

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
 Data File : BF093777.D
 Acq On : 20 Mar 2017 21:15
 Operator : SJ/MA
 Sample : I2304-05 2X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPA-B3(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	2.093	16	18	24	rVB2	64799	85173	2.42%	0.245%
2	5.007	270	273	278	rBV	480119	581965	16.50%	1.672%
3	5.430	307	310	312	rBV	3154418	3002818	85.15%	8.626%
4	5.842	343	346	348	rBV	38072	36713	1.04%	0.105%
5	6.459	397	400	403	rBV	2487739	3276901	92.92%	9.413%
6	6.596	410	412	415	rBV	2600873	3280516	93.02%	9.424%
7	6.836	430	433	435	rBV	1671636	1380378	39.14%	3.965%
8	6.996	444	447	449	rVB	2534329	2601337	73.76%	7.473%
9	7.396	479	482	484	rBV	2370240	2228305	63.18%	6.401%
10	7.636	498	503	506	rVB3	28749	59356	1.68%	0.171%
11	7.853	520	522	524	rBV2	21567	39859	1.13%	0.114%
12	8.116	543	545	548	rBV	1598859	1761909	49.96%	5.061%
13	8.722	596	598	602	rBV	34116	59662	1.69%	0.171%
14	9.202	637	640	642	rVB	3131358	3526659	100.00%	10.131%
15	9.293	645	648	650	rBV	79891	80912	2.29%	0.232%
16	9.453	660	662	666	rBV	30299	44686	1.27%	0.128%
17	9.533	666	669	672	rBV2	45070	98881	2.80%	0.284%
18	9.591	672	674	675	rVV	392941	349513	9.91%	1.004%
19	9.613	675	676	677	rVV	63005	54407	1.54%	0.156%
20	9.648	677	679	684	rVB4	21785	50341	1.43%	0.145%
21	9.819	693	694	696	rVB	119431	87075	2.47%	0.250%
22	9.876	696	699	701	rBV	1447166	1850546	52.47%	5.316%
23	10.071	712	716	718	rBV4	31394	71639	2.03%	0.206%
24	10.139	721	722	724	rVV2	34466	42007	1.19%	0.121%
25	10.288	730	735	736	rBV4	40518	85876	2.44%	0.247%
26	10.322	736	738	739	rVB	95153	111177	3.15%	0.319%
27	10.539	754	757	759	rBV	98290	113305	3.21%	0.325%
28	10.654	765	767	769	rVB	1608737	1520672	43.12%	4.368%
29	10.791	777	779	782	rBV	192477	320255	9.08%	0.920%
30	10.985	794	796	798	rBV2	24538	38542	1.09%	0.111%
31	11.236	816	818	819	rBV2	164671	136126	3.86%	0.391%
32	11.271	819	821	823	rVB	145441	151292	4.29%	0.435%
33	11.351	825	828	829	rBV	1633517	1615614	45.81%	4.641%
34	11.614	849	851	853	rBV	60465	80410	2.28%	0.231%

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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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
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35	11.659	853	855	857	rVB	178208	156291	4.43%	0.449%
36	11.842	867	871	873	rBV5	44400	130915	3.71%	0.376%
37	11.957	879	881	886	rBV4	43021	111027	3.15%	0.319%
38	12.071	889	891	893	rVV	67272	89900	2.55%	0.258%
39	12.345	913	915	918	rBV	89558	131582	3.73%	0.378%
40	12.562	932	934	935	rBV2	68762	95722	2.71%	0.275%
41	12.825	956	957	959	rBV	83632	75273	2.13%	0.216%
42	12.928	964	966	969	rVV	2247468	2224205	63.07%	6.389%
43	13.831	1043	1045	1052	rVB2	128556	309376	8.77%	0.889%
44	13.968	1055	1057	1059	rVB	917599	1035333	29.36%	2.974%
45	15.385	1178	1181	1183	rVB	661236	1006670	28.54%	2.892%
46	16.060	1238	1240	1249	rVB2	125474	334965	9.50%	0.962%
47	16.471	1273	1276	1281	rVB2	146133	285588	8.10%	0.820%

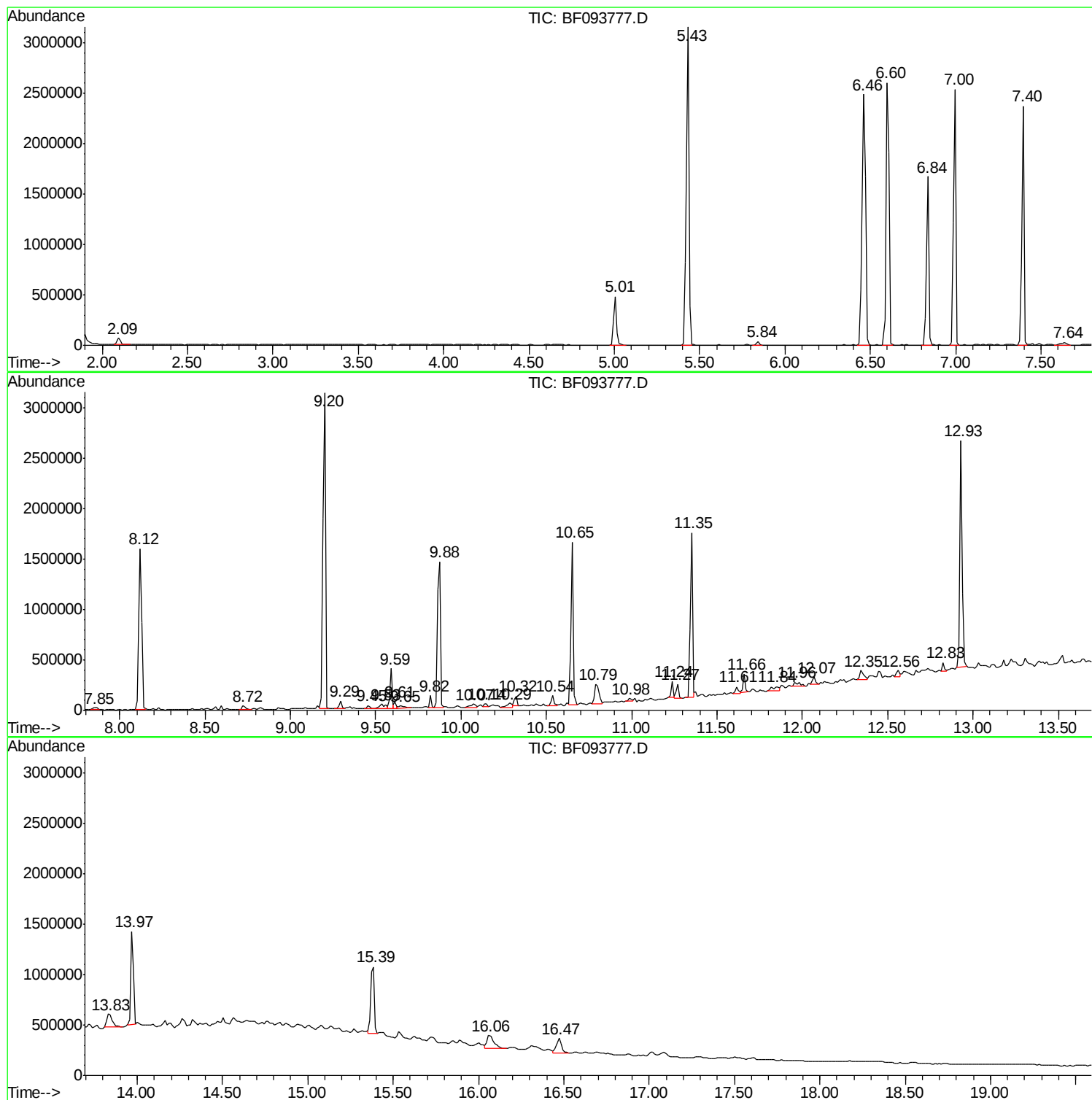
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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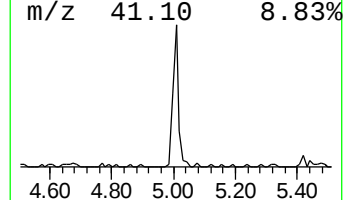
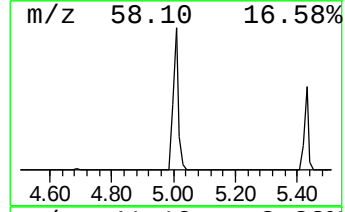
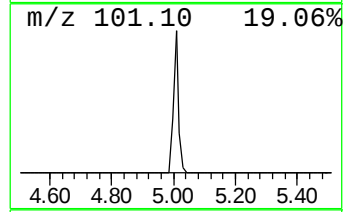
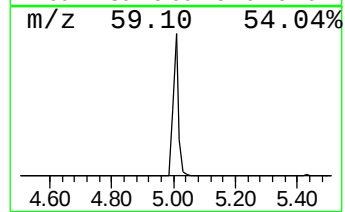
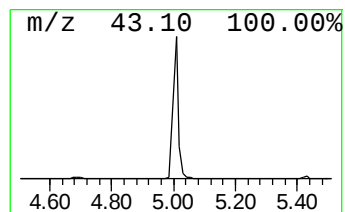
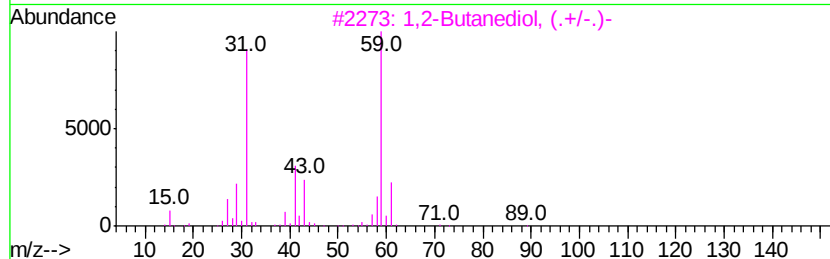
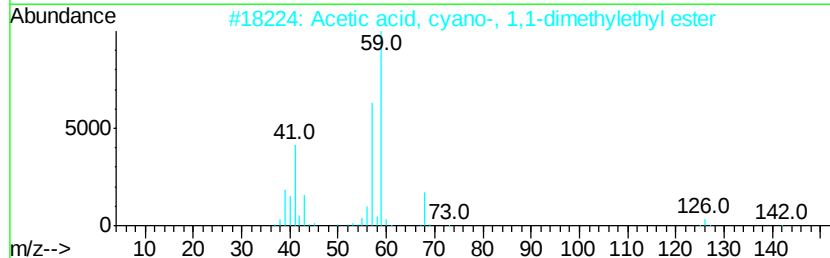
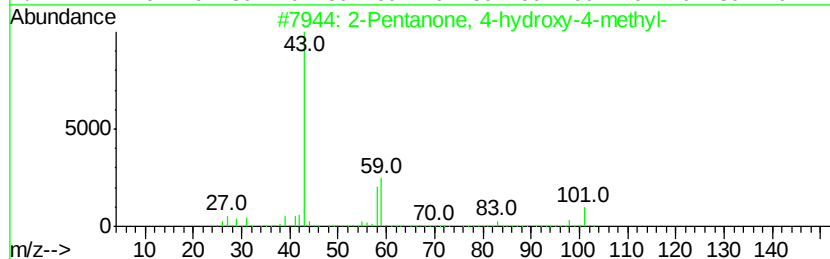
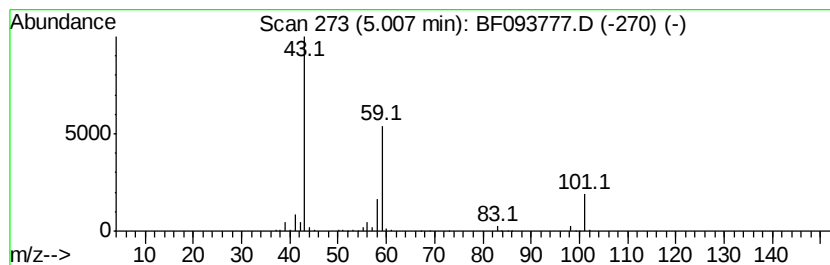
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	8.43 ng	581965	1,4-Dichlorobenzene-d4	6.84

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		1,2-Butanediol, (+/-)-	90	C4H10O2	026171-83-5	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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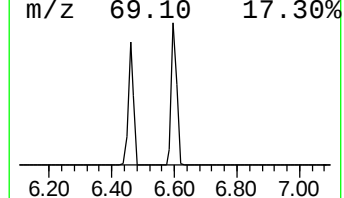
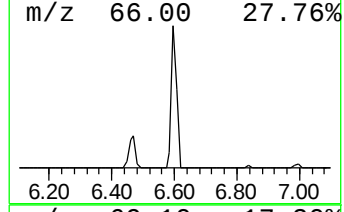
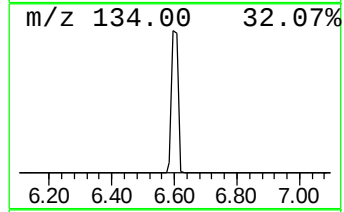
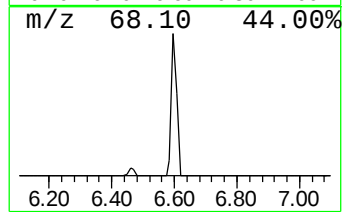
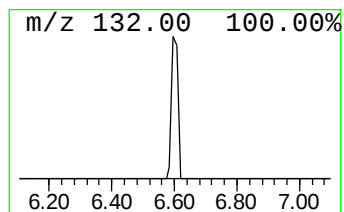
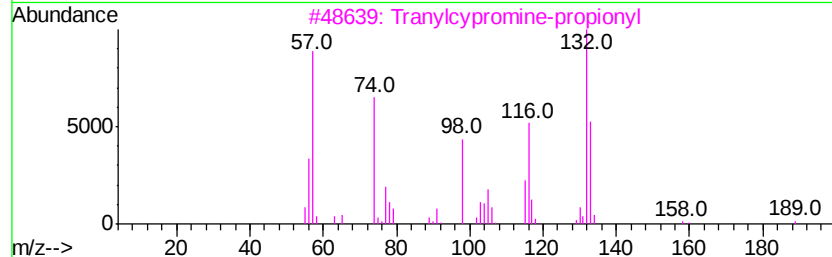
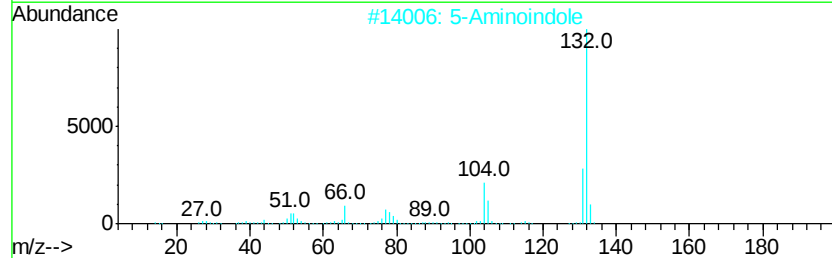
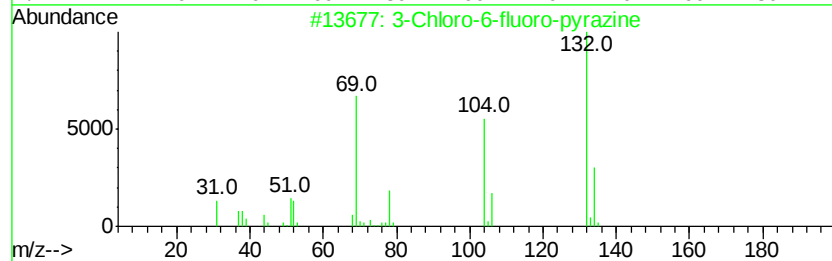
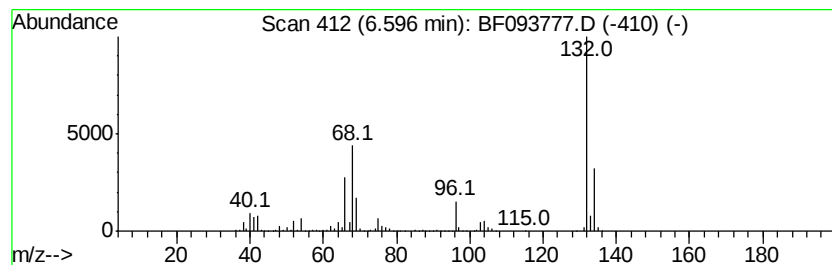
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	47.53 ng	3280520	1,4-Dichlorobenzene-d4	6.84

Hit#	of	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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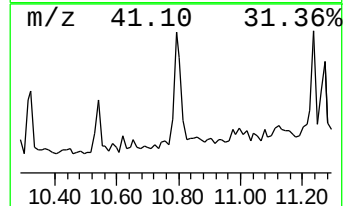
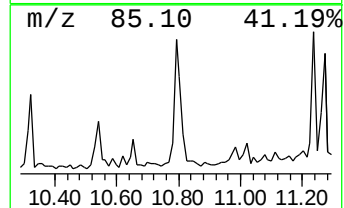
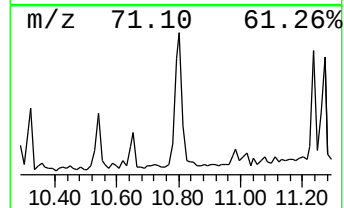
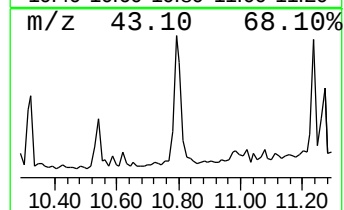
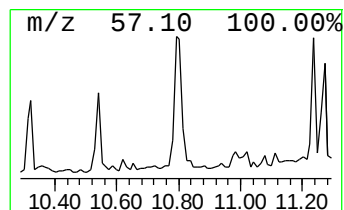
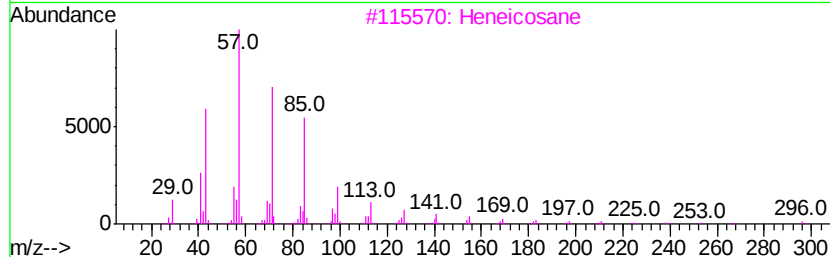
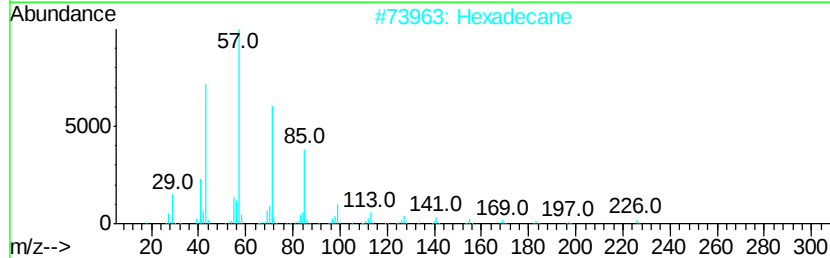
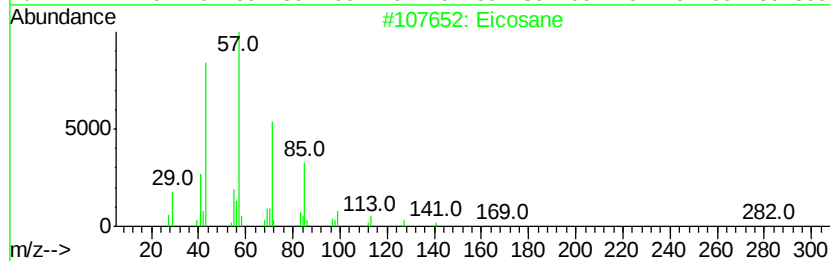
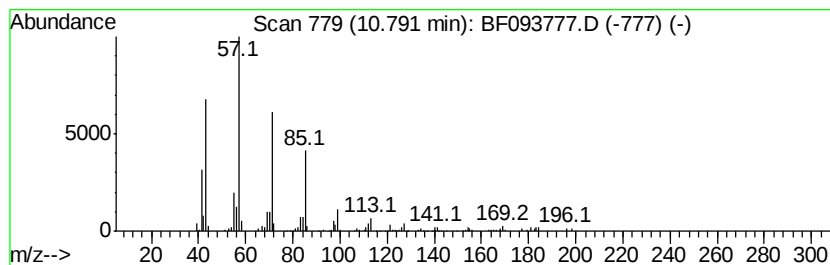
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	3.96 ng	320255	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Hexadecane	226	C16H34	000544-76-3	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptadecane	240	C17H36	000629-78-7	90
5		Heptacosane	380	C27H56	000593-49-7	87



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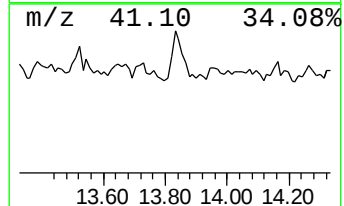
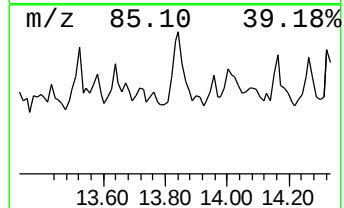
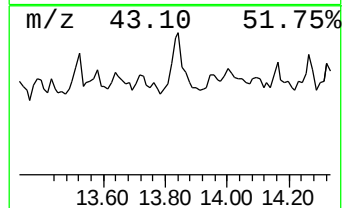
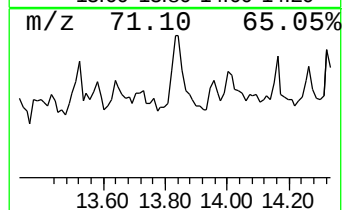
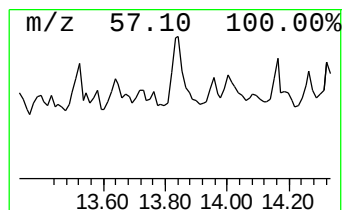
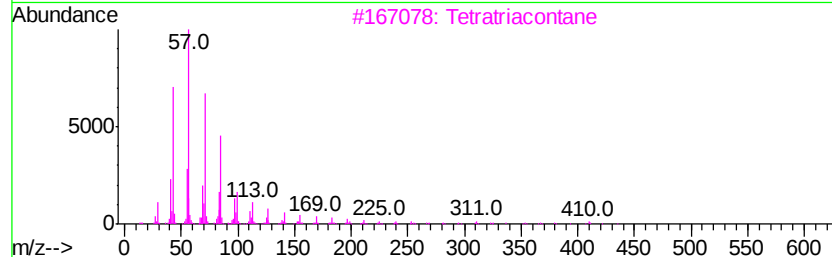
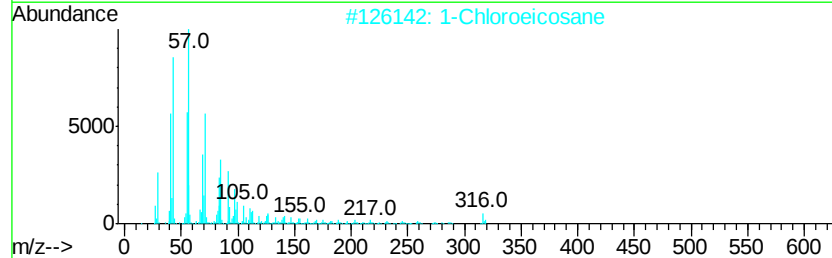
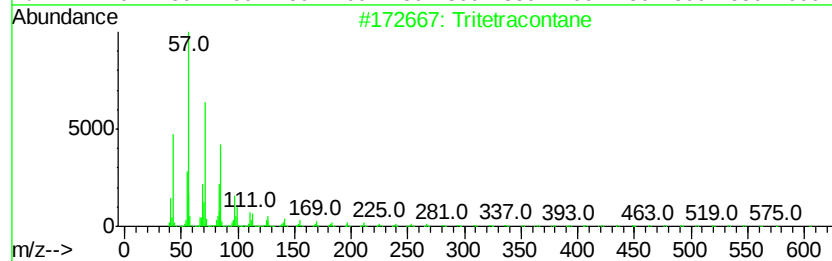
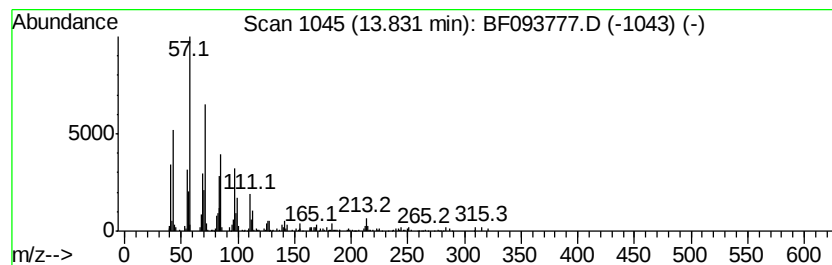
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tritetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.98 ng	309376	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tritetracontane	605	C43H88	007098-21-7	83
2		1-Chloroeicosane	316	C20H41Cl	042217-02-7	72
3		Tetratriacontane	479	C34H70	014167-59-0	72
4		Pentadecane	212	C15H32	000629-62-9	70
5		Octadecane	254	C18H38	000593-45-3	58



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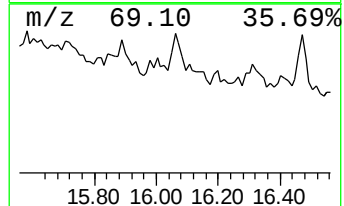
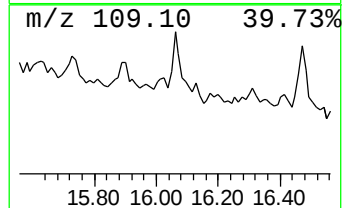
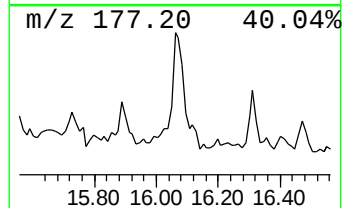
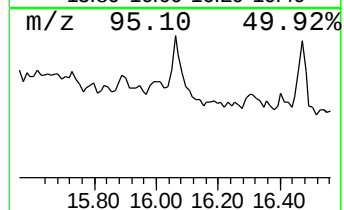
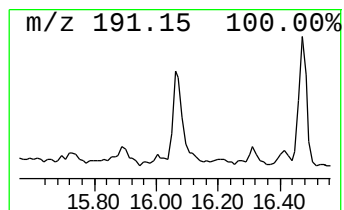
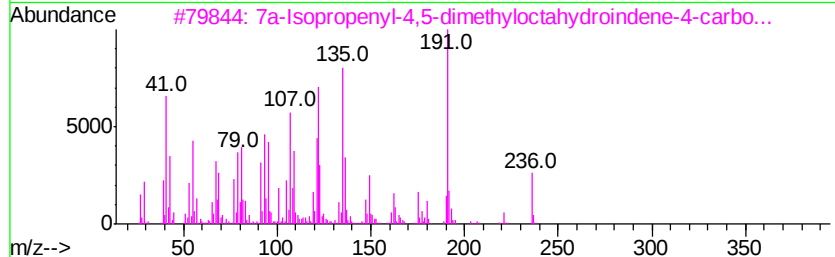
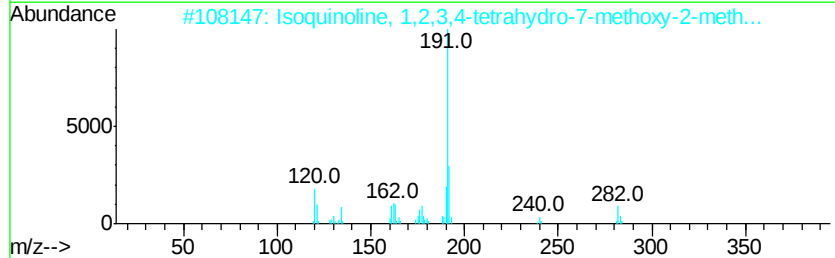
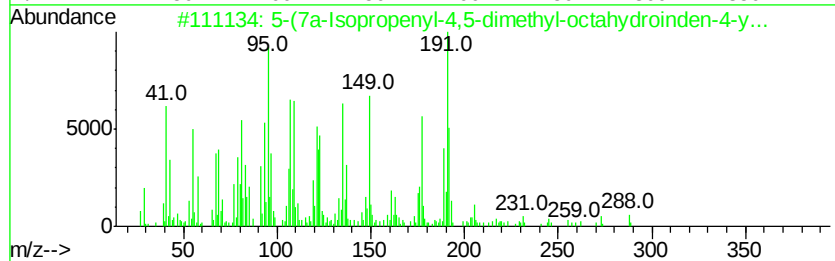
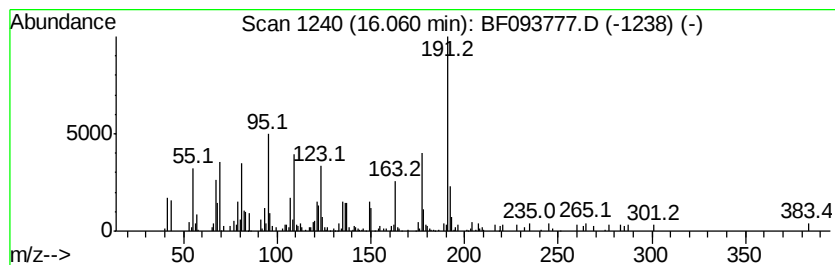
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-(7a-Isopropenyl-4,5-dimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	6.65 ng	334965	Perylene-d12	15.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-(7a-Isopropenyl-4,5-dimethyl-o...	288	C20H32O	1000193-54-1	50
2		Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	43
3		7a-Isopropenyl-4,5-dimethyloctah...	236	C15H24O2	1000192-14-7	42
4		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	32
5		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093777.D
Acq On : 20 Mar 2017 21:15
Operator : SJ/MA
Sample : I2304-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

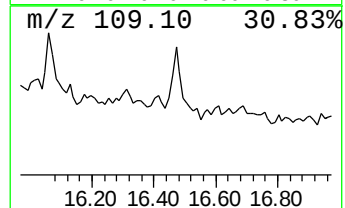
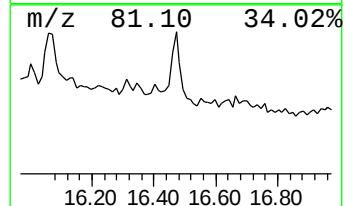
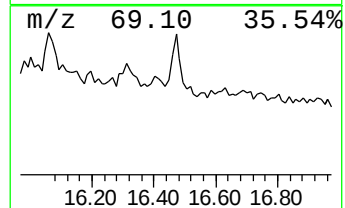
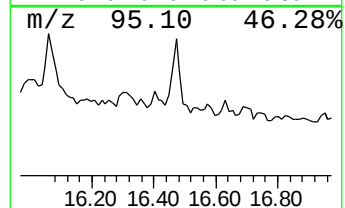
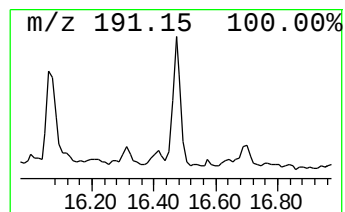
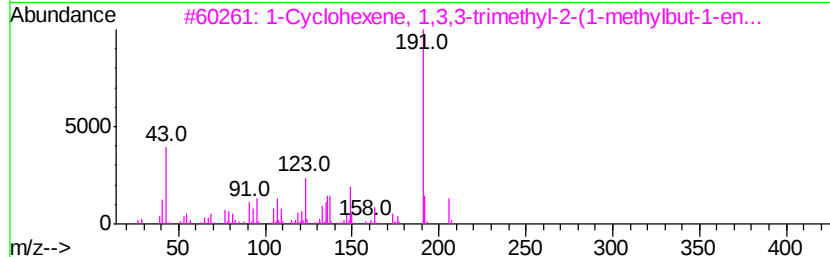
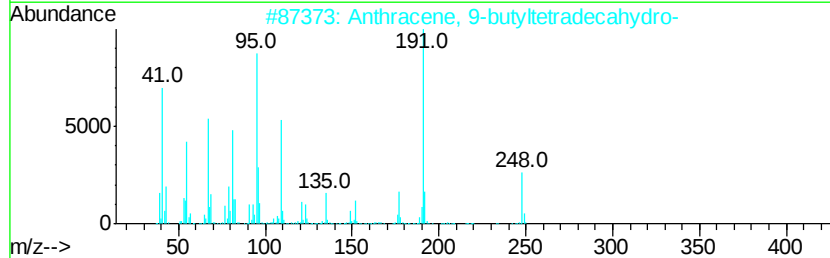
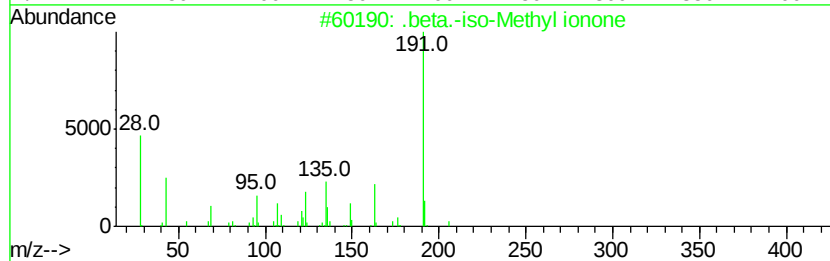
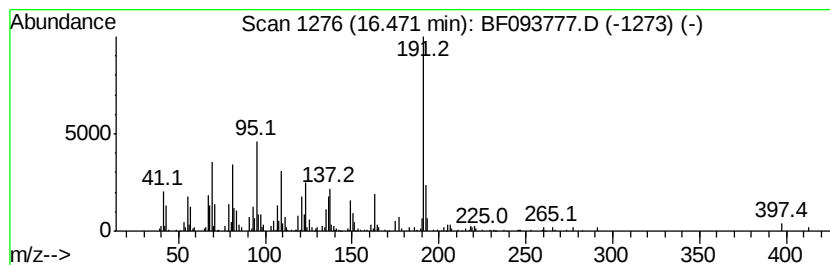
Instrument :
BNA_F
ClientSampleId :
SPA-B3(0-5)

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 unknown16.47 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.47	5.67 ng	285588	Perylene-d12	15.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	46
2	Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	40
3	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
4	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	37
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093777.D
Acq On : 20 Mar 2017 21:15
Operator : SJ/MA
Sample : I2304-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPA-B3(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	8.4	ng	581965	1	6.84	1380380	20.0
unknown6.60	6.60	47.5	ng	3280520	1	6.84	1380380	20.0
Eicosane	10.79	4.0	ng	320255	4	11.35	1615610	20.0
Tritetracontane	13.83	6.0	ng	309376	5	13.97	1035330	20.0
5-(7a-Isopropenyl...	16.06	6.7	ng	334965	6	15.39	1006670	20.0
unknown16.47	16.47	5.7	ng	285588	6	15.39	1006670	20.0