LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085449.D
Acq On : 15 Mar 2016 2:04
Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W170TH-SB-07-COMP(0.5-4.0)

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	5.144	247	250	258	rVB	223539	389268	7.26%	0.779%
2	5.544	281	285	287	rBV	3520357	5326814	99.31%	10.659%
3	6.562	371	374	377	rBV	3713335	4597214	85.70%	9.199%
4	6.699	383	386	388	rBV	4457997	5073368	94.58%	10.152%
5	6.927	403	406	408	rBV	1009997	1030842	19.22%	2.063%
6	7.087	417	420	422	rBV	3526519	4219526	78.66%	8.443%
7	7.487	452	455	457	rBV	2603748	3326302	62.01%	6.656%
8	8.207	516	518	521	rBV	1572343	1359361	25.34%	2.720%
9	9.293	610	613	615	rBV	4308368	5364063	100.00%	10.734%
10	9.682	645	647	648	rBV	959733	897138	16.72%	1.795%
11	9.899	663	666	668	rVB	98003	114938	2.14%	0.230%
12	9.968	670	672	674	rVB	1677618	1482770	27.64%	2.967%
13	10.162	687	689	692	rVB3	37552	64513	1.20%	0.129%
14	10.390	708	709	711	rVB	197576	191498	3.57%	0.383%
15	10.619	726	729	732	rBV	68924	143302	2.67%	0.287%
16	10.756	738	741	744	rBV	2907048	3029516	56.48%	6.062%
17	10.871	748	751	755	rBV	204543	290355	5.41%	0.581%
18	11.065	765	768	771	rBV4	28565	67523	1.26%	0.135%
19	11.316	787	790	791	rBV	125581	127337	2.37%	0.255%
20	11.453	799	802	803	rBV	1481419	1408649	26.26%	2.819%
21	11.476	803	804	806	rVV	269676	212132	3.95%	0.424%
22	11.522	806	808	810	rVB2	66287	71373	1.33%	0.143%
23	11.682	819	822	824	rBV2	28853	56155	1.05%	0.112%
24	11.979	844	848	850	rVV	355816	459346	8.56%	0.919%
25	12.059	853	855	859	rVB	81784	139483	2.60%	0.279%
26	12.162	860	864	867	rBV3	29614	84042	1.57%	0.168%
27	12.231	867	870	872	rBV2	50716	93893	1.75%	0.188%
28	12.505	891	894	895	rBV2	55414	79971	1.49%	0.160%
29	12.665	906	908	910	rBV	597974	585918	10.92%	1.172%
30	12.756	915	916	923	rVV4	155301	251899	4.70%	0.504%
31	12.859	923	925	926	rVV	95606	179748	3.35%	0.360%
32	12.894	926	928	930	rVV	530399	515728	9.61%	1.032%
33	12.928	930	931	934	rVB3	55395	74330	1.39%	0.149%
34	13.042	938	941	943	rVB	3412578	3853508	71.84%	7.711%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085449.D
Acq On : 15 Mar 2016 2:04
Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W170TH-SB-07-COMP(0.5-4.0)

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	13.111	943	947	951	rBV4	40353	56242	1.05%	0.113%
36	13.214	953	956	958	rVB2	39612	76100	1.42%	0.152%
37	13.282	958	962	964	rBV3	22751	58197	1.08%	0.116%
38	13.328	964	966	967	rBV2	44745	65435	1.22%	0.131%
39	13.557	985	986	988	rBV2	87453	80334	1.50%	0.161%
40	13.728	999	1001	1003	rVB	66012	82036	1.53%	0.164%
41	13.831	1008	1010	1012	rBV2	46502	71064	1.32%	0.142%
42	13.934	1017	1019	1021	rBV	192812	246377	4.59%	0.493%
43	14.082	1029	1032	1037	rBV2	786834	1488344	27.75%	2.978%
44	14.471	1064	1066	1068	rBV	52760	67733	1.26%	0.136%
45	14.551	1071	1073	1076	rBV4	64357	118113	2.20%	0.236%
46	14.837	1096	1098	1104	rVV2	241976	331301	6.18%	0.663%
47	14.928	1104	1106	1110	rVB2	116563	176643	3.29%	0.353%
48	15.122	1120	1123	1127	rVB	210851	400149	7.46%	0.801%
49	15.191	1127	1129	1131	rBV2	55501	65646	1.22%	0.131%
50	15.420	1147	1149	1152	rBV	102256	126722	2.36%	0.254%
51	15.488	1152	1155	1157	rVV	124798	207355	3.87%	0.415%
52	15.545	1157	1160	1168	rVB	642608	976858	18.21%	1.955%
53	16.997	1284	1287	1291	rVB2	57614	117714	2.19%	0.236%

Sum of corrected areas: 49974186

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Acq On : 15 Mar 2016 2:04
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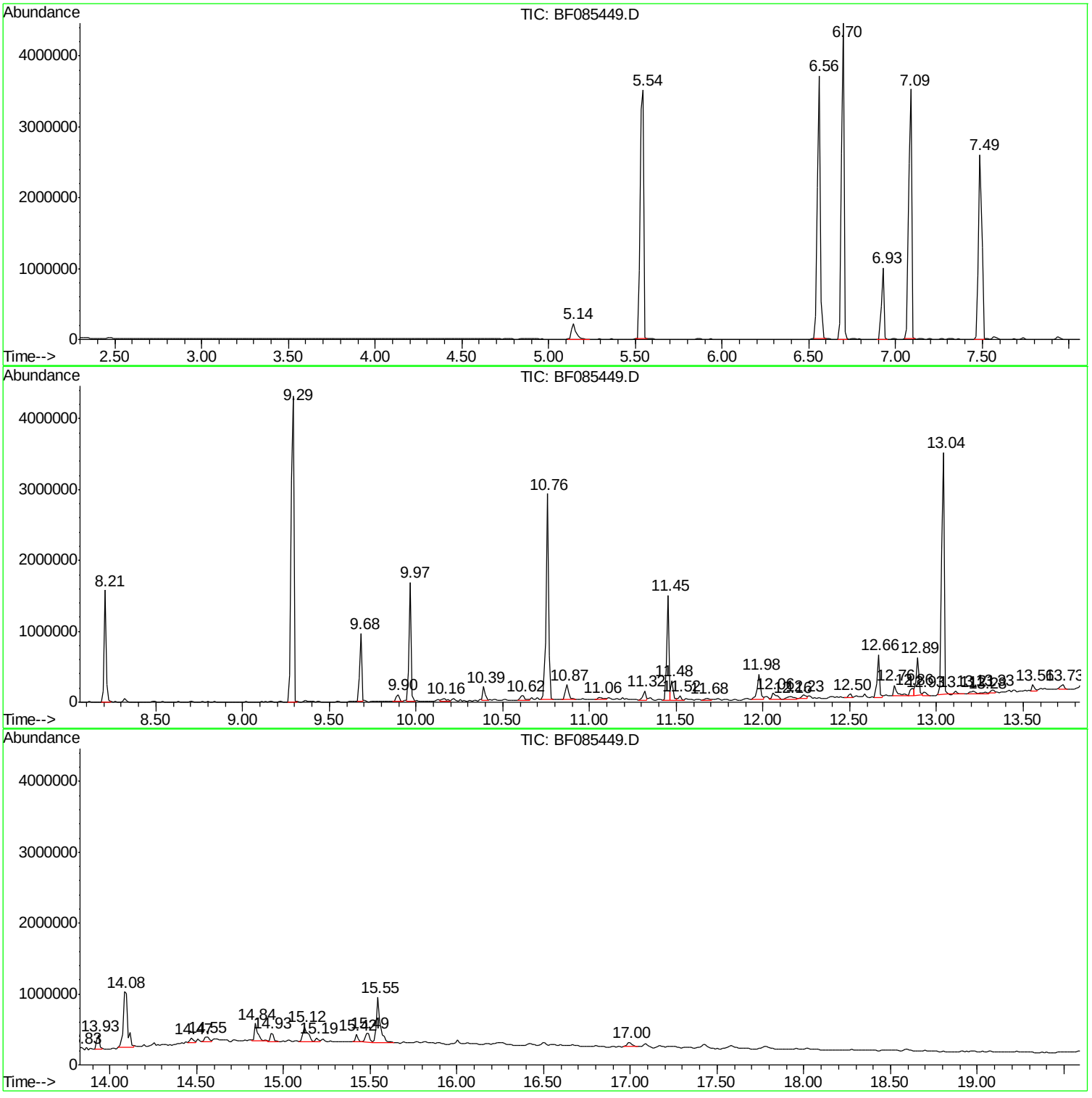
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-07-COMP(0.5-4.0)

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\BF031416\
Data File : BF085449.D
Acq On : 15 Mar 2016 2:04
Operator : UM/SJ
Sample : H1730-10
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Instrument : BNA_F
ClientSampleId : W170TH-SB-07-COMP(0.5-4.0)

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

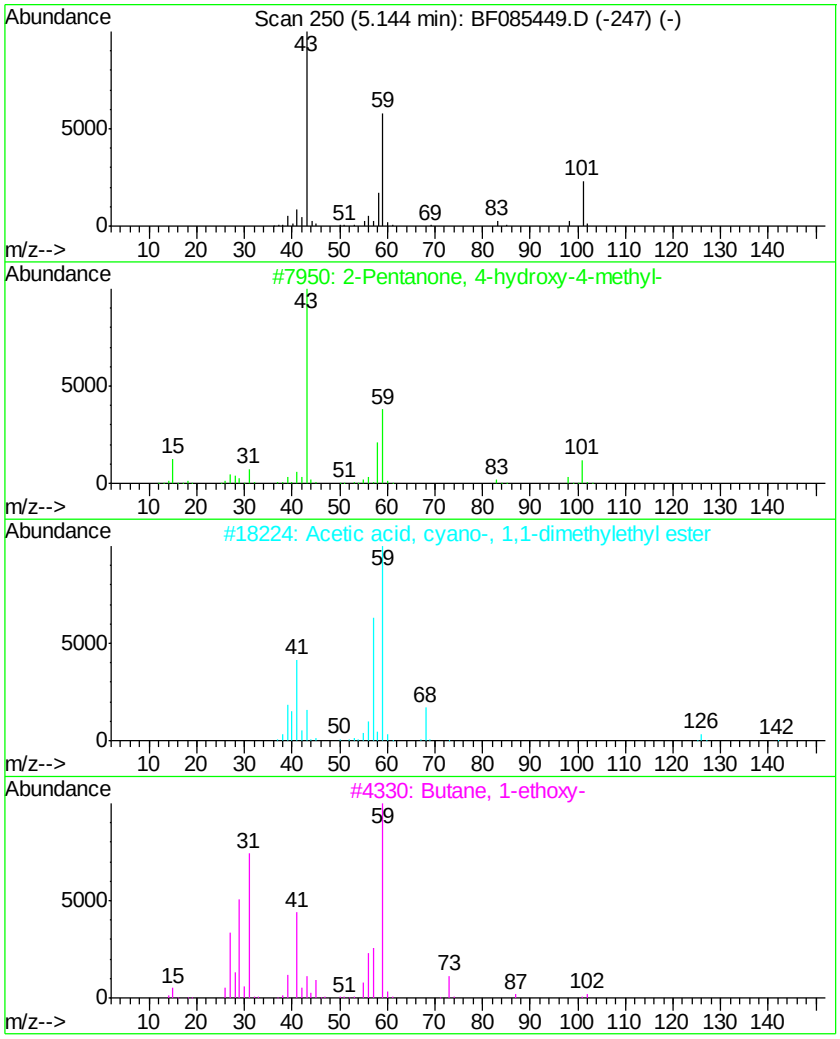
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

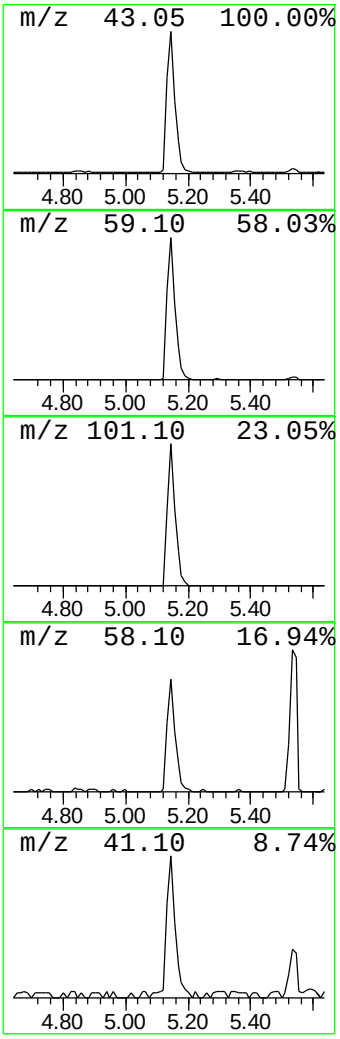
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	7.55 ng	389268	1,4-Dichlorobenzene-d4	6.93

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 : 15 Mar 2016 2:04
Operator : UM/SJ
Sample : H1730-10
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-07-COMP(0.5-4.0)

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

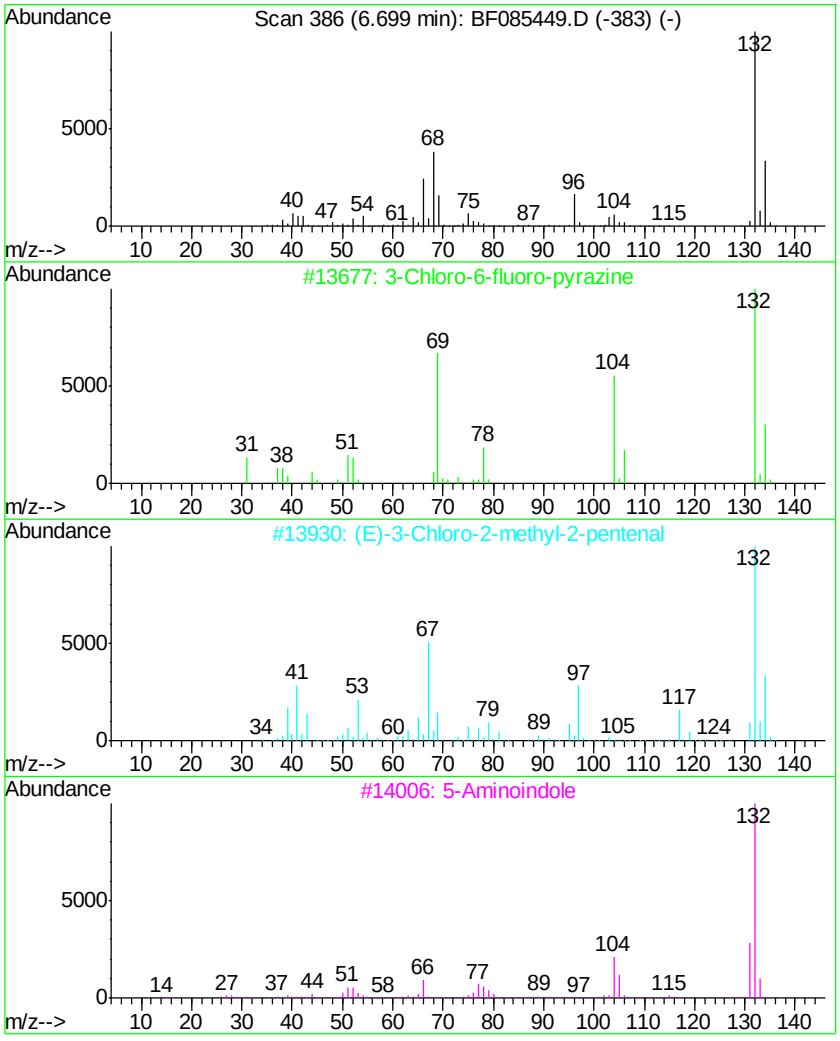
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

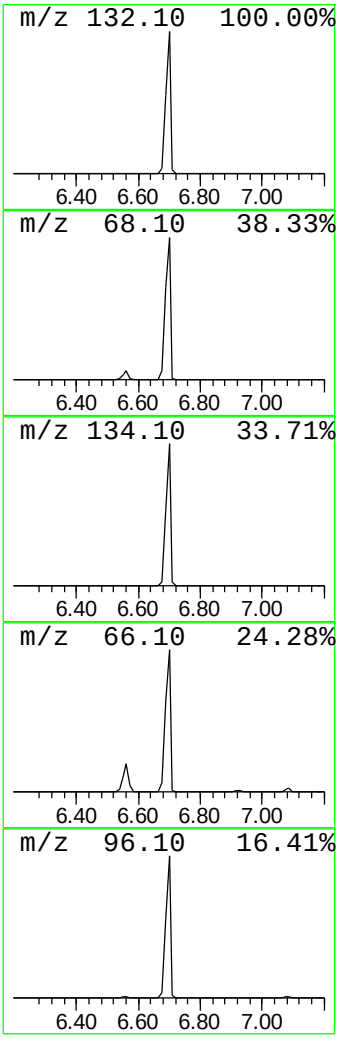
****

Peak Number 2 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	98.43 ng	5073370	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-07-COMP(0.5-4.0)

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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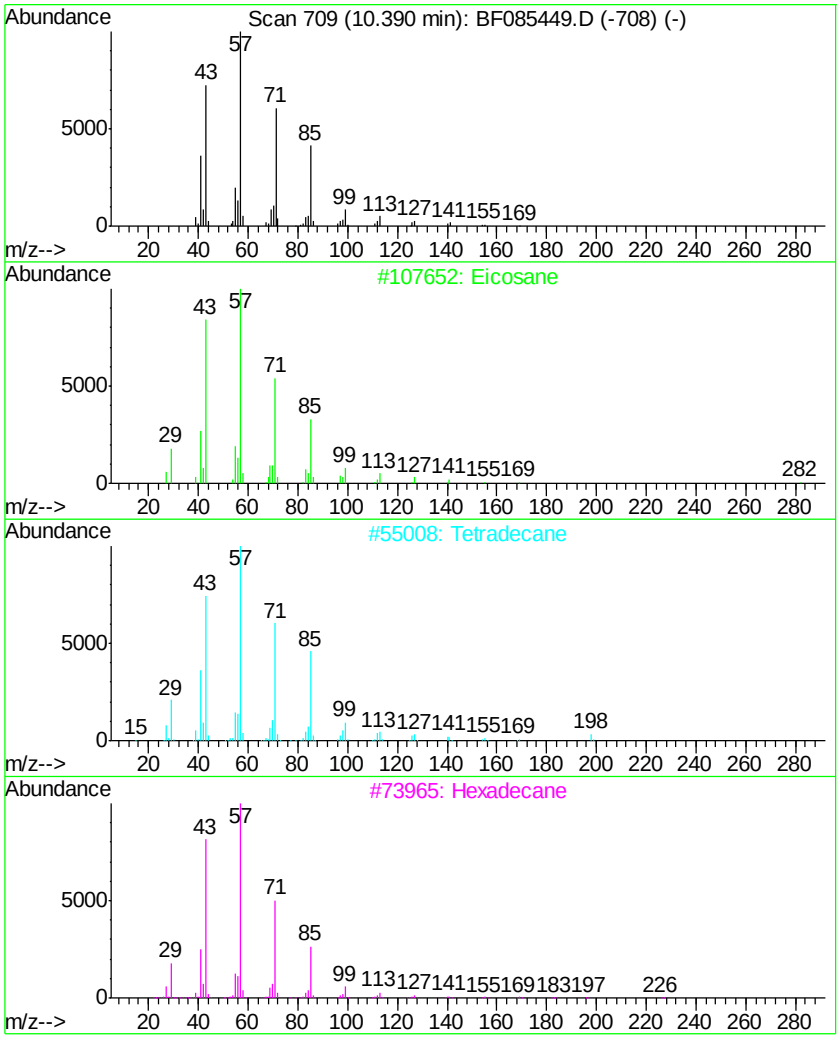
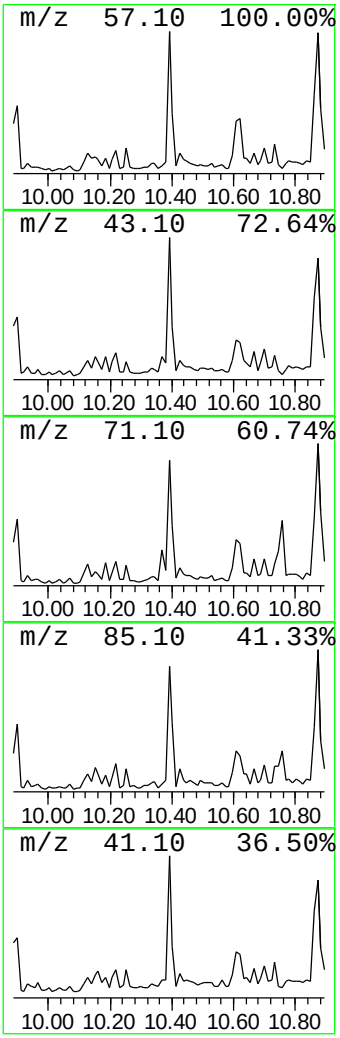
Peak Number 4 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.39	2.58 ng	191498	Acenaphthene-d10	9.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetradecane	198	C14H30	000629-59-4	83
3	Hexadecane	226	C16H34	000544-76-3	80
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	80
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085449.D
Acq On : 15 Mar 2016 2:04
Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-07-COMP(0.5-4.0)

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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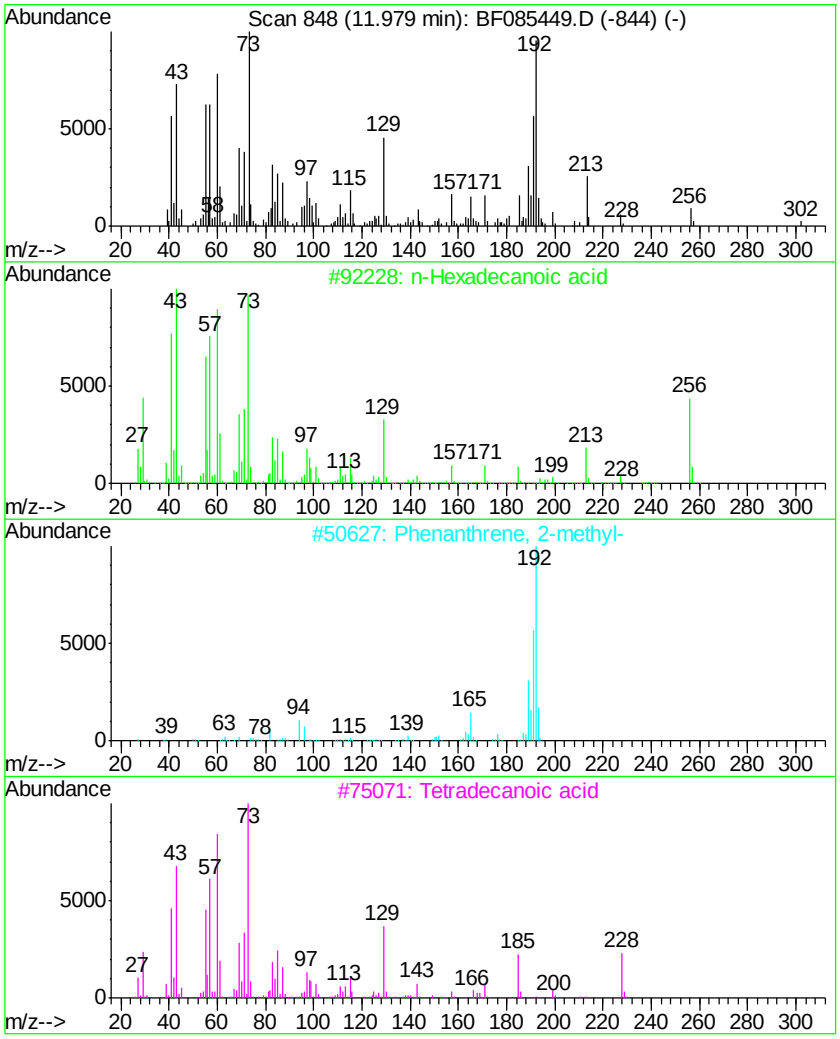
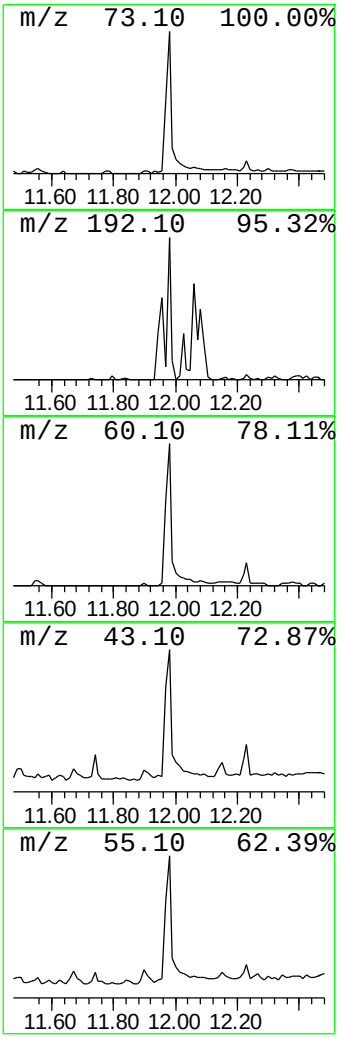
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	6.52 ng	459346	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	68





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Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-07-COMP(0.5-4.0)

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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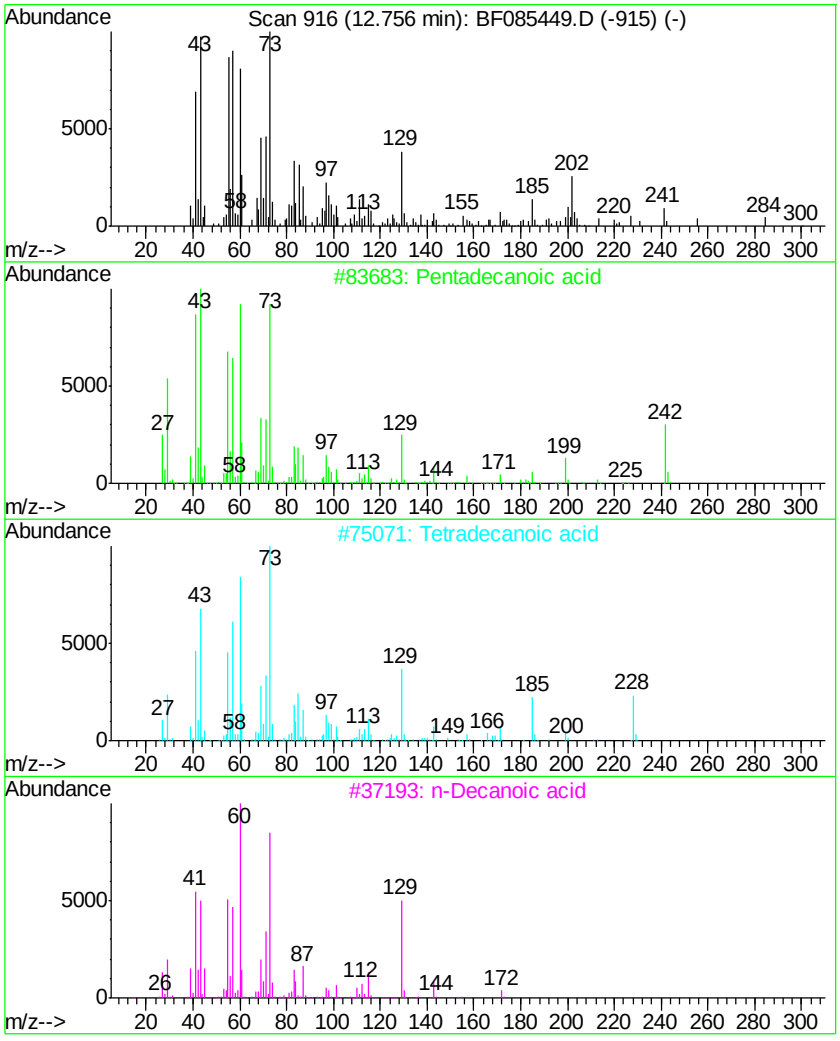
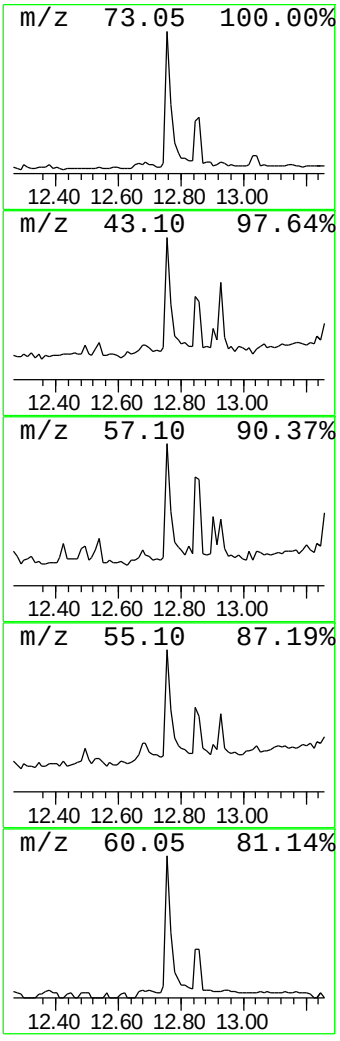
Peak Number 7 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	3.58 ng	251899	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	49
4	Dodecanoic acid	200	C12H24O2	000143-07-7	46
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085449.D
Acq On : 15 Mar 2016 2:04
Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-07-COMP(0.5-4.0)

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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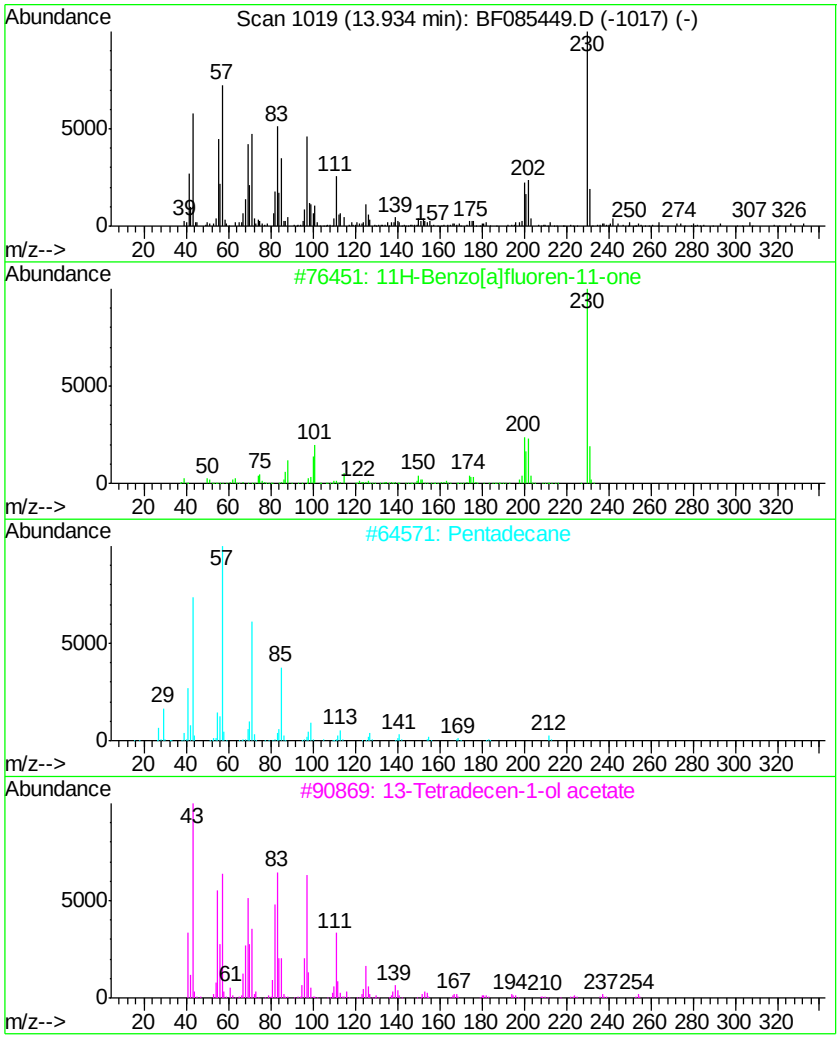
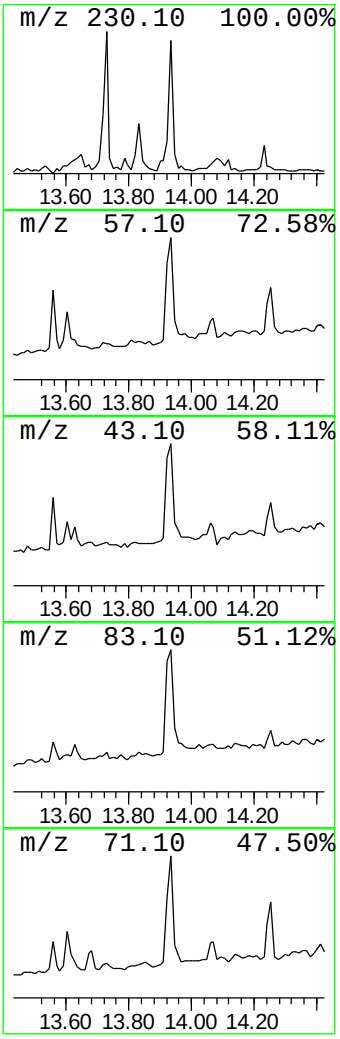
Peak Number 8 11H-Benzo[a]fluoren-11-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.31 ng	246377	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	60
2	Pentadecane	212	C15H32	000629-62-9	53
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	42
4	1-Octadecanol	270	C18H38O	000112-92-5	42
5	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	42





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Data File : BF085449.D
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Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W170TH-SB-07-COMP(0.5-4.0)

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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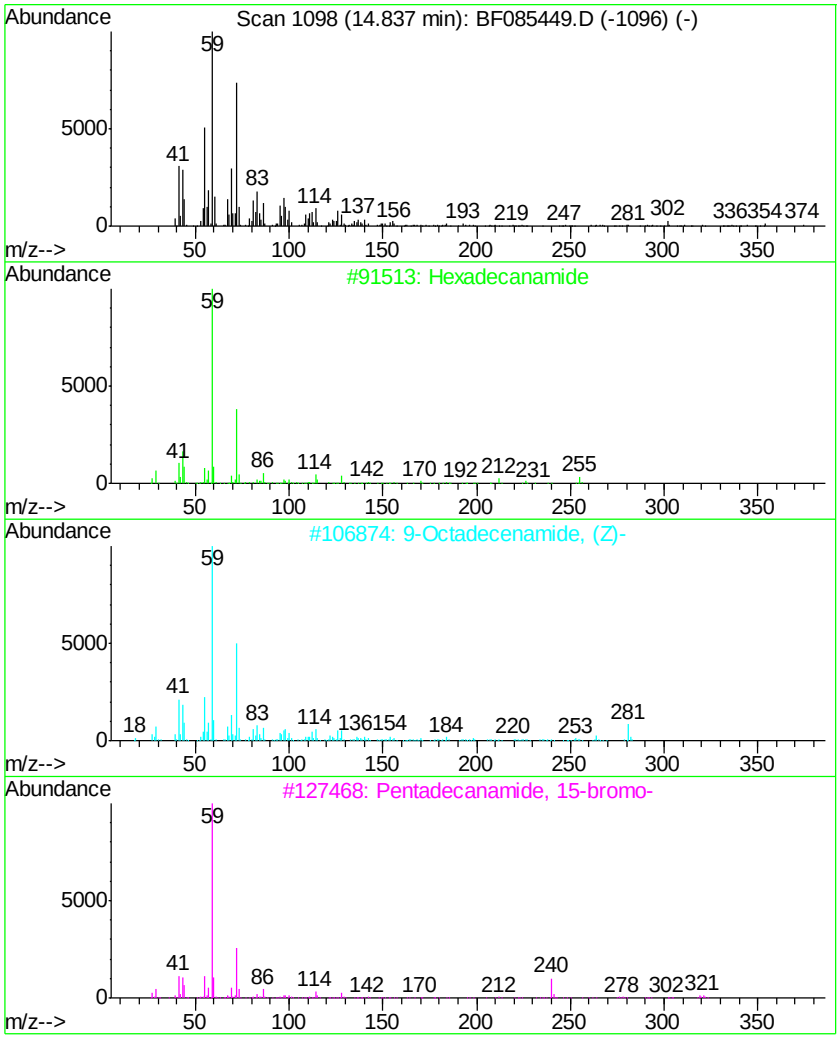
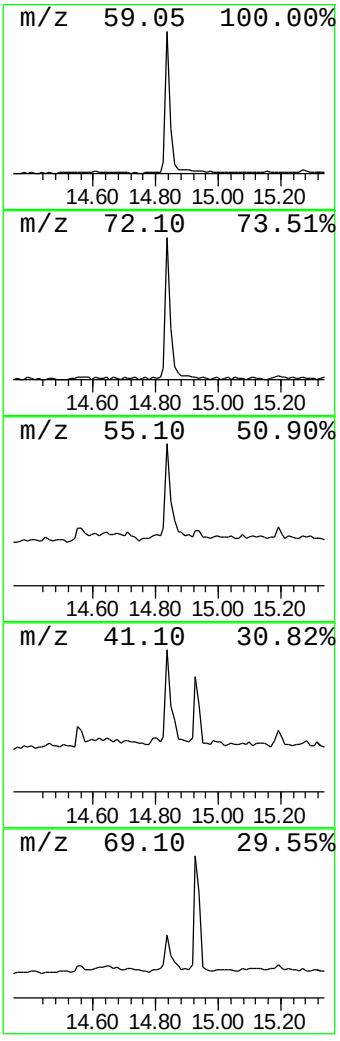
Peak Number 9 Hexadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	6.78 ng	331301	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	72
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	47
3	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	47
4	Dodecanamide	199	C12H25NO	001120-16-7	47
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	45





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085449.D
Acq On : 15 Mar 2016 2:04
Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-07-COMP(0.5-4.0)

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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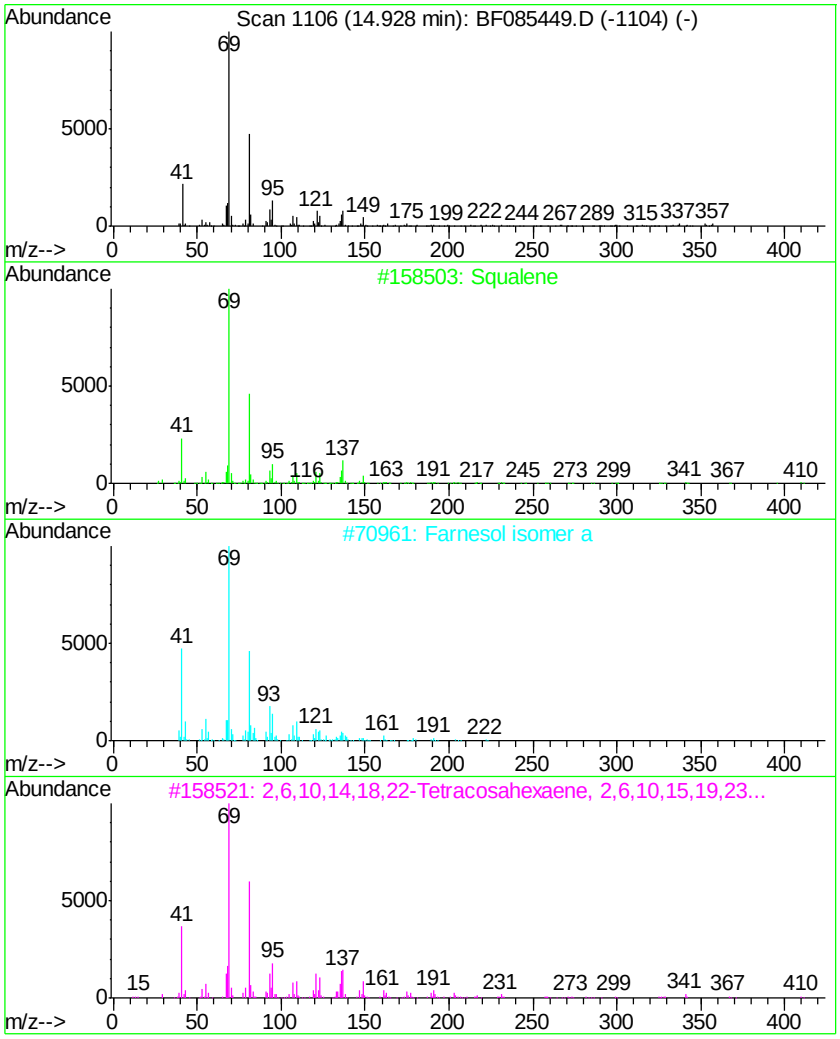
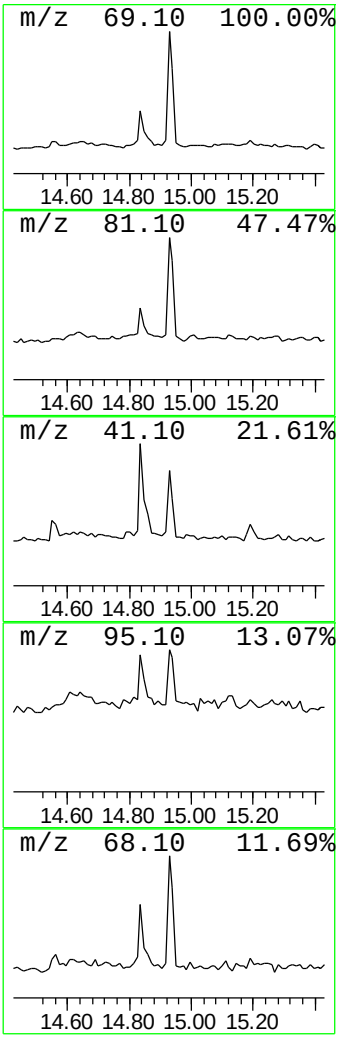
Peak Number 10 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	3.62 ng	176643	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	87
2	Farnesol isomer a	222	C15H26O	1000108-92-4	86
3	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86
4	.beta.-d-Mannofuranoside, O-geranyl	316	C16H28O6	1000154-77-2	78
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085449.D
Acq On : 15 Mar 2016 2:04
Operator : UM/SJ
Sample : H1730-10
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W170TH-SB-07-COMP(0.5-4.0)

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
2-Pentanone, 4-hy...	5.14	7.5	ng	389268	1	6.93	1030840	20.0
unknown6.70	6.70	98.4	ng	5073370	1	6.93	1030840	20.0
Eicosane	10.39	2.6	ng	191498	3	9.97	1482770	20.0
n-Hexadecanoic acid	11.98	6.5	ng	459346	4	11.45	1408650	20.0
Pentadecanoic acid	12.76	3.6	ng	251899	4	11.45	1408650	20.0
11H-Benzo[a]fluor...	13.93	3.3	ng	246377	5	14.09	1488340	20.0
Hexadecanamide	14.84	6.8	ng	331301	6	15.55	976858	20.0
Squalene	14.93	3.6	ng	176643	6	15.55	976858	20.0