

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016662.D
 Acq On : 02 Oct 2021 08:45
 Operator : CG/JU
 Sample : M3829-13
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE120D1-20210917

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016662.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	4	8	11	rBV	1348624	2620387	100.00%	59.006%
2	3.816	76	80	96	rVB	10637	44553	1.70%	1.003%
3	4.821	185	189	204	rVB	34620	80395	3.07%	1.810%
4	7.633	489	494	500	rVB2	51635	108732	4.15%	2.448%
5	7.864	515	519	525	rBV	14875	30100	1.15%	0.678%
6	8.784	601	605	610	rBV	22294	45786	1.75%	1.031%
7	10.407	729	733	736	rBV	101752	178260	6.80%	4.014%
8	12.003	918	931	942	rBV	45407	73692	2.81%	1.659%
9	12.886	1071	1074	1078	rBV	92974	150484	5.74%	3.389%
10	14.269	1180	1183	1186	rBV	135046	193325	7.38%	4.353%
11	17.017	1400	1403	1406	rBV	104562	160447	6.12%	3.613%
12	19.063	1688	1696	1721	rBV	127157	176690	6.74%	3.979%
13	19.678	1813	1820	1846	rBV	125706	162525	6.20%	3.660%
14	21.164	1993	1995	1998	rBV	24578	33048	1.26%	0.744%
15	21.227	1998	2001	2011	rVB	124127	188029	7.18%	4.234%
16	23.481	2415	2426	2459	rVB	99572	194401	7.42%	4.378%

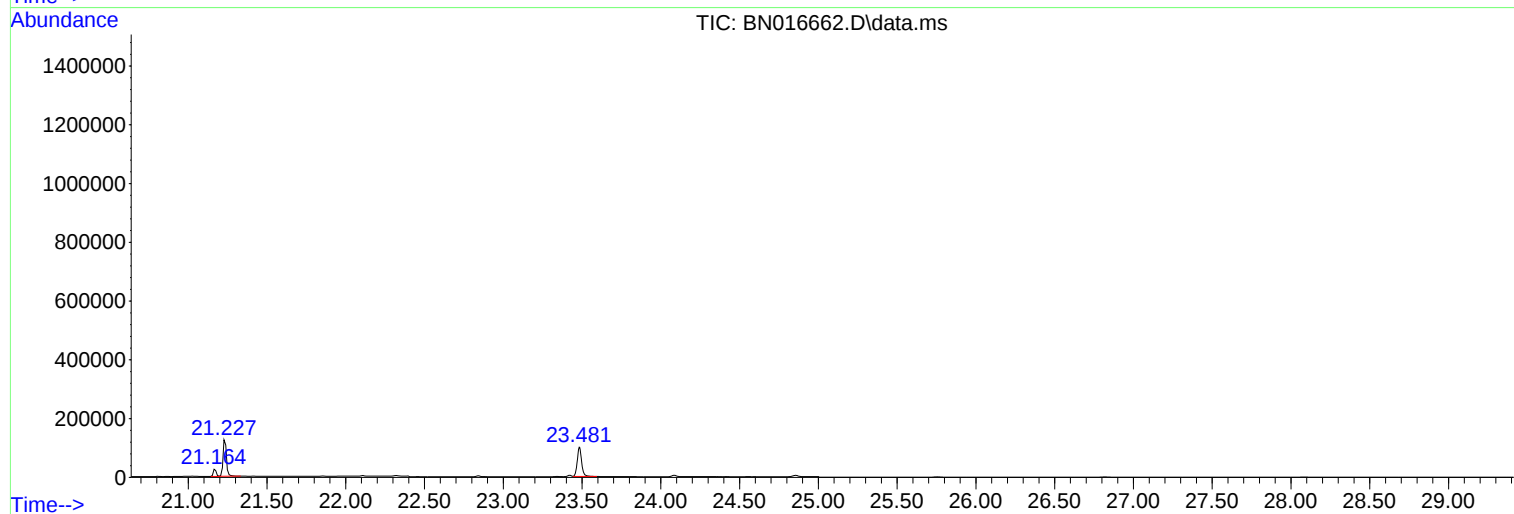
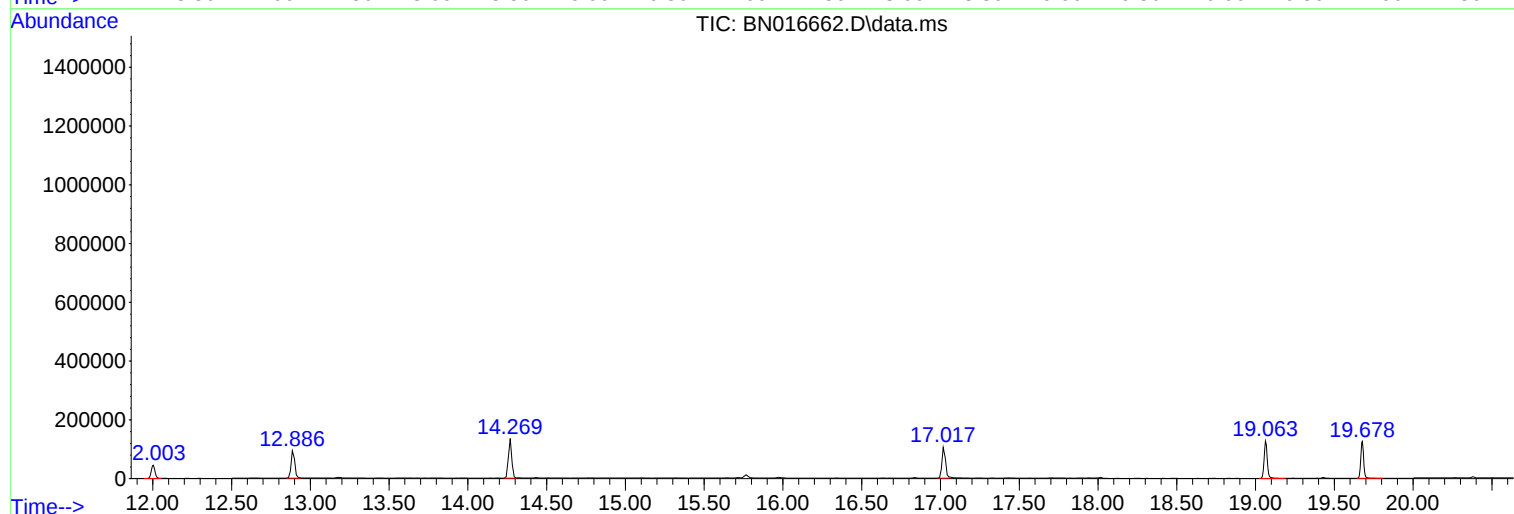
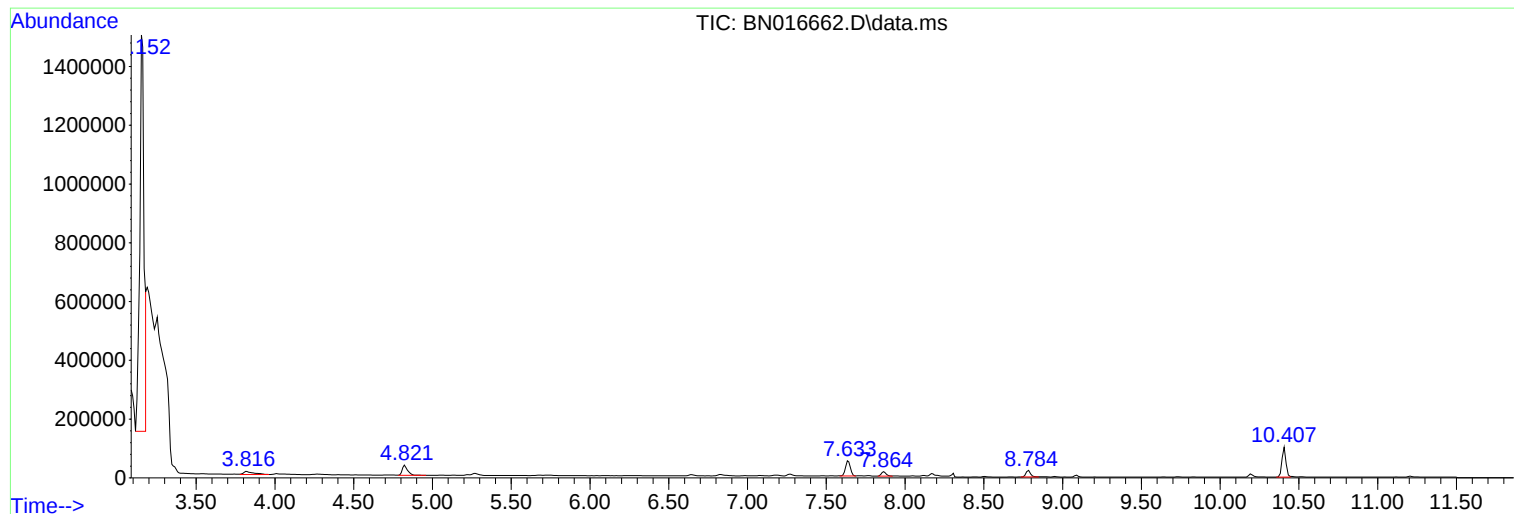
Sum of corrected areas: 4440854

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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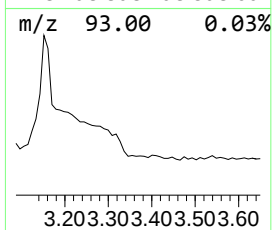
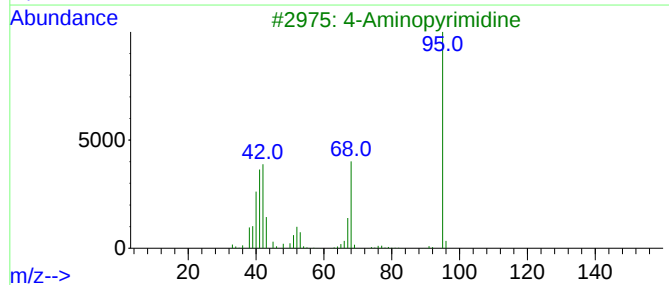
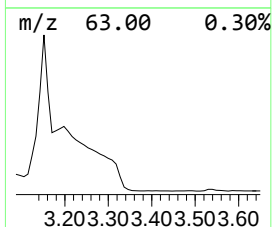
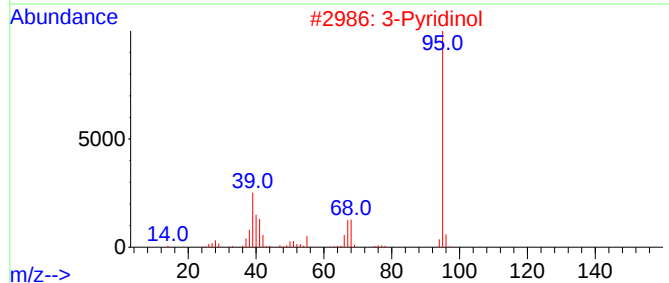
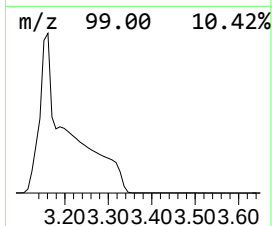
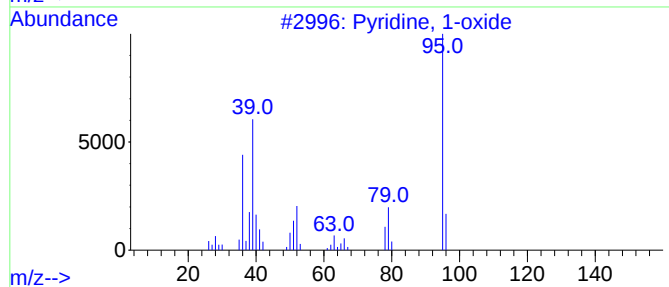
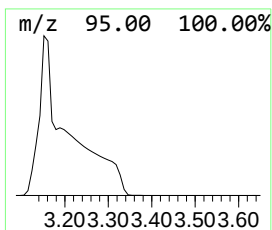
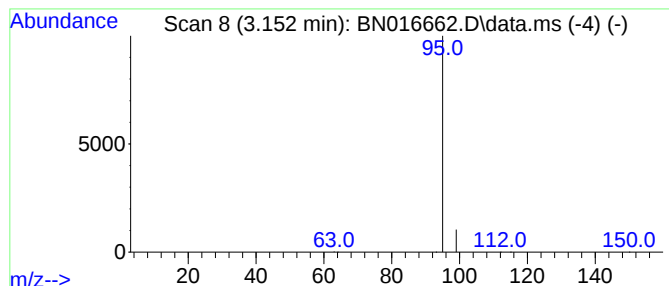
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	9.64 ng	2620390	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
2			3-Pyridinol	95	C5H5NO	000109-00-2	2
3			4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
4			4-Pyridinol	95	C5H5NO	000626-64-2	2
5			2-(Aminomethylene)aminoacrylonitrile	95	C4H5N3	167320-31-2	2



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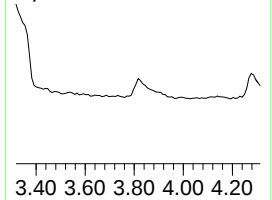
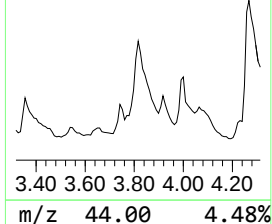
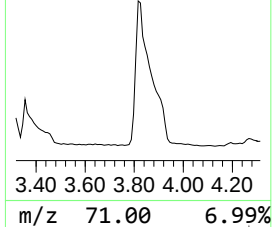
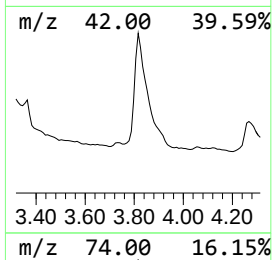
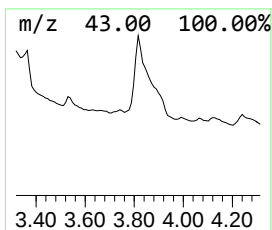
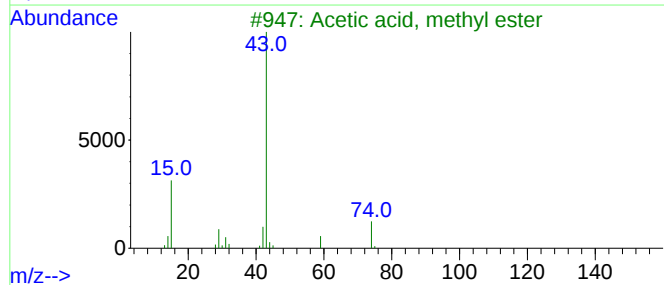
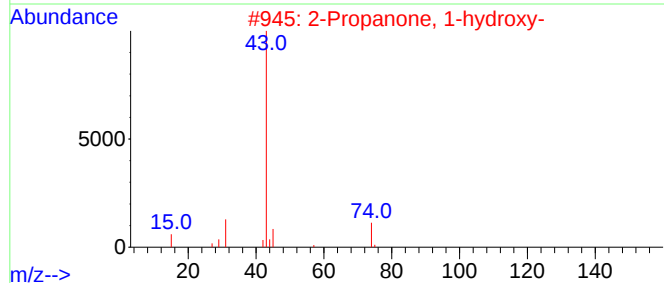
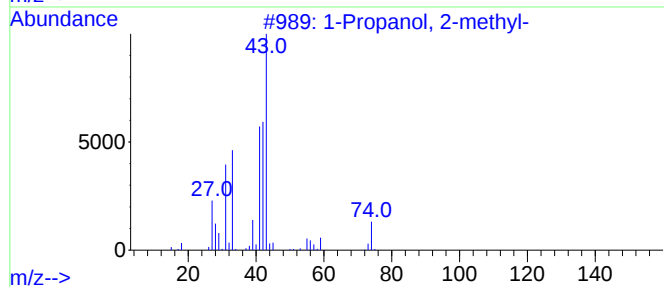
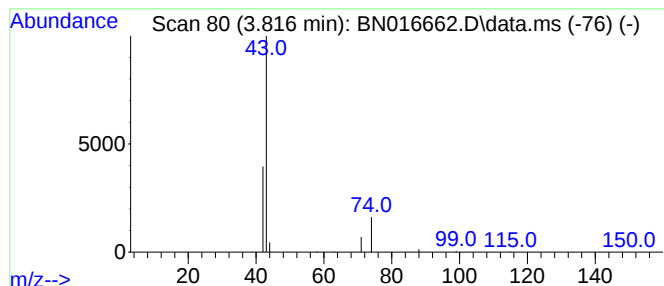
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.16 ng	44553	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
2			2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
3			Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
4			Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	4
5			Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	3



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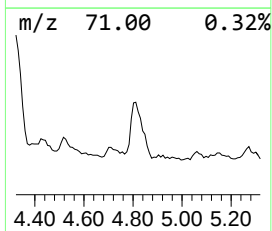
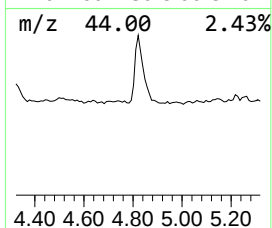
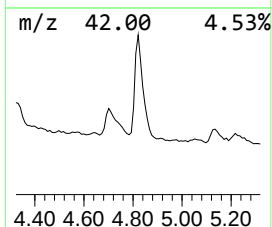
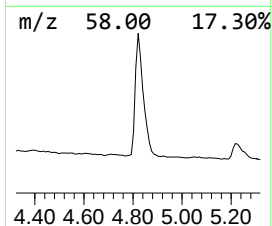
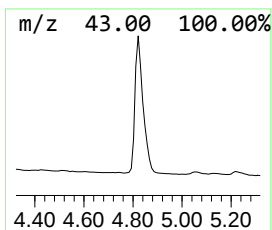
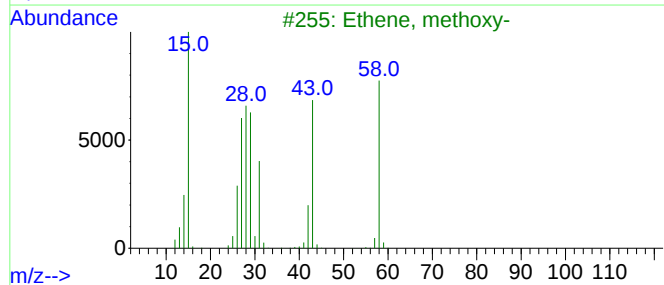
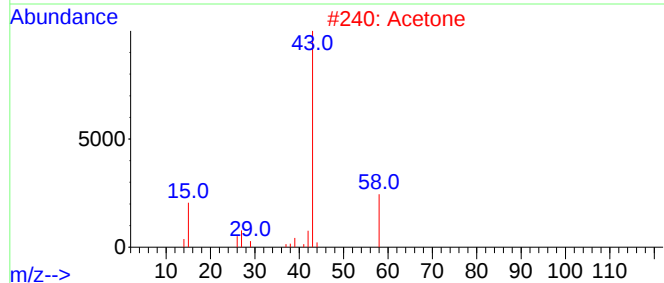
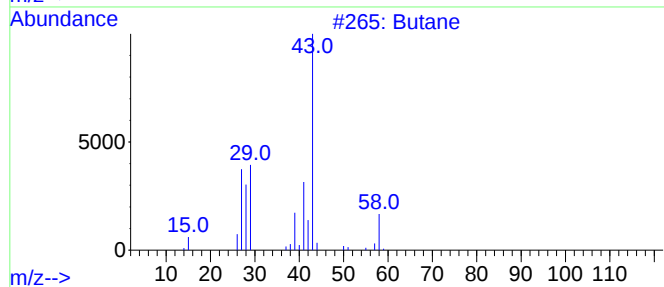
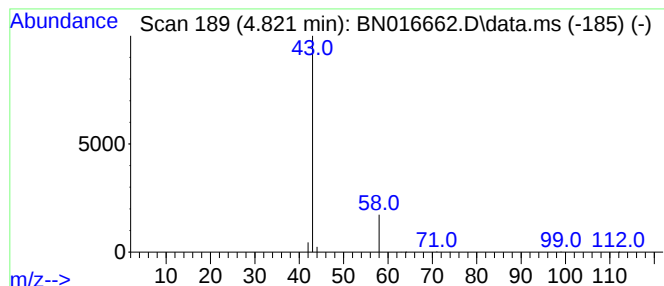
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Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.30 ng	80395	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Acetone	58	C3H6O	000067-64-1	4
3			Ethene, methoxy-	58	C3H6O	000107-25-5	3
4			Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5			Hydrogen isocyanate	43	CHNO	000075-13-8	2



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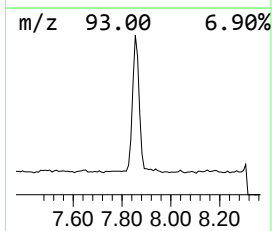
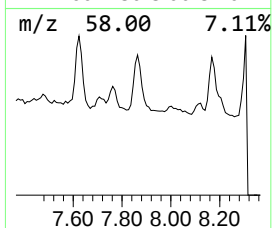
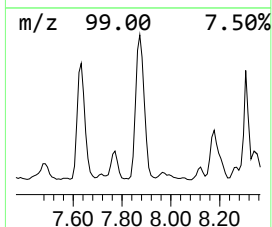
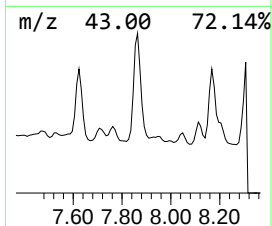
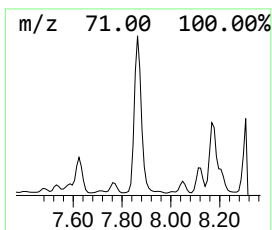
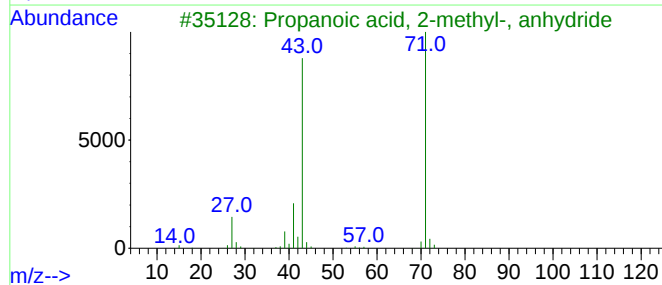
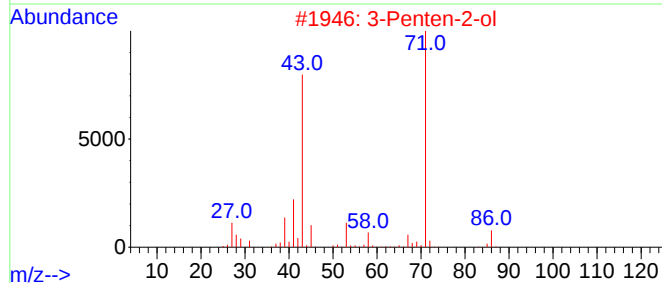
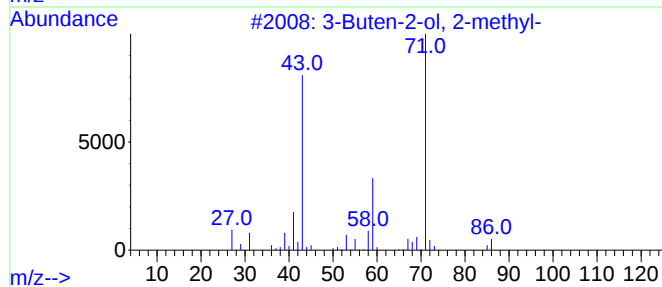
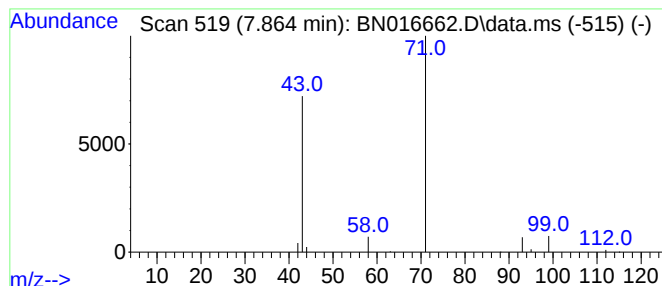
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Peak Number 4 3-Buten-2-ol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.11 ng	30100	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
2			3-Penten-2-ol	86	C5H10O	001569-50-2	4
3			Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
4			3-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4
5			Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pyridine, 1-oxide	3.152	9.6	ng	2620390	1	7.642	108732	0.4
1-Propanol, 2-m...	3.816	0.2	ng	44553	1	7.642	108732	0.4
Butane	4.821	0.3	ng	80395	1	7.642	108732	0.4
3-Buten-2-ol, 2...	7.864	0.1	ng	30100	1	7.642	108732	0.4