

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081623\
 Data File : BG058752.D
 Acq On : 16 Aug 2023 17:29
 Operator : MA/JU
 Sample : 03996-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EB-20230811

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.581	80	84	89	rBV	21799	28101	1.05%	0.288%
2	5.385	385	391	409	rBV	248736	421056	15.73%	4.315%
3	6.983	657	663	677	rVB	143804	254873	9.52%	2.612%
4	7.811	798	804	810	rBV	87974	149569	5.59%	1.533%
5	8.975	995	1002	1021	rBV	343688	645754	24.13%	6.618%
6	10.614	1270	1281	1291	rBV	116794	223982	8.37%	2.295%
7	11.137	1363	1370	1375	rBV	100792	160751	6.01%	1.647%
8	11.196	1375	1380	1392	rVB	116783	208942	7.81%	2.141%
9	12.494	1595	1601	1612	rBV3	15140	29323	1.10%	0.301%
10	13.076	1693	1700	1716	rBV	901377	1439265	53.78%	14.750%
11	13.346	1739	1746	1757	rBV	295484	469218	17.53%	4.809%
12	14.456	1929	1935	1953	rVB	186367	314659	11.76%	3.225%
13	15.949	2182	2189	2205	rBV	757819	1279555	47.81%	13.114%
14	17.206	2396	2403	2419	rBV	270572	442540	16.54%	4.535%
15	19.827	2842	2849	2863	rBV	1920375	2676138	100.00%	27.426%
16	21.448	3116	3125	3137	rBV	273515	490090	18.31%	5.023%
17	24.521	3637	3648	3668	rBV	157889	523692	19.57%	5.367%

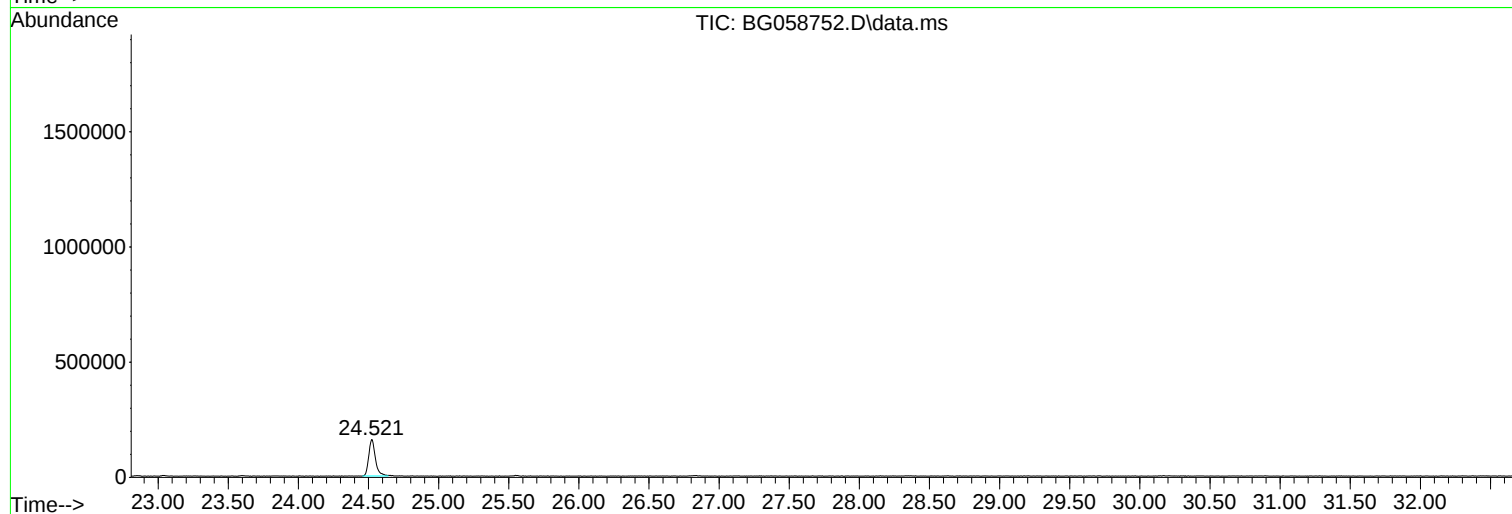
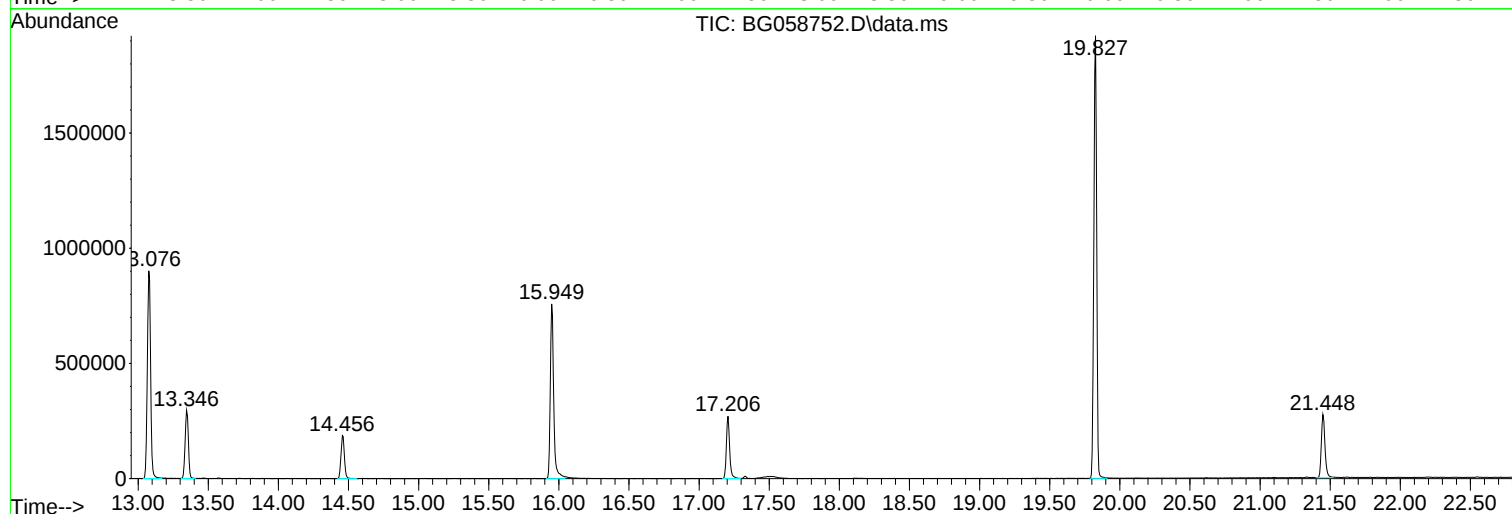
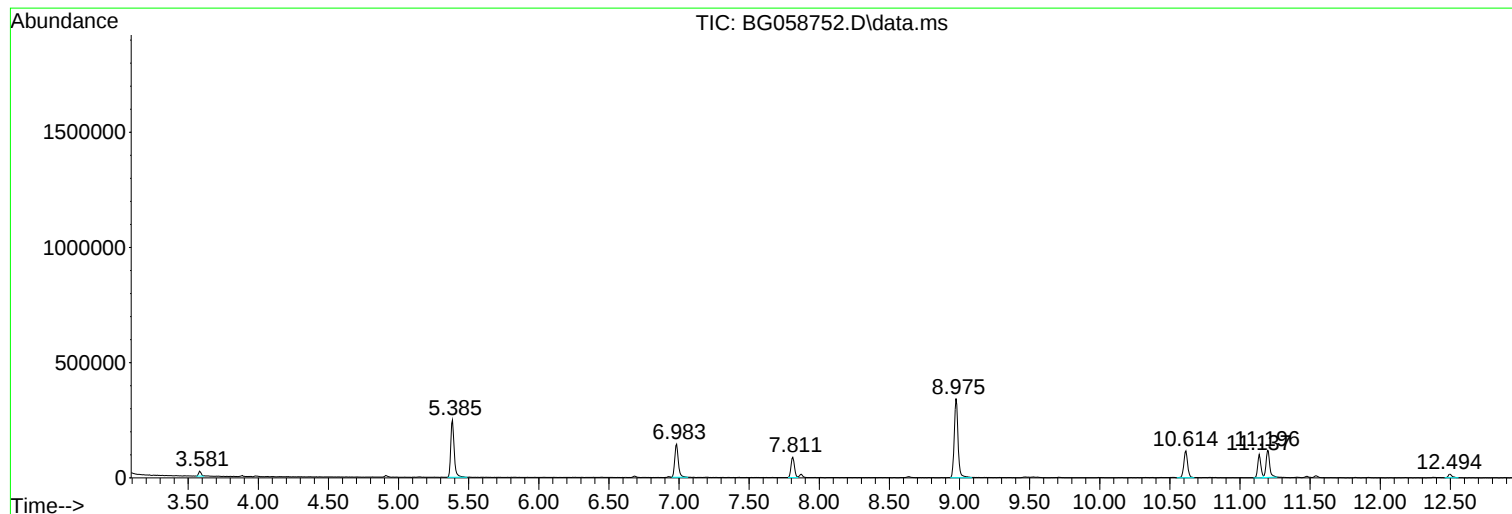
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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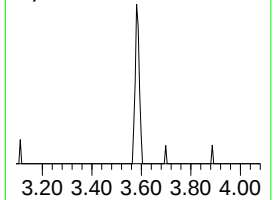
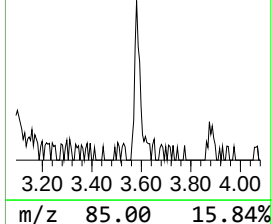
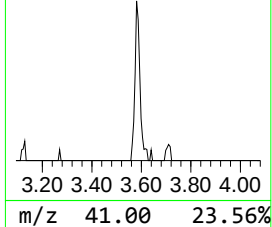
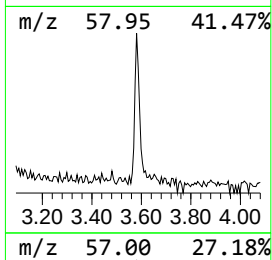
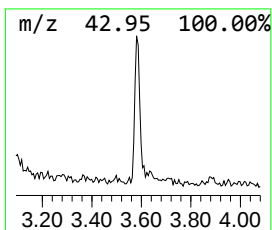
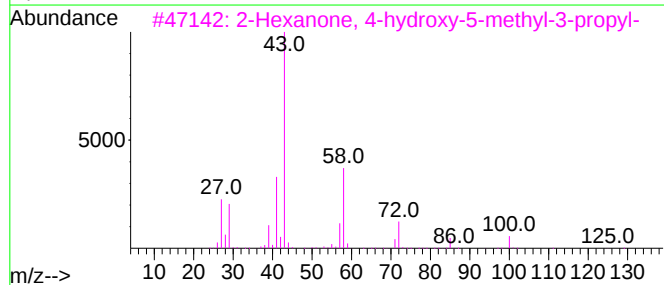
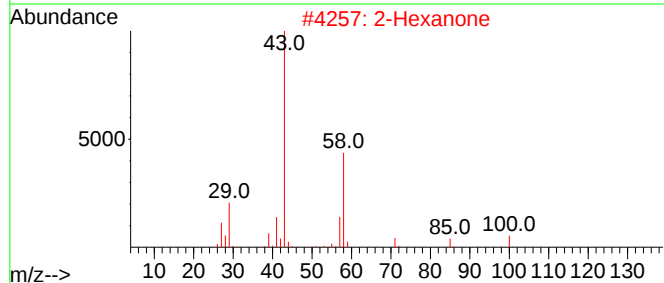
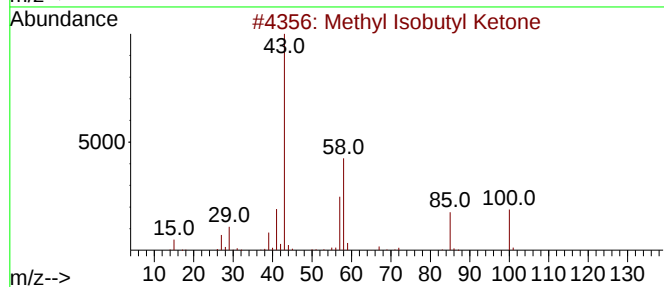
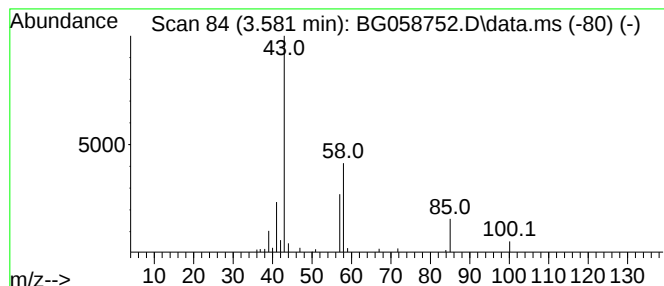
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Methyl Isobutyl Ketone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.581	3.76 ng	28101	1,4-Dichlorobenzene-d4	7.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	78
2			2-Hexanone	100	C6H12O	000591-78-6	78
3			2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	43
4			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	36
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12



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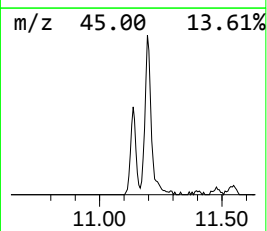
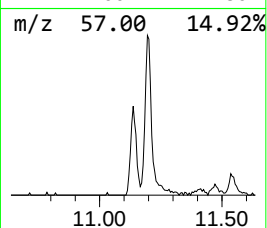
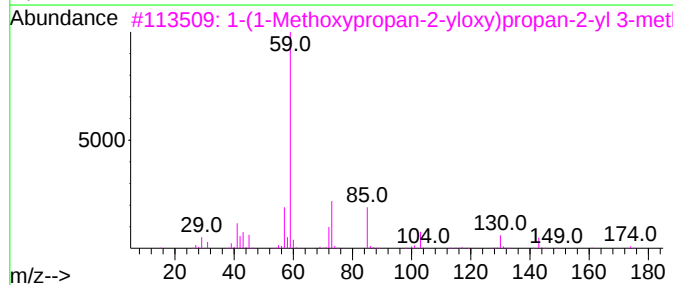
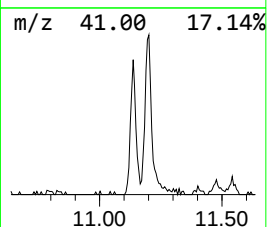
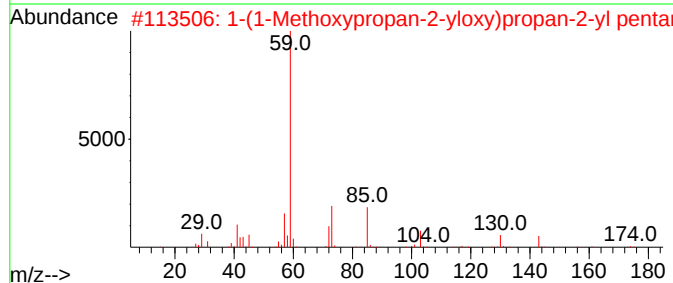
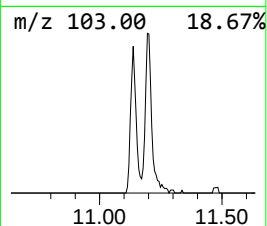
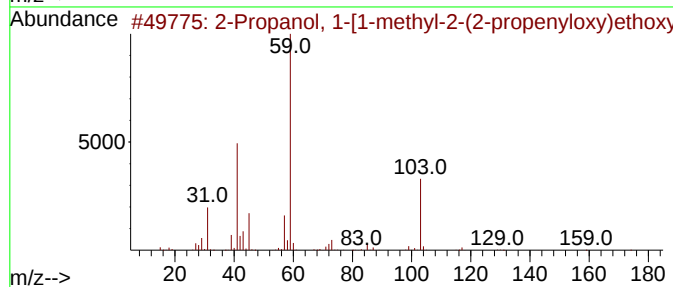
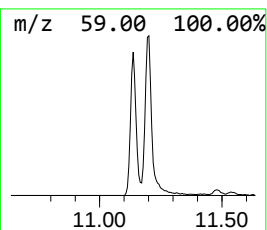
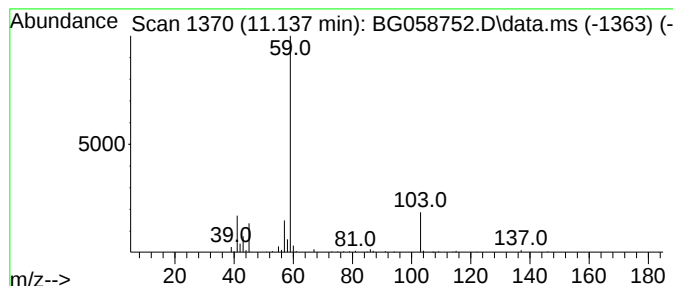
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.137	14.35 ng	160751	Naphthalene-d8	10.614

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78		
2	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	72		
3	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-13-2	72		
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64		
5	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	64		



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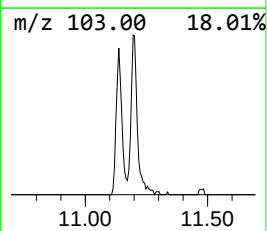
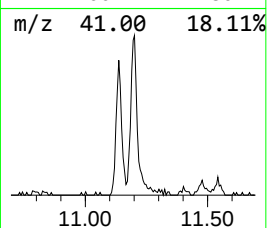
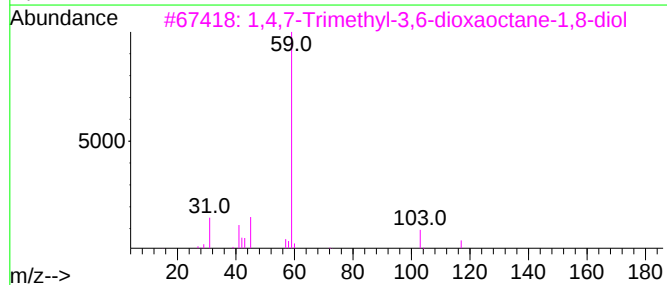
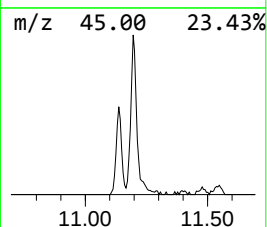
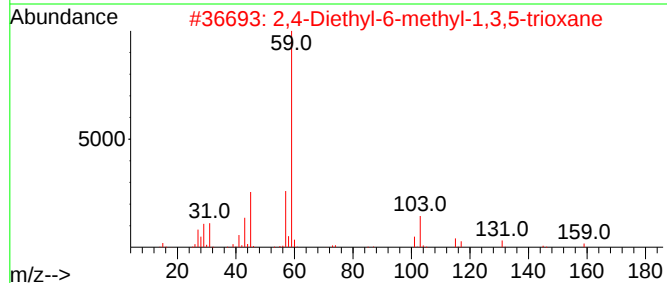
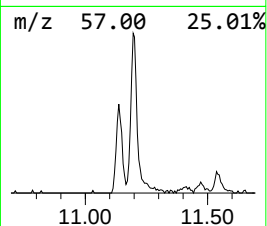
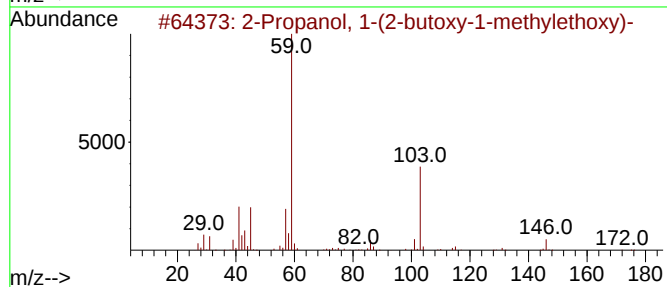
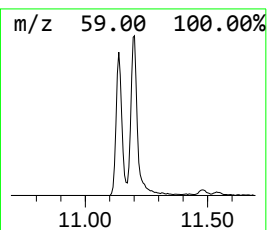
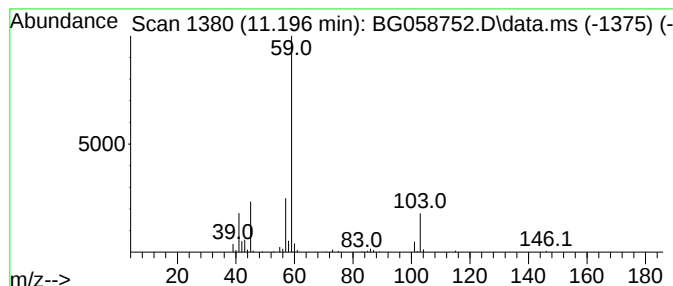
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.195	18.66 ng	208942	Naphthalene-d8	10.614	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	78
2	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	78
3	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	72
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64
5	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	64



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Instrument :
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ClientSampleId :
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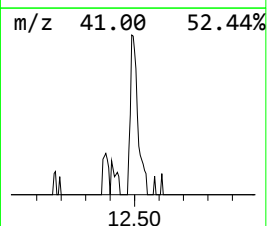
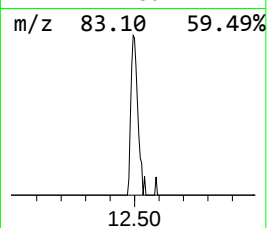
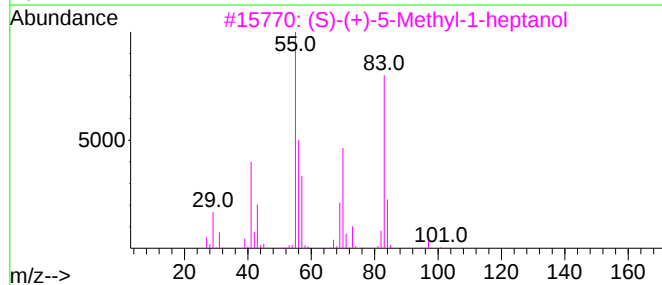
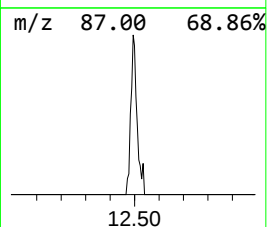
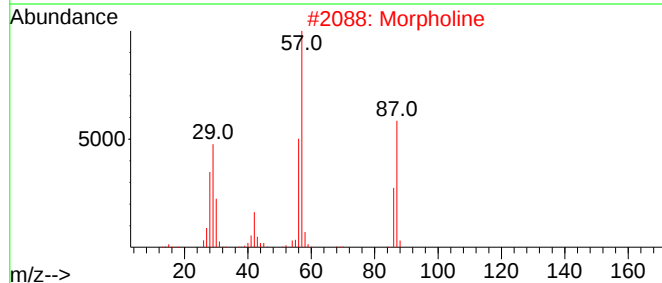
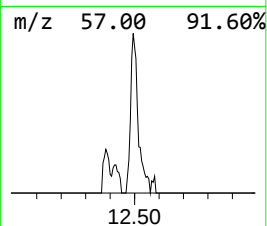
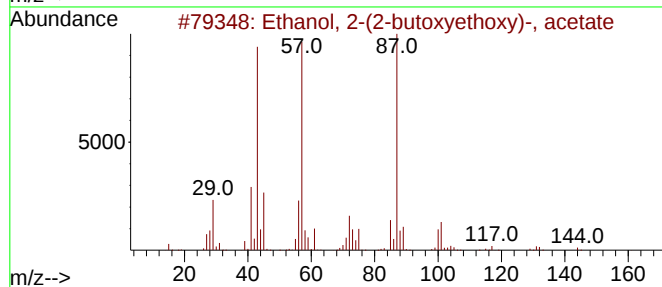
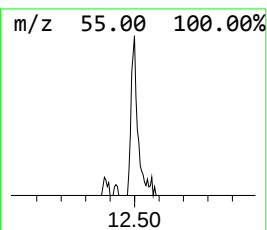
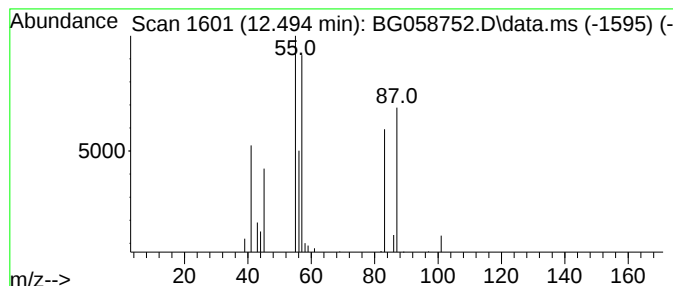
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Peak Number 4 unknown12.494 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.494	2.62 ng	29323	Naphthalene-d8	10.614

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	49
2			Morpholine	87	C4H9NO	000110-91-8	25
3			(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	25
4			3-Octanol, 1,1,2,2-tetrafluoro-	202	C8H14F4O	074810-72-3	23
5			2-Isobutoxyethyl acetate	160	C8H16O3	039220-44-5	12



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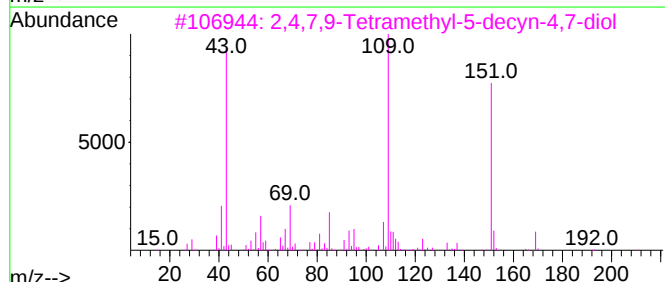
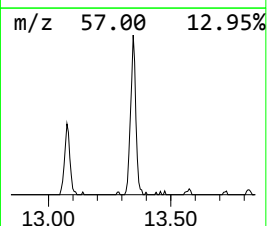
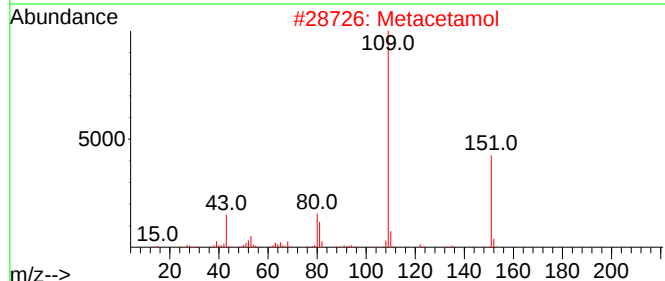
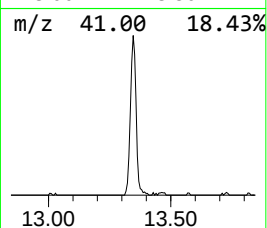
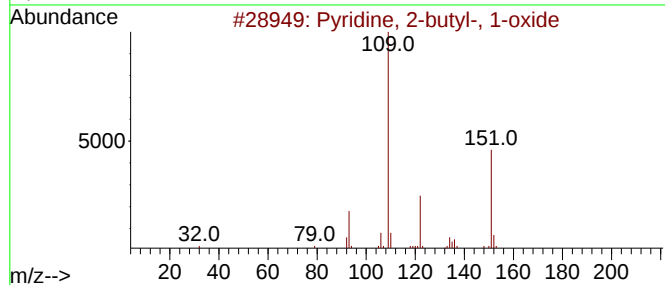
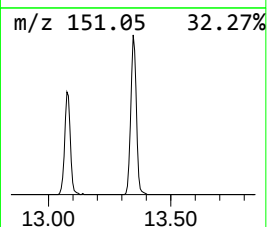
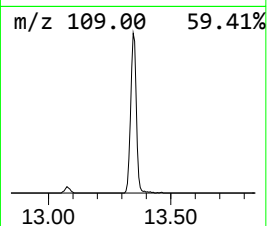
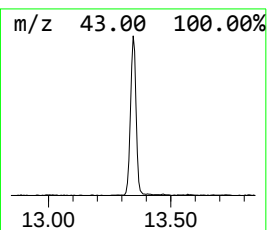
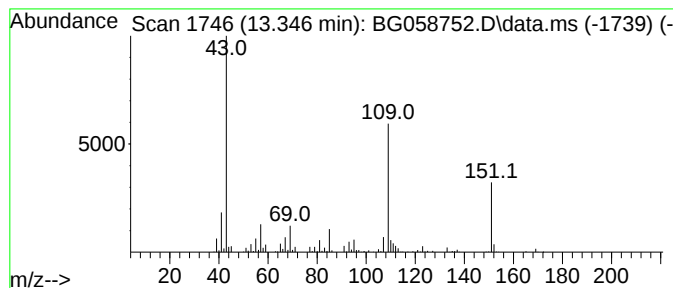
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pyridine, 2-butyl-, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.346	29.82 ng	469218	Acenaphthene-d10	14.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
2			Metacetamol	151	C8H9NO2	000621-42-1	47
3			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	47
4			Acetaminophen	151	C8H9NO2	000103-90-2	38
5			4-Amino-2-methylpyrimidine	109	C5H7N3	000074-69-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methyl Isobutyl...	3.581	3.8	ng	28101	1	7.811	149569	20.0
2-Propanol, 1-[...	11.137	14.4	ng	160751	2	10.614	223982	20.0
2-Propanol, 1-(...	11.195	18.7	ng	208942	2	10.614	223982	20.0
unknown12.494	12.494	2.6	ng	29323	2	10.614	223982	20.0
Pyridine, 2-but...	13.346	29.8	ng	469218	3	14.456	314659	20.0