

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
 Data File : BF095280.D
 Acq On : 20 May 2017 00:19
 Operator : SJ/MA
 Sample : I3177-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FLOOR-A

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-BF050217.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	5.137	540	544	563	rBV	159660	415206	12.43%	1.474%
2	5.731	641	645	677	rBV	1303550	2718466	81.38%	9.648%
3	7.307	908	913	929	rBV	1674659	2575459	77.10%	9.140%
4	7.431	929	934	943	rVB	1967441	2989952	89.51%	10.611%
5	7.766	987	991	1003	rBV	443051	544981	16.32%	1.934%
6	8.001	1026	1031	1052	rBV	1801538	2215958	66.34%	7.864%
7	8.666	1139	1144	1173	rBV	1094987	1728583	51.75%	6.135%
8	9.783	1330	1334	1354	rBV	449653	785038	23.50%	2.786%
9	11.554	1629	1635	1650	rBV	2356473	3340281	100.00%	11.855%
10	12.248	1749	1753	1767	rBV	275533	461023	13.80%	1.636%
11	12.613	1810	1815	1827	rBV2	617889	927739	27.77%	3.293%
12	13.448	1953	1957	1961	rBV	43678	50781	1.52%	0.180%
13	13.907	2030	2035	2047	rBV	1216808	2003039	59.97%	7.109%
14	14.218	2085	2088	2091	rBV2	35673	45563	1.36%	0.162%
15	14.424	2117	2123	2128	rBV9	17761	36562	1.09%	0.130%
16	14.642	2155	2160	2164	rBV5	31616	47552	1.42%	0.169%
17	14.824	2187	2191	2195	rBV4	24463	41813	1.25%	0.148%
18	15.012	2219	2223	2228	rBV2	548423	790010	23.65%	2.804%
19	15.054	2228	2230	2237	rVB	114081	174161	5.21%	0.618%
20	15.154	2243	2247	2255	rVB	40732	69662	2.09%	0.247%
21	15.807	2353	2358	2361	rBV	52832	73689	2.21%	0.262%
22	15.848	2361	2365	2371	rVB	76867	113432	3.40%	0.403%
23	15.912	2373	2376	2380	rVV2	48241	67034	2.01%	0.238%
24	15.971	2380	2386	2396	rVB3	107353	328560	9.84%	1.166%
25	16.595	2489	2492	2496	rBV	71638	88870	2.66%	0.315%
26	16.801	2523	2527	2532	rBV	192016	261963	7.84%	0.930%
27	16.936	2548	2550	2557	rVB	39648	60860	1.82%	0.216%
28	17.101	2574	2578	2584	rVB	213099	261528	7.83%	0.928%
29	17.336	2613	2618	2627	rVV	2319539	2809519	84.11%	9.971%
30	17.542	2648	2653	2654	rBV3	36748	57695	1.73%	0.205%
31	17.565	2654	2657	2661	rVB2	85109	104005	3.11%	0.369%
32	17.653	2668	2672	2676	rVB2	82416	101534	3.04%	0.360%
33	17.701	2676	2680	2685	rBV3	78688	129683	3.88%	0.460%
34	17.865	2704	2708	2711	rBV3	20386	37467	1.12%	0.133%

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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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.206	2762	2766	2769	rBV5	23378	40780	1.22%	0.145%
36	18.577	2824	2829	2840	rBV4	67877	170754	5.11%	0.606%
37	18.689	2842	2848	2852	rBV2	463200	691567	20.70%	2.454%
38	19.200	2932	2935	2939	rVB	37105	48746	1.46%	0.173%
39	19.359	2957	2962	2967	rBV8	21982	51305	1.54%	0.182%
40	19.965	3062	3065	3068	rBV	51983	64001	1.92%	0.227%
41	20.083	3081	3085	3092	rBV5	22562	44427	1.33%	0.158%
42	20.312	3122	3124	3129	rVB	47359	51940	1.55%	0.184%
43	20.365	3129	3133	3142	rBV	333286	476191	14.26%	1.690%
44	23.847	3719	3725	3735	rVB10	29455	79696	2.39%	0.283%

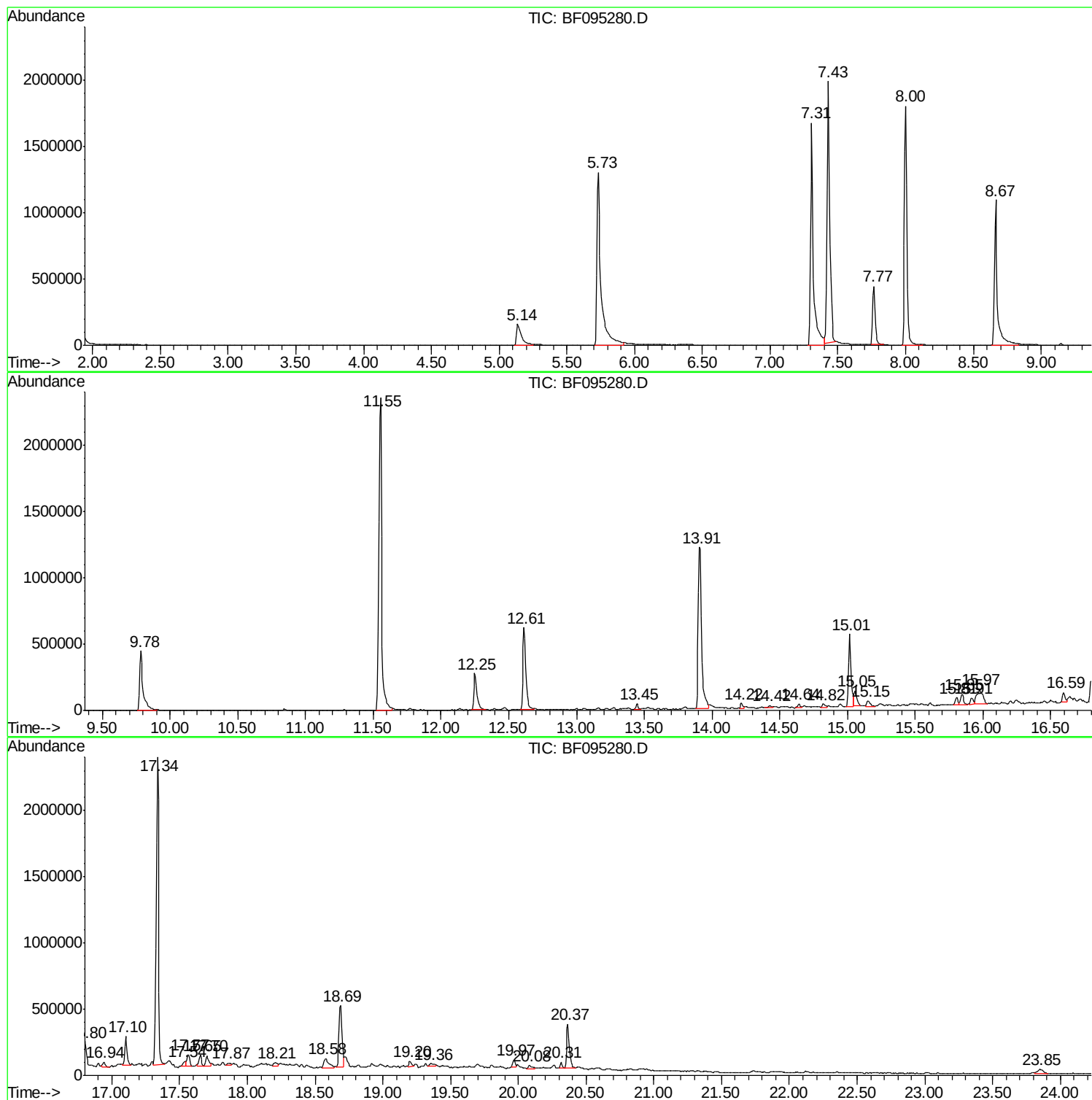
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : SJ/MA
Sample : I3177-04
Misc :
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Instrument :
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ClientSampleId :
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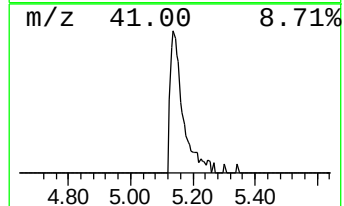
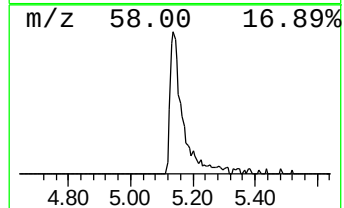
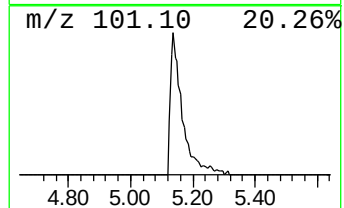
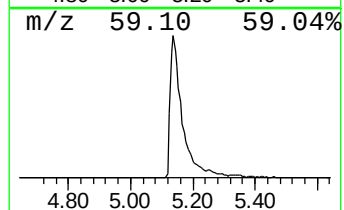
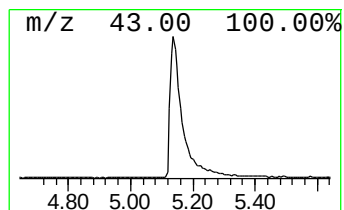
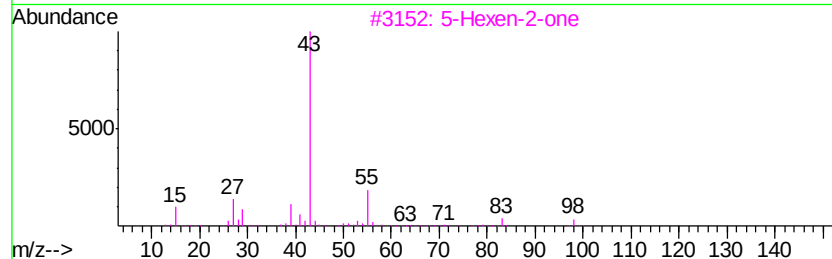
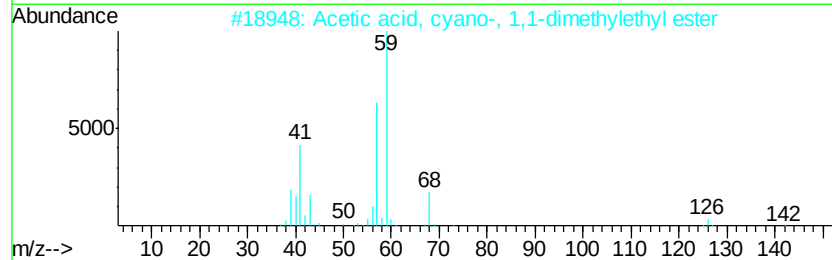
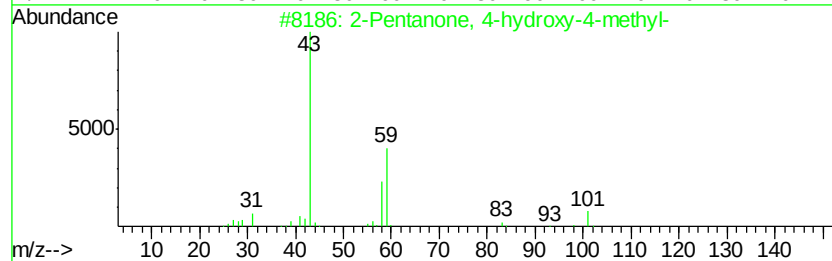
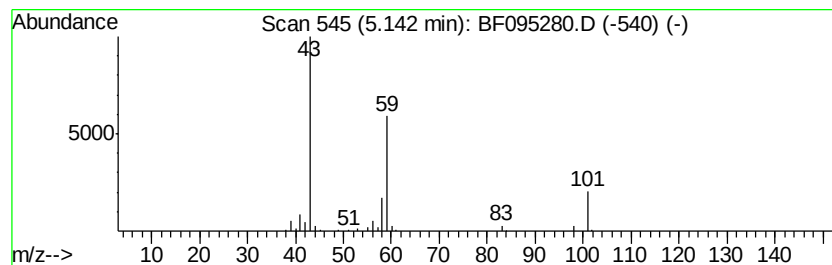
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	15.24 ng	415206	1,4-Dichlorobenzene-d4	7.77

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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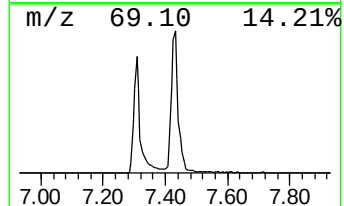
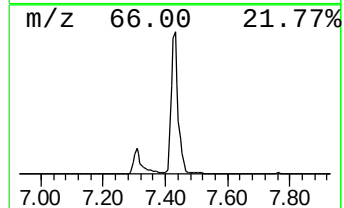
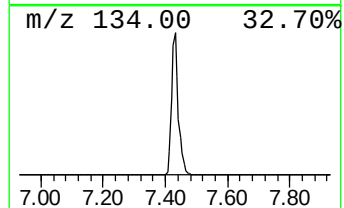
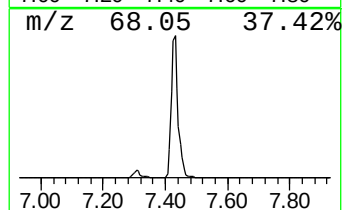
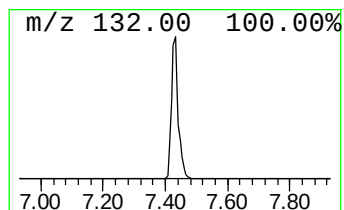
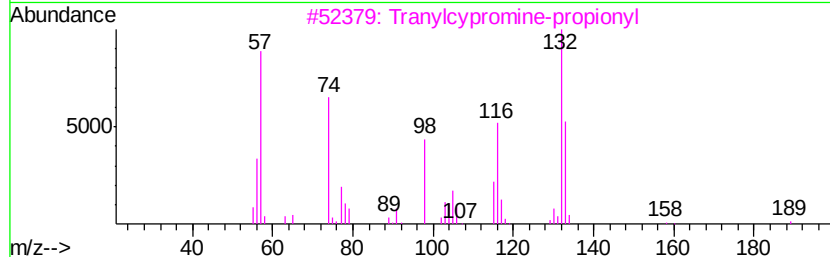
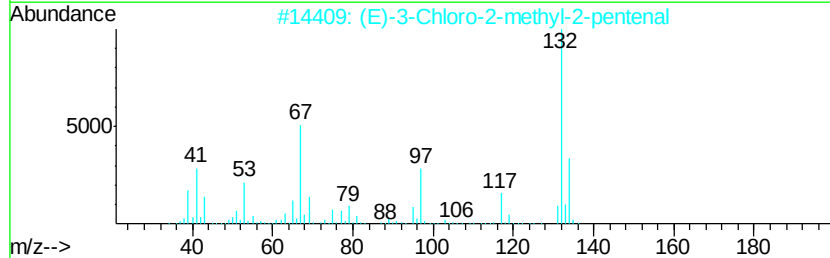
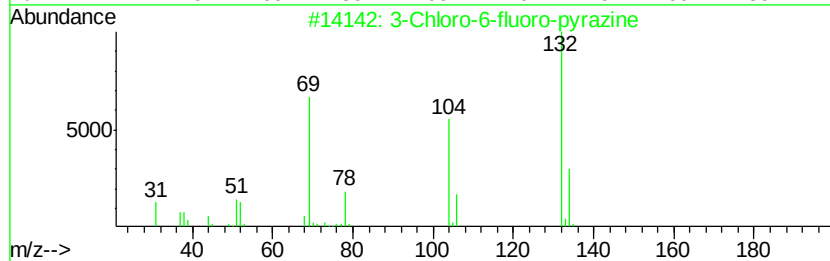
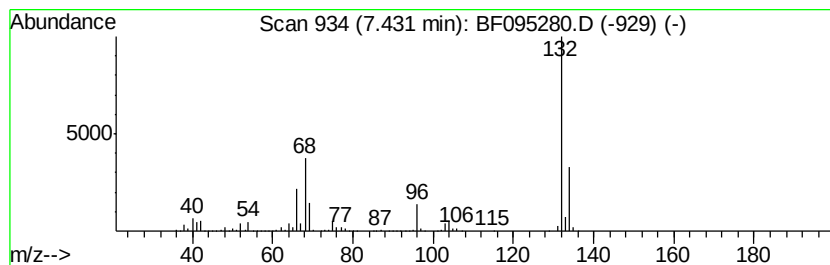
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Peak Number 2 unknown7.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	109.73 ng	2989950	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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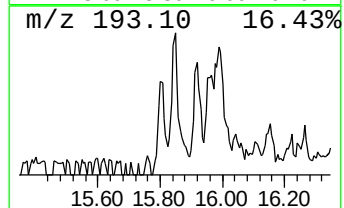
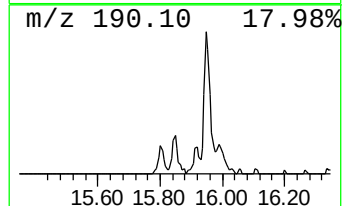
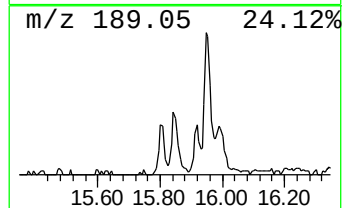
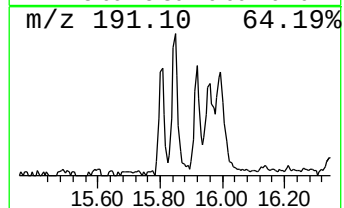
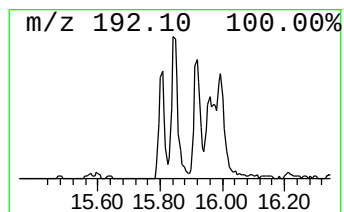
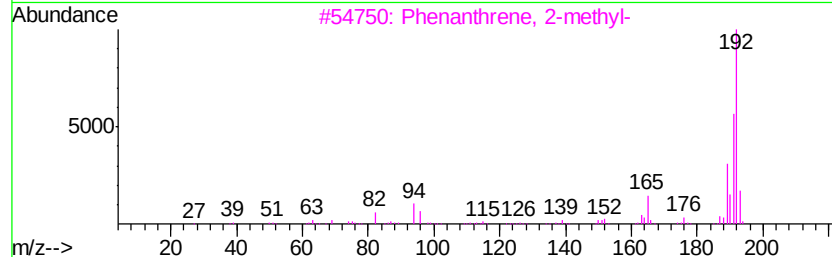
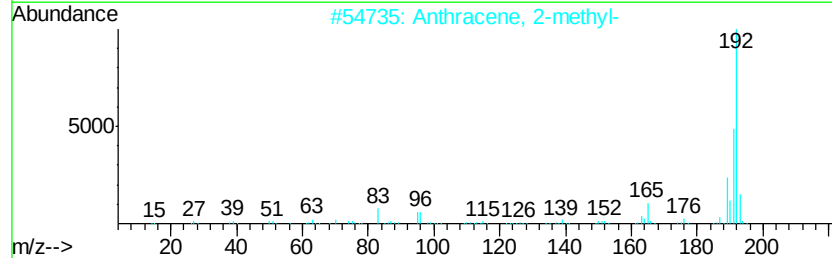
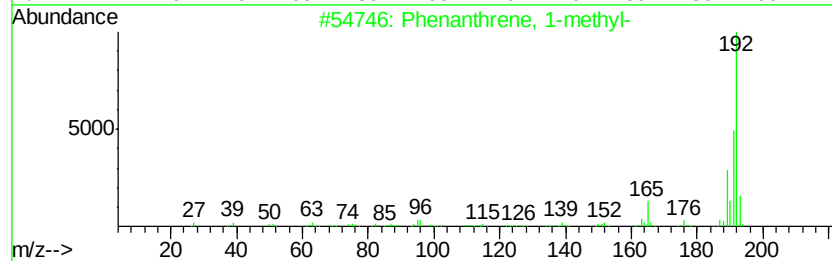
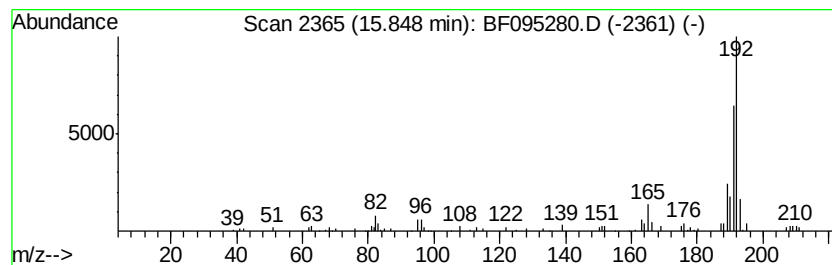
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.85	2.87 ng	113432	Phenanthrene-d10		15.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5	1H-Cyclopropa[l]phenanthrene, 1a, ...	192	C15H12	000949-41-7	89



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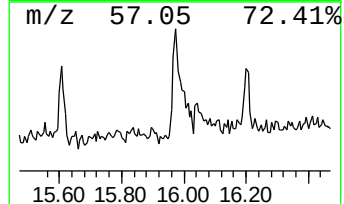
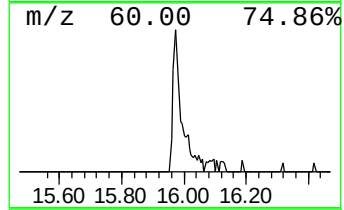
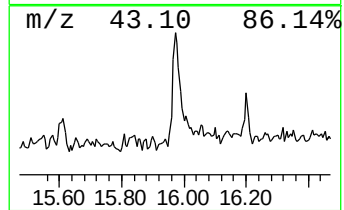
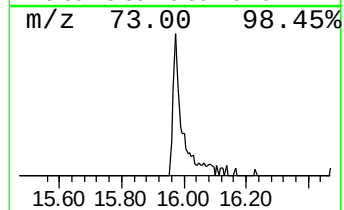
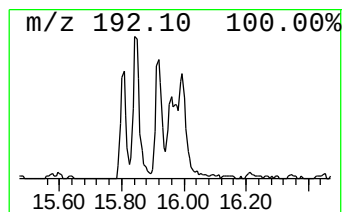
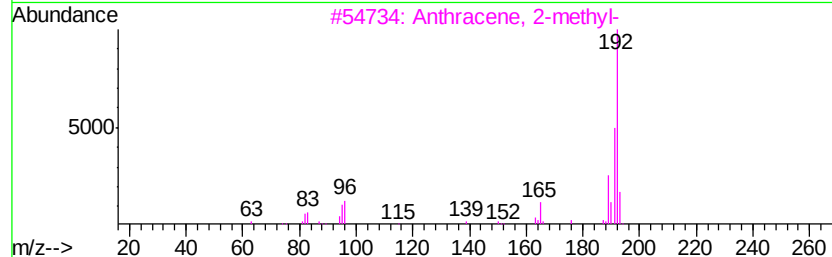
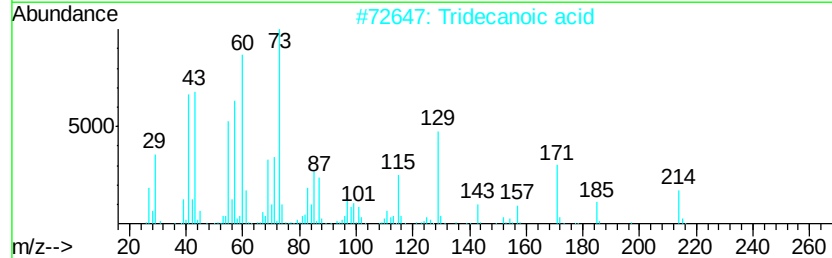
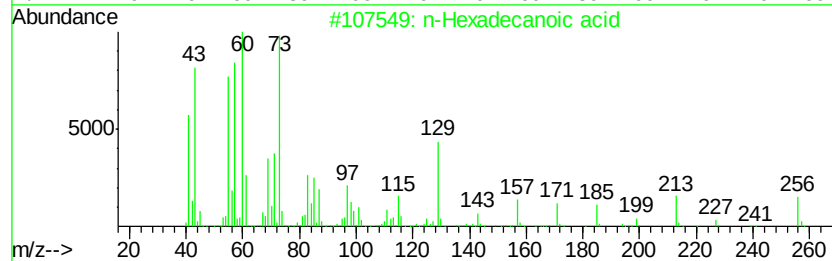
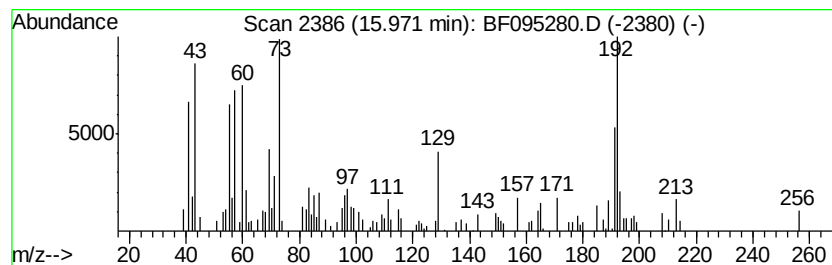
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.97	8.32 ng	328560	Phenanthrene-d10		15.01	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	70
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	55
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	46
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	45



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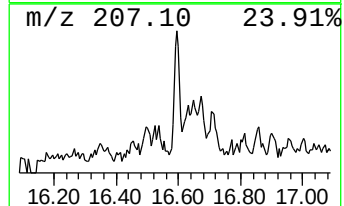
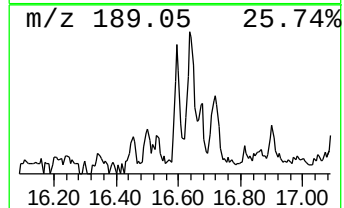
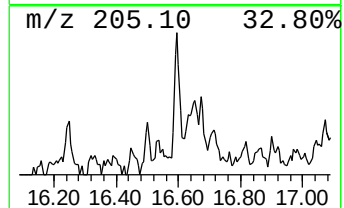
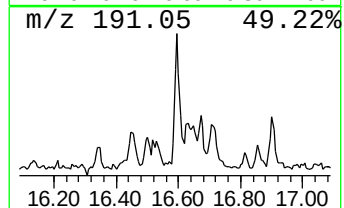
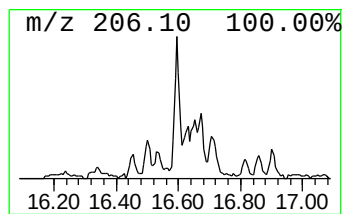
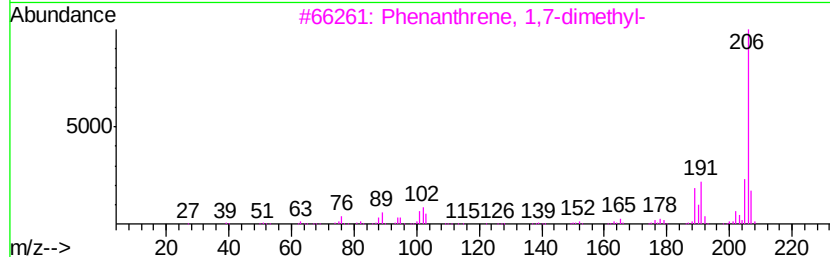
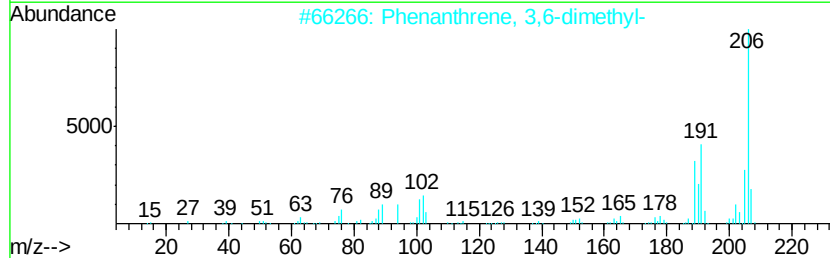
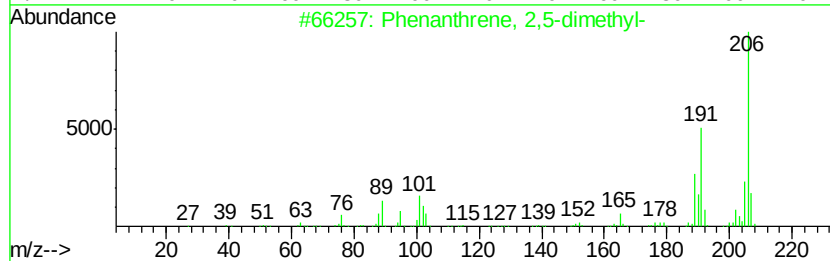
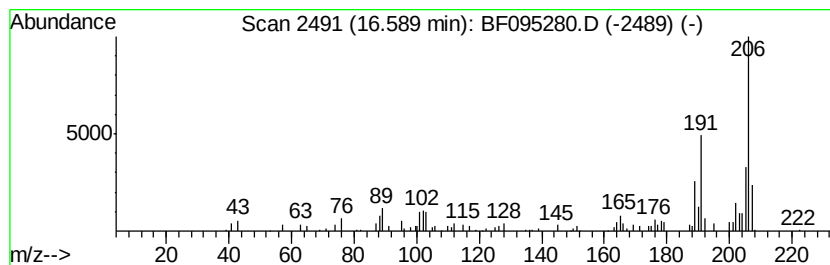
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.59	2.25 ng	88870	Phenanthrene-d10		15.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	95
3	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	95
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
5	9,10-Dimethylantracene	206	C16H14	000781-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095280.D
Acq On : 20 May 2017 00:19
Operator : SJ/MA
Sample : I3177-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

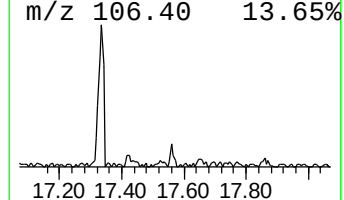
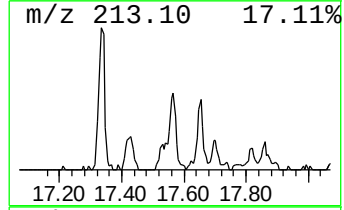
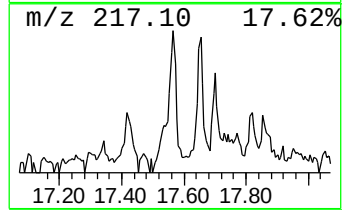
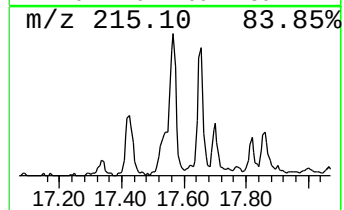
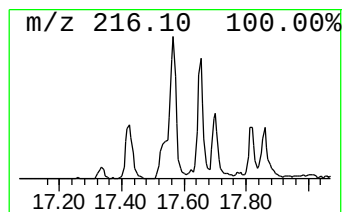
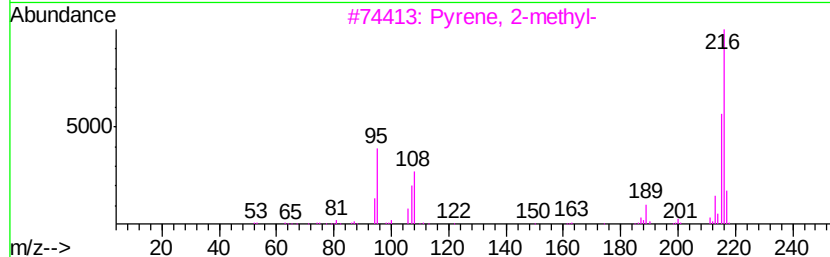
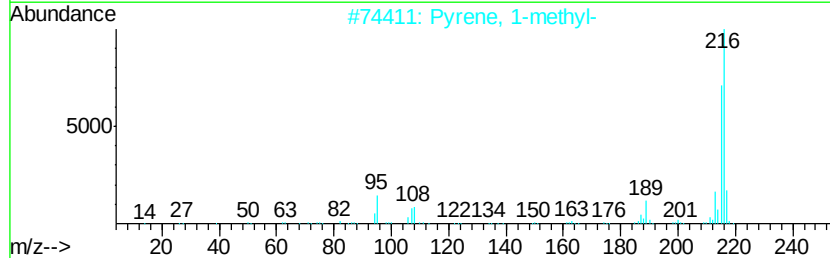
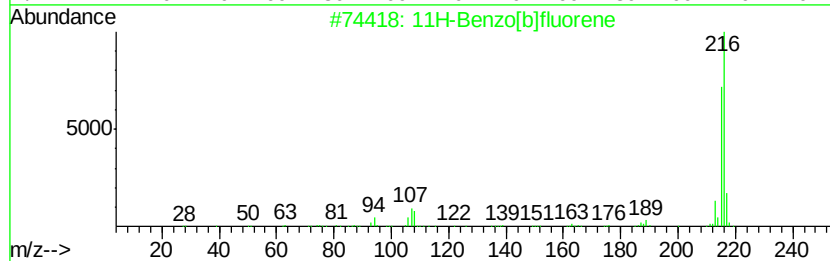
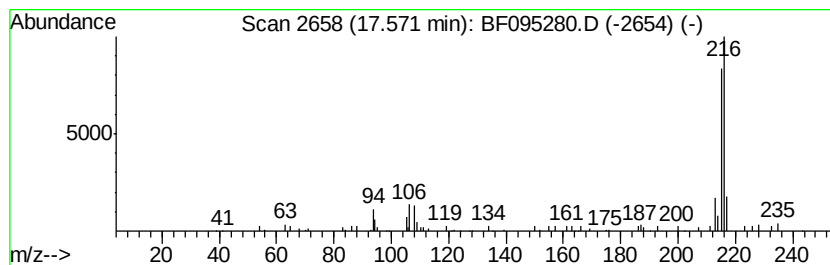
Instrument :
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ClientSampleId :
FLOOR-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.57	3.01 ng	104005	Chrysene-d12	18.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	86
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	80
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095280.D
Acq On : 20 May 2017 00:19
Operator : SJ/MA
Sample : I3177-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

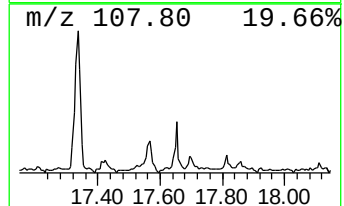
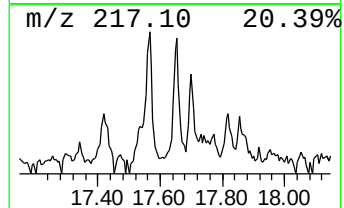
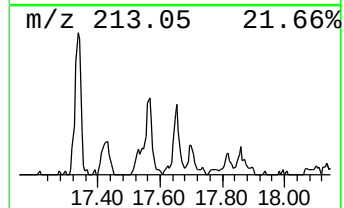
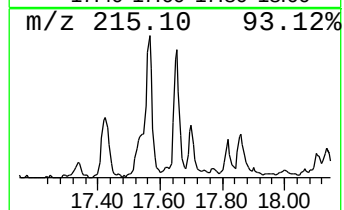
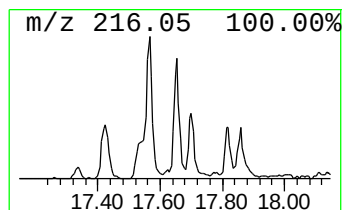
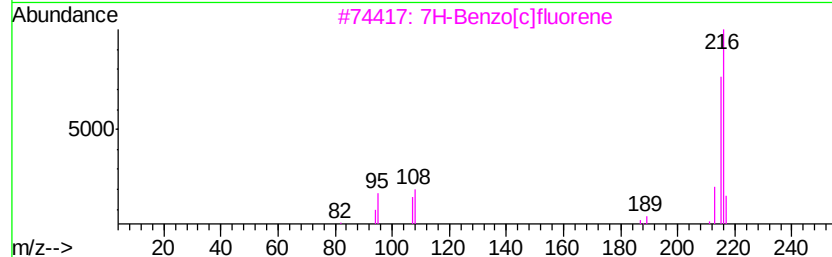
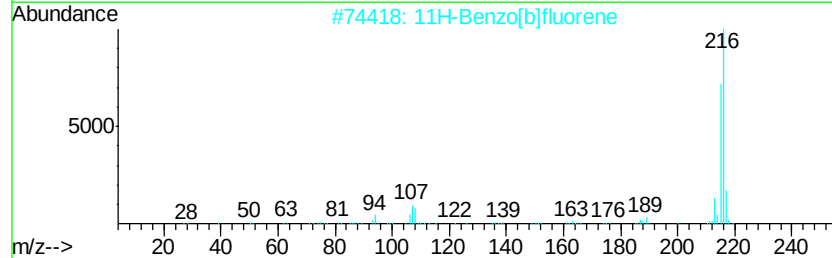
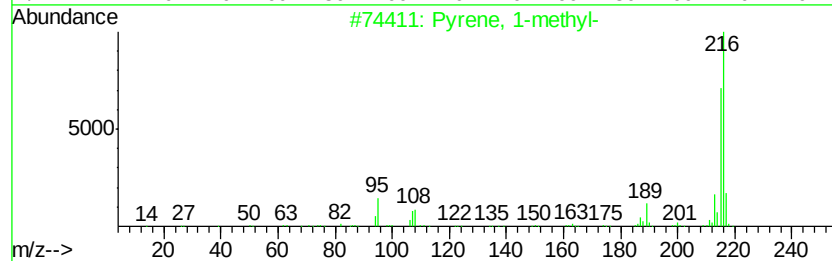
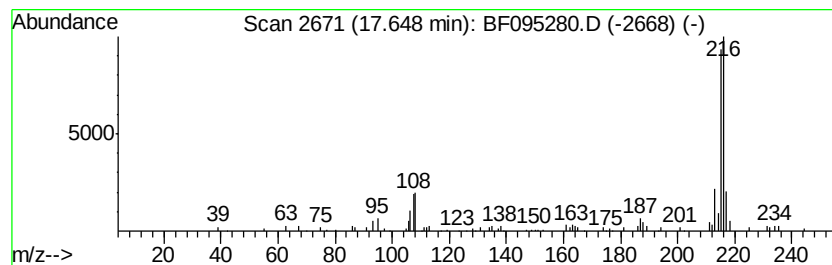
Instrument :
BNA_F
ClientSampleId :
FLOOR-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.65	2.94 ng	101534	Chrysene-d12		18.69
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
3	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	83
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095280.D
Acq On : 20 May 2017 00:19
Operator : SJ/MA
Sample : I3177-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FLOOR-A

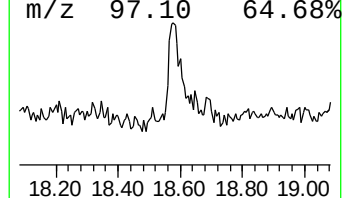
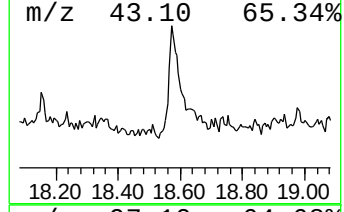
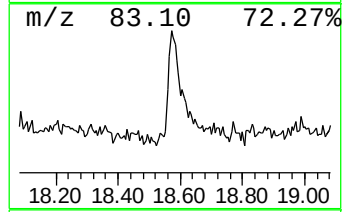
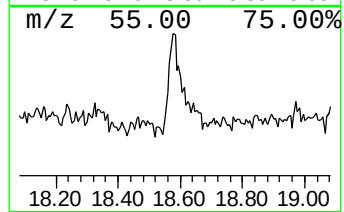
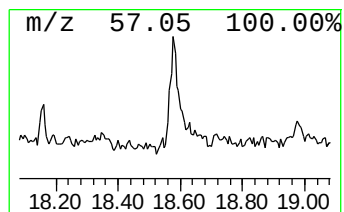
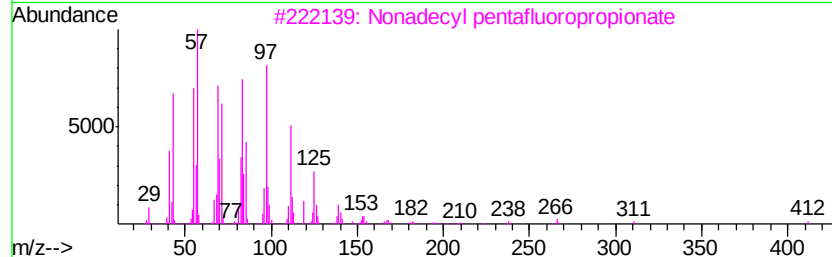
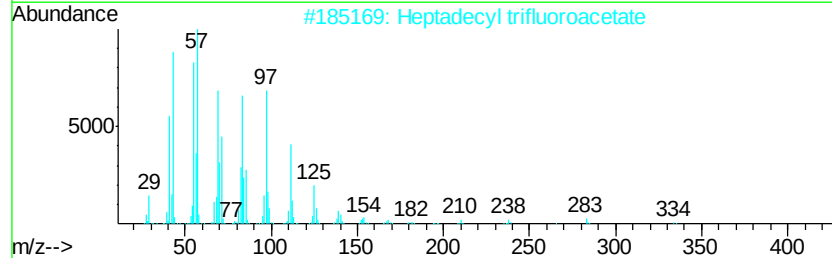
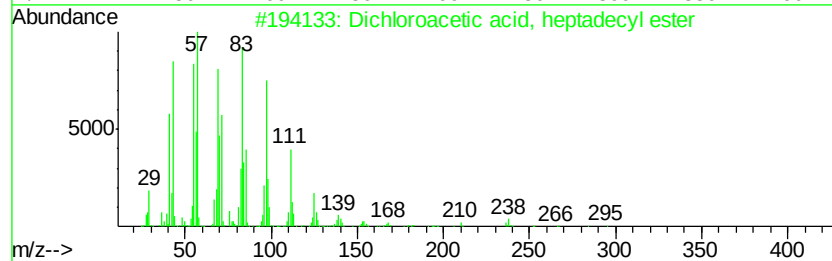
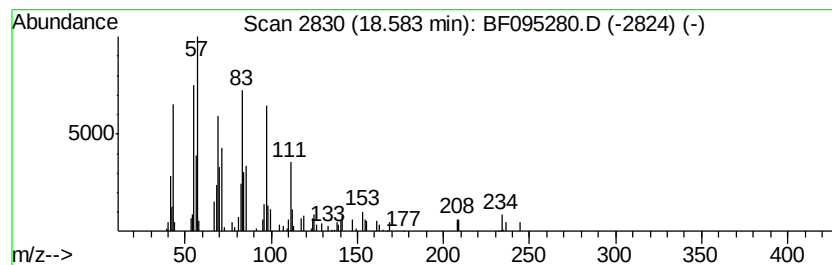
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dichloroacetic acid, heptadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	4.94 ng	170754	Chrysene-d12	18.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
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Acq On : 20 May 2017 00:19
Operator : SJ/MA
Sample : I3177-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FLOOR-A

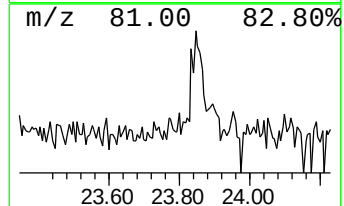
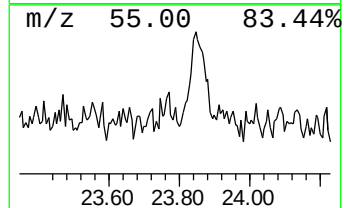
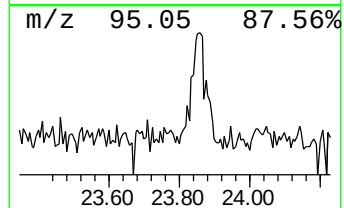
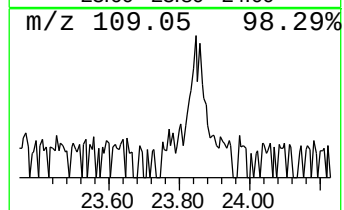
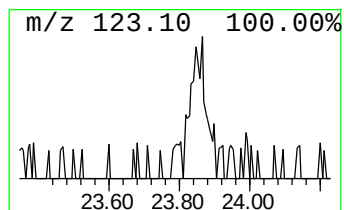
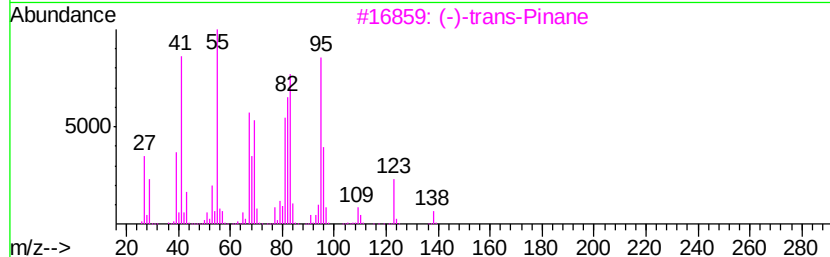
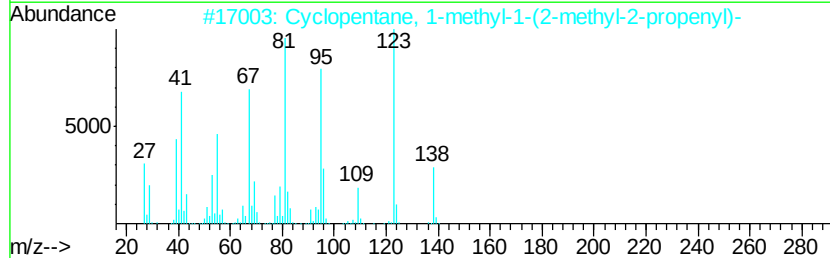
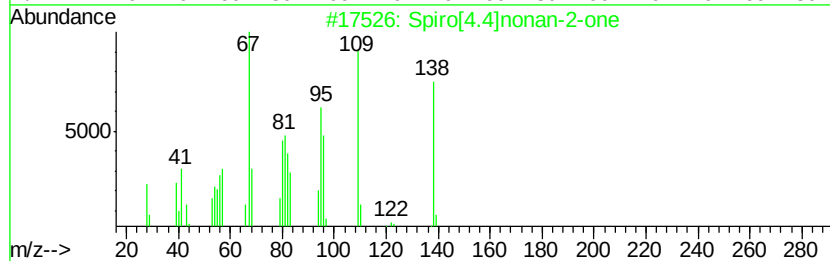
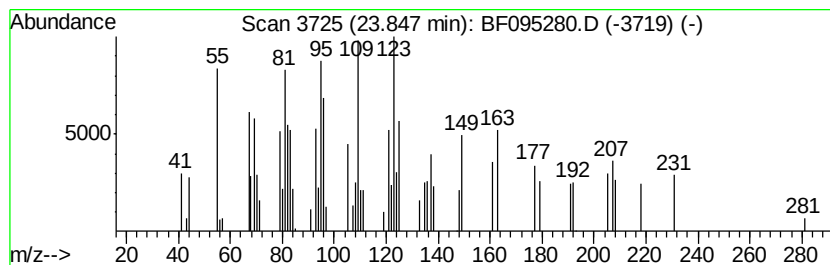
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown23.85 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.85	3.35 ng	79696	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Spiro[4.4]nonan-2-one	138	C9H14O	034177-18-9	38
2		Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	30
3		(-)-trans-Pinane	138	C10H18	033626-25-4	25
4		Cyclohexene, 4-(4-ethylcyclohexy...	262	C19H34	301643-32-3	22
5		Bicyclo[4.1.0]heptane-7-carboxyl...	258	C16H18O3	1000311-46-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
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Sample : I3177-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.14	15.2	ng	415206	1	7.77	544981	20.0
unknown7.43	7.43	109.7	ng	2989950	1	7.77	544981	20.0
Phenanthrene, 1-m...	15.85	2.9	ng	113432	4	15.01	790010	20.0
n-Hexadecanoic acid	15.97	8.3	ng	328560	4	15.01	790010	20.0
Phenanthrene, 2,5...	16.59	2.3	ng	88870	4	15.01	790010	20.0
11H-Benzo[b]fluorene	17.57	3.0	ng	104005	5	18.69	691567	20.0
Pyrene, 1-methyl-	17.65	2.9	ng	101534	5	18.69	691567	20.0
Dichloroacetic ac...	18.58	4.9	ng	170754	5	18.69	691567	20.0
unknown23.85	23.85	3.4	ng	79696	6	20.36	476191	20.0