

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
 Data File : VX039610.D
 Acq On : 03 Jan 2024 18:15
 Operator : JC/MD
 Sample : P1002-11
 Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1132

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\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039610.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	22	28	34	rBV2	4633	10459	1.47%	0.206%
2	1.575	68	80	81	rBV3	9530	25325	3.56%	0.500%
3	2.953	298	306	314	rBV2	3872	10146	1.43%	0.200%
4	5.391	694	706	719	rBV2	68015	207431	29.14%	4.094%
5	5.544	721	731	748	rVB	106157	308007	43.27%	6.078%
6	5.952	788	798	816	rBV	78707	225823	31.72%	4.457%
7	6.757	920	930	947	rBV	196102	490641	68.93%	9.683%
8	7.220	999	1006	1022	rVB3	2158	7888	1.11%	0.156%
9	8.647	1233	1240	1249	rBV	417380	679929	95.52%	13.418%
10	8.720	1249	1252	1256	rVB2	5226	7418	1.04%	0.146%
11	10.055	1465	1471	1484	rBV	466074	677093	95.12%	13.362%
12	10.305	1504	1512	1518	rBV2	9049	14961	2.10%	0.295%
13	11.079	1634	1639	1651	rBV	394986	541311	76.04%	10.683%
14	11.476	1701	1704	1709	rVB2	5447	7640	1.07%	0.151%
15	11.756	1746	1750	1759	rVB3	6851	11776	1.65%	0.232%
16	11.969	1782	1785	1789	rVB2	15571	18031	2.53%	0.356%
17	12.024	1789	1794	1800	rBV	539516	711841	100.00%	14.048%
18	12.097	1804	1806	1811	rVB4	6044	7376	1.04%	0.146%
19	12.317	1836	1842	1848	rVB8	7029	16165	2.27%	0.319%
20	12.421	1855	1859	1864	rBV	111393	125178	17.59%	2.470%
21	12.469	1864	1867	1872	rVB5	7334	13680	1.92%	0.270%
22	12.555	1875	1881	1882	rBV5	7322	12642	1.78%	0.249%
23	12.585	1882	1886	1892	rVV4	12285	20585	2.89%	0.406%
24	12.683	1898	1902	1905	rBV	17369	20939	2.94%	0.413%
25	12.817	1920	1924	1928	rVB3	12261	15336	2.15%	0.303%
26	12.890	1928	1936	1942	rBV5	36640	87515	12.29%	1.727%
27	12.939	1942	1944	1947	rBV	16719	20133	2.83%	0.397%
28	12.975	1947	1950	1957	rVB3	37608	49893	7.01%	0.985%
29	13.042	1957	1961	1965	rVB	30886	35052	4.92%	0.692%
30	13.085	1965	1968	1974	rVB7	4808	8331	1.17%	0.164%
31	13.140	1974	1977	1985	rBV4	20796	33391	4.69%	0.659%
32	13.207	1985	1988	1991	rBV4	6719	8361	1.17%	0.165%
33	13.262	1993	1997	2001	rBV	292154	358979	50.43%	7.084%
34	13.347	2008	2011	2013	rBV3	11767	13621	1.91%	0.269%
35	13.384	2013	2017	2020	rBV	68372	81007	11.38%	1.599%
36	13.414	2020	2022	2026	rVB4	9991	12654	1.78%	0.250%

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Integration Parameters: RTEINT.P

Integrator: RTE

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Start Thrs: 0.2

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Stop Thrs : 0

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37	13.493	2032	2035	2041	rBV6	7382	13057	1.83%	0.258%
38	13.591	2047	2051	2054	rBV5	4875	8555	1.20%	0.169%
39	13.682	2060	2066	2067	rBV4	11845	17232	2.42%	0.340%
40	13.701	2067	2069	2071	rVV2	14385	16221	2.28%	0.320%
41	13.731	2071	2074	2078	rVV2	21679	35004	4.92%	0.691%
42	13.768	2078	2080	2083	rVV4	12160	15499	2.18%	0.306%
43	13.798	2083	2085	2088	rVV3	8684	9361	1.32%	0.185%
44	13.835	2088	2091	2095	rVB4	12570	17685	2.48%	0.349%
45	14.036	2120	2124	2128	rVB	19751	20578	2.89%	0.406%
46	14.438	2186	2190	2193	rVB	8292	9926	1.39%	0.196%
47	14.755	2237	2242	2245	rBV4	5993	7533	1.06%	0.149%

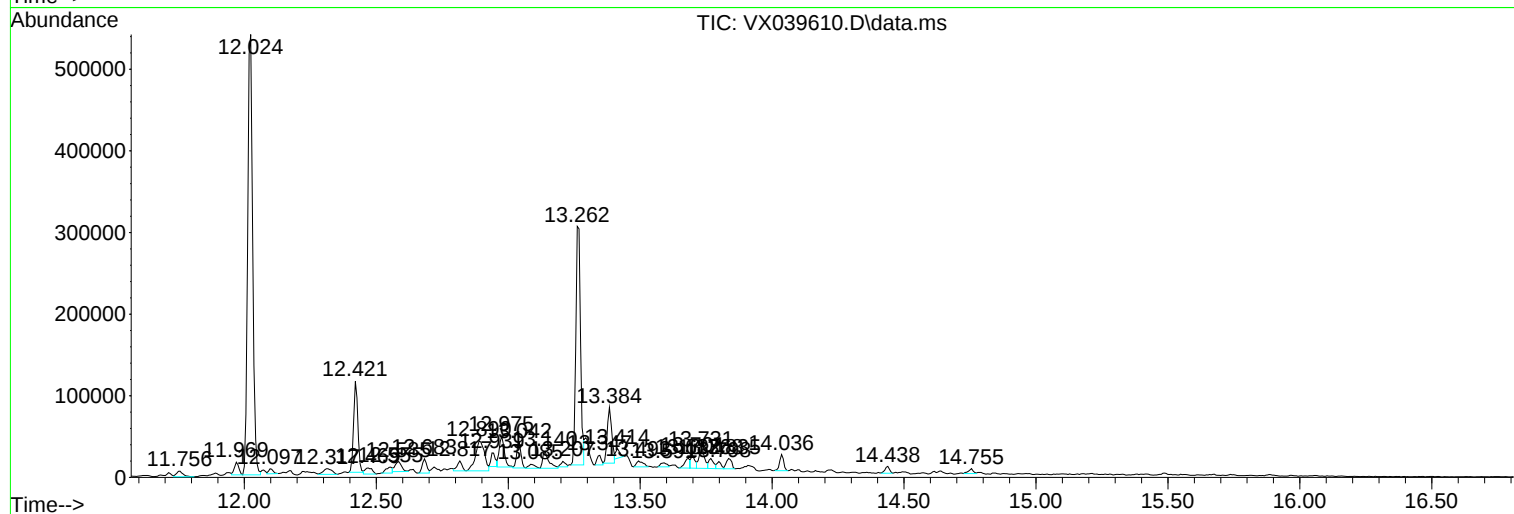
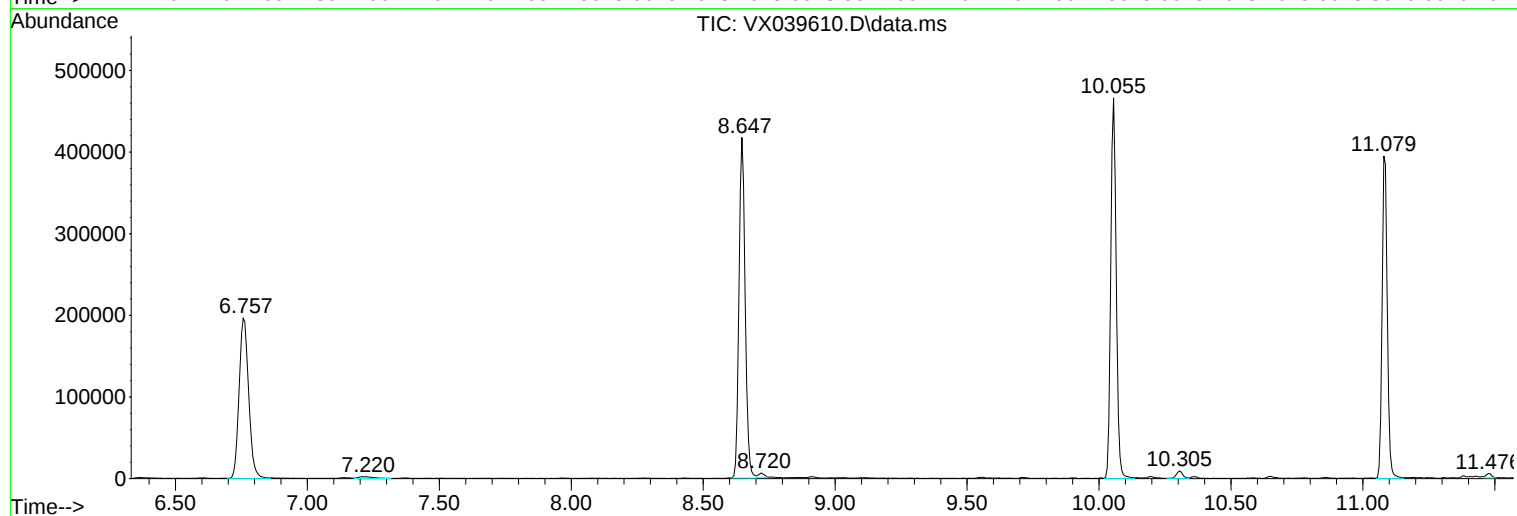
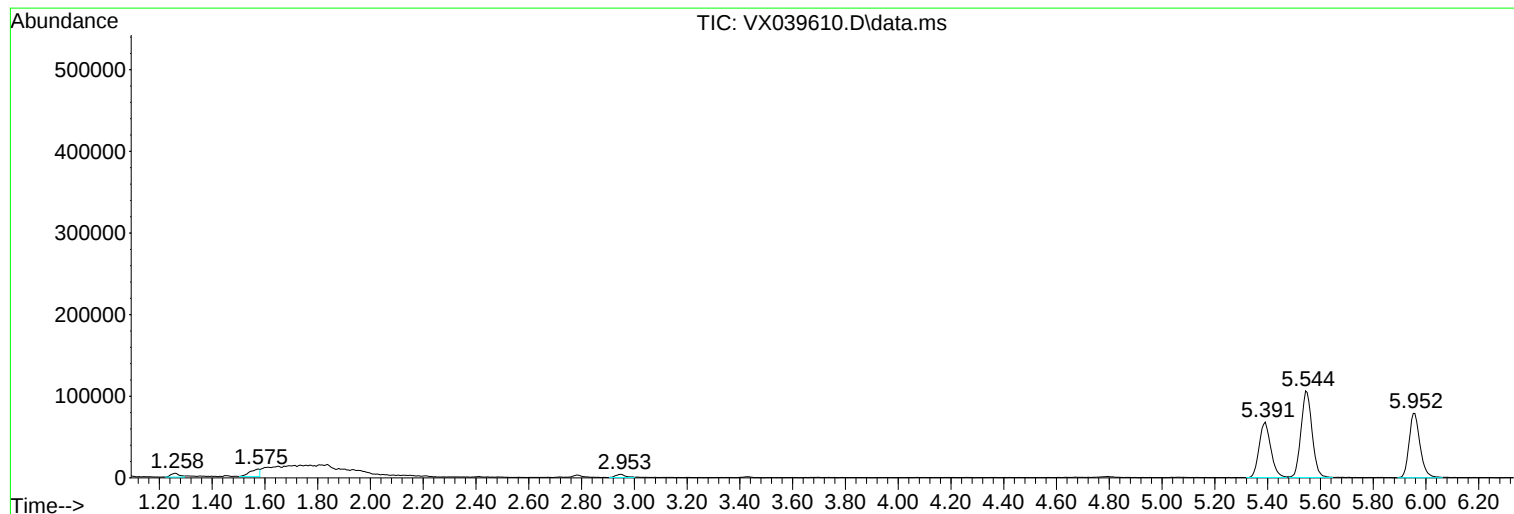
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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Instrument :
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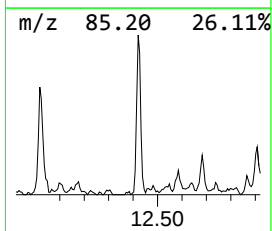
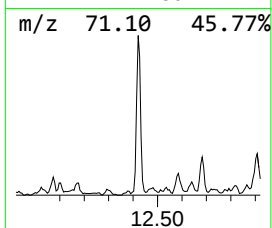
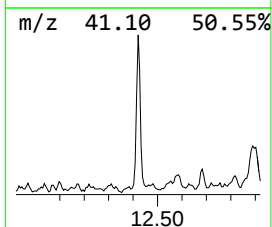
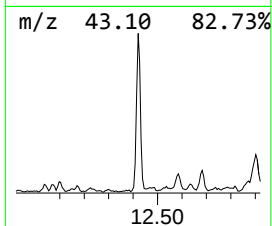
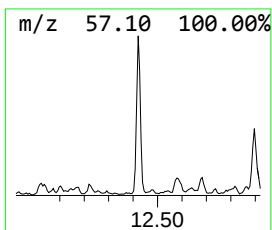
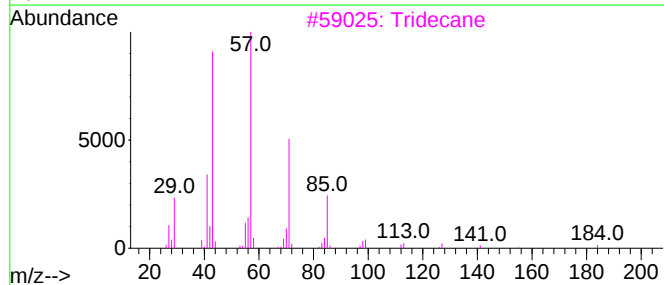
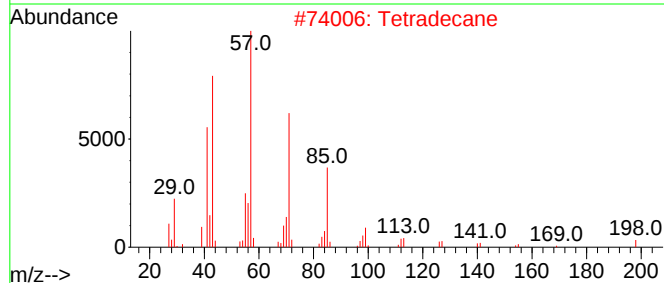
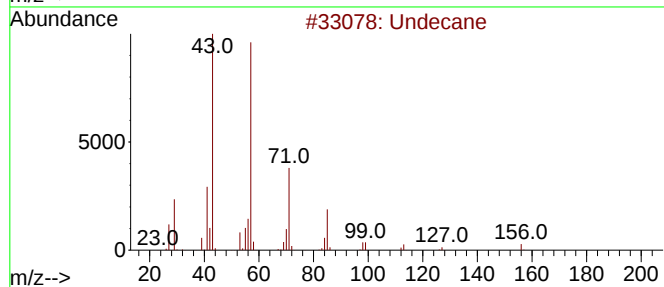
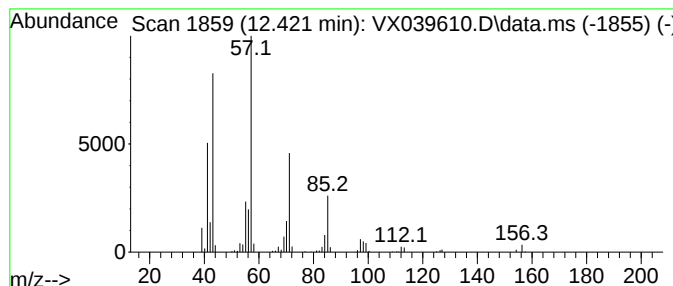
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	8.79 ug/l	125178	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane		156	C11H24	001120-21-4	91
2	Tetradecane		198	C14H30	000629-59-4	90
3	Tridecane		184	C13H28	000629-50-5	64
4	Decane, 2,3,7-trimethyl-		184	C13H28	062238-13-5	59
5	Nonadecane		268	C19H40	000629-92-5	53



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Instrument :
MSVOA_X
ClientSampleId :
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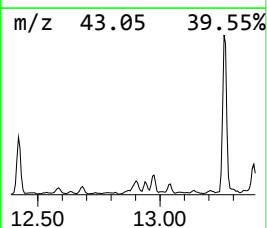
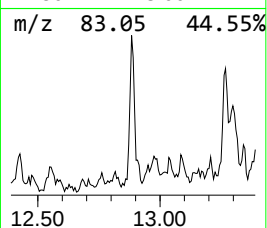
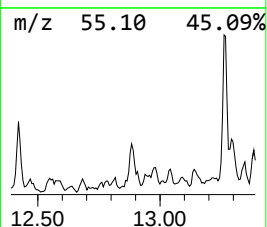
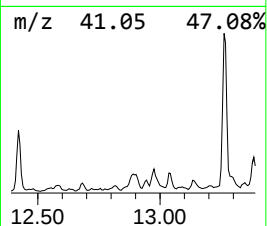
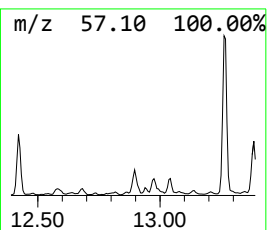
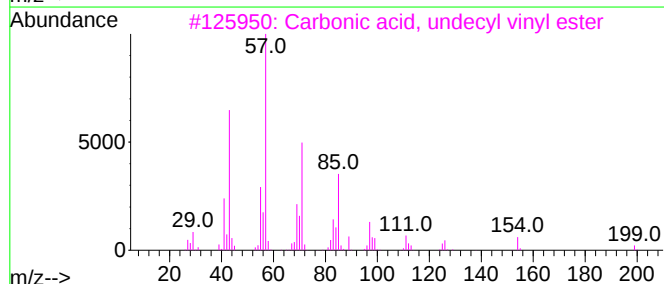
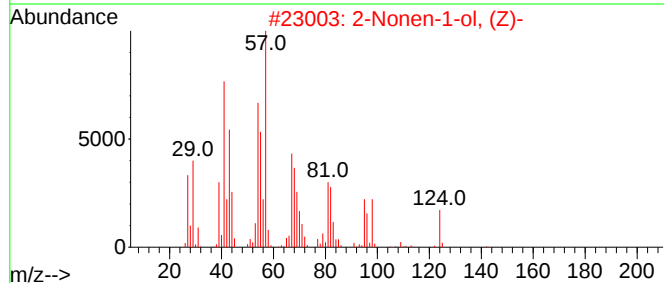
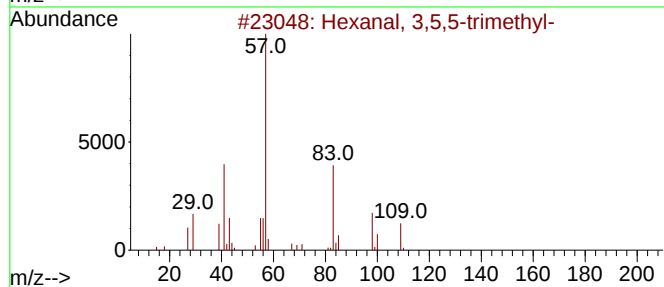
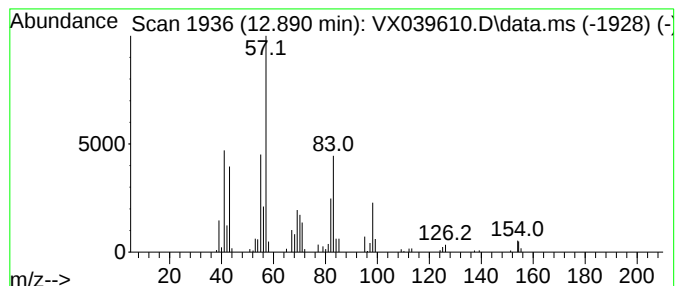
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.890 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	6.15 ug/l	87515	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	47
2			2-Nonen-1-ol, (Z)-	142	C9H18O	041453-56-9	38
3			Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	35
4			Octane, 4,5-dipropyl-	198	C14H30	020905-05-9	35
5			Propanoic acid, 2,2-dimethyl-, c...	184	C11H20O2	029878-49-7	32



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Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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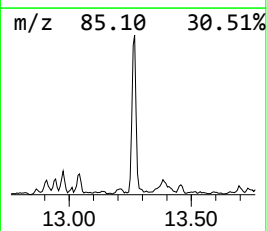
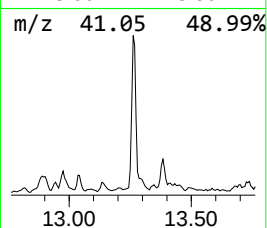
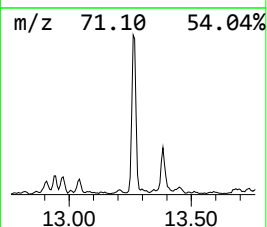
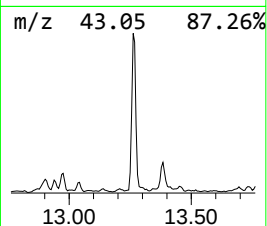
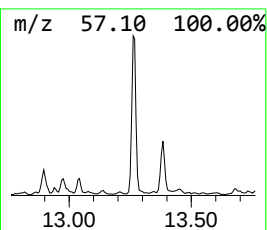
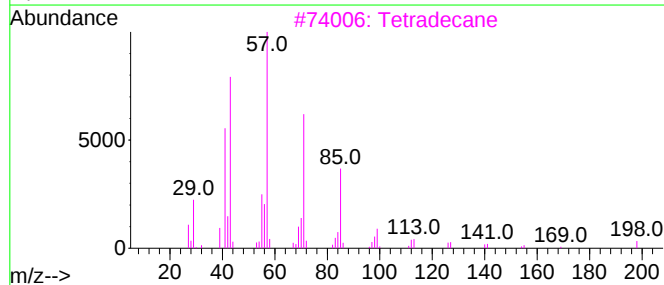
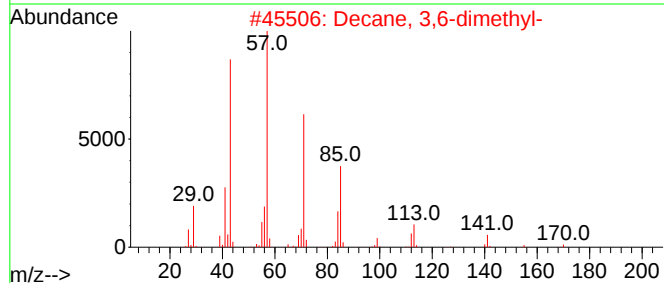
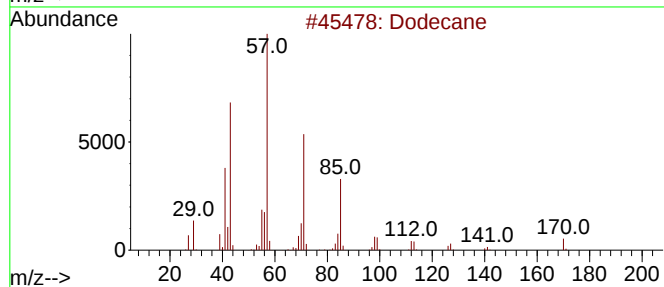
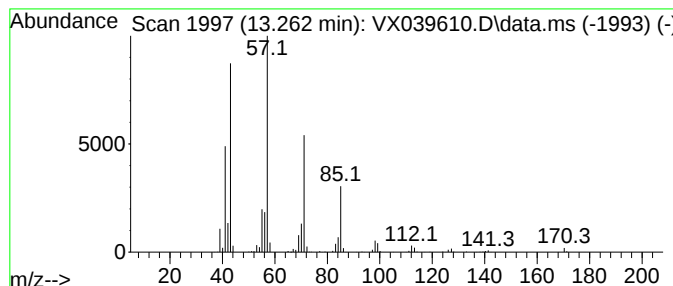
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 3 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.262	25.21 ug/l	358979	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	86
3			Tetradecane	198	C14H30	000629-59-4	83
4			2,6-Dimethyldecane	170	C12H26	013150-81-7	64
5			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	59



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ClientSampleId :
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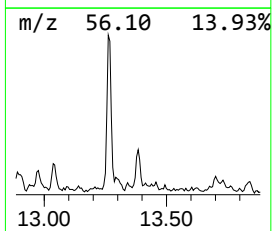
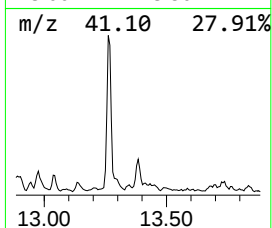
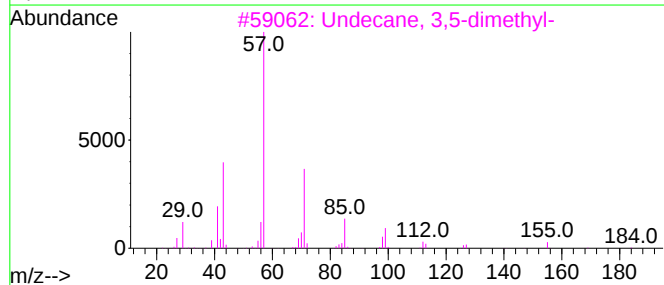
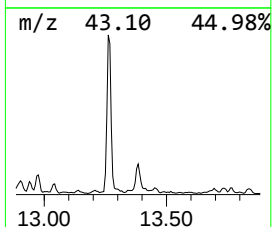
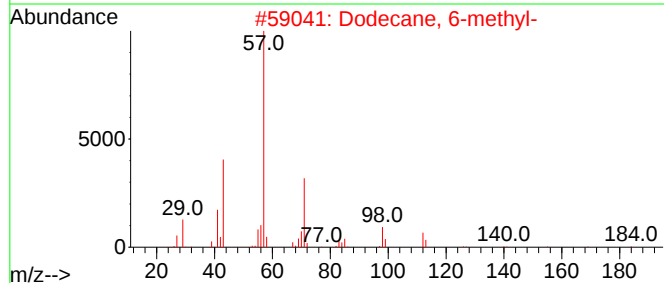
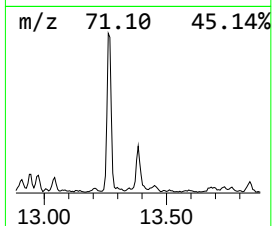
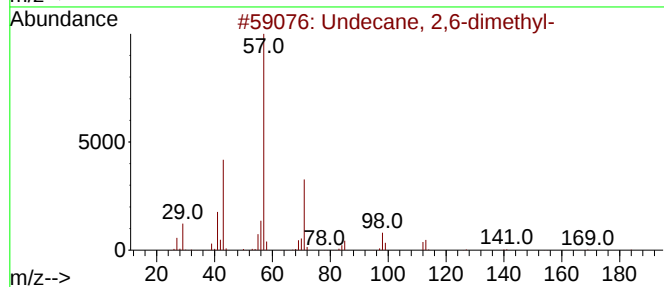
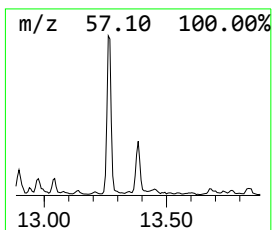
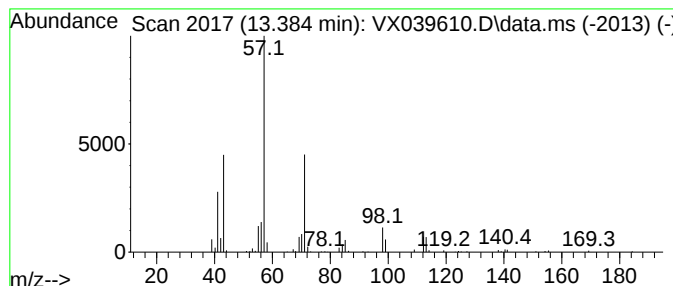
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Quant Title : SW846 8260

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

Peak Number 4 Undecane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.384	5.69 ug/l	81007	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	97
2			Dodecane, 6-methyl-	184	C13H28	006044-71-9	94
3			Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	80
4			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	80
5			5-Ethyldecane	170	C12H26	017302-36-2	78



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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
Undecane	12.421	8.8	ug/l	125178	4	12.024	711841	50.0
unknown12.890	12.890	6.2	ug/l	87515	4	12.024	711841	50.0
Dodecane	13.262	25.2	ug/l	358979	4	12.024	711841	50.0
Undecane, 2,6-d...	13.384	5.7	ug/l	81007	4	12.024	711841	50.0