

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
 Data File : BF092240.D
 Acq On : 13 Jan 2017 10:56
 Operator : UM/SJ
 Sample : I1131-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP

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-BF122116.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	3.981	190	192	197	rBV	27605	58862	1.07%	0.105%
2	4.713	253	256	271	rVB	1826000	3052965	55.47%	5.425%
3	5.182	295	297	313	rBV	4575645	5282566	95.99%	9.387%
4	6.256	388	391	398	rBV	4503209	5106531	92.79%	9.075%
5	6.359	398	400	403	rVV	4572790	4450655	80.87%	7.909%
6	6.587	418	420	422	rBV	1184226	1129637	20.53%	2.007%
7	6.747	431	434	436	rBV	3170177	4332170	78.72%	7.698%
8	7.159	467	470	472	rBV	3571003	3598231	65.38%	6.394%
9	7.296	480	482	488	rVB	58680	70994	1.29%	0.126%
10	7.867	530	532	535	rBV	1261259	1473618	26.78%	2.619%
11	8.828	614	616	622	rBV	59040	82199	1.49%	0.146%
12	8.953	624	627	629	rBV	5748165	5503334	100.00%	9.780%
13	9.353	660	662	664	rBV	1899603	1579330	28.70%	2.807%
14	9.616	683	685	688	rBV	1834888	2002634	36.39%	3.559%
15	10.039	716	722	723	rBV	148888	164780	2.99%	0.293%
16	10.073	723	725	726	rVB	104636	107910	1.96%	0.192%
17	10.291	741	744	745	rBV	50439	67696	1.23%	0.120%
18	10.416	752	755	757	rBV	3252250	4231145	76.88%	7.519%
19	10.542	764	766	772	rVB	174009	199406	3.62%	0.354%
20	10.988	803	805	806	rBV2	133820	132493	2.41%	0.235%
21	11.102	812	815	817	rBV	1508383	2029537	36.88%	3.607%
22	11.171	819	821	823	rBV	52503	61491	1.12%	0.109%
23	11.354	834	837	840	rBV2	161697	272509	4.95%	0.484%
24	11.411	840	842	844	rVB	58479	63324	1.15%	0.113%
25	11.605	854	859	860	rBV3	25320	66400	1.21%	0.118%
26	11.651	862	863	867	rVV2	479974	517219	9.40%	0.919%
27	11.708	867	868	873	rVB2	49571	83102	1.51%	0.148%
28	12.302	918	920	922	rBV	327945	303301	5.51%	0.539%
29	12.428	930	931	937	rBV2	66685	145089	2.64%	0.258%
30	12.531	937	940	942	rBV	255890	279957	5.09%	0.497%
31	12.691	951	954	956	rVB	4036884	5378803	97.74%	9.558%
32	12.862	965	969	971	rVB2	27865	56507	1.03%	0.100%
33	12.931	972	975	977	rBV	99342	112320	2.04%	0.200%
34	13.274	1002	1005	1009	rVB	56675	79160	1.44%	0.141%

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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

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35	13.605	1031	1034	1042	rBV2	255974	530837	9.65%	0.943%
36	13.720	1042	1044	1047	rBV	1081275	1499552	27.25%	2.665%
37	13.914	1059	1061	1069	rVB4	27330	65281	1.19%	0.116%
38	14.222	1083	1088	1089	rBV3	27070	68909	1.25%	0.122%
39	14.577	1116	1119	1122	rBV	125282	130495	2.37%	0.232%
40	14.725	1129	1132	1136	rBV	107401	297582	5.41%	0.529%
41	14.977	1152	1154	1157	rVB	58781	61591	1.12%	0.109%
42	15.034	1157	1159	1161	rVB	79376	90685	1.65%	0.161%
43	15.080	1161	1163	1166	rBV	957137	1253583	22.78%	2.228%
44	15.560	1202	1205	1207	rBV3	28316	64451	1.17%	0.115%
45	15.914	1233	1236	1243	rVB2	15950	55188	1.00%	0.098%
46	16.325	1269	1272	1276	rBV	43188	79348	1.44%	0.141%

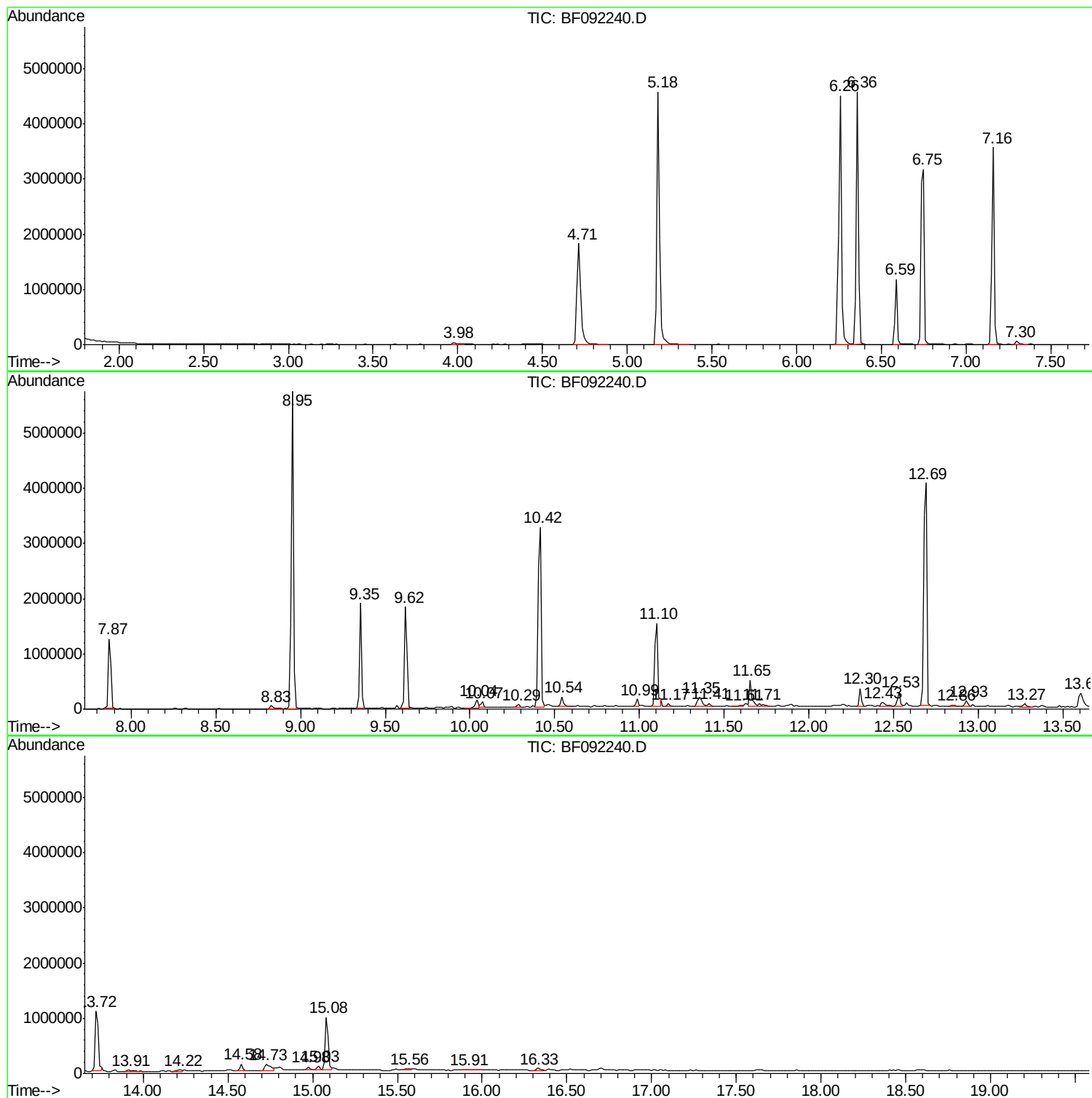
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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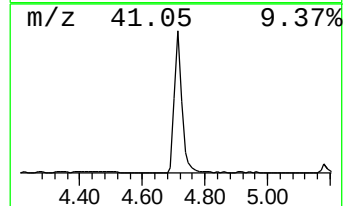
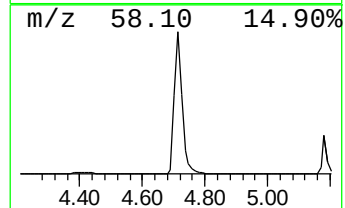
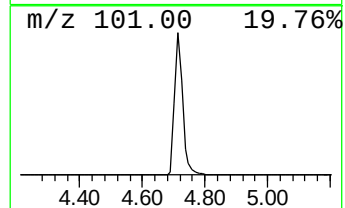
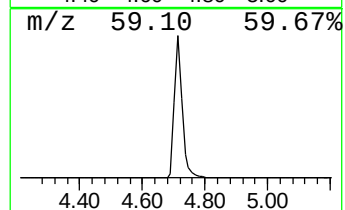
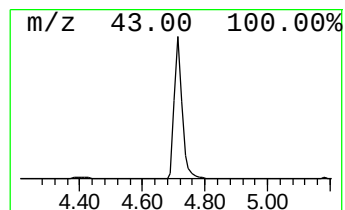
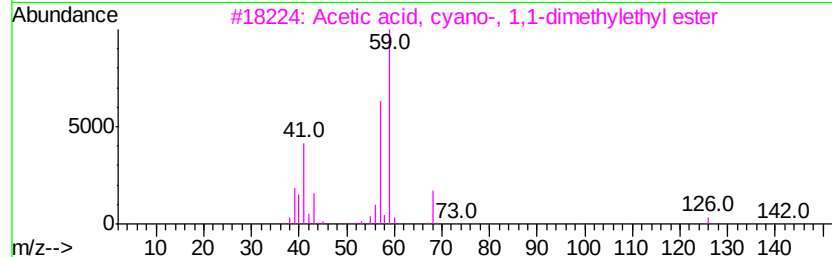
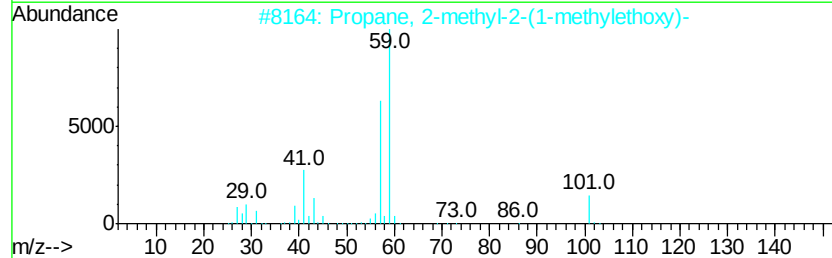
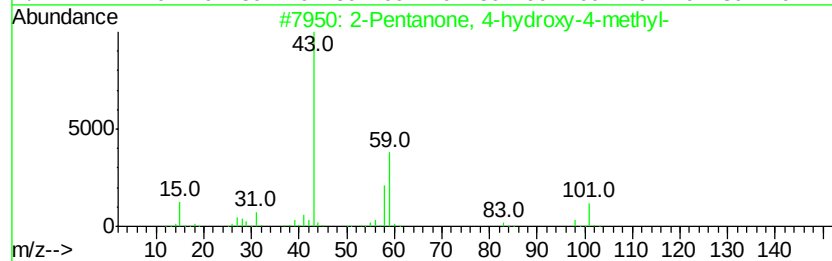
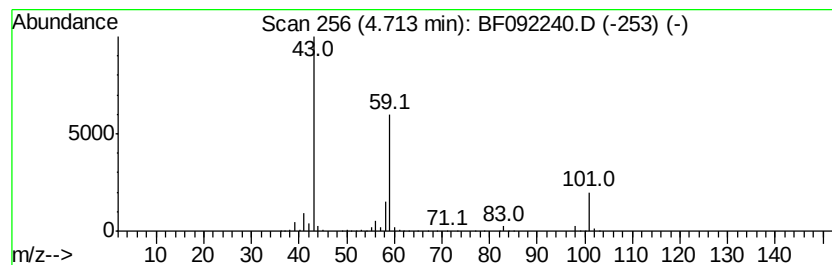
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	54.05 ng	3052970	1,4-Dichlorobenzene-d4	6.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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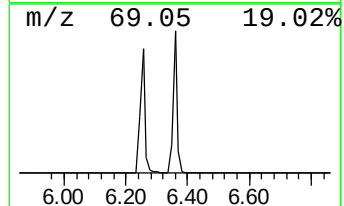
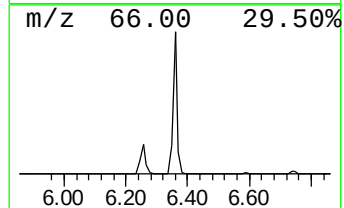
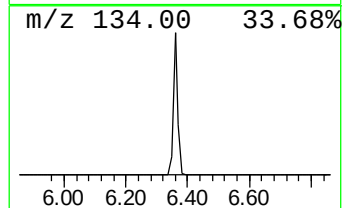
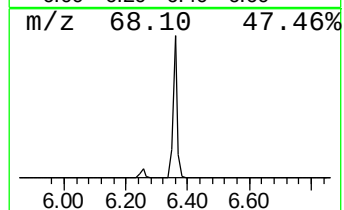
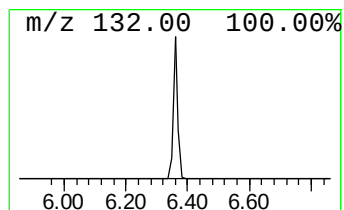
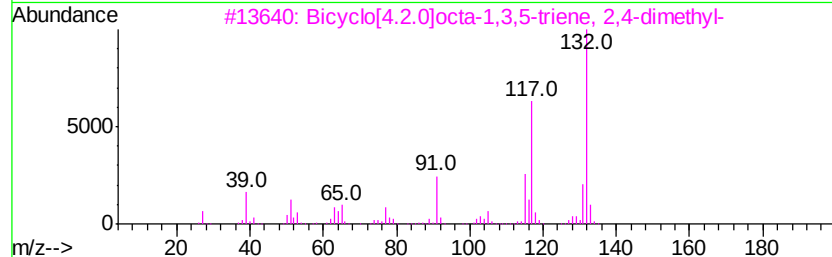
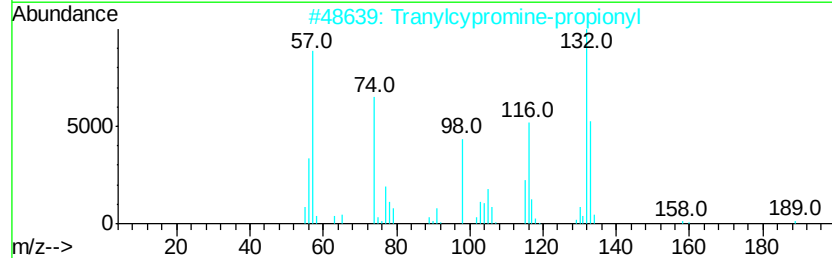
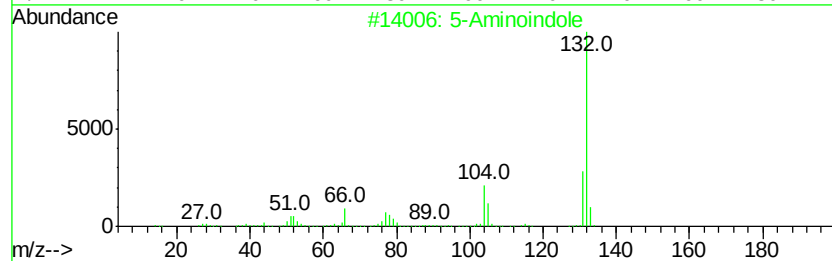
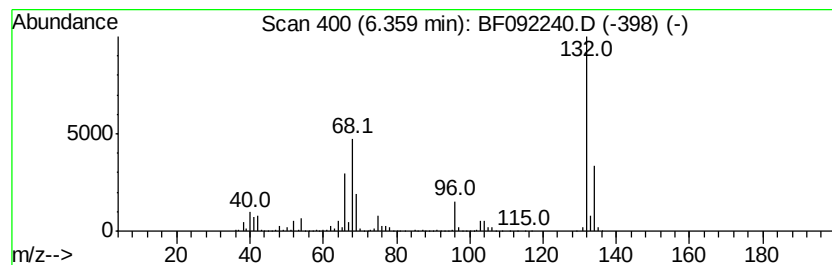
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Peak Number 2 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	78.80 ng	4450660	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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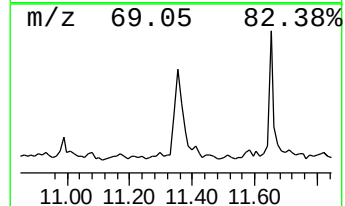
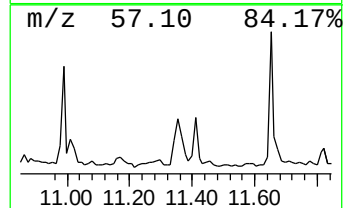
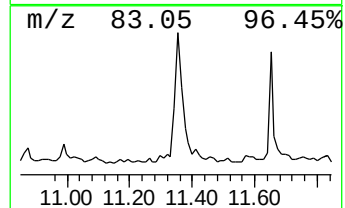
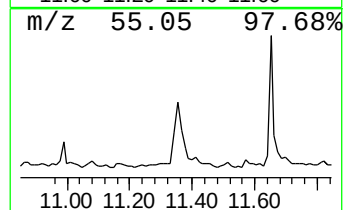
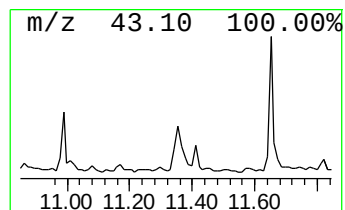
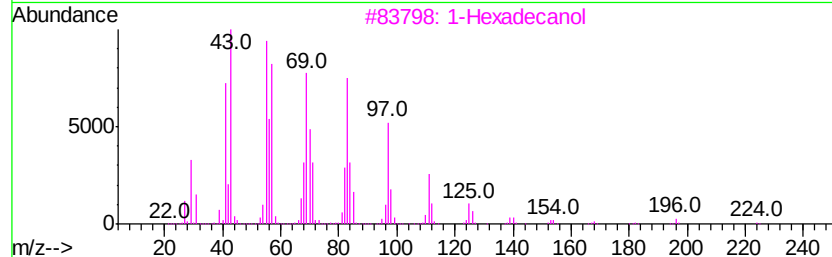
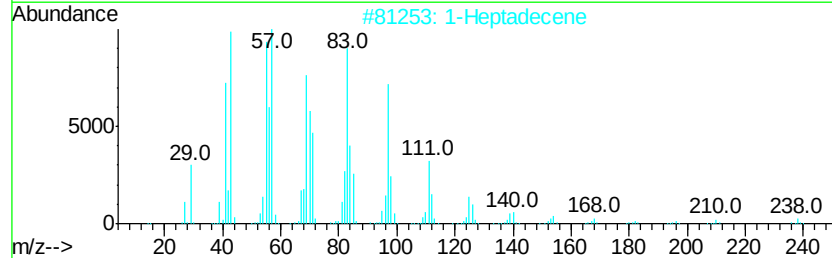
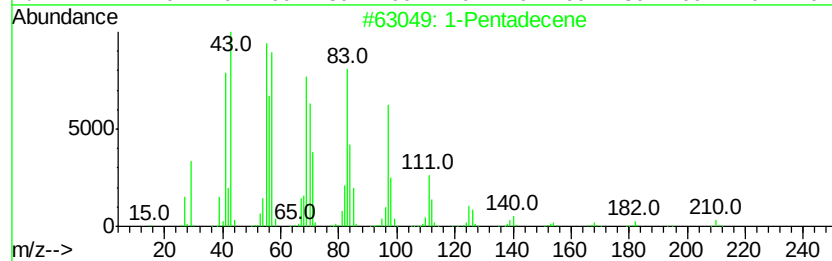
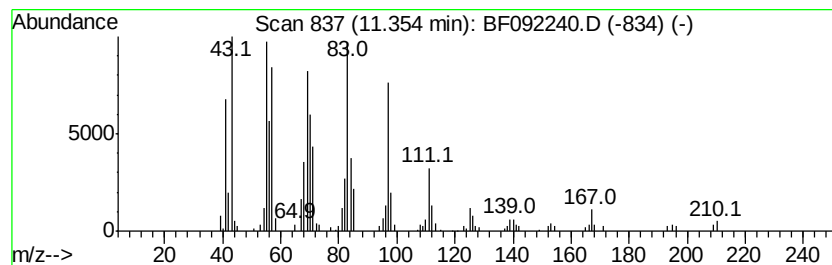
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Pentadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.35	2.69 ng	272509	Phenanthrene-d10	11.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene		210	C15H30	013360-61-7	97
2	1-Heptadecene		238	C17H34	006765-39-5	95
3	1-Hexadecanol		242	C16H34O	036653-82-4	93
4	5-Octadecene, (E)-		252	C18H36	007206-21-5	91
5	9-Eicosene, (E)-		280	C20H40	074685-29-3	91



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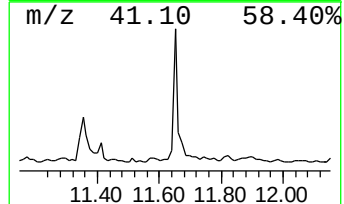
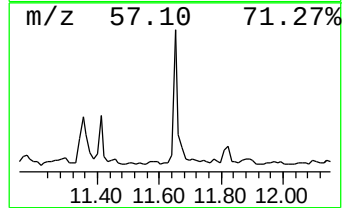
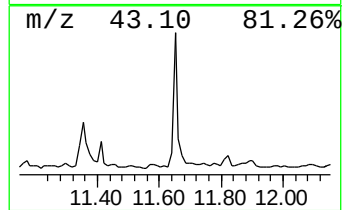
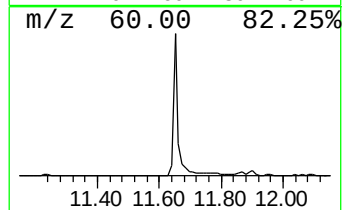
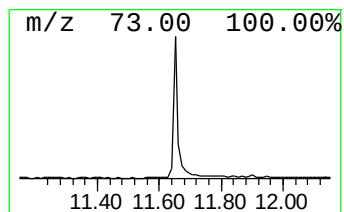
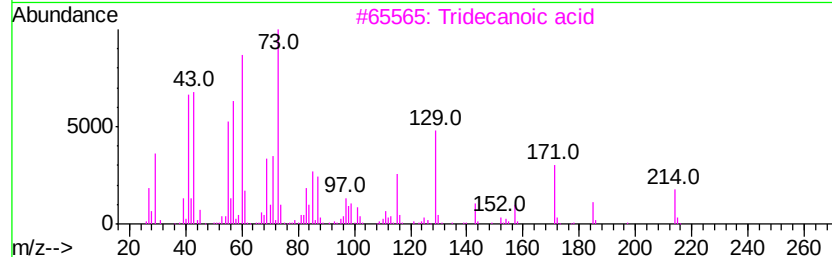
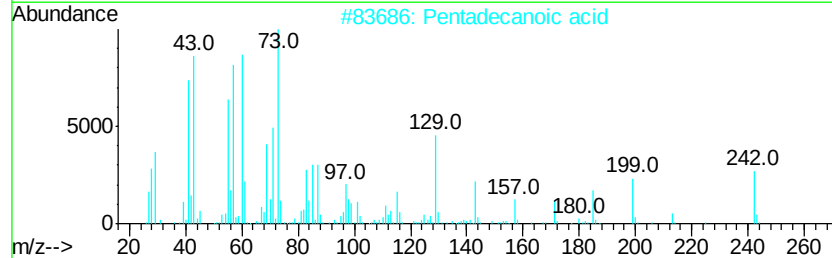
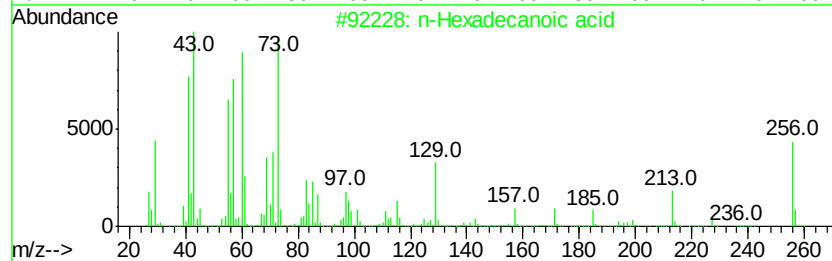
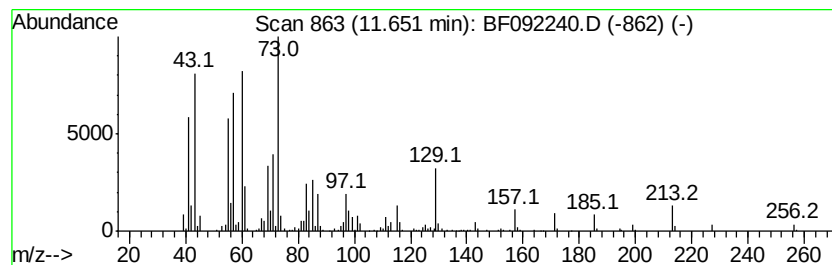
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	5.10 ng	517219	Phenanthrene-d10	11.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	50
4		Hexadecane	226	C16H34	000544-76-3	11
5		Nonanoic acid	158	C9H18O2	000112-05-0	11



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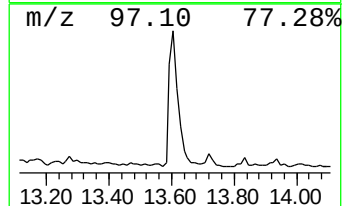
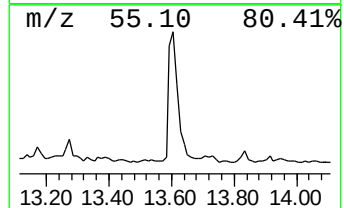
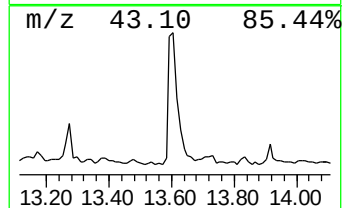
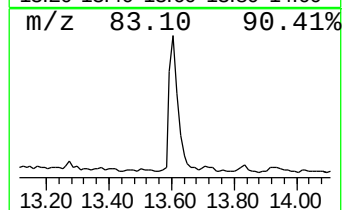
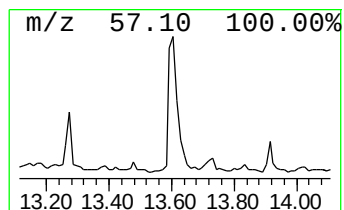
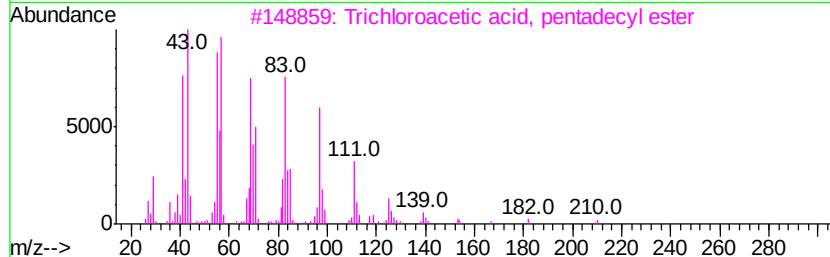
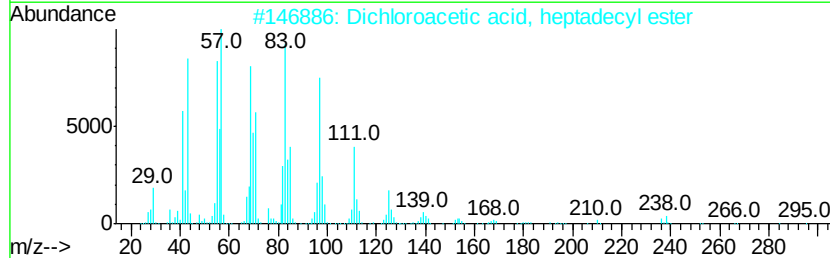
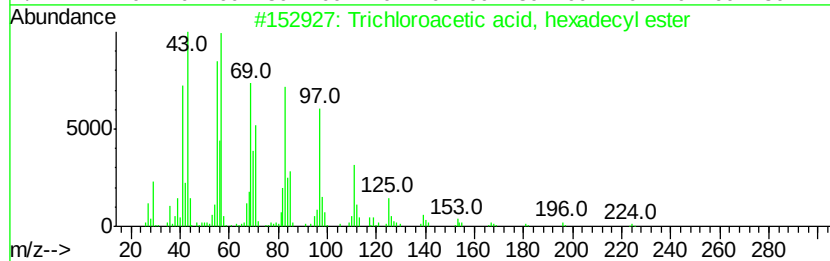
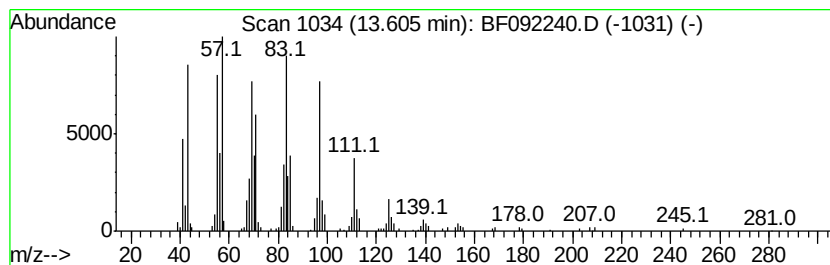
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	7.08 ng	530837	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		17-Pentatriacontene	491	C35H70	006971-40-0	91
5		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092240.D
Acq On : 13 Jan 2017 10:56
Operator : UM/SJ
Sample : I1131-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP

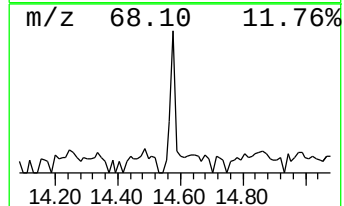
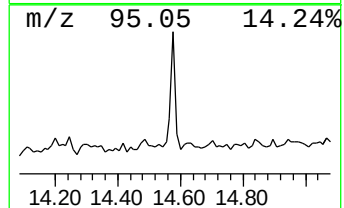
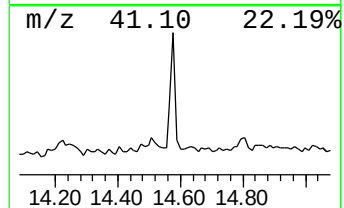
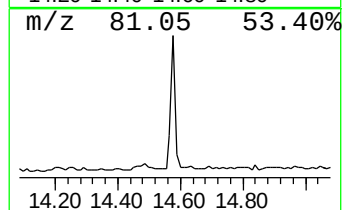
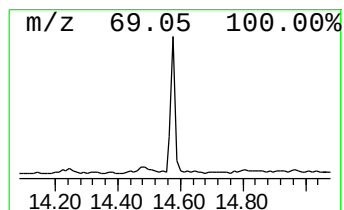
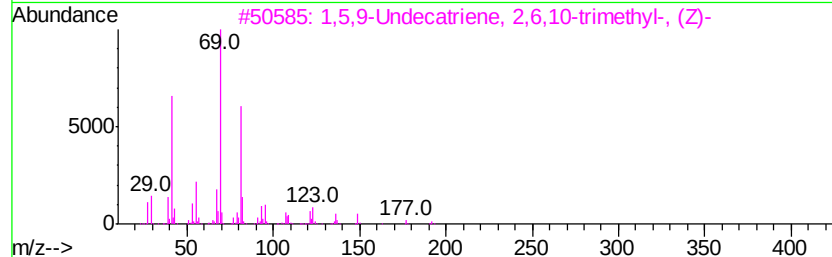
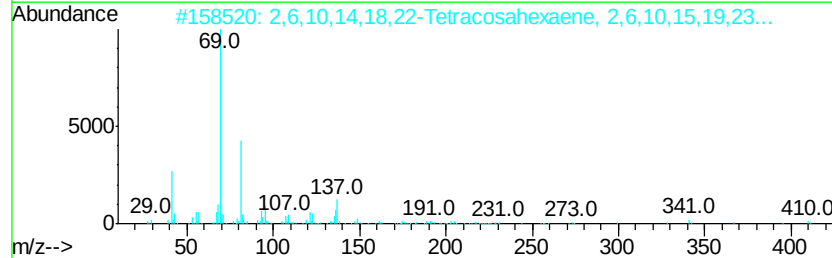
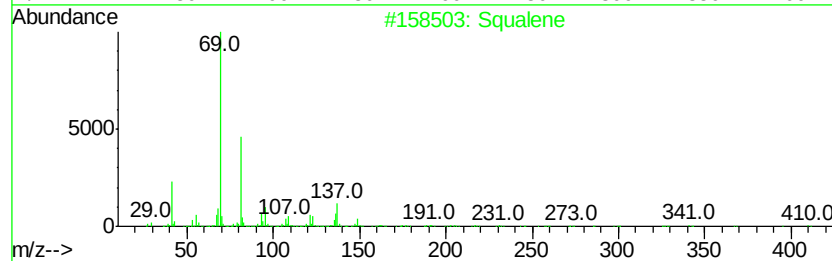
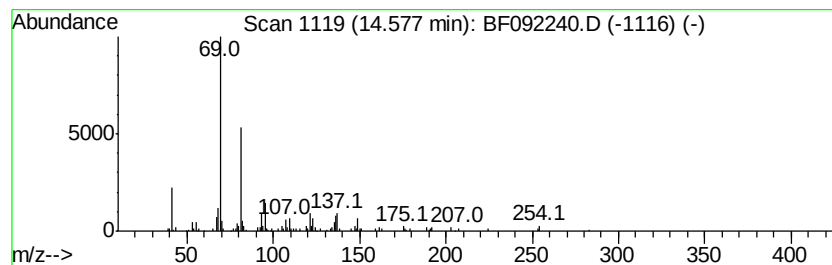
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.08 ng	130495	Perylene-d12	15.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	87
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	72
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092240.D
Acq On : 13 Jan 2017 10:56
Operator : UM/SJ
Sample : I1131-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
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
2-Pentanone, 4-hy...	4.71	54.0	ng	3052970	1	6.59	1129640	20.0
unknown6.36	6.36	78.8	ng	4450660	1	6.59	1129640	20.0
1-Pentadecene	11.35	2.7	ng	272509	4	11.10	2029540	20.0
n-Hexadecanoic acid	11.65	5.1	ng	517219	4	11.10	2029540	20.0
Trichloroacetic a...	13.61	7.1	ng	530837	5	13.73	1499550	20.0
Squalene	14.58	2.1	ng	130495	6	15.08	1253580	20.0