

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
 Data File : BF085521.D
 Acq On : 18 Mar 2016 6:12
 Operator : UM/SJ
 Sample : H1776-02
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-12(0.5-3.5)

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-BF031516.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	5.087	242	245	253	rVB	61793	94009	2.32%	0.233%
2	5.476	276	279	282	rBV	2855886	3639231	89.63%	9.001%
3	6.516	367	370	372	rBV	2905015	4060238	100.00%	10.042%
4	6.642	378	381	384	rBV	3127218	3661525	90.18%	9.056%
5	6.870	399	401	404	rBV	756716	792347	19.51%	1.960%
6	7.030	413	415	418	rBV	2898031	2786966	68.64%	6.893%
7	7.442	448	451	453	rBV	2365450	2473608	60.92%	6.118%
8	7.533	456	459	464	rVB	77202	101730	2.51%	0.252%
9	8.162	511	514	516	rBV	1164767	1074822	26.47%	2.658%
10	9.236	605	608	611	rBV	3305670	3570827	87.95%	8.832%
11	9.636	640	643	644	rBV	720469	793300	19.54%	1.962%
12	9.853	659	662	664	rVB	60342	80582	1.98%	0.199%
13	9.910	665	667	669	rVV	799937	1034946	25.49%	2.560%
14	10.345	704	705	707	rVB	145076	128845	3.17%	0.319%
15	10.562	722	724	728	rBV	48935	93871	2.31%	0.232%
16	10.711	734	737	739	rBV2	1797449	2465219	60.72%	6.097%
17	10.825	745	747	751	rBV	126739	211471	5.21%	0.523%
18	11.008	761	763	767	rBV4	26547	61913	1.52%	0.153%
19	11.271	782	786	787	rBV	98938	119652	2.95%	0.296%
20	11.293	787	788	792	rVB	46019	50687	1.25%	0.125%
21	11.396	795	797	801	rBV2	1111466	1366776	33.66%	3.380%
22	11.476	801	804	806	rVB2	67144	95136	2.34%	0.235%
23	11.693	821	823	825	rVB	65033	50077	1.23%	0.124%
24	11.899	839	841	842	rBV	78215	68160	1.68%	0.169%
25	11.922	842	843	846	rVV	142832	182975	4.51%	0.453%
26	12.014	849	851	855	rVB3	90917	171209	4.22%	0.423%
27	12.196	864	867	868	rBV	55005	55223	1.36%	0.137%
28	12.448	887	889	890	rBV	63043	63770	1.57%	0.158%
29	12.482	890	892	895	rVB3	33614	58511	1.44%	0.145%
30	12.528	895	896	901	rVB2	42873	57867	1.43%	0.143%
31	12.608	901	903	906	rBV	824057	712403	17.55%	1.762%
32	12.711	910	912	913	rBV2	42320	47056	1.16%	0.116%
33	12.802	918	920	921	rVV	163237	195828	4.82%	0.484%
34	12.836	921	923	926	rVV	772984	748616	18.44%	1.852%

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Integration Parameters: rteint.p
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35	12.882	926	927	930	rVB2	59938	65836	1.62%	0.163%
36	12.985	933	936	938	rVV	3000272	2836060	69.85%	7.014%
37	13.054	938	942	946	rVB3	48993	86254	2.12%	0.213%
38	13.168	948	952	953	rVB	56676	112783	2.78%	0.279%
39	13.236	953	958	959	rBV2	26013	61419	1.51%	0.152%
40	13.271	959	961	962	rBV	74837	83330	2.05%	0.206%
41	13.396	970	972	973	rBV	32572	44426	1.09%	0.110%
42	13.511	980	982	984	rBV	110233	93538	2.30%	0.231%
43	13.671	992	996	1000	rBV	53600	76822	1.89%	0.190%
44	13.785	1003	1006	1007	rBV2	46707	75737	1.87%	0.187%
45	13.877	1012	1014	1018	rVB2	174846	209725	5.17%	0.519%
46	14.037	1024	1028	1034	rBV3	835303	1559612	38.41%	3.857%
47	14.139	1034	1037	1038	rBV2	45100	48030	1.18%	0.119%
48	14.197	1040	1042	1045	rVV3	33313	51392	1.27%	0.127%
49	14.414	1059	1061	1063	rVB	42057	55609	1.37%	0.138%
50	14.505	1066	1069	1071	rBV3	72113	96972	2.39%	0.240%
51	14.779	1092	1093	1097	rBV2	102688	175954	4.33%	0.435%
52	14.882	1099	1102	1105	rBV3	20226	48219	1.19%	0.119%
53	15.054	1115	1117	1122	rBV	292799	580653	14.30%	1.436%
54	15.134	1122	1124	1125	rBV	64364	73924	1.82%	0.183%
55	15.157	1125	1126	1128	rVB	53766	56401	1.39%	0.139%
56	15.260	1132	1135	1138	rBV3	17098	58216	1.43%	0.144%
57	15.351	1140	1143	1146	rVB	163985	239655	5.90%	0.593%
58	15.408	1146	1148	1151	rBV	250660	312302	7.69%	0.772%
59	15.465	1151	1153	1155	rBV	490083	751616	18.51%	1.859%
60	15.922	1190	1193	1195	rVB	38105	61725	1.52%	0.153%
61	16.174	1210	1215	1226	rVB3	63430	277439	6.83%	0.686%
62	16.563	1247	1249	1257	rVB4	32751	75382	1.86%	0.186%
63	16.871	1273	1276	1281	rVB2	95450	206431	5.08%	0.511%
64	16.974	1281	1285	1288	rVB3	18496	46373	1.14%	0.115%
65	17.054	1289	1292	1294	rBV	22459	41075	1.01%	0.102%
66	17.111	1294	1297	1302	rBV3	17870	48751	1.20%	0.121%
67	17.305	1310	1314	1322	rBV	80110	179921	4.43%	0.445%
68	17.443	1323	1326	1331	rVV6	26157	83348	2.05%	0.206%
69	17.980	1371	1373	1380	rVB7	15961	44998	1.11%	0.111%
70	18.426	1409	1412	1423	rVB9	14343	53005	1.31%	0.131%
71	19.443	1496	1501	1510	rVB5	80428	289879	7.14%	0.717%

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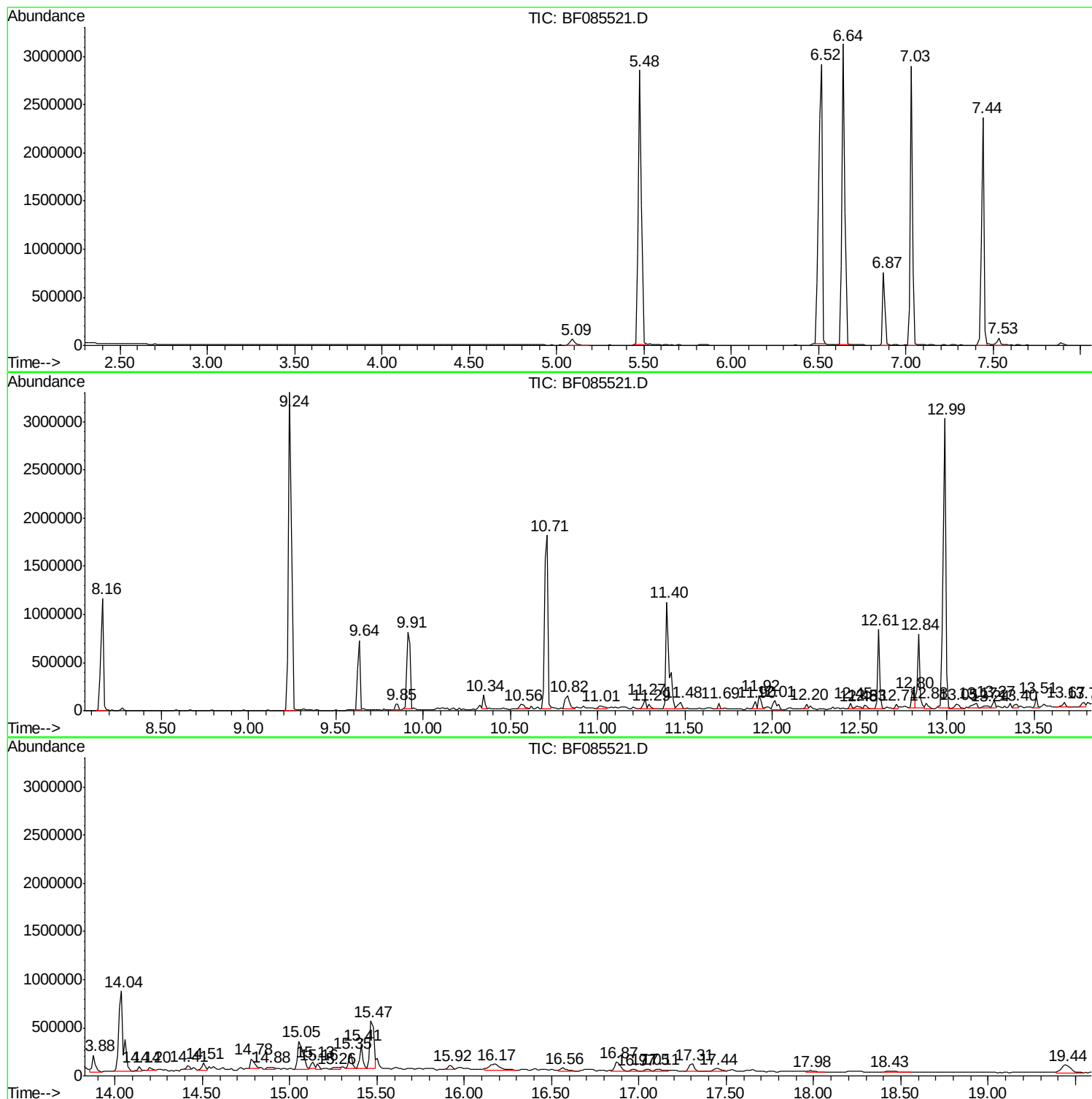
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
BNA_F
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W170TH-SB-12(0.5-3.5)

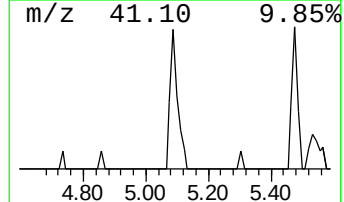
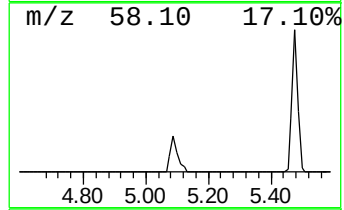
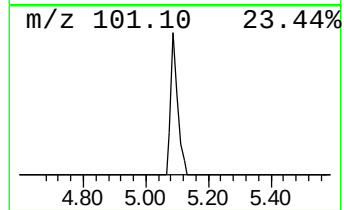
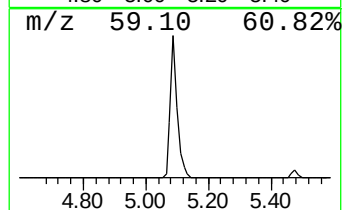
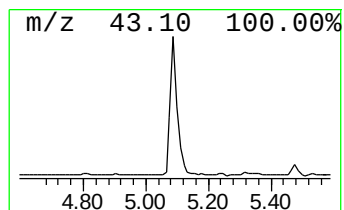
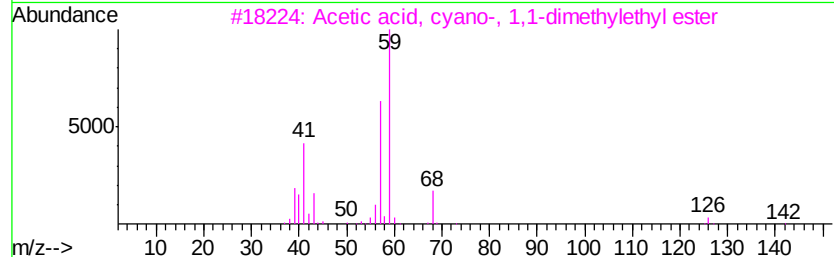
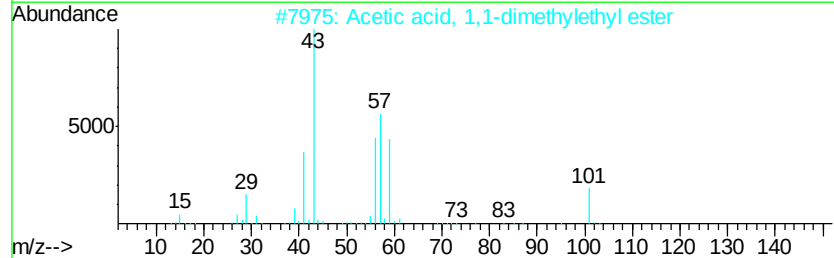
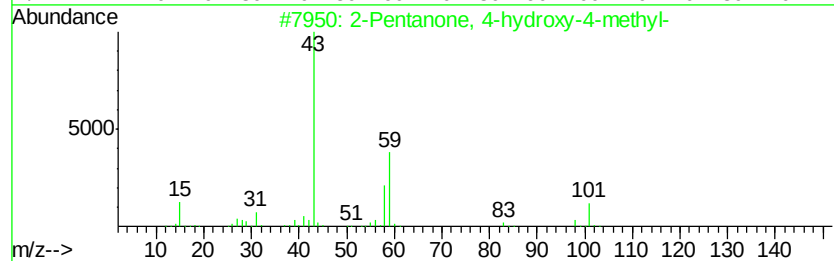
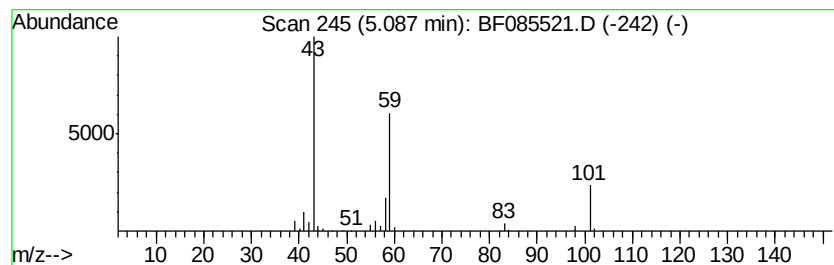
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.37 ng	94009	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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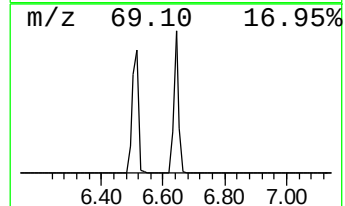
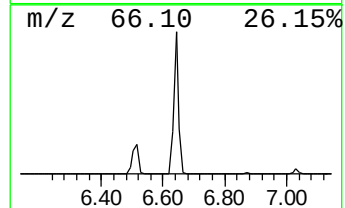
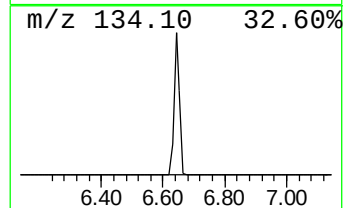
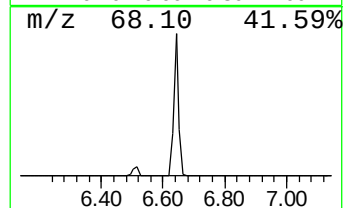
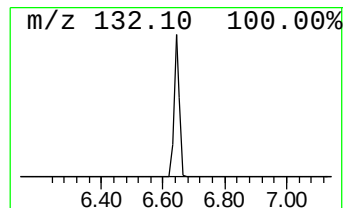
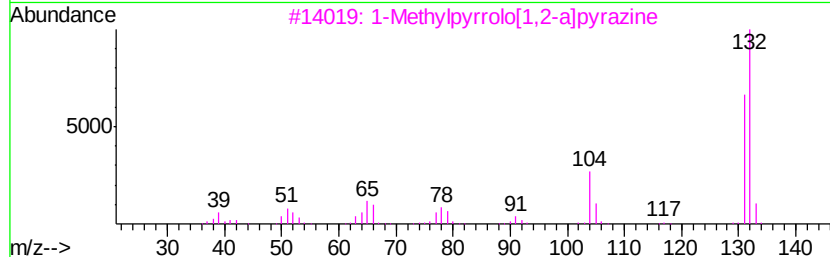
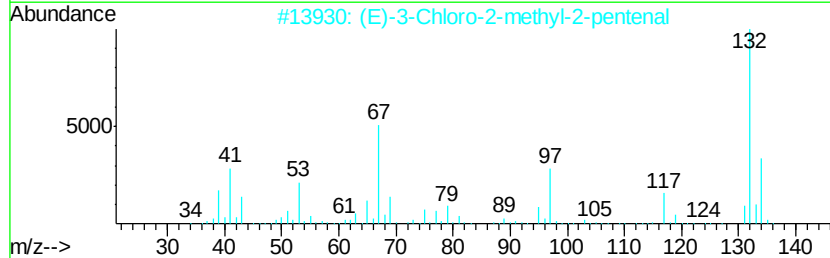
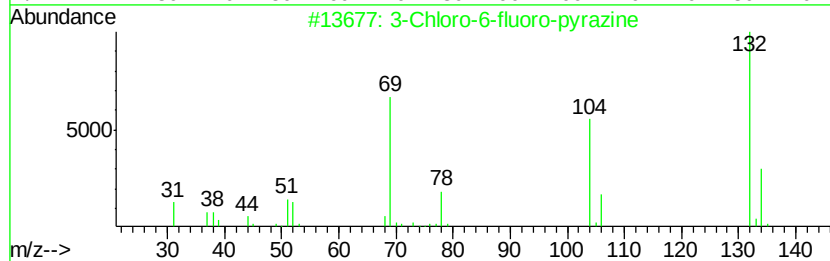
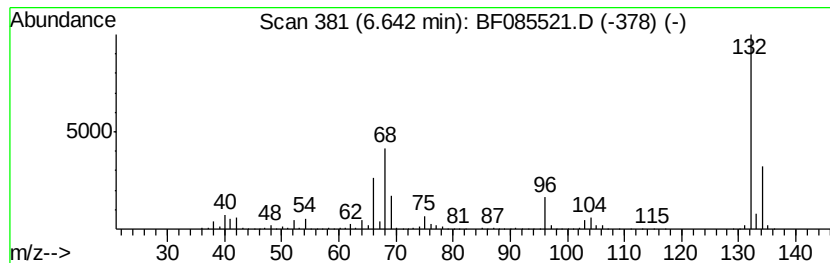
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	92.42 ng	3661530	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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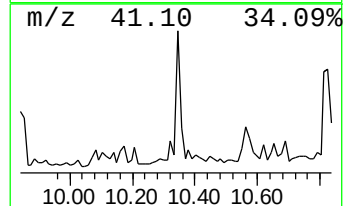
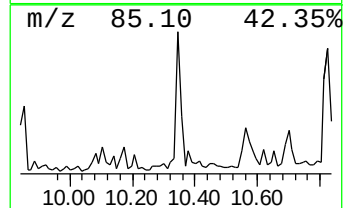
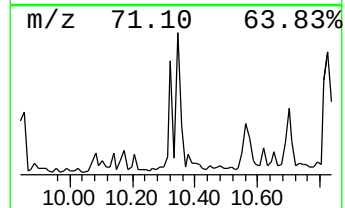
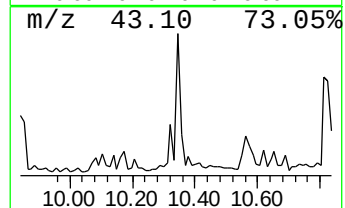
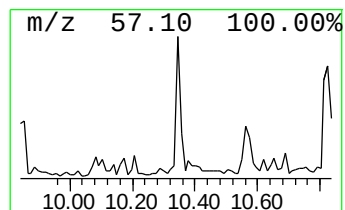
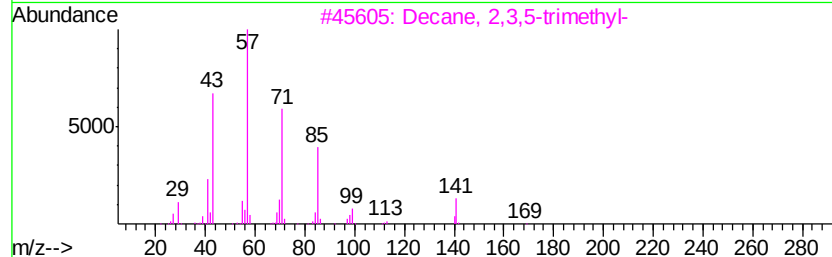
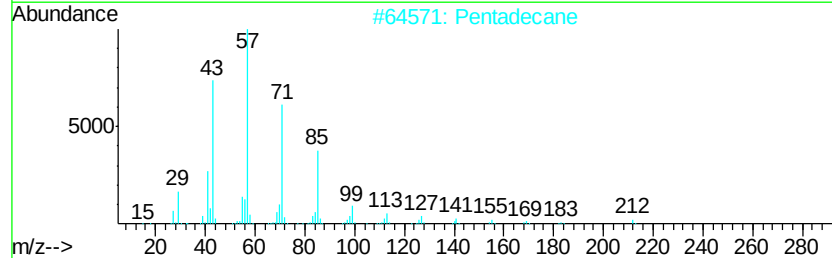
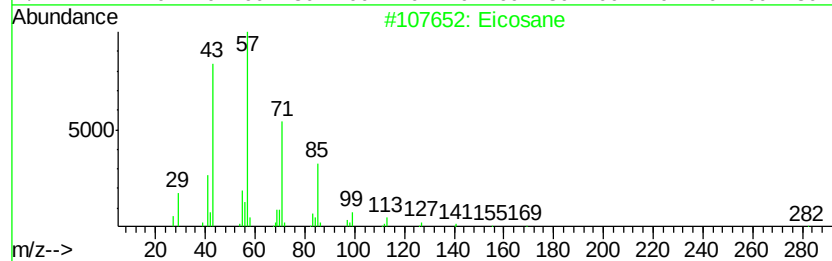
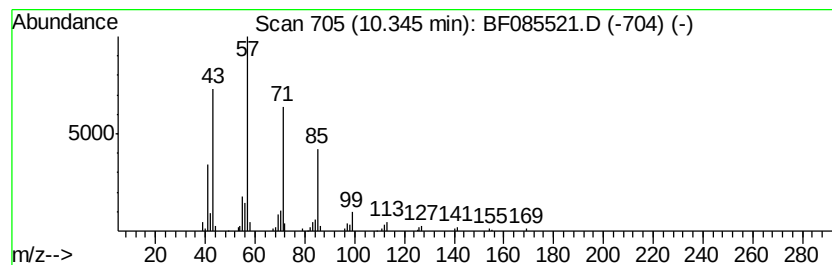
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.34	2.49 ng	128845	Acenaphthene-d10	9.91
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	91
2	Pentadecane	212 C15H32	000629-62-9	90
3	Decane, 2,3,5-trimethyl-	184 C13H28	062238-11-3	83
4	Hexadecane	226 C16H34	000544-76-3	83
5	Heptadecane	240 C17H36	000629-78-7	83



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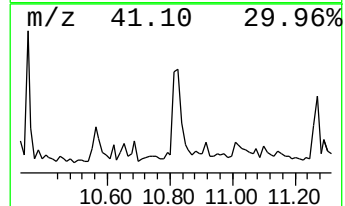
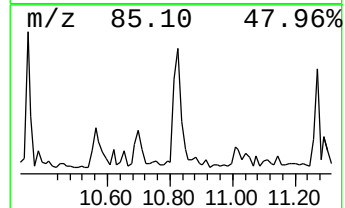
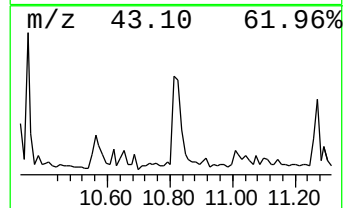
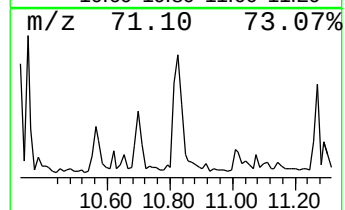
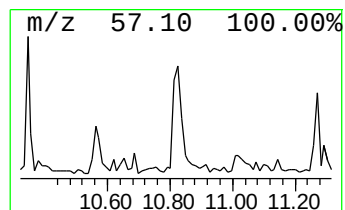
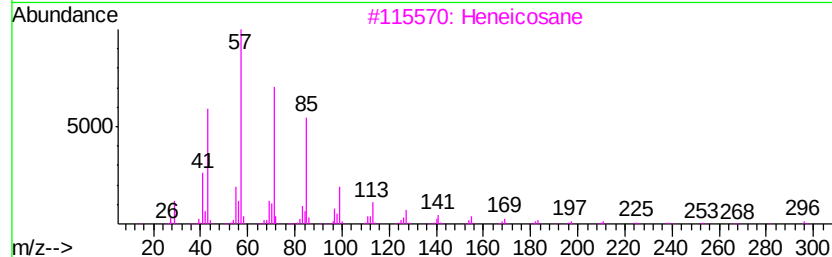
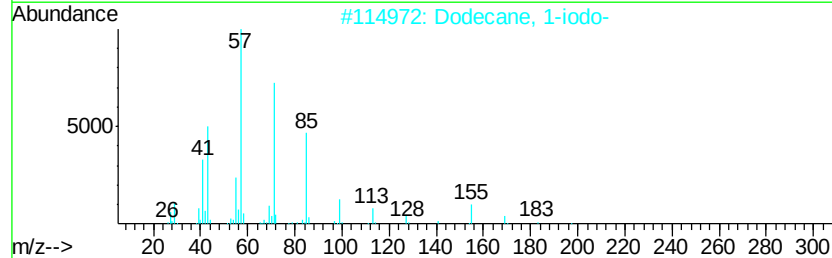
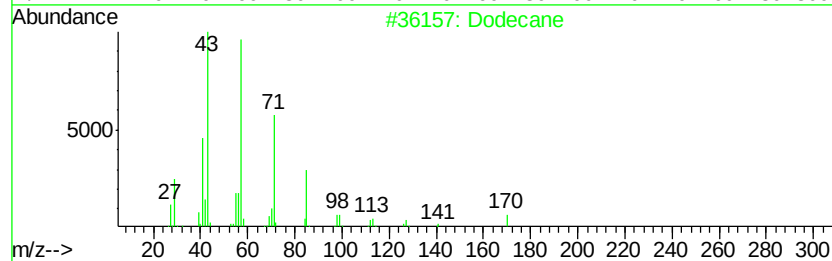
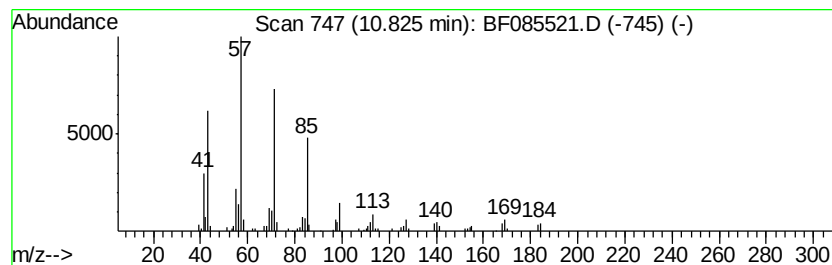
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.09 ng	211471	Phenanthrene-d10	11.40
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane	170 C12H26	000112-40-3	90
2	Dodecane, 1-iodo-	296 C12H25I	004292-19-7	74
3	Heneicosane	296 C21H44	000629-94-7	74
4	Heptadecane	240 C17H36	000629-78-7	74
5	Eicosane	282 C20H42	000112-95-8	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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Acq On : 18 Mar 2016 6:12
Operator : UM/SJ
Sample : H1776-02
Misc :
ALS Vial : 41 Sample Multiplier: 1

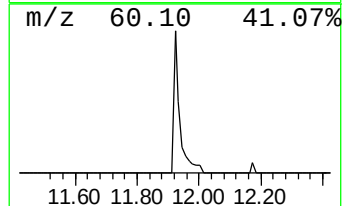
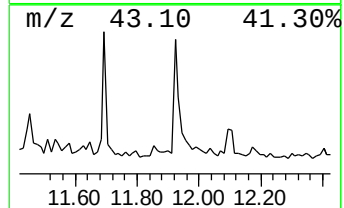
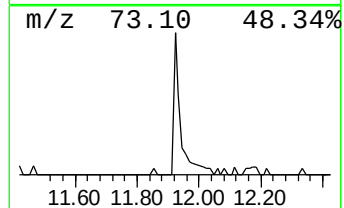
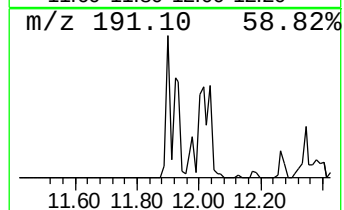
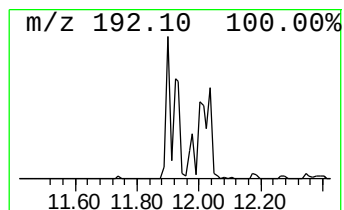
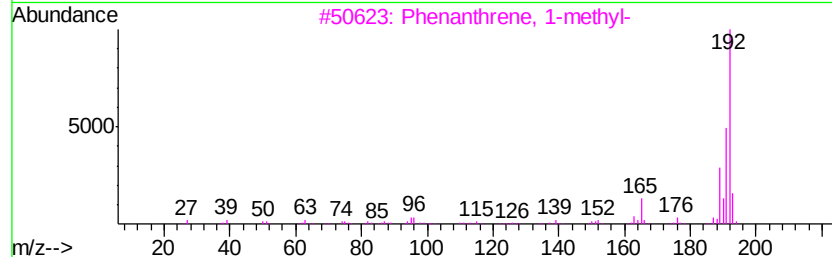
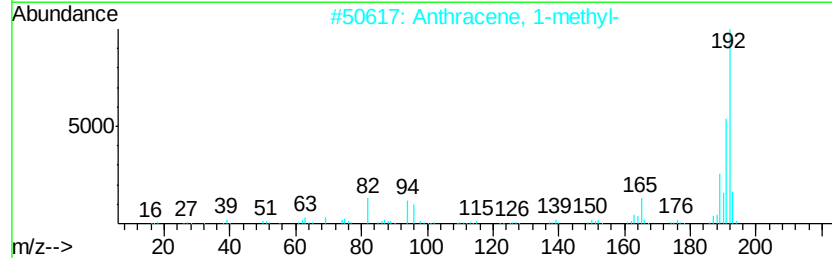
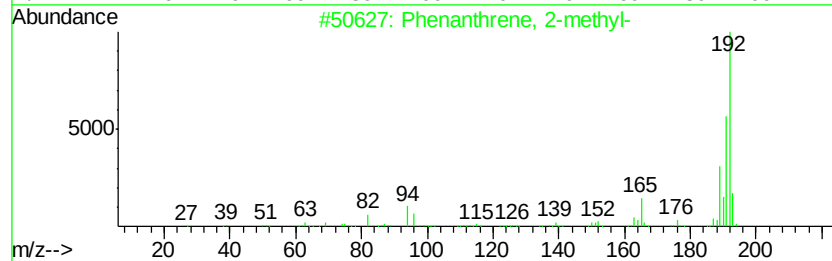
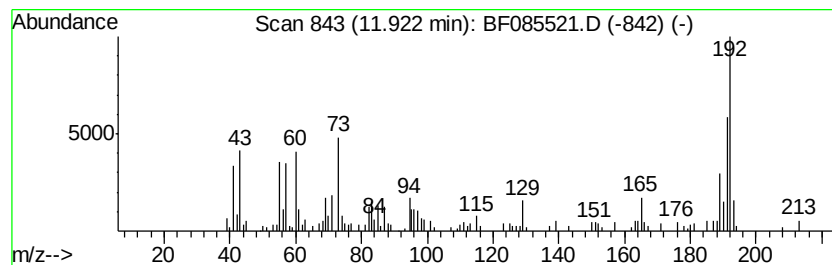
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	2.68 ng	182975	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	92
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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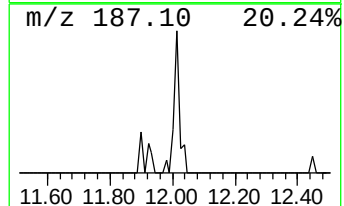
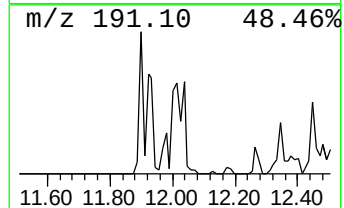
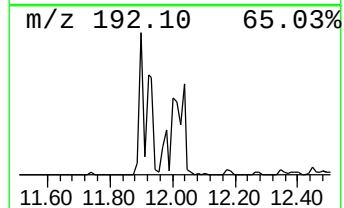
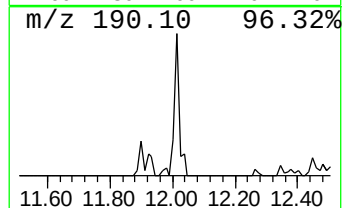
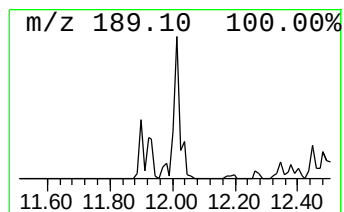
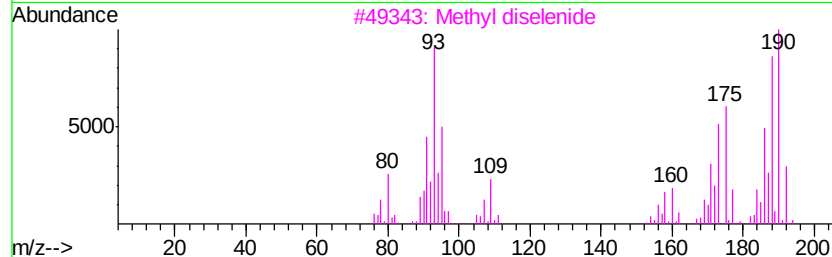
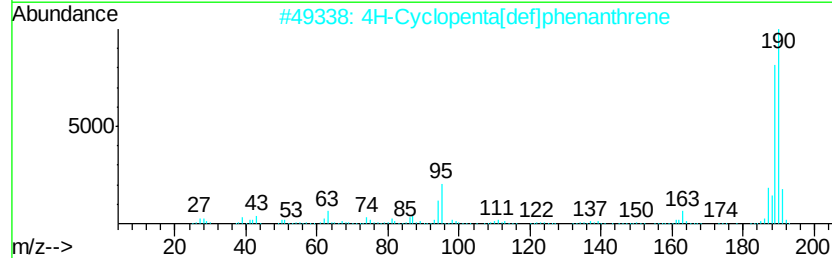
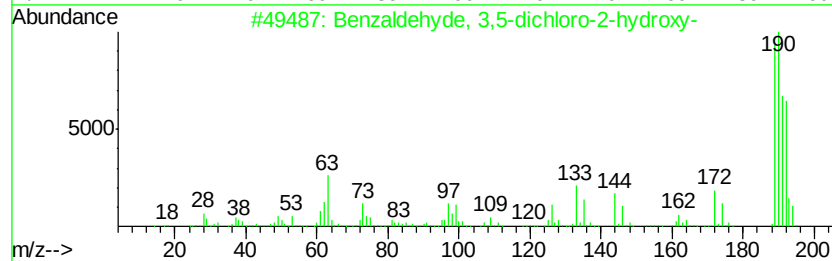
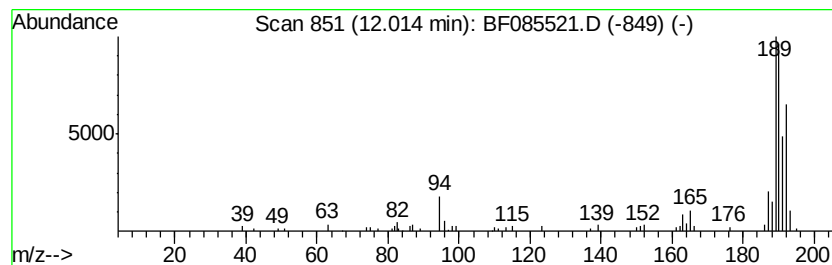
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzaldehyde, 3,5-dichloro-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.01	2.51 ng	171209	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
3	Methyl diselenide	190	C2H6Se2	007101-31-7	41
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085521.D
Acq On : 18 Mar 2016 6:12
Operator : UM/SJ
Sample : H1776-02
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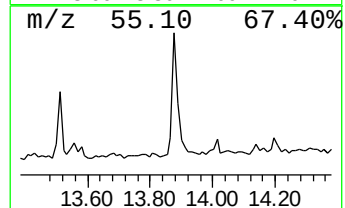
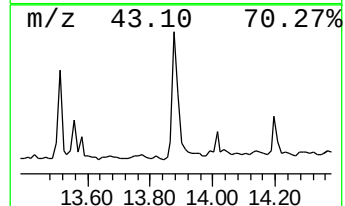
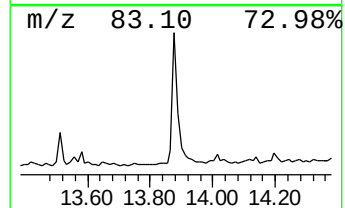
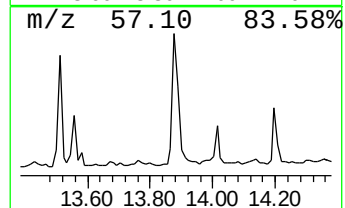
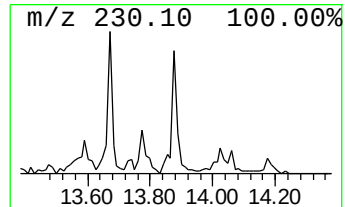
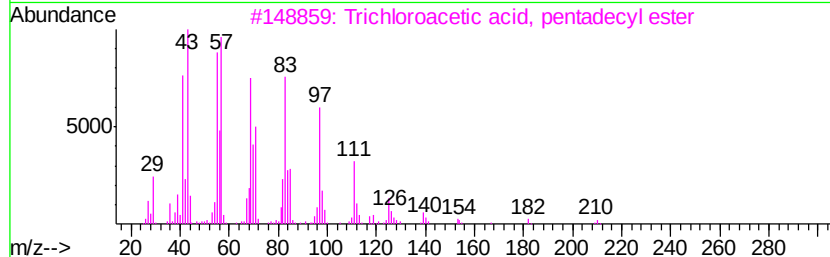
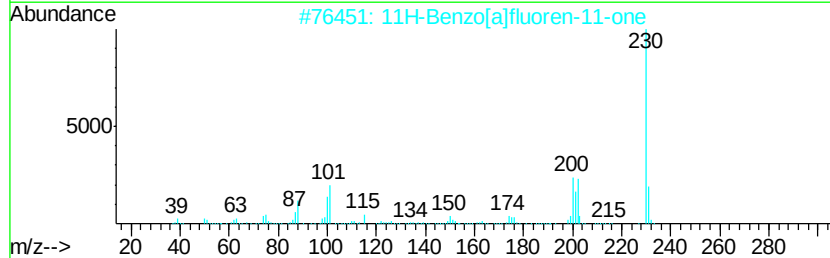
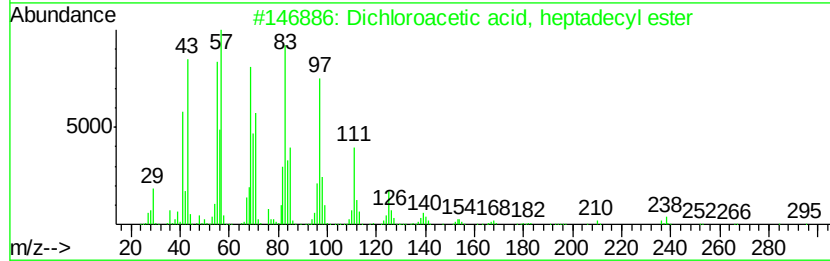
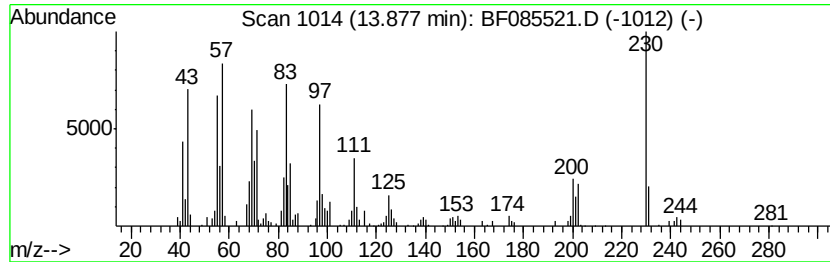
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	2.69 ng	209725	Chrysene-d12	14.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	89
2			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	56
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	55
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	55
5			1-Docosene	308	C22H44	001599-67-3	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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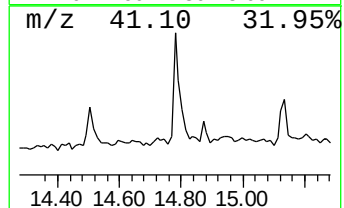
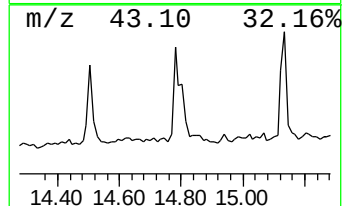
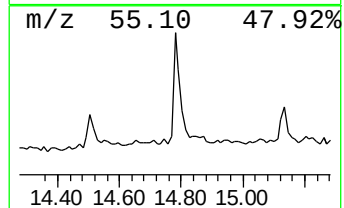
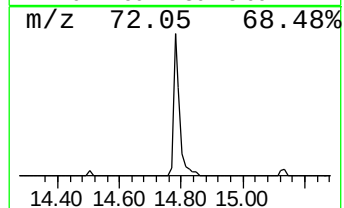
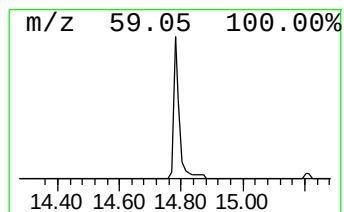
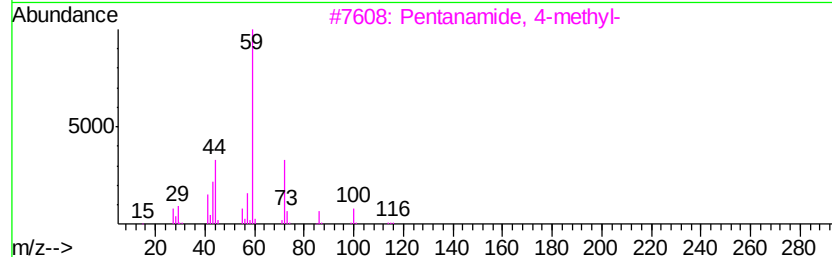
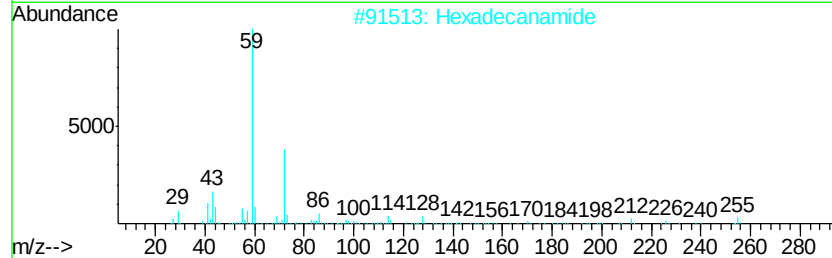
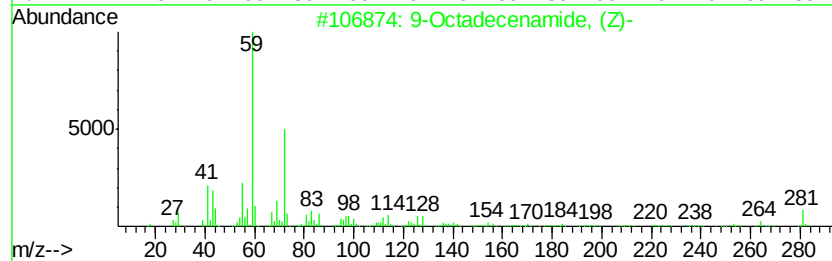
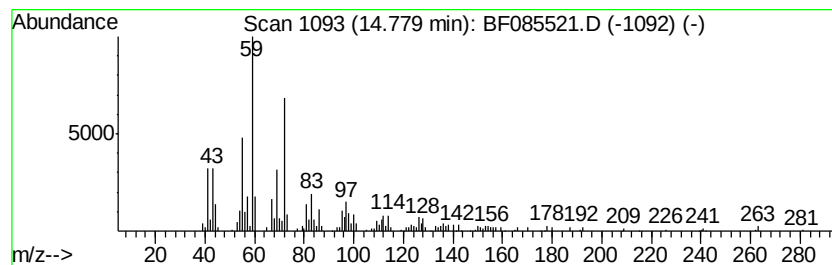
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.78	4.68 ng	175954	Perylene-d12	15.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2	Hexadecanamide	255	C16H33NO	000629-54-9	59
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
4	Dodecanamide	199	C12H25NO	001120-16-7	49
5	Decanamide-	171	C10H21NO	002319-29-1	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085521.D
Acq On : 18 Mar 2016 6:12
Operator : UM/SJ
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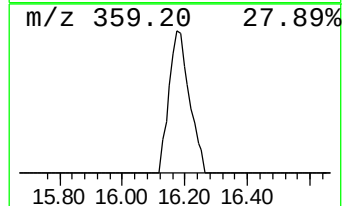
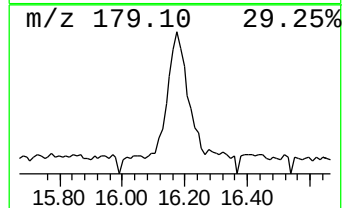
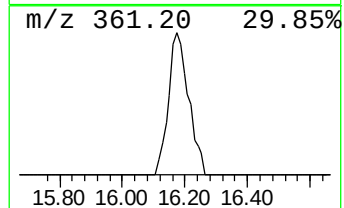
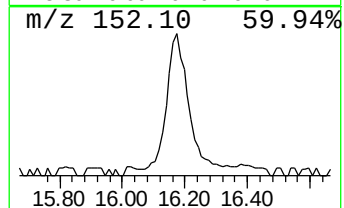
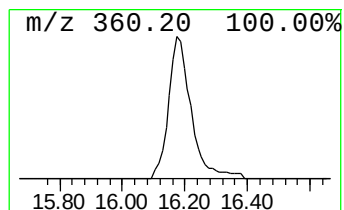
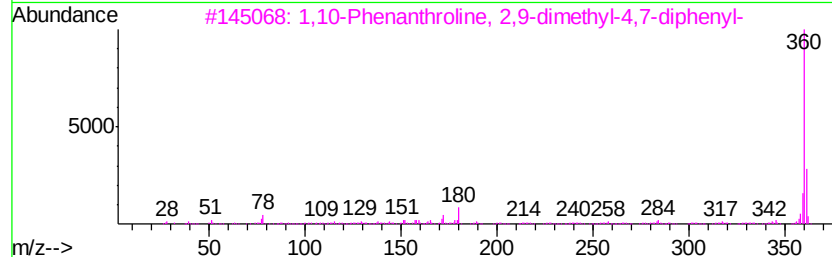
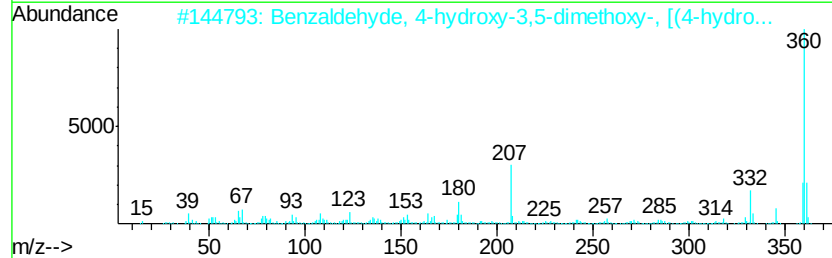
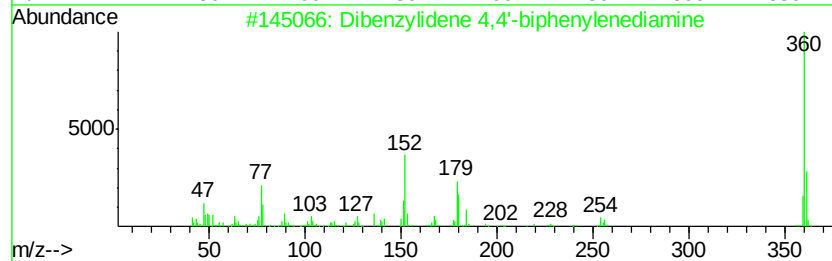
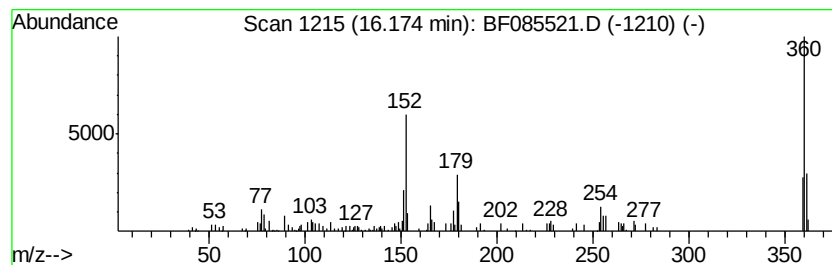
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	7.38 ng	277439	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	86
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	46
3		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
5		2-Cyclohexylamino-3-methyl(pheny...	360	C23H24N2O2	134614-17-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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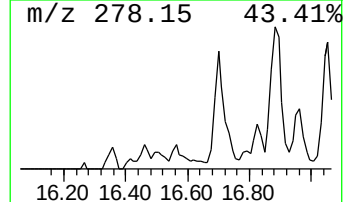
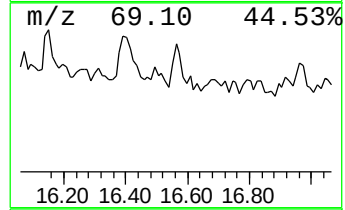
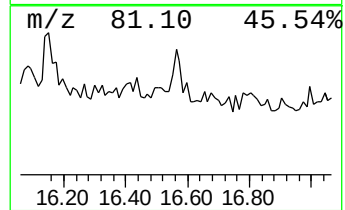
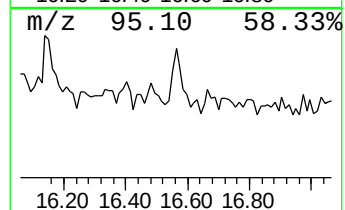
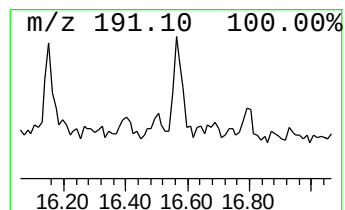
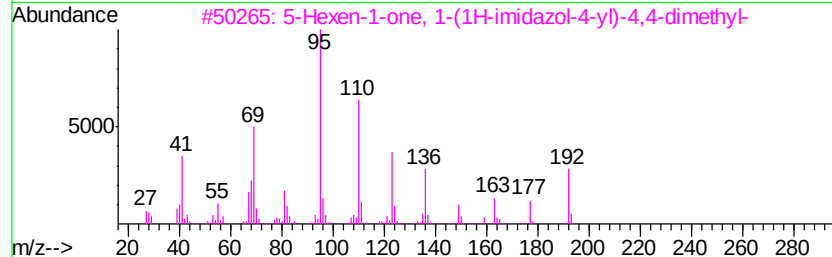
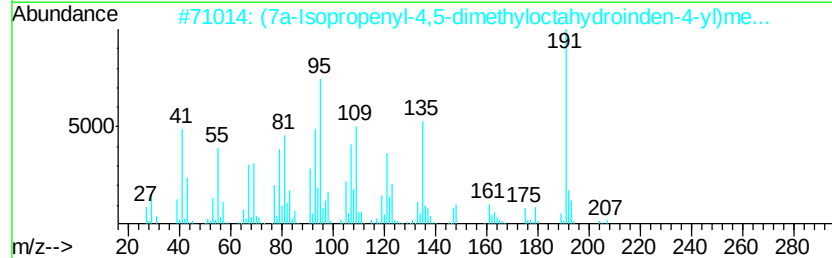
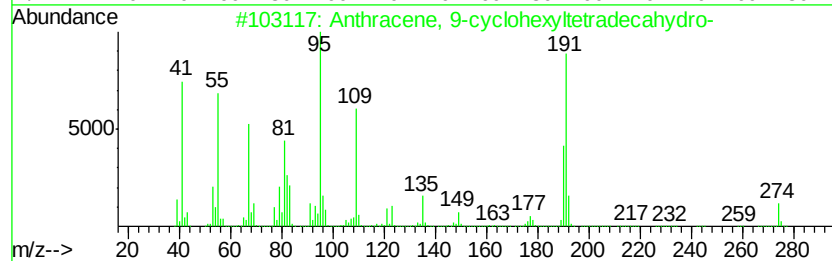
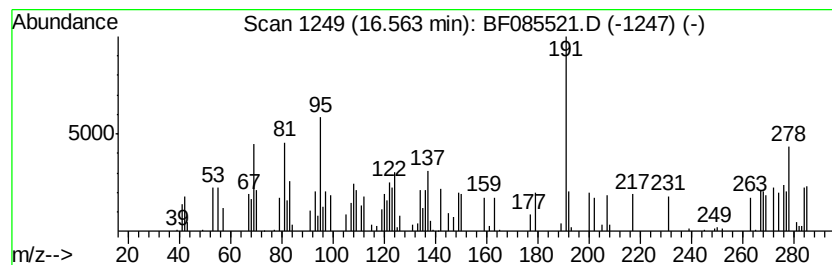
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.56 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	2.01 ng	75382	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Anthracene, 9-cyclohexyltetradec...	274 C20H34	055255-70-4 38
2		(7a-Isopropenyl-4,5-dimethylocta...	222 C15H26O	1000187-02-9 25
3		5-Hexen-1-one, 1-(1H-imidazol-4-...	192 C11H16N2O	069393-41-5 25
4		Silane, 1,3-decadiynyltrimethyl-	206 C13H22Si	084751-17-7 22
5		1-Penten-3-one, 1-(2,6,6-trimeth...	206 C14H22O	000127-43-5 22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085521.D
Acq On : 18 Mar 2016 6:12
Operator : UM/SJ
Sample : H1776-02
Misc :
ALS Vial : 41 Sample Multiplier: 1

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ClientSampleId :
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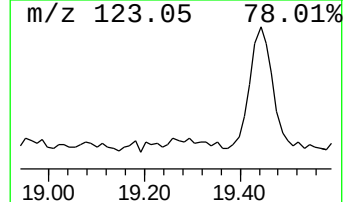
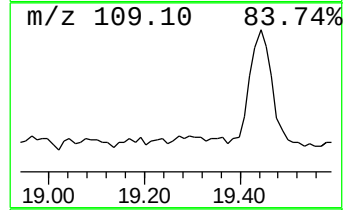
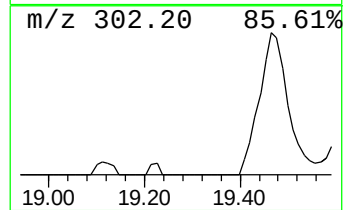
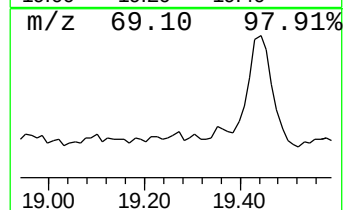
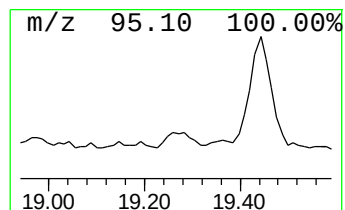
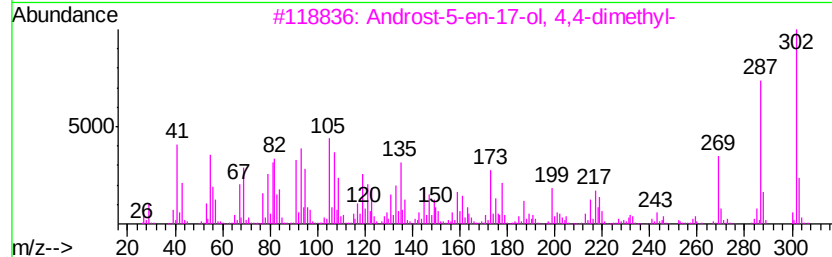
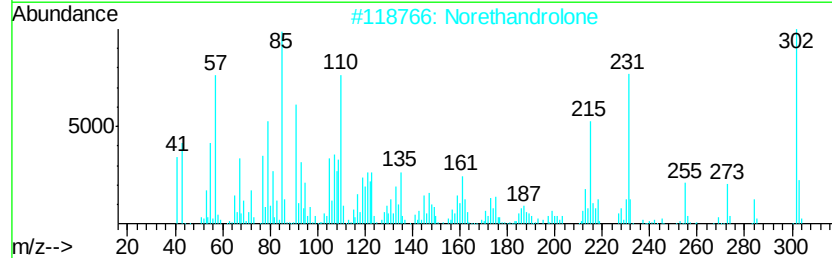
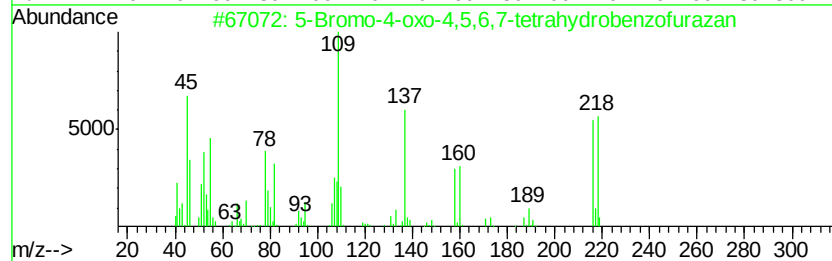
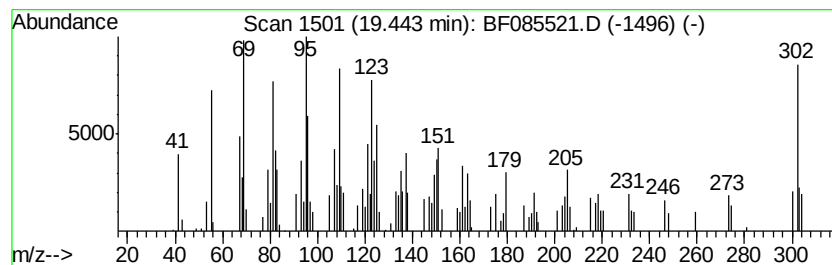
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.44	7.71 ng	289879	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
2		Norethandrolone	302	C20H30O2	000052-78-8	45
3		Androst-5-en-17-ol, 4,4-dimethyl-	302	C21H34O	1000195-76-3	41
4		(7,7-Dimethyl-2-oxobicyclo[2.2.1...]	246	C11H18O4S	1000197-55-6	41
5		2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
 Data File : BF085521.D
 Acq On : 18 Mar 2016 6:12
 Operator : UM/SJ
 Sample : H1776-02
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-12(0.5-3.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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...	5.09	2.4	ng	94009	1	6.87	792347	20.0
unknown6.64	6.64	92.4	ng	3661530	1	6.87	792347	20.0
Eicosane	10.34	2.5	ng	128845	3	9.91	1034950	20.0
Dodecane	10.82	3.1	ng	211471	4	11.40	1366780	20.0
Phenanthrene, 2-m...	11.92	2.7	ng	182975	4	11.40	1366780	20.0
Benzaldehyde, 3,5...	12.01	2.5	ng	171209	4	11.40	1366780	20.0
Dichloroacetic ac...	13.88	2.7	ng	209725	5	14.04	1559610	20.0
9-Octadecenamide,...	14.78	4.7	ng	175954	6	15.47	751616	20.0
Dibenzylidene 4,4...	16.17	7.4	ng	277439	6	15.47	751616	20.0
unknown16.56	16.56	2.0	ng	75382	6	15.47	751616	20.0
5-Bromo-4-oxo-4,5...	19.44	7.7	ng	289879	6	15.47	751616	20.0