LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

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-BF122116.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	4.081	189	192	196	rBV	50177	86552	1.24%	0.168%
2	4.778	251	253	265	rVB	726839	967969	13.88%	1.883%
3	5.247	292	294	306	rBV	3040966	2932852	42.07%	5.707%
4	6.310	384	387	393	rBV	1851389	2101499	30.14%	4.089%
5	6.424	394	397	399	rBV	5516081	5409559	77.59%	10.526%
6	6.653	414	417	419	rBV	1393894	1380554	19.80%	2.686%
7	6.813	428	431	433	rBV	3818298	5116406	73.39%	9.955%
8	7.224	464	467	469	rBV	4279756	4508559	64.67%	8.772%
9	7.933	527	529	532	rBV	1645533	1812465	26.00%	3.527%
10	9.019	621	624	626	rBV	7159647	6971609	100.00%	13.565%
11	9.419	657	659	661	rBV	152705	154196	2.21%	0.300%
12	9.682	680	682	685	rBV	1830899	2006291	28.78%	3.904%
13	10.128	718	721	723	rBV2	124853	166589	2.39%	0.324%
14	10.356	737	741	744	rBV	44553	78281	1.12%	0.152%
15	10.482	749	752	754	rBV	3186012	4439245	63.68%	8.638%
16	10.608	761	763	767	rBV	156717	230025	3.30%	0.448%
17	11.053	800	802	803	rBV	106950	115600	1.66%	0.225%
18	11.168	809	812	814	rBV	1639297	1899588	27.25%	3.696%
19	11.716	857	860	862	rBV	739240	739600	10.61%	1.439%
20	12.413	917	921	926	rBV4	27551	70967	1.02%	0.138%
21	12.493	926	928	931	rBV2	644261	851009	12.21%	1.656%
22	12.756	948	951	953	rBV	5738249	6225869	89.30%	12.114%
23	13.659	1027	1030	1035	rBV	99637	136789	1.96%	0.266%
24	13.796	1039	1042	1044	rBV	1237295	1512974	21.70%	2.944%
25	14.642	1112	1116	1118	rBV	181815	207925	2.98%	0.405%
26	15.065	1147	1153	1159	rBV3	34686	161059	2.31%	0.313%
27	15.157	1159	1161	1164	rBV	741299	1110517	15.93%	2.161%

Sum of corrected areas: 51394548

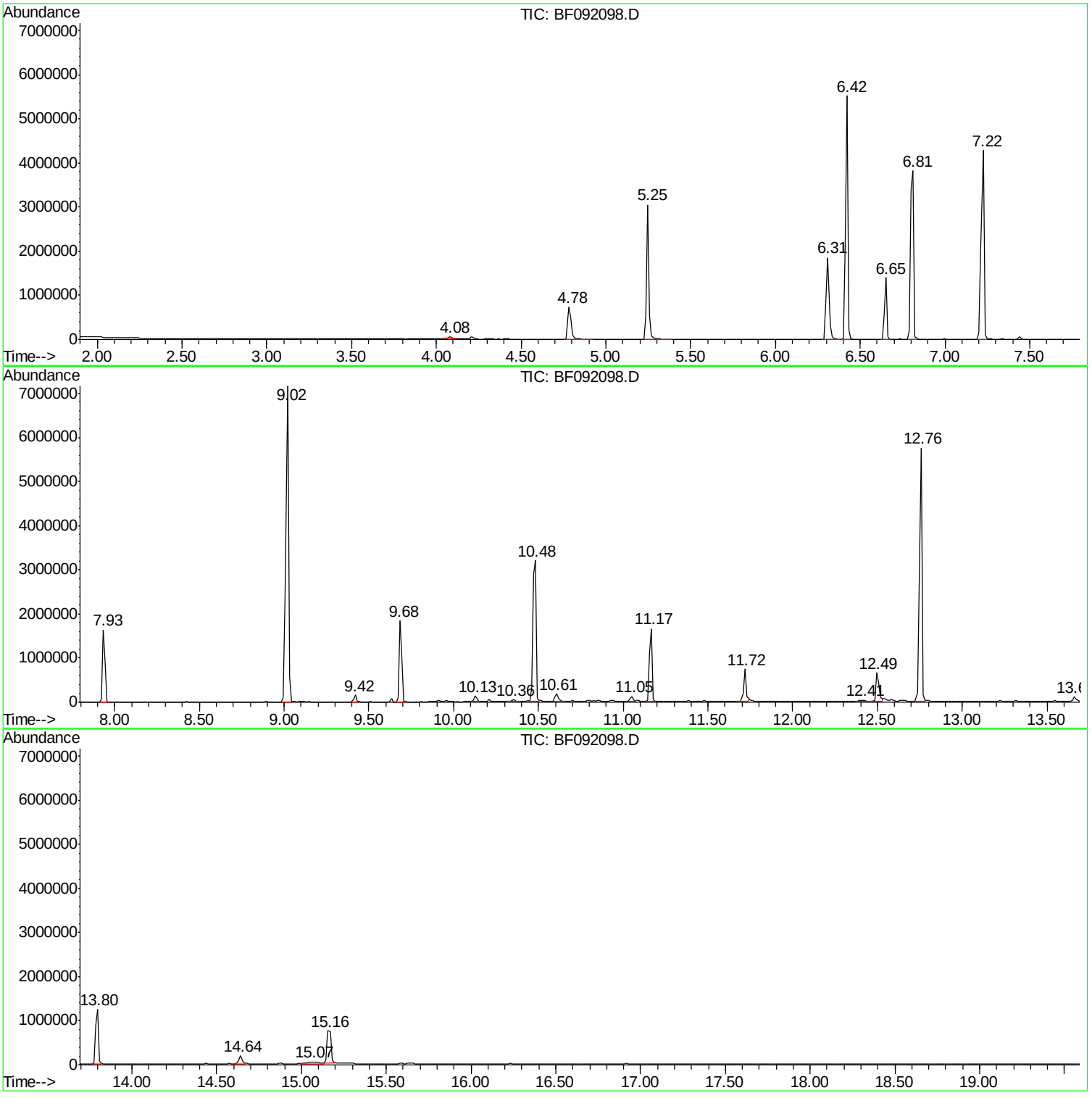
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

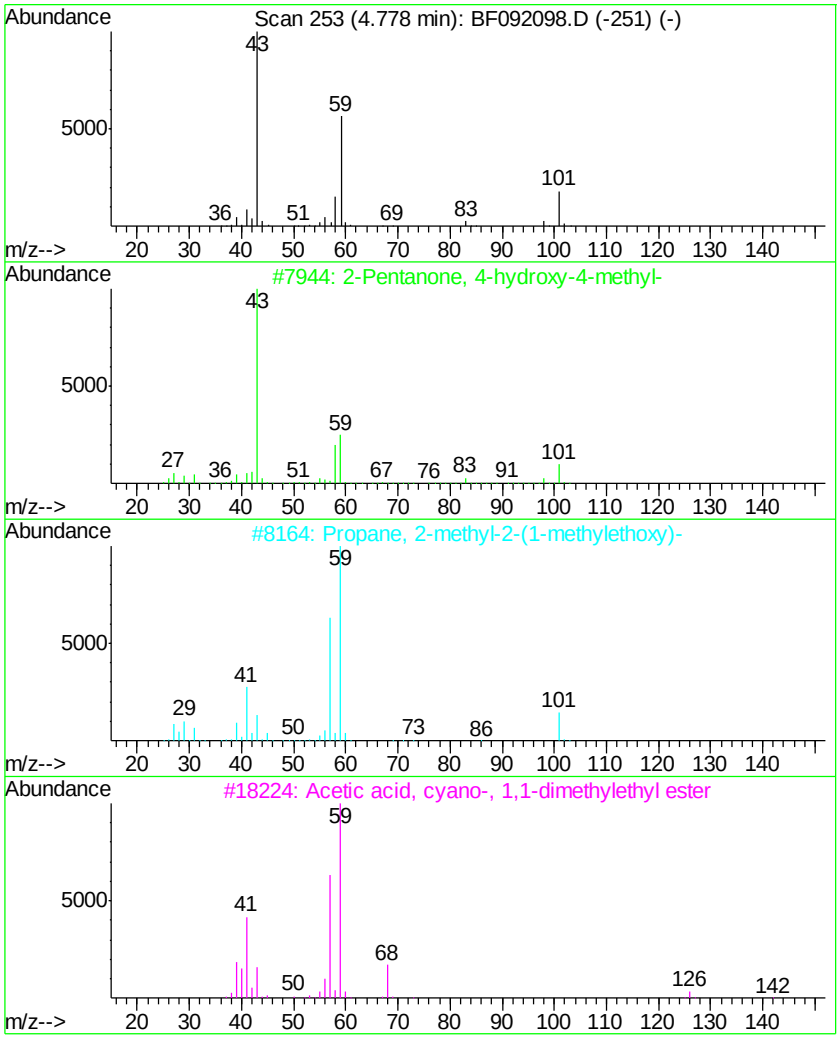
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

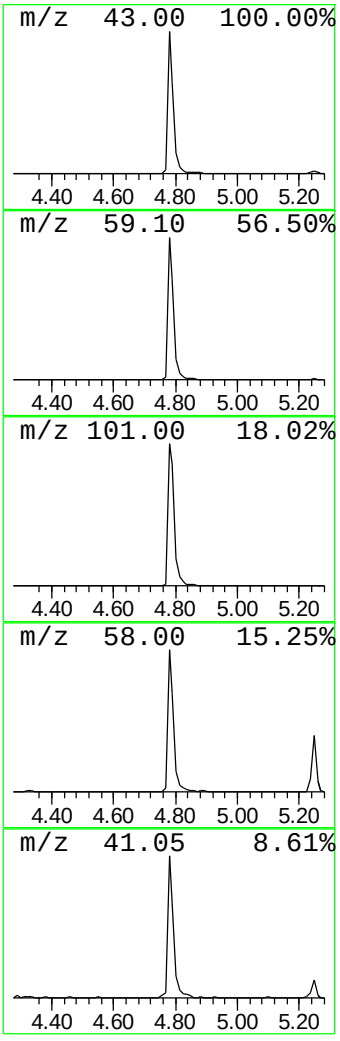
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	14.02 ng	967969	1,4-Dichlorobenzene-d4	6.65

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	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

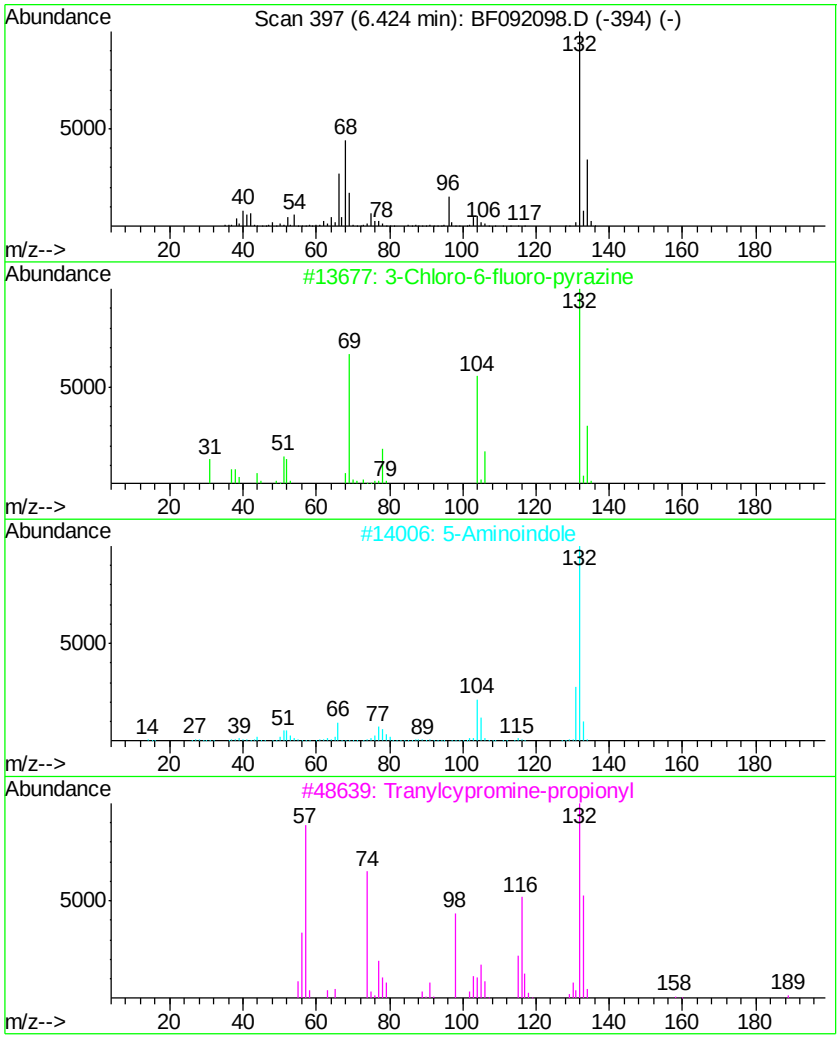
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

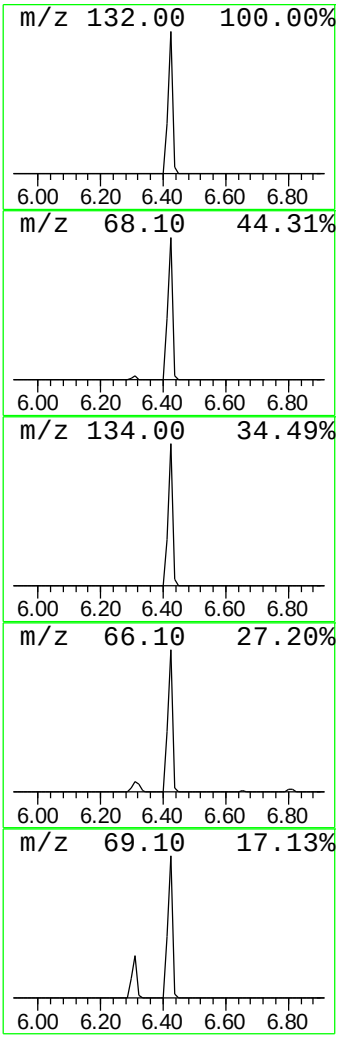
****

Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	78.37 ng	5409560	1,4-Dichlorobenzene-d4	6.65

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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

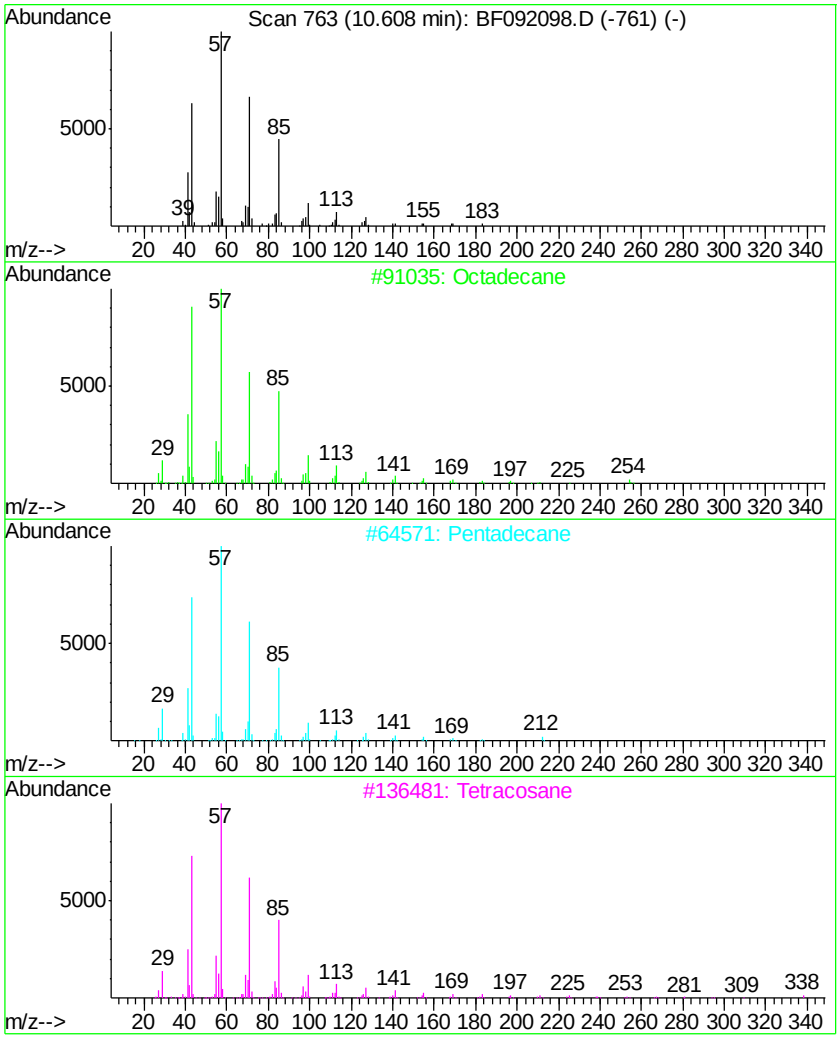
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

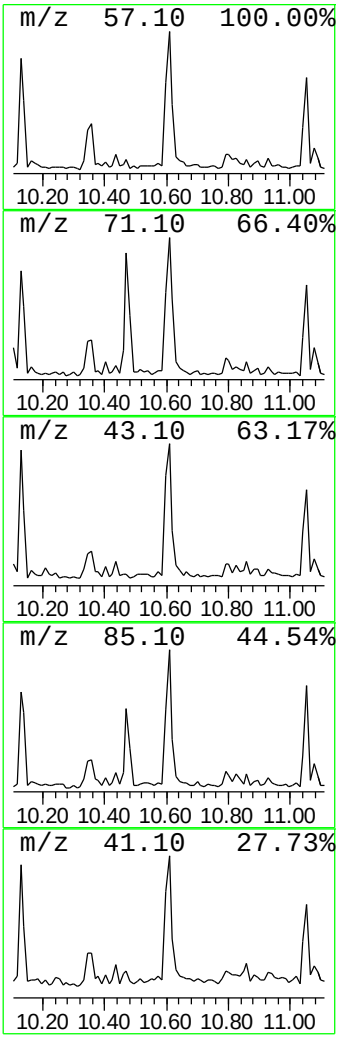
****

Peak Number 4 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	2.42 ng	230025	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Nonadecane	268	C19H40	000629-92-5	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

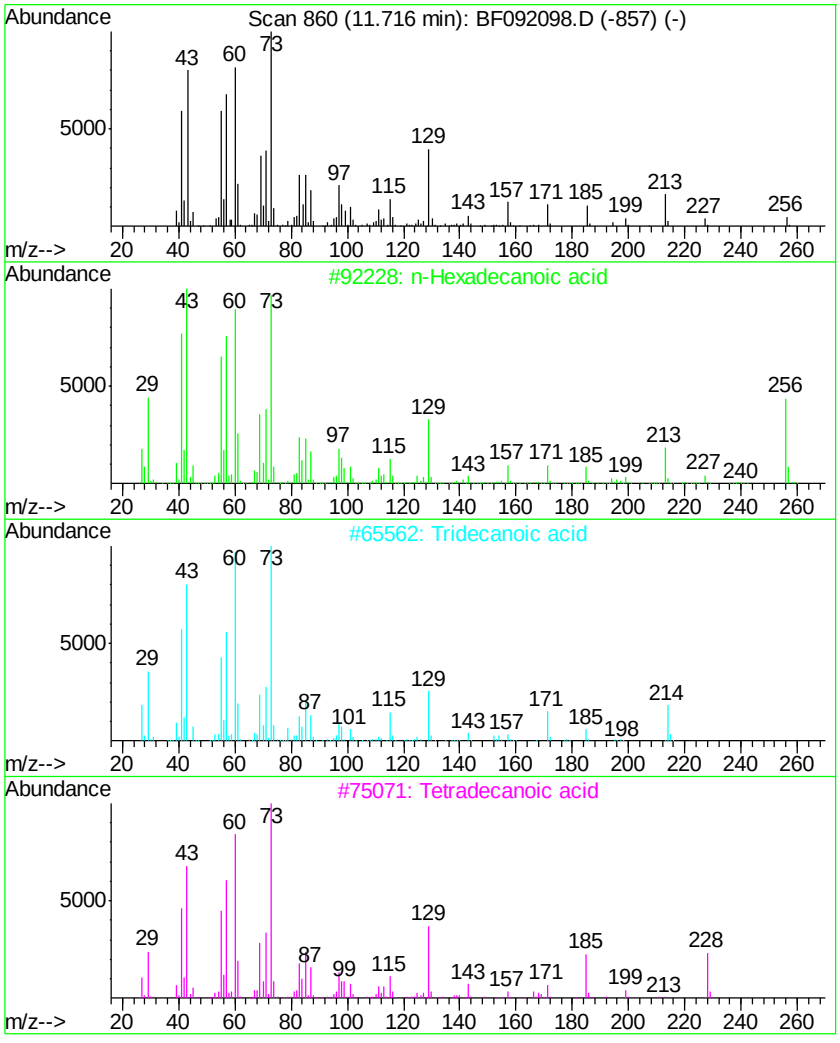
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

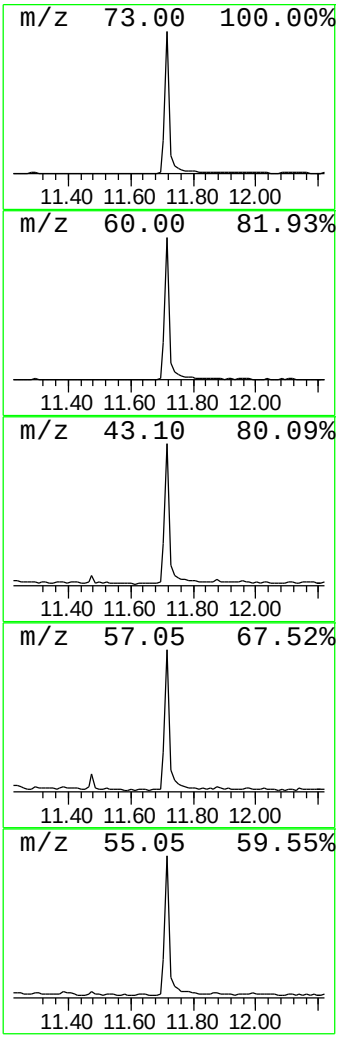
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	7.79 ng	739600	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Hexadecane	226	C16H34	000544-76-3	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

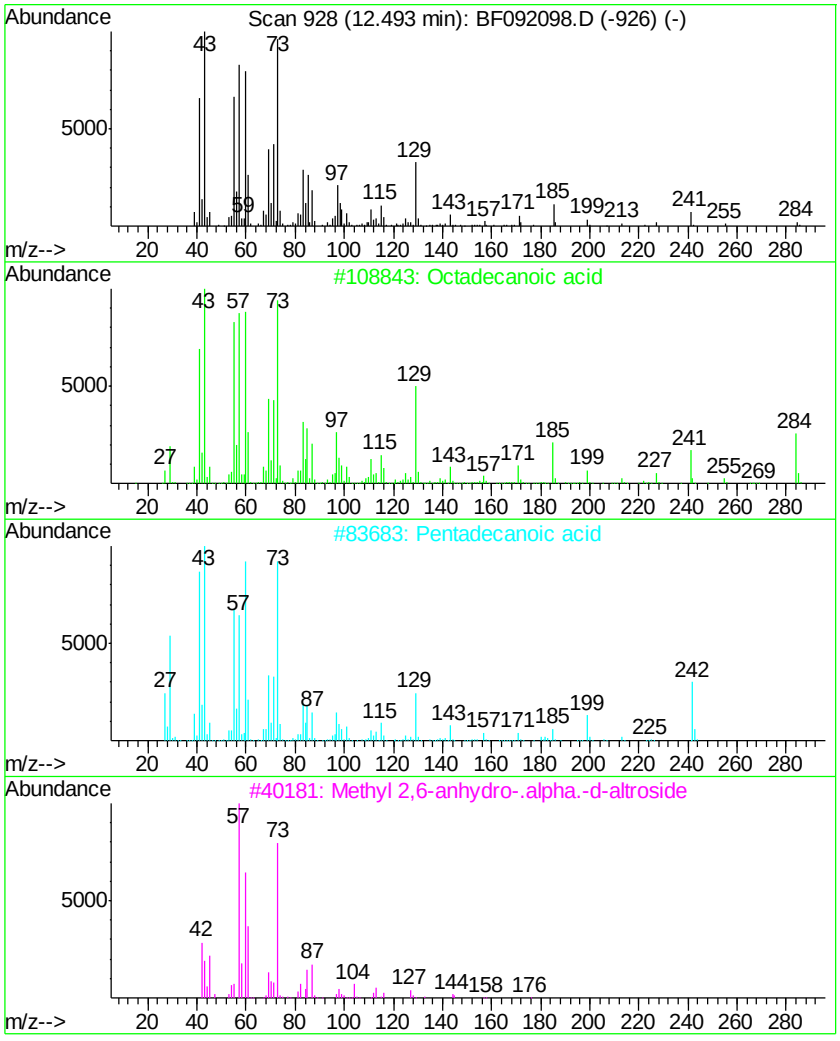
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

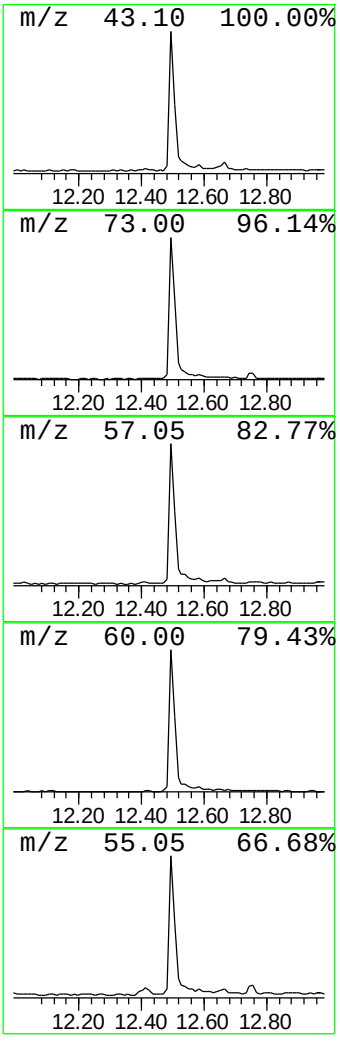
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	11.25 ng	851009	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	27
4	Undecane	156	C11H24	001120-21-4	11
5	Decane	142	C10H22	000124-18-5	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

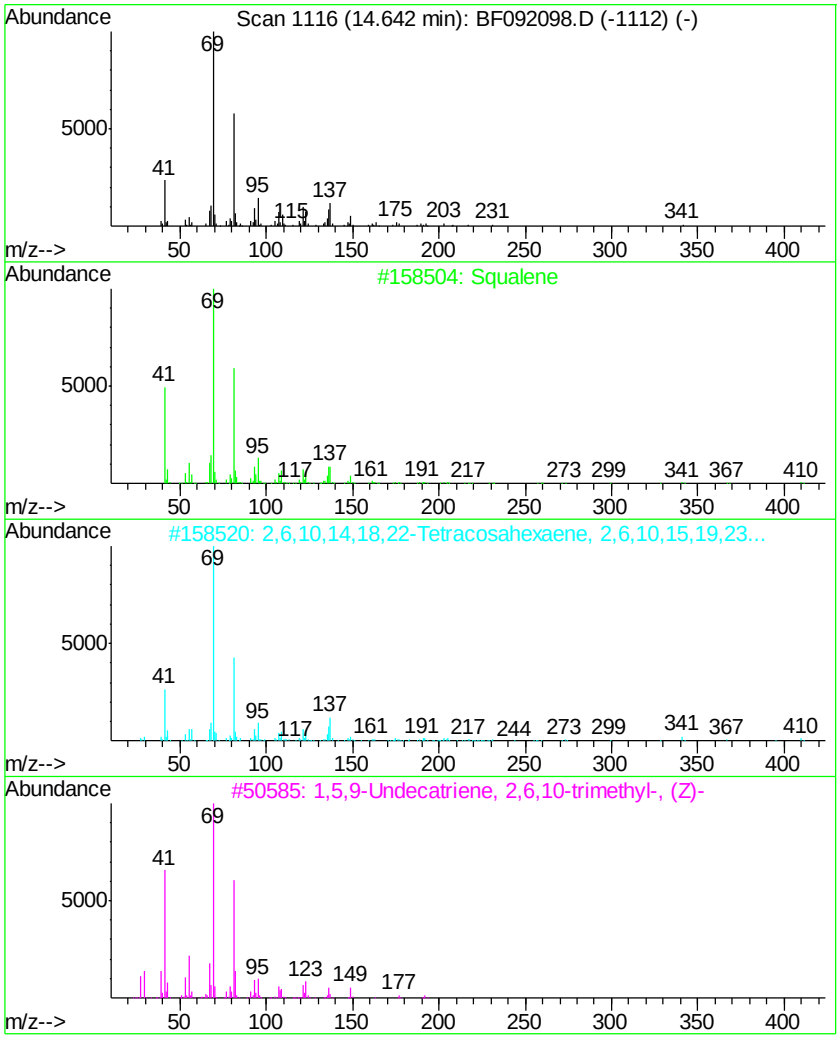
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

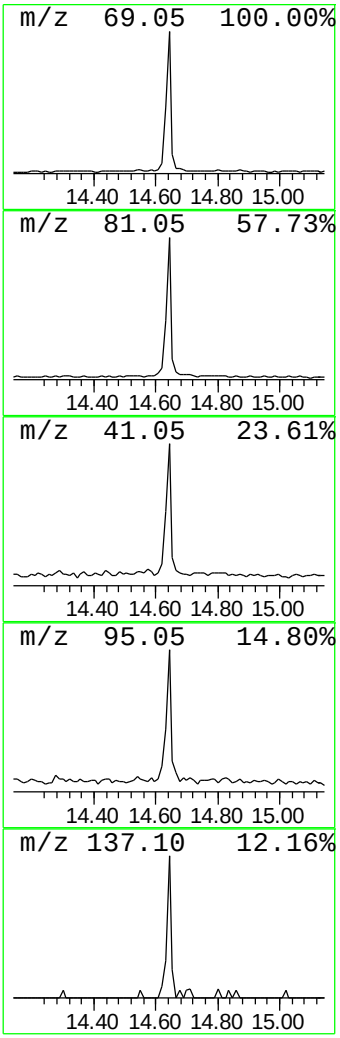
****

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.74 ng	207925	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

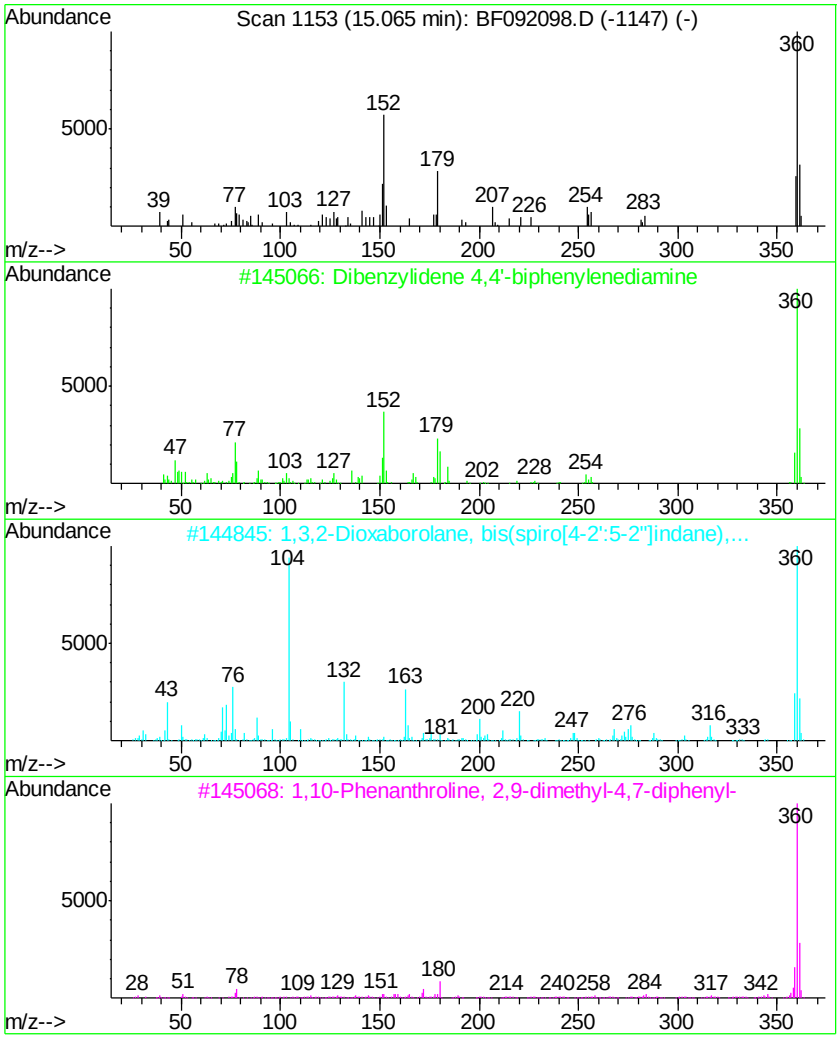
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

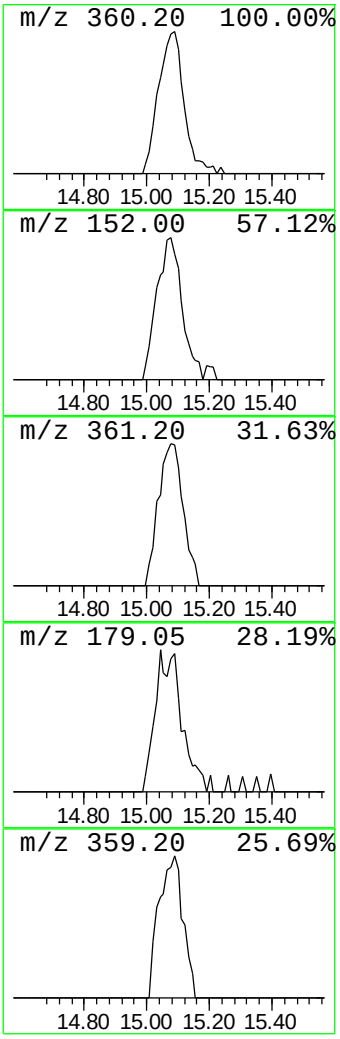
****

Peak Number 8 Dibenzylidene 4,4'-biphenyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.90 ng	161059	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	76
2	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	43
3	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	38
4	Benzoic acid, 4-(3,4-dihydro-2,4...	361	C20H15N3O4	317326-96-8	35
5	[2-(4-Methoxy-phenyl)-2H-benzo[g...	360	C22H20N2O3	1000188-59-8	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010517\
Data File : BF092098.D
Acq On : 5 Jan 2017 19:32
Operator : UM/SJ
Sample : I1004-08
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.78	14.0	ng	967969	1	6.65	1380550	20.0
unknown6.42	6.42	78.4	ng	5409560	1	6.65	1380550	20.0
Octadecane	10.61	2.4	ng	230025	4	11.17	1899590	20.0
n-Hexadecanoic acid	11.72	7.8	ng	739600	4	11.17	1899590	20.0
Octadecanoic acid	12.49	11.3	ng	851009	5	13.80	1512970	20.0
Squalene	14.64	3.7	ng	207925	6	15.17	1110520	20.0
Dibenzylidene 4,4...	15.07	2.9	ng	161059	6	15.17	1110520	20.0