

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
 Data File : BG049814.D
 Acq On : 12 Aug 2021 12:17
 Operator : CG/JU
 Sample : M3333-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 124055

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-BG080321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049814.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.132	11	16	21	rBV	62580	91520	6.06%	1.288%
2	5.106	347	352	358	rBV2	18173	29662	1.97%	0.417%
3	5.581	427	433	441	rBV	295142	482638	31.98%	6.793%
4	7.197	700	708	717	rBV	321915	559111	37.05%	7.869%
5	8.031	844	850	860	rBV	84689	144086	9.55%	2.028%
6	9.200	1041	1049	1062	rVB	194699	351732	23.30%	4.951%
7	10.616	1281	1290	1301	rBV3	24646	56050	3.71%	0.789%
8	10.857	1321	1331	1338	rBV	111247	210334	13.94%	2.960%
9	13.306	1739	1748	1754	rBV	523931	811005	53.73%	11.415%
10	14.687	1977	1983	1992	rVB	212439	338591	22.43%	4.766%
11	16.179	2230	2237	2244	rBV	639188	968363	64.16%	13.630%
12	17.436	2444	2451	2458	rBV	297552	468081	31.01%	6.588%
13	19.257	2758	2761	2765	rVB5	13841	18774	1.24%	0.264%
14	20.050	2890	2896	2903	rVB	1178364	1509270	100.00%	21.243%
15	21.354	3114	3118	3125	rBV4	31660	65040	4.31%	0.915%
16	21.430	3127	3131	3136	rBV	35179	57044	3.78%	0.803%
17	21.724	3175	3181	3187	rVB	266930	458386	30.37%	6.452%
18	25.002	3730	3739	3753	rVB2	166215	485141	32.14%	6.828%

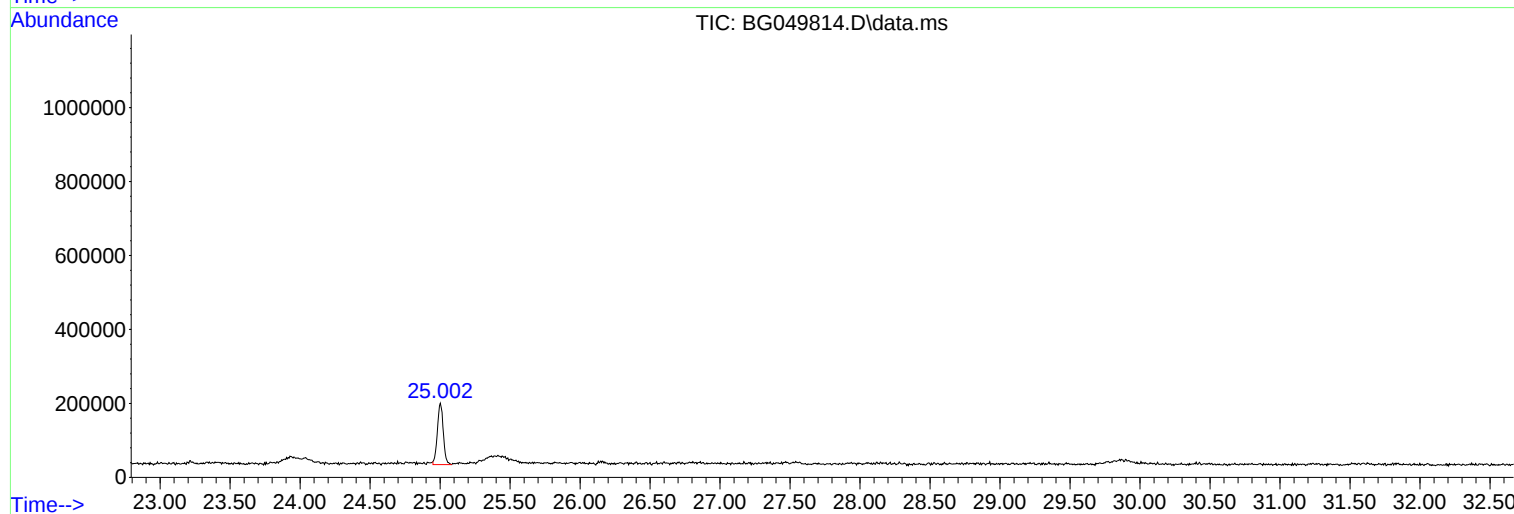
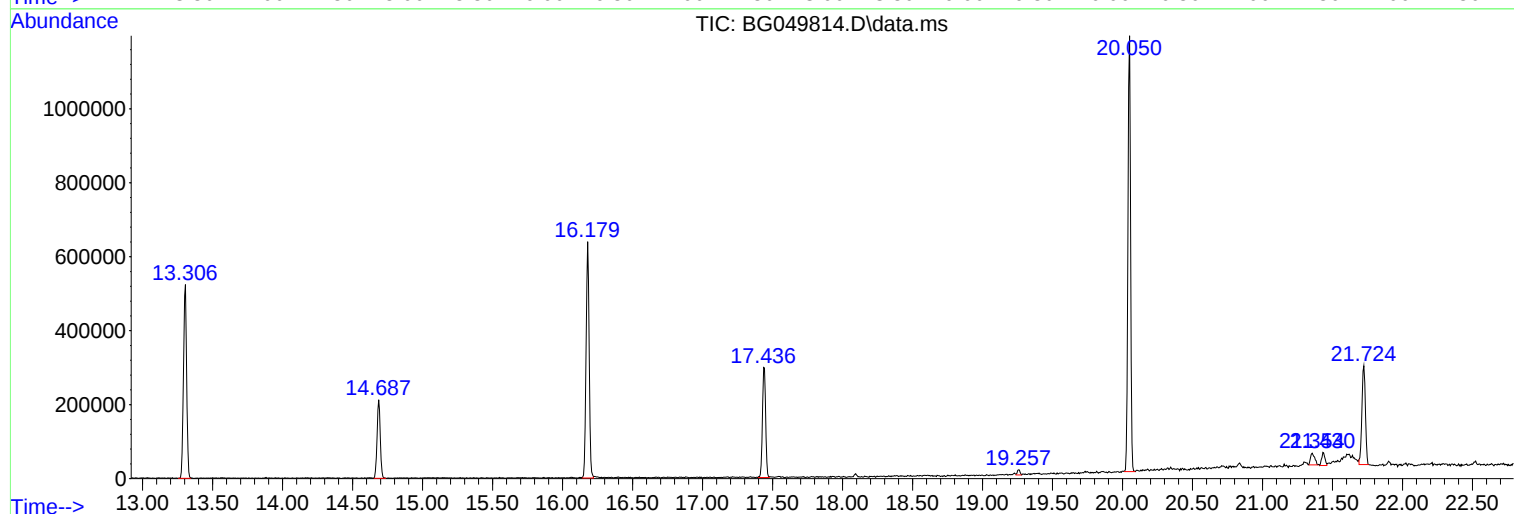
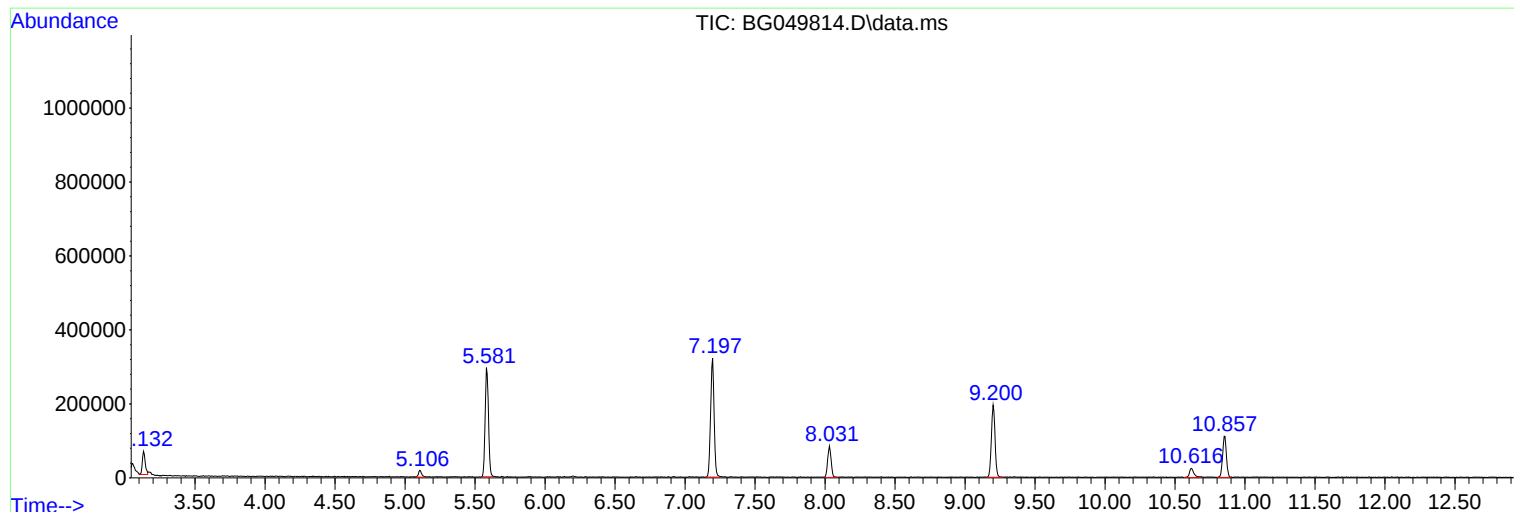
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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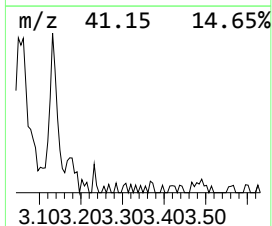
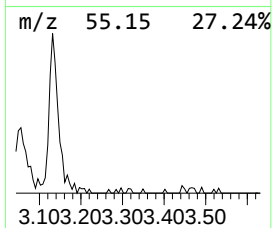
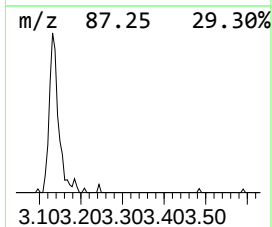
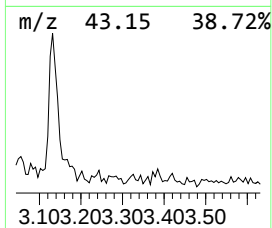
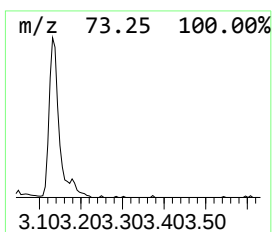
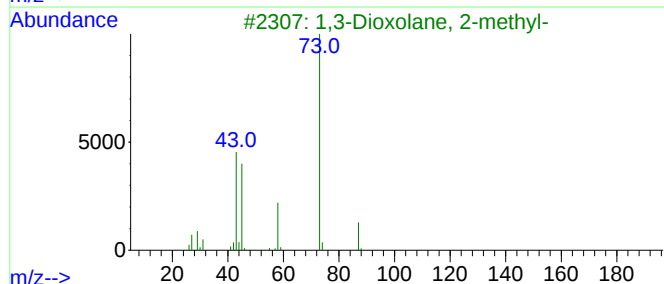
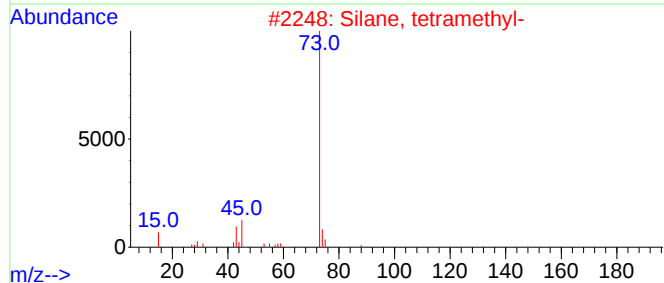
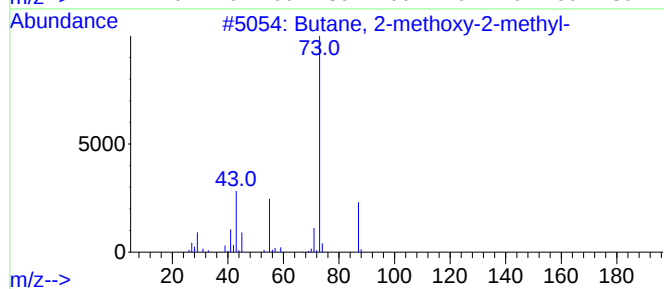
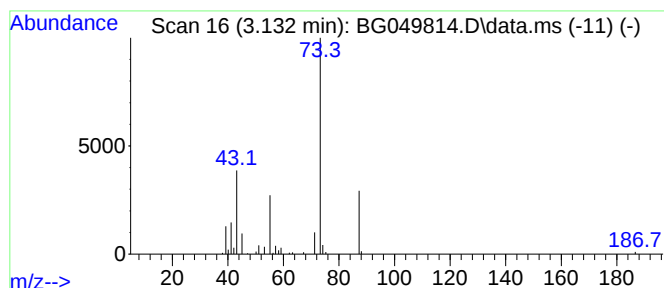
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.132	12.70 ng	91520	1,4-Dichlorobenzene-d4	8.031

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	9



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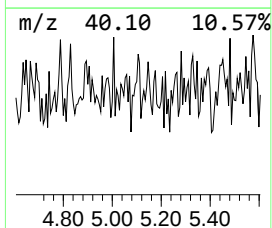
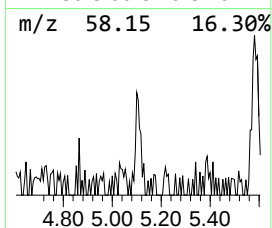
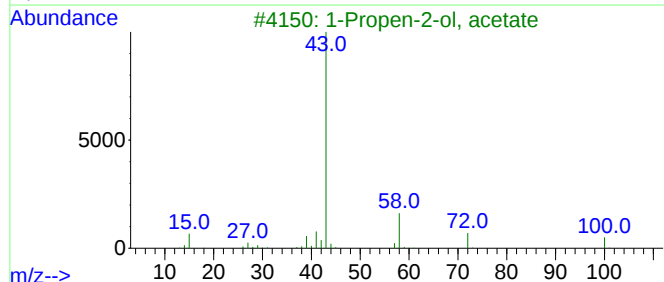
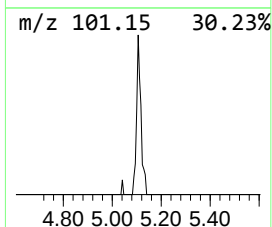
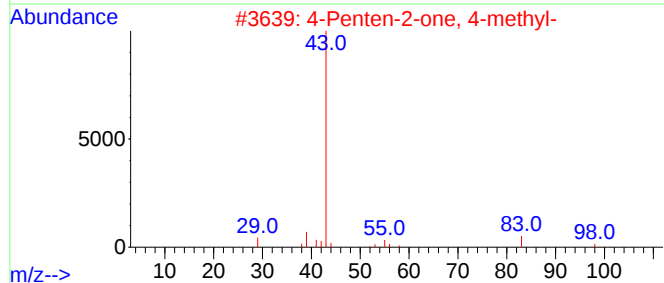
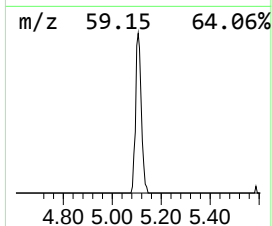
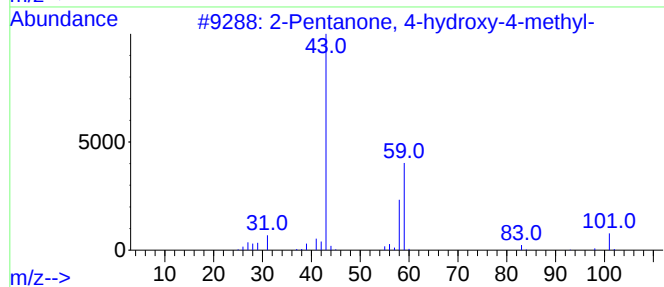
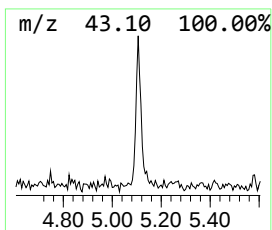
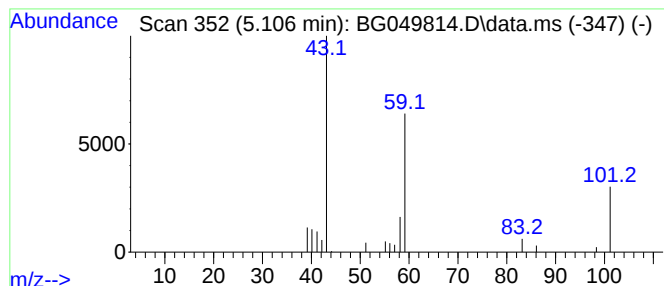
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.106	4.12 ng	29662	1,4-Dichlorobenzene-d4	8.031

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	9
5			Ethanol, 1-(methylenecyclopropyl)-	98	C6H10O	1000152-74-6	9



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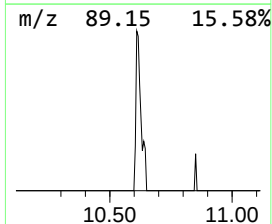
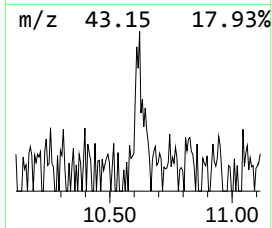
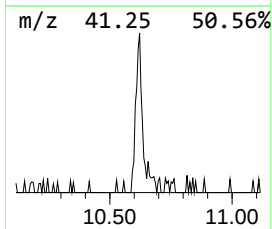
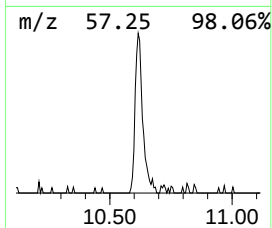
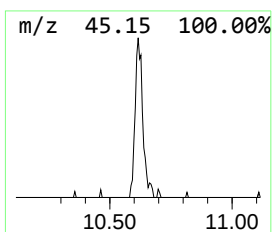
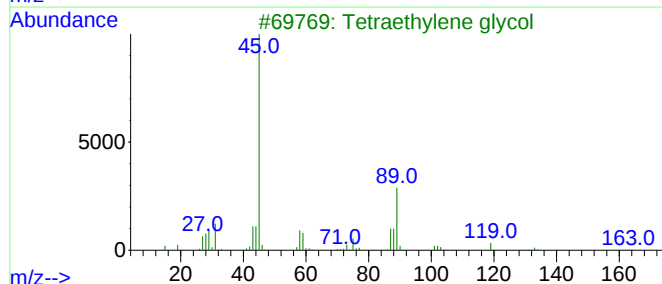
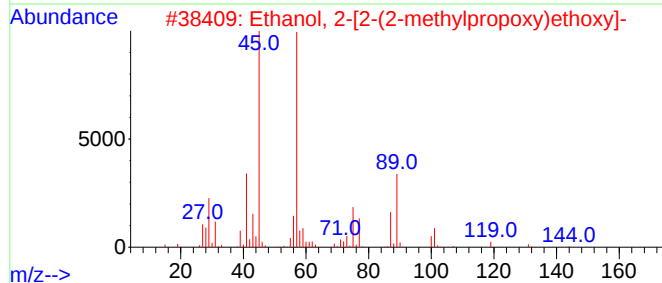
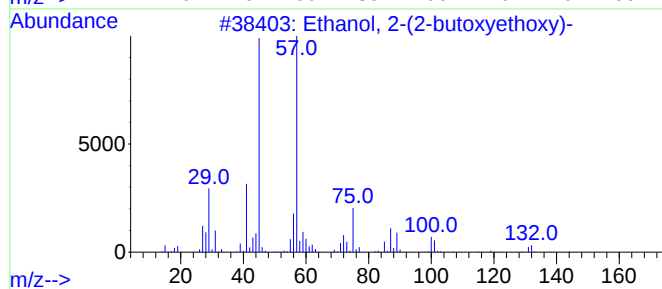
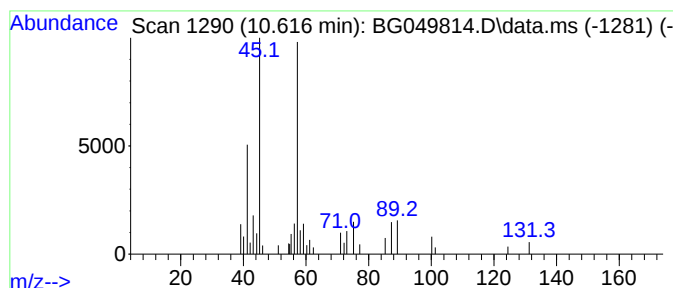
Instrument :
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.616	5.33 ng	56050	Naphthalene-d8	10.851	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	56
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	50
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	43



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
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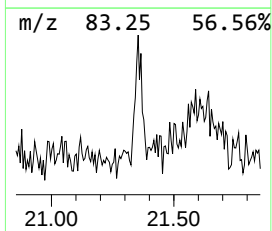
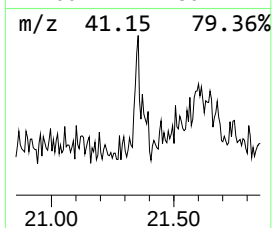
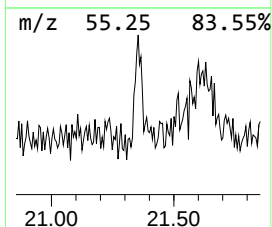
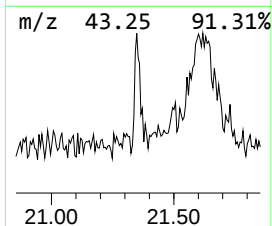
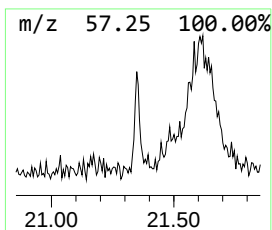
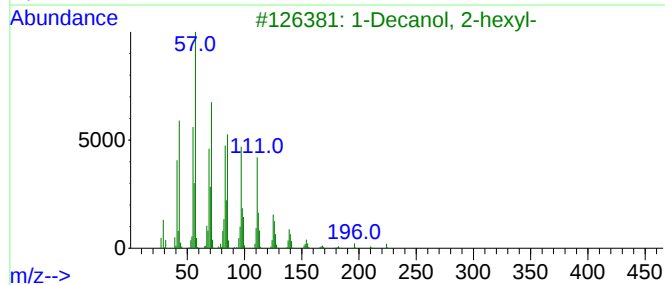
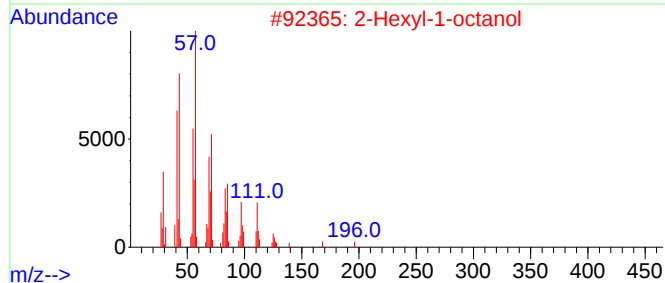
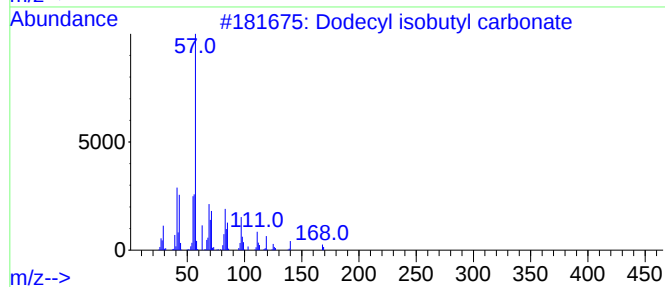
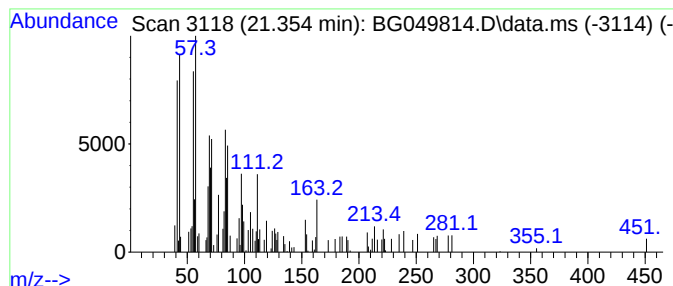
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Peak Number 4 Dodecyl isobutyl carbonate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.354	2.84 ng	65040	Chrysene-d12	21.724

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	72
2			2-Hexyl-1-octanol	214	C14H30O	019780-79-1	64
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	52
4			Carbonic acid, tridecyl 2,2,2-tr...	374	C16H29Cl3O3	1000314-55-9	52
5			Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	52



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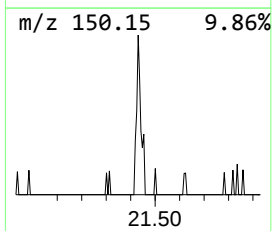
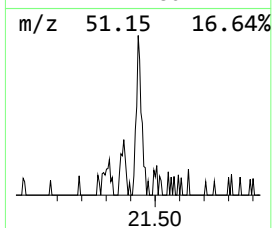
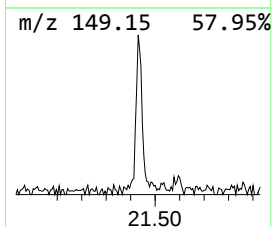
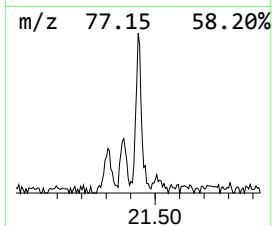
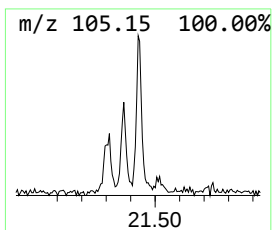
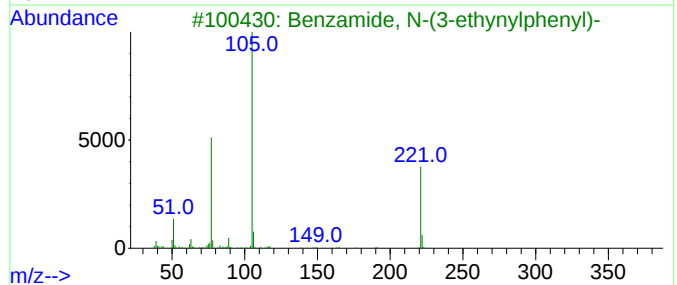
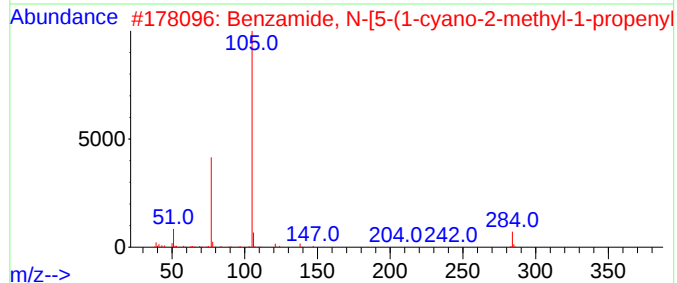
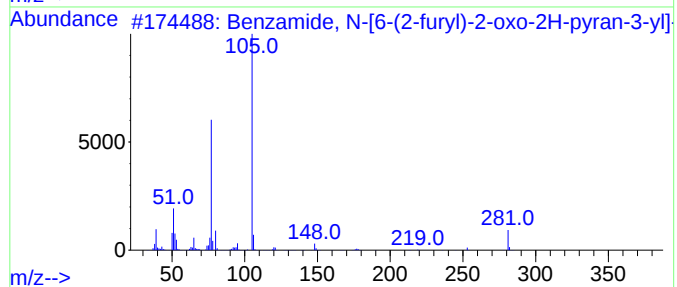
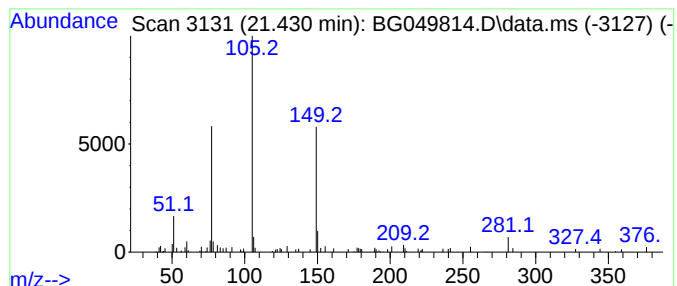
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Peak Number 5 unknown21.430 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.430	2.49 ng	57044	Chrysene-d12	21.724

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-[6-(2-furyl)-2-oxo-...	281	C16H11NO4	187749-77-5	43
2			Benzamide, N-[5-(1-cyano-2-methy...	284	C14H12N4OS	172535-11-4	38
3			Benzamide, N-(3-ethynylphenyl)-	221	C15H11NO	208943-24-2	38
4			4-Acetylphenylbenzoate	240	C15H12O3	001523-18-8	38
5			1,2,5-Benzothiadiazol, 4-benzamido-	255	C13H9N3OS	339302-44-2	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.132	12.7	ng	91520	1	8.031	144086	20.0
2-Pentanone, 4-...	5.106	4.1	ng	29662	1	8.031	144086	20.0
Ethanol, 2-(2-b...	10.616	5.3	ng	56050	2	10.851	210334	20.0
Dodecyl isobuty...	21.354	2.8	ng	65040	5	21.724	458386	20.0
unknown21.430	21.430	2.5	ng	57044	5	21.724	458386	20.0