

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
 Data File : VN075353.D
 Acq On : 21 Nov 2022 19:53
 Operator : JC\MD
 Sample : N5665-01 40X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COSTAL-DRUM-2DL

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\82N112122W.M

Title : SW846 8260

Signal : TIC: VN075353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.307	36	43	52	rBV2	17711	43930	2.21%	0.273%
2	2.495	69	75	82	rBV2	28120	67851	3.41%	0.422%
3	2.824	124	131	136	rBV4	11159	31253	1.57%	0.194%
4	4.442	396	406	415	rBV	14485	45428	2.28%	0.282%
5	5.530	579	591	607	rBV2	36871	135531	6.81%	0.842%
6	5.806	626	638	653	rVB2	55267	195946	9.84%	1.218%
7	6.689	775	788	807	rBV3	269076	907789	45.59%	5.641%
8	7.230	871	880	890	rBV3	32844	92540	4.65%	0.575%
9	7.347	890	900	910	rVV	58984	156921	7.88%	0.975%
10	8.171	1031	1040	1044	rBV	78922	183228	9.20%	1.138%
11	8.230	1044	1050	1060	rVB	209892	472225	23.72%	2.934%
12	8.612	1104	1115	1124	rVB2	305491	784953	39.42%	4.877%
13	8.818	1137	1150	1158	rBV5	25102	63934	3.21%	0.397%
14	9.106	1191	1199	1207	rBV	286238	582709	29.27%	3.621%
15	9.271	1219	1227	1237	rBV	50708	111320	5.59%	0.692%
16	9.371	1237	1244	1256	rVB2	49588	104324	5.24%	0.648%
17	9.653	1286	1292	1301	rVB5	13878	31616	1.59%	0.196%
18	9.747	1301	1308	1311	rVV	14857	29282	1.47%	0.182%
19	9.794	1311	1316	1325	rVB	57065	117436	5.90%	0.730%
20	9.883	1325	1331	1341	rVB4	19818	41477	2.08%	0.258%
21	10.288	1395	1400	1407	rVB3	15281	25709	1.29%	0.160%
22	10.565	1439	1447	1452	rBV	184897	358347	18.00%	2.227%
23	10.630	1452	1458	1471	rVV	1079040	1991024	100.00%	12.371%
24	10.730	1471	1475	1484	rVB6	11920	28086	1.41%	0.175%
25	10.959	1502	1514	1516	rBV	26605	53163	2.67%	0.330%
26	10.988	1516	1519	1526	rVV2	34084	59285	2.98%	0.368%
27	11.347	1574	1580	1589	rVB	119664	225848	11.34%	1.403%
28	11.541	1604	1613	1620	rBV	187065	332809	16.72%	2.068%
29	11.824	1655	1661	1662	rBV3	21438	32414	1.63%	0.201%
30	11.865	1662	1668	1678	rVB	408334	721862	36.26%	4.485%
31	11.965	1678	1685	1692	rVB	195333	331333	16.64%	2.059%
32	12.065	1692	1702	1713	rBV	933137	1732498	87.02%	10.765%
33	12.188	1715	1723	1737	rBV	151214	290163	14.57%	1.803%
34	12.400	1751	1759	1765	rBV	372703	654849	32.89%	4.069%
35	12.512	1770	1778	1798	rVV	173047	453058	22.76%	2.815%
36	12.659	1798	1803	1806	rVV6	9616	20140	1.01%	0.125%

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37	12.694	1806	1809	1816	rVB2	19499	29471	1.48%	0.183%
38	12.847	1826	1835	1846	rVB2	305366	618012	31.04%	3.840%
39	12.947	1846	1852	1857	rBV3	42345	80500	4.04%	0.500%
40	13.100	1872	1878	1886	rBV2	44936	119256	5.99%	0.741%
41	13.177	1886	1891	1895	rVB	30161	46784	2.35%	0.291%
42	13.259	1895	1905	1911	rBV10	10864	34808	1.75%	0.216%
43	13.335	1912	1918	1925	rBV	237712	387986	19.49%	2.411%
44	13.482	1939	1943	1948	rVB	38752	56352	2.83%	0.350%
45	13.688	1957	1978	1988	rBV3	137163	516772	25.96%	3.211%
46	13.794	1989	1996	2005	rVV	431691	813399	40.85%	5.054%
47	14.035	2025	2037	2046	rBV	155469	522858	26.26%	3.249%
48	14.171	2047	2060	2067	rVV3	301414	722938	36.31%	4.492%
49	14.329	2082	2087	2095	rVB9	8583	22616	1.14%	0.141%
50	14.494	2109	2115	2121	rBV5	23267	64612	3.25%	0.401%
51	14.600	2121	2133	2140	rVB6	58902	208499	10.47%	1.296%
52	14.765	2154	2161	2167	rBV2	64203	105986	5.32%	0.659%
53	14.871	2170	2179	2198	rVB4	27843	104074	5.23%	0.647%
54	15.100	2214	2218	2228	rVB7	7224	21757	1.09%	0.135%
55	15.518	2287	2289	2302	rVB4	6786	21226	1.07%	0.132%
56	15.641	2302	2310	2324	rBV4	16865	55741	2.80%	0.346%
57	16.482	2445	2453	2462	rBV3	12569	29937	1.50%	0.186%

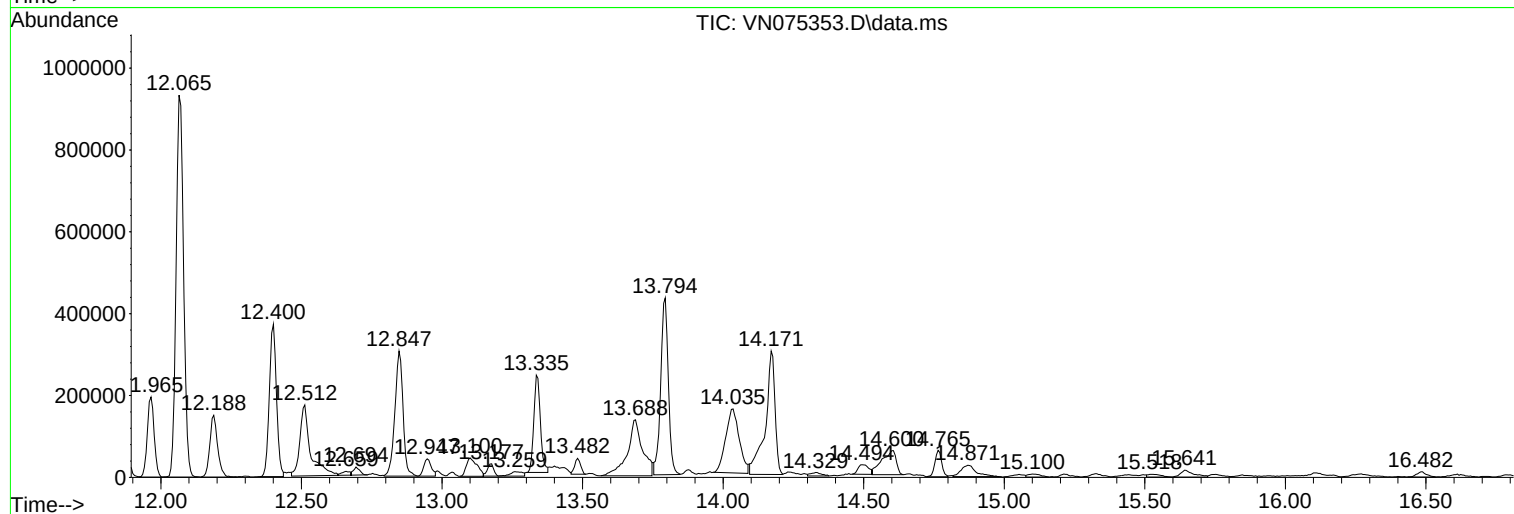
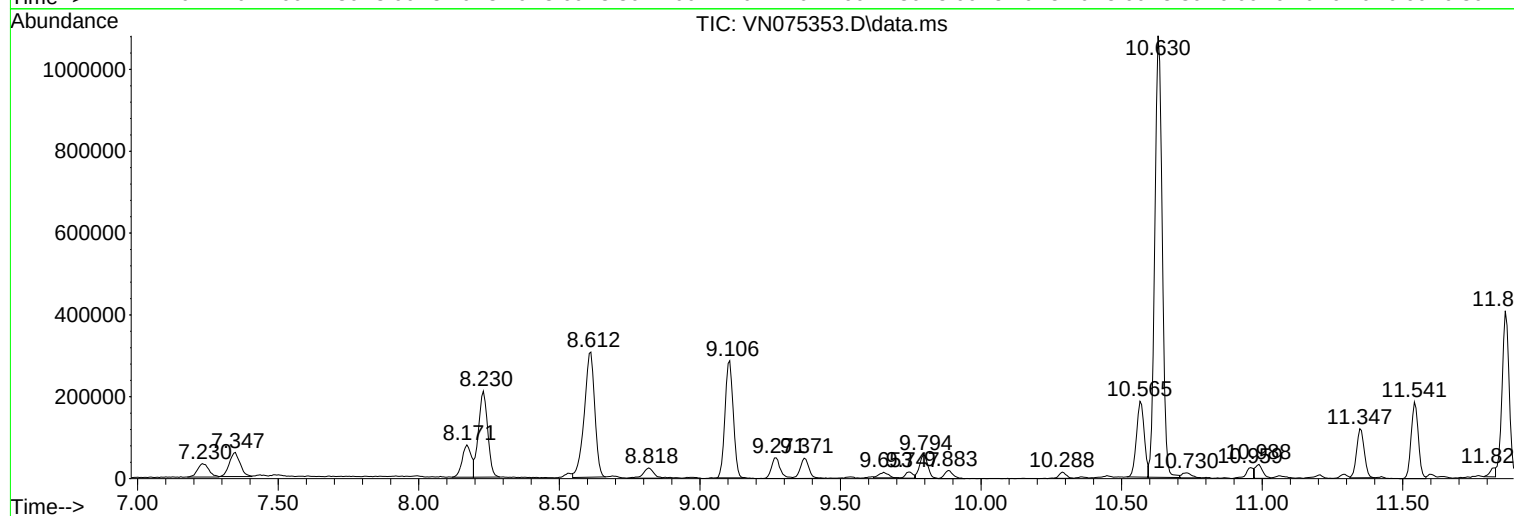
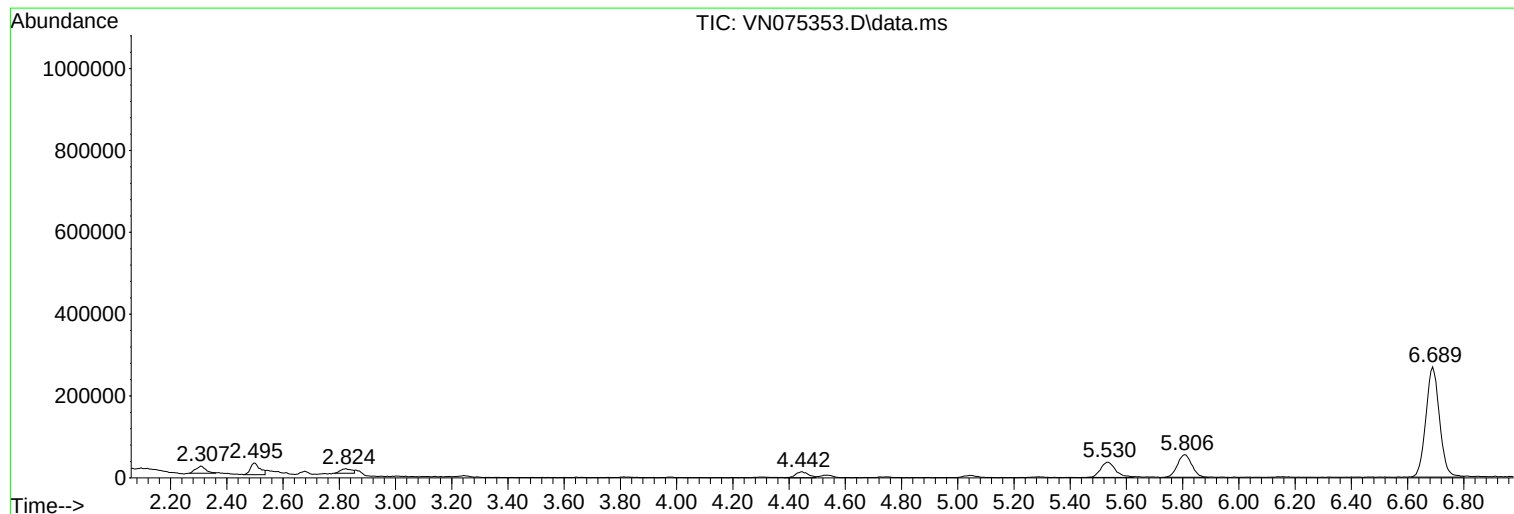
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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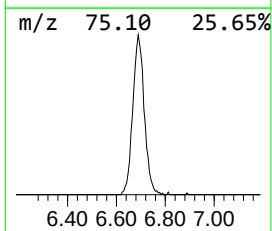
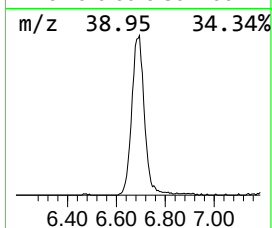
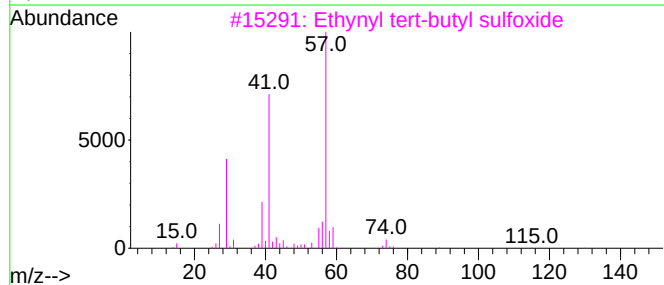
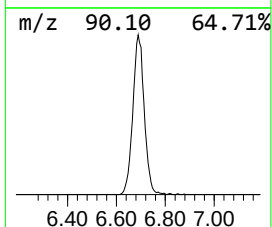
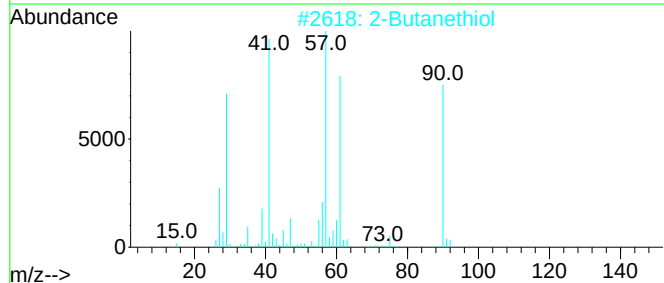
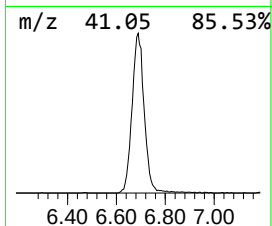
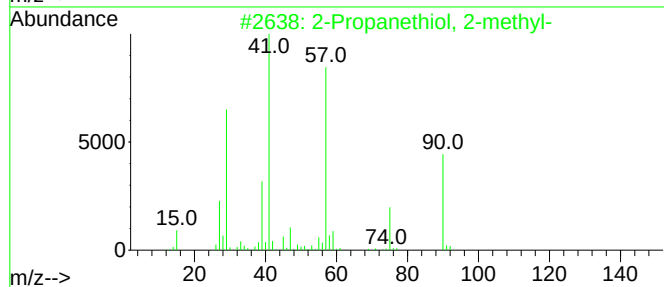
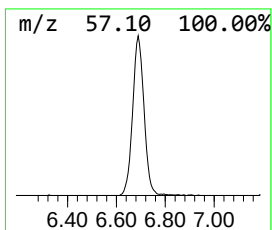
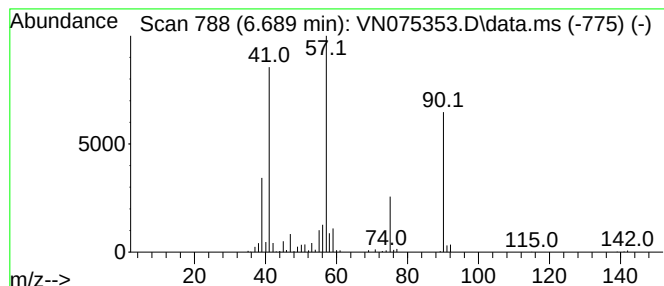
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.689	96.12 ug/l	907789	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-			90	C4H10S	000075-66-1	90
2	2-Butanethiol			90	C4H10S	000513-53-1	47
3	Ethynyl tert-butyl sulfoxide			130	C6H10OS	041463-34-7	25
4	Propane, 2-methyl-2-nitro-			103	C4H9NO2	000594-70-7	22
5	Propane, 2-bromo-2-methyl-			136	C4H9Br	000507-19-7	12



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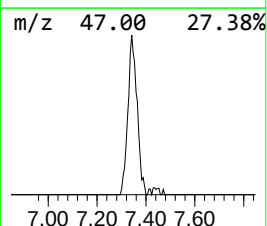
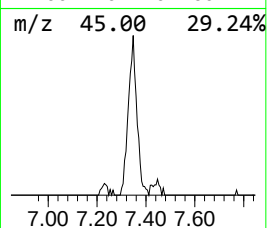
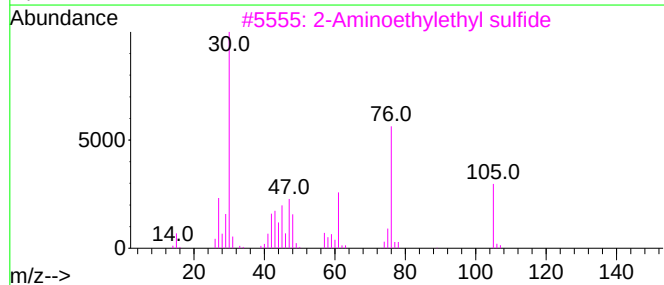
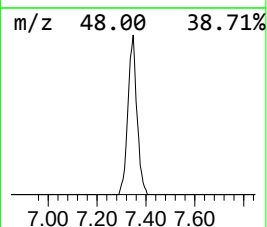
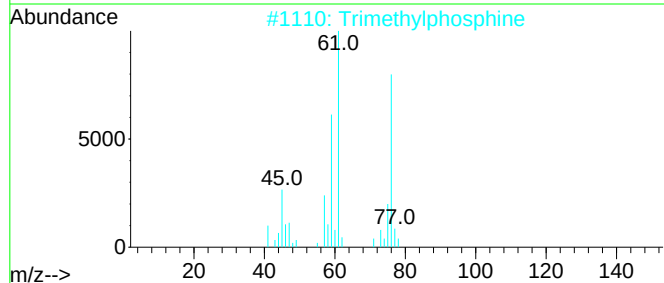
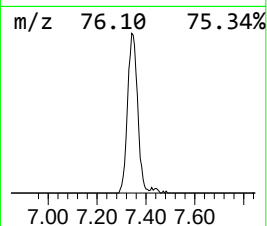
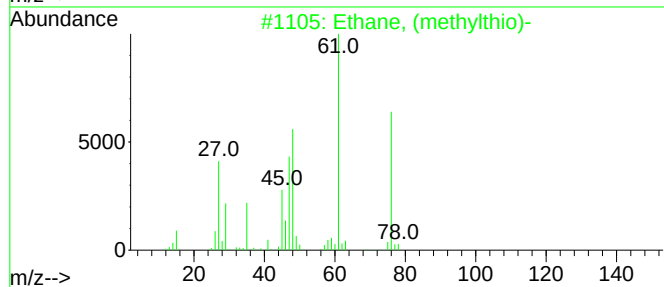
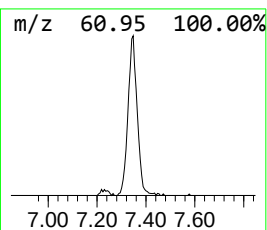
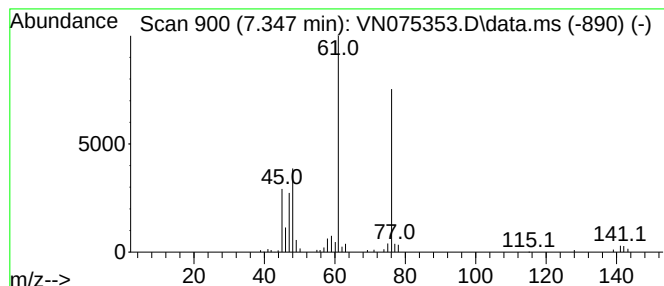
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethane, (methylthio)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.347	16.62 ug/l	156921	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, (methylthio)-	76	C3H8S	000624-89-5	91
2			Trimethylphosphine	76	C3H9P	000594-09-2	72
3			2-Aminoethylethyl sulfide	105	C4H11NS	036489-03-9	50
4			Monomethyl carbonotriithioate	124	C2H4S3	001113-26-4	38
5			Propane, 1-(ethenylsulfanyl)-	118	C5H10S	061926-31-6	36



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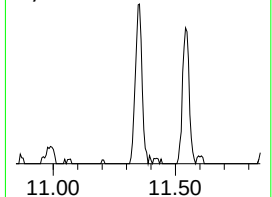
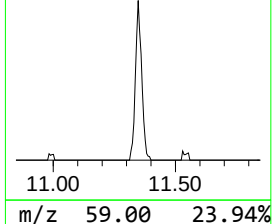
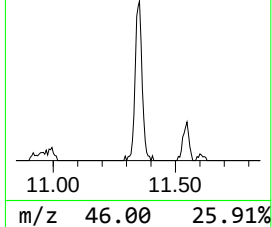
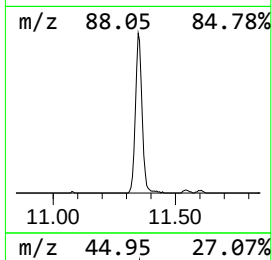
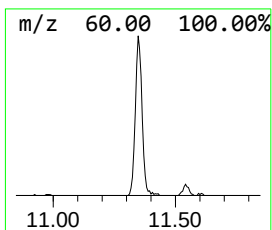
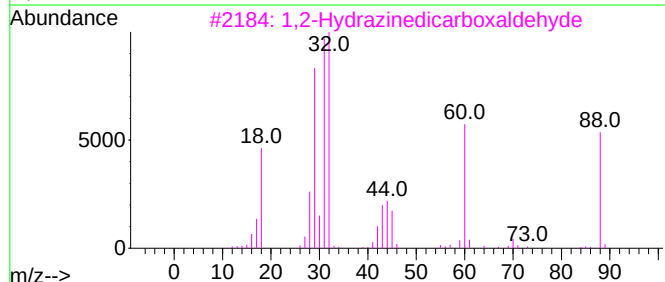
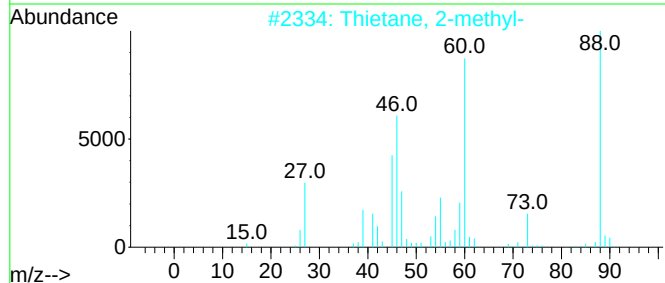
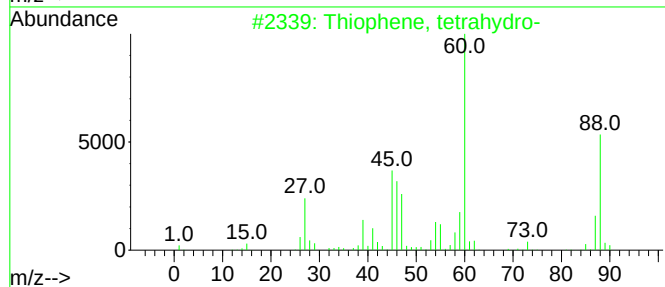
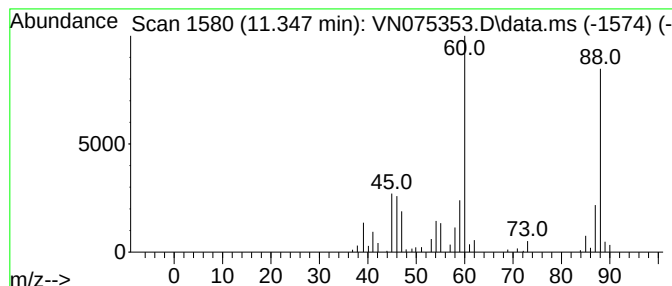
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Thiophene, tetrahydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.347	15.64 ug/l	225848	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	93
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	81
3			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
4			Sulfide, allyl methyl	88	C4H8S	010152-76-8	32
5			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	28



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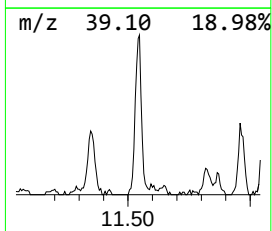
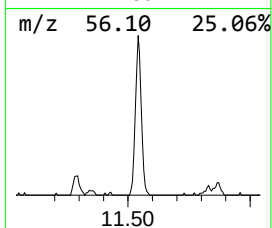
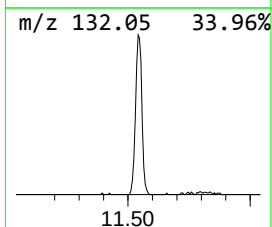
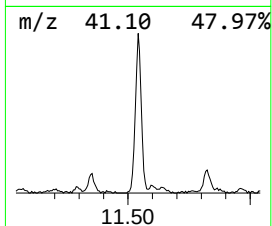
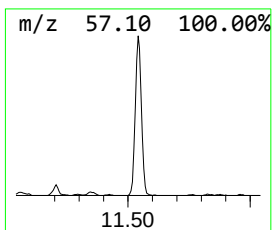
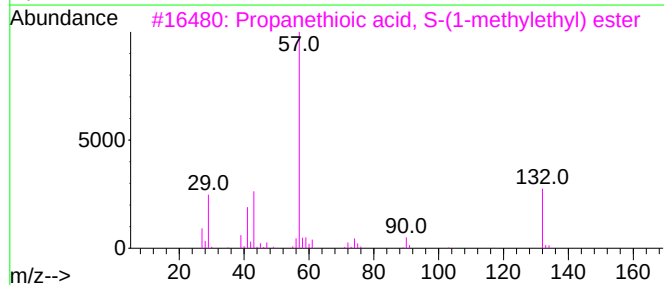
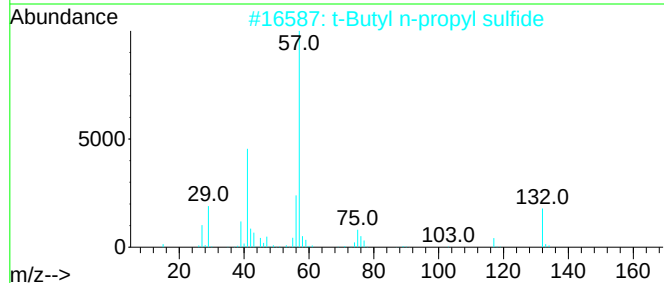
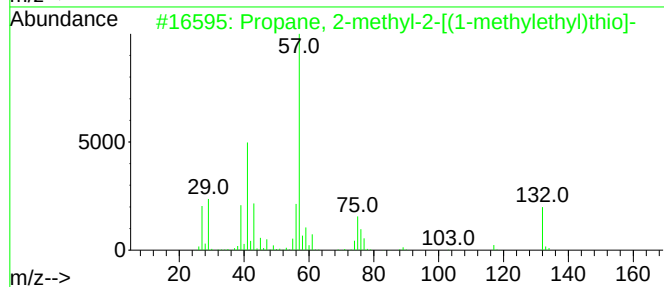
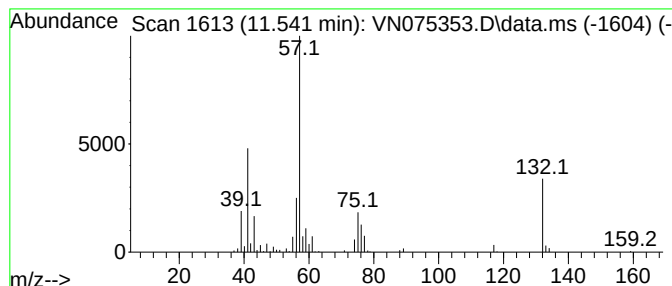
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Quant Title : SW846 8260

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

Peak Number 4 Propane, 2-methyl-2-[(1-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.541	23.05 ug/l	332809	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-[(1-methylet...	132	C7H16S	044657-76-3	91
2	t-Butyl n-propyl sulfide	132	C7H16S	1000343-63-5	64
3	Propanethioic acid, S-(1-methyle...	132	C6H12OS	002432-47-5	49
4	Phosphine, (1,1-dimethylethyl)(1...	132	C7H17P	060058-18-6	37
5	Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	25



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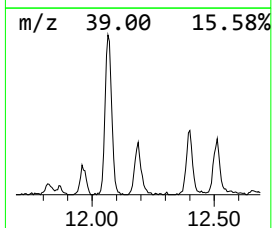
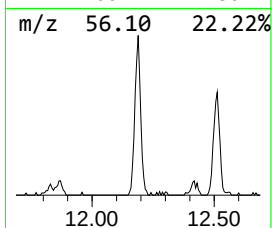
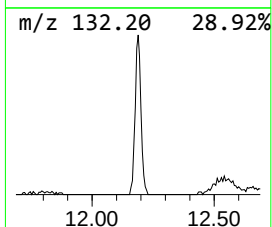
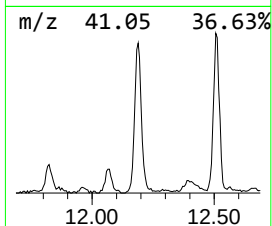
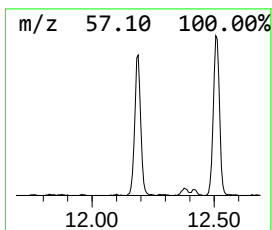
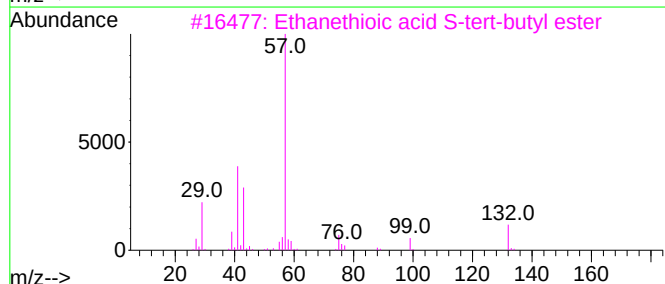
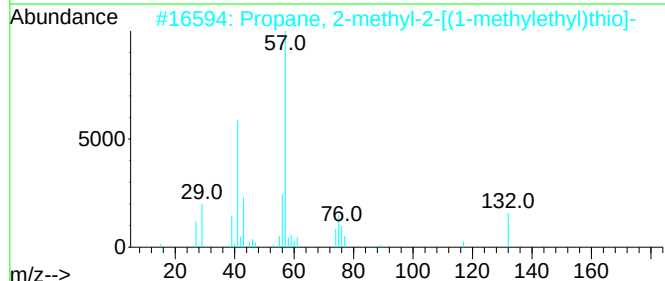
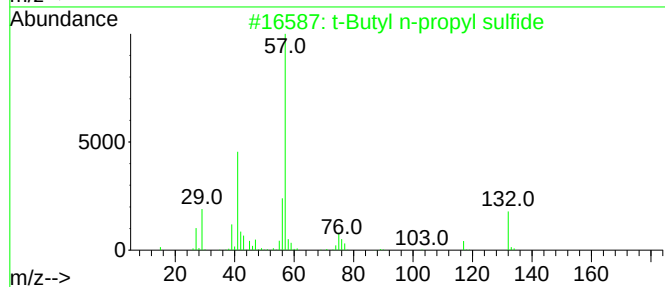
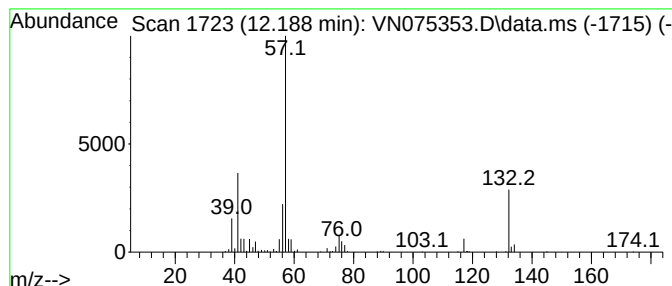
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Quant Title : SW846 8260

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

Peak Number 5 t-Butyl n-propyl sulfide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.188	20.10 ug/l	290163	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			t-Butyl n-propyl sulfide	132	C7H16S	1000343-63-5	83
2			Propane, 2-methyl-2-[(1-methylet...	132	C7H16S	044657-76-3	50
3			Ethanethioic acid S-tert-butyl e...	132	C6H12OS	000999-90-6	47
4			Propanethioic acid, S-(1-methyle...	132	C6H12OS	002432-47-5	47
5			Propanethioic acid, S-propyl ester	132	C6H12OS	002432-43-1	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075353.D
Acq On : 21 Nov 2022 19:53
Operator : JC\MD
Sample : N5665-01 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COSTAL-DRUM-2DL

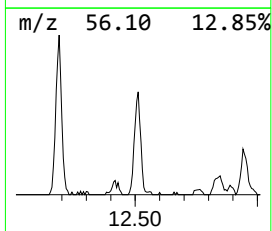
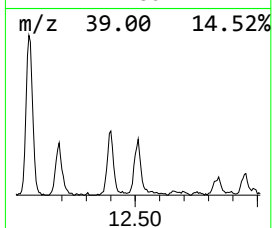
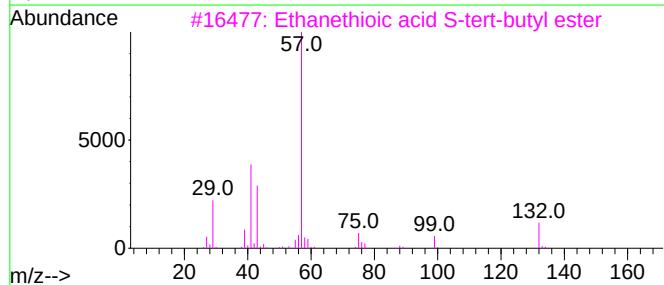
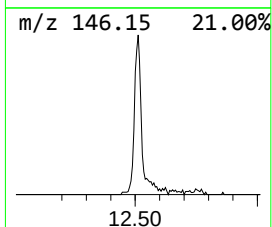
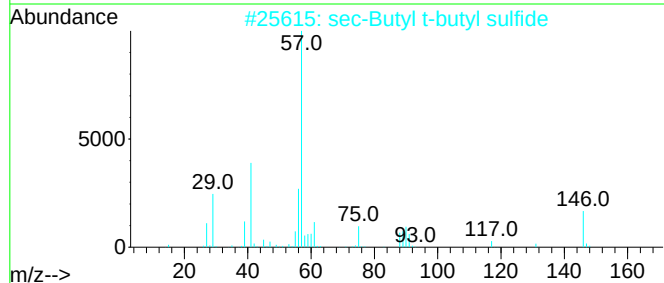
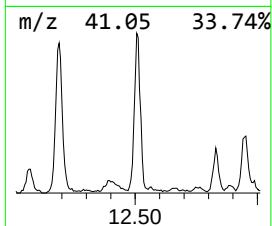
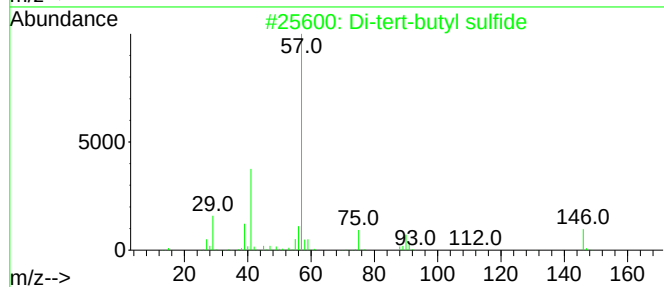
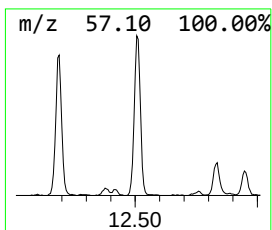
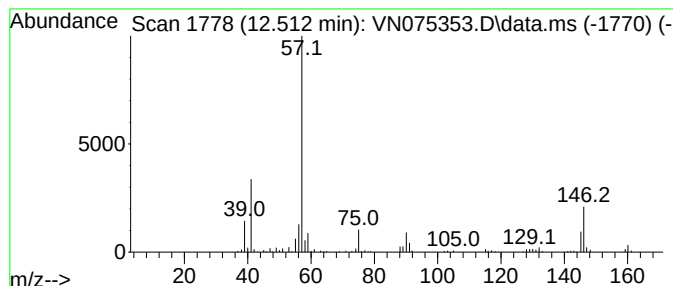
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Quant Title : SW846 8260

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

Peak Number 6 Di-tert-butyl sulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.512	31.38 ug/l	453058	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl sulfide	146	C8H18S	000107-47-1	87
2			sec-Butyl t-butyl sulfide	146	C8H18S	1000343-63-7	53
3			Ethanethioic acid S-tert-butyl e...	132	C6H12OS	000999-90-6	27
4			Propane, 1,1'-thiobis[2-methyl-	146	C8H18S	000592-65-4	27
5			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075353.D
Acq On : 21 Nov 2022 19:53
Operator : JC\MD
Sample : N5665-01 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COSTAL-DRUM-2DL

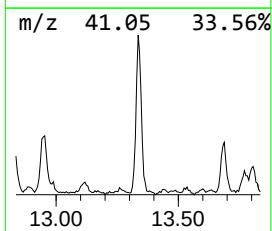
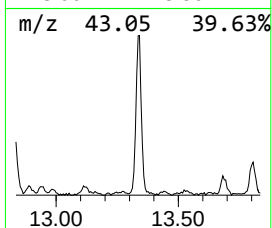
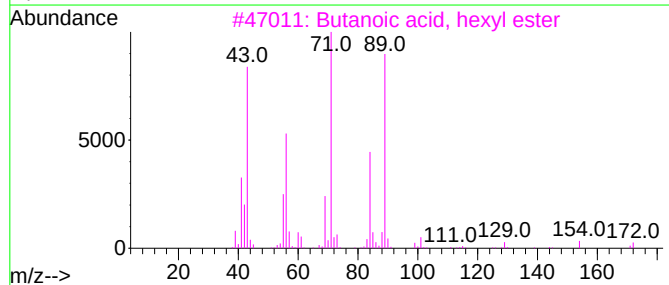
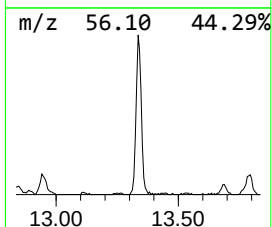
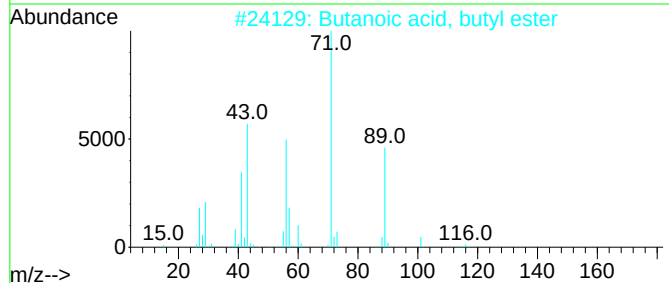
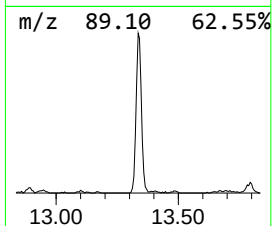
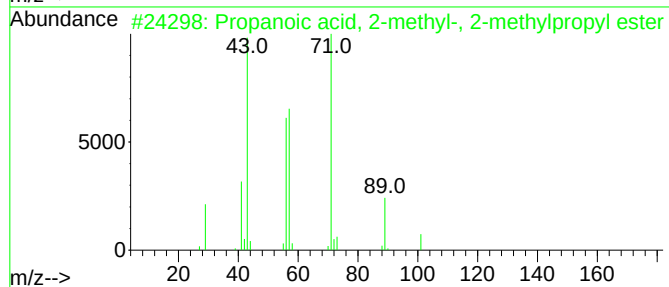
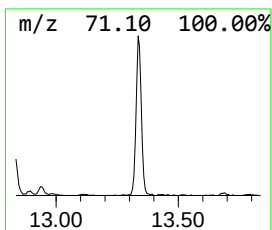
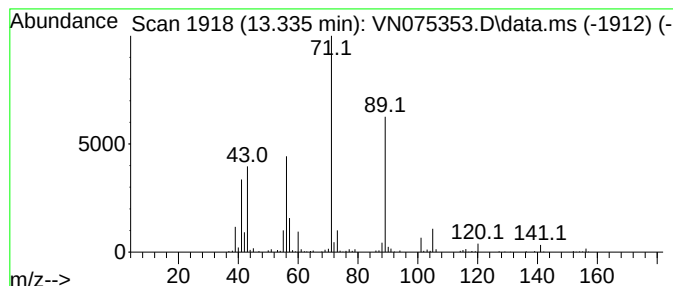
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Quant Title : SW846 8260

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

Peak Number 7 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	23.85 ug/l	387986	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
2			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	56
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	53
5			Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075353.D
Acq On : 21 Nov 2022 19:53
Operator : JC\MD
Sample : N5665-01 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COSTAL-DRUM-2DL

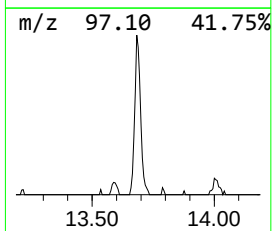
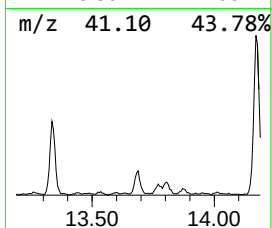
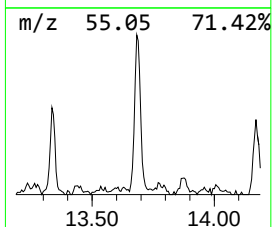
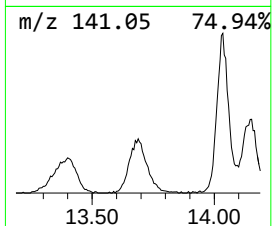
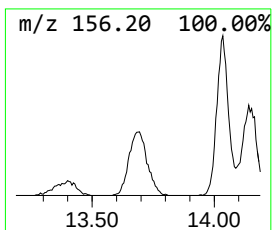
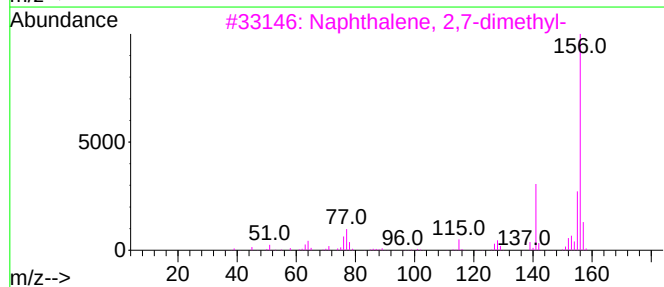
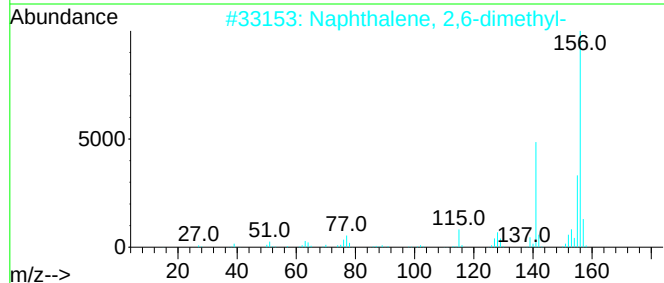
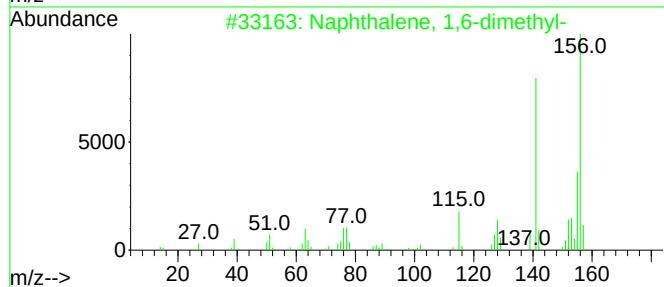
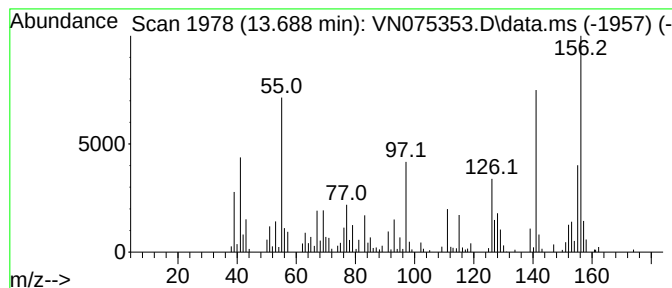
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	31.77 ug/l	516772	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	96
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	91
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	91
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075353.D
Acq On : 21 Nov 2022 19:53
Operator : JC\MD
Sample : N5665-01 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COSTAL-DRUM-2DL

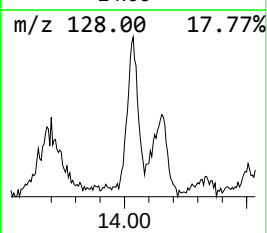
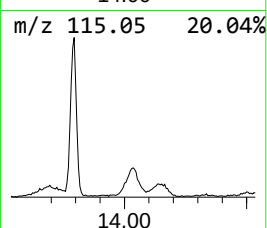
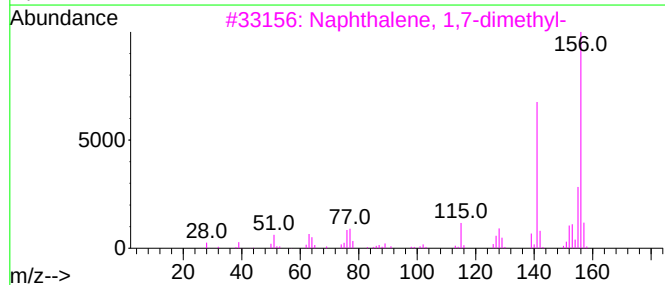
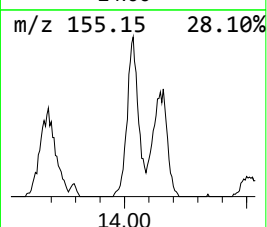
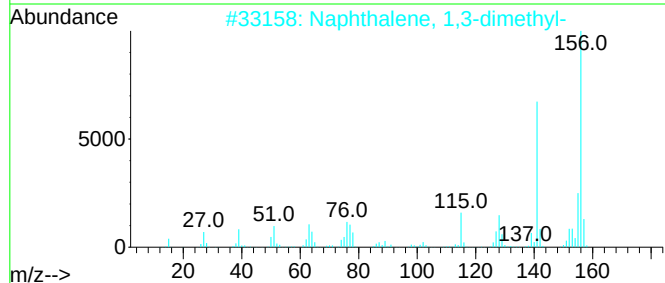
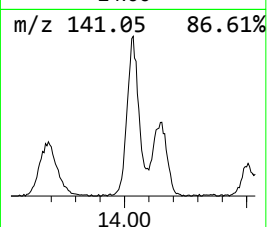
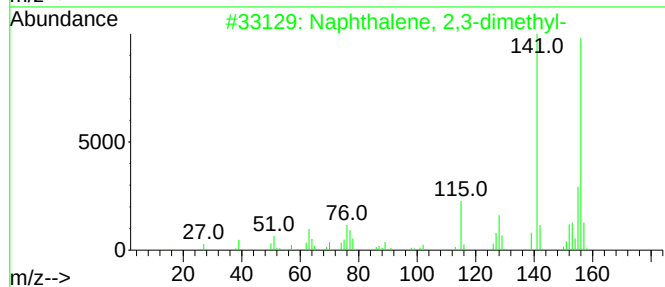
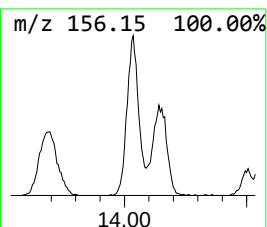
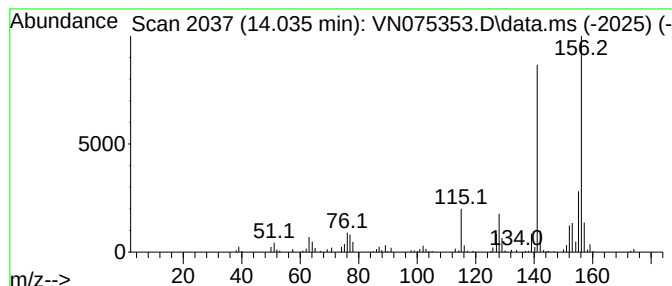
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.035	32.14 ug/l	522858	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075353.D
Acq On : 21 Nov 2022 19:53
Operator : JC\MD
Sample : N5665-01 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COSTAL-DRUM-2DL

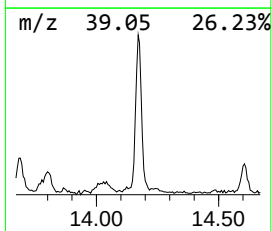
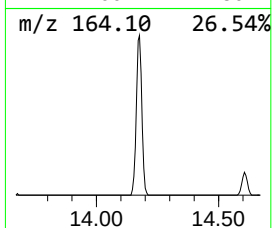
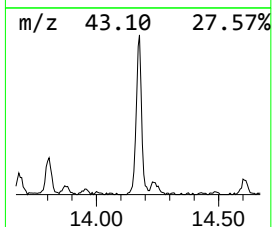
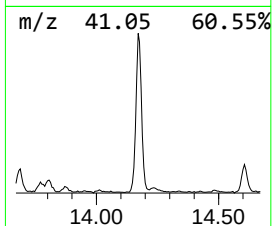
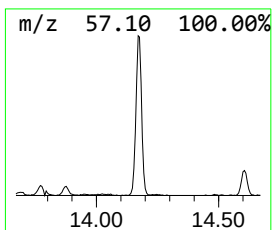
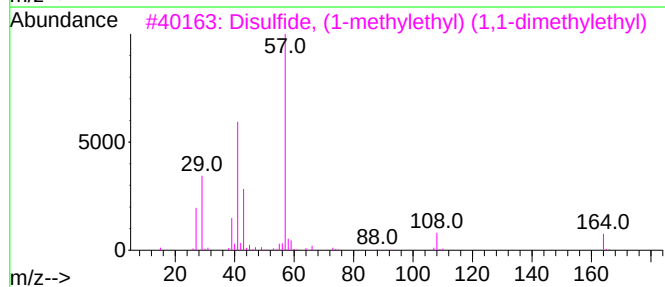
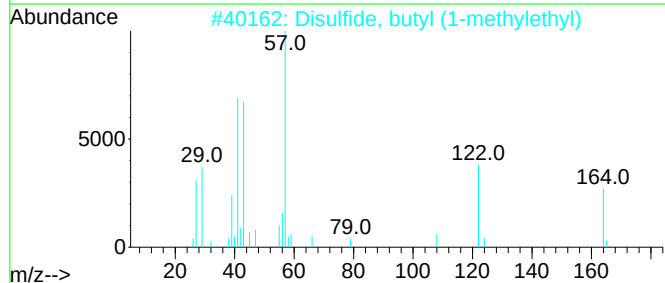
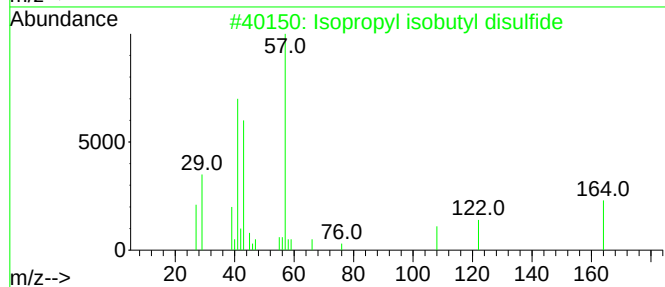
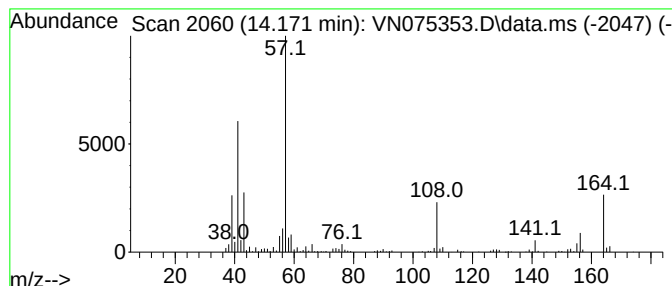
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 10 Isopropyl isobutyl disulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.171	44.44 ug/l	722938	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl isobutyl disulfide	164	C7H16S2	067421-82-3	64
2			Disulfide, butyl (1-methylethyl)	164	C7H16S2	072437-53-7	50
3			Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	49
4			Butane, 2-bromo-	136	C4H9Br	000078-76-2	14
5			Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112122\
Data File : VN075353.D
Acq On : 21 Nov 2022 19:53
Operator : JC\MD
Sample : N5665-01 40X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COSTAL-DRUM-2DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanethiol,...	6.689	96.1	ug/l	907789	1	8.230	472225	50.0
Ethane, (methyl...	7.347	16.6	ug/l	156921	1	8.230	472225	50.0
Thiophene, tetr...	11.347	15.6	ug/l	225848	3	11.865	721862	50.0
Propane, 2-meth...	11.541	23.1	ug/l	332809	3	11.865	721862	50.0
t-Butyl n-propy...	12.188	20.1	ug/l	290163	3	11.865	721862	50.0
Di-tert-butyl s...	12.512	31.4	ug/l	453058	3	11.865	721862	50.0
Propanoic acid,...	13.335	23.9	ug/l	387986	4	13.794	813399	50.0
Naphthalene, 1,...	13.688	31.8	ug/l	516772	4	13.794	813399	50.0
Naphthalene, 2,...	14.035	32.1	ug/l	522858	4	13.794	813399	50.0
Isopropyl isobu...	14.171	44.4	ug/l	722938	4	13.794	813399	50.0