

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051717\
 Data File : BF095214.D
 Acq On : 18 May 2017 8:39
 Operator : SJ/MA
 Sample : I3192-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 051617-02

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.119	538	541	559	rBV	142765	325725	15.71%	1.988%
2	5.743	643	647	684	rBV	779405	1804915	87.04%	11.017%
3	7.313	910	914	930	rBV	972897	1784504	86.06%	10.893%
4	7.437	930	935	952	rVB	1378420	2073595	100.00%	12.657%
5	7.772	988	992	1002	rBV	403282	477034	23.01%	2.912%
6	8.007	1027	1032	1044	rBV	1207350	1450459	69.95%	8.854%
7	8.666	1140	1144	1161	rBV	653463	1041172	50.21%	6.355%
8	9.789	1330	1335	1356	rBV	407057	620142	29.91%	3.785%
9	10.848	1510	1515	1521	rVB	71160	84547	4.08%	0.516%
10	11.560	1631	1636	1661	rBV	1290012	1907489	91.99%	11.643%
11	12.254	1750	1754	1765	rBV	237116	396311	19.11%	2.419%
12	12.342	1765	1769	1775	rVB	161322	200974	9.69%	1.227%
13	12.619	1812	1816	1834	rBV2	397285	608250	29.33%	3.713%
14	13.454	1955	1958	1962	rBV	20290	21123	1.02%	0.129%
15	13.919	2033	2037	2053	rBV	464104	817947	39.45%	4.993%
16	14.224	2085	2089	2092	rBV	22584	27693	1.34%	0.169%
17	14.960	2208	2214	2218	rBV	18335	22375	1.08%	0.137%
18	15.024	2218	2225	2237	rBV	311444	474433	22.88%	2.896%
19	17.342	2614	2619	2635	rBV	1098025	1358823	65.53%	8.294%
20	18.695	2845	2849	2862	rVB	334672	479330	23.12%	2.926%
21	19.812	3035	3039	3043	rBV	40672	42107	2.03%	0.257%
22	20.371	3130	3134	3145	rBV	243548	363532	17.53%	2.219%

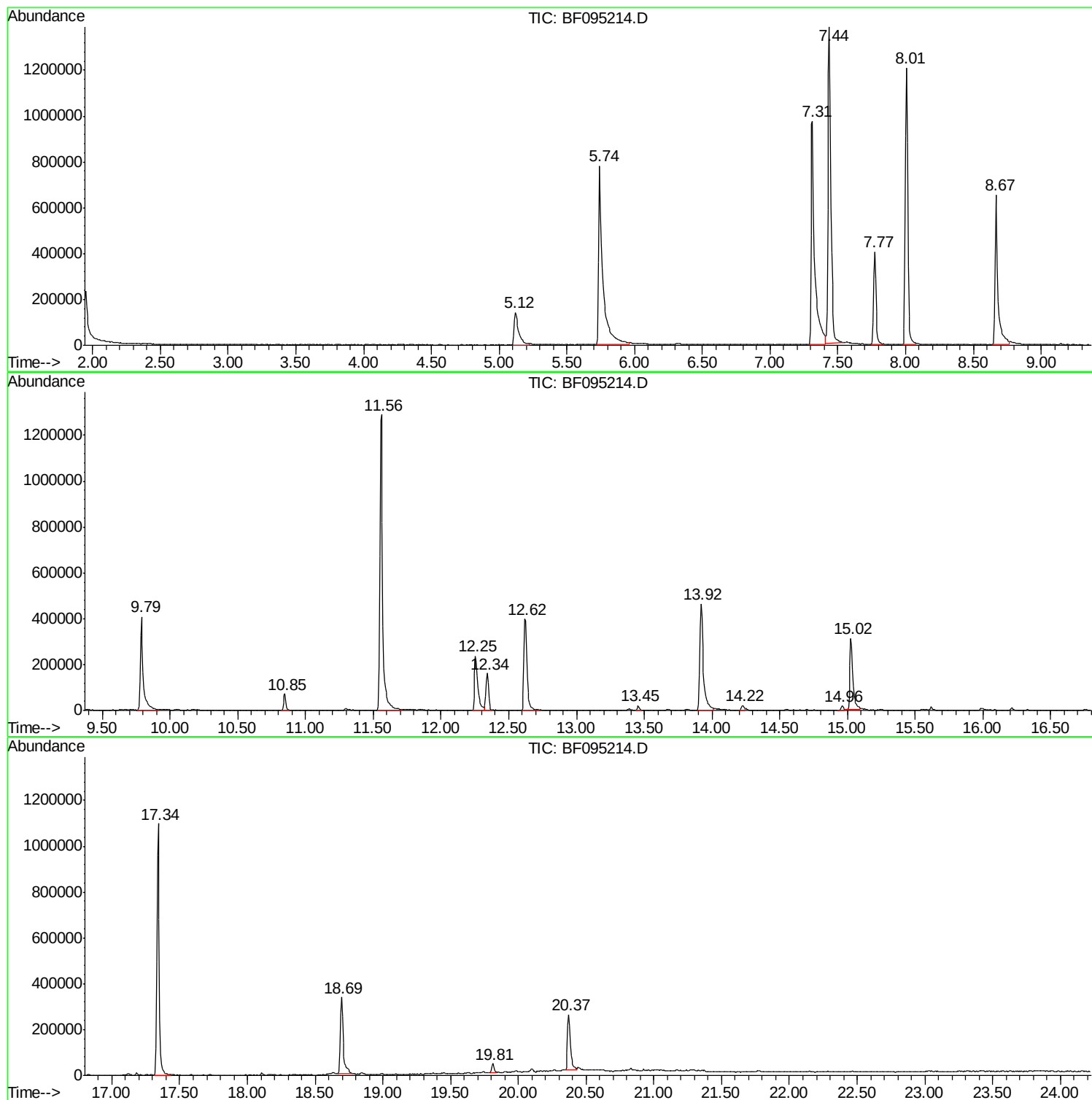
Sum of corrected areas: 16382480

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051717\
Data File : BF095214.D
Acq On : 18 May 2017 8:39
Operator : SJ/MA
Sample : I3192-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
051617-02

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\BF051717\
Data File : BF095214.D
Acq On : 18 May 2017 8:39
Operator : SJ/MA
Sample : I3192-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
051617-02

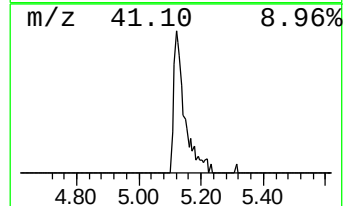
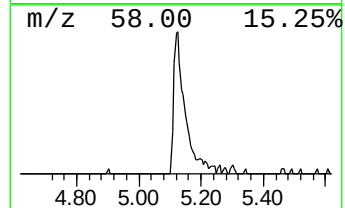
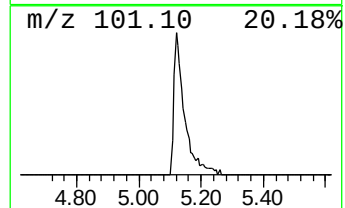
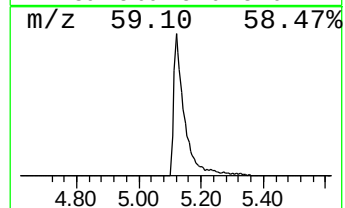
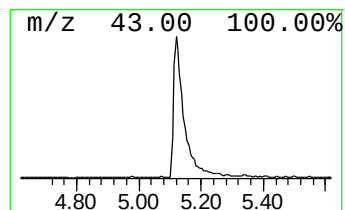
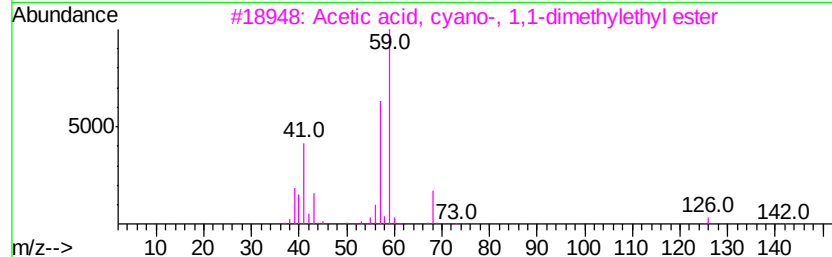
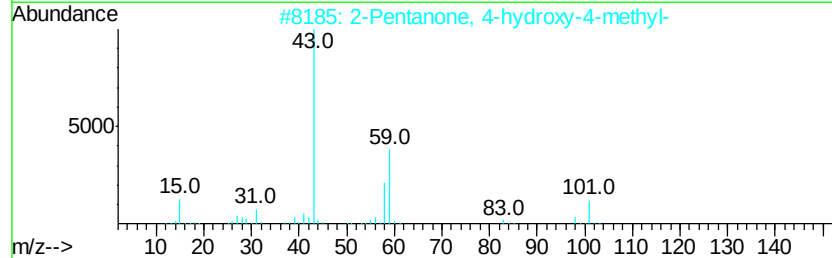
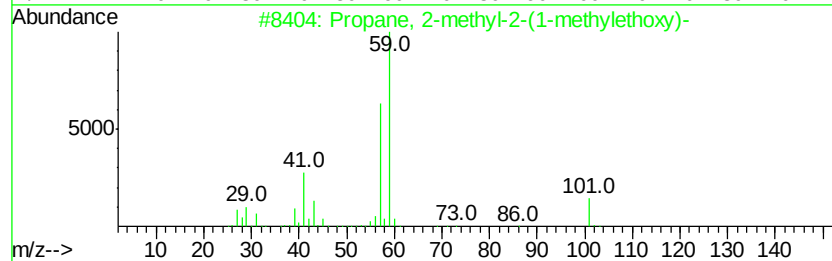
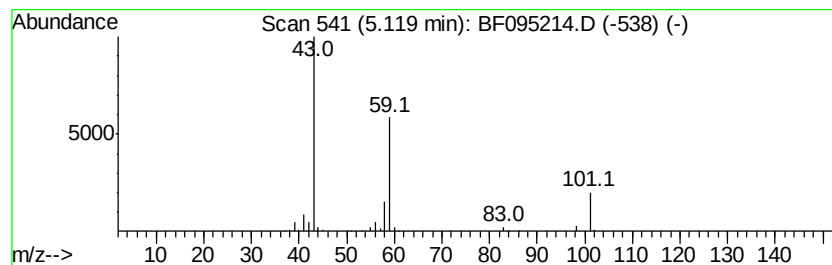
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	13.66 ng	325725	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051717\
Data File : BF095214.D
Acq On : 18 May 2017 8:39
Operator : SJ/MA
Sample : I3192-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
051617-02

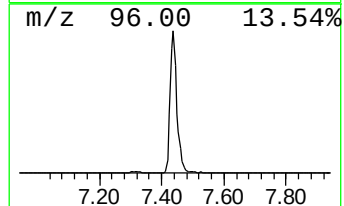
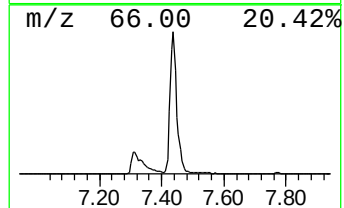
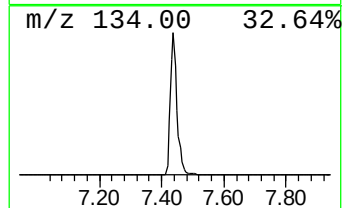
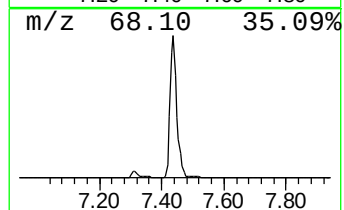
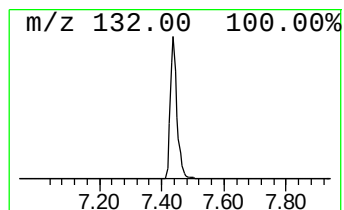
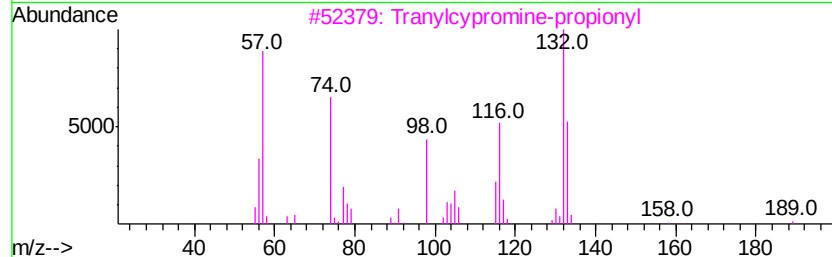
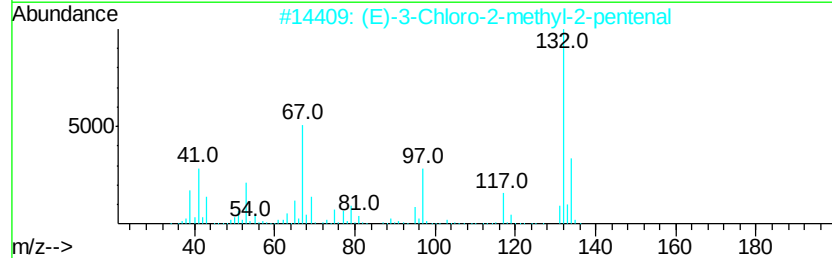
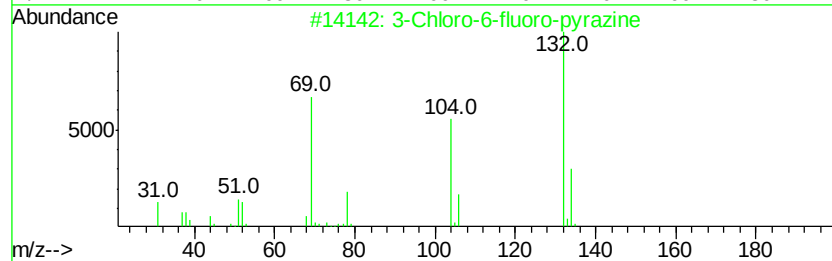
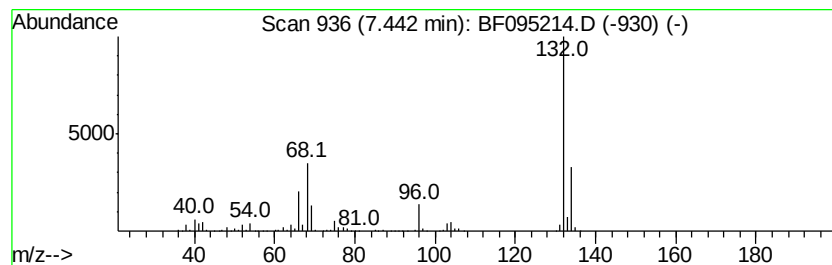
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	86.94 ng	2073600	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051717\
Data File : BF095214.D
Acq On : 18 May 2017 8:39
Operator : SJ/MA
Sample : I3192-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
051617-02

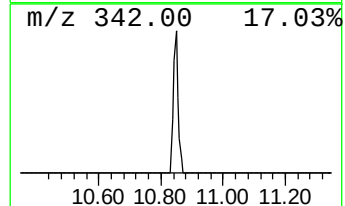
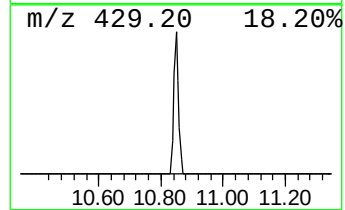
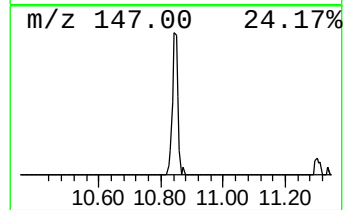
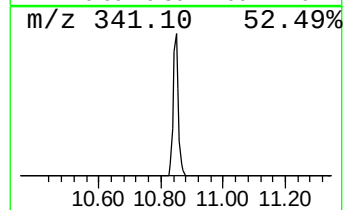
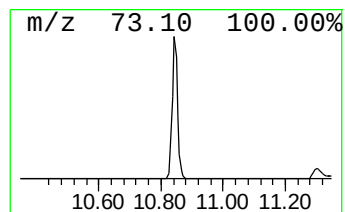
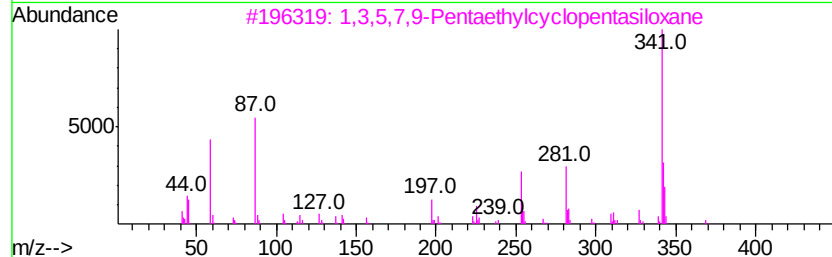
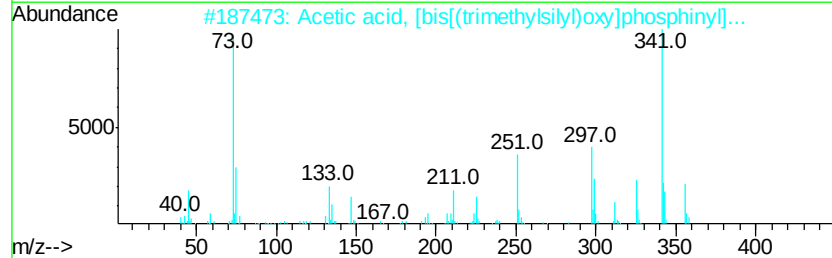
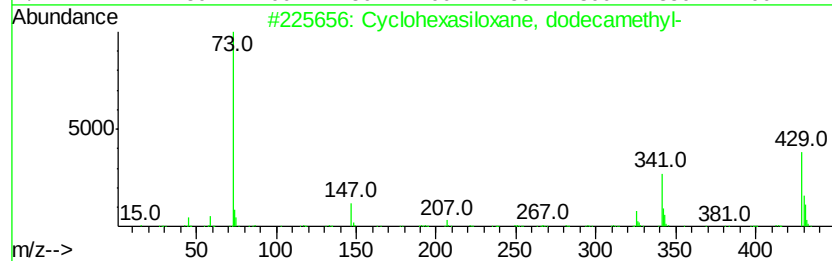
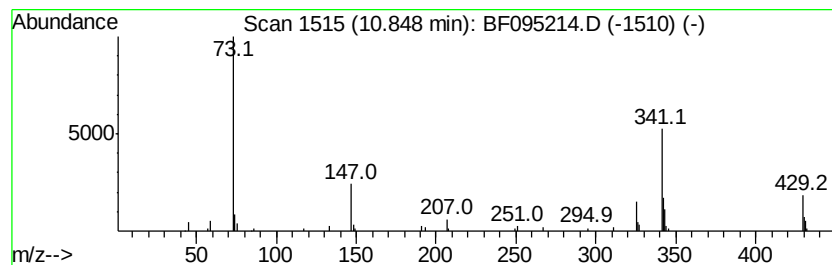
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclohexasiloxane, dodecane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	2.73 ng	84547	Naphthalene-d8	9.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	91
2		Acetic acid, [bis[(trimethylsilyl)oxy]phosphoryl]...	356	C11H29O5PSi3	053044-27-2	40
3		1,3,5,7,9-Pentaethylcyclopentasiloxane	370	C10H30O5Si5	017995-44-7	35
4		Morphinan, 7,8-didehydro-4,5-epo...	429	C23H35N3Si2	055449-66-6	18
5		Silane, trimethyl-[[[(17.alpha.)-...	356	C23H36OSi	056771-62-1	17



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051717\
Data File : BF095214.D
Acq On : 18 May 2017 8:39
Operator : SJ/MA
Sample : I3192-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

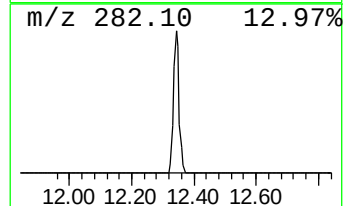
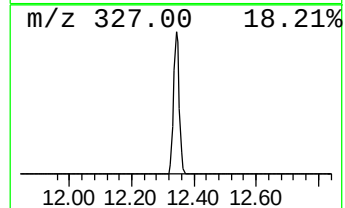
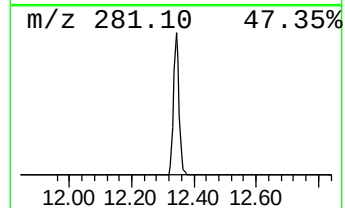
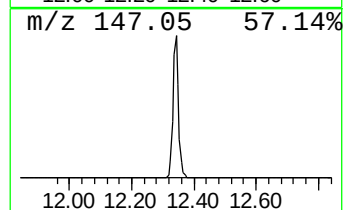
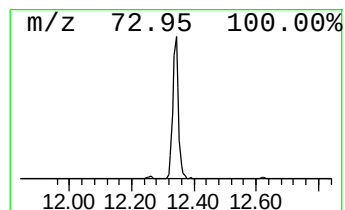
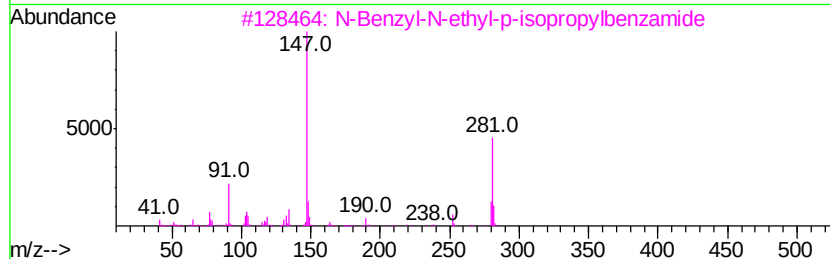
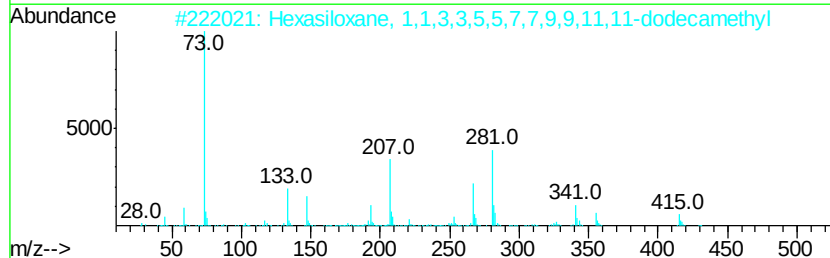
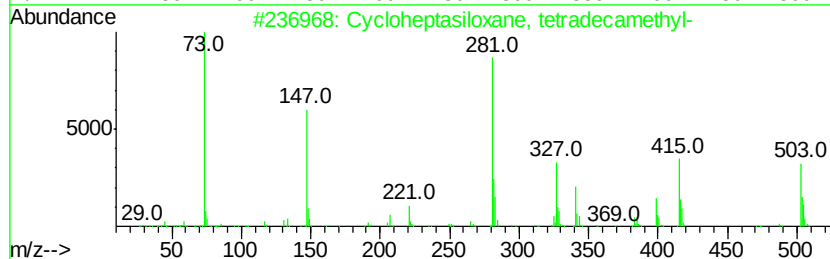
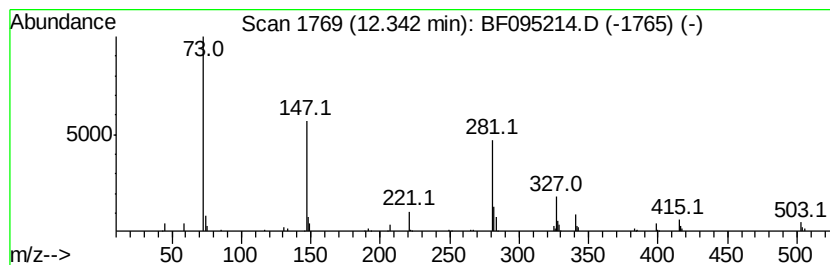
Instrument :
BNA_F
ClientSampleId :
051617-02

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 Cycloheptasiloxane, tetradec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	6.61 ng	200974	Acenaphthene-d10	12.62
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cycloheptasiloxane, tetradecamethyl-	518 C14H42O7Si7	000107-50-6 72
2		Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430 C12H38O5Si6	000995-82-4 50
3		N-Benzyl-N-ethyl-p-isopropylbenz...	281 C19H23NO	015089-22-2 47
4		2-(2',4',4',6',6',8',8'-Heptamet...	652 C16H48O10Si9	145344-72-5 38
5		Trisiloxane, 1,1,1,5,5,5-hexamet...	384 C12H36O4Si5	003555-47-3 37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051717\
Data File : BF095214.D
Acq On : 18 May 2017 8:39
Operator : SJ/MA
Sample : I3192-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

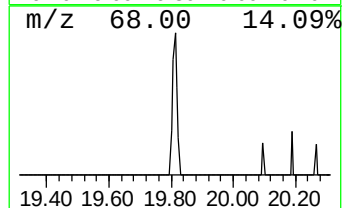
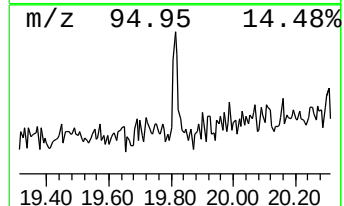
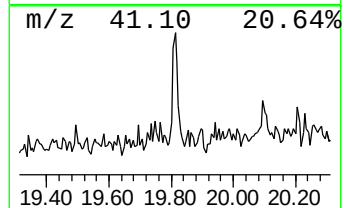
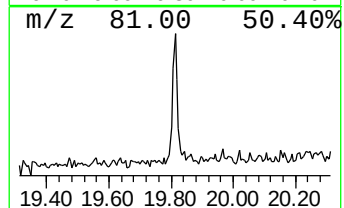
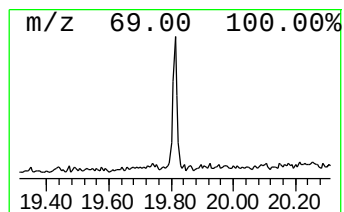
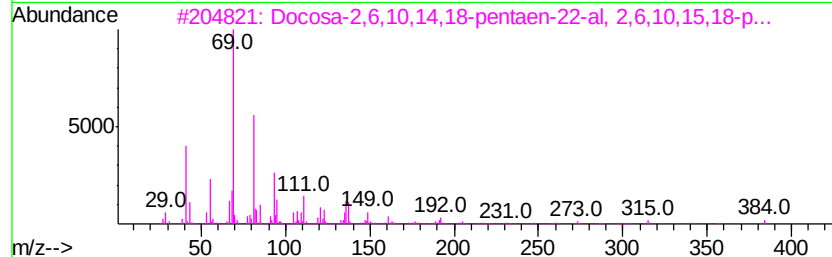
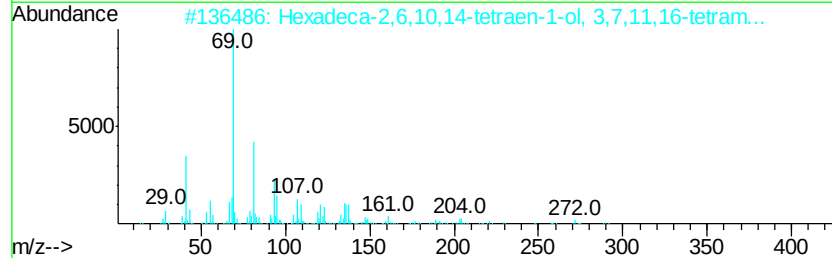
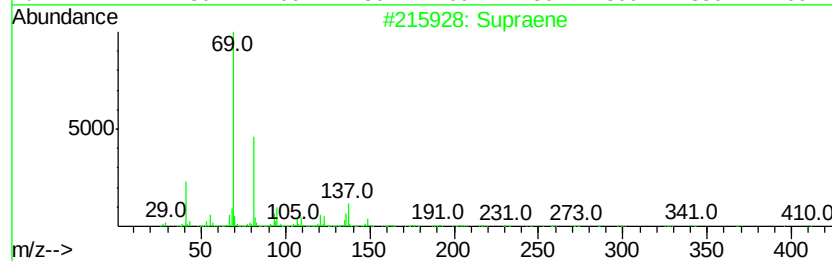
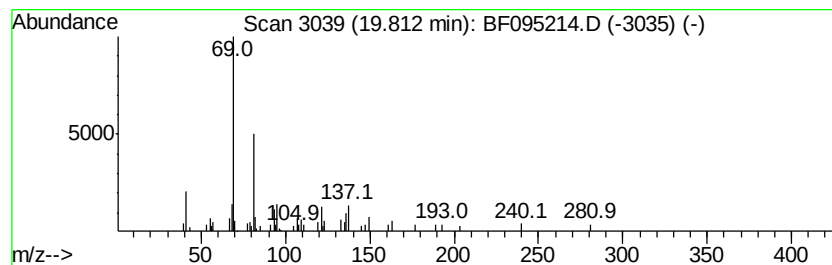
Instrument :
BNA_F
ClientSampleId :
051617-02

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 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.81	2.32 ng	42107	Perylene-d12	20.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	74
2	Hexadeca-2,6,10,14-tetraen-1-ol, ...	290	C20H34O	007614-21-3	72
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4	Squalene	410	C30H50	000111-02-4	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051717\
Data File : BF095214.D
Acq On : 18 May 2017 8:39
Operator : SJ/MA
Sample : I3192-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
051617-02

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
Propane, 2-methyl...	5.12	13.7	ng	325725	1	7.77	477034	20.0
unknown7.44	7.44	86.9	ng	2073600	1	7.77	477034	20.0
Cyclohexasiloxane...	10.85	2.7	ng	84547	2	9.79	620142	20.0
Cycloheptasiloxan...	12.34	6.6	ng	200974	3	12.62	608250	20.0
Supraene	19.81	2.3	ng	42107	6	20.37	363532	20.0