

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
 Data File : BF089811.D
 Acq On : 19 Aug 2016 22:13
 Operator : UM/SJ
 Sample : H4518-02
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-1(0-5)

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-BF081916.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	1.655	5	6	15	rVV	1750819	3412683	10.82%	2.151%
2	1.781	15	17	67	rVB	11191625	31553534	100.00%	19.884%
3	4.821	280	283	288	rBV	2389036	3555458	11.27%	2.241%
4	4.913	288	291	293	rVB	478341	637978	2.02%	0.402%
5	5.267	319	322	324	rBV	9797913	10256581	32.51%	6.463%
6	6.319	411	414	417	rBV	7823949	9436843	29.91%	5.947%
7	6.444	422	425	428	rVV	8509939	10577904	33.52%	6.666%
8	6.684	444	446	448	rBV	4024696	3319924	10.52%	2.092%
9	6.844	457	460	462	rBV	8097535	9075157	28.76%	5.719%
10	7.245	492	495	498	rBV	5287116	6126731	19.42%	3.861%
11	7.965	556	558	561	rBV	4496044	3983140	12.62%	2.510%
12	9.050	650	653	655	rBV	12381852	12292812	38.96%	7.747%
13	9.439	685	687	690	rBV	2264911	2250762	7.13%	1.418%
14	9.713	709	711	713	rBV	5170989	4348932	13.78%	2.741%
15	10.502	777	780	782	rBV2	4545348	5701859	18.07%	3.593%
16	10.639	790	792	796	rVB	300326	351940	1.12%	0.222%
17	11.188	838	840	844	rBV2	4081392	4165976	13.20%	2.625%
18	11.748	887	889	892	rVV2	961118	1640737	5.20%	1.034%
19	11.794	892	893	897	rVB	173120	328129	1.04%	0.207%
20	12.388	943	945	948	rBV	719716	883821	2.80%	0.557%
21	12.445	948	950	955	rVV3	175670	331117	1.05%	0.209%
22	12.525	955	957	962	rBV	1508828	1850172	5.86%	1.166%
23	12.616	962	965	967	rVB	1045216	1040271	3.30%	0.656%
24	12.777	977	979	982	rVV	7797088	7464752	23.66%	4.704%
25	12.891	986	989	990	rVV	959681	1107246	3.51%	0.698%
26	13.268	1019	1022	1024	rBV	3221058	3945858	12.51%	2.487%
27	13.714	1059	1061	1066	rBV2	280875	478806	1.52%	0.302%
28	13.839	1068	1072	1075	rBV3	3173356	6851571	21.71%	4.318%
29	14.388	1116	1120	1123	rBV4	282797	628329	1.99%	0.396%
30	14.457	1123	1126	1130	rBV	535598	1548707	4.91%	0.976%
31	14.880	1161	1163	1168	rVB	508272	1088253	3.45%	0.686%
32	15.142	1184	1186	1189	rVB	325002	411496	1.30%	0.259%
33	15.188	1189	1190	1192	rVV	382408	489376	1.55%	0.308%
34	15.257	1193	1196	1201	rVB	2559805	3592247	11.38%	2.264%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

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-BF081916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.394	1206	1208	1211	rBV2	240802	378732	1.20%	0.239%
36	15.897	1250	1252	1261	rVB	517669	1137297	3.60%	0.717%
37	16.274	1283	1285	1291	rVB	551318	1060091	3.36%	0.668%
38	16.525	1305	1307	1312	rVB2	255931	497198	1.58%	0.313%
39	16.788	1327	1330	1333	rVB	236721	457221	1.45%	0.288%
40	16.903	1338	1340	1346	rVB	214168	425857	1.35%	0.268%

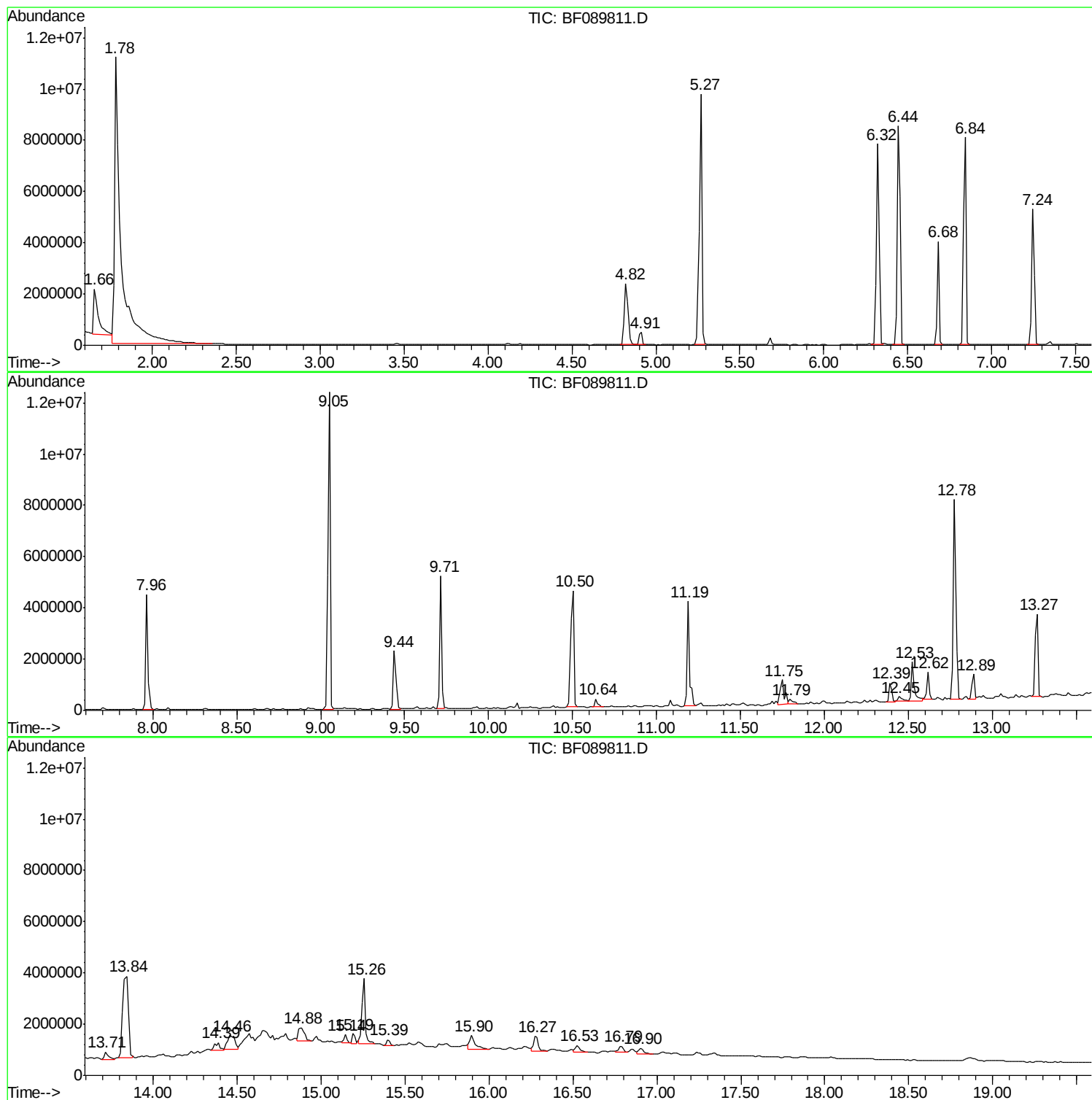
Sum of corrected areas: 158685498

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
A-1(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.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\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

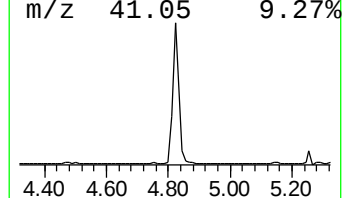
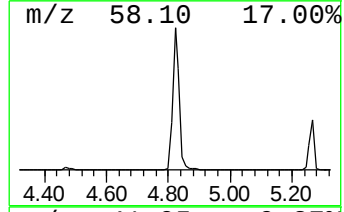
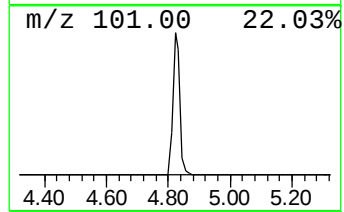
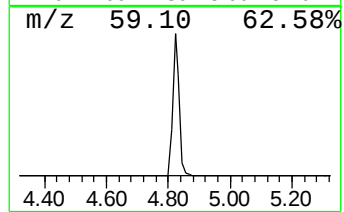
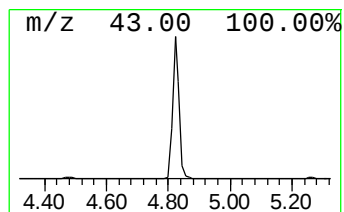
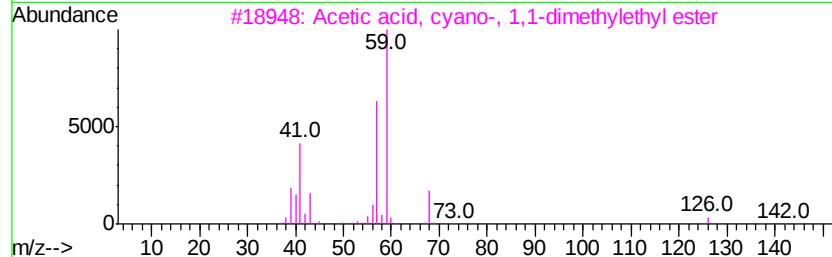
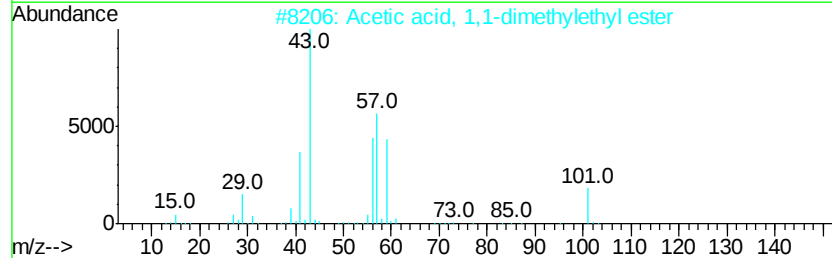
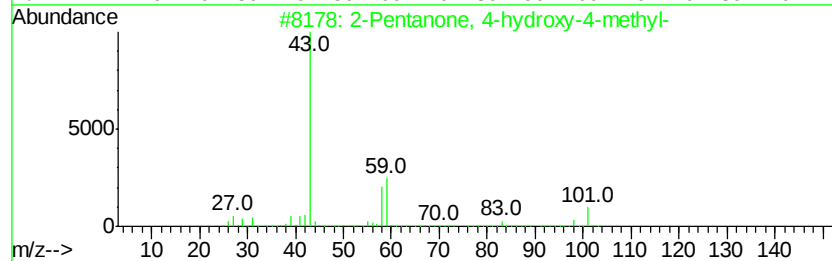
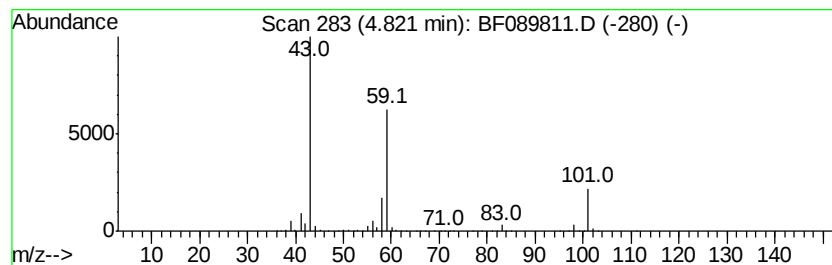
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	21.42 ng	3555460	1,4-Dichlorobenzene-d4	6.68

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

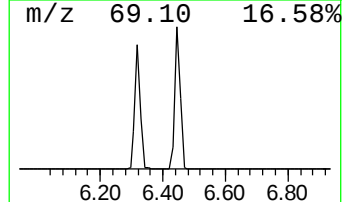
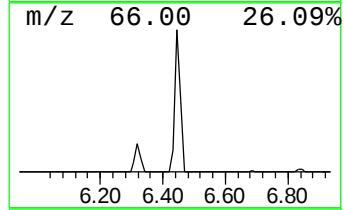
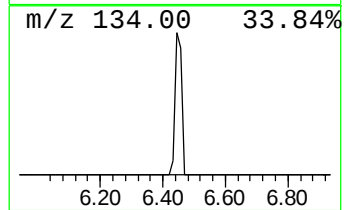
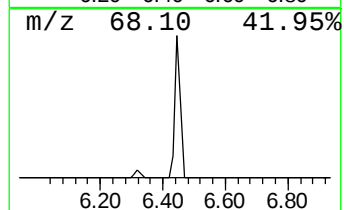
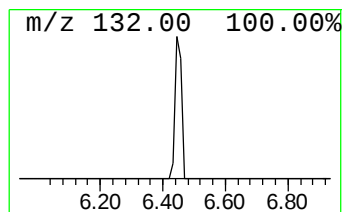
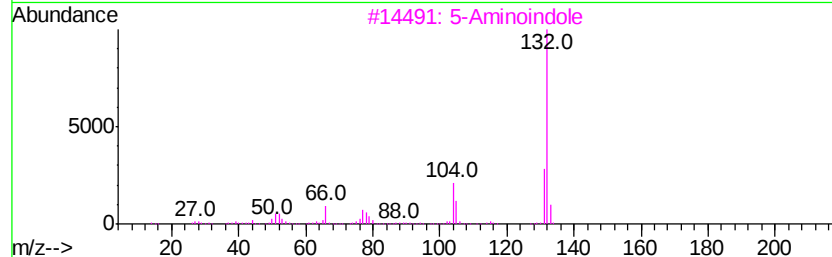
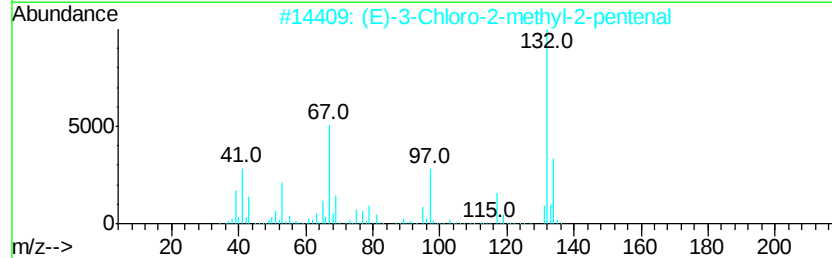
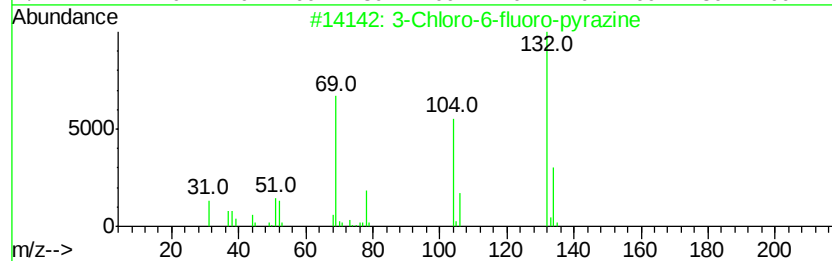
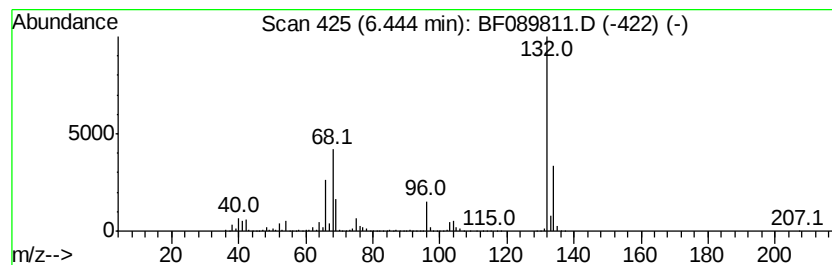
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	63.72 ng	10577900	1,4-Dichlorobenzene-d4	6.68

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

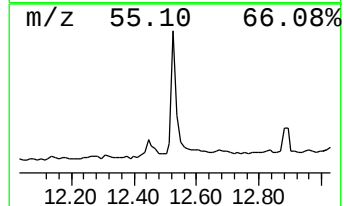
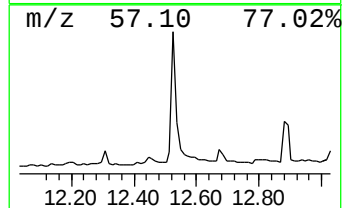
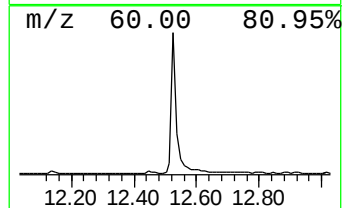
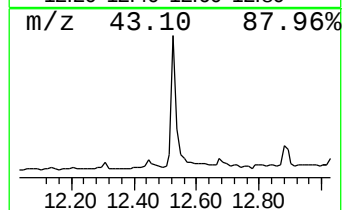
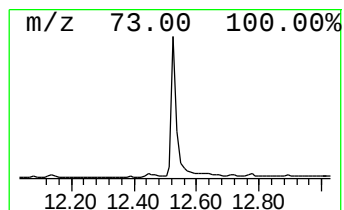
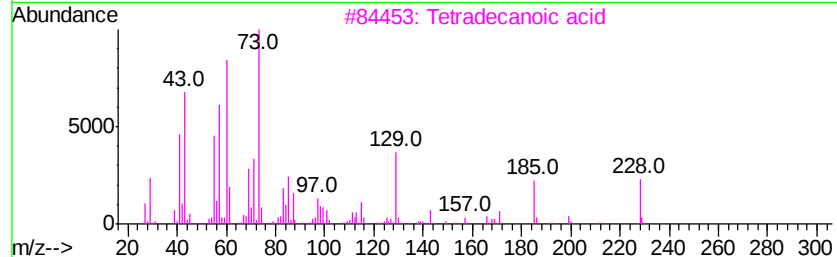
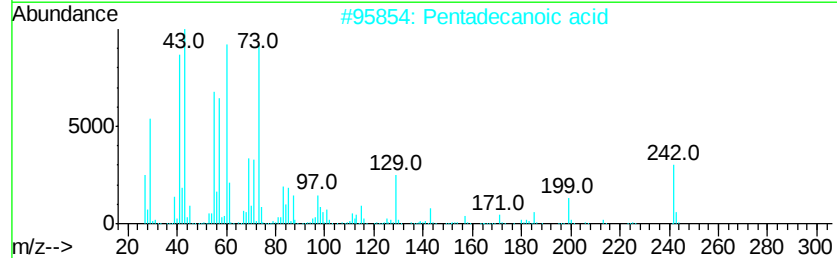
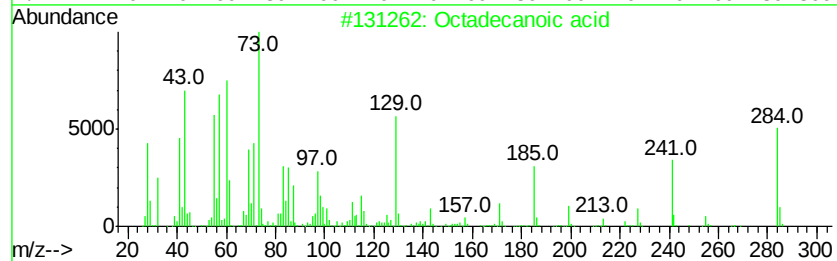
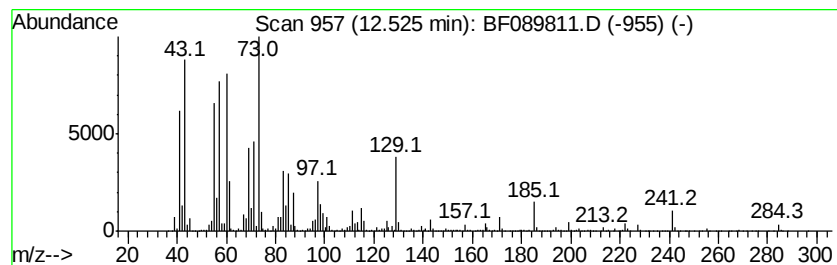
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	5.40 ng	1850170	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
5		Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

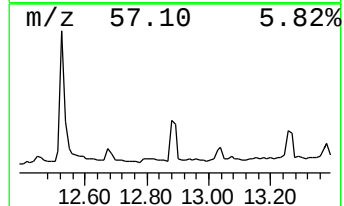
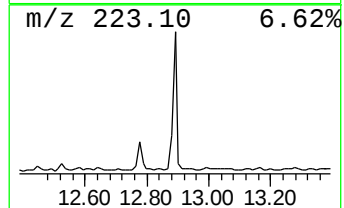
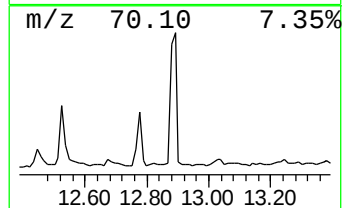
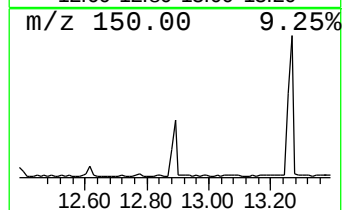
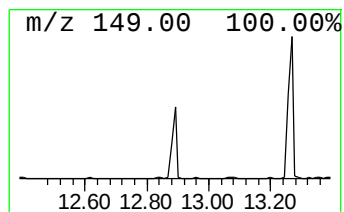
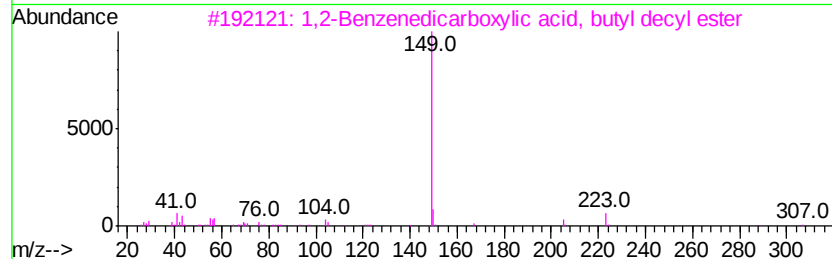
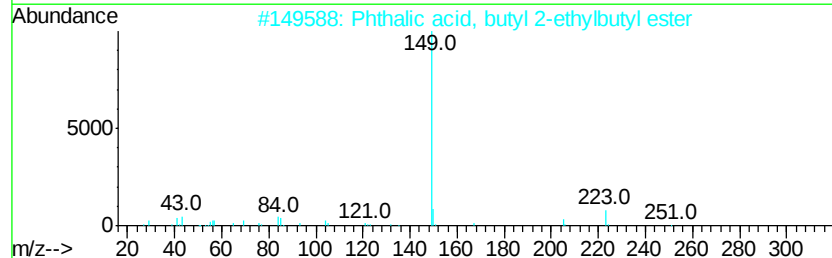
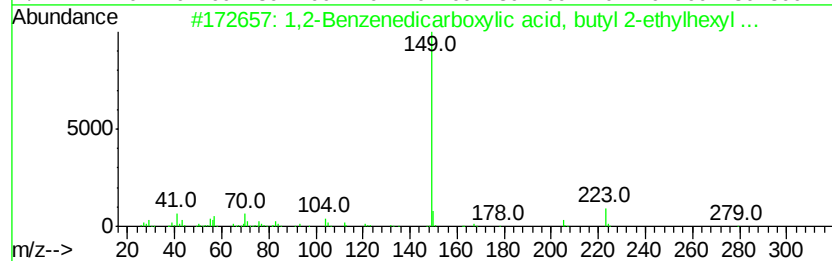
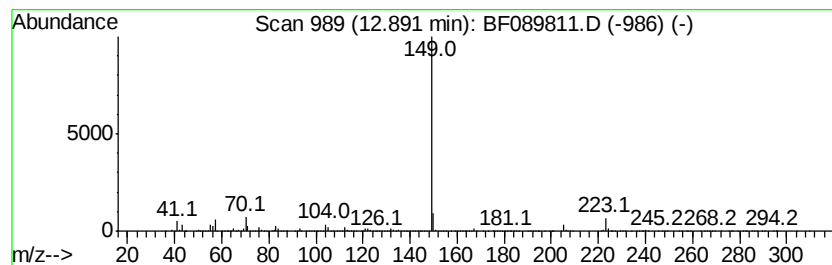
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	3.23 ng	1107250	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	91
2		Phthalic acid, butyl 2-ethylbuty...	306	C18H26O4	1000356-89-0	90
3		1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-19-0	90
4		Phthalic acid, isobutyl 4-methyl...	306	C18H26O4	1000356-87-2	86
5		Phthalic acid, butyl hexyl ester	306	C18H26O4	1000308-99-5	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

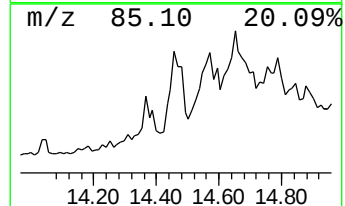
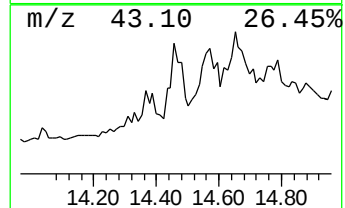
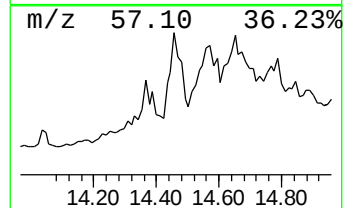
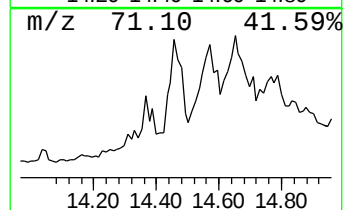
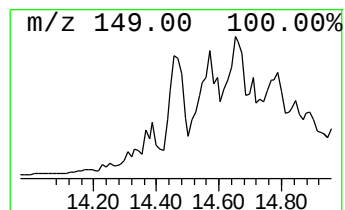
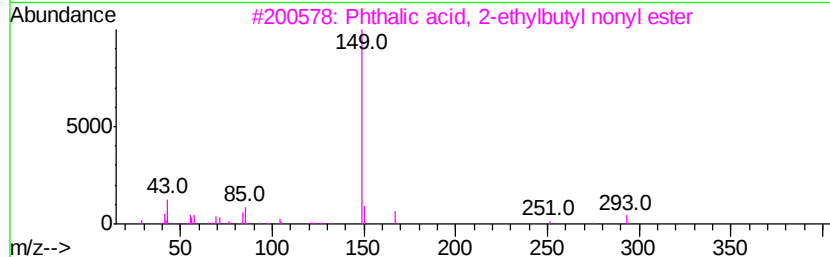
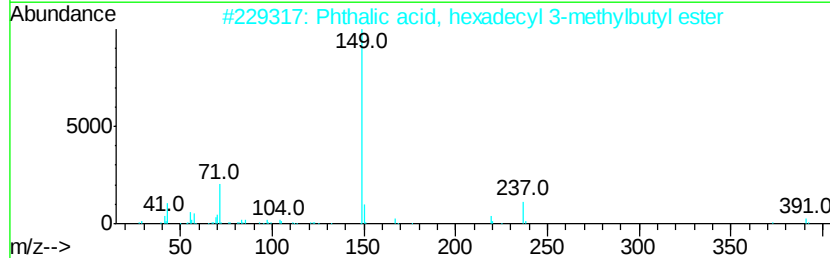
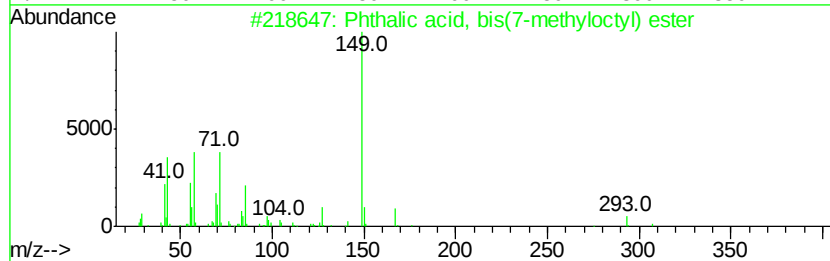
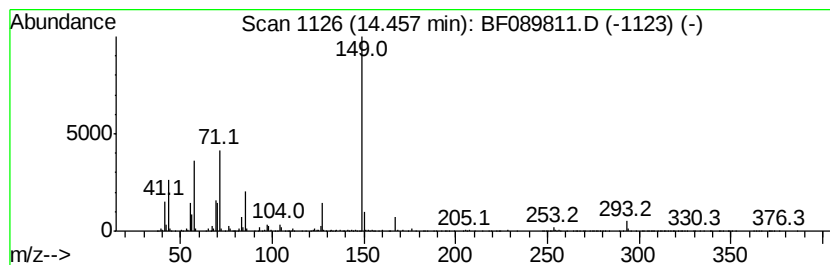
Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phthalic acid, bis(7-methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.46	4.52 ng	1548710	Chrysene-d12	13.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, bis(7-methyloctyl...	418	C26H42O4	020548-62-3	83	
2	Phthalic acid, hexadecyl 3-methy...	460	C29H48O4	1000356-81-7	59	
3	Phthalic acid, 2-ethylbutyl nonv...	376	C23H36O4	1000356-89-4	50	
4	1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	000146-50-9	50	
5	Phthalic acid, 2-ethylhexyl unde...	432	C27H44O4	1000308-97-4	47	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

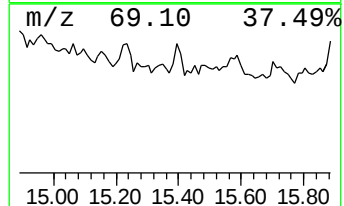
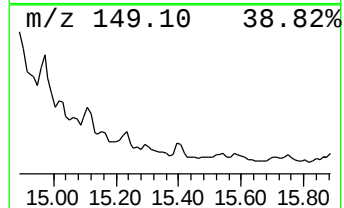
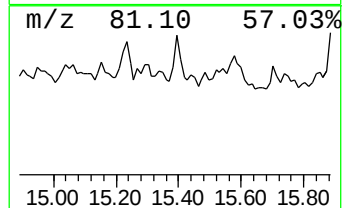
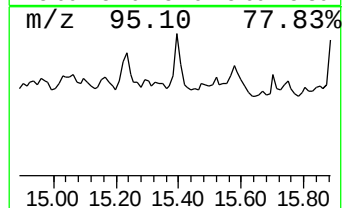
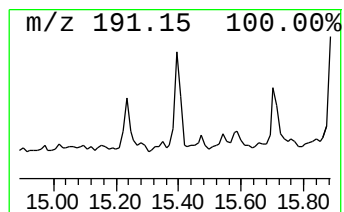
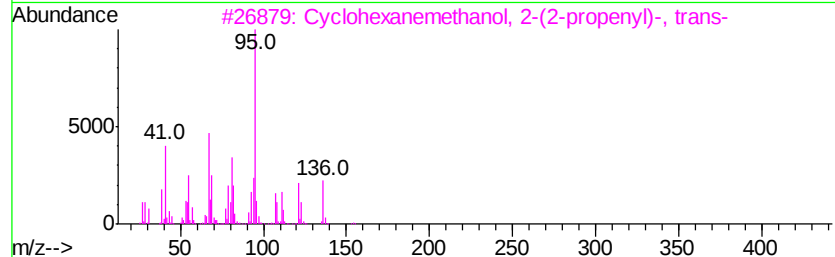
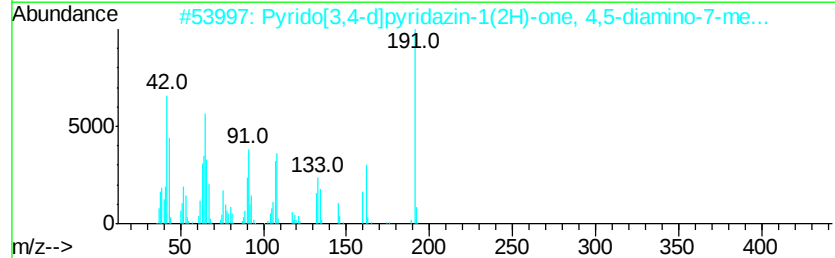
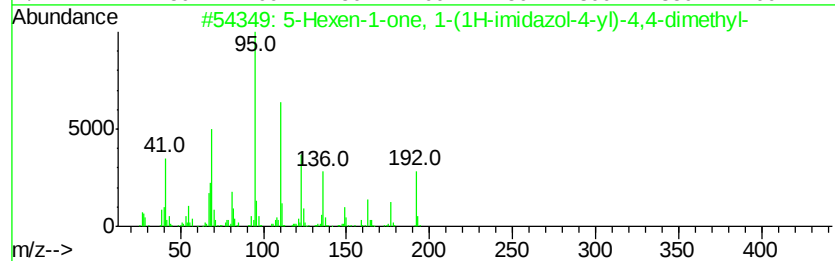
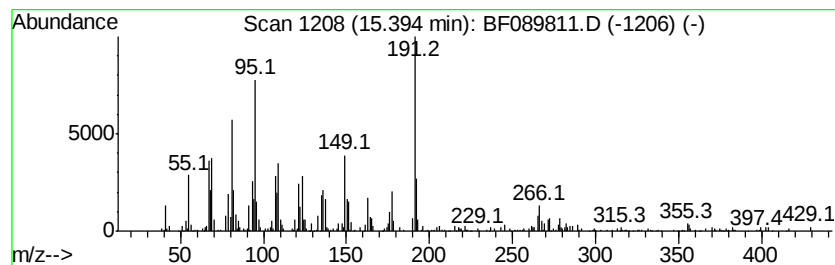
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.39 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	2.11 ng	378732	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	46
2		Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	35
3		Cyclohexanemethanol, 2-(2-propen...	154	C10H18O	134837-38-0	25
4		5-(1-Isopropenyl-4,5-dimethylbic...	332	C22H36O2	1000195-69-8	22
5		Succinic acid, di(2-methylphenyl...	298	C18H18O4	1000325-06-7	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

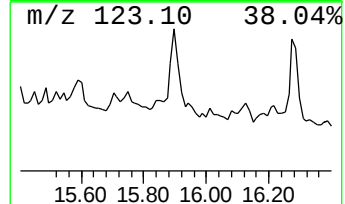
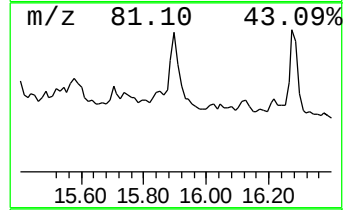
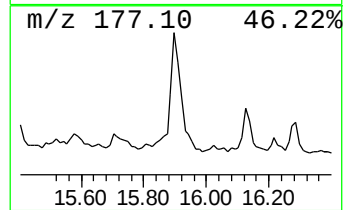
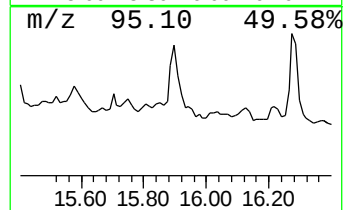
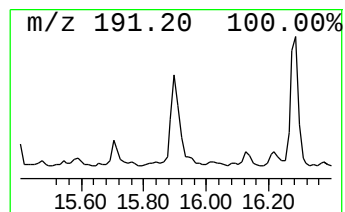
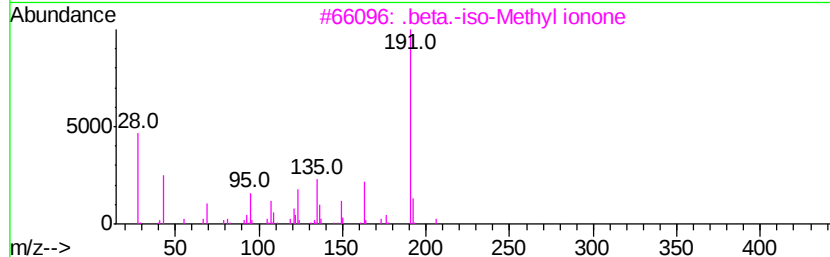
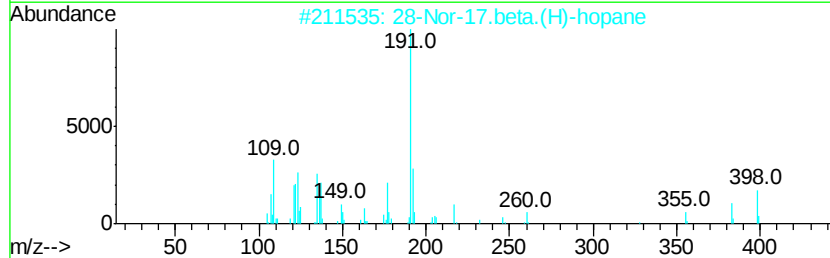
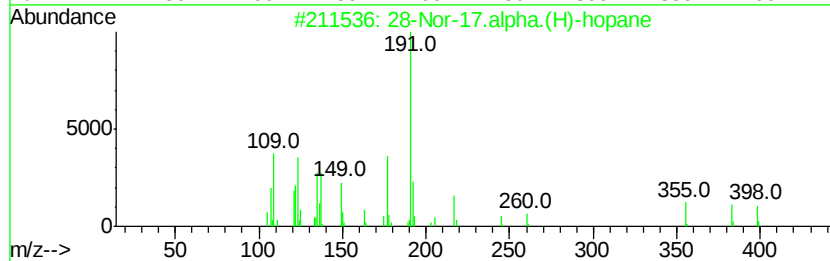
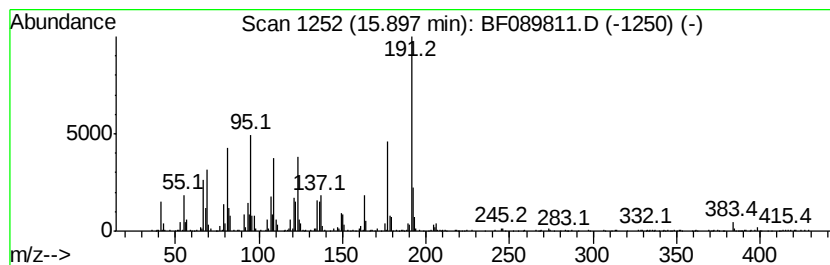
Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 28-Nor-17.alpha.(H)-hopane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.90	6.33 ng	1137300	Perylene-d12	15.26		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane		398	C29H50	053584-60-4	56
2	28-Nor-17.beta.(H)-hopane		398	C29H50	036728-72-0	50
3	.beta.-iso-Methyl ionone		206	C14H22O	1000285-40-2	37
4	4-(3H-Imidazo[4,5-b]pyridin-2-yl...)		342	C15H18N8S	1000276-08-2	35
5	5-(1-Isopropenyl-4,5-dimethylbic...		332	C22H36O2	1000195-69-8	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

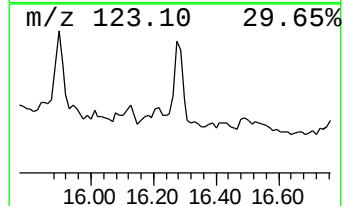
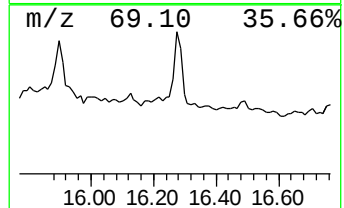
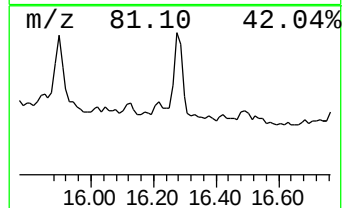
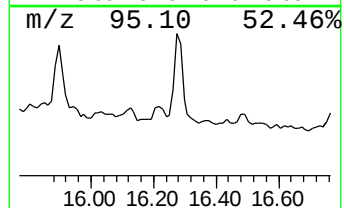
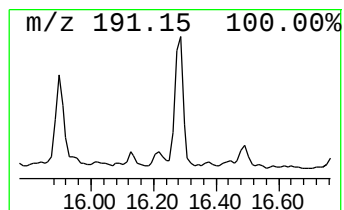
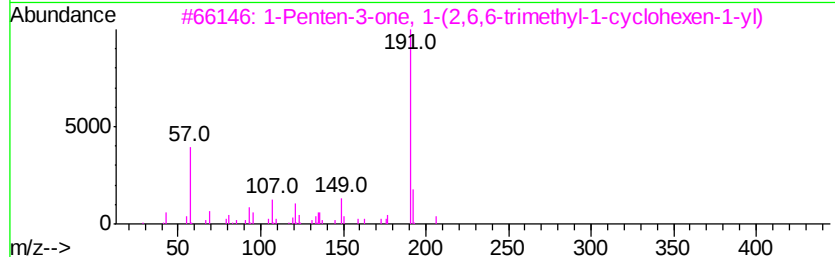
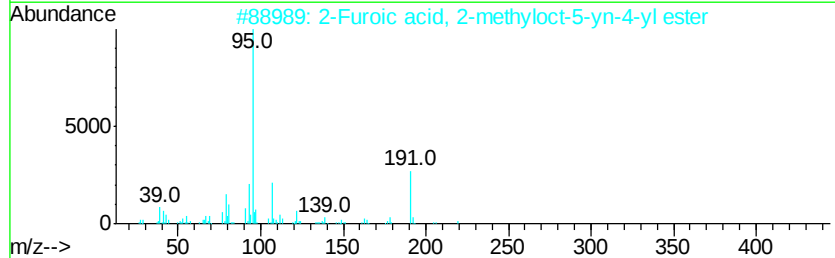
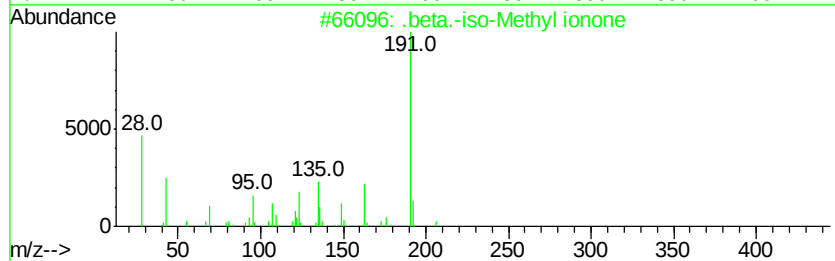
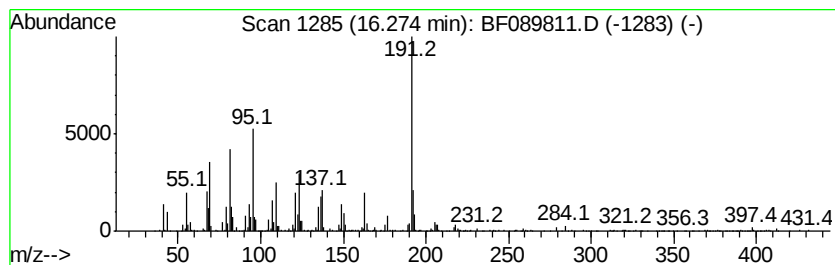
Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.27	5.90 ng	1060090	Perylene-d12	15.26		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	59
2		2-Furoic acid, 2-methyloct-5-yn-...	234	C14H18O3	1000299-23-7	43
3		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
4		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	38
5		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

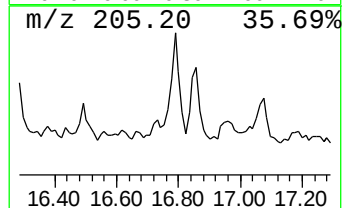
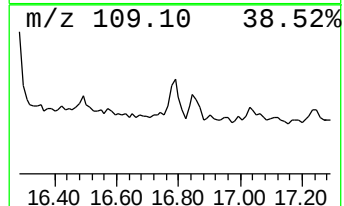
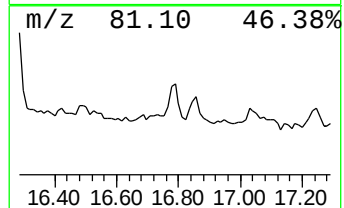
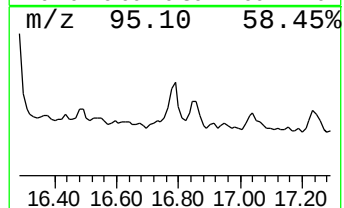
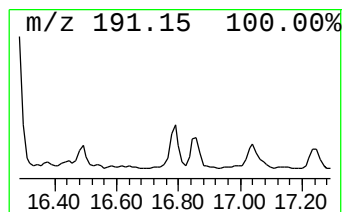
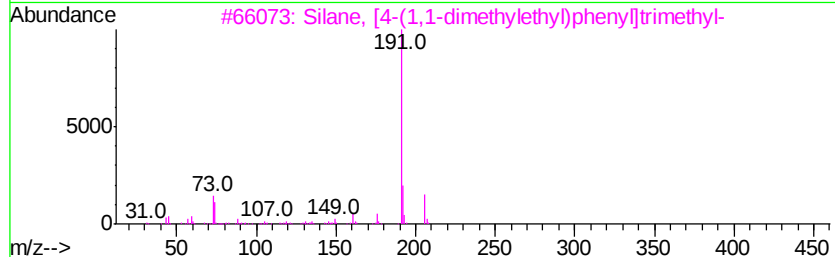
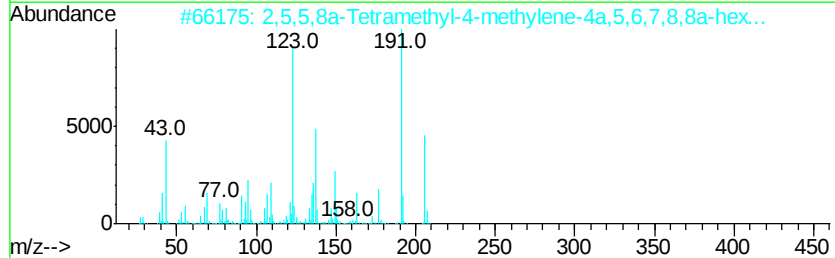
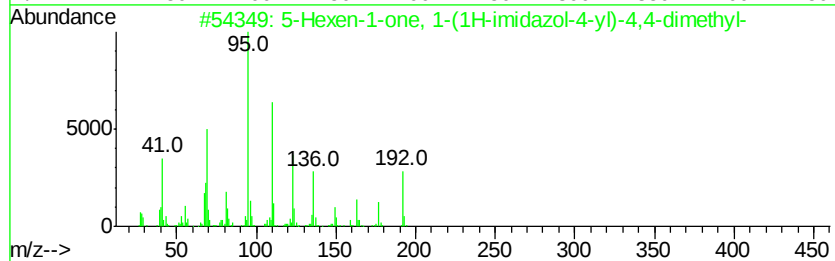
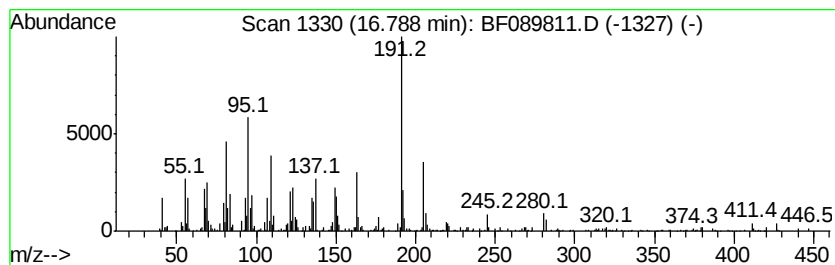
Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 5-Hexen-1-one, 1-(1H-imidaz... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.79	2.55 ng	457221	Perylene-d12	15.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	53
2	2,5,5,8a-Tetramethyl-4-methylene...	206	C14H22O	093175-76-9	38
3	Silane, [4-(1,1-dimethylethyl)ph...	206	C13H22Si	018412-68-5	35
4	2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	35
5	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081916\
Data File : BF089811.D
Acq On : 19 Aug 2016 22:13
Operator : UM/SJ
Sample : H4518-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.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...	4.82	21.4	ng	3555460	1	6.68	3319920	20.0
unknown6.44	6.44	63.7	ng	10577900	1	6.68	3319920	20.0
Octadecanoic acid	12.53	5.4	ng	1850170	5	13.83	6851570	20.0
1,2-Benzenedicarb...	12.89	3.2	ng	1107250	5	13.83	6851570	20.0
Phthalic acid, bi...	14.46	4.5	ng	1548710	5	13.83	6851570	20.0
unknown15.39	15.39	2.1	ng	378732	6	15.26	3592250	20.0
28-Nor-17.alpha.(...	15.90	6.3	ng	1137300	6	15.26	3592250	20.0
.beta.-iso-Methyl...	16.27	5.9	ng	1060090	6	15.26	3592250	20.0
5-Hexen-1-one, 1-...	16.79	2.5	ng	457221	6	15.26	3592250	20.0