LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028884.D
Acq On : 22 Sep 2017 21:20
Operator : SJ/JU
Sample : I5301-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170605-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	5.377	299	304	313	rBV	24442	38492	1.14%	0.269%
2	5.847	378	384	395	rBV	235231	406155	12.00%	2.833%
3	7.434	645	654	664	rBV	166209	328323	9.70%	2.290%
4	7.810	710	718	725	rBV	409526	720923	21.30%	5.029%
5	8.280	791	798	804	rBV	82753	147332	4.35%	1.028%
6	8.603	846	853	862	rBV	361433	650957	19.23%	4.541%
7	9.449	988	997	1008	rBV	297232	581737	17.19%	4.058%
8	11.094	1269	1277	1284	rBV	109128	205080	6.06%	1.431%
9	13.245	1636	1643	1650	rBV3	32110	55977	1.65%	0.391%
10	13.515	1678	1689	1696	rBV	1003045	1589209	46.95%	11.087%
11	13.762	1725	1731	1738	rVB2	32595	51560	1.52%	0.360%
12	14.332	1820	1828	1835	rBV	53300	85202	2.52%	0.594%
13	14.396	1835	1839	1848	rVB2	90798	127467	3.77%	0.889%
14	14.525	1856	1861	1868	rVB2	56599	82702	2.44%	0.577%
15	14.896	1917	1924	1931	rVB2	212908	360561	10.65%	2.515%
16	15.278	1984	1989	1998	rBV2	233794	334769	9.89%	2.335%
17	15.654	2048	2053	2059	rBV	539505	718018	21.21%	5.009%
18	16.382	2169	2177	2191	rBV	1126405	1778843	52.55%	12.409%
19	17.211	2314	2318	2325	rVB	54991	78346	2.31%	0.547%
20	17.569	2374	2379	2384	rBV2	49120	63873	1.89%	0.446%
21	17.645	2385	2392	2401	rVB2	372553	601103	17.76%	4.193%
22	18.286	2492	2501	2506	rBV3	145941	218695	6.46%	1.526%
23	19.884	2766	2773	2782	rBV2	84734	161367	4.77%	1.126%
24	20.231	2826	2832	2839	rBV	2584108	3385093	100.00%	23.615%
25	21.400	3023	3031	3040	rBV3	38037	104568	3.09%	0.729%
26	21.958	3119	3126	3135	rBV	416272	734348	21.69%	5.123%
27	25.407	3702	3713	3727	rVB3	235448	723836	21.38%	5.050%

Sum of corrected areas: 14334536

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Misc :
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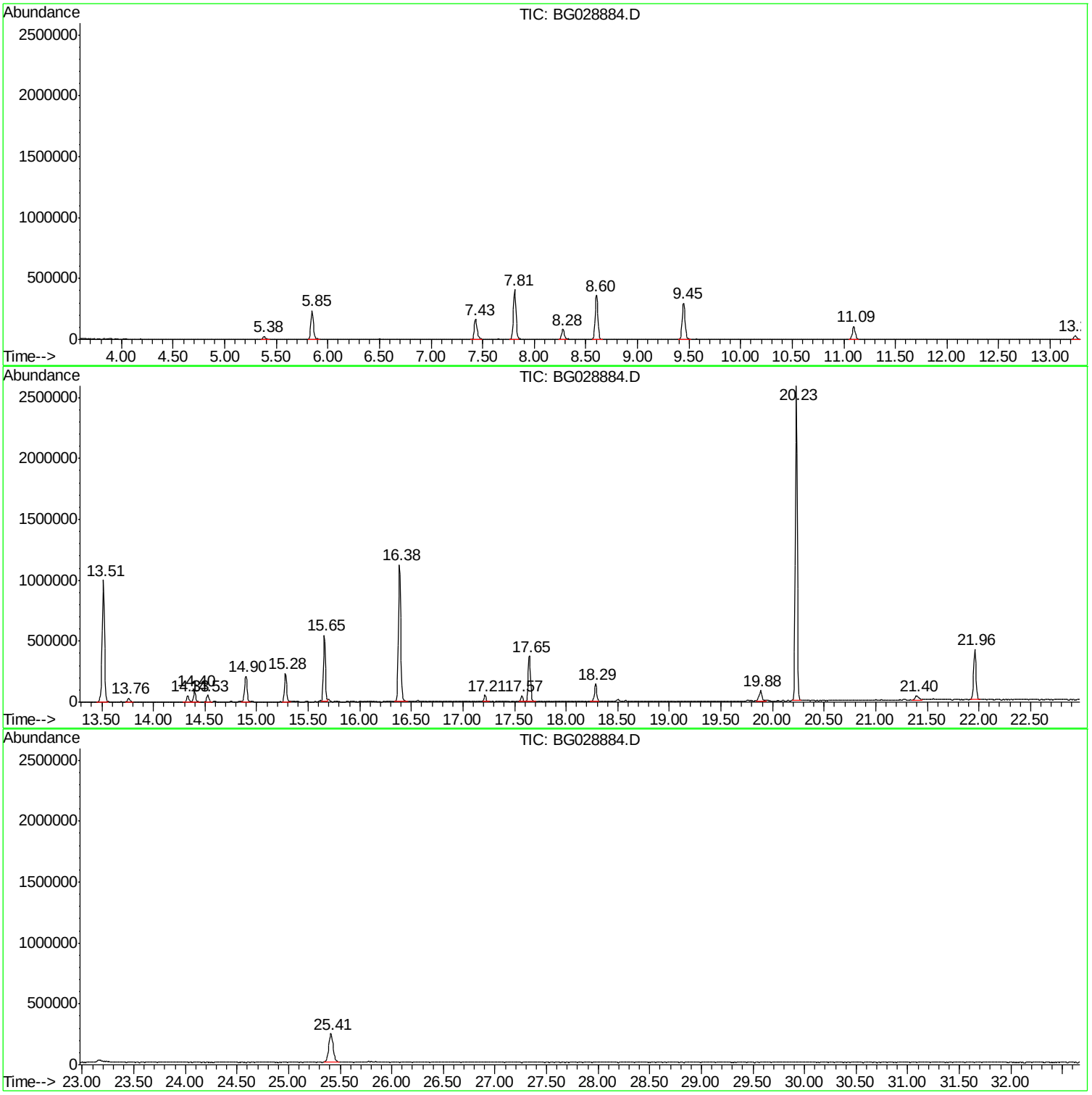
Instrument : BNA_G
ClientSampleId : 20170605-COMP-B

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



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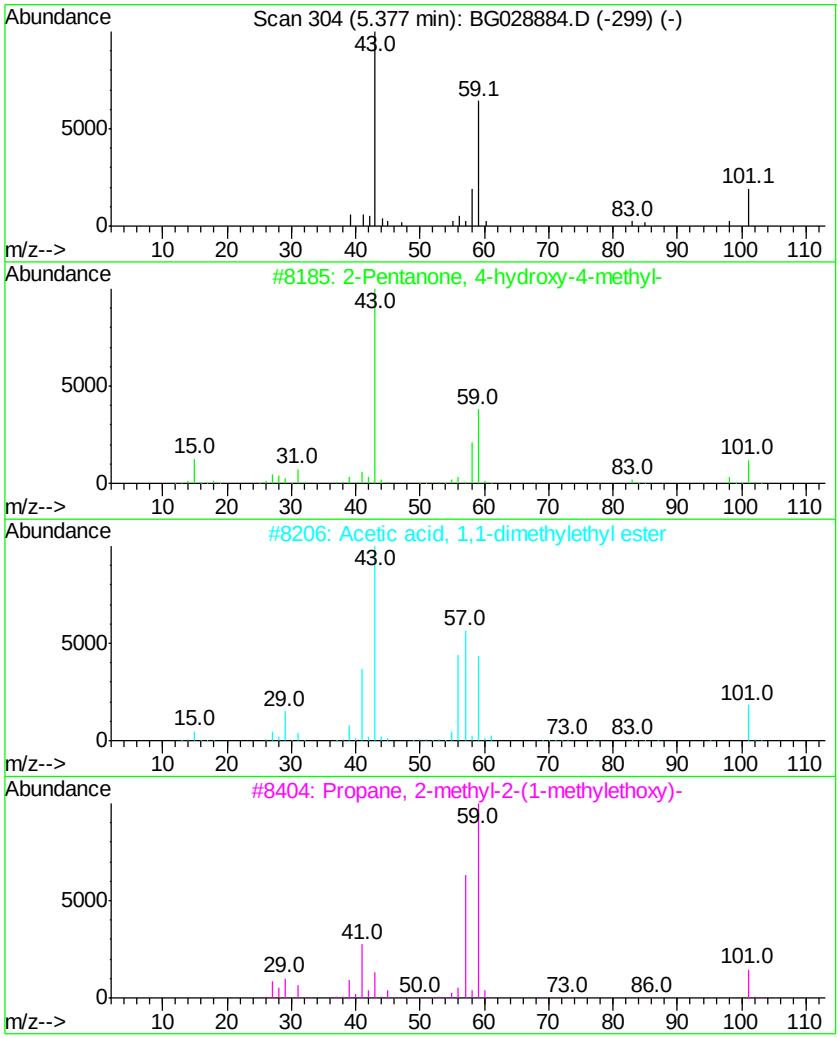
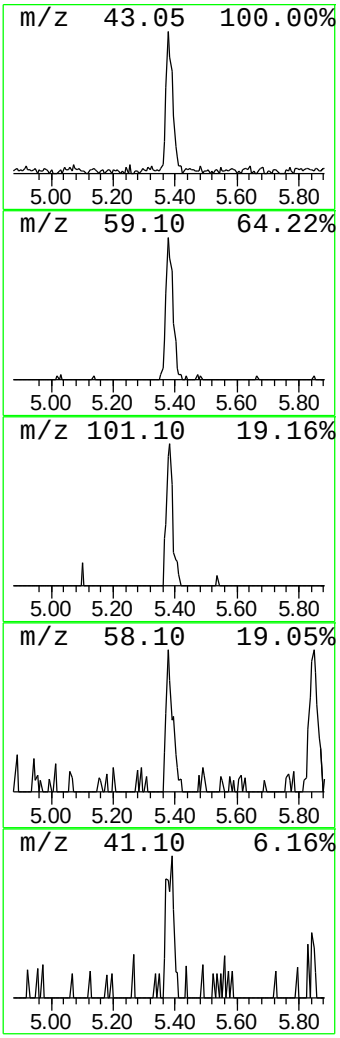
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	5.23 ng	38492	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	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5	3-Octanol	130	C8H18O	000589-98-0	23





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

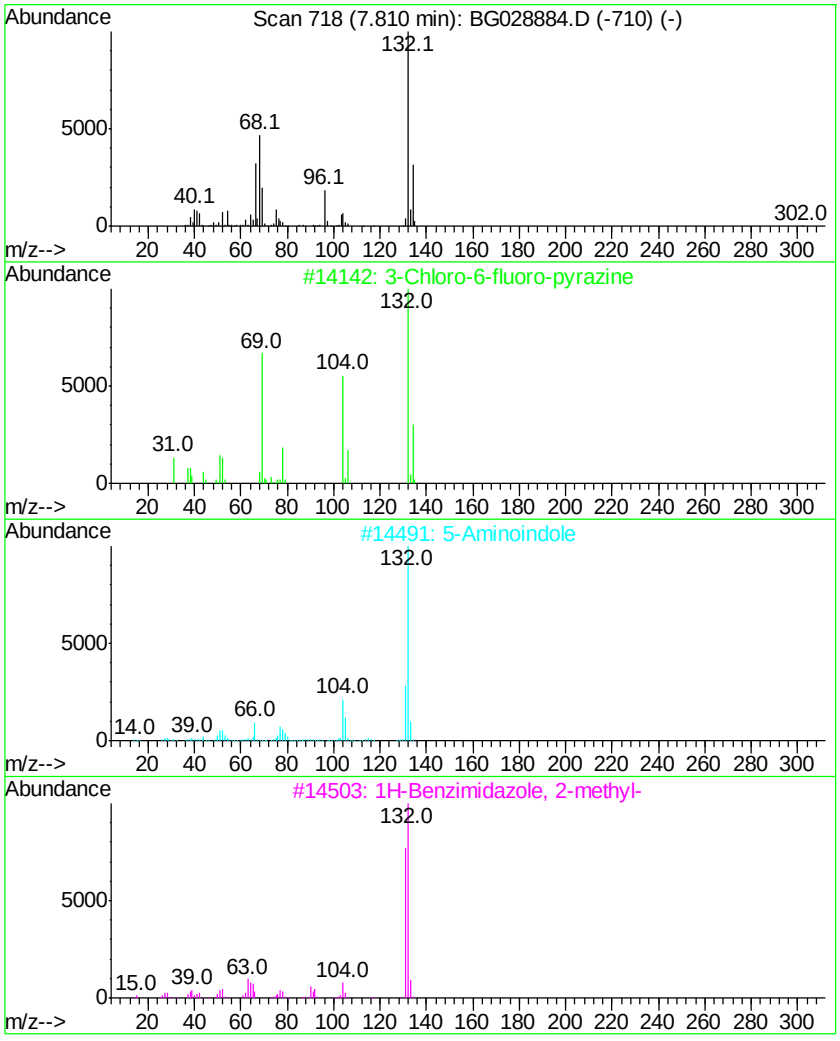
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

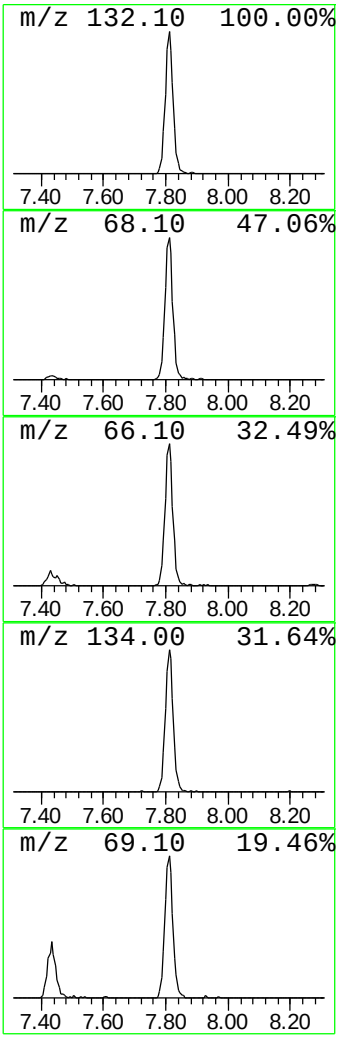
****

Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	97.86 ng	720923	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Benzenebutanal, .gamma.,4-dimethyl-	176	C12H16O	004895-19-6	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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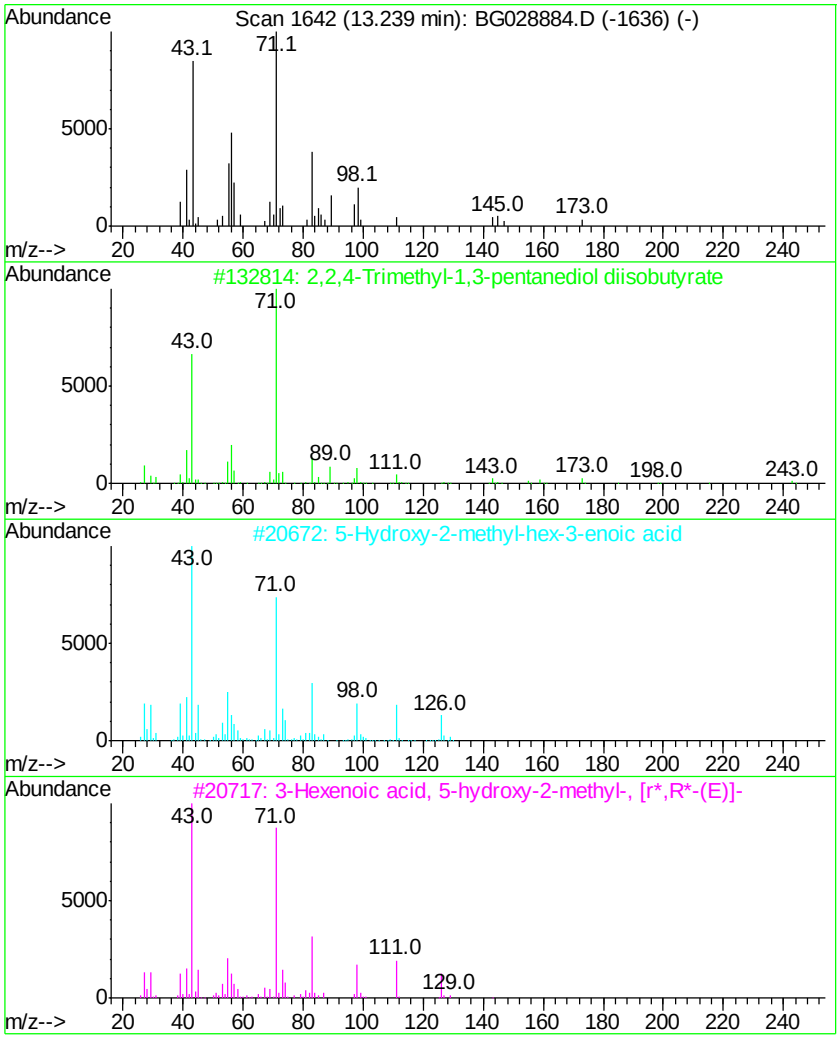
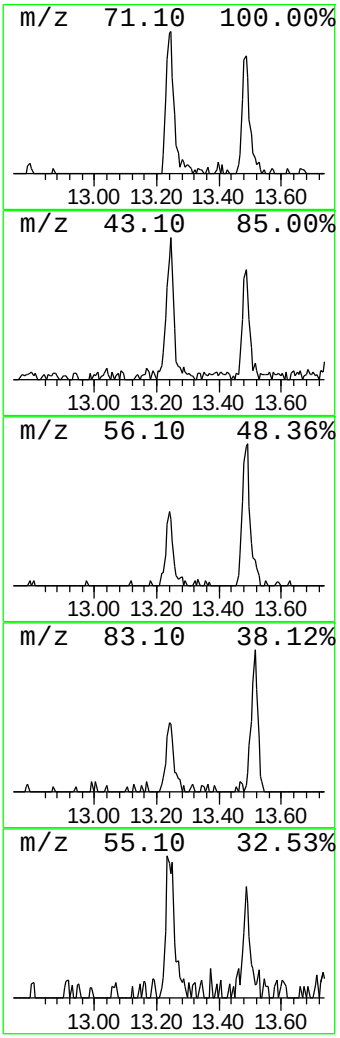
****

Peak Number 4 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	3.10 ng	55977	Acenaphthene-d10	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	50
2	5-Hydroxy-2-methyl-hex-3-enoic acid	144	C7H12O3	1000190-96-0	50
3	3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	47
4	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	40
5	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	40





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ClientSampleId : 20170605-COMP-B

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TIC Library : C:\Database\NIST11.L
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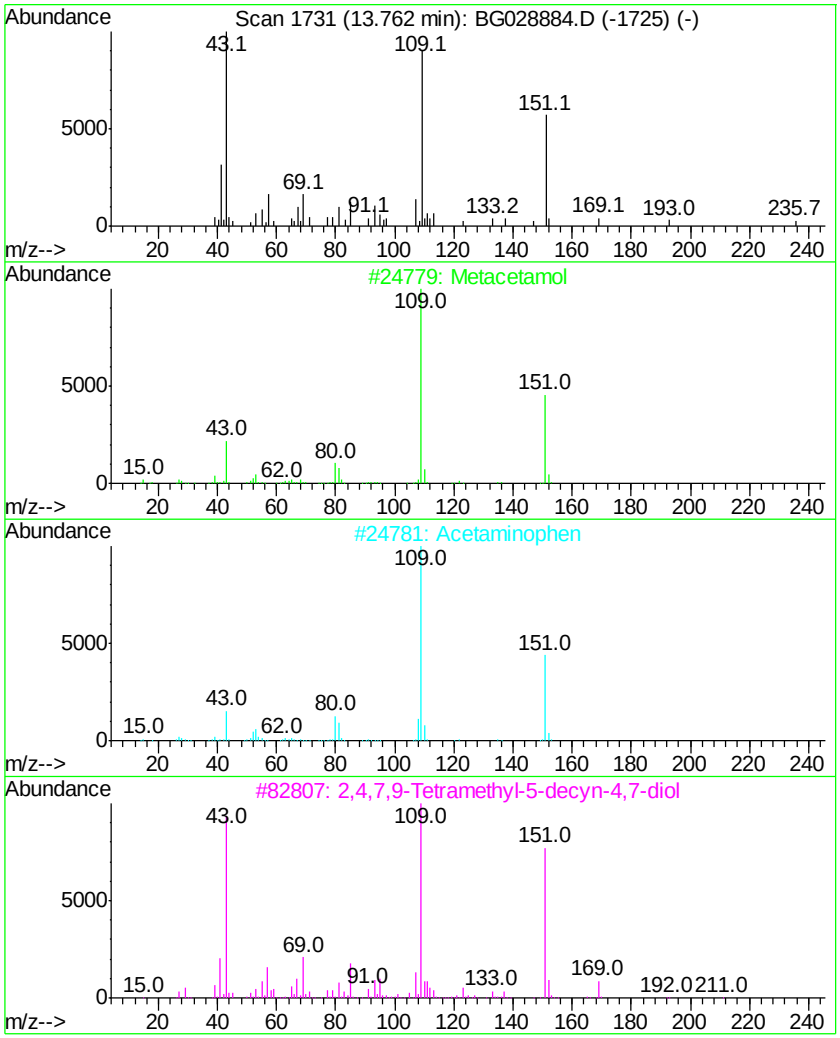
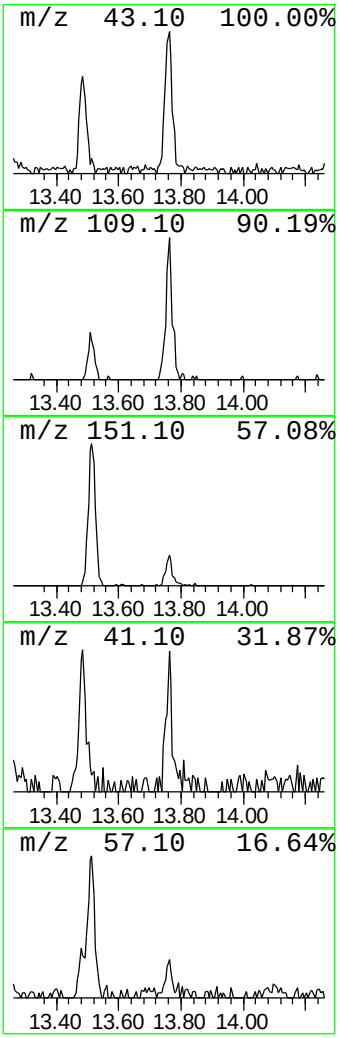
****

Peak Number 5 Metacetamol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	2.86 ng	51560	Acenaphthene-d10	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	59
2	Acetaminophen	151	C8H9NO2	000103-90-2	45
3	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43
4	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	39
5	Ethane-1,2-diamine, N,N'-(1-meth...	276	C12H16N6O2	1000276-72-1	38





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Sample : I5301-08
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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170605-COMP-B

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

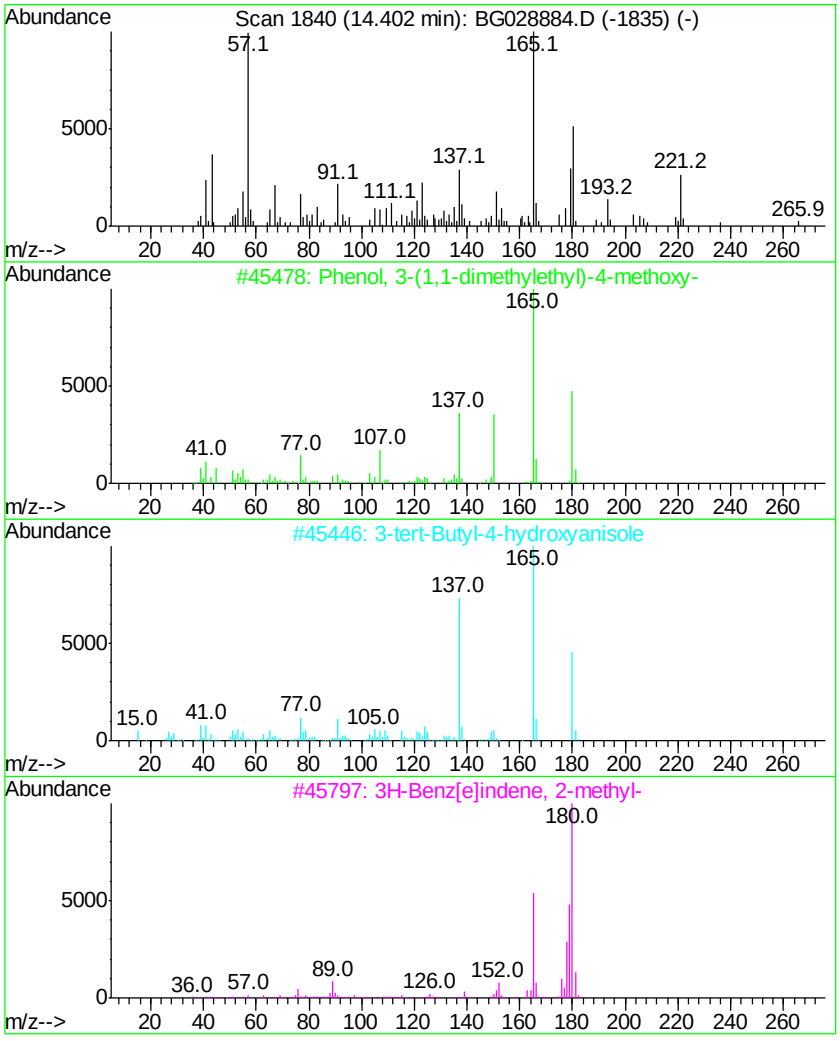
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

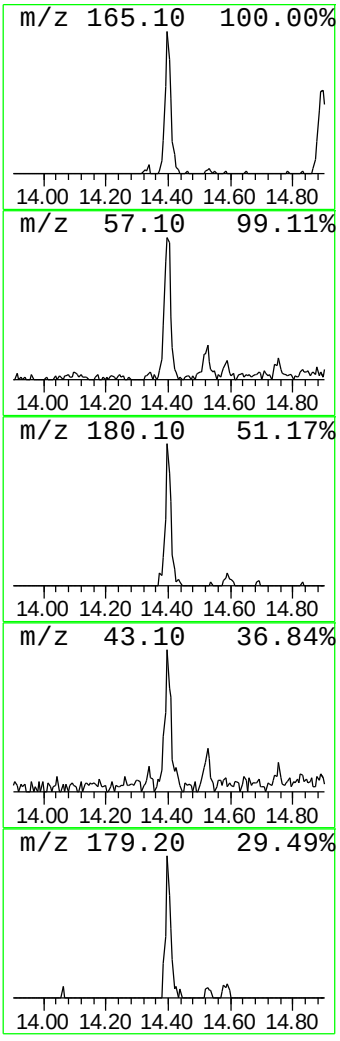
****

Peak Number 6 Phenol, 3-(1,1-dimethylethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	7.07 ng	127467	Acenaphthene-d10	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	64
2	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	58
3	3H-Benz[e]indene, 2-methyl-	180	C14H12	150096-60-9	58
4	Ethylene, 1,1-diphenyl-	180	C14H12	000530-48-3	52
5	Benzenamine, N-ethyl-N-methyl-4-...	180	C9H12N2O2	056269-48-8	49





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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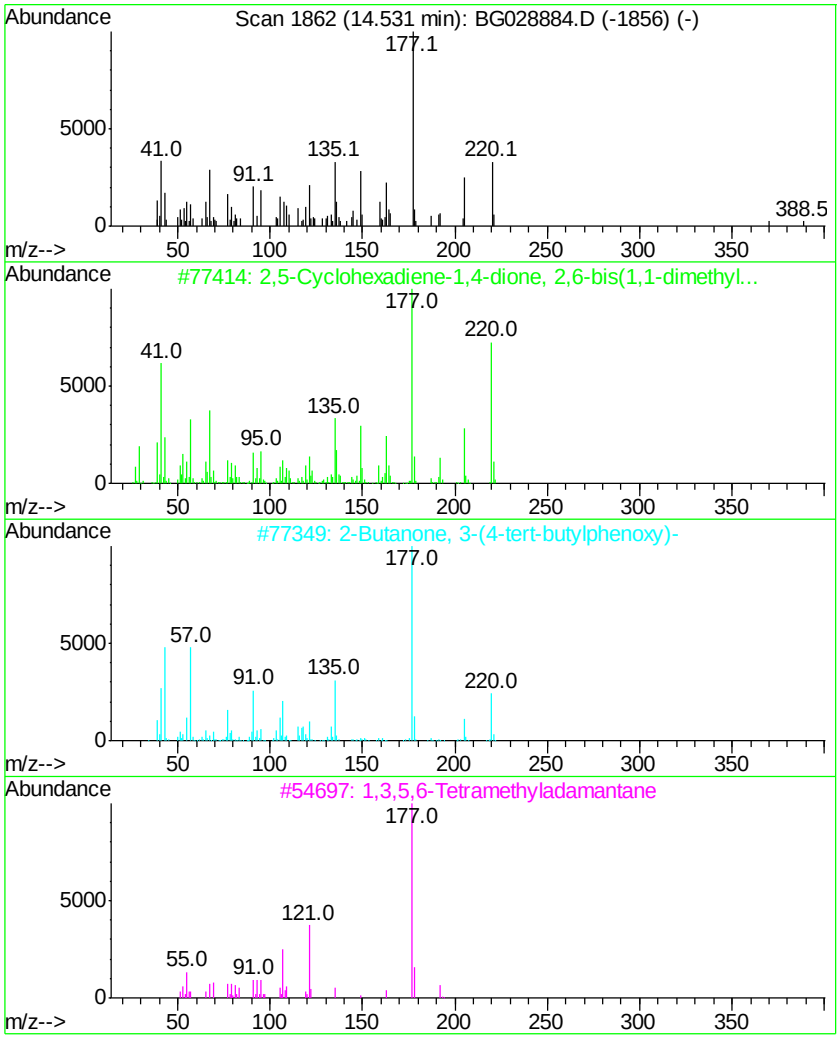
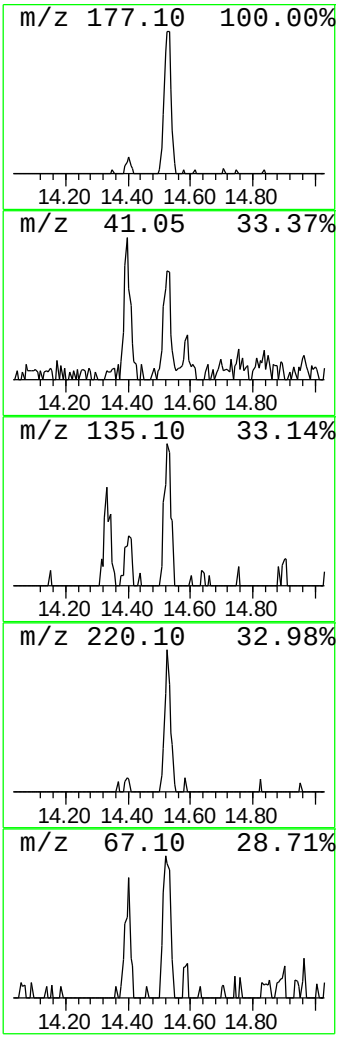
****

Peak Number 7 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	4.59 ng	82702	Acenaphthene-d10	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	91
2	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	64
3	1,3,5,6-Tetramethyladamantane	192	C14H24	034694-70-7	46
4	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	38
5	Benzeneacetic acid, 4-(1,1-dimet...	192	C12H16O2	032857-63-9	30





Library Search Compound Report

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TIC Library : C:\Database\NIST11.L
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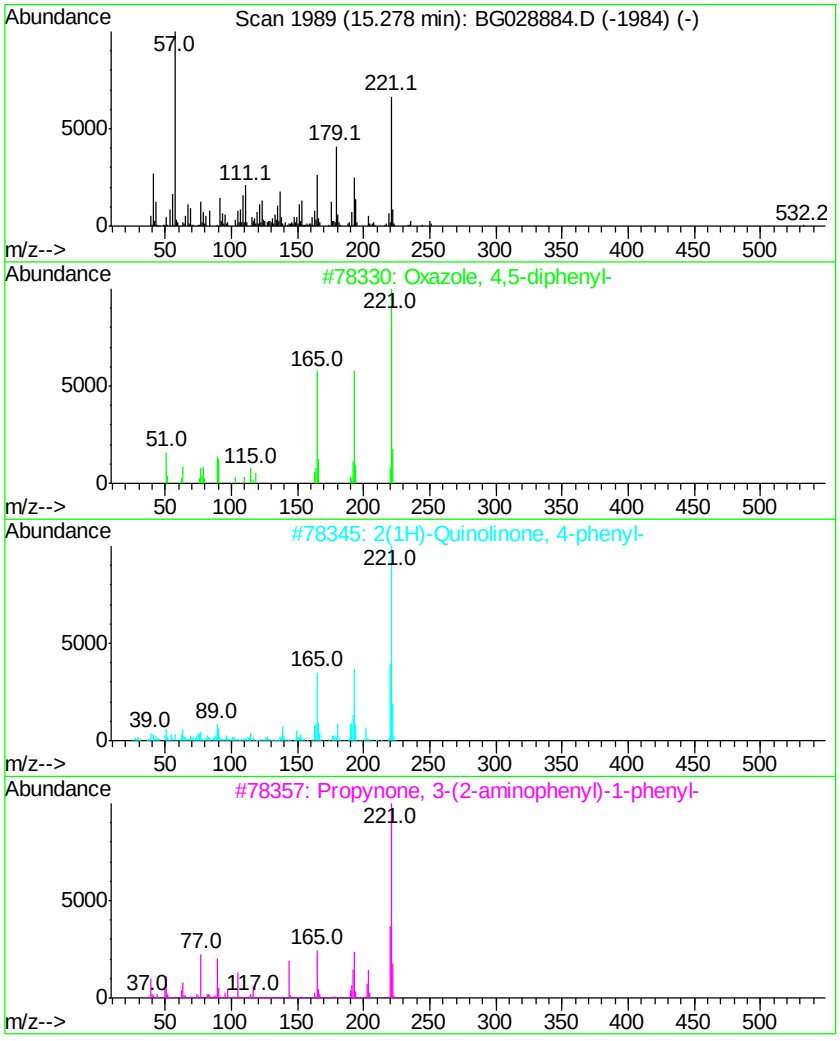
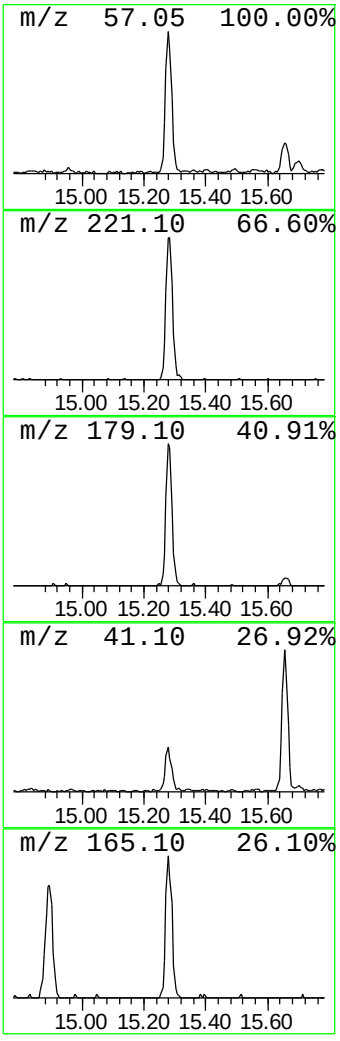
****

Peak Number 8 unknown15.28 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	18.57 ng	334769	Acenaphthene-d10	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazole, 4,5-diphenyl-	221	C15H11NO	004675-18-7	25
2	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	25
3	Propynone, 3-(2-aminophenyl)-1-p...	221	C15H11NO	1000311-26-1	22
4	3-Benzylidene-2-indolinone	221	C15H11NO	003359-49-7	22
5	8-Chloro-9-phenanthroic acid	256	C15H9ClO2	056988-44-4	16





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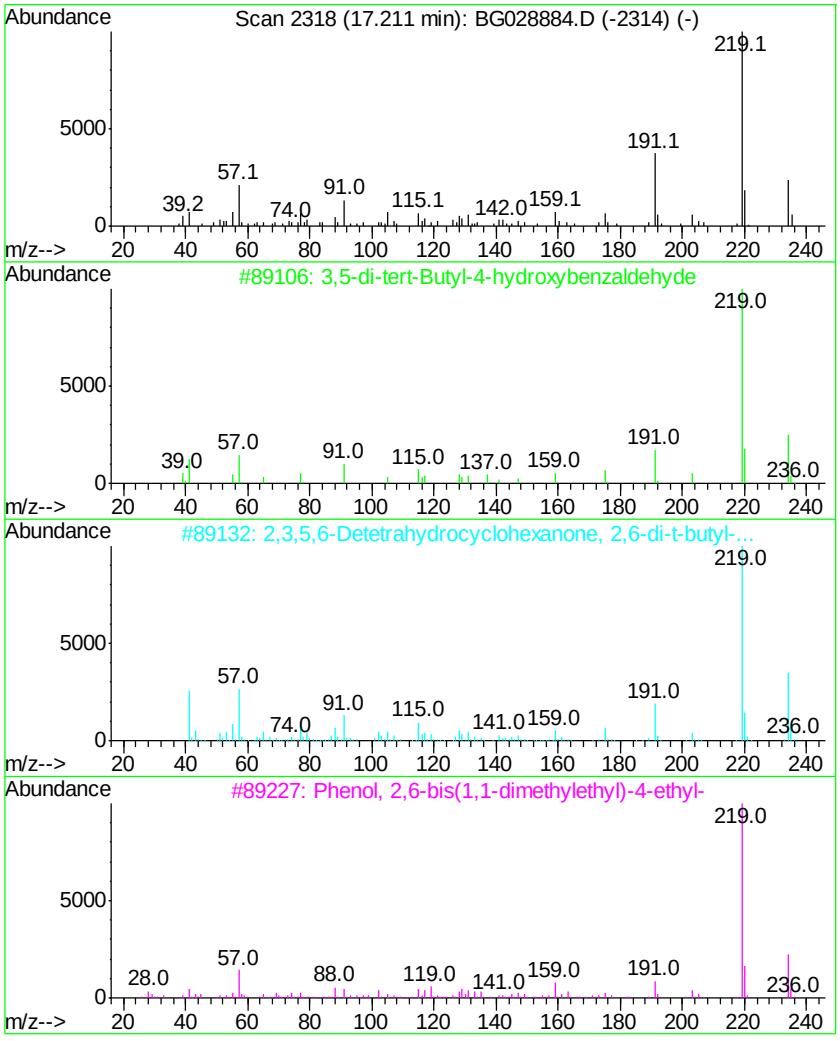
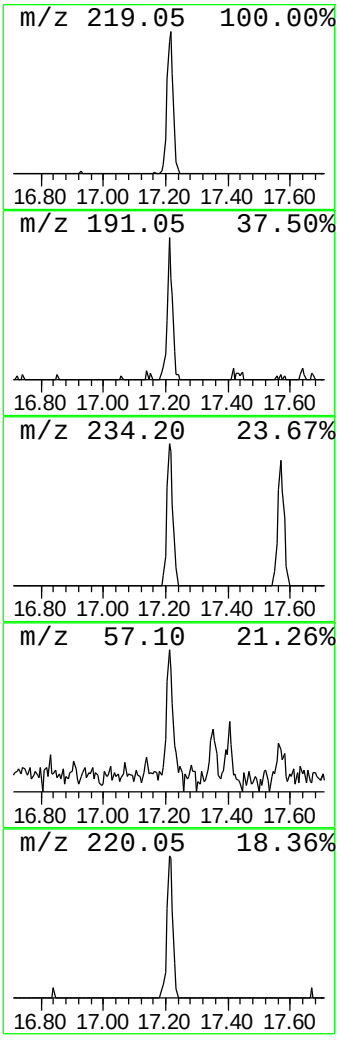
****

Peak Number 10 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	2.61 ng	78346	Phenanthrene-d10	17.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	96
2	2,3,5,6-Detetrahydrocyclohexanon...	234	C15H22O2	101100-38-3	93
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	87
4	6-Tert.butyl-2,3-dicyanonaphthalen	234	C16H14N2	032703-82-5	72
5	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	64





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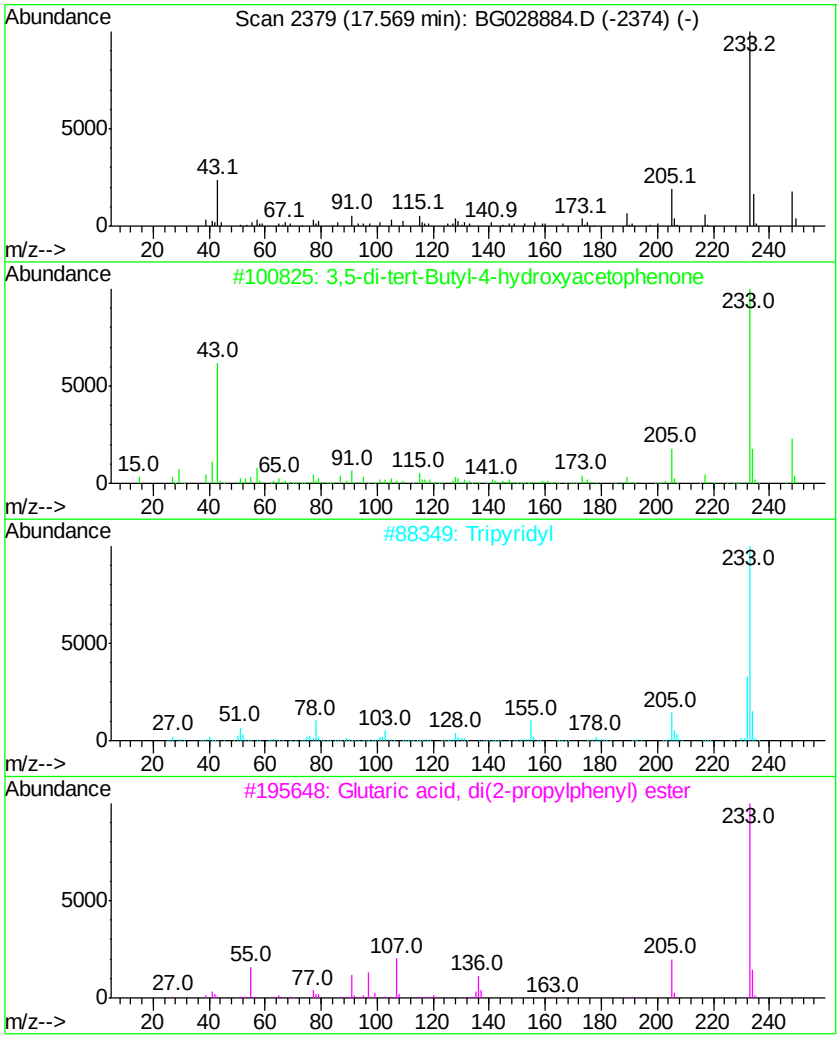
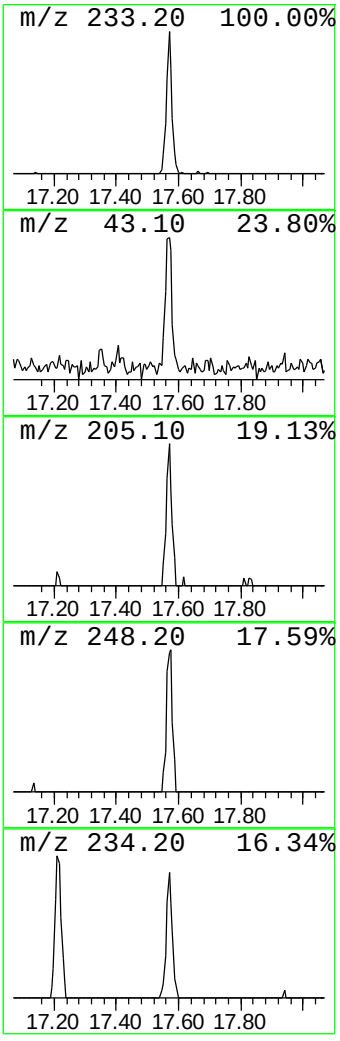
****

Peak Number 11 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	2.13 ng	63873	Phenanthrene-d10	17.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxyaceto...	248	C16H24O2	014035-33-7	95
2	Tripyridyl	233	C15H11N3	001148-79-4	64
3	Glutaric acid, di(2-propylphenyl...	368	C23H28O4	1000359-10-1	64
4	Ethanone, 1-(7-hydroxy-5-methoxy...	248	C14H16O4	000484-18-4	59
5	2-Phenyl-1H-1,3a,8-triaza-cyclop...	233	C15H11N3	1000300-58-5	53





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Instrument : BNA_G
ClientSampleId : 20170605-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

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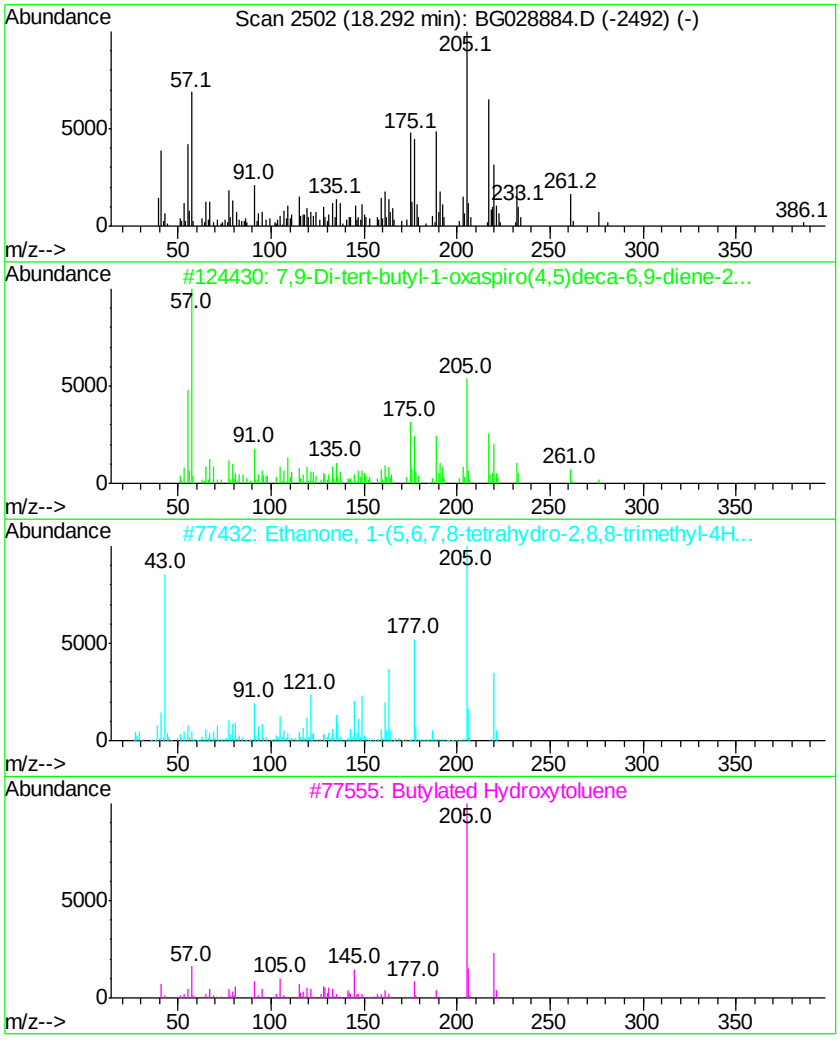
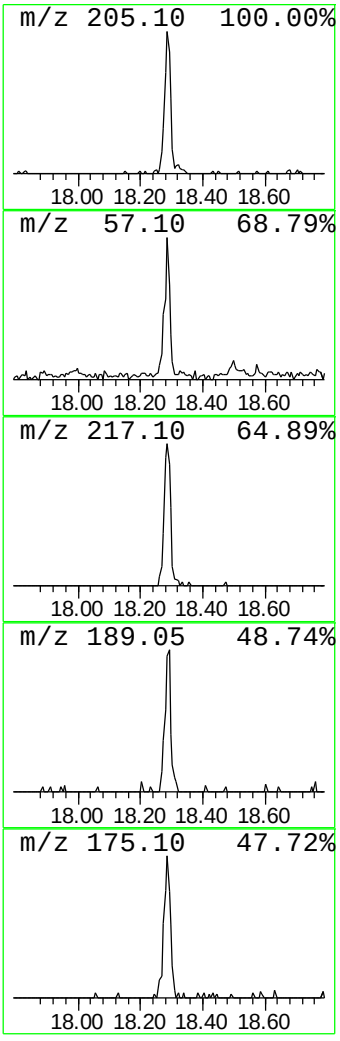
Peak Number 12 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	7.28 ng	218695	Phenanthrene-d10	17.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	95
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	52
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38
4	2,6-Bis(1,1-dimethylethyl)-4-met...	262	C18H30O	004278-82-4	30
5	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	30





Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028884.D
Acq On : 22 Sep 2017 21:20
Operator : SJ/JU
Sample : I5301-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170605-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

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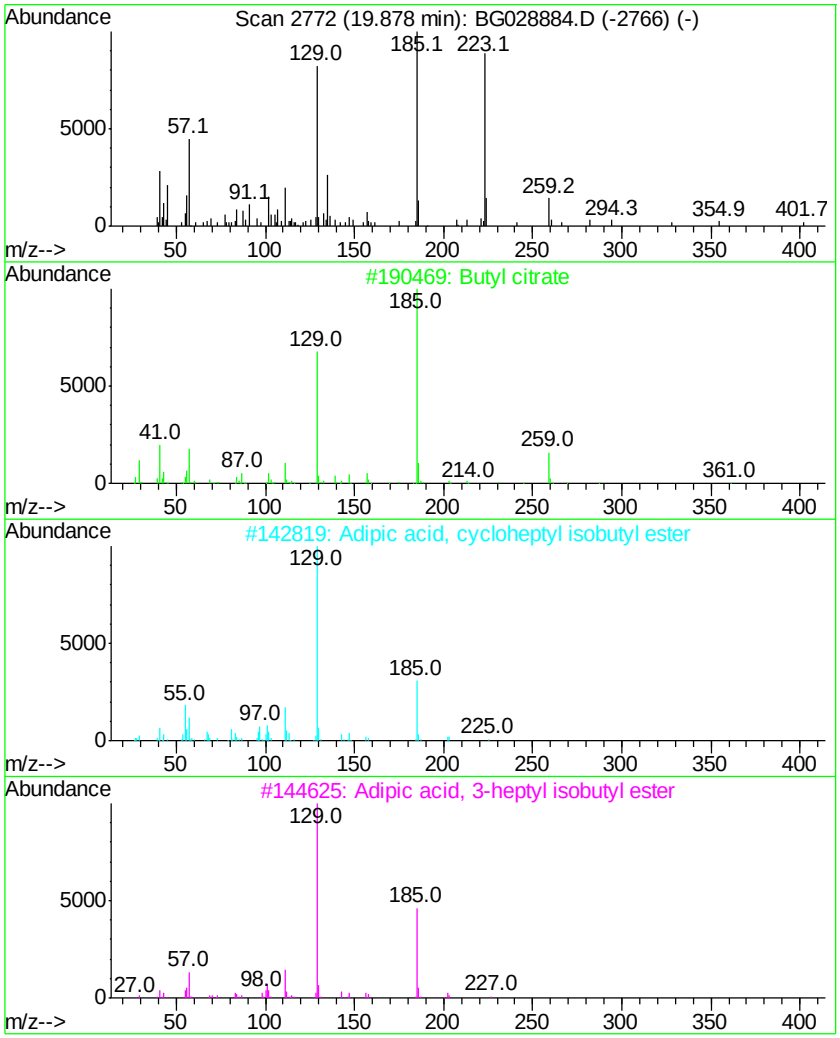
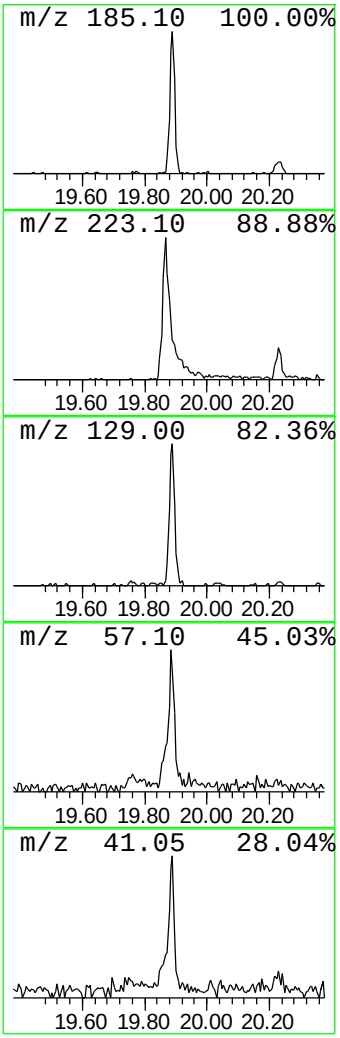
Peak Number 13 Butyl citrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.88	4.39 ng	161367	Chrysene-d12	21.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	76
2	Adipic acid, cycloheptyl isobuty...	298	C17H30O4	1000324-71-5	53
3	Adipic acid, 3-heptyl isobutyl e...	300	C17H32O4	1000353-64-8	53
4	Adipic acid, 2-hexyl isobutyl ester	286	C16H30O4	1000353-70-9	53
5	Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	53





Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028884.D
Acq On : 22 Sep 2017 21:20
Operator : SJ/JU
Sample : I5301-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170605-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

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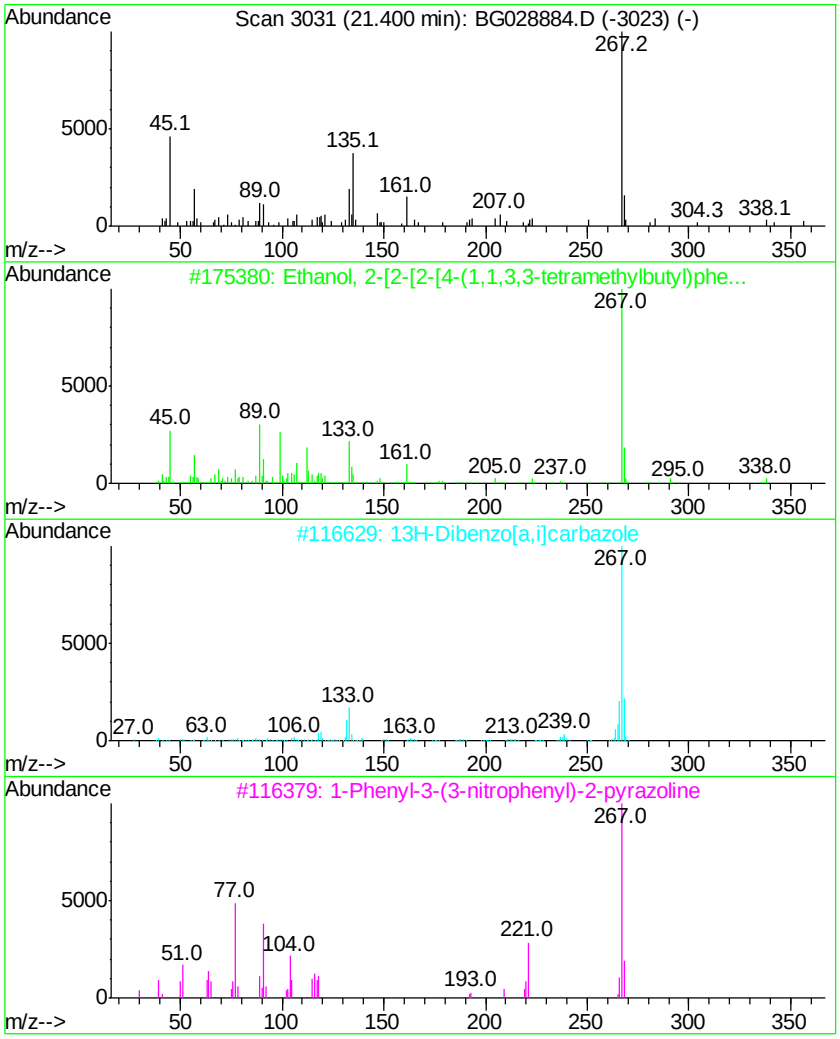
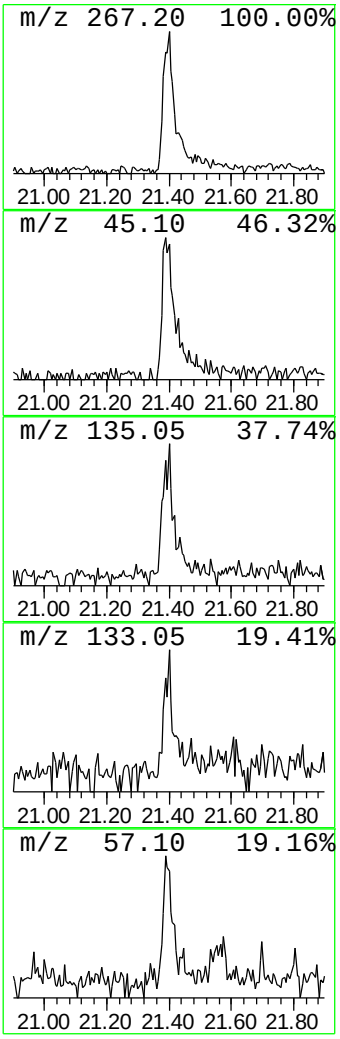
Peak Number 14 Ethanol, 2-[2-[2-[4-(1,1,3,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.85 ng	104568	Chrysene-d12	21.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[2-[4-(1,1,3,3-tet...	338	C20H34O4	002315-62-0	68
2	13H-Dibenzo[a,i]carbazole	267	C20H13N	000239-64-5	43
3	1-Phenyl-3-(3-nitrophenyl)-2-pyr...	267	C15H13N3O2	077242-45-6	38
4	Benzimidazole-2-methanol, .alpha...	298	C17H18N2O3	309724-70-7	38
5	7H-Dibenzo[c,g]carbazole	267	C20H13N	000194-59-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092217\
Data File : BG028884.D
Acq On : 22 Sep 2017 21:20
Operator : SJ/JU
Sample : I5301-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170605-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.38	5.2	ng	38492	1	8.28	147332	20.0
unknown7.81	7.81	97.9	ng	720923	1	8.28	147332	20.0
2,2,4-Trimethyl-1...	13.24	3.1	ng	55977	3	14.90	360561	20.0
Metacetamol	13.76	2.9	ng	51560	3	14.90	360561	20.0
Phenol, 3-(1,1-di...	14.40	7.1	ng	127467	3	14.90	360561	20.0
2,5-Cyclohexadien...	14.53	4.6	ng	82702	3	14.90	360561	20.0
unknown15.28	15.28	18.6	ng	334769	3	14.90	360561	20.0
3,5-di-tert-Butyl...	17.21	2.6	ng	78346	4	17.65	601103	20.0
3,5-di-tert-Butyl...	17.57	2.1	ng	63873	4	17.65	601103	20.0
7,9-Di-tert-butyl...	18.29	7.3	ng	218695	4	17.65	601103	20.0
Butyl citrate	19.88	4.4	ng	161367	5	21.96	734348	20.0
Ethanol, 2-[2-[2-...	21.40	2.9	ng	104568	5	21.96	734348	20.0