LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092317\
Data File : BG028892.D
Acq On : 23 Sep 2017 11:00
Operator : SJ/JU
Sample : I5321-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170610-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	5.383	299	305	311	rBV	30833	51587	1.38%	0.376%
2	5.847	377	384	395	rBV	271620	478751	12.77%	3.490%
3	7.433	646	654	666	rBV	205477	394680	10.52%	2.877%
4	7.809	709	718	727	rBV	461089	798874	21.30%	5.823%
5	8.279	791	798	804	rBV	87627	161247	4.30%	1.175%
6	8.602	846	853	863	rVB	378144	678503	18.09%	4.946%
7	9.448	988	997	1008	rBV	307909	589564	15.72%	4.298%
8	11.093	1270	1277	1285	rBV	118538	223136	5.95%	1.627%
9	13.514	1677	1689	1699	rBV	1018725	1621800	43.24%	11.822%
10	14.895	1917	1924	1931	rBV2	217419	365673	9.75%	2.666%
11	15.277	1984	1989	1994	rBV3	58844	80670	2.15%	0.588%
12	15.653	2049	2053	2058	rBV	113410	154260	4.11%	1.124%
13	16.381	2170	2177	2189	rBV	1116359	1820684	48.55%	13.272%
14	17.645	2385	2392	2401	rBV	401692	624251	16.64%	4.550%
15	18.285	2491	2501	2507	rBV3	135987	196442	5.24%	1.432%
16	19.889	2767	2774	2786	rVB	161984	217838	5.81%	1.588%
17	20.230	2825	2832	2842	rBV	2864170	3750454	100.00%	27.338%
18	21.957	3119	3126	3135	rVB2	428682	761063	20.29%	5.548%
19	25.412	3703	3714	3726	rVB2	240129	749222	19.98%	5.461%

Sum of corrected areas: 13718699

LSC Report - Integrated Chromatogram

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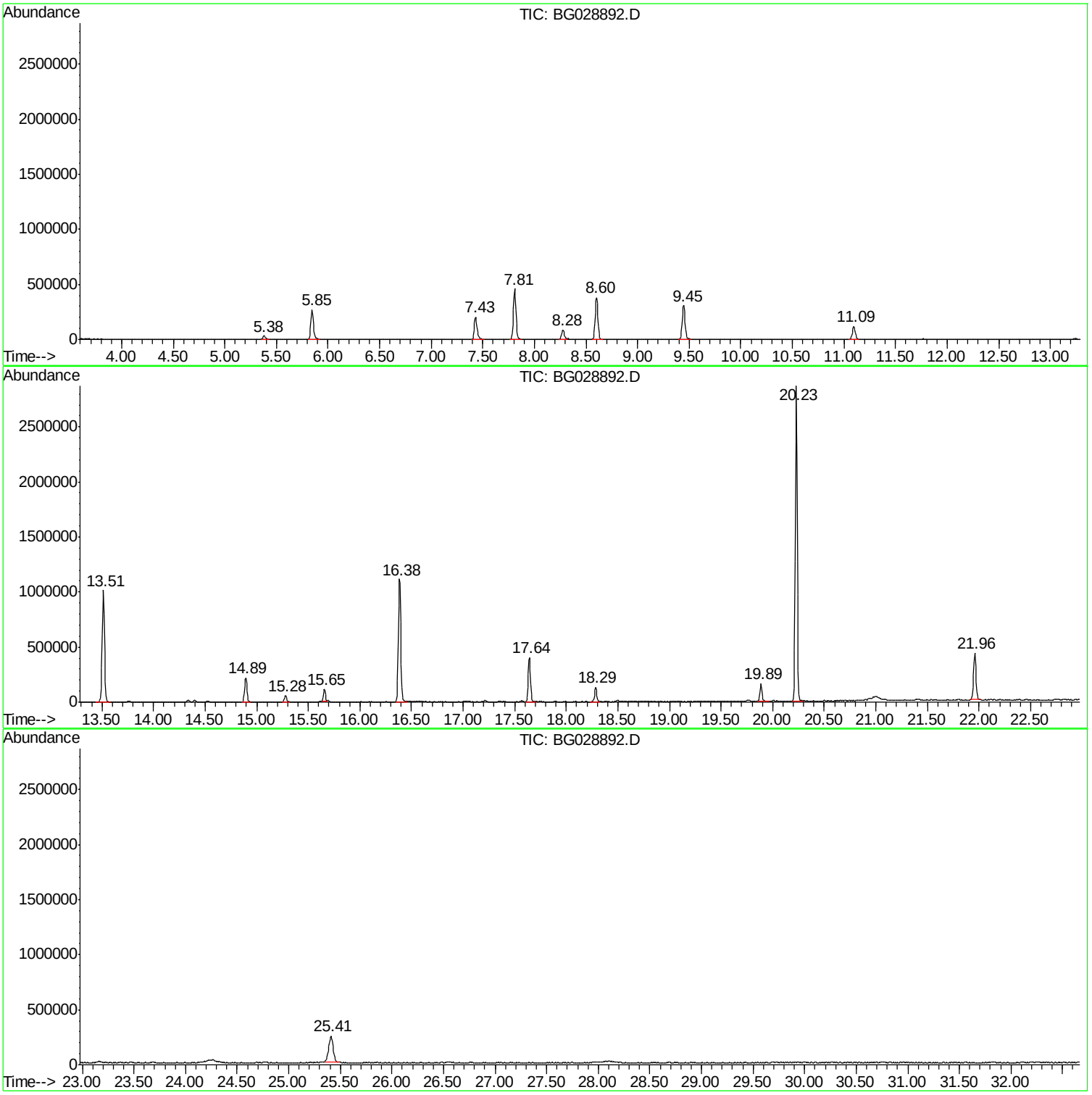
Instrument : BNA_G
ClientSampleId : 20170610-COMP-A

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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Operator : SJ/JU
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Instrument : BNA_G
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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

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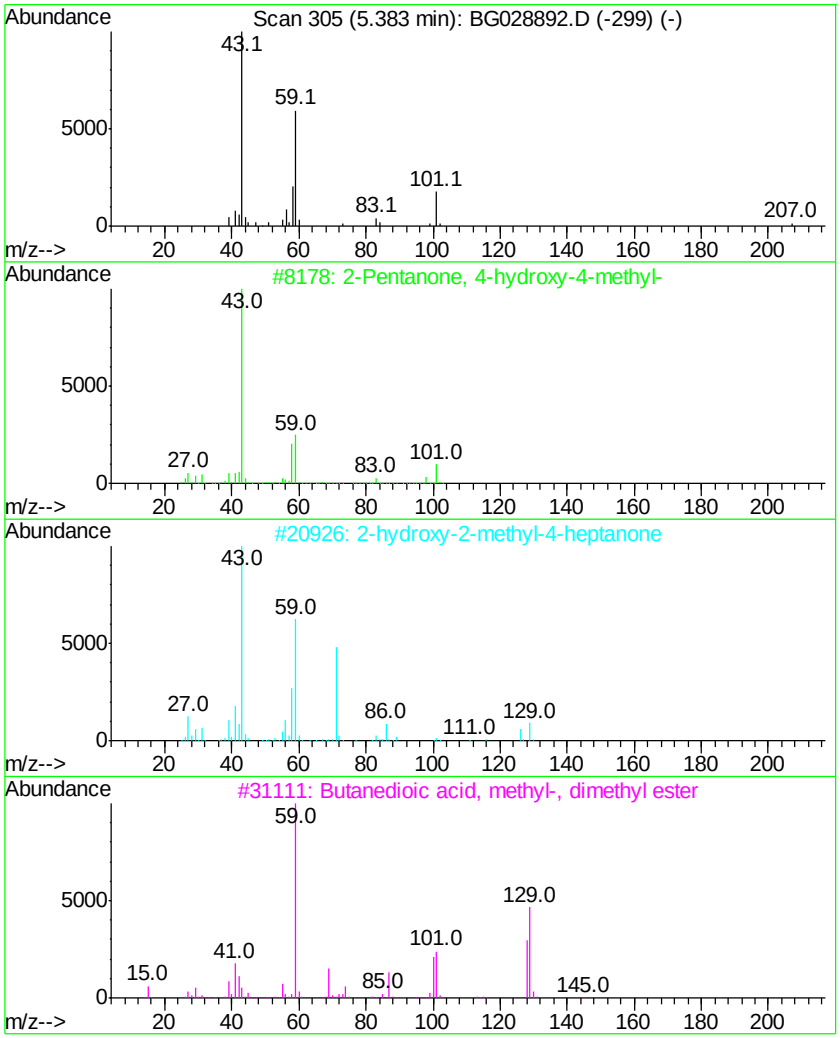
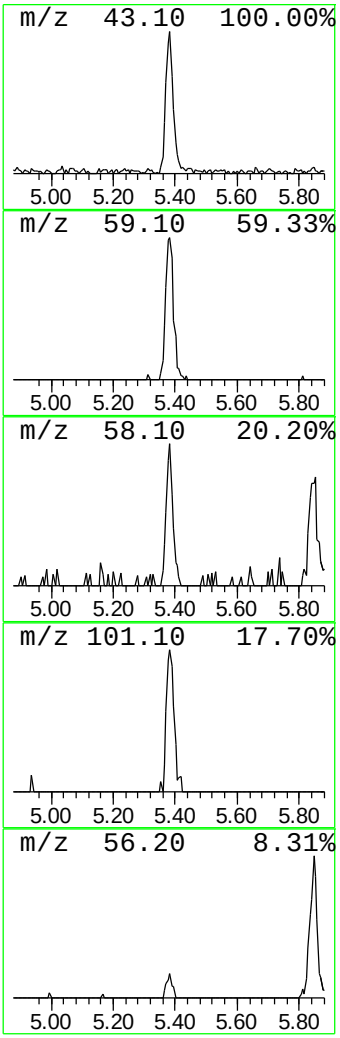
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	6.40 ng	51587	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	53
2	2-hydroxy-2-methyl-4-heptanone	144	C8H16O2	054862-91-8	45
3	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	32
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	25





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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170610-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
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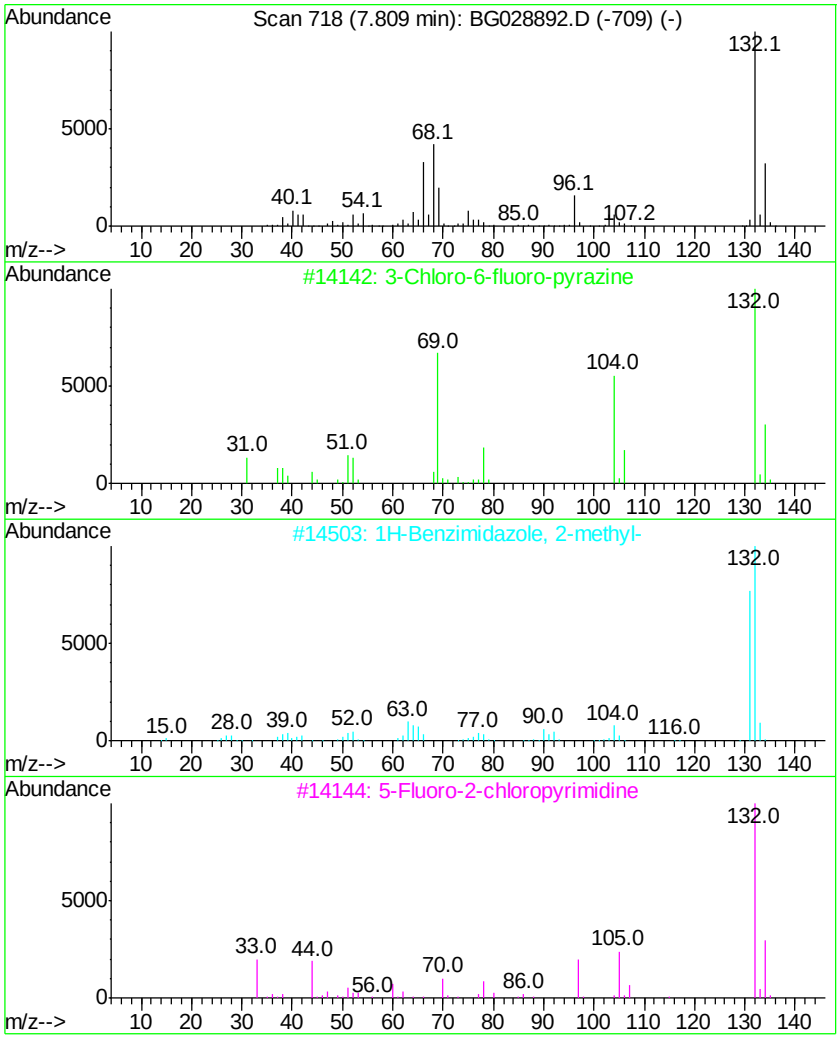
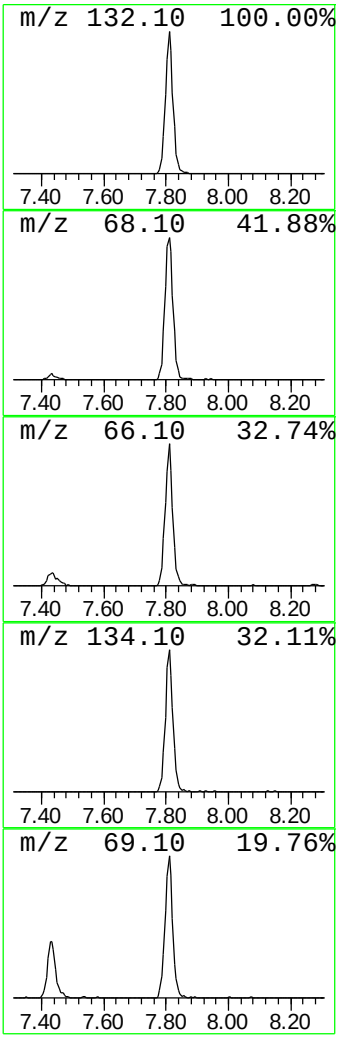
Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	99.09 ng	798874	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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092317\
Data File : BG028892.D
Acq On : 23 Sep 2017 11:00
Operator : SJ/JU
Sample : I5321-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170610-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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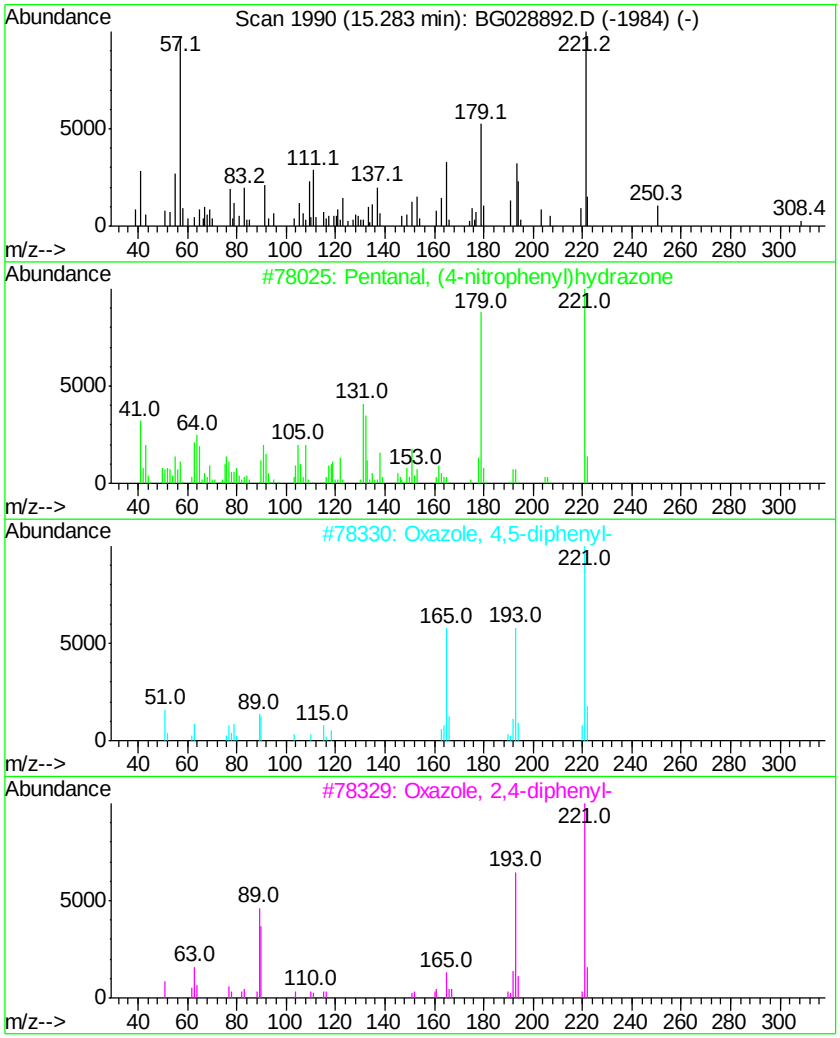
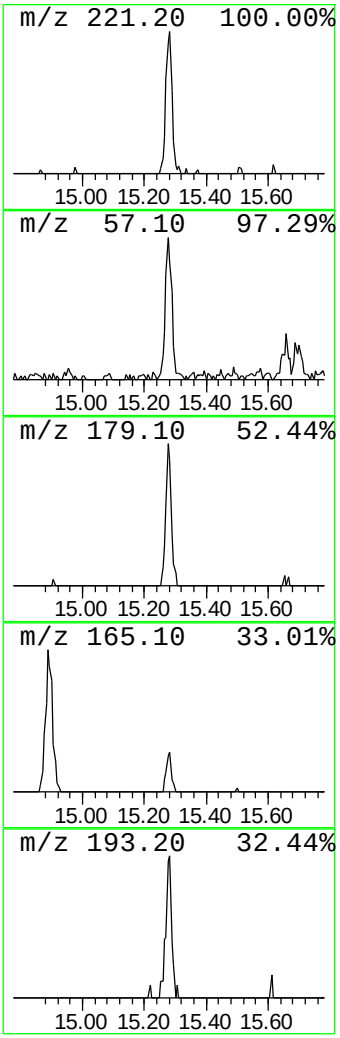
Peak Number 4 unknown15.28 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	4.41 ng	80670	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal, (4-nitrophenyl)hydrazone	221	C11H15N3O2	005873-64-3	46
2	Oxazole, 4,5-diphenyl-	221	C15H11NO	004675-18-7	43
3	Oxazole, 2,4-diphenyl-	221	C15H11NO	000838-41-5	43
4	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	43
5	2-(Trifluoromethyl)-7H-1,3,4-thi...	221	C6H2F3N3OS	094605-13-7	38





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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170610-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
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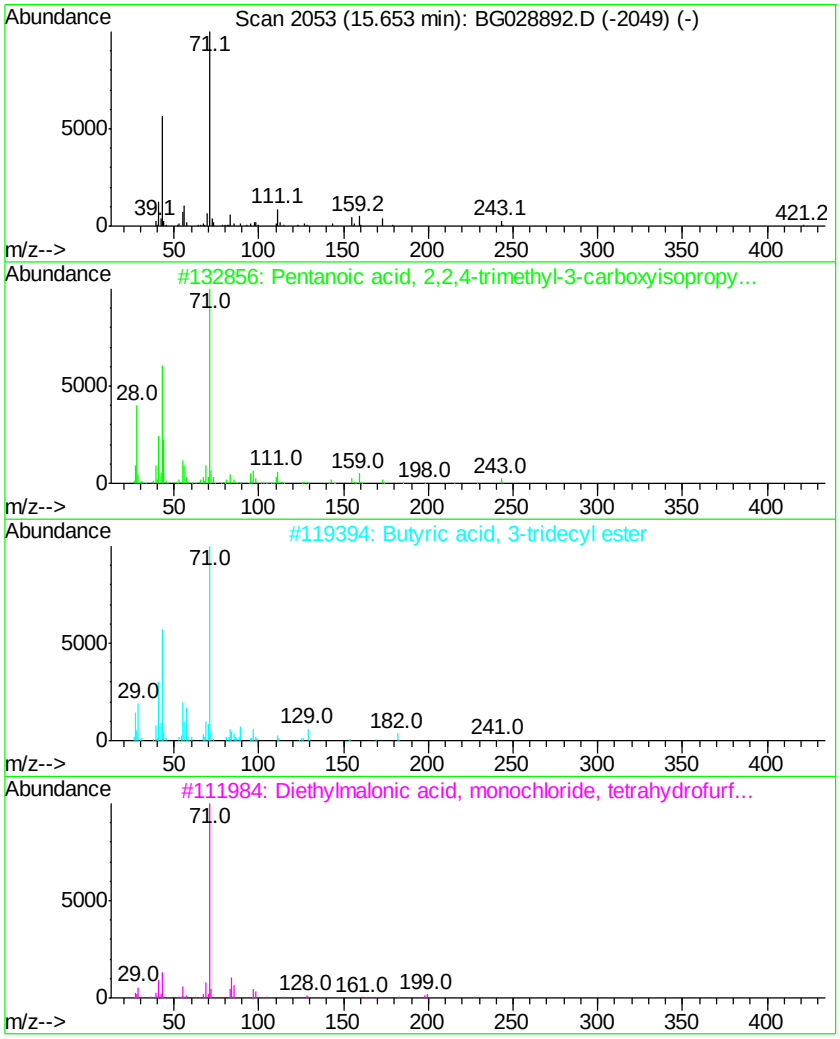
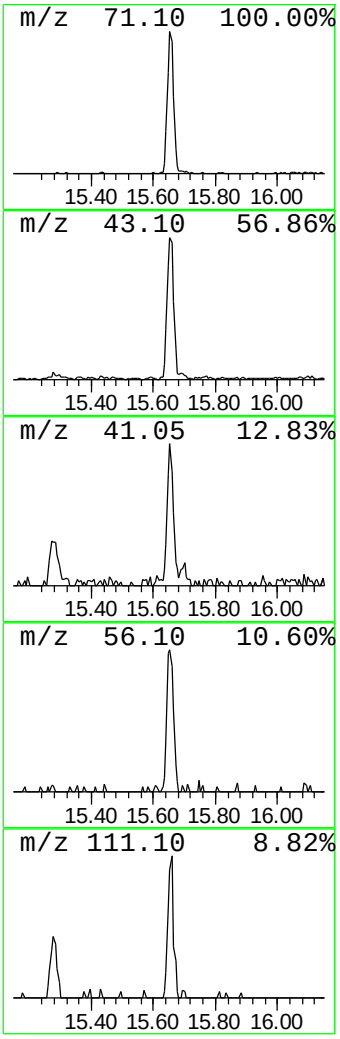
Peak Number 5 Pentanoic acid, 2,2,4-trime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	8.44 ng	154260	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	56
2	Butyric acid, 3-tridecyl ester	270	C17H34O2	1000280-56-8	50
3	Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	42
4	Butyric acid, thio-, S-decyl ester	244	C14H28OS	002432-55-5	36
5	4-Heptanone, 3-ethyl-	142	C9H18O	001528-25-2	36





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Instrument : BNA_G
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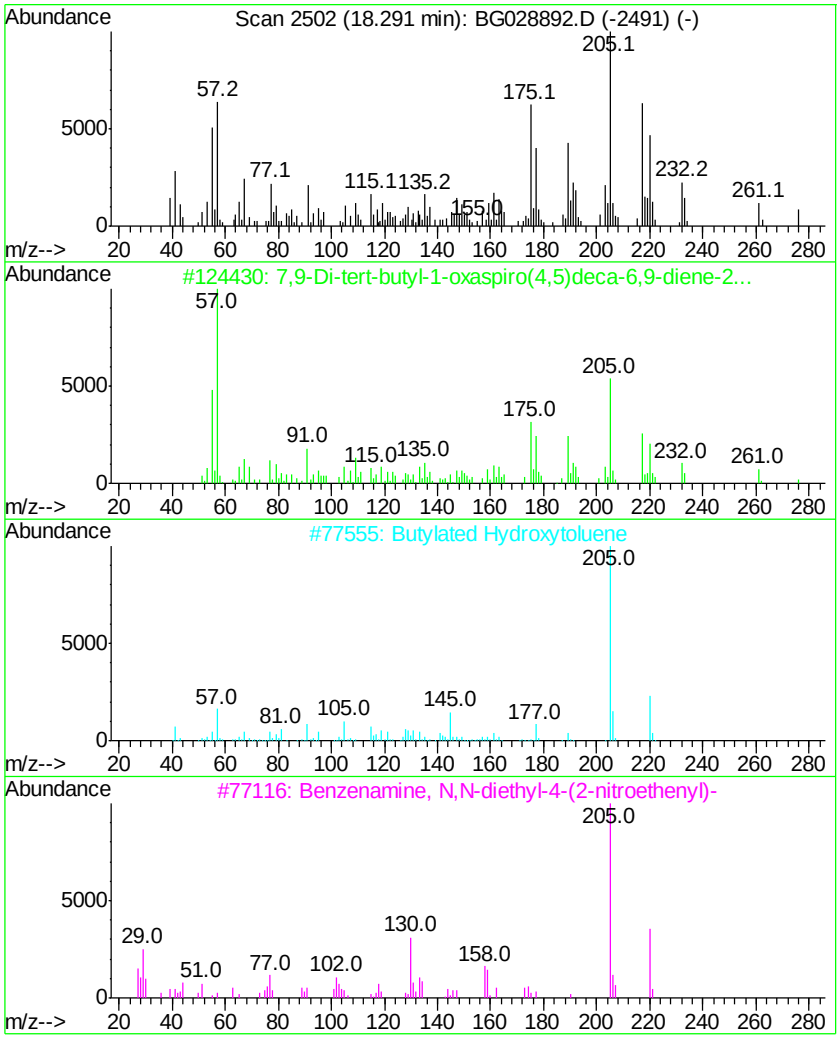
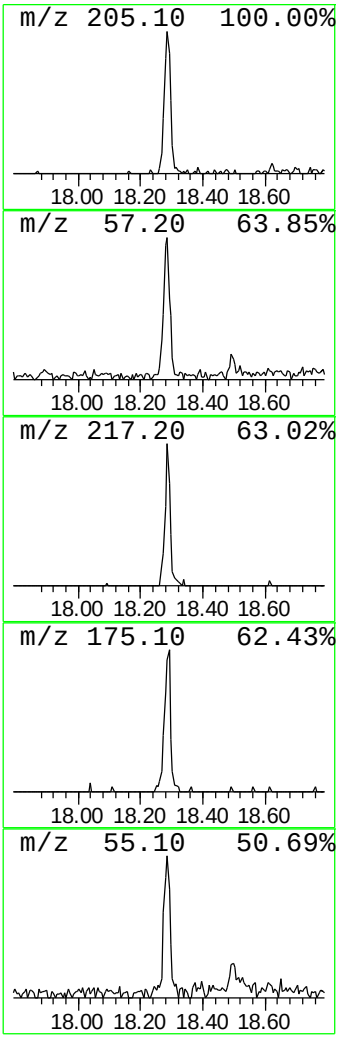
****

Peak Number 6 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	6.29 ng	196442	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	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38
3	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	35
4	1,4-Naphthoquinone, 6-acetyl-2,5...	232	C12H8O5	013378-90-0	30
5	Pyrido[3,4-d]pyridazin-1(2H)-one...	205	C9H11N5O	1000271-08-5	25





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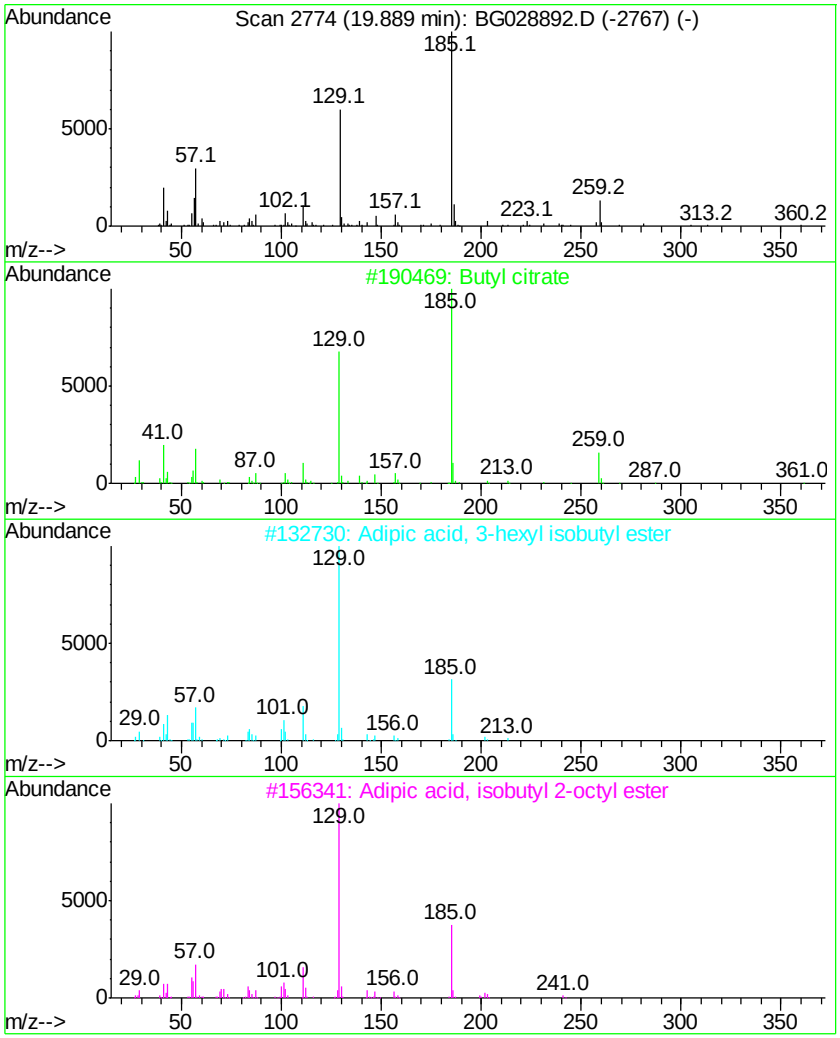
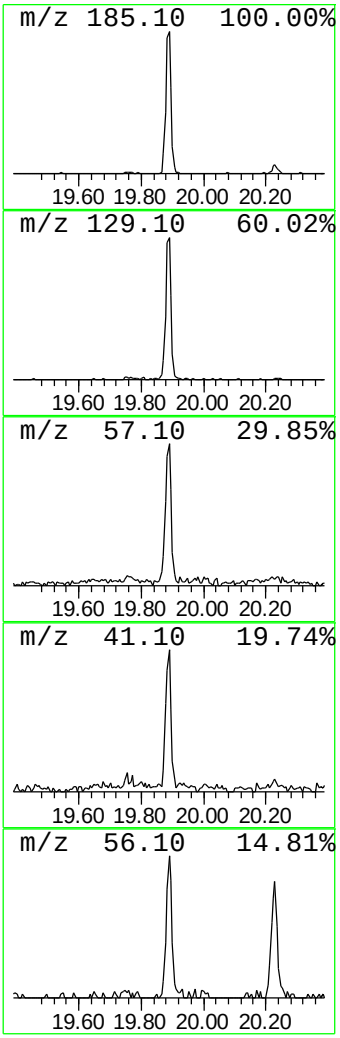
****

Peak Number 7 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	5.72 ng	217838	Chrysene-d12	21.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	72
3	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	72
4	Adipic acid, 2,4-dimethylpent-3-...	300	C17H32O4	1000349-77-6	64
5	Adipic acid, 4-bromophenyl butyl...	356	C16H21BrO4	1000324-37-9	64





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.38	6.4	ng	51587	1	8.28	161247	20.0
unknown7.81	7.81	99.1	ng	798874	1	8.28	161247	20.0
unknown15.28	15.28	4.4	ng	80670	3	14.89	365673	20.0
Pentanoic acid, 2...	15.65	8.4	ng	154260	3	14.89	365673	20.0
7,9-Di-tert-butyl...	18.29	6.3	ng	196442	4	17.64	624251	20.0
Butyl citrate	19.89	5.7	ng	217838	5	21.96	761063	20.0