

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121422\
 Data File : VN075801.D
 Acq On : 15 Dec 2022 05:39
 Operator : JC\MD
 Sample : N5990-10
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DUP120722-1

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\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN075801.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.301	35	42	59	rBV	77368	331784	18.69%	2.402%
2	2.818	126	130	140	rVB3	22831	60713	3.42%	0.439%
3	3.259	199	205	215	rVB3	20197	54111	3.05%	0.392%
4	5.530	579	591	607	rBV	67216	232650	13.10%	1.684%
5	5.812	624	639	654	rBV	261198	908544	51.17%	6.577%
6	6.677	777	786	798	rBV3	24453	83143	4.68%	0.602%
7	7.341	891	899	906	rBV7	9085	25201	1.42%	0.182%
8	8.171	1030	1040	1045	rBV	246304	602882	33.96%	4.364%
9	8.230	1045	1050	1062	rVB	496771	1108310	62.43%	8.023%
10	8.588	1101	1111	1121	rBV2	254174	664903	37.45%	4.813%
11	8.677	1121	1126	1136	rVB2	25636	59527	3.35%	0.431%
12	9.106	1190	1199	1209	rBV	647294	1314936	74.06%	9.519%
13	10.571	1439	1448	1462	rBV	968896	1775400	100.00%	12.852%
14	11.865	1660	1668	1678	rBV	820073	1491221	83.99%	10.795%
15	11.965	1679	1685	1695	rVV	98455	168715	9.50%	1.221%
16	12.076	1697	1704	1713	rVB3	76659	152883	8.61%	1.107%
17	12.400	1752	1759	1765	rBV	34132	55086	3.10%	0.399%
18	12.535	1770	1782	1783	rBV7	7975	19742	1.11%	0.143%
19	12.694	1803	1809	1825	rVB6	18425	58426	3.29%	0.423%
20	12.853	1827	1836	1845	rVB	654507	1109374	62.49%	8.031%
21	13.041	1860	1868	1873	rBV	26909	42705	2.41%	0.309%
22	13.100	1873	1878	1881	rVV	29766	48154	2.71%	0.349%
23	13.135	1881	1884	1888	rVV	29801	46342	2.61%	0.335%
24	13.176	1888	1891	1898	rVB	19808	29456	1.66%	0.213%
25	13.341	1909	1919	1924	rBV2	47916	122644	6.91%	0.888%
26	13.488	1938	1944	1951	rVB	110077	184701	10.40%	1.337%
27	13.694	1960	1979	1980	rBV3	59486	173012	9.74%	1.252%
28	13.794	1989	1996	2010	rVB	799869	1403119	79.03%	10.157%
29	14.035	2025	2037	2048	rVV4	131915	531002	29.91%	3.844%
30	14.153	2048	2057	2069	rVB5	50642	211351	11.90%	1.530%
31	14.335	2082	2088	2095	rVB2	21477	37432	2.11%	0.271%
32	14.447	2103	2107	2111	rBV4	11835	21069	1.19%	0.153%
33	14.506	2111	2117	2119	rVV4	12420	24332	1.37%	0.176%
34	14.576	2123	2129	2138	rVV5	32081	98527	5.55%	0.713%
35	14.659	2138	2143	2146	rVV2	15351	27578	1.55%	0.200%
36	14.694	2146	2149	2154	rVB2	15873	22944	1.29%	0.166%

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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_N\methods\82N121422W.M
Title : SW846 8260

37	14.882	2169	2181	2185	rBV8	13562	41928	2.36%	0.304%
38	14.929	2185	2189	2202	rVB3	16401	31785	1.79%	0.230%
39	15.053	2202	2210	2217	rBV4	29382	69888	3.94%	0.506%
40	15.641	2303	2310	2324	rVV	180919	368981	20.78%	2.671%

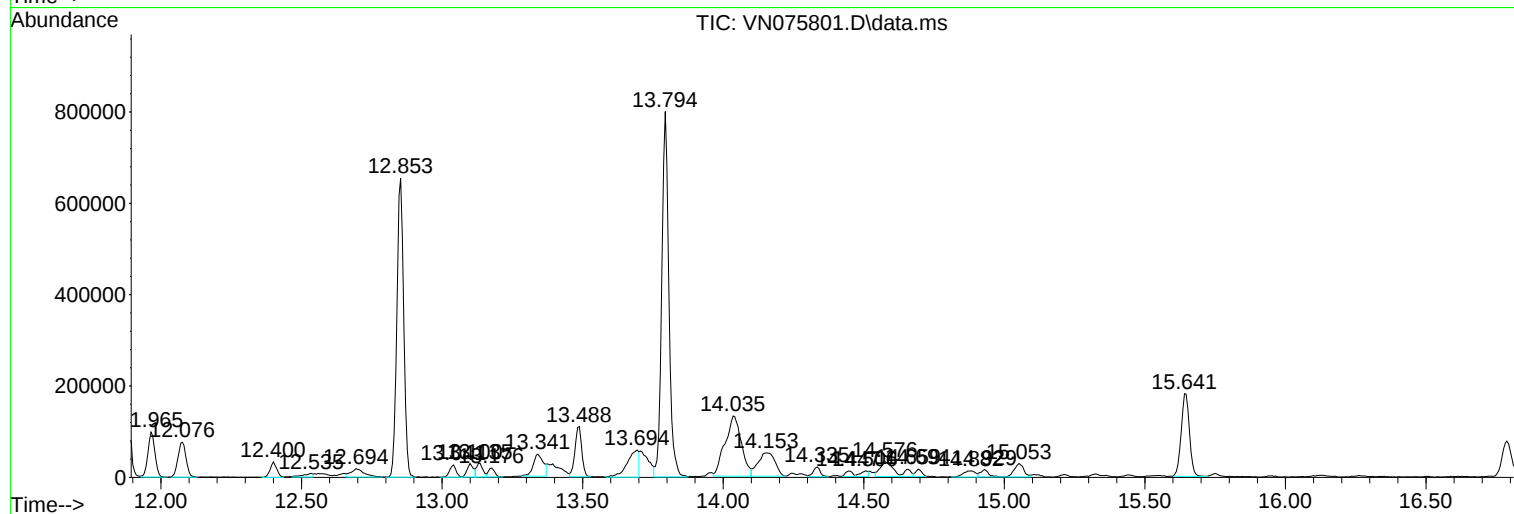
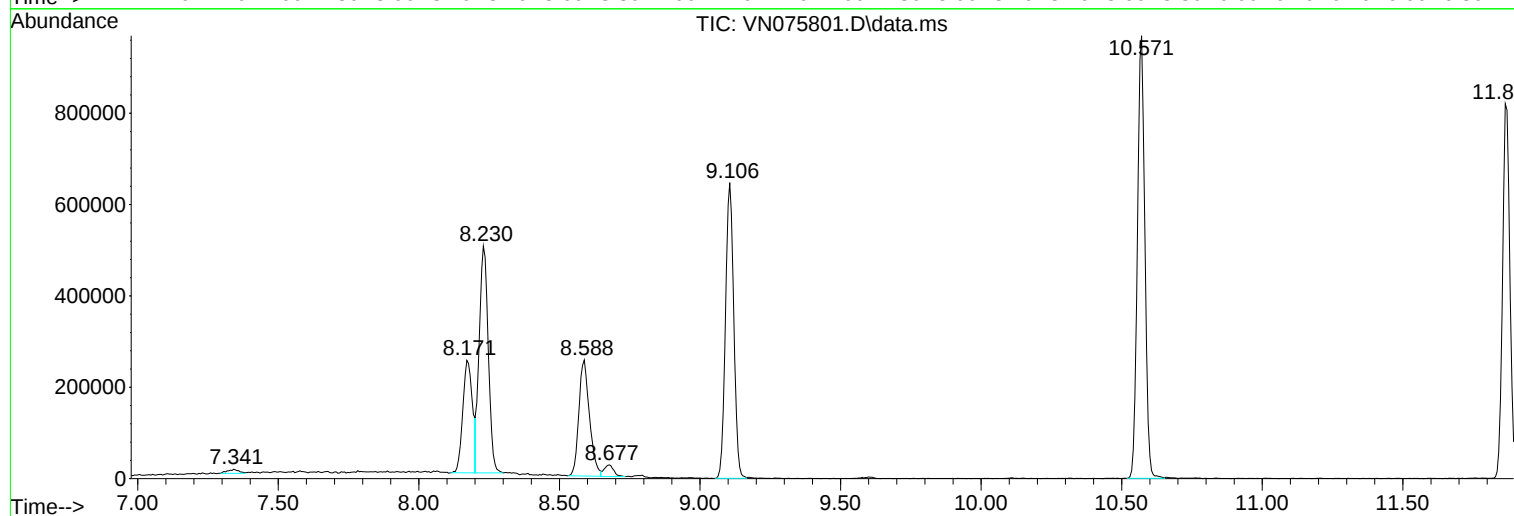
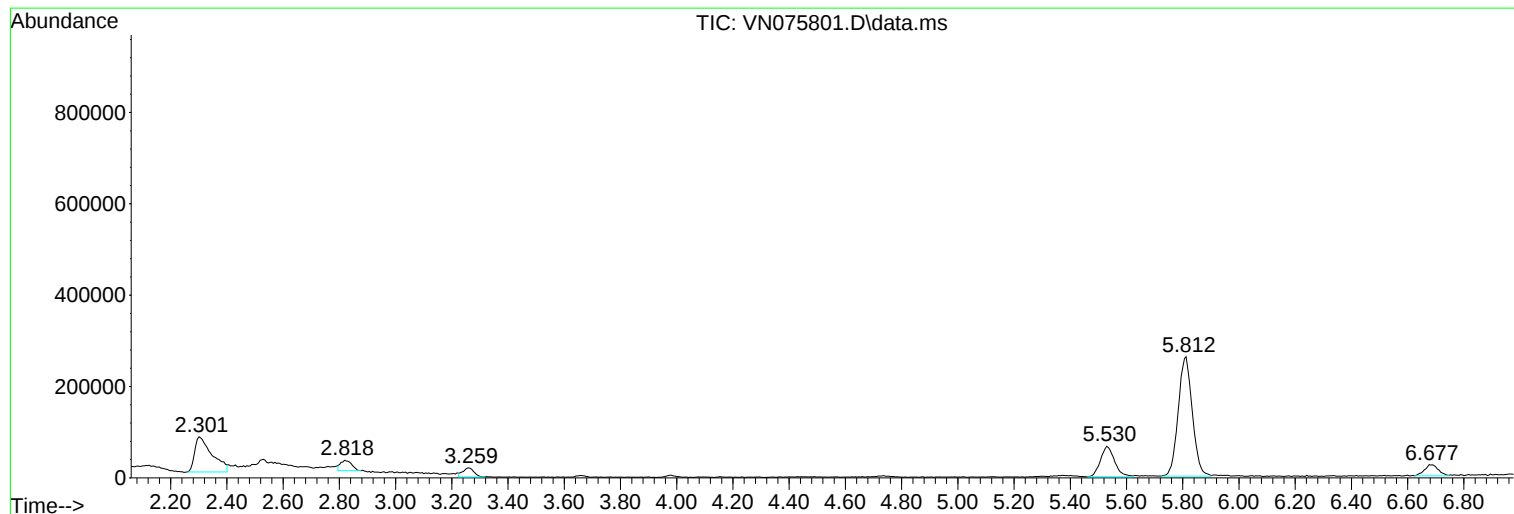
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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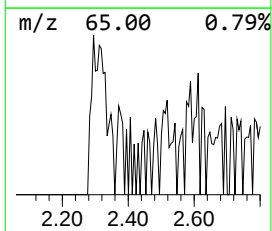
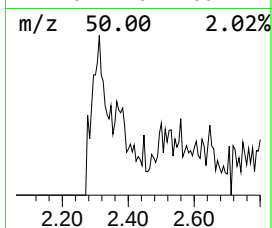
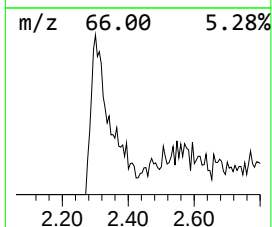
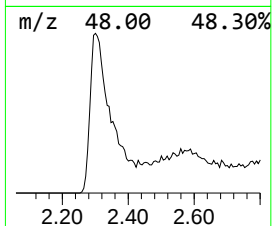
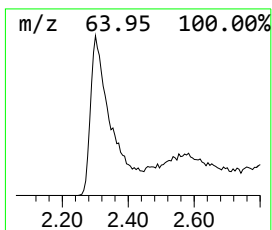
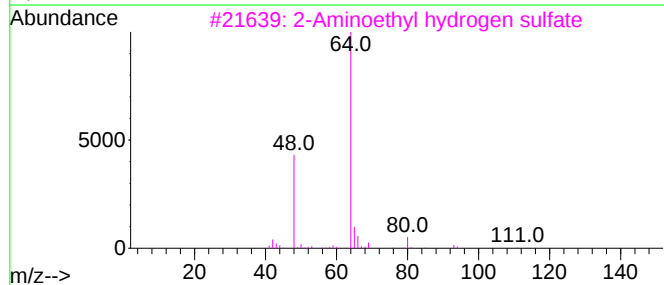
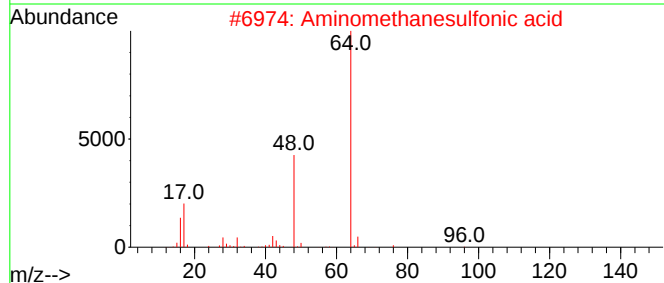
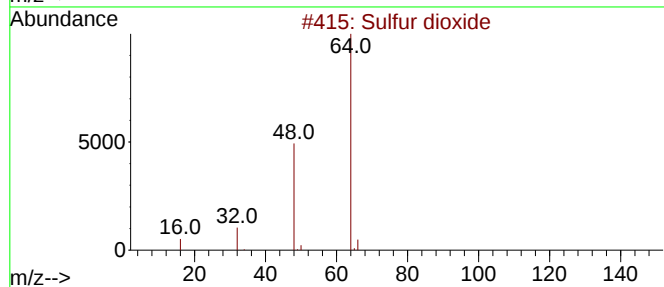
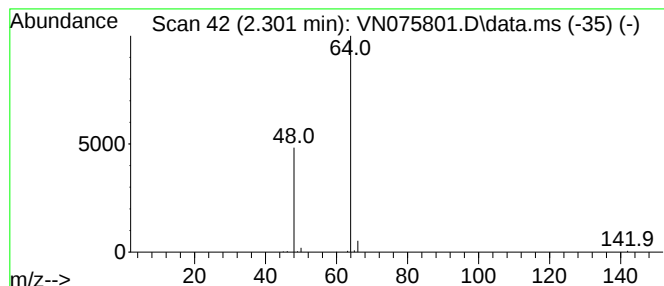
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.301	14.97 ug/l	331784	Pentafluorobenzene	8.230

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			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			1,1,1,2,2,3,3,4,4,5,5-Undecafluoro...	602	C10F22O2S	1000486-78-5	64
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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DUP120722-1

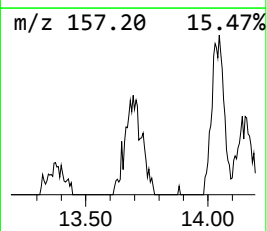
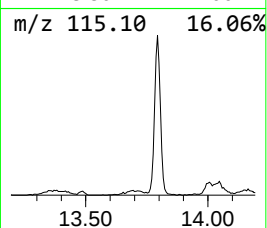
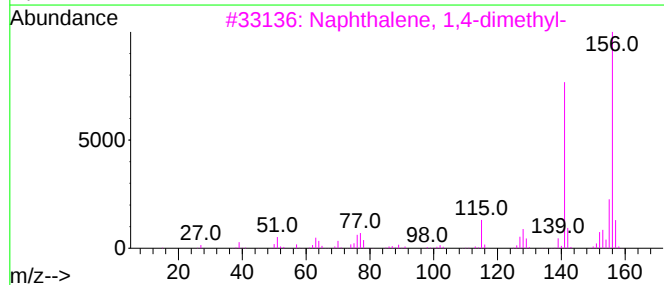
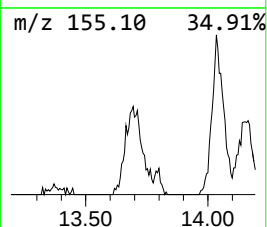
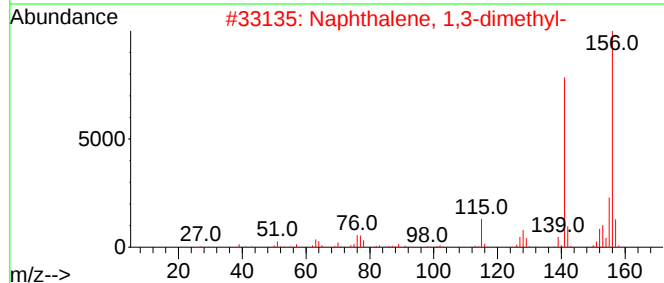
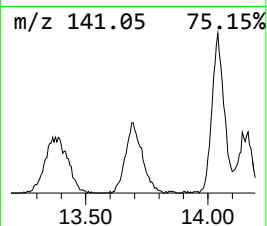
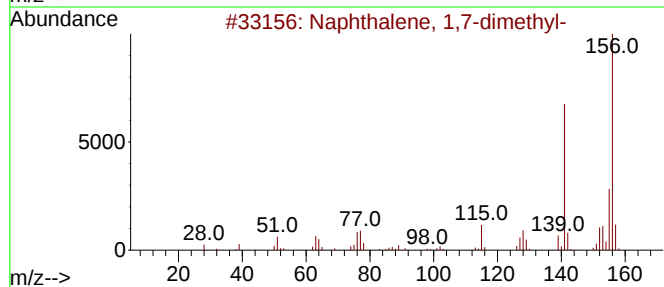
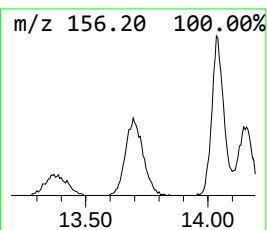
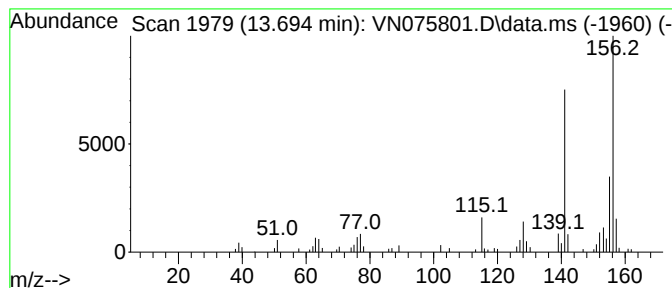
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 1,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.694	6.17 ug/l	173012	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96



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ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUP120722-1

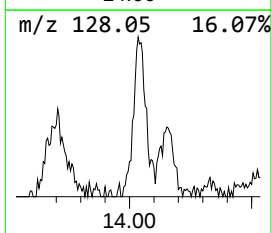
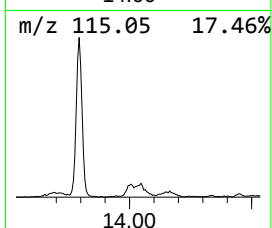
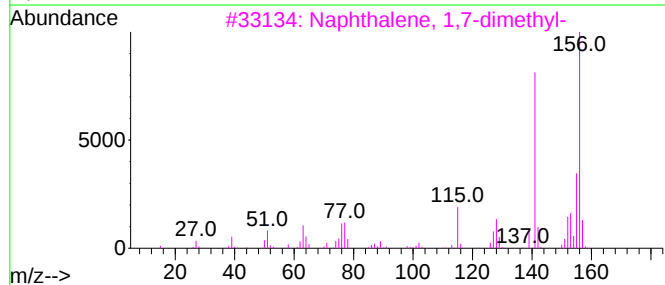
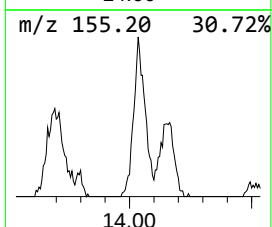
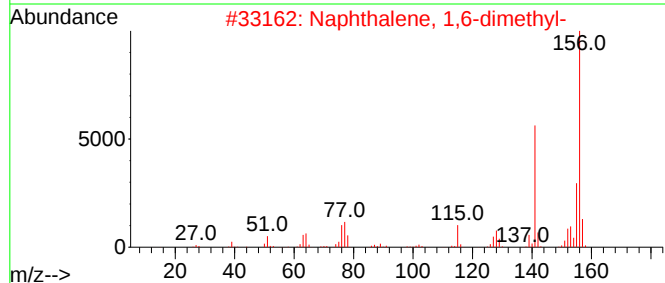
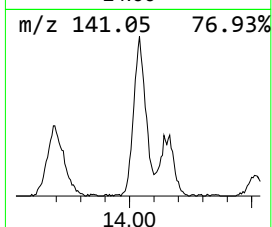
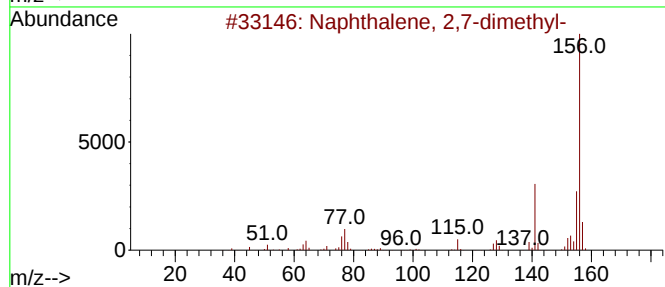
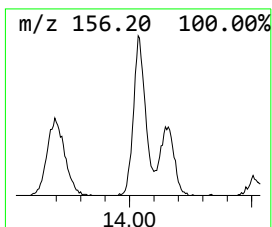
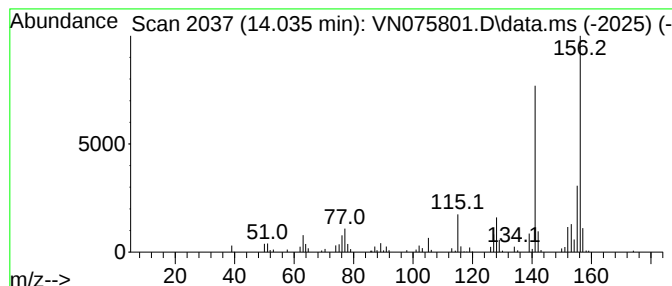
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 2,7-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.035	18.92 ug/l	531002	1,4-Dichlorobenzene-d4	13.794

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, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95



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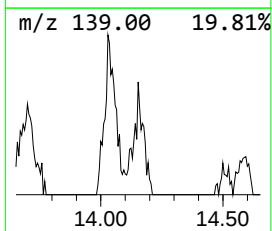
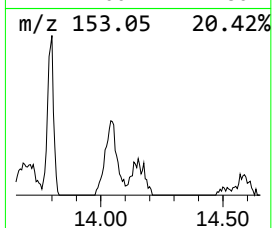
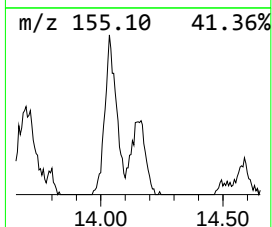
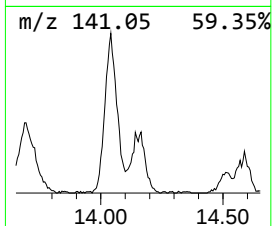
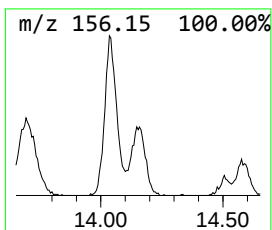
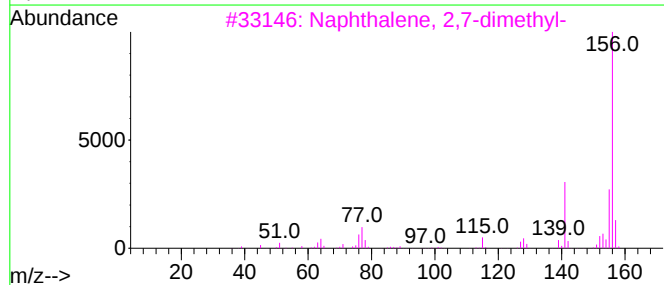
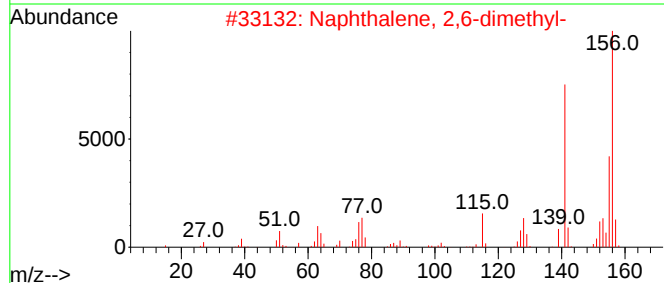
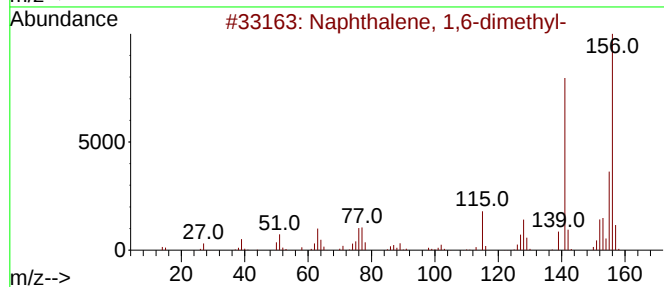
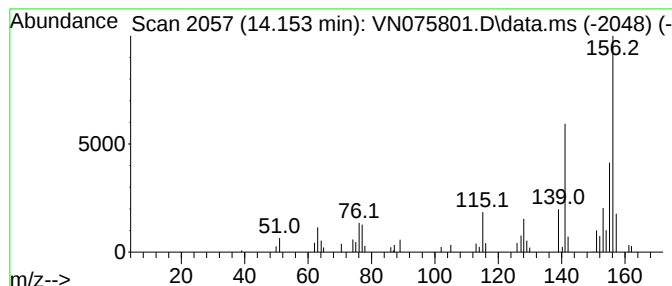
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.153	7.53 ug/l	211351	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	91
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	87
5			1,4-Dimethylazulene	156	C12H12	001127-69-1	83



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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	2.301	15.0	ug/l	331784	1	8.230	1108310	50.0
Naphthalene, 1,...	13.694	6.2	ug/l	173012	4	13.794	1403120	50.0
Naphthalene, 2,...	14.035	18.9	ug/l	531002	4	13.794	1403120	50.0
Naphthalene, 1,...	14.153	7.5	ug/l	211351	4	13.794	1403120	50.0