

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027958.D
 Acq On : 04 Apr 2022 15:24
 Operator : JC/MD
 Sample : N2249-03 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2D

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: VX027958.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	27	rBV	22175	26539	1.66%	0.269%
2	1.264	27	29	40	rVV	36705	38962	2.44%	0.396%
3	1.374	43	47	53	rBV	132815	136611	8.57%	1.387%
4	1.746	103	108	121	rVB	321728	447709	28.08%	4.546%
5	1.953	138	142	154	rVV2	93719	158008	9.91%	1.605%
6	2.069	155	161	169	rVV	60314	83814	5.26%	0.851%
7	2.166	171	177	181	rVV	28635	43058	2.70%	0.437%
8	2.215	181	185	197	rVB	64336	98741	6.19%	1.003%
9	2.782	260	278	281	rBV3	28956	85780	5.38%	0.871%
10	2.825	281	285	289	rVV	55602	114763	7.20%	1.165%
11	2.867	289	292	308	rVB4	31166	80962	5.08%	0.822%
12	3.105	322	331	343	rVB	43263	98850	6.20%	1.004%
13	3.319	359	366	376	rVB3	8390	19104	1.20%	0.194%
14	3.447	380	387	396	rBV2	12674	27789	1.74%	0.282%
15	3.593	402	411	416	rBV2	8077	19681	1.23%	0.200%
16	3.666	416	423	428	rVV3	9256	22662	1.42%	0.230%
17	3.733	428	434	443	rVB	17753	41701	2.62%	0.423%
18	3.837	443	451	457	rBV3	11359	28202	1.77%	0.286%
19	4.099	486	494	504	rVB3	15051	38948	2.44%	0.396%
20	4.306	518	528	541	rVB	50584	143912	9.03%	1.461%
21	5.190	663	673	687	rVB2	11455	36633	2.30%	0.372%
22	5.385	694	705	715	rBV	55628	165047	10.35%	1.676%
23	5.556	724	733	763	rVB2	100048	323195	20.27%	3.282%
24	5.958	788	799	813	rBV2	64205	167063	10.48%	1.696%
25	6.251	841	847	858	rVB5	9931	33553	2.10%	0.341%
26	6.763	922	931	940	rBV	146862	358332	22.48%	3.639%
27	6.842	940	944	955	rVB6	7266	21262	1.33%	0.216%
28	7.379	1021	1032	1043	rBV6	11023	31034	1.95%	0.315%
29	8.653	1232	1241	1247	rBV	303593	468752	29.40%	4.760%
30	8.720	1247	1252	1263	rVB	261836	399791	25.08%	4.060%
31	10.055	1461	1471	1478	rBV	301264	411910	25.84%	4.183%
32	10.195	1488	1494	1505	rBV	309937	404015	25.34%	4.103%
33	10.305	1505	1512	1523	rVB	1122400	1594357	100.00%	16.190%
34	10.640	1562	1567	1580	rVB	420427	553867	34.74%	5.624%
35	10.964	1616	1620	1625	rVB	22368	27938	1.75%	0.284%
36	11.079	1634	1639	1649	rVB	266565	355782	22.32%	3.613%

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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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37	11.305	1669	1676	1684	rBV	65692	79719	5.00%	0.810%
38	11.378	1684	1688	1690	rVV	133987	176679	11.08%	1.794%
39	11.403	1690	1692	1696	rVV	129293	136686	8.57%	1.388%
40	11.451	1696	1700	1708	rVB	151649	189678	11.90%	1.926%
41	11.616	1721	1727	1735	rBV	133046	169514	10.63%	1.721%
42	11.750	1744	1749	1756	rVB	594307	738754	46.34%	7.502%
43	12.024	1789	1794	1800	rBV	322318	388724	24.38%	3.947%
44	12.091	1800	1805	1810	rVB	143415	181236	11.37%	1.840%
45	12.244	1825	1830	1838	rBV2	115573	158697	9.95%	1.612%
46	12.317	1838	1842	1849	rVB2	35034	49404	3.10%	0.502%
47	12.530	1873	1877	1879	rBV	27116	33204	2.08%	0.337%
48	12.555	1879	1881	1886	rVB	22750	24610	1.54%	0.250%
49	12.616	1886	1891	1894	rBV	41744	50497	3.17%	0.513%
50	12.701	1900	1905	1913	rBV2	23891	32583	2.04%	0.331%
51	12.921	1937	1941	1945	rVV	24002	30490	1.91%	0.310%
52	12.963	1945	1948	1955	rVB	36100	42623	2.67%	0.433%
53	13.170	1977	1982	1988	rVB	26879	30572	1.92%	0.310%
54	13.292	1997	2002	2007	rVB2	51155	67626	4.24%	0.687%
55	13.774	2076	2081	2091	rVB	88766	115559	7.25%	1.173%
56	14.640	2219	2223	2231	rVB	21591	24437	1.53%	0.248%
57	14.780	2241	2246	2251	rBV	14718	17944	1.13%	0.182%

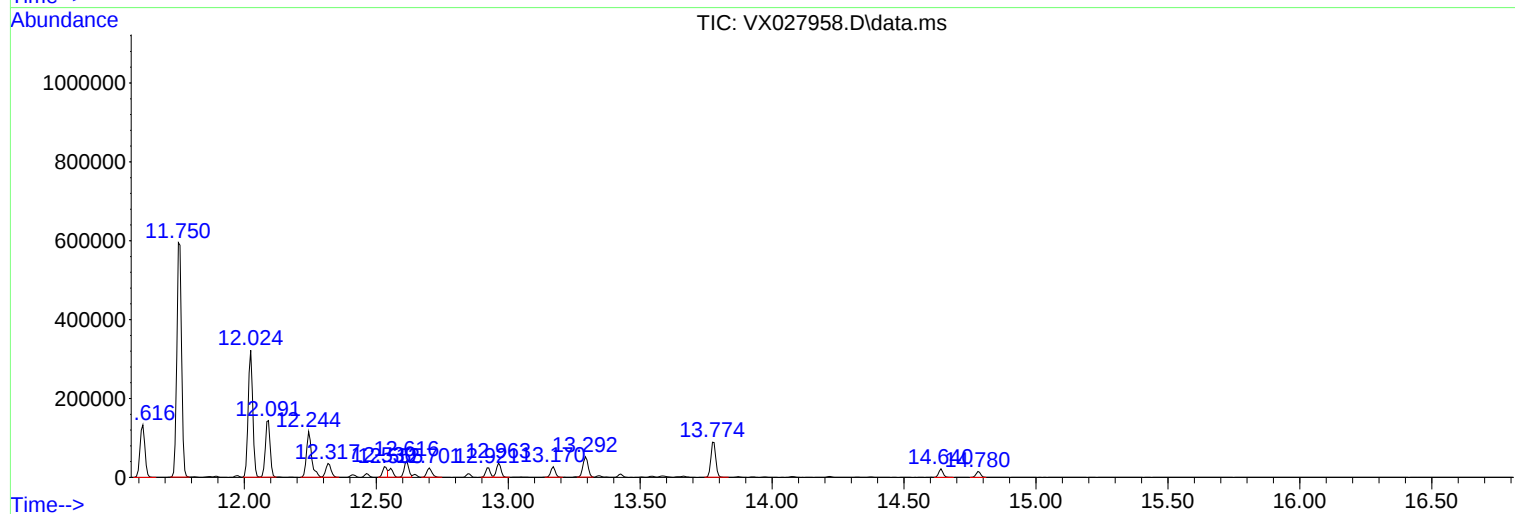
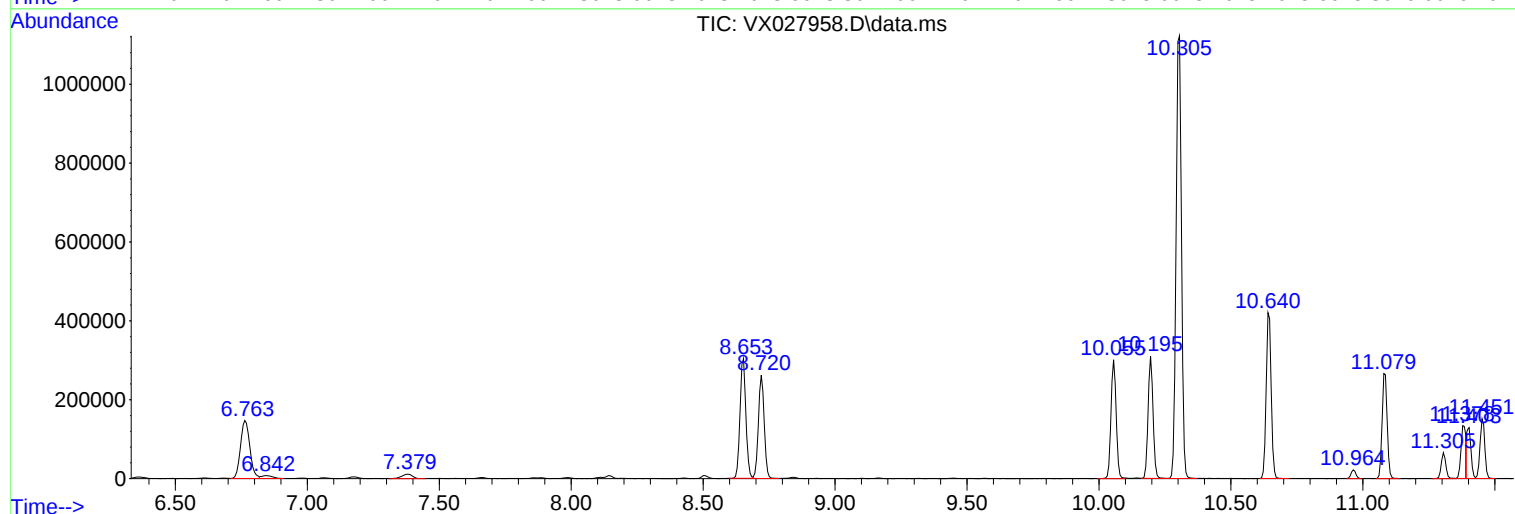
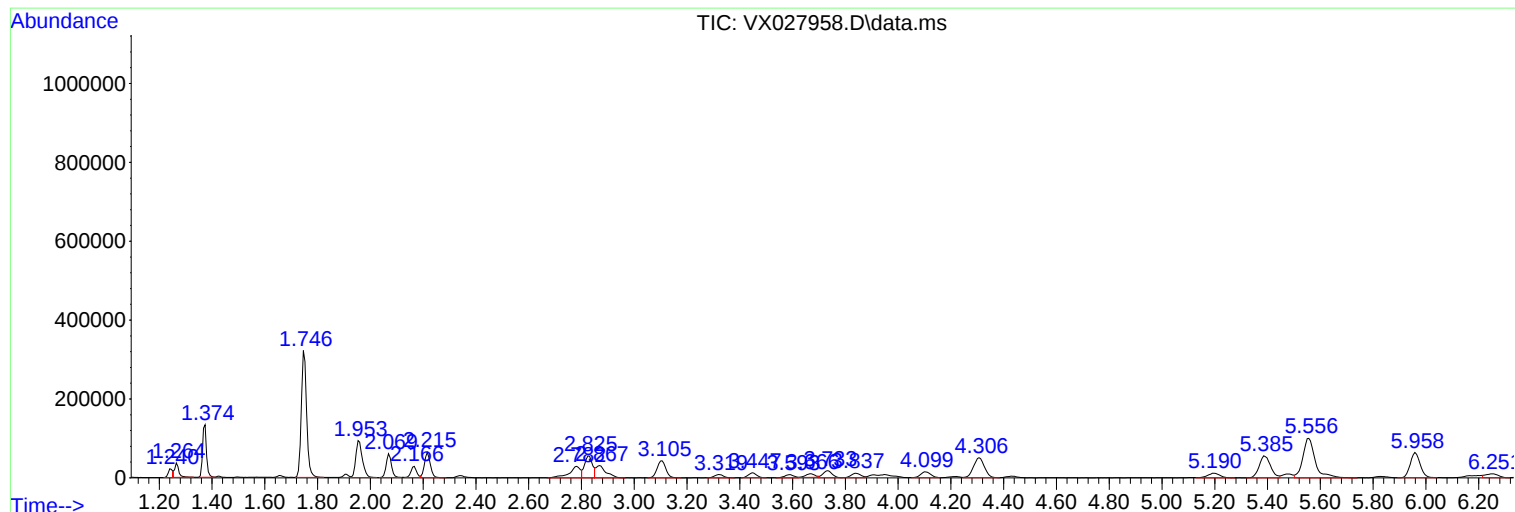
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Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
MSVOA_X
ClientSampleId :
MW-2D

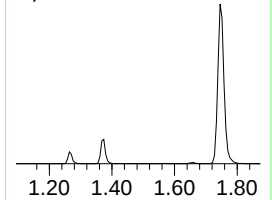
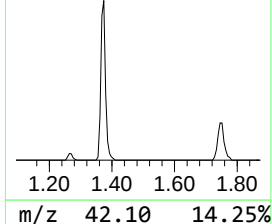
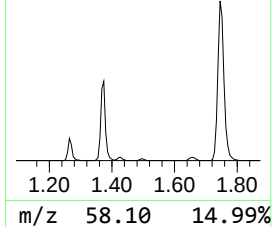
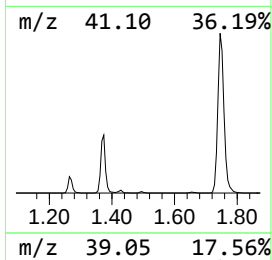
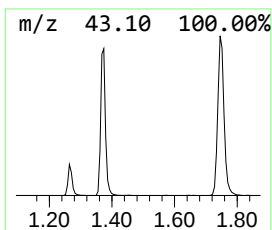
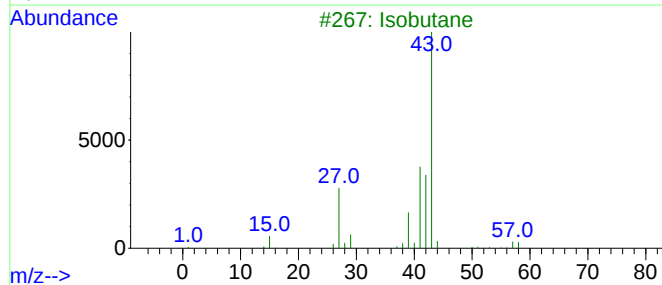
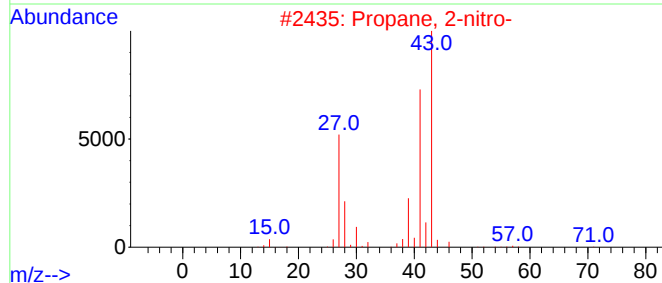
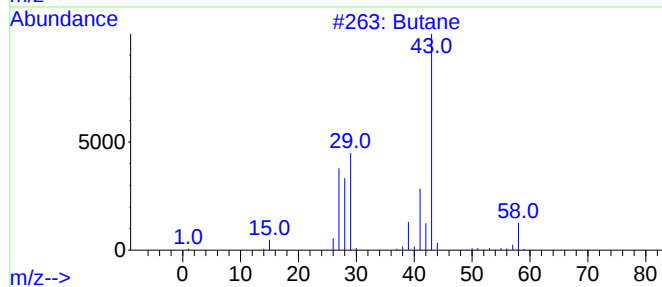
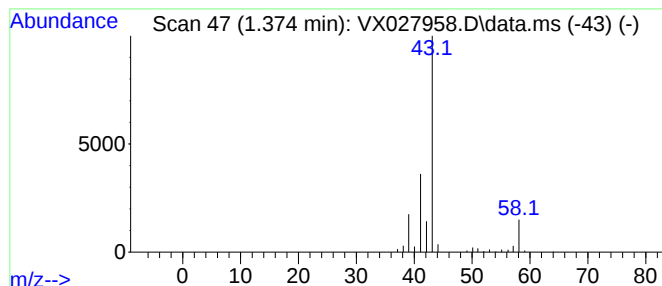
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	21.13 ug/l	136611	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2D

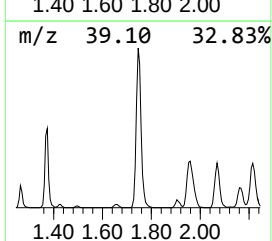
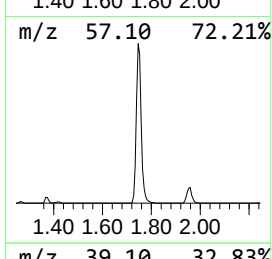
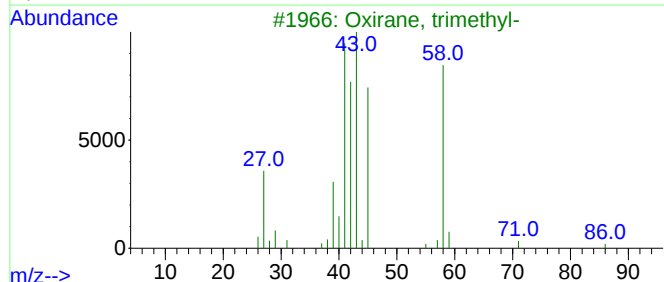
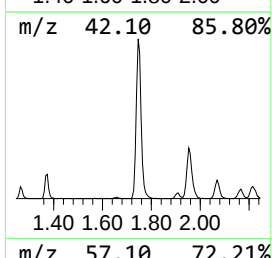
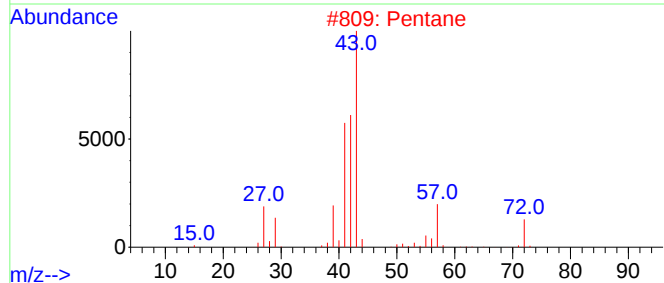
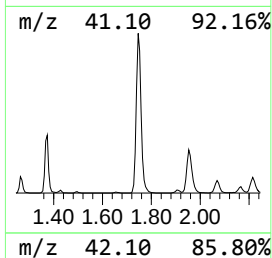
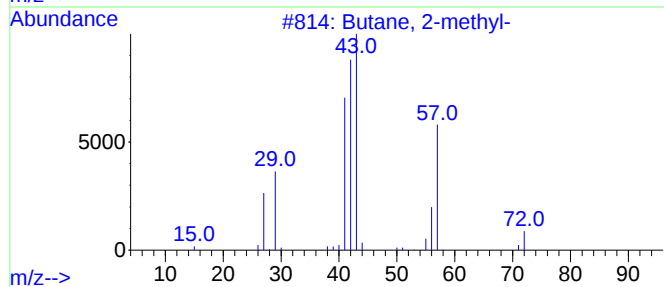
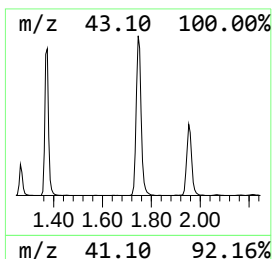
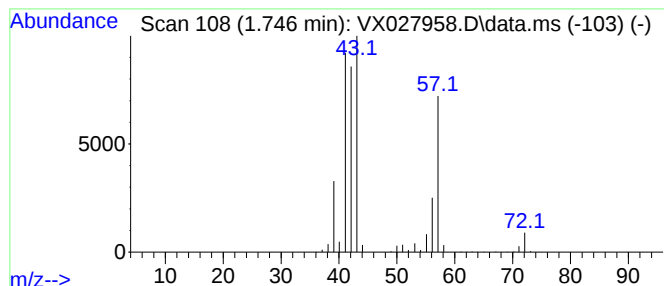
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	69.26 ug/l	447709	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			Pentane	72	C5H12	000109-66-0	36
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
4			3-Buten-1-ol	72	C4H8O	000627-27-0	33
5			1-Butene	56	C4H8	000106-98-9	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2D

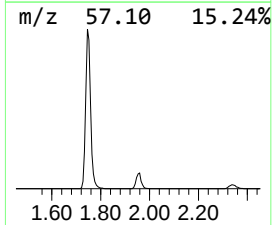
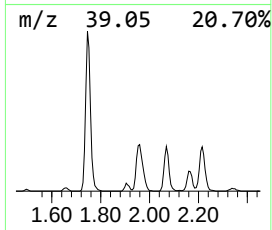
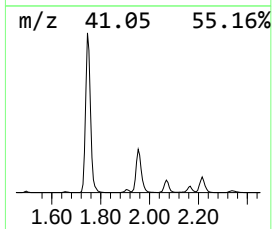
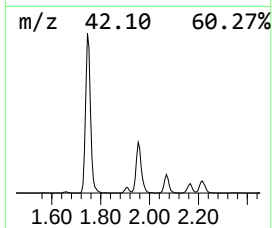
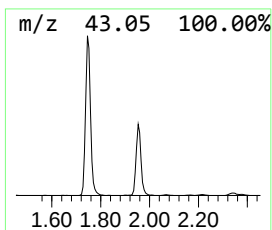
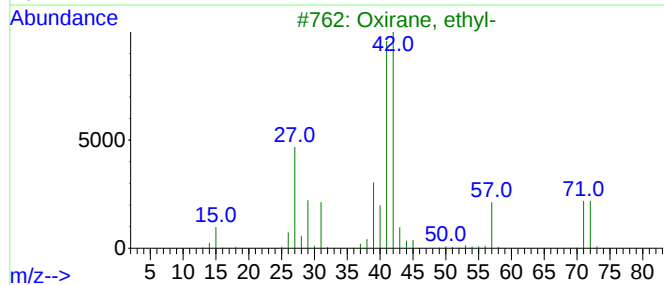
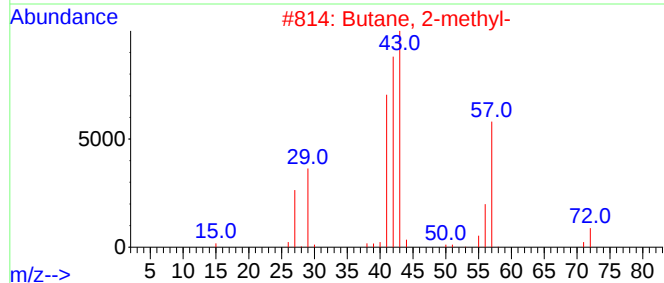
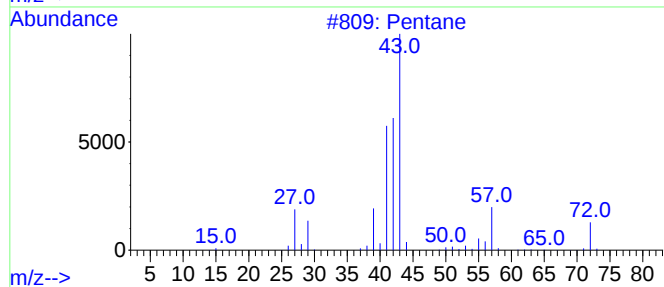
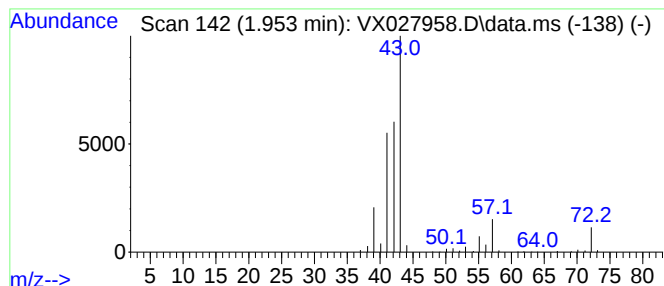
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	24.44 ug/l	158008	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	64
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-2D

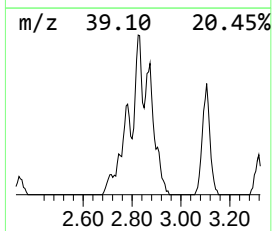
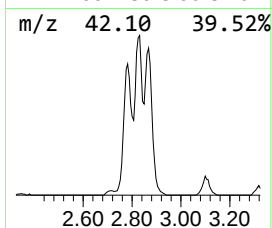
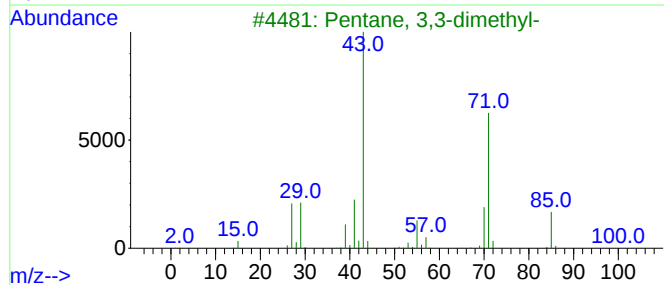
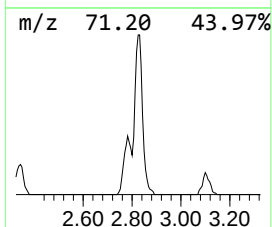
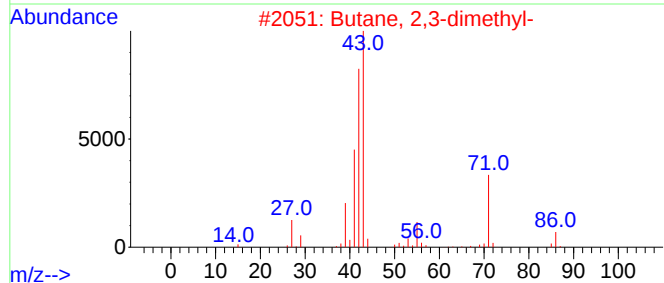
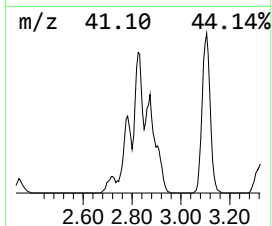
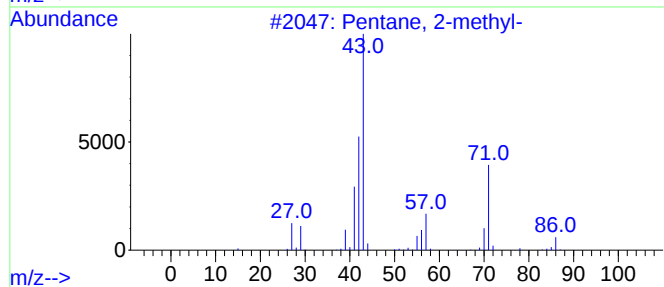
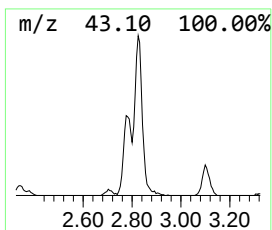
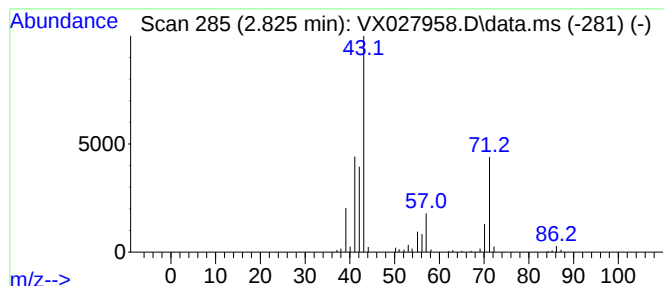
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	17.75 ug/l	114763	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	87
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
3			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28
5			Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	25



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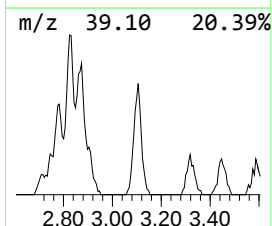
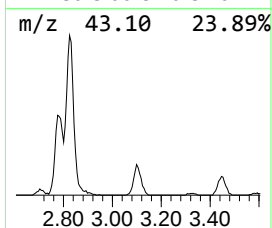
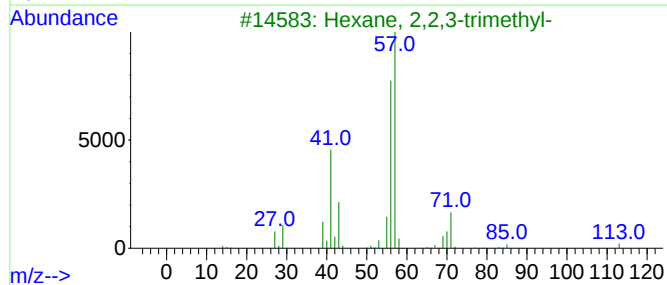
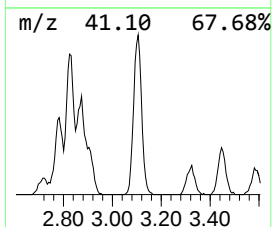
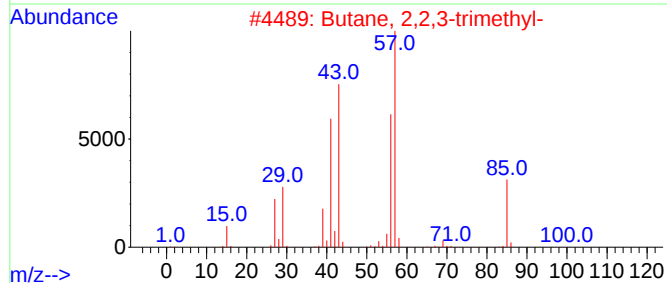
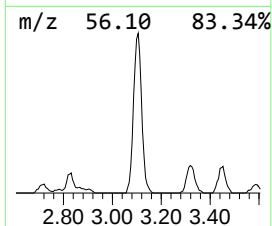
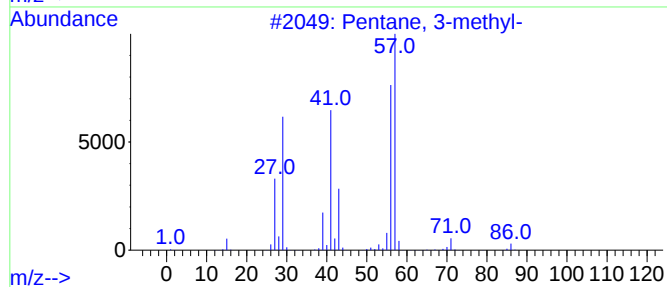
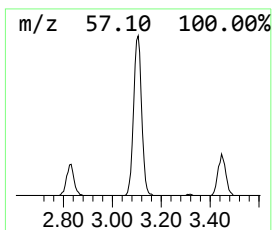
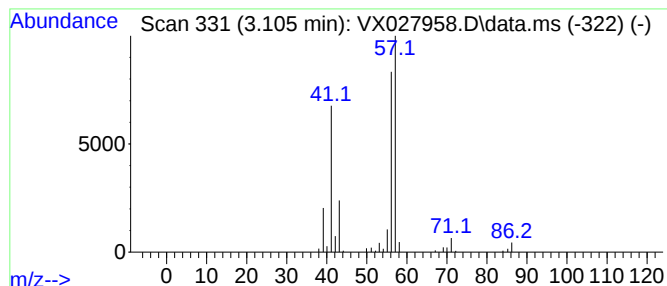
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	15.29 ug/l	98850	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
4			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	47
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO040422\
Data File : VX027958.D
Acq On : 04 Apr 2022 15:24
Operator : JC/MD
Sample : N2249-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2D

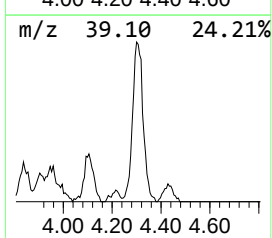
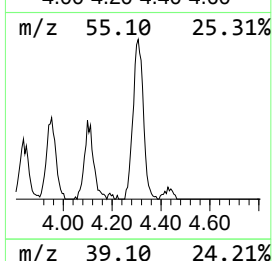
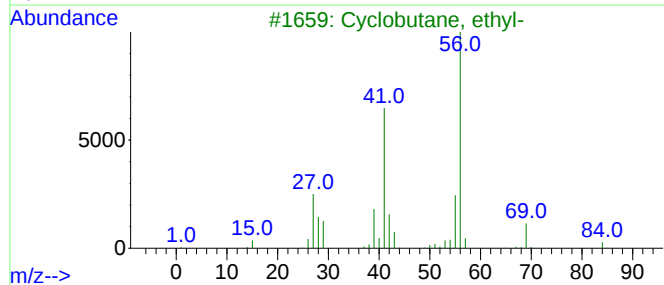
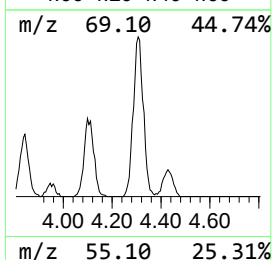
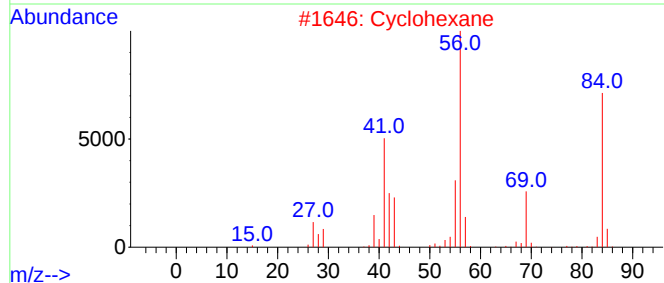
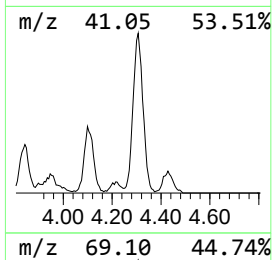
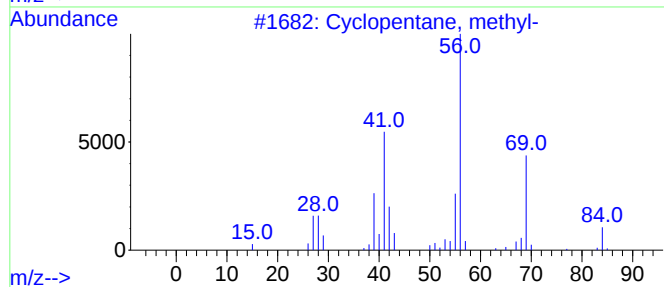
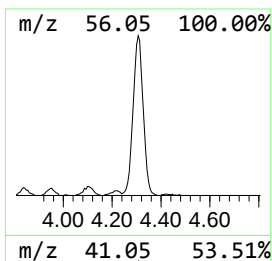
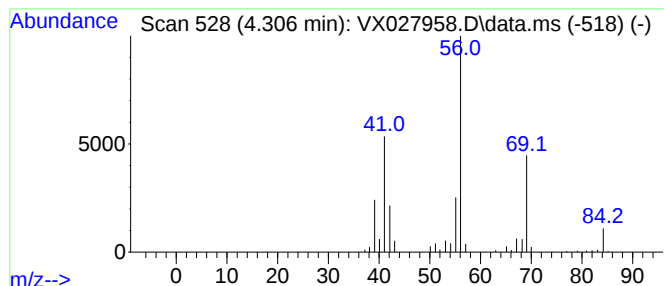
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	22.26 ug/l	143912	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclohexane	84	C6H12	000110-82-7	78
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027958.D
Acq On : 04 Apr 2022 15:24
Operator : JC/MD
Sample : N2249-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2D

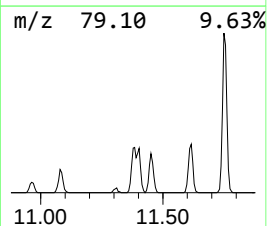
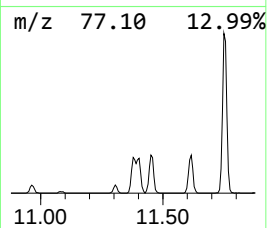
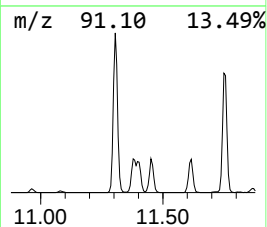
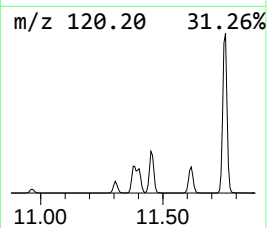
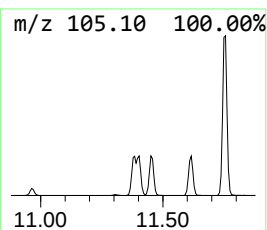
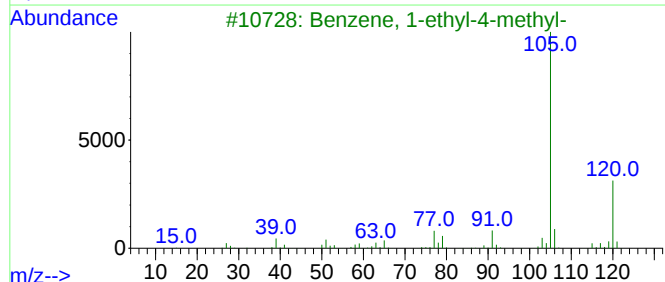
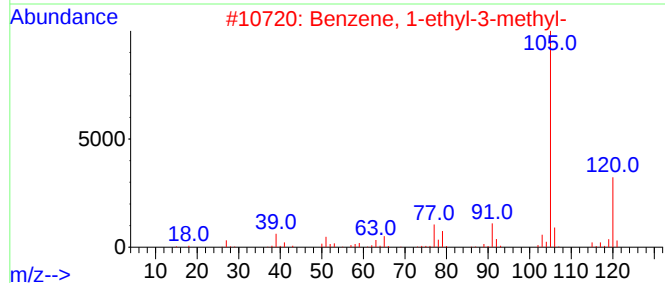
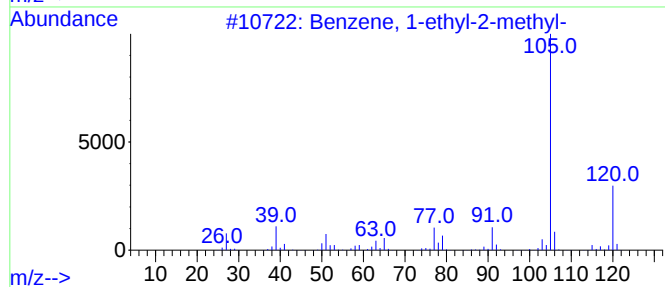
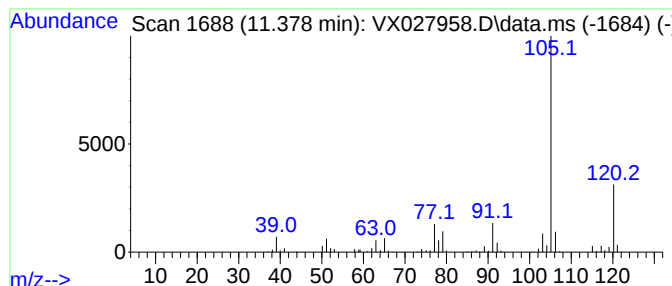
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	22.73 ug/l	176679	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO040422\
Data File : VX027958.D
Acq On : 04 Apr 2022 15:24
Operator : JC/MD
Sample : N2249-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2D

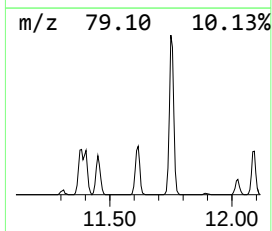
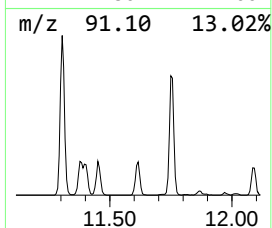
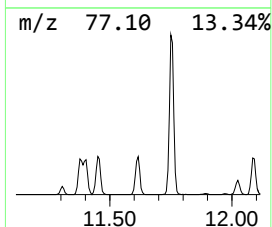
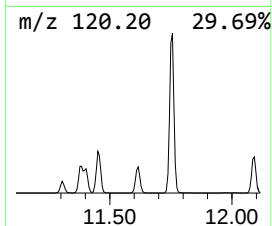
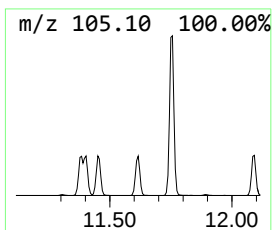
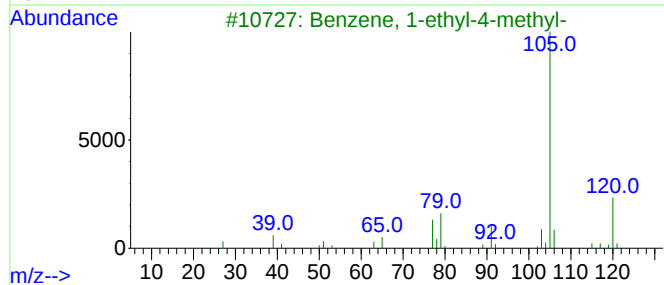
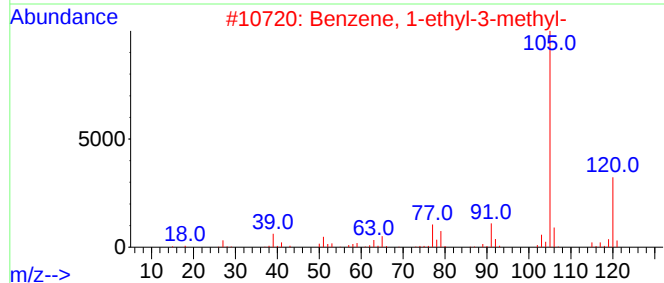
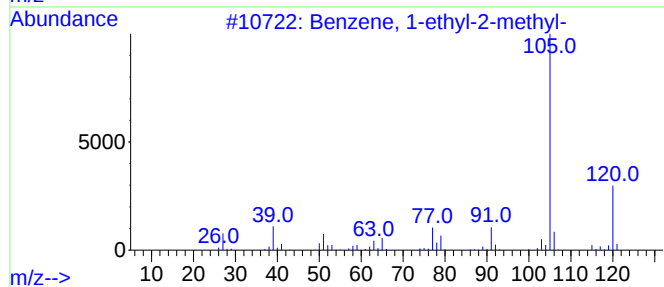
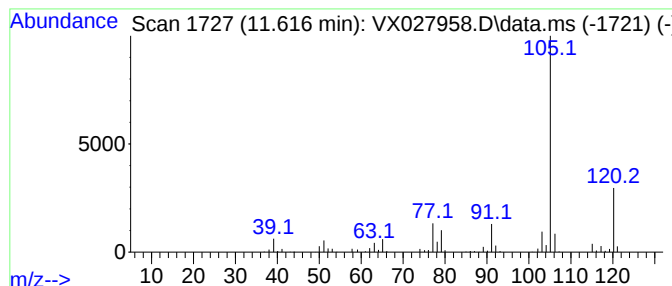
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	21.80 ug/l	169514	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-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027958.D
Acq On : 04 Apr 2022 15:24
Operator : JC/MD
Sample : N2249-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2D

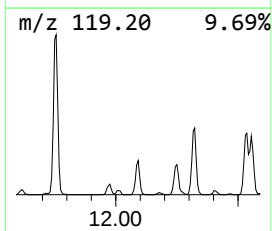
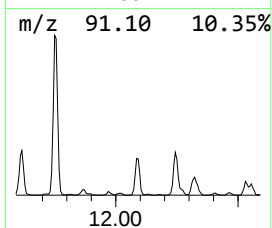
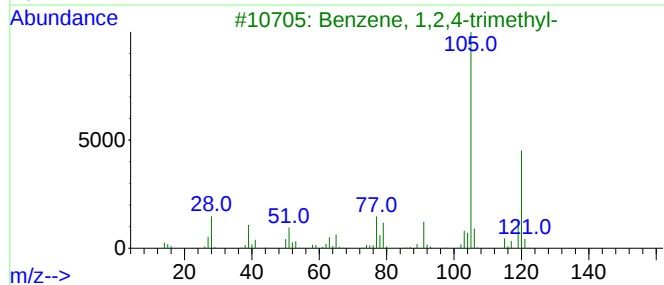
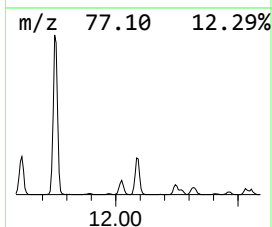
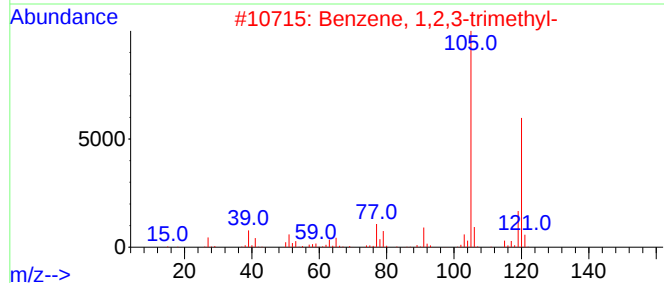
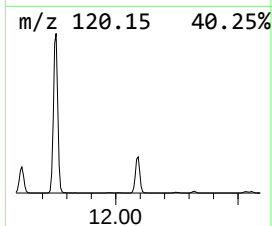
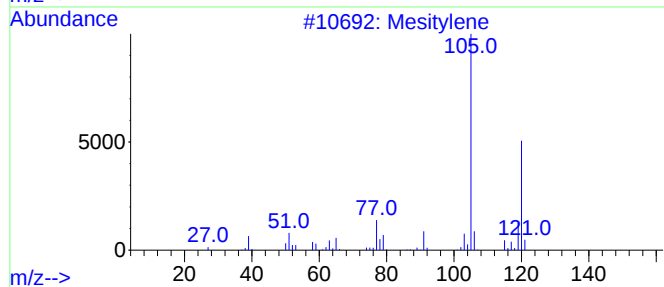
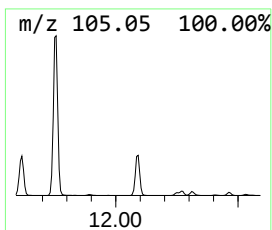
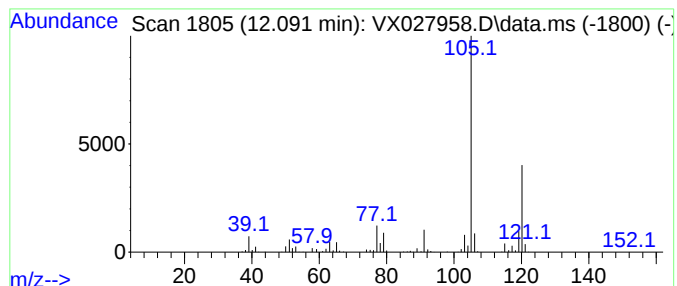
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Quant Title : SW846 8260

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

Peak Number 9 Mesitylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	23.31 ug/l	181236	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	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027958.D
Acq On : 04 Apr 2022 15:24
Operator : JC/MD
Sample : N2249-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2D

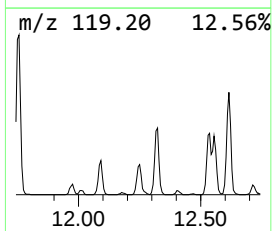
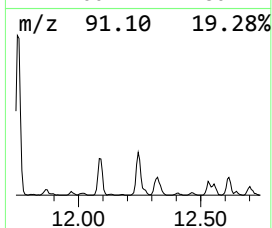
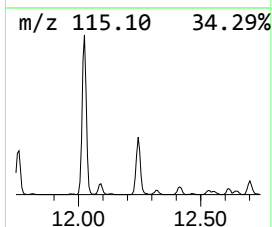
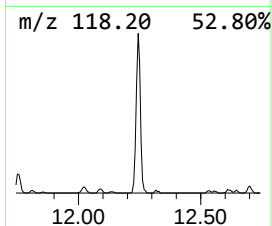
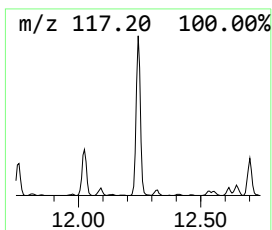
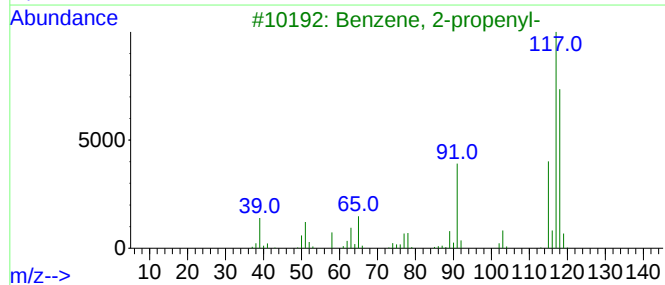
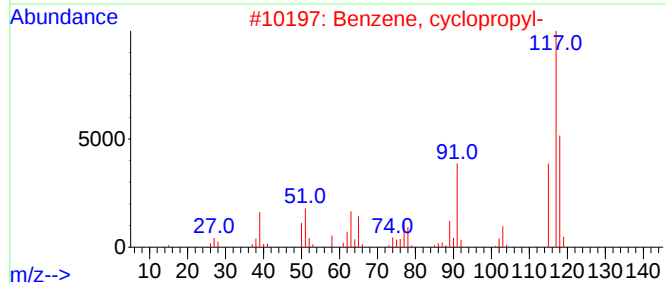
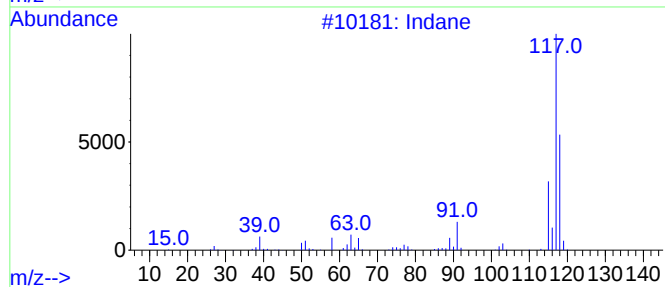
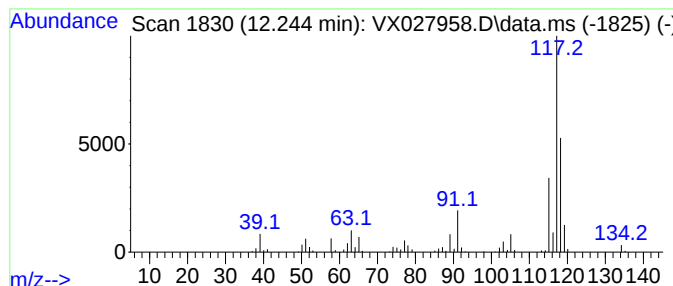
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	20.41 ug/l	158697	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
4			Delta-cyclene	118	C9H10	007785-10-6	53
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027958.D
Acq On : 04 Apr 2022 15:24
Operator : JC/MD
Sample : N2249-03 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2D

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	69.3	ug/l	447709	1	5.556	323195	50.0
Pentane	1.953	24.4	ug/l	158008	1	5.556	323195	50.0
Pentane, 2-methyl-	2.825	17.8	ug/l	114763	1	5.556	323195	50.0
Pentane, 3-methyl-	3.105	15.3	ug/l	98850	1	5.556	323195	50.0
Cyclopentane, m...	4.306	22.3	ug/l	143912	1	5.556	323195	50.0
Benzene, 1-ethy...	11.378	22.7	ug/l	176679	4	12.024	388724	50.0
Benzene, 1-ethy...	11.616	21.8	ug/l	169514	4	12.024	388724	50.0
Mesitylene	12.091	23.3	ug/l	181236	4	12.024	388724	50.0
Indane	12.244	20.4	ug/l	158697	4	12.024	388724	50.0