

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010917\
 Data File : BF092136.D
 Acq On : 9 Jan 2017 14:11
 Operator : UM/SJ
 Sample : H6244-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-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-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	4.059	187	190	193	rBV	20312	33459	1.03%	0.114%
2	4.127	193	196	201	rVB	47480	69849	2.15%	0.238%
3	4.767	249	252	256	rBV	713796	929576	28.64%	3.164%
4	5.167	284	287	291	rVB	28684	58565	1.80%	0.199%
5	5.236	291	293	301	rBV	1048815	1377256	42.43%	4.688%
6	6.150	371	373	378	rBV3	60234	112215	3.46%	0.382%
7	6.299	384	386	393	rBV	1236340	1265586	38.99%	4.308%
8	6.402	393	395	398	rBV	2008179	1926727	59.36%	6.558%
9	6.630	413	415	417	rBV	1440987	1330205	40.98%	4.528%
10	6.710	417	422	426	rVB2	29215	53257	1.64%	0.181%
11	6.790	426	429	431	rBV	2719181	3245913	100.00%	11.048%
12	7.202	462	465	467	rBV	1738875	1868354	57.56%	6.359%
13	7.236	467	468	470	rVB	71712	51932	1.60%	0.177%
14	7.659	503	505	507	rVB	241278	277052	8.54%	0.943%
15	7.739	507	512	516	rVB3	30607	66101	2.04%	0.225%
16	7.830	516	520	525	rBV2	36335	73635	2.27%	0.251%
17	7.922	525	528	530	rBV	633745	848766	26.15%	2.889%
18	8.070	538	541	545	rVV2	128378	161990	4.99%	0.551%
19	8.150	545	548	549	rVV	25313	33135	1.02%	0.113%
20	8.185	549	551	554	rVB2	38171	66333	2.04%	0.226%
21	8.505	577	579	582	rVB2	34231	37552	1.16%	0.128%
22	8.996	618	622	625	rVB	2753079	3225023	99.36%	10.977%
23	9.328	641	651	655	rBV8	21671	94190	2.90%	0.321%
24	9.396	655	657	659	rVV	453895	374460	11.54%	1.275%
25	9.613	673	676	678	rBV	42104	61642	1.90%	0.210%
26	9.671	678	681	683	rVV	974978	1003179	30.91%	3.415%
27	10.116	716	720	721	rBV2	38246	64881	2.00%	0.221%
28	10.459	747	750	752	rBV	639365	796023	24.52%	2.709%
29	10.585	759	761	764	rVB2	82208	93022	2.87%	0.317%
30	11.031	798	800	801	rBV	53605	47912	1.48%	0.163%
31	11.145	807	810	812	rBV	1104406	972031	29.95%	3.309%
32	11.214	812	816	819	rVB6	18799	41224	1.27%	0.140%
33	11.271	819	821	824	rVB4	15125	32785	1.01%	0.112%
34	11.362	828	829	830	rBV	31950	35527	1.09%	0.121%

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35	11.705	856	859	862	rBV2	281312	429077	13.22%	1.460%
36	12.151	896	898	901	rBV	54250	51179	1.58%	0.174%
37	12.402	917	920	925	rVB6	20974	42357	1.30%	0.144%
38	12.482	925	927	929	rBV	183604	191190	5.89%	0.651%
39	12.562	932	934	937	rVB2	89670	109744	3.38%	0.374%
40	12.631	937	940	946	rVB	60616	87999	2.71%	0.300%
41	12.734	946	949	952	rBV	2868895	3041698	93.71%	10.353%
42	12.974	966	970	971	rBV3	17673	34193	1.05%	0.116%
43	13.271	994	996	997	rBV	72974	111622	3.44%	0.380%
44	13.305	997	999	1001	rVV2	72466	160897	4.96%	0.548%
45	13.385	1004	1006	1008	rVV2	52916	125028	3.85%	0.426%
46	13.477	1012	1014	1016	rVV3	46653	102286	3.15%	0.348%
47	13.522	1016	1018	1021	rVV3	55369	128952	3.97%	0.439%
48	13.591	1021	1024	1027	rVV	243349	314537	9.69%	1.071%
49	13.637	1027	1028	1031	rVB	189291	263432	8.12%	0.897%
50	13.774	1037	1040	1043	rVB	1530979	1492703	45.99%	5.081%
51	14.265	1082	1083	1085	rBV2	29458	40474	1.25%	0.138%
52	14.562	1107	1109	1112	rVB2	43037	51216	1.58%	0.174%
53	14.620	1112	1114	1119	rVB	73240	91249	2.81%	0.311%
54	14.860	1132	1135	1137	rBV	53968	72830	2.24%	0.248%
55	15.145	1157	1160	1162	rBV	968175	1104486	34.03%	3.759%
56	15.191	1162	1164	1169	rVB	66840	106445	3.28%	0.362%
57	15.557	1194	1196	1198	rBV	72830	95524	2.94%	0.325%
58	15.603	1198	1200	1204	rVB4	17758	36974	1.14%	0.126%
59	15.991	1231	1234	1244	rVB2	61326	127821	3.94%	0.435%
60	16.483	1274	1277	1281	rVB	42299	87451	2.69%	0.298%
61	17.077	1326	1329	1337	rVB	33997	87005	2.68%	0.296%
62	17.763	1386	1389	1393	rBV4	21464	61453	1.89%	0.209%

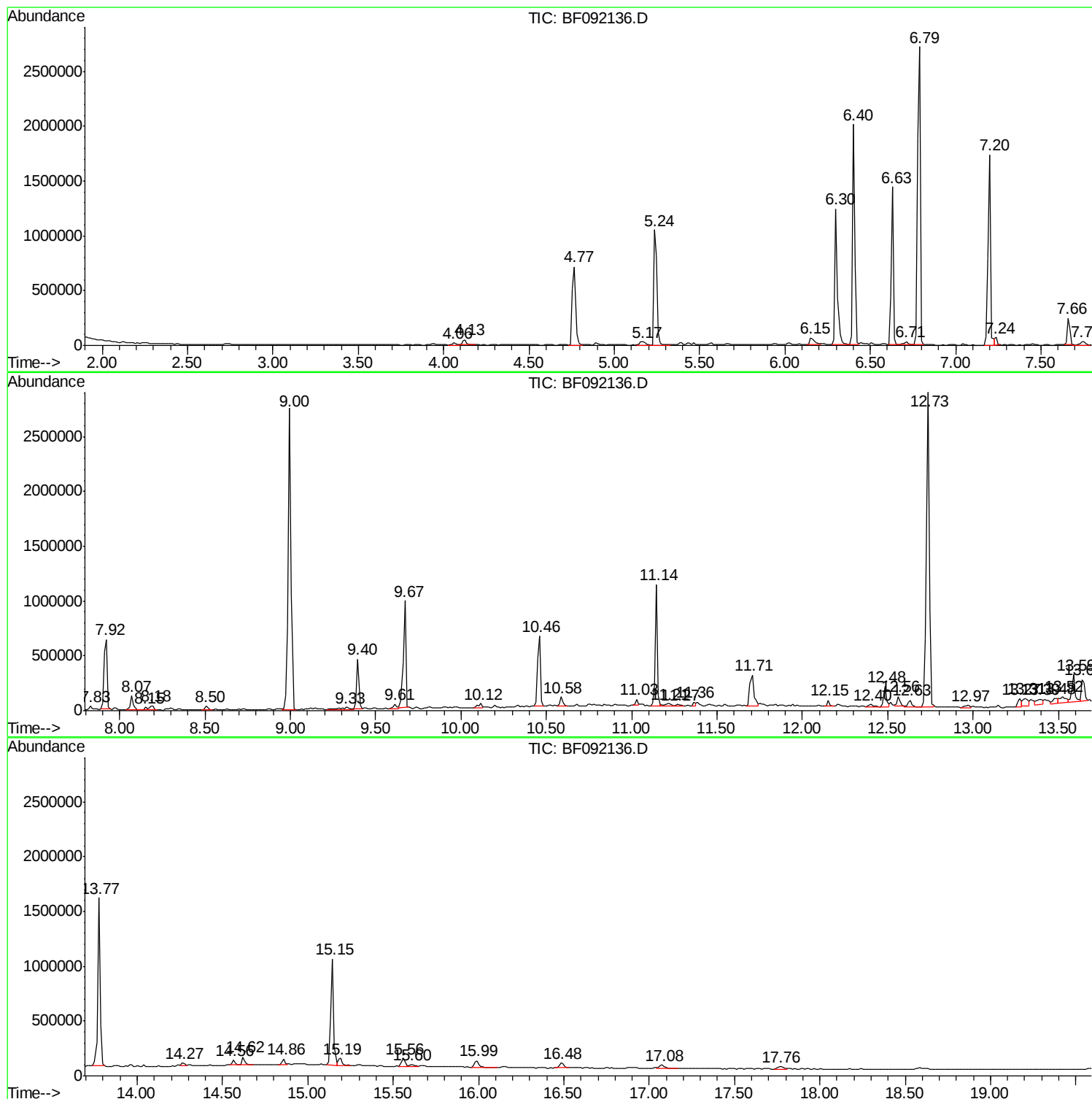
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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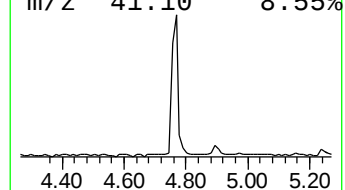
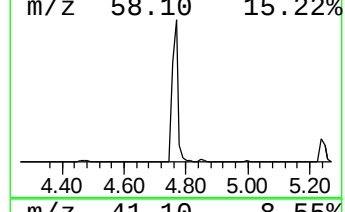
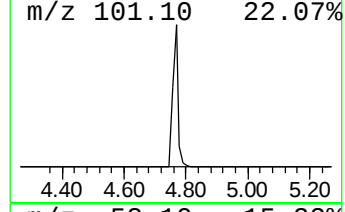
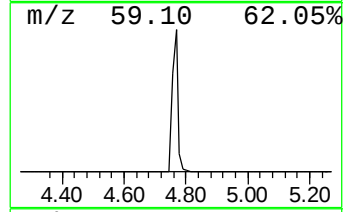
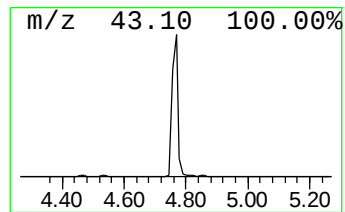
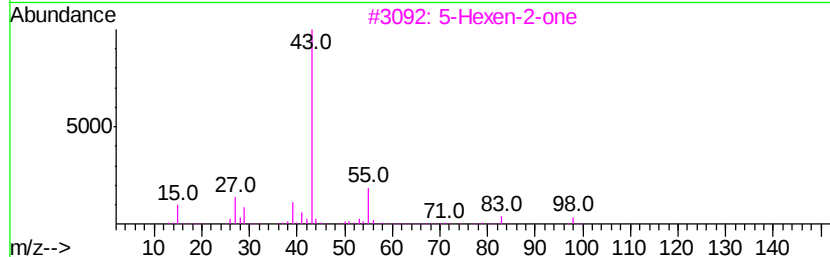
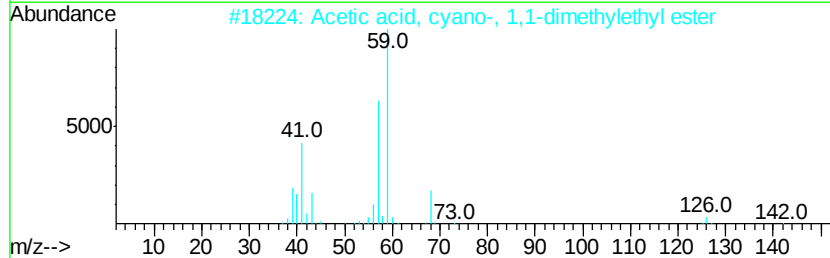
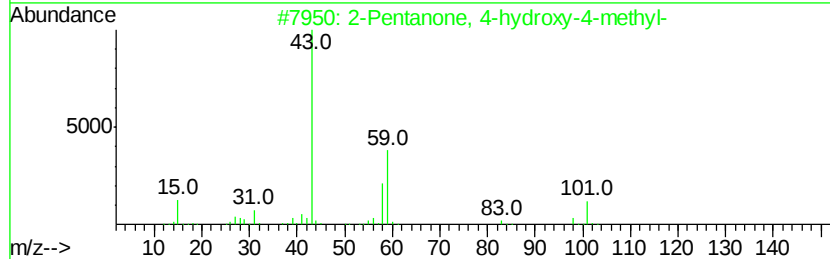
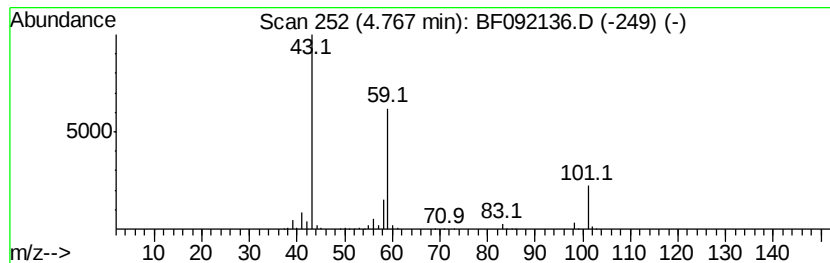
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	13.98 ng	929576	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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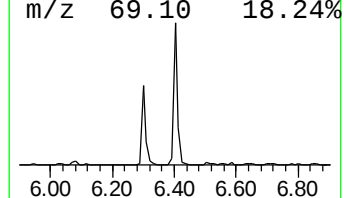
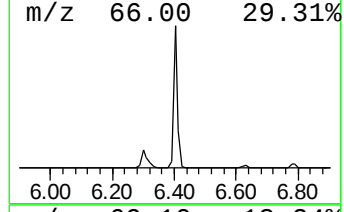
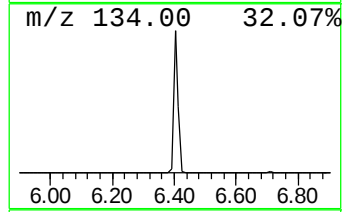
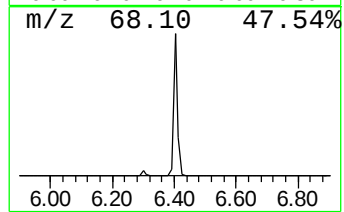
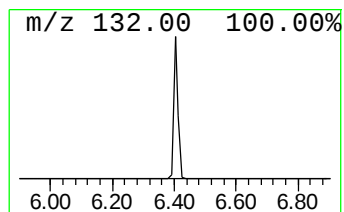
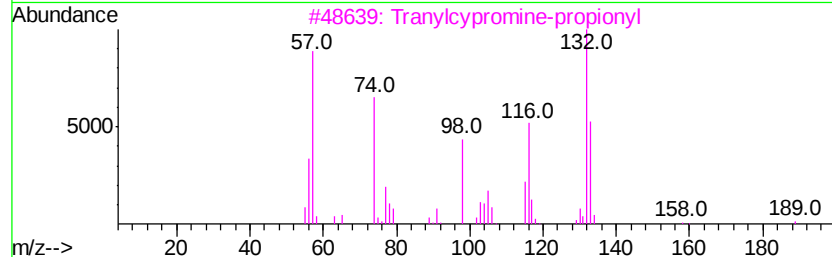
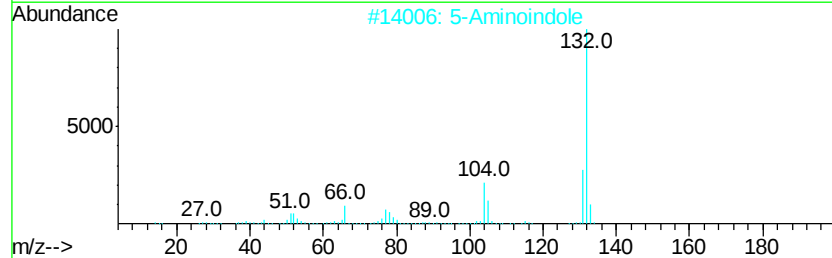
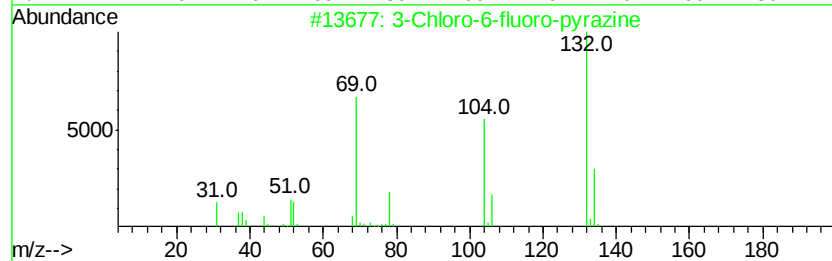
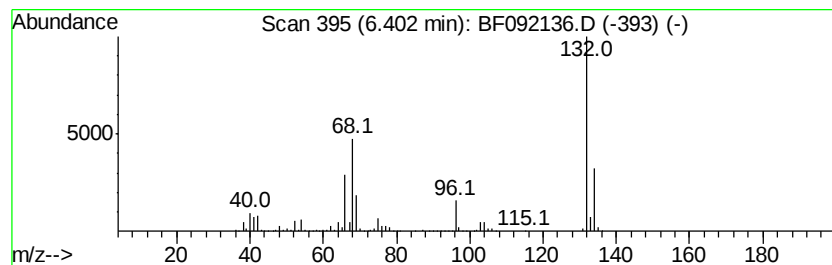
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	28.97 ng	1926730	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
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



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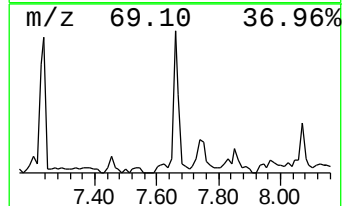
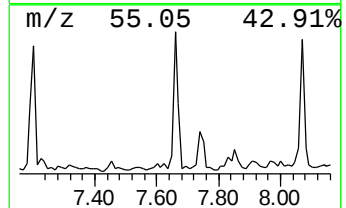
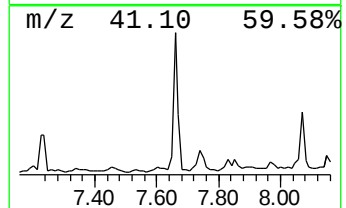
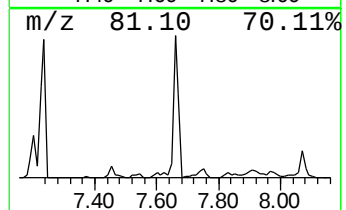
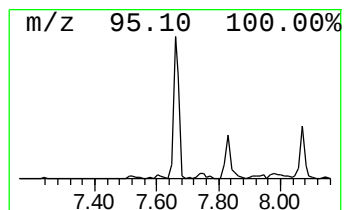
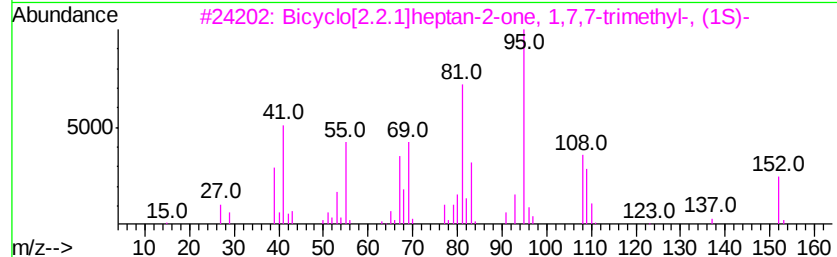
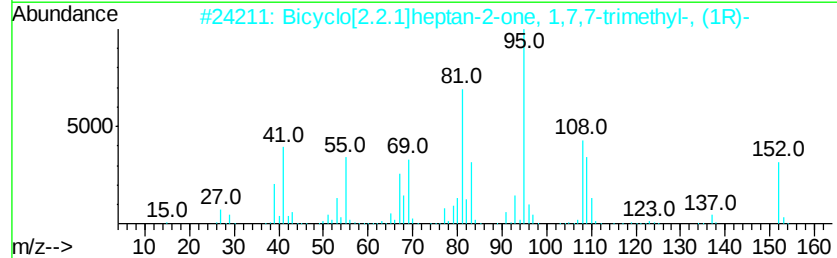
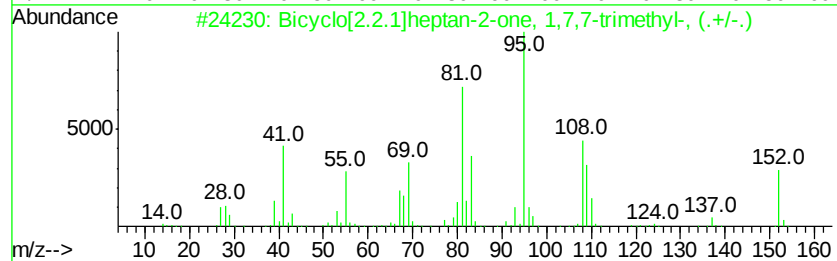
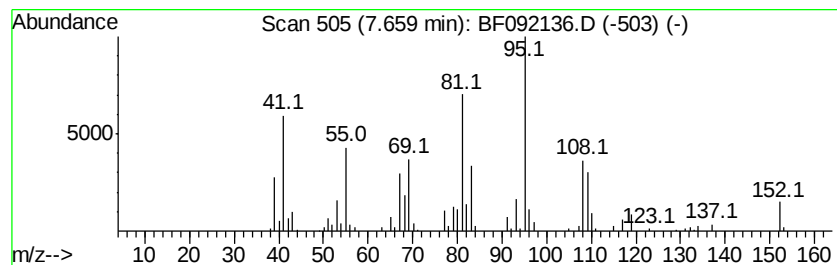
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Peak Number 4 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	6.53 ng	277052	Naphthalene-d8	7.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	021368-68-3	97
2		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	96
3		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
4		Camphor	152	C10H16O	000076-22-2	94
5		5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	53



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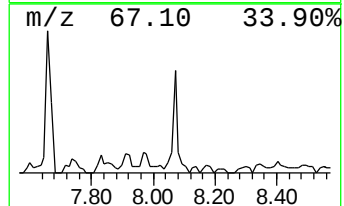
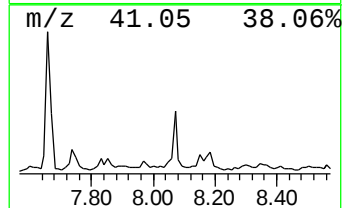
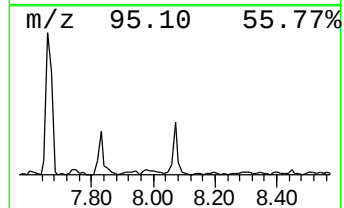
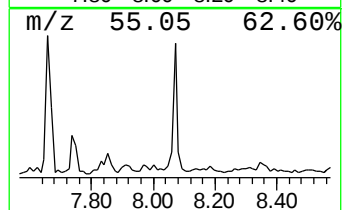
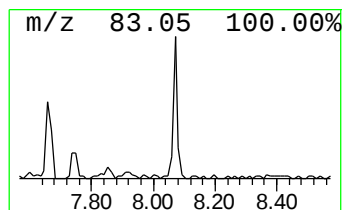
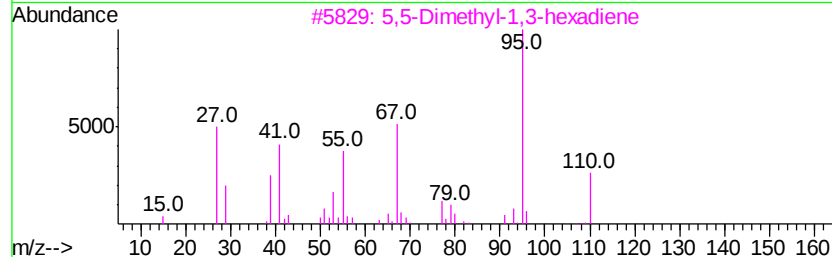
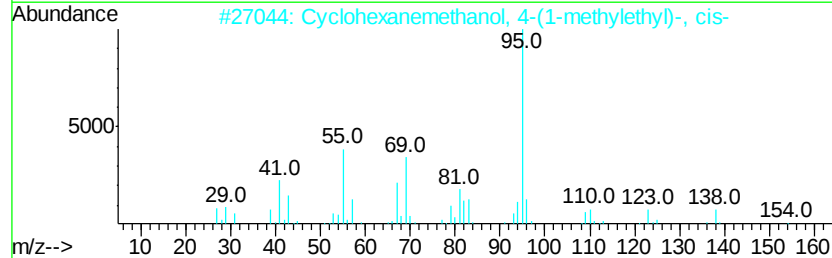
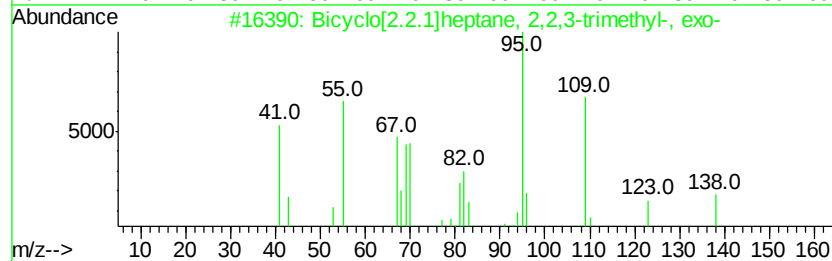
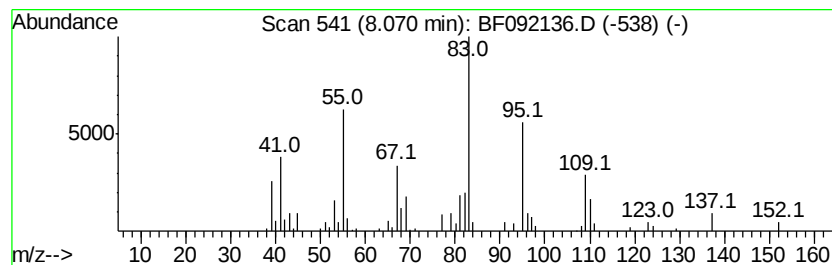
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown8.07 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.07	3.82 ng	161990	Naphthalene-d8	7.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	43
2		Cyclohexanemethanol, 4-(1-methyl...	156	C10H20O	013828-37-0	35
3		5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	30
4		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	30
5		Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	25



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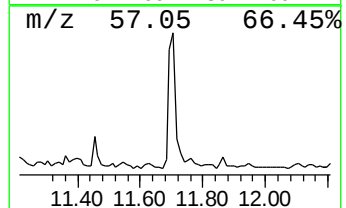
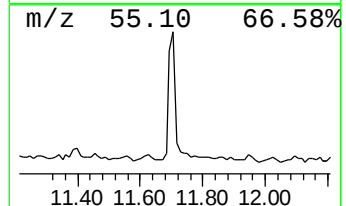
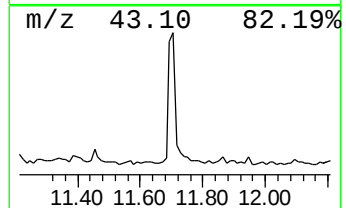
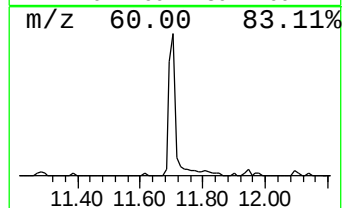
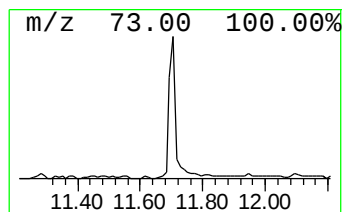
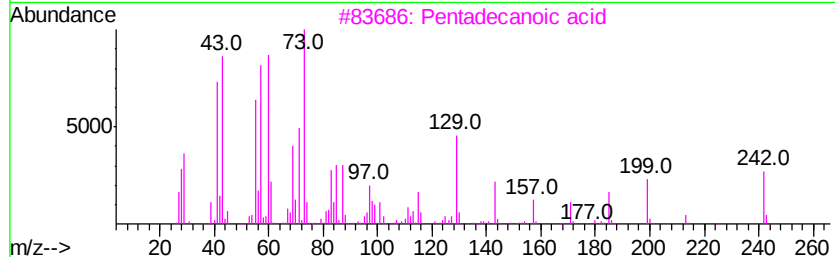
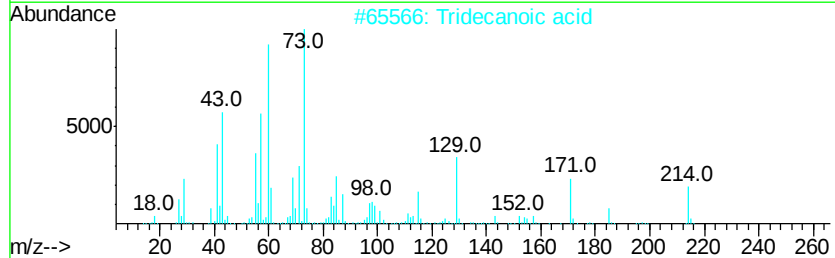
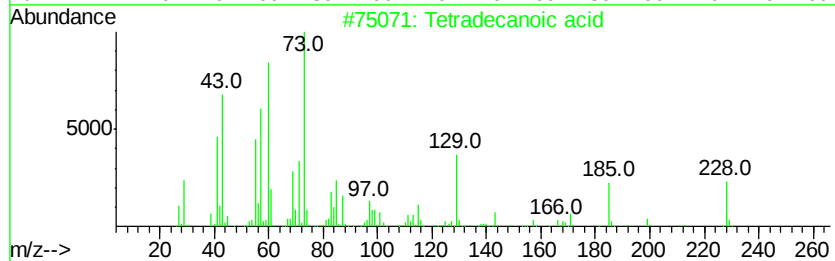
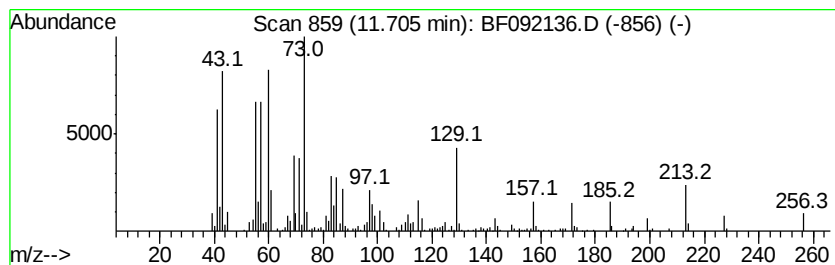
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	8.83 ng	429077	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092136.D
Acq On : 9 Jan 2017 14:11
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

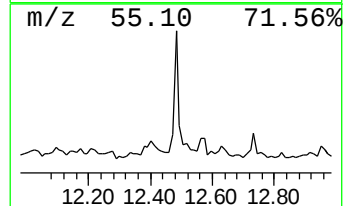
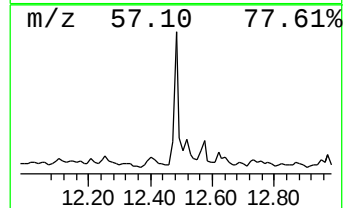
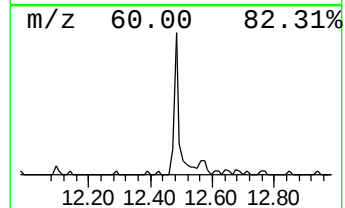
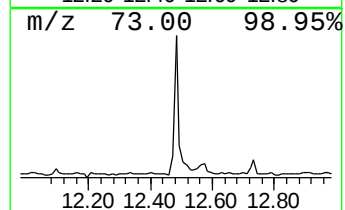
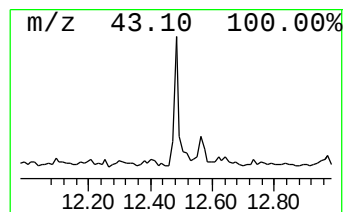
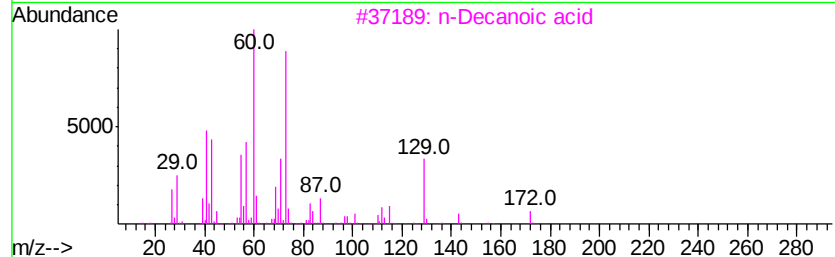
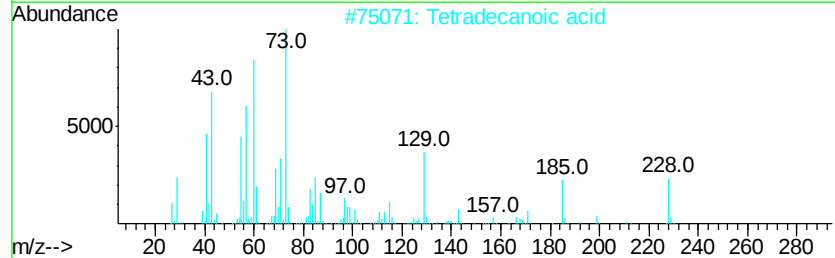
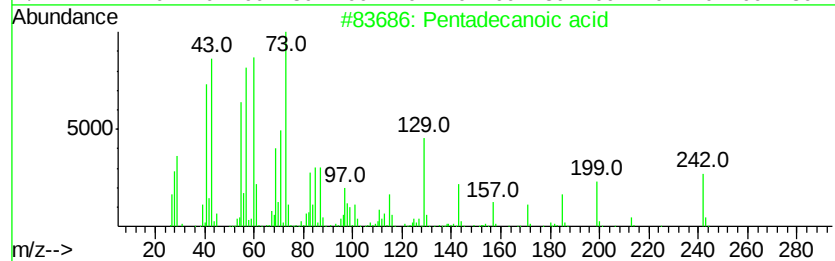
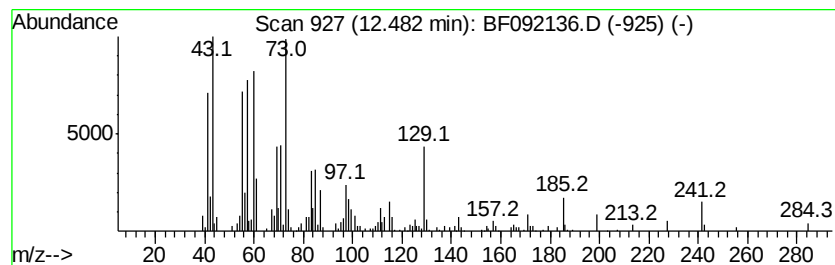
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	2.56 ng	191190	Chrysene-d12	13.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		n-Decanoic acid	172	C10H20O2	000334-48-5	76
4		Undecanoic acid	186	C11H22O2	000112-37-8	49
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010917\
Data File : BF092136.D
Acq On : 9 Jan 2017 14:11
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

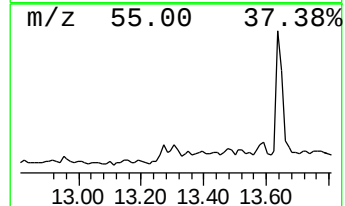
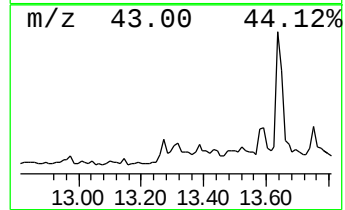
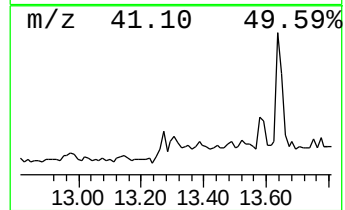
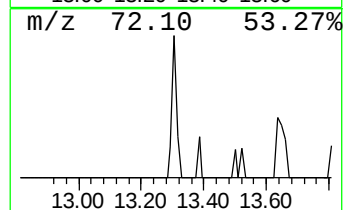
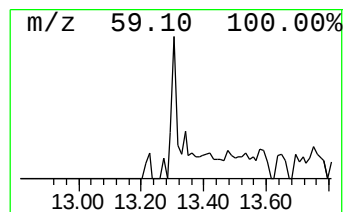
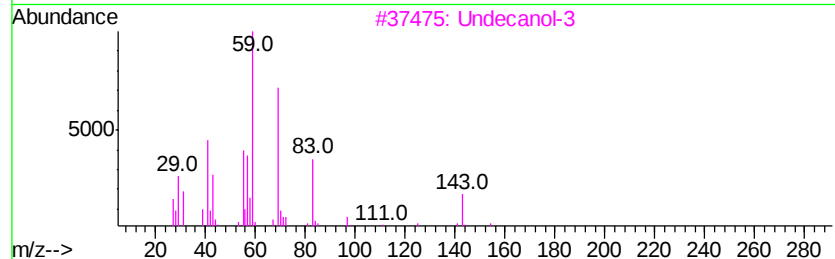
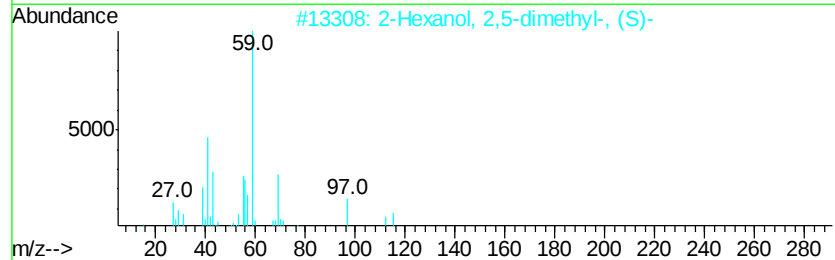
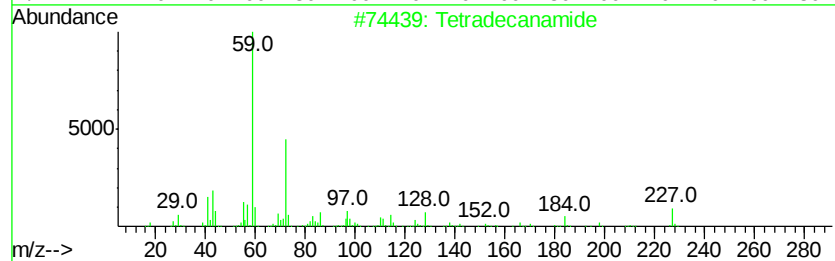
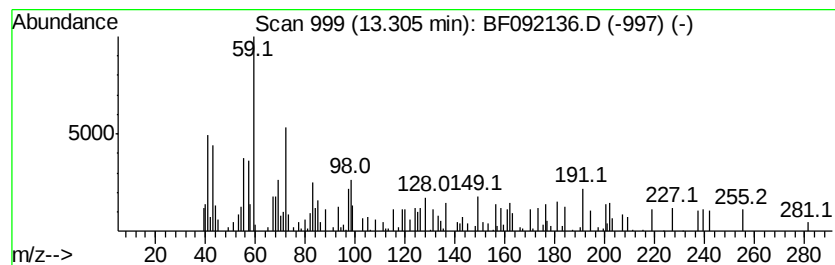
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.31 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.31	2.16 ng	160897	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecanamide	227	C14H29NO	000638-58-4	40
2		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	27
3		Undecanol-3	172	C11H24O	006929-08-4	27
4		3-Tridecanol	200	C13H28O	010289-68-6	25
5		3-Dodecanol	186	C12H26O	010203-30-2	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010917\
Data File : BF092136.D
Acq On : 9 Jan 2017 14:11
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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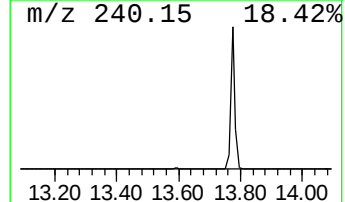
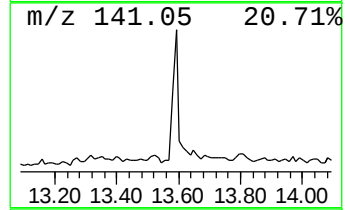
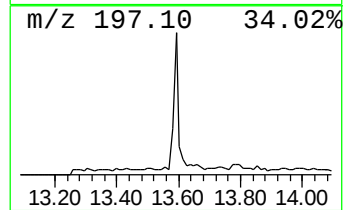
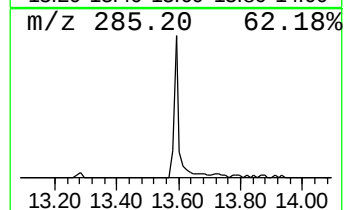
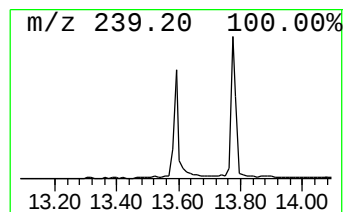
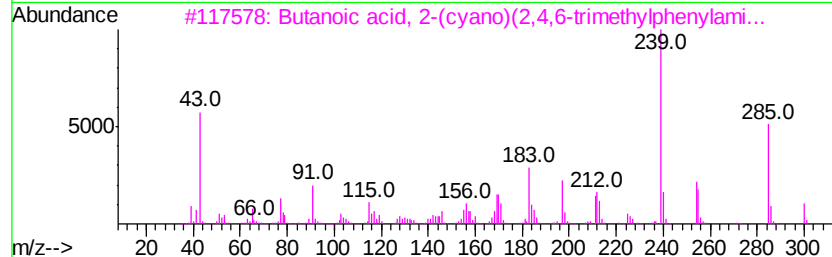
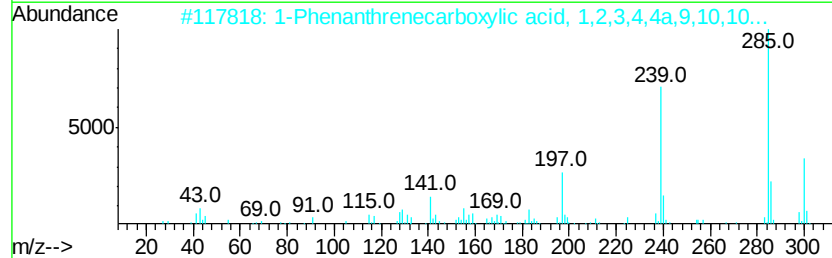
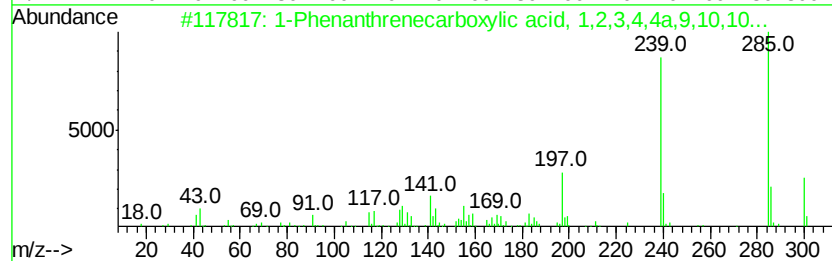
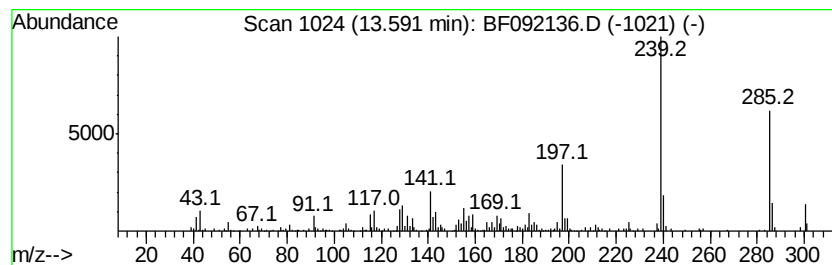
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Phenanthrenecarboxylic ac... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	4.21 ng	314537	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	001740-19-8	96
2		1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	93
3		Butanoic acid, 2-(cyano)(2,4,6-trimethylphenylami...	300	C17H20N2O3	1000267-71-7	80
4		Ethyl 4-hydroxy-7-trifluoromethyl...	285	C13H10F3N3	000391-02-6	52
5		3-Quinolinecarboxylic acid, 4-hy...	285	C13H10F3N3	023851-84-5	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092136.D
Acq On : 9 Jan 2017 14:11
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

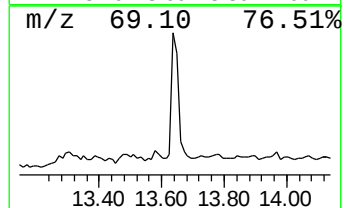
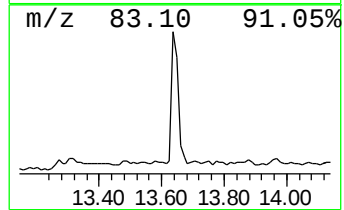
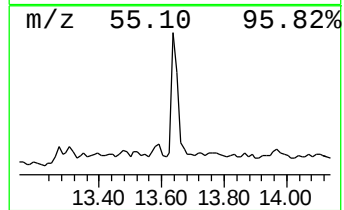
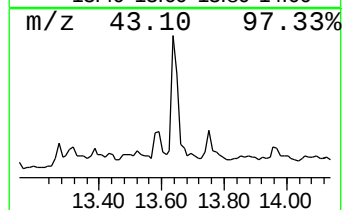
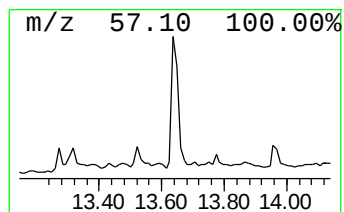
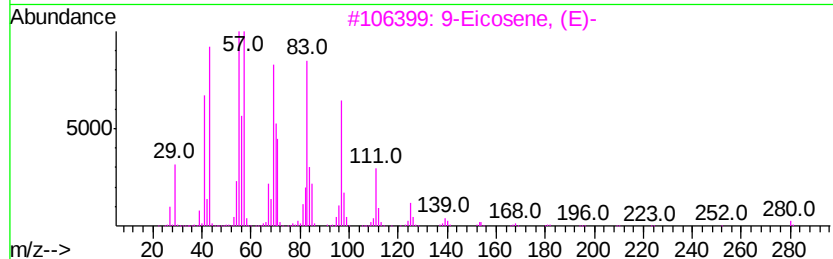
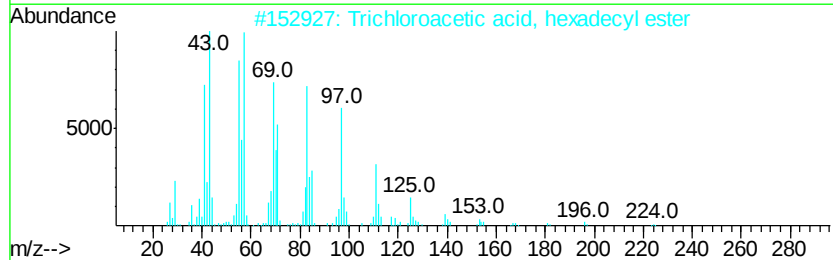
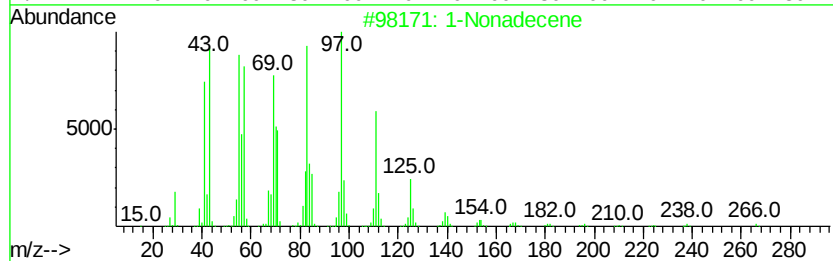
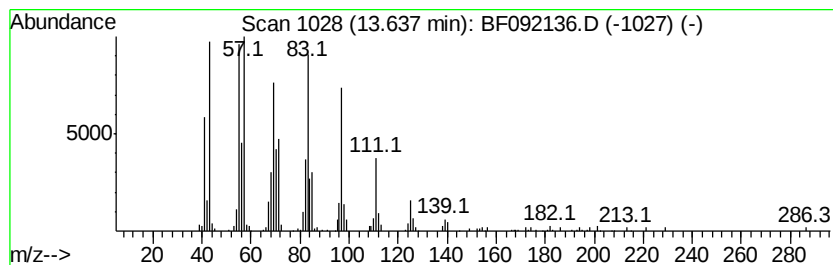
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Nonadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	3.53 ng	263432	Chrysene-d12	13.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	91
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4			1-Octadecanol	270	C18H38O	000112-92-5	90
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092136.D
Acq On : 9 Jan 2017 14:11
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

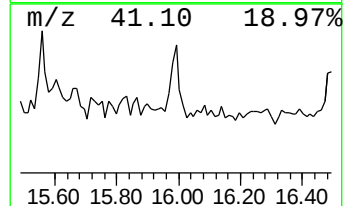
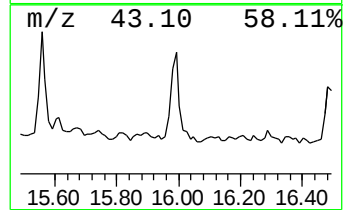
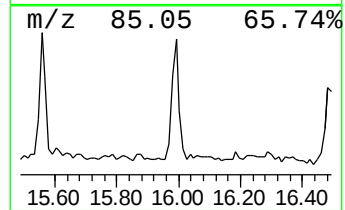
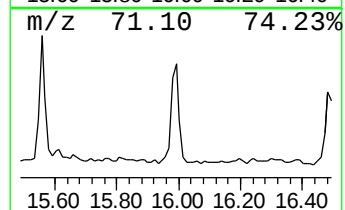
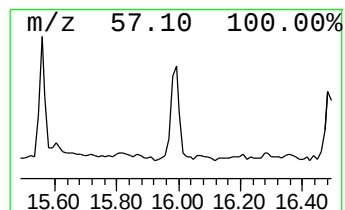
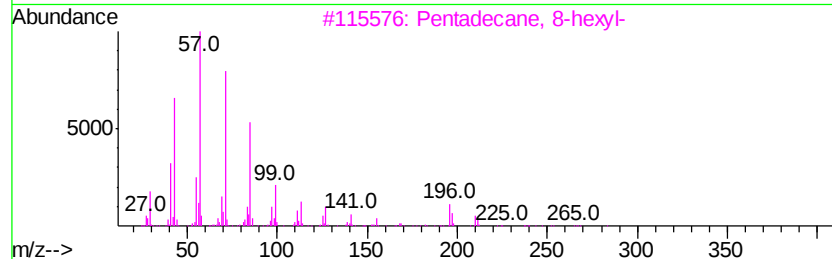
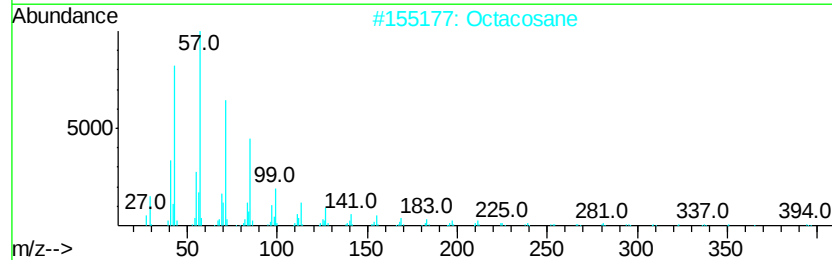
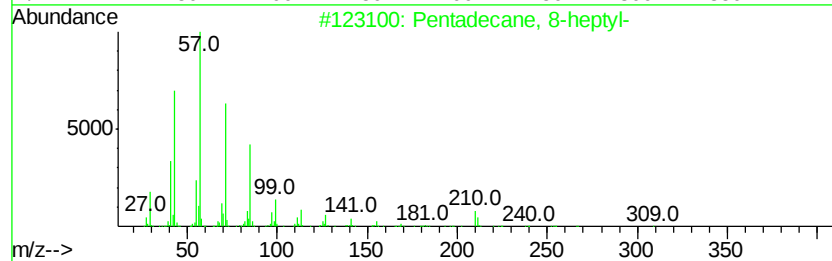
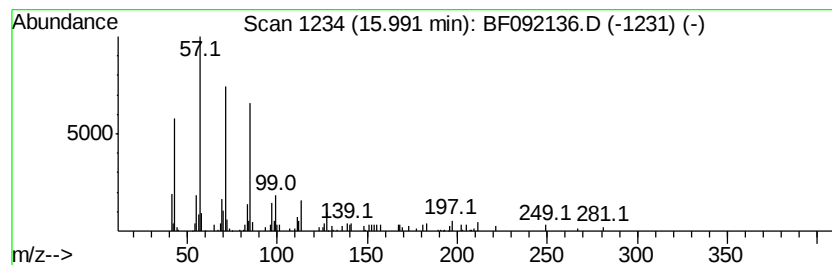
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecane, 8-heptyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.31 ng	127821	Perylene-d12	15.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
4		Pentacosane	352	C25H52	000629-99-2	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092136.D
Acq On : 9 Jan 2017 14:11
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

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
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unknown6.40	6.40	29.0	ng	1926730	1	6.63	1330210	20.0
Bicyclo[2.2.1]hep...	7.66	6.5	ng	277052	2	7.92	848766	20.0
unknown8.07	8.07	3.8	ng	161990	2	7.92	848766	20.0
Tetradecanoic acid	11.71	8.8	ng	429077	4	11.15	972031	20.0
Pentadecanoic acid	12.48	2.6	ng	191190	5	13.77	1492700	20.0
unknown13.31	13.31	2.2	ng	160897	5	13.77	1492700	20.0
1-Phenanthrenecar...	13.59	4.2	ng	314537	5	13.77	1492700	20.0
1-Nonadecene	13.64	3.5	ng	263432	5	13.77	1492700	20.0
Pentadecane, 8-he...	15.99	2.3	ng	127821	6	15.15	1104490	20.0