

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
 Data File : BF098920.D
 Acq On : 28 Sep 2017 21:31
 Operator : SJ/JU
 Sample : I5440-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-2

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-BF092317.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	2.234	21	25	35	rVB	121792	172990	4.33%	0.488%
2	5.151	516	521	534	rVB	774035	1092358	27.37%	3.082%
3	5.545	582	588	591	rBV	3433654	3897569	97.66%	10.997%
4	6.545	752	758	761	rBV	3292171	3991082	100.00%	11.261%
5	6.686	777	782	785	rBV	3749082	3973638	99.56%	11.212%
6	6.739	788	791	796	rVB	58208	47796	1.20%	0.135%
7	6.916	817	821	824	rBV	1205111	946118	23.71%	2.669%
8	7.075	843	848	851	rBV	3249439	2972234	74.47%	8.386%
9	7.480	911	917	920	rBV	2480698	2511590	62.93%	7.087%
10	8.198	1034	1039	1042	rBV	1498200	1219674	30.56%	3.441%
11	9.274	1216	1222	1225	rBV	4131346	3791323	94.99%	10.697%
12	9.663	1284	1288	1291	rBV	735556	582701	14.60%	1.644%
13	9.951	1333	1337	1341	rBV	1279730	1161386	29.10%	3.277%
14	10.374	1406	1409	1412	rVB	69824	52038	1.30%	0.147%
15	10.745	1467	1472	1475	rBV	1880494	1850272	46.36%	5.221%
16	10.845	1486	1489	1499	rBV	127820	128262	3.21%	0.362%
17	11.439	1586	1590	1593	rBV	1157485	925689	23.19%	2.612%
18	11.951	1673	1677	1682	rBV2	75876	73911	1.85%	0.209%
19	12.651	1793	1796	1801	rBV	142082	115733	2.90%	0.327%
20	12.880	1832	1835	1838	rVB	194061	158358	3.97%	0.447%
21	13.027	1855	1860	1863	rVB	2388616	2393786	59.98%	6.754%
22	13.904	2006	2009	2017	rVB2	218822	234292	5.87%	0.661%
23	14.080	2034	2039	2042	rBV2	859433	915189	22.93%	2.582%
24	14.104	2042	2043	2048	rVB	127729	84702	2.12%	0.239%
25	14.227	2060	2064	2067	rBV2	43966	47979	1.20%	0.135%
26	14.533	2113	2116	2123	rBV4	54641	74420	1.86%	0.210%
27	15.133	2213	2218	2221	rBV	147858	243833	6.11%	0.688%
28	15.239	2234	2236	2240	rVB	44455	47172	1.18%	0.133%
29	15.439	2267	2270	2277	rVB	93494	119007	2.98%	0.336%
30	15.503	2277	2281	2287	rVB	162055	206620	5.18%	0.583%
31	15.574	2287	2293	2304	rBV	656873	920185	23.06%	2.596%
32	16.027	2366	2370	2374	rBV	43024	57220	1.43%	0.161%
33	16.550	2456	2459	2466	rVB3	38380	58696	1.47%	0.166%
34	17.074	2543	2548	2554	rBV2	64854	124236	3.11%	0.351%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-2

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.168	2559	2564	2572	rVB6	34542	82671	2.07%	0.233%
36	17.533	2621	2626	2636	rVB	52573	109231	2.74%	0.308%
37	17.886	2682	2686	2694	rVB4	23418	57896	1.45%	0.163%

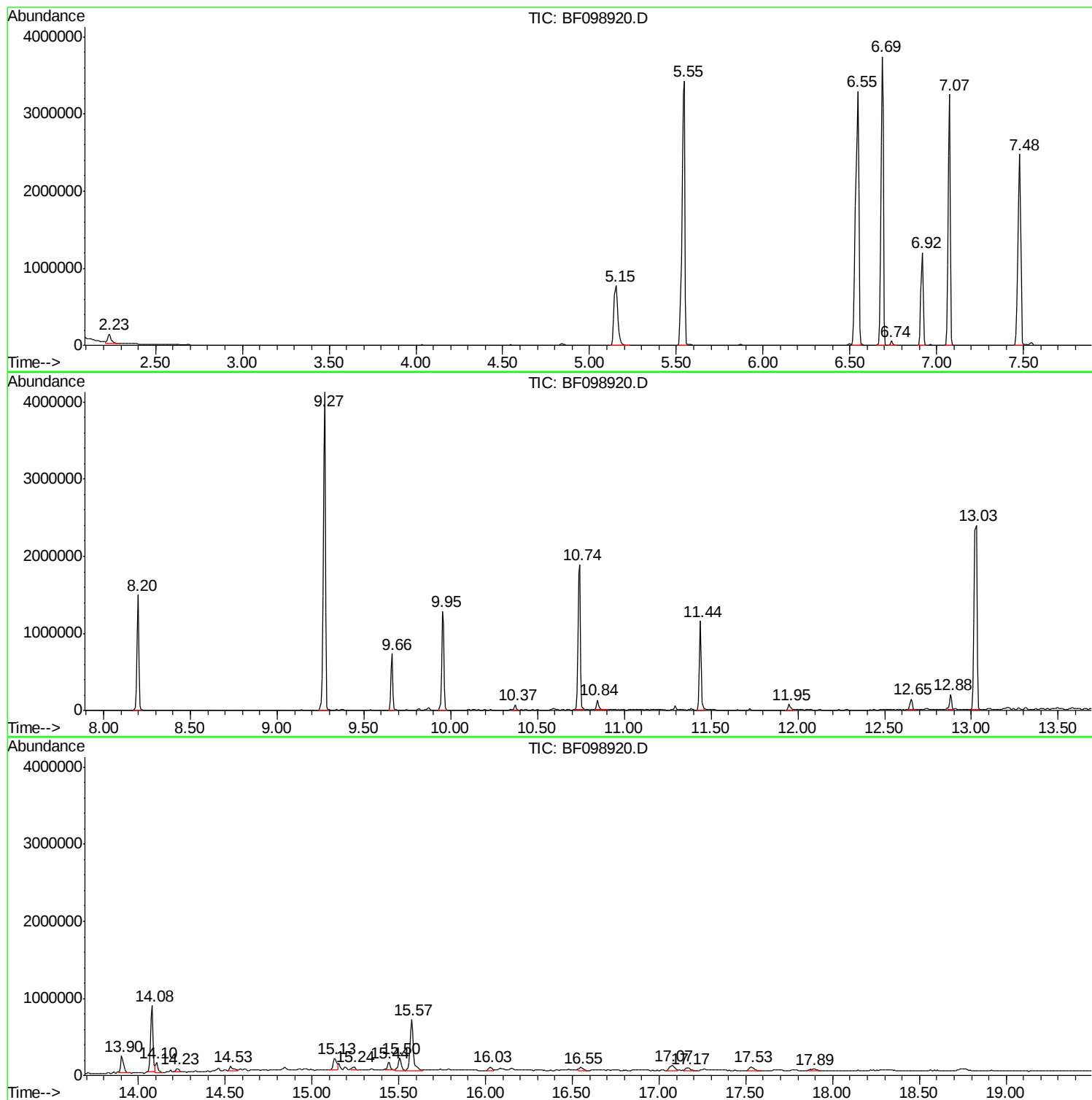
Sum of corrected areas: 35441857

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
W-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-2

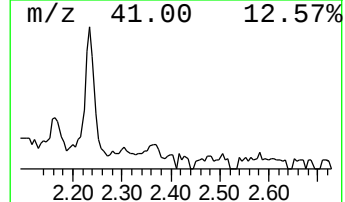
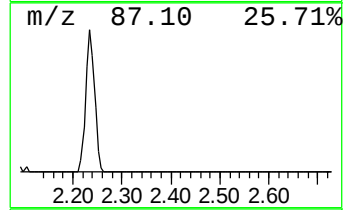
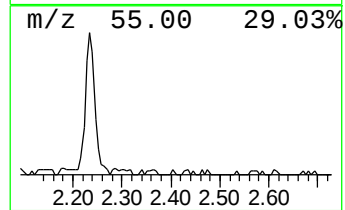
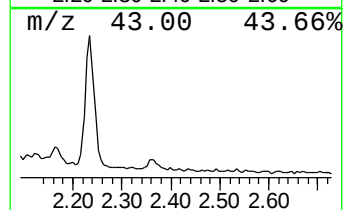
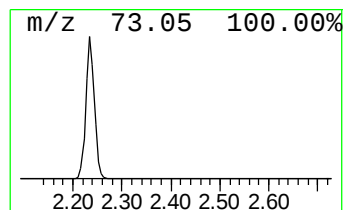
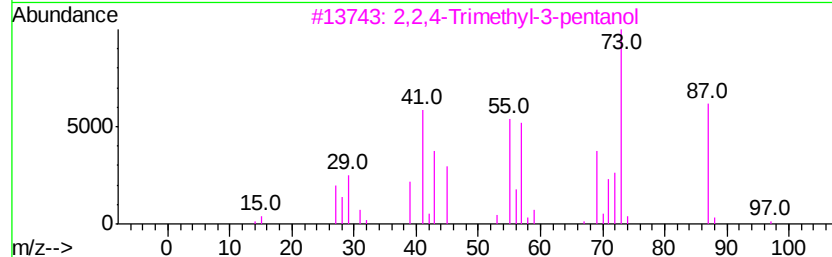
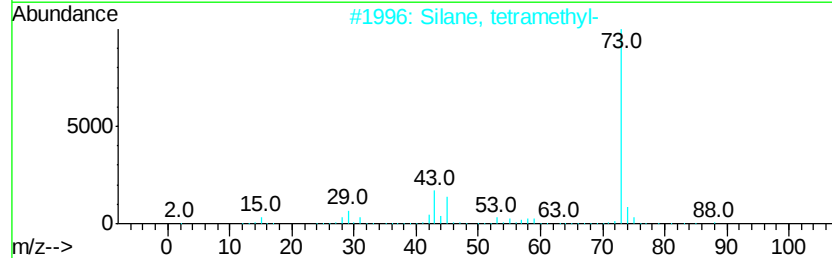
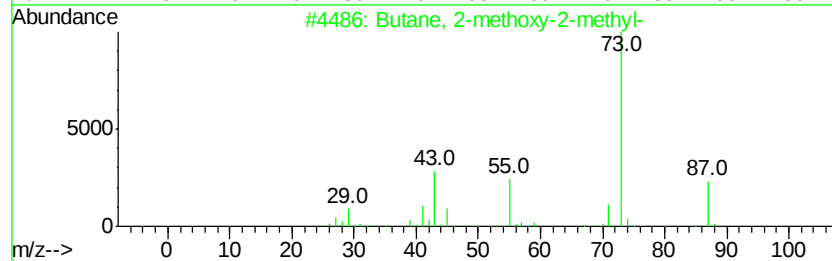
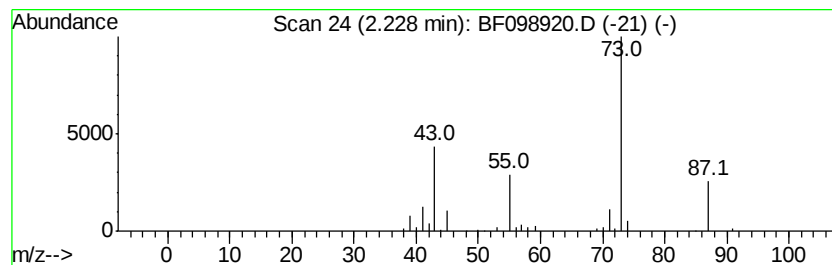
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	3.66 ng	172990	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	46
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-2

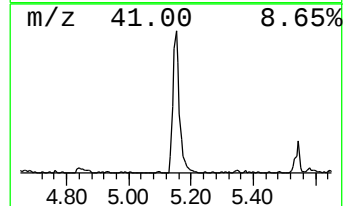
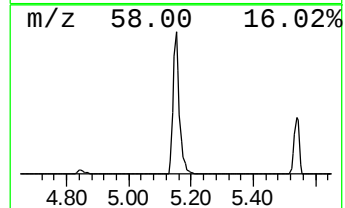
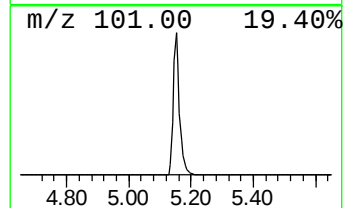
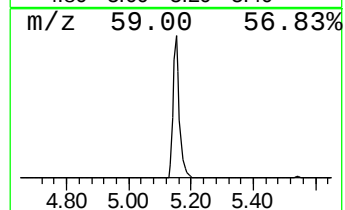
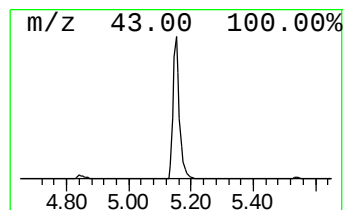
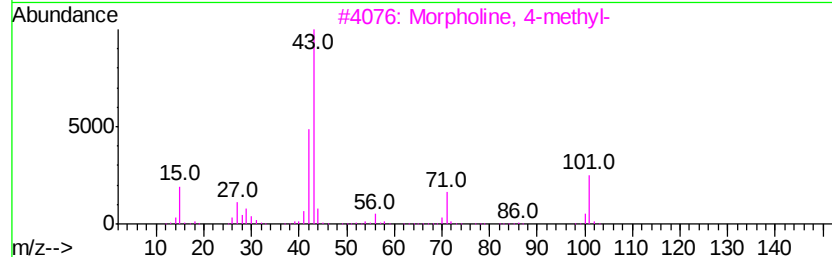
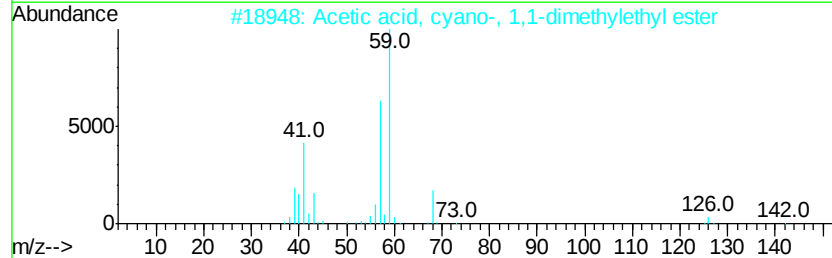
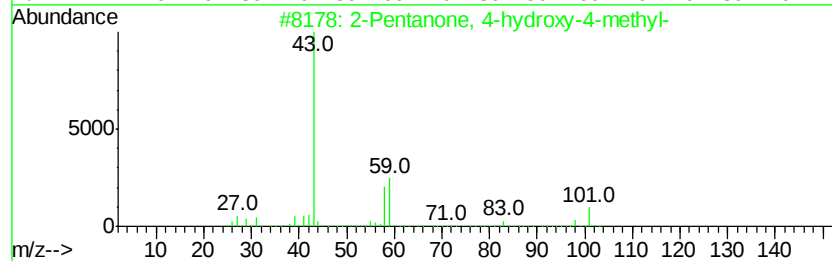
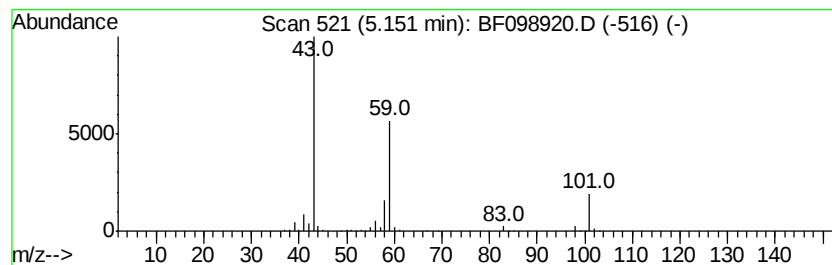
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	23.09 ng	1092360	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-2

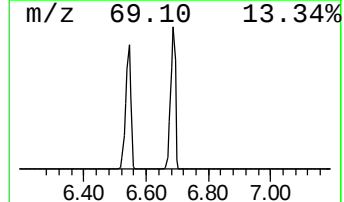
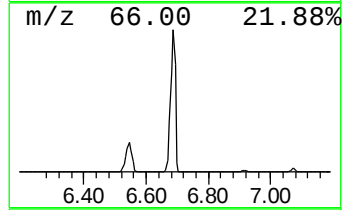
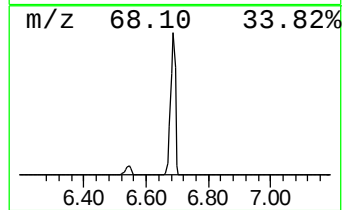
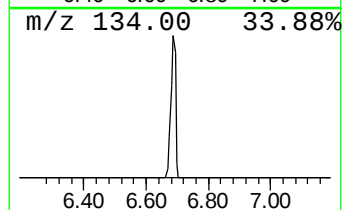
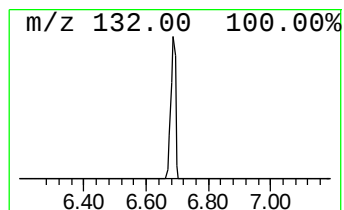
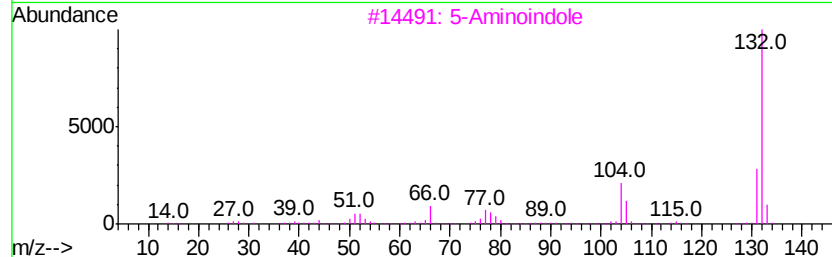
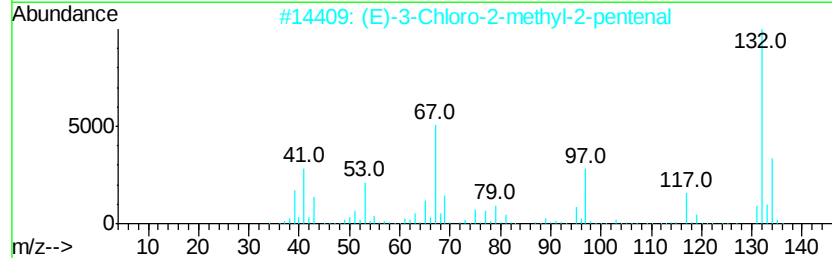
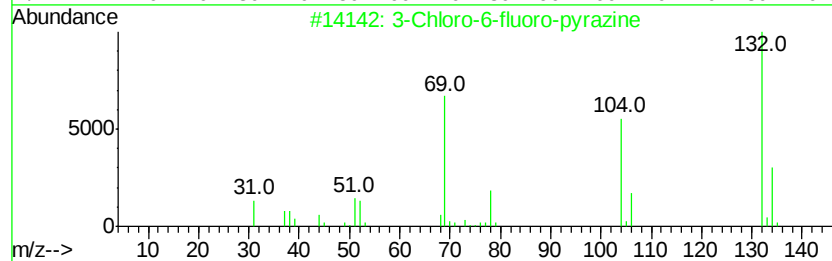
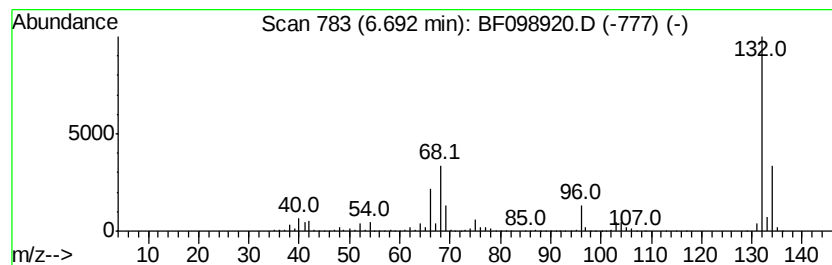
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	84.00 ng	3973640	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-2

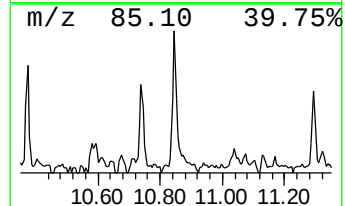
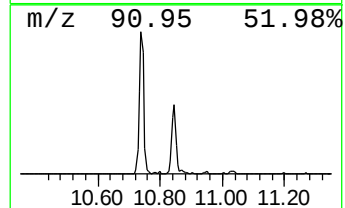
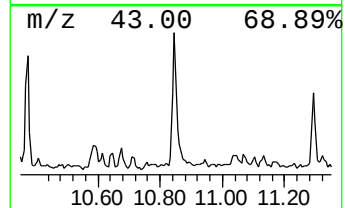
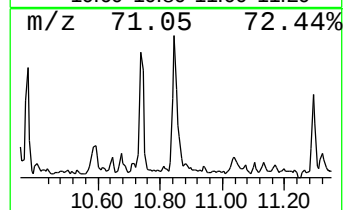
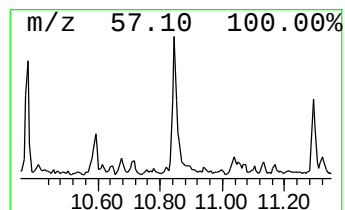
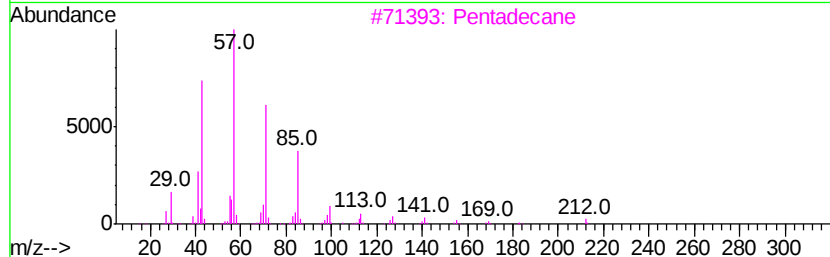
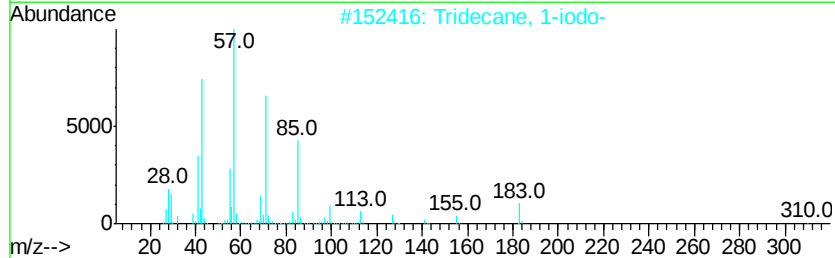
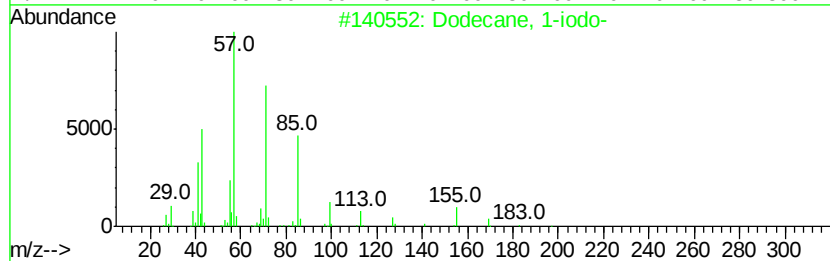
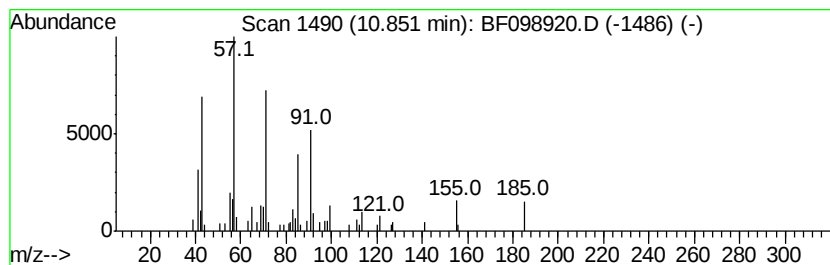
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dodecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	2.77 ng	128262	Phenanthrene-d10	11.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	58
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58
3		Pentadecane	212	C15H32	000629-62-9	52
4		Tetradecane	198	C14H30	000629-59-4	52
5		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-2

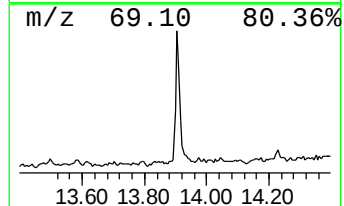
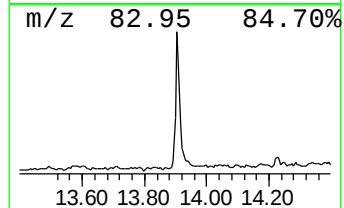
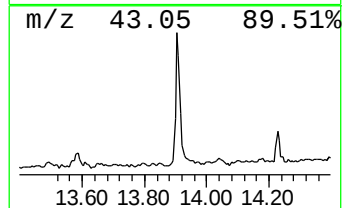
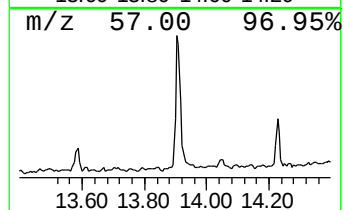
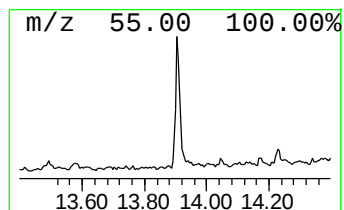
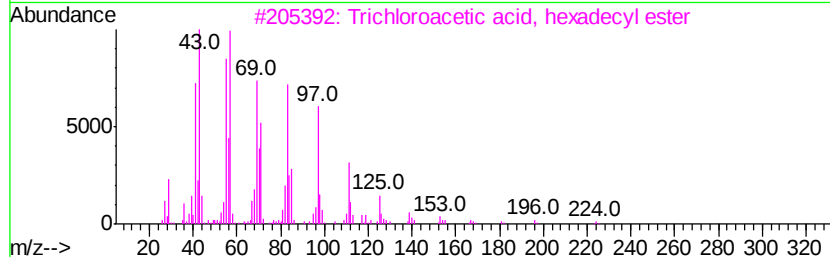
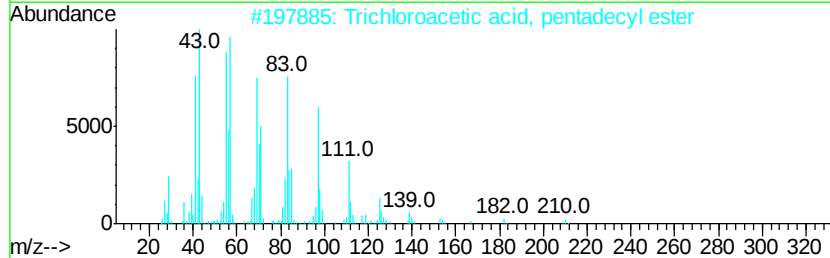
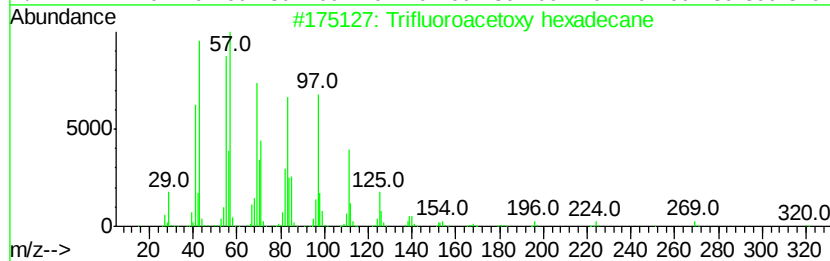
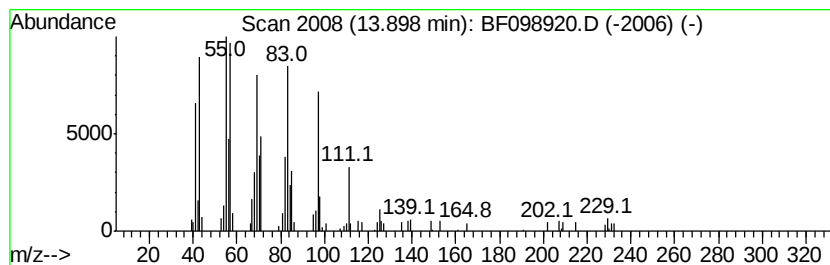
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	5.12 ng	234292	Chrysene-d12	14.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-2

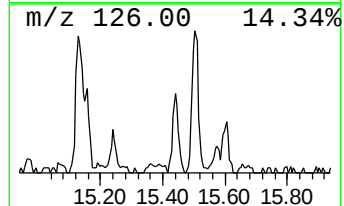
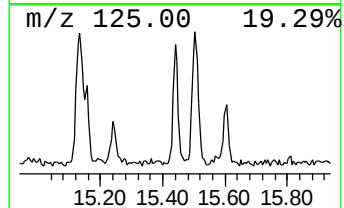
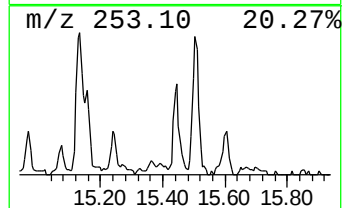
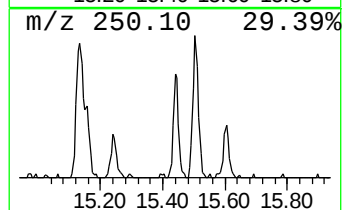
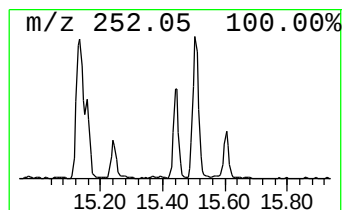
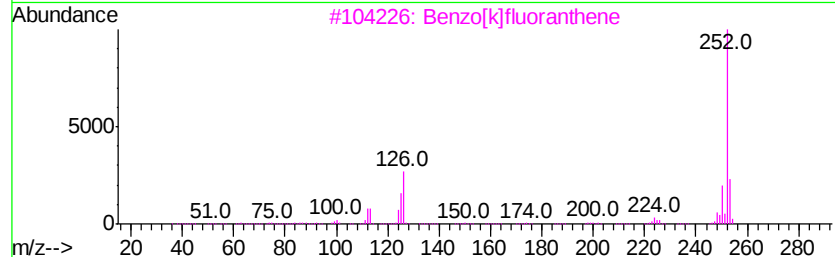
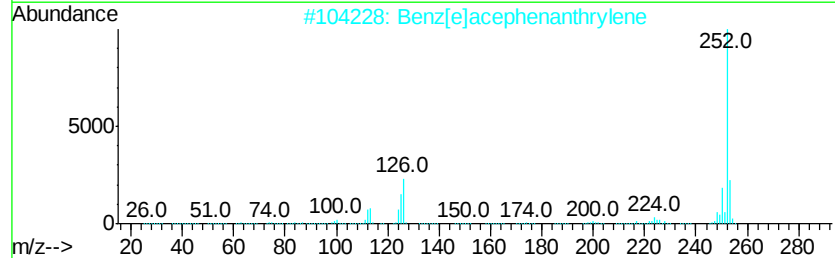
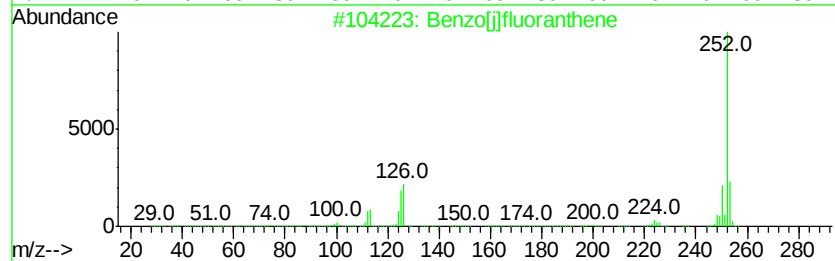
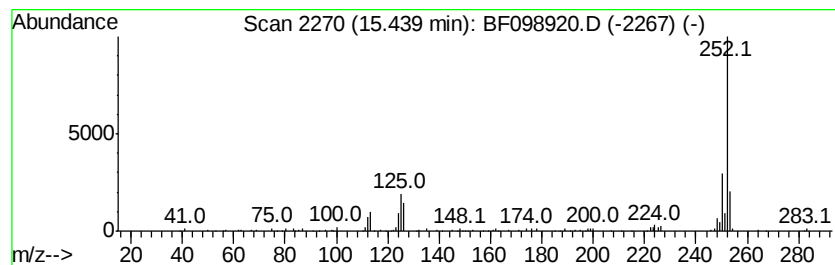
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[j]fluoranthene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	2.59 ng	119007	Perylene-d12	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[i]fluoranthene	252	C20H12	000205-82-3	93
2		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	93
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4		Benzo[e]pyrene	252	C20H12	000192-97-2	93
5		Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098920.D
Acq On : 28 Sep 2017 21:31
Operator : SJ/JU
Sample : I5440-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.23	3.7	ng	172990	1	6.92	946118	20.0
2-Pentanone, 4-hy...	5.15	23.1	ng	1092360	1	6.92	946118	20.0
unknown6.69	6.69	84.0	ng	3973640	1	6.92	946118	20.0
Dodecane, 1-iodo-	10.85	2.8	ng	128262	4	11.44	925689	20.0
Trifluoroacetoxy ...	13.90	5.1	ng	234292	5	14.08	915189	20.0
Benzo[j]fluoranthene	15.44	2.6	ng	119007	6	15.57	920185	20.0