

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071524\
 Data File : VX042324.D
 Acq On : 15 Jul 2024 14:01
 Operator : JC/MD
 Sample : P3224-01 20X
 Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 380AVEC-21

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\82X061824W.M
 Title : SW846 8260

Signal : TIC: VX042324.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.618	69	87	88	rBV5	7853	30108	4.22%	0.612%
2	5.391	692	706	721	rBV	92030	268792	37.68%	5.465%
3	5.550	721	732	748	rVV	123582	349115	48.94%	7.099%
4	5.958	789	799	809	rBV	90566	240863	33.77%	4.898%
5	6.037	809	812	830	rVB3	6996	18861	2.64%	0.384%
6	6.763	922	931	944	rBV	194683	458951	64.34%	9.332%
7	8.647	1234	1240	1248	rBV	368165	595697	83.51%	12.112%
8	8.720	1248	1252	1265	rVB	24144	41621	5.83%	0.846%
9	10.055	1465	1471	1490	rBV	376708	509534	71.43%	10.361%
10	10.305	1505	1512	1519	rBV	28368	41605	5.83%	0.846%
11	10.646	1563	1568	1578	rBV	20936	30831	4.32%	0.627%
12	11.085	1634	1640	1655	rBV	314630	417028	58.46%	8.480%
13	11.384	1682	1689	1696	rBV	5739	11082	1.55%	0.225%
14	11.451	1696	1700	1710	rVB	11990	18331	2.57%	0.373%
15	11.756	1745	1750	1756	rVB	24360	31485	4.41%	0.640%
16	12.024	1788	1794	1801	rBV	360653	453111	63.52%	9.213%
17	12.091	1801	1805	1811	rVB	13109	17890	2.51%	0.364%
18	12.244	1823	1830	1838	rBV5	3565	7531	1.06%	0.153%
19	12.420	1853	1859	1864	rBV2	18072	26883	3.77%	0.547%
20	12.969	1945	1949	1956	rVB2	6132	9327	1.31%	0.190%
21	13.268	1992	1998	2000	rBV	6923	9745	1.37%	0.198%
22	13.292	2000	2002	2008	rVB2	6510	7899	1.11%	0.161%
23	13.426	2020	2024	2032	rVB7	4388	9157	1.28%	0.186%
24	13.774	2076	2081	2090	rBV	555509	713305	100.00%	14.504%
25	13.871	2094	2097	2104	rVB	10703	13806	1.94%	0.281%
26	14.036	2120	2124	2128	rBV	9622	11068	1.55%	0.225%
27	14.640	2212	2223	2231	rVB	130893	178182	24.98%	3.623%
28	14.780	2239	2246	2253	rVB	105459	149302	20.93%	3.036%
29	15.207	2307	2316	2321	rBV	12748	20473	2.87%	0.416%
30	15.377	2334	2344	2347	rBV2	11650	20217	2.83%	0.411%
31	15.408	2347	2349	2354	rVV4	6288	9488	1.33%	0.193%
32	15.481	2354	2361	2374	rVV2	28761	55766	7.82%	1.134%
33	15.615	2374	2383	2386	rVV	36931	62404	8.75%	1.269%
34	15.652	2386	2389	2398	rVB	21434	32730	4.59%	0.666%
35	15.834	2410	2419	2426	rBV2	9306	26568	3.72%	0.540%
36	15.987	2438	2444	2449	rBV4	6223	10422	1.46%	0.212%

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ClientSampleId :
380AVEC-21

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\82X061824W.M
Title : SW846 8260

37	16.091	2455	2461	2469	rBV4	4844	8863	1.24%	0.180%
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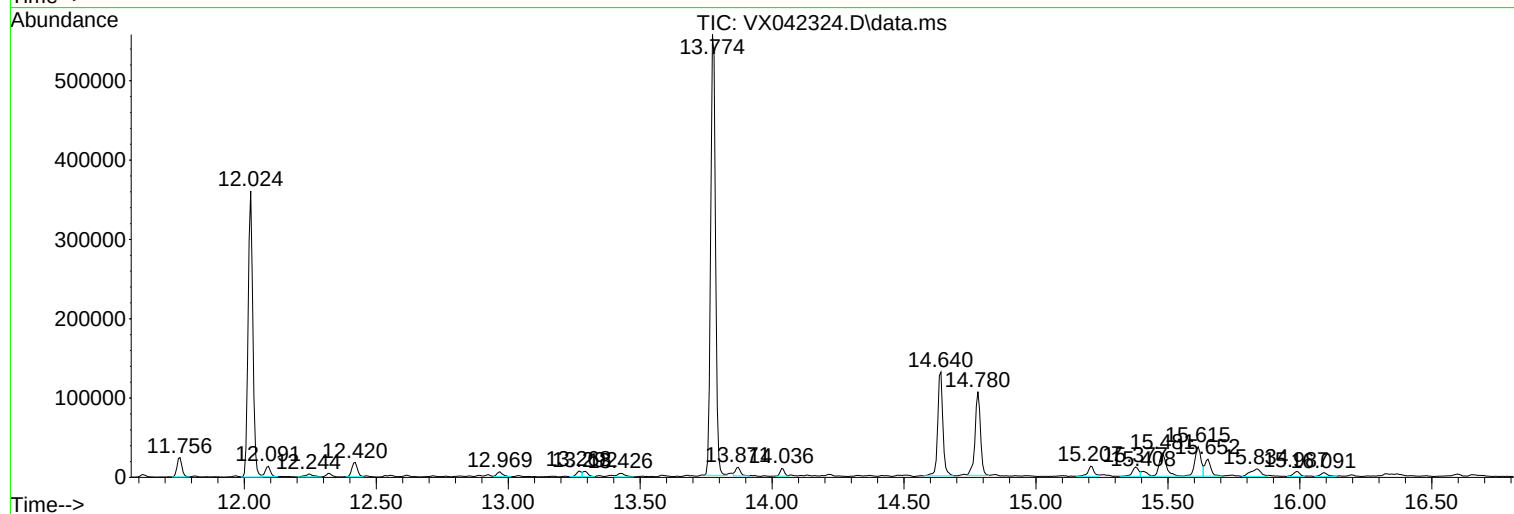
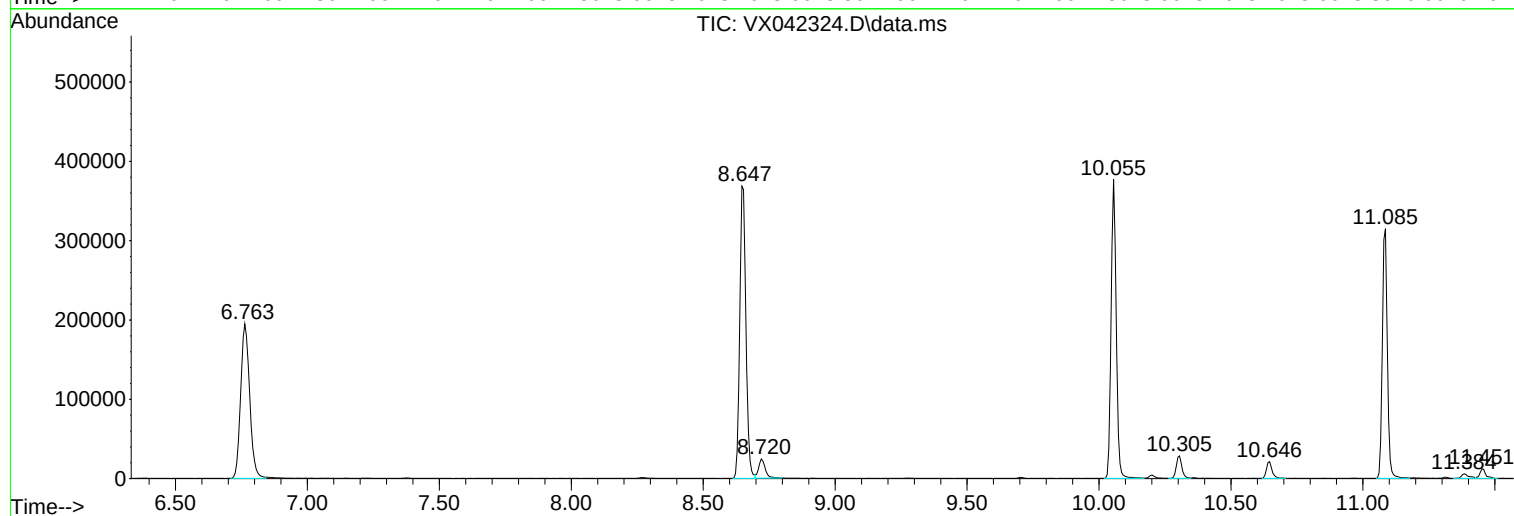
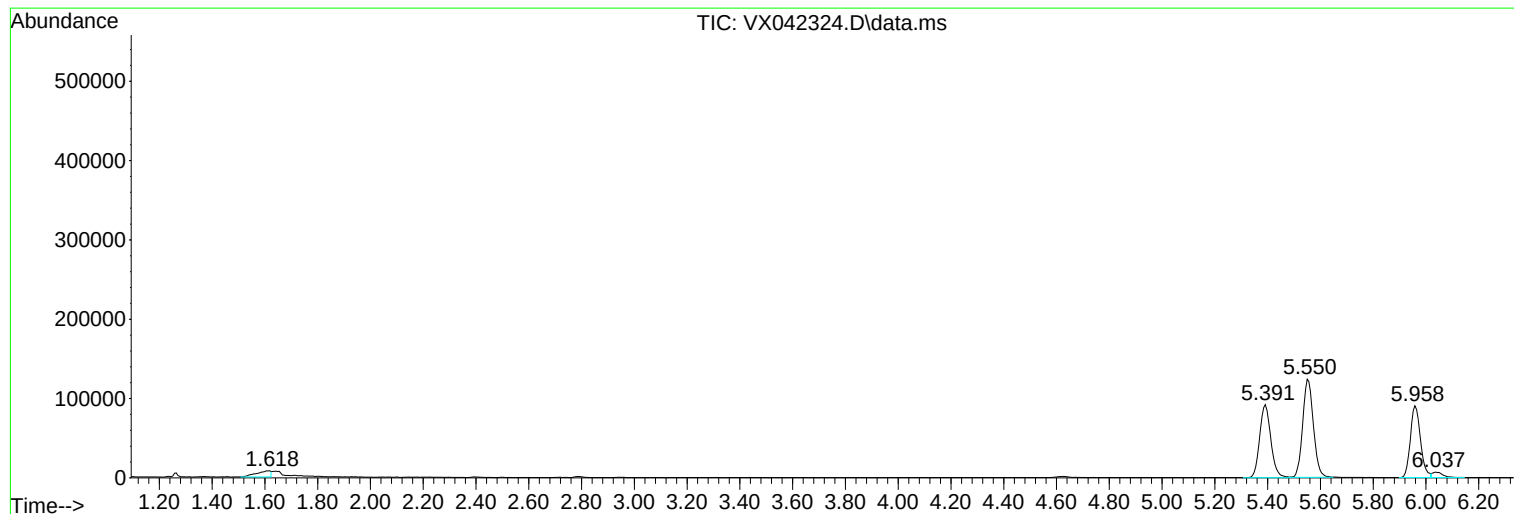
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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
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380AVEC-21

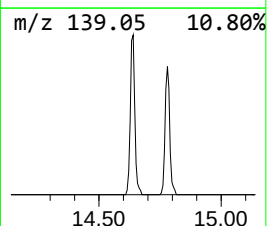
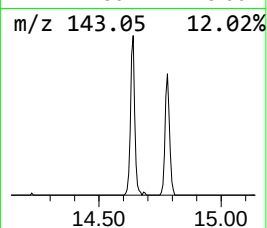
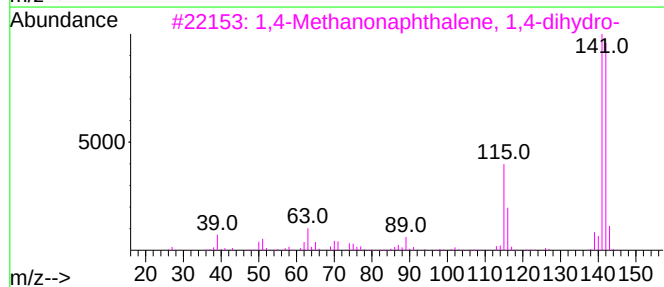
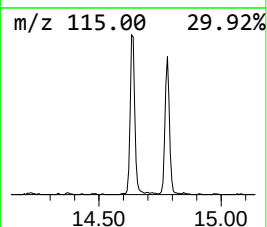
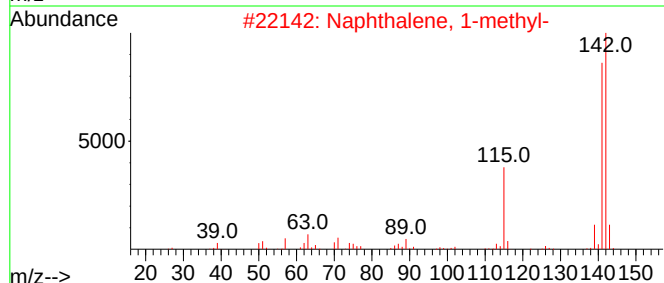
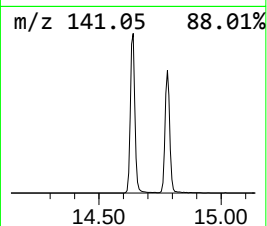
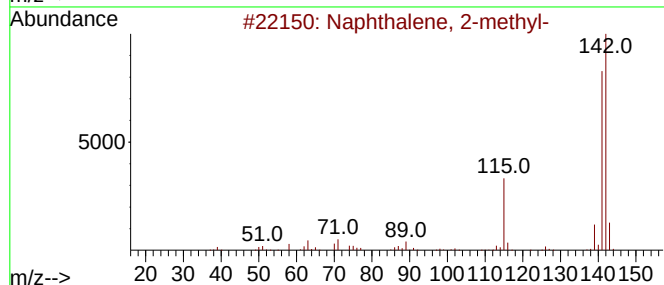
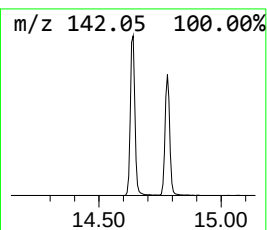
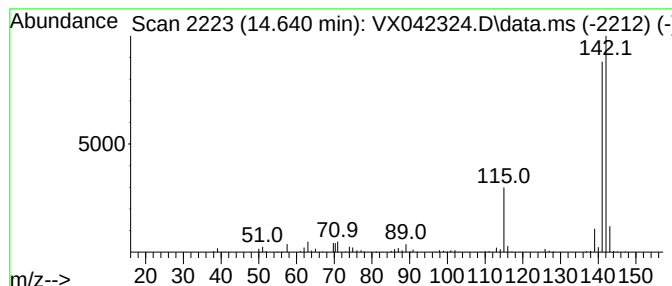
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	19.66 ug/l	178182	1,4-Dichlorobenzene-d4	12.024

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	64



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Sample : P3224-01 20X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-21

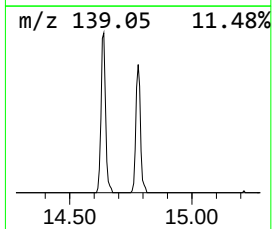
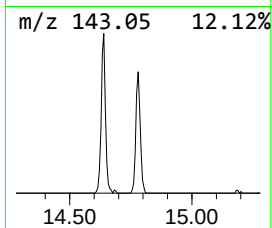
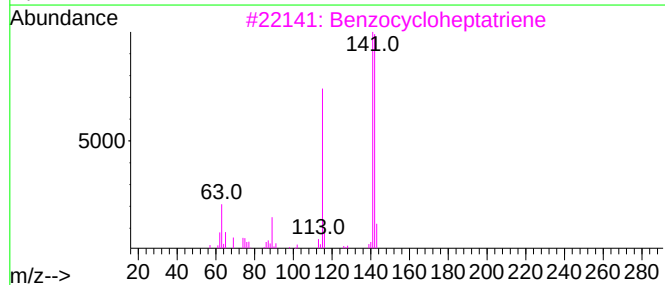
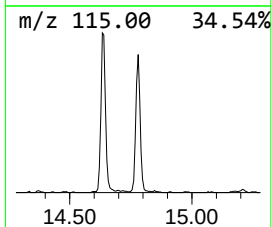
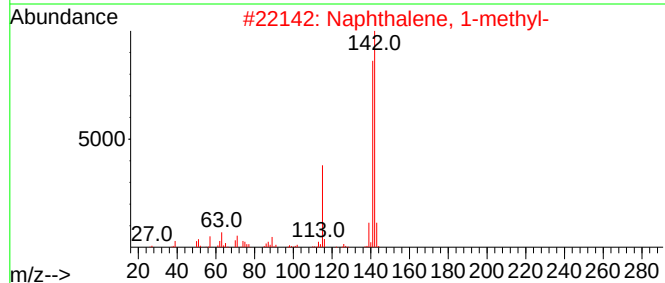
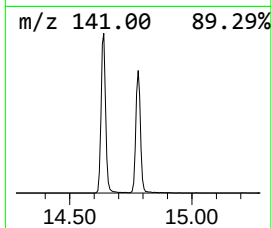
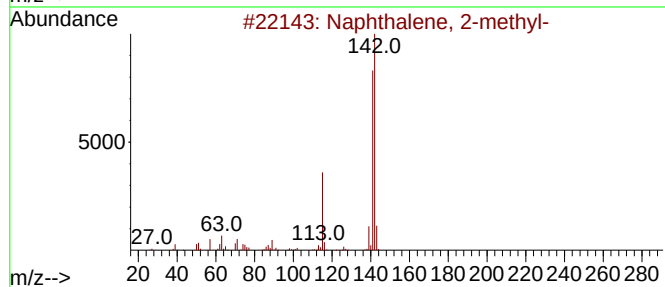
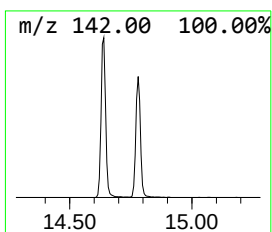
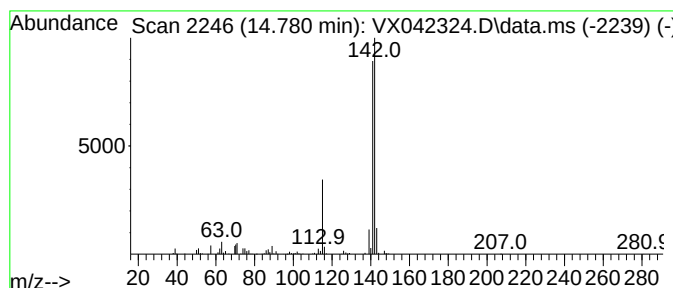
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	16.48 ug/l	149302	1,4-Dichlorobenzene-d4	12.024

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			3-Indolecarbonitrile	142	C9H6N2	005457-28-3	46



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Sample : P3224-01 20X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-21

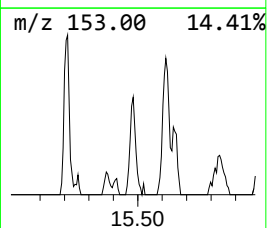
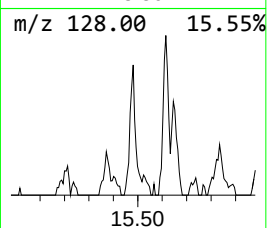
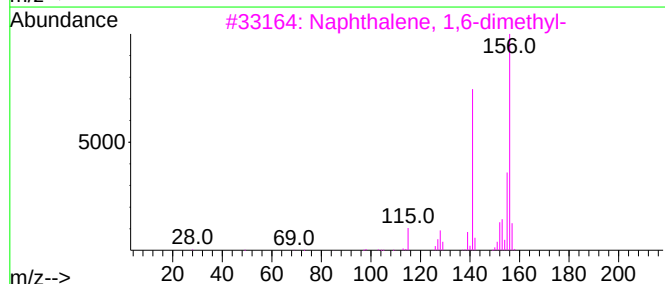
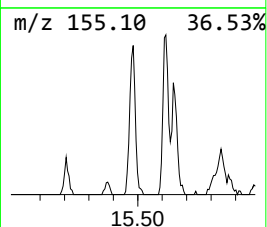
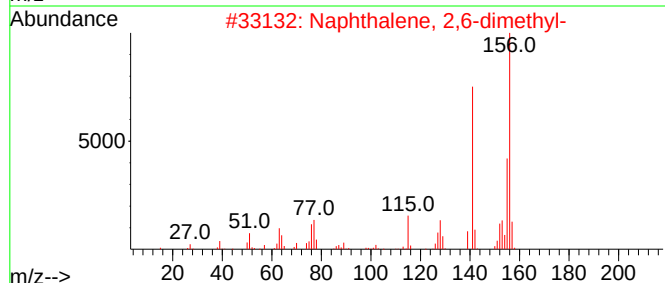
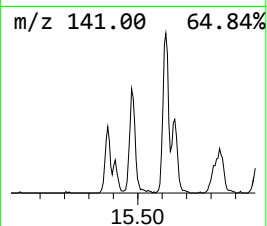
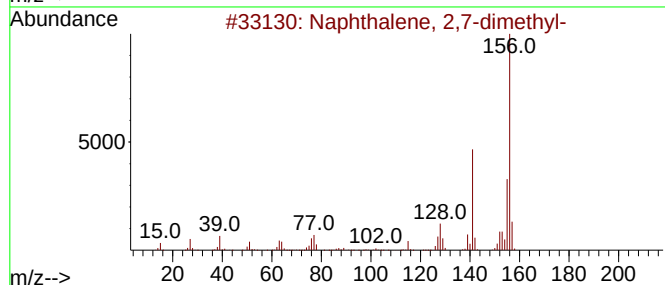
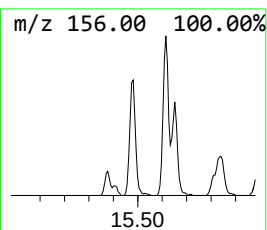
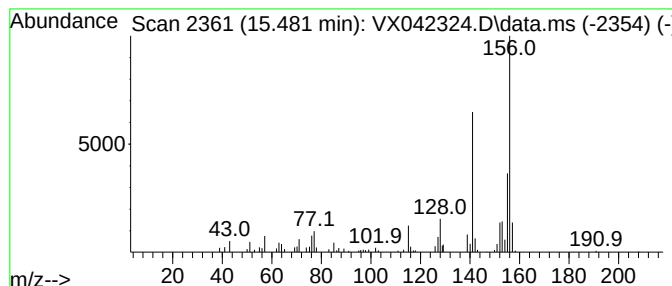
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 2,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	6.15 ug/l	55766	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	94



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Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
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Instrument :
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ClientSampleId :
380AVEC-21

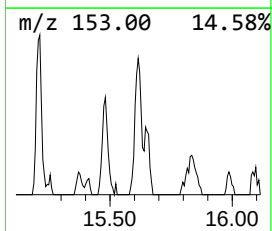
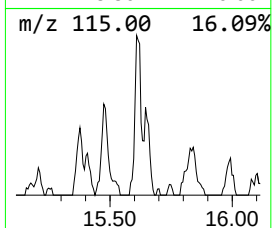
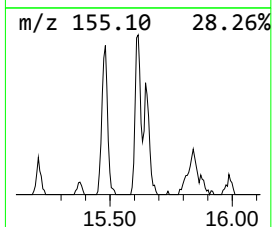
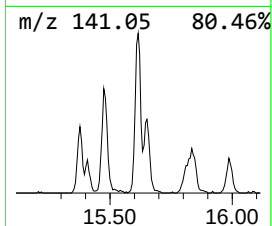
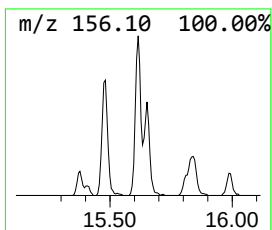
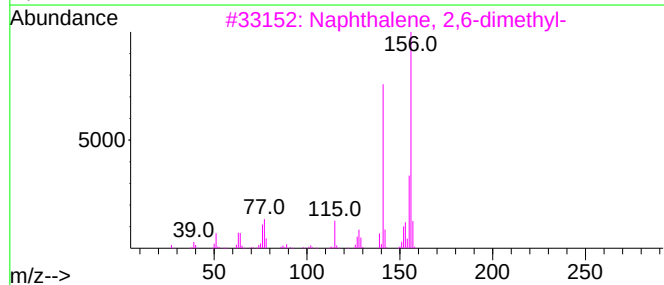
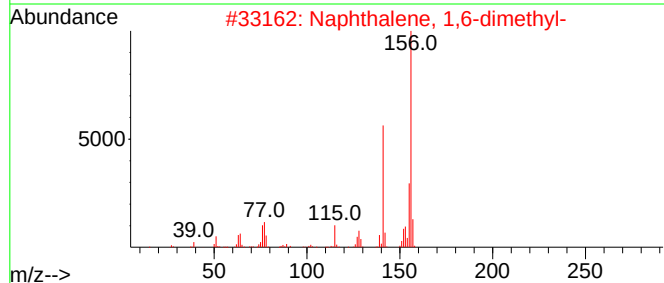
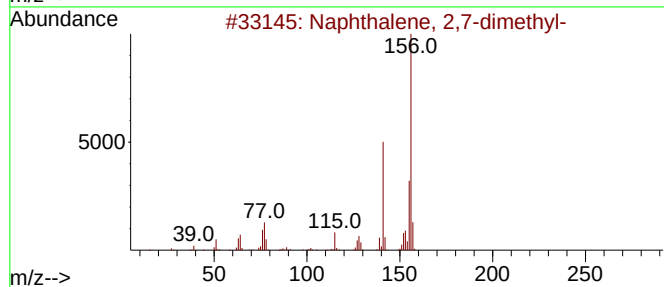
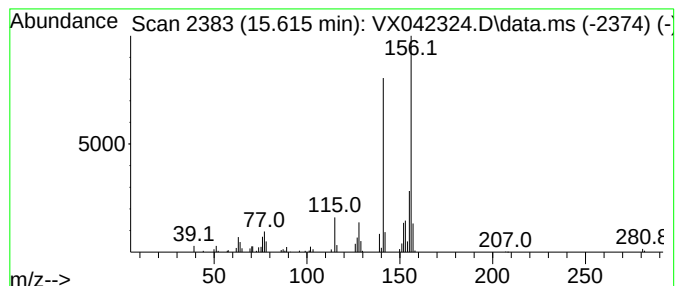
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	6.89 ug/l	62404	1,4-Dichlorobenzene-d4	12.024

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



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
380AVEC-21

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061824W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Naphthalene, 2-...	14.640	19.7	ug/l	178182	4	12.024	453111	50.0
Naphthalene, 1-...	14.780	16.5	ug/l	149302	4	12.024	453111	50.0
Naphthalene, 2,...	15.481	6.2	ug/l	55766	4	12.024	453111	50.0
Naphthalene, 1,...	15.615	6.9	ug/l	62404	4	12.024	453111	50.0