

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
 Data File : VX040235.D
 Acq On : 14 Feb 2024 20:54
 Operator : JC/MD
 Sample : P1427-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50240

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\82X020924W.M
 Title : SW846 8260

Signal : TIC: VX040235.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	53	rBV	745574	930318	2.30%	0.485%
2	1.447	57	59	65	rVB	777429	898246	2.22%	0.468%
3	1.752	103	109	122	rVB	525717	703410	1.74%	0.366%
4	2.117	151	169	172	rBV	5476321	17600716	43.43%	9.168%
5	3.111	322	332	353	rBV2	222102	547789	1.35%	0.285%
6	4.306	518	528	541	rVB3	216554	646667	1.60%	0.337%
7	4.708	581	594	615	rVB	233294	659106	1.63%	0.343%
8	5.470	711	719	727	rBV2	137626	432478	1.07%	0.225%
9	6.044	803	813	824	rVB	2553436	6695635	16.52%	3.488%
10	7.379	1021	1032	1041	rBV2	172698	430241	1.06%	0.224%
11	8.738	1246	1255	1261	rBV	21470290	40526020	100.00%	21.109%
12	10.055	1466	1471	1476	rVB	319768	423353	1.04%	0.221%
13	10.195	1488	1494	1505	rVB	7643163	10362759	25.57%	5.398%
14	10.311	1505	1513	1519	rBV	21138857	34242609	84.50%	17.836%
15	10.646	1561	1568	1578	rBV	12100531	16902240	41.71%	8.804%
16	10.963	1612	1620	1626	rBV	765999	978152	2.41%	0.510%
17	11.079	1634	1639	1644	rBV	334224	417793	1.03%	0.218%
18	11.305	1666	1676	1683	rBV	1839461	2241760	5.53%	1.168%
19	11.384	1683	1689	1696	rVV	6660549	12212496	30.13%	6.361%
20	11.451	1696	1700	1710	rVB	3399371	4063490	10.03%	2.117%
21	11.610	1721	1726	1737	rBV	2896638	3766590	9.29%	1.962%
22	11.756	1744	1750	1755	rBV	11341093	14287162	35.25%	7.442%
23	12.018	1789	1793	1799	rVB2	505756	676440	1.67%	0.352%
24	12.085	1799	1804	1810	rBV	3355086	4226067	10.43%	2.201%
25	12.244	1823	1830	1833	rBV	2076898	2905396	7.17%	1.513%
26	12.268	1833	1834	1838	rVV	842167	626380	1.55%	0.326%
27	12.317	1838	1842	1852	rVB3	1235374	1801248	4.44%	0.938%
28	12.463	1862	1866	1872	rVB	347765	421073	1.04%	0.219%
29	12.530	1872	1877	1879	rBV	779038	991622	2.45%	0.517%
30	12.555	1879	1881	1886	rVB	637450	658839	1.63%	0.343%
31	12.609	1886	1890	1894	rBV	1128651	1319588	3.26%	0.687%
32	12.701	1900	1905	1913	rBV2	529334	830853	2.05%	0.433%
33	12.847	1924	1929	1934	rVB	366012	432891	1.07%	0.225%
34	12.920	1934	1941	1944	rBV	715058	847729	2.09%	0.442%
35	12.963	1944	1948	1954	rVB	1057061	1261180	3.11%	0.657%
36	13.164	1977	1981	1986	rVB	584681	723367	1.78%	0.377%

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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\82X020924W.M
Title : SW846 8260

37	13.292	1997	2002	2007	rVB2	1161813	1581338	3.90%	0.824%
38	13.774	2075	2081	2088	rBV	1219469	1488925	3.67%	0.776%
39	14.633	2214	2222	2227	rBV	617858	808218	1.99%	0.421%
40	14.780	2240	2246	2250	rBV	334416	412275	1.02%	0.215%

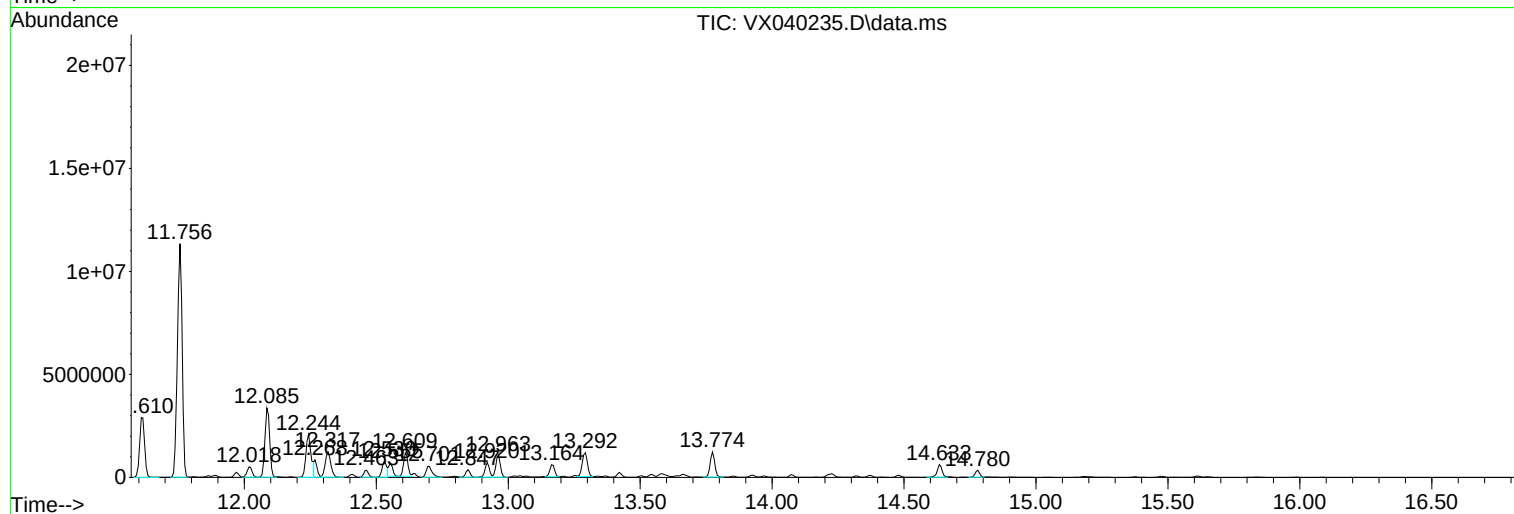
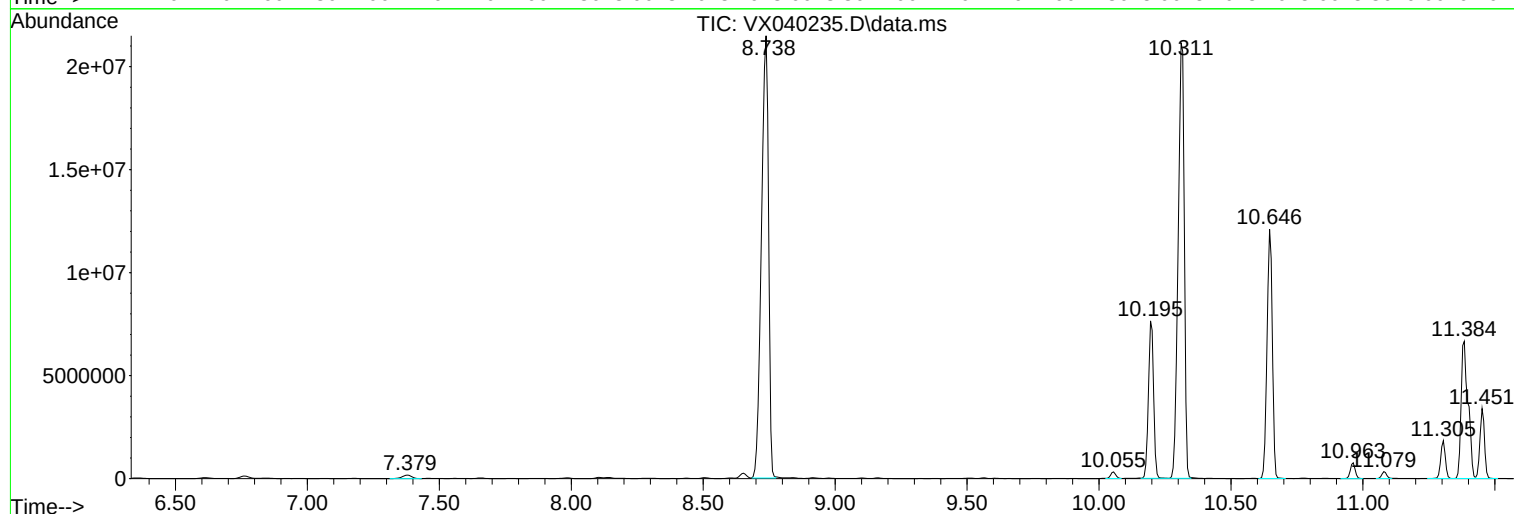
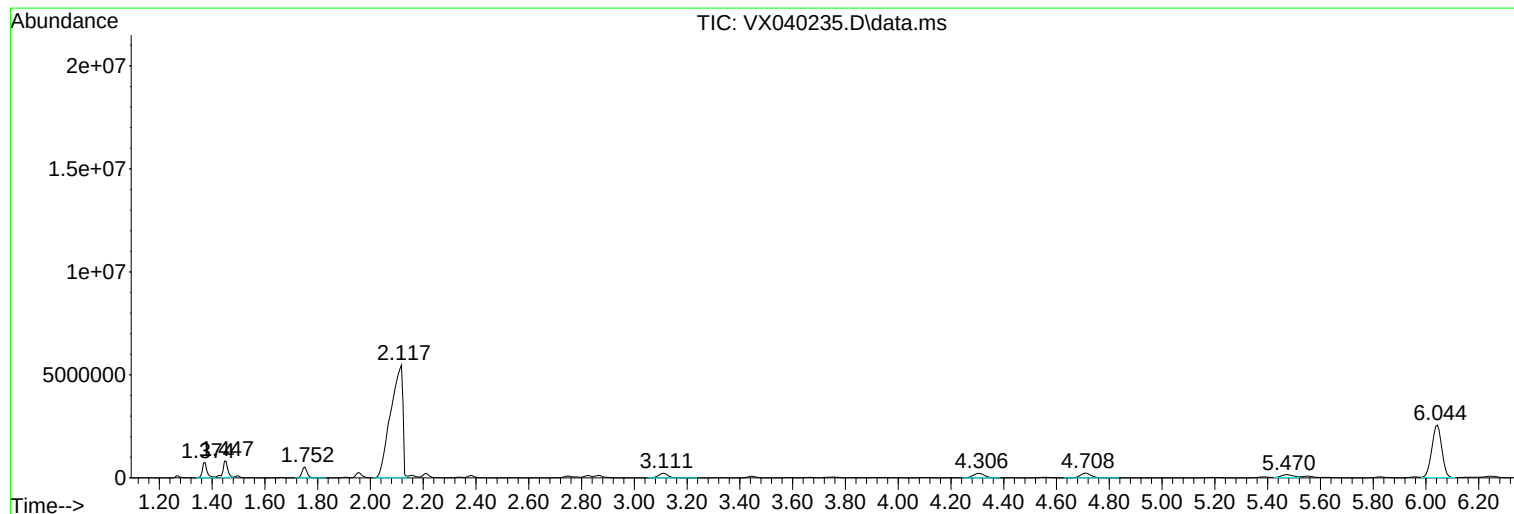
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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



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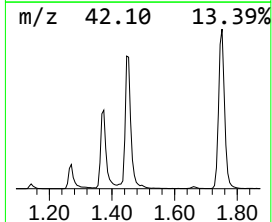
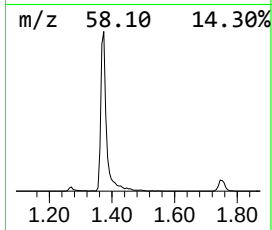
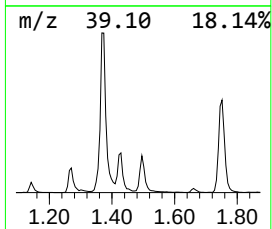
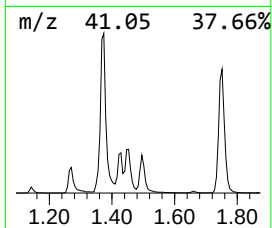
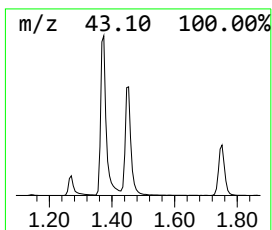
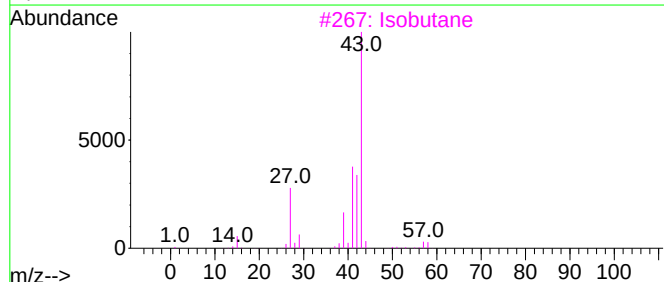
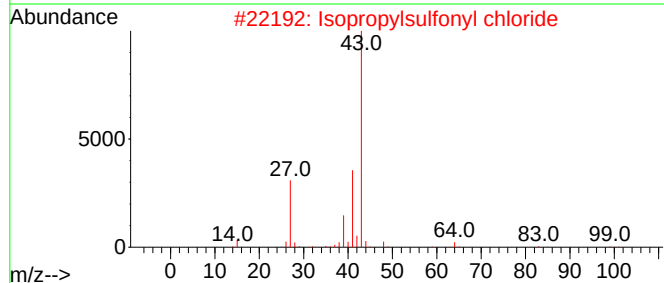
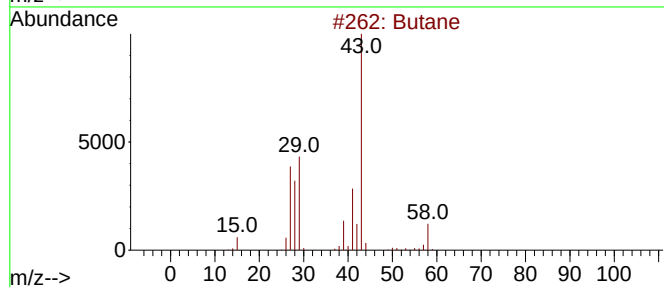
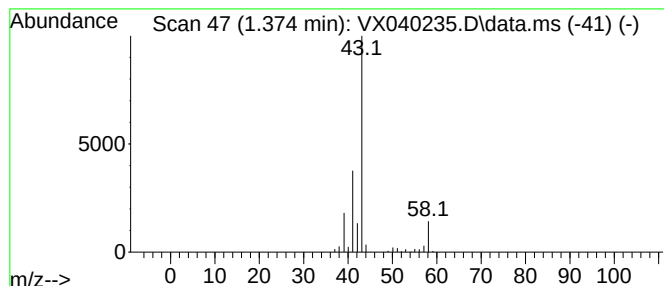
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	107.56 ug/l	930318	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane	58	C4H10	000106-97-8	80
2		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3		Isobutane	58	C4H10	000075-28-5	9
4		Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5		Diazene, dimethyl-	58	C2H6N2	000503-28-6	4



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Instrument :
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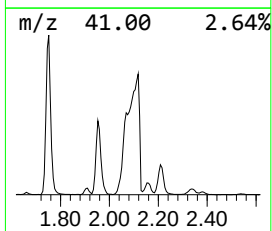
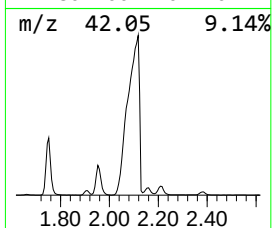
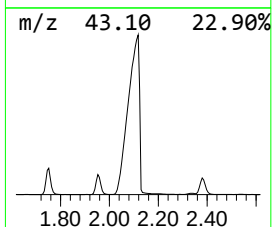
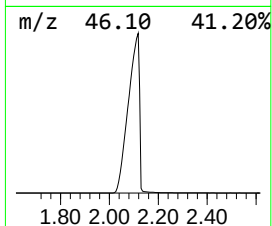
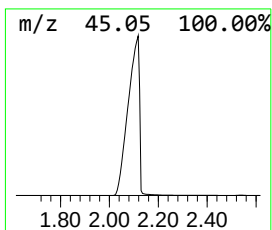
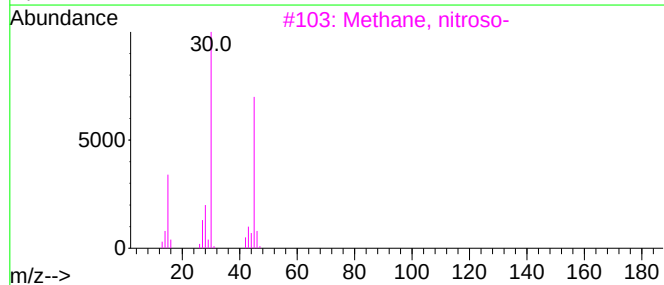
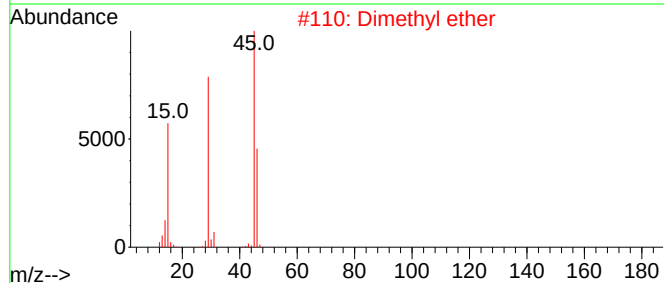
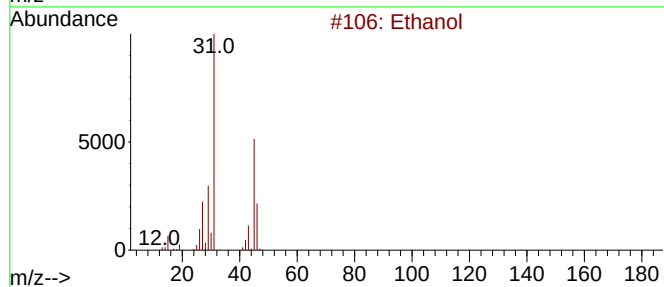
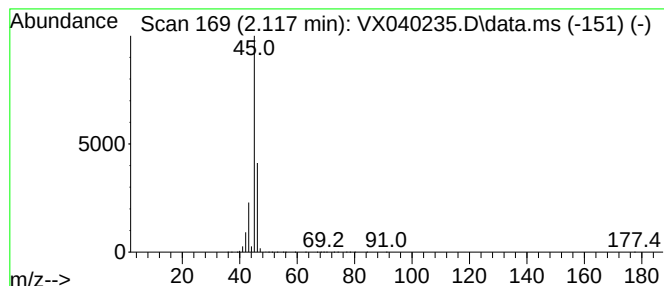
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.117	2034.87 ug/l	17600700	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	86
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Nitrogen dioxide			46	NO2	010102-44-0	2



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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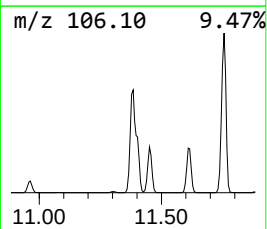
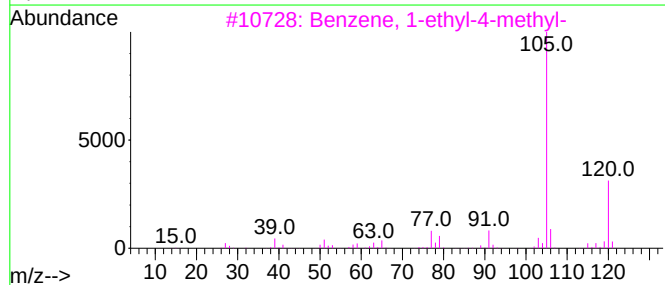
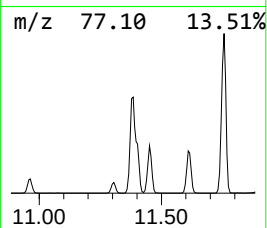
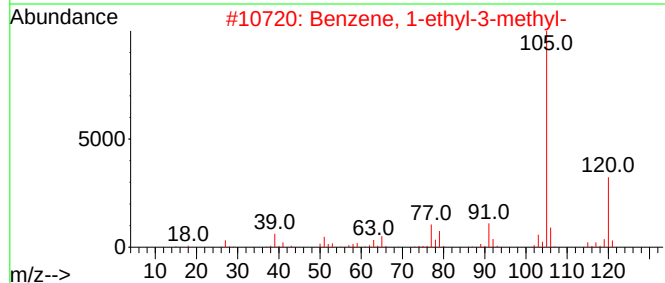
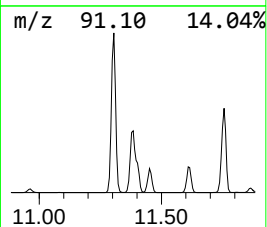
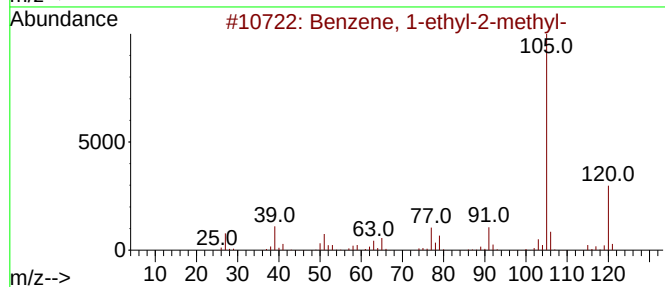
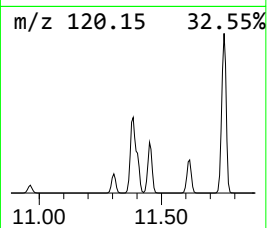
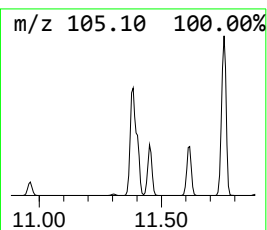
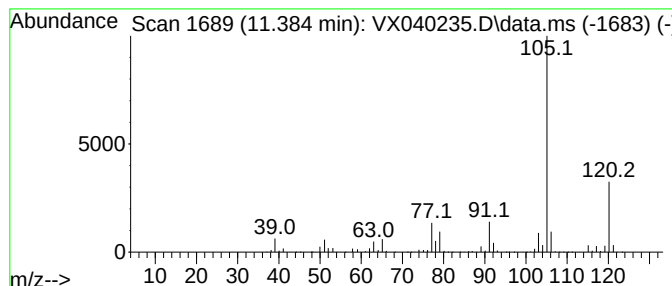
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	902.70 ug/l	12212500	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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ClientSampleId :
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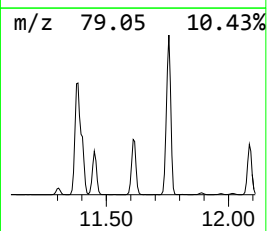
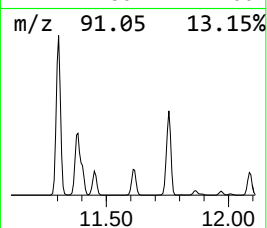
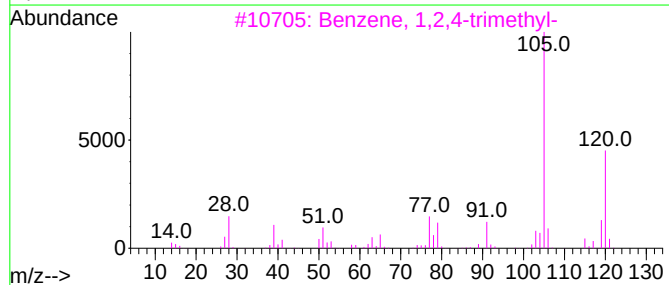
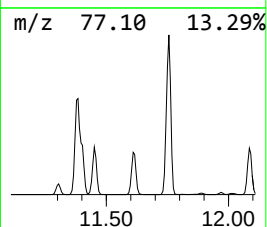
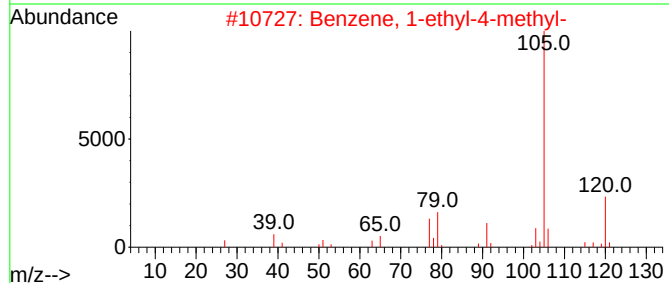
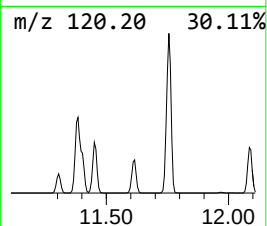
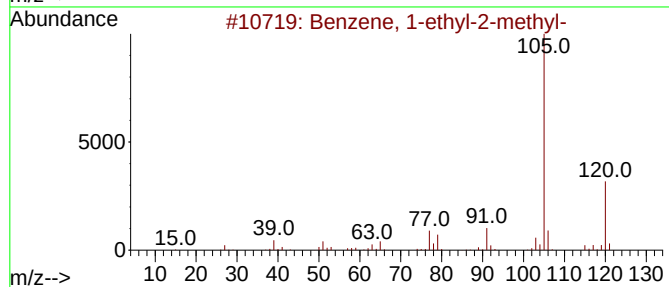
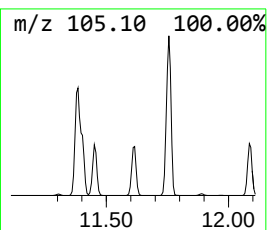
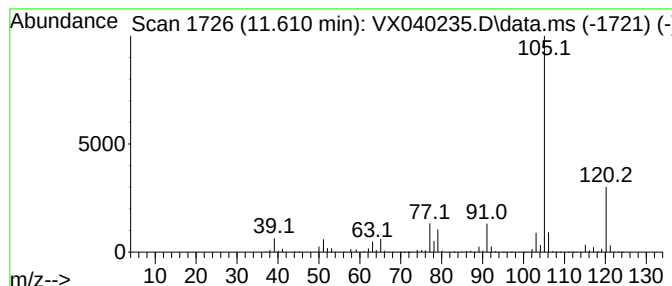
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	278.41 ug/l	3766590	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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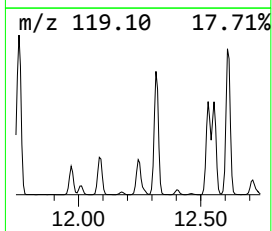
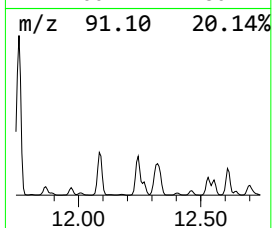
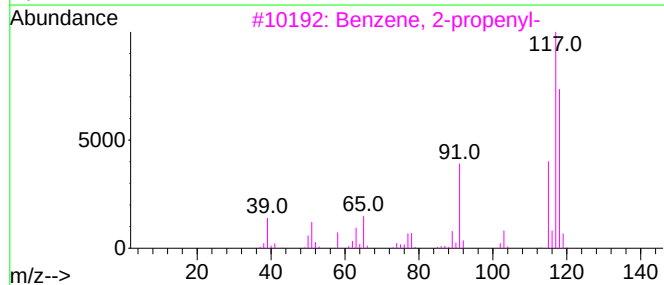
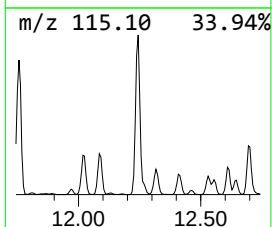
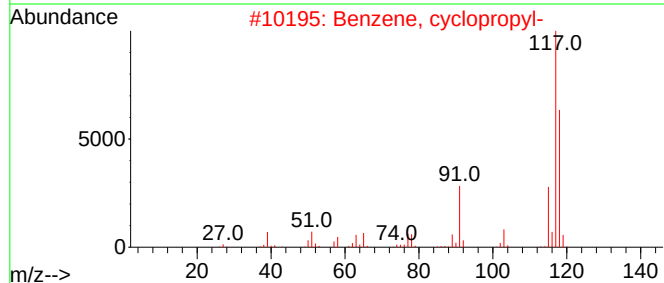
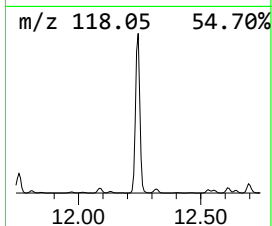
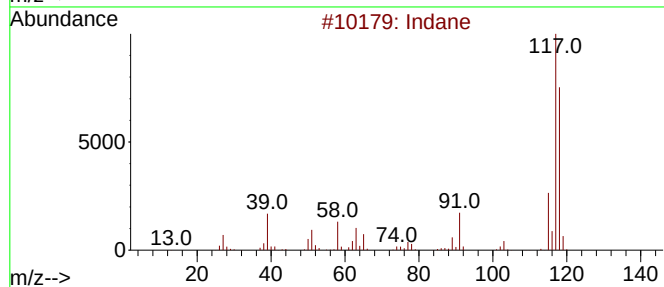
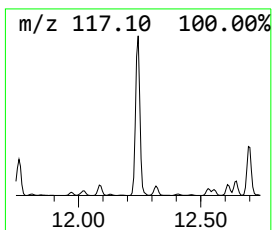
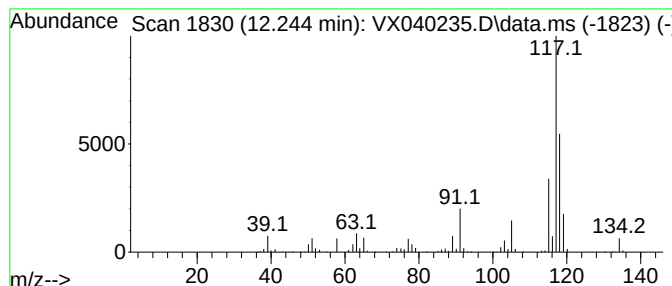
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	214.76 ug/l	2905400	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040235.D
Acq On : 14 Feb 2024 20:54
Operator : JC/MD
Sample : P1427-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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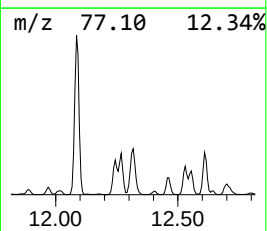
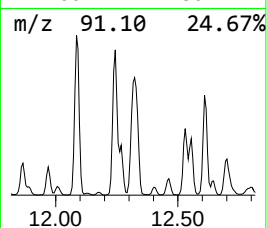
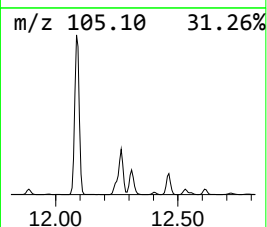
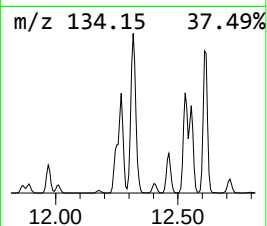
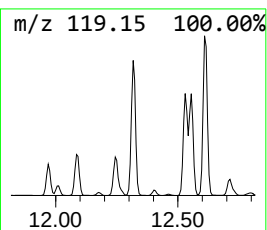
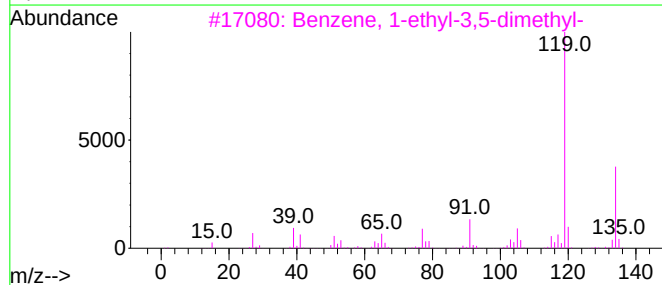
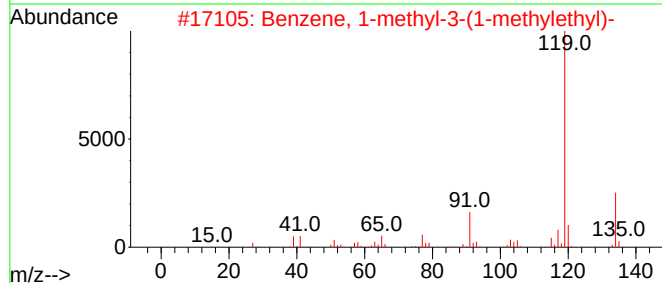
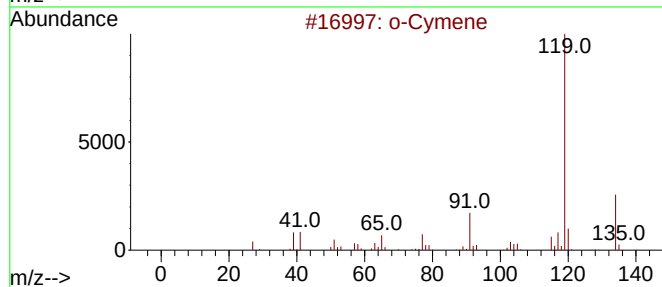
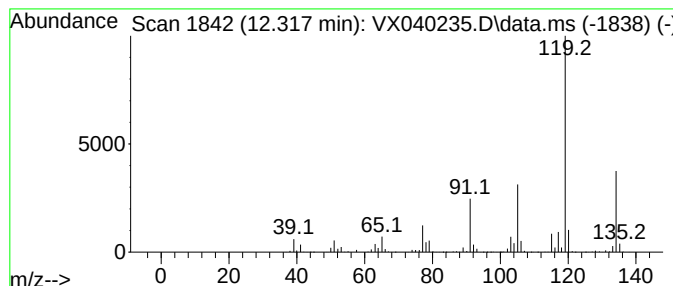
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Quant Title : SW846 8260

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

Peak Number 8 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	133.14 ug/l	1801250	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	95
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
3			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040235.D
Acq On : 14 Feb 2024 20:54
Operator : JC/MD
Sample : P1427-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50240

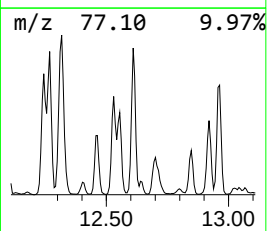
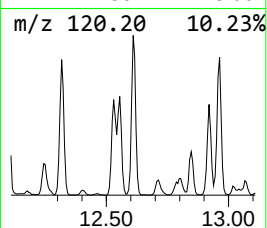
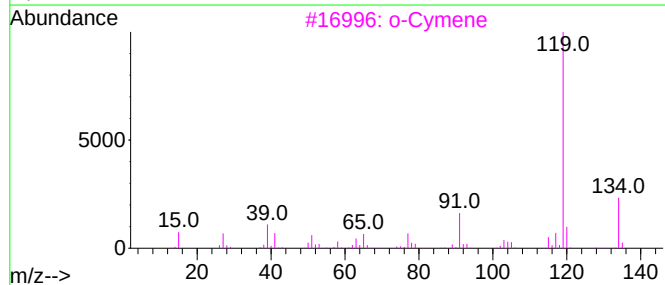
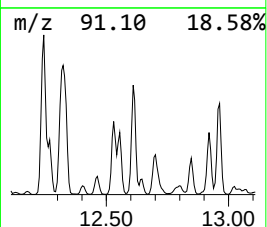
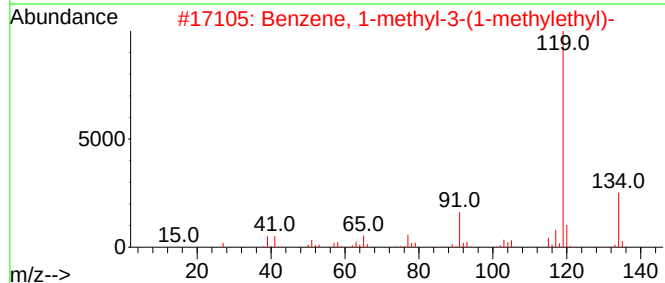
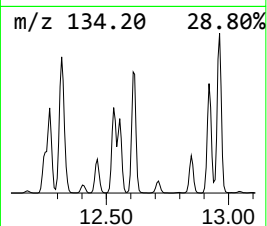
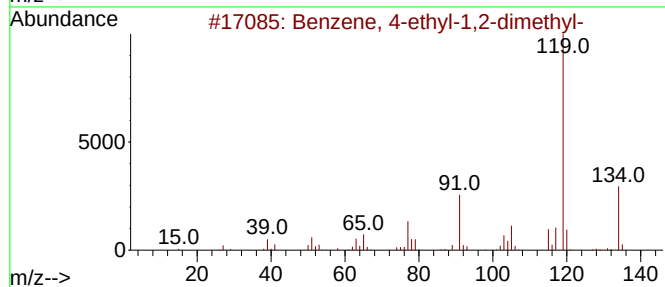
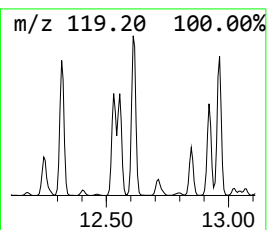
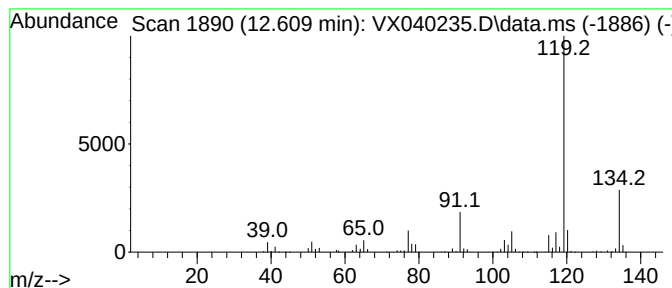
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.609	97.54 ug/l	1319590	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040235.D
Acq On : 14 Feb 2024 20:54
Operator : JC/MD
Sample : P1427-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50240

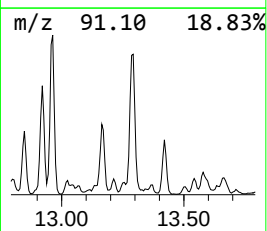
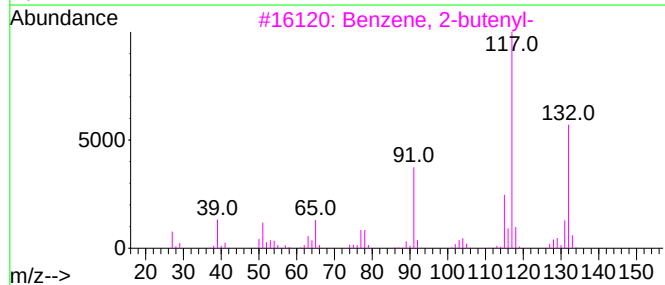
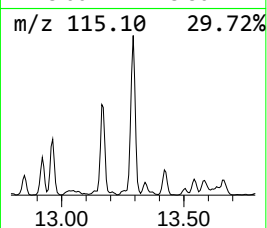
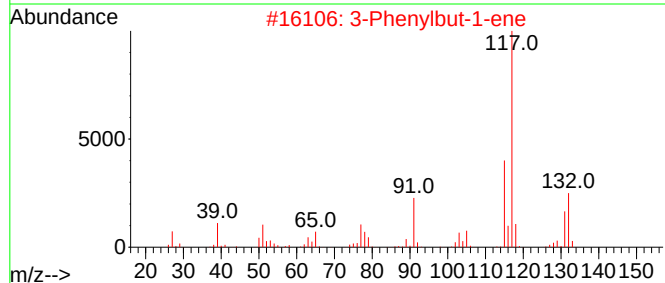
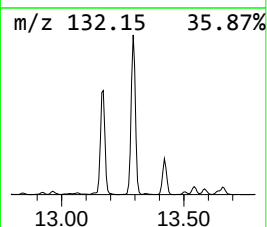
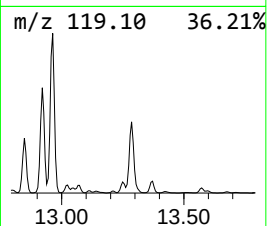
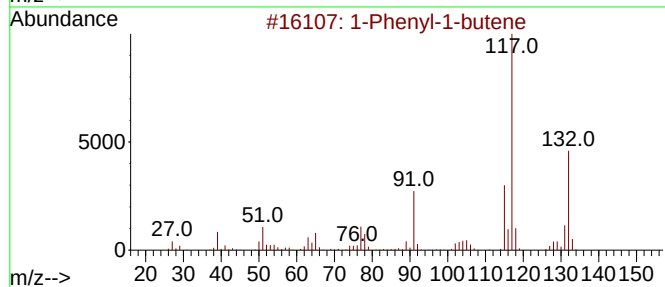
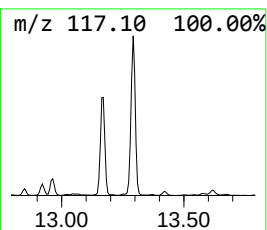
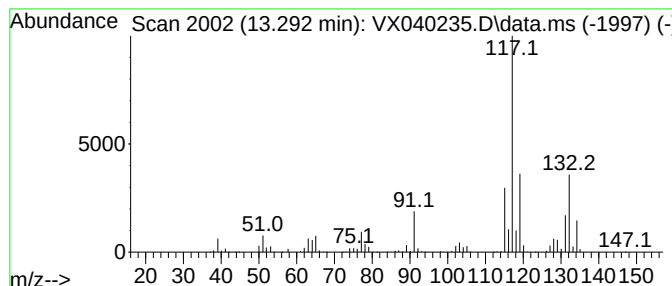
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Phenyl-1-butene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	116.89 ug/l	1581340	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenyl-1-butene	132	C10H12	000824-90-8	90
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
3		Benzene, 2-butenyl-	132	C10H12	001560-06-1	81
4		Indan, 1-methyl-	132	C10H12	000767-58-8	76
5		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040235.D
Acq On : 14 Feb 2024 20:54
Operator : JC/MD
Sample : P1427-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50240

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.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
Butane	1.374	107.6	ug/l	930318	1	5.550	432478	50.0
Ethanol	2.117	2034.9	ug/l	17600700	1	5.550	432478	50.0
Benzene, 1-ethy...	11.384	902.7	ug/l	12212500	4	12.024	676440	50.0
Benzene, 1-ethy...	11.610	278.4	ug/l	3766590	4	12.024	676440	50.0
Indane	12.244	214.8	ug/l	2905400	4	12.024	676440	50.0
o-Cymene	12.317	133.1	ug/l	1801250	4	12.024	676440	50.0
Benzene, 4-ethy...	12.609	97.5	ug/l	1319590	4	12.024	676440	50.0
1-Phenyl-1-butene	13.292	116.9	ug/l	1581340	4	12.024	676440	50.0