

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
 Data File : VY009518.D
 Acq On : 11 Jul 2022 18:12
 Operator : KP/MD
 Sample : N3648-01
 Misc : 4.58g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CMR-TP1-0708

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\82Y070722S.M

Title : SW846 8260

Signal : TIC: VY009518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.900	9	13	20	rVB	13522	18560	3.21%	0.521%
2	4.704	463	473	489	rBV4	15291	51441	8.89%	1.445%
3	5.728	632	641	654	rVB4	5532	17496	3.02%	0.492%
4	6.972	834	845	861	rBV	24154	76711	13.26%	2.155%
5	7.710	955	966	971	rBV3	76739	178030	30.77%	5.002%
6	7.783	971	978	994	rVB	172812	397298	68.67%	11.162%
7	8.130	1021	1035	1046	rBV2	75006	203856	35.24%	5.727%
8	8.685	1117	1126	1136	rVB	257408	511515	88.41%	14.370%
9	10.173	1363	1370	1379	rBV	215807	361539	62.49%	10.157%
10	10.575	1429	1436	1442	rBV	9054	16242	2.81%	0.456%
11	10.941	1490	1496	1505	rBV	16149	28310	4.89%	0.795%
12	11.313	1549	1557	1565	rVB3	5645	9839	1.70%	0.276%
13	11.484	1578	1585	1598	rBV	350957	578552	100.00%	16.254%
14	12.477	1739	1748	1757	rBV	225308	374447	64.72%	10.520%
15	12.624	1766	1772	1777	rBV4	5003	9343	1.61%	0.262%
16	12.831	1797	1806	1812	rBV7	5921	14914	2.58%	0.419%
17	13.063	1840	1844	1850	rVB	16864	28809	4.98%	0.809%
18	13.178	1857	1863	1870	rVB2	9790	16403	2.84%	0.461%
19	13.282	1870	1880	1885	rBV	30821	57096	9.87%	1.604%
20	13.422	1896	1903	1908	rBV	333846	512270	88.54%	14.392%
21	13.477	1908	1912	1926	rVB2	28083	63842	11.03%	1.794%
22	13.648	1930	1940	1945	rBV4	9012	19078	3.30%	0.536%
23	13.959	1985	1991	1995	rBV5	3573	6194	1.07%	0.174%
24	15.312	2208	2213	2218	rBV2	4983	7704	1.33%	0.216%

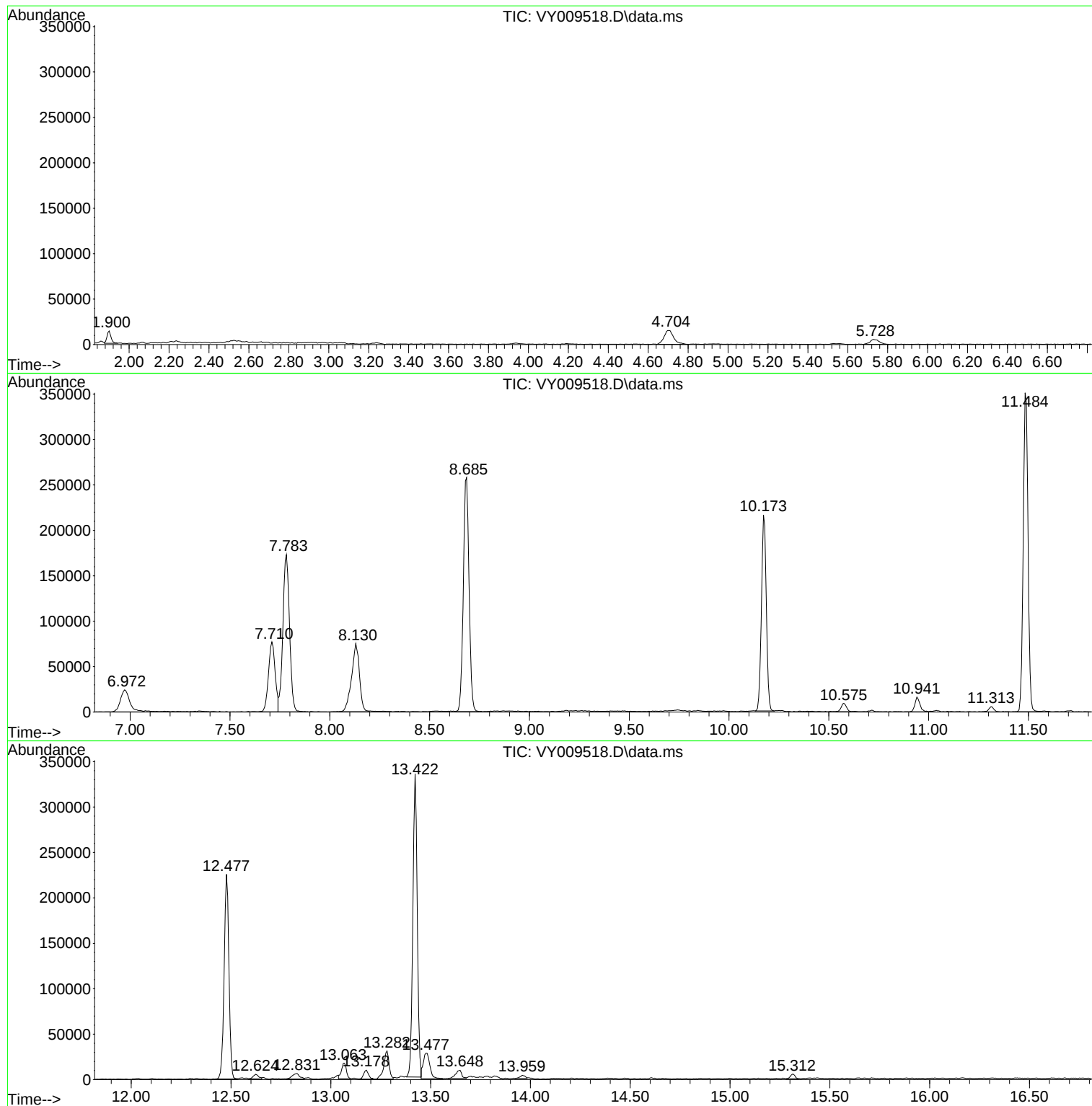
Sum of corrected areas: 3559489

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Quant Title : SW846 8260

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



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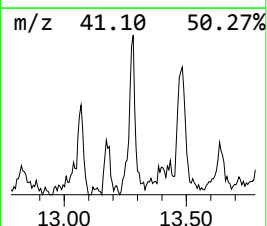
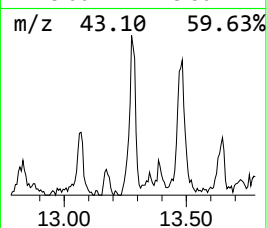
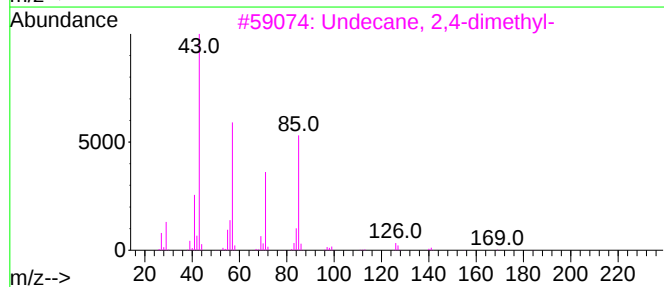
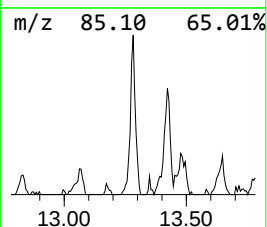
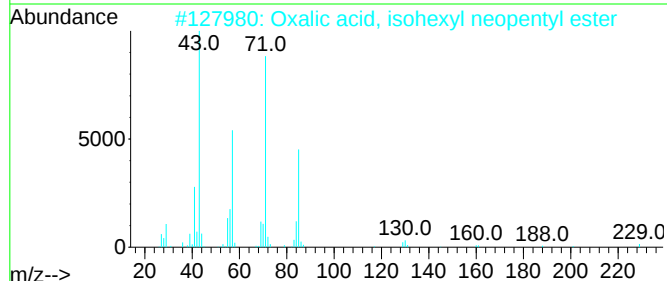
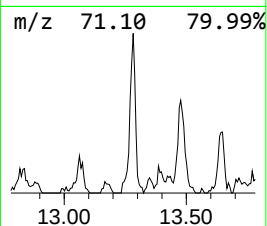
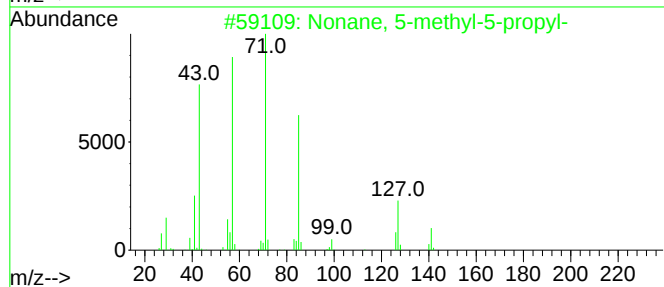
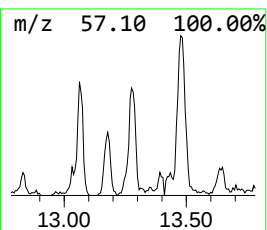
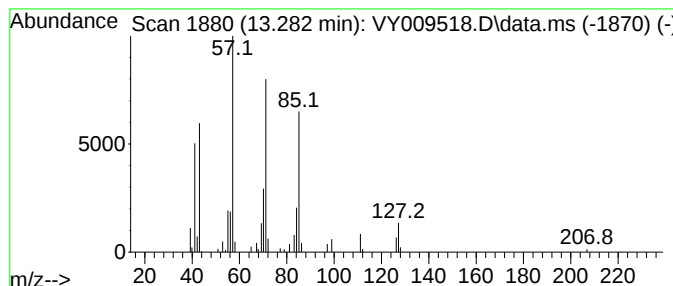
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 3 Nonane, 5-methyl-5-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	5.57 ug/l	57096	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	59
2			Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	53
3			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	53
4			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	53
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	49



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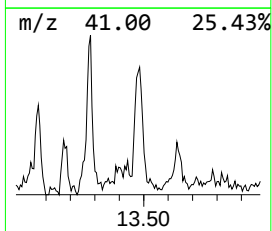
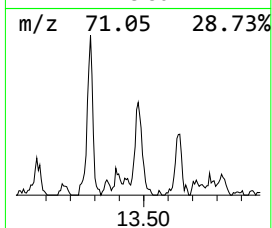
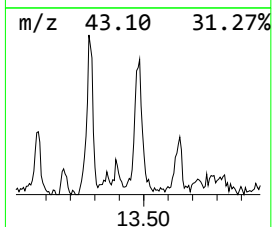
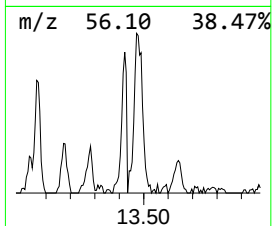
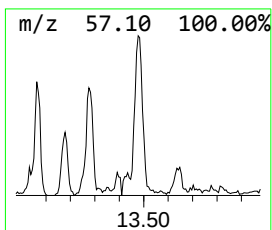
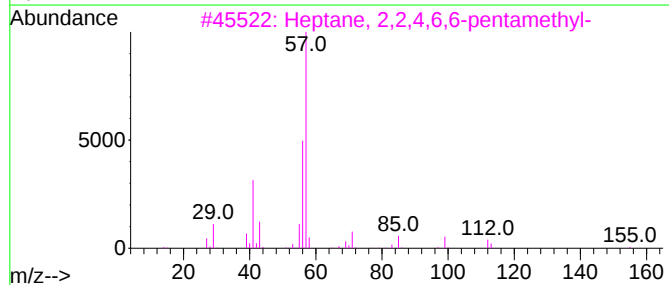
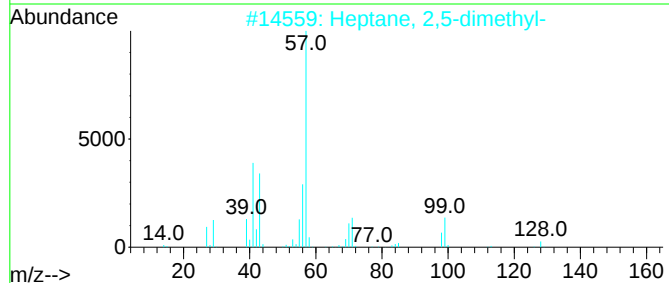
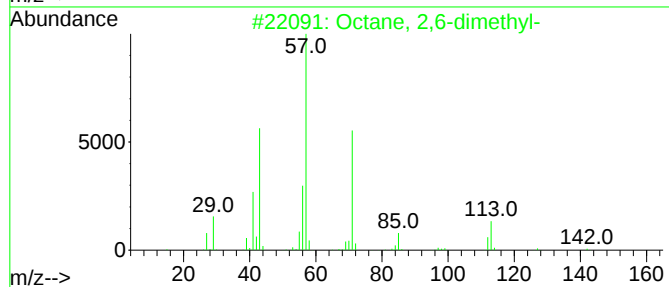
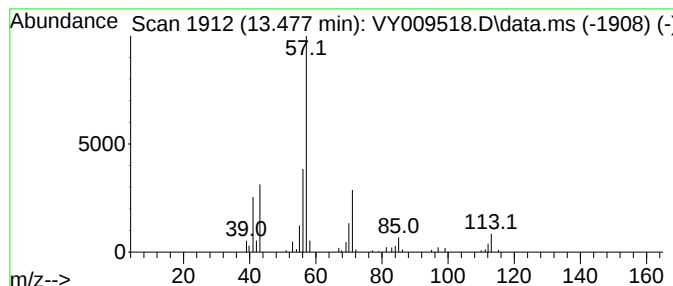
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Peak Number 4 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.477	6.23 ug/l	63842	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
2			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	53
3			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	53
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	47



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Nonane, 5-methy...	13.282	5.6	ug/l	57096	4	13.422	512270	50.0
Octane, 2,6-dim...	13.477	6.2	ug/l	63842	4	13.422	512270	50.0