LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092317\
Data File : BG028894.D
Acq On : 23 Sep 2017 12:19
Operator : SJ/JU
Sample : I5321-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170530-LOC-6

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	5.380	300	305	311	rBV2	26943	44786	1.21%	0.316%
2	5.844	377	384	396	rBV	239935	424231	11.44%	2.990%
3	7.430	646	654	665	rBV2	168102	332112	8.96%	2.341%
4	7.806	711	718	728	rBV	434914	788414	21.26%	5.558%
5	8.276	791	798	804	rBV2	91860	162652	4.39%	1.147%
6	8.599	846	853	861	rVB	412251	719573	19.41%	5.072%
7	9.445	990	997	1013	rBV	340914	638207	17.21%	4.499%
8	11.091	1270	1277	1285	rBV	119028	236216	6.37%	1.665%
9	13.511	1679	1689	1697	rBV	1123056	1751532	47.23%	12.347%
10	14.399	1835	1840	1848	rVB3	39554	54112	1.46%	0.381%
11	14.892	1918	1924	1932	rBV2	237406	393968	10.62%	2.777%
12	15.280	1983	1990	2000	rBV2	106899	155348	4.19%	1.095%
13	15.656	2049	2054	2059	rBV	229962	299454	8.08%	2.111%
14	16.384	2170	2178	2192	rBV	1213667	1876999	50.62%	13.231%
15	17.642	2386	2392	2398	rBV2	408034	628320	16.94%	4.429%
16	18.288	2493	2502	2510	rVB3	90817	137164	3.70%	0.967%
17	19.886	2764	2774	2779	rBV3	123767	188224	5.08%	1.327%
18	20.233	2826	2833	2840	rBV	2756891	3708136	100.00%	26.139%
19	21.390	3024	3030	3039	rBV4	28633	72939	1.97%	0.514%
20	21.960	3120	3127	3136	rVB2	429425	761876	20.55%	5.371%
21	23.159	3326	3331	3339	rBV10	20053	48363	1.30%	0.341%
22	25.409	3698	3714	3726	rBV2	238609	763402	20.59%	5.381%

Sum of corrected areas: 14186028

LSC Report - Integrated Chromatogram

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Misc :
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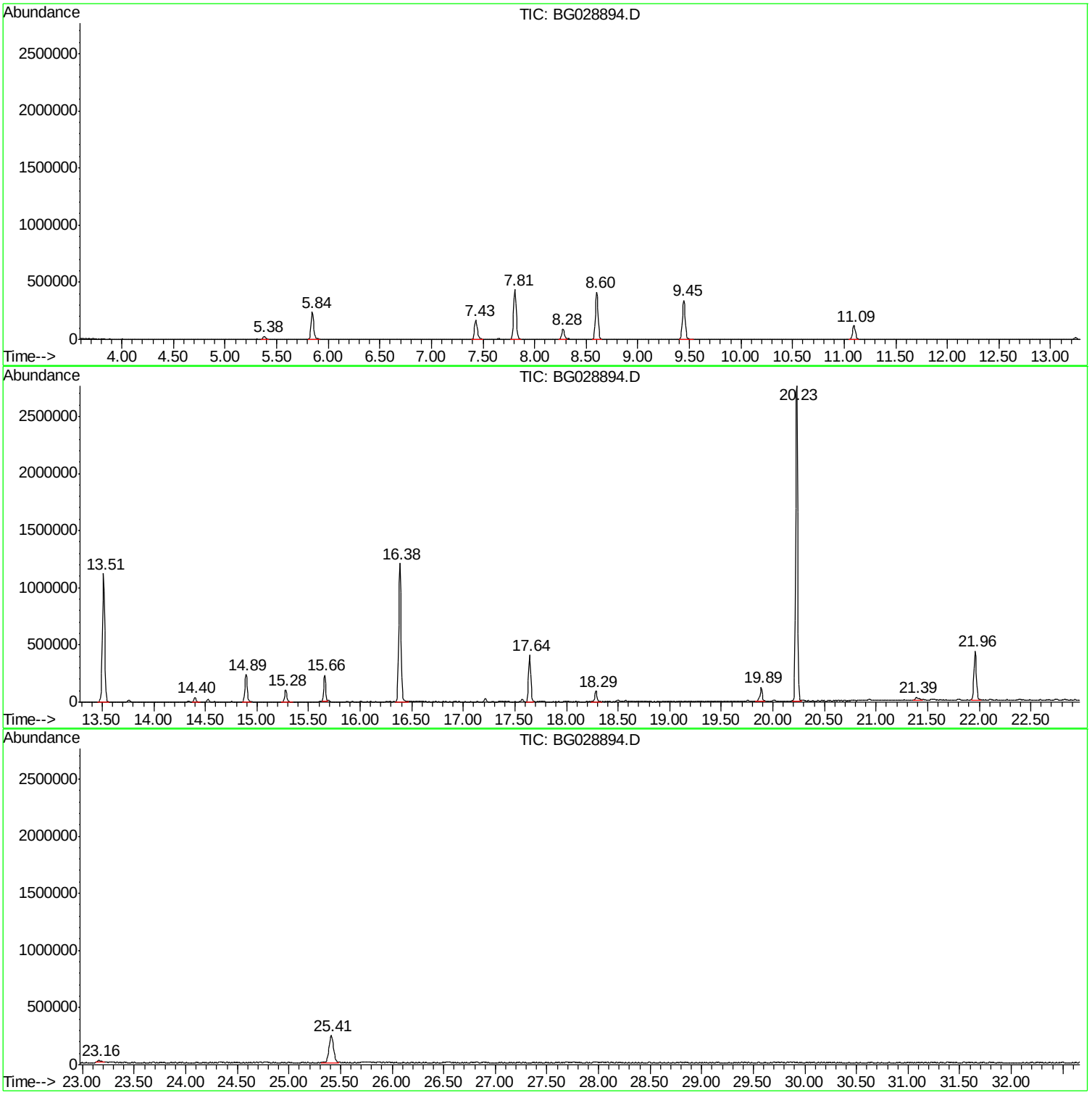
Instrument : BNA_G
ClientSampleId : 20170530-LOC-6

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



Library Search Compound Report

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Data File : BG028894.D
Acq On : 23 Sep 2017 12:19
Operator : SJ/JU
Sample : I5321-06
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

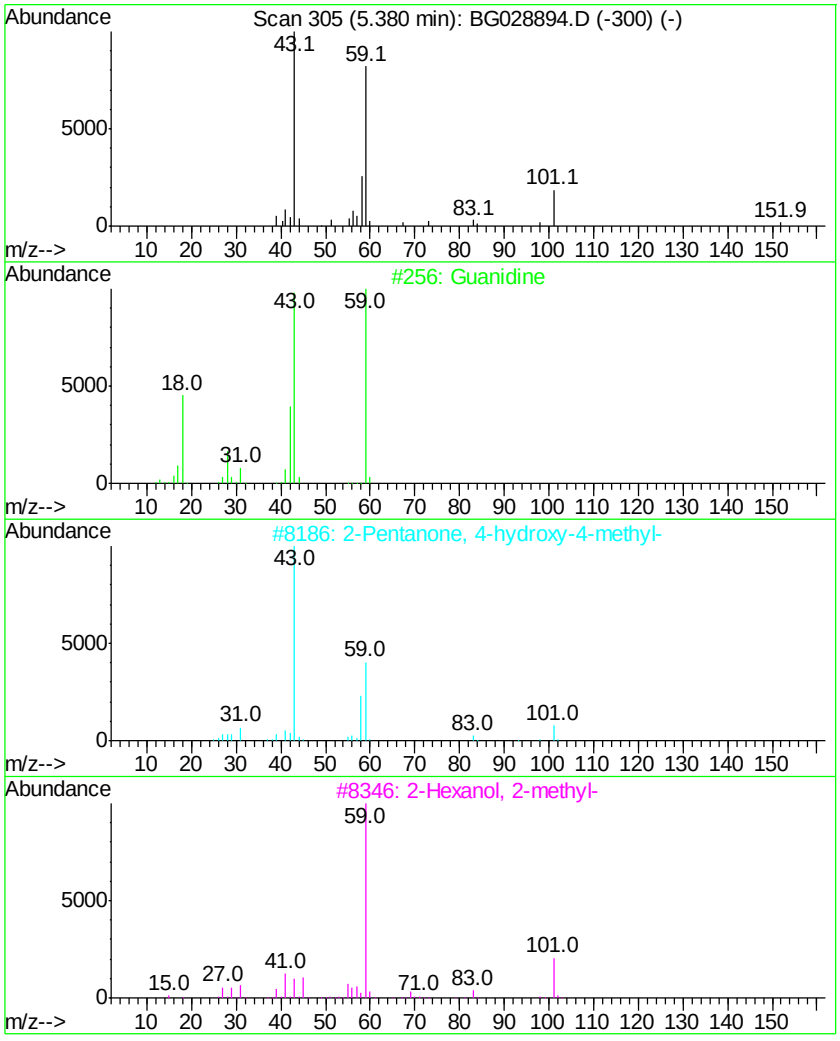
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

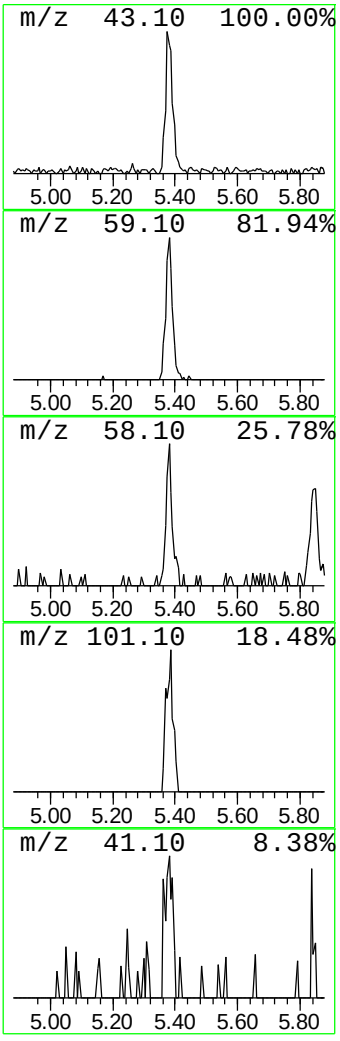
****

Peak Number 1 Guanidine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	5.51 ng	44786	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine	59	CH5N3	000113-00-8	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4	(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	40
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	40





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Sample : I5321-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170530-LOC-6

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

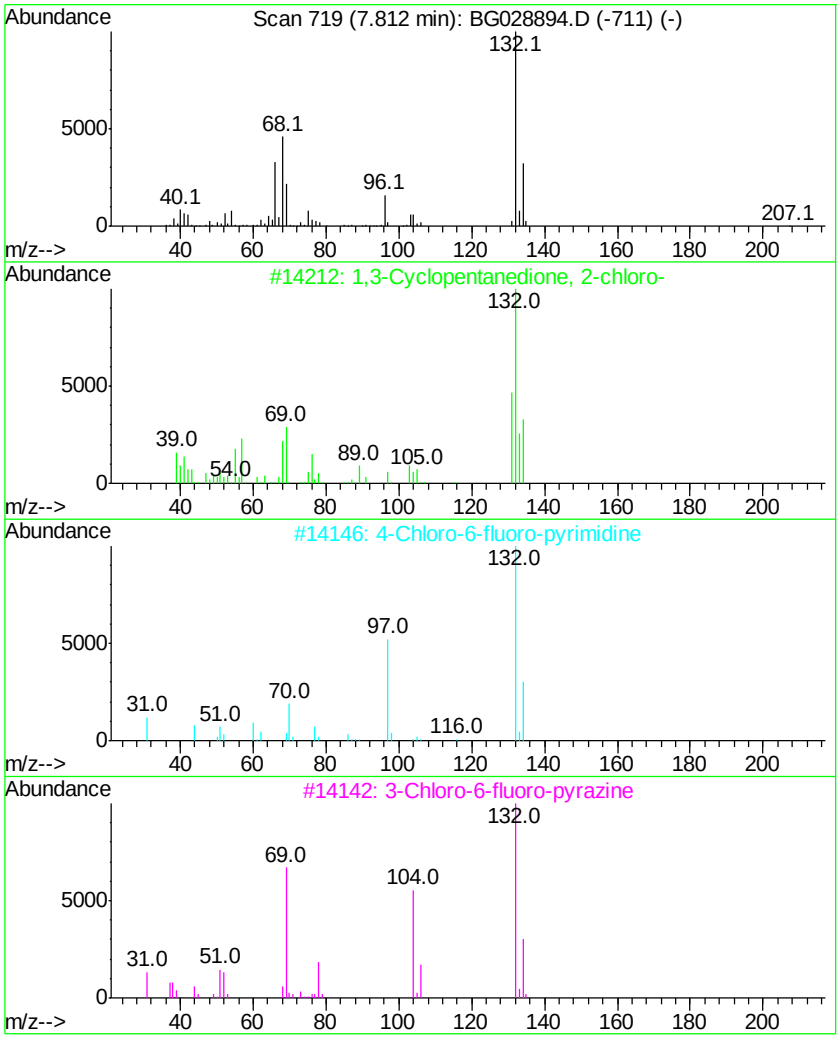
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

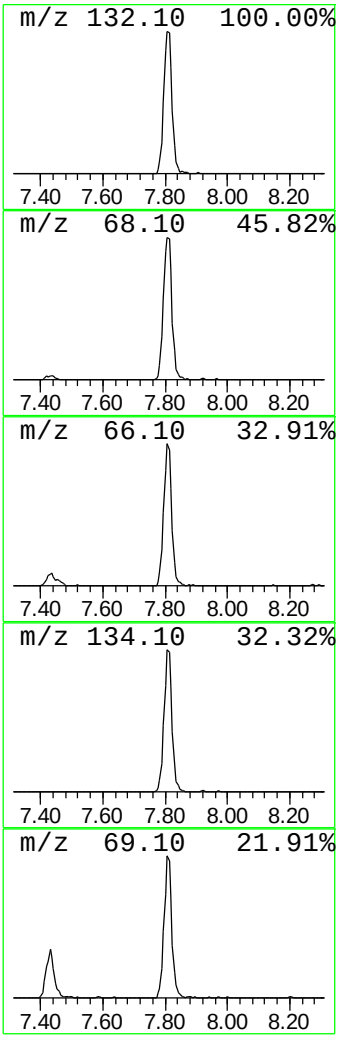
****

Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	96.94 ng	788414	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Data File : BG028894.D
Acq On : 23 Sep 2017 12:19
Operator : SJ/JU
Sample : I5321-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170530-LOC-6

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

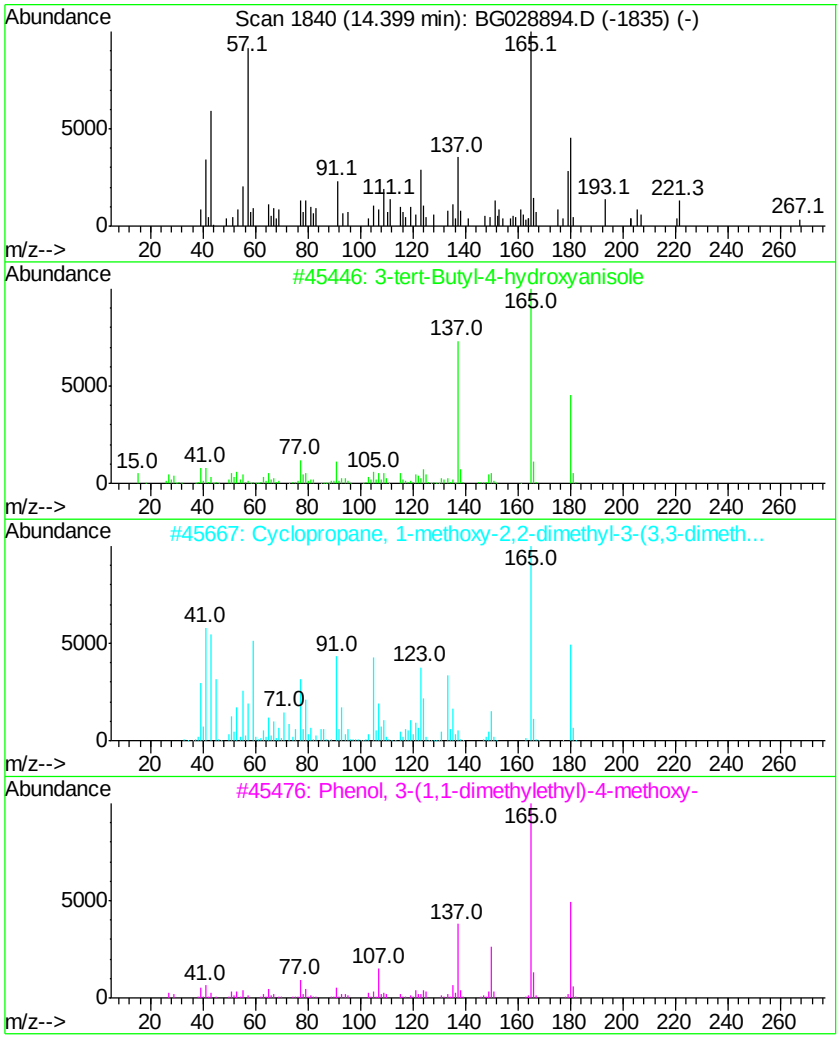
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

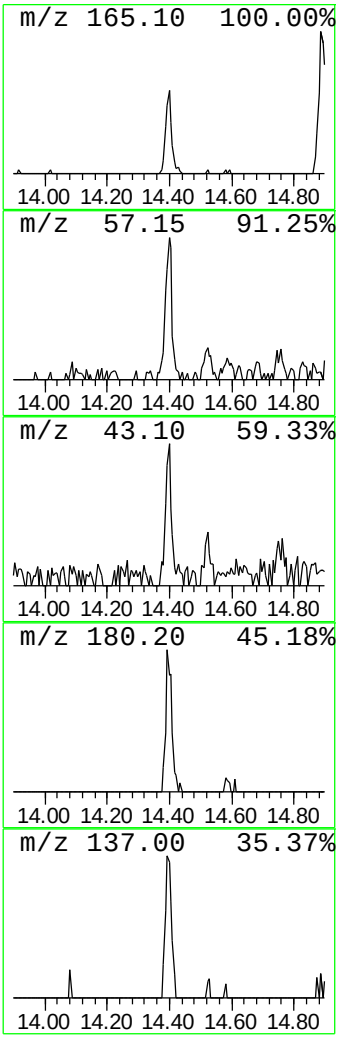
****

Peak Number 4 3-tert-Butyl-4-hydroxyanisole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	2.75 ng	54112	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	55
2	Cyclopropane, 1-methoxy-2,2-dime...	180	C12H20O	1000271-82-9	53
3	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	52
4	Ethanone, 1-(2,5-dimethoxyphenyl)-	180	C10H12O3	001201-38-3	49
5	2',4'-Dimethoxyacetophenone	180	C10H12O3	000829-20-9	49





Library Search Compound Report

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Data File : BG028894.D
Acq On : 23 Sep 2017 12:19
Operator : SJ/JU
Sample : I5321-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170530-LOC-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
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TIC Library : C:\Database\NIST11.L
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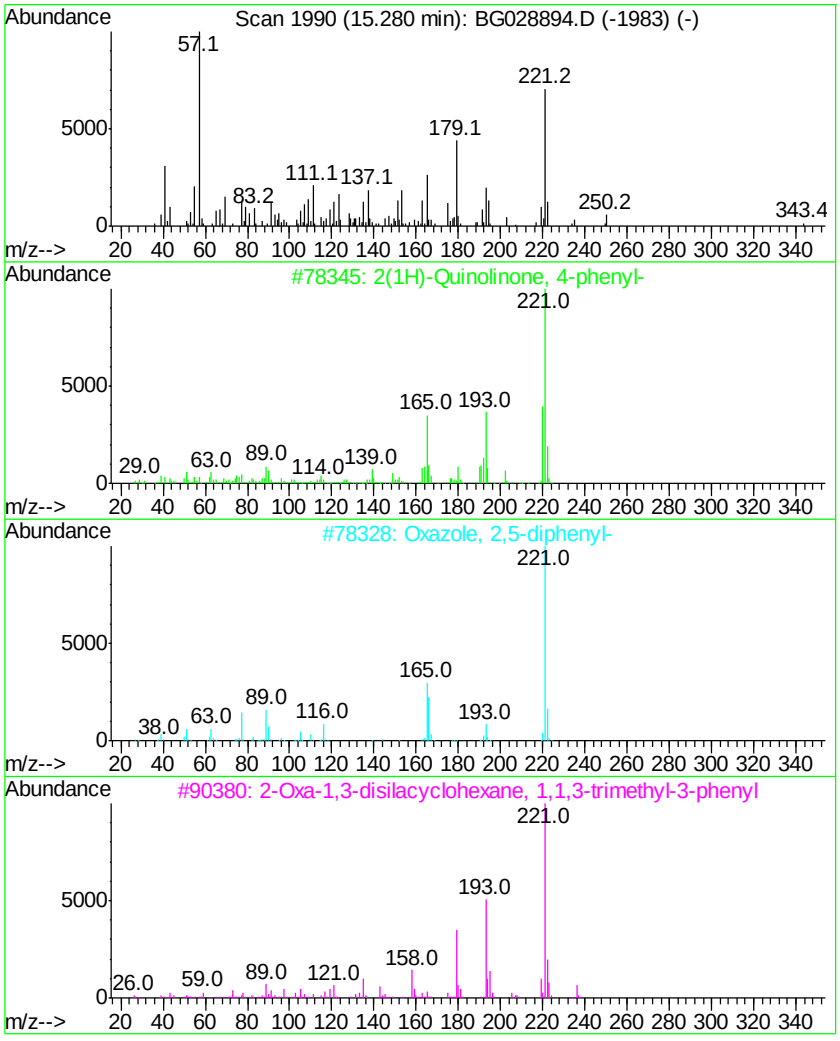
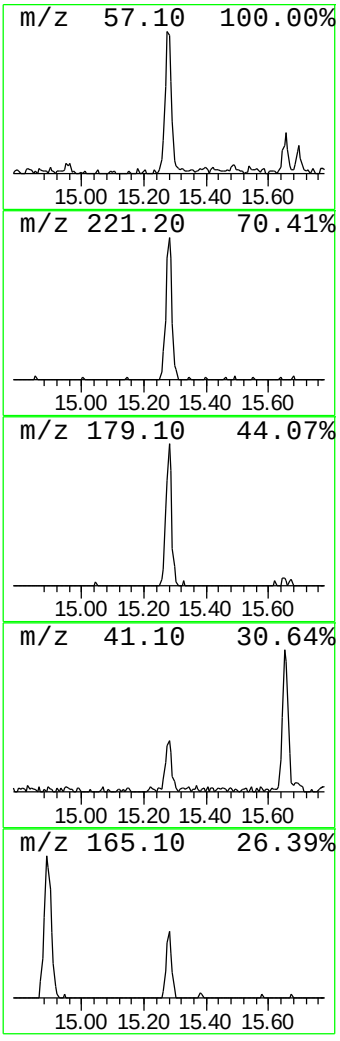
****

Peak Number 5 unknown15.28 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	7.89 ng	155348	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	45
2	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	41
3	2-Oxa-1,3-disilacyclohexane, 1,1...	236	C12H20OSi2	1000308-85-9	37
4	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	27
5	Benzo[h]quinoline, 2,3,4-trimethyl-	221	C16H15N	063042-66-0	22





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Sample : I5321-06
Misc :
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Instrument : BNA_G
ClientSampleId : 20170530-LOC-6

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
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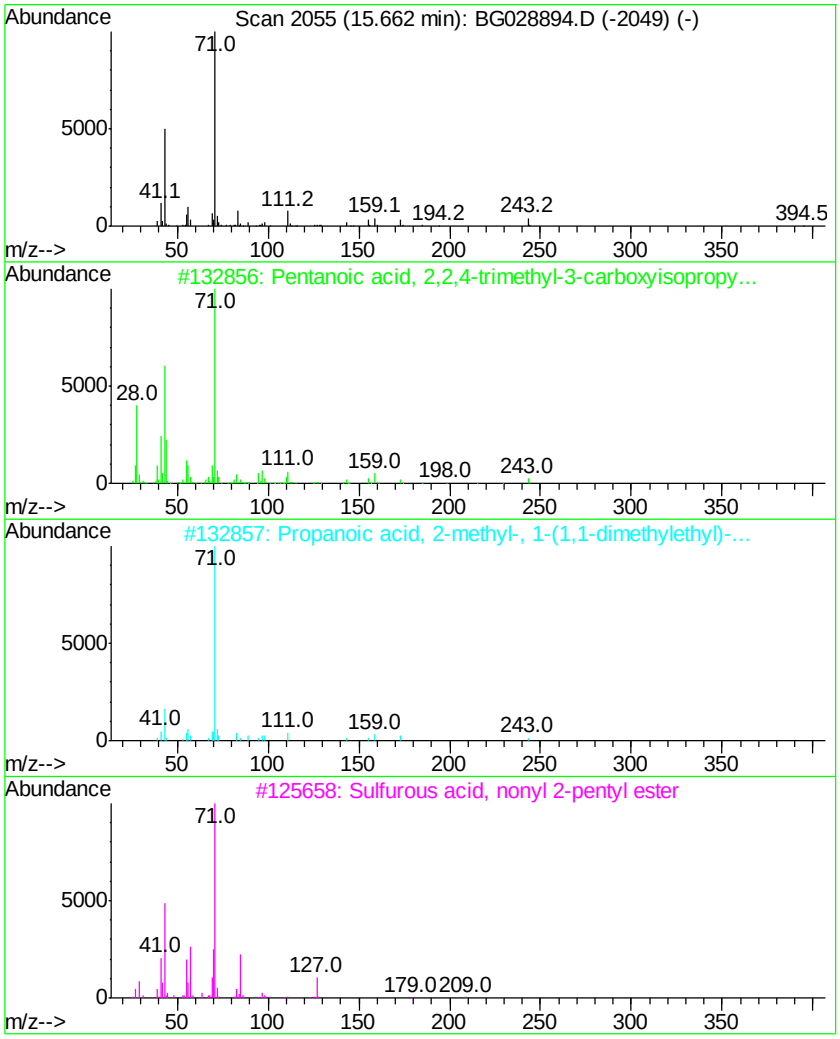
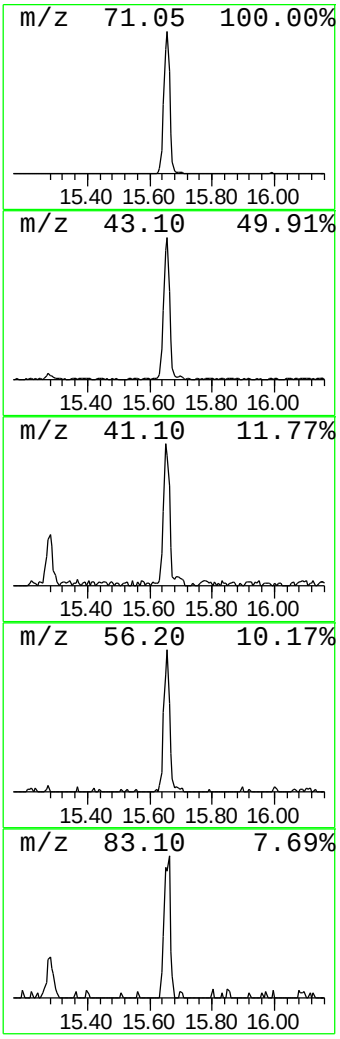
****

Peak Number 6 Pentanoic acid, 2,2,4-trime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	15.20 ng	299454	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	78
2	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	64
3	Sulfurous acid, nonyl 2-pentyl e...	278	C14H30O3S	1000309-15-8	45
4	3-Methyl-hepta-1,6-dien-3-ol	126	C8H14O	034780-69-3	45
5	Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	40





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

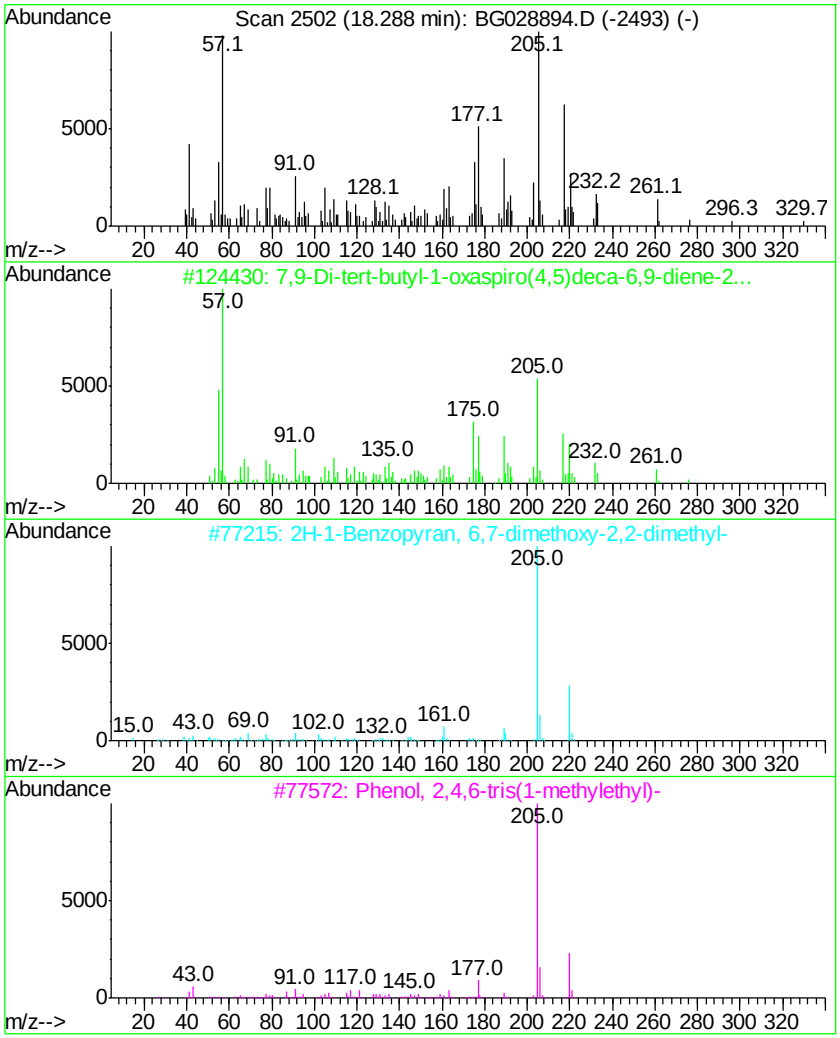
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

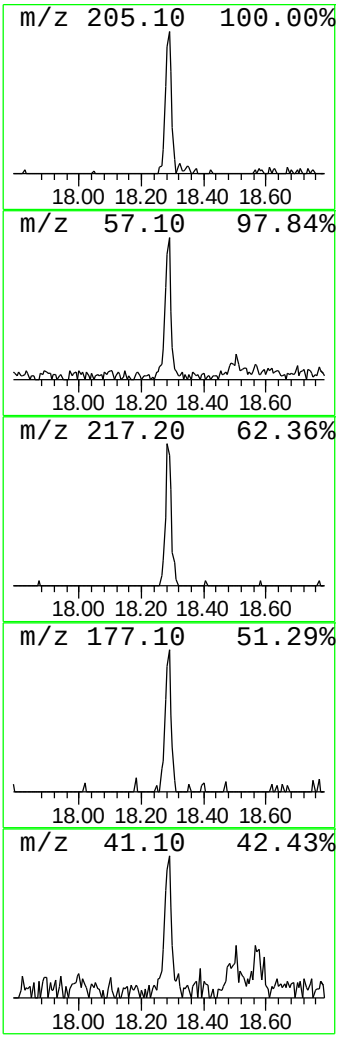
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	4.37 ng	137164	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	96
2	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	38
3	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	38
4	2-Acetylphenanthrene	220	C16H12O	005960-69-0	38
5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	35





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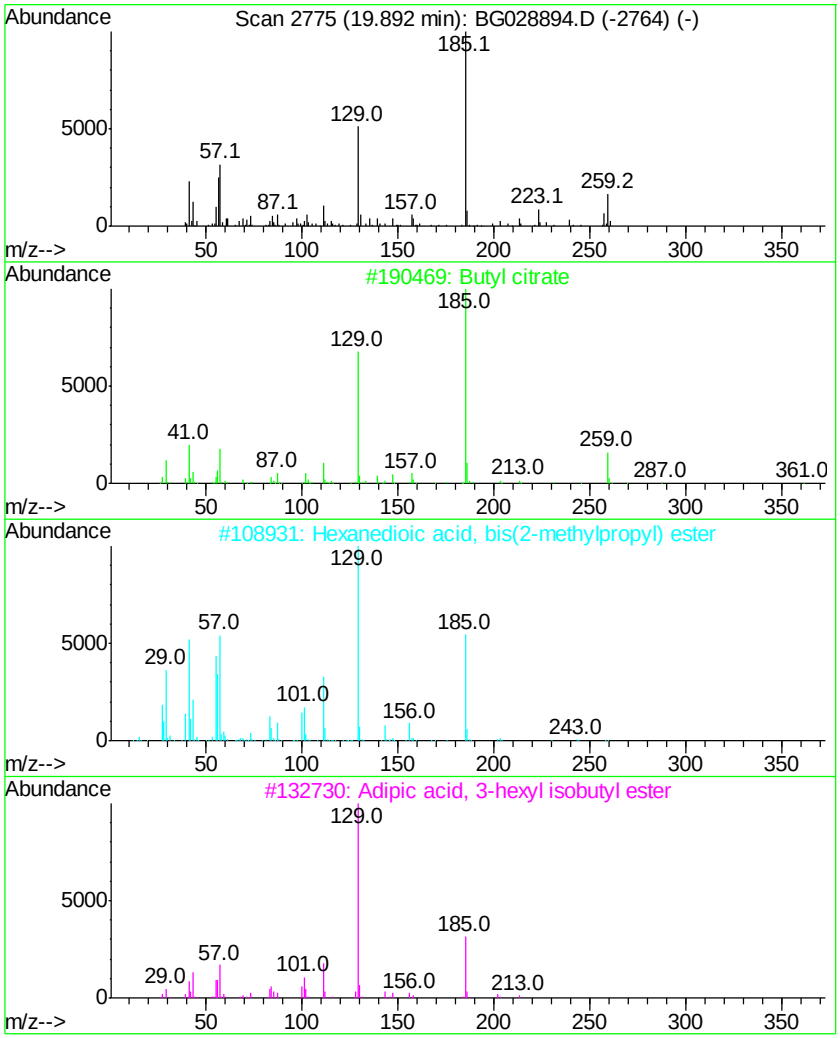
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

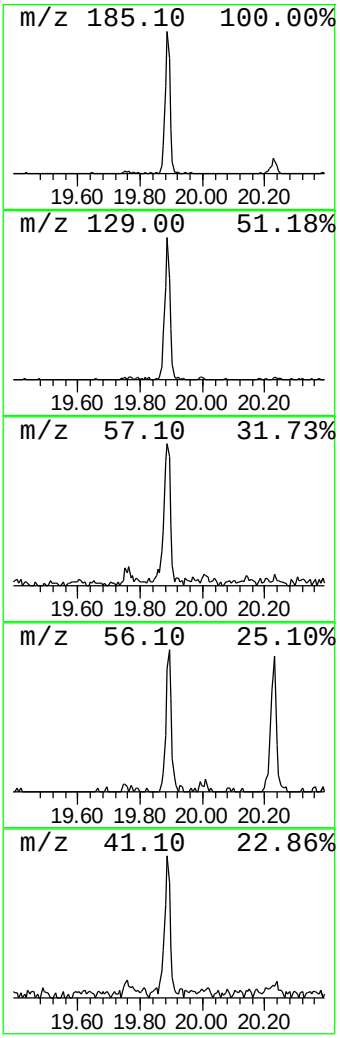
****

Peak Number 8 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	4.94 ng	188224	Chrysene-d12	21.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	90
2	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	74
3	Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	64
4	Adipic acid, butyl 2,4-dimethylp...	300	C17H32O4	1000349-77-7	64
5	O-Methyl-DL-serine, N-dimethylam...	230	C11H22N2O3	1000375-99-5	59





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Guanidine	5.38	5.5	ng	44786	1	8.28	162652	20.0
unknown7.81	7.81	96.9	ng	788414	1	8.28	162652	20.0
3-tert-Butyl-4-hy...	14.40	2.8	ng	54112	3	14.89	393968	20.0
unknown15.28	15.28	7.9	ng	155348	3	14.89	393968	20.0
Pentanoic acid, 2...	15.66	15.2	ng	299454	3	14.89	393968	20.0
7,9-Di-tert-butyl...	18.29	4.4	ng	137164	4	17.64	628320	20.0
Butyl citrate	19.89	4.9	ng	188224	5	21.96	761876	20.0