LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092317\
Data File : BG028893.D
Acq On : 23 Sep 2017 11:40
Operator : SJ/JU
Sample : I5321-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170611-COMP-B

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	rBV	24723	38566	1.01%	0.271%
2	5.844	377	384	398	rBV	286304	492495	12.86%	3.458%
3	7.430	646	654	667	rBV	187714	359042	9.37%	2.521%
4	7.806	711	718	730	rBV	463495	853414	22.28%	5.992%
5	8.276	791	798	805	rBV2	82817	159283	4.16%	1.118%
6	8.599	842	853	864	rBV	408946	736770	19.24%	5.173%
7	9.445	988	997	1008	rBV	338254	638133	16.66%	4.480%
8	11.096	1270	1278	1289	rBV	114413	217207	5.67%	1.525%
9	13.511	1679	1689	1697	rBV	1064515	1683851	43.96%	11.822%
10	14.398	1833	1840	1846	rBV3	30277	45061	1.18%	0.316%
11	14.892	1917	1924	1933	rVB	216227	359691	9.39%	2.525%
12	15.280	1984	1990	1996	rBV	91670	125522	3.28%	0.881%
13	15.656	2049	2054	2058	rBV	240154	307112	8.02%	2.156%
14	16.384	2171	2178	2195	rBV	1218185	1906645	49.78%	13.387%
15	17.642	2385	2392	2402	rBV2	380183	594093	15.51%	4.171%
16	18.282	2492	2501	2507	rBV3	176686	253226	6.61%	1.778%
17	19.886	2764	2774	2781	rBV2	121471	174203	4.55%	1.223%
18	20.233	2826	2833	2840	rBV	2892691	3830262	100.00%	26.892%
19	21.960	3120	3127	3136	rBV2	415512	747221	19.51%	5.246%
20	25.409	3702	3714	3724	rBV	236095	721243	18.83%	5.064%

Sum of corrected areas: 14243040

LSC Report - Integrated Chromatogram

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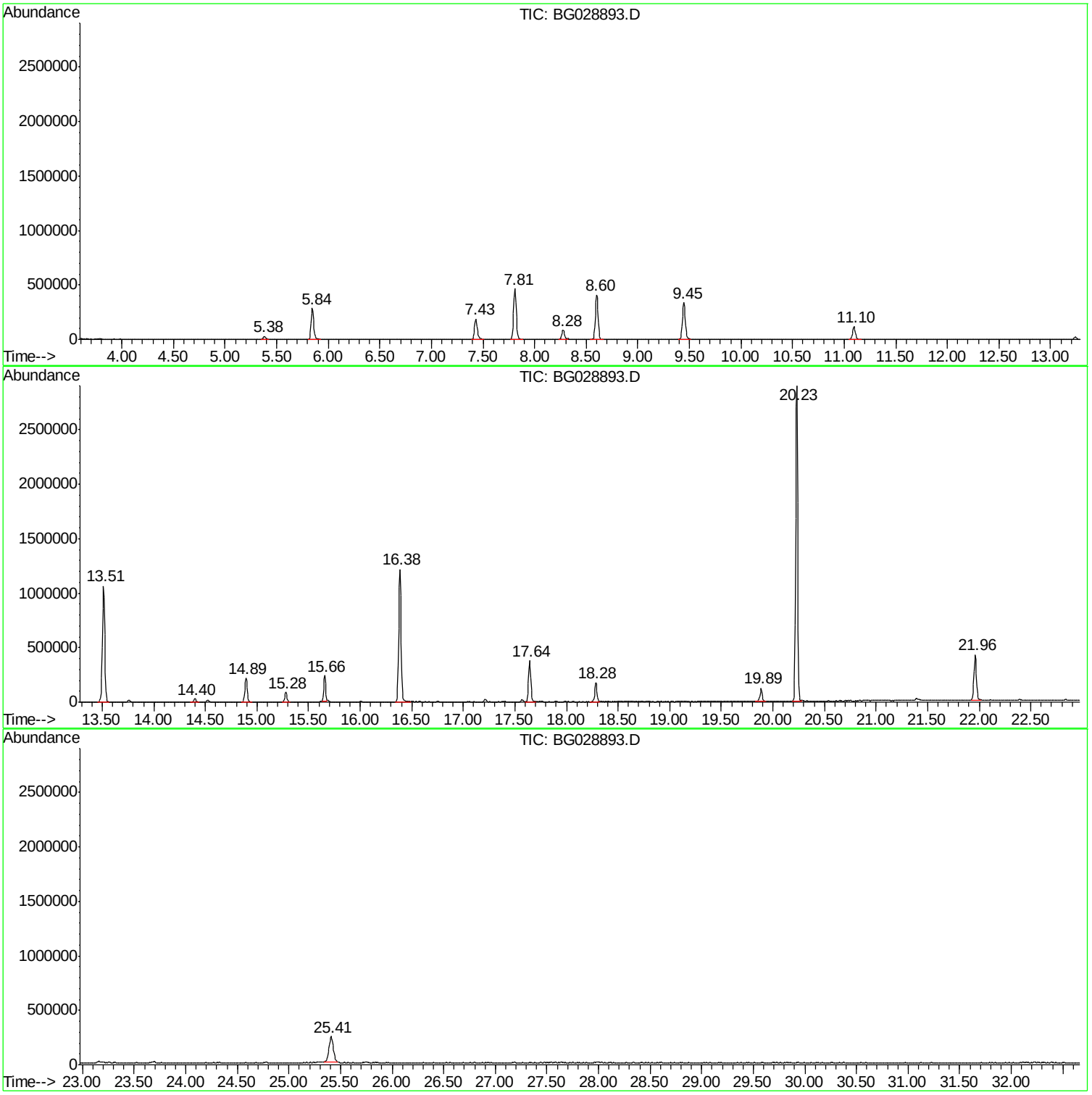
Instrument : BNA_G
ClientSampleId : 20170611-COMP-B

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG092317\
Data File : BG028893.D
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

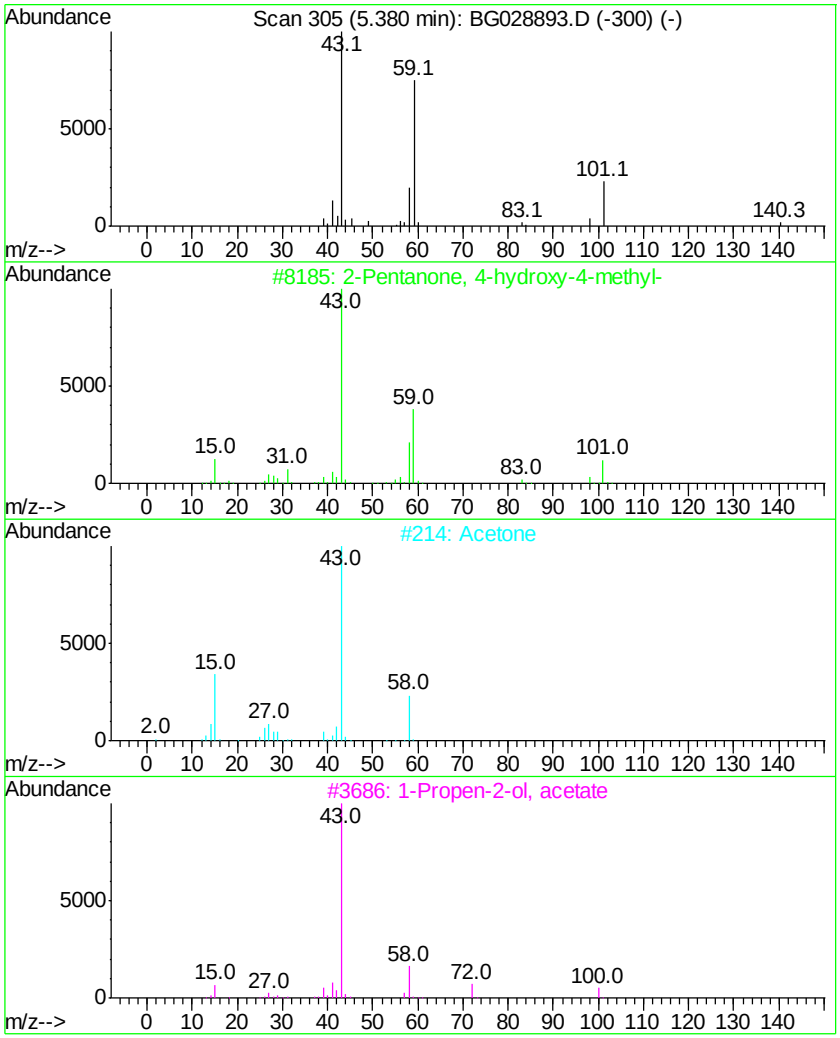
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

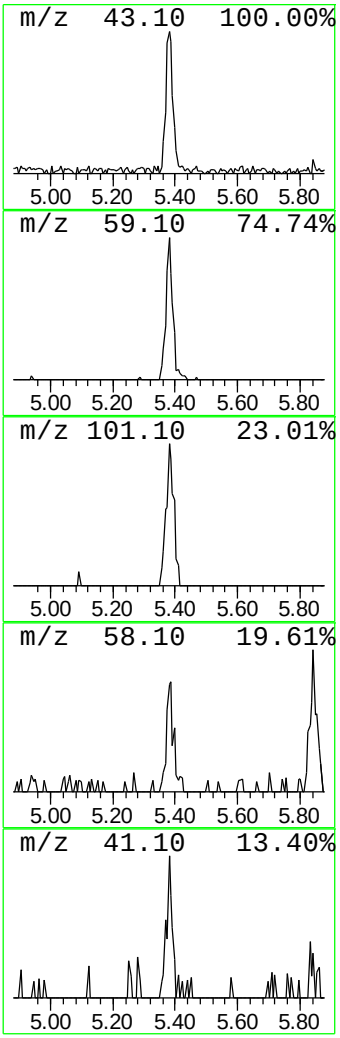
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	4.84 ng	38566	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
2	Acetone	58	C3H6O	000067-64-1	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	9





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Operator : SJ/JU
Sample : I5321-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170611-COMP-B

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

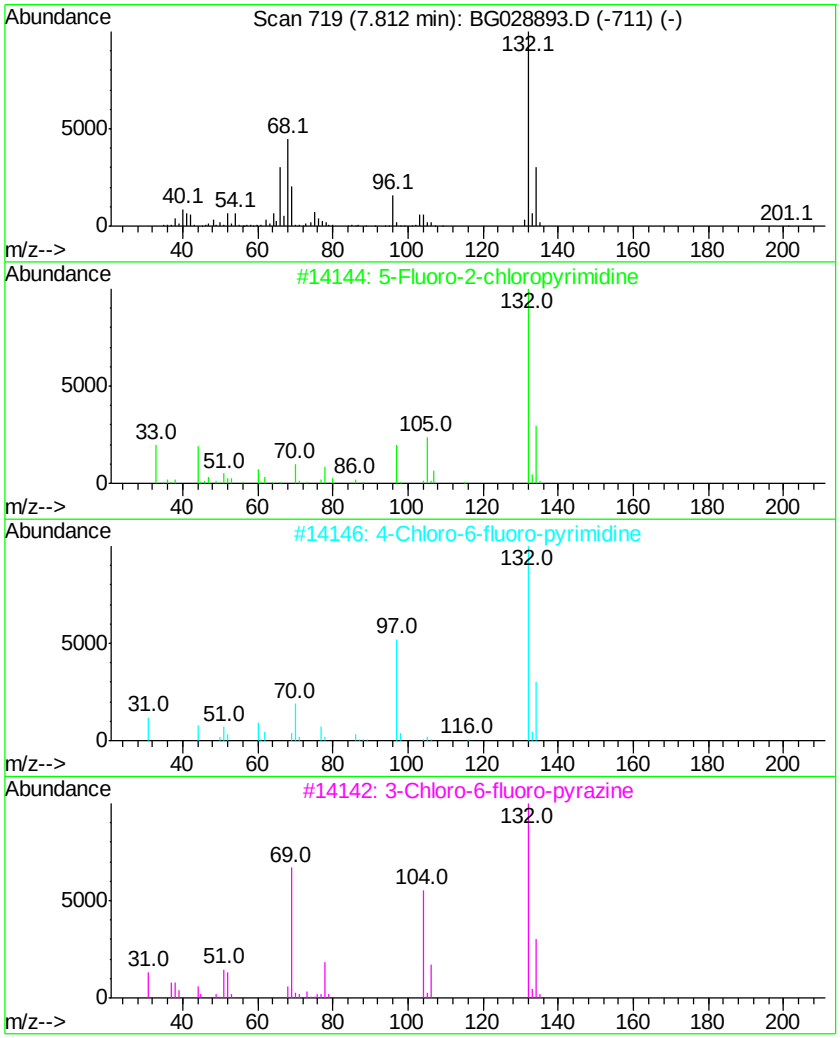
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

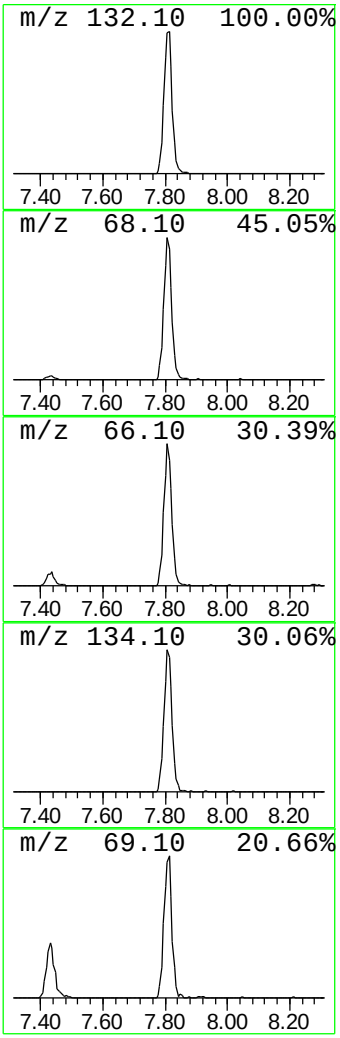
****

Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	107.16 ng	853414	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





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Misc :
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Instrument : BNA_G
ClientSampleId : 20170611-COMP-B

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

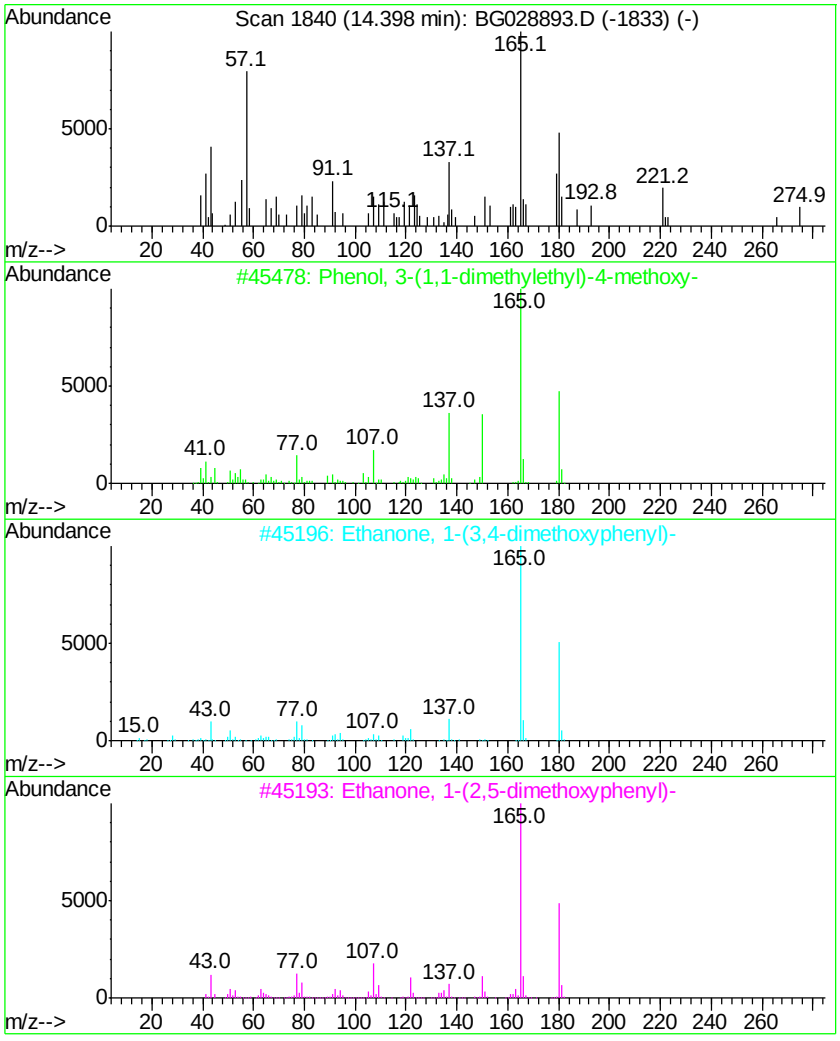
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

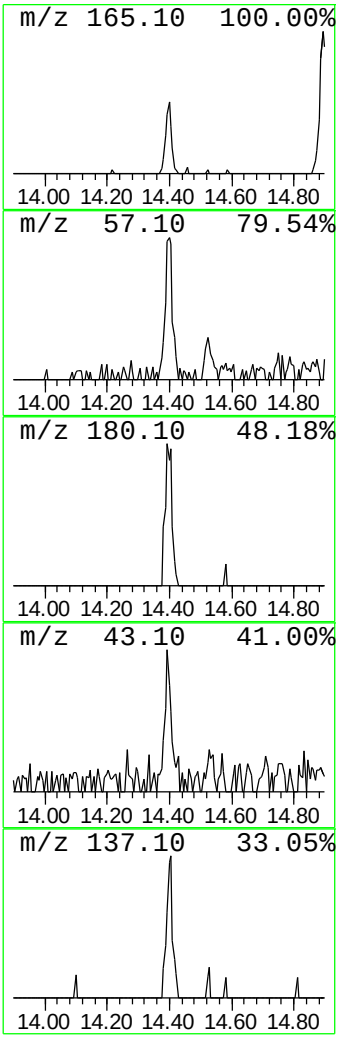
****

Peak Number 4 Phenol, 3-(1,1-dimethylethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	2.51 ng	45061	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	52
2	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	001131-62-0	49
3	Ethanone, 1-(2,5-dimethoxyphenyl)-	180	C10H12O3	001201-38-3	49
4	9H-Fluorene, 9-methyl-	180	C14H12	002523-37-7	49
5	9H-Fluorene, 4-methyl-	180	C14H12	001556-99-6	49





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092317\
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Misc :
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Instrument : BNA_G
ClientSampleId : 20170611-COMP-B

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

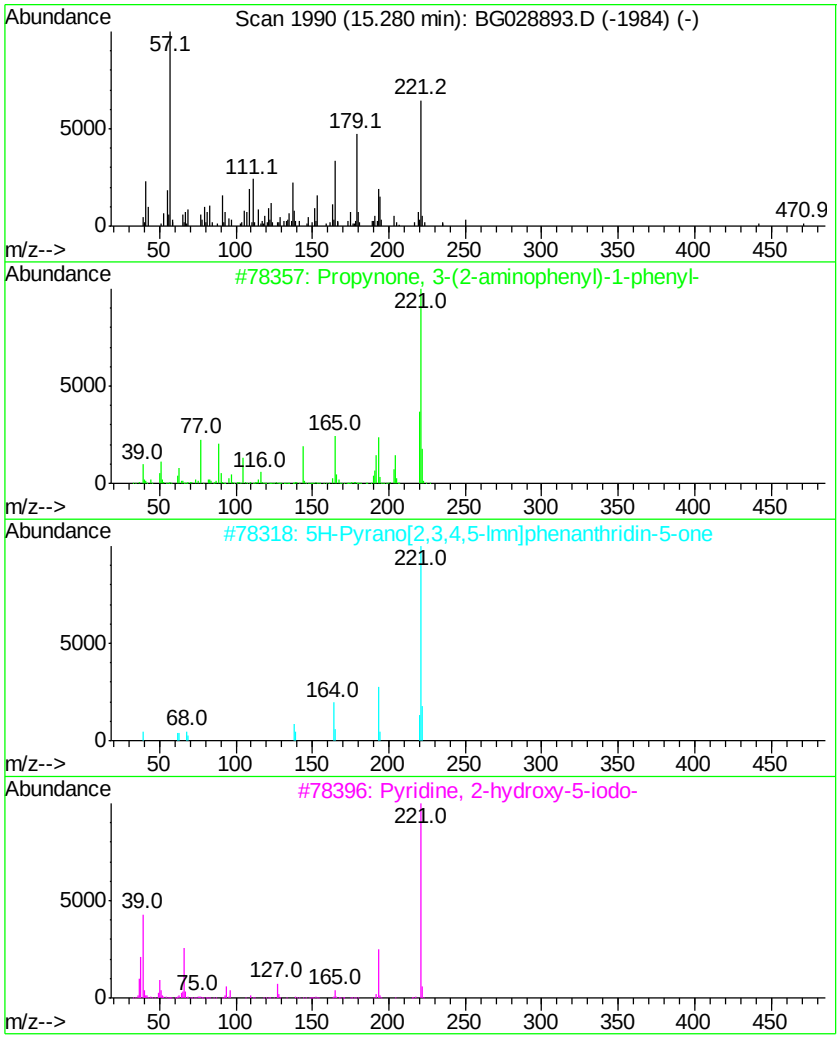
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

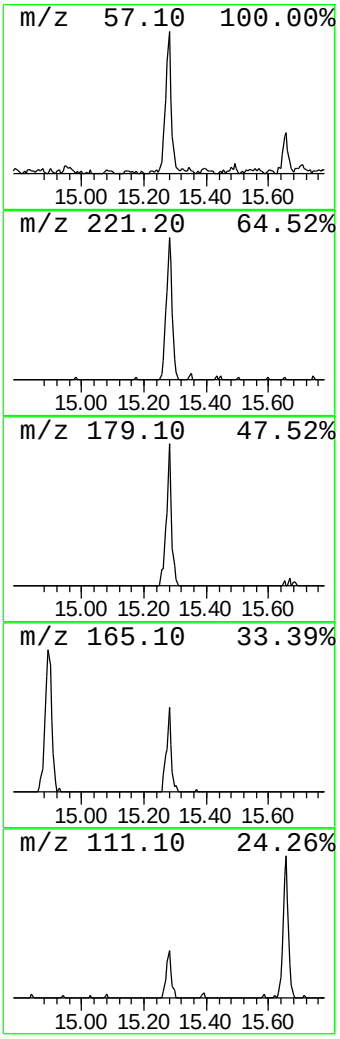
****

Peak Number 5 unknown15.28 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	6.98 ng	125522	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propynone, 3-(2-aminophenyl)-1-p...	221	C15H11NO	1000311-26-1	25
2	5H-Pyrano[2,3,4,5-lmn]phenanthri...	221	C14H7NO2	004733-28-2	14
3	Pyridine, 2-hydroxy-5-iodo-	221	C5H4INO	013472-79-2	14
4	Silane, chlorodiethyloctyloxy-	250	C12H27ClOSi	1000363-08-4	12
5	(E)-2-Hydroxy-4'-cyano-stilbene	221	C15H11NO	1000147-85-5	12





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ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170611-COMP-B

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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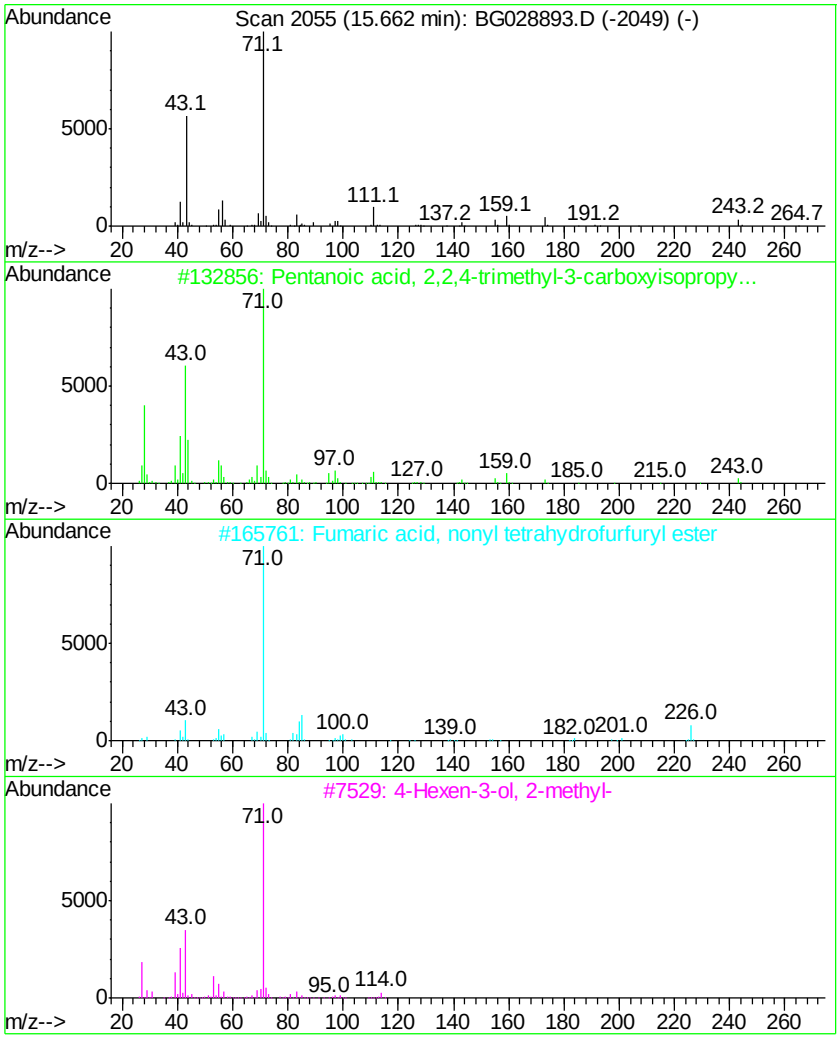
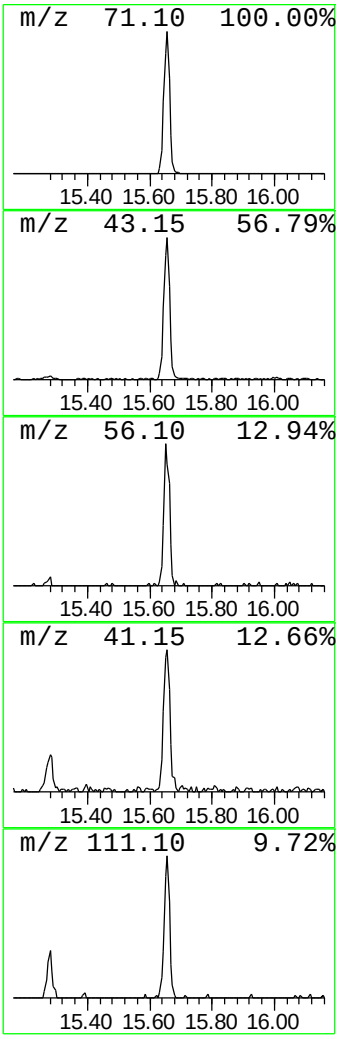
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	17.08 ng	307112	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	Fumaric acid, nonyl tetrahydrofu...	326	C18H30O5	1000330-58-3	50
3	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	50
4	Sulfurous acid, nonyl pentyl ester	278	C14H30O3S	1000309-14-2	45
5	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	45





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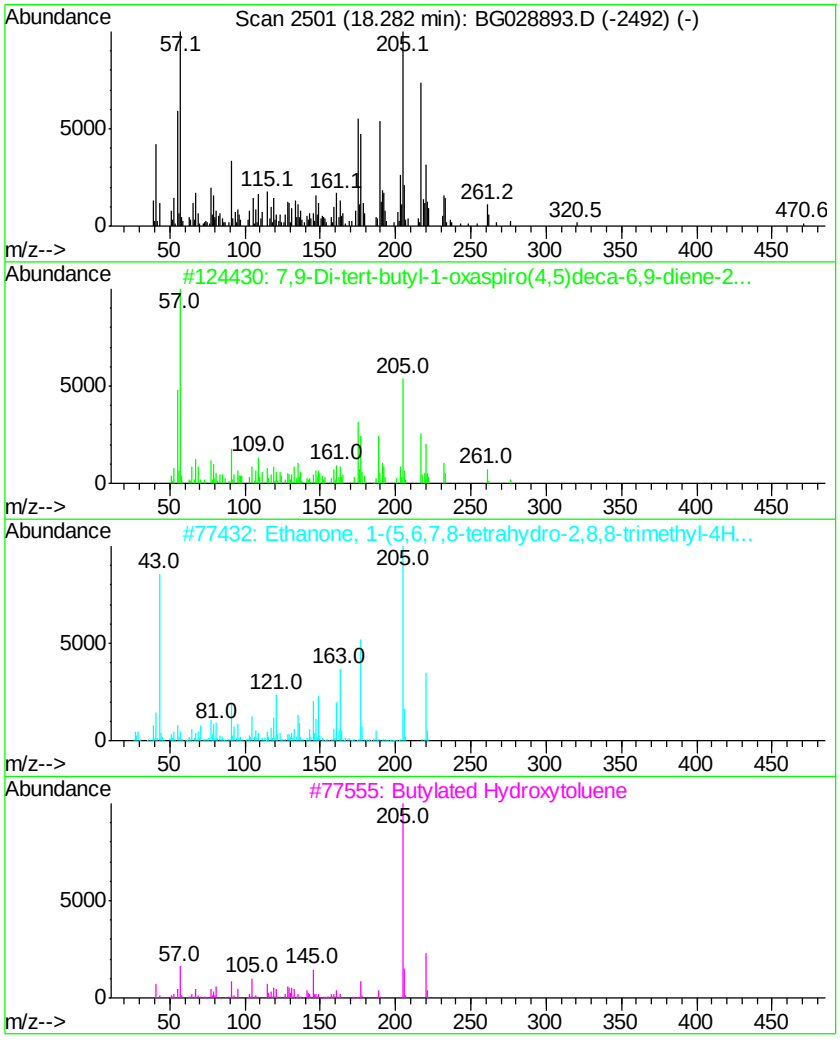
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

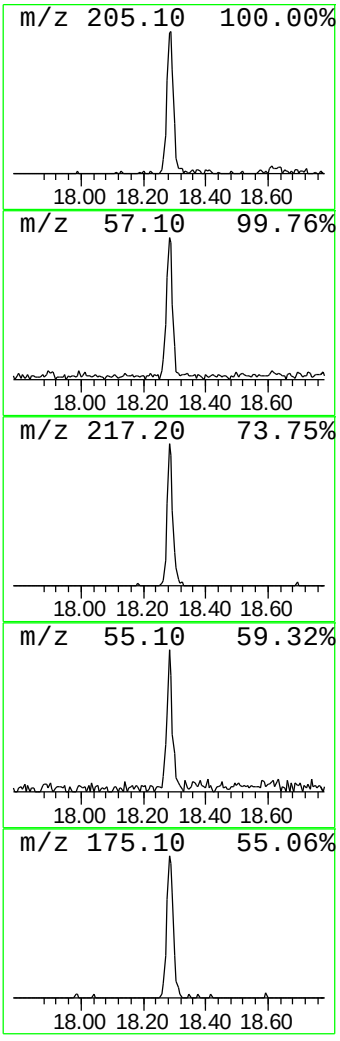
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	8.52 ng	253226	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	83
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	42
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38
4	4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	30
5	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	30





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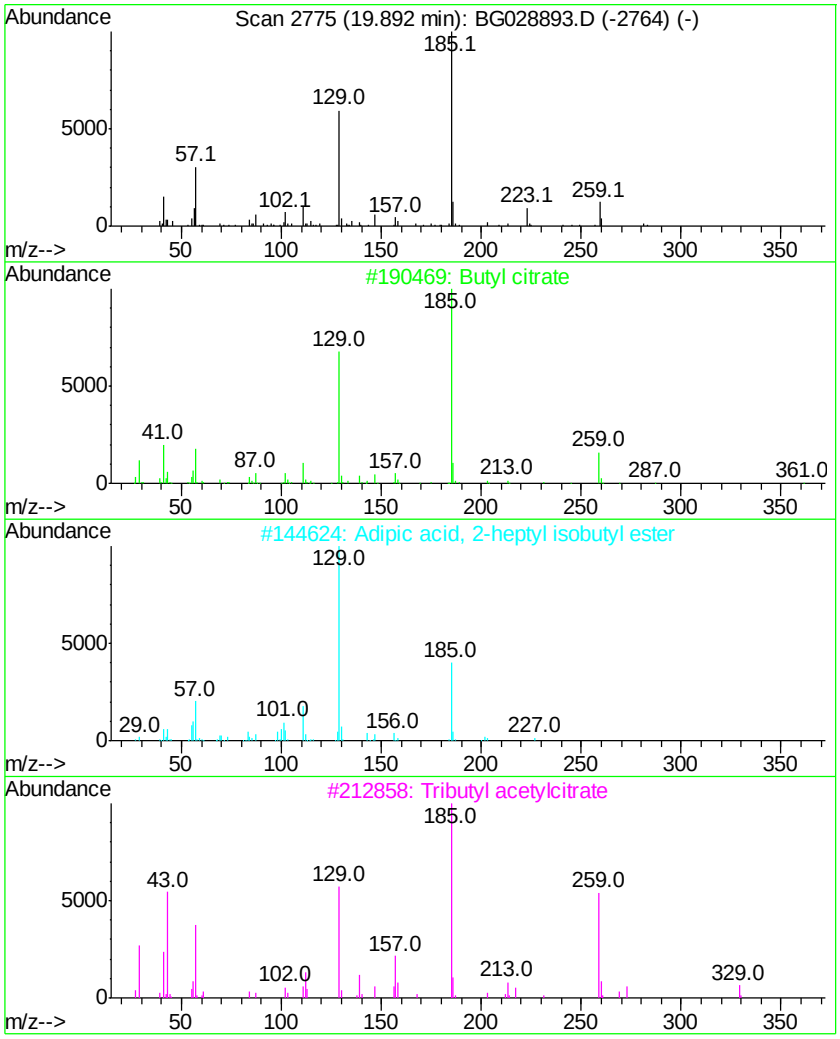
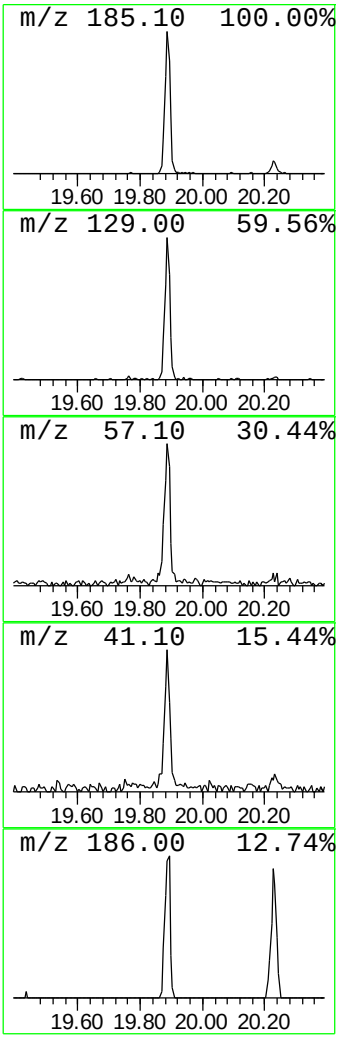
****

Peak Number 8 Butyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	4.66 ng	174203	Chrysene-d12	21.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	58
2	Adipic acid, 2-heptyl isobutyl e...	300	C17H32O4	1000353-64-3	56
3	Tributyl acetylcitrate	402	C20H34O8	000077-90-7	56
4	Adipic acid, 3,3-dimethylbut-2-y...	286	C16H30O4	1000353-66-7	56
5	Adipic acid, cyclohexyl isobutyl...	284	C16H28O4	1000324-25-8	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
2-Pentanone, 4-hy...	5.38	4.8	ng	38566	1	8.28	159283	20.0
unknown7.81	7.81	107.2	ng	853414	1	8.28	159283	20.0
Phenol, 3-(1,1-di...	14.40	2.5	ng	45061	3	14.89	359691	20.0
unknown15.28	15.28	7.0	ng	125522	3	14.89	359691	20.0
Pentanoic acid, 2...	15.66	17.1	ng	307112	3	14.89	359691	20.0
7,9-Di-tert-butyl...	18.28	8.5	ng	253226	4	17.64	594093	20.0
Butyl citrate	19.89	4.7	ng	174203	5	21.96	747221	20.0