

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
 Data File : VX035081.D
 Acq On : 14 Apr 2023 14:22
 Operator : JC/MD
 Sample : 02345-01
 Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 14 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: VX035081.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.416	209	218	255	rBV	2273770	5838711	14.64%	6.023%
2	5.111	642	660	675	rBV2	149727	545404	1.37%	0.563%
3	5.391	695	706	711	rBV	138442	405695	1.02%	0.418%
4	5.495	711	723	735	rVV2	1739165	6109972	15.32%	6.302%
5	5.611	735	742	759	rVB2	606404	1928744	4.84%	1.989%
6	5.812	761	775	790	rBV	2408701	7036962	17.65%	7.259%
7	5.952	790	798	811	rBV	169781	444635	1.12%	0.459%
8	6.178	820	835	842	rBV4	282073	1056996	2.65%	1.090%
9	6.605	892	905	922	rBV	2247362	5434357	13.63%	5.606%
10	6.757	922	930	952	rVB	422927	1034690	2.60%	1.067%
11	7.373	1019	1031	1041	rVB3	292065	756357	1.90%	0.780%
12	8.647	1235	1240	1245	rBV	832370	1305825	3.28%	1.347%
13	8.726	1245	1253	1259	rBV	22912737	39871079	100.00%	41.127%
14	10.055	1466	1471	1479	rVB	867697	1163481	2.92%	1.200%
15	10.195	1488	1494	1499	rBV	459720	601952	1.51%	0.621%
16	10.299	1502	1511	1517	rVV	1474814	2051625	5.15%	2.116%
17	10.640	1562	1567	1577	rBV	445905	611642	1.53%	0.631%
18	11.085	1634	1640	1652	rBV	730202	1117142	2.80%	1.152%
19	11.378	1684	1688	1695	rBV	387416	718306	1.80%	0.741%
20	11.451	1695	1700	1702	rVV2	238825	423289	1.06%	0.437%
21	11.476	1702	1704	1710	rVB	391472	441010	1.11%	0.455%
22	11.750	1746	1749	1759	rVB	800526	1207997	3.03%	1.246%
23	11.945	1776	1781	1784	rBV2	337640	504334	1.26%	0.520%
24	12.024	1789	1794	1800	rBV2	936400	1356233	3.40%	1.399%
25	12.097	1800	1806	1812	rBV3	244948	623895	1.56%	0.644%
26	12.250	1825	1831	1832	rBV	283474	414253	1.04%	0.427%
27	12.317	1837	1842	1848	rVB4	538012	1075160	2.70%	1.109%
28	12.427	1855	1860	1864	rVB	1690223	2000067	5.02%	2.063%
29	12.469	1864	1867	1873	rVB4	422548	725112	1.82%	0.748%
30	12.555	1874	1881	1884	rBV3	462543	980970	2.46%	1.012%
31	12.689	1899	1903	1906	rBV3	223847	411644	1.03%	0.425%
32	12.817	1921	1924	1931	rVB2	574206	798322	2.00%	0.823%
33	12.884	1931	1935	1939	rBV2	684902	1060183	2.66%	1.094%
34	12.988	1943	1952	1956	rVB4	654831	1342065	3.37%	1.384%
35	13.042	1956	1961	1964	rBV4	314175	403500	1.01%	0.416%
36	13.170	1975	1982	1986	rBV3	288628	618844	1.55%	0.638%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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Title : SW846 8260

37	13.268	1994	1998	2000	rBV	798026	972178	2.44%	1.003%
38	13.292	2000	2002	2008	rVB3	780657	1041960	2.61%	1.075%
39	13.420	2019	2023	2032	rVB5	423810	983313	2.47%	1.014%
40	14.225	2149	2155	2162	rBV4	295526	571340	1.43%	0.589%
41	14.640	2220	2223	2226	rVB	377270	479212	1.20%	0.494%
42	15.188	2307	2313	2320	rBV3	243215	477786	1.20%	0.493%

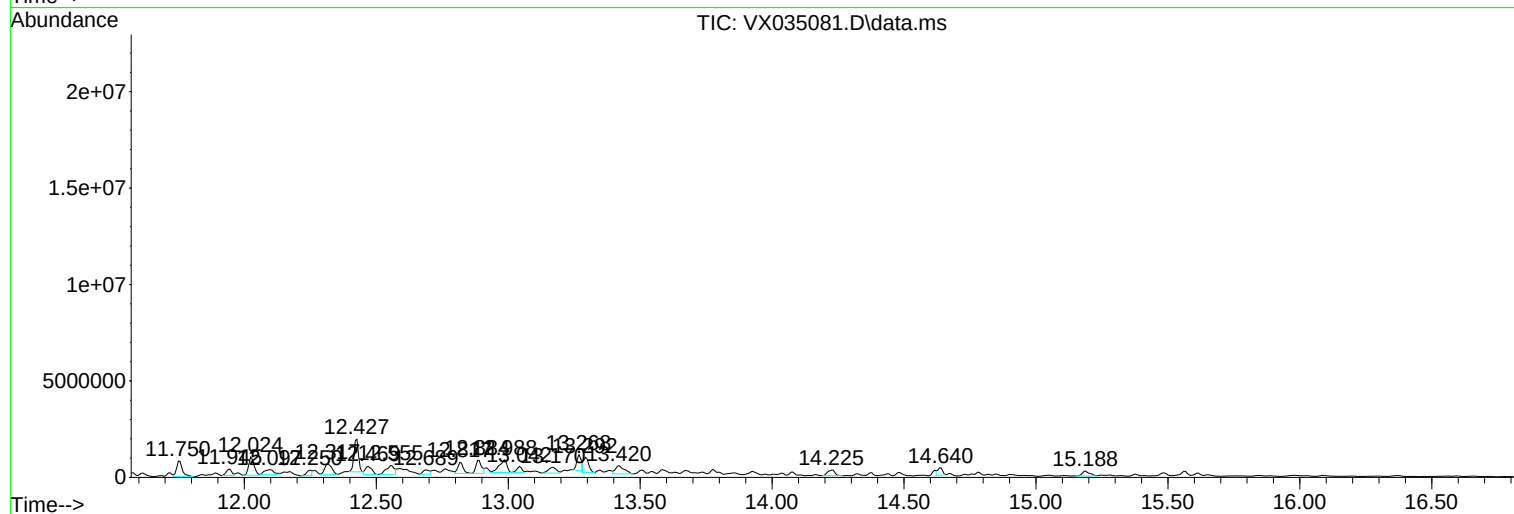
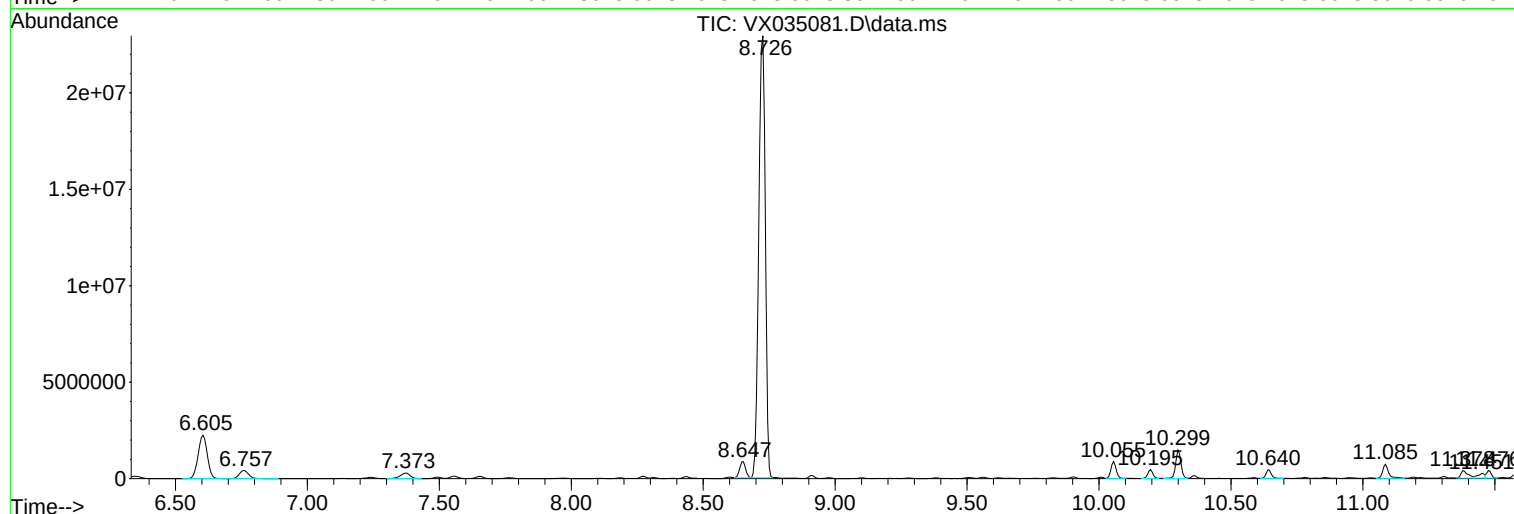
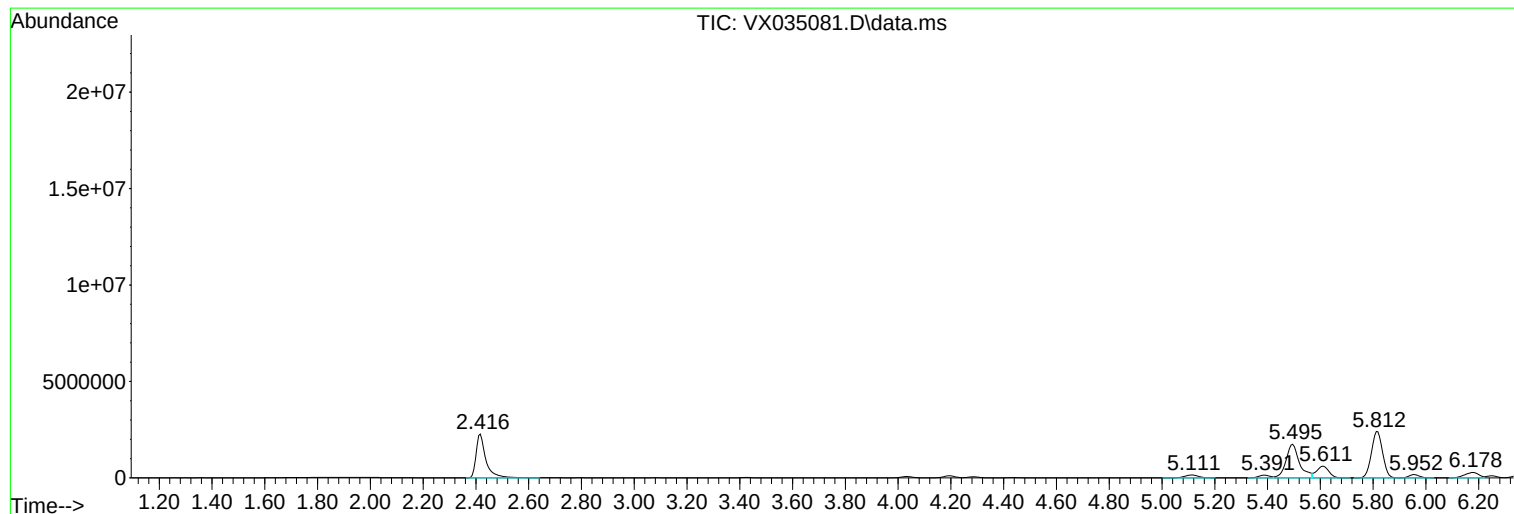
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
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1595

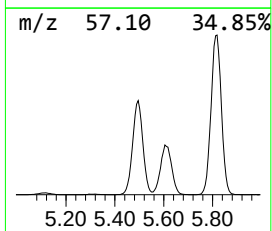
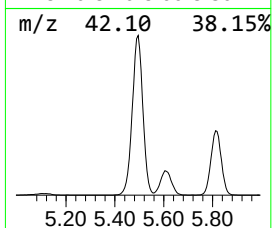
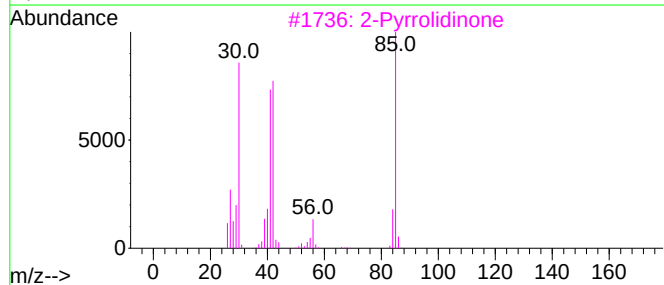
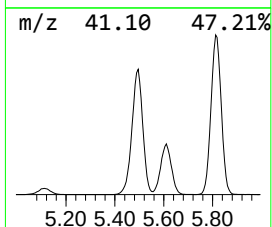
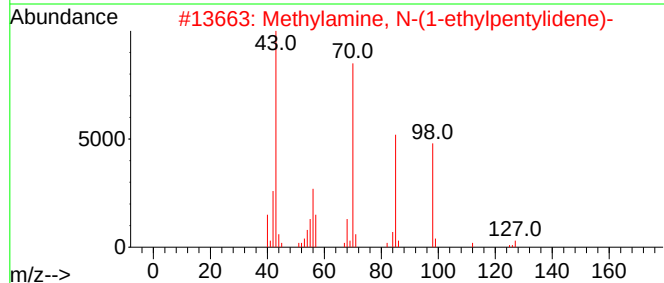
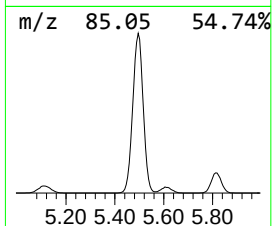
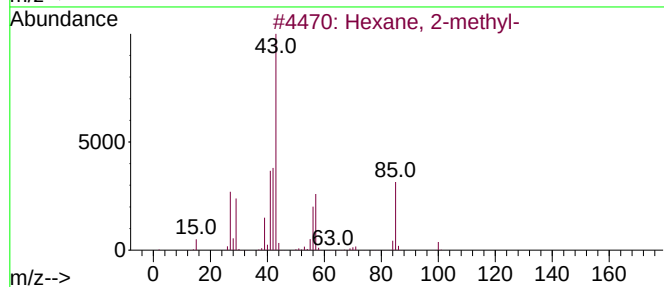
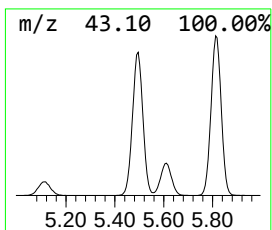
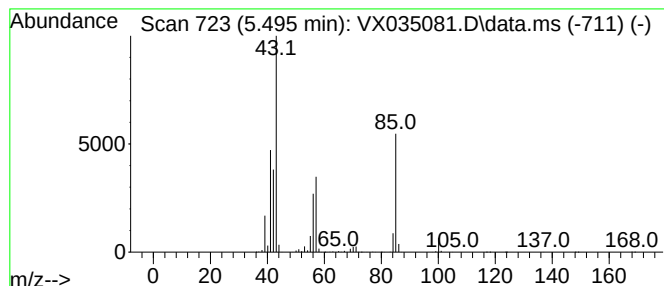
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.495	50.00 ug/l	6109970	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2-methyl-	100	C7H16	000591-76-4	90
2			Methylamine, N-(1-ethylpentylide...	127	C8H17N	018641-73-1	64
3			2-Pyrrolidinone	85	C4H7NO	000616-45-5	53
4			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	50
5			2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	50



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

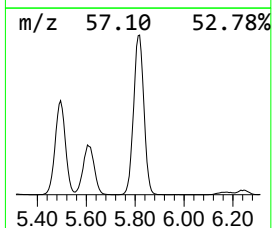
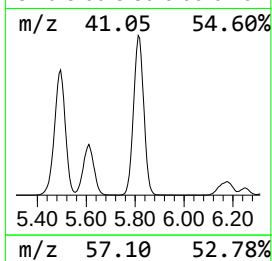
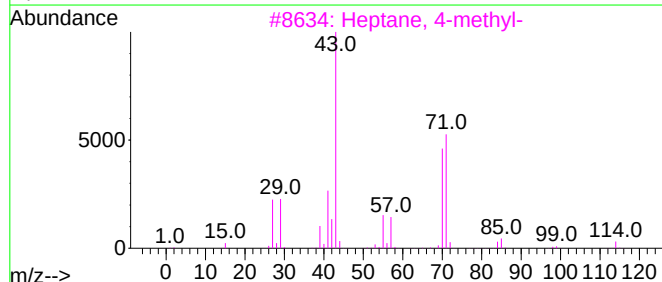
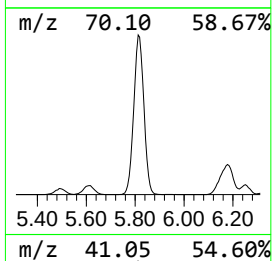
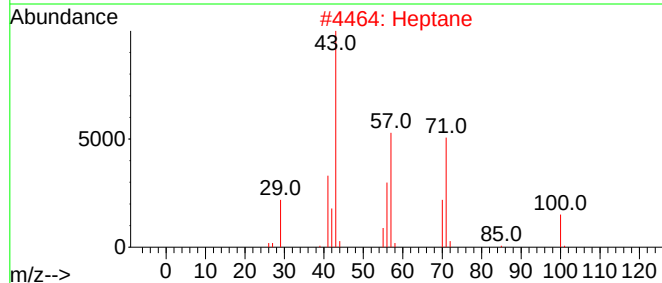
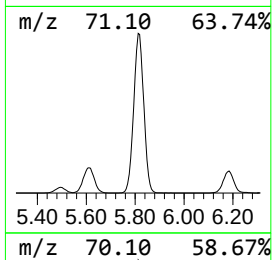
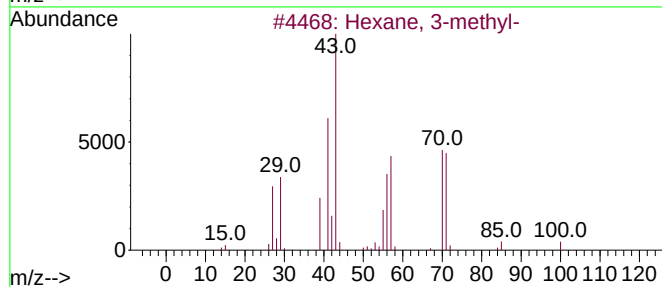
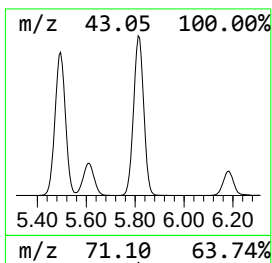
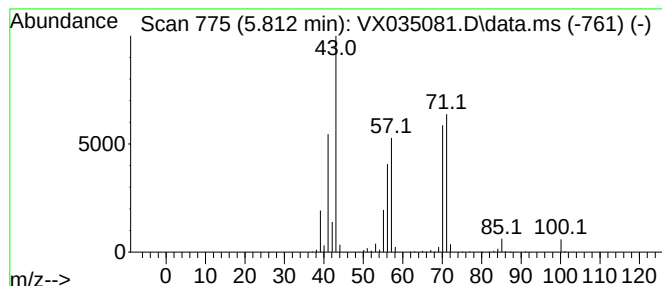
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 2 Hexane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	57.59 ug/l	7036960	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53



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ALS Vial : 14 Sample Multiplier: 1

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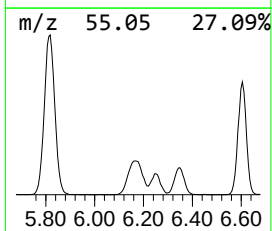
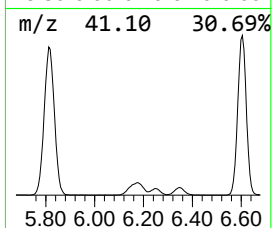
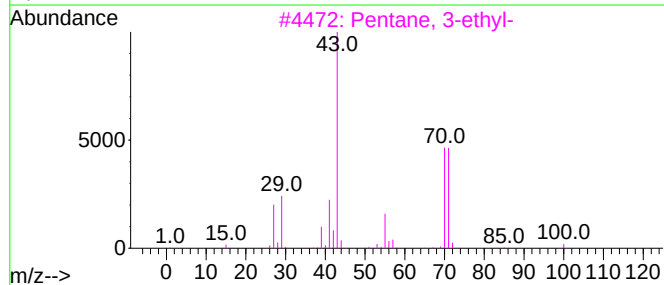
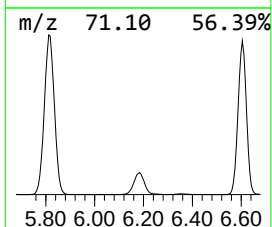
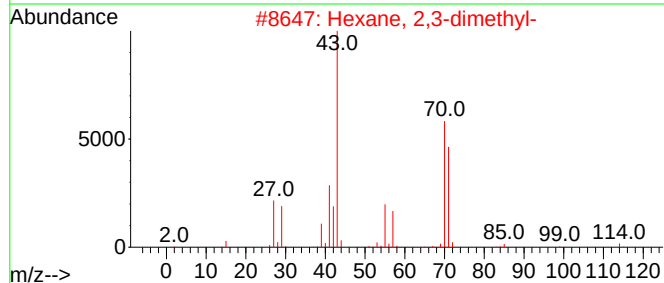
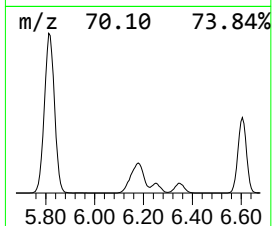
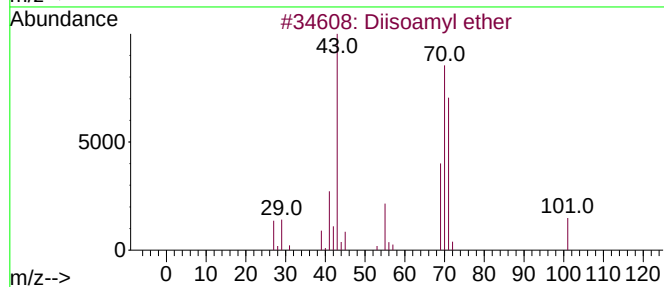
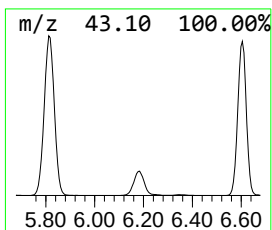
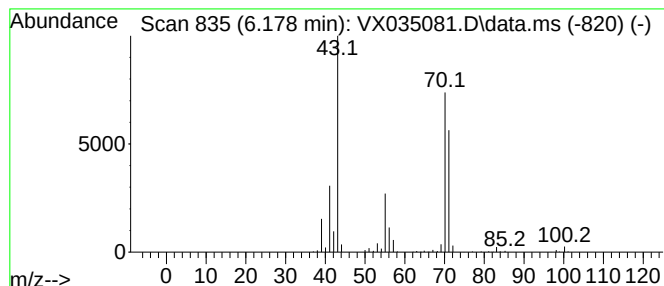
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 3 Diisoamyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.178	51.08 ug/l	1057000	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisoamyl ether	158	C10H22O	000544-01-4	72
2			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	72
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	72
4			Pyrrolidine	71	C4H9N	000123-75-1	64
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



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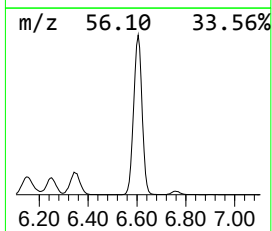
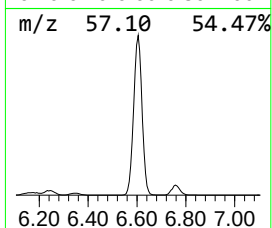
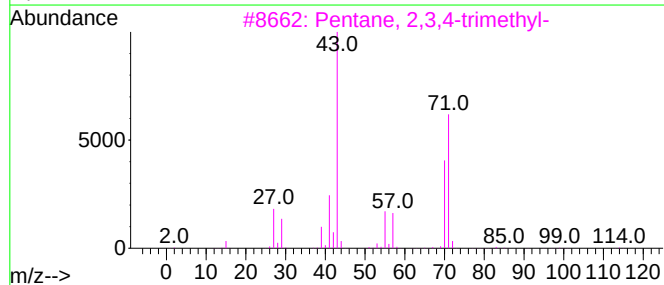
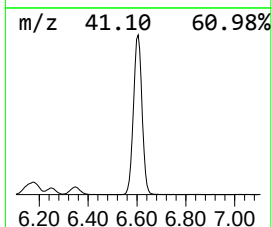
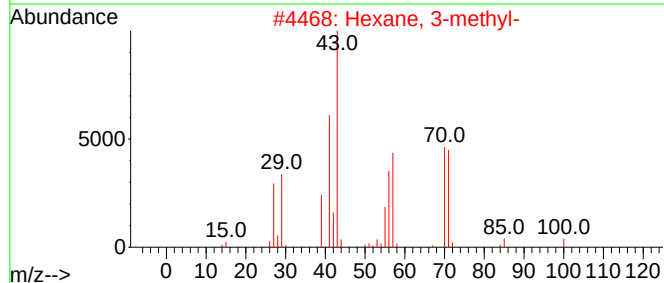
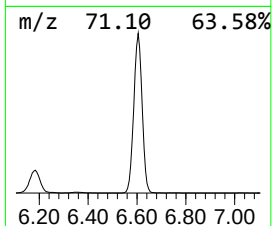
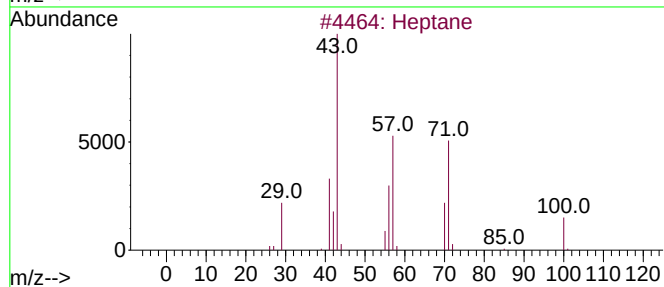
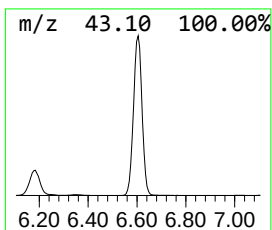
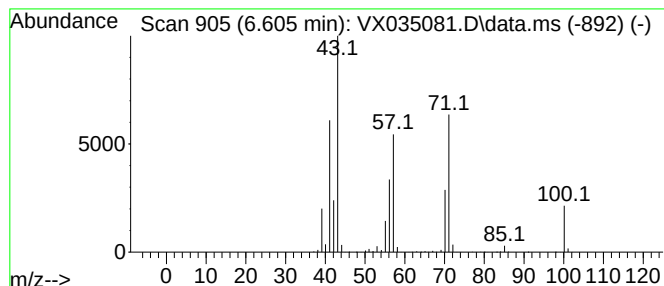
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Quant Title : SW846 8260

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

Peak Number 4 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.605	262.61 ug/l	5434360	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40
4			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38
5			Pentane, 2-methyl-	86	C6H14	000107-83-5	37



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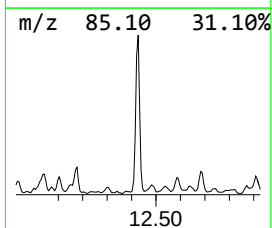
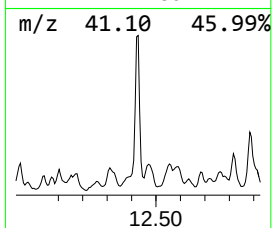
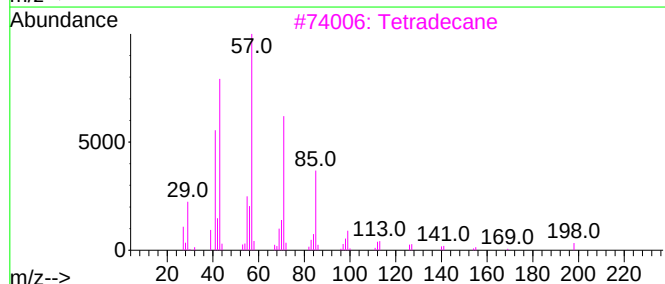
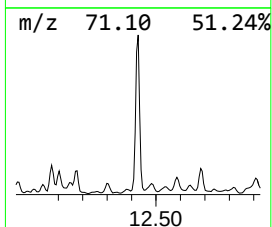
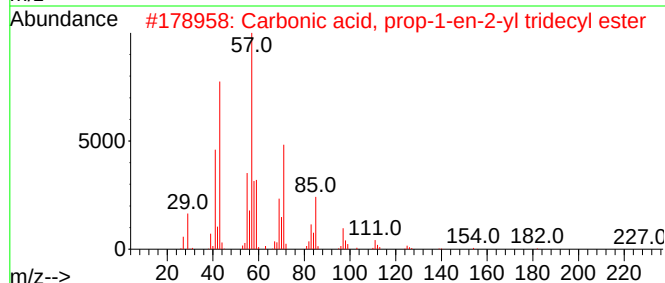
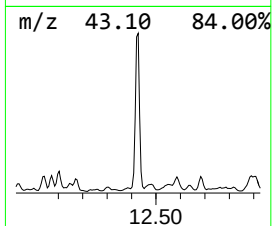
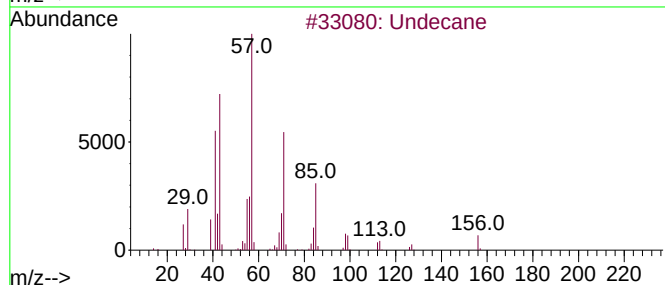
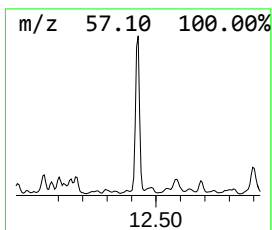
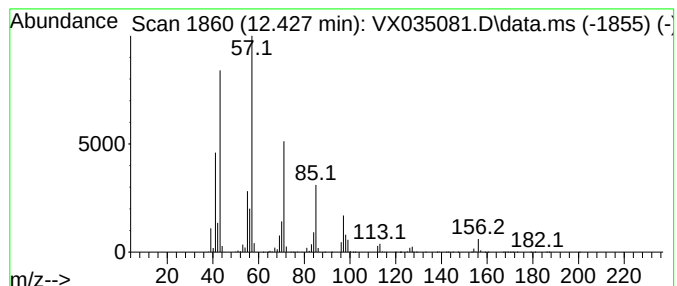
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Quant Title : SW846 8260

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

Peak Number 5 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	73.74 ug/l	2000070	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	Tetradecane			198	C14H30	000629-59-4	80
4	Hexadecane			226	C16H34	000544-76-3	72
5	Tridecane			184	C13H28	000629-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035081.D
Acq On : 14 Apr 2023 14:22
Operator : JC/MD
Sample : 02345-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

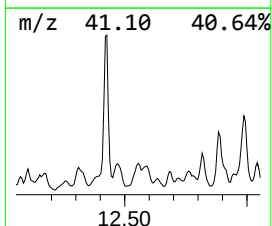
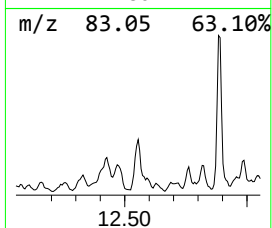
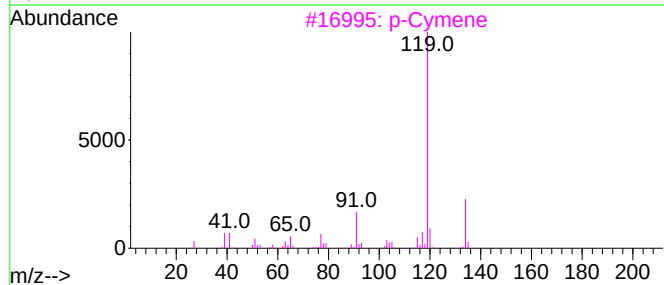
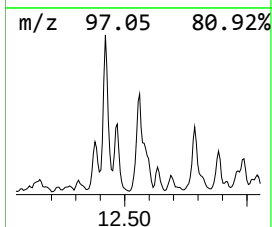
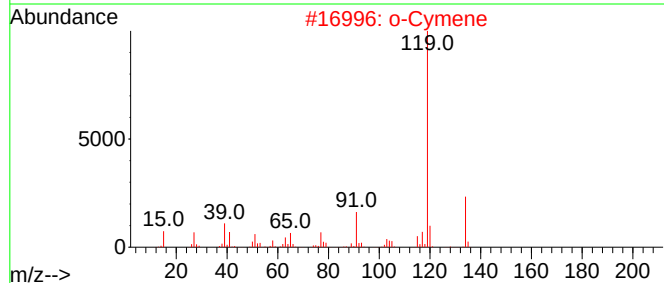
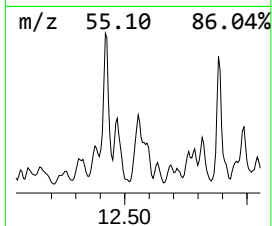
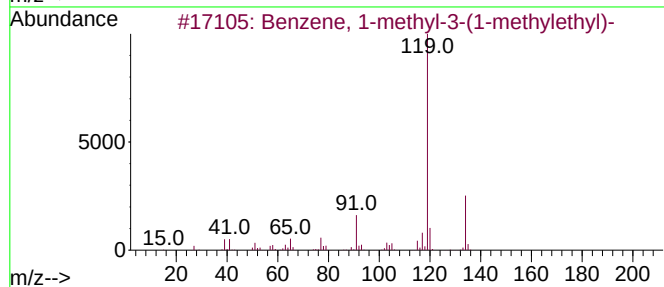
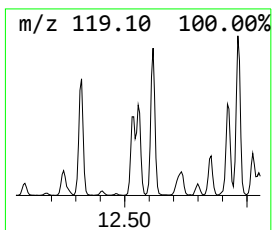
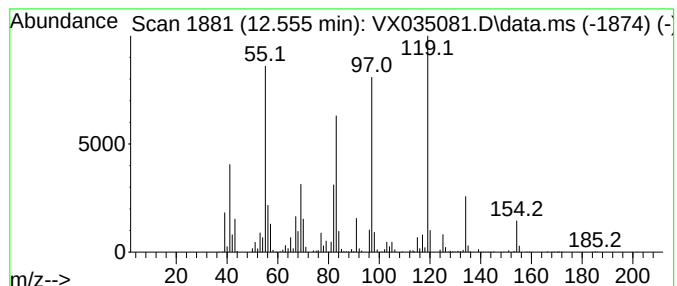
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-methyl-3-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.555	36.17 ug/l	980970	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	78
2			o-Cymene	134	C10H14	000527-84-4	78
3			p-Cymene	134	C10H14	000099-87-6	78
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	70
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	51



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035081.D
Acq On : 14 Apr 2023 14:22
Operator : JC/MD
Sample : 02345-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

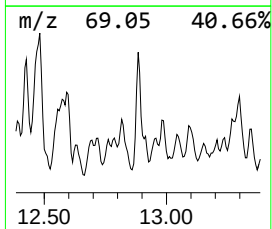
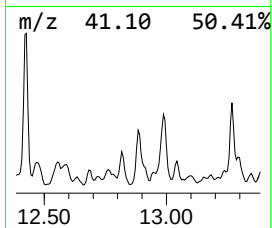
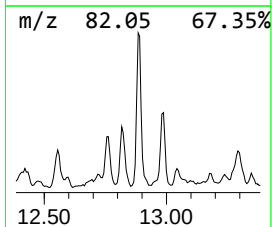
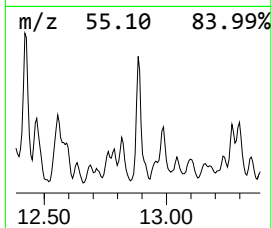
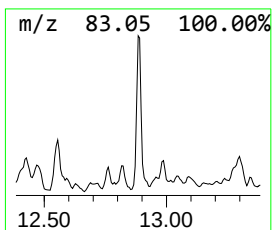
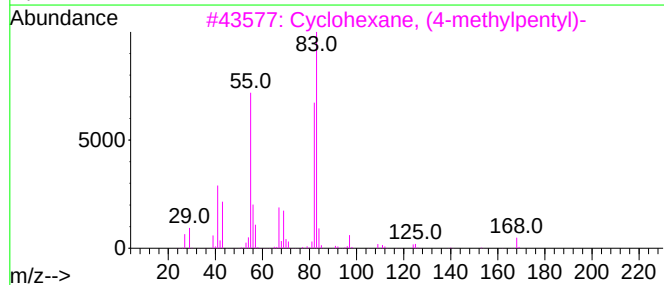
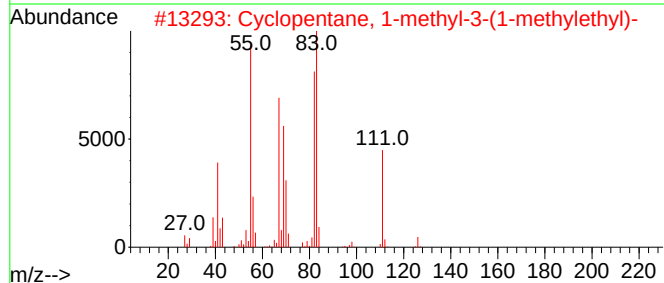
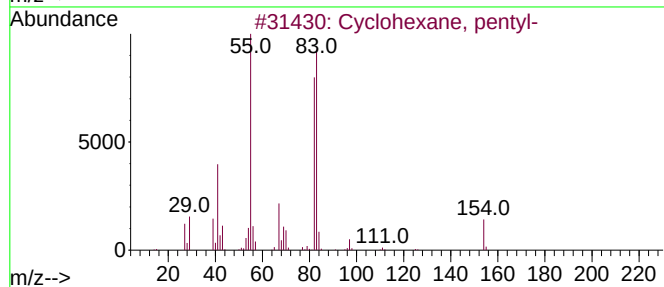
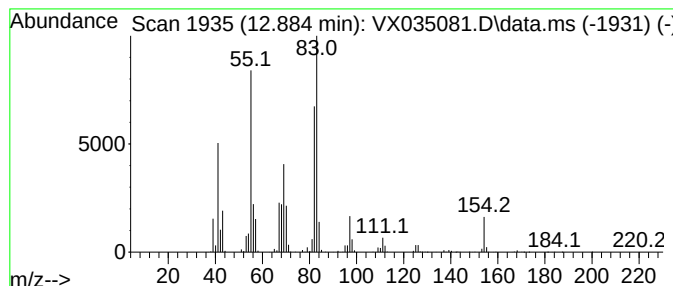
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, pentyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	39.09 ug/l	1060180	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, pentyl-	154	C11H22	004292-92-6	74
2			Cyclopentane, 1-methyl-3-(1-meth...	126	C9H18	053771-88-3	70
3			Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	68
4			Cyclohexane, propyl-	126	C9H18	001678-92-8	59
5			Cyclohexane, hexyl-	168	C12H24	004292-75-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035081.D
Acq On : 14 Apr 2023 14:22
Operator : JC/MD
Sample : 02345-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

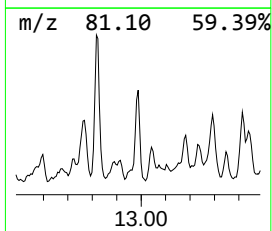
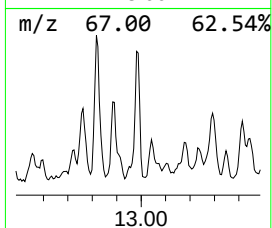
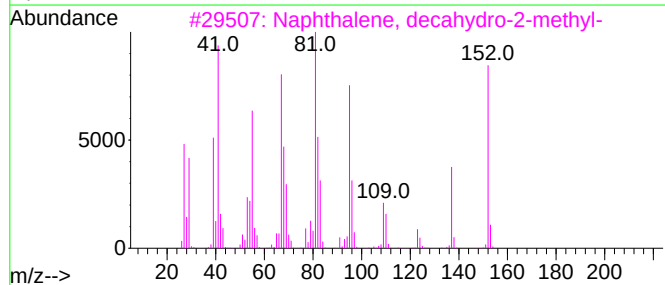
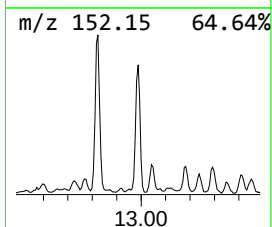
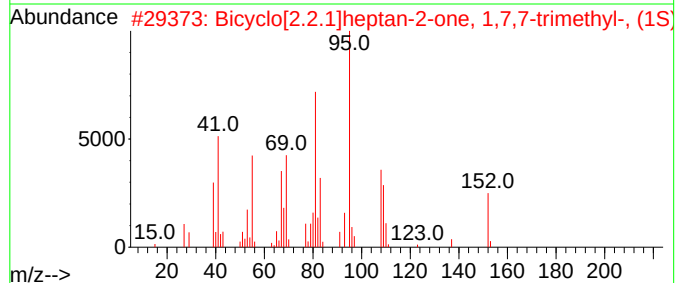
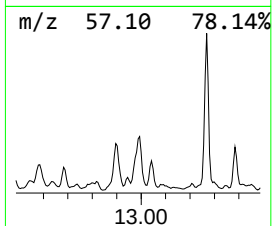
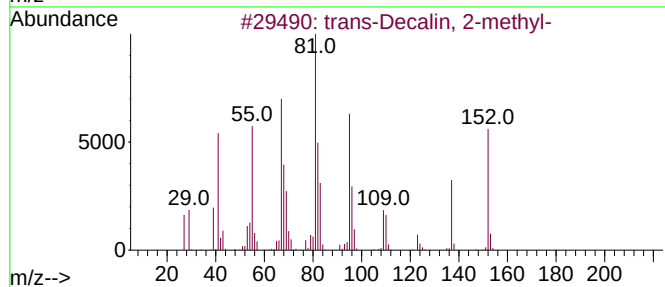
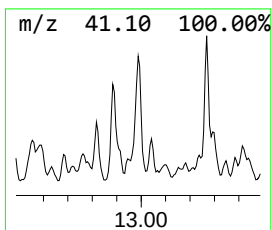
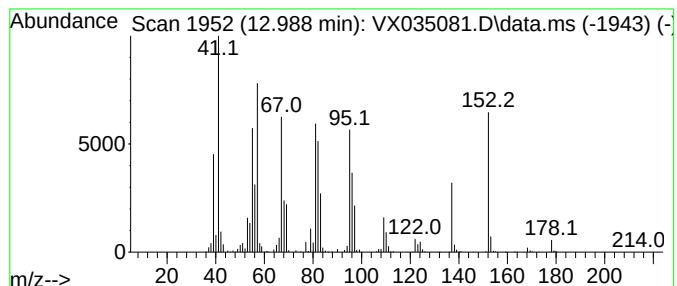
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Quant Title : SW846 8260

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

Peak Number 8 trans-Decalin, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.988	49.48 ug/l	1342070	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	72
2			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	70
3			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	70
4			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	64
5			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035081.D
Acq On : 14 Apr 2023 14:22
Operator : JC/MD
Sample : 02345-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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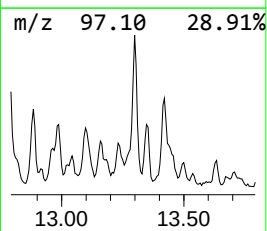
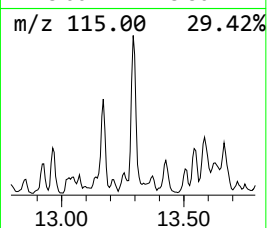
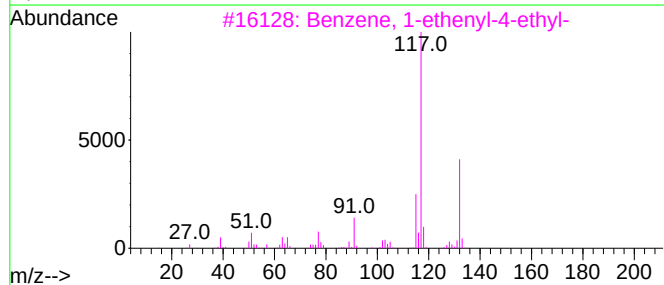
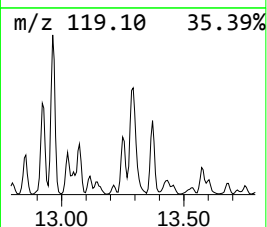
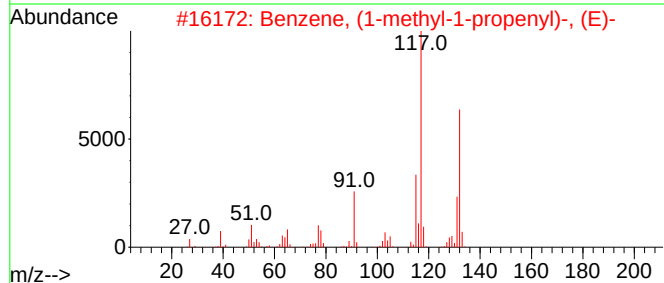
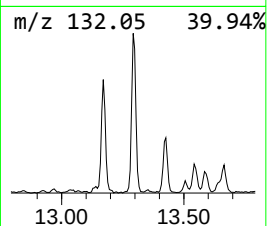
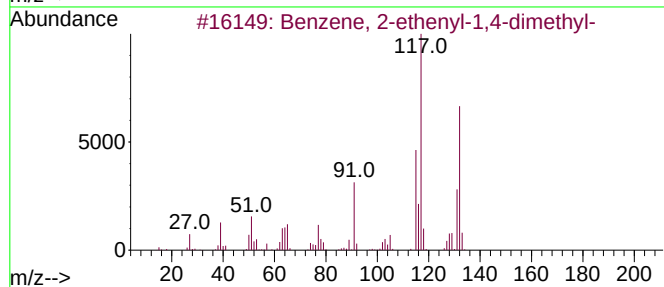
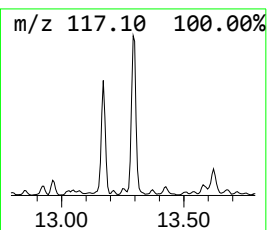
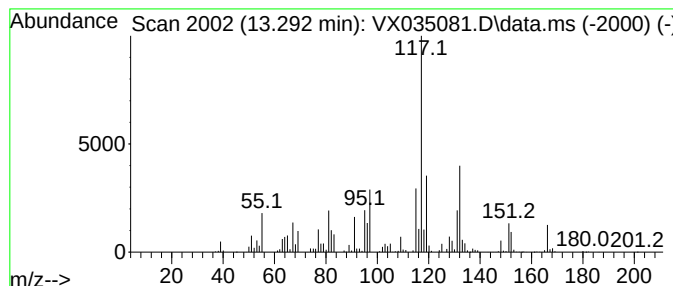
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	38.41 ug/l	1041960	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	94
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	78
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	60
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035081.D
Acq On : 14 Apr 2023 14:22
Operator : JC/MD
Sample : 02345-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1595

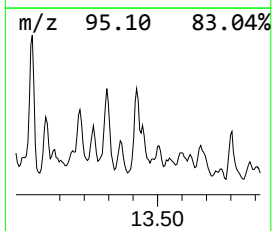
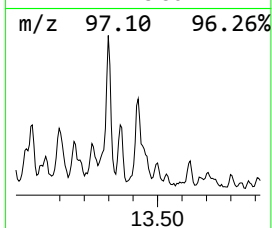
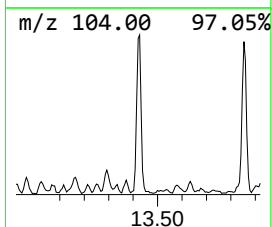
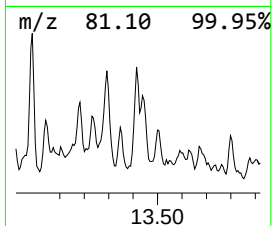
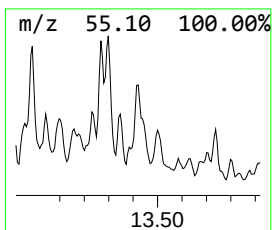
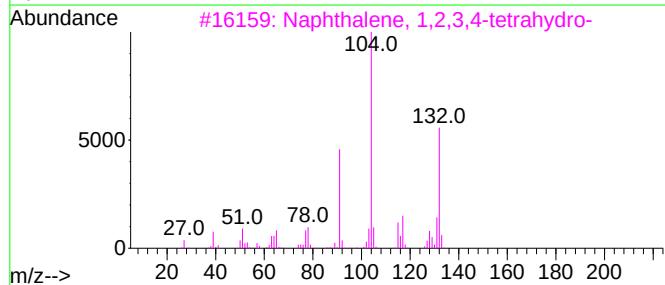
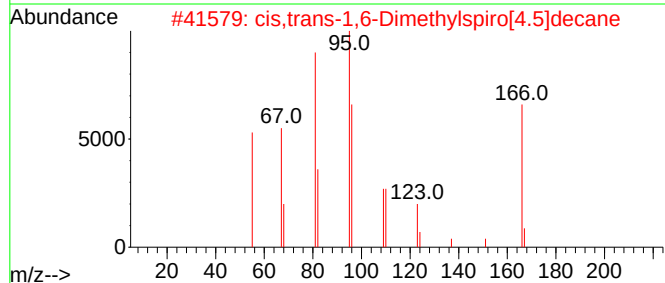
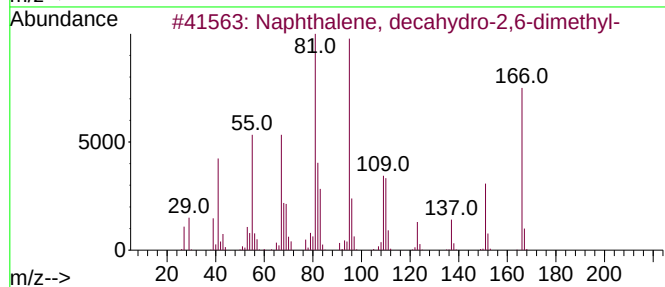
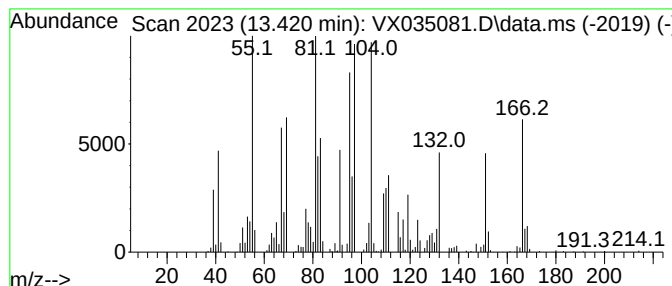
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, decahydro-2,6-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	36.25 ug/l	983313	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	66
2			cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	56
3			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	45
4			1,3-Hexadiene, 2,5-dimethyl-	110	C8H14	029253-64-3	25
5			Cyclopropane, tetramethylmethylene-	110	C8H14	054376-39-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035081.D
Acq On : 14 Apr 2023 14:22
Operator : JC/MD
Sample : 02345-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 2-methyl-	5.495	50.0	ug/l	6109970	1	5.550	6109970	50.0
Hexane, 3-methyl-	5.812	57.6	ug/l	7036960	1	5.550	6109970	50.0
Diisoamyl ether	6.178	51.1	ug/l	1057000	2	6.757	1034690	50.0
Heptane	6.605	262.6	ug/l	5434360	2	6.757	1034690	50.0
Undecane	12.427	73.7	ug/l	2000070	4	12.024	1356230	50.0
Benzene, 1-meth...	12.555	36.2	ug/l	980970	4	12.024	1356230	50.0
Cyclohexane, pe...	12.884	39.1	ug/l	1060180	4	12.024	1356230	50.0
trans-Decalin, ...	12.988	49.5	ug/l	1342070	4	12.024	1356230	50.0
Benzene, 2-ethe...	13.292	38.4	ug/l	1041960	4	12.024	1356230	50.0
Naphthalene, de...	13.420	36.3	ug/l	983313	4	12.024	1356230	50.0