

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053116\
 Data File : BF087608.D
 Acq On : 1 Jun 2016 6:36
 Operator : UM/SJ
 Sample : H3323-06
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04-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-BF052316.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	4.673	268	270	284	rBV	124938	414340	10.67%	1.150%
2	5.347	326	329	364	rBV	1441395	3238154	83.40%	8.985%
3	7.016	472	475	480	rBV	1636114	3037093	78.23%	8.428%
4	7.096	480	482	503	rVB	2081521	3882467	100.00%	10.773%
5	7.439	510	512	523	rVB	653460	920216	23.70%	2.553%
6	7.668	530	532	545	rVB	1468425	2489338	64.12%	6.908%
7	8.365	591	593	613	rBV	1265446	2276929	58.65%	6.318%
8	9.473	688	690	705	rBV	712697	1160356	29.89%	3.220%
9	11.245	842	845	848	rBV	2695955	3332042	85.82%	9.246%
10	11.451	860	863	868	rVB	59361	79681	2.05%	0.221%
11	11.954	905	907	914	rVB	114739	222678	5.74%	0.618%
12	12.297	934	937	941	rBV	785051	1133504	29.20%	3.145%
13	12.354	941	942	948	rVB	42300	70204	1.81%	0.195%
14	12.685	968	971	974	rBV2	22561	45943	1.18%	0.127%
15	13.131	1007	1010	1012	rVB	72739	91723	2.36%	0.255%
16	13.211	1015	1017	1021	rVB2	29925	51191	1.32%	0.142%
17	13.485	1038	1041	1043	rBV	43140	68963	1.78%	0.191%
18	13.588	1048	1050	1060	rBV2	910211	1630202	41.99%	4.524%
19	13.897	1075	1077	1082	rBV	80945	184332	4.75%	0.511%
20	14.365	1117	1118	1127	rVB6	15404	47665	1.23%	0.132%
21	14.628	1137	1141	1143	rBV	59495	77000	1.98%	0.214%
22	14.708	1146	1148	1150	rVV	541830	892524	22.99%	2.477%
23	14.743	1150	1151	1157	rVB	285095	429502	11.06%	1.192%
24	14.857	1158	1161	1165	rVV	60427	124946	3.22%	0.347%
25	15.314	1198	1201	1203	rVB	31882	50728	1.31%	0.141%
26	15.520	1216	1219	1221	rBV	48626	76674	1.97%	0.213%
27	15.565	1221	1223	1228	rVV	53802	95814	2.47%	0.266%
28	15.657	1228	1231	1233	rBV2	74118	151244	3.90%	0.420%
29	15.703	1233	1235	1238	rVB2	40123	78940	2.03%	0.219%
30	15.908	1251	1253	1255	rBV	31868	43636	1.12%	0.121%
31	15.965	1255	1258	1260	rVV	33157	57535	1.48%	0.160%
32	16.320	1286	1289	1291	rBV2	52491	87740	2.26%	0.243%
33	16.468	1300	1302	1305	rVB3	31413	49180	1.27%	0.136%
34	16.514	1305	1306	1312	rBV	460306	793582	20.44%	2.202%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.731	1323	1325	1328	rBV2	23088	51331	1.32%	0.142%
36	16.823	1330	1333	1337	rVV	565637	795375	20.49%	2.207%
37	16.903	1337	1340	1342	rVB2	93938	121183	3.12%	0.336%
38	16.948	1342	1344	1345	rBV2	25476	47776	1.23%	0.133%
39	17.063	1351	1354	1356	rBV	1638826	2373371	61.13%	6.586%
40	17.268	1367	1372	1373	rBV4	44905	114332	2.94%	0.317%
41	17.303	1373	1375	1379	rVB	60699	84224	2.17%	0.234%
42	17.394	1380	1383	1385	rBV	44184	70580	1.82%	0.196%
43	17.440	1385	1387	1389	rBV	109281	150400	3.87%	0.417%
44	17.554	1395	1397	1399	rBV	34384	41701	1.07%	0.116%
45	17.600	1399	1401	1403	rBV	48494	56546	1.46%	0.157%
46	17.714	1409	1411	1414	rBV	89018	131406	3.38%	0.365%
47	17.829	1419	1421	1424	rVV3	69763	119835	3.09%	0.333%
48	17.886	1424	1426	1428	rVB	45866	56541	1.46%	0.157%
49	18.126	1445	1447	1449	rBV2	47505	78931	2.03%	0.219%
50	18.309	1461	1463	1468	rVB3	57593	112765	2.90%	0.313%
51	18.411	1470	1472	1475	rBV2	653783	1218271	31.38%	3.381%
52	18.457	1475	1476	1483	rVV2	272595	507738	13.08%	1.409%
53	18.560	1483	1485	1488	rVB	64320	90048	2.32%	0.250%
54	19.429	1559	1561	1567	rBV2	305223	521588	13.43%	1.447%
55	19.703	1584	1585	1588	rBV	239666	404490	10.42%	1.122%
56	19.817	1593	1595	1600	rVB2	104832	197353	5.08%	0.548%
57	20.000	1609	1611	1614	rBV	156476	195043	5.02%	0.541%
58	20.069	1614	1617	1619	rVB	157140	262624	6.76%	0.729%
59	20.103	1619	1620	1623	rBV	385467	568180	14.63%	1.577%
60	20.926	1690	1692	1695	rVB2	98310	133469	3.44%	0.370%
61	21.749	1762	1764	1769	rVB	70276	146452	3.77%	0.406%

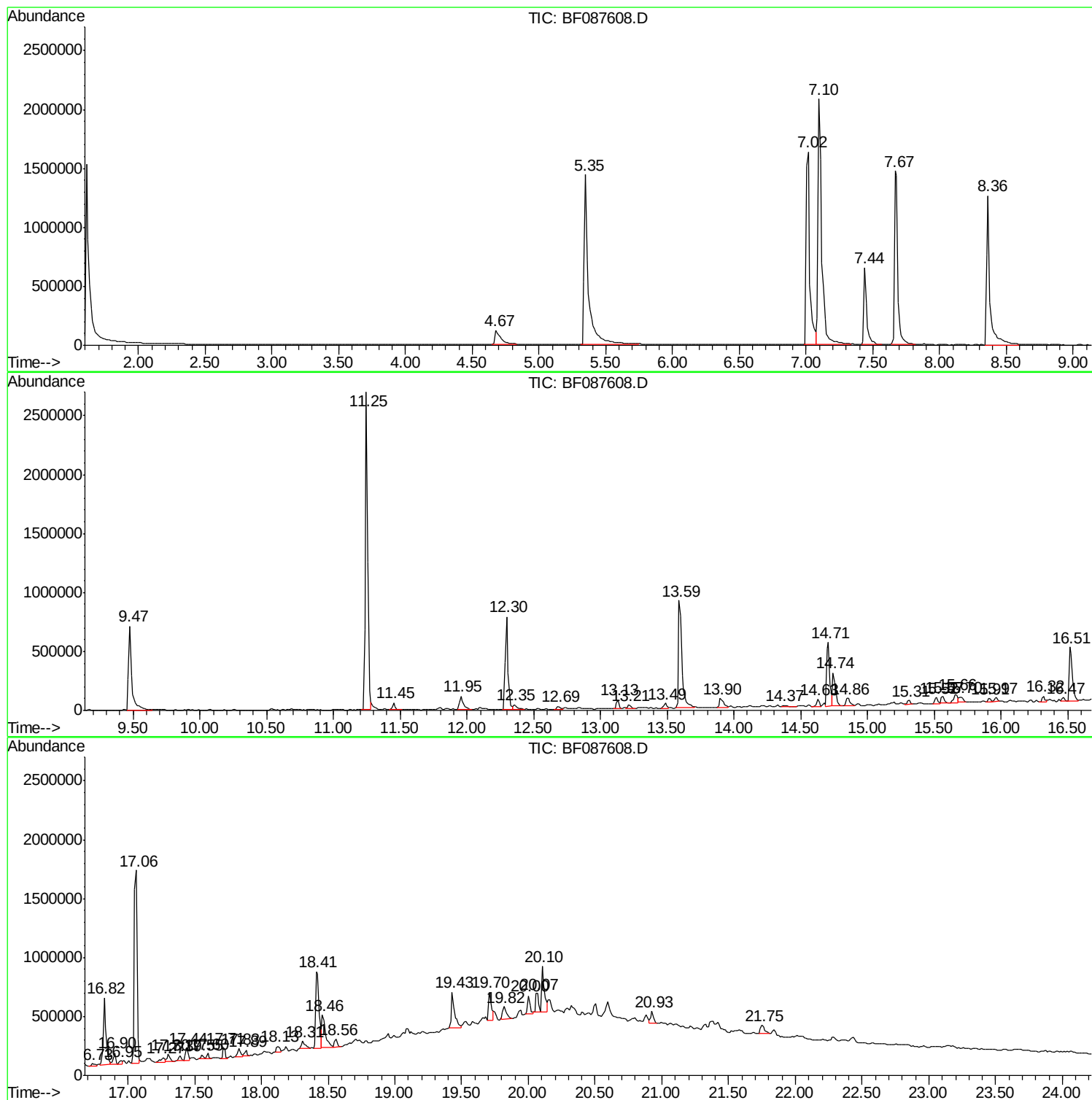
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ClientSampled :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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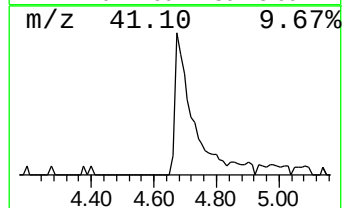
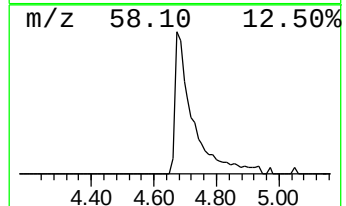
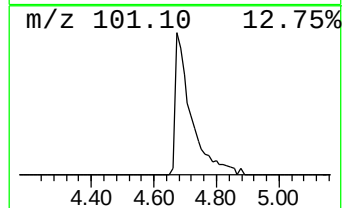
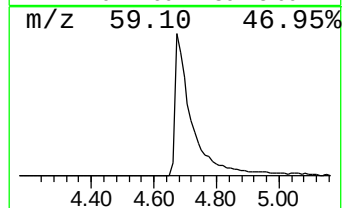
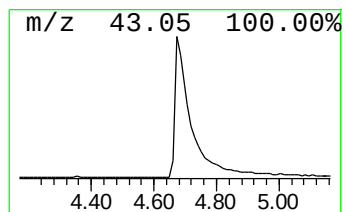
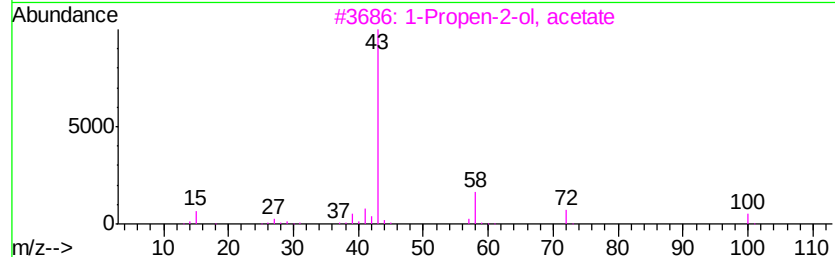
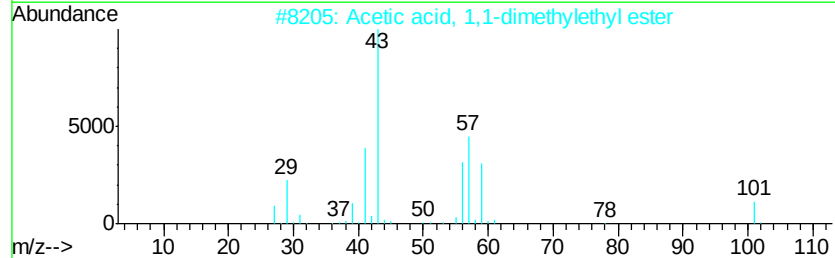
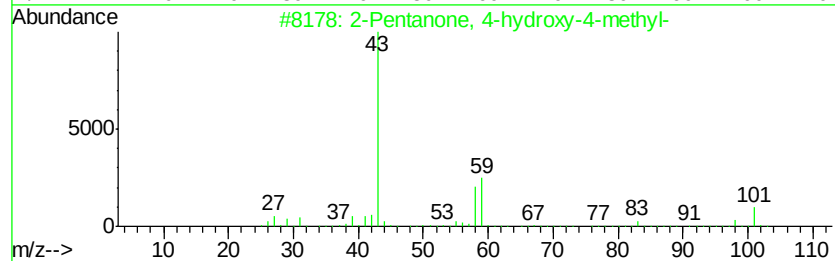
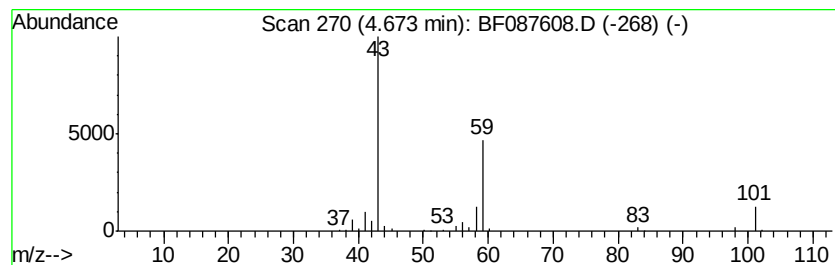
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	9.01 ng	414340	1,4-Dichlorobenzene-d4	7.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane	58	C4H10	000106-97-8	9



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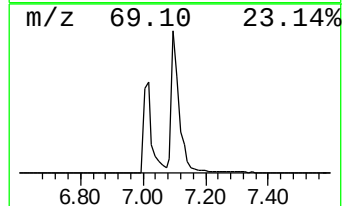
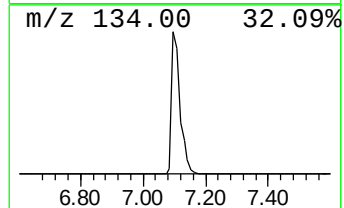
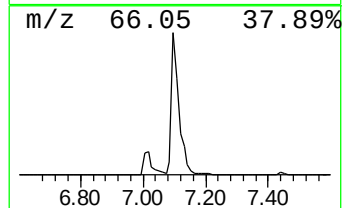
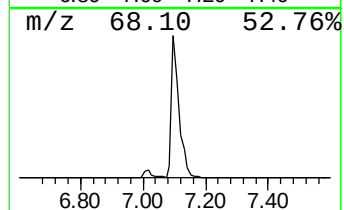
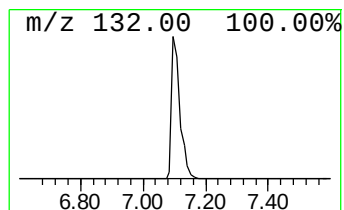
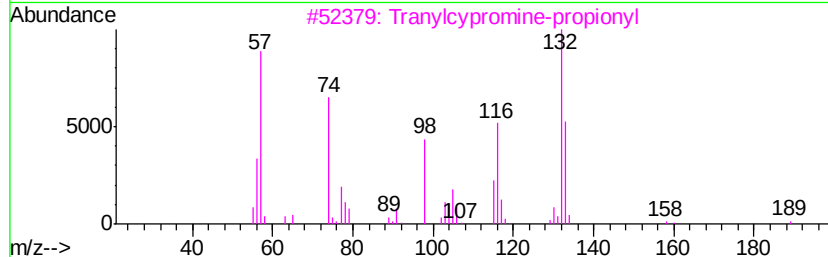
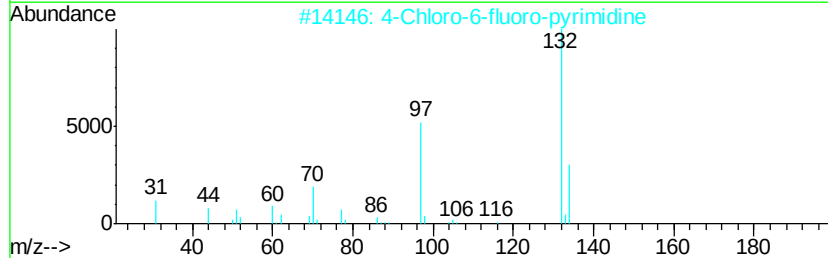
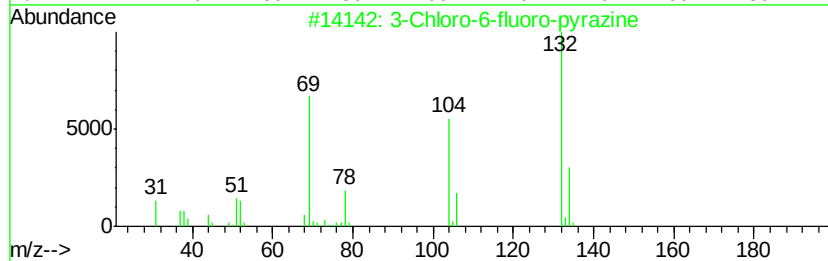
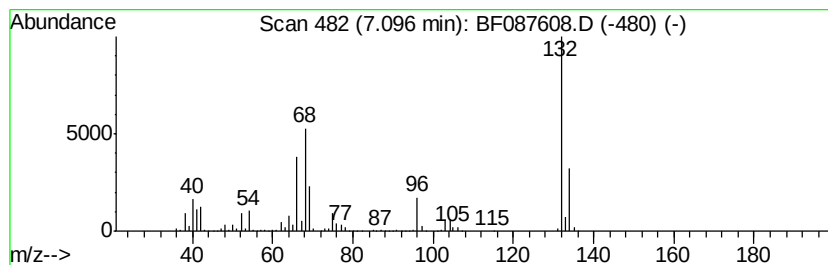
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	84.38 ng	3882470	1,4-Dichlorobenzene-d4	7.44

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		Tranvlcypropine-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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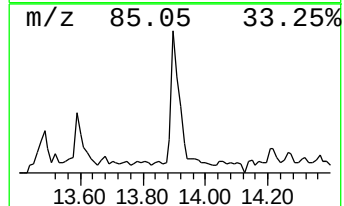
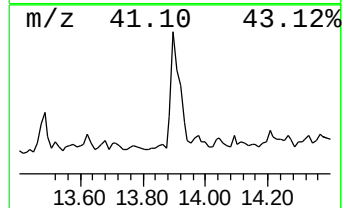
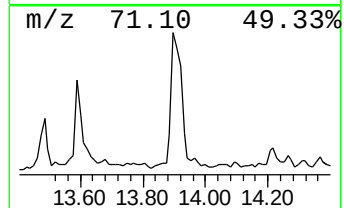
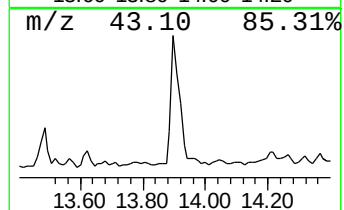
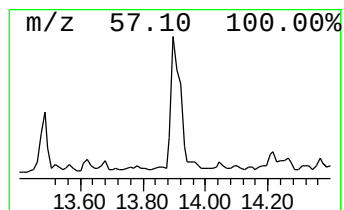
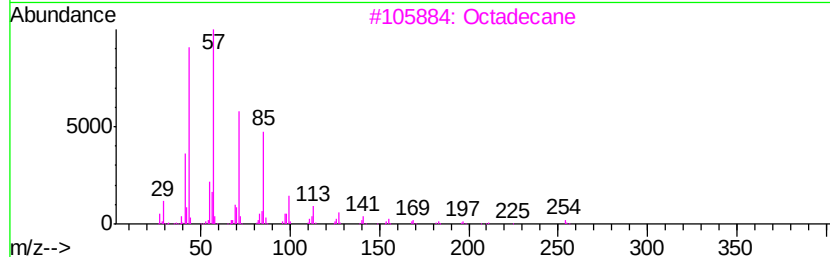
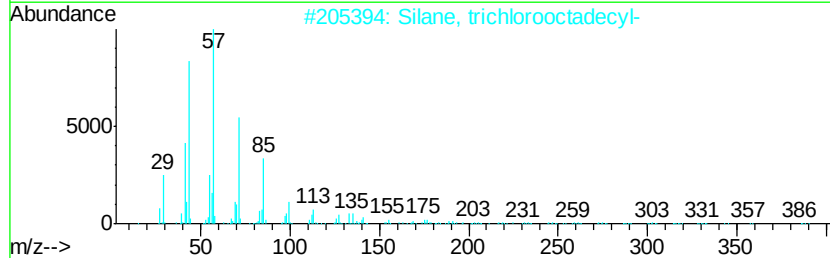
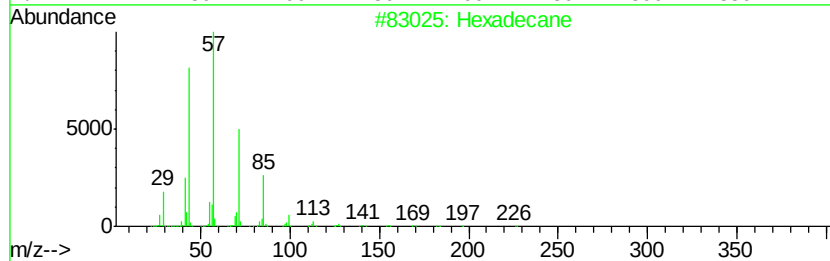
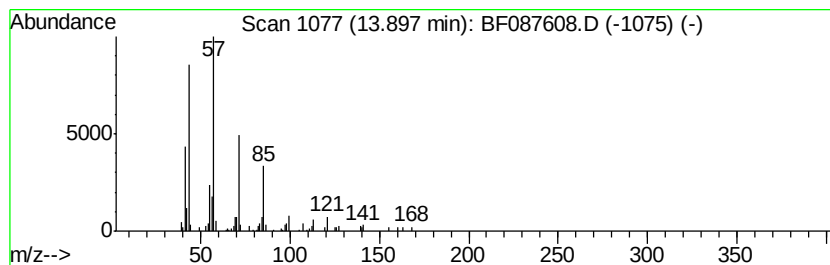
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.13 ng	184332	Phenanthrene-d10	14.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	86
2	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	80
3	Octadecane		254	C18H38	000593-45-3	80
4	Pentadecane		212	C15H32	000629-62-9	80
5	Tridecane		184	C13H28	000629-50-5	72



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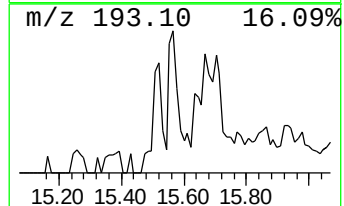
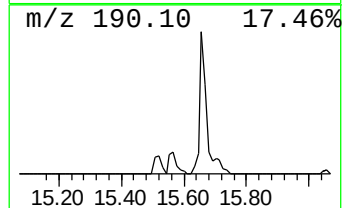
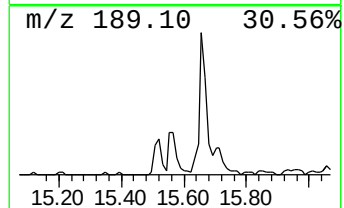
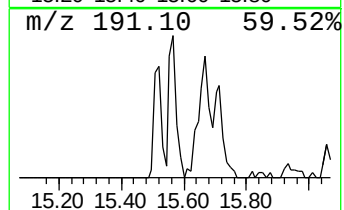
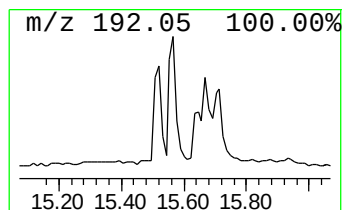
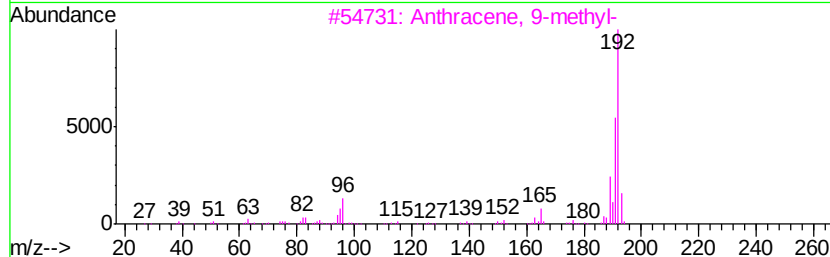
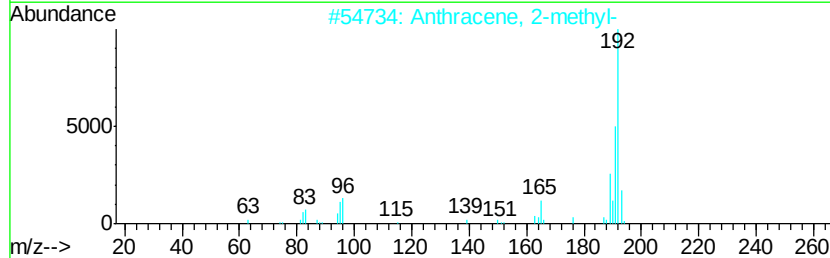
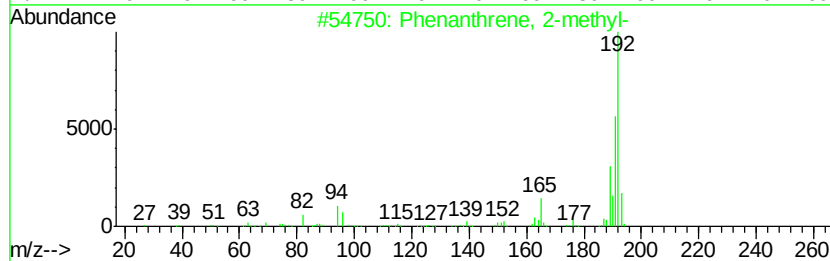
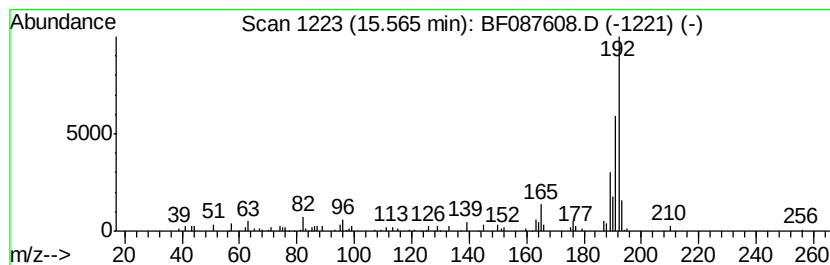
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.15 ng	95814	Phenanthrene-d10	14.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
2		Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3		Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
4		Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	91
5		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91



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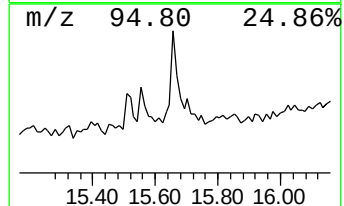
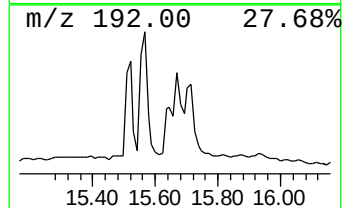
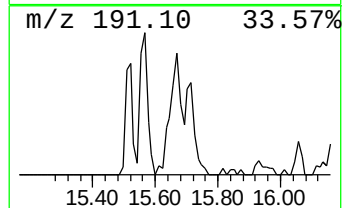
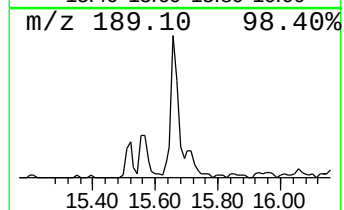
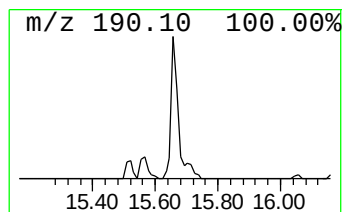
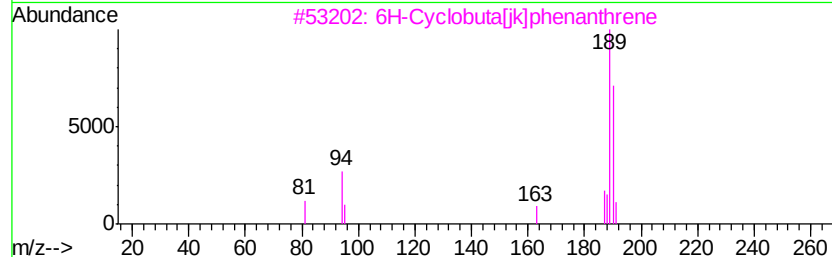
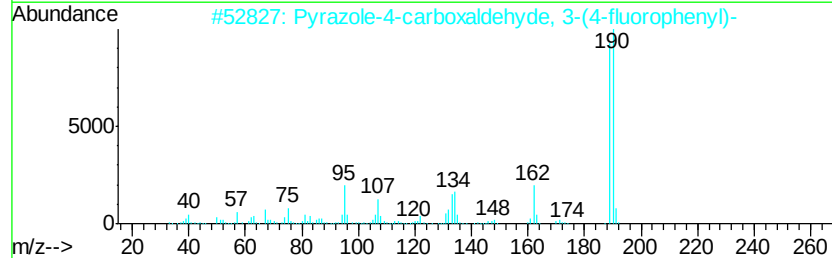
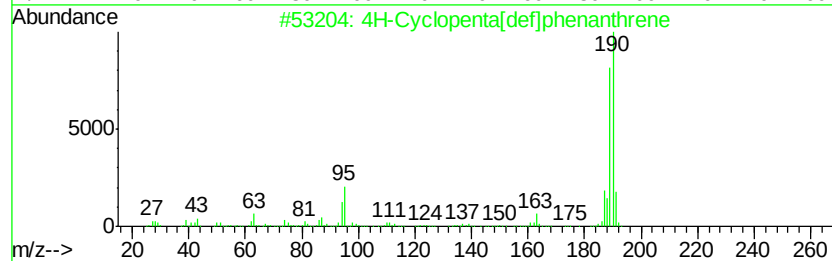
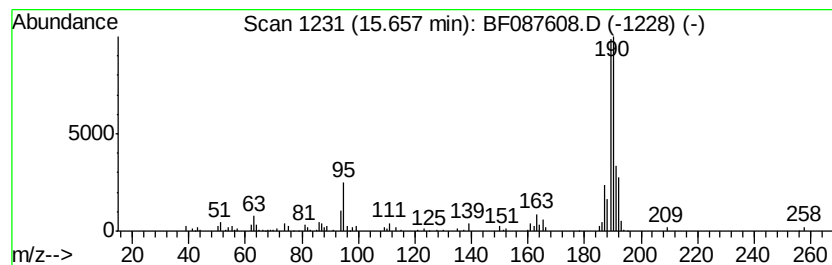
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ClientSampleId :
SB-04-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.66	3.39 ng	151244	Phenanthrene-d10	14.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	58
3	6H-Cyclobuta[flk]phenanthrene	190	C15H10	083469-43-6	45
4	1-Aminocyclopentanecarboxylic ac...	297	C11H17Cl2N04	1000329-17-6	27
5	4-Oxo-2-(4-fluorophenyl)-3,4-dih...	190	C10H7FN2O	076128-79-5	17



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053116\
Data File : BF087608.D
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Operator : UM/SJ
Sample : H3323-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-COMP

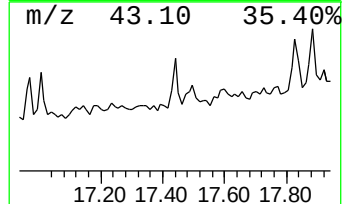
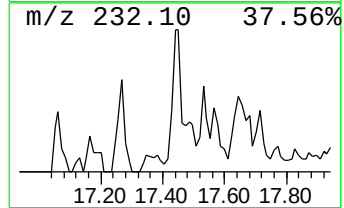
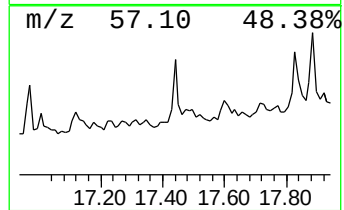
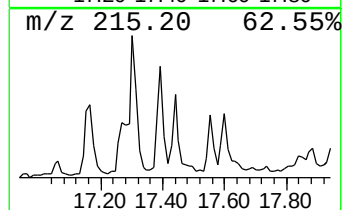
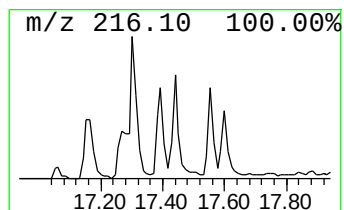
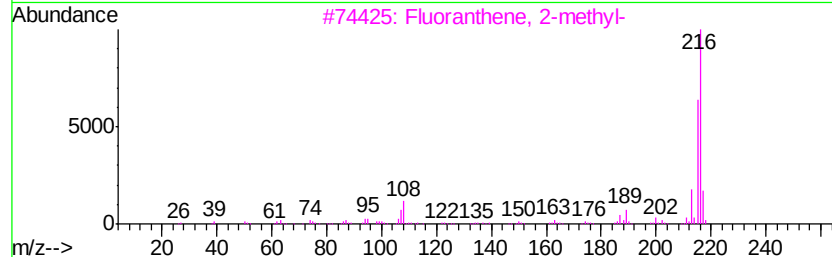
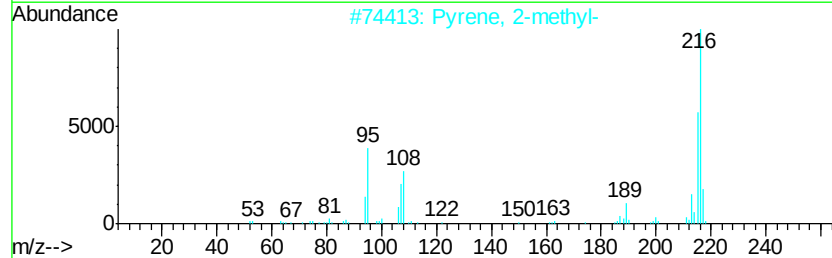
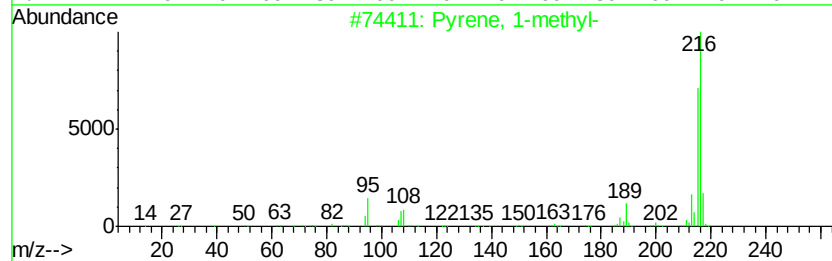
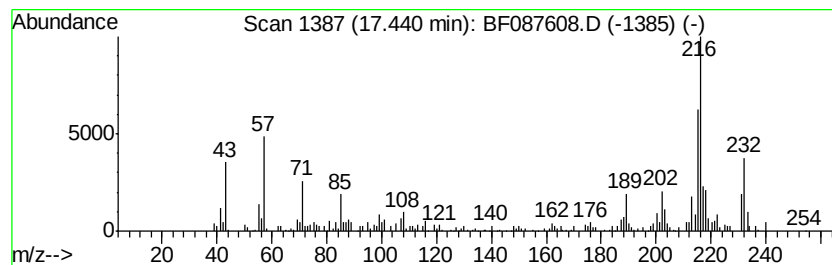
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	2.47 ng	150400	Chrysene-d12	18.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	92
2		Pyrene, 2-methyl-	216	C17H12	003442-78-2	78
3		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	60
4		11H-Benzo[<i>a</i>]fluorene	216	C17H12	000238-84-6	49
5		Pyrene, 4-methyl-	216	C17H12	003353-12-6	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF053116\
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Acq On : 1 Jun 2016 6:36
Operator : UM/SJ
Sample : H3323-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-COMP

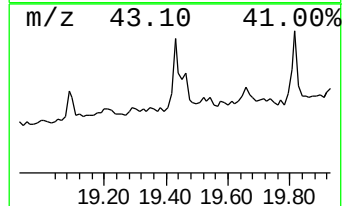
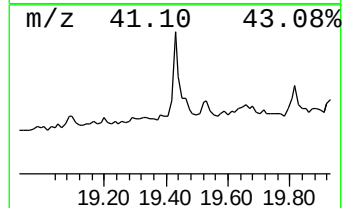
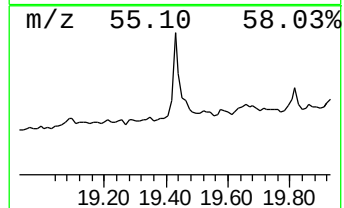
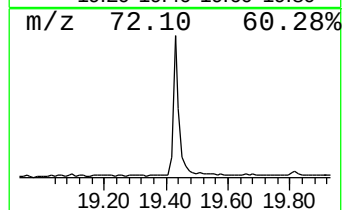
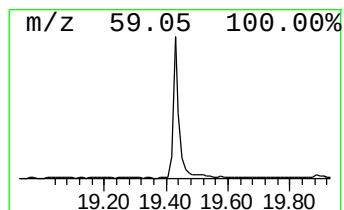
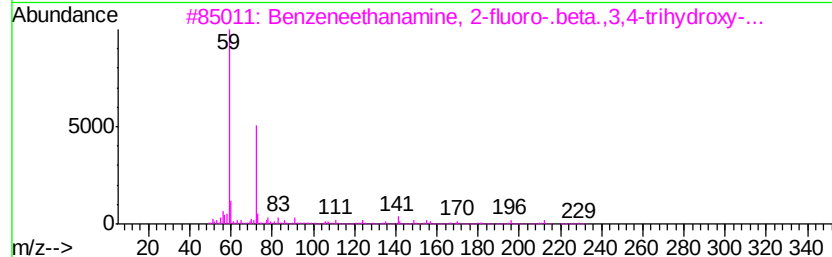
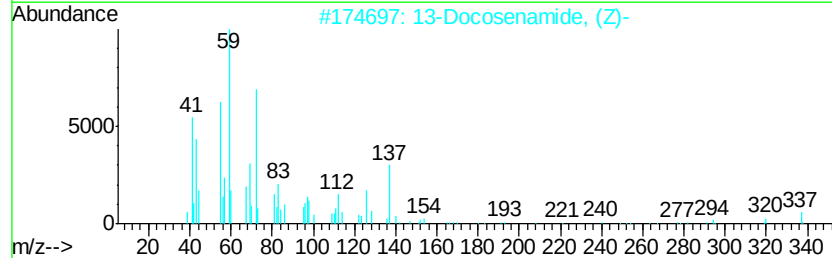
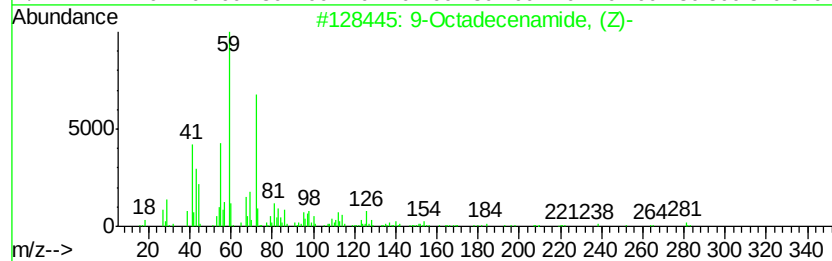
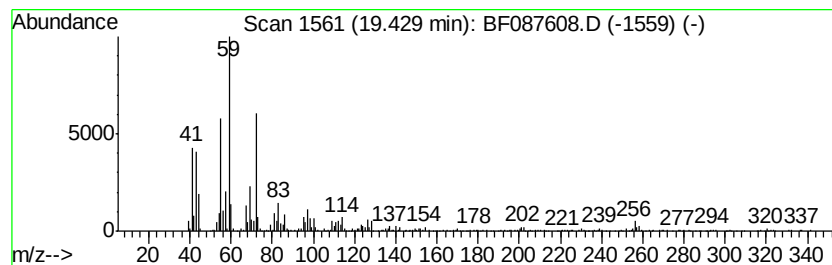
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	18.36 ng	521588	Perylene-d12	20.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	72
4		Dodecanamide	199	C12H25NO	001120-16-7	62
5		Hexanamide	115	C6H13NO	000628-02-4	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053116\
Data File : BF087608.D
Acq On : 1 Jun 2016 6:36
Operator : UM/SJ
Sample : H3323-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

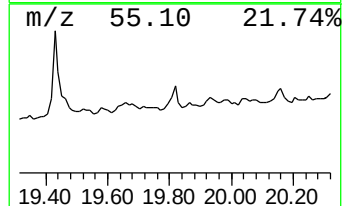
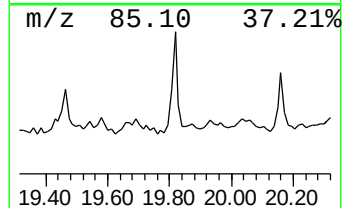
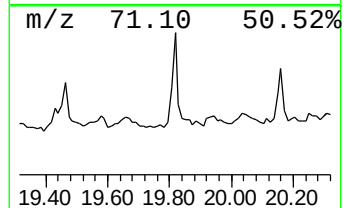
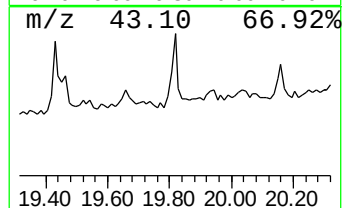
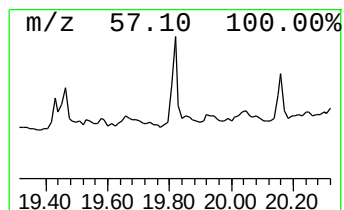
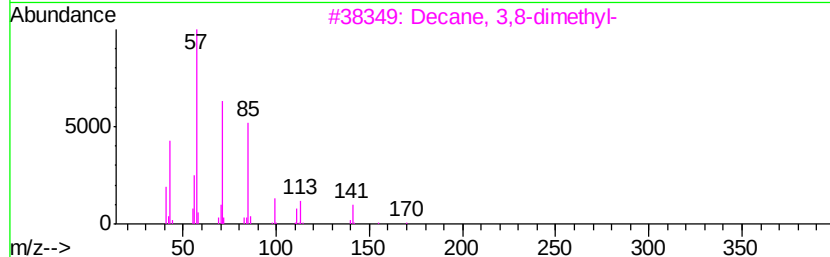
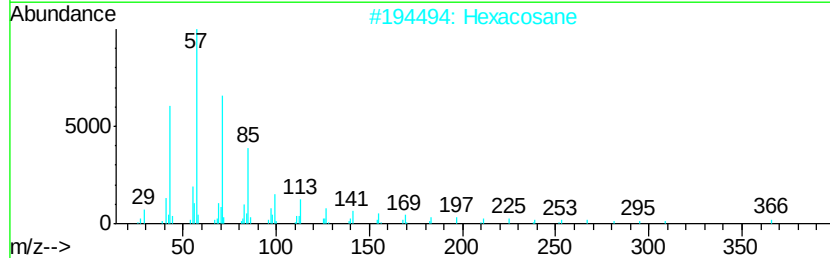
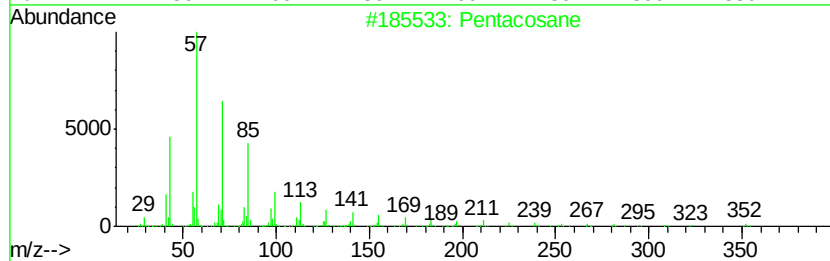
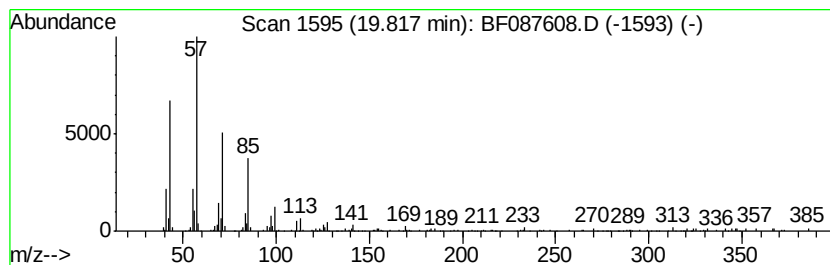
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.82	6.95 ng	197353	Perylene-d12	20.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	95
2	Hexacosane	366	C26H54	000630-01-3	91
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
4	Nonadecane, 1-bromo-	346	C19H39Br	004434-66-6	87
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	83



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Sample : H3323-06
Misc :
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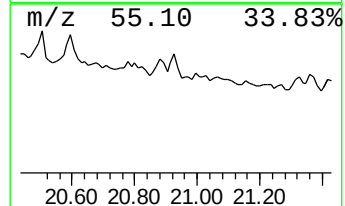
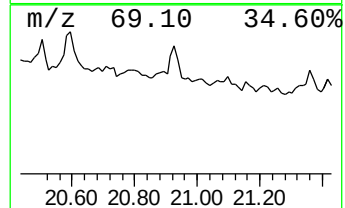
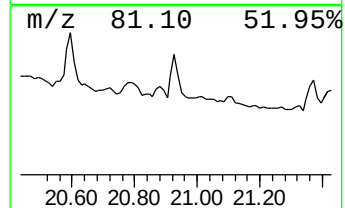
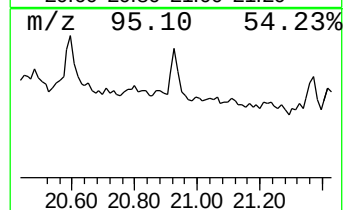
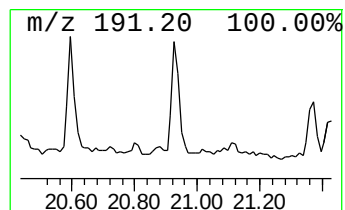
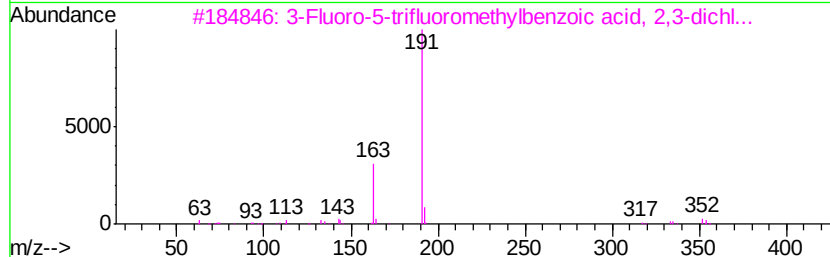
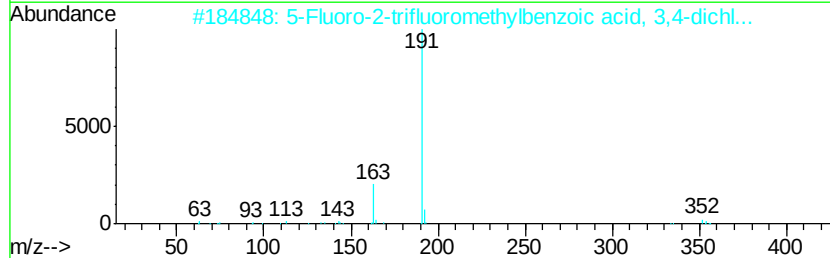
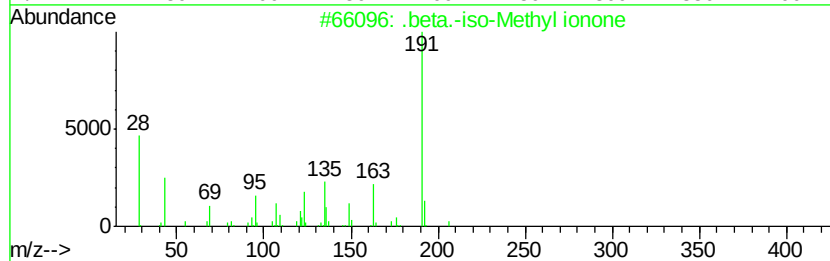
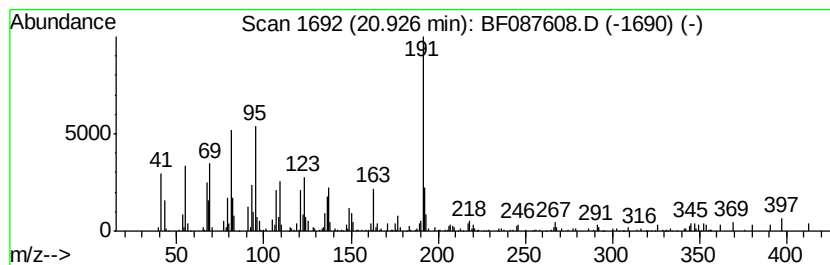
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.93	4.70 ng	133469	Perylene-d12	20.10		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	62
2		5-Fluoro-2-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-63-5	30
3		3-Fluoro-5-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-34-4	30
4		3-Fluoro-4-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-94-6	30
5		2-Fluoro-6-trifluoromethylbenzoi...	290	C14H14F4O2	1000357-69-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053116\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.67	9.0 ng		414340	1	7.44	920216	20.0
unknown7.10	7.10	84.4 ng		3882470	1	7.44	920216	20.0
Hexadecane	13.90	4.1 ng		184332	4	14.71	892524	20.0
Phenanthrene, 2-m...	15.57	2.1 ng		95814	4	14.71	892524	20.0
4H-Cyclopenta[def...	15.66	3.4 ng		151244	4	14.71	892524	20.0
Pyrene, 1-methyl-	17.44	2.5 ng		150400	5	18.42	1218270	20.0
9-Octadecenamide, ...	19.43	18.4 ng		521588	6	20.10	568180	20.0
Pentacosane	19.82	7.0 ng		197353	6	20.10	568180	20.0
.beta.-iso-Methyl...	20.93	4.7 ng		133469	6	20.10	568180	20.0