LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085185.D
Acq On : 4 Mar 2016 4:41
Operator : SJ/UM
Sample : H1661-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-51-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	261	rVB	807791	1107714	24.50%	2.762%
2	5.590	286	289	291	rBV	3966047	4120948	91.15%	10.274%
3	6.607	375	378	380	rBV	3853769	4363187	96.51%	10.878%
4	6.744	387	390	393	rBV	3507399	4520873	100.00%	11.271%
5	6.984	408	411	413	rVB	771090	933025	20.64%	2.326%
6	7.133	422	424	427	rVB	2726570	3512557	77.70%	8.757%
7	7.544	457	460	462	rBV	3037911	3118497	68.98%	7.775%
8	7.613	464	466	469	rVB	50111	60397	1.34%	0.151%
9	8.265	520	523	525	rBV	1536781	1279033	28.29%	3.189%
10	9.339	614	617	620	rBV	4480127	4333247	95.85%	10.803%
11	9.728	649	651	653	rBV	902157	758672	16.78%	1.891%
12	9.945	668	670	672	rVB	110973	94941	2.10%	0.237%
13	10.025	674	677	679	rVB	1014919	1198444	26.51%	2.988%
14	10.425	710	712	713	rBV	42368	50905	1.13%	0.127%
15	10.448	713	714	716	rVB	159255	111930	2.48%	0.279%
16	10.665	730	733	736	rBV	43385	71023	1.57%	0.177%
17	10.802	743	745	748	rBV2	1726482	2463312	54.49%	6.141%
18	10.916	754	755	762	rBV	127066	170543	3.77%	0.425%
19	11.362	792	794	796	rBV	66626	74909	1.66%	0.187%
20	11.499	804	806	809	rBV2	903842	1080534	23.90%	2.694%
21	11.556	809	811	814	rVB2	35310	63652	1.41%	0.159%
22	12.025	849	852	857	rBV2	265915	334957	7.41%	0.835%
23	12.116	857	860	864	rVB	36309	74418	1.65%	0.186%
24	12.196	865	867	869	rBV2	39934	51348	1.14%	0.128%
25	12.299	872	876	878	rBV2	23439	48076	1.06%	0.120%
26	12.711	911	912	915	rBV	58485	77059	1.70%	0.192%
27	12.814	919	921	923	rVV	33216	52570	1.16%	0.131%
28	12.939	930	932	936	rBV2	36220	63741	1.41%	0.159%
29	13.088	942	945	948	rBV	3415510	3238455	71.63%	8.074%
30	13.979	1020	1023	1026	rBV	224332	354529	7.84%	0.884%
31	14.139	1033	1037	1039	rBV	976990	990856	21.92%	2.470%
32	14.894	1100	1103	1110	rVB	335310	472360	10.45%	1.178%
33	15.614	1163	1166	1172	rBV	641324	864285	19.12%	2.155%

LSC Area Percent Report

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Data File : BF085185.D
Acq On : 4 Mar 2016 4:41
Operator : SJ/UM
Sample : H1661-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-51-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

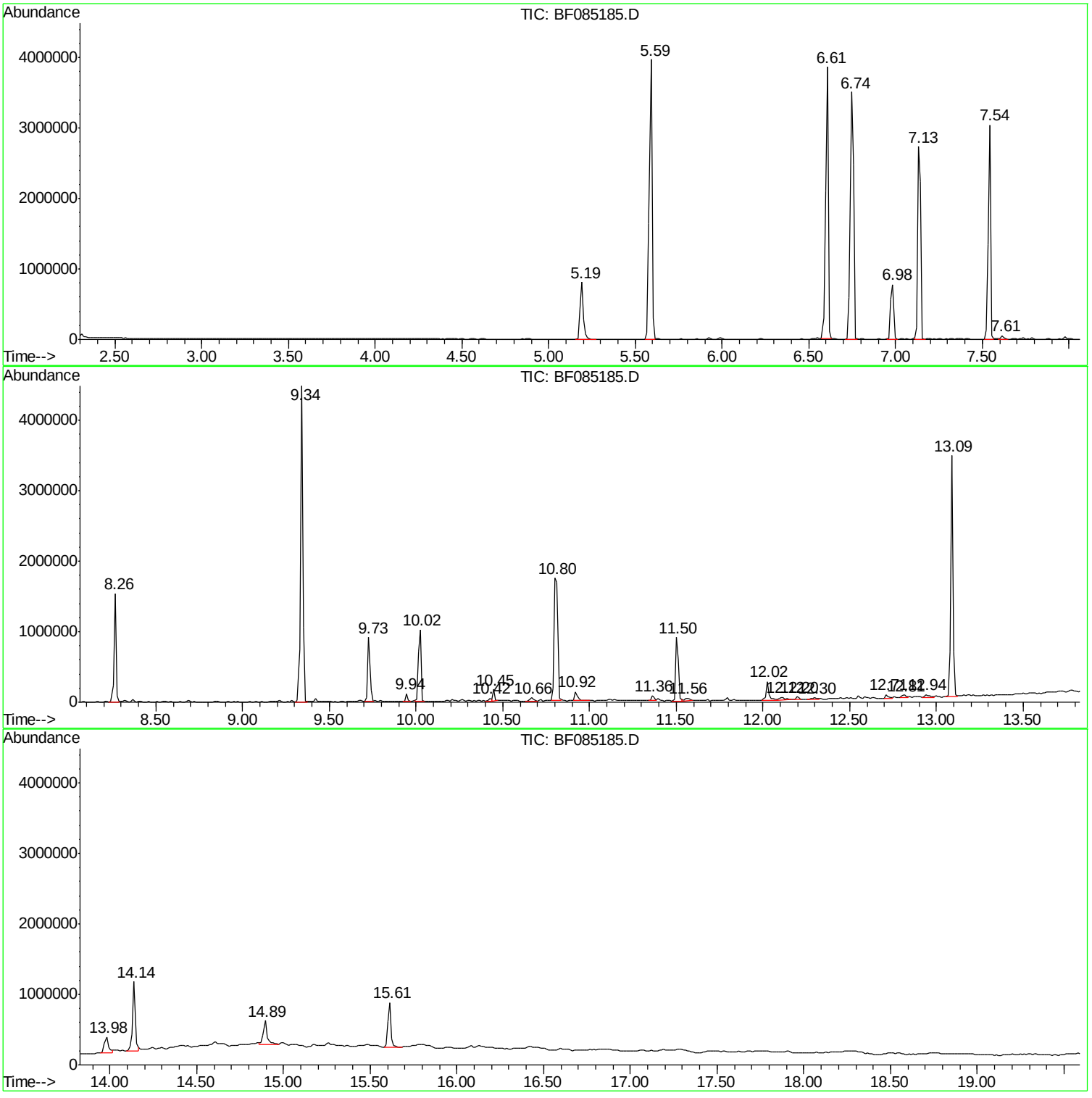
Sum of corrected areas: 40110997

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
Data File : BF085185.D
Acq On : 4 Mar 2016 4:41
Operator : SJ/UM
Sample : H1661-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-51-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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TIC Library : C:\DATABASE\NIST02.L
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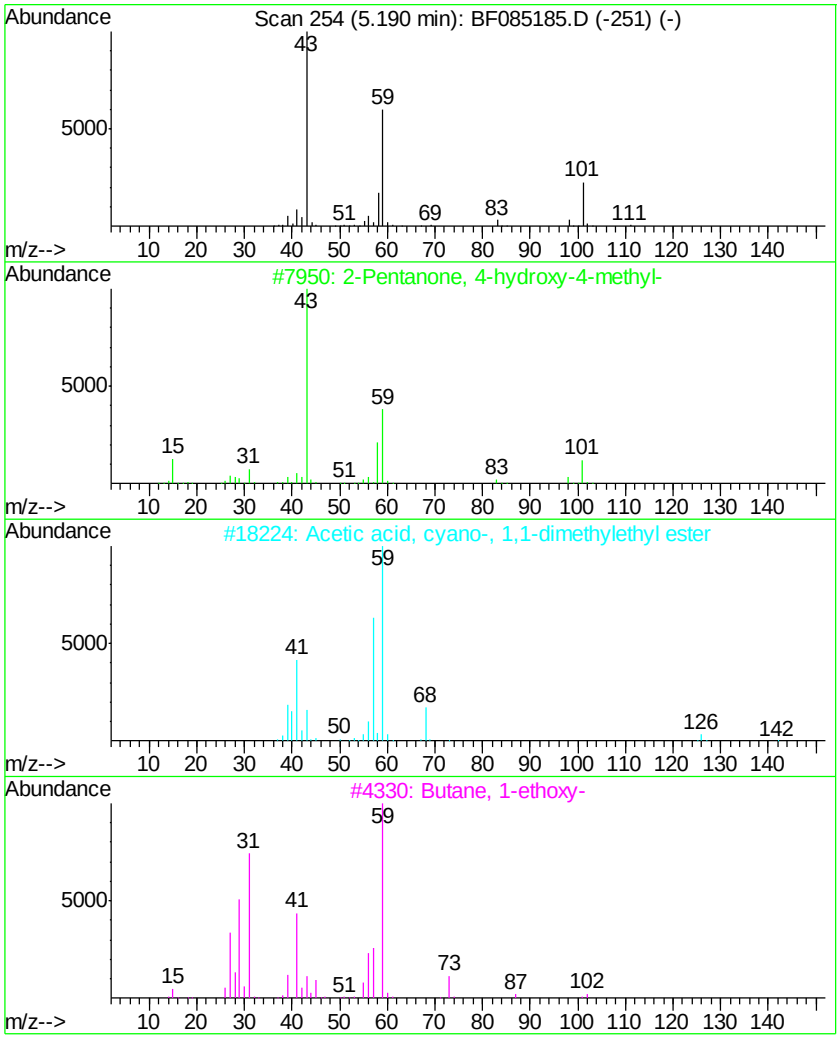
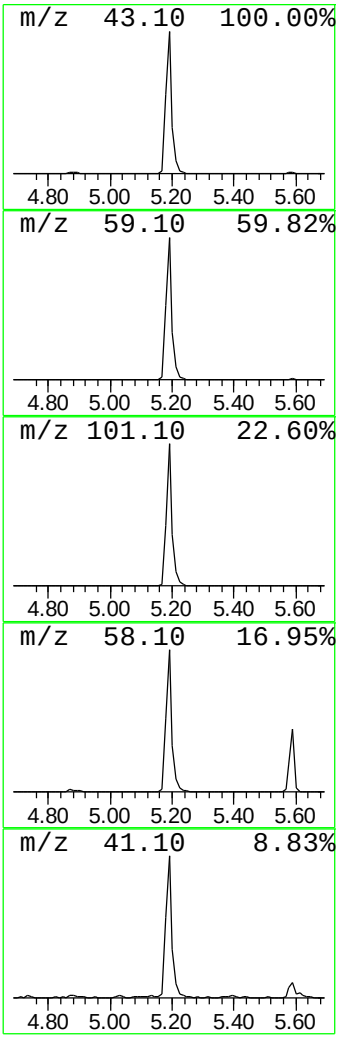
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	23.74 ng	1107710	1,4-Dichlorobenzene-d4	6.98

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	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF085185.D
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Operator : SJ/UM
Sample : H1661-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-51-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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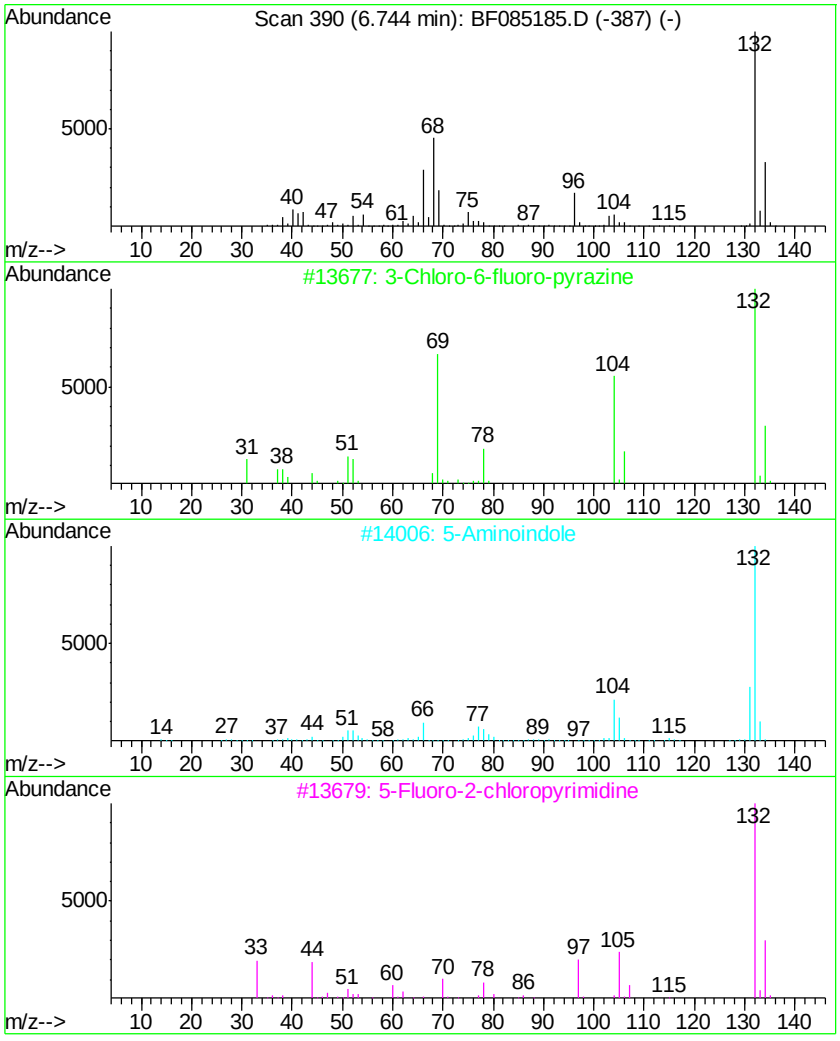
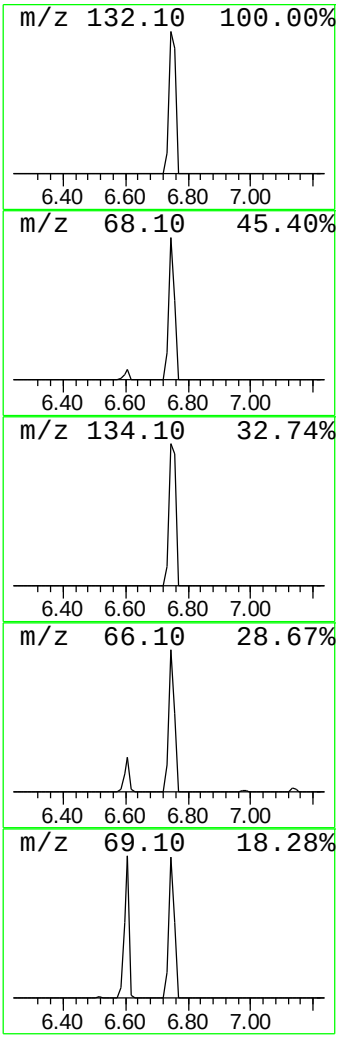
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	96.91 ng	4520870	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Sample : H1661-06
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Instrument : BNA_F
ClientSampleId : SB-51-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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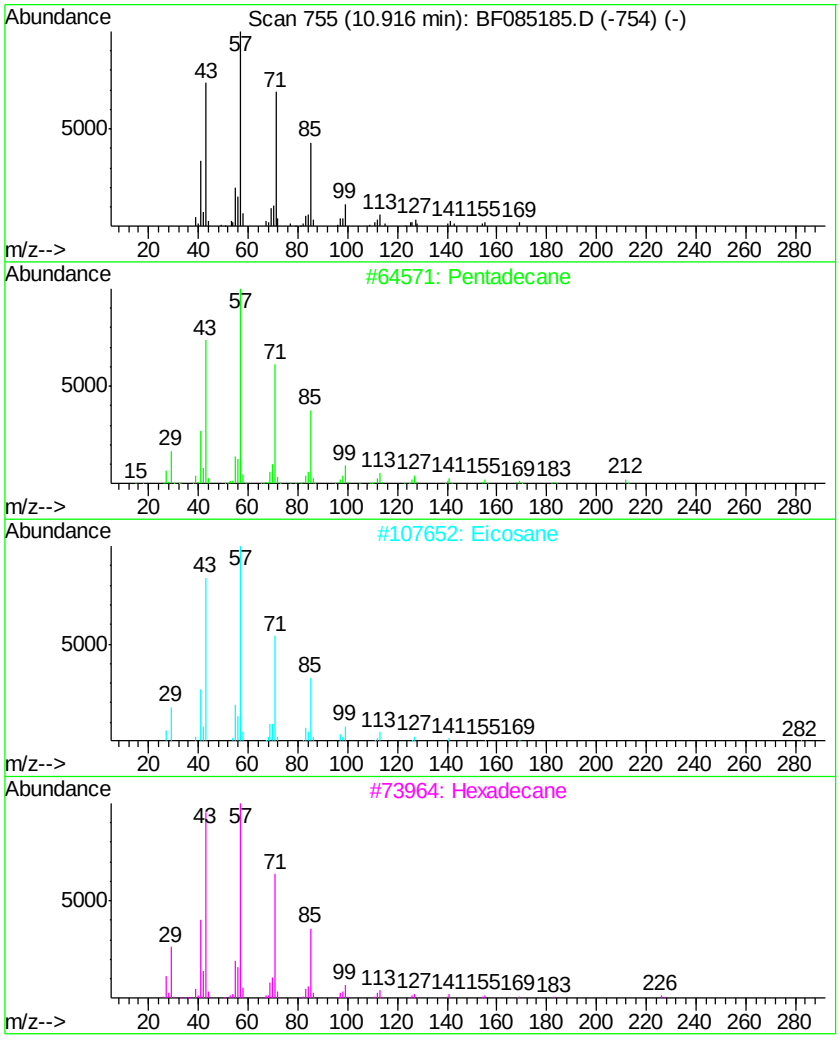
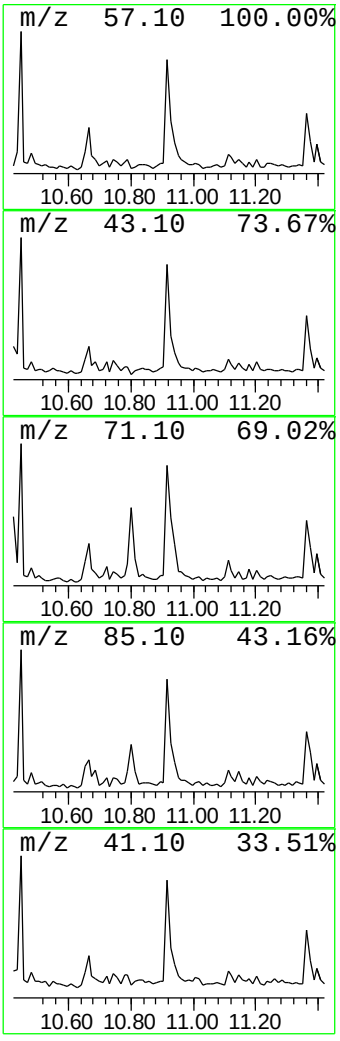
Peak Number 4 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.92	3.16 ng	170543	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tetradecane	198	C14H30	000629-59-4	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
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Operator : SJ/UM
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Instrument : BNA_F
ClientSampleId : SB-51-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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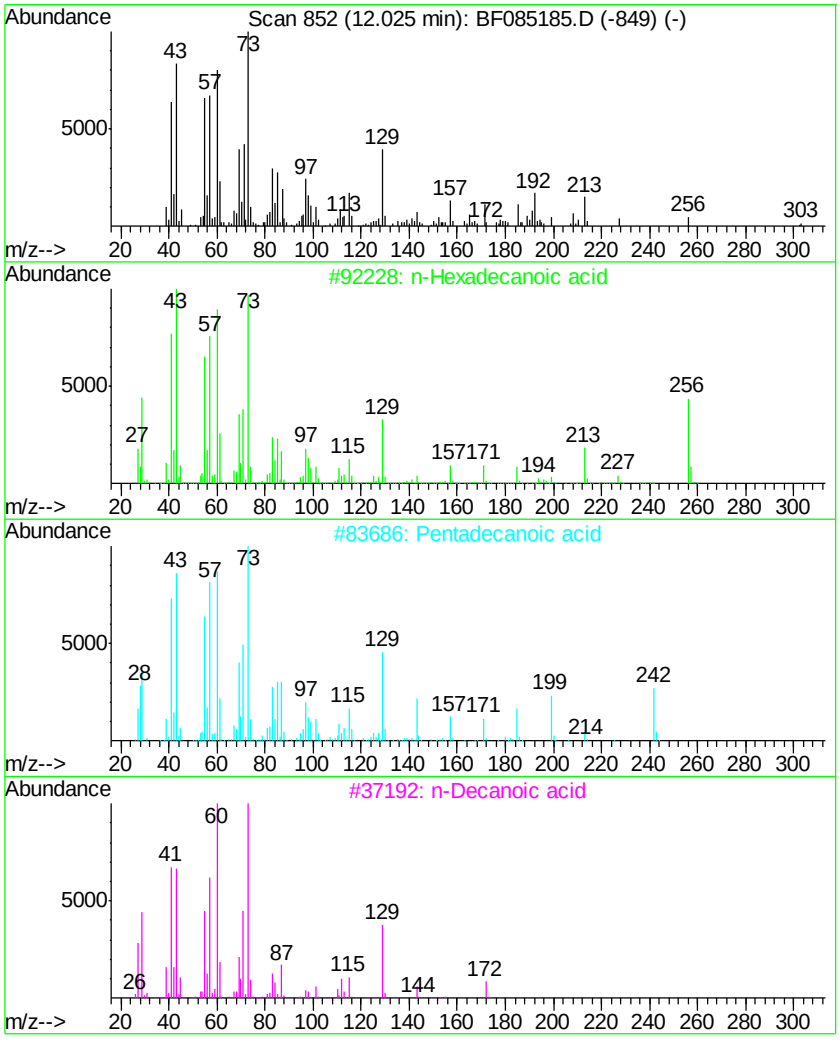
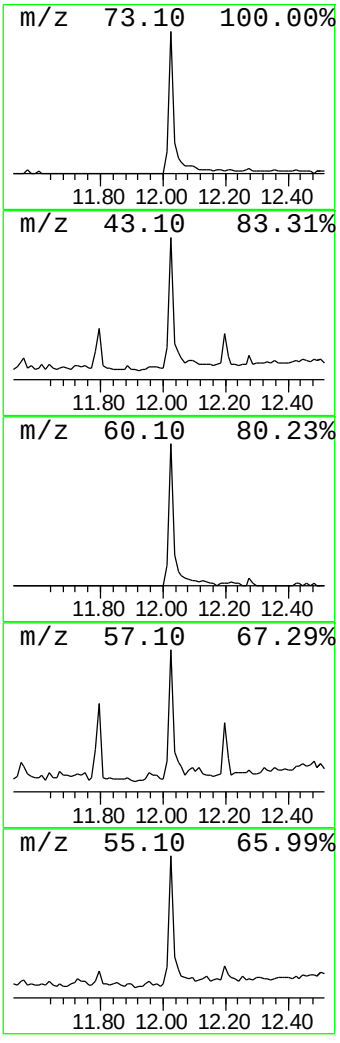
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	6.20 ng	334957	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Pentadecane	212	C15H32	000629-62-9	11





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TIC Library : C:\DATABASE\NIST02.L
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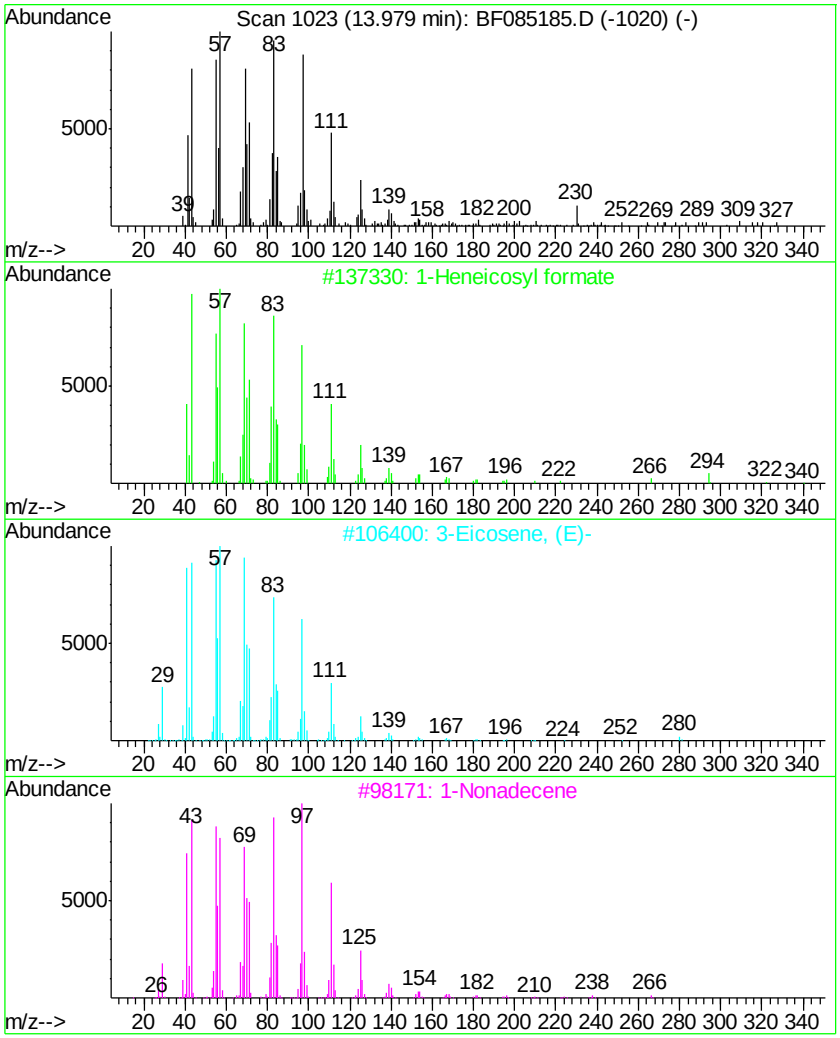
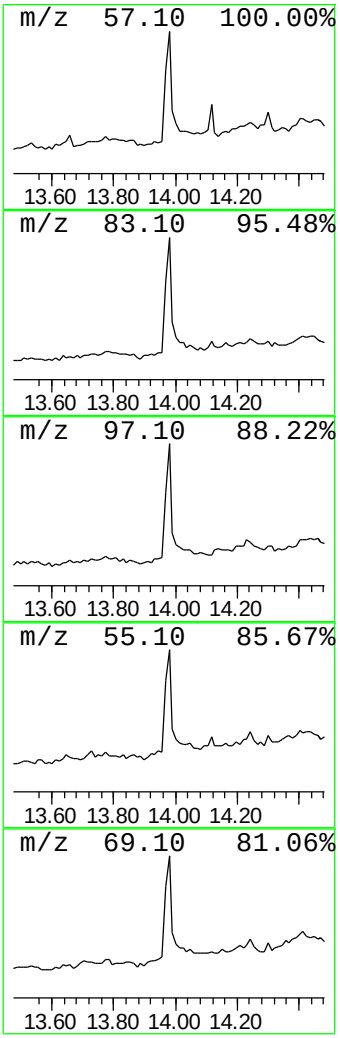
Peak Number 6 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	7.16 ng	354529	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
5	1-Octadecene	252	C18H36	000112-88-9	89





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Instrument : BNA_F
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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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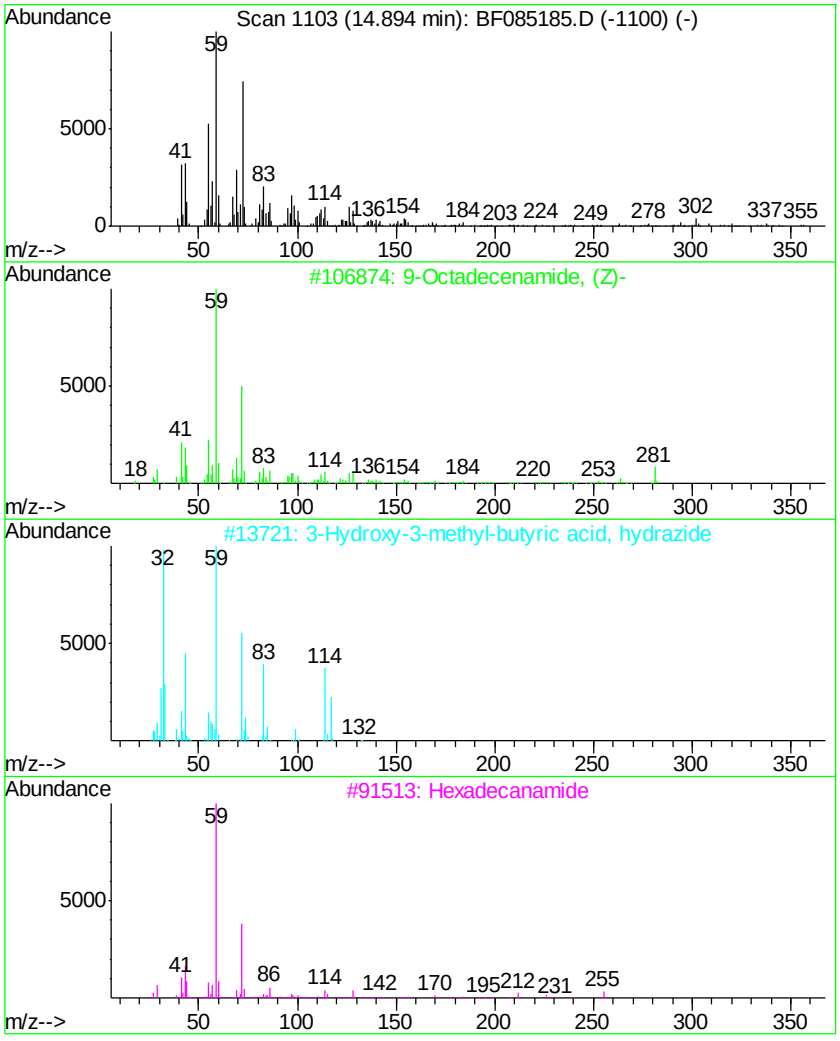
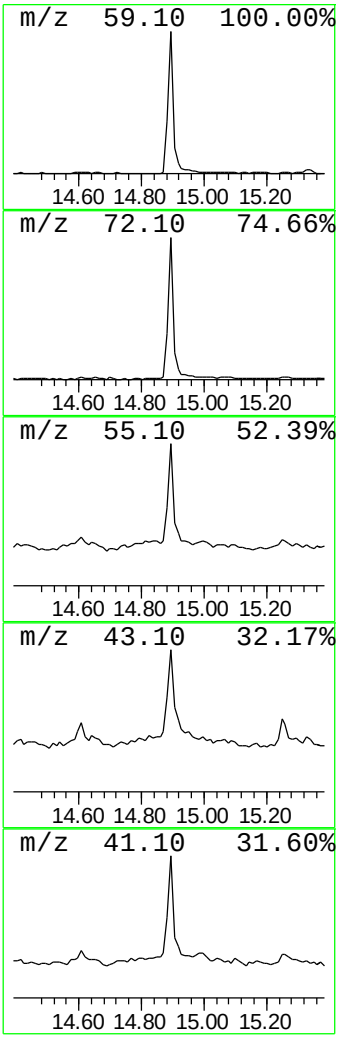
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	10.93 ng	472360	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	3-Hydroxy-3-methyl-butyric acid,...	132	C5H12N2O2	1000193-80-2	53
3	Hexadecanamide	255	C16H33NO	000629-54-9	53
4	Dodecanamide	199	C12H25NO	001120-16-7	47
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	40





Tentatively Identified Compound (LSC) summary

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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	23.7	ng	1107710	1	6.98	933025	20.0
unknown6.74	6.74	96.9	ng	4520870	1	6.98	933025	20.0
Pentadecane	10.92	3.2	ng	170543	4	11.50	1080530	20.0
n-Hexadecanoic acid	12.02	6.2	ng	334957	4	11.50	1080530	20.0
1-Heneicosyl formate	13.98	7.2	ng	354529	5	14.14	990856	20.0
9-Octadecenamide,...	14.89	10.9	ng	472360	6	15.61	864285	20.0