

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
 Data File : BF095546.D
 Acq On : 30 May 2017 20:57
 Operator : SJ/MA
 Sample : I3302-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM16-COMP-6-18

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	5.096	533	537	550	rBV	65401	155466	7.04%	0.877%
2	5.707	637	641	673	rBV	695919	1910359	86.48%	10.775%
3	7.289	906	910	926	rBV	658676	1593574	72.14%	8.988%
4	7.407	926	930	952	rVB	1221441	2209054	100.00%	12.459%
5	7.737	982	986	997	rVB	415299	509651	23.07%	2.875%
6	7.972	1021	1026	1042	rBV	1207291	1551503	70.23%	8.751%
7	8.642	1136	1140	1182	rBV	446096	1118653	50.64%	6.309%
8	9.766	1326	1331	1358	rBV	282547	678237	30.70%	3.825%
9	11.530	1626	1631	1653	rBV	992559	1854188	83.94%	10.458%
10	12.242	1747	1752	1768	rBV	94087	188572	8.54%	1.064%
11	12.595	1807	1812	1829	rBV2	357698	665765	30.14%	3.755%
12	13.419	1947	1952	1958	rBV2	25916	31770	1.44%	0.179%
13	13.901	2029	2034	2057	rBV	404652	832904	37.70%	4.698%
14	14.195	2080	2084	2087	rBV	26682	32877	1.49%	0.185%
15	15.001	2217	2221	2241	rVV3	279211	574235	25.99%	3.239%
16	15.842	2360	2364	2370	rBV4	15794	28171	1.28%	0.159%
17	15.954	2379	2383	2395	rVB5	85712	146389	6.63%	0.826%
18	16.783	2521	2524	2533	rBV	137089	184098	8.33%	1.038%
19	17.042	2564	2568	2572	rBV4	29971	45787	2.07%	0.258%
20	17.089	2572	2576	2586	rVB	147258	215536	9.76%	1.216%
21	17.312	2610	2614	2625	rBV	1012113	1213182	54.92%	6.843%
22	17.554	2651	2655	2659	rVB2	17636	25766	1.17%	0.145%
23	17.636	2665	2669	2673	rBV	16692	25481	1.15%	0.144%
24	17.695	2674	2679	2685	rVB4	18596	33726	1.53%	0.190%
25	18.430	2799	2804	2808	rBV4	10551	25307	1.15%	0.143%
26	18.553	2821	2825	2836	rBV5	45856	95490	4.32%	0.539%
27	18.671	2839	2845	2850	rBV2	484811	712358	32.25%	4.018%
28	18.806	2862	2868	2873	rVB7	25082	37360	1.69%	0.211%
29	19.342	2955	2959	2966	rBV8	21703	54198	2.45%	0.306%
30	19.783	3030	3034	3041	rVB3	55483	94223	4.27%	0.531%
31	19.947	3058	3062	3065	rBV	85312	124627	5.64%	0.703%
32	20.065	3079	3082	3086	rBV3	37025	49550	2.24%	0.279%
33	20.242	3108	3112	3118	rBV	59639	98301	4.45%	0.554%
34	20.300	3119	3122	3126	rVV	66835	84561	3.83%	0.477%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-6-18

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	20.353	3127	3131	3139	rVV	300213	419782	19.00%	2.368%
36	21.718	3357	3363	3370	rBV8	49556	109312	4.95%	0.617%

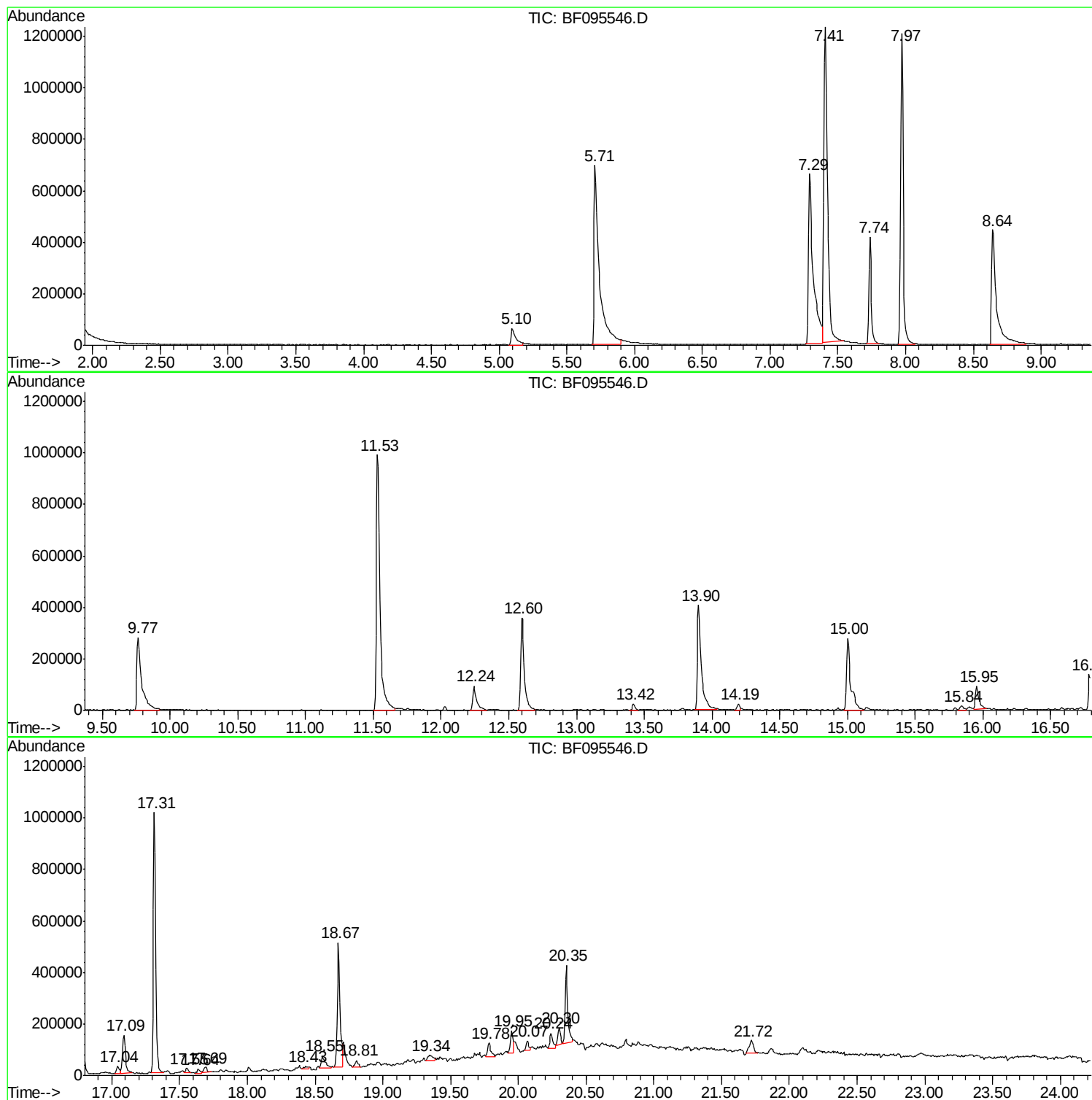
Sum of corrected areas: 17730013

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
NM16-COMP-6-18

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\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-6-18

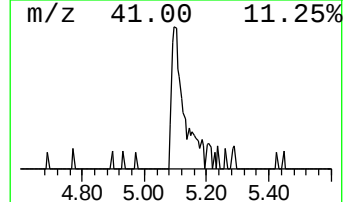
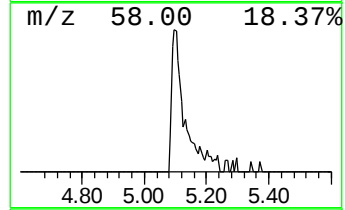
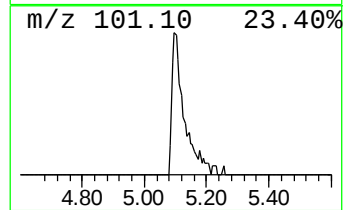
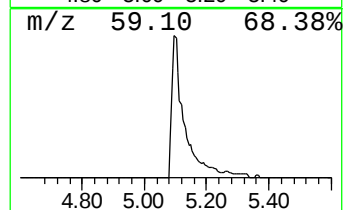
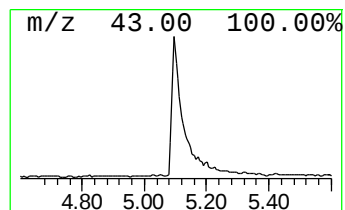
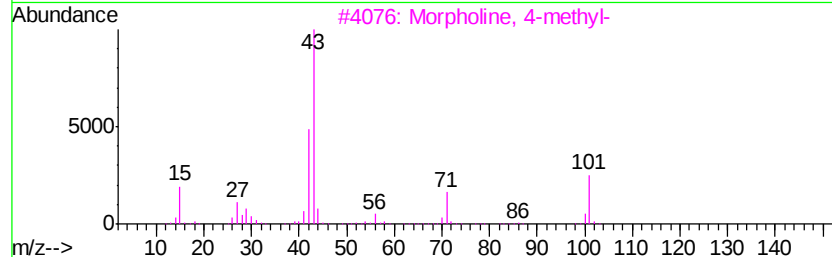
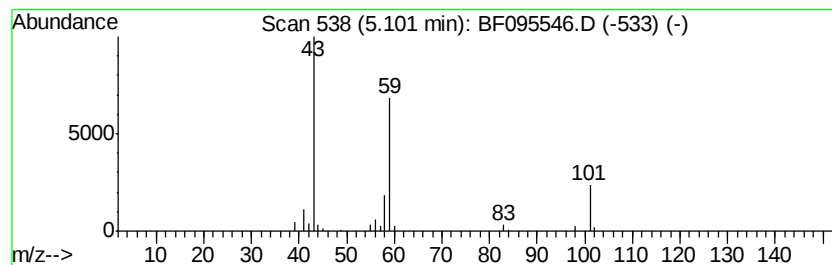
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	6.10 ng	155466	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	45
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-6-18

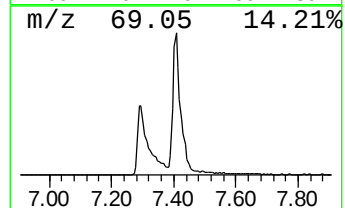
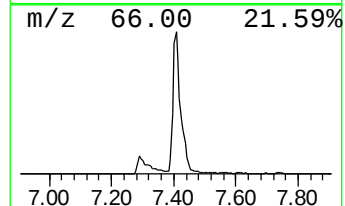
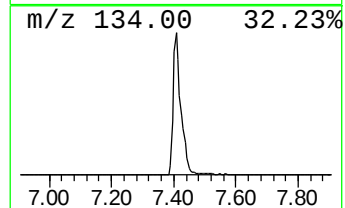
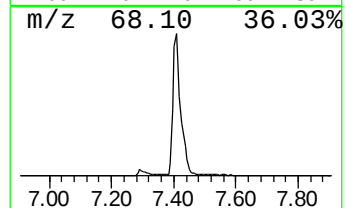
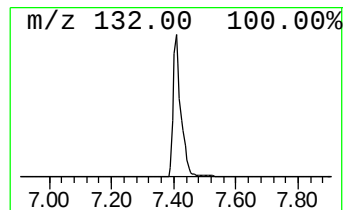
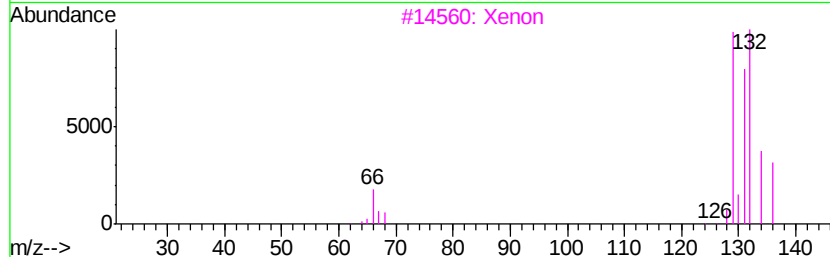
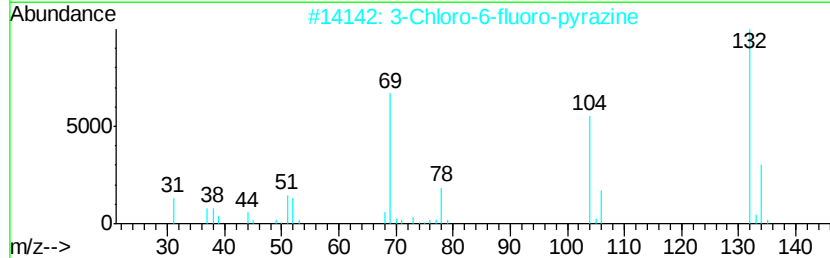
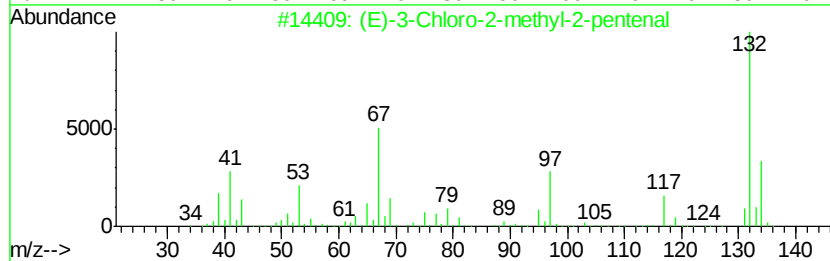
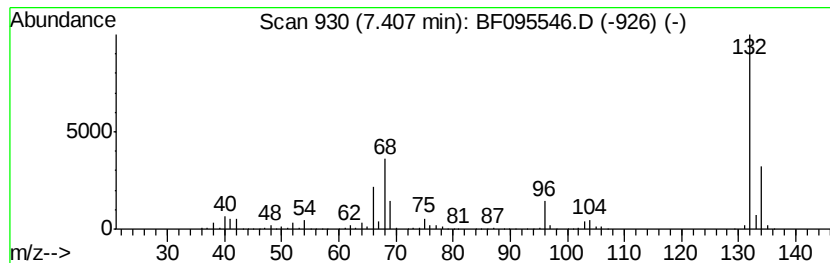
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	86.69 ng	2209050	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		Xenon	132	Xe	007440-63-3	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

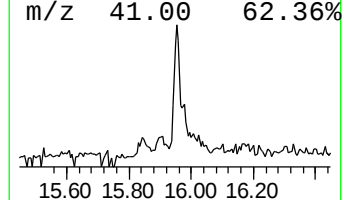
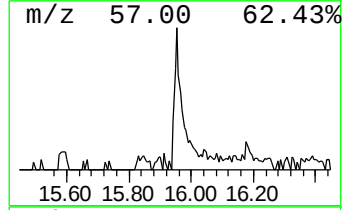
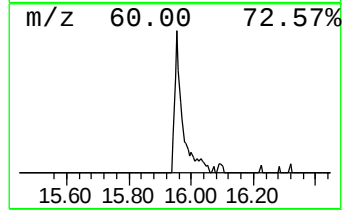
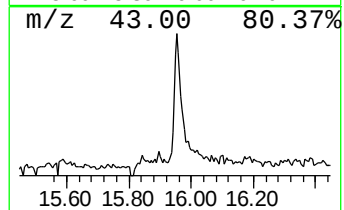
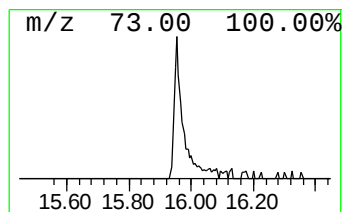
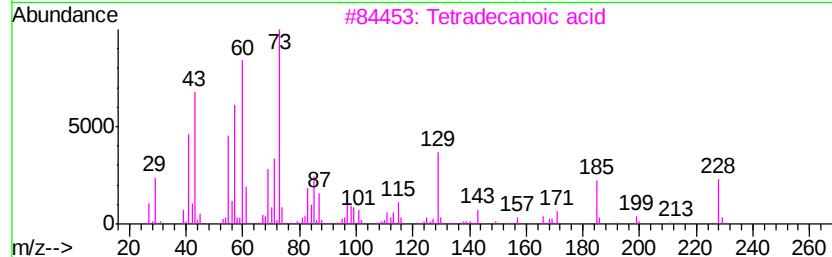
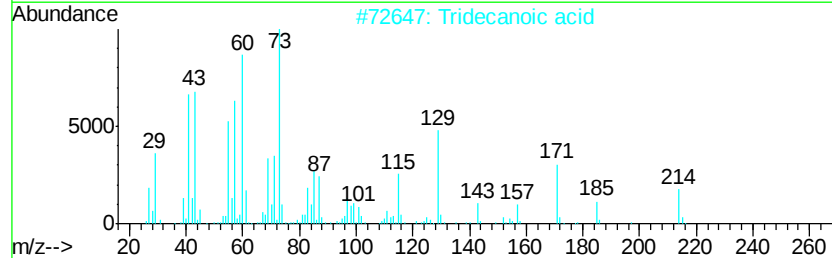
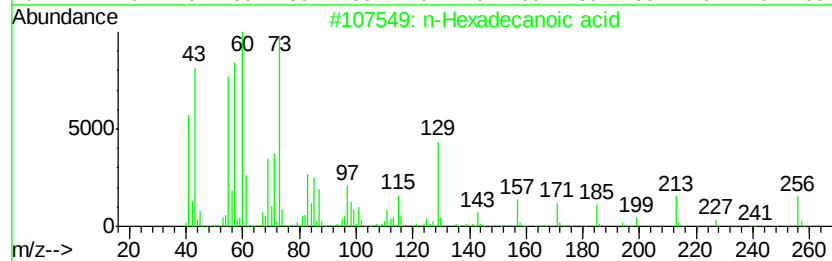
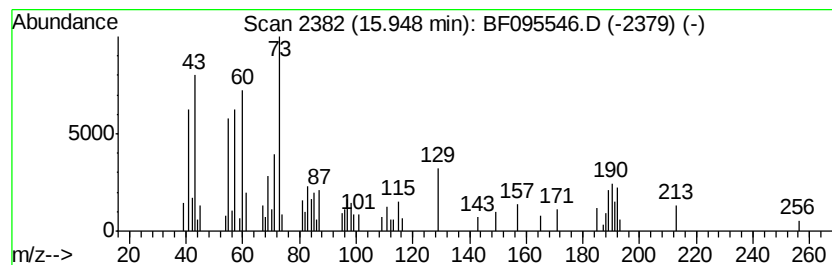
Instrument :
BNA_F
ClientSampleId :
NM16-COMP-6-18

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 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.95	5.10 ng	146389	Phenanthrene-d10		15.00	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	72
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5		.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

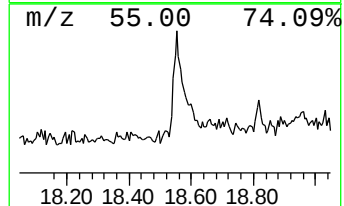
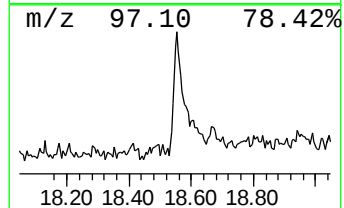
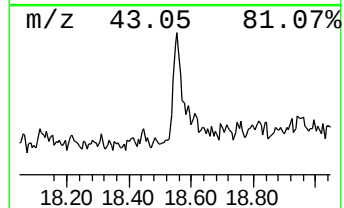
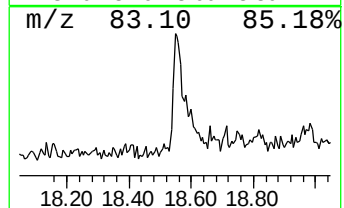
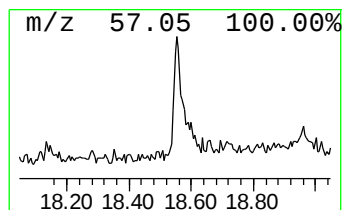
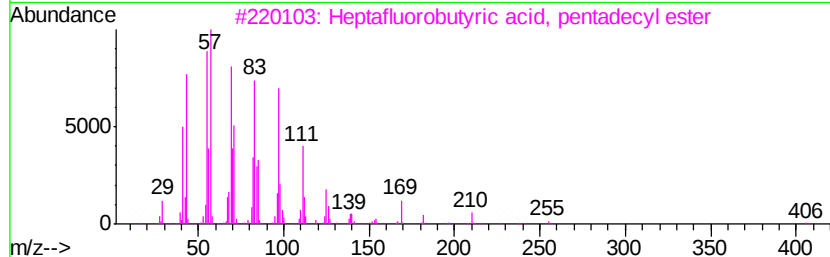
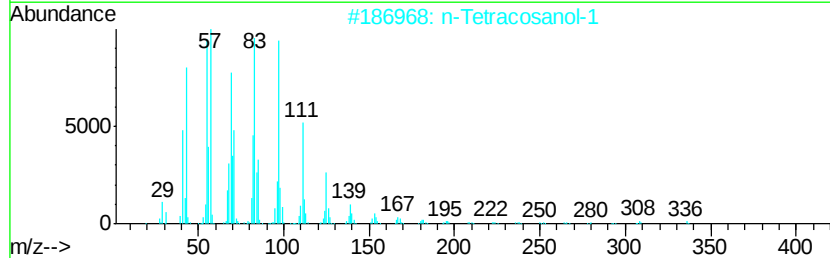
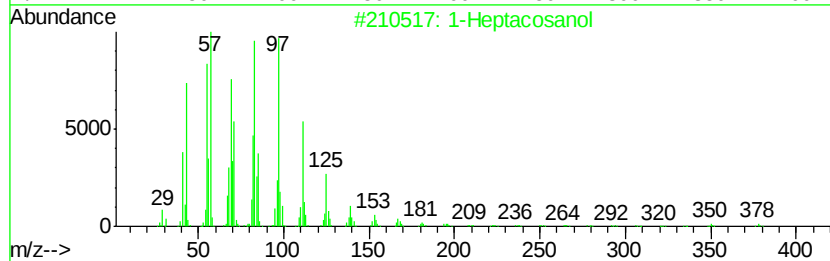
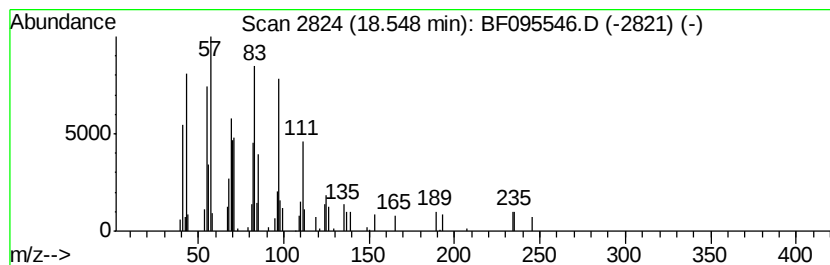
Instrument :
BNA_F
ClientSampleId :
NM16-COMP-6-18

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 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.55	2.68 ng	95490	Chrysene-d12		18.67
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-6-18

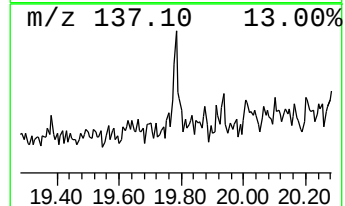
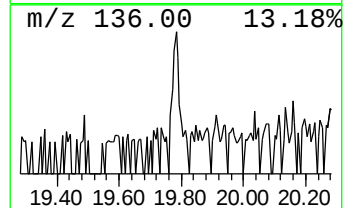
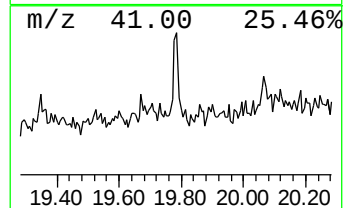
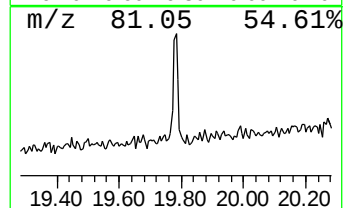
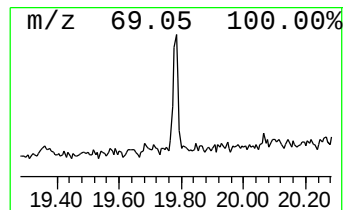
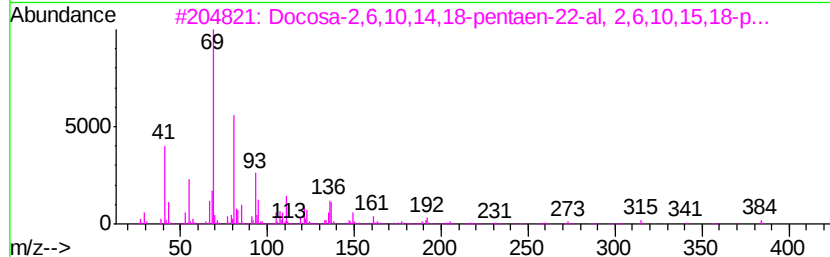
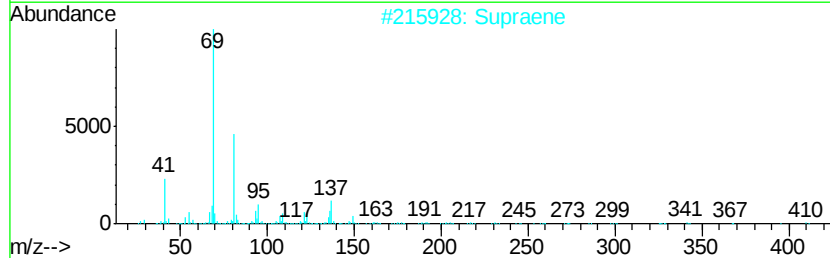
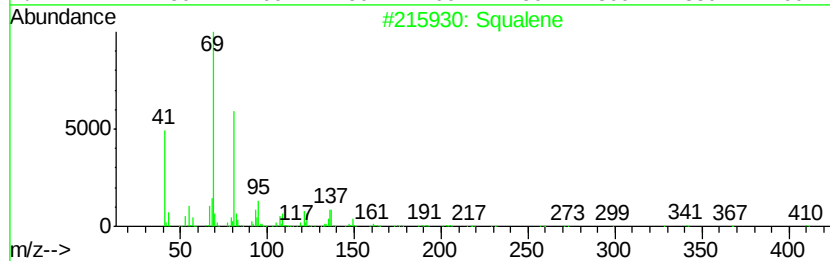
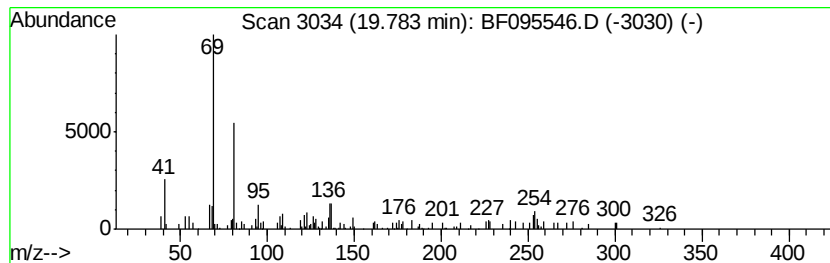
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	4.49 ng	94223	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	68
2		Supraene	410	C30H50	007683-64-9	64
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	53
5		trans-Farnesol	222	C15H26O	000106-28-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

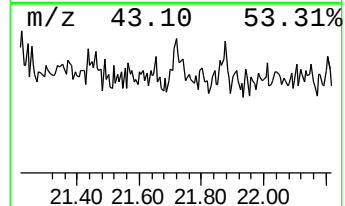
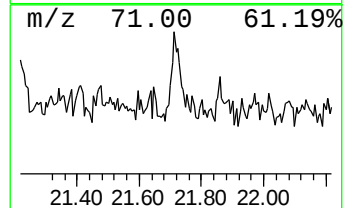
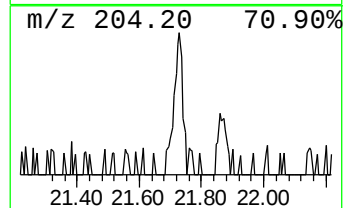
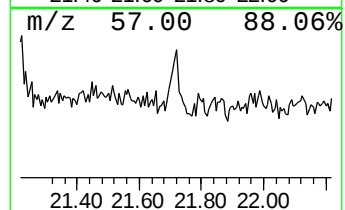
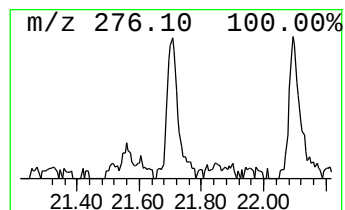
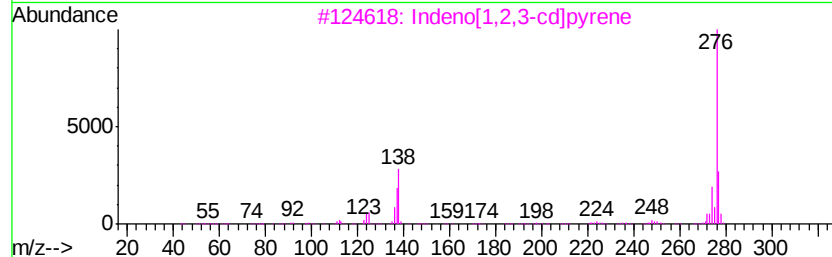
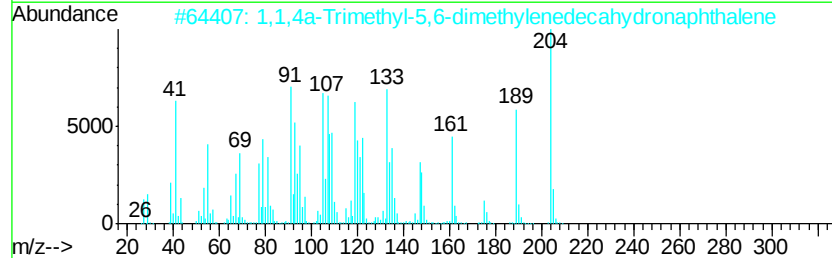
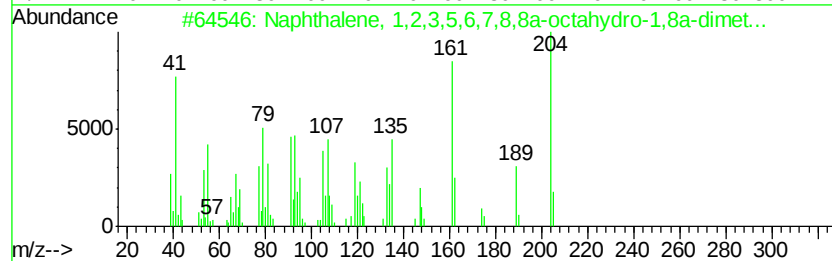
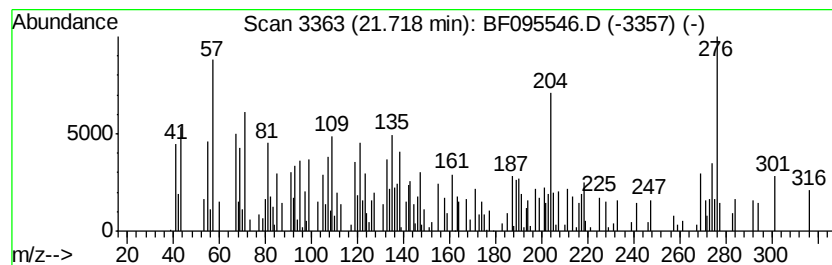
Instrument :
BNA_F
ClientSampleID :
NM16-COMP-6-18

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 unknown21.72 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	5.21 ng	109312	Perylene-d12	20.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204 C15H24	004630-07-3 22
2		1,1,4a-Trimethyl-5,6-dimethylene...	204 C15H24	1000193-60-8 22
3		Indeno[1,2,3-cd]pyrene	276 C22H12	000193-39-5 22
4		Naphthalene, decahydro-4a-methyl...	204 C15H24	017066-67-0 15
5		Naphthalen-1-yl-(3-nitro-benzyl)...	276 C17H12N2O2	200421-53-0 15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095546.D
Acq On : 30 May 2017 20:57
Operator : SJ/MA
Sample : I3302-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-6-18

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	6.1 ng		155466	1	7.74	509651	20.0
unknown7.41	7.41	86.7 ng		2209050	1	7.74	509651	20.0
n-Hexadecanoic acid	15.95	5.1 ng		146389	4	15.00	574235	20.0
1-Heptacosanol	18.55	2.7 ng		95490	5	18.67	712358	20.0
Squalene	19.78	4.5 ng		94223	6	20.35	419782	20.0
unknown21.72	21.72	5.2 ng		109312	6	20.35	419782	20.0