

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027956.D
 Acq On : 04 Apr 2022 14:38
 Operator : JC/MD
 Sample : N2249-01 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-1R

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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\82X032922W.M
 Title : SW846 8260

Signal : TIC: VX027956.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	22	29	43	rBV	89692	315302	19.97%	3.936%
2	1.374	44	47	53	rVB2	11541	20543	1.30%	0.256%
3	1.746	104	108	130	rVB2	62121	105363	6.67%	1.315%
4	1.953	138	142	151	rVB	20033	30715	1.95%	0.383%
5	2.825	281	285	289	rBV2	8932	16226	1.03%	0.203%
6	2.867	289	292	304	rVB3	9091	23319	1.48%	0.291%
7	3.105	323	331	342	rVB2	10458	24131	1.53%	0.301%
8	4.306	517	528	539	rVB2	22606	64810	4.11%	0.809%
9	5.391	694	706	716	rBV2	56012	162874	10.32%	2.033%
10	5.556	724	733	753	rVB	100015	294373	18.65%	3.675%
11	5.958	788	799	811	rBV	62772	160375	10.16%	2.002%
12	6.763	922	931	942	rBV	150669	353680	22.40%	4.415%
13	8.653	1234	1241	1248	rBV	276740	440351	27.89%	5.497%
14	8.720	1248	1252	1260	rVB	15332	23990	1.52%	0.299%
15	10.055	1462	1471	1481	rBV	292796	396424	25.11%	4.949%
16	10.195	1488	1494	1501	rBV	312963	407399	25.81%	5.086%
17	10.305	1505	1512	1523	rBV	1149449	1578652	100.00%	19.706%
18	10.646	1562	1568	1574	rBV	77398	103330	6.55%	1.290%
19	10.963	1615	1620	1628	rVB	21398	26759	1.70%	0.334%
20	11.079	1634	1639	1654	rVB	284580	376650	23.86%	4.702%
21	11.305	1671	1676	1683	rBV	50147	61071	3.87%	0.762%
22	11.378	1683	1688	1690	rBV	215627	277930	17.61%	3.469%
23	11.451	1696	1700	1712	rVB	124281	152146	9.64%	1.899%
24	11.616	1721	1727	1737	rVB	178739	218765	13.86%	2.731%
25	11.750	1744	1749	1757	rBV	587359	732799	46.42%	9.148%
26	12.024	1789	1794	1800	rBV	323348	387411	24.54%	4.836%
27	12.085	1800	1804	1810	rVB	216301	265963	16.85%	3.320%
28	12.244	1824	1830	1838	rBV	236869	298638	18.92%	3.728%
29	12.317	1838	1842	1850	rVB2	28114	40575	2.57%	0.506%
30	12.530	1872	1877	1880	rBV	21948	32159	2.04%	0.401%
31	12.616	1886	1891	1894	rBV	43563	51433	3.26%	0.642%
32	12.701	1900	1905	1915	rVB2	29267	39579	2.51%	0.494%
33	12.920	1936	1941	1945	rBV	23202	30004	1.90%	0.375%
34	12.963	1945	1948	1953	rVB	32833	37531	2.38%	0.469%
35	13.170	1977	1982	1988	rVB	29933	35094	2.22%	0.438%
36	13.292	1997	2002	2008	rVB2	62944	82165	5.20%	1.026%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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

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Title : SW846 8260

37	13.780	2076	2082	2088	rBV	222433	284492	18.02%	3.551%
38	14.640	2219	2223	2230	rVB	28707	35240	2.23%	0.440%
39	14.780	2242	2246	2253	rVB	17579	22610	1.43%	0.282%

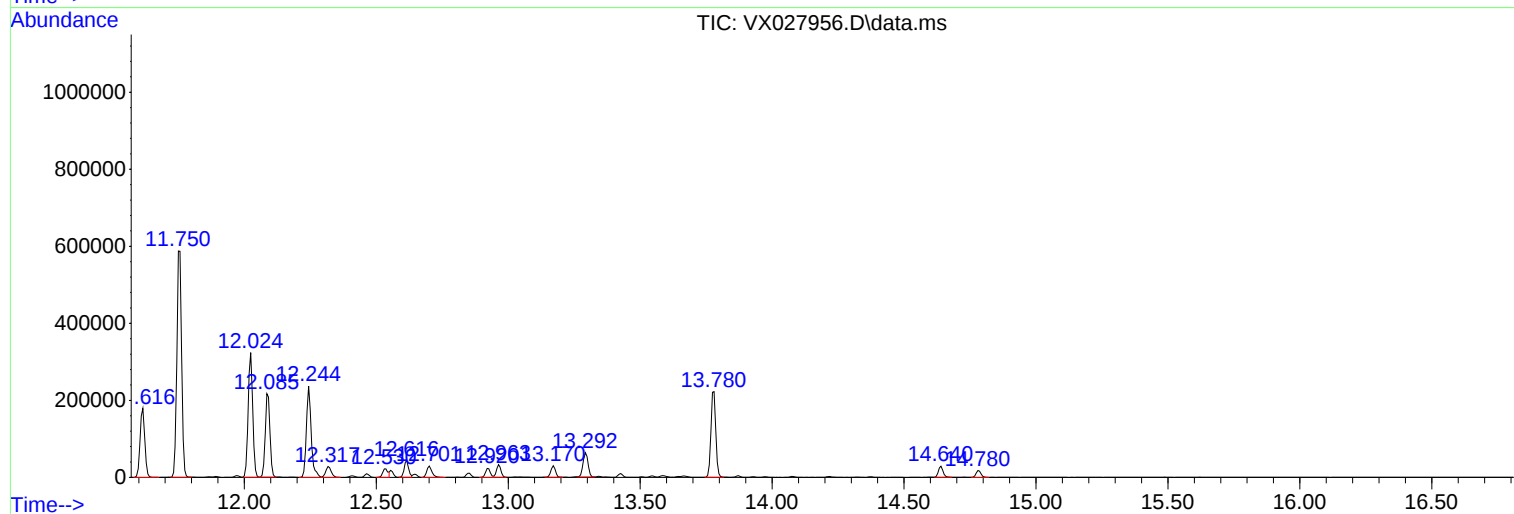
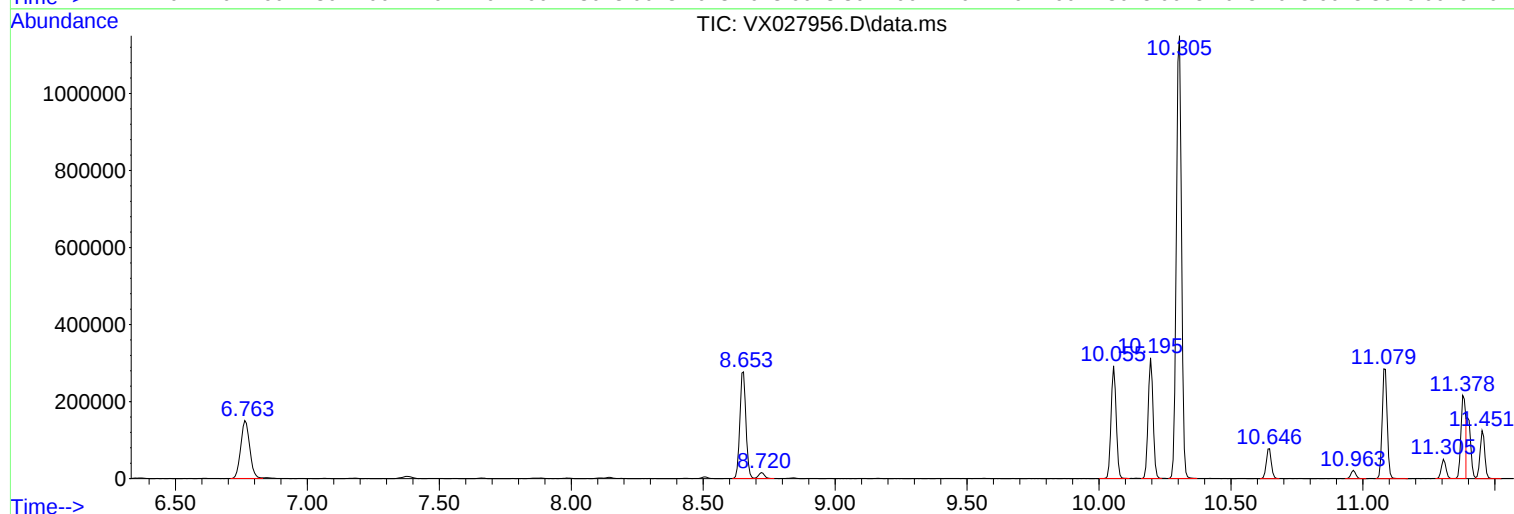
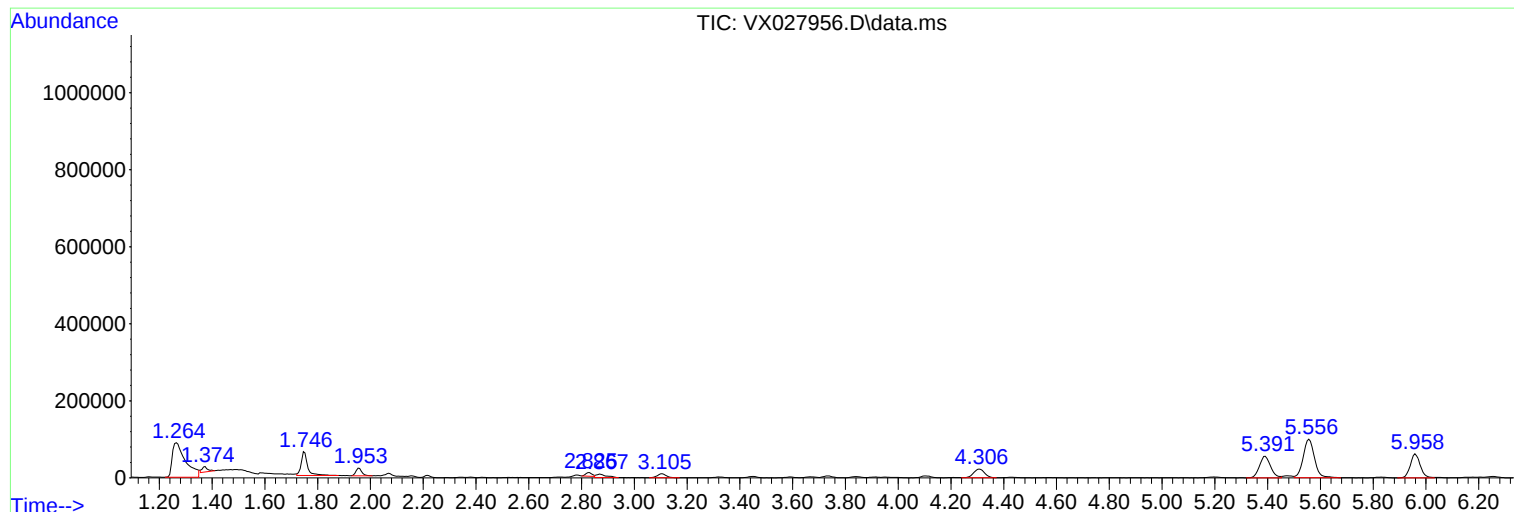
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



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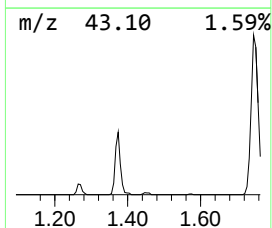
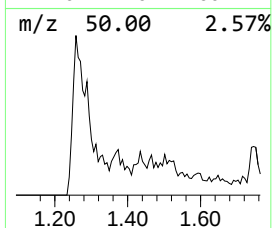
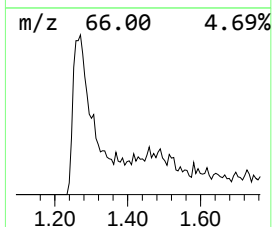
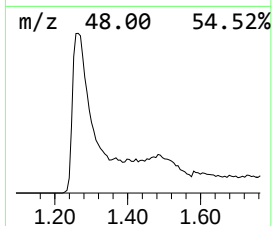
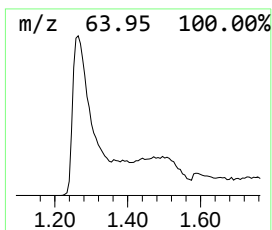
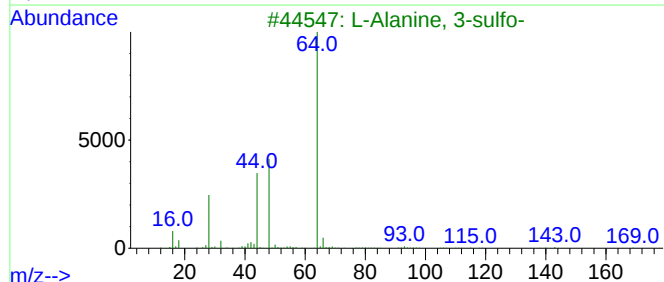
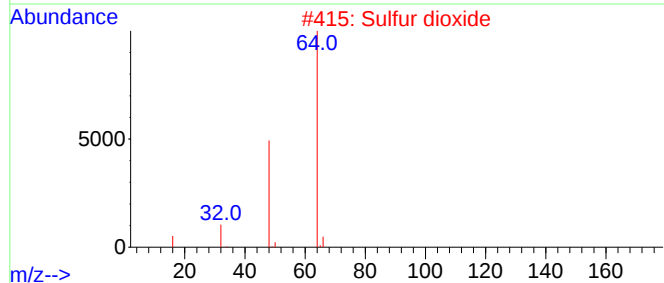
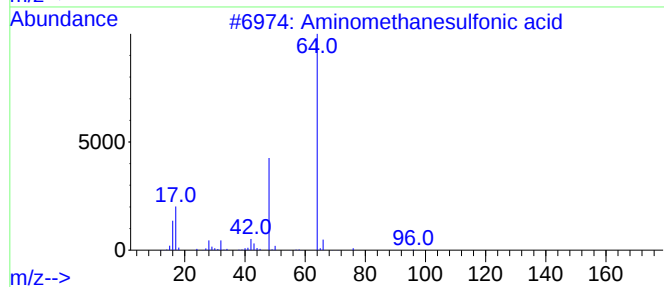
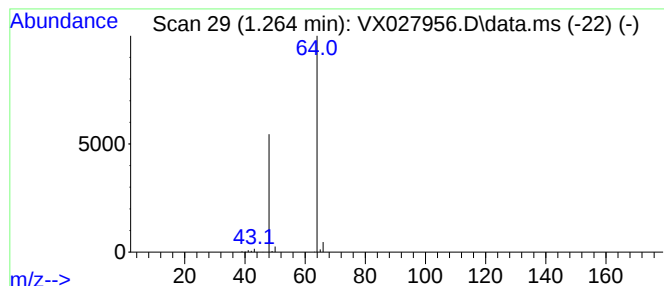
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	53.55 ug/l	315302	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4



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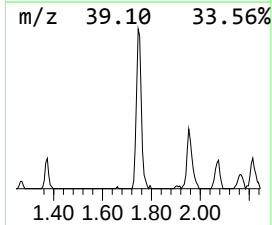
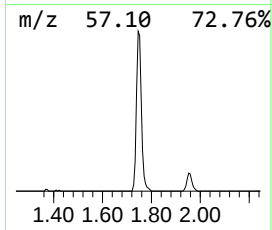
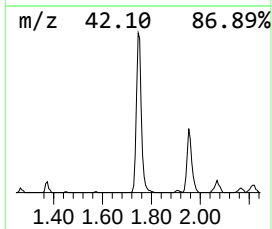
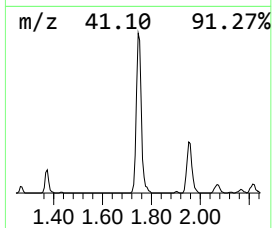
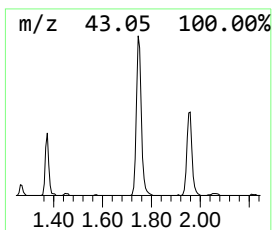
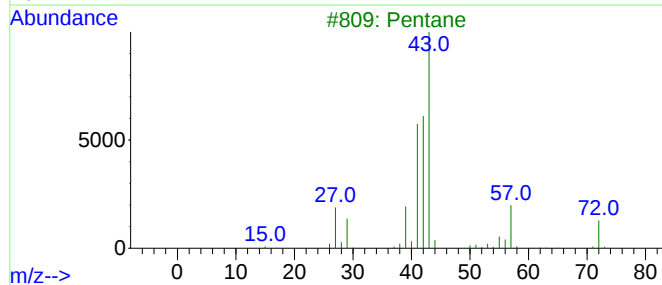
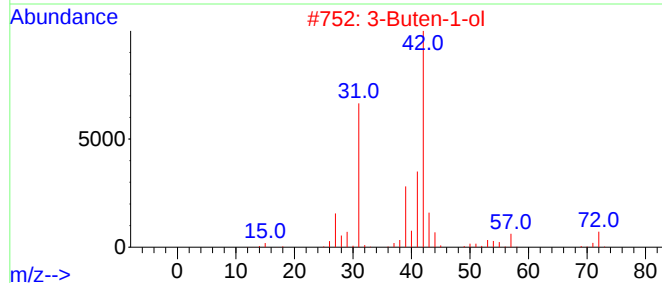
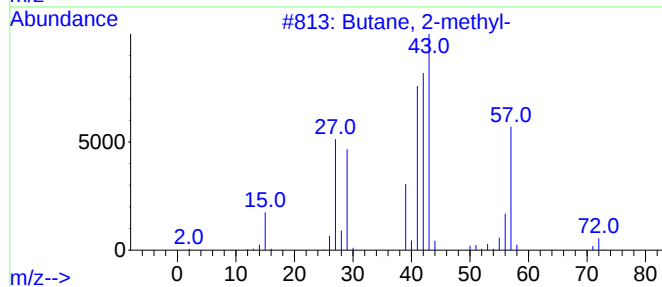
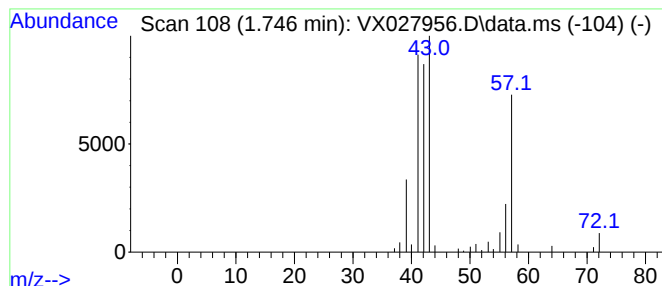
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	17.90 ug/l	105363	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	37
3			Pentane	72	C5H12	000109-66-0	33
4			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	25



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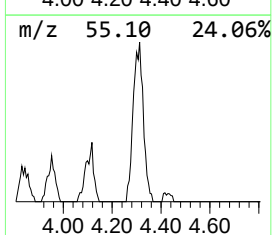
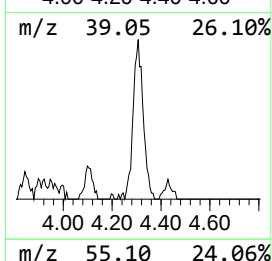
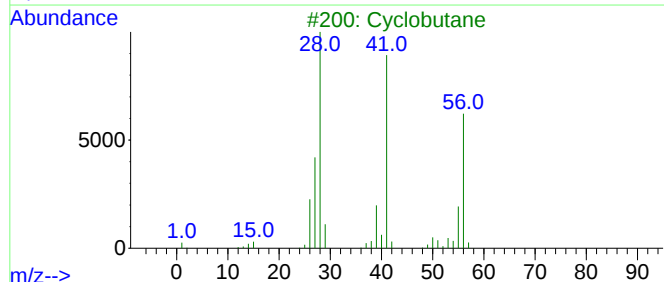
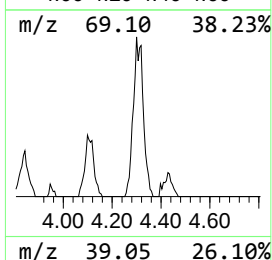
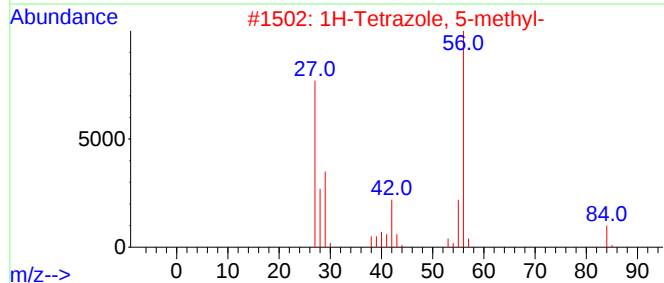
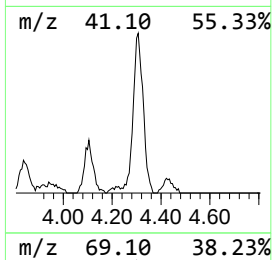
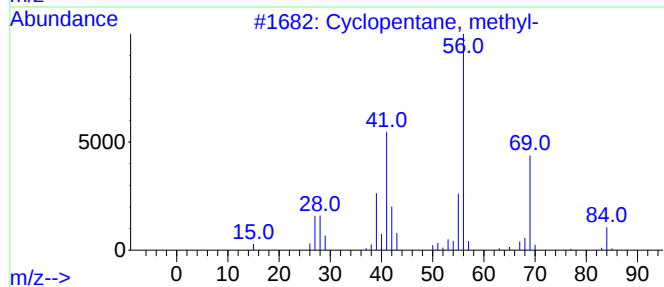
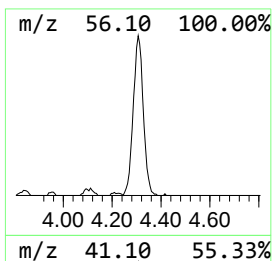
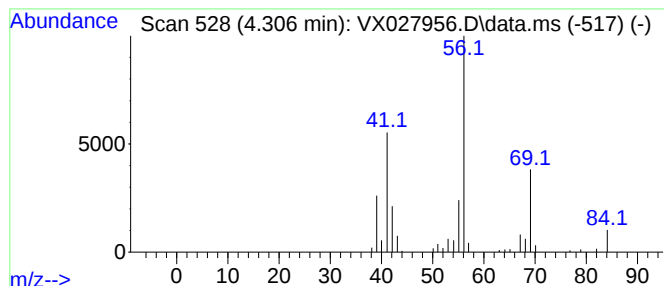
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	11.01 ug/l	64810	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3			Cyclobutane	56	C4H8	000287-23-0	50
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
5			Cyclobutane, butyl-	112	C8H16	013152-44-8	42



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ClientSampleId :
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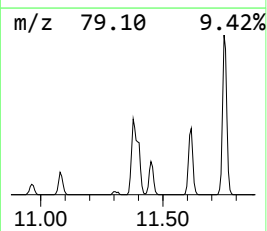
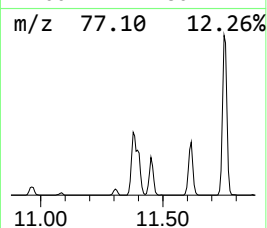
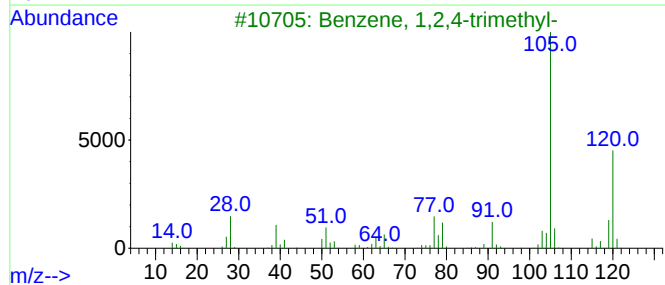
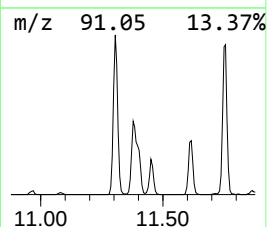
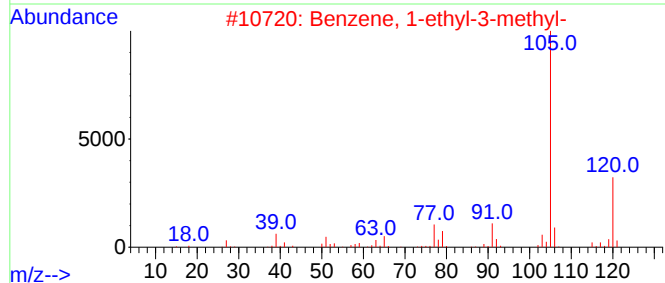
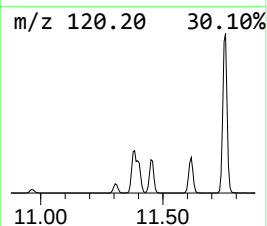
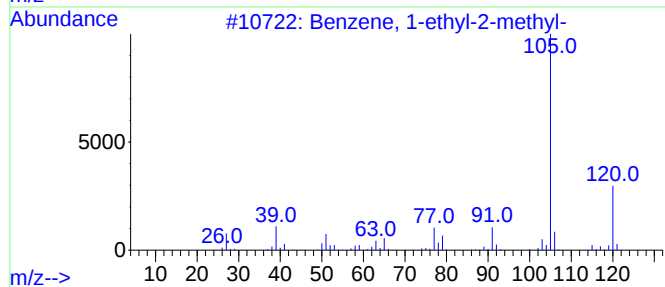
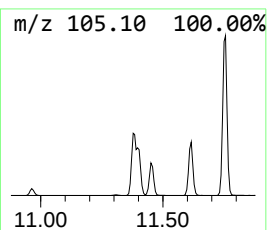
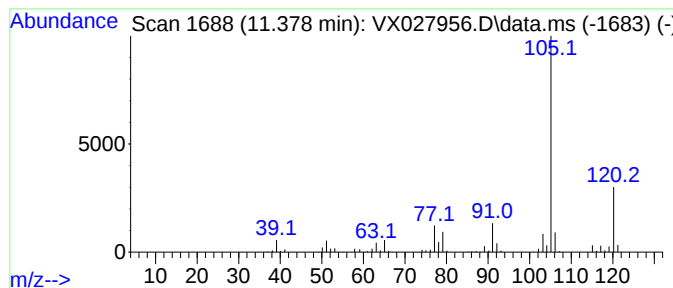
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	35.87 ug/l	277930	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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ClientSampleId :
MW-1R

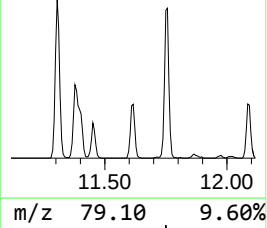
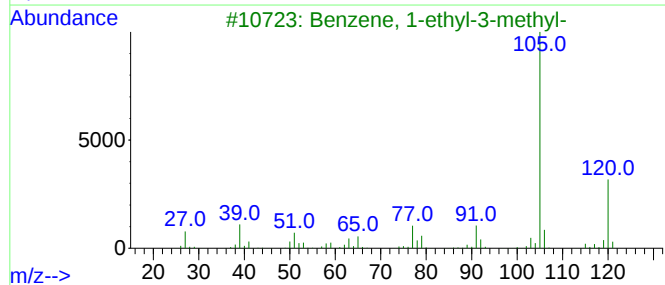
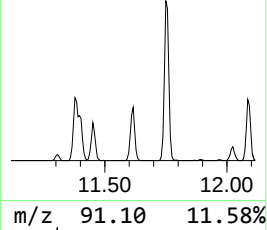
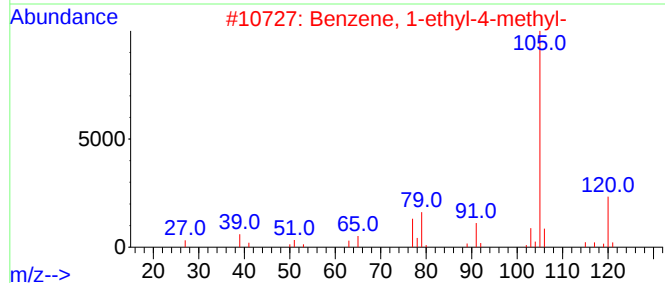
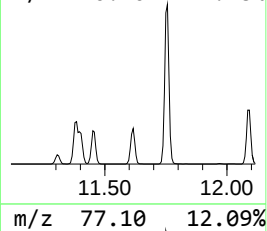
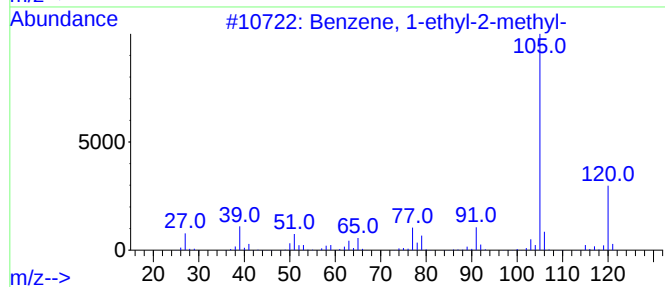
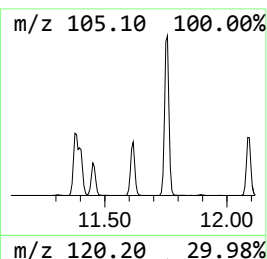
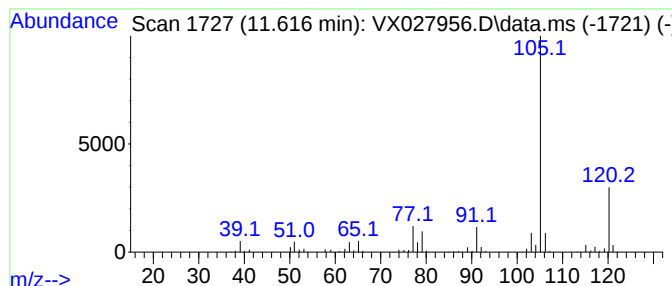
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	28.23 ug/l	218765	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	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO040422\
Data File : VX027956.D
Acq On : 04 Apr 2022 14:38
Operator : JC/MD
Sample : N2249-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

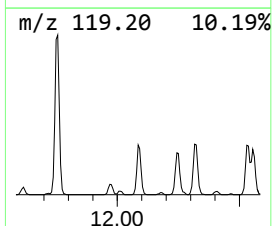
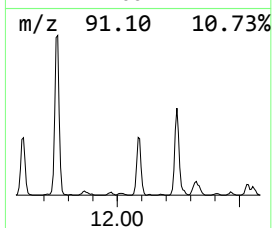
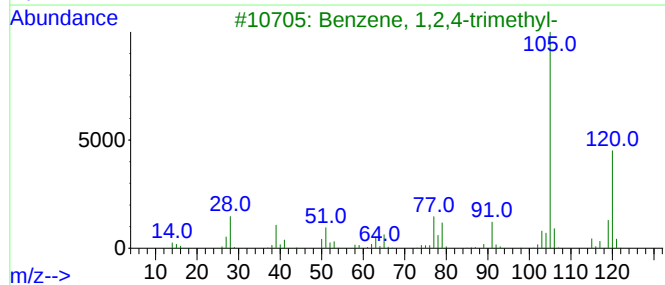
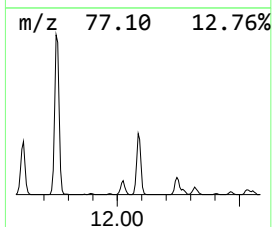
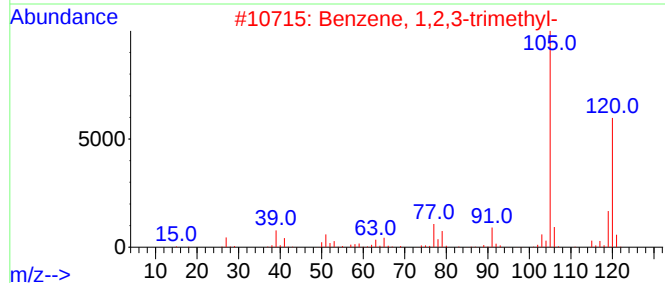
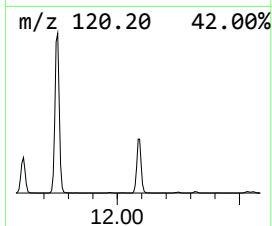
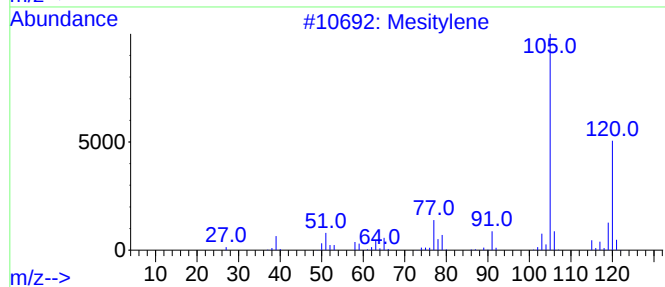
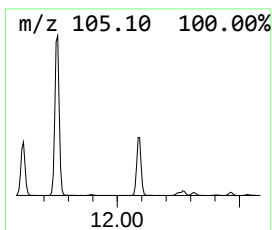
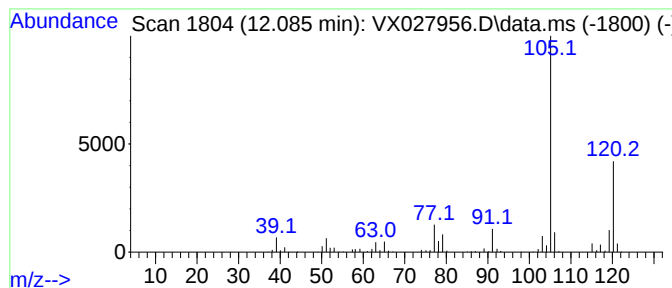
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Quant Title : SW846 8260

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

Peak Number 6 Mesitylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	34.33 ug/l	265963	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027956.D
Acq On : 04 Apr 2022 14:38
Operator : JC/MD
Sample : N2249-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

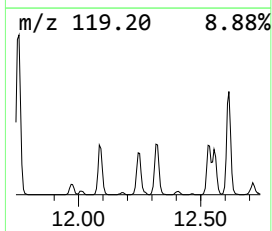
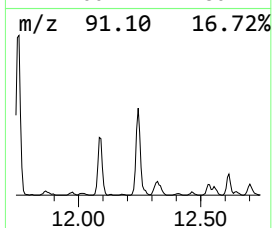
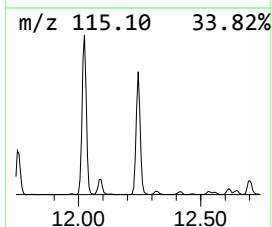
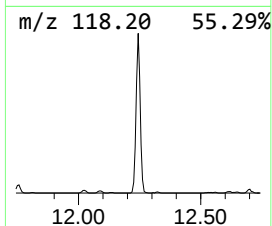
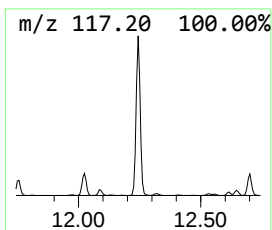
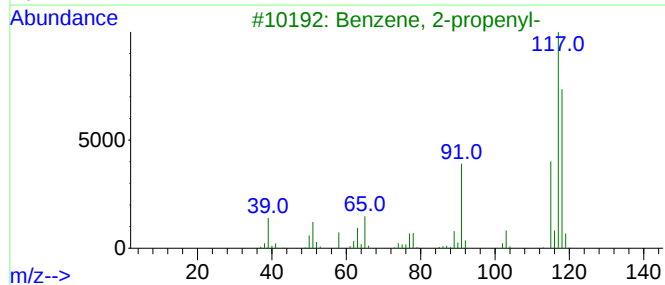
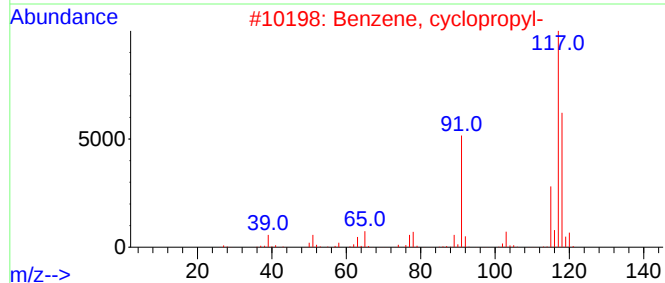
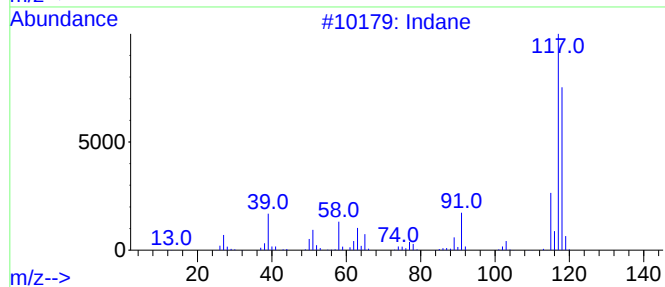
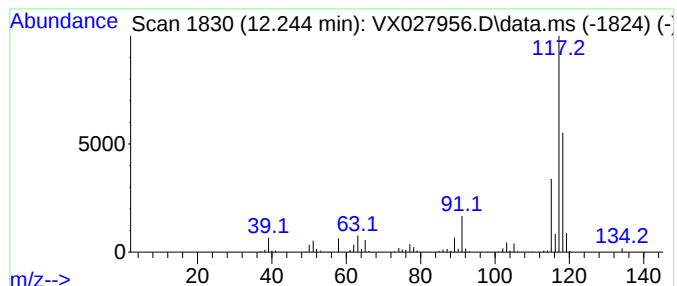
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	38.54 ug/l	298638	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO040422\
Data File : VX027956.D
Acq On : 04 Apr 2022 14:38
Operator : JC/MD
Sample : N2249-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

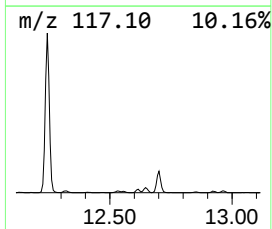
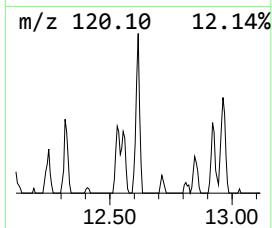
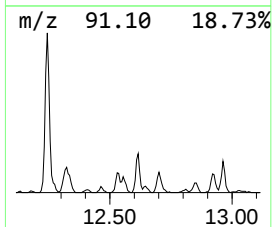
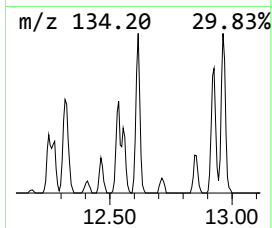
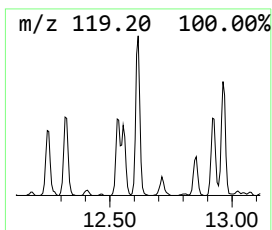
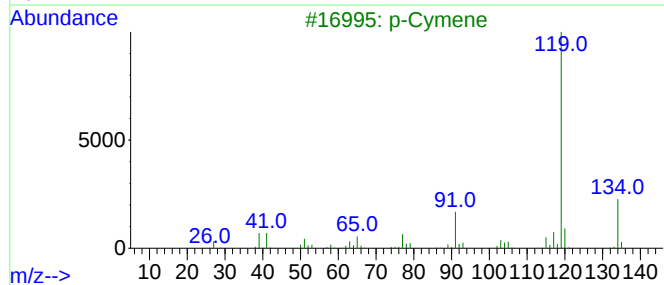
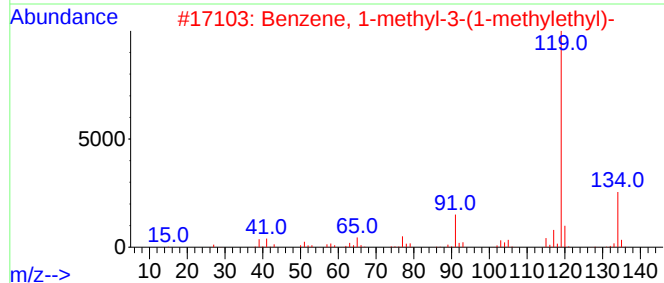
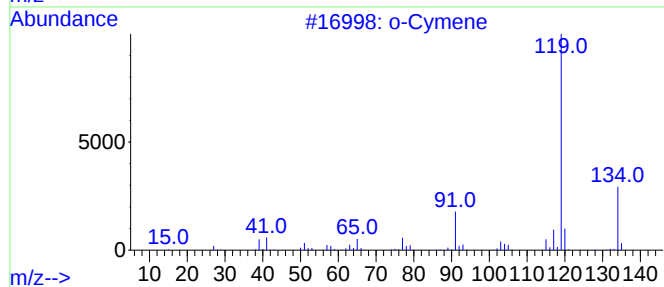
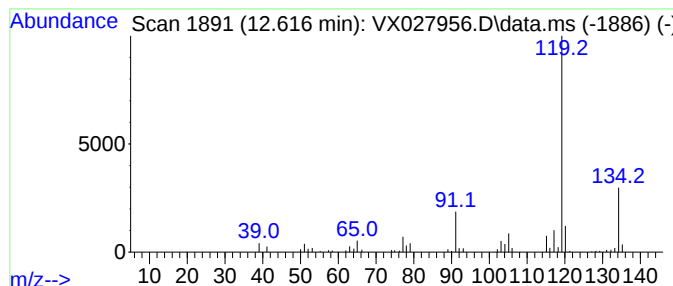
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Quant Title : SW846 8260

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

Peak Number 8 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	6.64 ug/l	51433	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	97
3			p-Cymene	134	C10H14	000099-87-6	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX040422\
Data File : VX027956.D
Acq On : 04 Apr 2022 14:38
Operator : JC/MD
Sample : N2249-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

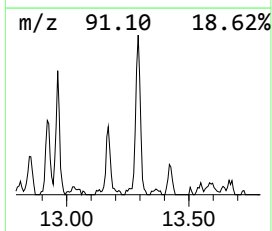
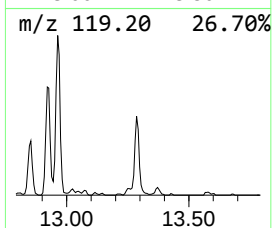
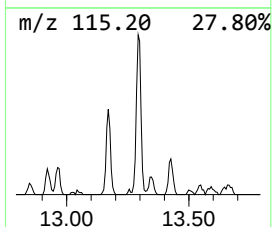
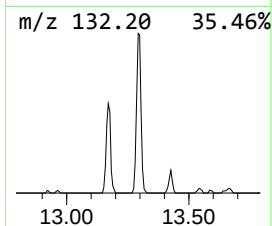
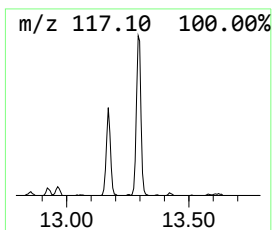
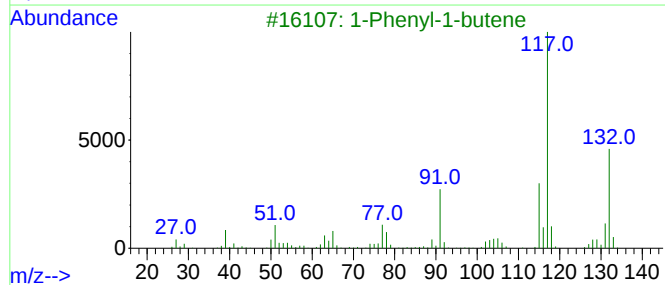
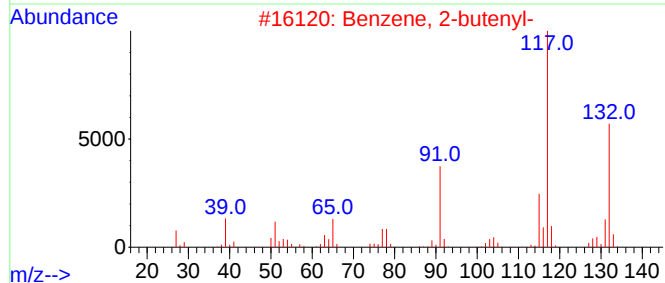
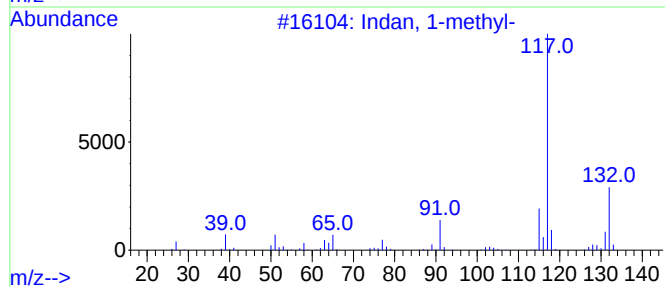
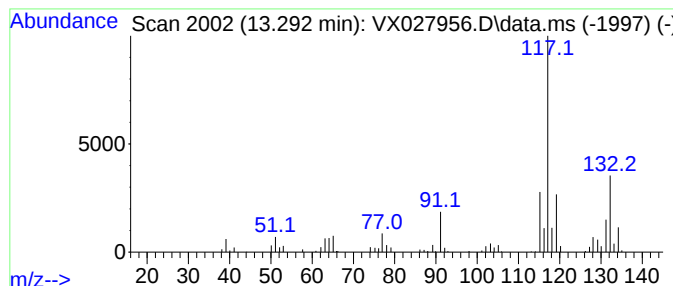
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Quant Title : SW846 8260

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

Peak Number 9 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	10.60 ug/l	82165	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	93
2			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027956.D
Acq On : 04 Apr 2022 14:38
Operator : JC/MD
Sample : N2249-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

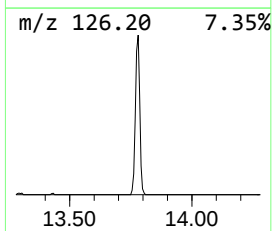
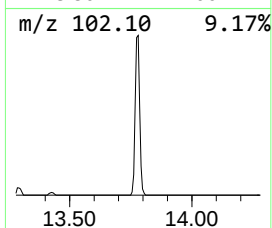
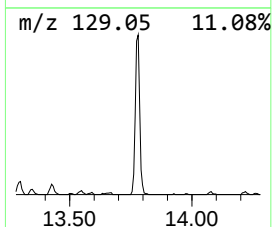
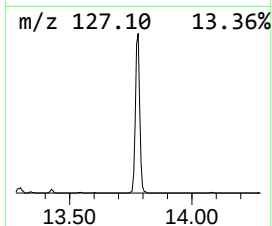
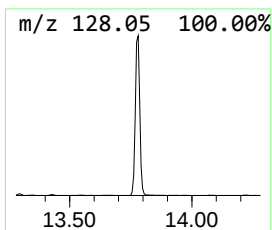
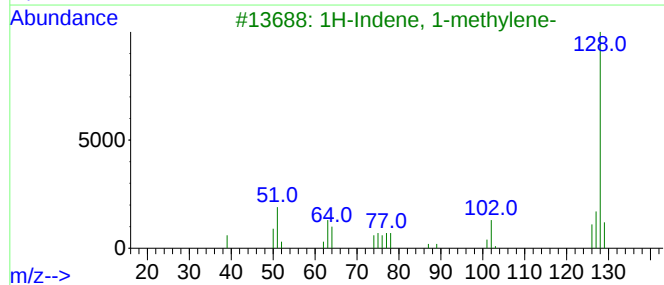
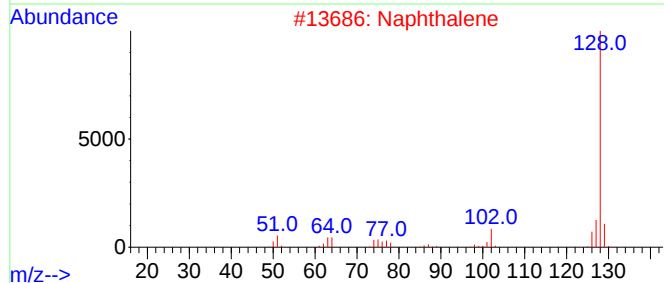
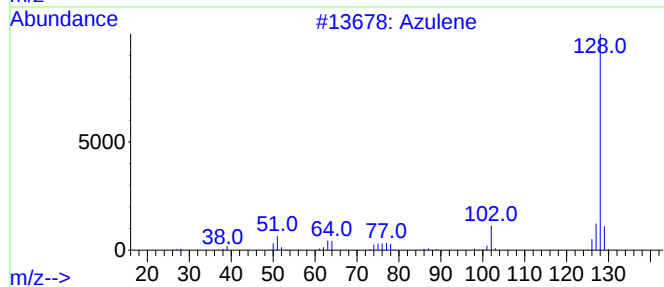
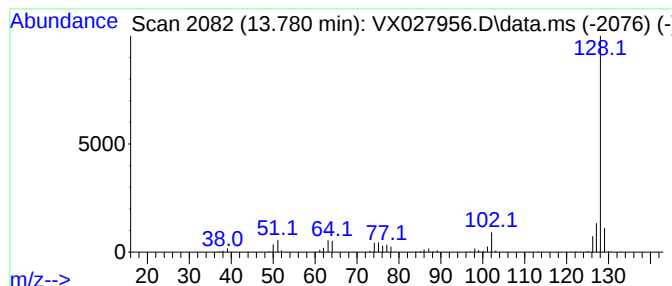
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Quant Title : SW846 8260

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

Peak Number 10 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	36.72 ug/l	284492	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027956.D
Acq On : 04 Apr 2022 14:38
Operator : JC/MD
Sample : N2249-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-1R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.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
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Butane, 2-methyl-	1.746	17.9	ug/l	105363	1	5.556	294373	50.0
Cyclopentane, m...	4.306	11.0	ug/l	64810	1	5.556	294373	50.0
Benzene, 1-ethy...	11.378	35.9	ug/l	277930	4	12.024	387411	50.0
Benzene, 1-ethy...	11.616	28.2	ug/l	218765	4	12.024	387411	50.0
Mesitylene	12.085	34.3	ug/l	265963	4	12.024	387411	50.0
Indane	12.244	38.5	ug/l	298638	4	12.024	387411	50.0
o-Cymene	12.616	6.6	ug/l	51433	4	12.024	387411	50.0
Indan, 1-methyl-	13.292	10.6	ug/l	82165	4	12.024	387411	50.0
Azulene	13.780	36.7	ug/l	284492	4	12.024	387411	50.0