LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX042018\
Data File : VX001007.D
Acq On : 20 Apr 2018 14:36
Operator : JC/MD
Sample : J2387-05
Misc : 5.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20180243-COMPOSITE-E

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.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	1.069	70	79	93	rBV	573116	668539	51.51%	3.817%
2	1.636	155	172	174	rBV4	11386	33434	2.58%	0.191%
3	5.513	794	808	822	rBV	129789	375583	28.94%	2.144%
4	5.665	822	833	851	rVV	215162	608456	46.88%	3.474%
5	6.074	889	900	918	rBV	148576	389589	30.02%	2.224%
6	6.866	1020	1030	1045	rBV	300248	735198	56.64%	4.197%
7	8.720	1327	1334	1350	rBV	729456	1190164	91.70%	6.794%
8	10.122	1558	1564	1580	rVB	637609	922715	71.09%	5.268%
9	10.256	1580	1586	1593	rVB	28626	40903	3.15%	0.234%
10	10.841	1674	1682	1686	rBV	18647	27789	2.14%	0.159%
11	10.951	1697	1700	1705	rVB	16097	21643	1.67%	0.124%
12	11.146	1726	1732	1742	rVB	789603	1011269	77.91%	5.773%
13	11.280	1751	1754	1759	rVB3	10769	15315	1.18%	0.087%
14	11.439	1776	1780	1786	rBV	35790	74895	5.77%	0.428%
15	11.676	1814	1819	1825	rVB3	17003	31380	2.42%	0.179%
16	11.743	1825	1830	1832	rBV4	8823	13020	1.00%	0.074%
17	11.774	1832	1835	1838	rVV	31178	34931	2.69%	0.199%
18	11.811	1838	1841	1848	rVB4	16754	29817	2.30%	0.170%
19	11.951	1857	1864	1868	rVB3	23449	38836	2.99%	0.222%
20	12.006	1868	1873	1874	rBV3	14844	20063	1.55%	0.115%
21	12.030	1874	1877	1881	rVV2	33270	41767	3.22%	0.238%
22	12.085	1881	1886	1892	rVB	1052548	1297923	100.00%	7.410%
23	12.225	1903	1909	1913	rBV5	10582	18988	1.46%	0.108%
24	12.310	1918	1923	1930	rBV6	21382	47109	3.63%	0.269%
25	12.378	1930	1934	1940	rBV2	37096	66411	5.12%	0.379%
26	12.481	1947	1951	1956	rVB3	21114	26129	2.01%	0.149%
27	12.530	1956	1959	1965	rVB4	21247	40377	3.11%	0.231%
28	12.615	1966	1973	1976	rBV2	30255	68942	5.31%	0.394%
29	12.670	1980	1982	1990	rVB	44449	65071	5.01%	0.371%
30	12.743	1990	1994	2002	rBV4	38381	84327	6.50%	0.481%
31	12.859	2009	2013	2014	rBV2	20970	23284	1.79%	0.133%
32	12.944	2023	2027	2030	rBV3	31475	45352	3.49%	0.259%
33	12.981	2031	2033	2037	rVB2	21830	21029	1.62%	0.120%
34	13.024	2037	2040	2042	rBV	26455	29702	2.29%	0.170%

LSC Area Percent Report

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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20180243-COMPOSITE-E

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

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Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Title : SW846 8260

35	13.103	2050	2053	2056	rBV3	12874	16808	1.29%	0.096%
36	13.158	2058	2062	2067	rVB2	31171	44657	3.44%	0.255%
37	13.274	2077	2081	2084	rBV2	19738	24096	1.86%	0.138%
38	13.353	2084	2094	2099	rBV6	73278	156753	12.08%	0.895%
39	13.408	2099	2103	2105	rVV2	43221	51262	3.95%	0.293%
40	13.444	2105	2109	2112	rVV2	72950	99323	7.65%	0.567%
41	13.487	2112	2116	2124	rVB4	74506	163601	12.60%	0.934%
42	13.609	2132	2136	2139	rBV	41534	64312	4.95%	0.367%
43	13.737	2154	2157	2159	rBV4	24795	31973	2.46%	0.183%
44	13.767	2159	2162	2165	rVV2	30649	38562	2.97%	0.220%
45	13.841	2170	2174	2181	rBV	142698	215471	16.60%	1.230%
46	13.902	2181	2184	2191	rBV3	52459	74392	5.73%	0.425%
47	13.969	2191	2195	2197	rBV3	26062	39139	3.02%	0.223%
48	14.054	2206	2209	2211	rBV3	17639	22946	1.77%	0.131%
49	14.133	2219	2222	2224	rBV3	36837	43205	3.33%	0.247%
50	14.164	2224	2227	2230	rVV3	50190	57783	4.45%	0.330%
51	14.200	2230	2233	2238	rVV5	29367	42228	3.25%	0.241%
52	14.280	2243	2246	2250	rBV3	55740	71423	5.50%	0.408%
53	14.383	2259	2263	2269	rBV2	46009	71937	5.54%	0.411%
54	14.584	2293	2296	2299	rVB2	22259	23087	1.78%	0.132%
55	14.700	2308	2315	2320	rBV	852934	1063374	81.93%	6.071%
56	14.792	2327	2330	2332	rBV3	17683	21184	1.63%	0.121%
57	14.847	2332	2339	2347	rVV	824613	1086531	83.71%	6.203%
58	14.914	2347	2350	2353	rVV3	15231	17738	1.37%	0.101%
59	15.005	2362	2365	2366	rBV2	12668	15311	1.18%	0.087%
60	15.279	2406	2410	2415	rVB	116704	159144	12.26%	0.909%
61	15.334	2415	2419	2425	rVB3	33449	57928	4.46%	0.331%
62	15.450	2430	2438	2442	rBV	506860	766999	59.09%	4.379%
63	15.554	2450	2455	2460	rBV	751884	1189709	91.66%	6.792%
64	15.694	2469	2478	2482	rBV	756999	1272610	98.05%	7.265%
65	15.731	2482	2484	2493	rVB	385856	552542	42.57%	3.154%
66	15.822	2495	2499	2506	rVB3	30459	59915	4.62%	0.342%
67	15.920	2506	2515	2520	rBV	203042	554301	42.71%	3.164%
68	16.078	2536	2541	2552	rVB	120856	218219	16.81%	1.246%
69	16.182	2552	2558	2564	rBV	102685	175383	13.51%	1.001%
70	16.291	2572	2576	2582	rVB	46786	82120	6.33%	0.469%
71	16.426	2593	2598	2607	rVB2	149266	345664	26.63%	1.973%

LSC Area Percent Report

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Misc : 5.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20180243-COMPOSITE-E

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

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Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Title : SW846 8260

72	16.578	2618	2623	2628	rBV2	20536	34384	2.65%	0.196%
73	16.657	2628	2636	2639	rBV3	38033	111285	8.57%	0.635%
74	16.700	2639	2643	2648	rVB2	67042	116905	9.01%	0.667%
75	16.761	2648	2653	2657	rBV	63724	102829	7.92%	0.587%

Sum of corrected areas: 17516983

LSC Report - Integrated Chromatogram

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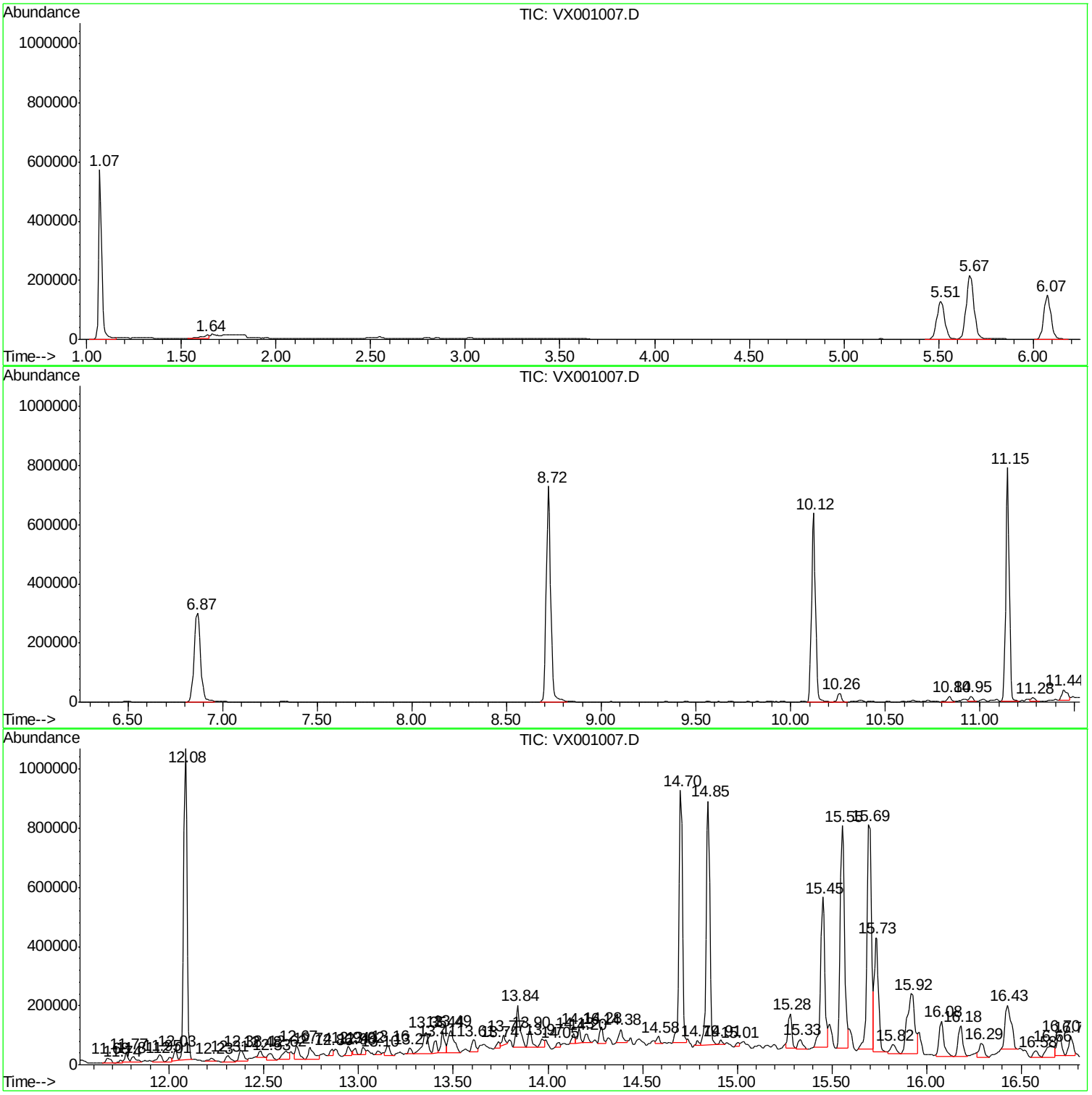
Sample : J2387-05
Misc : 5.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20180243-COMPOSITE-E

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Quant Title : SW846 8260

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



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX042018\
Data File : VX001007.D
Acq On : 20 Apr 2018 14:36
Operator : JC/MD
Sample : J2387-05
Misc : 5.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20180243-COMPOSITE-E

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Quant Title : SW846 8260

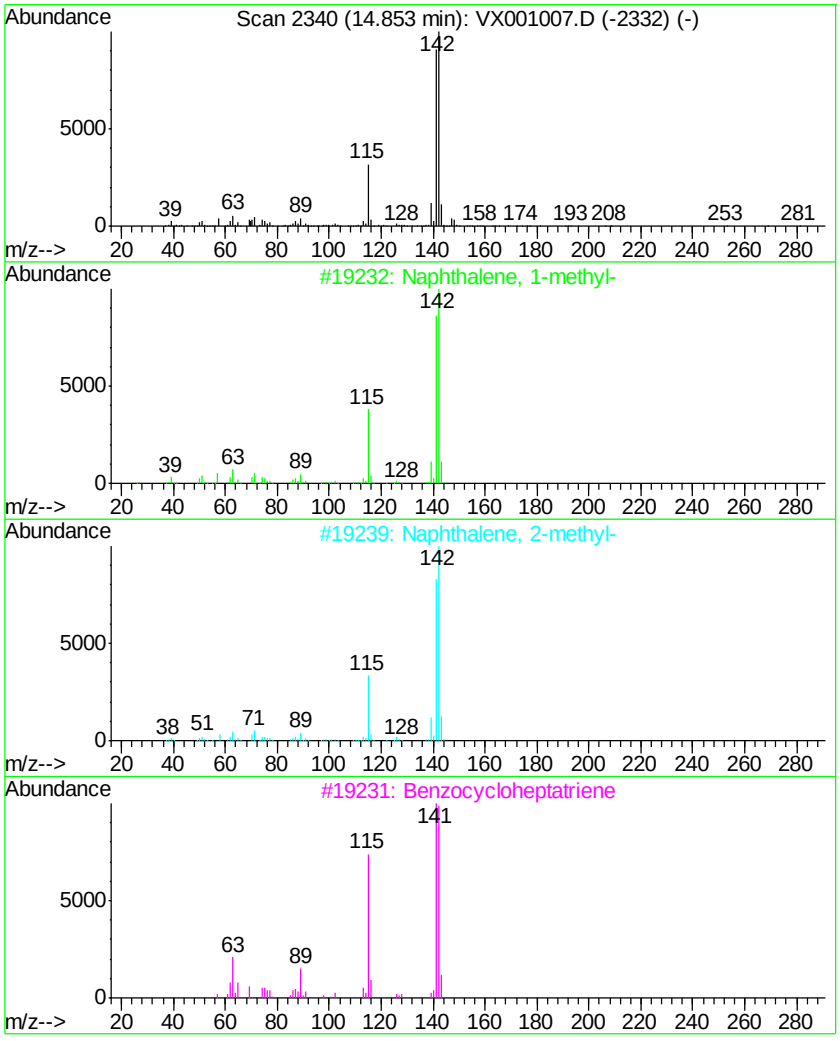
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

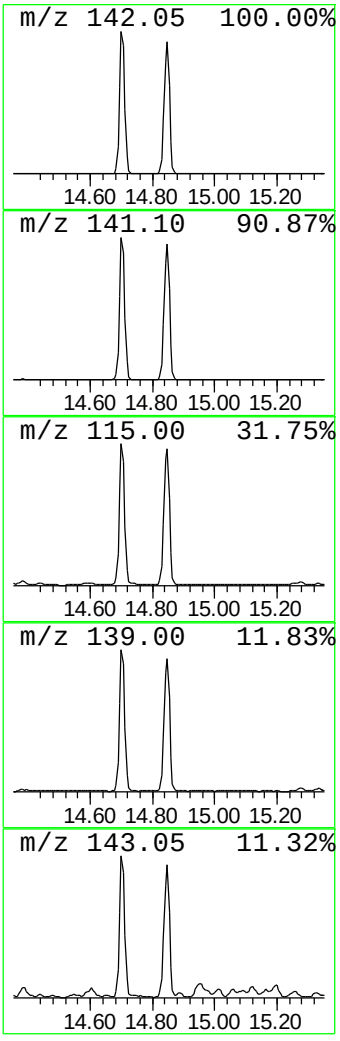
****

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	41.86 ug/l	1086530	1,4-Dichlorobenzene-d4	12.08

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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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 20180243-COMPOSITE-E

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Quant Title : SW846 8260

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

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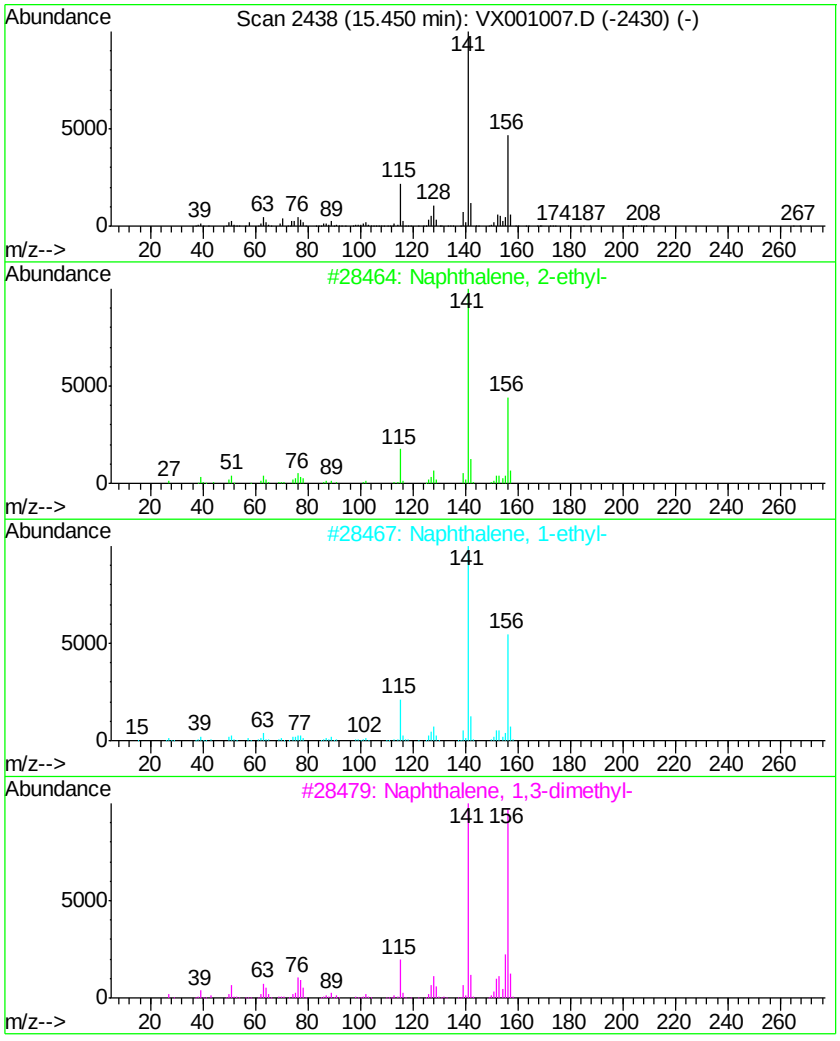
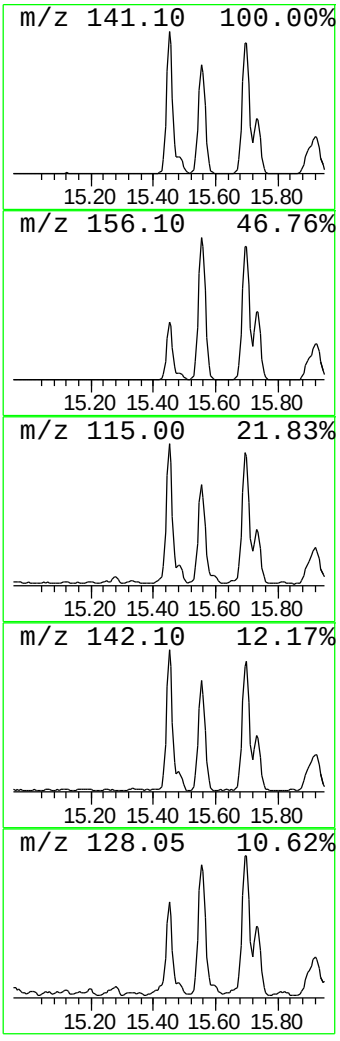
Peak Number 4 Naphthalene, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	29.55 ug/l	766999	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	97
2	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91
4	2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	59
5	Naphthalene, 1-propyl-	170	C13H14	002765-18-6	59





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX042018\
Data File : VX001007.D
Acq On : 20 Apr 2018 14:36
Operator : JC/MD
Sample : J2387-05
Misc : 5.05g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20180243-COMPOSITE-E

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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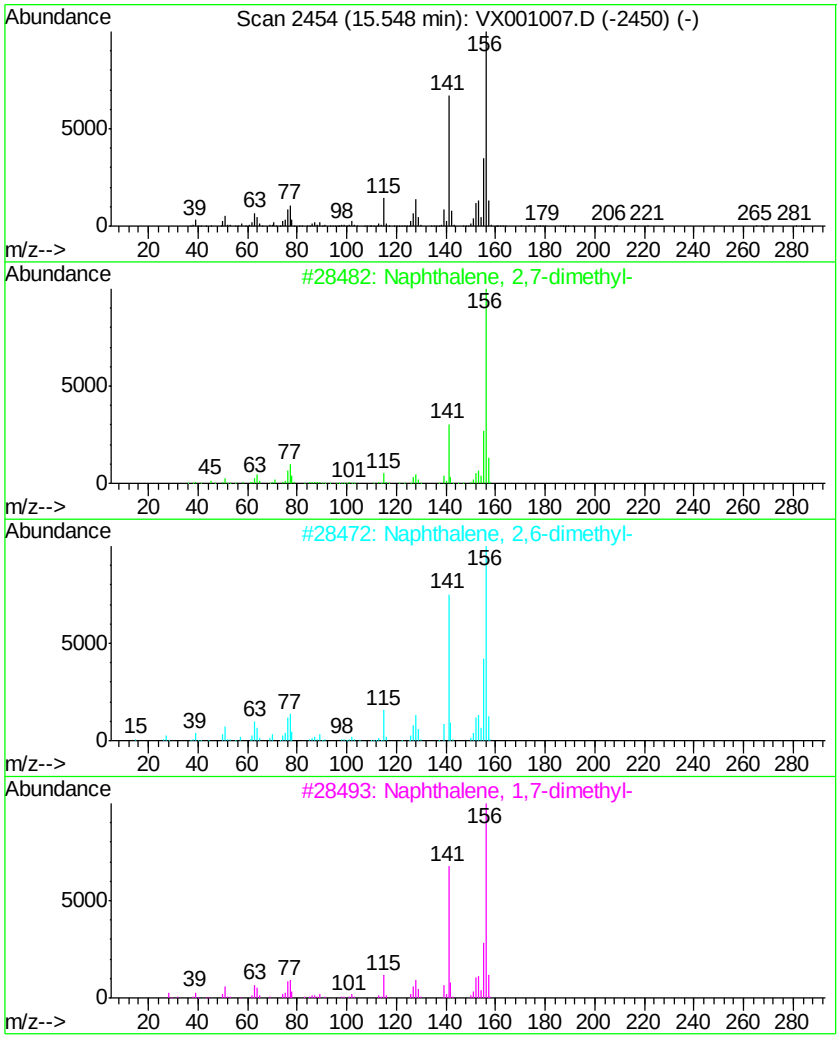
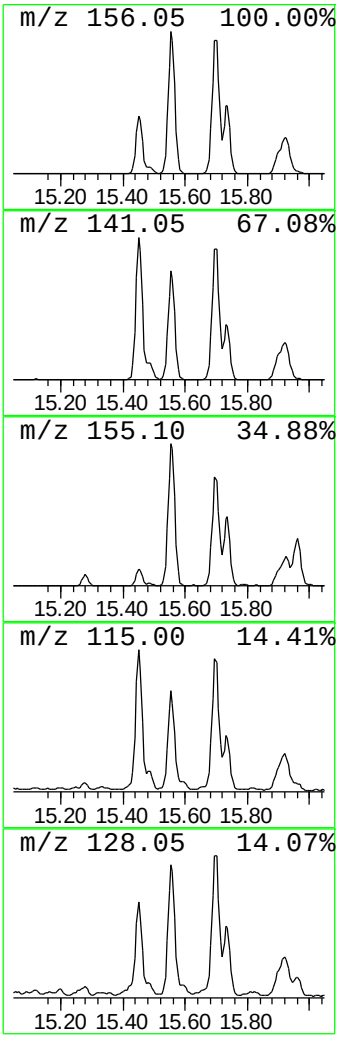
Peak Number 5 Naphthalene, 2,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	45.83 ug/l	1189710	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97





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MSVOA_X
ClientSampleId :
20180243-COMPOSITE-E

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Quant Title : SW846 8260

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

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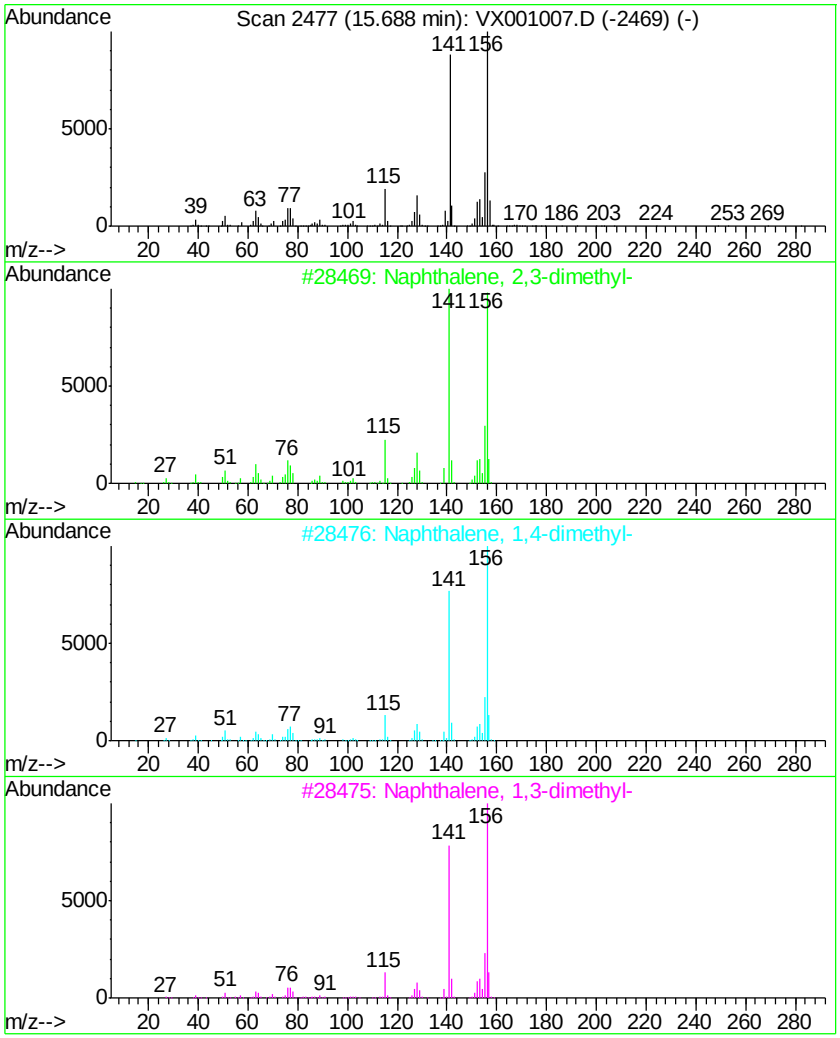
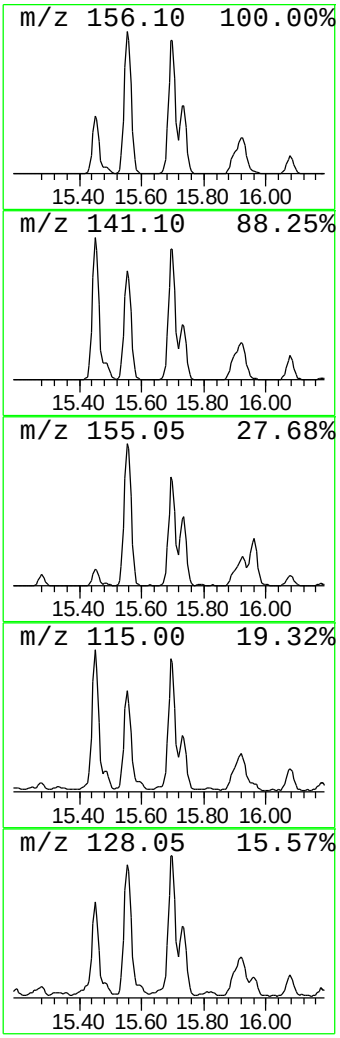
Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	49.02 ug/l	1272610	1,4-Dichlorobenzene-d4	12.08

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, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96





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Instrument :
MSVOA_X
ClientSampleId :
20180243-COMPOSITE-E

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.M
Quant Title : SW846 8260

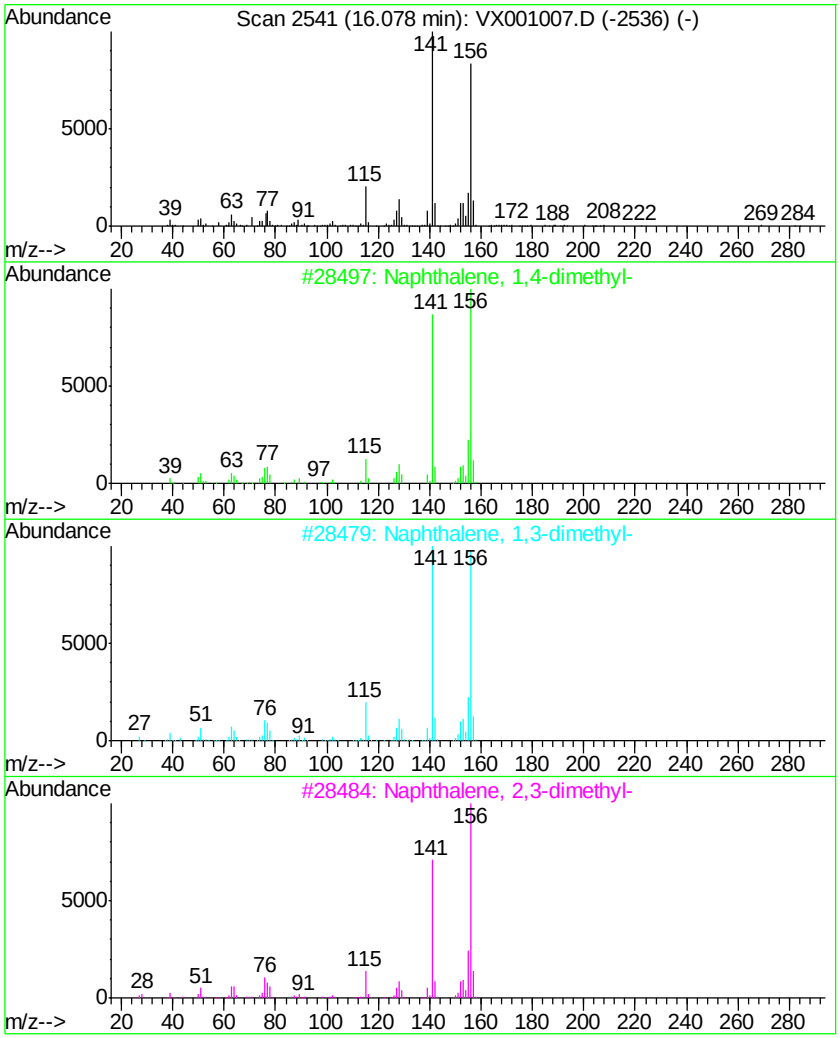
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

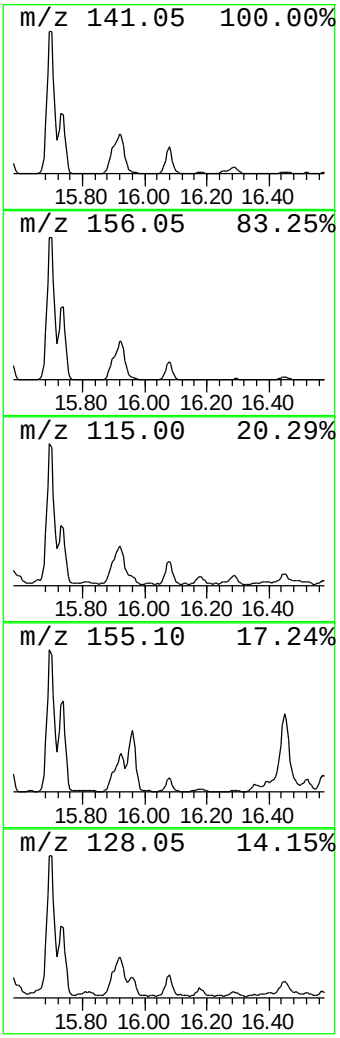
****

Peak Number 9 Naphthalene, 1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	8.41 ug/l	218219	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, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	95
5	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	94





Tentatively Identified Compound (LSC) summary

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Instrument : MSVOA_X
ClientSampleId : 20180243-COMPOSITE-E

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041918W.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
Naphthalene, 1-me...	14.85	41.9	ug/l	1086530	4	12.08	1297920	50.0
Naphthalene, 2-et...	15.45	29.6	ug/l	766999	4	12.08	1297920	50.0
Naphthalene, 2,7-...	15.55	45.8	ug/l	1189710	4	12.08	1297920	50.0
Naphthalene, 2,3-...	15.69	49.0	ug/l	1272610	4	12.08	1297920	50.0
Naphthalene, 1,4-...	16.08	8.4	ug/l	218219	4	12.08	1297920	50.0