

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
 Data File : VN074312.D
 Acq On : 03 Sep 2022 02:16
 Operator : JC\MD
 Sample : N4355-08
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-16R

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_N\methods\82N090222W.M
 Title : SW846 8260

Signal : TIC: VN074312.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	49	65	70	rBV	402910	1391481	55.65%	7.050%
2	2.699	133	138	151	rVB3	141459	433708	17.35%	2.197%
3	3.457	261	267	275	rVB6	10961	26216	1.05%	0.133%
4	4.222	391	397	405	rBV2	20078	58286	2.33%	0.295%
5	5.275	567	576	578	rBV2	24851	46747	1.87%	0.237%
6	5.293	578	579	591	rVB	25464	34513	1.38%	0.175%
7	5.540	606	621	633	rBV3	102093	367362	14.69%	1.861%
8	6.410	763	769	779	rVB6	8080	25212	1.01%	0.128%
9	7.063	864	880	890	rVB7	13761	57584	2.30%	0.292%
10	7.263	902	914	925	rBV	38043	102710	4.11%	0.520%
11	7.951	1020	1031	1036	rBV	317856	761118	30.44%	3.856%
12	8.016	1036	1042	1055	rVB	528182	1210274	48.40%	6.132%
13	8.375	1092	1103	1114	rBV3	427949	1224683	48.98%	6.205%
14	8.904	1182	1193	1209	rBV	774510	1599207	63.96%	8.102%
15	9.110	1220	1228	1235	rBV3	14607	28935	1.16%	0.147%
16	10.380	1435	1444	1451	rBV	1143598	2056537	82.25%	10.419%
17	10.445	1451	1455	1465	rVB	39249	77486	3.10%	0.393%
18	10.545	1465	1472	1476	rBV	26335	46257	1.85%	0.234%
19	11.680	1658	1665	1676	rBV	1127657	2033781	81.34%	10.304%
20	11.786	1676	1683	1695	rVV2	88968	246731	9.87%	1.250%
21	11.892	1695	1701	1709	rVB	153489	302730	12.11%	1.534%
22	12.216	1750	1756	1763	rVB3	27713	46991	1.88%	0.238%
23	12.521	1802	1808	1813	rBV6	13241	26192	1.05%	0.133%
24	12.669	1822	1833	1844	rBV	957463	1789895	71.58%	9.068%
25	12.863	1861	1866	1870	rVB2	19305	33896	1.36%	0.172%
26	12.921	1870	1876	1879	rBV	40091	67180	2.69%	0.340%
27	12.998	1885	1889	1892	rBV4	19834	29632	1.19%	0.150%
28	13.098	1892	1906	1913	rBV4	98770	443202	17.73%	2.245%
29	13.304	1935	1941	1948	rBV	105106	169195	6.77%	0.857%
30	13.498	1958	1974	1987	rBV4	202434	883175	35.32%	4.475%
31	13.610	1987	1993	2015	rVB	1284055	2500413	100.00%	12.668%
32	13.816	2023	2028	2032	rBV3	42725	71936	2.88%	0.364%
33	14.021	2054	2063	2065	rBV6	28277	70871	2.83%	0.359%
34	14.104	2068	2077	2092	rVB8	66700	294950	11.80%	1.494%
35	14.268	2100	2105	2110	rVB5	15196	28034	1.12%	0.142%
36	14.445	2121	2135	2143	rBV6	36845	146783	5.87%	0.744%

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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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37	14.515	2143	2147	2151	rVB6	14887	26161	1.05%	0.133%
38	14.680	2166	2175	2177	rBV9	12599	33828	1.35%	0.171%
39	14.868	2200	2207	2213	rBV8	26089	62277	2.49%	0.316%
40	15.015	2226	2232	2238	rBV7	11922	33126	1.32%	0.168%
41	15.427	2290	2302	2310	rBV2	164550	358112	14.32%	1.814%
42	16.527	2481	2489	2501	rVB	128625	303241	12.13%	1.536%
43	16.733	2516	2524	2533	rVB2	78392	187094	7.48%	0.948%

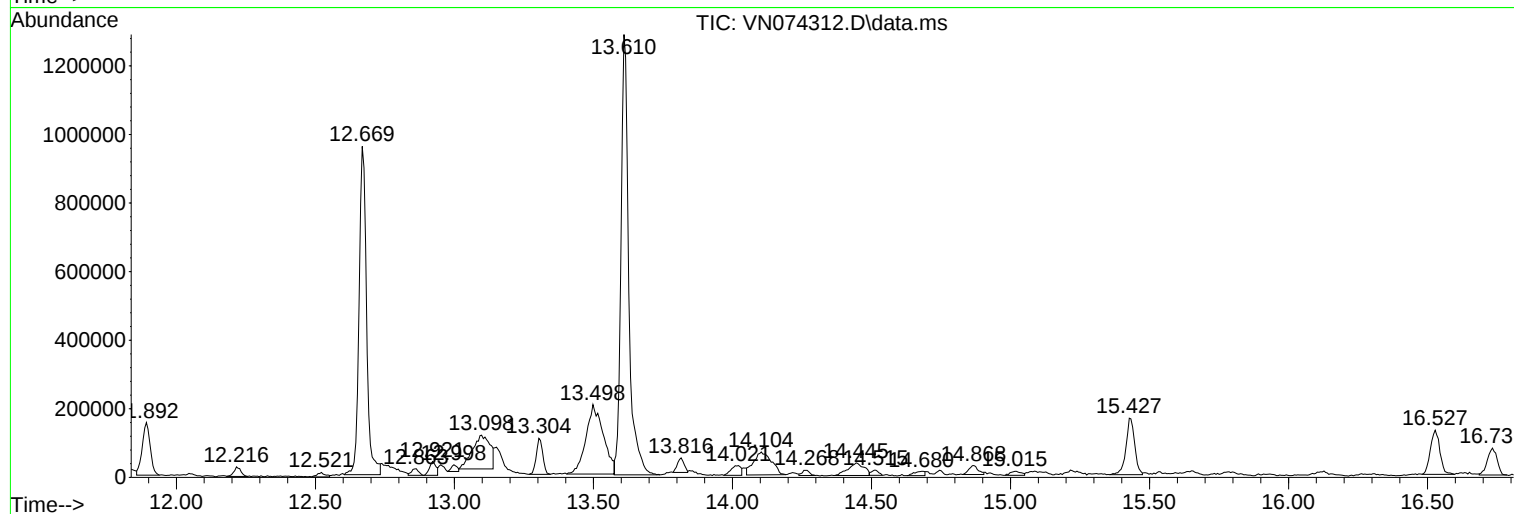
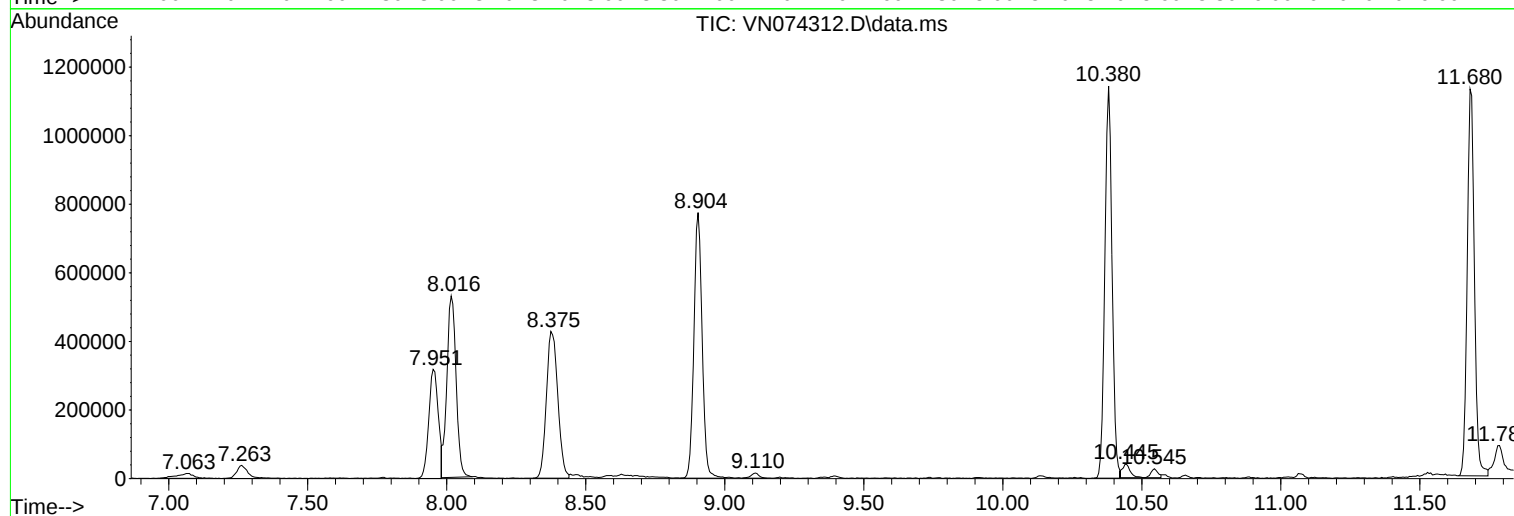
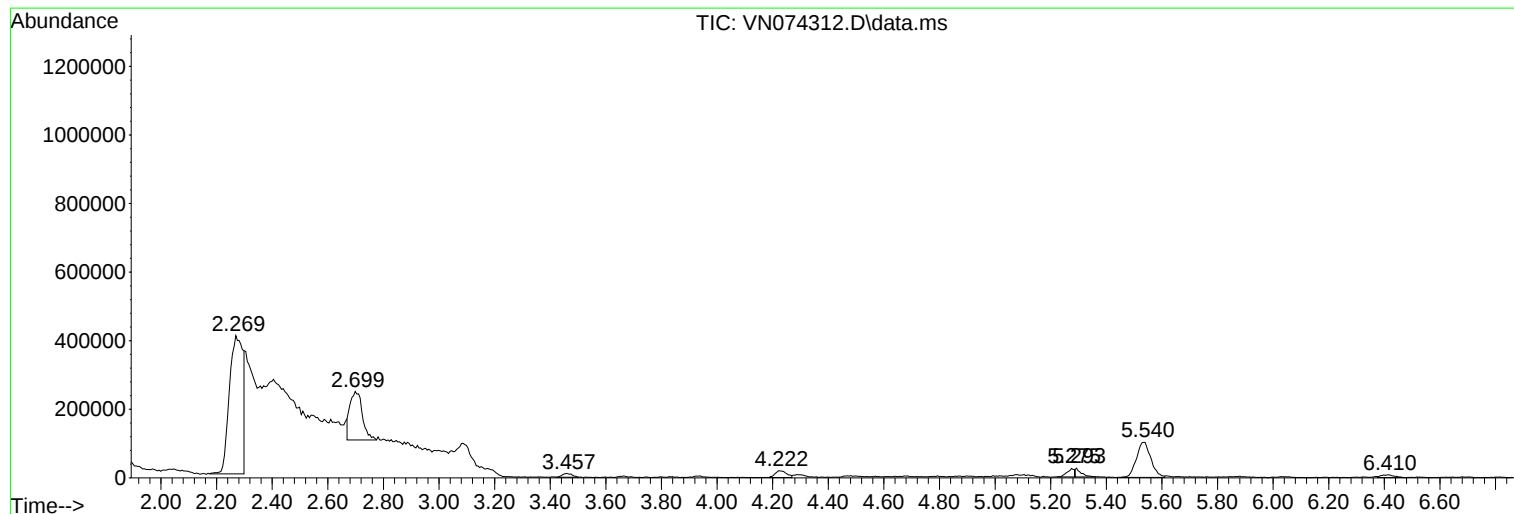
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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



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Instrument :
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MW-16R

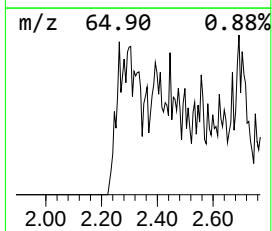
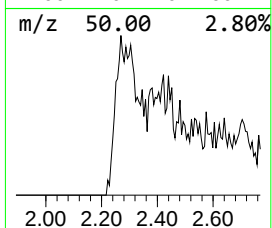
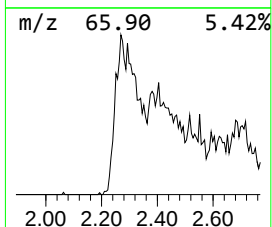
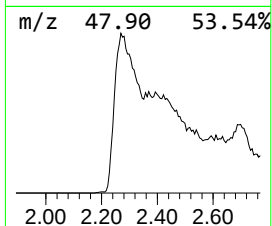
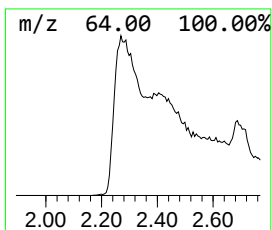
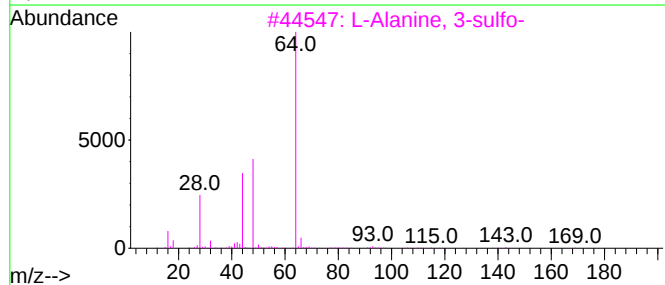
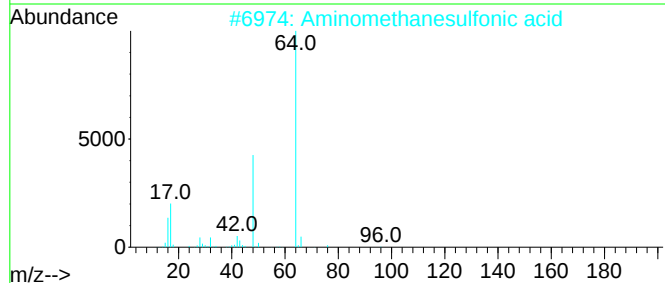
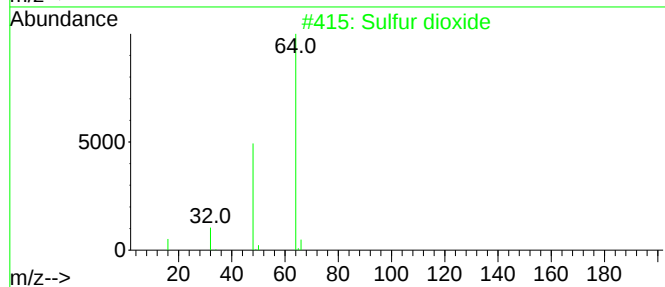
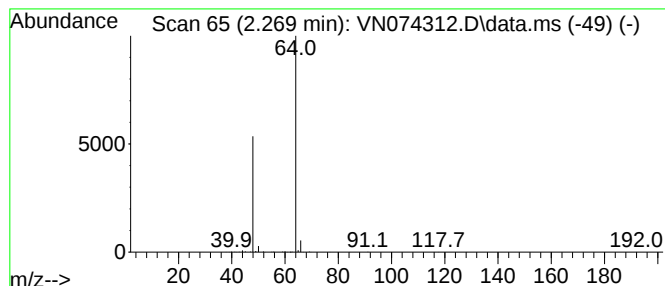
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	57.49 ug/l	1391480	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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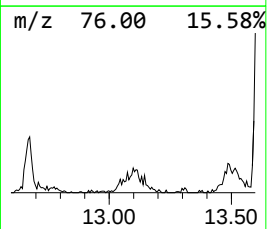
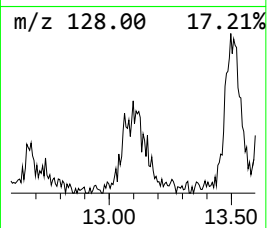
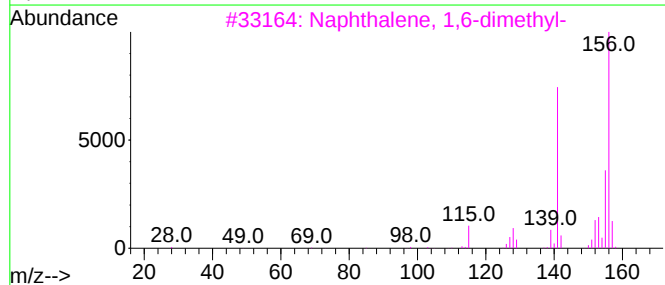
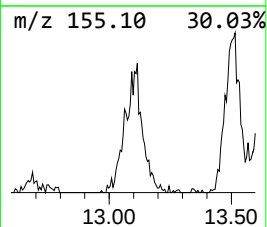
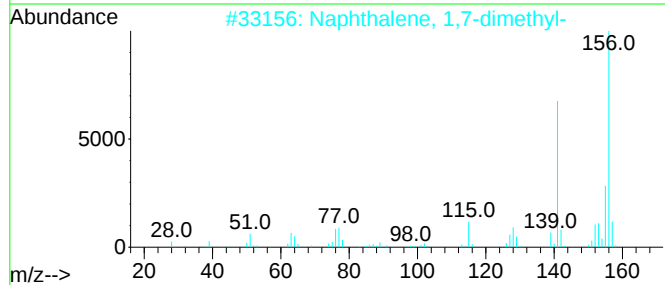
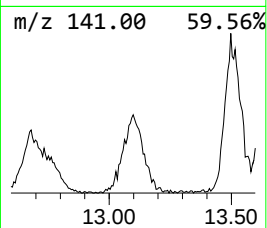
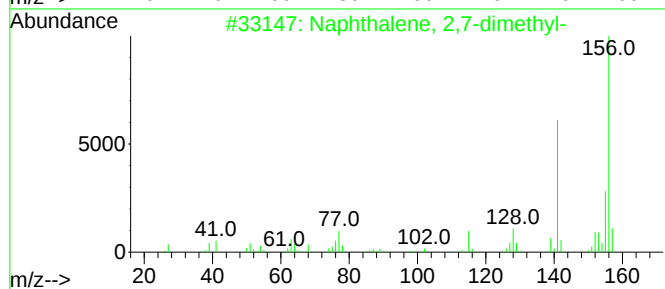
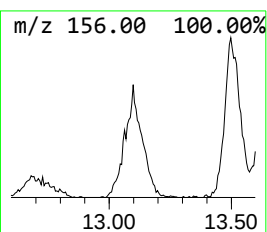
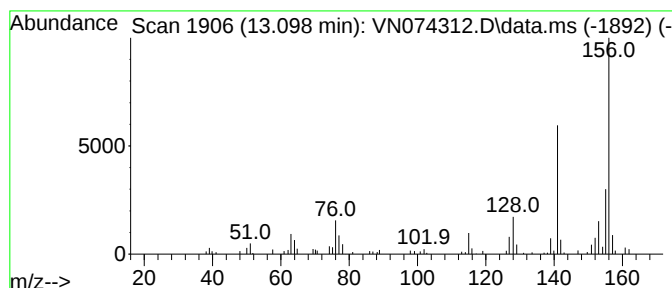
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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.
13.098	8.86 ug/l	443202	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	91
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91



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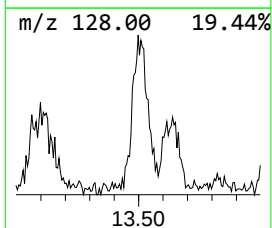
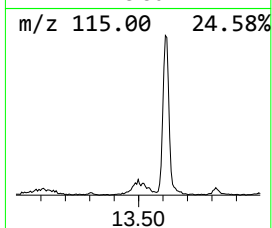
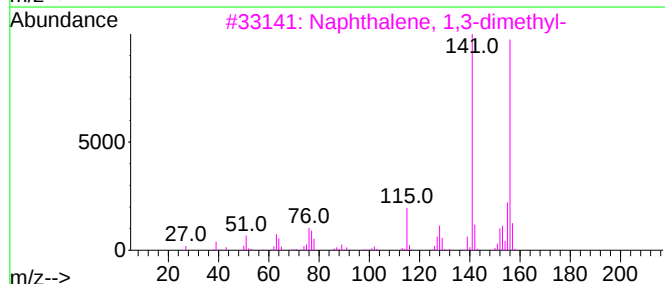
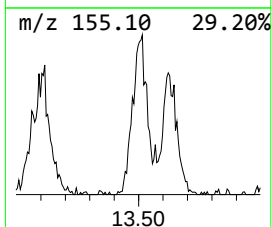
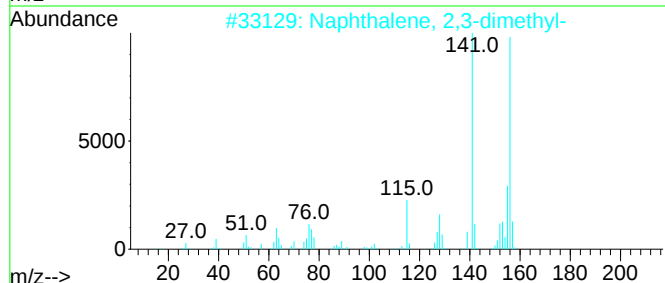
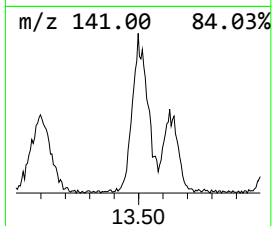
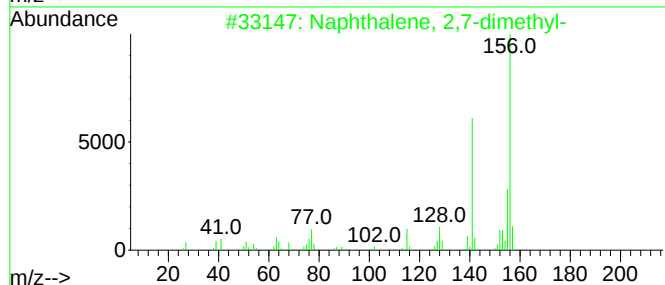
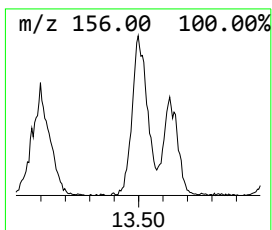
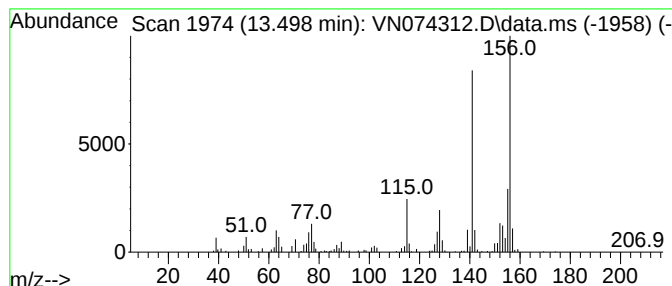
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	17.66 ug/l	883175	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96



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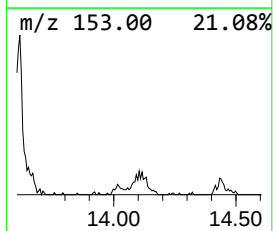
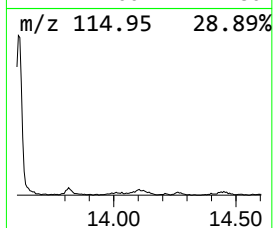
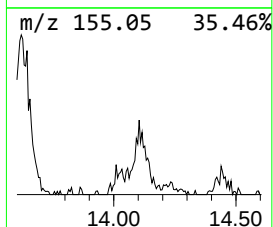
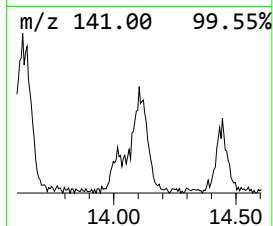
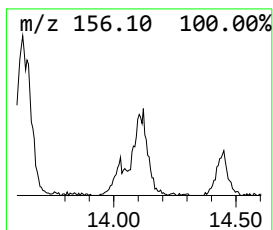
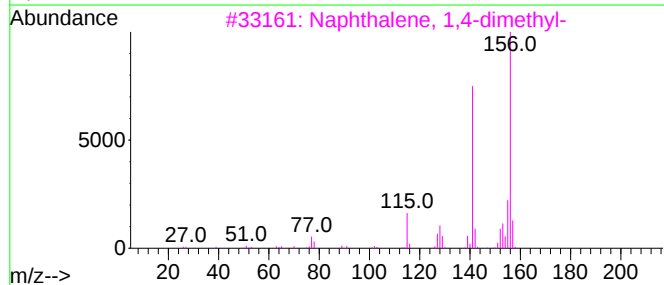
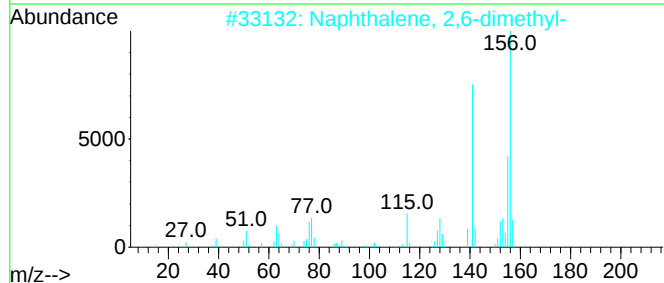
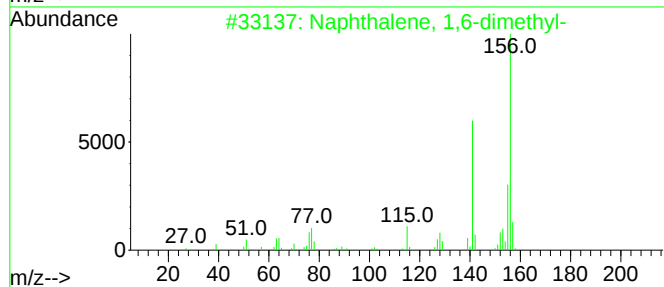
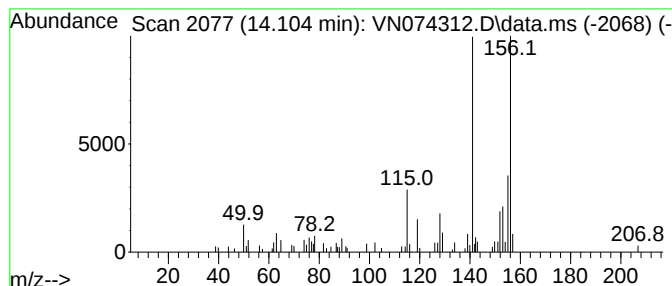
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	5.90 ug/l	294950	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	91
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	91
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	87
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	87
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	83



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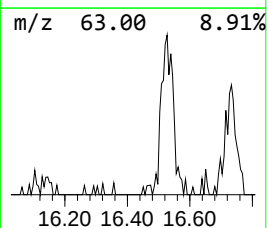
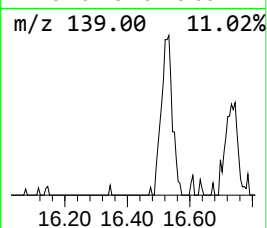
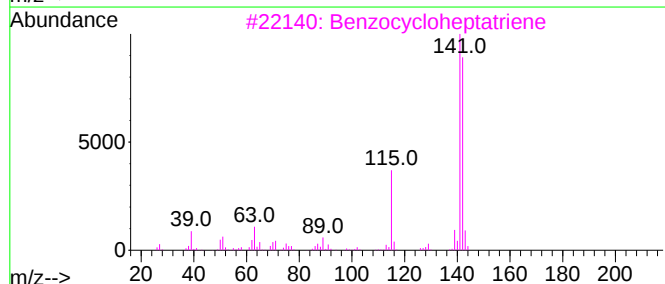
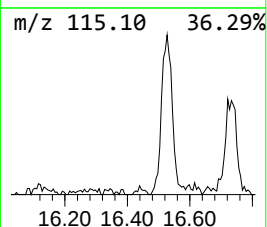
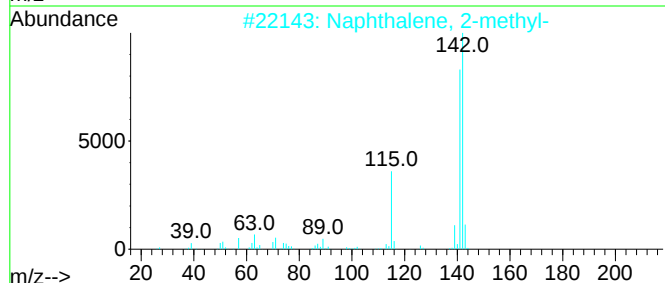
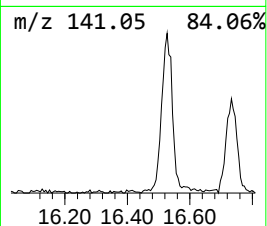
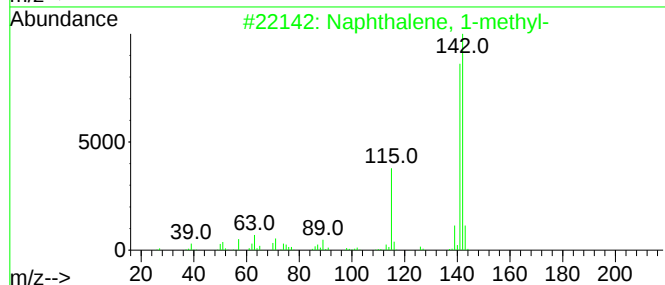
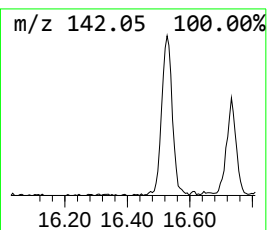
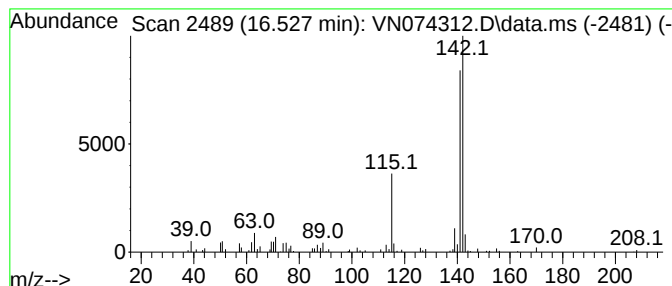
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	6.06 ug/l	303241	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
3			Benzocycloheptatriene	142	C11H10	000264-09-5	94
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87
5			Naphthalene, 1-[(2-propenyloxy)m...	198	C14H14O	074685-39-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074312.D
Acq On : 03 Sep 2022 02:16
Operator : JC\MD
Sample : N4355-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.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
Sulfur dioxide	2.269	57.5	ug/l	1391480	1	8.016	1210270	50.0
Naphthalene, 2,...	13.098	8.9	ug/l	443202	4	13.616	2500410	50.0
Naphthalene, 2,...	13.498	17.7	ug/l	883175	4	13.616	2500410	50.0
Naphthalene, 1,...	14.104	5.9	ug/l	294950	4	13.616	2500410	50.0
Benzocyclohepta...	16.527	6.1	ug/l	303241	4	13.616	2500410	50.0