

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081221\
 Data File : VY005626.D
 Acq On : 12 Aug 2021 16:38
 Operator : SY/MD
 Sample : M3343-08
 Misc : 5.00G/5ML/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20210582-COM-5

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_Y\methods\82Y080221S.M

Title : SW846 8260

Signal : TIC: VY005626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.869	4	8	17	rVB3	20544	35081	2.47%	0.329%
2	2.229	60	67	69	rBV3	11011	19392	1.37%	0.182%
3	3.954	342	350	358	rBV	35418	97077	6.85%	0.910%
4	4.040	358	364	379	rVV2	37089	100166	7.07%	0.939%
5	4.204	379	391	405	rVB2	21949	61027	4.31%	0.572%
6	4.729	466	477	488	rBV	21624	70228	4.95%	0.658%
7	5.759	635	646	658	rBV3	9711	28949	2.04%	0.271%
8	6.996	838	849	861	rBV	13629	38463	2.71%	0.361%
9	7.728	957	969	974	rBV	183959	437415	30.86%	4.100%
10	7.795	974	980	991	rVB	300653	680125	47.98%	6.375%
11	8.149	1028	1038	1049	rBV	198039	439612	31.01%	4.120%
12	8.697	1118	1128	1137	rBV	500230	975423	68.81%	9.142%
13	9.752	1292	1301	1308	rBV2	8126	17741	1.25%	0.166%
14	10.185	1365	1372	1381	rBV	829887	1417497	100.00%	13.286%
15	11.496	1579	1587	1595	rBV	781808	1303197	91.94%	12.215%
16	11.685	1613	1618	1623	rBV4	7075	14473	1.02%	0.136%
17	11.746	1623	1628	1639	rVB4	14401	33754	2.38%	0.316%
18	12.002	1663	1670	1677	rVV5	13322	39225	2.77%	0.368%
19	12.124	1682	1690	1695	rVB	31689	62713	4.42%	0.588%
20	12.233	1695	1708	1714	rBV3	48645	135387	9.55%	1.269%
21	12.325	1714	1723	1726	rBV7	19069	44852	3.16%	0.420%
22	12.374	1729	1731	1737	rVB3	16016	25904	1.83%	0.243%
23	12.483	1741	1749	1756	rVB3	781915	1357115	95.74%	12.720%
24	12.575	1756	1764	1768	rBV4	26651	59965	4.23%	0.562%
25	12.642	1768	1775	1783	rVB3	41761	117954	8.32%	1.106%
26	12.733	1783	1790	1796	rBV6	29245	87196	6.15%	0.817%
27	12.843	1796	1808	1817	rBV4	82829	238385	16.82%	2.234%
28	13.001	1829	1834	1837	rBV3	20924	36367	2.57%	0.341%
29	13.069	1837	1845	1853	rVB	71787	140536	9.91%	1.317%
30	13.172	1858	1862	1868	rBV	42809	75774	5.35%	0.710%
31	13.221	1868	1870	1873	rVV3	15787	22631	1.60%	0.212%
32	13.288	1873	1881	1885	rVV	137178	262181	18.50%	2.457%
33	13.355	1889	1892	1896	rVV3	23972	39520	2.79%	0.370%
34	13.428	1897	1904	1909	rVV	886972	1373048	96.86%	12.869%
35	13.477	1909	1912	1923	rVB	107118	221851	15.65%	2.079%
36	13.568	1923	1927	1931	rBV4	18607	28757	2.03%	0.270%

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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	13.648	1936	1940	1944	rVB3	27290	39001	2.75%	0.366%
38	13.751	1953	1957	1961	rVB5	22073	34203	2.41%	0.321%
39	13.965	1982	1992	1996	rBV3	69327	134702	9.50%	1.263%
40	14.074	2007	2010	2014	rVB3	12951	17369	1.23%	0.163%
41	14.148	2016	2022	2028	rVB5	19125	42741	3.02%	0.401%
42	14.202	2028	2031	2035	rVB5	8875	14454	1.02%	0.135%
43	14.257	2035	2040	2046	rBV6	27905	60151	4.24%	0.564%
44	14.391	2056	2062	2065	rBV5	27013	58427	4.12%	0.548%
45	14.477	2072	2076	2081	rVB7	12317	20694	1.46%	0.194%
46	14.733	2114	2118	2124	rVB7	17081	33877	2.39%	0.318%
47	14.940	2148	2152	2156	rVB6	9367	17818	1.26%	0.167%
48	15.123	2179	2182	2190	rVB7	11499	19128	1.35%	0.179%
49	15.214	2194	2197	2202	rVB3	12524	19091	1.35%	0.179%
50	16.153	2349	2351	2358	rVB6	9727	18614	1.31%	0.174%

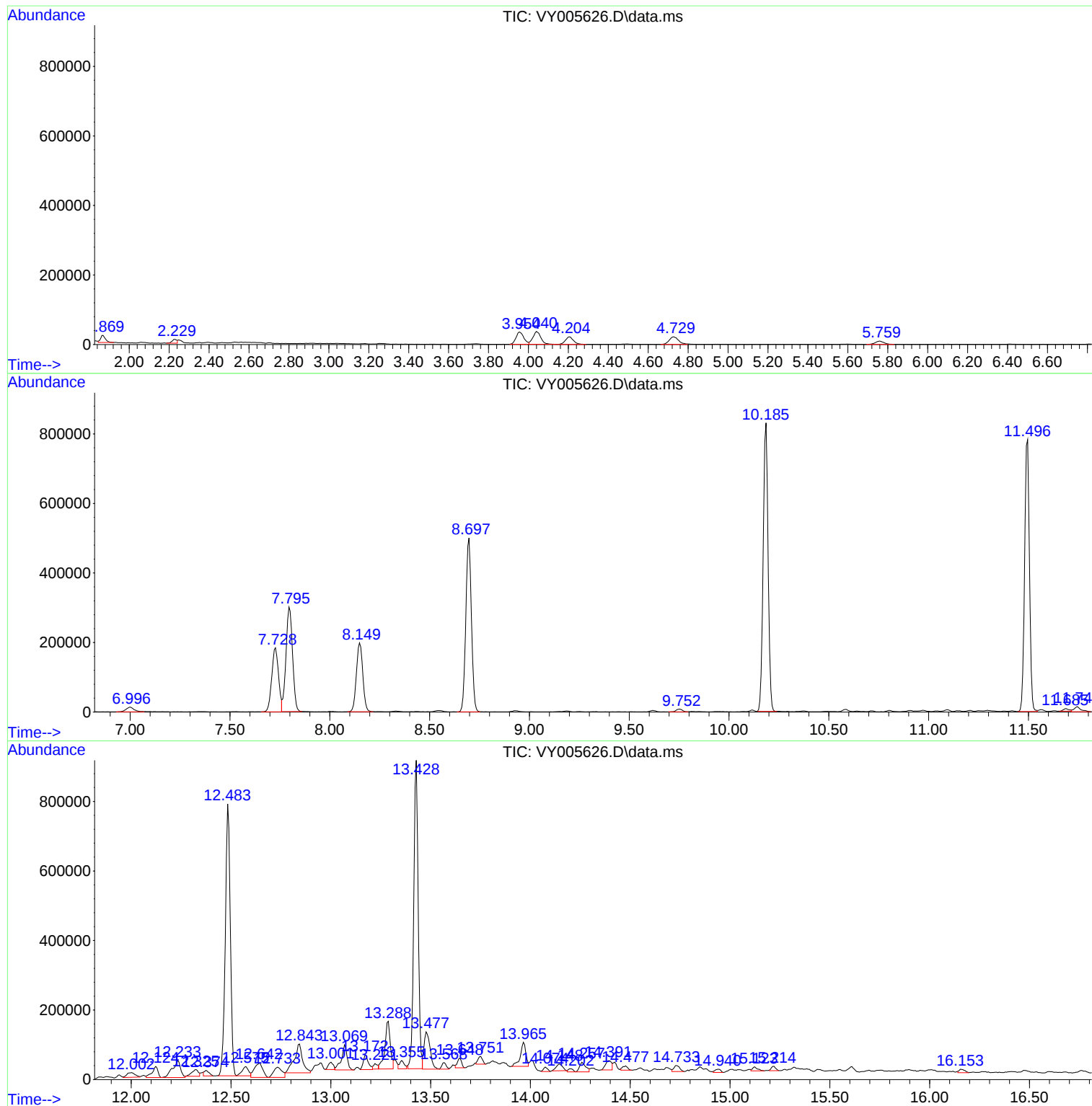
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080221S.M
Quant Title : SW846 8260

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



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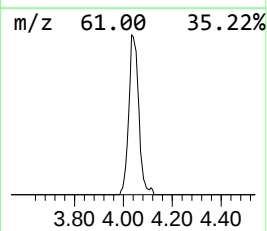
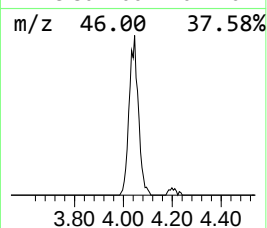
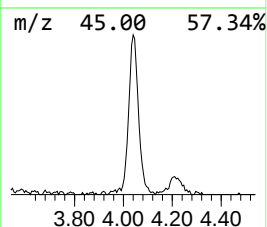
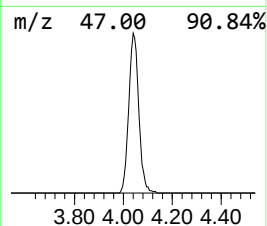
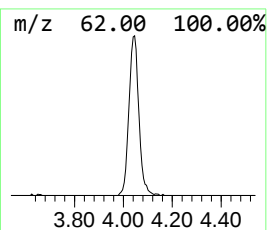
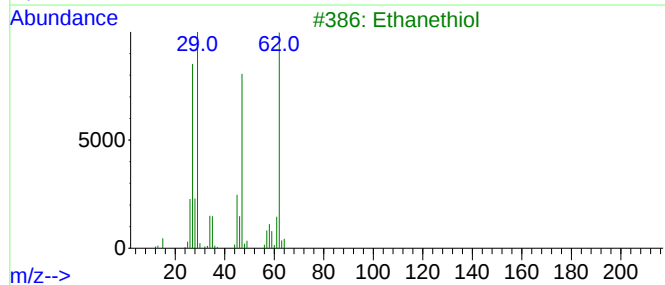
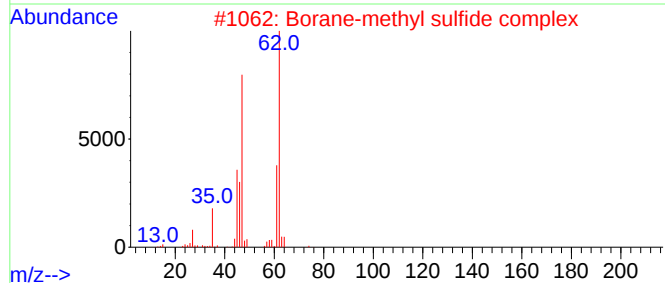
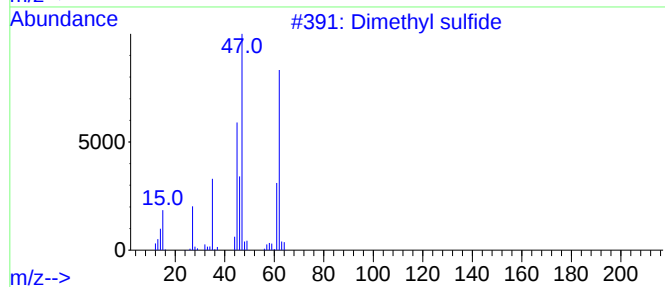
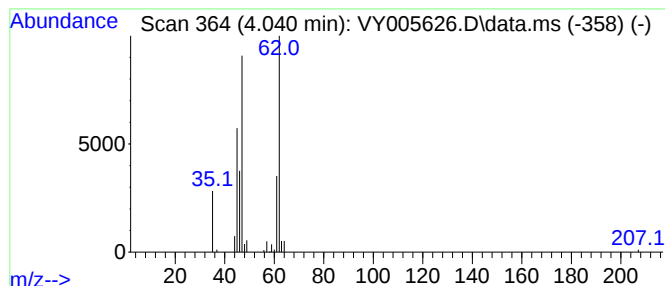
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Quant Title : SW846 8260

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

Peak Number 1 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.040	7.36 ug/l	100166	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	97
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	80
3			Ethanethiol	62	C2H6S	000075-08-1	64
4			Carbonodithioic acid, O,S-diethy...	150	C5H10OS2	000623-79-0	40
5			Acetic acid, 2,2'-thiobis-	150	C4H6O4S	000123-93-3	10



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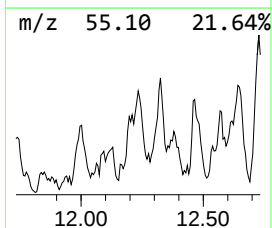
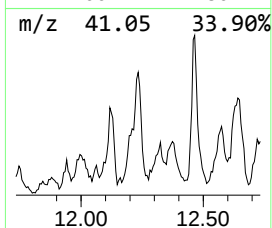
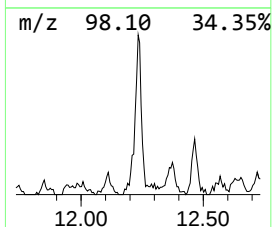
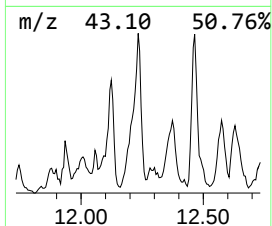
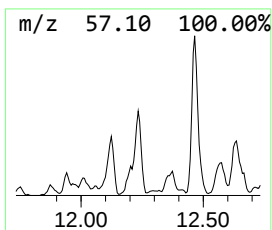
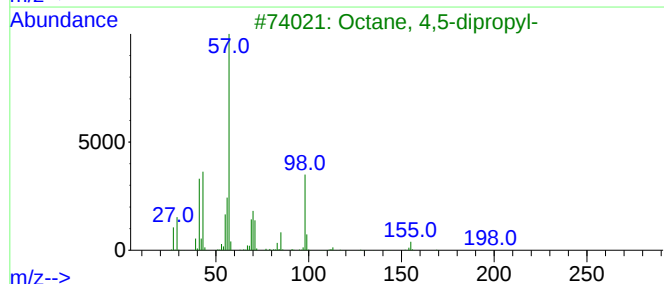
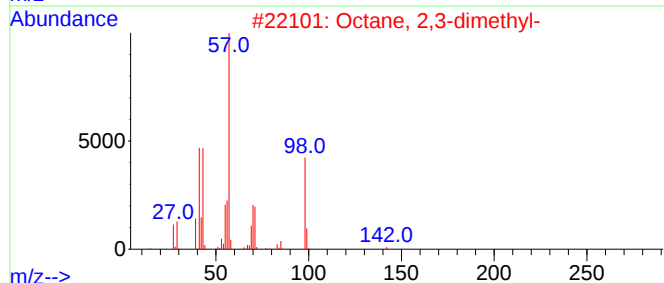
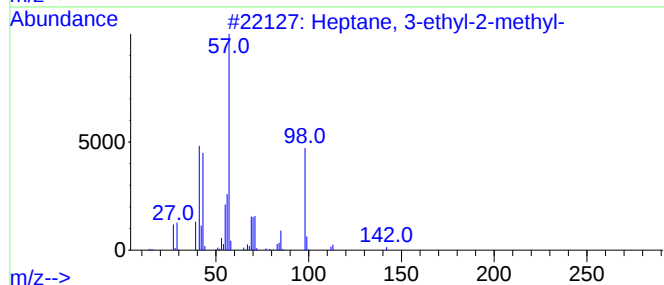
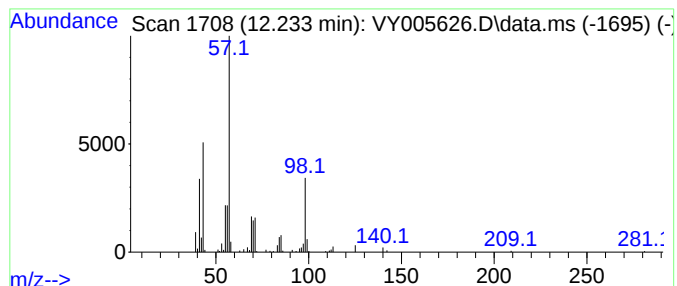
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080221S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptane, 3-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	5.19 ug/l	135387	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	87
2			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	83
3			Octane, 4,5-dipropyl-	198	C14H30	020905-05-9	78
4			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	59
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50



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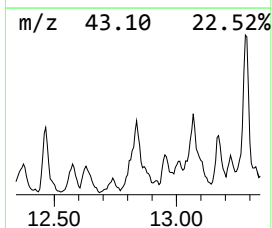
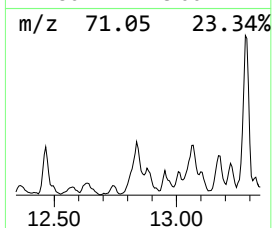
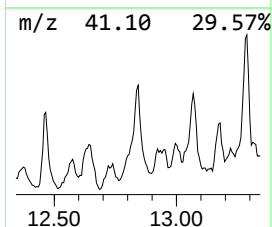
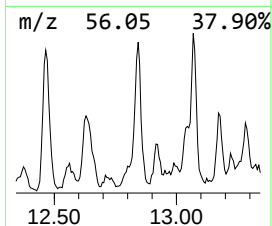
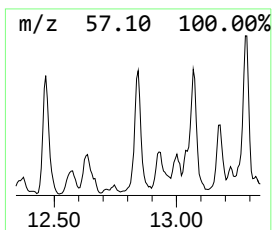
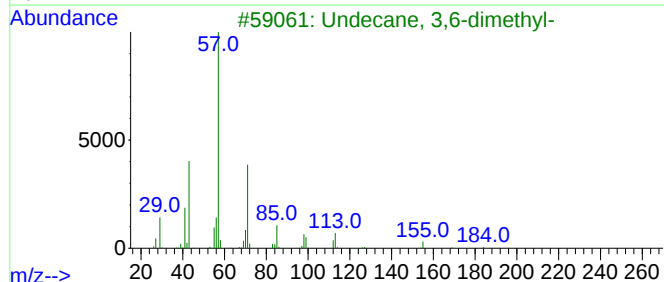
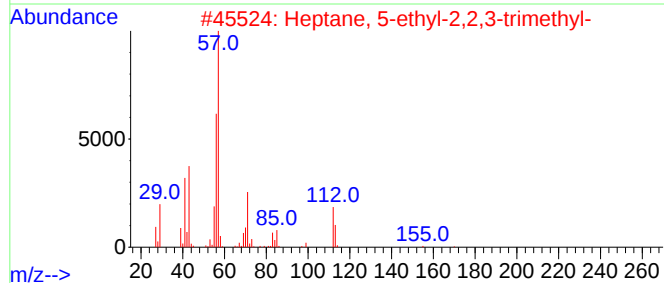
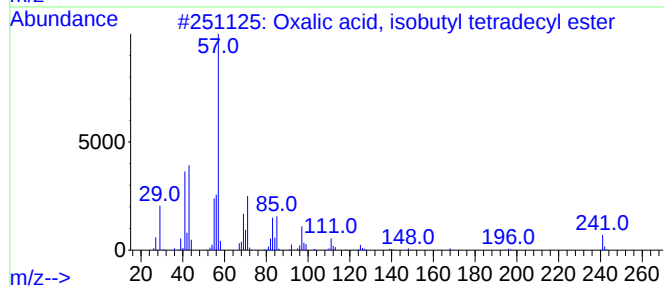
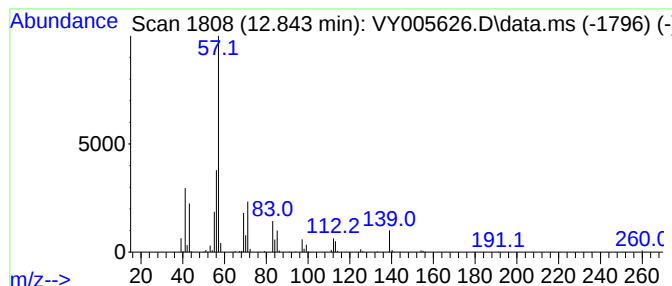
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Oxalic acid, isobutyl tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.843	8.68 ug/l	238385	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	53
2			Heptane, 5-ethyl-2,2,3-trimethyl-	170	C12H26	062199-06-8	53
3			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	53
4			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	50
5			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	47



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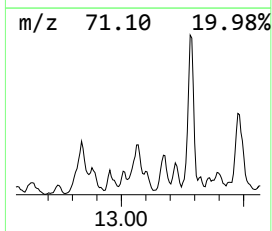
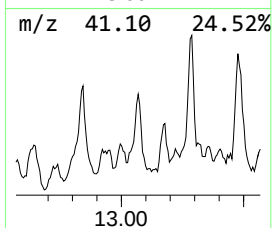
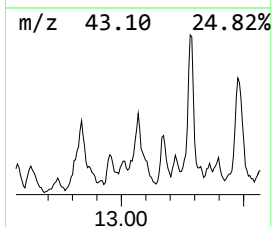
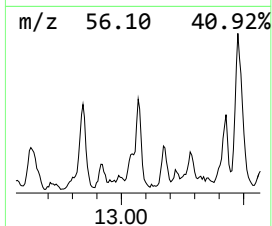
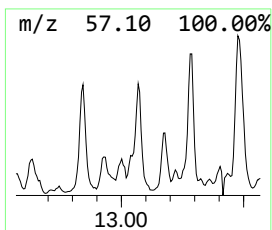
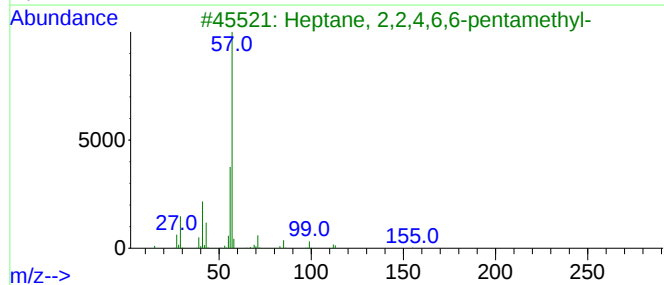
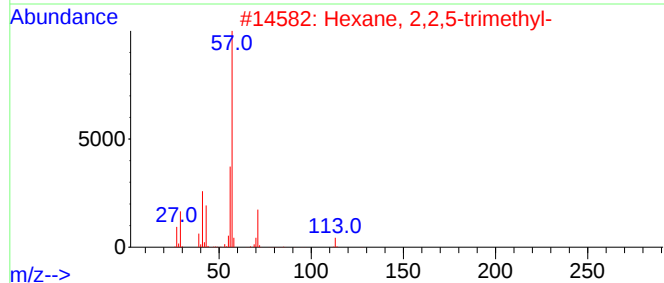
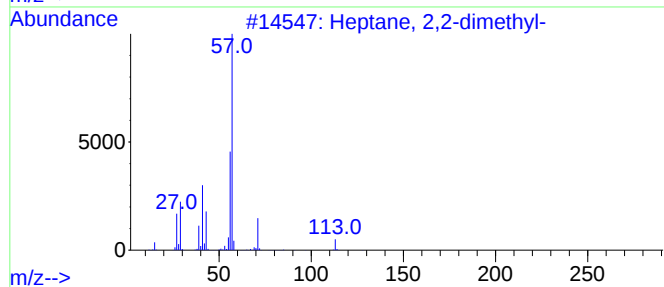
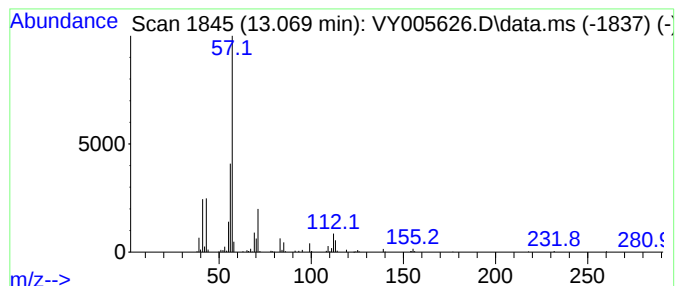
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Peak Number 5 Heptane, 2,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.069	5.12 ug/l	140536	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	59
2			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59
3			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53
4			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	53
5			2,2-Dimethyleicosane	310	C22H46	1000360-43-4	45



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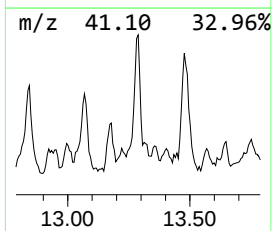
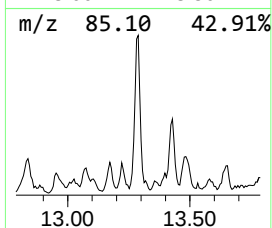
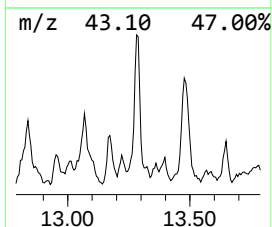
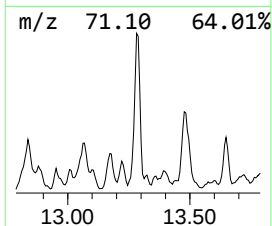
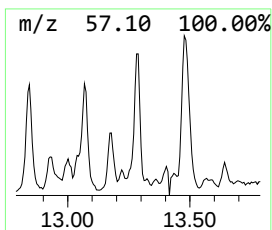
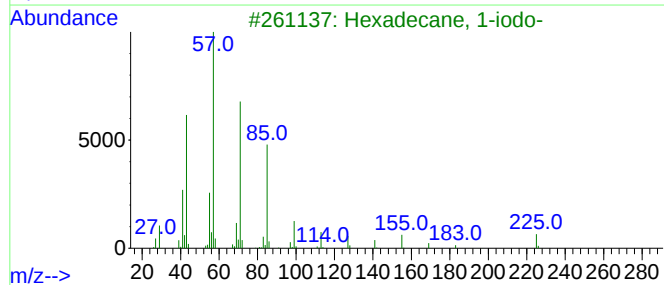
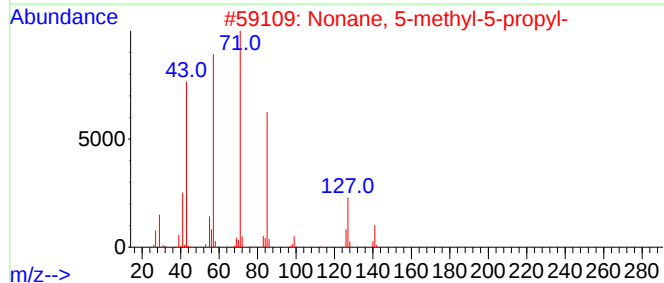
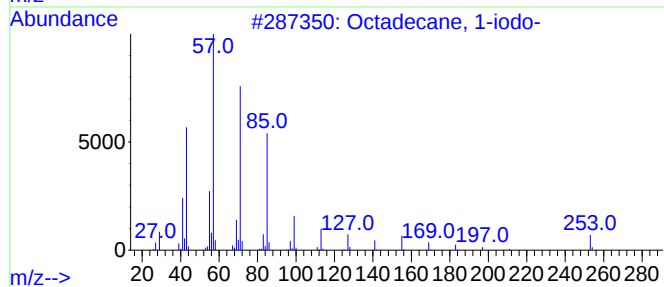
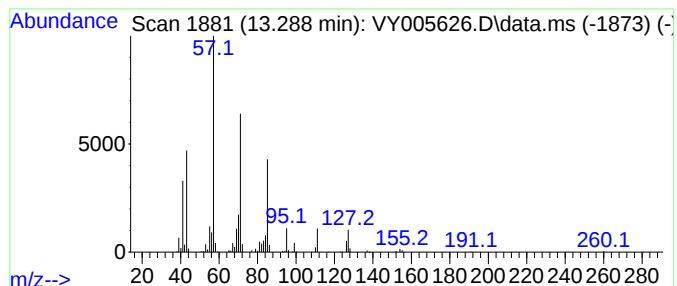
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080221S.M
Quant Title : SW846 8260

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

Peak Number 6 Octadecane, 1-iodo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.288	9.55 ug/l	262181	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64
2			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	59
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	59
4			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	58
5			Nonane, 5-butyl-	184	C13H28	017312-63-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081221\
Data File : VY005626.D
Acq On : 12 Aug 2021 16:38
Operator : SY/MD
Sample : M3343-08
Misc : 5.00G/5ML/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20210582-COM-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080221S.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
Dimethyl sulfide	4.040	7.4	ug/l	100166	1	7.795	680125	50.0
Heptane, 3-ethy...	12.233	5.2	ug/l	135387	3	11.496	1303200	50.0
Oxalic acid, is...	12.843	8.7	ug/l	238385	4	13.428	1373050	50.0
Heptane, 2,2-di...	13.069	5.1	ug/l	140536	4	13.428	1373050	50.0
Octadecane, 1-i...	13.288	9.6	ug/l	262181	4	13.428	1373050	50.0