

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032918\
 Data File : VX000511.D
 Acq On : 29 Mar 2018 14:41
 Operator : JC/MD
 Sample : J2066-01
 Misc : 6.15g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RO-CV-2036

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	73	79	92	rBV	280367	345184	48.68%	6.000%
2	1.636	156	172	176	rBV3	37962	118890	16.76%	2.067%
3	2.489	305	312	314	rBV2	4488	8949	1.26%	0.156%
4	5.519	796	809	821	rBV	71747	210316	29.66%	3.656%
5	5.666	823	833	847	rVB	110621	312111	44.01%	5.425%
6	6.080	889	901	915	rBV	83778	226061	31.88%	3.930%
7	6.867	1019	1030	1044	rBV2	193538	469829	66.25%	8.167%
8	8.720	1326	1334	1342	rBV	406224	674822	95.16%	11.730%
9	10.122	1557	1564	1579	rBV	426698	633858	89.38%	11.018%
10	11.152	1725	1733	1744	rBV	370096	510830	72.03%	8.880%
11	12.091	1881	1887	1895	rVB	552125	709156	100.00%	12.327%
12	12.396	1930	1937	1941	rBV6	6840	14778	2.08%	0.257%
13	12.878	2013	2016	2021	rVB2	10061	14670	2.07%	0.255%
14	12.987	2030	2034	2038	rBV2	7654	9684	1.37%	0.168%
15	13.359	2091	2095	2101	rVB5	11008	17696	2.50%	0.308%
16	13.469	2109	2113	2122	rBV8	13567	35257	4.97%	0.613%
17	13.585	2128	2132	2136	rBV3	8489	14224	2.01%	0.247%
18	13.658	2140	2144	2146	rVB5	6997	9441	1.33%	0.164%
19	13.743	2154	2158	2160	rBV5	4969	7266	1.02%	0.126%
20	13.841	2171	2174	2176	rVB3	6919	7891	1.11%	0.137%
21	13.865	2176	2178	2182	rVB2	11946	13784	1.94%	0.240%
22	13.914	2182	2186	2192	rBV5	21374	34063	4.80%	0.592%
23	13.993	2194	2199	2202	rBV6	8646	13898	1.96%	0.242%
24	14.134	2218	2222	2226	rBV6	22392	33550	4.73%	0.583%
25	14.237	2234	2239	2243	rBV6	16767	32630	4.60%	0.567%
26	14.286	2243	2247	2252	rVB7	21648	38879	5.48%	0.676%
27	14.554	2288	2291	2298	rVB8	19411	44295	6.25%	0.770%
28	14.652	2304	2307	2309	rBV4	14121	14958	2.11%	0.260%
29	14.682	2309	2312	2314	rBV3	51036	64451	9.09%	1.120%
30	14.743	2319	2322	2325	rBV4	24946	36273	5.11%	0.631%
31	14.822	2332	2335	2337	rBV3	33885	40136	5.66%	0.698%
32	14.847	2337	2339	2343	rVB2	36777	48024	6.77%	0.835%
33	14.914	2348	2350	2353	rVB3	26818	28089	3.96%	0.488%
34	15.249	2402	2405	2409	rBV5	50822	91273	12.87%	1.587%

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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

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35	15.499	2442	2446	2450	rVB3	53492	83364	11.76%	1.449%
36	15.566	2452	2457	2461	rBV4	69969	142131	20.04%	2.471%
37	15.700	2475	2479	2482	rBV	68262	93433	13.18%	1.624%
38	15.743	2482	2486	2488	rBV4	38375	62560	8.82%	1.087%
39	15.828	2496	2500	2507	rVB2	112695	203683	28.72%	3.541%
40	16.188	2555	2559	2569	rBV10	67102	168329	23.74%	2.926%
41	16.377	2585	2590	2591	rBV5	69793	114023	16.08%	1.982%

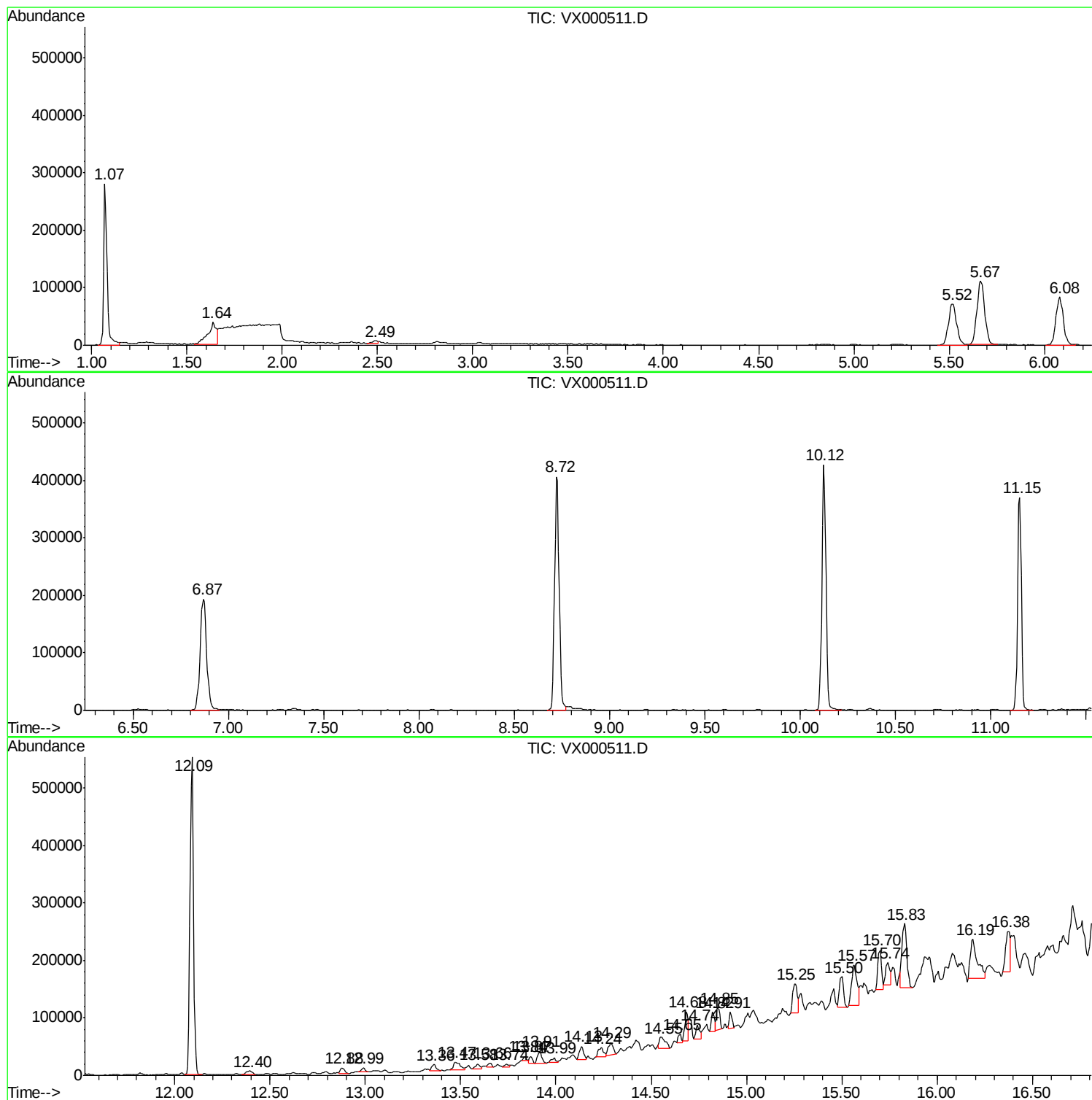
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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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



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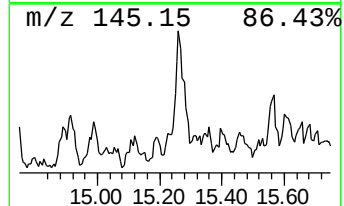
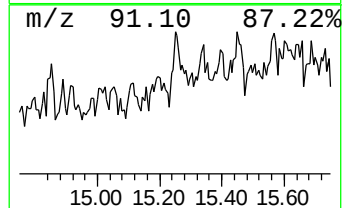
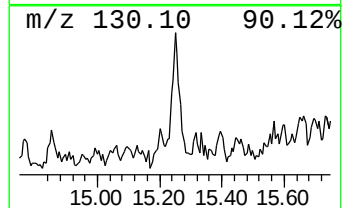
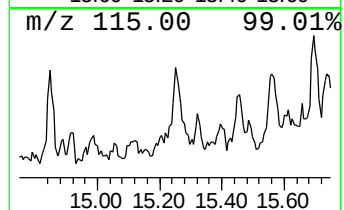
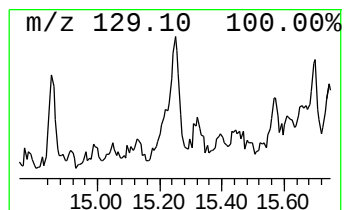
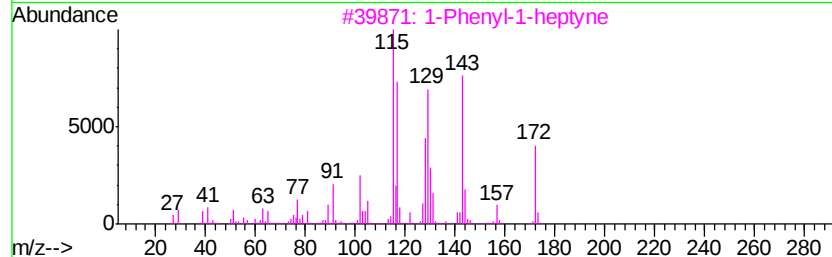
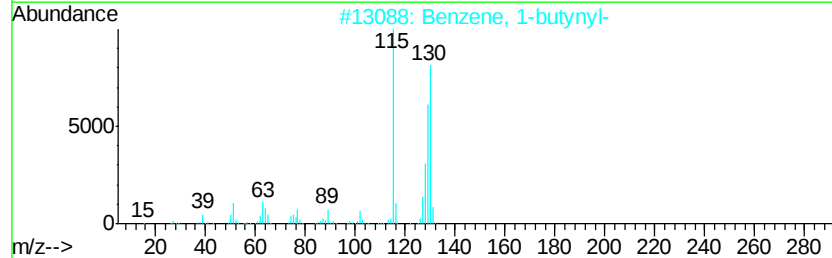
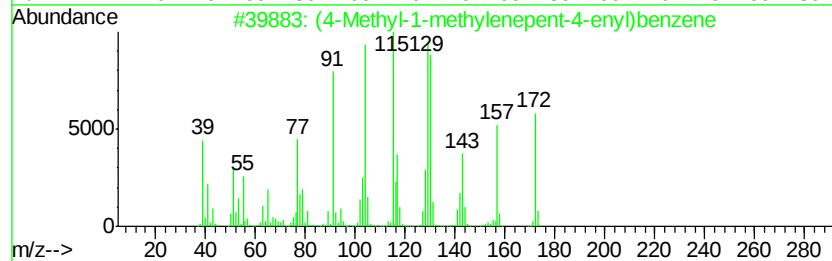
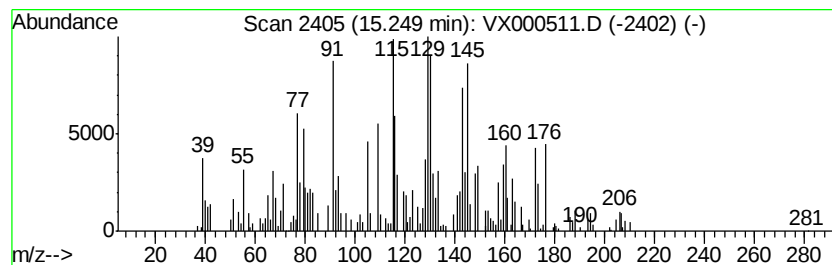
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown15.25 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	6.44 ug/l	91273	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(4-Methyl-1-methylenepent-4-enyl)...	172	C13H16	063942-88-1	43
2		Benzene, 1-butylnyl-	130	C10H10	000622-76-4	38
3		1-Phenyl-1-heptyne	172	C13H16	014374-45-9	38
4		6-Methyl benzobicyclo[2.2.1] hep...	172	C12H12O	140224-88-0	30
5		Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	30



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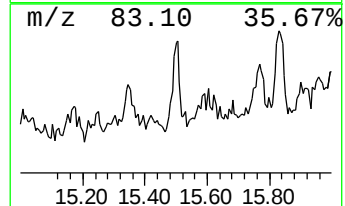
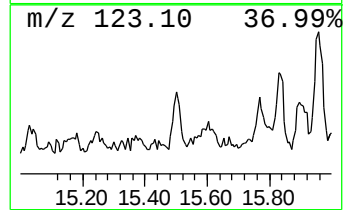
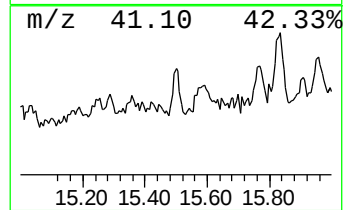
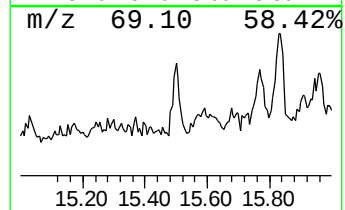
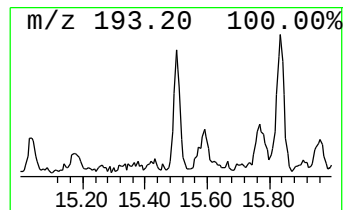
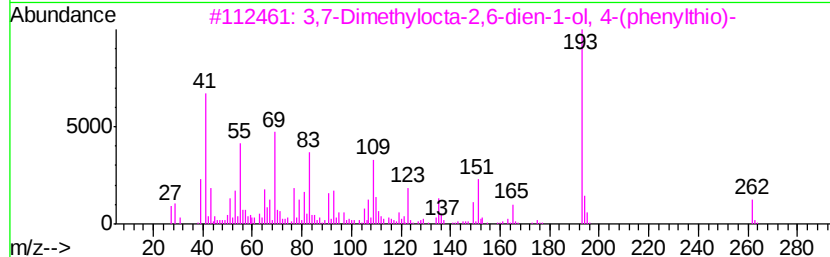
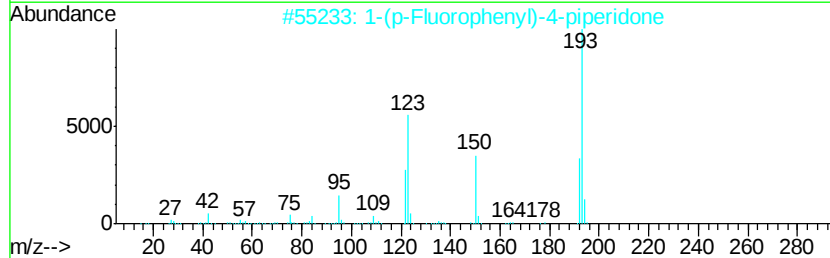
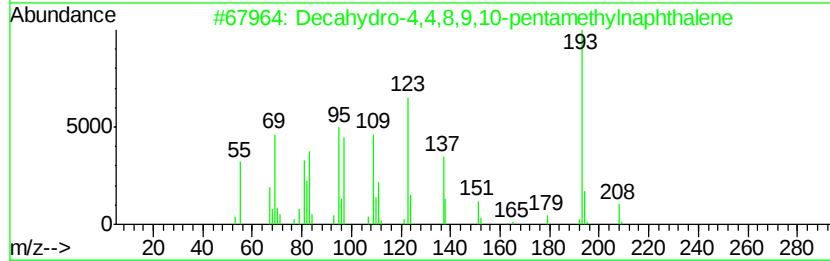
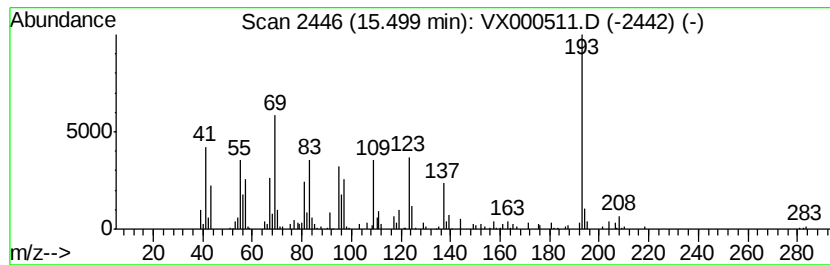
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Decahydro-4,4,8,9,10-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.50	5.88 ug/l	83364	1,4-Dichlorobenzene-d4	12.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	68
2		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	47
3		3,7-Dimethylocta-2,6-dien-1-ol, ...	262	C16H22OS	1000196-46-7	43
4		2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	42
5		2-Amino-4-butylthiomethyl-6-pipe...	281	C13H23NS	022362-21-6	38



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Instrument :
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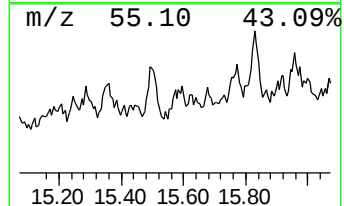
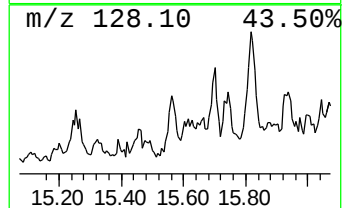
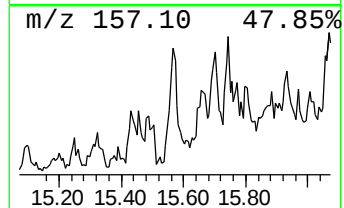
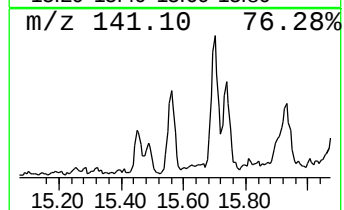
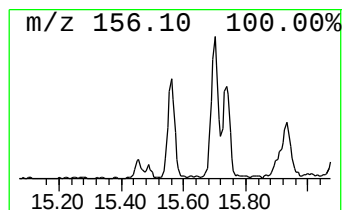
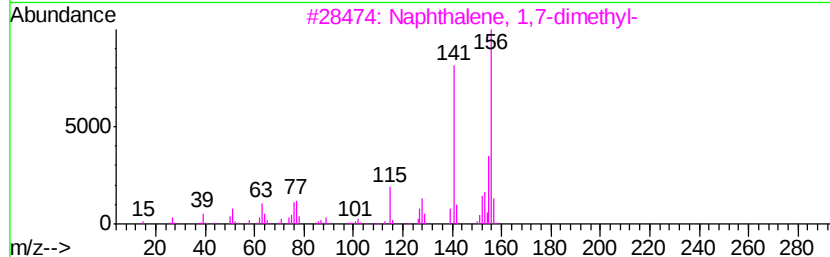
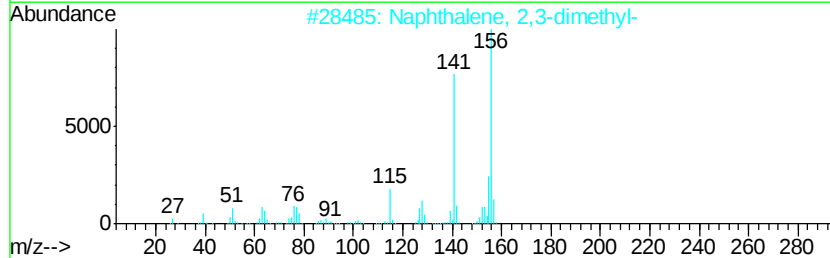
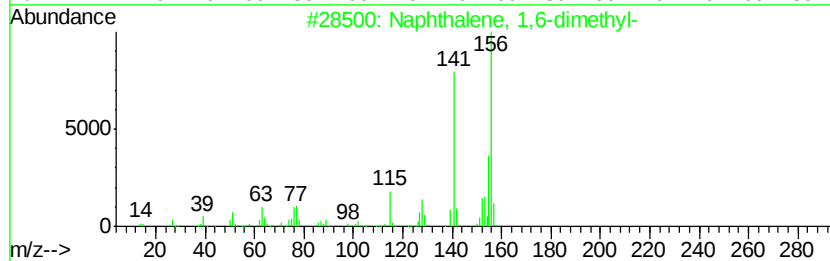
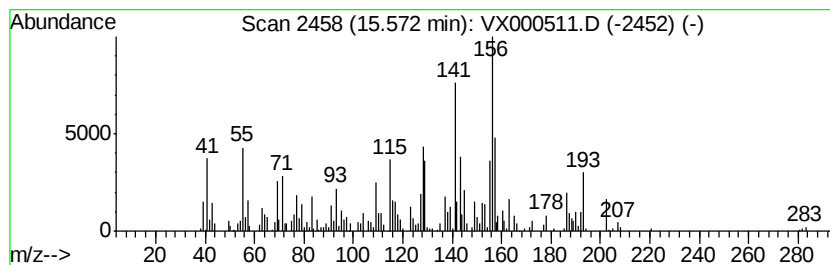
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	10.02 ug/l	142131	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	91
2		Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	91
3		Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	91
4		Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	91
5		Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	64



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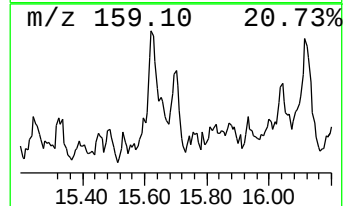
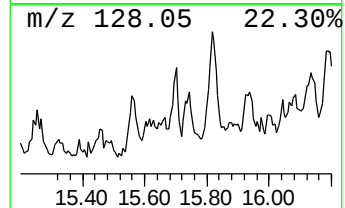
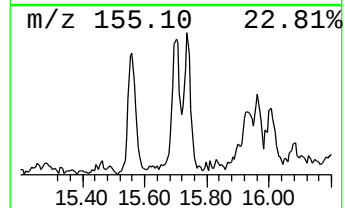
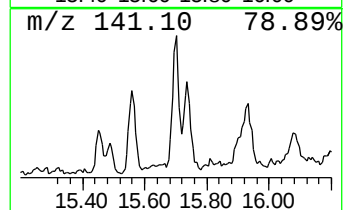
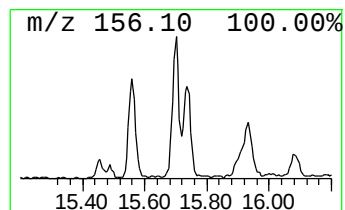
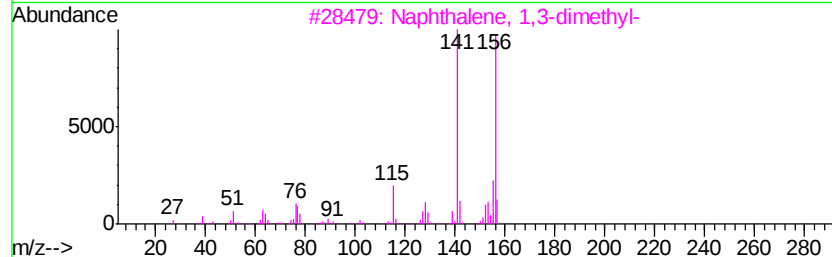
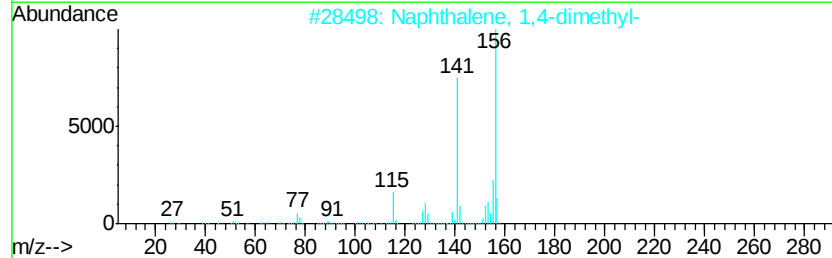
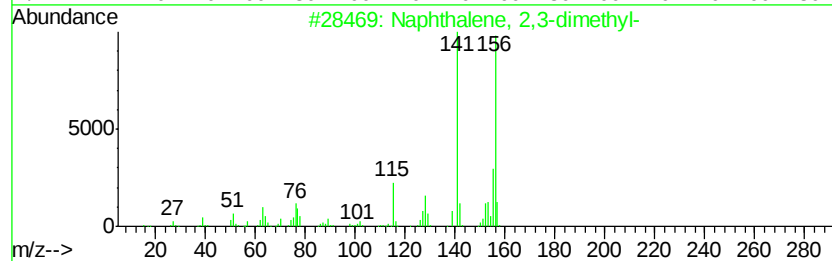
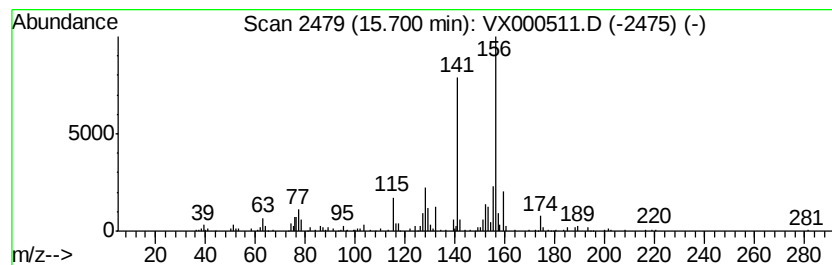
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	6.59 ug/l	93433	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	90
2		Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	76
3		Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	68
4		Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	62
5		Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	60



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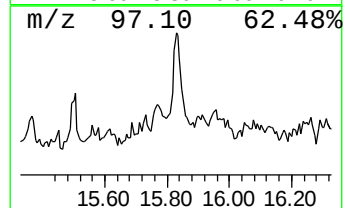
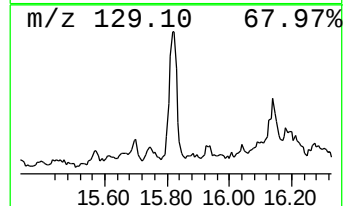
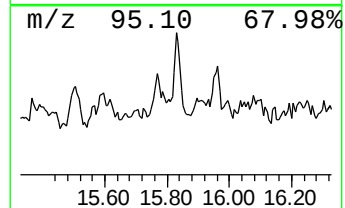
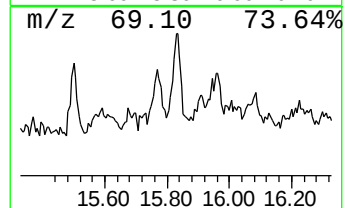
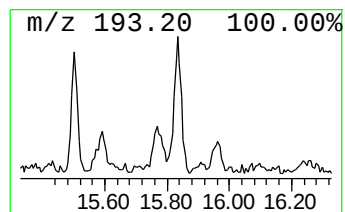
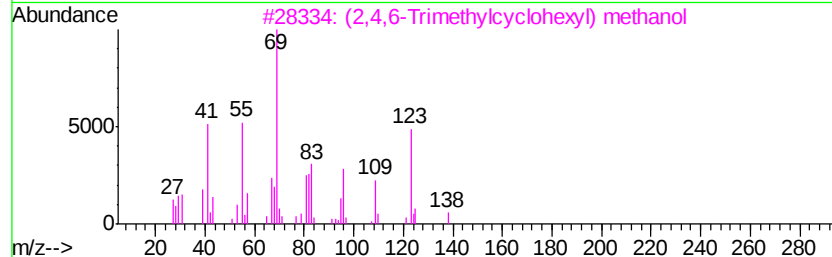
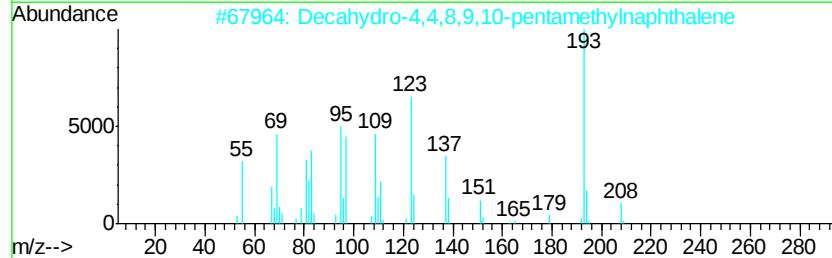
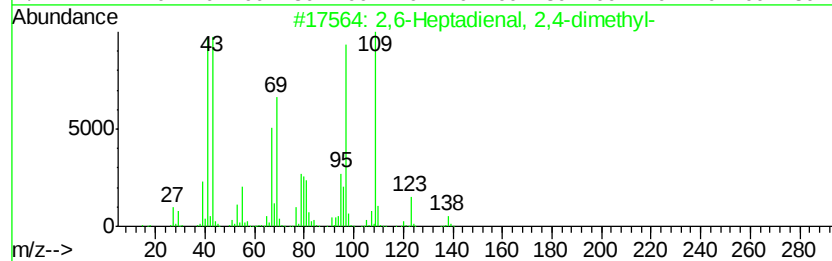
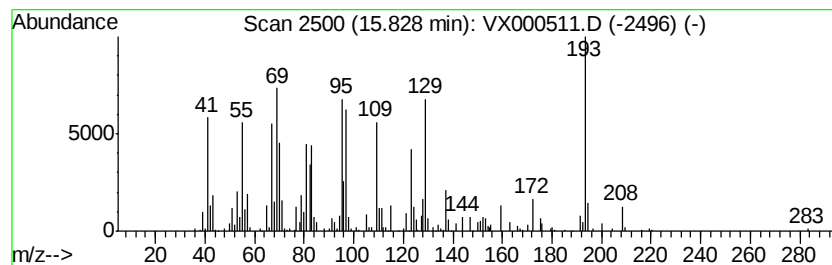
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Quant Title : SW846 8260

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

Peak Number 6 unknown15.83 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	14.36 ug/l	203683	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	41
2		Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
3		(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
4		2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	14
5		Cyclopentanecarboxylic acid, 4-p...	324	C21H40O2	1000280-59-2	14



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032918\
Data File : VX000511.D
Acq On : 29 Mar 2018 14:41
Operator : JC/MD
Sample : J2066-01
Misc : 6.15µL/5mL/100µL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RO-CV-2036

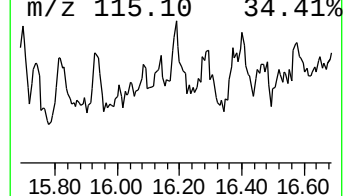
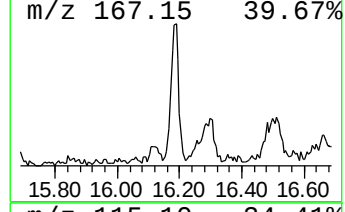
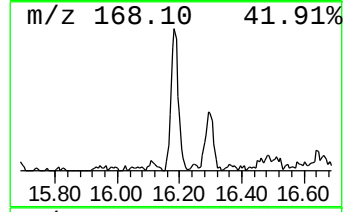
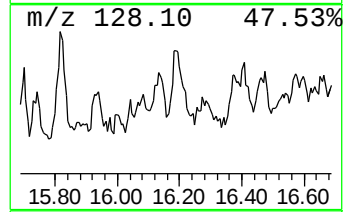
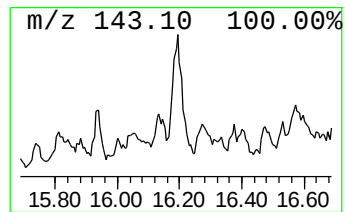
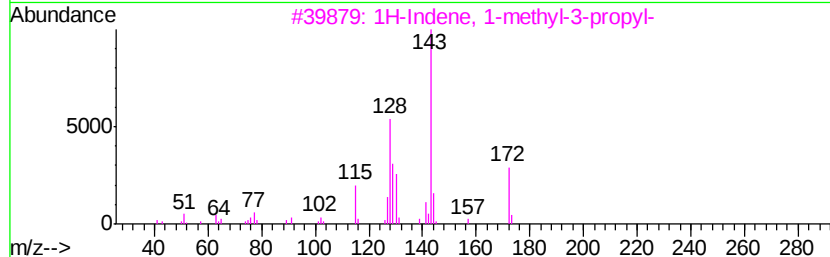
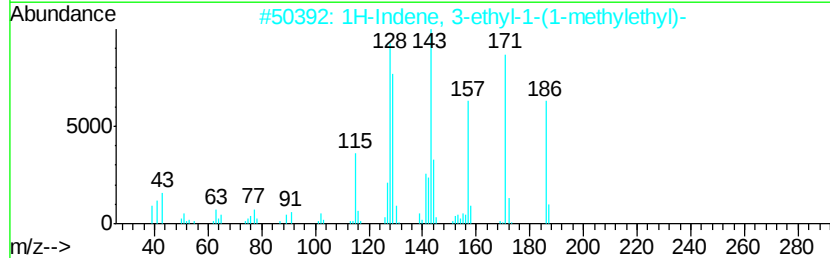
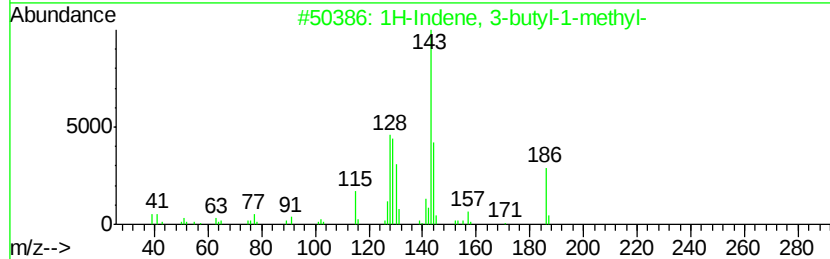
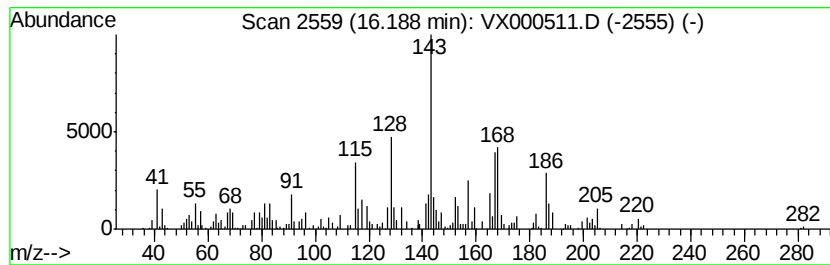
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 7 unknown16.19 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	11.87 ug/l	168329	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 3-butyl-1-methyl-	186	C14H18	111400-84-1	46
2		1H-Indene, 3-ethyl-1-(1-methylethyl)-	186	C14H18	111400-85-2	38
3		1H-Indene, 1-methyl-3-propyl-	172	C13H16	111400-83-0	35
4		Benzene, 1,3,5-trimethyl-2-(1,2-dimethyl-ethyl)-	158	C12H14	029555-07-5	35
5		2-Methyl-1,2,3,4-tetrahydro-.bet...	186	C12H14N2	013100-00-0	30



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032918\
Data File : VX000511.D
Acq On : 29 Mar 2018 14:41
Operator : JC/MD
Sample : J2066-01
Misc : 6.15uL/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
RO-CV-2036

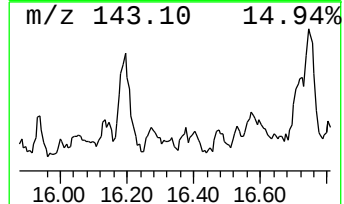
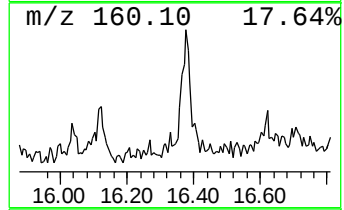
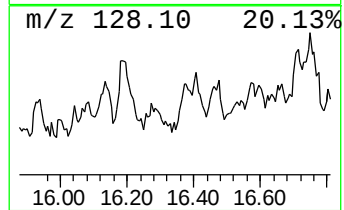
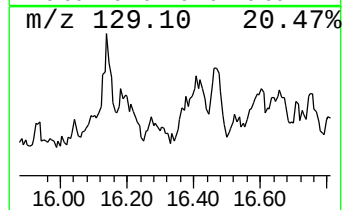
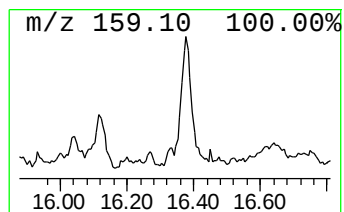
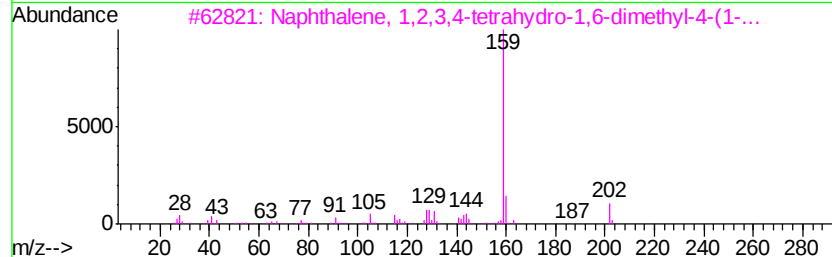
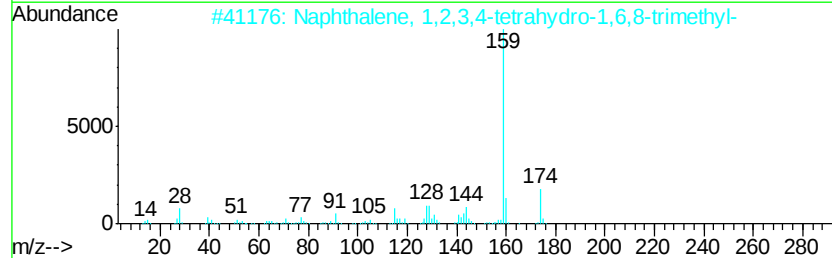
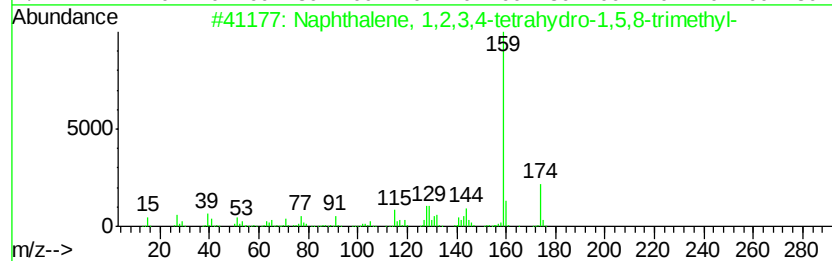
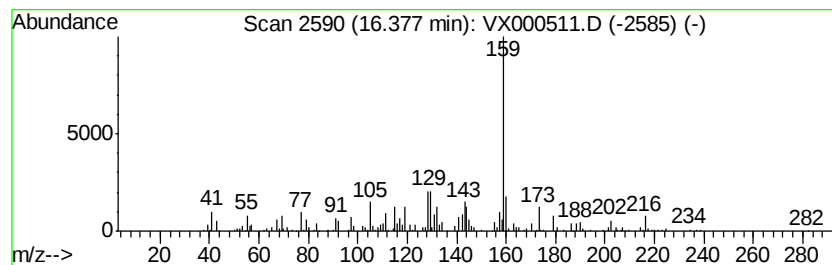
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	8.04 ug/l	114023	1,4-Dichlorobenzene-d4	12.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-51-6	93
2		Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	76
3		Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	76
4		Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	76
5		trans-calamenene	202	C15H22	1000374-17-3	72



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032918\
Data File : VX000511.D
Acq On : 29 Mar 2018 14:41
Operator : JC/MD
Sample : J2066-01
Misc : 6.15g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RO-CV-2036

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown15.25	15.25	6.4	ug/l	91273	4	12.09	709156	50.0
Decahydro-4,4,8,9...	15.50	5.9	ug/l	83364	4	12.09	709156	50.0
Naphthalene, 1,6-...	15.57	10.0	ug/l	142131	4	12.09	709156	50.0
Naphthalene, 2,3-...	15.70	6.6	ug/l	93433	4	12.09	709156	50.0
unknown15.83	15.83	14.4	ug/l	203683	4	12.09	709156	50.0
unknown16.19	16.19	11.9	ug/l	168329	4	12.09	709156	50.0
Naphthalene, 1,2,...	16.38	8.0	ug/l	114023	4	12.09	709156	50.0