

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
 Data File : BF097170.D
 Acq On : 28 Jul 2017 22:50
 Operator : SJ/JU
 Sample : I4456-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-8D24

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	4.628	461	466	478	rBV	551849	783188	29.23%	3.447%
2	5.087	540	544	562	rBV	2338601	2536920	94.69%	11.166%
3	6.151	720	725	739	rBV	2584672	2679176	100.00%	11.792%
4	6.257	739	743	747	rBV	2330574	2356803	87.97%	10.373%
5	6.486	778	782	792	rBV	880325	748123	27.92%	3.293%
6	6.645	804	809	812	rBV	1953963	1939415	72.39%	8.536%
7	7.057	874	879	882	rBV	1937316	1782394	66.53%	7.845%
8	7.769	996	1000	1008	rBV	1173775	968977	36.17%	4.265%
9	8.845	1179	1183	1187	rBV	2199971	2073175	77.38%	9.125%
10	9.245	1248	1251	1257	rBV	505750	394833	14.74%	1.738%
11	9.516	1293	1297	1301	rBV	958337	851495	31.78%	3.748%
12	9.969	1371	1374	1377	rVB	43644	33960	1.27%	0.149%
13	10.186	1404	1411	1414	rBV2	18301	27086	1.01%	0.119%
14	10.298	1427	1430	1438	rBV	1046956	939981	35.08%	4.137%
15	10.439	1451	1454	1461	rBV	67355	76808	2.87%	0.338%
16	10.886	1525	1530	1532	rBV	40207	38894	1.45%	0.171%
17	10.986	1543	1547	1550	rBV	715618	626213	23.37%	2.756%
18	11.010	1550	1551	1555	rVB	103876	63225	2.36%	0.278%
19	11.539	1639	1641	1649	rBV2	67595	72310	2.70%	0.318%
20	12.192	1749	1752	1755	rBV	120793	103625	3.87%	0.456%
21	12.416	1786	1790	1797	rBV	166512	150776	5.63%	0.664%
22	12.568	1812	1816	1820	rBV	1387227	1243162	46.40%	5.472%
23	13.480	1967	1971	1977	rBV2	96733	123205	4.60%	0.542%
24	13.610	1988	1993	1996	rBV	657577	625197	23.34%	2.752%
25	13.633	1996	1997	2003	rVB	44568	40615	1.52%	0.179%
26	14.374	2120	2123	2126	rBV3	24261	29521	1.10%	0.130%
27	14.604	2158	2162	2169	rVB	64048	107179	4.00%	0.472%
28	14.692	2173	2177	2183	rBV2	35324	49064	1.83%	0.216%
29	14.857	2202	2205	2207	rBV	29340	30291	1.13%	0.133%
30	14.909	2211	2214	2218	rVB	42189	45927	1.71%	0.202%
31	14.957	2218	2222	2227	rBV	413540	486557	18.16%	2.142%
32	15.004	2228	2230	2234	rVB	54351	56900	2.12%	0.250%
33	15.362	2287	2291	2296	rVB	61814	78394	2.93%	0.345%
34	15.774	2357	2361	2367	rVB	82109	125832	4.70%	0.554%

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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	16.186	2426	2431	2433	rBV3	23477	38020	1.42%	0.167%
36	16.251	2437	2442	2449	rVB	73174	139933	5.22%	0.616%
37	16.809	2532	2537	2544	rVB	73761	143983	5.37%	0.634%
38	17.474	2646	2650	2661	rVB4	43467	108389	4.05%	0.477%

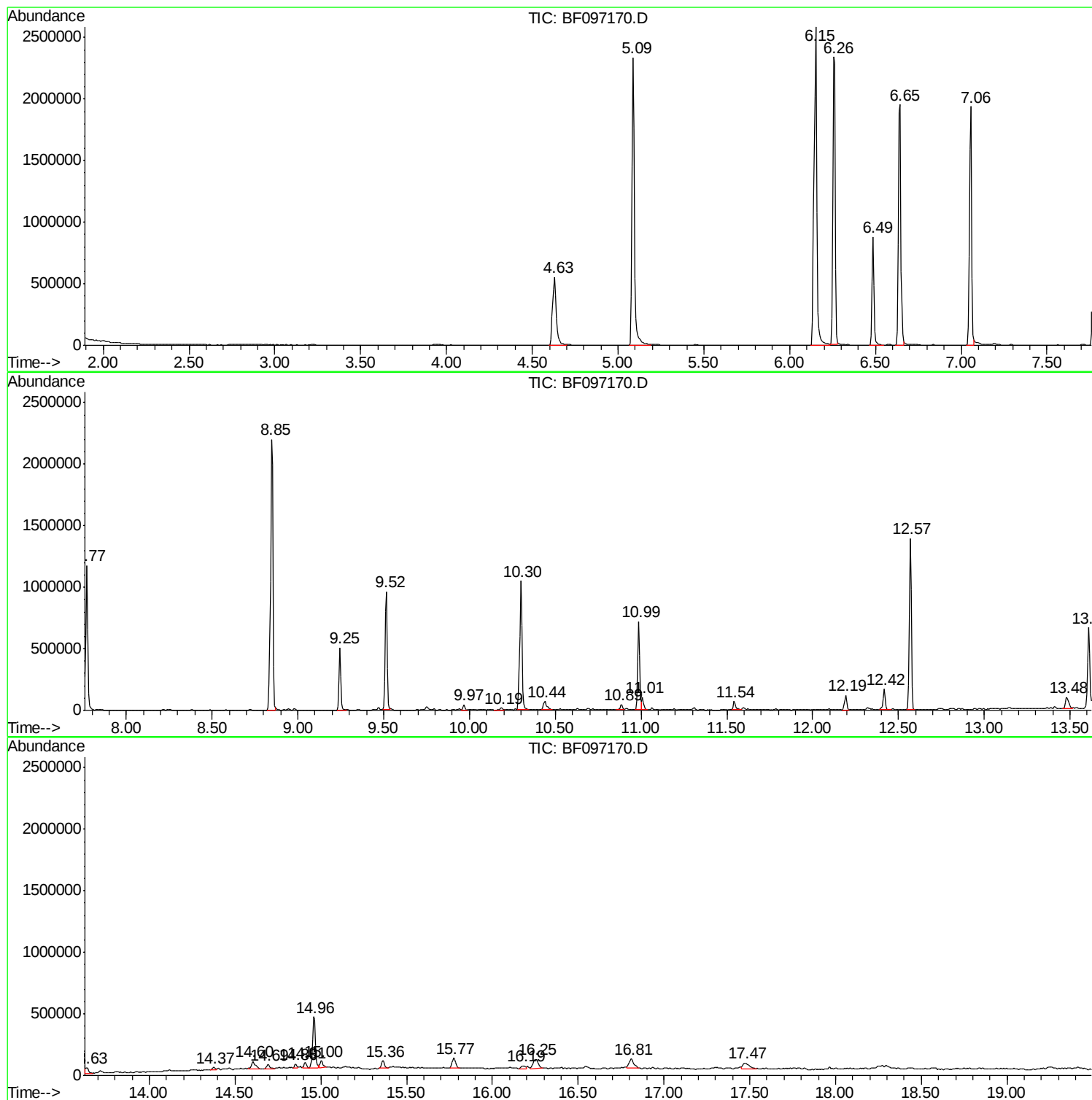
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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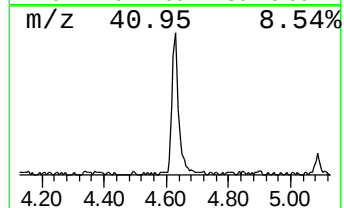
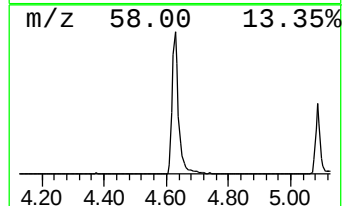
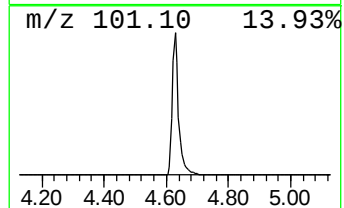
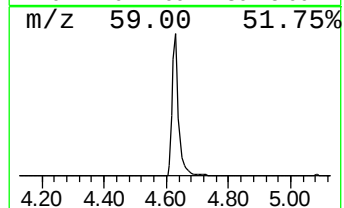
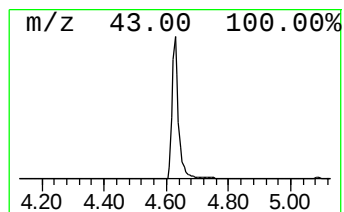
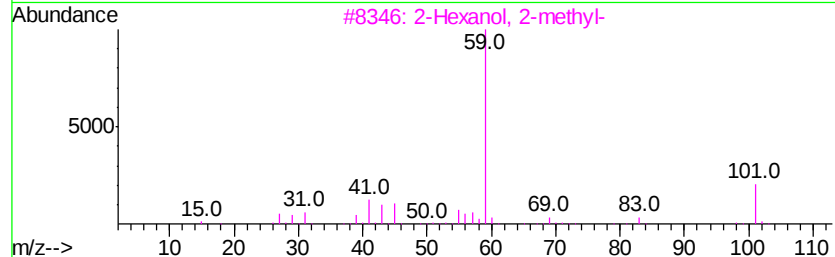
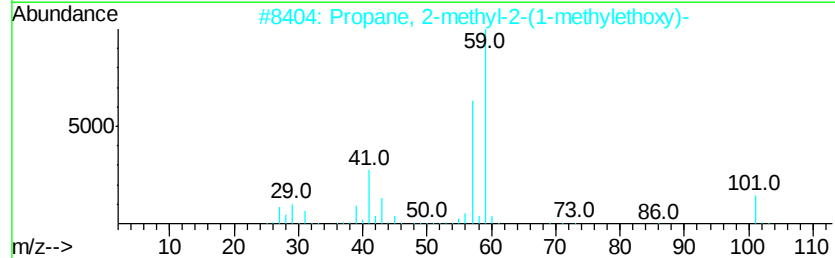
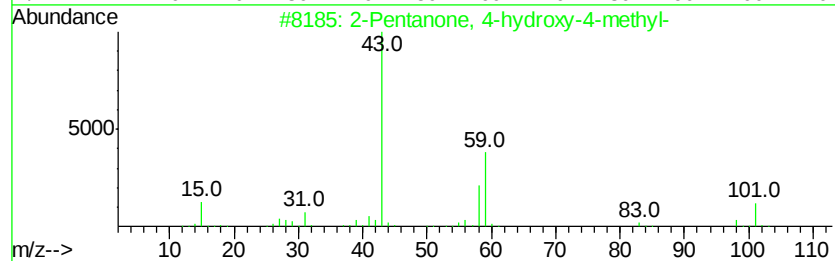
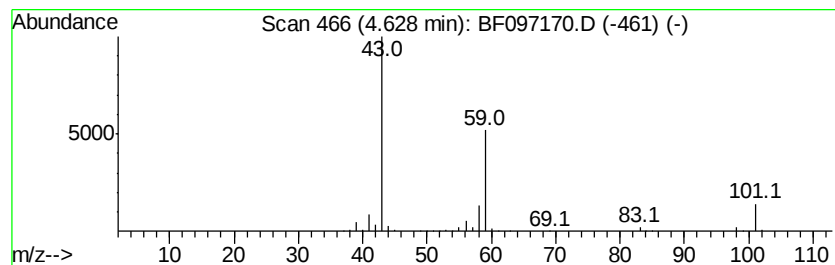
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	20.94 ng	783188	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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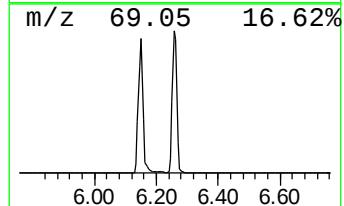
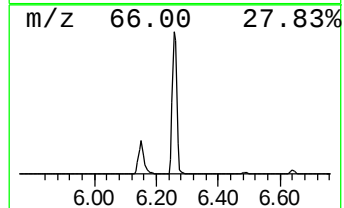
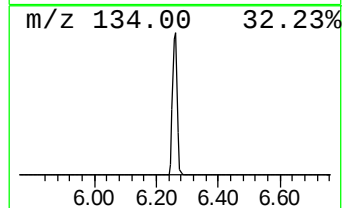
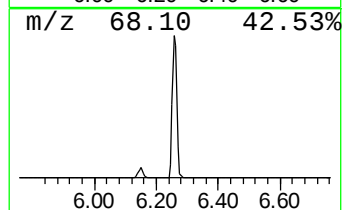
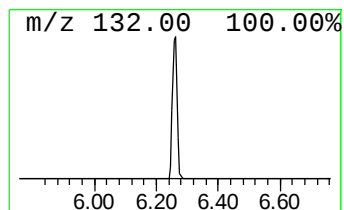
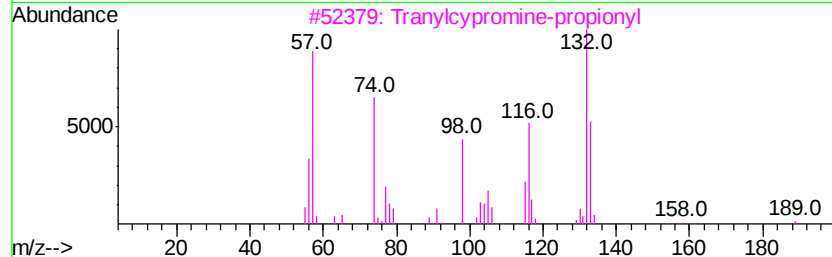
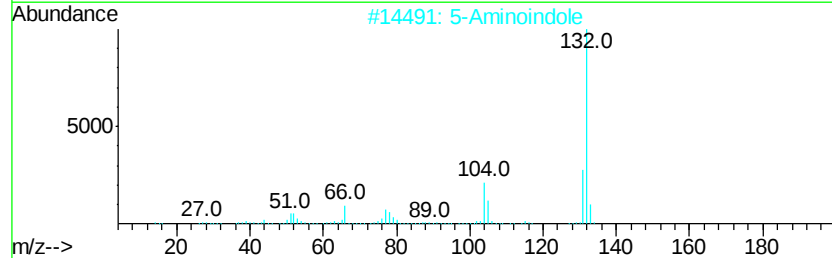
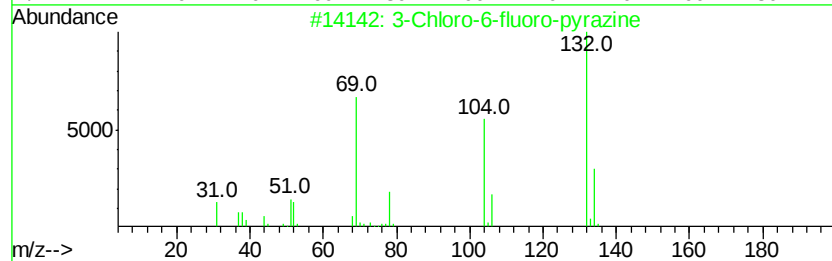
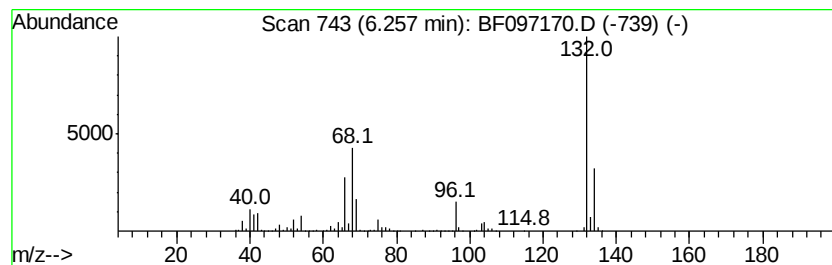
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	63.01 ng	2356800	1,4-Dichlorobenzene-d4	6.49

Hit#	of	5	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			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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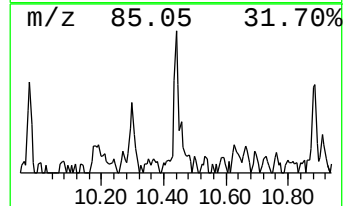
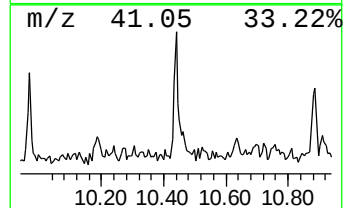
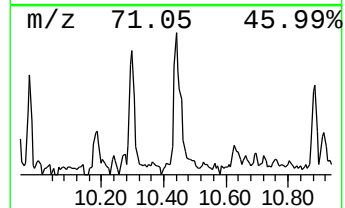
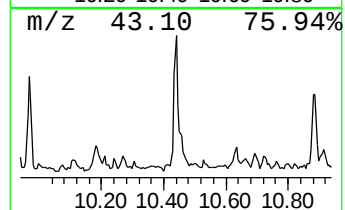
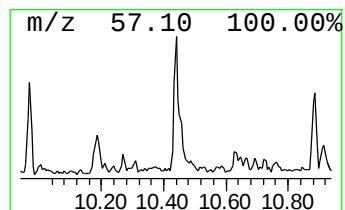
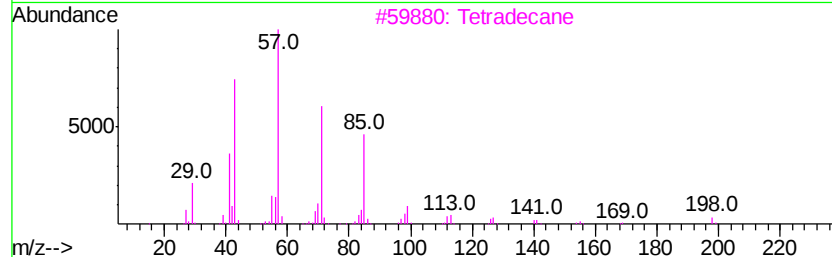
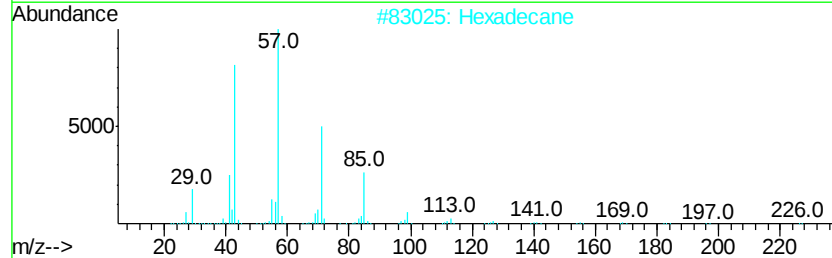
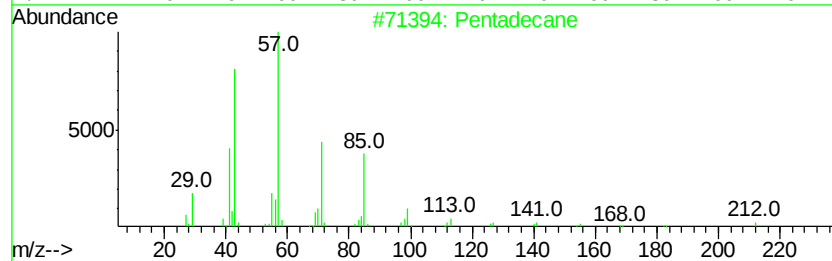
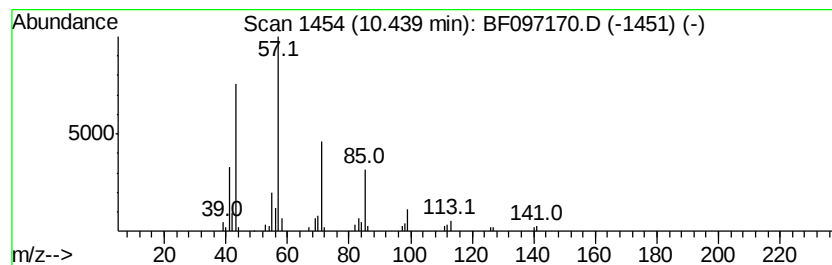
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.45 ng	76808	Phenanthrene-d10	10.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	87
2		Hexadecane	226	C16H34	000544-76-3	86
3		Tetradecane	198	C14H30	000629-59-4	86
4		Tridecane	184	C13H28	000629-50-5	86
5		Octadecane	254	C18H38	000593-45-3	80



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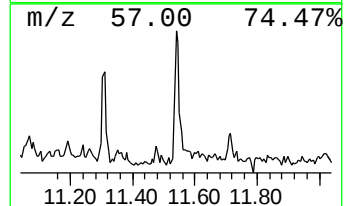
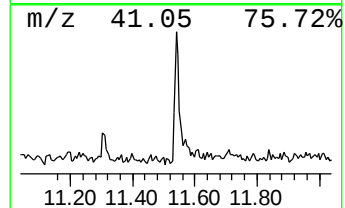
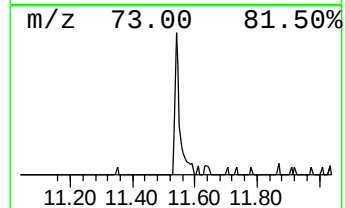
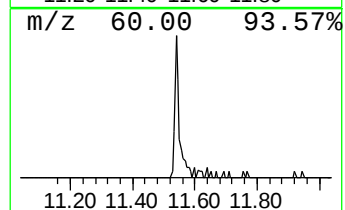
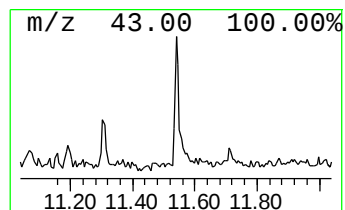
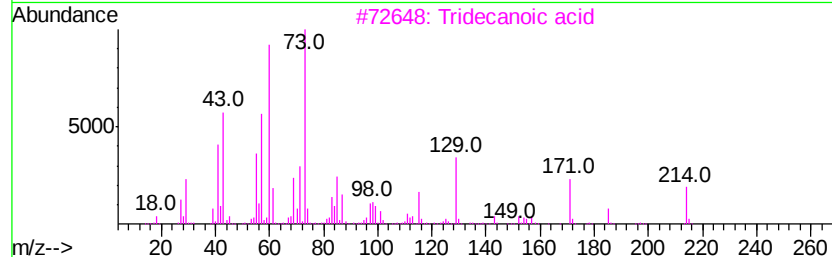
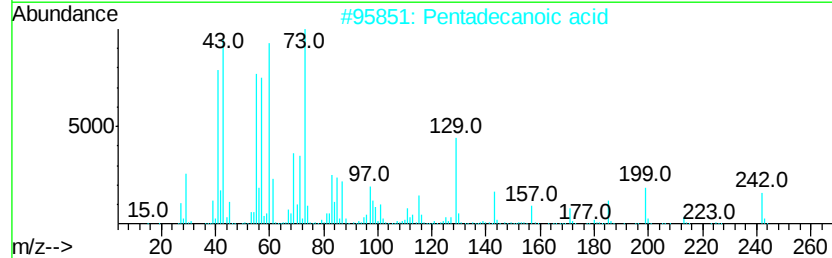
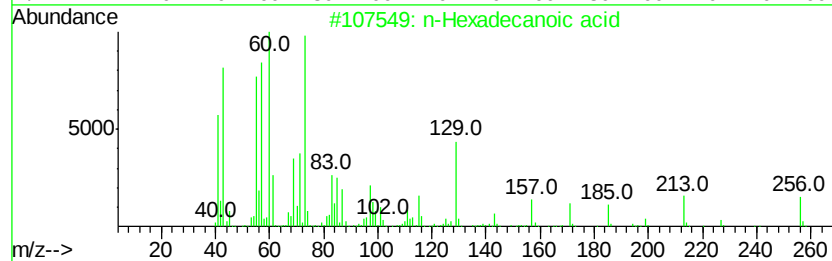
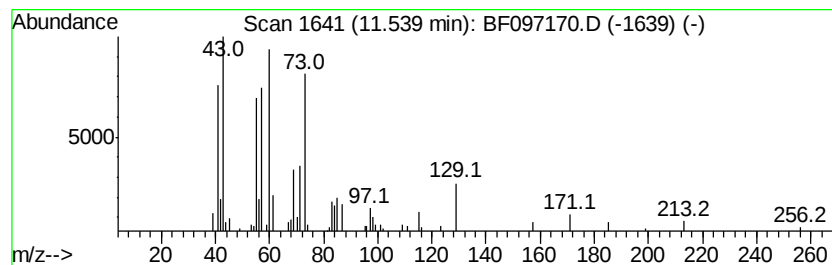
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.31 ng	72310	Phenanthrene-d10	10.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Undecanoic acid	186	C11H22O2	000112-37-8	86
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	86



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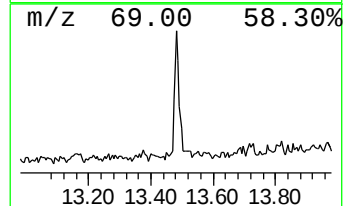
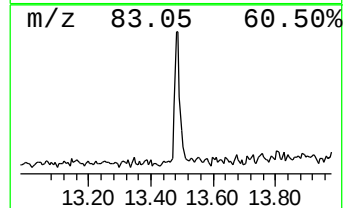
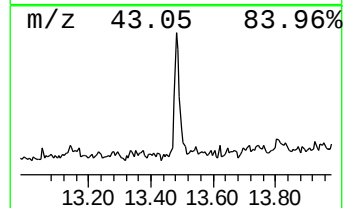
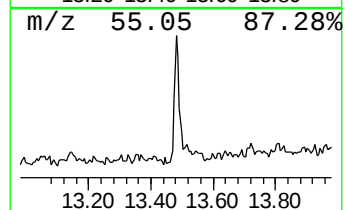
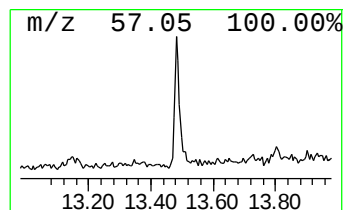
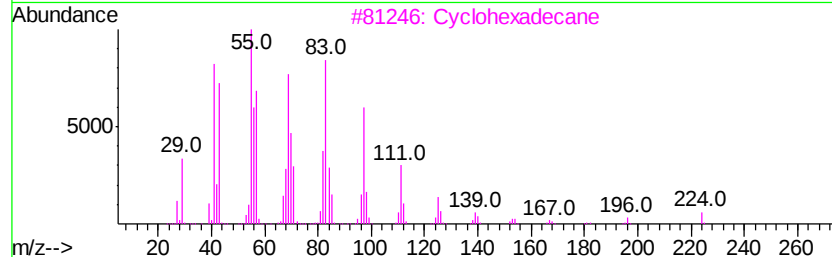
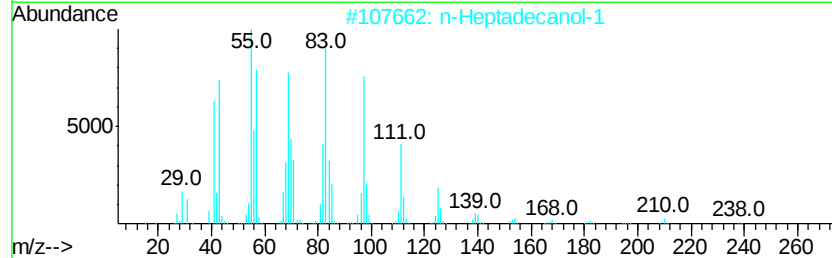
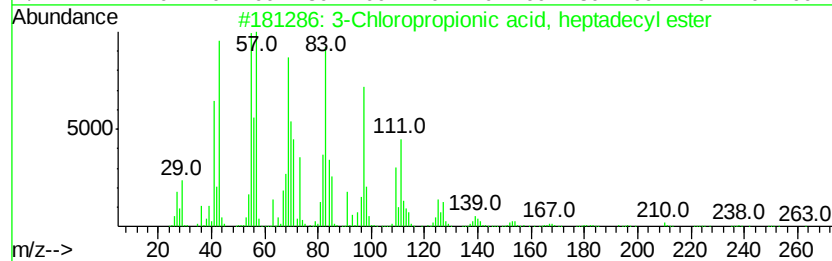
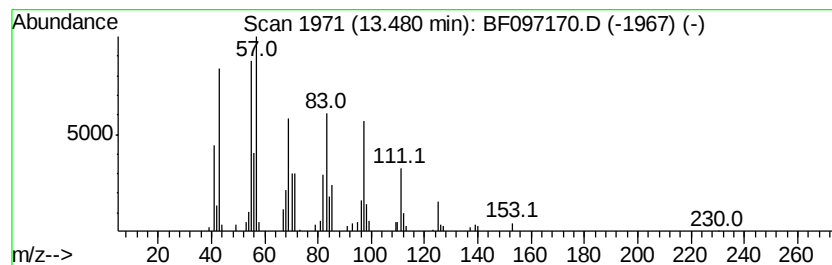
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Chloropropionic acid, hep... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	3.94 ng	123205	Chrysene-d12	13.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3		Cyclohexadecane	224	C16H32	000295-65-8	91
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



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Acq On : 28 Jul 2017 22:50
Operator : SJ/JU
Sample : I4456-03
Misc :
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Instrument :
BNA_F
ClientSampleId :
TP-8D24

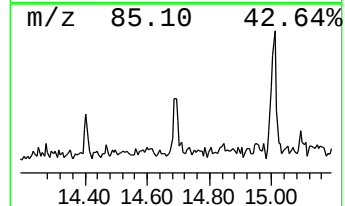
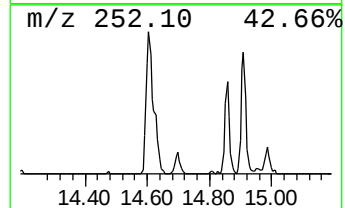
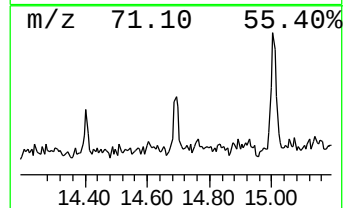
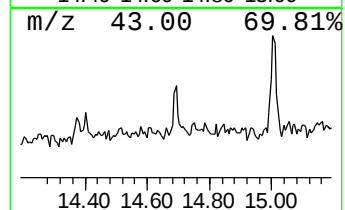
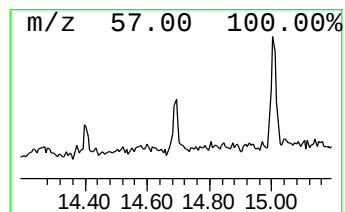
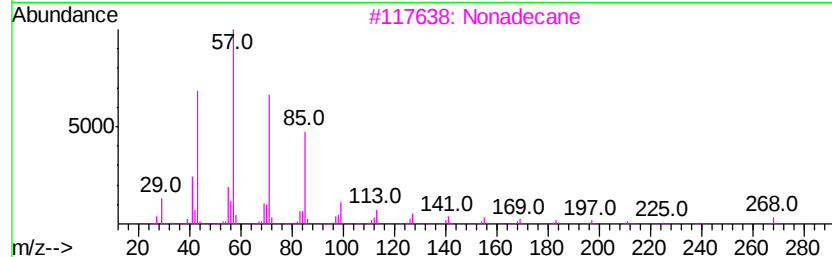
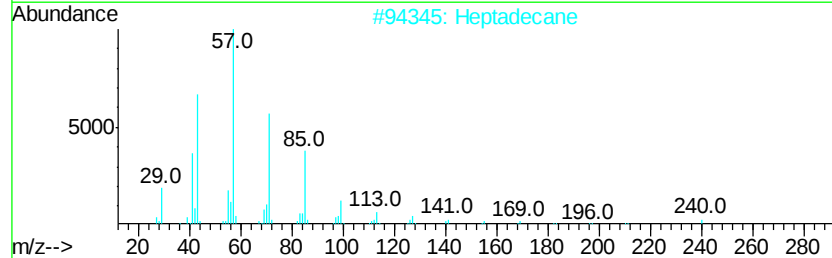
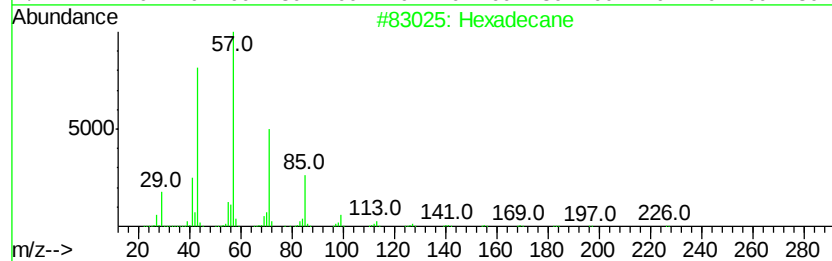
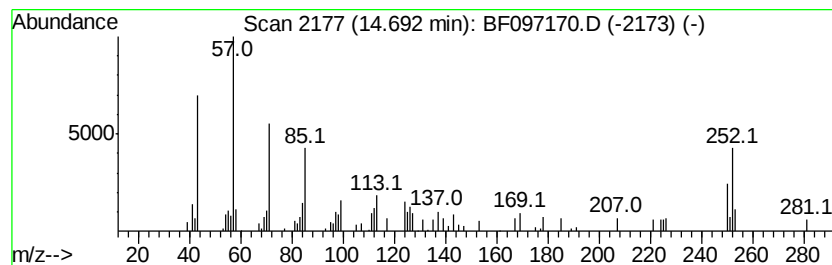
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.02 ng	49064	Perylene-d12	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	42
2		Heptadecane	240	C17H36	000629-78-7	35
3		Nonadecane	268	C19H40	000629-92-5	27
4		3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	27
5		Heneicosane	296	C21H44	000629-94-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
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Acq On : 28 Jul 2017 22:50
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Misc :
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ClientSampleId :
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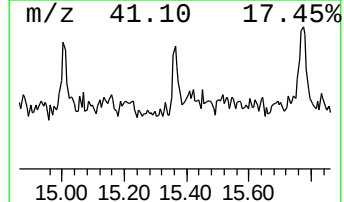
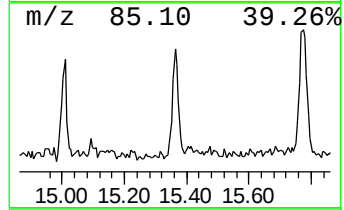
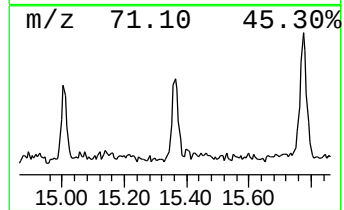
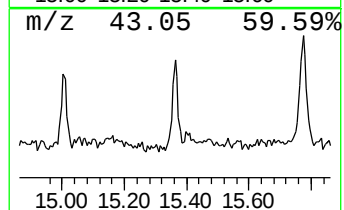
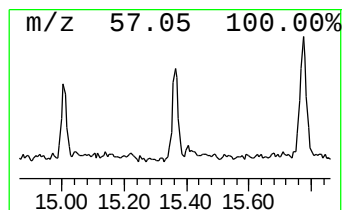
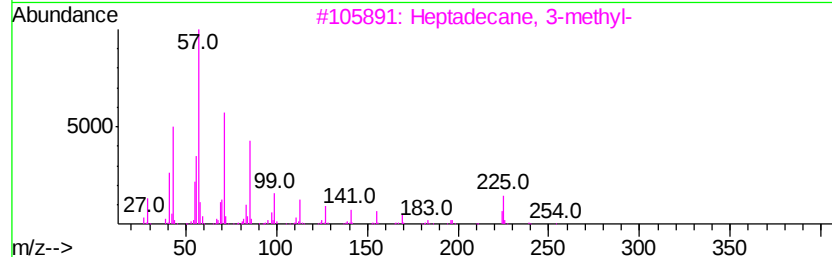
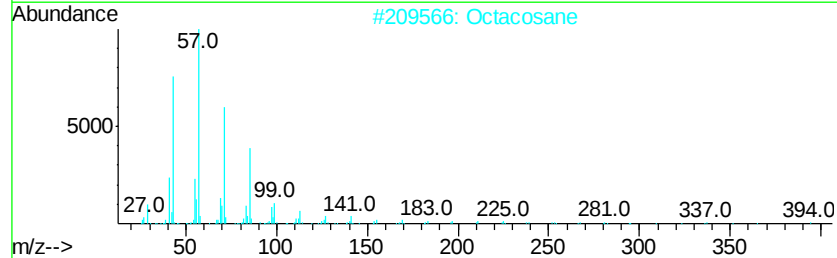
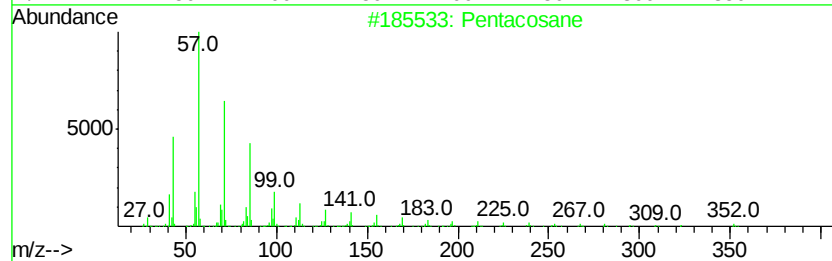
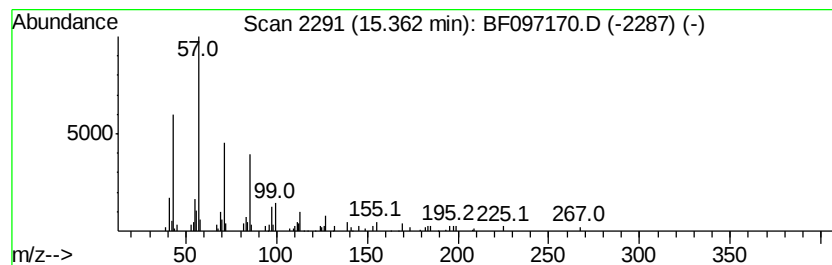
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	3.22 ng	78394	Perylene-d12	14.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	91
2	Octacosane		394	C28H58	000630-02-4	86
3	Heptadecane, 3-methyl-		254	C18H38	006418-44-6	86
4	triacontane		422	C30H62	000638-68-6	80
5	Tetracosane		338	C24H50	000646-31-1	80



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Sample : I4456-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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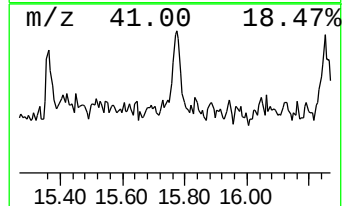
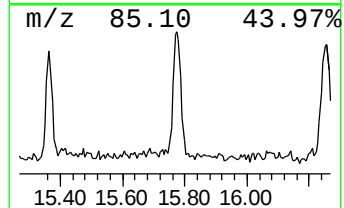
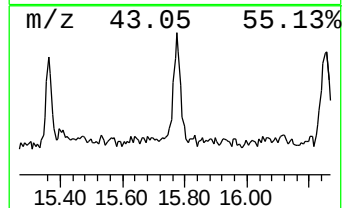
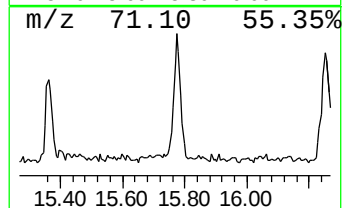
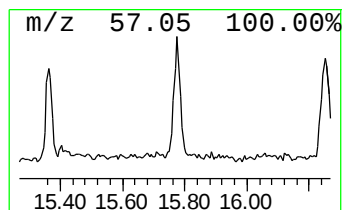
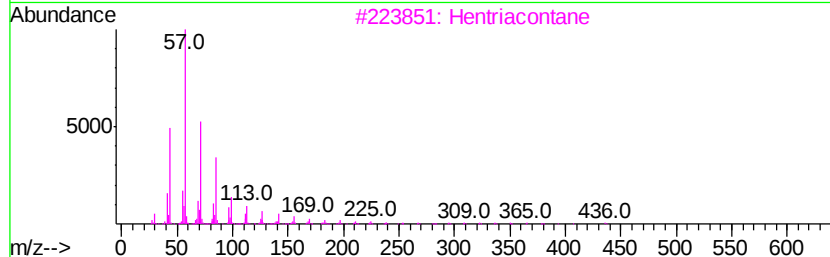
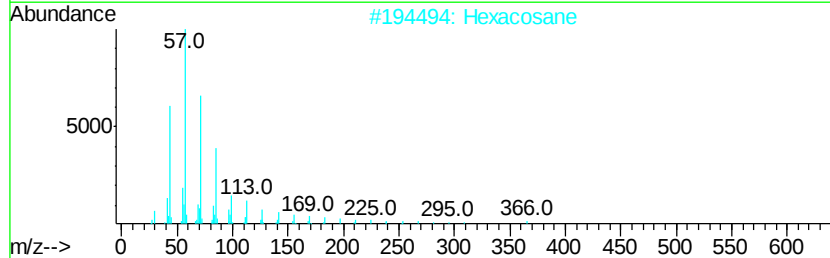
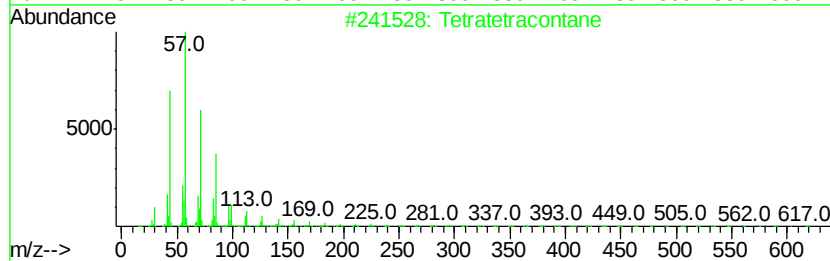
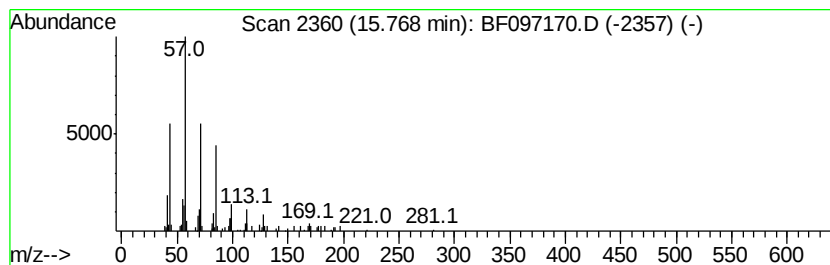
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	5.17 ng	125832	Perylene-d12	14.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	90
2		Hexacosane	366	C26H54	000630-01-3	86
3		Hentriacontane	437	C31H64	000630-04-6	86
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5		2-methyloctacosane	408	C29H60	1000376-72-8	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
Data File : BF097170.D
Acq On : 28 Jul 2017 22:50
Operator : SJ/JU
Sample : I4456-03
Misc :
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Instrument :
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ClientSampleId :
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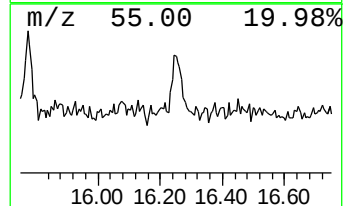
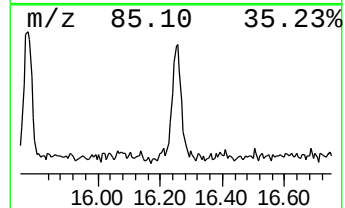
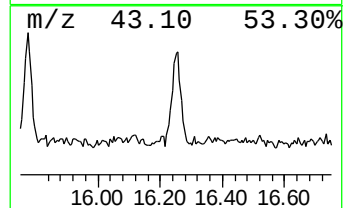
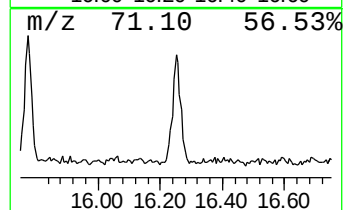
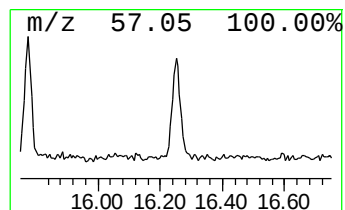
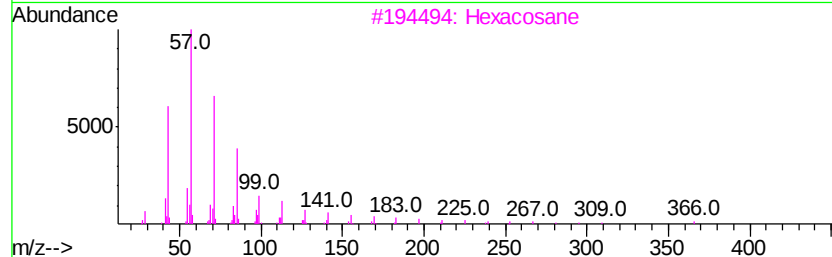
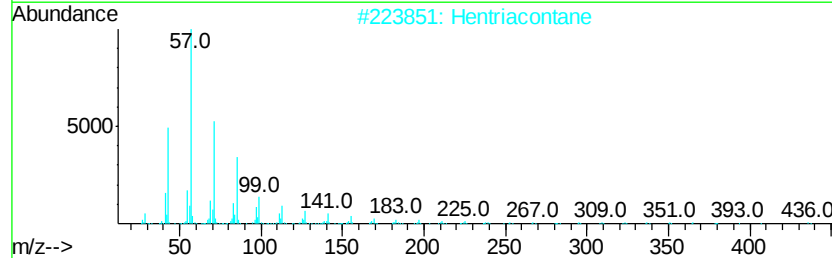
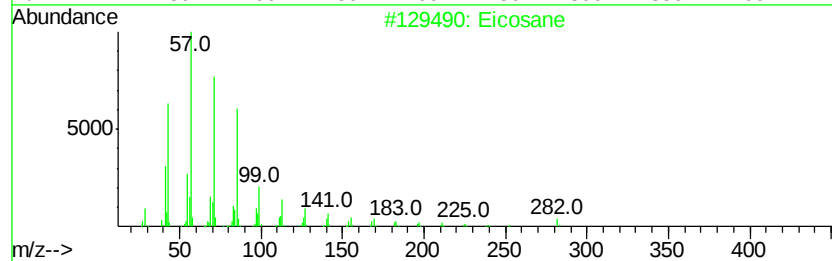
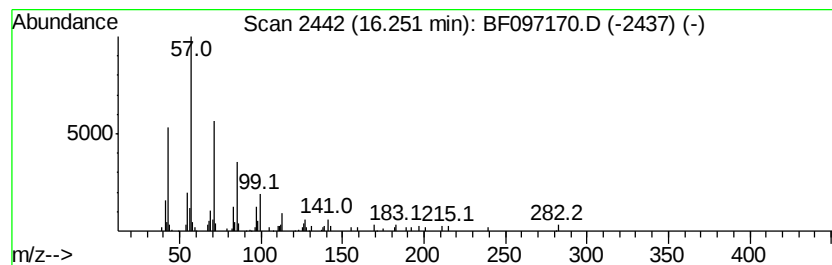
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	5.75 ng	139933	Perylene-d12	14.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Hentriacontane		437	C31H64	000630-04-6	90
3	Hexacosane		366	C26H54	000630-01-3	87
4	Tridecanol, 2-ethyl-2-methyl-		242	C16H34O	1000115-66-1	86
5	Docosane		310	C22H46	000629-97-0	86



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Sample : I4456-03
Misc :
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ClientSampleId :
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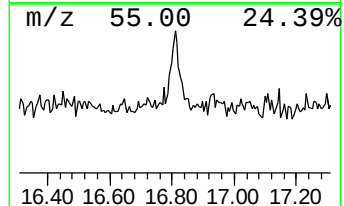
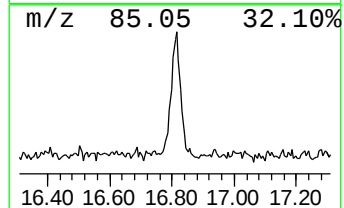
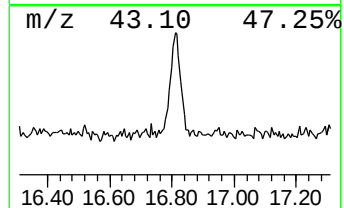
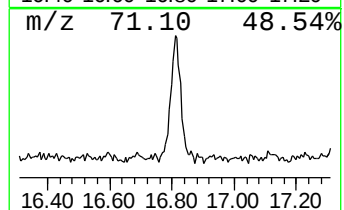
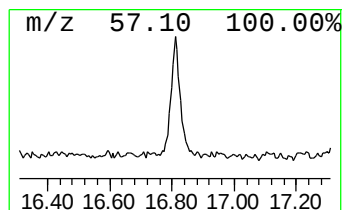
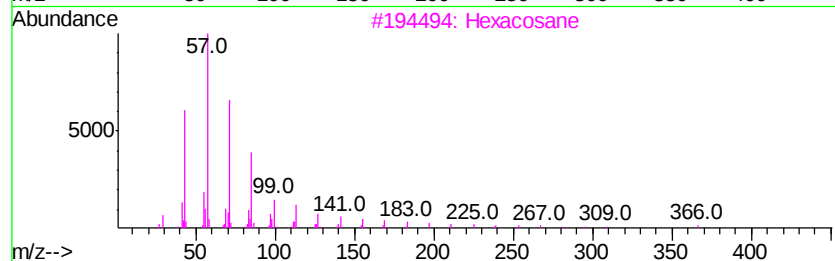
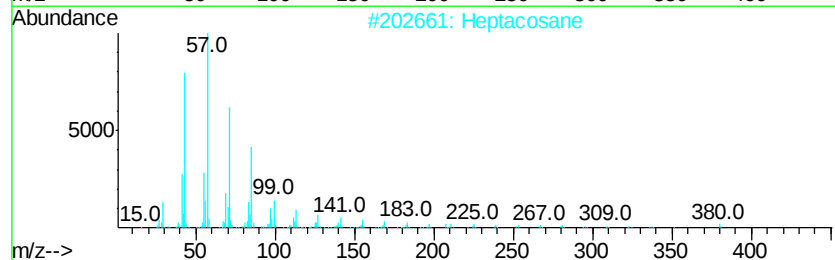
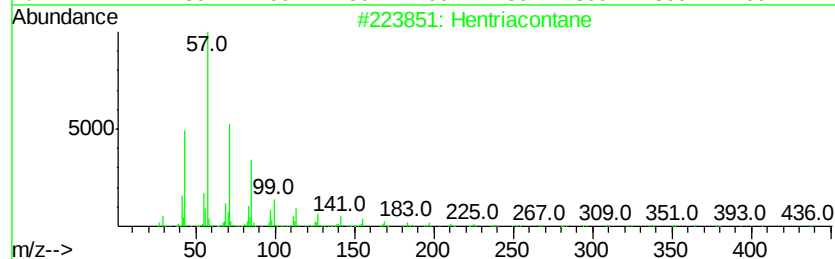
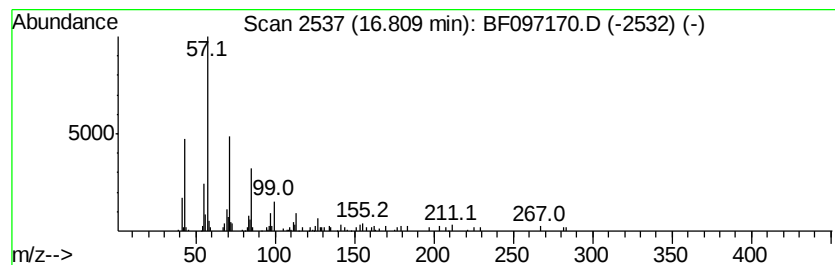
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	5.92 ng	143983	Perylene-d12	14.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Heptacosane	380	C27H56	000593-49-7	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5			Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
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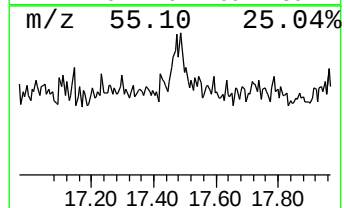
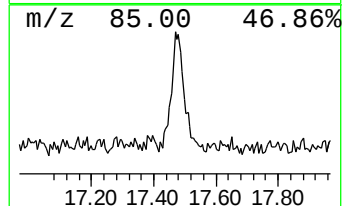
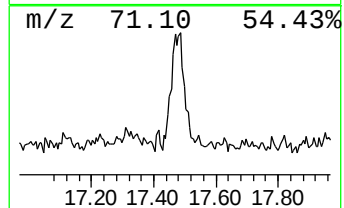
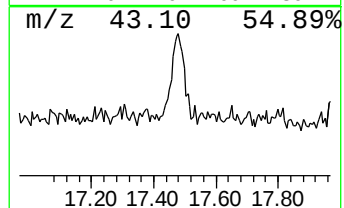
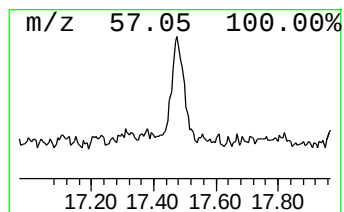
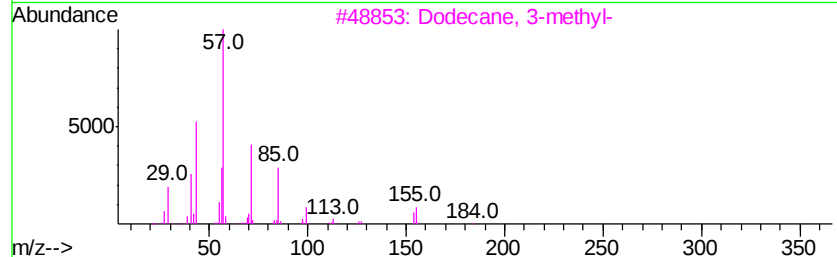
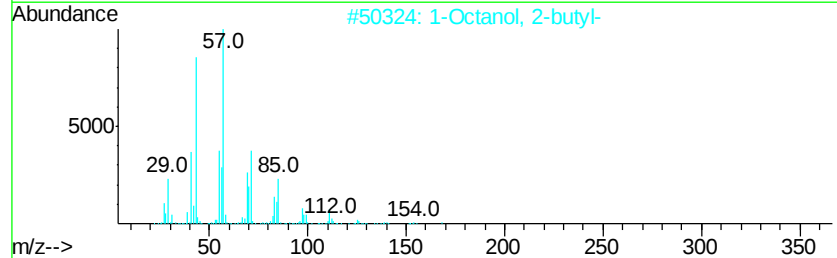
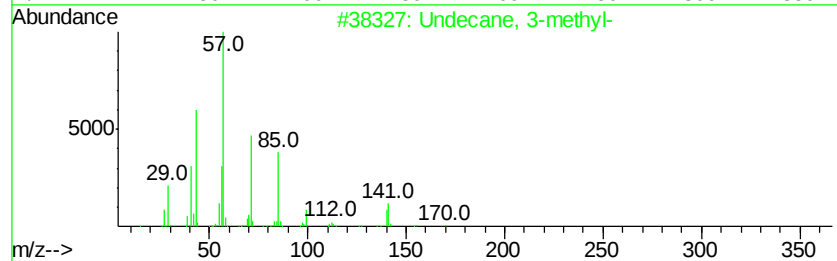
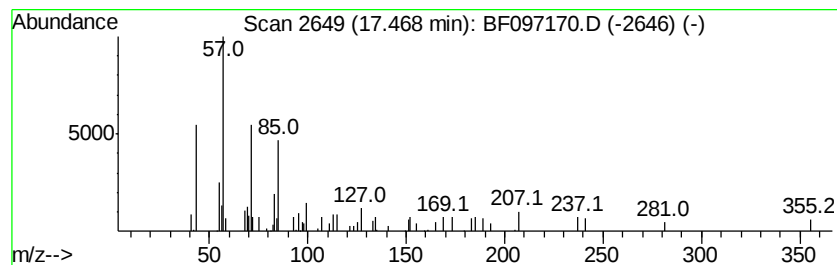
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Undecane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	4.46 ng	108389	Perylene-d12	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 3-methyl-	170	C12H26	001002-43-3	59
2		1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	59
3		Dodecane, 3-methyl-	184	C13H28	017312-57-1	59
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	59
5		3,5-Dimethyldodecane	198	C14H30	107770-99-0	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.26	6.26	63.0	ng	2356800	1	6.49	748123	20.0
Pentadecane	10.44	2.5	ng	76808	4	10.99	626213	20.0
n-Hexadecanoic acid	11.54	2.3	ng	72310	4	10.99	626213	20.0
3-Chloropropionic...	13.48	3.9	ng	123205	5	13.61	625197	20.0
Hexadecane	14.69	2.0	ng	49064	6	14.96	486557	20.0
Pentacosane	15.36	3.2	ng	78394	6	14.96	486557	20.0
Tetratetracontane	15.77	5.2	ng	125832	6	14.96	486557	20.0
Eicosane	16.25	5.8	ng	139933	6	14.96	486557	20.0
Hentriacontane	16.81	5.9	ng	143983	6	14.96	486557	20.0
Undecane, 3-methyl-	17.47	4.5	ng	108389	6	14.96	486557	20.0