

Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
 Data File : BF097904.D
 Acq On : 21 Aug 2017 14:07
 Operator : SJ/JU
 Sample : I4873-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-BE3-3-10-COMP

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-BF081517.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	3.140	176	179	192	rBV	20172	53209	1.76%	0.205%
2	4.946	482	486	497	rVB	229905	316829	10.47%	1.220%
3	5.357	551	556	560	rBV	2611278	2851307	94.24%	10.976%
4	6.387	725	731	735	rBV	2680769	3025542	100.00%	11.647%
5	6.516	748	753	756	rBV	2940534	2843312	93.98%	10.945%
6	6.745	789	792	796	rBV	1004813	823233	27.21%	3.169%
7	6.904	815	819	822	rBV	2539223	2131621	70.45%	8.206%
8	7.310	883	888	891	rBV	1887330	1815349	60.00%	6.988%
9	8.028	1006	1010	1014	rBV	1233167	1067975	35.30%	4.111%
10	9.110	1188	1194	1197	rBV	2999705	2949251	97.48%	11.353%
11	9.498	1256	1260	1263	rBV	395273	298487	9.87%	1.149%
12	9.722	1295	1298	1301	rVB	52244	44088	1.46%	0.170%
13	9.781	1301	1308	1312	rBV2	1256513	1083543	35.81%	4.171%
14	10.216	1379	1382	1385	rVB	85071	72196	2.39%	0.278%
15	10.439	1415	1420	1422	rBV2	25329	32845	1.09%	0.126%
16	10.569	1437	1442	1445	rBV	1596234	1535303	50.74%	5.910%
17	10.692	1459	1463	1470	rBV	83664	93070	3.08%	0.358%
18	11.139	1536	1539	1541	rBV	48899	35554	1.18%	0.137%
19	11.263	1556	1560	1563	rBV	1085089	928388	30.69%	3.574%
20	12.845	1825	1829	1833	rBV	2060116	1981821	65.50%	7.629%
21	13.327	1906	1911	1918	rBV	115290	126510	4.18%	0.487%
22	13.745	1978	1982	1989	rBV	141988	148265	4.90%	0.571%
23	13.892	2002	2007	2010	rBV2	887355	844844	27.92%	3.252%
24	14.745	2148	2152	2156	rVB	76051	78917	2.61%	0.304%
25	15.310	2243	2248	2253	rBV	601958	690763	22.83%	2.659%
26	15.815	2330	2334	2339	rVB6	22430	33702	1.11%	0.130%
27	16.245	2404	2407	2411	rVB4	23065	31531	1.04%	0.121%
28	16.798	2497	2501	2509	rBV5	17530	40148	1.33%	0.155%

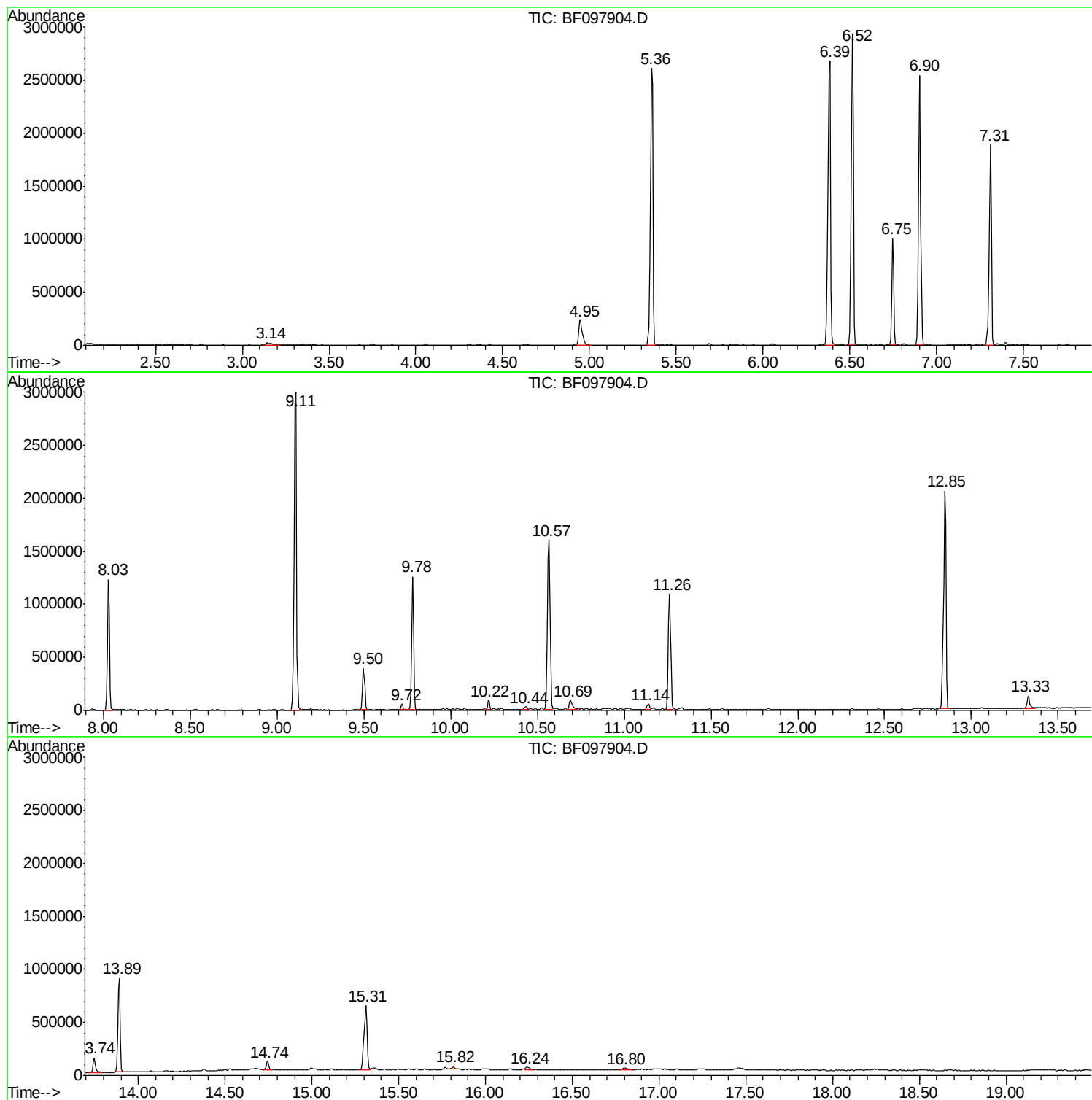
Sum of corrected areas: 25977603

Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097904.D
Acq On : 21 Aug 2017 14:07
Operator : SJ/JU
Sample : I4873-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BE3-3-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097904.D
Acq On : 21 Aug 2017 14:07
Operator : SJ/JU
Sample : I4873-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BE3-3-10-COMP

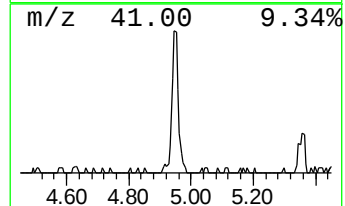
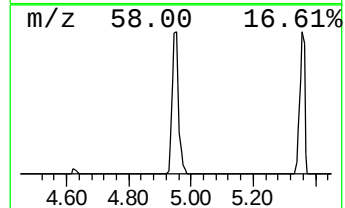
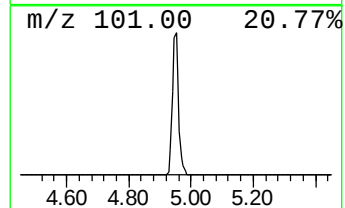
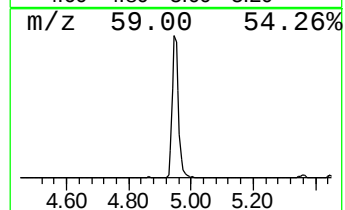
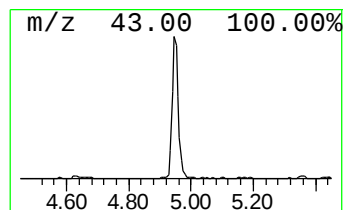
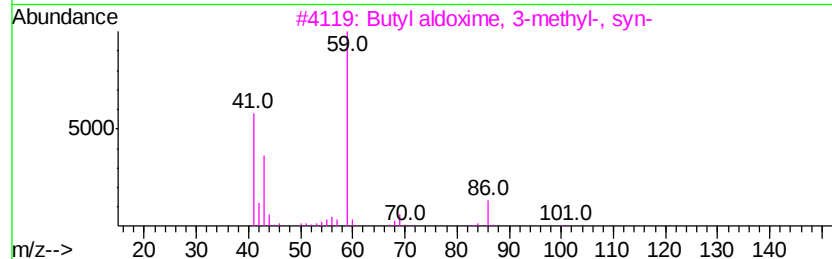
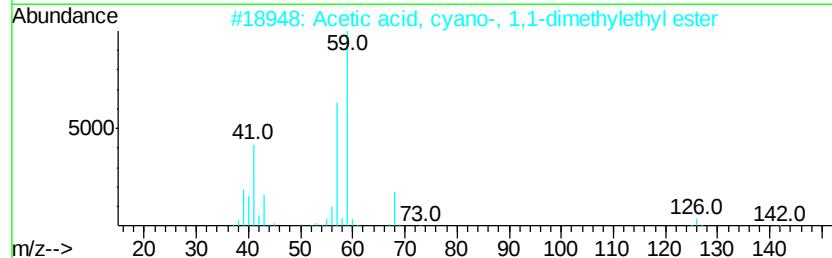
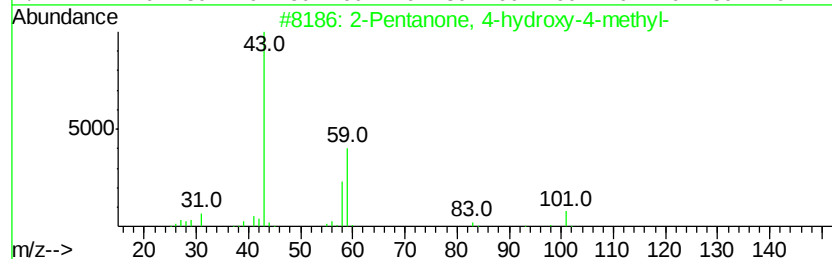
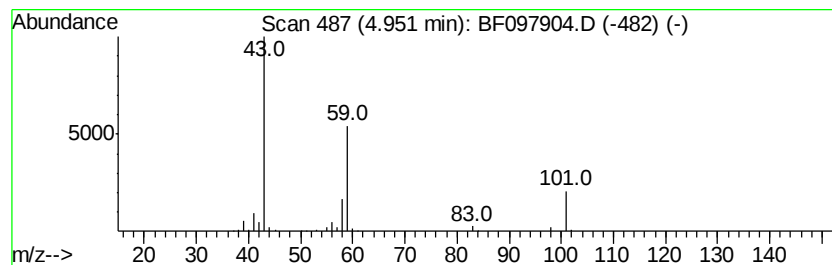
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.95	7.70 ng	316829	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097904.D
Acq On : 21 Aug 2017 14:07
Operator : SJ/JU
Sample : I4873-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BE3-3-10-COMP

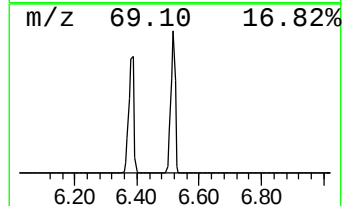
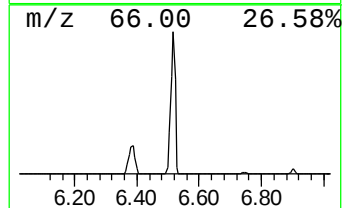
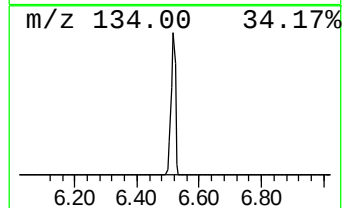
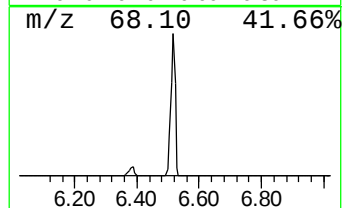
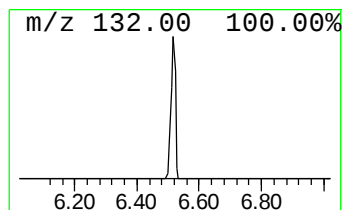
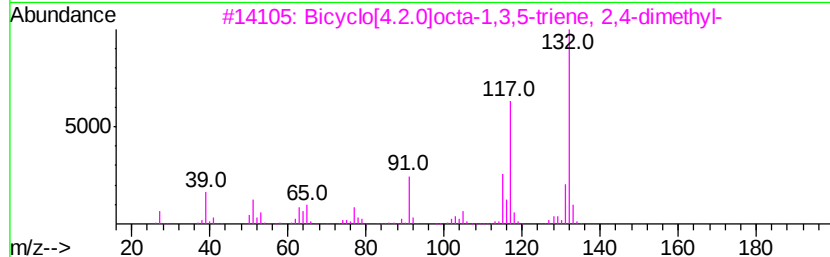
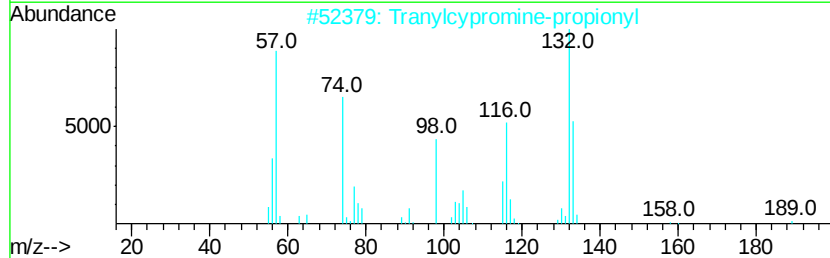
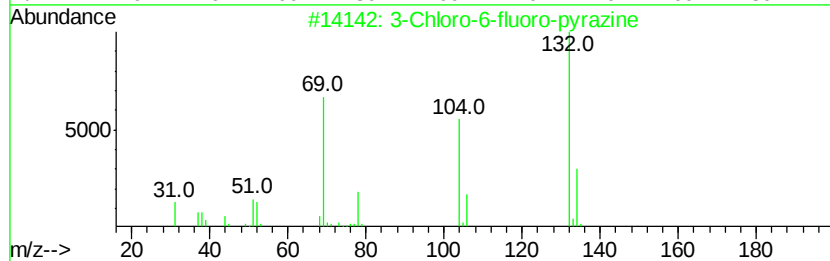
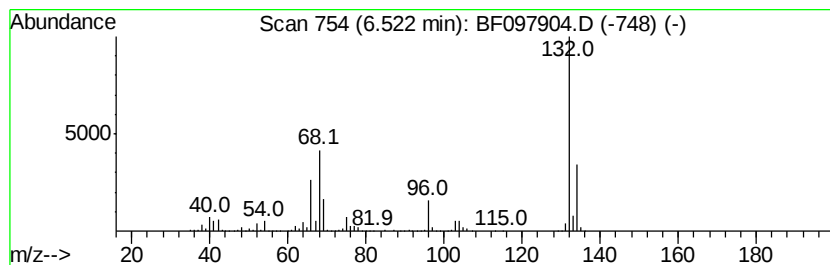
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	69.08 ng	2843310	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
Data File : BF097904.D
Acq On : 21 Aug 2017 14:07
Operator : SJ/JU
Sample : I4873-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

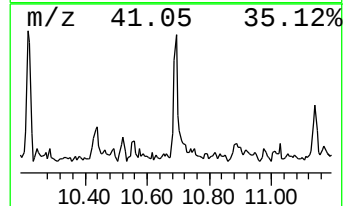
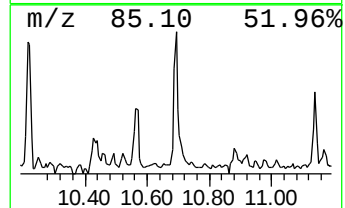
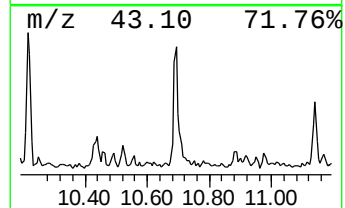
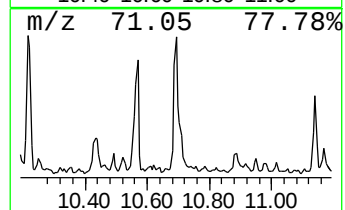
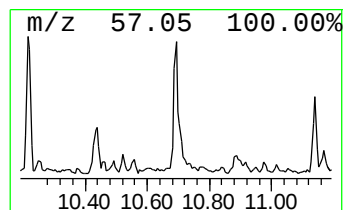
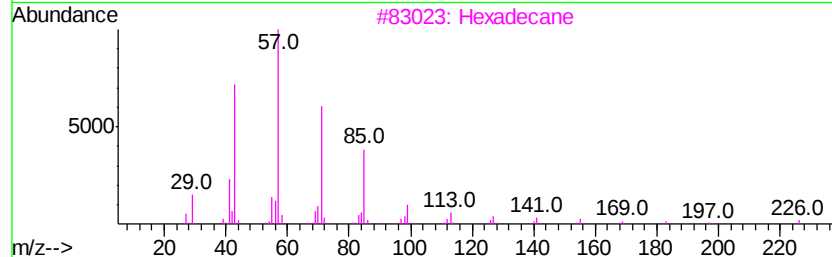
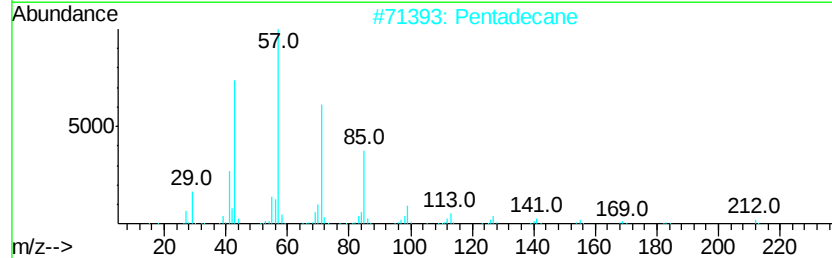
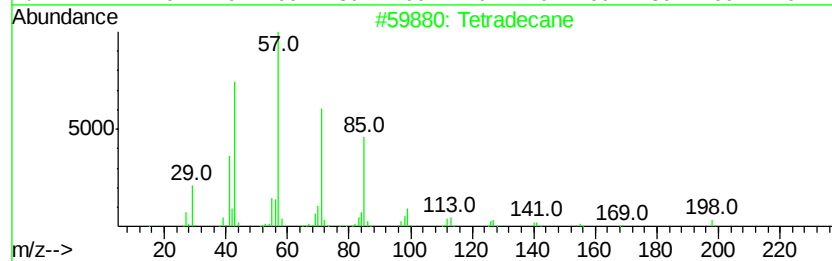
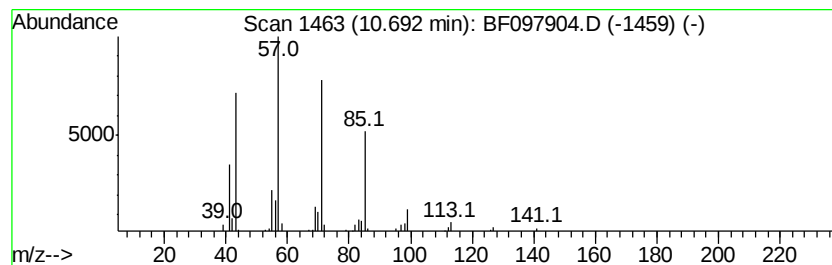
Instrument :
BNA_F
ClientSampleId :
TEC-BE3-3-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.69	2.00 ng	93070	Phenanthrene-d10	11.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	83
5	Heptacosane	380	C27H56	000593-49-7	72



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097904.D
Acq On : 21 Aug 2017 14:07
Operator : SJ/JU
Sample : I4873-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

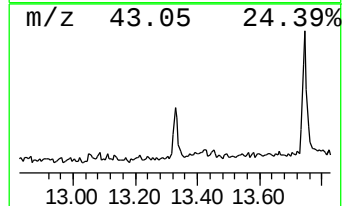
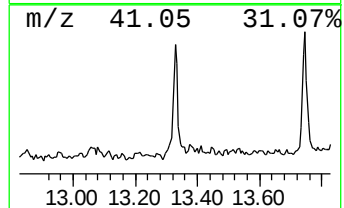
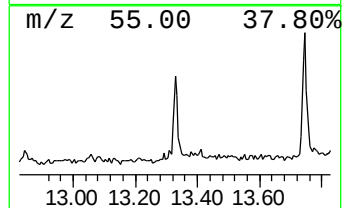
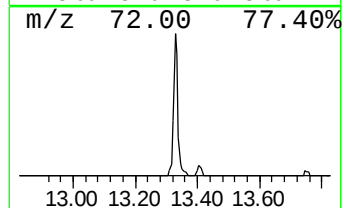
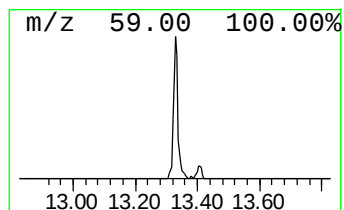
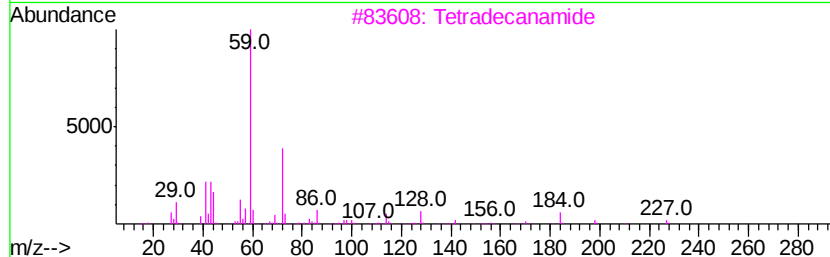
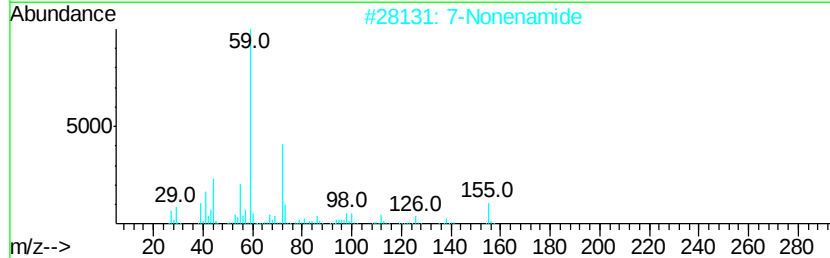
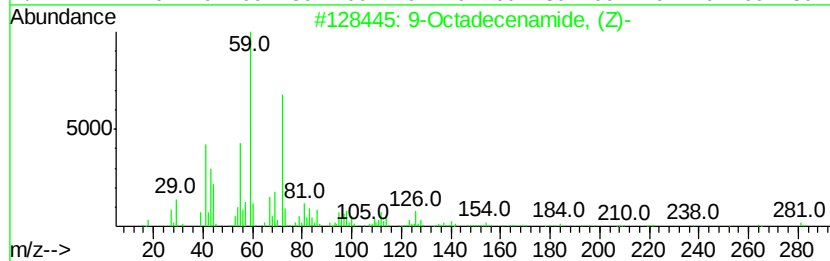
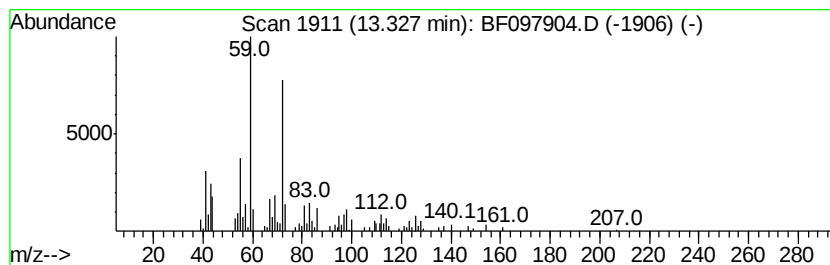
Instrument :
BNA_F
ClientSampleId :
TEC-BE3-3-10-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.33	2.99 ng	126510	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	7-Nonenamide	155	C9H17NO	090949-53-4	78
3	Tetradecanamide	227	C14H29NO	000638-58-4	72
4	Hexadecanamide	255	C16H33NO	000629-54-9	53
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097904.D
Acq On : 21 Aug 2017 14:07
Operator : SJ/JU
Sample : I4873-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BE3-3-10-COMP

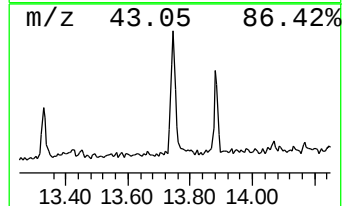
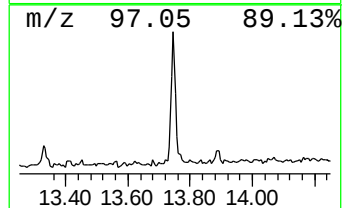
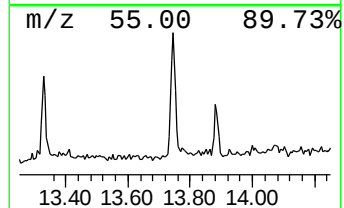
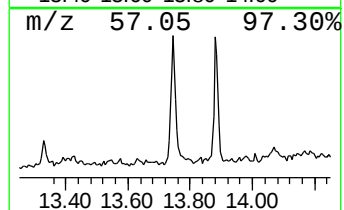
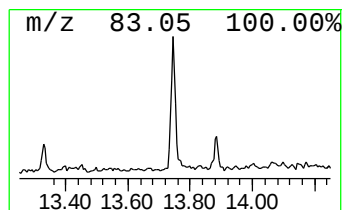
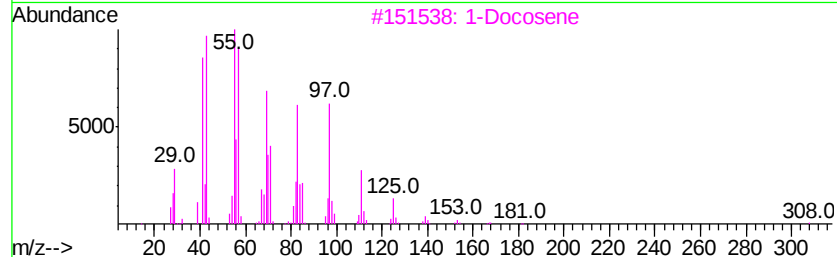
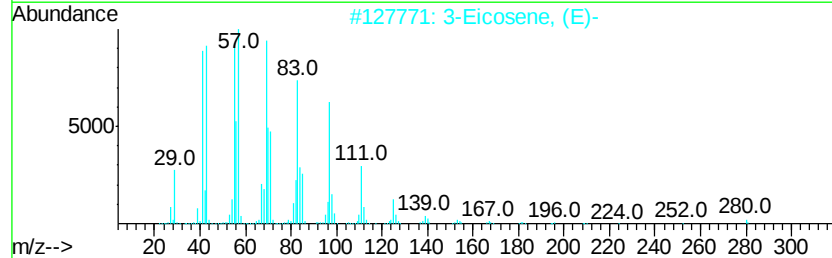
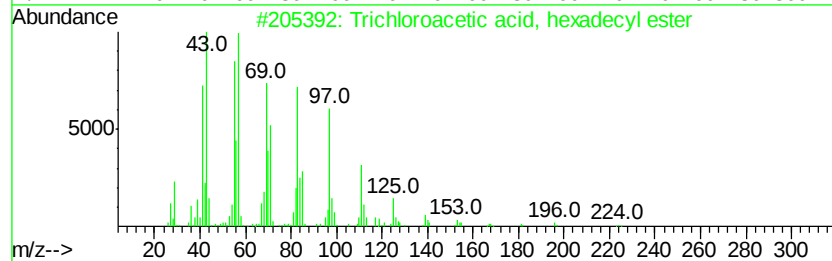
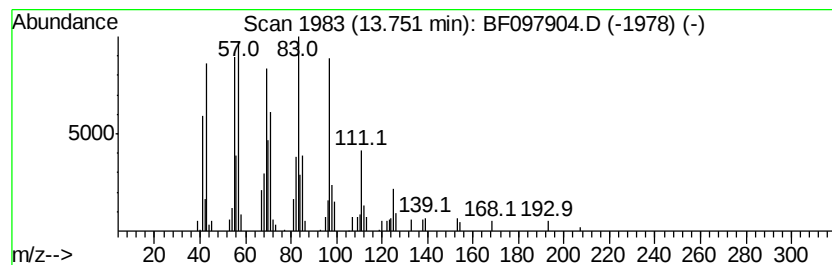
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.51 ng	148265	Chrysene-d12	13.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3			1-Docosene	308	C22H44	001599-67-3	81
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	81
5			1-Heneicosanol	312	C21H44O	015594-90-8	76



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
Data File : BF097904.D
Acq On : 21 Aug 2017 14:07
Operator : SJ/JU
Sample : I4873-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BE3-3-10-COMP

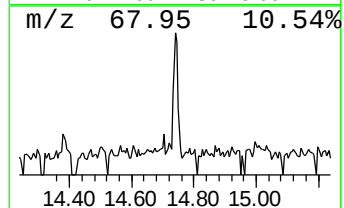
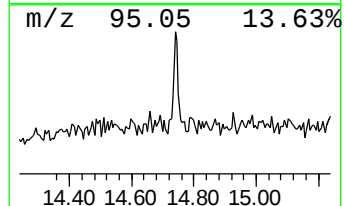
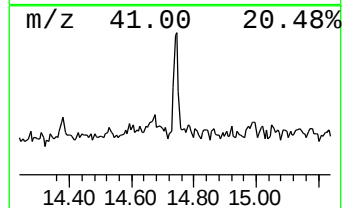
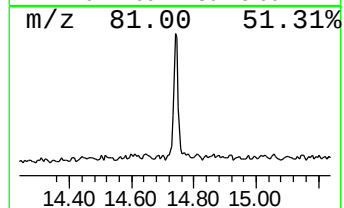
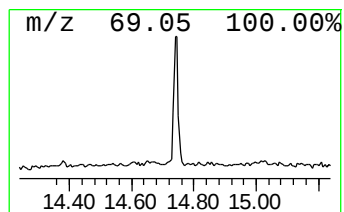
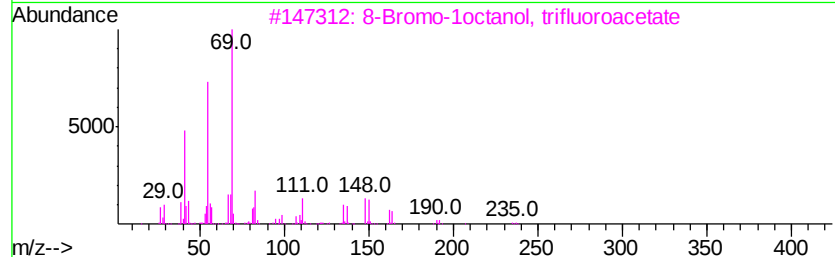
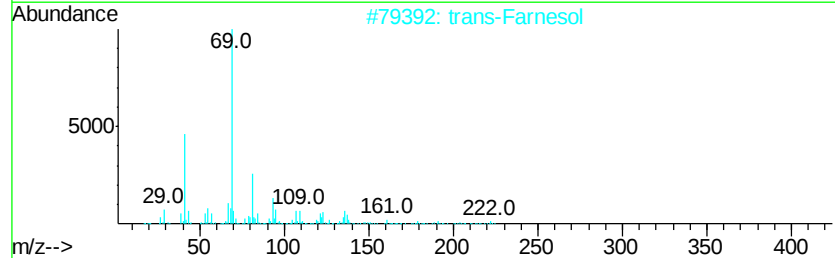
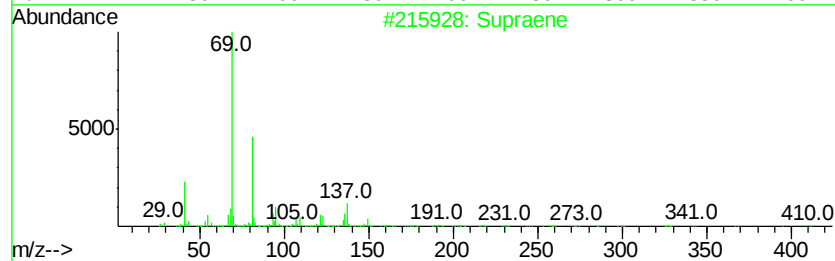
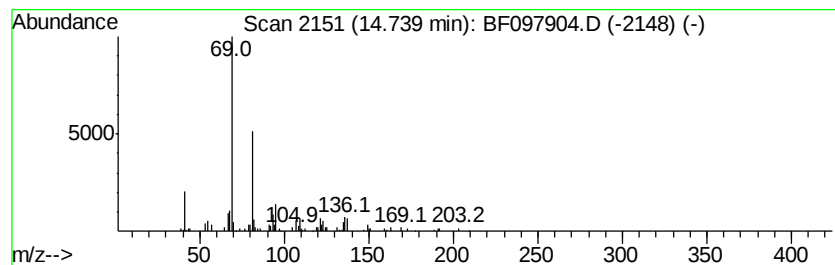
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.28 ng	78917	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	83
2		trans-Farnesol	222	C15H26O	000106-28-5	83
3		8-Bromo-1octanol, trifluoroacetate	304	C10H16BrF3O2	1000365-19-4	59
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	42
5		1,5-Heptadiene, 3,3-dimethyl-, (E)-	124	C9H16	067682-47-7	40



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
Data File : BF097904.D
Acq On : 21 Aug 2017 14:07
Operator : SJ/JU
Sample : I4873-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BE3-3-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.95	7.7	ng	316829	1	6.75	823233	20.0
unknown6.52	6.52	69.1	ng	2843310	1	6.75	823233	20.0
Tetradecane	10.69	2.0	ng	93070	4	11.26	928388	20.0
9-Octadecenamide,...	13.33	3.0	ng	126510	5	13.89	844844	20.0
Trichloroacetic a...	13.75	3.5	ng	148265	5	13.89	844844	20.0
Supraene	14.74	2.3	ng	78917	6	15.31	690763	20.0