

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
 Data File : BF101273.D
 Acq On : 9 Dec 2017 9:45
 Operator : SJ/JU
 Sample : I6744-02
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PROS-3-E(4-5)

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-BF113017.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	5.051	501	504	518	rBB	38961	50686	5.14%	0.569%
2	5.451	568	572	580	rBV	975458	897353	91.00%	10.074%
3	6.469	741	745	756	rBV2	966434	986123	100.00%	11.070%
4	6.598	763	767	771	rBV	1015798	956198	96.97%	10.734%
5	6.828	803	806	810	rBV	323649	254000	25.76%	2.851%
6	6.986	829	833	836	rBV	855319	748928	75.95%	8.408%
7	7.392	898	902	905	rBV	567992	492440	49.94%	5.528%
8	8.110	1020	1024	1037	rVB	385202	306880	31.12%	3.445%
9	9.186	1203	1207	1210	rBV	1237770	965737	97.93%	10.842%
10	9.257	1216	1219	1222	rBV	16566	12808	1.30%	0.144%
11	9.580	1268	1274	1280	rBV	83559	77788	7.89%	0.873%
12	9.786	1305	1309	1312	rVB	35531	26001	2.64%	0.292%
13	9.869	1319	1323	1326	rBV	350246	291200	29.53%	3.269%
14	10.286	1392	1394	1397	rVB	35664	25418	2.58%	0.285%
15	10.504	1427	1431	1434	rBV4	9157	12926	1.31%	0.145%
16	10.663	1454	1458	1461	rBV	493701	448738	45.51%	5.038%
17	10.763	1472	1475	1479	rBV	25029	29891	3.03%	0.336%
18	11.210	1548	1551	1553	rBV	14860	12859	1.30%	0.144%
19	11.357	1573	1576	1579	rBV	322945	277100	28.10%	3.111%
20	11.380	1579	1580	1585	rVV	71493	46832	4.75%	0.526%
21	11.433	1586	1589	1594	rVB	15969	16884	1.71%	0.190%
22	11.633	1620	1623	1628	rVB3	14669	16483	1.67%	0.185%
23	11.874	1659	1664	1665	rBV2	14042	22816	2.31%	0.256%
24	11.974	1677	1681	1683	rBV3	17820	21722	2.20%	0.244%
25	12.110	1699	1704	1707	rBV7	6133	12443	1.26%	0.140%
26	12.192	1714	1718	1721	rBV6	12353	14055	1.43%	0.158%
27	12.574	1780	1783	1786	rBV	138352	115574	11.72%	1.297%
28	12.716	1804	1807	1811	rBV4	8621	15783	1.60%	0.177%
29	12.751	1811	1813	1817	rVV3	19002	17848	1.81%	0.200%
30	12.804	1817	1822	1829	rVV	138162	144745	14.68%	1.625%
31	12.945	1838	1846	1849	rBV	943555	784652	79.57%	8.809%
32	13.139	1872	1879	1881	rBV3	18745	32290	3.27%	0.362%
33	13.239	1893	1896	1899	rBV2	13621	14596	1.48%	0.164%
34	13.827	1994	1996	2000	rVB3	44112	43360	4.40%	0.487%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101273.D
Acq On : 9 Dec 2017 9:45
Operator : SJ/JU
Sample : I6744-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-3-E(4-5)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.968	2017	2020	2023	rBV	186756	157492	15.97%	1.768%
36	14.010	2023	2027	2029	rVV2	281312	300314	30.45%	3.371%
37	14.033	2029	2031	2036	rVB	61845	55579	5.64%	0.624%
38	15.421	2264	2267	2271	rVB	32967	39379	3.99%	0.442%
39	15.480	2274	2277	2282	rVB	132214	161825	16.41%	1.817%

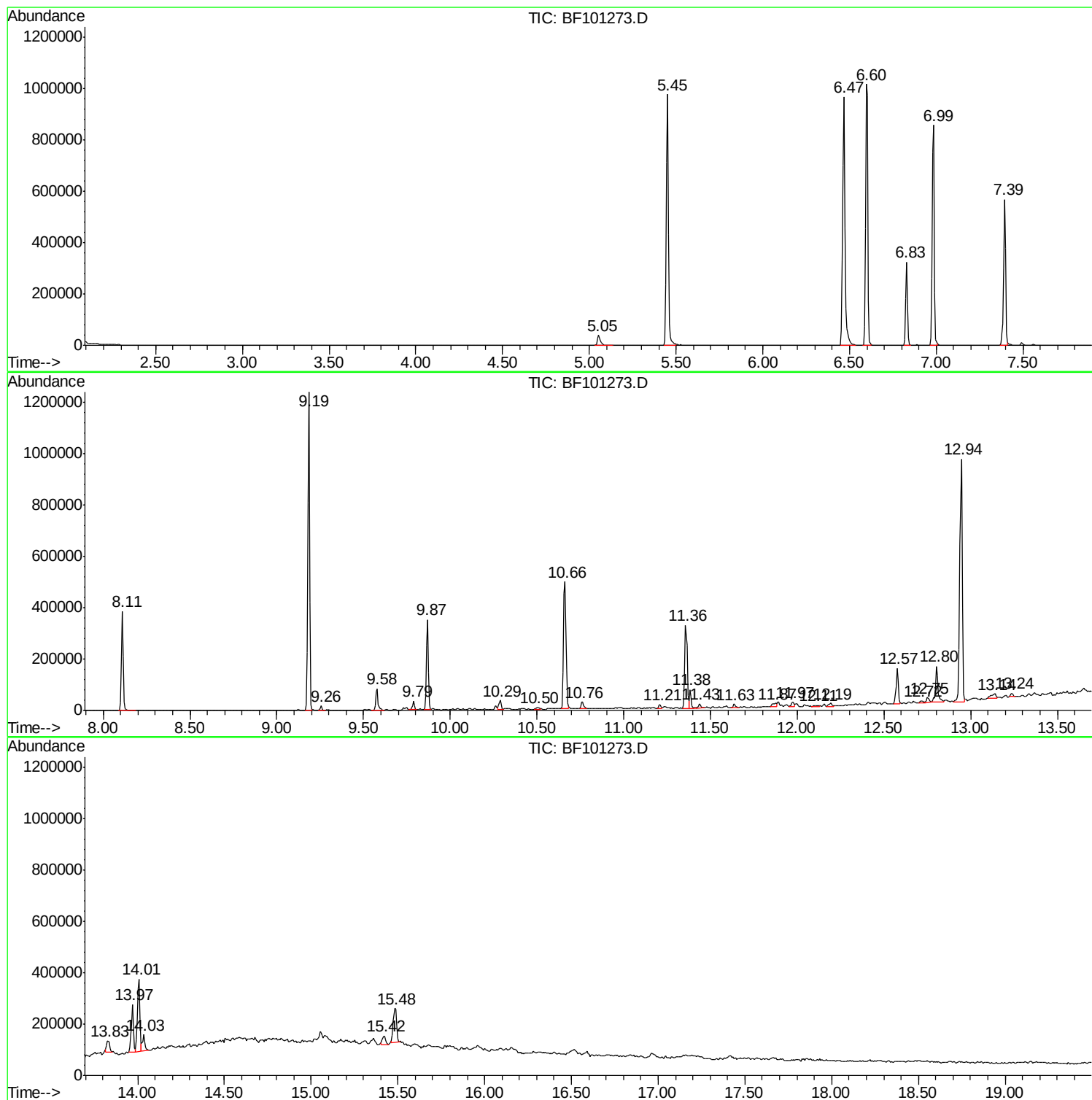
Sum of corrected areas: 8907746

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101273.D
Acq On : 9 Dec 2017 9:45
Operator : SJ/JU
Sample : I6744-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PROS-3-E(4-5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101273.D
Acq On : 9 Dec 2017 9:45
Operator : SJ/JU
Sample : I6744-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-3-E(4-5)

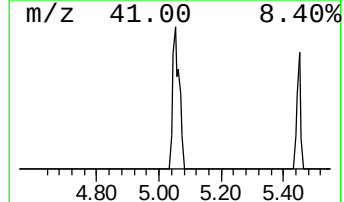
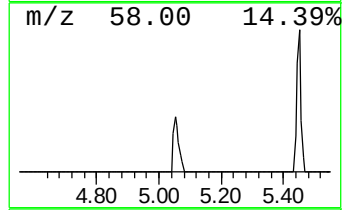
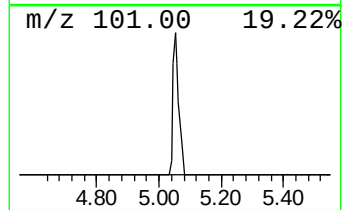
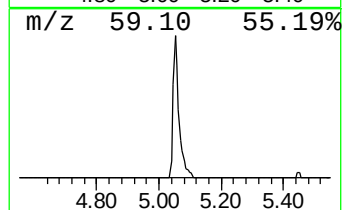
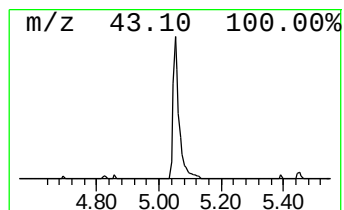
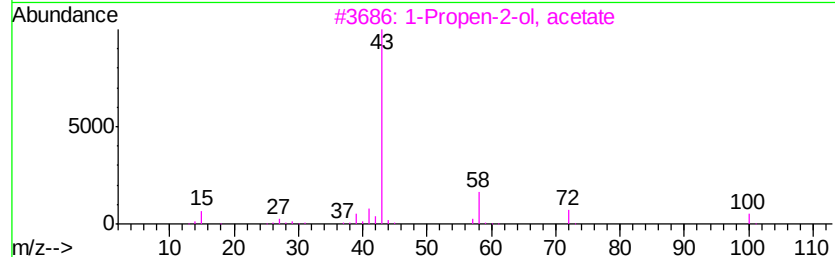
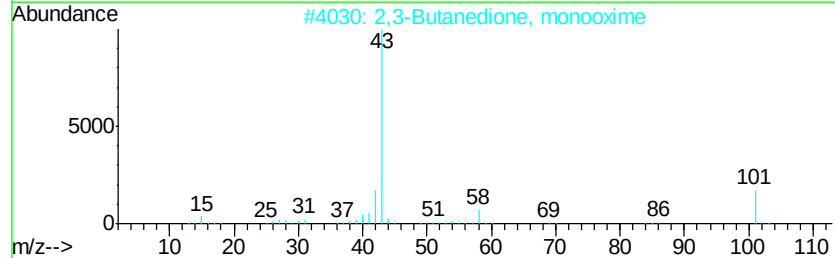
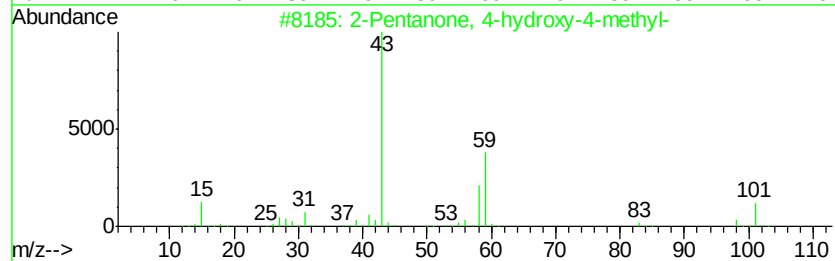
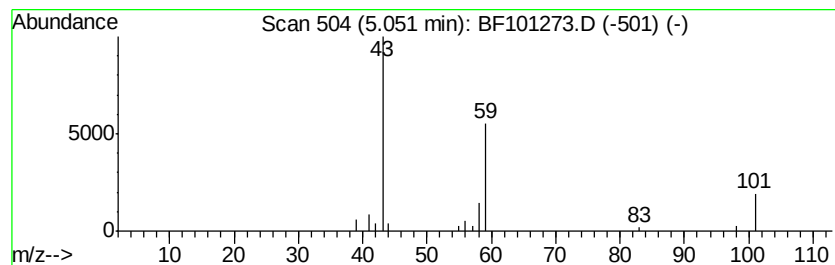
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	3.99 ng	50686	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			3-Hexanol	102	C6H14O	000623-37-0	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120817\
Data File : BF101273.D
Acq On : 9 Dec 2017 9:45
Operator : SJ/JU
Sample : I6744-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-3-E(4-5)

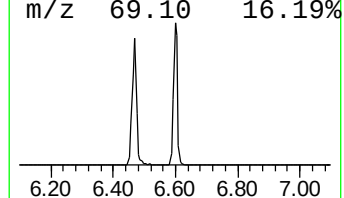
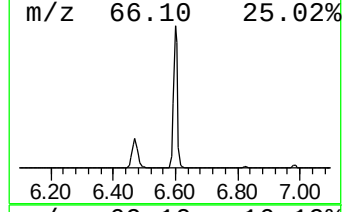
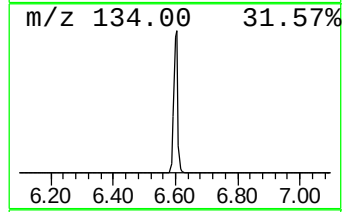
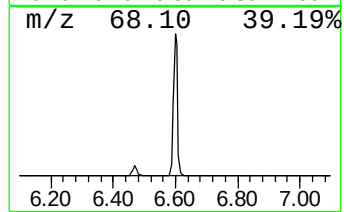
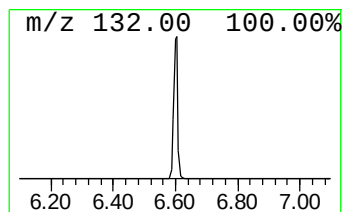
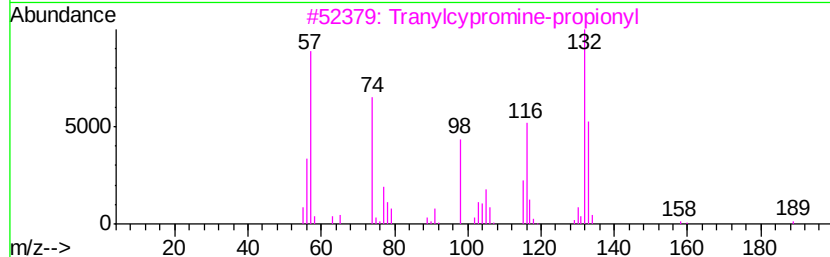
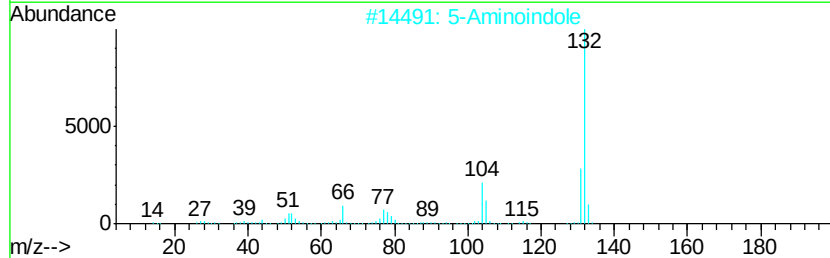
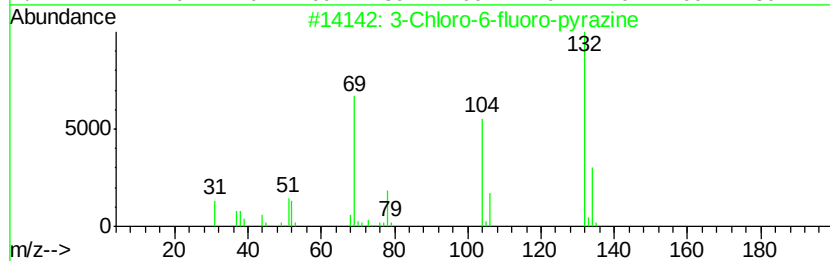
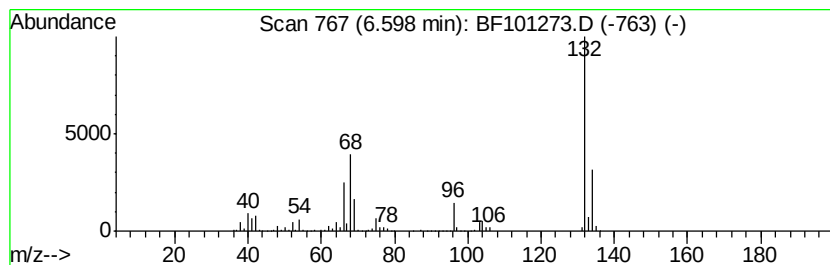
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	75.29 ng	956198	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101273.D
Acq On : 9 Dec 2017 9:45
Operator : SJ/JU
Sample : I6744-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-3-E(4-5)

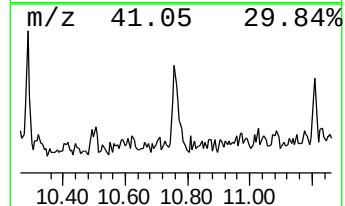
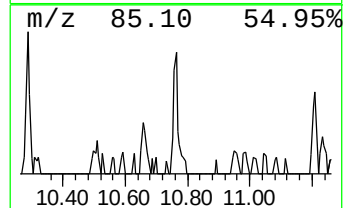
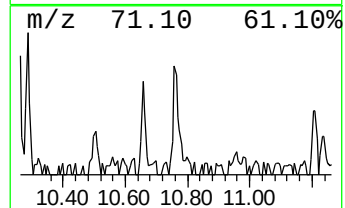
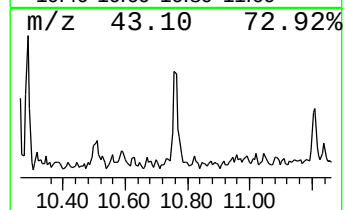
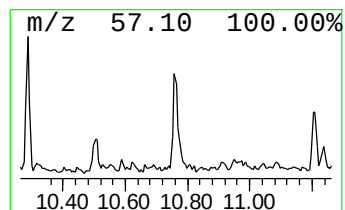
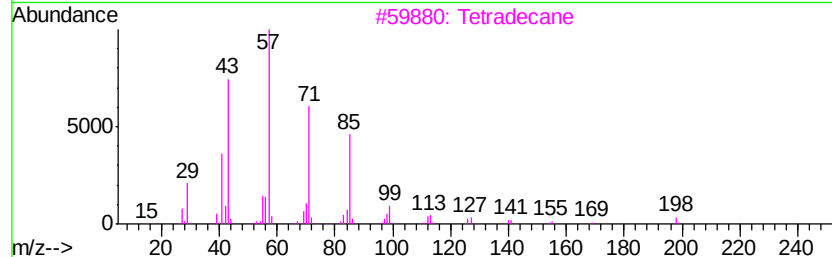
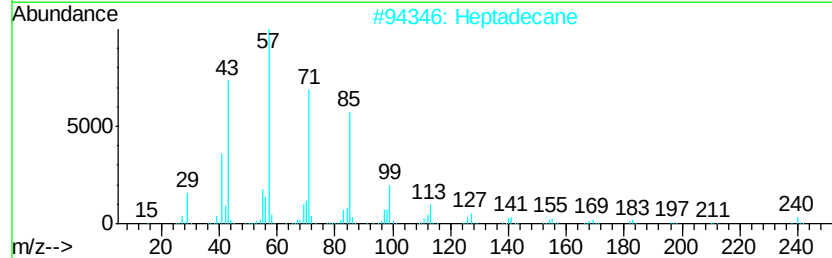
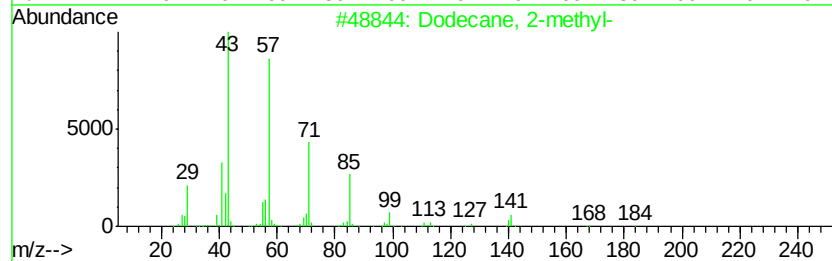
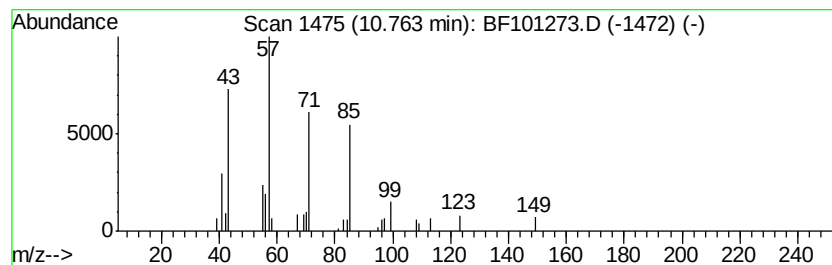
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dodecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.16 ng	29891	Phenanthrene-d10	11.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72
2		Heptadecane	240	C17H36	000629-78-7	64
3		Tetradecane	198	C14H30	000629-59-4	64
4		Pentadecane	212	C15H32	000629-62-9	64
5		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101273.D
Acq On : 9 Dec 2017 9:45
Operator : SJ/JU
Sample : I6744-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-3-E(4-5)

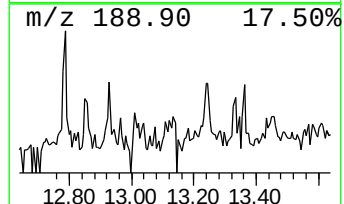
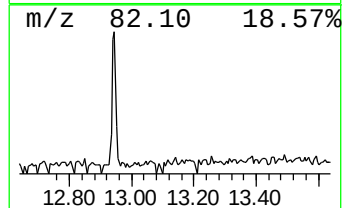
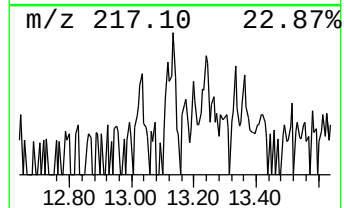
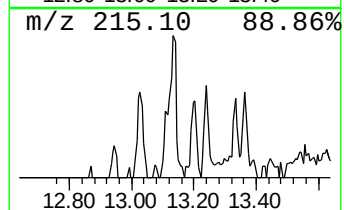
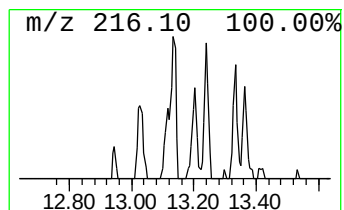
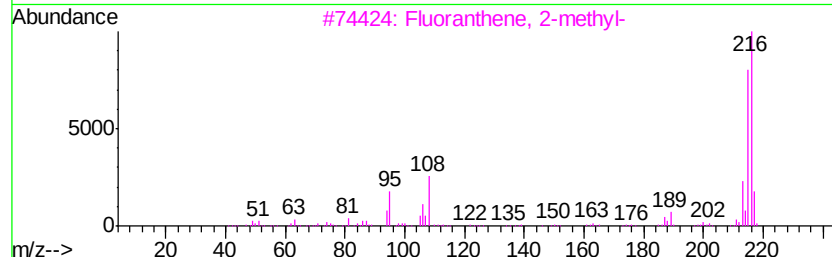
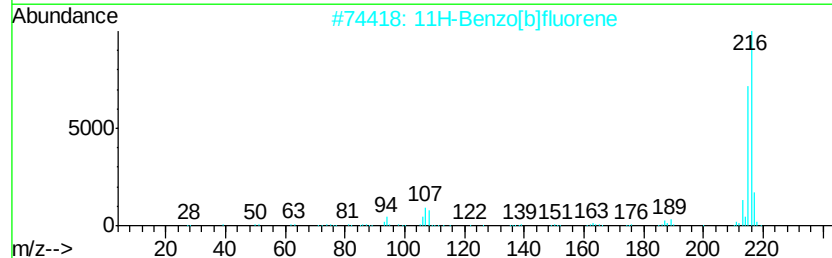
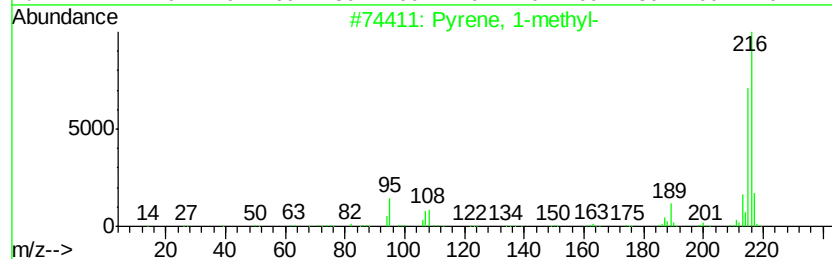
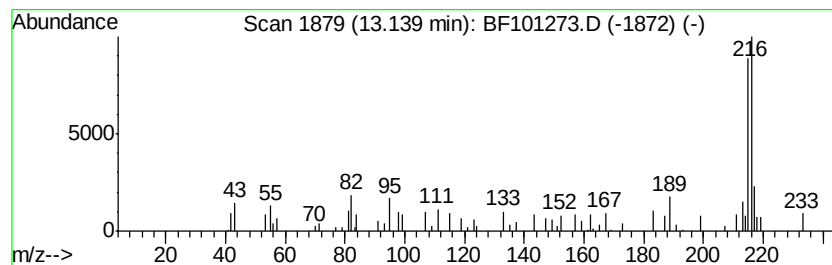
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	2.15 ng	32290	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrene, 1-methyl-	216	C17H12	002381-21-7	74
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	74
3		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	68
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101273.D
Acq On : 9 Dec 2017 9:45
Operator : SJ/JU
Sample : I6744-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-3-E(4-5)

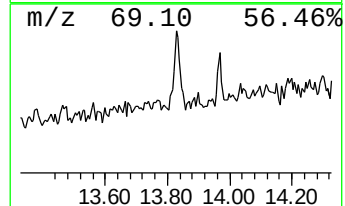
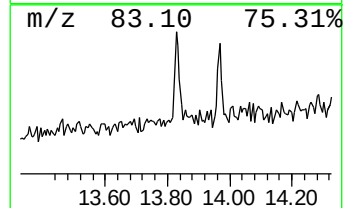
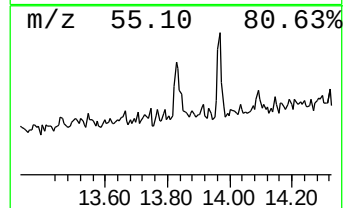
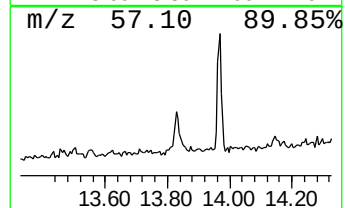
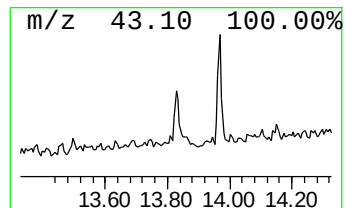
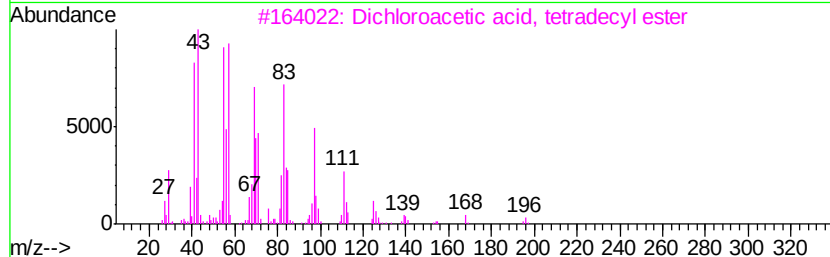
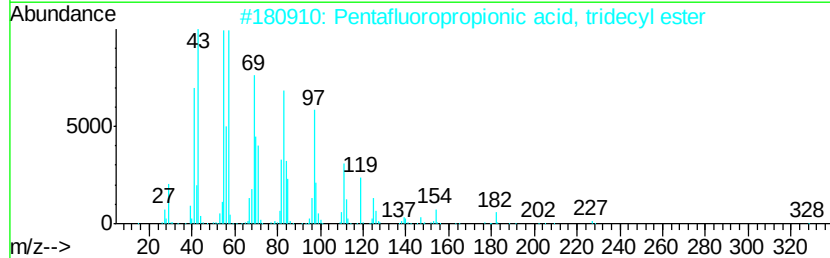
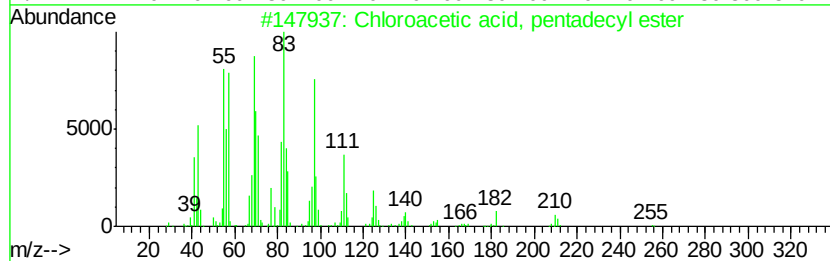
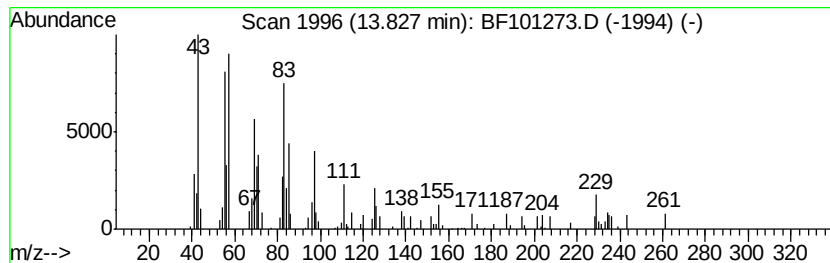
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Chloroacetic acid, pentadec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.89 ng	43360	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	62
2		Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	53
3		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	49
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	49
5		1-Docosene	308	C22H44	001599-67-3	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120817\
Data File : BF101273.D
Acq On : 9 Dec 2017 9:45
Operator : SJ/JU
Sample : I6744-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PROS-3-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.05	4.0	ng	50686	1	6.83	254000	20.0
unknown6.60	6.60	75.3	ng	956198	1	6.83	254000	20.0
Dodecane, 2-methyl-	10.76	2.2	ng	29891	4	11.36	277100	20.0
Pyrene, 1-methyl-	13.14	2.1	ng	32290	5	14.01	300314	20.0
Chloroacetic acid...	13.83	2.9	ng	43360	5	14.01	300314	20.0