LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028889.D
Acq On : 23 Sep 2017 00:38
Operator : SJ/JU
Sample : I5301-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170609-COMP-A

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-BG091217.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	5.379	300	305	312	rBV	29319	45045	1.13%	0.315%
2	5.844	378	384	397	rBV	280865	490890	12.30%	3.438%
3	7.430	647	654	665	rBV	192778	368685	9.24%	2.582%
4	7.812	711	719	732	rBV	475553	859187	21.52%	6.017%
5	8.276	792	798	804	rBV2	94342	165117	4.14%	1.156%
6	8.605	845	854	863	rBV	412476	765348	19.17%	5.360%
7	9.445	988	997	1010	rBV	339240	660451	16.54%	4.625%
8	11.096	1270	1278	1290	rBV	120589	227490	5.70%	1.593%
9	13.511	1680	1689	1700	rBV	1055165	1693752	42.43%	11.861%
10	14.892	1918	1924	1936	rVB2	217891	360060	9.02%	2.521%
11	15.280	1977	1990	1997	rBV2	58848	87724	2.20%	0.614%
12	15.656	2050	2054	2058	rBV	118652	148253	3.71%	1.038%
13	16.384	2170	2178	2190	rBV	1217802	1903052	47.67%	13.327%
14	17.642	2385	2392	2402	rBV	386976	593216	14.86%	4.154%
15	18.288	2493	2502	2510	rBV2	142666	209506	5.25%	1.467%
16	19.886	2767	2774	2782	rBV	131680	171479	4.30%	1.201%
17	20.233	2826	2833	2840	rBV	2956418	3992223	100.00%	27.957%
18	21.960	3121	3127	3136	rVB	442441	774346	19.40%	5.423%
19	25.415	3704	3715	3727	rVB	243294	763992	19.14%	5.350%

Sum of corrected areas: 14279816

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Data File : BG028889.D
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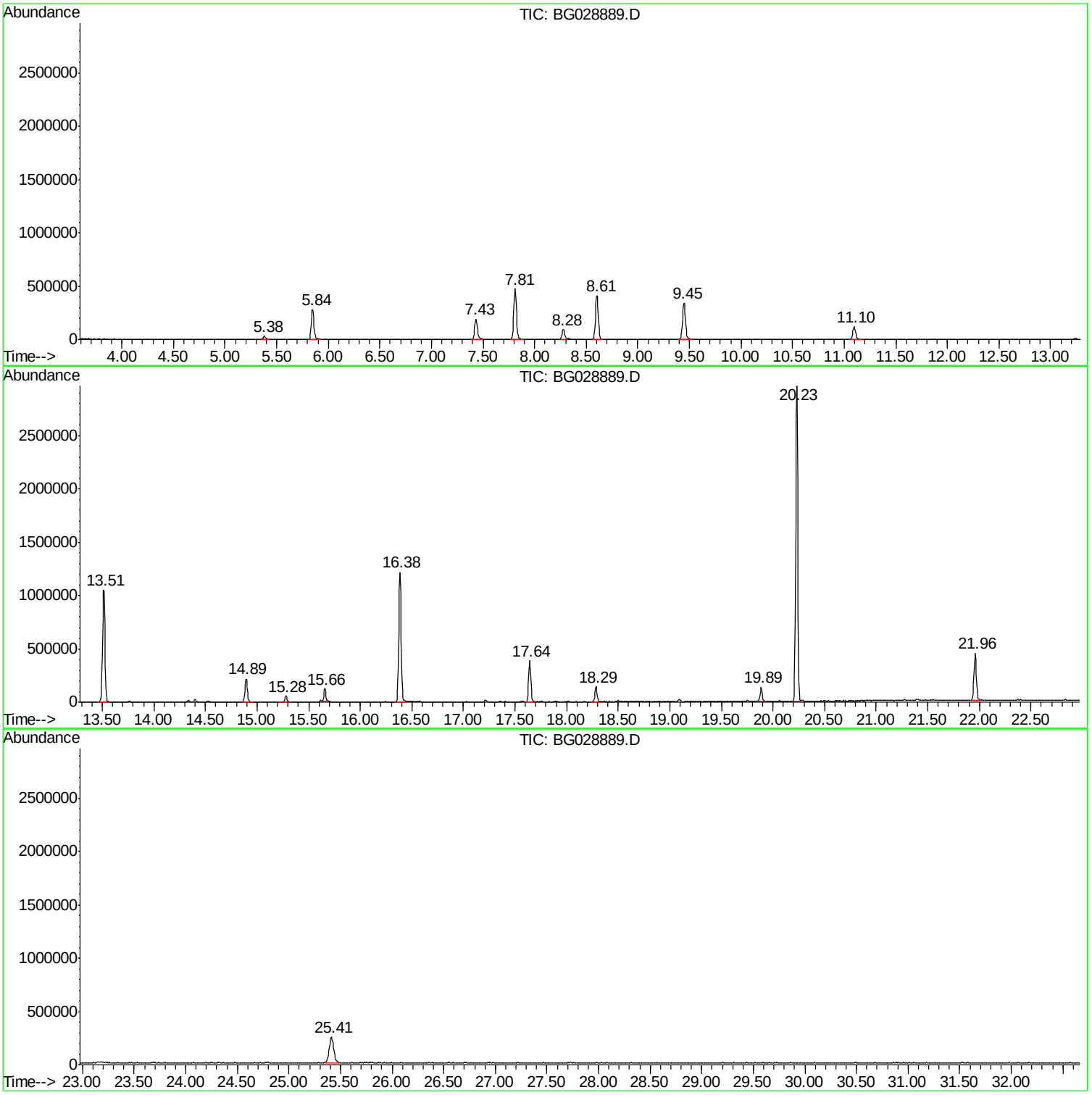
Sample : I5301-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20170609-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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Data File : BG028889.D
Acq On : 23 Sep 2017 00:38
Operator : SJ/JU
Sample : I5301-13
Misc :
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Instrument : BNA_G
ClientSampleId : 20170609-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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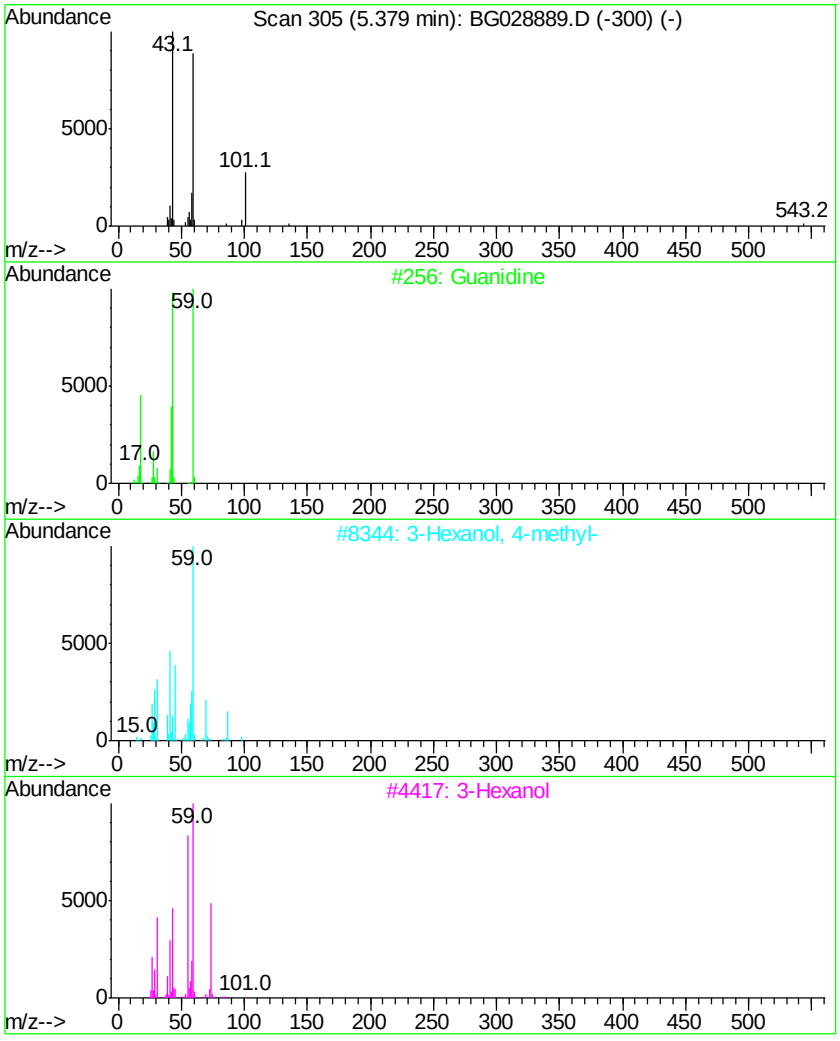
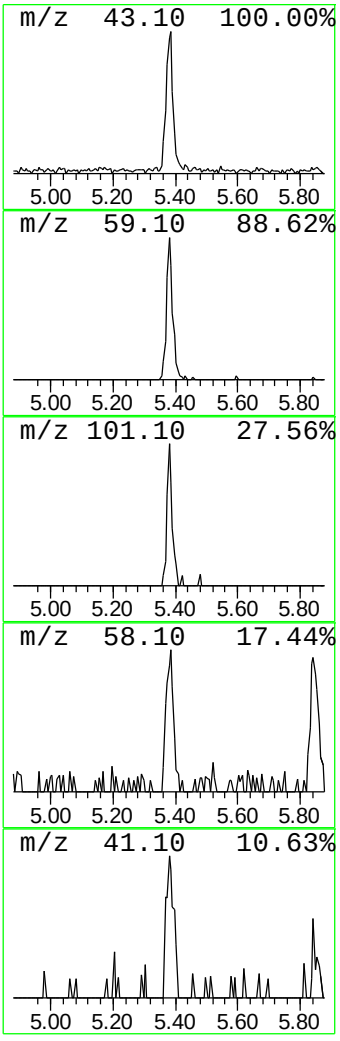
Peak Number 1 Guanidine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	5.46 ng	45045	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine	59	CH5N3	000113-00-8	53
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	36
3	3-Hexanol	102	C6H14O	000623-37-0	36
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	28
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	28





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028889.D
Acq On : 23 Sep 2017 00:38
Operator : SJ/JU
Sample : I5301-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170609-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

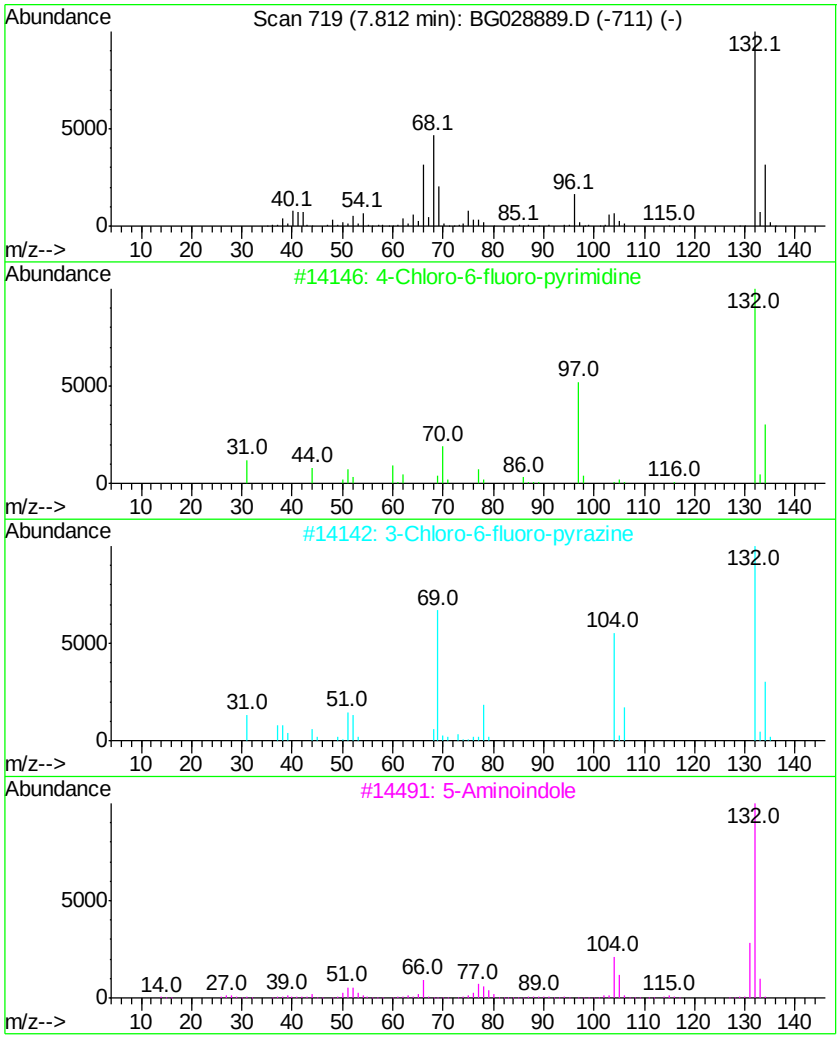
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

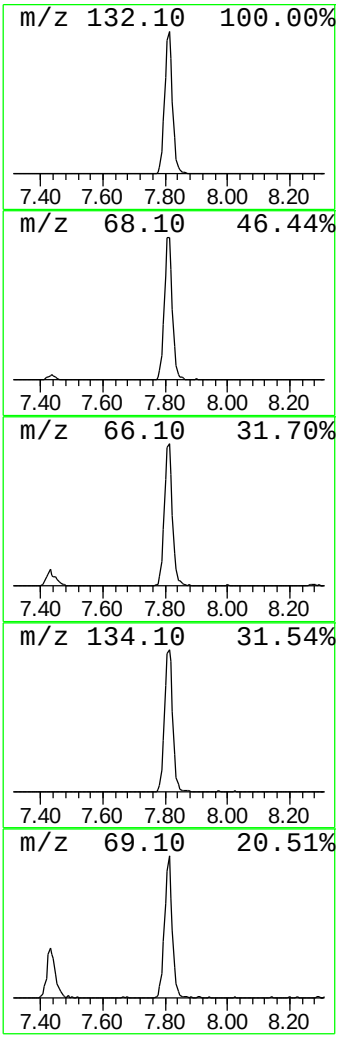
****

Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	104.07 ng	859187	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
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Acq On : 23 Sep 2017 00:38
Operator : SJ/JU
Sample : I5301-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170609-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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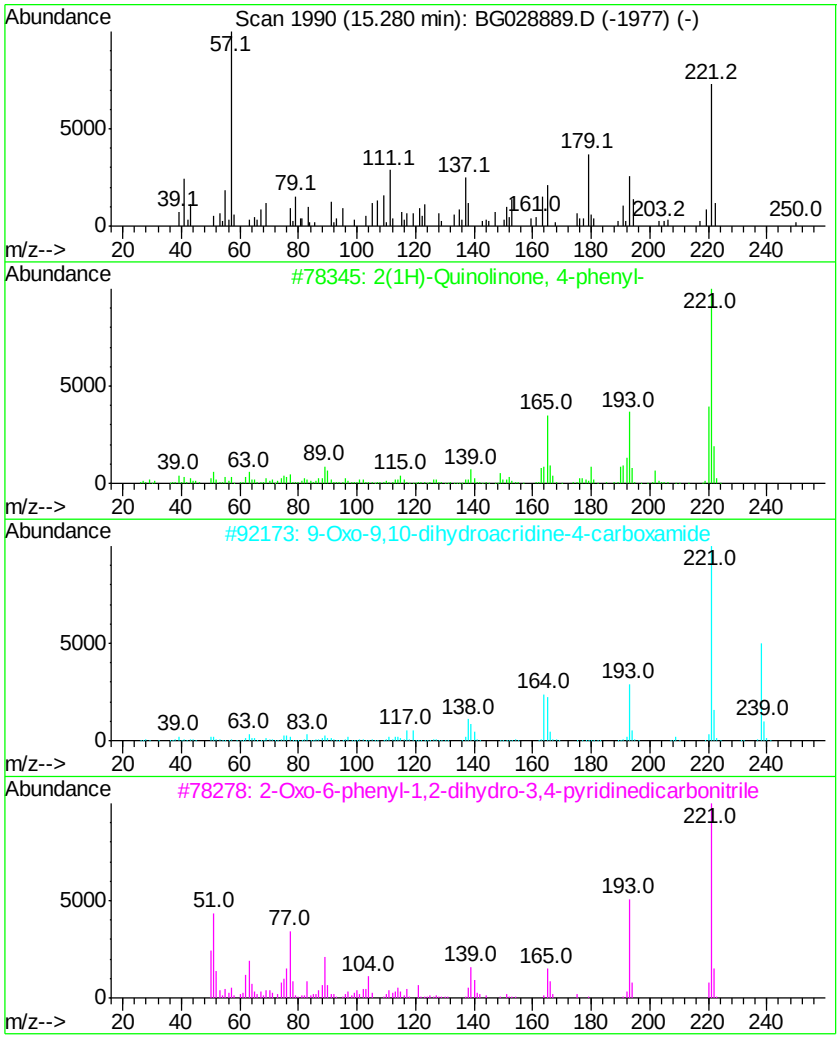
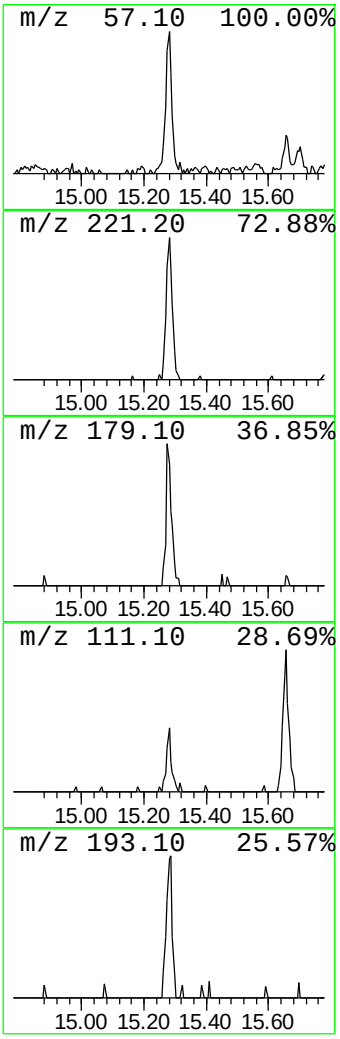
Peak Number 4 unknown15.28 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	4.87 ng	87724	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	49
2	9-Oxo-9,10-dihydroacridine-4-car...	238	C14H10N2O2	037760-72-8	38
3	2-Oxo-6-phenyl-1,2-dihydro-3,4-p...	221	C13H7N3O	1000327-01-8	35
4	2-Oxa-1,3-disilacyclohexane, 1,1...	236	C12H20OSi2	1000308-85-9	35
5	1H-1,2,3-Triazole, 4,5-diphenyl-	221	C14H11N3	005533-73-3	30





Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
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Sample : I5301-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170609-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

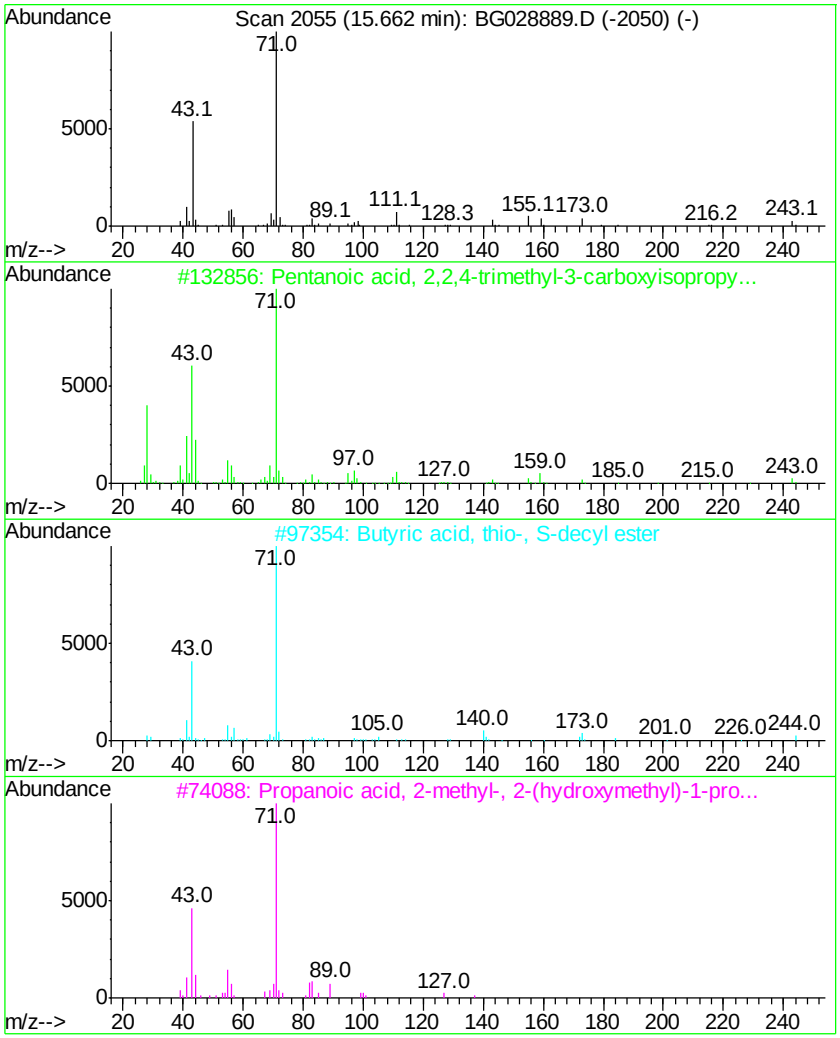
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

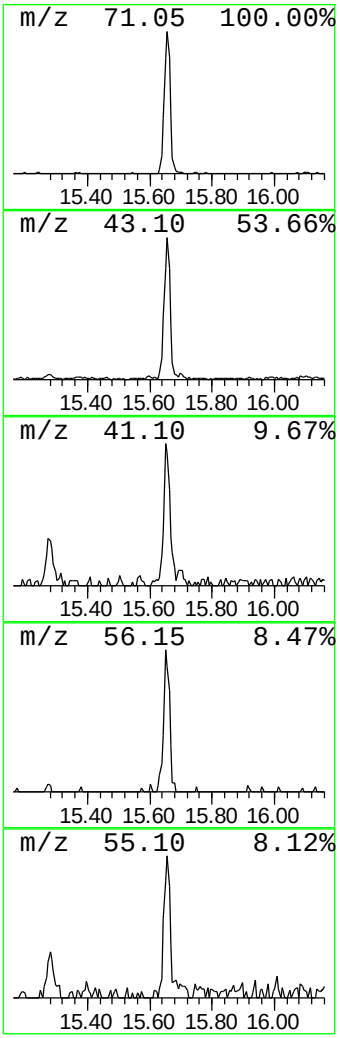
****

Peak Number 5 Pentanoic acid, 2,2,4-trime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	8.23 ng	148253	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	64
2	Butyric acid, thio-, S-decyl ester	244	C14H28OS	002432-55-5	59
3	Propanoic acid, 2-methyl-, 2-(hy...	216	C12H24O3	074367-32-1	53
4	Fumaric acid, nonyl tetrahydrofu...	326	C18H30O5	1000330-58-3	53
5	Propanoic acid, 2-methyl-, 1,2,3...	302	C15H26O6	014295-64-8	53





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Data File : BG028889.D
Acq On : 23 Sep 2017 00:38
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Sample : I5301-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170609-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

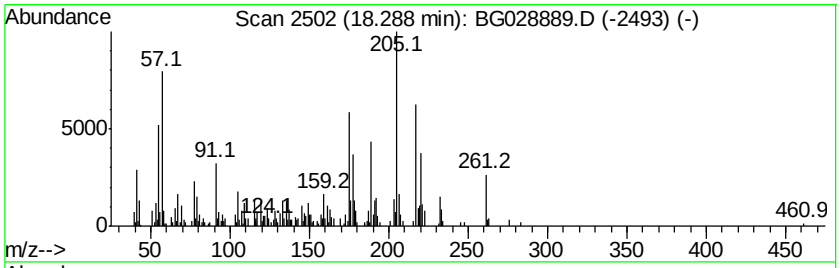
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

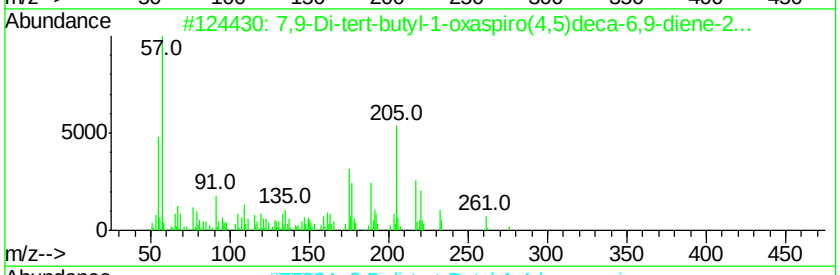
****

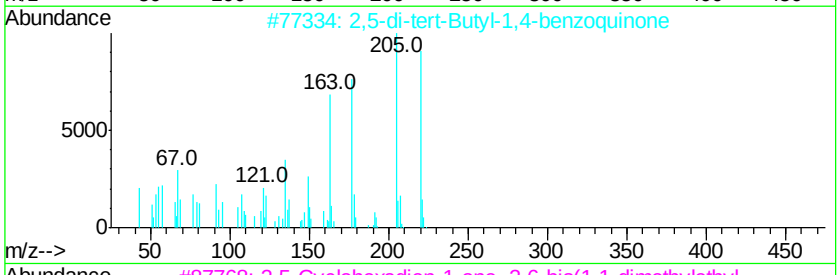
Peak Number 6 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 4

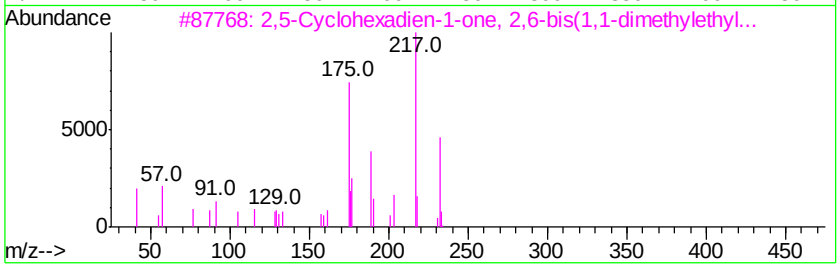
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	7.06 ng	209506	Phenanthrene-d10	17.64

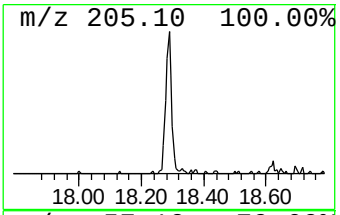
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
2	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	53
3	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	42
4	Thiophene, 2-(4-nitrophenyl)-	205	C10H7NO2S	059156-21-7	38
5	2,6-Bis(1,1-dimethylethyl)-4-met...	262	C18H30O	004278-82-4	30

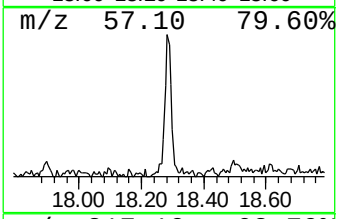


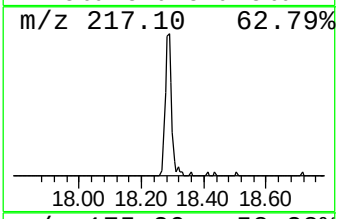


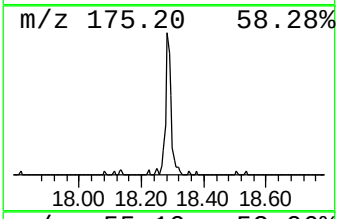


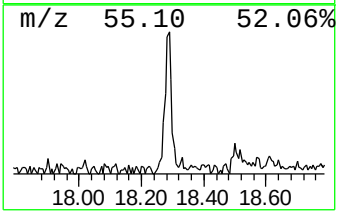












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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

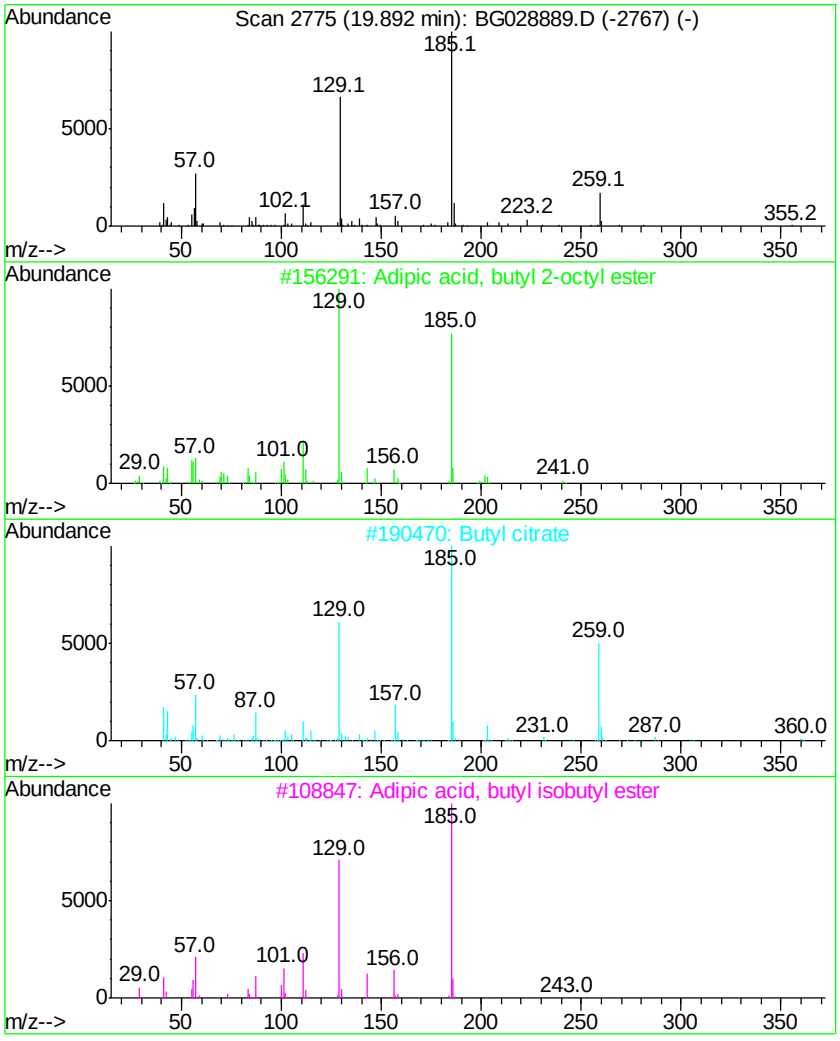
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

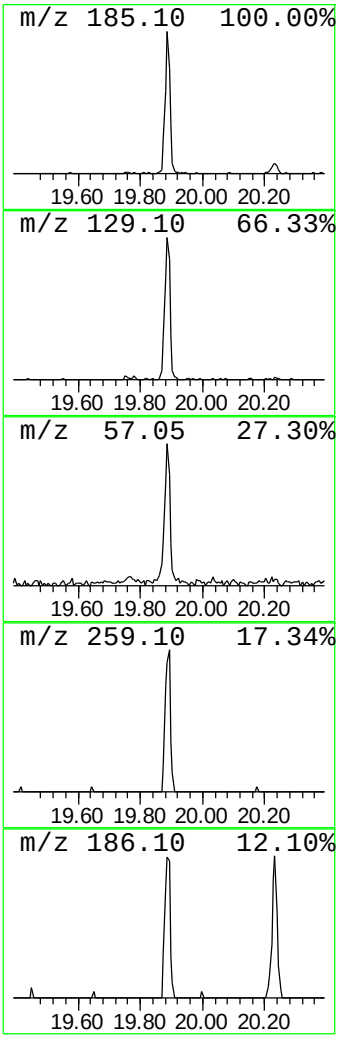
****

Peak Number 7 Adipic acid, butyl 2-octyl ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	4.43 ng	171479	Chrysene-d12	21.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, butyl 2-octyl ester	314	C18H34O4	1000324-44-6	64
2	Butyl citrate	360	C18H32O7	000077-94-1	64
3	Adipic acid, butyl isobutyl ester	258	C14H26O4	1000324-09-3	64
4	Adipic acid, isobutyl 3-pentyl e...	272	C15H28O4	1000324-60-4	50
5	Adipic acid, butyl 3-hexyl ester	286	C16H30O4	1000353-62-3	50





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Guanidine	5.38	5.5	ng	45045	1	8.28	165117	20.0
unknown7.81	7.81	104.1	ng	859187	1	8.28	165117	20.0
unknown15.28	15.28	4.9	ng	87724	3	14.89	360060	20.0
Pentanoic acid, 2...	15.66	8.2	ng	148253	3	14.89	360060	20.0
7,9-Di-tert-butyl...	18.29	7.1	ng	209506	4	17.64	593216	20.0
Adipic acid, buty...	19.89	4.4	ng	171479	5	21.96	774346	20.0