

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042921\
 Data File : VY004673.D
 Acq On : 29 Apr 2021 20:41
 Operator : SY/MD
 Sample : M2217-06
 Misc : 4.92G/5ML/MSVOA_Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 HPCR2-COMP-CF03-01

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\82Y041221S.M
 Title : SW846 8260

Signal : TIC: VY004673.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.077	37	42	47	rBV2	7558	11968	1.19%	0.160%
2	2.253	67	71	79	rVB	17969	29202	2.90%	0.389%
3	2.912	172	179	186	rVB3	14179	30297	3.01%	0.404%
4	3.259	230	236	244	rVB3	9750	23038	2.29%	0.307%
5	4.729	465	477	497	rBV4	32798	122013	12.14%	1.627%
6	5.759	636	646	660	rVB3	14325	42643	4.24%	0.568%
7	6.801	803	817	828	rVB4	7598	24601	2.45%	0.328%
8	7.728	959	969	974	rBV2	123060	292125	29.06%	3.894%
9	7.795	974	980	990	rVB	236708	543859	54.09%	7.250%
10	8.002	1007	1014	1021	rBV5	5356	13700	1.36%	0.183%
11	8.149	1021	1038	1048	rVV2	163699	508070	50.53%	6.773%
12	8.551	1096	1104	1113	rVB3	15976	31947	3.18%	0.426%
13	8.697	1120	1128	1137	rBV	350175	677736	67.41%	9.035%
14	9.185	1195	1208	1215	rBV	48339	105754	10.52%	1.410%
15	9.612	1270	1278	1286	rVB3	7759	16793	1.67%	0.224%
16	9.752	1293	1301	1307	rBV2	17222	35308	3.51%	0.471%
17	9.819	1307	1312	1323	rVB6	8122	23041	2.29%	0.307%
18	9.959	1327	1335	1339	rBV4	6793	15653	1.56%	0.209%
19	10.185	1365	1372	1381	rBV	582394	1005397	100.00%	13.403%
20	10.264	1381	1385	1389	rBV3	10667	19673	1.96%	0.262%
21	10.374	1396	1403	1408	rVB6	9431	20918	2.08%	0.279%
22	10.581	1431	1437	1454	rVB2	35601	82038	8.16%	1.094%
23	11.038	1505	1512	1517	rBV2	16140	26106	2.60%	0.348%
24	11.093	1517	1521	1526	rVB2	8611	13593	1.35%	0.181%
25	11.319	1547	1558	1564	rVB2	43702	84747	8.43%	1.130%
26	11.489	1579	1586	1596	rBV	520836	861328	85.67%	11.482%
27	11.593	1596	1603	1606	rBV5	5112	10141	1.01%	0.135%
28	11.709	1612	1622	1624	rBV8	6276	16268	1.62%	0.217%
29	11.739	1624	1627	1632	rVV2	10083	19516	1.94%	0.260%
30	12.002	1664	1670	1679	rBV8	7943	20935	2.08%	0.279%
31	12.245	1705	1710	1716	rVB4	10607	21780	2.17%	0.290%
32	12.483	1740	1749	1756	rBV3	464814	819291	81.49%	10.922%
33	12.575	1756	1764	1768	rBV5	8352	19774	1.97%	0.264%
34	12.630	1768	1773	1783	rVB3	30001	76543	7.61%	1.020%
35	12.727	1783	1789	1796	rBV10	5499	15623	1.55%	0.208%
36	12.837	1796	1807	1814	rBV4	30123	89248	8.88%	1.190%

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Instrument :
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 ClientSampleId :
 HTRCV2-COMP-CF03-01

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	13.044	1833	1841	1842	rVV2	20727	42071	4.18%	0.561%
38	13.068	1842	1845	1853	rVB	94014	136034	13.53%	1.813%
39	13.178	1858	1863	1870	rBV2	47519	77540	7.71%	1.034%
40	13.282	1870	1880	1885	rBV	136863	254738	25.34%	3.396%
41	13.428	1895	1904	1909	rBV	524550	824486	82.01%	10.991%
42	13.483	1909	1913	1923	rVB	114065	239121	23.78%	3.188%
43	13.648	1932	1940	1948	rBV2	36487	74733	7.43%	0.996%
44	13.971	1987	1993	2006	rVB3	17956	45811	4.56%	0.611%
45	14.257	2036	2040	2047	rVB7	6351	10810	1.08%	0.144%
46	14.422	2063	2067	2074	rVB8	6938	11081	1.10%	0.148%
47	15.318	2209	2214	2221	rVB	8632	14360	1.43%	0.191%

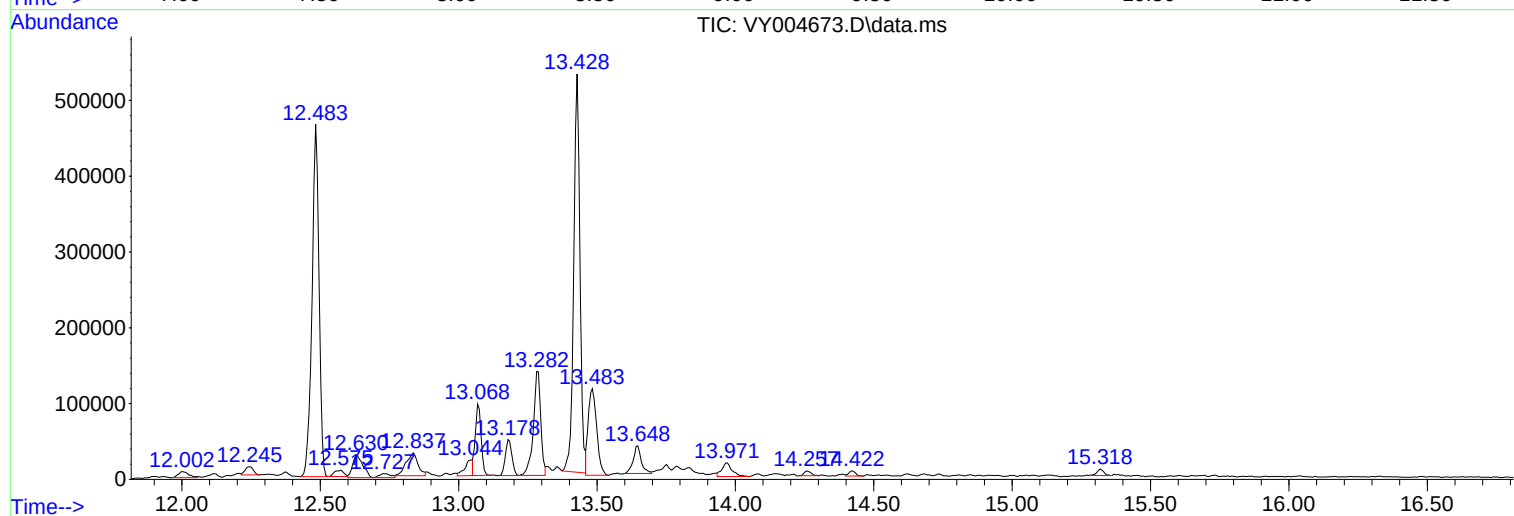
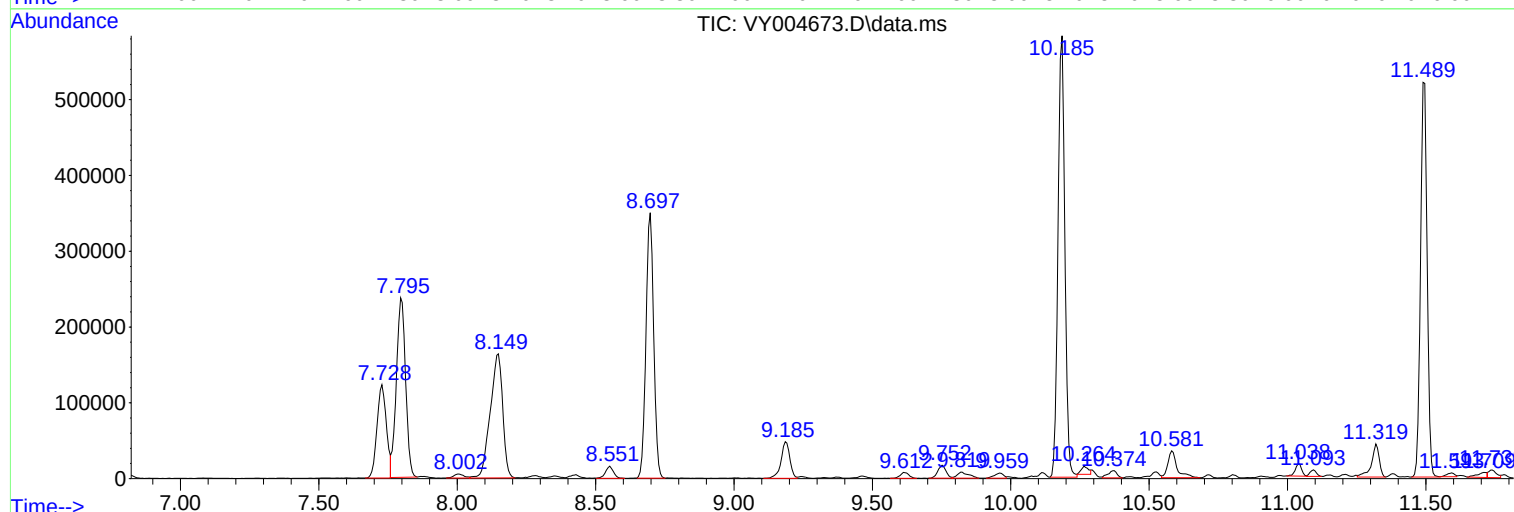
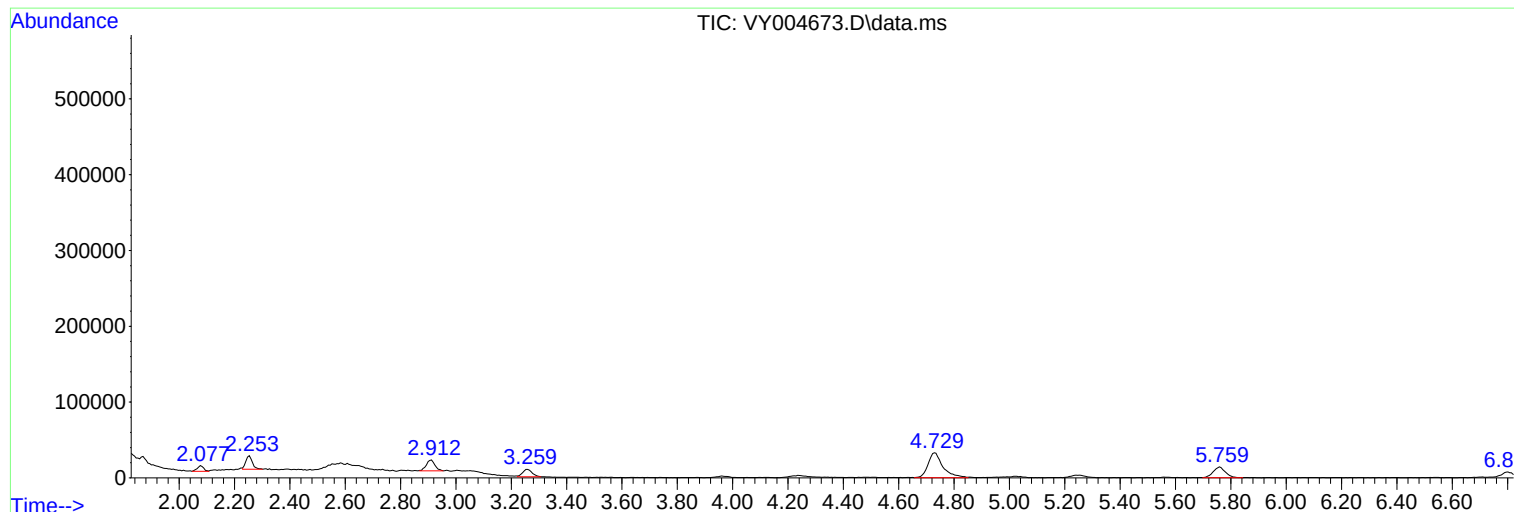
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ClientSampleId :
HTCRV2-COMP-CF03-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_Y
ClientSampleId :
HTCRV2-COMP-CF03-01

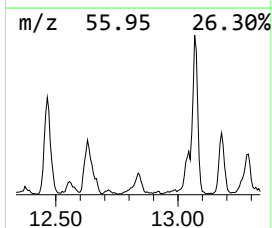
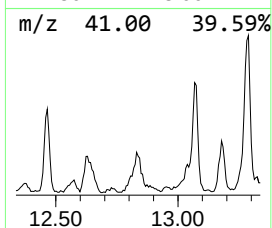
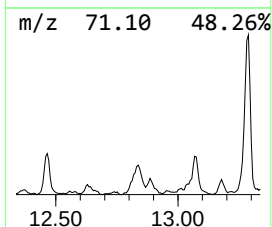
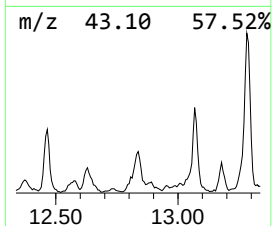
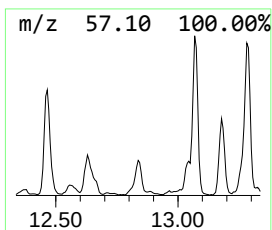
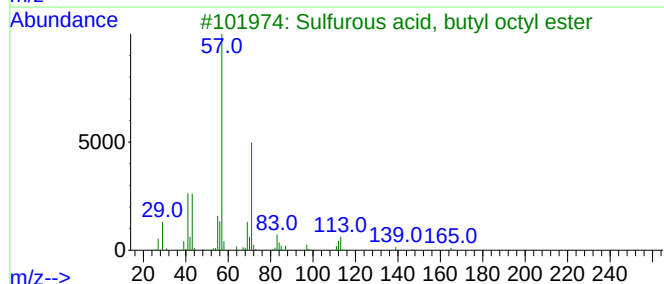
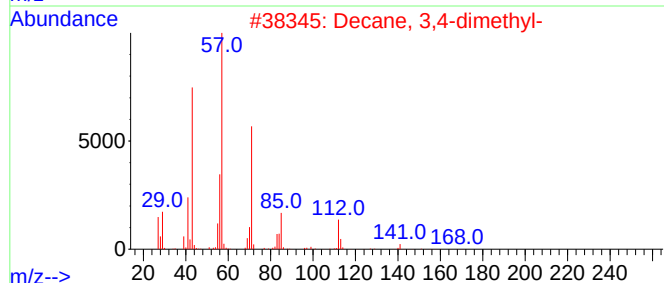
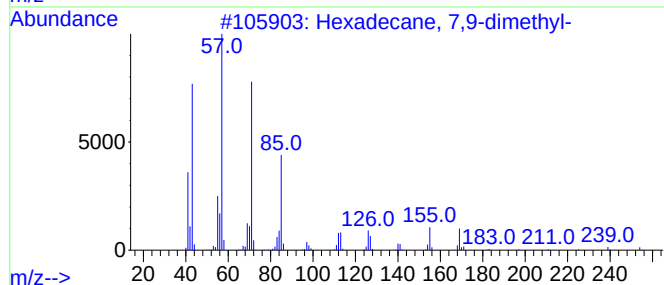
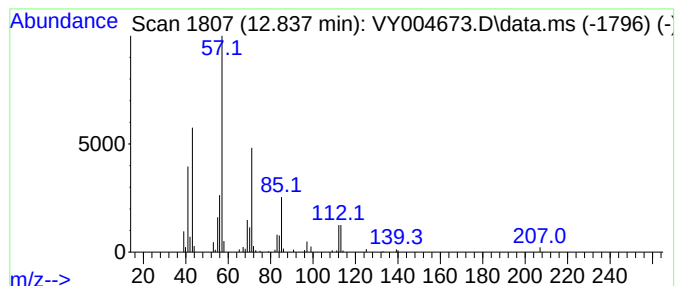
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecane, 7,9-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.837	5.41 ug/l	89248	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	64
2			Decane, 3,4-dimethyl-	170	C12H26	017312-45-7	64
3			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	59
4			Nonane, 3-methyl-	142	C10H22	005911-04-6	53
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	53



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Instrument :
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ClientSampleId :
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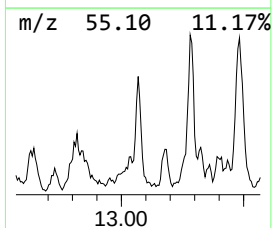
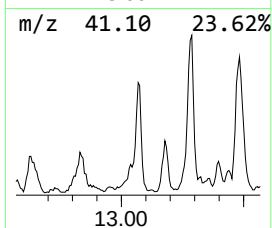
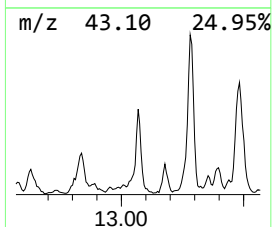
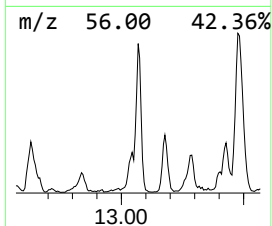
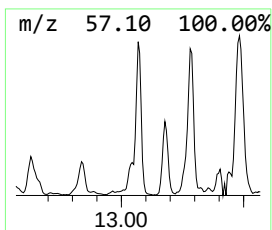
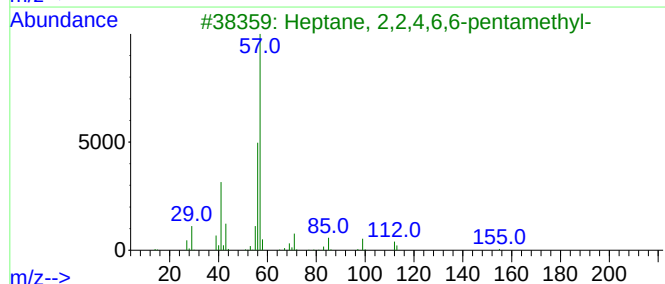
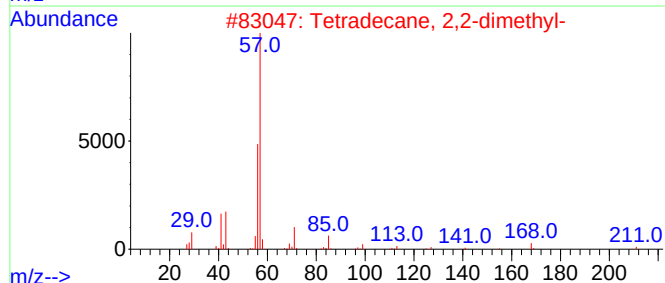
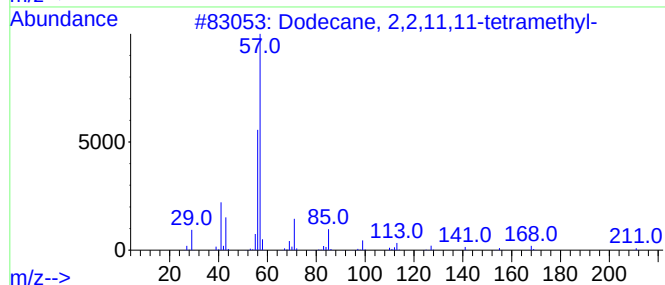
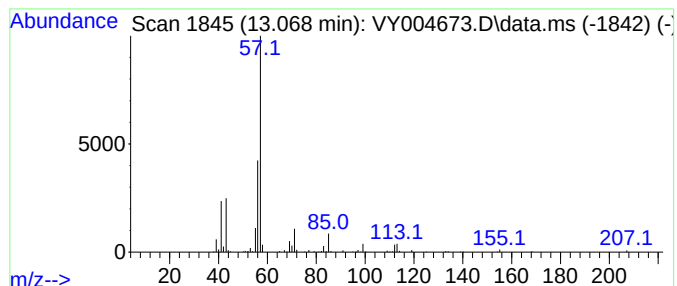
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane, 2,2,11,11-tetrame... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.069	8.25 ug/l	136034	1,4-Dichlorobenzene-d4	13.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	72
2		Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	72
3		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
4		Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	64
5		2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	64



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Instrument :
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ClientSampleId :
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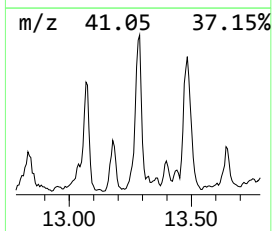
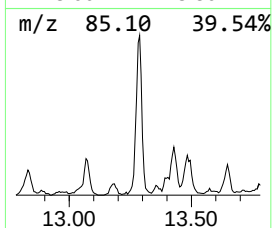
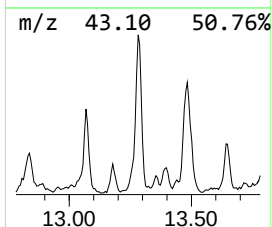
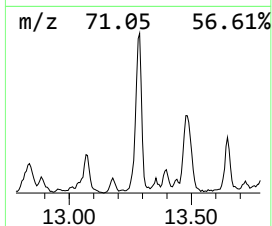
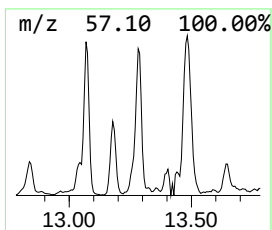
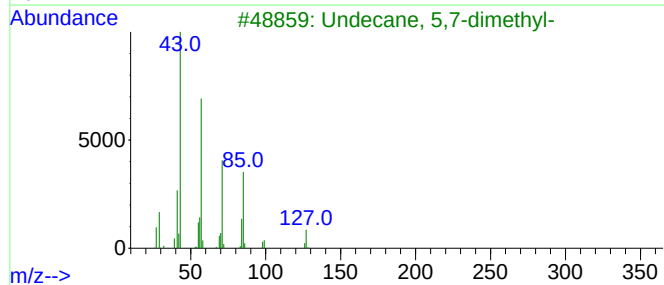
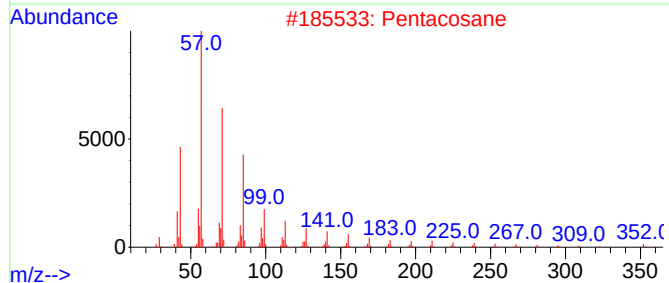
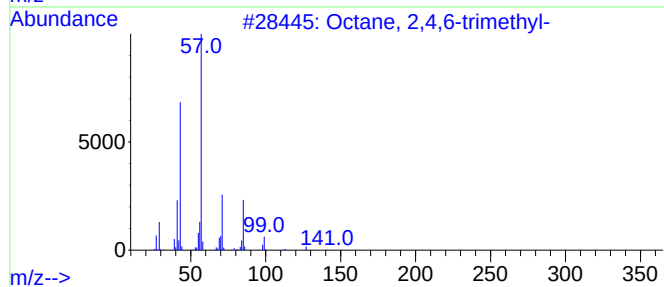
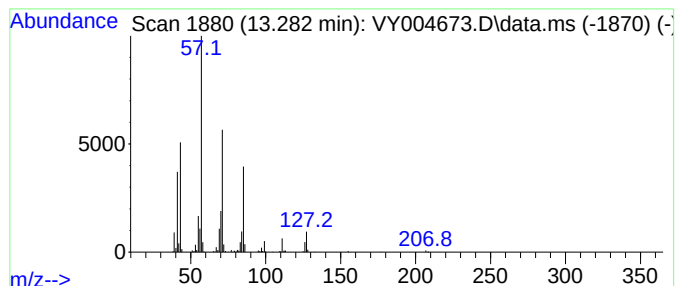
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041221S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octane, 2,4,6-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	15.45 ug/l	254738	1,4-Dichlorobenzene-d4	13.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
2		Pentacosane	352	C25H52	000629-99-2	78
3		Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	78
4		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
5		Undecane	156	C11H24	001120-21-4	64



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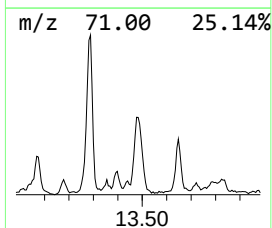
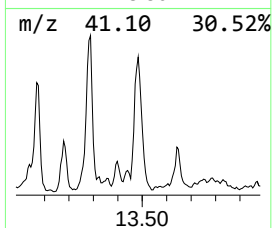
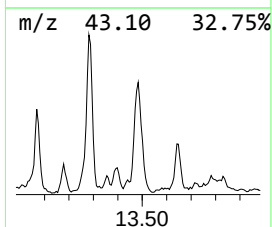
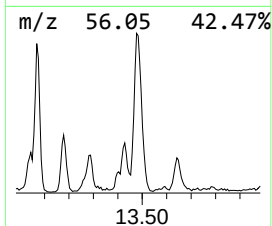
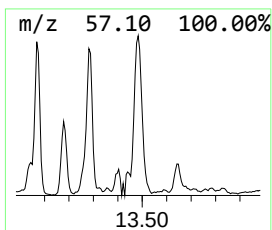
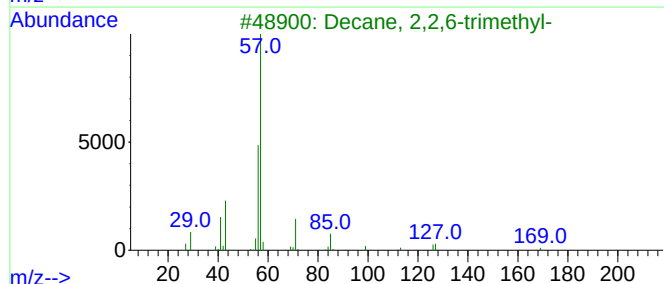
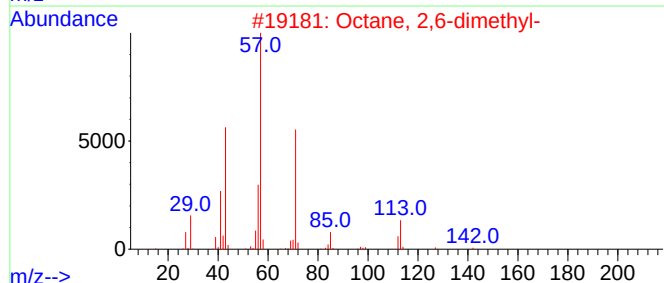
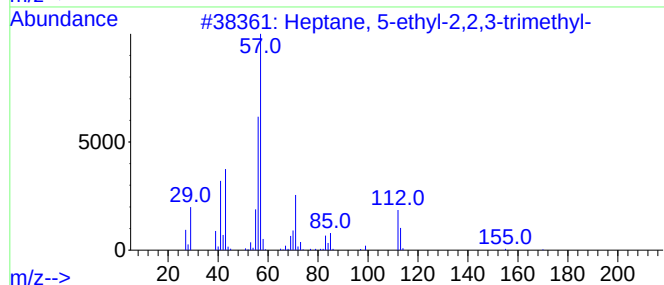
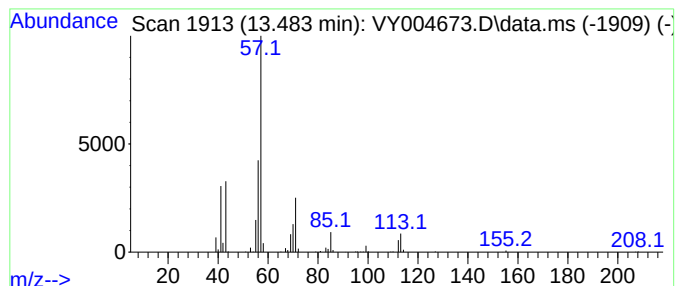
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptane, 5-ethyl-2,2,3-trim... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.483	14.50 ug/l	239121	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 5-ethyl-2,2,3-trimethyl-	170	C12H26	062199-06-8	78
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3			Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	59
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	59
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecane, 7,9...	12.837	5.4	ug/l	89248	4	13.428	824486	50.0
Dodecane, 2,2,1...	13.069	8.3	ug/l	136034	4	13.428	824486	50.0
Octane, 2,4,6-t...	13.282	15.4	ug/l	254738	4	13.428	824486	50.0
Heptane, 5-ethy...	13.483	14.5	ug/l	239121	4	13.428	824486	50.0