

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111616\
 Data File : BF091192.D
 Acq On : 16 Nov 2016 17:09
 Operator : UM/SJ
 Sample : H5636-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CPS043041

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-BF110316.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	4.738	265	267	285	rBV	558183	710766	9.75%	1.629%
2	5.196	305	307	325	rBV	1343368	1977588	27.13%	4.531%
3	6.270	399	401	409	rBV	1178309	1341869	18.41%	3.075%
4	6.384	409	411	414	rBV	3608231	3472402	47.63%	7.956%
5	6.613	429	431	441	rVB	874711	1116341	15.31%	2.558%
6	6.773	443	445	448	rBV	4355780	4299285	58.98%	9.851%
7	7.196	479	482	484	rBV	3173094	3844709	52.74%	8.809%
8	7.904	542	544	547	rBV	1544391	1530224	20.99%	3.506%
9	8.316	579	580	588	rBV	150778	244164	3.35%	0.559%
10	8.990	636	639	642	rBV	5817029	6376864	87.48%	14.611%
11	9.390	672	674	676	rBV	359075	308873	4.24%	0.708%
12	9.653	695	697	700	rBV	1348665	1607169	22.05%	3.682%
13	10.453	764	767	769	rBV	2610379	3151529	43.23%	7.221%
14	11.139	824	827	829	rBV	1928234	1710859	23.47%	3.920%
15	11.379	846	848	852	rVV	276428	320333	4.39%	0.734%
16	12.202	917	920	923	rBV	655484	759135	10.41%	1.739%
17	12.728	963	966	969	rBV	4863981	7289824	100.00%	16.703%
18	13.185	1004	1006	1007	rBV	77292	76621	1.05%	0.176%
19	13.642	1043	1046	1055	rBV	125293	175242	2.40%	0.402%
20	13.768	1055	1057	1060	rBV	1286530	1617179	22.18%	3.705%
21	14.237	1096	1098	1105	rBV	254984	294937	4.05%	0.676%
22	14.625	1129	1132	1134	rBV	110896	155280	2.13%	0.356%
23	15.140	1175	1177	1180	rBV	975496	1262664	17.32%	2.893%

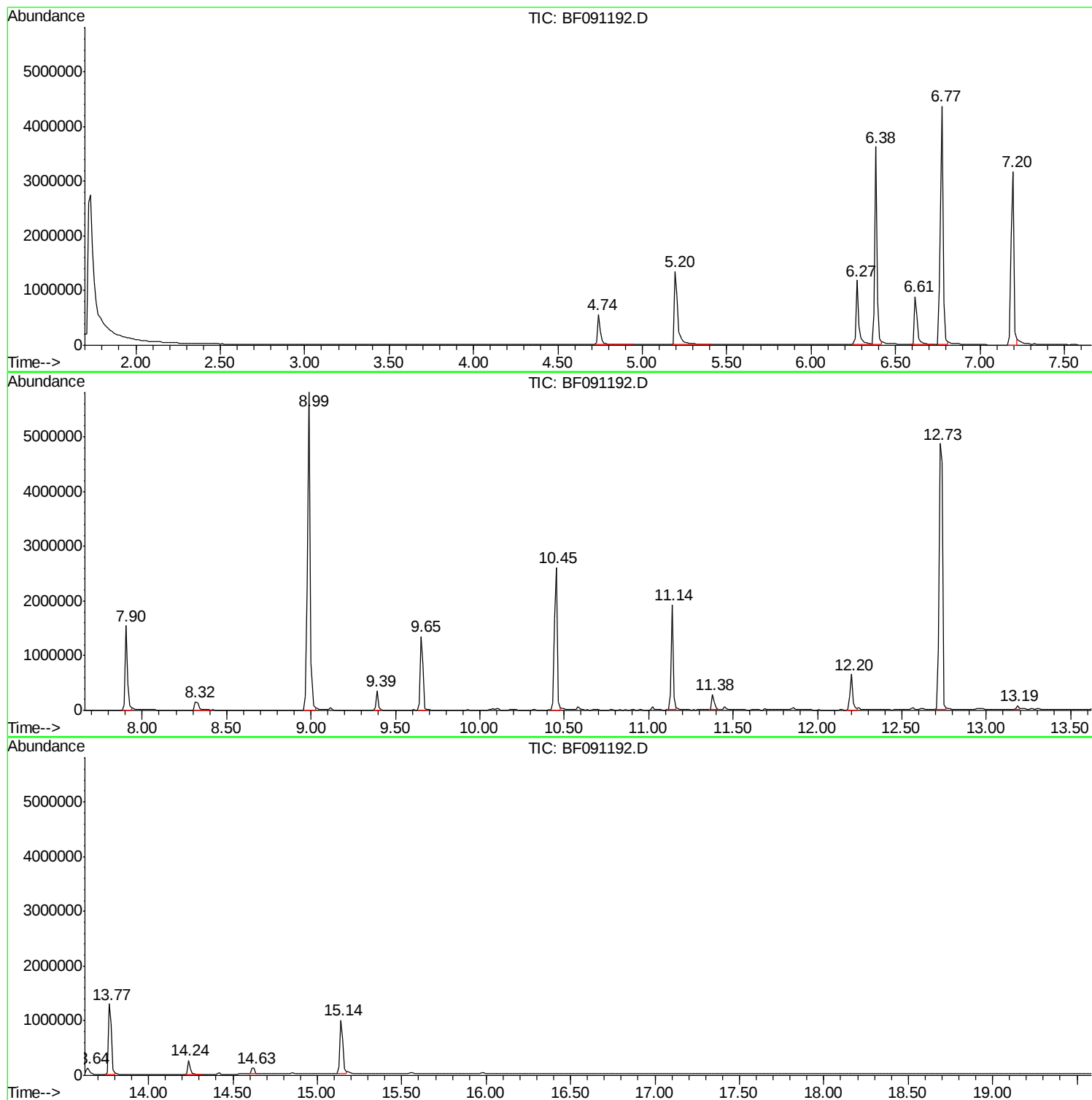
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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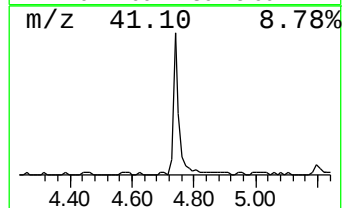
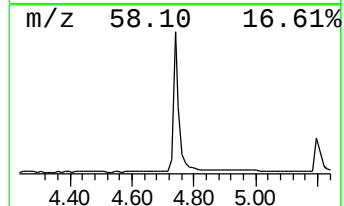
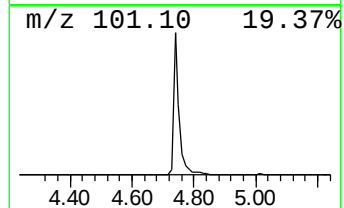
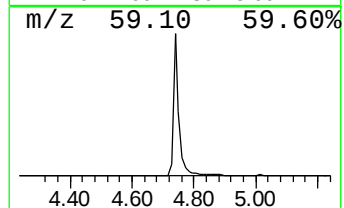
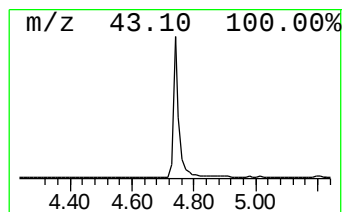
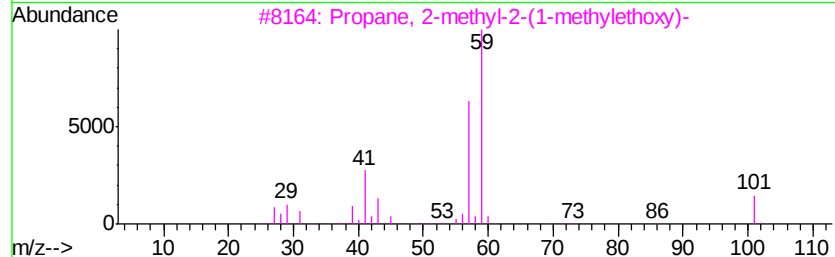
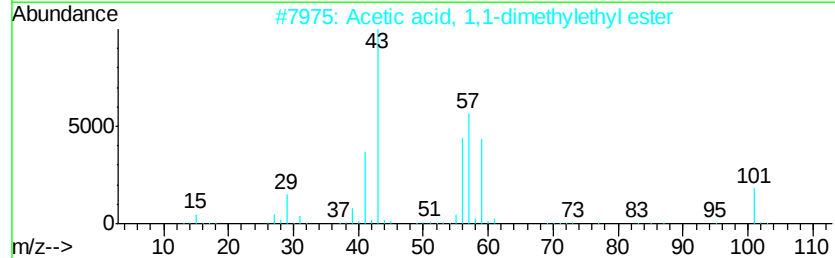
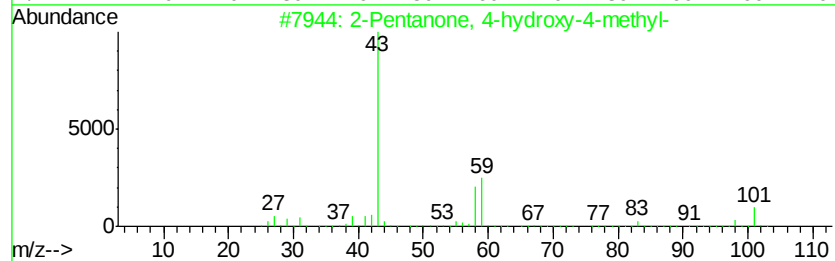
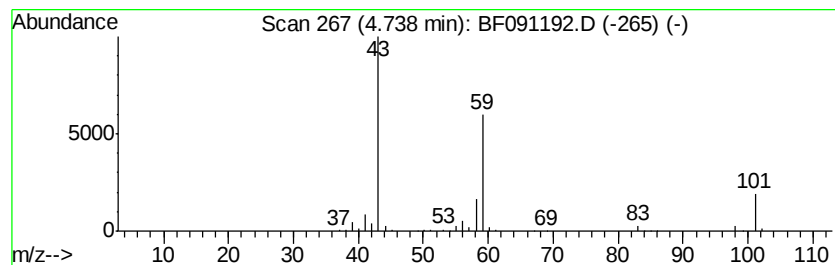
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.74	12.73 ng	710766	1,4-Dichlorobenzene-d4	6.61

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		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Acetone	58	C3H6O	000067-64-1	9



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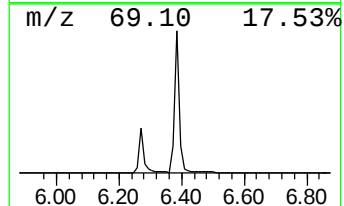
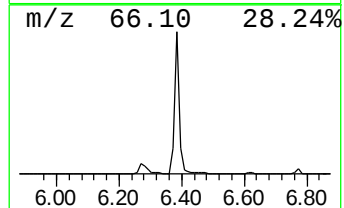
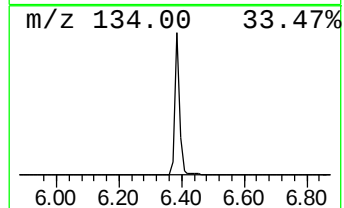
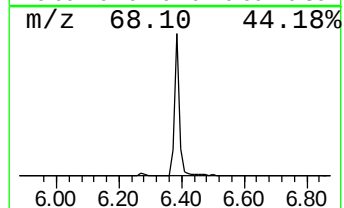
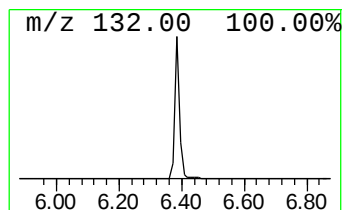
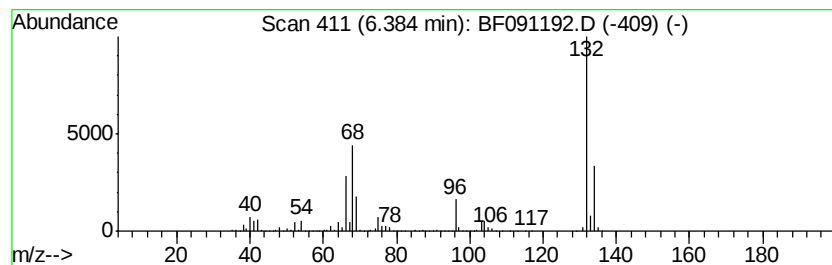
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	62.21 ng	3472400	1,4-Dichlorobenzene-d4	6.61

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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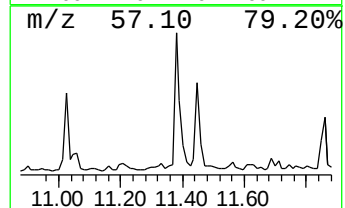
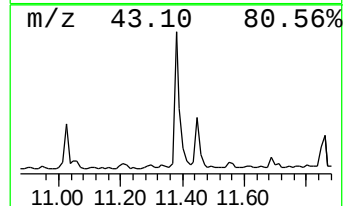
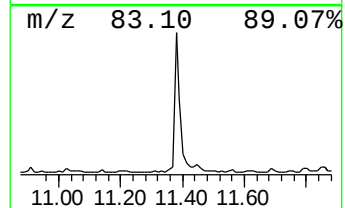
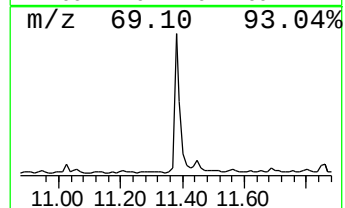
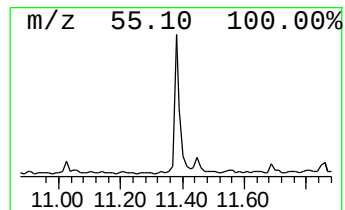
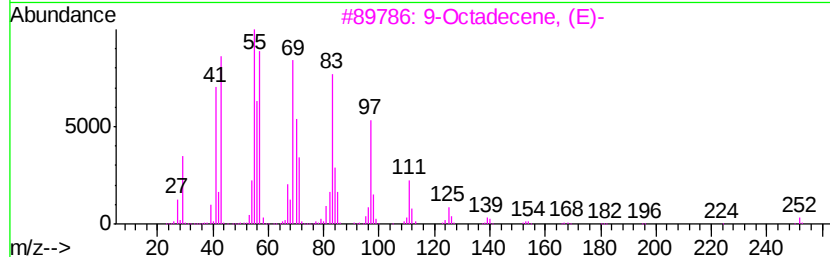
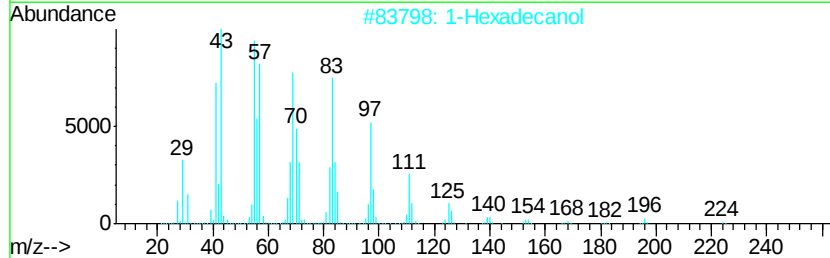
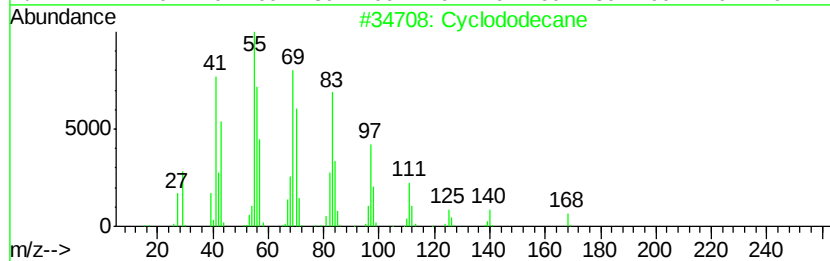
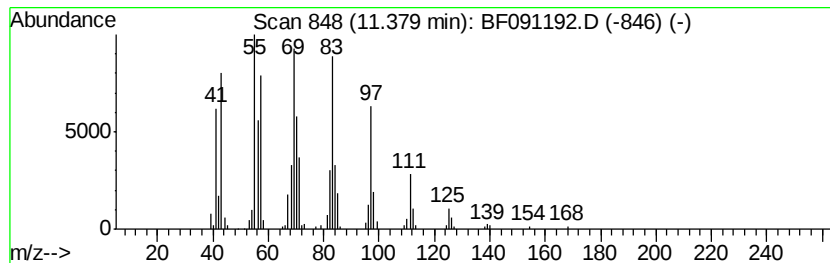
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Peak Number 4 Cyclododecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.38	3.74 ng	320333	Phenanthrene-d10	11.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclododecane	168	C12H24	000294-62-2	95
2		1-Hexadecanol	242	C16H34O	036653-82-4	94
3		9-Octadecene, (E)-	252	C18H36	007206-25-9	91
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5		1-Tridecanol	200	C13H28O	000112-70-9	91



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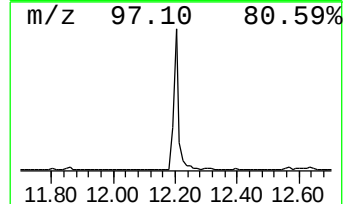
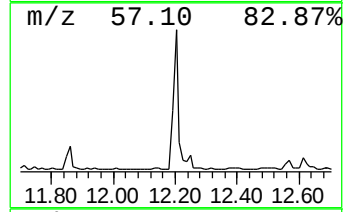
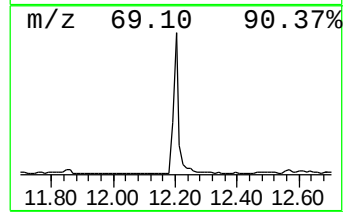
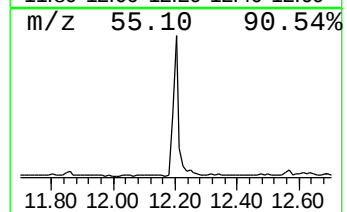
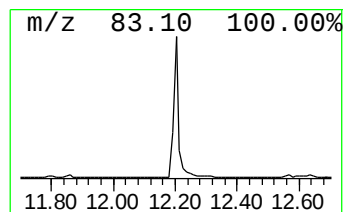
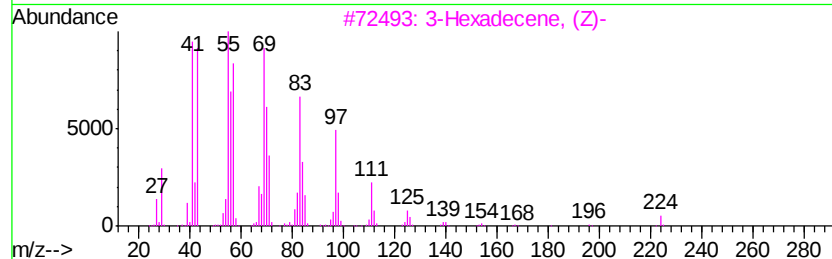
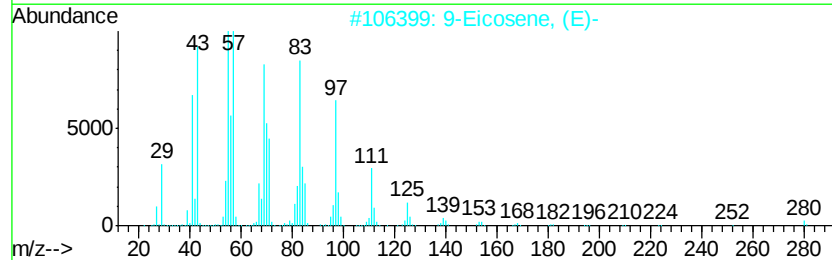
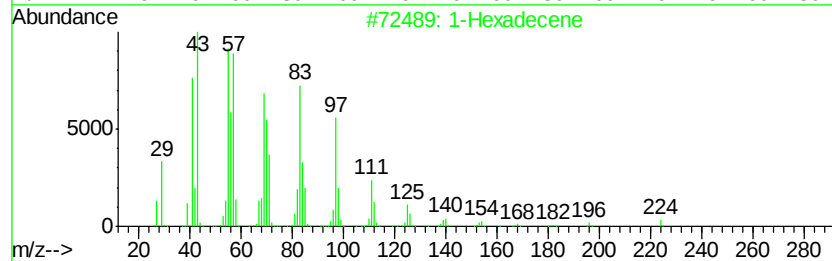
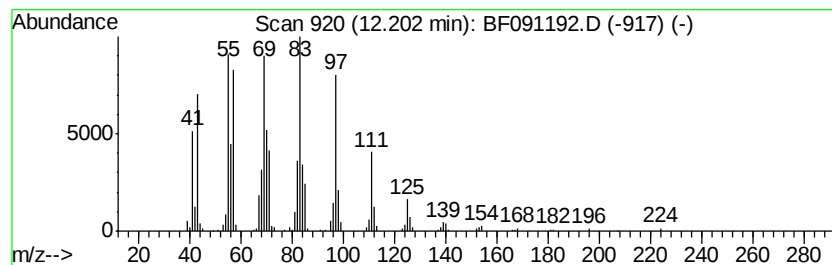
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.20	8.87 ng	759135	Phenanthrene-d10	11.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecene		224	C16H32	000629-73-2	92
2	9-Eicosene, (E)-		280	C20H40	074685-29-3	91
3	3-Hexadecene, (Z)-		224	C16H32	034303-81-6	91
4	9-Octadecene, (E)-		252	C18H36	007206-25-9	91
5	5-Octadecene, (E)-		252	C18H36	007206-21-5	91



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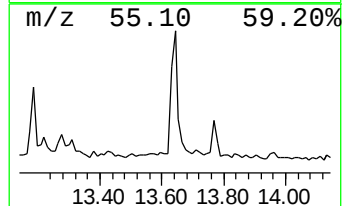
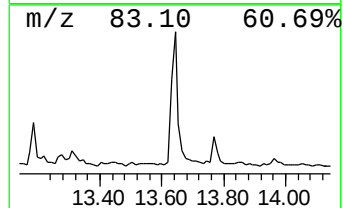
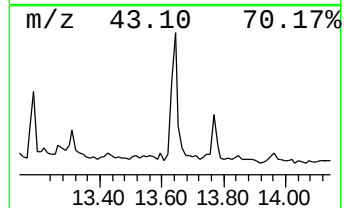
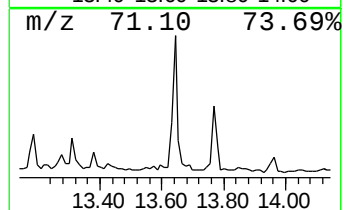
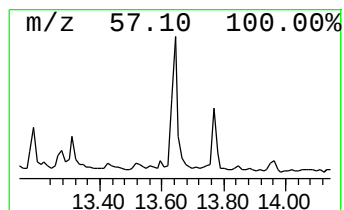
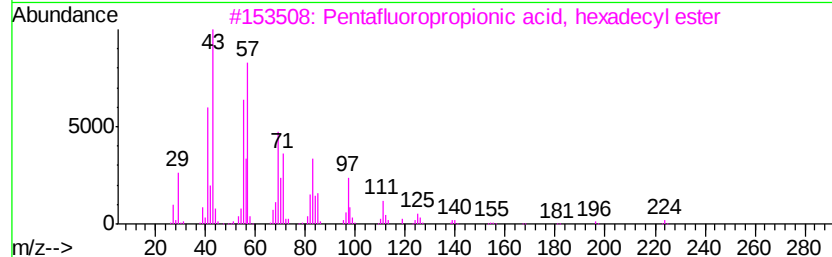
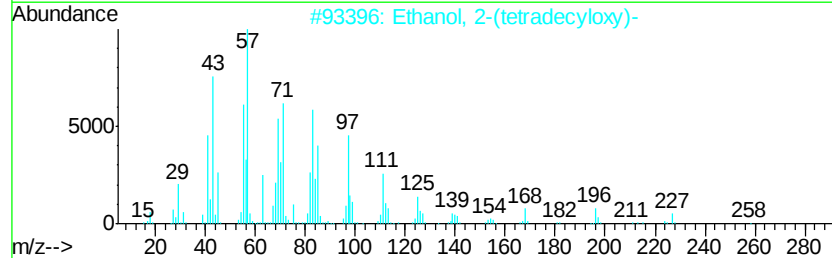
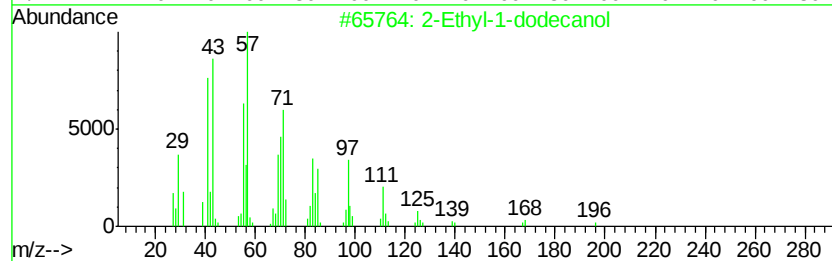
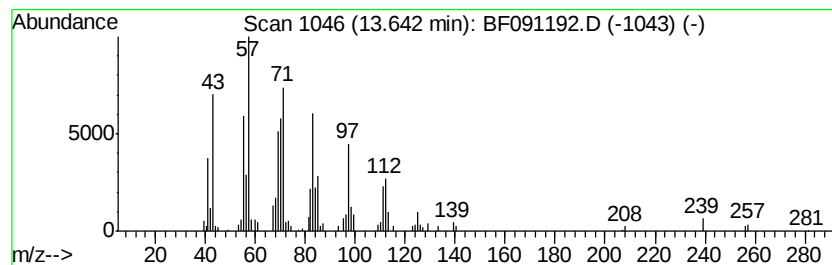
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Peak Number 6 2-Ethyl-1-dodecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	2.17 ng	175242	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	83
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	62
3		Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	62
4		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	1000280-07-7	62
5		Trichloroacetic acid, pentadecyl ester	372	C17H31Cl3O2	074339-53-0	58



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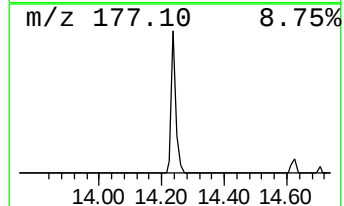
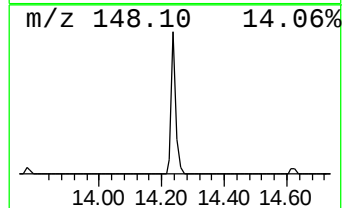
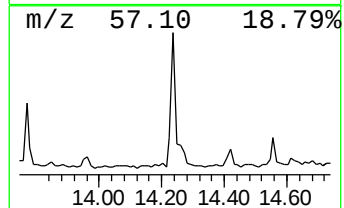
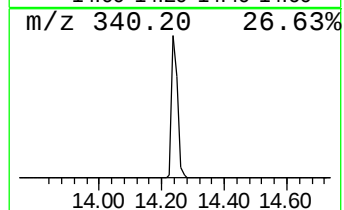
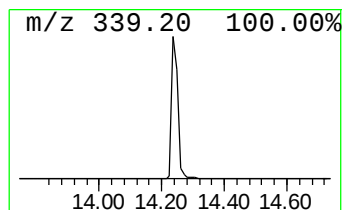
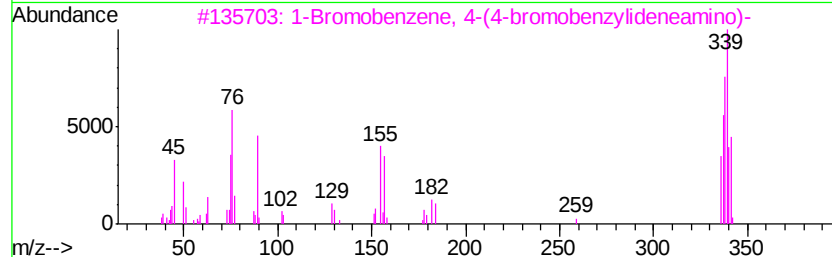
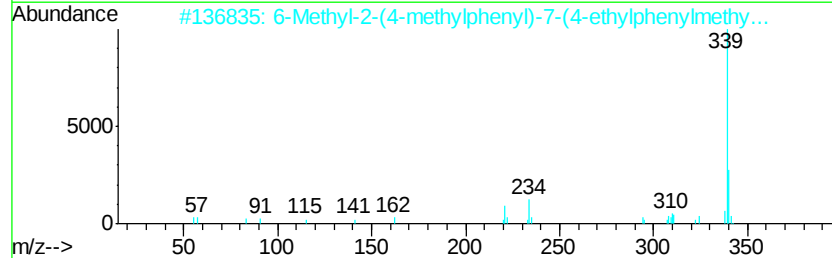
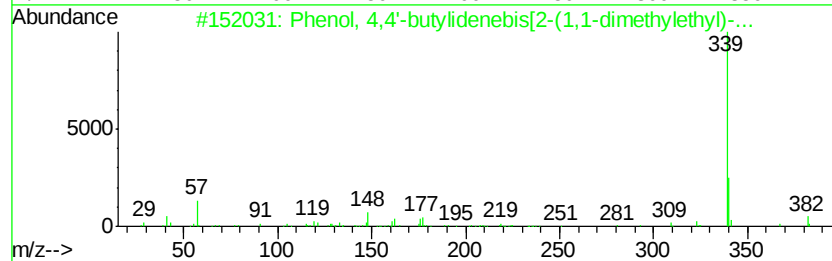
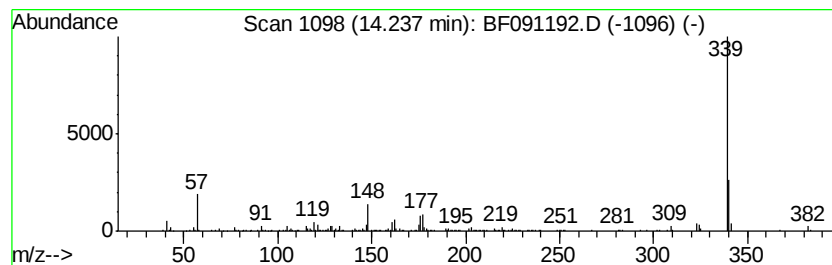
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Phenol, 4,4'-butylidenebis[... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	3.65 ng	294937	Chrysene-d12	13.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-butylidenebis[2-(1,...	382	C26H38O2	000085-60-9	98
2			6-Methyl-2-(4-methylphenyl)-7-(4...	339	C25H25N	080193-45-9	72
3			1-Bromobenzene, 4-(4-bromobenzyl...	337	C13H9Br2N	1000221-92-9	68
4			1-(2,6-Dimethylphenyl)iminomethyl...	339	C23H17N02	129086-91-5	64
5			6-Methyl-2-phenyl-7-(2,4,5-trime...	339	C25H25N	064002-76-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111616\
Data File : BF091192.D
Acq On : 16 Nov 2016 17:09
Operator : UM/SJ
Sample : H5636-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPS043041

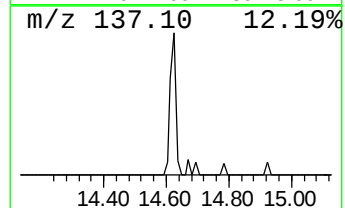
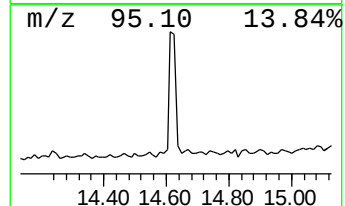
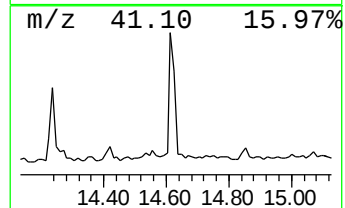
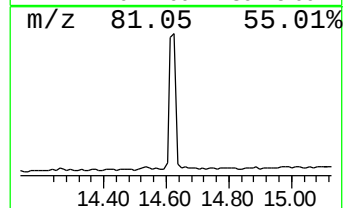
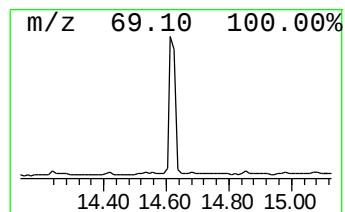
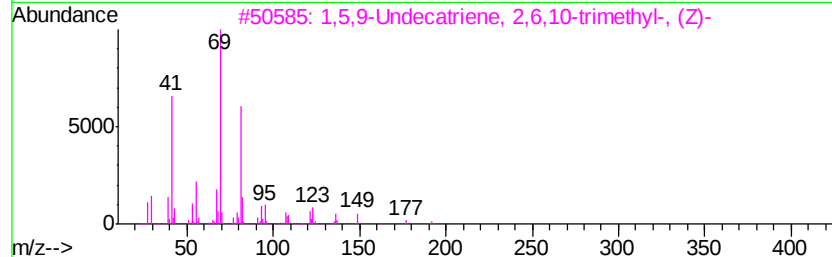
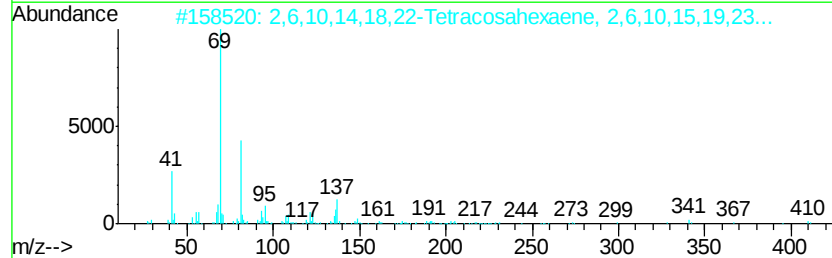
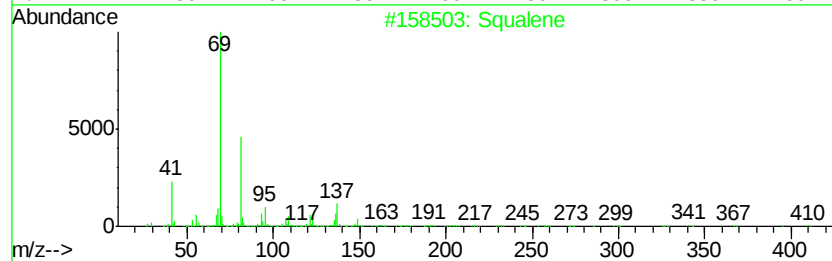
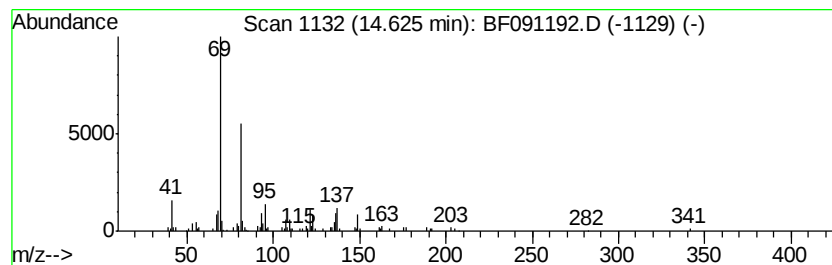
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.46 ng	155280	Perylene-d12	15.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
4		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111616\
Data File : BF091192.D
Acq On : 16 Nov 2016 17:09
Operator : UM/SJ
Sample : H5636-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CPS043041

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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...	4.74	12.7	ng	710766	1	6.61	1116340	20.0
unknown6.38	6.38	62.2	ng	3472400	1	6.61	1116340	20.0
Cyclododecane	11.38	3.7	ng	320333	4	11.14	1710860	20.0
1-Hexadecene	12.20	8.9	ng	759135	4	11.14	1710860	20.0
2-Ethyl-1-dodecanol	13.64	2.2	ng	175242	5	13.77	1617180	20.0
Phenol, 4,4'-buty...	14.24	3.6	ng	294937	5	13.77	1617180	20.0
Squalene	14.63	2.5	ng	155280	6	15.14	1262660	20.0