LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033018\
Data File : VX000579.D
Acq On : 30 Mar 2018 23:29
Operator : JC/MD
Sample : J2048-03
Misc : 11.75g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SB-106(2-3)

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\82X032018W.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	76	79	92	rBV	302124	380817	46.66%	5.617%
2	1.636	156	172	176	rBV3	29266	103304	12.66%	1.524%
3	2.818	358	366	369	rBV2	13004	32502	3.98%	0.479%
4	3.026	395	400	409	rBV4	4080	9061	1.11%	0.134%
5	5.513	798	808	822	rBV2	79611	230921	28.30%	3.406%
6	5.665	822	833	847	rBV2	130707	366258	44.88%	5.402%
7	6.074	890	900	915	rBV	89721	243445	29.83%	3.591%
8	6.866	1019	1030	1051	rBV	208874	511165	62.64%	7.539%
9	8.720	1327	1334	1343	rBV	442956	731208	89.60%	10.785%
10	10.122	1557	1564	1575	rBV	470669	694124	85.05%	10.238%
11	11.146	1726	1732	1740	rBV	435098	578388	70.87%	8.531%
12	11.677	1815	1819	1826	rBV2	6904	9231	1.13%	0.136%
13	11.817	1838	1842	1848	rVB	13160	17498	2.14%	0.258%
14	12.091	1881	1887	1893	rVV	614329	816096	100.00%	12.037%
15	12.152	1893	1897	1902	rVB2	10813	14888	1.82%	0.220%
16	12.311	1917	1923	1929	rBV4	17236	27659	3.39%	0.408%
17	12.378	1930	1934	1940	rVB2	13375	22246	2.73%	0.328%
18	12.481	1947	1951	1955	rBV5	7569	9576	1.17%	0.141%
19	12.530	1955	1959	1964	rVB5	5815	8506	1.04%	0.125%
20	12.615	1971	1973	1978	rVB3	8439	8624	1.06%	0.127%
21	12.676	1979	1983	1989	rVB2	23431	28388	3.48%	0.419%
22	12.768	1993	1998	2002	rVV6	6085	13526	1.66%	0.199%
23	12.811	2003	2005	2010	rVB3	9322	11941	1.46%	0.176%
24	12.981	2025	2033	2037	rBV3	12186	21645	2.65%	0.319%
25	13.030	2037	2041	2048	rVV	25253	44479	5.45%	0.656%
26	13.109	2049	2054	2056	rVV5	7552	13637	1.67%	0.201%
27	13.158	2060	2062	2066	rVB3	7712	8479	1.04%	0.125%
28	13.231	2071	2074	2078	rVB	9359	13392	1.64%	0.198%
29	13.353	2090	2094	2099	rVB2	35531	50901	6.24%	0.751%
30	13.408	2099	2103	2106	rBV2	16472	19426	2.38%	0.287%
31	13.487	2109	2116	2122	rBV	44721	78316	9.60%	1.155%
32	13.615	2132	2137	2139	rBV5	6721	11591	1.42%	0.171%
33	13.743	2154	2158	2160	rBV2	10165	13826	1.69%	0.204%
34	13.768	2160	2162	2165	rVV4	8487	10327	1.27%	0.152%

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Instrument : MSVOA_X
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Integration Parameters: RTEINT.P
Integrator: RTE
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Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Title : SW846 8260

35	13.816	2167	2170	2171	rVV3	8618	9309	1.14%	0.137%
36	13.841	2171	2174	2182	rVB	41026	73364	8.99%	1.082%
37	13.920	2182	2187	2192	rBV9	8895	21252	2.60%	0.313%
38	13.993	2196	2199	2204	rVB3	10983	16786	2.06%	0.248%
39	14.042	2204	2207	2210	rBV5	4981	8546	1.05%	0.126%
40	14.140	2219	2223	2225	rBV5	11933	17577	2.15%	0.259%
41	14.170	2225	2228	2230	rVV4	10715	14463	1.77%	0.213%
42	14.201	2230	2233	2237	rVV5	12662	22351	2.74%	0.330%
43	14.243	2237	2240	2243	rVV5	12721	17250	2.11%	0.254%
44	14.286	2243	2247	2251	rVV4	34338	56066	6.87%	0.827%
45	14.329	2251	2254	2258	rVV5	13499	18306	2.24%	0.270%
46	14.383	2258	2263	2269	rVV3	42218	69998	8.58%	1.032%
47	14.438	2269	2272	2275	rVV4	16146	21384	2.62%	0.315%
48	14.487	2275	2280	2286	rVB8	11208	21030	2.58%	0.310%
49	14.548	2286	2290	2294	rBV5	11637	19512	2.39%	0.288%
50	14.591	2294	2297	2300	rVV2	11606	14384	1.76%	0.212%
51	14.670	2304	2310	2312	rVV	18418	35800	4.39%	0.528%
52	14.700	2313	2315	2319	rVV	26816	33322	4.08%	0.491%
53	14.737	2319	2321	2325	rVB4	7414	8263	1.01%	0.122%
54	14.847	2332	2339	2348	rBV	200275	284826	34.90%	4.201%
55	15.054	2371	2373	2377	rVB5	9387	9780	1.20%	0.144%
56	15.261	2403	2407	2408	rBV4	9684	12539	1.54%	0.185%
57	15.432	2429	2435	2436	rBV5	10919	18910	2.32%	0.279%
58	15.456	2436	2439	2442	rVB	21013	25364	3.11%	0.374%
59	15.493	2442	2445	2450	rVB4	21080	30266	3.71%	0.446%
60	15.560	2450	2456	2460	rBV	57946	100494	12.31%	1.482%
61	15.658	2469	2472	2474	rBV4	9812	12284	1.51%	0.181%
62	15.700	2474	2479	2482	rVV	113565	176492	21.63%	2.603%
63	15.737	2482	2485	2491	rVB3	47243	75281	9.22%	1.110%
64	15.834	2496	2501	2506	rVB8	14138	28593	3.50%	0.422%
65	15.901	2507	2512	2514	rBV2	31601	52623	6.45%	0.776%
66	16.078	2537	2541	2547	rBV2	24765	45805	5.61%	0.676%
67	16.188	2553	2559	2565	rBV2	29599	54961	6.73%	0.811%
68	16.395	2585	2593	2594	rBV7	11365	22965	2.81%	0.339%
69	16.426	2595	2598	2604	rVV3	20042	41563	5.09%	0.613%
70	16.493	2606	2609	2613	rVB5	7658	11421	1.40%	0.168%
71	16.578	2619	2623	2629	rVB7	8185	15474	1.90%	0.228%

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Instrument : MSVOA_X
ClientSampleId : SB-106(2-3)

Integration Parameters: RTEINT.P
Integrator: RTE
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Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Title : SW846 8260

72	16.663	2630	2637	2639	rBV8	11088	23928	2.93%	0.353%
73	16.706	2639	2644	2649	rVB3	27024	50380	6.17%	0.743%
74	16.767	2649	2654	2657	rBV2	18830	31841	3.90%	0.470%

Sum of corrected areas: 6780144

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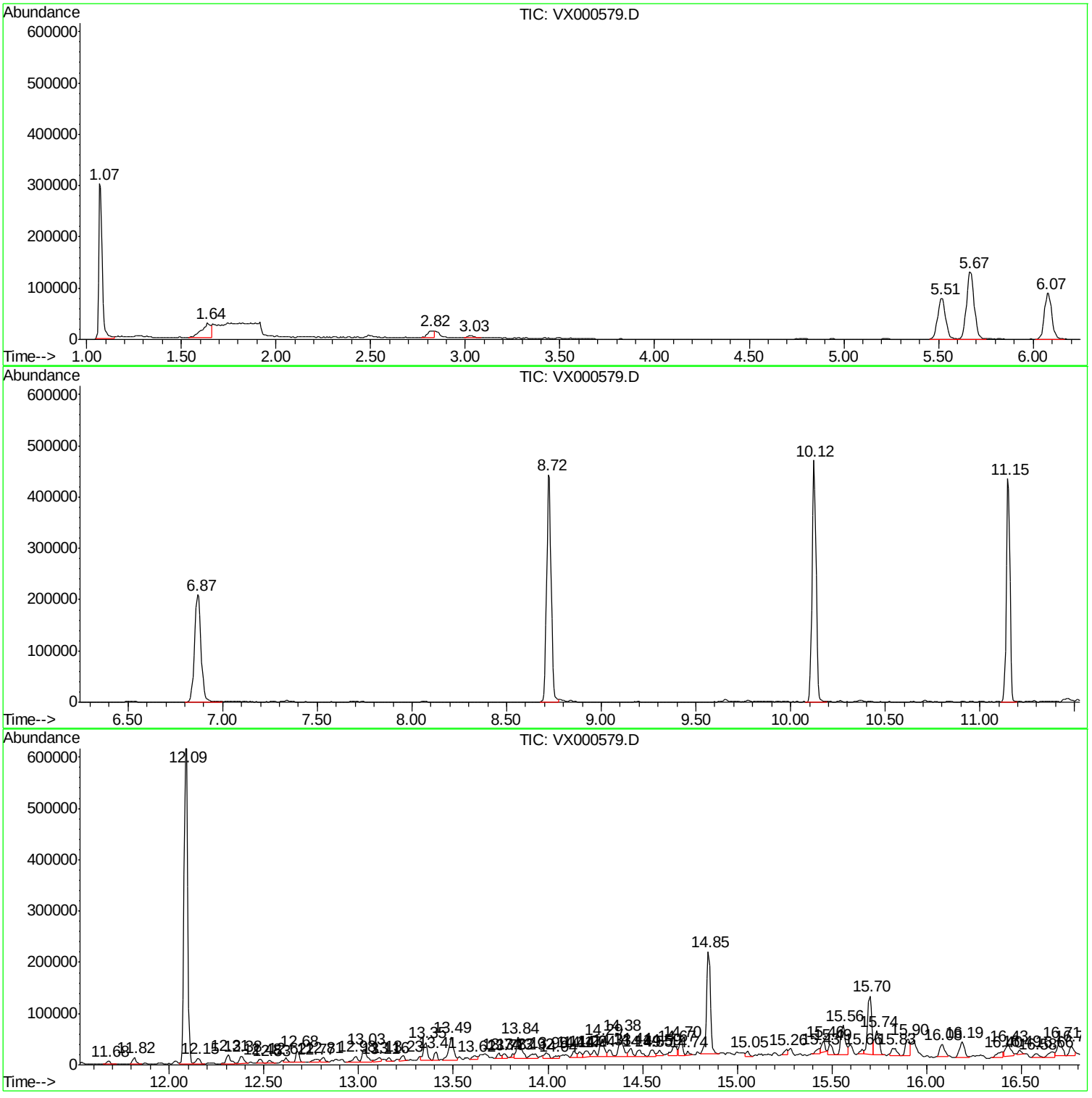
MSVOA_X
ClientSampleId :
SB-106(2-3)

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033018\
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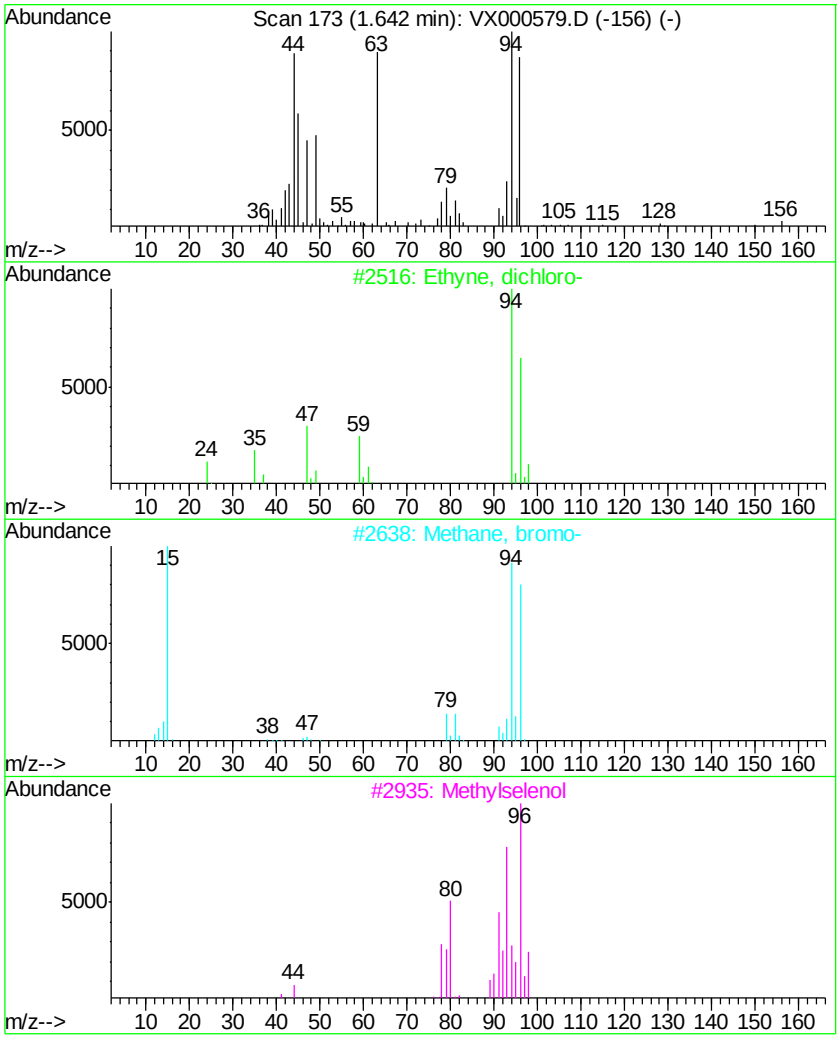
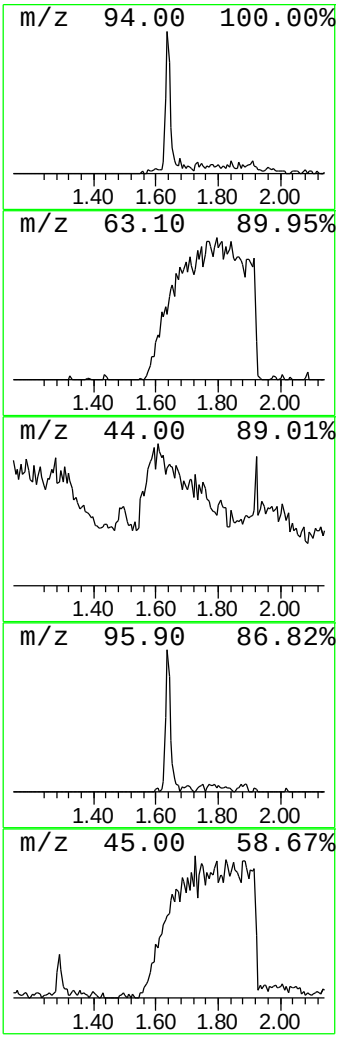
****

Peak Number 2 unknown1.64 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.64	14.10 ug/l	103304	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyne, dichloro-	94	C2Cl2	007572-29-4	14
2	Methane, bromo-	94	CH3Br	000074-83-9	11
3	Methylselenol	96	CH4Se	006486-05-1	9
4	Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	9
5	Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	9





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TIC Integration Parameters: LSCINT.P

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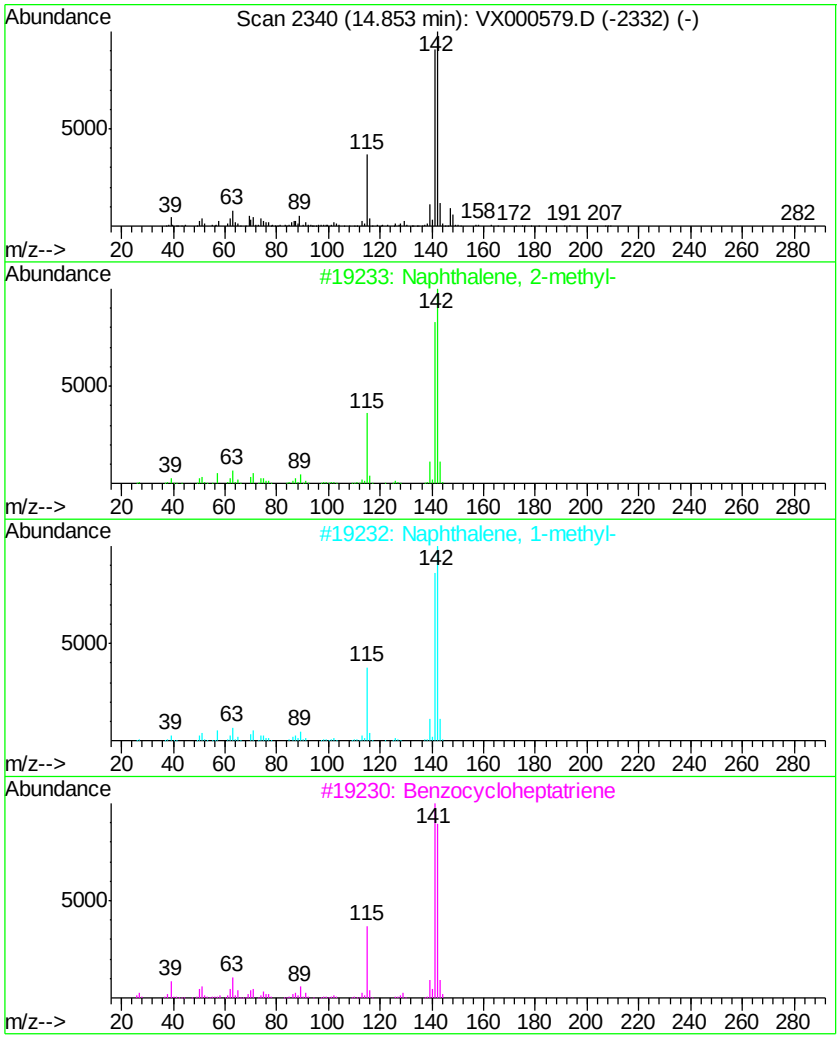
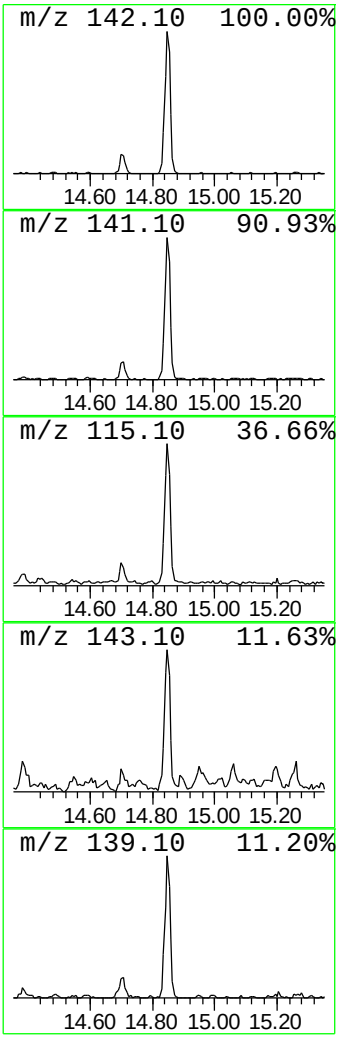
Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	17.45 ug/l	284826	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	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90





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Instrument : MSVOA_X
ClientSampleId : SB-106(2-3)

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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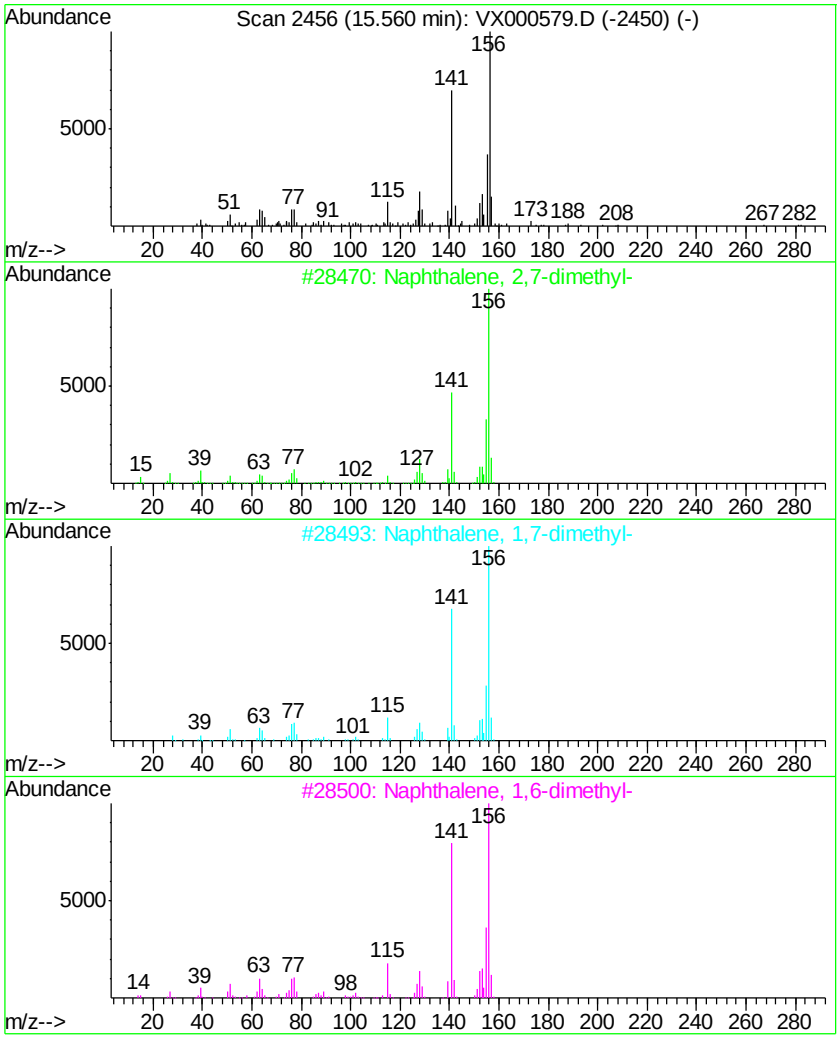
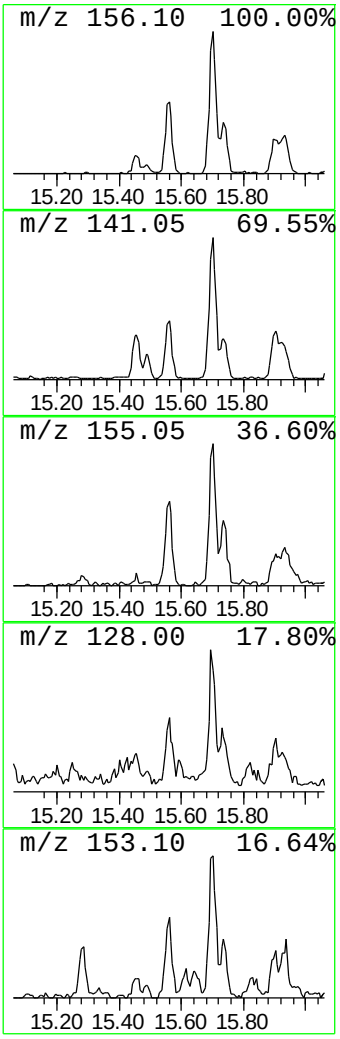
Peak Number 4 Naphthalene, 2,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	6.16 ug/l	100494	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	94





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Quant Title : SW846 8260

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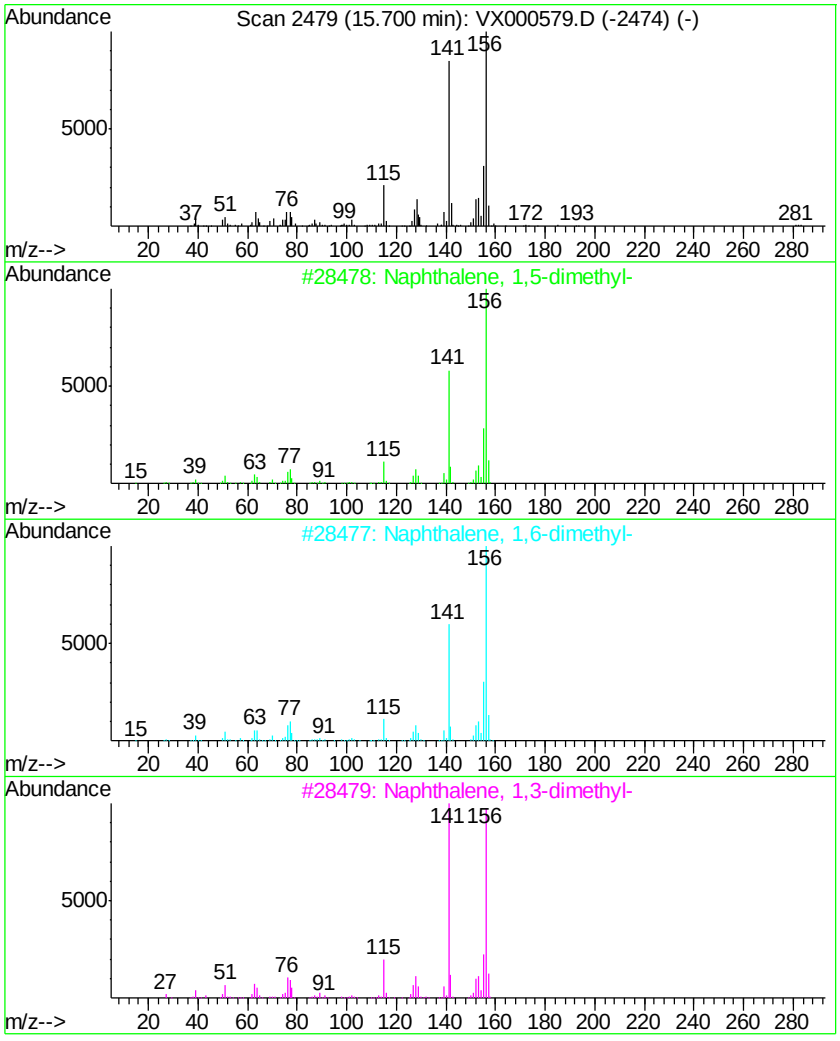
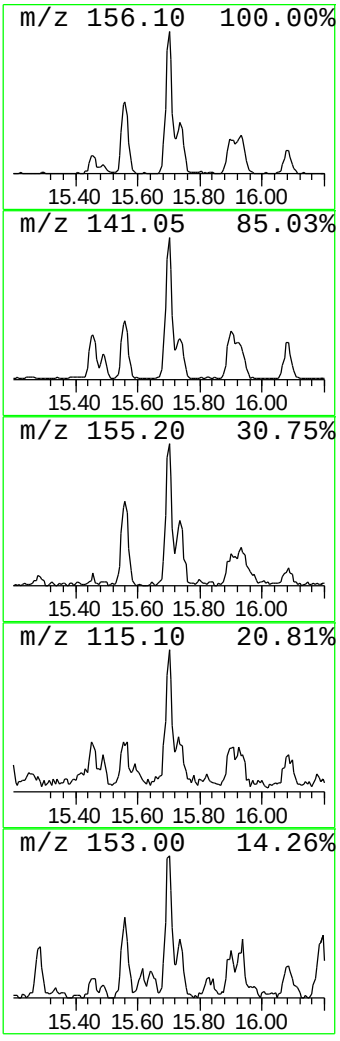
Peak Number 5 Naphthalene, 1,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	10.81 ug/l	176492	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95





Tentatively Identified Compound (LSC) summary

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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
unknown1.64	1.64	14.1	ug/l	103304	1	5.67	366258	50.0
Naphthalene, 1-me...	14.85	17.4	ug/l	284826	4	12.09	816096	50.0
Naphthalene, 2,7-...	15.56	6.2	ug/l	100494	4	12.09	816096	50.0
Naphthalene, 1,5-...	15.70	10.8	ug/l	176492	4	12.09	816096	50.0