

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112321\
 Data File : VX025286.D
 Acq On : 23 Nov 2021 19:48
 Operator : JC/MD
 Sample : M4817-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A6879

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025286.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	22	27	34	rBV2	81194	91335	8.63%	1.396%
2	2.380	204	212	227	rBV	429522	693236	65.49%	10.594%
3	2.532	230	237	248	rVB	17018	32857	3.10%	0.502%
4	4.556	558	569	587	rBV	385863	1058514	100.00%	16.176%
5	5.001	630	642	664	rBV	325630	1010708	95.48%	15.446%
6	5.391	694	706	720	rBV	63127	182750	17.26%	2.793%
7	5.556	723	733	749	rVB	91638	257476	24.32%	3.935%
8	5.958	789	799	811	rBV	60511	161527	15.26%	2.468%
9	6.763	921	931	946	rBV	154083	368950	34.86%	5.638%
10	8.653	1234	1241	1249	rBV	330600	525117	49.61%	8.025%
11	9.580	1388	1393	1408	rBV	3612	11050	1.04%	0.169%
12	10.055	1465	1471	1485	rBV	346979	468503	44.26%	7.160%
13	11.085	1634	1640	1651	rVB	274930	365727	34.55%	5.589%
14	12.024	1789	1794	1801	rBV	349581	432314	40.84%	6.607%
15	12.091	1801	1805	1810	rVB	12563	15592	1.47%	0.238%
16	12.963	1944	1948	1953	rVB	11827	14270	1.35%	0.218%
17	13.170	1978	1982	1986	rVB2	9199	11472	1.08%	0.175%
18	13.292	1998	2002	2007	rVB2	29650	39144	3.70%	0.598%
19	13.426	2019	2024	2029	rBB	22884	30035	2.84%	0.459%
20	13.585	2046	2050	2056	rVV4	6875	13257	1.25%	0.203%
21	13.780	2074	2082	2089	rBV	195544	253926	23.99%	3.880%
22	13.926	2101	2106	2110	rBV2	8954	11768	1.11%	0.180%
23	14.079	2127	2131	2134	rBV2	8375	10914	1.03%	0.167%
24	14.231	2148	2156	2162	rBV2	20068	38041	3.59%	0.581%
25	14.371	2175	2179	2184	rVB2	10142	11901	1.12%	0.182%
26	14.481	2192	2197	2202	rBV2	15340	21071	1.99%	0.322%
27	14.640	2214	2223	2227	rBV	108722	144947	13.69%	2.215%
28	14.780	2240	2246	2251	rBV	92562	116814	11.04%	1.785%
29	15.188	2305	2313	2314	rBV	9989	13277	1.25%	0.203%
30	15.207	2314	2316	2321	rVB	10743	12716	1.20%	0.194%
31	15.377	2339	2344	2347	rBV	9149	13237	1.25%	0.202%
32	15.481	2354	2361	2365	rBV	16287	25605	2.42%	0.391%
33	15.615	2374	2383	2387	rBV	30693	49998	4.72%	0.764%
34	15.652	2387	2389	2397	rVB2	14360	18879	1.78%	0.289%
35	15.835	2410	2419	2426	rBV4	5863	16717	1.58%	0.255%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Title : SW846 8260

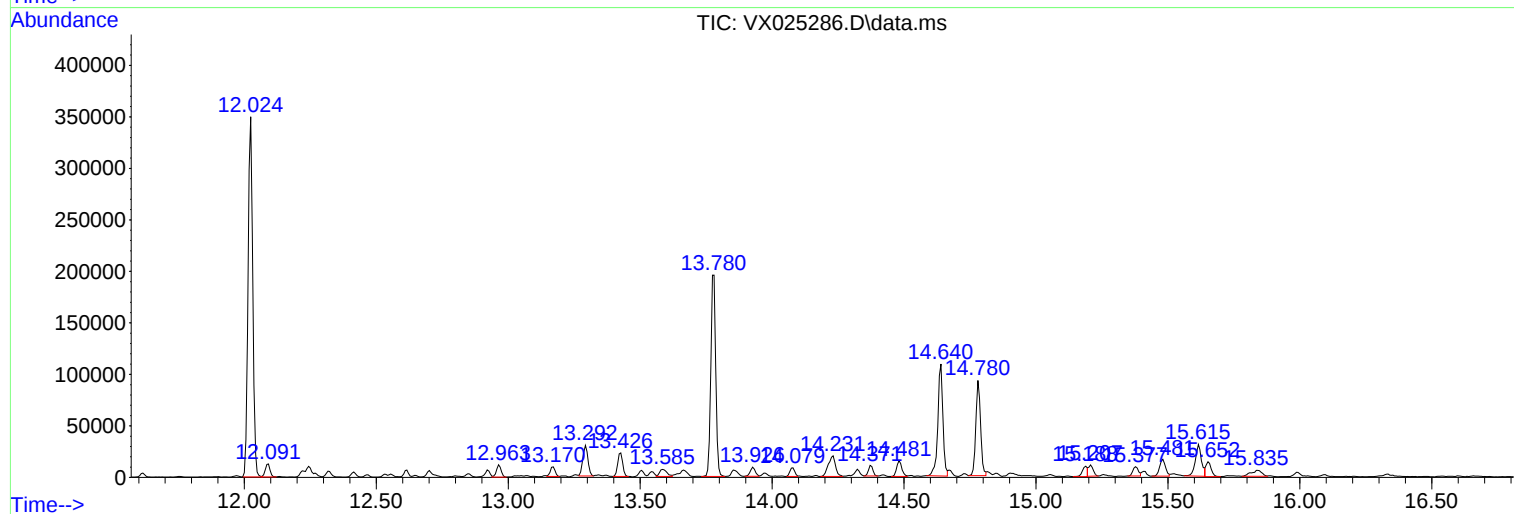
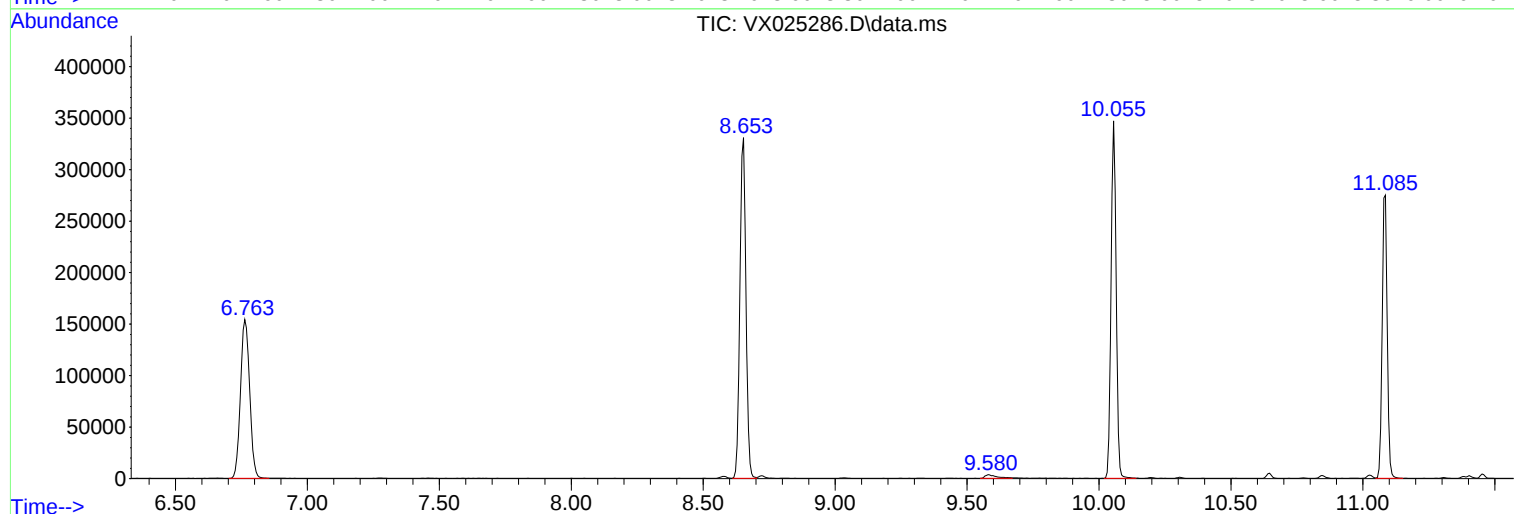
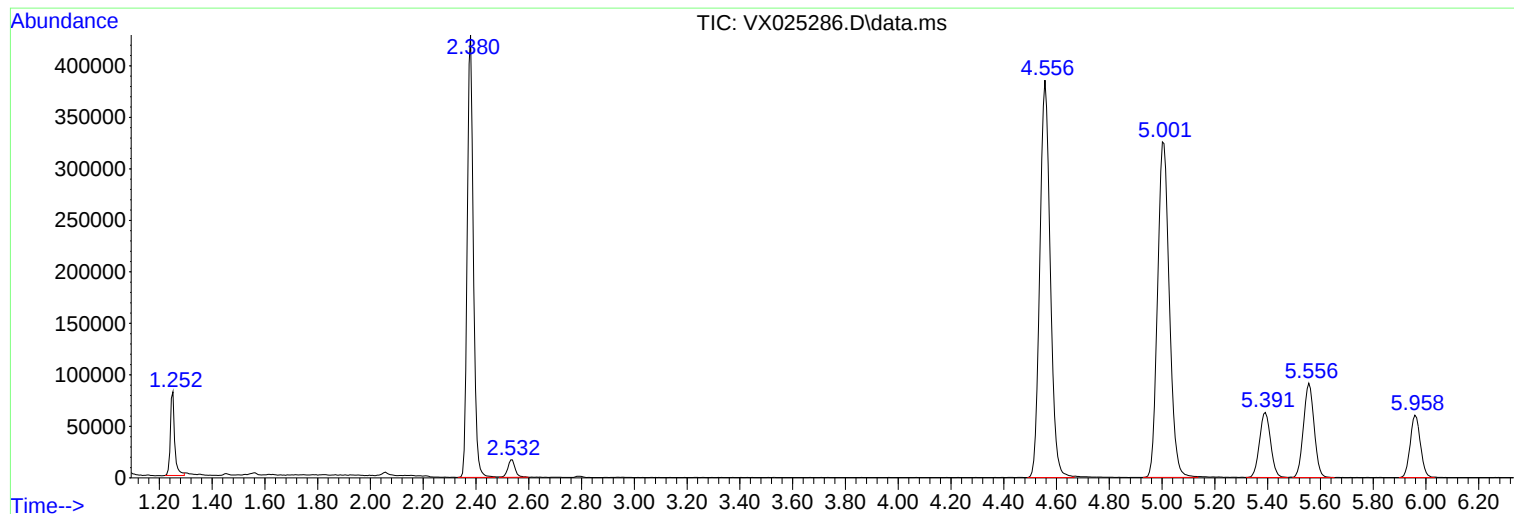
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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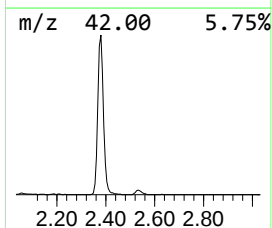
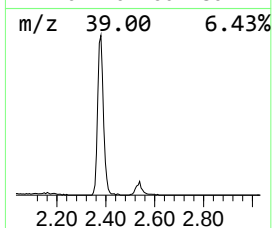
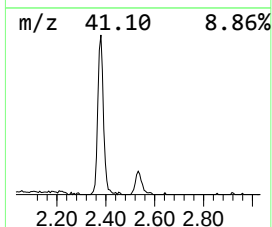
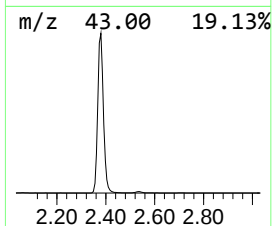
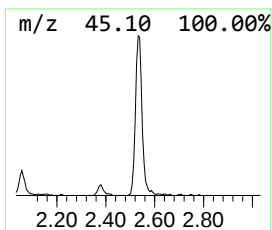
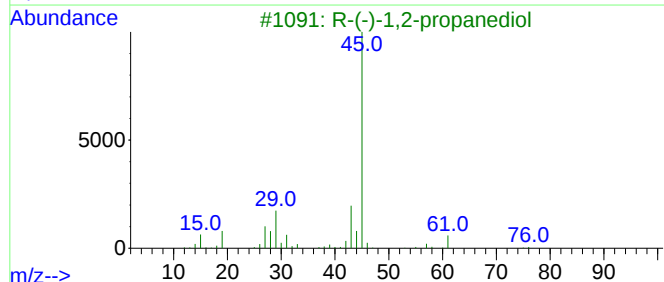
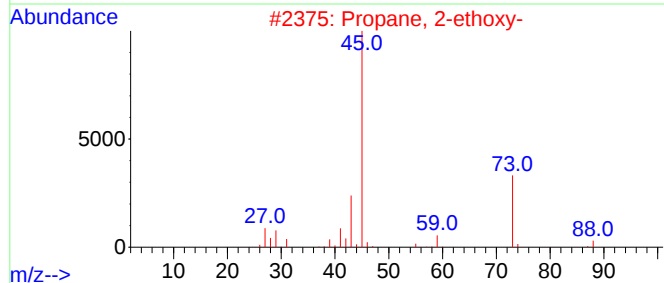
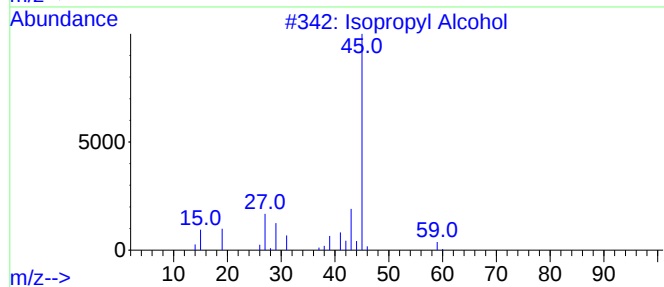
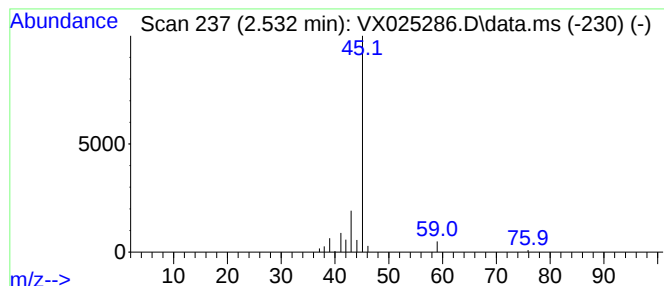
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	6.38 ug/l	32857	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	9
5			2-Pentanol	88	C5H12O	006032-29-7	9



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Instrument :
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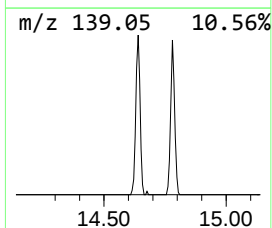
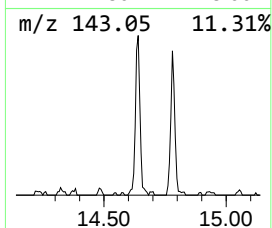
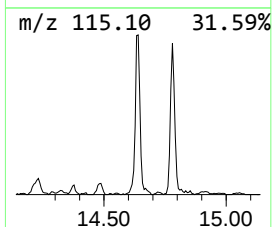
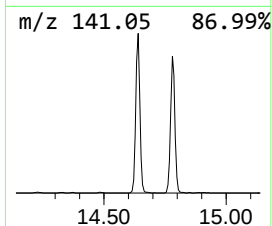
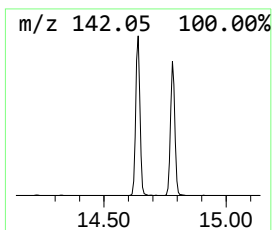
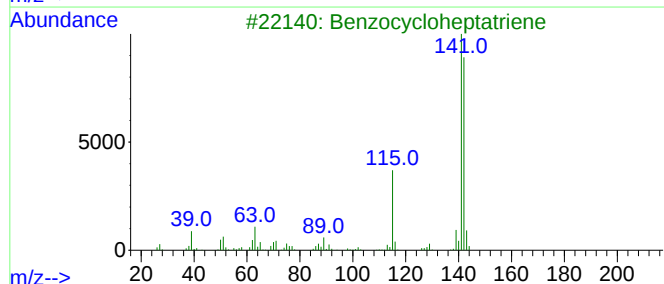
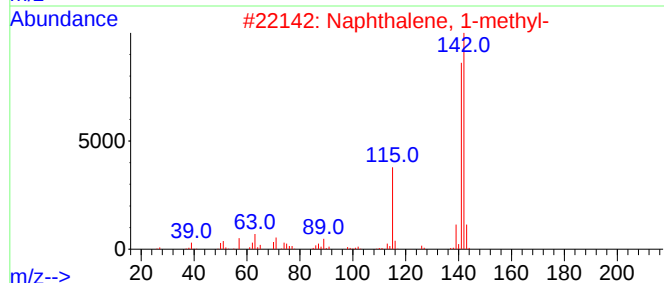
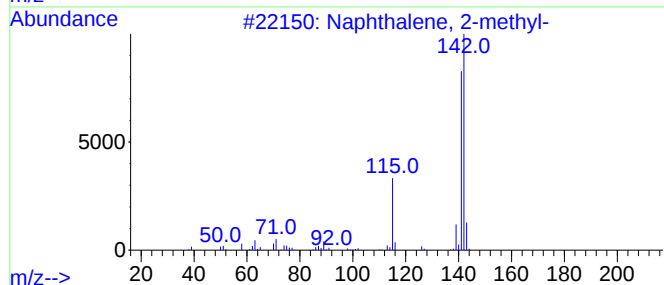
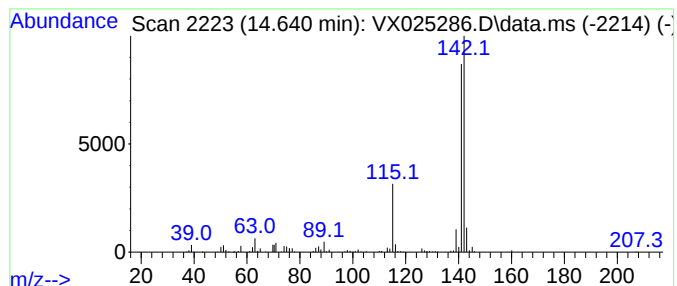
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	16.76 ug/l	144947	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			1H-Indole-4-carbonitrile	142	C9H6N2	016136-52-0	46



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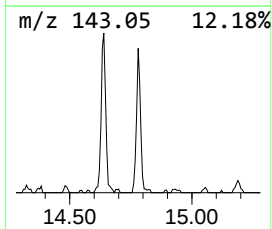
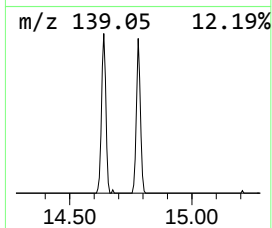
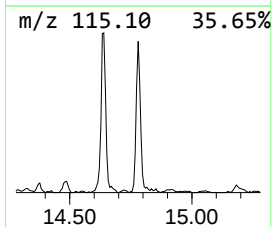
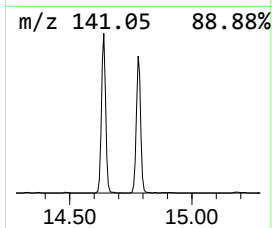
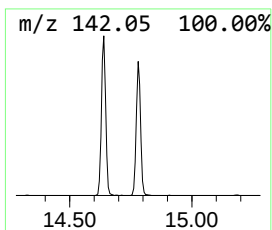
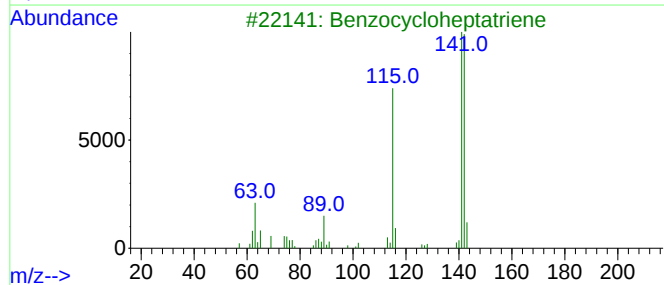
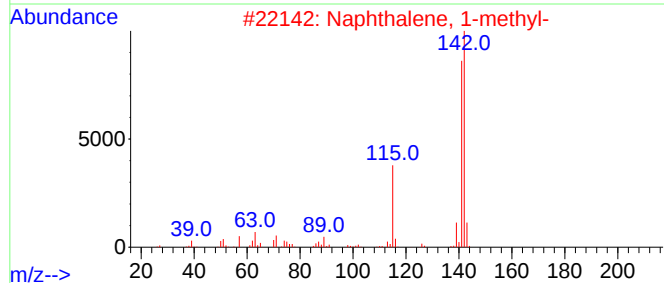
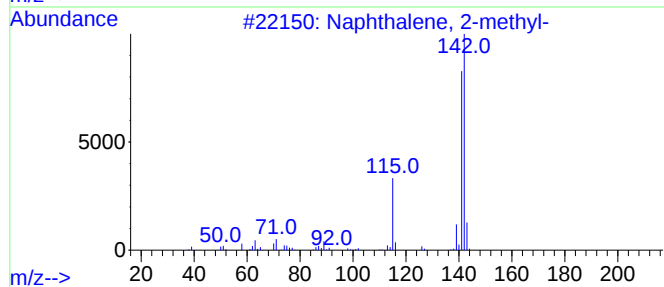
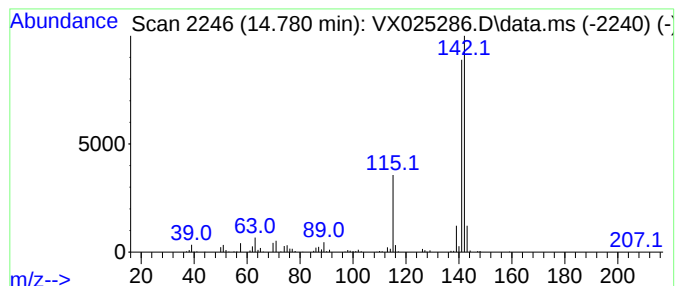
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	13.51 ug/l	116814	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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



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Instrument :
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ClientSampleId :
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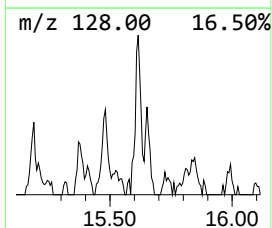
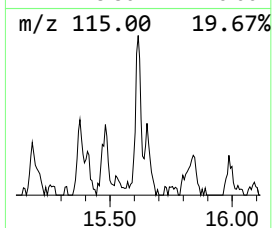
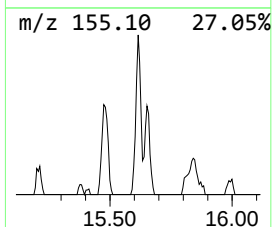
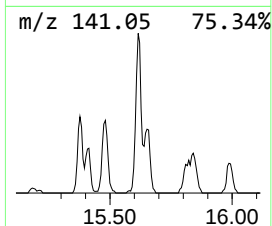
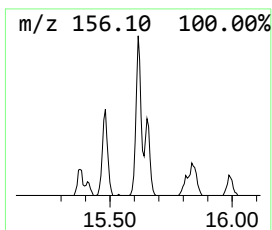
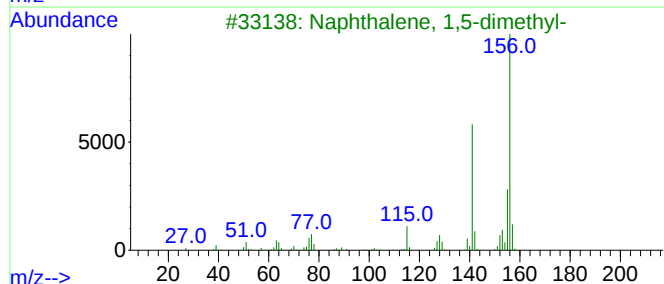
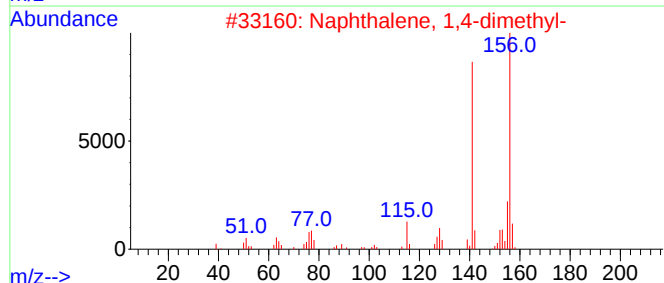
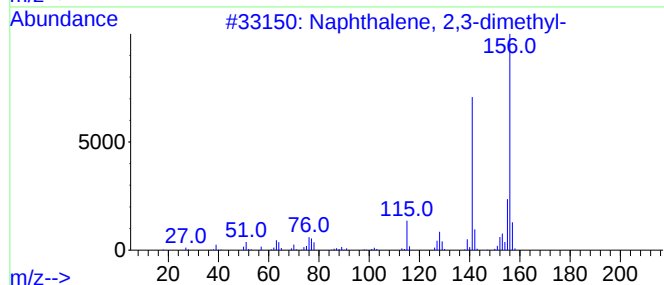
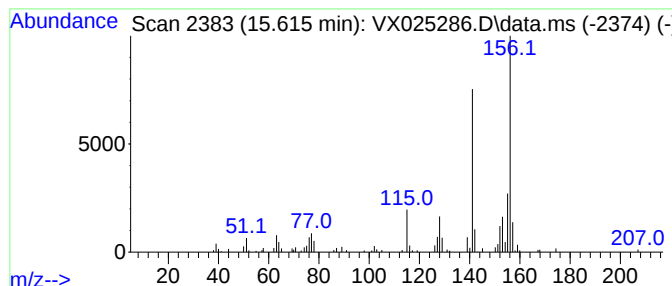
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	5.78 ug/l	49998	1,4-Dichlorobenzene-d4	12.024

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, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	95



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.532	6.4	ug/l	32857	1	5.556	257476	50.0
Naphthalene, 1-...	14.640	16.8	ug/l	144947	4	12.024	432314	50.0
Benzocyclohepta...	14.780	13.5	ug/l	116814	4	12.024	432314	50.0
Naphthalene, 2,...	15.615	5.8	ug/l	49998	4	12.024	432314	50.0