

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
 Data File : VX029646.D
 Acq On : 21 Jun 2022 07:18
 Operator : JC/MD
 Sample : N3354-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-53

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	18	rVB	56341	55044	4.27%	0.516%
2	1.264	26	29	43	rBV	646540	667043	51.76%	6.250%
3	1.367	43	46	53	rVV	658279	710721	55.15%	6.659%
4	1.752	104	109	114	rBV	36412	50326	3.91%	0.472%
5	2.136	167	172	179	rVB3	7123	15473	1.20%	0.145%
6	2.215	180	185	194	rVB	9537	16006	1.24%	0.150%
7	2.562	230	242	251	rBV2	8701	29147	2.26%	0.273%
8	2.782	268	278	285	rBV6	5650	14137	1.10%	0.132%
9	2.867	285	292	300	rBV	39672	79618	6.18%	0.746%
10	2.971	300	309	324	rVV	224363	603315	46.82%	5.653%
11	3.117	324	333	347	rVB	182013	428818	33.28%	4.018%
12	3.763	429	439	448	rBV3	25151	66859	5.19%	0.626%
13	5.391	693	706	717	rBV2	149421	431647	33.49%	4.045%
14	5.556	723	733	749	rVB2	270196	766468	59.48%	7.182%
15	5.958	788	799	806	rBV	155656	417707	32.41%	3.914%
16	6.043	806	813	830	rVB	218394	581796	45.15%	5.451%
17	6.245	834	846	858	rBV	144642	428612	33.26%	4.016%
18	6.763	920	931	951	rVB	413721	984359	76.38%	9.223%
19	8.433	1199	1205	1212	rVV	14419	25260	1.96%	0.237%
20	8.506	1212	1217	1225	rVB3	8194	14537	1.13%	0.136%
21	8.653	1233	1241	1248	rBV	832915	1288692	100.00%	12.075%
22	8.720	1248	1252	1260	rVB2	10797	19065	1.48%	0.179%
23	9.445	1365	1371	1378	rBV2	10731	19306	1.50%	0.181%
24	10.055	1466	1471	1484	rVB	828276	1096702	85.10%	10.276%
25	10.878	1600	1606	1614	rBV	14464	23852	1.85%	0.223%
26	11.085	1634	1640	1649	rBV	622509	799978	62.08%	7.496%
27	11.171	1649	1654	1661	rVB2	23360	31818	2.47%	0.298%
28	11.494	1702	1707	1714	rVB	16088	23048	1.79%	0.216%
29	12.024	1788	1794	1804	rBV	817667	982991	76.28%	9.211%

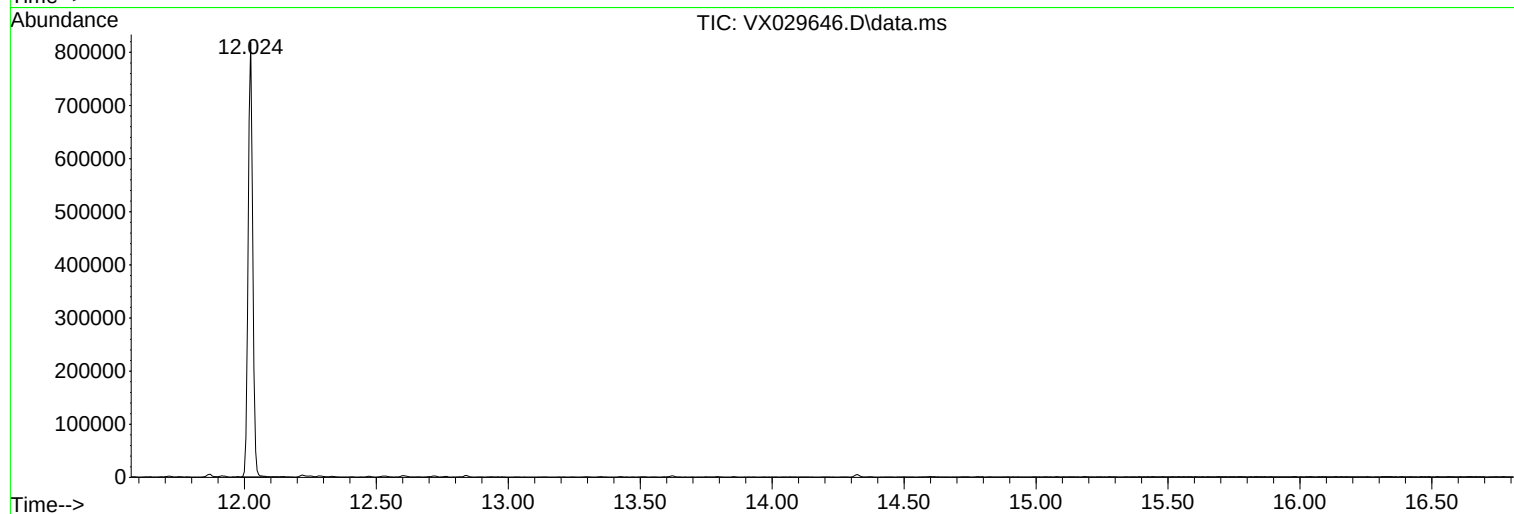
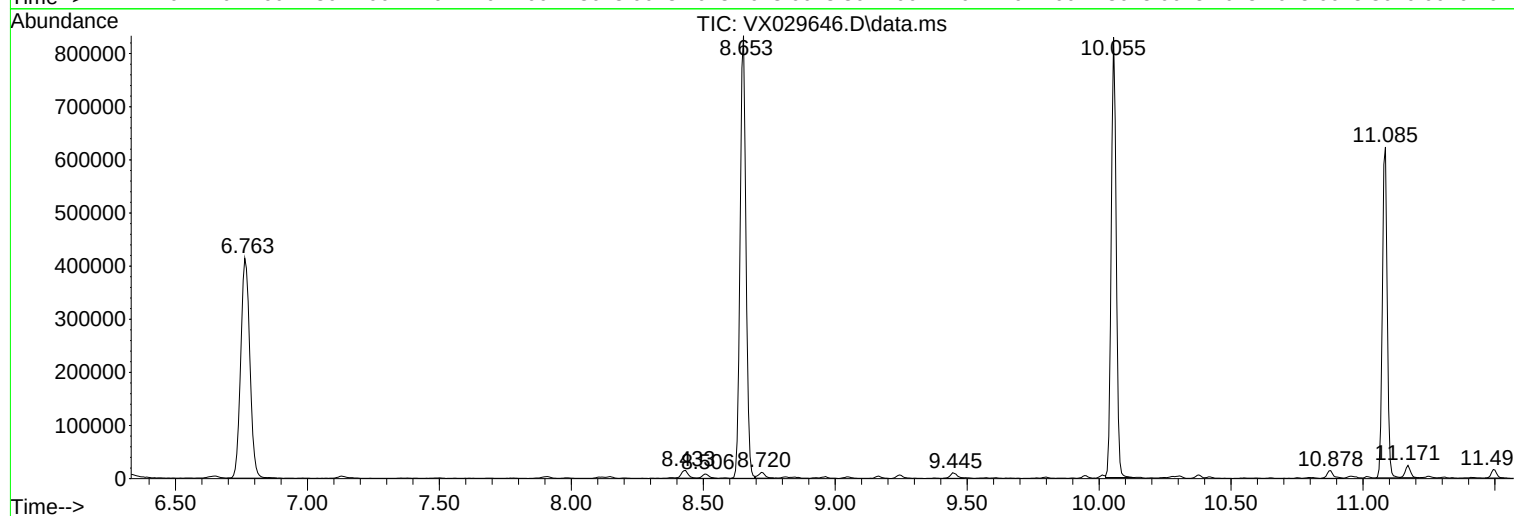
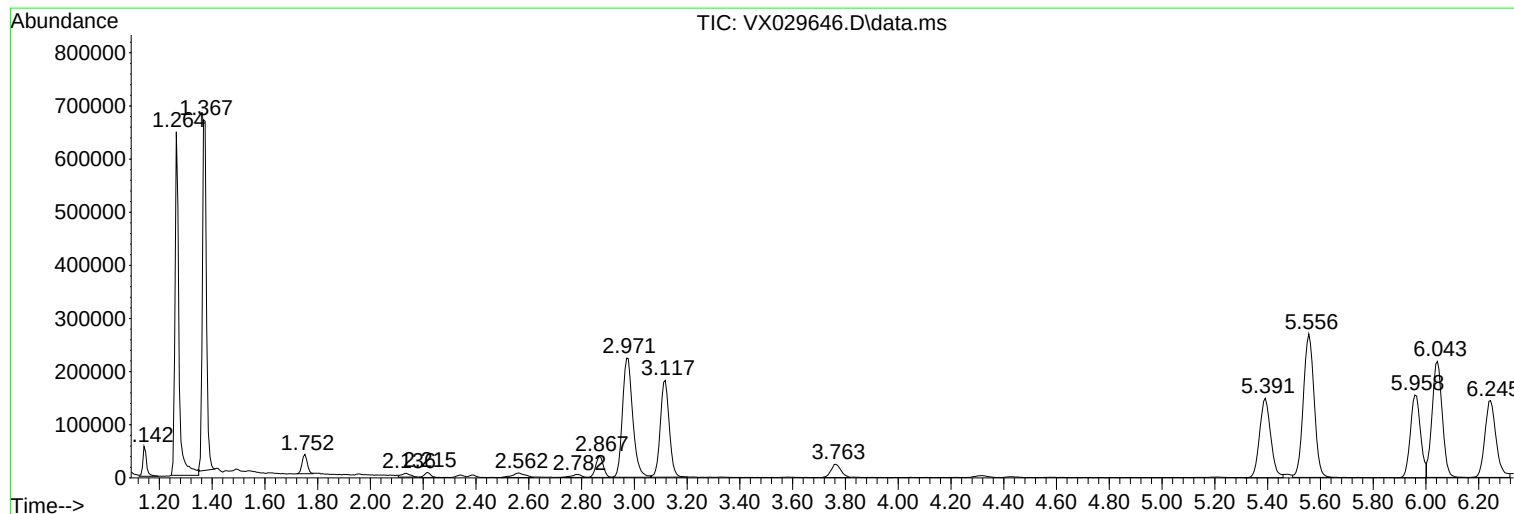
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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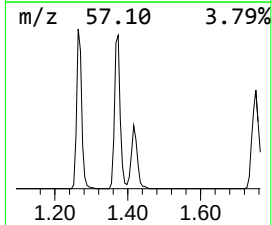
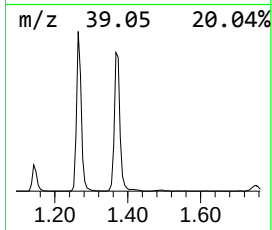
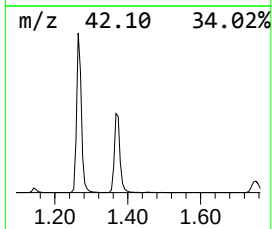
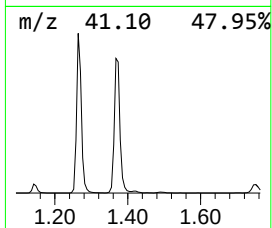
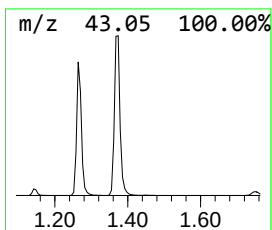
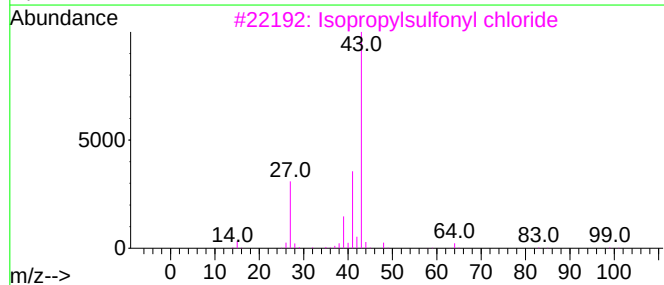
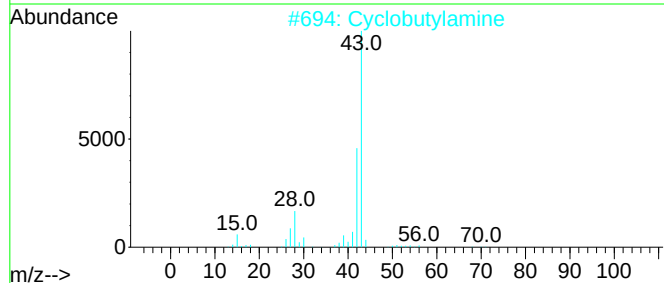
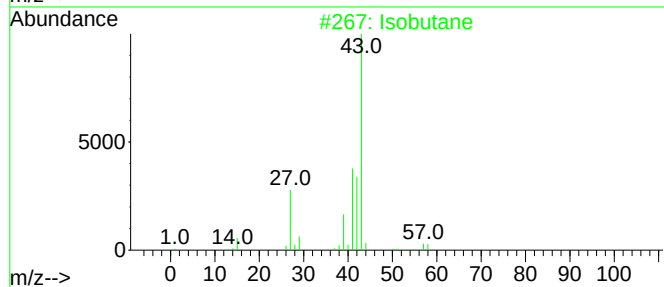
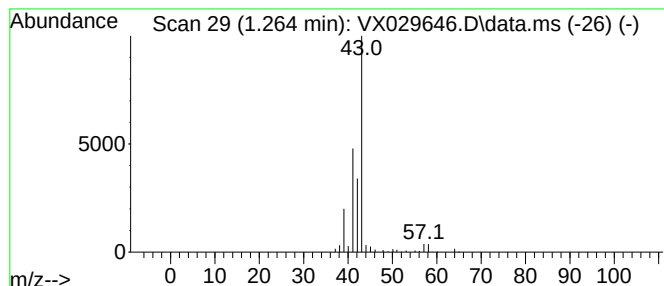
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	43.51 ug/l	667043	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	80
2		Cyclobutylamine	71	C4H9N	002516-34-9	9
3		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4		Hydrogen isocyanate	43	CHNO	000075-13-8	4
5		Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4



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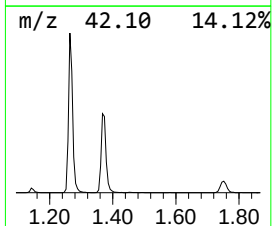
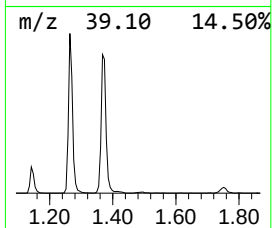
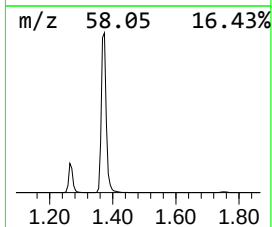
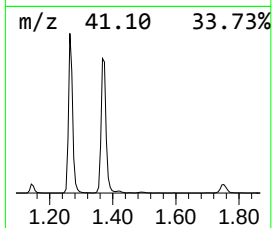
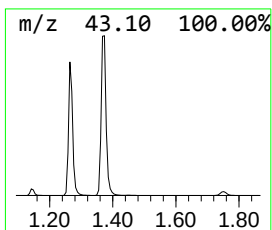
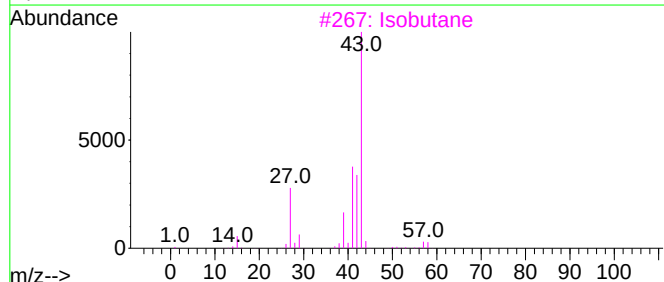
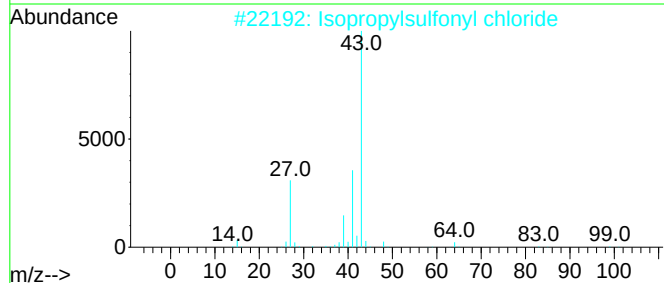
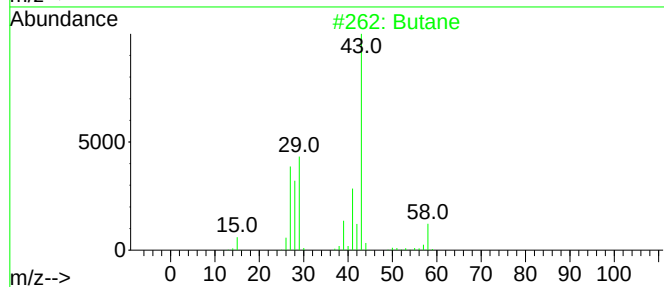
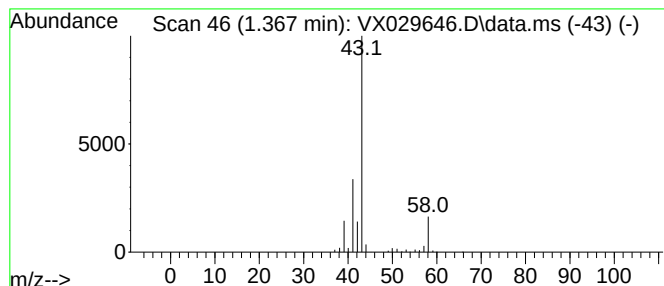
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	46.36 ug/l	710721	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Acetone	58	C3H6O	000067-64-1	4



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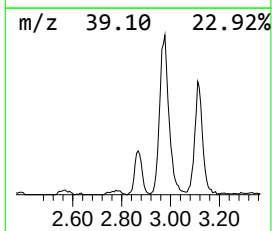
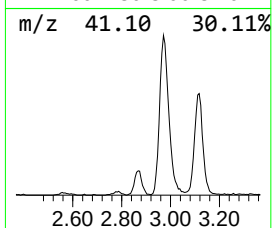
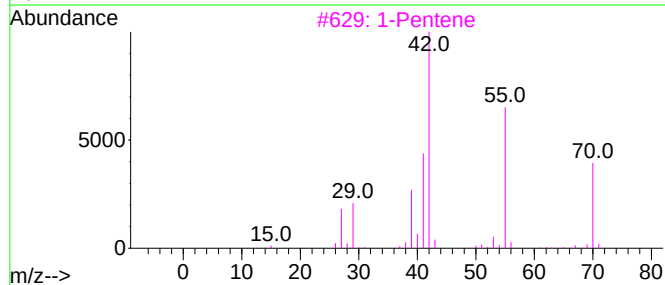
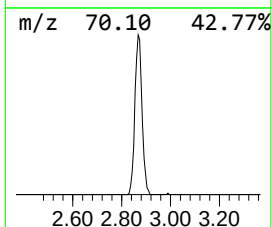
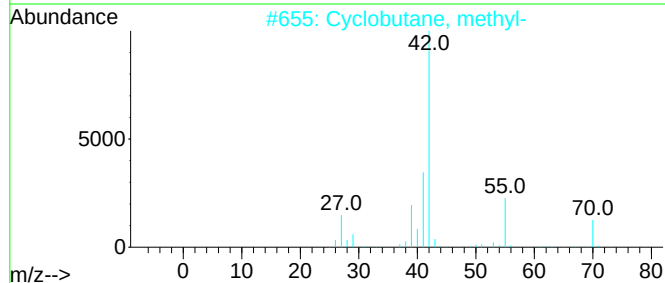
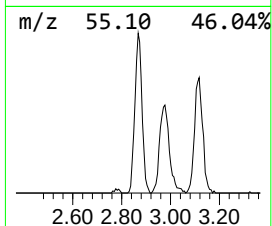
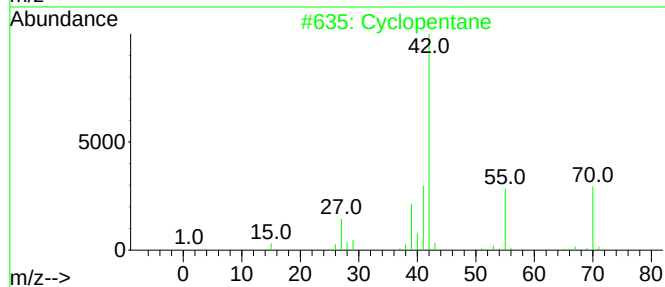
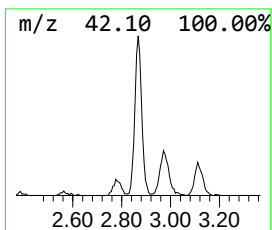
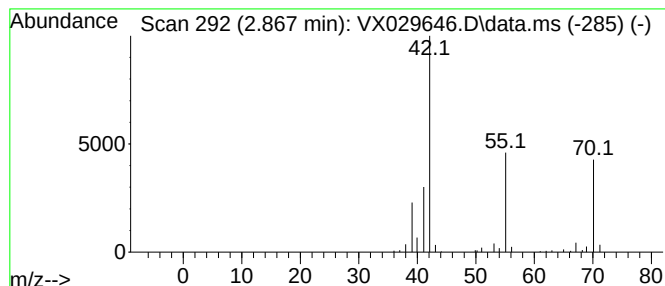
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Peak Number 3 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	5.19 ug/l	79618	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	78
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	78
3			1-Pentene	70	C5H10	000109-67-1	72
4			Methyl propargyl ether	70	C4H6O	000627-41-8	9
5			Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	9



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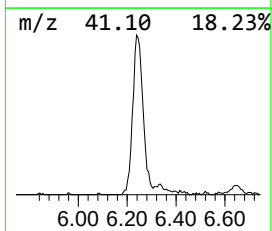
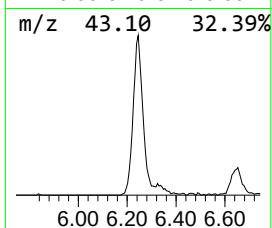
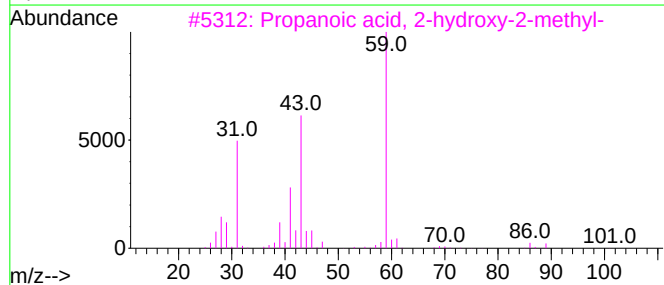
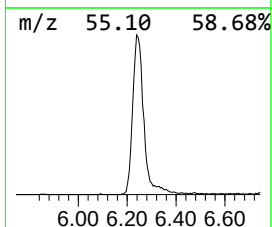
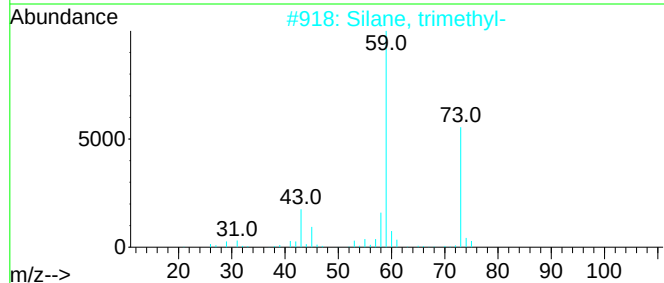
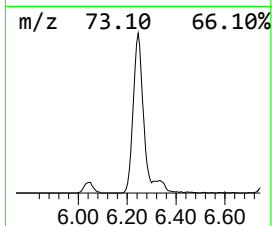
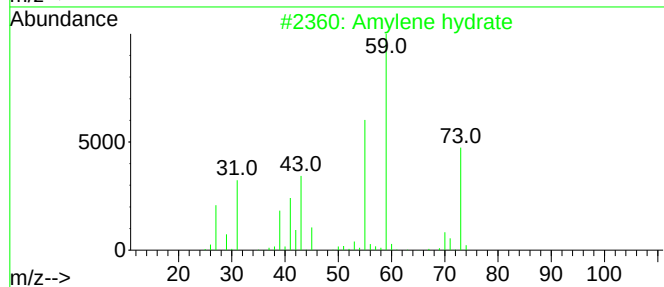
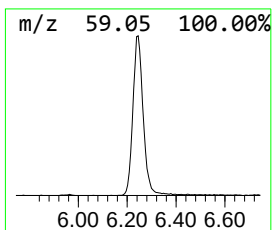
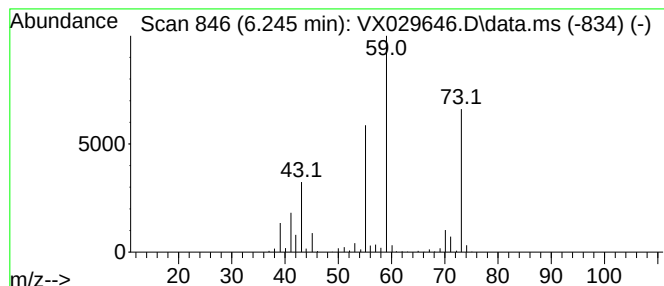
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Peak Number 4 Amylene hydrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	21.77 ug/l	428612	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			Silane, trimethyl-	74	C3H10Si	000993-07-7	38
3			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	33
4			Butanamide	87	C4H9NO	000541-35-5	9
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isobutane	1.264	43.5	ug/l	667043	1	5.556	766468	50.0
Butane	1.367	46.4	ug/l	710721	1	5.556	766468	50.0
Cyclopentane	2.867	5.2	ug/l	79618	1	5.556	766468	50.0
Amylene hydrate	6.245	21.8	ug/l	428612	2	6.763	984359	50.0