LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085404.D
Acq On : 12 Mar 2016 7:34
Operator : UM/SJ
Sample : H1730-04 5X
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W170TH-SB-18-COMP(0.5-1.5)

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-BF030316.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	5.110	245	247	254	rVB	62674	80704	5.48%	0.389%
2	5.521	281	283	286	rBV	863021	1044953	71.01%	5.032%
3	6.550	371	373	376	rBV	999969	1005964	68.36%	4.844%
4	6.699	383	386	388	rBV	1424513	1214489	82.53%	5.848%
5	6.939	404	407	409	rBV	735263	932594	63.37%	4.491%
6	7.087	418	420	423	rVB	1043994	903875	61.42%	4.352%
7	7.499	453	456	458	rBV	552172	667017	45.33%	3.212%
8	8.219	517	519	522	rBV	1377443	1211716	82.34%	5.835%
9	8.493	541	543	546	rBV	11161	15486	1.05%	0.075%
10	9.293	611	613	616	rBV	1269332	1135493	77.16%	5.468%
11	9.636	640	643	646	rBV2	16562	23805	1.62%	0.115%
12	9.693	646	648	650	rVV	153239	145447	9.88%	0.700%
13	9.842	658	661	663	rBV	28312	28737	1.95%	0.138%
14	9.910	663	667	668	rVV	26344	25541	1.74%	0.123%
15	9.979	670	673	675	rVV	1426547	1206752	82.00%	5.811%
16	10.013	675	676	677	rVB	28539	19602	1.33%	0.094%
17	10.185	688	691	693	rVV3	16124	23299	1.58%	0.112%
18	10.219	693	694	697	rVB2	12788	14855	1.01%	0.072%
19	10.402	706	710	712	rBV	29574	43761	2.97%	0.211%
20	10.528	719	721	724	rVB	37780	41387	2.81%	0.199%
21	10.631	726	730	732	rVV3	14235	24966	1.70%	0.120%
22	10.768	739	742	744	rBV	498099	564276	38.34%	2.717%
23	10.882	749	752	756	rBV	49721	60399	4.10%	0.291%
24	11.076	766	769	770	rBV	17858	23841	1.62%	0.115%
25	11.202	778	780	784	rBV2	9813	18706	1.27%	0.090%
26	11.328	788	791	793	rBV2	29173	39087	2.66%	0.188%
27	11.362	793	794	797	rVB	24246	20727	1.41%	0.100%
28	11.465	801	803	804	rBV	1170291	1007523	68.46%	4.851%
29	11.488	804	805	807	rVV	379257	280450	19.06%	1.350%
30	11.533	807	809	811	rVB	77318	96286	6.54%	0.464%
31	11.693	820	823	824	rBV	20034	22736	1.54%	0.109%
32	11.762	827	829	831	rBV2	13324	17273	1.17%	0.083%
33	11.991	844	849	851	rBV2	102153	168797	11.47%	0.813%
34	12.036	851	853	855	rVV2	33038	46719	3.17%	0.225%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H1730-04 5X
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W170TH-SB-18-COMP(0.5-1.5)

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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.082	855	857	861	rVB	89142	147890	10.05%	0.712%
36	12.162	861	864	869	rBV3	28002	63397	4.31%	0.305%
37	12.265	869	873	877	rVB3	35864	75575	5.14%	0.364%
38	12.414	883	886	887	rBV2	16659	17655	1.20%	0.085%
39	12.436	887	888	889	rBV	12176	14879	1.01%	0.072%
40	12.516	892	895	896	rBV	50259	57737	3.92%	0.278%
41	12.551	896	898	901	rVB	43383	58739	3.99%	0.283%
42	12.596	901	902	907	rVB2	25684	40643	2.76%	0.196%
43	12.676	907	909	911	rBV	592308	501494	34.08%	2.415%
44	12.722	911	913	916	rVB4	12271	21346	1.45%	0.103%
45	12.768	916	917	921	rBV2	27047	51689	3.51%	0.249%
46	12.871	924	926	927	rBV	367637	324868	22.08%	1.564%
47	12.905	927	929	932	rVV	474753	512600	34.83%	2.468%
48	12.951	932	933	936	rVB2	74256	73174	4.97%	0.352%
49	13.054	939	942	944	rVB	517348	737665	50.13%	3.552%
50	13.122	944	948	952	rBV3	36303	69615	4.73%	0.335%
51	13.236	954	958	959	rBV	81011	108019	7.34%	0.520%
52	13.305	959	964	965	rBV2	62327	106410	7.23%	0.512%
53	13.339	965	967	968	rBV	66093	68327	4.64%	0.329%
54	13.431	973	975	976	rVB	36592	30729	2.09%	0.148%
55	13.465	976	978	980	rBV	30075	41209	2.80%	0.198%
56	13.579	986	988	989	rBV	216820	203683	13.84%	0.981%
57	13.625	989	992	996	rVV3	58216	109715	7.46%	0.528%
58	13.739	1000	1002	1005	rVB	26901	29381	2.00%	0.141%
59	13.854	1009	1012	1013	rBV2	51824	78477	5.33%	0.378%
60	13.945	1018	1020	1023	rVV2	111251	145907	9.91%	0.703%
61	14.002	1023	1025	1026	rVV	46288	65984	4.48%	0.318%
62	14.105	1030	1034	1039	rBV2	1038764	1471606	100.00%	7.086%
63	14.208	1041	1043	1045	rVV2	43298	48899	3.32%	0.235%
64	14.265	1046	1048	1052	rVB2	79960	106157	7.21%	0.511%
65	14.494	1066	1068	1069	rVB	44114	40996	2.79%	0.197%
66	14.528	1069	1071	1072	rVB2	22934	22419	1.52%	0.108%
67	14.574	1073	1075	1077	rVV2	98737	127211	8.64%	0.613%
68	14.619	1077	1079	1082	rVB4	37971	72562	4.93%	0.349%
69	14.757	1089	1091	1093	rBV	657325	640789	43.54%	3.085%
70	14.882	1098	1102	1104	rVB2	73314	135811	9.23%	0.654%
71	15.145	1122	1125	1129	rBV	186378	376214	25.56%	1.812%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : W170TH-SB-18-COMP(0.5-1.5)

Integration Parameters: rteint.p
Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	15.214	1129	1131	1133	rBV	75342	105478	7.17%	0.508%
73	15.442	1149	1151	1154	rVB	96514	146470	9.95%	0.705%
74	15.511	1154	1157	1160	rBV	137163	204103	13.87%	0.983%
75	15.568	1160	1162	1168	rBV	442208	806740	54.82%	3.885%
76	16.037	1200	1203	1205	rBV	56675	79889	5.43%	0.385%
77	16.540	1245	1247	1250	rVB	39696	62325	4.24%	0.300%
78	17.031	1287	1290	1295	rVB2	57135	130019	8.84%	0.626%
79	17.465	1325	1328	1333	rBV	42069	91877	6.24%	0.442%
80	17.625	1338	1342	1346	rVB4	57595	148535	10.09%	0.715%
81	17.968	1370	1372	1373	rBV2	19425	15822	1.08%	0.076%

Sum of corrected areas: 20767992

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Sample : H1730-04 5X
Misc :
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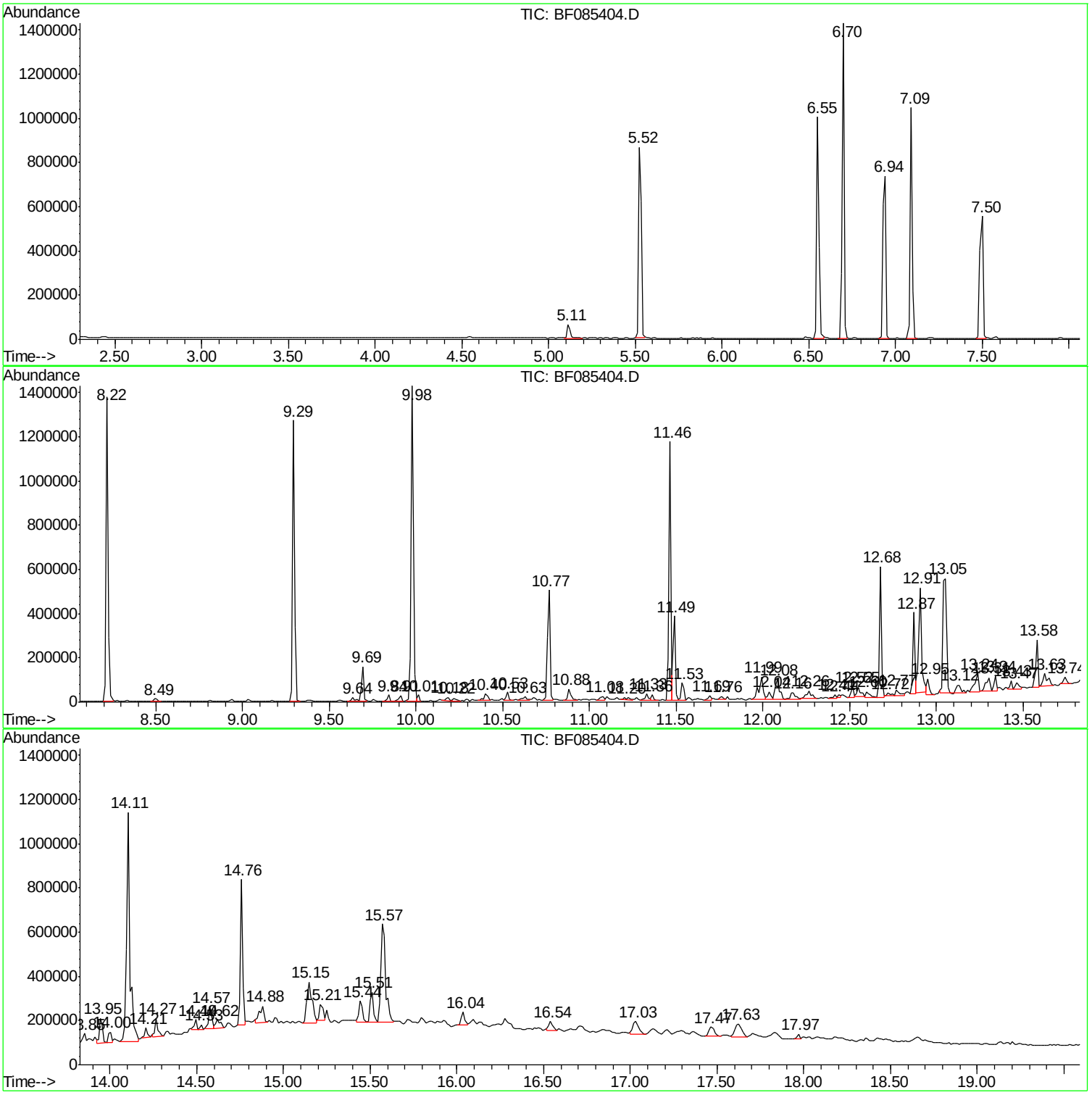
Instrument :
BNA_F
ClientSampleId :
W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085404.D
Acq On : 12 Mar 2016 7:34
Operator : UM/SJ
Sample : H1730-04 5X
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Instrument :
BNA_F
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W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

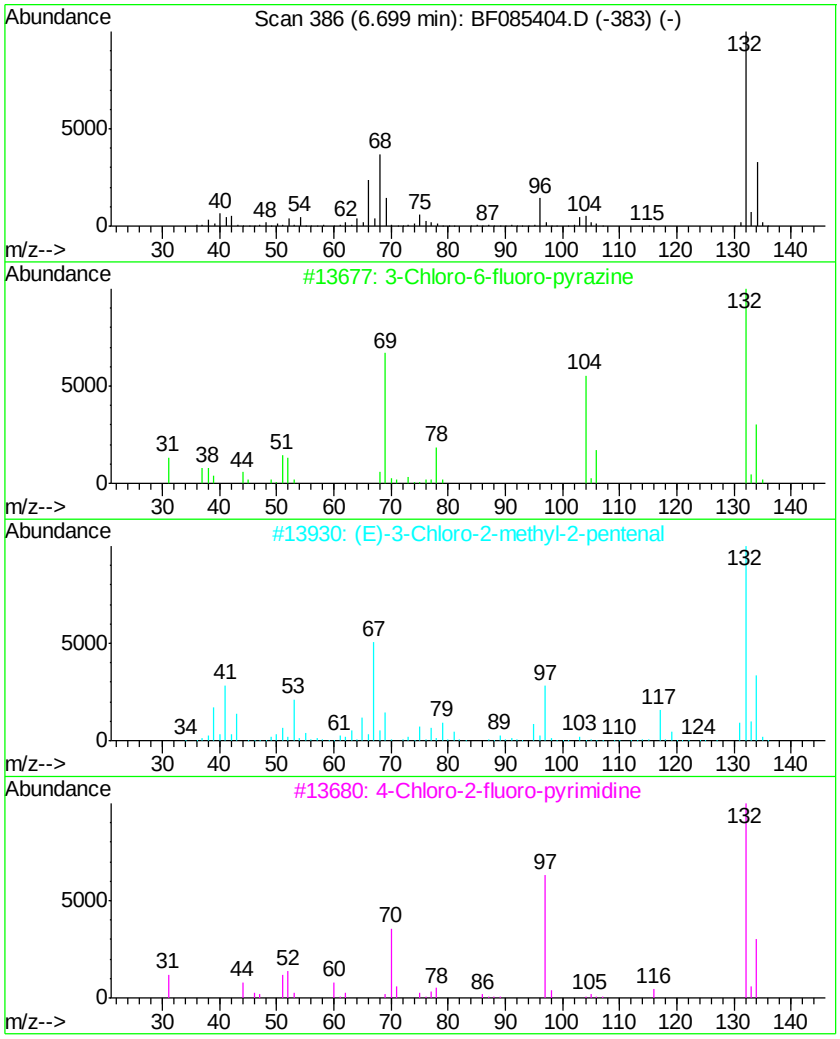
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

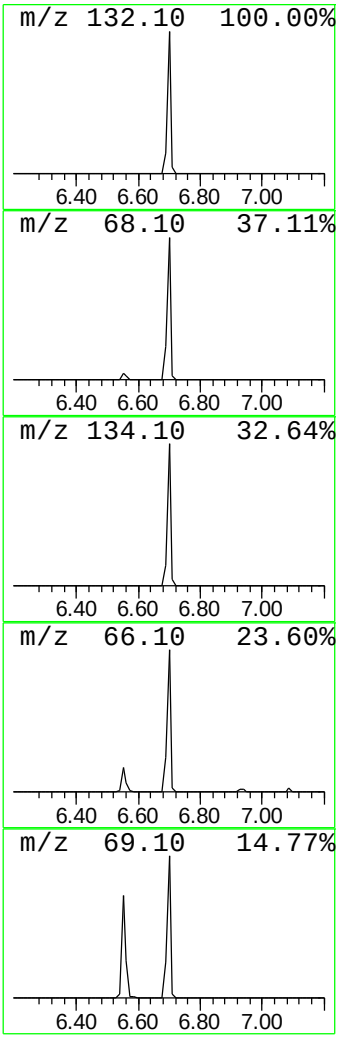
****

Peak Number 1 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	26.05 ng	1214490	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Acq On : 12 Mar 2016 7:34
Operator : UM/SJ
Sample : H1730-04 5X
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

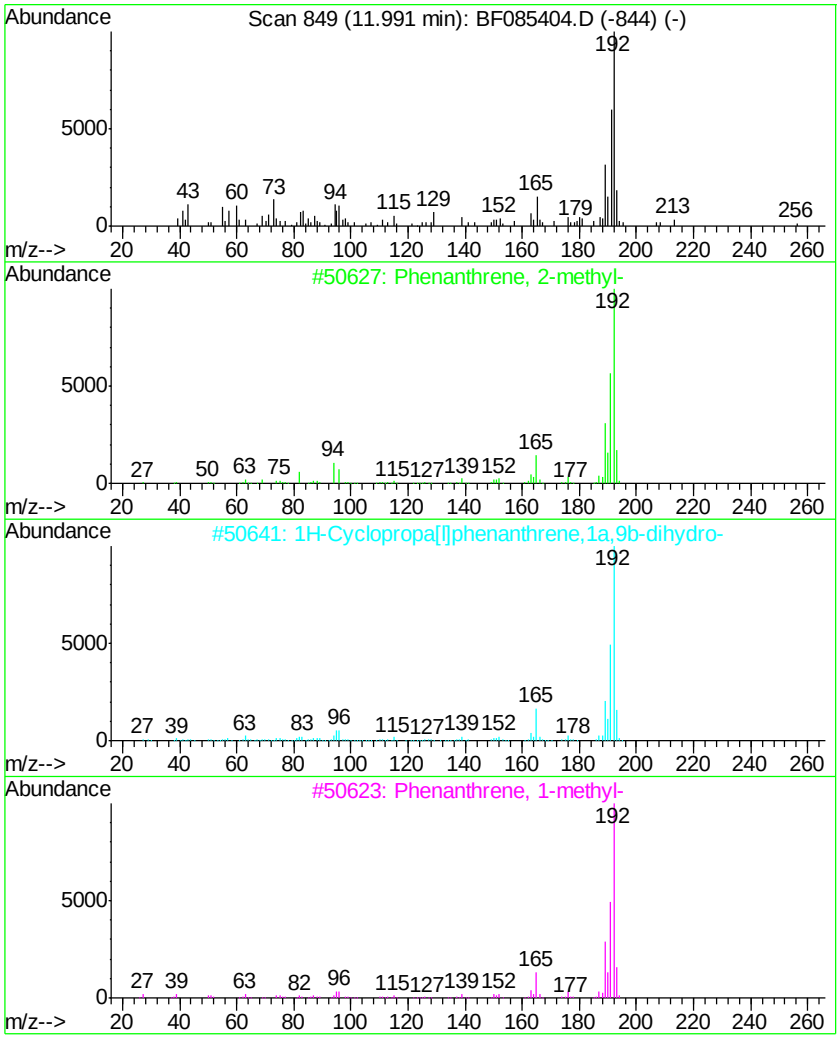
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

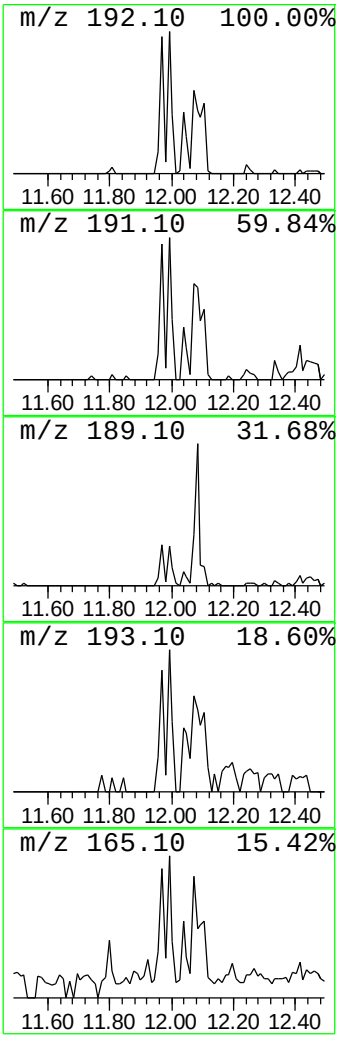
****

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	3.35 ng	168797	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
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Sample : H1730-04 5X
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

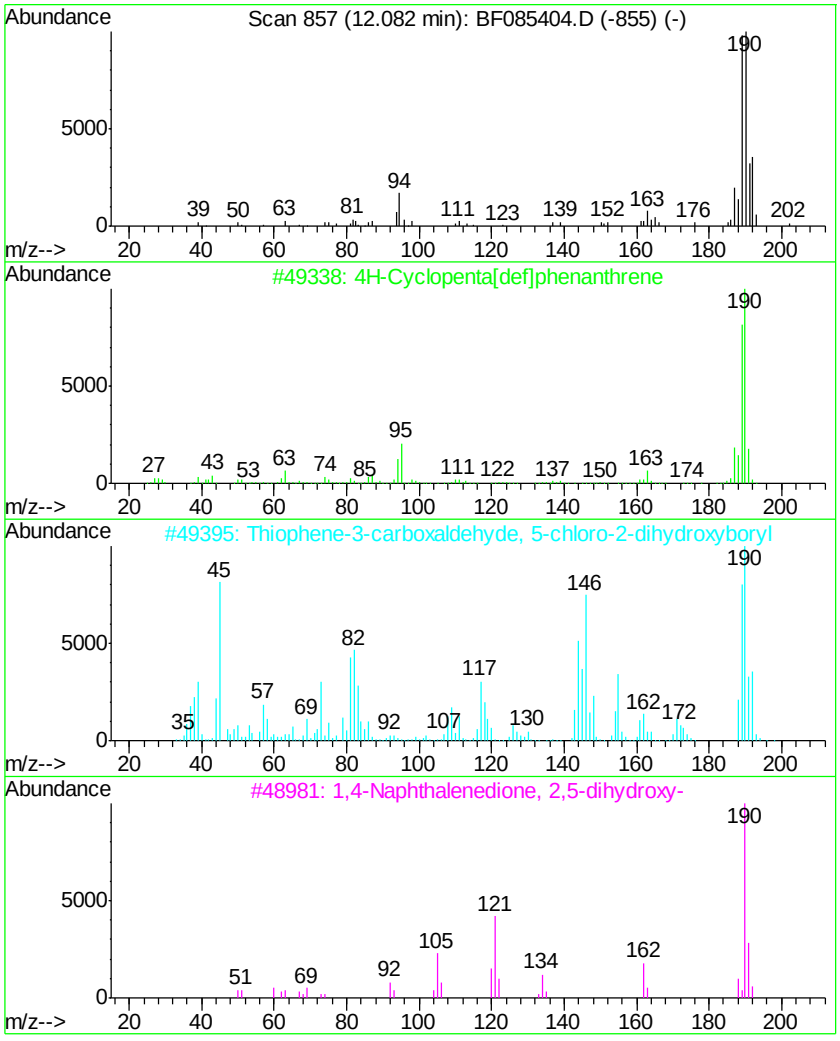
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

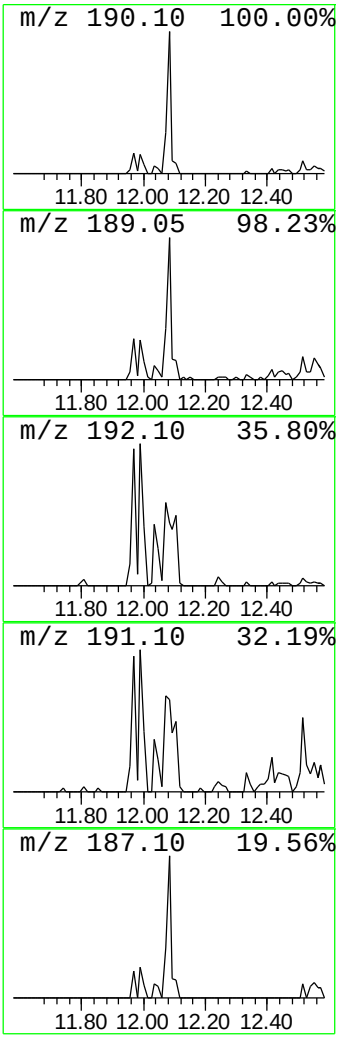
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	2.94 ng	147890	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	89
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
3	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	17
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	16
5	Methyl diselenide	190	C2H6Se2	007101-31-7	12





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Sample : H1730-04 5X
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BNA_F
ClientSampleId :
W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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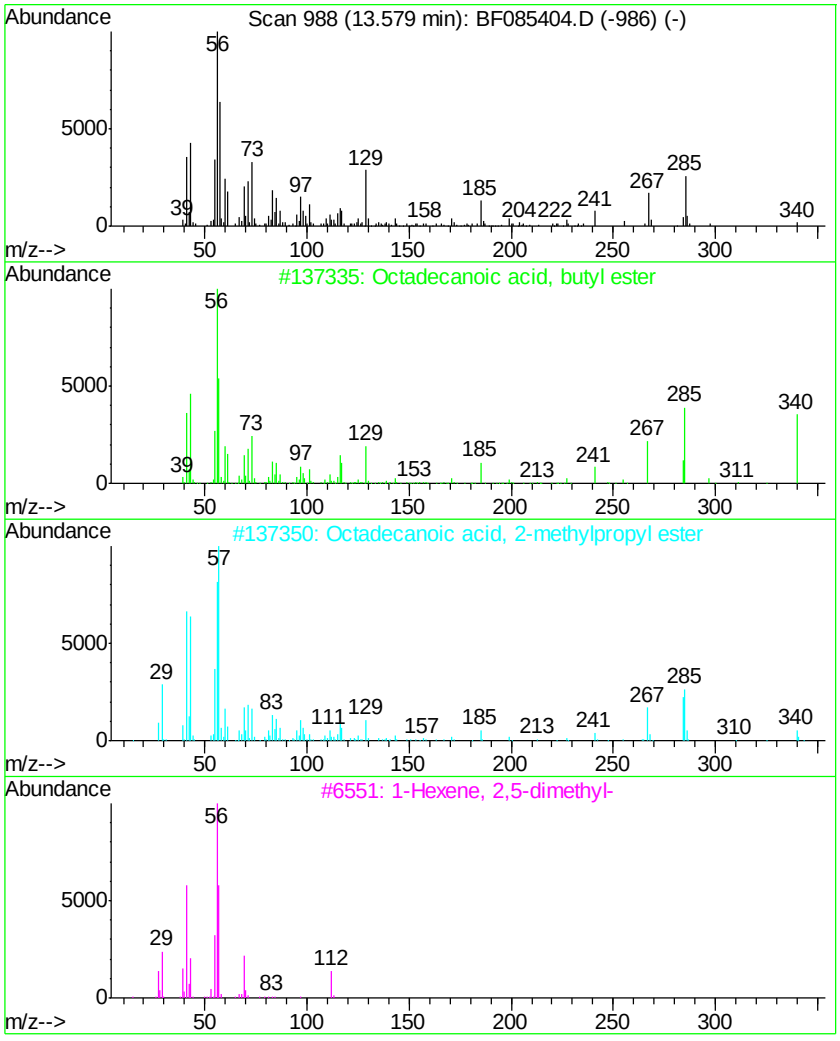
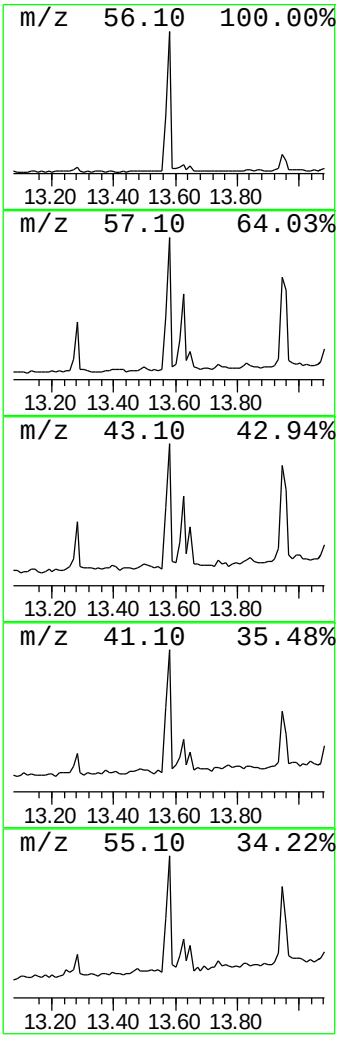
Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	2.77 ng	203683	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	80
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	30
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27





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Acq On : 12 Mar 2016 7:34
Operator : UM/SJ
Sample : H1730-04 5X
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

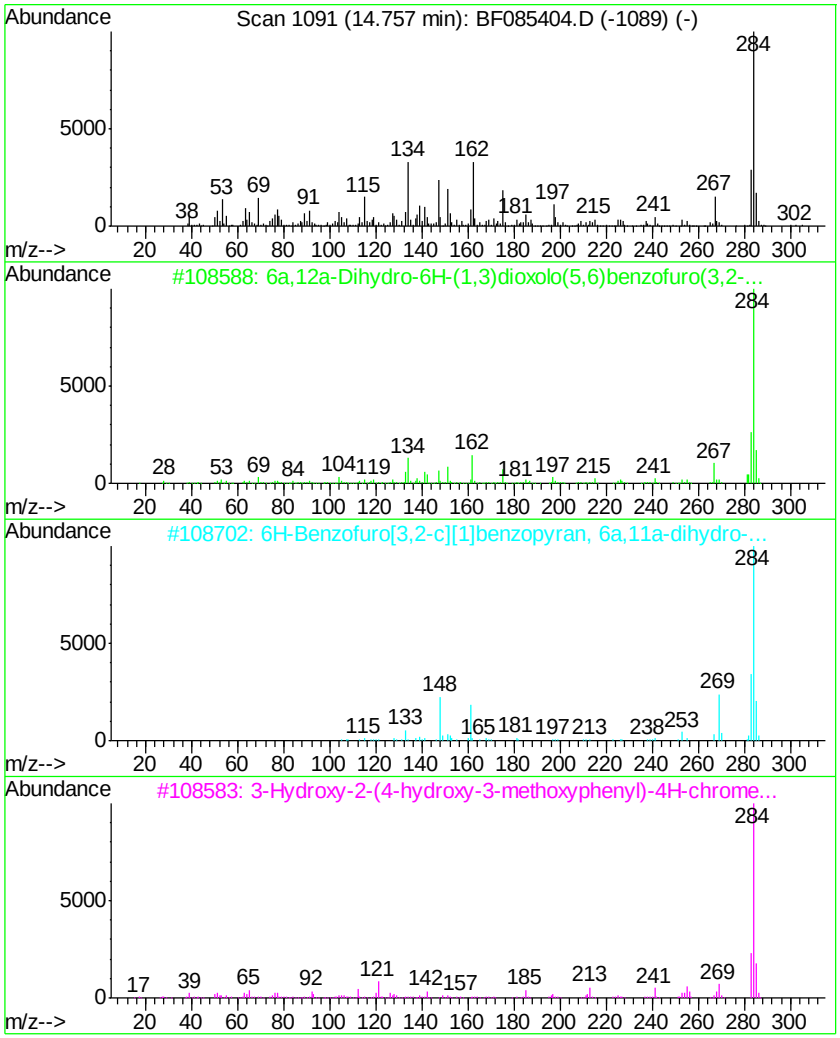
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

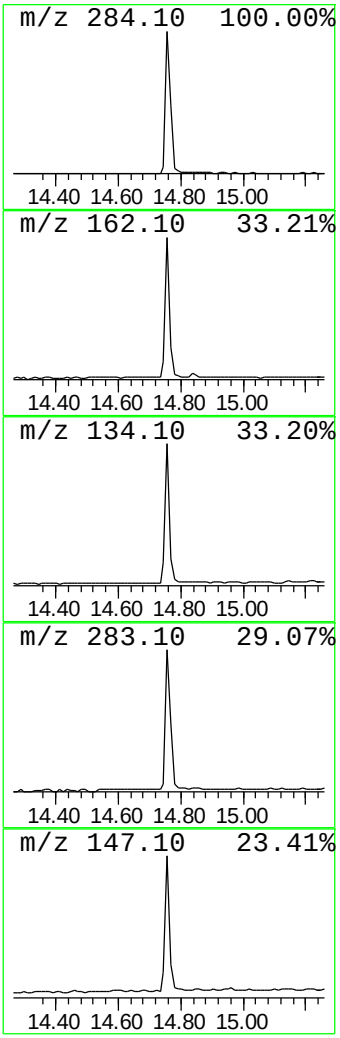
****

Peak Number 6 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	8.71 ng	640789	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	022091-18-5	93
2	6H-Benzofuro[3,2-c][1]benzopyran...	284	C17H16O4	000606-91-7	45
3	3-Hydroxy-2-(4-hydroxy-3-methoxy...	284	C16H12O5	159184-95-9	43
4	Benzo-1,3,2-dioxaborolane, 2-[2'...	284	C16H17BO4	1000164-23-9	38
5	2-(4-Biphenylyl)-6-methylimidazo...	284	C20H16N2	324741-46-0	35





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BNA_F
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W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

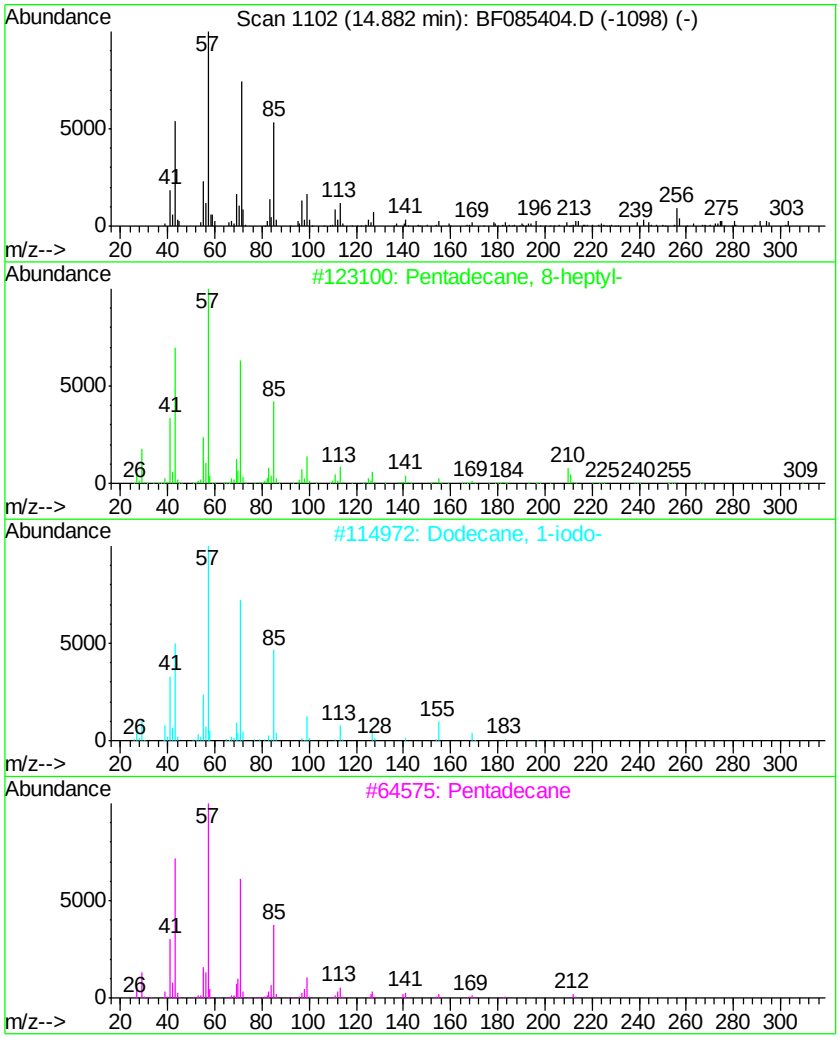
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

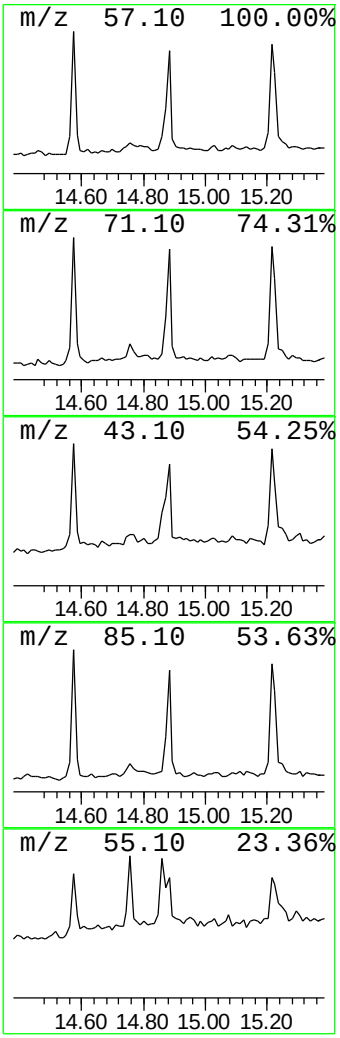
****

Peak Number 7 Pentadecane, 8-heptyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	3.37 ng	135811	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
3	Pentadecane	212	C15H32	000629-62-9	80
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	80





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Data File : BF085404.D
Acq On : 12 Mar 2016 7:34
Operator : UM/SJ
Sample : H1730-04 5X
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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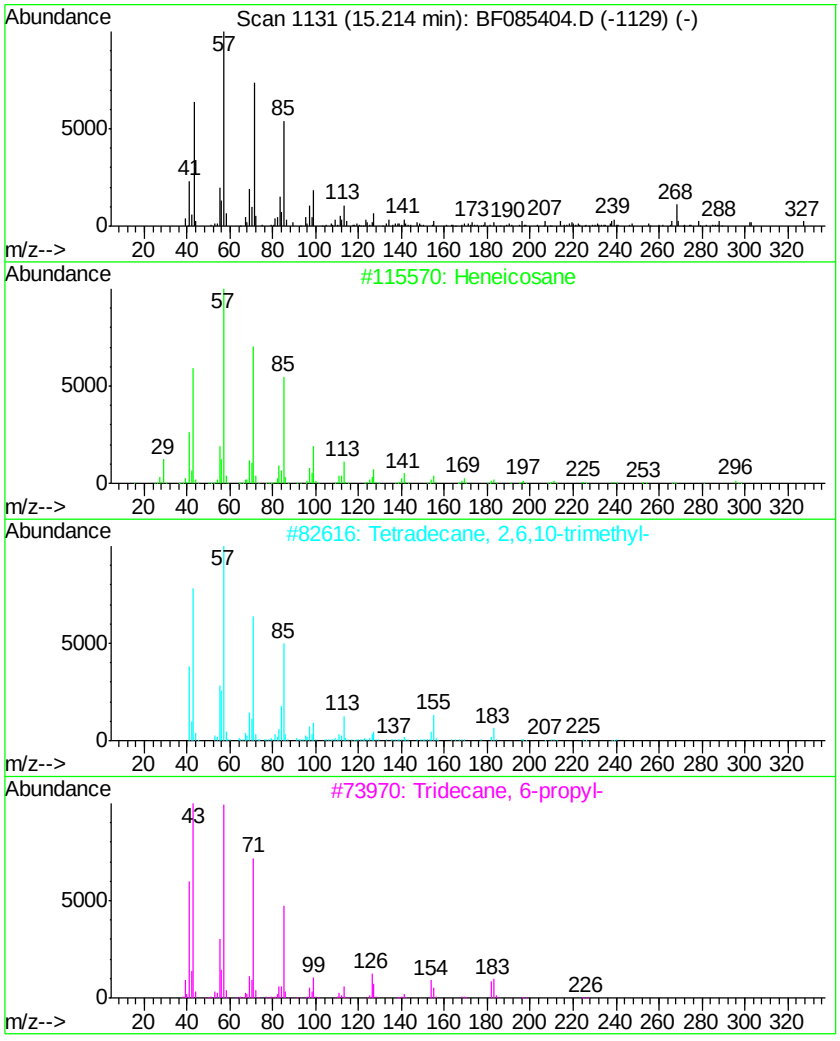
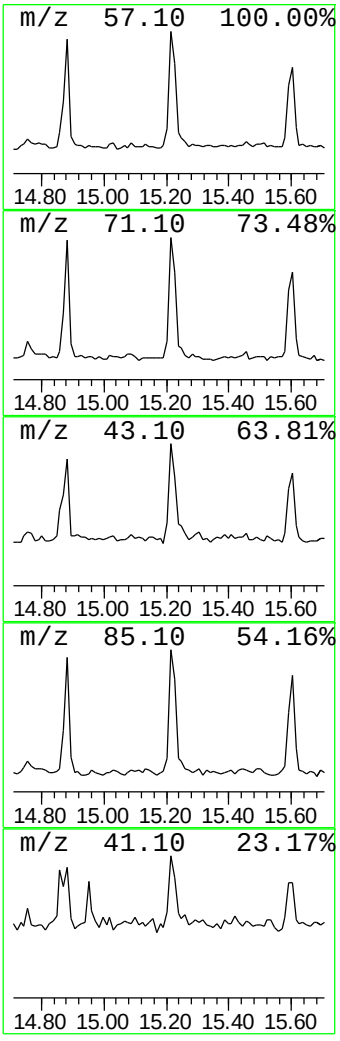
Peak Number 8 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.61 ng	105478	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
3	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085404.D
Acq On : 12 Mar 2016 7:34
Operator : UM/SJ
Sample : H1730-04 5X
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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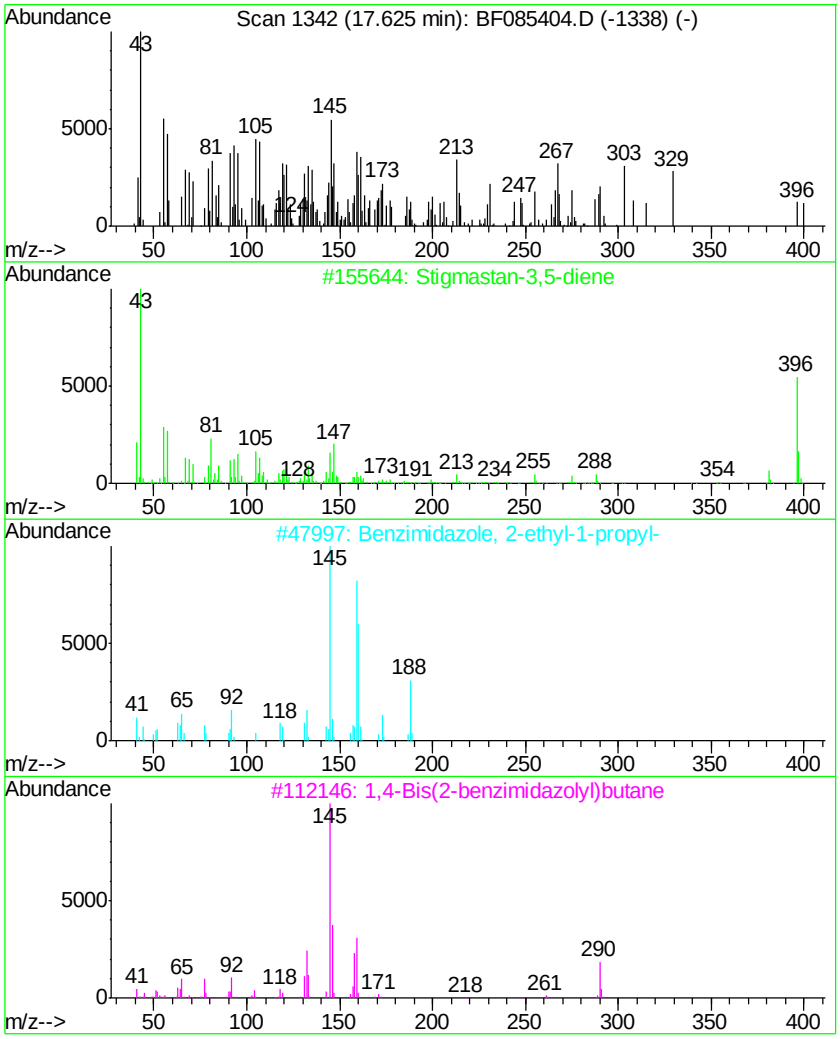
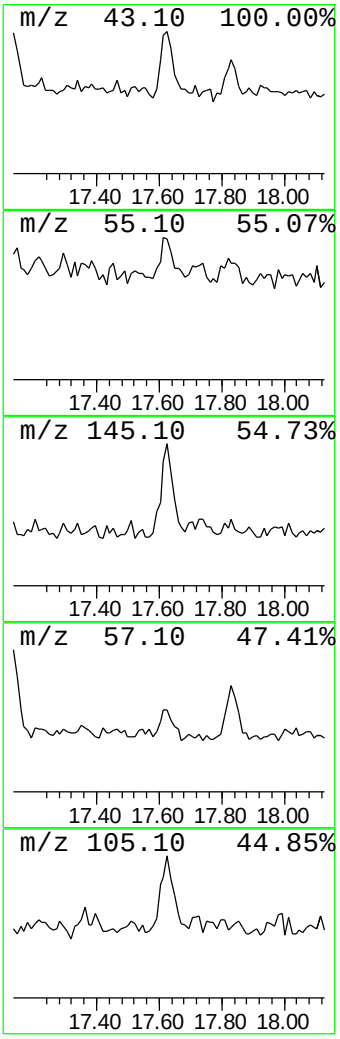
Peak Number 10 unknown17.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.63	3.68 ng	148535	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	41
2	Benzimidazole, 2-ethyl-1-propyl-	188	C12H16N2	024103-02-4	30
3	1,4-Bis(2-benzimidazolyl)butane	290	C18H18N4	004746-56-9	20
4	Corticosterone 21-acetate	388	C23H32O5	001173-26-8	16
5	N-(3-Chloro-4-fluoro-phenyl)-2-(...	329	C14H10Cl2FNOS	1000295-12-7	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085404.D
Acq On : 12 Mar 2016 7:34
Operator : UM/SJ
Sample : H1730-04 5X
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W170TH-SB-18-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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
unknown6.70	6.70	26.1	ng	1214490	1	6.94	932594	20.0
Phenanthrene, 2-m...	11.99	3.4	ng	168797	4	11.46	1007520	20.0
4H-Cyclopenta[def...	12.08	2.9	ng	147890	4	11.46	1007520	20.0
Octadecanoic acid...	13.58	2.8	ng	203683	5	14.11	1471610	20.0
6a,12a-Dihydro-6H...	14.76	8.7	ng	640789	5	14.11	1471610	20.0
Pentadecane, 8-he...	14.88	3.4	ng	135811	6	15.57	806740	20.0
Heneicosane	15.21	2.6	ng	105478	6	15.57	806740	20.0
unknown17.63	17.63	3.7	ng	148535	6	15.57	806740	20.0