

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071917\
 Data File : BF096870.D
 Acq On : 19 Jul 2017 15:19
 Operator : SJ/JU
 Sample : I4199-09
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3569-SPP4

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-BF071317.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	4.746	462	469	476	rBV	99148	128971	4.22%	0.610%
2	5.187	540	544	552	rBV	1189240	1130751	37.01%	5.346%
3	6.234	718	722	729	rBV	701599	688670	22.54%	3.256%
4	6.357	738	743	746	rBV	2239077	2041492	66.81%	9.652%
5	6.587	778	782	785	rBV	678735	603614	19.75%	2.854%
6	6.745	804	809	812	rBV	2068837	2035231	66.61%	9.622%
7	7.151	872	878	881	rBV	1636581	1828879	59.85%	8.646%
8	7.869	995	1000	1003	rBV	991371	829840	27.16%	3.923%
9	8.145	1042	1047	1050	rBV	471474	436049	14.27%	2.062%
10	8.951	1178	1184	1187	rBV	2916429	3055576	100.00%	14.446%
11	9.616	1291	1297	1301	rBV2	998579	896593	29.34%	4.239%
12	10.404	1425	1431	1434	rBV	1630201	1672760	54.74%	7.908%
13	11.092	1543	1548	1552	rBV	1013772	848828	27.78%	4.013%
14	11.639	1636	1641	1644	rBV	98094	113901	3.73%	0.538%
15	12.363	1758	1764	1769	rVB2	17588	41891	1.37%	0.198%
16	12.422	1771	1774	1779	rBV	58480	65612	2.15%	0.310%
17	12.516	1787	1790	1793	rVB2	37283	34155	1.12%	0.161%
18	12.680	1812	1818	1822	rBV	2543800	2957075	96.78%	13.980%
19	13.239	1912	1913	1920	rVB5	24896	37916	1.24%	0.179%
20	13.586	1970	1972	1976	rBV4	59670	80169	2.62%	0.379%
21	13.716	1990	1994	1998	rBV	772749	749084	24.52%	3.541%
22	14.163	2066	2070	2073	rBV5	29201	41319	1.35%	0.195%
23	14.368	2101	2105	2109	rBV4	38344	51079	1.67%	0.241%
24	14.568	2138	2139	2143	rVB	61736	44577	1.46%	0.211%
25	14.657	2151	2154	2162	rVB9	28415	53177	1.74%	0.251%
26	15.004	2210	2213	2218	rBV7	22643	50884	1.67%	0.241%
27	15.086	2223	2227	2231	rBV	473079	532689	17.43%	2.518%
28	15.557	2305	2307	2316	rVB7	35854	68300	2.24%	0.323%
29	15.957	2371	2375	2378	rBV4	24303	32688	1.07%	0.155%

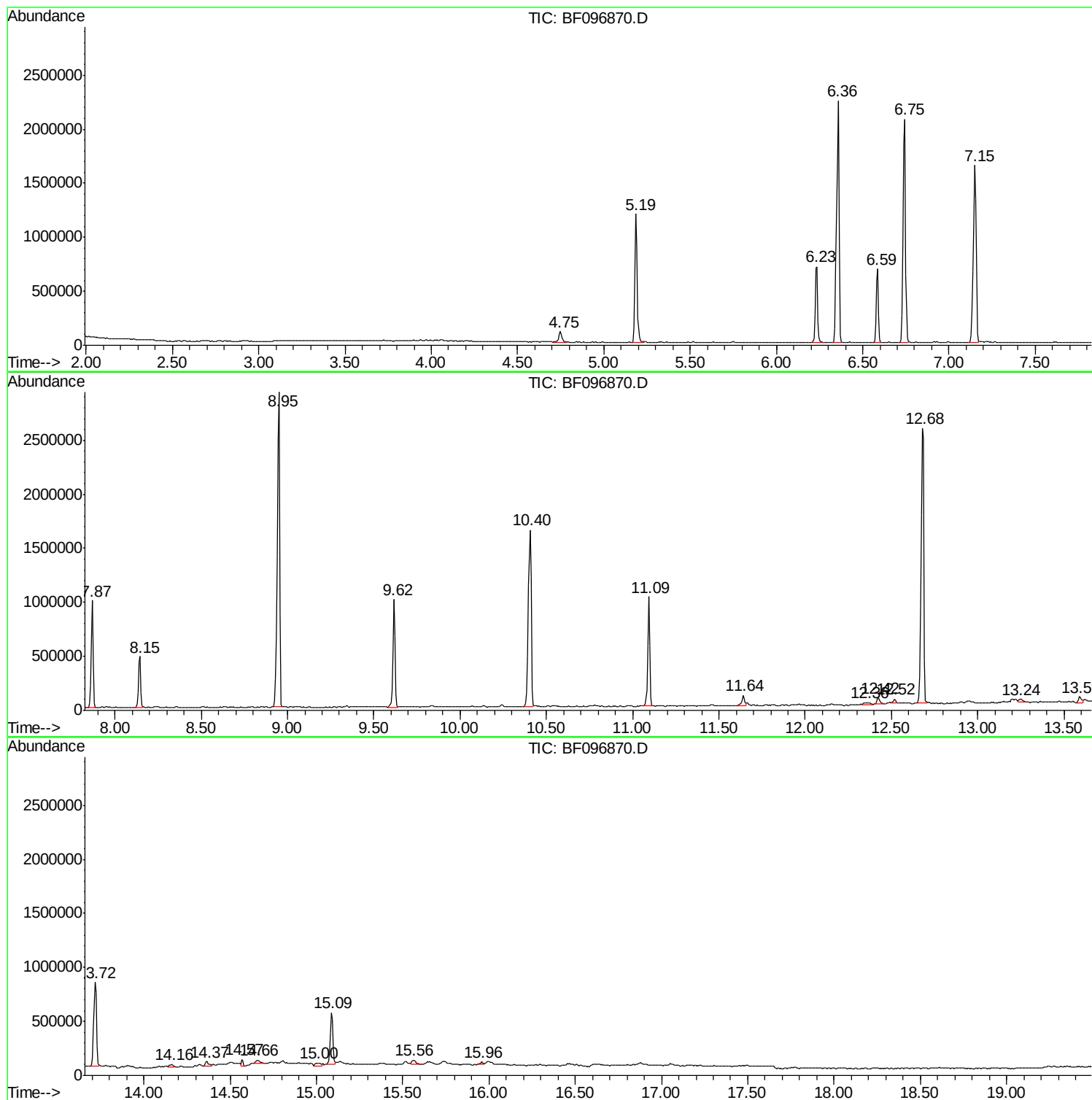
Sum of corrected areas: 21151770

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
Data File : BF096870.D
Acq On : 19 Jul 2017 15:19
Operator : SJ/JU
Sample : I4199-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3569-SPP4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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\BF071917\
Data File : BF096870.D
Acq On : 19 Jul 2017 15:19
Operator : SJ/JU
Sample : I4199-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3569-SPP4

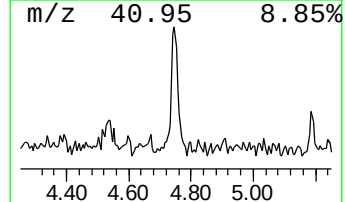
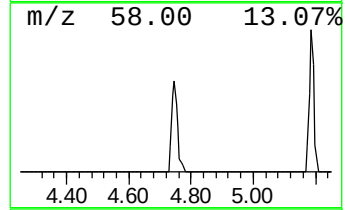
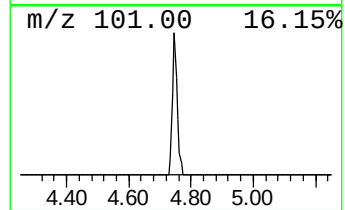
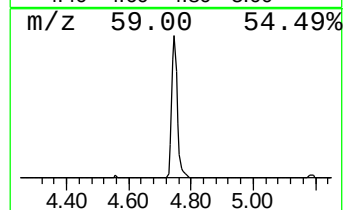
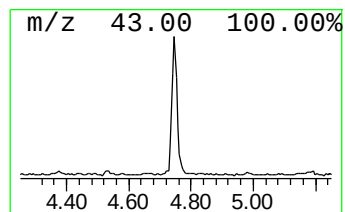
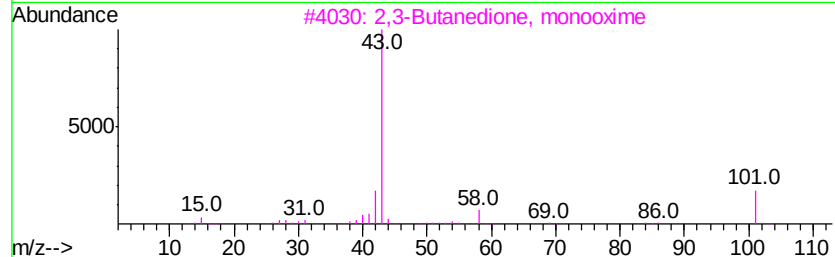
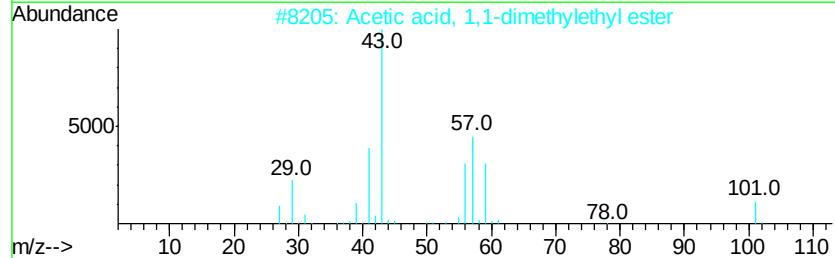
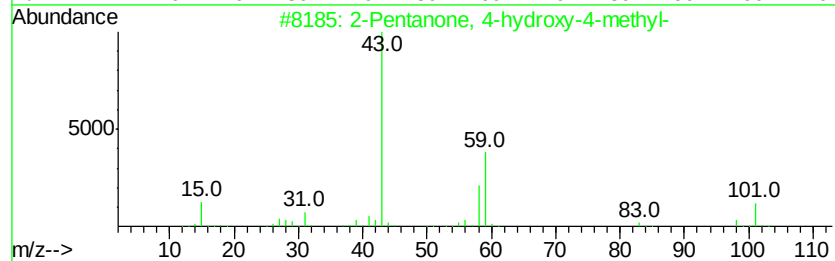
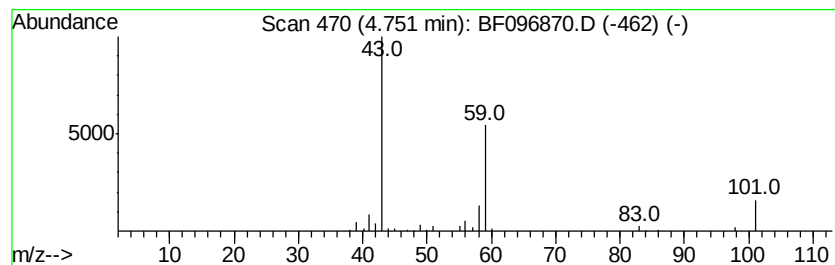
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	4.27 ng	128971	1,4-Dichlorobenzene-d4	6.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5			Silane, trimethyl-	74	C3H10Si	000993-07-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
Data File : BF096870.D
Acq On : 19 Jul 2017 15:19
Operator : SJ/JU
Sample : I4199-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3569-SPP4

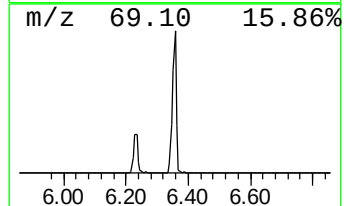
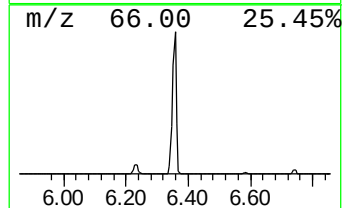
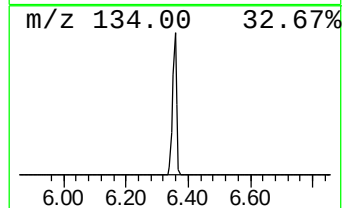
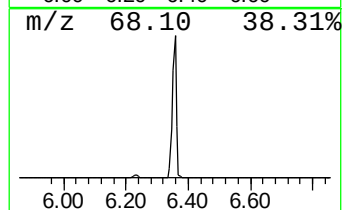
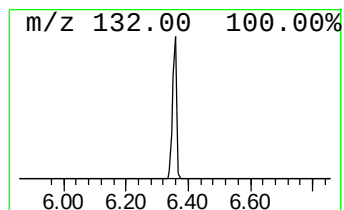
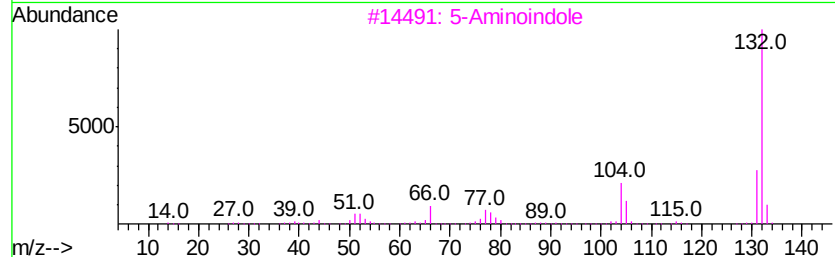
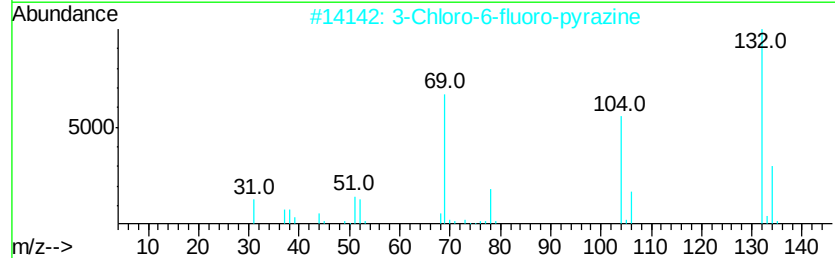
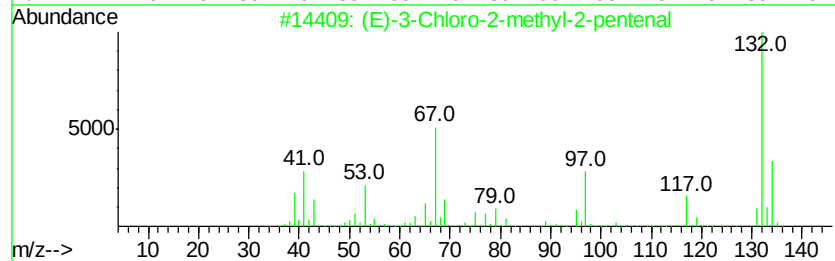
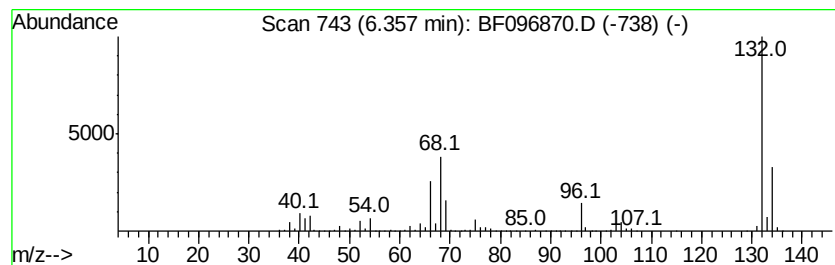
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	67.64 ng	2041490	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
Data File : BF096870.D
Acq On : 19 Jul 2017 15:19
Operator : SJ/JU
Sample : I4199-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3569-SPP4

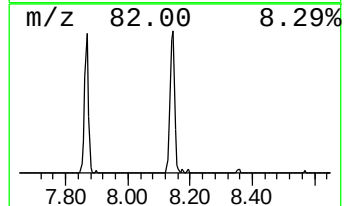
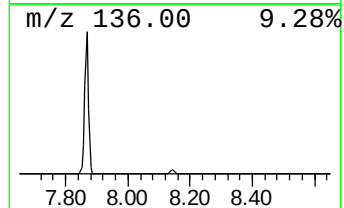
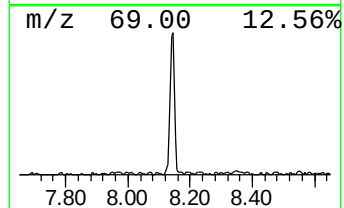
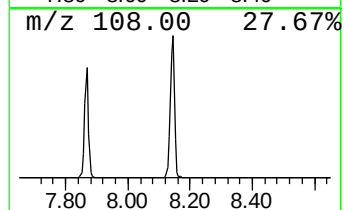
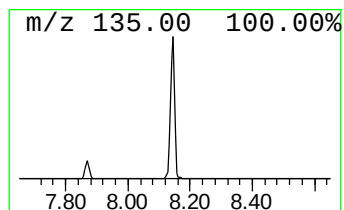
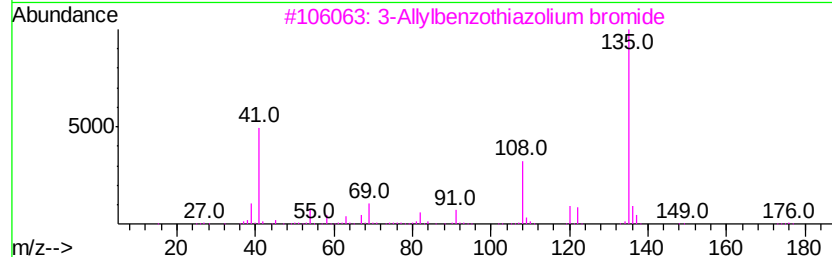
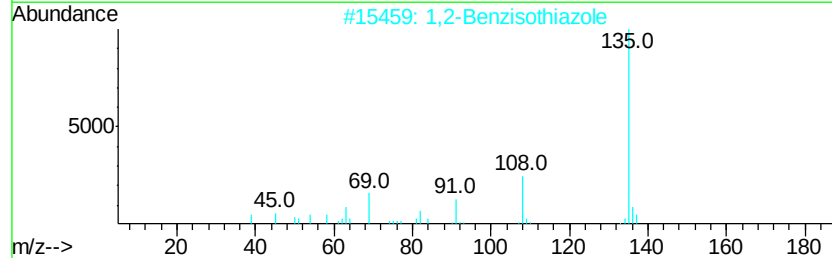
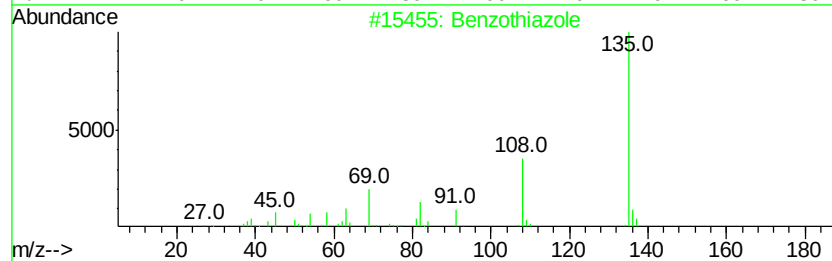
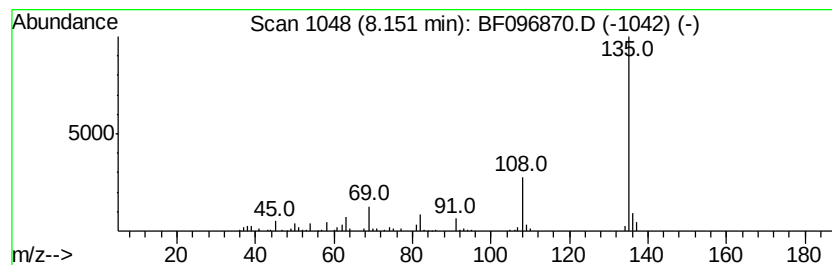
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	10.51 ng	436049	Napthalene-d8	7.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	95
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	90
4		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
5		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071917\
Data File : BF096870.D
Acq On : 19 Jul 2017 15:19
Operator : SJ/JU
Sample : I4199-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

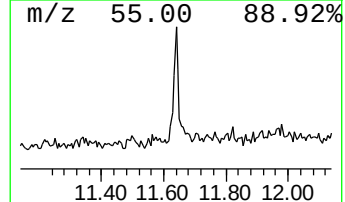
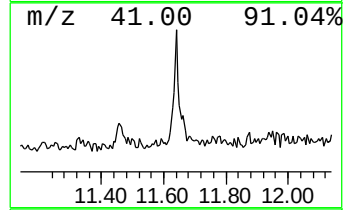
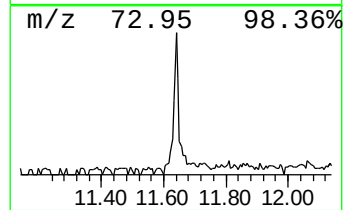
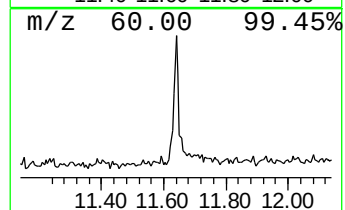
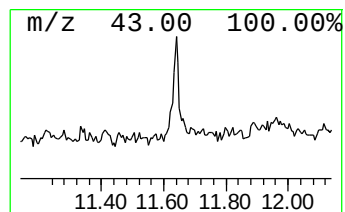
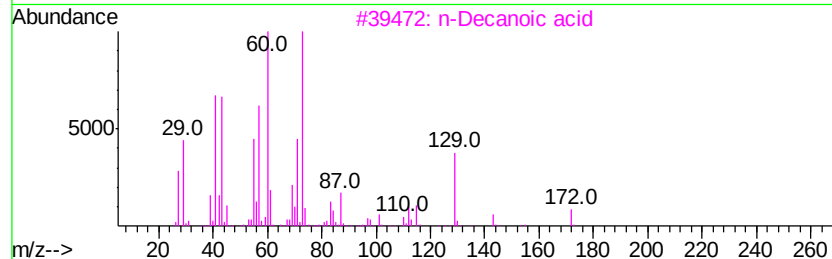
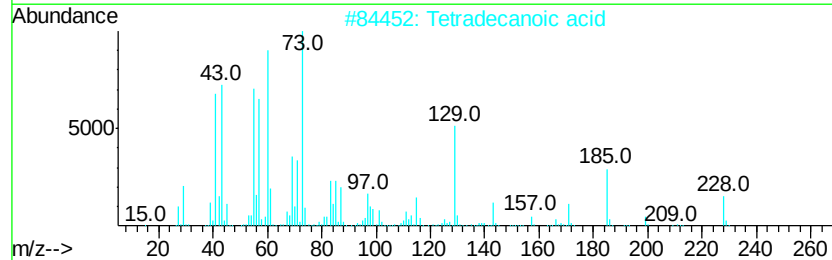
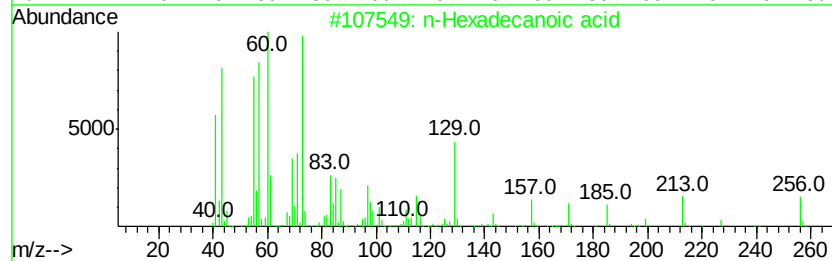
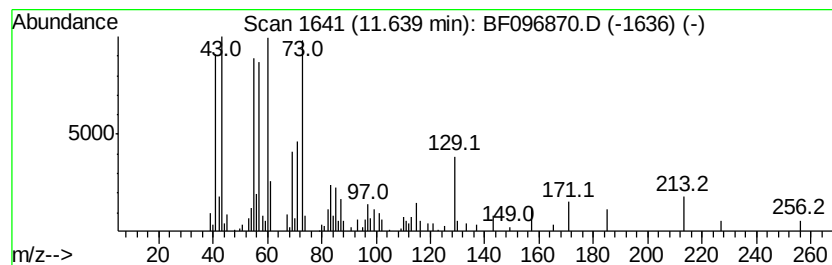
Instrument :
BNA_F
ClientSampleId :
3569-SPP4

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.64	2.68 ng	113901	Phenanthrene-d10		11.09
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
Data File : BF096870.D
Acq On : 19 Jul 2017 15:19
Operator : SJ/JU
Sample : I4199-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3569-SPP4

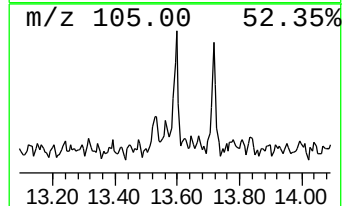
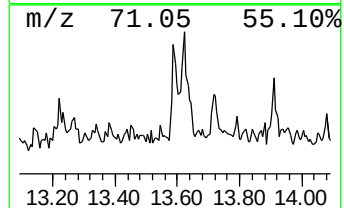
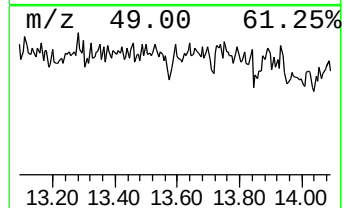
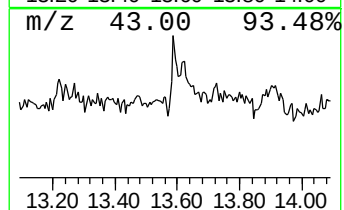
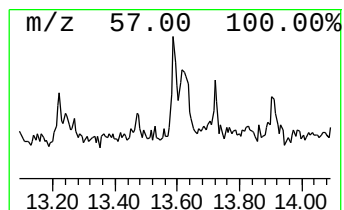
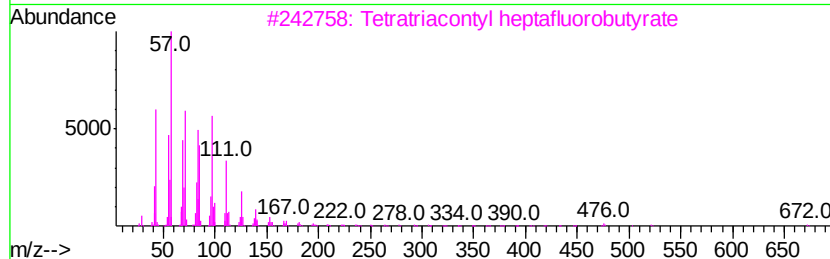
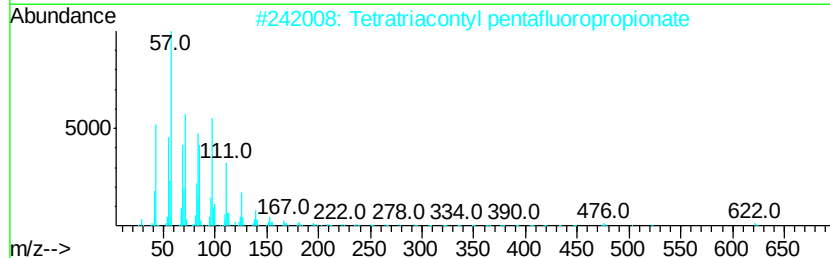
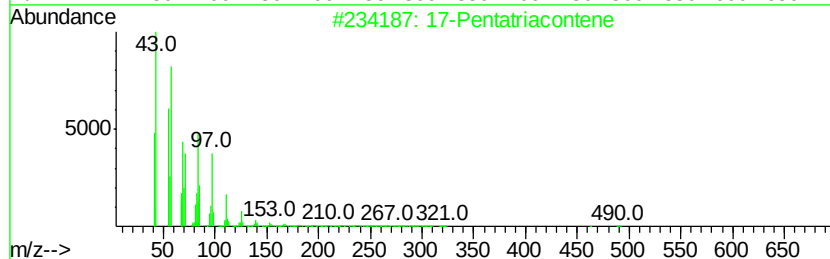
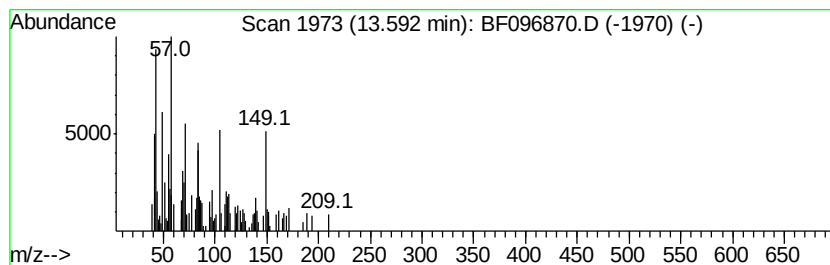
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	2.14 ng	80169	Chrysene-d12	13.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	50
2		Tetratriacontyl pentafluoropropi...	641	C37H69F502	1000351-81-5	43
3		Tetratriacontyl heptafluorobutyrate	691	C38H69F702	1000351-84-1	43
4		Octatriacontyl trifluoroacetate	647	C40H77F302	1000351-88-7	43
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
Data File : BF096870.D
Acq On : 19 Jul 2017 15:19
Operator : SJ/JU
Sample : I4199-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

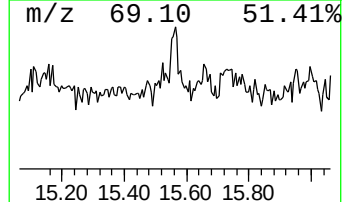
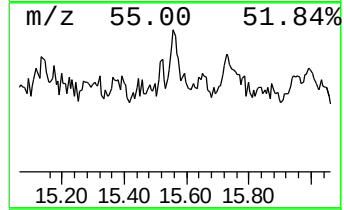
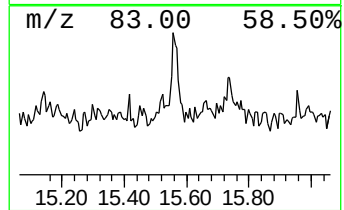
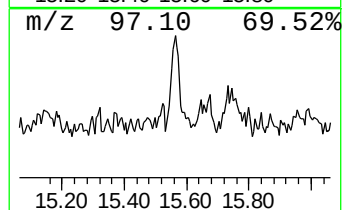
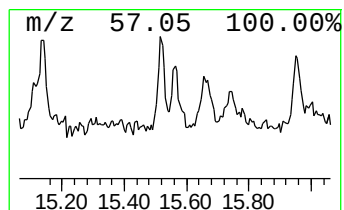
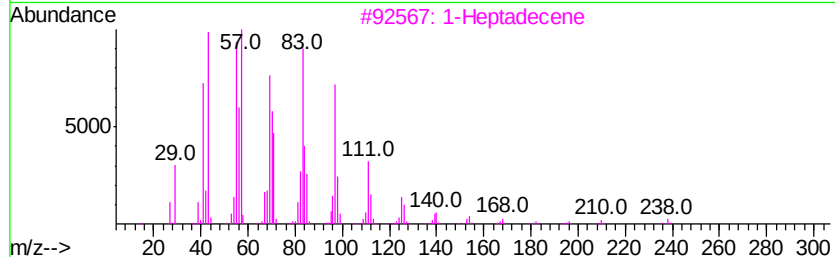
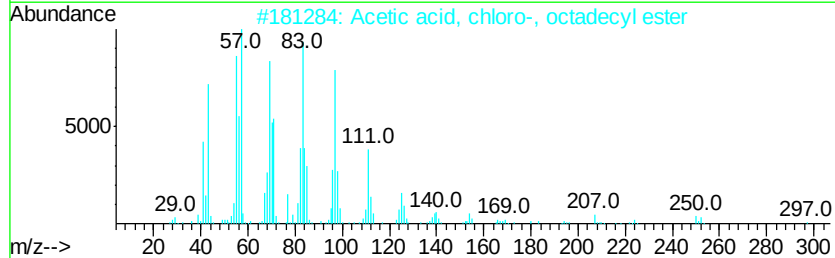
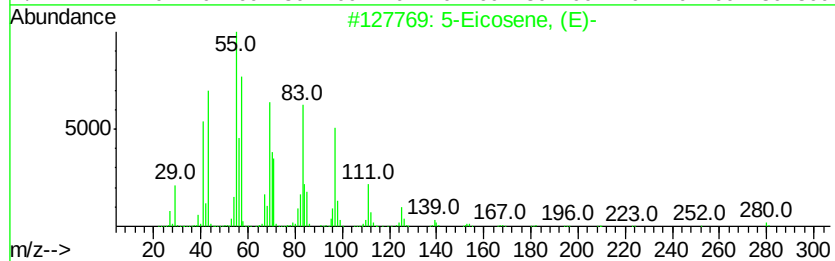
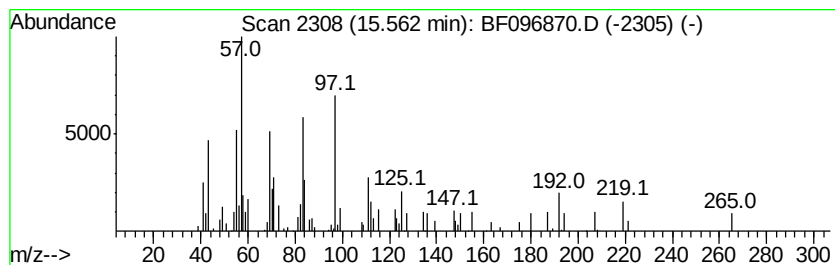
Instrument :
BNA_F
ClientSampled :
3569-SPP4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.56	2.56 ng	68300	Perylene-d12	15.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	58
2	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	53
3	1-Heptadecene	238	C17H34	006765-39-5	53
4	n-Pentadecanol	228	C15H32O	000629-76-5	52
5	Cyclohexane, 1,2,3,4,5,6-hexaethyl-	252	C18H36	001795-14-8	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
Data File : BF096870.D
Acq On : 19 Jul 2017 15:19
Operator : SJ/JU
Sample : I4199-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3569-SPP4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	4.75	4.3	ng	128971	1	6.59	603614	20.0
unknown6.36	6.36	67.6	ng	2041490	1	6.59	603614	20.0
Benzothiazole	8.15	10.5	ng	436049	2	7.87	829840	20.0
n-Hexadecanoic acid	11.64	2.7	ng	113901	4	11.09	848828	20.0
17-Pentatriacontene	13.59	2.1	ng	80169	5	13.72	749084	20.0
5-Eicosene, (E)-	15.56	2.6	ng	68300	6	15.09	532689	20.0