LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020416\
Data File : BF084850.D
Acq On : 5 Feb 2016 1:20
Operator : SJ/IZ
Sample : H1320-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B011(25-28)

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-BF020116.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	4.121	176	178	183	rVB	55239	76307	1.43%	0.178%
2	4.830	237	240	253	rVB	1254236	1953711	36.53%	4.554%
3	5.276	276	279	281	rBV	4431347	5347680	100.00%	12.466%
4	5.676	312	314	317	rBV	64691	58374	1.09%	0.136%
5	6.327	368	371	374	rBV	4134656	4540619	84.91%	10.584%
6	6.441	378	381	384	rBV	4421061	4638708	86.74%	10.813%
7	6.670	399	401	404	rBV	1073966	901377	16.86%	2.101%
8	6.830	412	415	417	rBV	4232330	3751522	70.15%	8.745%
9	7.242	448	451	454	rBV	2441462	2983035	55.78%	6.954%
10	7.962	511	514	516	rBV	1357431	1223102	22.87%	2.851%
11	9.036	605	608	611	rBV	3396569	4559957	85.27%	10.629%
12	9.436	641	643	645	rBV	610091	524134	9.80%	1.222%
13	9.653	660	662	664	rVB	109614	102923	1.92%	0.240%
14	9.710	664	667	669	rBV	1470365	1273309	23.81%	2.968%
15	10.156	704	706	708	rVB	193565	146242	2.73%	0.341%
16	10.373	722	725	728	rBV	52355	82755	1.55%	0.193%
17	10.499	733	736	738	rBV	3163947	3015159	56.38%	7.028%
18	10.625	745	747	752	rVB	154970	167631	3.13%	0.391%
19	11.185	794	796	799	rVB	1145537	1049796	19.63%	2.447%
20	12.774	933	935	938	rBV	3146366	3074184	57.49%	7.166%
21	13.688	1012	1015	1024	rBV	495119	941288	17.60%	2.194%
22	13.814	1024	1026	1029	rVB	846337	849042	15.88%	1.979%
23	14.317	1065	1070	1077	rBV	111335	275676	5.16%	0.643%
24	14.671	1098	1101	1103	rBV	87720	98744	1.85%	0.230%
25	15.185	1144	1146	1148	rBV	551054	816927	15.28%	1.904%
26	15.665	1186	1188	1191	rBV2	62566	148957	2.79%	0.347%
27	15.848	1201	1204	1209	rVB	31162	65876	1.23%	0.154%
28	17.025	1300	1307	1311	rBV8	52858	165177	3.09%	0.385%
29	18.740	1454	1457	1463	rVB7	27496	67330	1.26%	0.157%

Sum of corrected areas: 42899542

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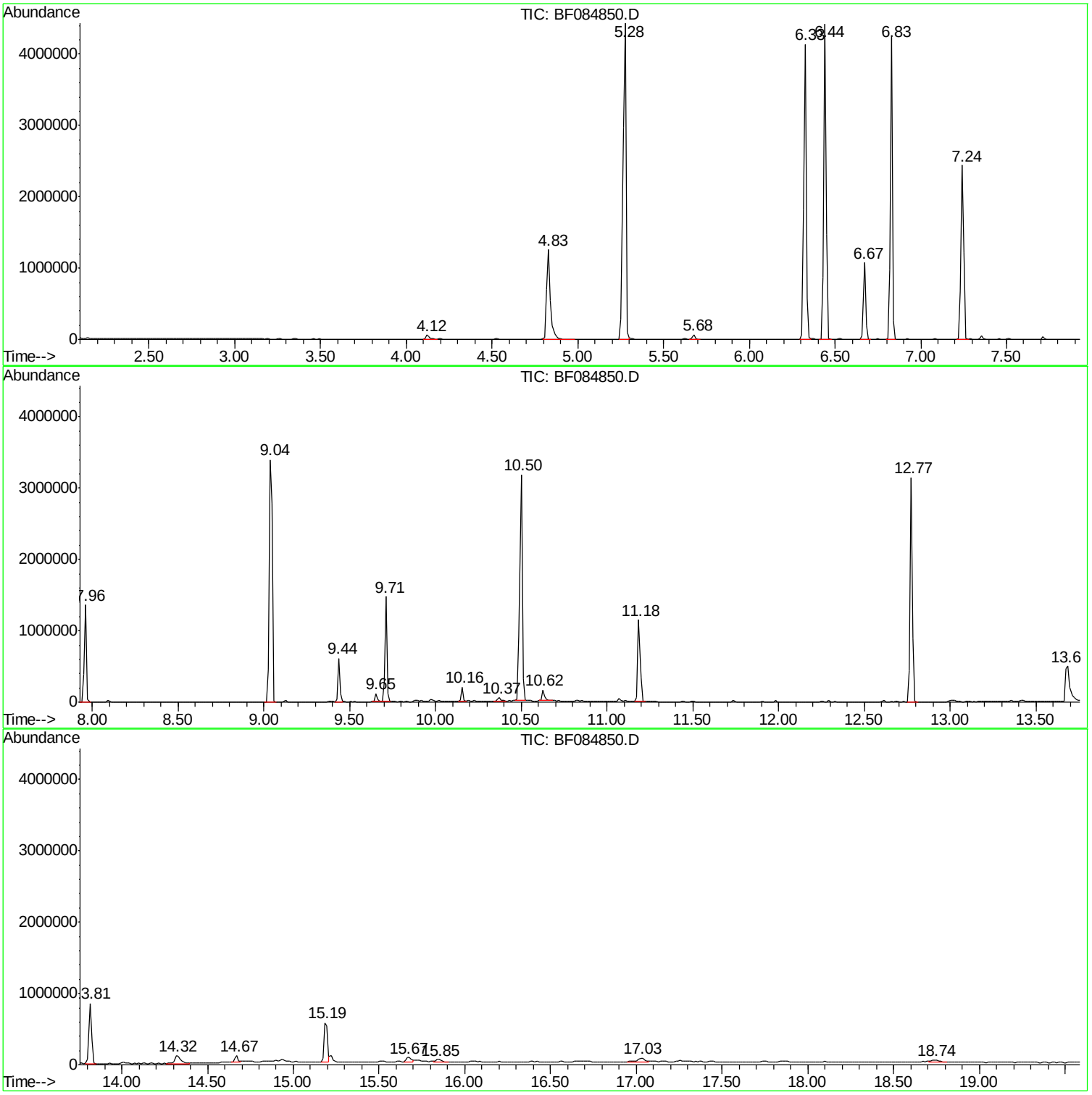
ClientSampleId :
S4-B011(25-28)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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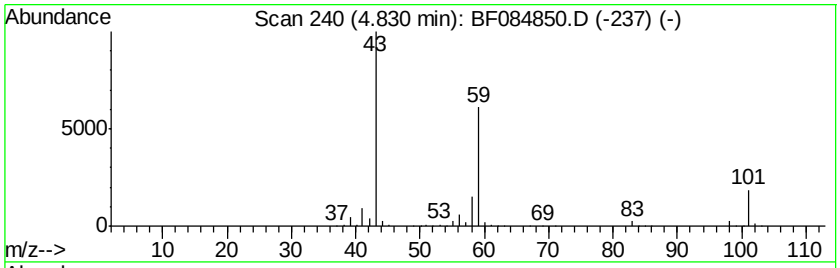
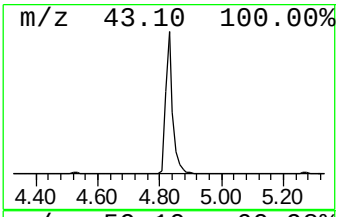
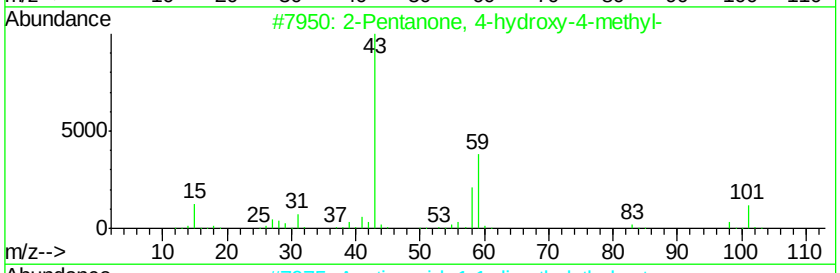
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

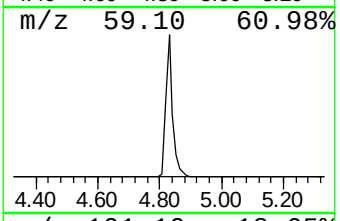
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	43.35 ng	1953710	1,4-Dichlorobenzene-d4	6.67

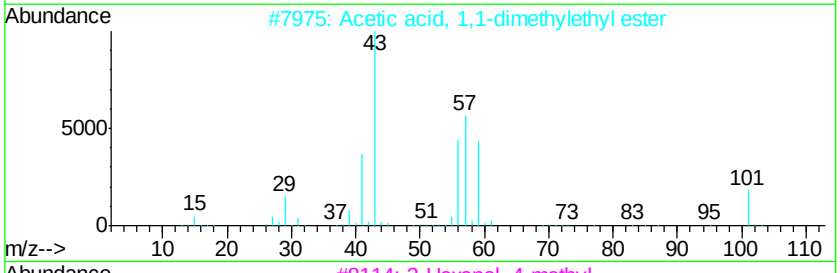
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

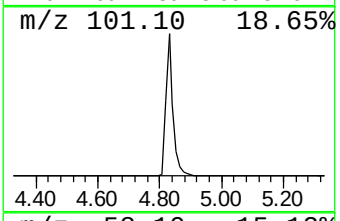


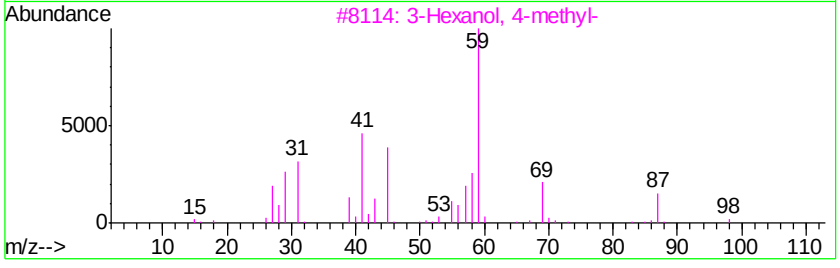


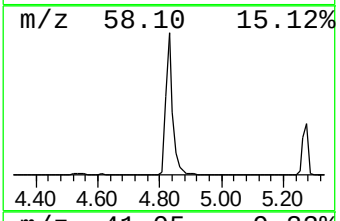


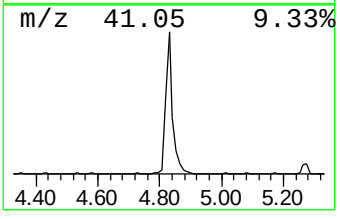












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Instrument : BNA_F
ClientSampleId : S4-B011(25-28)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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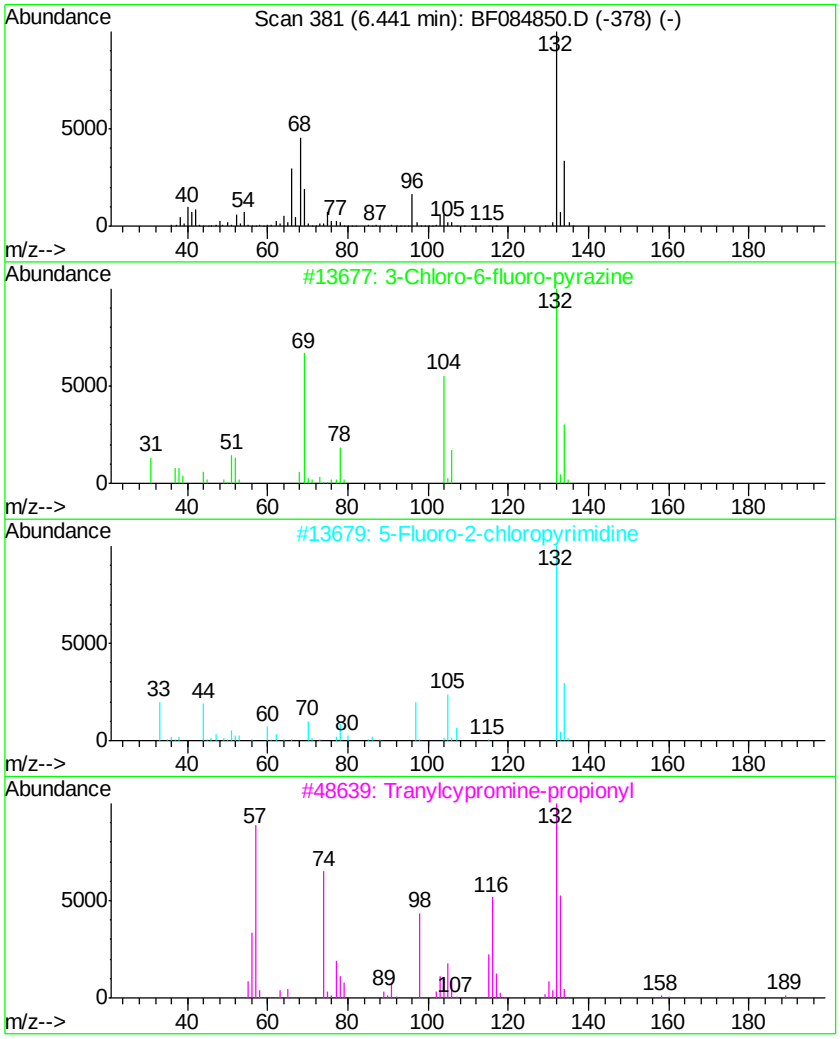
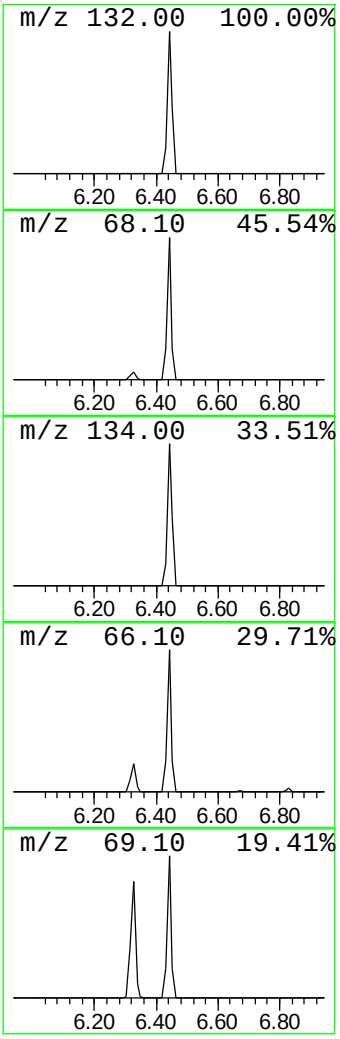
Peak Number 2 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	102.93 ng	4638710	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





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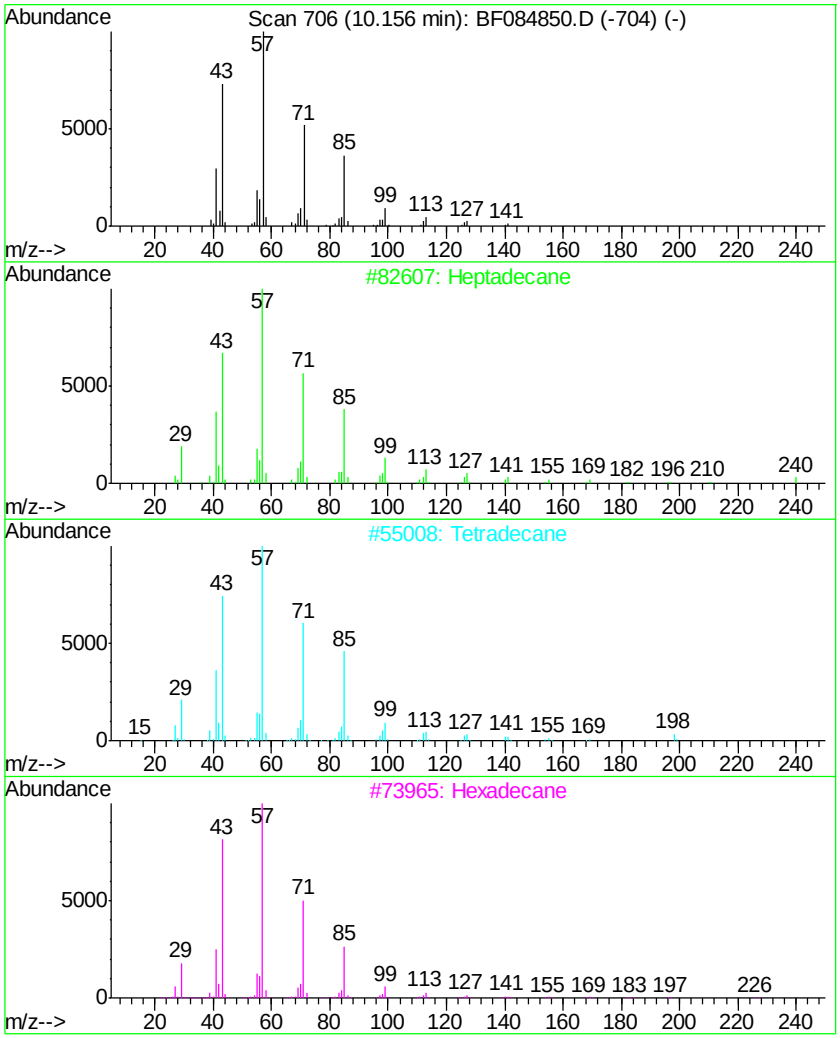
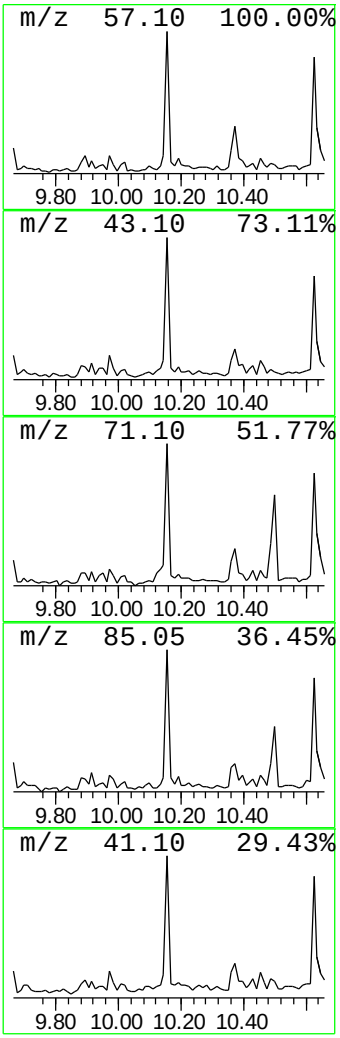
Peak Number 4 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	2.30 ng	146242	Acenaphthene-d10	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tetratetracontane	619	C44H90	007098-22-8	83
5	Pentadecane	212	C15H32	000629-62-9	78





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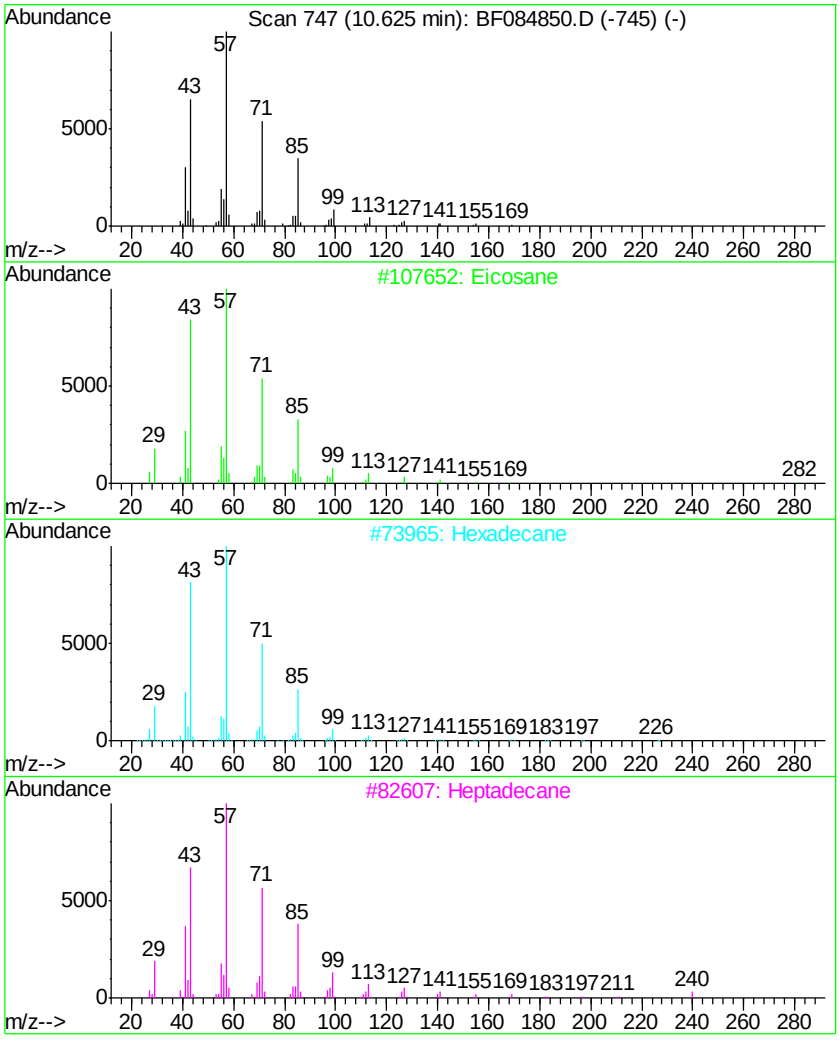
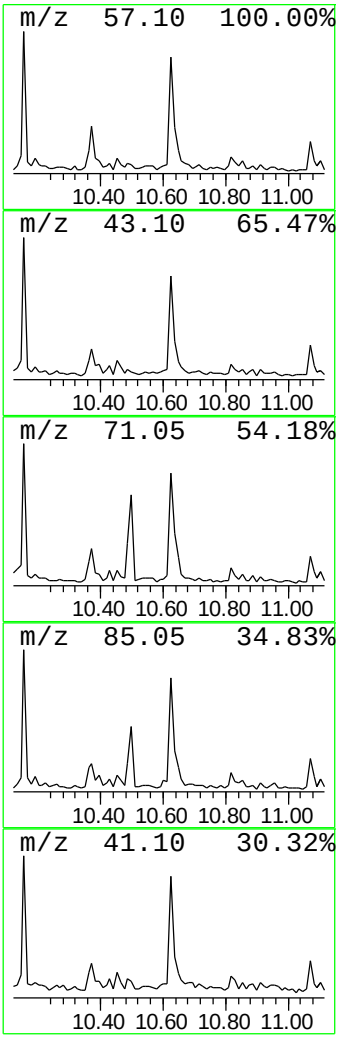
Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	3.19 ng	167631	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptadecane	240	C17H36	000629-78-7	83
4	Tetradecane	198	C14H30	000629-59-4	80
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	78





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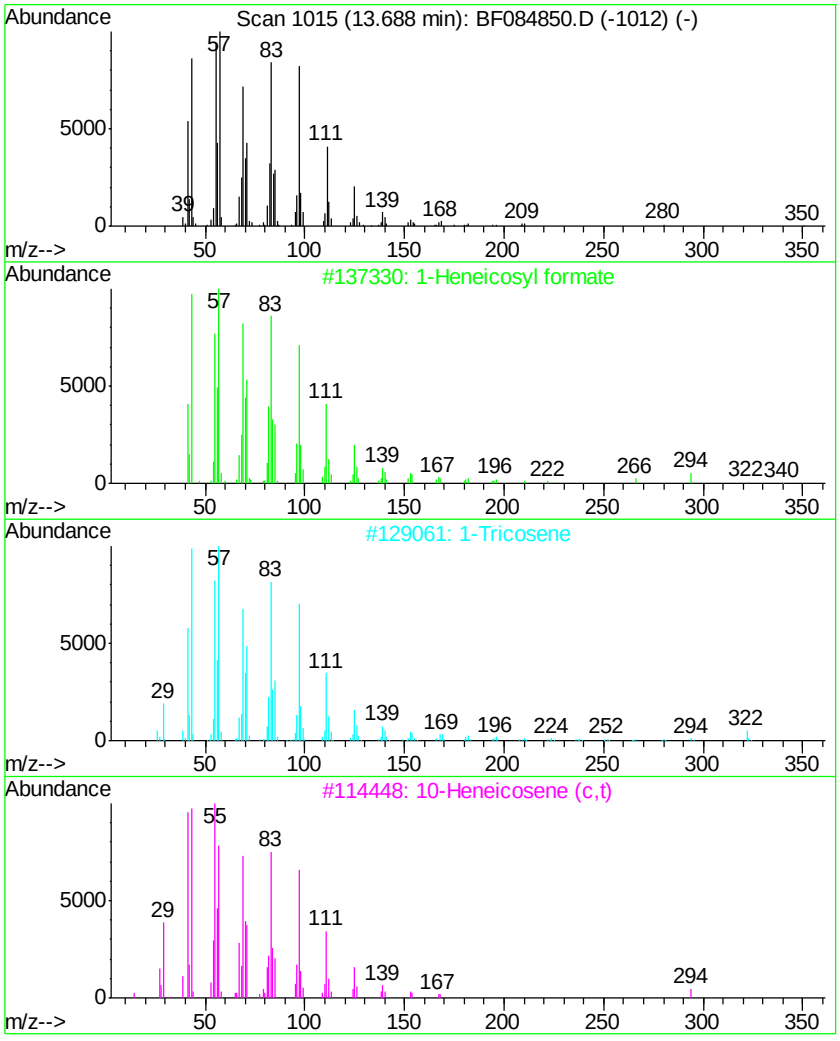
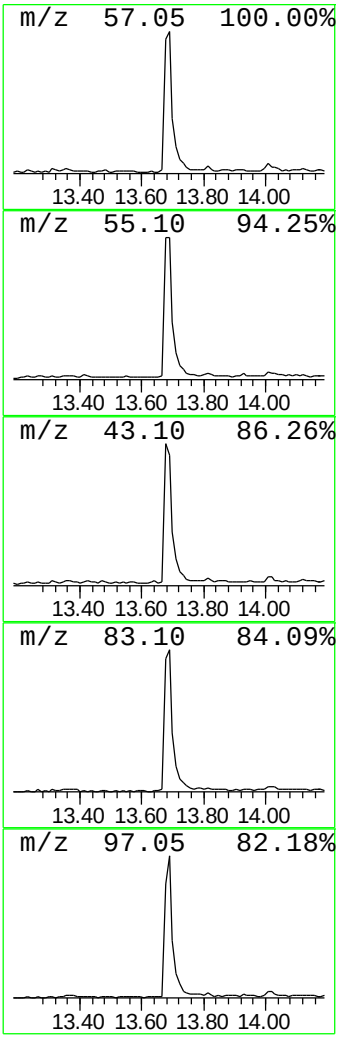
Peak Number 6 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	22.17 ng	941288	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2	1-Tricosene	322	C23H46	018835-32-0	91
3	10-Heneicosene (c,t)	294	C21H42	095008-11-0	91
4	Cyclotetracosane	336	C24H48	000297-03-0	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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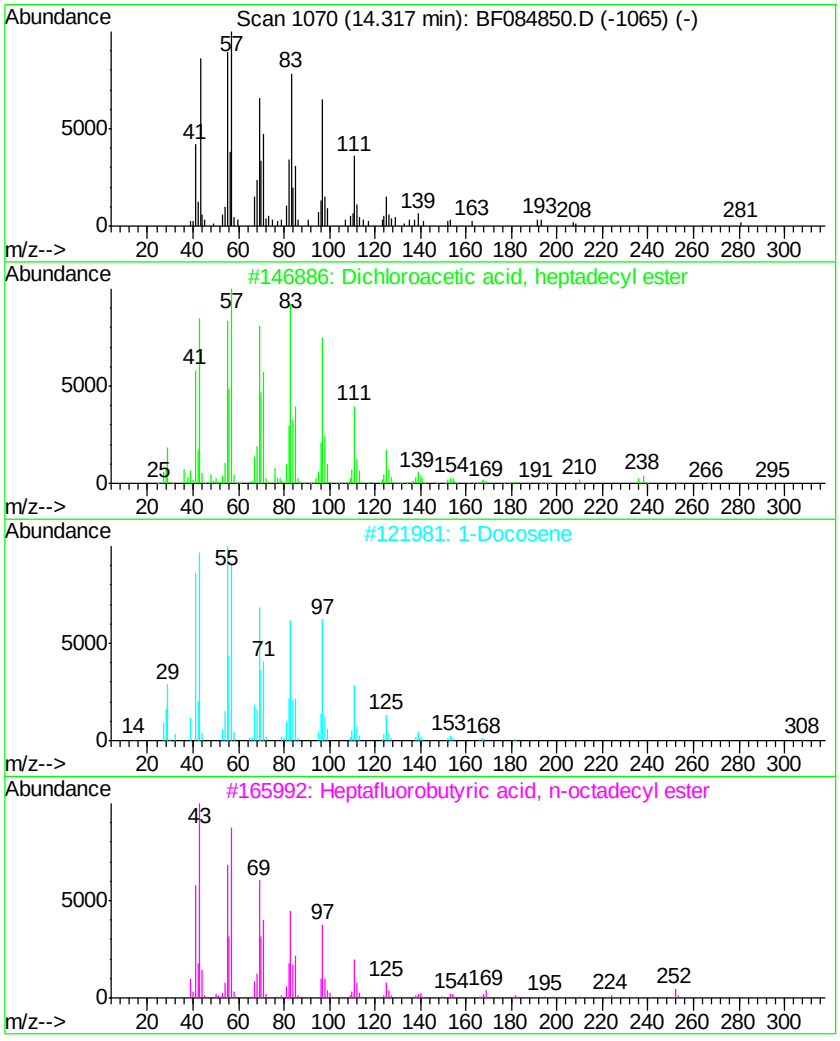
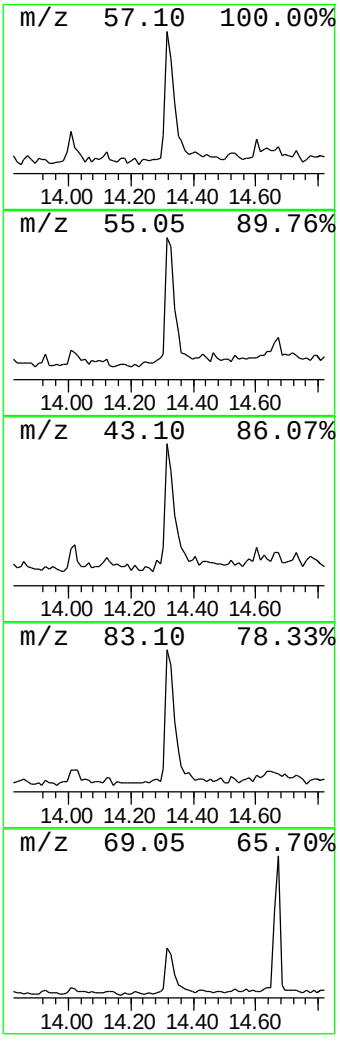
Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	6.49 ng	275676	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90





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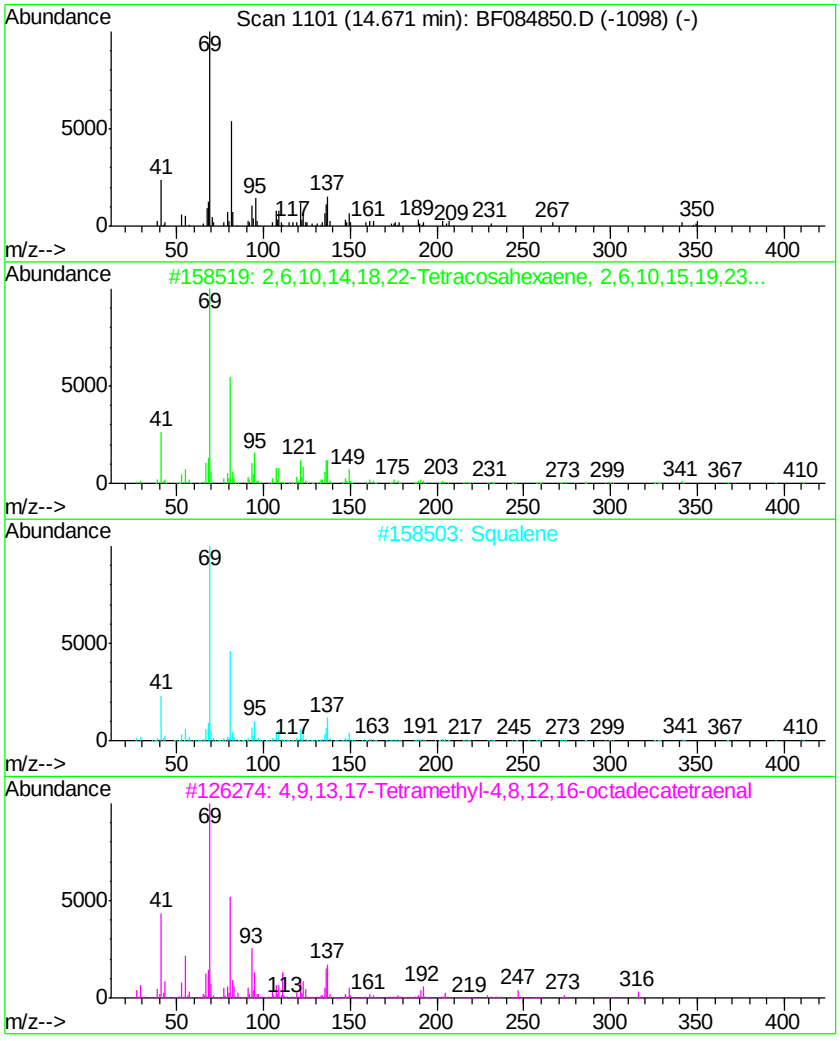
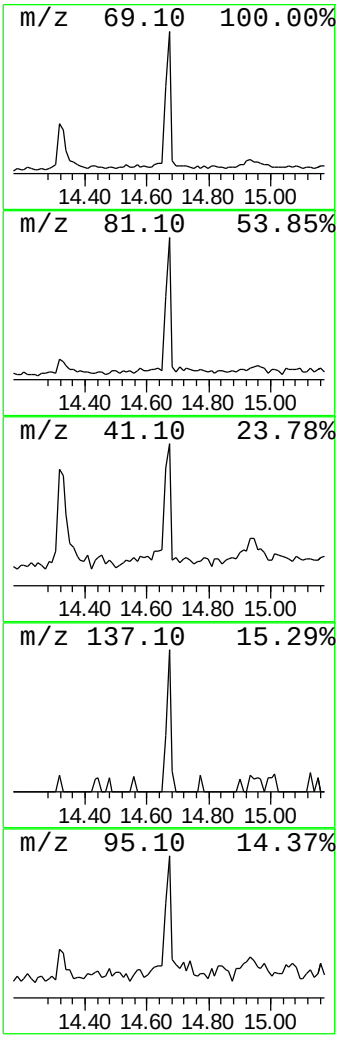
****

Peak Number 8 2,6,10,14,18,22-Tetracosahe... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.42 ng	98744	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
2	Squalene	410	C30H50	007683-64-9	87
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	72
5	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72





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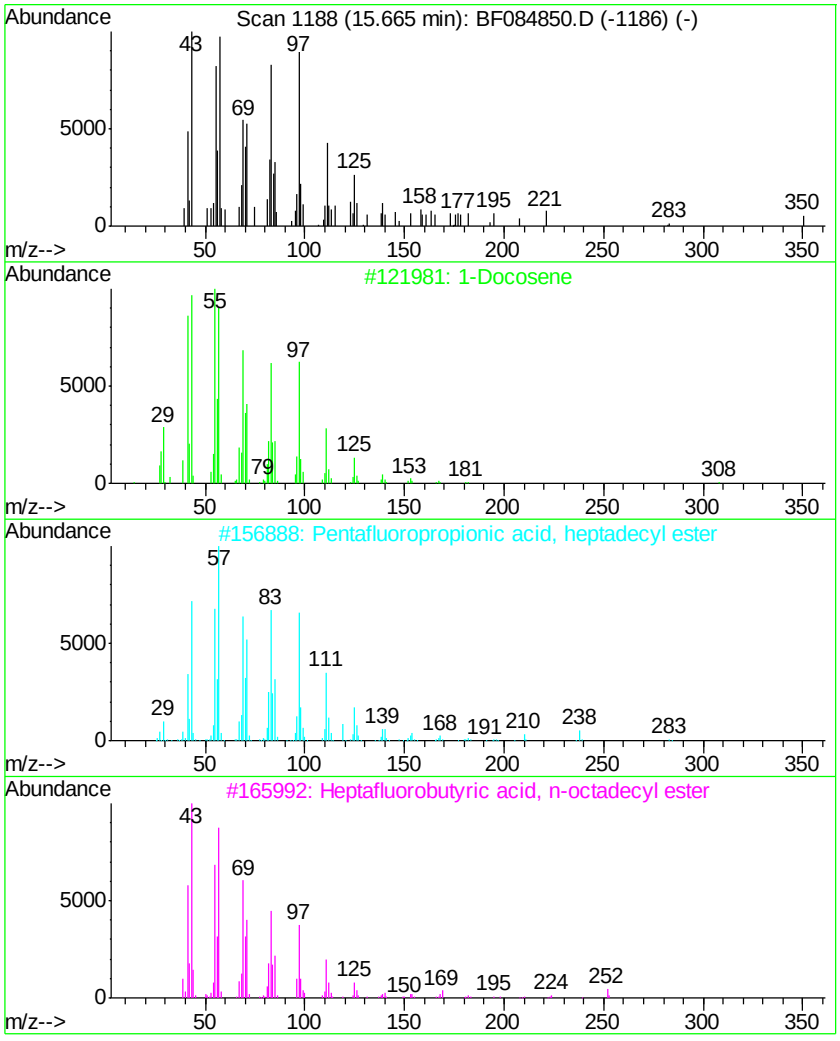
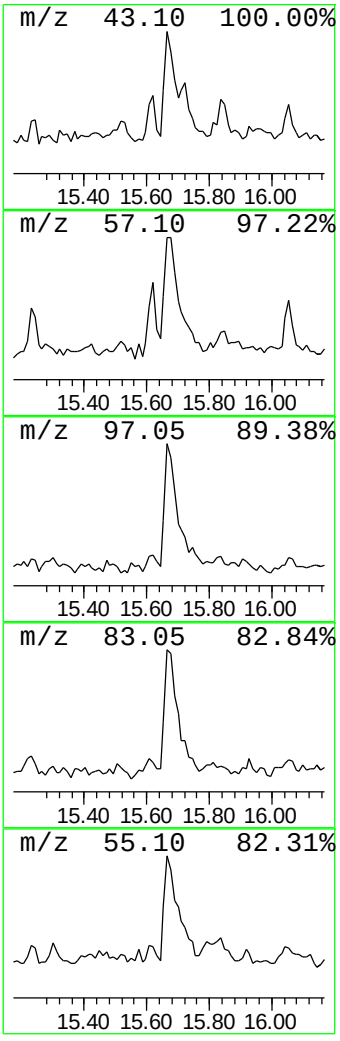
Peak Number 9 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	3.65 ng	148957	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Cyclotetracosane	336	C24H48	000297-03-0	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	87





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Sample : H1320-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B011(25-28)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

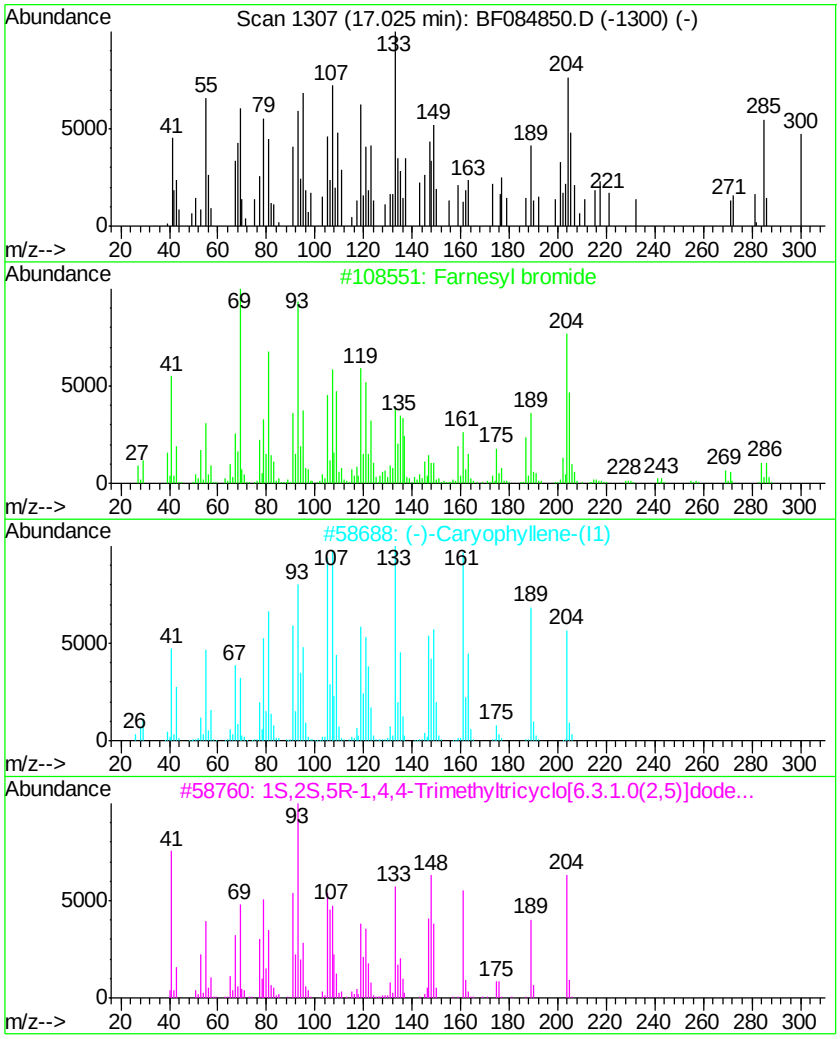
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

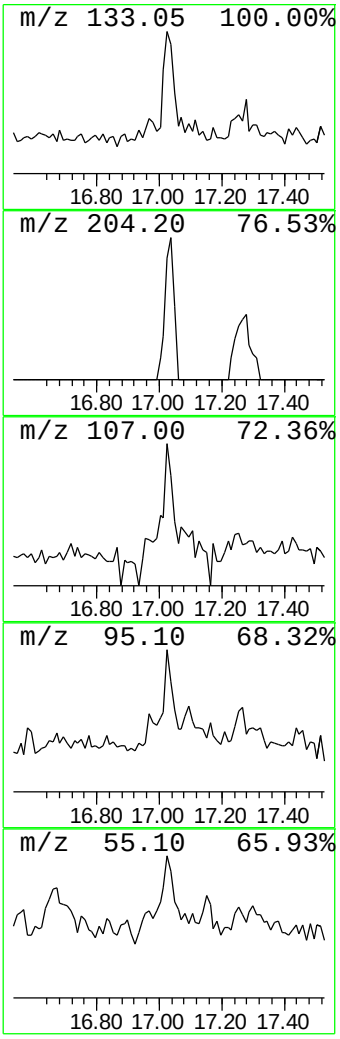
****

Peak Number 10 unknown17.03 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	4.04 ng	165177	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesyl bromide	284	C15H25Br	006874-67-5	46
2	(-)-Caryophyllene-(I1)	204	C15H24	1000156-13-1	46
3	1S,2S,5R-1,4,4-Trimethyltricyclo...	204	C15H24	1000140-07-5	43
4	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	42
5	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020416\
Data File : BF084850.D
Acq On : 5 Feb 2016 1:20
Operator : SJ/IZ
Sample : H1320-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B011(25-28)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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...	4.83	43.4	ng	1953710	1	6.67	901377	20.0
unknown6.44	6.44	102.9	ng	4638710	1	6.67	901377	20.0
Heptadecane	10.16	2.3	ng	146242	3	9.71	1273310	20.0
Eicosane	10.62	3.2	ng	167631	4	11.18	1049800	20.0
1-Heneicosyl formate	13.69	22.2	ng	941288	5	13.81	849042	20.0
Dichloroacetic ac...	14.32	6.5	ng	275676	5	13.81	849042	20.0
2,6,10,14,18,22-T...	14.67	2.4	ng	98744	6	15.20	816927	20.0
1-Docosene	15.67	3.6	ng	148957	6	15.20	816927	20.0
unknown17.03	17.03	4.0	ng	165177	6	15.20	816927	20.0