

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110725\
 Data File : VN088230.D
 Acq On : 07 Nov 2025 13:51
 Operator : JC\MD
 Sample : Q3518-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 50831

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\82N102325W.M
 Title : SW846 8260

Signal : TIC: VN088230.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.101	19	25	28	rBV	132010	226541	3.02%	0.676%
2	2.683	116	124	137	rBV	811117	1587687	21.20%	4.737%
3	3.789	300	312	338	rBV	1090288	3331353	44.48%	9.940%
4	4.283	387	396	408	rBV2	52760	164131	2.19%	0.490%
5	4.424	411	420	432	rVV2	165975	530972	7.09%	1.584%
6	4.706	455	468	491	rBV	634508	2025069	27.04%	6.042%
7	6.718	799	810	833	rBV2	234896	793591	10.60%	2.368%
8	7.212	881	894	905	rBV	224712	663982	8.87%	1.981%
9	7.471	921	938	952	rBV	100921	294045	3.93%	0.877%
10	8.147	1043	1053	1058	rBV	229351	558598	7.46%	1.667%
11	8.206	1058	1063	1073	rVB	316210	698698	9.33%	2.085%
12	8.559	1111	1123	1137	rBV2	266637	715525	9.55%	2.135%
13	9.082	1202	1212	1223	rBV	592722	1190786	15.90%	3.553%
14	9.253	1232	1241	1259	rBV	3247320	6930374	92.54%	20.679%
15	10.429	1434	1441	1450	rBV	84584	170361	2.27%	0.508%
16	10.547	1450	1461	1468	rVV	919177	1734732	23.16%	5.176%
17	10.606	1468	1471	1483	rVB	76000	142896	1.91%	0.426%
18	11.841	1671	1681	1695	rBV	823077	1549244	20.69%	4.623%
19	12.829	1841	1849	1862	rBV	627488	1190159	15.89%	3.551%
20	13.770	1994	2009	2017	rBV	838699	1526182	20.38%	4.554%
21	13.859	2017	2024	2062	rBV	2553129	7489191	100.00%	22.346%

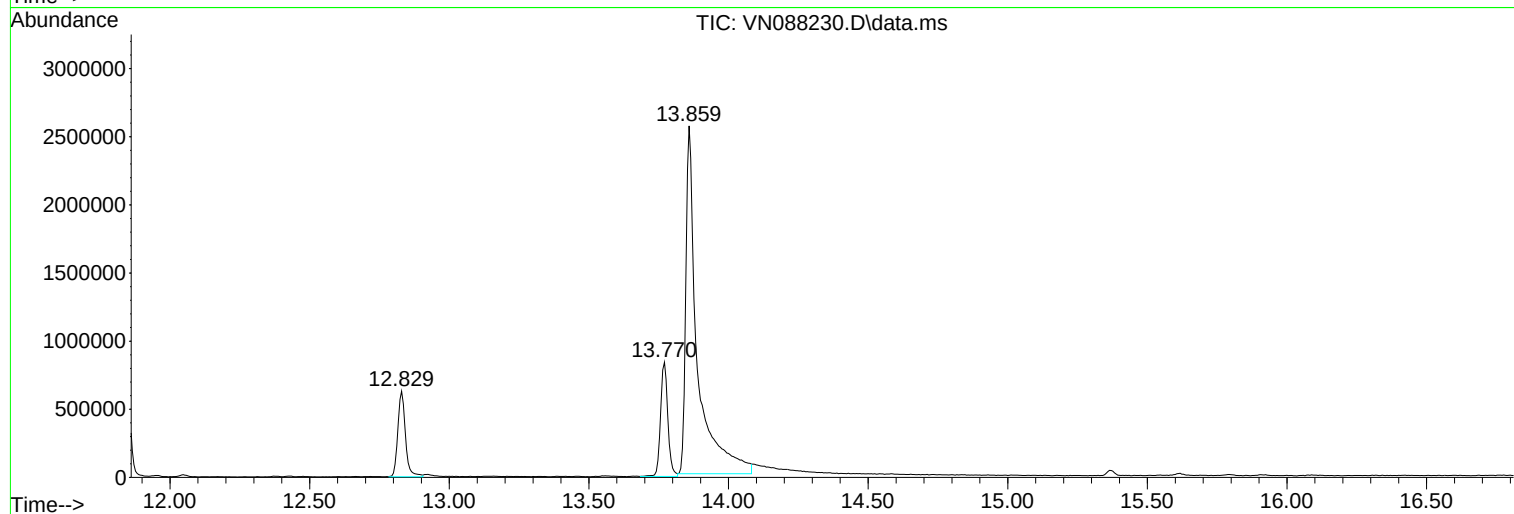
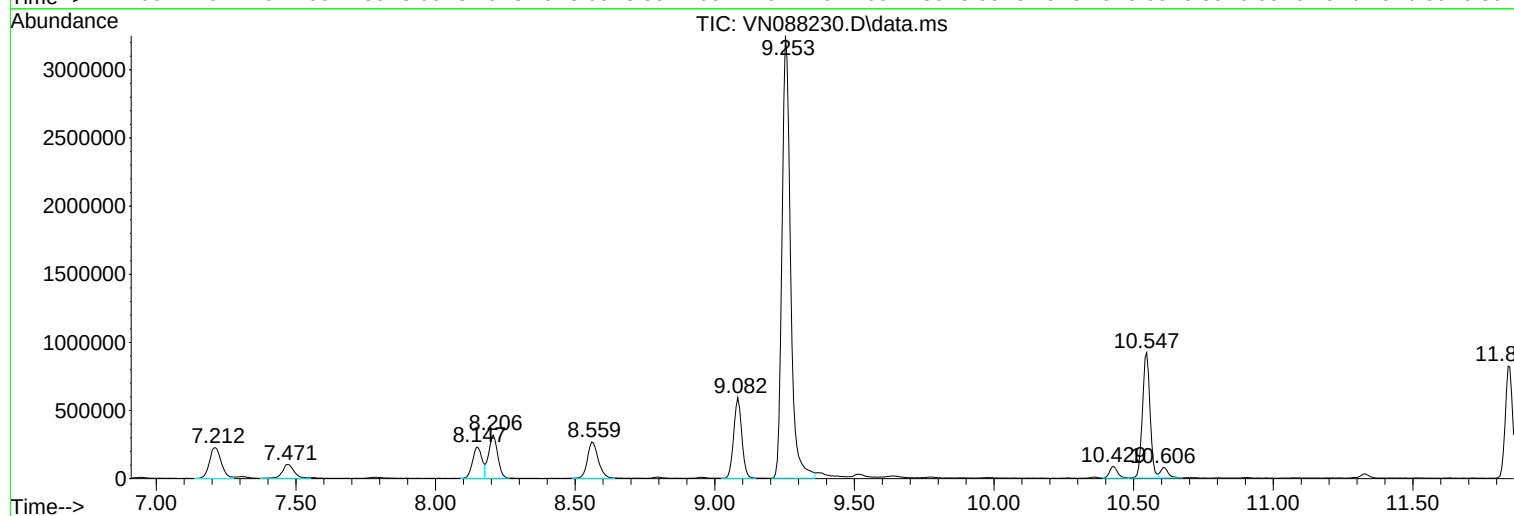
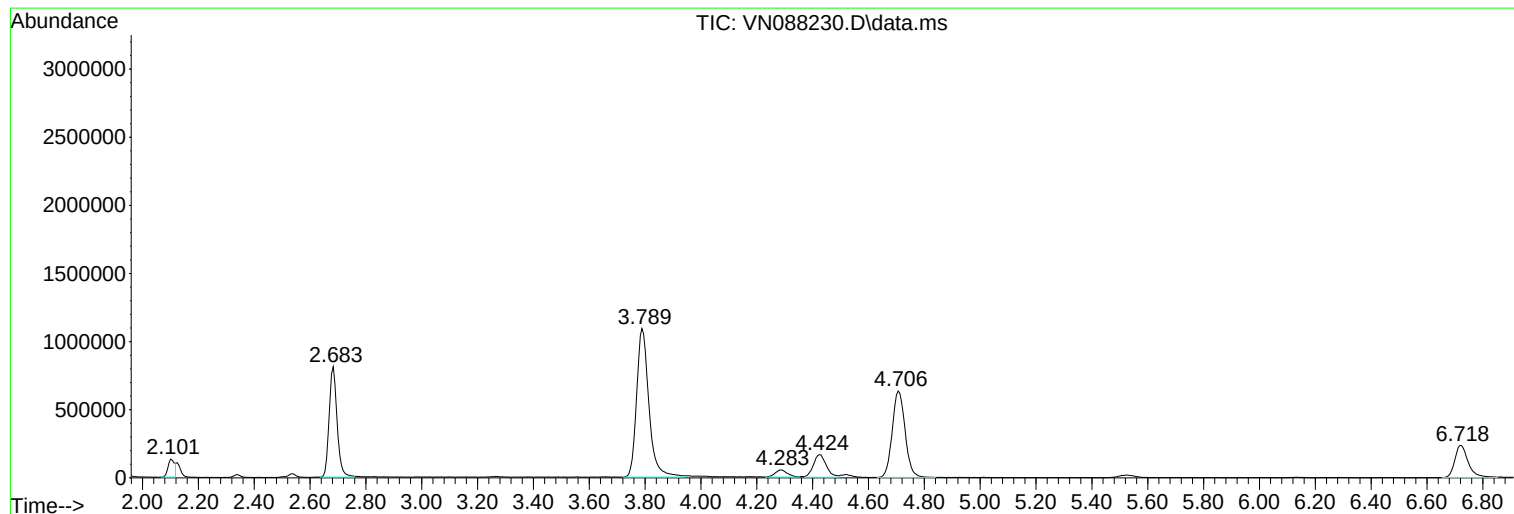
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TIC Library : C:\Database\NIST20.L
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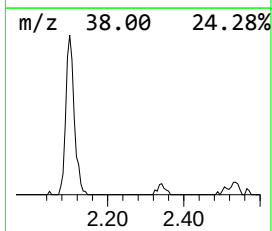
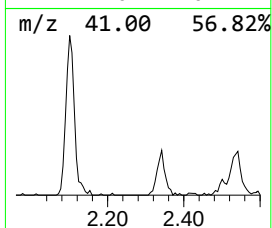
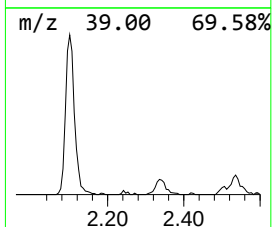
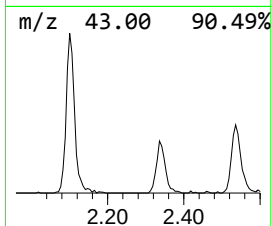
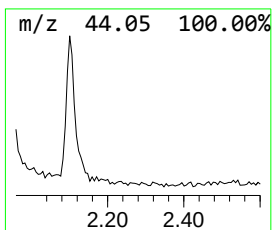
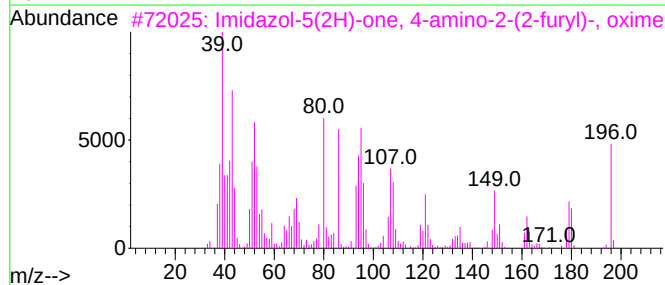
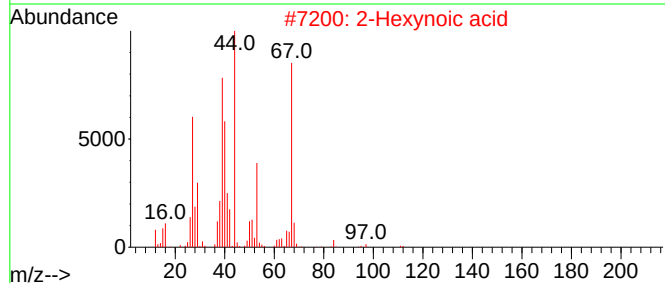
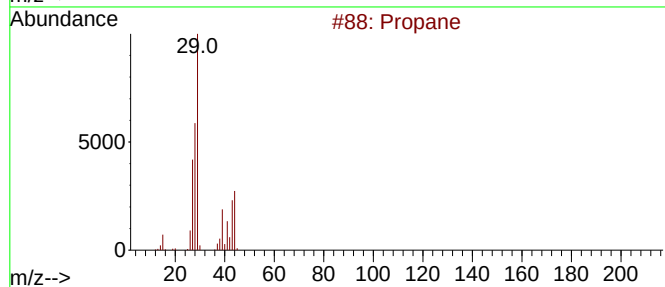
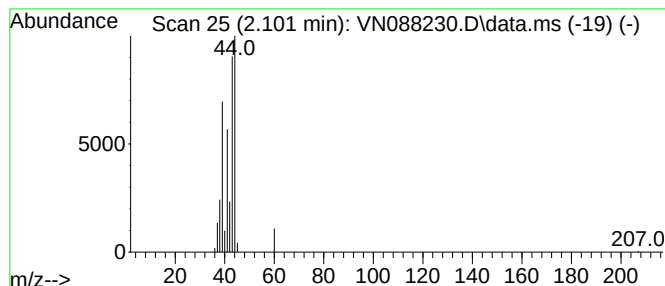
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.101	16.21 ug/l	226541	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	90
2	2-Hexynoic acid			112	C6H8O2	000764-33-0	39
3	Imidazol-5(2H)-one, 4-amino-2-(2...			196	C7H8N4O3	318259-17-5	38
4	2-Butenal, (E)-			70	C4H6O	000123-73-9	38
5	Acetoacetic acid, 1-thio-, S-all...			158	C7H10O2S	015780-65-1	33



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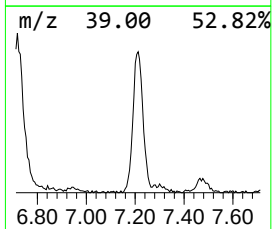
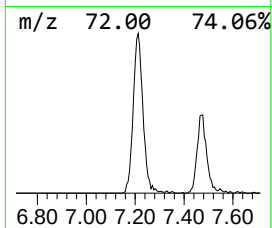
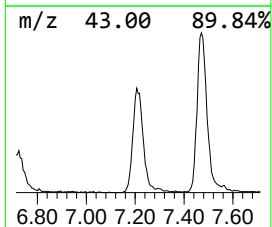
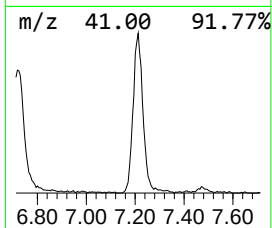
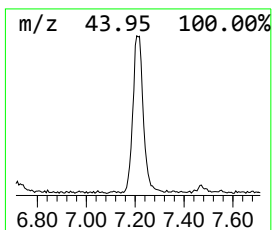
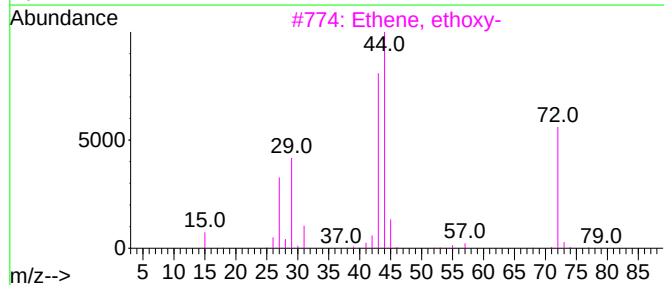
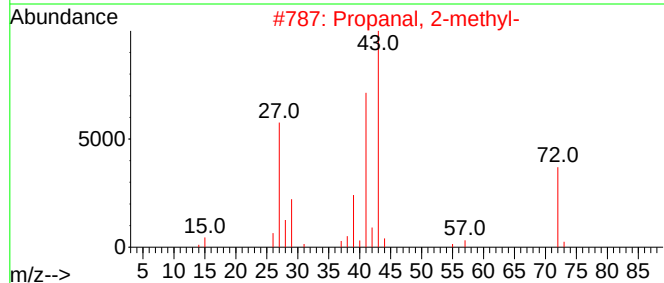
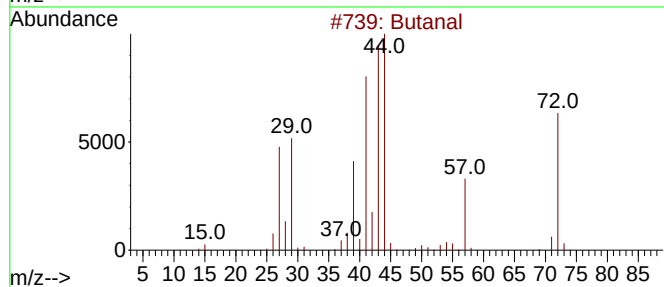
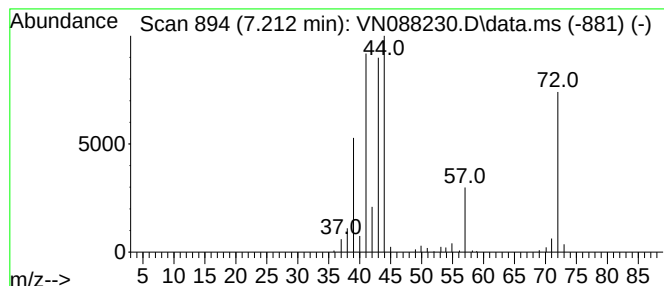
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Peak Number 6 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.212	47.52 ug/l	663982	Pentafluorobenzene	8.206	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5	Acetaldehyde, methylhydrazone	72	C3H8N2	017167-73-6	27



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Instrument :
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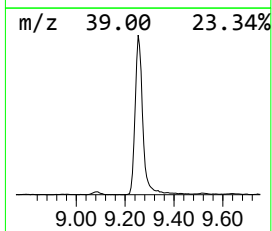
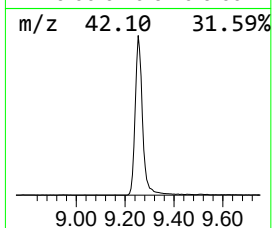
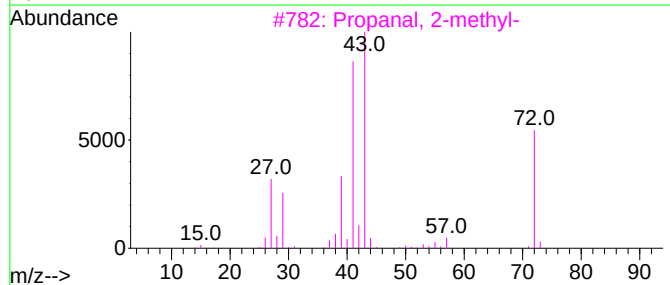
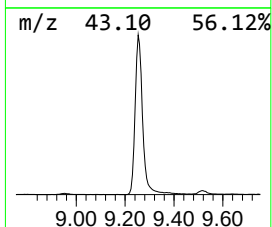
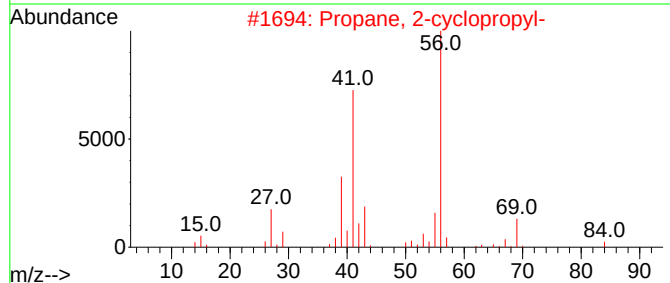
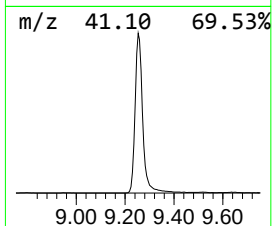
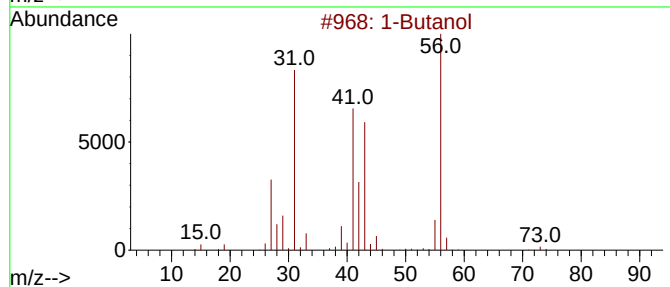
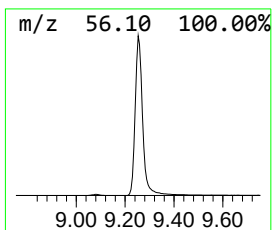
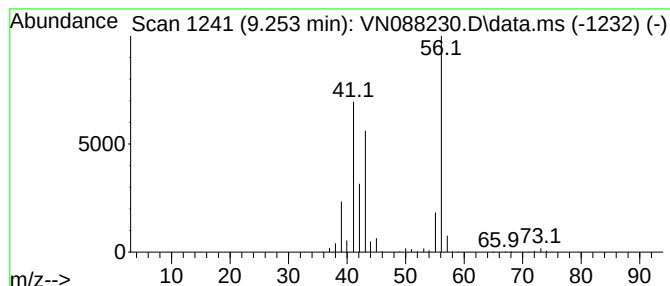
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Peak Number 7 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.253	291.00 ug/l	6930370	1,4-Difluorobenzene	9.082

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	10
4			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9



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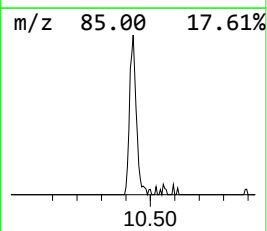
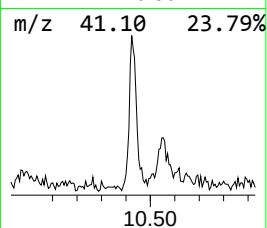
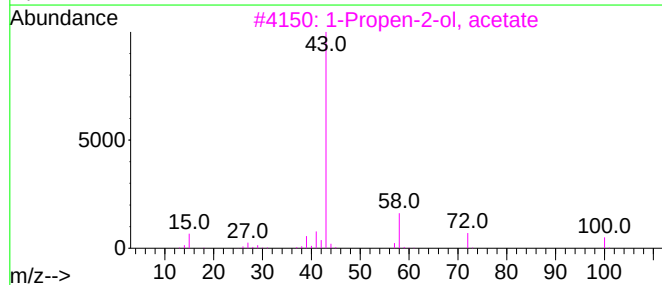
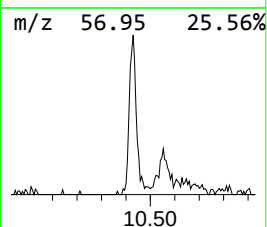
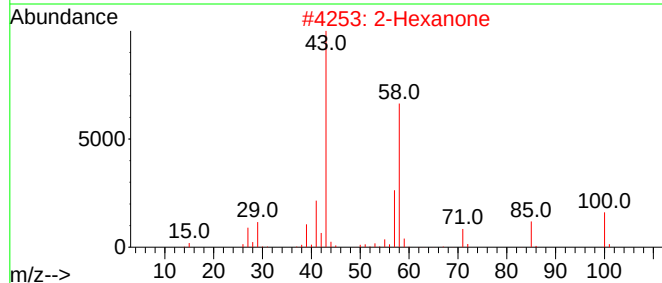
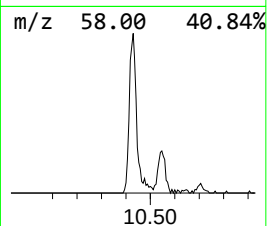
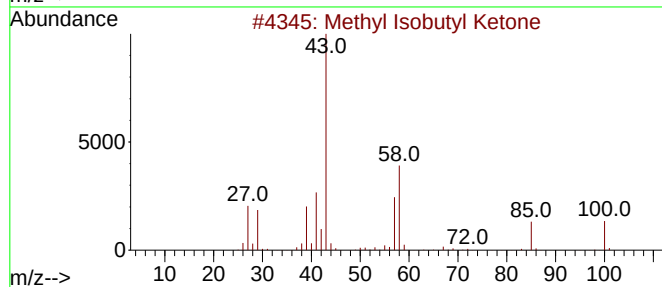
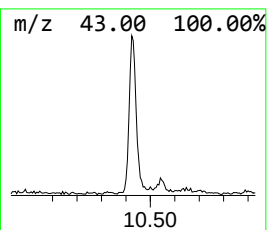
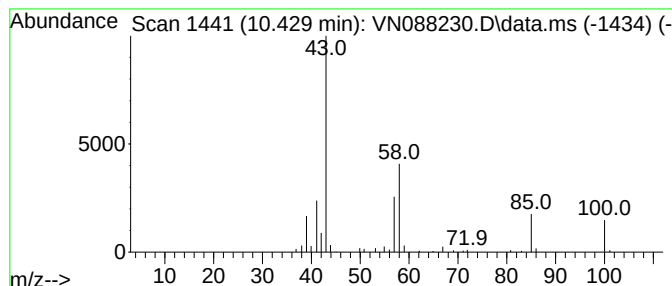
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Peak Number 8 Methyl Isobutyl Ketone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.430	7.15 ug/l	170361	1,4-Difluorobenzene	9.082

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	90
2			2-Hexanone	100	C6H12O	000591-78-6	80
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	50
4			2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	40
5			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	36



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane	2.101	16.2	ug/l	226541	1	8.206	698698	50.0
Butanal	7.212	47.5	ug/l	663982	1	8.206	698698	50.0
1-Butanol	9.253	291.0	ug/l	6930370	2	9.082	1190790	50.0
Methyl Isobutyl...	10.430	7.2	ug/l	170361	2	9.082	1190790	50.0