LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030416\
Data File : BF085233.D
Acq On : 5 Mar 2016 5:26
Operator : SJ/IZ
Sample : H1661-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-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	3.201	74	80	81	rBV3	856360	3000186	71.43%	6.100%
2	3.395	94	97	98	rVB3	764436	1563840	37.23%	3.180%
3	3.441	98	101	102	rBV2	756191	1921946	45.76%	3.908%
4	3.864	137	138	143	rVB3	298324	275977	6.57%	0.561%
5	4.047	150	154	155	rBV4	76240	135812	3.23%	0.276%
6	4.093	155	158	160	rVV	81057	122050	2.91%	0.248%
7	4.127	160	161	165	rVB2	206173	262613	6.25%	0.534%
8	5.178	251	253	260	rVB	690210	975381	23.22%	1.983%
9	5.578	285	288	290	rBV	3380930	3696991	88.02%	7.517%
10	6.596	374	377	379	rVV	3646537	4156813	98.96%	8.452%
11	6.733	386	389	392	rBV	3296809	4094706	97.49%	8.326%
12	6.973	407	410	412	rBV	778562	943756	22.47%	1.919%
13	7.121	421	423	426	rVB	2756358	3146441	74.91%	6.398%
14	7.533	456	459	461	rBV	2753949	2977443	70.89%	6.054%
15	7.613	461	466	468	rVB	75641	118075	2.81%	0.240%
16	8.253	519	522	524	rBV	1516115	1313407	31.27%	2.671%
17	9.327	613	616	619	rBV	3708057	4200299	100.00%	8.541%
18	9.716	648	650	652	rBV	664037	904608	21.54%	1.839%
19	9.933	667	669	671	rVB	98131	109373	2.60%	0.222%
20	10.013	673	676	678	rVB	1296159	1413089	33.64%	2.873%
21	10.413	709	711	712	rBV	46663	50307	1.20%	0.102%
22	10.436	712	713	715	rVB	193122	146915	3.50%	0.299%
23	10.653	729	732	736	rBV	53549	102751	2.45%	0.209%
24	10.802	742	745	747	rBV	2659015	3051242	72.64%	6.204%
25	10.905	753	754	759	rBV	127074	204788	4.88%	0.416%
26	11.362	791	794	795	rBV	78406	94132	2.24%	0.191%
27	11.499	803	806	808	rBV	1051874	1439090	34.26%	2.926%
28	11.545	809	810	814	rVB2	29203	59036	1.41%	0.120%
29	11.785	829	831	833	rBV	55115	45216	1.08%	0.092%
30	12.013	849	851	858	rBV	232119	237614	5.66%	0.483%
31	12.699	910	911	914	rBV	69575	80854	1.92%	0.164%
32	12.802	918	920	924	rBV2	45272	72385	1.72%	0.147%
33	12.893	927	928	930	rVV	76194	72188	1.72%	0.147%
34	12.928	930	931	934	rVV2	59025	78533	1.87%	0.160%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030416\
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Acq On : 5 Mar 2016 5:26
Operator : SJ/IZ
Sample : H1661-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-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	12.973	934	935	937	rVB	59915	44212	1.05%	0.090%
36	13.076	941	944	947	rBV	3488196	4115324	97.98%	8.368%
37	13.305	957	964	965	rBV3	26398	53974	1.29%	0.110%
38	13.648	991	994	998	rVB2	51660	92375	2.20%	0.188%
39	13.968	1019	1022	1032	rBV	673308	837525	19.94%	1.703%
40	14.128	1032	1036	1038	rBV	1142597	1096998	26.12%	2.231%
41	14.288	1048	1050	1054	rBV	91755	95046	2.26%	0.193%
42	14.597	1074	1077	1080	rBV	103795	128970	3.07%	0.262%
43	14.848	1097	1099	1100	rBV	50126	65372	1.56%	0.133%
44	14.882	1100	1102	1106	rVV2	145493	259368	6.17%	0.527%
45	15.237	1131	1133	1136	rBV	62626	91386	2.18%	0.186%
46	15.591	1161	1164	1167	rBV	498426	746905	17.78%	1.519%
47	16.060	1202	1205	1207	rBV	45712	70222	1.67%	0.143%
48	16.117	1207	1210	1214	rVB	40004	83448	1.99%	0.170%
49	16.574	1246	1250	1252	rBV2	36407	73759	1.76%	0.150%
50	17.168	1299	1302	1306	rBV	27832	57472	1.37%	0.117%
51	17.660	1341	1345	1351	rBV5	23558	70640	1.68%	0.144%
52	17.877	1358	1364	1368	rVB2	24996	67187	1.60%	0.137%
53	18.711	1433	1437	1442	rBV3	18142	61557	1.47%	0.125%

Sum of corrected areas: 49179597

LSC Report - Integrated Chromatogram

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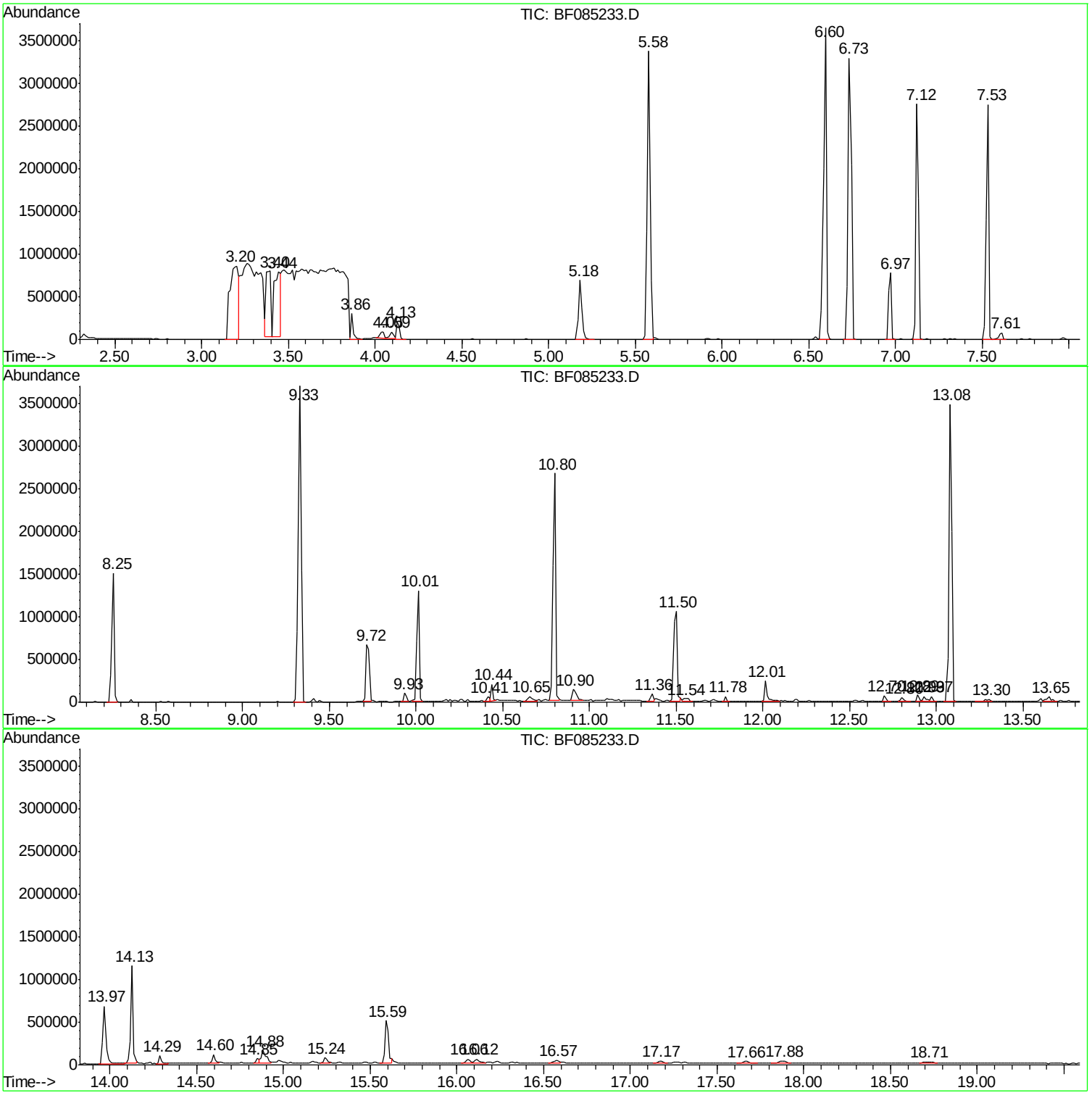
Operator : SJ/IZ
Sample : H1661-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030416\
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Acq On : 5 Mar 2016 5:26
Operator : SJ/IZ
Sample : H1661-03
Misc :
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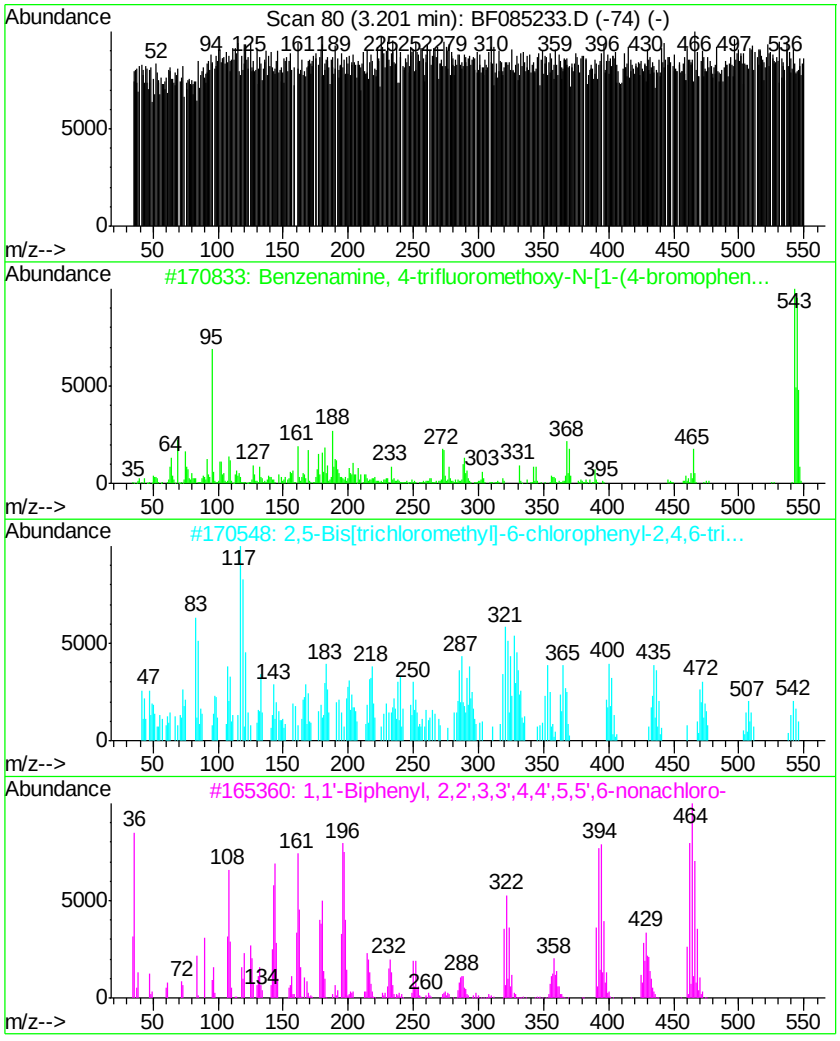
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

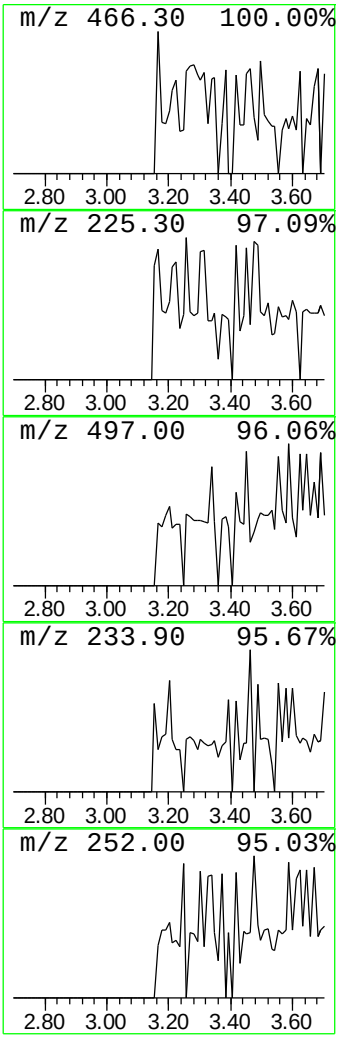
****

Peak Number 1 Benzenamine, 4-trifluoromet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	63.58 ng	3000190	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 4-trifluoromethoxy-...	544	C23H15BrF6N2O2	284495-96-1	55
2	2,5-Bis[trichloromethyl]-6-chlor...	538	C14H4Cl10O	1000254-09-6	45
3	1,1'-Biphenyl, 2,2',3,3',4,4',5,...	460	C12HCl9	040186-72-9	35
4	4,5-Dichloropyridazin-3(2H)-one	164	C4H2Cl2N2O	000932-22-9	20
5	1,2,4-Oxadiazol-5(4H)-one, 3-(2,...	307	C13H7Cl2N3O2	288246-51-5	20





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Operator : SJ/IZ
Sample : H1661-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-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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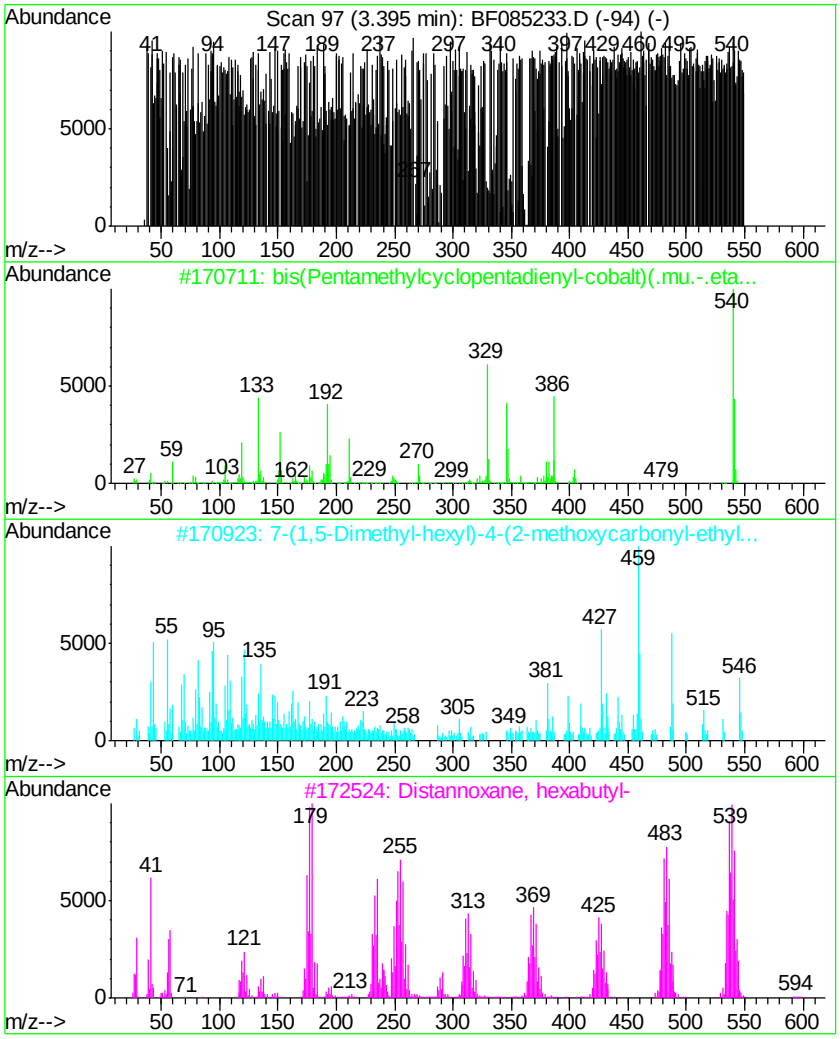
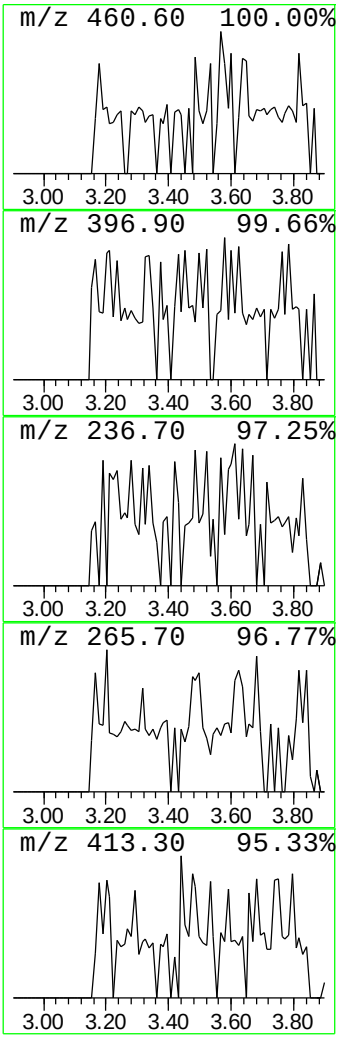
Peak Number 2 unknown3.40 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.40	33.14 ng	1563840	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	bis(Pentamethylcyclopentadienyl-...	540	C32H38Co2	1000157-66-1	25
2	7-(1,5-Dimethyl-hexyl)-4-(2-meth...	546	C32H50O7	1000194-67-5	25
3	Distannoxane, hexabutyl-	598	C24H54OSn2	000056-35-9	22
4	Nickel, bis[1,2-diphenyl-1,2-eth...	542	C28H20NiS4	028984-20-5	15
5	Tris(benzo[b]selenopheno)[2,3:2'...	540	C24H12Se3	107210-82-2	15





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Sample : H1661-03
Misc :
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Instrument : BNA_F
ClientSampleId : SB-46-COMP

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

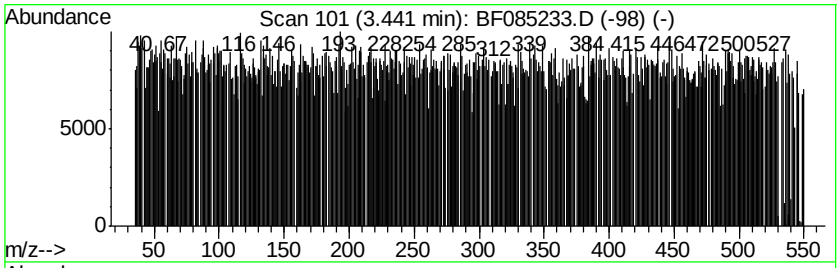
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

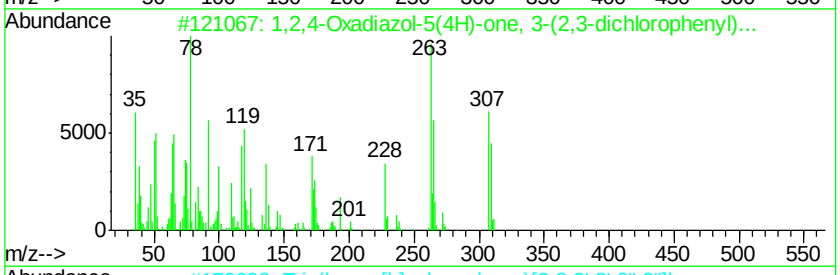
****

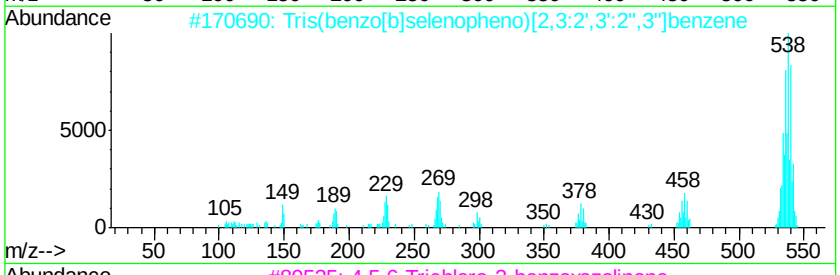
Peak Number 3 1,2,4-Oxadiazol-5(4H)-one, ... Concentration Rank 4

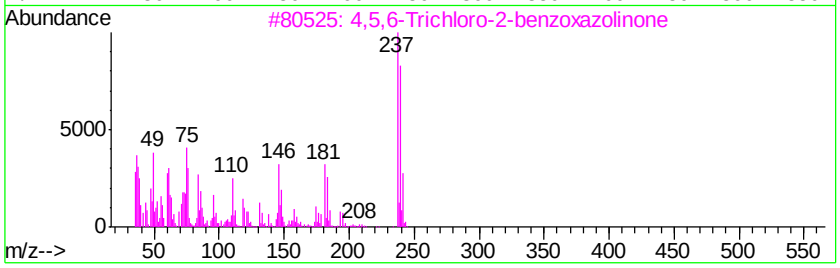
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.44	40.73 ng	1921950	1,4-Dichlorobenzene-d4	6.97

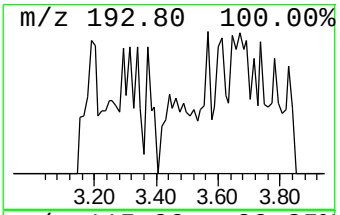
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Oxadiazol-5(4H)-one, 3-(2,...	307	C13H7Cl2N3O2	288246-51-5	50
2	Tris(benzo[b]selenopheno)[2,3:2'...	540	C24H12Se3	107210-82-2	43
3	4,5,6-Trichloro-2-benzoxazolinone	237	C7H2Cl3NO2	050995-94-3	35
4	Isothiazolo[5,4-b]pyridine, 3-ch...	170	C6H3ClN2S	1000294-14-7	35
5	3-Amino-4-methyl-6-phenylpyridazine	185	C11H11N3	081819-90-1	20

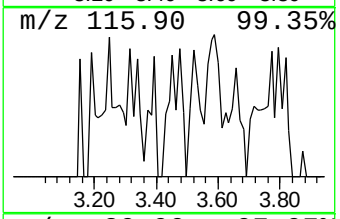


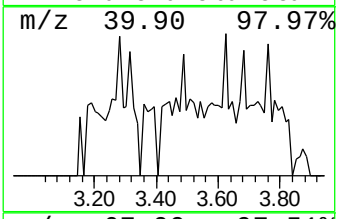


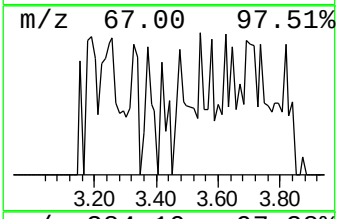


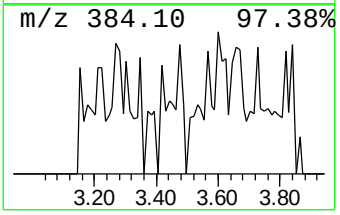












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030416\
Data File : BF085233.D
Acq On : 5 Mar 2016 5:26
Operator : SJ/IZ
Sample : H1661-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-COMP

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

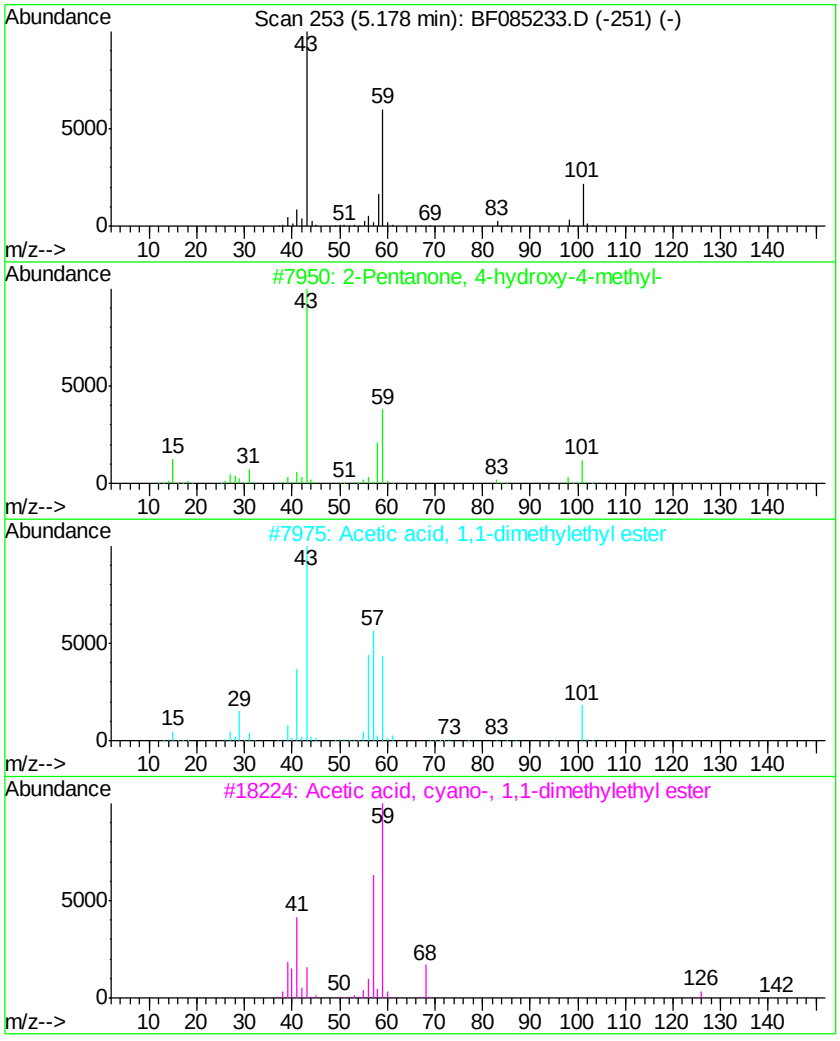
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

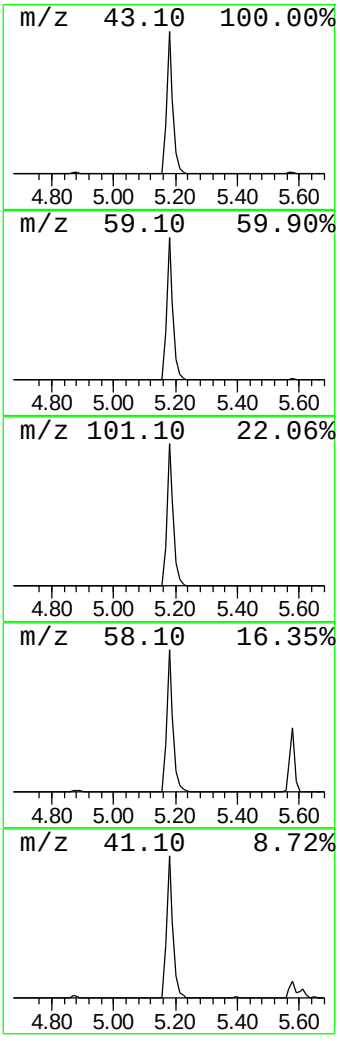
****

Peak Number 8 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	20.67 ng	975381	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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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ClientSampleId : SB-46-COMP

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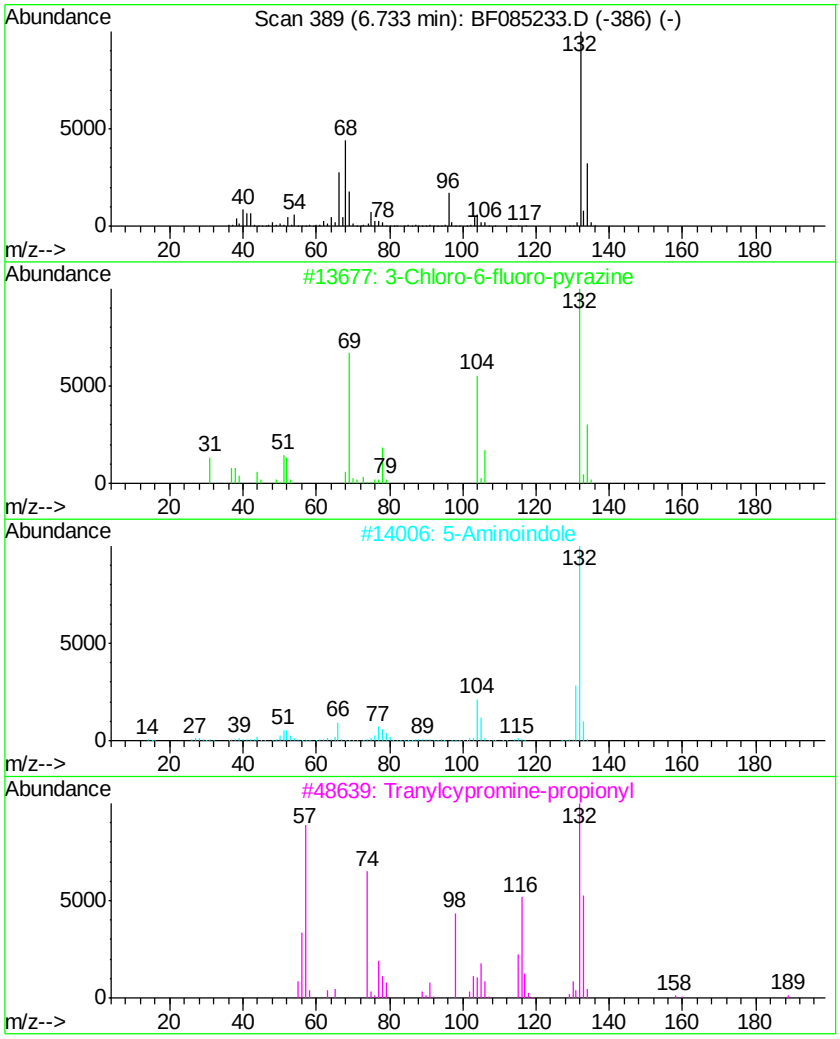
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

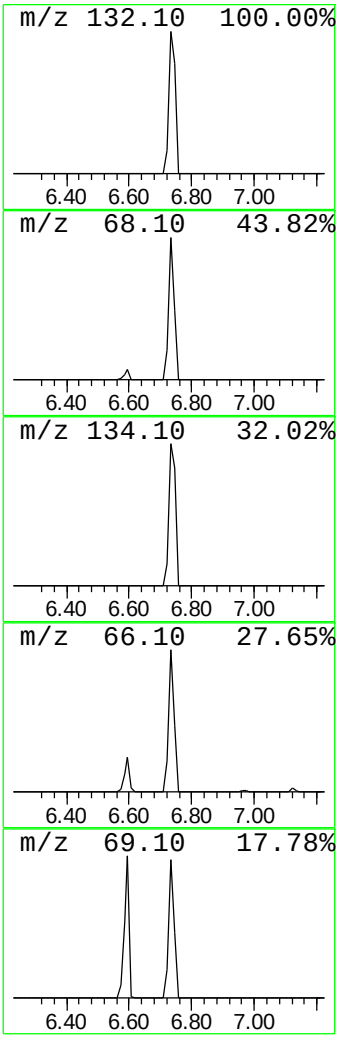
****

Peak Number 9 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	86.77 ng	4094710	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	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
ClientSampleId : SB-46-COMP

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

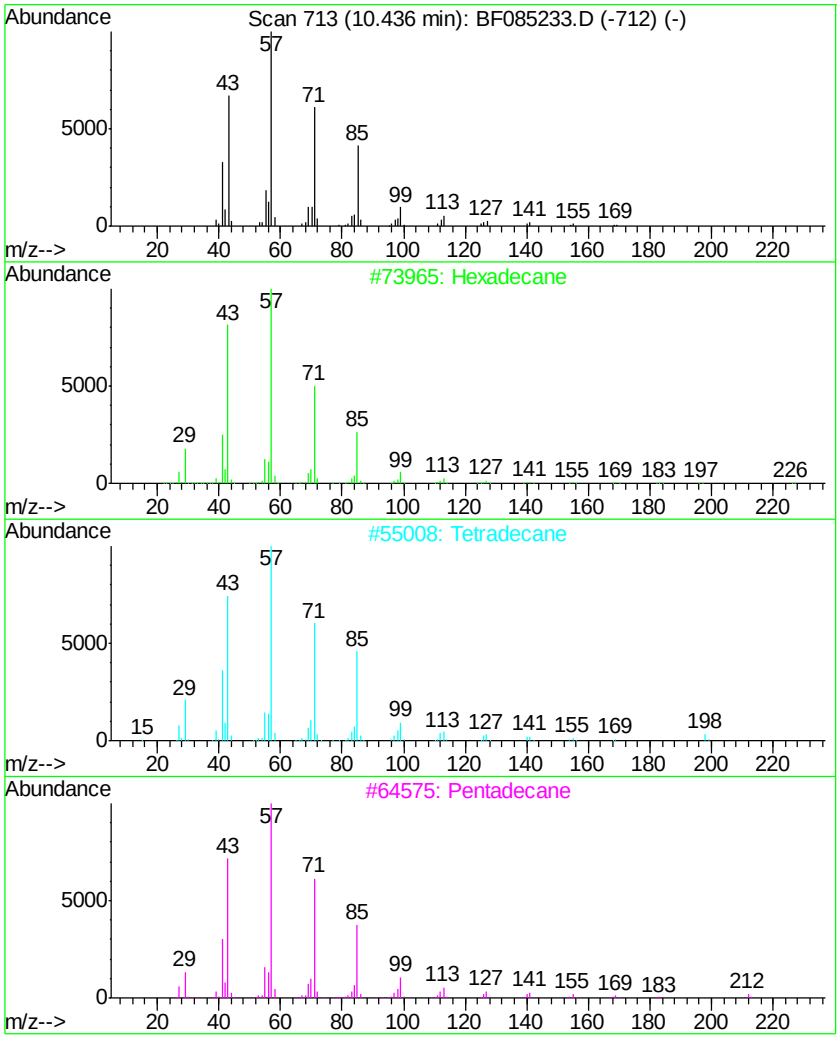
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

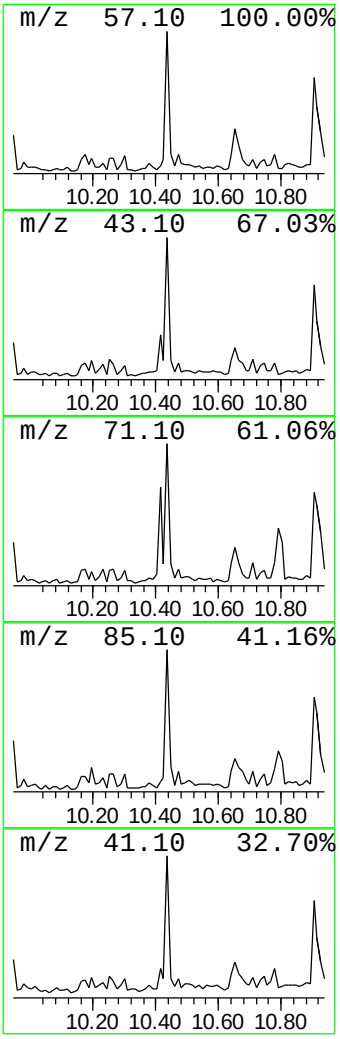
****

Peak Number 11 Hexadecane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.08 ng	146915	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	87
3	Pentadecane	212	C15H32	000629-62-9	86
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5	Eicosane	282	C20H42	000112-95-8	83





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Instrument : BNA_F
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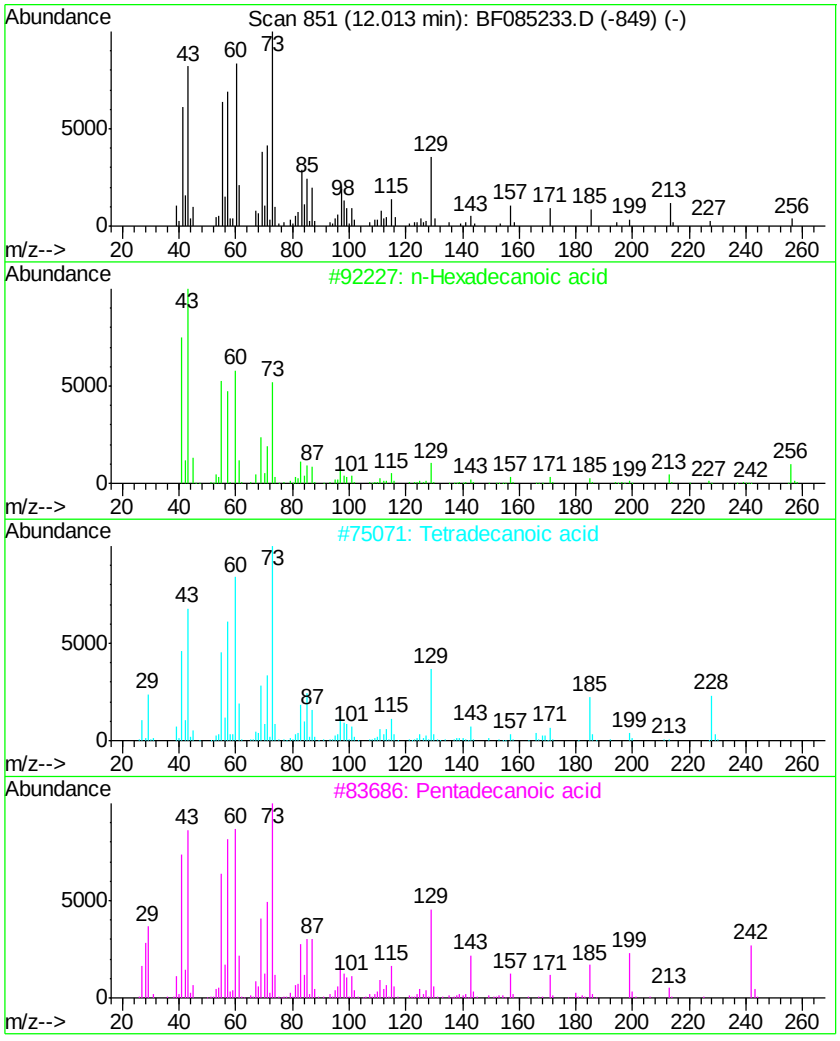
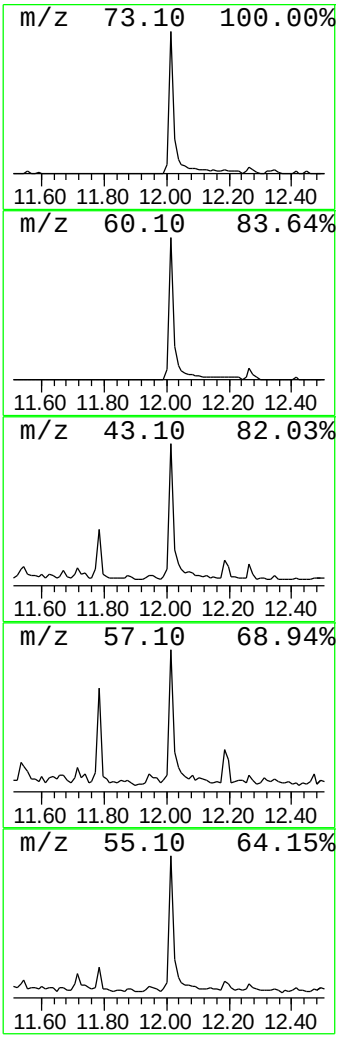
Peak Number 13 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	3.30 ng	237614	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	11





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Acq On : 5 Mar 2016 5:26
Operator : SJ/IZ
Sample : H1661-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-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

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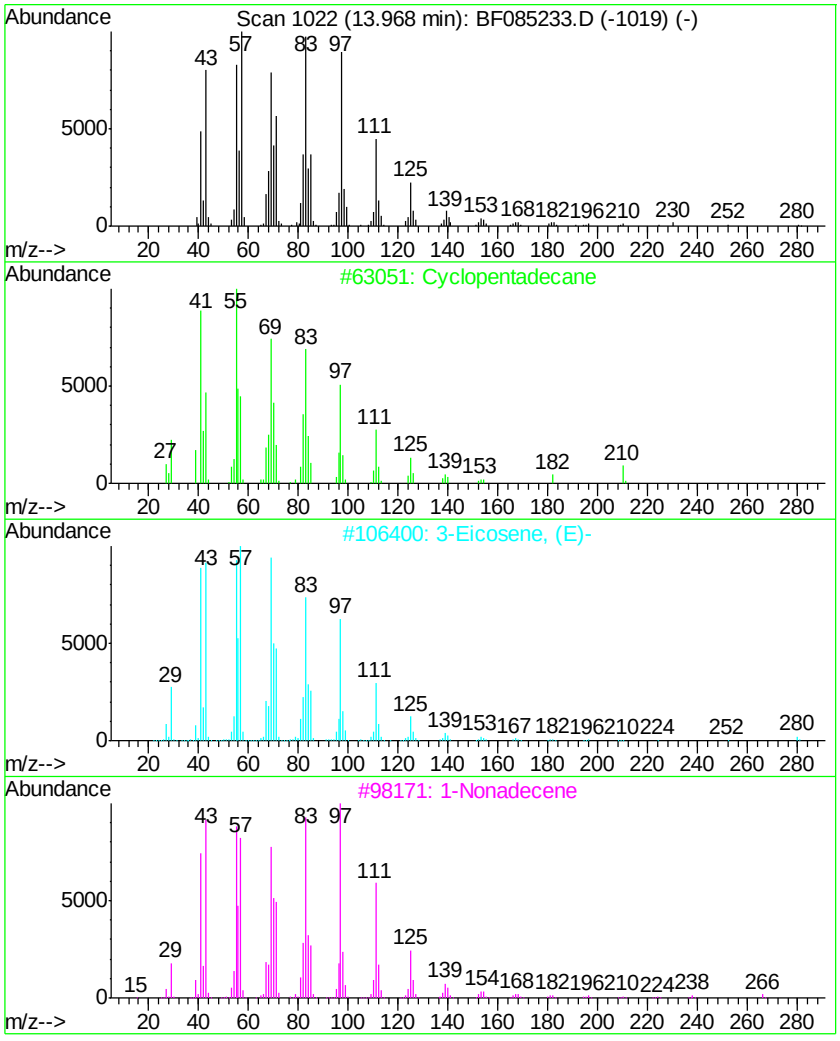
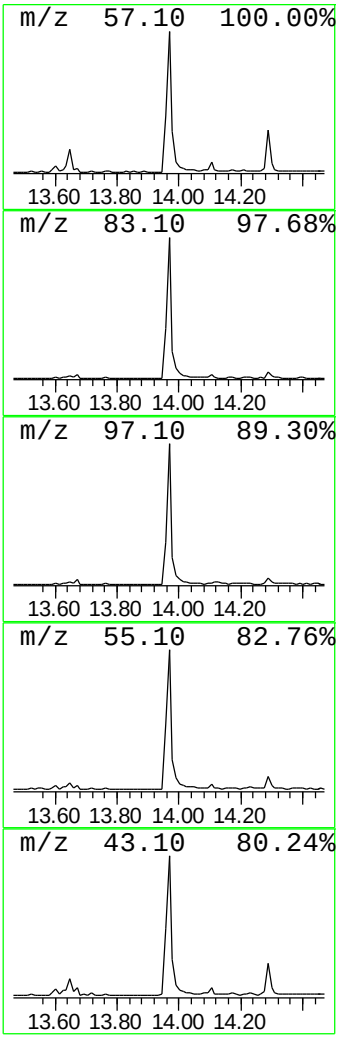
Peak Number 14 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	15.27 ng	837525	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91





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ClientSampleId : SB-46-COMP

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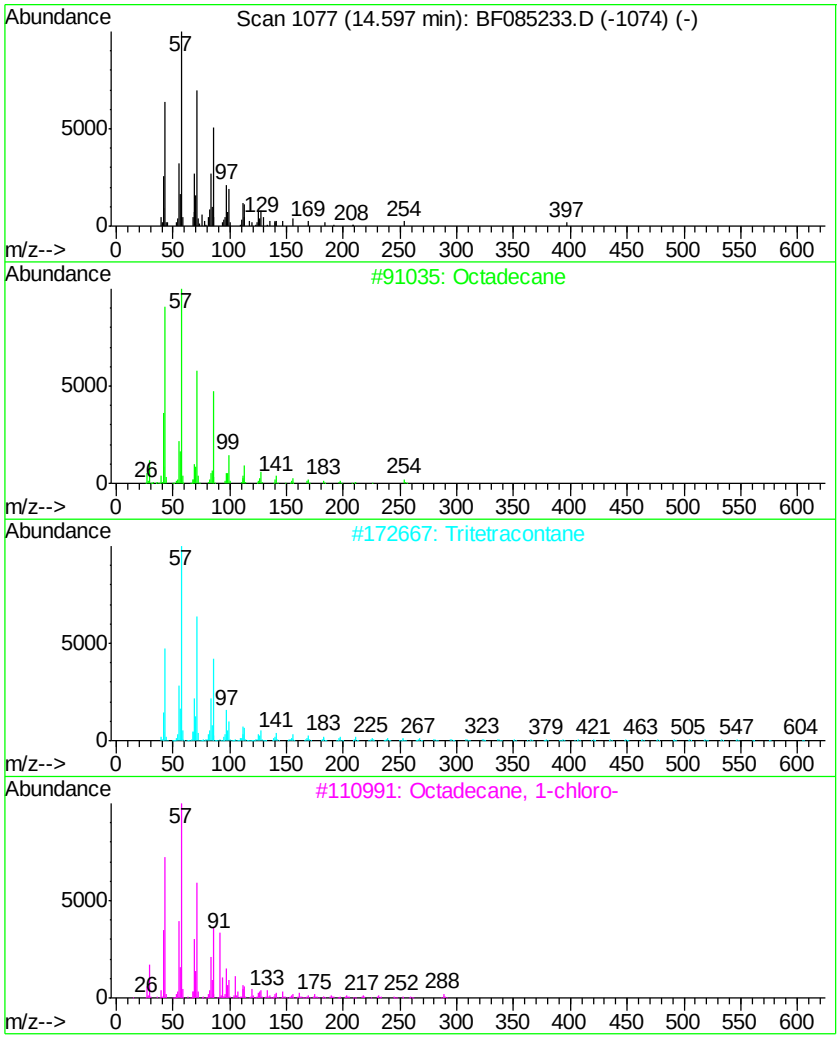
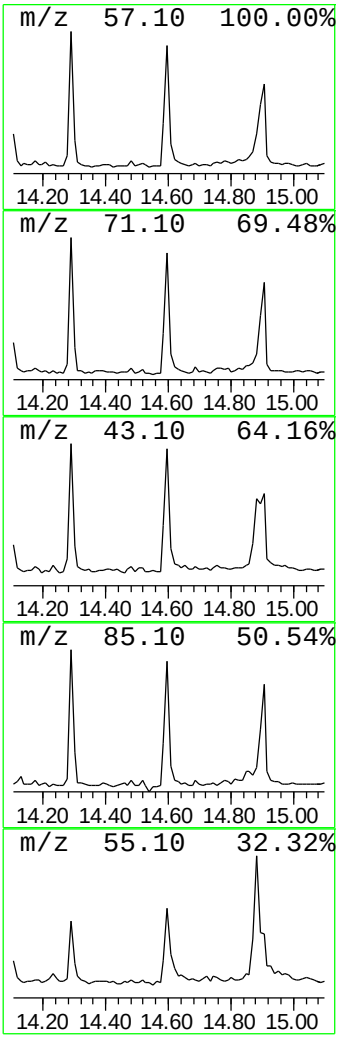
Peak Number 15 Octadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.35 ng	128970	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Tritetracontane	605	C43H88	007098-21-7	87
3	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83
5	Heptadecane	240	C17H36	000629-78-7	68





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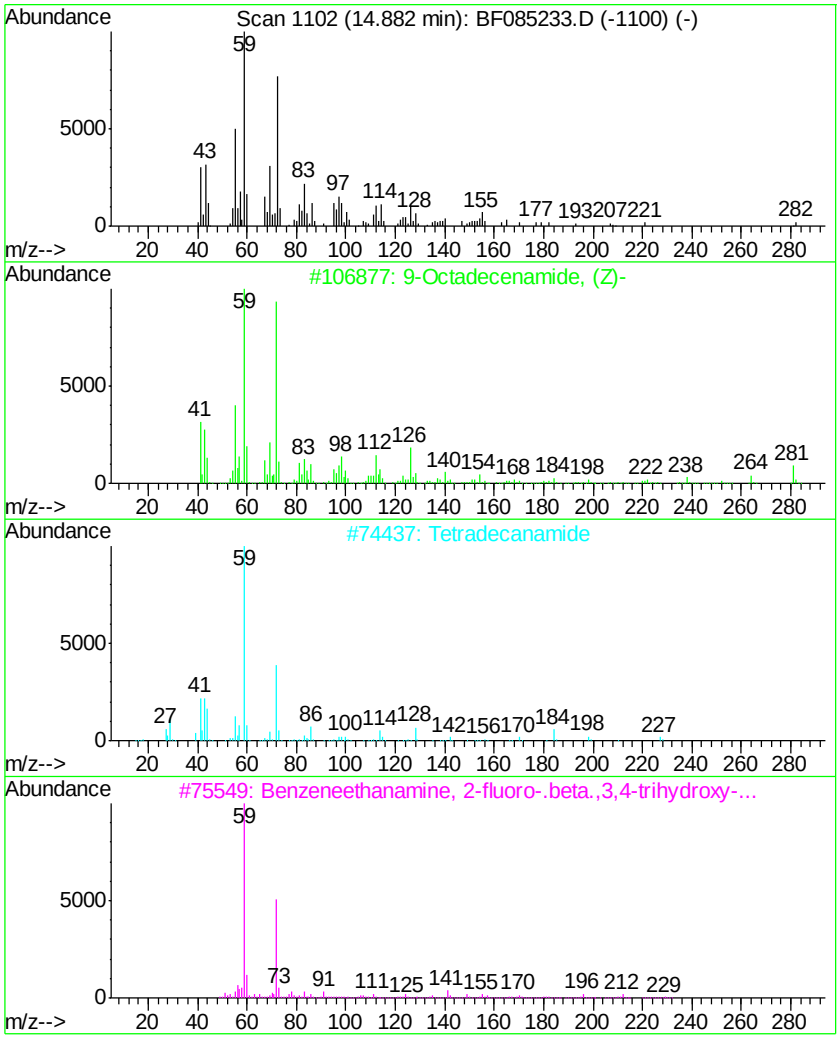
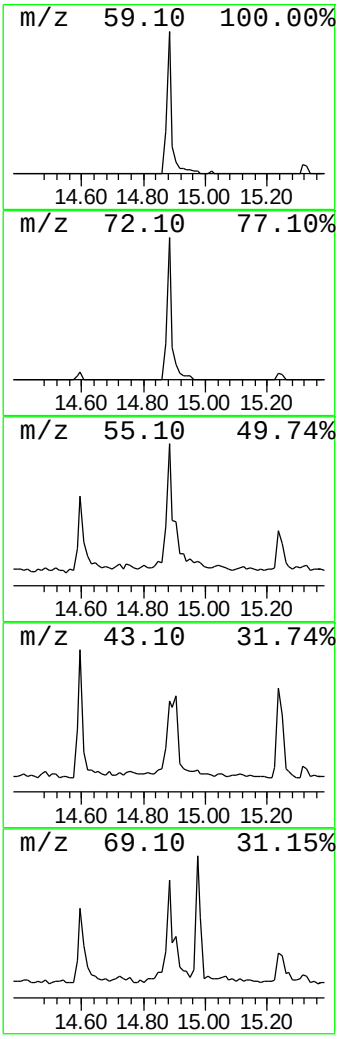
Peak Number 16 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	6.95 ng	259368	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
2	Tetradecanamide	227	C14H29NO	000638-58-4	59
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	38
4	2-Methyl-2-decanol	172	C11H24O	003396-02-9	35
5	Dodecanamide	199	C12H25NO	001120-16-7	35





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Sample : H1661-03
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ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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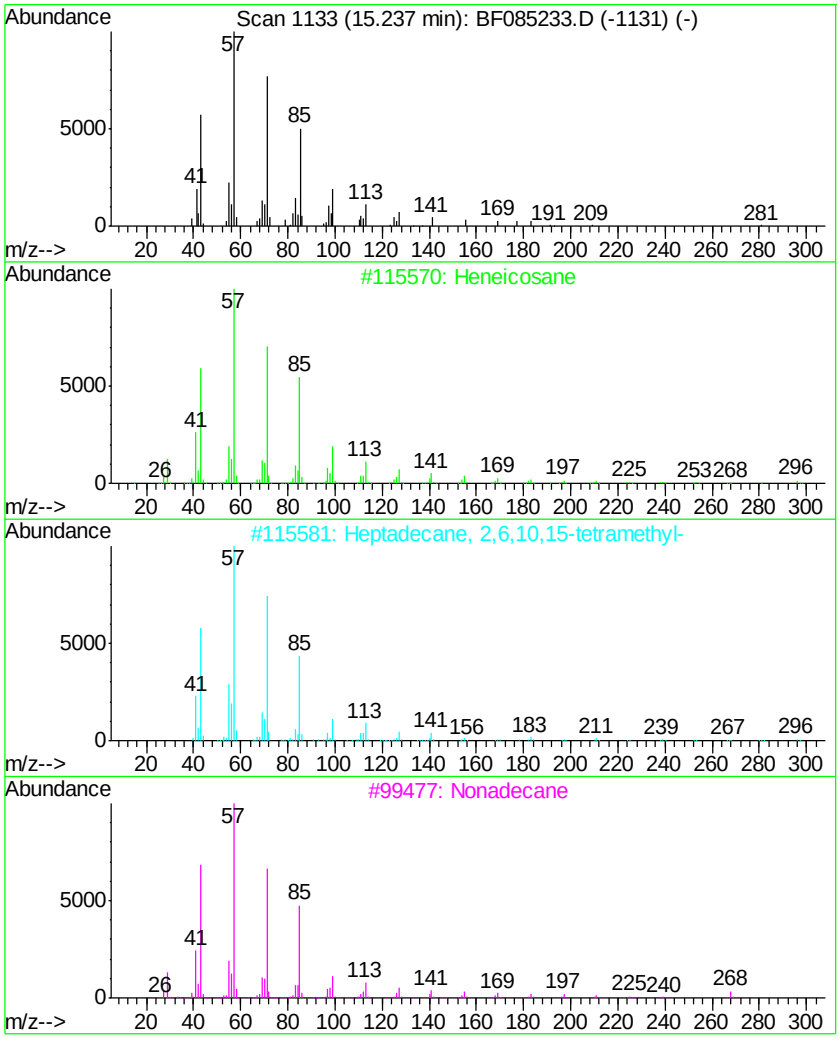
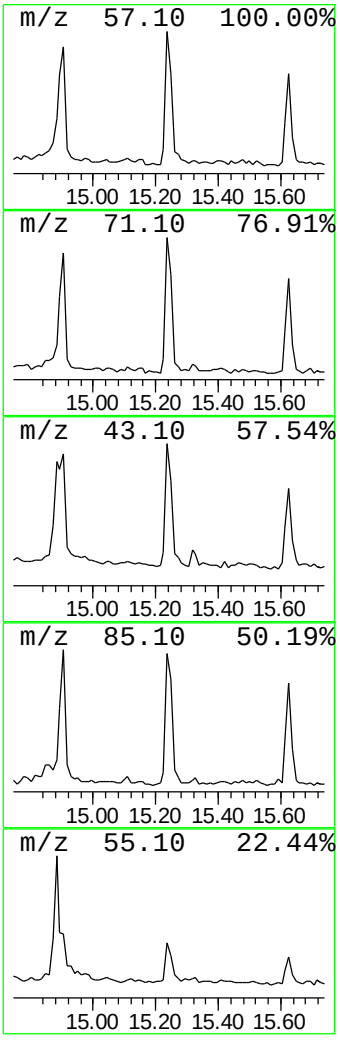
Peak Number 17 Heneicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.45 ng	91386	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3	Nonadecane	268	C19H40	000629-92-5	90
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5	Eicosane	282	C20H42	000112-95-8	90





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Sample : H1661-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-COMP

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

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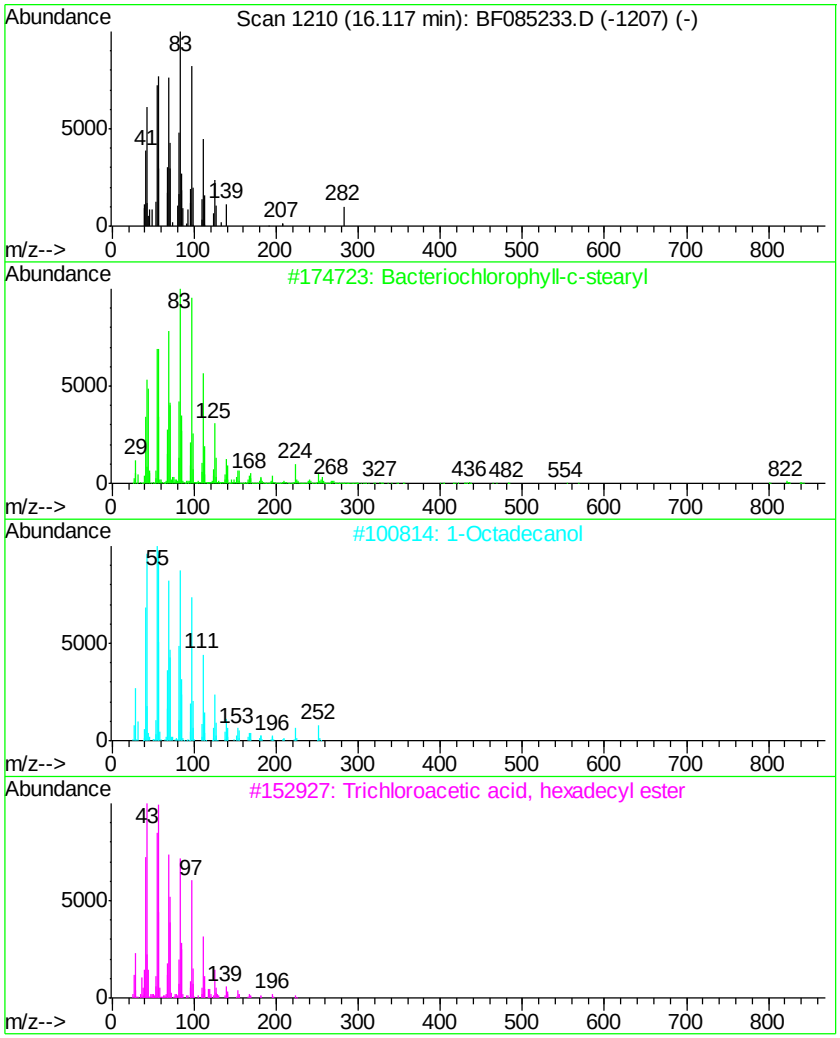
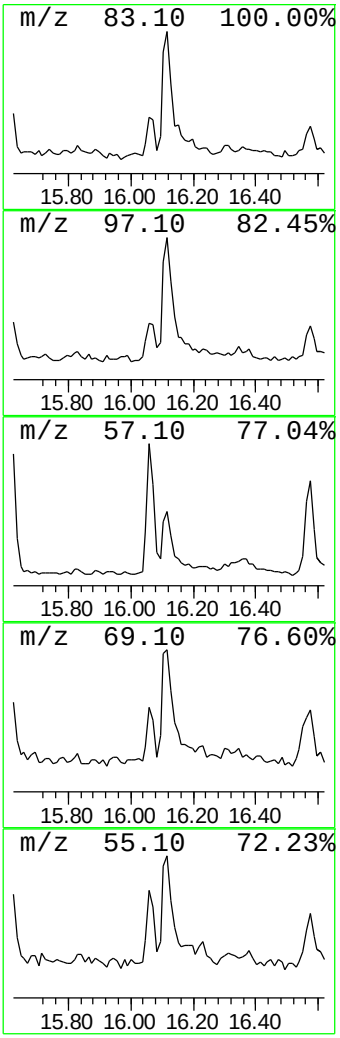
Peak Number 18 Bacteriochlorophyll-c-stearyl Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.23 ng	83448	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	90
2	1-Octadecanol	270	C18H38O	000112-92-5	87
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	80
4	1-Hexadecanol	242	C16H34O	036653-82-4	72
5	1-Eicosanol	298	C20H42O	000629-96-9	64





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-46-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzenamine, 4-tr...	3.20	63.6	ng	3000190	1	6.97	943756	20.0
unknown3.40	3.40	33.1	ng	1563840	1	6.97	943756	20.0
1,2,4-Oxadiazol-5...	3.44	40.7	ng	1921950	1	6.97	943756	20.0
2-Pentanone, 4-hy...	5.18	20.7	ng	975381	1	6.97	943756	20.0
unknown6.73	6.73	86.8	ng	4094710	1	6.97	943756	20.0
Hexadecane	10.44	2.1	ng	146915	3	10.01	1413090	20.0
n-Hexadecanoic acid	12.01	3.3	ng	237614	4	11.50	1439090	20.0
Cyclopentadecane	13.97	15.3	ng	837525	5	14.13	1097000	20.0
Octadecane	14.60	2.4	ng	128970	5	14.13	1097000	20.0
9-Octadecenamide,...	14.88	7.0	ng	259368	6	15.59	746905	20.0
Heneicosane	15.24	2.5	ng	91386	6	15.59	746905	20.0
Bacteriochlorophy...	16.12	2.2	ng	83448	6	15.59	746905	20.0