

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
 Data File : BF091598.D
 Acq On : 14 Dec 2016 21:41
 Operator : UM/SJ
 Sample : H6006-12
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-7-0-5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.235	11	13	16	rVB2	67335	94809	1.31%	0.133%
2	4.956	248	251	254	rBV	1592672	2562884	35.52%	3.582%
3	5.390	286	289	292	rBV	4848689	6206932	86.03%	8.675%
4	6.441	377	381	383	rVB	4909154	7084847	98.20%	9.902%
5	6.567	389	392	394	rBV	5714180	6774163	93.90%	9.467%
6	6.796	409	412	414	rBV	1794140	1750002	24.26%	2.446%
7	6.944	423	425	428	rBV	3723783	4852095	67.25%	6.781%
8	7.356	458	461	464	rBV	3843051	3803819	52.72%	5.316%
9	8.076	522	524	527	rBV	2484639	2284056	31.66%	3.192%
10	9.162	616	619	621	rBV	7021788	7214537	100.00%	10.083%
11	9.276	628	629	632	rVB	89170	106260	1.47%	0.149%
12	9.550	651	653	656	rVB	871507	730214	10.12%	1.021%
13	9.836	675	678	679	rBV	2403855	2566593	35.58%	3.587%
14	10.248	711	714	715	rBV	97539	96611	1.34%	0.135%
15	10.625	744	747	749	rBV	3638404	4466460	61.91%	6.242%
16	10.750	756	758	762	rVB	88414	152798	2.12%	0.214%
17	11.196	792	797	802	rBV4	115426	276174	3.83%	0.386%
18	11.310	805	807	811	rVV2	2488092	3126408	43.33%	4.369%
19	11.390	811	814	815	rVB	130830	178706	2.48%	0.250%
20	11.505	819	824	825	rBV2	60291	111324	1.54%	0.156%
21	11.551	825	828	830	rVV3	522067	548590	7.60%	0.767%
22	11.619	832	834	835	rBV	159013	130945	1.82%	0.183%
23	11.813	849	851	852	rBV	187308	158308	2.19%	0.221%
24	11.848	852	854	856	rVV2	248143	348589	4.83%	0.487%
25	11.882	856	857	859	rVV	90252	102014	1.41%	0.143%
26	11.928	859	861	865	rVV3	169263	357233	4.95%	0.499%
27	12.019	868	869	874	rVV	76744	126411	1.75%	0.177%
28	12.111	874	877	881	rVB2	109269	196578	2.72%	0.275%
29	12.259	887	890	891	rBV2	62497	74202	1.03%	0.104%
30	12.362	897	899	901	rBV	536742	611637	8.48%	0.855%
31	12.442	905	906	911	rVB3	65390	96685	1.34%	0.135%
32	12.522	911	913	915	rBV	876916	820998	11.38%	1.147%
33	12.636	921	923	925	rBV2	43203	83699	1.16%	0.117%
34	12.751	930	933	934	rVV	668980	846298	11.73%	1.183%

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Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
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35	12.785	934	936	942	rVB3	182803	244324	3.39%	0.341%
36	12.899	944	946	949	rVV	5430742	5414860	75.05%	7.568%
37	12.968	949	952	956	rVB4	67634	111022	1.54%	0.155%
38	13.071	958	961	963	rVB	82944	180454	2.50%	0.252%
39	13.139	963	967	969	rBV	230004	268760	3.73%	0.376%
40	13.185	969	971	972	rBV	80719	103771	1.44%	0.145%
41	13.482	992	997	1000	rBV3	118714	204265	2.83%	0.285%
42	13.585	1003	1006	1010	rVB2	53409	99832	1.38%	0.140%
43	13.688	1013	1015	1017	rBV2	61107	89363	1.24%	0.125%
44	13.802	1022	1025	1029	rVB3	256641	324673	4.50%	0.454%
45	13.939	1034	1037	1043	rVB	1539378	2389007	33.11%	3.339%
46	14.328	1069	1071	1073	rBV	73368	83886	1.16%	0.117%
47	14.431	1076	1080	1081	rBV4	42658	99984	1.39%	0.140%
48	14.671	1099	1101	1109	rBV3	145918	304939	4.23%	0.426%
49	14.797	1110	1112	1117	rVB2	49306	77717	1.08%	0.109%
50	14.957	1123	1126	1131	rVB	182286	361236	5.01%	0.505%
51	15.242	1148	1151	1153	rVB	87207	134950	1.87%	0.189%
52	15.288	1153	1155	1158	rBV	113121	165612	2.30%	0.231%
53	15.357	1158	1161	1164	rBV	1420161	1678801	23.27%	2.346%
54	16.705	1276	1279	1284	rVB2	69617	145486	2.02%	0.203%
55	17.117	1312	1315	1323	rVB	51559	127366	1.77%	0.178%

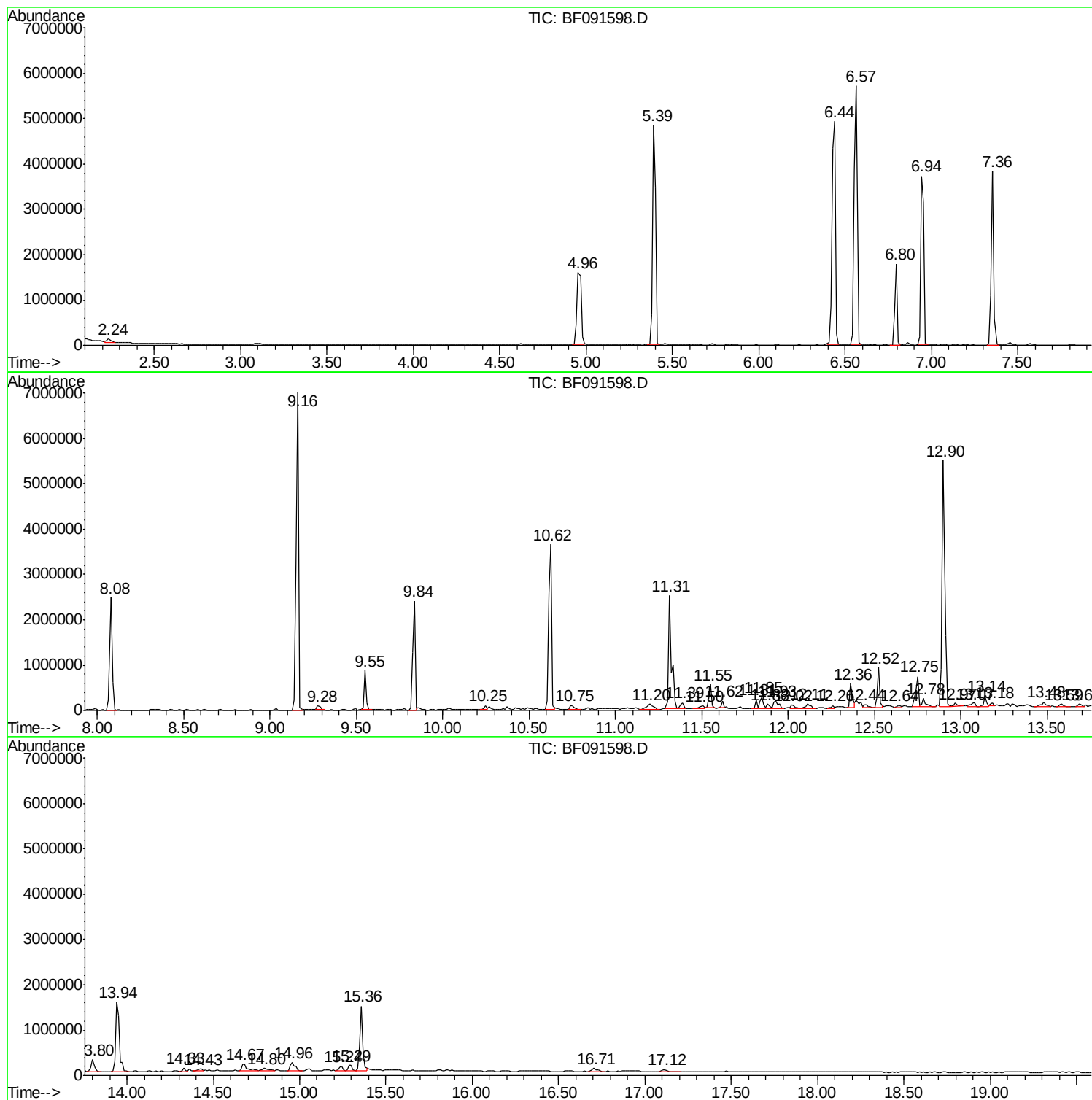
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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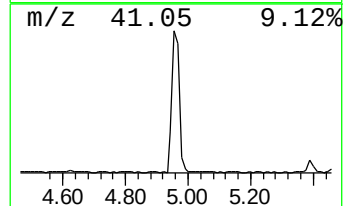
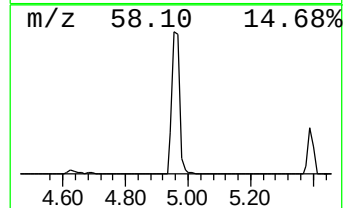
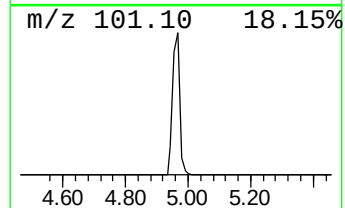
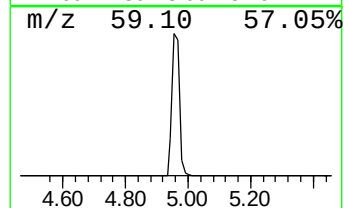
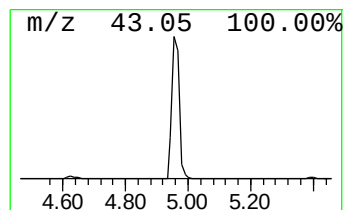
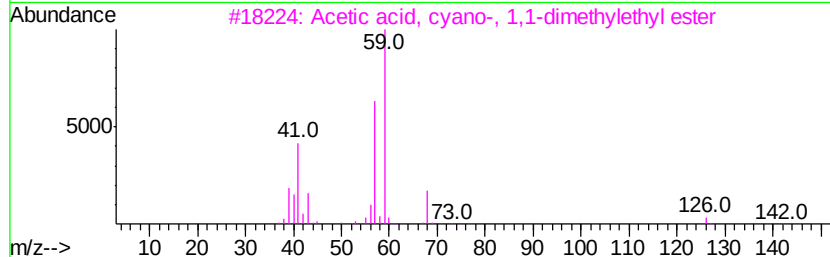
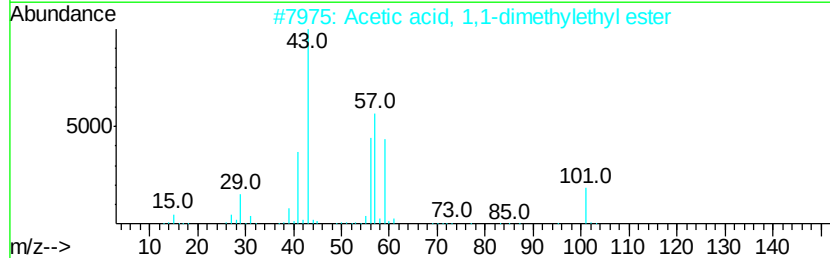
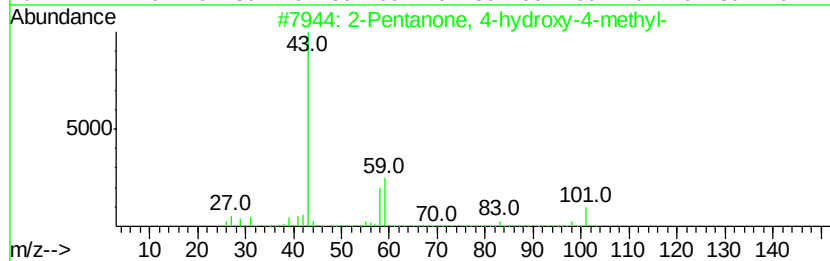
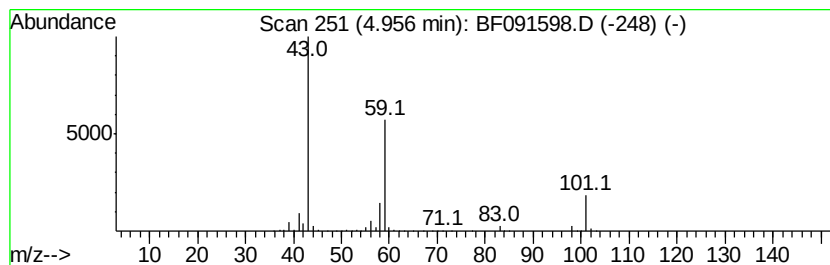
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	29.29 ng	2562880	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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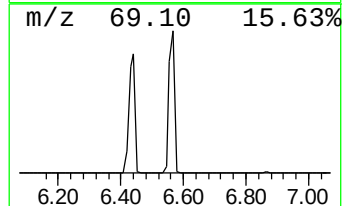
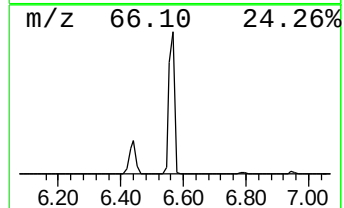
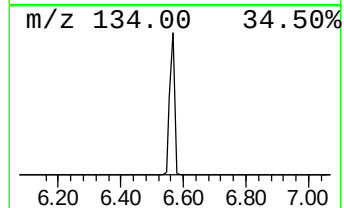
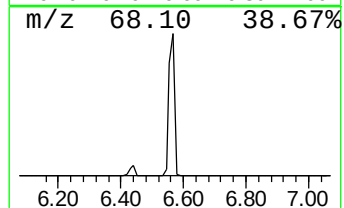
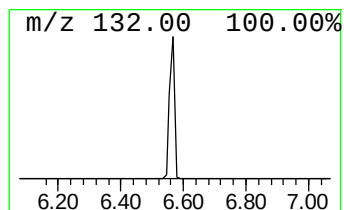
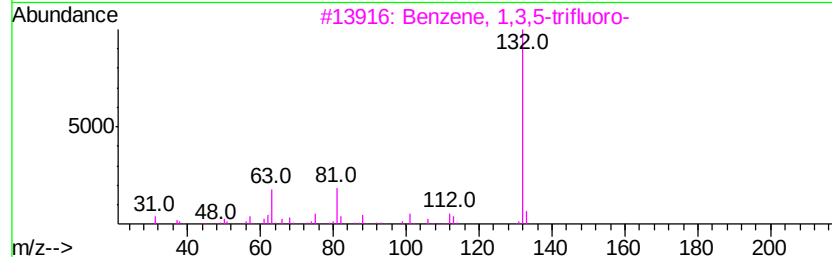
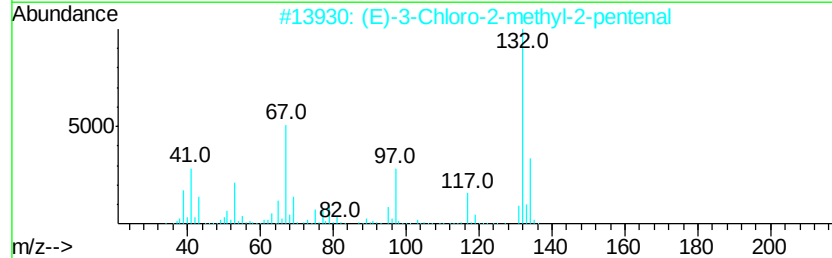
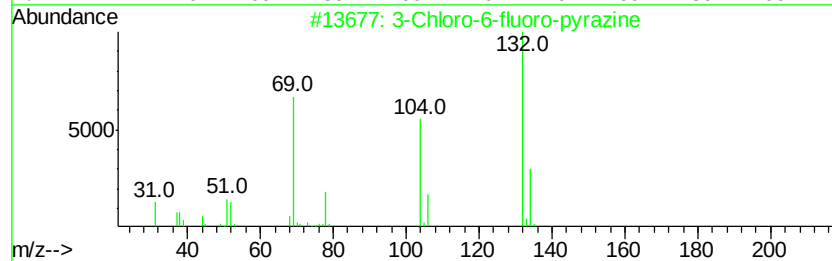
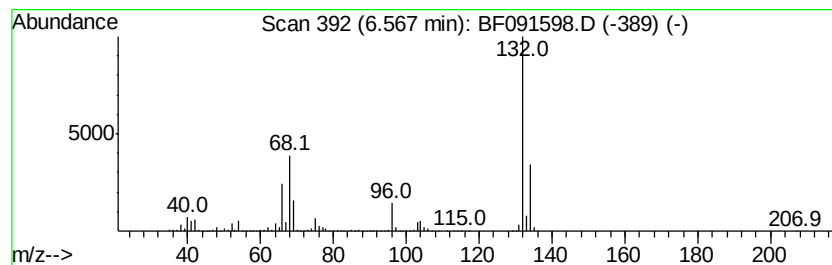
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	77.42 ng	6774160	1,4-Dichlorobenzene-d4	6.80

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		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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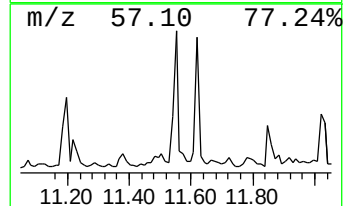
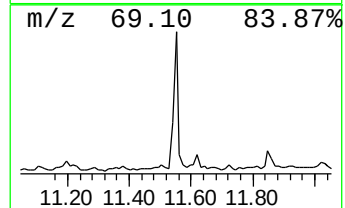
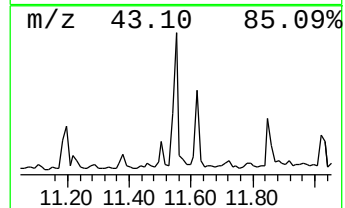
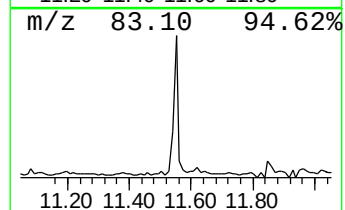
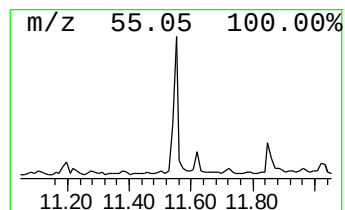
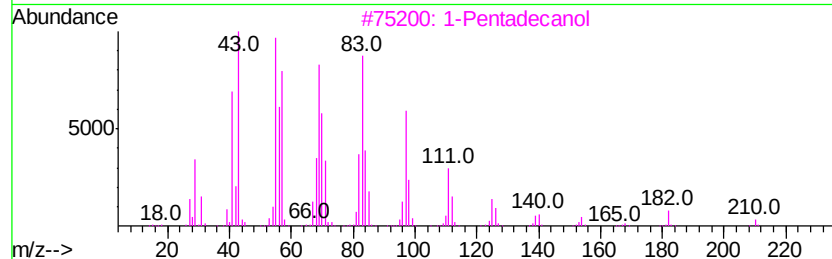
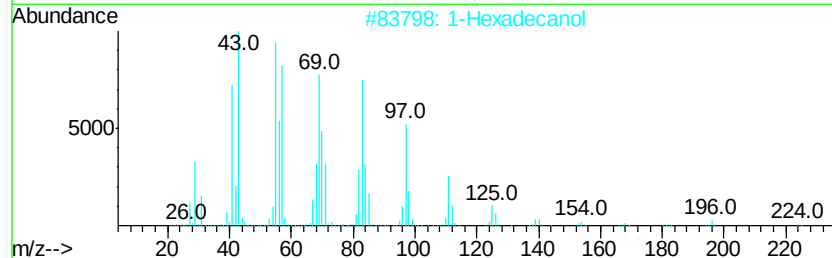
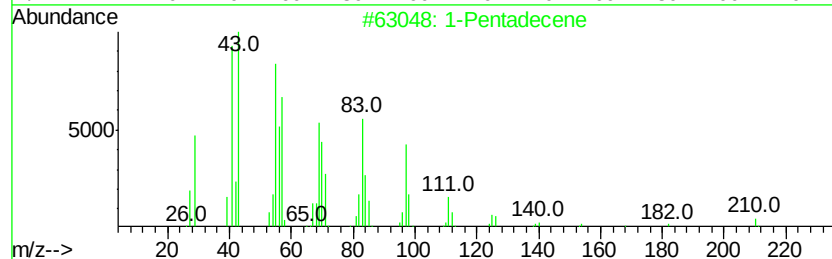
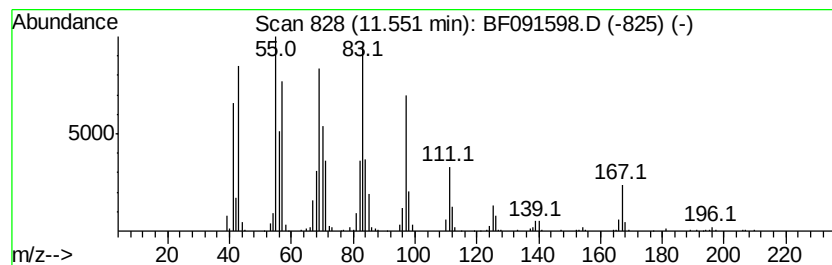
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Pentadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	3.51 ng	548590	Phenanthrene-d10	11.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene		210	C15H30	013360-61-7	95
2	1-Hexadecanol		242	C16H34O	036653-82-4	94
3	1-Pentadecanol		228	C15H32O	000629-76-5	94
4	1-Heptadecene		238	C17H34	006765-39-5	94
5	Cyclotetradecane		196	C14H28	000295-17-0	93



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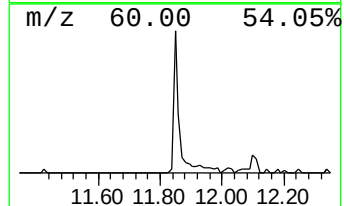
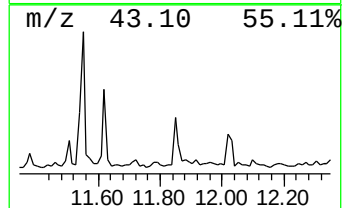
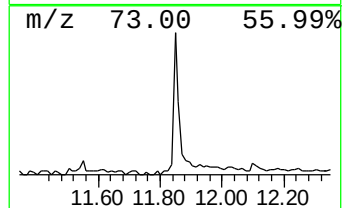
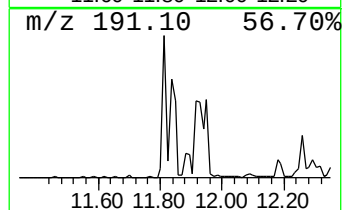
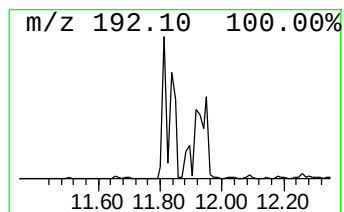
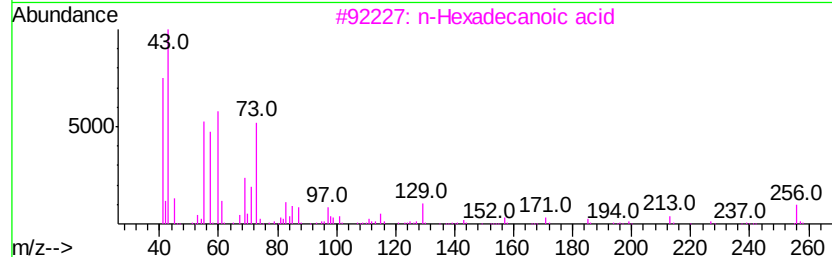
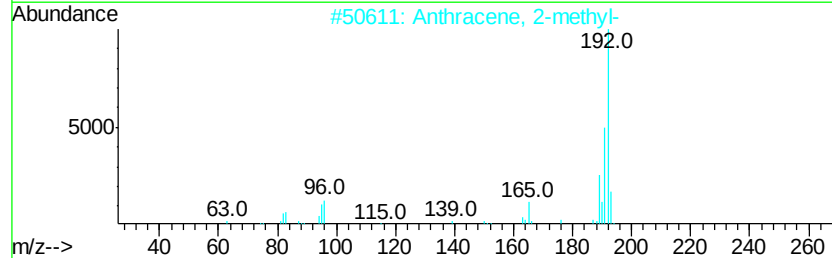
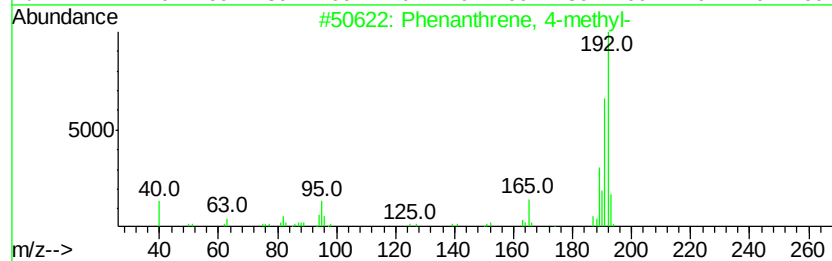
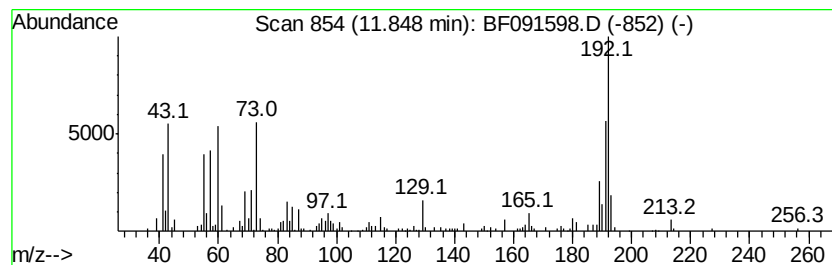
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Phenanthrene, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	2.23 ng	348589	Phenanthrene-d10	11.31	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	91
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	83
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	83



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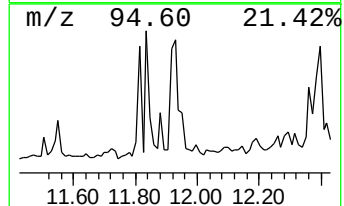
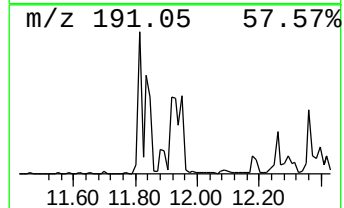
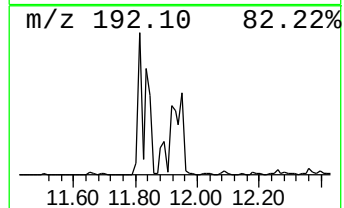
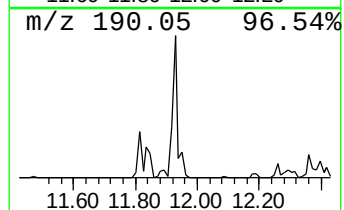
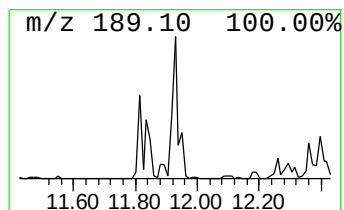
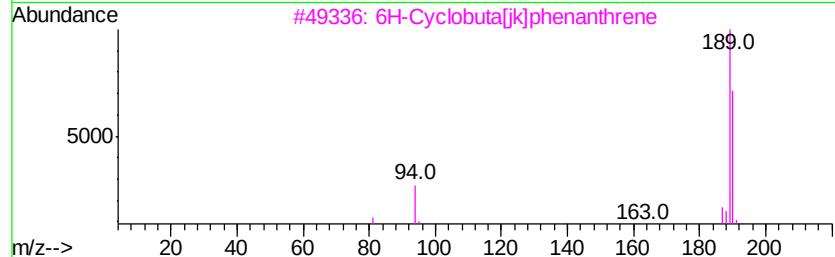
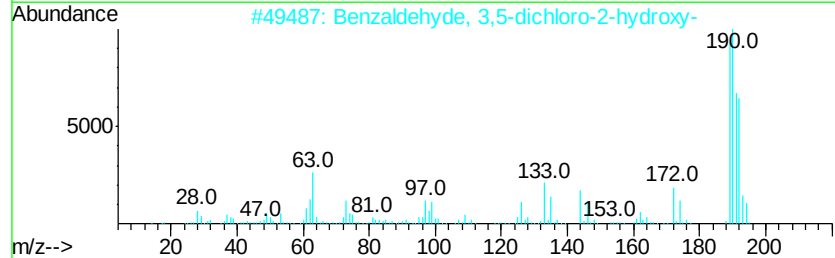
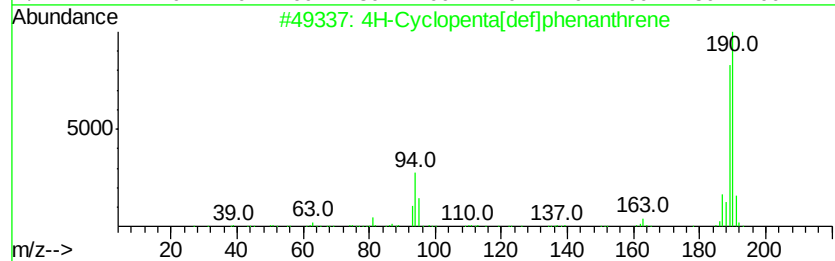
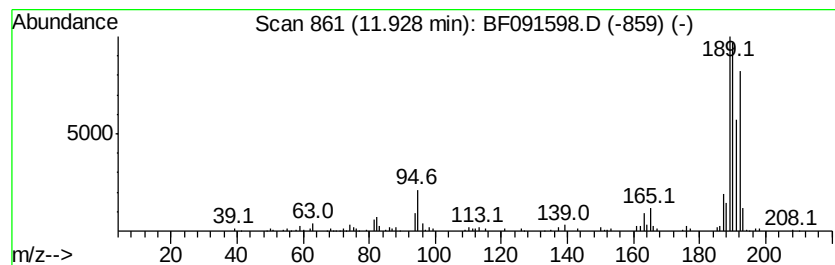
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ClientSampleId :
WC-7-0-5

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.93	2.29 ng	357233	Phenanthrene-d10	11.31	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	58
3	6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	49
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	35
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
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Acq On : 14 Dec 2016 21:41
Operator : UM/SJ
Sample : H6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

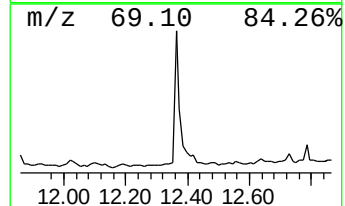
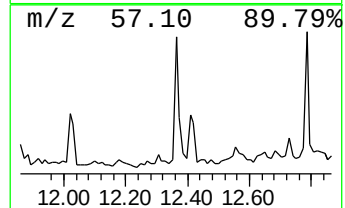
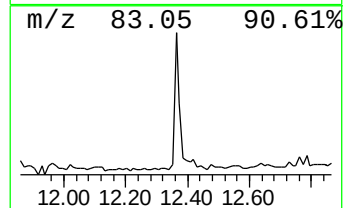
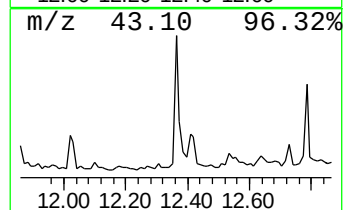
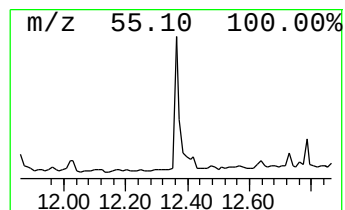
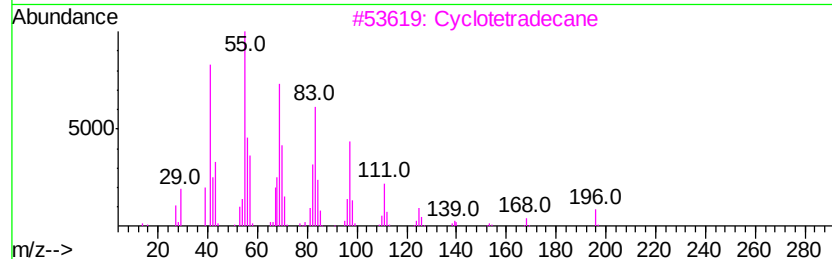
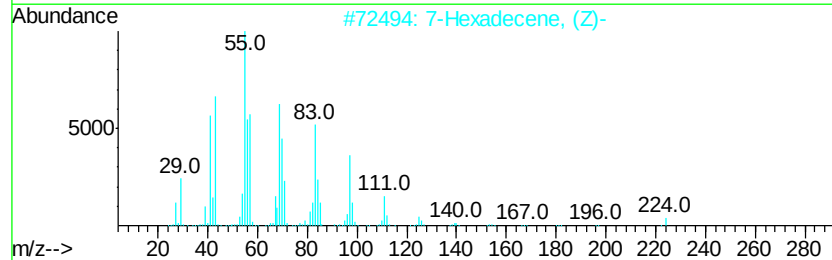
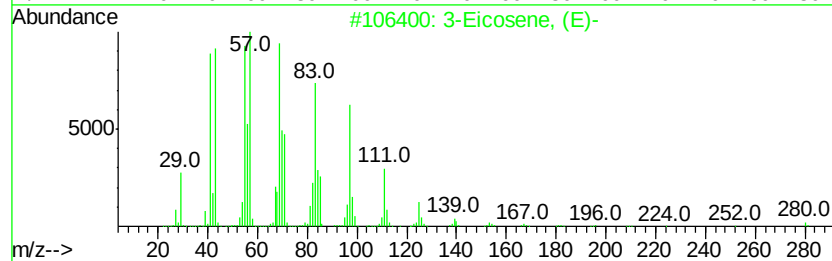
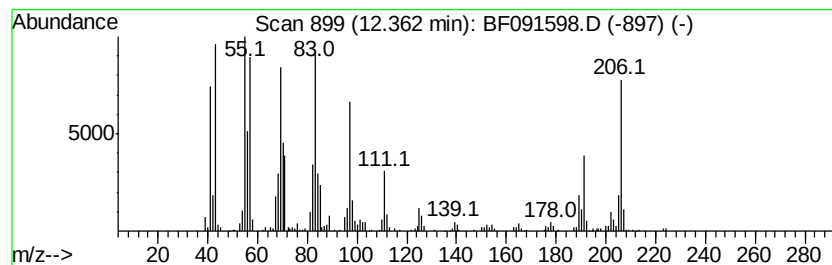
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
12.36	3.91 ng	611637	Phenanthrene-d10		11.31		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Eicosene, (E)-	280	C20H40	074685-33-9	93	
2	7	Hexadecene, (Z)-	224	C16H32	035507-09-6	91	
3		Cyclotetradecane	196	C14H28	000295-17-0	90	
4	5	Eicosene, (E)-	280	C20H40	074685-30-6	89	
5	1	Hexadecanol	242	C16H34O	036653-82-4	86	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
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Sample : H6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

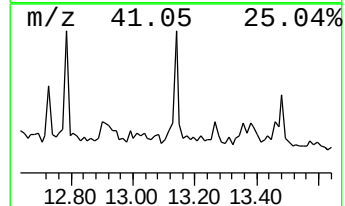
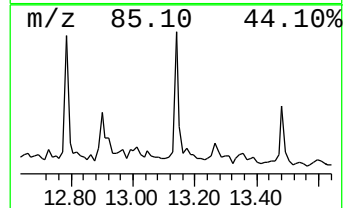
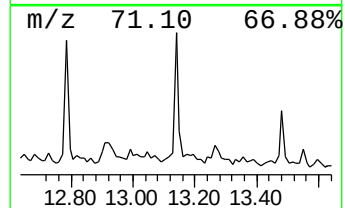
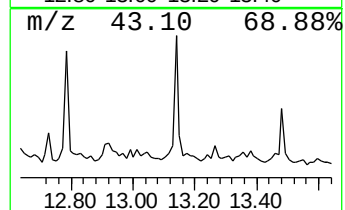
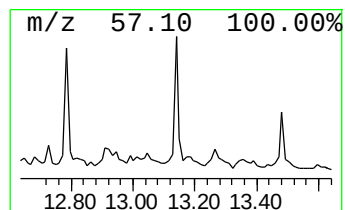
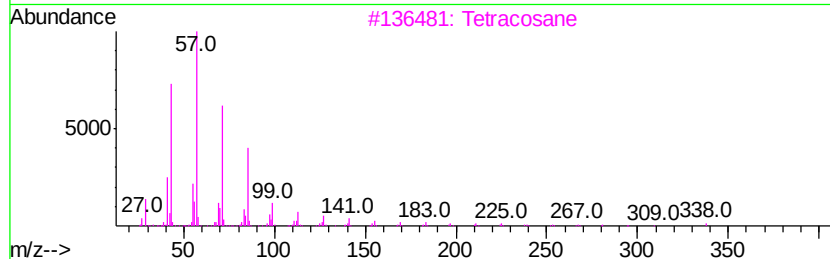
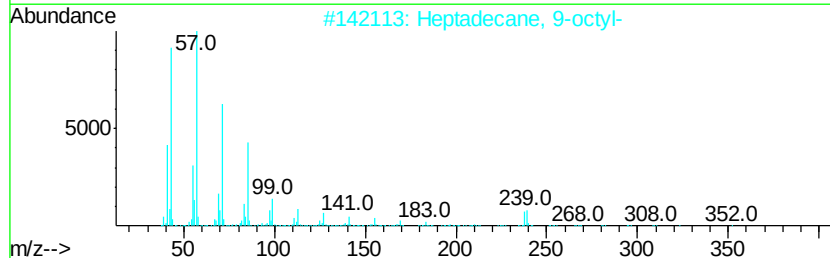
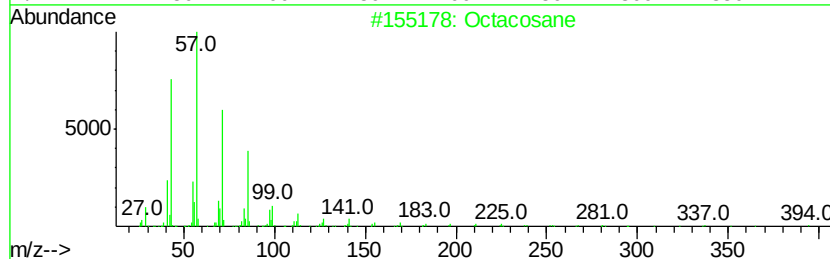
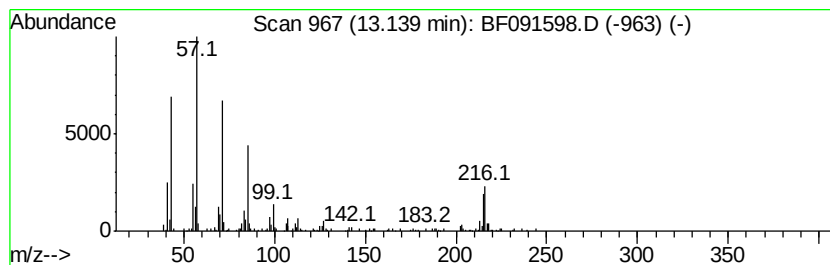
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	2.25 ng	268760	Chrysene-d12	13.95
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394 C28H58	000630-02-4	62
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	62
3	Tetracosane	338 C24H50	000646-31-1	62
4	Heptacosane	380 C27H56	000593-49-7	62
5	Eicosane	282 C20H42	000112-95-8	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
Data File : BF091598.D
Acq On : 14 Dec 2016 21:41
Operator : UM/SJ
Sample : H6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

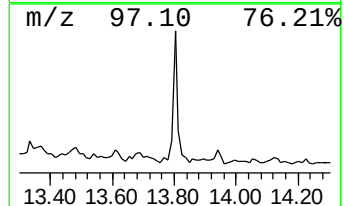
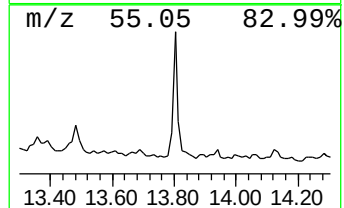
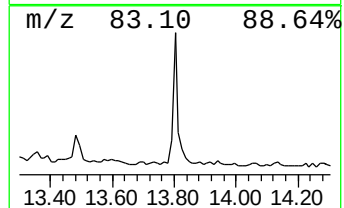
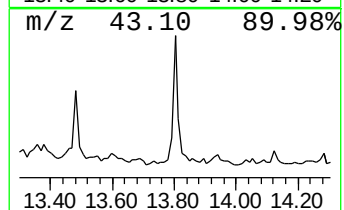
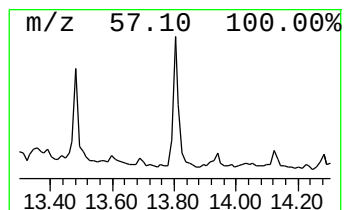
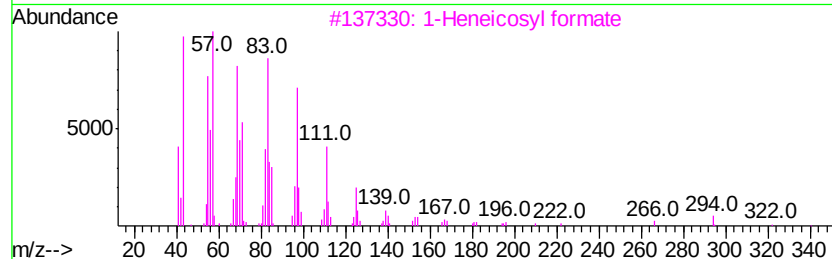
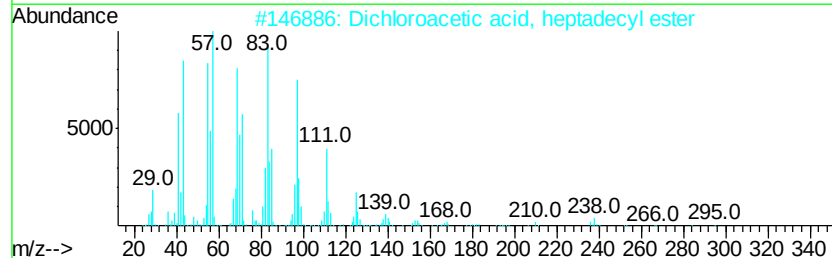
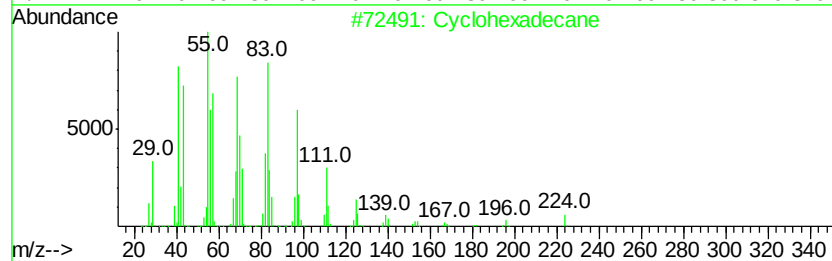
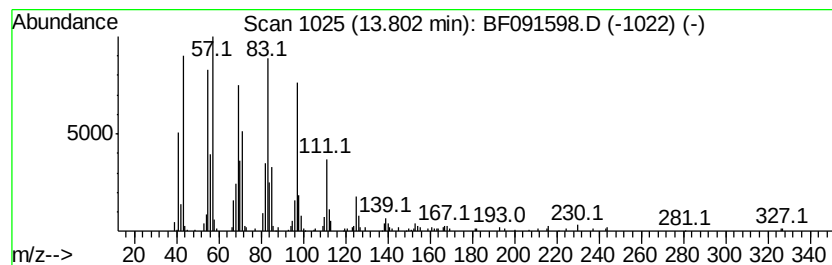
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.80	2.72 ng	324673	Chrysene-d12	13.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
Data File : BF091598.D
Acq On : 14 Dec 2016 21:41
Operator : UM/SJ
Sample : H6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

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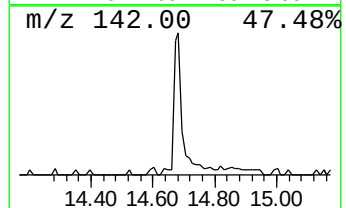
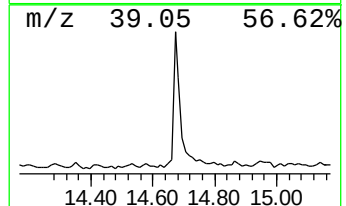
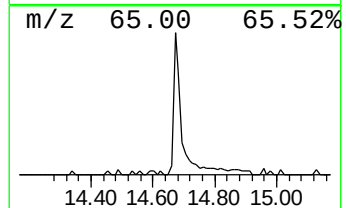
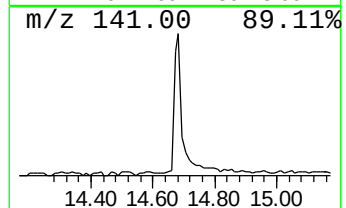
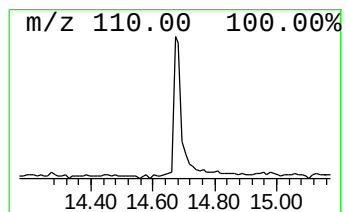
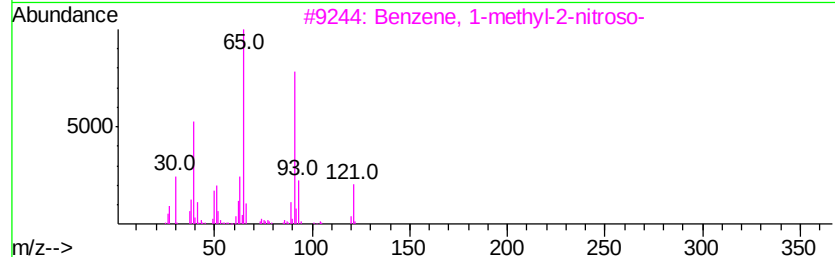
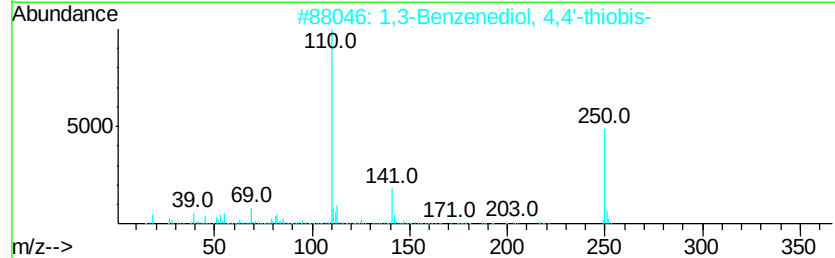
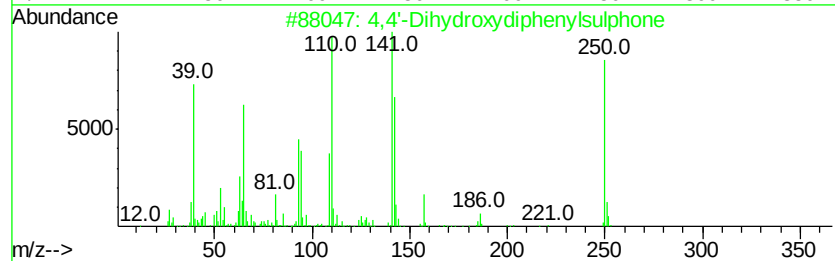
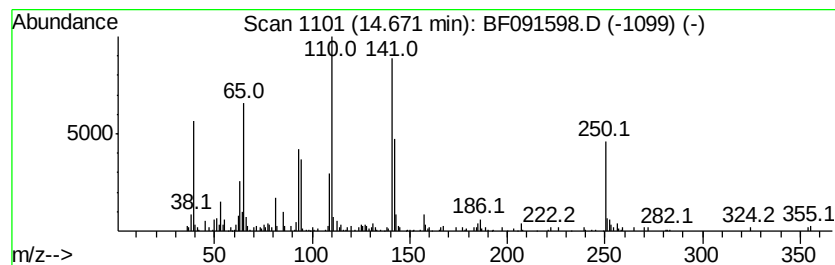
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.67 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	3.63 ng	304939	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	38
2		1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	38
3		Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	12
4		Phenoxyacetone nitrile	133	C8H7NO	003598-14-9	12
5		Benzene, 1-nitro-2-(p-methylphen...	247	C13H10FN03	028987-57-7	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
Data File : BF091598.D
Acq On : 14 Dec 2016 21:41
Operator : UM/SJ
Sample : H6006-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-7-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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...	4.96	29.3	ng	2562880	1	6.80	1750000	20.0
unknown6.57	6.57	77.4	ng	6774160	1	6.80	1750000	20.0
1-Pentadecene	11.55	3.5	ng	548590	4	11.31	3126410	20.0
Phenanthrene, 4-m...	11.85	2.2	ng	348589	4	11.31	3126410	20.0
4H-Cyclopenta[def...	11.93	2.3	ng	357233	4	11.31	3126410	20.0
3-Eicosene, (E)-	12.36	3.9	ng	611637	4	11.31	3126410	20.0
Octacosane	13.14	2.3	ng	268760	5	13.95	2389010	20.0
Cyclohexadecane	13.80	2.7	ng	324673	5	13.95	2389010	20.0
unknown14.67	14.67	3.6	ng	304939	6	15.36	1678800	20.0