

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110325\
 Data File : VX048464.D
 Acq On : 03 Nov 2025 17:44
 Operator : JC/MD
 Sample : Q3500-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 461-LIQUID

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\82X102925W.M
 Title : SW846 8260

Signal : TIC: VX048464.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.148	8	10	28	rVB	71108	148895	28.10%	2.502%
2	1.368	42	46	55	rVB2	21673	37024	6.99%	0.622%
3	1.459	58	61	67	rVV	7636	10012	1.89%	0.168%
4	1.557	71	77	88	rVB	22776	36844	6.95%	0.619%
5	2.374	205	211	215	rBV	40719	71395	13.47%	1.200%
6	2.428	215	220	229	rVV	46784	93186	17.59%	1.566%
7	2.520	229	235	251	rVB	51492	103655	19.56%	1.742%
8	2.934	296	303	313	rBV2	9900	25564	4.82%	0.430%
9	4.014	471	480	489	rBV6	4429	12049	2.27%	0.202%
10	4.221	501	514	523	rBV5	3168	11346	2.14%	0.191%
11	4.544	555	567	591	rBV2	13354	48163	9.09%	0.809%
12	5.373	691	703	720	rBV2	65498	214686	40.51%	3.607%
13	5.538	720	730	750	rVB	97217	309780	58.46%	5.205%
14	5.946	786	797	819	rBV	69001	206618	38.99%	3.472%
15	6.330	851	860	870	rBV4	3127	9341	1.76%	0.157%
16	6.617	897	907	915	rBV2	3460	10552	1.99%	0.177%
17	6.745	920	928	943	rBV	154079	402145	75.89%	6.757%
18	7.281	1011	1016	1023	rVB4	3790	8296	1.57%	0.139%
19	7.403	1025	1036	1039	rVV6	9526	25148	4.75%	0.423%
20	7.440	1039	1042	1059	rVV2	14037	38323	7.23%	0.644%
21	7.562	1059	1062	1069	rVV4	2647	6593	1.24%	0.111%
22	7.635	1069	1074	1083	rVB2	2705	6388	1.21%	0.107%
23	7.885	1108	1115	1132	rVB2	30272	70162	13.24%	1.179%
24	8.562	1220	1226	1230	rBV	10846	18242	3.44%	0.307%
25	8.635	1230	1238	1247	rBV	318871	529917	100.00%	8.904%
26	9.025	1297	1302	1311	rVB5	3271	7645	1.44%	0.128%
27	9.226	1329	1335	1339	rVV2	4877	8320	1.57%	0.140%
28	9.293	1339	1346	1352	rVB2	6577	13434	2.54%	0.226%
29	9.421	1361	1367	1375	rBV2	12555	25324	4.78%	0.426%
30	9.506	1377	1381	1390	rVB3	7160	13242	2.50%	0.223%
31	10.037	1458	1468	1481	rBV	334592	489349	92.34%	8.223%
32	10.195	1489	1494	1496	rBV4	4040	6486	1.22%	0.109%
33	10.226	1496	1499	1506	rVV6	5183	11710	2.21%	0.197%
34	10.287	1506	1509	1515	rVB3	4836	7450	1.41%	0.125%
35	10.366	1515	1522	1530	rBV4	8642	22592	4.26%	0.380%
36	10.488	1537	1542	1546	rBV3	4976	6683	1.26%	0.112%

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37	10.671	1568	1572	1579	rVB	6497	10552	1.99%	0.177%
38	10.750	1579	1585	1596	rBV	23612	44205	8.34%	0.743%
39	10.860	1596	1603	1611	rVV6	11637	33906	6.40%	0.570%
40	11.061	1631	1636	1647	rBV	247976	352409	66.50%	5.922%
41	11.153	1647	1651	1657	rVB7	4984	10463	1.97%	0.176%
42	11.415	1690	1694	1696	rBV3	5586	8176	1.54%	0.137%
43	11.457	1697	1701	1709	rVB	48992	69169	13.05%	1.162%
44	11.543	1711	1715	1719	rBV	19981	25757	4.86%	0.433%
45	11.598	1719	1724	1727	rBV4	6136	11975	2.26%	0.201%
46	11.738	1743	1747	1751	rVV2	11530	15494	2.92%	0.260%
47	11.823	1756	1761	1765	rBV2	16735	25460	4.80%	0.428%
48	11.884	1766	1771	1773	rBV3	8458	13150	2.48%	0.221%
49	11.915	1773	1776	1780	rVV5	6314	10019	1.89%	0.168%
50	11.951	1780	1782	1785	rVB4	6972	8124	1.53%	0.137%
51	12.006	1785	1791	1797	rBV	283024	380593	71.82%	6.395%
52	12.085	1797	1804	1809	rBV3	9604	22122	4.17%	0.372%
53	12.201	1818	1823	1830	rBV	104484	156869	29.60%	2.636%
54	12.299	1835	1839	1844	rVB5	11420	22904	4.32%	0.385%
55	12.408	1852	1857	1867	rBV5	27905	64778	12.22%	1.088%
56	12.494	1868	1871	1874	rBV2	9713	14395	2.72%	0.242%
57	12.567	1880	1883	1890	rVB4	33608	45831	8.65%	0.770%
58	12.677	1896	1901	1904	rBV6	11856	16138	3.05%	0.271%
59	12.756	1909	1914	1917	rBV5	9318	19581	3.70%	0.329%
60	12.841	1924	1928	1931	rBV3	19646	23494	4.43%	0.395%
61	12.890	1931	1936	1940	rBV6	13113	21244	4.01%	0.357%
62	12.927	1940	1942	1943	rBV	7565	6103	1.15%	0.103%
63	12.957	1943	1947	1953	rVB4	27883	41955	7.92%	0.705%
64	13.024	1953	1958	1961	rBV5	25110	37102	7.00%	0.623%
65	13.085	1964	1968	1969	rBV	32011	37779	7.13%	0.635%
66	13.109	1969	1972	1977	rVB3	27135	40079	7.56%	0.673%
67	13.195	1982	1986	1991	rBV2	27914	39775	7.51%	0.668%
68	13.250	1991	1995	1997	rBV	42897	51768	9.77%	0.870%
69	13.274	1997	1999	2004	rVB3	34332	41313	7.80%	0.694%
70	13.402	2012	2020	2028	rVB7	50314	107958	20.37%	1.814%
71	13.481	2029	2033	2035	rBV4	14745	24716	4.66%	0.415%
72	13.567	2044	2047	2050	rBV5	18409	25210	4.76%	0.424%
73	13.603	2050	2053	2058	rVB6	19008	31860	6.01%	0.535%
74	13.676	2058	2065	2068	rBV5	45471	87646	16.54%	1.473%
75	13.713	2068	2071	2074	rVV2	31881	43406	8.19%	0.729%
76	13.750	2074	2077	2079	rVV	31590	35758	6.75%	0.601%

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77	13.780	2079	2082	2084	rVV3	17461	21999	4.15%	0.370%
78	13.811	2084	2087	2095	rVV3	49045	92958	17.54%	1.562%
79	13.890	2095	2100	2108	rVB6	23111	53969	10.18%	0.907%
80	14.018	2118	2121	2124	rBV	35506	34027	6.42%	0.572%
81	14.079	2128	2131	2134	rVB	34235	38716	7.31%	0.651%
82	14.115	2134	2137	2140	rBV4	12751	13518	2.55%	0.227%
83	14.152	2140	2143	2146	rVV5	10085	13859	2.62%	0.233%
84	14.207	2147	2152	2157	rVB6	28152	51114	9.65%	0.859%
85	14.390	2178	2182	2184	rBV4	21997	29709	5.61%	0.499%
86	14.414	2184	2186	2189	rVB3	20951	19288	3.64%	0.324%
87	14.457	2189	2193	2194	rBV3	23808	28296	5.34%	0.475%
88	14.542	2204	2207	2212	rVB2	16248	21164	3.99%	0.356%
89	14.591	2212	2215	2218	rBV2	35295	45276	8.54%	0.761%
90	14.652	2222	2225	2226	rVV2	19183	20288	3.83%	0.341%
91	14.676	2226	2229	2233	rVV	37424	50100	9.45%	0.842%
92	14.731	2235	2238	2241	rVV4	31370	38790	7.32%	0.652%
93	14.768	2241	2244	2249	rVB5	21827	27948	5.27%	0.470%
94	14.908	2264	2267	2279	rVB5	26115	64046	12.09%	1.076%
95	15.048	2286	2290	2299	rVB3	39077	75345	14.22%	1.266%
96	15.121	2299	2302	2306	rBV3	8151	15175	2.86%	0.255%
97	15.353	2337	2340	2342	rBV4	4849	6297	1.19%	0.106%
98	15.390	2343	2346	2353	rVB6	13030	18602	3.51%	0.313%
99	15.743	2401	2404	2410	rVB	11170	15632	2.95%	0.263%
100	15.835	2415	2419	2423	rVB4	5426	9228	1.74%	0.155%

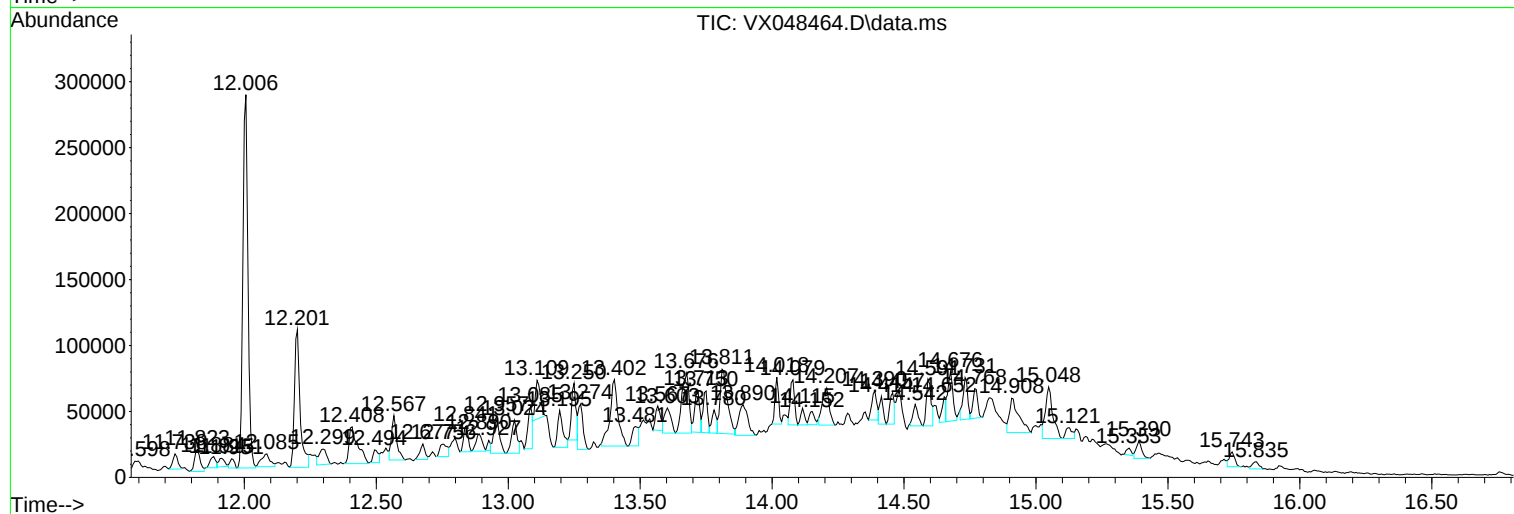
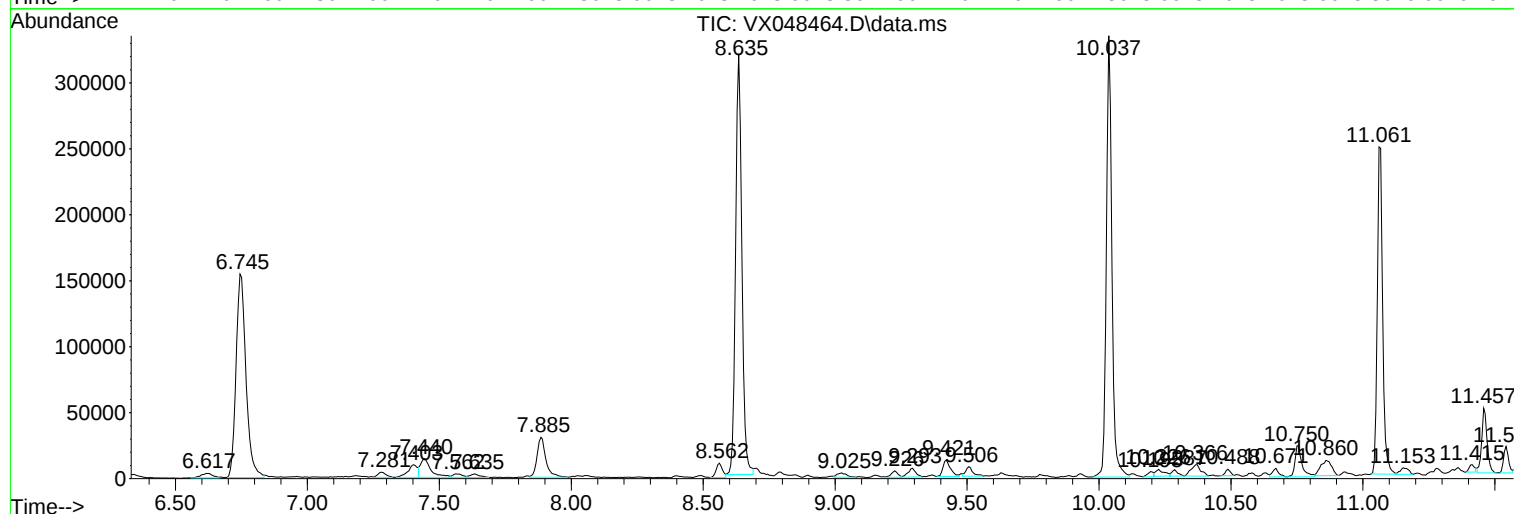
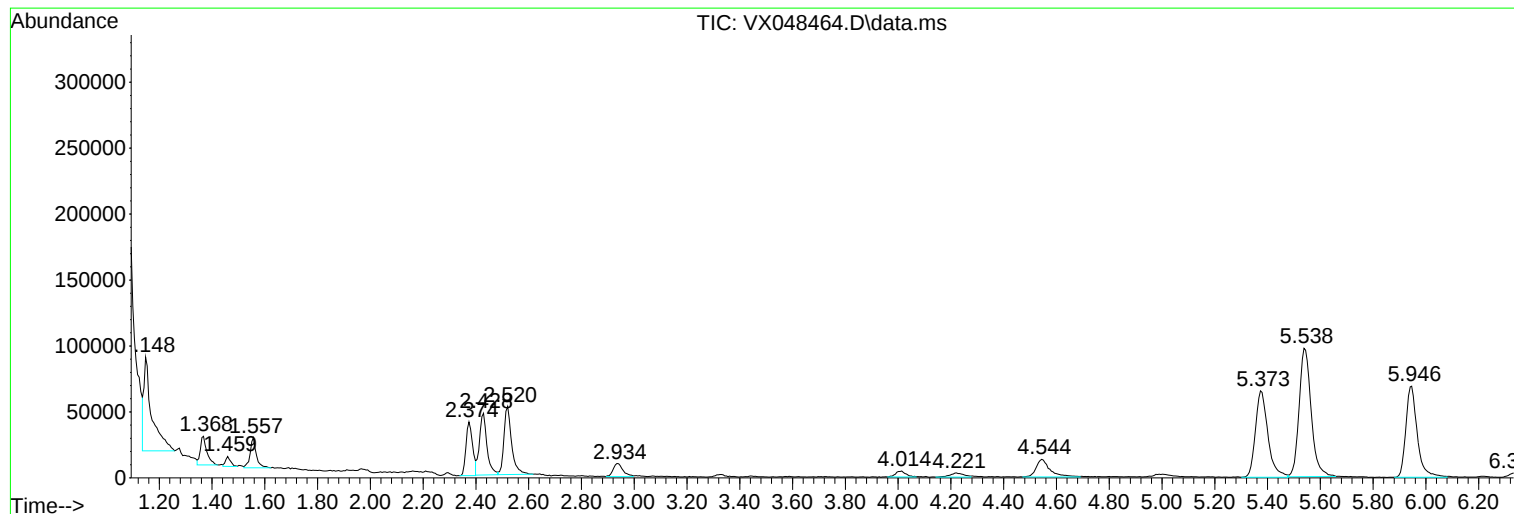
Sum of corrected areas: 5951139

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

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



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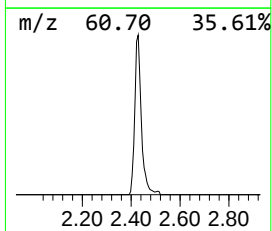
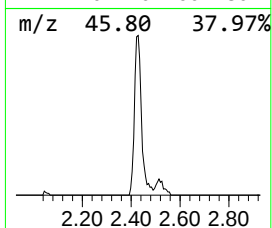
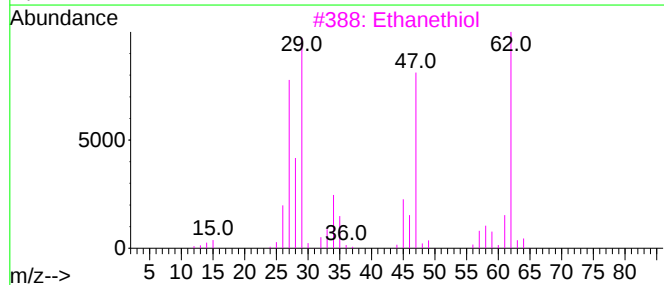
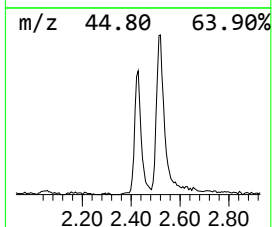
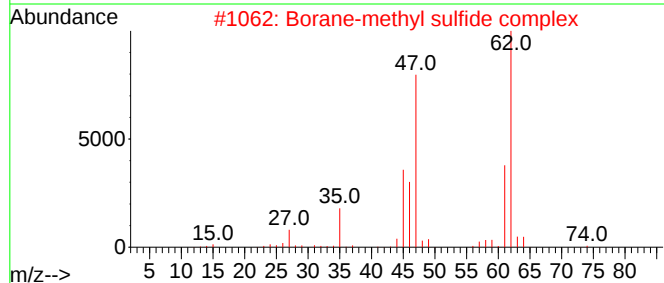
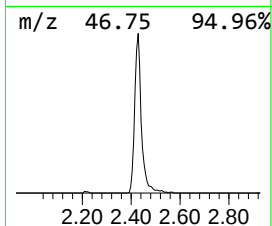
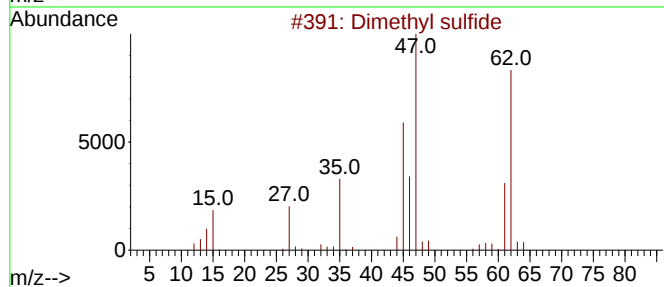
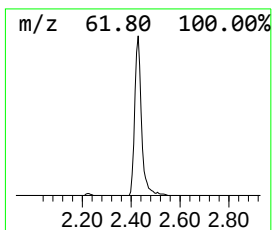
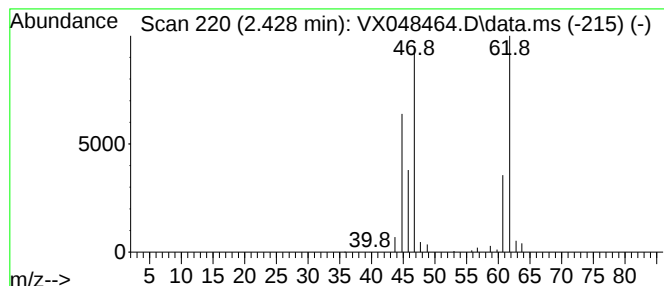
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

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

Peak Number 2 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.428	15.04 ug/l	93186	Pentafluorobenzene	5.538

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			Ethene, chloro-	62	C2H3Cl	000075-01-4	50
5			Boric acid	62	BH3O3	010043-35-3	5



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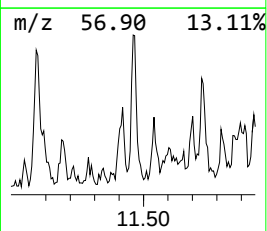
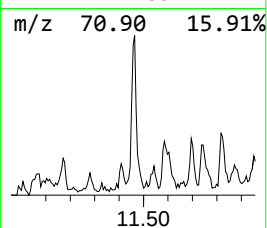
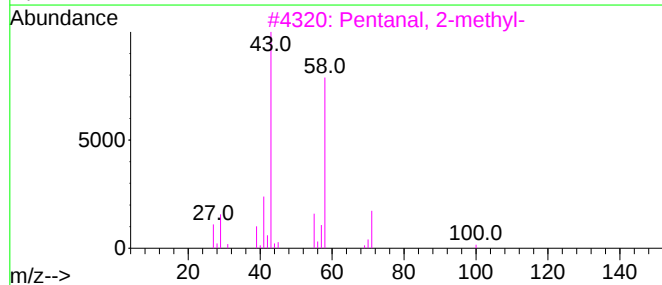
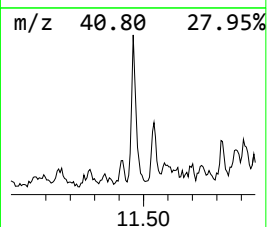
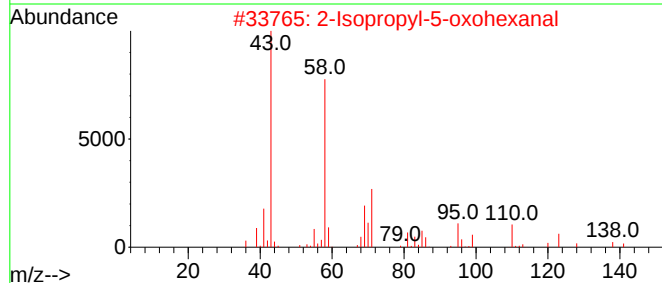
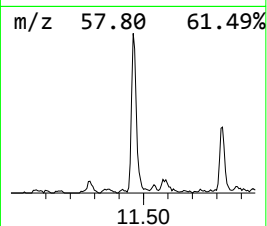
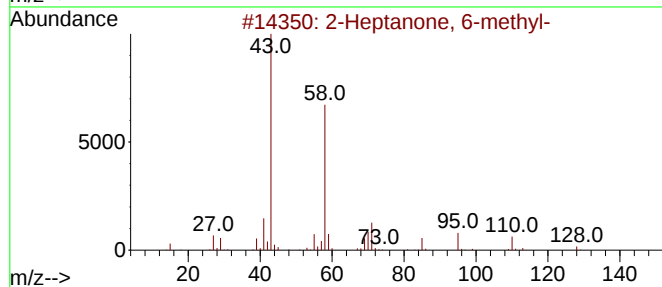
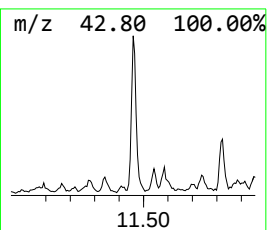
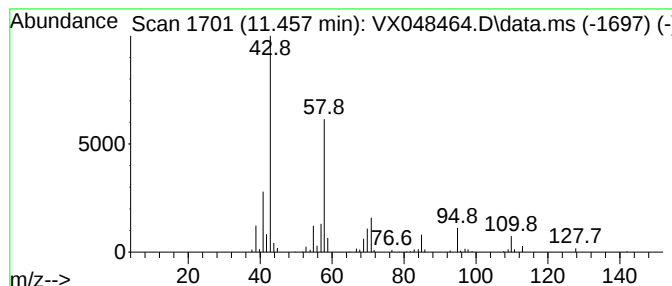
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Quant Title : SW846 8260

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

Peak Number 4 2-Heptanone, 6-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.457	9.09 ug/l	69169	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	91
2			2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	64
3			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	53
4			2-Hexanone	100	C6H12O	000591-78-6	47
5			Butanimidamide	86	C4H10N2	000107-90-4	40



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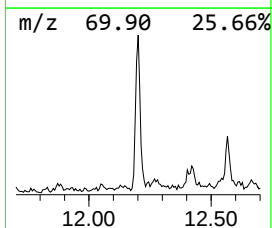
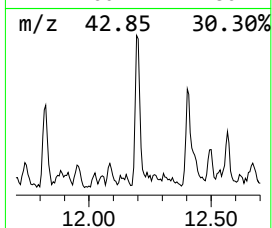
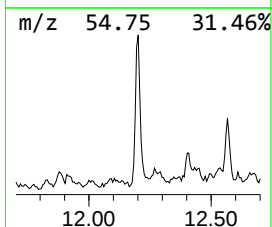
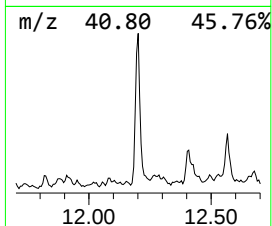
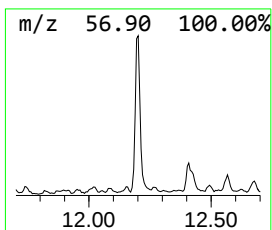
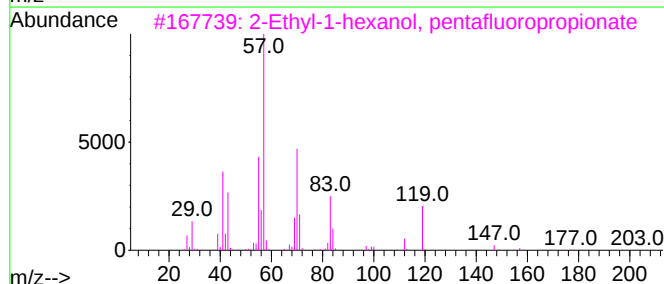
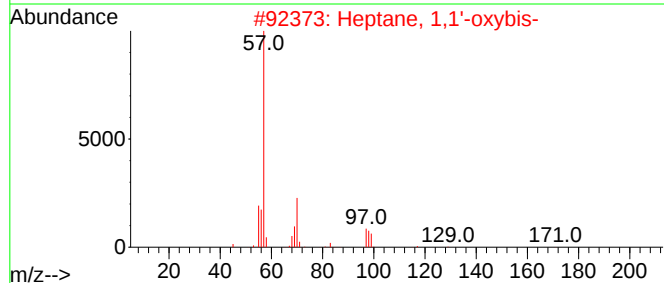
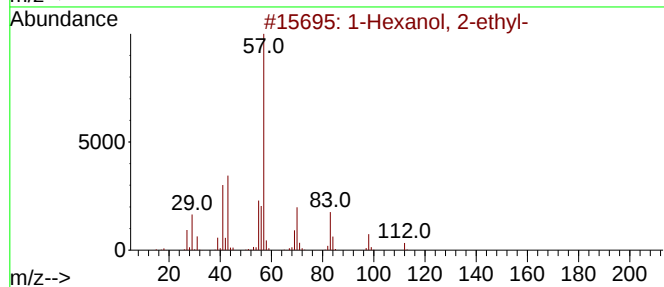
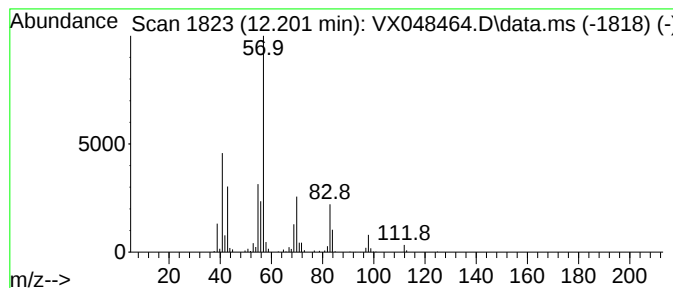
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.201	20.61 ug/l	156869	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	50
4			Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110325\
Data File : VX048464.D
Acq On : 03 Nov 2025 17:44
Operator : JC/MD
Sample : Q3500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461-LIQUID

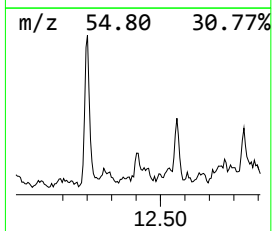
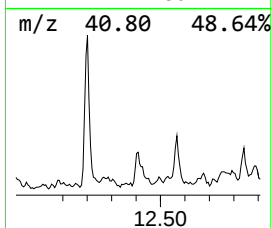
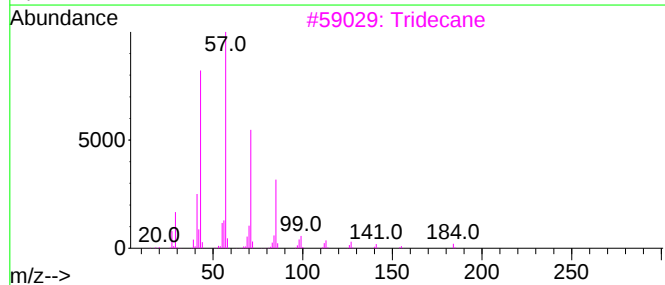
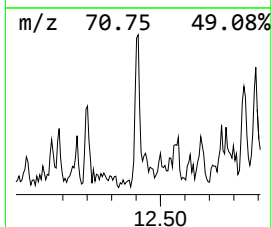
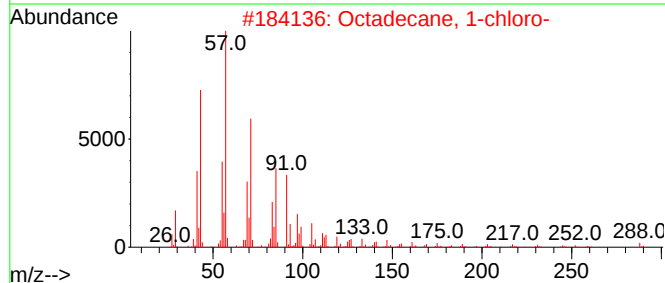
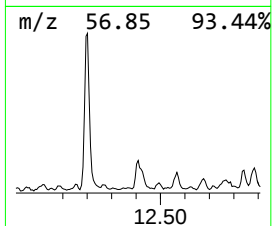
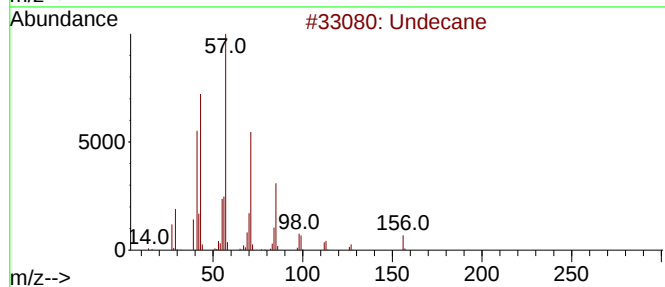
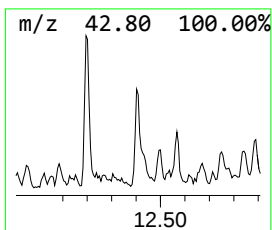
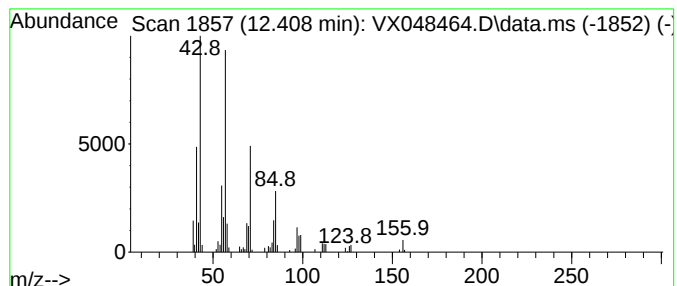
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

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

Peak Number 6 Undecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.408	8.51 ug/l	64778	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	95
2			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	78
3			Tridecane	184	C13H28	000629-50-5	72
4			Tetradecane	198	C14H30	000629-59-4	72
5			Dotriacontane	451	C32H66	000544-85-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110325\
Data File : VX048464.D
Acq On : 03 Nov 2025 17:44
Operator : JC/MD
Sample : Q3500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461-LIQUID

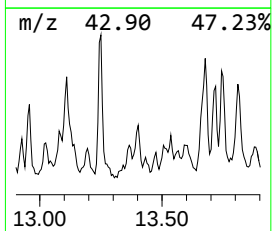
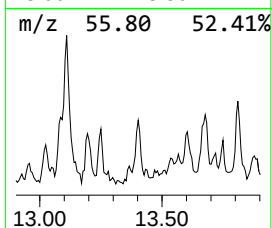
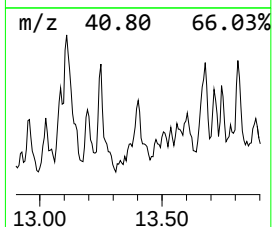
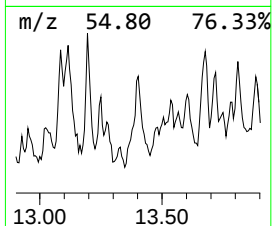
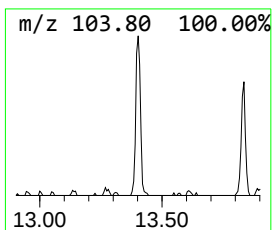
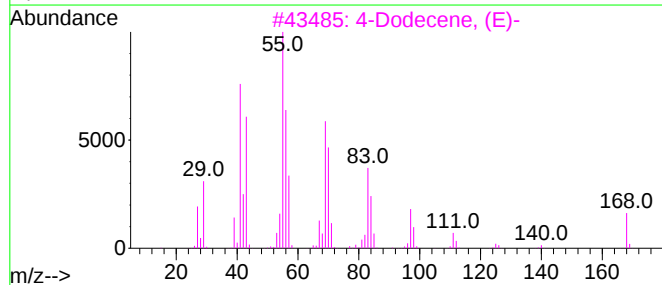
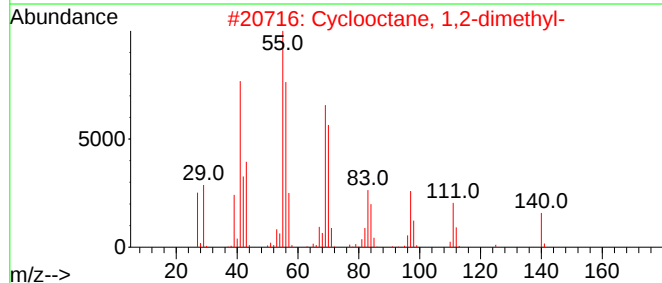
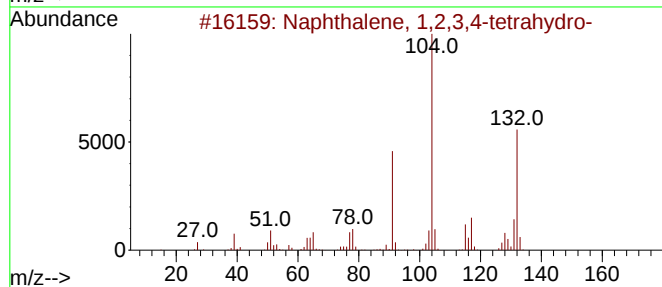
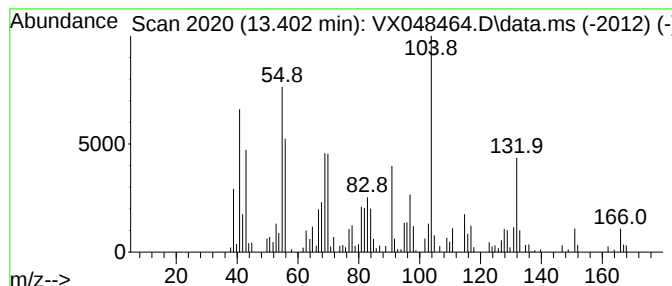
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.402	14.18 ug/l	107958	1,4-Dichlorobenzene-d4	12.006

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	89
2		Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	42
3		4-Dodecene, (E)-	168	C12H24	007206-15-7	42
4		4-Dodecene, (Z)-	168	C12H24	007206-27-1	42
5		Cyclododecane	168	C12H24	000294-62-2	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110325\
Data File : VX048464.D
Acq On : 03 Nov 2025 17:44
Operator : JC/MD
Sample : Q3500-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461-LIQUID

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.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
Dimethyl sulfide	2.428	15.0	ug/l	93186	1	5.538	309780	50.0
2-Heptanone, 6-...	11.457	9.1	ug/l	69169	4	12.006	380593	50.0
1-Hexanol, 2-et...	12.201	20.6	ug/l	156869	4	12.006	380593	50.0
Undecane	12.408	8.5	ug/l	64778	4	12.006	380593	50.0
Naphthalene, 1,...	13.402	14.2	ug/l	107958	4	12.006	380593	50.0