

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034799.D
 Acq On : 28 Mar 2023 17:36
 Operator : JC/MD
 Sample : 02073-01
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TRE-1715ME

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\82X031023W.M
 Title : SW846 8260

Signal : TIC: VX034799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.179	174	179	193	rVB	124706	193390	1.03%	0.322%
2	2.416	208	218	264	rBV	2420440	9525847	50.77%	15.869%
3	5.385	695	705	713	rBV	166580	497066	2.65%	0.828%
4	5.489	713	722	726	rVV	290529	838686	4.47%	1.397%
5	5.544	727	731	734	rVV2	343309	782508	4.17%	1.304%
6	5.623	734	744	765	rVV	3122989	10699437	57.02%	17.824%
7	5.812	765	775	788	rVB	394976	1143804	6.10%	1.905%
8	5.958	788	799	809	rBV	222221	598491	3.19%	0.997%
9	6.598	890	904	921	rBV	387116	942947	5.03%	1.571%
10	6.757	921	930	949	rVB	529423	1295103	6.90%	2.157%
11	7.123	976	990	1022	rBV	190935	862562	4.60%	1.437%
12	8.647	1234	1240	1245	rBV	1062443	1703804	9.08%	2.838%
13	8.720	1245	1252	1265	rVB	11925655	18764221	100.00%	31.259%
14	10.055	1466	1471	1482	rVB	971853	1465873	7.81%	2.442%
15	10.604	1555	1561	1567	rBV	180296	335119	1.79%	0.558%
16	11.085	1634	1640	1653	rVB	755882	1166176	6.21%	1.943%
17	11.543	1710	1715	1723	rBV	356197	471496	2.51%	0.785%
18	12.024	1789	1794	1800	rBV	1068745	1419068	7.56%	2.364%
19	12.317	1836	1842	1848	rVB6	124632	274763	1.46%	0.458%
20	12.421	1856	1859	1863	rVV	305587	338719	1.81%	0.564%
21	12.616	1887	1891	1899	rVB	115026	194454	1.04%	0.324%
22	12.920	1938	1941	1945	rVV	157784	211215	1.13%	0.352%
23	12.963	1945	1948	1955	rVB	287586	422676	2.25%	0.704%
24	13.164	1975	1981	1986	rBV3	196757	336453	1.79%	0.560%
25	13.213	1986	1989	1992	rBV2	157411	213835	1.14%	0.356%
26	13.262	1992	1997	1999	rVV3	200145	359008	1.91%	0.598%
27	13.292	1999	2002	2007	rVB3	360688	507893	2.71%	0.846%
28	13.420	2019	2023	2032	rVB4	170946	371522	1.98%	0.619%
29	13.579	2039	2049	2055	rBV3	384856	1014119	5.40%	1.689%
30	13.774	2078	2081	2087	rVB	195617	243421	1.30%	0.406%
31	13.847	2087	2093	2099	rVB6	186777	522358	2.78%	0.870%
32	13.926	2100	2106	2112	rBV4	229038	556593	2.97%	0.927%
33	14.036	2121	2124	2127	rVB3	207634	237249	1.26%	0.395%
34	14.225	2149	2155	2160	rVB3	302739	570594	3.04%	0.951%
35	14.323	2167	2171	2176	rBV	126099	189307	1.01%	0.315%
36	14.481	2193	2197	2205	rVB4	192404	384036	2.05%	0.640%

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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\82X031023W.M

Title : SW846 8260

37	14.615	2215	2219	2221	rBV	279701	375268	2.00%	0.625%
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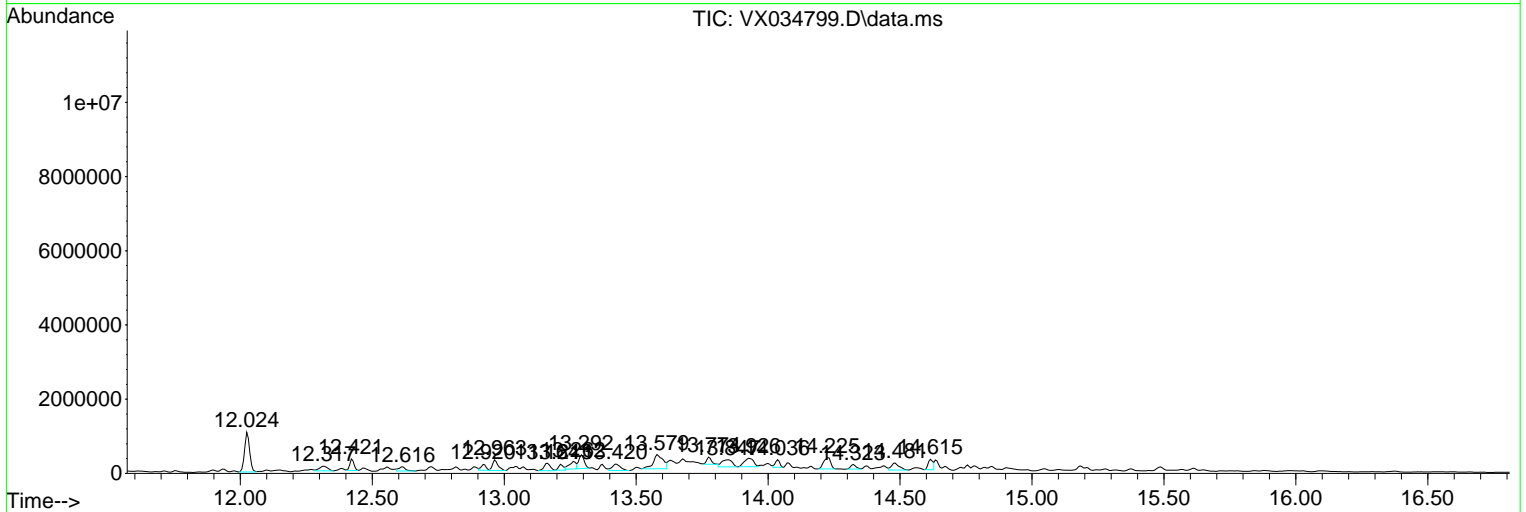
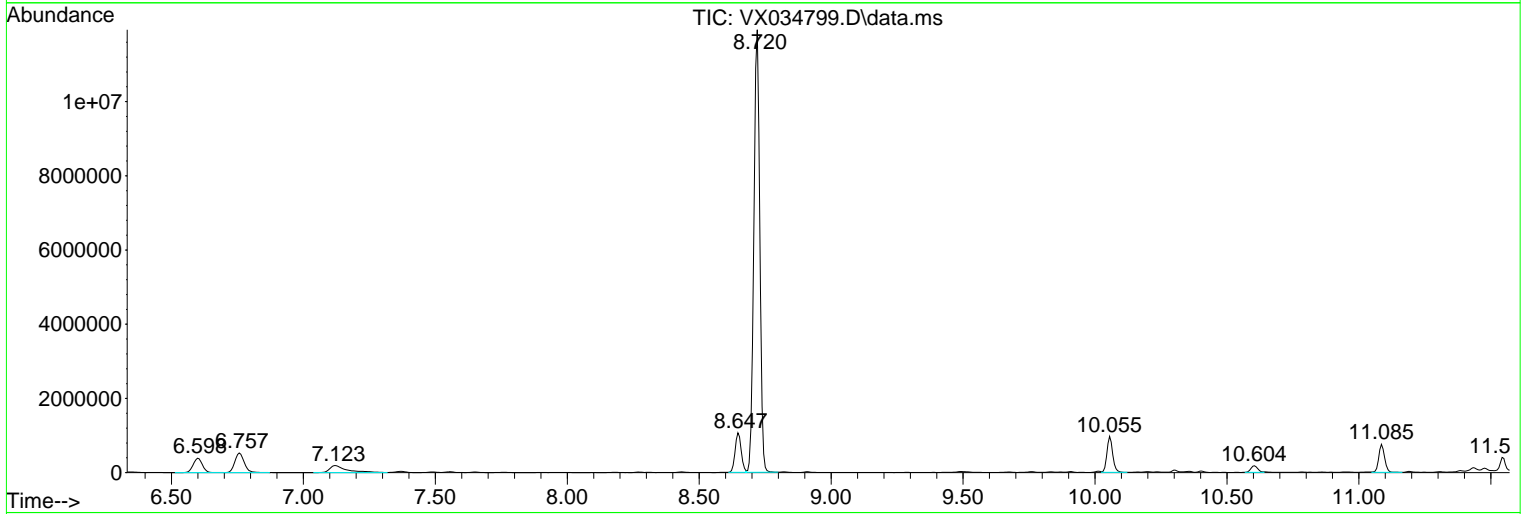
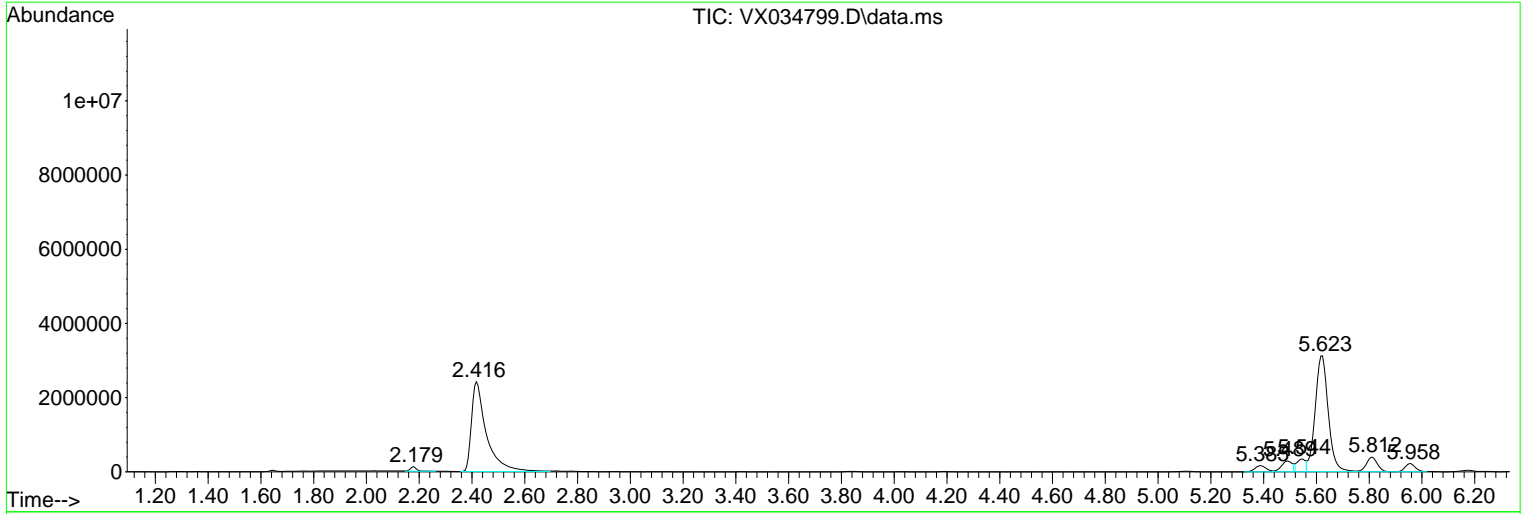
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 Quant Title : SW846 8260

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



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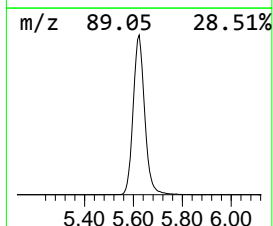
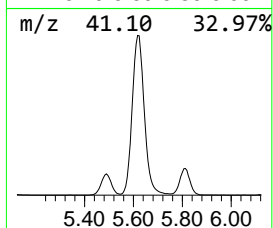
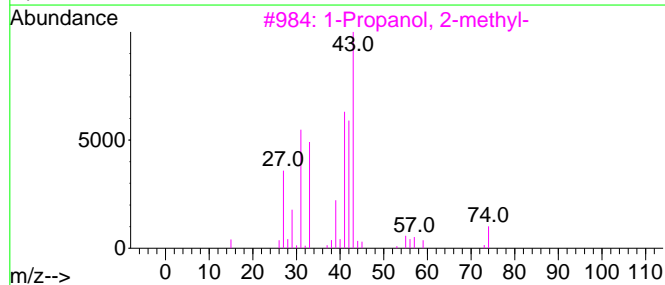
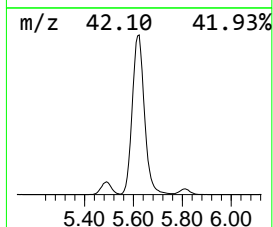
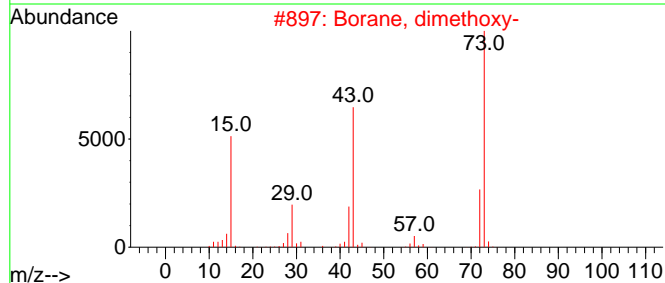
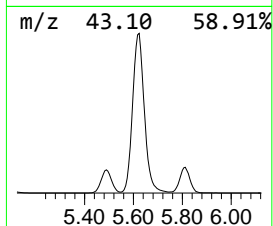
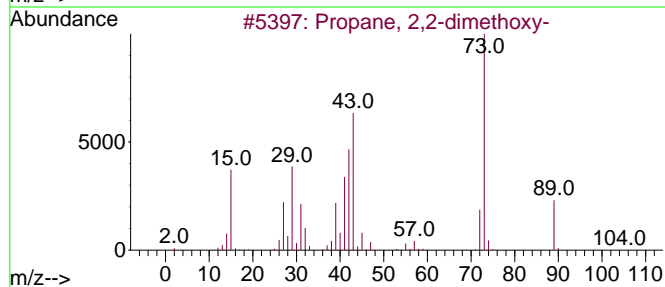
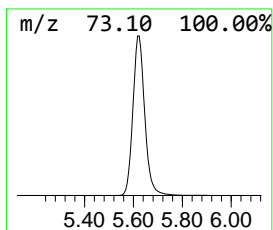
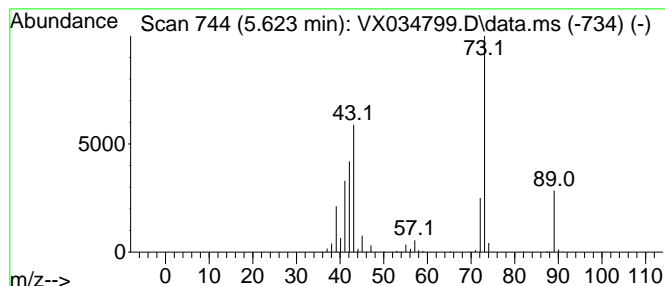
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
 Quant Title : SW846 8260

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

 Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	683.66 ug/l	10699400	Pentafluorobenzene	5.544

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	59
2		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	38
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	12
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	10
5		Guanidine, methyl-	73	C2H7N3	000471-29-4	9



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Instrument :
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 ClientSampleId :
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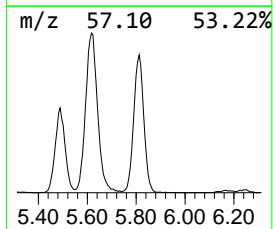
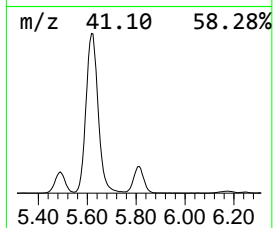
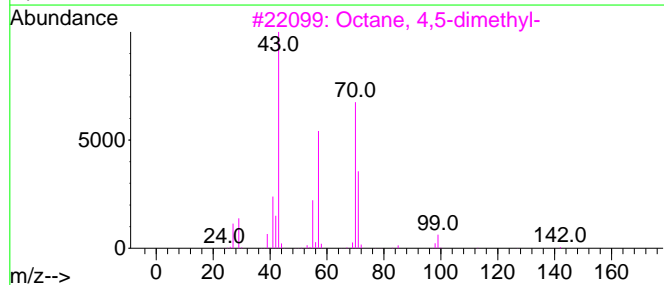
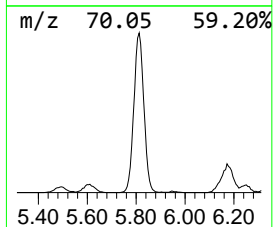
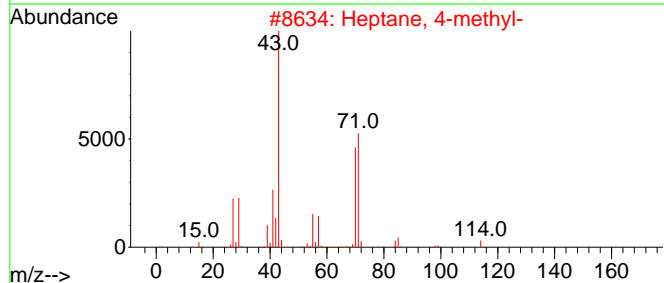
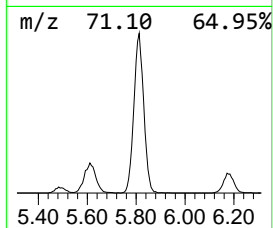
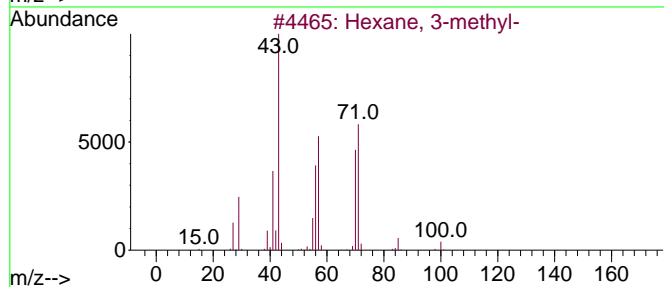
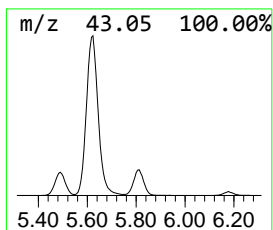
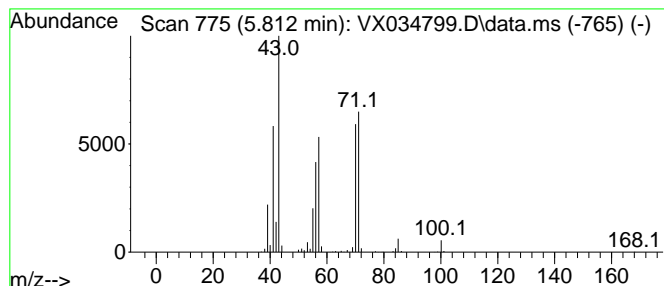
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	73.09 ug/l	1143800	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
3			Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	47
4			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	45
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	43



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Instrument :
 MSVOA_X
 ClientSampleId :
 TRE-1715ME

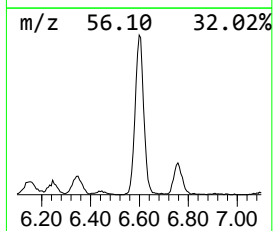
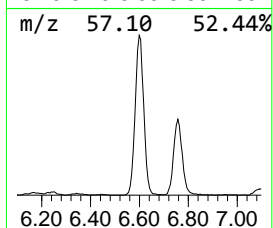
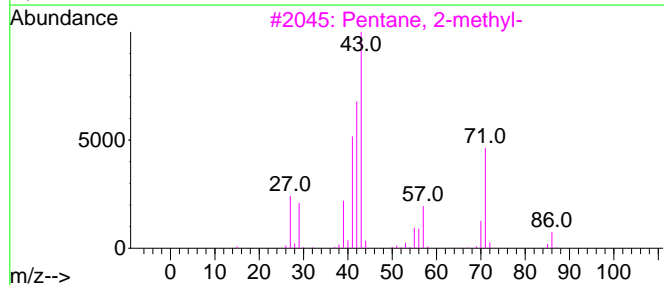
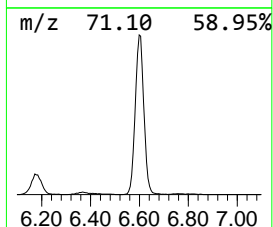
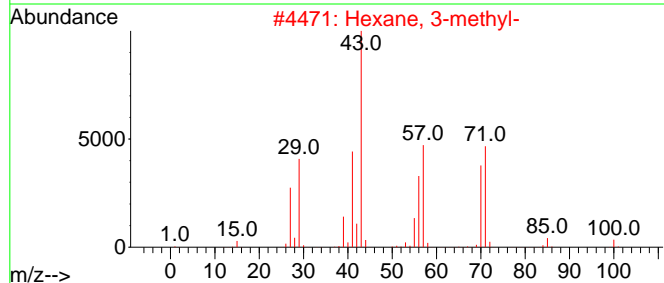
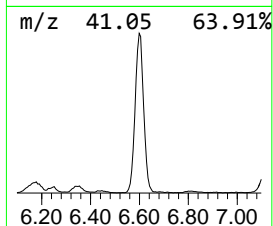
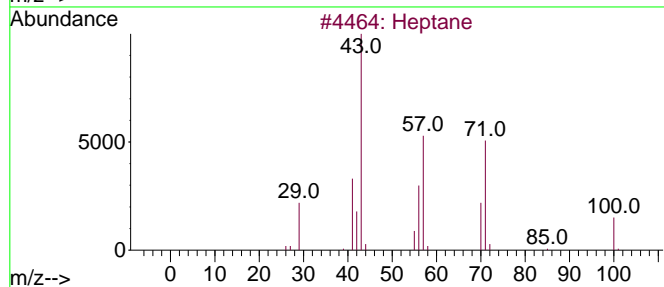
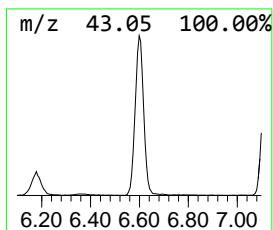
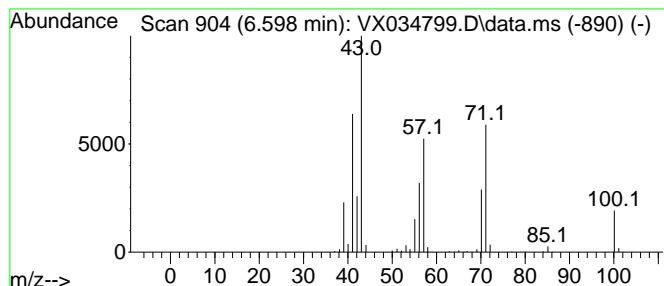
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	36.40 ug/l	942947	1,4-Difluorobenzene	6.757

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	91
2		Hexane, 3-methyl-	100	C7H16	000589-34-4	50
3		Pentane, 2-methyl-	86	C6H14	000107-83-5	43
4		Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	43
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40



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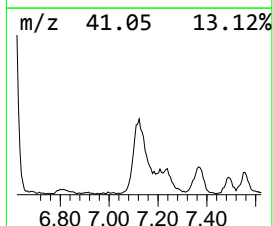
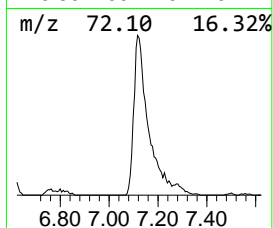
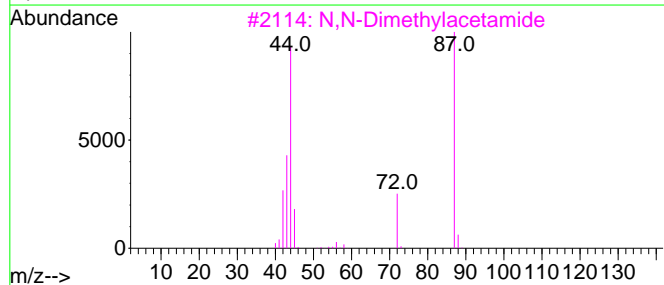
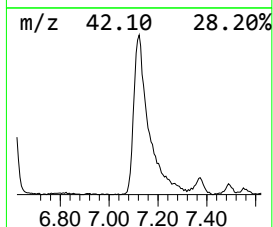
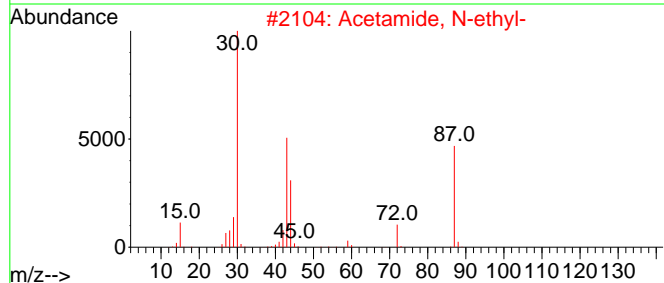
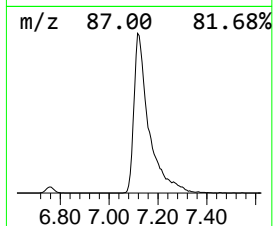
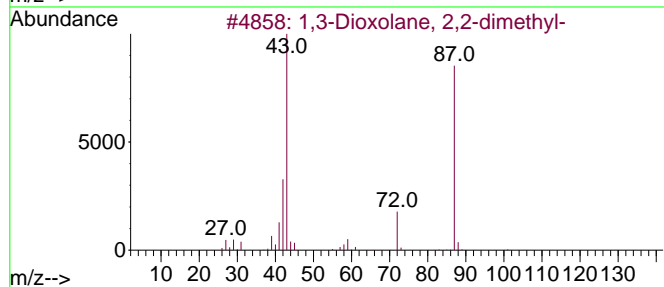
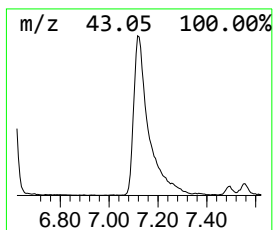
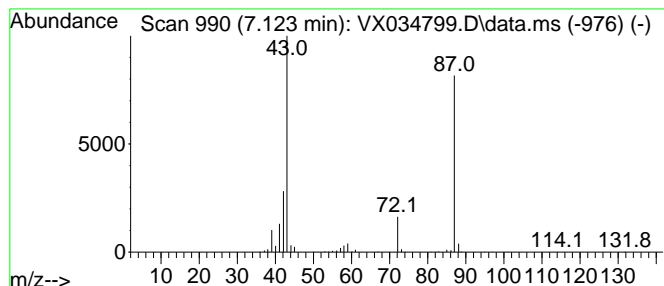
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 1,3-Dioxolane, 2,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.123	33.30 ug/l	862562	1,4-Difluorobenzene	6.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	90
2		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	72
3		N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	53
4		Isobutane	58	C4H10	000075-28-5	9
5		Oxirane, trimethyl-	86	C5H10O	005076-19-7	9



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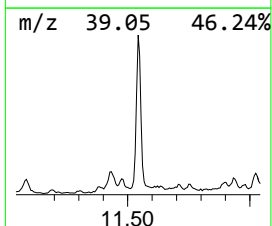
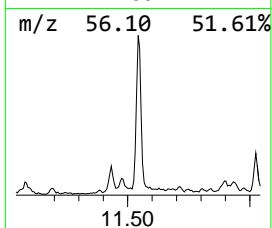
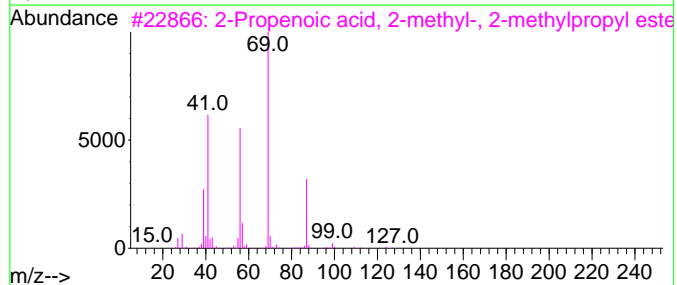
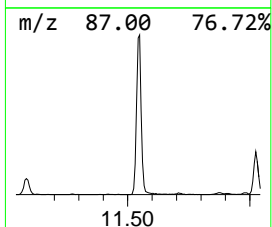
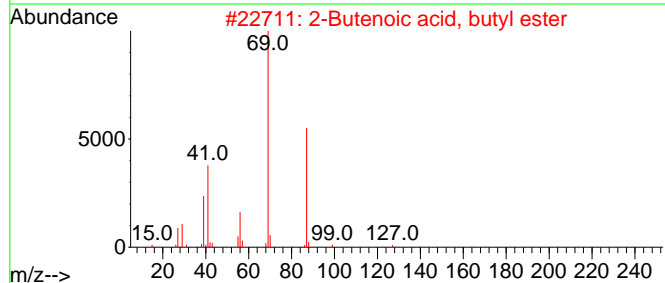
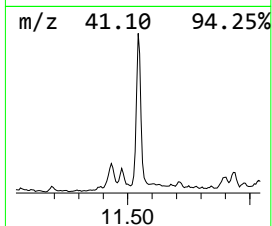
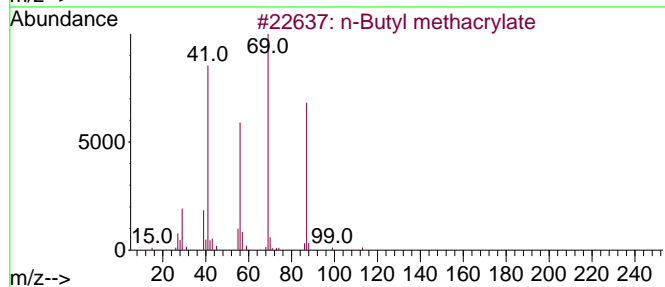
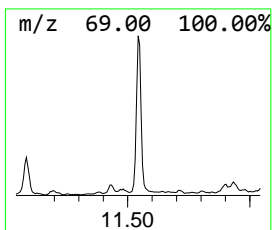
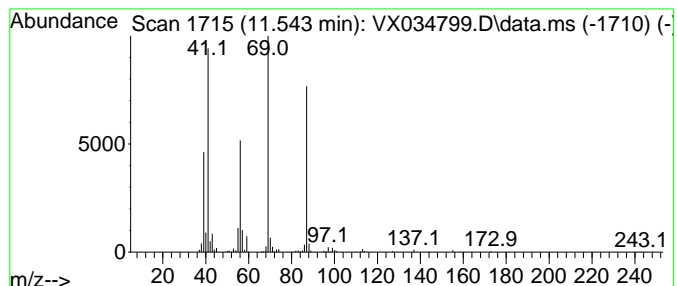
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 Quant Title : SW846 8260

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

 Peak Number 5 n-Butyl methacrylate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.543	16.61 ug/l	471496	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Butyl methacrylate	142	C8H14O2	000097-88-1	80
2			2-Butenoic acid, butyl ester	142	C8H14O2	007299-91-4	80
3			2-Propenoic acid, 2-methyl-, 2-m...	142	C8H14O2	000097-86-9	72
4			2-Propenoic acid, 2-methyl-, hex...	170	C10H18O2	000142-09-6	64
5			Amyl crotonate	156	C9H16O2	1000429-17-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034799.D
 Acq On : 28 Mar 2023 17:36
 Operator : JC/MD
 Sample : 02073-01
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TRE-1715ME

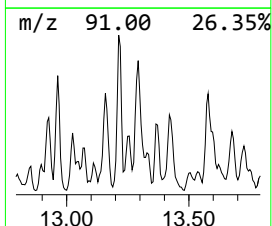
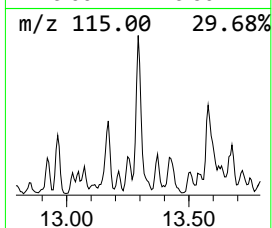
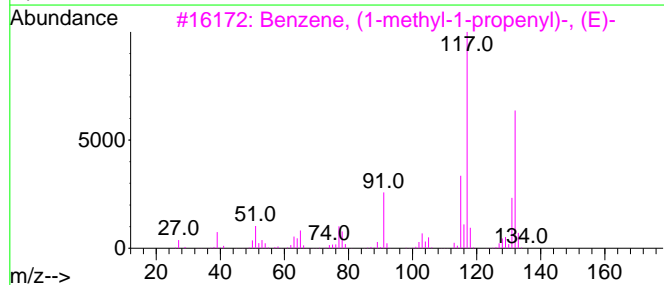
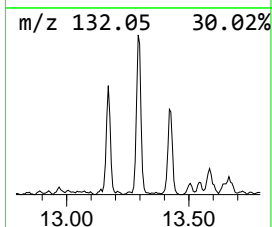
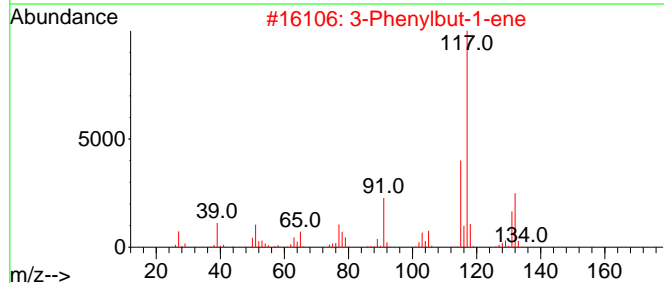
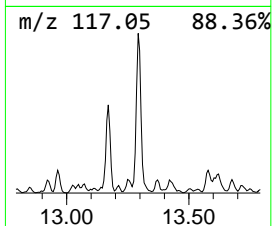
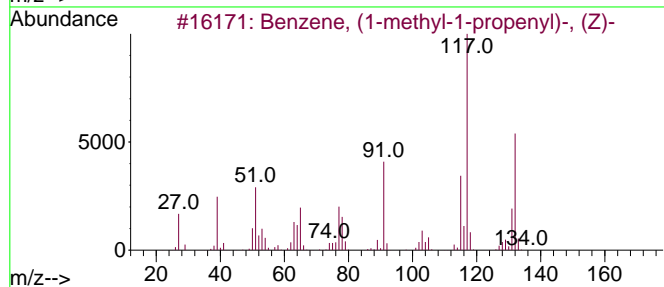
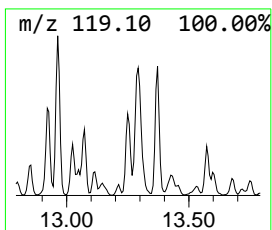
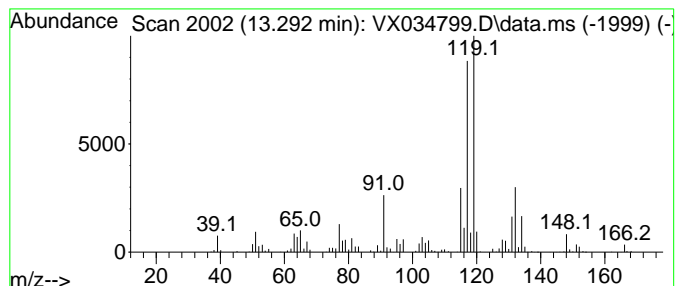
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 Quant Title : SW846 8260

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

 Peak Number 6 Benzene, (1-methyl-1-propen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	17.90 ug/l	507893	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	70
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
3		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	55
4		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	50
5		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034799.D
 Acq On : 28 Mar 2023 17:36
 Operator : JC/MD
 Sample : 02073-01
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TRE-1715ME

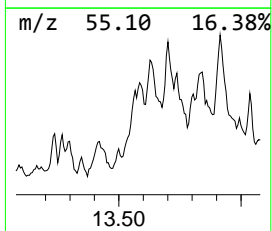
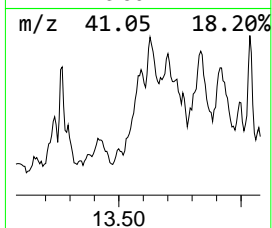
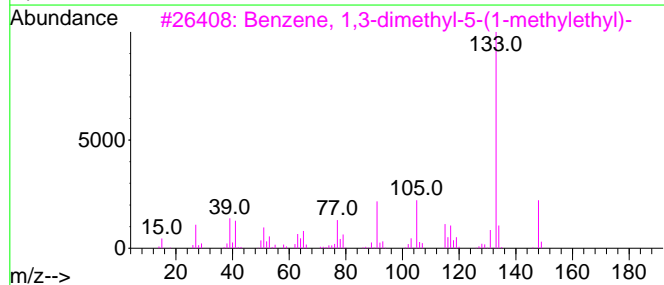
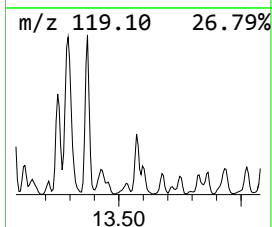
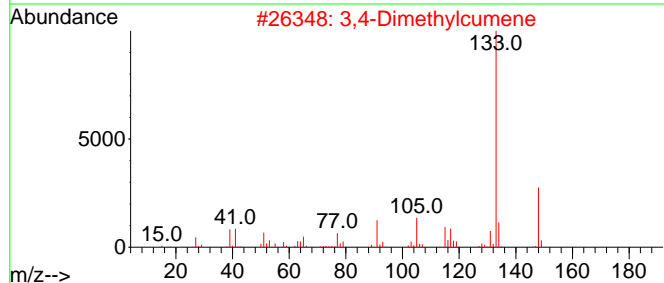
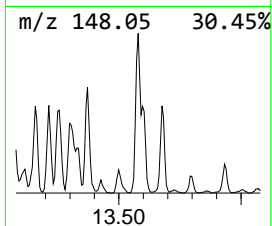
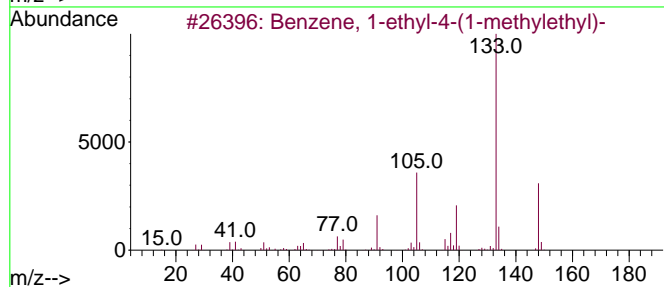
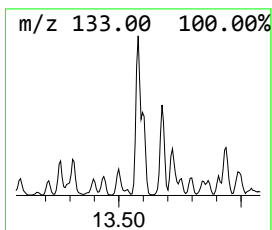
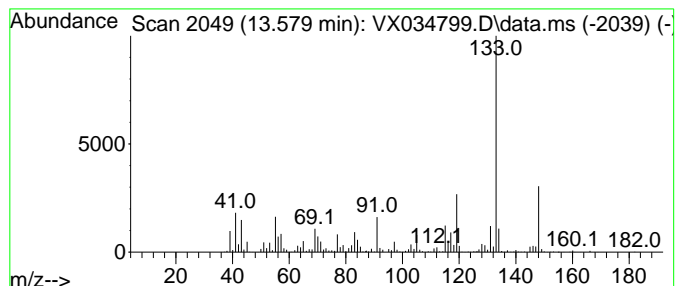
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 Quant Title : SW846 8260

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

 Peak Number 7 Benzene, 1-ethyl-4-(1-methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.579	35.73 ug/l	1014120	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	90
2		3,4-Dimethylcumene	148	C11H16	1000370-34-1	87
3		Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	83
4		4-tert-Butyltoluene	148	C11H16	000098-51-1	74
5		Benzene, 1-ethyl-2,4,5-trimethyl-	148	C11H16	017851-27-3	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034799.D
 Acq On : 28 Mar 2023 17:36
 Operator : JC/MD
 Sample : 02073-01
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TRE-1715ME

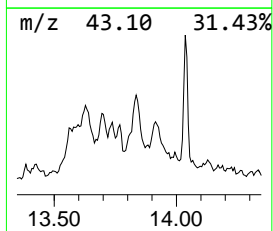
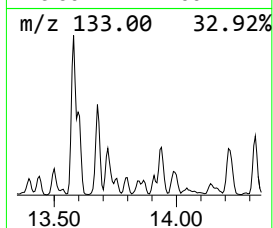
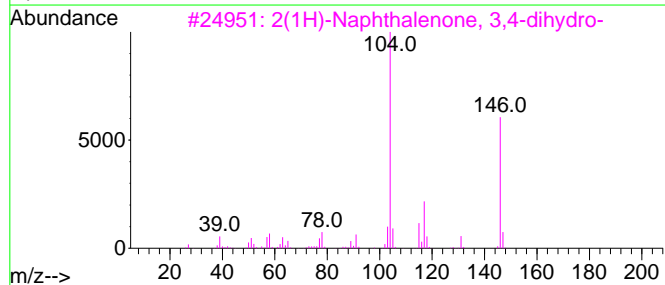
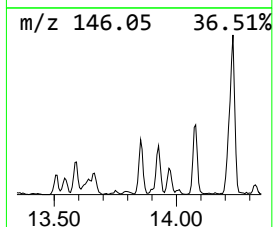
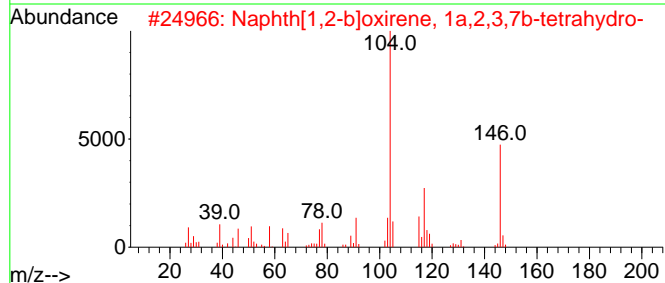
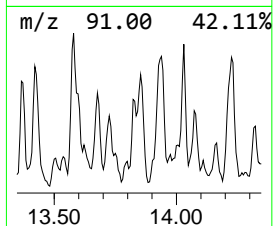
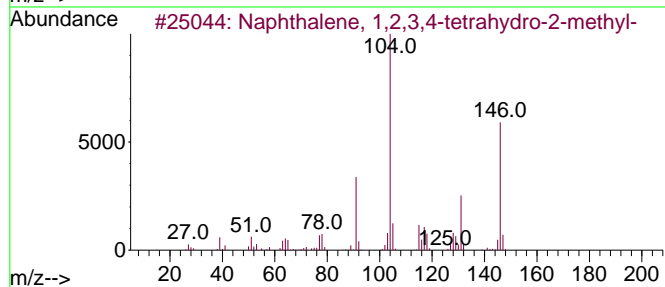
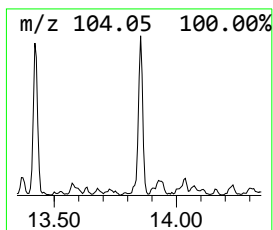
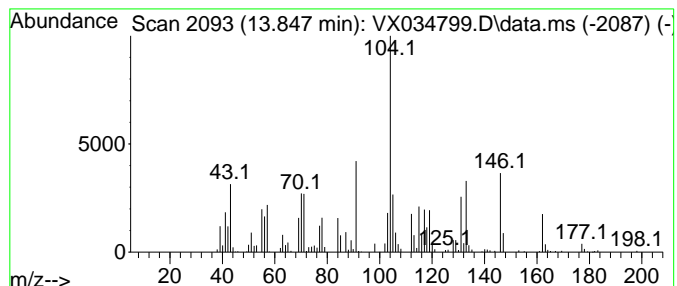
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 Quant Title : SW846 8260

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

 Peak Number 8 Naphthalene, 1,2,3,4-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.847	18.41 ug/l	522358	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	50
2			Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	49
3			2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	49
4			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	38
5			2-Azetidinone, 4-phenyl-	147	C9H9NO	005661-55-2	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034799.D
 Acq On : 28 Mar 2023 17:36
 Operator : JC/MD
 Sample : 02073-01
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
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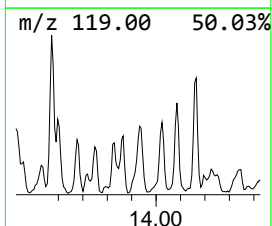
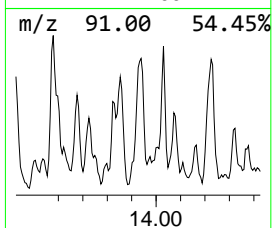
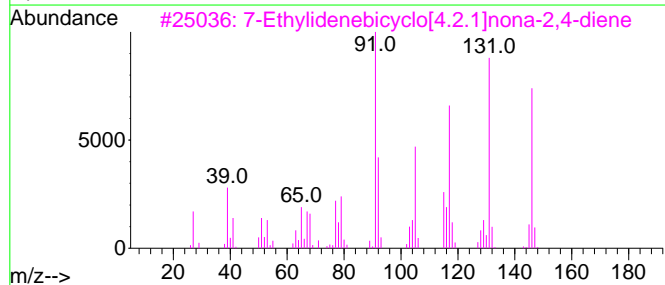
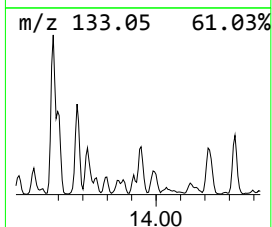
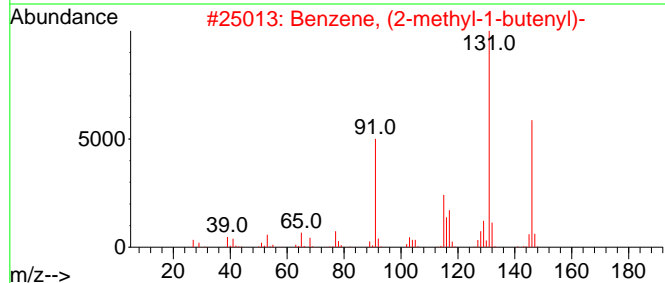
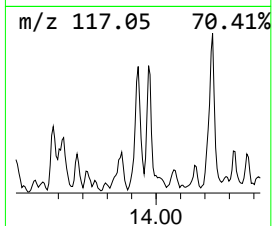
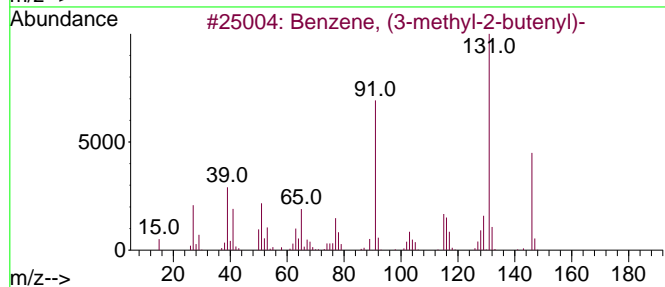
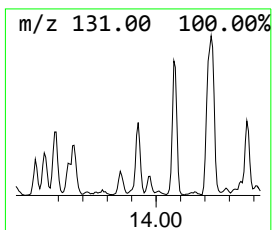
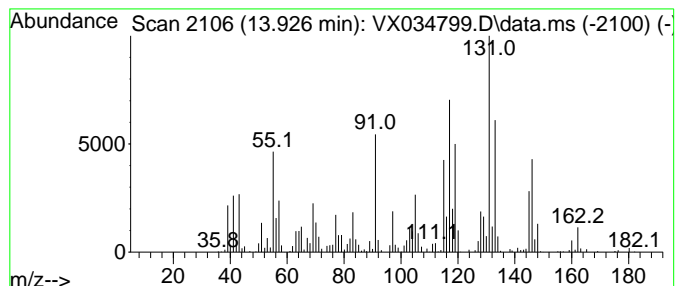
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 Quant Title : SW846 8260

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

 Peak Number 9 Benzene, (3-methyl-2-butenyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	19.61 ug/l	556593	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	55
2		Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	55
3		7-Ethylidenebicyclo[4.2.1]nona-2...	146	C11H14	094400-10-9	55
4		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	49
5		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034799.D
 Acq On : 28 Mar 2023 17:36
 Operator : JC/MD
 Sample : 02073-01
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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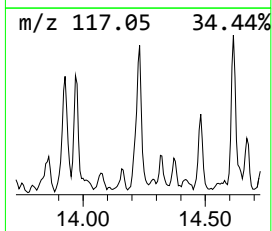
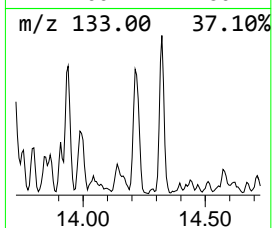
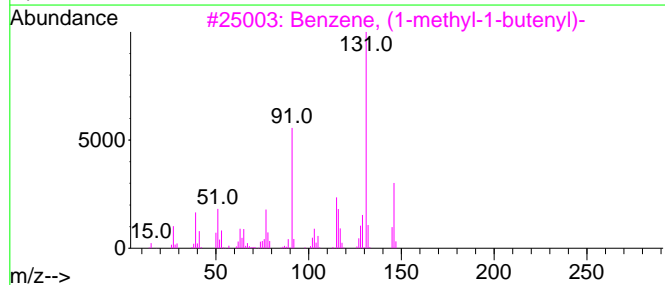
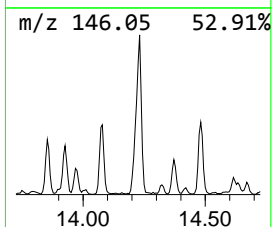
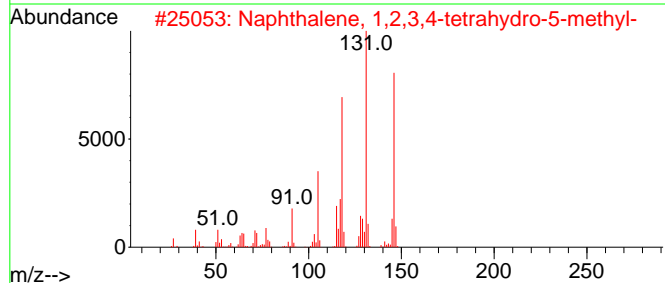
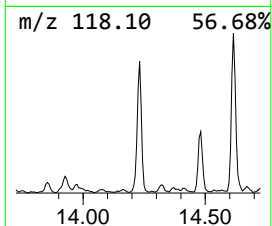
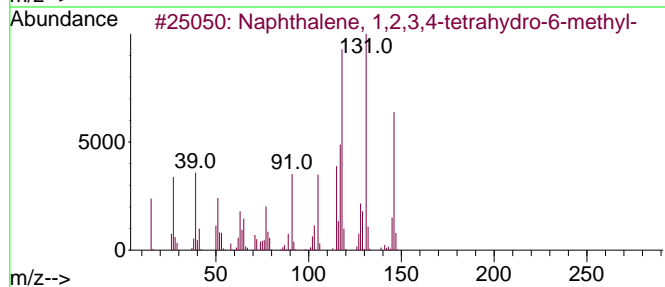
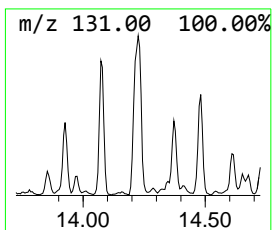
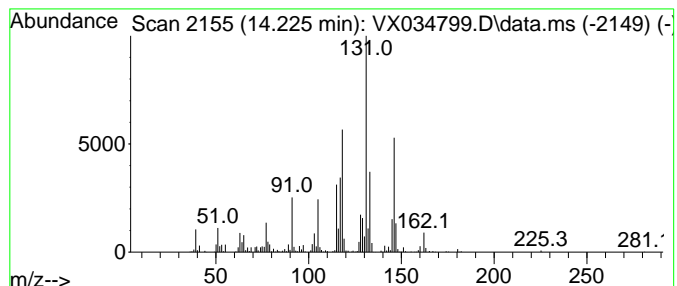
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 Quant Title : SW846 8260

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

 Peak Number 10 Naphthalene, 1,2,3,4-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.225	20.10 ug/l	570594	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
2		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
3		Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	78
4		Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	64
5		2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034799.D
 Acq On : 28 Mar 2023 17:36
 Operator : JC/MD
 Sample : 02073-01
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
 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
Propane, 2,2-di...	5.623	683.7	ug/l	10699400	1	5.544	782508	50.0
Hexane, 3-methyl-	5.812	73.1	ug/l	1143800	1	5.544	782508	50.0
Heptane	6.598	36.4	ug/l	942947	2	6.757	1295100	50.0
1,3-Dioxolane, ...	7.123	33.3	ug/l	862562	2	6.757	1295100	50.0
n-Butyl methacr...	11.543	16.6	ug/l	471496	4	12.024	1419070	50.0
Benzene, (1-met...	13.292	17.9	ug/l	507893	4	12.024	1419070	50.0
Benzene, 1-ethy...	13.579	35.7	ug/l	1014120	4	12.024	1419070	50.0
Naphthalene, 1,...	13.847	18.4	ug/l	522358	4	12.024	1419070	50.0
Benzene, (3-met...	13.926	19.6	ug/l	556593	4	12.024	1419070	50.0
Naphthalene, 1,...	14.225	20.1	ug/l	570594	4	12.024	1419070	50.0