LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028886.D
Acq On : 22 Sep 2017 22:39
Operator : SJ/JU
Sample : I5301-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170604-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	5.375	300	304	310	rBV	26542	42658	1.11%	0.298%
2	5.845	376	384	398	rBV	283666	485743	12.68%	3.396%
3	7.431	645	654	664	rBV	194034	382549	9.99%	2.675%
4	7.807	711	718	728	rBV	466302	835728	21.82%	5.843%
5	8.277	792	798	803	rBV	85226	149455	3.90%	1.045%
6	8.601	845	853	861	rBV	395695	712821	18.61%	4.984%
7	9.447	989	997	1011	rBV	337349	634328	16.56%	4.435%
8	11.098	1270	1278	1287	rBV2	110677	207668	5.42%	1.452%
9	13.512	1680	1689	1696	rBV	1075170	1653627	43.18%	11.561%
10	14.400	1835	1840	1846	rVB3	45139	56720	1.48%	0.397%
11	14.893	1918	1924	1932	rBV3	214558	355515	9.28%	2.486%
12	15.281	1984	1990	1995	rBV	116847	165571	4.32%	1.158%
13	15.657	2049	2054	2059	rBV	228926	288019	7.52%	2.014%
14	16.386	2170	2178	2190	rBV	1226865	1908870	49.85%	13.346%
15	17.214	2313	2319	2324	rVB2	24902	40162	1.05%	0.281%
16	17.643	2385	2392	2399	rBV2	379769	591673	15.45%	4.137%
17	18.283	2494	2501	2507	rBV3	84505	136376	3.56%	0.953%
18	19.887	2764	2774	2780	rBV	209034	277804	7.25%	1.942%
19	20.228	2826	2832	2839	rBV	2811178	3829527	100.00%	26.774%
20	21.397	3025	3031	3039	rBV4	24907	66591	1.74%	0.466%
21	21.961	3120	3127	3136	rBV	443408	763178	19.93%	5.336%
22	25.410	3704	3714	3725	rBV	238327	718334	18.76%	5.022%

Sum of corrected areas: 14302917

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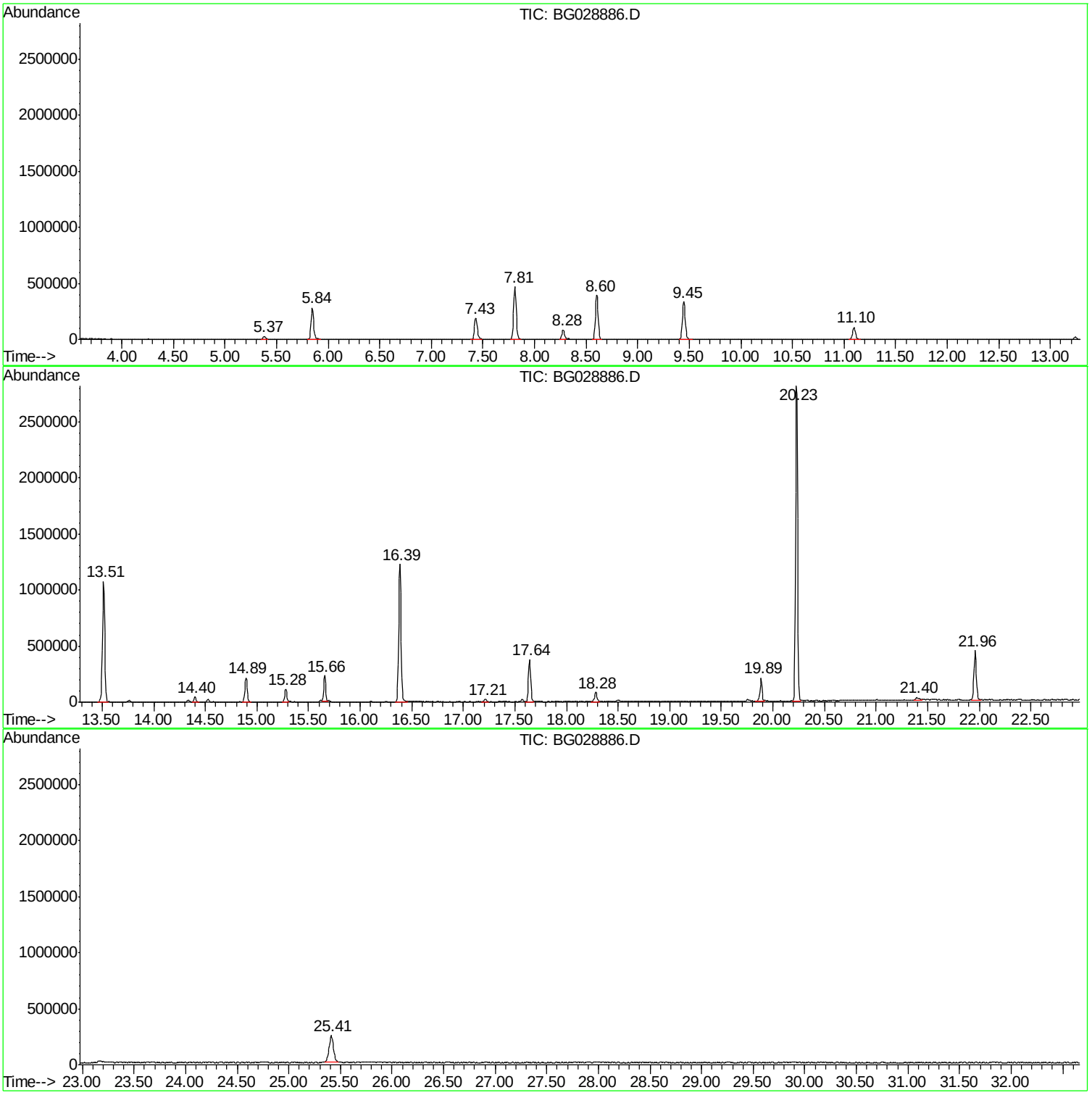
20170604-COMP-A

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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TIC Library : C:\Database\NIST11.L
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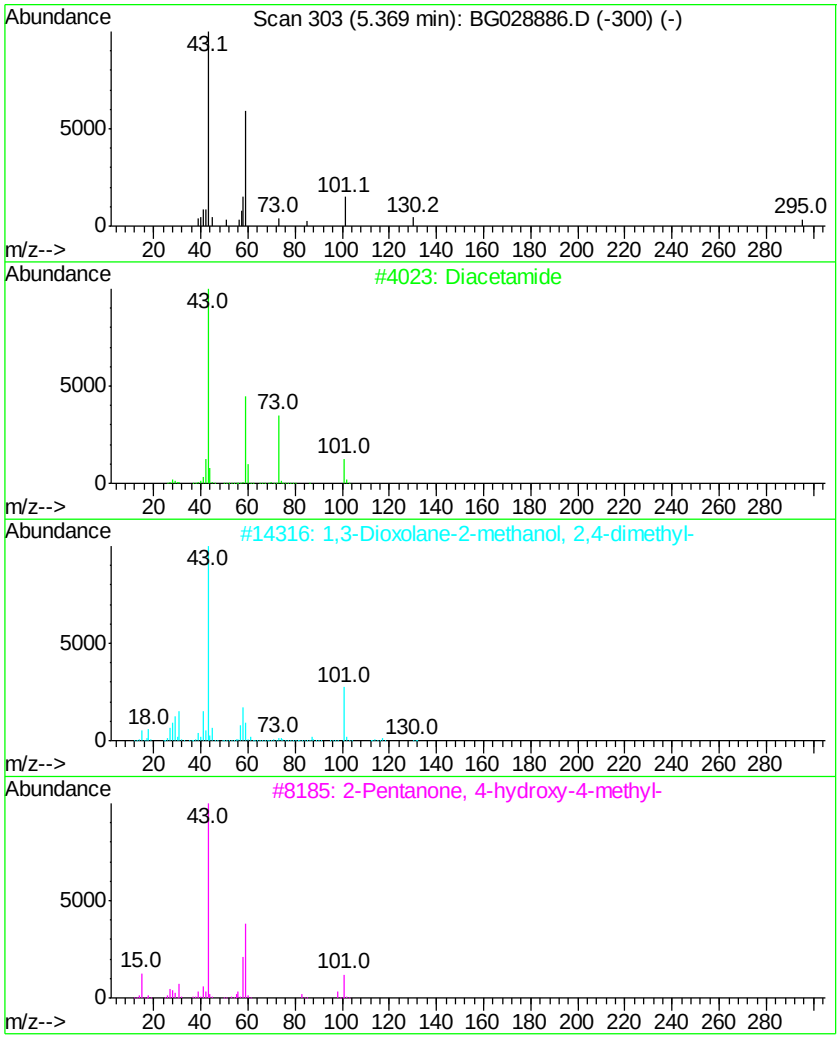
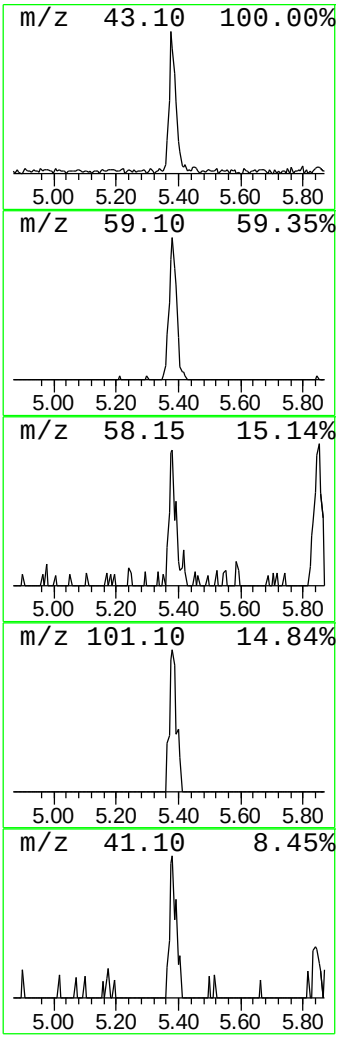
Peak Number 1 unknown5.37 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.37	5.71 ng	42658	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diacetamide	101	C4H7NO2	000625-77-4	9
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	7
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7





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TIC Library : C:\Database\NIST11.L
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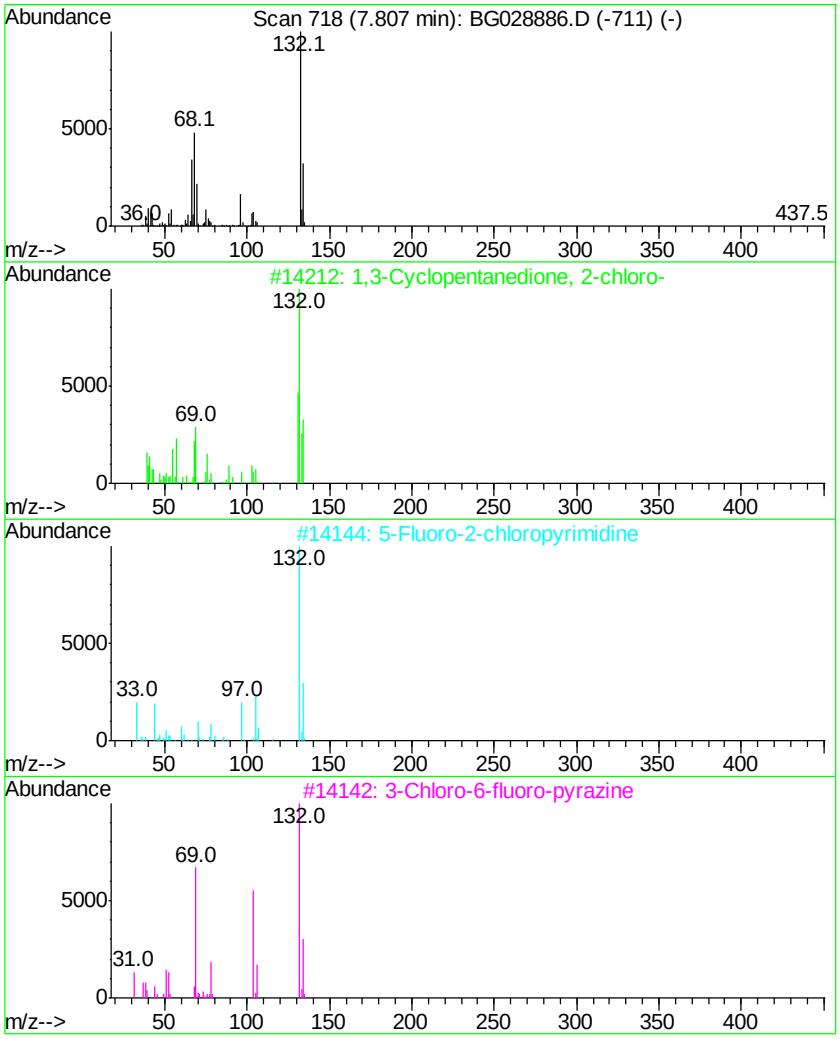
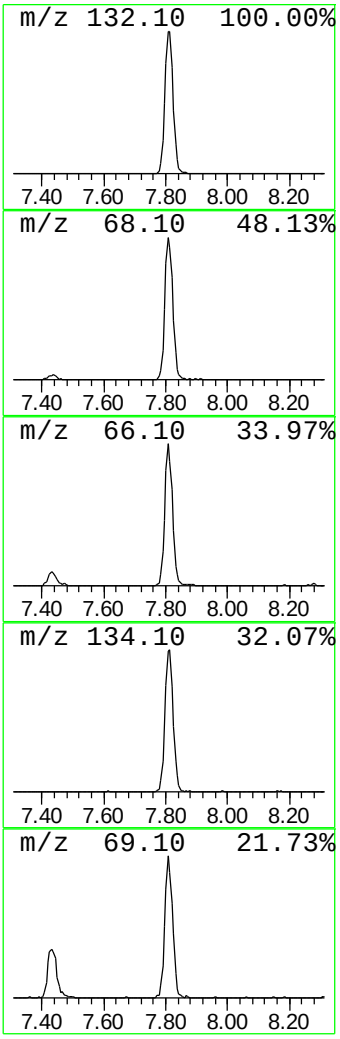
Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	111.84 ng	835728	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Sample : I5301-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170604-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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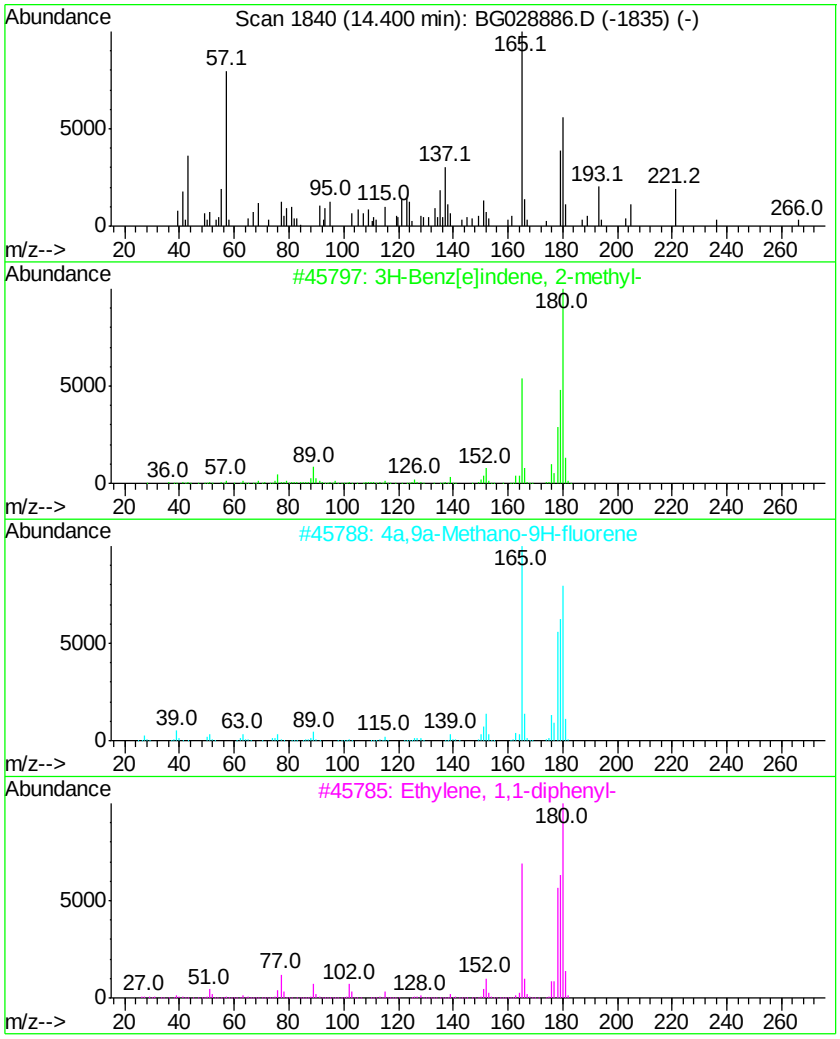
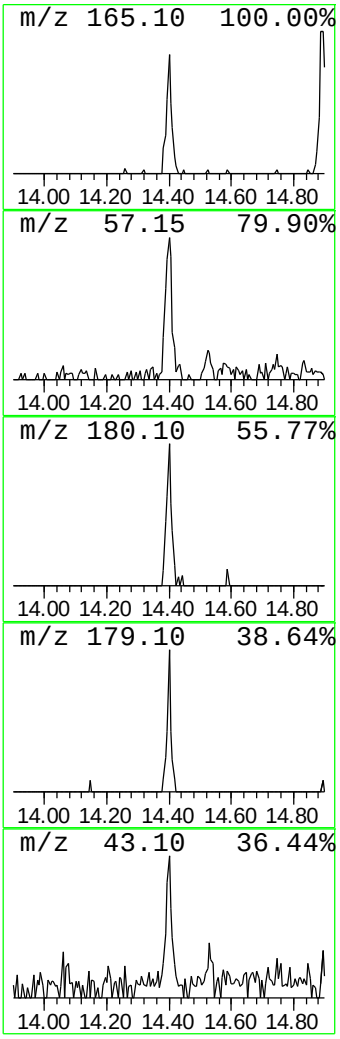
Peak Number 4 3H-Benz[e]indene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	3.19 ng	56720	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-Benz[e]indene, 2-methyl-	180	C14H12	150096-60-9	62
2	4a,9a-Methano-9H-fluorene	180	C14H12	019540-84-2	58
3	Ethylene, 1,1-diphenyl-	180	C14H12	000530-48-3	58
4	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	53
5	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	001131-62-0	49





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170604-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
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TIC Library : C:\Database\NIST11.L
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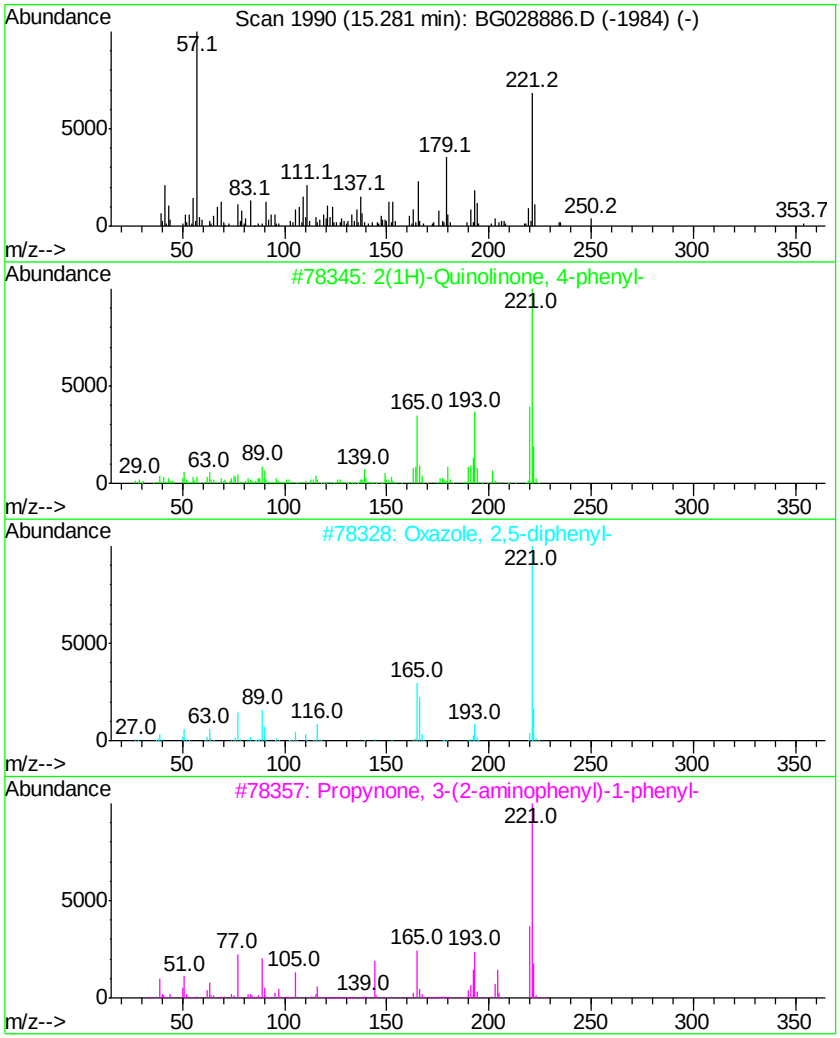
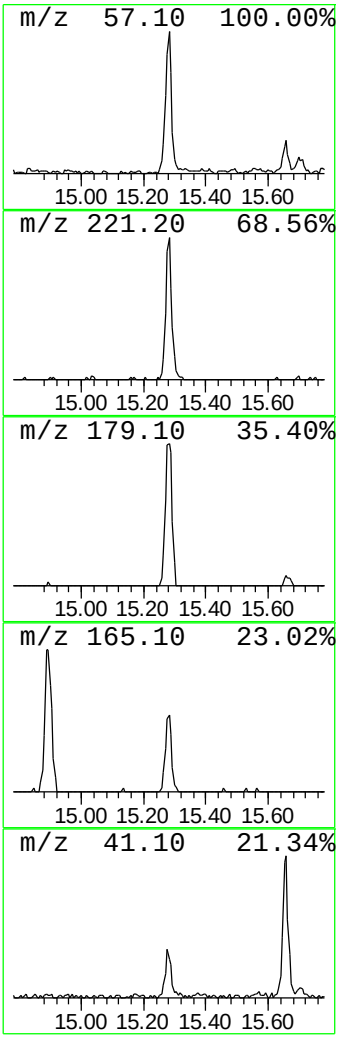
Peak Number 5 unknown15.28 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	9.31 ng	165571	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	46
2	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	43
3	Propynone, 3-(2-aminophenyl)-1-p...	221	C15H11NO	1000311-26-1	35
4	9-Oxo-9,10-dihydroacridine-4-car...	238	C14H10N2O2	037760-72-8	35
5	8-Chloro-9-phenanthroic acid	256	C15H9ClO2	056988-44-4	35





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Sample : I5301-10
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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
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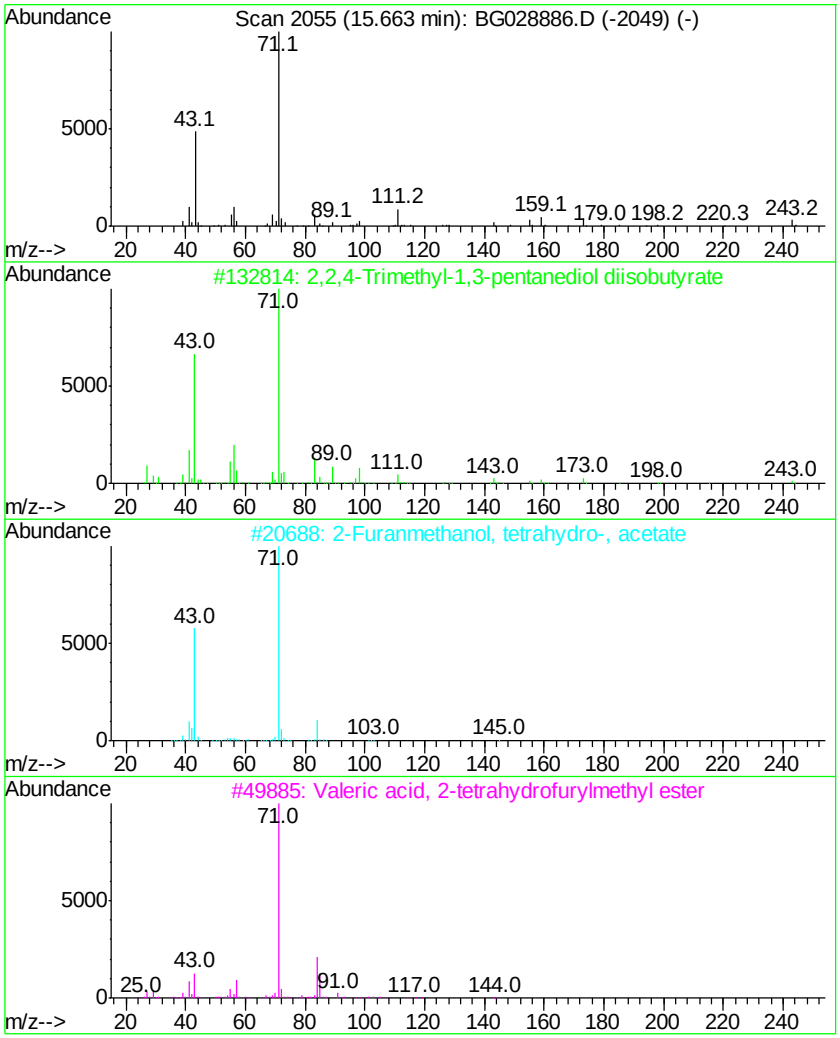
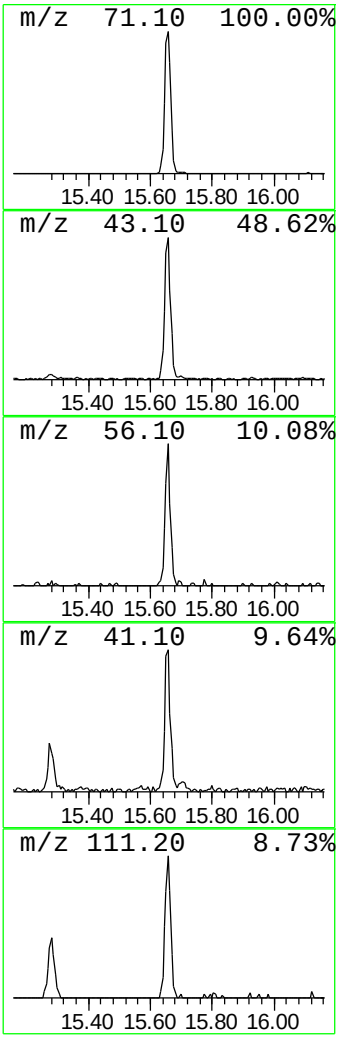
Peak Number 6 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	16.20 ng	288019	Acenaphthene-d10	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	56
2	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	42
3	Valeric acid, 2-tetrahydrofurylm...	186	C10H18O3	005451-86-5	42
4	Propanoic acid, 2-methyl-, 2-eth...	286	C16H30O4	074367-30-9	40
5	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	40





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Instrument : BNA_G
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TIC Library : C:\Database\NIST11.L
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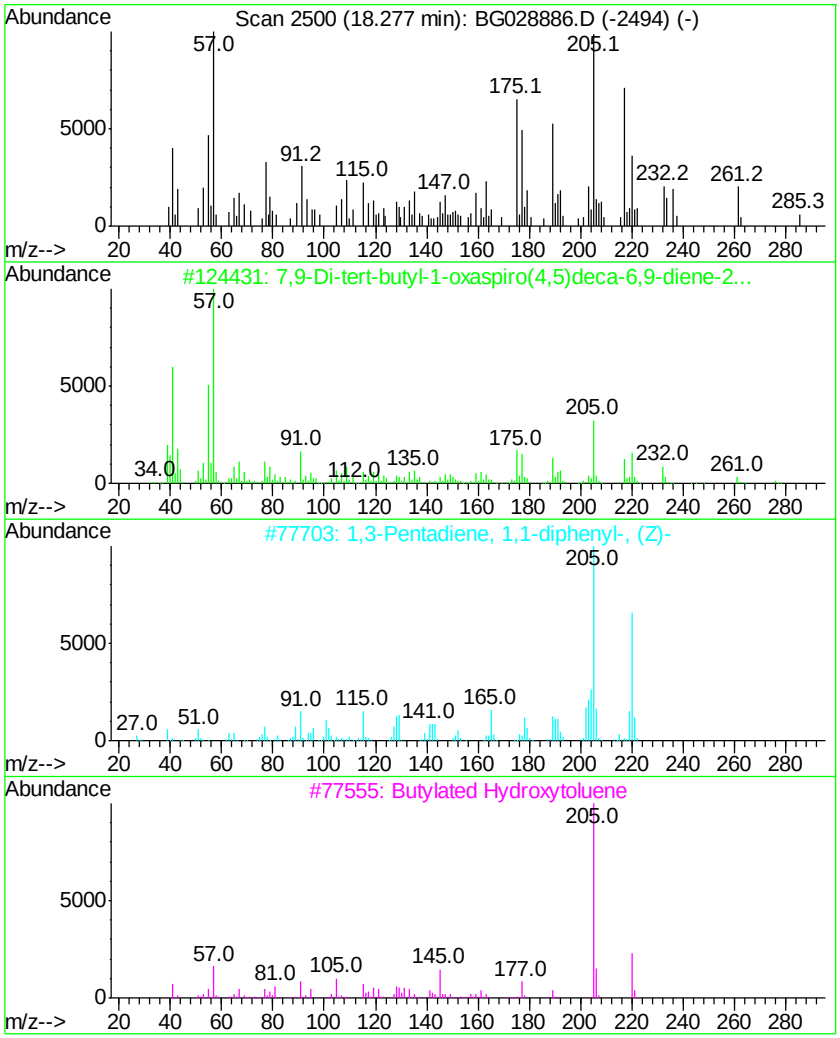
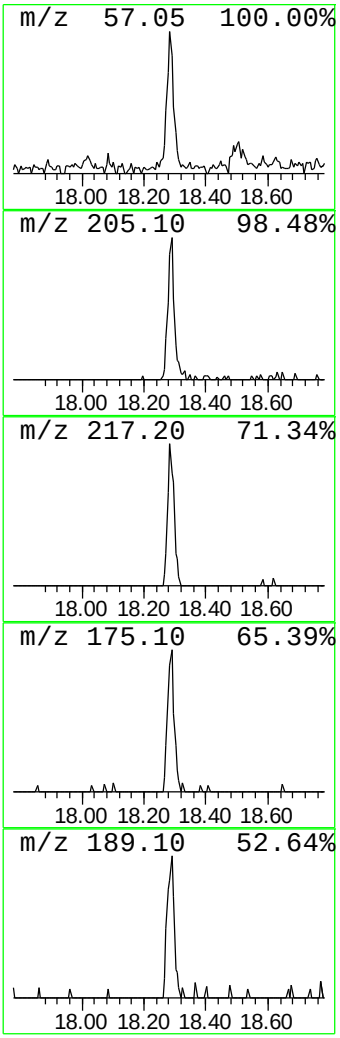
Peak Number 7 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	4.61 ng	136376	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	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	50
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	46
4	Benzene, 1,1'-(1-methyl-2-butynyl...	220	C17H16	054372-84-8	45
5	1-Ethyl-2-methylphenanthrene	220	C17H16	061983-53-7	42





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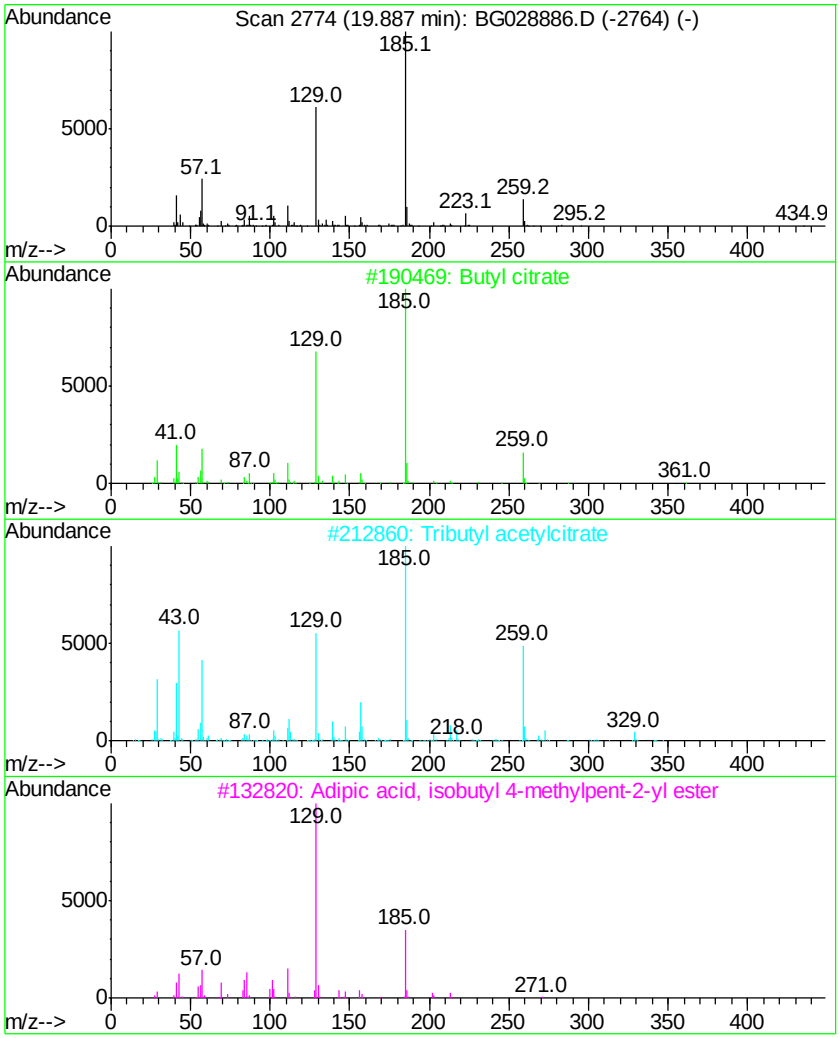
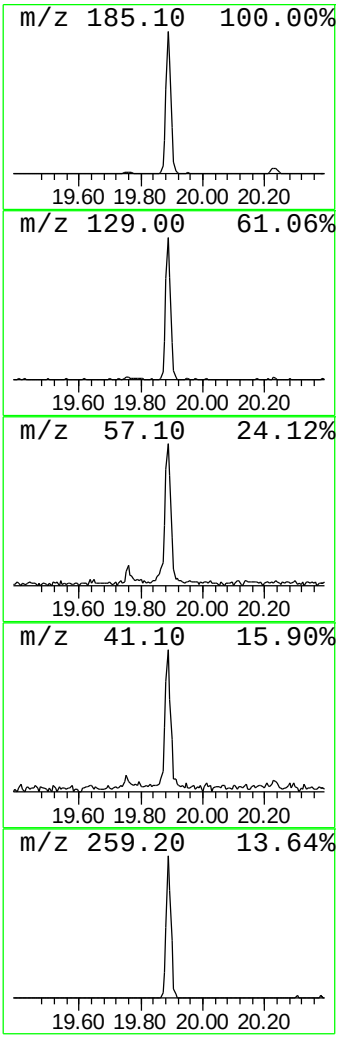
Peak Number 8 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	7.28 ng	277804	Chrysene-d12	21.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Tributyl acetylcitrate	402	C20H34O8	000077-90-7	59
3	Adipic acid, isobutyl 4-methylpe...	286	C16H30O4	1000353-50-1	56
4	Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	56
5	Adipic acid, 2-heptyl isobutyl e...	300	C17H32O4	1000353-64-3	56





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.37	5.37	5.7	ng	42658	1	8.27	149455	20.0
unknown7.81	7.81	111.8	ng	835728	1	8.27	149455	20.0
3H-Benz[e]indene,...	14.40	3.2	ng	56720	3	14.89	355515	20.0
unknown15.28	15.28	9.3	ng	165571	3	14.89	355515	20.0
2,2,4-Trimethyl-1...	15.66	16.2	ng	288019	3	14.89	355515	20.0
7,9-Di-tert-butyl...	18.28	4.6	ng	136376	4	17.64	591673	20.0
Butyl citrate	19.89	7.3	ng	277804	5	21.96	763178	20.0