

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
 Data File : BF097102.D
 Acq On : 27 Jul 2017 3:43
 Operator : SJ/JU
 Sample : I4414-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-03-072417

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-BF072517.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	4.640	464	468	481	rBV	150400	233290	10.02%	1.183%
2	5.093	541	545	562	rBV	2168629	2269500	97.48%	11.504%
3	6.157	722	726	741	rBV	2016252	2328248	100.00%	11.802%
4	6.269	741	745	748	rBV	2485595	2283150	98.06%	11.574%
5	6.492	780	783	788	rBV	560613	528428	22.70%	2.679%
6	6.651	806	810	820	rBV	1752912	1541250	66.20%	7.813%
7	7.063	876	880	883	rBV	1485932	1316875	56.56%	6.675%
8	7.781	998	1002	1006	rBV	853910	736279	31.62%	3.732%
9	8.228	1073	1078	1082	rBV	49133	48339	2.08%	0.245%
10	8.392	1102	1106	1109	rBV	61136	54702	2.35%	0.277%
11	8.822	1177	1179	1181	rVB	41337	27986	1.20%	0.142%
12	8.857	1181	1185	1188	rBV	2102342	1822043	78.26%	9.236%
13	8.957	1199	1202	1206	rVB	89866	72708	3.12%	0.369%
14	9.257	1247	1253	1255	rBV	211288	201189	8.64%	1.020%
15	9.480	1288	1291	1294	rVB	103251	88309	3.79%	0.448%
16	9.522	1294	1298	1302	rBV	684219	660714	28.38%	3.349%
17	9.804	1343	1346	1349	rVB	27570	24726	1.06%	0.125%
18	9.980	1373	1376	1379	rVB	103766	76566	3.29%	0.388%
19	10.198	1409	1413	1416	rBV	38442	45866	1.97%	0.233%
20	10.310	1428	1432	1442	rVB	1116327	1017885	43.72%	5.160%
21	10.451	1453	1456	1457	rBV	93429	77545	3.33%	0.393%
22	10.898	1528	1532	1535	rBV	48072	45015	1.93%	0.228%
23	10.998	1545	1549	1552	rBV	600268	518052	22.25%	2.626%
24	11.557	1641	1644	1650	rBV2	87701	94977	4.08%	0.481%
25	12.204	1751	1754	1758	rVB	97697	81640	3.51%	0.414%
26	12.339	1774	1777	1784	rBV2	78986	94722	4.07%	0.480%
27	12.427	1788	1792	1796	rVV	112789	107927	4.64%	0.547%
28	12.586	1815	1819	1822	rBV	1604176	1462417	62.81%	7.413%
29	13.498	1968	1974	1978	rBV3	102492	150953	6.48%	0.765%
30	13.627	1991	1996	1999	rBV	544134	579156	24.88%	2.936%
31	13.651	1999	2000	2003	rVB	47556	29329	1.26%	0.149%
32	13.827	2027	2030	2032	rBV3	39870	40860	1.75%	0.207%
33	14.127	2078	2081	2091	rBV3	74436	165828	7.12%	0.841%
34	14.421	2128	2131	2134	rBV	41314	45649	1.96%	0.231%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.927	2215	2217	2221	rBV2	38338	47148	2.03%	0.239%
36	14.974	2222	2225	2232	rVV	301760	358523	15.40%	1.817%
37	15.274	2275	2276	2281	rVB3	43512	42694	1.83%	0.216%
38	15.386	2292	2295	2298	rBV2	36093	52592	2.26%	0.267%
39	15.562	2322	2325	2330	rVB6	43374	53800	2.31%	0.273%
40	16.474	2478	2480	2487	rVB7	30764	40794	1.75%	0.207%
41	17.133	2590	2592	2593	rBV2	36481	33231	1.43%	0.168%
42	17.480	2649	2651	2653	rBV3	22724	24883	1.07%	0.126%
43	18.074	2750	2752	2756	rBV4	31613	52995	2.28%	0.269%
44	18.386	2803	2805	2812	rBV7	26468	43035	1.85%	0.218%
45	18.727	2861	2863	2871	rBV8	18788	33657	1.45%	0.171%
46	18.868	2886	2887	2892	rBV4	28725	38892	1.67%	0.197%
47	19.439	2982	2984	2988	rBV4	23394	32913	1.41%	0.167%

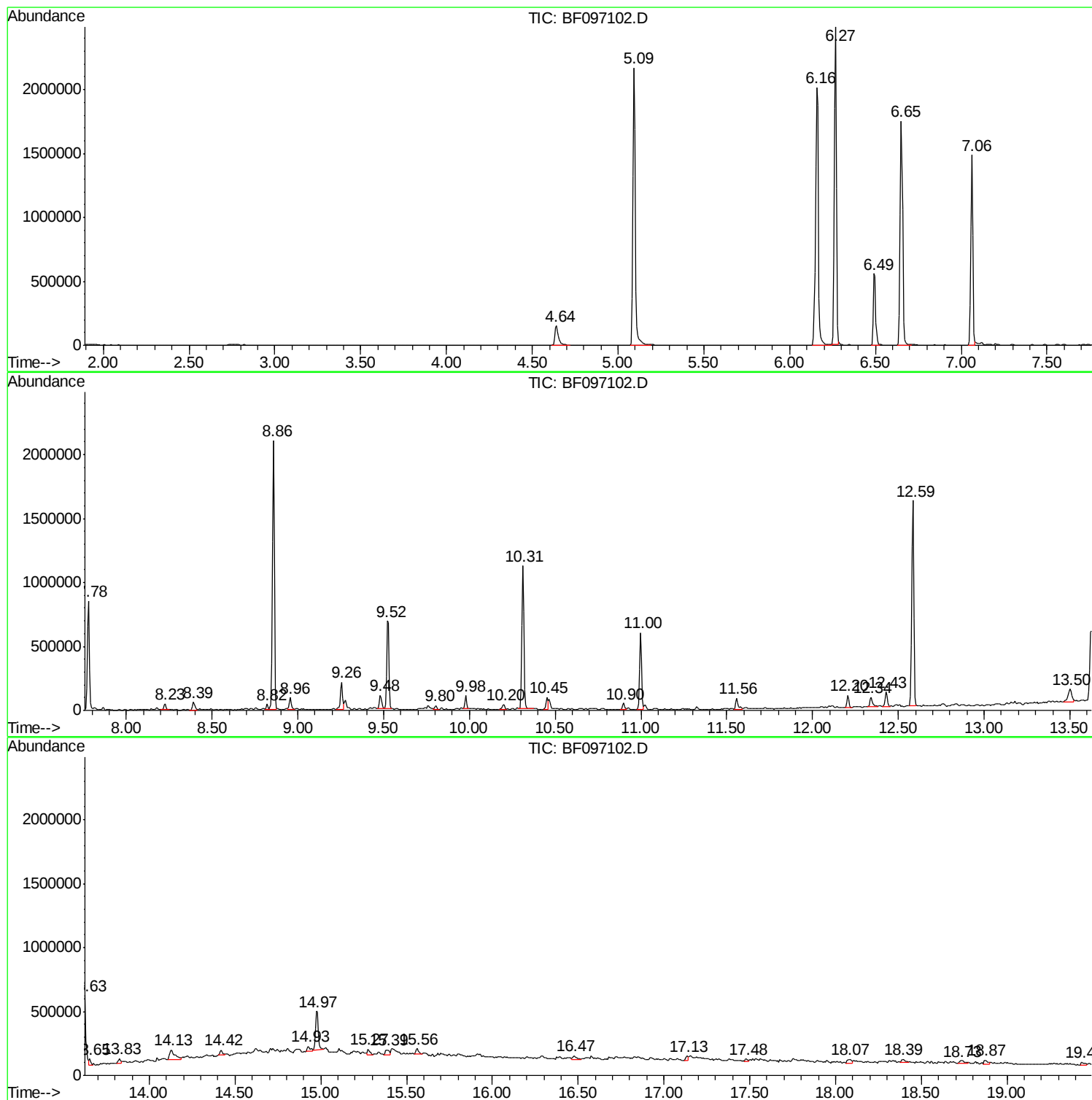
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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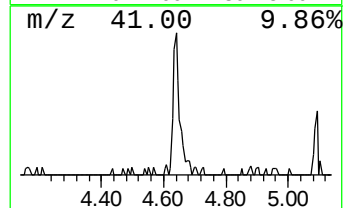
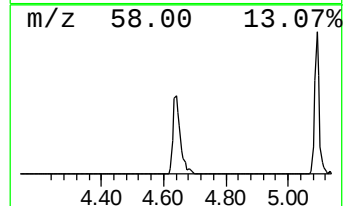
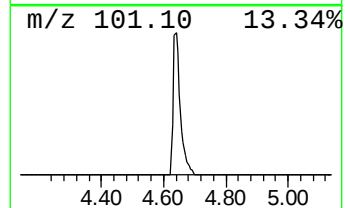
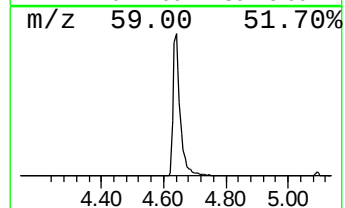
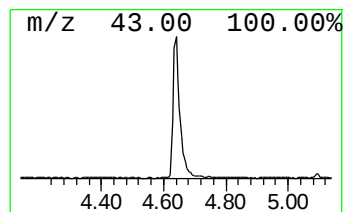
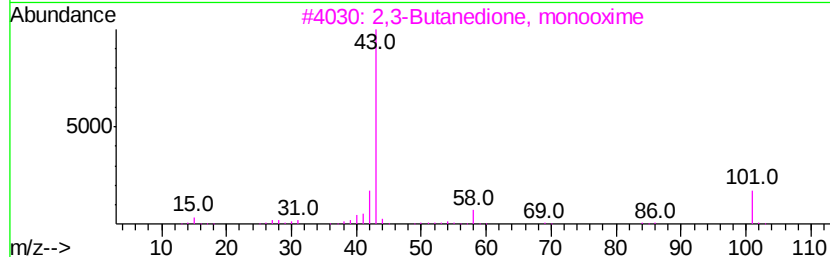
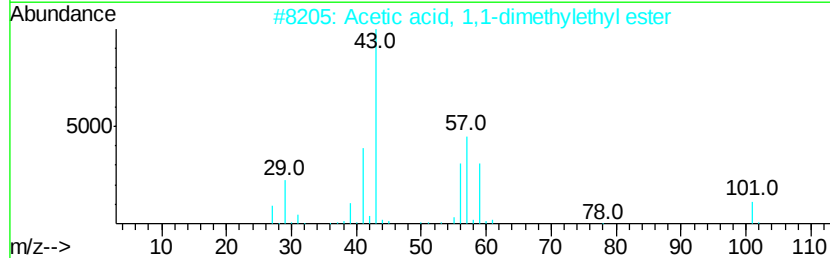
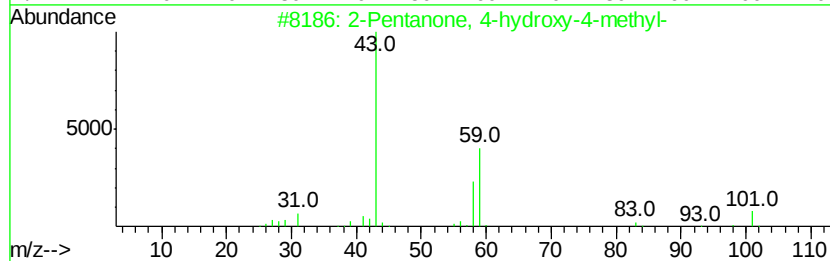
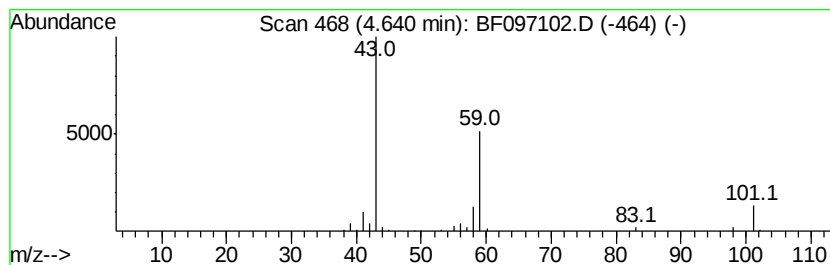
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.64	8.83 ng	233290	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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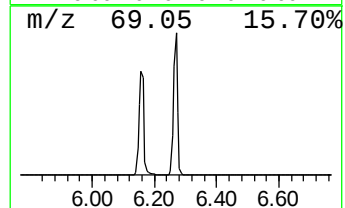
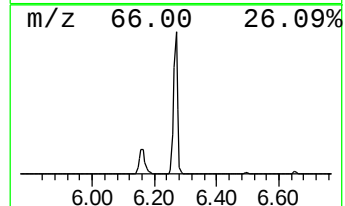
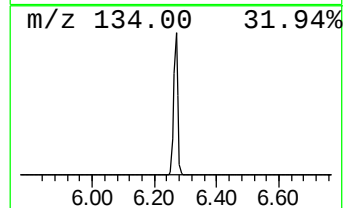
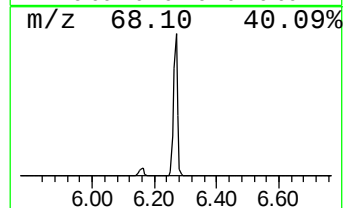
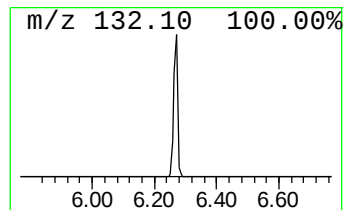
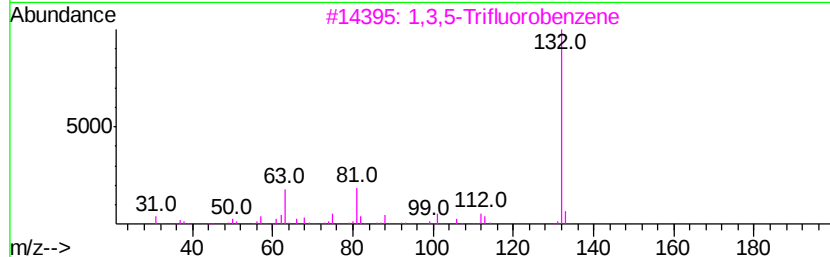
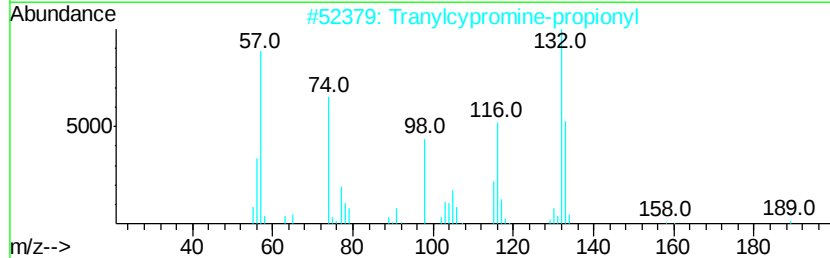
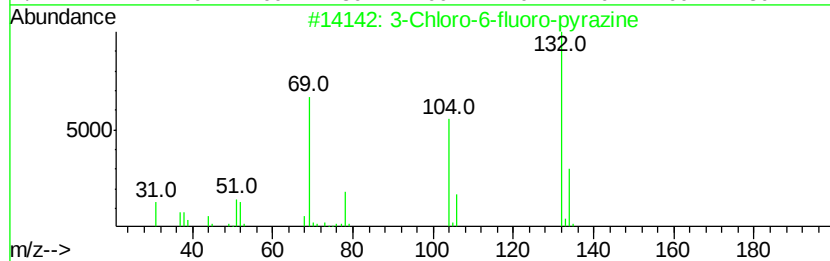
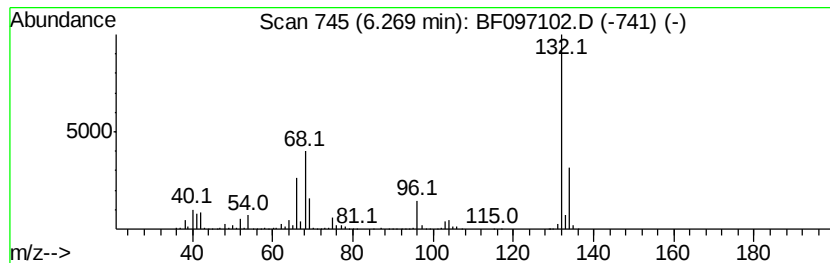
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	86.41 ng	2283150	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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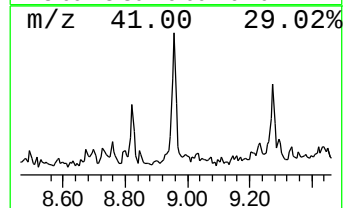
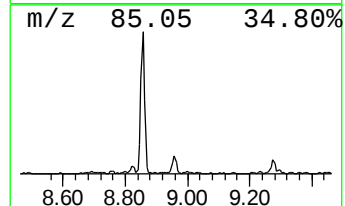
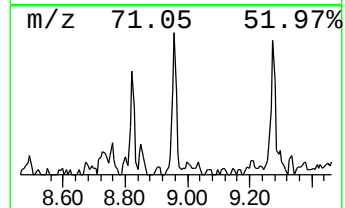
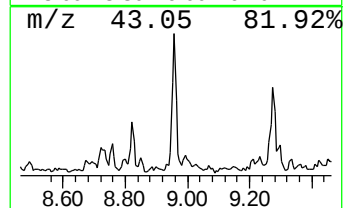
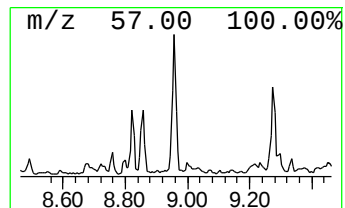
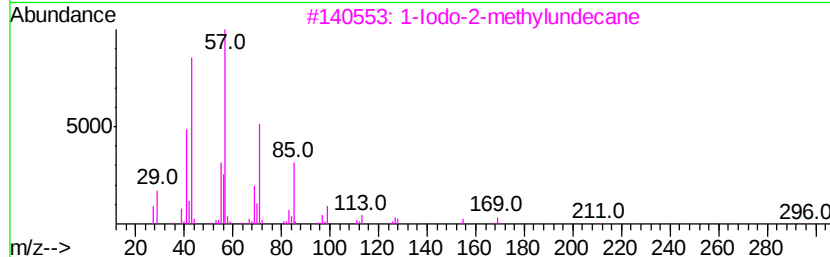
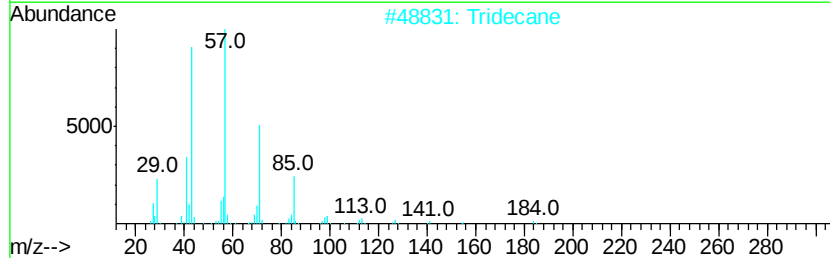
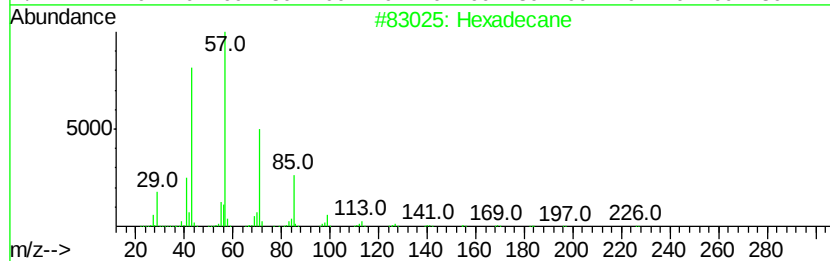
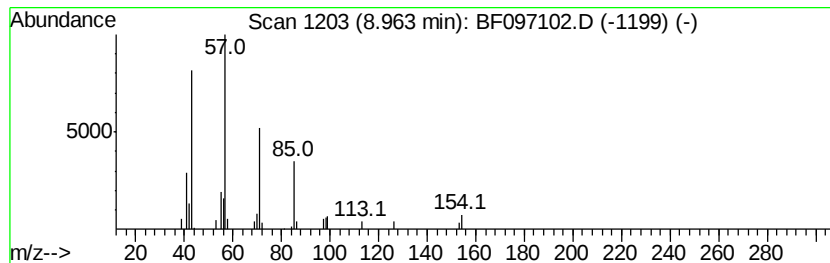
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	2.20 ng	72708	Acenaphthene-d10	9.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	86
2		Tridecane	184	C13H28	000629-50-5	86
3		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80
4		Tetradecane	198	C14H30	000629-59-4	78
5		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72



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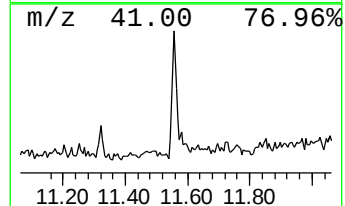
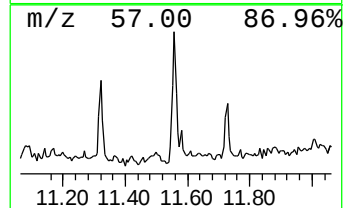
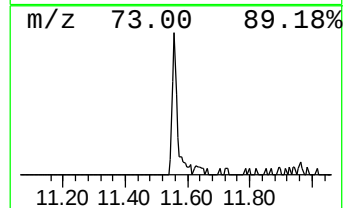
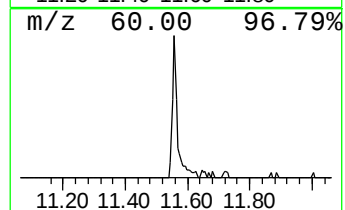
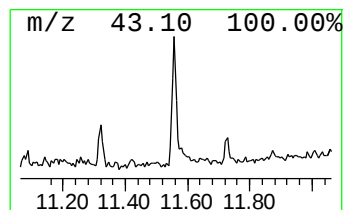
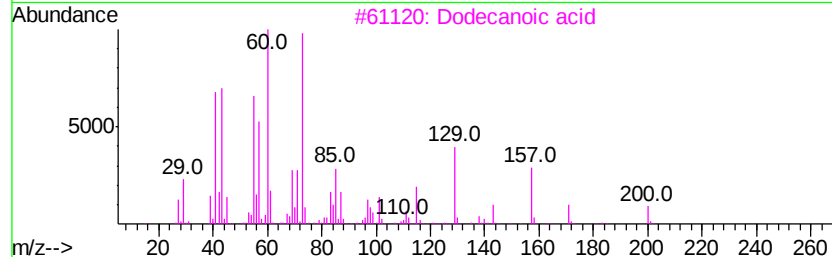
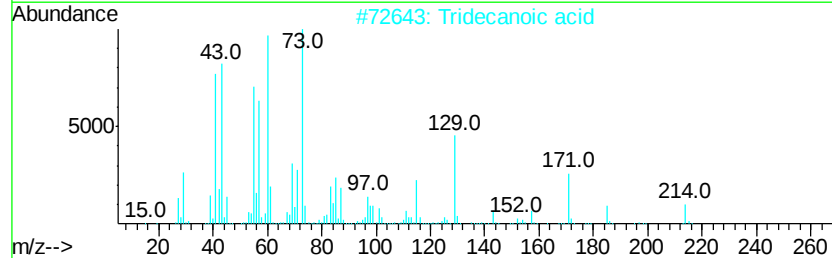
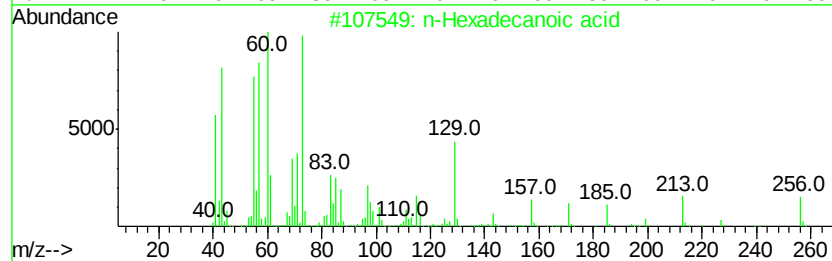
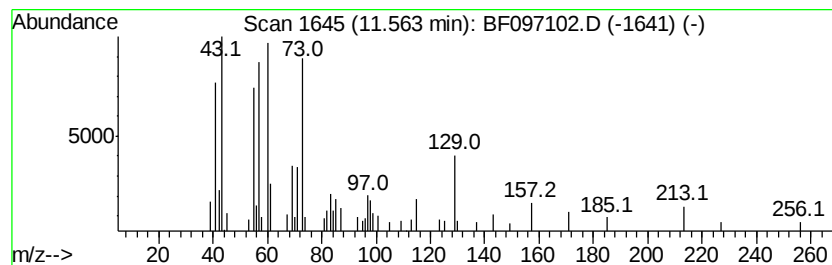
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	3.67 ng	94977	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Dodecanoic acid	200	C12H24O2	000143-07-7	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



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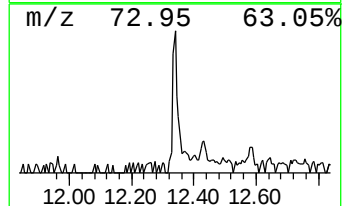
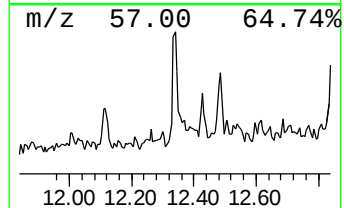
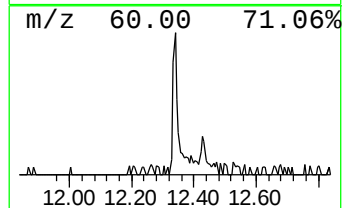
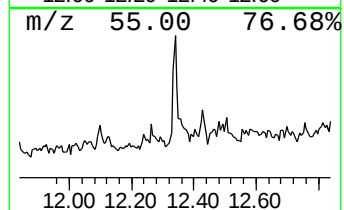
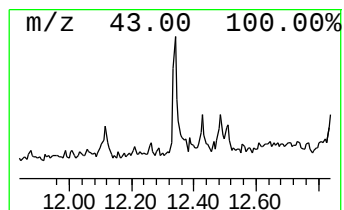
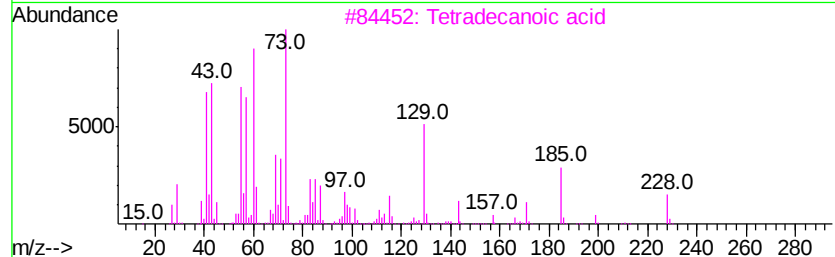
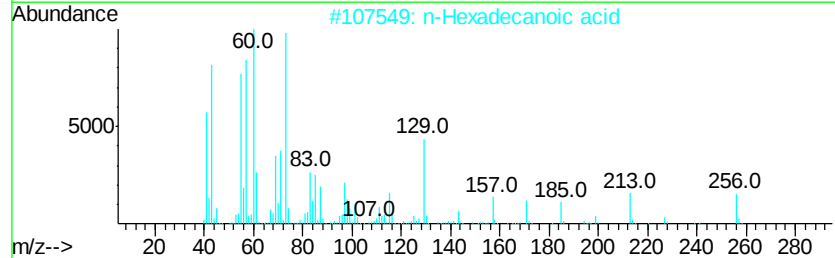
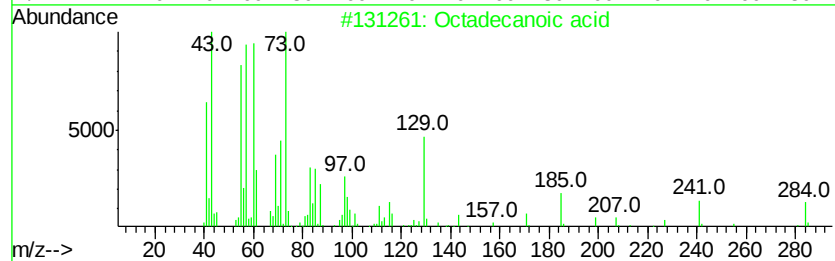
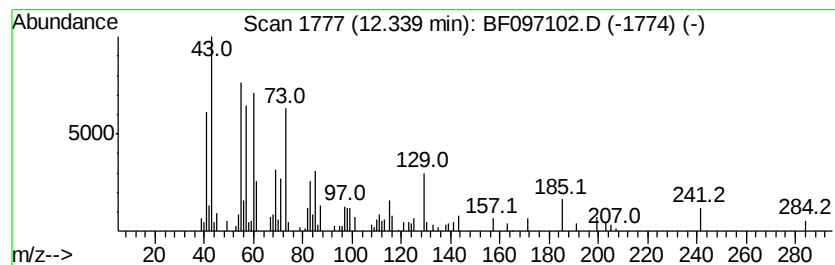
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	3.27 ng	94722	Chrysene-d12	13.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	81
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
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Acq On : 27 Jul 2017 3:43
Operator : SJ/JU
Sample : I4414-01
Misc :
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ClientSampleId :
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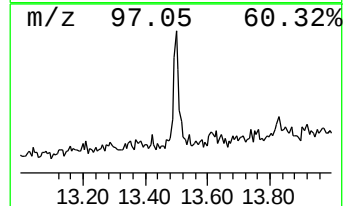
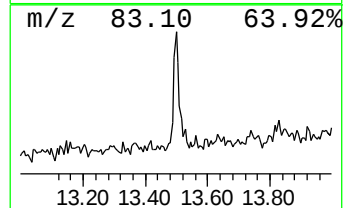
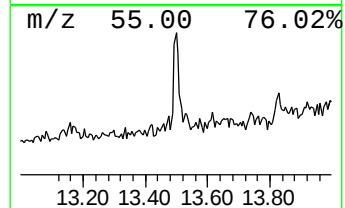
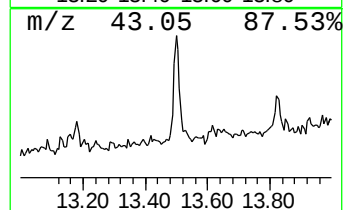
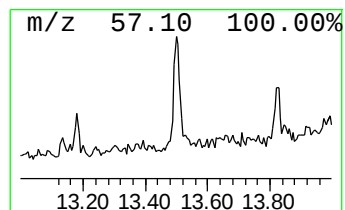
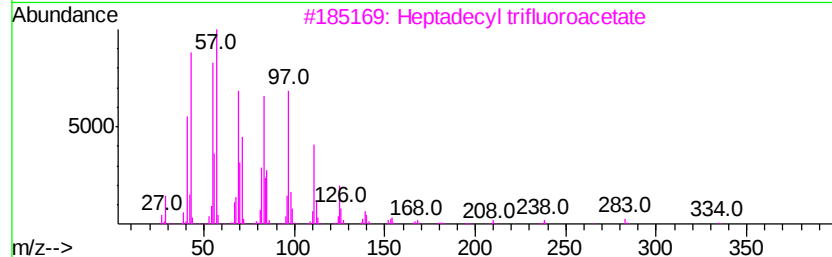
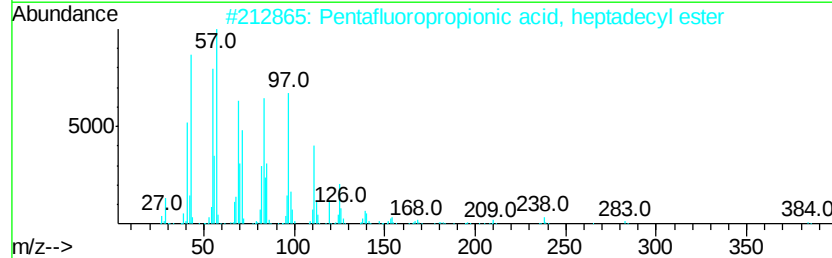
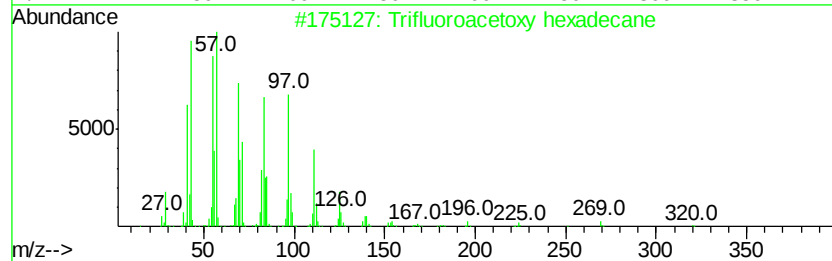
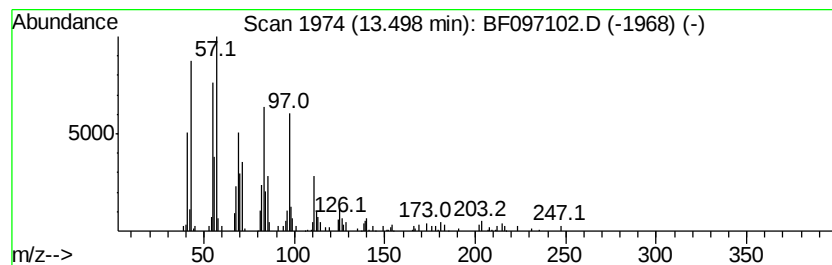
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	5.21 ng	150953	Chrysene-d12	13.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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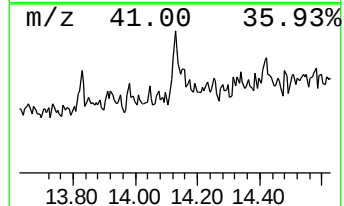
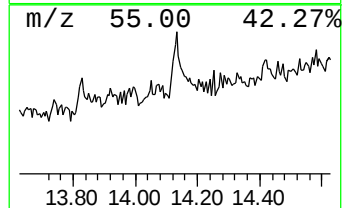
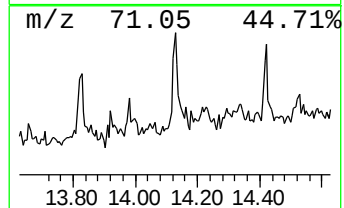
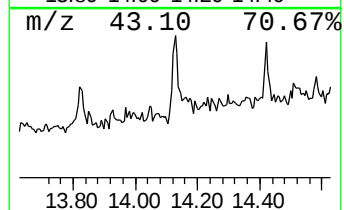
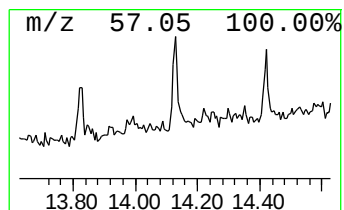
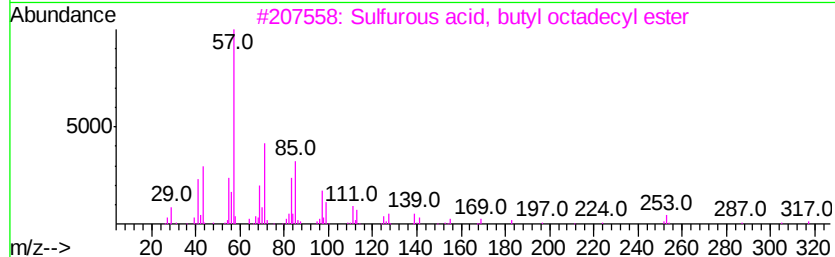
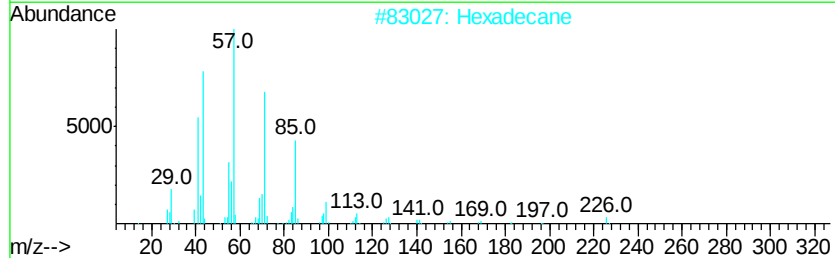
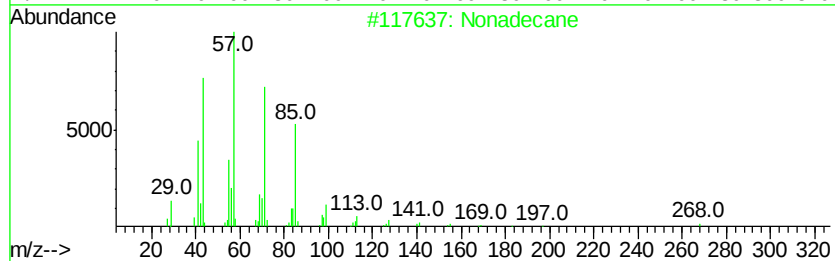
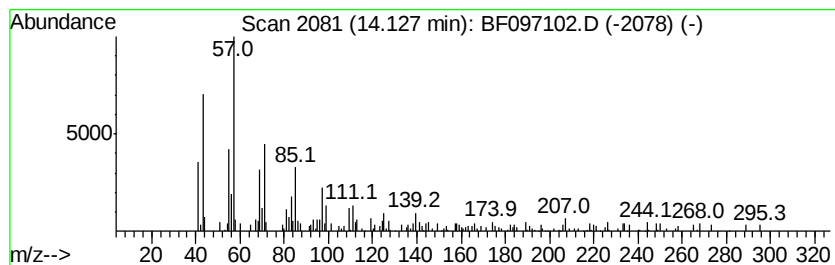
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.13	5.73 ng	165828	Chrysene-d12	13.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	78
2	Hexadecane	226	C16H34	000544-76-3	70
3	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	58
4	Tridecane	184	C13H28	000629-50-5	55
5	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
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Operator : SJ/JU
Sample : I4414-01
Misc :
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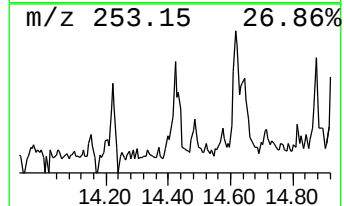
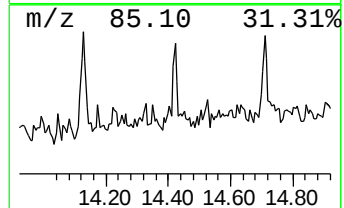
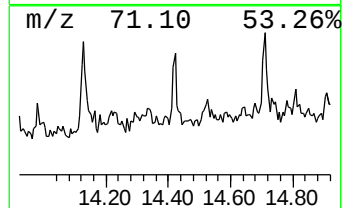
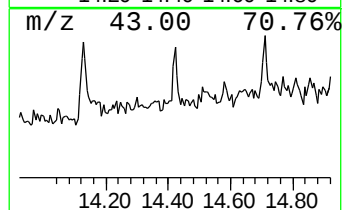
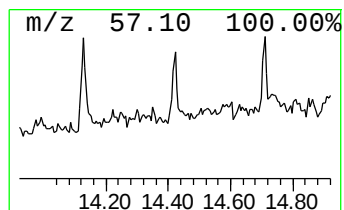
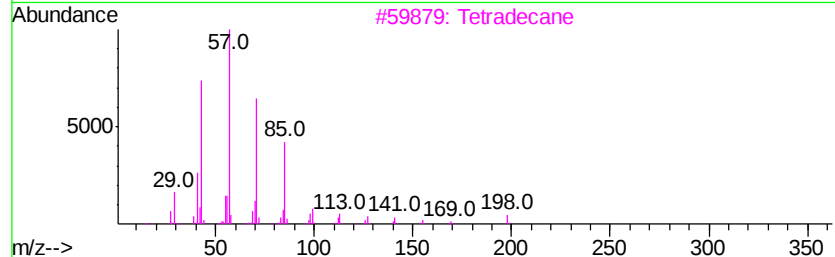
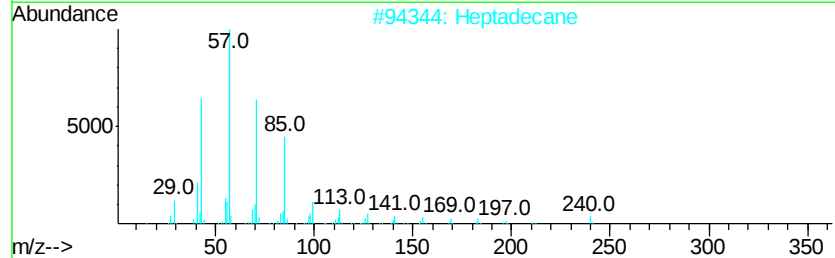
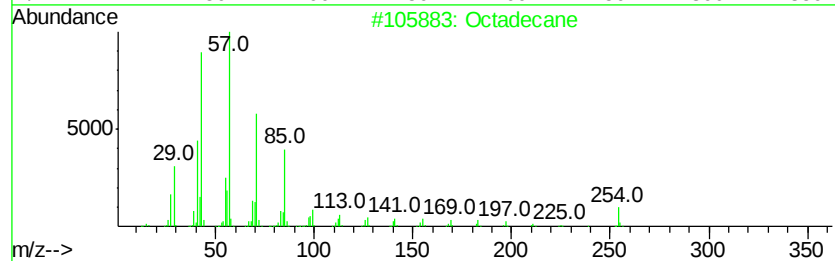
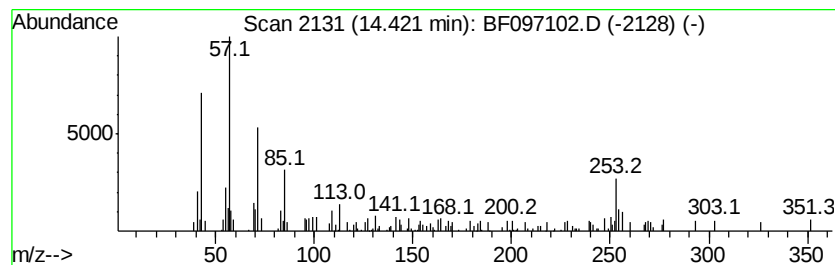
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.42	2.55 ng	45649	Perylene-d12		14.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	70
2	Heptadecane	240	C17H36	000629-78-7	64
3	Tetradecane	198	C14H30	000629-59-4	50
4	Nonadecane	268	C19H40	000629-92-5	50
5	Tridecane	184	C13H28	000629-50-5	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
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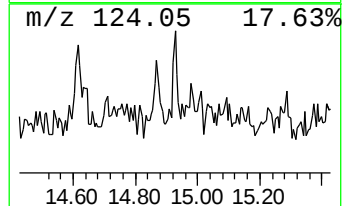
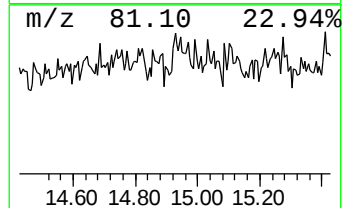
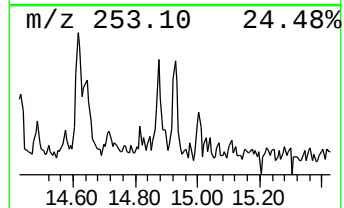
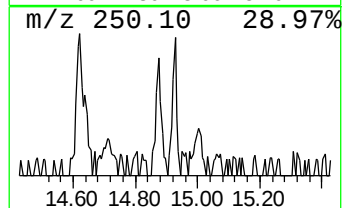
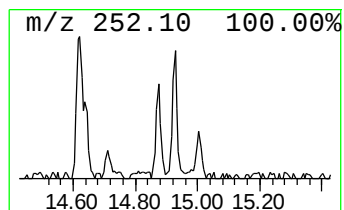
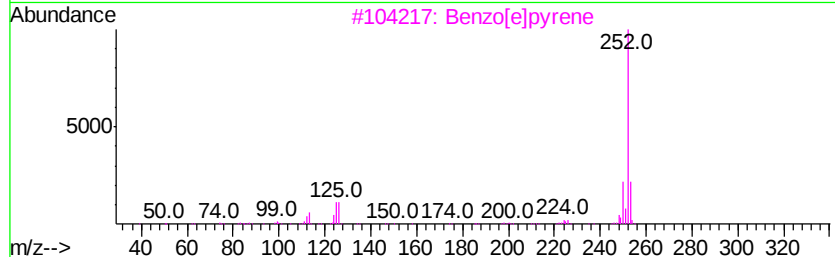
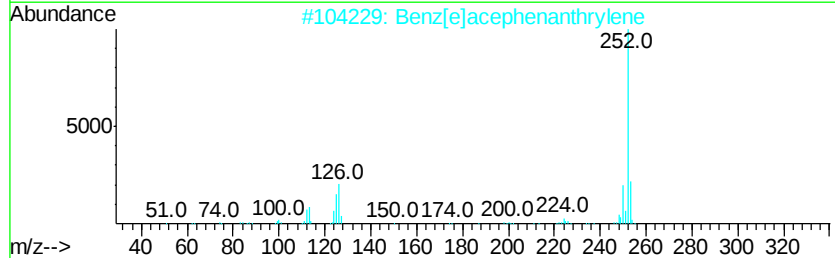
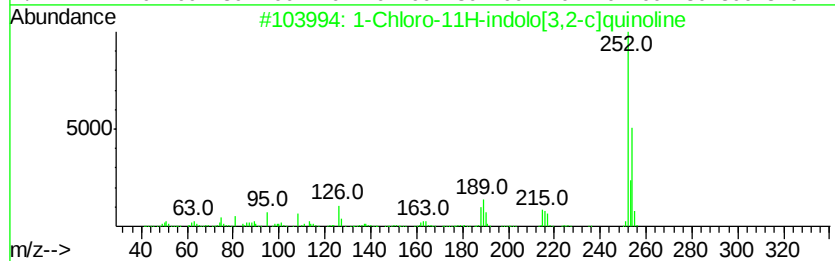
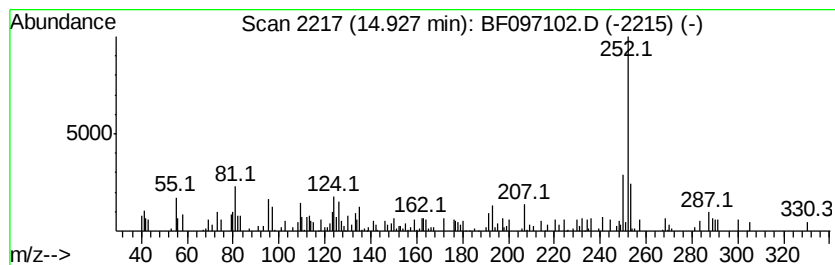
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown14.93 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.63 ng	47148	Perylene-d12	14.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Chloro-11H-indolo[3,2-c]quinoline	252	C15H9ClN2	155249-51-7	49
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	49
3		Benzo[e]pyrene	252	C20H12	000192-97-2	49
4		Benzo[a]pyrene	252	C20H12	000050-32-8	49
5		Thiazole, 2-amino-4,5-diphenyl-	252	C15H12N2S	006318-74-7	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown15.27 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	2.38 ng	42694	Perylene-d12	14.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2	N-(2-Benzoyl-4-bromo-phenyl)-acr...	329	C16H12BrN02	1000318-48-5	14
2		Ethalfuralin	333	C13H14F3N3O4	055283-68-6	9

