LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027346.D
Acq On : 9 Jun 2017 10:50
Operator : SJ/MA
Sample : I3460-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-118

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_G\METHODS\8270-BG060517.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	5.703	337	343	353	rVB2	41977	70135	1.59%	0.357%
2	6.143	411	418	426	rBV	402632	715720	16.27%	3.647%
3	7.689	670	681	692	rBV	282010	530484	12.06%	2.703%
4	8.088	741	749	759	rBV	727933	1318125	29.96%	6.716%
5	8.552	821	828	837	rBV	154704	288590	6.56%	1.470%
6	8.881	876	884	893	rBV	511494	952452	21.65%	4.853%
7	9.716	1016	1026	1040	rBV	516311	1016395	23.10%	5.179%
8	11.373	1300	1308	1317	rBV	246437	472462	10.74%	2.407%
9	11.866	1387	1392	1397	rBV	38311	60272	1.37%	0.307%
10	11.925	1397	1402	1412	rVB	42415	74616	1.70%	0.380%
11	13.764	1707	1715	1722	rBV	1585148	2585815	58.77%	13.175%
12	14.569	1846	1852	1857	rBV	45869	74391	1.69%	0.379%
13	15.139	1942	1949	1955	rBV2	416790	724717	16.47%	3.693%
14	16.308	2143	2148	2155	rBV	41904	84766	1.93%	0.432%
15	16.619	2194	2201	2212	rVB	1560413	2486559	56.52%	12.670%
16	16.849	2235	2240	2247	rVB3	49704	105337	2.39%	0.537%
17	17.236	2303	2306	2317	rVB9	23201	44748	1.02%	0.228%
18	17.889	2410	2417	2425	rVB	563202	937425	21.31%	4.776%
19	18.729	2555	2560	2568	rBV	131996	195166	4.44%	0.994%
20	19.986	2769	2774	2783	rBV	110287	172088	3.91%	0.877%
21	20.127	2795	2798	2804	rVB3	34329	48034	1.09%	0.245%
22	20.462	2849	2855	2865	rBV	3015296	4399526	100.00%	22.416%
23	21.831	3083	3088	3096	rBV2	33459	68463	1.56%	0.349%
24	22.272	3156	3163	3172	rVB	590346	1131833	25.73%	5.767%
25	25.956	3779	3790	3804	rVB3	326380	1068199	24.28%	5.443%

Sum of corrected areas: 19626318

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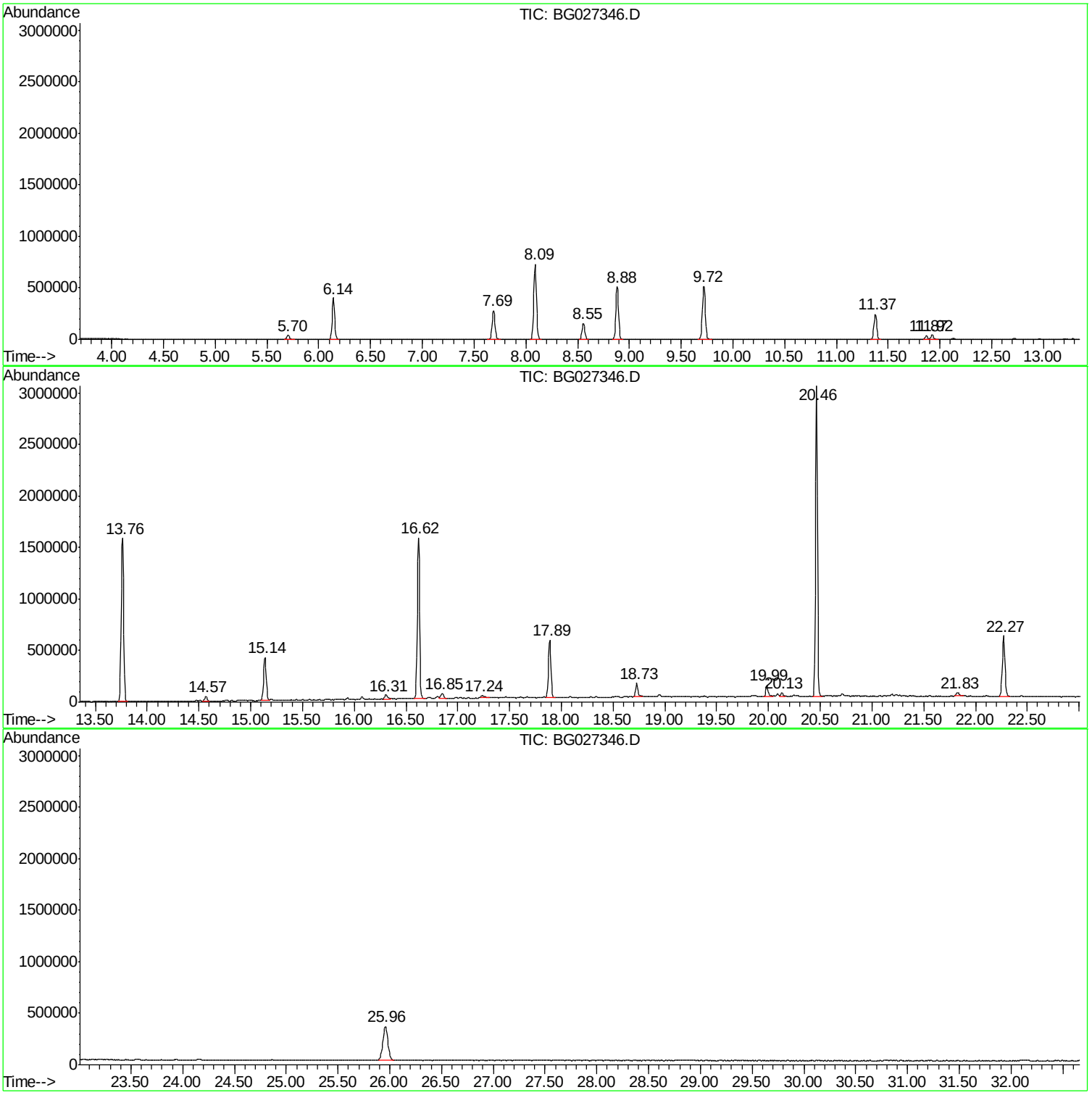
Instrument : BNA_G
ClientSampleId : MW-118

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Operator : SJ/MA
Sample : I3460-09
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ClientSampleId : MW-118

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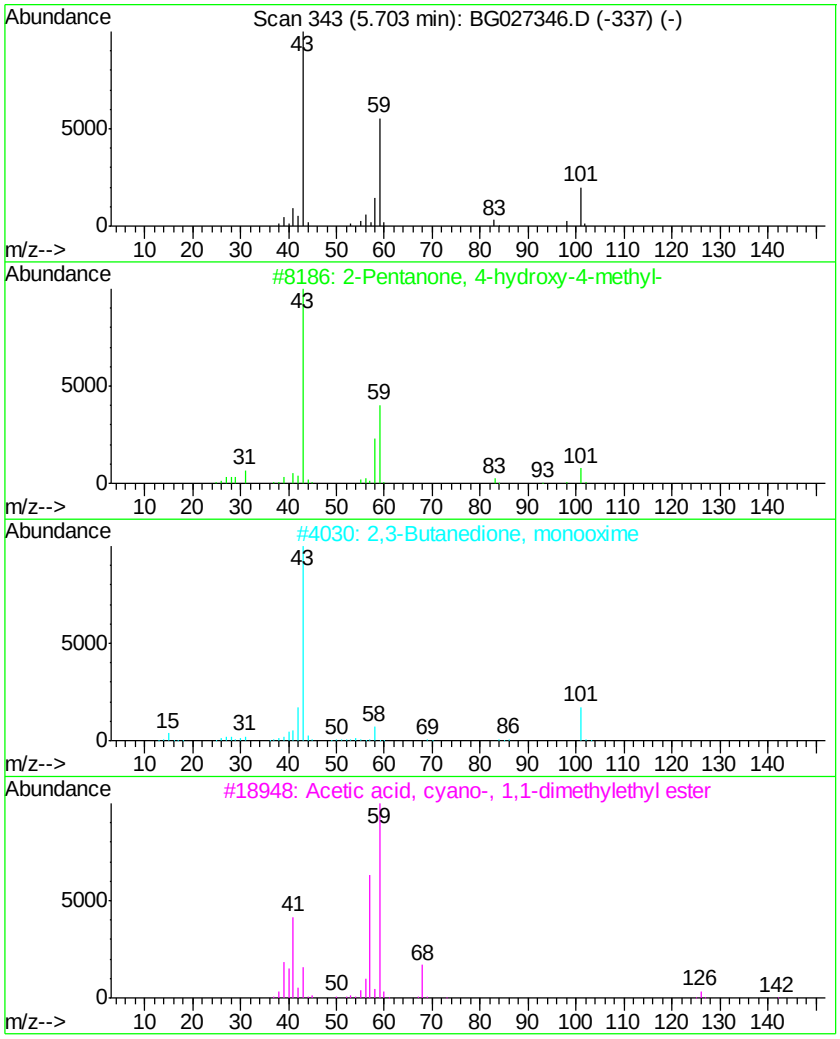
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

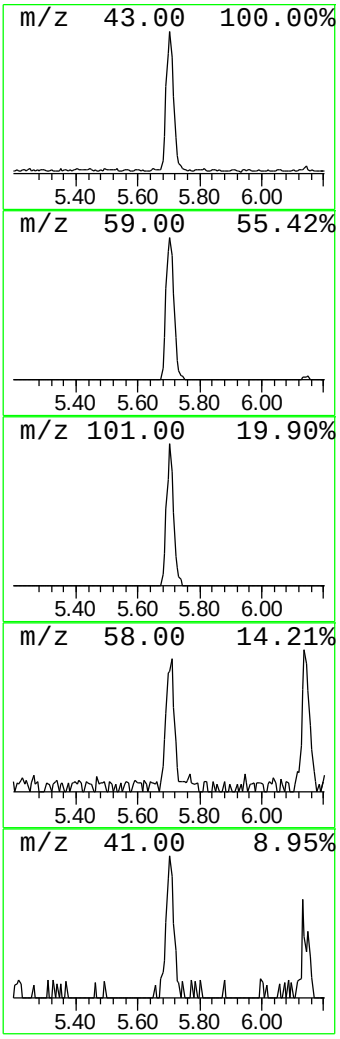
****

Peak Number 1 unknown5.70 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	4.86 ng	70135	1,4-Dichlorobenzene-d4	8.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
Data File : BG027346.D
Acq On : 9 Jun 2017 10:50
Operator : SJ/MA
Sample : I3460-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-118

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

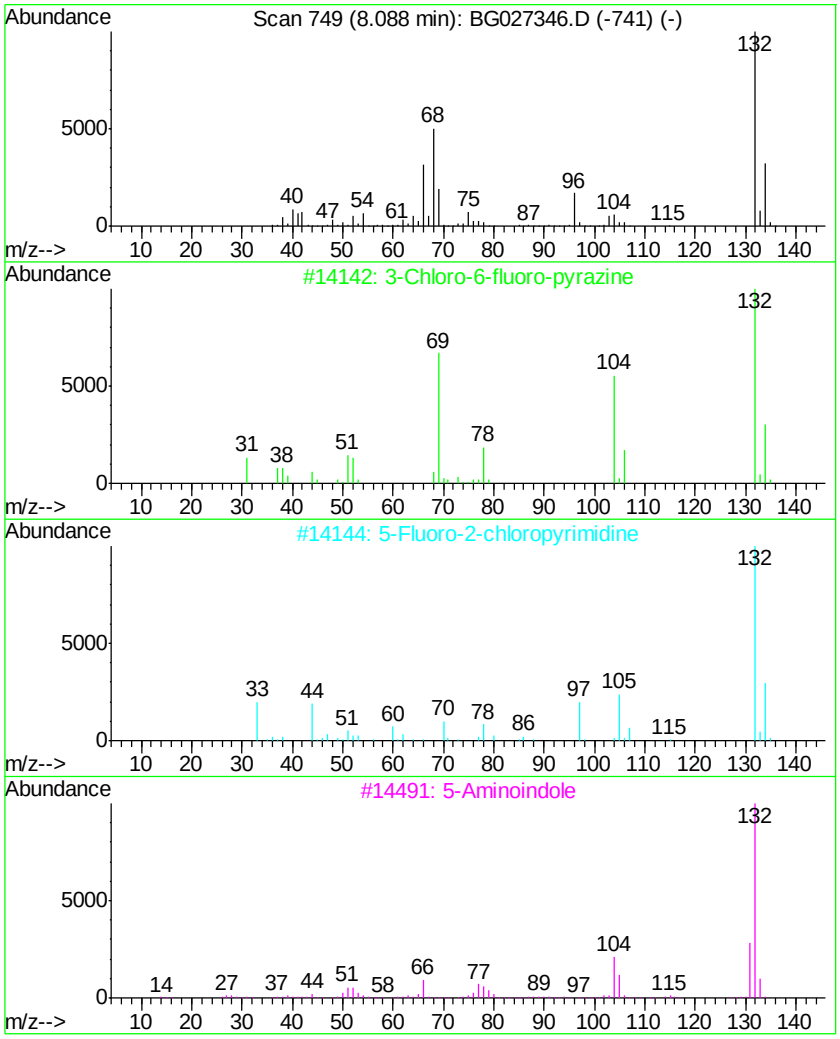
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

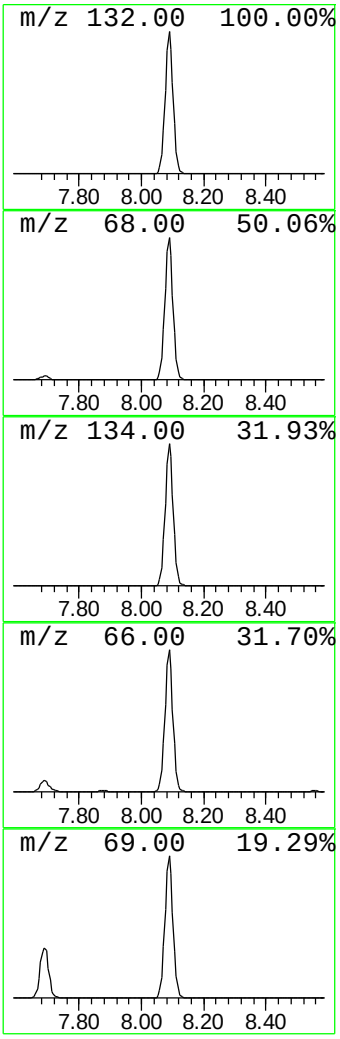
****

Peak Number 2 unknown8.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	91.35 ng	1318130	1,4-Dichlorobenzene-d4	8.56

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





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Data File : BG027346.D
Acq On : 9 Jun 2017 10:50
Operator : SJ/MA
Sample : I3460-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-118

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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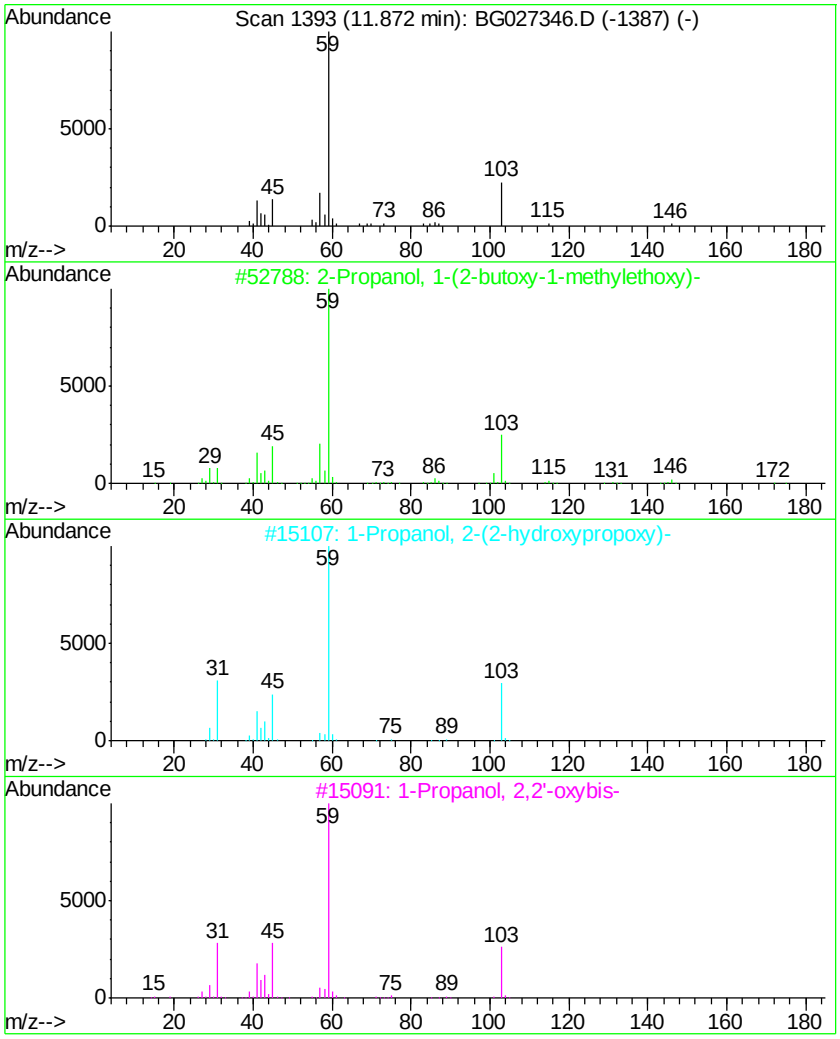
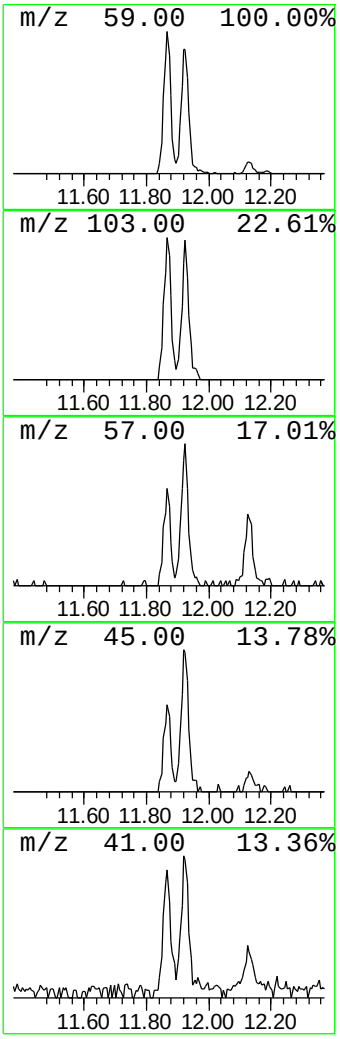
Peak Number 4 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.55 ng	60272	Naphthalene-d8	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	78
4	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	56
5	2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	56





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Data File : BG027346.D
Acq On : 9 Jun 2017 10:50
Operator : SJ/MA
Sample : I3460-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-118

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

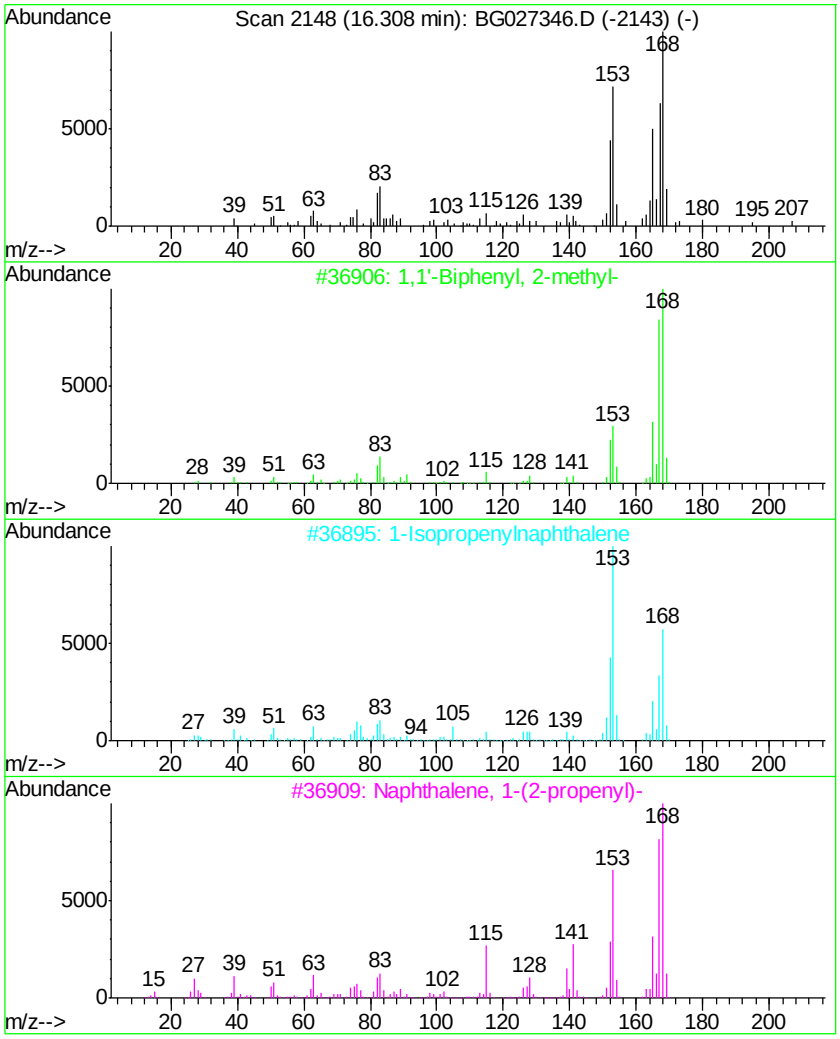
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

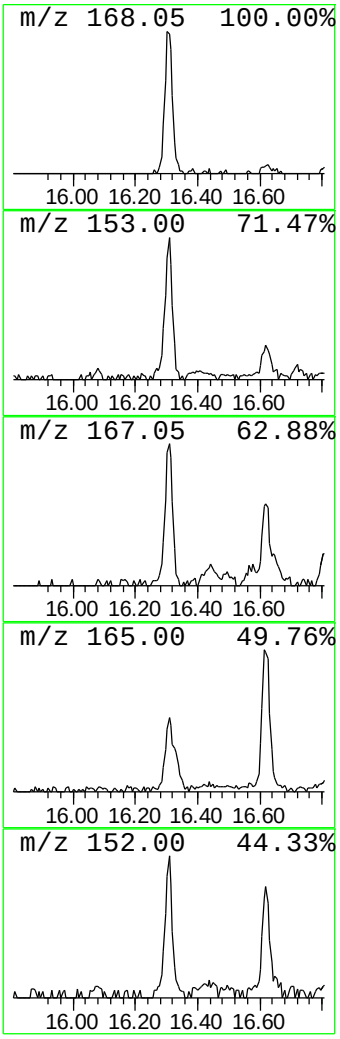
****

Peak Number 6 1,1'-Biphenyl, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	2.34 ng	84766	Acenaphthene-d10	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	72
2	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	62
3	Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	58
4	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	58
5	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	49





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Sample : I3460-09
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-118

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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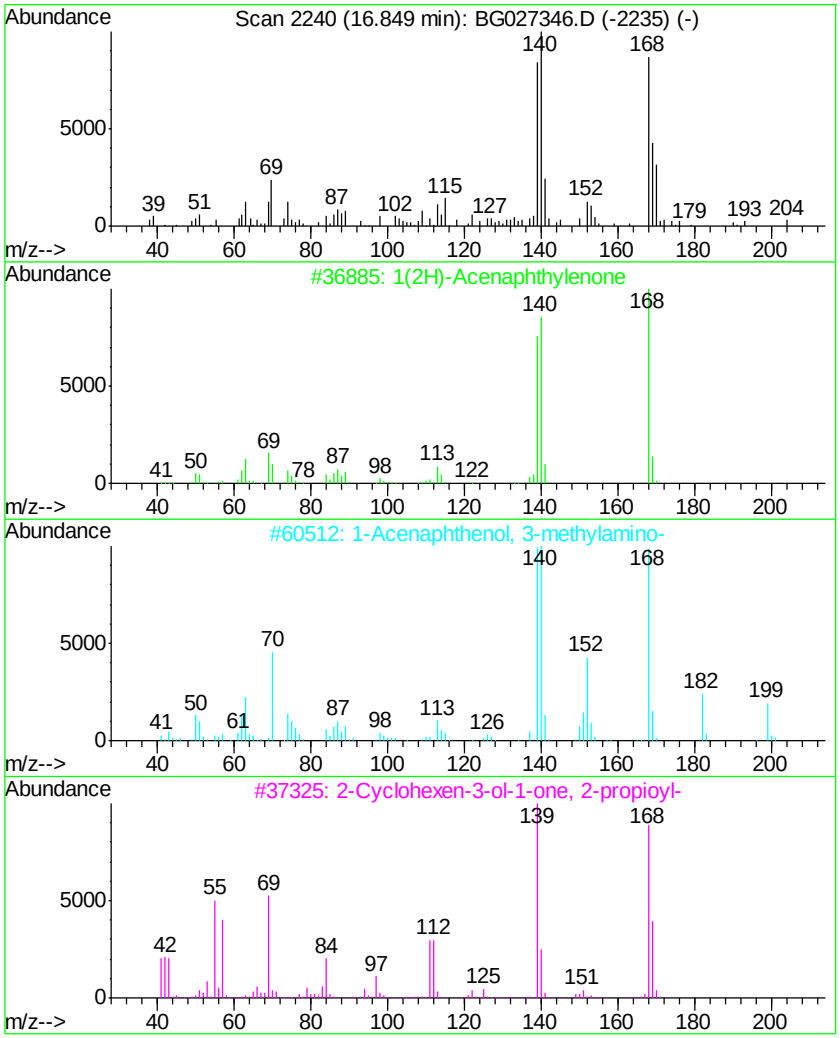
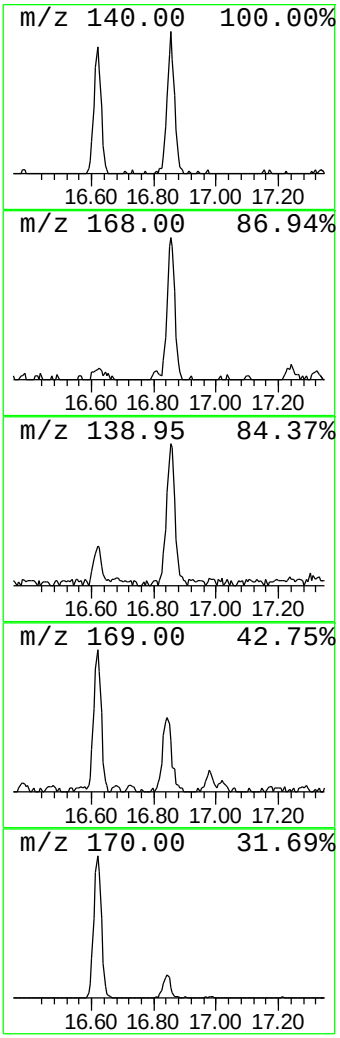
Peak Number 7 1(2H)-Acenaphthylenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.85	2.25 ng	105337	Phenanthrene-d10	17.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	94
2	1-Acenaphthenol, 3-methylamino-	199	C13H13NO	1000129-22-6	64
3	2-Cyclohexen-3-ol-1-one, 2-propi...	168	C9H12O3	062847-90-9	50
4	Dibenzofuran	168	C12H8O	000132-64-9	45
5	Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	43





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Operator : SJ/MA
Sample : I3460-09
Misc :
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Instrument : BNA_G
ClientSampleId : MW-118

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

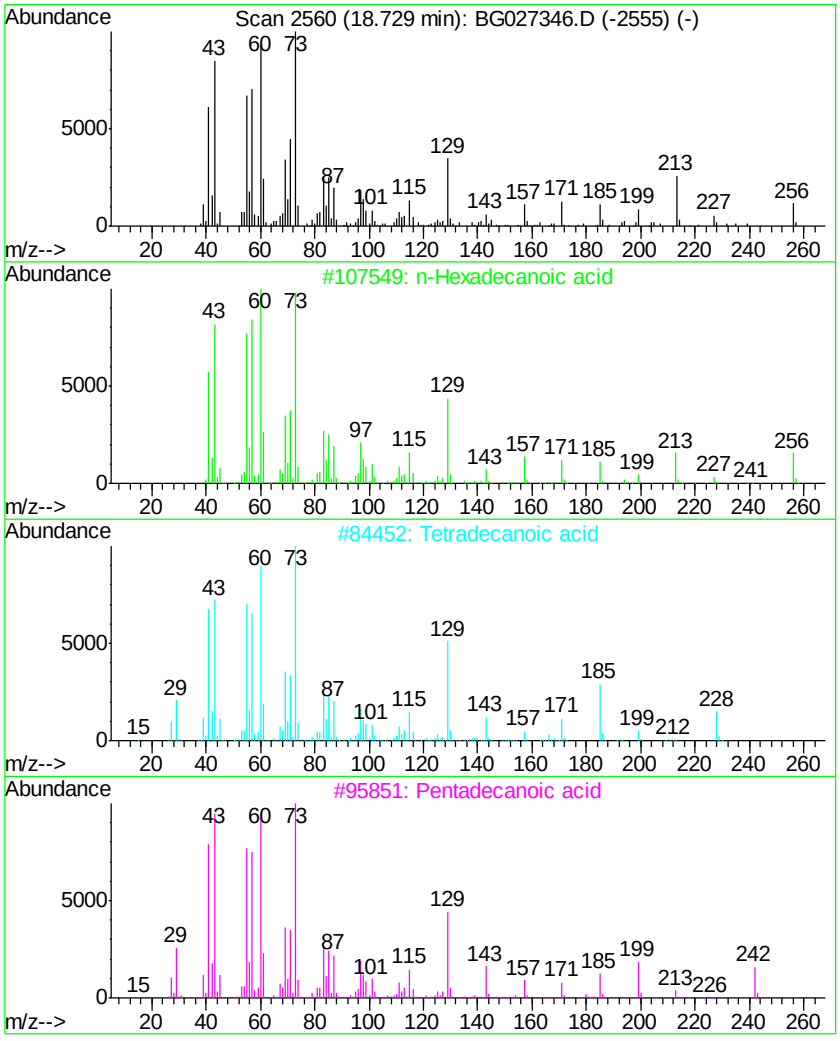
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

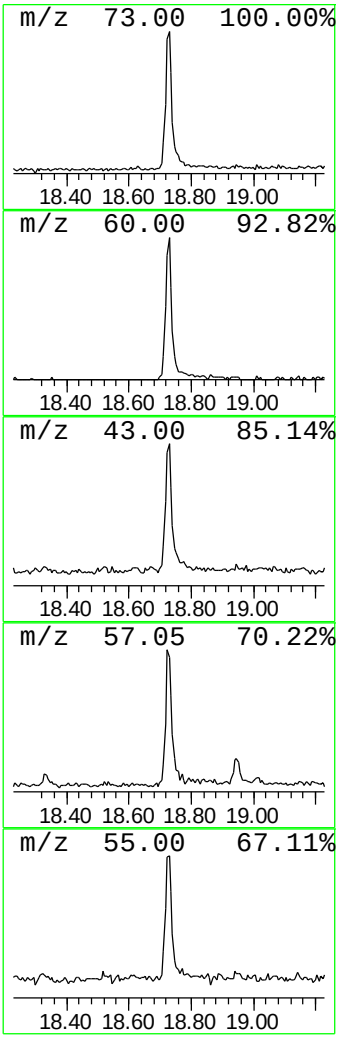
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	4.16 ng	195166	Phenanthrene-d10	17.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Instrument : BNA_G
ClientSampleId : MW-118

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

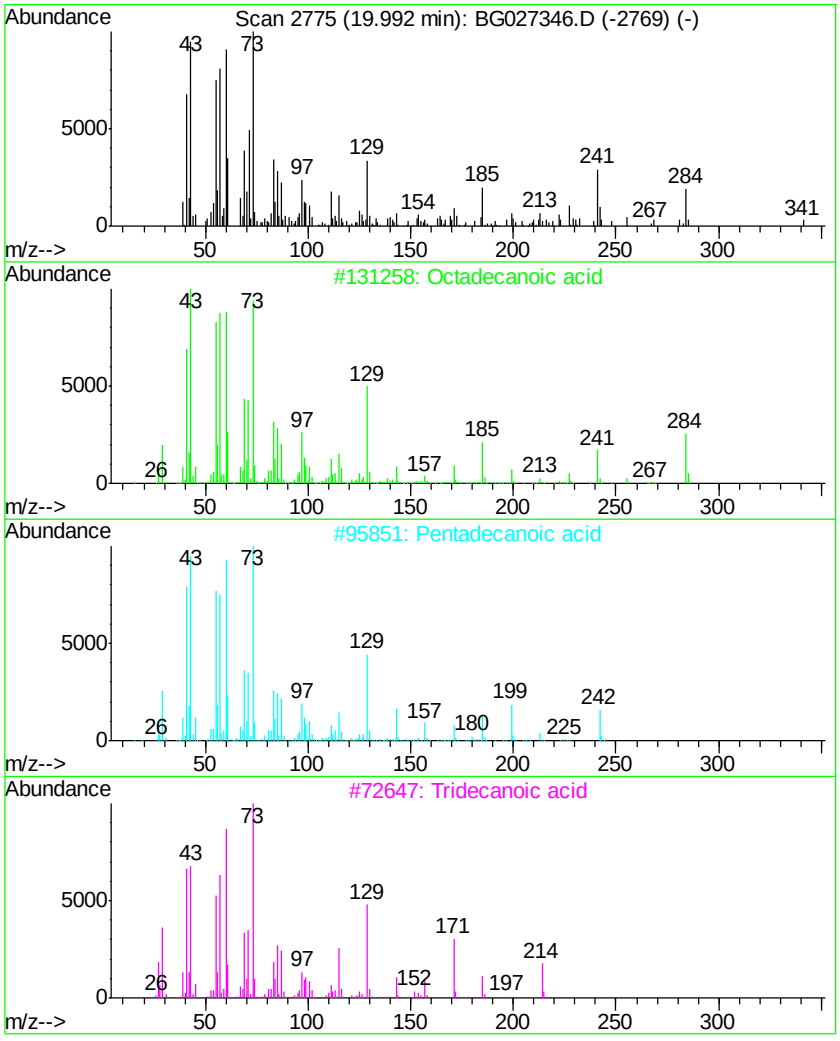
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

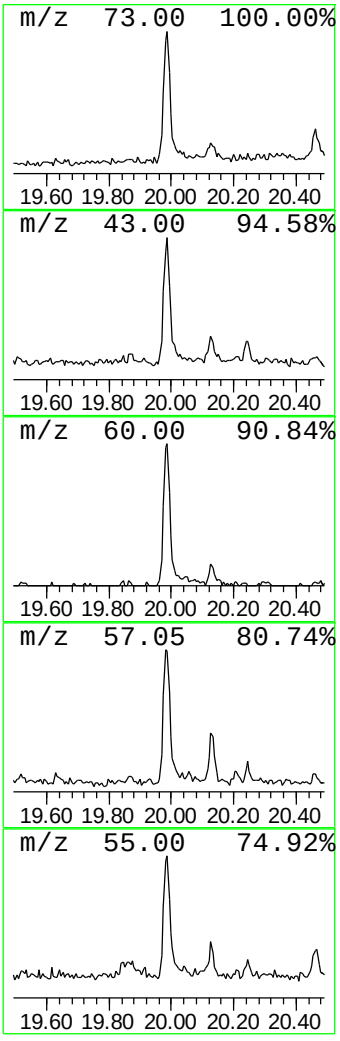
****

Peak Number 9 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.99	3.67 ng	172088	Phenanthrene-d10	17.89

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	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecane	184	C13H28	000629-50-5	56





Tentatively Identified Compound (LSC) summary

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MW-118

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.70	5.70	4.9	ng	70135	1	8.56	288590	20.0
unknown8.09	8.09	91.3	ng	1318130	1	8.56	288590	20.0
2-Propanol, 1-(2-...	11.87	2.5	ng	60272	2	11.37	472462	20.0
1,1'-Biphenyl, 2-...	16.31	2.3	ng	84766	3	15.13	724717	20.0
1(2H)-Acenaphthyl...	16.85	2.3	ng	105337	4	17.89	937425	20.0
n-Hexadecanoic acid	18.73	4.2	ng	195166	4	17.89	937425	20.0
Octadecanoic acid	19.99	3.7	ng	172088	4	17.89	937425	20.0