LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

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-BF090115.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	4.421	246	248	258	rVB	263113	407705	16.59%	2.657%
2	4.924	290	292	295	rBV	573660	776992	31.63%	5.064%
3	6.044	388	390	397	rVB	560617	503244	20.48%	3.280%
4	6.147	397	399	402	rBV	1198749	1319941	53.72%	8.602%
5	6.387	418	420	422	rBV	490605	439443	17.89%	2.864%
6	6.547	431	434	436	rBV	1307024	1559904	63.49%	10.166%
7	6.970	467	471	473	rBV	1192216	1478589	60.18%	9.636%
8	7.679	530	533	535	rBV	623455	581372	23.66%	3.789%
9	8.765	625	628	630	rBV	2227191	2456847	100.00%	16.012%
10	8.936	639	643	645	rVB3	10171	24641	1.00%	0.161%
11	9.165	661	663	665	rVB	48117	50275	2.05%	0.328%
12	9.279	670	673	675	rBV4	13059	25936	1.06%	0.169%
13	9.416	683	685	687	rBV	717923	631450	25.70%	4.115%
14	10.022	734	738	742	rBV3	30987	76435	3.11%	0.498%
15	10.205	751	754	756	rVB	967236	1201111	48.89%	7.828%
16	10.788	804	805	807	rBV2	21526	30788	1.25%	0.201%
17	10.879	811	813	815	rBV	642918	583892	23.77%	3.805%
18	11.154	835	837	840	rVB	40921	42083	1.71%	0.274%
19	11.211	840	842	845	rBV2	26749	36816	1.50%	0.240%
20	11.462	862	864	871	rVB	219439	252968	10.30%	1.649%
21	12.239	929	932	937	rBV	77947	94825	3.86%	0.618%
22	12.468	949	952	955	rBV	1660862	1775586	72.27%	11.572%
23	13.394	1031	1033	1036	rVB	114724	134575	5.48%	0.877%
24	13.485	1039	1041	1044	rBV	385497	458026	18.64%	2.985%
25	14.365	1116	1118	1120	rVB	40015	40246	1.64%	0.262%
26	14.800	1154	1156	1159	rBV	326988	323978	13.19%	2.111%
27	15.234	1192	1194	1202	rVB4	13879	36241	1.48%	0.236%

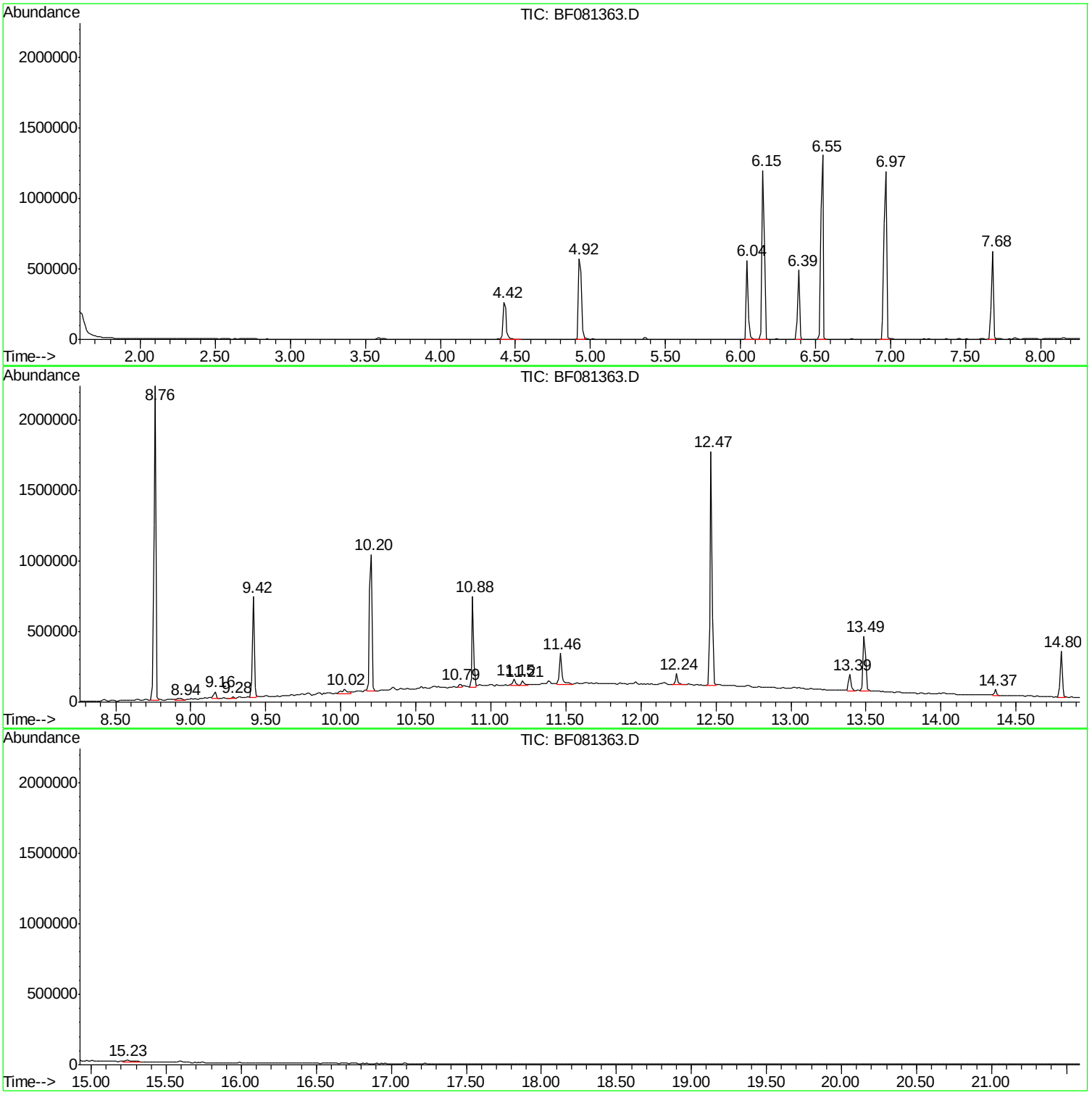
Sum of corrected areas: 15343909

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

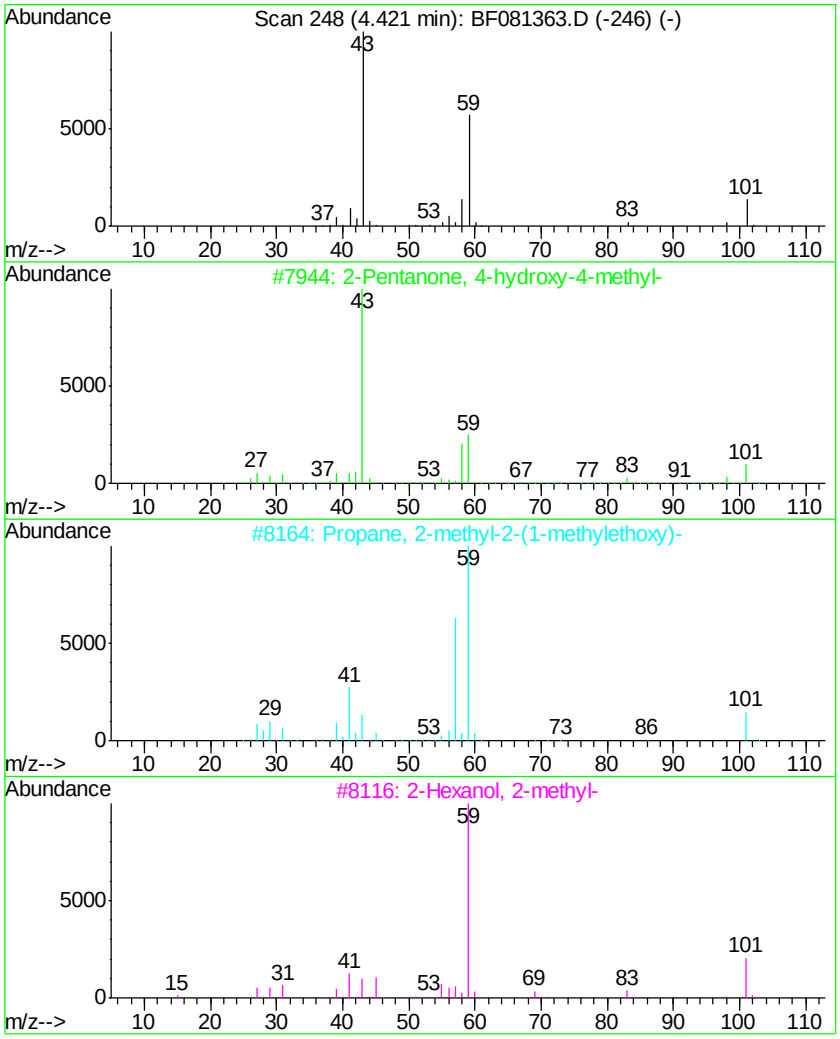
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

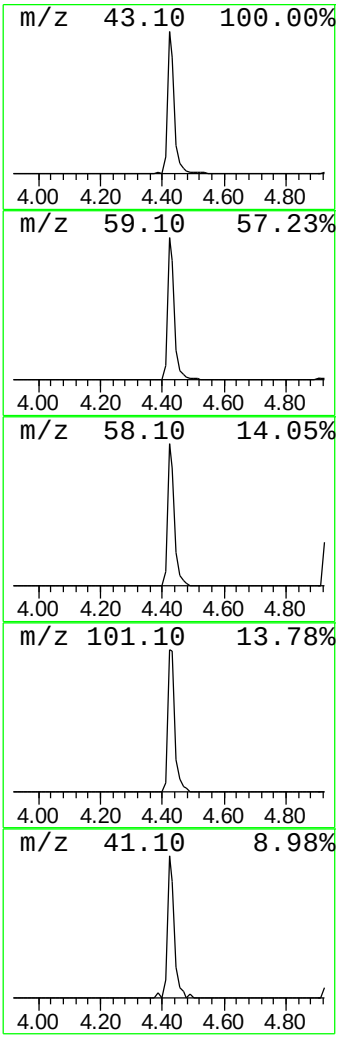
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	18.56 ng	407705	1,4-Dichlorobenzene-d4	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

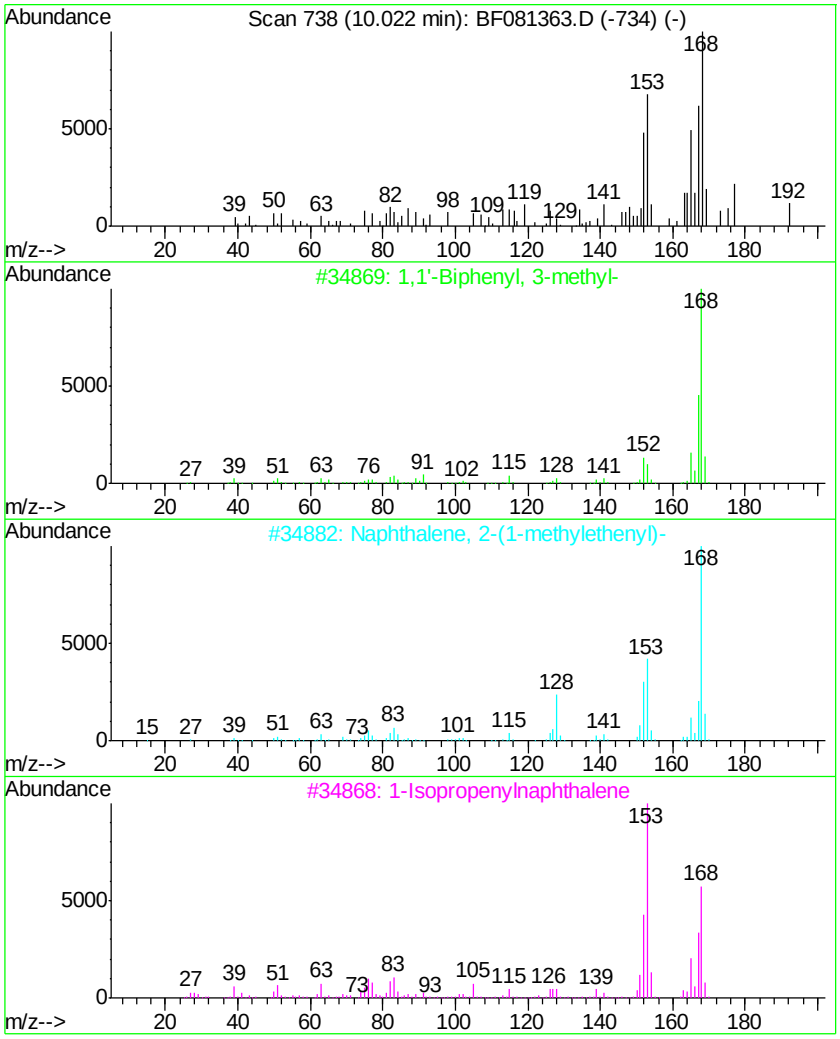
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

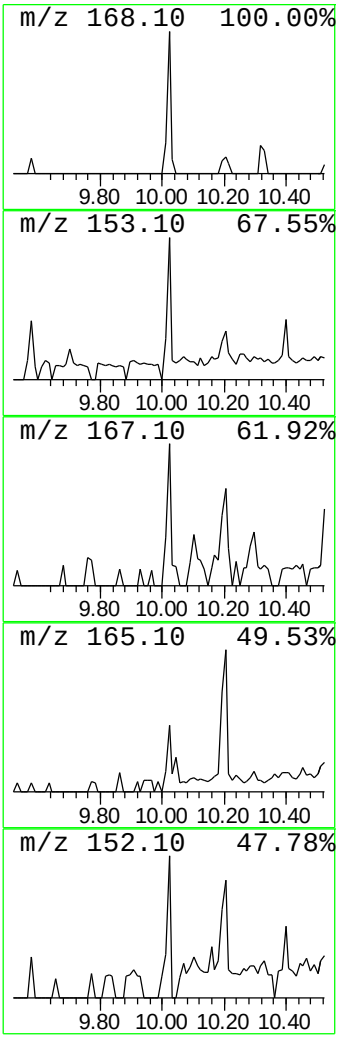
****

Peak Number 4 1,1'-Biphenyl, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	2.42 ng	76435	Acenaphthene-d10	9.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	58
2	Naphthalene, 2-(1-methylethenyl)-	168	C13H12	003710-23-4	53
3	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	52
4	Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	52
5	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	50





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

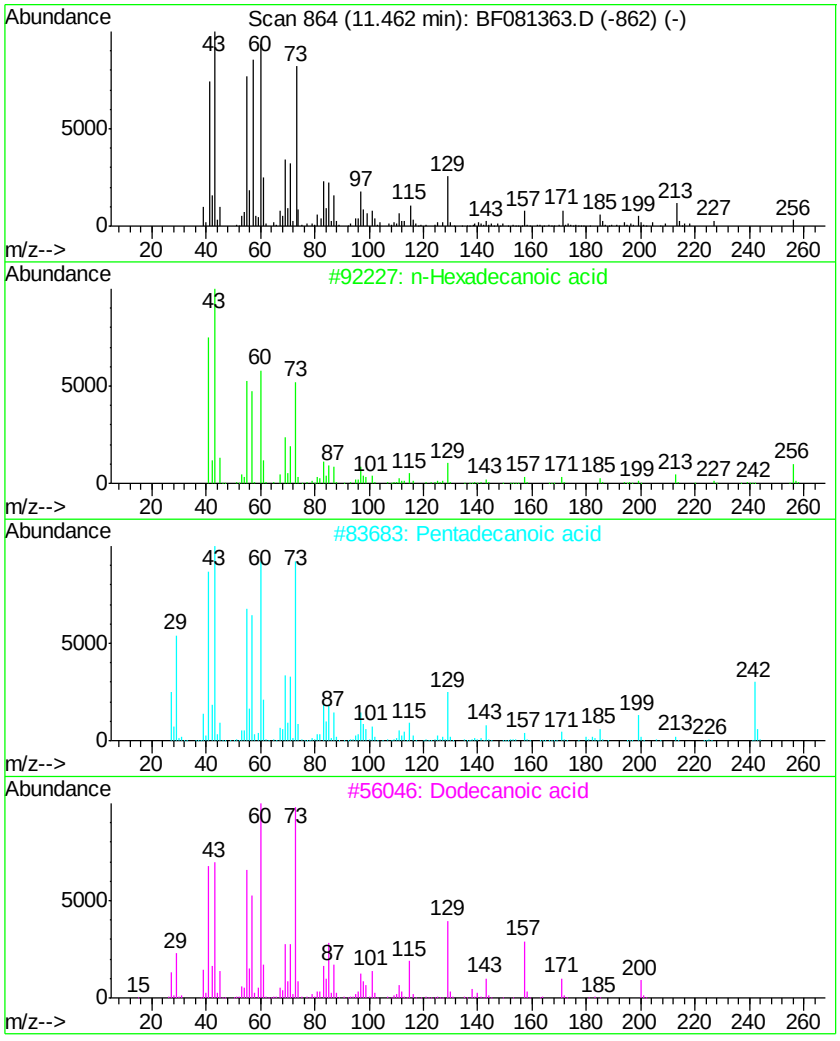
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

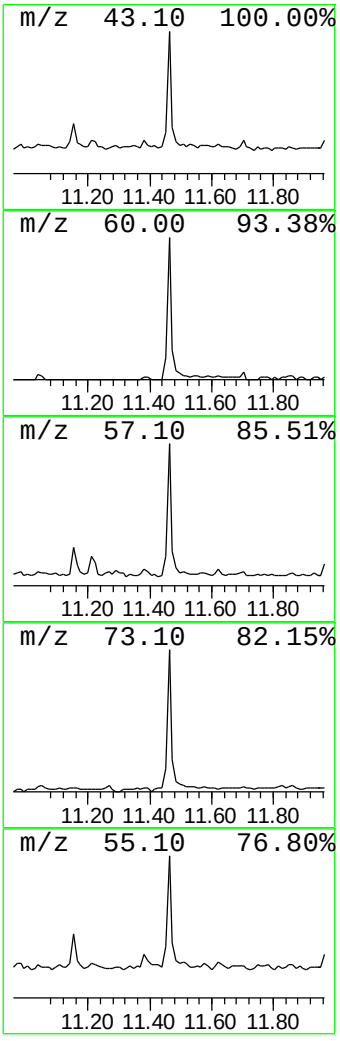
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	8.66 ng	252968	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Dodecanoic acid	200	C12H24O2	000143-07-7	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	68
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

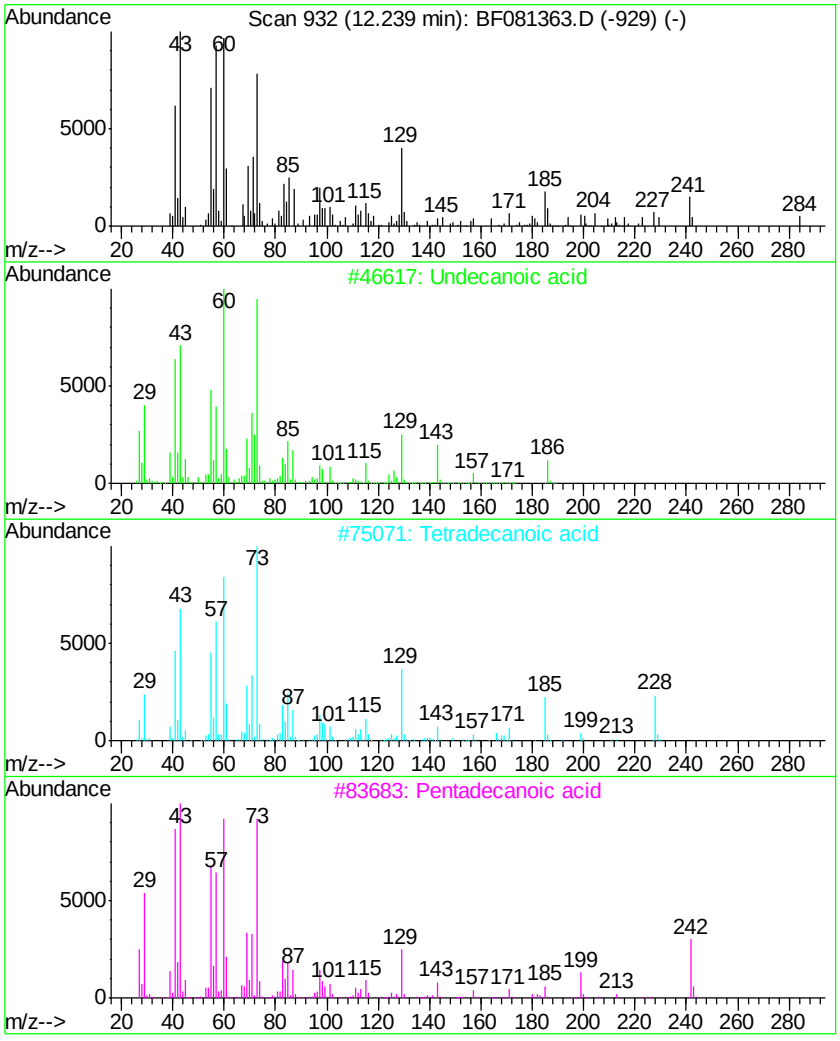
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

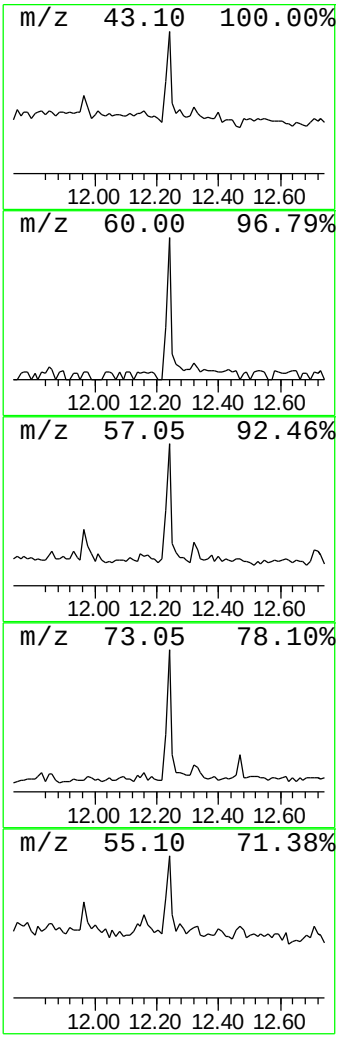
****

Peak Number 6 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.24	4.14 ng	94825	Chrysene-d12	13.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	76
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

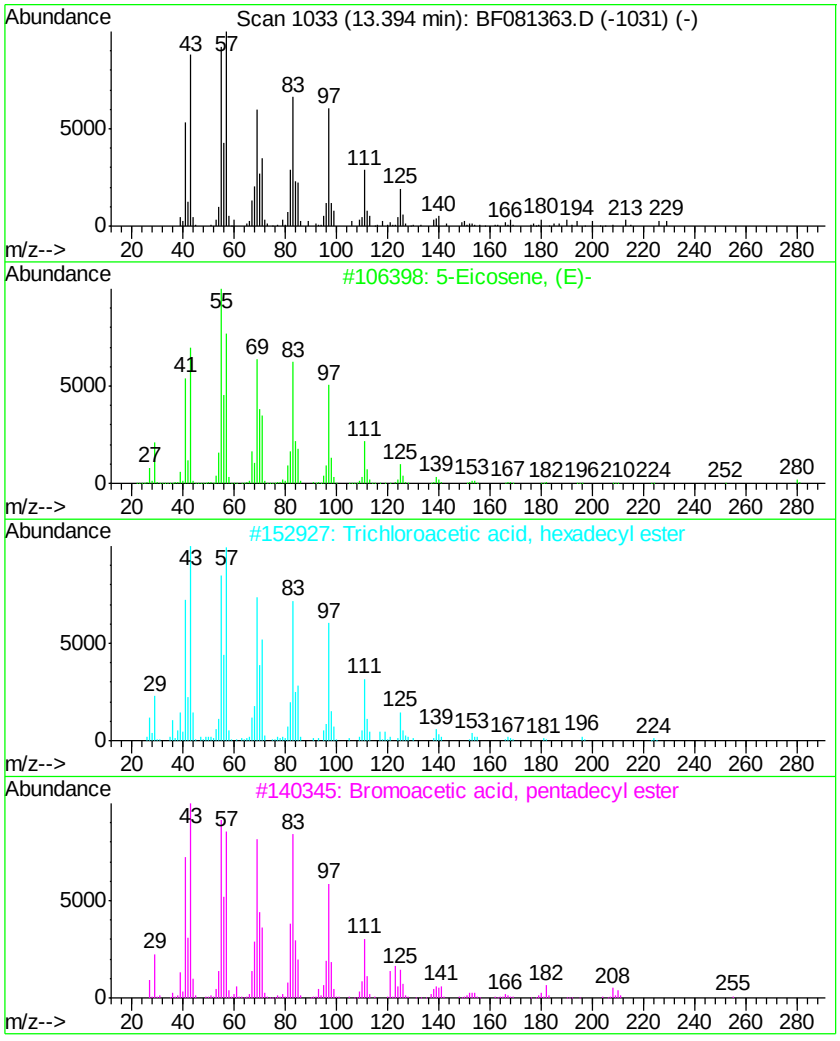
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

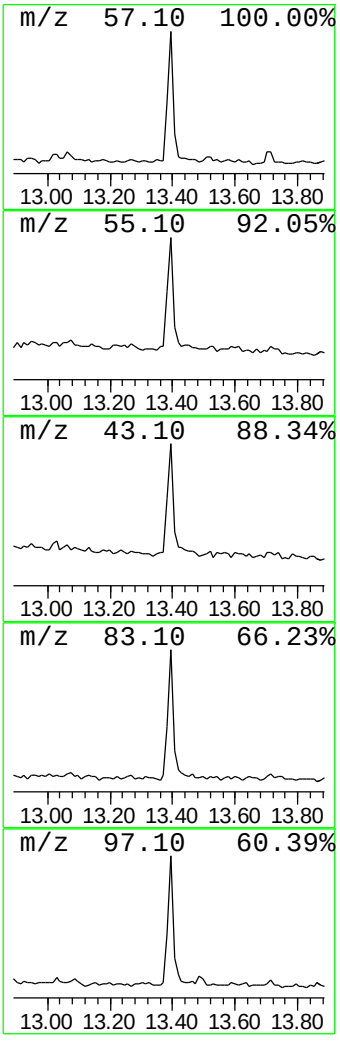
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	5.88 ng	134575	Chrysene-d12	13.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	74
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	72
5	11-Tricosene	322	C23H46	052078-56-5	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

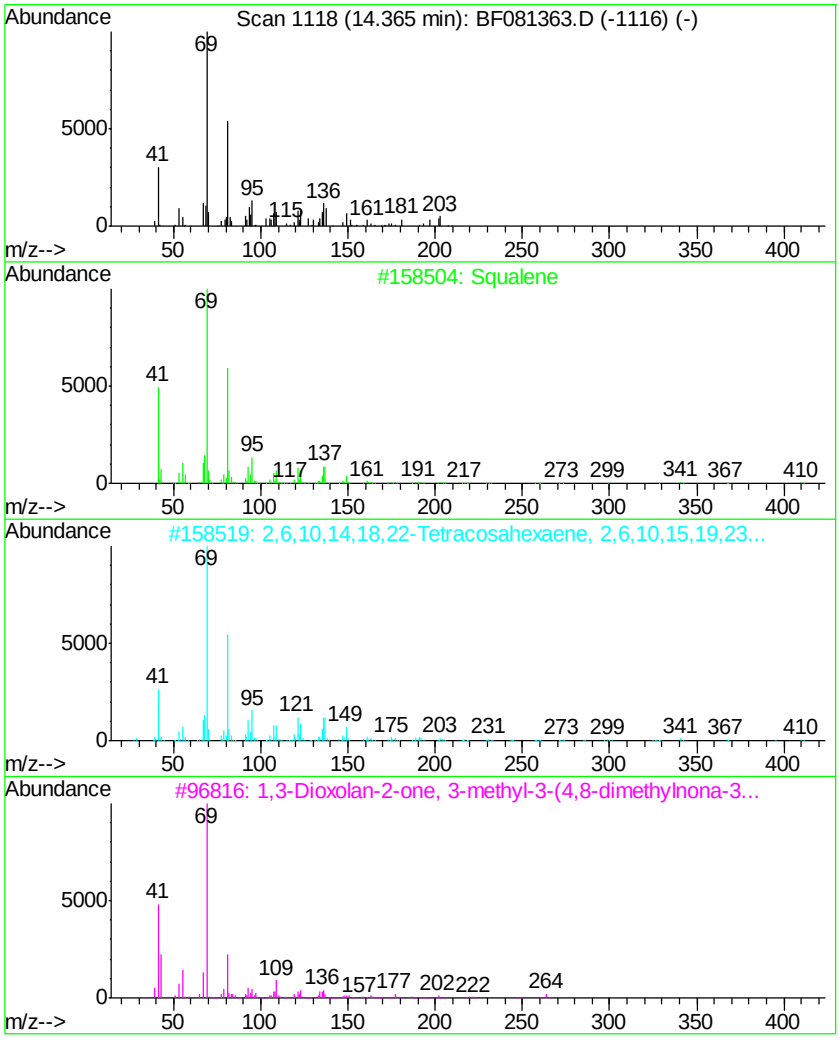
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

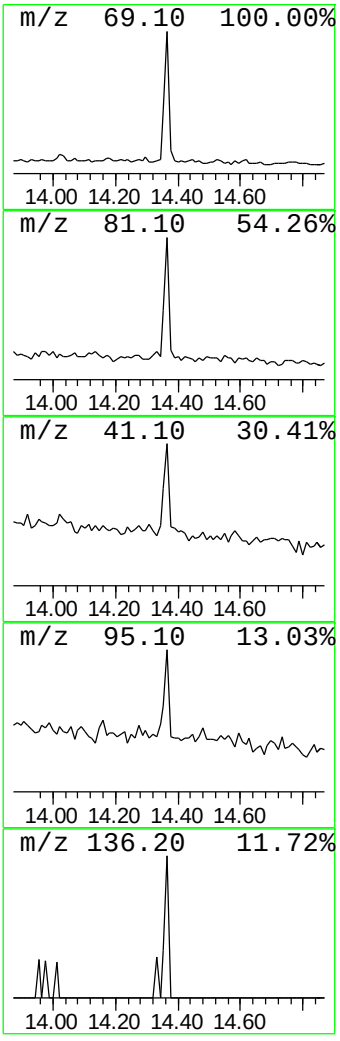
****

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	2.48 ng	40246	Perylene-d12	14.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	83
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	80
3	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	72
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	53





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

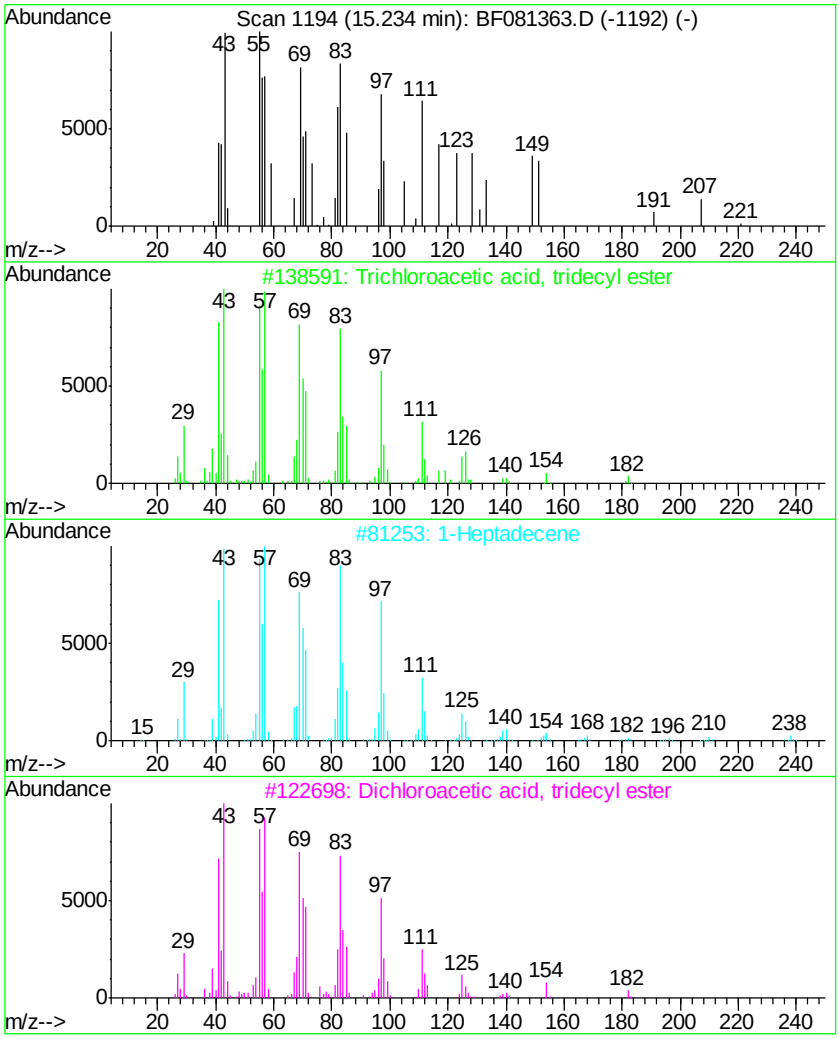
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

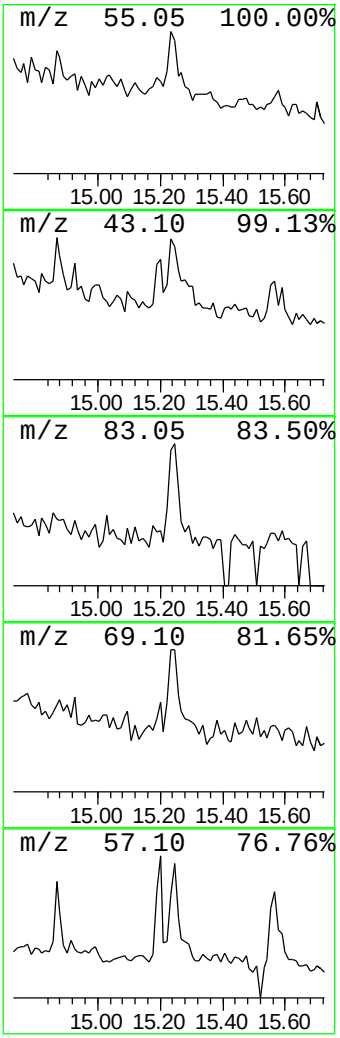
****

Peak Number 9 unknown15.23 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	2.24 ng	36241	Perylene-d12	14.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	47
2	1-Heptadecene	238	C17H34	006765-39-5	47
3	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	47
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	47
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081363.D
Acq On : 2 Sep 2015 22:49
Operator : UM/IZ
Sample : G3474-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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...	4.42	18.6	ng	407705	1	6.39	439443	20.0
1,1'-Biphenyl, 3-...	10.02	2.4	ng	76435	3	9.42	631450	20.0
n-Hexadecanoic acid	11.46	8.7	ng	252968	4	10.88	583892	20.0
Undecanoic acid	12.24	4.1	ng	94825	5	13.49	458026	20.0
5-Eicosene, (E)-	13.39	5.9	ng	134575	5	13.49	458026	20.0
Squalene	14.37	2.5	ng	40246	6	14.80	323978	20.0
unknown15.23	15.23	2.2	ng	36241	6	14.80	323978	20.0