LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006089.D
Acq On : 19 Nov 2018 14:21
Operator : JC/MD
Sample : J5767-11
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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	1.666	65	84	86	rBV2	13127	48106	1.95%	0.276%
2	5.507	702	714	728	rBV2	71662	204923	8.31%	1.176%
3	5.659	728	739	757	rVB	132705	367243	14.89%	2.107%
4	6.061	793	805	823	rBV2	76347	207200	8.40%	1.189%
5	6.854	925	935	953	rBV2	188190	449488	18.22%	2.579%
6	8.713	1233	1240	1248	rBV	329328	525141	21.29%	3.013%
7	10.116	1464	1470	1488	rBV	327746	460954	18.69%	2.645%
8	11.140	1632	1638	1652	rBV	293044	385223	15.62%	2.210%
9	11.810	1743	1748	1753	rBV	41756	53643	2.17%	0.308%
10	12.079	1787	1792	1799	rBV	402791	510608	20.70%	2.930%
11	12.146	1799	1803	1807	rVB	20763	25178	1.02%	0.144%
12	12.298	1823	1828	1836	rBV	120564	163949	6.65%	0.941%
13	12.371	1836	1840	1846	rVB3	18615	27857	1.13%	0.160%
14	13.017	1943	1946	1952	rVB	30150	39860	1.62%	0.229%
15	13.225	1976	1980	1984	rVB	38850	45212	1.83%	0.259%
16	13.353	1990	2001	2005	rBV2	86568	137567	5.58%	0.789%
17	13.402	2005	2009	2013	rVV	72427	91182	3.70%	0.523%
18	13.481	2017	2022	2030	rVB	106833	148626	6.02%	0.853%
19	13.834	2074	2080	2087	rBV	1036082	1247220	50.56%	7.156%
20	13.926	2087	2095	2100	rVB2	22375	42540	1.72%	0.244%
21	14.133	2125	2129	2132	rBV	21174	28108	1.14%	0.161%
22	14.279	2149	2153	2156	rBV2	35487	57434	2.33%	0.330%
23	14.377	2163	2169	2175	rBV	44467	76882	3.12%	0.441%
24	14.657	2211	2215	2217	rBV	33463	46162	1.87%	0.265%
25	14.700	2217	2222	2231	rVB	1901271	2466937	100.00%	14.155%
26	14.785	2232	2236	2239	rBV	24368	32629	1.32%	0.187%
27	14.840	2240	2245	2254	rVB	1795580	2185310	88.58%	12.539%
28	15.273	2308	2316	2321	rBV	150822	211836	8.59%	1.215%
29	15.322	2321	2324	2331	rVB2	24211	36846	1.49%	0.211%
30	15.444	2335	2344	2347	rBV2	199721	333616	13.52%	1.914%
31	15.480	2347	2350	2355	rVB	75480	105389	4.27%	0.605%
32	15.547	2355	2361	2367	rBV	892475	1475922	59.83%	8.469%
33	15.688	2373	2384	2388	rBV	1056289	1790997	72.60%	10.276%
34	15.724	2388	2390	2399	rVV	655471	939658	38.09%	5.392%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
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Operator : JC/MD
Sample : J5767-11
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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

35	15.810	2399	2404	2411	rVV2	24203	48546	1.97%	0.279%
36	15.919	2411	2422	2432	rVB	278558	803340	32.56%	4.609%
37	16.072	2440	2447	2457	rVB	218400	392904	15.93%	2.254%
38	16.169	2457	2463	2470	rBV	118312	195345	7.92%	1.121%
39	16.279	2471	2481	2487	rVB3	57367	122248	4.96%	0.701%
40	16.438	2494	2507	2512	rBV2	103920	295047	11.96%	1.693%
41	16.566	2524	2528	2534	rVB2	37806	65276	2.65%	0.375%
42	16.657	2534	2543	2544	rBV3	52947	99621	4.04%	0.572%
43	16.694	2544	2549	2554	rVB	122599	223420	9.06%	1.282%
44	16.755	2554	2559	2564	rBV	120050	213066	8.64%	1.223%

Sum of corrected areas: 17428259

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Operator : JC/MD
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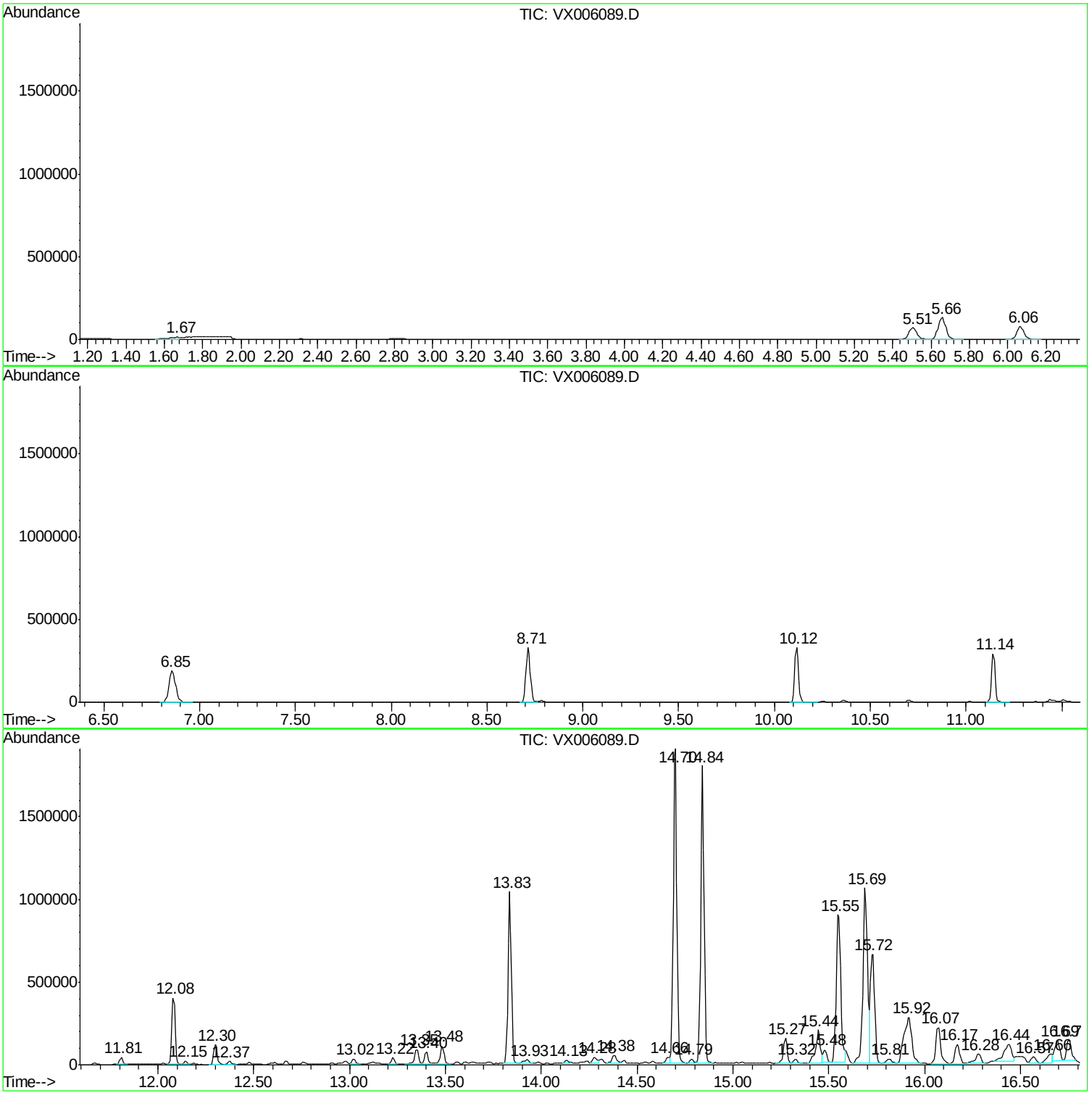
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-01-111418-B

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006089.D
Acq On : 19 Nov 2018 14:21
Operator : JC/MD
Sample : J5767-11
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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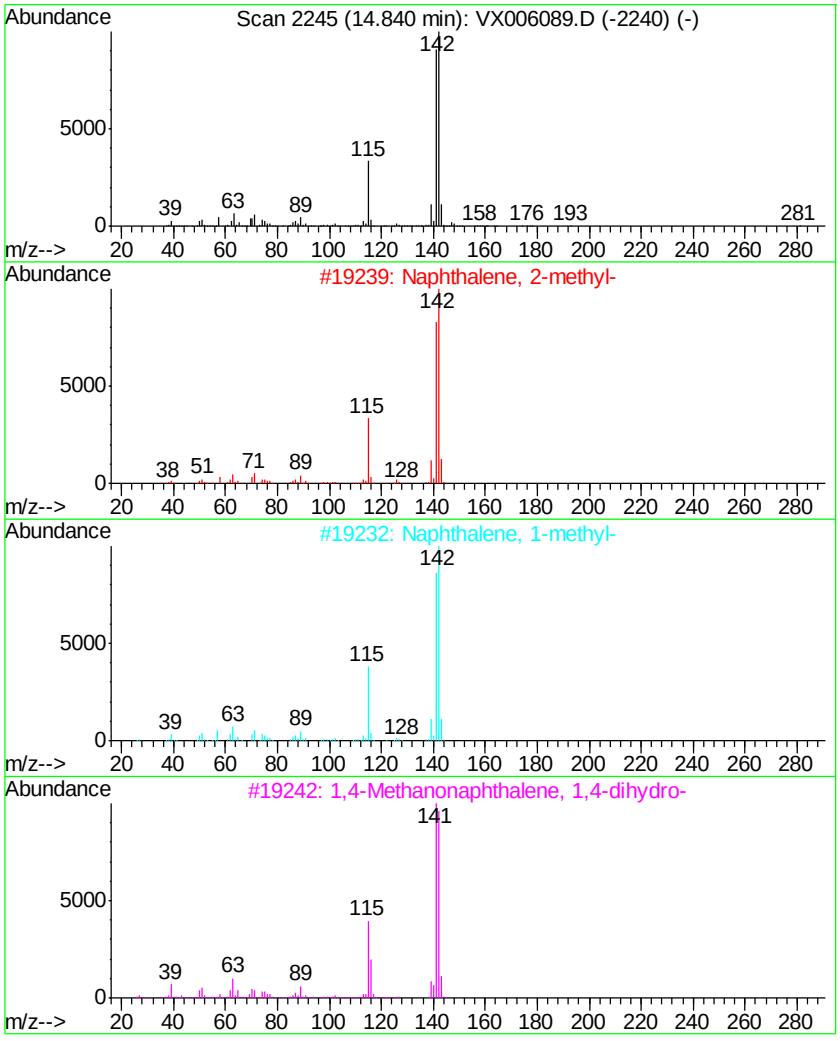
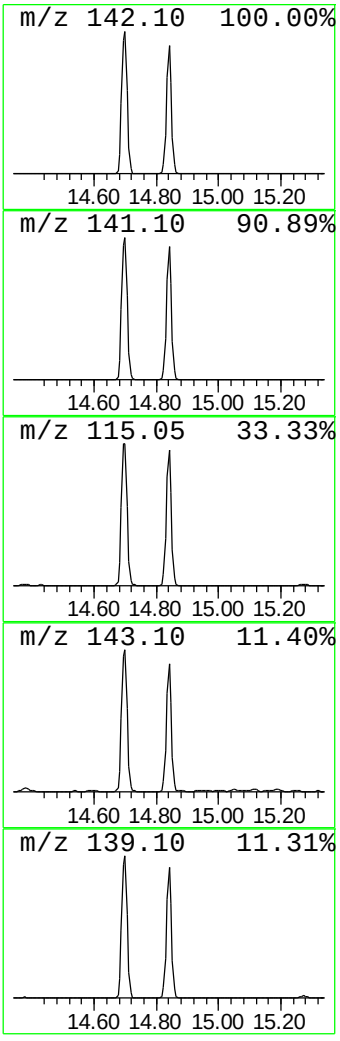
Peak Number 2 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	213.99 ug/l	2185310	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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006089.D
Acq On : 19 Nov 2018 14:21
Operator : JC/MD
Sample : J5767-11
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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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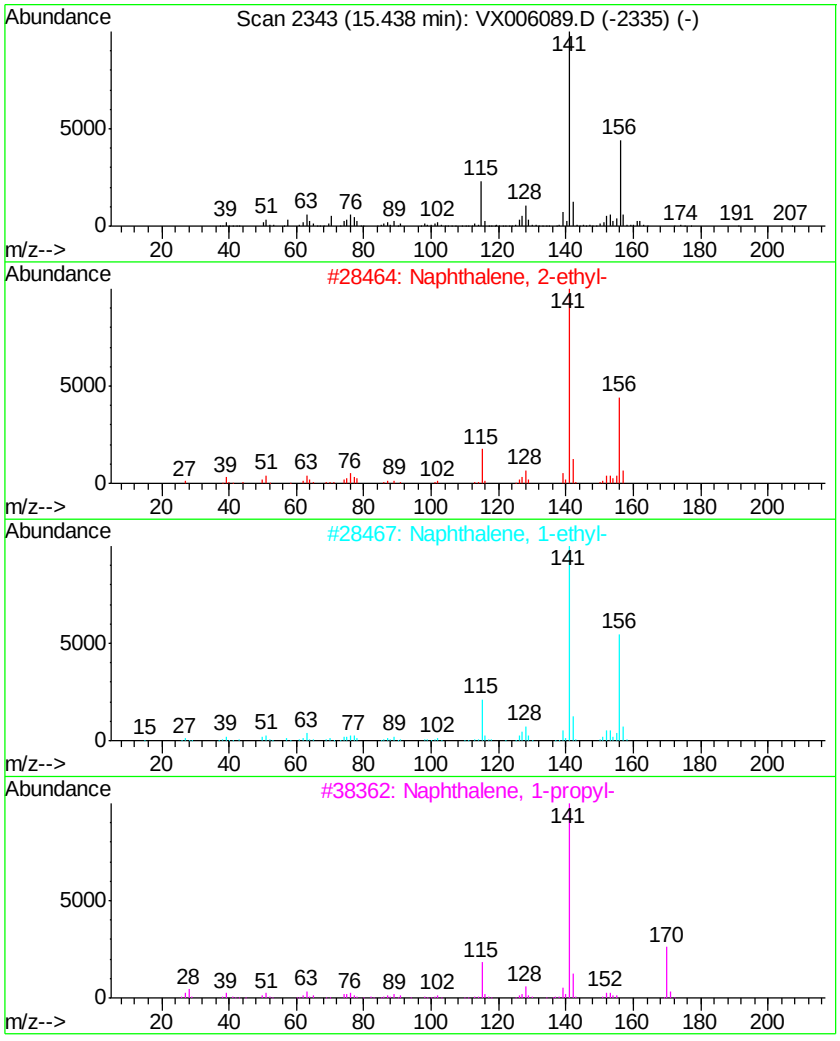
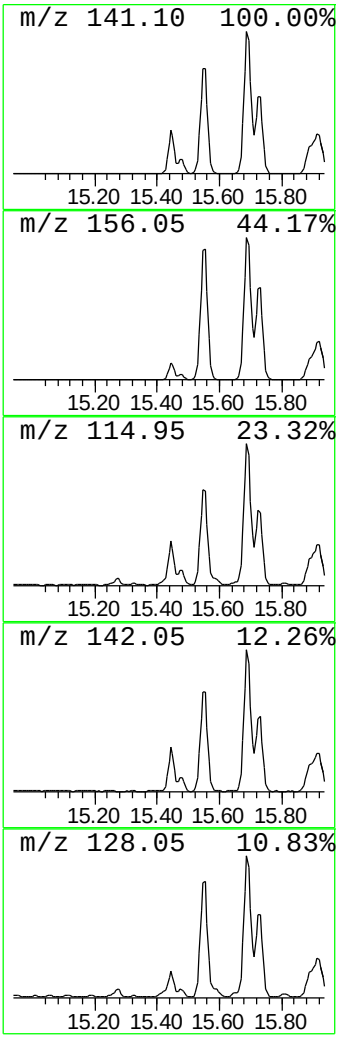
Peak Number 3 Naphthalene, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	32.67 ug/l	333616	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
2	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
3	Naphthalene, 1-propyl-	170	C13H14	002765-18-6	59
4	2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	59
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
Data File : VX006089.D
Acq On : 19 Nov 2018 14:21
Operator : JC/MD
Sample : J5767-11
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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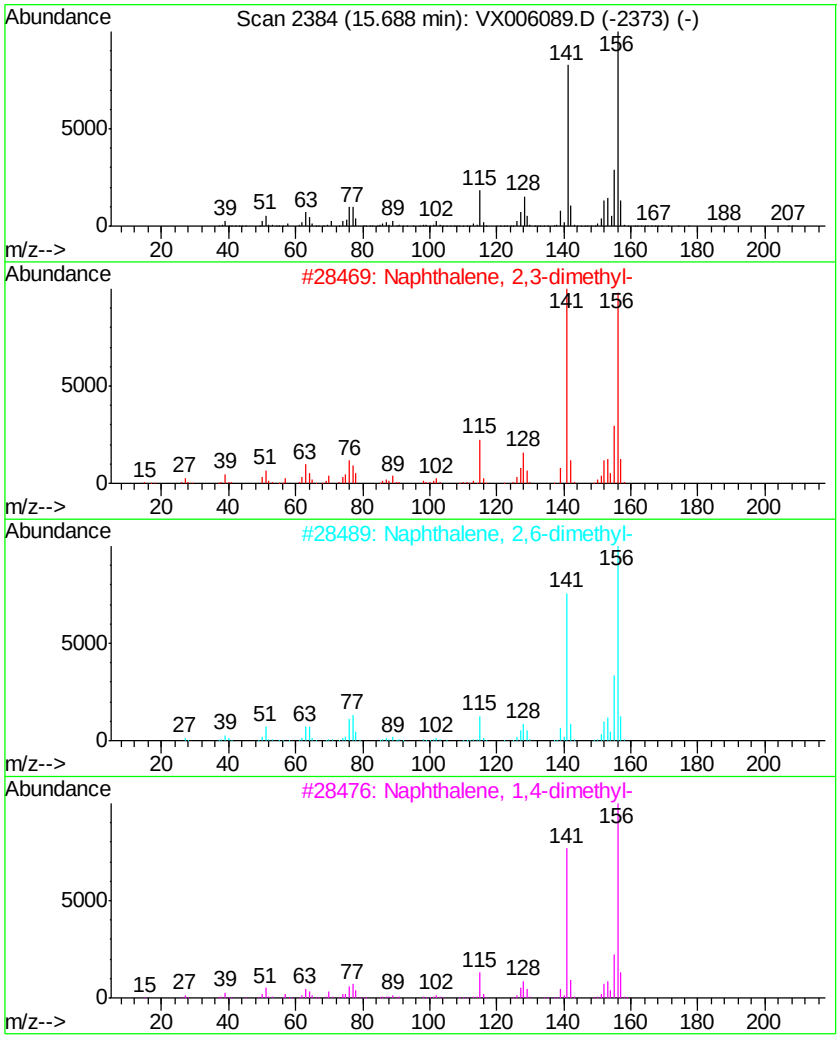
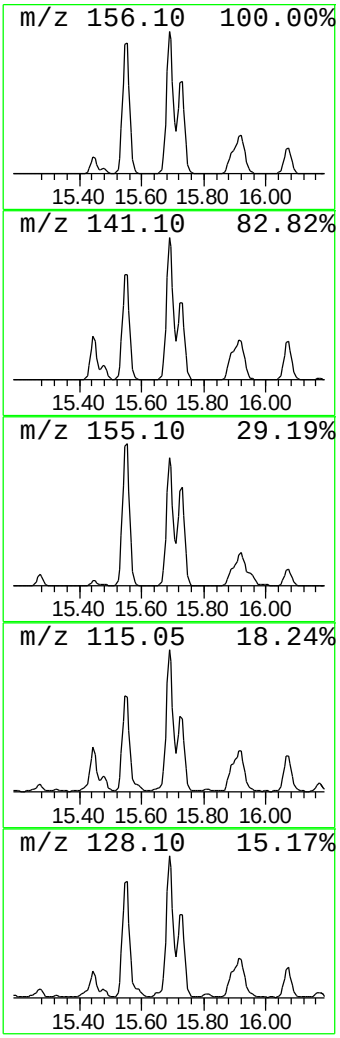
Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	175.38 ug/l	1791000	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, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97





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Data File : VX006089.D
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Operator : JC/MD
Sample : J5767-11
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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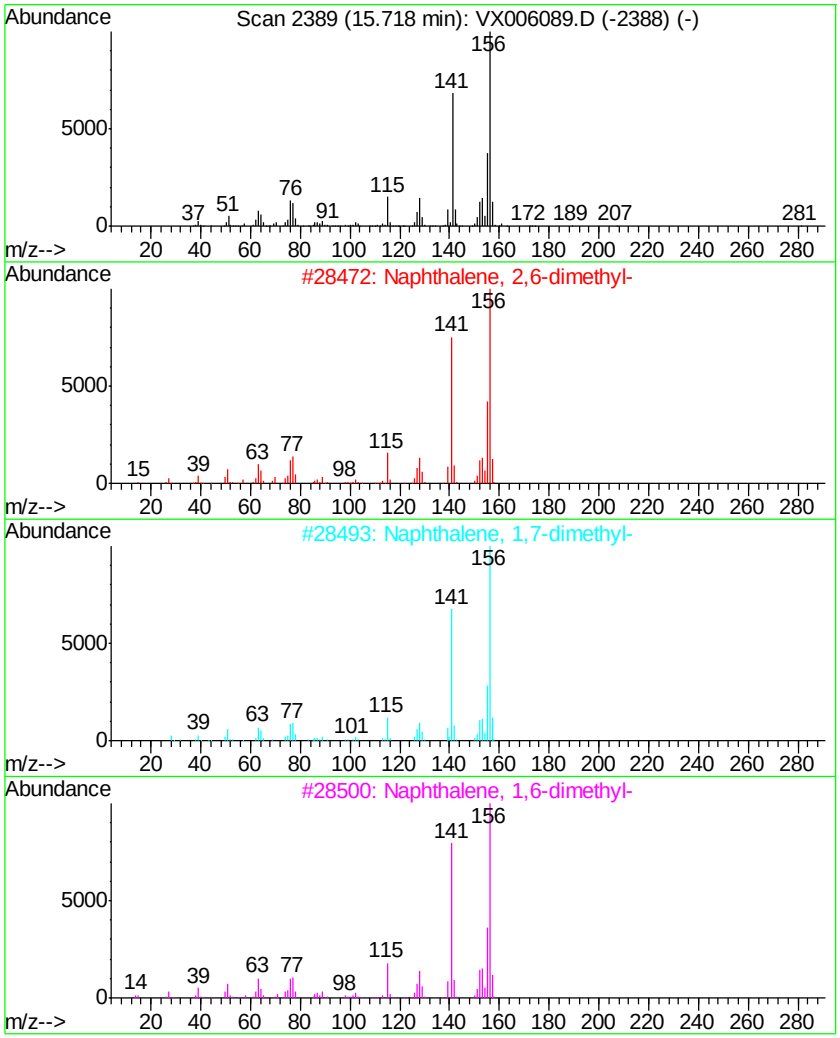
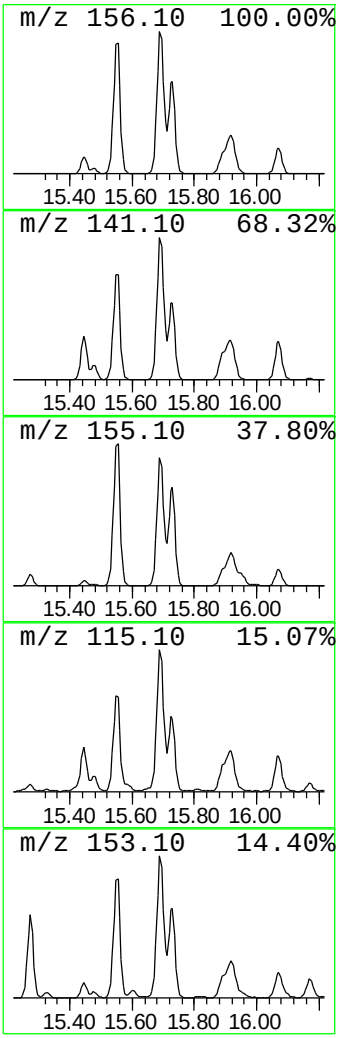
Peak Number 6 Naphthalene, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	92.01 ug/l	939658	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, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96





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Operator : JC/MD
Sample : J5767-11
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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

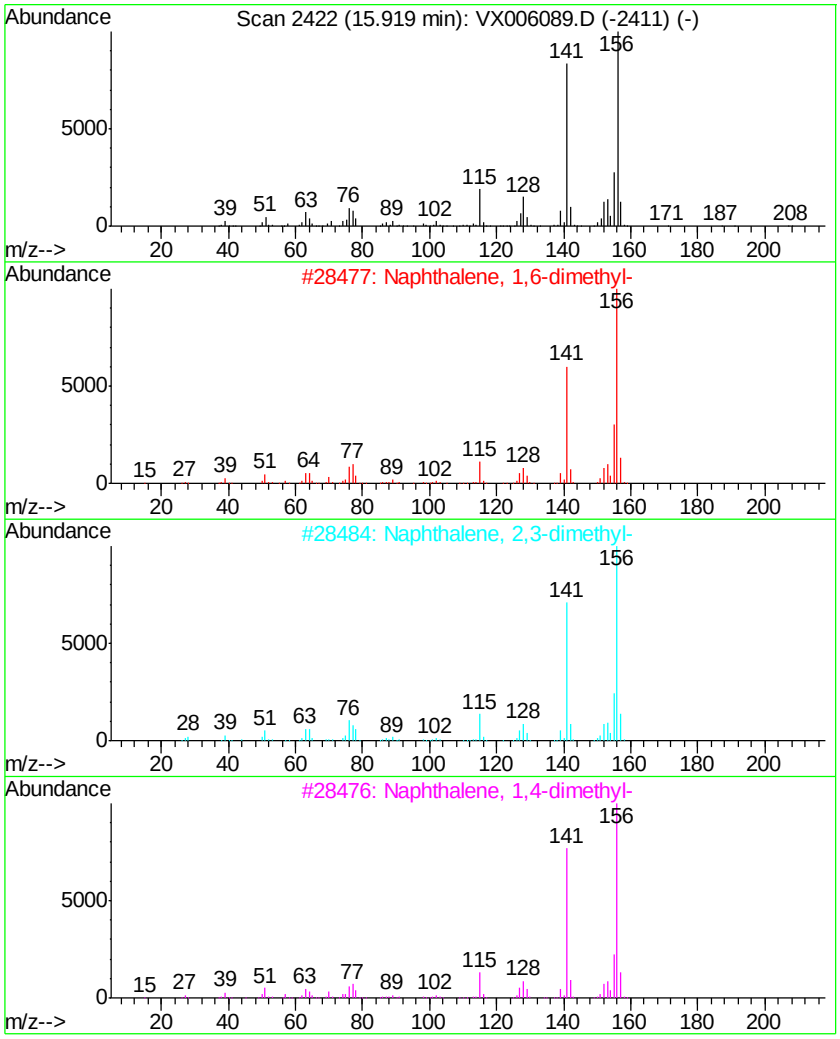
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

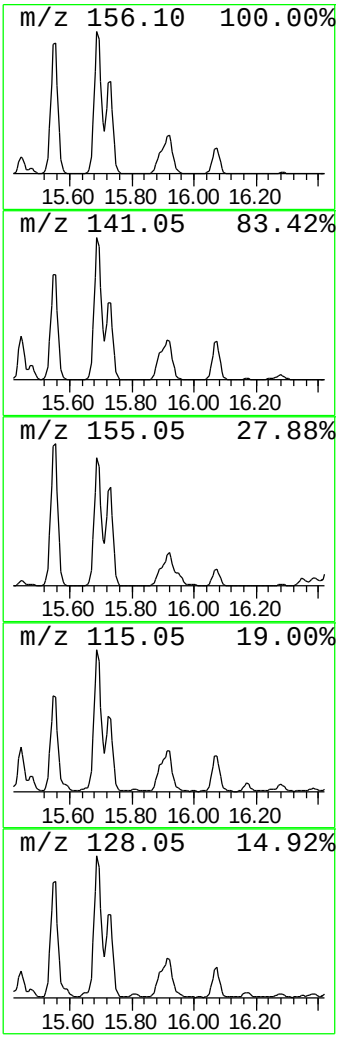
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	78.67 ug/l	803340	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
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Sample : J5767-11
Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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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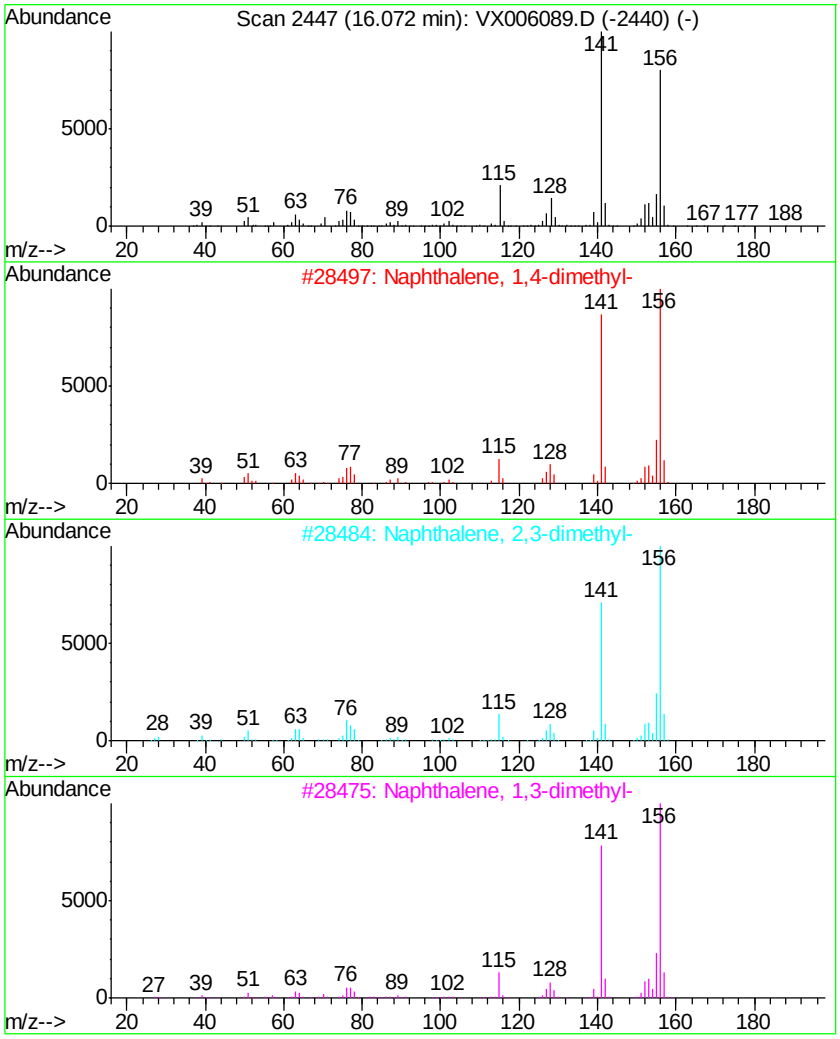
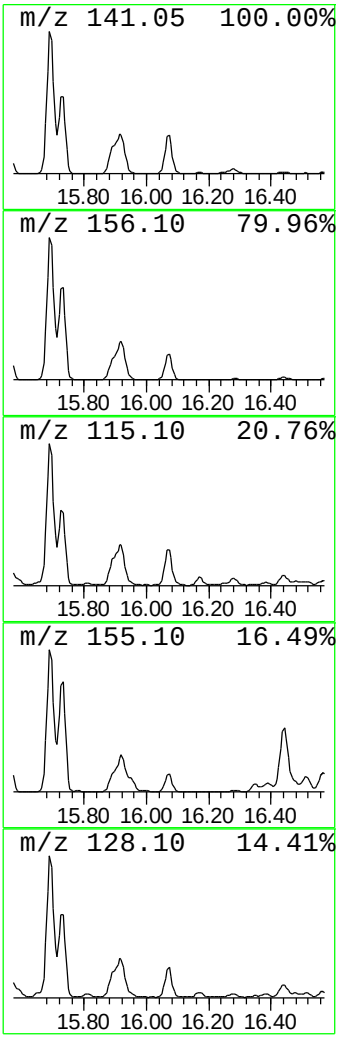
Peak Number 8 Naphthalene, 1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	38.47 ug/l	392904	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	96
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	95
5	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	94





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Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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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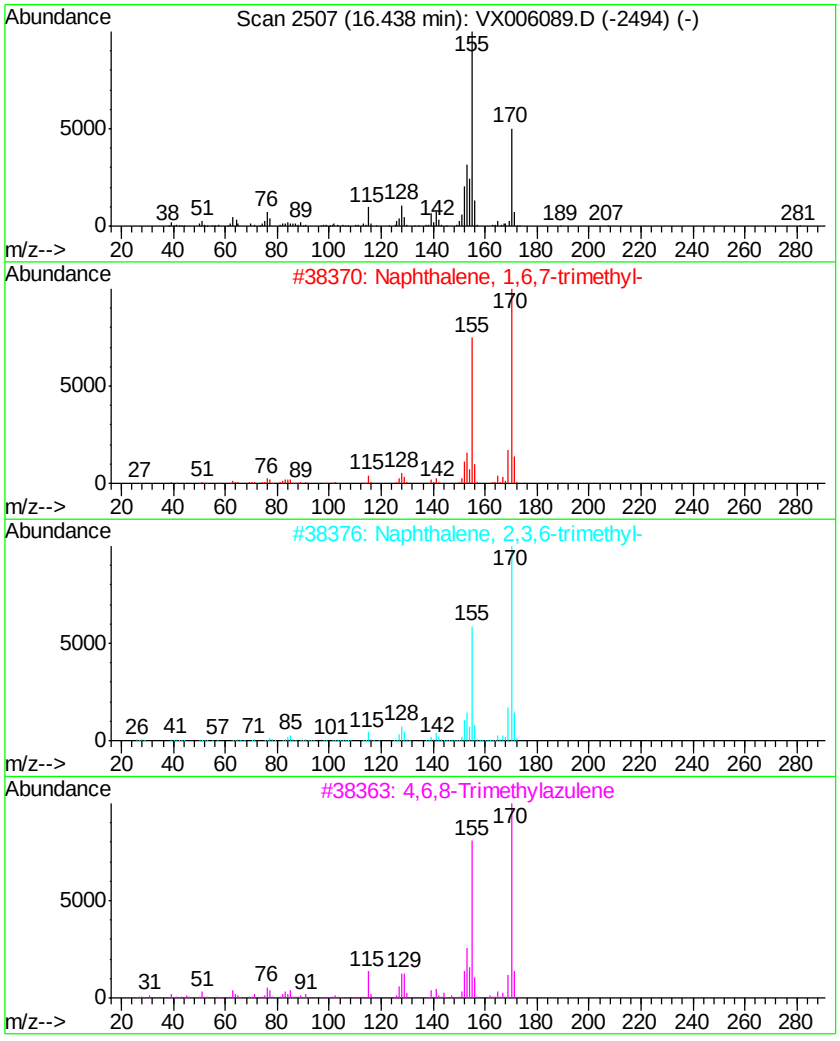
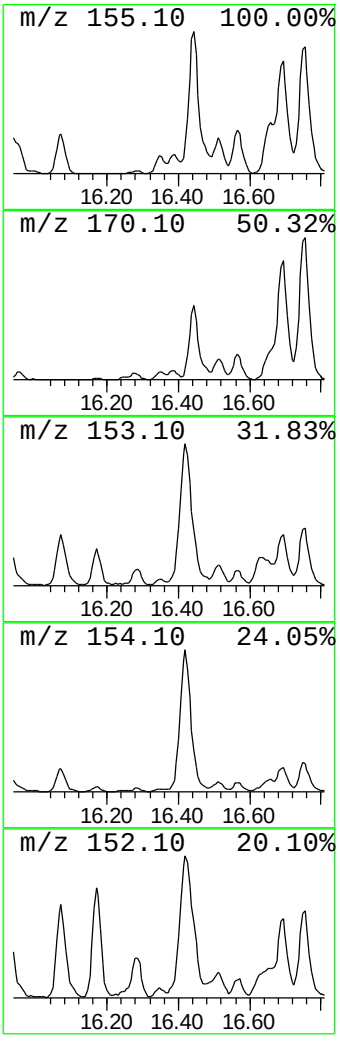
Peak Number 9 Naphthalene, 1,6,7-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	28.89 ug/l	295047	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	91
2	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	90
3	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	90
4	Naphthalene, 1-(1-methylethyl)-	170	C13H14	006158-45-8	80
5	Naphthalene, 2-(1-methylethyl)-	170	C13H14	002027-17-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX111918\
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Misc : 6.61g/5mL/100uL/5.00ml/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : CL-01-111418-B

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
Naphthalene, 1-me...	14.84	214.0	ug/l	2185310	4	12.08	510608	50.0
Naphthalene, 2-et...	15.44	32.7	ug/l	333616	4	12.08	510608	50.0
Naphthalene, 2,3-...	15.69	175.4	ug/l	1791000	4	12.08	510608	50.0
Naphthalene, 2,6-...	15.72	92.0	ug/l	939658	4	12.08	510608	50.0
Naphthalene, 1,6-...	15.92	78.7	ug/l	803340	4	12.08	510608	50.0
Naphthalene, 1,4-...	16.07	38.5	ug/l	392904	4	12.08	510608	50.0
Naphthalene, 1,6,...	16.44	28.9	ug/l	295047	4	12.08	510608	50.0