

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
 Data File : BF092229.D
 Acq On : 13 Jan 2017 2:23
 Operator : UM/SJ
 Sample : I1131-01
 Misc :
 ALS Vial : 24 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	3.990	182	184	194	rVB	24844	54411	1.00%	0.112%
2	4.401	215	220	234	rVB2	18542	64157	1.18%	0.132%
3	4.733	245	249	262	rBV	1287552	2588770	47.64%	5.318%
4	5.190	287	289	292	rBV	3282331	4780976	87.98%	9.821%
5	6.264	380	383	390	rBV	4483579	5156065	94.88%	10.591%
6	6.367	390	392	395	rVB	5321508	5434062	100.00%	11.162%
7	6.596	410	412	414	rBV	1009519	956979	17.61%	1.966%
8	6.756	423	426	428	rBV	2961495	3991405	73.45%	8.199%
9	7.167	459	462	464	rBV	3130907	3248875	59.79%	6.674%
10	7.304	472	474	479	rBV	55286	78553	1.45%	0.161%
11	7.876	522	524	527	rBV	1183734	1393272	25.64%	2.862%
12	8.836	605	608	612	rBV	50032	63940	1.18%	0.131%
13	8.962	616	619	621	rBV	4773942	4726813	86.98%	9.709%
14	9.362	651	654	656	rBV	1330367	1126226	20.73%	2.313%
15	9.625	675	677	680	rBV	1329131	1374896	25.30%	2.824%
16	10.048	709	714	715	rBV	99296	99994	1.84%	0.205%
17	10.082	715	717	718	rVB	58275	72278	1.33%	0.148%
18	10.425	744	747	749	rBV2	2219488	3206591	59.01%	6.587%
19	10.550	756	758	762	rVB	99015	123436	2.27%	0.254%
20	10.996	795	797	798	rBV	72470	76645	1.41%	0.157%
21	11.110	804	807	809	rBV	965081	1396615	25.70%	2.869%
22	11.362	827	829	833	rBV	102510	195380	3.60%	0.401%
23	11.659	853	855	859	rVB2	257008	251769	4.63%	0.517%
24	12.311	910	912	914	rBV	219110	201121	3.70%	0.413%
25	12.436	922	923	929	rBV2	38392	82334	1.52%	0.169%
26	12.539	929	932	934	rVB	158967	183023	3.37%	0.376%
27	12.585	934	936	941	rVB	43642	55341	1.02%	0.114%
28	12.688	943	945	948	rVB	2837889	3854096	70.92%	7.917%
29	12.939	963	967	968	rBV	63330	74810	1.38%	0.154%
30	13.602	1023	1025	1034	rBV2	165296	370984	6.83%	0.762%
31	13.728	1034	1036	1041	rVB	1030087	1189929	21.90%	2.444%
32	14.517	1097	1105	1109	rBV3	40112	117798	2.17%	0.242%
33	14.585	1109	1111	1115	rVB	83519	106535	1.96%	0.219%
34	14.734	1121	1124	1127	rBV	79197	192599	3.54%	0.396%

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35	14.814	1127	1131	1139	rVB4	63244	214239	3.94%	0.440%
36	15.042	1148	1151	1153	rBV	58999	69274	1.27%	0.142%
37	15.088	1153	1155	1158	rBV	869796	1081159	19.90%	2.221%
38	15.568	1194	1197	1200	rBV4	40799	114508	2.11%	0.235%
39	16.334	1261	1264	1268	rBV	27652	56521	1.04%	0.116%
40	16.528	1276	1281	1290	rBV8	25220	132552	2.44%	0.272%
41	16.711	1294	1297	1303	rBV2	37650	123627	2.28%	0.254%

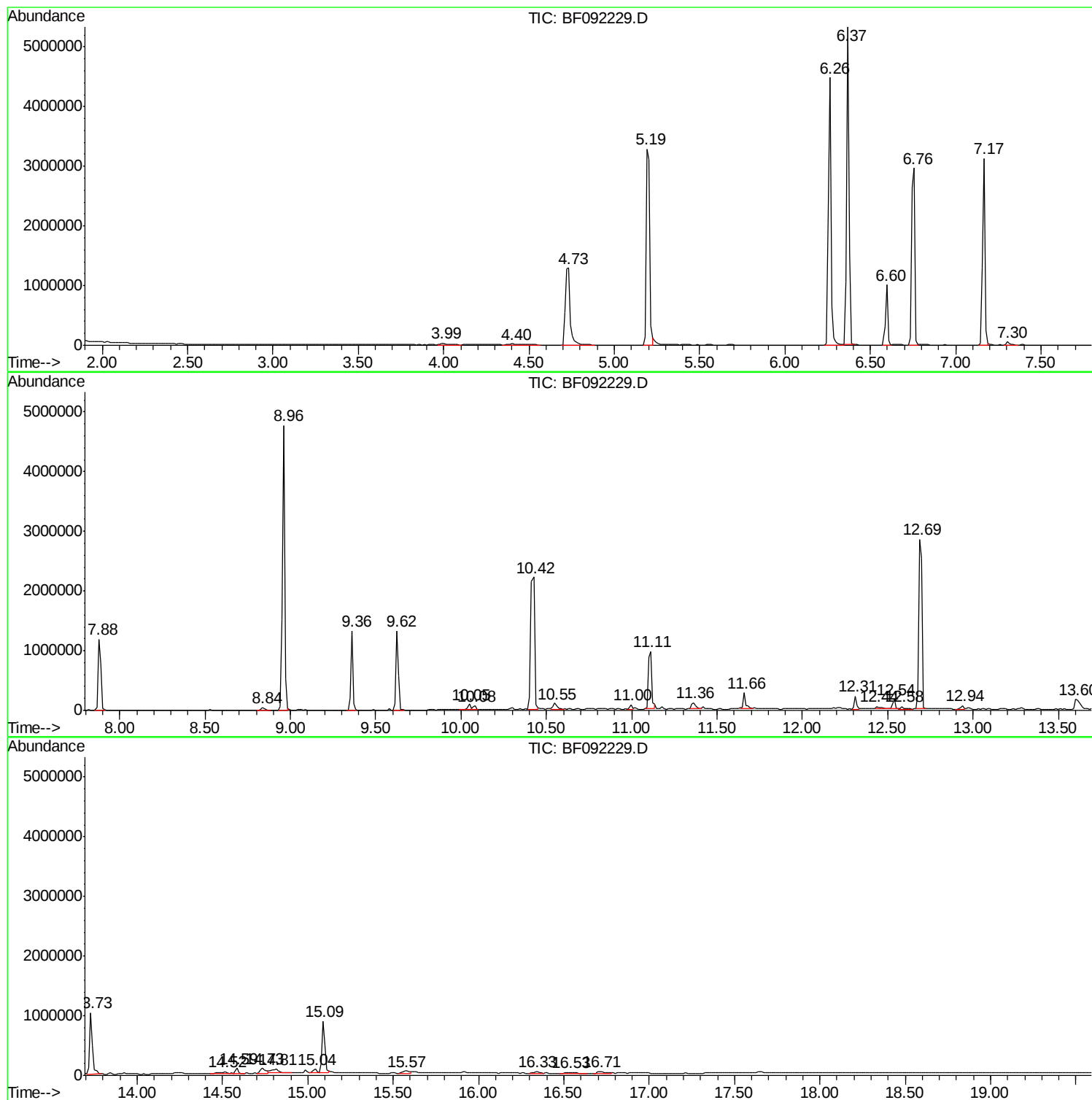
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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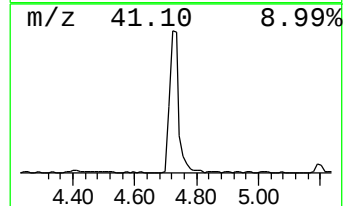
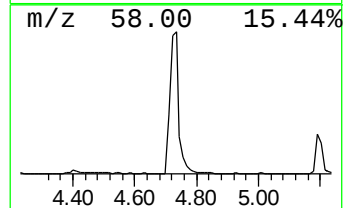
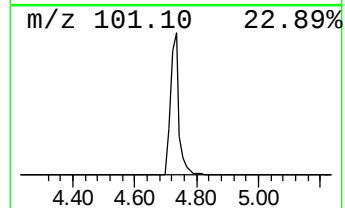
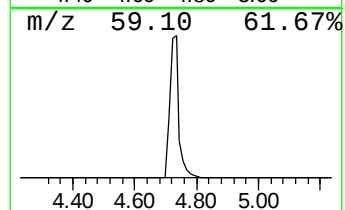
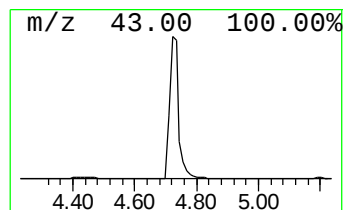
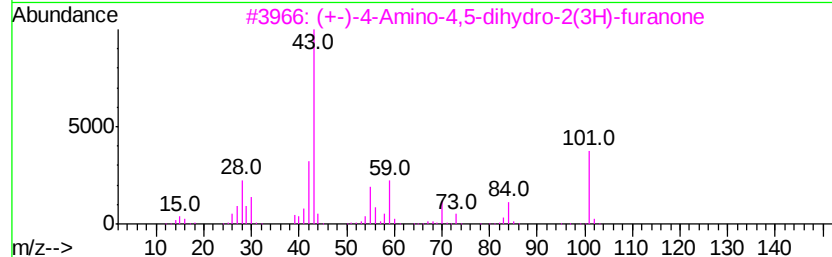
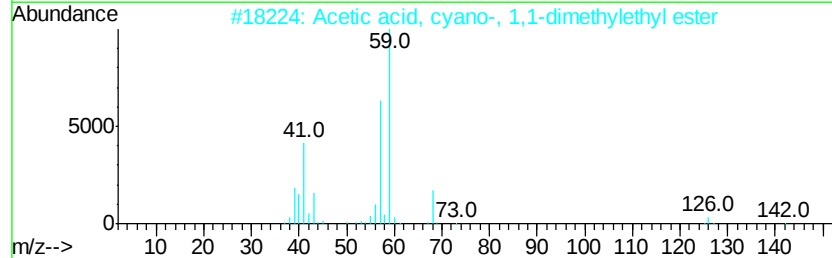
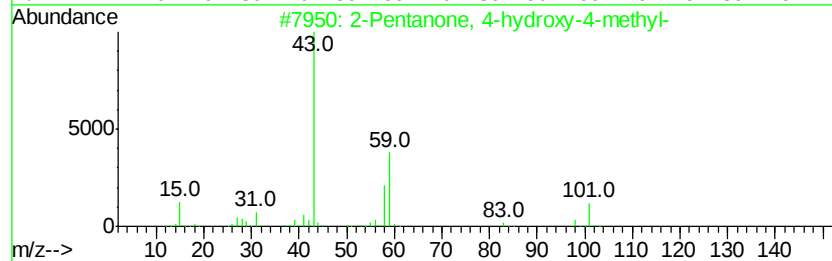
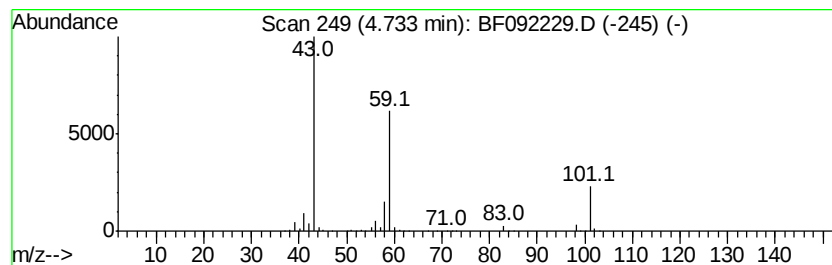
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	54.10 ng	2588770	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
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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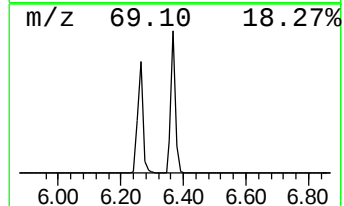
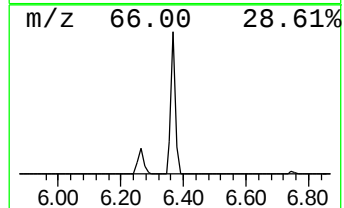
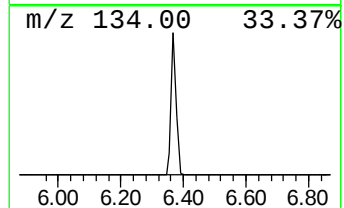
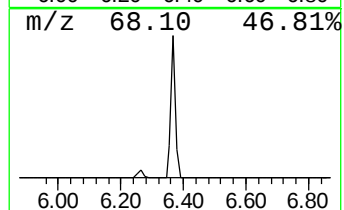
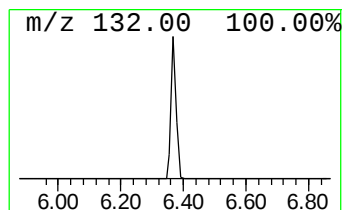
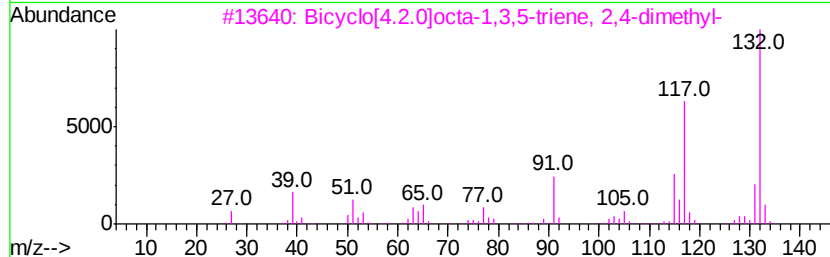
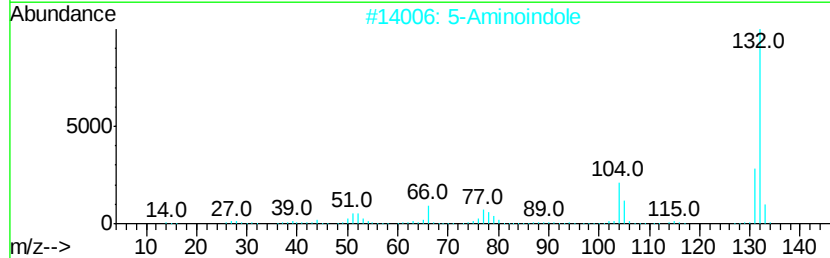
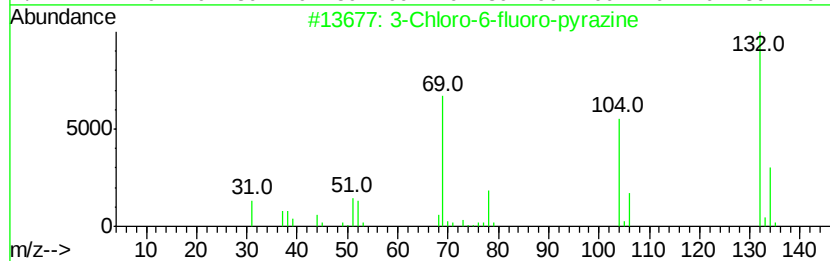
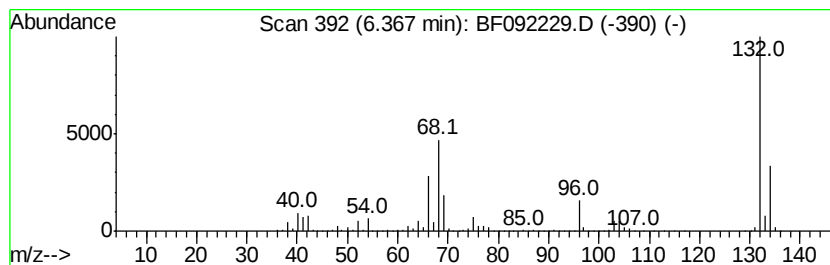
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Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	113.57 ng	5434060	1,4-Dichlorobenzene-d4	6.60

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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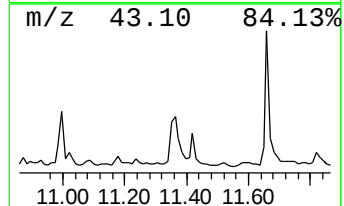
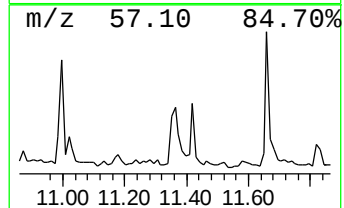
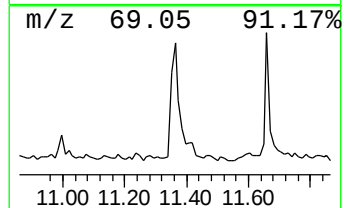
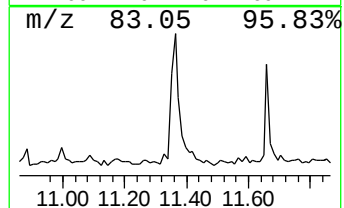
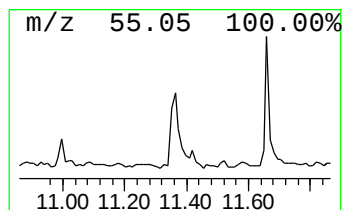
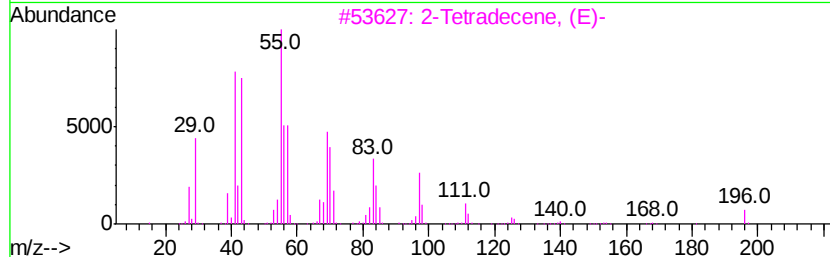
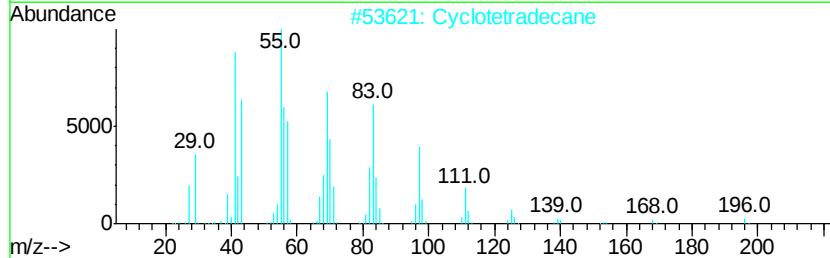
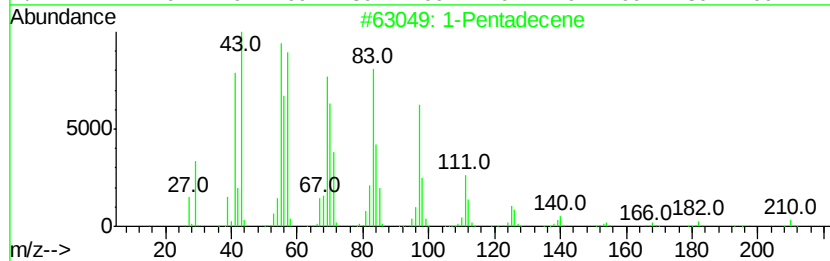
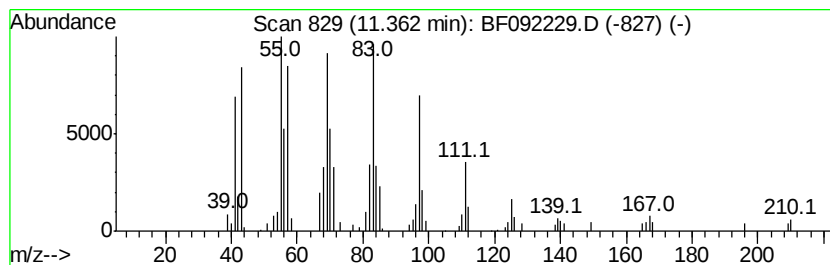
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Pentadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.36	2.80 ng	195380	Phenanthrene-d10	11.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene		210	C15H30	013360-61-7	99
2	Cyclotetradecane		196	C14H28	000295-17-0	98
3	2-Tetradecene, (E)-		196	C14H28	035953-53-8	95
4	1-Hexadecanol		242	C16H34O	036653-82-4	94
5	Bromoacetic acid, pentadecyl ester		348	C17H33BrO2	131143-01-6	94



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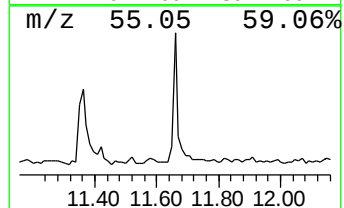
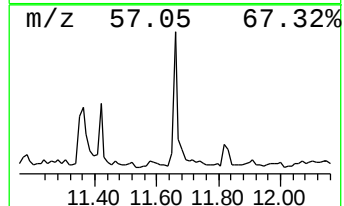
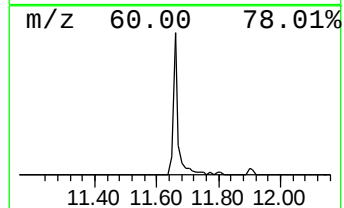
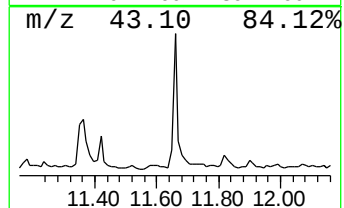
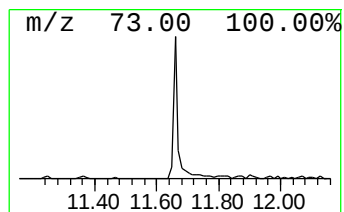
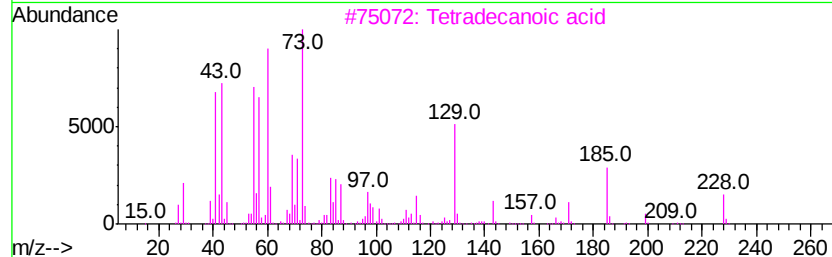
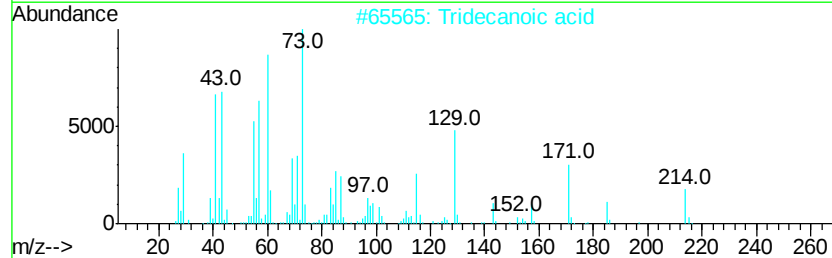
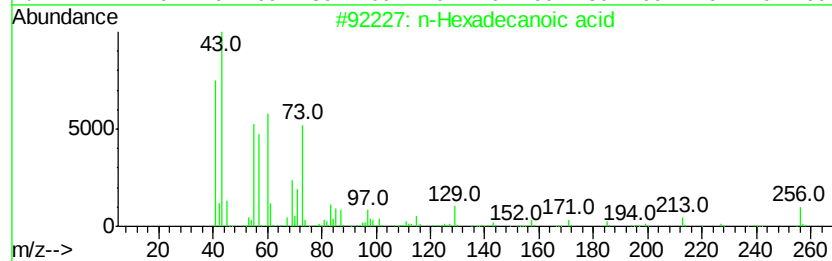
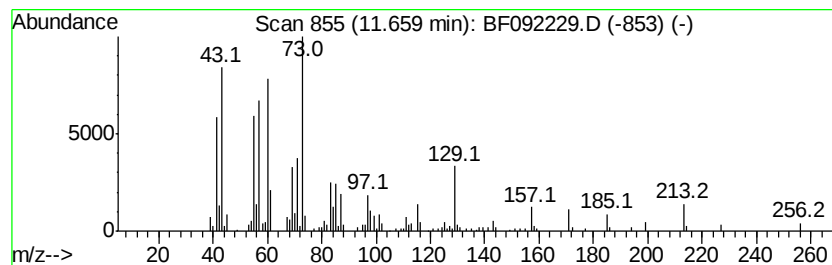
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	3.61 ng	251769	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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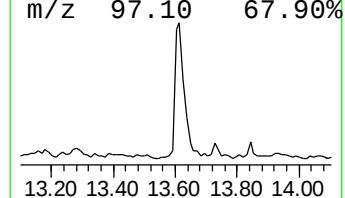
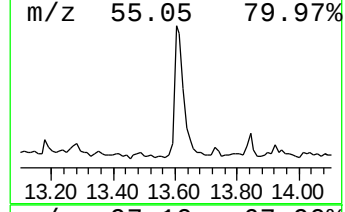
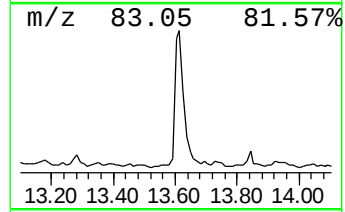
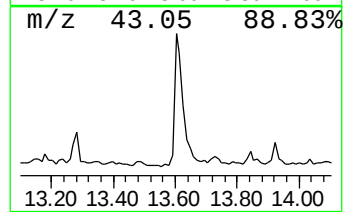
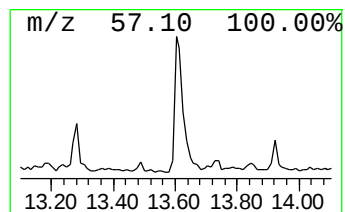
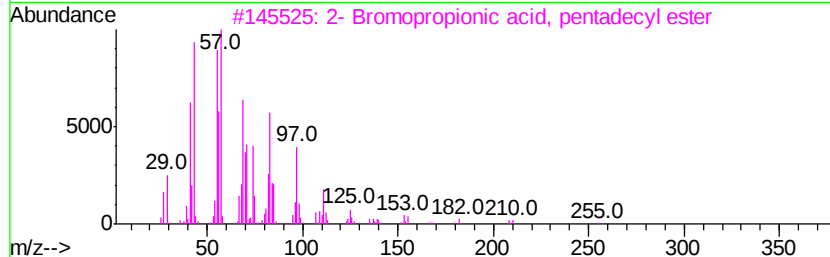
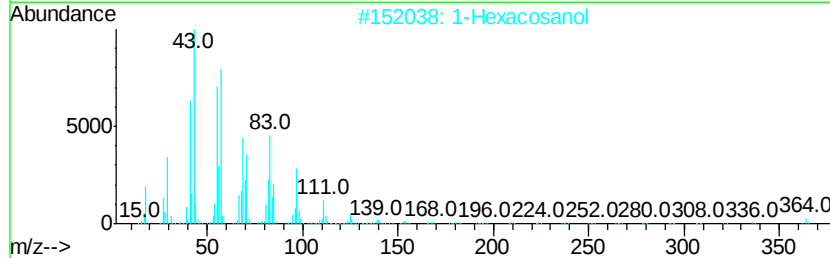
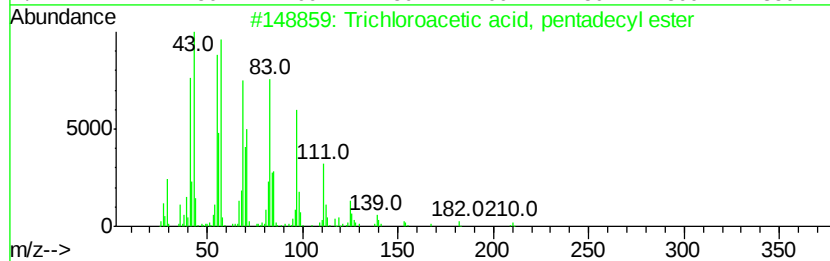
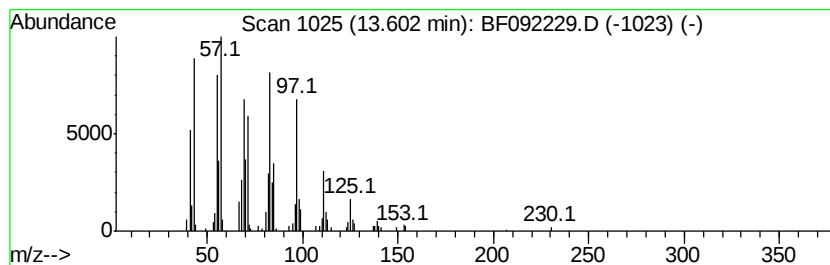
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	6.24 ng	370984	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		1-Hexacosanol	382	C26H54O	000506-52-5	91
3		2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
4		1-Heptadecanol	256	C17H36O	001454-85-9	87
5		1-Octadecanol	270	C18H38O	000112-92-5	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092229.D
Acq On : 13 Jan 2017 2:23
Operator : UM/SJ
Sample : I1131-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

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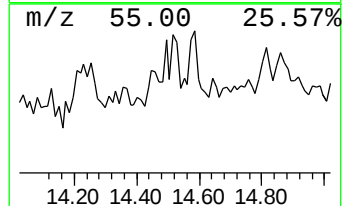
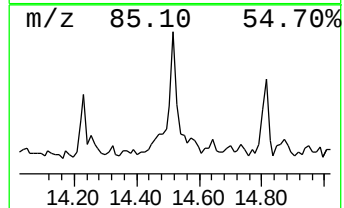
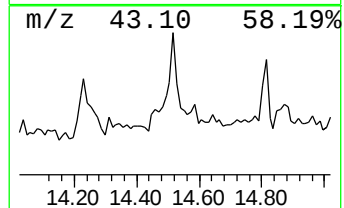
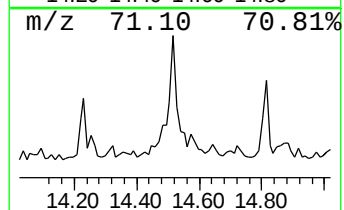
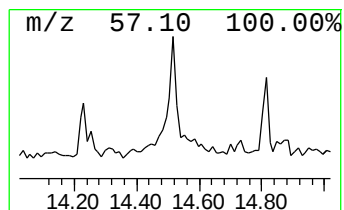
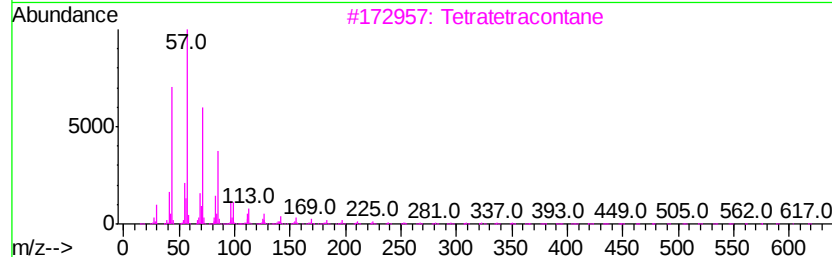
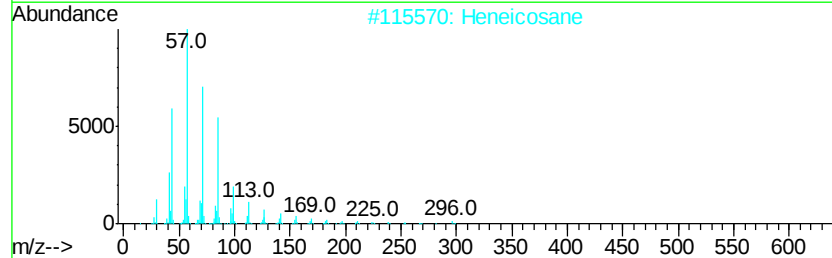
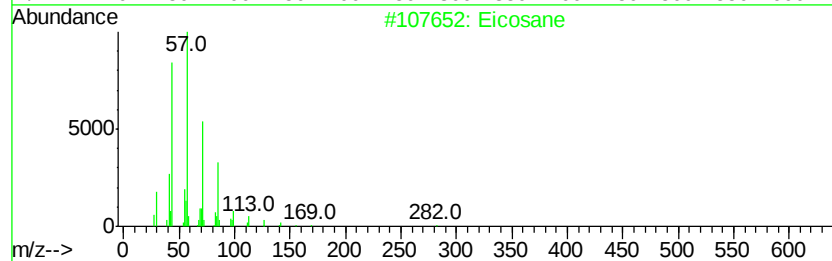
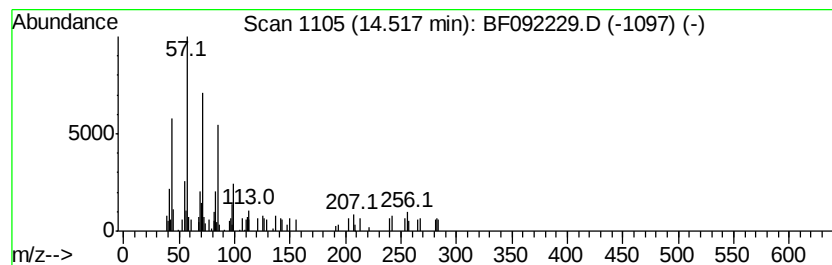
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.18 ng	117798	Perylene-d12	15.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	76
2	Heneicosane		296	C21H44	000629-94-7	64
3	Tetratetracontane		619	C44H90	007098-22-8	59
4	Eicosane, 9-octyl-		394	C28H58	013475-77-9	59
5	Heptadecane		240	C17H36	000629-78-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
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Acq On : 13 Jan 2017 2:23
Operator : UM/SJ
Sample : I1131-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP

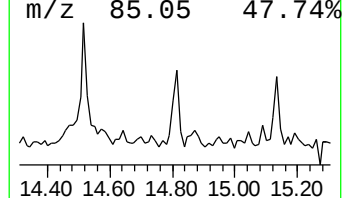
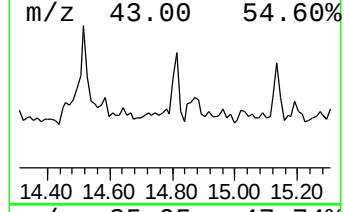
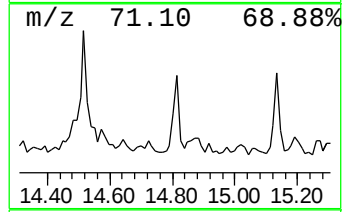
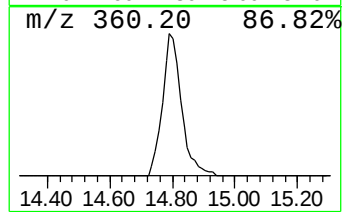
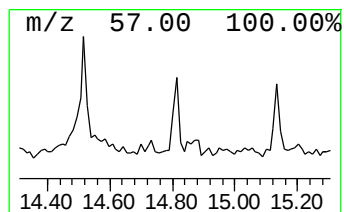
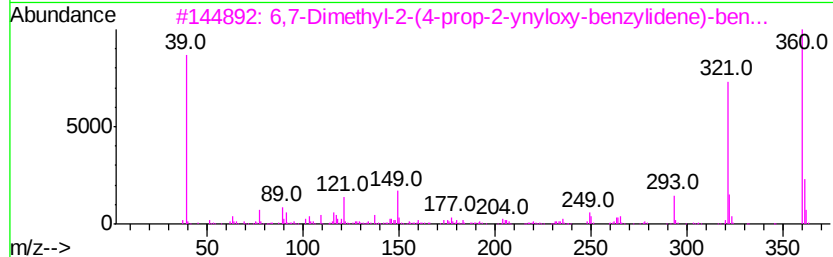
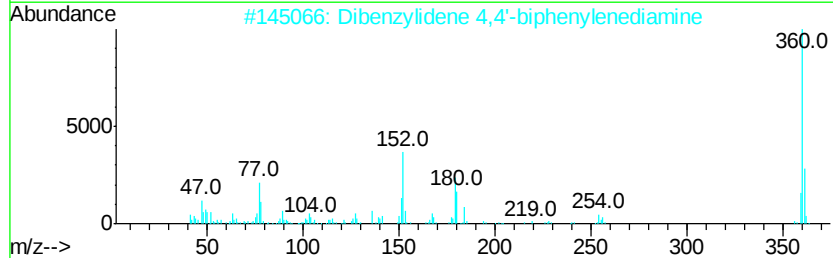
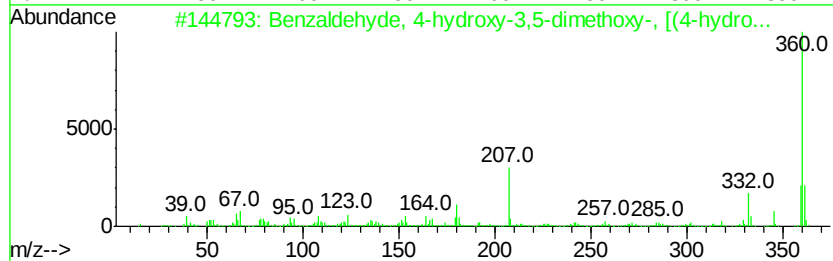
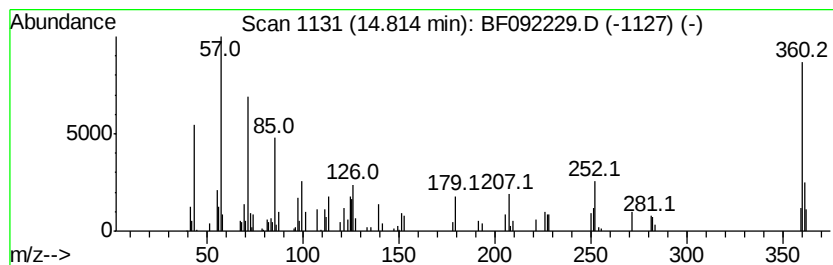
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.81 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	3.96 ng	214239	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	38
2		Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	38
3		6,7-Dimethyl-2-(4-prop-2-ynvloxv...	360	C21H16N2O2S	1000296-51-8	35
4		3-Amino-6-nitro-4-phenylsulfanyl...	360	C16H12N2O4S2	1000275-36-3	27
5		Melatonin, pentafluoropropionyl ...	360	C16H13F5N2O2	066012-87-1	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092229.D
Acq On : 13 Jan 2017 2:23
Operator : UM/SJ
Sample : I1131-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

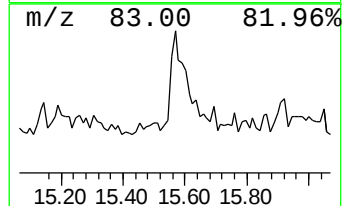
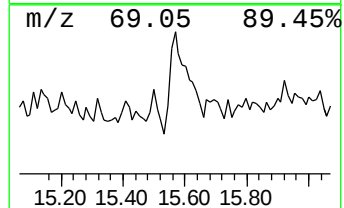
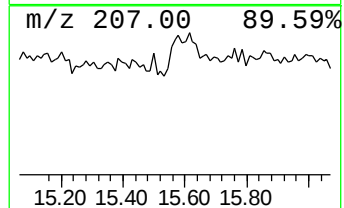
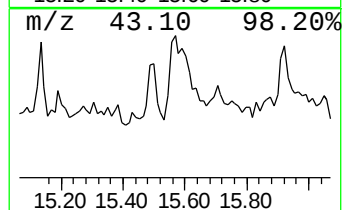
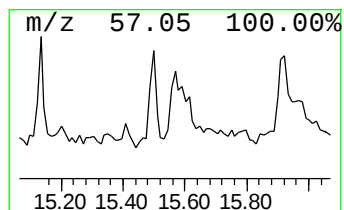
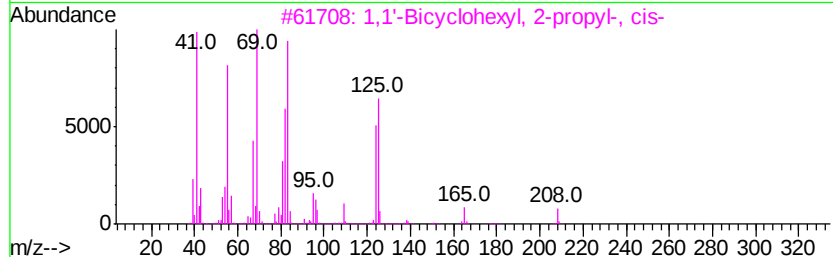
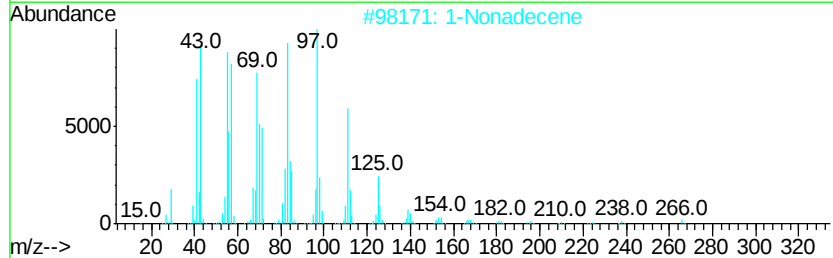
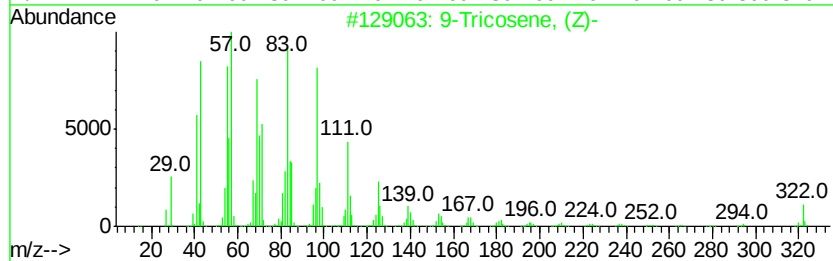
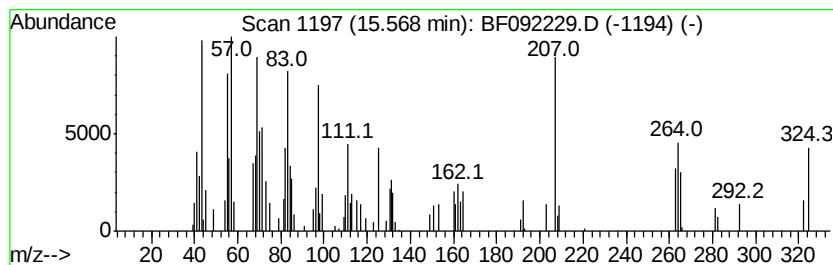
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Tricosene, (Z)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.12 ng	114508	Perylene-d12	15.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Tricosene, (Z)-	322 C23H46	027519-02-4	81
2	1-Nonadecene	266 C19H38	018435-45-5	80
3	1,1'-Bicyclohexyl, 2-propyl-, cis-	208 C15H28	054934-88-2	56
4	1-Tricosene	322 C23H46	018835-32-0	55
5	1-Nonadecanol	284 C19H40O	001454-84-8	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
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Acq On : 13 Jan 2017 2:23
Operator : UM/SJ
Sample : I1131-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

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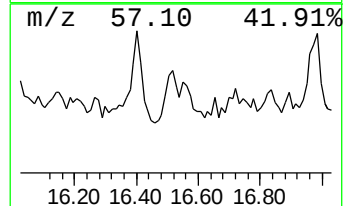
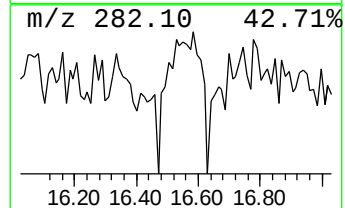
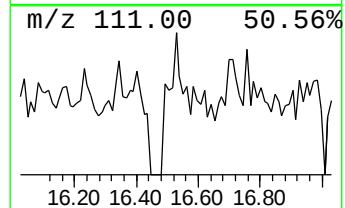
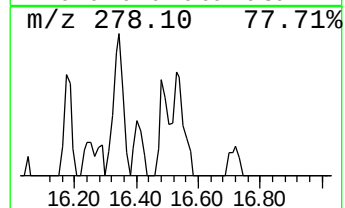
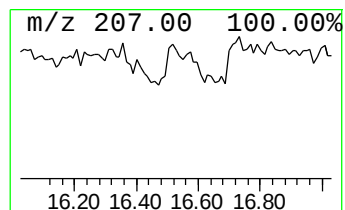
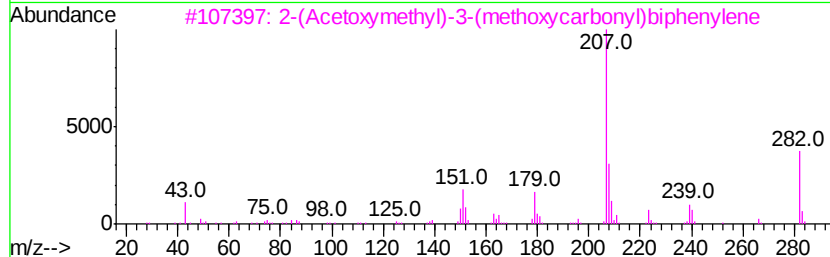
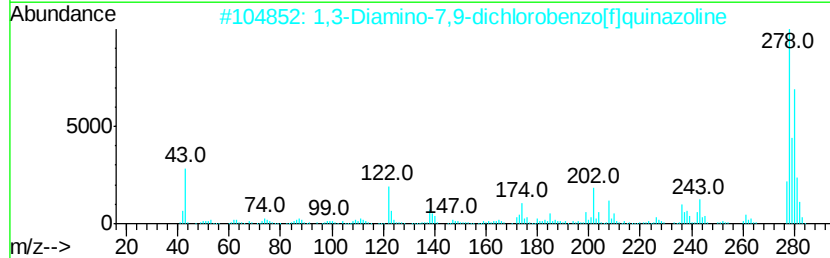
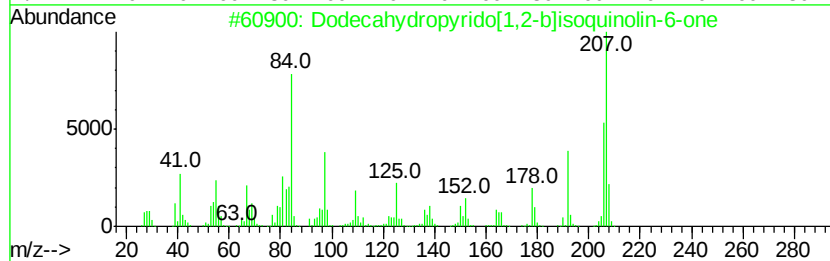
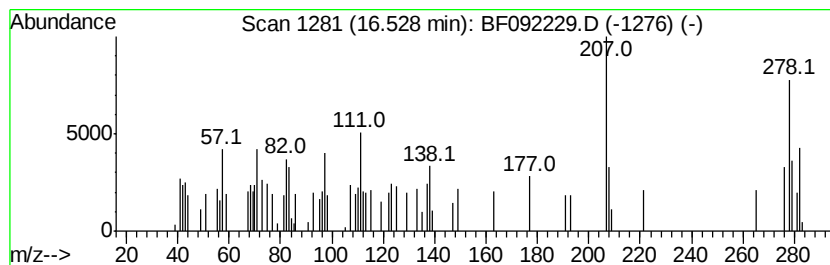
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.53 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.45 ng	132552	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecahydropyrido[1,2-b]isoquinoline...	207	C13H21NO	108873-36-5	25
2		1,3-Diamino-7,9-dichlorobenzo[f]...	278	C12H8Cl2N4	037521-58-7	22
3		2-(Acetoxymethyl)-3-(methoxycarbonyl)...	282	C17H14O4	093103-70-9	22
4		11H-Dibenzo[c,f][1,2]diazepine, ...	278	C13H8Cl2N2O	000958-71-4	22
5		Disulfide, bis(2-methoxyphenyl)	278	C14H14O2S2	013920-94-0	18



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 Misc :
 ALS Vial : 24 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...	4.73	54.1	ng	2588770	1	6.60	956979	20.0
unknown6.37	6.37	113.6	ng	5434060	1	6.60	956979	20.0
1-Pentadecene	11.36	2.8	ng	195380	4	11.11	1396620	20.0
n-Hexadecanoic acid	11.66	3.6	ng	251769	4	11.11	1396620	20.0
Trichloroacetic a...	13.60	6.2	ng	370984	5	13.73	1189930	20.0
Eicosane	14.52	2.2	ng	117798	6	15.09	1081160	20.0
unknown14.81	14.81	4.0	ng	214239	6	15.09	1081160	20.0
9-Tricosene, (Z)-	15.57	2.1	ng	114508	6	15.09	1081160	20.0
unknown16.53	16.53	2.5	ng	132552	6	15.09	1081160	20.0