

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060625\
 Data File : VN086877.D
 Acq On : 06 Jun 2025 19:28
 Operator : JC\MD
 Sample : Q2216-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 3888

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\82N060625W.M
 Title : SW846 8260

Signal : TIC: VN086877.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.447	413	424	434	rBV	75381	240117	12.84%	2.054%
2	4.547	434	441	453	rVB2	34888	108217	5.79%	0.926%
3	4.741	463	474	485	rBV	18839	66466	3.55%	0.568%
4	6.977	842	854	862	rBV3	17303	50139	2.68%	0.429%
5	7.494	934	942	955	rVB	88452	229512	12.27%	1.963%
6	7.800	985	994	1004	rBV2	16807	44666	2.39%	0.382%
7	8.177	1047	1058	1062	rBV	232778	539396	28.84%	4.613%
8	8.235	1062	1068	1079	rVB	429502	985042	52.66%	8.424%
9	8.588	1116	1128	1139	rBV	262074	599116	32.03%	5.124%
10	8.971	1184	1193	1203	rBV2	14417	33180	1.77%	0.284%
11	9.106	1205	1216	1234	rBV	648439	1355177	72.45%	11.590%
12	9.406	1260	1267	1274	rBV3	16784	35205	1.88%	0.301%
13	9.535	1283	1289	1295	rBV	16443	34302	1.83%	0.293%
14	9.606	1295	1301	1308	rVV2	38537	72109	3.85%	0.617%
15	9.912	1346	1353	1362	rVB2	22542	46192	2.47%	0.395%
16	10.453	1437	1445	1454	rBV2	14854	33827	1.81%	0.289%
17	10.570	1457	1465	1473	rBV	1010007	1870533	100.00%	15.997%
18	11.176	1564	1568	1572	rBV3	13917	20963	1.12%	0.179%
19	11.865	1678	1685	1697	rBV	845599	1545509	82.62%	13.218%
20	12.412	1768	1778	1786	rVB2	81696	160554	8.58%	1.373%
21	12.494	1786	1792	1796	rBV2	23777	39392	2.11%	0.337%
22	12.547	1796	1801	1806	rVV6	16861	31969	1.71%	0.273%
23	12.617	1807	1813	1821	rVB7	7578	19682	1.05%	0.168%
24	12.735	1828	1833	1842	rVB	18964	35997	1.92%	0.308%
25	12.847	1845	1852	1867	rBV	636301	1161622	62.10%	9.935%
26	13.170	1898	1907	1911	rBV6	11899	27742	1.48%	0.237%
27	13.259	1917	1922	1929	rVB3	19188	28922	1.55%	0.247%
28	13.482	1955	1960	1968	rVB	15185	30548	1.63%	0.261%
29	13.600	1976	1980	1985	rBV4	21147	35173	1.88%	0.301%
30	13.794	2005	2013	2020	rBV	853424	1484810	79.38%	12.699%
31	13.853	2020	2023	2028	rVB3	36521	58463	3.13%	0.500%
32	13.935	2029	2037	2042	rBV4	23508	74636	3.99%	0.638%
33	14.376	2108	2112	2120	rVB7	13751	31502	1.68%	0.269%
34	14.500	2123	2133	2140	rBV5	43125	114217	6.11%	0.977%
35	14.764	2166	2178	2191	rVV5	97096	326966	17.48%	2.796%
36	14.982	2211	2215	2217	rBV5	15601	22127	1.18%	0.189%

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Instrument :
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ClientSampleId :
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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	15.376	2277	2282	2289	rBV4	43496	98792	5.28%	0.845%
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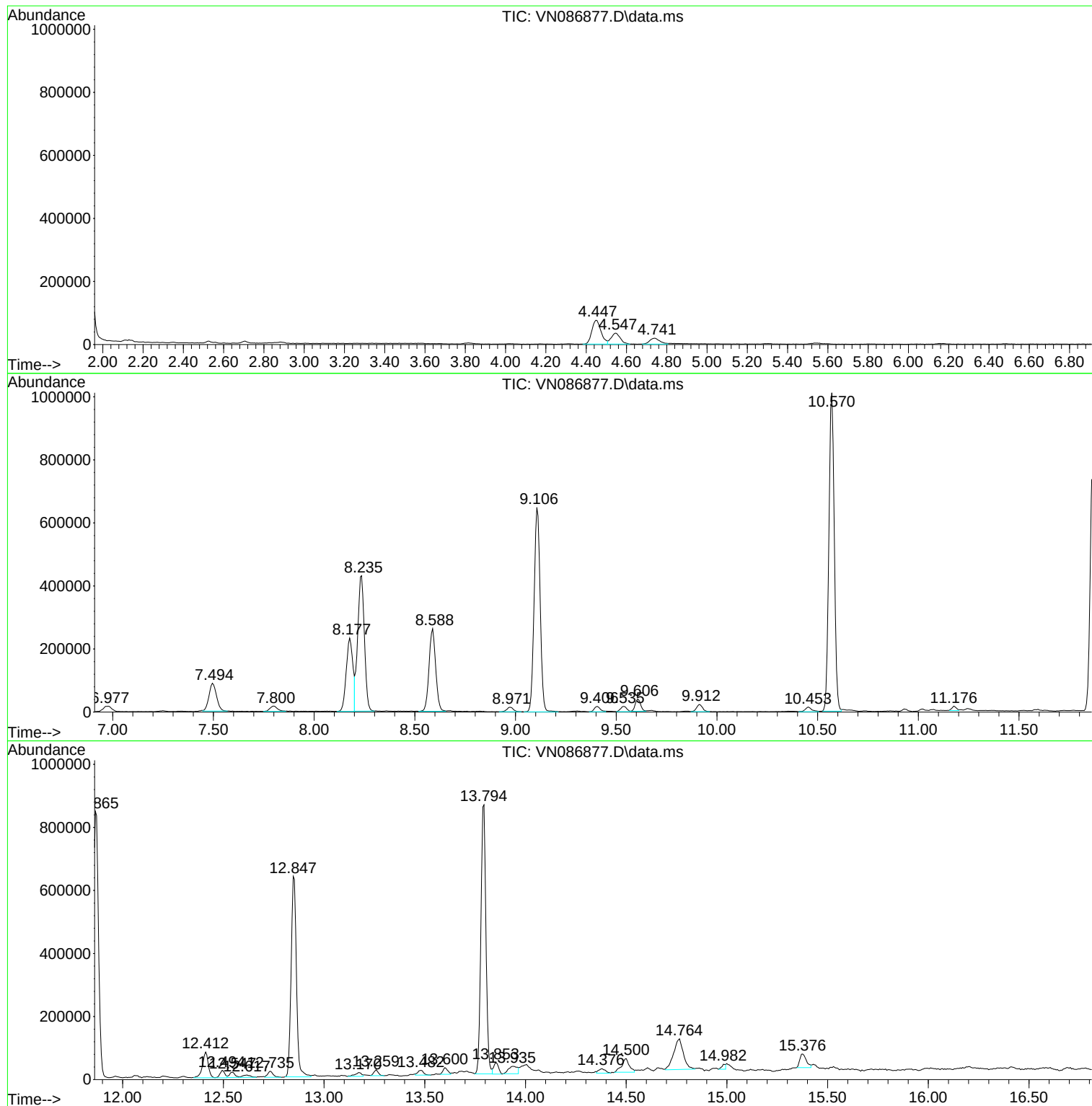
Sum of corrected areas: 11692782

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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



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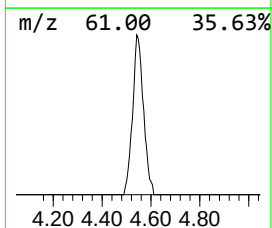
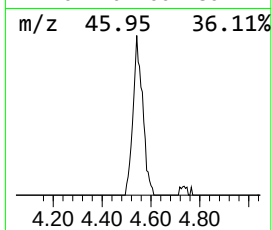
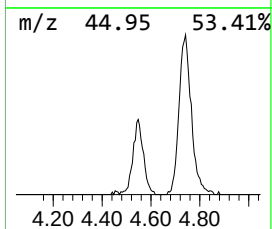
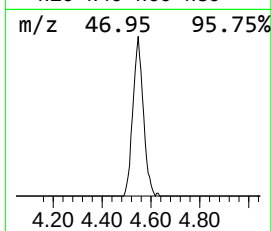
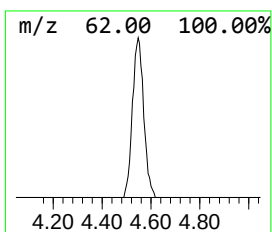
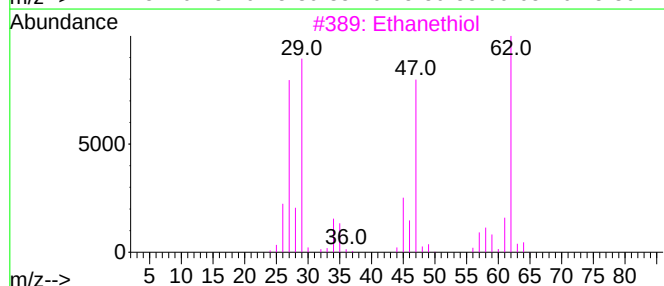
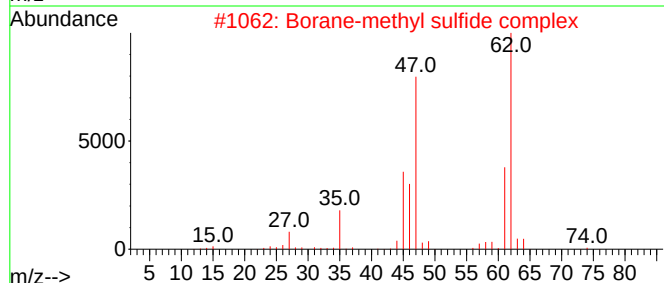
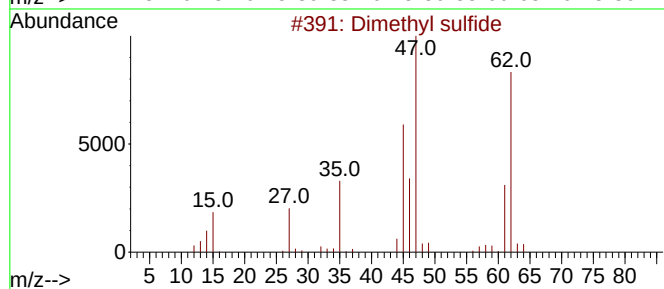
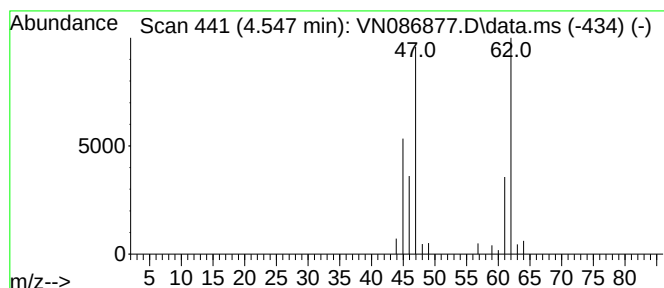
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Peak Number 1 Dimethyl sulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.547	5.49 ug/l	108217	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3			Ethanethiol	62	C2H6S	000075-08-1	78
4			Methanethiol	48	CH4S	000074-93-1	9
5			Boric acid	62	BH3O3	010043-35-3	5



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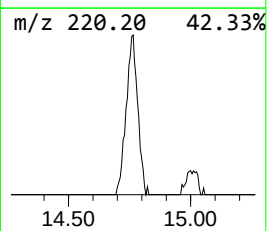
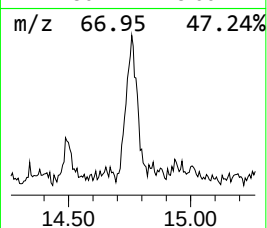
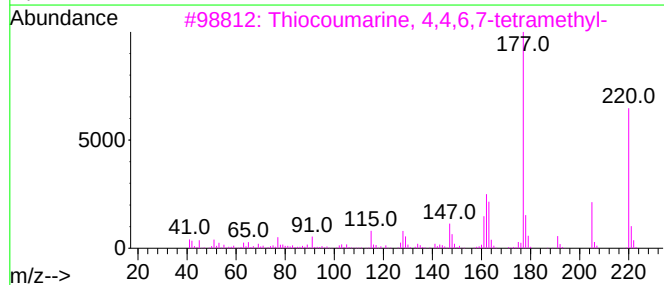
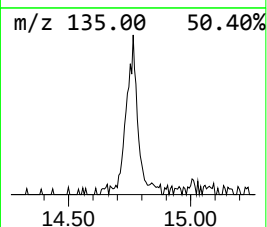
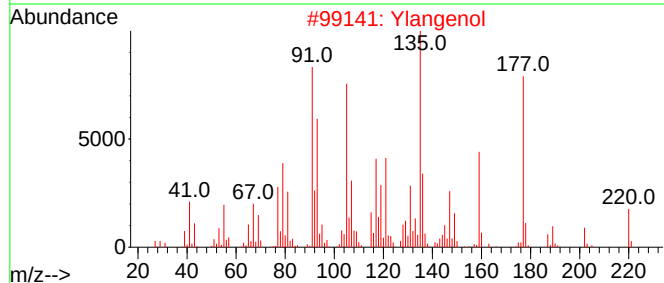
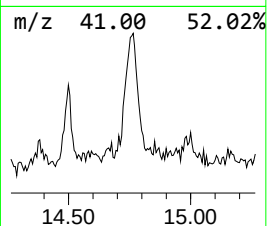
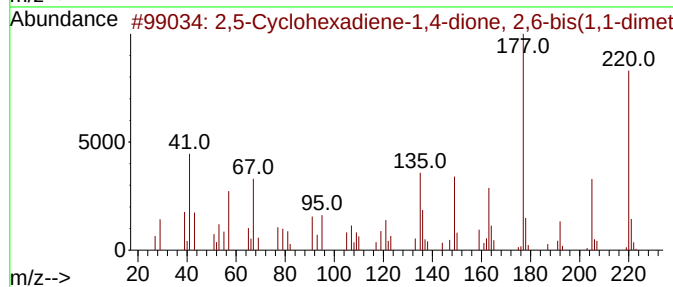
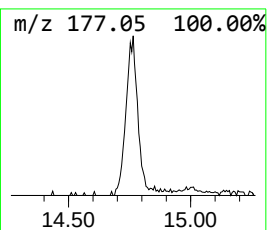
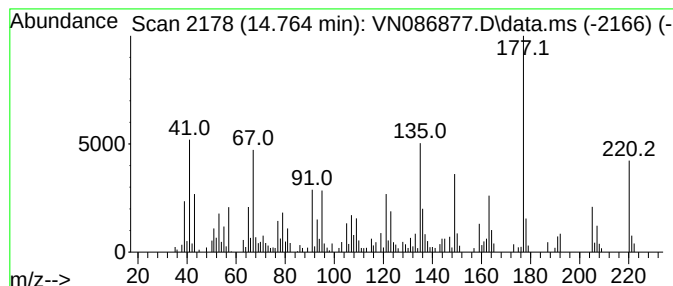
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.764	11.01 ug/l	326966	1,4-Dichlorobenzene-d4	13.794	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2	Ylangelol	220	C15H24O	041610-69-9	60
3	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	55
4	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	46
5	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F4O2	1000461-12-2	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl sulfide	4.547	5.5	ug/l	108217	1	8.235	985042	50.0
2,5-Cyclohexadi...	14.764	11.0	ug/l	326966	4	13.794	1484810	50.0