

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
 Data File : BF079998.D
 Acq On : 16 Jun 2015 18:53
 Operator : TP/IZ
 Sample : G2646-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1506053196

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.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	5.567	215	217	221	rBV	164887	154954	8.01%	1.214%
2	5.956	249	251	254	rBV	732042	670277	34.64%	5.252%
3	6.950	335	338	340	rBV	963939	796732	41.18%	6.243%
4	7.110	350	352	355	rBV	554702	725726	37.51%	5.686%
5	7.350	371	373	375	rBV	325365	257834	13.33%	2.020%
6	7.396	375	377	379	rVV	31700	26721	1.38%	0.209%
7	7.510	385	387	389	rBV	773437	614493	31.76%	4.815%
8	7.910	419	422	424	rBV	307019	402883	20.82%	3.157%
9	8.607	481	483	484	rBV	37234	27968	1.45%	0.219%
10	8.642	484	486	488	rVB	437875	351406	18.16%	2.753%
11	9.145	528	530	535	rVB	18577	22664	1.17%	0.178%
12	9.213	535	536	538	rVB	117922	119160	6.16%	0.934%
13	9.590	567	569	571	rBV	20278	21268	1.10%	0.167%
14	9.716	578	580	582	rVB	1383186	1076387	55.63%	8.434%
15	10.105	612	614	615	rVB	150160	112983	5.84%	0.885%
16	10.196	619	622	625	rBV2	14695	24950	1.29%	0.195%
17	10.276	627	629	632	rBV2	14263	34167	1.77%	0.268%
18	10.413	639	641	644	rVB	500003	419304	21.67%	3.285%
19	10.802	672	675	678	rBV2	15434	34290	1.77%	0.269%
20	11.145	704	705	708	rVV	23681	20782	1.07%	0.163%
21	11.202	708	710	712	rVV	671749	642812	33.22%	5.037%
22	11.271	714	716	717	rVV	27114	30487	1.58%	0.239%
23	11.305	717	719	722	rVV	22624	40597	2.10%	0.318%
24	11.408	726	728	730	rVB3	16785	21931	1.13%	0.172%
25	11.625	746	747	750	rVV3	10879	23023	1.19%	0.180%
26	11.671	750	751	756	rVV3	13683	23639	1.22%	0.185%
27	11.922	770	773	775	rBV	408352	441457	22.82%	3.459%
28	12.071	784	786	788	rVB3	90112	117911	6.09%	0.924%
29	12.185	795	796	799	rVB	15014	22123	1.14%	0.173%
30	12.471	818	821	825	rVV2	11375	20295	1.05%	0.159%
31	12.562	825	829	830	rVB2	12497	21041	1.09%	0.165%
32	13.202	881	885	887	rBV2	22412	22541	1.16%	0.177%
33	13.602	917	920	922	rBV	1020716	1333251	68.91%	10.447%
34	14.139	962	967	973	rBV	73519	181079	9.36%	1.419%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.642	1008	1011	1018	rBV2	48519	102976	5.32%	0.807%
36	14.860	1027	1030	1032	rVB	363516	480509	24.83%	3.765%
37	14.974	1038	1040	1045	rBV	78459	128830	6.66%	1.009%
38	15.820	1111	1114	1123	rBV	1429830	1934901	100.00%	15.161%
39	15.945	1123	1125	1136	rVB	43275	108765	5.62%	0.852%
40	16.277	1152	1154	1160	rBV6	11131	29991	1.55%	0.235%
41	16.723	1190	1193	1196	rBV	321213	486345	25.14%	3.811%
42	18.849	1374	1379	1390	rBV	86117	255589	13.21%	2.003%
43	19.374	1420	1425	1433	rBV2	128305	377355	19.50%	2.957%

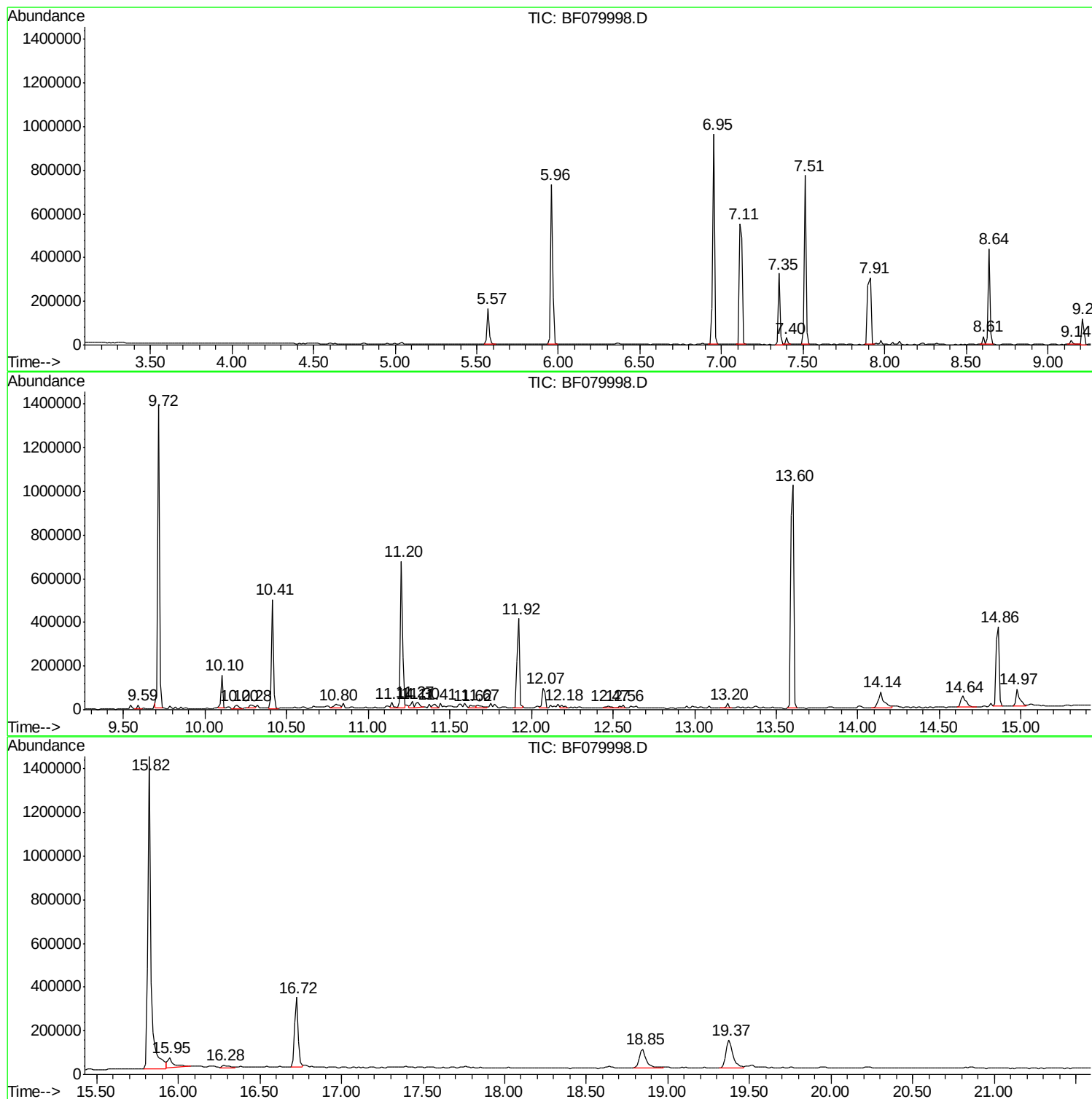
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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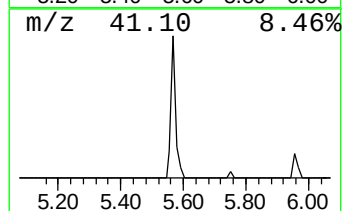
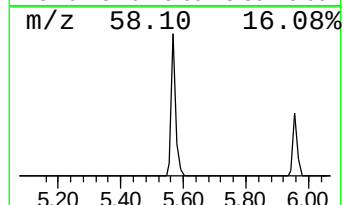
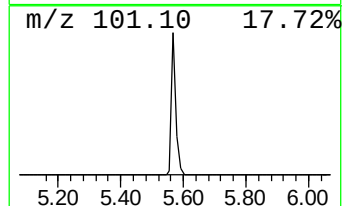
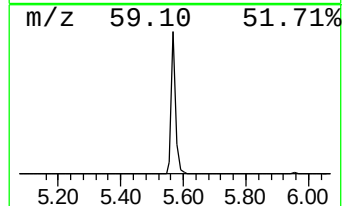
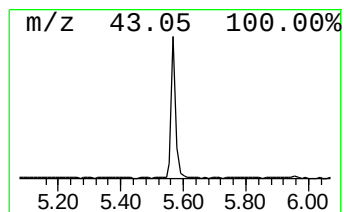
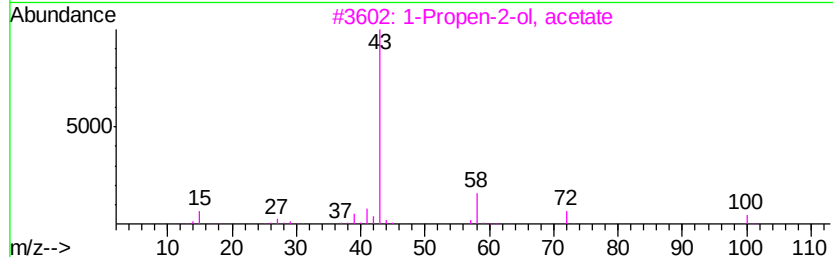
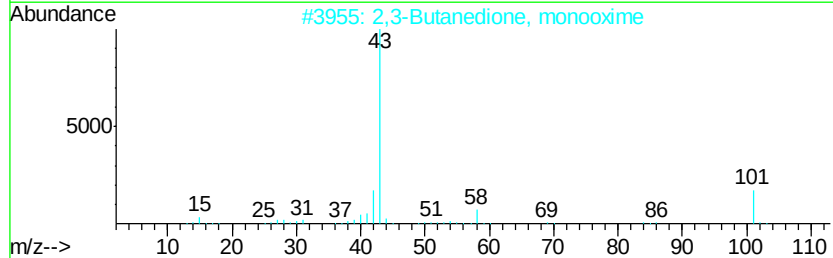
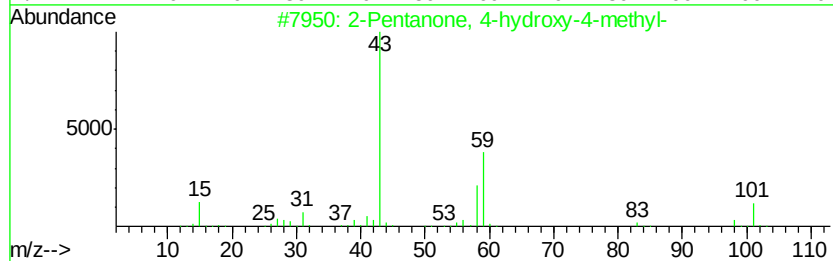
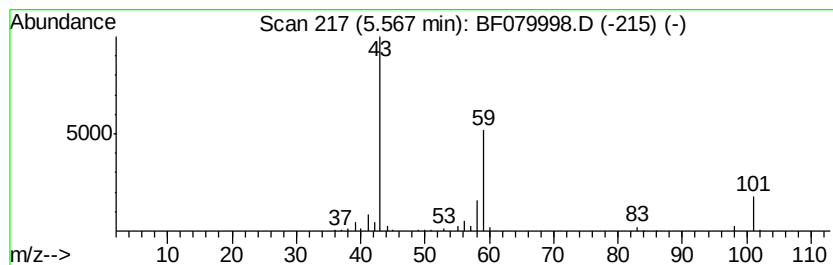
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.57	12.02 ng	154954	1,4-Dichlorobenzene-d4	7.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Butane	58	C4H10	000106-97-8	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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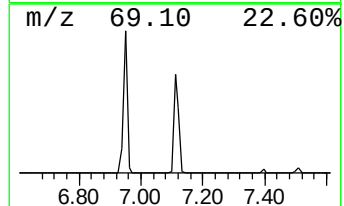
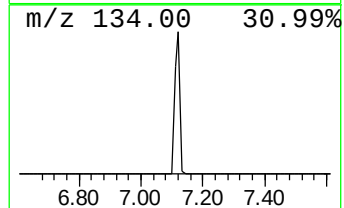
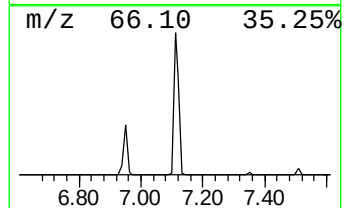
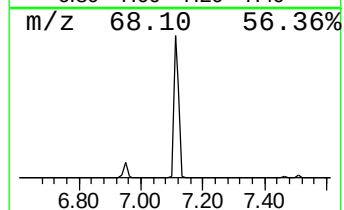
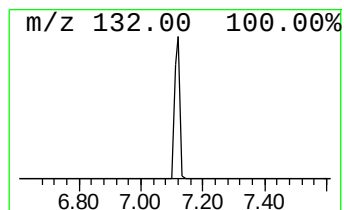
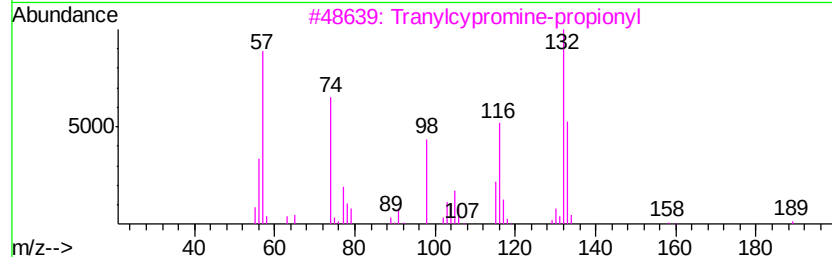
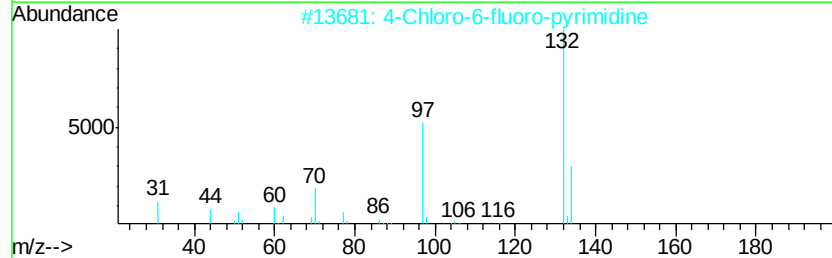
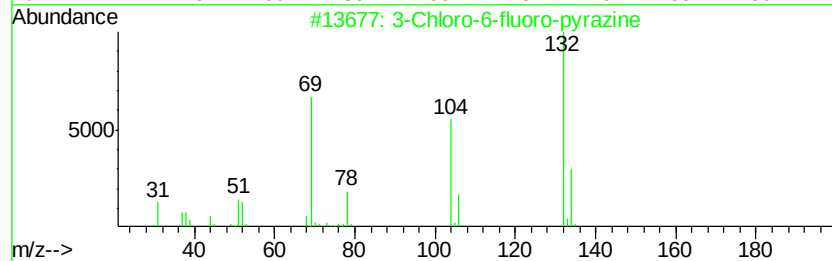
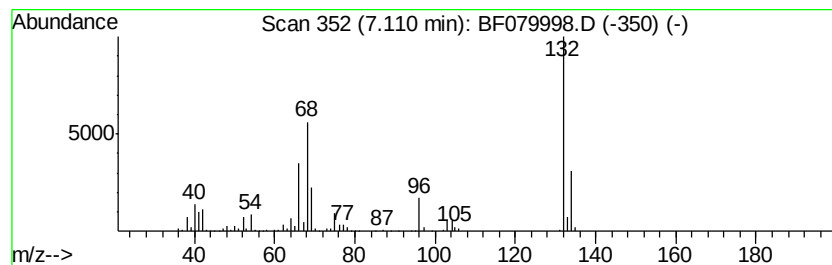
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.11 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.11	56.29 ng	725726	1,4-Dichlorobenzene-d4	7.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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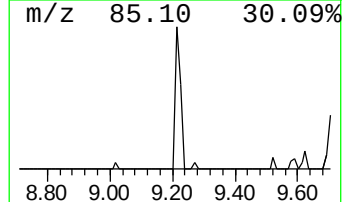
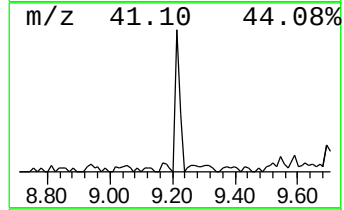
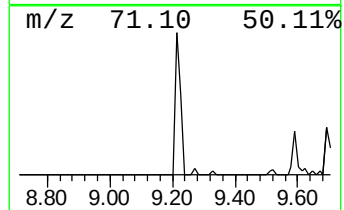
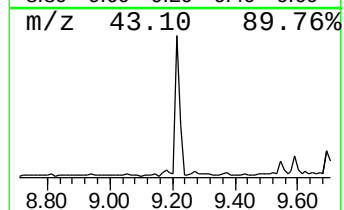
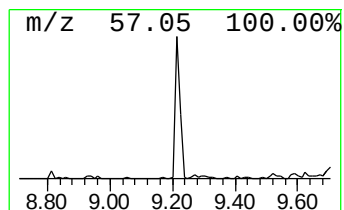
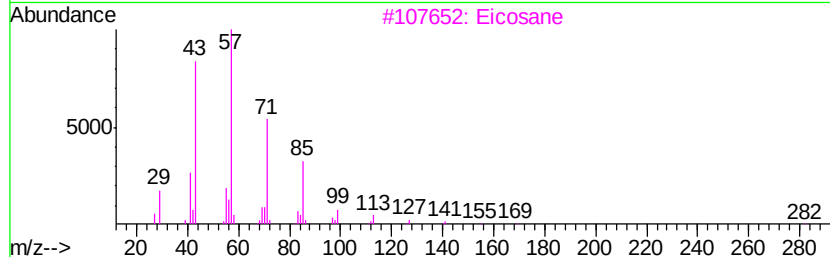
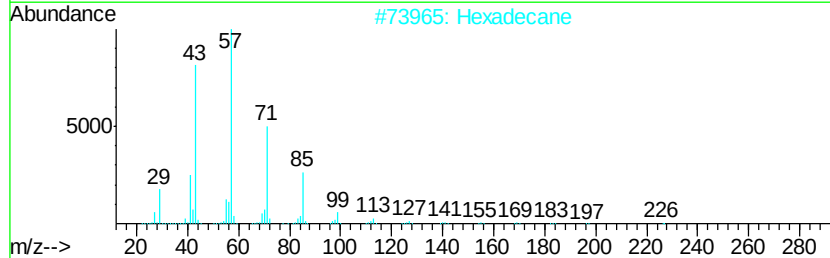
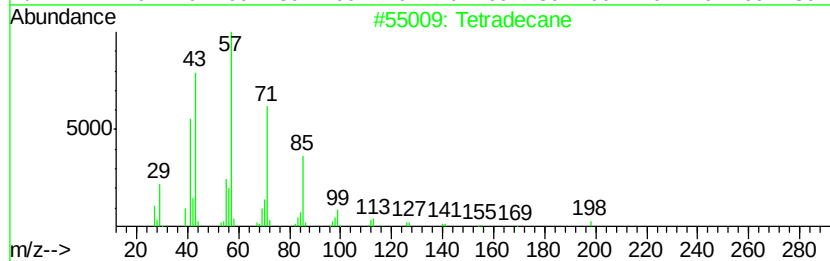
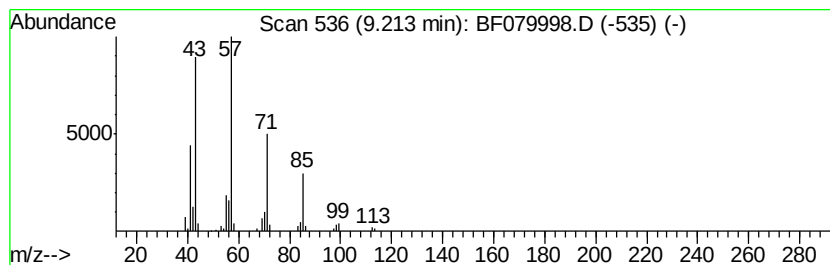
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.21	6.78 ng	119160	Naphthalene-d8	8.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	90
2			Hexadecane	226	C16H34	000544-76-3	90
3			Eicosane	282	C20H42	000112-95-8	83
4			Tridecane	184	C13H28	000629-50-5	83
5			Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	64



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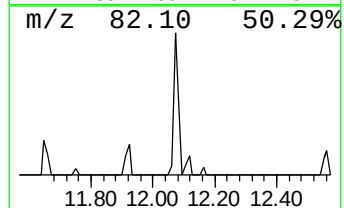
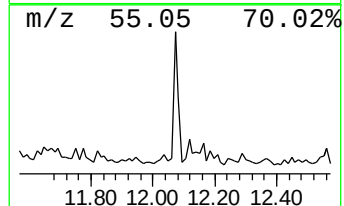
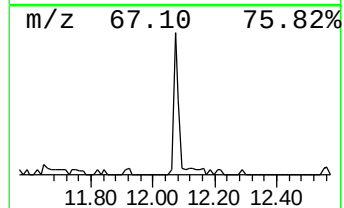
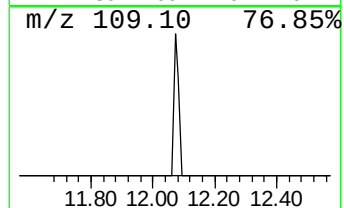
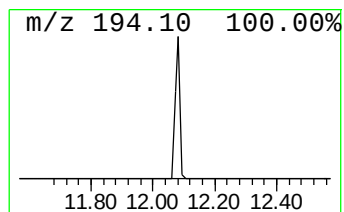
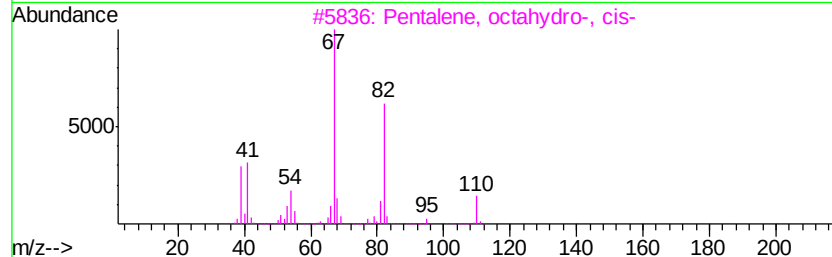
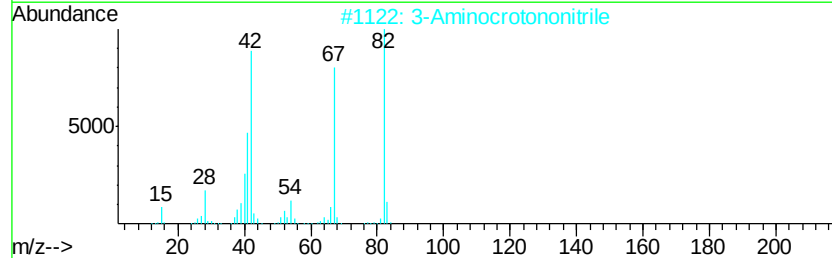
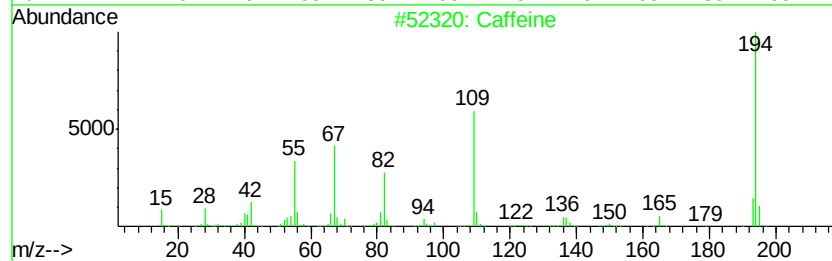
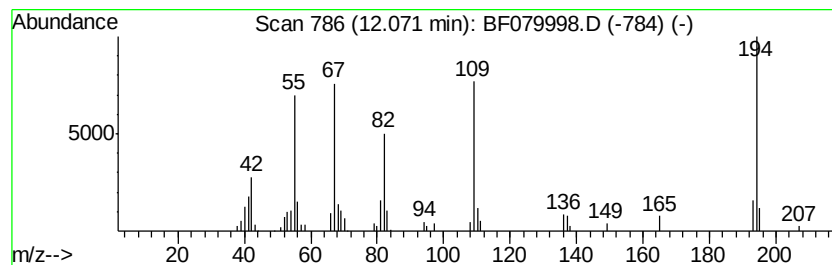
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Caffeine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	5.34 ng	117911	Phenanthrene-d10	11.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine		194	C8H10N4O2	000058-08-2	97
2	3-Aminocrotononitrile		82	C4H6N2	001118-61-2	42
3	Pentalene, octahydro-, cis-		110	C8H14	001755-05-1	42
4	Pentalene, octahydro-		110	C8H14	000694-72-4	27
5	2,6-Pyridinediamine		109	C5H7N3	000141-86-6	27



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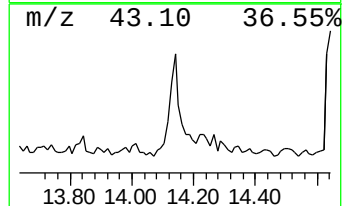
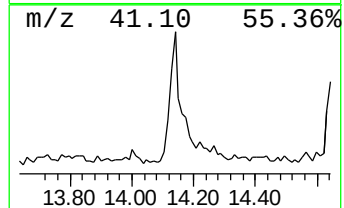
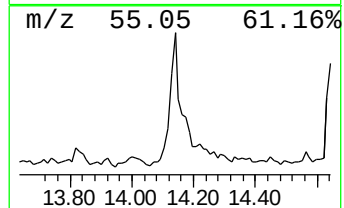
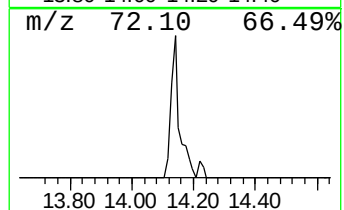
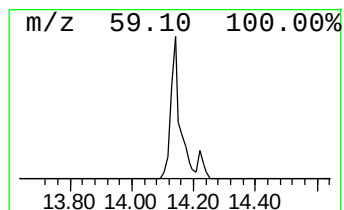
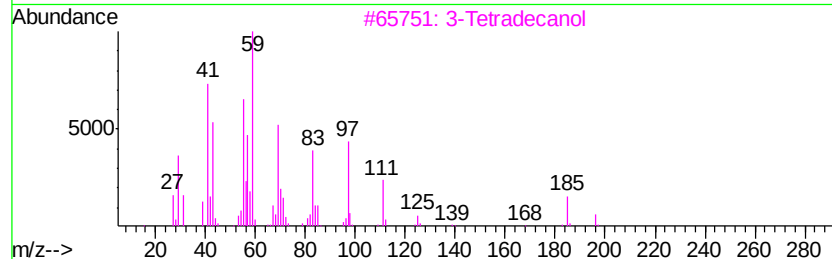
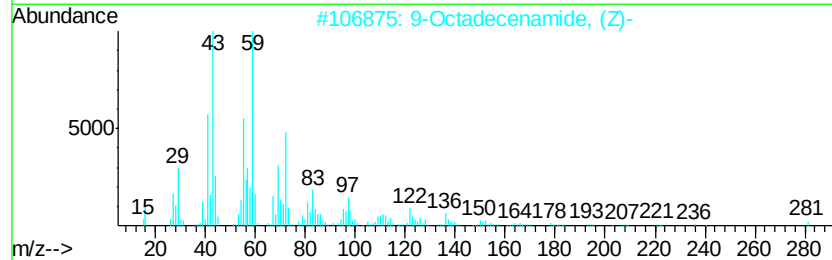
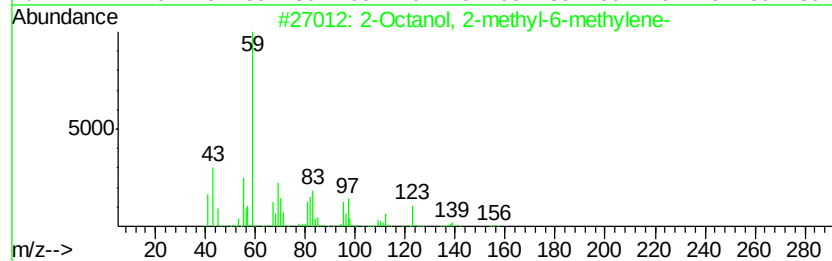
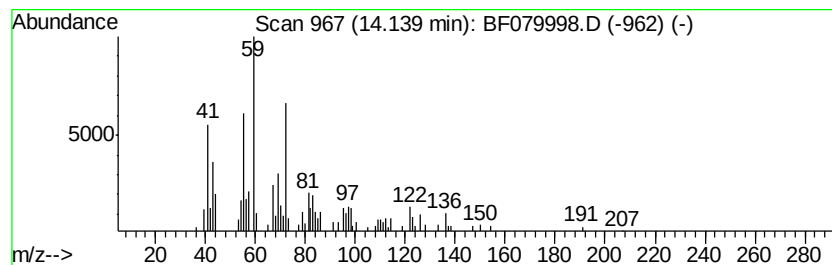
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.14 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	7.54 ng	181079	Chrysene-d12	14.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	43		
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	38		
3	3-Tetradecanol	214	C14H30O	001653-32-3	38		
4	Propane, 1-chloro-3-ethoxy-	122	C5H11ClO	036865-38-0	35		
5	3-Butenoic acid, 2-methyl-, meth...	114	C6H10O2	051747-33-2	35		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
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Acq On : 16 Jun 2015 18:53
Operator : TP/IZ
Sample : G2646-01
Misc :
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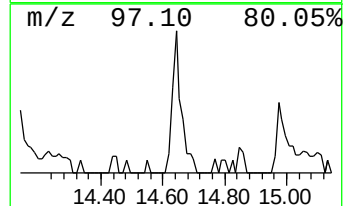
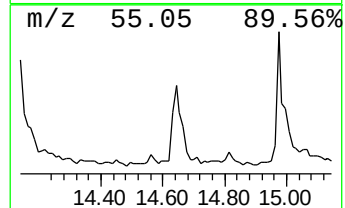
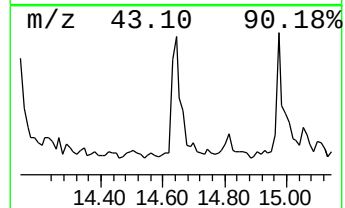
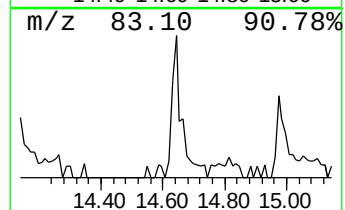
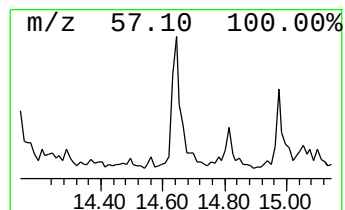
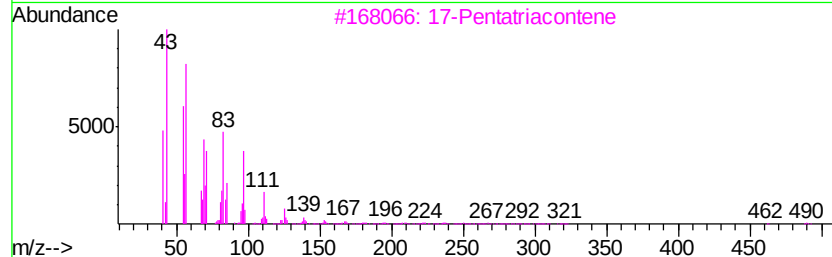
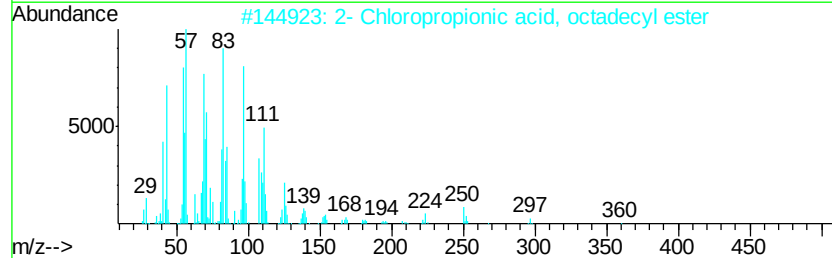
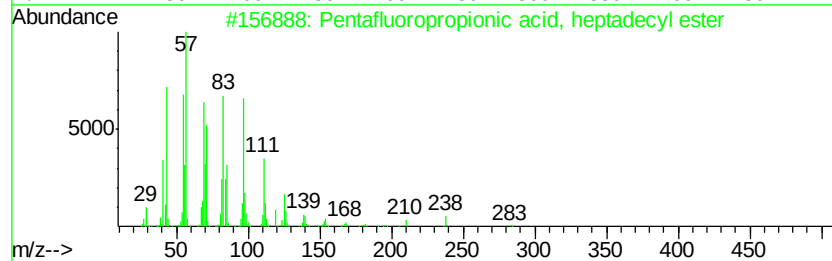
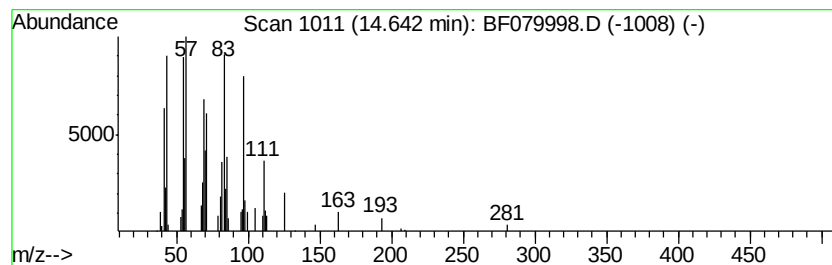
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.64	4.29 ng	102976	Chrysene-d12	14.86		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		1-Octadecanol	270	C18H38O	000112-92-5	87
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
Data File : BF079998.D
Acq On : 16 Jun 2015 18:53
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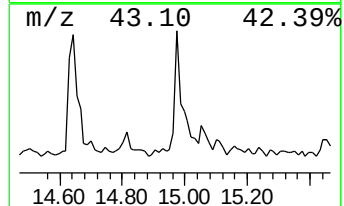
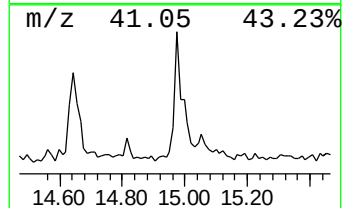
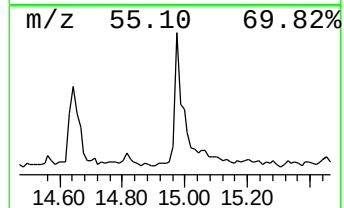
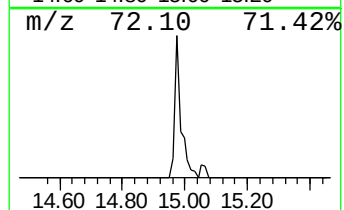
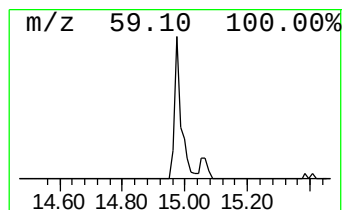
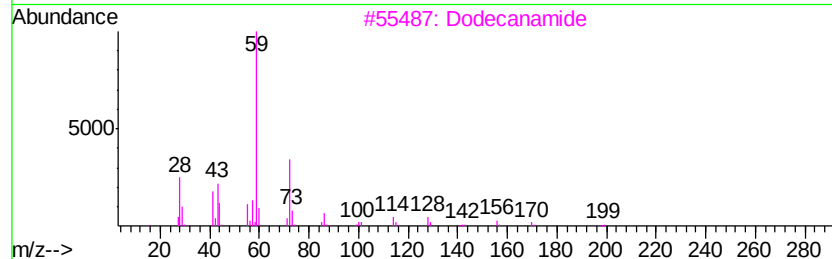
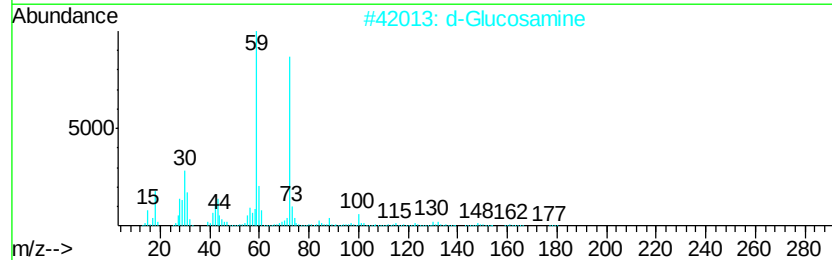
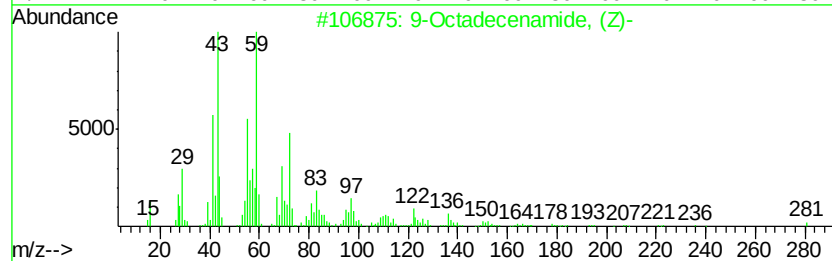
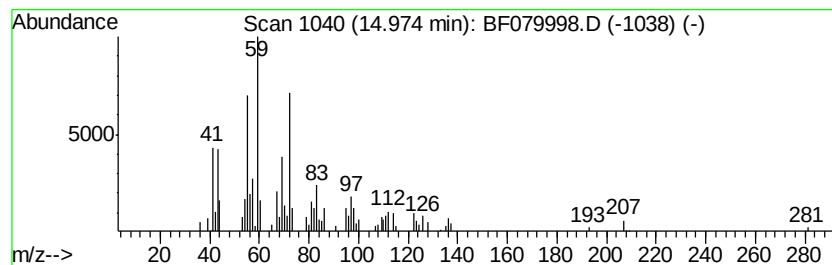
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	5.36 ng	128830	Chrysene-d12	14.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		d-Glucosamine	179	C6H13NO5	000090-77-7	43
3		Dodecanamide	199	C12H25NO	001120-16-7	43
4		Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	35
5		1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
Data File : BF079998.D
Acq On : 16 Jun 2015 18:53
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Sample : G2646-01
Misc :
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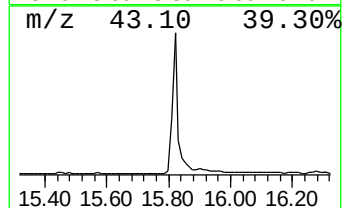
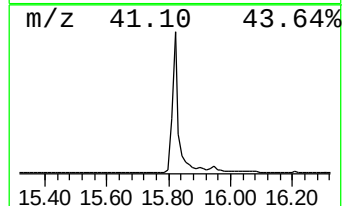
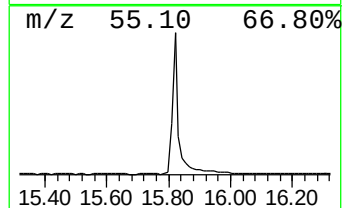
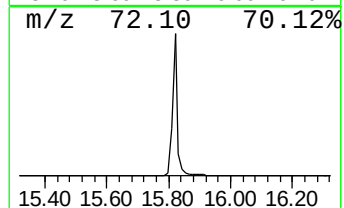
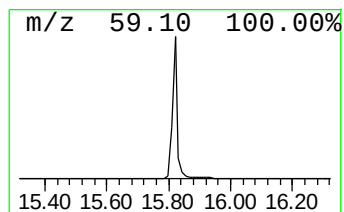
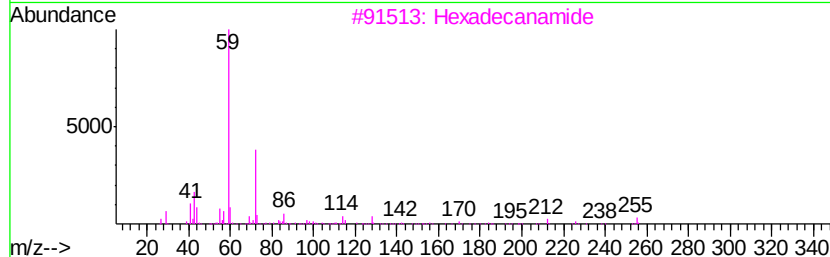
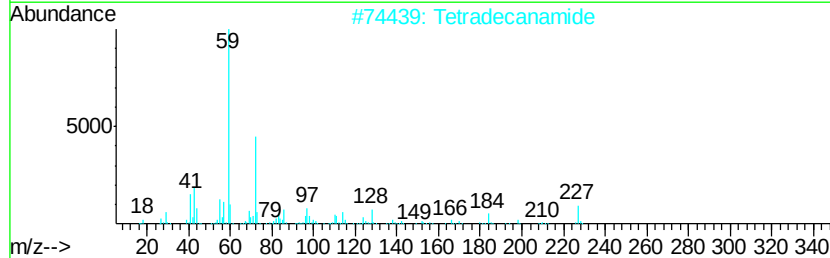
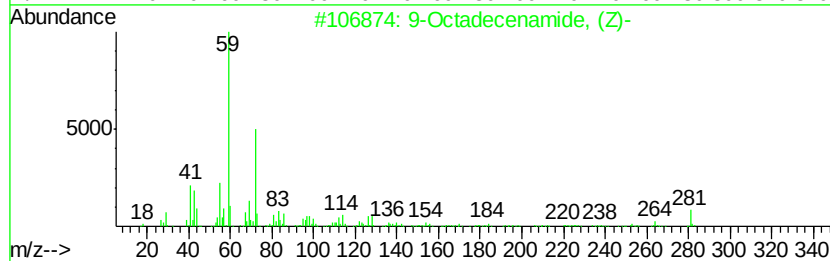
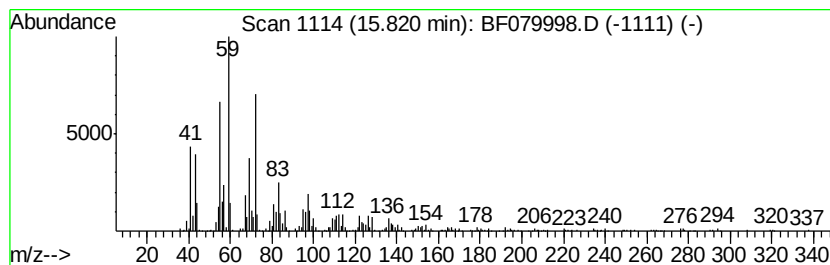
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Tetradecanamide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	79.57 ng	1934900	Perylene-d12	16.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
2		Tetradecanamide	227	C14H29NO	000638-58-4	59
3		Hexadecanamide	255	C16H33NO	000629-54-9	53
4		Dodecanamide	199	C12H25NO	001120-16-7	43
5		3-Dodecanol	186	C12H26O	010203-30-2	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
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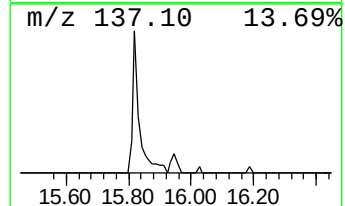
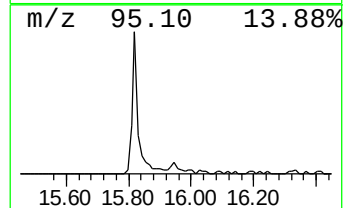
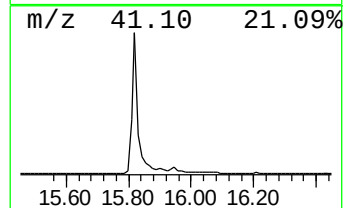
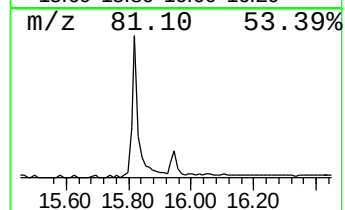
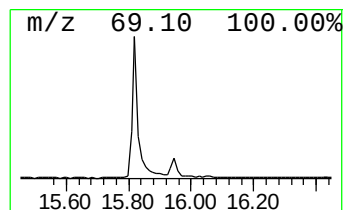
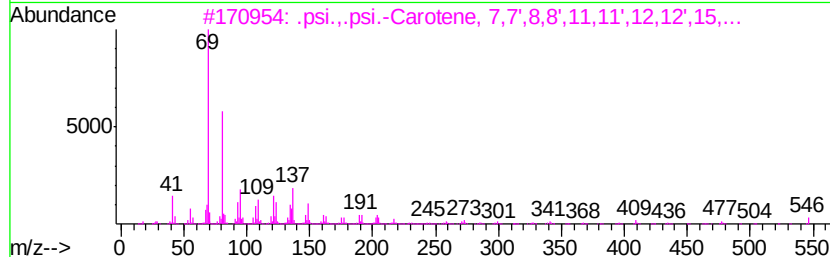
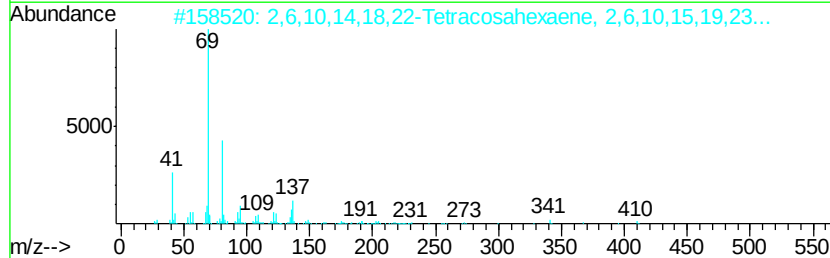
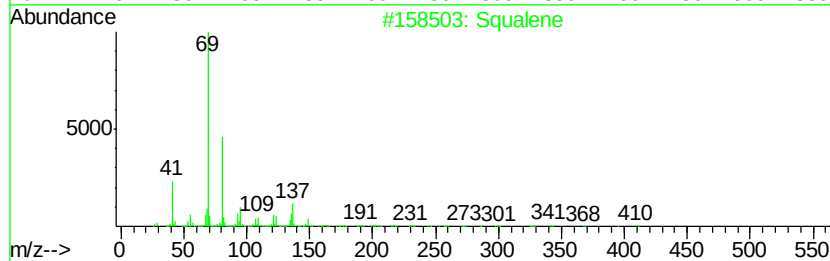
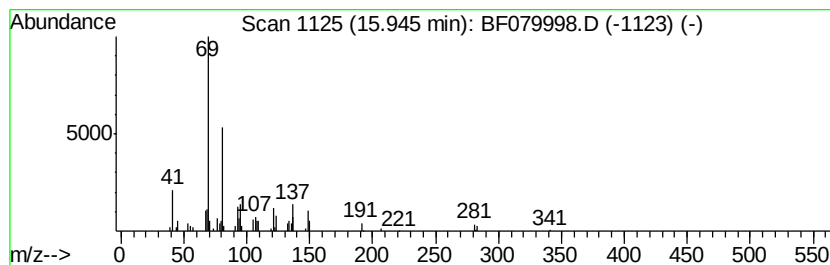
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	4.47 ng	108765	Perylene-d12	16.72
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 83
2	2,6,10,14,18,22-Tetracosahexaene...		410 C30H50	000111-02-4 72
3	.psi.,.psi.-Carotene, 7,7',8,8',...		547 C40H66	000502-62-5 64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...		222 C15H26O	004602-84-0 59
5	4,8,12-Tetradecatrienal, 5,9,13-...		248 C17H28O	066408-55-7 59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
Data File : BF079998.D
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Operator : TP/IZ
Sample : G2646-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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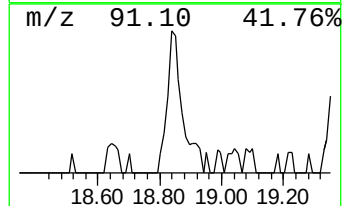
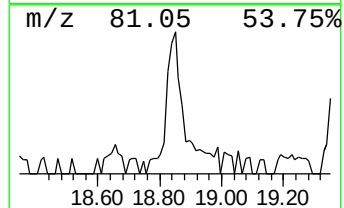
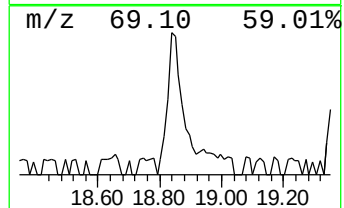
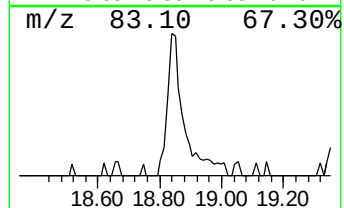
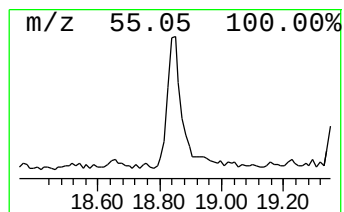
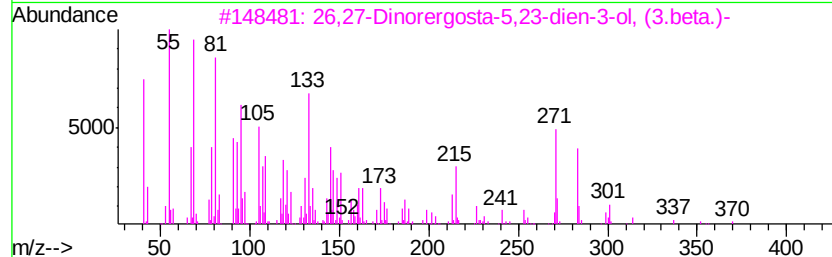
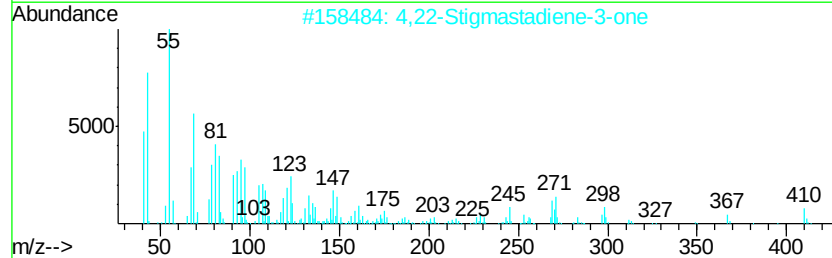
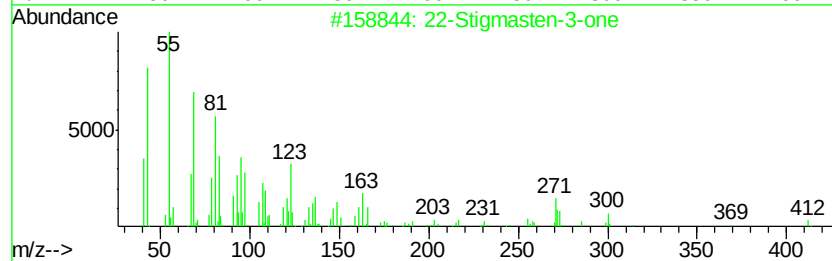
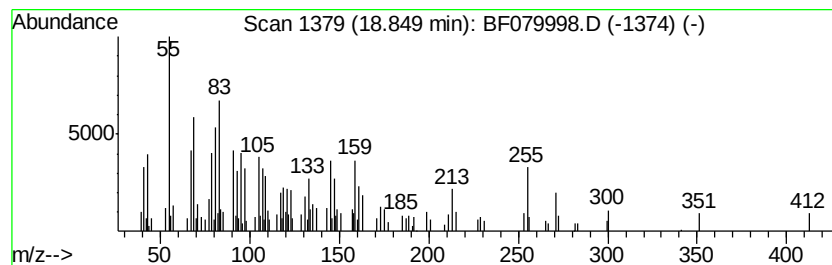
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown18.85 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.85	10.51 ng	255589	Perylene-d12	16.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	22	Stigmasten-3-one	412	C29H48O	004736-95-2	38
2	4,22	Stigmastadiene-3-one	410	C29H46O	020817-72-5	25
3	26,27	Dinoregosta-5,23-dien-3-o...	370	C26H42O	035882-88-3	12
4	Phosphinous	chloride, phenyl(1,7...	280	C16H22ClP	074630-27-6	9
5	Piperazine,	1-(2-furanylcarbonyl)-	180	C9H12N2O2	040172-95-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
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Acq On : 16 Jun 2015 18:53
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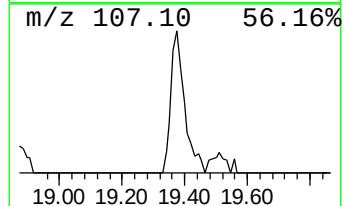
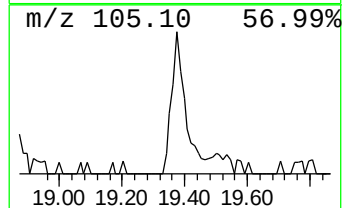
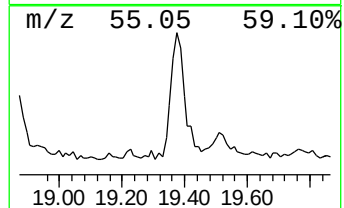
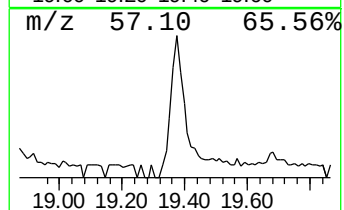
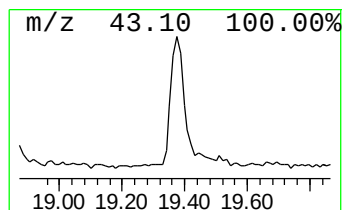
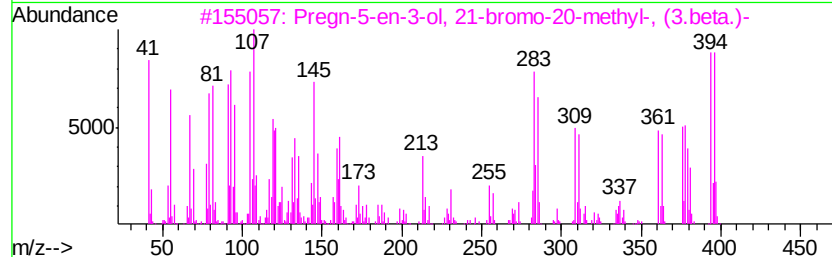
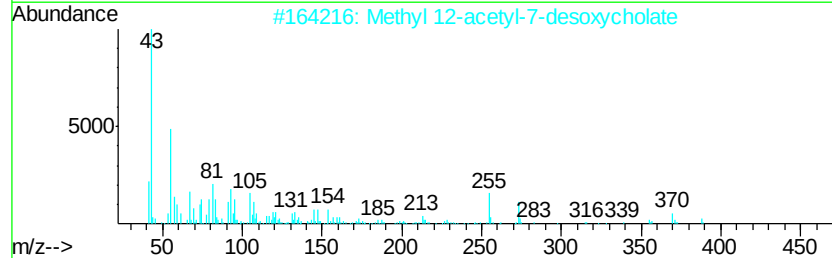
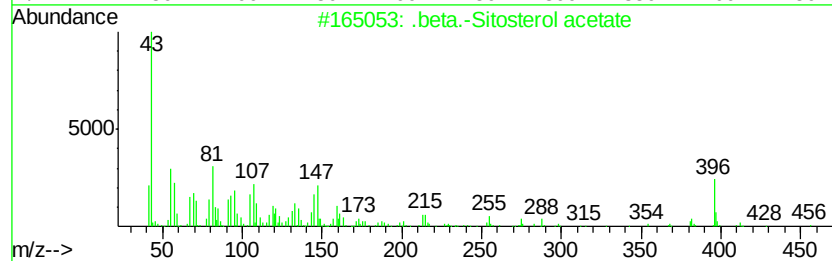
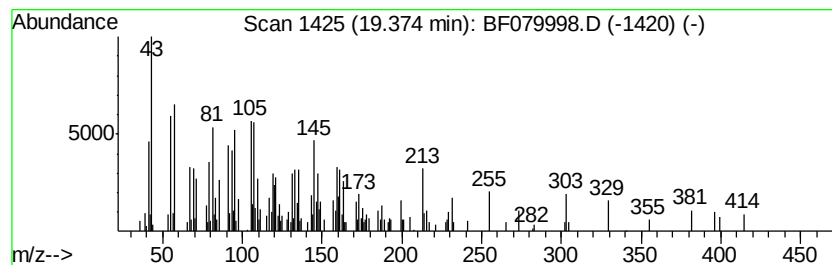
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown19.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	15.52 ng	377355	Perylene-d12	16.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	49
2		Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	35
3		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	27
4		3,3,3-Trifluoro-N-(2-pyrimidinyl...	273	C8H5F6N3O	340137-97-5	10
5		8-Phthalimido-6-methoxy-2-[1-met...	414	C23H18N4O4	1000213-30-0	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown7.11	7.11	56.3	ng	725726	1	7.35	257834	20.0
Tetradecane	9.21	6.8	ng	119160	2	8.64	351406	20.0
Caffeine	12.07	5.3	ng	117911	4	11.92	441457	20.0
unknown14.14	14.14	7.5	ng	181079	5	14.86	480509	20.0
Pentafluoropropio...	14.64	4.3	ng	102976	5	14.86	480509	20.0
9-Octadecenamide,...	14.97	5.4	ng	128830	5	14.86	480509	20.0
Tetradecanamide	15.82	79.6	ng	1934900	6	16.72	486345	20.0
Squalene	15.95	4.5	ng	108765	6	16.72	486345	20.0
unknown18.85	18.85	10.5	ng	255589	6	16.72	486345	20.0
unknown19.37	19.37	15.5	ng	377355	6	16.72	486345	20.0