

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
 Data File : BF093776.D
 Acq On : 20 Mar 2017 20:47
 Operator : SJ/MA
 Sample : I2304-03 2X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPA-B2(0-5)

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-BF032017.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	2.104	17	19	30	rVB	79647	123054	3.20%	0.316%
2	3.121	105	108	114	rVB	39107	71201	1.85%	0.183%
3	5.007	270	273	278	rBV	550472	660663	17.16%	1.698%
4	5.430	307	310	313	rBV	3105898	3277121	85.11%	8.421%
5	5.842	342	346	348	rBV	45964	45958	1.19%	0.118%
6	6.459	397	400	403	rBV	2559829	3850421	100.00%	9.894%
7	6.596	410	412	415	rBV	2790976	3730897	96.90%	9.587%
8	6.836	430	433	435	rBV	1677842	1440297	37.41%	3.701%
9	6.996	444	447	449	rVB	2720286	2850039	74.02%	7.324%
10	7.396	479	482	484	rBV	2550181	2465397	64.03%	6.335%
11	7.636	499	503	506	rVB2	46281	95913	2.49%	0.246%
12	7.865	520	523	524	rBV2	31948	56303	1.46%	0.145%
13	8.116	543	545	548	rBV	1706731	1895795	49.24%	4.872%
14	8.230	553	555	558	rVB	32699	39579	1.03%	0.102%
15	8.562	581	584	586	rBV	34863	43608	1.13%	0.112%
16	8.722	596	598	602	rBV2	39116	70000	1.82%	0.180%
17	8.825	605	607	609	rVB2	32319	45941	1.19%	0.118%
18	8.928	614	616	620	rVV2	27769	39307	1.02%	0.101%
19	9.156	635	636	637	rBV	47800	38579	1.00%	0.099%
20	9.202	637	640	642	rVB	3323356	3727617	96.81%	9.579%
21	9.293	645	648	650	rBV	105041	110385	2.87%	0.284%
22	9.453	660	662	666	rBV	42285	65644	1.70%	0.169%
23	9.533	666	669	672	rBV2	65324	143664	3.73%	0.369%
24	9.591	672	674	675	rVV	423706	380449	9.88%	0.978%
25	9.613	675	676	677	rVV	87445	76241	1.98%	0.196%
26	9.648	677	679	684	rVB2	31129	68307	1.77%	0.176%
27	9.819	693	694	696	rVB	149069	108318	2.81%	0.278%
28	9.876	696	699	701	rBV	1647813	2028969	52.69%	5.214%
29	9.979	706	708	710	rBV	24582	41083	1.07%	0.106%
30	10.071	712	716	718	rBV4	50784	110645	2.87%	0.284%
31	10.139	721	722	724	rBV2	48807	60352	1.57%	0.155%
32	10.185	724	726	728	rBV2	24048	50617	1.31%	0.130%
33	10.288	730	735	736	rBV5	54402	107314	2.79%	0.276%
34	10.322	736	738	739	rVV	95498	127554	3.31%	0.328%

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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 >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.368	739	742	745	rVV4	19696	47333	1.23%	0.122%
36	10.539	754	757	759	rBV	120269	134662	3.50%	0.346%
37	10.619	763	764	765	rBV	34735	43058	1.12%	0.111%
38	10.653	765	767	769	rVB	1815671	1670777	43.39%	4.293%
39	10.802	777	780	782	rBV	227847	399519	10.38%	1.027%
40	11.236	816	818	819	rBV2	190818	168038	4.36%	0.432%
41	11.271	819	821	823	rVB	148619	160447	4.17%	0.412%
42	11.351	826	828	829	rBV	1686407	1697027	44.07%	4.361%
43	11.374	829	830	831	rVB	71090	50689	1.32%	0.130%
44	11.614	849	851	853	rBV2	58731	73580	1.91%	0.189%
45	11.659	853	855	857	rVV	154109	124610	3.24%	0.320%
46	11.842	867	871	873	rBV4	56195	171517	4.45%	0.441%
47	11.888	873	875	876	rVV2	71325	116641	3.03%	0.300%
48	11.957	880	881	887	rVB5	62065	174280	4.53%	0.448%
49	12.345	913	915	918	rBV	80555	108292	2.81%	0.278%
50	12.551	932	933	935	rBV2	77535	123374	3.20%	0.317%
51	12.928	964	966	969	rBV	2383617	2340974	60.80%	6.015%
52	13.831	1043	1045	1049	rBV	152233	312179	8.11%	0.802%
53	13.968	1055	1057	1059	rBV	995192	1084734	28.17%	2.787%
54	15.374	1178	1180	1183	rVB	662358	1034688	26.87%	2.659%
55	15.534	1192	1194	1200	rVB3	88316	175890	4.57%	0.452%
56	16.060	1238	1240	1249	rVB3	133015	351873	9.14%	0.904%
57	16.471	1273	1276	1283	rVB	149236	304588	7.91%	0.783%

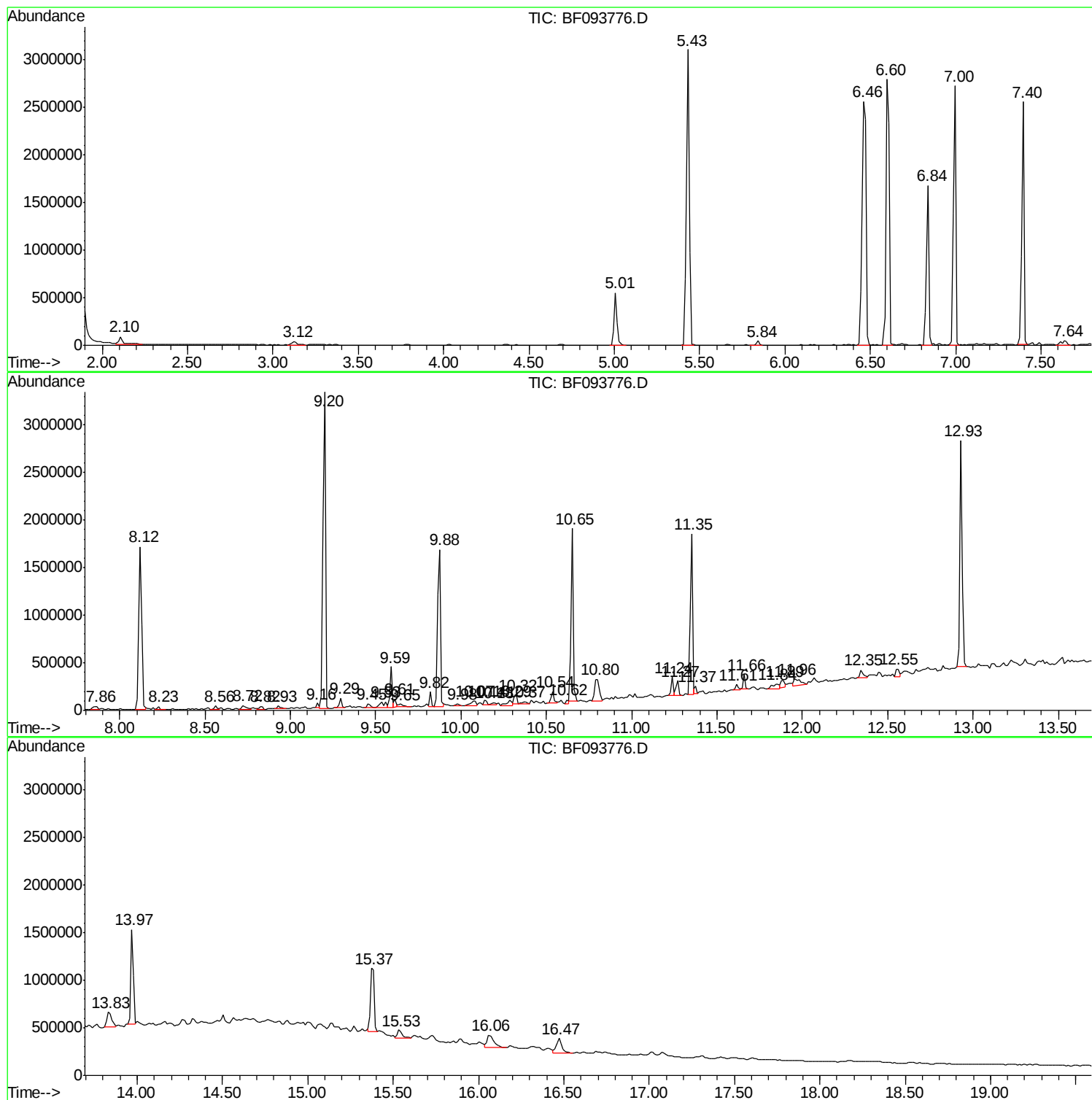
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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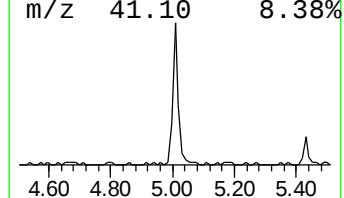
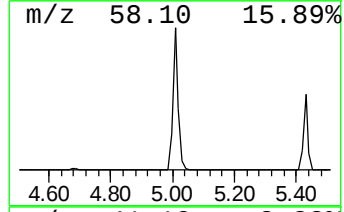
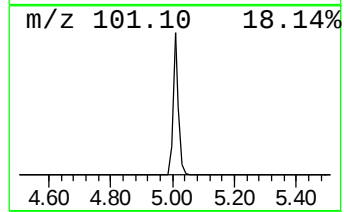
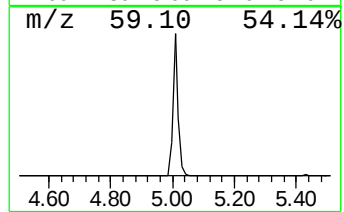
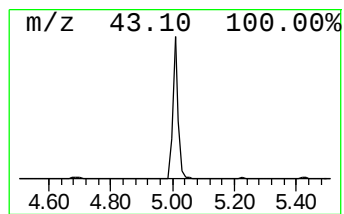
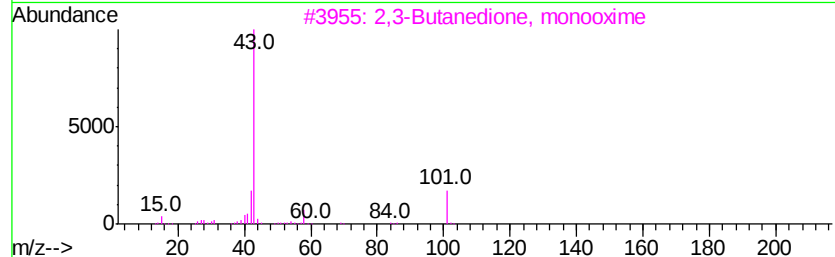
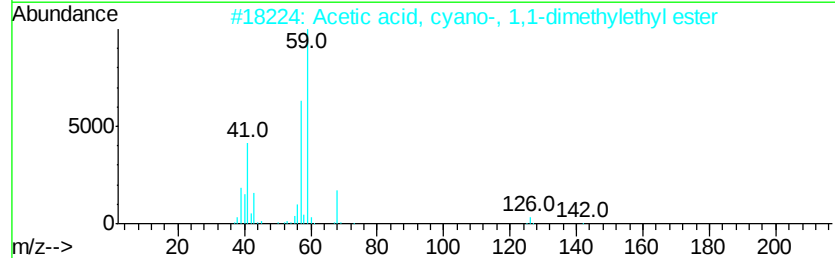
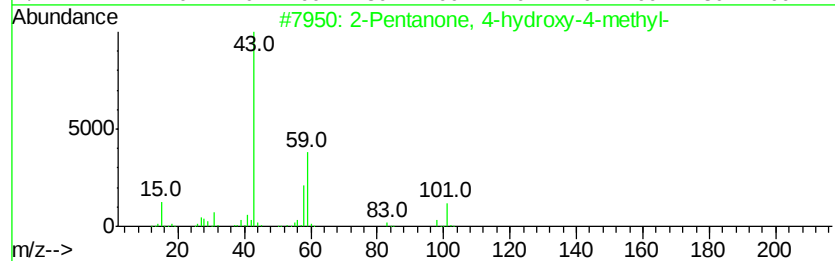
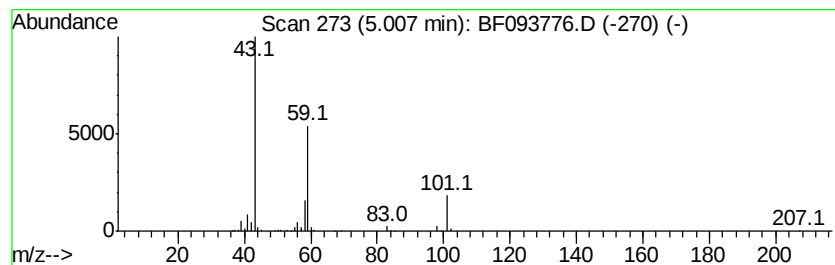
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.01	9.17 ng	660663	1,4-Dichlorobenzene-d4	6.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane	58	C4H10	000106-97-8	9



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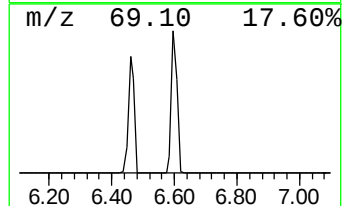
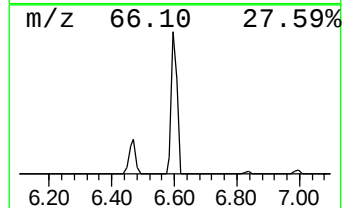
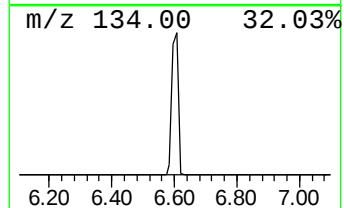
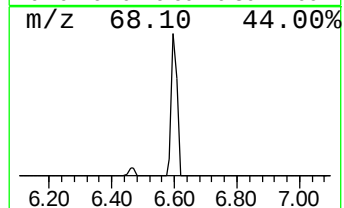
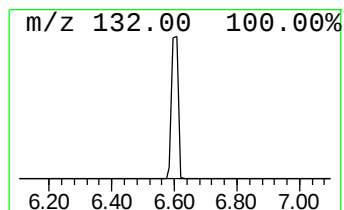
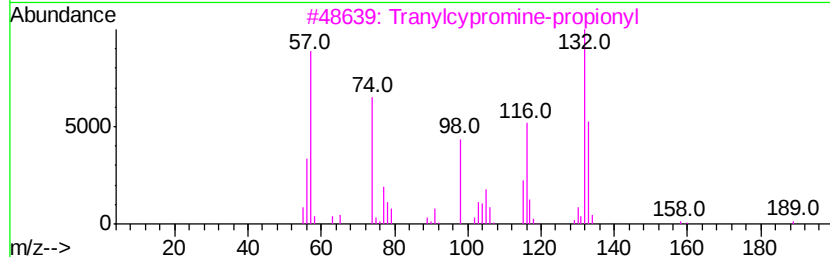
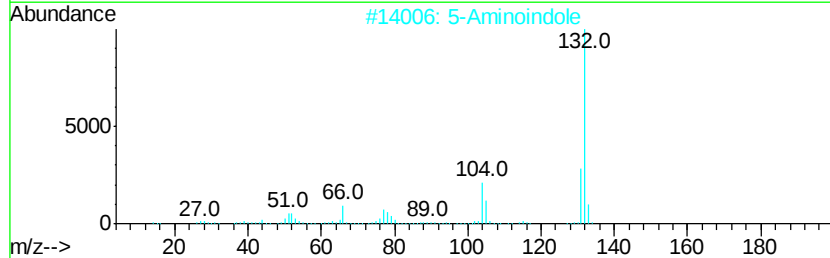
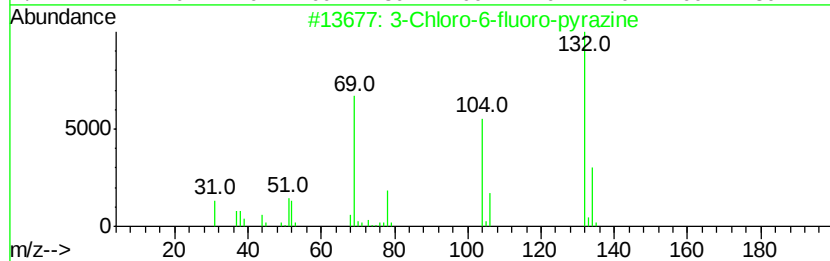
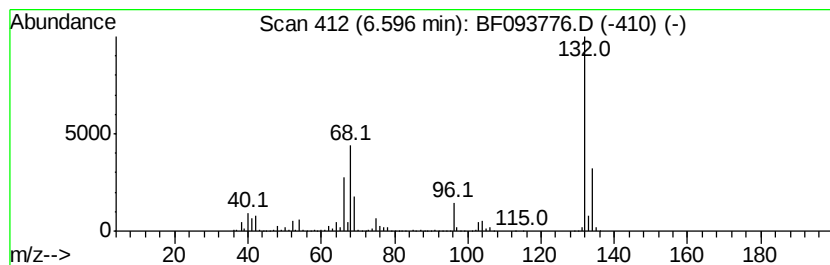
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	51.81 ng	3730900	1,4-Dichlorobenzene-d4	6.84

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			Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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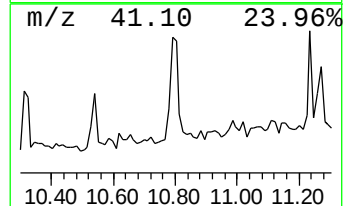
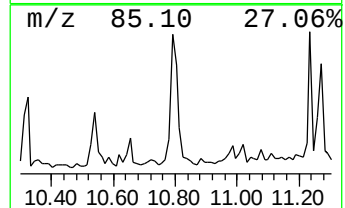
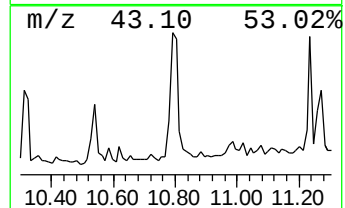
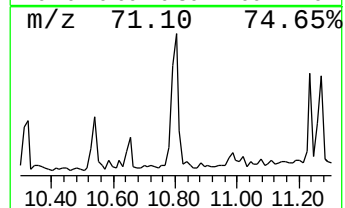
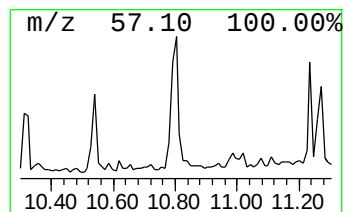
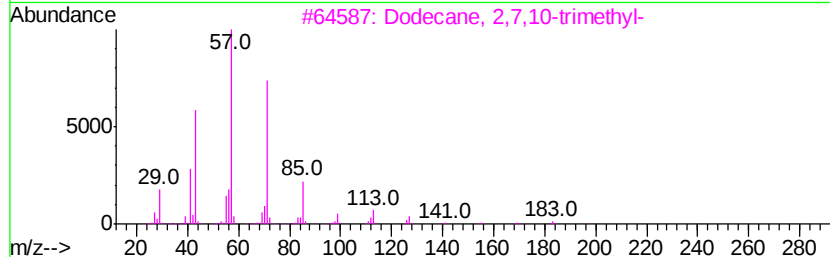
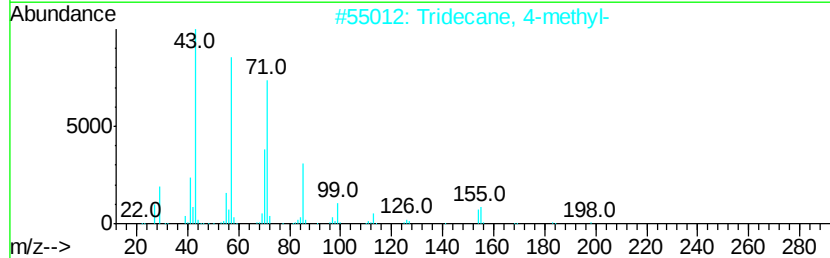
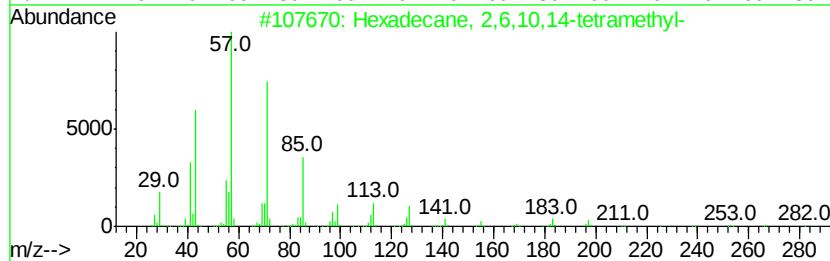
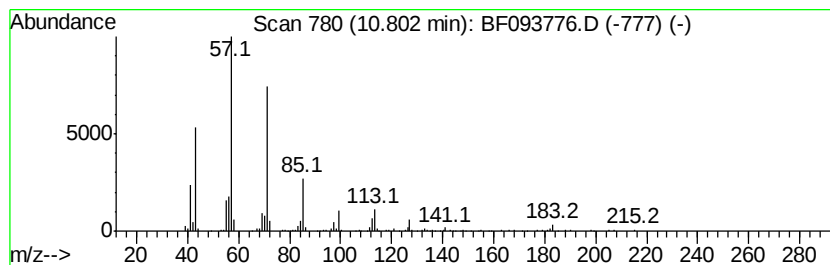
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane, 2,6,10,14-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	4.71 ng	399519	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2		Tridecane, 4-methyl-	198	C14H30	026730-12-1	87
3		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	78
5		Heptadecane, 7-methyl-	254	C18H38	020959-33-5	78



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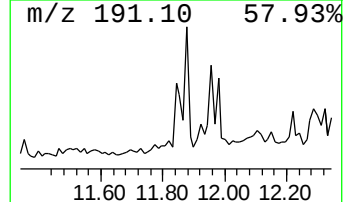
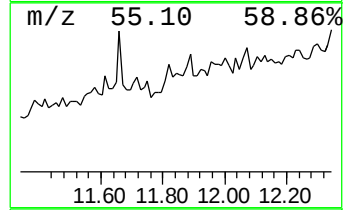
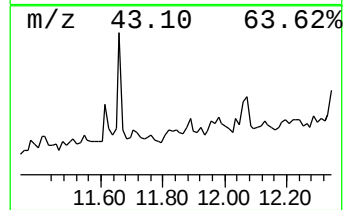
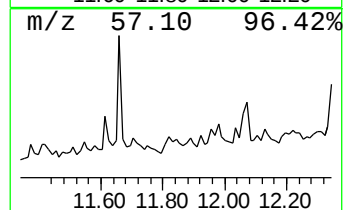
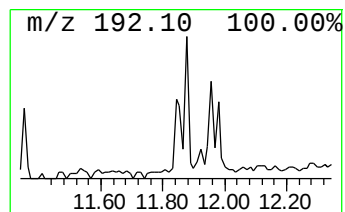
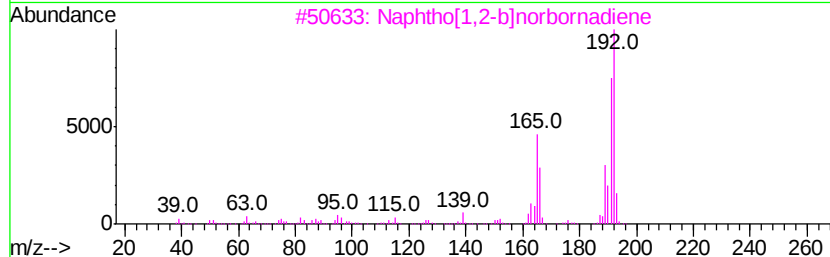
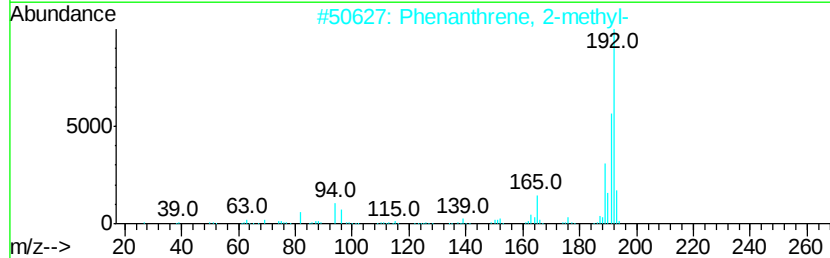
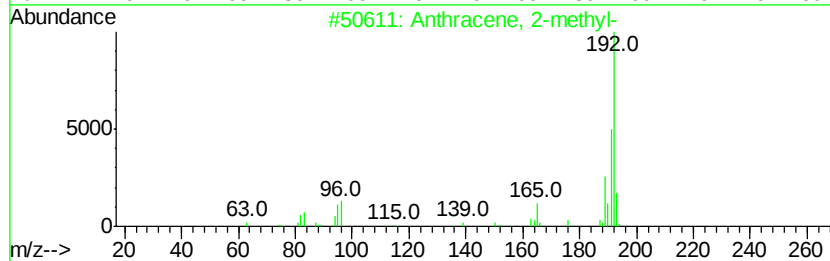
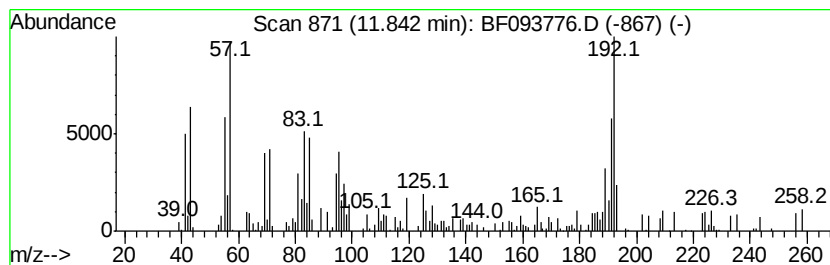
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Anthracene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.02 ng	171517	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 2-methyl-	192	C15H12	000613-12-7	55
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	50
3		Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	49
4		Anthracene, 1-methyl-	192	C15H12	000610-48-0	46
5		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46



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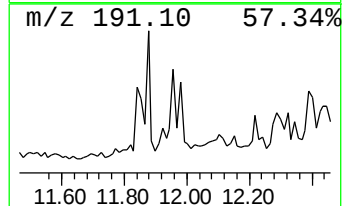
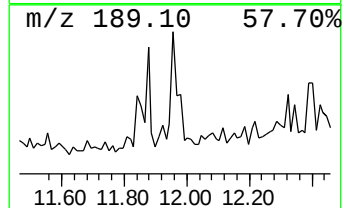
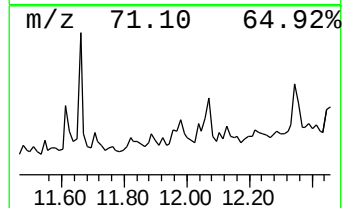
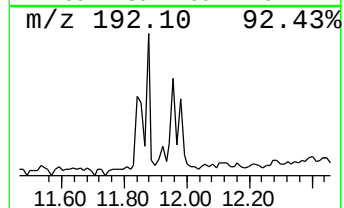
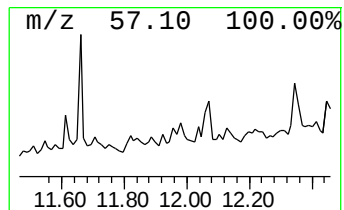
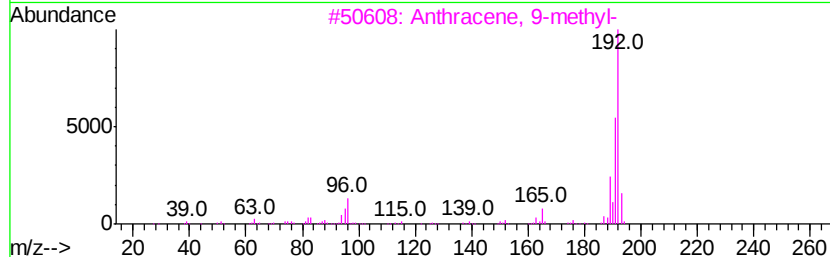
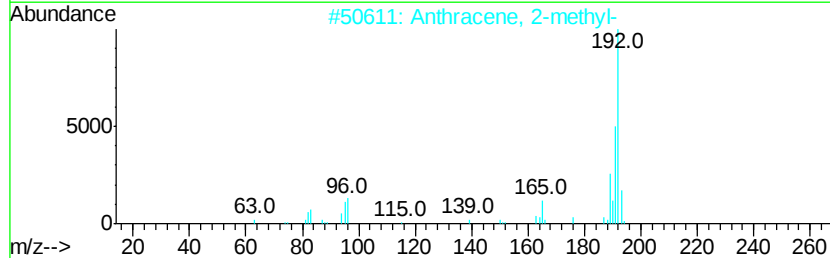
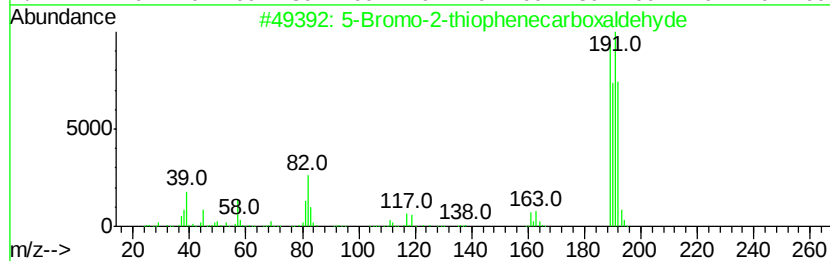
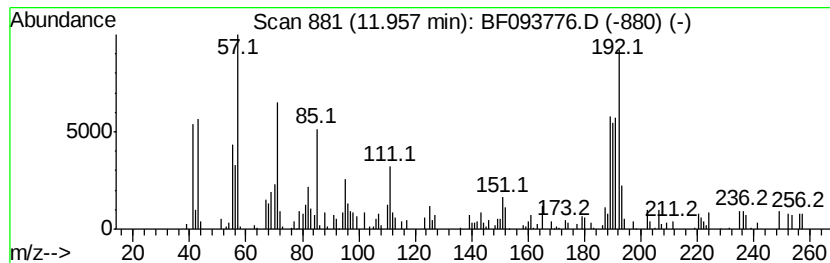
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown11.96 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.05 ng	174280	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Bromo-2-thiophenecarboxaldehde	190	C5H3BrOS	004701-17-1	49
2		Anthracene, 2-methyl-	192	C15H12	000613-12-7	43
3		Anthracene, 9-methyl-	192	C15H12	000779-02-2	35
4		5-Chloro-1,2-trimethylene benzim...	192	C10H9ClN2	010252-95-6	35
5		Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093776.D
Acq On : 20 Mar 2017 20:47
Operator : SJ/MA
Sample : I2304-03 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

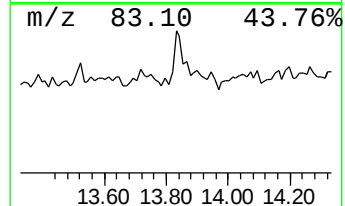
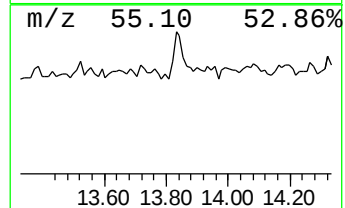
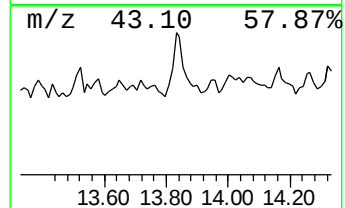
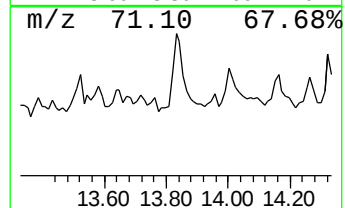
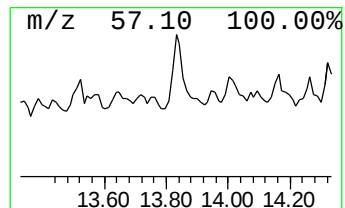
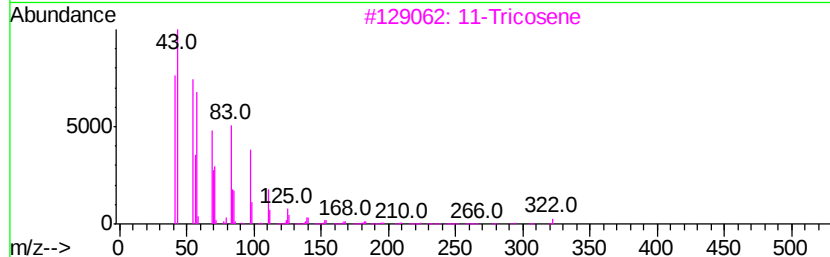
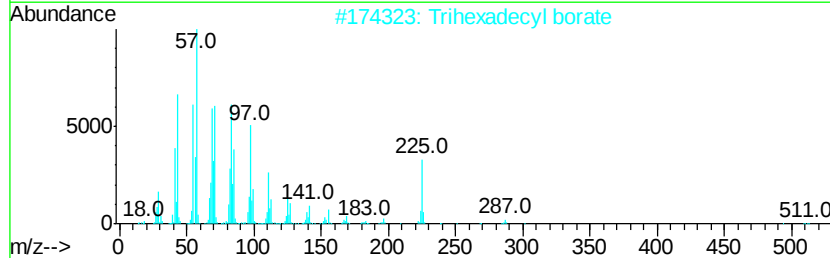
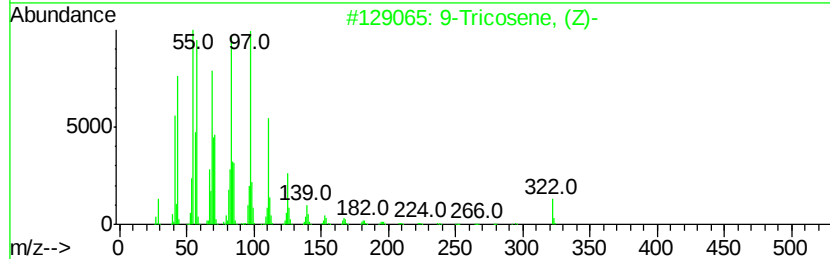
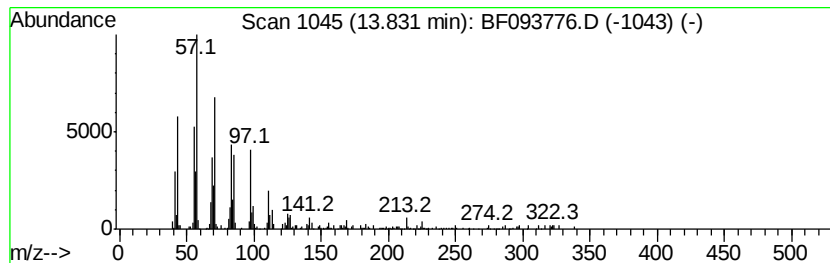
Instrument :
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ClientSampleId :
SPA-B2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Tricosene, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.83	5.76 ng	312179	Chrysene-d12	13.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-		322	C23H46	027519-02-4	83
2	Trihexadecyl borate		735	C48H99B03	002665-11-4	83
3	11-Tricosene		322	C23H46	052078-56-5	70
4	1-Tricosene		322	C23H46	018835-32-0	58
5	Trichloroacetic acid, pentadecyl...		372	C17H31Cl302	074339-53-0	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093776.D
Acq On : 20 Mar 2017 20:47
Operator : SJ/MA
Sample : I2304-03 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPA-B2(0-5)

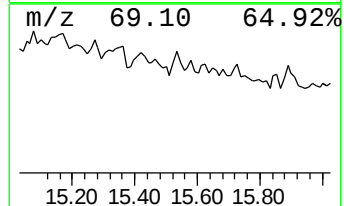
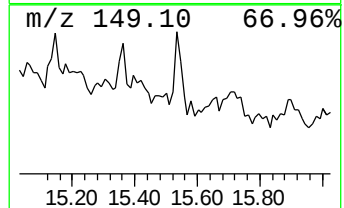
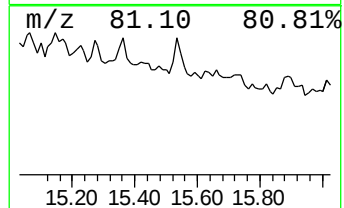
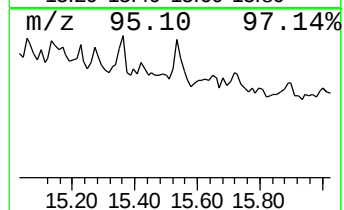
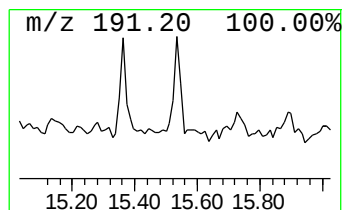
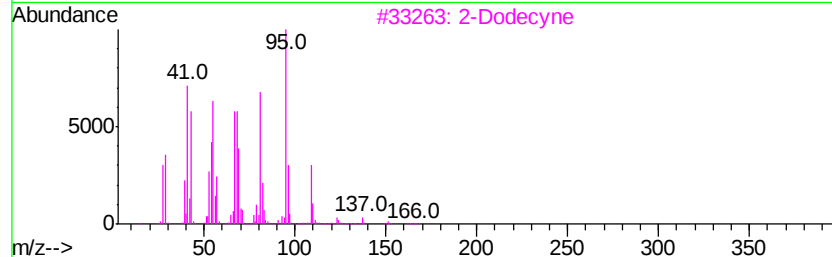
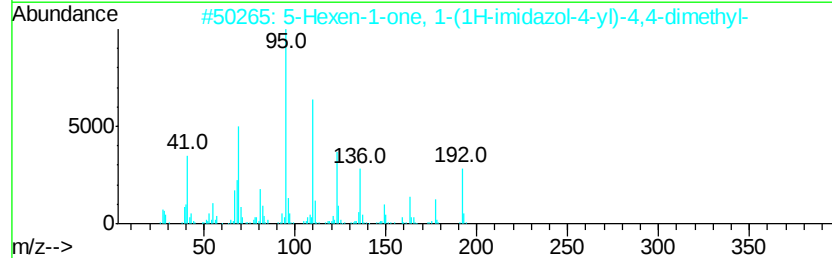
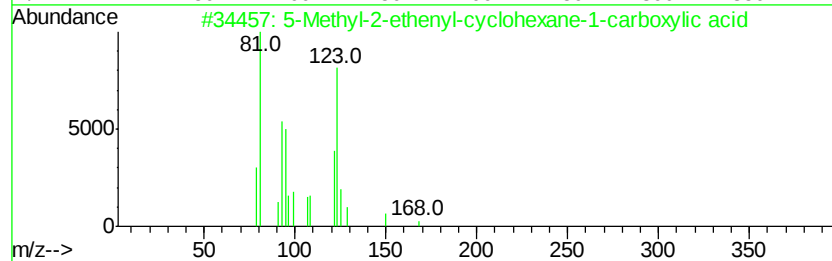
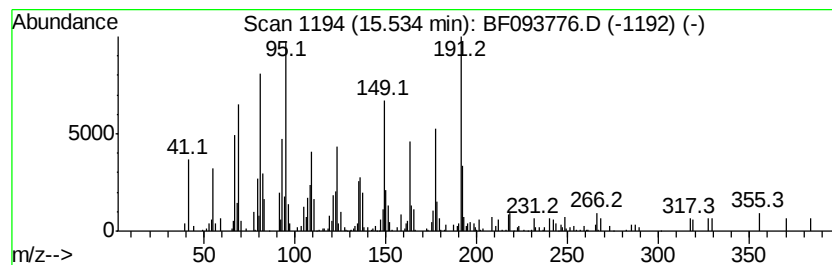
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.53 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	3.40 ng	175890	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Methyl-2-ethenyl-cyclohexane-1...	168	C10H16O2	1000144-53-6	25
2		5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	25
3		2-Dodecyne	166	C12H22	000629-49-2	22
4		N-Acrylonitril-2,2,5,5-tetrameth...	192	C11H16N2O	077376-89-7	15
5		Acetic acid, 1,7,7-trimethyl-bic...	196	C12H20O2	092618-89-8	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093776.D
Acq On : 20 Mar 2017 20:47
Operator : SJ/MA
Sample : I2304-03 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPA-B2(0-5)

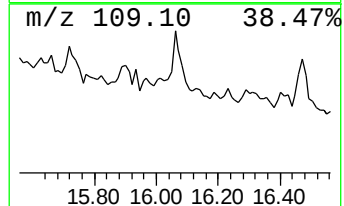
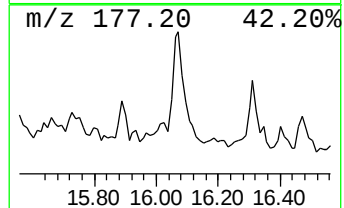
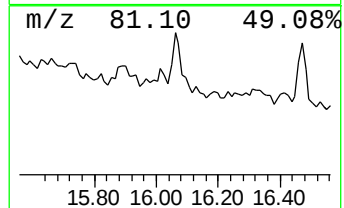
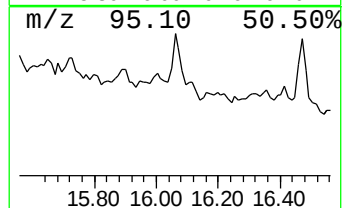
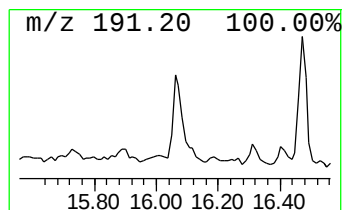
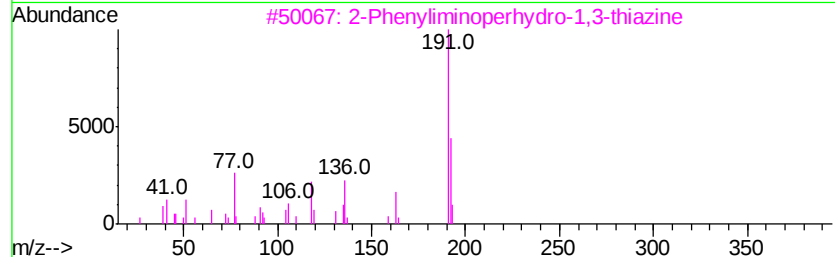
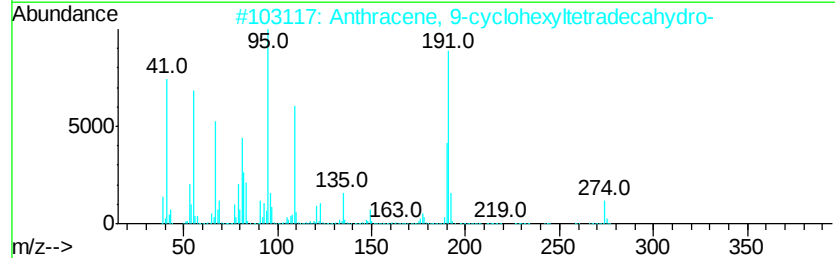
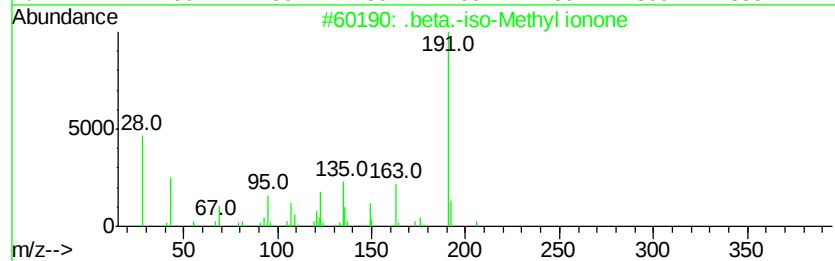
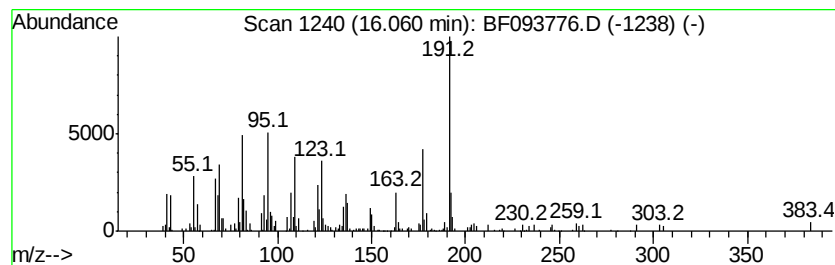
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.06 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	6.80 ng	351873	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
2		Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	35
3		2-Phenyliminoperhydro-1,3-thiazine	192	C10H12N2S	1000138-91-3	27
4		2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	25
5		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093776.D
Acq On : 20 Mar 2017 20:47
Operator : SJ/MA
Sample : I2304-03 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPA-B2(0-5)

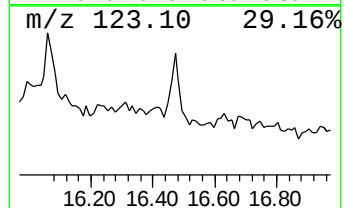
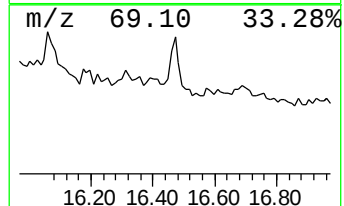
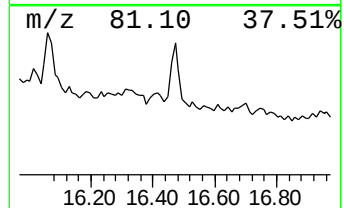
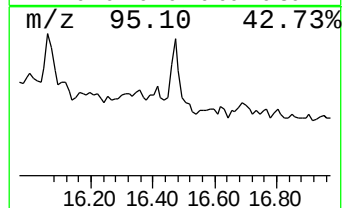
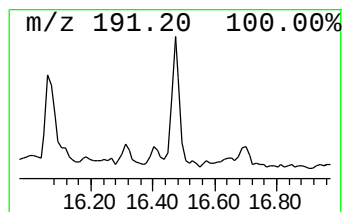
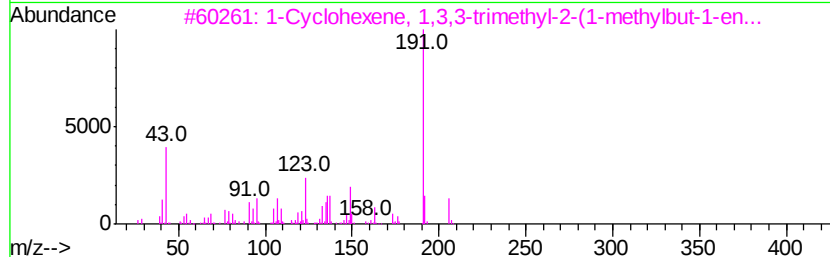
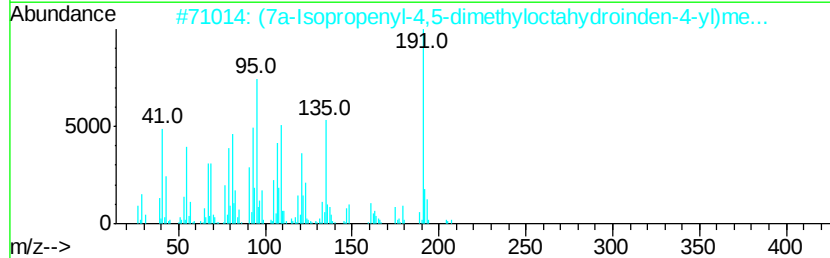
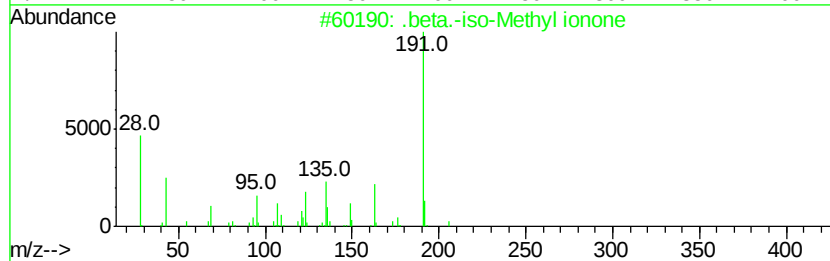
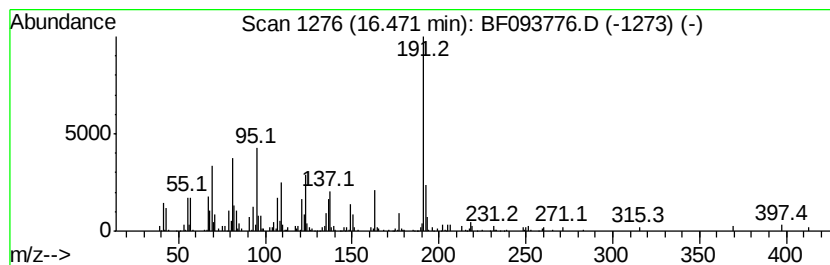
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .beta.-iso-Methyl ionone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	5.89 ng	304588	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	76
2		(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1000187-02-9	40
3		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
4		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	37
5		Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093776.D
Acq On : 20 Mar 2017 20:47
Operator : SJ/MA
Sample : I2304-03 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPA-B2(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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...	5.01	9.2 ng		660663	1	6.84	1440300	20.0
unknown6.60	6.60	51.8 ng		3730900	1	6.84	1440300	20.0
Hexadecane, 2,6,1...	10.80	4.7 ng		399519	4	11.35	1697030	20.0
Anthracene, 2-met...	11.84	2.0 ng		171517	4	11.35	1697030	20.0
unknown11.96	11.96	2.0 ng		174280	4	11.35	1697030	20.0
9-Tricosene, (Z)-	13.83	5.8 ng		312179	5	13.97	1084730	20.0
unknown15.53	15.53	3.4 ng		175890	6	15.39	1034690	20.0
unknown16.06	16.06	6.8 ng		351873	6	15.39	1034690	20.0
.beta.-iso-Methyl...	16.47	5.9 ng		304588	6	15.39	1034690	20.0