LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020084.D
Acq On : 10 Dec 2015 20:33
Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

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-BG120215.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	2.990	21	26	45	rVB	1207119	1740000	100.00%	17.730%
2	3.131	45	50	55	rBV3	11904	22261	1.28%	0.227%
3	5.182	393	399	408	rVB	63320	97445	5.60%	0.993%
4	5.658	473	480	490	rBV	301272	470250	27.03%	4.792%
5	7.262	745	753	763	rBV	331041	558373	32.09%	5.689%
6	7.638	808	817	827	rBV	322379	538988	30.98%	5.492%
7	8.108	889	897	904	rVB	71485	118470	6.81%	1.207%
8	8.437	944	953	960	rBV	211968	366029	21.04%	3.730%
9	9.277	1088	1096	1102	rBV	204849	355099	20.41%	3.618%
10	10.928	1370	1377	1384	rBV	106652	182723	10.50%	1.862%
11	12.303	1602	1611	1620	rBV2	72506	129666	7.45%	1.321%
12	13.366	1782	1792	1799	rBV	506438	785162	45.12%	8.000%
13	14.183	1925	1931	1938	rBV	134777	186697	10.73%	1.902%
14	14.741	2019	2026	2033	rVB2	168005	273131	15.70%	2.783%
15	15.564	2163	2166	2171	rVB	16284	19132	1.10%	0.195%
16	16.222	2267	2278	2289	rBV	517338	750071	43.11%	7.643%
17	16.427	2309	2313	2316	rBV2	20717	27238	1.57%	0.278%
18	17.479	2486	2492	2498	rBV	231695	345431	19.85%	3.520%
19	17.843	2549	2554	2558	rBV2	13763	20447	1.18%	0.208%
20	18.354	2635	2641	2649	rBV	94307	136941	7.87%	1.395%
21	19.206	2781	2786	2793	rBV	22879	34476	1.98%	0.351%
22	19.506	2828	2837	2845	rBV2	173455	292647	16.82%	2.982%
23	19.618	2851	2856	2862	rBV2	36142	47034	2.70%	0.479%
24	19.888	2898	2902	2909	rVB2	22410	36463	2.10%	0.372%
25	20.082	2929	2935	2940	rBV	1017731	1302058	74.83%	13.267%
26	20.834	3060	3063	3072	rVB6	7994	18387	1.06%	0.187%
27	21.380	3151	3156	3161	rBV	54811	86310	4.96%	0.879%
28	21.750	3212	3219	3225	rBV	280896	464234	26.68%	4.730%
29	25.029	3767	3777	3788	rBV	150053	408962	23.50%	4.167%

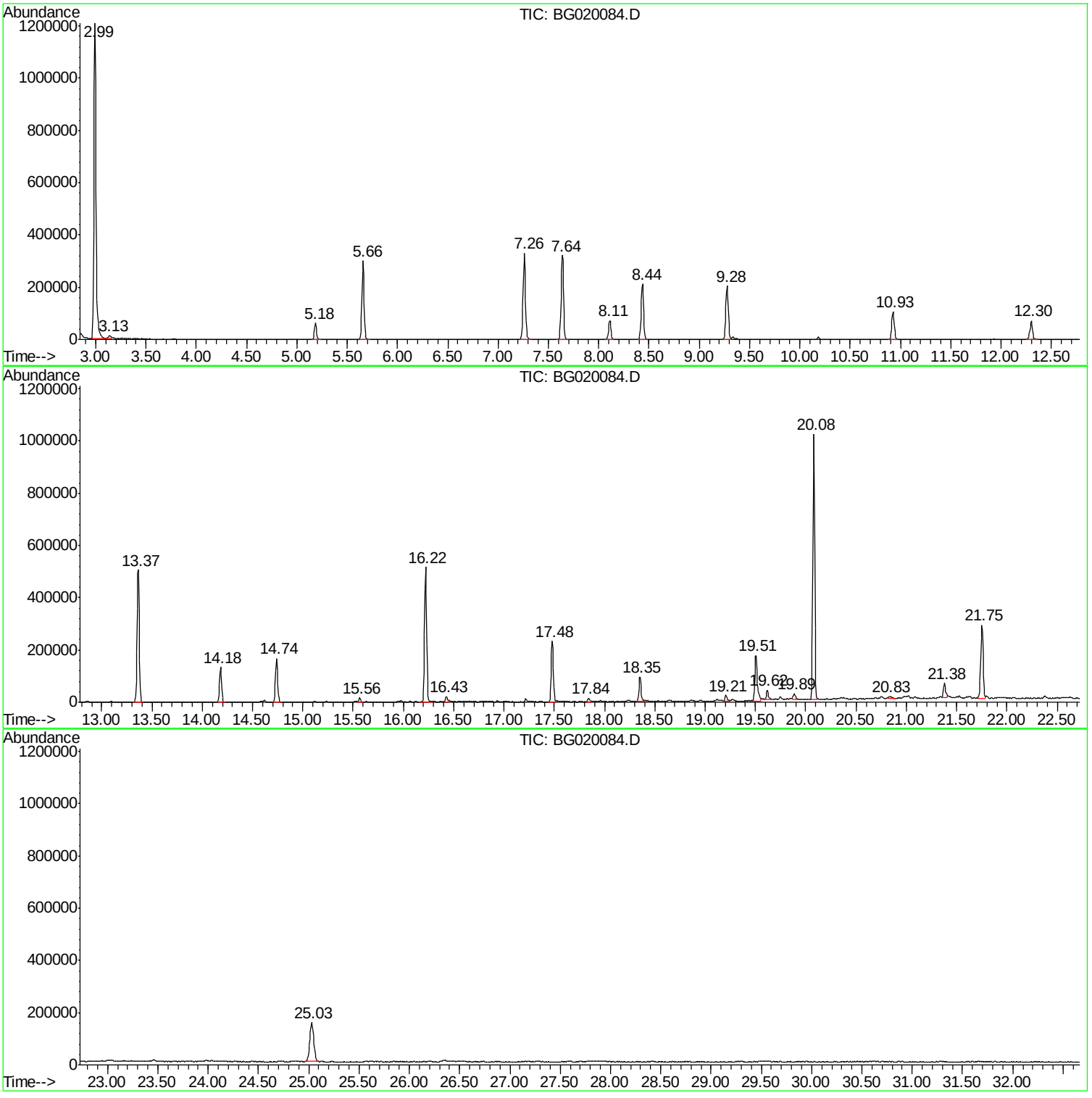
Sum of corrected areas: 9814125

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020084.D
Acq On : 10 Dec 2015 20:33
Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020084.D
Acq On : 10 Dec 2015 20:33
Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

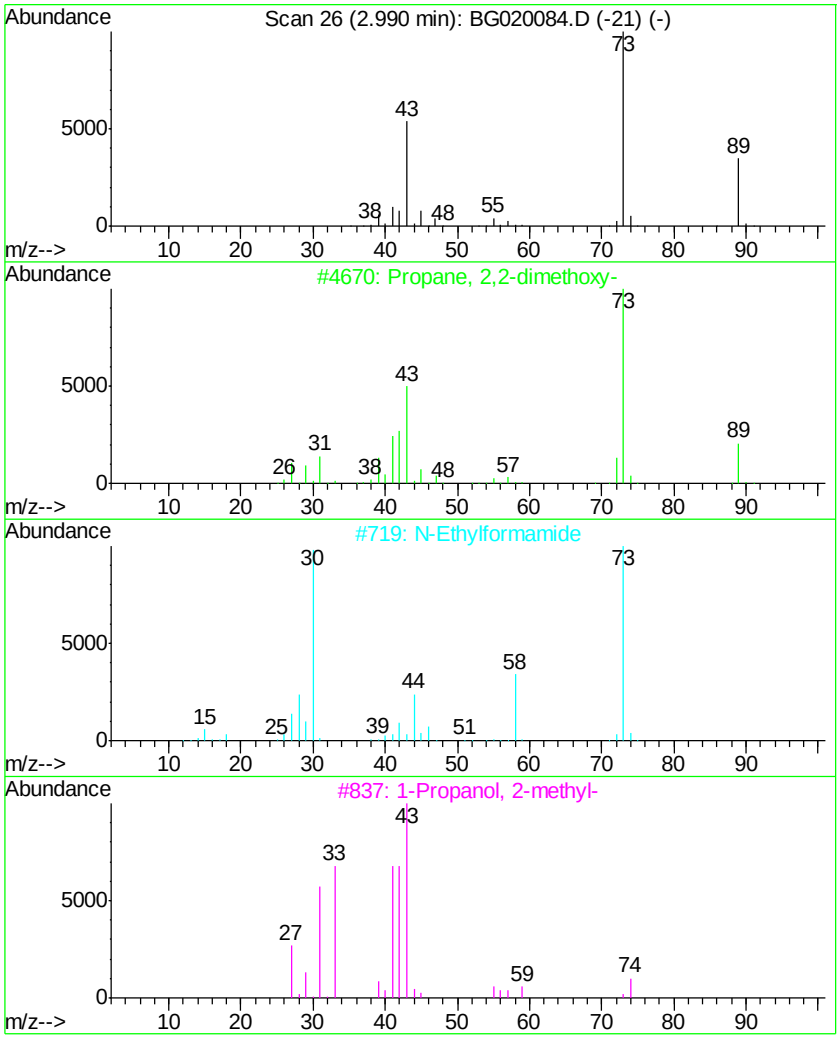
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

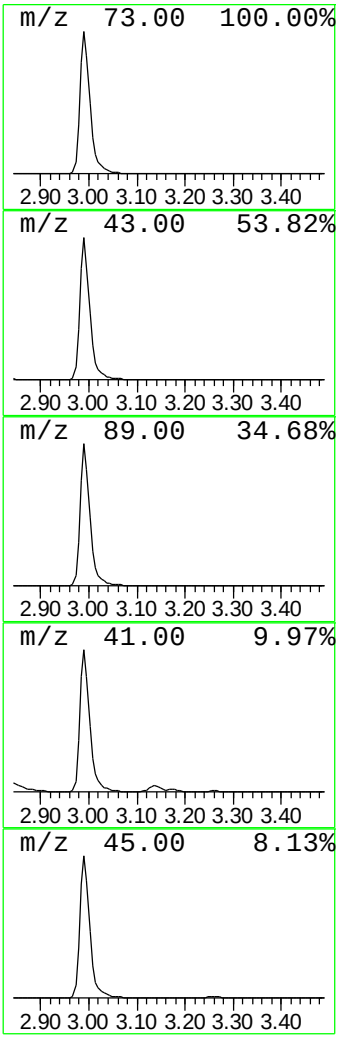
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	293.75 ng	1740000	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020084.D
Acq On : 10 Dec 2015 20:33
Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

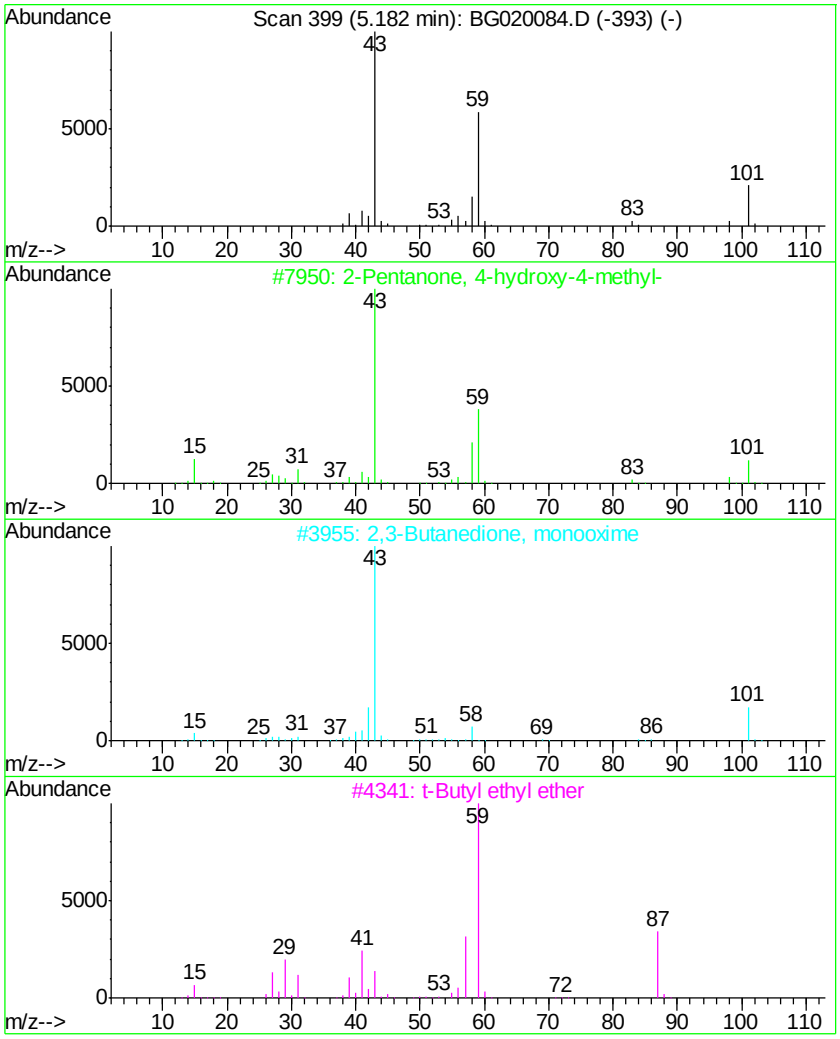
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

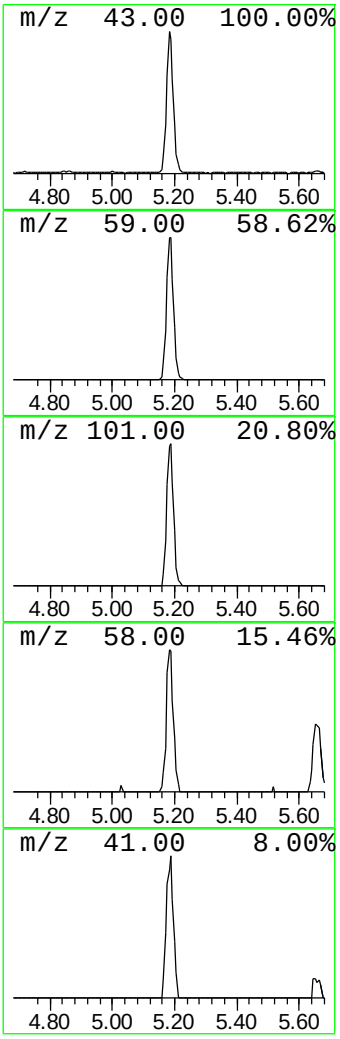
****

Peak Number 3 unknown5.18 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	16.45 ng	97445	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	t-Butyl ethyl ether	102	C6H14O	1000118-18-4	17
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17





Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020084.D
Acq On : 10 Dec 2015 20:33
Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

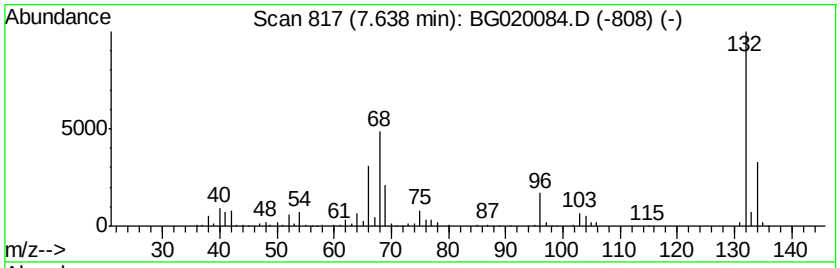
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

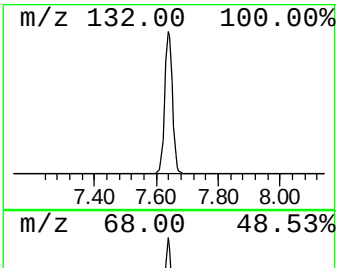
****

Peak Number 4 unknown7.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	90.99 ng	538988	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020084.D
Acq On : 10 Dec 2015 20:33
Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

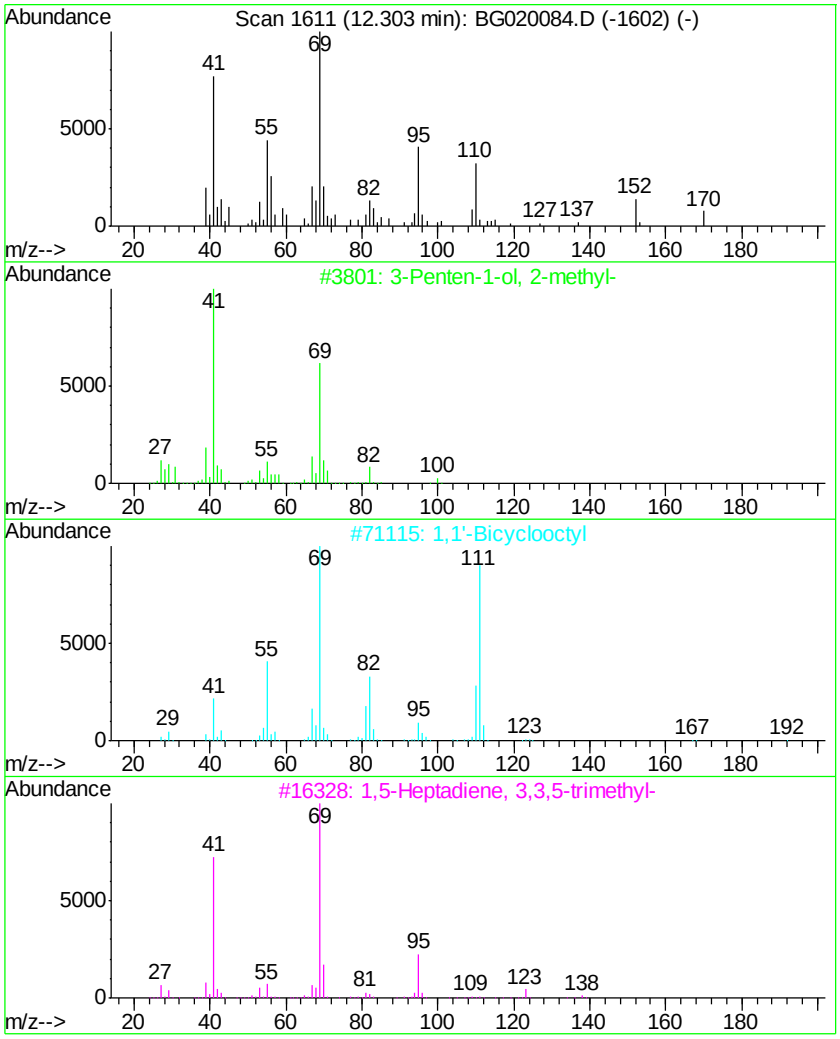
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

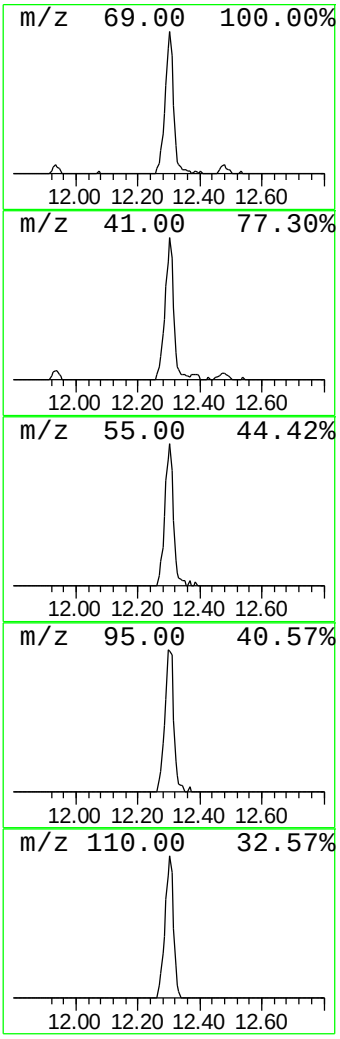
****

Peak Number 6 unknown12.30 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	14.19 ng	129666	Naphthalene-d8	10.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-1-ol, 2-methyl-	100	C6H12O	062238-37-3	49
2	1,1'-Bicyclooctyl	222	C16H30	006708-17-4	47
3	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	47
4	Cyclopentane, 1-butyl-2-ethyl-	154	C11H22	072993-32-9	38
5	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	37





Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020084.D
Acq On : 10 Dec 2015 20:33
Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

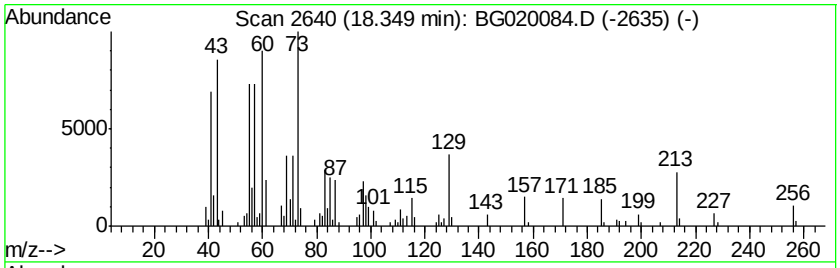
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

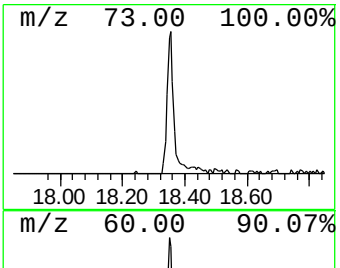
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	7.93 ng	136941	Phenanthrene-d10	17.48

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	76
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121115\
Data File : BG020084.D
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Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

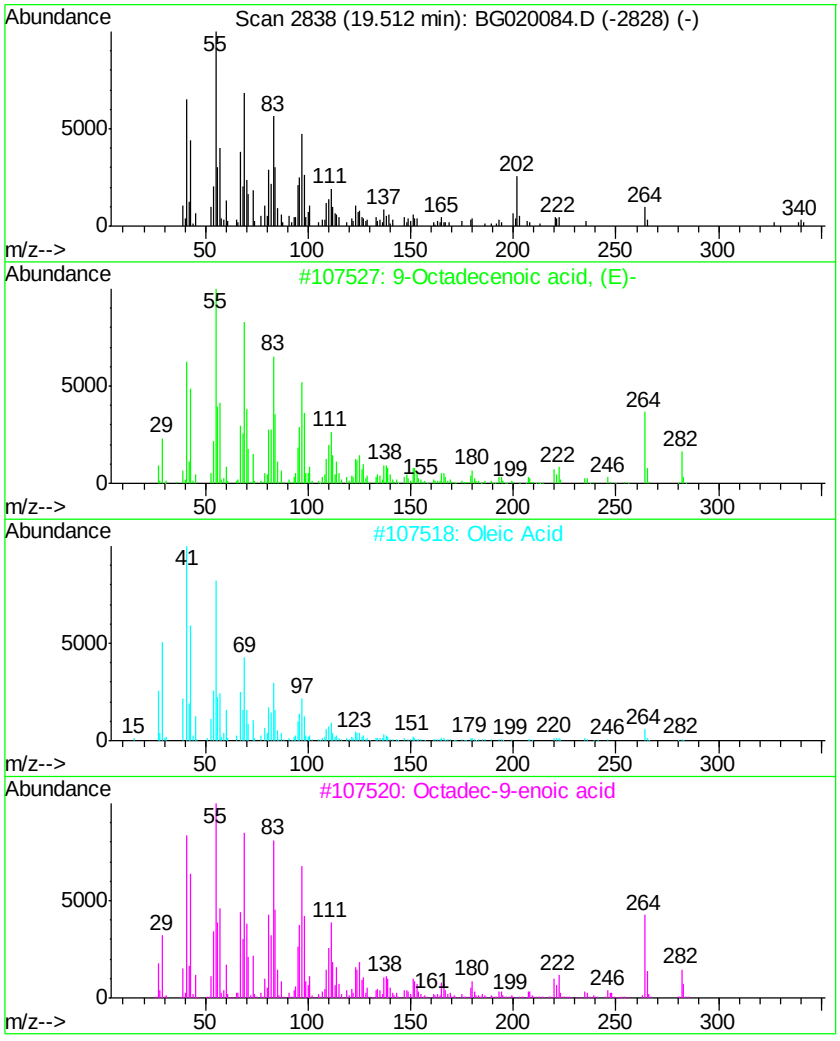
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

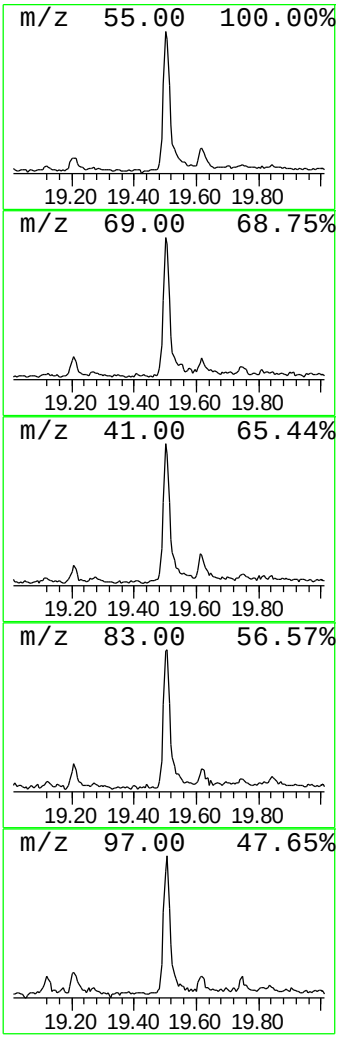
****

Peak Number 8 9-Octadecenoic acid, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.51	16.94 ng	292647	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	95
2	Oleic Acid	282	C18H34O2	000112-80-1	92
3	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	91
4	7-Heptadecene, 1-chloro-	272	C17H33Cl	056554-78-0	58
5	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	55





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Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

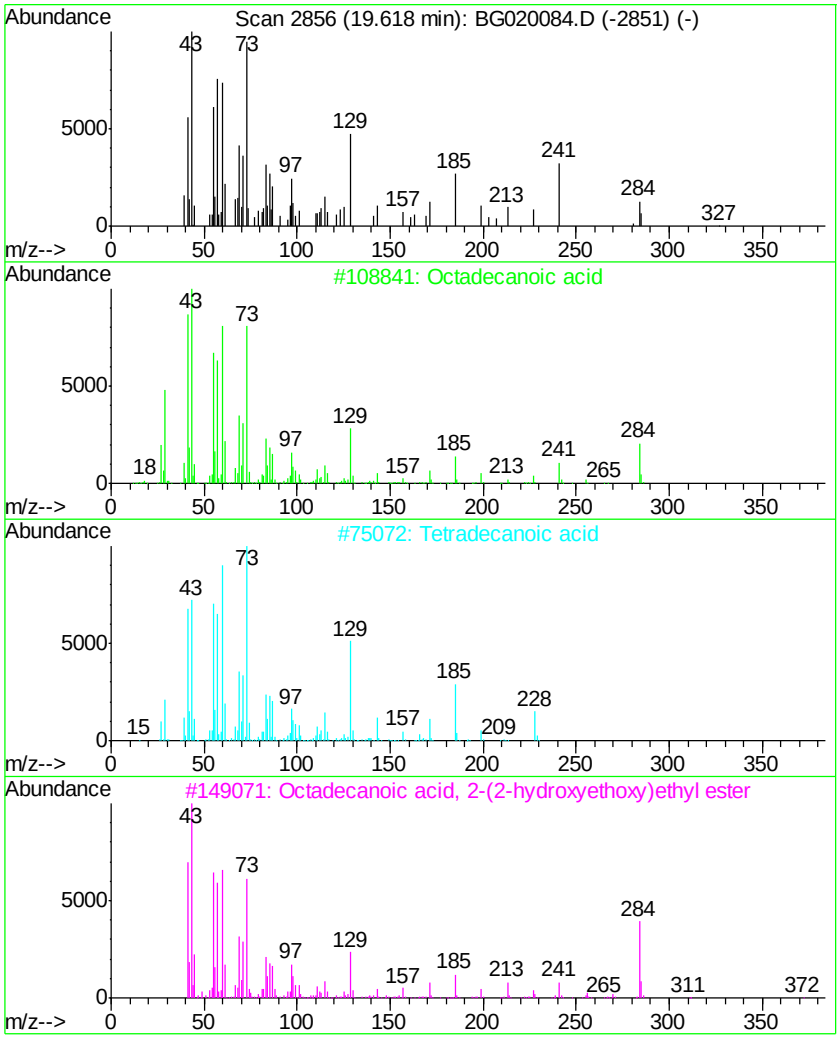
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

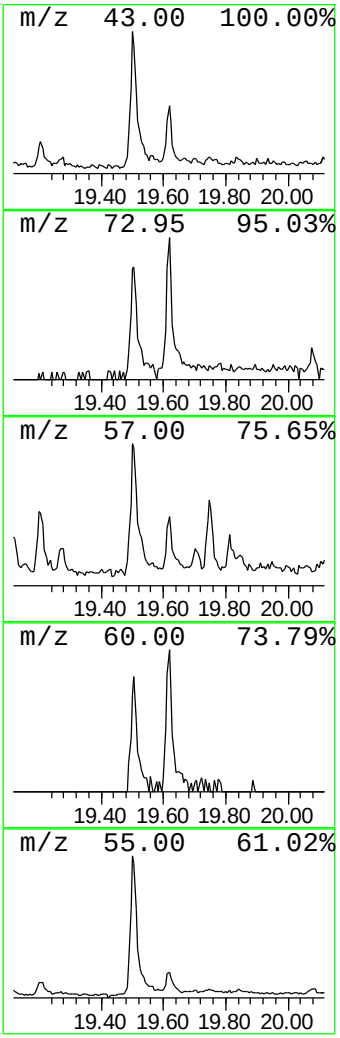
****

Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.03 ng	47034	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	50
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

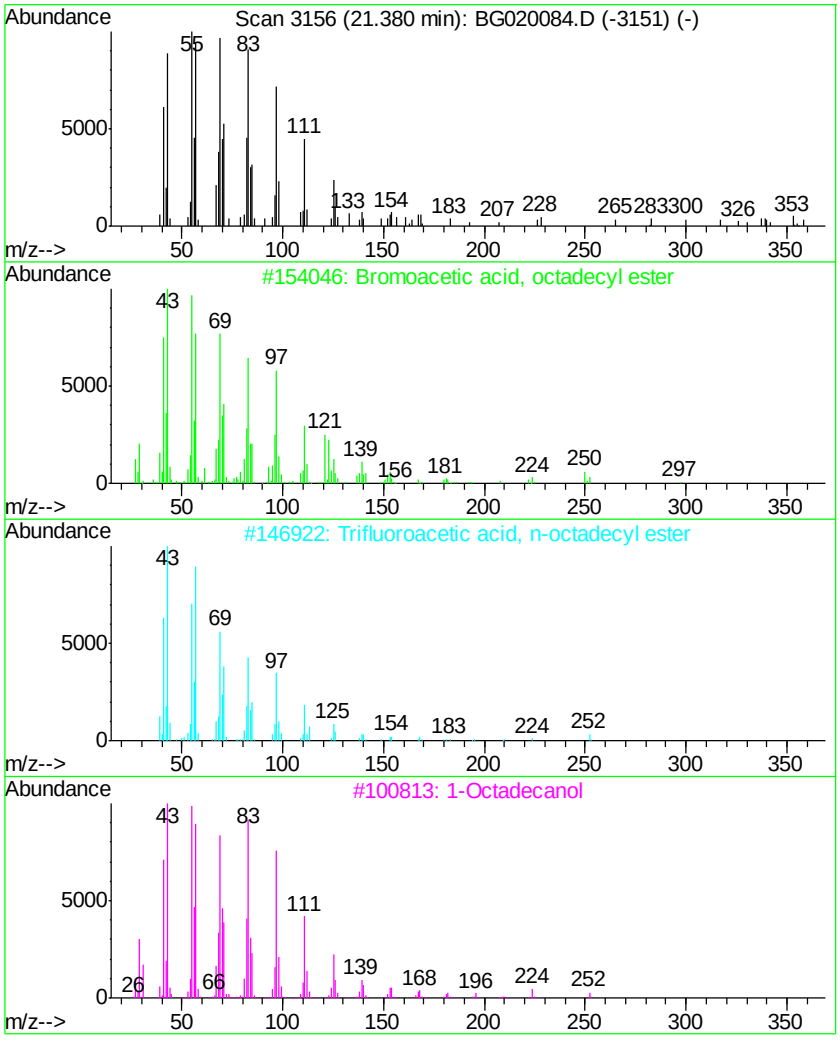
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

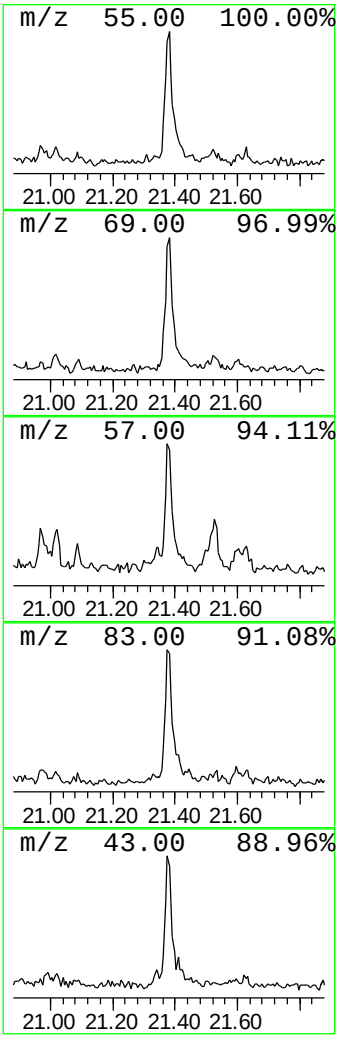
****

Peak Number 10 Bromoacetic acid, octadecyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	3.72 ng	86310	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3	1-Octadecanol	270	C18H38O	000112-92-5	91
4	1-Nonadecanol	284	C19H40O	001454-84-8	91
5	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG121115\
Data File : BG020084.D
Acq On : 10 Dec 2015 20:33
Operator : UM/SJ
Sample : G4683-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S11-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2,2-dime...	2.99	293.8	ng	1740000	1	8.11	118470	20.0
unknown5.18	5.18	16.4	ng	97445	1	8.11	118470	20.0
unknown7.64	7.64	91.0	ng	538988	1	8.11	118470	20.0
unknown12.30	12.30	14.2	ng	129666	2	10.93	182723	20.0
n-Hexadecanoic acid	18.35	7.9	ng	136941	4	17.48	345431	20.0
9-Octadecenoic ac...	19.51	16.9	ng	292647	4	17.48	345431	20.0
Octadecanoic acid	19.62	2.0	ng	47034	5	21.75	464234	20.0
Bromoacetic acid,...	21.38	3.7	ng	86310	5	21.75	464234	20.0