

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
 Data File : BF092214.D
 Acq On : 12 Jan 2017 18:17
 Operator : UM/SJ
 Sample : I1029-15
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-008

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-BF122116.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	3.990	181	184	188	rBV	60640	106081	2.38%	0.270%
2	4.721	245	248	259	rVB	1530678	2150356	48.22%	5.471%
3	5.190	287	289	296	rBV	3227806	3442527	77.20%	8.758%
4	6.265	380	383	385	rBV	3756674	4459145	100.00%	11.344%
5	6.367	390	392	394	rBV	4673191	4278333	95.95%	10.884%
6	6.596	409	412	414	rBV	1132954	1106787	24.82%	2.816%
7	6.745	423	425	428	rBV	2527199	3036801	68.10%	7.726%
8	7.167	459	462	464	rBV	2401319	2526180	56.65%	6.427%
9	7.876	522	524	527	rBV	1116147	1274512	28.58%	3.242%
10	8.962	616	619	621	rBV	4318633	4061786	91.09%	10.334%
11	9.362	652	654	656	rBV	313986	271738	6.09%	0.691%
12	9.625	675	677	680	rBV	1370448	1385760	31.08%	3.526%
13	10.082	715	717	718	rVB	48487	63092	1.41%	0.161%
14	10.413	744	746	749	rBV2	2025133	2436468	54.64%	6.199%
15	10.551	756	758	761	rBV	104375	132170	2.96%	0.336%
16	10.996	795	797	798	rBV2	76582	75308	1.69%	0.192%
17	11.099	804	806	809	rBV	1050367	1390395	31.18%	3.537%
18	11.659	853	855	859	rBV2	313824	303911	6.82%	0.773%
19	12.437	921	923	929	rBV	73825	90911	2.04%	0.231%
20	12.539	929	932	934	rVB2	44242	58479	1.31%	0.149%
21	12.688	943	945	948	rVB	2887889	3335702	74.81%	8.486%
22	13.602	1022	1025	1034	rBV	185134	283443	6.36%	0.721%
23	13.728	1034	1036	1039	rBV	950574	1008559	22.62%	2.566%
24	14.231	1077	1080	1086	rBV	57110	116163	2.61%	0.296%
25	14.517	1101	1105	1109	rBV3	19073	48479	1.09%	0.123%
26	14.642	1114	1116	1119	rVV	54059	56937	1.28%	0.145%
27	14.814	1128	1131	1132	rBV	38123	57467	1.29%	0.146%
28	14.837	1132	1133	1138	rVB2	38741	68271	1.53%	0.174%
29	15.088	1152	1155	1158	rBV	733571	850713	19.08%	2.164%
30	15.385	1178	1181	1188	rVB7	14928	45812	1.03%	0.117%
31	15.500	1188	1191	1193	rBV	49163	70569	1.58%	0.180%
32	15.557	1193	1196	1198	rBV3	23491	60581	1.36%	0.154%
33	16.448	1271	1274	1280	rVB3	66786	146524	3.29%	0.373%
34	16.551	1280	1283	1284	rVV	45701	97566	2.19%	0.248%

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ALS Vial : 11 Sample Multiplier: 1

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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

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35	16.586	1284	1286	1291	rVB	117188	226329	5.08%	0.576%
36	16.814	1302	1306	1312	rVB5	42565	113200	2.54%	0.288%
37	17.466	1360	1363	1367	rBV5	19611	69652	1.56%	0.177%

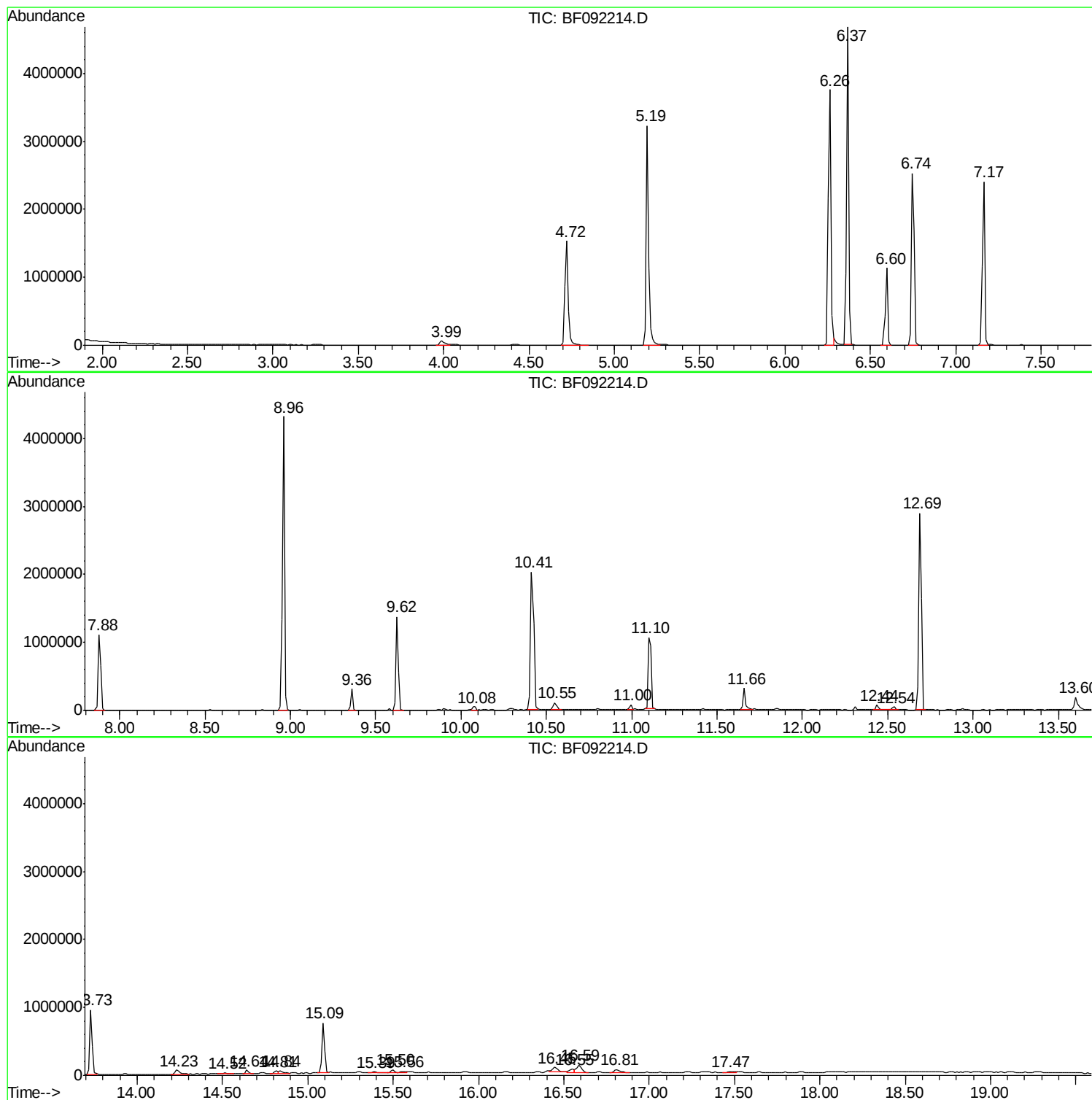
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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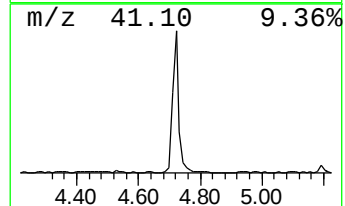
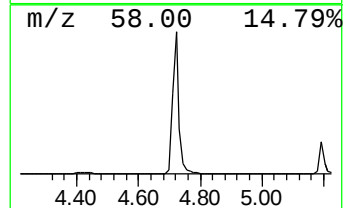
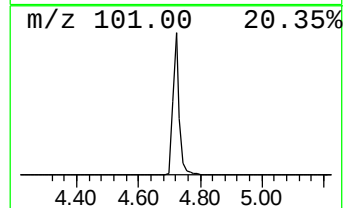
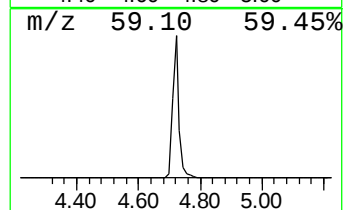
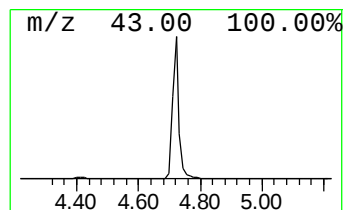
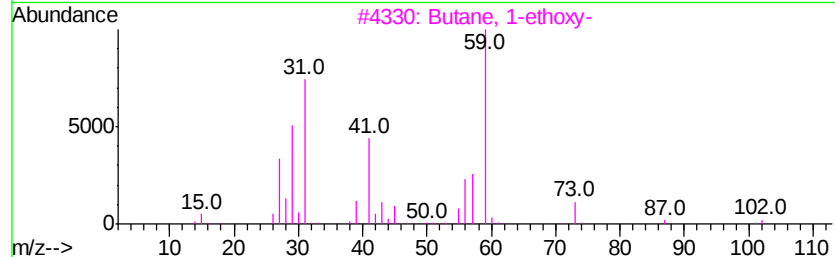
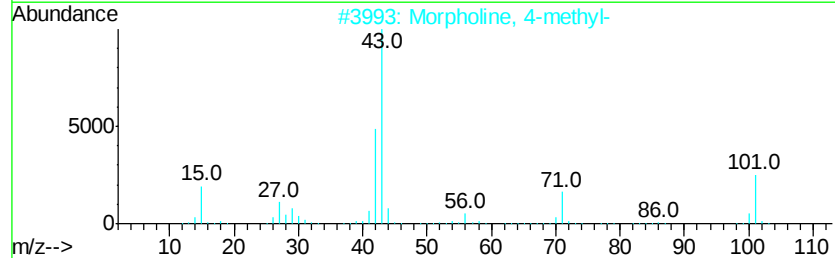
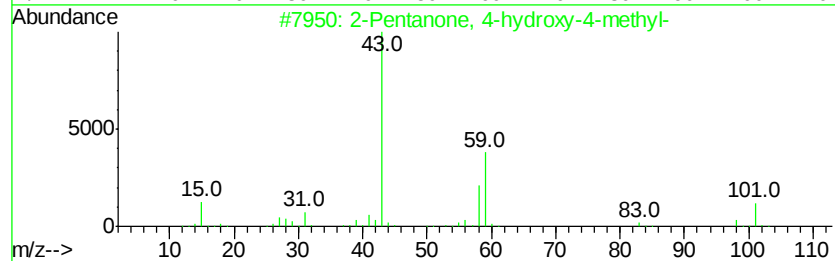
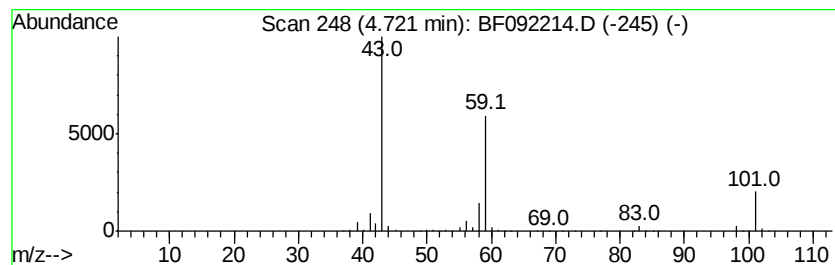
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.72	38.86 ng	2150360	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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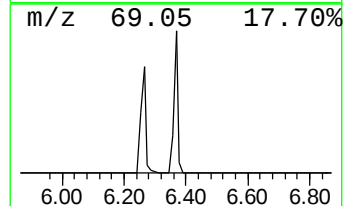
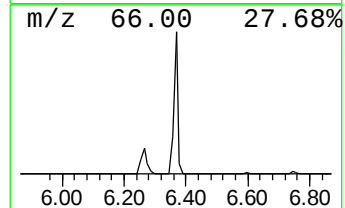
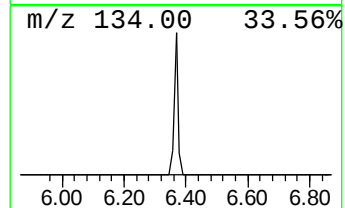
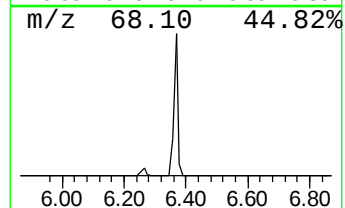
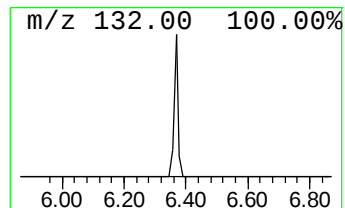
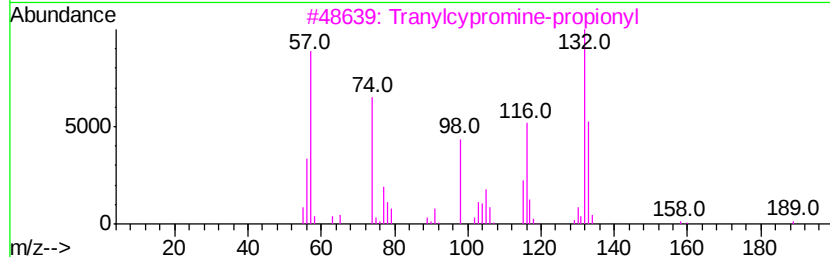
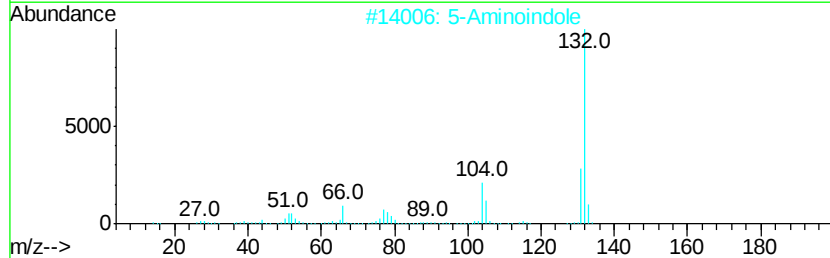
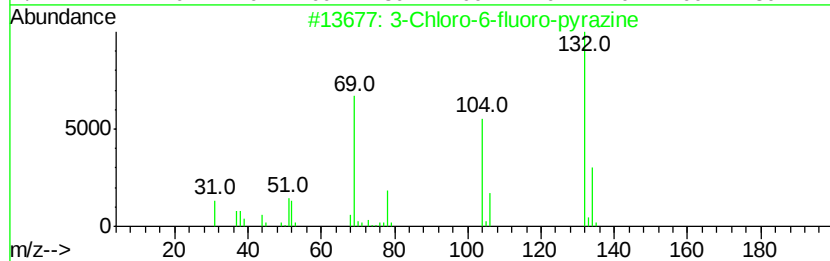
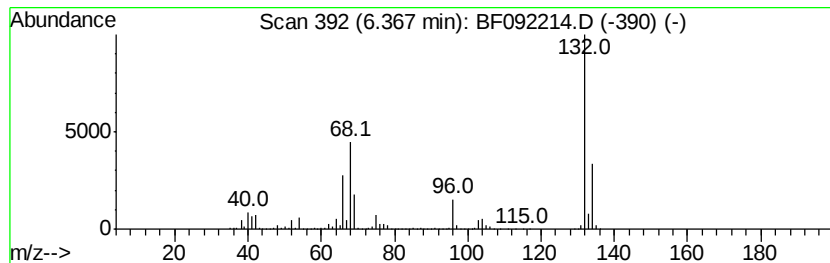
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	77.31 ng	4278330	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9	
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	



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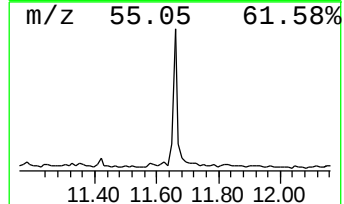
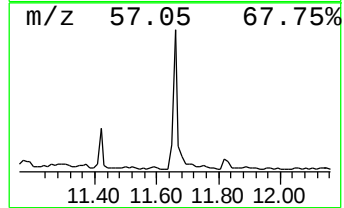
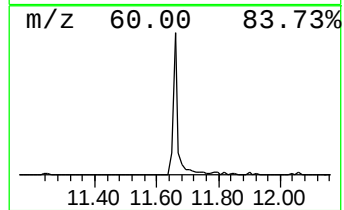
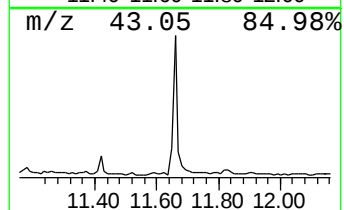
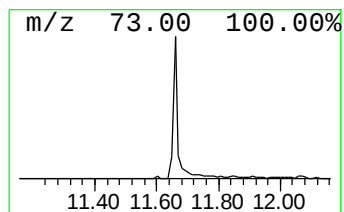
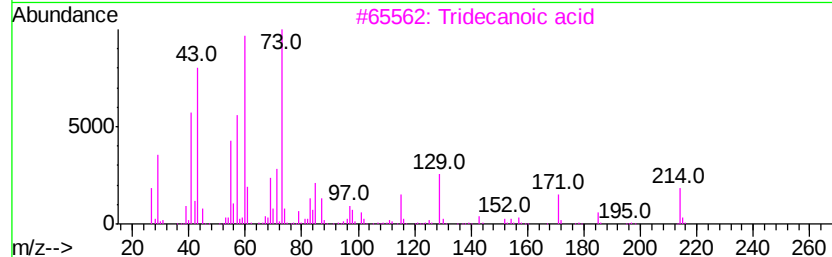
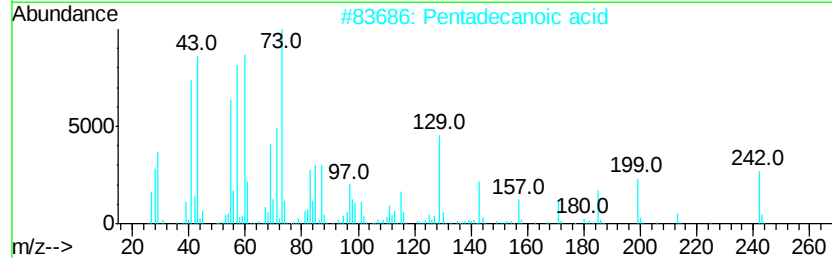
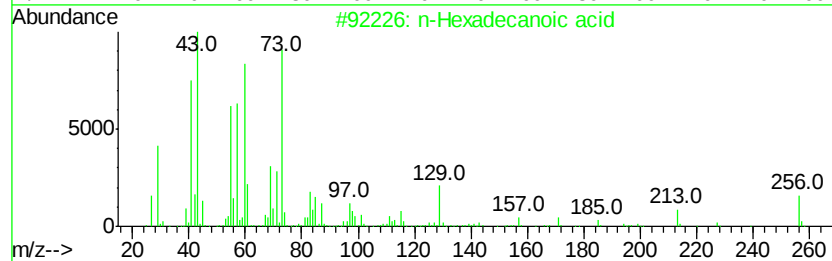
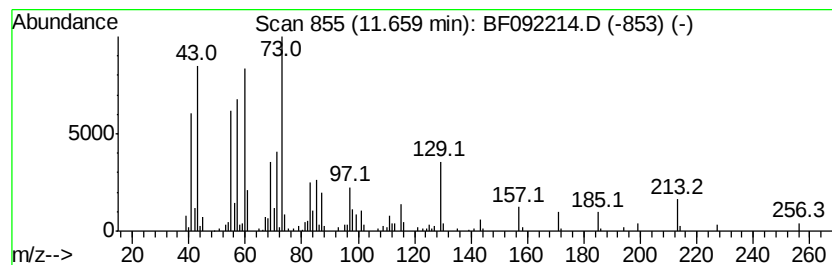
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	4.37 ng	303911	Phenanthrene-d10	11.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Nonanoic acid	158	C9H18O2	000112-05-0	43



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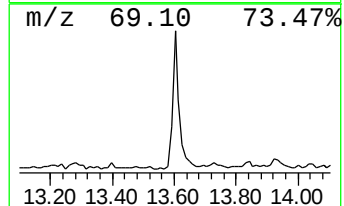
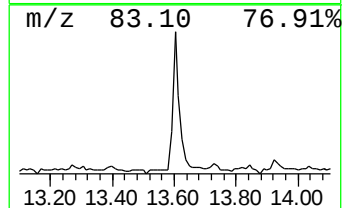
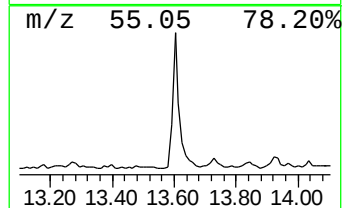
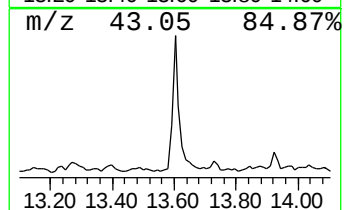
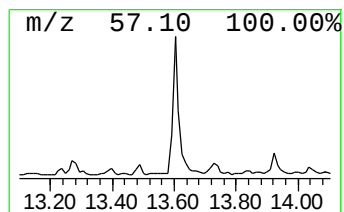
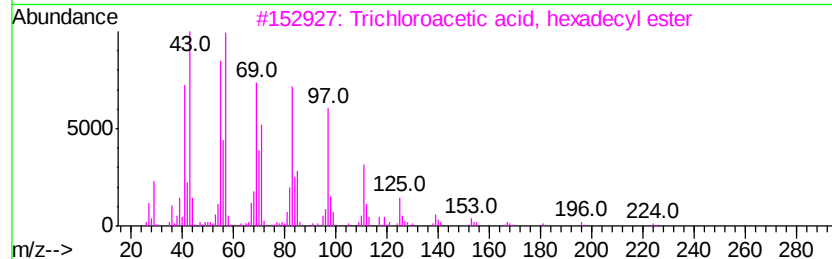
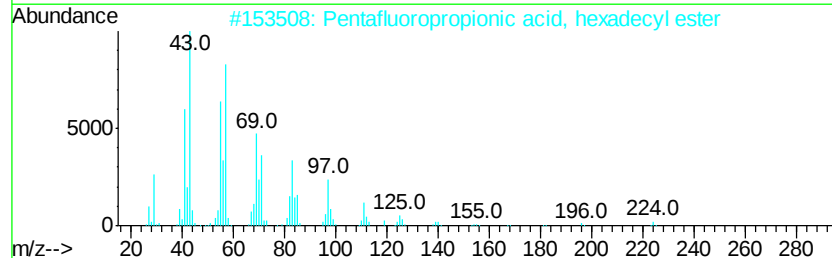
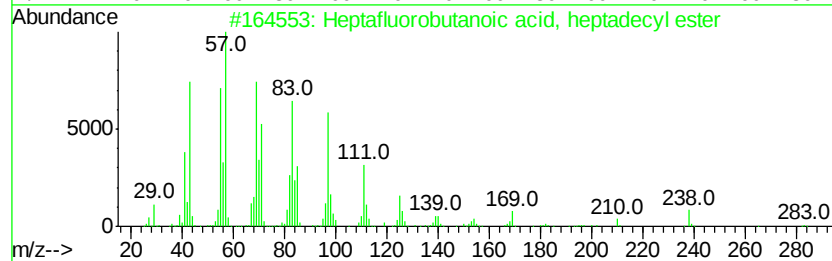
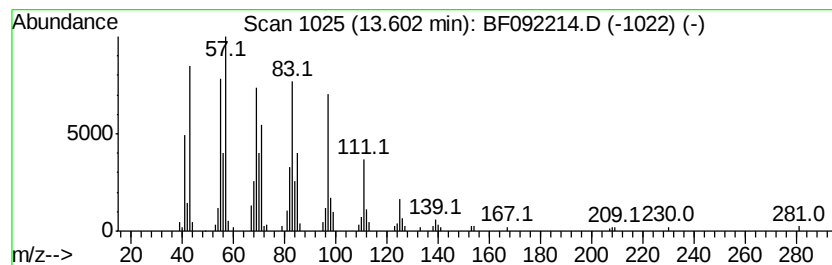
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutanoic acid, h... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	5.62 ng	283443	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91



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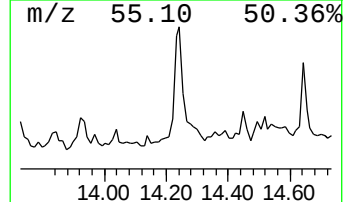
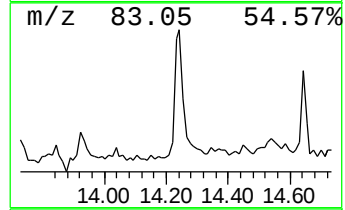
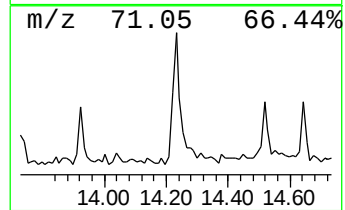
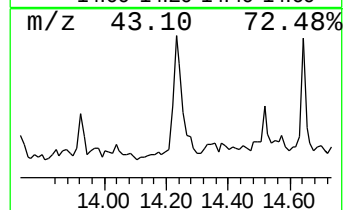
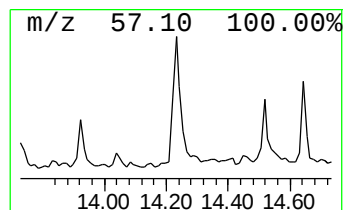
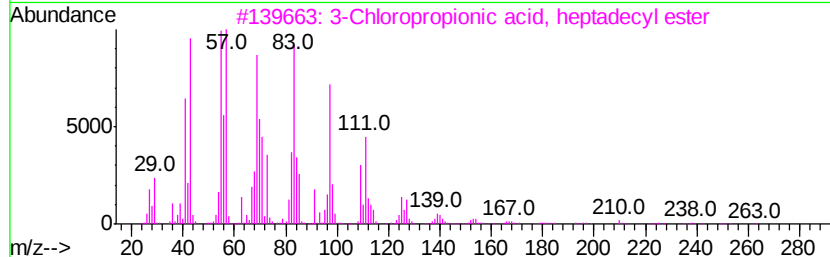
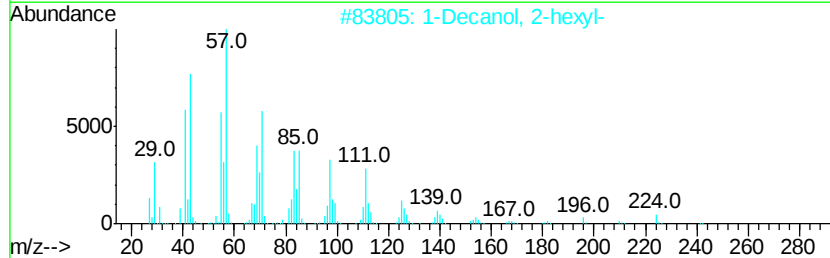
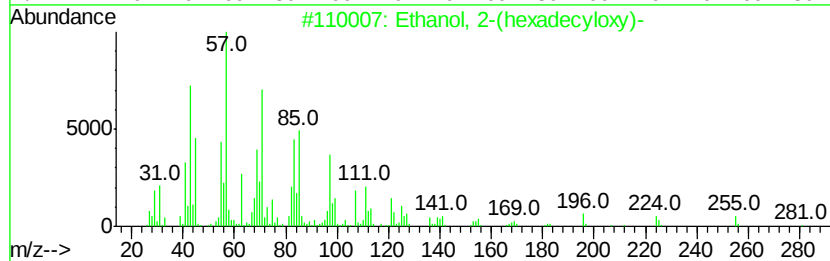
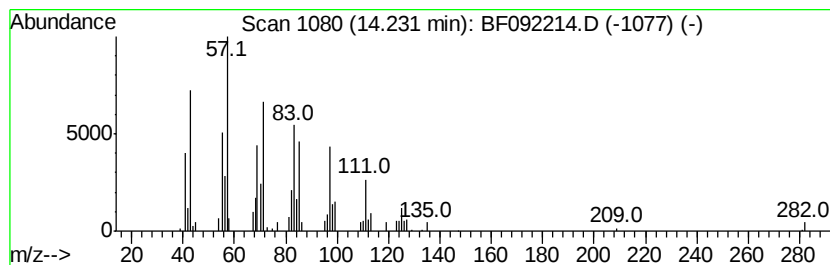
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Peak Number 6 Ethanol, 2-(hexadecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.30 ng	116163	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	80
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	70
4		1-Octadecanol	270	C18H38O	000112-92-5	64
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	62



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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-008

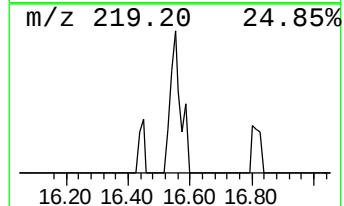
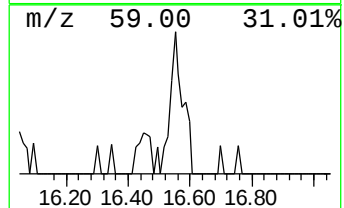
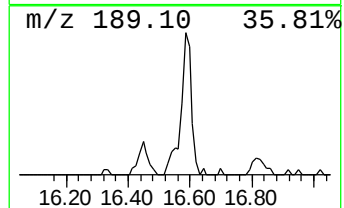
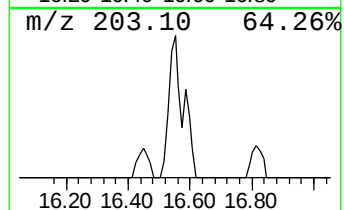
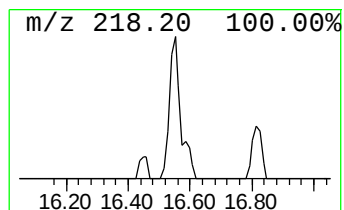
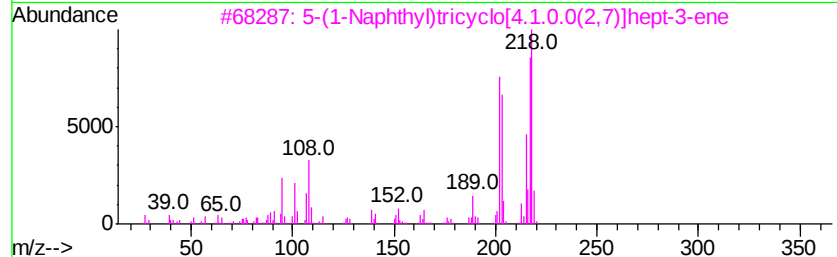
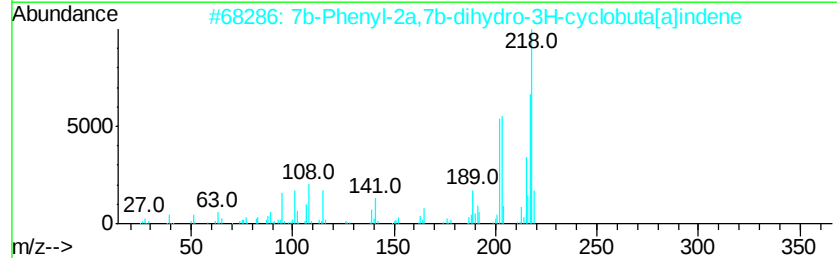
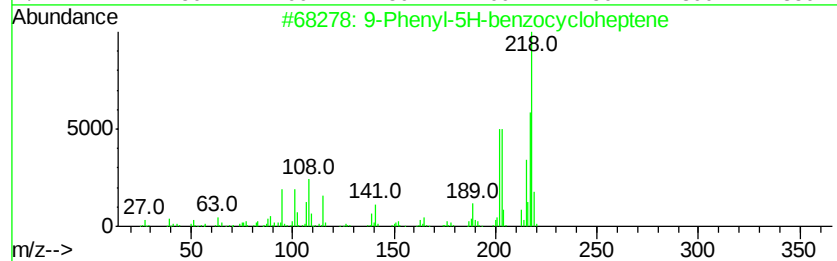
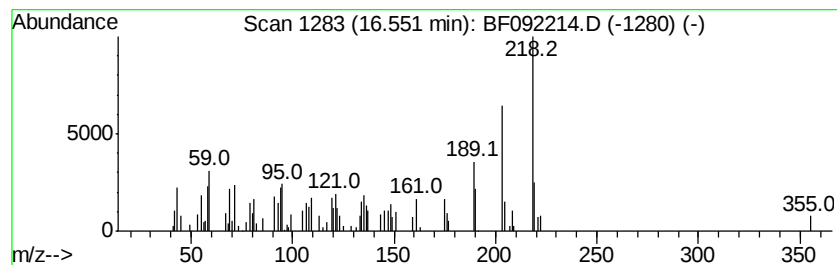
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 9-Phenyl-5H-benzocycloheptene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.29 ng	97566	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	52
2		7b-Phenyl-2a,7b-dihydro-3H-cyclo...	218	C17H14	138089-70-0	50
3		5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	50
4		4,4,9,9-Tetramethyl-4,9-disilatr...	218	C12H18Si2	1000280-67-7	47
5		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092214.D
Acq On : 12 Jan 2017 18:17
Operator : UM/SJ
Sample : I1029-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-008

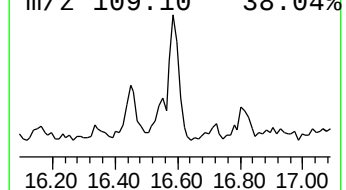
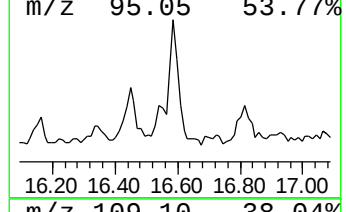
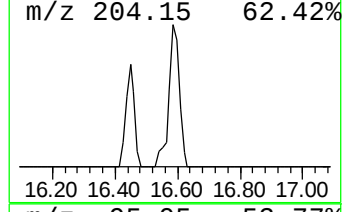
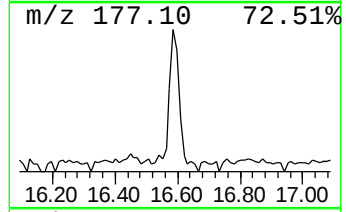
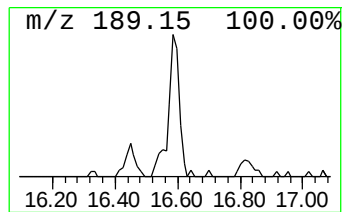
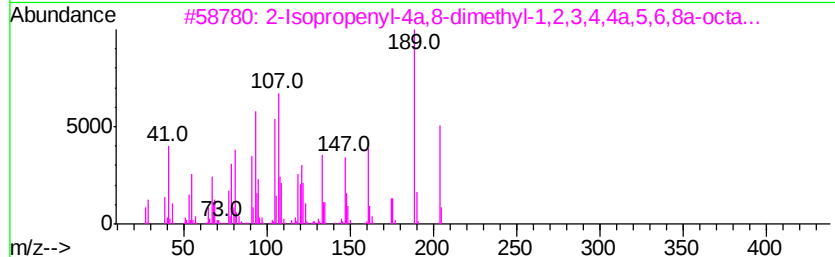
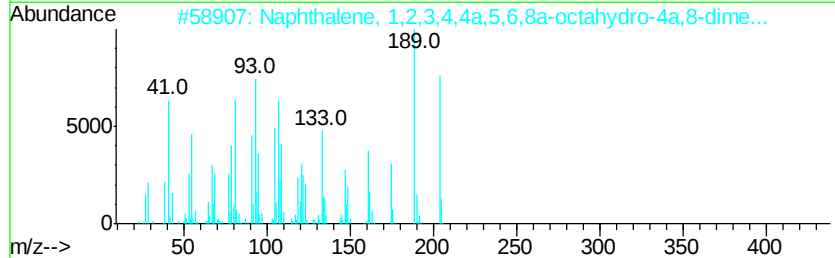
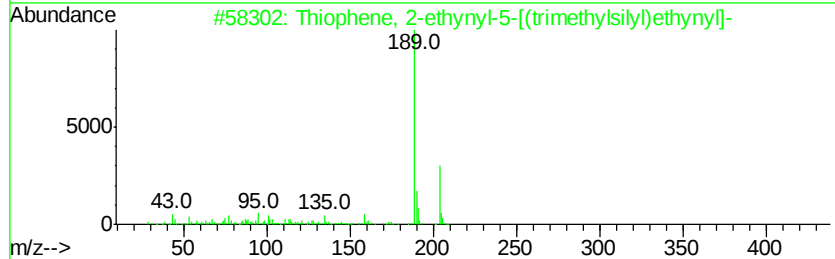
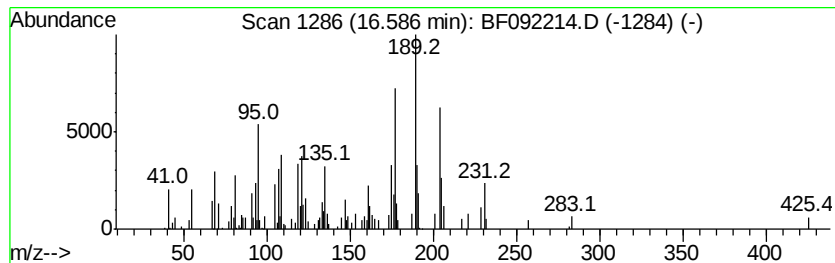
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Thiophene, 2-ethynyl-5-[(tr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	5.32 ng	226329	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	50
2		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	49
3		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	43
4		3H-1,2-Dithiole-3-thione, 5-tert...	204	C8H12S3	013120-76-8	43
5		1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092214.D
Acq On : 12 Jan 2017 18:17
Operator : UM/SJ
Sample : I1029-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-008

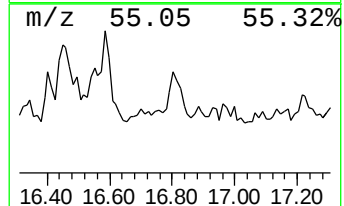
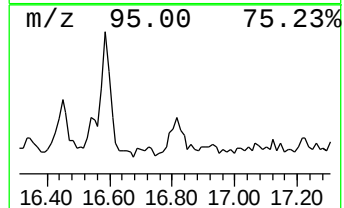
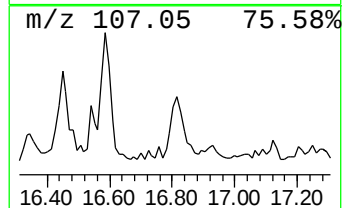
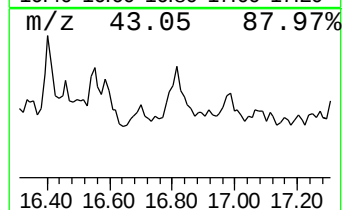
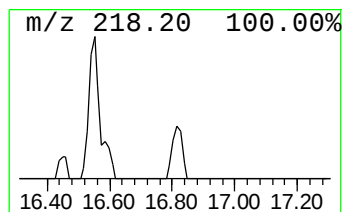
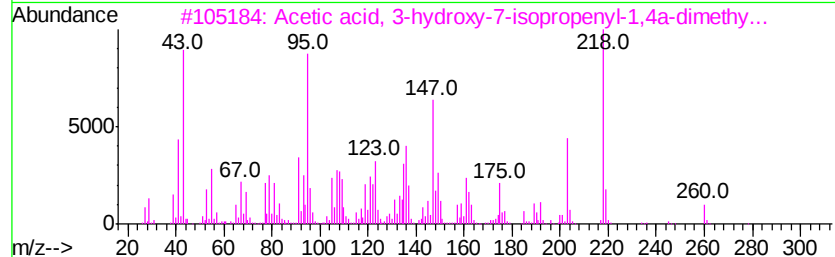
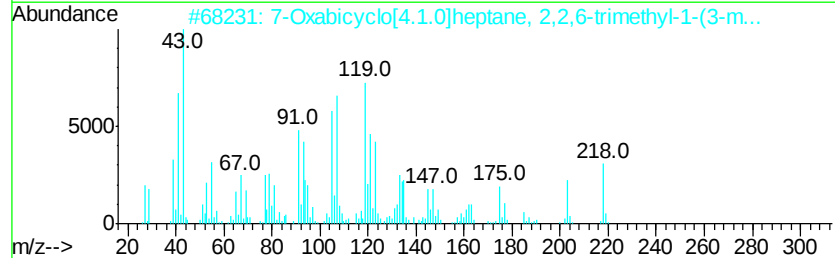
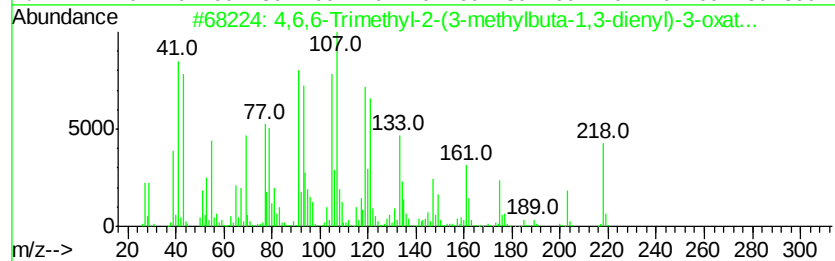
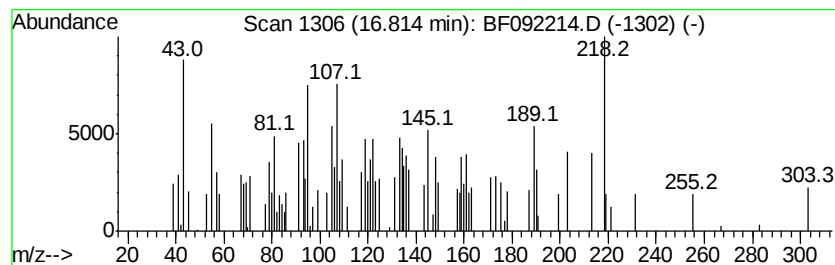
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 4,6,6-Trimethyl-2-(3-methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	2.66 ng	113200	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,6,6-Trimethyl-2-(3-methylbuta-...	218	C15H22O	1000190-22-2	64
2			7-Oxabicyclo[4.1.0]heptane, 2,2,...	218	C15H22O	070038-20-9	49
3			Acetic acid, 3-hydroxy-7-isoprop...	278	C17H26O3	1000187-37-6	38
4			6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	38
5			5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
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Operator : UM/SJ
Sample : I1029-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-008

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.72	38.9	ng	2150360	1	6.60	1106790	20.0
unknown6.37	6.37	77.3	ng	4278330	1	6.60	1106790	20.0
n-Hexadecanoic acid	11.66	4.4	ng	303911	4	11.11	1390400	20.0
Heptafluorobutano...	13.60	5.6	ng	283443	5	13.73	1008560	20.0
Ethanol, 2-(hexad...	14.23	2.3	ng	116163	5	13.73	1008560	20.0
1,1,4a-Trimethyl-...	16.45	3.4	ng	146524	6	15.09	850713	20.0
9-Phenyl-5H-benzo...	16.55	2.3	ng	97566	6	15.09	850713	20.0
Thiophene, 2-ethy...	16.59	5.3	ng	226329	6	15.09	850713	20.0
4,6,6-Trimethyl-2...	16.81	2.7	ng	113200	6	15.09	850713	20.0