

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102521\
 Data File : BG050711.D
 Acq On : 25 Oct 2021 15:18
 Operator : CG/JU
 Sample : M4313-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 1-3-TOTES

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-BG100621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050711.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.269	126	133	141	rBV3	6465	13111	1.10%	0.173%
2	5.315	303	311	317	rBV4	15046	26353	2.21%	0.349%
3	5.791	385	392	401	rVB	178482	297104	24.89%	3.931%
4	6.290	470	477	482	rBV3	7201	13437	1.13%	0.178%
5	7.389	655	664	677	rBV	109236	203735	17.07%	2.696%
6	8.247	804	810	817	rBV	117616	208216	17.45%	2.755%
7	9.422	1002	1010	1018	rBV	248749	461181	38.64%	6.102%
8	10.820	1240	1248	1259	rBV	168093	313919	26.30%	4.154%
9	11.073	1283	1291	1299	rBV	162390	299550	25.10%	3.964%
10	11.637	1379	1387	1392	rBV4	6597	12243	1.03%	0.162%
11	11.725	1395	1402	1409	rBV2	21364	39405	3.30%	0.521%
12	13.493	1692	1703	1710	rBV	574200	907784	76.06%	12.011%
13	14.786	1917	1923	1930	rBV	41880	66176	5.54%	0.876%
14	14.868	1930	1937	1944	rVB	252294	405993	34.02%	5.372%
15	15.256	1998	2003	2010	rVB	40267	64286	5.39%	0.851%
16	15.350	2015	2019	2028	rVB7	6824	14519	1.22%	0.192%
17	15.485	2035	2042	2047	rBV2	33452	54787	4.59%	0.725%
18	16.355	2183	2190	2197	rBV	387772	615417	51.57%	8.143%
19	16.549	2216	2223	2231	rBV10	7008	18893	1.58%	0.250%
20	17.260	2338	2344	2352	rBV	152385	252904	21.19%	3.346%
21	17.612	2398	2404	2412	rVB	307567	474033	39.72%	6.272%
22	17.724	2418	2423	2428	rBV3	15309	23159	1.94%	0.306%
23	18.247	2509	2512	2518	rVB2	31106	39098	3.28%	0.517%
24	18.470	2545	2550	2556	rBV2	46083	69609	5.83%	0.921%
25	19.404	2707	2709	2713	rVB4	13613	13340	1.12%	0.177%
26	20.197	2839	2844	2851	rBV	874440	1193456	100.00%	15.791%
27	21.508	3062	3067	3079	rBV2	126076	258364	21.65%	3.419%
28	21.608	3081	3084	3092	rVB	32162	48608	4.07%	0.643%
29	21.913	3130	3136	3144	rVB	296769	519785	43.55%	6.878%
30	25.327	3707	3717	3729	rBV3	189355	629177	52.72%	8.325%

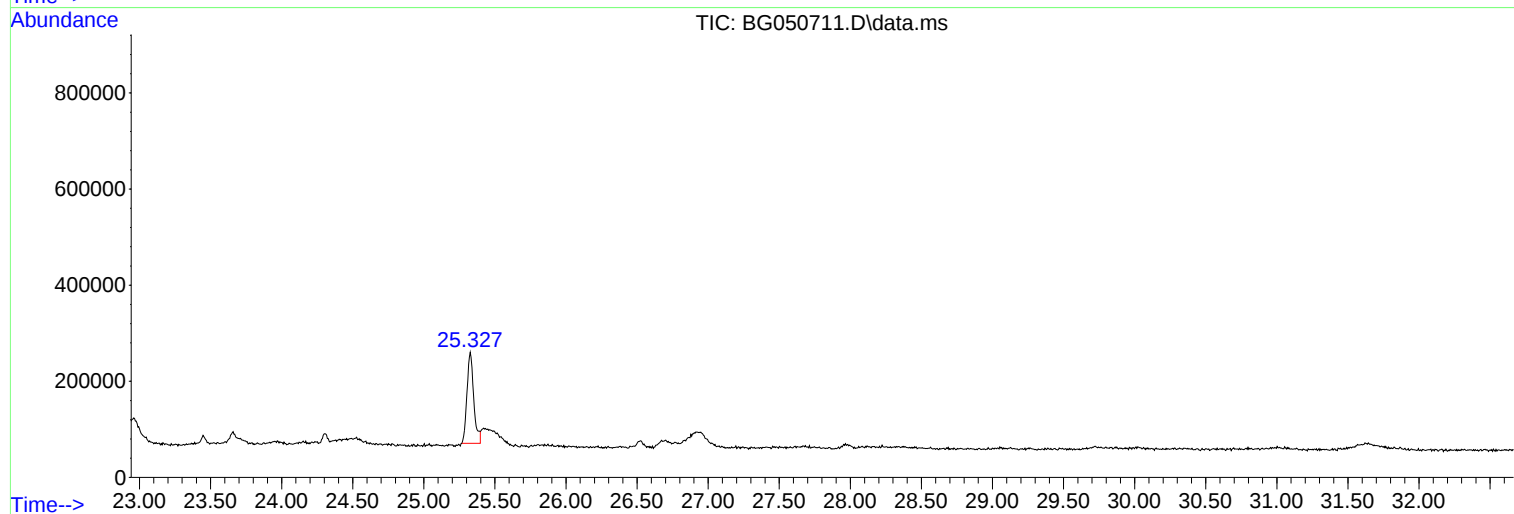
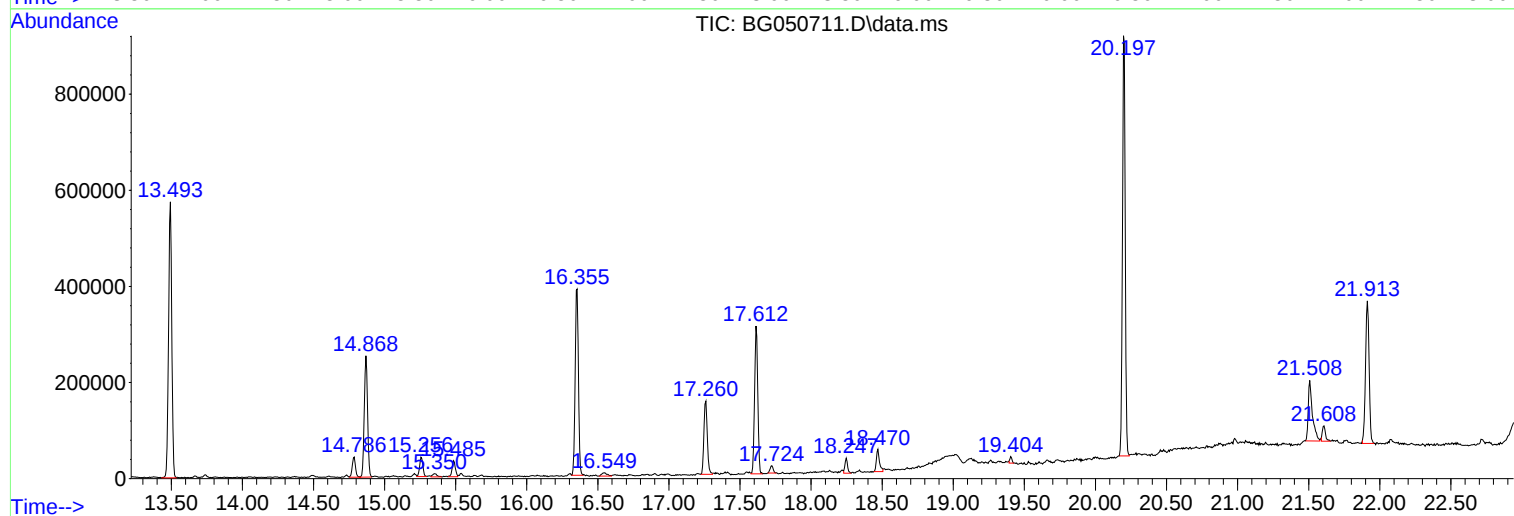
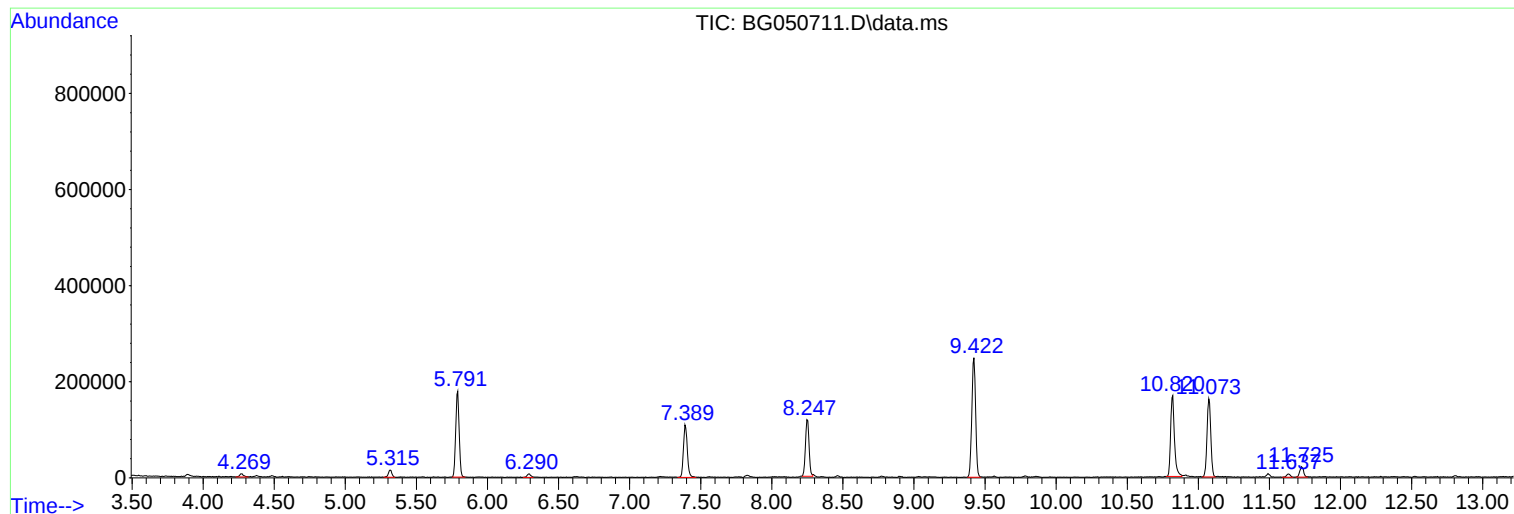
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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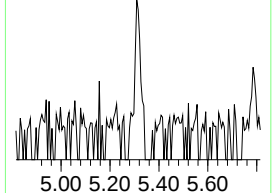
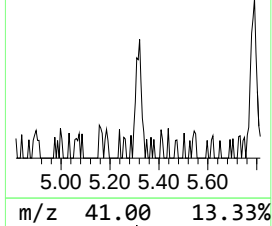
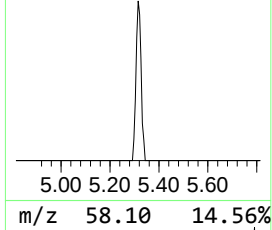
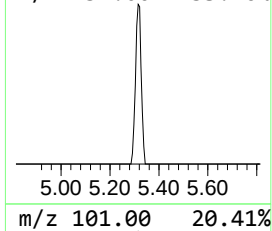
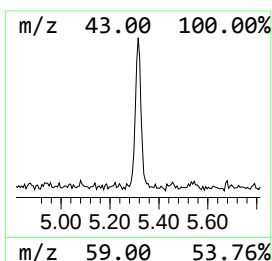
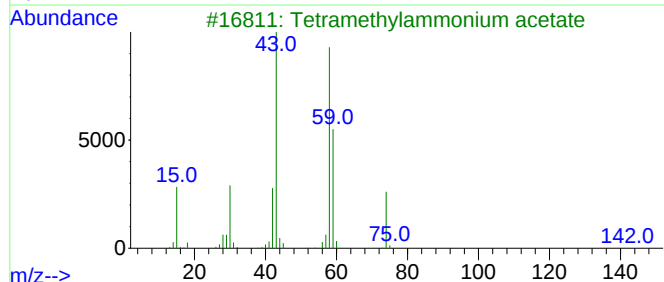
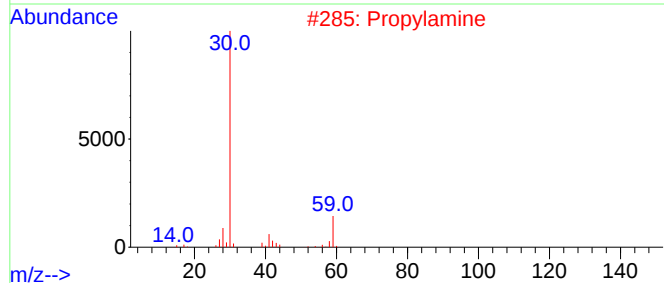
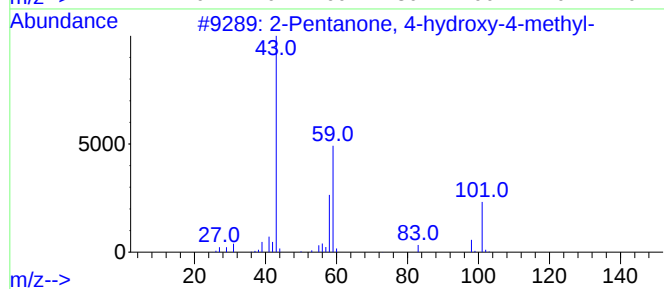
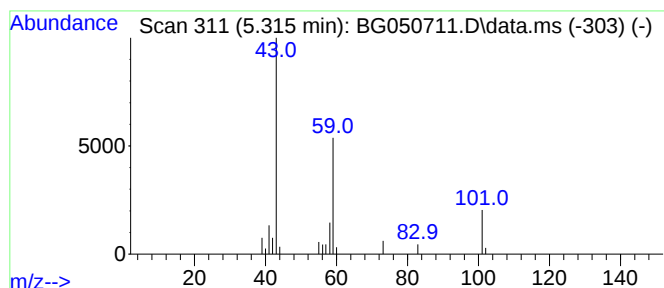
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.315	2.53 ng	26353	1,4-Dichlorobenzene-d4	8.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Propylamine	59	C3H9N	000107-10-8	37		
3	Tetramethylammonium acetate	133	C6H15NO2	010581-12-1	28		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25		
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	25		



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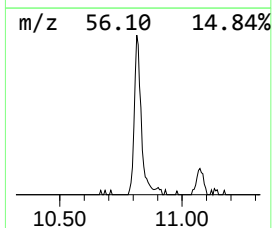
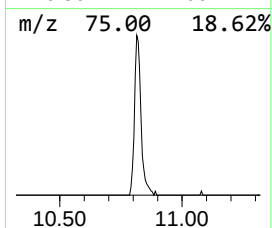
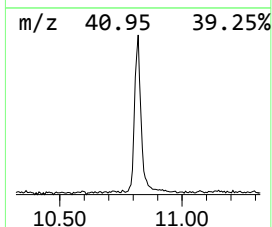
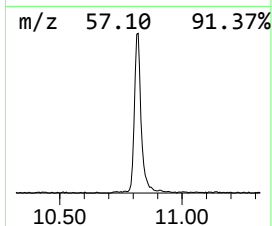
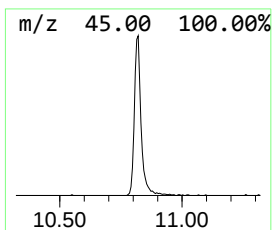
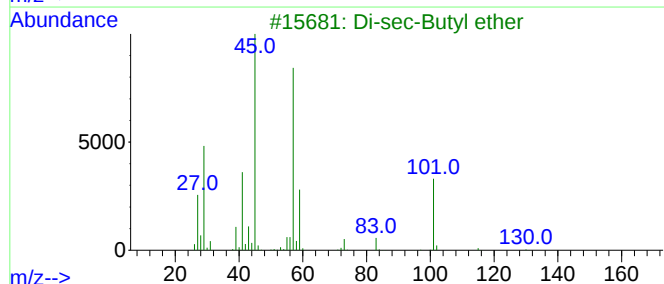
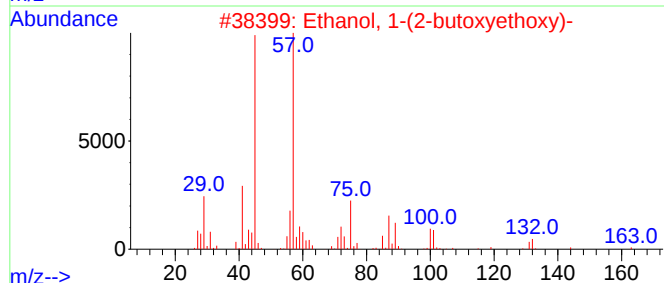
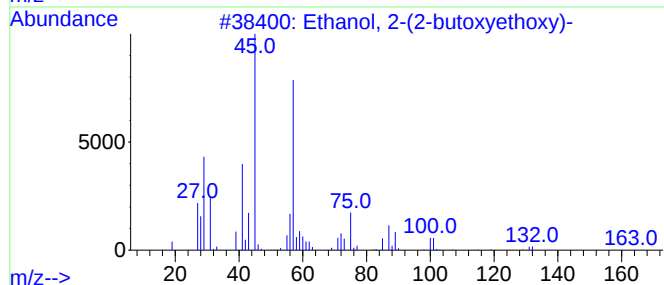
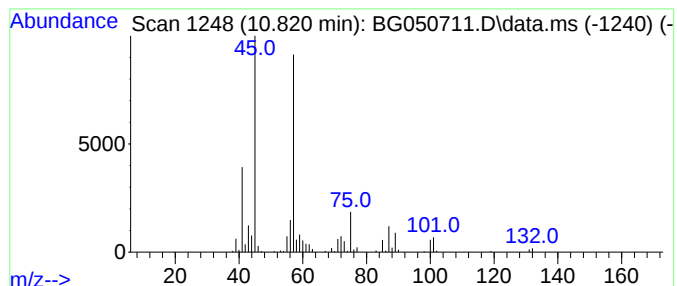
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.820	20.96 ng	313919	Naphthalene-d8	11.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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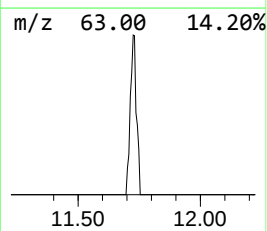
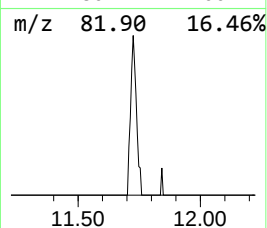
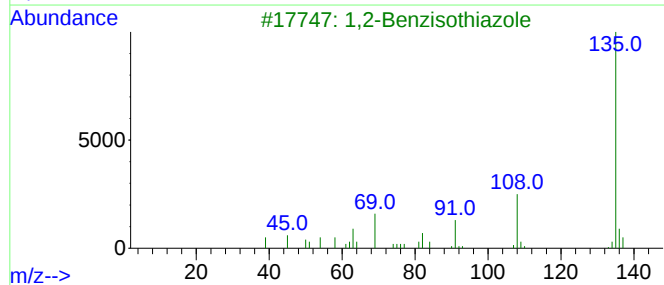
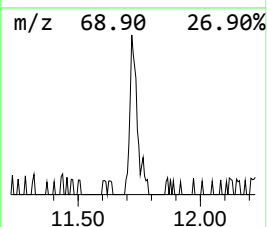
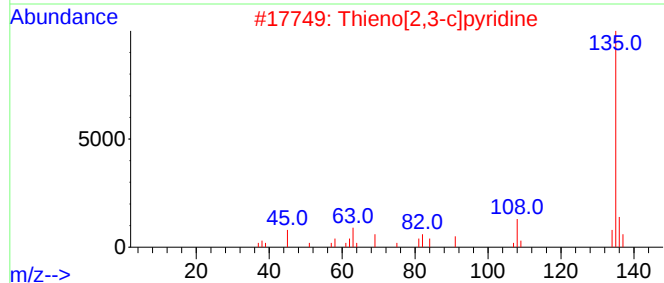
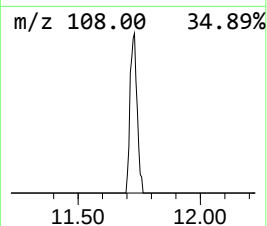
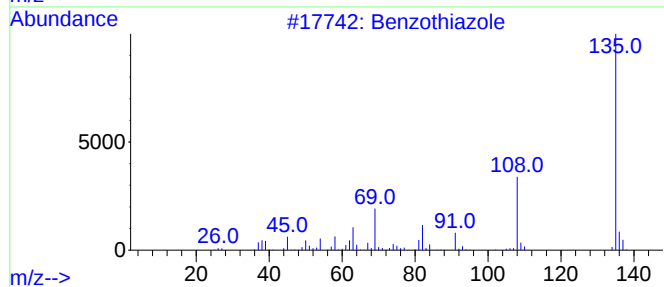
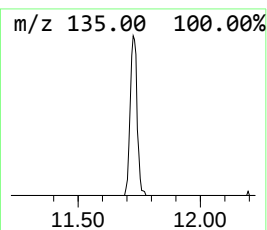
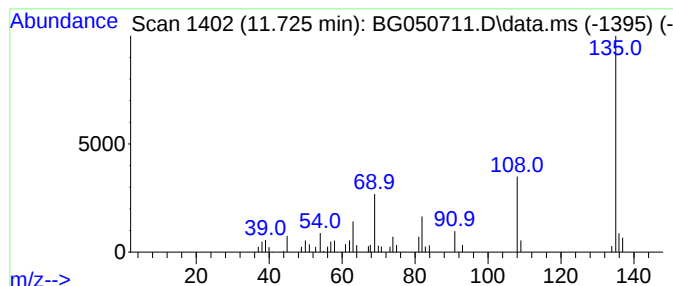
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.725	2.63 ng	39405	Naphthalene-d8	11.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzothiazole	135	C7H5NS	000095-16-9	94
2			Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	90
3			1,2-Benzisothiazole	135	C7H5NS	000272-16-2	83
4			3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
5			Thiocyanic acid, phenyl ester	135	C7H5NS	005285-87-0	59



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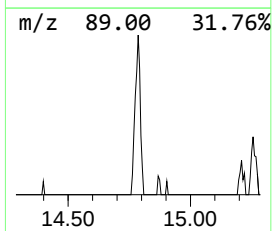
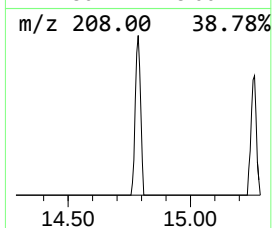
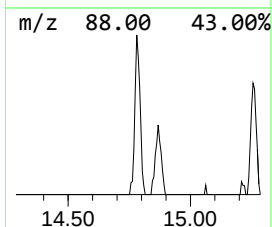
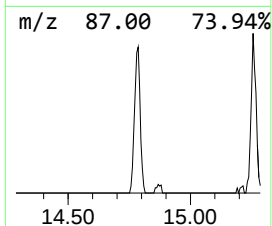
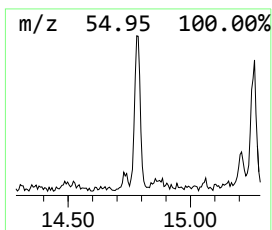
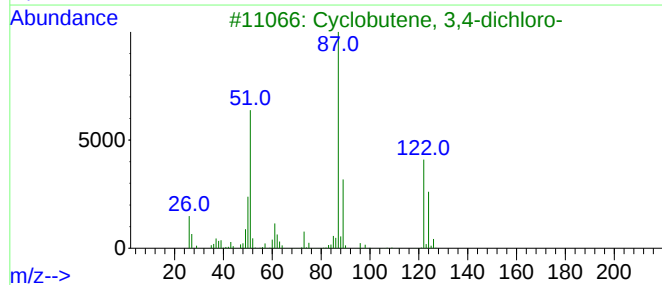
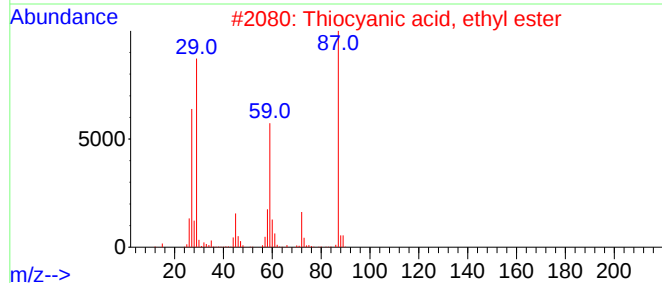
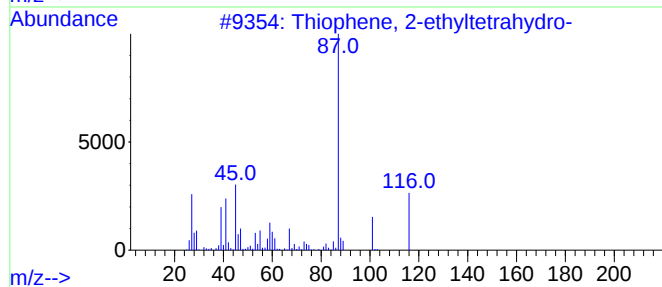
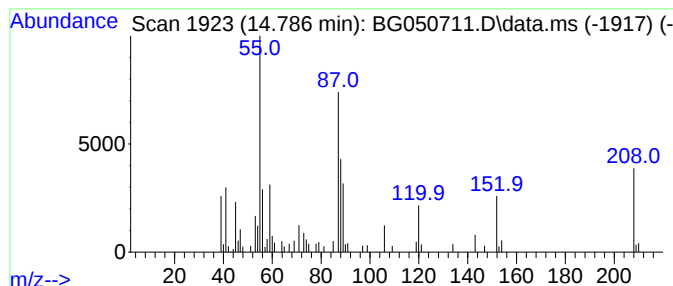
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Peak Number 4 unknown14.786 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	3.26 ng	66176	Acenaphthene-d10	14.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	27
2			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	16
3			Cyclobutene, 3,4-dichloro-	122	C4H4Cl2	041326-64-1	16
4			1,2,4-Trithiolane, 3,5-bis(1-met...	208	C8H16S3	054934-99-5	14
5			2-[2-[2-(2-(2-Butoxyethoxy)ethox...	336	C16H32O7	1000351-94-0	12



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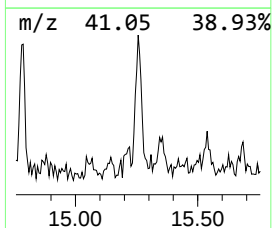
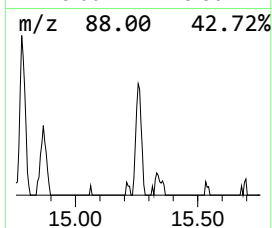
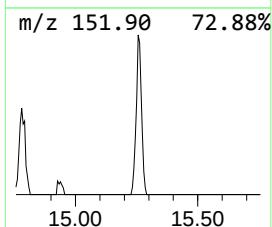
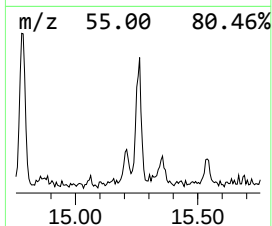
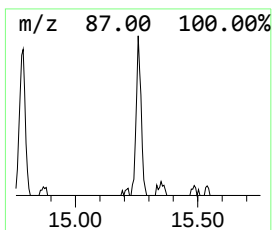
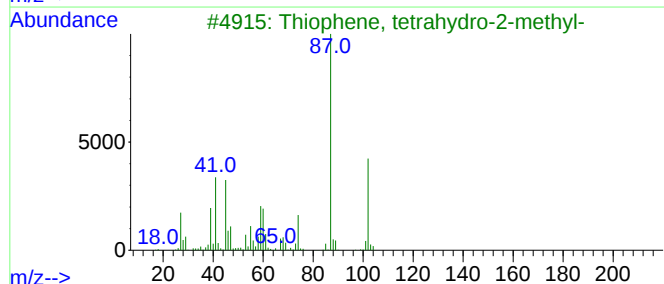
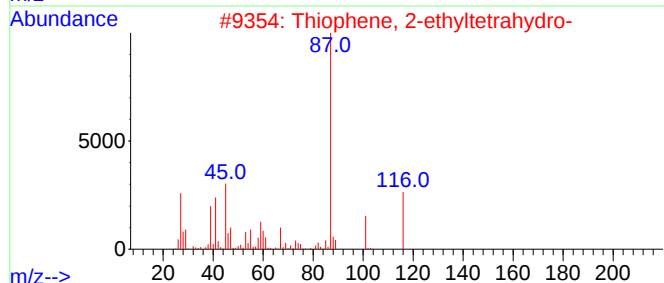
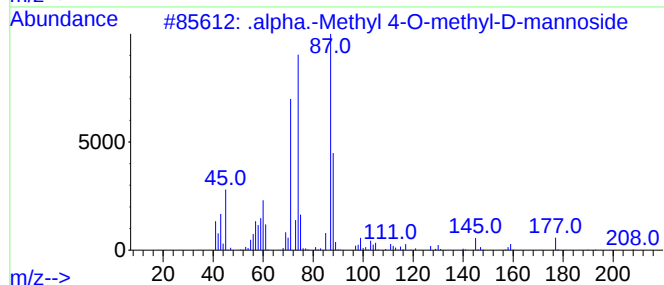
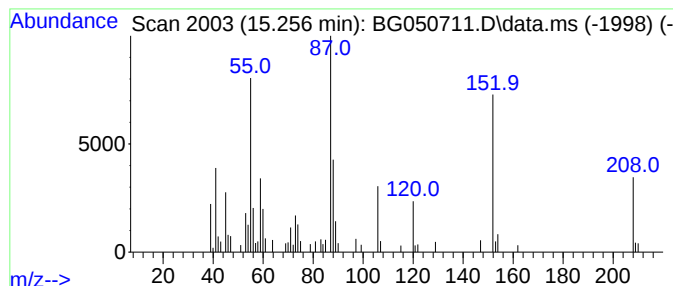
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Peak Number 5 unknown15.256 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.256	3.17 ng	64286	Acenaphthene-d10	14.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Methyl 4-O-methyl-D-mann...	208	C8H16O6	1000127-87-5	37
2			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	22
3			Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	22
4			1,2,5-Trithiepane	152	C4H8S3	006576-93-8	14
5			2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	558	C25H50O13	1000351-91-9	12



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1-3-TOTES

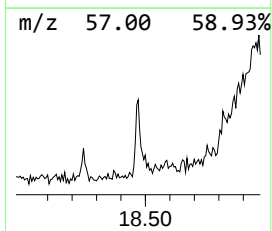
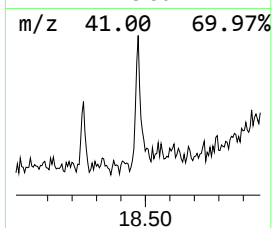
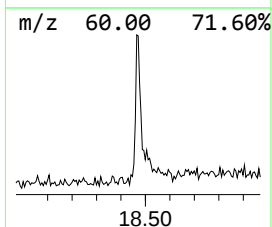
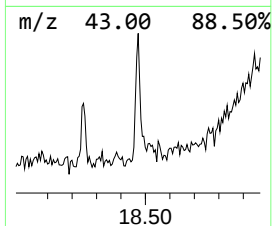
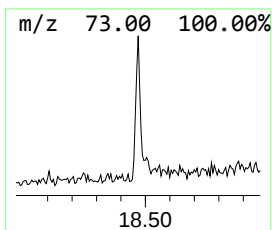
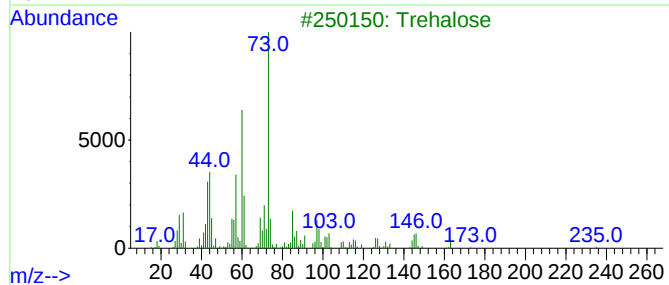
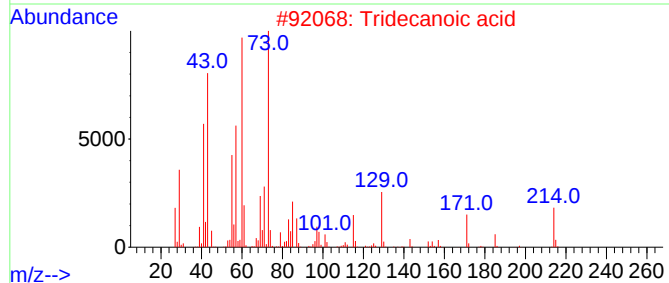
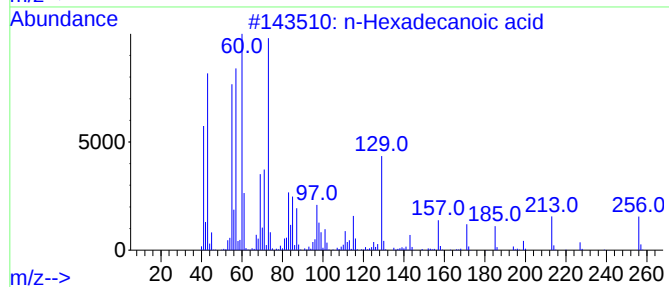
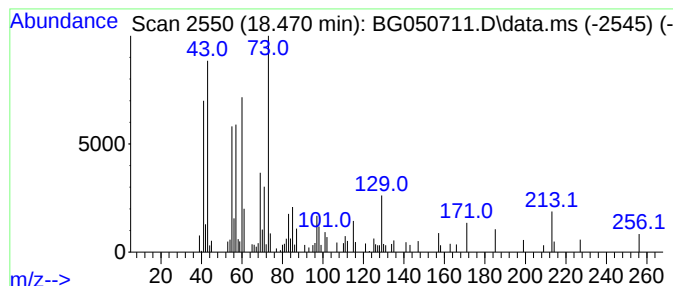
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.470	2.94 ng	69609	Phenanthrene-d10	17.612

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Trehalose	342	C12H22O11	000099-20-7	50
4		Dodecanoic acid	200	C12H24O2	000143-07-7	47
5		Nonanoic acid	158	C9H18O2	000112-05-0	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102521\
Data File : BG050711.D
Acq On : 25 Oct 2021 15:18
Operator : CG/JU
Sample : M4313-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

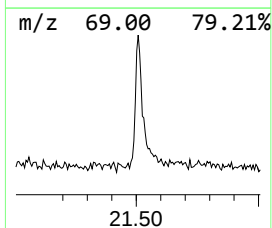
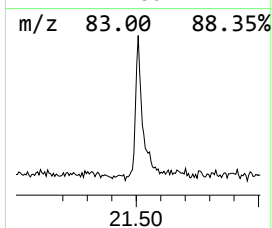
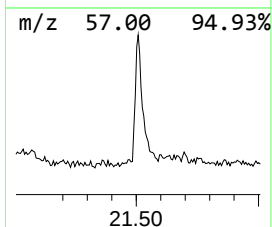
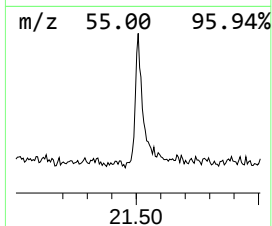
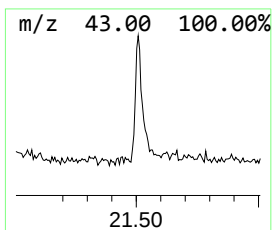
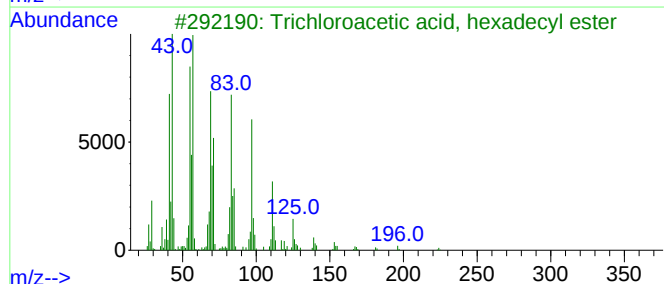
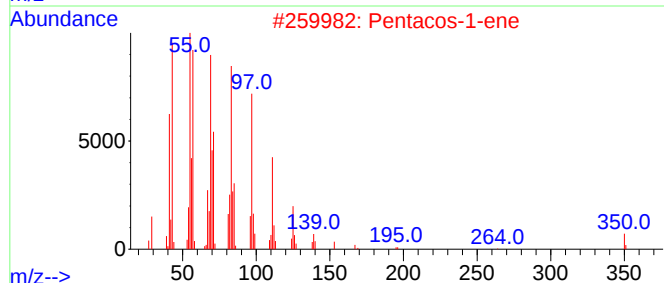
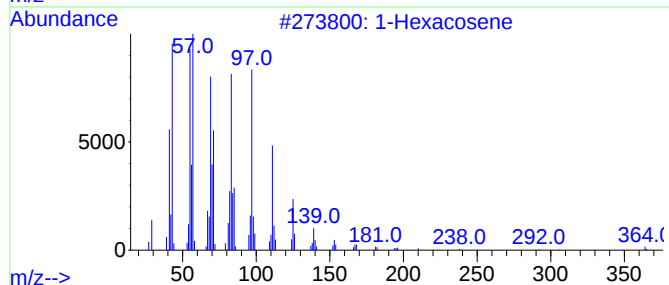
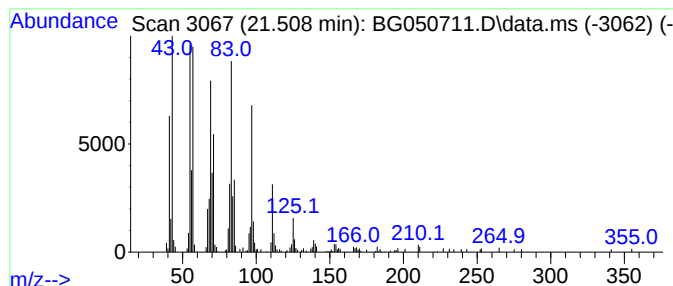
Instrument :
BNA_G
ClientSampleId :
1-3-TOTES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.508	9.94 ng	258364	Chrysene-d12	21.913	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
5	1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102521\
Data File : BG050711.D
Acq On : 25 Oct 2021 15:18
Operator : CG/JU
Sample : M4313-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1-3-TOTES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.315	2.5	ng	26353	1	8.253	208216	20.0
Ethanol, 2-(2-b...	10.820	21.0	ng	313919	2	11.073	299550	20.0
Benzothiazole	11.725	2.6	ng	39405	2	11.073	299550	20.0
unknown14.786	14.786	3.3	ng	66176	3	14.868	405993	20.0
unknown15.256	15.256	3.2	ng	64286	3	14.868	405993	20.0
n-Hexadecanoic ...	18.470	2.9	ng	69609	4	17.612	474033	20.0
1-Hexacosene	21.508	9.9	ng	258364	5	21.913	519785	20.0