LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014858.D
Acq On : 06 Feb 2020 19:16
Operator : JC/SP
Sample : L1390-01
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SB-1

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\82X012220W.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	5.581	760	770	776	rVV4	404693	1719052	5.60%	0.426%
2	5.655	776	782	809	rVB3	426021	1829923	5.96%	0.453%
3	5.911	812	824	838	rBV4	567685	1744722	5.68%	0.432%
4	6.441	902	911	923	rVB	566817	1630453	5.31%	0.404%
5	6.691	942	952	963	rBV	1868972	4470450	14.55%	1.107%
6	6.856	969	979	986	rBV	581932	1757614	5.72%	0.435%
7	7.447	1065	1076	1088	rVB	3159276	7535443	24.53%	1.866%
8	8.337	1216	1222	1225	rVV	2567510	4421427	14.39%	1.095%
9	8.374	1225	1228	1235	rVB3	981149	1630151	5.31%	0.404%
10	8.496	1243	1248	1253	rBV	1488866	2453669	7.99%	0.608%
11	8.660	1268	1275	1278	rBV2	2485953	4424180	14.40%	1.096%
12	8.703	1278	1282	1293	rVB2	1538911	3625203	11.80%	0.898%
13	8.831	1293	1303	1307	rBV2	901663	1805620	5.88%	0.447%
14	8.965	1320	1325	1331	rBV	4233688	6136917	19.98%	1.520%
15	9.038	1331	1337	1348	rVB2	1796889	3517335	11.45%	0.871%
16	9.160	1348	1357	1362	rBV	993287	1863942	6.07%	0.462%
17	9.441	1397	1403	1407	rBV	1495173	2192569	7.14%	0.543%
18	9.562	1417	1423	1428	rBV3	1289683	2807047	9.14%	0.695%
19	9.617	1428	1432	1436	rVB	2745307	3681355	11.98%	0.912%
20	9.672	1436	1441	1445	rBV	2477391	3845808	12.52%	0.952%
21	9.812	1459	1464	1469	rBV2	1193557	1800017	5.86%	0.446%
22	9.873	1469	1474	1480	rBV3	1522554	3642551	11.86%	0.902%
23	9.953	1483	1487	1492	rVV	2939378	4222697	13.75%	1.046%
24	10.062	1497	1505	1509	rVB	3229916	4522130	14.72%	1.120%
25	10.111	1509	1513	1517	rBV	1240651	1733893	5.64%	0.429%
26	10.245	1529	1535	1540	rVV2	986809	1815143	5.91%	0.450%
27	10.324	1540	1548	1552	rVV3	1242870	2642027	8.60%	0.654%
28	10.373	1552	1556	1559	rVV	1758047	2549131	8.30%	0.631%
29	10.410	1559	1562	1572	rVB2	1505834	2929098	9.54%	0.725%
30	10.507	1572	1578	1587	rBV3	684561	1291426	4.20%	0.320%
31	10.635	1593	1599	1607	rVB4	1983514	3612051	11.76%	0.895%
32	10.721	1607	1613	1618	rBV5	677563	1274141	4.15%	0.316%
33	10.830	1623	1631	1635	rBV2	3337413	5511876	17.94%	1.365%
34	10.910	1635	1644	1648	rBV3	3395015	5910476	19.24%	1.464%

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Integrator: RTE
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Title : SW846 8260

35	10.946	1648	1650	1655	rVB	1200409	1321962	4.30%	0.327%
36	11.013	1655	1661	1664	rBV2	906752	1557428	5.07%	0.386%
37	11.135	1675	1681	1687	rBV5	2449413	4581735	14.92%	1.135%
38	11.239	1692	1698	1701	rBV	1600576	2532763	8.25%	0.627%
39	11.269	1701	1703	1708	rVB3	1775313	2215330	7.21%	0.549%
40	11.355	1713	1717	1720	rBV	1221263	1574796	5.13%	0.390%
41	11.440	1727	1731	1734	rBV3	917184	1414540	4.61%	0.350%
42	11.483	1734	1738	1742	rVB	1999418	2368735	7.71%	0.587%
43	11.532	1742	1746	1750	rVB3	1148839	1852004	6.03%	0.459%
44	11.666	1763	1768	1775	rVB4	1573290	3137725	10.22%	0.777%
45	11.916	1801	1809	1810	rBV4	811091	1529357	4.98%	0.379%
46	11.940	1810	1813	1818	rVV2	1758330	2742614	8.93%	0.679%
47	11.995	1818	1822	1825	rVV	3248162	4163230	13.55%	1.031%
48	12.074	1830	1835	1840	rVV3	1774185	3218726	10.48%	0.797%
49	12.141	1840	1846	1851	rVV3	1471033	2677424	8.72%	0.663%
50	12.220	1855	1859	1867	rVB5	1042362	2251464	7.33%	0.558%
51	12.300	1867	1872	1878	rBV	2470857	3673258	11.96%	0.910%
52	12.367	1878	1883	1890	rVB2	3229028	6338798	20.64%	1.570%
53	12.464	1892	1899	1904	rBV4	1067149	2686045	8.74%	0.665%
54	12.513	1904	1907	1913	rVB3	2825305	4220611	13.74%	1.045%
55	12.666	1928	1932	1935	rVB	3224726	3662876	11.92%	0.907%
56	12.757	1941	1947	1948	rBV	1999000	2948662	9.60%	0.730%
57	12.873	1962	1966	1969	rVV2	2729965	4163652	13.56%	1.031%
58	12.940	1973	1977	1980	rBV3	1888356	3084749	10.04%	0.764%
59	12.976	1980	1983	1988	rVB2	2853793	3733209	12.15%	0.925%
60	13.037	1988	1993	1996	rBV2	2555067	3352468	10.91%	0.830%
61	13.080	1996	2000	2006	rVB4	1997669	3620604	11.79%	0.897%
62	13.147	2007	2011	2016	rBV2	1078161	2026250	6.60%	0.502%
63	13.220	2020	2023	2027	rVB	1766831	1927134	6.27%	0.477%
64	13.342	2039	2043	2048	rVV2	7000699	10607331	34.53%	2.627%
65	13.385	2048	2050	2053	rVV2	1051457	1306229	4.25%	0.323%
66	13.421	2053	2056	2059	rVV	1570102	1699314	5.53%	0.421%
67	13.476	2059	2065	2074	rVB6	4087146	8511657	27.71%	2.108%
68	13.562	2074	2079	2081	rBV2	1532086	2266734	7.38%	0.561%
69	13.598	2081	2085	2087	rVV	2174153	2911384	9.48%	0.721%
70	13.635	2087	2091	2095	rVV4	3206935	5013931	16.32%	1.242%
71	13.696	2095	2101	2102	rVV5	1016171	2104300	6.85%	0.521%

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Integrator: RTE
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Title : SW846 8260

72	13.720	2102	2105	2110	rVB3	2906447	4552118	14.82%	1.127%
73	13.830	2120	2123	2130	rVB	3691637	5121955	16.67%	1.268%
74	13.909	2132	2136	2141	rVB2	3106879	4790002	15.59%	1.186%
75	13.982	2141	2148	2152	rBV3	4068470	6876645	22.39%	1.703%
76	14.025	2152	2155	2158	rBV3	1534036	2130467	6.94%	0.528%
77	14.129	2167	2172	2175	rBV3	3534226	4711664	15.34%	1.167%
78	14.214	2183	2186	2190	rBV	1175913	1294065	4.21%	0.320%
79	14.281	2190	2197	2204	rBV3	6271095	12995525	42.31%	3.218%
80	14.373	2209	2212	2218	rBV2	2846048	4002528	13.03%	0.991%
81	14.427	2218	2221	2225	rVB	4255515	4873597	15.87%	1.207%
82	14.470	2225	2228	2234	rVB5	1676627	2858186	9.31%	0.708%
83	14.537	2234	2239	2247	rBV3	4531571	8030636	26.14%	1.989%
84	14.696	2257	2265	2268	rVV2	18014891	30716427	100.00%	7.607%
85	14.726	2268	2270	2274	rVB	3772996	4328620	14.09%	1.072%
86	14.781	2274	2279	2283	rBV4	2443505	3715806	12.10%	0.920%
87	14.836	2284	2288	2292	rVV	9833409	12850253	41.84%	3.182%
88	14.872	2292	2294	2296	rVV3	2103679	2260800	7.36%	0.560%
89	14.903	2296	2299	2304	rVV3	2206448	3026137	9.85%	0.749%
90	14.958	2304	2308	2315	rVV3	1606216	3592511	11.70%	0.890%
91	15.104	2326	2332	2336	rBV3	1114944	2157965	7.03%	0.534%
92	15.244	2349	2355	2362	rVB	3576754	6395819	20.82%	1.584%
93	15.311	2362	2366	2369	rBV4	734051	1349400	4.39%	0.334%
94	15.439	2382	2387	2390	rBV	4065959	5727396	18.65%	1.418%
95	15.470	2390	2392	2397	rVB2	988999	1391616	4.53%	0.345%
96	15.543	2398	2404	2410	rBV	8652326	13008499	42.35%	3.221%
97	15.683	2421	2427	2430	rBV	7498334	11455701	37.30%	2.837%
98	15.720	2430	2433	2441	rVB	4576128	7238465	23.57%	1.793%
99	15.909	2456	2464	2479	rVB2	1660558	4995485	16.26%	1.237%
100	16.061	2484	2489	2501	rVB2	858505	1808488	5.89%	0.448%

Sum of corrected areas: 403805342

LSC Report - Integrated Chromatogram

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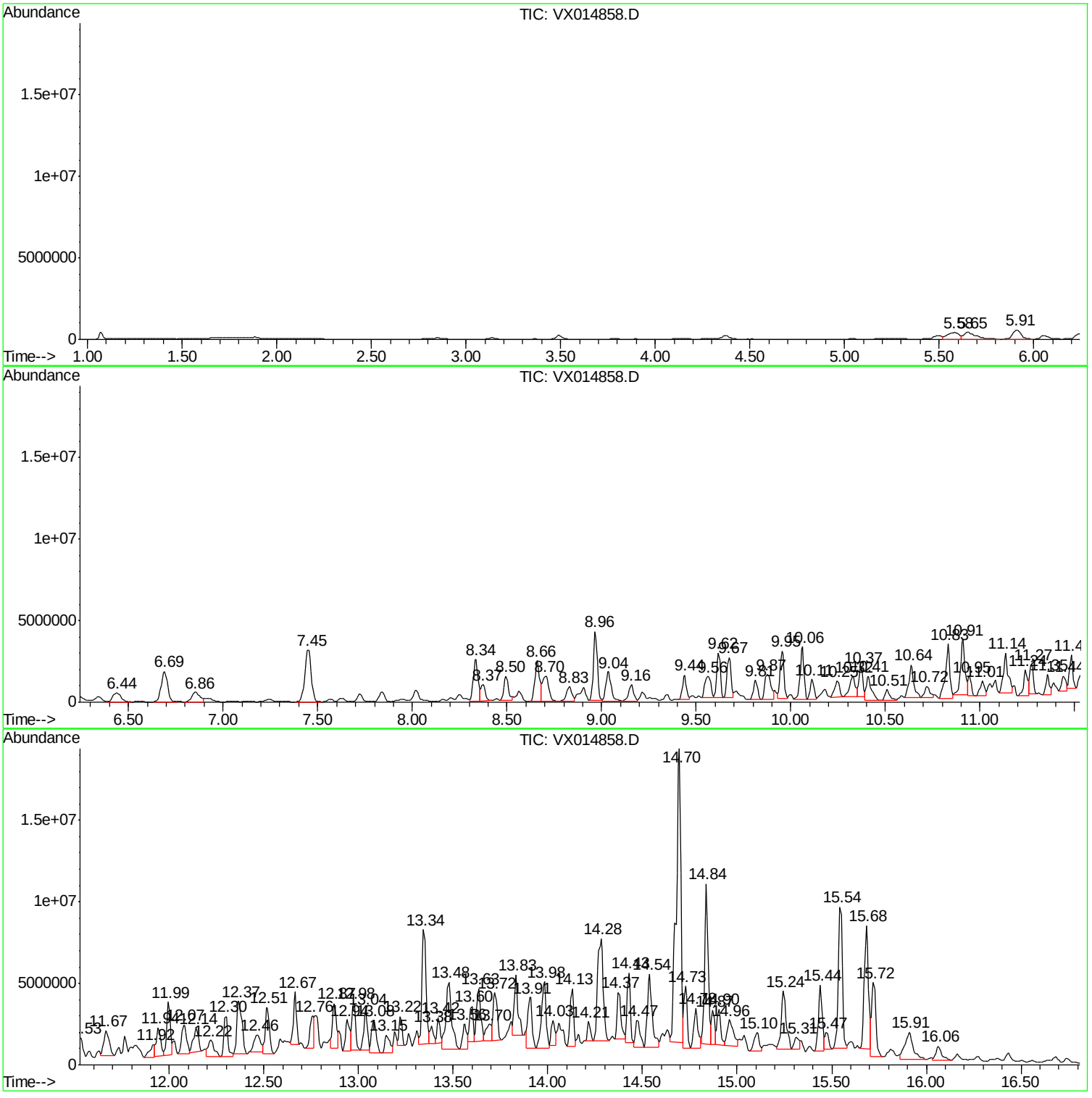
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SB-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Quant Title : SW846 8260

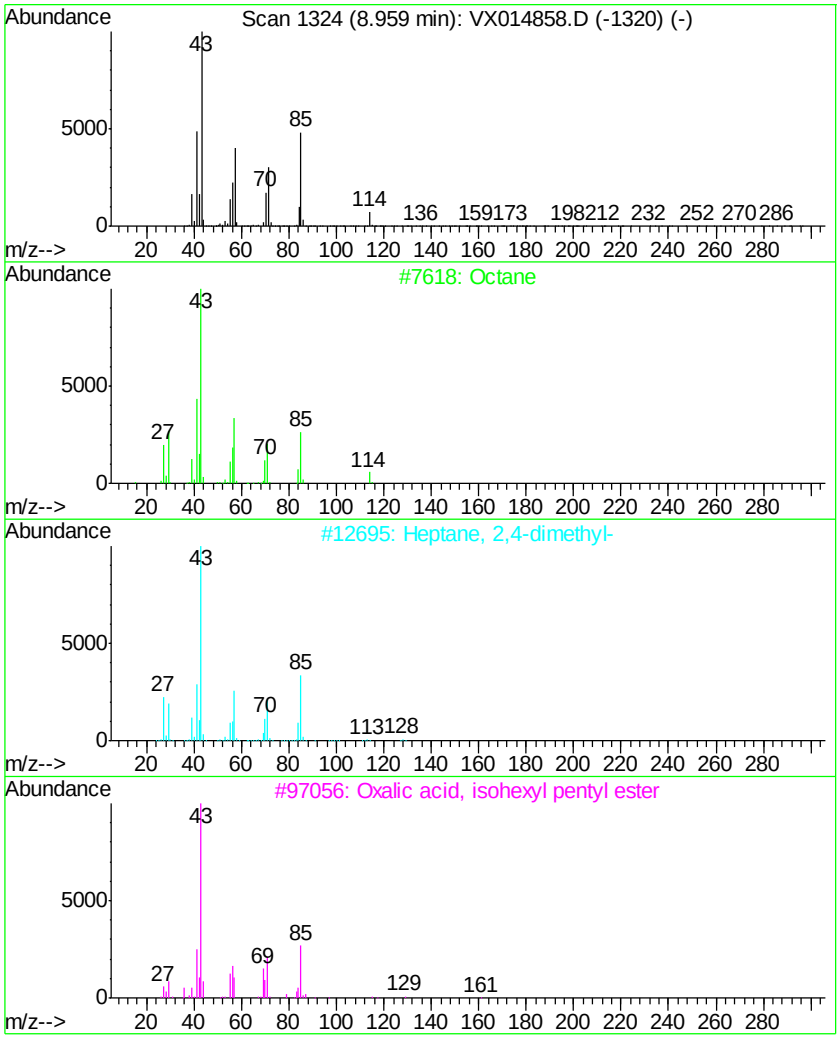
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

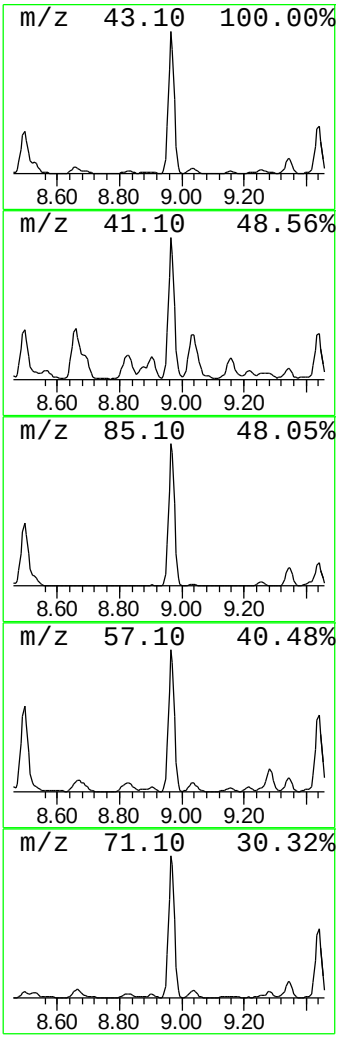
****

Peak Number 1 Octane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	176.97 ug/l	6136920	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	94
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	90
3	Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	83
4	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	64
5	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	64





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ClientSampleId : SB-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

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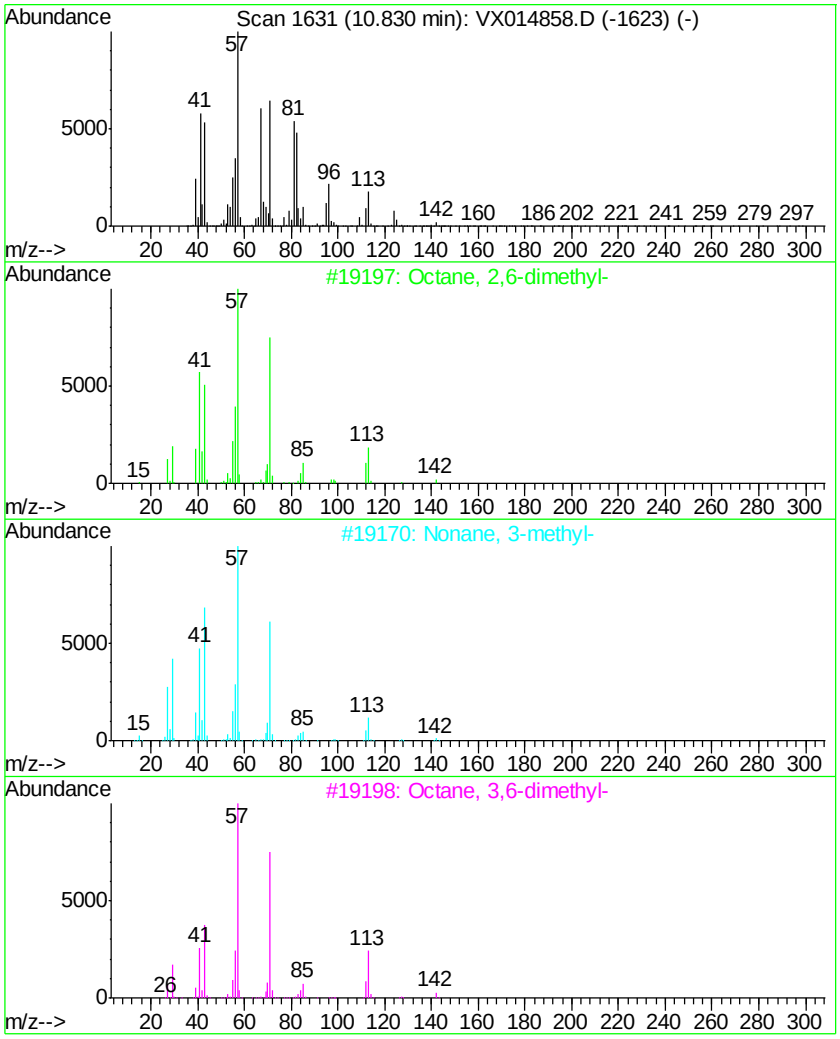
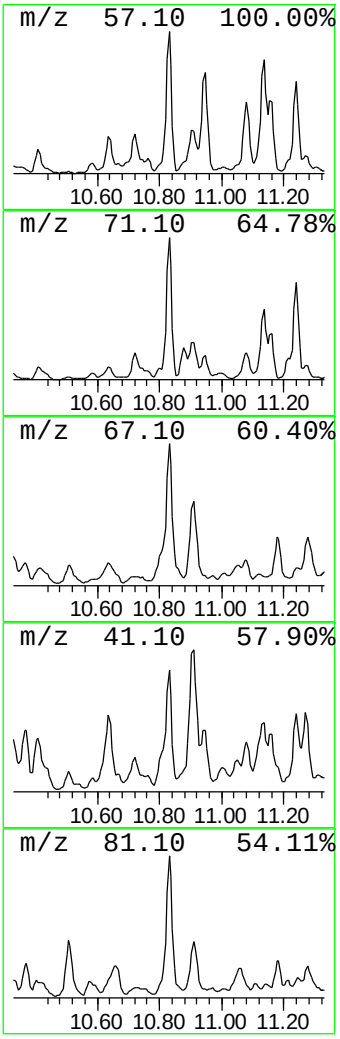
Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	158.95 ug/l	5511880	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	86
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	50
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	46
4	1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	42
5	Heptanoic acid, 3-hexenyl ester,...	212	C13H24O2	061444-39-1	35





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Instrument : MSVOA_X
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

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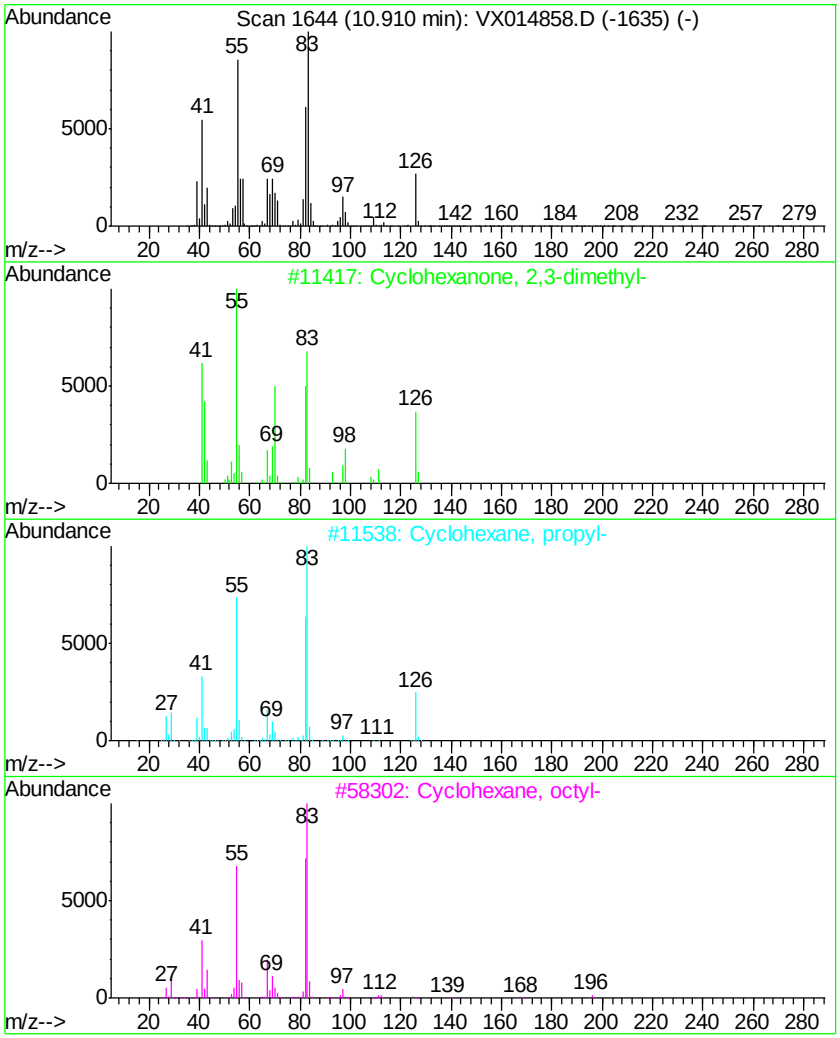
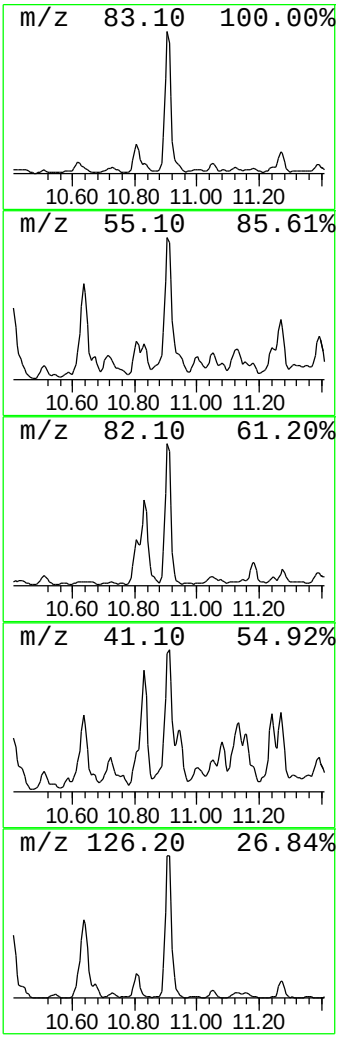
Peak Number 3 Cyclohexanone, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	170.44 ug/l	5910480	Chlorobenzene-d5	10.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	91
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	74
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	64
4	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	64
5	Acetic acid, mercapto-, cyclohex...	174	C8H14O2S	016849-98-2	53





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Quant Title : SW846 8260

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

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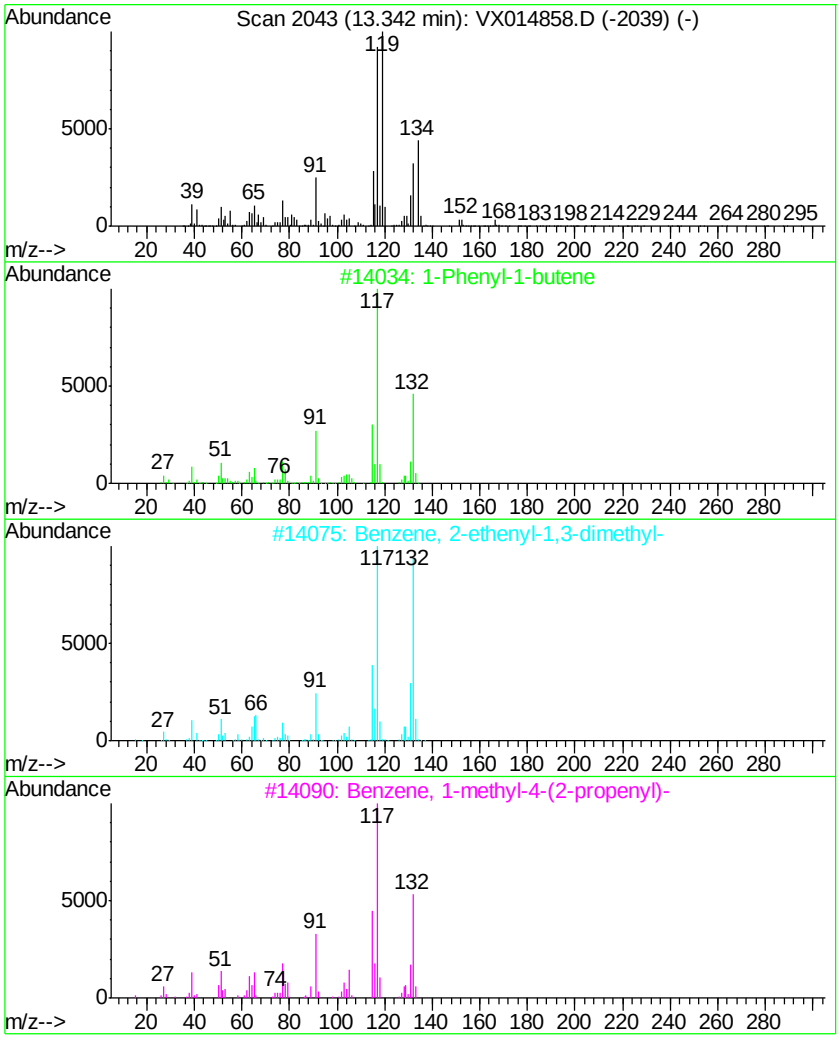
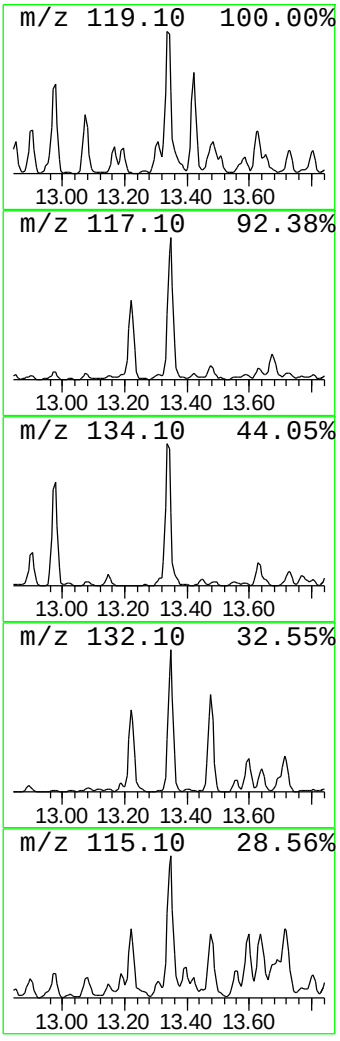
Peak Number 4 1-Phenyl-1-butene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	164.78 ug/l	10607300	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
2	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	64
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	64
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	50





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Quant Title : SW846 8260

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

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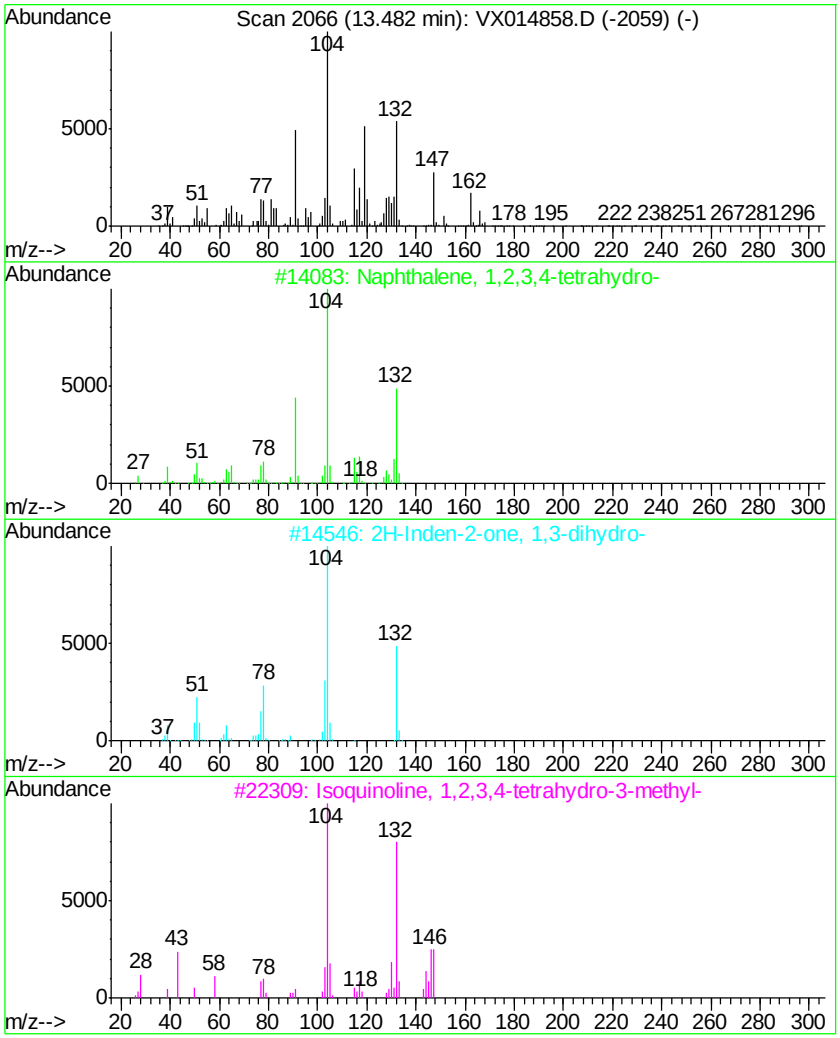
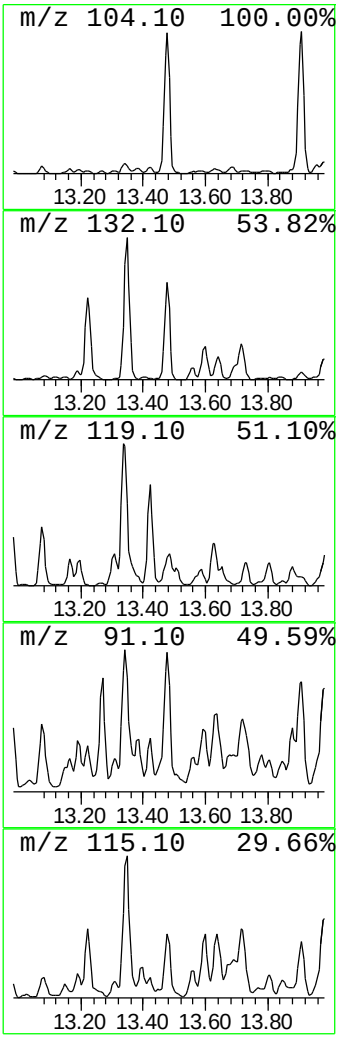
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	132.22 ug/l	8511660	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	93
2	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	43
3	Isoquinoline, 1,2,3,4-tetrahydro...	147	C10H13N	029726-60-1	38
4	Benzeneethanol, .alpha.,.alpha.-...	162	C11H14O	025982-72-3	35
5	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014858.D
Acq On : 06 Feb 2020 19:16
Operator : JC/SP
Sample : L1390-01
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SB-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

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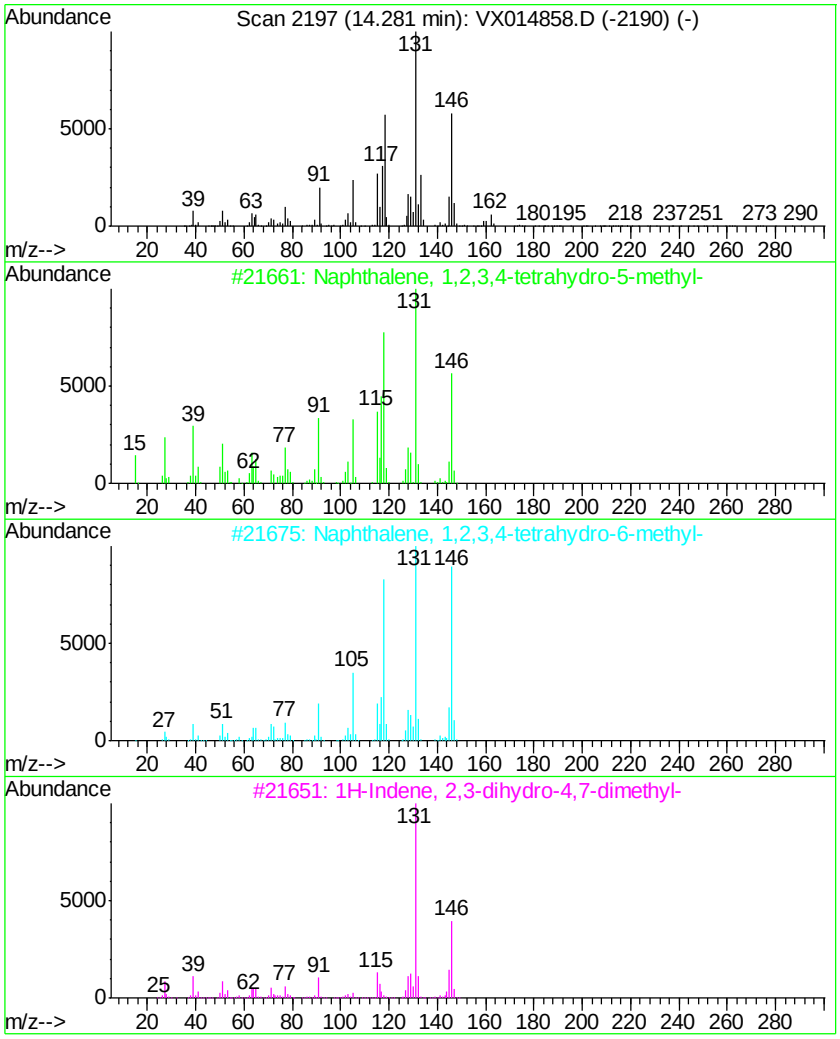
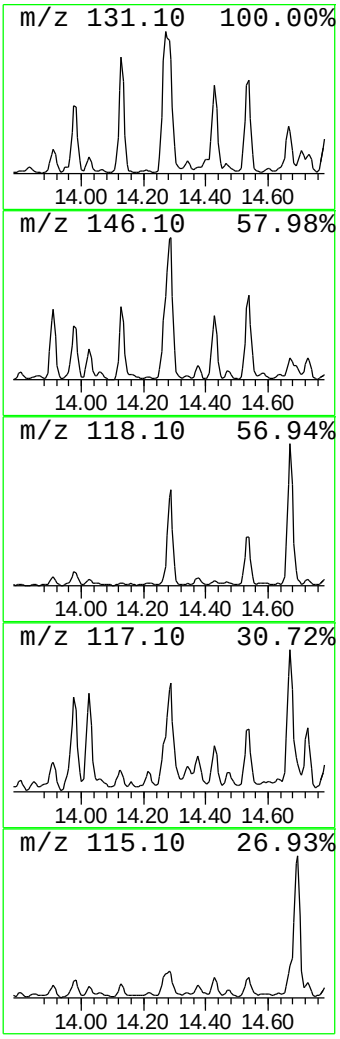
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	201.87 ug/l	12995500	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	92
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	91
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	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 : VX014858.D
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Operator : JC/SP
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Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SB-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

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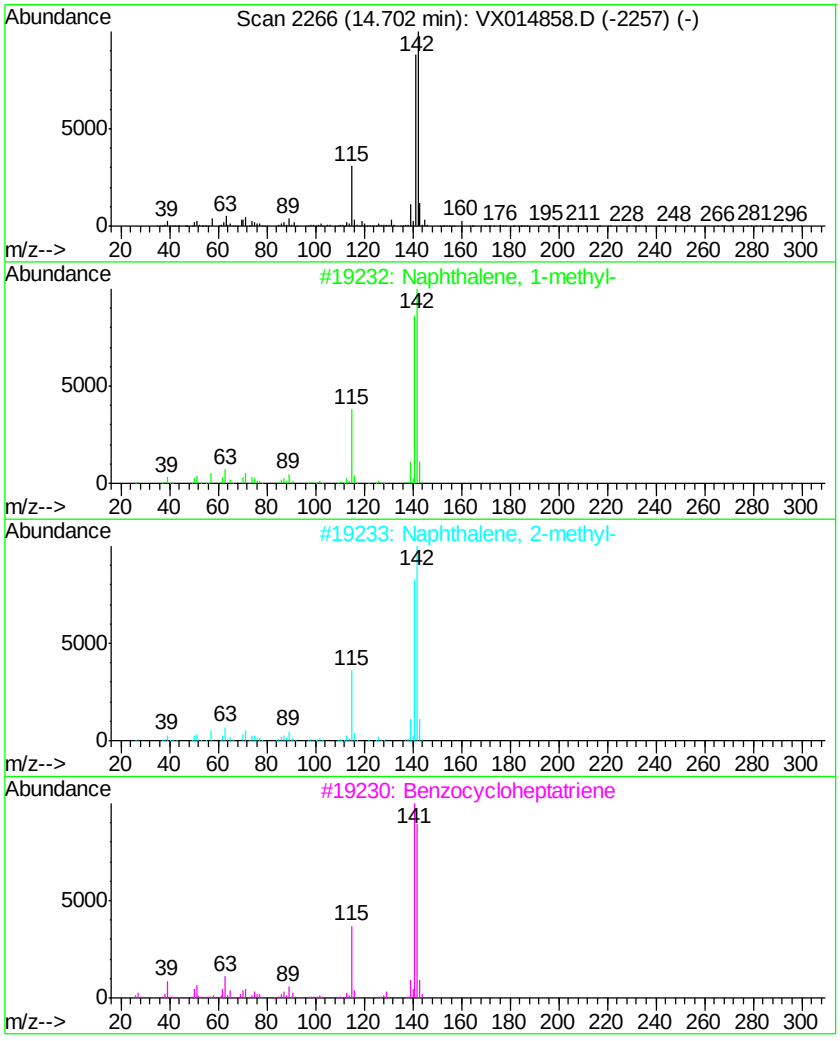
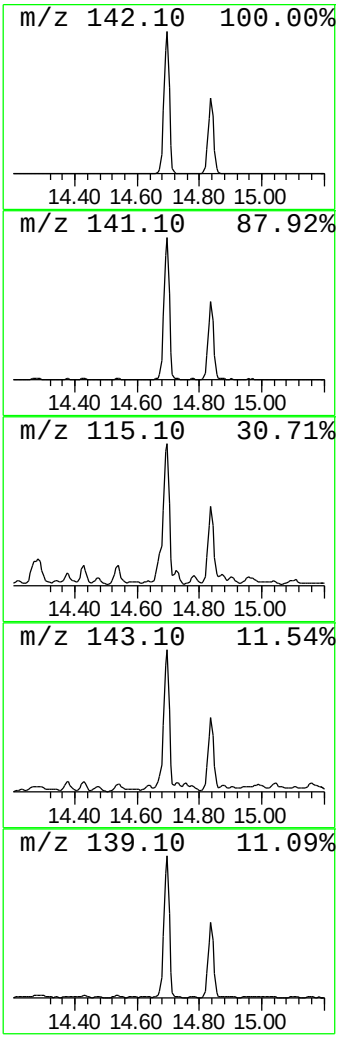
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	477.15 ug/l	30716400	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	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





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Data File : VX014858.D
Acq On : 06 Feb 2020 19:16
Operator : JC/SP
Sample : L1390-01
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SB-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

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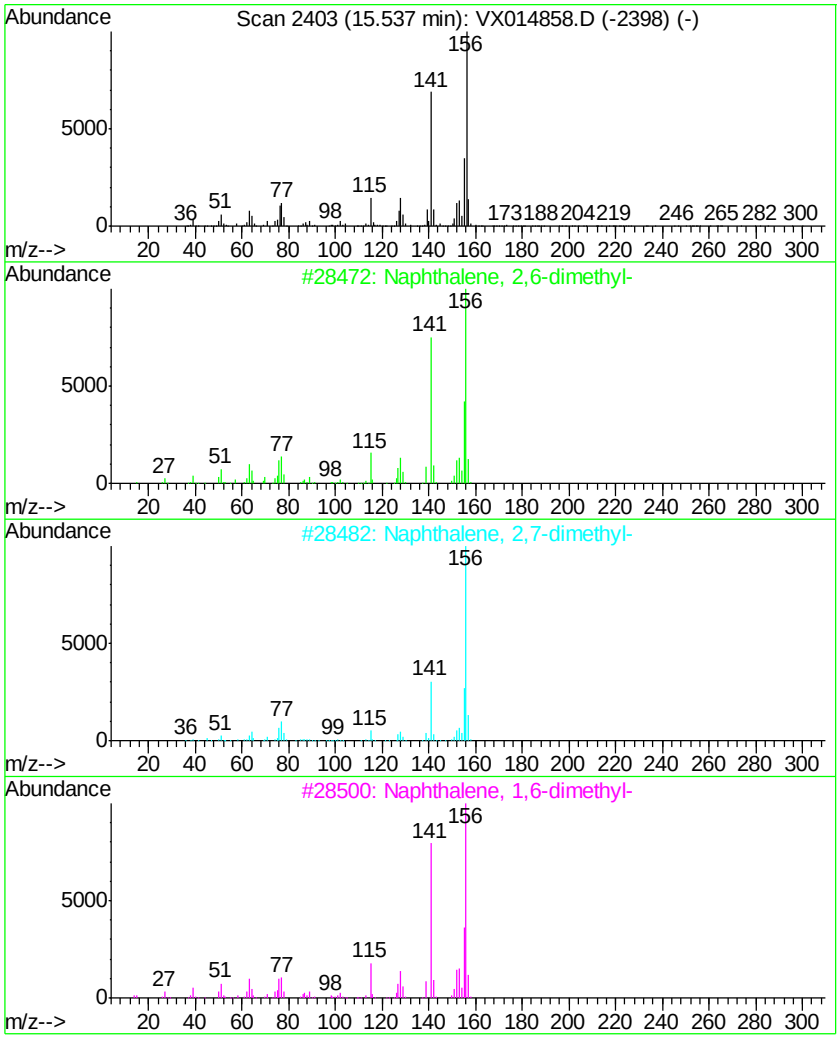
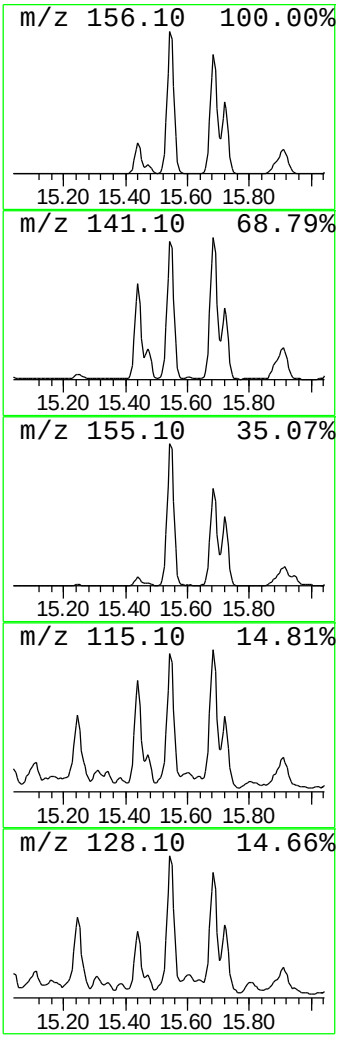
Peak Number 9 Naphthalene, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	202.08 ug/l	13008500	1,4-Dichlorobenzene-d4	12.07

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, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97





Library Search Compound Report

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Data File : VX014858.D
Acq On : 06 Feb 2020 19:16
Operator : JC/SP
Sample : L1390-01
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SB-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

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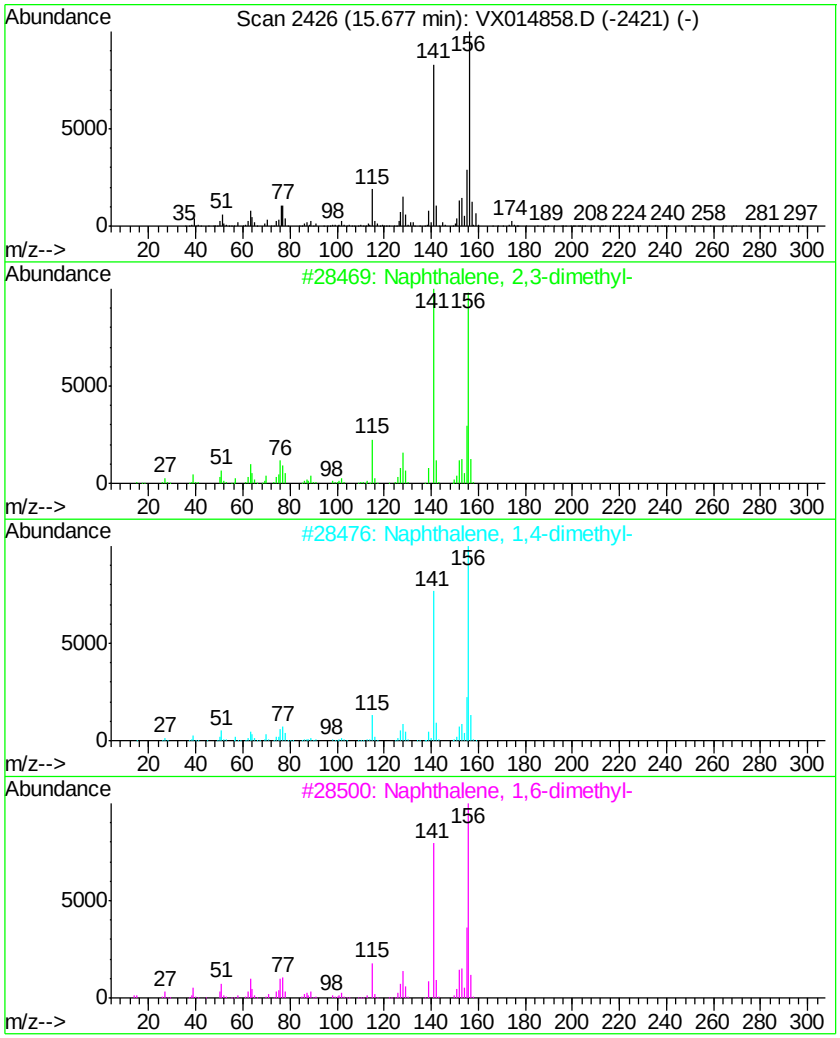
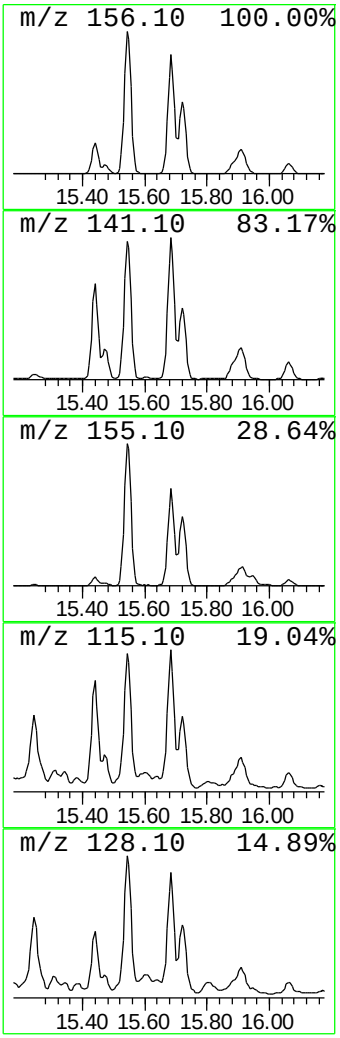
Peak Number 10 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	177.95 ug/l	11455700	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014858.D
Acq On : 06 Feb 2020 19:16
Operator : JC/SP
Sample : L1390-01
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ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SB-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.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	8.96	177.0	ug/l	6136920	3	10.11	1733890	50.0
Octane, 2,6-dimet...	10.83	158.9	ug/l	5511880	3	10.11	1733890	50.0
Cyclohexanone, 2,...	10.91	170.4	ug/l	5910480	3	10.11	1733890	50.0
1-Phenyl-1-butene	13.34	164.8	ug/l	10607300	4	12.07	3218730	50.0
Naphthalene, 1,2,...	13.48	132.2	ug/l	8511660	4	12.07	3218730	50.0
Naphthalene, 1,2,...	14.28	201.9	ug/l	12995500	4	12.07	3218730	50.0
Naphthalene, 1-me...	14.70	477.1	ug/l	30716400	4	12.07	3218730	50.0
Naphthalene, 2,6-...	15.54	202.1	ug/l	13008500	4	12.07	3218730	50.0
Naphthalene, 2,3-...	15.68	177.9	ug/l	11455700	4	12.07	3218730	50.0