

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
 Data File : BG028805.D
 Acq On : 18 Sep 2017 21:39
 Operator : SJ/JU
 Sample : I5259-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20170603-COMP-D

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:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.858	379	386	397	rVB	282034	480369	14.08%	3.206%
2	7.445	649	656	668	rBV	197870	379826	11.14%	2.535%
3	7.821	713	720	731	rBV	488219	872870	25.59%	5.825%
4	8.291	793	800	805	rBV	106615	186585	5.47%	1.245%
5	8.614	848	855	865	rBV	438617	772742	22.66%	5.157%
6	9.460	991	999	1009	rBV	366505	690658	20.25%	4.609%
7	11.111	1271	1280	1288	rBV	143584	271569	7.96%	1.812%
8	13.255	1639	1645	1651	rBV2	23238	39349	1.15%	0.263%
9	13.526	1680	1691	1703	rBV	1177075	1850637	54.26%	12.351%
10	13.767	1725	1732	1740	rVB2	21448	40238	1.18%	0.269%
11	14.413	1837	1842	1848	rBV2	62525	90293	2.65%	0.603%
12	14.542	1859	1864	1868	rVB2	28575	37883	1.11%	0.253%
13	14.906	1918	1926	1935	rBV2	269289	436634	12.80%	2.914%
14	15.294	1986	1992	1999	rBV	167457	245249	7.19%	1.637%
15	15.670	2051	2056	2060	rBV	269792	363628	10.66%	2.427%
16	16.399	2172	2180	2191	rBV	1123598	1816993	53.27%	12.127%
17	17.227	2316	2321	2328	rVB2	35808	53368	1.56%	0.356%
18	17.586	2376	2382	2388	rBV	38290	55618	1.63%	0.371%
19	17.656	2388	2394	2403	rBV2	419005	668495	19.60%	4.461%
20	18.302	2495	2504	2512	rBV3	108298	173437	5.09%	1.158%
21	18.508	2535	2539	2545	rBV5	26061	41781	1.23%	0.279%
22	19.901	2767	2776	2785	rBV3	85774	175667	5.15%	1.172%
23	20.247	2829	2835	2847	rBV	2581823	3410611	100.00%	22.762%
24	21.405	3027	3032	3043	rBV2	58949	128233	3.76%	0.856%
25	21.557	3054	3058	3068	rBV2	16404	46289	1.36%	0.309%
26	21.980	3122	3130	3141	rBV	438375	789016	23.13%	5.266%
27	23.185	3328	3335	3347	rBV6	40879	133638	3.92%	0.892%
28	25.447	3707	3720	3736	rBV2	229277	731971	21.46%	4.885%

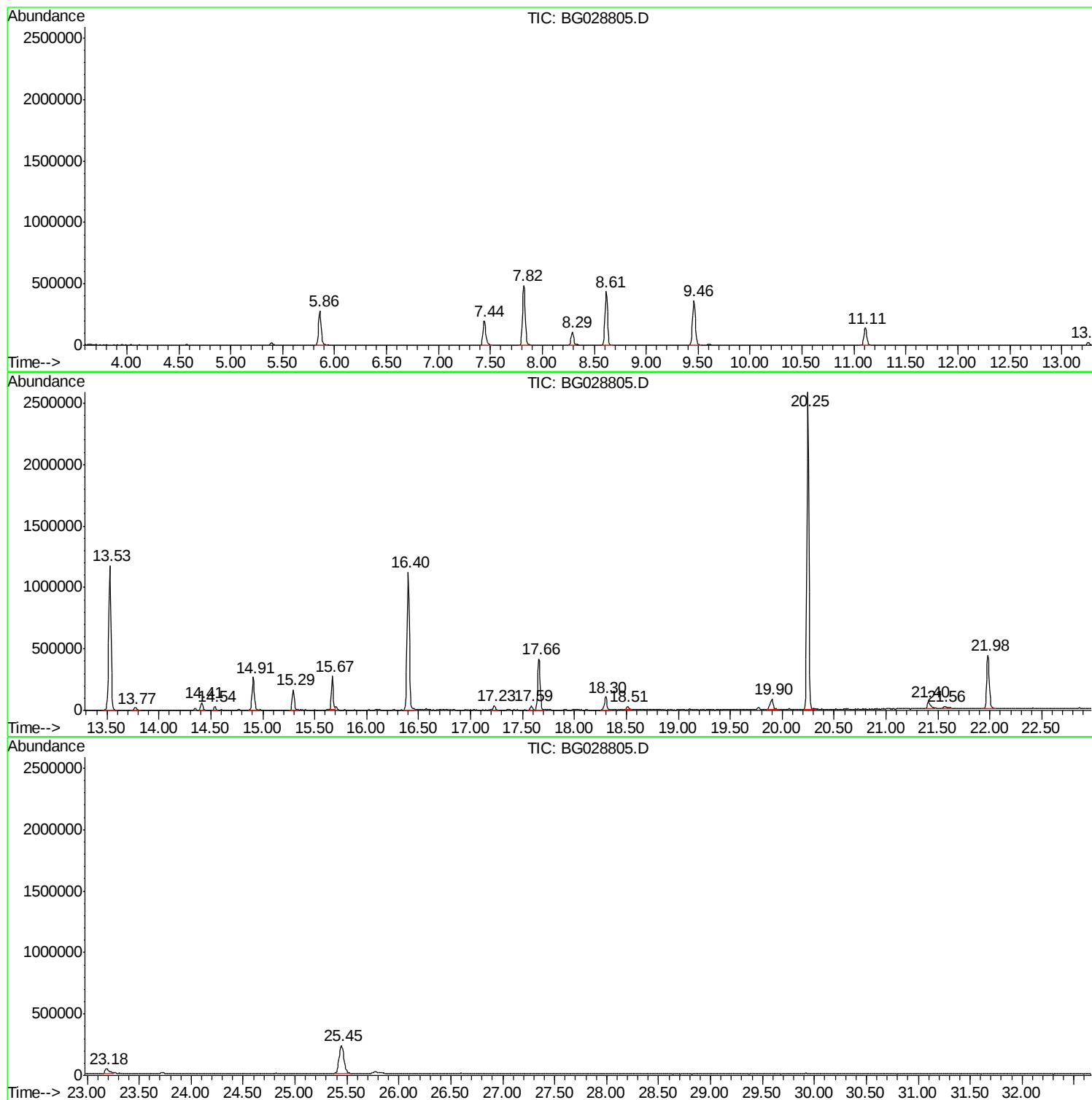
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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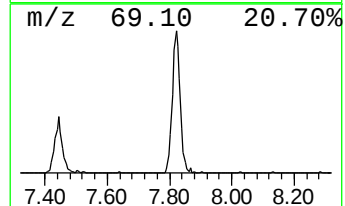
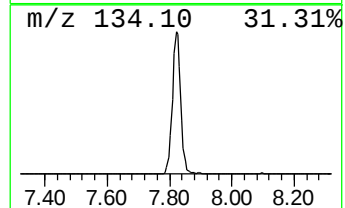
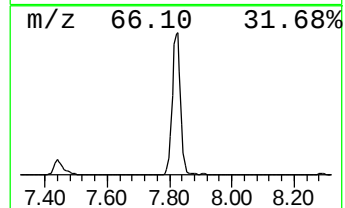
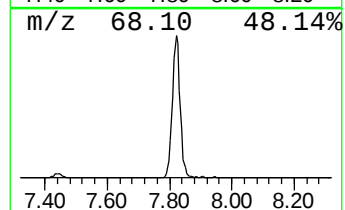
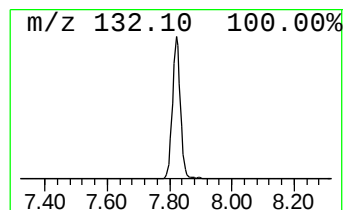
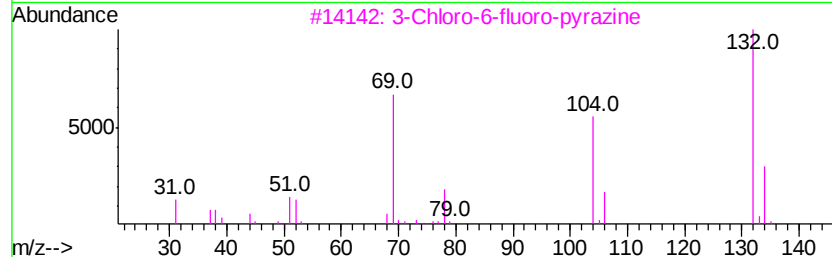
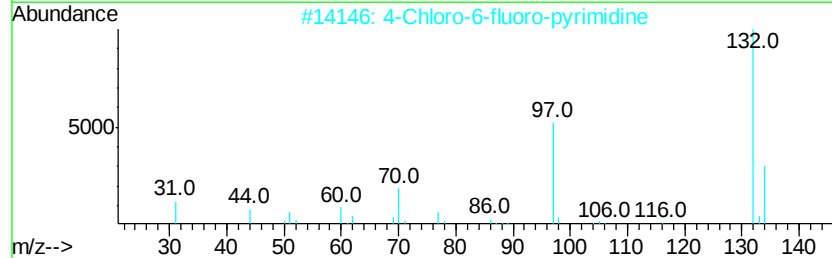
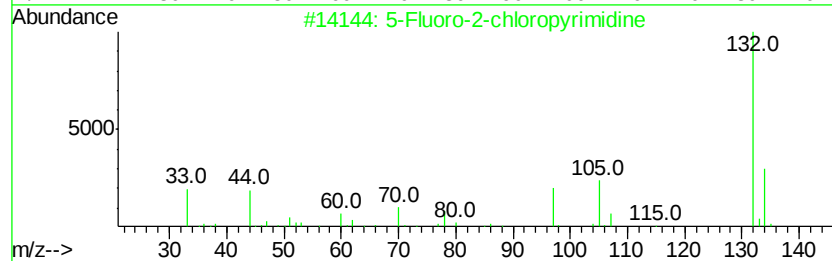
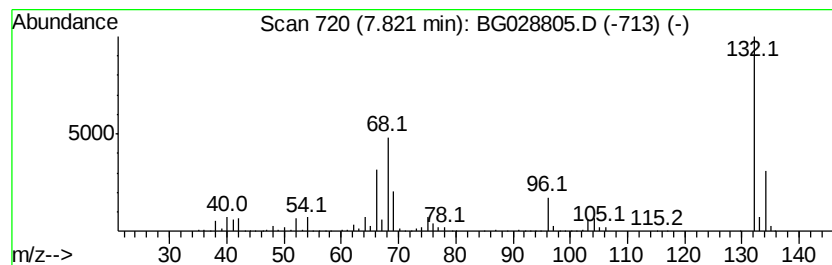
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	93.56 ng	872870	1,4-Dichlorobenzene-d4	8.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10



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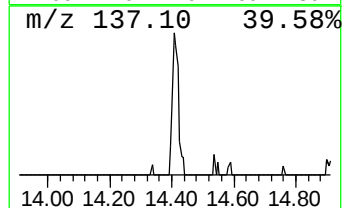
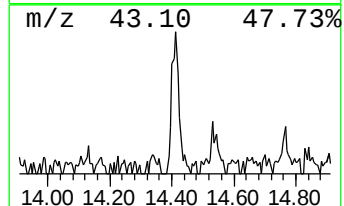
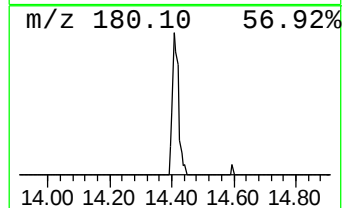
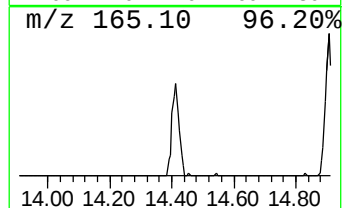
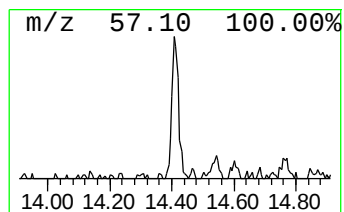
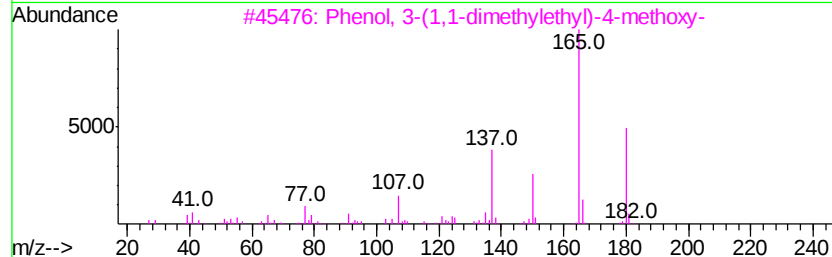
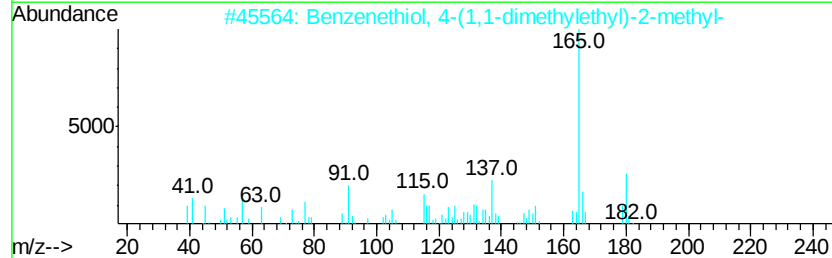
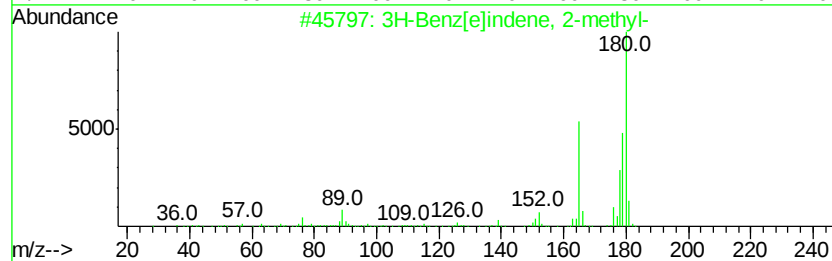
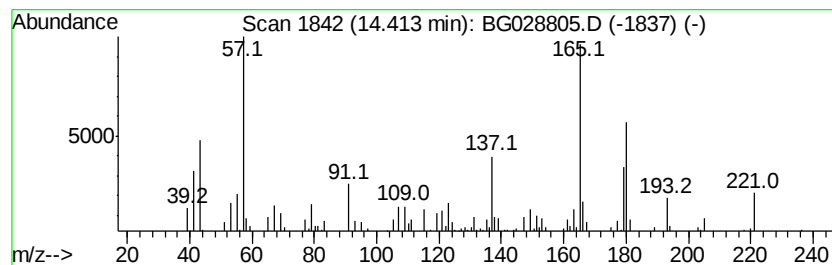
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Peak Number 3 3H-Benz[e]indene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.41	4.14 ng	90293	Acenaphthene-d10		14.91
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-Benz[elindene, 2-methyl-	180	C14H12	150096-60-9	62
2	Benzenethiol, 4-(1,1-dimethyleth...	180	C11H16S	015570-10-2	62
3	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	62
4	3',5'-Dimethoxvacetophenone	180	C10H12O3	039151-19-4	58
5	Pentacyclo[6.4.0.1(1,8).1(2,7)]t...	180	C14H12	086120-84-5	53



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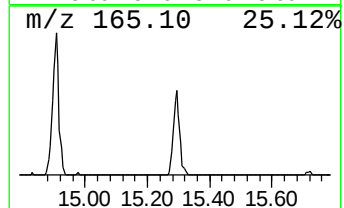
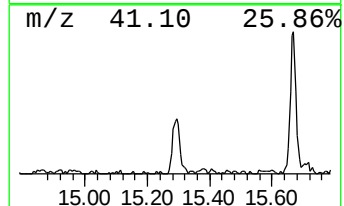
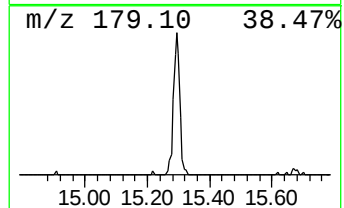
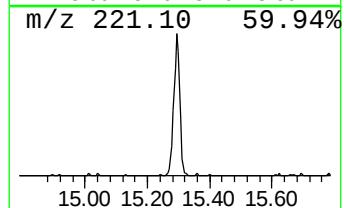
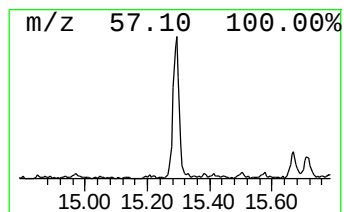
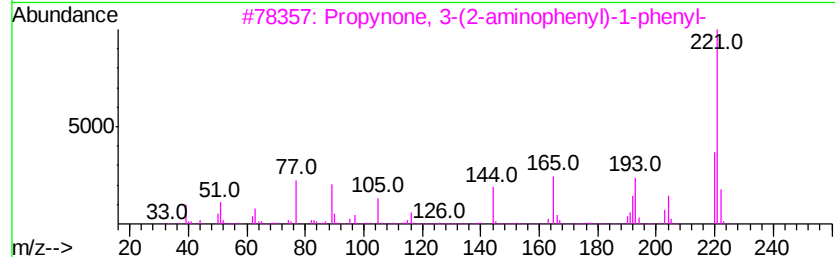
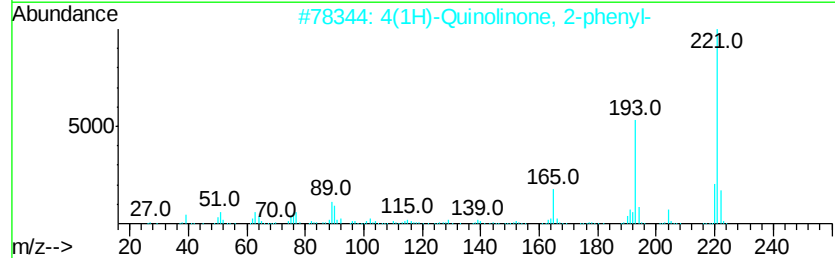
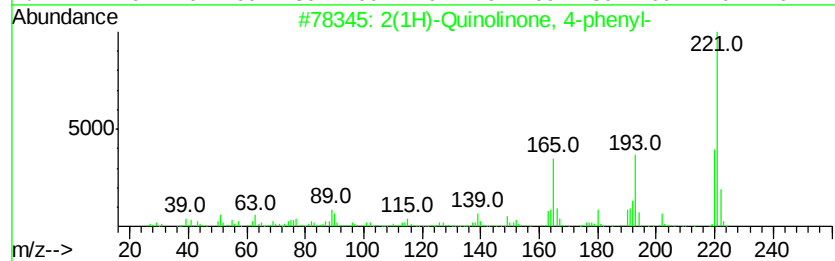
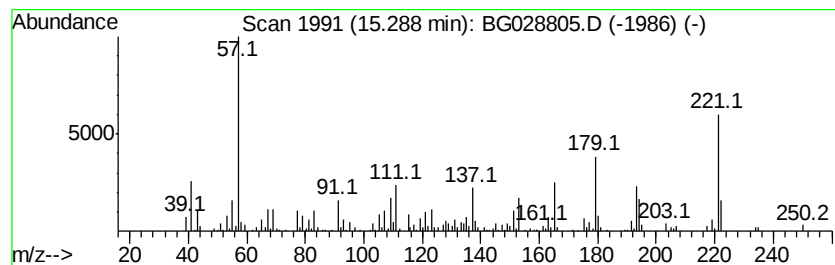
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Peak Number 4 unknown15.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	11.23 ng	245249	Acenaphthene-d10	14.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	38
2		4(1H)-Quinolinone, 2-phenyl-	221	C15H11NO	014802-18-7	27
3		Propynone, 3-(2-aminophenyl)-1-phenyl-	221	C15H11NO	1000311-26-1	22
4		4-Quinolinol, 2-phenyl-	221	C15H11NO	001144-20-3	16
5		4H-Pyrido[1,2-a]pyrimidine-3-carboxamide	221	C11H15N3O2	064399-29-7	15



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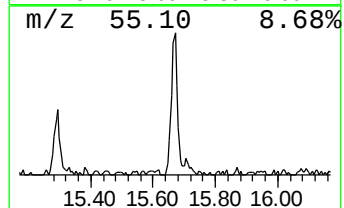
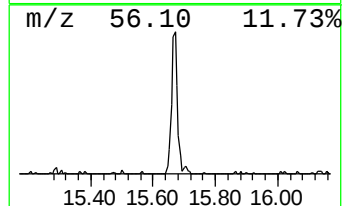
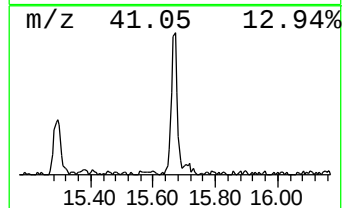
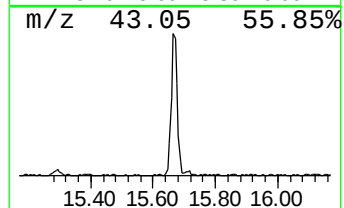
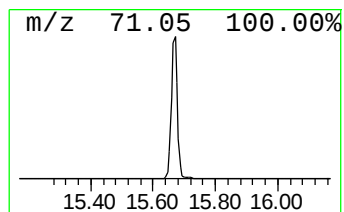
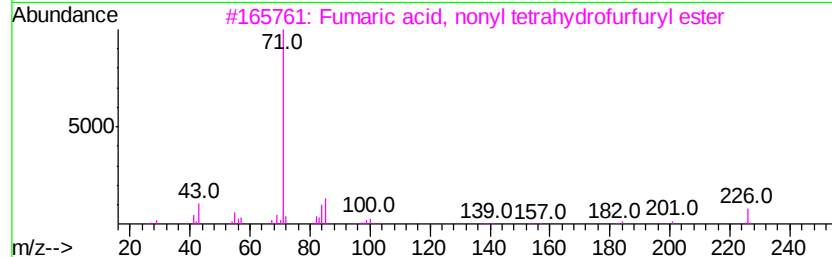
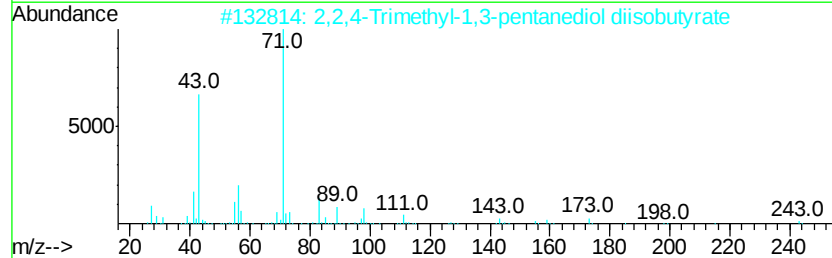
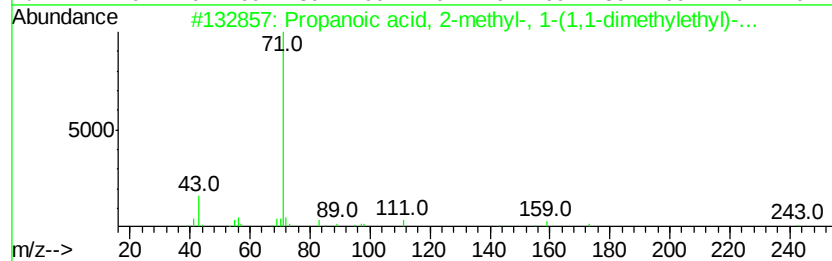
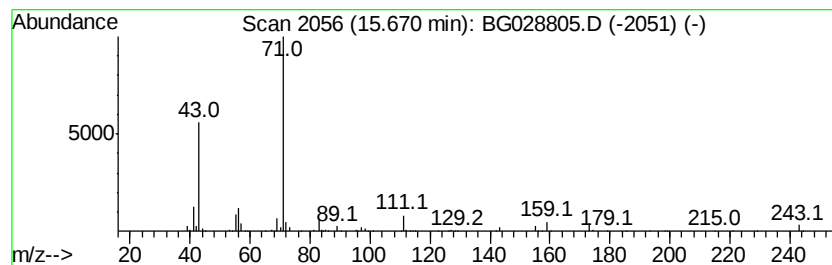
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Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	16.66 ng	363628	Acenaphthene-d10	14.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	64
2		2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	56
3		Fumaric acid, nonyl tetrahydrofu...	326	C18H30O5	1000330-58-3	53
4		Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	47
5		3-Methyl-hepta-1,6-dien-3-ol	126	C8H14O	034780-69-3	45



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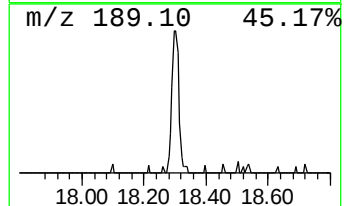
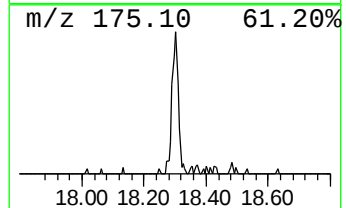
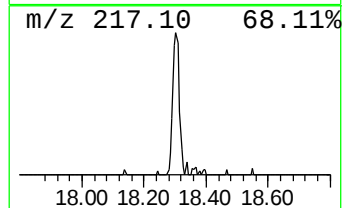
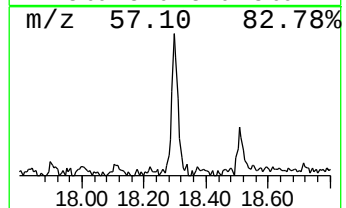
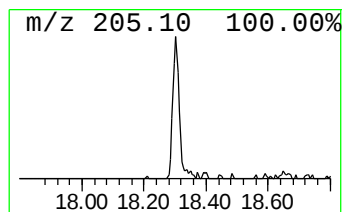
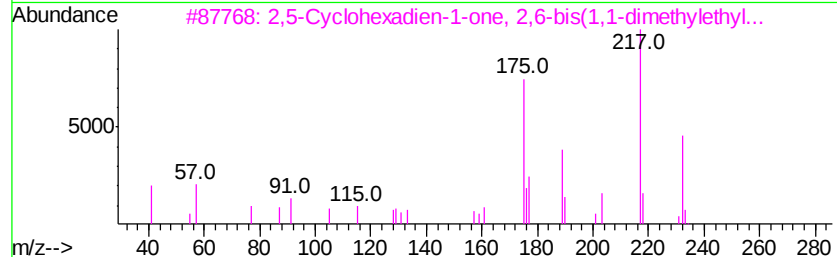
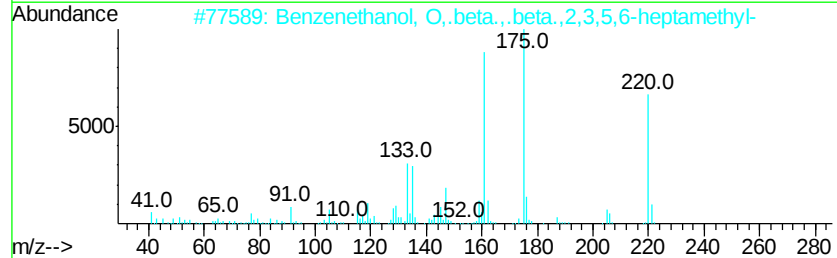
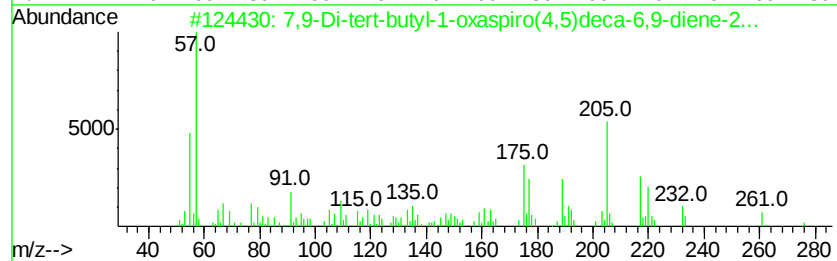
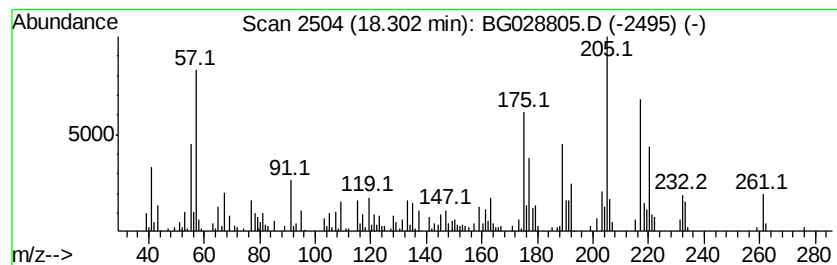
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Peak Number 6 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 5

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18.30	5.19 ng	173437	Phenanthrene-d10	17.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
2	Benzenethanol, 0,.beta.,.beta.,2...	220	C15H24O	1000128-94-8	56
3	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	47
4	Benzene, 1,1'-(1-methyl-2-butynv...	220	C17H16	054372-84-8	38
5	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38



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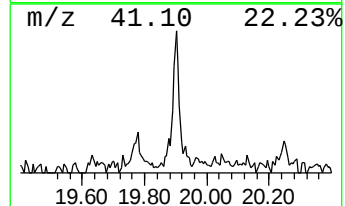
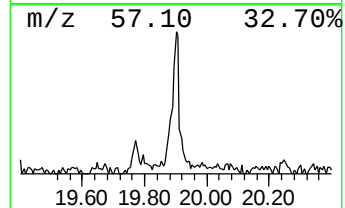
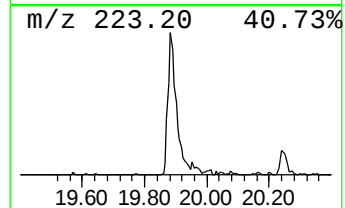
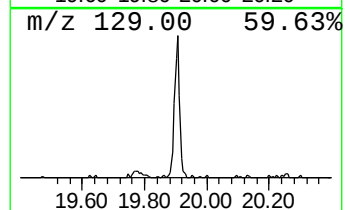
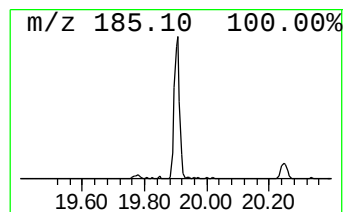
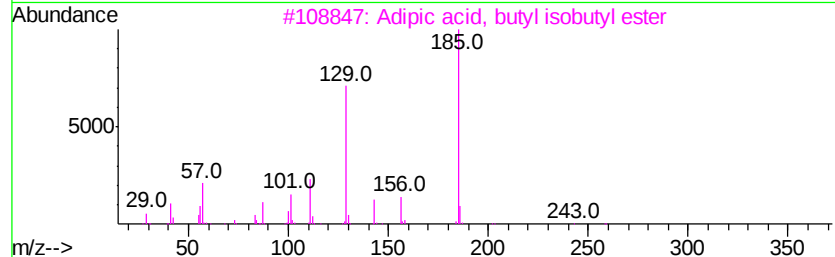
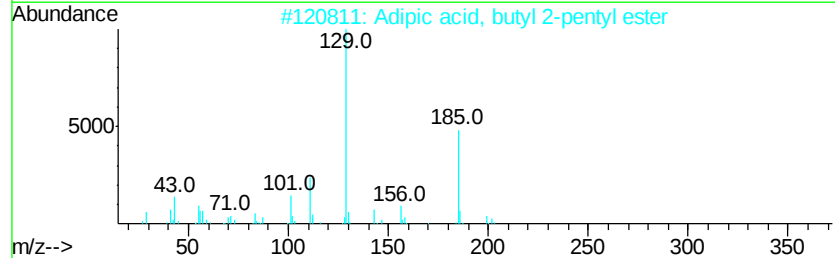
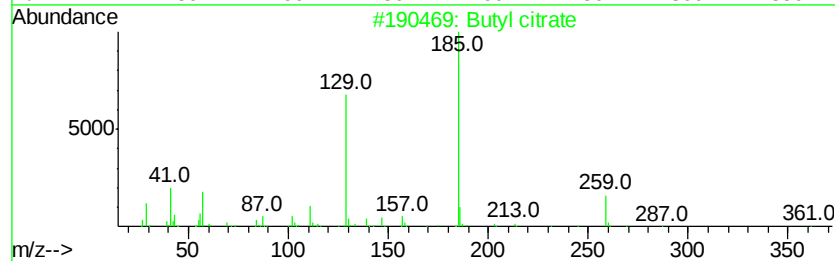
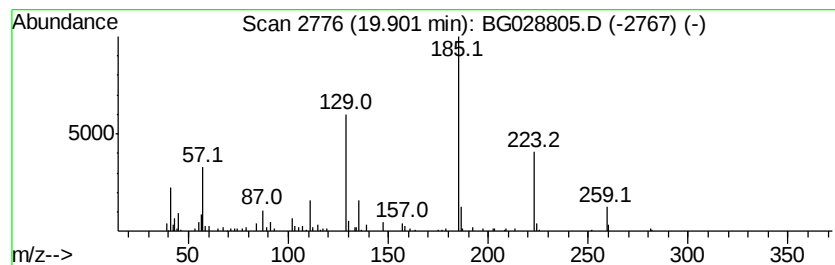
Instrument :
BNA_G
ClientSampleId :
20170603-COMP-D

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	4.45 ng	175667	Chrysene-d12	21.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1 70	
2	Adipic acid, butyl 2-pentyl ester	272 C15H28O4	1000324-15-7 50	
3	Adipic acid, butyl isobutyl ester	258 C14H26O4	1000324-09-3 50	
4	Hexanedioic acid, bis(2-methylpr...	258 C14H26O4	000141-04-8 50	
5	Adipic acid, isobutyl pent-4-en-...	270 C15H26O4	1000354-11-8 47	



Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
Data File : BG028805.D
Acq On : 18 Sep 2017 21:39
Operator : SJ/JU
Sample : I5259-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

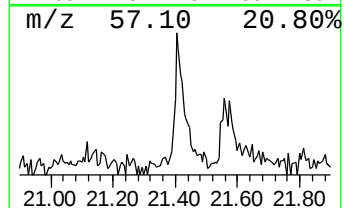
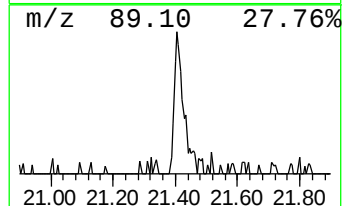
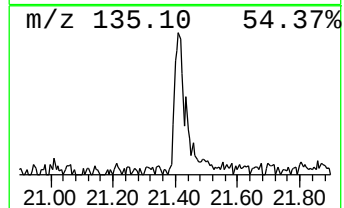
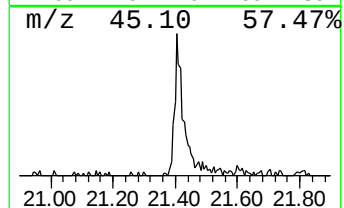
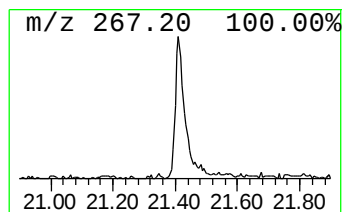
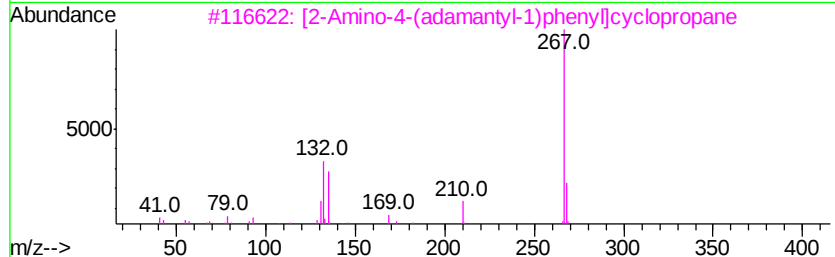
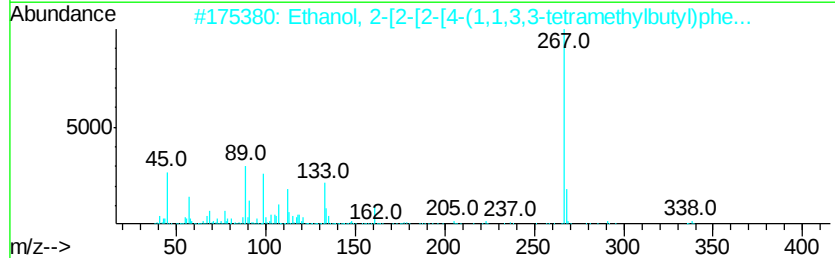
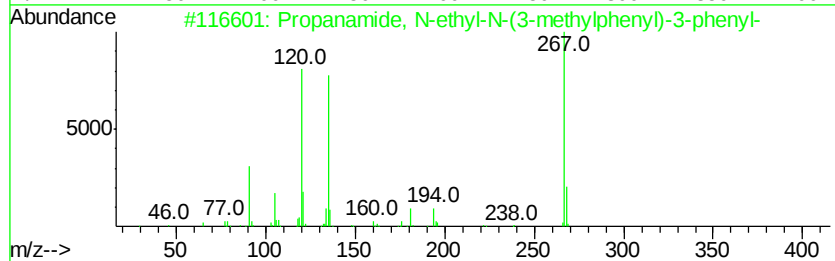
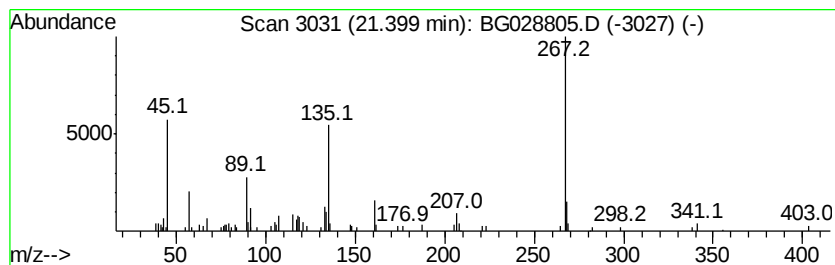
Instrument :
BNA_G
ClientSampleId :
20170603-COMP-D

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown21.40 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.40	3.25 ng	128233	Chrysene-d12	21.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanamide, N-ethyl-N-(3-methyl...	267	C18H21NO	1000308-21-3	43
2	Ethanol, 2-[2-[2-[4-(1,1,3,3-tet...	338	C20H34O4	002315-62-0	43
3	[2-Amino-4-(adamantyl-1)phenyl]c...	267	C19H25N	1000140-61-3	43
4	13H-Dibenzo[a,i]carbazole	267	C20H13N	000239-64-5	38
5	7H-Dibenzo(a,g)carbazole	267	C20H13N	000207-84-1	35



Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
Data File : BG028805.D
Acq On : 18 Sep 2017 21:39
Operator : SJ/JU
Sample : I5259-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20170603-COMP-D

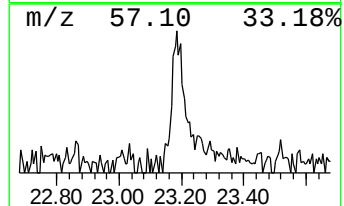
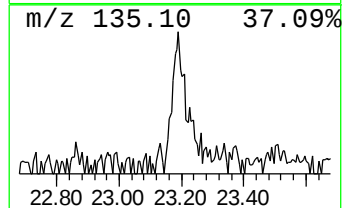
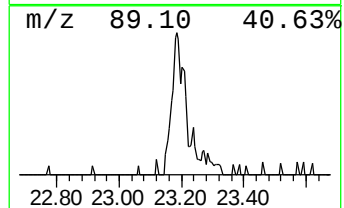
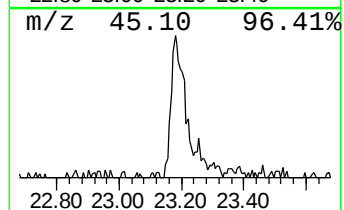
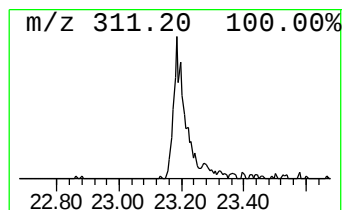
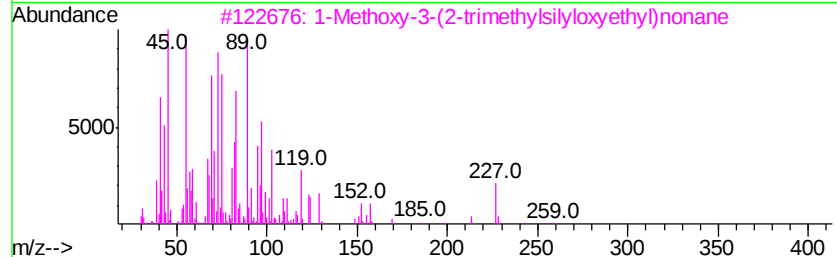
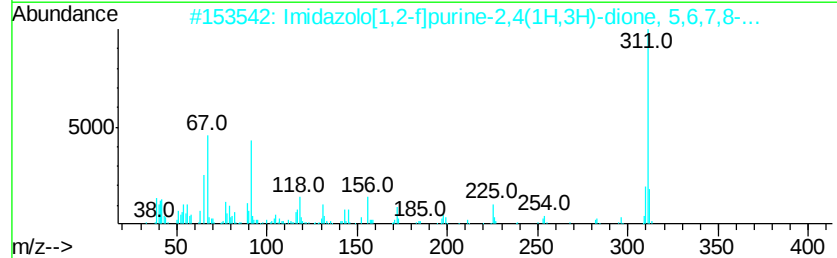
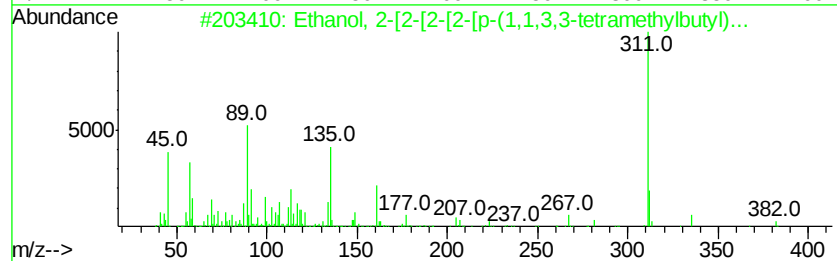
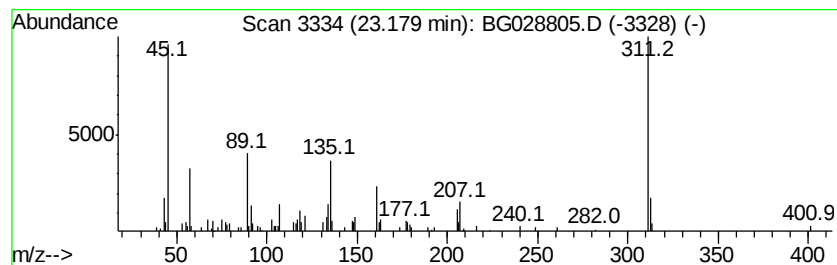
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown23.18 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	3.39 ng	133638	Chrysene-d12	21.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-[2-[2-[2-[p-(1,1,3,3-...	382	C22H38O5	002315-63-1	40
2		Imidazolo[1,2-f]purine-2,4(1H,3H...	311	C16H17N5O2	1000293-98-4	23
3		1-Methoxy-3-(2-trimethylsilyloxy...	274	C15H34O2Si	1000216-82-7	14
4		1,4,7,10,13,16-Hexaoxanonadecane...	320	C16H32O6	1000163-65-3	10
5		2-[2-[2-[2-(tert-Butyldimethylsi...	308	C14H32O5Si	1000352-10-2	10



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091817\
Data File : BG028805.D
Acq On : 18 Sep 2017 21:39
Operator : SJ/JU
Sample : I5259-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20170603-COMP-D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.82	7.82	93.6	ng	872870	1	8.29	186585	20.0
3H-Benz[e]indene,...	14.41	4.1	ng	90293	3	14.91	436634	20.0
unknown15.29	15.29	11.2	ng	245249	3	14.91	436634	20.0
Propanoic acid, 2...	15.67	16.7	ng	363628	3	14.91	436634	20.0
7,9-Di-tert-butyl...	18.30	5.2	ng	173437	4	17.66	668495	20.0
Butyl citrate	19.90	4.5	ng	175667	5	21.98	789016	20.0
unknown21.40	21.40	3.3	ng	128233	5	21.98	789016	20.0
unknown23.18	23.18	3.4	ng	133638	5	21.98	789016	20.0