

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062922\
 Data File : VX029893.D
 Acq On : 30 Jun 2022 04:50
 Operator : JC/MD
 Sample : N3481-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-30

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\82X062822W.M
 Title : SW846 8260

Signal : TIC: VX029893.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	24	30	43	rBV	213544	644425	49.17%	6.137%
2	1.367	43	46	51	rVV2	62265	87256	6.66%	0.831%
3	1.752	104	109	118	rVB	59955	83641	6.38%	0.797%
4	1.953	138	142	151	rVB	21890	30600	2.33%	0.291%
5	2.136	168	172	181	rVB4	9662	21385	1.63%	0.204%
6	2.215	181	185	194	rVB	25121	37445	2.86%	0.357%
7	2.751	266	273	278	rBV3	12972	29970	2.29%	0.285%
8	2.825	281	285	288	rVV4	9492	17989	1.37%	0.171%
9	2.867	288	292	301	rVV2	18712	38063	2.90%	0.362%
10	2.971	301	309	323	rVV	68592	179793	13.72%	1.712%
11	3.117	323	333	345	rVB	405189	927775	70.79%	8.835%
12	3.763	428	439	448	rBV2	18296	51472	3.93%	0.490%
13	4.306	519	528	541	rVB2	18520	52223	3.98%	0.497%
14	5.391	693	706	716	rBV2	125653	363756	27.76%	3.464%
15	5.556	724	733	755	rVB	225033	646319	49.32%	6.155%
16	5.958	789	799	805	rBV	138259	364141	27.78%	3.468%
17	6.043	805	813	831	rVB	471924	1310582	100.00%	12.481%
18	6.251	842	847	854	rVB3	7348	19858	1.52%	0.189%
19	6.763	921	931	944	rBV	360062	866937	66.15%	8.256%
20	7.385	1022	1033	1041	rBV6	7493	18141	1.38%	0.173%
21	8.653	1234	1241	1248	rVV	739665	1158956	88.43%	11.037%
22	8.720	1248	1252	1260	rVB	55123	90717	6.92%	0.864%
23	9.963	1451	1456	1463	rBV2	8726	14472	1.10%	0.138%
24	10.055	1463	1471	1482	rVV	737654	977633	74.60%	9.310%
25	10.195	1489	1494	1500	rVB	172381	218766	16.69%	2.083%
26	10.305	1507	1512	1520	rVB	121150	152541	11.64%	1.453%
27	10.640	1563	1567	1576	rVB	16112	21846	1.67%	0.208%
28	11.085	1633	1640	1650	rBV	536121	687767	52.48%	6.550%
29	11.305	1672	1676	1683	rVB	24193	31834	2.43%	0.303%
30	11.402	1685	1692	1696	rBV	26726	45495	3.47%	0.433%
31	11.451	1696	1700	1707	rVB	18492	26199	2.00%	0.249%
32	11.616	1721	1727	1733	rBV	13481	17091	1.30%	0.163%
33	11.756	1745	1750	1756	rBV	47247	60471	4.61%	0.576%
34	12.024	1788	1794	1800	rBV	702082	874485	66.72%	8.328%
35	12.091	1800	1805	1811	rVB	22013	29757	2.27%	0.283%
36	12.244	1822	1830	1838	rBV3	46941	80091	6.11%	0.763%

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Title : SW846 8260

37	12.317	1838	1842	1849	rVB4	9617	15624	1.19%	0.149%
38	12.701	1901	1905	1913	rVB2	12570	18026	1.38%	0.172%
39	12.963	1945	1948	1956	rVB	10296	13329	1.02%	0.127%
40	13.292	1997	2002	2007	rVB3	23400	29775	2.27%	0.284%
41	13.774	2076	2081	2088	rBV	96392	127347	9.72%	1.213%
42	14.780	2241	2246	2253	rBV	12427	16855	1.29%	0.161%

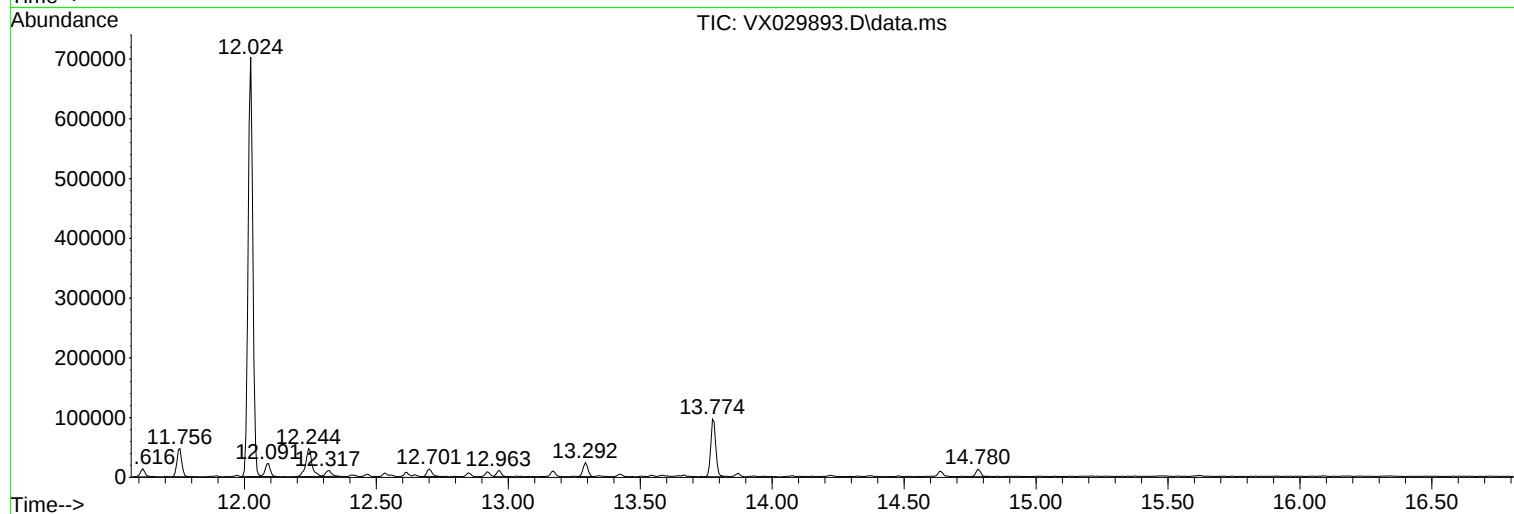
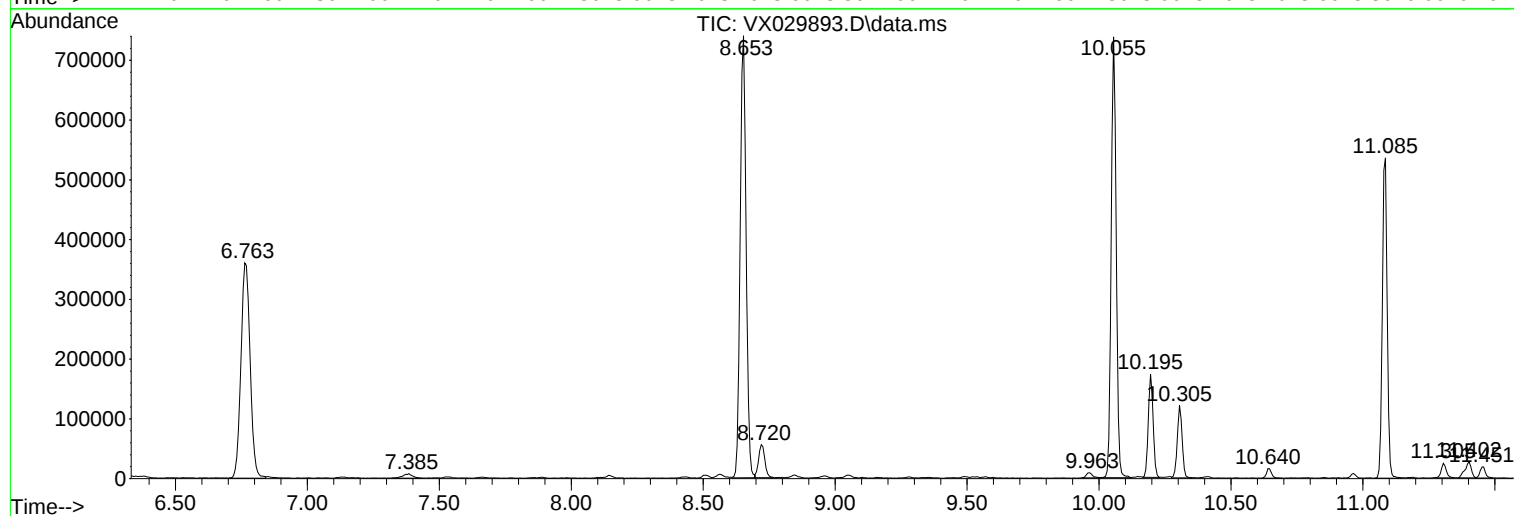
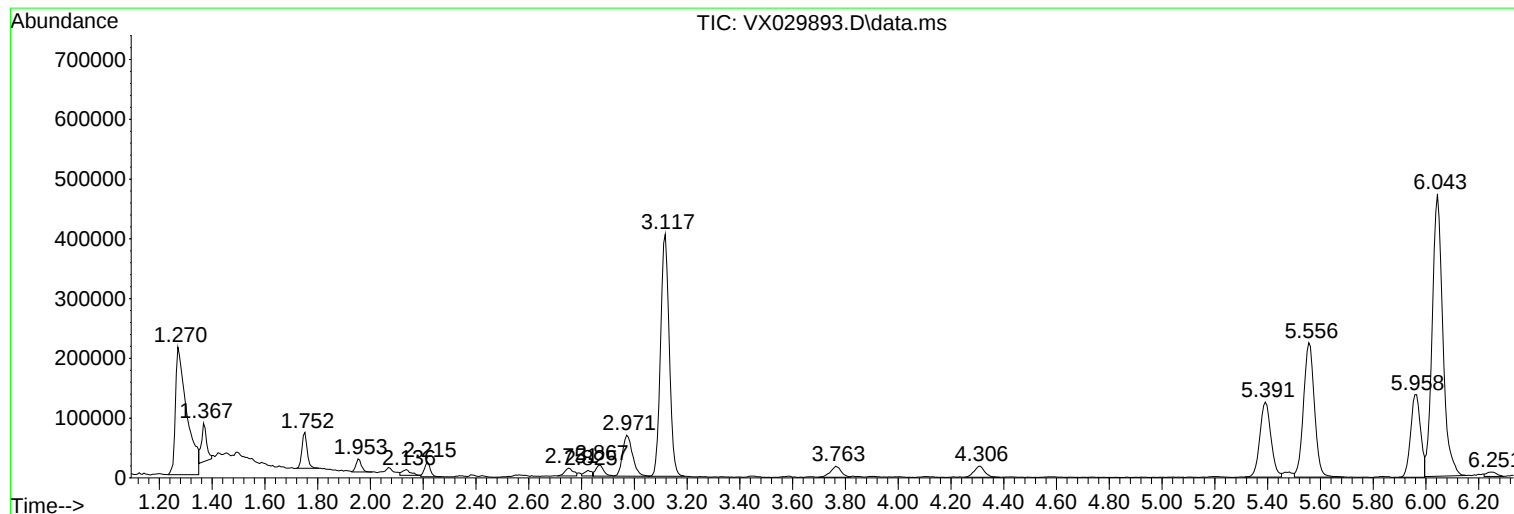
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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



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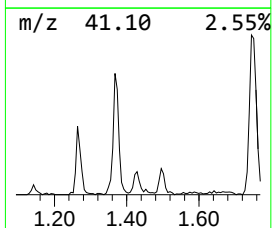
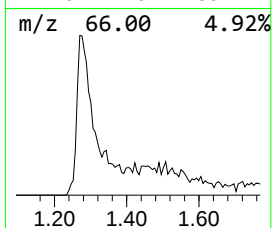
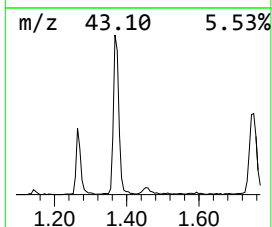
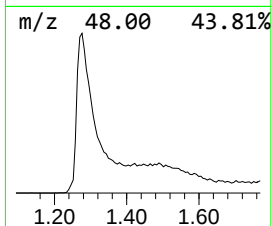
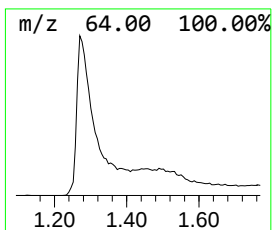
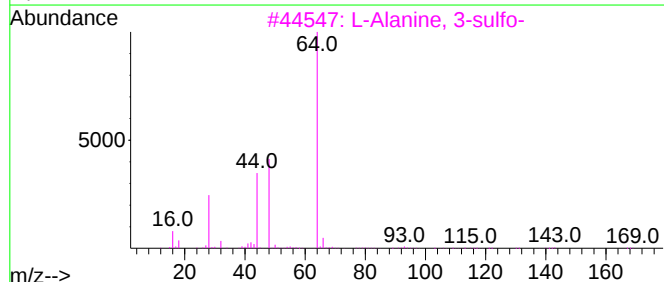
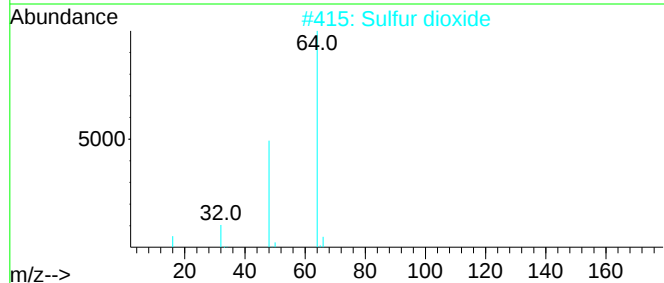
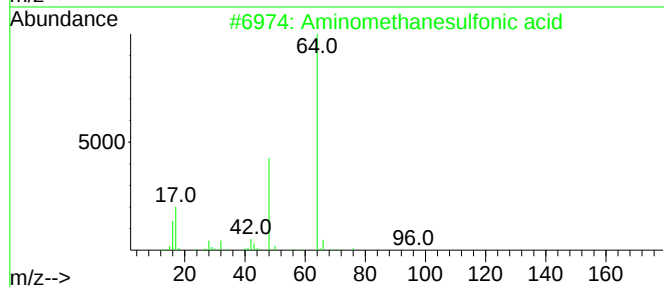
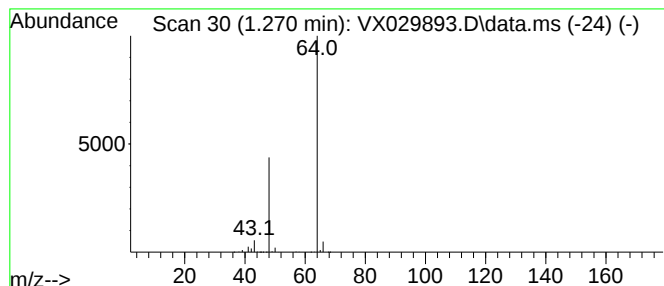
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	49.85 ug/l	644425	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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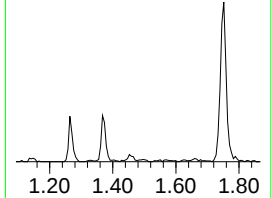
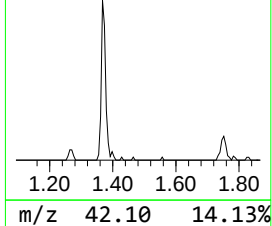
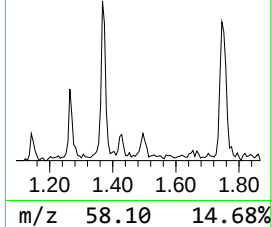
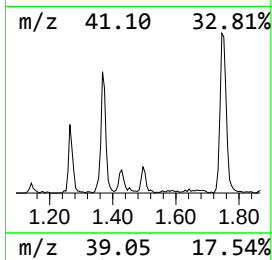
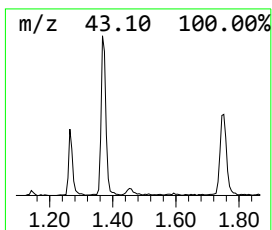
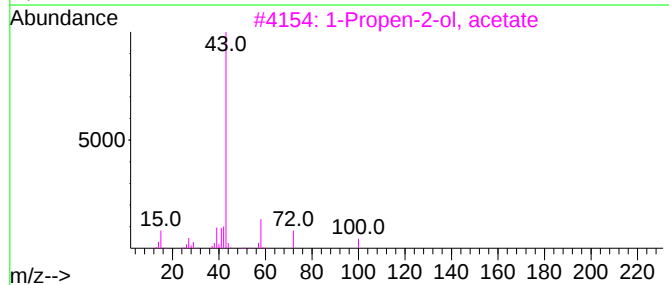
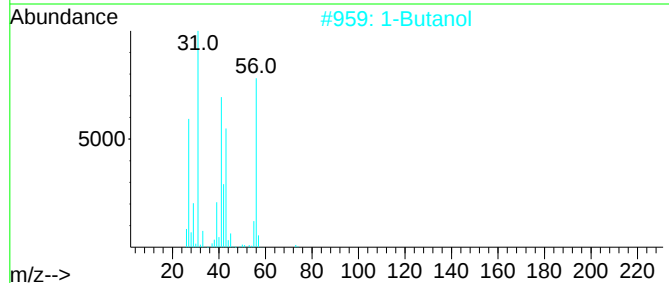
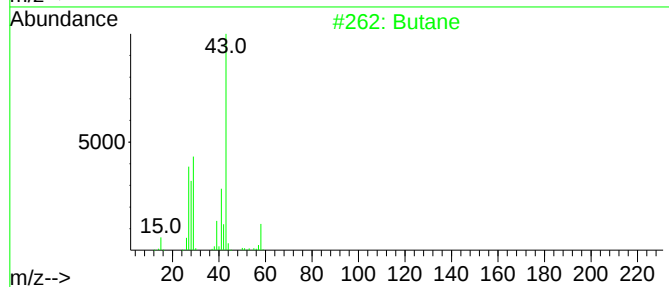
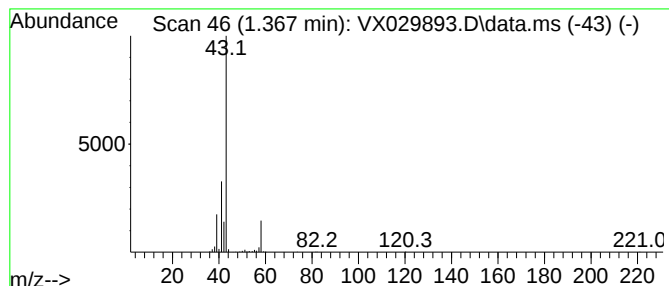
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	6.75 ug/l	87256	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	59
2			1-Butanol	74	C4H10O	000071-36-3	9
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	5



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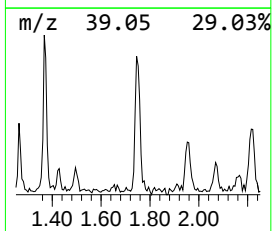
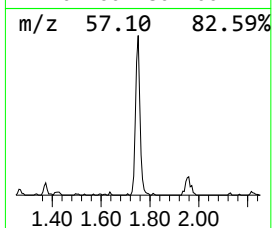
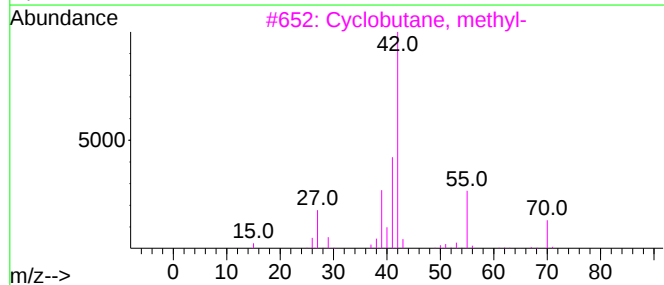
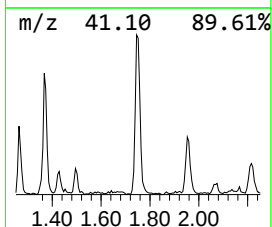
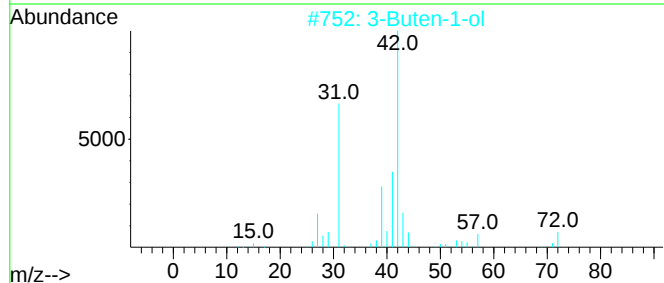
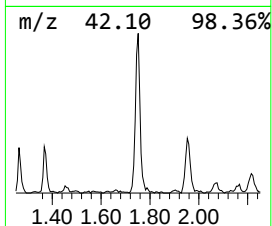
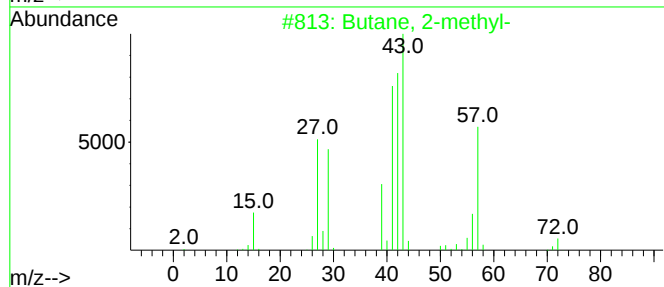
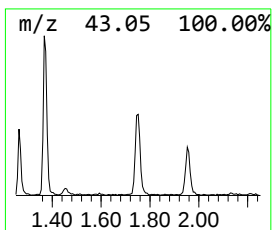
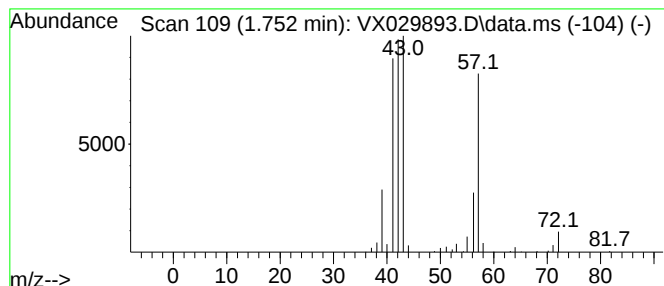
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Peak Number 3 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	6.47 ug/l	83641	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	43
4			Isobutylene epoxide	72	C4H8O	000558-30-5	38
5			Pentane	72	C5H12	000109-66-0	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.270	49.9	ug/l	644425	1	5.556	646319	50.0
Butane	1.367	6.8	ug/l	87256	1	5.556	646319	50.0
Butane, 2-methyl-	1.752	6.5	ug/l	83641	1	5.556	646319	50.0