LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085183.D
Acq On : 4 Mar 2016 3:45
Operator : SJ/UM
Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(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-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	5.190	251	254	262	rBV	798321	1099618	22.52%	2.352%
2	5.590	286	289	291	rBV	4059138	4369467	89.48%	9.348%
3	6.607	374	378	380	rBV	3923609	4883115	100.00%	10.447%
4	6.745	387	390	393	rBV	3876865	4420185	90.52%	9.456%
5	6.973	408	410	413	rBV	738538	889075	18.21%	1.902%
6	7.133	422	424	427	rVB	3350755	3478162	71.23%	7.441%
7	7.545	456	460	462	rBV	2970697	3373624	69.09%	7.217%
8	8.265	520	523	525	rBV	1362923	1251704	25.63%	2.678%
9	9.339	614	617	619	rBV	4849726	4467948	91.50%	9.558%
10	9.728	649	651	653	rBV	1005422	817354	16.74%	1.749%
11	9.945	668	670	672	rVB	182288	141393	2.90%	0.302%
12	10.013	674	676	678	rVB2	1106058	1179982	24.16%	2.524%
13	10.173	687	690	692	rBV	34271	58922	1.21%	0.126%
14	10.448	710	714	715	rBV	246290	243523	4.99%	0.521%
15	10.665	730	733	736	rBV	82442	130689	2.68%	0.280%
16	10.802	742	745	748	rBV	2411745	2749301	56.30%	5.882%
17	10.916	753	755	760	rVV	270494	305475	6.26%	0.654%
18	11.111	770	772	774	rBV	37945	52596	1.08%	0.113%
19	11.362	792	794	796	rBV	103148	93634	1.92%	0.200%
20	11.499	804	806	810	rBV2	1265785	1270950	26.03%	2.719%
21	11.568	810	812	814	rVB2	34056	62844	1.29%	0.134%
22	12.025	848	852	858	rBV3	232114	356512	7.30%	0.763%
23	12.116	858	860	863	rVB2	45554	81404	1.67%	0.174%
24	12.276	872	874	880	rVB3	41901	92928	1.90%	0.199%
25	12.551	895	898	899	rBV2	43678	60137	1.23%	0.129%
26	12.711	910	912	914	rBV	335391	289116	5.92%	0.619%
27	12.802	919	920	924	rBV2	68434	98832	2.02%	0.211%
28	12.939	929	932	935	rVB	489235	466926	9.56%	0.999%
29	13.088	942	945	947	rBV	3717135	3536496	72.42%	7.566%
30	13.157	947	951	955	rVB2	32085	55076	1.13%	0.118%
31	13.271	957	961	962	rBV	32944	64587	1.32%	0.138%
32	13.374	968	970	971	rBV	66279	63566	1.30%	0.136%
33	13.557	984	986	988	rVB	72066	57540	1.18%	0.123%
34	13.877	1012	1014	1016	rBV2	29901	57728	1.18%	0.123%

LSC Area Percent Report

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Data File : BF085183.D
Acq On : 4 Mar 2016 3:45
Operator : SJ/UM
Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.980	1021	1023	1028	rVB2	145684	236189	4.84%	0.505%
36	14.140	1032	1037	1038	rBV3	758691	1380057	28.26%	2.952%
37	14.277	1047	1049	1050	rBV	44673	49969	1.02%	0.107%
38	14.517	1066	1070	1072	rBV2	66602	177963	3.64%	0.381%
39	14.768	1089	1092	1095	rBV4	36013	63989	1.31%	0.137%
40	14.860	1098	1100	1101	rBV	35917	49332	1.01%	0.106%
41	14.985	1109	1111	1113	rBV	248888	302533	6.20%	0.647%
42	15.180	1125	1128	1133	rBV	189981	415592	8.51%	0.889%
43	15.283	1136	1137	1140	rVB	56699	54844	1.12%	0.117%
44	15.477	1152	1154	1157	rBV	192924	277087	5.67%	0.593%
45	15.545	1157	1160	1163	rVV	263942	352784	7.22%	0.755%
46	15.603	1163	1165	1171	rVB2	501672	919035	18.82%	1.966%
47	15.991	1196	1199	1202	rVB2	347059	493901	10.11%	1.057%
48	16.494	1241	1243	1248	rVB5	39706	88947	1.82%	0.190%
49	17.077	1290	1294	1298	rVB2	117803	243609	4.99%	0.521%
50	17.260	1307	1310	1313	rBV	36785	85451	1.75%	0.183%
51	17.523	1329	1333	1339	rBV	154904	338837	6.94%	0.725%
52	17.683	1343	1347	1351	rVV6	33715	94461	1.93%	0.202%
53	17.751	1351	1353	1360	rVB	38272	102022	2.09%	0.218%
54	17.888	1362	1365	1373	rVB7	32868	108213	2.22%	0.232%
55	18.026	1373	1377	1383	rBV4	97942	288393	5.91%	0.617%

Sum of corrected areas: 46743617

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Sample : H1648-10
Misc :
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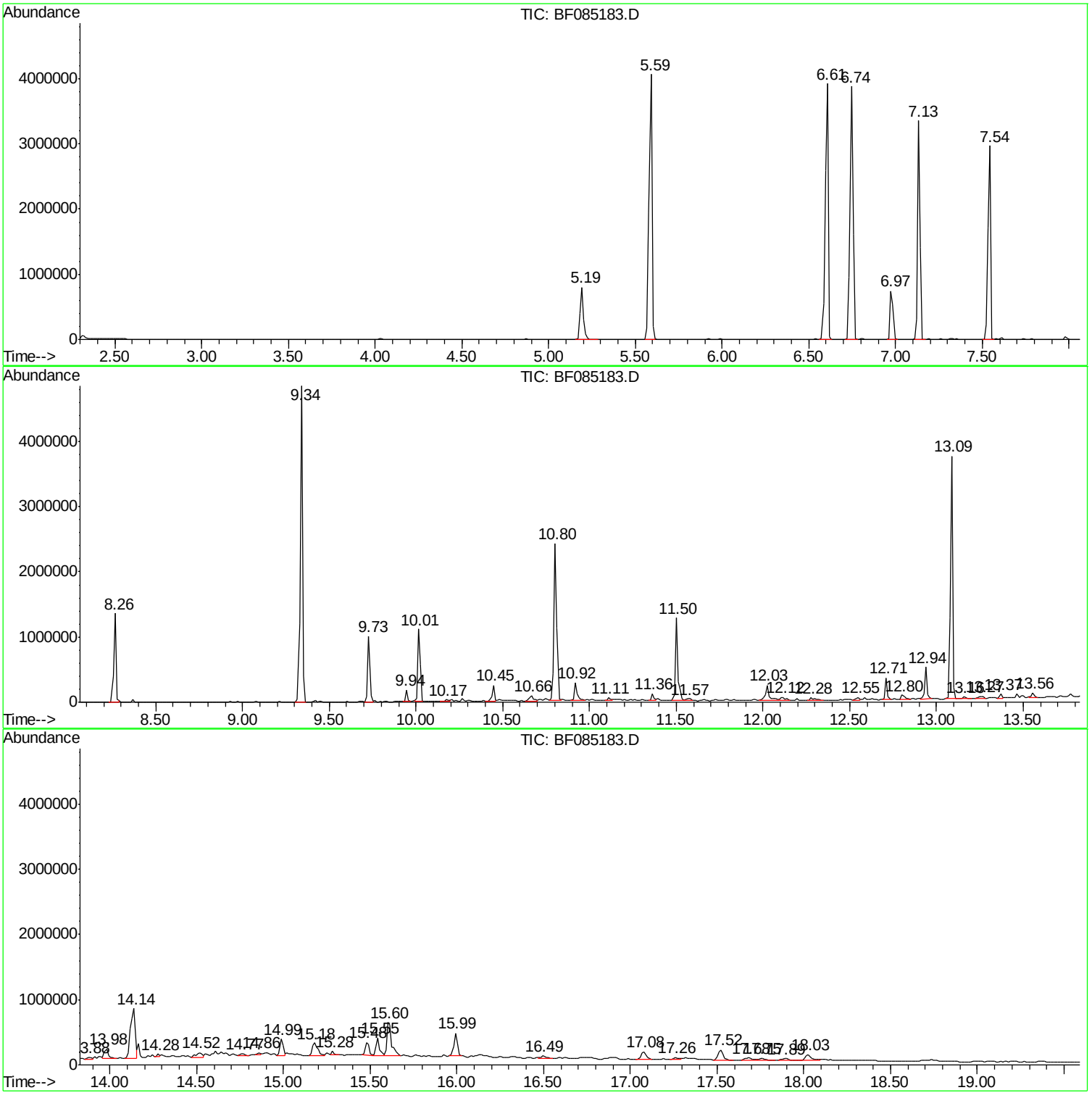
Instrument :
BNA_F
ClientSampleId :
SB-52(COMP)

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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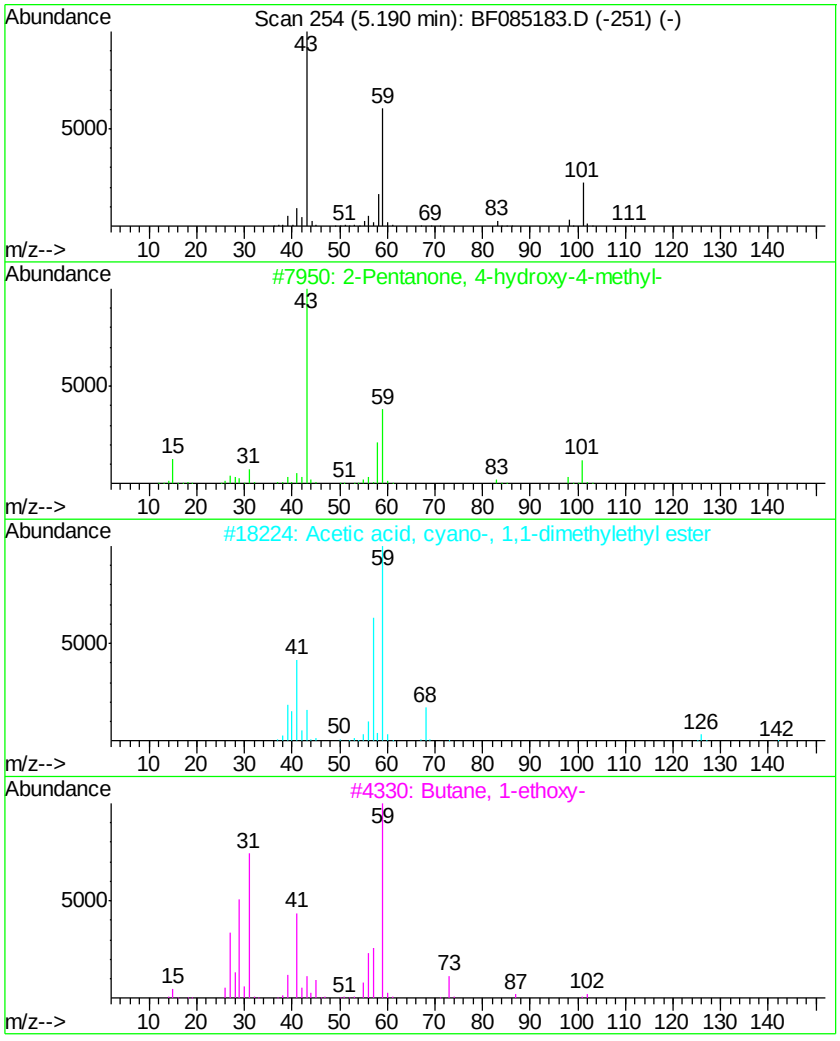
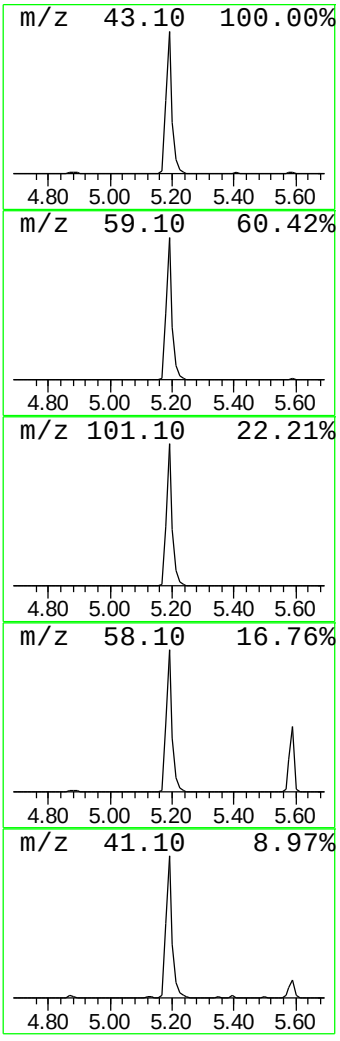
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	24.74 ng	1099620	1,4-Dichlorobenzene-d4	6.97

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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Acq On : 4 Mar 2016 3:45
Operator : SJ/UM
Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

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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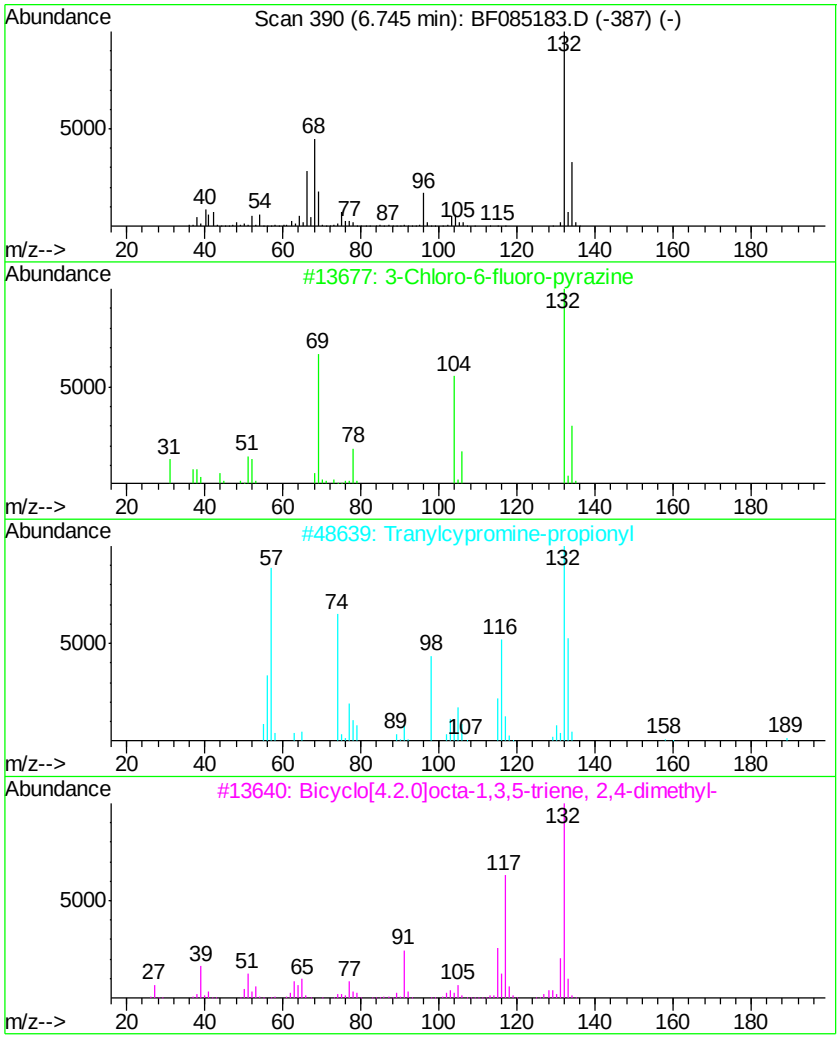
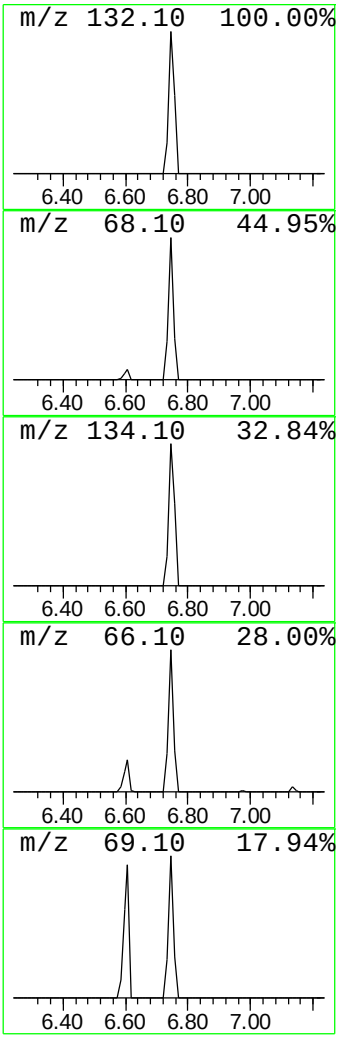
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	99.43 ng	4420190	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Data File : BF085183.D
Acq On : 4 Mar 2016 3:45
Operator : SJ/UM
Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

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
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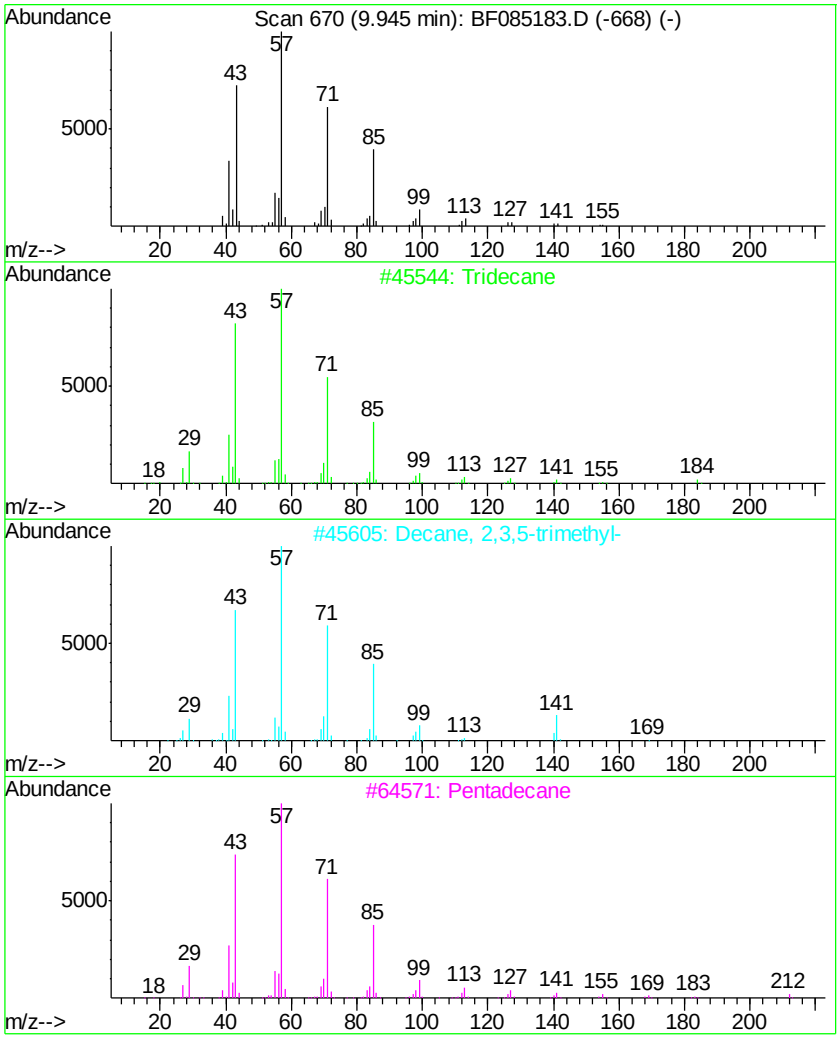
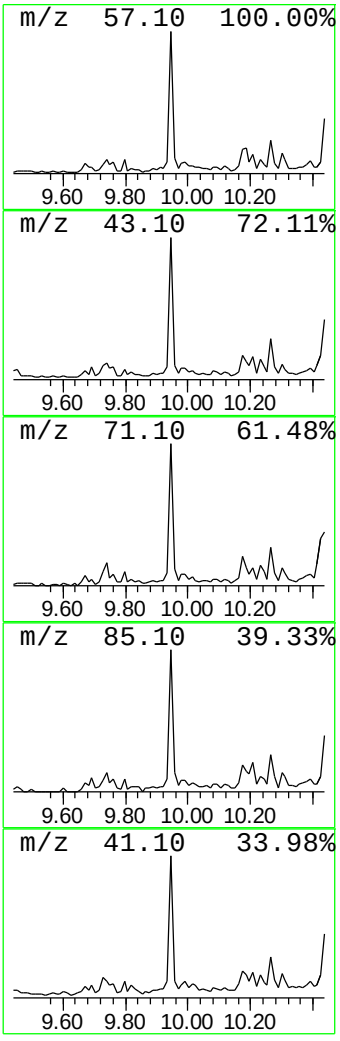
Peak Number 4 Tridecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.94	2.40 ng	141393	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
3	Pentadecane	212	C15H32	000629-62-9	83
4	Hexadecane	226	C16H34	000544-76-3	80
5	Tetradecane	198	C14H30	000629-59-4	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085183.D
Acq On : 4 Mar 2016 3:45
Operator : SJ/UM
Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

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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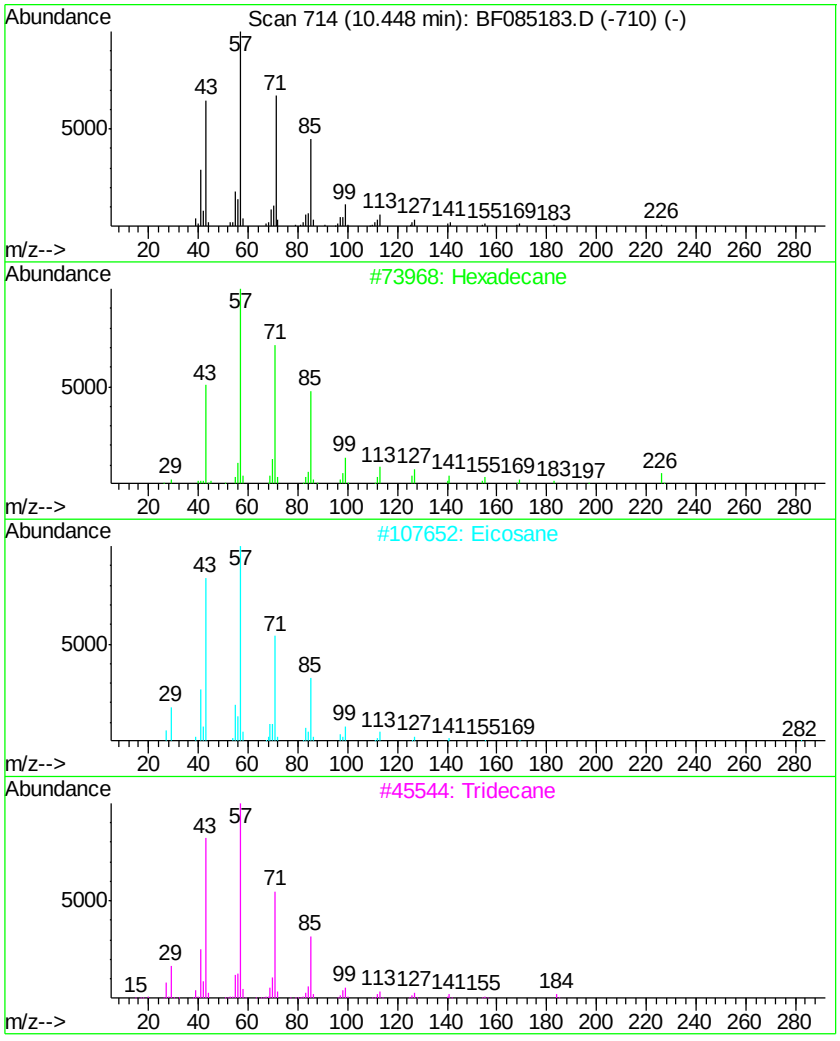
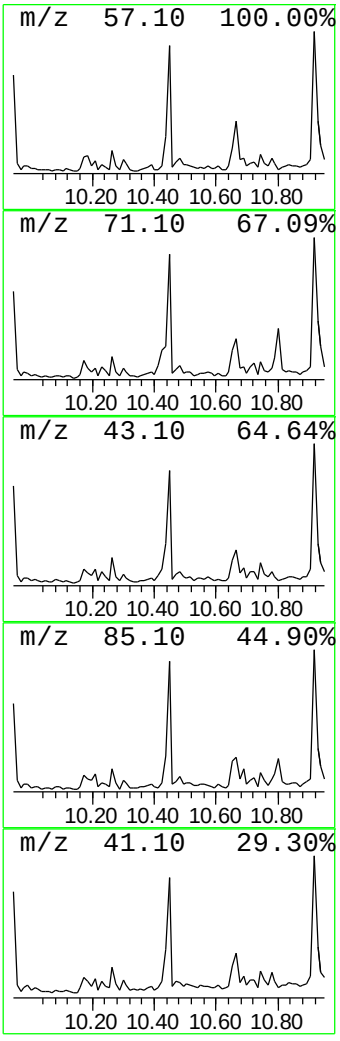
Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	4.13 ng	243523	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Eicosane	282	C20H42	000112-95-8	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetradecane	198	C14H30	000629-59-4	87





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Sample : H1648-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-52(COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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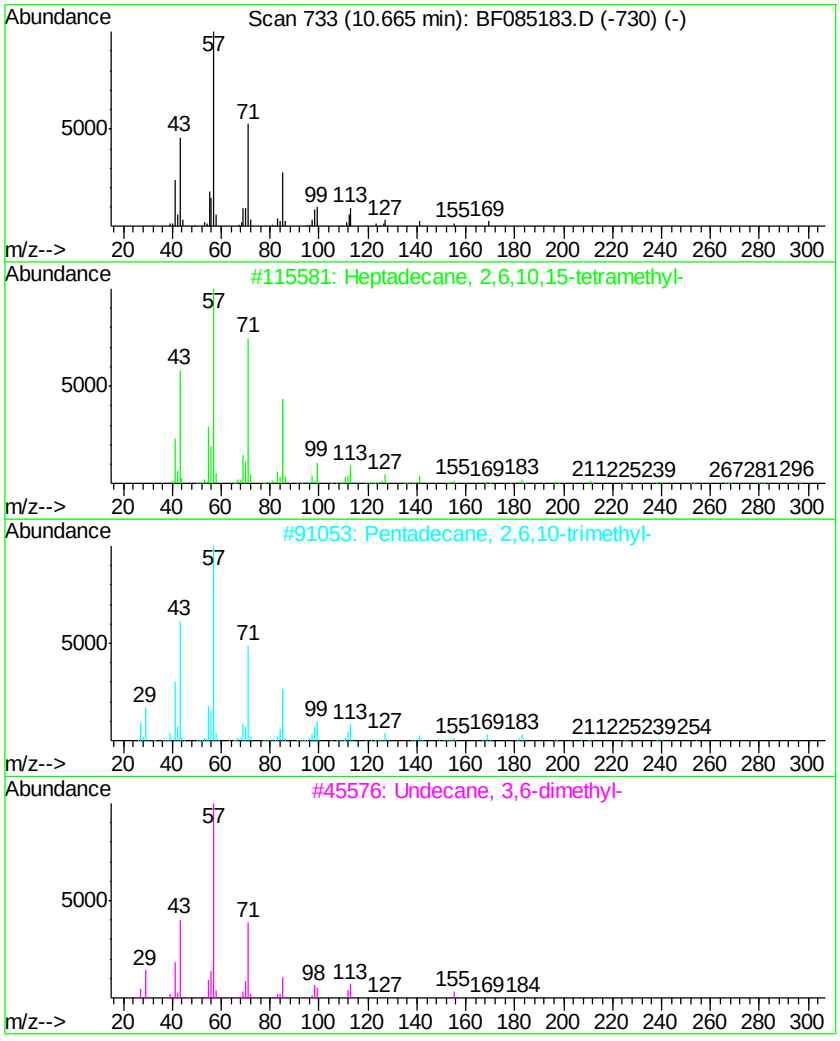
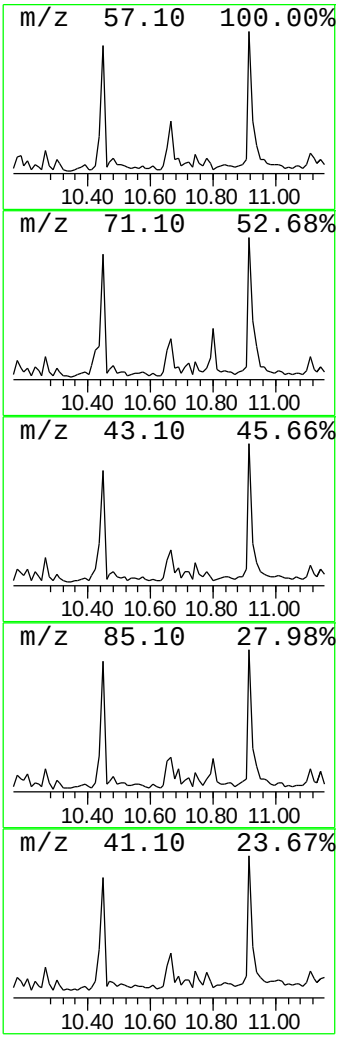
Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.22 ng	130689	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	80
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	78
4	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	72
5	Heptacosane	380	C27H56	000593-49-7	72





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Instrument : BNA_F
ClientSampleId : SB-52(COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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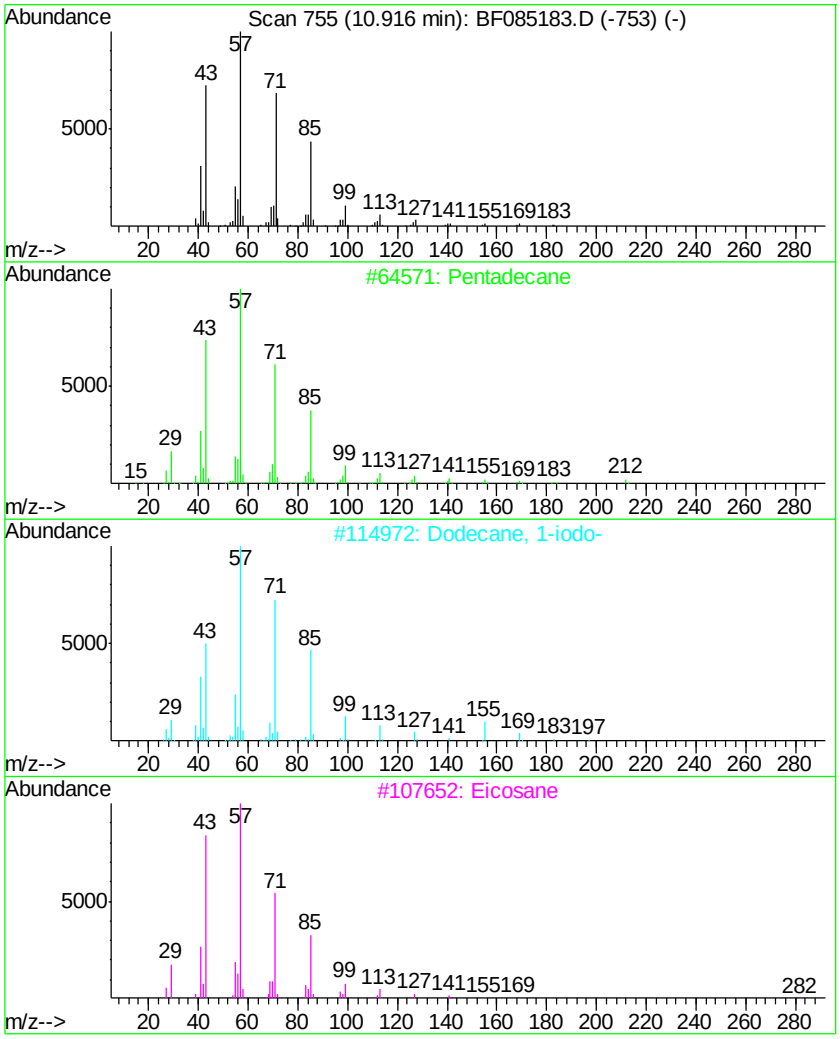
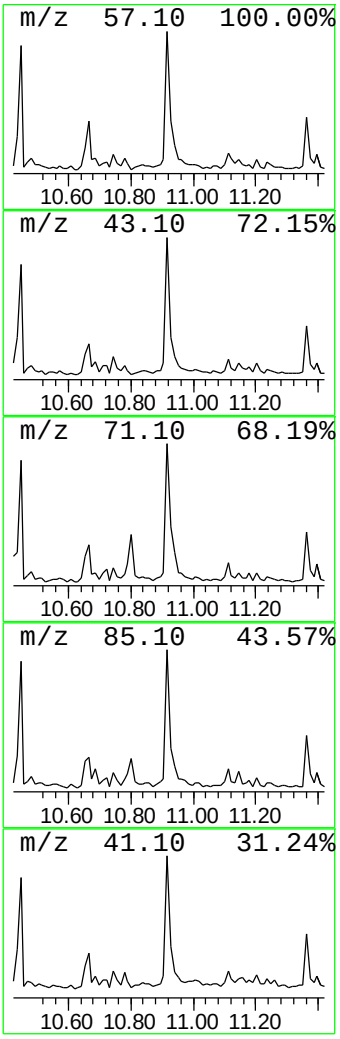
Peak Number 7 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.92	4.81 ng	305475	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Eicosane	282	C20H42	000112-95-8	83
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5	Hexadecane	226	C16H34	000544-76-3	80





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ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

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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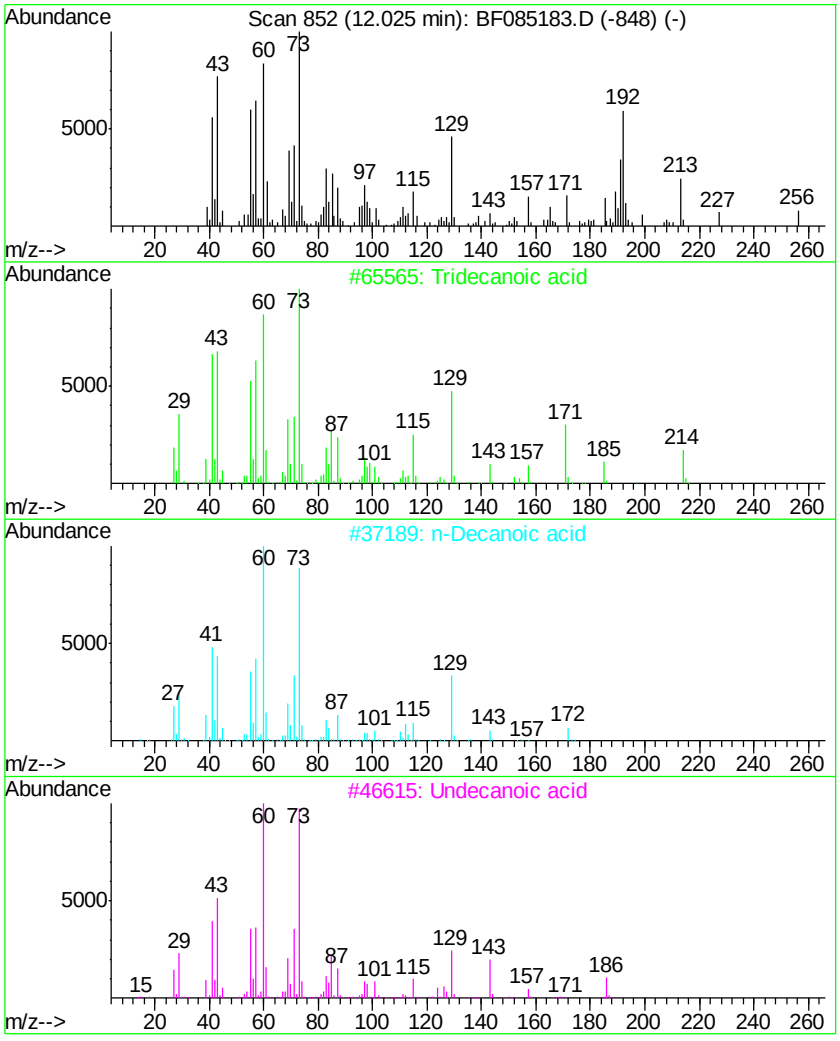
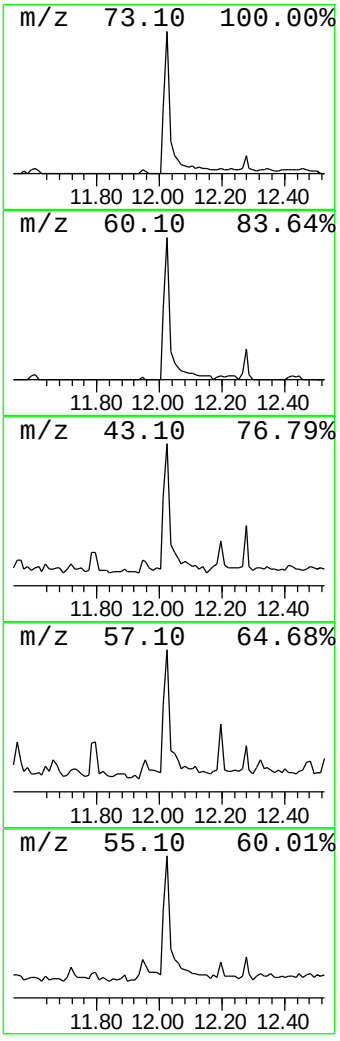
Peak Number 8 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	5.61 ng	356512	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	92
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	58
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085183.D
Acq On : 4 Mar 2016 3:45
Operator : SJ/UM
Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

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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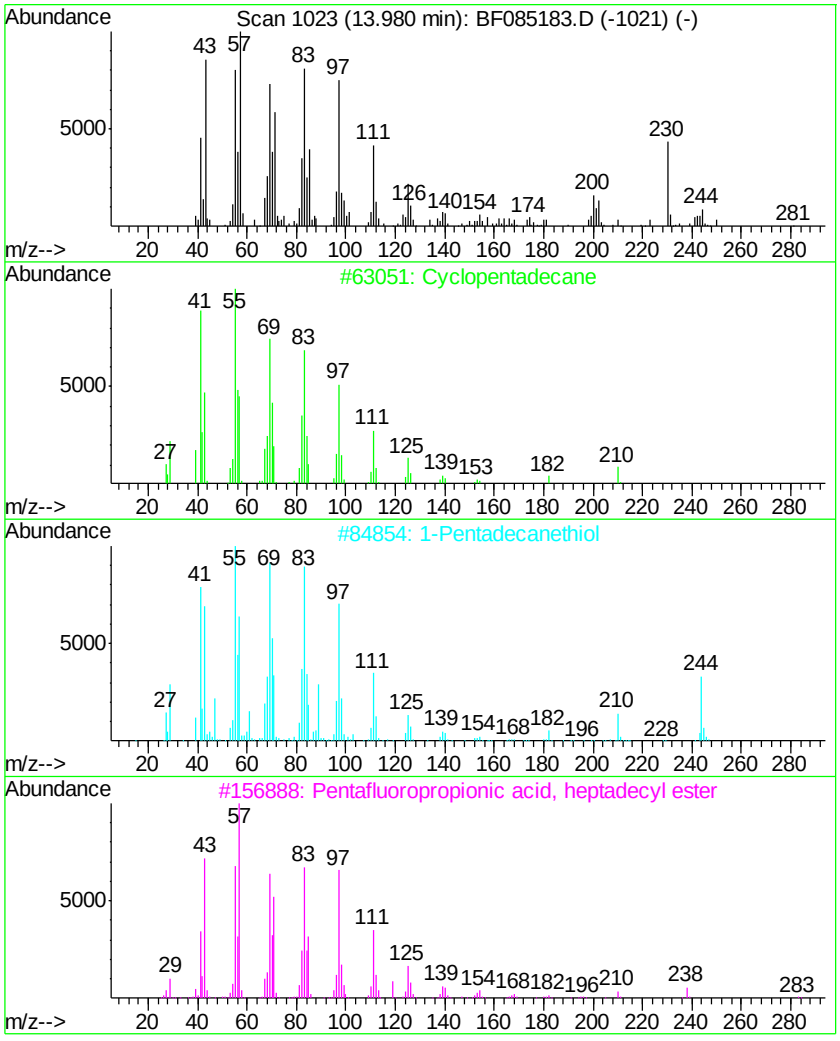
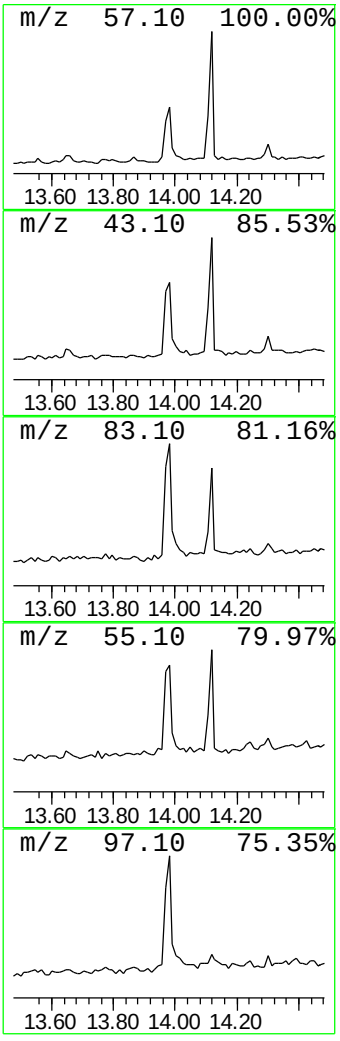
Peak Number 9 Cyclopentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	3.42 ng	236189	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	1-Pentadecanethiol	244	C15H32S	025276-70-4	93
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	93
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93





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Data File : BF085183.D
Acq On : 4 Mar 2016 3:45
Operator : SJ/UM
Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

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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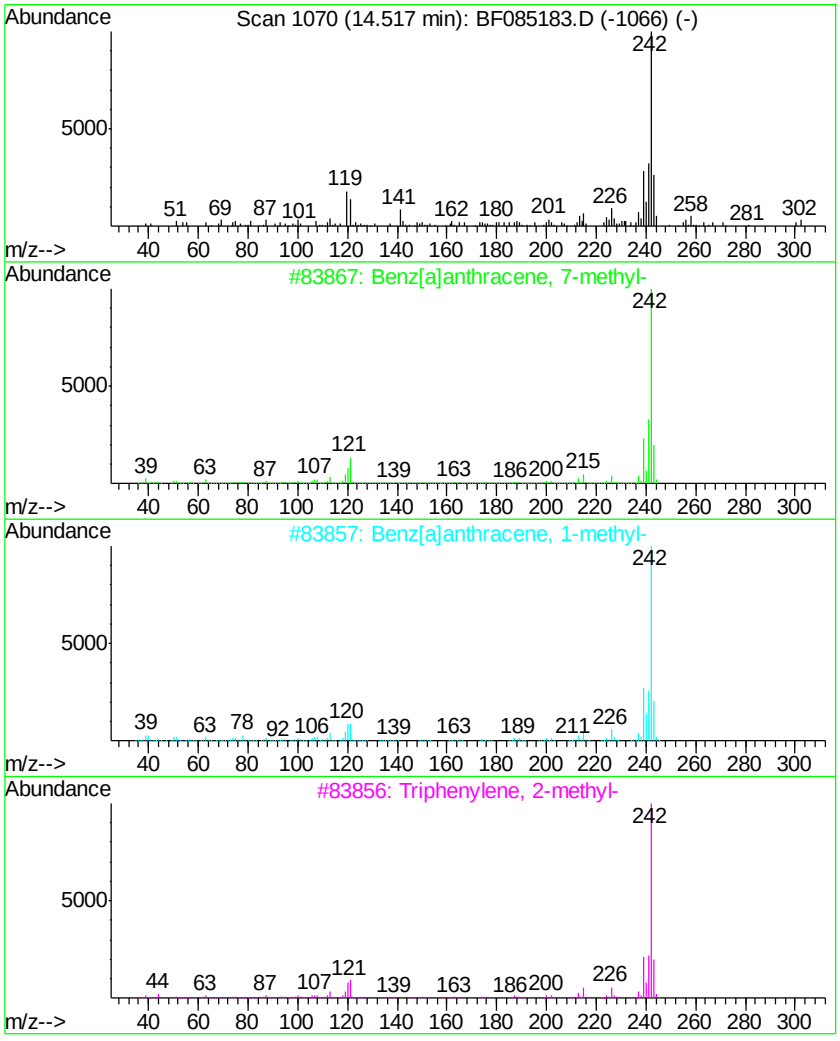
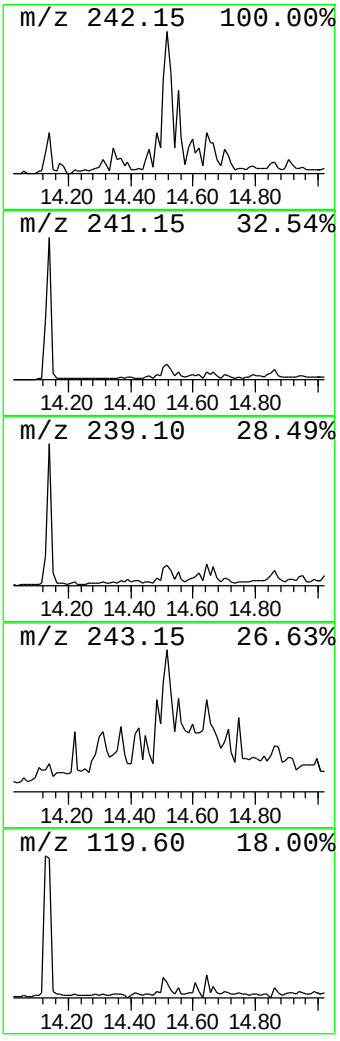
Peak Number 10 Benz[a]anthracene, 7-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.58 ng	177963	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	95
2	Benz[a]anthracene, 1-methyl-	242	C19H14	002498-77-3	94
3	Triphenylene, 2-methyl-	242	C19H14	001705-84-6	93
4	Benz[a]anthracene, 8-methyl-	242	C19H14	002381-31-9	92
5	Chrysene, 6-methyl-	242	C19H14	003697-24-3	90





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Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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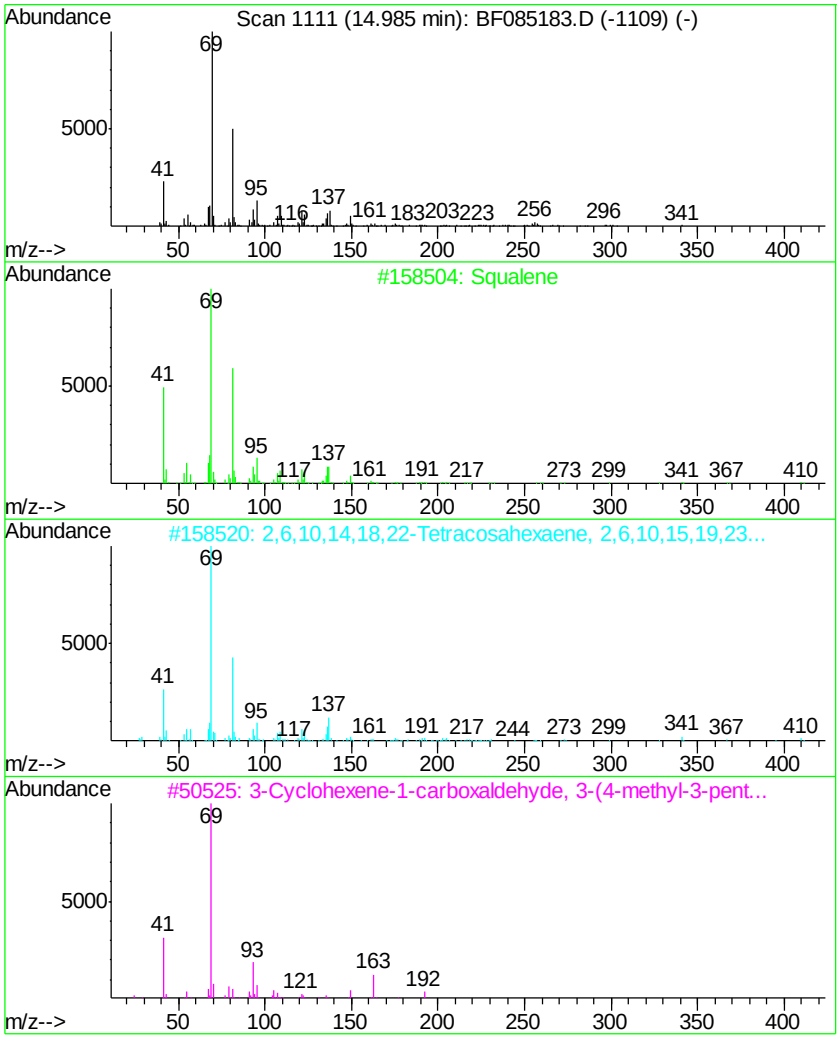
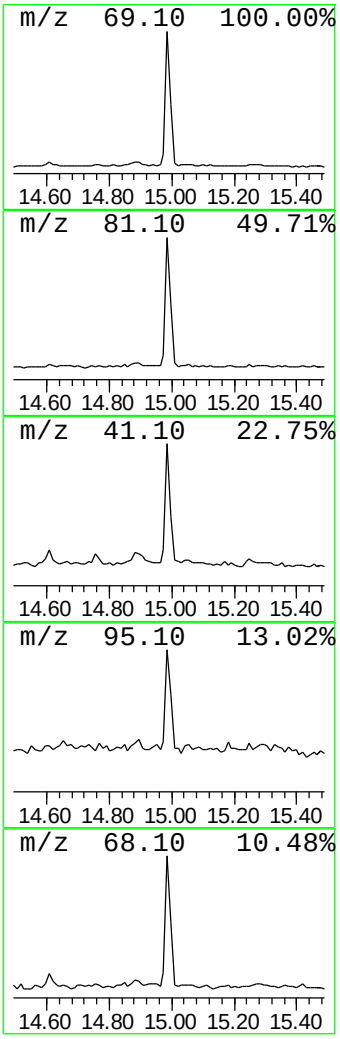
Peak Number 11 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	6.58 ng	302533	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	64
4	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	53





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Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Integration Parameters: LSCINT.P

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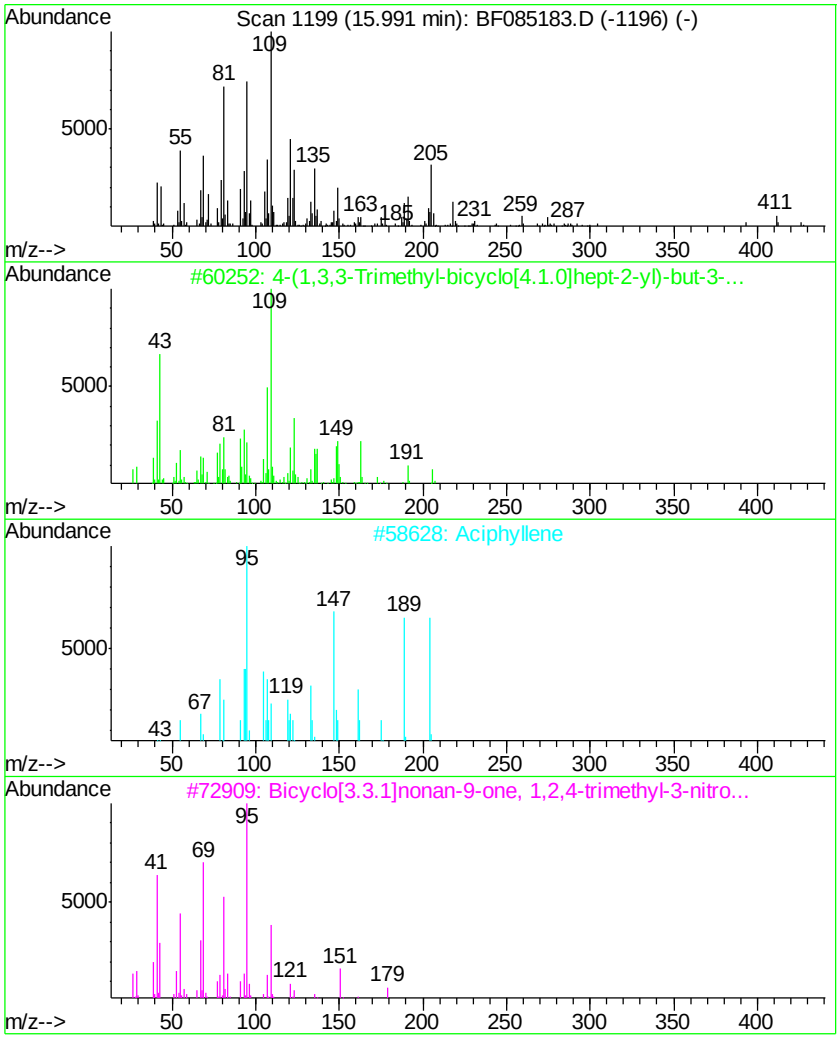
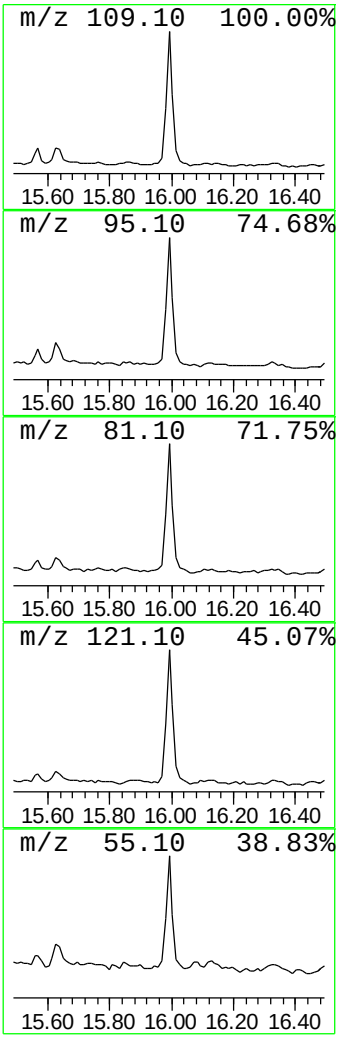
Peak Number 13 unknown15.99 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	10.75 ng	493901	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	47
2	Aciphyllene	204	C15H24	087745-31-1	30
3	Bicyclo[3.3.1]nonan-9-one, 1,2,4...	225	C12H19NO3	129967-65-3	27
4	5,9-Undecadien-2-ol, 6,10-dimethyl-	196	C13H24O	053837-34-6	27
5	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	22





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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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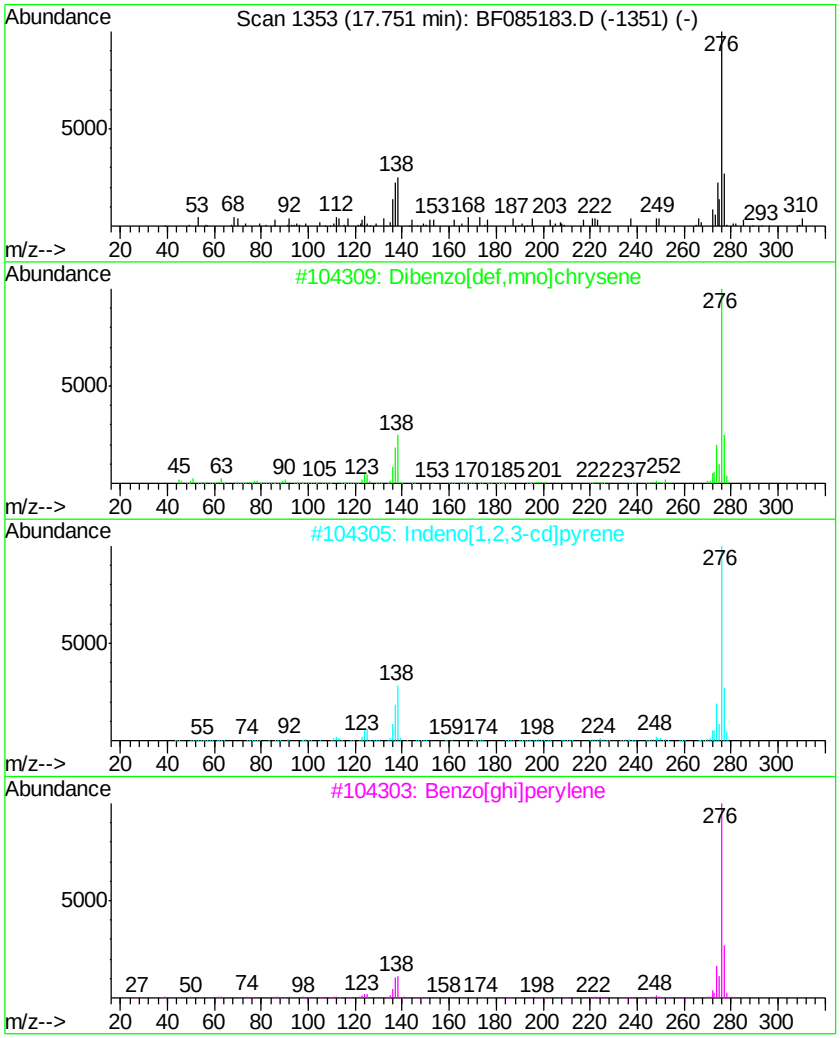
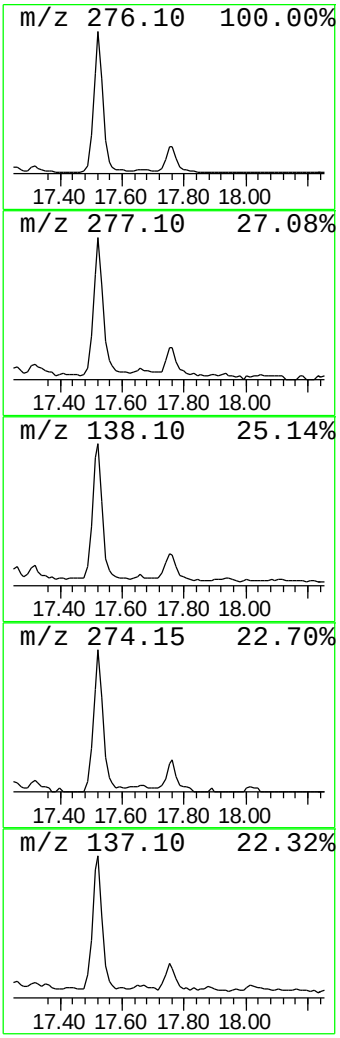
Peak Number 15 Dibenzo[def,mno]chrysene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	2.22 ng	102022	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	91
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	91
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	91
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	74
5	Dithiocarbonic acid, S-methyl es...	383	C20H33NO2S2	1000202-13-0	32





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Operator : SJ/UM
Sample : H1648-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-52(COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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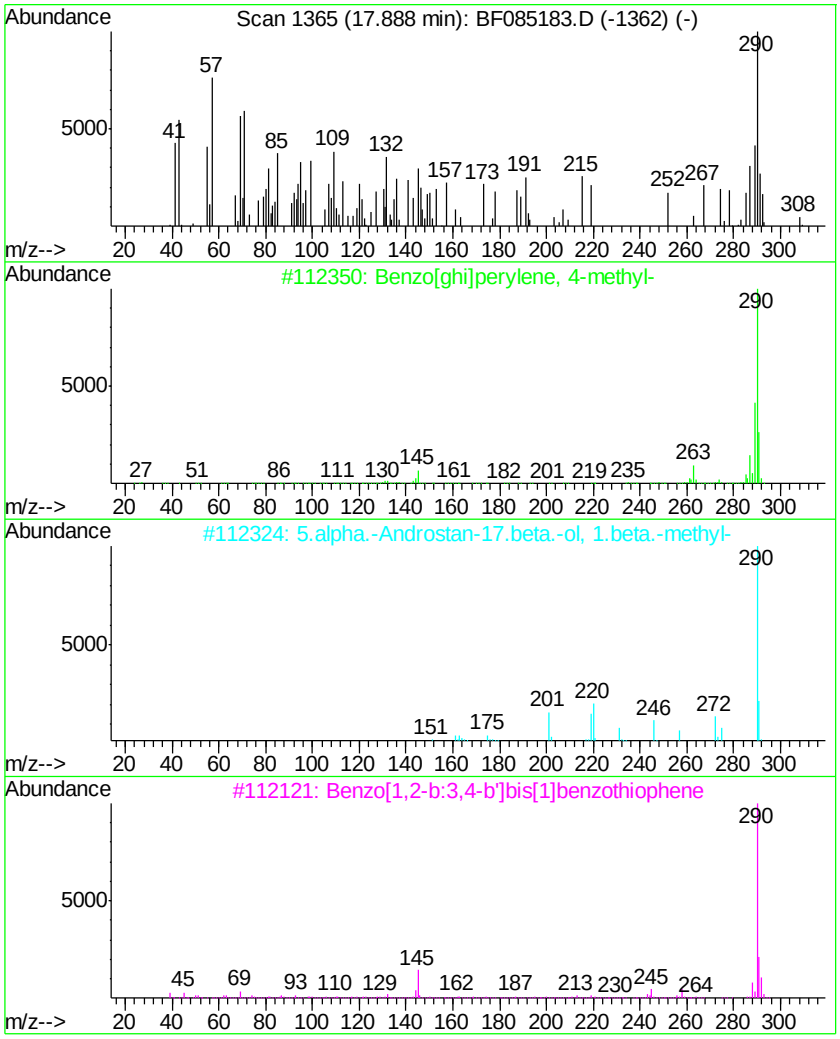
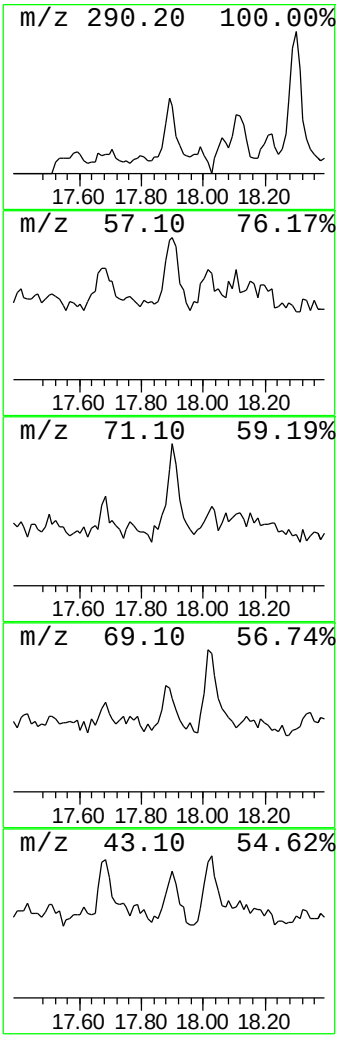
Peak Number 16 unknown17.89 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	2.35 ng	108213	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[ghi]perylene, 4-methyl-	290	C23H14	019224-38-5	43
2	5.alpha.-Androstan-17.beta.-ol, ...	290	C20H34O	005846-88-8	35
3	Benzo[1,2-b:3,4-b']bis[1]benzoth...	290	C18H10S2	000198-89-0	35
4	Benzo[2,1-b:3,4-b']bis[1]benzoth...	290	C18H10S2	000222-24-2	30
5	Androstane-3,12,17-triol, (3.bet...	308	C19H32O3	053608-26-7	30





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Instrument : BNA_F
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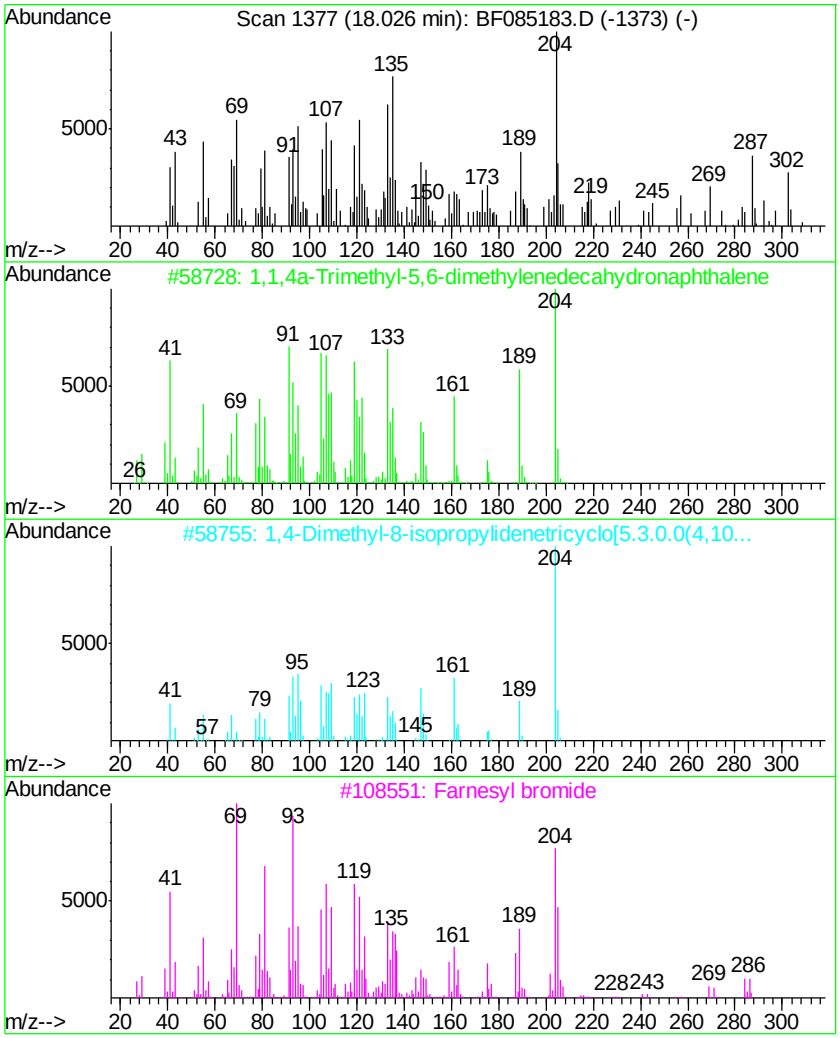
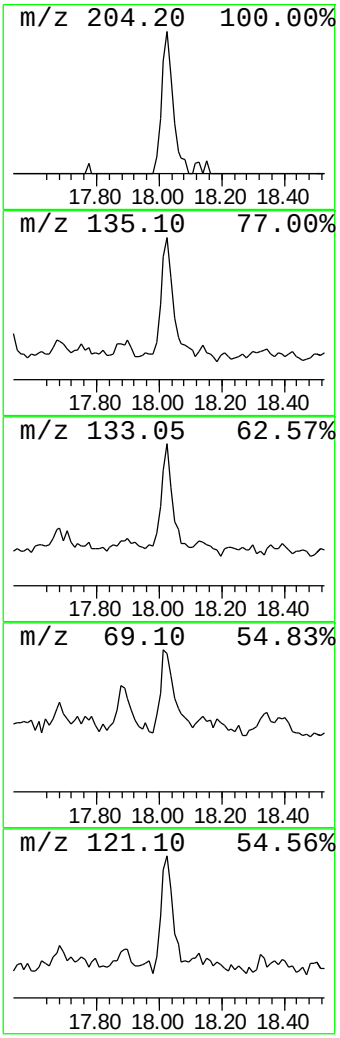
Peak Number 17 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	6.28 ng	288393	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	60
2	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	58
3	Farnesyl bromide	284	C15H25Br	006874-67-5	53
4	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49
5	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	49





Tentatively Identified Compound (LSC) summary

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Operator : SJ/UM
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Misc :
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Instrument : BNA_F
ClientSampleId : SB-52(COMP)

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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...	5.19	24.7	ng	1099620	1	6.97	889075	20.0
unknown6.74	6.74	99.4	ng	4420190	1	6.97	889075	20.0
Tridecane	9.94	2.4	ng	141393	3	10.01	1179980	20.0
Hexadecane	10.45	4.1	ng	243523	3	10.01	1179980	20.0
Heptadecane, 2,6,...	10.66	2.2	ng	130689	3	10.01	1179980	20.0
Pentadecane	10.92	4.8	ng	305475	4	11.50	1270950	20.0
Tridecanoic acid	12.03	5.6	ng	356512	4	11.50	1270950	20.0
Cyclopentadecane	13.98	3.4	ng	236189	5	14.14	1380060	20.0
Benz[a]anthracene...	14.52	2.6	ng	177963	5	14.14	1380060	20.0
Squalene	14.99	6.6	ng	302533	6	15.61	919035	20.0
unknown15.99	15.99	10.8	ng	493901	6	15.61	919035	20.0
Dibenzo[def,mno]c...	17.75	2.2	ng	102022	6	15.61	919035	20.0
unknown17.89	17.89	2.4	ng	108213	6	15.61	919035	20.0
1,1,4a-Trimethyl-...	18.03	6.3	ng	288393	6	15.61	919035	20.0