

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111821\
 Data File : VN069554.D
 Acq On : 18 Nov 2021 15:43
 Operator : JC/MD
 Sample : M4739-01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-3R

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: VN069554.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.443	158	169	185	rVB	288313	466645	2.34%	0.549%
2	3.140	410	429	456	rBV2	872053	1992167	10.01%	2.343%
3	3.510	550	567	593	rBV4	388750	994432	4.99%	1.169%
4	5.079	1130	1152	1159	rBV3	76347	220415	1.11%	0.259%
5	5.621	1319	1354	1415	rBV	3636472	12769637	64.14%	15.016%
6	6.501	1660	1682	1705	rVB4	184137	627499	3.15%	0.738%
7	7.147	1902	1923	1945	rBV2	264761	773430	3.88%	0.909%
8	7.329	1968	1991	2022	rBV	273901	751907	3.78%	0.884%
9	8.024	2224	2250	2261	rBV	941520	2300356	11.55%	2.705%
10	8.088	2261	2274	2294	rVV	1894100	4445802	22.33%	5.228%
11	8.180	2297	2308	2332	rVB5	95177	245306	1.23%	0.288%
12	8.461	2385	2413	2439	rBV3	7831657	19910225	100.00%	23.413%
13	8.971	2581	2603	2650	rBV	2832195	6030953	30.29%	7.092%
14	9.217	2678	2695	2730	rVB6	110700	313184	1.57%	0.368%
15	9.459	2757	2785	2798	rBV6	106697	309449	1.55%	0.364%
16	9.883	2930	2943	2964	rVB4	113205	235563	1.18%	0.277%
17	10.017	2968	2993	3022	rBV2	147229	336669	1.69%	0.396%
18	10.443	3134	3152	3169	rBV	4404008	8251046	41.44%	9.702%
19	11.747	3619	3638	3660	rBV	4244462	7678549	38.57%	9.029%
20	11.846	3661	3675	3698	rVB	2338346	4030937	20.25%	4.740%
21	12.581	3936	3949	3966	rBV	160525	272062	1.37%	0.320%
22	12.734	3987	4006	4034	rBV	3108816	5557706	27.91%	6.535%
23	12.921	4061	4076	4092	rBV	316870	540784	2.72%	0.636%
24	13.678	4340	4358	4386	rBV	3390170	5985877	30.06%	7.039%

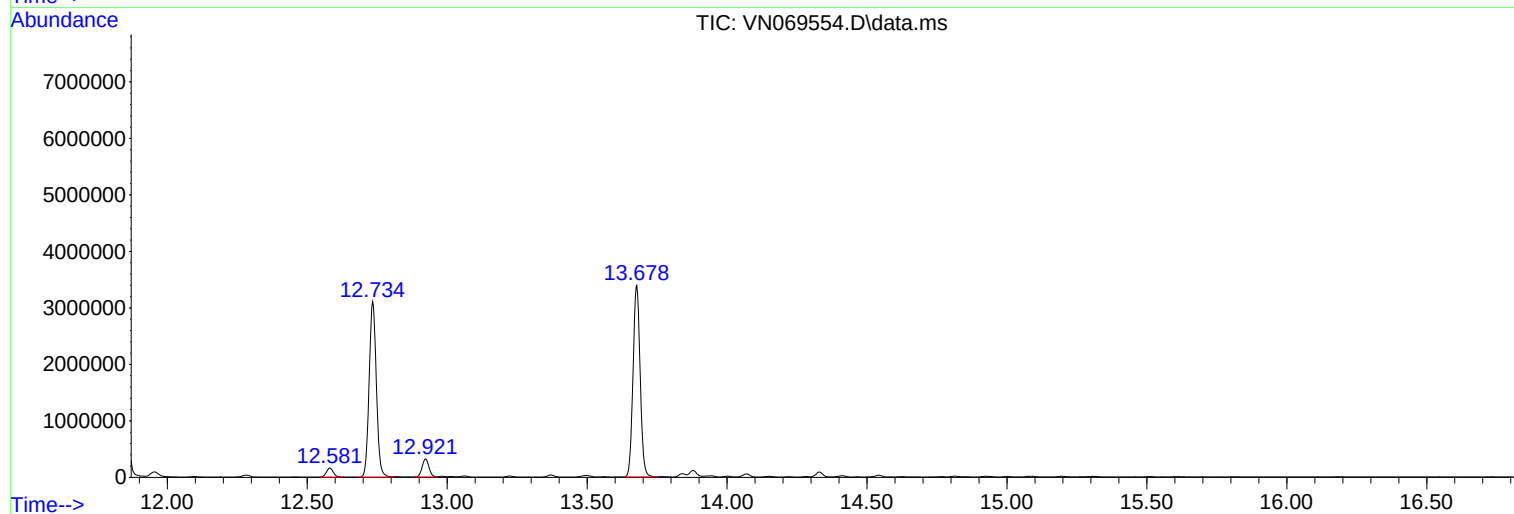
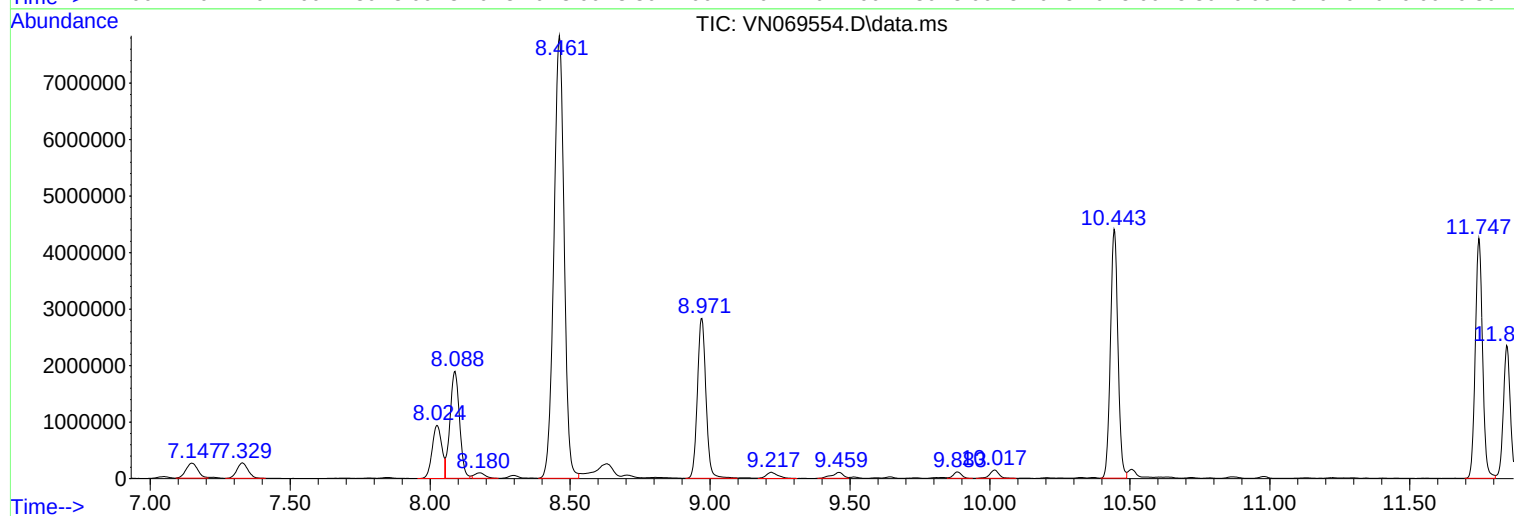
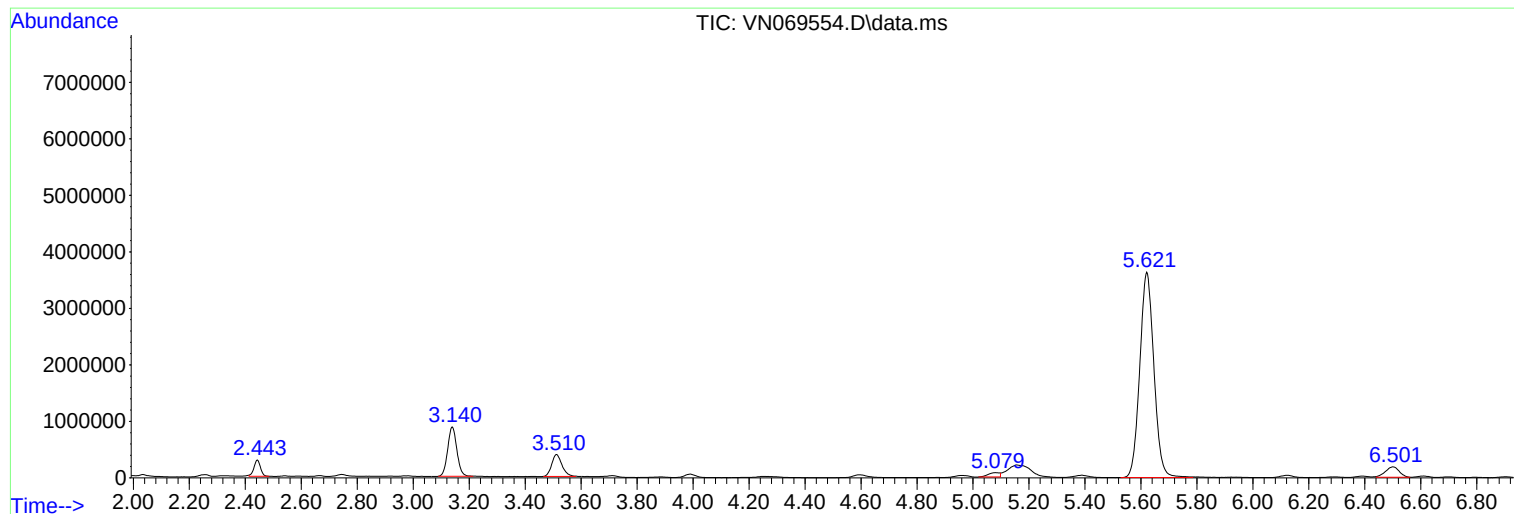
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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



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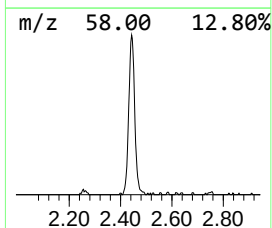
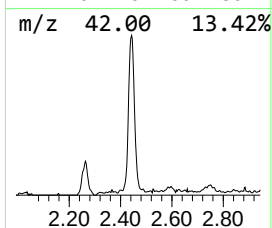
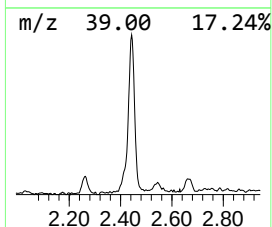
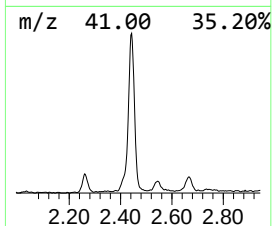
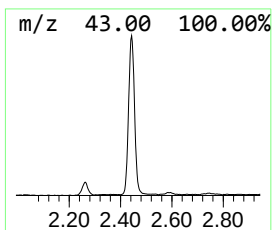
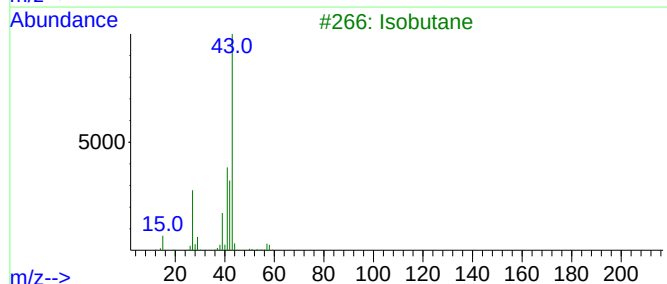
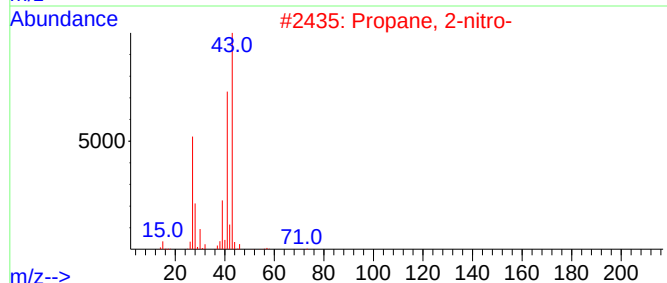
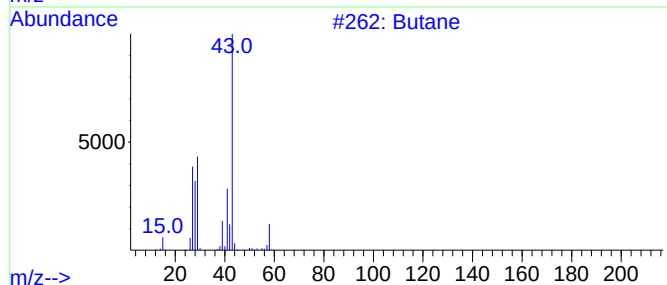
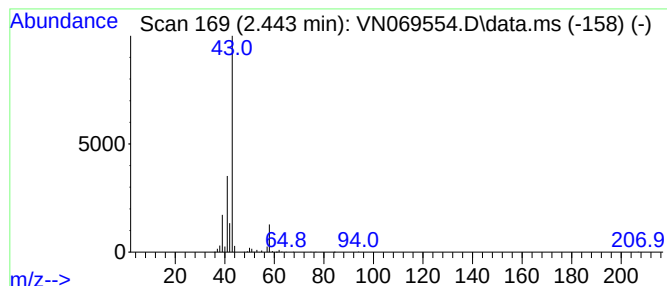
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.443	5.25 ug/l	466645	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	59
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9



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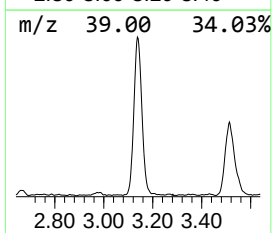
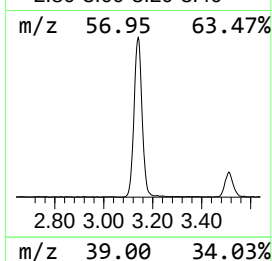
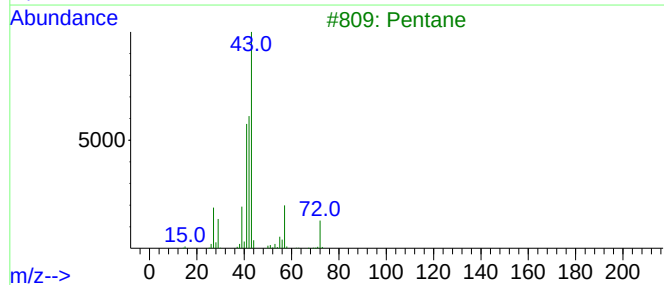
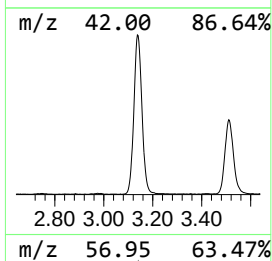
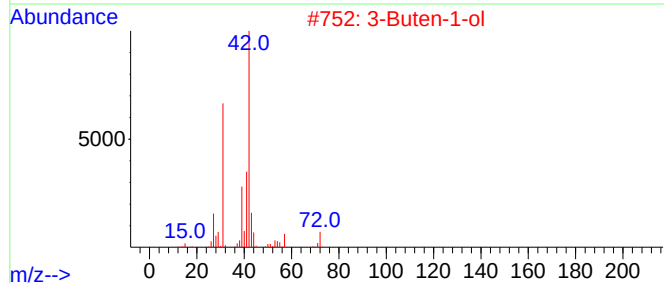
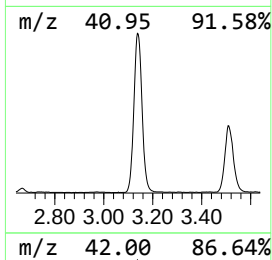
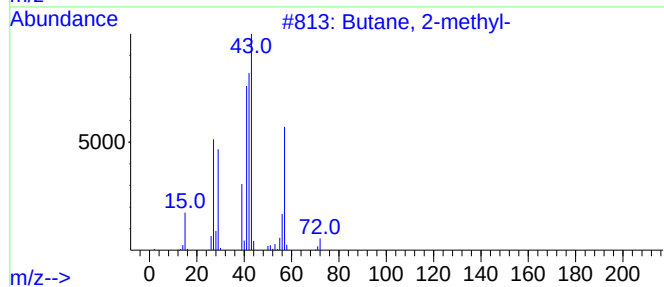
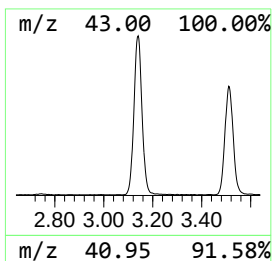
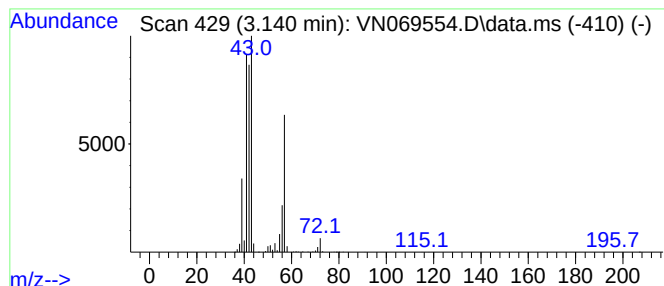
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	22.41 ug/l	1992170	Pentafluorobenzene	8.088

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	42
4			2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	25
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	14



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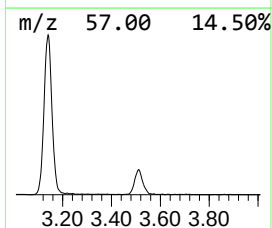
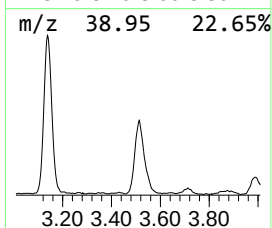
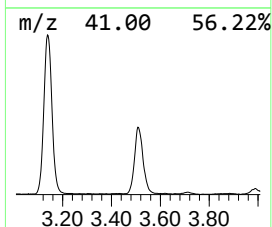
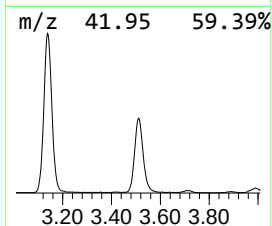
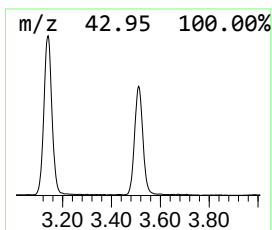
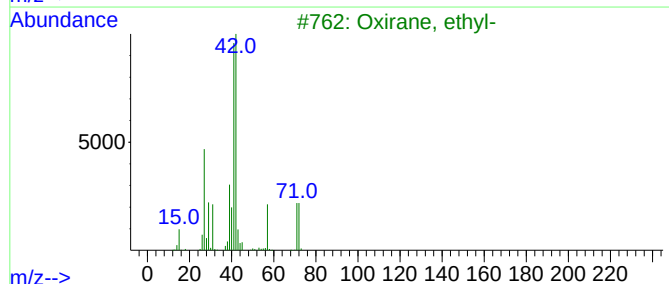
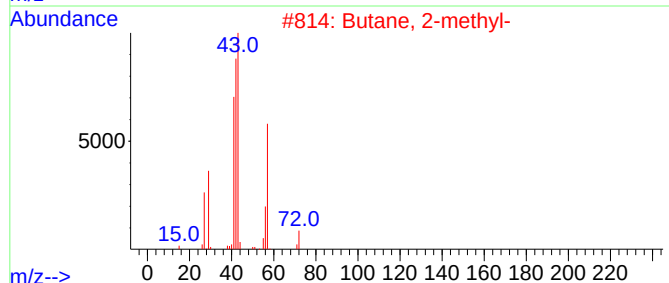
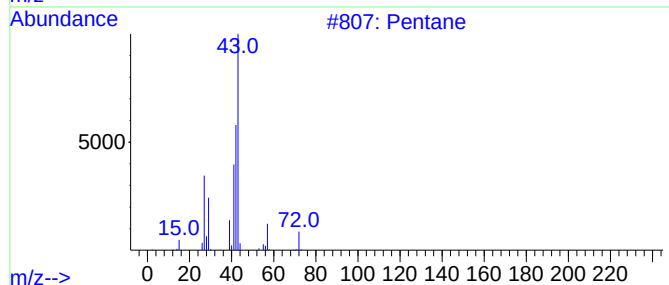
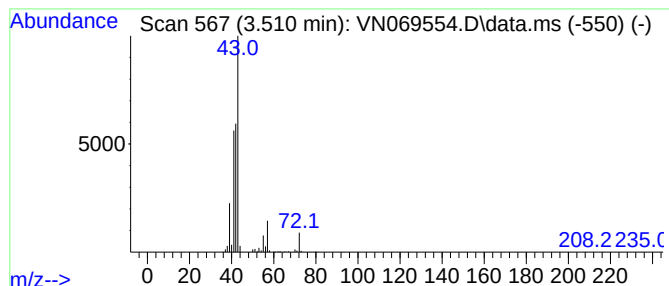
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Peak Number 3 Pentane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.510	11.18 ug/l	994432	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	80
2			Butane, 2-methyl-	72	C5H12	000078-78-4	64
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	42
4			Isobutyl nitrite	103	C4H9NO2	000542-56-3	17
5			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9



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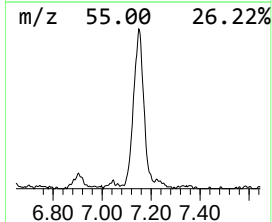
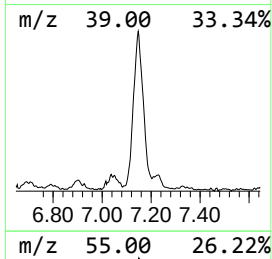
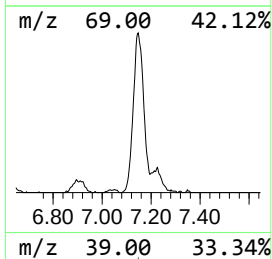
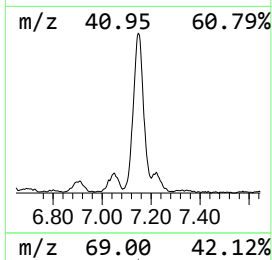
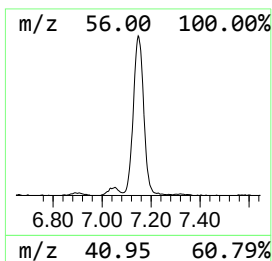
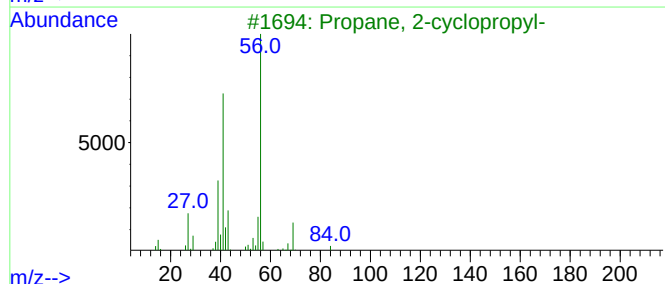
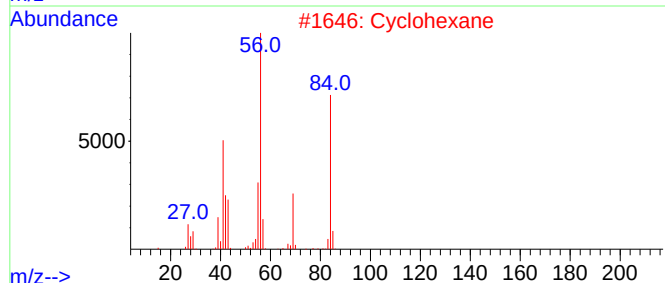
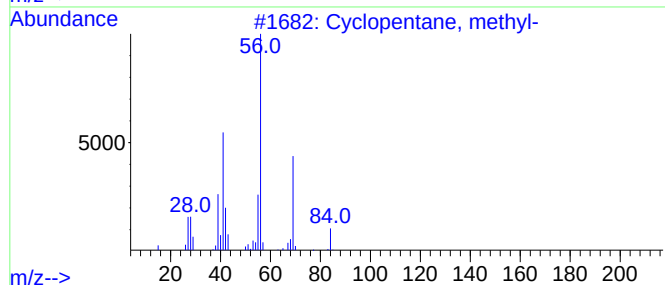
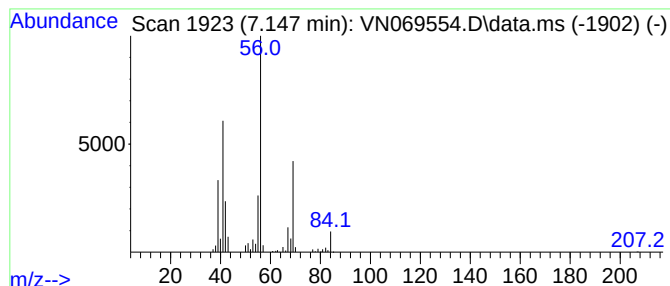
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	8.70 ug/l	773430	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2			Cyclohexane	84	C6H12	000110-82-7	64
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	59
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
5			Cyclobutane	56	C4H8	000287-23-0	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	2.443	5.3	ug/l	466645	1	8.088	4445800	50.0
Butane, 2-methyl-	3.140	22.4	ug/l	1992170	1	8.088	4445800	50.0
Pentane	3.510	11.2	ug/l	994432	1	8.088	4445800	50.0
Cyclopentane, m...	7.147	8.7	ug/l	773430	1	8.088	4445800	50.0