

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
 Data File : BF088724.D
 Acq On : 6 Jul 2016 1:34
 Operator : UM/SJ
 Sample : H3881-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 Q6-B1-0-6-C

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-BF063016.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	1.724	10	12	17	rVB	11932	23733	1.05%	0.106%
2	1.850	21	23	33	rVB	343125	642130	28.51%	2.876%
3	4.936	290	293	296	rBV	90796	134715	5.98%	0.603%
4	5.359	327	330	333	rBV	1530521	1607117	71.35%	7.198%
5	6.410	419	422	424	rBV	1860249	1936441	85.97%	8.674%
6	6.536	431	433	436	rBV	1615764	1816031	80.62%	8.134%
7	6.776	451	454	456	rBV	720121	662095	29.39%	2.966%
8	6.936	465	468	470	rBV	1063330	1481109	65.75%	6.634%
9	7.336	500	503	506	rBV	1193076	1127769	50.07%	5.051%
10	8.056	564	566	569	rBV	971665	854235	37.92%	3.826%
11	9.142	658	661	663	rBV	1609003	2252513	100.00%	10.089%
12	9.530	693	695	697	rBV	370340	331657	14.72%	1.486%
13	9.748	712	714	717	rBV	32180	32693	1.45%	0.146%
14	9.805	717	719	721	rBV	953244	857680	38.08%	3.842%
15	10.216	753	755	757	rBV	24212	31882	1.42%	0.143%
16	10.250	757	758	760	rVB	59519	41835	1.86%	0.187%
17	10.468	774	777	780	rBV	19748	29623	1.32%	0.133%
18	10.593	785	788	790	rBV	1042685	1120374	49.74%	5.018%
19	10.719	797	799	803	rBV	71634	77996	3.46%	0.349%
20	10.913	813	816	818	rBV	11722	24309	1.08%	0.109%
21	11.165	836	838	840	rVV	105169	106148	4.71%	0.475%
22	11.199	840	841	844	rVV	22966	25934	1.15%	0.116%
23	11.279	846	848	852	rVV	741234	865402	38.42%	3.876%
24	11.359	852	855	856	rVB3	43811	69921	3.10%	0.313%
25	11.588	873	875	879	rVB	61472	71240	3.16%	0.319%
26	11.805	893	894	897	rVB	26040	26383	1.17%	0.118%
27	11.851	897	898	900	rVB	25202	24139	1.07%	0.108%
28	11.896	900	902	906	rBV2	27292	53056	2.36%	0.238%
29	11.999	906	911	913	rBV2	15514	25286	1.12%	0.113%
30	12.079	917	918	922	rVB3	16305	31335	1.39%	0.140%
31	12.331	938	940	942	rBV	21745	28634	1.27%	0.128%
32	12.388	942	945	946	rBV2	17581	26537	1.18%	0.119%
33	12.491	952	954	956	rBV	218810	225256	10.00%	1.009%
34	12.708	971	973	975	rBV2	172716	241305	10.71%	1.081%

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35	12.754	975	977	983	rVB3	16729	25604	1.14%	0.115%
36	12.868	985	987	989	rVB	1745552	1626521	72.21%	7.285%
37	12.936	989	993	996	rVB3	21134	24622	1.09%	0.110%
38	13.016	997	1000	1001	rBV3	30126	51375	2.28%	0.230%
39	13.108	1006	1008	1010	rBV	44706	48336	2.15%	0.217%
40	13.142	1010	1011	1015	rVB	40598	48328	2.15%	0.216%
41	13.234	1017	1019	1021	rBV	26928	27537	1.22%	0.123%
42	13.451	1036	1038	1040	rBV2	22947	29522	1.31%	0.132%
43	13.542	1044	1046	1049	rVV2	32015	48863	2.17%	0.219%
44	13.657	1054	1056	1058	rBV3	33837	60507	2.69%	0.271%
45	13.782	1065	1067	1071	rBV2	77546	138541	6.15%	0.621%
46	13.908	1075	1078	1079	rBV2	697450	801277	35.57%	3.589%
47	14.114	1095	1096	1099	rBV2	22077	41419	1.84%	0.186%
48	14.285	1109	1111	1113	rBV2	24068	41845	1.86%	0.187%
49	14.399	1119	1121	1122	rBV	28238	45039	2.00%	0.202%
50	14.434	1122	1124	1126	rVB2	46875	80702	3.58%	0.361%
51	14.822	1156	1158	1160	rVB	114353	99734	4.43%	0.447%
52	14.902	1163	1165	1170	rBV	159509	324609	14.41%	1.454%
53	15.005	1171	1174	1175	rBV2	105623	117087	5.20%	0.524%
54	15.040	1175	1177	1185	rVB3	56274	136578	6.06%	0.612%
55	15.177	1187	1189	1192	rVB	90168	122797	5.45%	0.550%
56	15.234	1192	1194	1197	rVB	106865	123851	5.50%	0.555%
57	15.302	1197	1200	1202	rBV	400378	569446	25.28%	2.551%
58	15.531	1218	1220	1223	rVB2	55028	69707	3.09%	0.312%
59	15.748	1236	1239	1242	rBV	129950	208565	9.26%	0.934%
60	16.468	1299	1302	1308	rVB2	88494	193965	8.61%	0.869%
61	16.617	1313	1315	1319	rVB2	46504	90263	4.01%	0.404%
62	16.743	1324	1326	1329	rBV	23909	40926	1.82%	0.183%
63	17.017	1348	1350	1356	rVB	42516	79027	3.51%	0.354%
64	17.211	1364	1367	1373	rVB5	29567	102833	4.57%	0.461%

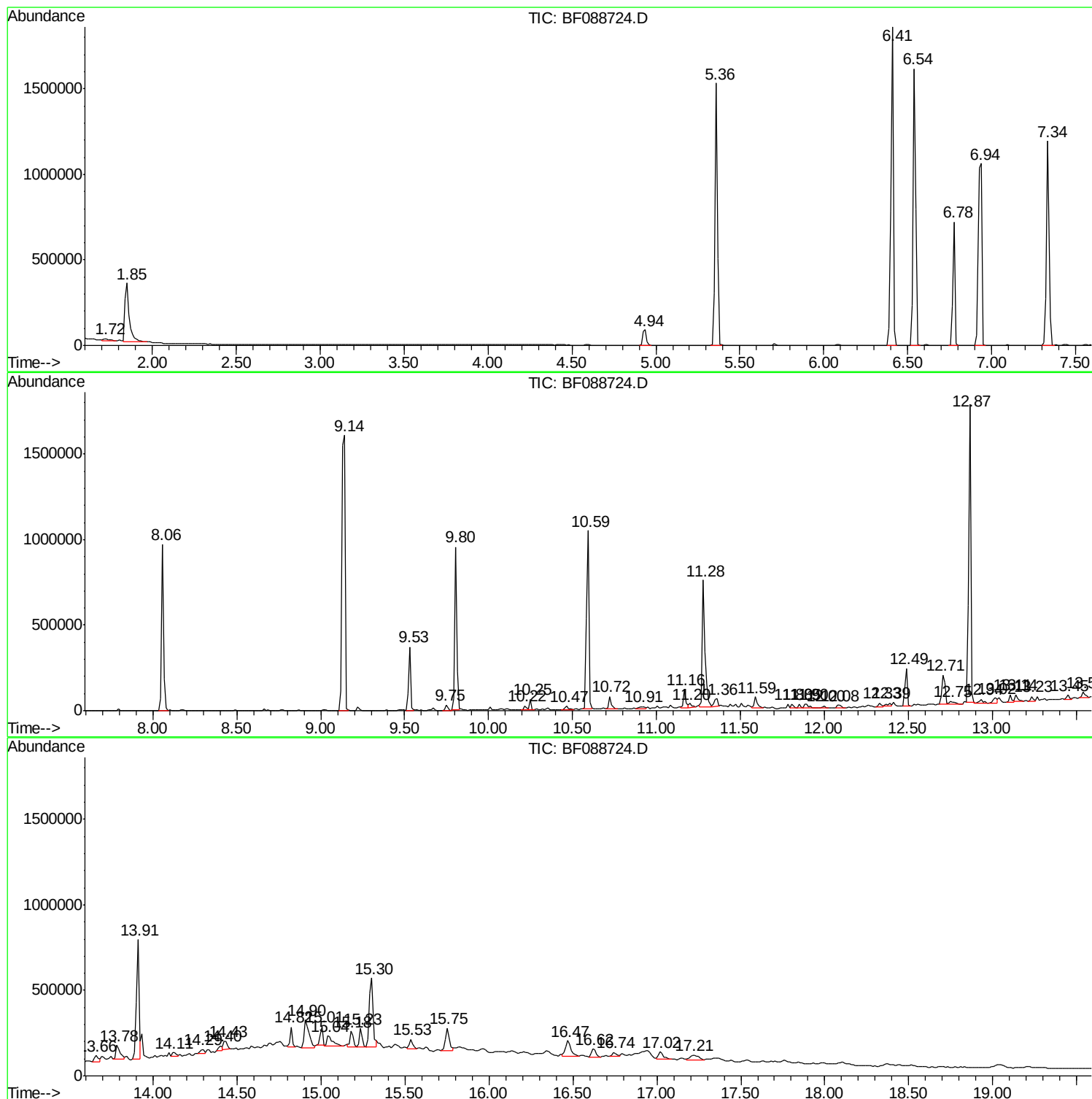
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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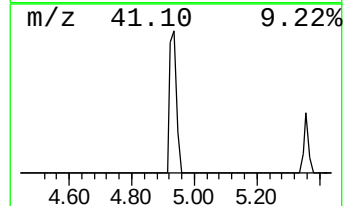
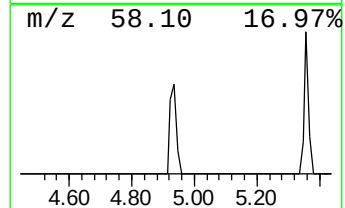
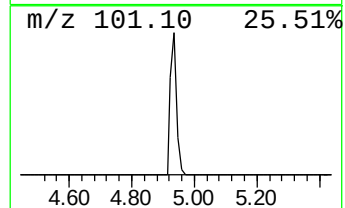
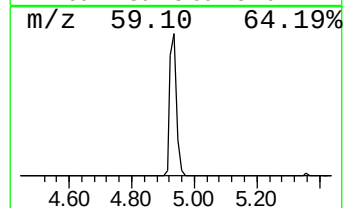
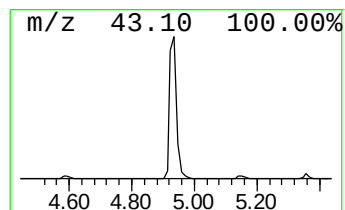
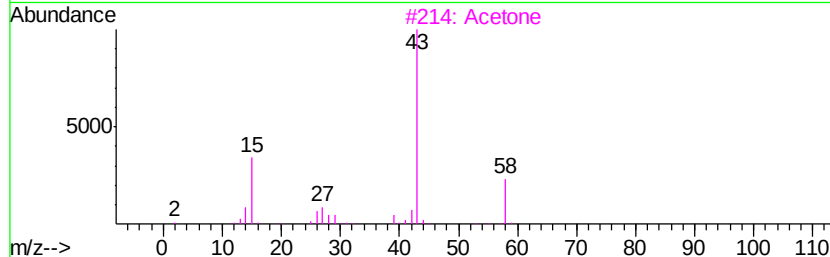
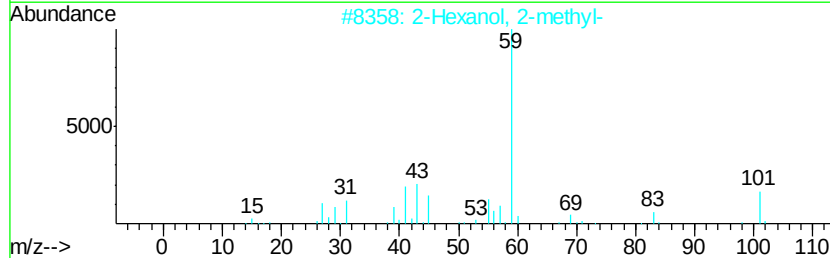
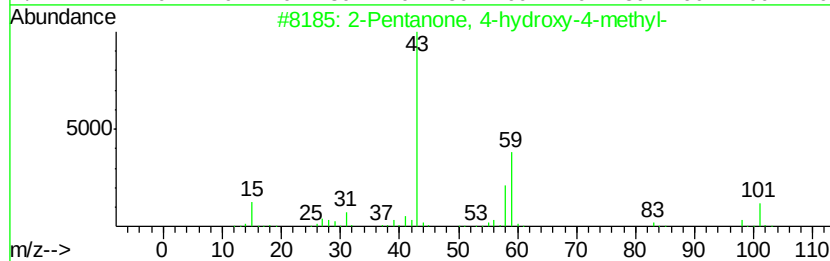
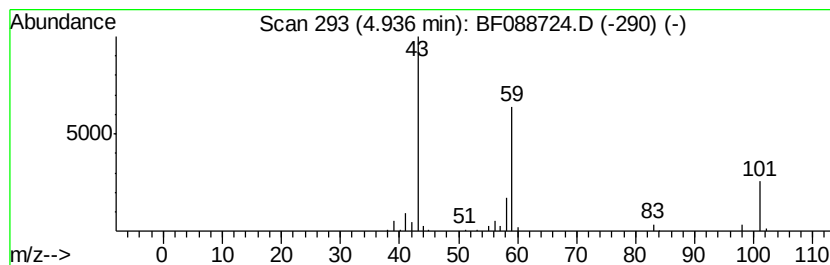
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	4.07 ng	134715	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		Acetone	58	C3H6O	000067-64-1	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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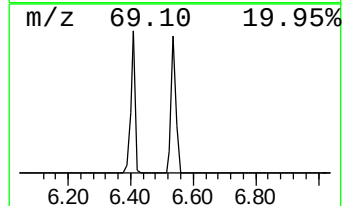
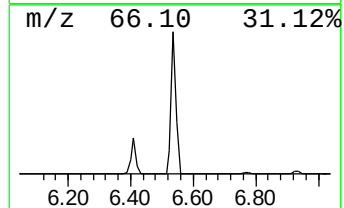
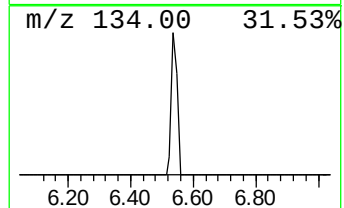
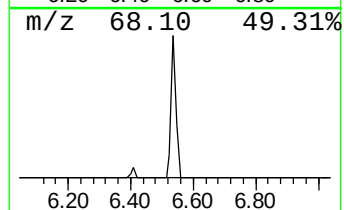
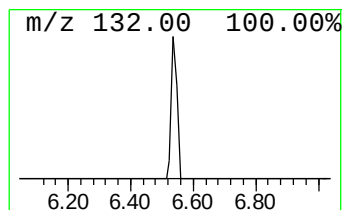
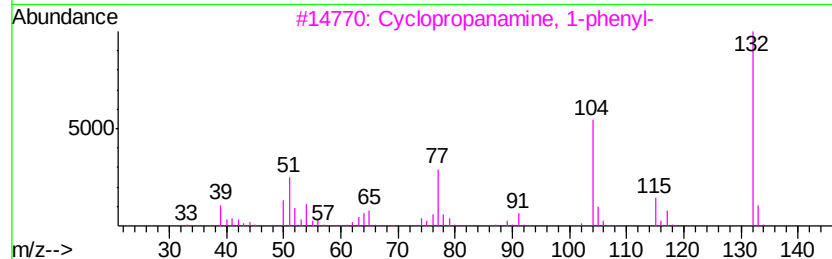
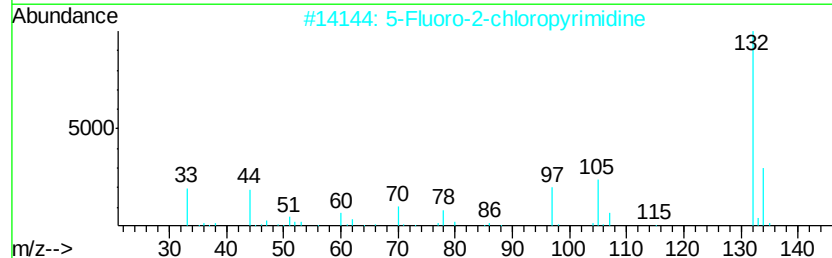
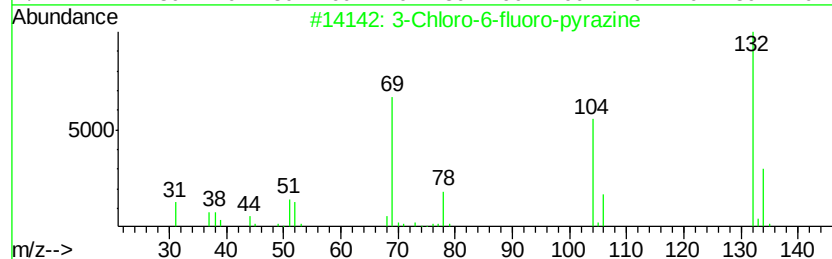
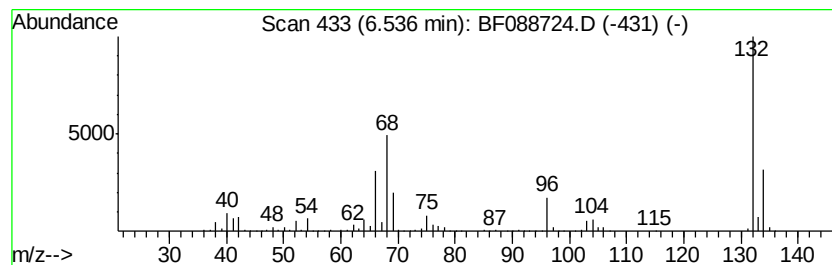
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	54.86 ng	1816030	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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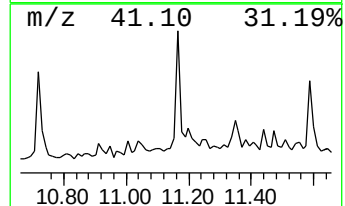
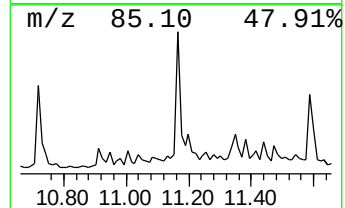
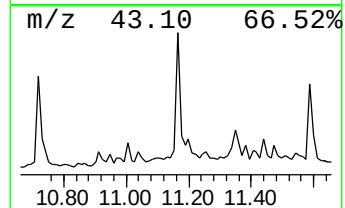
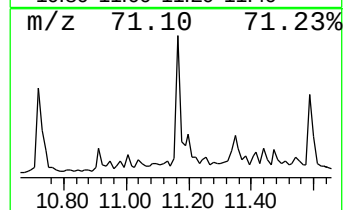
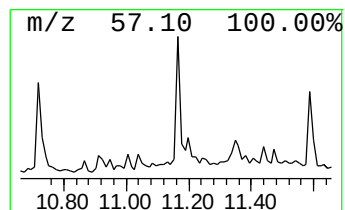
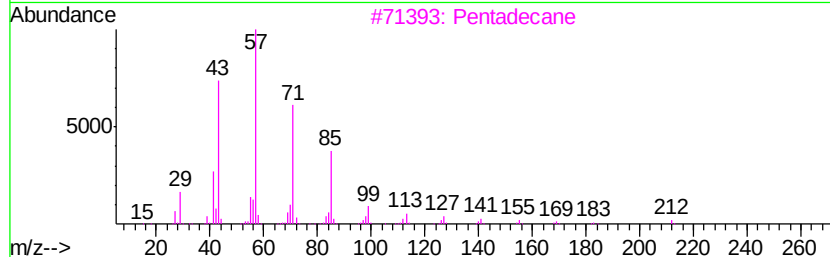
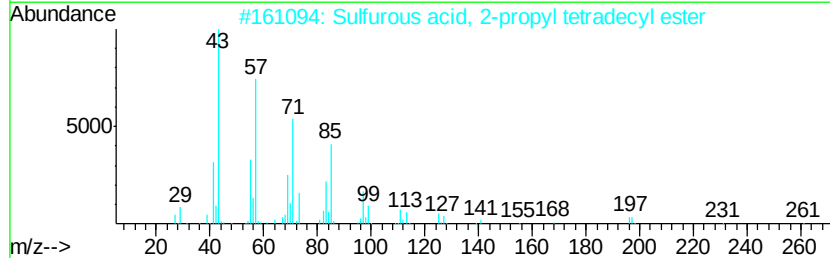
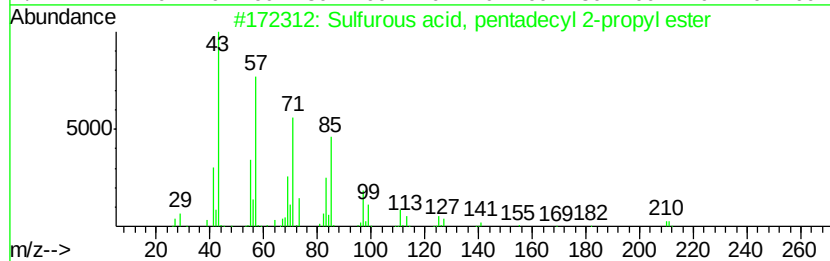
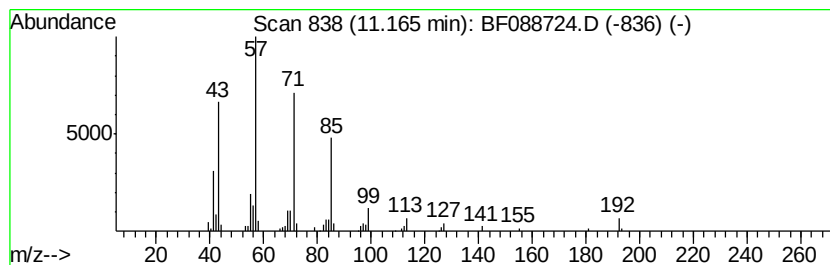
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Peak Number 5 Sulfurous acid, pentadecyl ... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	2.45 ng	106148	Phenanthrene-d10	11.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	86
2		Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
3		Pentadecane	212	C15H32	000629-62-9	86
4		Eicosane	282	C20H42	000112-95-8	86
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



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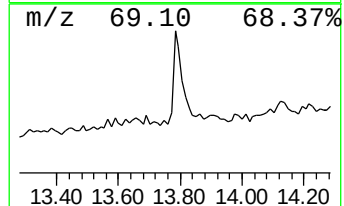
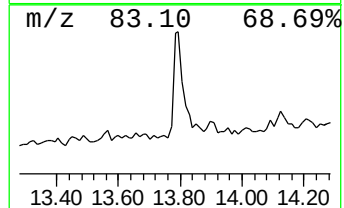
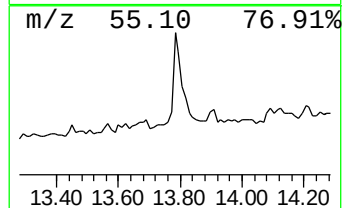
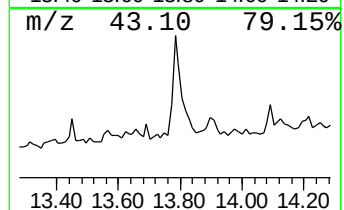
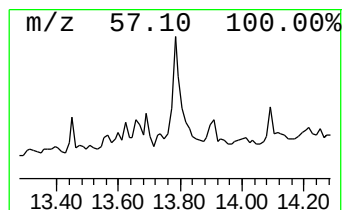
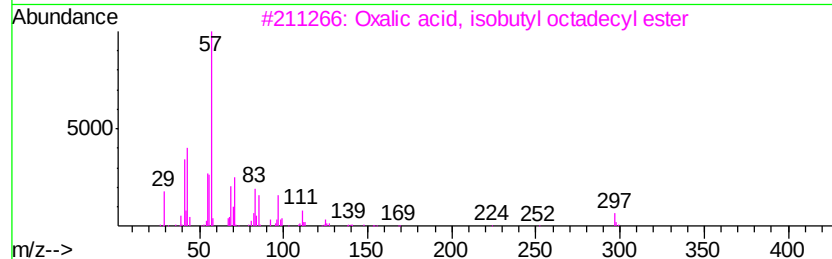
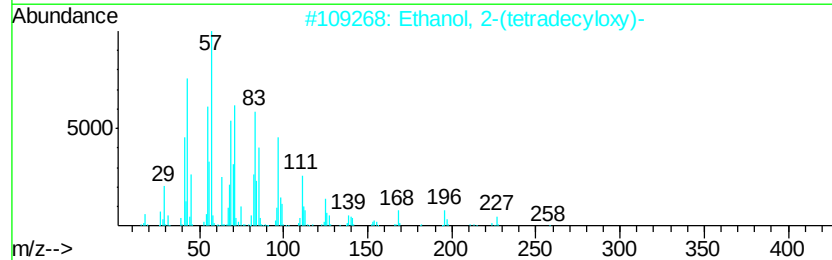
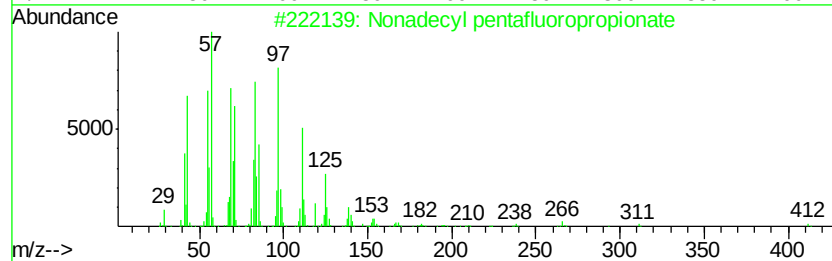
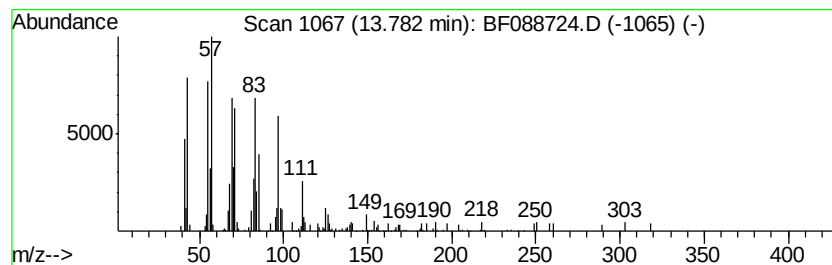
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Nonadecyl pentafluoropropio... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	3.46 ng	138541	Chrysene-d12	13.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3		Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
4		Triacetyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	74
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70



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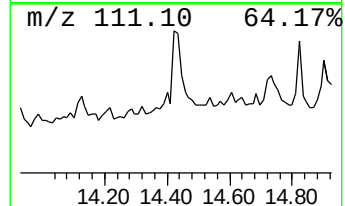
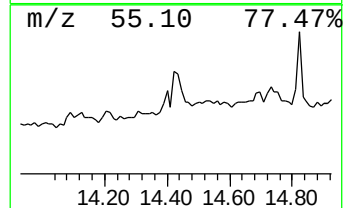
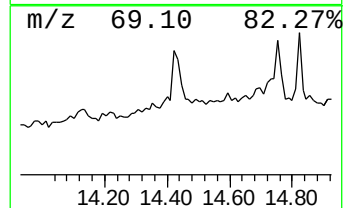
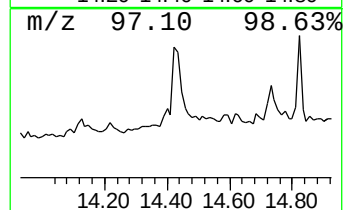
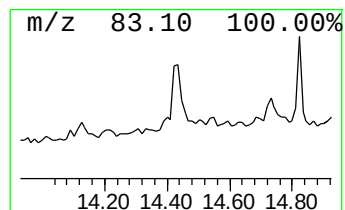
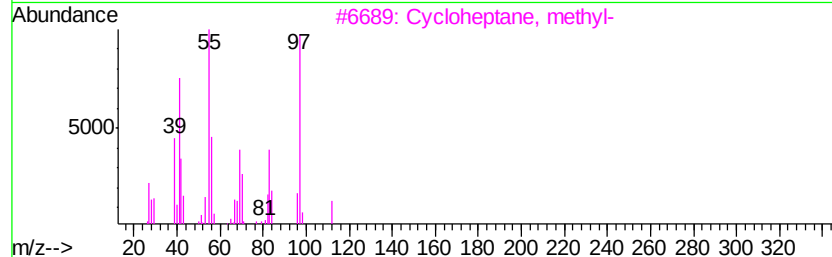
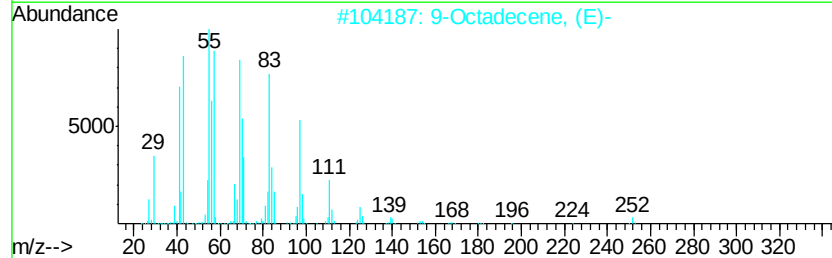
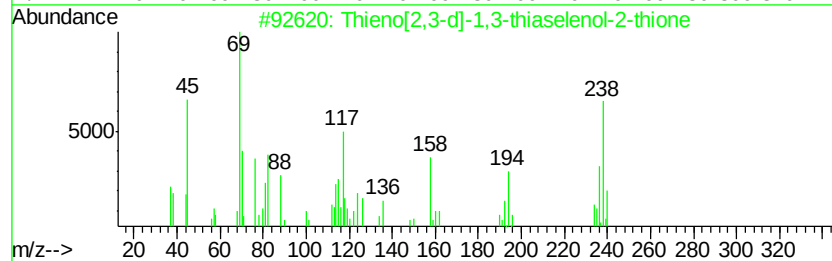
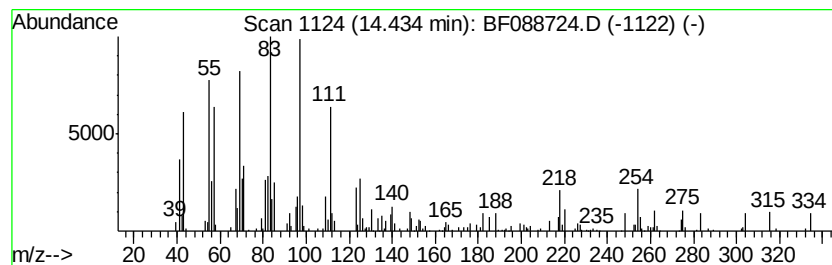
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Thieno[2,3-d]-1,3-thiaselen... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.01 ng	80702	Chrysene-d12	13.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	56
2		9-Octadecene, (E)-	252	C18H36	007206-25-9	53
3		Cycloheptane, methyl-	112	C8H16	004126-78-7	35
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	20
5		1-Heptacosanol	396	C27H56O	002004-39-9	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
Data File : BF088724.D
Acq On : 6 Jul 2016 1:34
Operator : UM/SJ
Sample : H3881-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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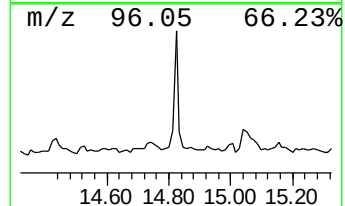
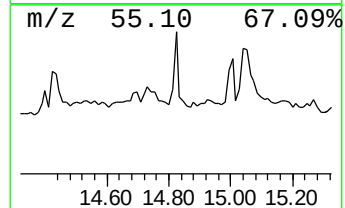
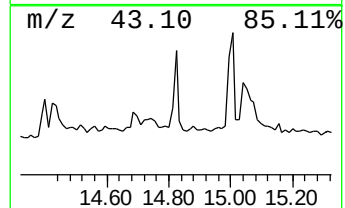
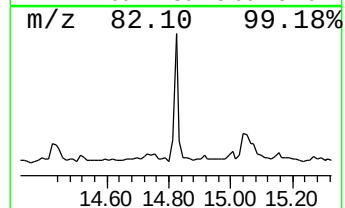
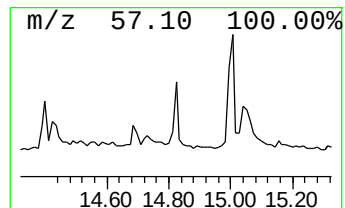
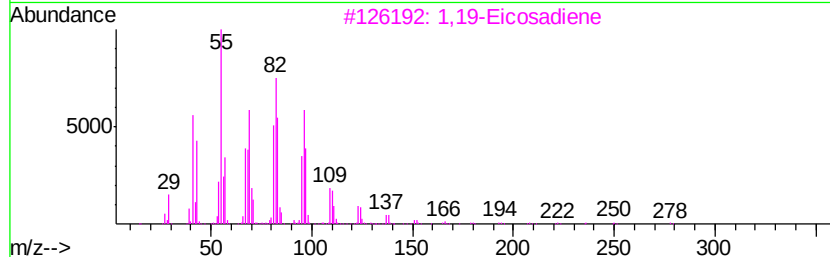
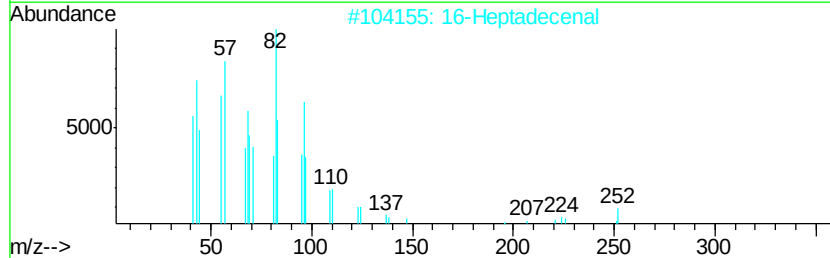
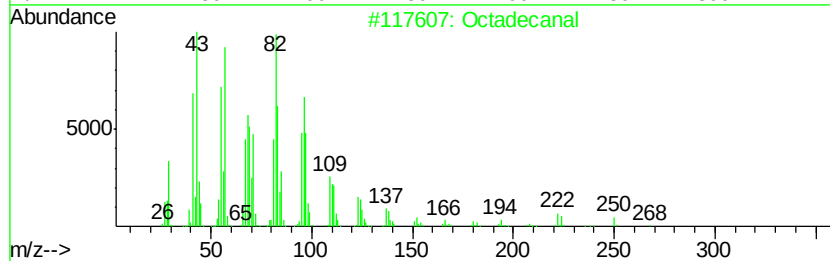
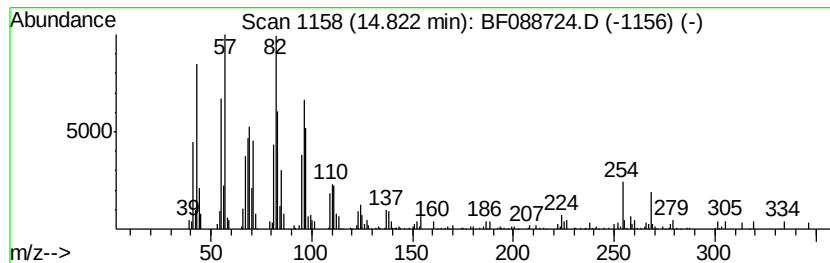
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	3.50 ng	99734	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	91
2		16-Heptadecenal	252	C17H32O	1000144-57-9	86
3		1,19-Eicosadiene	278	C20H38	014811-95-1	81
4		2-Heptadecenal	252	C17H32O	1000143-48-6	70
5		14-Heptadecenal	252	C17H32O	1000144-58-0	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
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Sample : H3881-07
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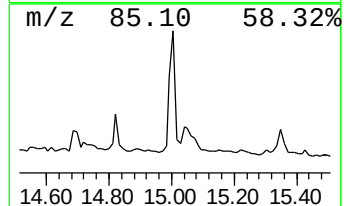
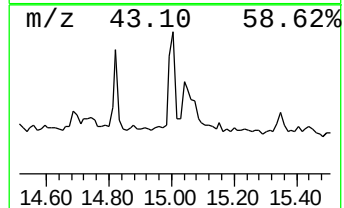
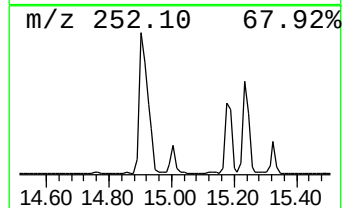
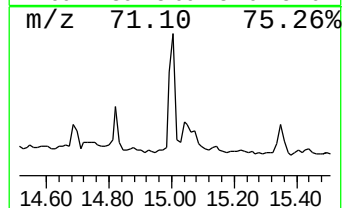
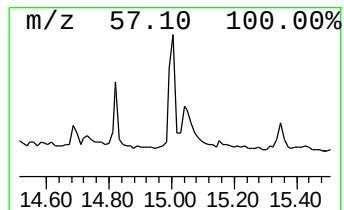
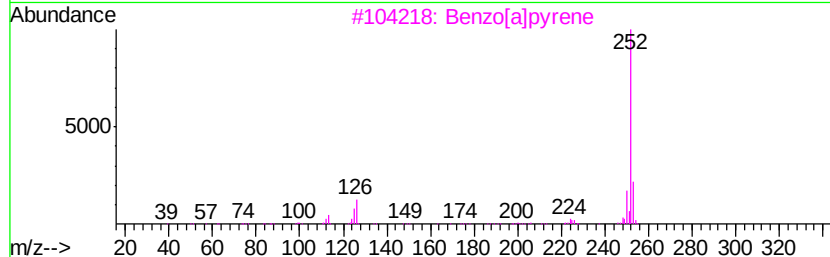
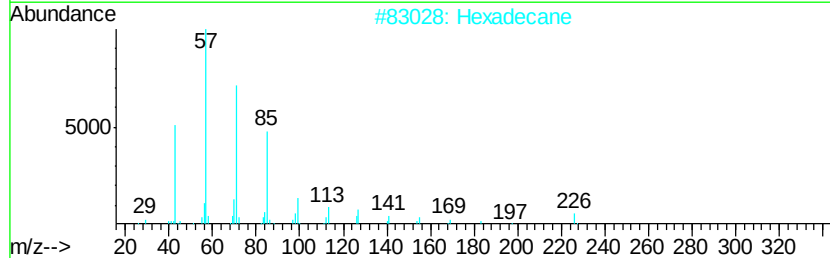
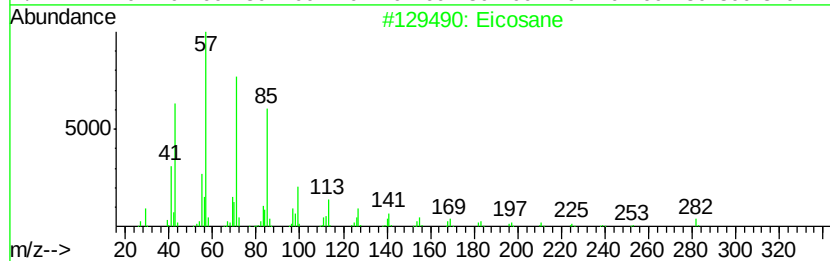
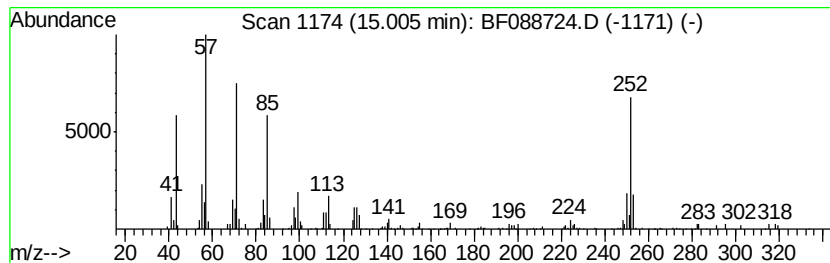
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.01	4.11 ng	117087	Perylene-d12	15.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Benzo[alpyrene	252	C20H12	000050-32-8	70
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
Data File : BF088724.D
Acq On : 6 Jul 2016 1:34
Operator : UM/SJ
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Misc :
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ClientSampleId :
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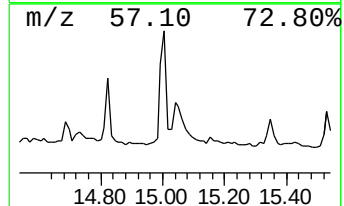
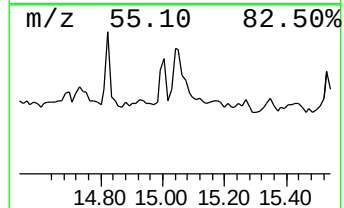
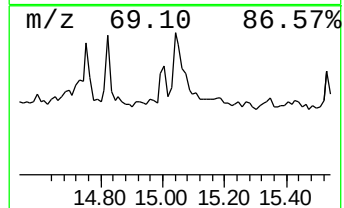
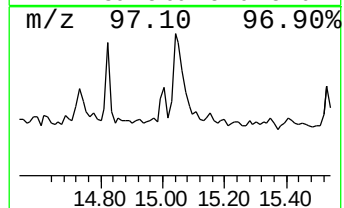
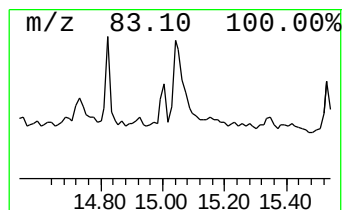
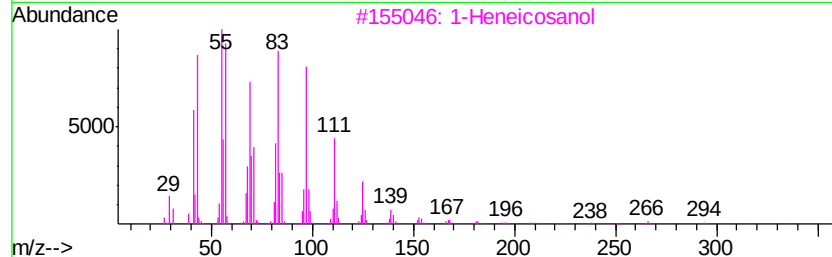
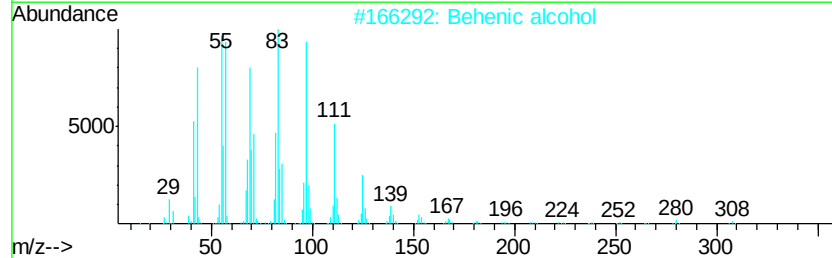
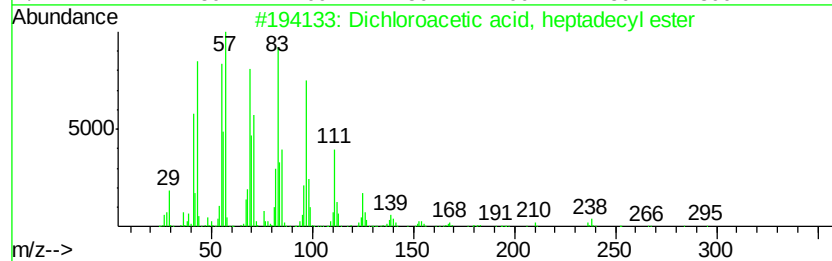
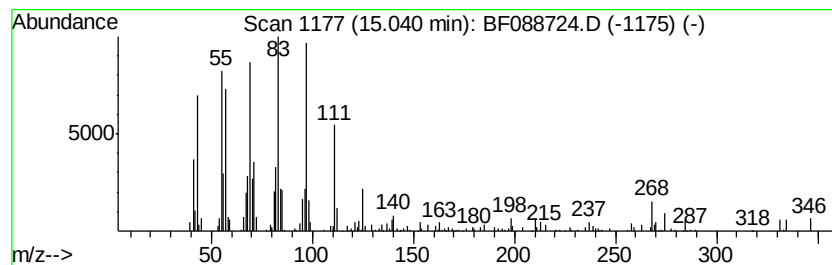
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	4.80 ng	136578	Perylene-d12	15.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	80
2			Behenic alcohol	326	C22H46O	000661-19-8	60
3			1-Heneicosanol	312	C21H44O	015594-90-8	46
4			3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	43
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	41



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070516\
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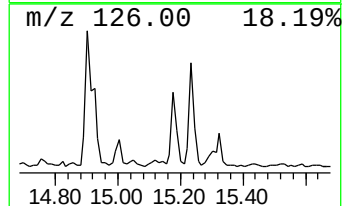
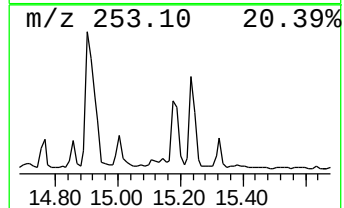
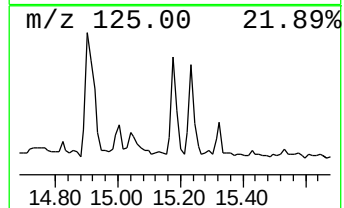
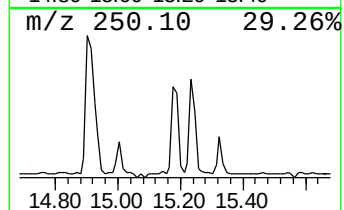
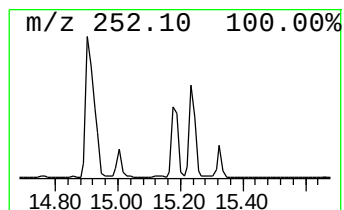
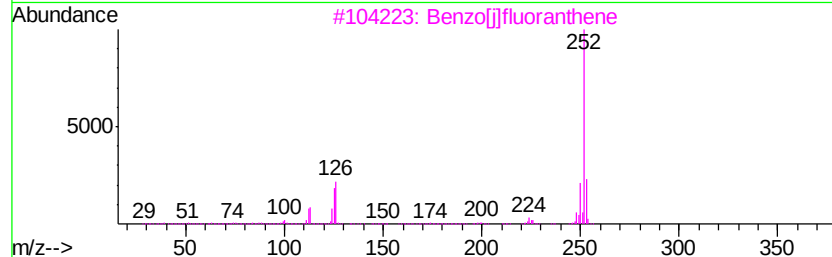
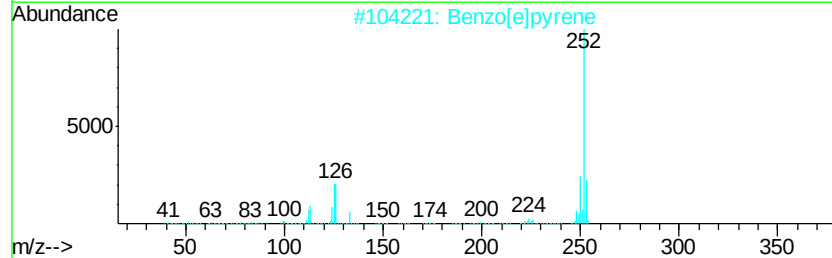
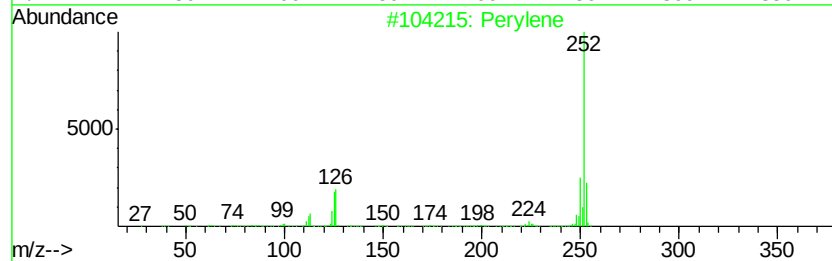
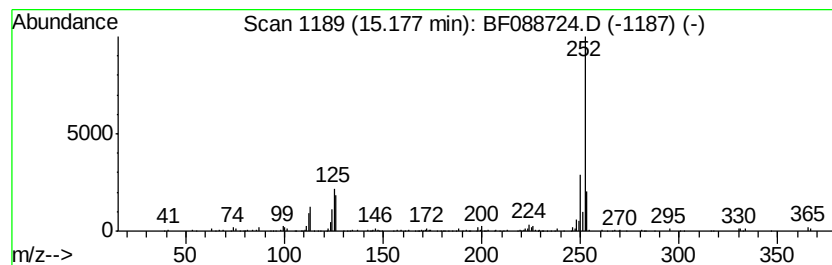
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	4.31 ng	122797	Perylene-d12	15.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene		252	C20H12	000198-55-0	94
2	Benzo[e]pyrene		252	C20H12	000192-97-2	94
3	Benzo[i]fluoranthene		252	C20H12	000205-82-3	94
4	Benzo[k]fluoranthene		252	C20H12	000207-08-9	93
5	Benzo[a]pyrene		252	C20H12	000050-32-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
Data File : BF088724.D
Acq On : 6 Jul 2016 1:34
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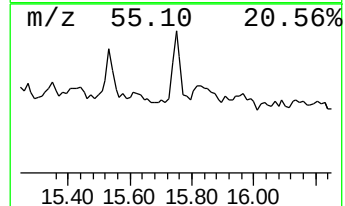
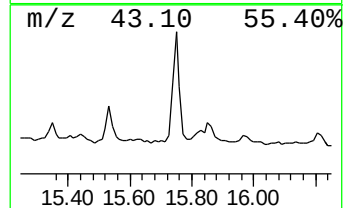
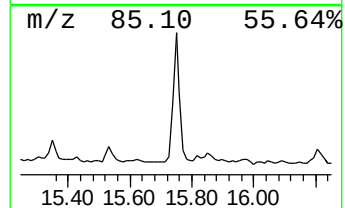
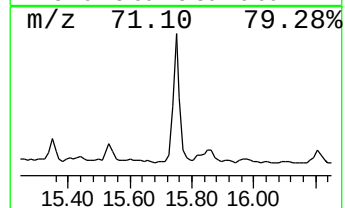
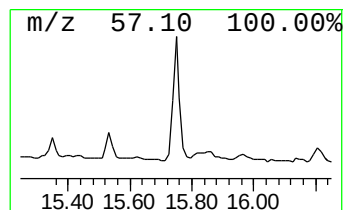
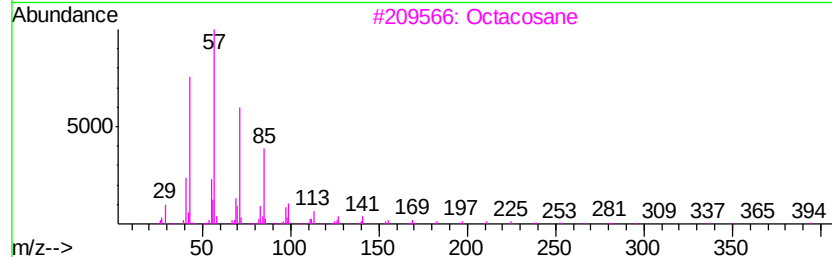
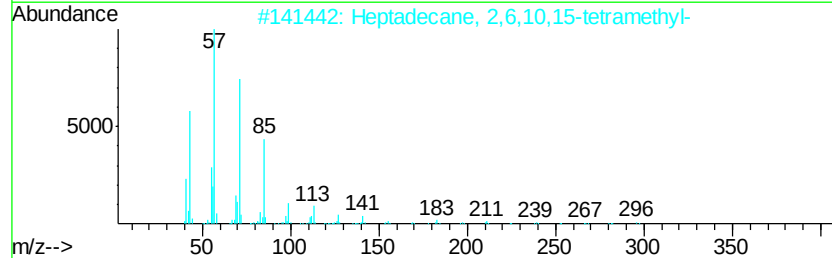
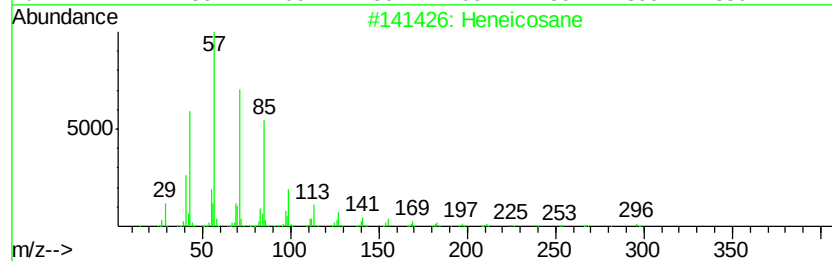
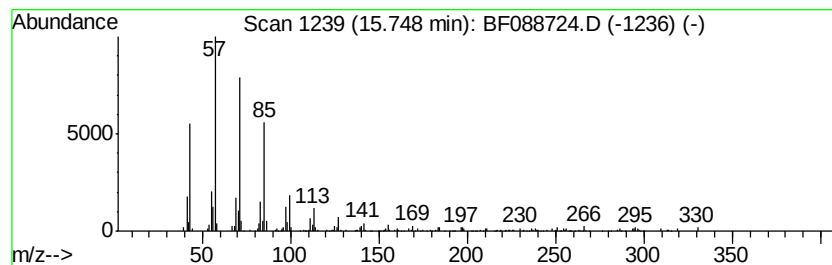
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	7.33 ng	208565	Perylene-d12	15.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	99
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3			Octacosane	394	C28H58	000630-02-4	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
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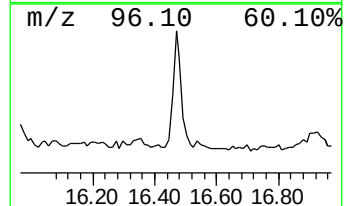
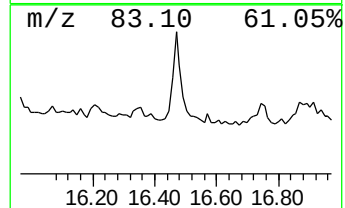
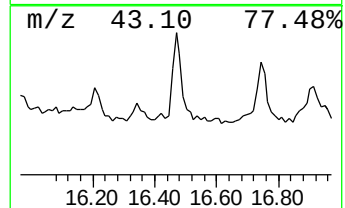
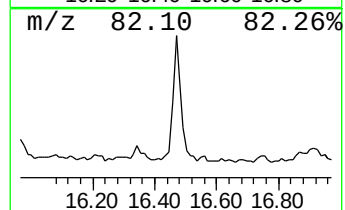
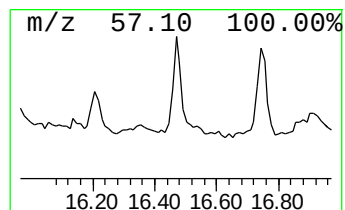
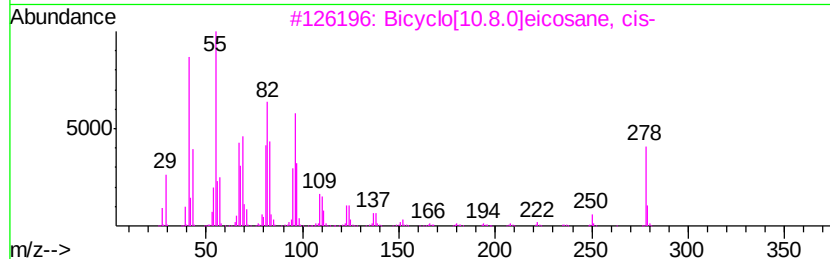
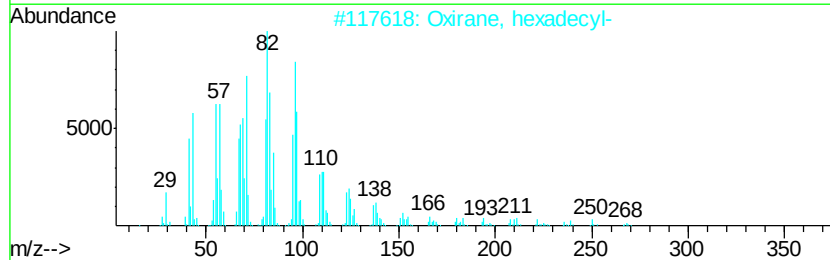
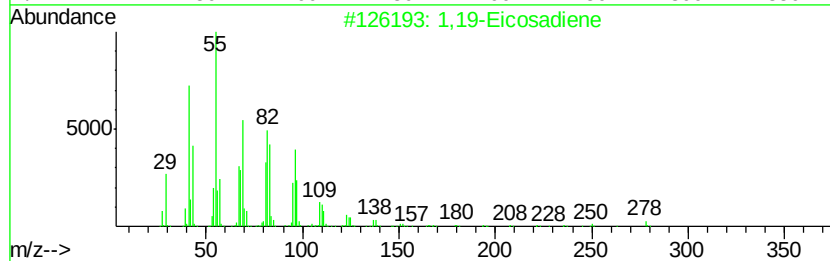
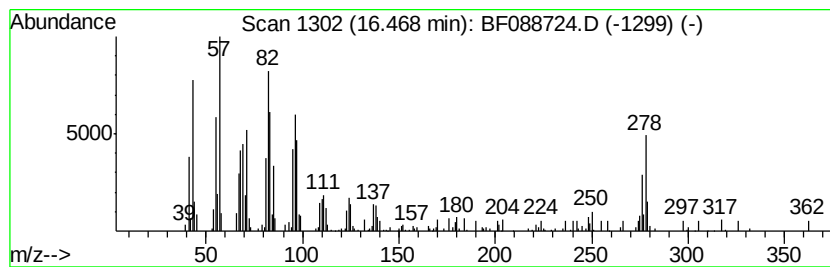
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 1,19-Eicosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.47	6.81 ng	193965	Perylene-d12	15.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	68
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	58
3	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	58
4	8-Octadecenal	266	C18H34O	056554-94-0	52
5	Octadecanal	268	C18H36O	000638-66-4	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
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Acq On : 6 Jul 2016 1:34
Operator : UM/SJ
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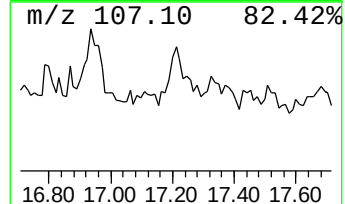
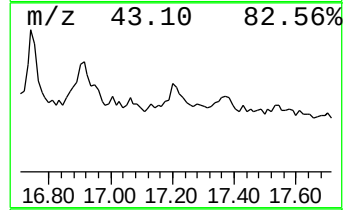
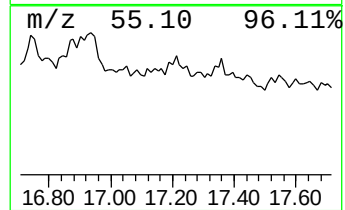
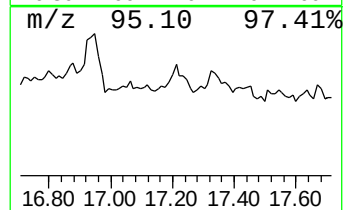
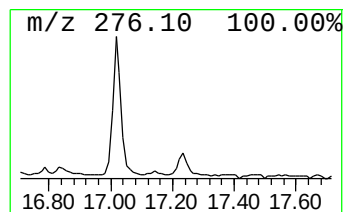
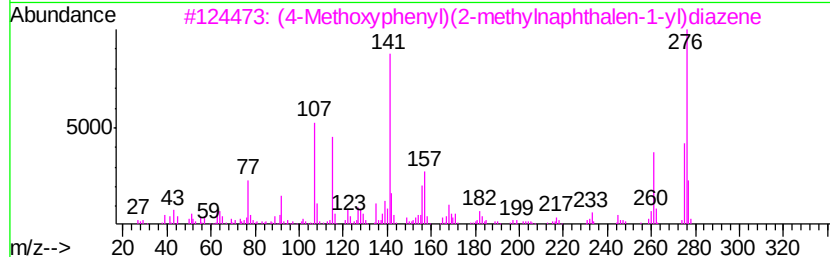
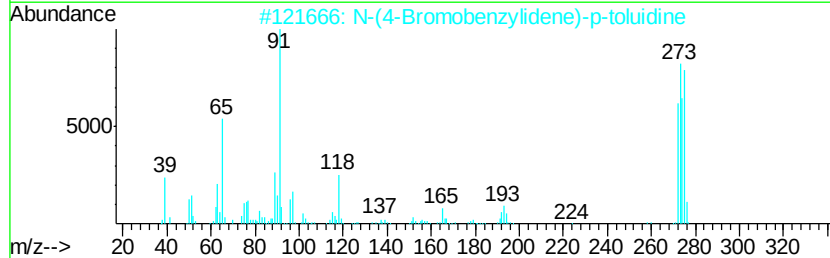
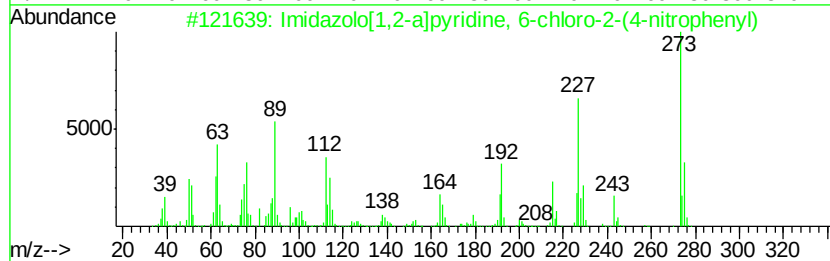
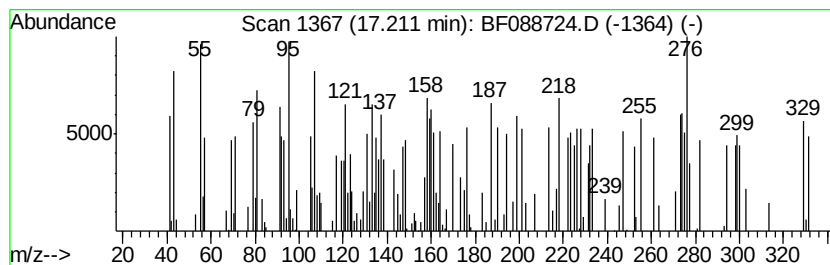
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown17.21 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	3.61 ng	102833	Perylene-d12	15.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Imidazo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	25
2			N-(4-Bromobenzylidene)-p-toluidine	273	C14H12BrN	039128-27-3	11
3			(4-Methoxyphenyl)(2-methylnaphth...	276	C18H16N2O	083733-40-8	11
4			Cyclopropanecarbonitrile, 2-[p-(...	276	C19H20N2	032589-51-8	10
5			Phenolphthalein	318	C20H14O4	000077-09-8	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070516\
 Data File : BF088724.D
 Acq On : 6 Jul 2016 1:34
 Operator : UM/SJ
 Sample : H3881-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 Q6-B1-0-6-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	4.1 ng		134715	1	6.78	662095	20.0
unknown6.54	6.54	54.9 ng		1816030	1	6.78	662095	20.0
Sulfurous acid, p...	11.16	2.5 ng		106148	4	11.28	865402	20.0
Nonadecyl pentafl...	13.78	3.5 ng		138541	5	13.91	801277	20.0
Thieno[2,3-d]-1,3...	14.43	2.0 ng		80702	5	13.91	801277	20.0
Octadecanal	14.82	3.5 ng		99734	6	15.30	569446	20.0
Eicosane	15.01	4.1 ng		117087	6	15.30	569446	20.0
Dichloroacetic ac...	15.04	4.8 ng		136578	6	15.30	569446	20.0
Perylene	15.18	4.3 ng		122797	6	15.30	569446	20.0
Heneicosane	15.75	7.3 ng		208565	6	15.30	569446	20.0
1,19-Eicosadiene	16.47	6.8 ng		193965	6	15.30	569446	20.0
unknown17.21	17.21	3.6 ng		102833	6	15.30	569446	20.0