

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
 Data File : VX033054.D
 Acq On : 24 Nov 2022 11:02
 Operator : JC/MD
 Sample : N5747-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-29

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033054.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	25	29	41	rBV	29219	54074	3.66%	0.521%
2	1.373	41	47	53	rVB	50962	58742	3.98%	0.566%
3	1.751	104	109	118	rVB	68586	88465	5.99%	0.853%
4	1.965	138	144	155	rVB3	34339	72129	4.89%	0.695%
5	2.074	157	162	169	rVV	19330	29980	2.03%	0.289%
6	2.166	169	177	181	rVV	17269	27879	1.89%	0.269%
7	2.215	181	185	195	rVB	53201	82507	5.59%	0.795%
8	2.751	262	273	282	rBV	30071	66378	4.50%	0.640%
9	2.867	287	292	304	rVV2	30217	70808	4.80%	0.683%
10	2.989	304	312	324	rVV3	7303	25525	1.73%	0.246%
11	3.111	324	332	342	rVB2	24858	58167	3.94%	0.561%
12	3.733	426	434	444	rBV2	9264	24532	1.66%	0.236%
13	3.903	457	462	469	rVV	6392	16287	1.10%	0.157%
14	4.105	486	495	504	rVB4	6101	15360	1.04%	0.148%
15	4.306	518	528	538	rVB2	22565	63375	4.29%	0.611%
16	5.196	662	674	687	rVB2	9247	26280	1.78%	0.253%
17	5.385	692	705	714	rBV	65548	187398	12.70%	1.806%
18	5.476	714	720	724	rVV3	14621	40783	2.76%	0.393%
19	5.549	724	732	748	rVB	137996	391959	26.56%	3.778%
20	5.958	788	799	804	rBV	69952	179094	12.14%	1.726%
21	6.037	804	812	826	rVB	562190	1475779	100.00%	14.226%
22	6.202	830	839	846	rBV2	9014	25118	1.70%	0.242%
23	6.763	920	931	942	rBV	210481	503412	34.11%	4.853%
24	7.378	1021	1032	1041	rBV4	6290	15726	1.07%	0.152%
25	8.646	1234	1240	1247	rBV	323092	506793	34.34%	4.885%
26	8.720	1247	1252	1260	rVB	162126	249921	16.93%	2.409%
27	9.457	1366	1373	1378	rBV2	11119	17626	1.19%	0.170%
28	9.945	1448	1453	1460	rBV	13181	18807	1.27%	0.181%
29	10.055	1465	1471	1484	rVV	440490	585765	39.69%	5.647%
30	10.195	1488	1494	1505	rBV	883142	1132303	76.73%	10.915%
31	10.299	1505	1511	1521	rVB	843508	1155816	78.32%	11.142%
32	10.640	1562	1567	1577	rVB	204656	261035	17.69%	2.516%
33	10.963	1615	1620	1625	rBV	34643	43178	2.93%	0.416%
34	11.079	1634	1639	1650	rBV	286100	359042	24.33%	3.461%
35	11.304	1671	1676	1682	rBV	63062	75539	5.12%	0.728%
36	11.378	1683	1688	1690	rVV	73628	101357	6.87%	0.977%

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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

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37	11.396	1690	1691	1696	rVV	88027	88535	6.00%	0.853%
38	11.451	1696	1700	1706	rVB	51600	62656	4.25%	0.604%
39	11.615	1721	1727	1733	rBV	86021	111358	7.55%	1.073%
40	11.750	1744	1749	1756	rBV	438066	539490	36.56%	5.200%
41	12.024	1788	1794	1799	rBV	450095	567100	38.43%	5.467%
42	12.085	1799	1804	1809	rVB	164234	202057	13.69%	1.948%
43	12.243	1824	1830	1838	rBV	183454	229293	15.54%	2.210%
44	12.316	1838	1842	1849	rVB3	11878	17547	1.19%	0.169%
45	12.414	1853	1858	1862	rBV	16931	22751	1.54%	0.219%
46	12.530	1873	1877	1879	rBV	14217	17130	1.16%	0.165%
47	12.615	1886	1891	1894	rBV	22216	27491	1.86%	0.265%
48	12.701	1900	1905	1912	rVB2	23451	32782	2.22%	0.316%
49	12.920	1935	1941	1945	rBV	13407	16385	1.11%	0.158%
50	12.963	1945	1948	1955	rVB	18847	21517	1.46%	0.207%
51	13.170	1978	1982	1987	rVB	18015	20989	1.42%	0.202%
52	13.292	1997	2002	2008	rVB2	43553	56678	3.84%	0.546%
53	13.420	2019	2023	2029	rBV2	14781	18660	1.26%	0.180%
54	13.774	2076	2081	2087	rBV	139227	172292	11.67%	1.661%
55	14.639	2219	2223	2231	rVB	14364	19116	1.30%	0.184%
56	14.779	2241	2246	2255	rVB	18762	23083	1.56%	0.223%

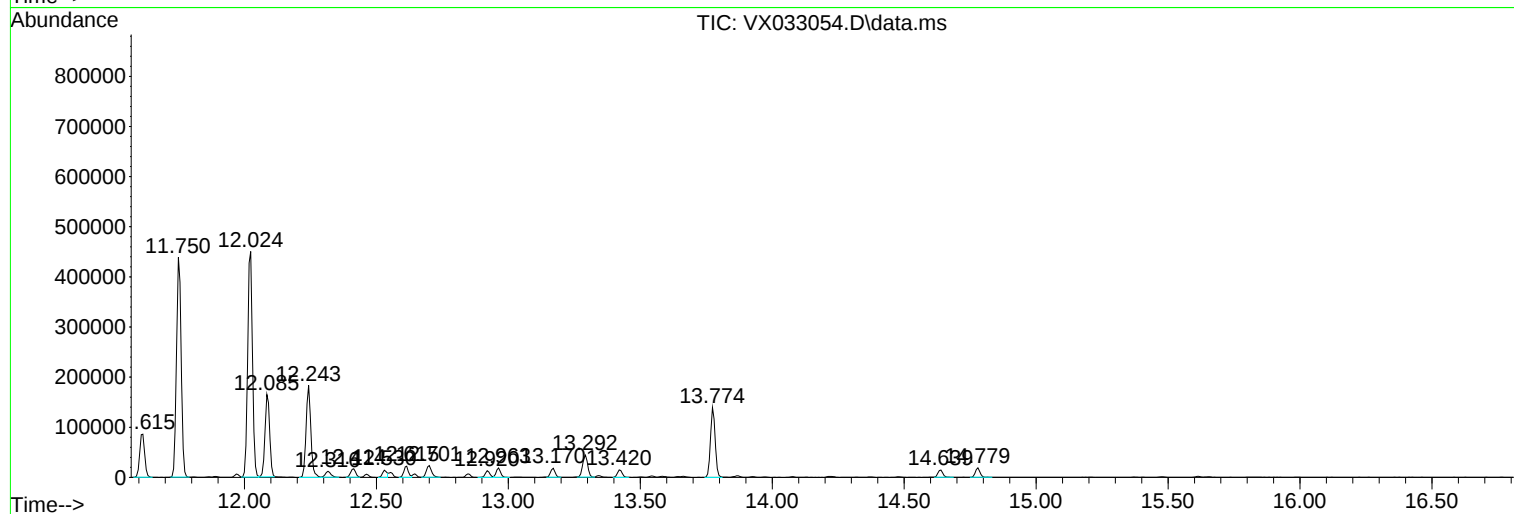
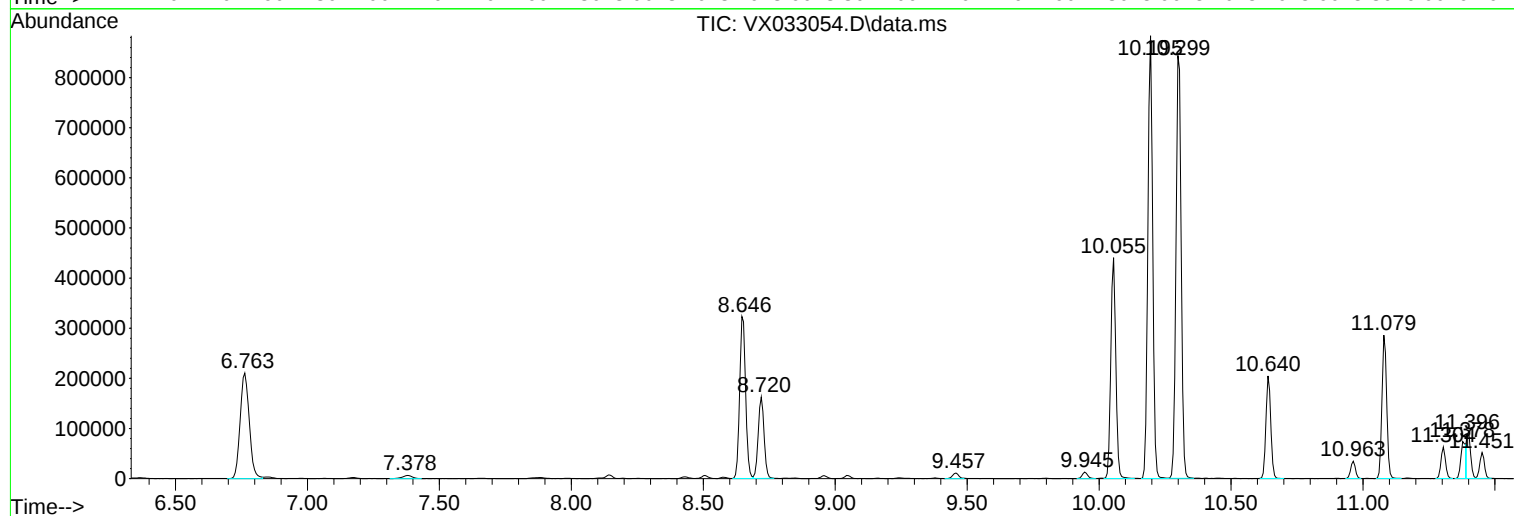
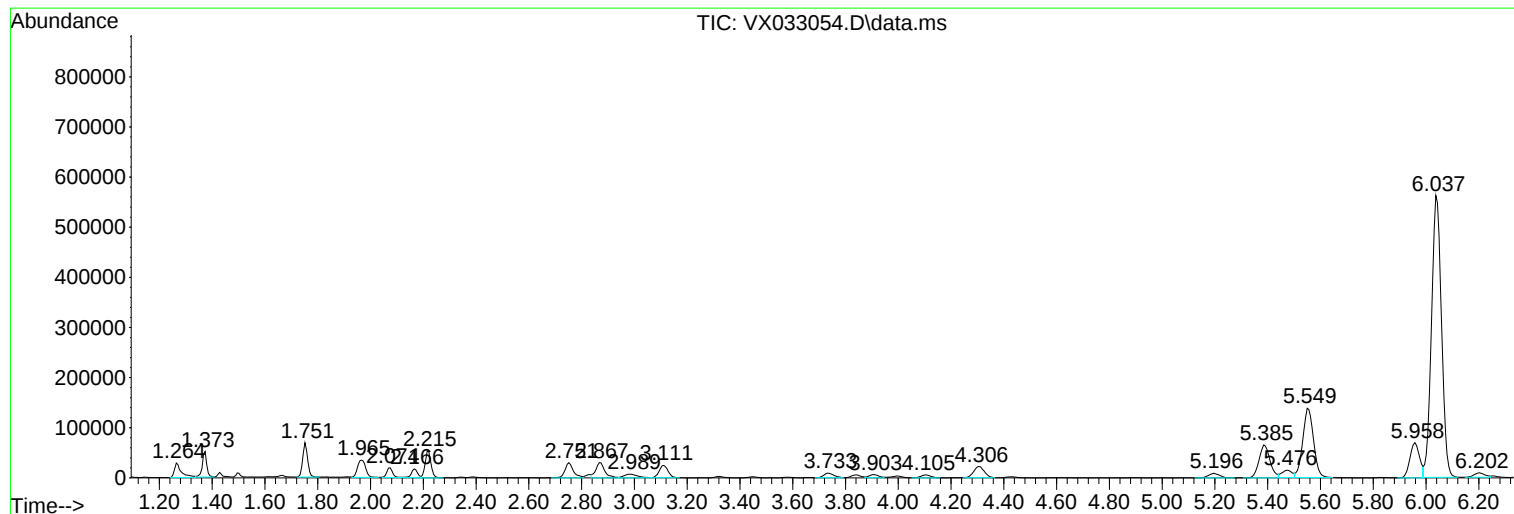
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
MW-29

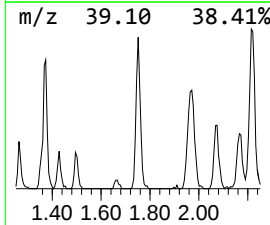
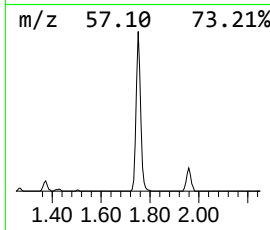
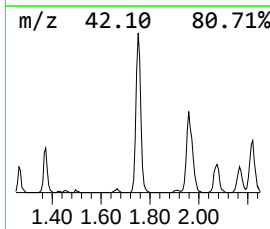
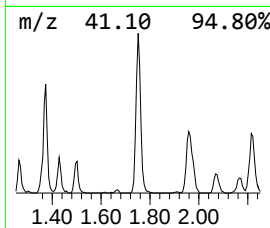
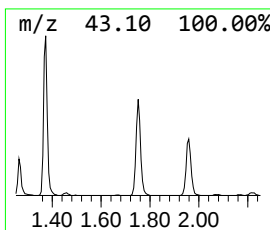
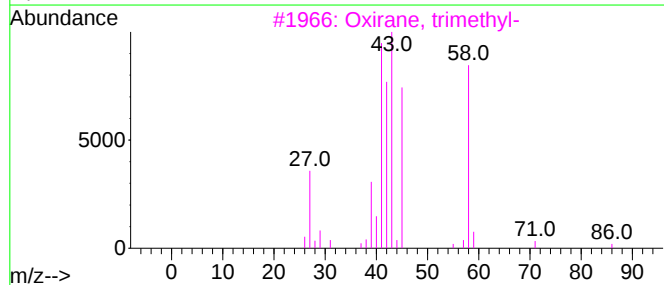
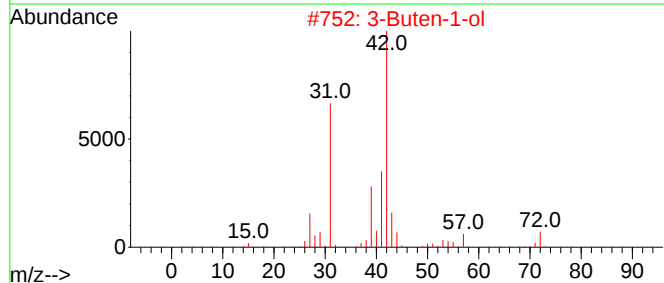
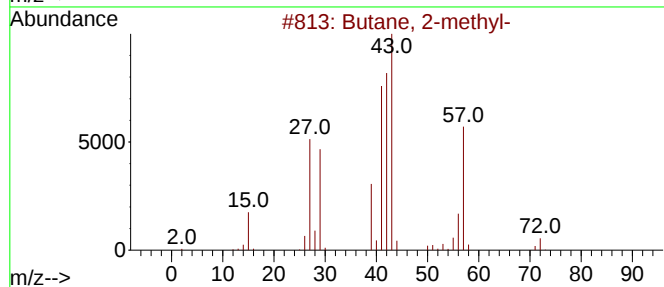
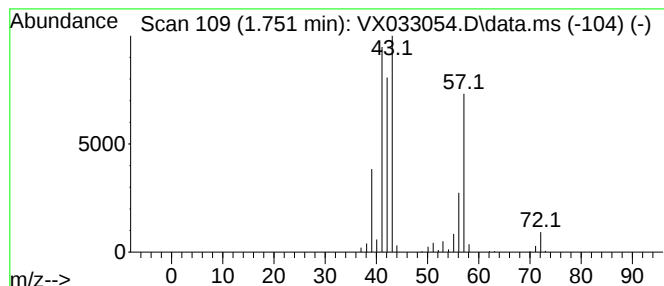
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.751	11.29 ug/l	88465	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			3-Buten-1-ol	72	C4H8O	000627-27-0	38
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	37
4			1-Butene	56	C4H8	000106-98-9	27
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	27



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ALS Vial : 49 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-29

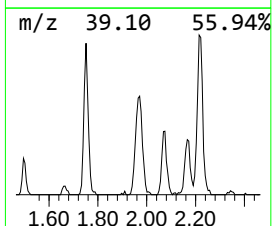
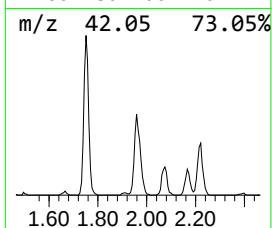
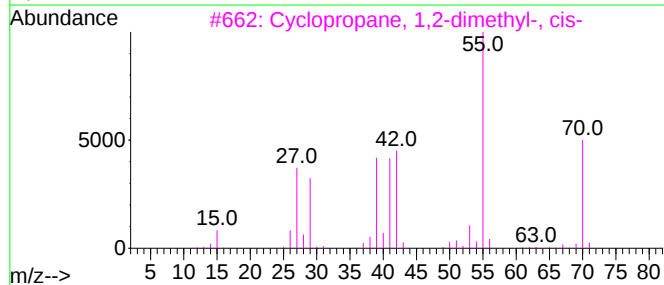
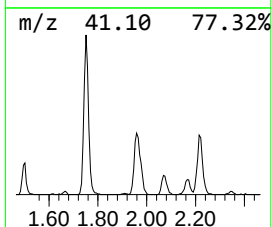
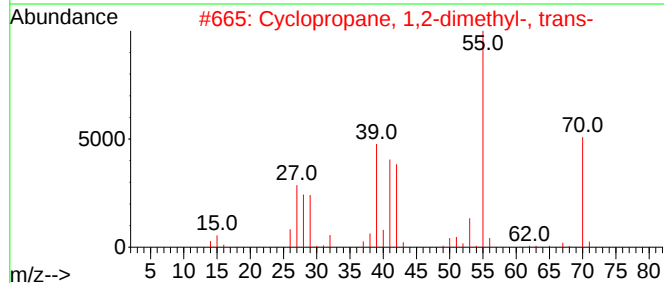
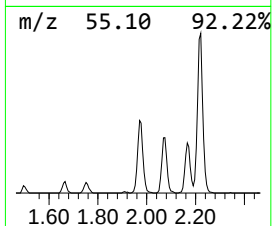
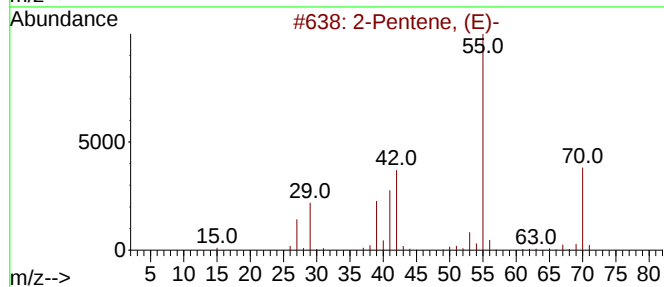
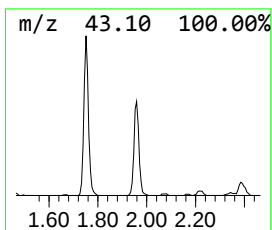
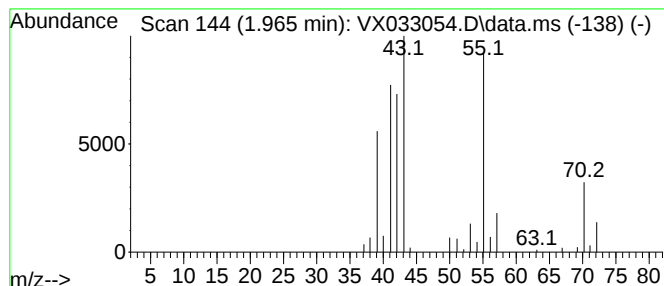
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Quant Title : SW846 8260

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

Peak Number 2 2-Pentene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.965	9.20 ug/l	72129	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-			70	C5H10	000646-04-8	58
2	Cyclopropane, 1,2-dimethyl-, trans-			70	C5H10	002402-06-4	53
3	Cyclopropane, 1,2-dimethyl-, cis-			70	C5H10	000930-18-7	52
4	1-Butanol, 3-methyl-			88	C5H12O	000123-51-3	47
5	1-Butene, 3-methyl-			70	C5H10	000563-45-1	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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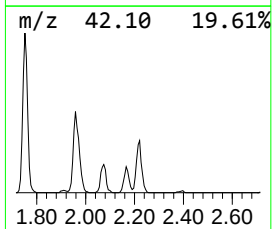
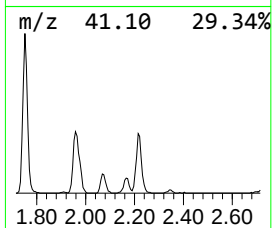
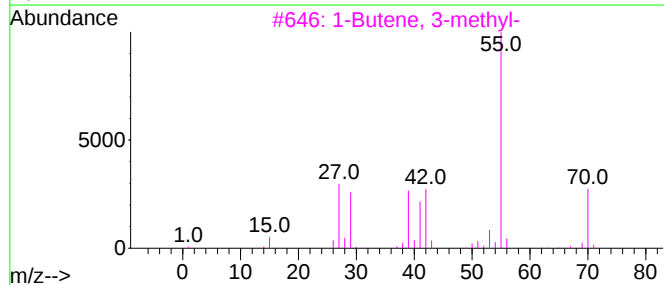
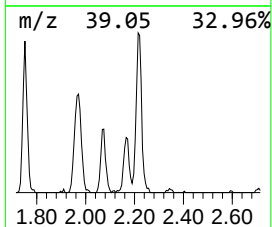
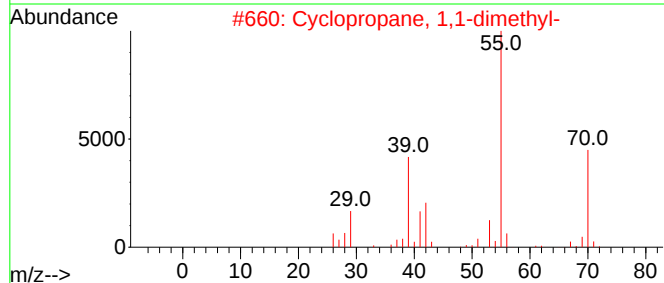
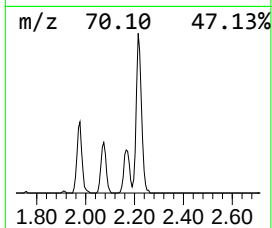
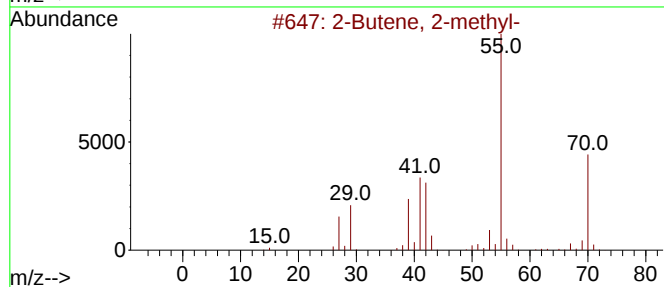
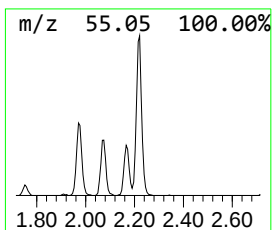
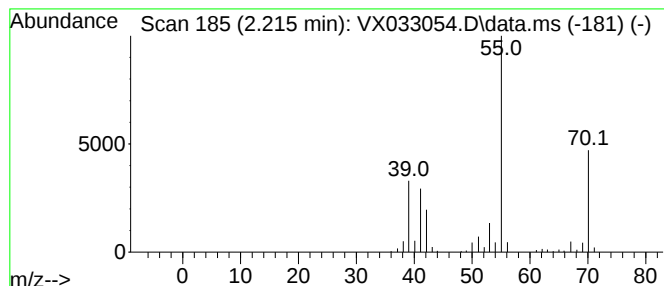
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Butene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	10.53 ug/l	82507	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-			70	C5H10	000513-35-9	90
2	Cyclopropane, 1,1-dimethyl-			70	C5H10	001630-94-0	83
3	1-Butene, 3-methyl-			70	C5H10	000563-45-1	78
4	Cyclopropane, 1,2-dimethyl-, cis-			70	C5H10	000930-18-7	68
5	2-Pentene, (E)-			70	C5H10	000646-04-8	64



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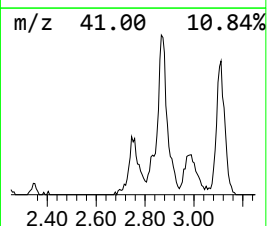
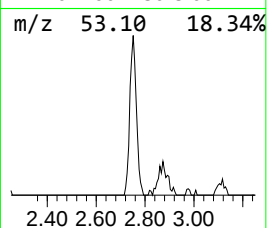
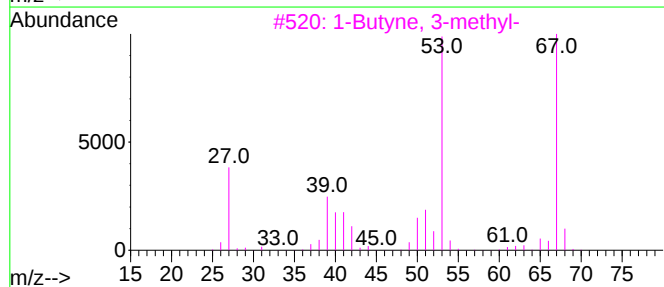
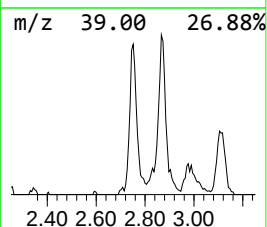
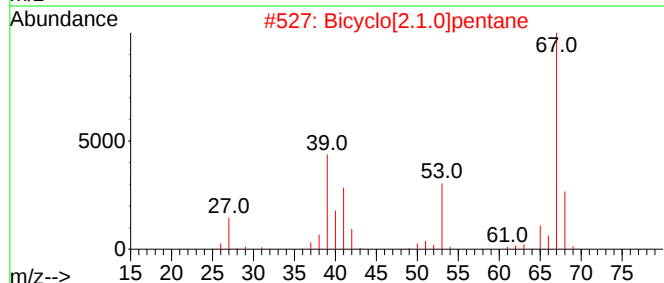
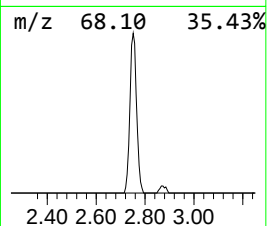
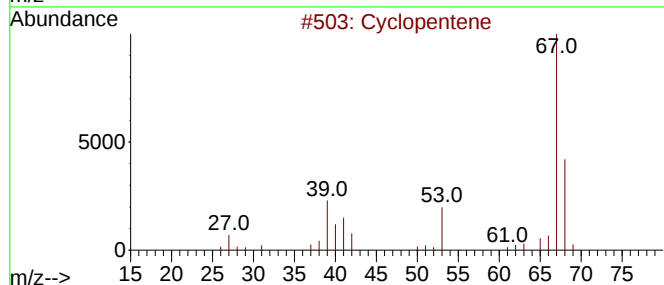
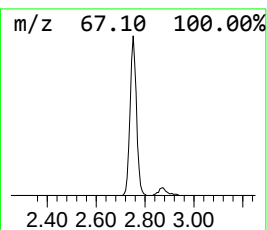
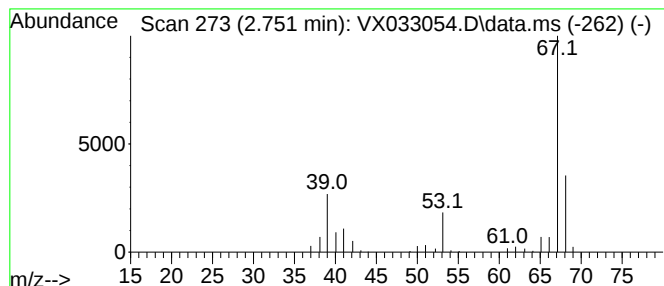
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopentene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.751	8.47 ug/l	66378	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene	68	C5H8	000142-29-0	91
2			Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	78
3			1-Butyne, 3-methyl-	68	C5H8	000598-23-2	64
4			1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	53
5			1,3-Pentadiene	68	C5H8	000504-60-9	50



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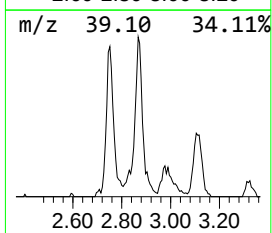
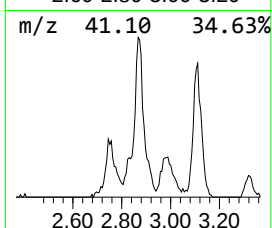
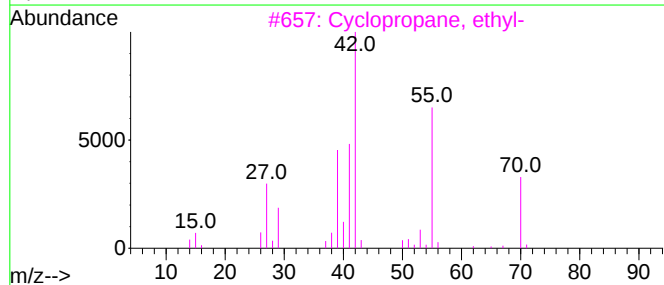
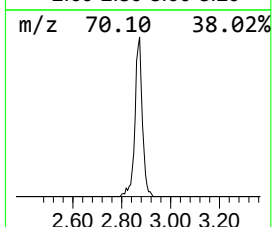
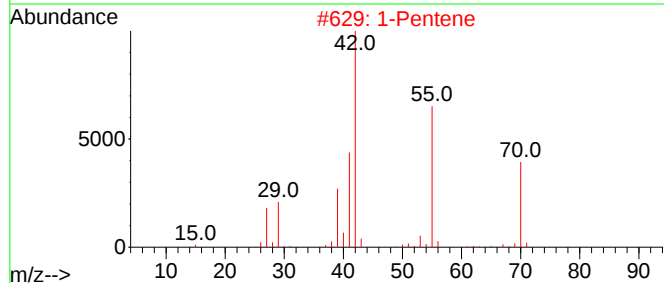
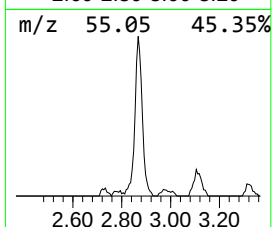
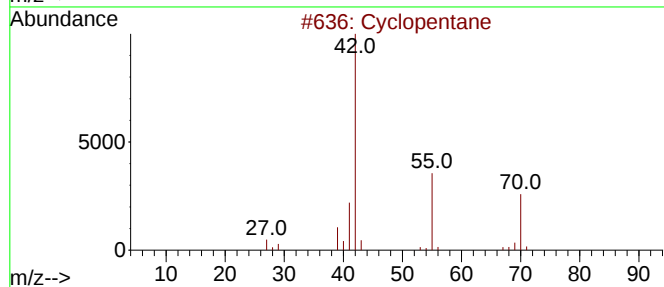
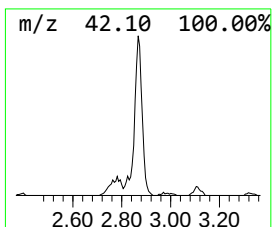
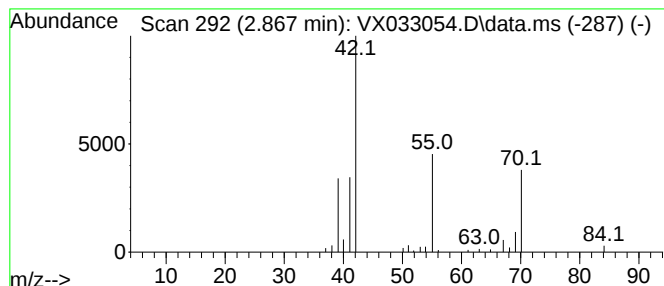
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	9.03 ug/l	70808	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	78
2			1-Pentene	70	C5H10	000109-67-1	64
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	39
4			3-Buten-1-ol	72	C4H8O	000627-27-0	9
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033054.D
Acq On : 24 Nov 2022 11:02
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

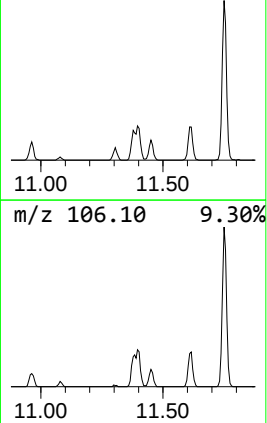
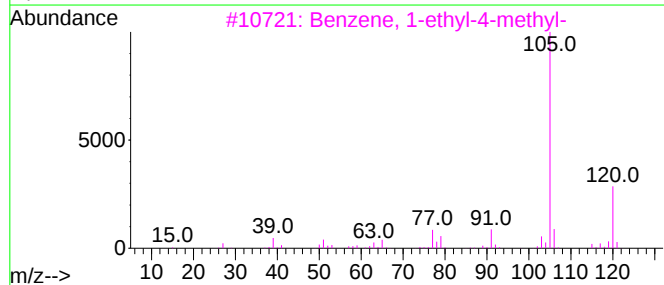
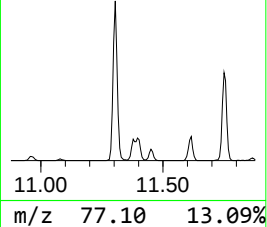
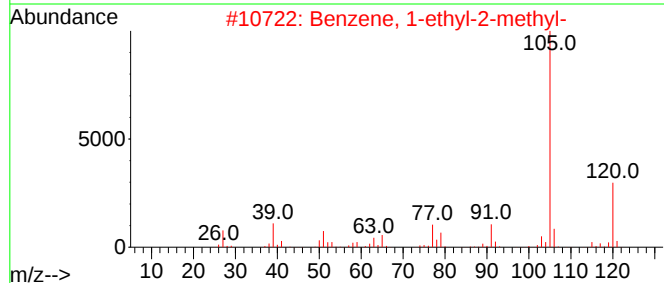
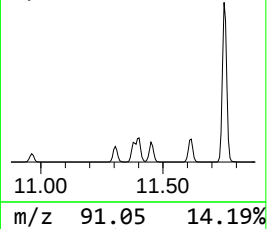
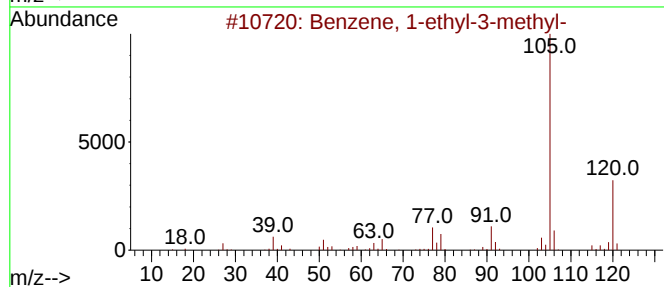
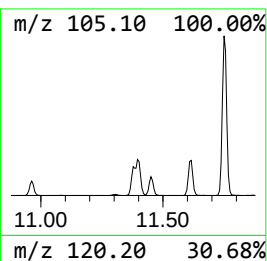
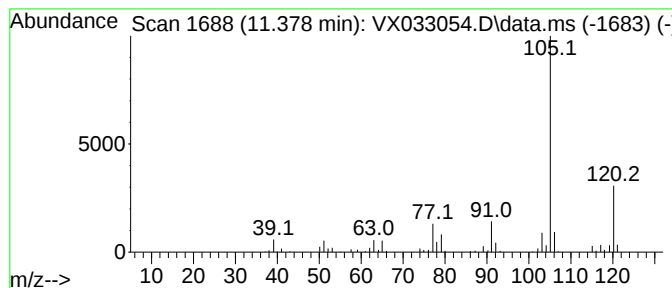
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	8.94 ug/l	101357	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
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			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033054.D
Acq On : 24 Nov 2022 11:02
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

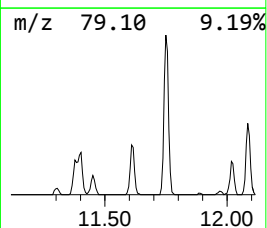
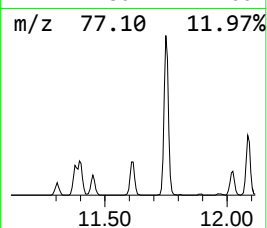
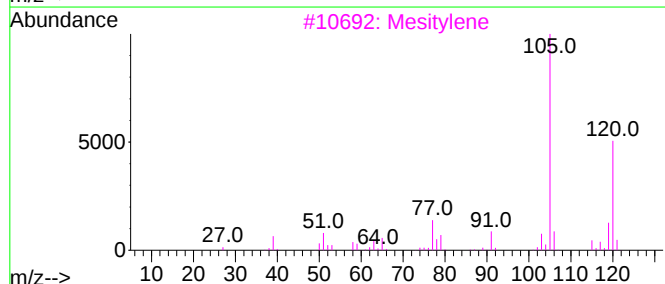
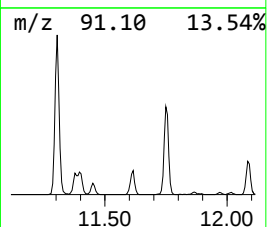
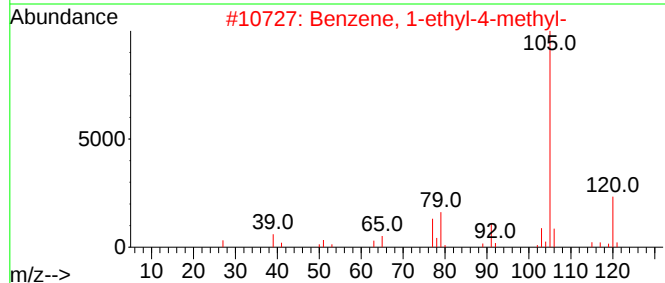
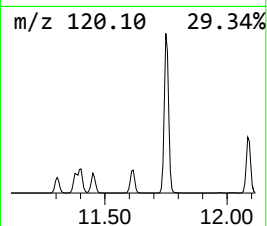
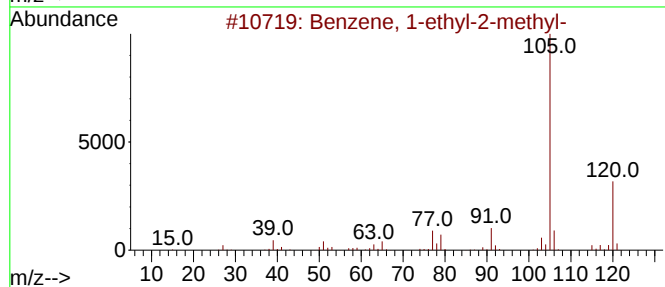
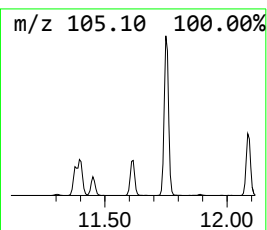
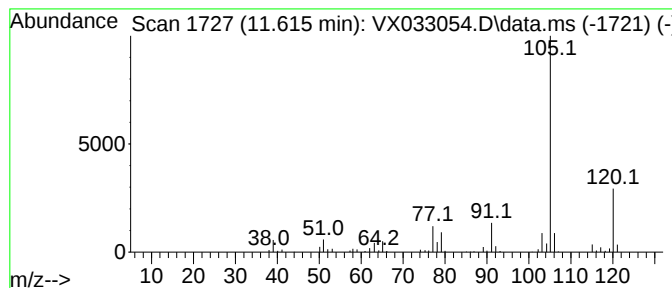
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.615	9.82 ug/l	111358	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			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033054.D
Acq On : 24 Nov 2022 11:02
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

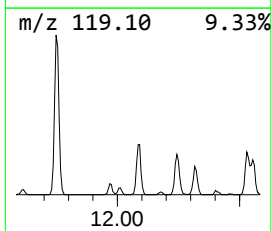
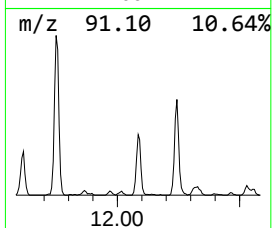
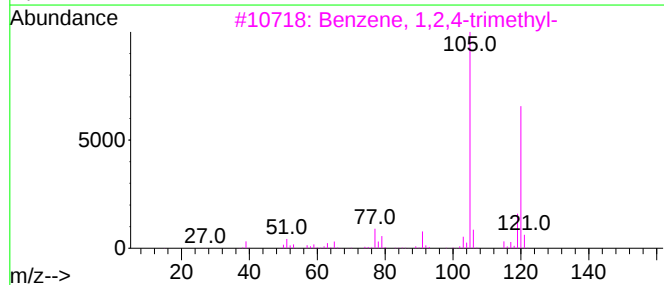
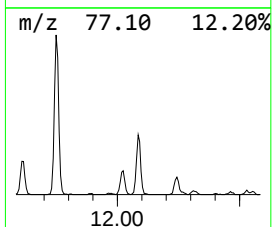
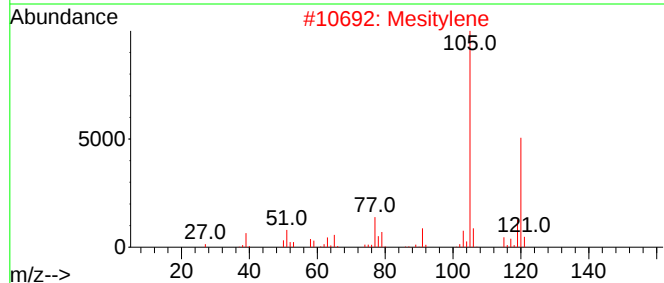
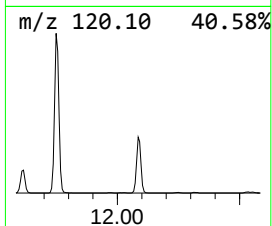
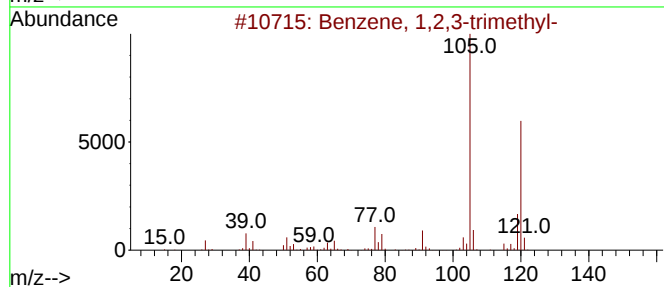
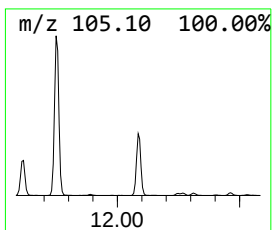
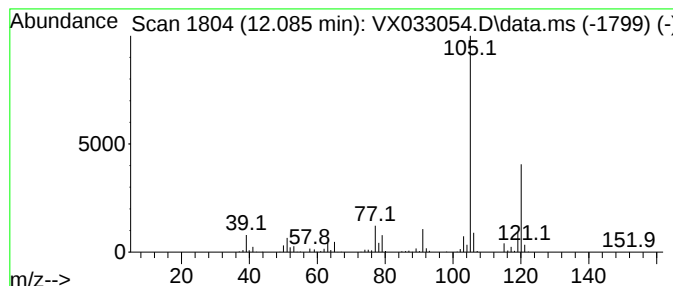
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	17.81 ug/l	202057	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2			Mesitylene	120	C9H12	000108-67-8	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033054.D
Acq On : 24 Nov 2022 11:02
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

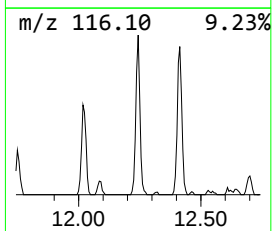
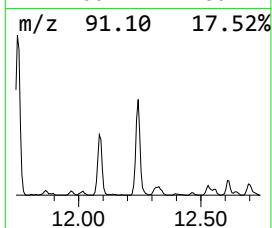
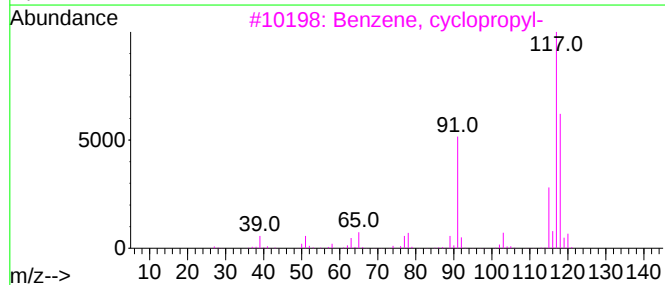
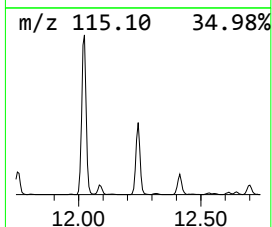
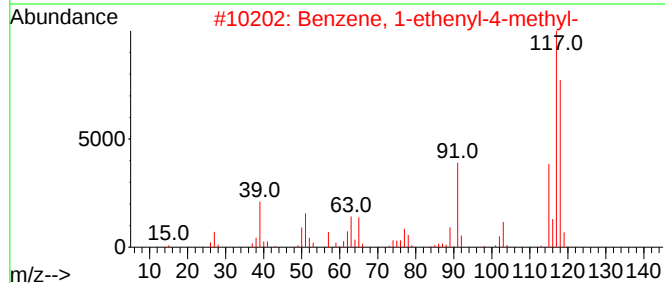
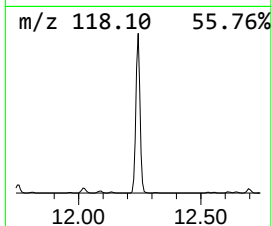
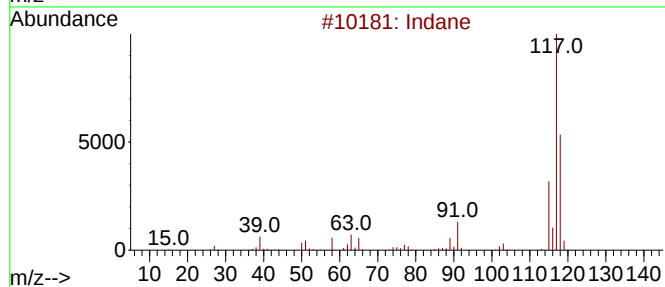
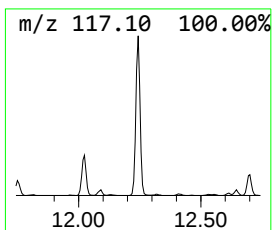
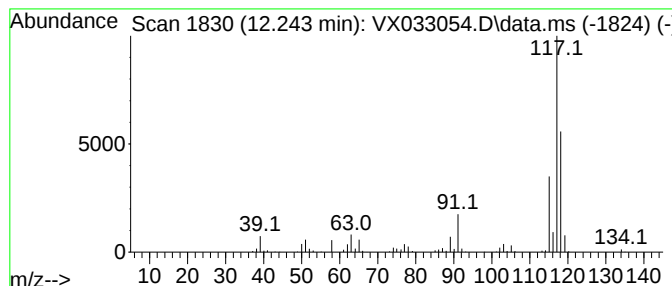
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	20.22 ug/l	229293	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4			Delatacyclene	118	C9H10	007785-10-6	72
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033054.D
Acq On : 24 Nov 2022 11:02
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

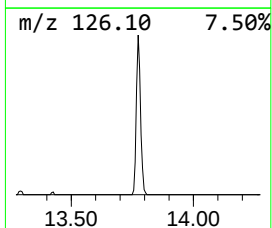
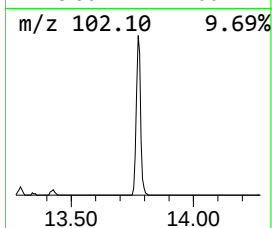
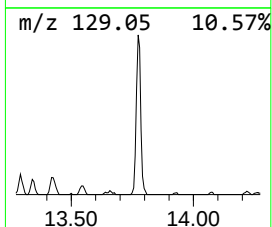
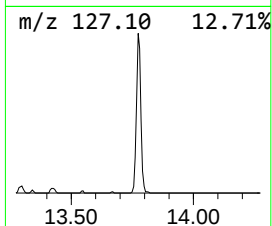
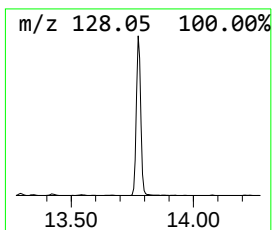
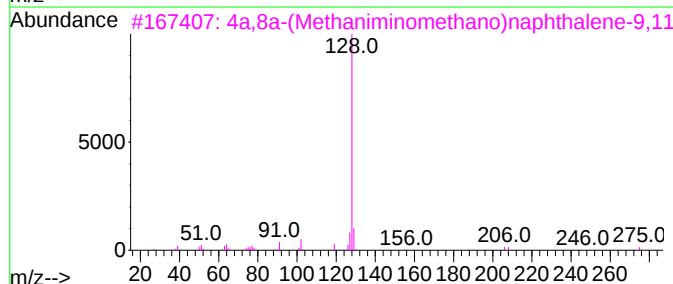
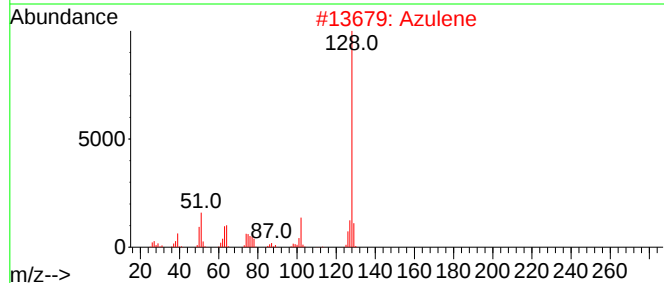
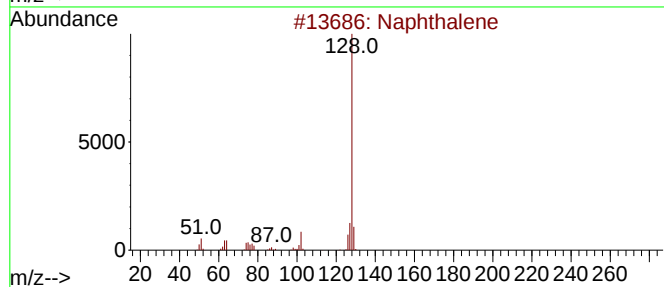
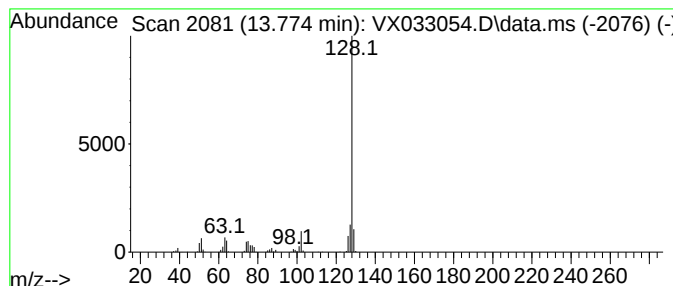
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Quant Title : SW846 8260

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.
13.774	15.19 ug/l	172292	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	52
5			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033054.D
Acq On : 24 Nov 2022 11:02
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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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2-Pentene, (E)-	1.965	9.2	ug/l	72129	1	5.549	391959	50.0
2-Butene, 2-met...	2.215	10.5	ug/l	82507	1	5.549	391959	50.0
Cyclopentene	2.751	8.5	ug/l	66378	1	5.549	391959	50.0
Cyclopentane	2.867	9.0	ug/l	70808	1	5.549	391959	50.0
Benzene, 1-ethy...	11.378	8.9	ug/l	101357	4	12.024	567100	50.0
Benzene, 1-ethy...	11.615	9.8	ug/l	111358	4	12.024	567100	50.0
Benzene, 1,2,3-...	12.085	17.8	ug/l	202057	4	12.024	567100	50.0
Indane	12.243	20.2	ug/l	229293	4	12.024	567100	50.0
Azulene	13.774	15.2	ug/l	172292	4	12.024	567100	50.0