

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
 Data File : BF085192.D
 Acq On : 4 Mar 2016 7:55
 Operator : SJ/UM
 Sample : H1661-03
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-46-COMP

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-BF030316.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	5.190	251	254	262	rVB	698285	907294	22.26%	2.522%
2	5.590	286	289	291	rBV	3521531	3624956	88.94%	10.078%
3	6.607	375	378	380	rBV	3409846	4075790	100.00%	11.331%
4	6.744	387	390	393	rBV	3297554	3696808	90.70%	10.278%
5	6.984	408	411	413	rVB	698940	865915	21.25%	2.407%
6	7.133	422	424	427	rVB	2526007	2888653	70.87%	8.031%
7	7.544	457	460	462	rBV	2573976	2767671	67.91%	7.695%
8	7.624	462	467	469	rVB	68149	95619	2.35%	0.266%
9	8.264	520	523	525	rBV	1396797	1173360	28.79%	3.262%
10	9.339	614	617	620	rBV	4009733	3678624	90.26%	10.227%
11	9.727	649	651	653	rBV	895832	792582	19.45%	2.203%
12	9.945	668	670	672	rVB	115030	96840	2.38%	0.269%
13	10.025	674	677	679	rVB	901789	1114702	27.35%	3.099%
14	10.425	710	712	713	rBV	32741	45928	1.13%	0.128%
15	10.448	713	714	715	rVB	171710	118991	2.92%	0.331%
16	10.665	730	733	736	rBV	50219	80712	1.98%	0.224%
17	10.802	743	745	748	rVB2	1620806	2009296	49.30%	5.586%
18	10.916	754	755	762	rVB	147809	176227	4.32%	0.490%
19	11.362	792	794	796	rBV	64581	75463	1.85%	0.210%
20	11.499	804	806	809	rBV2	851886	996656	24.45%	2.771%
21	12.025	849	852	859	rBV	90208	117757	2.89%	0.327%
22	12.711	910	912	914	rBV	54787	59180	1.45%	0.165%
23	12.813	919	921	925	rBV4	22948	45046	1.11%	0.125%
24	13.088	942	945	947	rBV	3029883	2786920	68.38%	7.748%
25	13.294	957	963	966	rBV3	16171	46057	1.13%	0.128%
26	13.979	1021	1023	1028	rBV	444778	666151	16.34%	1.852%
27	14.139	1033	1037	1039	rBV	911390	897704	22.03%	2.496%
28	14.242	1044	1046	1049	rVV2	45604	72890	1.79%	0.203%
29	14.299	1049	1051	1054	rVV2	57813	84280	2.07%	0.234%
30	14.608	1076	1078	1085	rBV2	83586	148272	3.64%	0.412%
31	14.859	1098	1100	1101	rBV	89140	101461	2.49%	0.282%
32	14.894	1101	1103	1110	rVB2	178293	272628	6.69%	0.758%
33	15.179	1125	1128	1132	rVB	19775	46778	1.15%	0.130%
34	15.248	1132	1134	1136	rBV	50186	79570	1.95%	0.221%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.614	1163	1166	1171	rVB	628397	865591	21.24%	2.406%
36	16.082	1204	1207	1209	rBV	35484	62642	1.54%	0.174%
37	16.128	1209	1211	1215	rVV	56655	98719	2.42%	0.274%
38	16.585	1248	1251	1254	rBV2	24453	59051	1.45%	0.164%
39	17.683	1344	1347	1352	rVB5	33214	81636	2.00%	0.227%
40	18.734	1435	1439	1444	rBV5	25378	94925	2.33%	0.264%

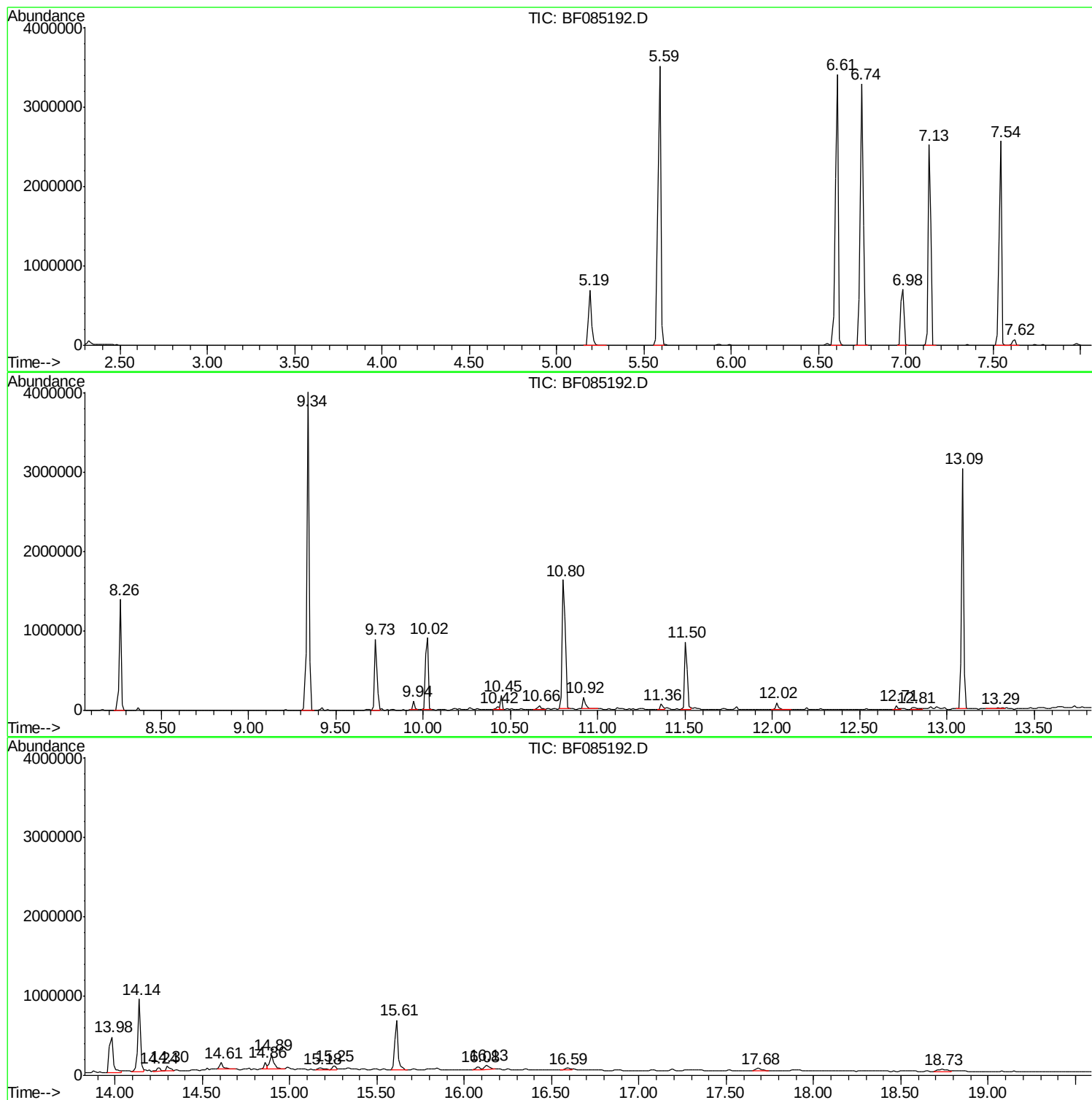
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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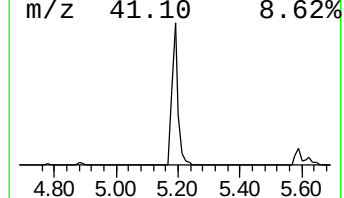
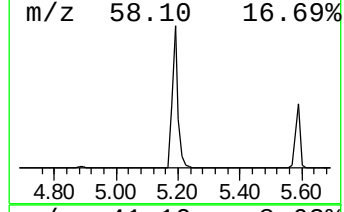
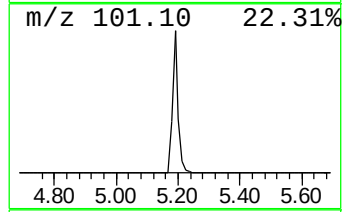
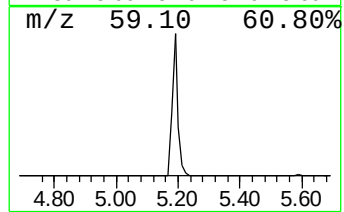
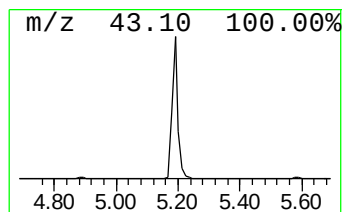
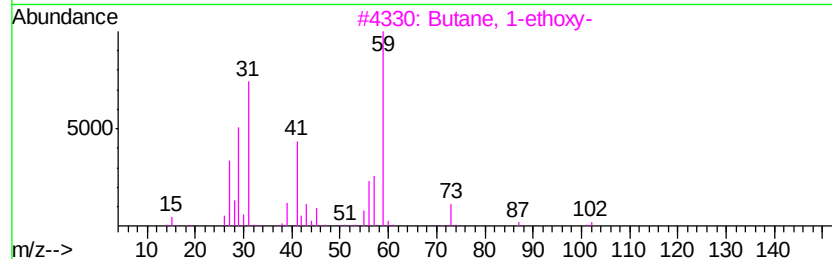
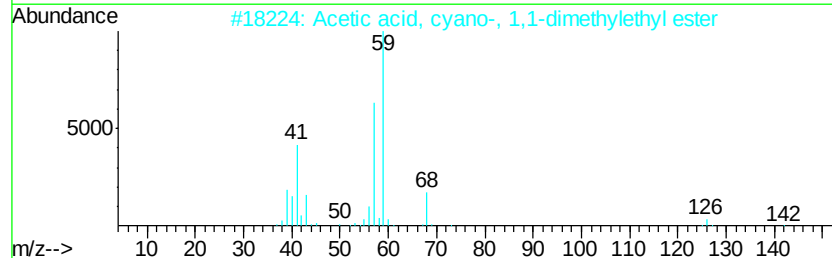
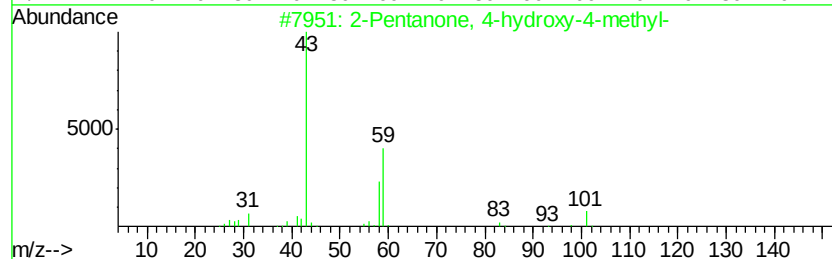
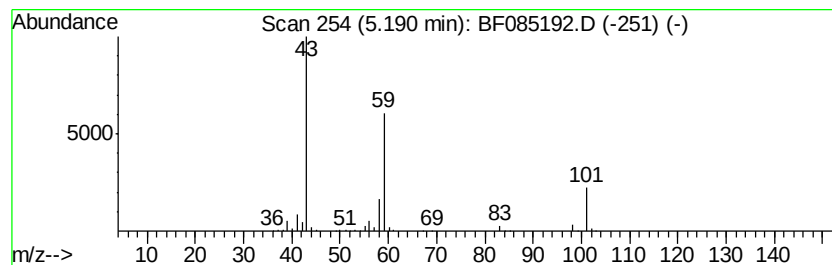
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	20.96 ng	907294	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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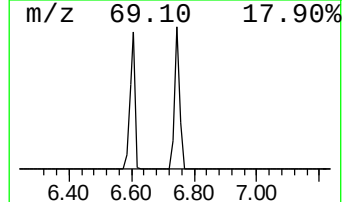
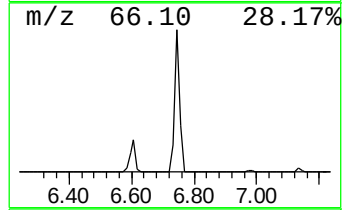
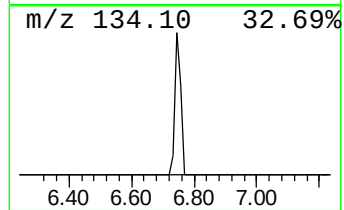
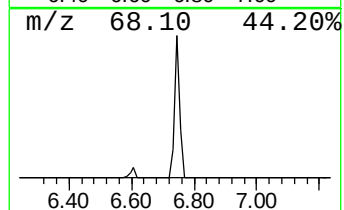
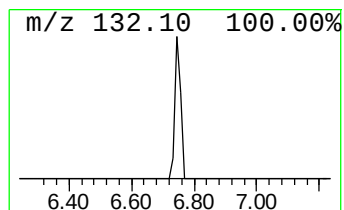
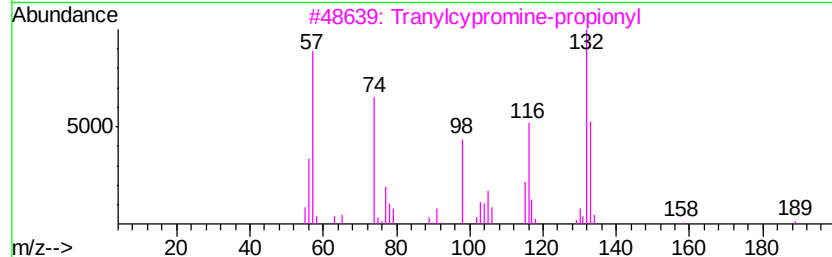
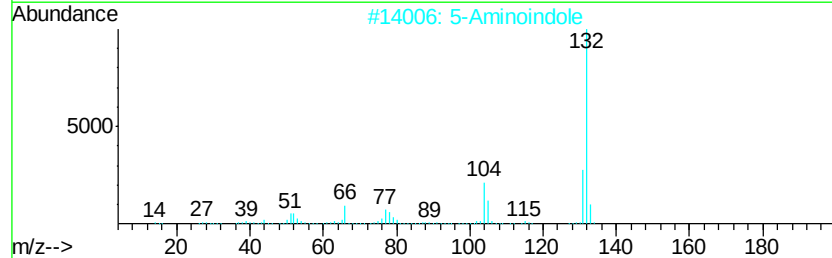
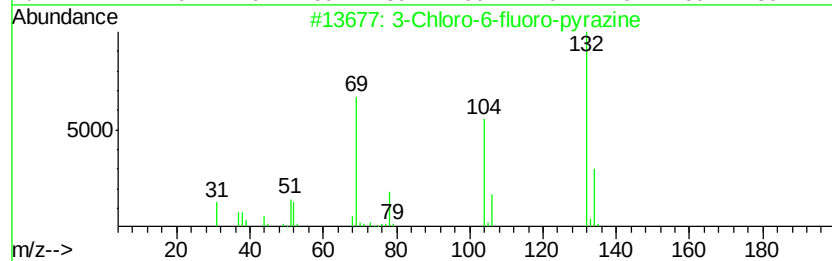
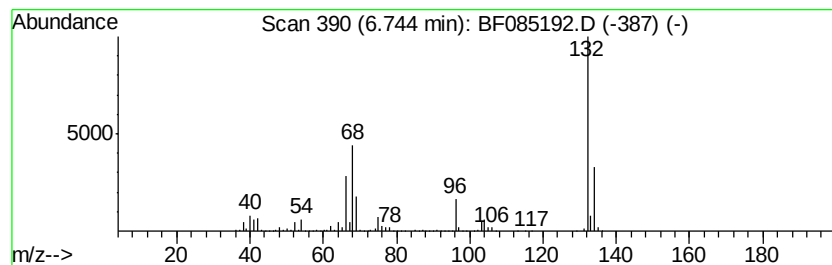
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	85.39 ng	3696810	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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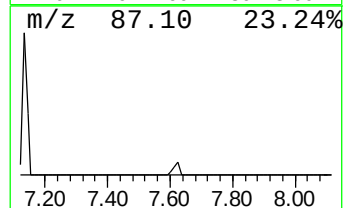
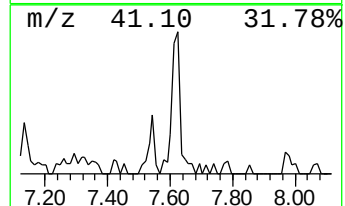
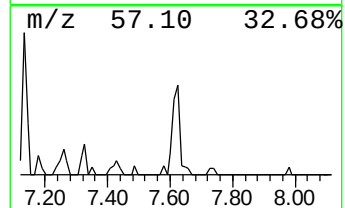
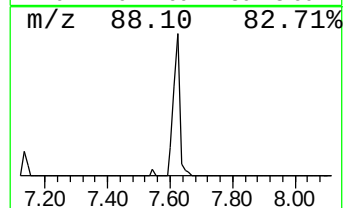
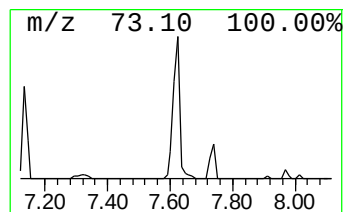
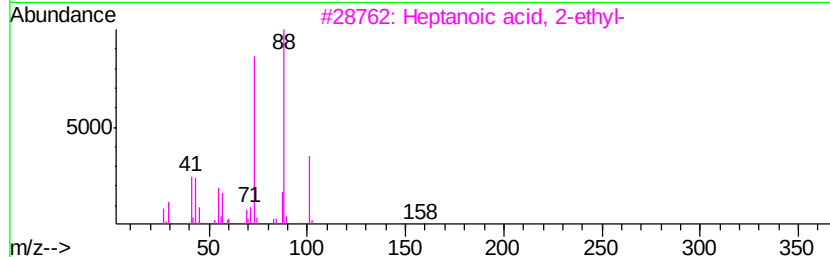
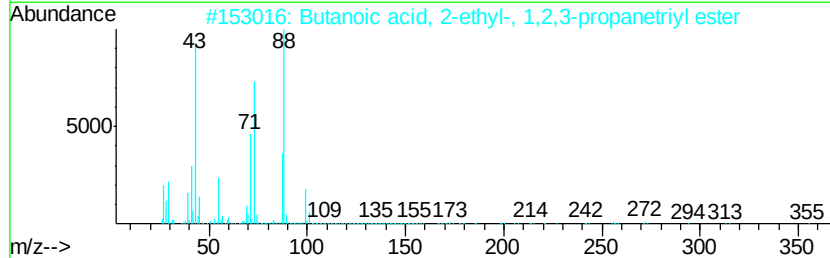
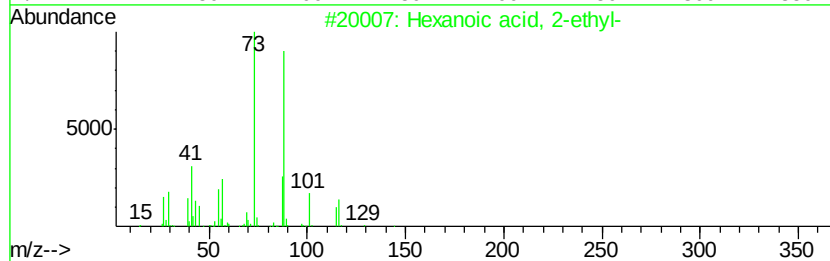
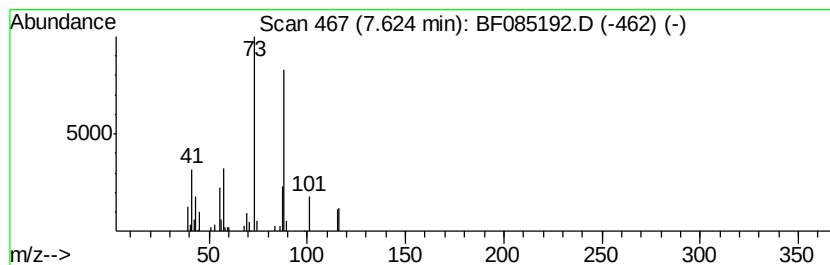
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	2.21 ng	95619	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
4		1,4-Dioxane	88	C4H8O2	000123-91-1	37
5		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	33



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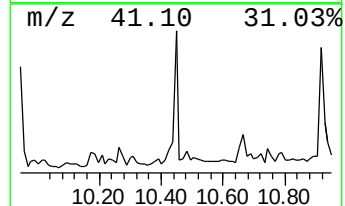
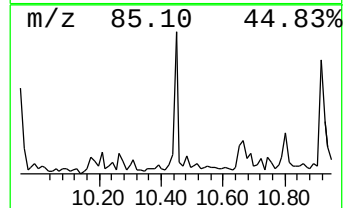
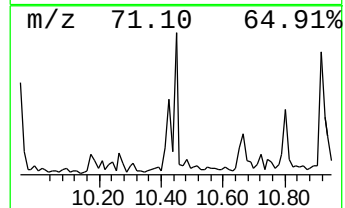
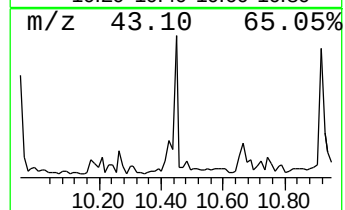
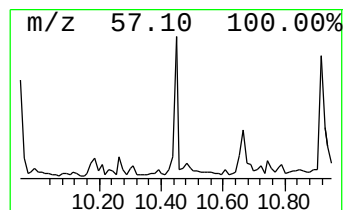
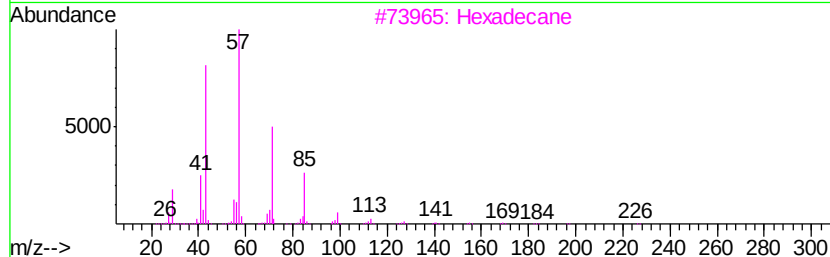
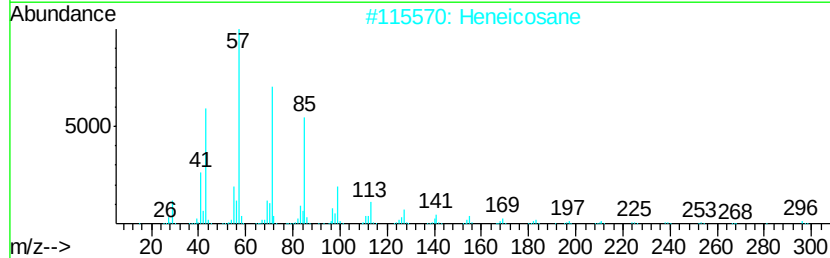
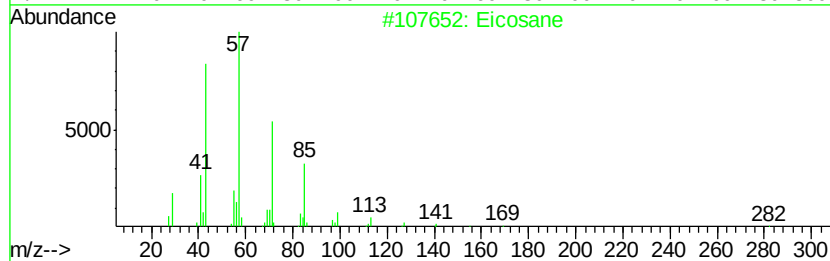
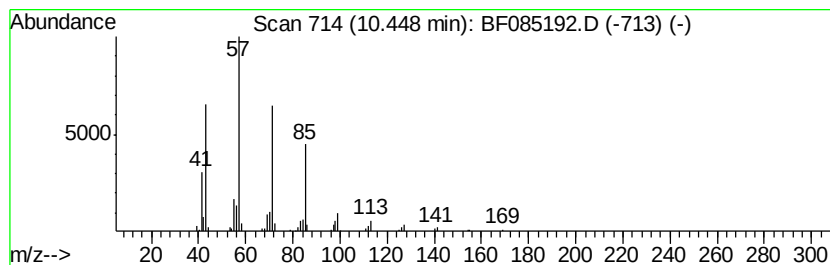
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.13 ng	118991	Acenaphthene-d10	10.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	91
2	Heneicosane	296 C21H44	000629-94-7	90
3	Hexadecane	226 C16H34	000544-76-3	90
4	Tridecane	184 C13H28	000629-50-5	90
5	Tetradecane	198 C14H30	000629-59-4	87



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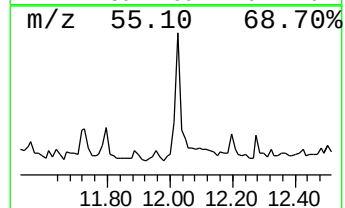
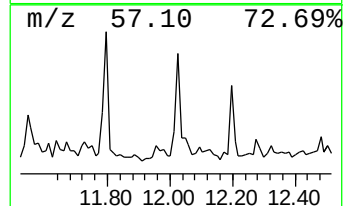
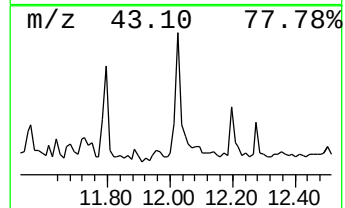
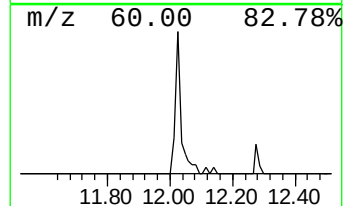
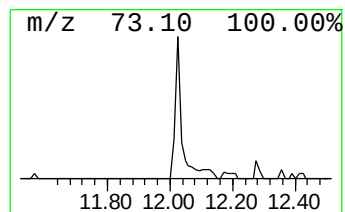
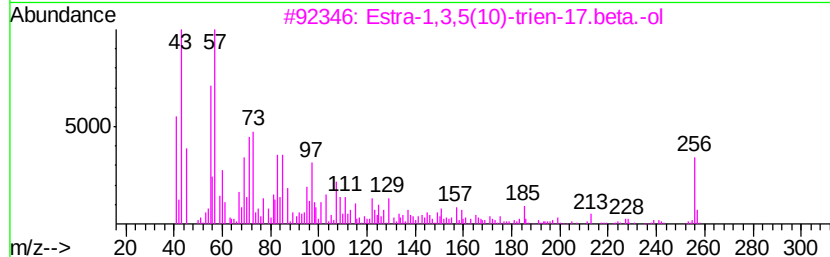
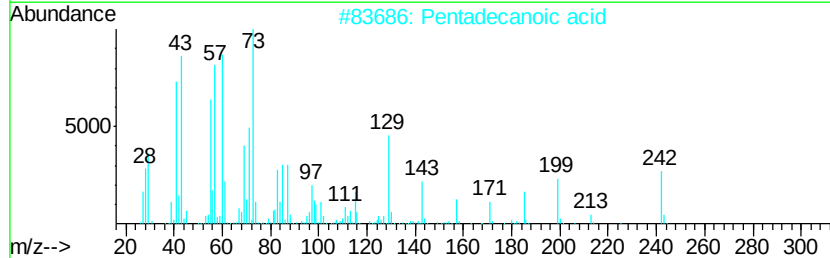
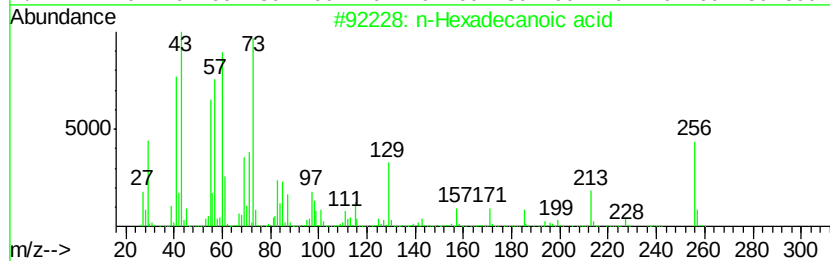
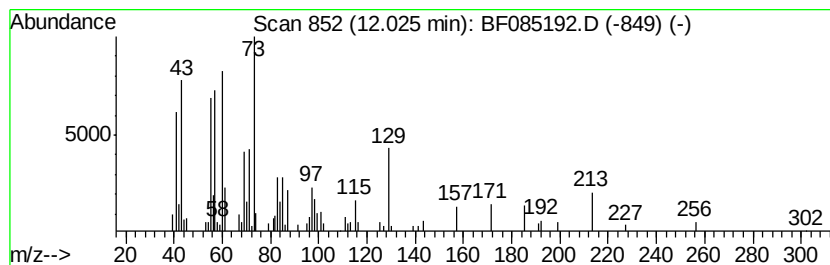
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.36 ng	117757	Phenanthrene-d10	11.50

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	80
3	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	20
4	.alpha.-D-Glucopyranoside, 0-.al...	504	C18H32O16	000597-12-6	14
5	Dodecane	170	C12H26	000112-40-3	11



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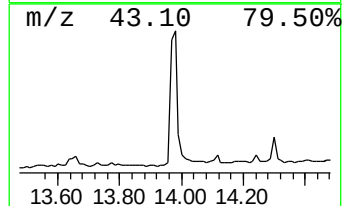
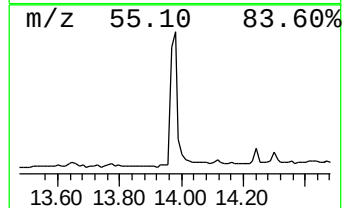
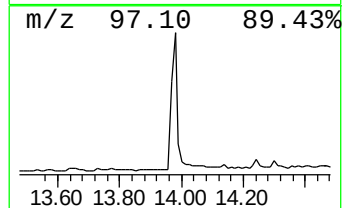
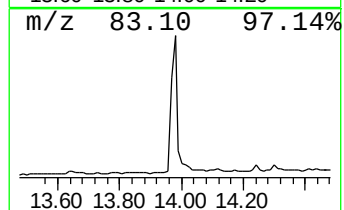
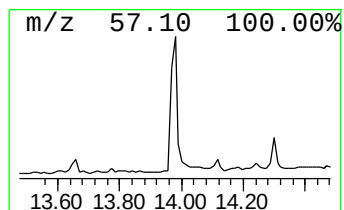
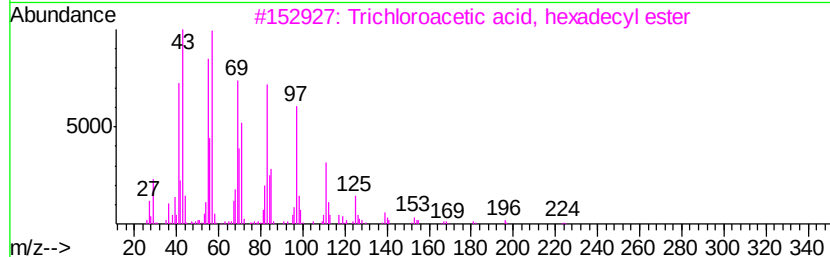
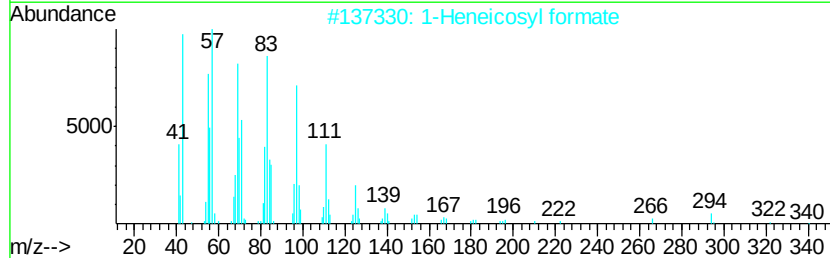
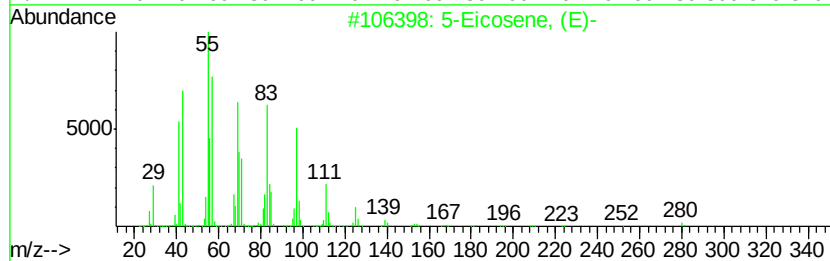
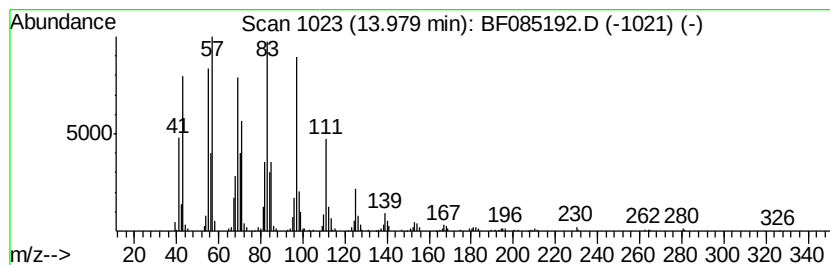
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.98	14.84 ng	666151	Chrysene-d12	14.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085192.D
Acq On : 4 Mar 2016 7:55
Operator : SJ/UM
Sample : H1661-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-46-COMP

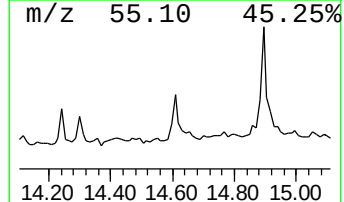
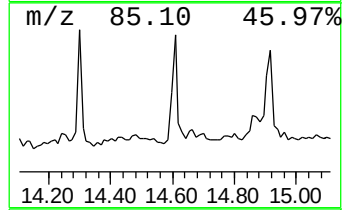
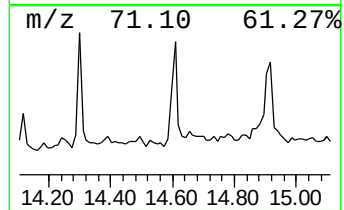
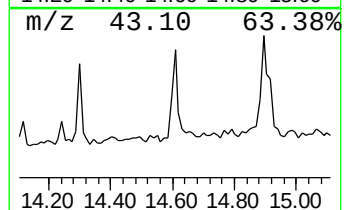
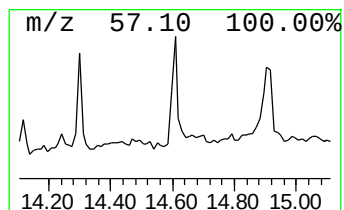
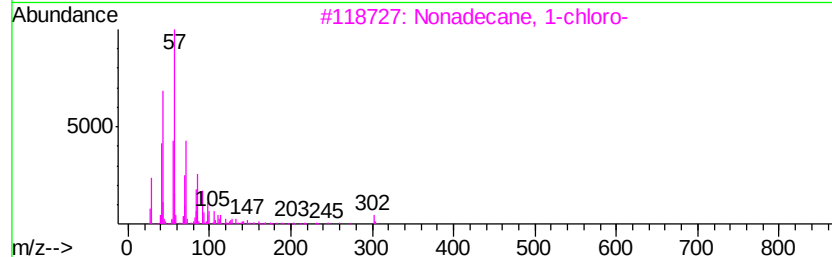
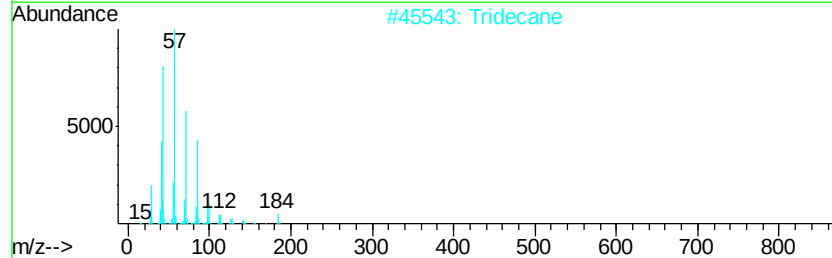
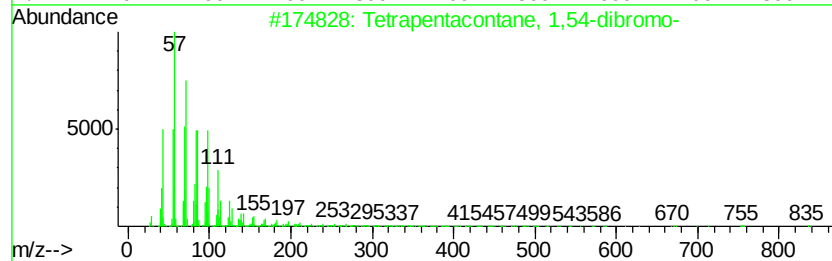
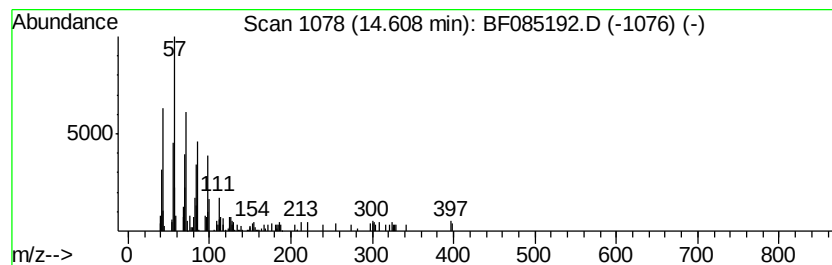
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetrapentacontane, 1,54-dib... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	3.30 ng	148272	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	68
2		Tridecane	184	C13H28	000629-50-5	64
3		Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	58
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	46
5		Nonadecane	268	C19H40	000629-92-5	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085192.D
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Sample : H1661-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
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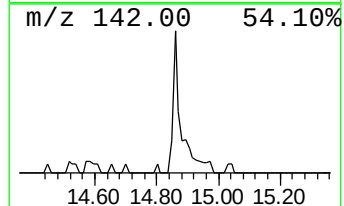
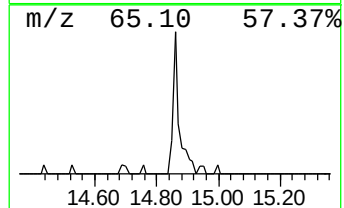
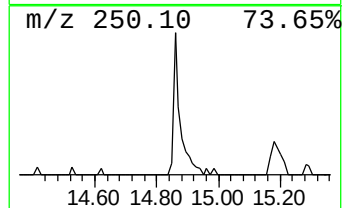
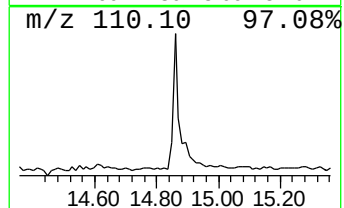
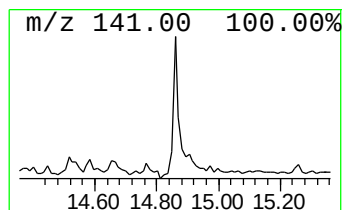
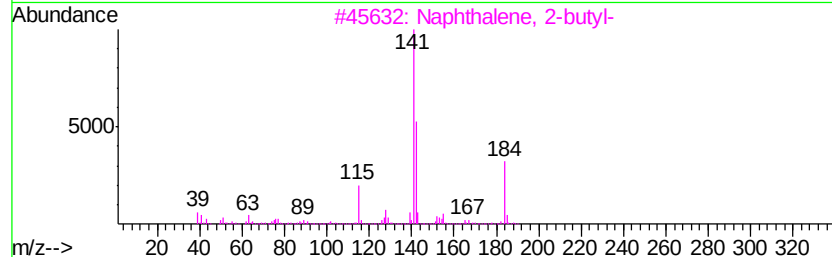
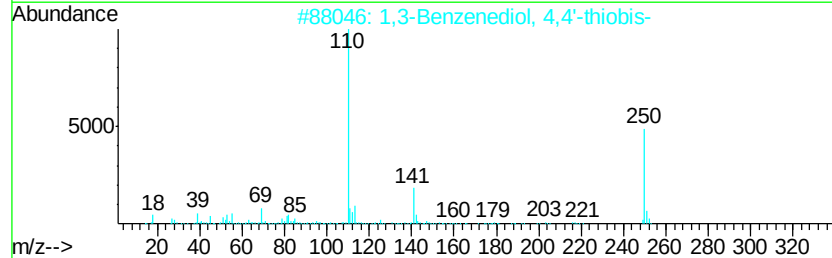
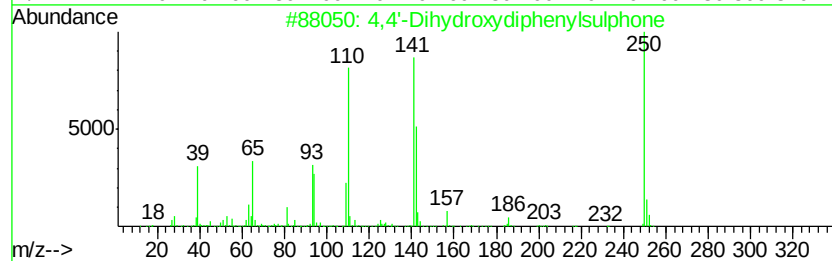
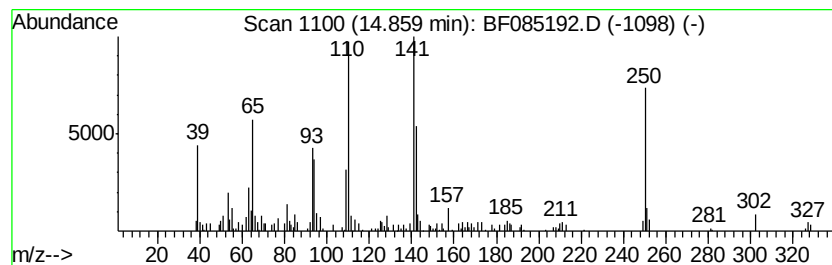
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 4,4'-Dihydroxydiphenylsulphone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	2.26 ng	101461	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	99
2		1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	45
3		Naphthalene, 2-butyl-	184	C14H16	001134-62-9	25
4		Phenoxyacetone nitrile	133	C8H7NO	003598-14-9	22
5		n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
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Acq On : 4 Mar 2016 7:55
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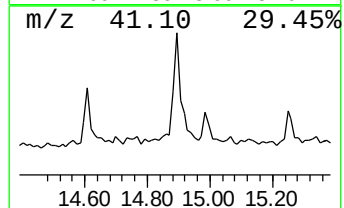
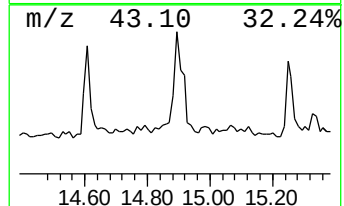
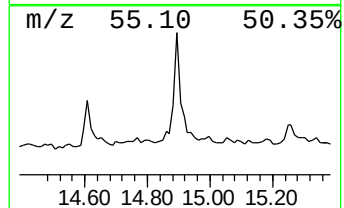
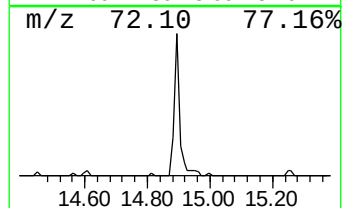
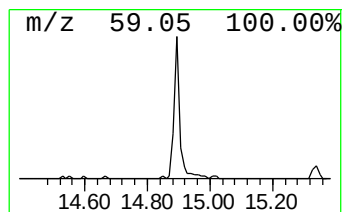
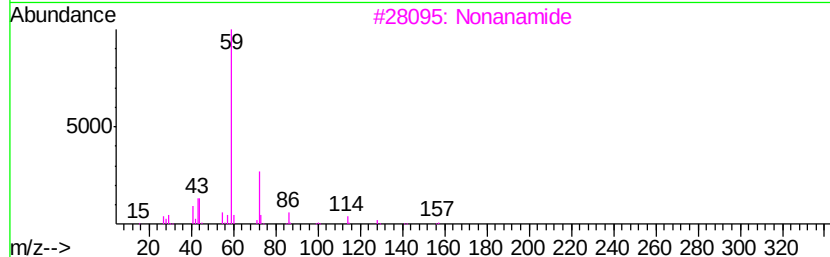
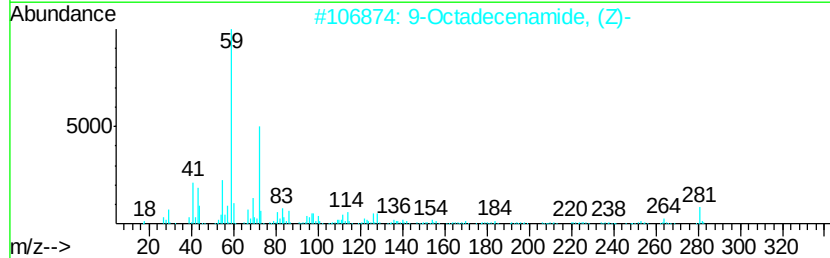
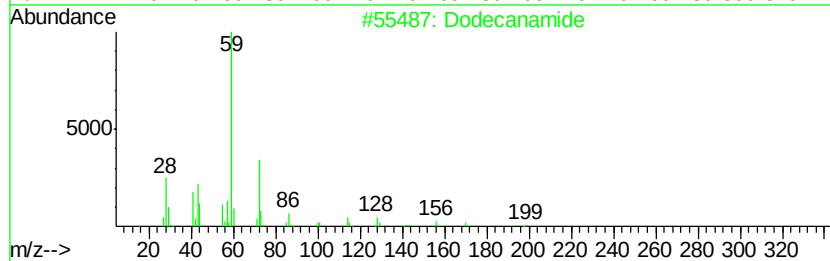
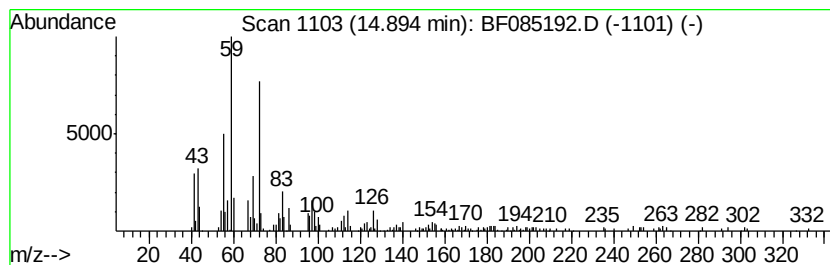
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dodecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.89	6.30 ng	272628	Perylene-d12	15.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanamide	199	C12H25NO	001120-16-7	50
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	49
3	Nonanamide	157	C9H19NO	001120-07-6	38
4	Tetradecanamide	227	C14H29NO	000638-58-4	38
5	Cyclohexane, (ethoxymethoxy)-	158	C9H18O2	054699-29-5	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085192.D
Acq On : 4 Mar 2016 7:55
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Instrument :
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ClientSampled :
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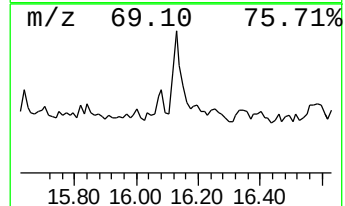
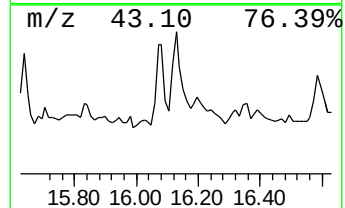
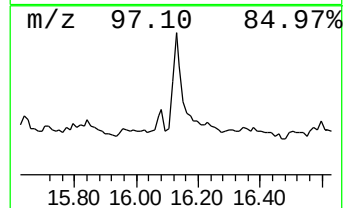
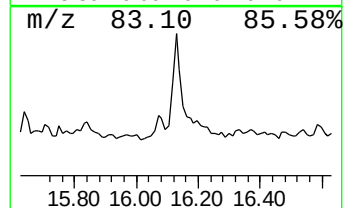
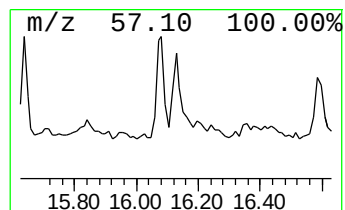
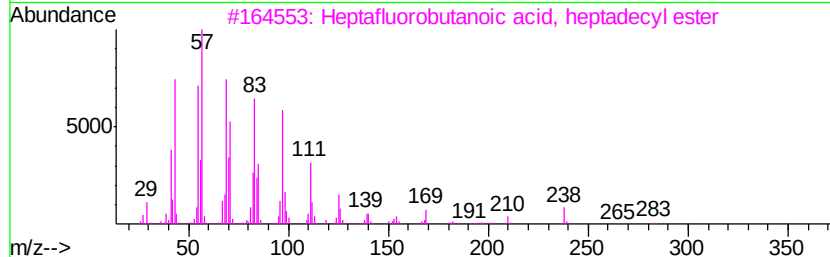
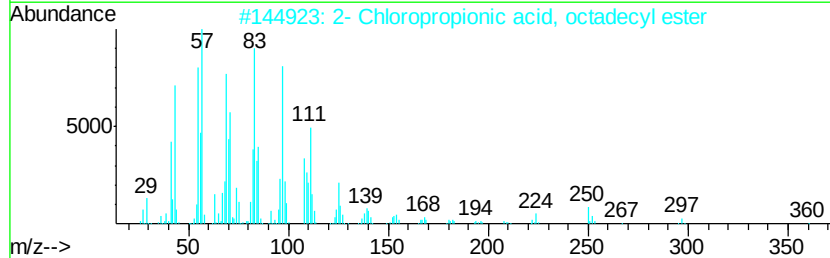
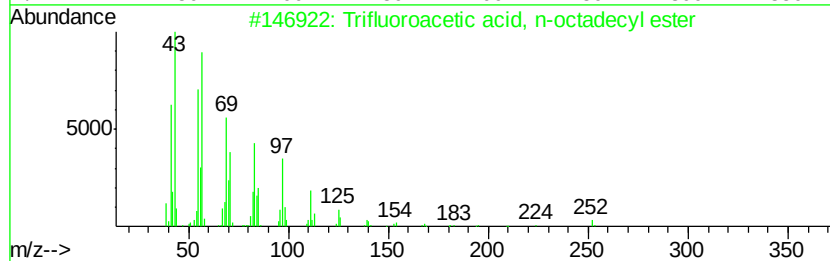
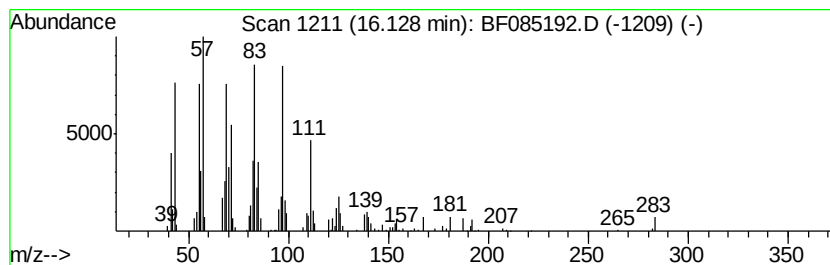
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Trifluoroacetic acid, n-oct... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.28 ng	98719	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	83
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	76
5		1-Docosene	308	C22H44	001599-67-3	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
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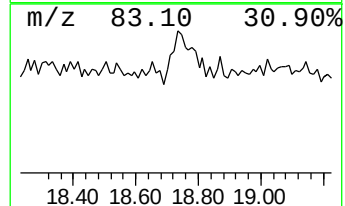
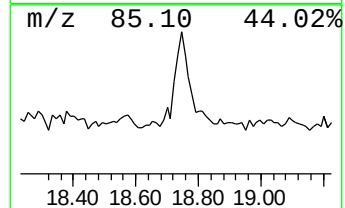
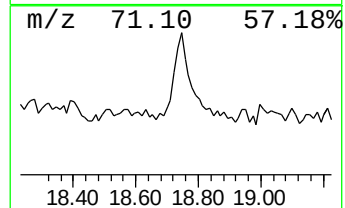
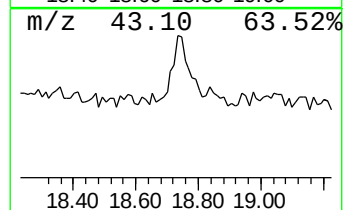
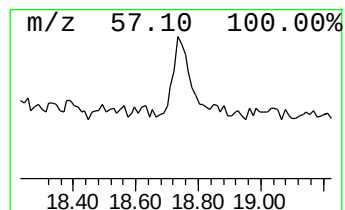
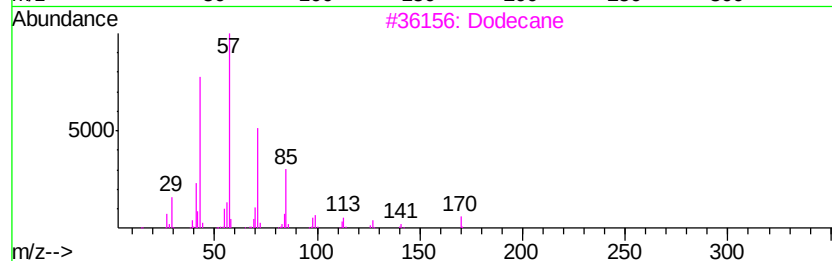
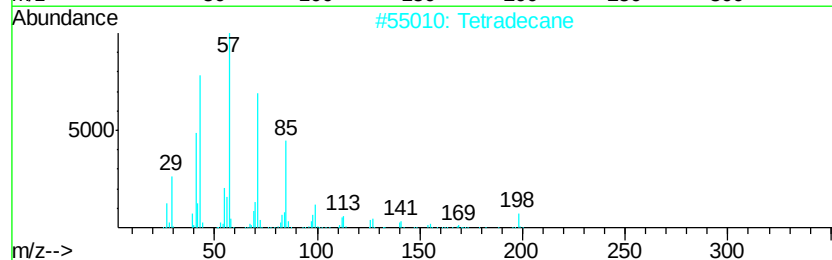
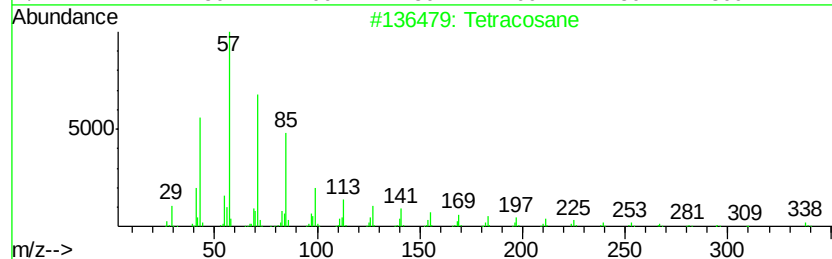
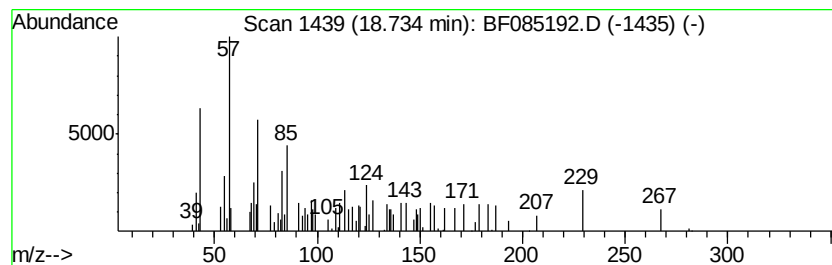
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.73 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	2.19 ng	94925	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	38
2		Tetradecane	198	C14H30	000629-59-4	35
3		Dodecane	170	C12H26	000112-40-3	35
4		Dotriacontane	451	C32H66	000544-85-4	35
5		2,5-Heptanedione, 3,3,6-trimethyl-	170	C10H18O2	051513-40-7	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085192.D
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Sample : H1661-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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...	5.19	21.0	ng	907294	1	6.98	865915	20.0
unknown6.74	6.74	85.4	ng	3696810	1	6.98	865915	20.0
Hexanoic acid, 2-...	7.62	2.2	ng	95619	1	6.98	865915	20.0
Eicosane	10.45	2.1	ng	118991	3	10.02	1114700	20.0
n-Hexadecanoic acid	12.02	2.4	ng	117757	4	11.50	996656	20.0
5-Eicosene, (E)-	13.98	14.8	ng	666151	5	14.14	897704	20.0
Tetrapentacontane...	14.61	3.3	ng	148272	5	14.14	897704	20.0
4,4'-Dihydroxydip...	14.86	2.3	ng	101461	5	14.14	897704	20.0
Dodecanamide	14.89	6.3	ng	272628	6	15.61	865591	20.0
Trifluoroacetic a...	16.13	2.3	ng	98719	6	15.61	865591	20.0
unknown18.73	18.73	2.2	ng	94925	6	15.61	865591	20.0