LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006094.D
Acq On : 19 Nov 2018 16:34
Operator : JC/MD
Sample : J5951-03 10X
Misc : 5.04g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-04(10-12)

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	701	714	722	rBV3	74442	219127	7.30%	0.419%
2	5.665	731	740	761	rVB	137396	416171	13.86%	0.796%
3	6.068	795	806	825	rVV2	82687	218017	7.26%	0.417%
4	6.860	925	936	947	rBV	198366	471113	15.69%	0.902%
5	7.458	1021	1034	1045	rBV2	145390	339862	11.32%	0.650%
6	8.342	1174	1179	1182	rVV	88851	143314	4.77%	0.274%
7	8.500	1200	1205	1213	rBV	82869	154480	5.15%	0.296%
8	8.665	1225	1232	1235	rBV2	162355	287001	9.56%	0.549%
9	8.713	1235	1240	1251	rVB	391182	691919	23.05%	1.324%
10	9.043	1288	1294	1305	rVB	128209	221359	7.37%	0.424%
11	9.165	1305	1314	1319	rBV	77736	133738	4.45%	0.256%
12	9.445	1354	1360	1364	rBV	117368	176075	5.86%	0.337%
13	9.561	1374	1379	1385	rBV4	114696	255852	8.52%	0.490%
14	9.622	1385	1389	1393	rVV	231849	327352	10.90%	0.626%
15	9.677	1393	1398	1402	rVV	224473	350996	11.69%	0.672%
16	9.878	1426	1431	1437	rBV3	145494	361679	12.05%	0.692%
17	9.957	1440	1444	1449	rVB	225768	316802	10.55%	0.606%
18	10.067	1455	1462	1466	rBV	254907	364744	12.15%	0.698%
19	10.116	1466	1470	1474	rVB	350151	466891	15.55%	0.893%
20	10.335	1497	1506	1509	rBV2	140441	280092	9.33%	0.536%
21	10.378	1509	1513	1516	rVV	173269	229122	7.63%	0.438%
22	10.408	1516	1518	1530	rVB	130756	251738	8.38%	0.482%
23	10.640	1549	1556	1564	rBV3	265549	510927	17.02%	0.978%
24	10.725	1564	1570	1575	rBV3	116317	209802	6.99%	0.401%
25	10.835	1580	1588	1592	rBV2	542273	831371	27.69%	1.591%
26	10.908	1592	1600	1604	rBV3	500551	858600	28.60%	1.643%
27	10.951	1604	1607	1612	rVB	254987	337825	11.25%	0.646%
28	11.018	1612	1618	1621	rBV2	164892	256988	8.56%	0.492%
29	11.085	1626	1629	1632	rVB	132078	156113	5.20%	0.299%
30	11.140	1632	1638	1643	rBV2	608178	813920	27.11%	1.558%
31	11.243	1648	1655	1657	rBV	221249	326503	10.88%	0.625%
32	11.274	1657	1660	1669	rVB3	369929	566541	18.87%	1.084%
33	11.359	1670	1674	1677	rBV	300028	363652	12.11%	0.696%
34	11.445	1684	1688	1691	rBV2	137847	185866	6.19%	0.356%

LSC Area Percent Report

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Misc : 5.04g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-04(10-12)

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

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Title : SW846 8260

35	11.487	1691	1695	1699	rBV	363901	452611	15.08%	0.866%
36	11.536	1699	1703	1707	rVB3	200439	328054	10.93%	0.628%
37	11.682	1720	1727	1732	rVB5	198484	444760	14.81%	0.851%
38	11.737	1732	1736	1738	rBV2	164507	205820	6.86%	0.394%
39	11.768	1738	1741	1744	rBV	534763	576908	19.22%	1.104%
40	11.890	1757	1761	1763	rBV2	132020	180275	6.00%	0.345%
41	11.945	1763	1770	1775	rVB2	491167	846501	28.20%	1.620%
42	11.999	1775	1779	1782	rBV	574238	689428	22.96%	1.319%
43	12.030	1782	1784	1788	rVB2	126431	142053	4.73%	0.272%
44	12.079	1788	1792	1798	rBV2	475753	852979	28.41%	1.632%
45	12.128	1798	1800	1803	rVB2	198312	195245	6.50%	0.374%
46	12.219	1812	1815	1824	rVB6	196385	486728	16.21%	0.931%
47	12.304	1824	1829	1833	rBV	591276	848598	28.26%	1.624%
48	12.371	1835	1840	1842	rBV	634956	989320	32.95%	1.893%
49	12.463	1850	1855	1862	rBV3	255143	632039	21.05%	1.210%
50	12.524	1862	1865	1870	rVB4	330598	561853	18.71%	1.075%
51	12.615	1874	1880	1881	rBV5	224497	391103	13.03%	0.748%
52	12.670	1885	1889	1892	rVB	712610	786222	26.19%	1.505%
53	12.755	1897	1903	1911	rBV6	406624	1128248	37.58%	2.159%
54	12.822	1911	1914	1918	rVB4	101224	153798	5.12%	0.294%
55	12.877	1918	1923	1929	rVB4	599885	993190	33.08%	1.901%
56	12.944	1929	1934	1937	rBV3	632009	1050899	35.00%	2.011%
57	12.981	1937	1940	1946	rVB2	640123	843835	28.11%	1.615%
58	13.042	1946	1950	1953	rBV2	435956	525985	17.52%	1.007%
59	13.079	1953	1956	1963	rVB2	334326	571710	19.04%	1.094%
60	13.152	1964	1968	1973	rBV2	257372	505669	16.84%	0.968%
61	13.194	1973	1975	1978	rBV2	248282	265543	8.84%	0.508%
62	13.225	1978	1980	1983	rVB	153965	143832	4.79%	0.275%
63	13.316	1991	1995	1996	rBV2	124072	148327	4.94%	0.284%
64	13.347	1996	2000	2006	rVB2	1594331	2451646	81.66%	4.692%
65	13.402	2006	2009	2011	rBV3	128654	152663	5.08%	0.292%
66	13.432	2011	2014	2018	rVV2	267741	474838	15.82%	0.909%
67	13.475	2018	2021	2030	rVB5	424818	1099789	36.63%	2.105%
68	13.566	2031	2036	2038	rBV2	268963	398298	13.27%	0.762%
69	13.603	2038	2042	2044	rVB	170114	204016	6.80%	0.390%
70	13.639	2044	2048	2052	rBV3	474608	631360	21.03%	1.208%
71	13.688	2052	2056	2059	rBV5	182309	364683	12.15%	0.698%

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Title : SW846 8260

72	13.725	2059	2062	2066	rVB2	353894	522043	17.39%	0.999%
73	13.804	2071	2075	2080	rVB3	298857	524457	17.47%	1.004%
74	13.859	2080	2084	2087	rBV2	365112	496280	16.53%	0.950%
75	13.908	2087	2092	2097	rVB4	437727	765372	25.49%	1.465%
76	13.987	2097	2105	2109	rVB5	563294	1049649	34.96%	2.009%
77	14.036	2109	2113	2116	rBV4	191361	345468	11.51%	0.661%
78	14.127	2124	2128	2131	rBV2	261823	353554	11.78%	0.677%
79	14.164	2131	2134	2137	rVV2	152280	171776	5.72%	0.329%
80	14.219	2141	2143	2146	rVV	149992	202995	6.76%	0.388%
81	14.286	2148	2154	2160	rVB5	740054	1443708	48.09%	2.763%
82	14.383	2166	2170	2175	rVB2	195954	267783	8.92%	0.512%
83	14.432	2175	2178	2182	rVB	267808	310464	10.34%	0.594%
84	14.481	2182	2186	2191	rVB3	213174	331226	11.03%	0.634%
85	14.542	2191	2196	2204	rVB4	593147	1009480	33.62%	1.932%
86	14.700	2214	2222	2225	rBV	1960277	3002298	100.00%	5.745%
87	14.731	2225	2227	2231	rVB3	397344	449553	14.97%	0.860%
88	14.786	2231	2236	2239	rBV3	202366	297672	9.91%	0.570%
89	14.840	2241	2245	2249	rVV	1272130	1594086	53.10%	3.051%
90	14.907	2253	2256	2260	rVB2	229760	267698	8.92%	0.512%
91	15.109	2285	2289	2293	rBV3	100611	162210	5.40%	0.310%
92	15.249	2307	2312	2315	rBV3	224891	372696	12.41%	0.713%
93	15.444	2340	2344	2348	rBV	300380	457262	15.23%	0.875%
94	15.481	2348	2350	2354	rVV2	99175	135514	4.51%	0.259%
95	15.548	2356	2361	2367	rVB	697019	1105411	36.82%	2.115%
96	15.688	2379	2384	2388	rBV	671300	1128542	37.59%	2.160%
97	15.724	2388	2390	2398	rVB	545681	813014	27.08%	1.556%
98	15.919	2414	2422	2432	rVB	182013	500992	16.69%	0.959%
99	16.072	2443	2447	2459	rVB4	94671	208239	6.94%	0.399%
100	16.694	2545	2549	2554	rVV	85141	151794	5.06%	0.290%

Sum of corrected areas: 52255614

LSC Report - Integrated Chromatogram

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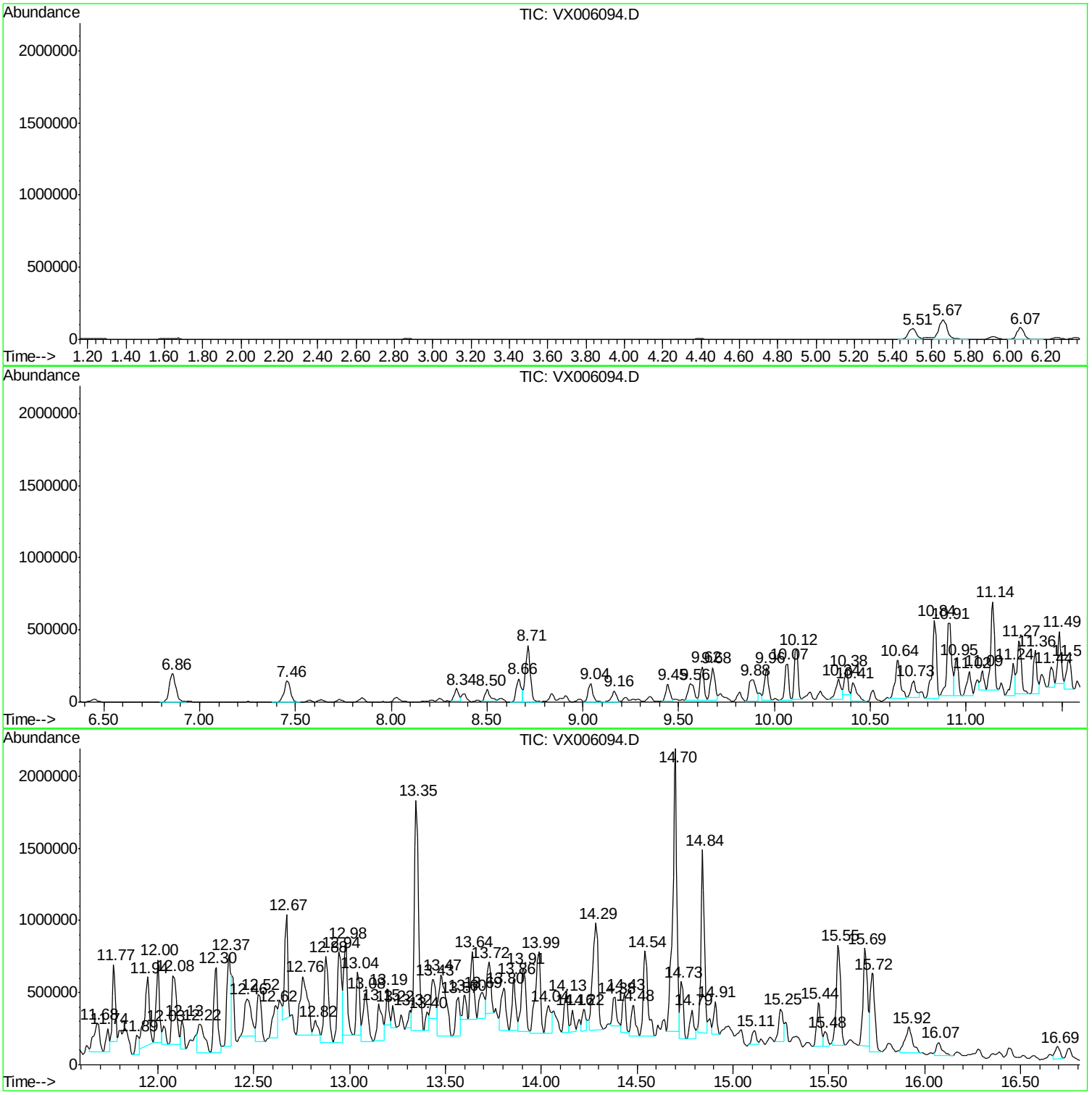
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FDSB-04(10-12)

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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Quant Title : SW846 8260

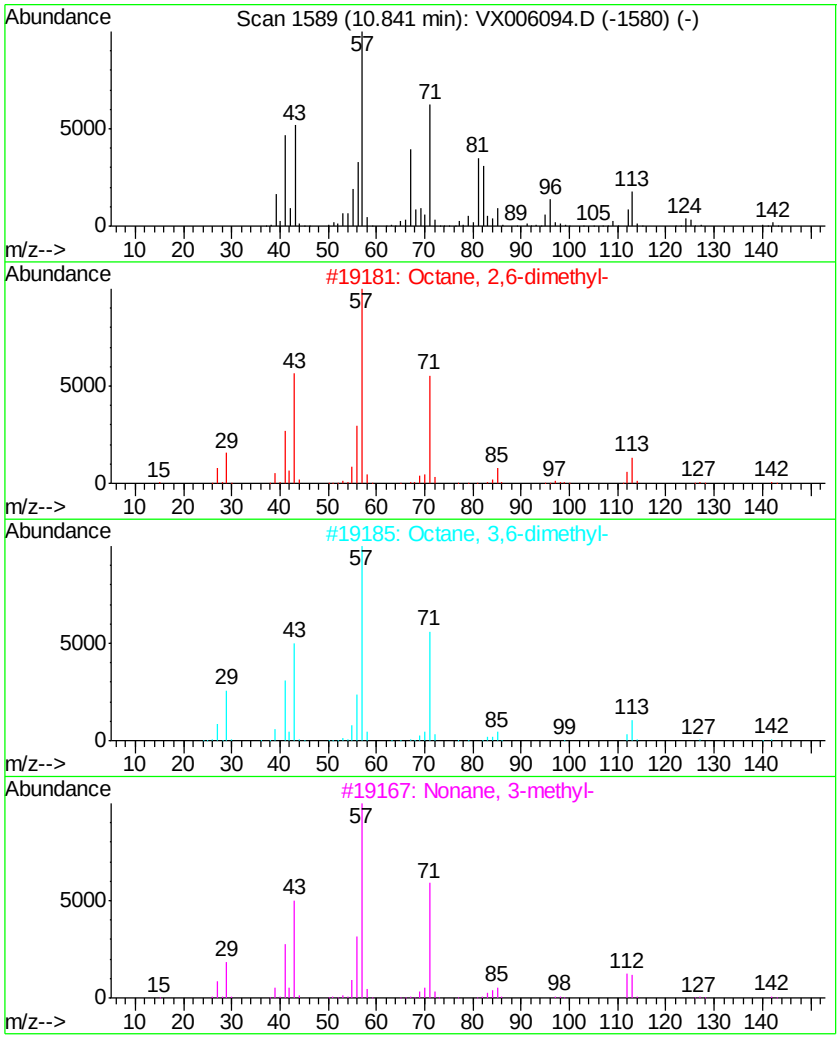
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

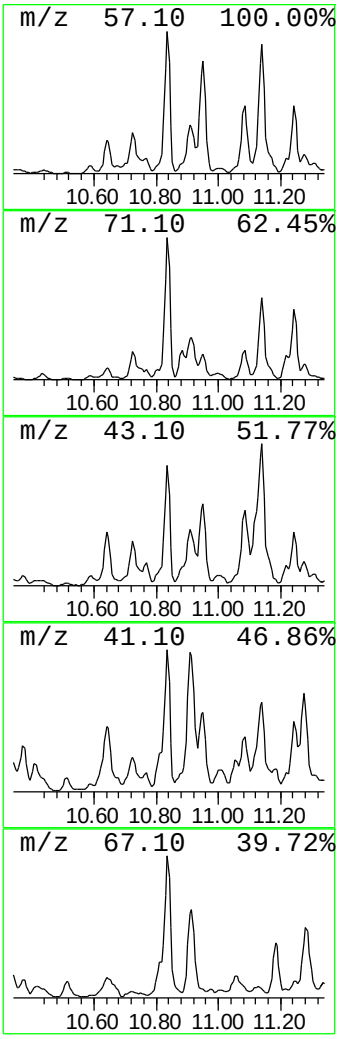
****

Peak Number 1 Octane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	89.03 ug/l	831371	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	60
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	60
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	46
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	43





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ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-04(10-12)

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

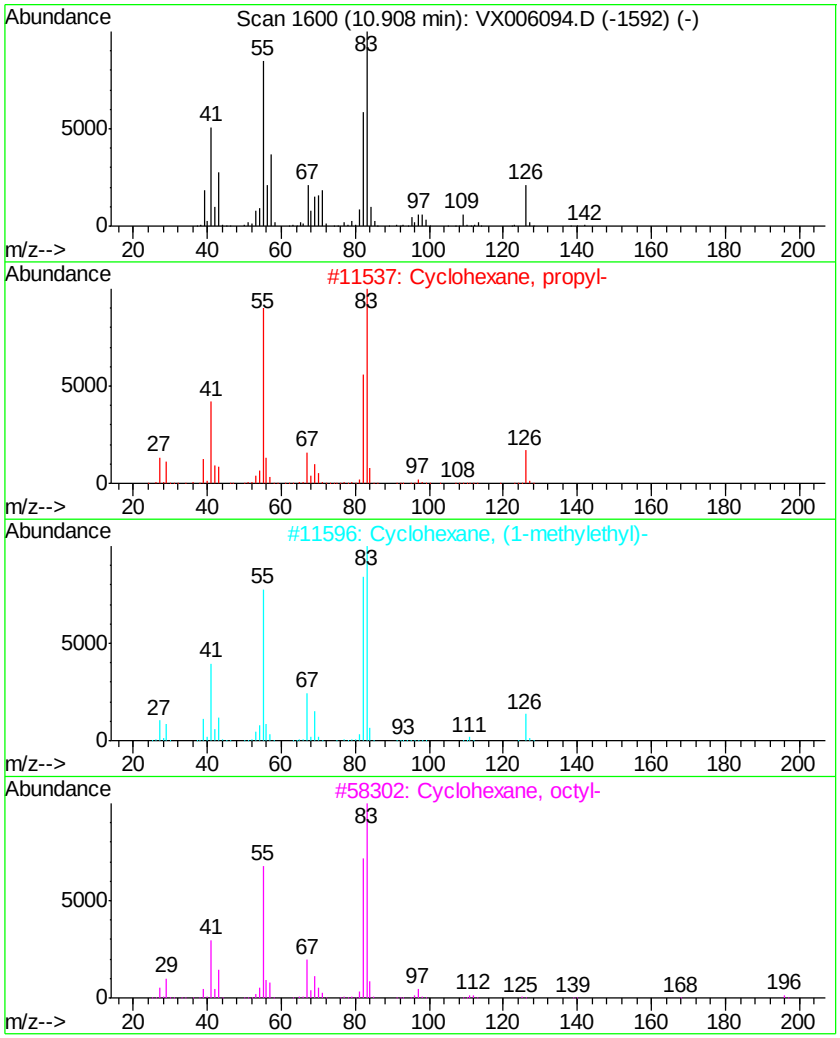
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

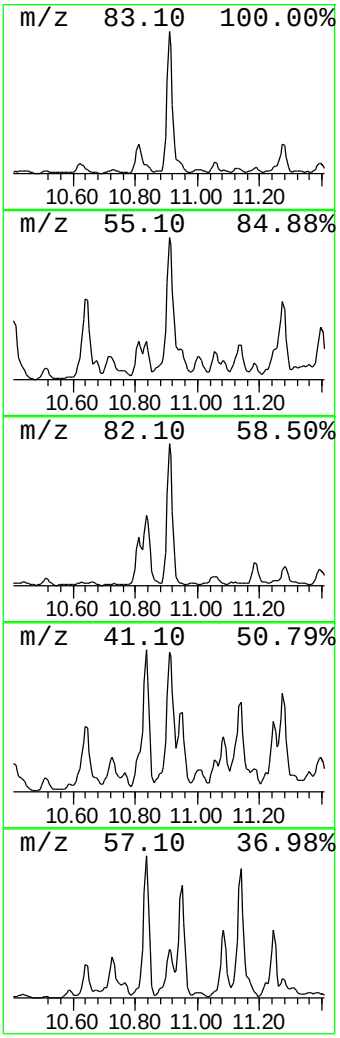
****

Peak Number 2 Cyclohexane, propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	91.95 ug/l	858600	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	64
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	64
4	Cyclohexane, undecyl-	238	C17H34	054105-66-7	64
5	Cyclohexane, butyl-	140	C10H20	001678-93-9	64





Library Search Compound Report

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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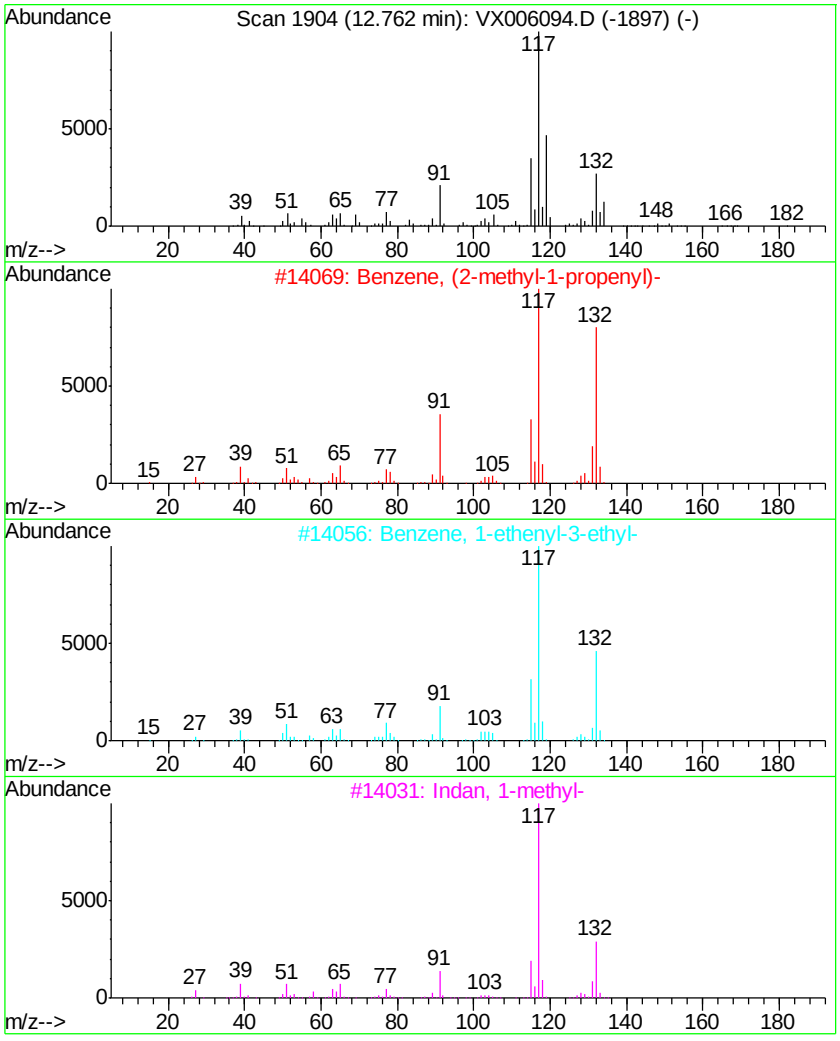
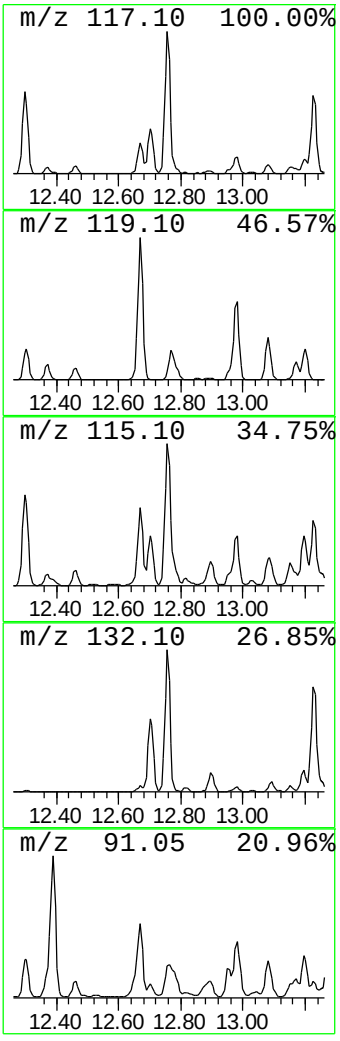
****
Peak Number 3 Benzene, (2-methyl-1-propen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	66.14 ug/l	1128250	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	81
4	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	74
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	74





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

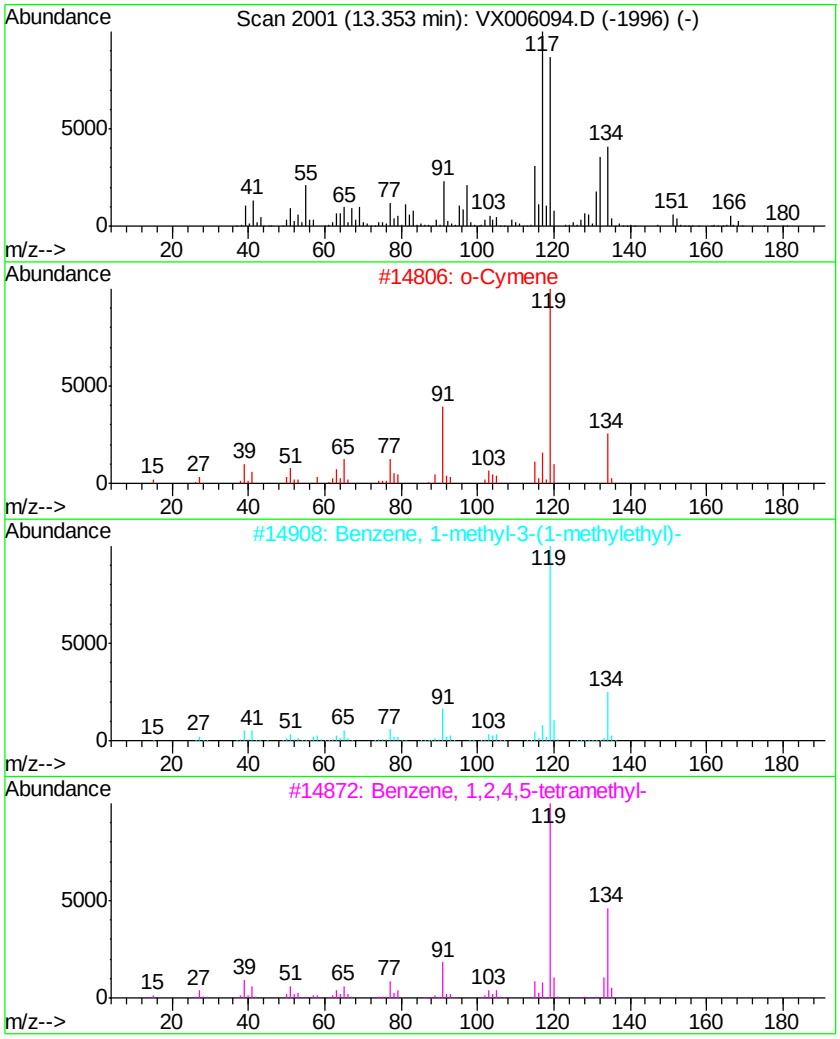
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

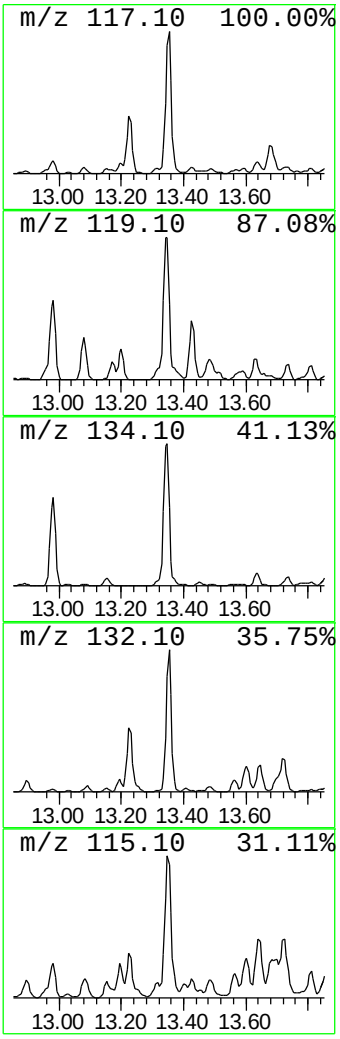
****

Peak Number 4 o-Cymene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	143.71 ug/l	2451650	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	76
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	70
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	70
4	p-Cymene	134	C10H14	000099-87-6	62
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	62





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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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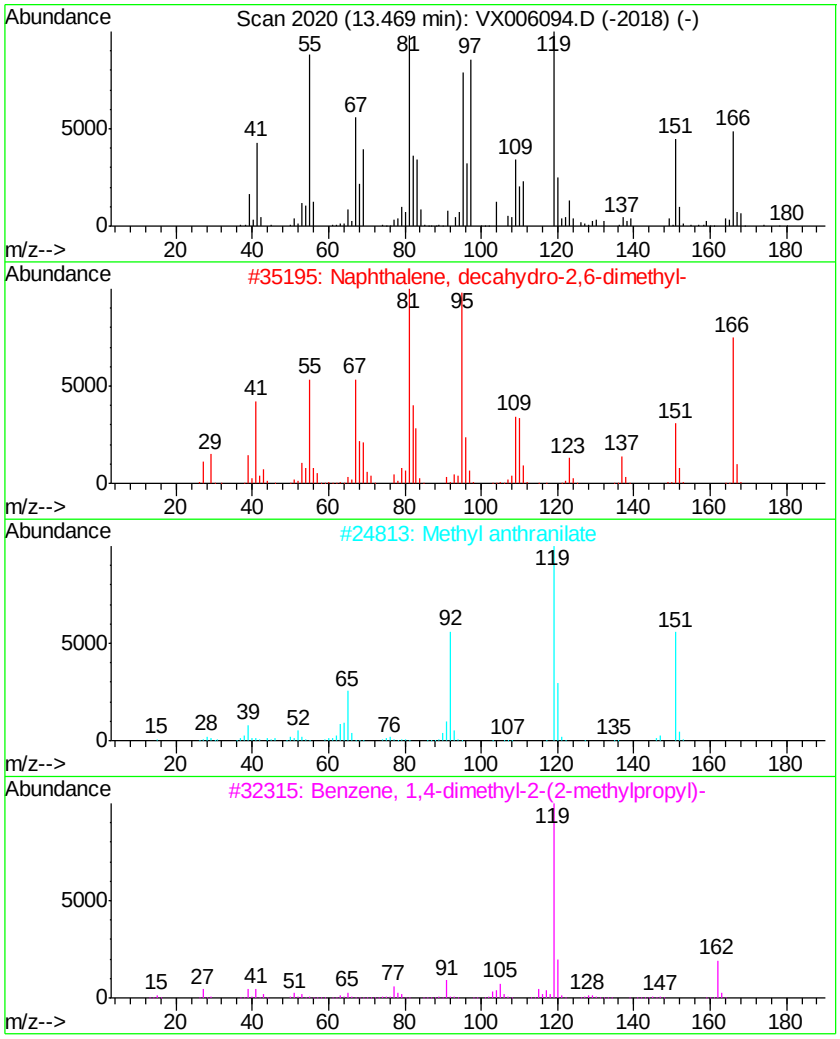
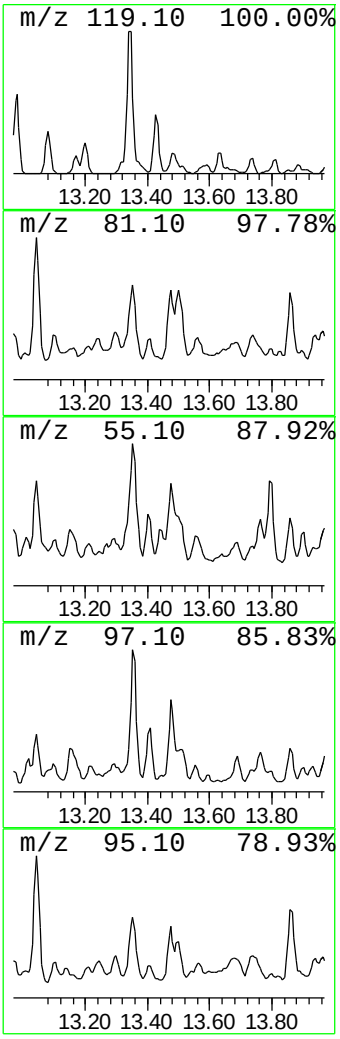
****

Peak Number 5 unknown13.47 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	64.47 ug/l	1099790	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	42
2	Methyl anthranilate	151	C8H9NO2	000134-20-3	27
3	Benzene, 1,4-dimethyl-2-(2-methy...	162	C12H18	055669-88-0	22
4	2-n-Heptylfuran	166	C11H18O	003777-71-7	22
5	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	14





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006094.D
Acq On : 19 Nov 2018 16:34
Operator : JC/MD
Sample : J5951-03 10X
Misc : 5.04g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-04(10-12)

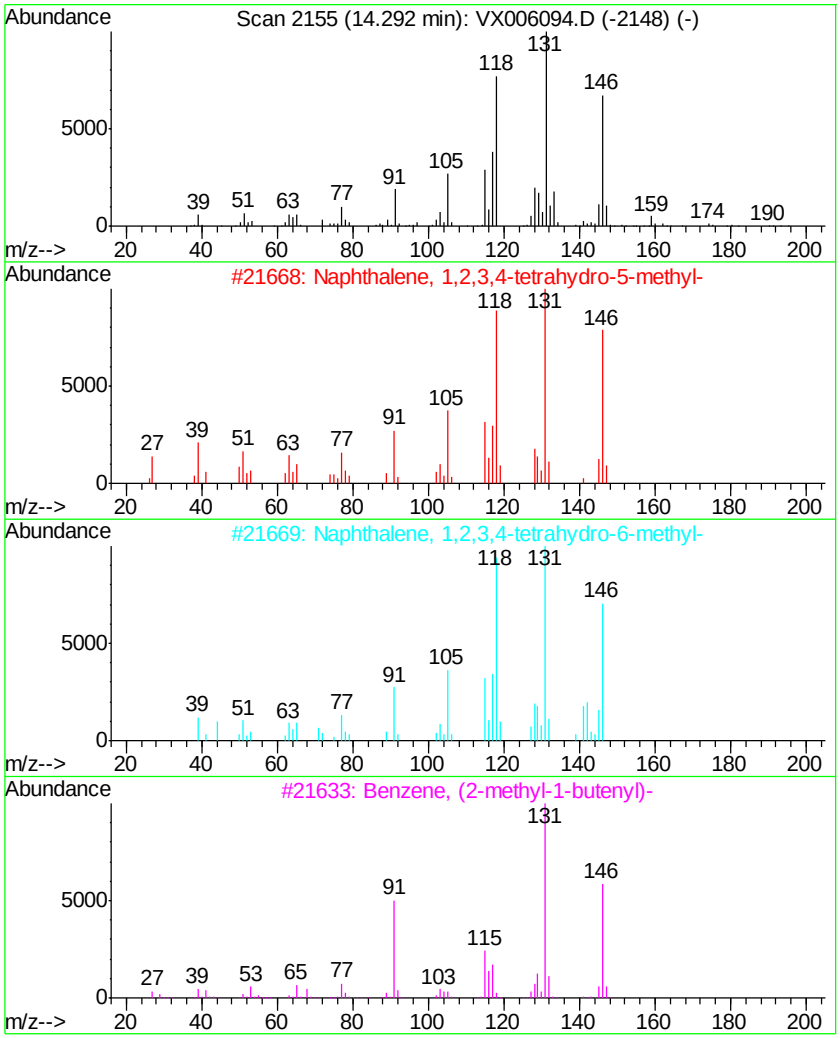
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X110718W.M
Quant Title : SW846 8260

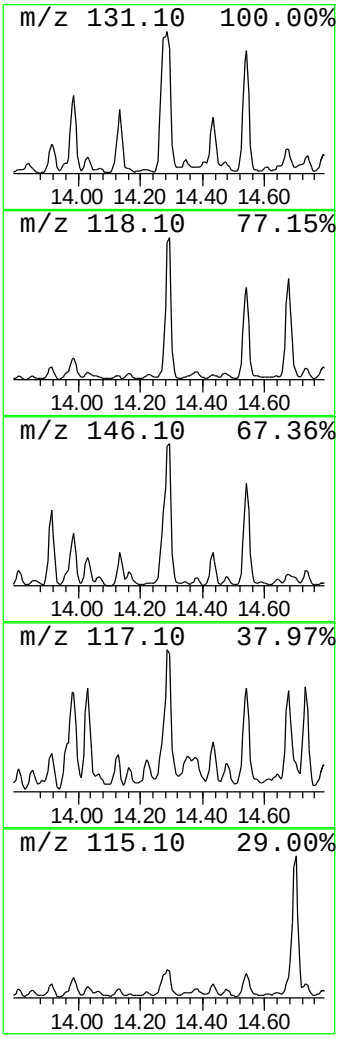
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	84.63 ug/l	1443710	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	96
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	93
3	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	70
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70
5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	64





Library Search Compound Report

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Data File : VX006094.D
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Operator : JC/MD
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Misc : 5.04g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-04(10-12)

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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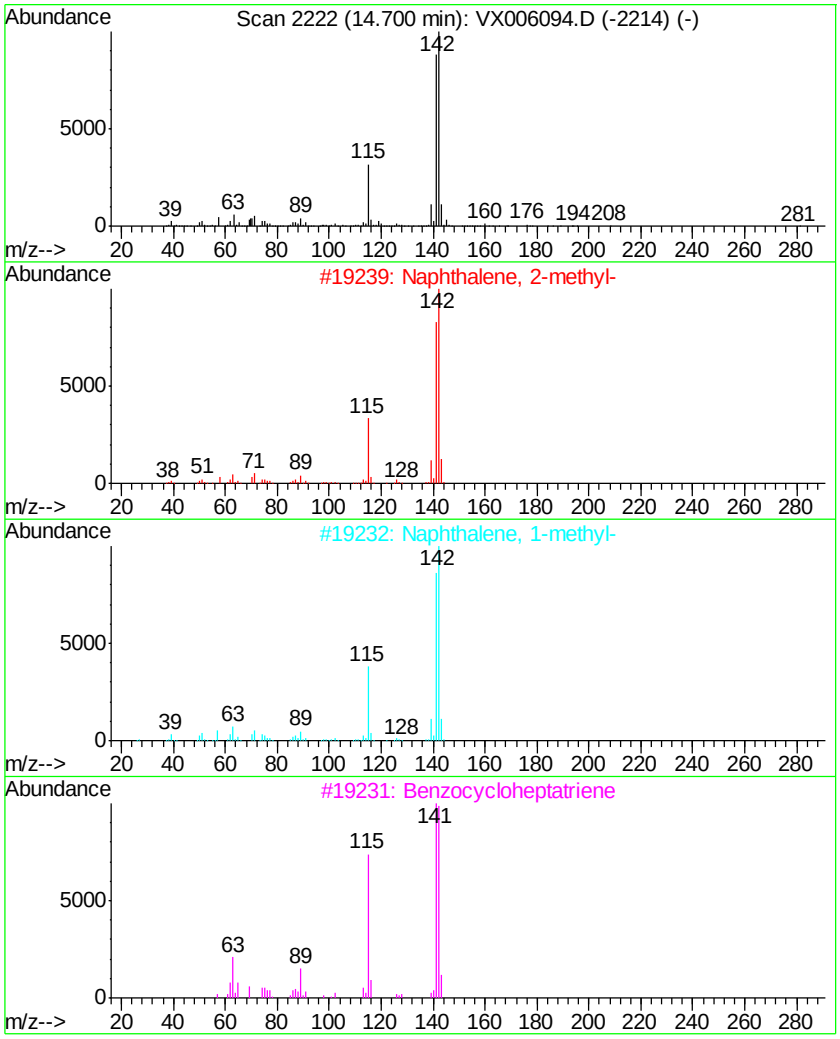
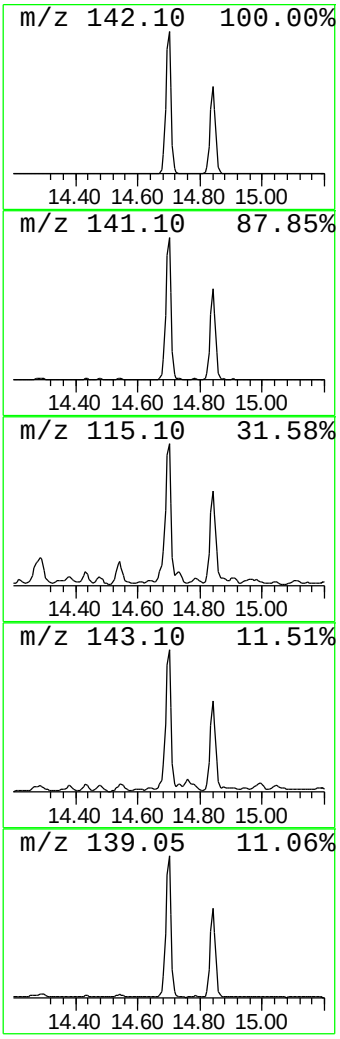
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	175.99 ug/l	3002300	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





Library Search Compound Report

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Data File : VX006094.D
Acq On : 19 Nov 2018 16:34
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Sample : J5951-03 10X
Misc : 5.04g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-04(10-12)

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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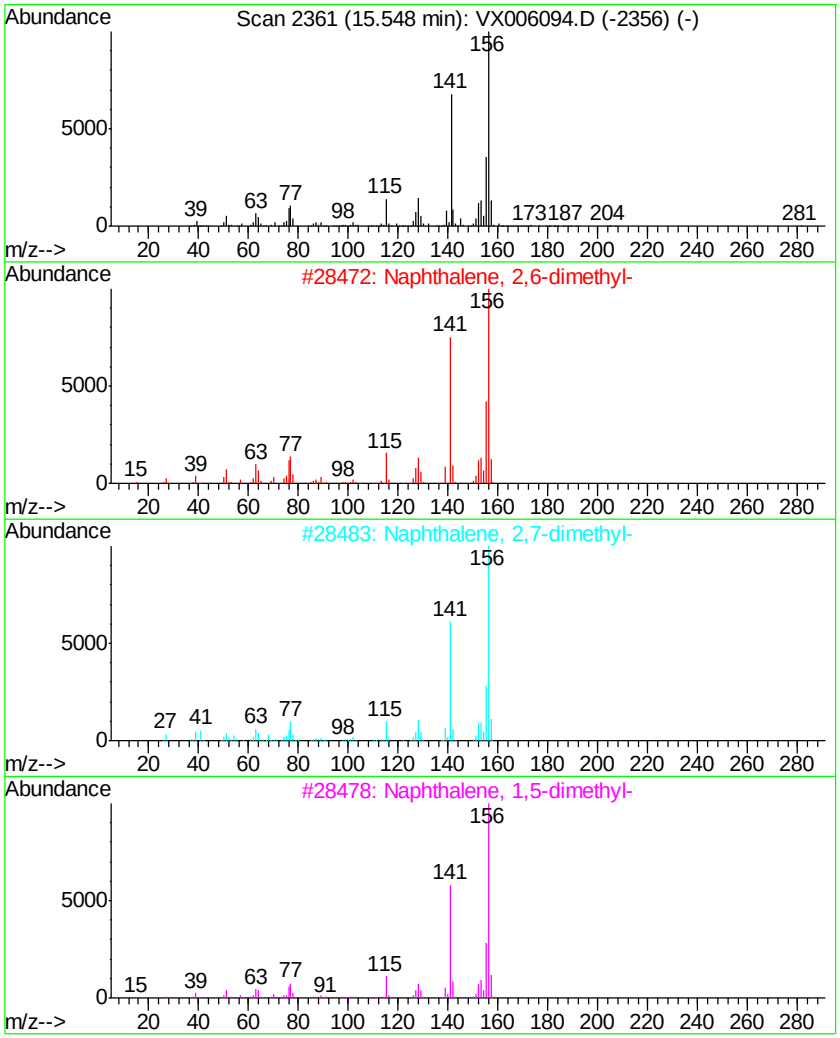
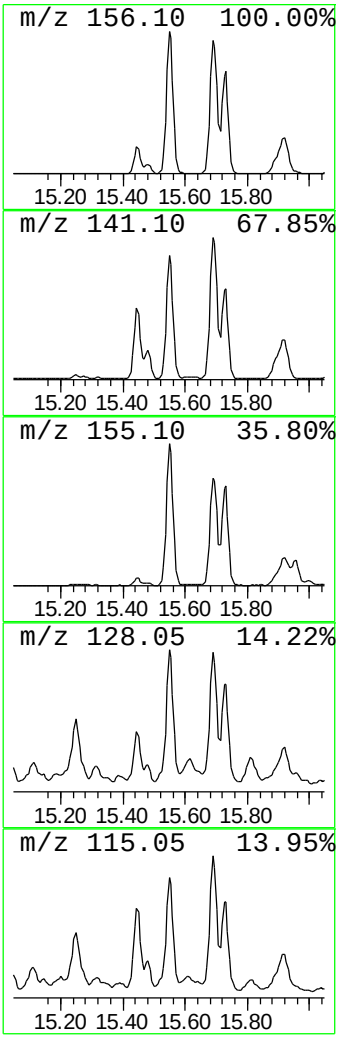
Peak Number 9 Naphthalene, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	64.80 ug/l	1105410	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97





Library Search Compound Report

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Misc : 5.04g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-04(10-12)

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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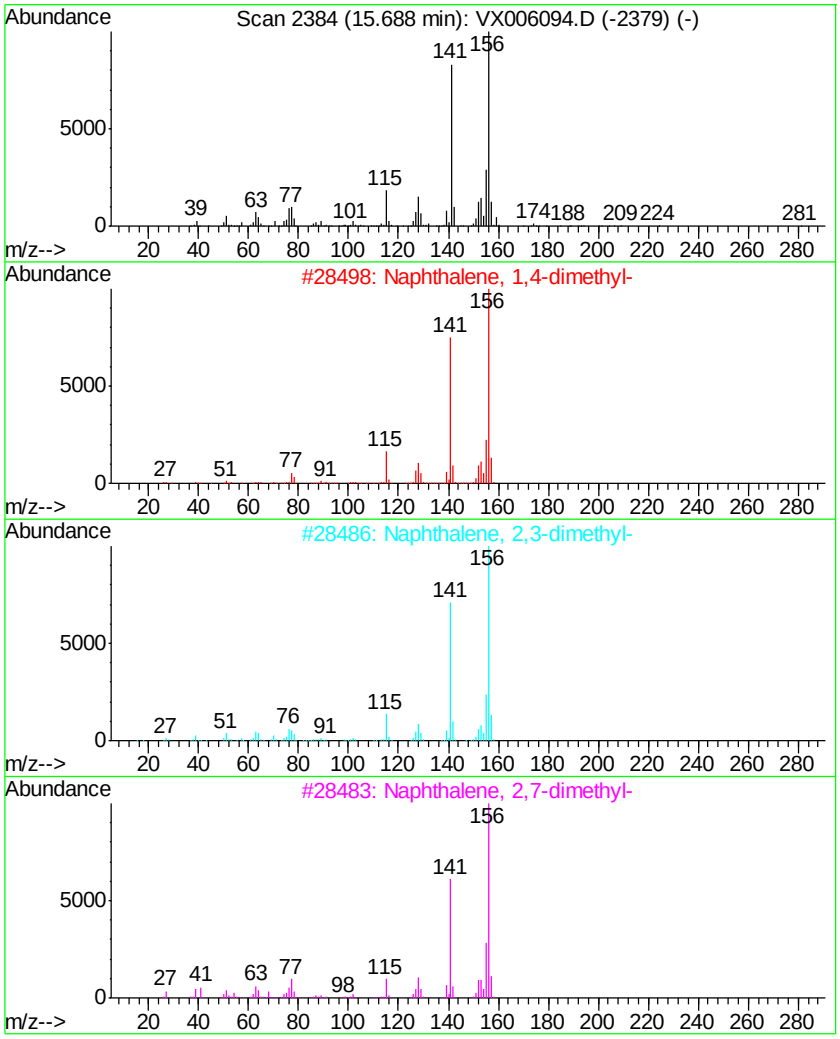
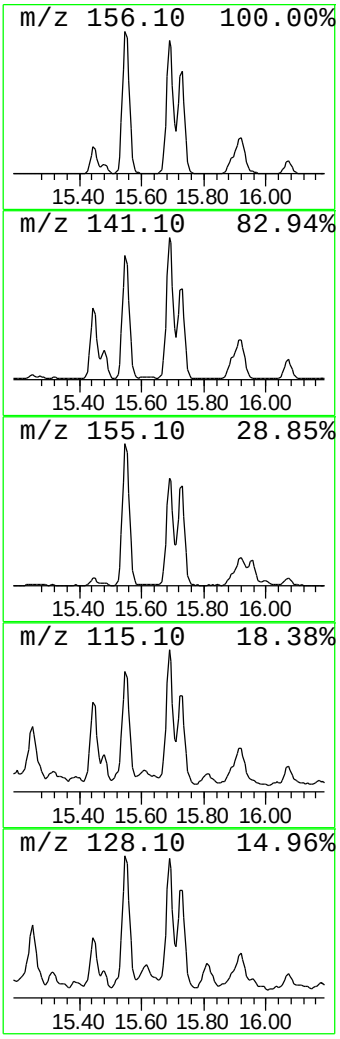
Peak Number 10 Naphthalene, 1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	66.15 ug/l	1128540	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006094.D
Acq On : 19 Nov 2018 16:34
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Sample : J5951-03 10X
Misc : 5.04g/10mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FDSB-04(10-12)

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
Octane, 2,6-dimet...	10.84	89.0	ug/l	831371	3	10.12	466891	50.0
Cyclohexane, propyl-	10.91	92.0	ug/l	858600	3	10.12	466891	50.0
Benzene, (2-methy...	12.76	66.1	ug/l	1128250	4	12.08	852979	50.0
o-Cymene	13.35	143.7	ug/l	2451650	4	12.08	852979	50.0
unknown13.47	13.47	64.5	ug/l	1099790	4	12.08	852979	50.0
Naphthalene, 1,2,...	14.29	84.6	ug/l	1443710	4	12.08	852979	50.0
Naphthalene, 1-me...	14.70	176.0	ug/l	3002300	4	12.08	852979	50.0
Naphthalene, 2,6-...	15.55	64.8	ug/l	1105410	4	12.08	852979	50.0
Naphthalene, 1,4-...	15.69	66.2	ug/l	1128540	4	12.08	852979	50.0