

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
 Data File : VX043180.D
 Acq On : 26 Sep 2024 15:57
 Operator : JC/MD
 Sample : P4172-04
 Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 CHRT-20425

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\82X092324W.M
 Title : SW846 8260

Signal : TIC: VX043180.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	32	rBV2	5969	8077	1.71%	0.284%
2	1.563	68	78	79	rBV3	4586	10325	2.19%	0.363%
3	2.947	296	305	313	rBV	4596	11576	2.46%	0.407%
4	5.385	694	705	721	rBV	53066	158098	33.54%	5.557%
5	5.544	721	731	744	rVV	81213	227815	48.32%	8.007%
6	5.952	787	798	815	rBV	62618	169782	36.01%	5.968%
7	6.757	919	930	945	rBV	143308	343245	72.81%	12.064%
8	8.647	1233	1240	1249	rBV	301051	471428	100.00%	16.570%
9	10.055	1465	1471	1483	rBV	294269	411620	87.31%	14.468%
10	11.079	1634	1639	1655	rBV	237077	318488	67.56%	11.194%
11	12.024	1789	1794	1805	rBV	287255	379387	80.48%	13.335%
12	12.896	1929	1937	1942	rBV6	4979	12432	2.64%	0.437%
13	13.292	1996	2002	2008	rVB7	5001	9217	1.96%	0.324%
14	13.384	2013	2017	2026	rVV	27366	41279	8.76%	1.451%
15	13.457	2026	2029	2032	rVB4	4644	6390	1.36%	0.225%
16	13.554	2041	2045	2048	rBV6	3692	5063	1.07%	0.178%
17	13.609	2048	2054	2056	rBV6	2623	5786	1.23%	0.203%
18	13.676	2062	2065	2067	rBV4	4051	5022	1.07%	0.177%
19	13.737	2071	2075	2077	rVV4	8137	10956	2.32%	0.385%
20	13.768	2077	2080	2082	rVV3	6387	7500	1.59%	0.264%
21	13.798	2083	2085	2088	rVV3	6268	6940	1.47%	0.244%
22	13.841	2088	2092	2098	rVV	38060	48791	10.35%	1.715%
23	13.908	2099	2103	2110	rVB10	4907	10228	2.17%	0.359%
24	14.188	2145	2149	2152	rBV	11974	13593	2.88%	0.478%
25	14.408	2182	2185	2187	rBV2	6355	7842	1.66%	0.276%
26	14.609	2215	2218	2222	rBV2	26864	34816	7.39%	1.224%
27	14.755	2238	2242	2244	rBV5	7229	8363	1.77%	0.294%
28	14.792	2246	2248	2253	rVB5	7619	9987	2.12%	0.351%
29	14.963	2272	2276	2283	rVB9	10319	18840	4.00%	0.662%
30	15.213	2314	2317	2320	rVB	15011	16807	3.57%	0.591%
31	15.414	2346	2350	2356	rVB3	10704	16051	3.40%	0.564%
32	15.743	2400	2404	2410	rVB3	11511	19330	4.10%	0.679%
33	15.865	2421	2424	2430	rVB6	5611	7940	1.68%	0.279%
34	16.706	2558	2562	2568	rVB6	5956	12095	2.57%	0.425%

Sum of corrected areas: 2845109

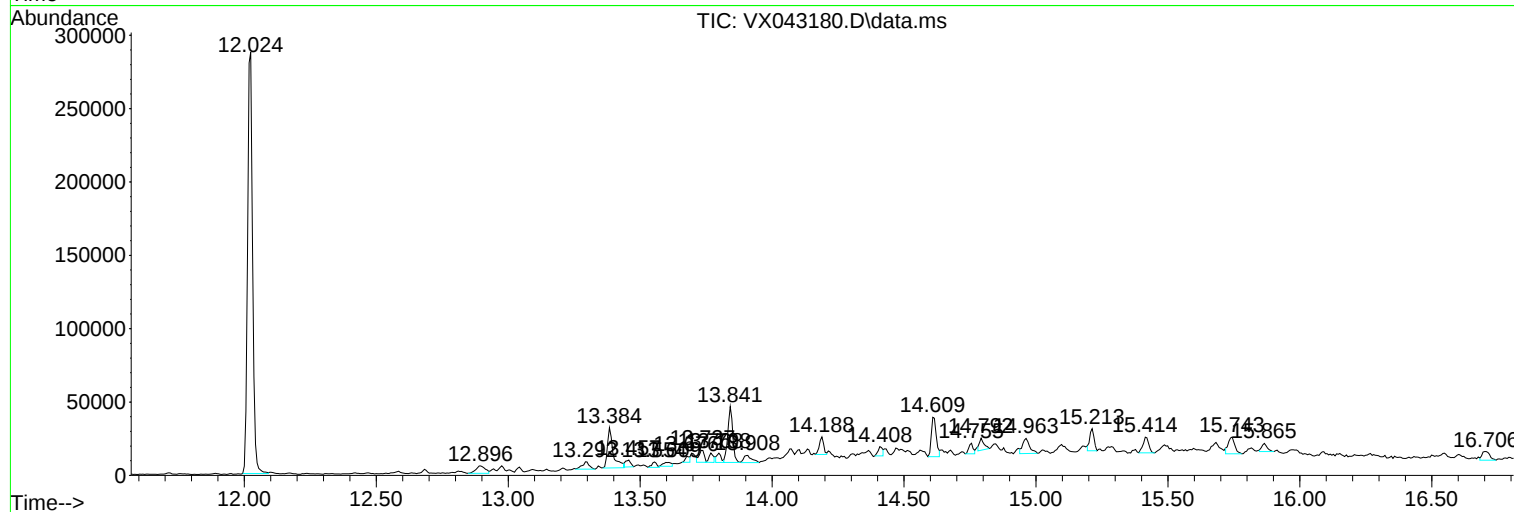
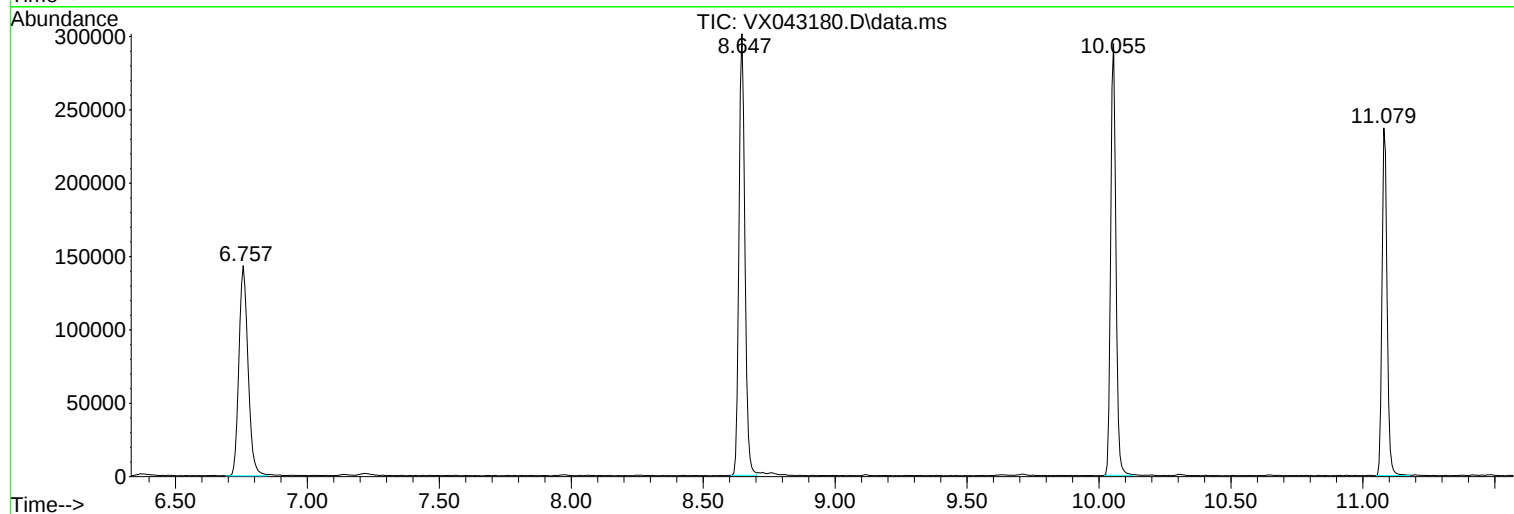
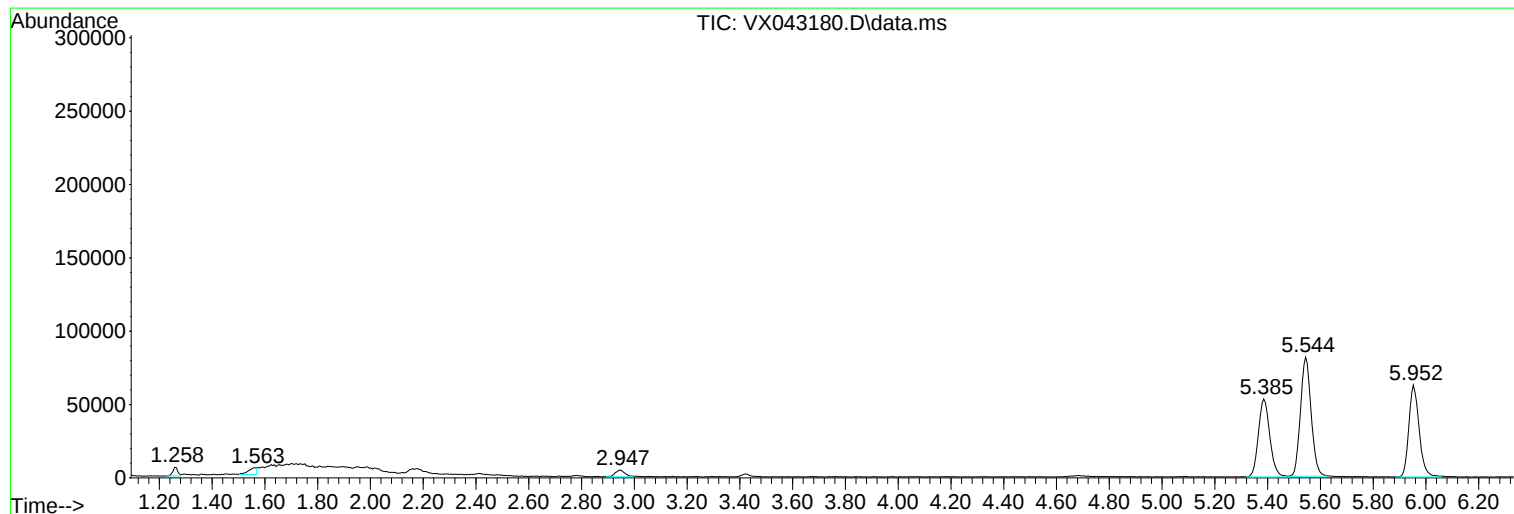
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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



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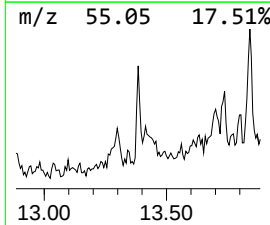
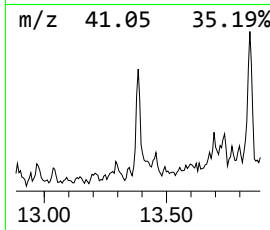
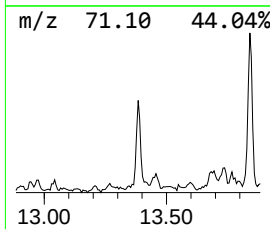
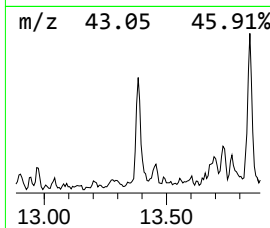
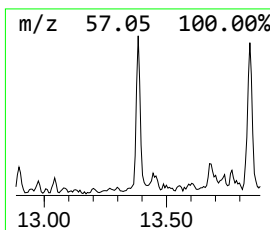
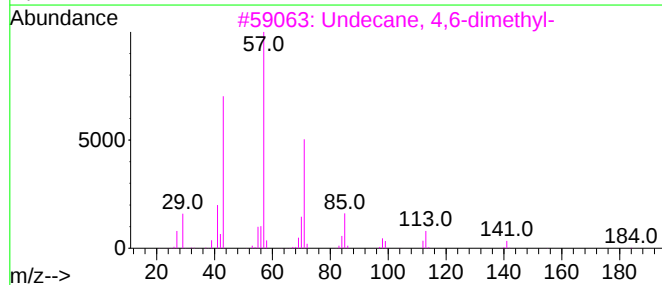
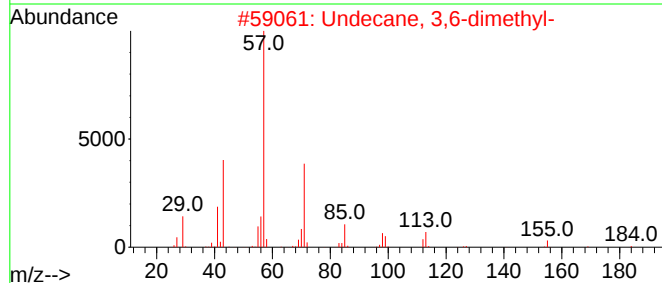
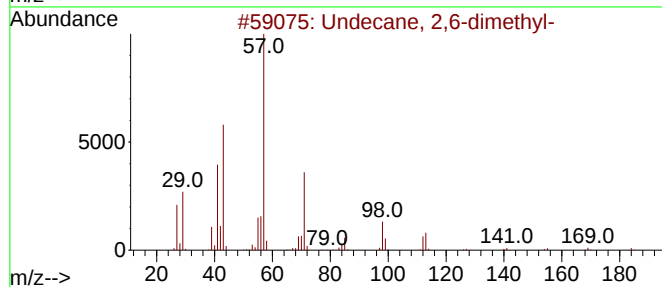
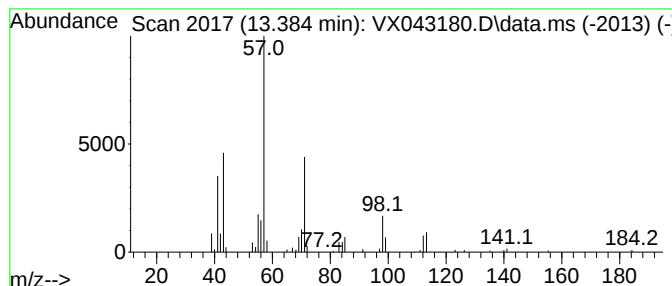
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Undecane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.384	5.44 ug/l	41279	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	91		
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	90		
3	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	86		
4	Dodecane, 6-methyl-	184	C13H28	006044-71-9	81		
5	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	70		



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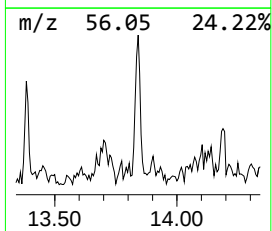
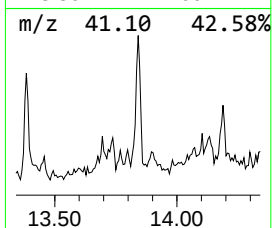
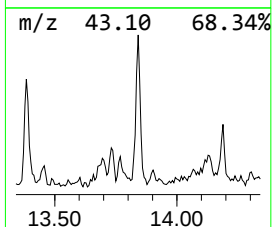
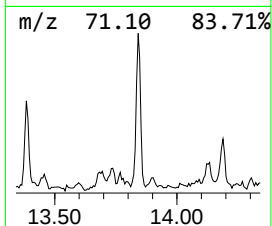
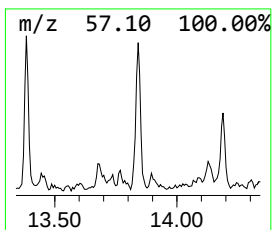
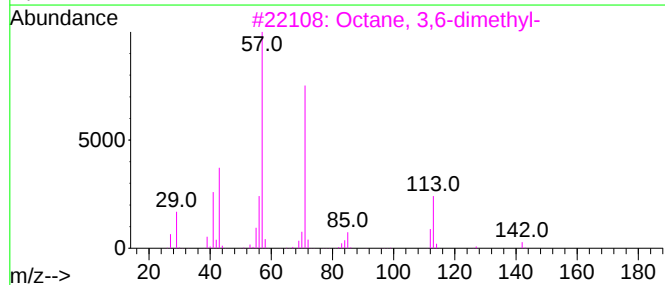
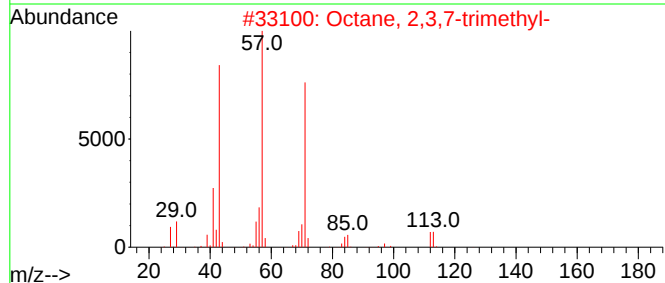
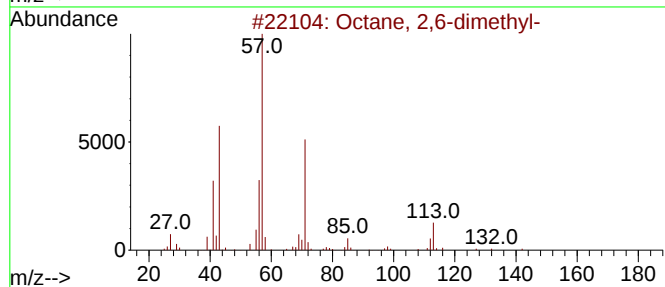
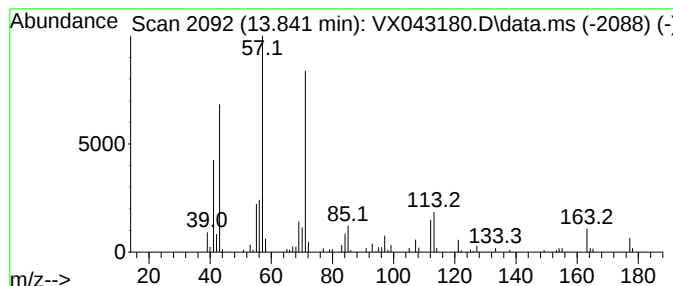
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	6.43 ug/l	48791	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
2			Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	72
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	72
4			Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	64
5			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Undecane, 2,6-d...	13.384	5.4	ug/l	41279	4	12.024	379387	50.0
Octane, 2,6-dim...	13.841	6.4	ug/l	48791	4	12.024	379387	50.0