LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

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-BG072616.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	3.472	102	108	115	rBV	391581	618549	4.93%	0.984%
2	5.193	394	401	412	rBV	1175136	1769912	14.11%	2.817%
3	5.675	474	483	494	rBV	1281738	2128075	16.97%	3.387%
4	7.284	748	757	769	rBV	1130560	2038332	16.25%	3.244%
5	7.660	810	821	831	rBV	1945536	3499303	27.90%	5.569%
6	8.136	894	902	908	rBV	577563	1003854	8.00%	1.598%
7	8.459	948	957	968	rBV	2162982	3803272	30.33%	6.053%
8	9.311	1094	1102	1112	rBV	1965683	3533312	28.17%	5.623%
9	10.974	1377	1385	1393	rBV	882521	1585930	12.65%	2.524%
10	11.755	1513	1518	1528	rBV	66101	133041	1.06%	0.212%
11	13.423	1794	1802	1816	rVB	5371335	8752519	69.79%	13.929%
12	14.246	1936	1942	1949	rBV	529925	772040	6.16%	1.229%
13	14.810	2031	2038	2047	rBV2	1501122	2505309	19.98%	3.987%
14	16.302	2286	2292	2307	rBV	3297388	5315117	42.38%	8.459%
15	16.501	2321	2326	2335	rBV2	113711	222178	1.77%	0.354%
16	17.570	2501	2508	2518	rBV2	2005396	3197199	25.49%	5.088%
17	18.440	2651	2656	2667	rBV	278579	534049	4.26%	0.850%
18	19.709	2868	2872	2879	rBV3	216165	367231	2.93%	0.584%
19	19.856	2893	2897	2902	rVB	621504	707388	5.64%	1.126%
20	20.179	2946	2952	2959	rBV	9288691	12541154	100.00%	19.959%
21	20.901	3070	3075	3079	rBV	435296	519265	4.14%	0.826%
22	21.888	3237	3243	3253	rVB2	2088682	3539752	28.23%	5.633%
23	23.639	3536	3541	3549	rVB2	124381	252659	2.01%	0.402%
24	25.295	3813	3823	3837	rVB2	1189140	3495217	27.87%	5.563%

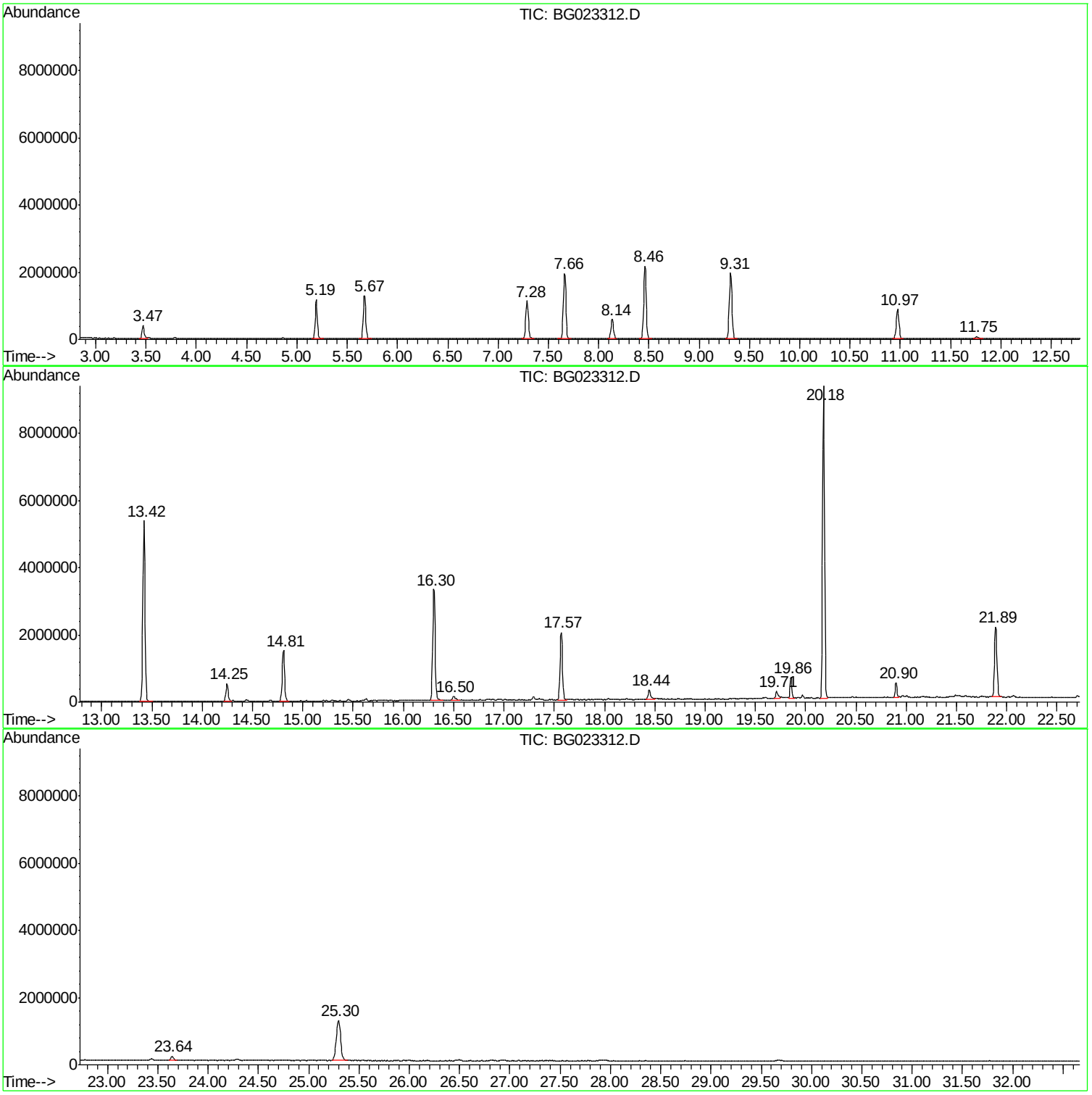
Sum of corrected areas: 62834657

Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

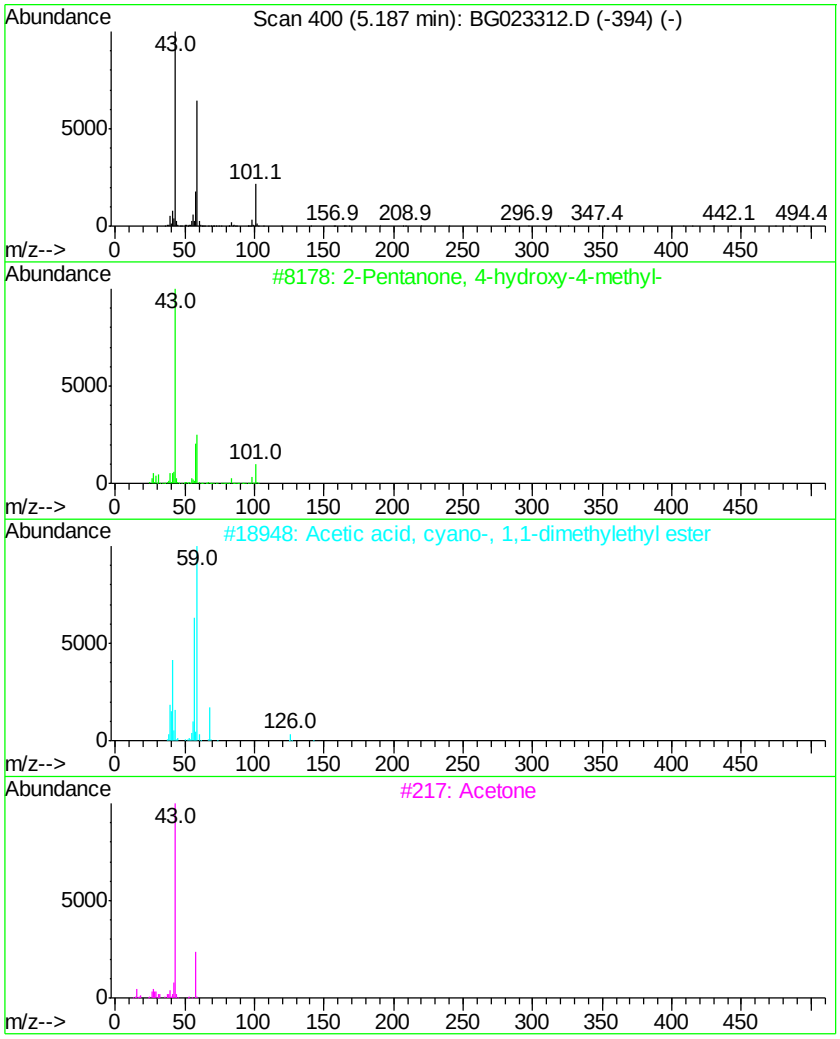
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

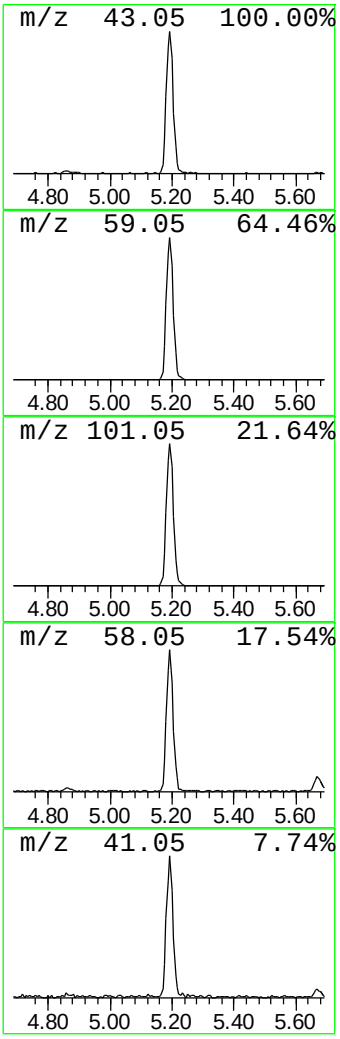
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	35.26 ng	1769910	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

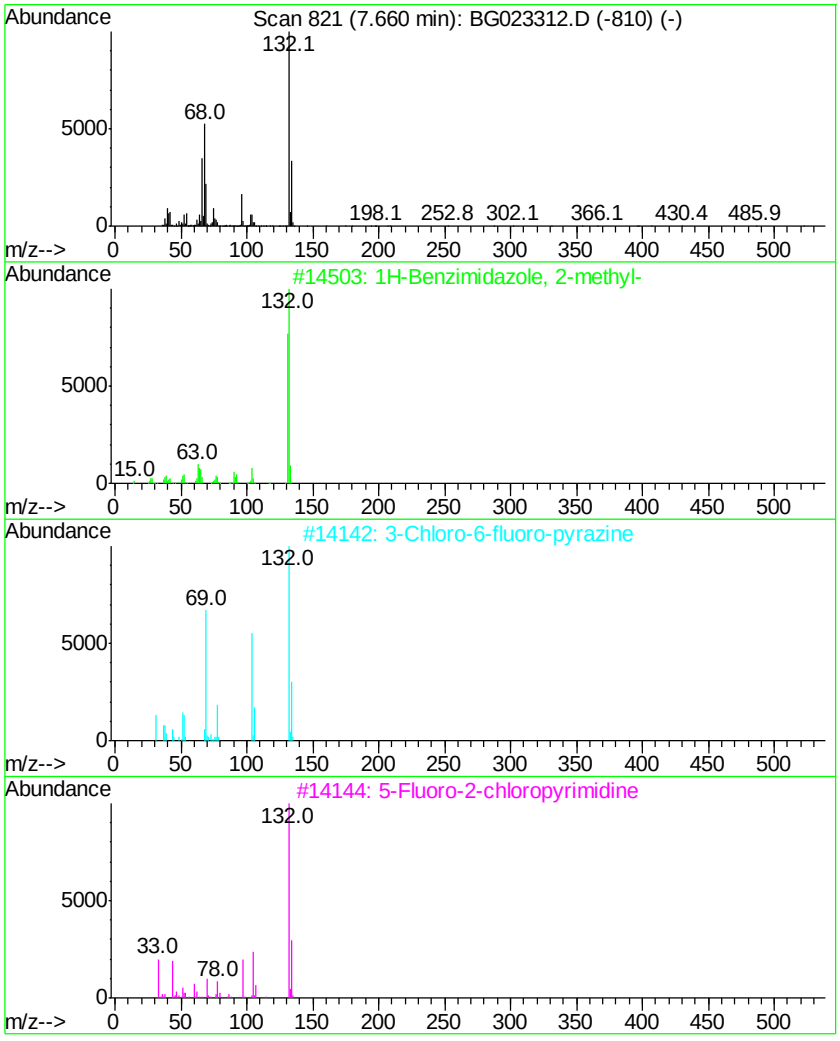
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

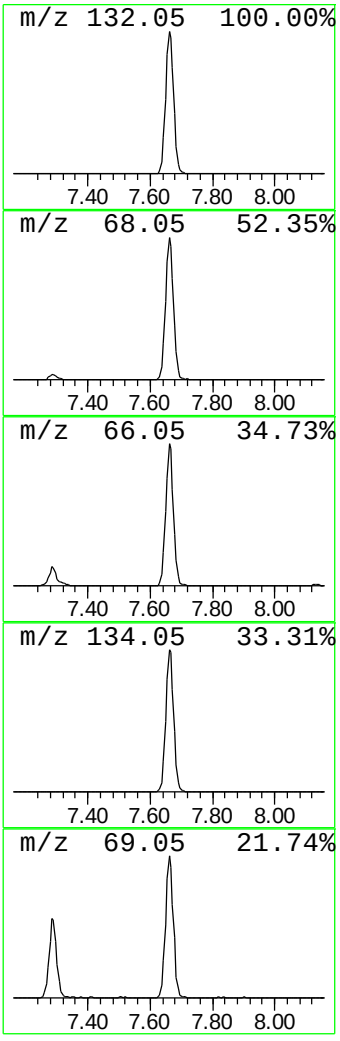
****

Peak Number 3 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	69.72 ng	3499300	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

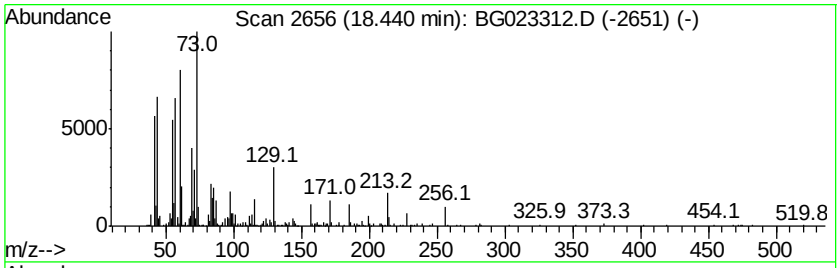
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

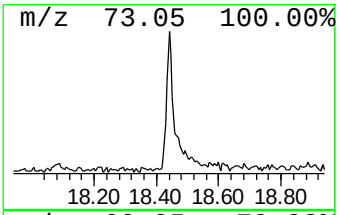
****

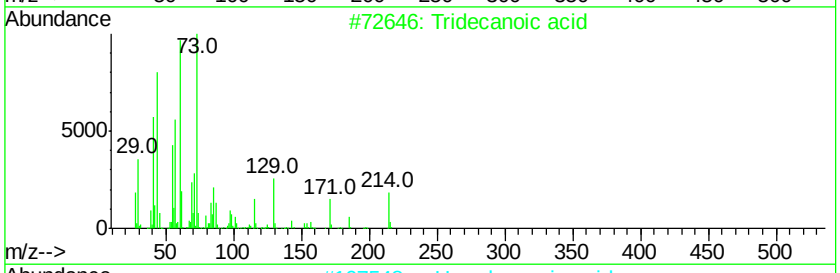
Peak Number 5 Tridecanoic acid Concentration Rank 6

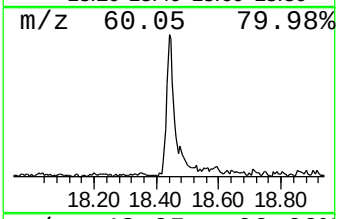
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.44	3.34 ng	534049	Phenanthrene-d10	17.57

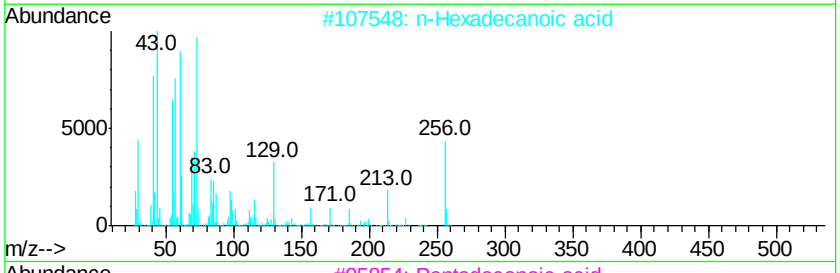
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	.alpha.-d-6,3-Furanose, methyl-....	192	C7H12O6	1000149-62-6	53

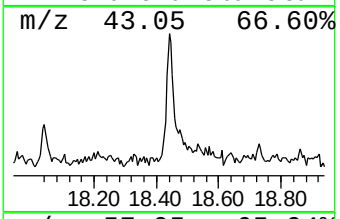


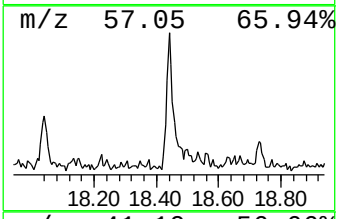


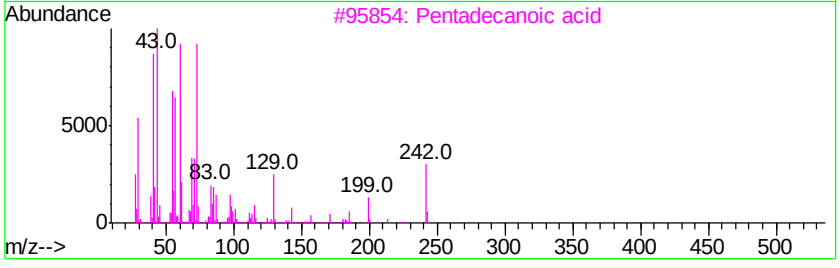


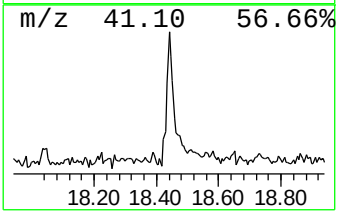












Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

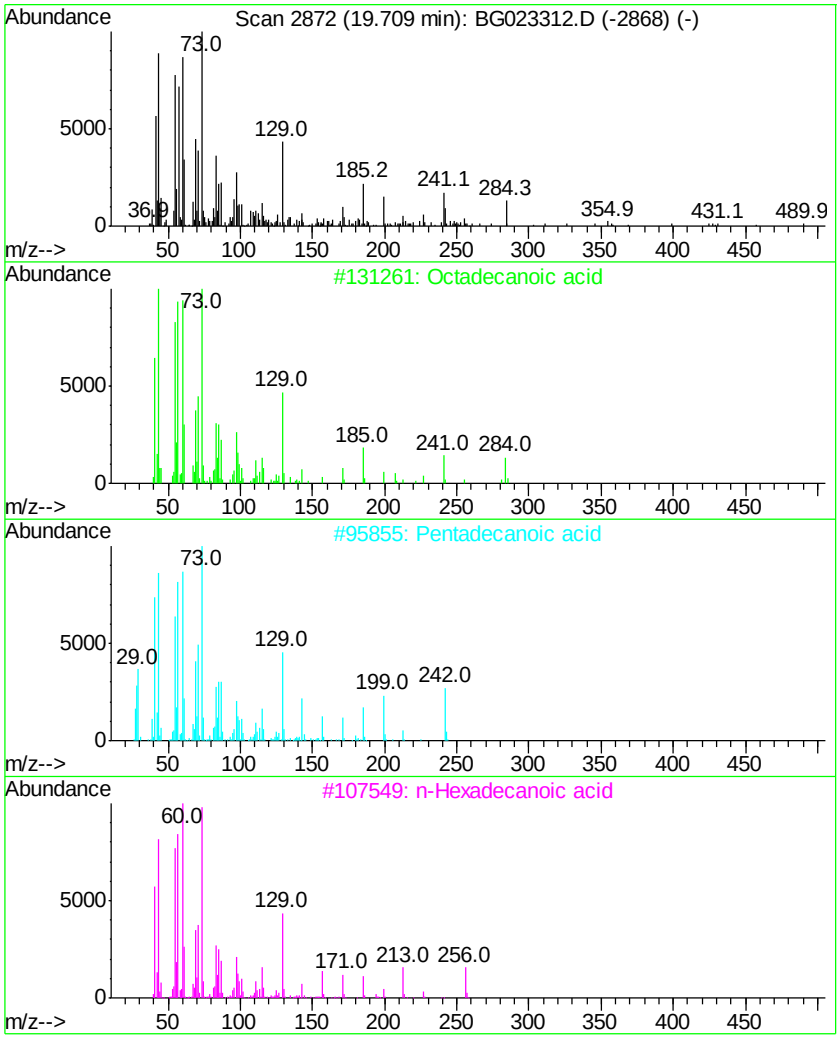
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

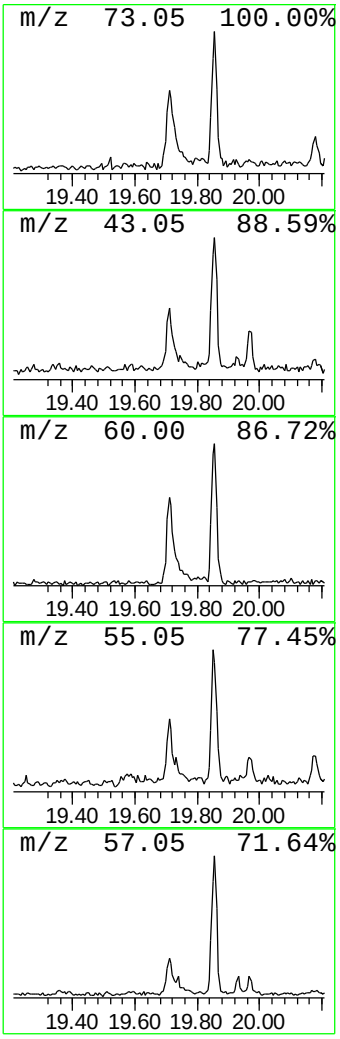
****

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.71	2.30 ng	367231	Phenanthrene-d10	17.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

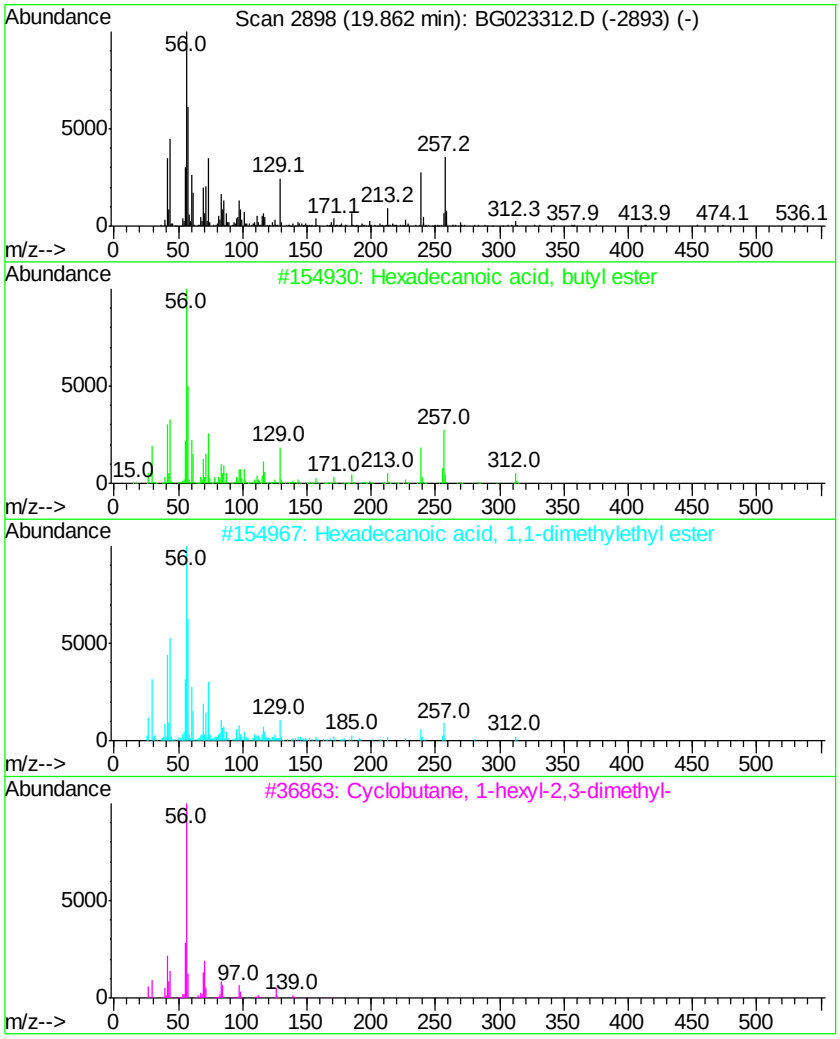
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

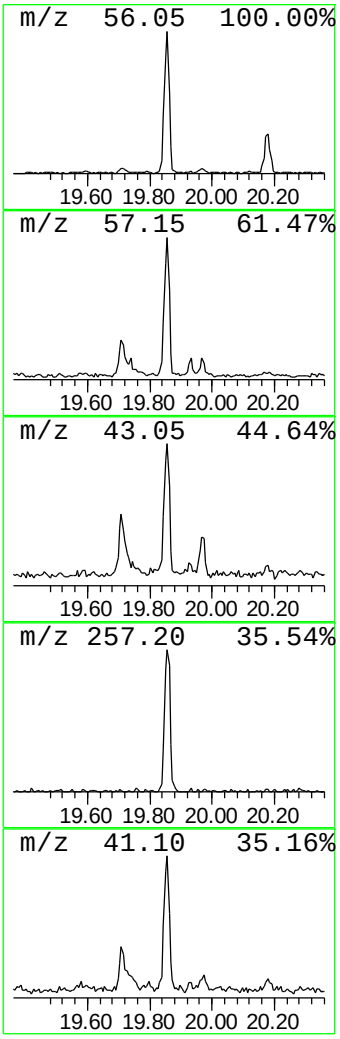
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.86	4.00 ng	707388	Chrysene-d12	21.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32





Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

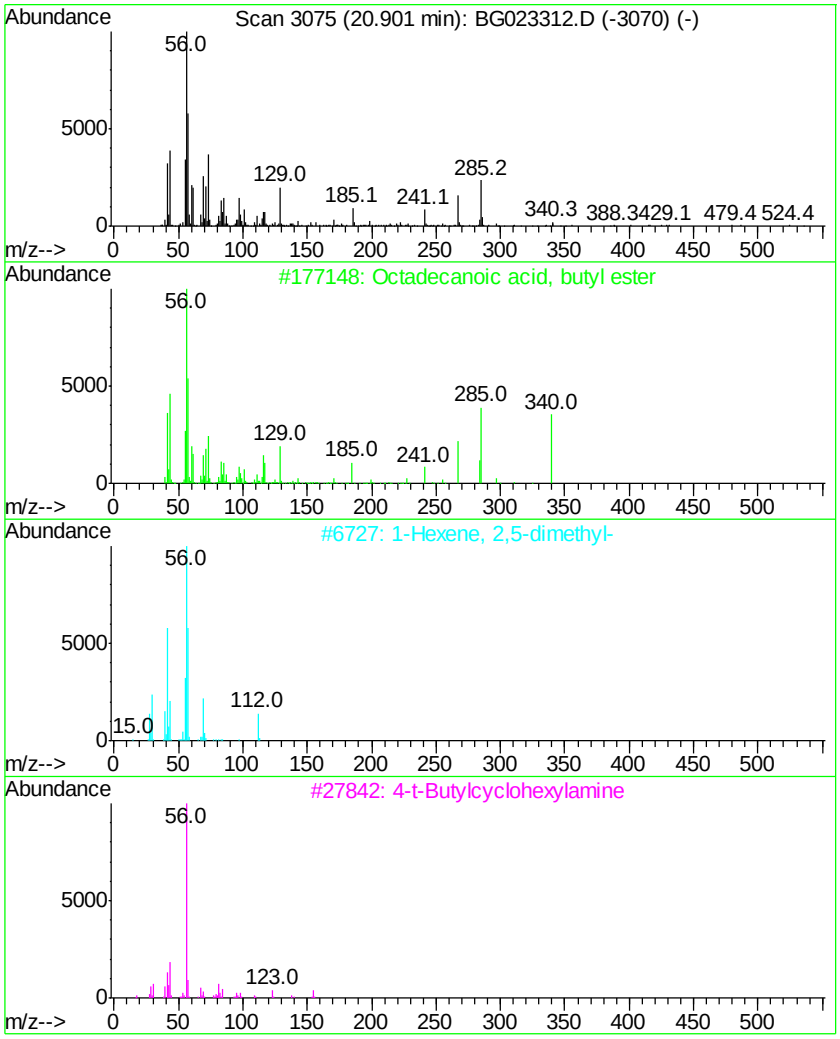
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

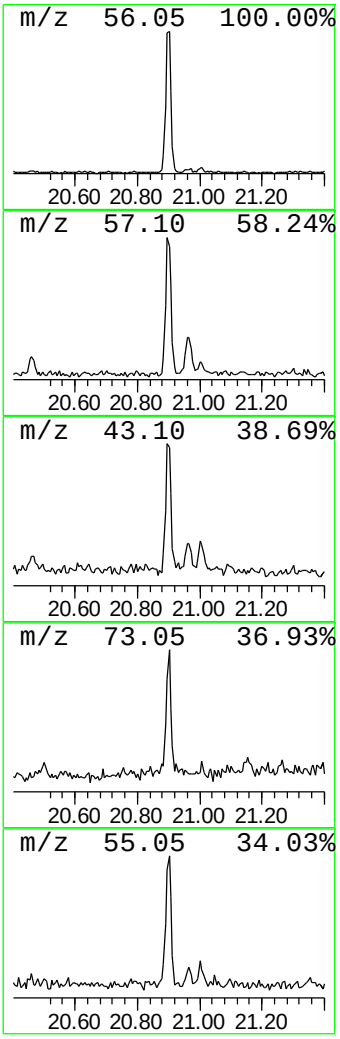
****

Peak Number 8 unknown20.90 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.90	2.93 ng	519265	Chrysene-d12	21.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	35
2	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
3	4-t-Butylcyclohexylamine	155	C10H21N	005400-88-4	27
4	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	27
5	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072816\
Data File : BG023312.D
Acq On : 28 Jul 2016 18:26
Operator : UM/SJ
Sample : H4205-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-40-5.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
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
2-Pentanone, 4-hy...	5.19	35.3	ng	1769910	1	8.14	1003850	20.0
unknown7.66	7.66	69.7	ng	3499300	1	8.14	1003850	20.0
Tridecanoic acid	18.44	3.3	ng	534049	4	17.57	3197200	20.0
Octadecanoic acid	19.71	2.3	ng	367231	4	17.57	3197200	20.0
Hexadecanoic acid...	19.86	4.0	ng	707388	5	21.89	3539750	20.0
unknown20.90	20.90	2.9	ng	519265	5	21.89	3539750	20.0