

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034812.D
 Acq On : 28 Mar 2023 22:38
 Operator : JC/MD
 Sample : 02084-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PMW-2

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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

Signal : TIC: VX034812.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	39	rBV	48079	47957	2.53%	0.287%
2	1.374	43	47	52	rVV	244916	258697	13.65%	1.547%
3	1.416	52	54	59	rVB	20454	22469	1.19%	0.134%
4	1.752	103	109	123	rVB	1451118	1894742	100.00%	11.331%
5	1.959	137	143	155	rVB	227848	332716	17.56%	1.990%
6	2.215	181	185	190	rVB	14936	22927	1.21%	0.137%
7	2.343	197	206	218	rBV	76532	153860	8.12%	0.920%
8	2.782	270	278	282	rBV	153906	333560	17.60%	1.995%
9	2.825	282	285	297	rVB2	149643	296926	15.67%	1.776%
10	3.105	320	331	344	rBV	205578	464353	24.51%	2.777%
11	3.446	379	387	397	rBV	26125	55948	2.95%	0.335%
12	3.837	443	451	461	rBV3	11987	31825	1.68%	0.190%
13	4.214	502	513	518	rBV2	11047	30598	1.61%	0.183%
14	4.306	518	528	539	rVB2	140466	401946	21.21%	2.404%
15	4.434	539	549	550	rBV4	11238	23417	1.24%	0.140%
16	5.123	649	662	671	rBV6	9073	42531	2.24%	0.254%
17	5.385	692	705	713	rBV	195378	568710	30.02%	3.401%
18	5.470	713	719	724	rVV2	41063	104157	5.50%	0.623%
19	5.550	724	732	741	rVV	311900	825519	43.57%	4.937%
20	5.842	766	780	790	rBV5	39752	134773	7.11%	0.806%
21	5.952	790	798	810	rBV	230738	600140	31.67%	3.589%
22	6.159	824	832	841	rBV4	36275	113722	6.00%	0.680%
23	6.257	841	848	856	rVV2	38628	108879	5.75%	0.651%
24	6.354	856	864	876	rVB2	53486	152326	8.04%	0.911%
25	6.763	921	931	941	rBV	533186	1305525	68.90%	7.807%
26	7.171	991	998	1007	rVB3	16204	35526	1.87%	0.212%
27	7.372	1019	1031	1044	rVB3	106945	289449	15.28%	1.731%
28	7.659	1072	1078	1089	rVV5	12261	26783	1.41%	0.160%
29	7.775	1089	1097	1104	rVB	35287	71478	3.77%	0.427%
30	7.952	1121	1126	1141	rVB8	14825	54704	2.89%	0.327%
31	8.104	1143	1151	1155	rBV2	13011	28843	1.52%	0.172%
32	8.226	1161	1171	1176	rVB9	7397	19625	1.04%	0.117%
33	8.317	1176	1186	1193	rBV4	30154	64036	3.38%	0.383%
34	8.506	1211	1217	1225	rVB4	16508	35952	1.90%	0.215%
35	8.604	1225	1233	1235	rBV2	28904	53910	2.85%	0.322%
36	8.647	1235	1240	1247	rVV	1128357	1756933	92.73%	10.507%

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Integrator: RTE

Smoothing : ON

Filtering: 5

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Max Peaks: 100

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Peak Location: TOP

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37	8.720	1247	1252	1257	rVV	100644	165380	8.73%	0.989%
38	8.775	1257	1261	1265	rVB	30773	49206	2.60%	0.294%
39	8.921	1281	1285	1289	rBV2	13947	23008	1.21%	0.138%
40	8.976	1289	1294	1300	rVB	91966	145853	7.70%	0.872%
41	9.098	1306	1314	1319	rBV	23798	42795	2.26%	0.256%
42	9.159	1319	1324	1335	rVB	50341	86721	4.58%	0.519%
43	9.427	1364	1368	1371	rBV3	14754	23597	1.25%	0.141%
44	9.506	1377	1381	1386	rVB2	26159	43564	2.30%	0.261%
45	9.659	1402	1406	1416	rVB3	18019	35690	1.88%	0.213%
46	9.762	1416	1423	1430	rBV6	15657	31722	1.67%	0.190%
47	9.835	1430	1435	1444	rBV2	17874	34839	1.84%	0.208%
48	10.055	1465	1471	1477	rVV	1090734	1512910	79.85%	9.048%
49	10.122	1479	1482	1486	rVV	20690	35772	1.89%	0.214%
50	10.195	1489	1494	1503	rVV	29365	52845	2.79%	0.316%
51	10.299	1503	1511	1518	rVB	94009	168994	8.92%	1.011%
52	10.457	1531	1537	1546	rVB2	19291	37804	2.00%	0.226%
53	10.585	1551	1558	1564	rBV5	20893	58533	3.09%	0.350%
54	10.646	1564	1568	1573	rVV2	21639	30926	1.63%	0.185%
55	10.780	1579	1590	1593	rBV4	19937	41052	2.17%	0.245%
56	10.860	1598	1603	1610	rVV9	9188	20740	1.09%	0.124%
57	11.079	1634	1639	1645	rBV	900765	1173539	61.94%	7.018%
58	11.122	1645	1646	1650	rVB3	20277	21337	1.13%	0.128%
59	11.384	1684	1689	1697	rBV	25774	58688	3.10%	0.351%
60	11.616	1723	1727	1734	rVB	22029	32173	1.70%	0.192%
61	11.750	1745	1749	1755	rVB	55790	70907	3.74%	0.424%
62	11.890	1769	1772	1777	rVB	14800	19964	1.05%	0.119%
63	12.018	1788	1793	1801	rBV	1034113	1385510	73.12%	8.286%
64	12.250	1825	1831	1832	rBV2	24198	33402	1.76%	0.200%
65	12.268	1832	1834	1837	rVV	23894	26856	1.42%	0.161%
66	12.317	1837	1842	1852	rVB4	42201	72919	3.85%	0.436%
67	12.463	1862	1866	1872	rVB2	14472	21085	1.11%	0.126%
68	12.530	1872	1877	1879	rBV	16971	22030	1.16%	0.132%
69	12.615	1886	1891	1894	rVB	34223	44054	2.33%	0.263%
70	12.920	1933	1941	1945	rBV	31176	49927	2.64%	0.299%
71	12.963	1945	1948	1955	rVB2	24312	32642	1.72%	0.195%
72	13.030	1955	1959	1964	rBV4	15932	34200	1.80%	0.205%
73	13.292	1998	2002	2007	rVB4	26162	40590	2.14%	0.243%
74	13.579	2046	2049	2054	rBV3	18362	30030	1.58%	0.180%
75	13.664	2060	2063	2070	rVB2	17781	26820	1.42%	0.160%
76	13.780	2074	2082	2090	rVB2	22608	48159	2.54%	0.288%

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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

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Title : SW846 8260

77	14.213	2149	2153	2163	rBV2	10922	21092	1.11%	0.126%
78	14.639	2215	2223	2227	rBV	18775	27976	1.48%	0.167%
79	14.780	2242	2246	2253	rVB	13426	20506	1.08%	0.123%

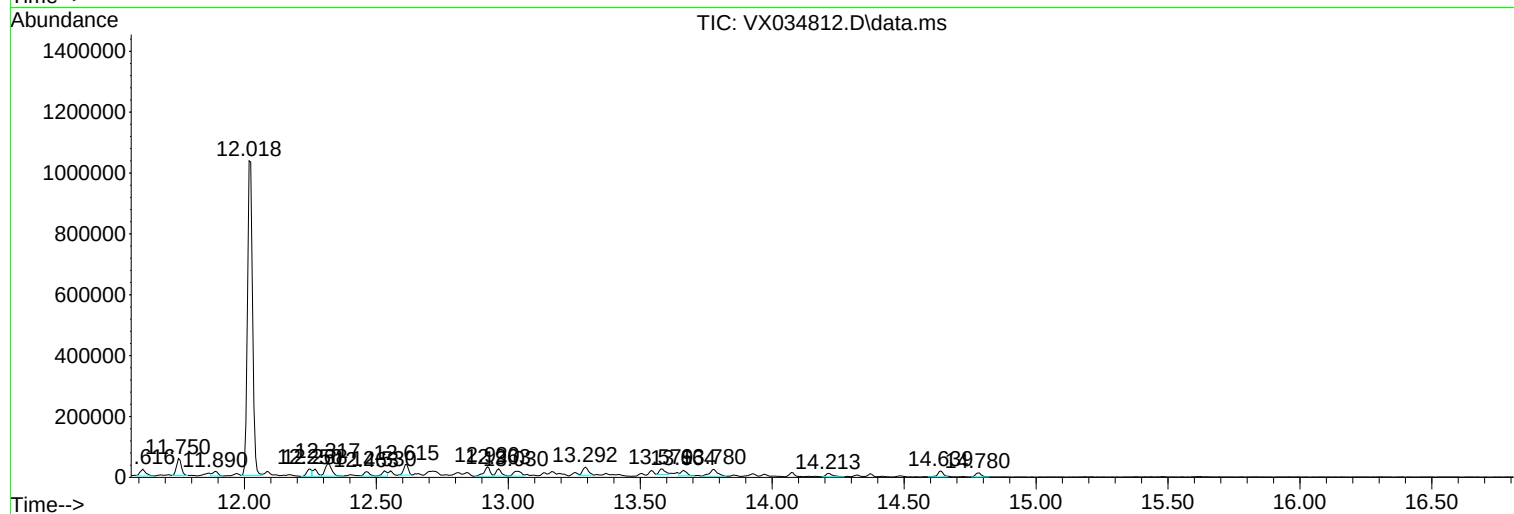
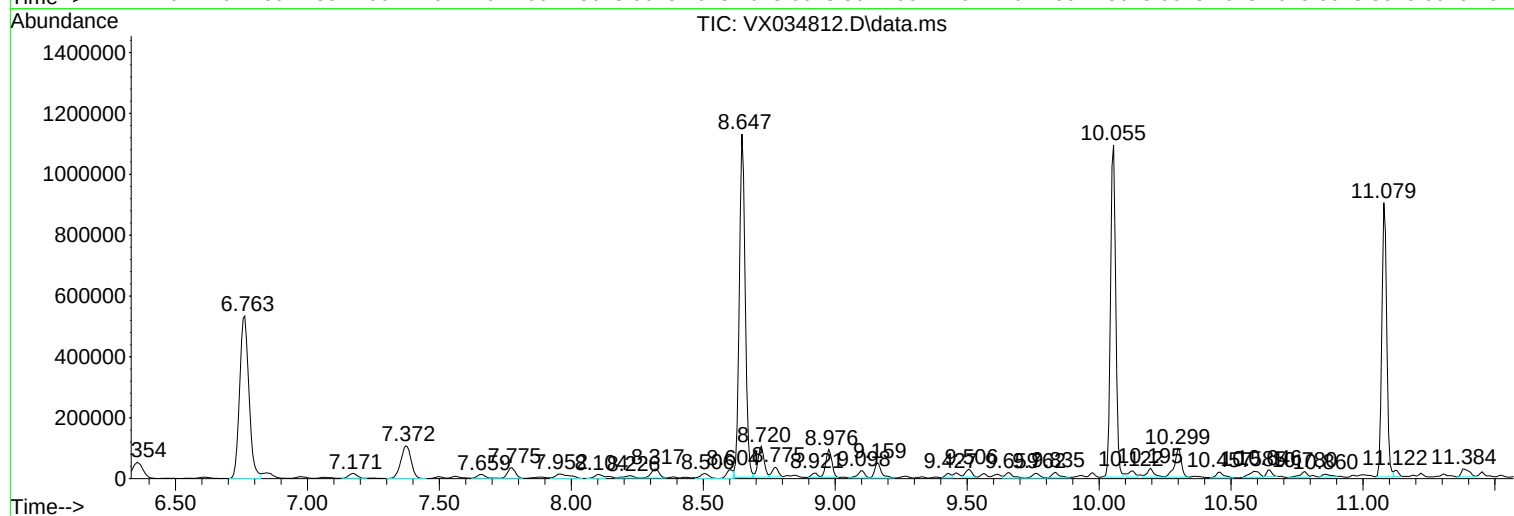
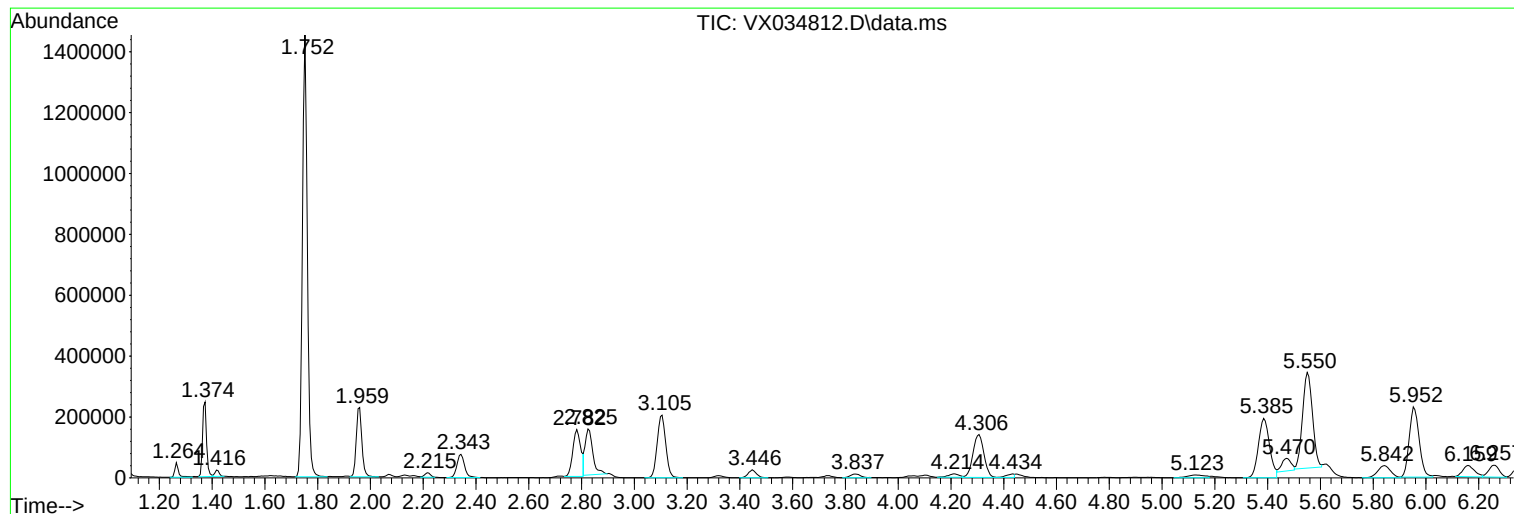
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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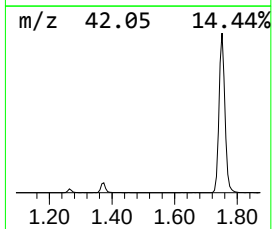
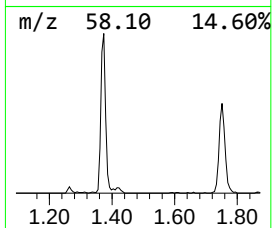
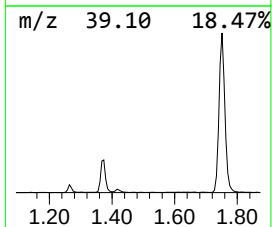
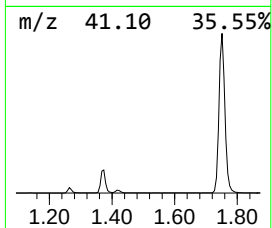
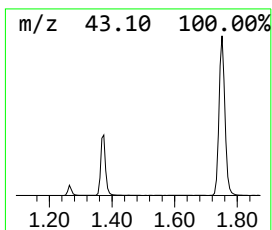
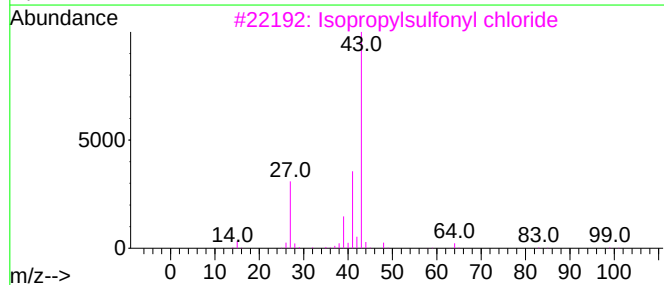
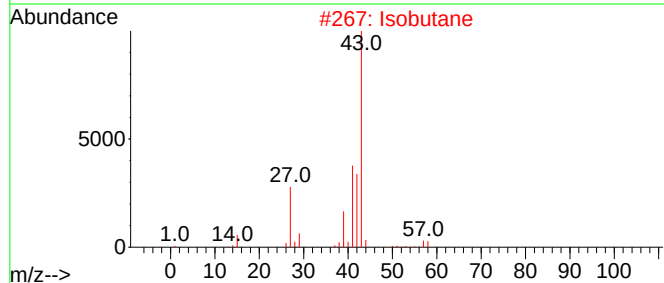
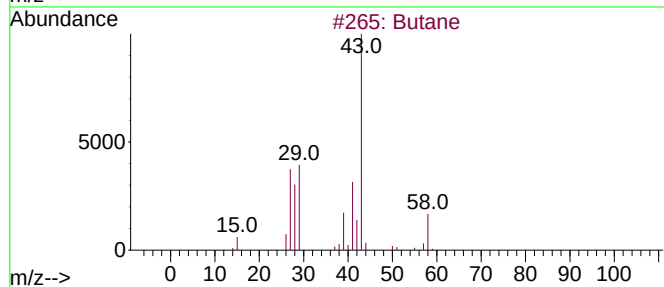
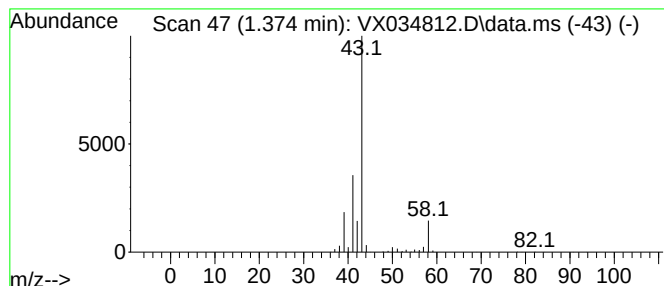
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	15.67 ug/l	258697	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane		58	C4H10	000106-97-8	72
2	Isobutane		58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride		142	C3H7ClO2S	010147-37-2	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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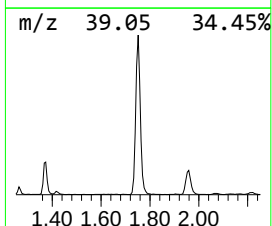
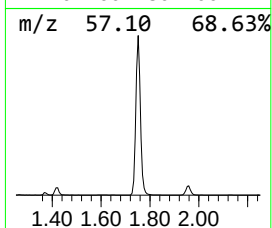
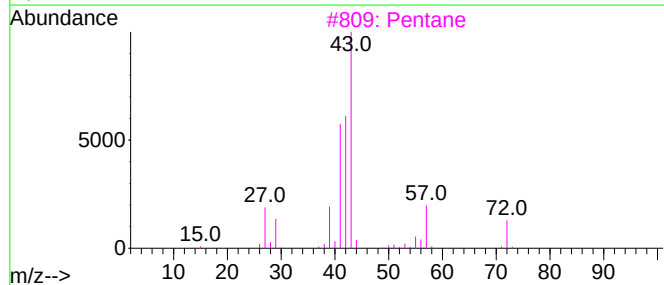
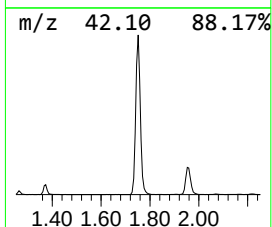
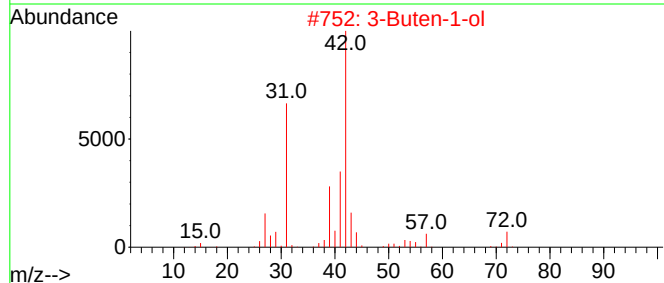
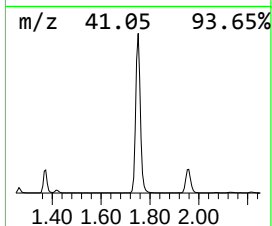
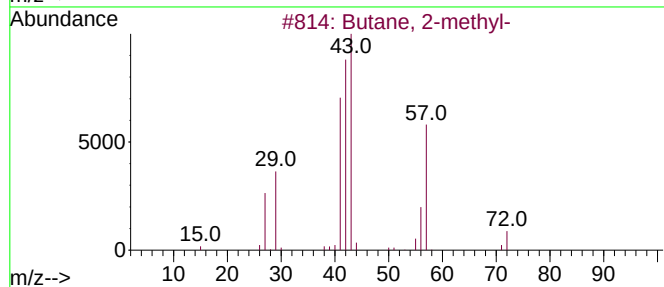
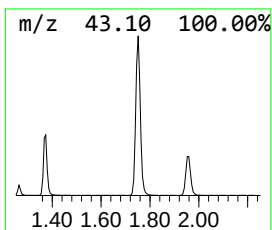
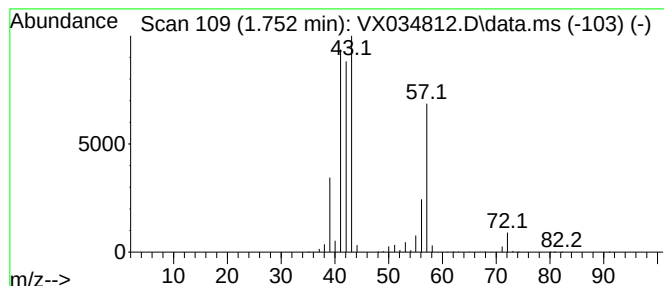
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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.
1.752	114.76 ug/l	1894740	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			1-Butene	56	C4H8	000106-98-9	10
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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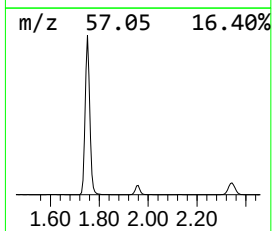
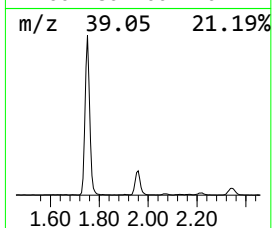
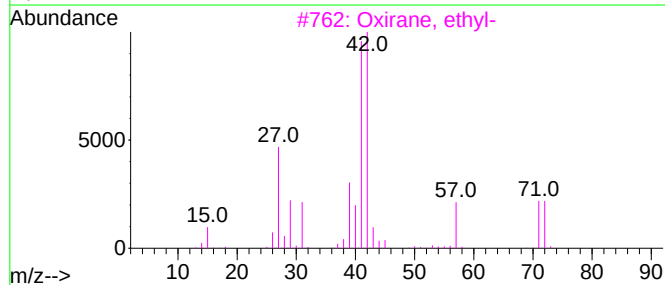
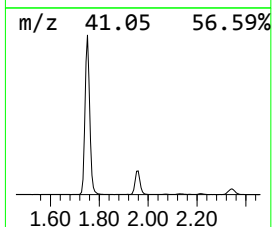
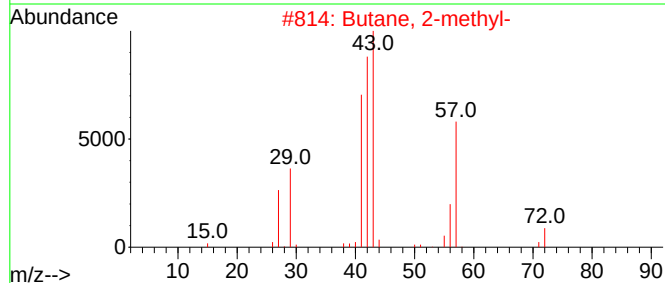
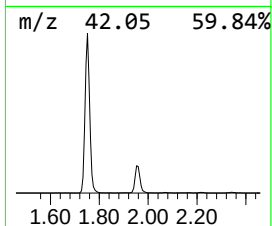
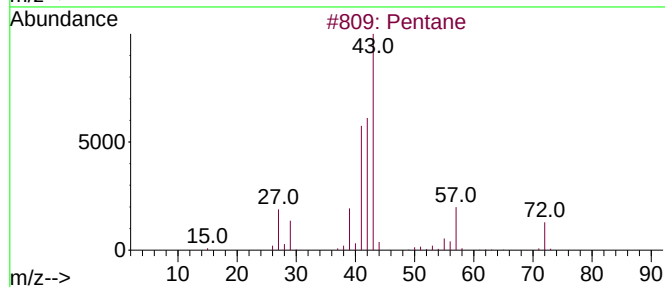
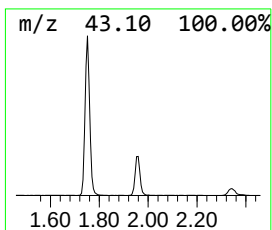
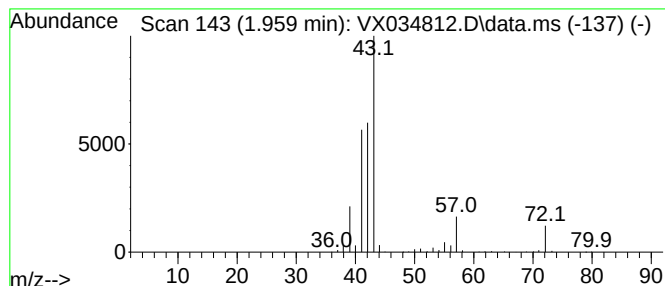
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	20.15 ug/l	332716	Pentafluorobenzene	5.550

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	35
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	9



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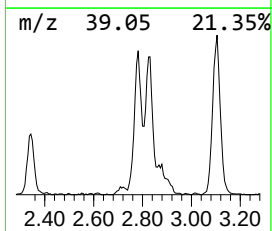
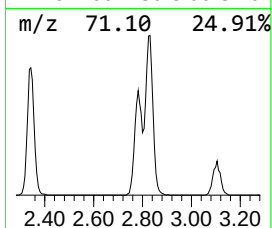
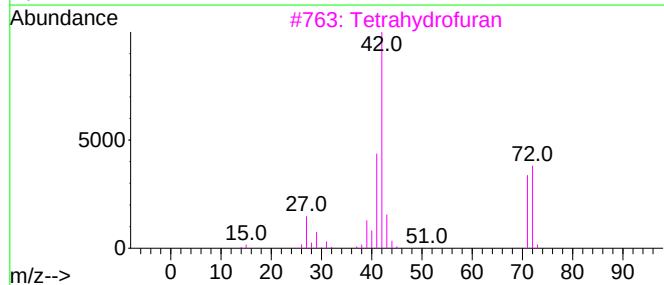
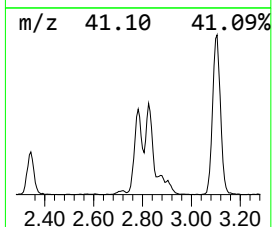
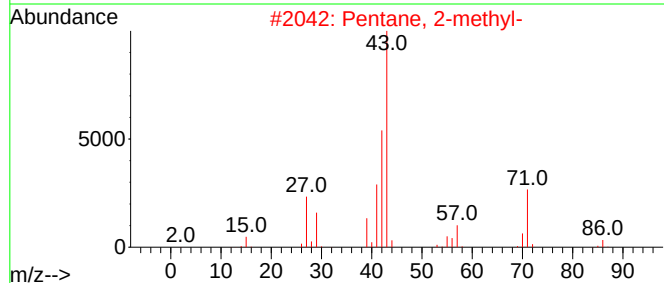
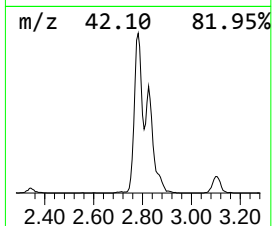
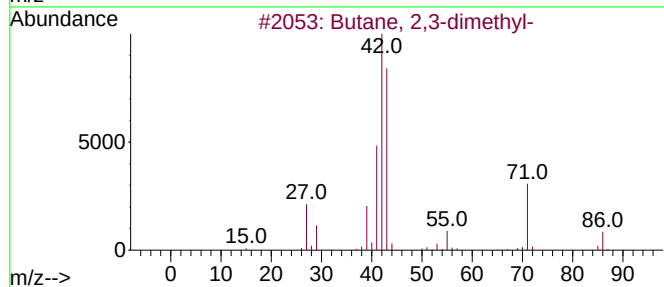
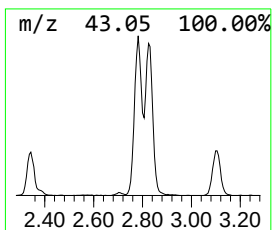
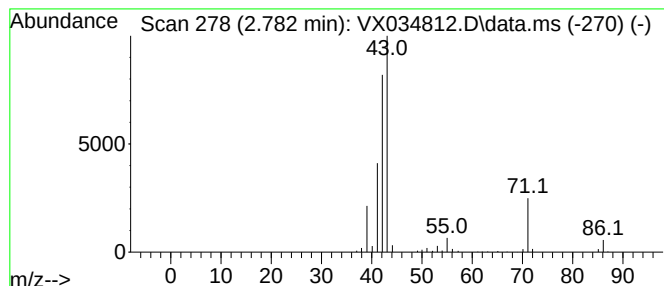
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Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	20.20 ug/l	333560	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3			Tetrahydrofuran	72	C4H8O	000109-99-9	38
4			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	12
5			Pyrrolidine	71	C4H9N	000123-75-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034812.D
Acq On : 28 Mar 2023 22:38
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

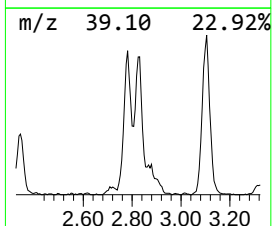
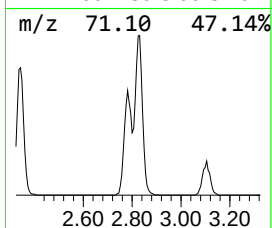
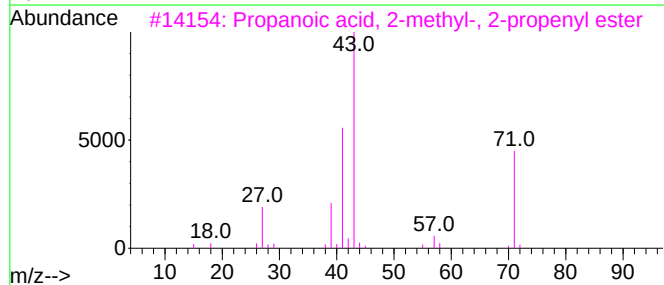
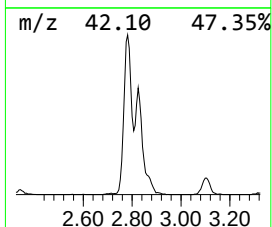
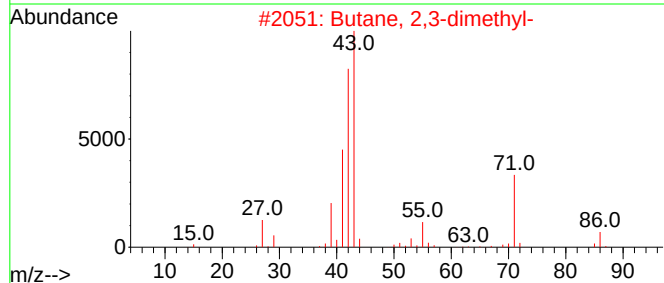
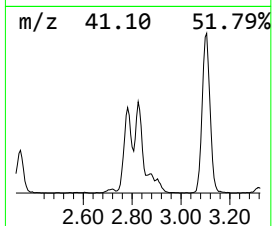
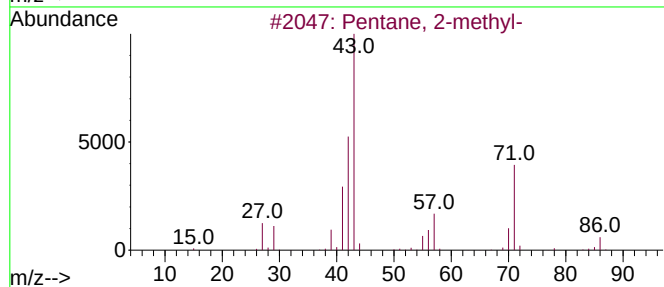
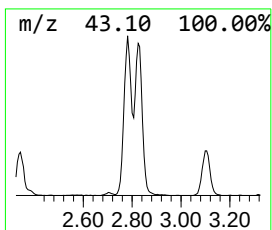
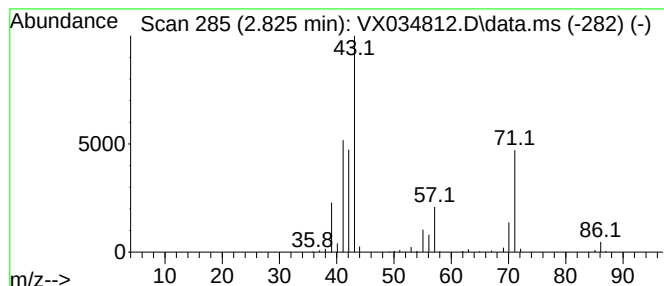
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	17.98 ug/l	296926	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	64
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	38
3			Propanoic acid, 2-methyl-, 2-pro...	128	C7H12O2	015727-77-2	28
4			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	25
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034812.D
Acq On : 28 Mar 2023 22:38
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

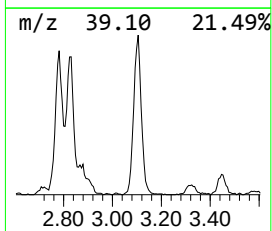
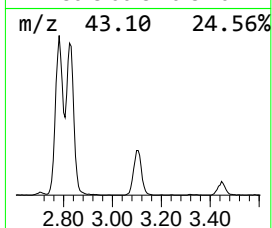
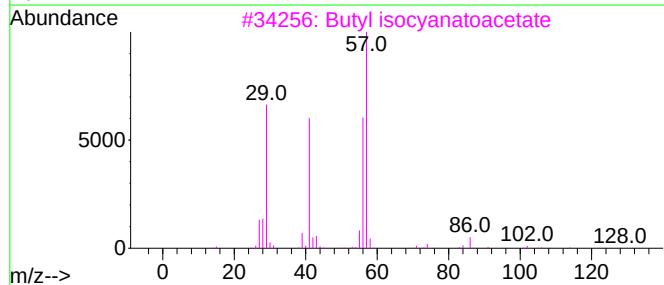
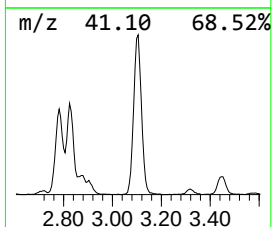
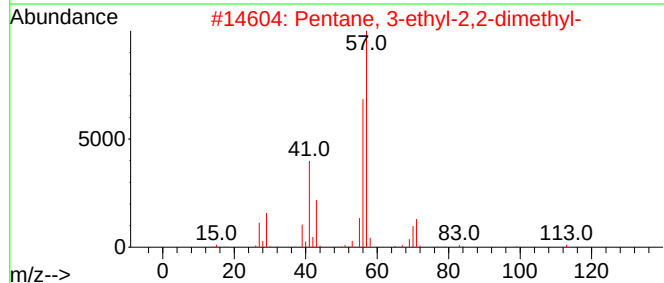
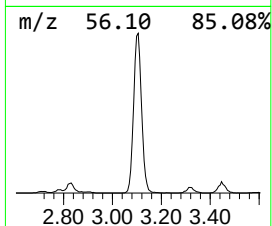
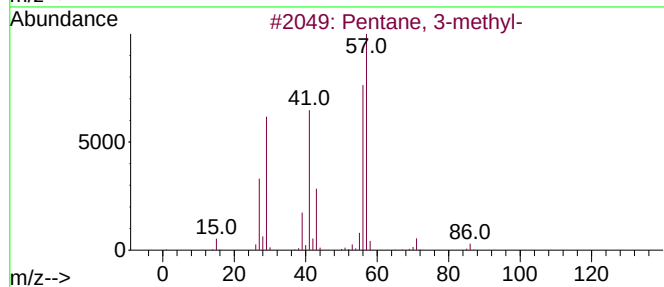
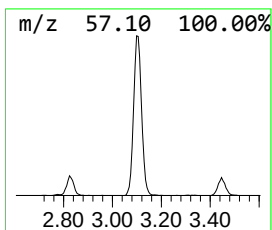
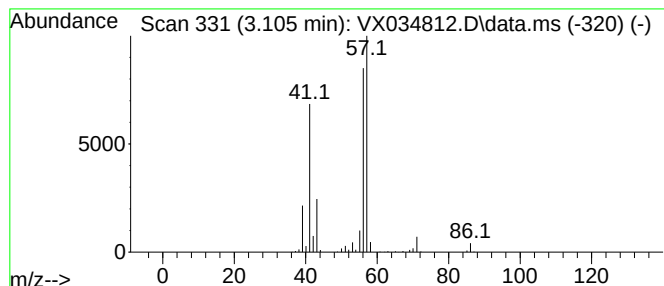
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	28.12 ug/l	464353	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
3			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40
4			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	39
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034812.D
Acq On : 28 Mar 2023 22:38
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

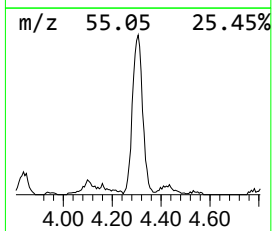
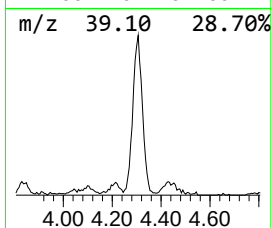
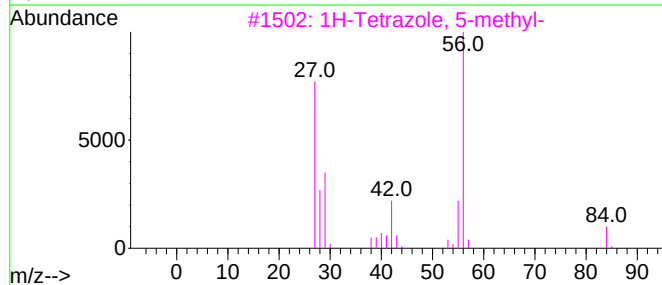
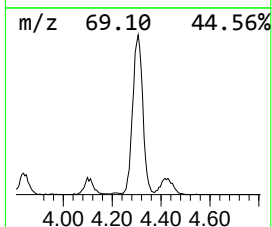
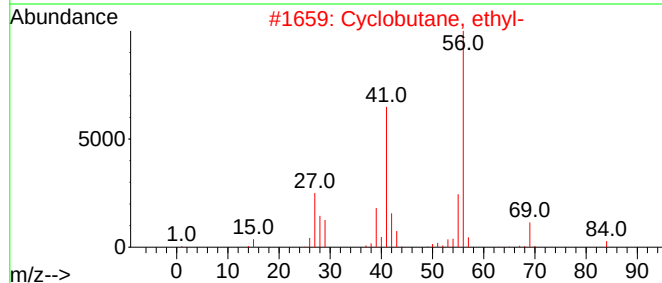
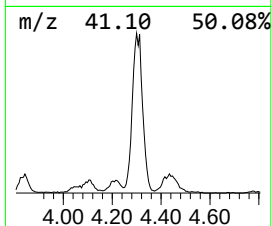
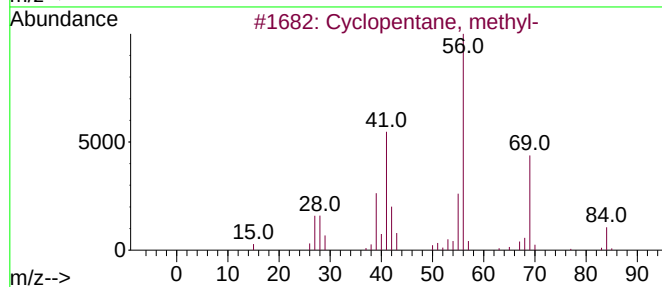
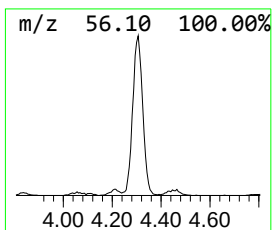
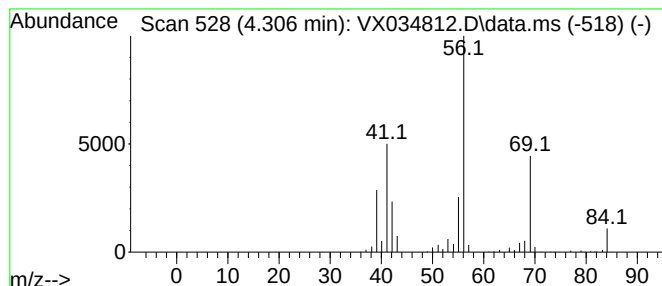
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	24.34 ug/l	401946	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4			Cyclobutane	56	C4H8	000287-23-0	50
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034812.D
Acq On : 28 Mar 2023 22:38
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

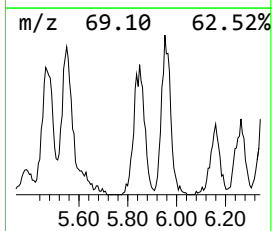
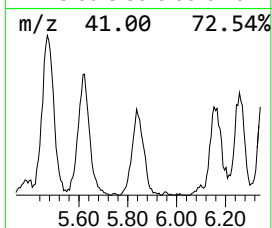
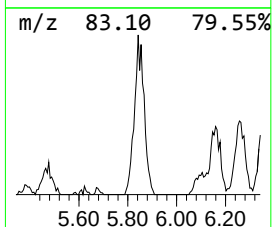
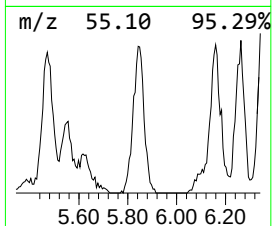
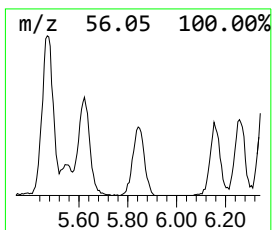
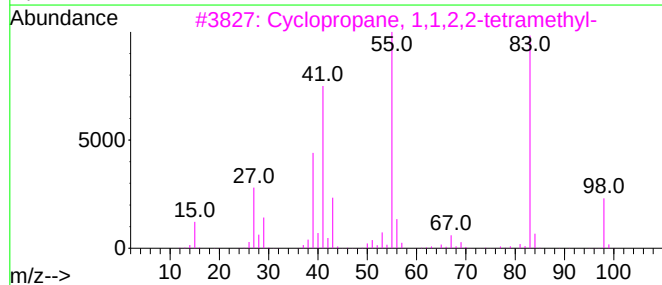
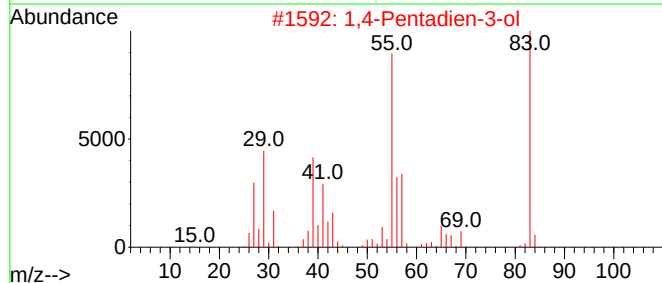
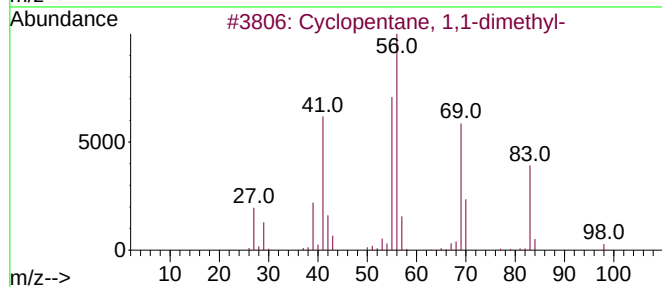
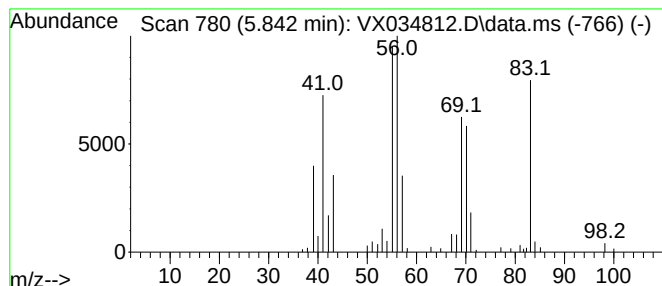
Instrument :
MSVOA_X
ClientSampleId :
PMW-2

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

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

Peak Number 8 unknown5.842 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.842	8.16 ug/l	134773	Pentafluorobenzene	5.550	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	49
2	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	47
3	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	46
4	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	43
5	1-Heptene	98	C7H14	000592-76-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034812.D
Acq On : 28 Mar 2023 22:38
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

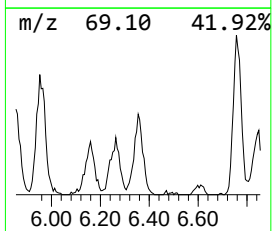
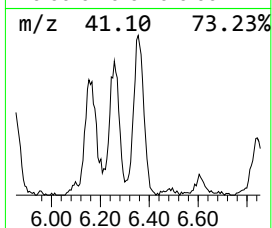
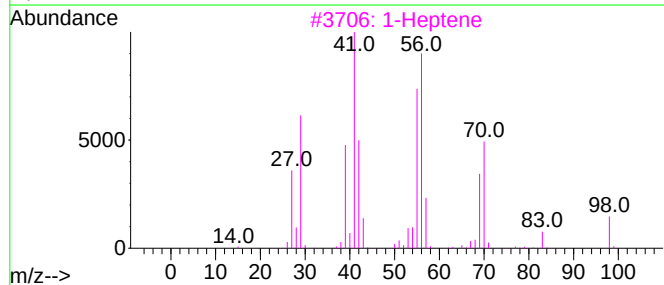
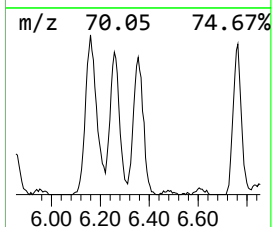
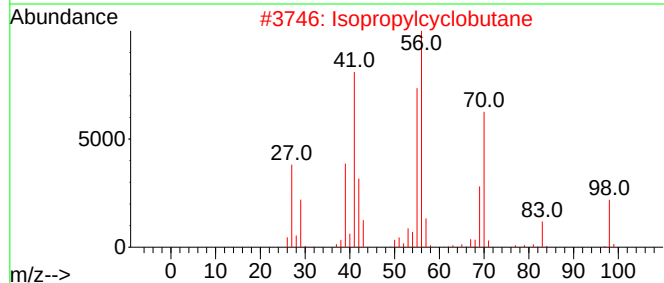
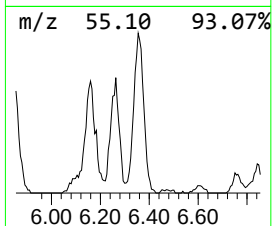
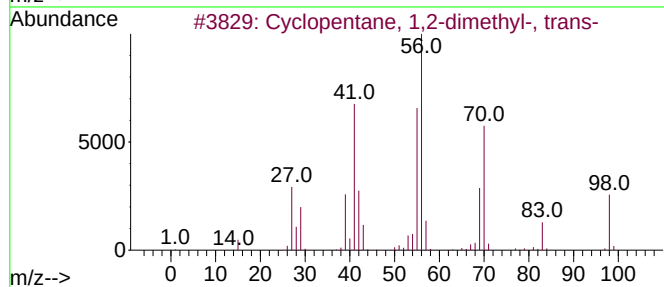
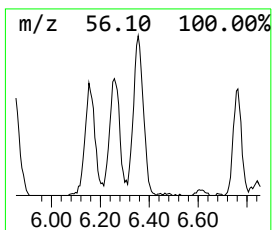
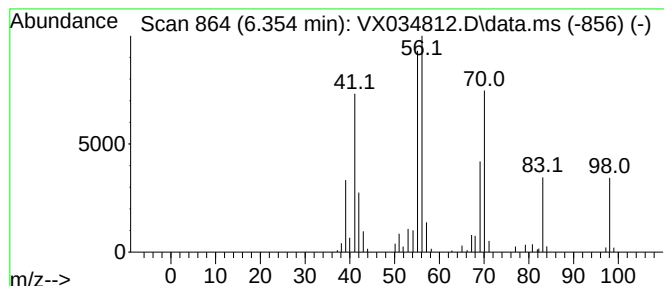
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopentane, 1,2-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.354	5.83 ug/l	152326	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
2		Isopropylcyclobutane	98	C7H14	000872-56-0	90
3		1-Heptene	98	C7H14	000592-76-7	87
4		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	86
5		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034812.D
Acq On : 28 Mar 2023 22:38
Operator : JC/MD
Sample : 02084-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PMW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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-	1.752	114.8	ug/l	1894740	1	5.550	825519	50.0
Pentane	1.959	20.1	ug/l	332716	1	5.550	825519	50.0
Butane, 2,3-dim...	2.782	20.2	ug/l	333560	1	5.550	825519	50.0
Pentane, 2-methyl-	2.825	18.0	ug/l	296926	1	5.550	825519	50.0
Pentane, 3-methyl-	3.105	28.1	ug/l	464353	1	5.550	825519	50.0
Cyclopentane, m...	4.306	24.3	ug/l	401946	1	5.550	825519	50.0
unknown5.842	5.842	8.2	ug/l	134773	1	5.550	825519	50.0
Cyclopentane, 1...	6.354	5.8	ug/l	152326	2	6.763	1305530	50.0