LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-7B-16.5-17-BGS

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-BG101617.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	5.245	326	333	342	rBV	206196	312114	6.70%	1.151%
2	5.721	407	414	430	rVB	1167940	1840798	39.54%	6.788%
3	7.325	678	687	704	rBV	1196636	2187749	47.00%	8.067%
4	7.701	743	751	759	rBV	1164428	2009552	43.17%	7.410%
5	8.171	824	831	837	rBV	228154	382543	8.22%	1.411%
6	8.494	878	886	897	rVB	836736	1451676	31.18%	5.353%
7	9.334	1020	1029	1037	rBV	715229	1273486	27.36%	4.696%
8	10.985	1301	1310	1320	rBV	356293	624379	13.41%	2.302%
9	12.283	1524	1531	1538	rBV	65101	108207	2.32%	0.399%
10	13.412	1716	1723	1731	rBV	2085381	3279460	70.45%	12.093%
11	14.228	1855	1862	1868	rBV	207626	296172	6.36%	1.092%
12	14.786	1950	1957	1967	rVB2	598387	957074	20.56%	3.529%
13	16.132	2179	2186	2197	rVB	316579	454284	9.76%	1.675%
14	16.267	2202	2209	2223	rBV	1844074	2710412	58.22%	9.994%
15	17.524	2411	2423	2431	rBV2	791599	1185075	25.46%	4.370%
16	18.394	2566	2571	2582	rBV	185970	270870	5.82%	0.999%
17	19.651	2780	2785	2793	rBV	71645	106648	2.29%	0.393%
18	19.798	2807	2810	2816	rVB2	47135	55313	1.19%	0.204%
19	20.115	2858	2864	2874	rBV	3561756	4655140	100.00%	17.165%
20	21.420	3081	3086	3099	rBV	140163	265349	5.70%	0.978%
21	21.796	3143	3150	3159	rBV2	794561	1360751	29.23%	5.018%
22	25.104	3702	3713	3728	rBV2	428635	1332395	28.62%	4.913%

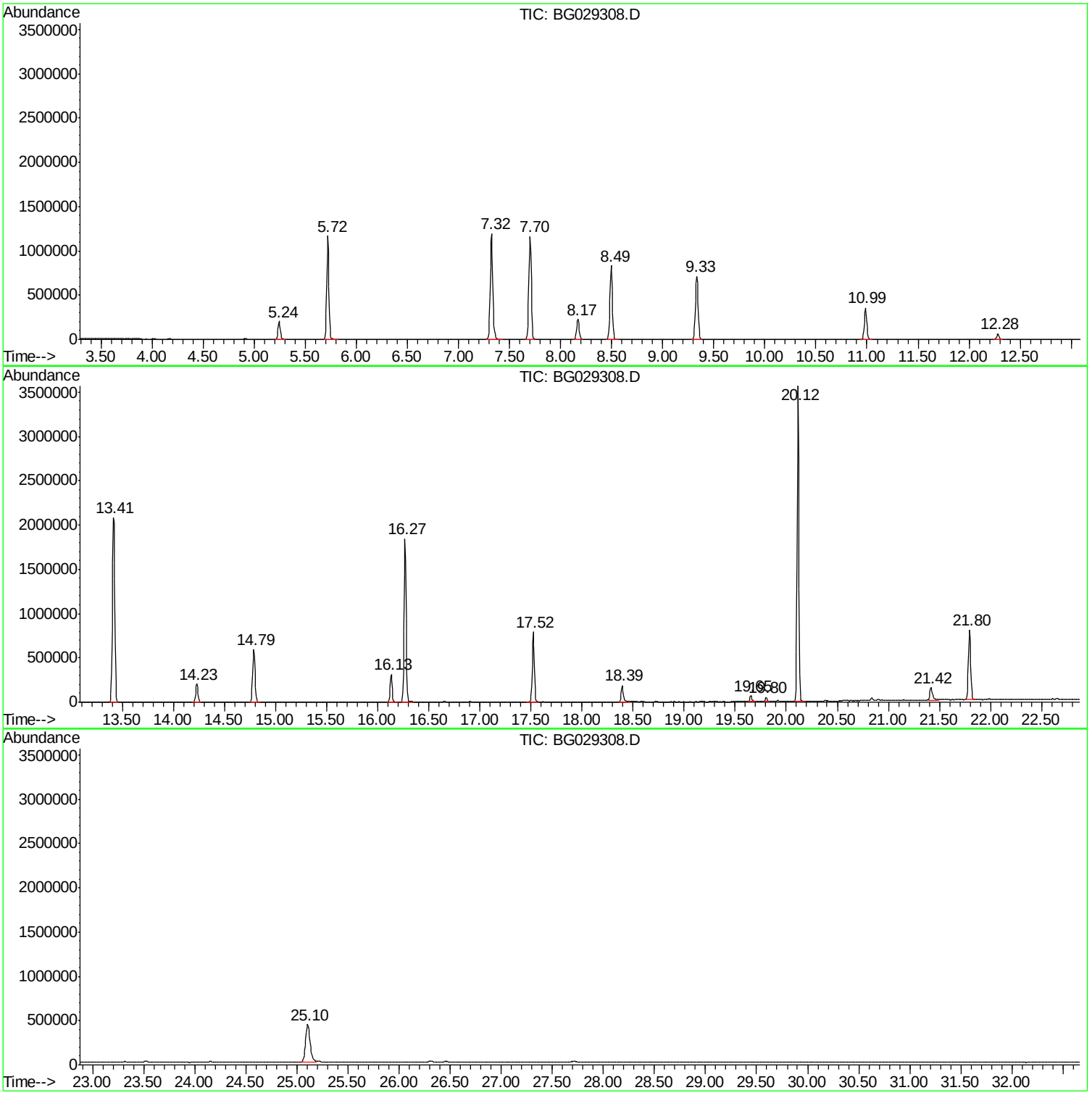
Sum of corrected areas: 27119447

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WPSB-7B-16.5-17-BGS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.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\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-7B-16.5-17-BGS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

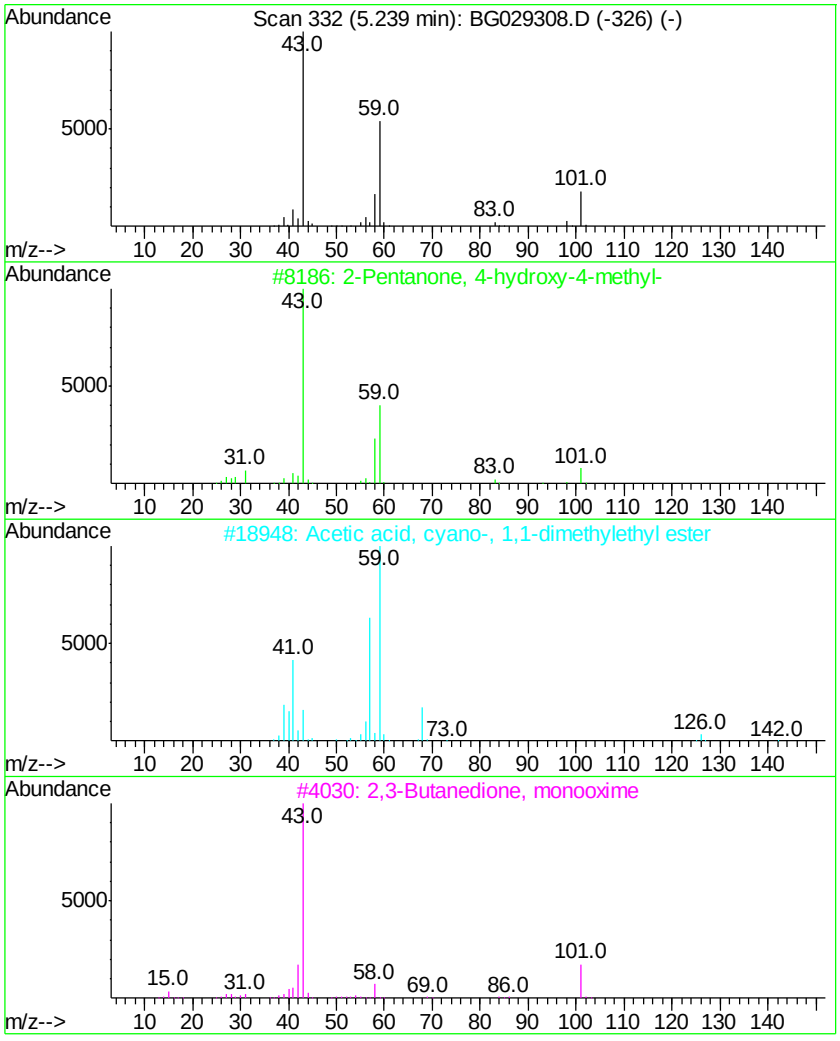
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

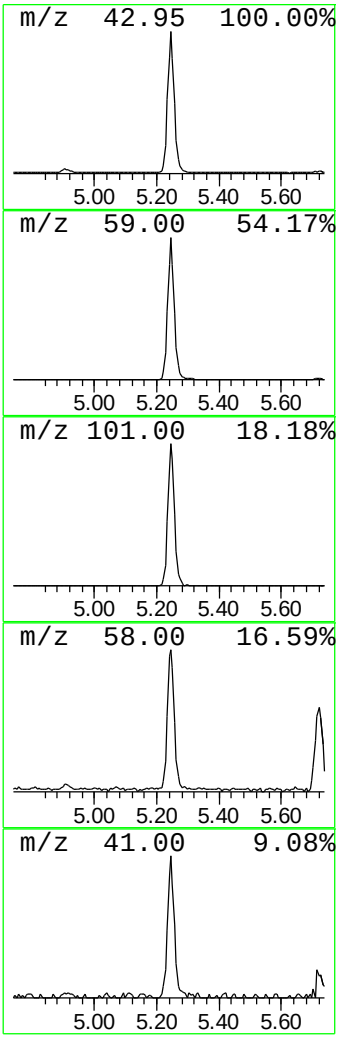
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	16.32 ng	312114	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-7B-16.5-17-BGS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

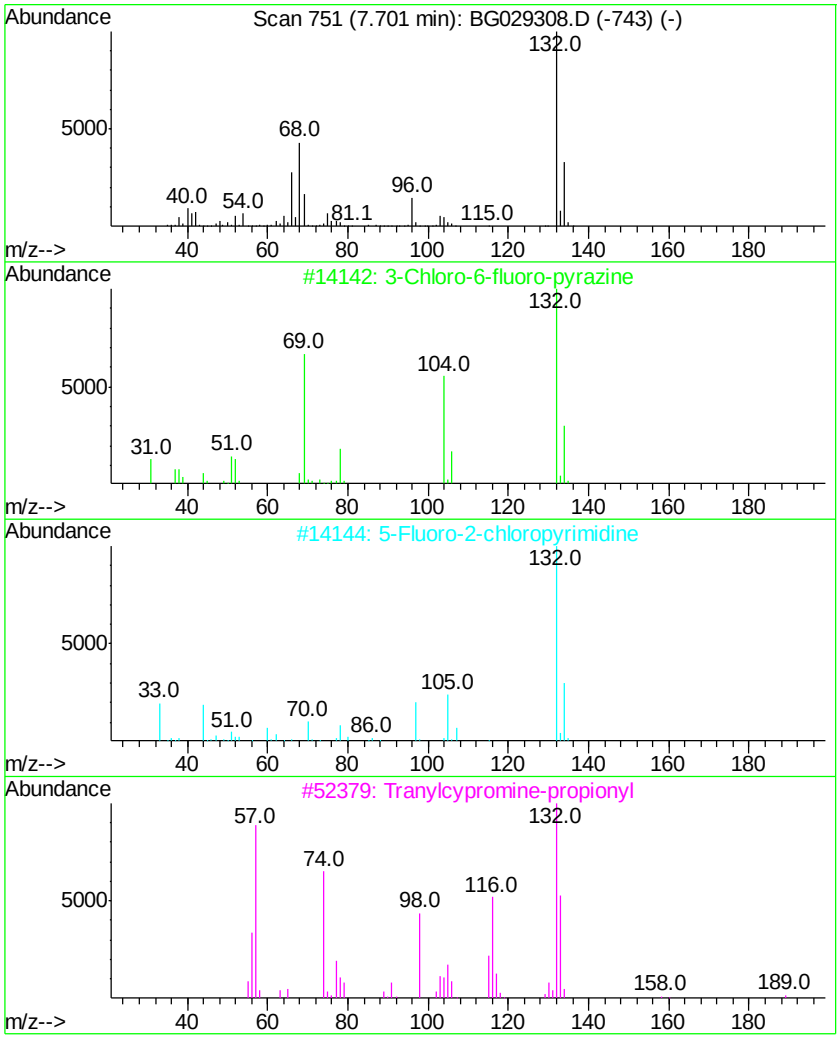
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

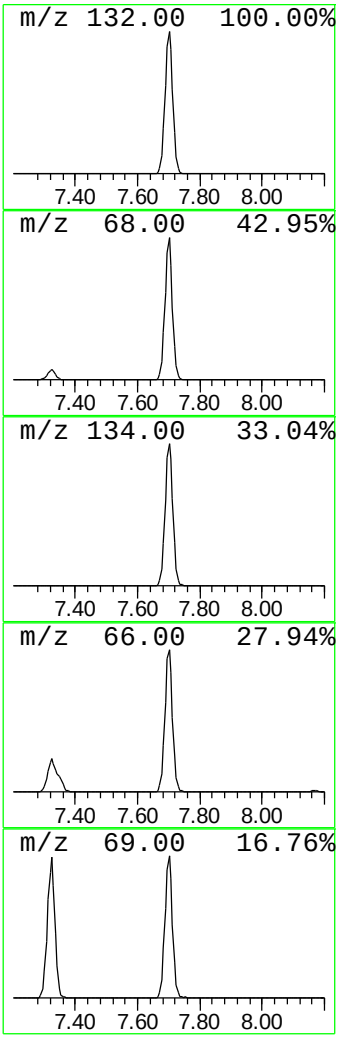
****

Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	105.06 ng	2009550	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-7B-16.5-17-BGS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

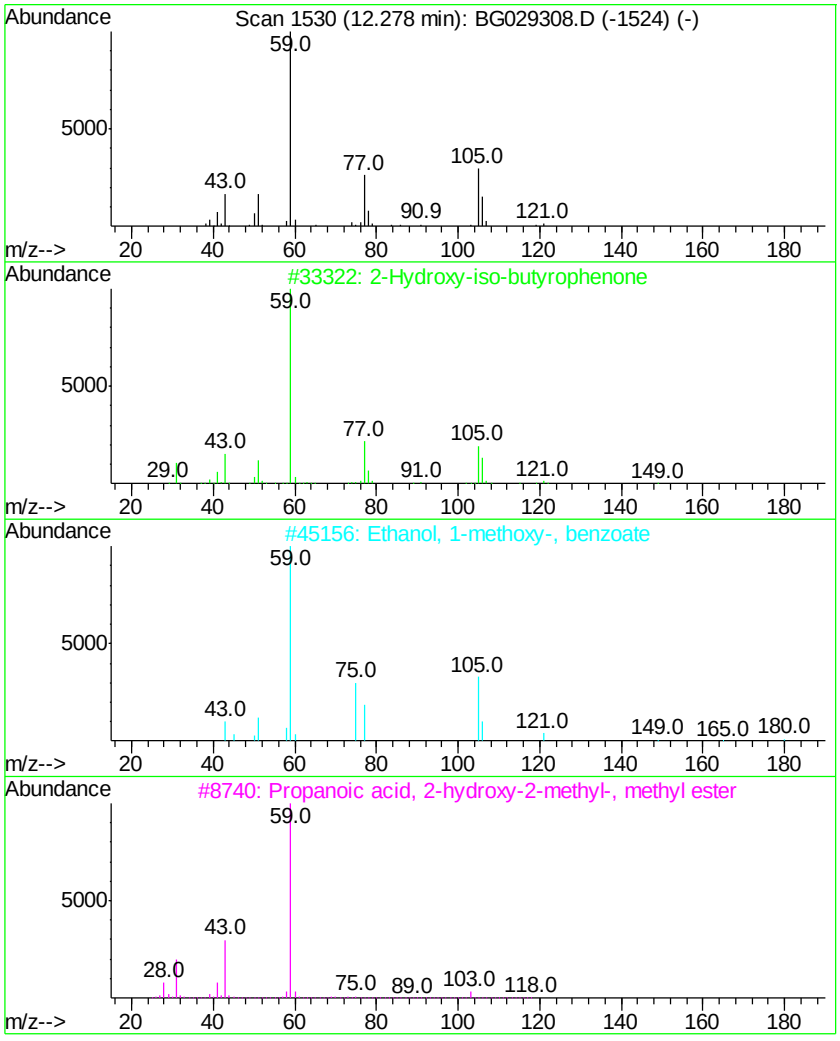
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

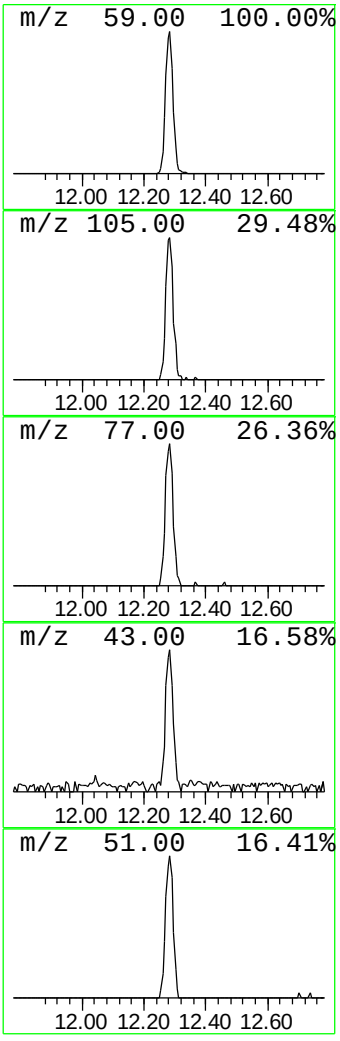
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	3.47 ng	108207	Naphthalene-d8	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Propanoic acid, 2-hydroxy-2-meth...	118	C5H10O3	002110-78-3	9
4	Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5





Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-7B-16.5-17-BGS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

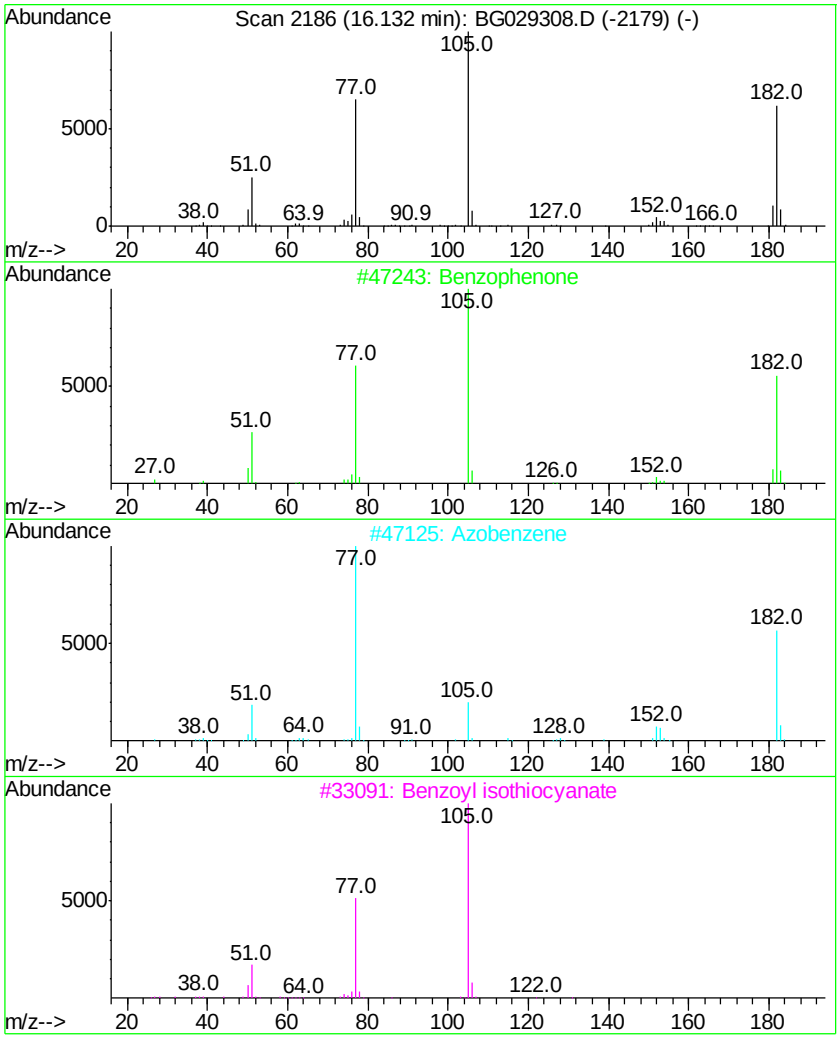
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

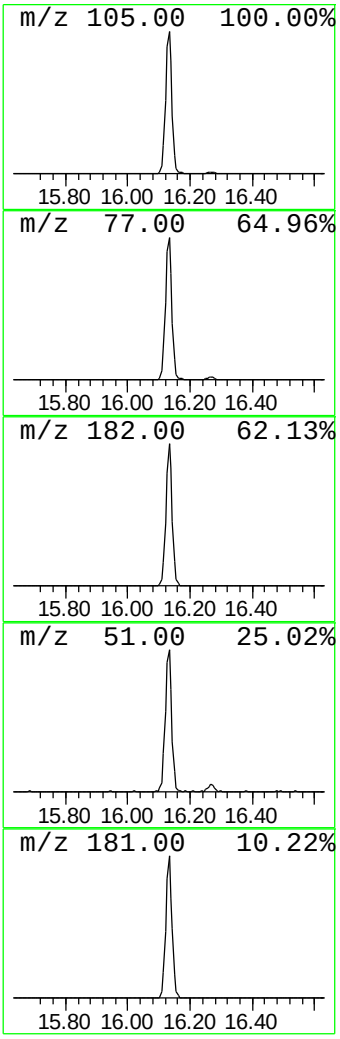
****

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	9.49 ng	454284	Acenaphthene-d10	14.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	Methyl benzilate	242	C15H14O3	000076-89-1	47





Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-7B-16.5-17-BGS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

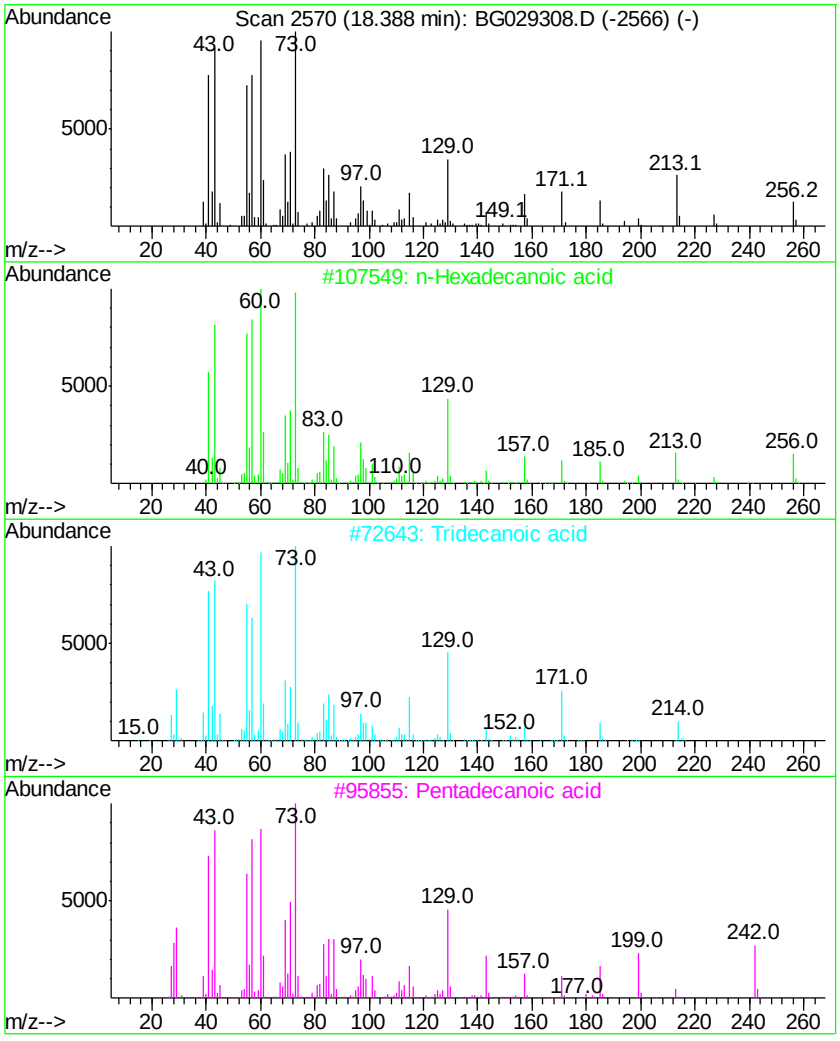
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

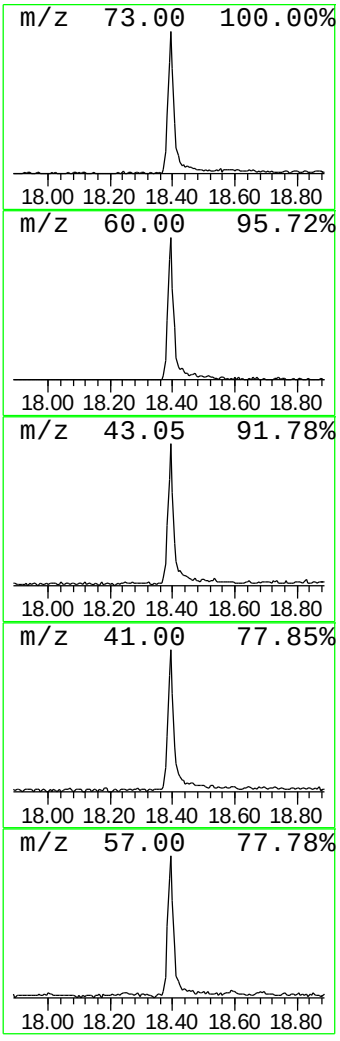
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	4.57 ng	270870	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-7B-16.5-17-BGS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

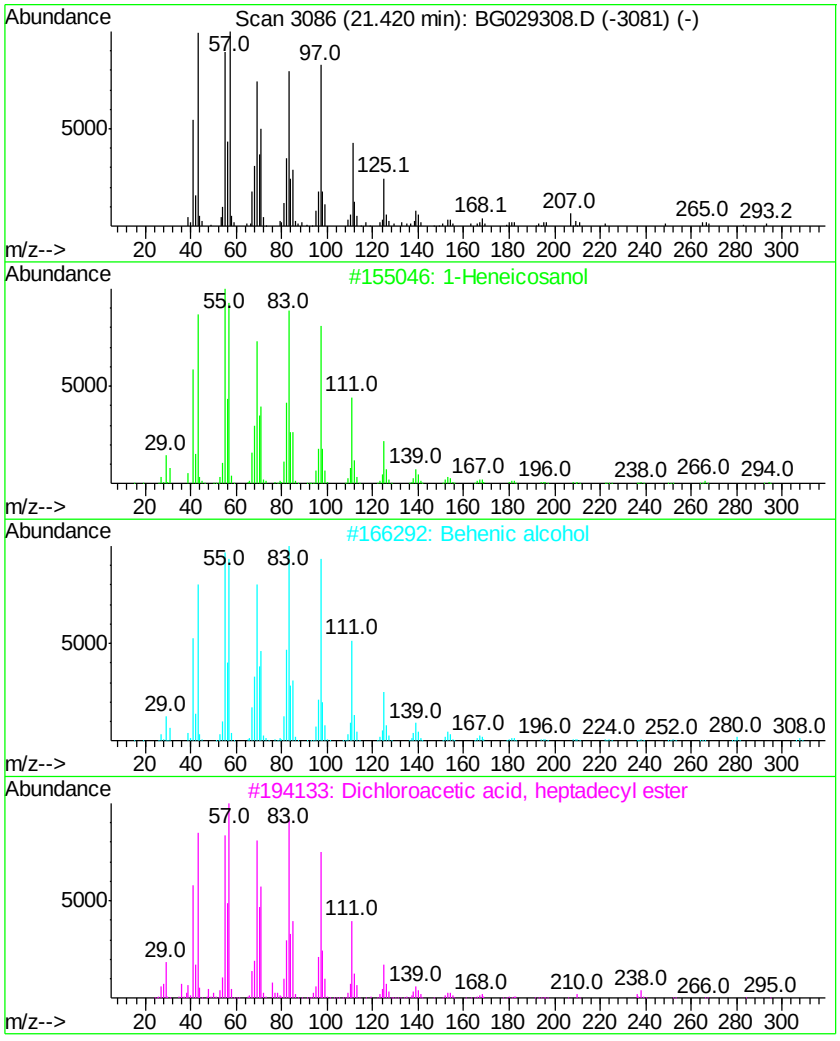
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

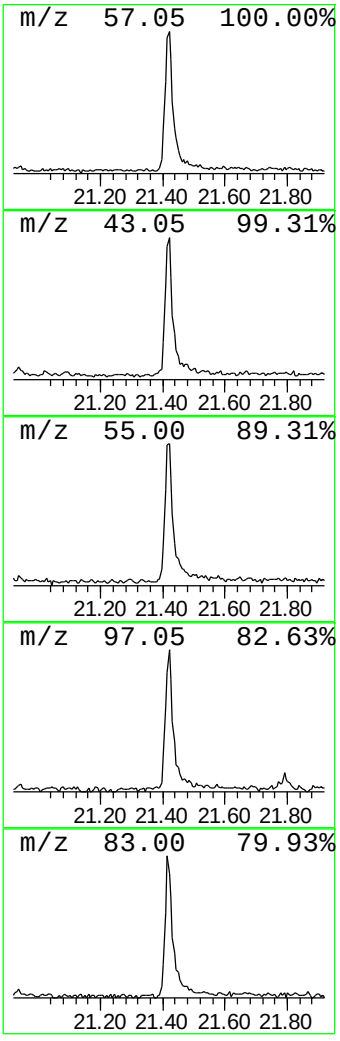
****

Peak Number 7 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	3.90 ng	265349	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101717\
Data File : BG029308.D
Acq On : 17 Oct 2017 19:32
Operator : SJ/JU
Sample : I5821-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WPSB-7B-16.5-17-BGS

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.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...	5.24	16.3	ng	312114	1	8.17	382543	20.0
unknown7.70	7.70	105.1	ng	2009550	1	8.17	382543	20.0
2-Hydroxy-iso-but...	12.28	3.5	ng	108207	2	10.98	624379	20.0
Benzophenone	16.13	9.5	ng	454284	3	14.79	957074	20.0
n-Hexadecanoic acid	18.39	4.6	ng	270870	4	17.52	1185080	20.0
1-Heneicosanol	21.42	3.9	ng	265349	5	21.80	1360750	20.0