

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111821\
 Data File : VN069556.D
 Acq On : 18 Nov 2021 16:34
 Operator : JC/MD
 Sample : M4739-03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-14

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_N\methods\82N110921W.M
 Title : SW846 8260

Signal : TIC: VN069556.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.258	85	100	109	rBV6	37613	88111	1.04%	0.147%
2	2.443	160	169	185	rVB	151997	236247	2.80%	0.394%
3	3.140	412	429	454	rVB2	529116	1183008	14.02%	1.972%
4	4.291	816	858	889	rBV4	118278	571786	6.78%	0.953%
5	4.594	950	971	996	rBV	39681	130957	1.55%	0.218%
6	5.076	1125	1151	1174	rBV2	214946	850689	10.08%	1.418%
7	5.390	1242	1268	1302	rBV3	56106	201200	2.39%	0.335%
8	5.621	1321	1354	1389	rBV2	580745	2053768	24.35%	3.423%
9	6.501	1652	1682	1712	rBV2	1473562	4724794	56.01%	7.874%
10	7.045	1867	1885	1905	rBV4	60778	177637	2.11%	0.296%
11	7.147	1905	1923	1940	rVV2	54166	158361	1.88%	0.264%
12	7.327	1972	1990	2019	rVB6	37285	119695	1.42%	0.199%
13	7.847	2172	2184	2203	rVB6	37699	92886	1.10%	0.155%
14	8.027	2224	2251	2261	rBV2	957368	2296705	27.23%	3.828%
15	8.088	2262	2274	2297	rVB	1841880	4191299	49.68%	6.985%
16	8.440	2386	2405	2429	rBV	1165409	2809744	33.31%	4.683%
17	8.542	2430	2443	2458	rVV7	126503	352619	4.18%	0.588%
18	8.619	2462	2472	2494	rVB2	170936	452410	5.36%	0.754%
19	8.971	2582	2603	2632	rBV	2899986	6111078	72.44%	10.185%
20	9.424	2756	2772	2782	rBV8	45018	112135	1.33%	0.187%
21	9.885	2930	2944	2960	rVB2	104471	205934	2.44%	0.343%
22	10.017	2982	2993	3021	rVB2	205310	456858	5.42%	0.761%
23	10.207	3048	3064	3066	rBV3	104148	154068	1.83%	0.257%
24	10.443	3134	3152	3183	rBV	4492078	8435906	100.00%	14.059%
25	10.556	3184	3194	3207	rVB	117622	220925	2.62%	0.368%
26	10.644	3213	3227	3241	rBV	823064	1459631	17.30%	2.433%
27	10.719	3241	3255	3273	rVB	929798	1647729	19.53%	2.746%
28	10.859	3294	3307	3328	rVB3	95177	200556	2.38%	0.334%
29	11.620	3572	3591	3613	rBV5	81097	217141	2.57%	0.362%
30	11.747	3621	3638	3671	rBV	4400585	8015406	95.02%	13.358%
31	11.865	3671	3682	3699	rVB6	68681	160728	1.91%	0.268%
32	12.581	3941	3949	3967	rVB4	50541	100164	1.19%	0.167%
33	12.733	3989	4006	4035	rBV	3155579	5616440	66.58%	9.360%
34	12.849	4040	4049	4065	rVV6	50494	128655	1.53%	0.214%
35	12.921	4069	4076	4099	rVB	46595	90837	1.08%	0.151%
36	13.678	4341	4358	4382	rBV	3322422	5843492	69.27%	9.739%

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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	13.879	4422	4433	4449	rVB2	73371	133552	1.58%	0.223%
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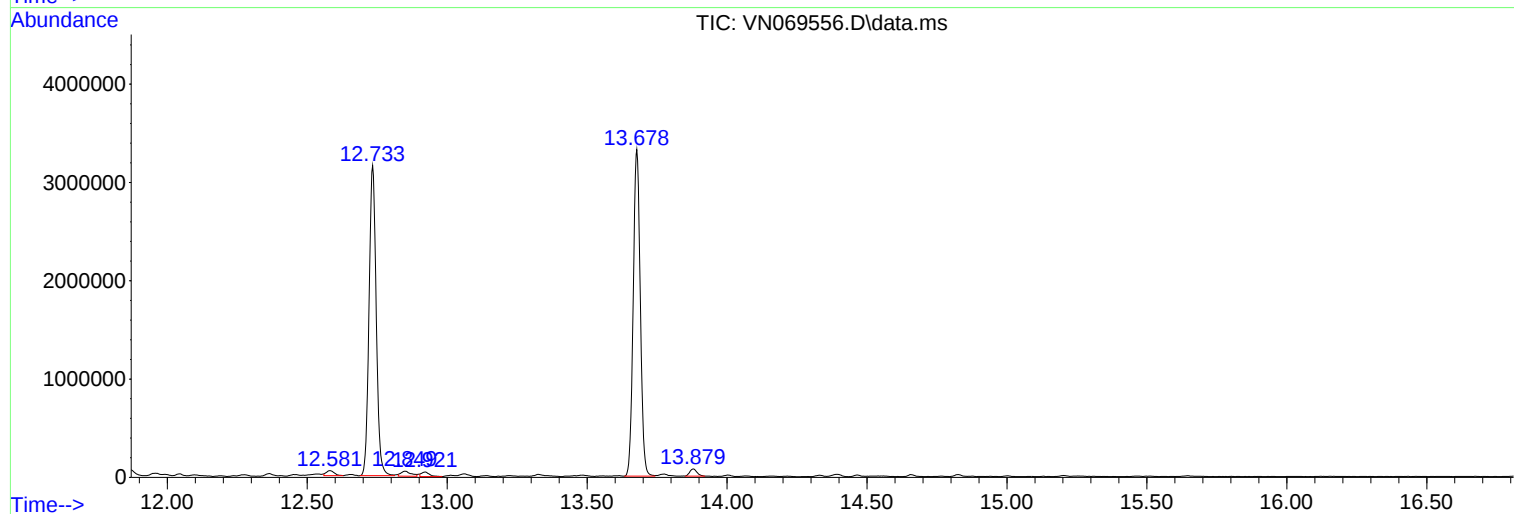
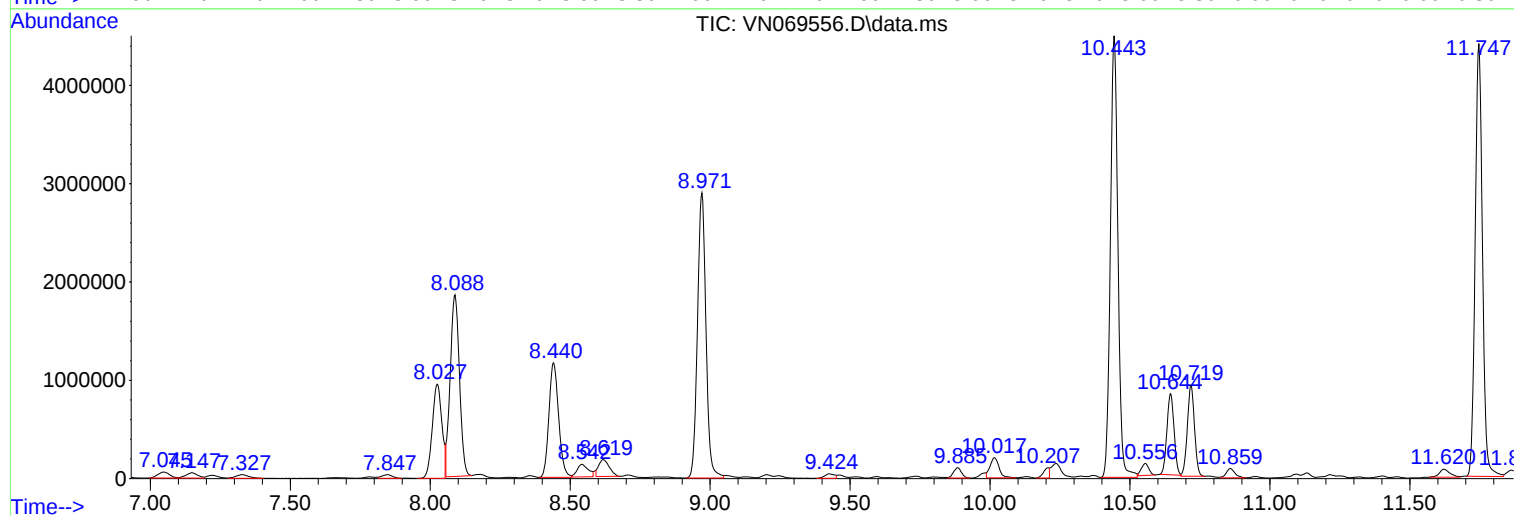
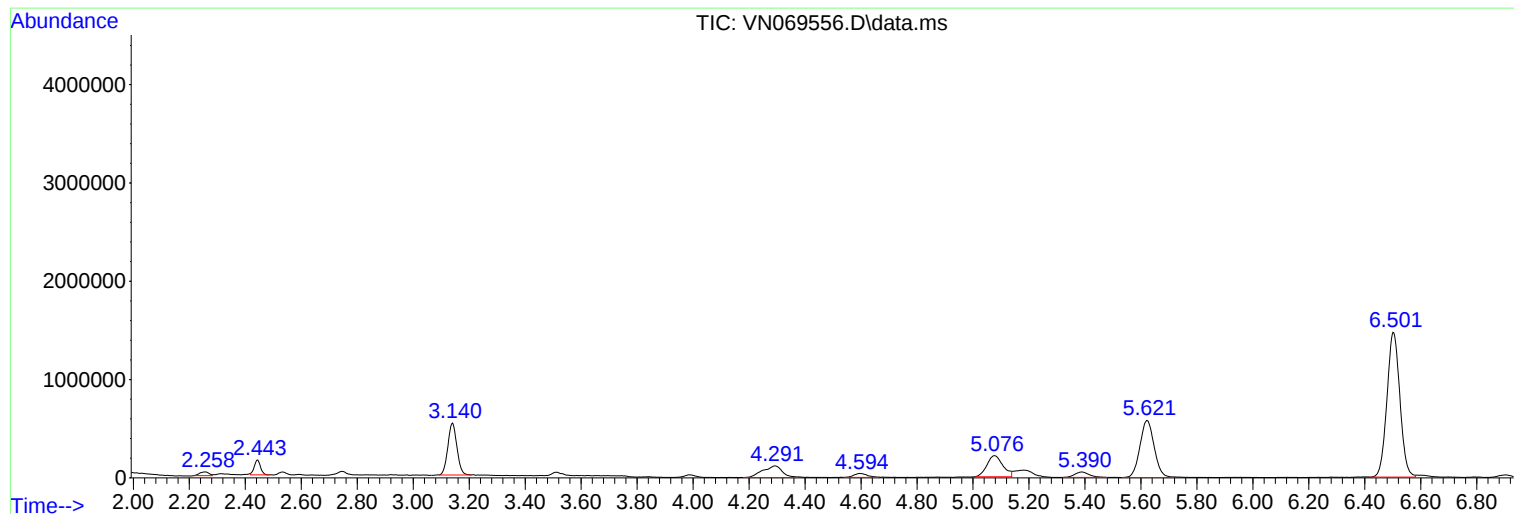
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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



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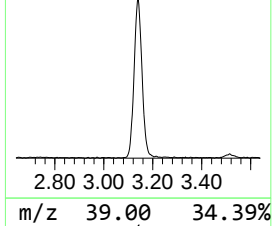
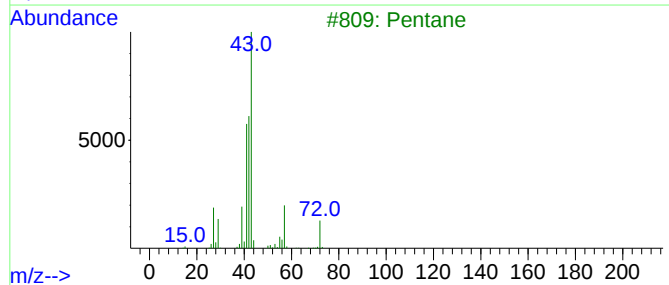
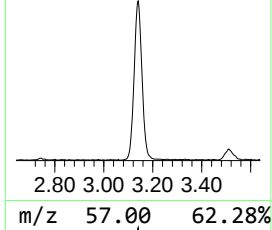
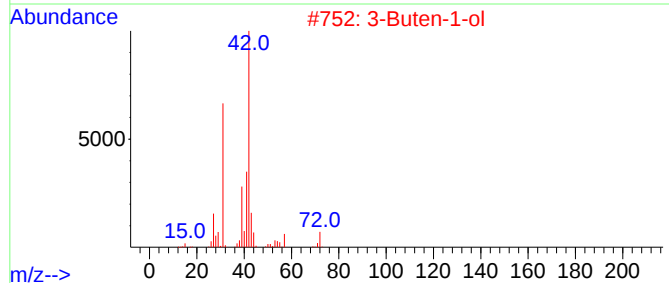
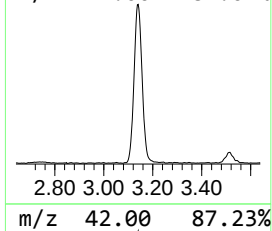
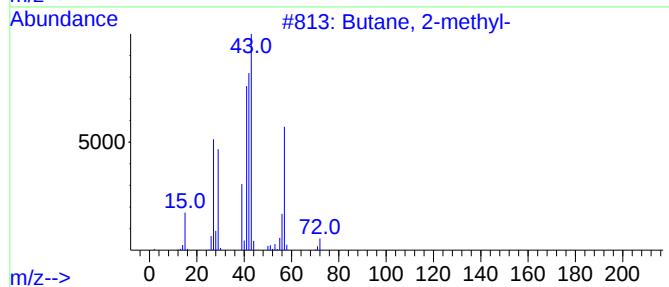
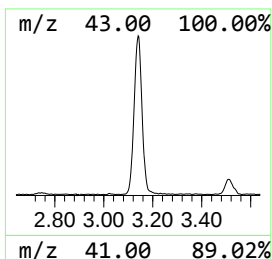
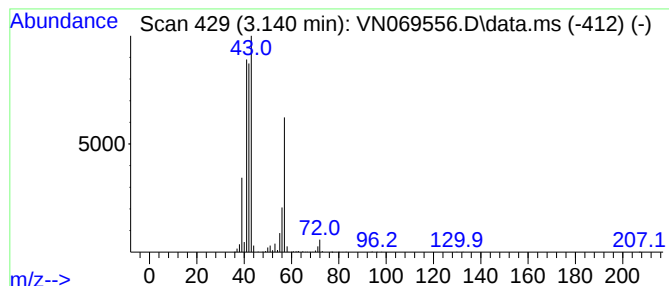
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	14.11 ug/l	1183010	Pentafluorobenzene	8.088

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	47
3			Pentane	72	C5H12	000109-66-0	36
4			Butane, 1-isocyano-	83	C5H9N	002769-64-4	16
5			1-Butene	56	C4H8	000106-98-9	14



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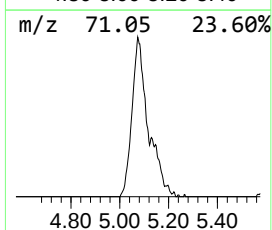
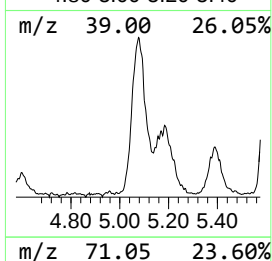
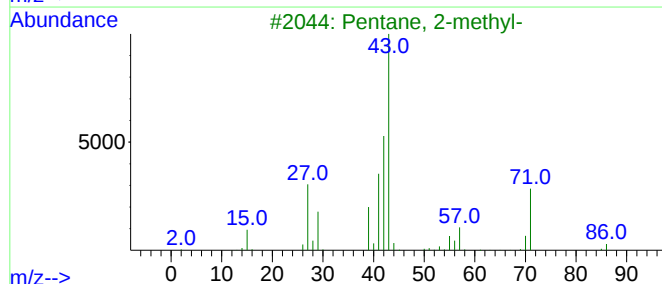
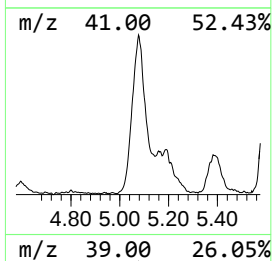
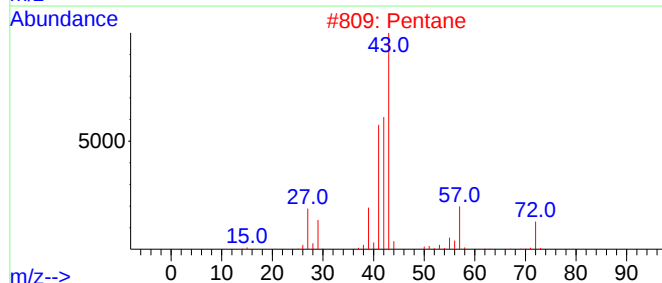
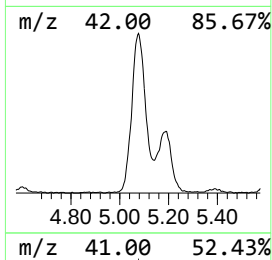
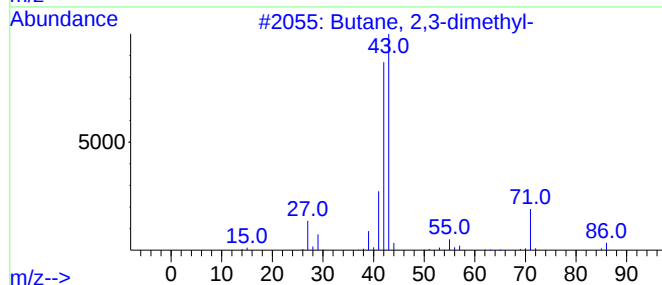
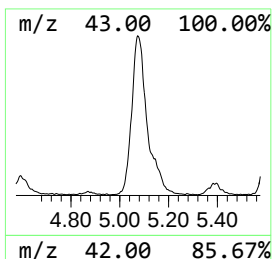
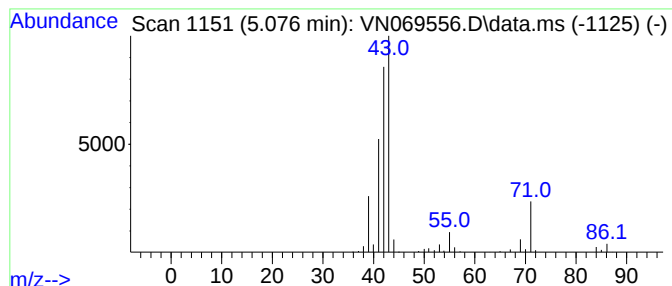
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.076	10.15 ug/l	850689	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2			Pentane	72	C5H12	000109-66-0	17
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	17
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	12
5			Pyrrolidine	71	C4H9N	000123-75-1	9



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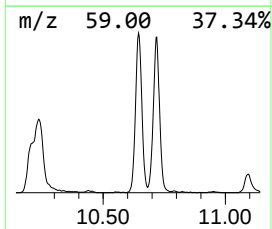
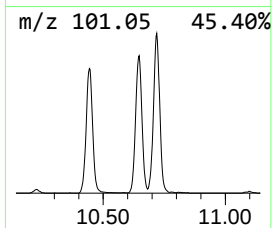
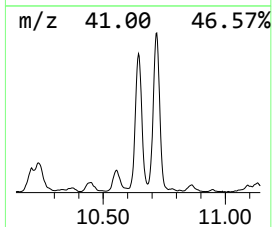
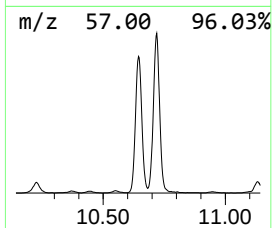
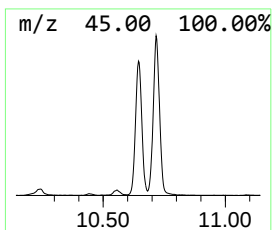
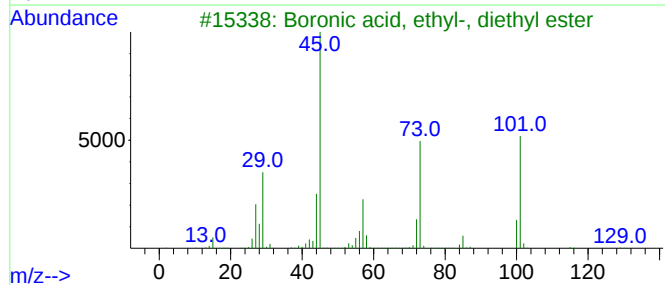
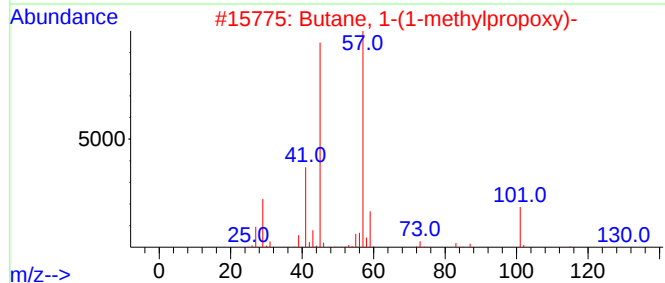
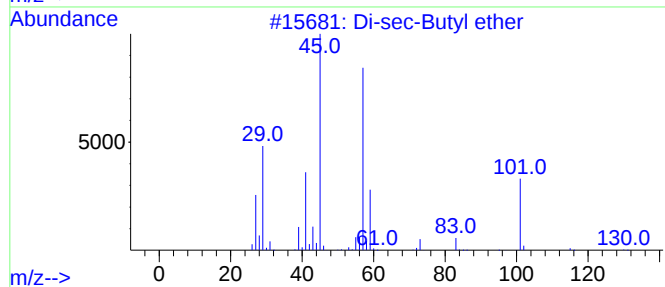
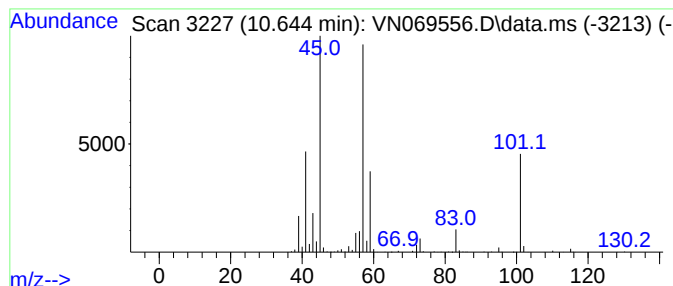
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Di-sec-Butyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.644	9.11 ug/l	1459630	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	56
3			Boronic acid, ethyl-, diethyl ester	130	C6H15B02	053907-92-9	42
4			trans-2-Hexenyl lactate	172	C9H16O3	1000431-56-9	37
5			Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	33



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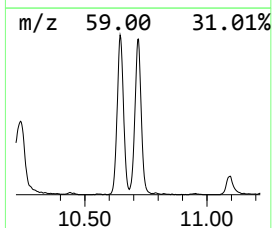
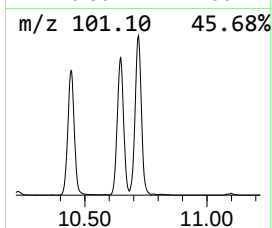
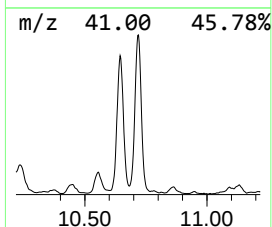
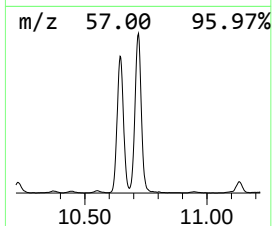
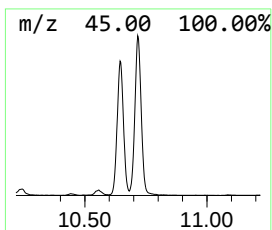
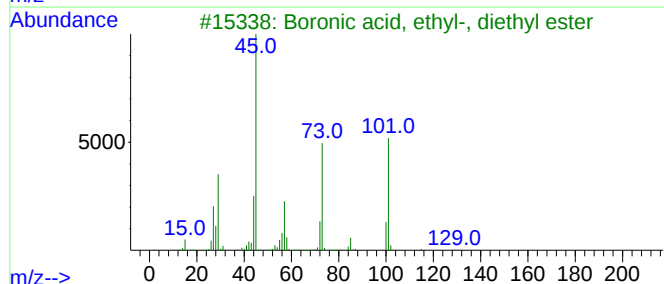
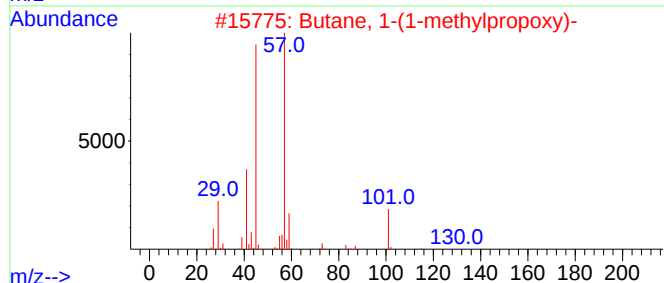
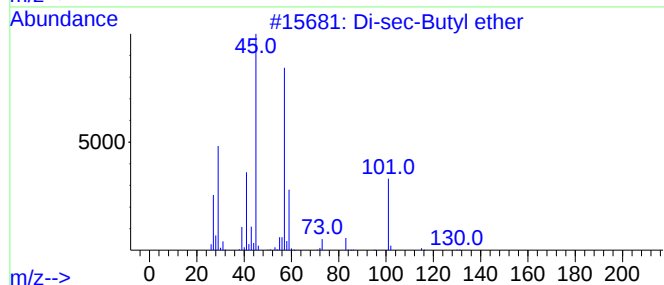
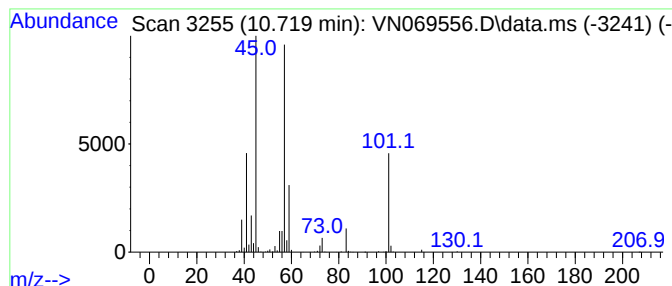
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 1-(1-methylpropoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.719	10.28 ug/l	1647730	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	64
3			Boronic acid, ethyl-, diethyl ester	130	C6H15B02	053907-92-9	45
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38
5			Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	33



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.140	14.1	ug/l	1183010	1	8.088	4191300	50.0
Butane, 2,3-dim...	5.076	10.2	ug/l	850689	1	8.088	4191300	50.0
Di-sec-Butyl ether	10.644	9.1	ug/l	1459630	3	11.746	8015410	50.0
Butane, 1-(1-me...	10.719	10.3	ug/l	1647730	3	11.746	8015410	50.0