

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
 Data File : VX035088.D
 Acq On : 14 Apr 2023 17:06
 Operator : JC/MD
 Sample : 02345-01 10X
 Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1595

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\82X032923W.M
 Title : SW846 8260

Signal : TIC: VX035088.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.386	206	213	229	rBV	387322	670939	18.57%	4.508%
2	5.391	694	706	716	rBV2	147980	431298	11.94%	2.898%
3	5.550	716	732	741	rBV2	268325	991574	27.44%	6.662%
4	5.824	765	777	789	rBV2	129441	373976	10.35%	2.512%
5	5.958	789	799	813	rVV	165930	446089	12.35%	2.997%
6	6.190	824	837	844	rBV4	15934	59345	1.64%	0.399%
7	6.610	895	906	921	rBV2	100964	250585	6.94%	1.684%
8	6.763	921	931	948	rBV	427406	1014806	28.09%	6.818%
9	7.379	1021	1032	1041	rBV4	19372	49832	1.38%	0.335%
10	8.647	1234	1240	1246	rBV	848791	1348374	37.32%	9.059%
11	8.720	1246	1252	1271	rVB	2385725	3613012	100.00%	24.273%
12	10.055	1465	1471	1488	rVB	864366	1140530	31.57%	7.662%
13	10.195	1488	1494	1502	rVB	34249	46203	1.28%	0.310%
14	10.299	1502	1511	1518	rBV	113118	158355	4.38%	1.064%
15	10.640	1562	1567	1577	rBV	33002	48617	1.35%	0.327%
16	11.079	1634	1639	1653	rBV	656762	882217	24.42%	5.927%
17	11.378	1684	1688	1696	rBV	25498	55384	1.53%	0.372%
18	11.475	1702	1704	1710	rVB	31614	39454	1.09%	0.265%
19	11.750	1746	1749	1759	rVB2	63765	100550	2.78%	0.676%
20	11.939	1776	1780	1784	rBV5	25889	41979	1.16%	0.282%
21	12.024	1789	1794	1800	rVV	793739	1032437	28.58%	6.936%
22	12.103	1804	1807	1812	rVV4	33496	54581	1.51%	0.367%
23	12.177	1816	1819	1825	rVB2	30085	43034	1.19%	0.289%
24	12.250	1825	1831	1837	rBV4	23195	60845	1.68%	0.409%
25	12.317	1837	1842	1848	rVB7	33321	65918	1.82%	0.443%
26	12.427	1855	1860	1864	rVV	295470	360234	9.97%	2.420%
27	12.469	1864	1867	1873	rVB4	37541	70301	1.95%	0.472%
28	12.555	1873	1881	1883	rBV5	41062	85774	2.37%	0.576%
29	12.585	1883	1886	1893	rVB4	33374	58706	1.62%	0.394%
30	12.683	1898	1902	1906	rBV3	47318	66572	1.84%	0.447%
31	12.817	1921	1924	1929	rVB3	40437	56568	1.57%	0.380%
32	12.890	1931	1936	1943	rBV5	91939	202346	5.60%	1.359%
33	12.945	1943	1945	1947	rVV	36072	45073	1.25%	0.303%
34	12.975	1947	1950	1956	rVV4	80410	132845	3.68%	0.892%
35	13.042	1958	1961	1965	rVB2	54943	61173	1.69%	0.411%
36	13.164	1976	1981	1986	rBV7	22903	45090	1.25%	0.303%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Title : SW846 8260

37	13.268	1994	1998	2001	rBV	326732	378139	10.47%	2.540%
38	13.384	2014	2017	2020	rVV	74618	94468	2.61%	0.635%
39	13.420	2020	2023	2032	rVB5	54624	126958	3.51%	0.853%
40	14.042	2121	2125	2128	rVB	34787	36523	1.01%	0.245%
41	15.493	2357	2363	2367	rBV2	25677	44012	1.22%	0.296%

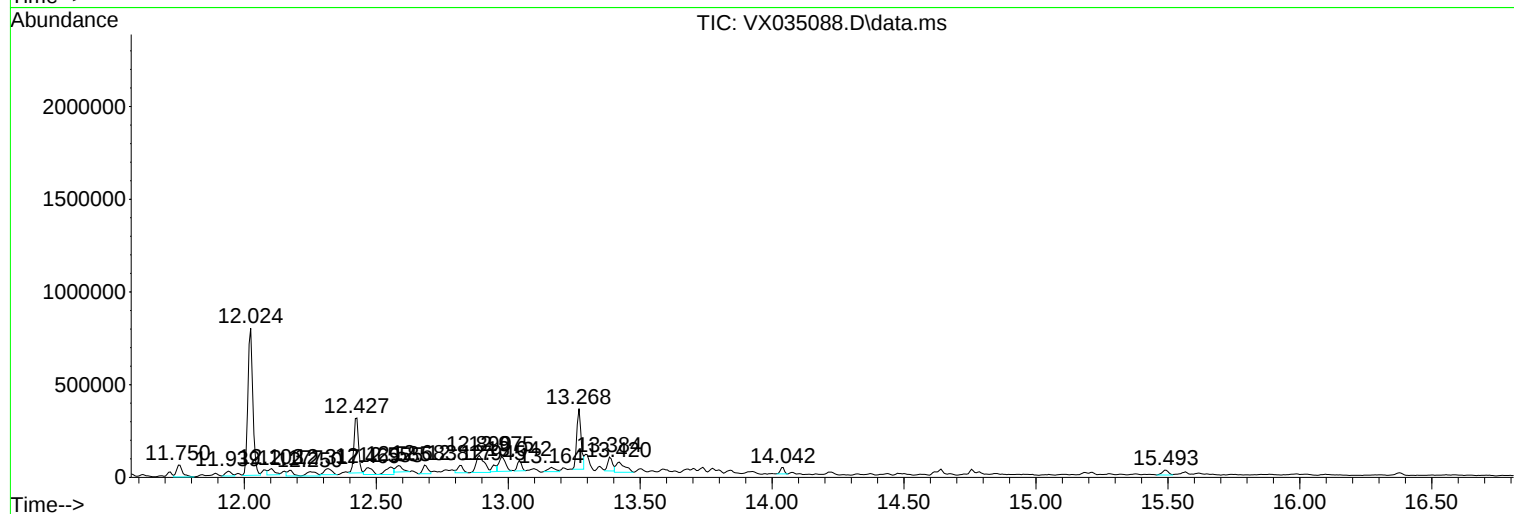
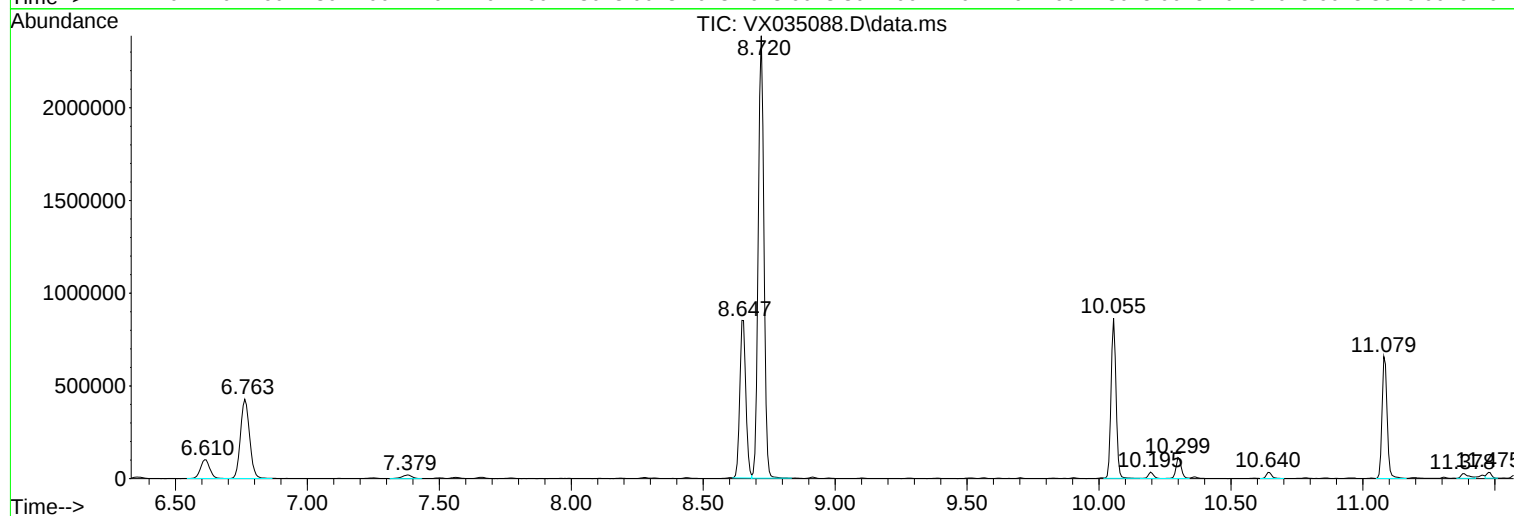
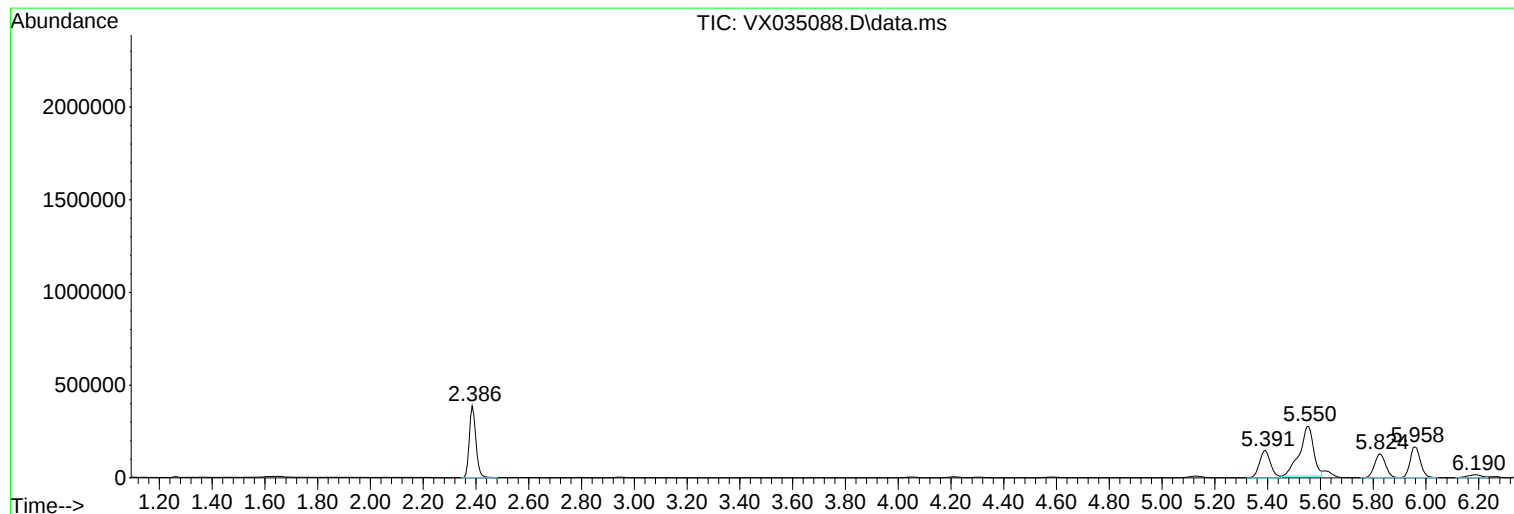
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX041523\
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

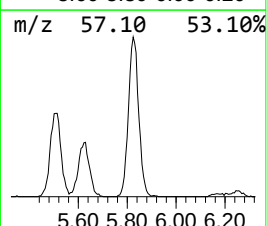
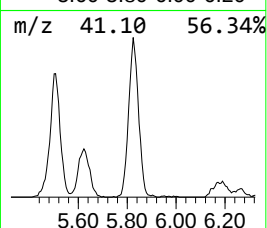
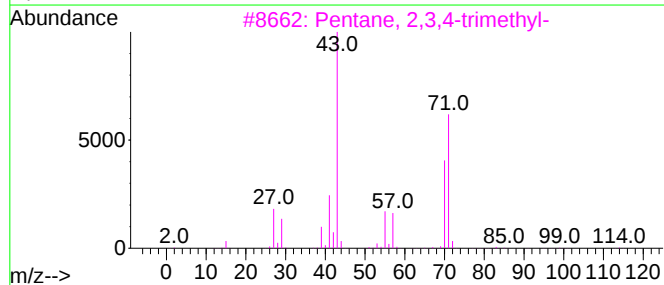
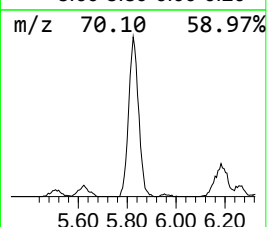
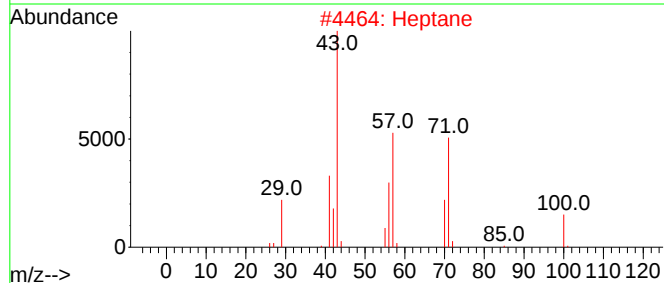
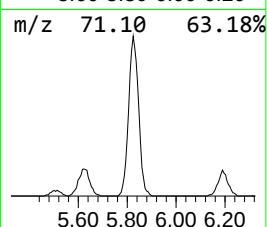
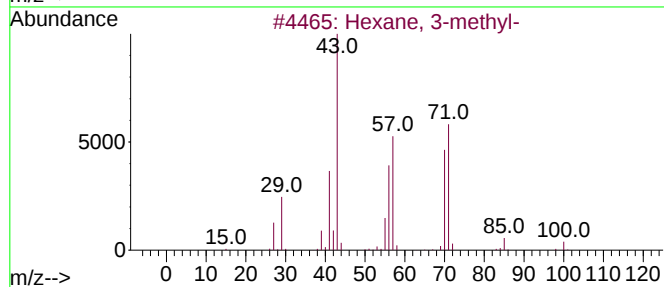
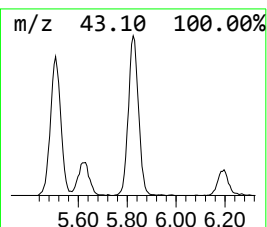
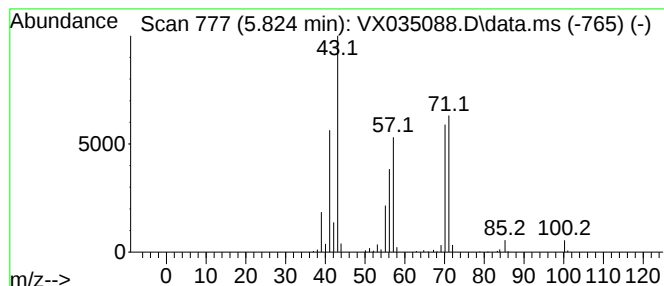
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.824	18.86 ug/l	373976	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	80
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	53



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Instrument :
MSVOA_X
ClientSampleId :
1595

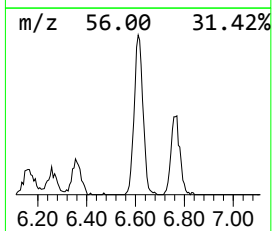
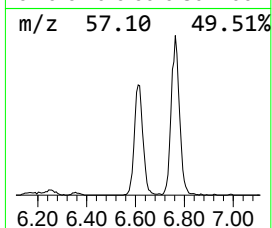
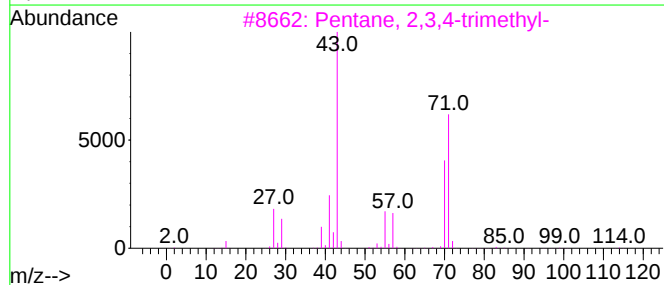
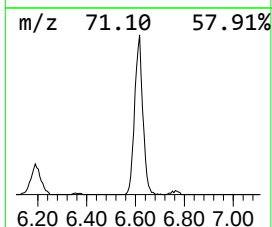
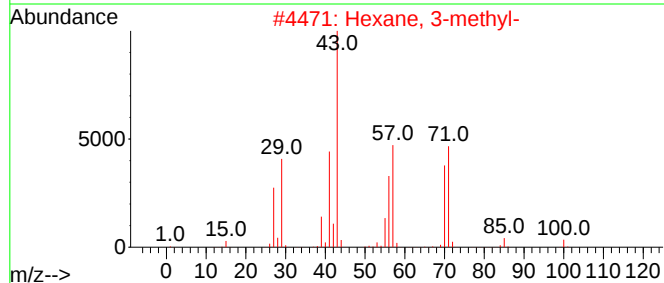
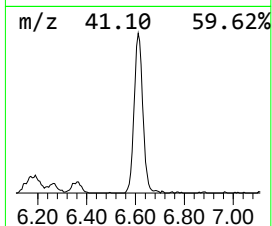
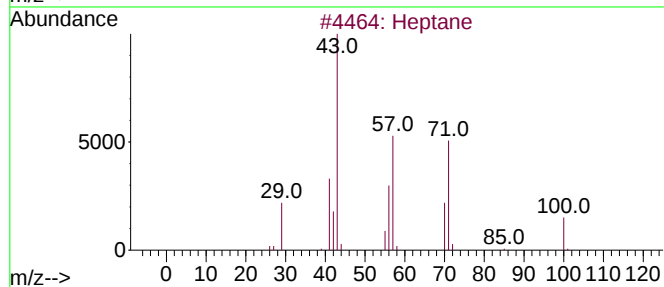
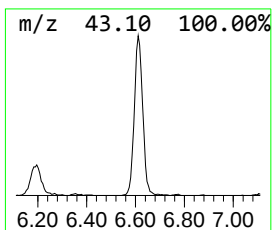
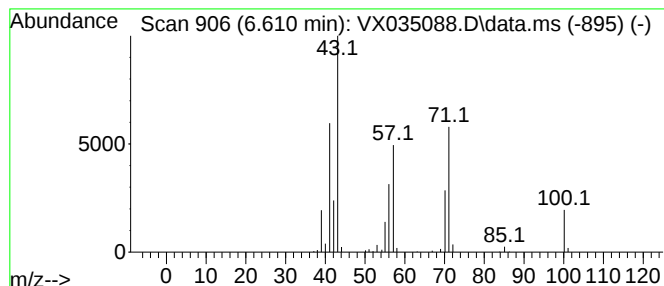
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.610	12.35 ug/l	250585	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	87
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	50
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
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Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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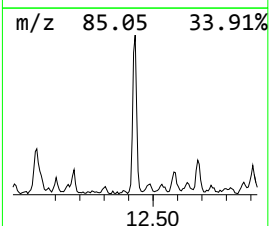
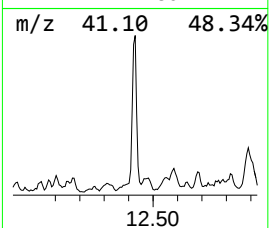
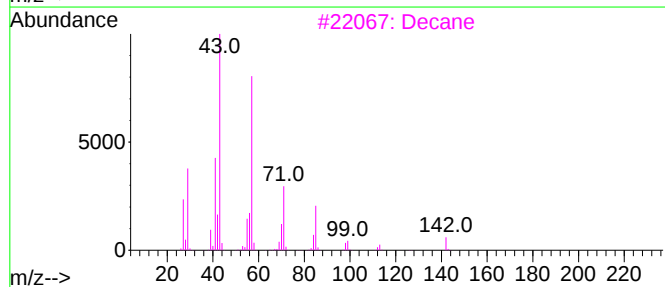
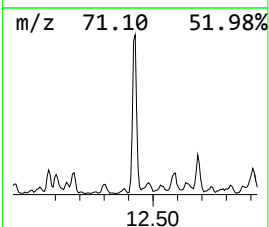
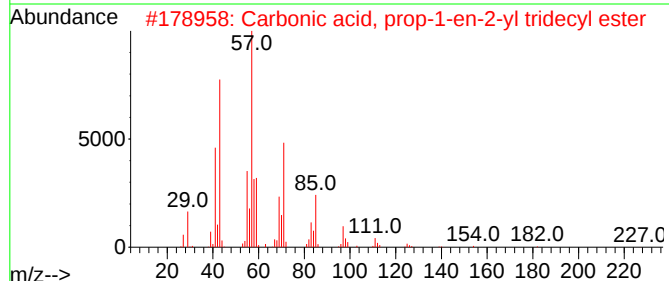
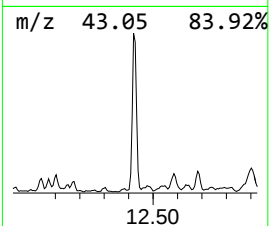
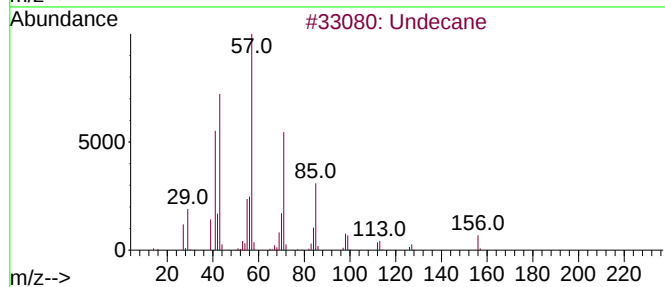
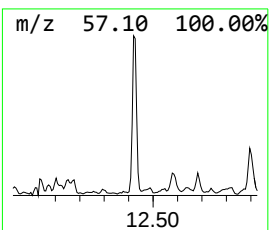
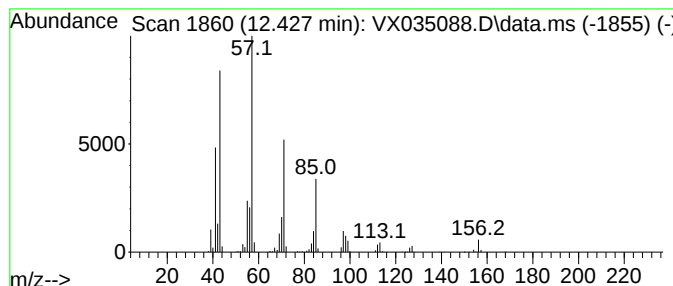
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	17.45 ug/l	360234	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	96
2	Carbonic acid, prop-1-en-2-yl tr...			284	C17H32O3	1000382-90-8	86
3	Decane			142	C10H22	000124-18-5	80
4	Tetradecane			198	C14H30	000629-59-4	78
5	Heptadecane, 2,6,10,14-tetramethyl-			296	C21H44	018344-37-1	64



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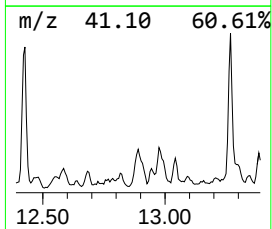
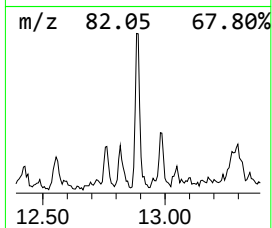
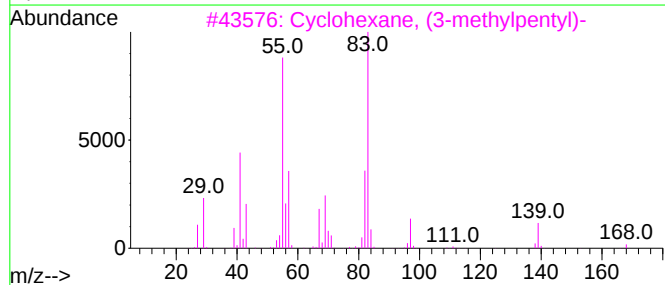
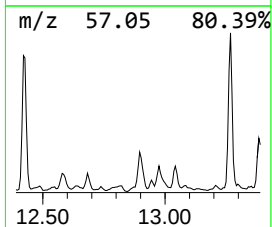
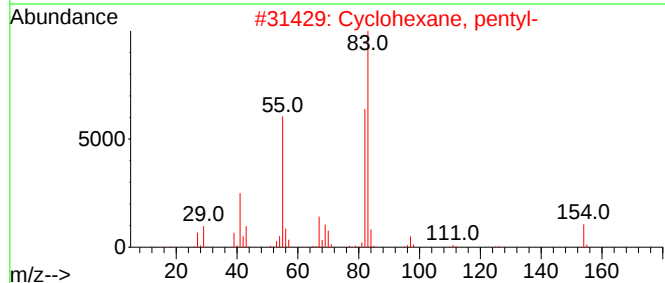
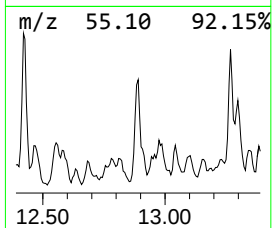
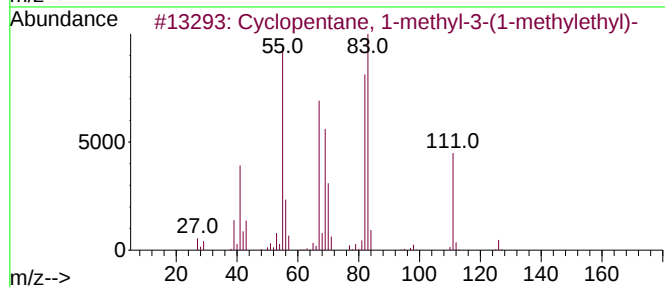
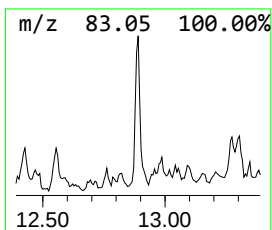
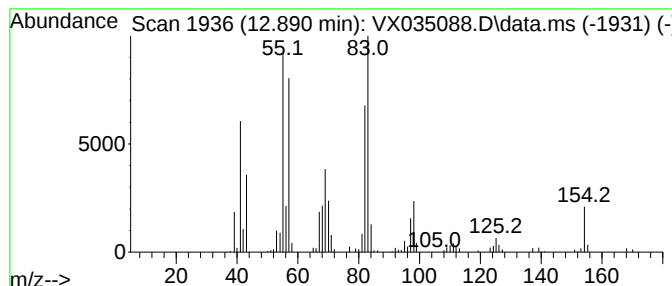
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, 1-methyl-3-(1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	9.80 ug/l	202346	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-3-(1-meth...	126	C9H18	053771-88-3	64
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	52
3			Cyclohexane, (3-methylpentyl)-	168	C12H24	061142-38-9	49
4			Cyclohexane, methyl-	98	C7H14	000108-87-2	47
5			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	43



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ClientSampleId :
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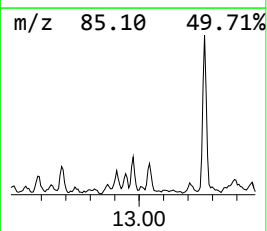
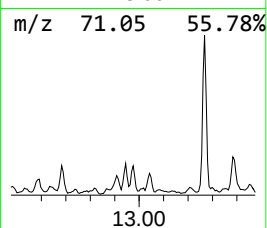
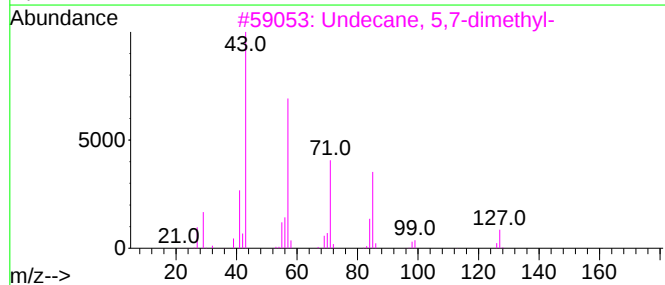
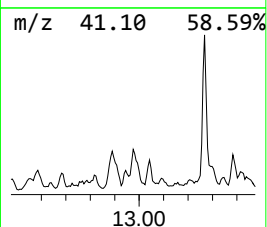
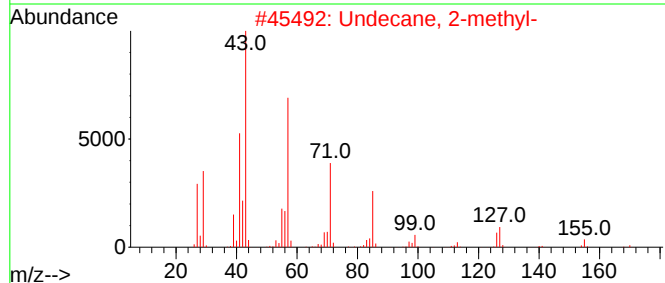
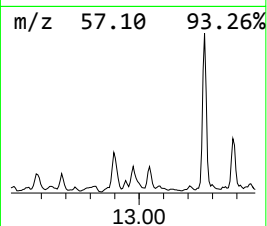
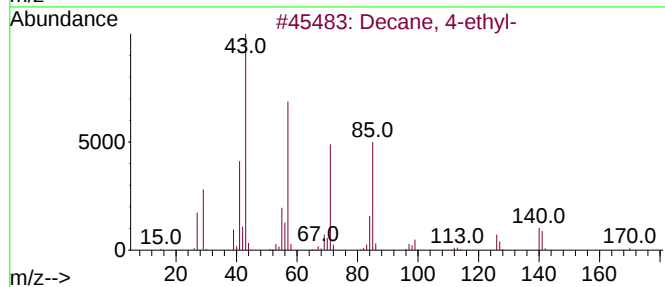
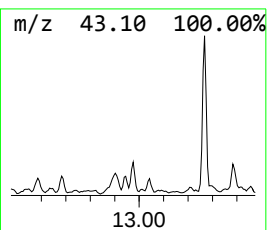
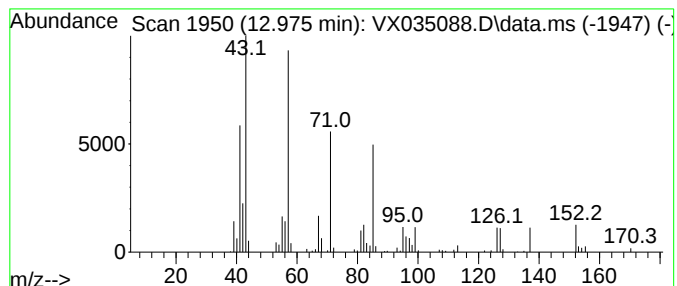
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Quant Title : SW846 8260

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

Peak Number 5 Decane, 4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.975	6.43 ug/l	132845	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-ethyl-	170	C12H26	001636-44-8	58
2			Undecane, 2-methyl-	170	C12H26	007045-71-8	58
3			Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	50
4			Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	47
5			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035088.D
Acq On : 14 Apr 2023 17:06
Operator : JC/MD
Sample : 02345-01 10X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

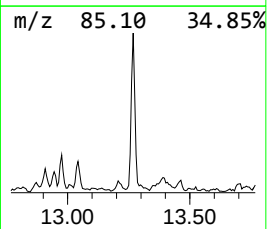
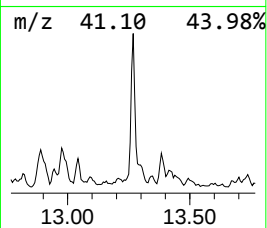
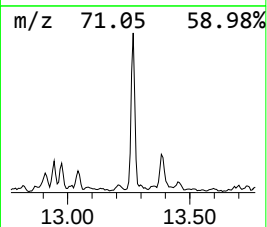
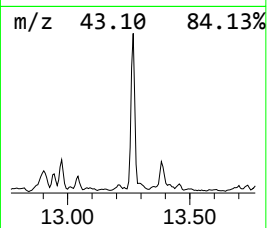
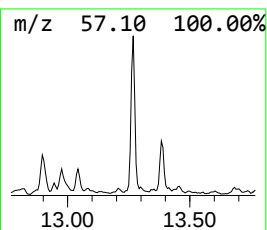
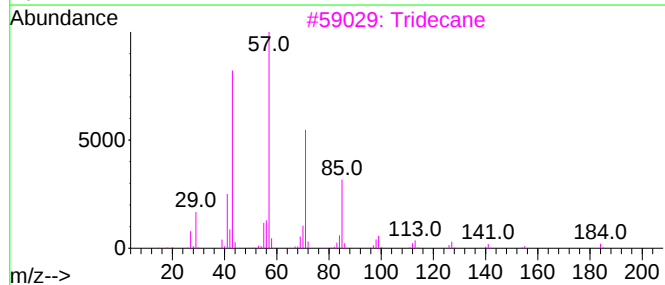
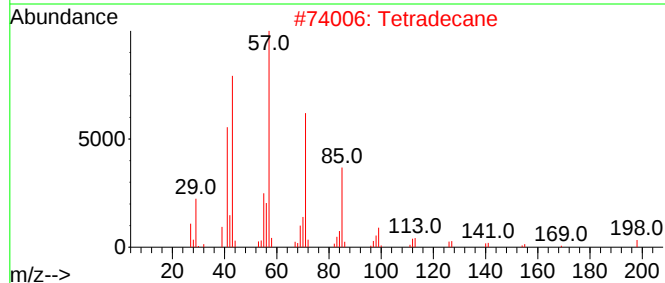
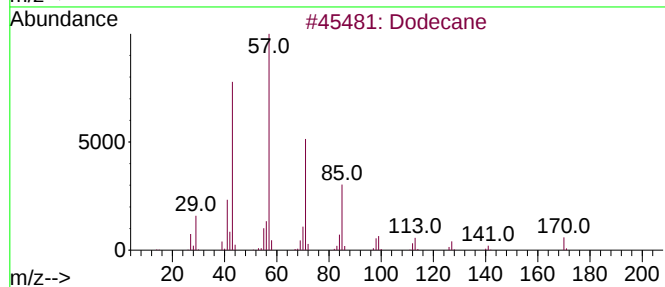
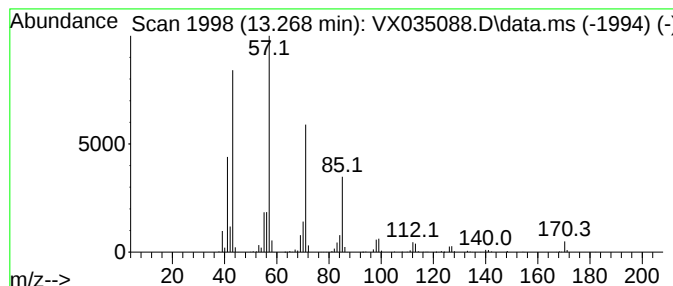
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	18.31 ug/l	378139	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Tetradecane	198	C14H30	000629-59-4	90
3			Tridecane	184	C13H28	000629-50-5	90
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
5			Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035088.D
Acq On : 14 Apr 2023 17:06
Operator : JC/MD
Sample : 02345-01 10X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

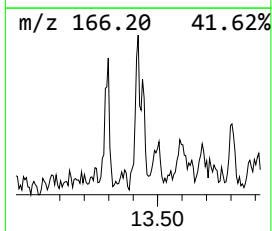
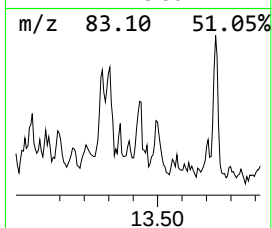
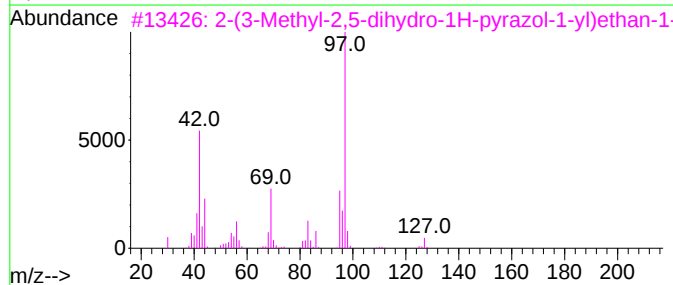
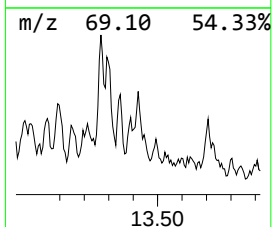
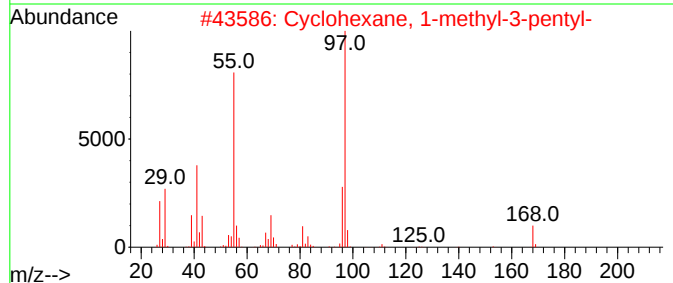
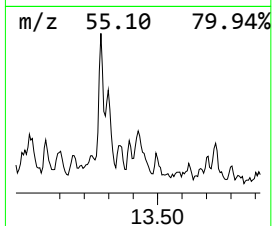
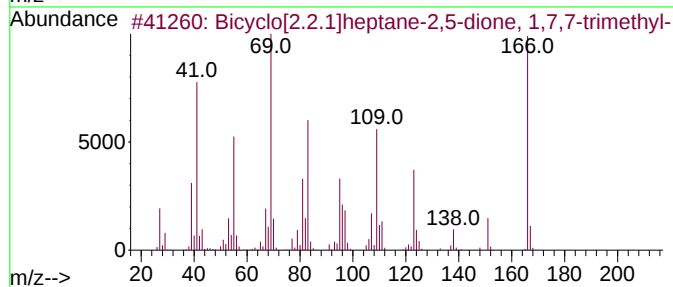
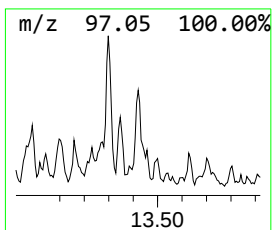
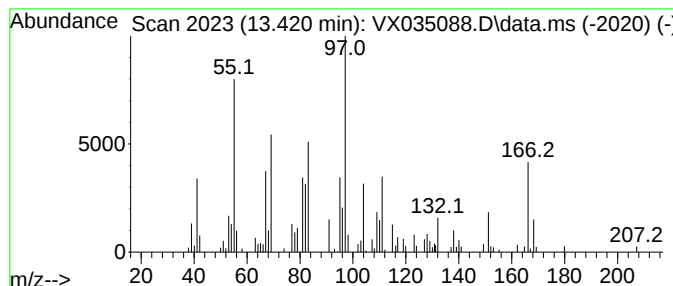
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.420 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	6.15 ug/l	126958	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane-2,5-dione,...	166	C10H14O2	004230-32-4	43
2			Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	38
3			2-(3-Methyl-2,5-dihydro-1H-pyraz...	127	C6H13N3	1000387-20-9	35
4			1-Cyclohexanone, 3,5,5-trimethyl...	166	C11H18O	027749-07-1	27
5			4-Methylcyclohexanecetic acid (...)	156	C9H16O2	1000453-59-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035088.D
Acq On : 14 Apr 2023 17:06
Operator : JC/MD
Sample : 02345-01 10X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	5.824	18.9	ug/l	373976	1	5.556	991574	50.0
Heptane	6.610	12.4	ug/l	250585	2	6.763	1014810	50.0
Undecane	12.427	17.4	ug/l	360234	4	12.024	1032440	50.0
Cyclopentane, 1...	12.890	9.8	ug/l	202346	4	12.024	1032440	50.0
Decane, 4-ethyl-	12.975	6.4	ug/l	132845	4	12.024	1032440	50.0
Dodecane	13.268	18.3	ug/l	378139	4	12.024	1032440	50.0
unknown13.420	13.420	6.2	ug/l	126958	4	12.024	1032440	50.0