LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-4(40)

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-BG011218.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	3.406	14	20	31	rBV2	40572	94060	2.75%	0.526%
2	3.500	31	36	46	rVB	37206	61403	1.80%	0.343%
3	5.686	401	408	416	rVB	34752	57613	1.69%	0.322%
4	6.191	486	494	507	rBV	629841	1102022	32.26%	6.162%
5	7.871	772	780	791	rBV	627521	1191716	34.89%	6.664%
6	8.277	840	849	859	rBV	671617	1227144	35.92%	6.862%
7	8.764	925	932	942	rBB	129684	238979	7.00%	1.336%
8	9.099	977	989	1004	rBB	505434	960129	28.11%	5.369%
9	9.963	1128	1136	1152	rBV	366172	693909	20.31%	3.880%
10	11.649	1414	1423	1435	rVB	171844	323545	9.47%	1.809%
11	12.906	1629	1637	1644	rBV	54678	90377	2.65%	0.505%
12	14.023	1816	1827	1839	rBV	1210226	1961288	57.42%	10.967%
13	14.822	1954	1963	1969	rBV	262328	391464	11.46%	2.189%
14	15.398	2054	2061	2071	rVB2	299856	500014	14.64%	2.796%
15	16.726	2279	2287	2296	rBV	550278	822815	24.09%	4.601%
16	16.872	2304	2312	2323	rBV	1218359	1949146	57.06%	10.899%
17	18.130	2518	2526	2537	rVB	462915	722234	21.14%	4.038%
18	18.941	2659	2664	2672	rBV2	66619	104393	3.06%	0.584%
19	20.180	2870	2875	2883	rBV6	18738	34174	1.00%	0.191%
20	20.662	2951	2957	2966	rBV	2537084	3415976	100.00%	19.101%
21	22.008	3178	3186	3191	rBV3	31404	55668	1.63%	0.311%
22	22.466	3256	3264	3273	rBV2	506424	942617	27.59%	5.271%
23	26.179	3884	3896	3914	rBV	284841	943365	27.62%	5.275%

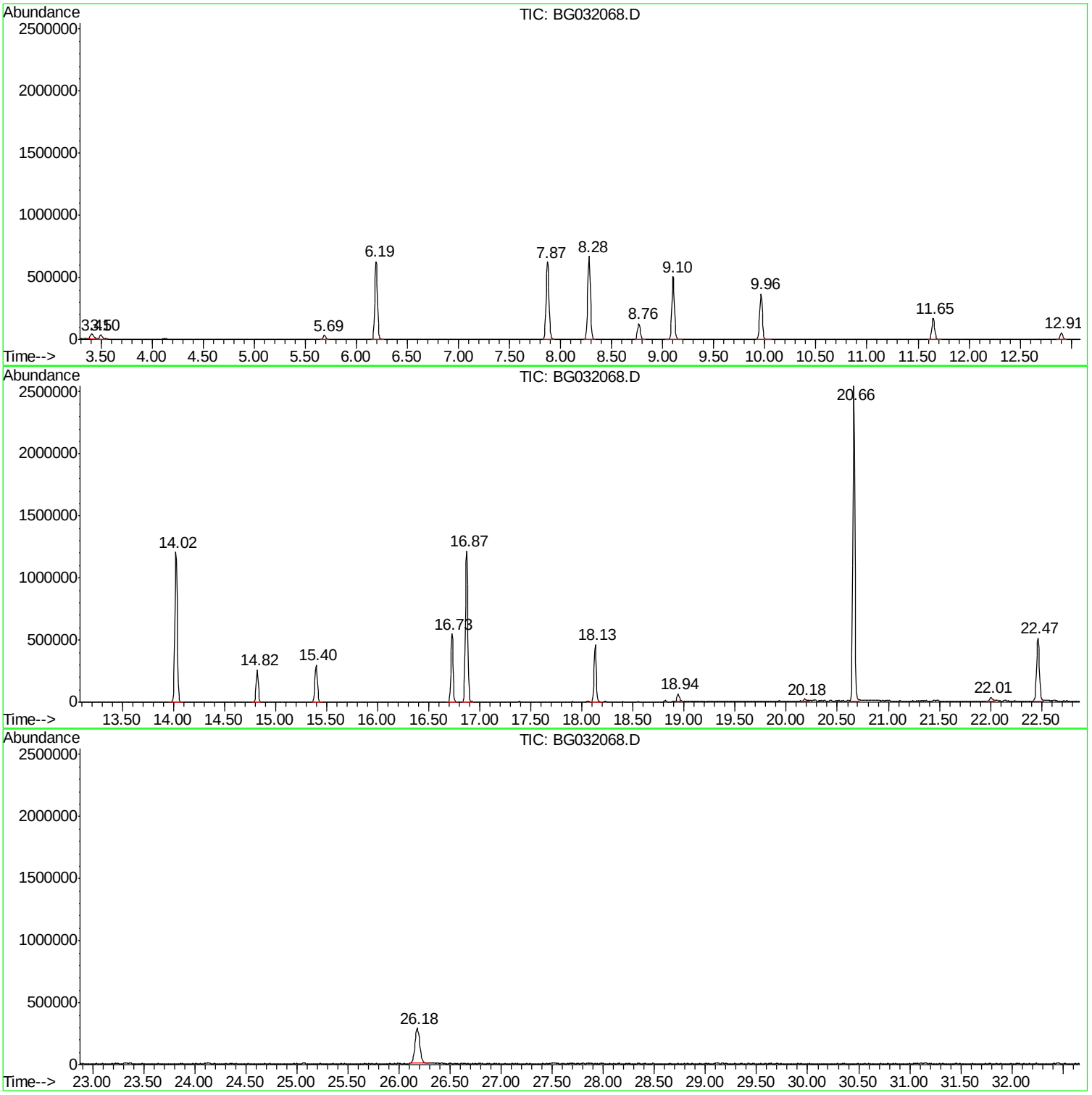
Sum of corrected areas: 17884051

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-4(40)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-4(40)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

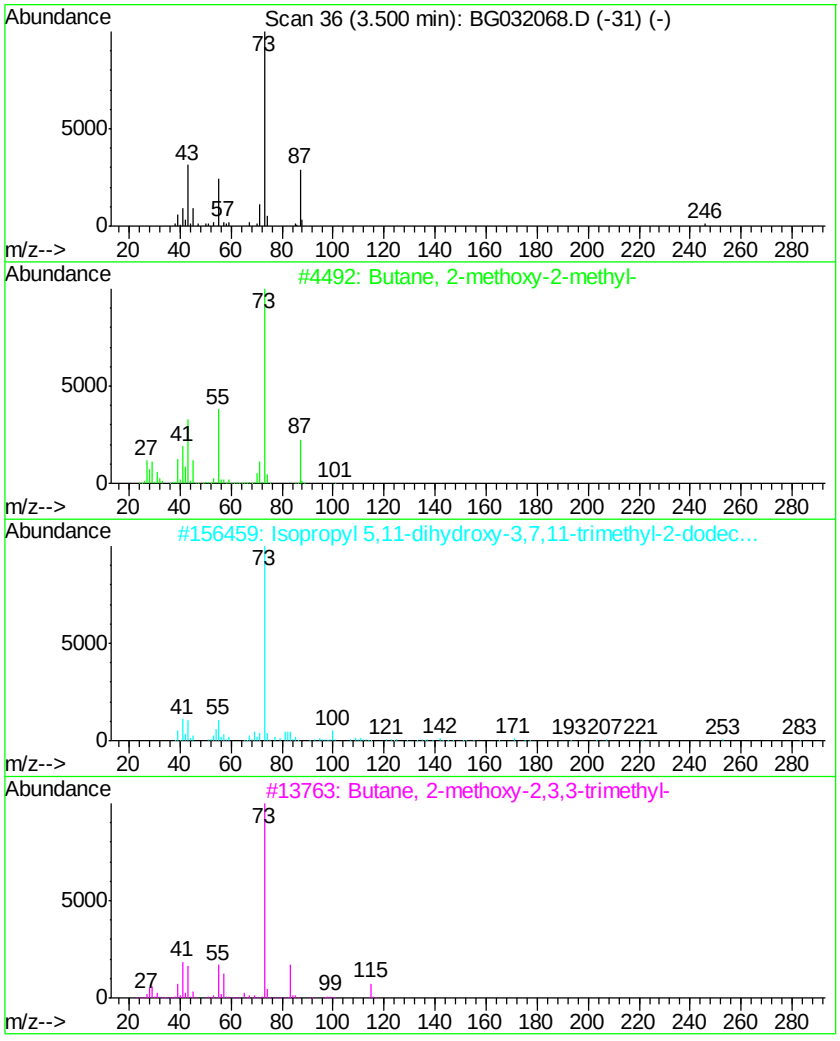
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

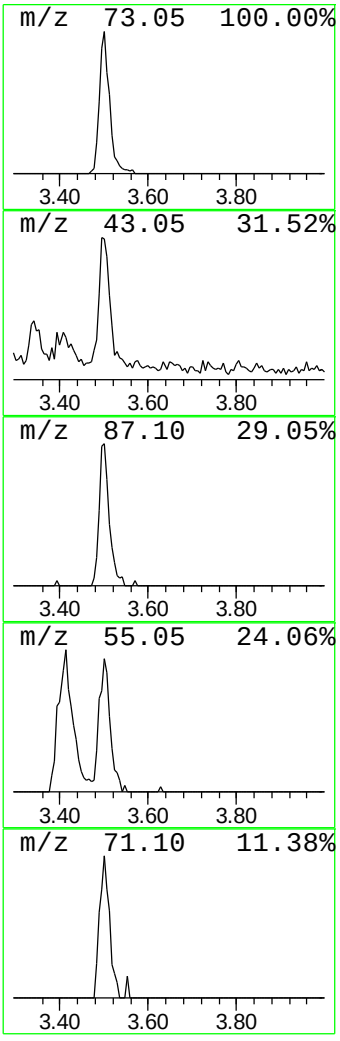
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	5.14 ng	61403	1,4-Dichlorobenzene-d4	8.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Isopropyl 5,11-dihydroxy-3,7,11-...	314	C18H34O4	1000223-34-1	12
3	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	10
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-4(40)

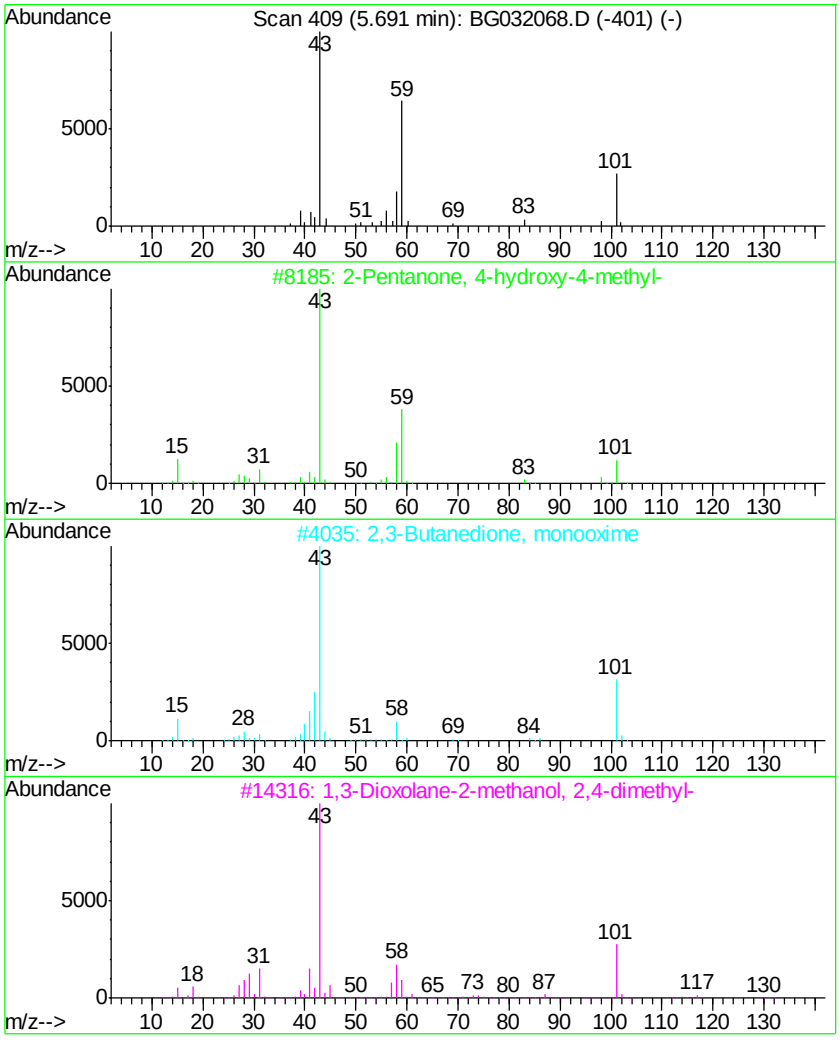
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

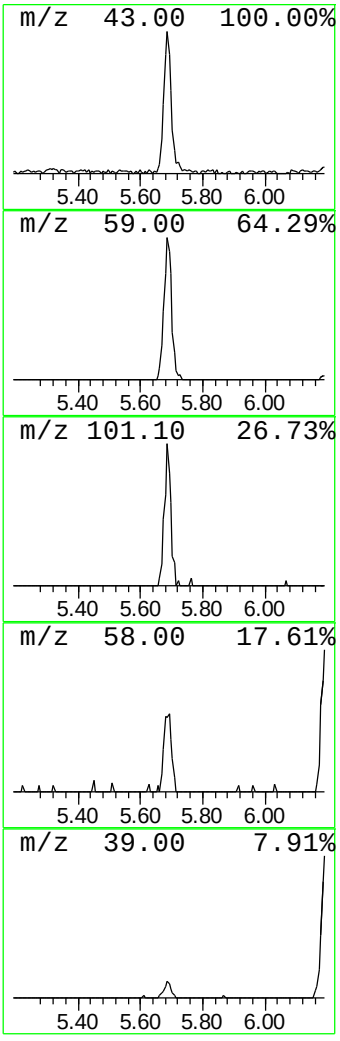
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	4.82 ng	57613	1,4-Dichlorobenzene-d4	8.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-4(40)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

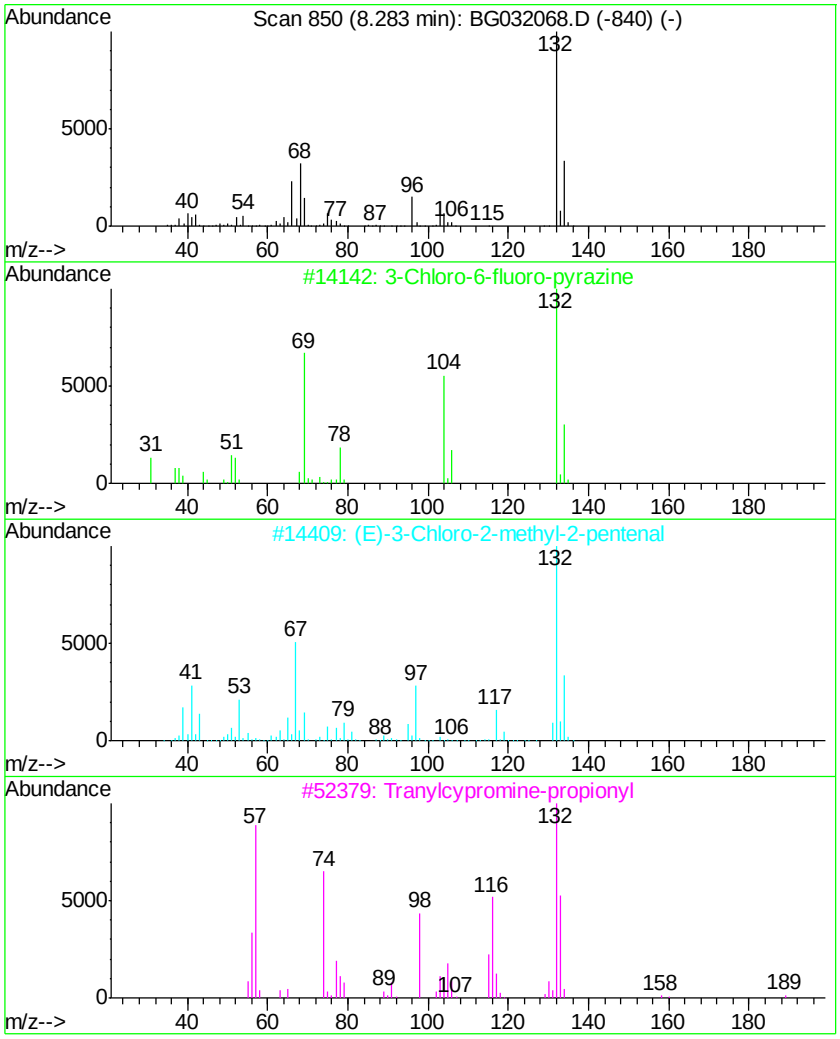
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

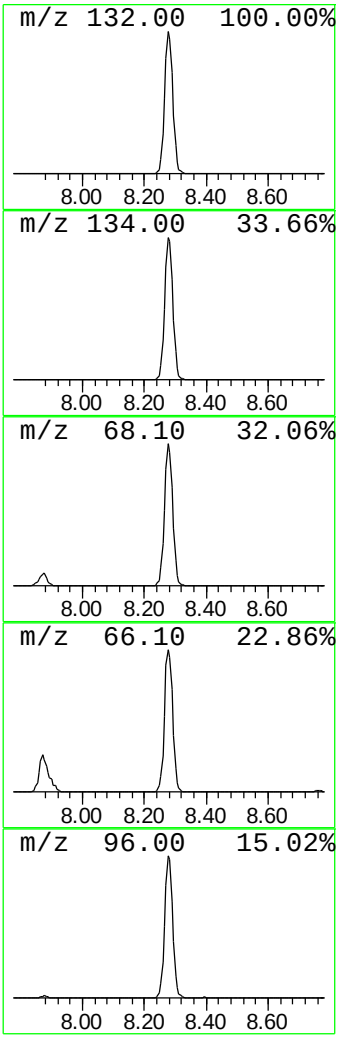
****

Peak Number 4 unknown8.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	102.70 ng	1227140	1,4-Dichlorobenzene-d4	8.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
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





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-4(40)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

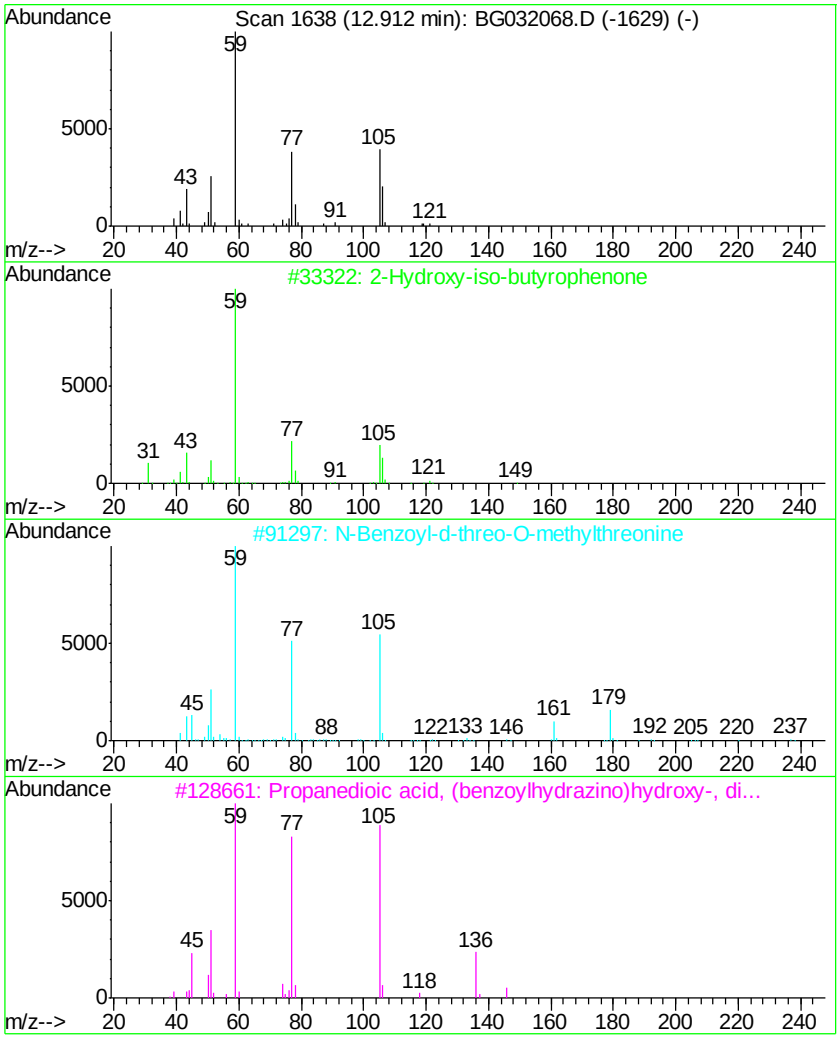
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

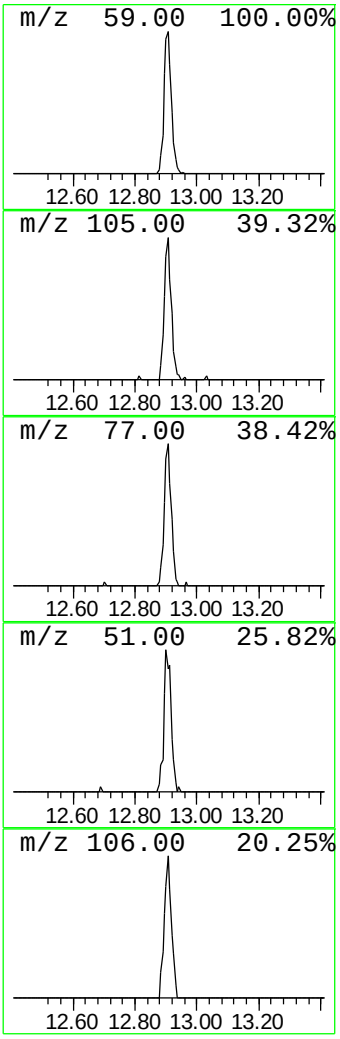
****

Peak Number 6 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	5.59 ng	90377	Naphthalene-d8	11.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	59
2	N-Benzoyl-d-threo-O-methylthreonine	237	C12H15NO4	131644-54-7	50
3	Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	40
4	Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	12
5	Carbonic acid, 2-methoxyethyl ph...	196	C10H12O4	1000357-86-8	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-4(40)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

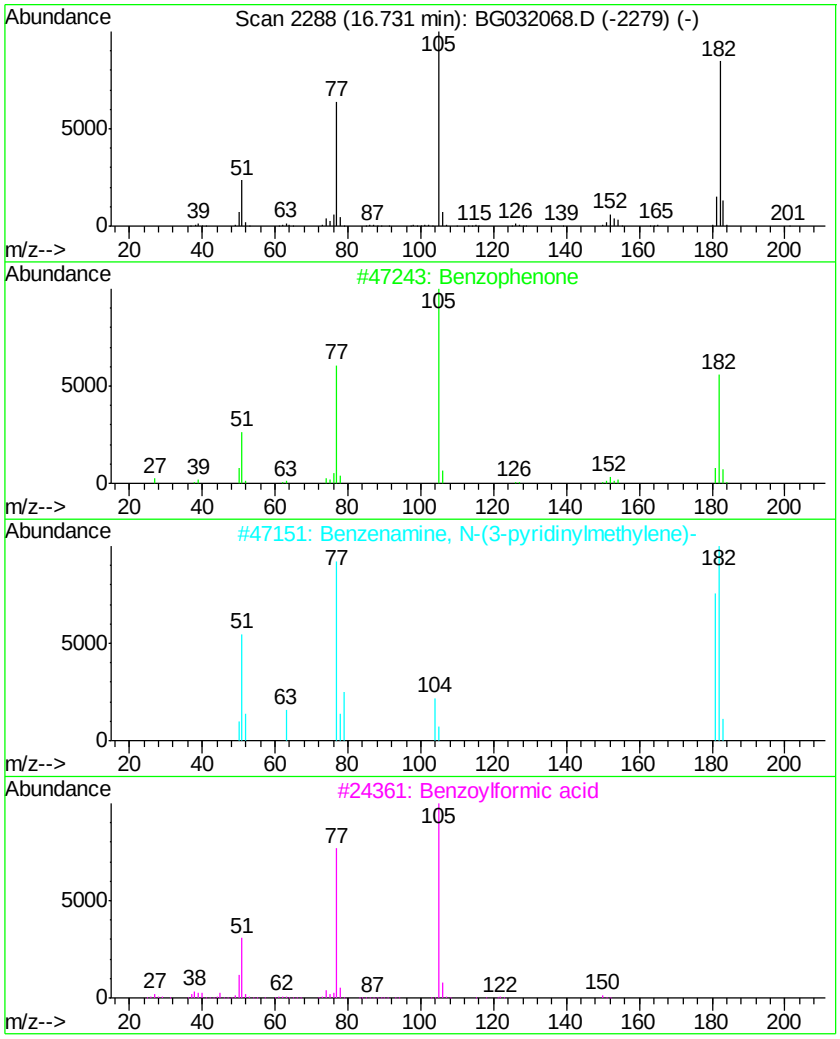
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

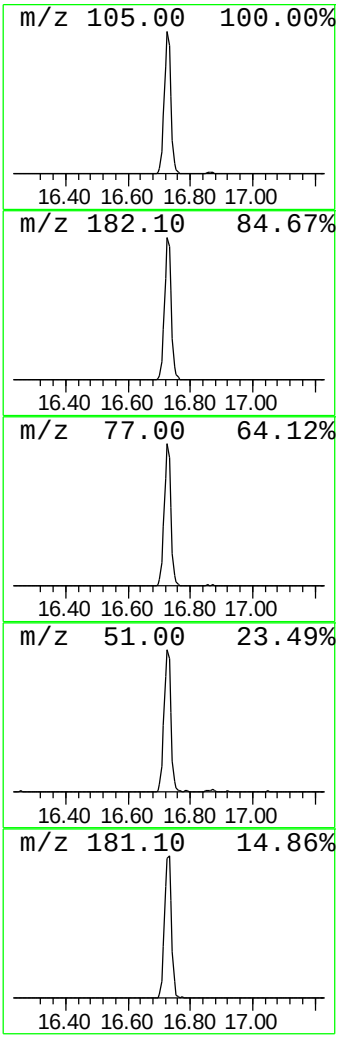
****

Peak Number 7 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	32.91 ng	822815	Acenaphthene-d10	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	59
3	Benzoylformic acid	150	C8H6O3	000611-73-4	41
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	38
5	1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	38





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-4(40)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

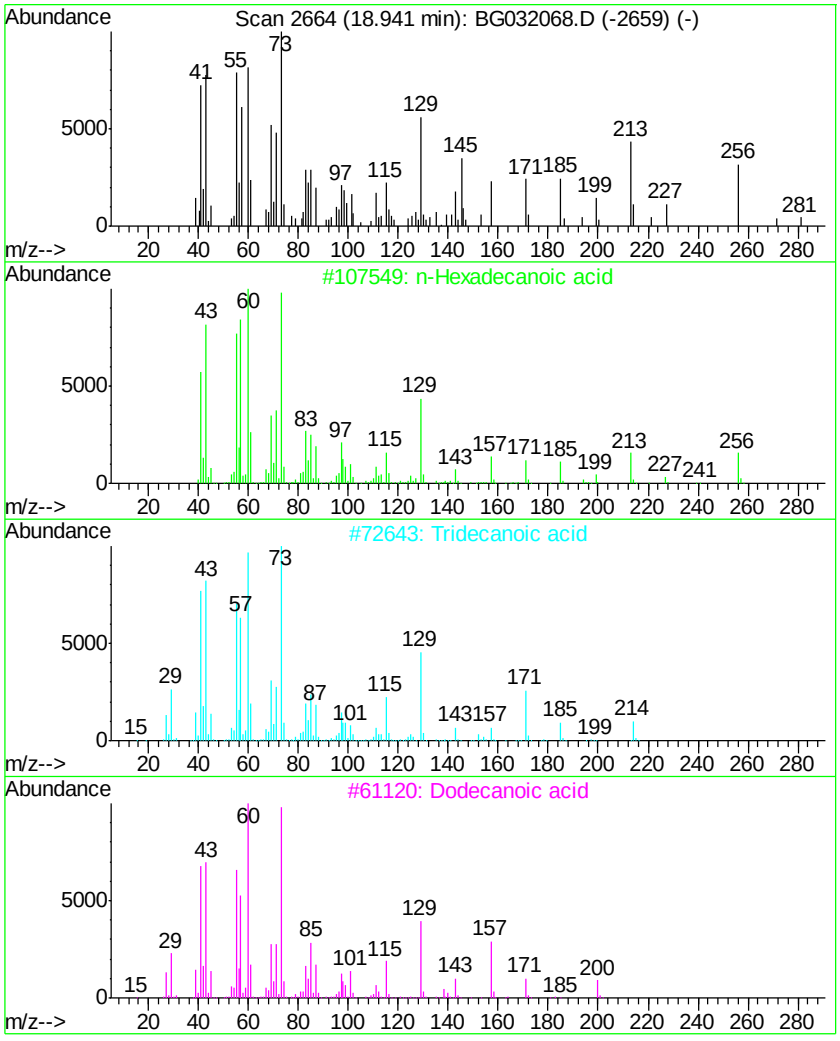
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

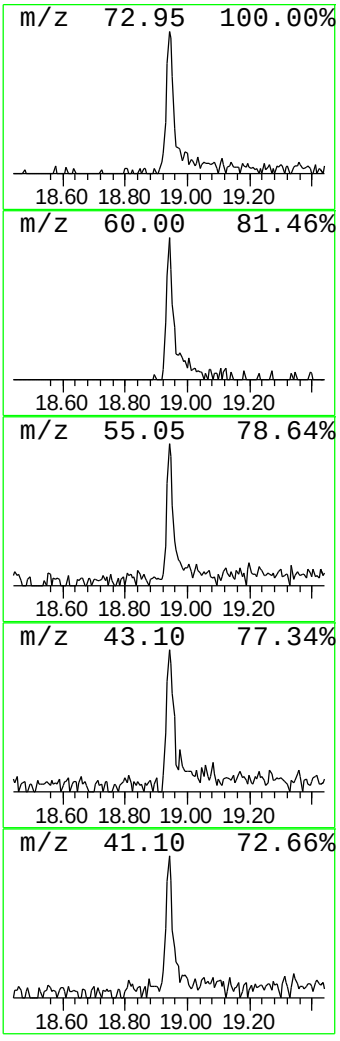
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.94	2.89 ng	104393	Phenanthrene-d10	18.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	38





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032068.D
Acq On : 16 Jan 2018 14:14
Operator : SJ/JU
Sample : J1123-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-4(40)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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
Butane, 2-methoxy...	3.50	5.1	ng	61403	1	8.77	238979	20.0
2-Pentanone, 4-hy...	5.69	4.8	ng	57613	1	8.77	238979	20.0
unknown8.28	8.28	102.7	ng	1227140	1	8.77	238979	20.0
2-Hydroxy-iso-but...	12.91	5.6	ng	90377	2	11.65	323545	20.0
Benzophenone	16.73	32.9	ng	822815	3	15.40	500014	20.0
n-Hexadecanoic acid	18.94	2.9	ng	104393	4	18.13	722234	20.0