

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
 Data File : VN070494.D
 Acq On : 5 Jan 2022 17:12
 Operator : JC/MD
 Sample : N1012-11
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31243

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\82N122721W.M

Title : SW846 8260

Signal : TIC: VN070494.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	77	92	149	rBV2	20387069	34451294	100.00%	58.732%
2	7.064	1864	1892	1945	rBV2	1361468	4018180	11.66%	6.850%
3	8.021	2227	2249	2260	rBV2	608130	1461445	4.24%	2.491%
4	8.083	2261	2272	2301	rVB	797439	1847931	5.36%	3.150%
5	8.437	2381	2404	2440	rBV	845757	2036806	5.91%	3.472%
6	8.965	2581	2601	2629	rBV	1361940	2858925	8.30%	4.874%
7	9.164	2656	2675	2711	rBV3	135314	427675	1.24%	0.729%
8	10.440	3131	3151	3164	rBV	1741782	3253540	9.44%	5.547%
9	10.502	3164	3174	3192	rVB	587961	1088636	3.16%	1.856%
10	11.186	3413	3429	3480	rBV	425255	992438	2.88%	1.692%
11	11.744	3612	3637	3664	rBV	1403709	2748420	7.98%	4.685%
12	12.731	3990	4005	4033	rVB	967486	1772001	5.14%	3.021%
13	13.581	4309	4322	4341	rBV2	264572	439237	1.27%	0.749%
14	13.675	4341	4357	4379	rVB	708209	1261735	3.66%	2.151%

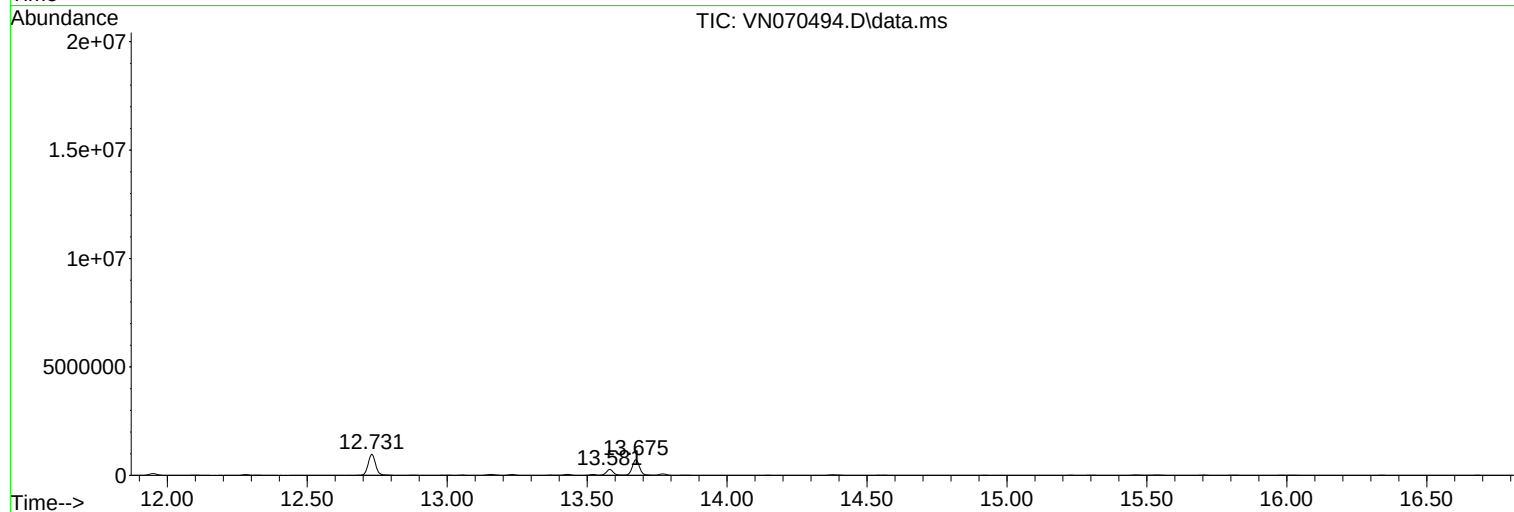
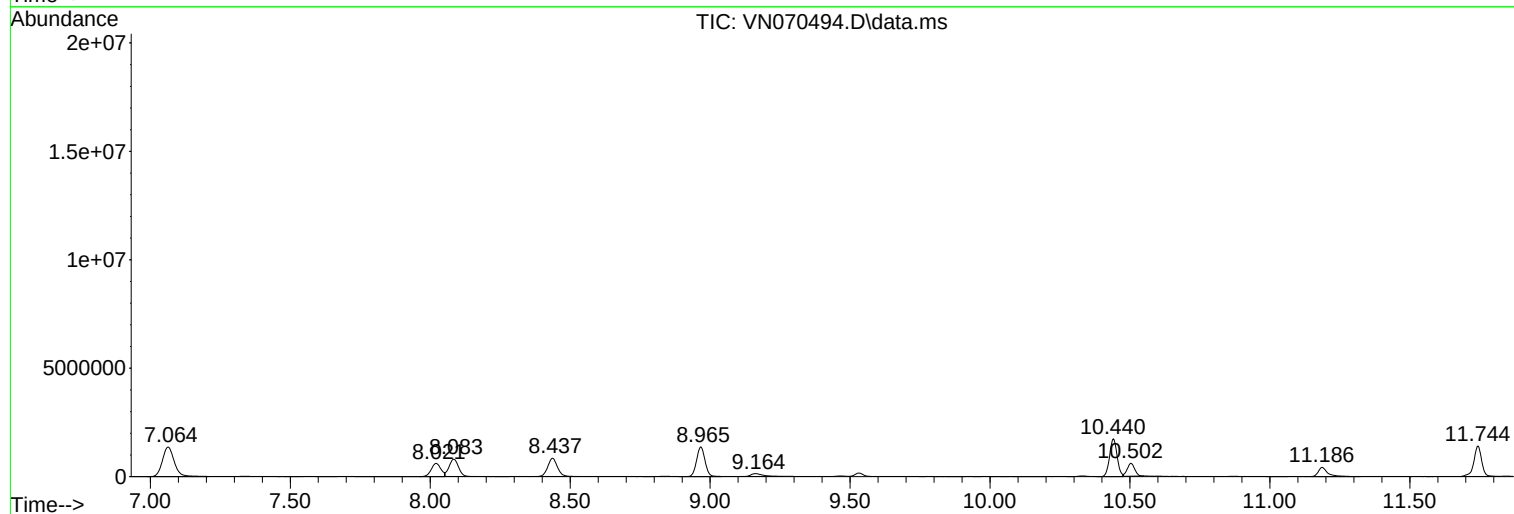
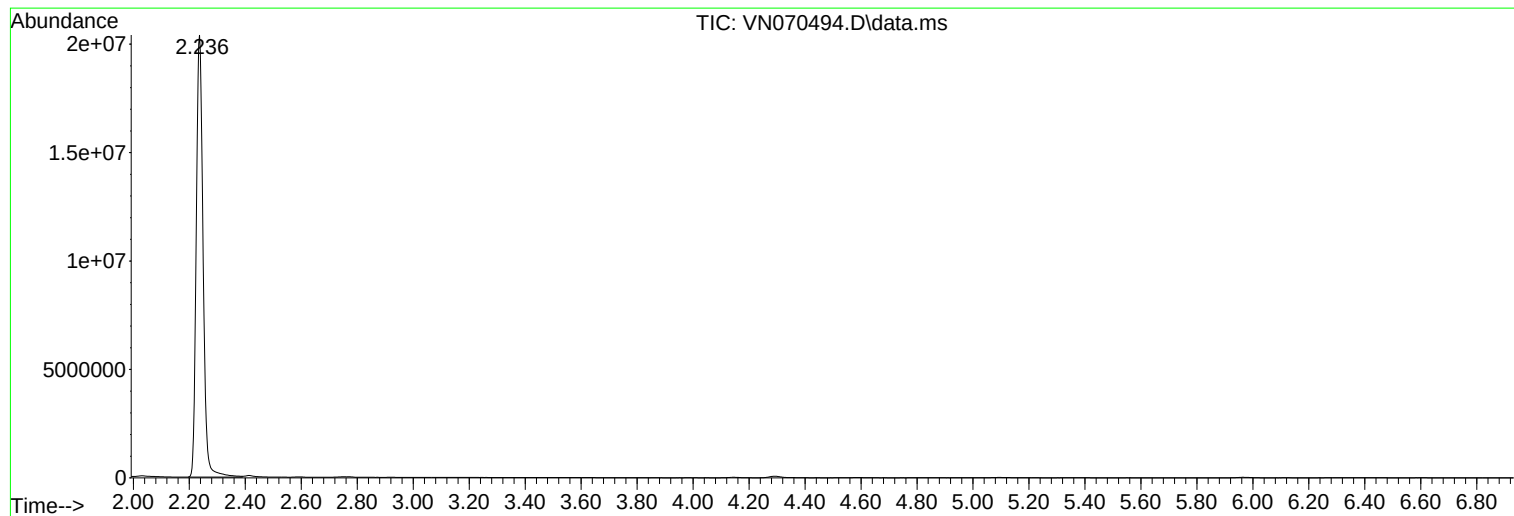
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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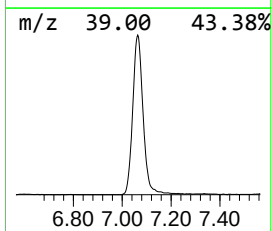
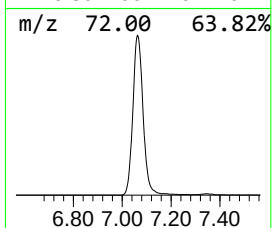
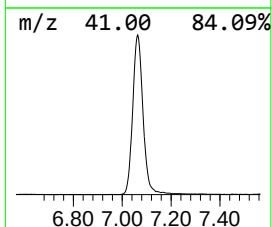
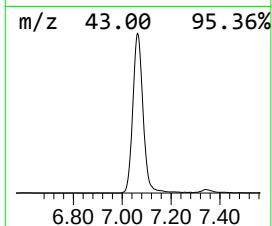
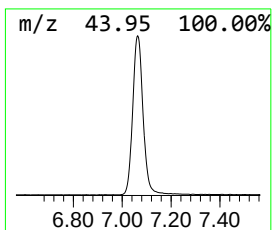
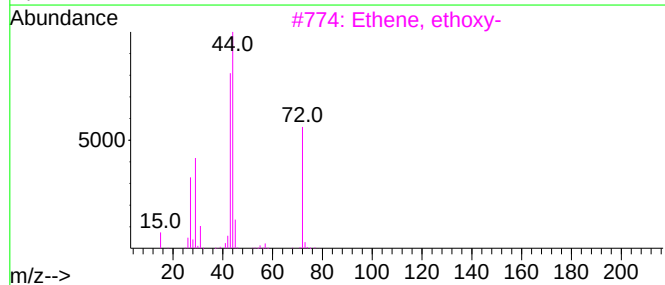
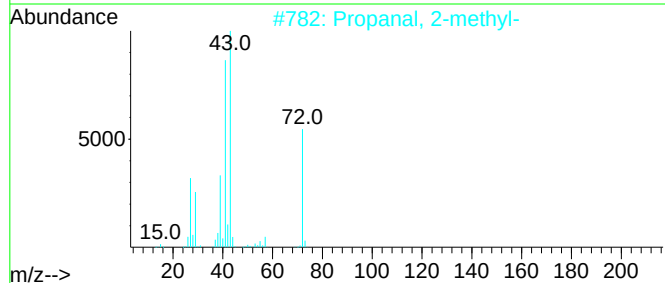
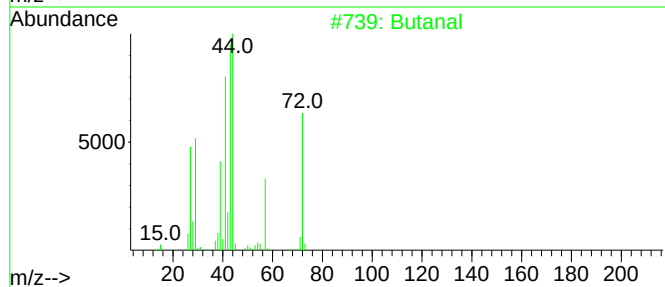
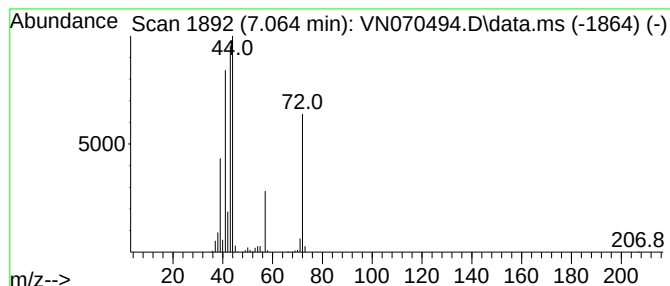
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.064	108.72 ug/l	4018180	Pentafluorobenzene	8.086

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	49
4		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
5		2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23



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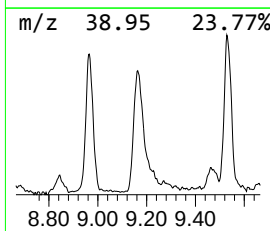
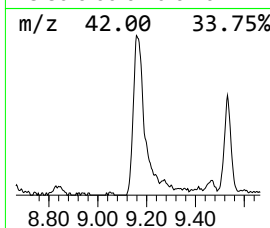
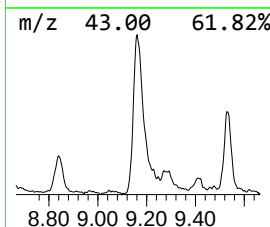
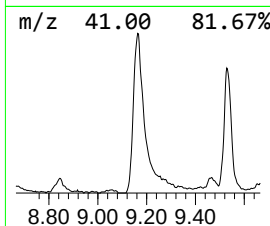
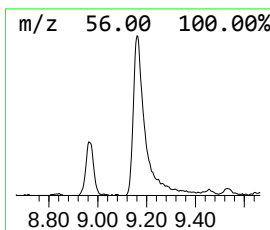
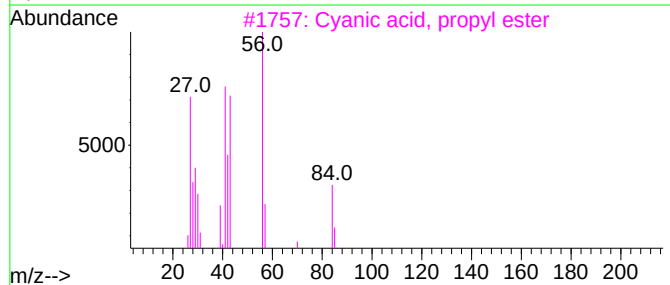
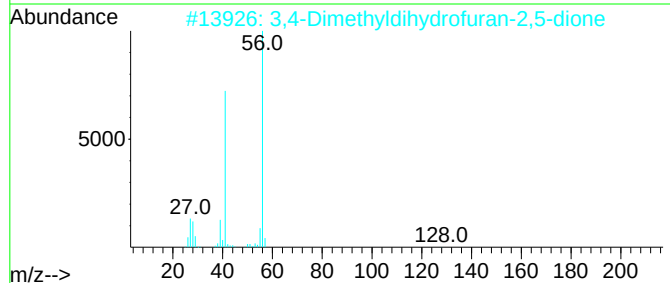
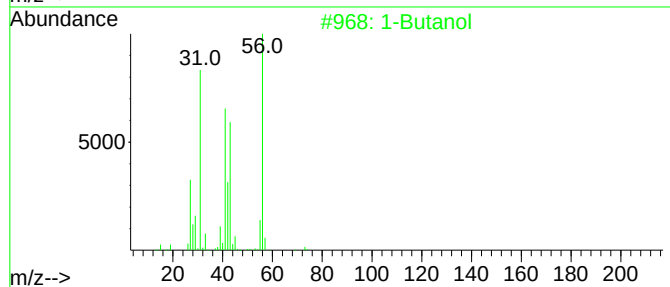
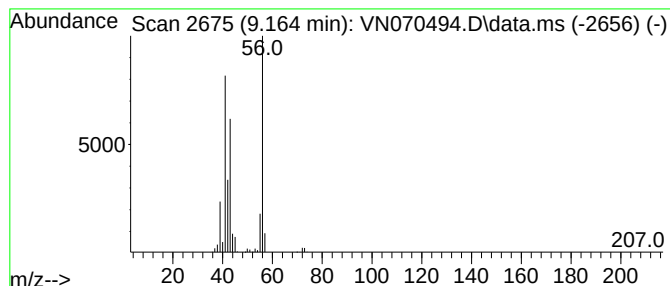
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Peak Number 3 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.164	7.48 ug/l	427675	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	59
3			Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	50
4			Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	45
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39



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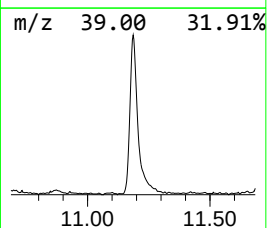
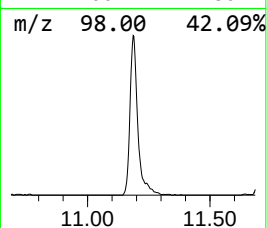
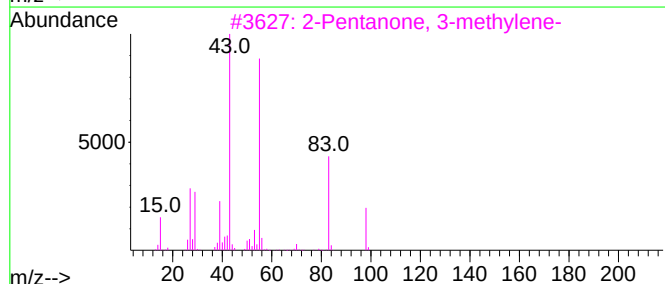
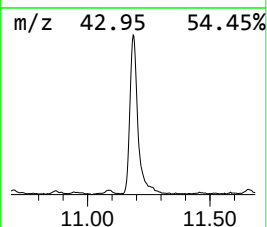
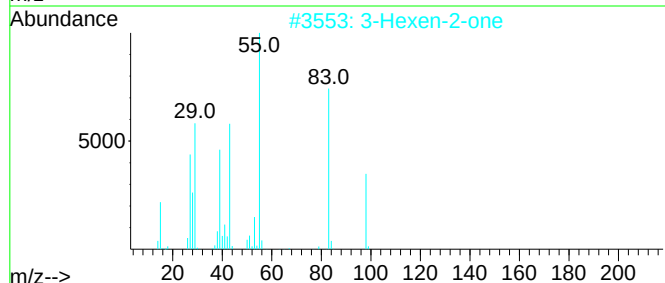
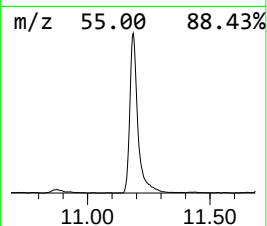
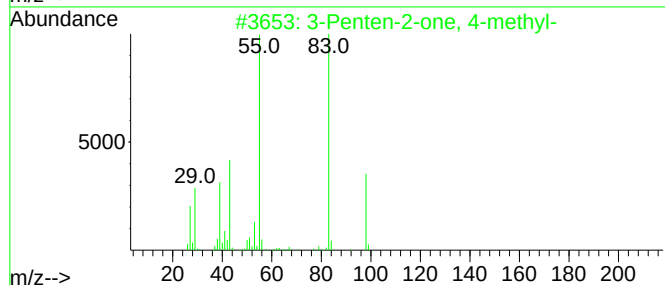
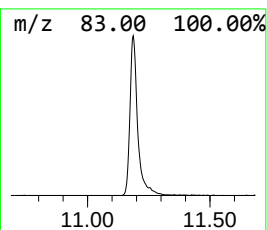
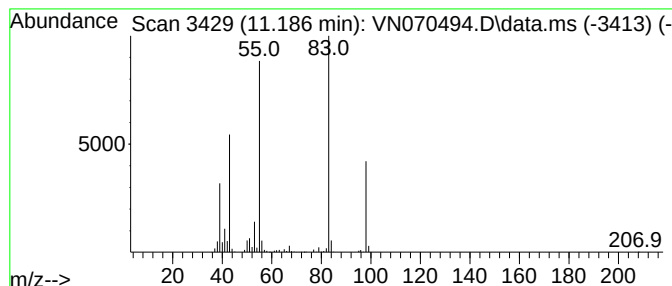
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Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.186	18.05 ug/l	992438	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	91
4			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	86
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



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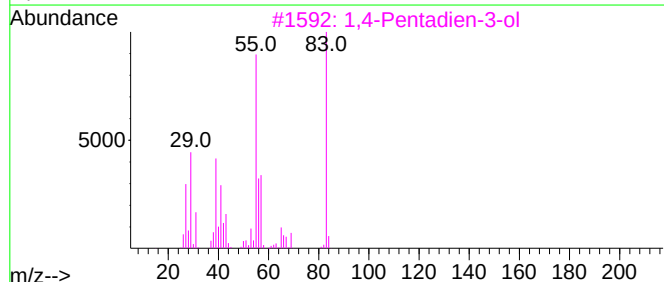
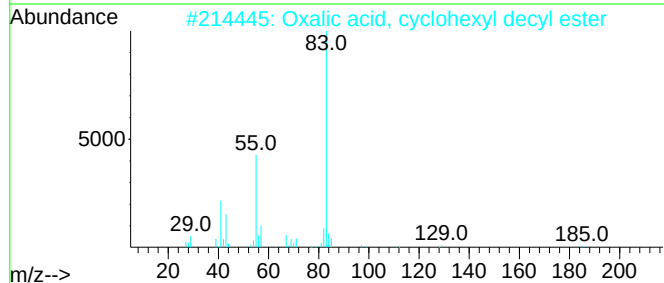
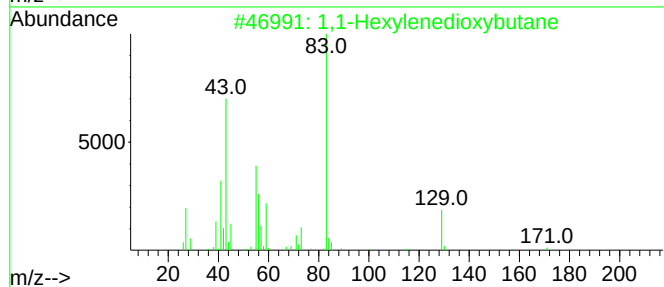
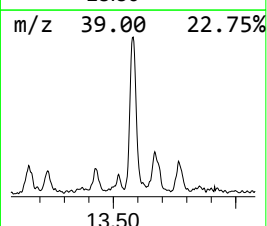
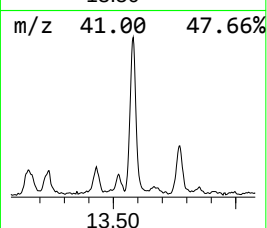
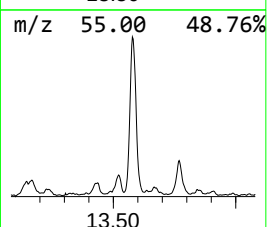
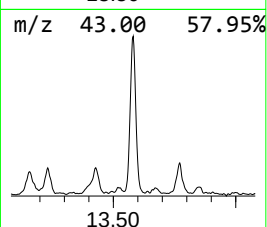
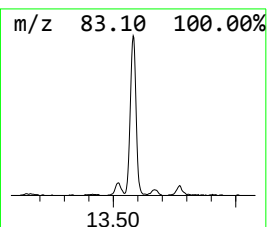
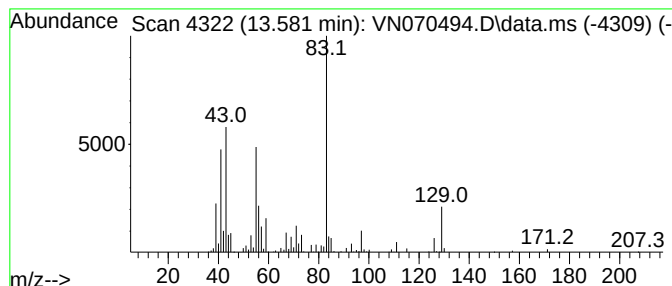
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Peak Number 5 1,1-Hexylenedioxybutane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.581	17.41 ug/l	439237	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	64
2			Oxalic acid, cyclohexyl decyl ester	312	C18H32O4	1000309-31-2	47
3			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	47
4			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	47
5			Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.064	108.7	ug/l	4018180	1	8.086	1847930	50.0
1-Butanol	9.164	7.5	ug/l	427675	2	8.968	2858930	50.0
3-Penten-2-one,...	11.186	18.1	ug/l	992438	3	11.744	2748420	50.0
1,1-Hexylenedio...	13.581	17.4	ug/l	439237	4	13.675	1261740	50.0