LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

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\82X041018W.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	75	79	93	rBV	512303	569129	45.30%	4.635%
2	1.636	162	172	174	rBV4	8022	16485	1.31%	0.134%
3	5.513	797	808	822	rBV	136084	391008	31.12%	3.184%
4	5.665	822	833	852	rBV	225854	644886	51.33%	5.252%
5	6.074	888	900	918	rVB	146820	396459	31.56%	3.229%
6	6.866	1020	1030	1052	rBV	314520	767445	61.09%	6.250%
7	8.720	1327	1334	1350	rBV	744994	1235808	98.37%	10.065%
8	10.122	1558	1564	1577	rBV	653876	940941	74.90%	7.663%
9	11.146	1726	1732	1743	rBV	784516	1002293	79.78%	8.163%
10	11.445	1777	1781	1787	rBV	10615	22321	1.78%	0.182%
11	11.536	1789	1796	1801	rVB2	25435	45648	3.63%	0.372%
12	11.677	1814	1819	1826	rVB2	9824	16754	1.33%	0.136%
13	11.817	1838	1842	1851	rVB	37255	53279	4.24%	0.434%
14	12.085	1881	1886	1892	rBV	1019626	1256332	100.00%	10.232%
15	12.152	1892	1897	1902	rVB3	18425	30995	2.47%	0.252%
16	12.231	1902	1910	1917	rVB4	11249	21678	1.73%	0.177%
17	12.311	1917	1923	1924	rBV	15052	20433	1.63%	0.166%
18	12.329	1924	1926	1930	rVB2	15608	17777	1.41%	0.145%
19	12.378	1930	1934	1941	rVB3	32013	53427	4.25%	0.435%
20	12.481	1941	1951	1955	rBV	88993	104090	8.29%	0.848%
21	12.524	1955	1958	1965	rVB2	16275	24515	1.95%	0.200%
22	12.597	1965	1970	1971	rBV	14781	19052	1.52%	0.155%
23	12.676	1980	1983	1987	rVB	14774	15693	1.25%	0.128%
24	12.792	1991	2002	2005	rBV4	13967	45817	3.65%	0.373%
25	12.884	2010	2017	2020	rBV4	15751	23830	1.90%	0.194%
26	12.951	2024	2028	2031	rBV3	14379	23859	1.90%	0.194%
27	13.030	2038	2041	2047	rVB3	27322	44782	3.56%	0.365%
28	13.103	2047	2053	2056	rBV3	22002	35396	2.82%	0.288%
29	13.225	2067	2073	2078	rBV4	26326	51319	4.08%	0.418%
30	13.274	2078	2081	2084	rBV	18082	21139	1.68%	0.172%
31	13.329	2084	2090	2092	rBV2	75178	99333	7.91%	0.809%
32	13.359	2092	2095	2099	rVB2	71968	93374	7.43%	0.760%
33	13.445	2105	2109	2112	rBV2	10855	15016	1.20%	0.122%
34	13.487	2112	2116	2124	rVB4	50965	93057	7.41%	0.758%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

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\82X041018W.M
Title : SW846 8260

35	13.566	2124	2129	2132	rBV2	18183	26917	2.14%	0.219%
36	13.609	2132	2136	2139	rBV	15002	20645	1.64%	0.168%
37	13.652	2139	2143	2147	rBV3	21631	36400	2.90%	0.296%
38	13.737	2153	2157	2161	rBV3	18516	31641	2.52%	0.258%
39	13.841	2169	2174	2180	rVB	282859	351166	27.95%	2.860%
40	13.920	2180	2187	2192	rVB5	42393	91175	7.26%	0.743%
41	13.993	2192	2199	2204	rBV4	40648	83997	6.69%	0.684%
42	14.097	2213	2216	2220	rVB3	56669	63318	5.04%	0.516%
43	14.140	2220	2223	2226	rBV2	34525	41662	3.32%	0.339%
44	14.292	2242	2248	2254	rBV3	93118	165620	13.18%	1.349%
45	14.390	2260	2264	2269	rBV4	20558	30620	2.44%	0.249%
46	14.438	2269	2272	2277	rVV2	34676	45010	3.58%	0.367%
47	14.481	2277	2279	2285	rVB6	10758	19810	1.58%	0.161%
48	14.548	2285	2290	2298	rVB4	57299	104681	8.33%	0.853%
49	14.621	2298	2302	2307	rBV6	12923	29415	2.34%	0.240%
50	14.707	2308	2316	2320	rVV	451037	677183	53.90%	5.515%
51	14.737	2320	2321	2326	rVB3	42475	41925	3.34%	0.341%
52	14.792	2326	2330	2332	rBV3	23631	33018	2.63%	0.269%
53	14.847	2335	2339	2344	rVV	382224	483711	38.50%	3.939%
54	14.914	2348	2350	2356	rVV4	26633	34089	2.71%	0.278%
55	14.969	2356	2359	2370	rVB5	17968	38622	3.07%	0.315%
56	15.121	2379	2384	2388	rVB5	12729	20686	1.65%	0.168%
57	15.261	2402	2407	2408	rBV	44895	62947	5.01%	0.513%
58	15.280	2408	2410	2414	rVB	57946	68289	5.44%	0.556%
59	15.456	2434	2439	2442	rBV	68507	99570	7.93%	0.811%
60	15.487	2442	2444	2449	rVB2	18911	23360	1.86%	0.190%
61	15.560	2450	2456	2468	rVB	181154	311808	24.82%	2.539%
62	15.700	2473	2479	2482	rVV	210454	332001	26.43%	2.704%
63	15.737	2482	2485	2493	rVB	114061	175630	13.98%	1.430%
64	15.926	2507	2516	2531	rVB2	50392	167131	13.30%	1.361%
65	16.078	2537	2541	2553	rVB	29916	67313	5.36%	0.548%
66	16.182	2553	2558	2564	rBV	24878	42143	3.35%	0.343%
67	16.292	2572	2576	2583	rVB3	11403	22628	1.80%	0.184%
68	16.432	2593	2599	2609	rVB2	67262	151169	12.03%	1.231%
69	16.651	2629	2635	2637	rBV6	7647	16988	1.35%	0.138%
70	16.700	2640	2643	2649	rVB4	15692	26086	2.08%	0.212%
71	16.767	2649	2654	2656	rBV2	16028	26876	2.14%	0.219%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

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\82X041018W.M
Title : SW846 8260

Sum of corrected areas: 12278620

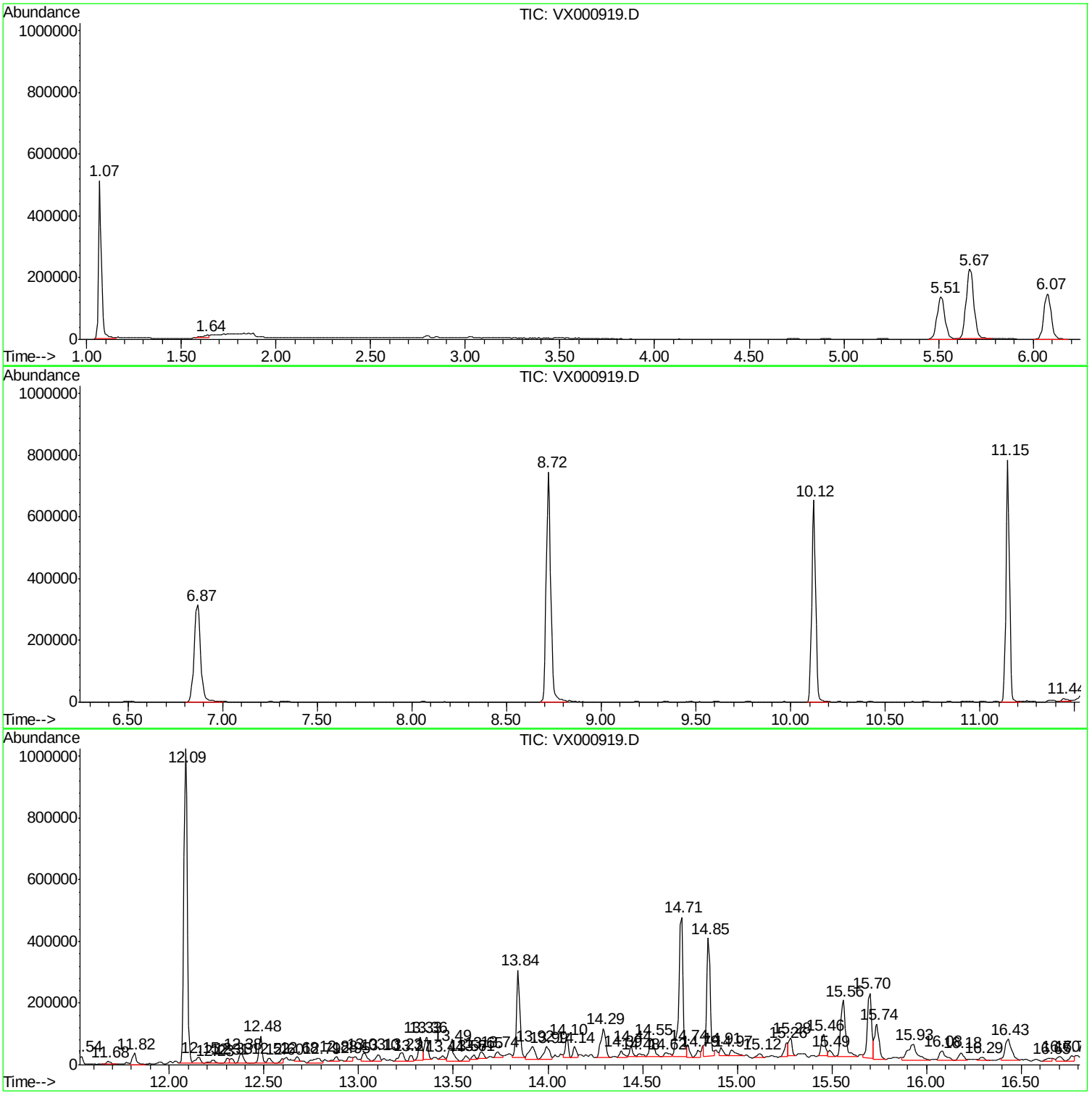
LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041018W.M
Quant Title : SW846 8260

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



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041018W.M
Quant Title : SW846 8260

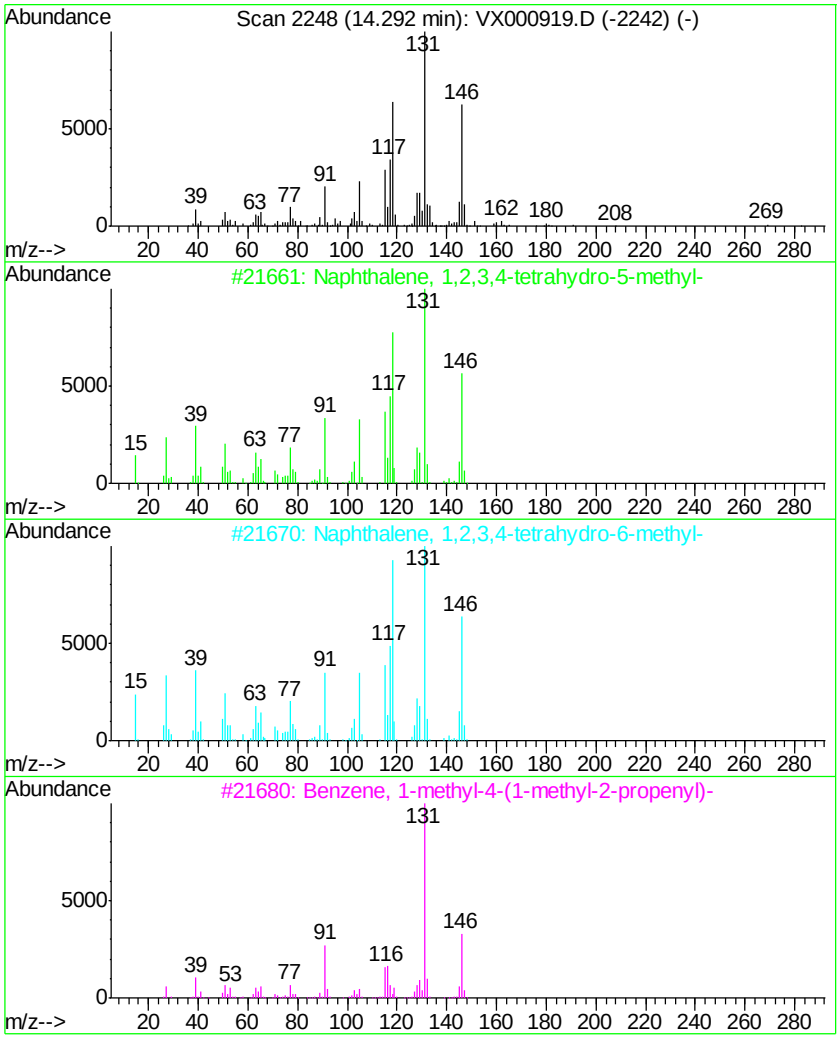
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

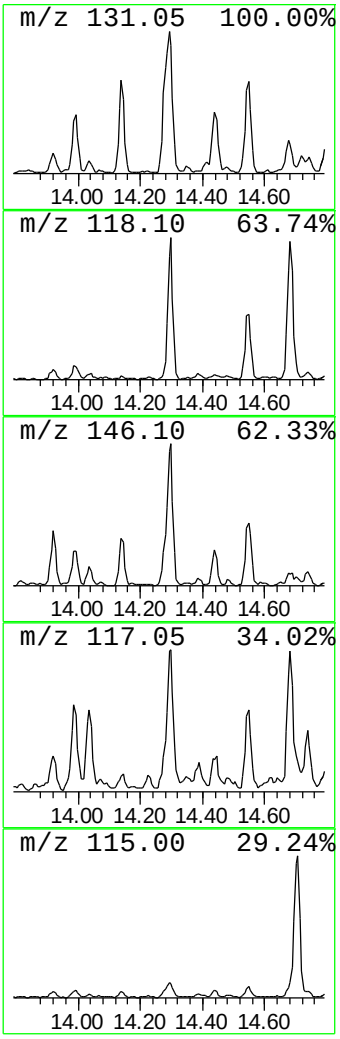
****

Peak Number 2 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	6.59 ug/l	165620	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	97
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
3	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	70
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	70





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041018W.M
Quant Title : SW846 8260

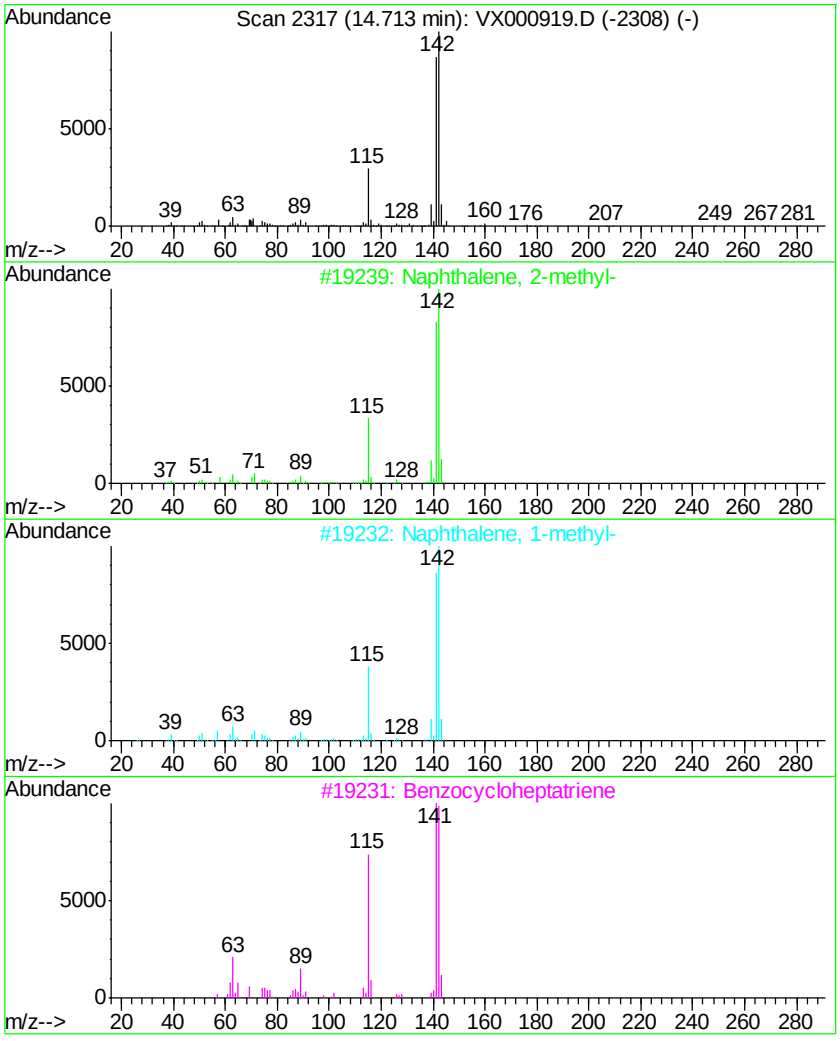
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

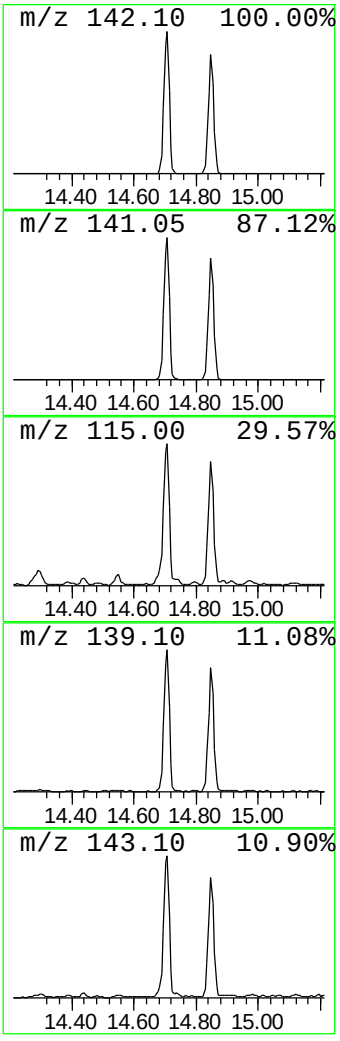
****

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	26.95 ug/l	677183	1,4-Dichlorobenzene-d4	12.09

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





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041018W.M
Quant Title : SW846 8260

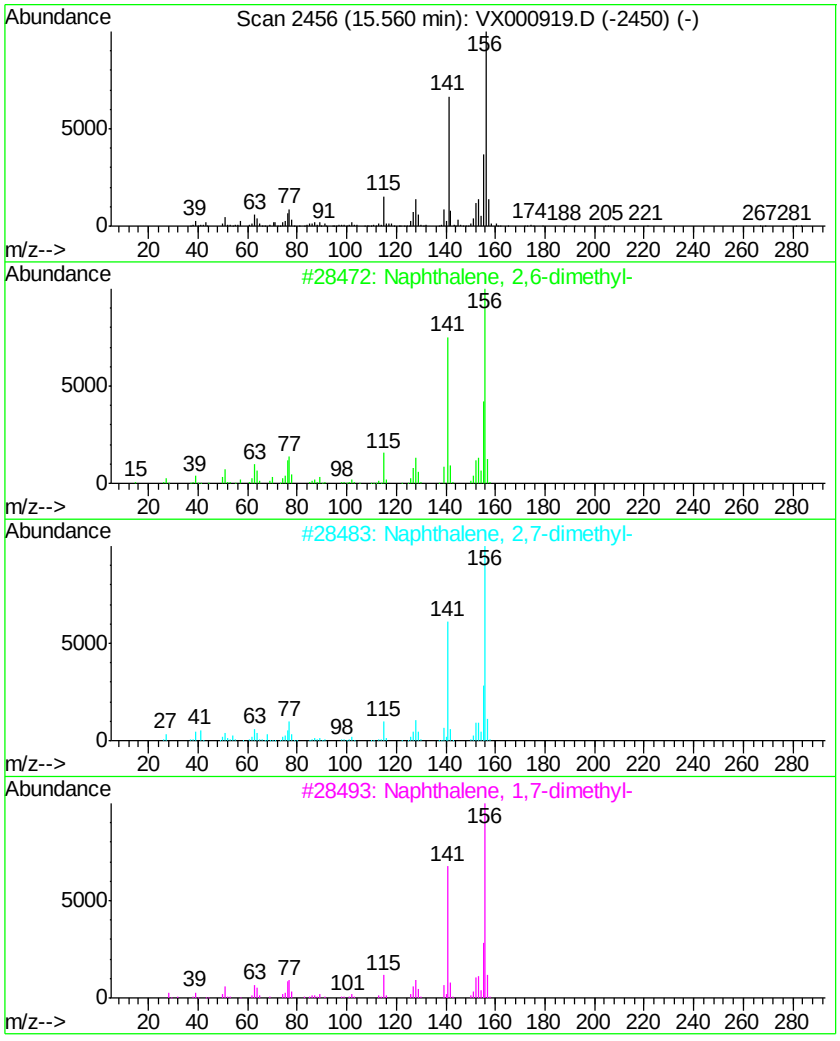
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

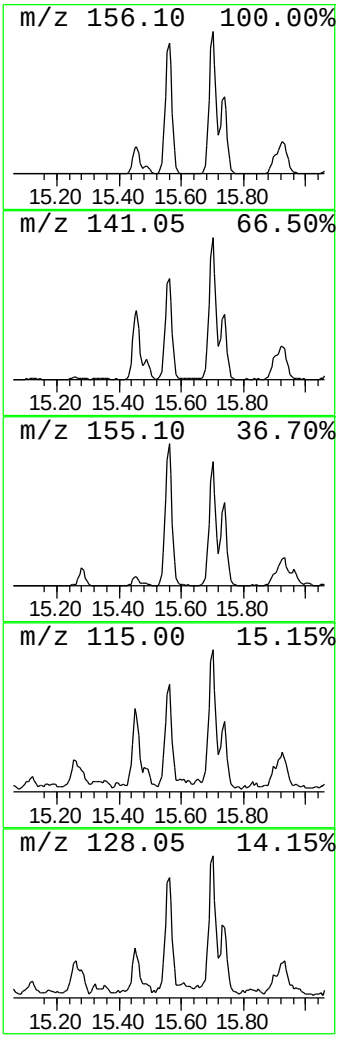
****

Peak Number 5 Naphthalene, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	12.41 ug/l	311808	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041018W.M
Quant Title : SW846 8260

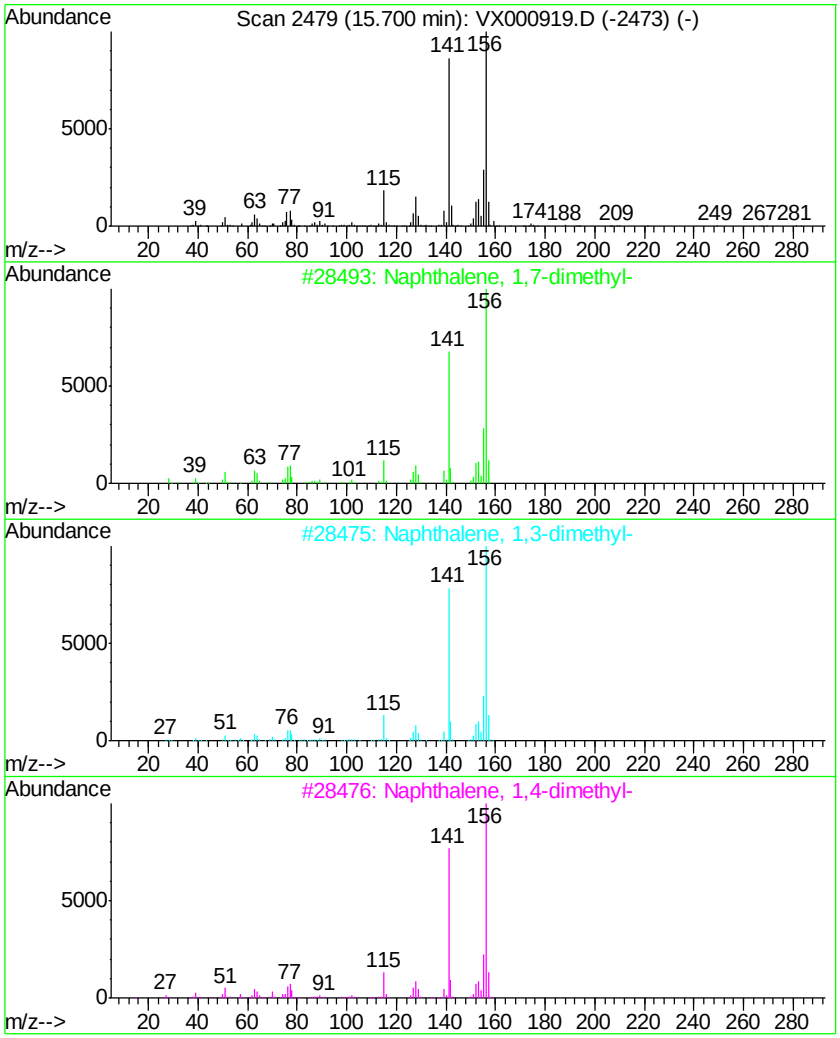
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

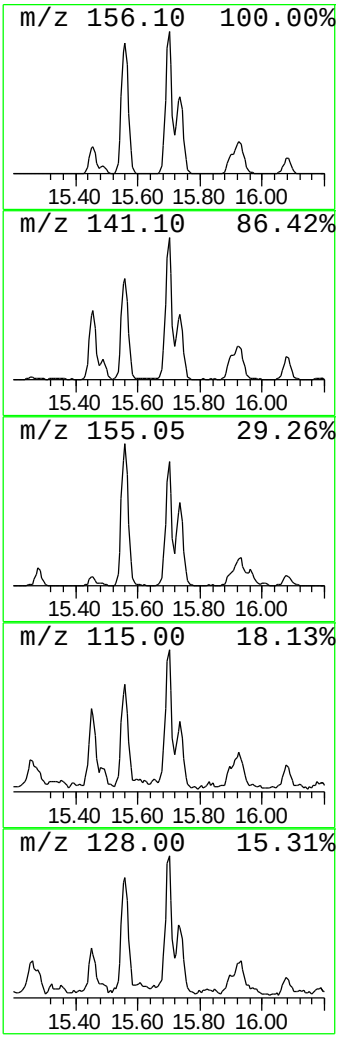
****

Peak Number 6 Naphthalene, 1,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	13.21 ug/l	332001	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
2	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041018W.M
Quant Title : SW846 8260

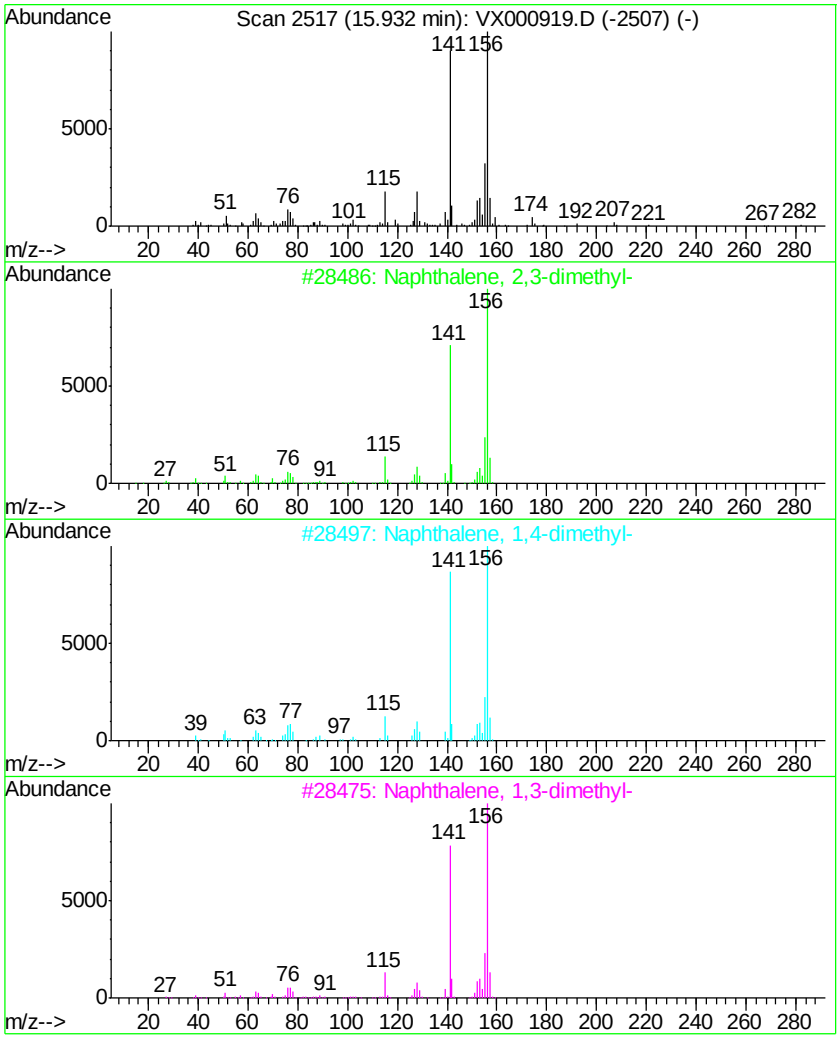
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

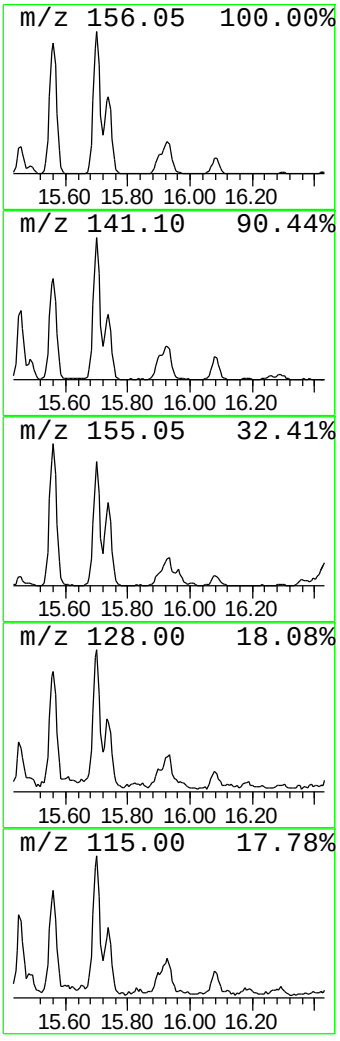
****

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	6.65 ug/l	167131	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93





Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX041618\
Data File : VX000919.D
Acq On : 16 Apr 2018 15:24
Operator : JC/MD
Sample : J2163-01
Misc : 5.73g/5.0mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PL-01-041118-A

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X041018W.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, 1,2,...	14.29	6.6	ug/l	165620	4	12.09	1256330	50.0
Naphthalene, 1-me...	14.71	26.9	ug/l	677183	4	12.09	1256330	50.0
Naphthalene, 2,6-...	15.56	12.4	ug/l	311808	4	12.09	1256330	50.0
Naphthalene, 1,7-...	15.70	13.2	ug/l	332001	4	12.09	1256330	50.0
Naphthalene, 2,3-...	15.93	6.7	ug/l	167131	4	12.09	1256330	50.0