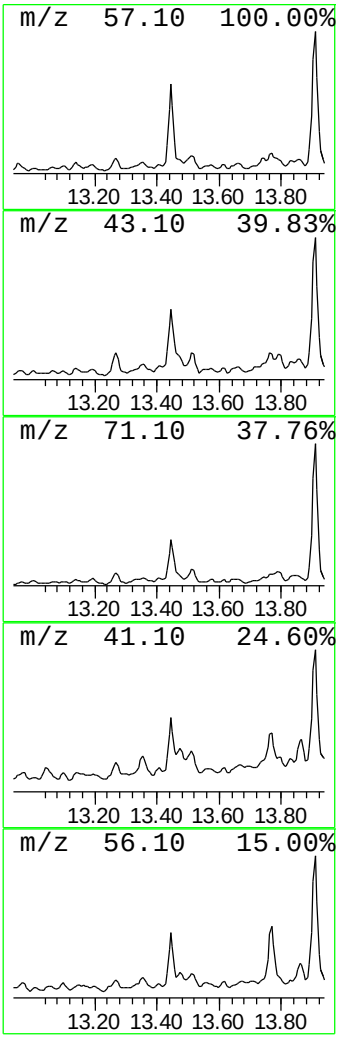
****

Peak Number 2 Dodecane, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	259.98 ug/l	3318050	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 6-methyl-	184	C13H28	006044-71-9	97
2	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	95
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	93
4	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	72
5	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

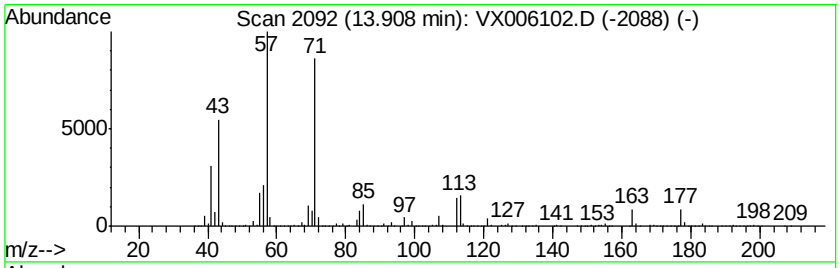
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

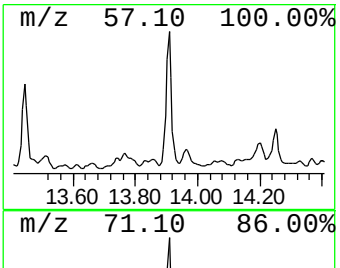
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Sulfurous acid, dodecyl 2-e... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	519.15 ug/l	6625820	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	72
2	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64
3	Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	64
4	Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	64
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

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

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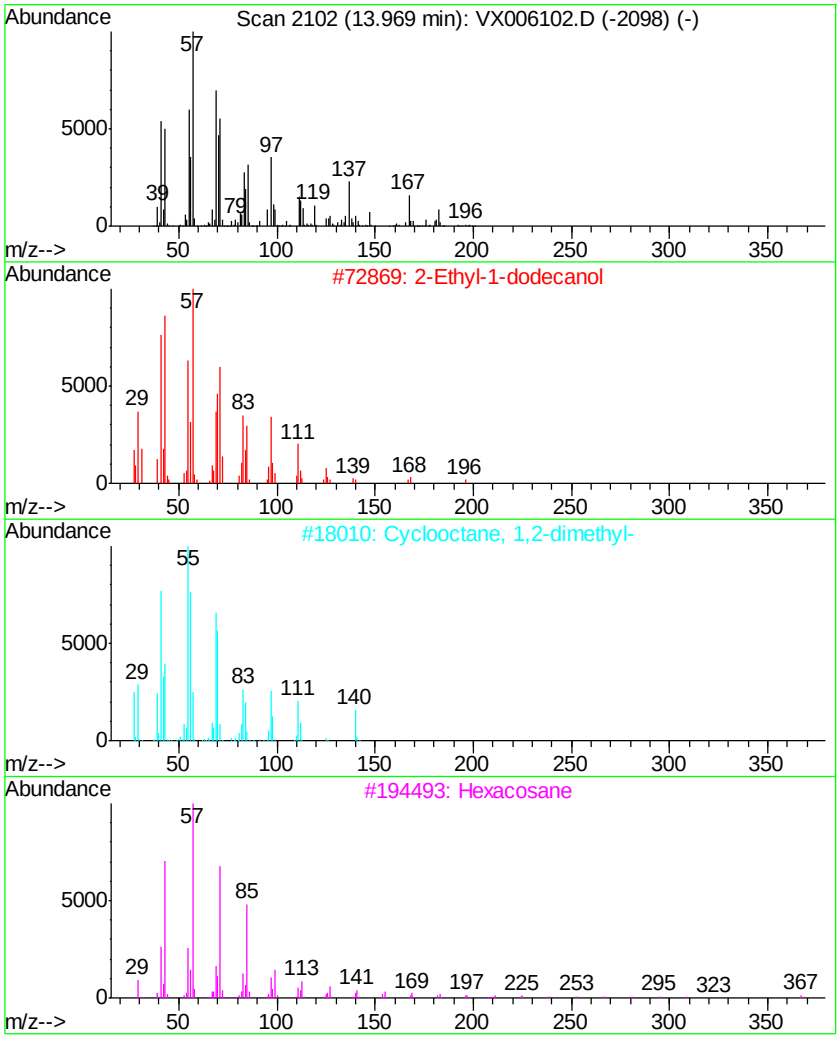
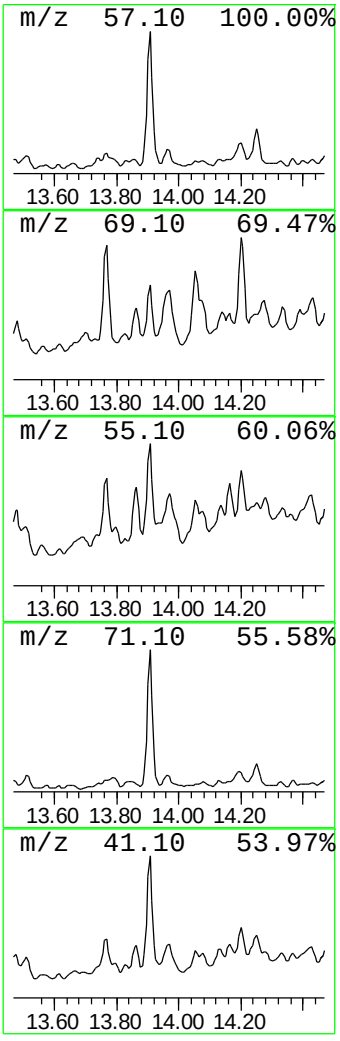
Peak Number 4 2-Ethyl-1-dodecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	211.86 ug/l	2703970	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	58
2	Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	38
3	Hexacosane	366	C26H54	000630-01-3	35
4	Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	30
5	Tetracosane	338	C24H50	000646-31-1	27





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
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Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

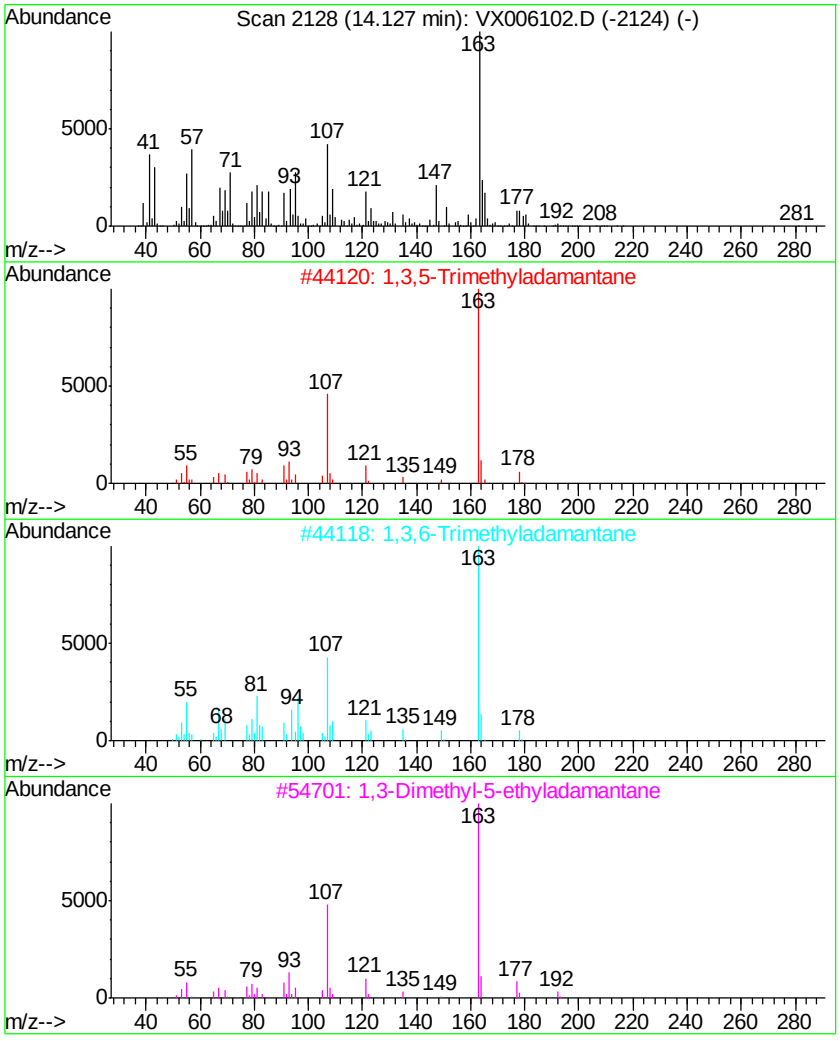
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

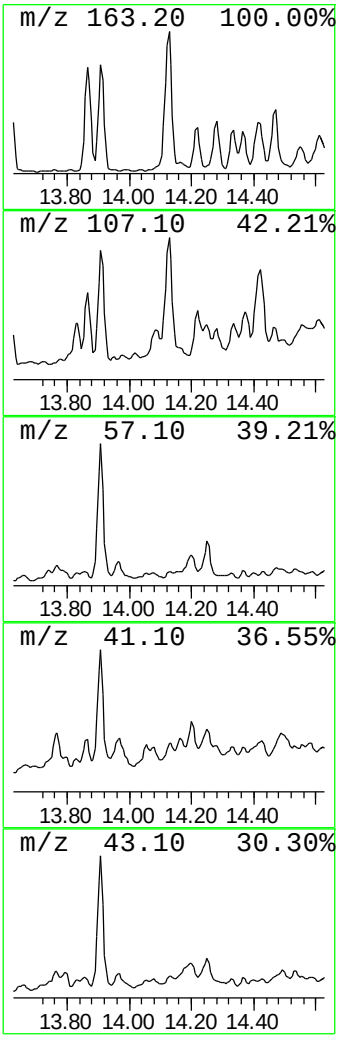
****

Peak Number 5 1,3,5-Trimethyladamantane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	157.02 ug/l	2004060	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	53
2	1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	52
3	1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	47
4	1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	38
5	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	38





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ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

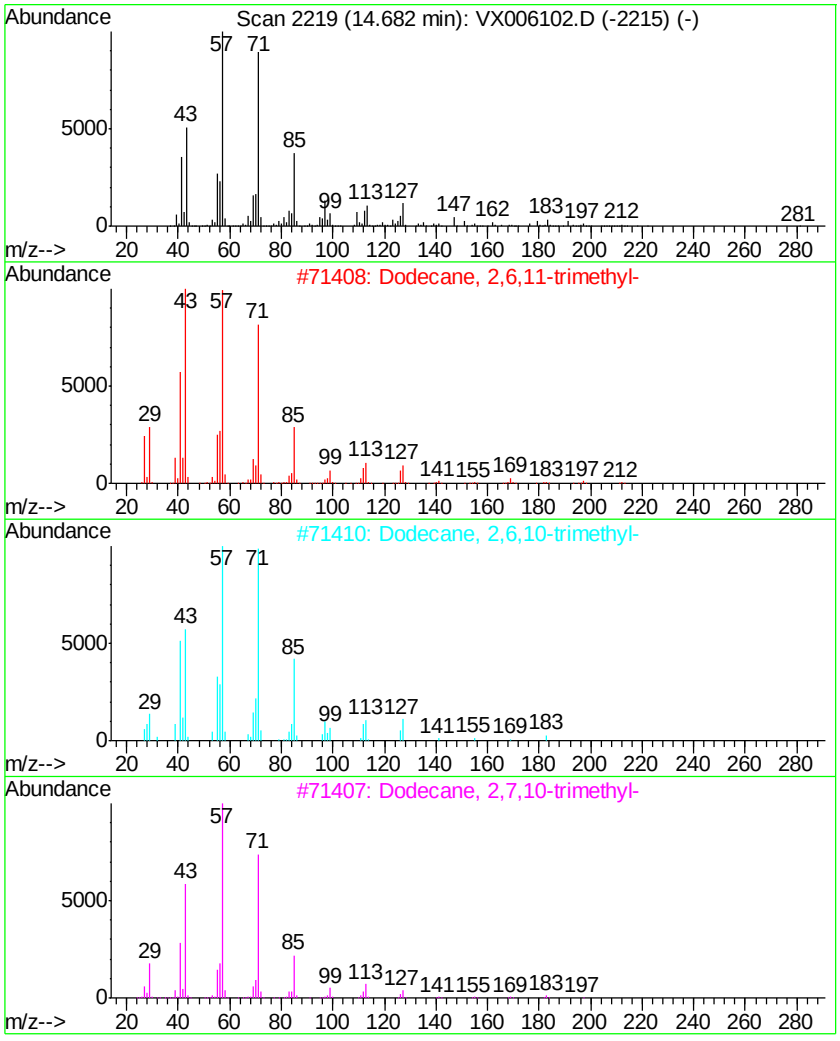
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

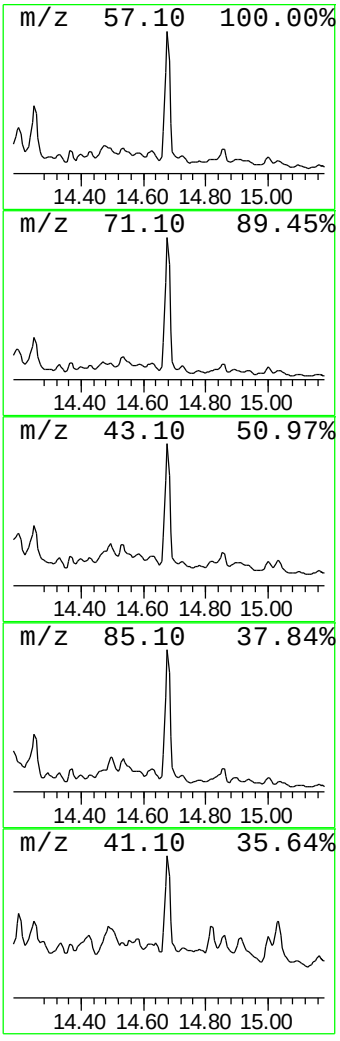
****

Peak Number 6 Dodecane, 2,6,11-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	374.22 ug/l	4776080	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	94
2	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	91
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	83





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

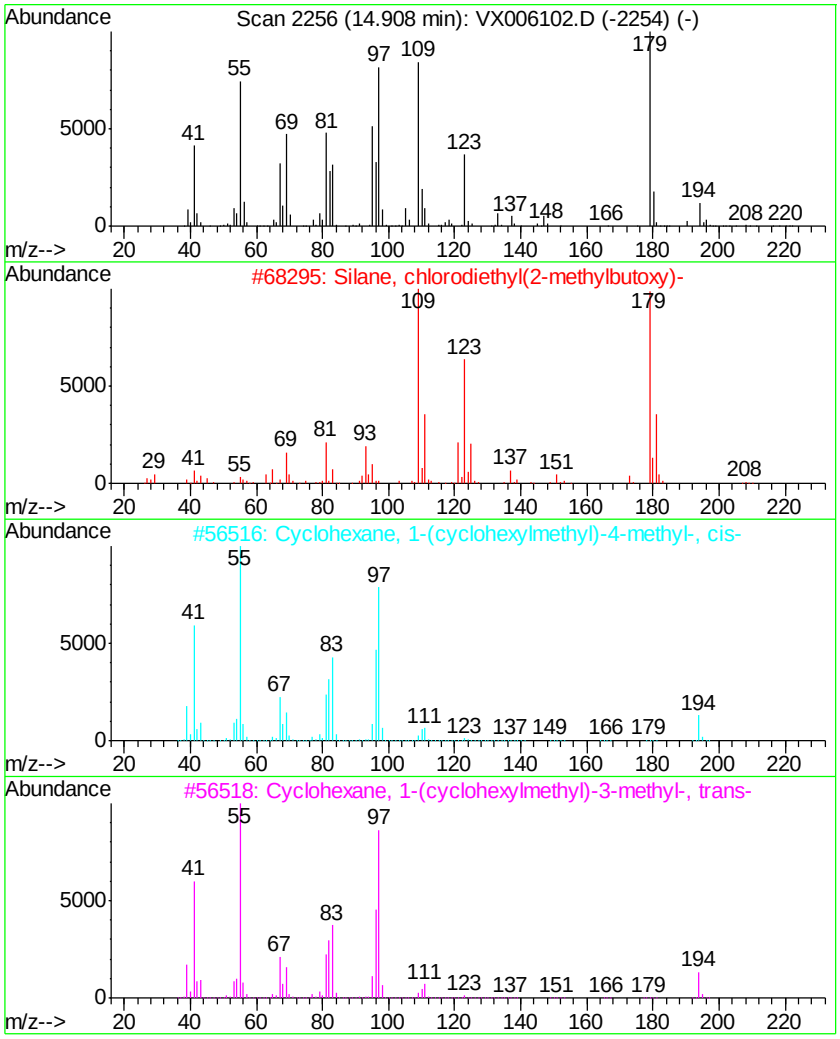
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

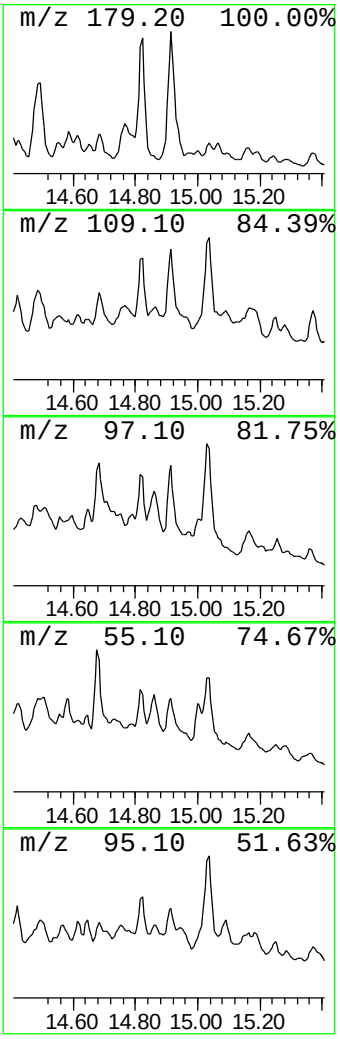
****

Peak Number 7 unknown14.91 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	210.92 ug/l	2691950	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorodiethyl(2-methylbu...	208	C9H21ClOSi	1000363-11-1	38
2	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-97-1	25
3	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-95-9	25
4	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-96-0	25
5	1,4-Bis[.alpha.-methoxyethyl]ben...	194	C12H18O2	129770-42-9	22





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

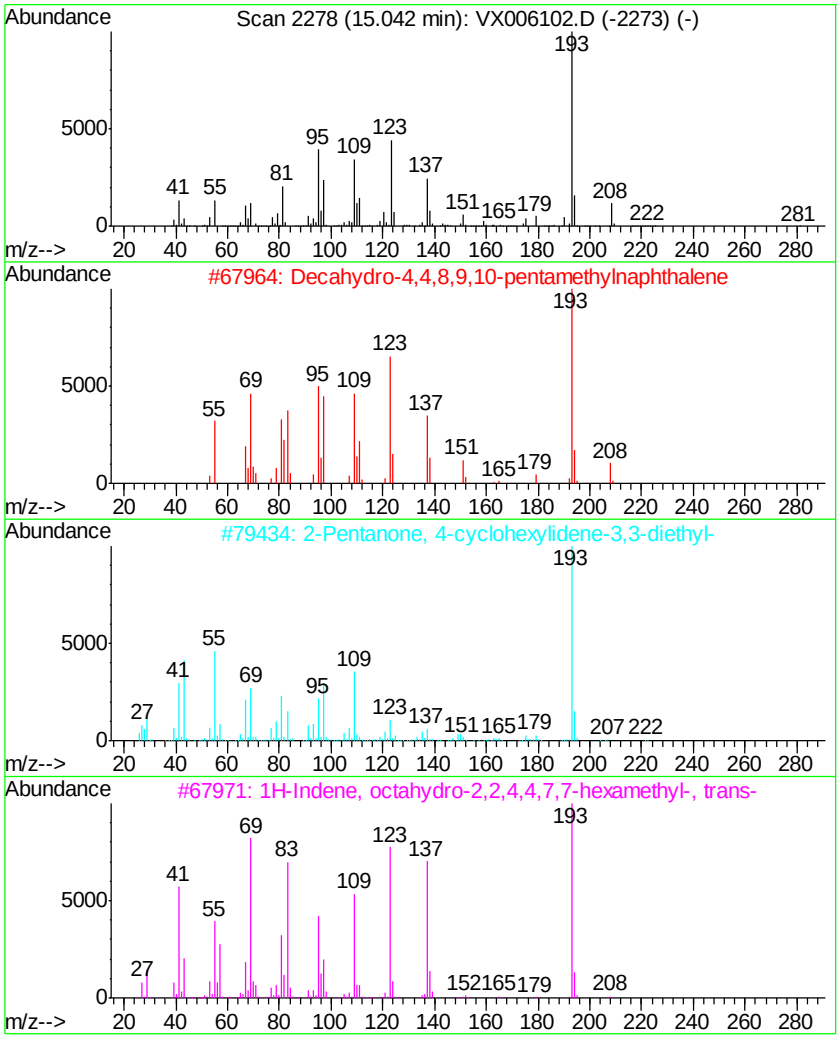
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

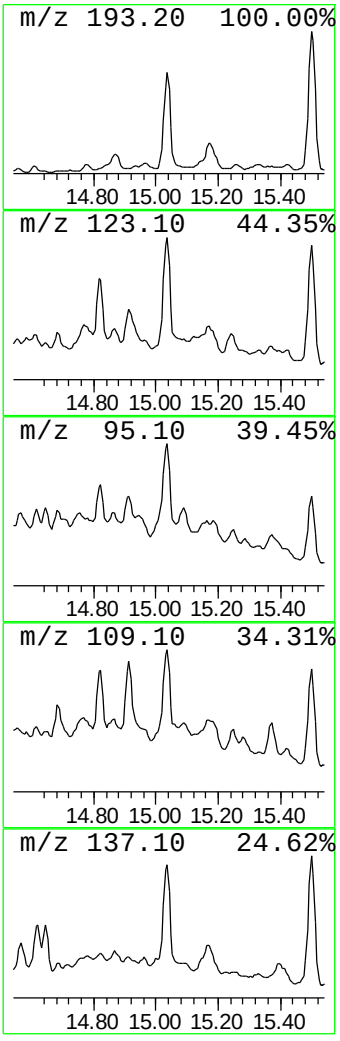
****

Peak Number 8 Decahydro-4,4,8,9,10-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	312.17 ug/l	3984140	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	86
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	50
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	37
5	Silane, tetra-2-propenyl-	192	C12H20Si	001112-66-9	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006102.D
Acq On : 19 Nov 2018 20:07
Operator : JC/MD
Sample : J5967-03
Misc : 5.03g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-14(5.5-7.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.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
1,4-Dimethyladama...	12.98	180.8	ug/l	2308010	4	12.08	638140	50.0
Dodecane, 6-methyl-	13.44	260.0	ug/l	3318050	4	12.08	638140	50.0
Sulfurous acid, d...	13.91	519.1	ug/l	6625820	4	12.08	638140	50.0
2-Ethyl-1-dodecanol	13.97	211.9	ug/l	2703970	4	12.08	638140	50.0
1,3,5-Trimethylad...	14.13	157.0	ug/l	2004060	4	12.08	638140	50.0
Dodecane, 2,6,11-...	14.68	374.2	ug/l	4776080	4	12.08	638140	50.0
unknown14.91	14.91	210.9	ug/l	2691950	4	12.08	638140	50.0
Decahydro-4,4,8,9...	15.04	312.2	ug/l	3984140	4	12.08	638140	50.0