

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
 Data File : BF096910.D
 Acq On : 20 Jul 2017 17:19
 Operator : SJ/JU
 Sample : I4282-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-GF-02-007-A

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-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	4.740	463	468	480	rVB	192078	306466	9.63%	1.207%
2	5.181	537	543	546	rBV	2383890	2705980	85.00%	10.653%
3	6.222	714	720	732	rBV	2623577	3183641	100.00%	12.534%
4	6.340	735	740	743	rBV	2894357	2945296	92.51%	11.595%
5	6.569	775	779	782	rBV	752977	658621	20.69%	2.593%
6	6.728	801	806	809	rBV	2147980	2170315	68.17%	8.544%
7	7.134	869	875	878	rBV	1839959	1872496	58.82%	7.372%
8	7.851	992	997	1000	rBV	1033518	928375	29.16%	3.655%
9	8.928	1175	1180	1184	rBV	2494190	2600376	81.68%	10.237%
10	9.239	1229	1233	1235	rBV	45837	45243	1.42%	0.178%
11	9.322	1243	1247	1250	rBV	341991	285175	8.96%	1.123%
12	9.598	1289	1294	1298	rBV	980383	851362	26.74%	3.352%
13	10.051	1367	1371	1374	rVB	49623	39837	1.25%	0.157%
14	10.269	1401	1408	1411	rBV	62684	66733	2.10%	0.263%
15	10.386	1422	1428	1431	rBV	1666857	1688125	53.02%	6.646%
16	10.522	1447	1451	1458	rVB	63209	86857	2.73%	0.342%
17	11.074	1540	1545	1548	rBV	1017648	891203	27.99%	3.509%
18	12.274	1746	1749	1753	rBV	54811	52921	1.66%	0.208%
19	12.504	1783	1788	1792	rBV	62077	63844	2.01%	0.251%
20	12.663	1810	1815	1818	rBV	2174806	2209685	69.41%	8.699%
21	13.086	1884	1887	1891	rBV	79602	76550	2.40%	0.301%
22	13.568	1965	1969	1977	rBV	86948	113577	3.57%	0.447%
23	13.698	1986	1991	1995	rBV	666654	609221	19.14%	2.398%
24	14.204	2073	2077	2084	rBV3	39492	53763	1.69%	0.212%
25	14.692	2157	2160	2162	rBV2	28426	32808	1.03%	0.129%
26	14.957	2201	2205	2208	rBV2	26567	33212	1.04%	0.131%
27	15.062	2219	2223	2230	rVB	468118	572269	17.98%	2.253%
28	15.186	2242	2244	2251	rVB8	20189	32384	1.02%	0.127%
29	15.680	2324	2328	2333	rBV5	32942	49702	1.56%	0.196%
30	16.051	2387	2391	2396	rVB4	52430	78385	2.46%	0.309%
31	17.515	2634	2640	2652	rBV4	35892	96197	3.02%	0.379%

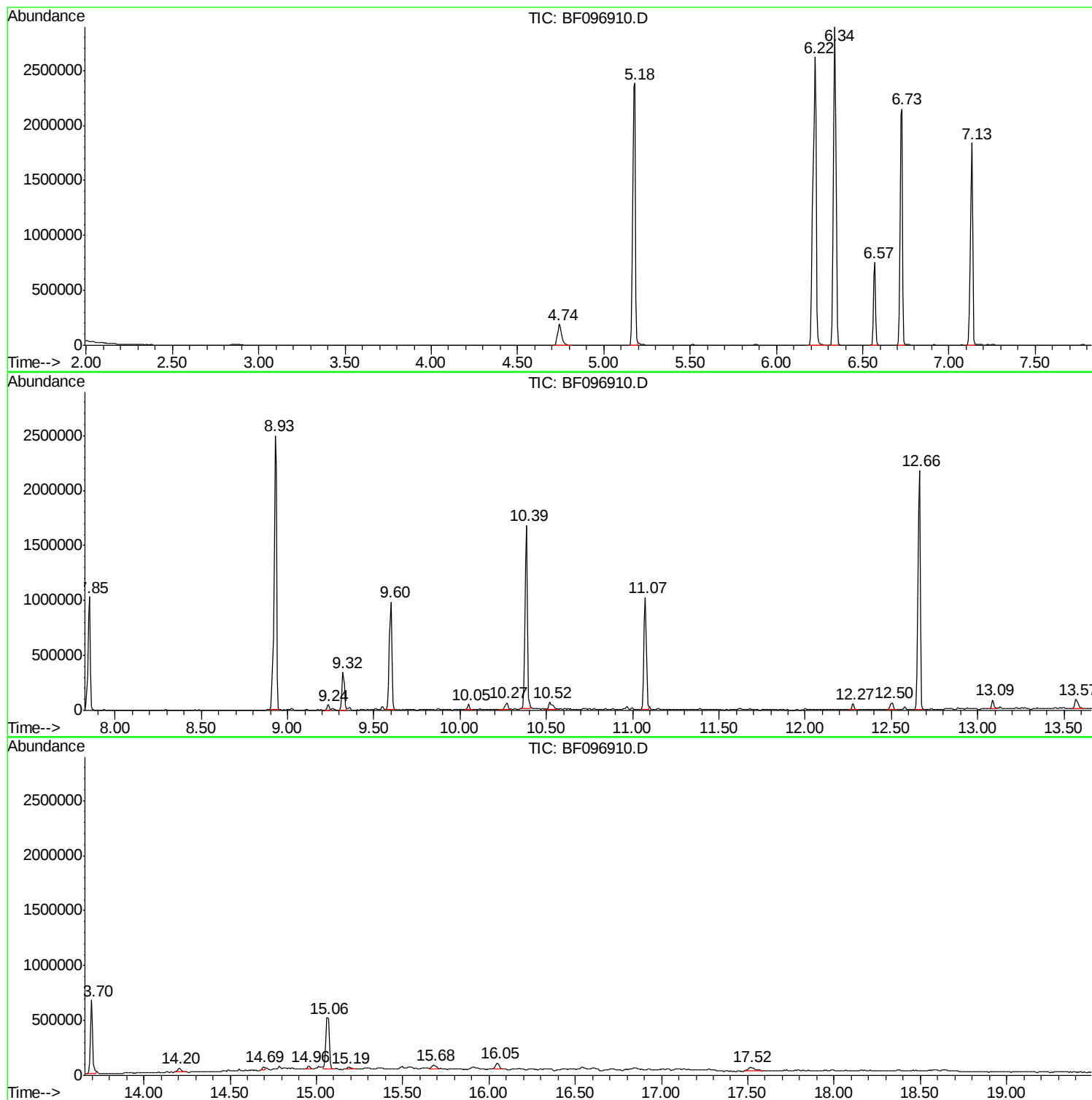
Sum of corrected areas: 25400619

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072017\
Data File : BF096910.D
Acq On : 20 Jul 2017 17:19
Operator : SJ/JU
Sample : I4282-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-007-A

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\BF072017\
Data File : BF096910.D
Acq On : 20 Jul 2017 17:19
Operator : SJ/JU
Sample : I4282-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-007-A

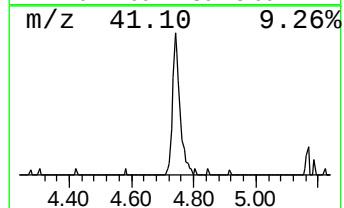
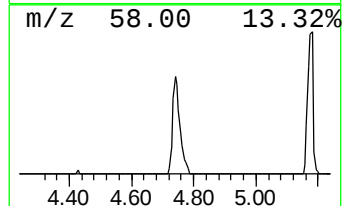
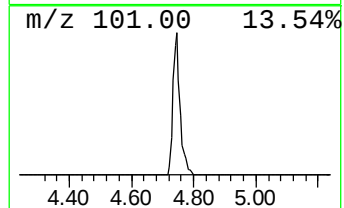
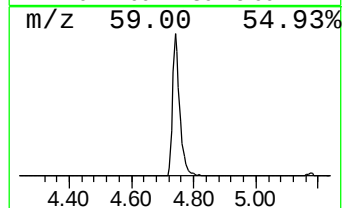
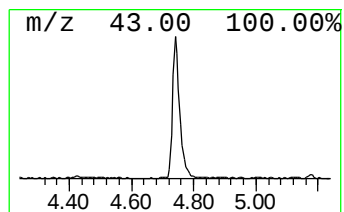
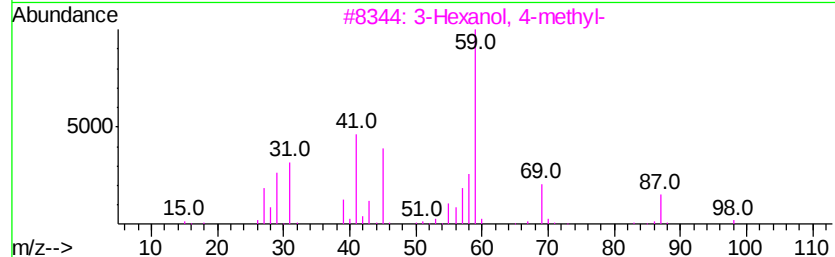
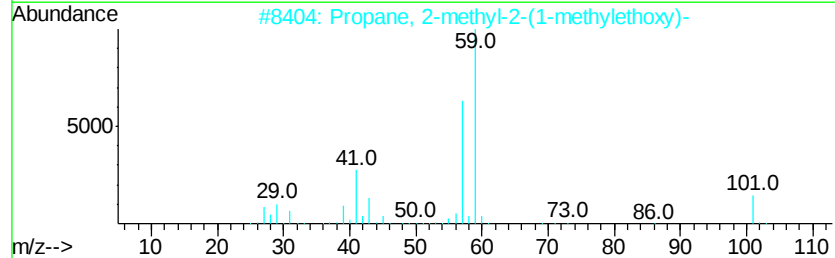
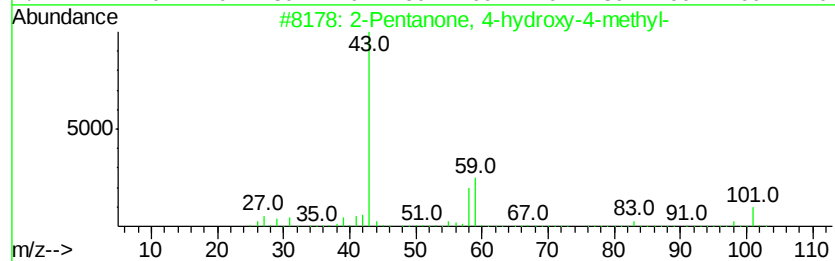
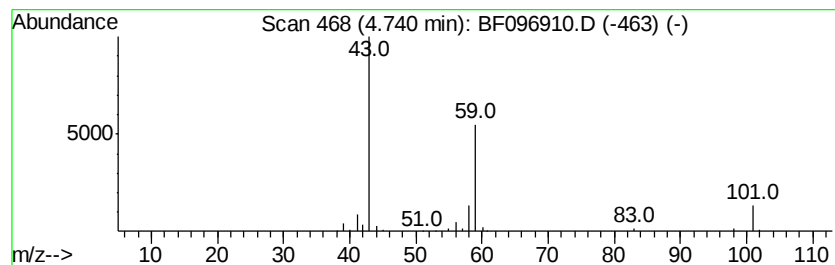
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	9.31 ng	306466	1,4-Dichlorobenzene-d4	6.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072017\
Data File : BF096910.D
Acq On : 20 Jul 2017 17:19
Operator : SJ/JU
Sample : I4282-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-007-A

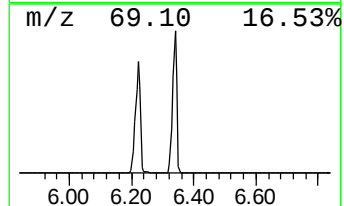
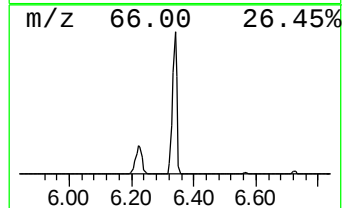
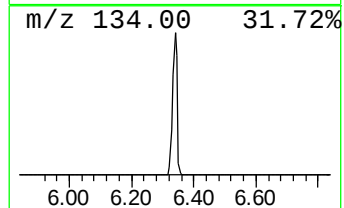
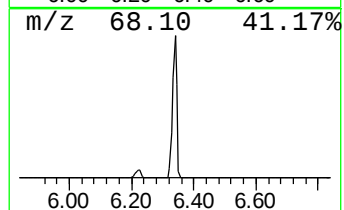
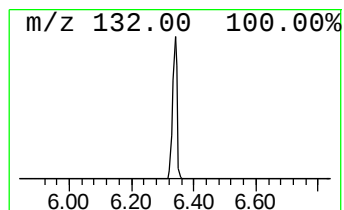
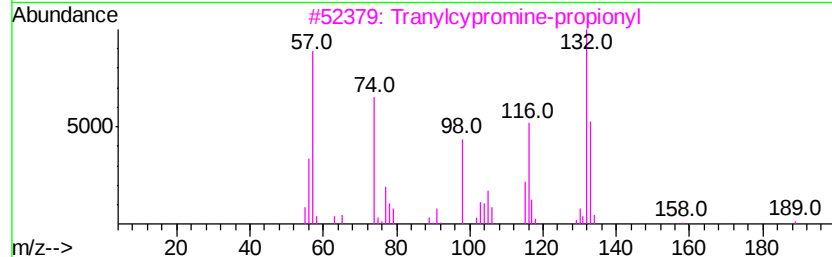
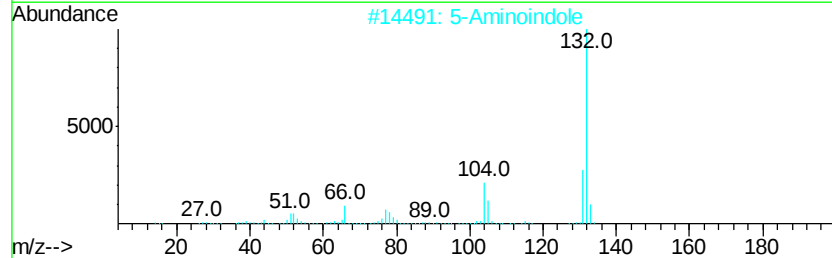
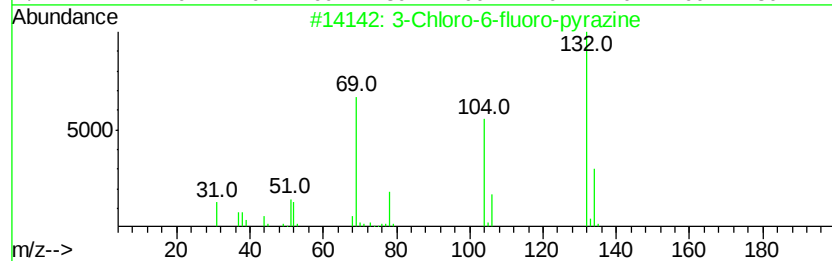
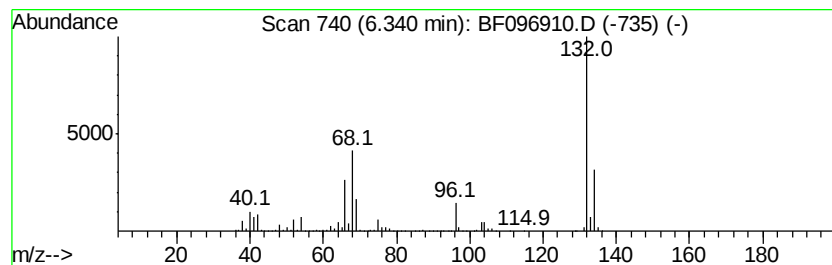
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	89.44 ng	2945300	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
Data File : BF096910.D
Acq On : 20 Jul 2017 17:19
Operator : SJ/JU
Sample : I4282-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-007-A

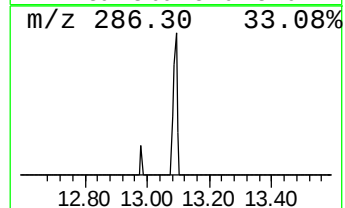
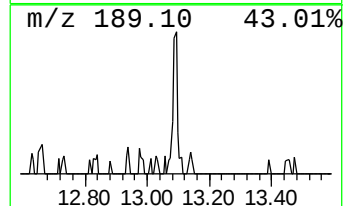
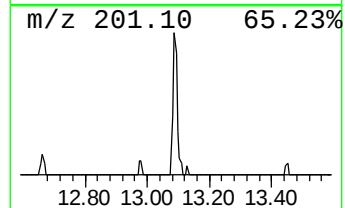
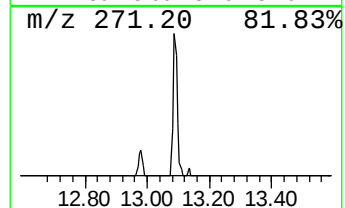
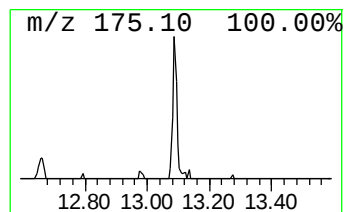
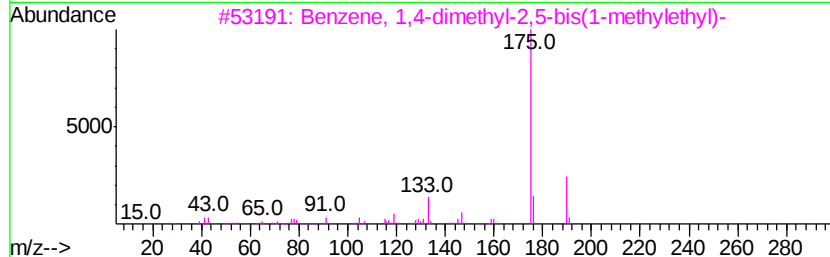
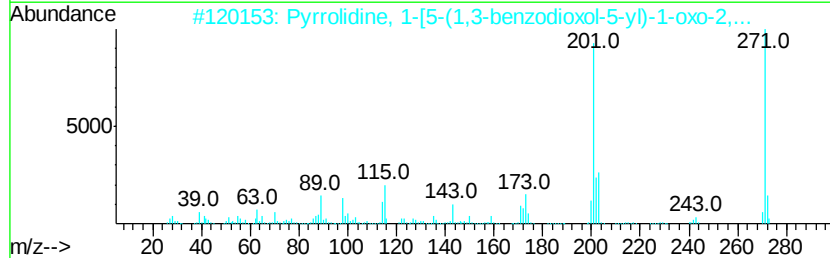
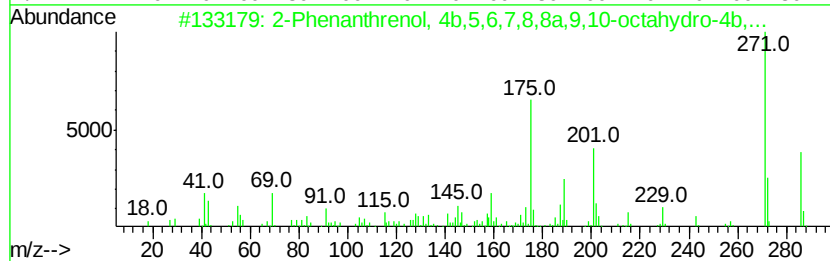
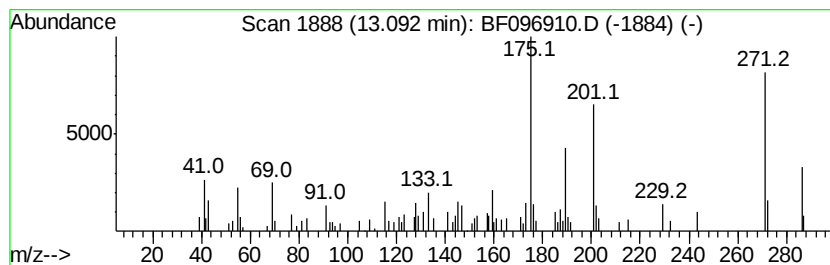
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	2.51 ng	76550	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	95
2		Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	27
3		Benzene, 1,4-dimethyl-2,5-bis(1-...	190	C14H22	010375-96-9	25
4		m-Cymene, 5-tert-butyl-	190	C14H22	029577-19-3	22
5		1H-Pyrrole-2,5-dione, 2,5-dihydr...	201	C12H11NO2	065833-09-2	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072017\
Data File : BF096910.D
Acq On : 20 Jul 2017 17:19
Operator : SJ/JU
Sample : I4282-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-007-A

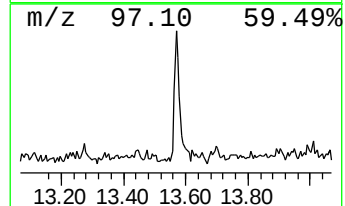
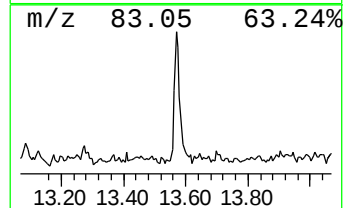
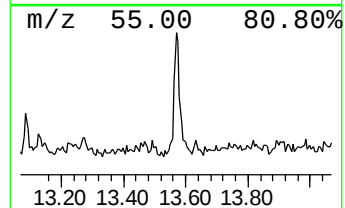
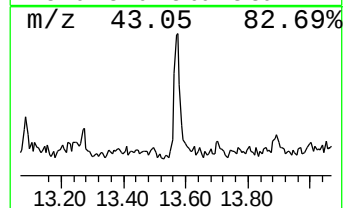
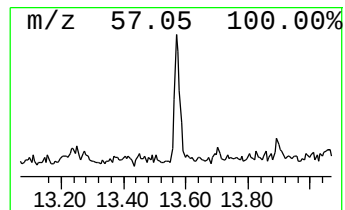
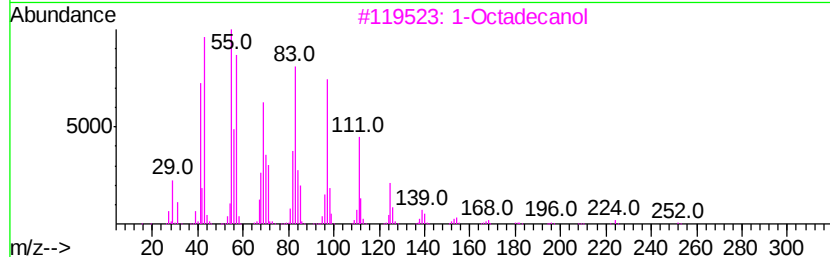
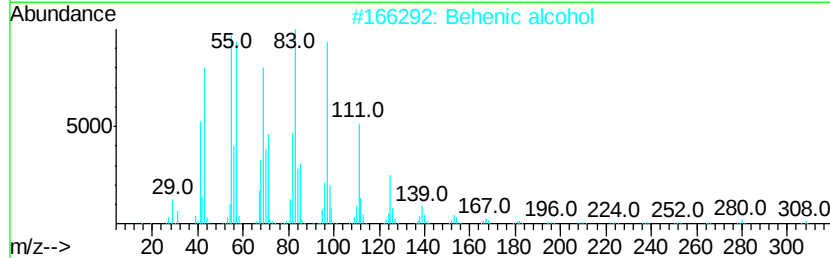
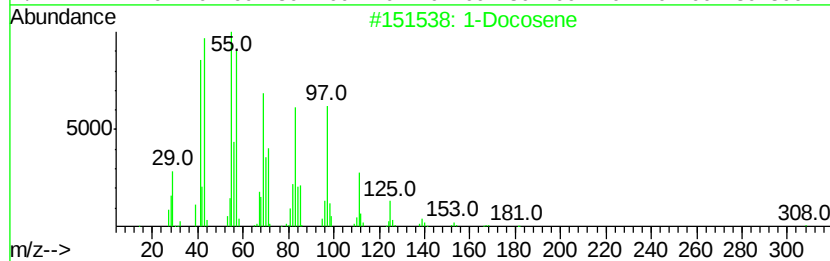
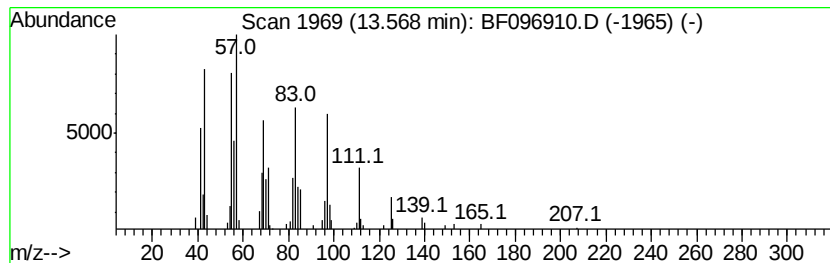
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	3.73 ng	113577	Chrysene-d12	13.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		Behenic alcohol	326	C22H46O	000661-19-8	91
3		1-Octadecanol	270	C18H38O	000112-92-5	91
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072017\
Data File : BF096910.D
Acq On : 20 Jul 2017 17:19
Operator : SJ/JU
Sample : I4282-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
FK-GF-02-007-A

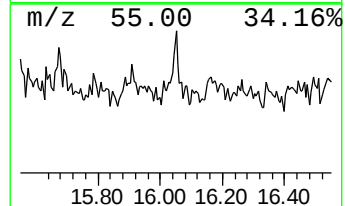
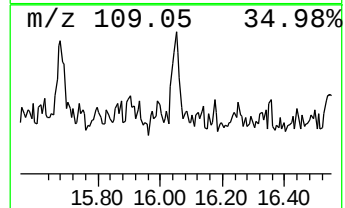
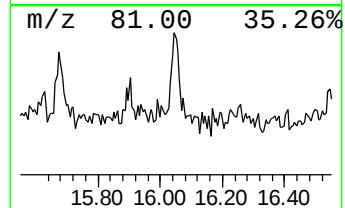
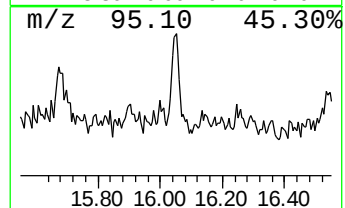
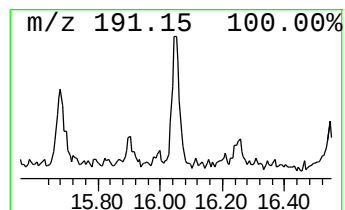
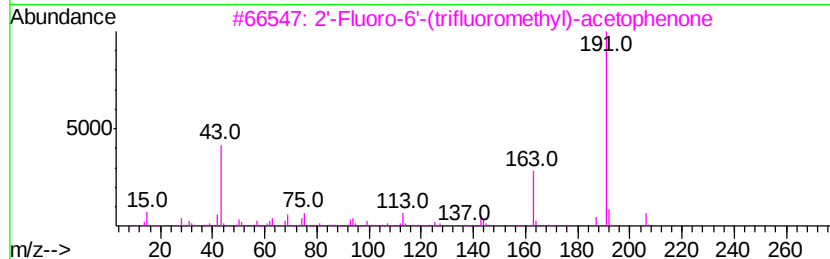
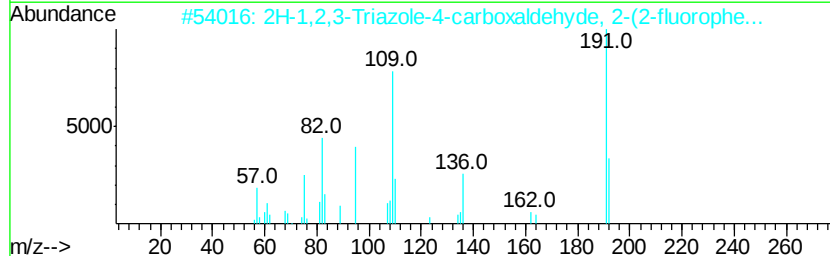
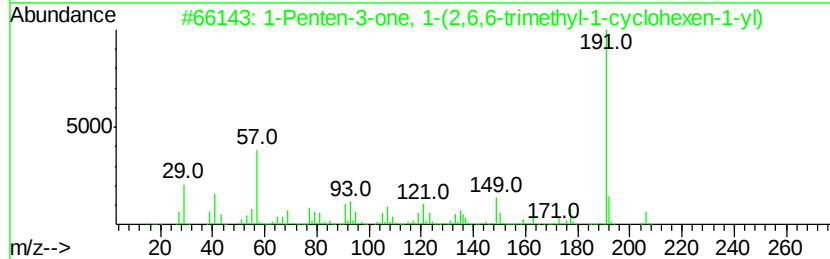
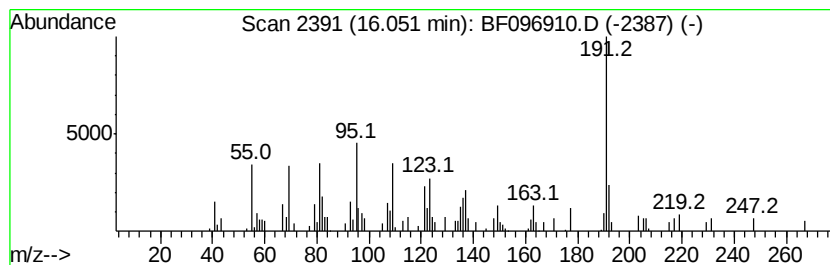
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.05 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	2.74 ng	78385	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
2		2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	38
3		2'-Fluoro-6'-(trifluoromethyl)-a...	206	C9H6F4O	174013-29-7	30
4		4-Fluoro-3-trifluoromethylbenzoi...	404	C22H32F4O2	1000338-68-3	27
5		3-Fluoro-5-trifluoromethylbenzoi...	376	C20H28F4O2	1000338-65-5	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072017\
Data File : BF096910.D
Acq On : 20 Jul 2017 17:19
Operator : SJ/JU
Sample : I4282-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-007-A

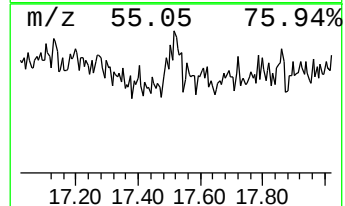
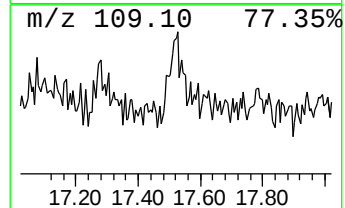
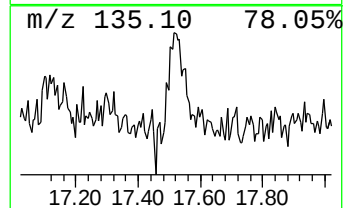
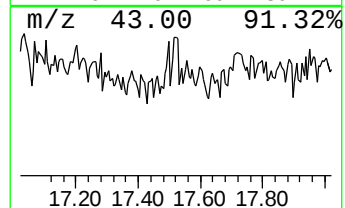
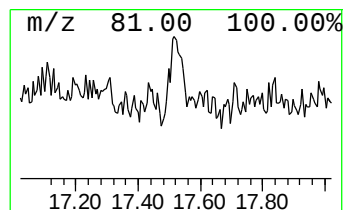
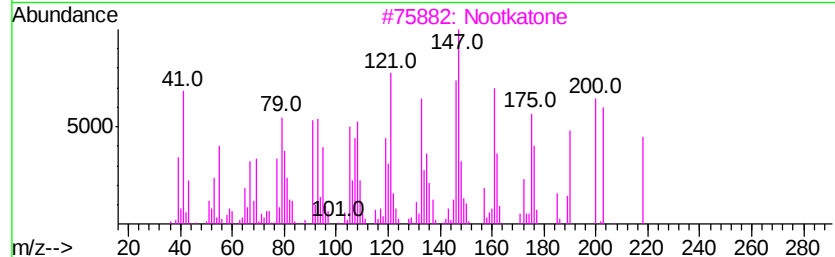
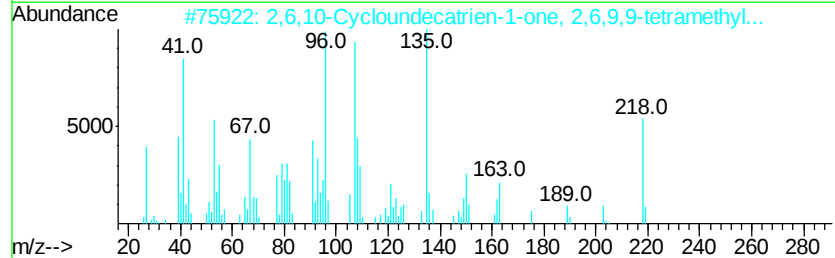
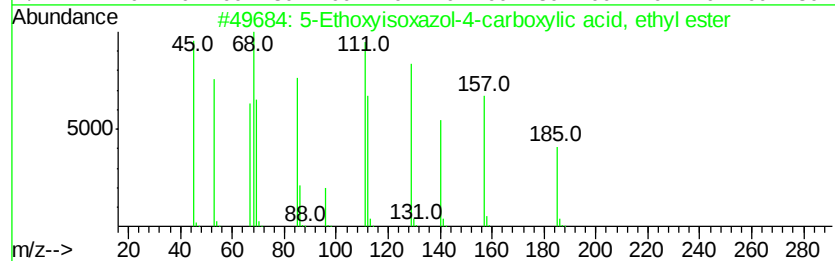
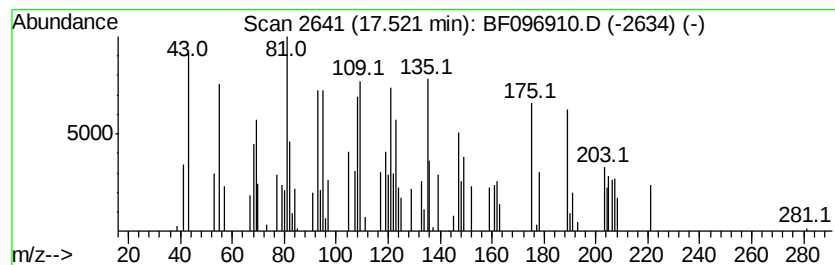
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Ethoxyisoxazol-4-carboxyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.52	3.36 ng	96197	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Ethoxyisoxazol-4-carboxylic ac...	185	C8H11N04	1000306-38-6	60
2		2,6,10-Cycloundecatrien-1-one, 2...	218	C15H22O	000471-05-6	45
3		Nootkatone	218	C15H22O	004674-50-4	40
4		1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	021391-98-0	35
5		3a,7-Methano-3aH-cyclopentacyclo...	206	C15H26	000469-91-0	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072017\
Data File : BF096910.D
Acq On : 20 Jul 2017 17:19
Operator : SJ/JU
Sample : I4282-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-007-A

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...	4.74	9.3	ng	306466	1	6.57	658621	20.0
unknown6.34	6.34	89.4	ng	2945300	1	6.57	658621	20.0
2-Phenanthrenol, ...	13.09	2.5	ng	76550	5	13.70	609221	20.0
1-Docosene	13.57	3.7	ng	113577	5	13.70	609221	20.0
unknown16.05	16.05	2.7	ng	78385	6	15.07	572269	20.0
5-Ethoxyisoxazol-...	17.52	3.4	ng	96197	6	15.07	572269	20.0