LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092387.D
Acq On : 20 Jan 2017 22:05
Operator : UM/SJ
Sample : I1329-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.621	245	248	262	rBV	640983	1038577	35.95%	2.898%
2	5.101	288	290	306	rBV	2011486	2889065	100.00%	8.062%
3	6.187	383	385	392	rVB	1902998	2444553	84.61%	6.822%
4	6.290	392	394	397	rBV	2311110	2717220	94.05%	7.583%
5	6.519	412	414	417	rBV	771784	730356	25.28%	2.038%
6	6.679	426	428	430	rBV	1771409	1718285	59.48%	4.795%
7	7.102	462	465	467	rBV	1491166	1998987	69.19%	5.578%
8	7.810	525	527	531	rBV2	1622002	1901453	65.82%	5.306%
9	7.890	531	534	538	rVB	22286	32535	1.13%	0.091%
10	8.530	587	590	592	rBV	142147	168876	5.85%	0.471%
11	8.622	596	598	603	rVB	113871	108466	3.75%	0.303%
12	8.896	619	622	624	rBV	2386099	2812074	97.34%	7.848%
13	8.987	627	630	632	rBV	68530	75101	2.60%	0.210%
14	9.159	642	645	648	rBV	22713	35071	1.21%	0.098%
15	9.227	648	651	652	rBV	38938	49589	1.72%	0.138%
16	9.296	655	657	659	rVV	652664	589449	20.40%	1.645%
17	9.342	659	661	664	rVB	22567	32675	1.13%	0.091%
18	9.422	666	668	670	rBV	96259	85069	2.94%	0.237%
19	9.513	674	676	677	rBV	37321	33097	1.15%	0.092%
20	9.559	677	680	682	rVV	1484629	1369350	47.40%	3.821%
21	9.593	682	683	685	rVB	195630	144558	5.00%	0.403%
22	9.765	695	698	700	rBV	199063	175639	6.08%	0.490%
23	9.810	700	702	706	rVB2	19347	34331	1.19%	0.096%
24	9.982	713	717	718	rBV2	29766	50439	1.75%	0.141%
25	10.005	718	719	721	rVB2	40788	50160	1.74%	0.140%
26	10.108	726	728	730	rBV	201508	205346	7.11%	0.573%
27	10.268	740	742	744	rVB	36309	42394	1.47%	0.118%
28	10.348	747	749	752	rBV	1474146	1417534	49.07%	3.956%
29	10.485	758	761	764	rVB2	65980	106978	3.70%	0.299%
30	10.656	773	776	779	rBV2	22303	43581	1.51%	0.122%
31	10.805	786	789	792	rVB2	21860	38475	1.33%	0.107%
32	10.930	798	800	805	rVB	122516	147665	5.11%	0.412%
33	11.033	807	809	810	rBV	1205746	1125333	38.95%	3.140%
34	11.113	813	816	818	rVB	235890	246461	8.53%	0.688%

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Sample : I1329-03
Misc :
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Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.159	818	820	822	rBV2	21040	37947	1.31%	0.106%
36	11.273	828	830	832	rBV2	60911	97752	3.38%	0.273%
37	11.353	836	837	842	rVB2	71837	79089	2.74%	0.221%
38	11.536	851	853	854	rBV	102827	92661	3.21%	0.259%
39	11.571	854	856	857	rVV	91203	114009	3.95%	0.318%
40	11.616	857	860	861	rVV2	59375	91645	3.17%	0.256%
41	11.651	861	863	868	rVB2	129762	254526	8.81%	0.710%
42	11.753	871	872	875	rVB	41767	50330	1.74%	0.140%
43	11.833	875	879	881	rBV	100273	102426	3.55%	0.286%
44	11.868	881	882	887	rVB2	23137	30530	1.06%	0.085%
45	11.982	889	892	893	rBV	33919	40058	1.39%	0.112%
46	12.085	898	901	902	rBV	67100	73409	2.54%	0.205%
47	12.142	902	906	907	rVB2	39841	51152	1.77%	0.143%
48	12.176	907	909	913	rVB	51655	66031	2.29%	0.184%
49	12.245	913	915	917	rBV	1336222	1257770	43.54%	3.510%
50	12.291	917	919	922	rBV2	29194	61200	2.12%	0.171%
51	12.336	922	923	925	rVB	57356	56225	1.95%	0.157%
52	12.393	925	928	929	rBV	58502	71808	2.49%	0.200%
53	12.462	932	934	937	rBV	910701	1211440	41.93%	3.381%
54	12.519	937	939	944	rVB2	56896	82924	2.87%	0.231%
55	12.622	945	948	950	rVB	1908921	1903015	65.87%	5.311%
56	12.691	951	954	956	rBV2	61403	95789	3.32%	0.267%
57	12.794	960	963	965	rVB2	90930	190451	6.59%	0.531%
58	12.862	968	969	971	rBV	78965	80593	2.79%	0.225%
59	12.896	971	972	976	rVB2	68831	111582	3.86%	0.311%
60	12.988	979	980	982	rVB	38317	46607	1.61%	0.130%
61	13.022	982	983	988	rBV2	53753	71240	2.47%	0.199%
62	13.205	993	999	1004	rBV6	36786	148605	5.14%	0.415%
63	13.319	1007	1009	1012	rVB	43684	68616	2.38%	0.191%
64	13.411	1015	1017	1018	rBV	55691	84048	2.91%	0.235%
65	13.525	1025	1027	1029	rBV2	46317	53936	1.87%	0.151%
66	13.582	1029	1032	1035	rVB2	30566	61242	2.12%	0.171%
67	13.662	1036	1039	1044	rBV2	1142969	1823609	63.12%	5.089%
68	13.765	1046	1048	1050	rBV	81395	85059	2.94%	0.237%
69	14.051	1069	1073	1075	rBV2	67001	131458	4.55%	0.367%
70	14.142	1078	1081	1083	rBV3	32256	81802	2.83%	0.228%
71	14.531	1111	1115	1116	rBV2	48598	98244	3.40%	0.274%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.657	1124	1126	1131	rBV	282498	568323	19.67%	1.586%
73	14.748	1132	1134	1137	rVB2	51600	80846	2.80%	0.226%
74	14.908	1146	1148	1151	rBV	138369	185327	6.41%	0.517%
75	14.965	1151	1153	1155	rBV	258668	271894	9.41%	0.759%
76	15.011	1155	1157	1159	rBV	477185	644970	22.32%	1.800%
77	16.234	1261	1264	1271	rBV	107878	210971	7.30%	0.589%
78	16.588	1293	1295	1300	rVB	75642	153950	5.33%	0.430%

Sum of corrected areas: 35833851

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
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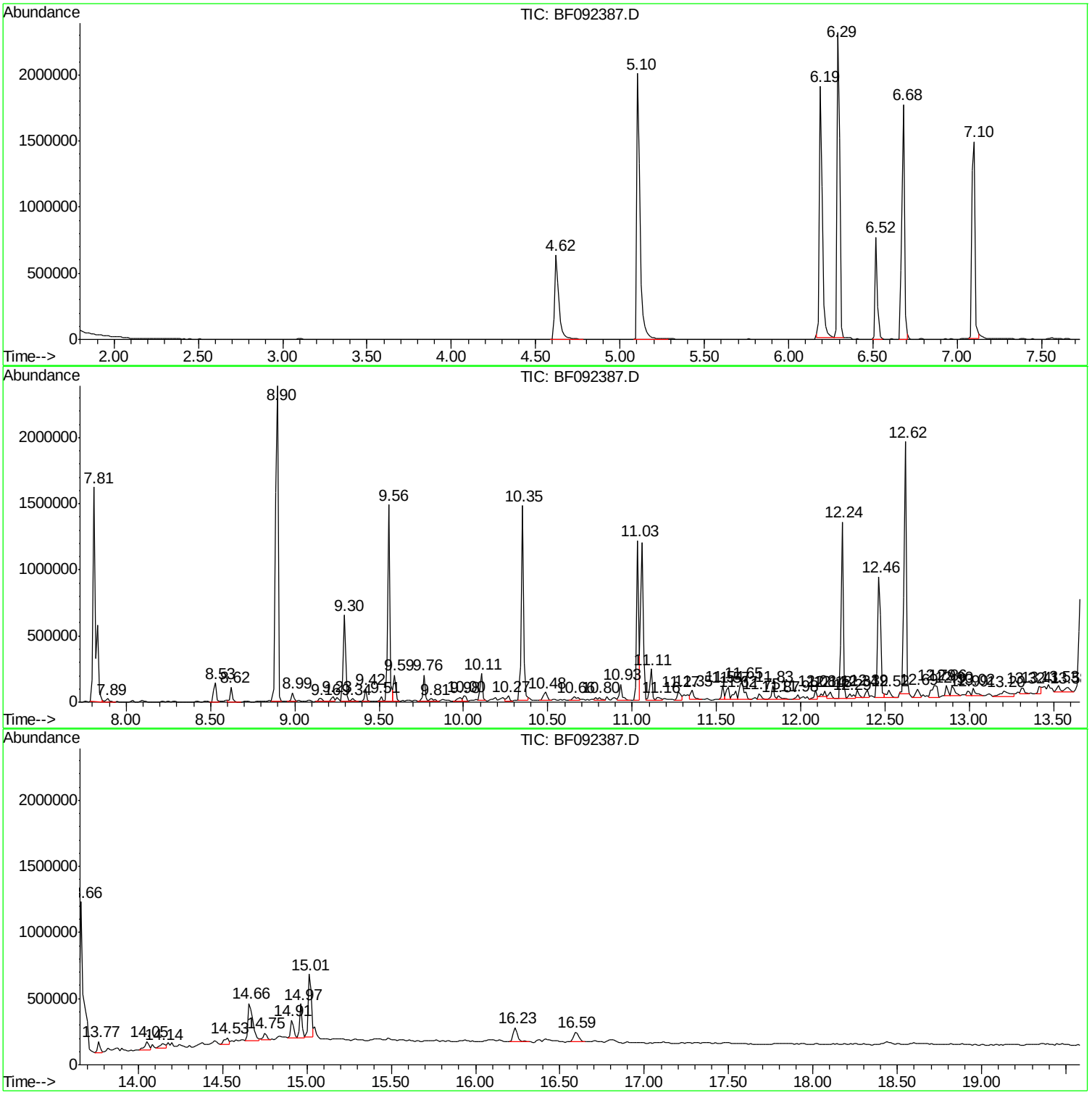
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092387.D
Acq On : 20 Jan 2017 22:05
Operator : UM/SJ
Sample : I1329-03
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

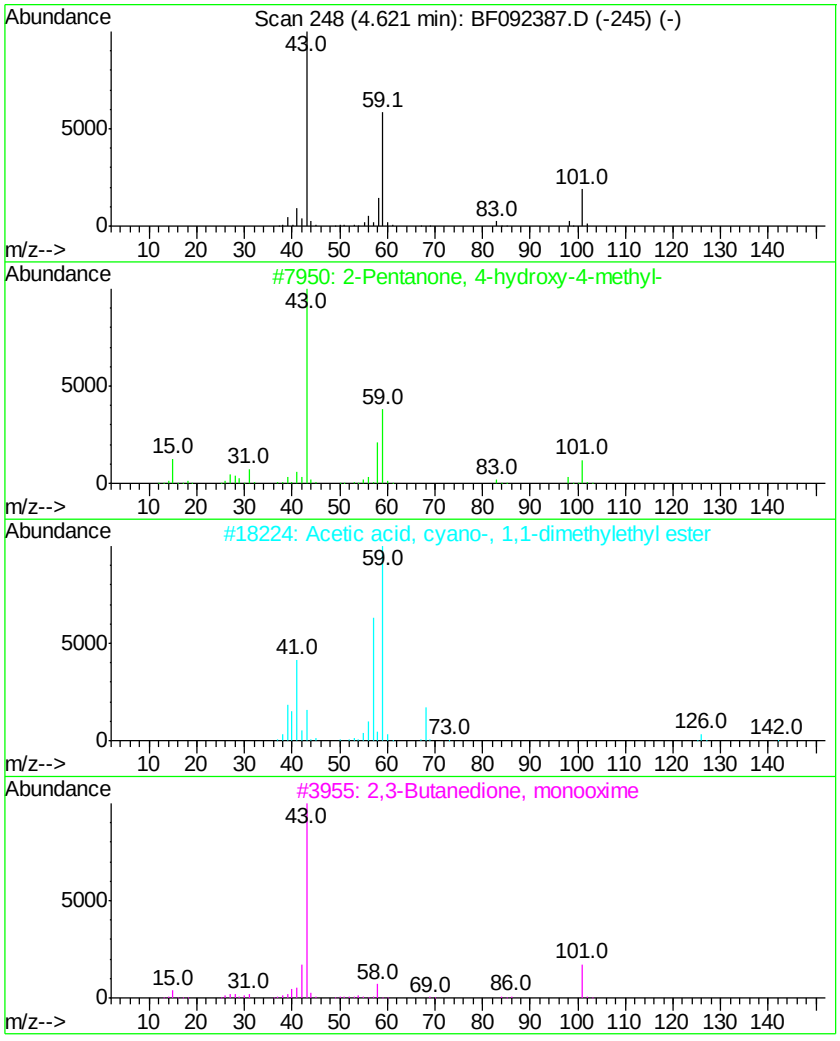
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

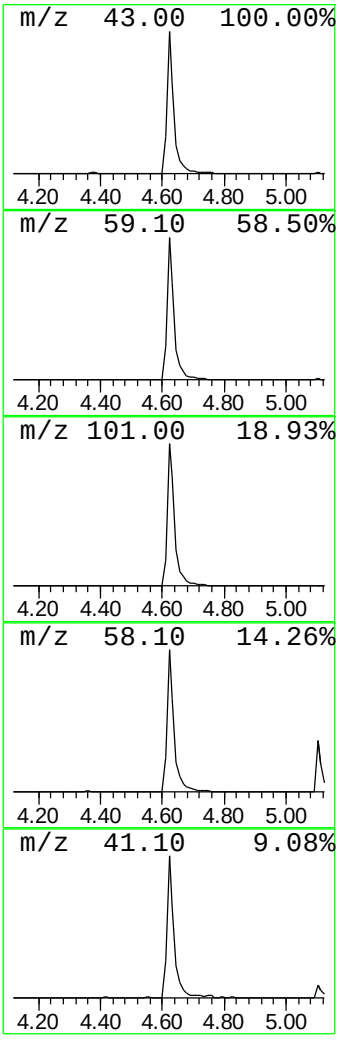
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	28.44 ng	1038580	1,4-Dichlorobenzene-d4	6.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
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Sample : I1329-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

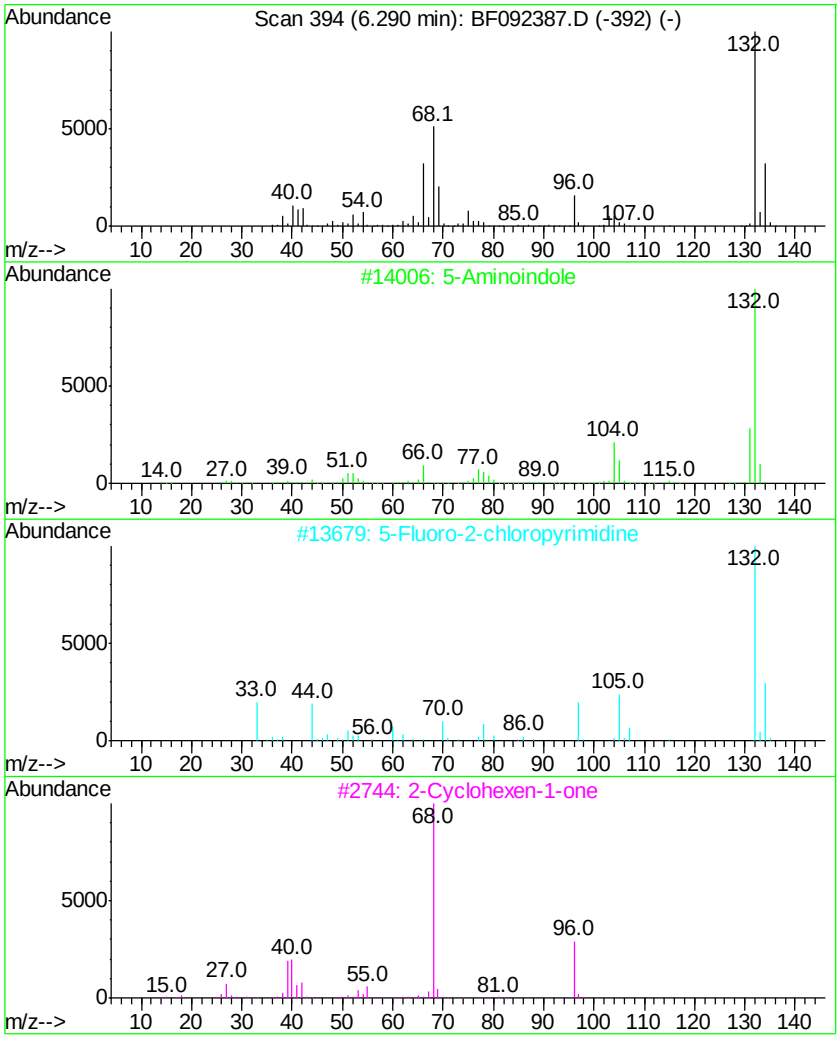
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

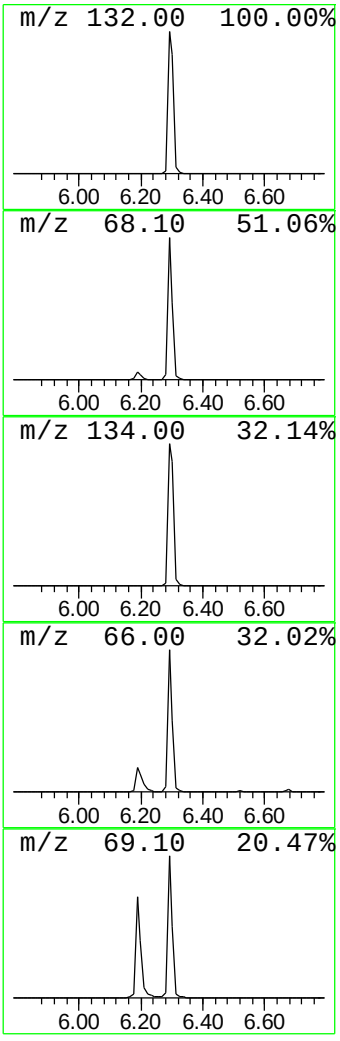
****

Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	74.41 ng	2717220	1,4-Dichlorobenzene-d4	6.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092387.D
Acq On : 20 Jan 2017 22:05
Operator : UM/SJ
Sample : I1329-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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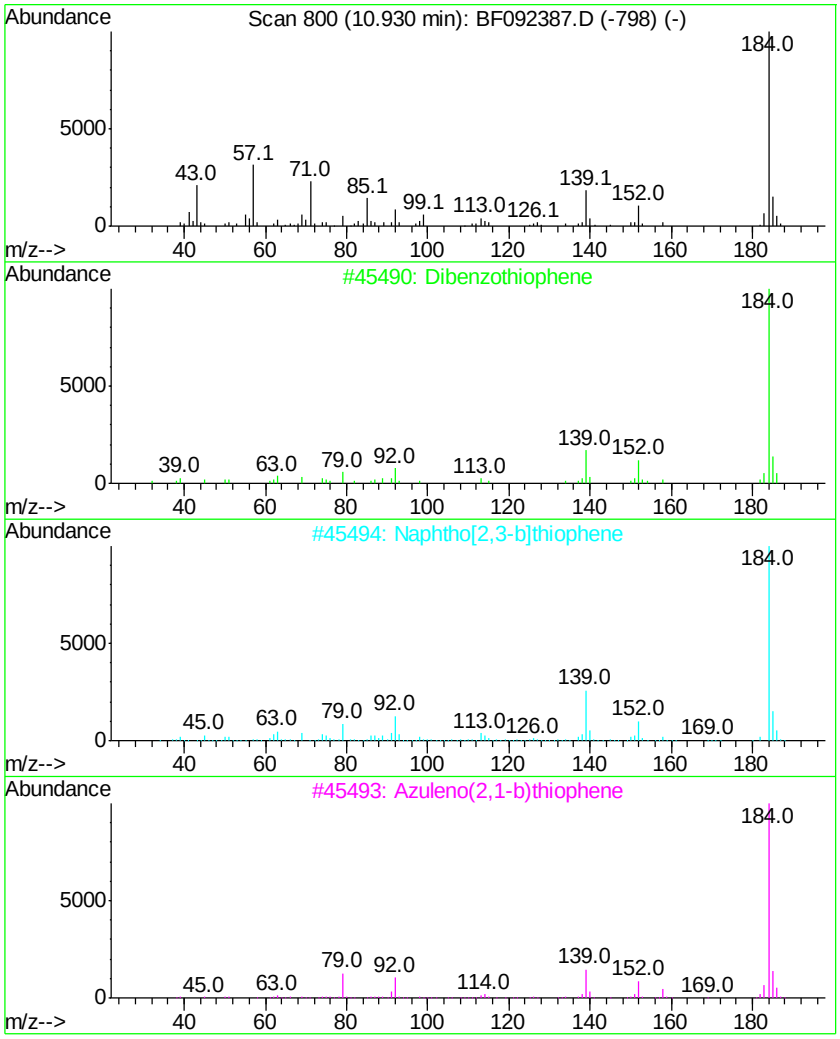
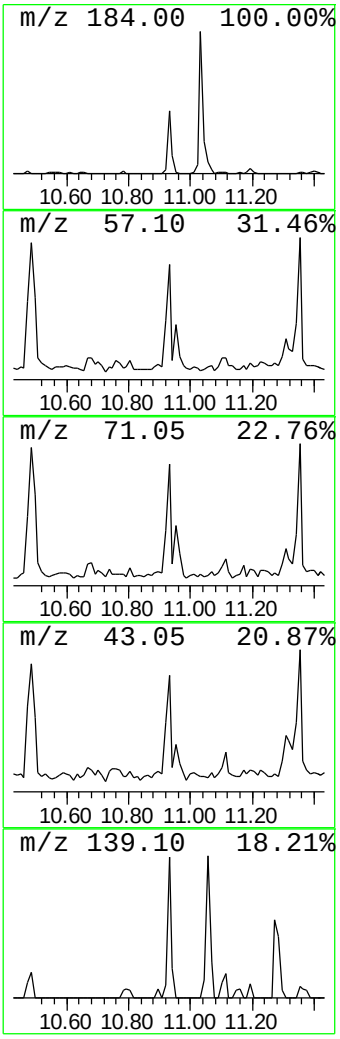
****

Peak Number 4 Dibenzothiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	2.62 ng	147665	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	95
2	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	89
3	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	81
4	Naphthalene, 2-ethenyl-6-methoxy-	184	C13H12O	063444-51-9	58
5	1,1'-Biphenyl, 2-methoxy-	184	C13H12O	000086-26-0	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
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Operator : UM/SJ
Sample : I1329-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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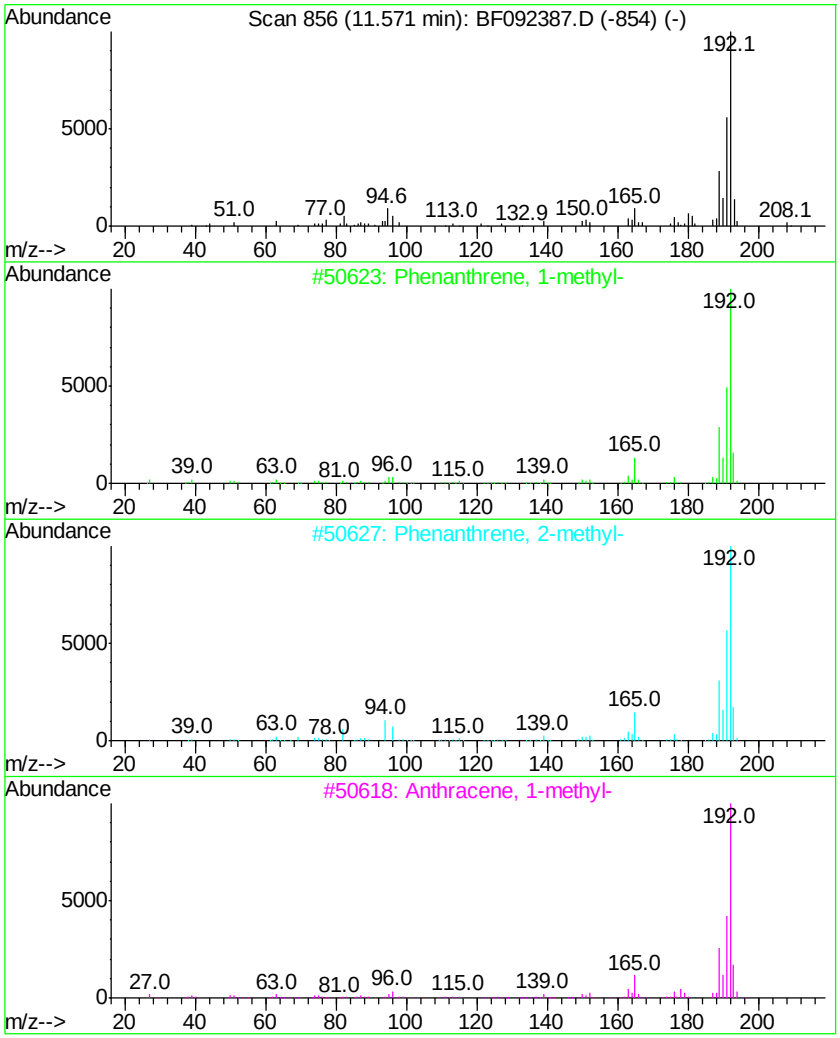
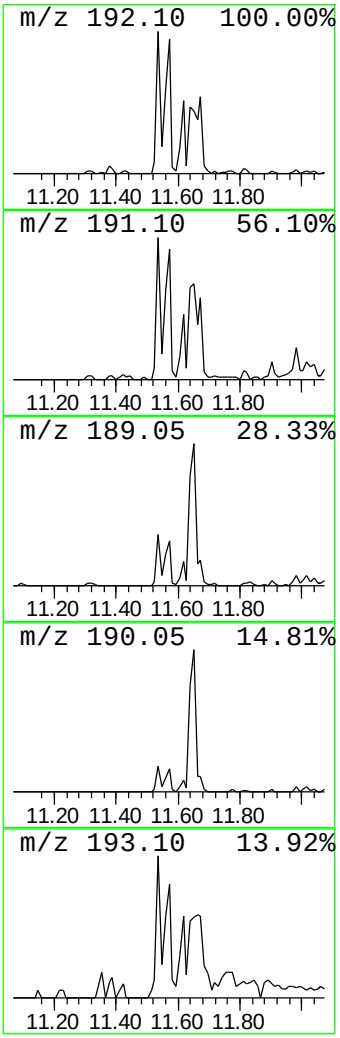
Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	2.03 ng	114009	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	81





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Sample : I1329-03
Misc :
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Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

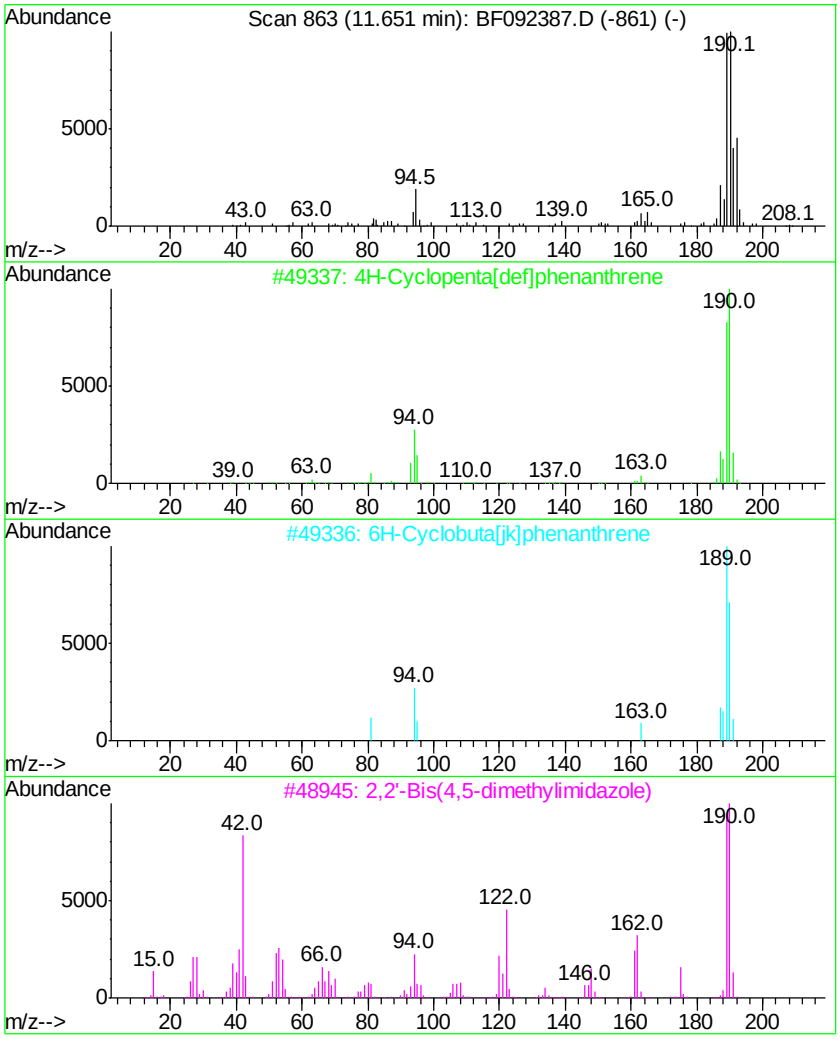
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

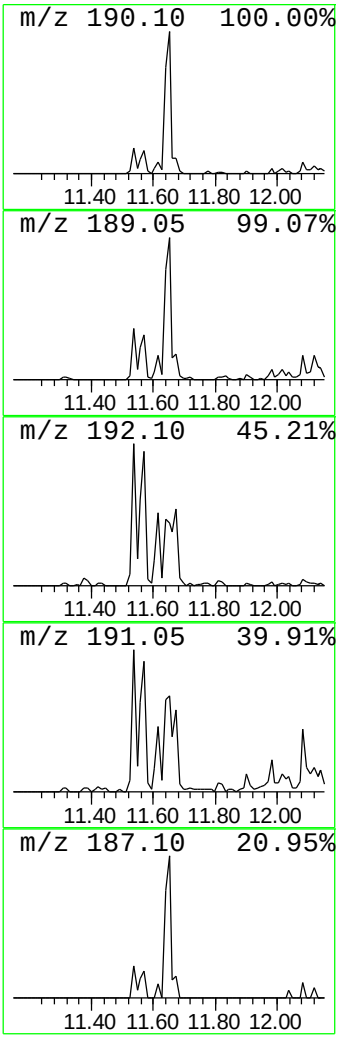
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	4.52 ng	254526	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	42
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	4,4'-Difluorobiphenyl	190	C12H8F2	000398-23-2	23
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	17





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Data File : BF092387.D
Acq On : 20 Jan 2017 22:05
Operator : UM/SJ
Sample : I1329-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

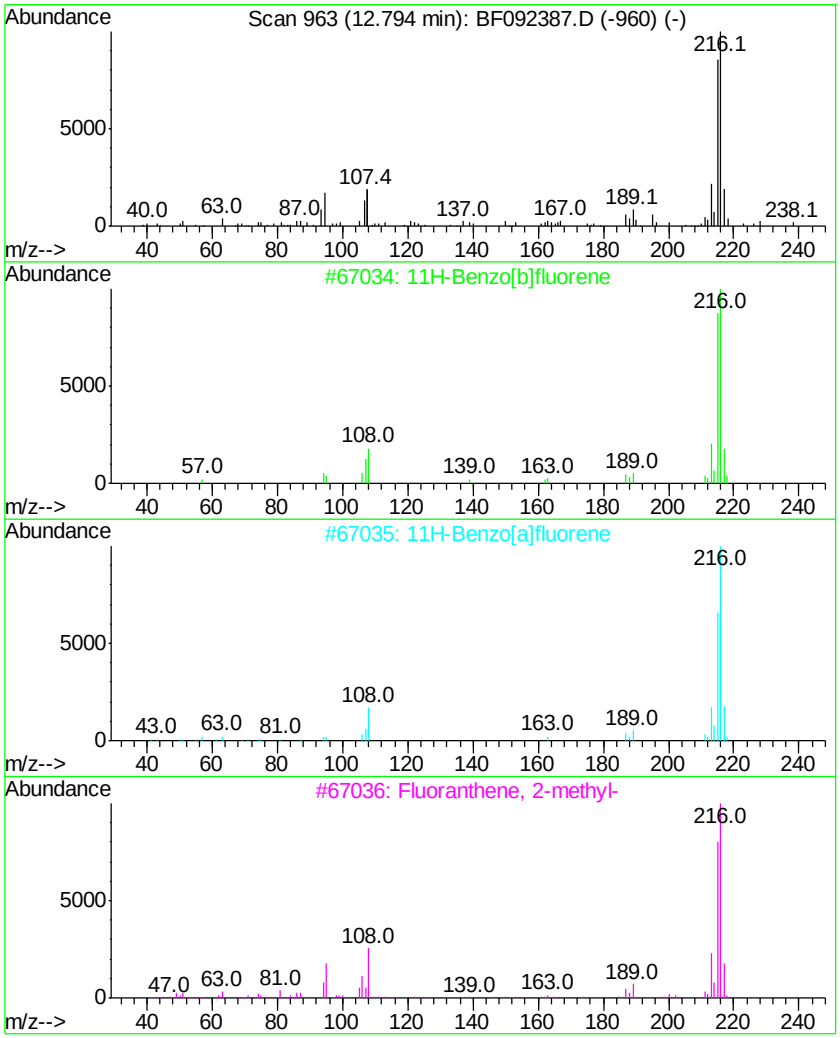
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

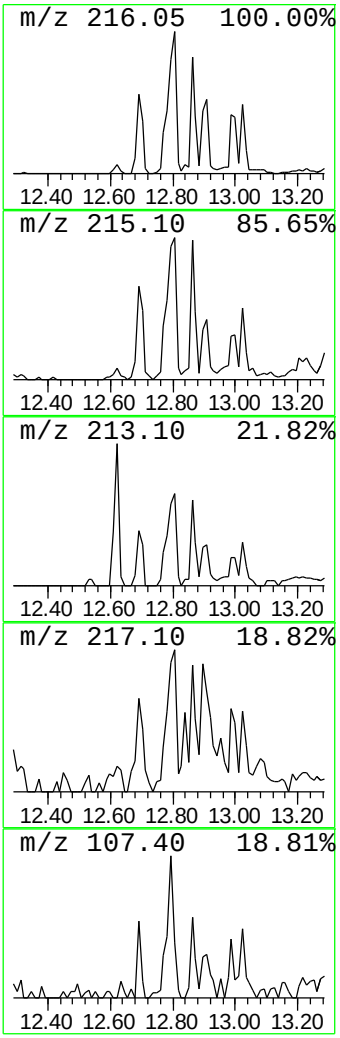
****

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	2.09 ng	190451	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092387.D
Acq On : 20 Jan 2017 22:05
Operator : UM/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

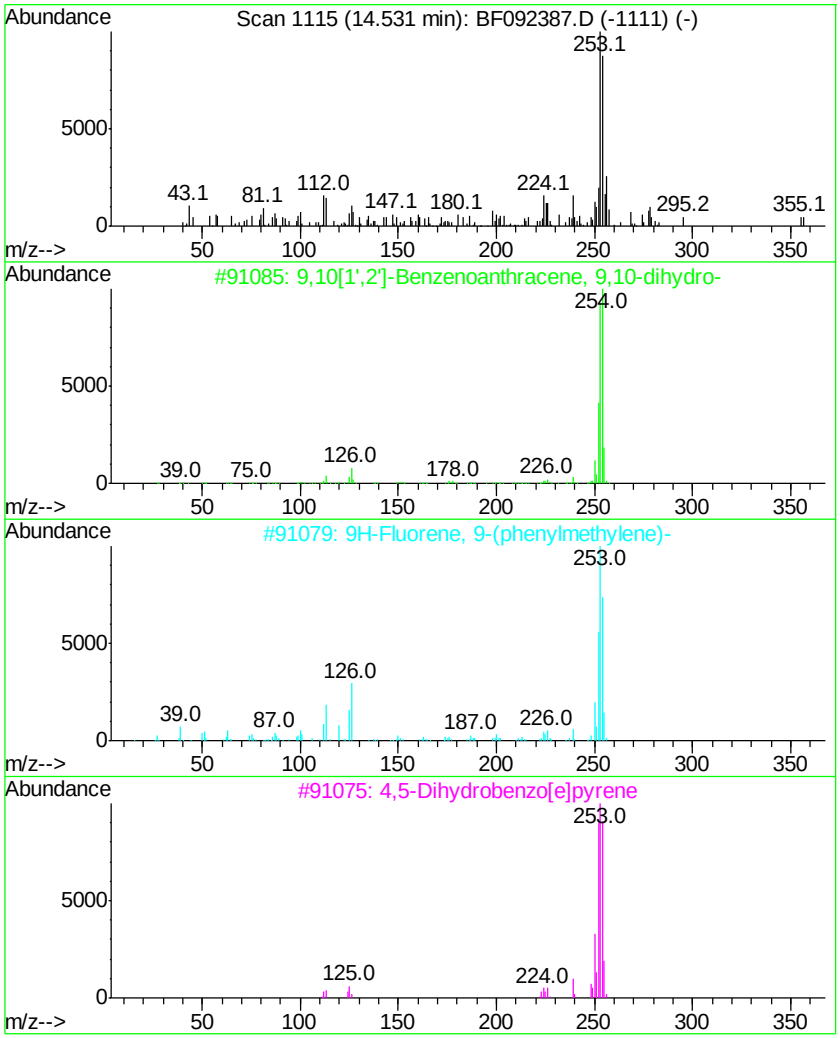
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

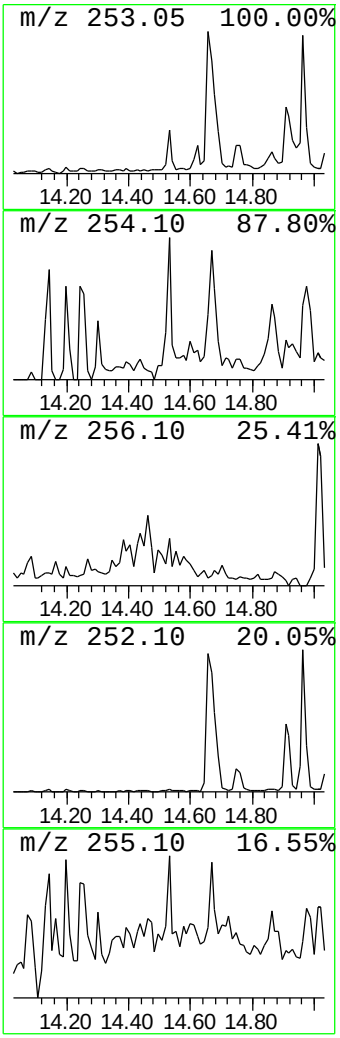
****

Peak Number 8 9,10[1',2']-Benzenoanthrace... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	3.05 ng	98244	Perylene-d12	15.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10[1',2']-Benzenoanthracene, 9...	254	C20H14	000477-75-8	70
2	9H-Fluorene, 9-(phenylmethylene)-	254	C20H14	001836-87-9	70
3	4,5-Dihydrobenzo[e]pyrene	254	C20H14	095676-42-9	62
4	1,2-Dihydrobenzo[b]fluoranthene	254	C20H14	100516-13-0	58
5	1,2'-Binaphthalene	254	C20H14	004325-74-0	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092387.D
Acq On : 20 Jan 2017 22:05
Operator : UM/SJ
Sample : I1329-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLACK-FILL2-0-5FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.62	28.4	ng	1038580	1	6.52	730356	20.0
unknown6.29	6.29	74.4	ng	2717220	1	6.52	730356	20.0
Dibenzothiophene	10.93	2.6	ng	147665	4	11.03	1125330	20.0
Phenanthrene, 1-m...	11.57	2.0	ng	114009	4	11.03	1125330	20.0
4H-Cyclopenta[def...	11.65	4.5	ng	254526	4	11.03	1125330	20.0
11H-Benzo[b]fluorene	12.79	2.1	ng	190451	5	13.66	1823610	20.0
9,10[1',2']-Benze...	14.53	3.0	ng	98244	6	15.01	644970	20.0