LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
Data File : BG031679.D
Acq On : 21 Dec 2017 18:44
Operator : SJ/JU
Sample : I6961-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(15-17)

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-BG122117.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	3.448	19	27	38	rBV3	45741	96023	2.73%	0.524%
2	5.746	412	418	425	rBV	32738	56075	1.59%	0.306%
3	6.245	495	503	513	rBV	631961	1095633	31.10%	5.981%
4	7.925	780	789	800	rBV	642062	1223596	34.73%	6.679%
5	8.343	851	860	869	rBV	670273	1239632	35.19%	6.767%
6	8.830	935	943	951	rBV	153904	275337	7.82%	1.503%
7	9.165	992	1000	1012	rVB	489697	922043	26.17%	5.033%
8	10.029	1138	1147	1158	rBV	350002	643035	18.25%	3.510%
9	11.721	1426	1435	1442	rBV	216550	402623	11.43%	2.198%
10	12.972	1642	1648	1656	rVB	42191	69180	1.96%	0.378%
11	14.095	1831	1839	1854	rVB	1255418	1991371	56.53%	10.870%
12	14.888	1968	1974	1982	rVB	157387	237727	6.75%	1.298%
13	15.464	2065	2072	2082	rVB2	385768	653429	18.55%	3.567%
14	16.797	2292	2299	2307	rVB	289832	416999	11.84%	2.276%
15	16.938	2316	2323	2336	rBV	1160036	1857571	52.73%	10.140%
16	18.196	2530	2537	2545	rBV2	578229	907801	25.77%	4.955%
17	19.024	2673	2678	2686	rBV2	67532	104631	2.97%	0.571%
18	20.258	2884	2888	2893	rBV5	38509	57214	1.62%	0.312%
19	20.734	2963	2969	2978	rBV	2586807	3522929	100.00%	19.230%
20	22.115	3199	3204	3213	rBV	101823	167601	4.76%	0.915%
21	22.561	3271	3280	3289	rBV	613341	1187517	33.71%	6.482%
22	26.351	3913	3925	3937	rVB2	367350	1191955	33.83%	6.506%

Sum of corrected areas: 18319922

LSC Report - Integrated Chromatogram

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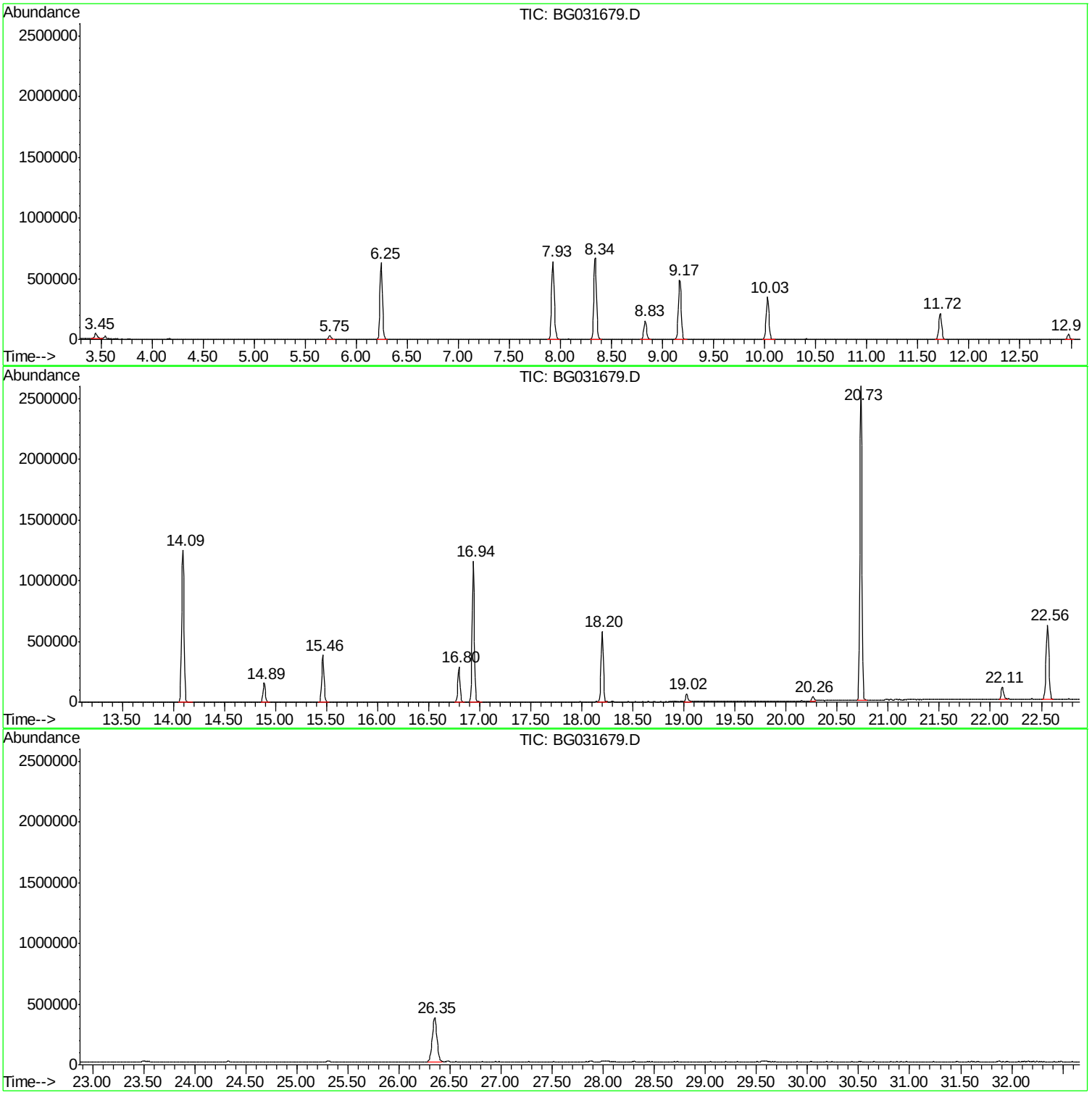
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(15-17)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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\BG122117\
Data File : BG031679.D
Acq On : 21 Dec 2017 18:44
Operator : SJ/JU
Sample : I6961-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(15-17)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

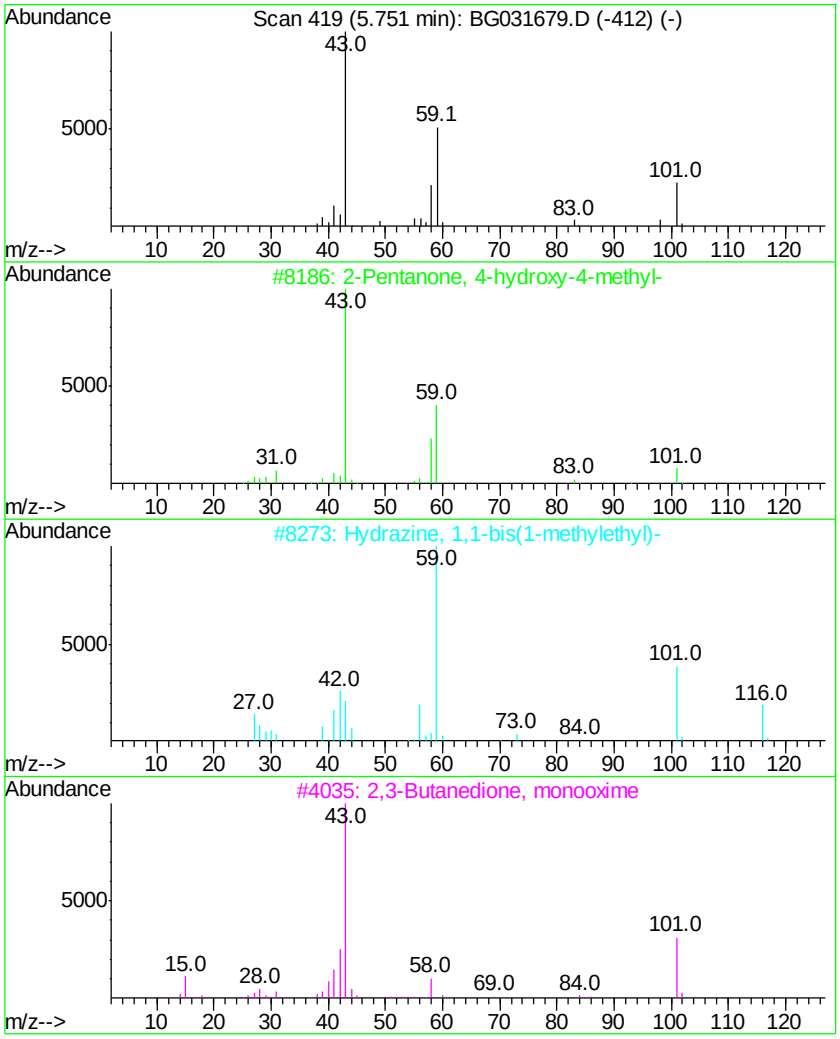
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

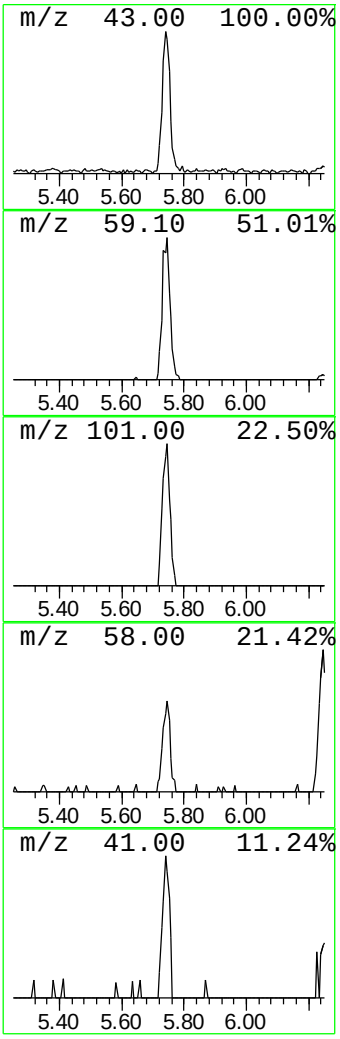
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.75	4.07 ng	56075	1,4-Dichlorobenzene-d4	8.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	22
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	17





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Data File : BG031679.D
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Operator : SJ/JU
Sample : I6961-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(15-17)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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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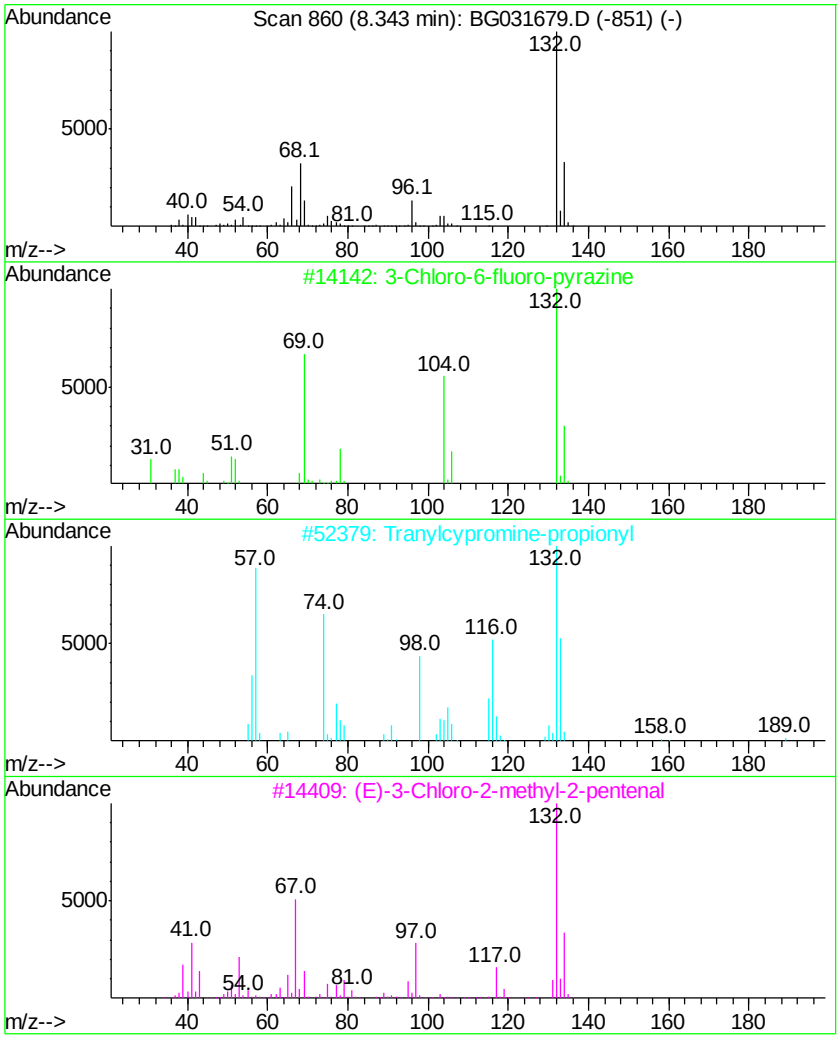
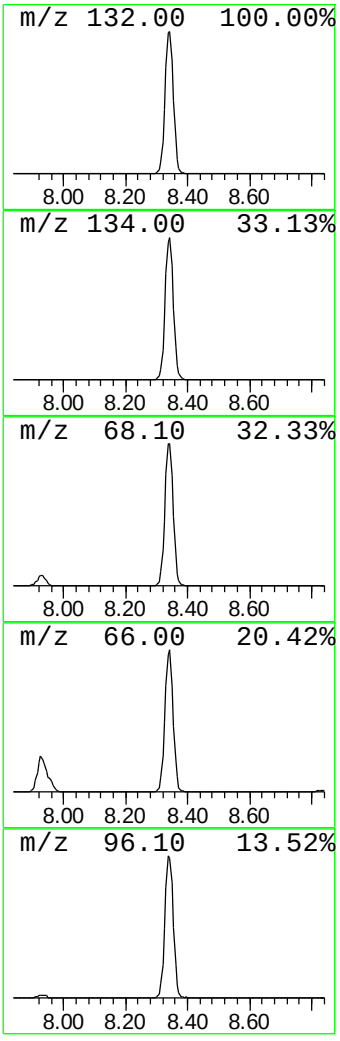
Peak Number 3 unknown8.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	90.04 ng	1239630	1,4-Dichlorobenzene-d4	8.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Xenon	132	Xe	007440-63-3	9





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Data File : BG031679.D
Acq On : 21 Dec 2017 18:44
Operator : SJ/JU
Sample : I6961-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(15-17)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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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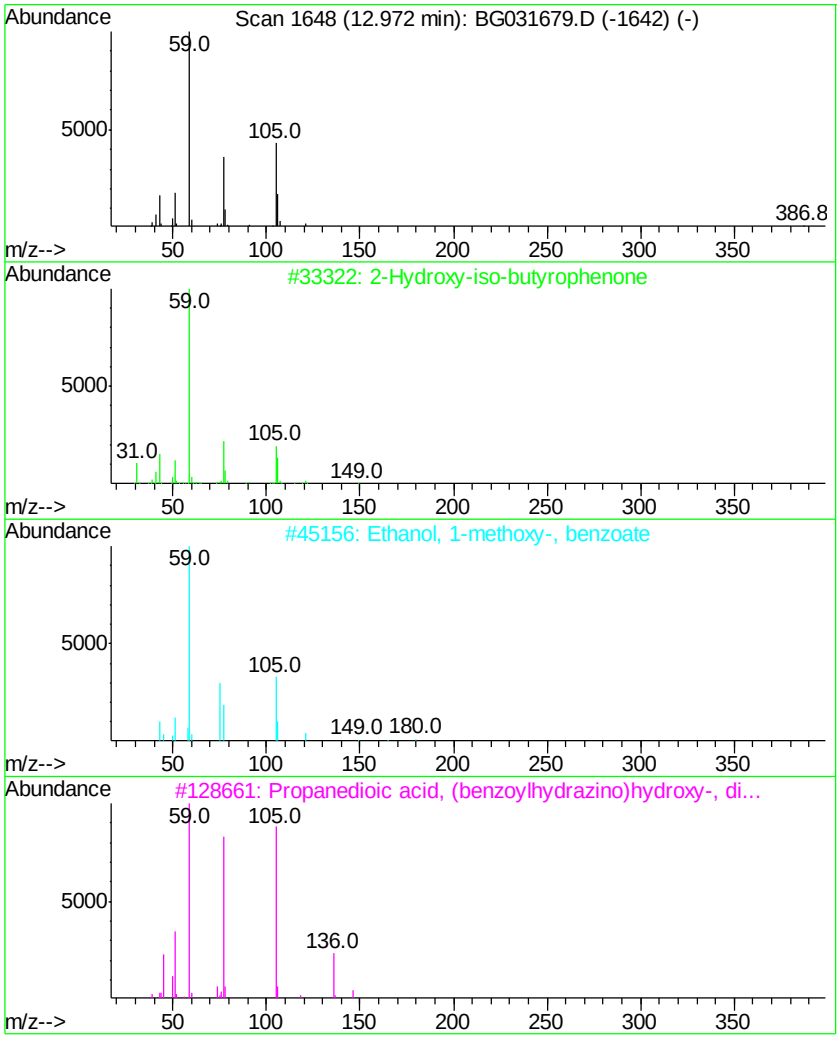
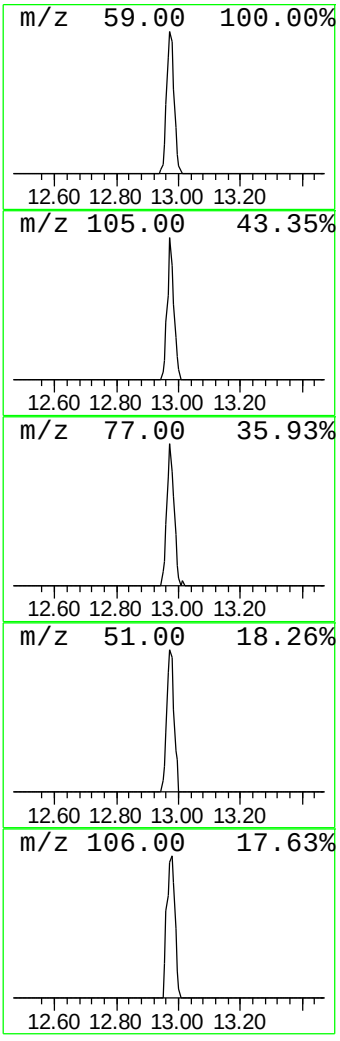
Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	3.44 ng	69180	Naphthalene-d8	11.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3	Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	38
4	.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	9
5	N-Benzoyl-d-threo-O-methylthreonine	237	C12H15NO4	131644-54-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
Data File : BG031679.D
Acq On : 21 Dec 2017 18:44
Operator : SJ/JU
Sample : I6961-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(15-17)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

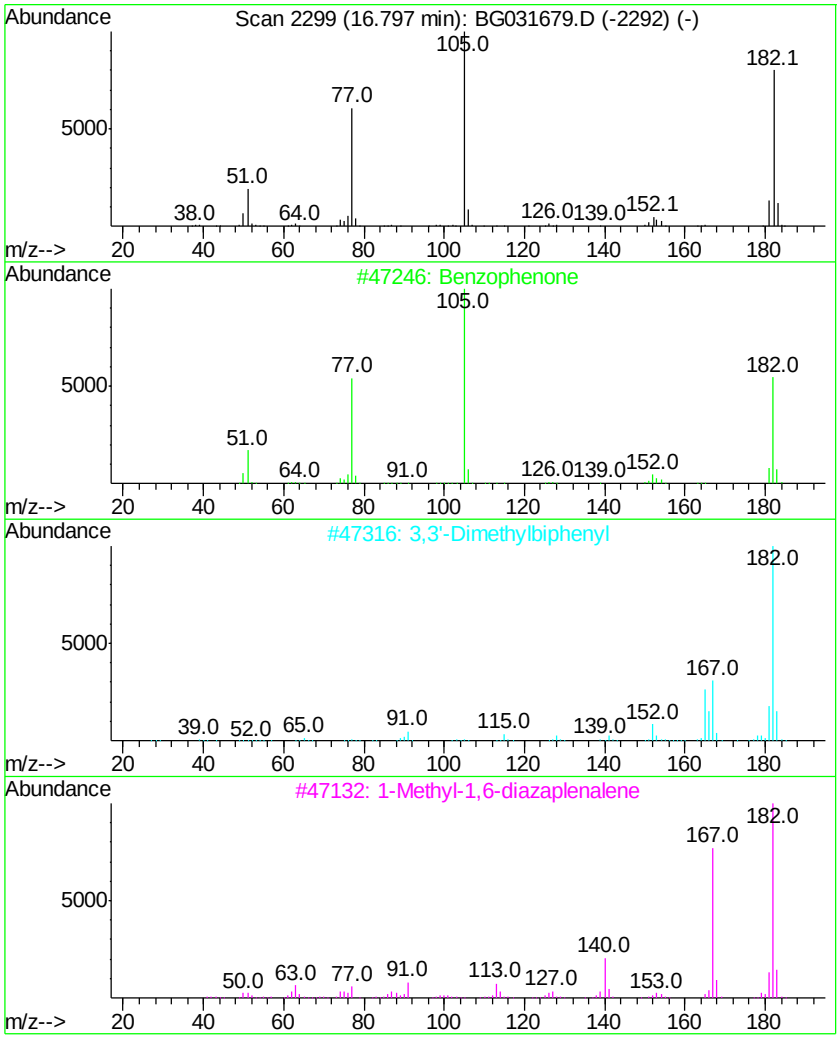
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

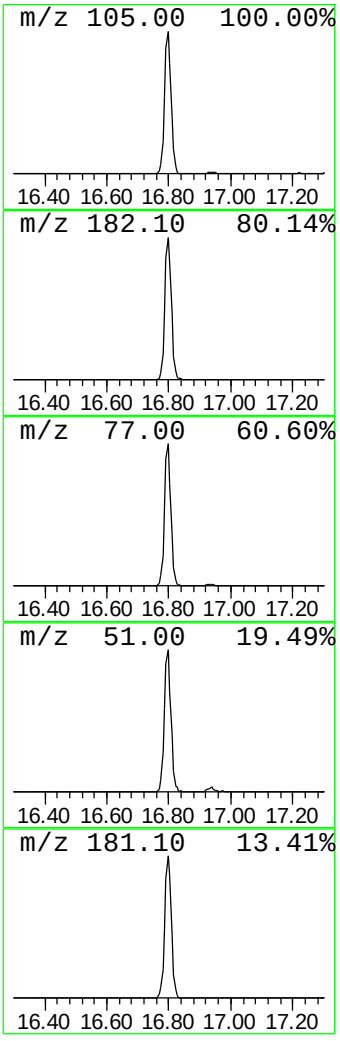
****

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	12.76 ng	416999	Acenaphthene-d10	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
3	1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	38
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	38
5	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	38





Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
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Operator : SJ/JU
Sample : I6961-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(15-17)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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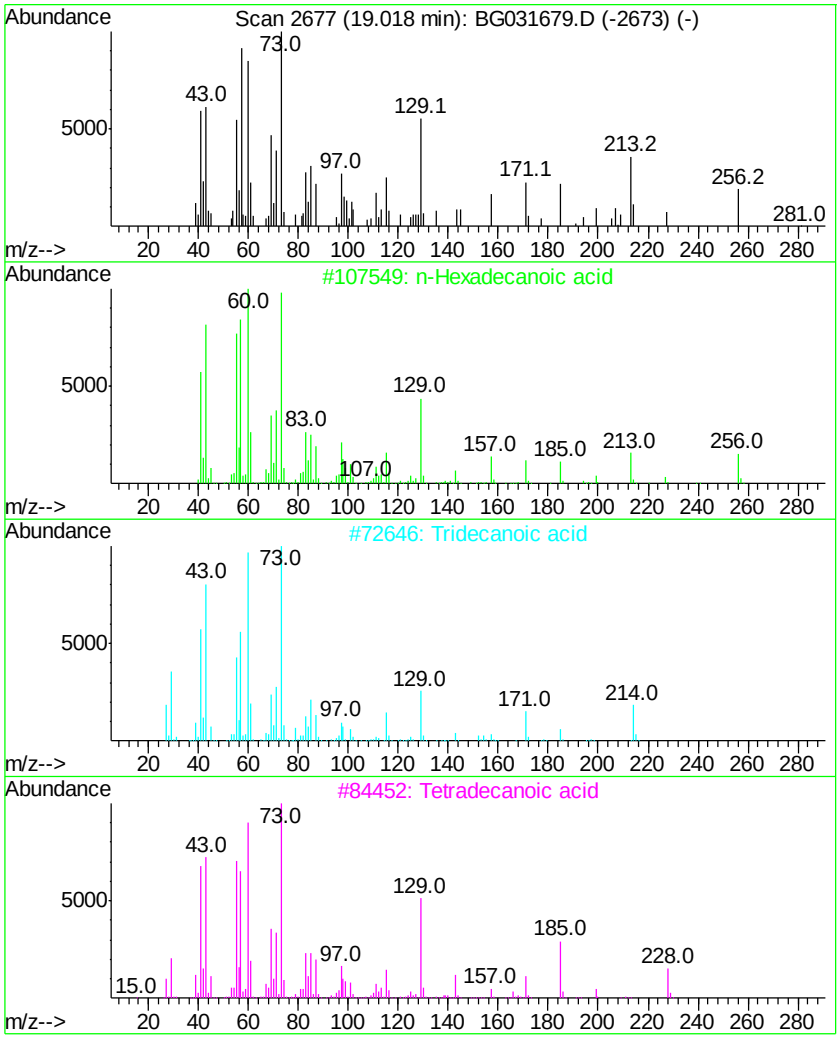
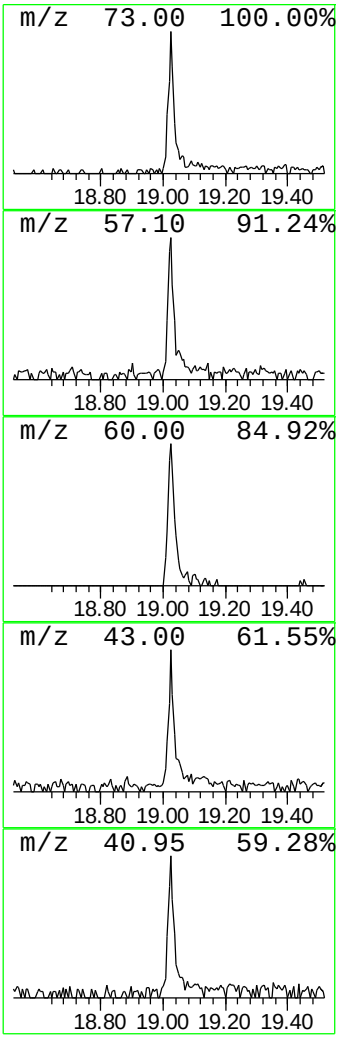
Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	2.31 ng	104631	Phenanthrene-d10	18.20

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





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Misc :
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Instrument : BNA_G
ClientSampleId : EPE-108-1(15-17)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

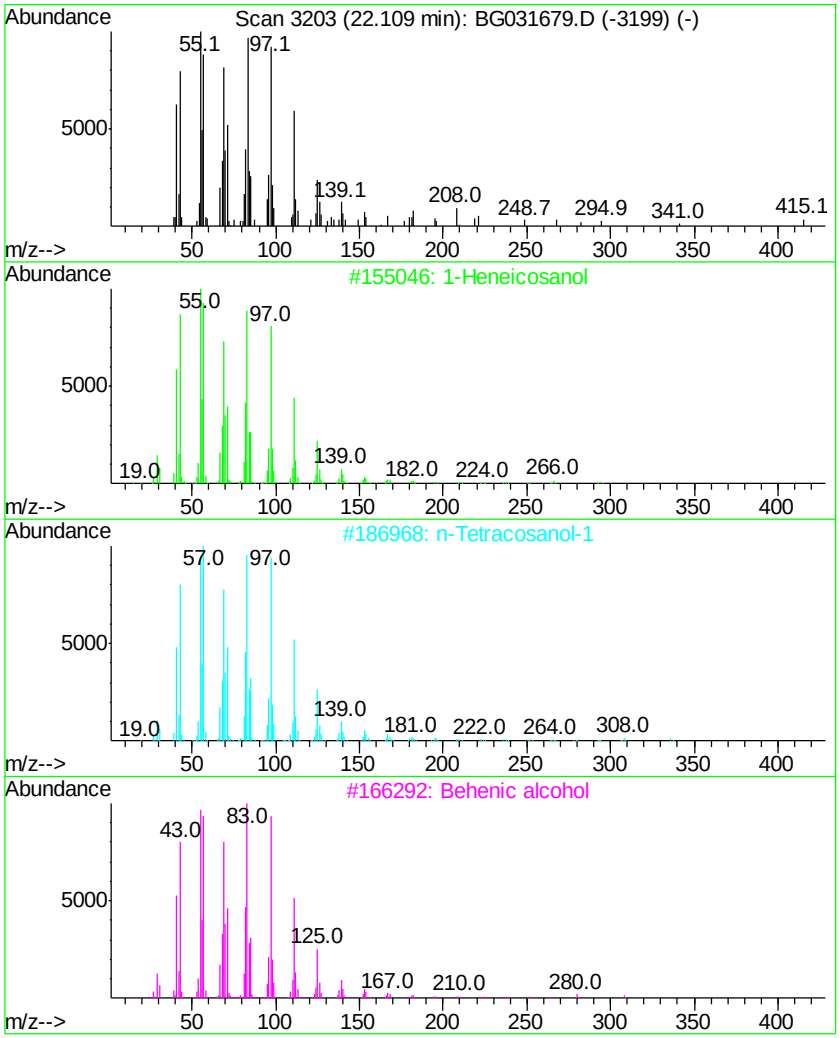
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

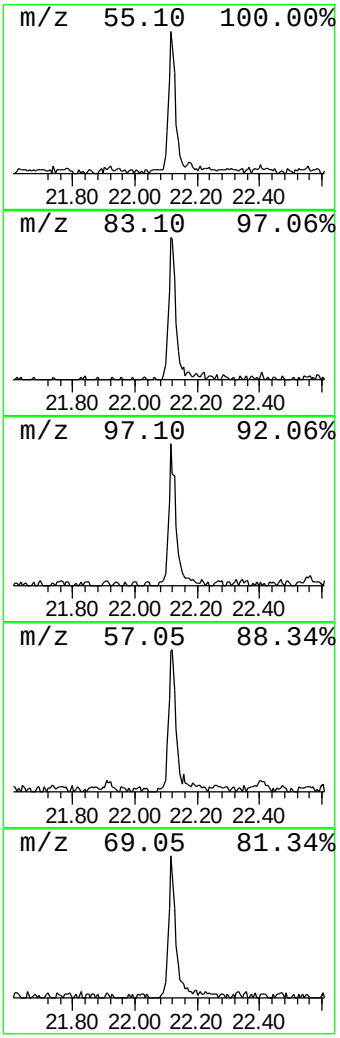
****

Peak Number 8 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	2.82 ng	167601	Chrysene-d12	22.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	1-Nonadecene	266	C19H38	018435-45-5	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.75	4.1	ng	56075	1	8.83	275337	20.0
unknown8.34	8.34	90.0	ng	1239630	1	8.83	275337	20.0
2-Hydroxy-iso-but...	12.97	3.4	ng	69180	2	11.72	402623	20.0
Benzophenone	16.80	12.8	ng	416999	3	15.46	653429	20.0
n-Hexadecanoic acid	19.02	2.3	ng	104631	4	18.20	907801	20.0
1-Heneicosanol	22.11	2.8	ng	167601	5	22.56	1187520	20.0