LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
Data File : BG031680.D
Acq On : 21 Dec 2017 19:21
Operator : SJ/JU
Sample : I6961-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(50-52)

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	3.446	22	27	36	rBV2	40846	83582	1.92%	0.382%
2	5.744	412	418	427	rBV	40459	70004	1.61%	0.320%
3	6.249	496	504	517	rBV	784179	1371847	31.59%	6.263%
4	7.929	779	790	801	rBV	805577	1538180	35.42%	7.023%
5	8.341	851	860	872	rBV	848921	1547307	35.63%	7.065%
6	8.828	936	943	953	rVB	157399	276962	6.38%	1.265%
7	9.169	991	1001	1012	rBV	636126	1158964	26.69%	5.291%
8	10.027	1139	1147	1158	rBV	435795	812765	18.72%	3.711%
9	11.719	1427	1435	1444	rBV	217446	407082	9.37%	1.859%
10	12.976	1640	1649	1660	rVB	67077	109538	2.52%	0.500%
11	14.093	1831	1839	1851	rVB	1632725	2657597	61.20%	12.134%
12	14.892	1968	1975	1982	rBV	232201	354051	8.15%	1.616%
13	15.462	2063	2072	2083	rVB3	378382	654769	15.08%	2.989%
14	16.801	2293	2300	2310	rVB	440997	676693	15.58%	3.090%
15	16.936	2316	2323	2336	rBV	1463711	2331307	53.69%	10.644%
16	18.200	2531	2538	2545	rBV2	587347	924498	21.29%	4.221%
17	19.028	2674	2679	2690	rBV3	62582	105363	2.43%	0.481%
18	20.262	2885	2889	2896	rBV4	39251	53100	1.22%	0.242%
19	20.738	2961	2970	2980	rBV	3121540	4342317	100.00%	19.826%
20	22.124	3201	3206	3212	rBV3	69954	115596	2.66%	0.528%
21	22.565	3273	3281	3290	rBV2	606414	1152633	26.54%	5.263%
22	26.366	3916	3928	3942	rVB3	353586	1158284	26.67%	5.288%

Sum of corrected areas: 21902439

LSC Report - Integrated Chromatogram

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Operator : SJ/JU
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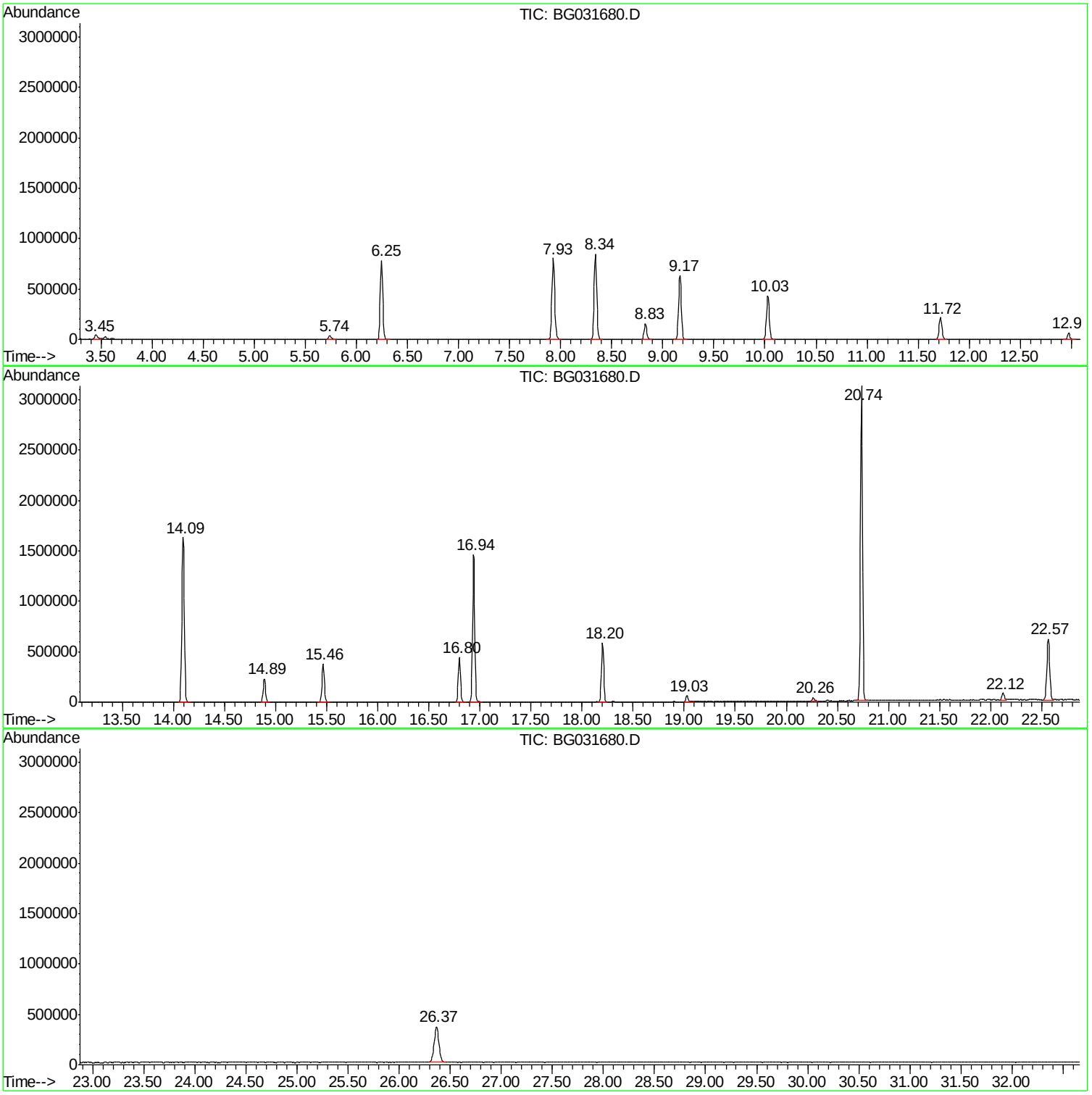
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(50-52)

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 : BG031680.D
Acq On : 21 Dec 2017 19:21
Operator : SJ/JU
Sample : I6961-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(50-52)

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

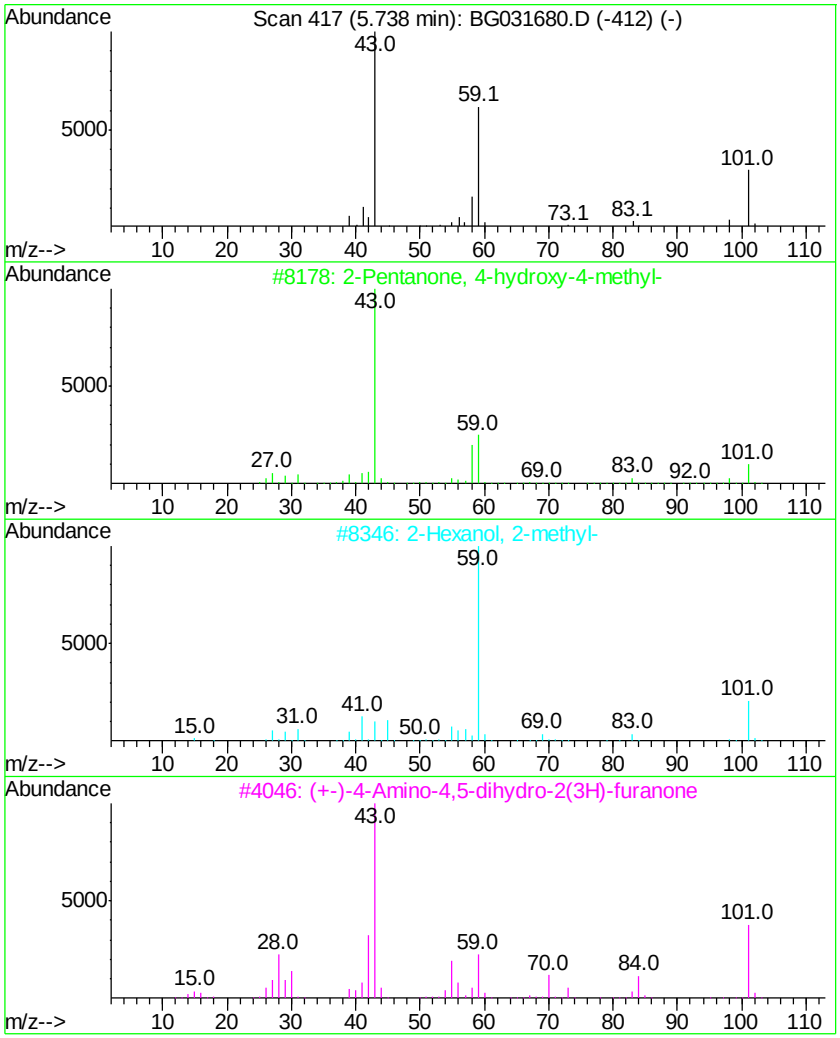
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

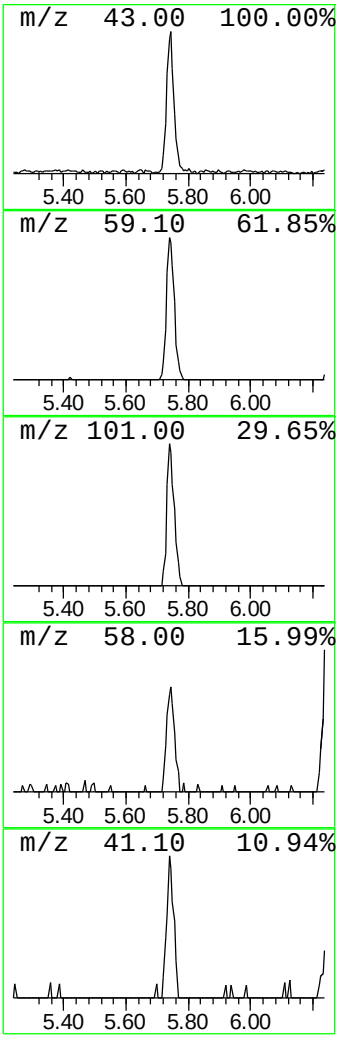
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	5.06 ng	70004	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	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28





Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
Data File : BG031680.D
Acq On : 21 Dec 2017 19:21
Operator : SJ/JU
Sample : I6961-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(50-52)

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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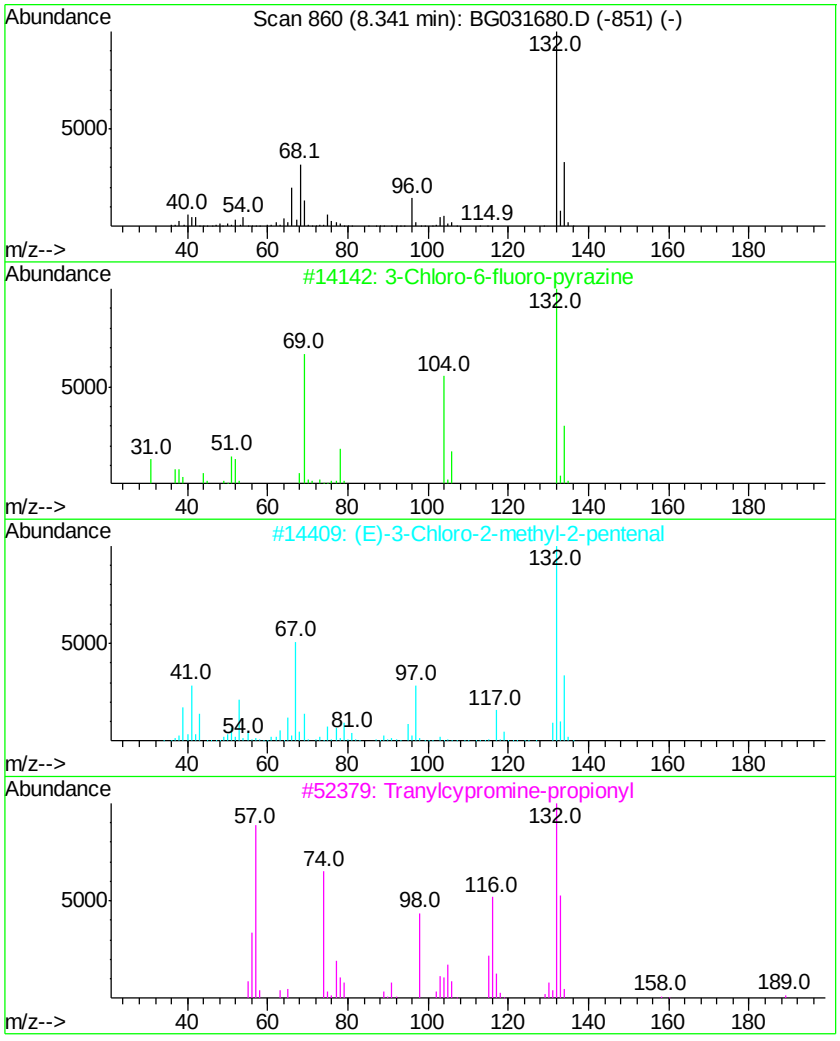
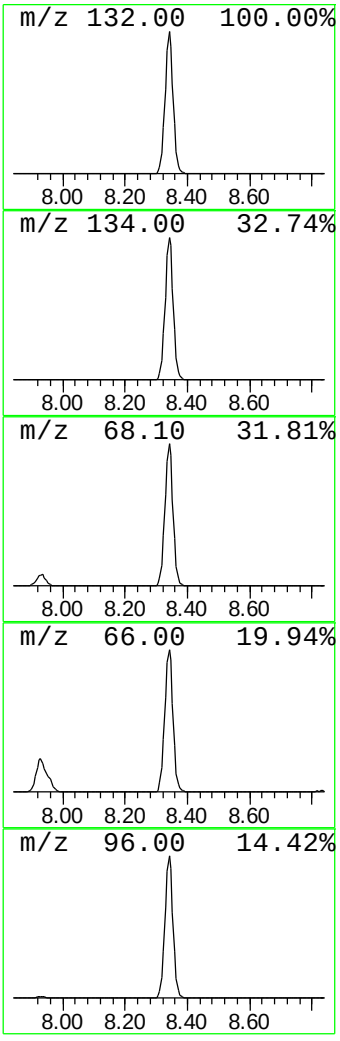
Peak Number 3 unknown8.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	111.73 ng	1547310	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
Data File : BG031680.D
Acq On : 21 Dec 2017 19:21
Operator : SJ/JU
Sample : I6961-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(50-52)

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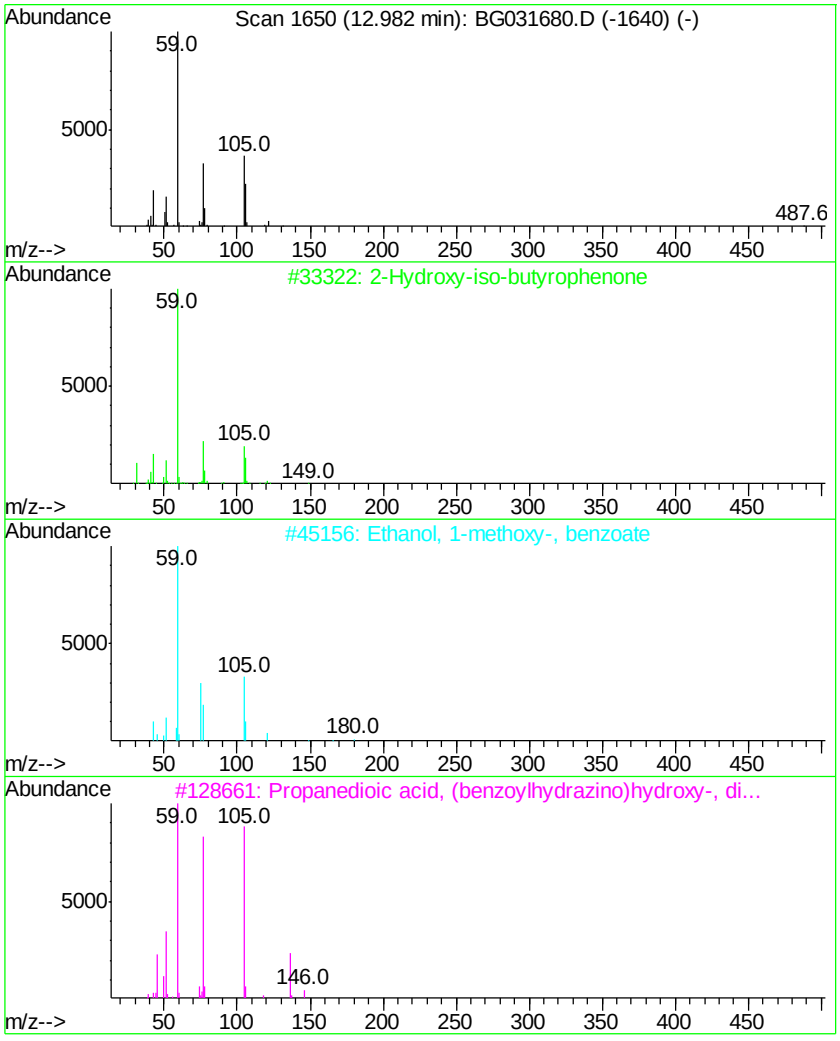
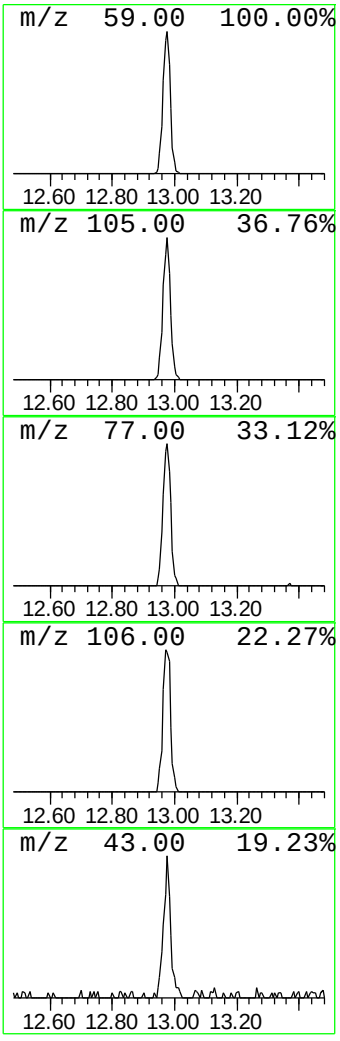
Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	5.38 ng	109538	Naphthalene-d8	11.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	74
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3	Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	25
4	Carbonic acid, 2-methoxyethyl ph...	196	C10H12O4	1000357-86-8	9
5	Guanidine	59	CH5N3	000113-00-8	7





Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
Data File : BG031680.D
Acq On : 21 Dec 2017 19:21
Operator : SJ/JU
Sample : I6961-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(50-52)

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

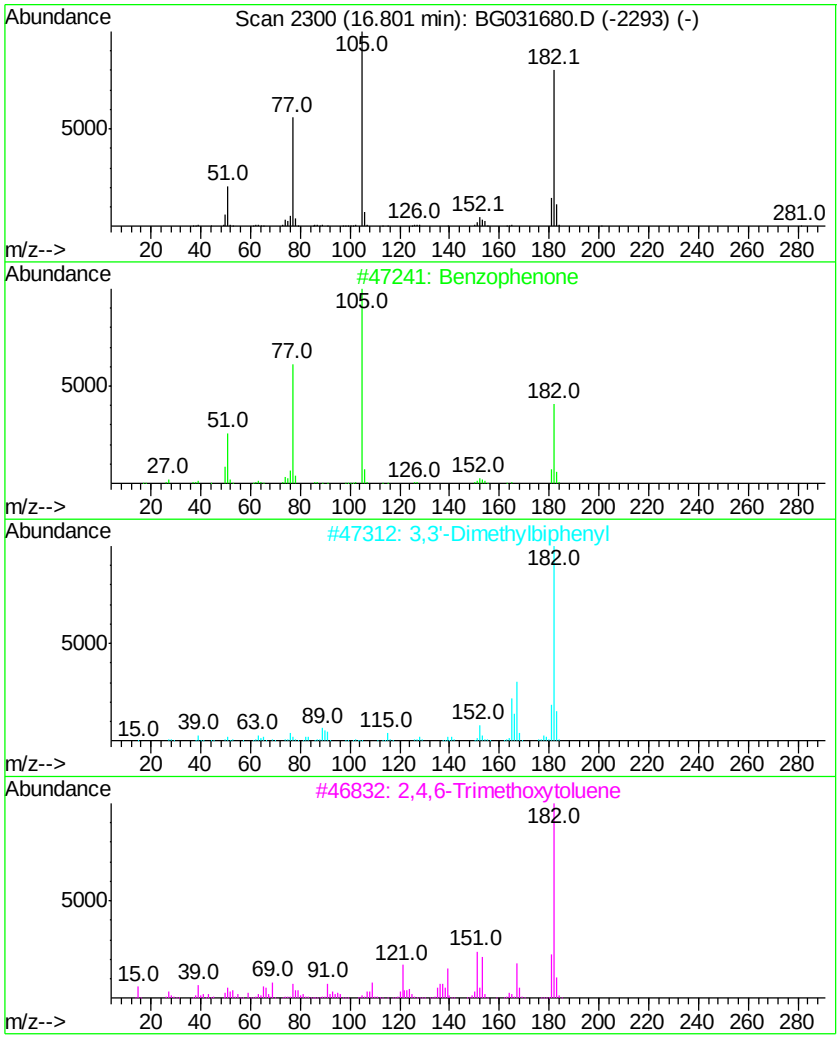
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

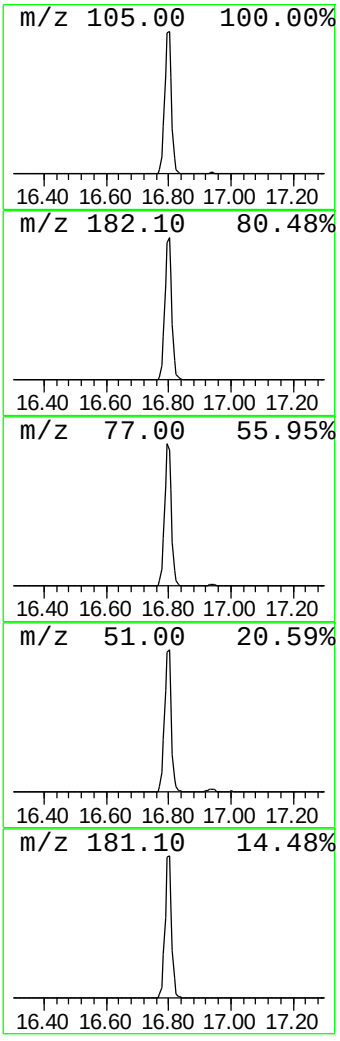
****

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	20.67 ng	676693	Acenaphthene-d10	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
3	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
4	1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	38
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122117\
Data File : BG031680.D
Acq On : 21 Dec 2017 19:21
Operator : SJ/JU
Sample : I6961-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(50-52)

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

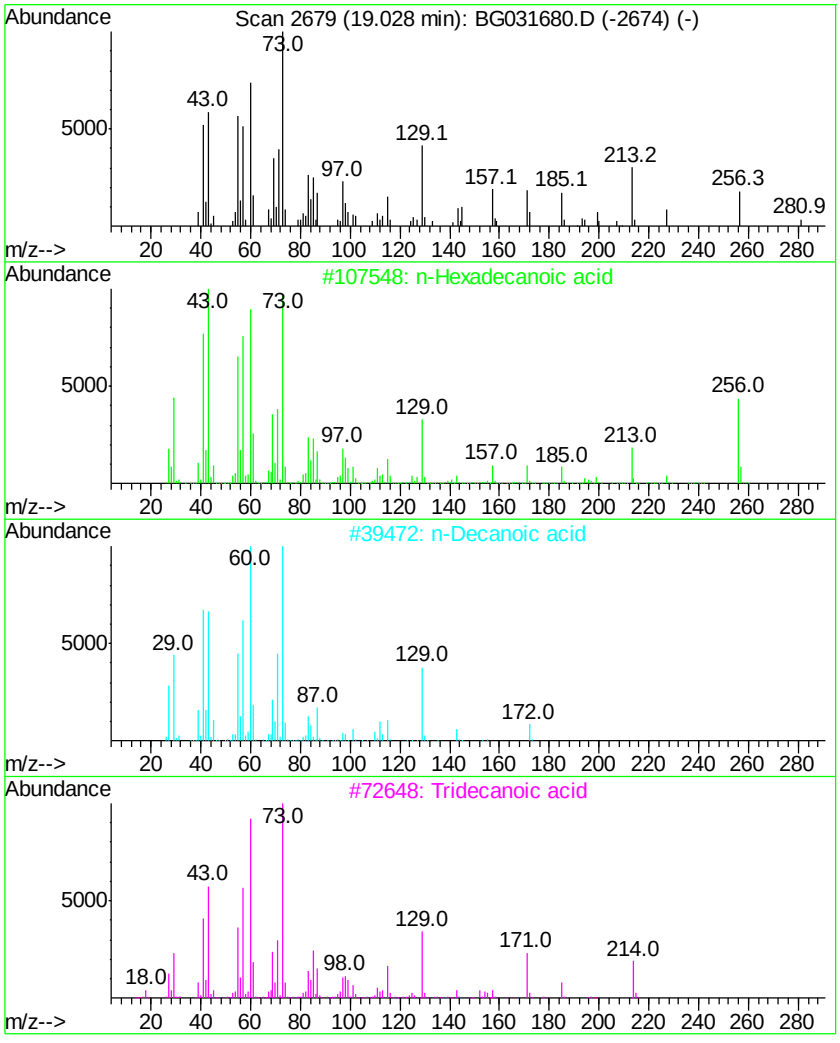
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

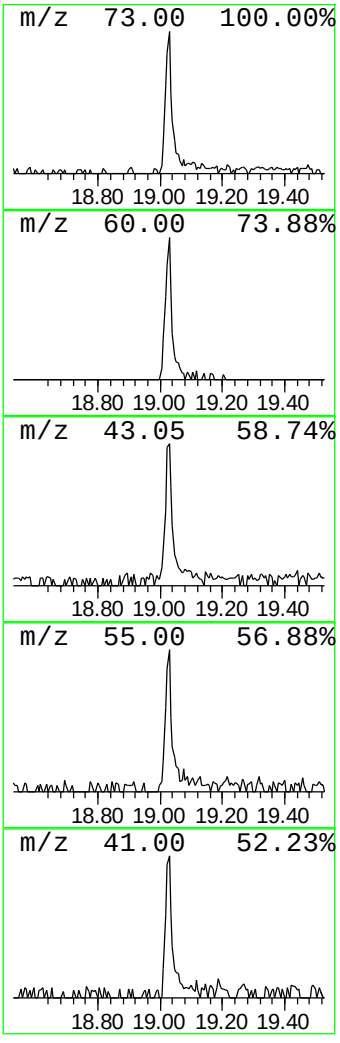
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	2.28 ng	105363	Phenanthrene-d10	18.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	n-Decanoic acid	172	C10H20O2	000334-48-5	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Dodecanoic acid	200	C12H24O2	000143-07-7	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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Sample : I6961-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EPE-108-1(50-52)

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

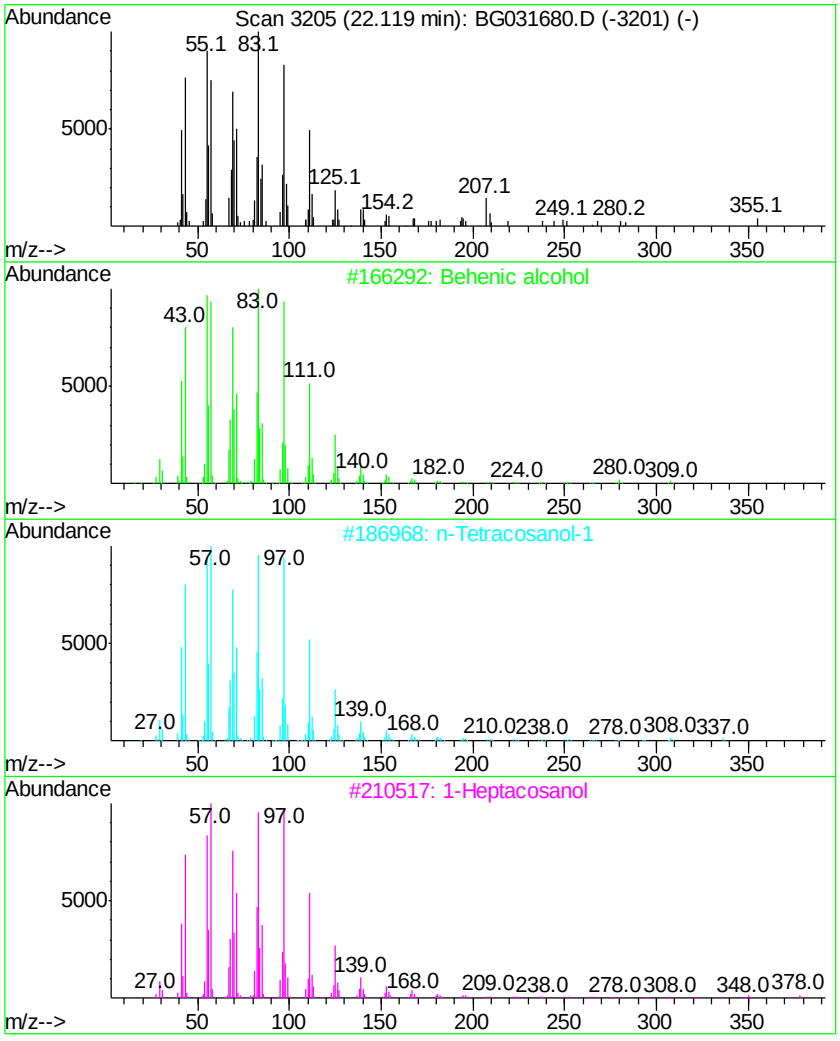
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

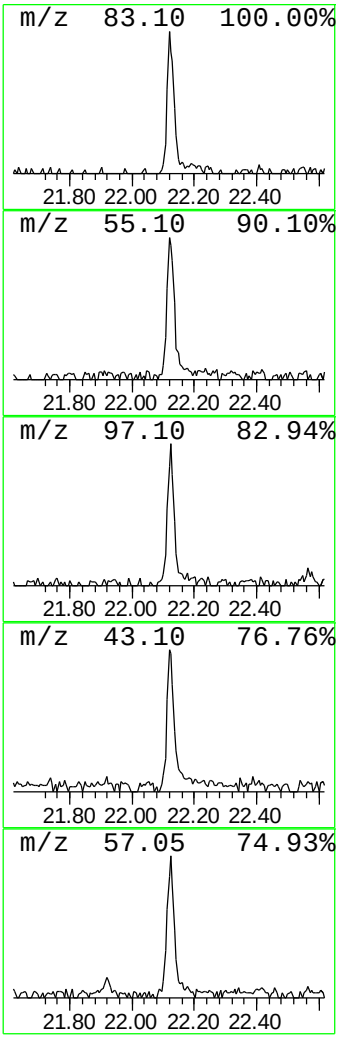
****

Peak Number 8 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.12	2.01 ng	115596	Chrysene-d12	22.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	Octacosanol	410	C28H58O	000557-61-9	90
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90





Tentatively Identified Compound (LSC) summary

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Data File : BG031680.D
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ClientSampleId : EPE-108-1(50-52)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.74	5.1	ng	70004	1	8.83	276962	20.0
unknown8.34	8.34	111.7	ng	1547310	1	8.83	276962	20.0
2-Hydroxy-iso-but...	12.98	5.4	ng	109538	2	11.72	407082	20.0
Benzophenone	16.80	20.7	ng	676693	3	15.46	654769	20.0
n-Hexadecanoic acid	19.03	2.3	ng	105363	4	18.20	924498	20.0
Behenic alcohol	22.12	2.0	ng	115596	5	22.57	1152630	20.0