

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
 Data File : BF097494.D
 Acq On : 9 Aug 2017 3:15
 Operator : SJ/JU
 Sample : I4655-02 5X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP8N-WC1

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	4.528	463	466	474	rBV	9470	18344	3.26%	0.330%
2	5.010	545	548	561	rBV	131021	261082	46.34%	4.695%
3	6.093	728	732	745	rBV	135118	263605	46.78%	4.740%
4	6.187	745	748	759	rVB	217850	285905	50.74%	5.141%
5	6.404	782	785	798	rBV	489185	463278	82.22%	8.331%
6	6.563	809	812	827	rBV	168596	174230	30.92%	3.133%
7	6.981	881	883	900	rBV	78379	128841	22.87%	2.317%
8	7.687	1000	1003	1018	rBV	572171	563457	100.00%	10.132%
9	8.769	1183	1187	1196	rBV	221874	200396	35.57%	3.604%
10	9.169	1252	1255	1263	rBV	37995	39307	6.98%	0.707%
11	9.433	1296	1300	1309	rVB	601687	491581	87.24%	8.840%
12	9.886	1374	1377	1380	rBV2	7121	7540	1.34%	0.136%
13	10.228	1431	1435	1441	rBV	102203	116151	20.61%	2.089%
14	10.357	1454	1457	1460	rBV4	6653	8034	1.43%	0.144%
15	10.904	1547	1550	1554	rBV	454440	443635	78.73%	7.978%
16	11.045	1572	1574	1577	rBV3	9996	11280	2.00%	0.203%
17	11.263	1609	1611	1619	rVB8	10581	17692	3.14%	0.318%
18	11.327	1619	1622	1623	rBV3	6513	7237	1.28%	0.130%
19	11.345	1623	1625	1627	rBV3	9731	8032	1.43%	0.144%
20	11.369	1627	1629	1632	rVB3	11449	8831	1.57%	0.159%
21	11.422	1632	1638	1640	rBV6	22418	44528	7.90%	0.801%
22	11.874	1712	1715	1718	rBV5	18605	24521	4.35%	0.441%
23	12.116	1753	1756	1759	rBV	30759	31240	5.54%	0.562%
24	12.339	1792	1794	1796	rBV	22462	17953	3.19%	0.323%
25	12.433	1808	1810	1814	rBV5	26792	41669	7.40%	0.749%
26	12.486	1816	1819	1825	rVV	190894	205742	36.51%	3.700%
27	12.921	1890	1893	1896	rVB4	50749	44789	7.95%	0.805%
28	12.951	1896	1898	1899	rBV2	28499	19810	3.52%	0.356%
29	13.045	1910	1914	1918	rBV7	42876	91703	16.28%	1.649%
30	13.339	1962	1964	1965	rBV2	42049	38116	6.76%	0.685%
31	13.533	1993	1997	2001	rBV	513009	493990	87.67%	8.883%
32	14.874	2222	2225	2229	rVB	317799	321946	57.14%	5.789%
33	15.745	2371	2373	2377	rVB2	87931	88852	15.77%	1.598%
34	15.974	2410	2412	2417	rVB5	46023	51150	9.08%	0.920%

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Integration Parameters: rteint.p
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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	16.104	2432	2434	2441	rBV8	40898	71549	12.70%	1.287%
36	16.204	2448	2451	2456	rVB5	66592	86444	15.34%	1.554%
37	16.539	2506	2508	2509	rBV2	32830	18064	3.21%	0.325%
38	16.598	2516	2518	2522	rBV4	45608	85936	15.25%	1.545%
39	16.839	2557	2559	2560	rBV2	32212	32633	5.79%	0.587%
40	17.756	2712	2715	2718	rBV4	23347	23787	4.22%	0.428%
41	17.786	2718	2720	2721	rBV	19774	8141	1.44%	0.146%
42	17.909	2739	2741	2743	rBV2	24615	19730	3.50%	0.355%
43	17.939	2744	2746	2753	rVB8	33786	52913	9.39%	0.951%
44	17.992	2753	2755	2758	rBV4	27218	30512	5.42%	0.549%
45	18.033	2760	2762	2770	rVB9	25849	37743	6.70%	0.679%
46	18.156	2782	2783	2784	rBV	31940	16842	2.99%	0.303%
47	18.262	2799	2801	2802	rBV2	24886	22204	3.94%	0.399%
48	18.733	2878	2881	2882	rBV2	19946	20080	3.56%	0.361%

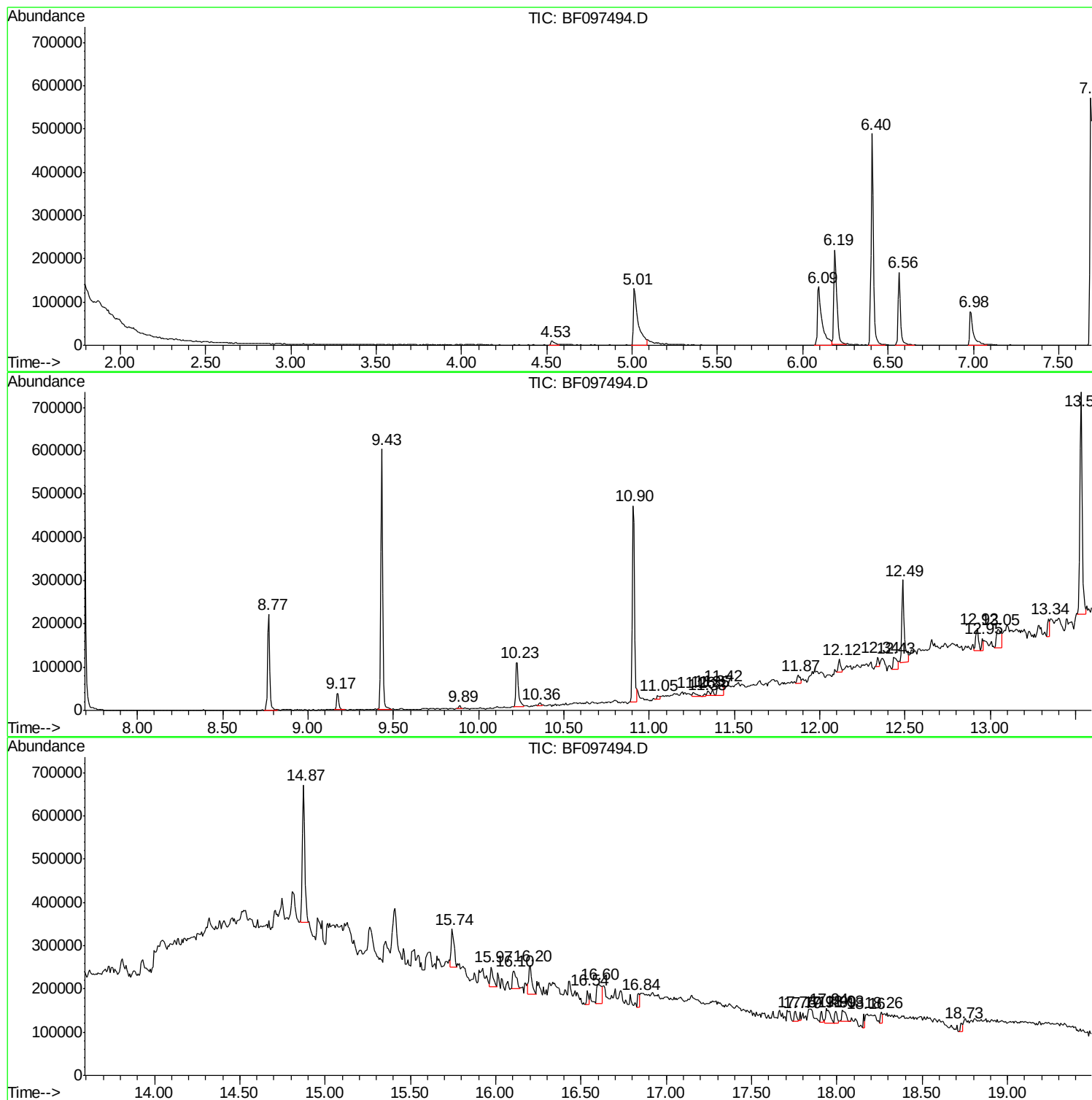
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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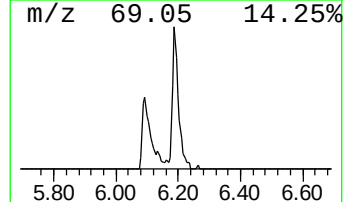
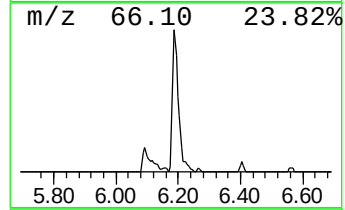
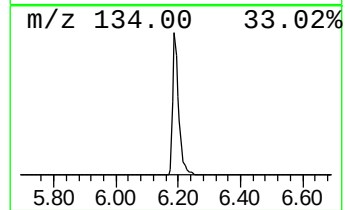
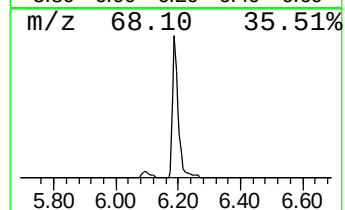
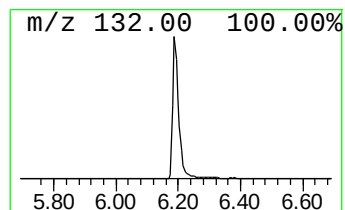
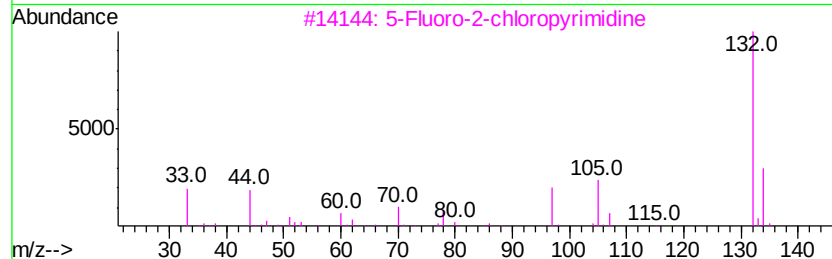
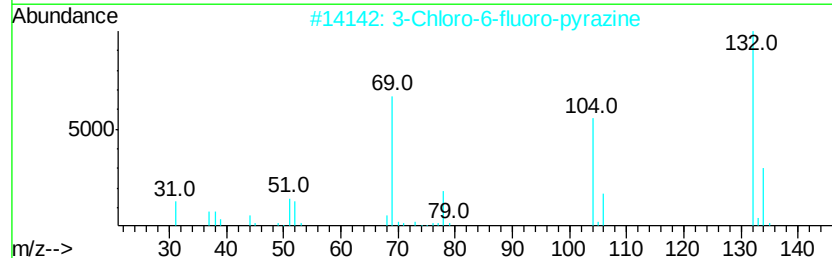
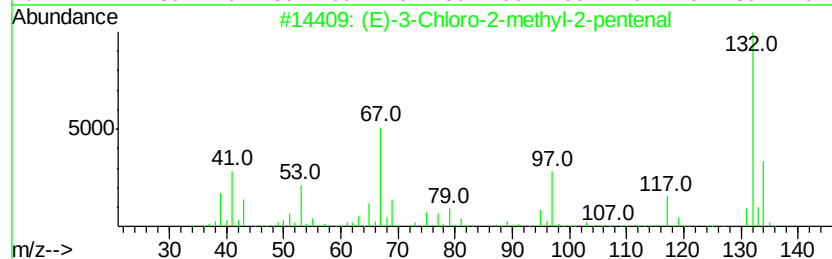
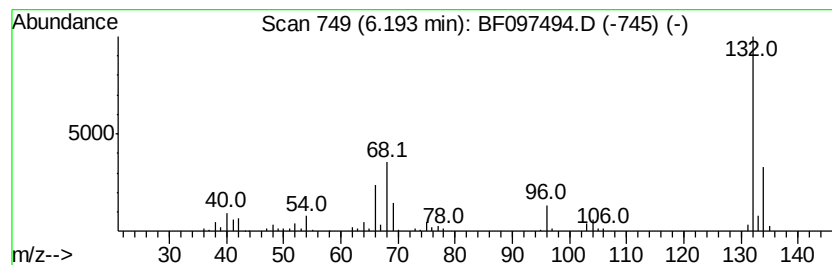
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	12.34 ng	285905	1,4-Dichlorobenzene-d4	6.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Amphetaminil	250	C17H18N2	017590-01-1	10



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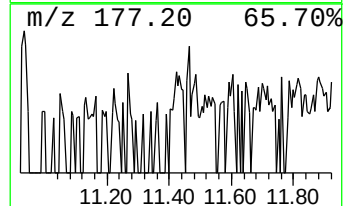
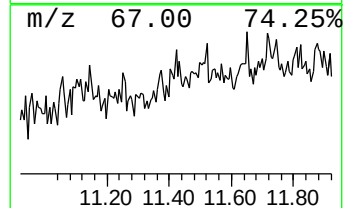
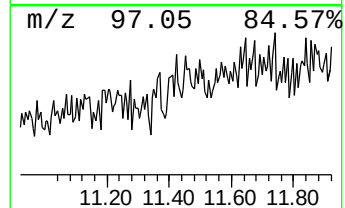
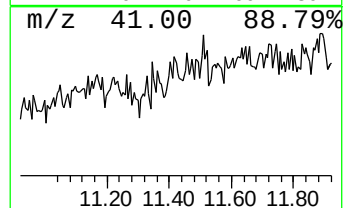
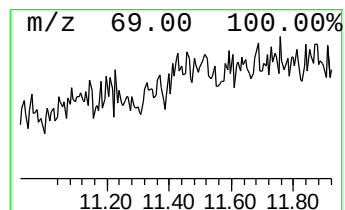
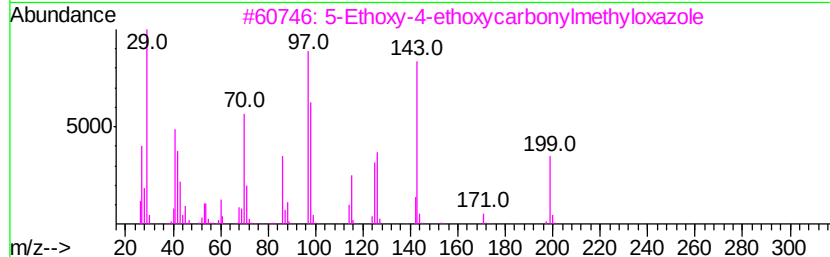
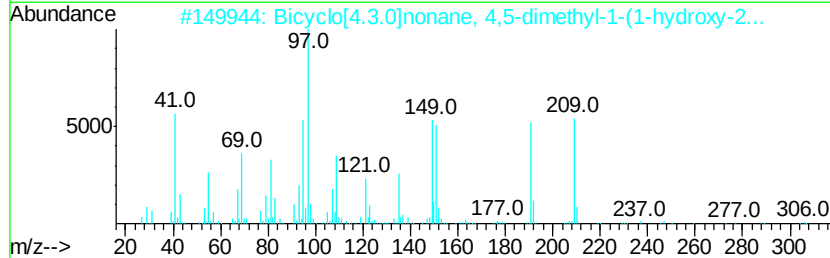
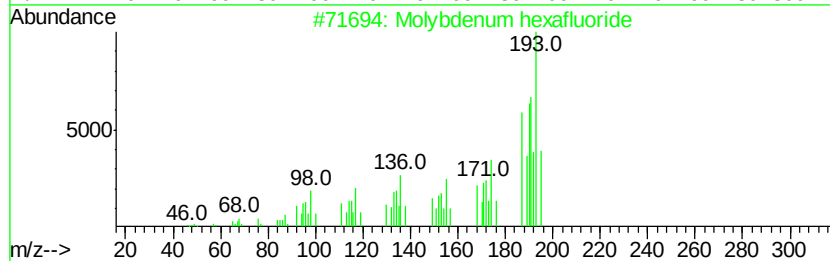
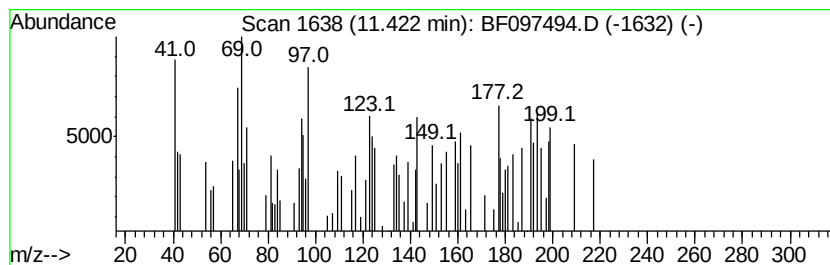
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Peak Number 3 unknown11.42 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.42	2.01 ng	44528	Phenanthrene-d10	10.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Molybdenum hexafluoride	212	F6Mo	007783-77-9	12
2	Bicyclo[4.3.0]nonane, 4,5-dimeth...	306	C20H34O2	1000195-46-7	10
3	5-Ethoxy-4-ethoxycarbonylmethyl...	199	C9H13NO4	010500-74-0	9
4	Carbophenothion sulfone	374	C11H16ClO4PS3	016662-85-4	9
5	2-Fluoro-6-trifluoromethylbenzoi...	404	C22H32F4O2	1000338-53-6	9



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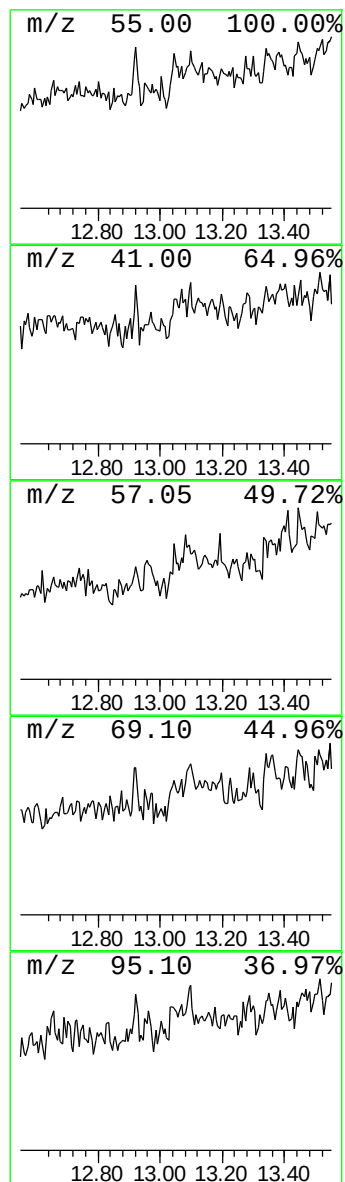
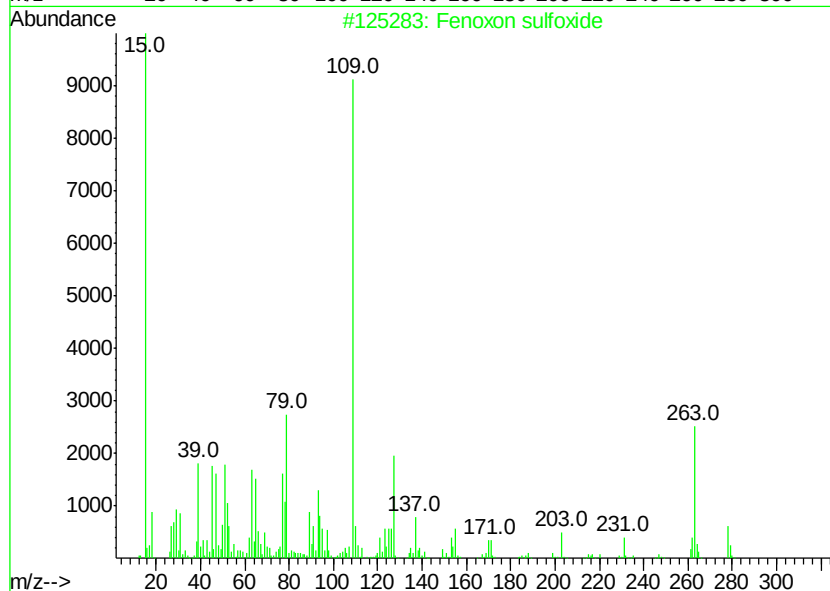
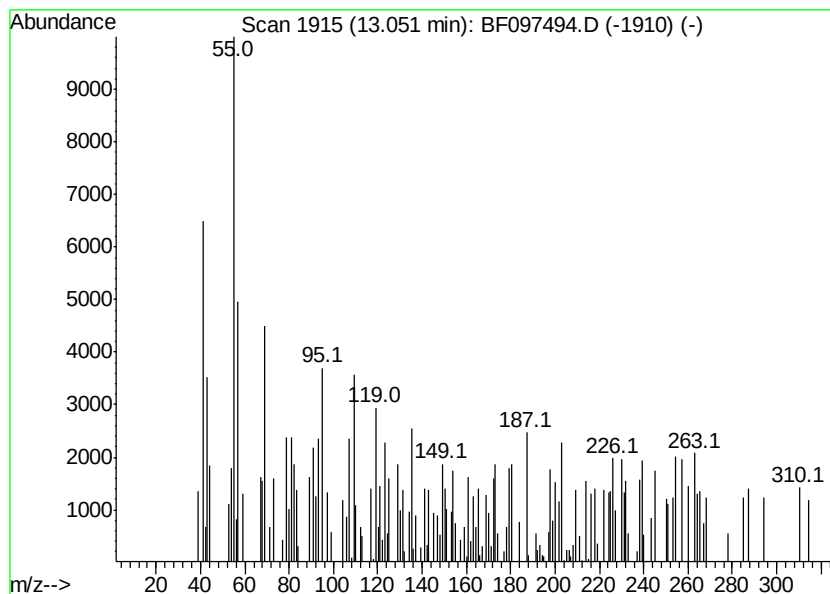
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown13.05 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.05	3.71 ng	91703	Chrysene-d12	13.53
Hit# of	1	Tentative ID	MW MolForm	CAS# Qual
1	Fenoxon sulfoxide		278 C10H15O5PS	006552-13-2 1



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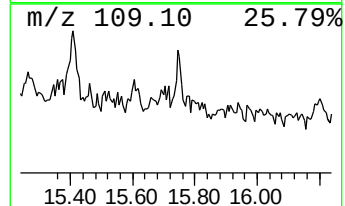
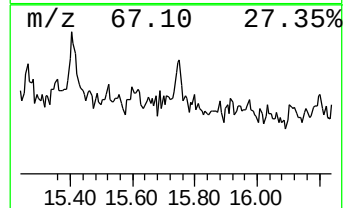
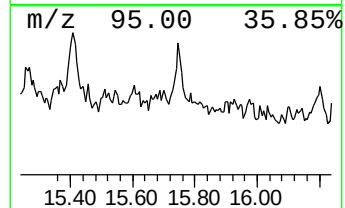
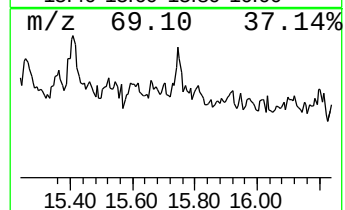
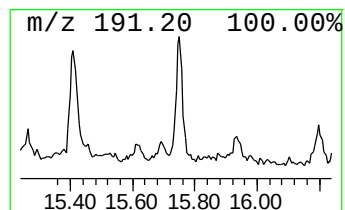
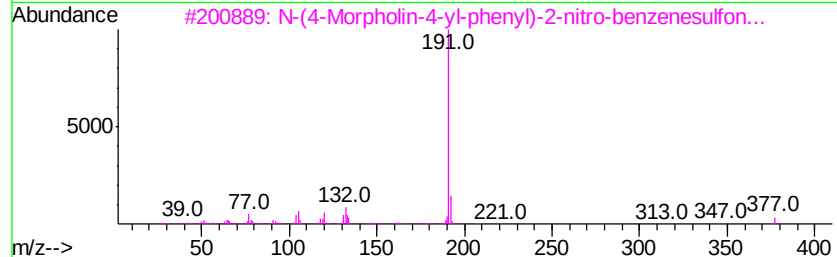
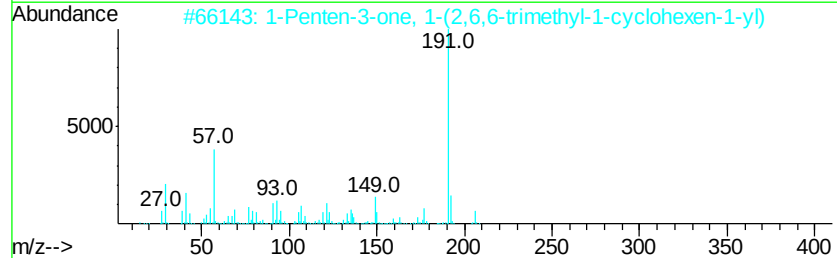
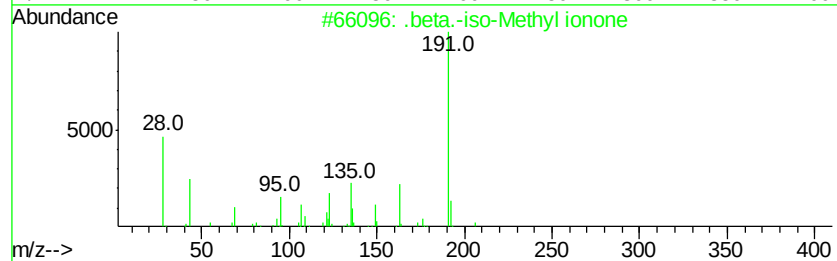
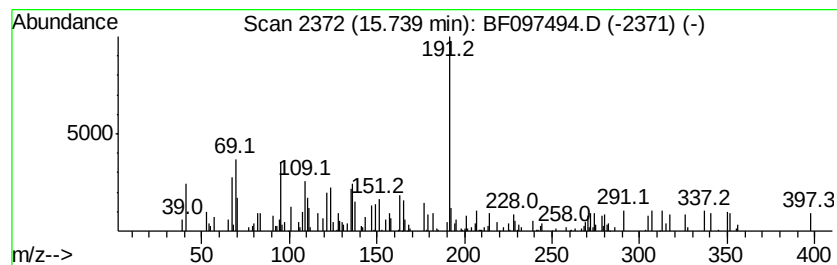
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.74 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	5.52 ng	88852	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
3		N-(4-Morpholin-4-yl-phenyl)-2-ni...	377	C17H19N3O5S	1000374-81-7	41
4		Terephthalic acid, 4-bromophenyl...	362	C17H15BrO4	1000323-67-7	38
5		Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	35



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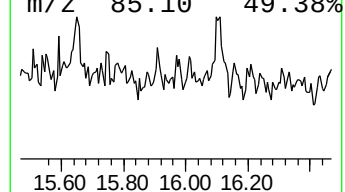
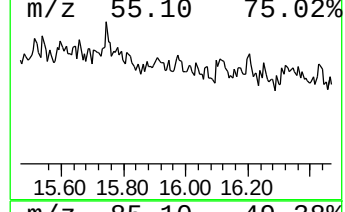
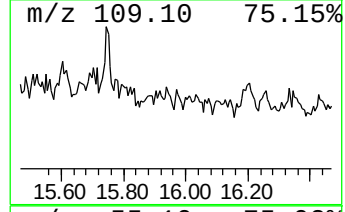
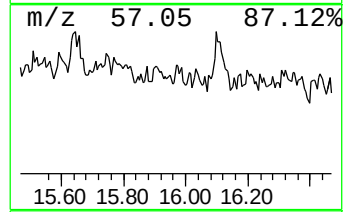
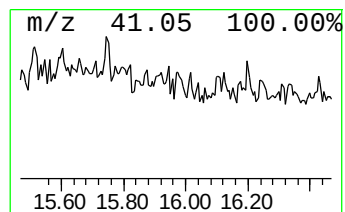
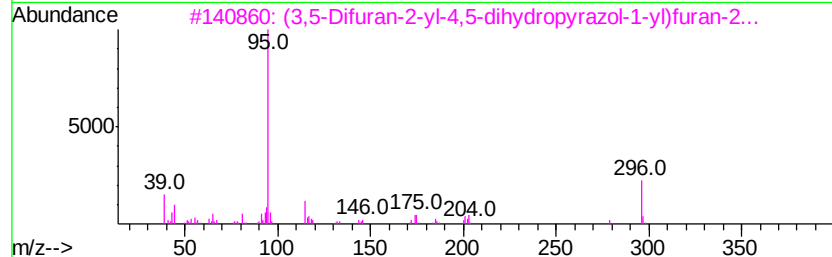
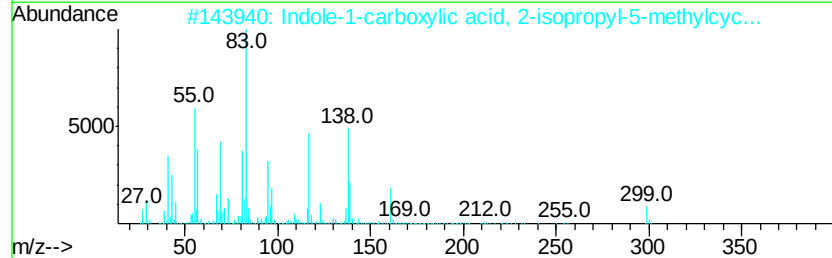
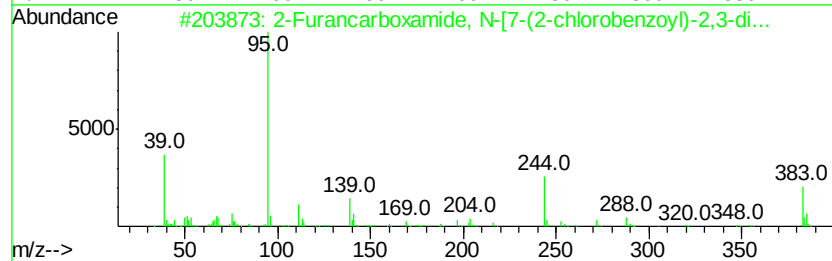
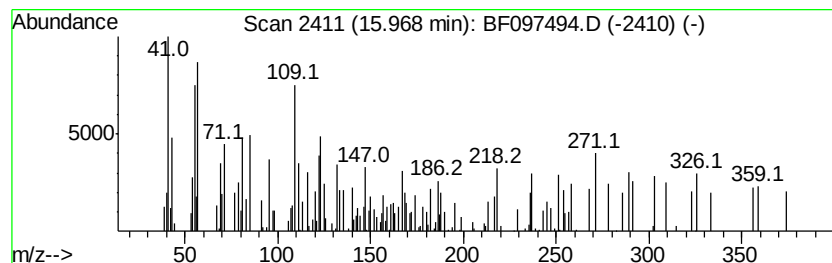
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown15.97 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	3.18 ng	51150	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Furancarboxamide, N-[7-(2-chlo...	383	C20H14ClN05	1000319-07-5	12
2		Indole-1-carboxylic acid, 2-isop...	299	C19H25N02	1000210-71-4	11
3		(3,5-Difuran-2-yl-4,5-dihydropr...	296	C16H12N204	1000322-07-8	11
4		3-(Furan-2-carbonyl)-5-p-tolyl-3...	323	C17H13N304	1000296-77-7	11
5		(-)-Pinane-3-carboxylic acid	182	C11H1802	064284-84-0	11



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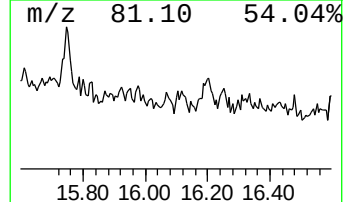
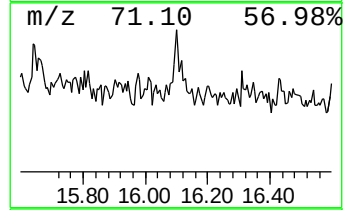
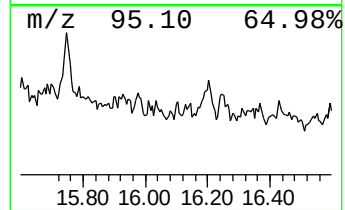
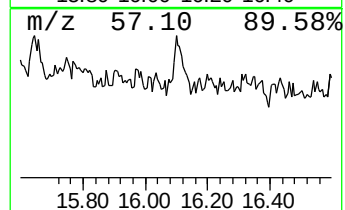
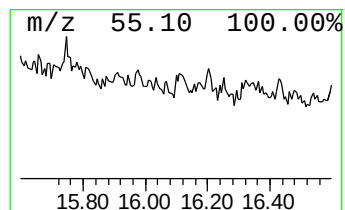
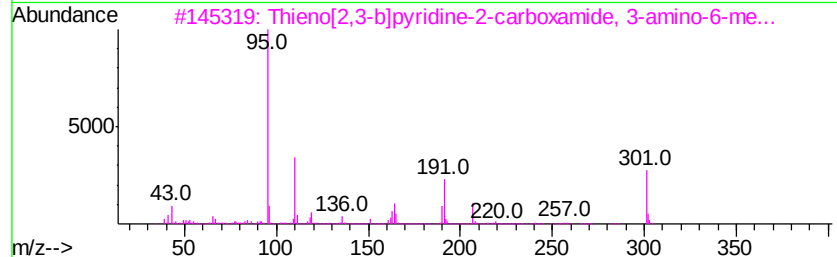
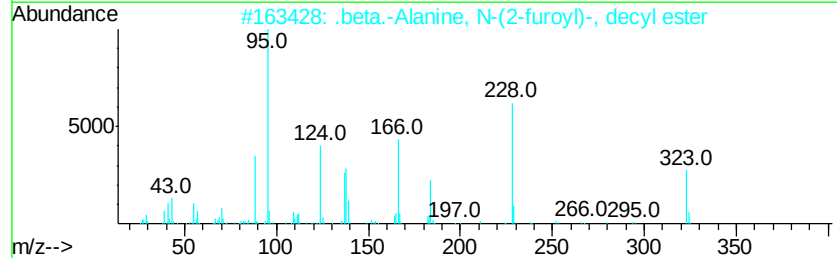
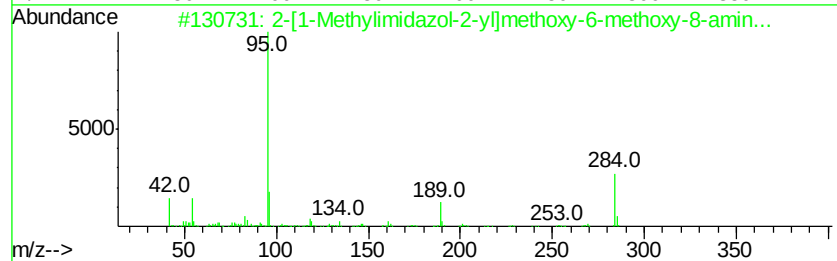
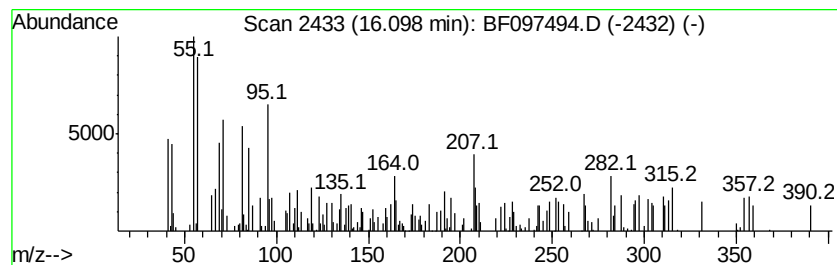
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.10 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	4.44 ng	71549	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-[1-Methylimidazol-2-yl]methoxy...	284	C15H16N4O2	1000213-40-6	30
2		.beta.-Alanine, N-(2-furoyl)-, d...	323	C18H29N04	1000321-98-0	27
3		Thieno[2,3-b]pyridine-2-carboxam...	301	C15H15N3O2S	1000350-91-4	27
4		Pyridine, 3-(5-furan-2-yl)-[1,2,4...	319	C18H13N3O3	1000317-00-3	16
5		Methyl 2-octylcyclopropene-1-hep...	294	C19H34O2	005026-66-4	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097494.D
Acq On : 9 Aug 2017 3:15
Operator : SJ/JU
Sample : I4655-02 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP8N-WC1

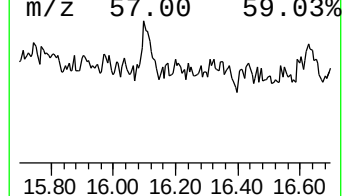
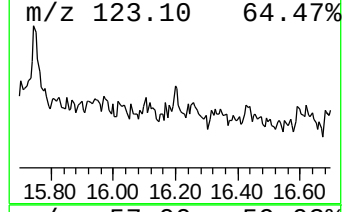
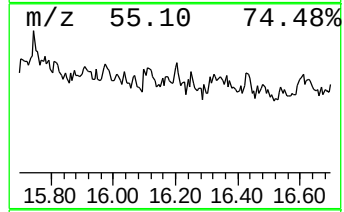
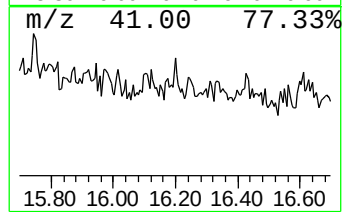
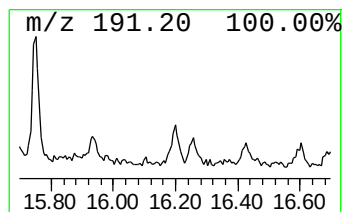
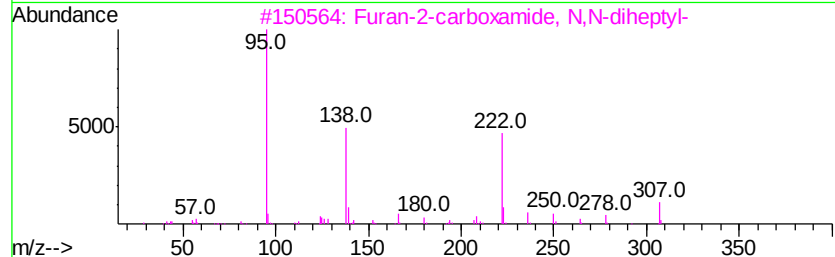
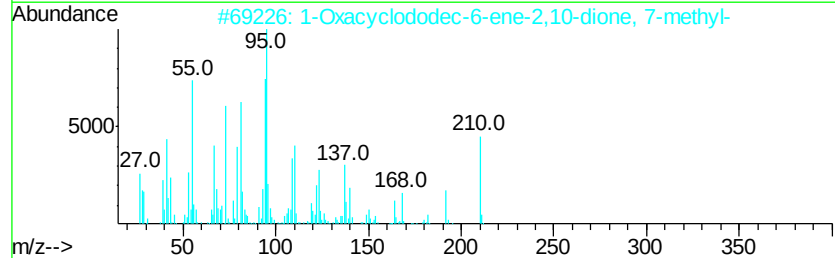
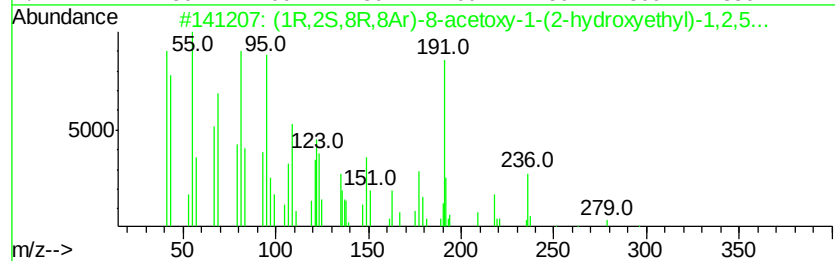
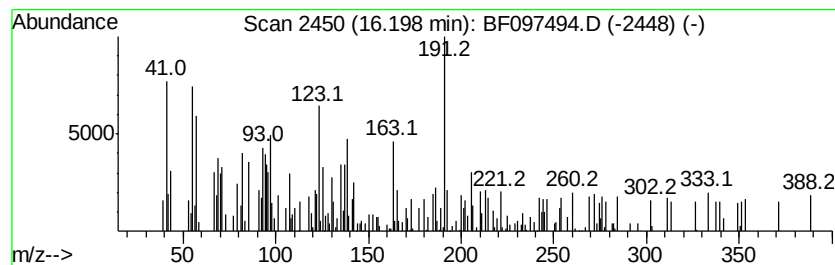
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.20 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	5.37 ng	86444	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1R,2S,8R,8Ar)-8-acetoxv-1-(2-hv...	296	C18H32O3	1000298-98-4	35
2		1-Oxacyclododec-6-ene-2,10-dione...	210	C12H18O3	1000197-15-7	27
3		Furan-2-carboxamide, N,N-diheptyl-	307	C19H33NO2	1000308-20-7	27
4		4,8a-Dimethyl-6-(2-methyl-oxiran...	234	C15H22O2	1000189-11-4	20
5		2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097494.D
Acq On : 9 Aug 2017 3:15
Operator : SJ/JU
Sample : I4655-02 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP8N-WC1

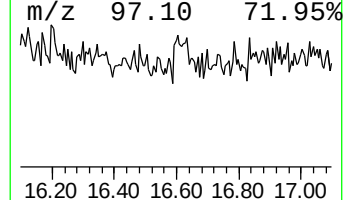
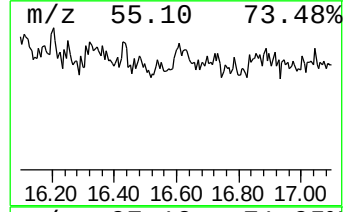
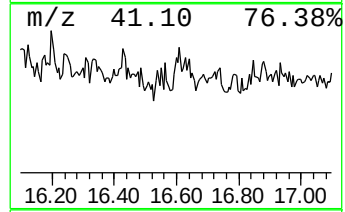
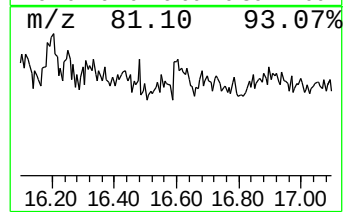
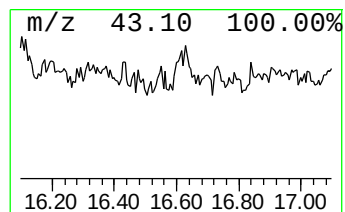
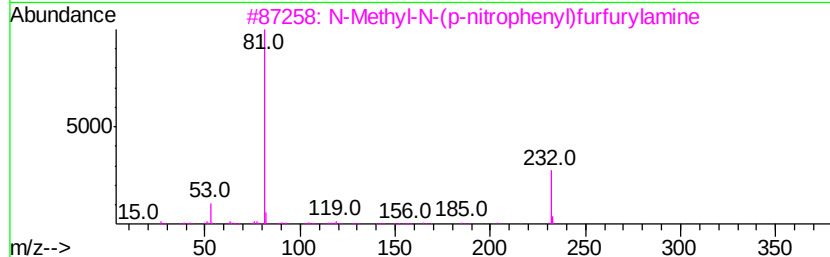
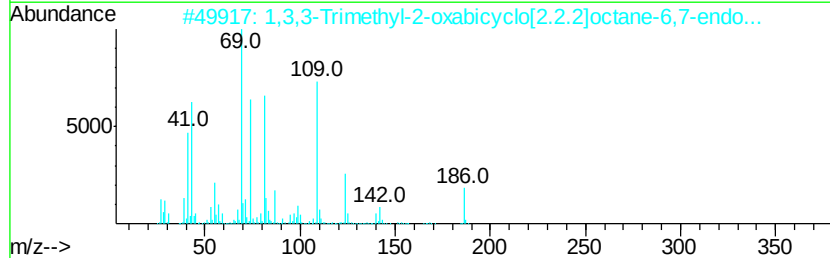
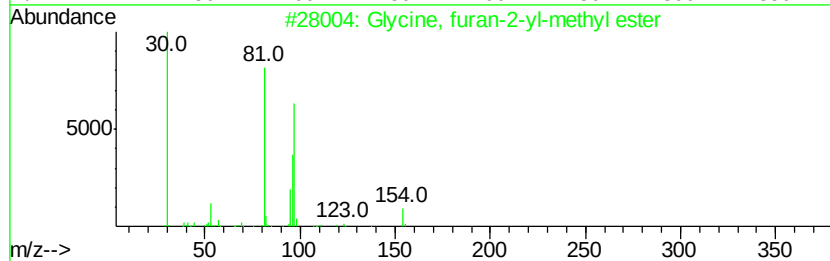
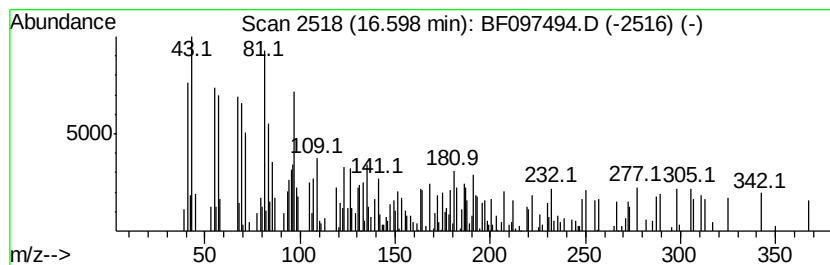
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.60 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	5.34 ng	85936	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Glycine, furan-2-yl-methyl ester	155	C7H9NO3	1000306-78-7	25
2		1,3,3-Trimethyl-2-oxabicyclo[2.2...	186	C10H18O3	056084-15-2	22
3		N-Methyl-N-(p-nitrophenyl)furfur...	232	C12H12N2O3	1000243-99-7	22
4		E-11(12-Cyclopropyl)dodecen-1-ol...	266	C17H30O2	1000130-71-0	20
5		Z-11(12-Cyclopropyl)dodecen-1-ol...	266	C17H30O2	1000130-71-1	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097494.D
Acq On : 9 Aug 2017 3:15
Operator : SJ/JU
Sample : I4655-02 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP8N-WC1

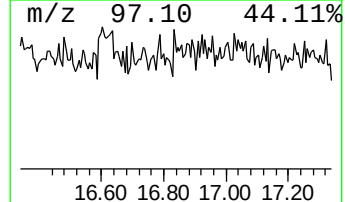
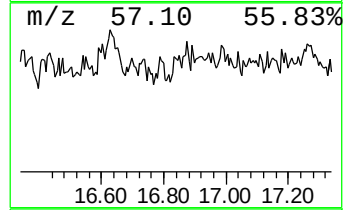
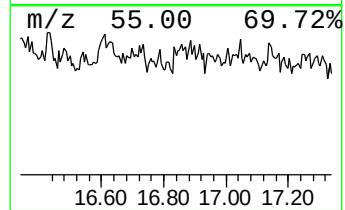
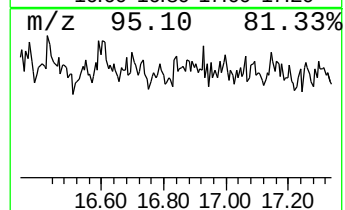
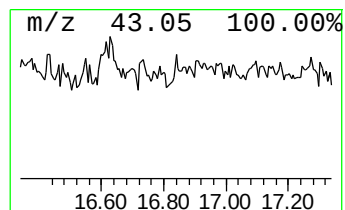
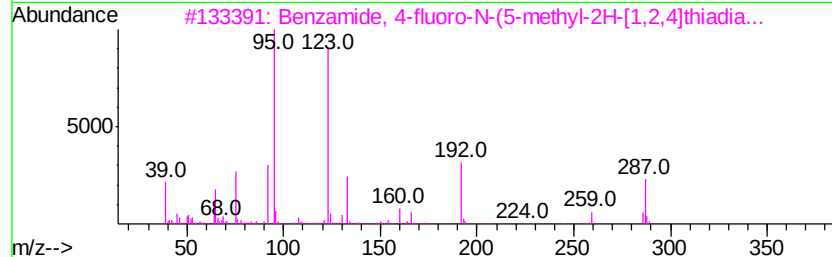
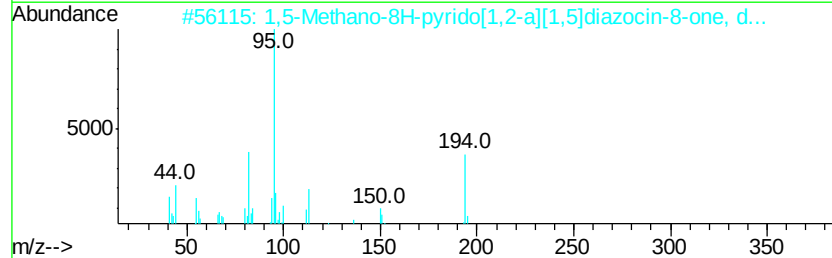
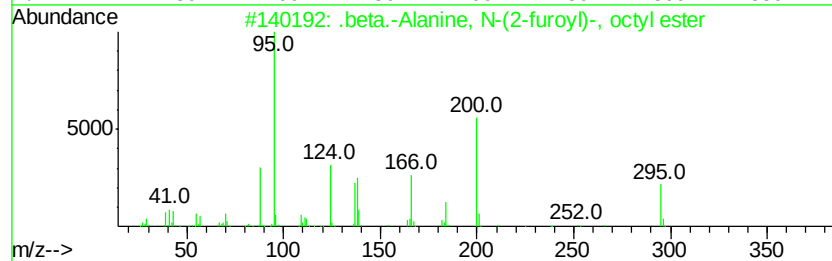
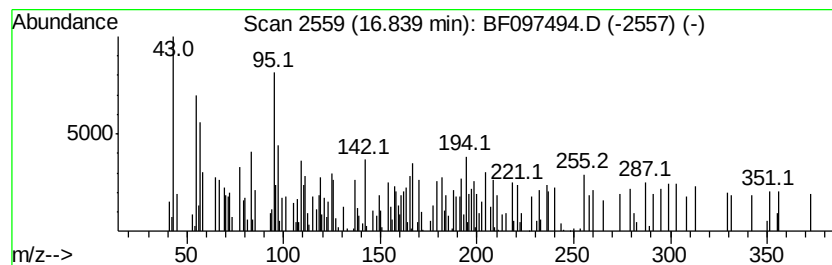
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.84 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	2.03 ng	32633	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Alanine, N-(2-furoyl)-, o...	295	C16H25N04	1000321-97-8	22
2		1,5-Methano-8H-pyrido[1,2-a][1,5...	194	C11H18N2O	018161-94-9	16
3		Benzamide, 4-fluoro-N-(5-methyl-...	287	C14H10FN3OS	1000350-88-6	12
4		Furan-2-carboxylic acid 4-methan...	344	C15H24N2O5S	1000300-98-9	12
5		Octane-1,8-diamine, N,N'-bis(2-f...	332	C18H24N2O4	300717-17-3	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097494.D
Acq On : 9 Aug 2017 3:15
Operator : SJ/JU
Sample : I4655-02 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP8N-WC1

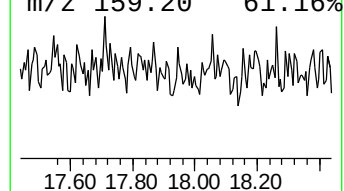
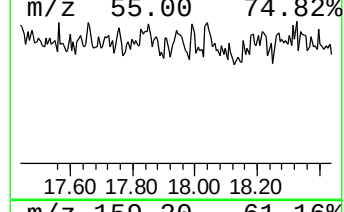
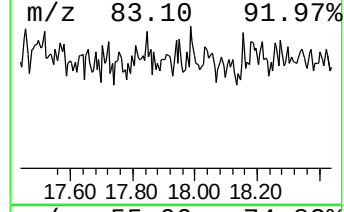
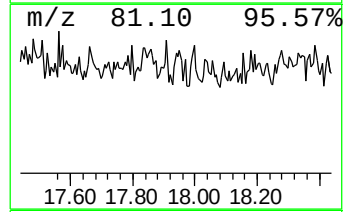
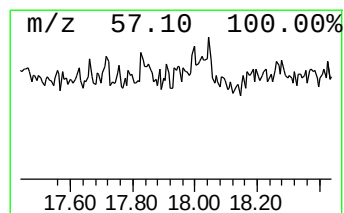
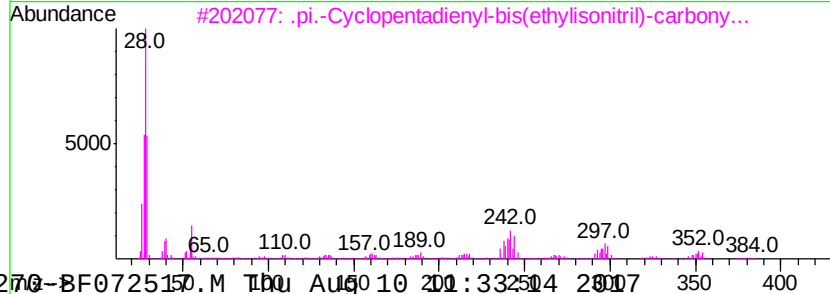
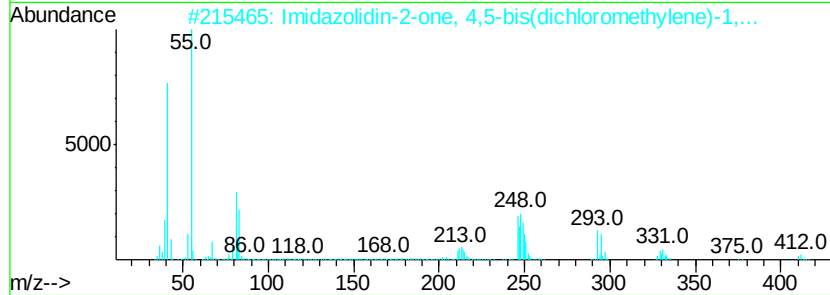
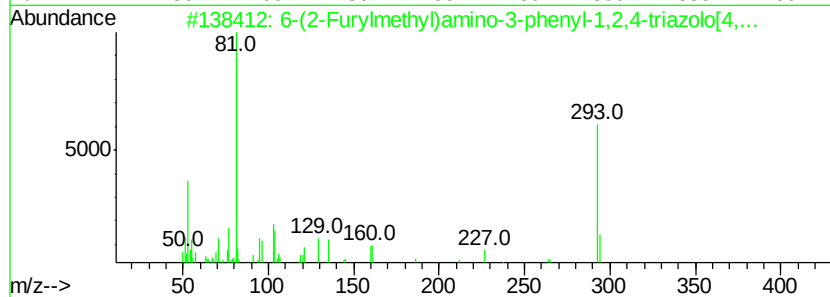
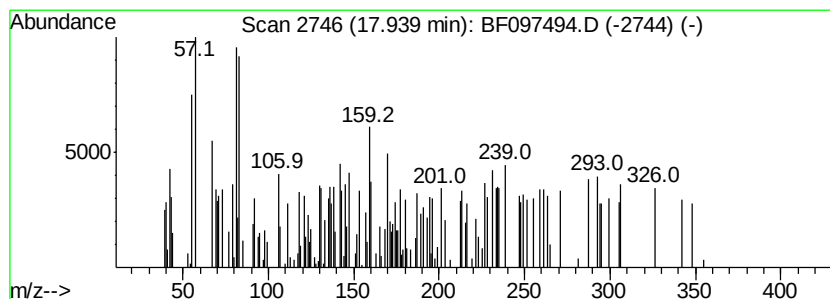
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.94 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	3.29 ng	52913	Perylene-d12	14.87

Hit#	of	4	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(2-Furylmethyl)amino-3-phenyl-	293	C14H11N7O	1000284-82-3	9		
2	Imidazolidin-2-one, 4,5-bis(dichloromethyl)-	410	C17H22Cl4N2O	134126-49-1	4		
3	.pi.-Cyclopentadienyl-bis(ethylmethylammonium)-	380	C12H15BrMoN2O	1000287-47-6	2		
4	4,7-Dichloro-2-(ethyloxy)-2-[(1-ethoxy-2-methyl-5-oxo-1,2,3,4-tetrahydropyridin-4-ylidene)amino]-	366	C12H12Cl2N2O3S	194228-11-0	1		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097494.D
Acq On : 9 Aug 2017 3:15
Operator : SJ/JU
Sample : I4655-02 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

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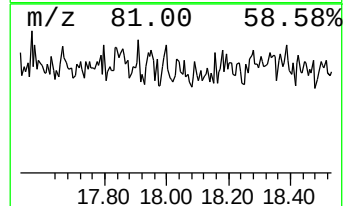
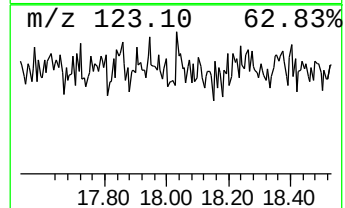
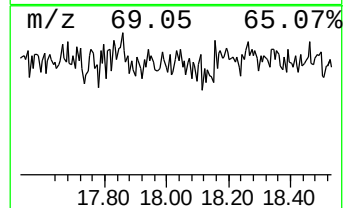
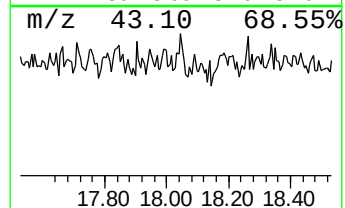
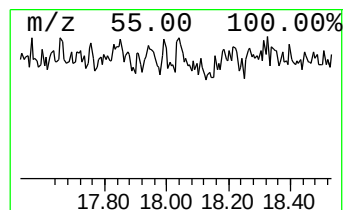
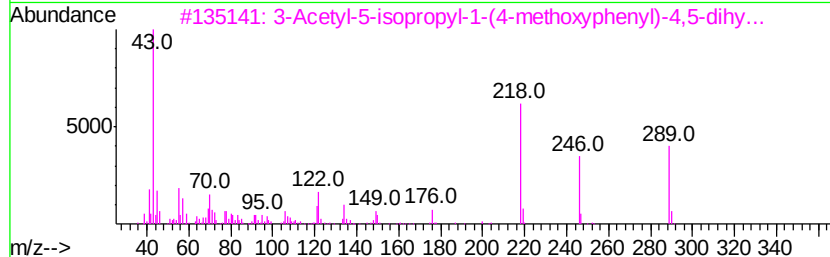
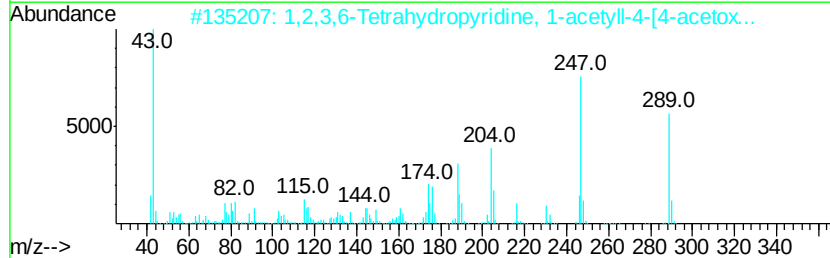
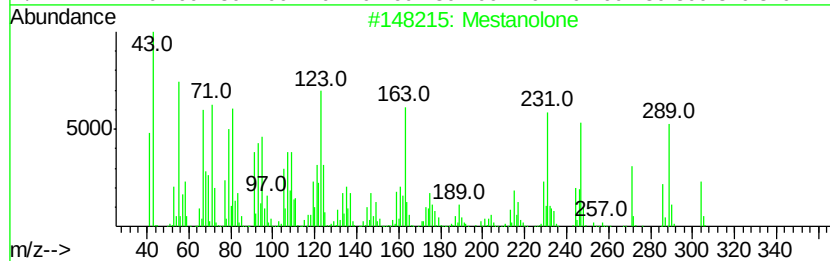
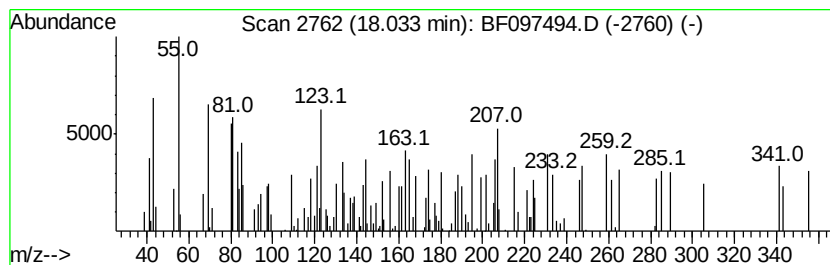
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown18.03 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	2.34 ng	37743	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mestanolone	304	C20H32O2	000521-11-9	10
2		1,2,3,6-Tetrahydropyridine, 1-ac...	289	C16H19N04	094427-33-5	10
3		3-Acetyl-5-isopropyl-1-(4-methox...	289	C15H19N3O3	1000210-22-0	10
4		17.beta.-Hydroxy-5.alpha.-andros...	305	C19H31NO2	002436-48-8	9
5		Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	288	C21H36	078578-98-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097494.D
Acq On : 9 Aug 2017 3:15
Operator : SJ/JU
Sample : I4655-02 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP8N-WC1

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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					#	RT	Resp	Conc
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unknown13.05	13.05	3.7	ng	91703	5	13.53	493990	20.0
unknown15.74	15.74	5.5	ng	88852	6	14.87	321946	20.0
unknown15.97	15.97	3.2	ng	51150	6	14.87	321946	20.0
unknown16.10	16.10	4.4	ng	71549	6	14.87	321946	20.0
unknown16.20	16.20	5.4	ng	86444	6	14.87	321946	20.0
unknown16.60	16.60	5.3	ng	85936	6	14.87	321946	20.0
unknown16.84	16.84	2.0	ng	32633	6	14.87	321946	20.0
unknown17.94	17.94	3.3	ng	52913	6	14.87	321946	20.0
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