

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
 Data File : BF095512.D
 Acq On : 27 May 2017 23:25
 Operator : SJ/MA
 Sample : I3244-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM6-COMP-0-6

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-BF050217.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	5.101	535	538	552	rBV	58785	157386	7.52%	0.892%
2	5.707	637	641	675	rBV	515466	1616560	77.23%	9.157%
3	7.284	906	909	926	rBV	554436	1447182	69.14%	8.198%
4	7.407	926	930	955	rVB	1068639	2093255	100.00%	11.858%
5	7.737	983	986	1002	rBV	392137	526373	25.15%	2.982%
6	7.972	1022	1026	1055	rBV	971429	1338162	63.93%	7.580%
7	8.648	1137	1141	1163	rBV	334131	933262	44.58%	5.287%
8	9.772	1328	1332	1362	rBV	246470	704429	33.65%	3.990%
9	11.536	1627	1632	1657	rBV	930095	1861123	88.91%	10.543%
10	12.248	1746	1753	1770	rBV	80765	183004	8.74%	1.037%
11	12.601	1808	1813	1827	rBV2	525502	965919	46.14%	5.472%
12	13.424	1948	1953	1959	rBV	25065	29337	1.40%	0.166%
13	13.901	2030	2034	2052	rBV	412284	946635	45.22%	5.362%
14	14.195	2081	2084	2095	rVB	21822	33649	1.61%	0.191%
15	15.007	2217	2222	2244	rVV2	316670	744573	35.57%	4.218%
16	15.954	2379	2383	2398	rVB4	47524	108078	5.16%	0.612%
17	16.795	2522	2526	2534	rBV	117122	179890	8.59%	1.019%
18	17.095	2573	2577	2585	rVV	123360	192348	9.19%	1.090%
19	17.312	2610	2614	2627	rBV	814666	1051638	50.24%	5.957%
20	17.424	2627	2633	2641	rVB3	10199	24677	1.18%	0.140%
21	17.706	2676	2681	2688	rVB4	16038	25900	1.24%	0.147%
22	18.553	2820	2825	2829	rBV4	30018	58433	2.79%	0.331%
23	18.677	2840	2846	2851	rBV2	347902	573856	27.41%	3.251%
24	18.812	2864	2869	2872	rBV4	15144	21813	1.04%	0.124%
25	19.195	2928	2934	2938	rBV2	16499	30832	1.47%	0.175%
26	19.342	2957	2959	2963	rBV4	15619	22213	1.06%	0.126%
27	19.783	3031	3034	3037	rBV4	12577	21313	1.02%	0.121%
28	19.865	3044	3048	3051	rVB4	37316	45259	2.16%	0.256%
29	19.953	3059	3063	3066	rBV	101058	139545	6.67%	0.790%
30	20.065	3078	3082	3086	rBV2	87176	118315	5.65%	0.670%
31	20.195	3102	3104	3108	rVB5	19181	21480	1.03%	0.122%
32	20.242	3109	3112	3117	rVV	69013	92381	4.41%	0.523%
33	20.300	3119	3122	3127	rVV	93129	123622	5.91%	0.700%
34	20.353	3127	3131	3145	rVB	332388	611794	29.23%	3.466%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.583	3166	3170	3177	rBV9	42591	79024	3.78%	0.448%
36	20.789	3200	3205	3211	rBV2	105117	161148	7.70%	0.913%
37	21.459	3315	3319	3322	rVB6	20171	25188	1.20%	0.143%
38	21.718	3358	3363	3369	rBV4	138724	240838	11.51%	1.364%
39	22.112	3425	3430	3440	rVB3	39665	102642	4.90%	0.581%

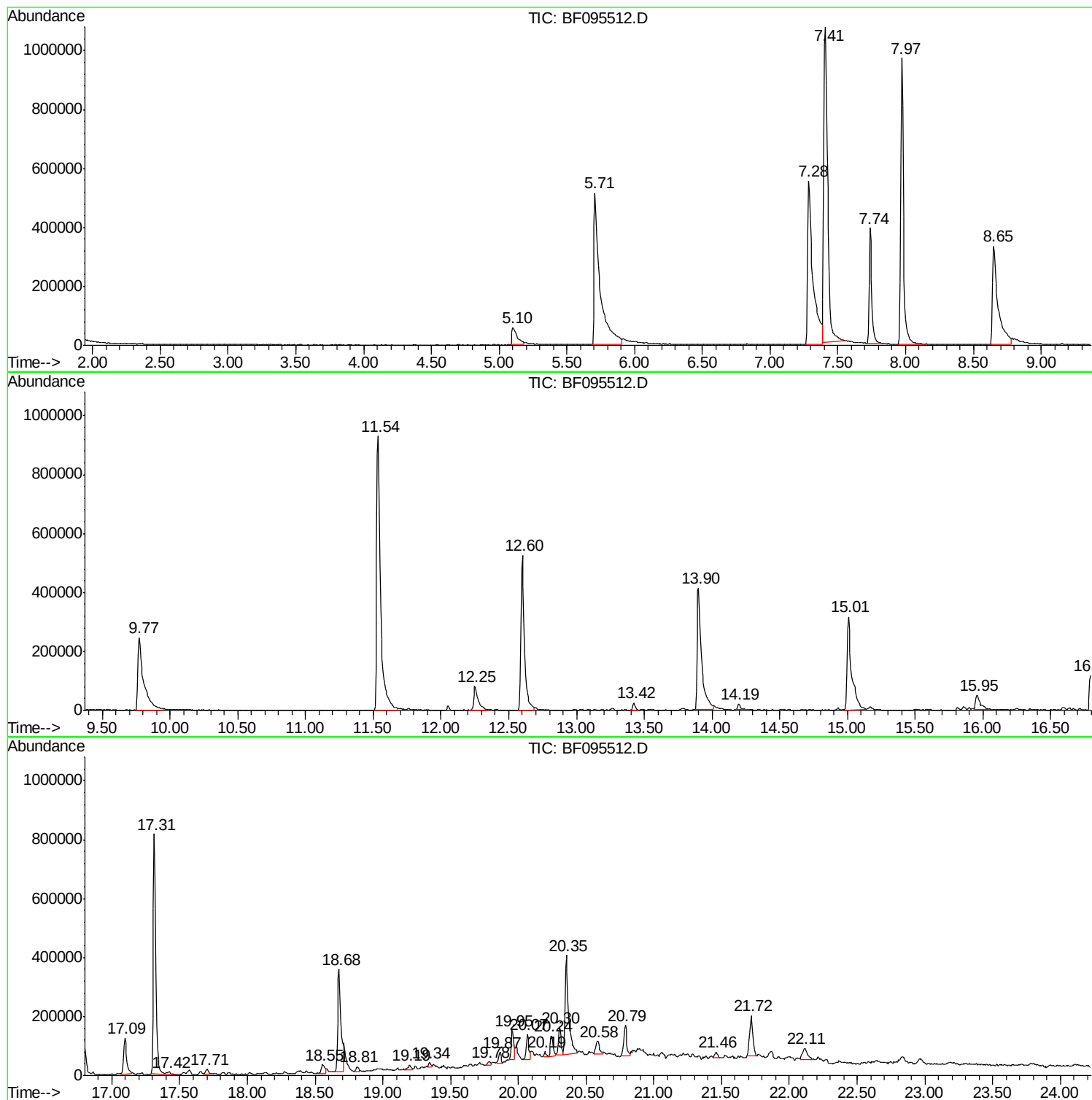
Sum of corrected areas: 17653076

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

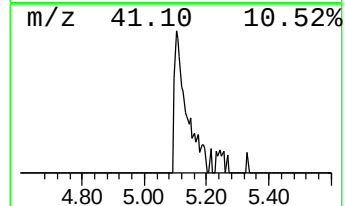
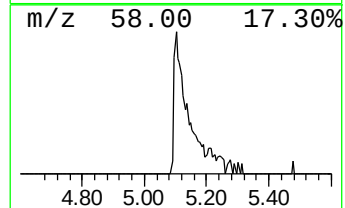
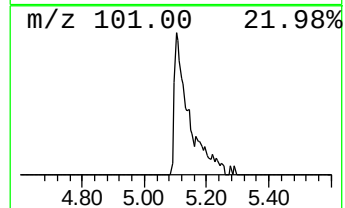
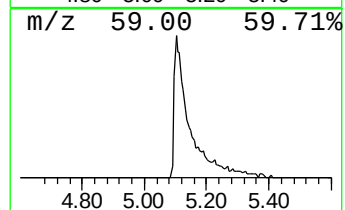
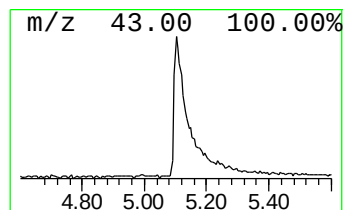
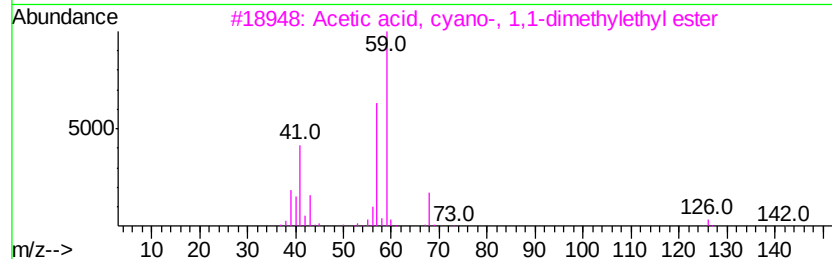
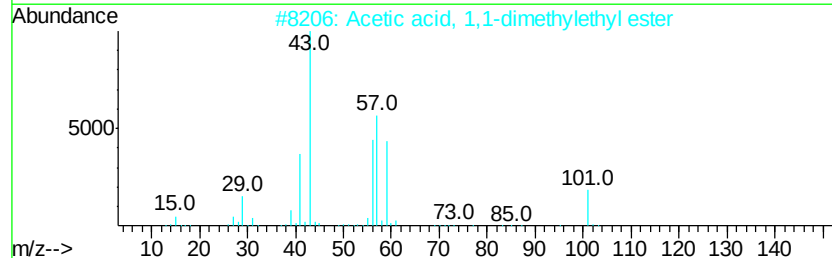
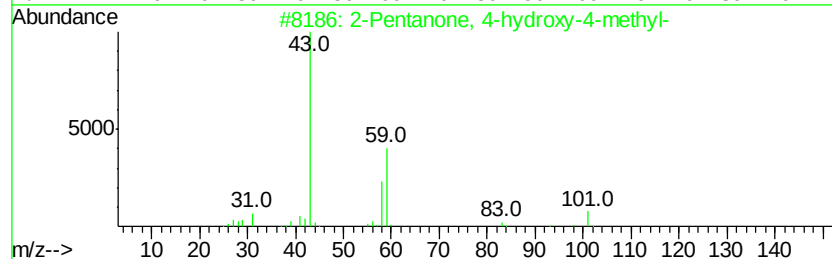
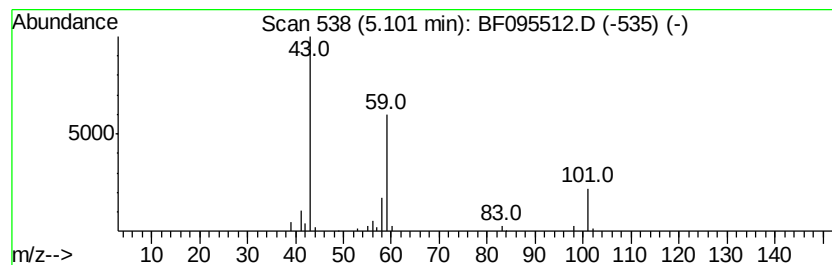
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.10	5.98 ng	157386	1,4-Dichlorobenzene-d4	7.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

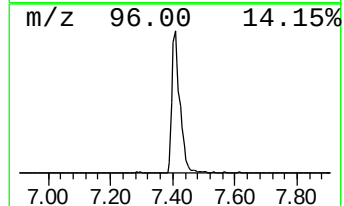
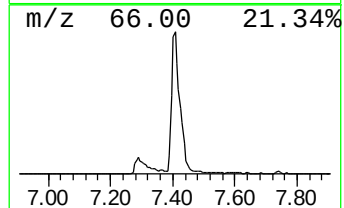
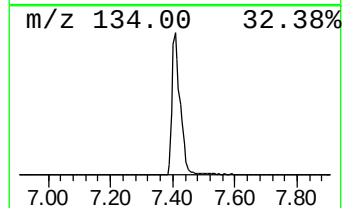
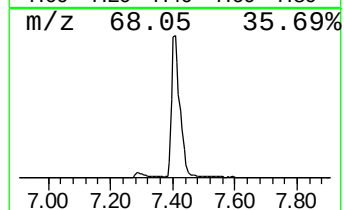
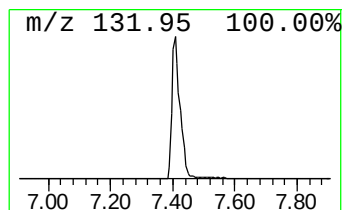
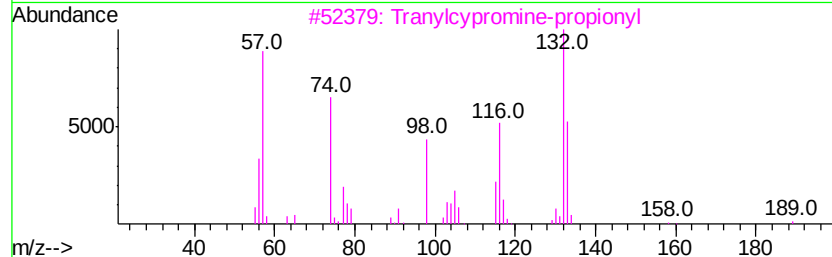
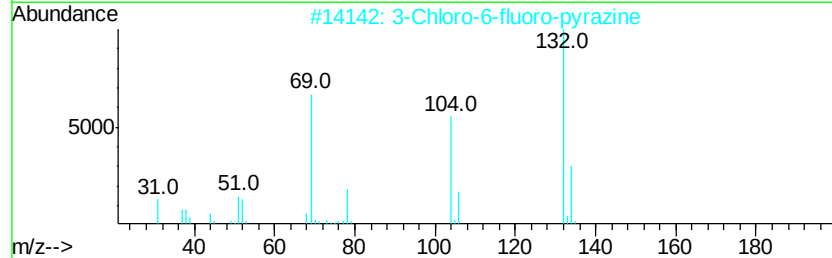
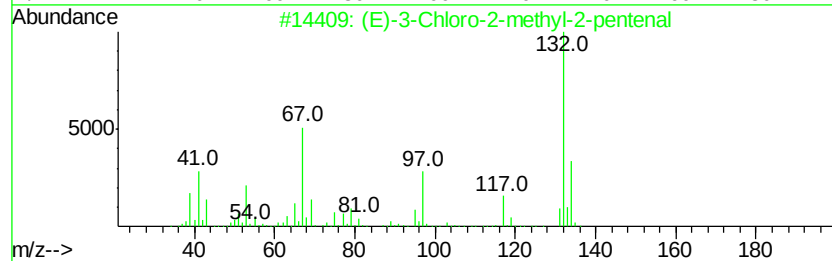
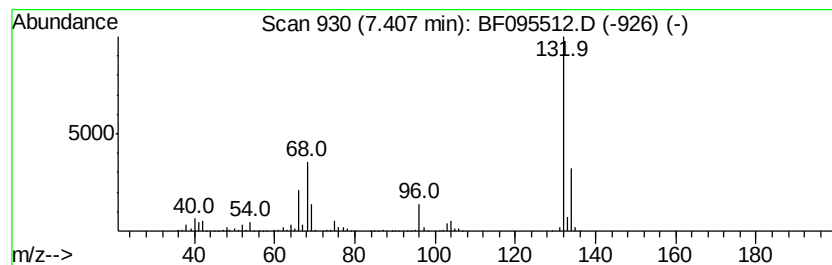
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	79.54 ng	2093260	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Aminoindan	133	C9H11N	034698-41-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

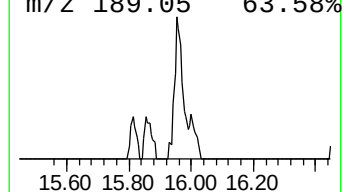
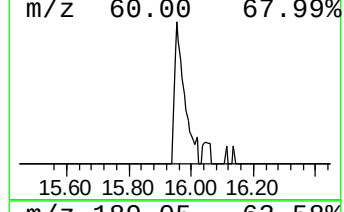
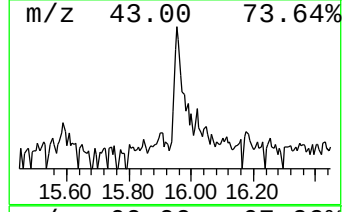
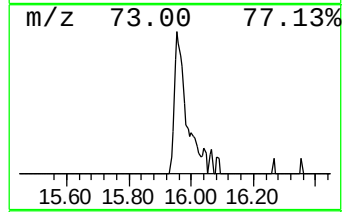
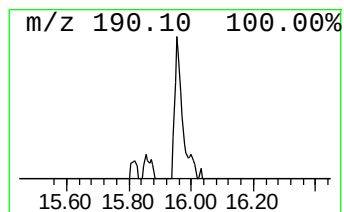
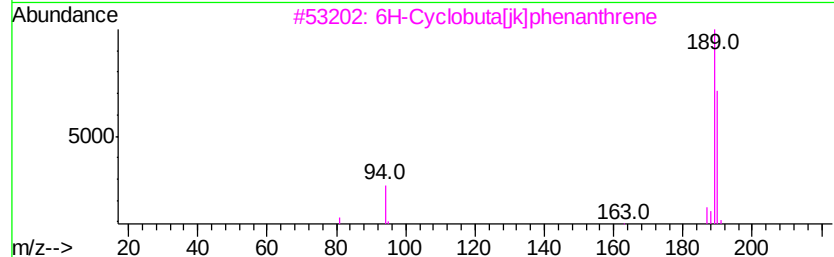
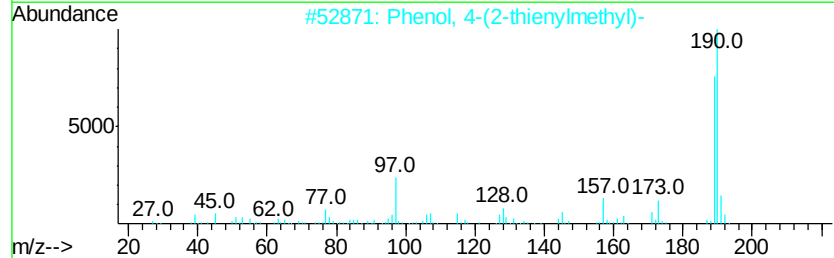
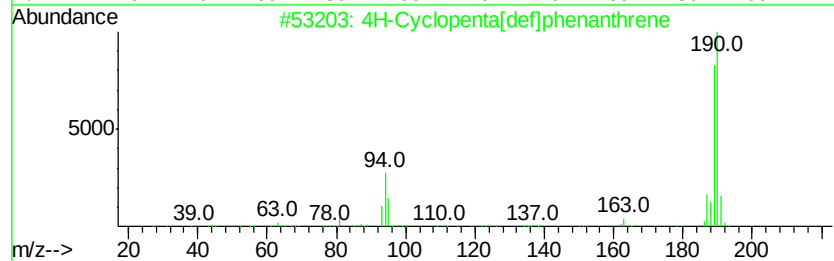
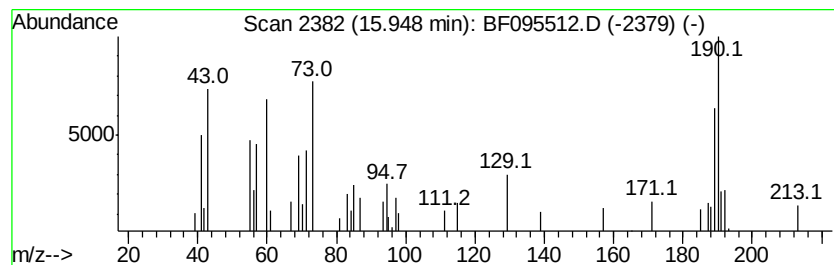
Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.95	2.90 ng	108078	Phenanthrene-d10	15.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	46
3	6H-Cyclobuta[ikl]phenanthrene	190	C15H10	083469-43-6	43
4	8H-Cyclopenta[d][1,2,4]triazolo[...]	190	C9H10N4O	1000337-56-4	32
5	Cyclohepta[cd][2]benzothiophene, ...	190	C12H14S	199807-57-3	16



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

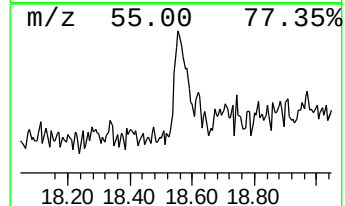
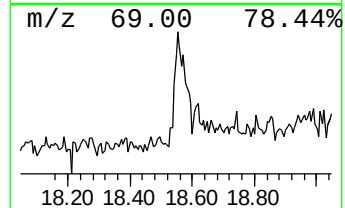
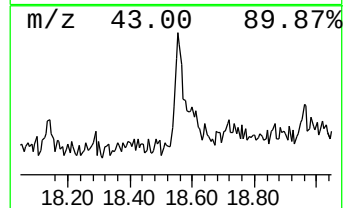
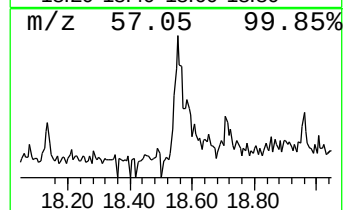
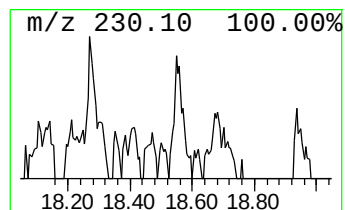
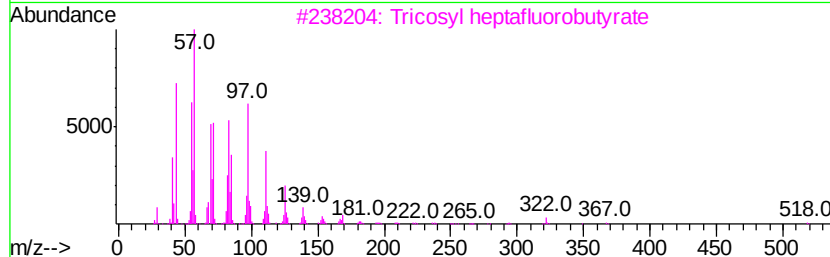
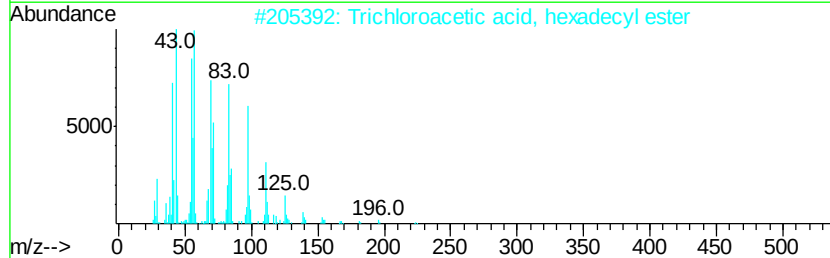
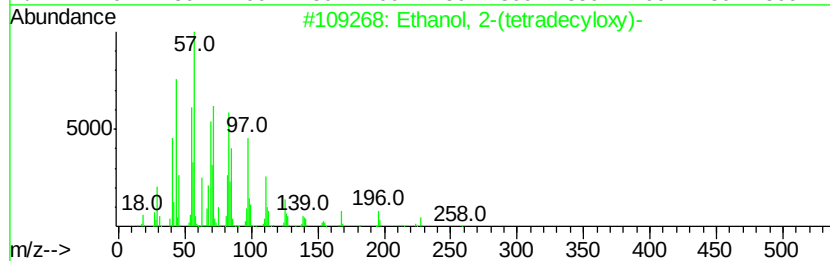
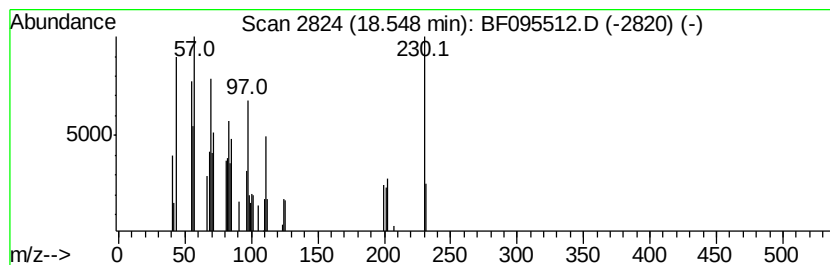
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	2.04 ng	58433	Chrysene-d12	18.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	70
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	58
3		Tricosyl heptafluorobutrate	536	C27H47F7O2	1000351-83-4	58
4		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	58
5		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	55



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

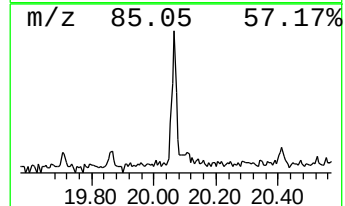
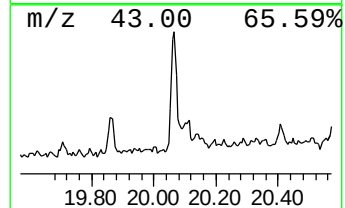
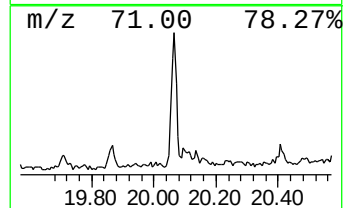
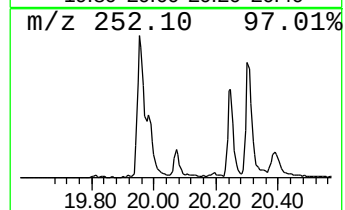
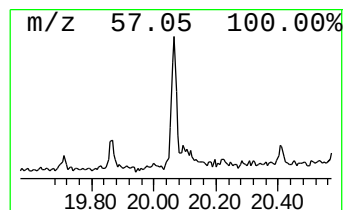
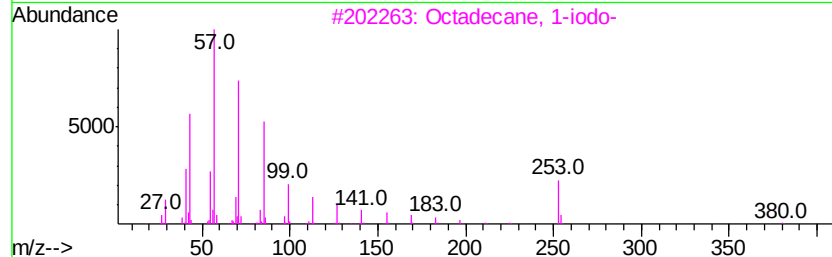
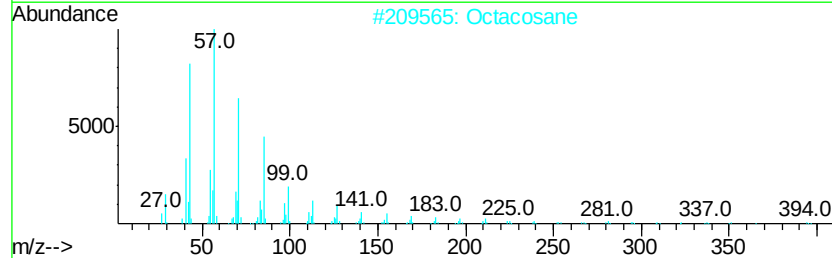
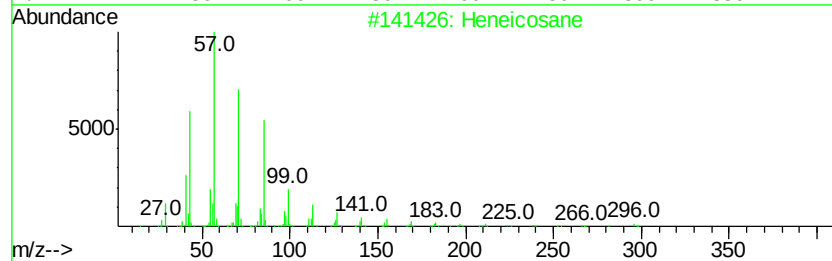
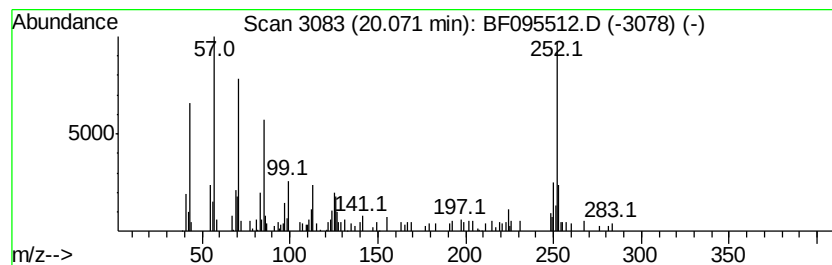
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	3.87 ng	118315	Perylene-d12	20.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	53
2	Octacosane		394	C28H58	000630-02-4	52
3	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	52
4	Hexacosane		366	C26H54	000630-01-3	49
5	Pentacosane		352	C25H52	000629-99-2	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

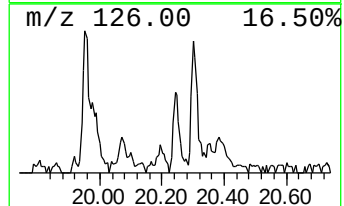
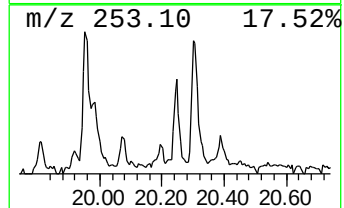
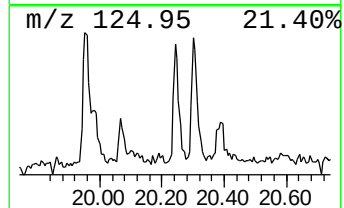
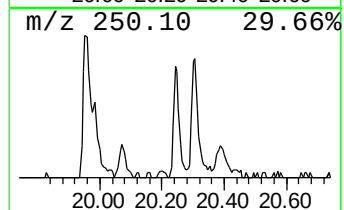
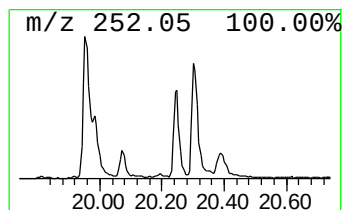
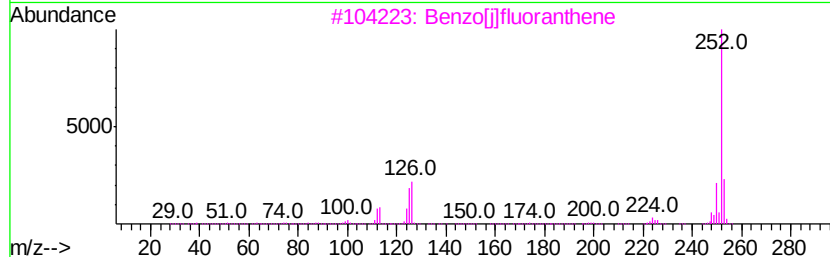
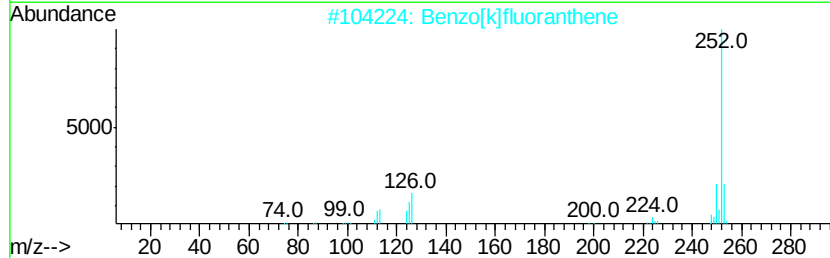
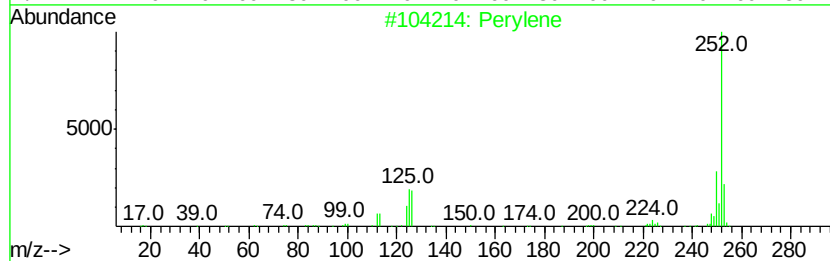
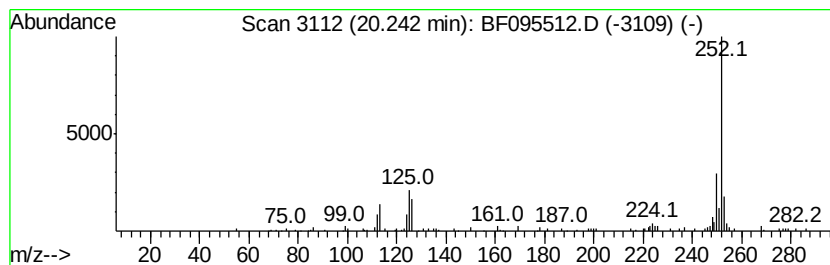
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.24	3.02 ng	92381	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	98
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3		Benzo[i]fluoranthene	252	C20H12	000205-82-3	95
4		Benzo[a]pyrene	252	C20H12	000050-32-8	94
5		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

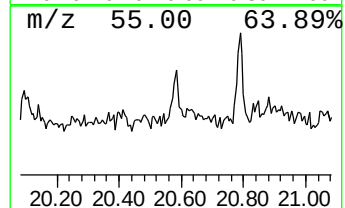
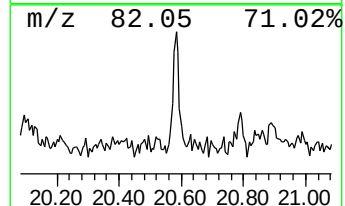
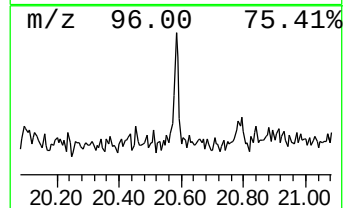
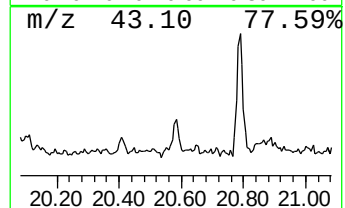
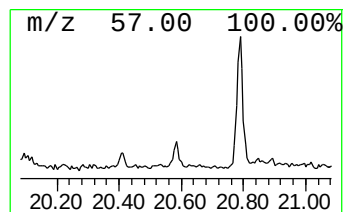
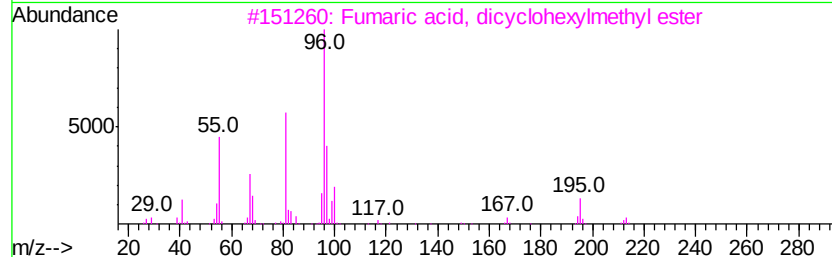
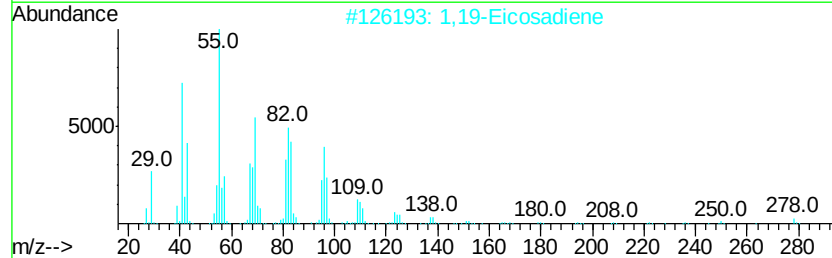
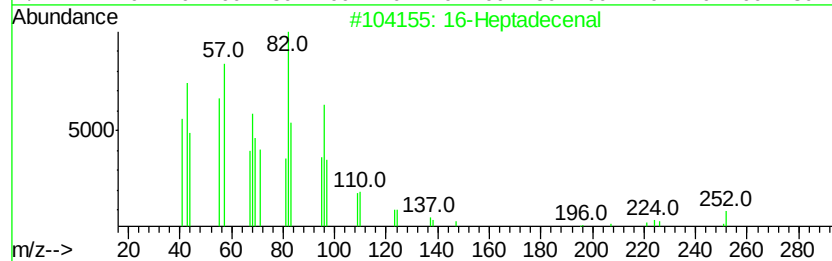
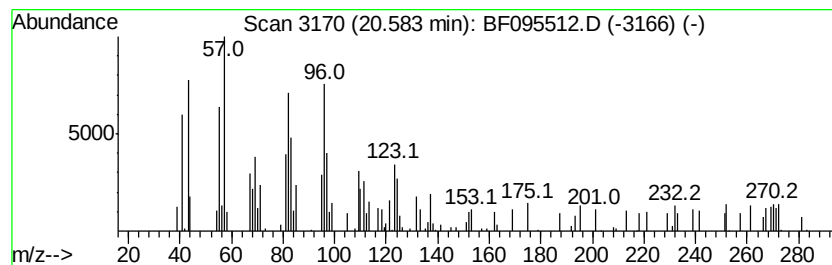
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 16-Heptadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.58	2.58 ng	79024	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	16-Heptadecenal	252	C17H32O	1000144-57-9	52
2		1,19-Eicosadiene	278	C20H38	014811-95-1	46
3		Fumaric acid, dicyclohexylmethyl...	308	C18H28O4	1000345-05-9	43
4		1,1'-Bicycloheptyl	194	C14H26	023183-11-1	43
5		1H-Indene, octahydro-	124	C9H16	000496-10-6	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

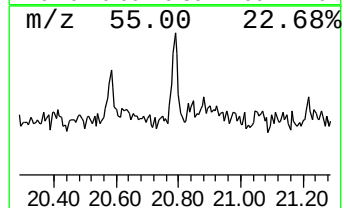
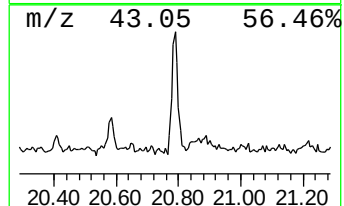
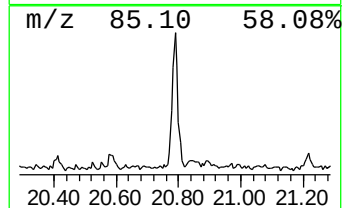
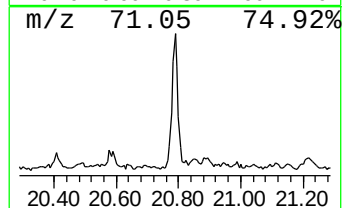
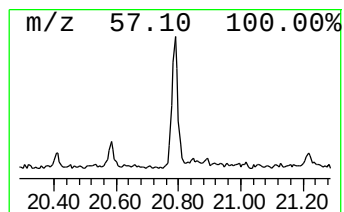
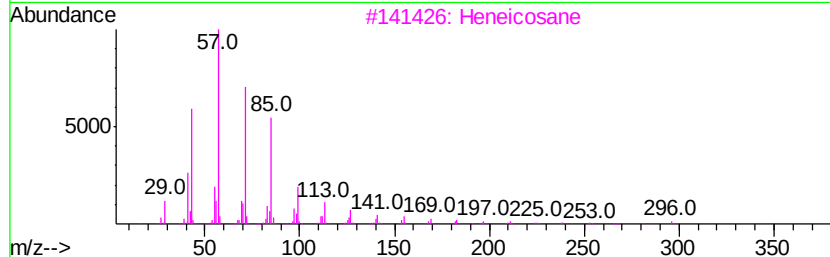
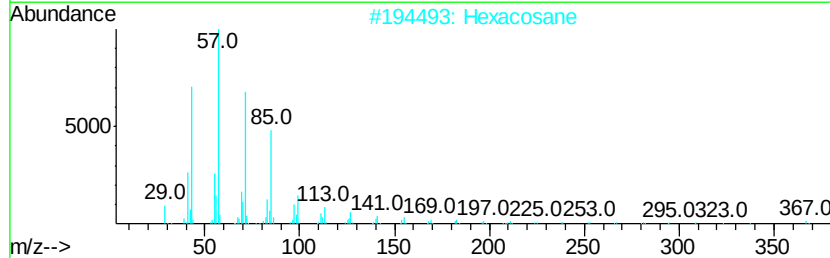
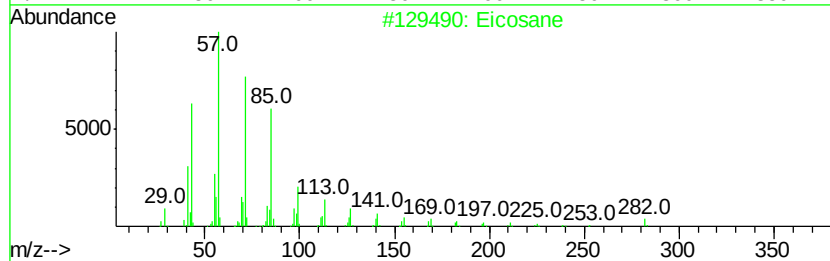
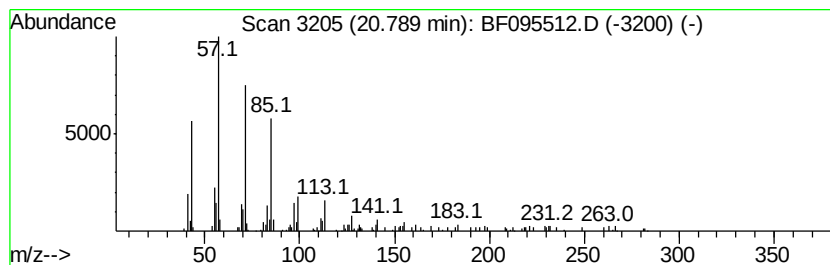
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	5.27 ng	161148	Perylene-d12	20.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	97
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	triacontane		422	C30H62	000638-68-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
Data File : BF095512.D
Acq On : 27 May 2017 23:25
Operator : SJ/MA
Sample : I3244-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM6-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.10	6.0	ng	157386	1	7.74	526373	20.0
unknown7.41	7.41	79.5	ng	2093260	1	7.74	526373	20.0
4H-Cyclopenta[def...	15.95	2.9	ng	108078	4	15.01	744573	20.0
Ethanol, 2-(tetra...	18.55	2.0	ng	58433	5	18.68	573856	20.0
Heneicosane	20.07	3.9	ng	118315	6	20.35	611794	20.0
Perylene	20.24	3.0	ng	92381	6	20.35	611794	20.0
16-Heptadecenal	20.58	2.6	ng	79024	6	20.35	611794	20.0
Eicosane	20.79	5.3	ng	161148	6	20.35	611794	20.0