

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
 Data File : BF099189.D
 Acq On : 7 Oct 2017 12:50
 Operator : SJ/JU
 Sample : I5585-17
 Misc :
 ALS Vial : 6 Sample Multiplier: 2

Instrument :
 BNA_F
 ClientSampleId :
 G71-0-1.5

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-BF092317.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	2.152	6	11	18	rVB	113391	143980	5.05%	0.466%
2	5.087	507	510	523	rVB	362462	482528	16.91%	1.560%
3	5.487	574	578	582	rBV	2517503	2547762	89.28%	8.237%
4	6.498	745	750	753	rBV	2388566	2546635	89.24%	8.234%
5	6.634	769	773	777	rBV	2701563	2645968	92.72%	8.555%
6	6.863	808	812	816	rBV	1875472	1557181	54.57%	5.035%
7	7.022	834	839	842	rBV	2304442	2090026	73.24%	6.757%
8	7.428	903	908	911	rBV	1741073	1626813	57.01%	5.260%
9	8.145	1026	1030	1033	rBV	2373401	2045038	71.66%	6.612%
10	9.222	1207	1213	1216	rBV	3184339	2853608	100.00%	9.226%
11	9.610	1276	1279	1282	rBV	370072	271581	9.52%	0.878%
12	9.822	1307	1315	1318	rBV	40871	38852	1.36%	0.126%
13	9.904	1324	1329	1332	rBV	2062233	2055563	72.03%	6.646%
14	10.322	1397	1400	1403	rVB	66679	57357	2.01%	0.185%
15	10.539	1431	1437	1439	rBV	22901	32146	1.13%	0.104%
16	10.686	1458	1462	1472	rVB	1386879	1335353	46.80%	4.317%
17	10.792	1477	1480	1489	rVB	85371	99581	3.49%	0.322%
18	11.239	1553	1556	1558	rBV	55344	38794	1.36%	0.125%
19	11.386	1577	1581	1584	rBV	1945879	1735841	60.83%	5.612%
20	11.410	1584	1585	1587	rVB	72559	35024	1.23%	0.113%
21	11.592	1611	1616	1619	rBV	42232	50831	1.78%	0.164%
22	11.904	1663	1669	1674	rBV2	46858	81763	2.87%	0.264%
23	12.598	1784	1787	1790	rBV	116360	94482	3.31%	0.305%
24	12.780	1815	1818	1821	rBV3	43986	38373	1.34%	0.124%
25	12.851	1821	1830	1841	rBV2	760314	1190874	41.73%	3.850%
26	12.969	1846	1850	1853	rBV	2099934	1833744	64.26%	5.929%
27	13.439	1926	1930	1935	rBV	199519	189505	6.64%	0.613%
28	13.851	1997	2000	2008	rVB2	120992	144567	5.07%	0.467%
29	14.027	2025	2030	2033	rBV	1412713	1337474	46.87%	4.324%
30	15.063	2203	2206	2213	rVB	69726	108252	3.79%	0.350%
31	15.374	2256	2259	2265	rVB	46370	63190	2.21%	0.204%
32	15.433	2266	2269	2273	rVV	55392	78381	2.75%	0.253%
33	15.504	2276	2281	2298	rVB	971986	1318896	46.22%	4.264%
34	15.939	2352	2355	2359	rVB2	53731	67577	2.37%	0.218%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099189.D
Acq On : 7 Oct 2017 12:50
Operator : SJ/JU
Sample : I5585-17
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
G71-0-1.5

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.439	2437	2440	2447	rVB2	59180	91897	3.22%	0.297%
----	--------	------	------	------	------	-------	-------	-------	--------

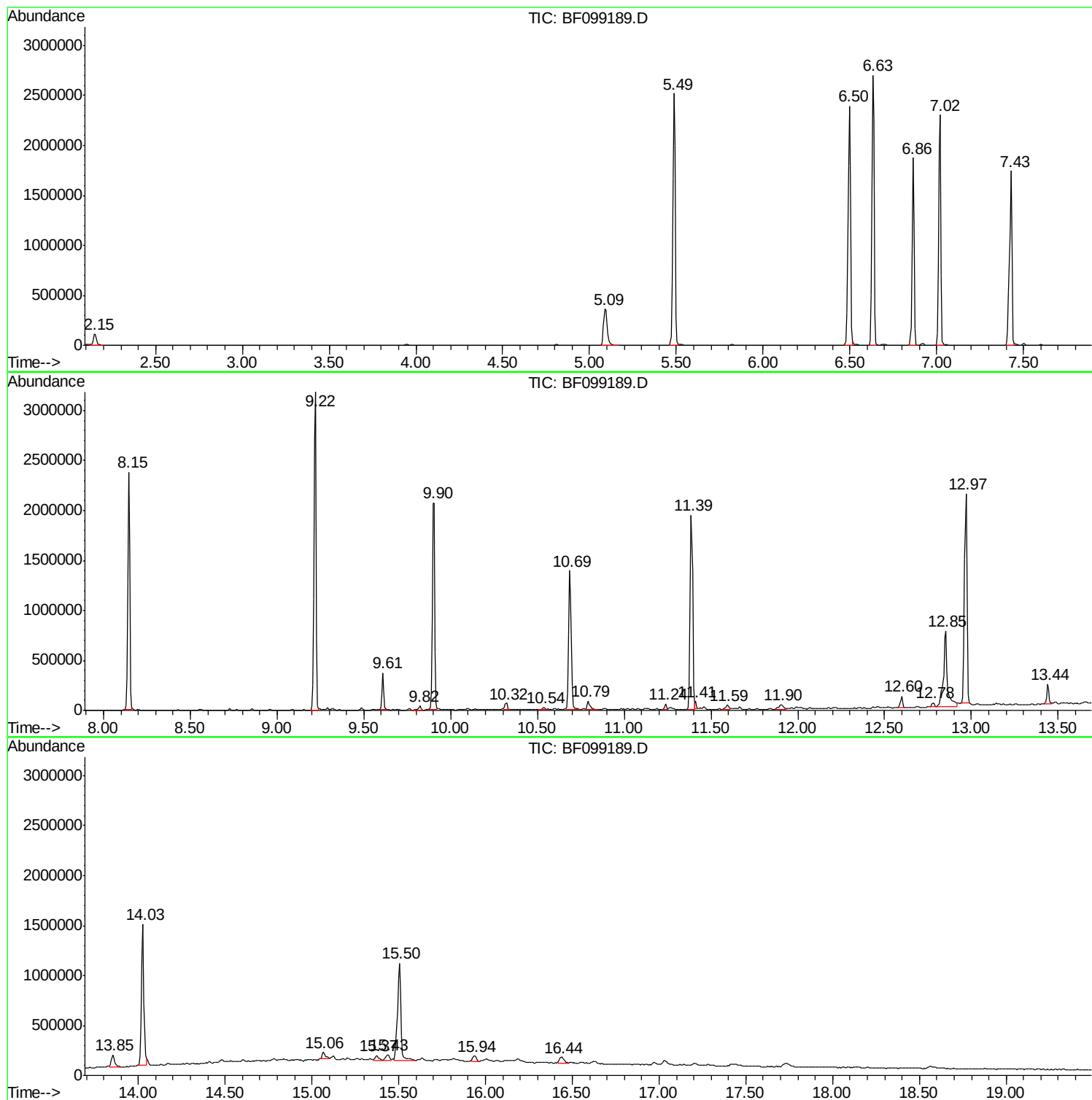
Sum of corrected areas: 30929437

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099189.D
Acq On : 7 Oct 2017 12:50
Operator : SJ/JU
Sample : I5585-17
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
G71-0-1.5

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.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\BF100717\
Data File : BF099189.D
Acq On : 7 Oct 2017 12:50
Operator : SJ/JU
Sample : I5585-17
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
G71-0-1.5

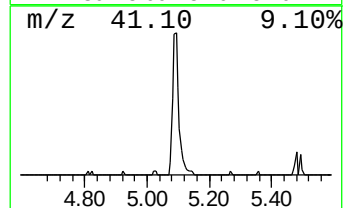
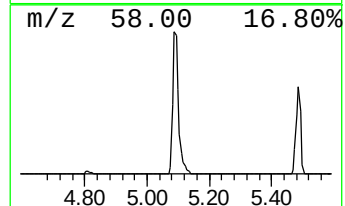
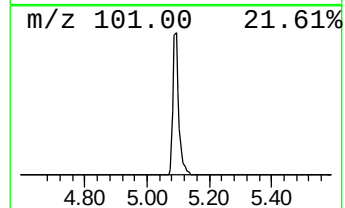
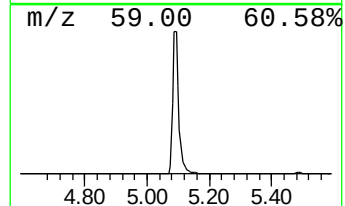
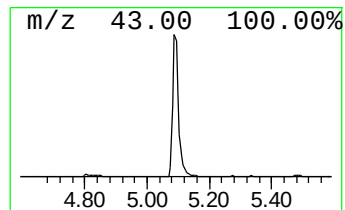
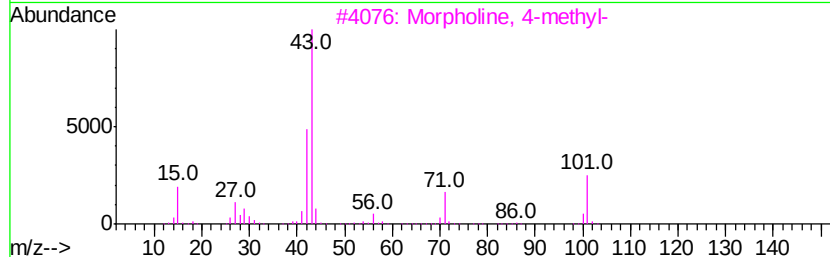
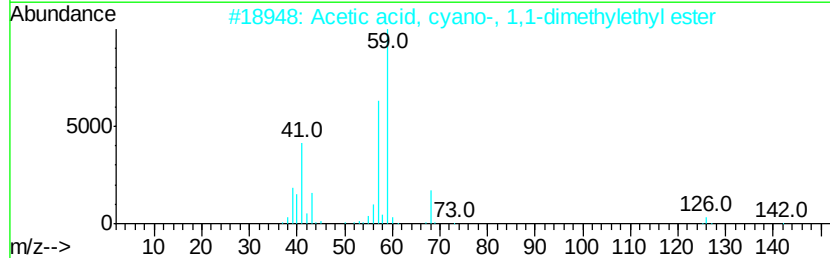
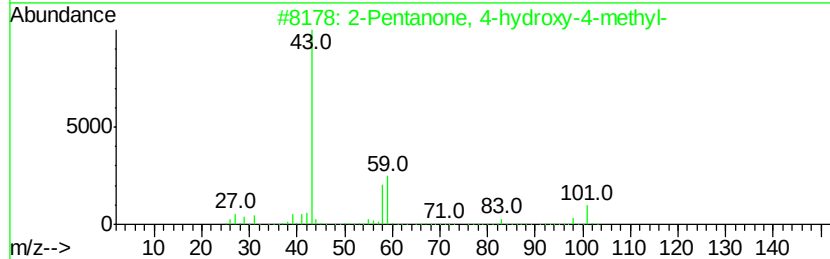
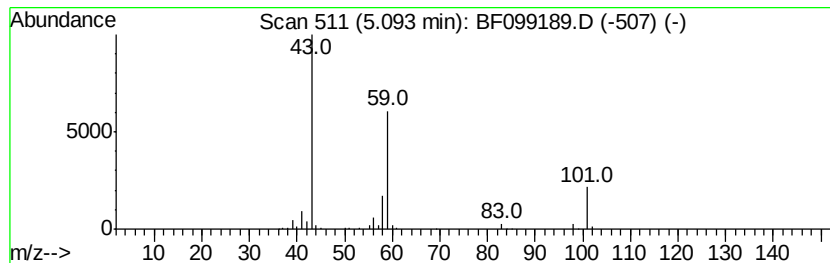
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.09	6.20 ng	482528	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100717\
Data File : BF099189.D
Acq On : 7 Oct 2017 12:50
Operator : SJ/JU
Sample : I5585-17
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
G71-0-1.5

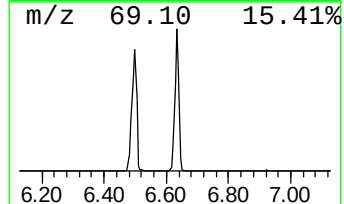
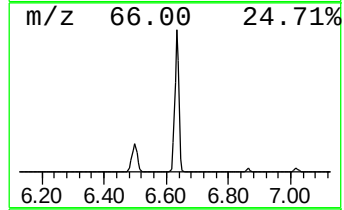
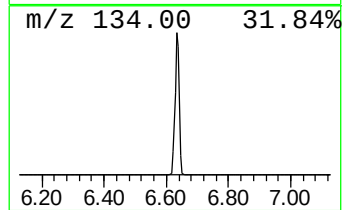
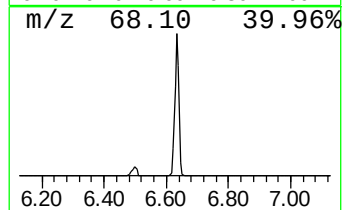
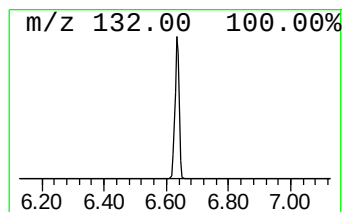
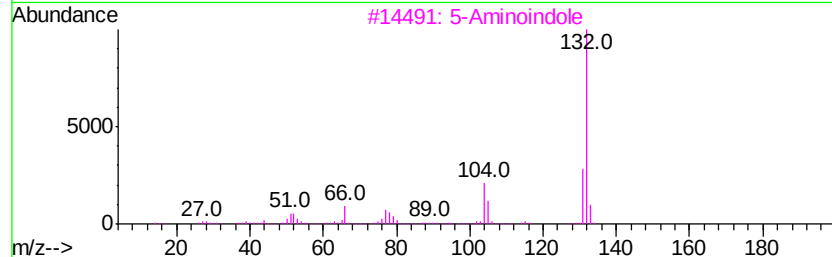
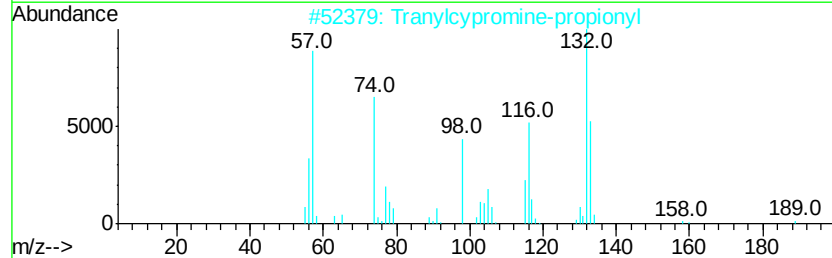
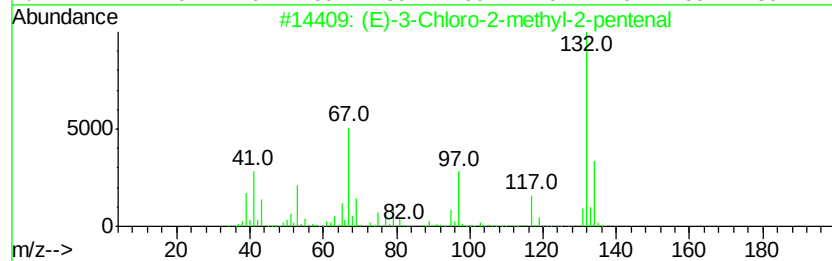
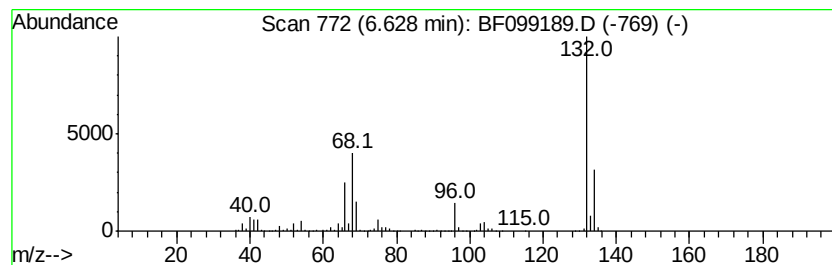
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	33.98 ng	2645970	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12	
3	5-Aminoindole	132	C8H8N2	005192-03-0	12	
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100717\
Data File : BF099189.D
Acq On : 7 Oct 2017 12:50
Operator : SJ/JU
Sample : I5585-17
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
G71-0-1.5

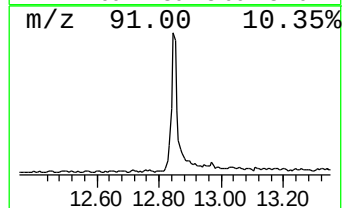
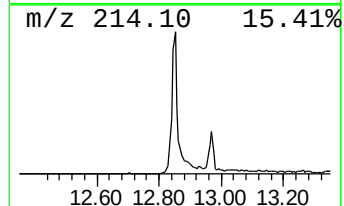
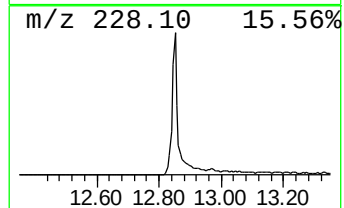
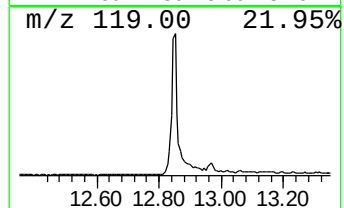
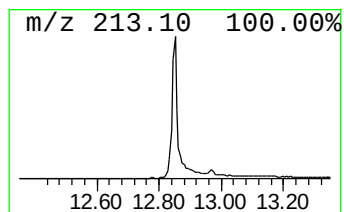
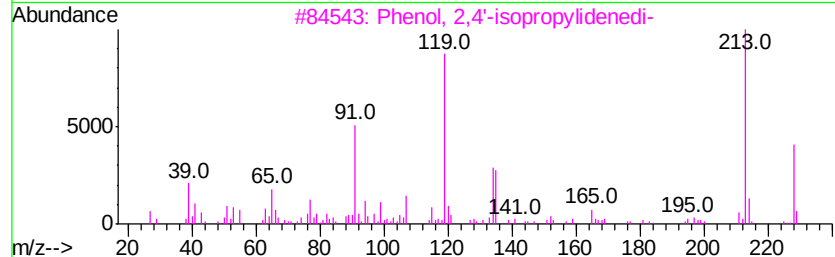
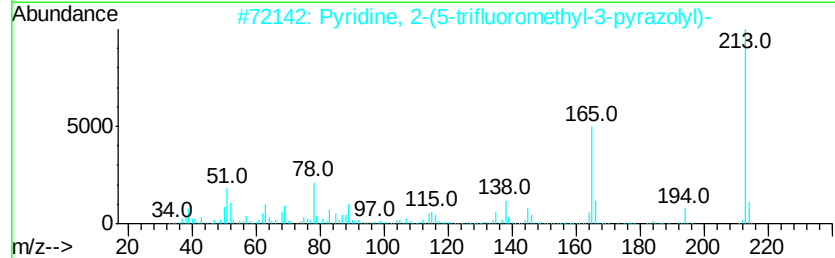
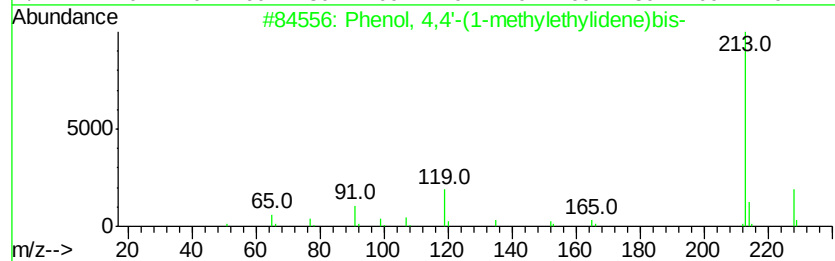
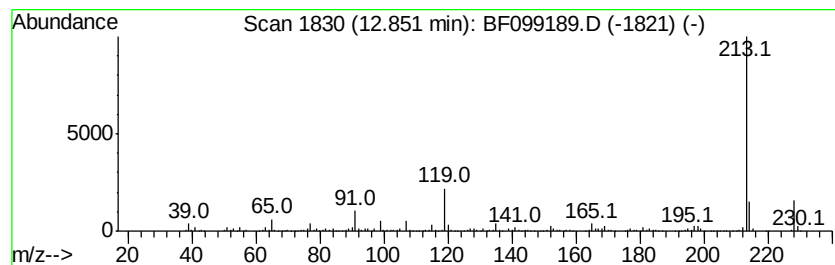
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	17.81 ng	1190870	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	96
2		Pyridine, 2-(5-trifluoromethyl-3-pyrazolyl)-	213	C9H6F3N3	003974-71-8	50
3		Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	50
4		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	50
5		2,5-bis(Trimethylsilyl)thiophene	228	C10H20Si2	017906-71-7	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099189.D
Acq On : 7 Oct 2017 12:50
Operator : SJ/JU
Sample : I5585-17
Misc :
ALS Vial : 6 Sample Multiplier: 2

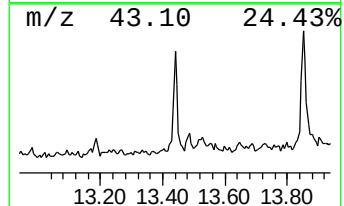
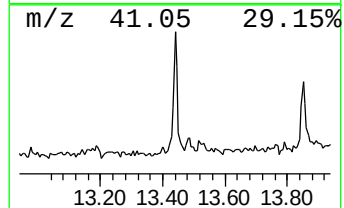
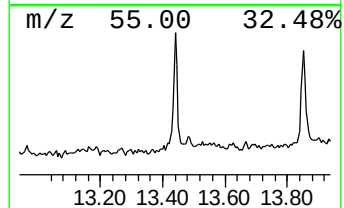
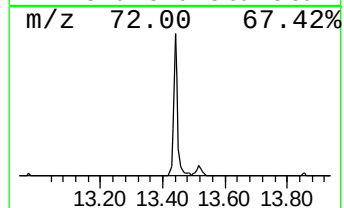
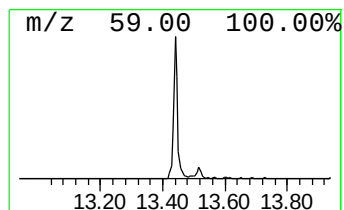
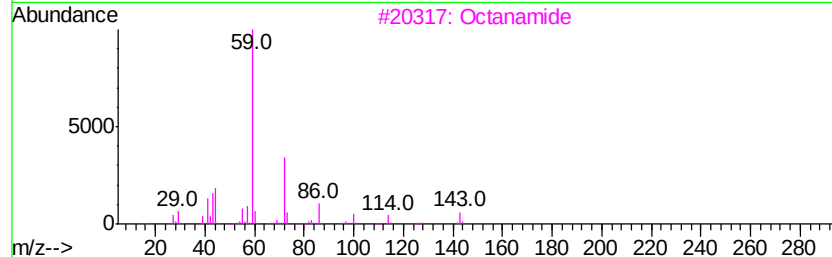
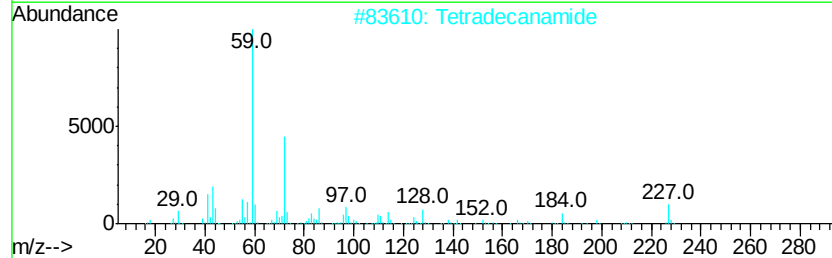
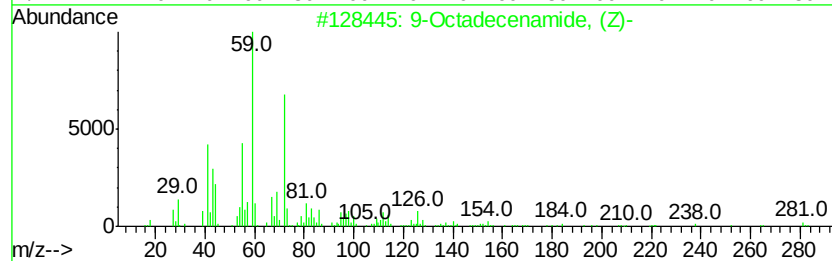
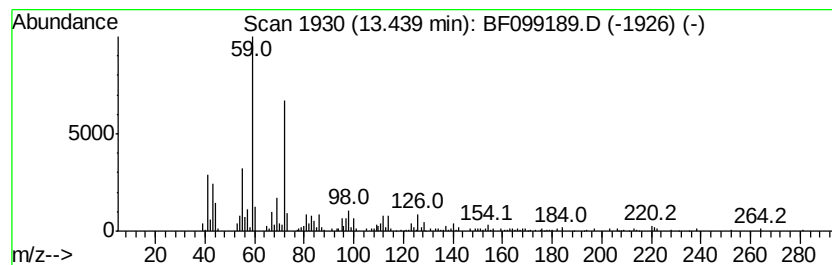
Instrument :
BNA_F
ClientSampleId :
G71-0-1.5

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.44	2.83 ng	189505	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Tetradecanamide	227	C14H29NO	000638-58-4	59
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Dodecanamide	199	C12H25NO	001120-16-7	53
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099189.D
Acq On : 7 Oct 2017 12:50
Operator : SJ/JU
Sample : I5585-17
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
G71-0-1.5

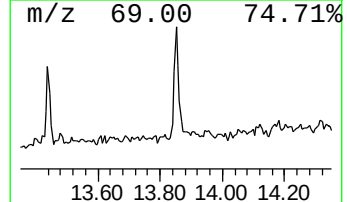
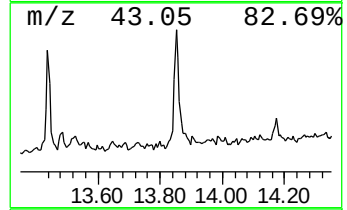
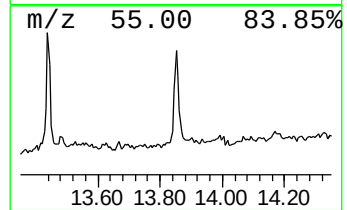
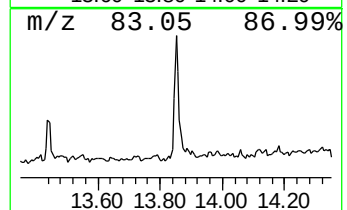
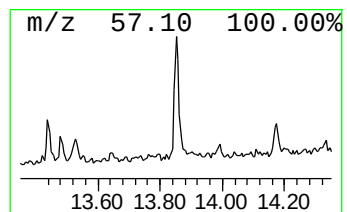
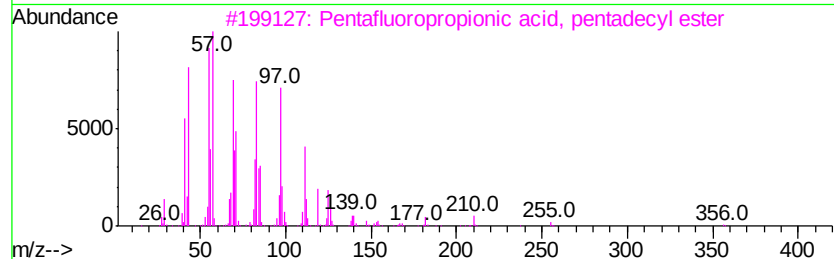
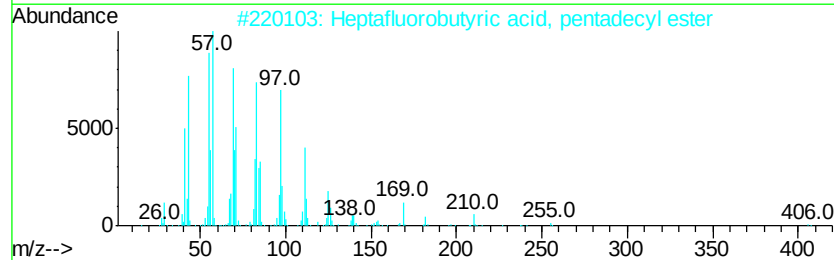
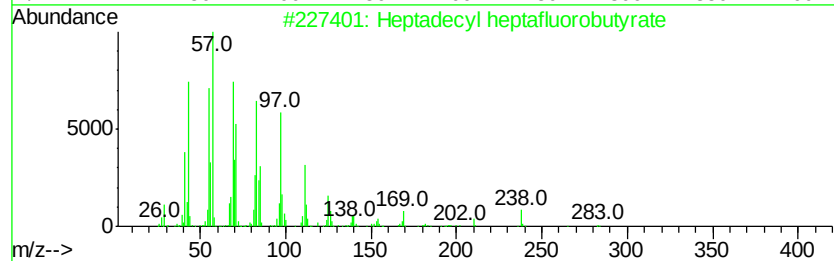
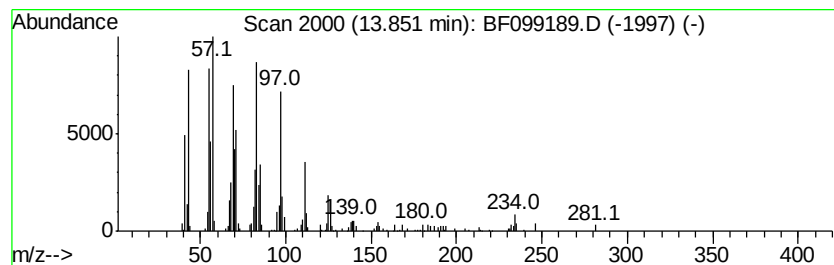
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.16 ng	144567	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Heptafluorobutyric acid, pentadecyl...	424	C19H31F7O2	959261-23-5	93
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100717\
Data File : BF099189.D
Acq On : 7 Oct 2017 12:50
Operator : SJ/JU
Sample : I5585-17
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
G71-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.09	6.2	ng	482528	1	6.86	1557180	20.0
unknown6.63	6.63	34.0	ng	2645970	1	6.86	1557180	20.0
Phenol, 4,4'-(1-m...	12.85	17.8	ng	1190870	5	14.03	1337470	20.0
9-Octadecenamide,...	13.44	2.8	ng	189505	5	14.03	1337470	20.0
Heptadecyl heptaf...	13.85	2.2	ng	144567	5	14.03	1337470	20.0