LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
Data File : BG028806.D
Acq On : 18 Sep 2017 22:19
Operator : SJ/JU
Sample : I5259-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170602-COMP-C

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	5.392	302	307	316	rVB	22258	38589	1.12%	0.269%
2	5.856	379	386	395	rBV	280517	474428	13.79%	3.309%
3	7.442	649	656	668	rBV2	201437	385768	11.21%	2.691%
4	7.818	714	720	731	rBV	479248	864347	25.12%	6.029%
5	8.288	792	800	811	rBV	113391	200129	5.82%	1.396%
6	8.617	845	856	864	rBV	441991	812095	23.60%	5.664%
7	9.458	992	999	1008	rBV	367221	697835	20.28%	4.867%
8	11.109	1273	1280	1290	rBV	143397	273038	7.94%	1.904%
9	13.529	1679	1692	1705	rBV	1198238	1897257	55.14%	13.233%
10	14.411	1837	1842	1846	rBV3	38887	53319	1.55%	0.372%
11	14.910	1919	1927	1935	rBV3	256931	438600	12.75%	3.059%
12	15.292	1987	1992	2000	rBV3	112336	153746	4.47%	1.072%
13	15.668	2049	2056	2061	rBV	221877	299834	8.71%	2.091%
14	16.397	2173	2180	2194	rBV	1048877	1735328	50.44%	12.103%
15	17.660	2388	2395	2403	rVV2	413183	650497	18.91%	4.537%
16	18.300	2495	2504	2517	rBV5	76467	125578	3.65%	0.876%
17	19.904	2769	2777	2782	rBV3	107937	160488	4.66%	1.119%
18	20.245	2829	2835	2849	rBV	2495388	3440713	100.00%	23.998%
19	21.408	3029	3033	3040	rBV4	36227	69783	2.03%	0.487%
20	21.984	3123	3131	3141	rBV2	411057	767851	22.32%	5.356%
21	23.183	3329	3335	3340	rBV5	26548	59353	1.73%	0.414%
22	25.451	3709	3721	3735	rBV2	228379	738889	21.47%	5.154%

Sum of corrected areas: 14337465

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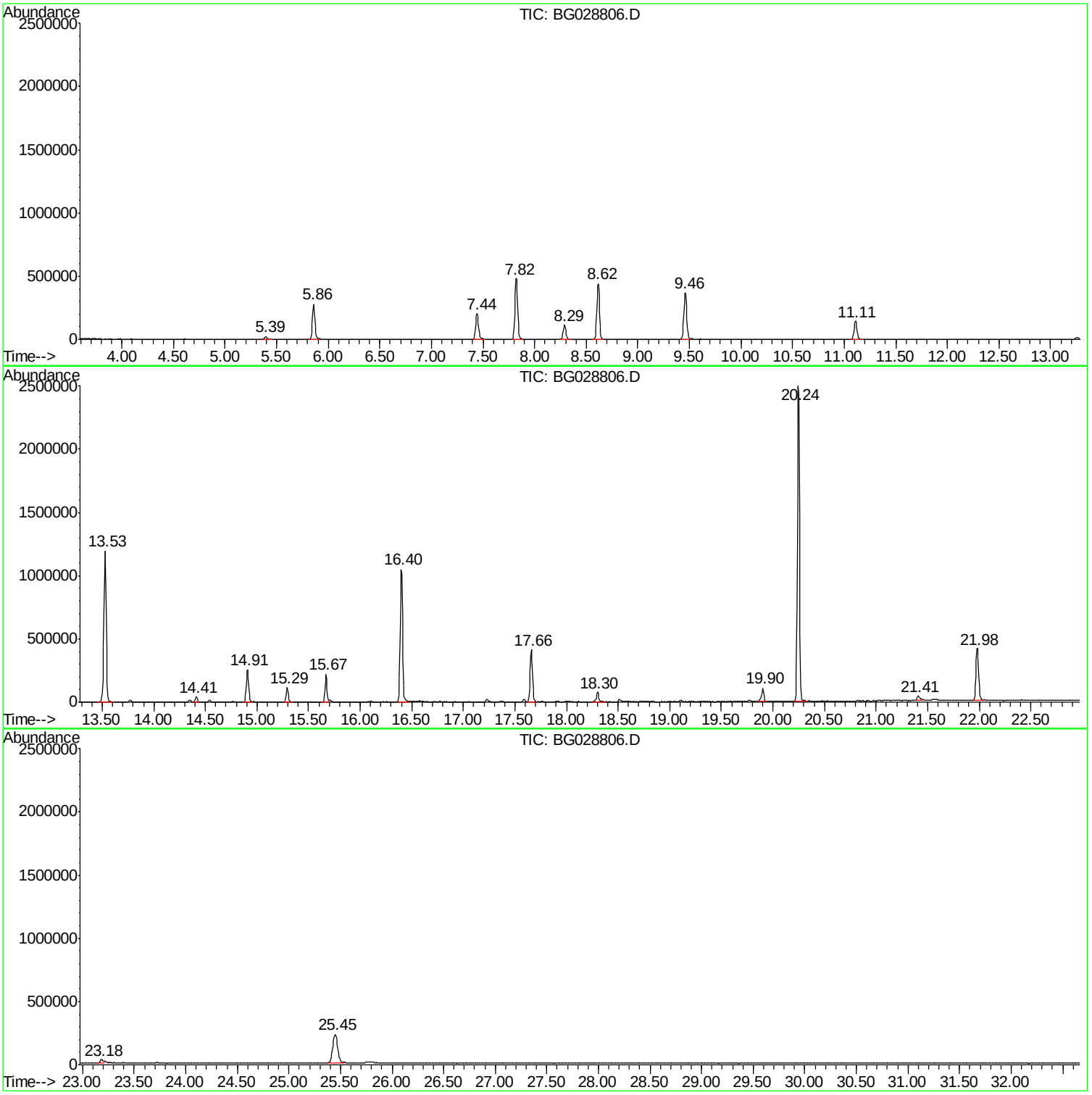
BNA_G
ClientSampleId :
20170602-COMP-C

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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Data File : BG028806.D
Acq On : 18 Sep 2017 22:19
Operator : SJ/JU
Sample : I5259-06
Misc :
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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

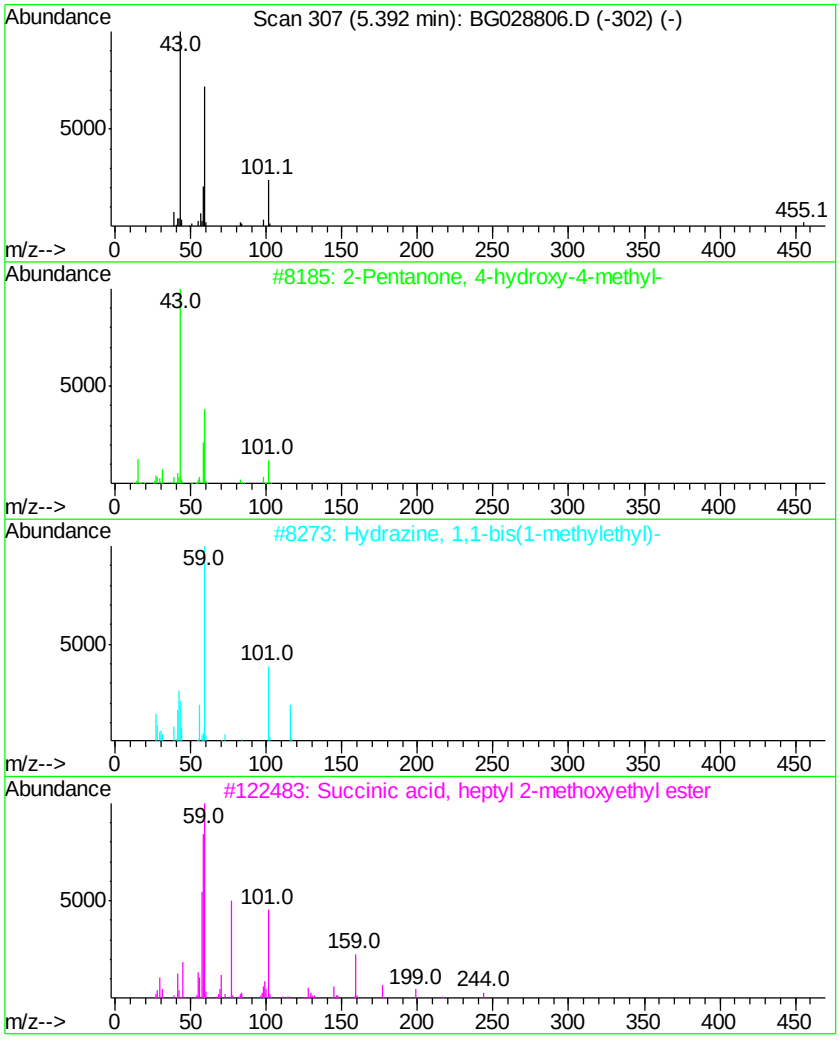
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

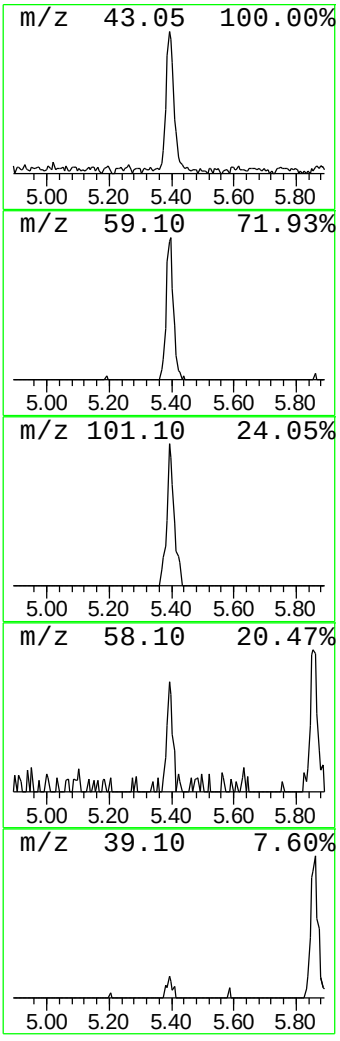
****

Peak Number 1 unknown5.39 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.39	3.86 ng	38589	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
3	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	3-Hexanol	102	C6H14O	000623-37-0	17





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Sample : I5259-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170602-COMP-C

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

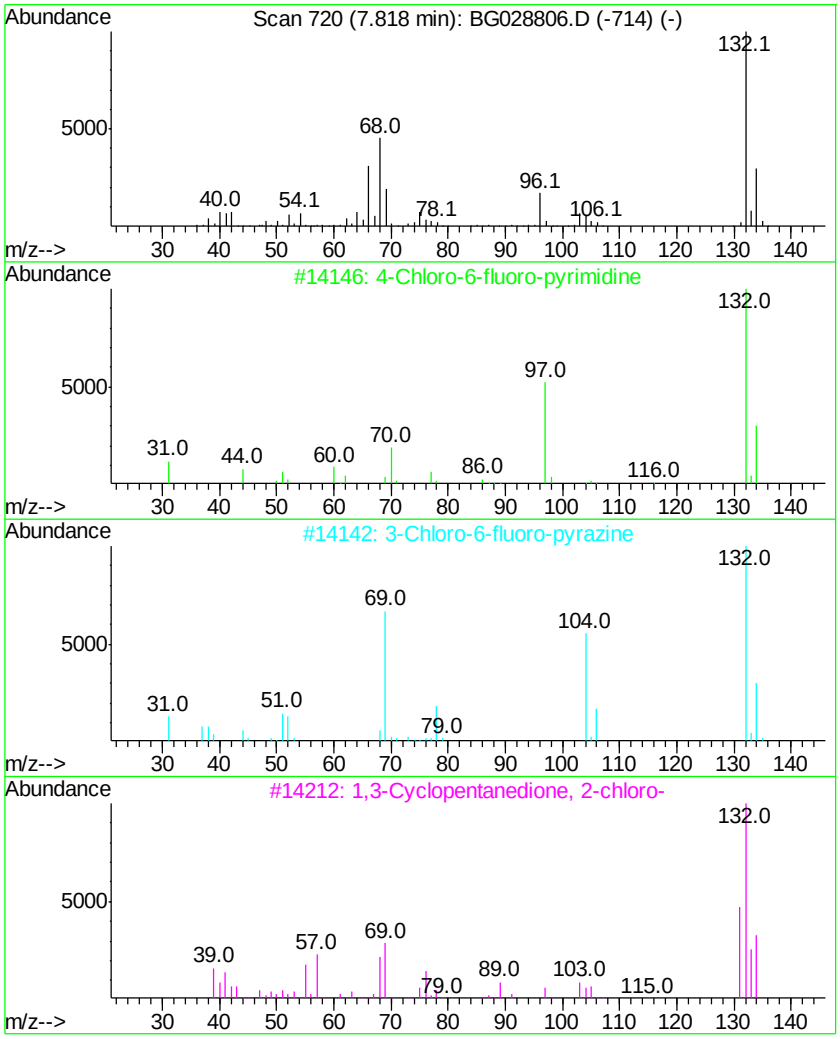
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

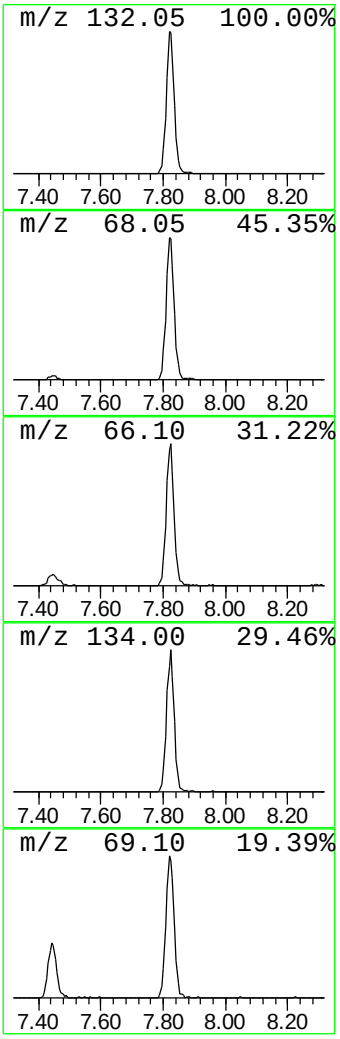
****

Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	86.38 ng	864347	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Library Search Compound Report

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Acq On : 18 Sep 2017 22:19
Operator : SJ/JU
Sample : I5259-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170602-COMP-C

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

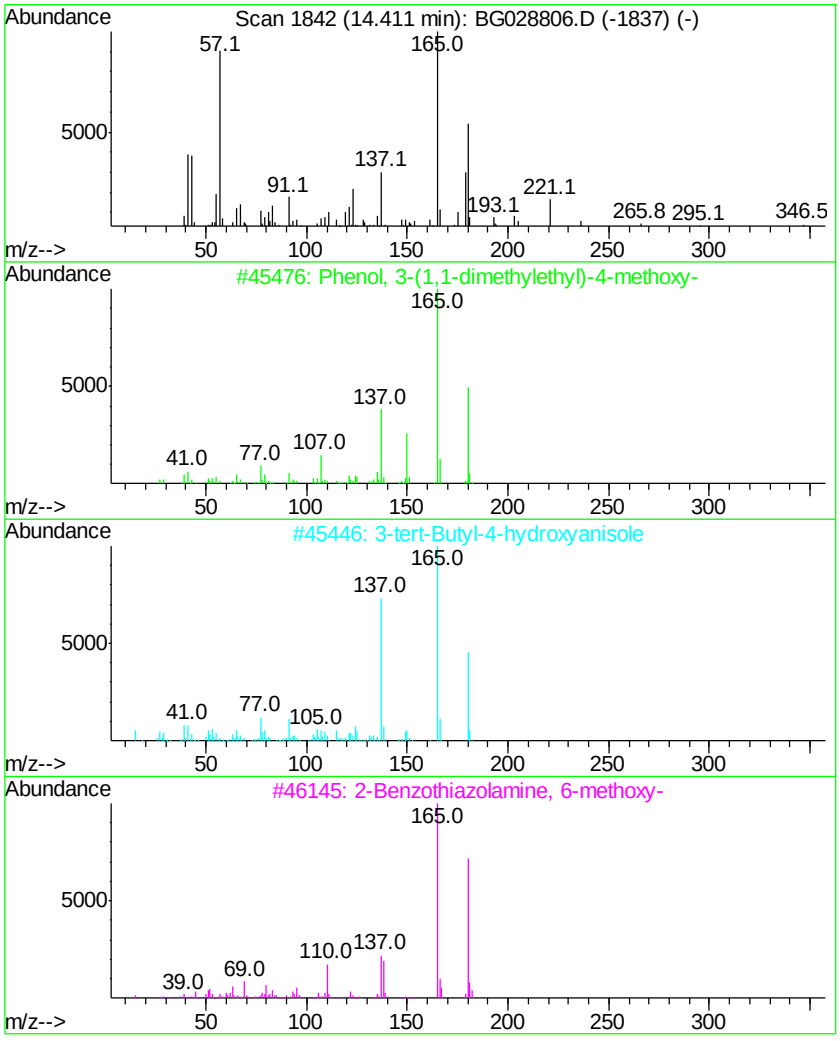
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

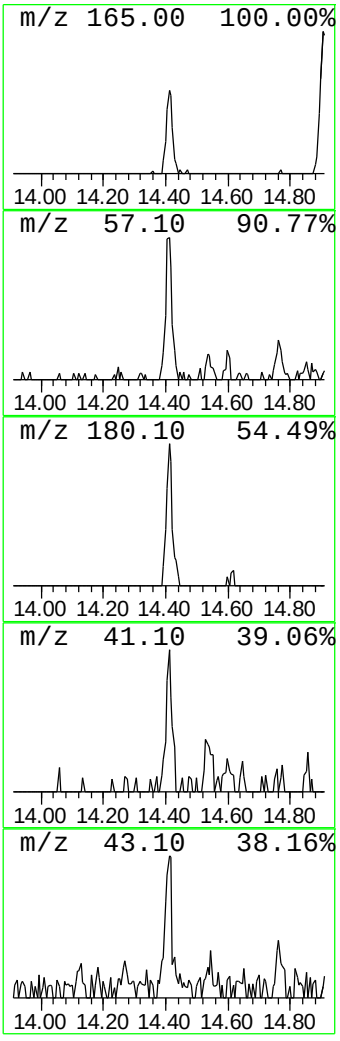
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	2.43 ng	53319	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	55
3	2-Benzothiazolamine, 6-methoxy-	180	C8H8N2OS	001747-60-0	52
4	2-Amino-4-(tert-butyl)thiophene-...	180	C9H12N2S	010413-34-0	49
5	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	001131-62-0	49





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Sample : I5259-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170602-COMP-C

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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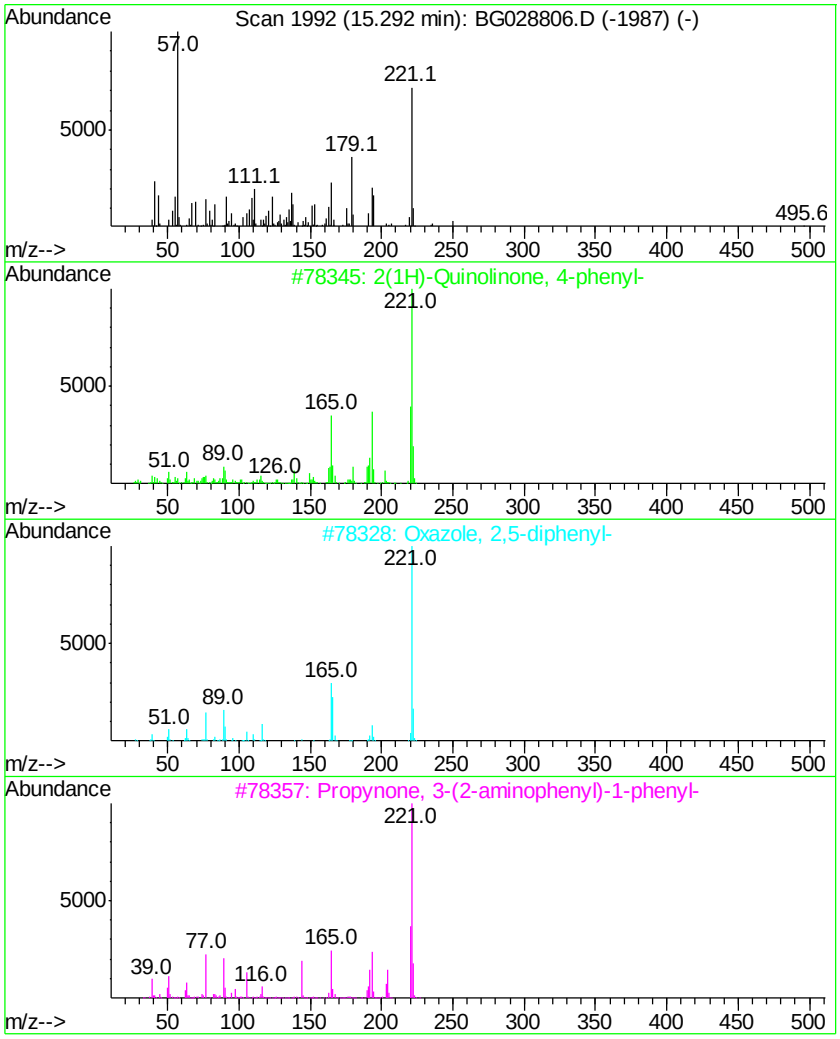
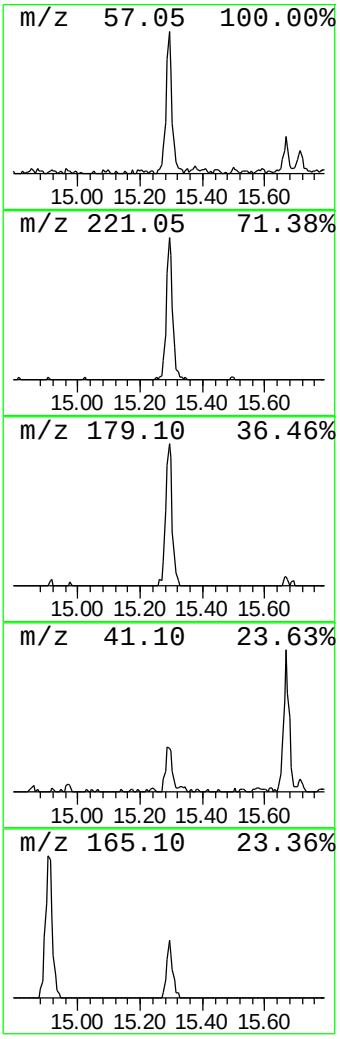
****

Peak Number 5 unknown15.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	7.01 ng	153746	Acenaphthene-d10	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	38
2	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	38
3	Propynone, 3-(2-aminophenyl)-1-p...	221	C15H11NO	1000311-26-1	35
4	Methanone, cyclohexyl(2,5-diprop...	304	C19H28O3	076185-90-5	35
5	9-Oxo-9,10-dihydroacridine-4-car...	238	C14H10N2O2	037760-72-8	32





Library Search Compound Report

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ClientSampleId : 20170602-COMP-C

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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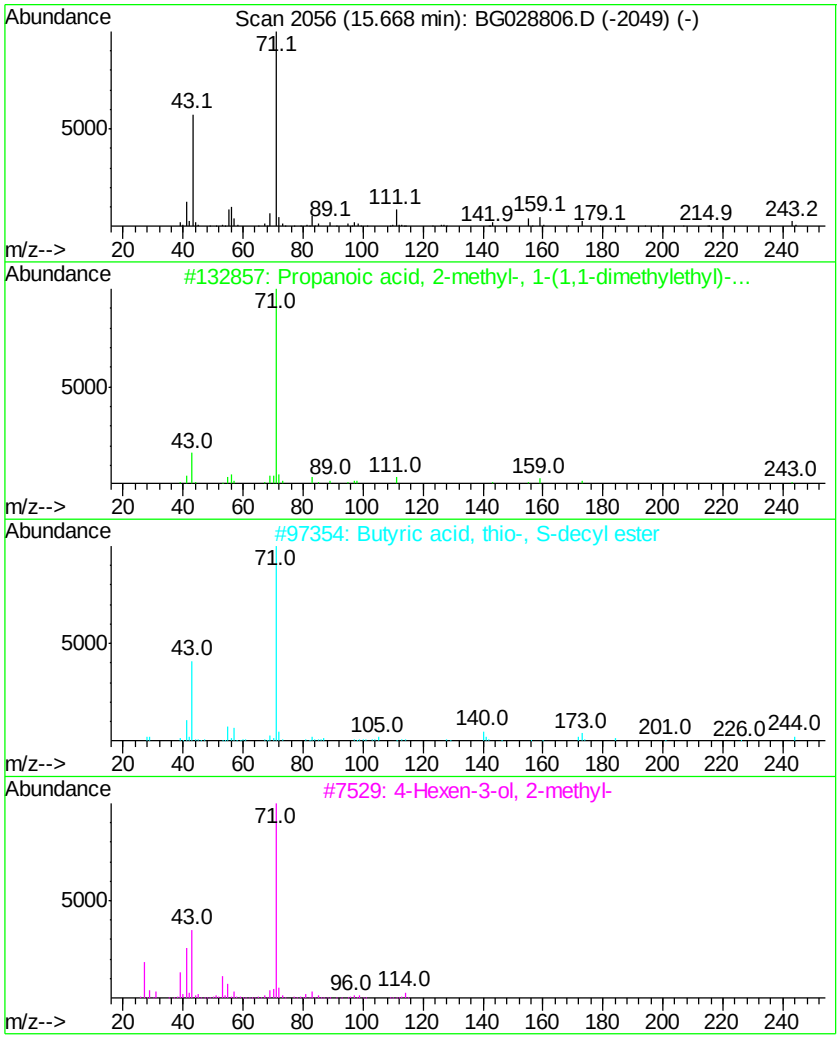
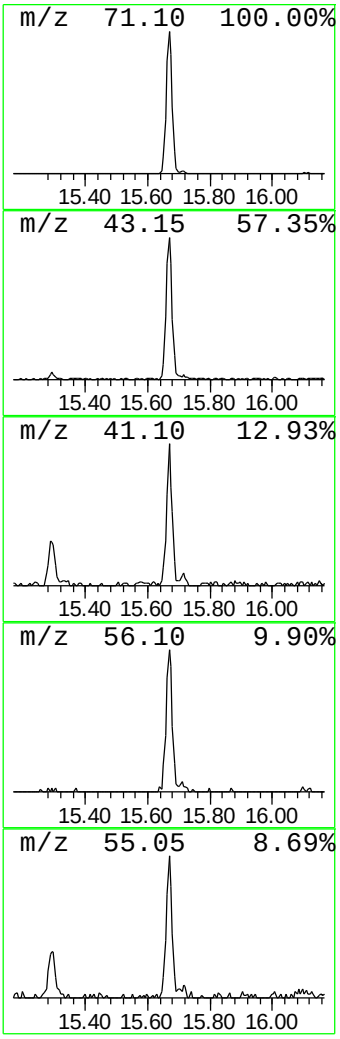
****

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	13.67 ng	299834	Acenaphthene-d10	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	72
2	Butyric acid, thio-, S-decyl ester	244	C14H28OS	002432-55-5	53
3	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	53
4	Sulfurous acid, nonyl pentyl ester	278	C14H30O3S	1000309-14-2	50
5	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	45





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ClientSampleId : 20170602-COMP-C

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

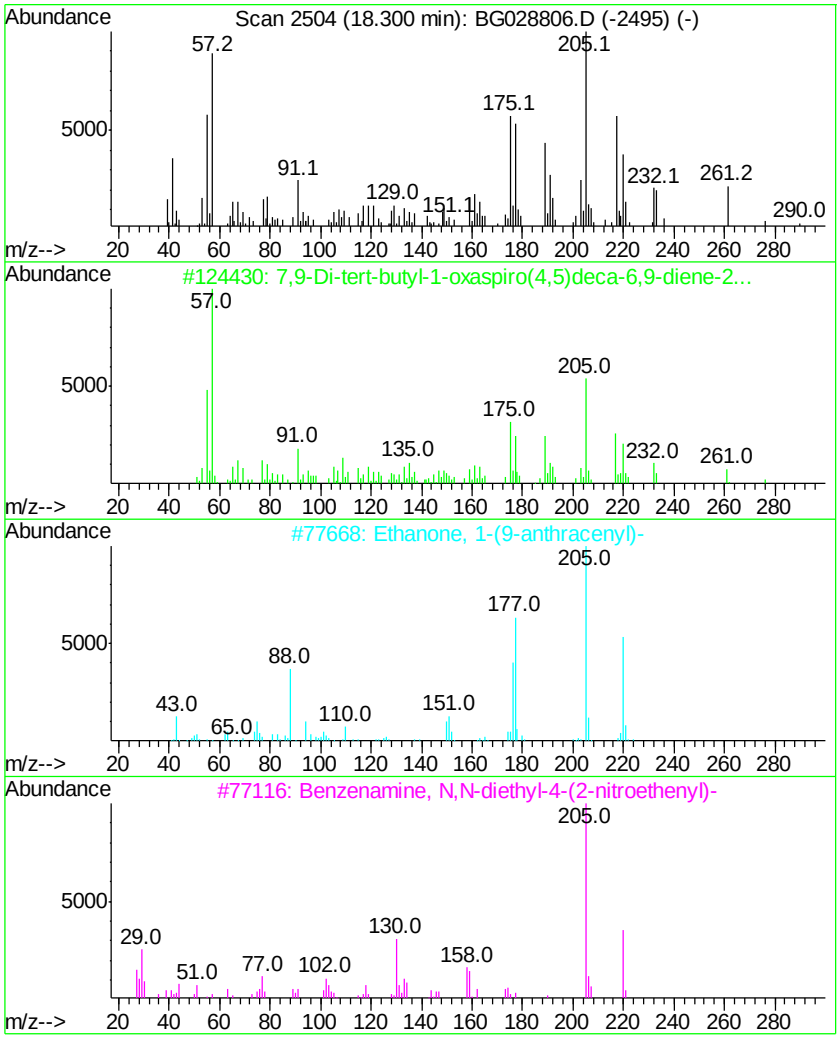
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

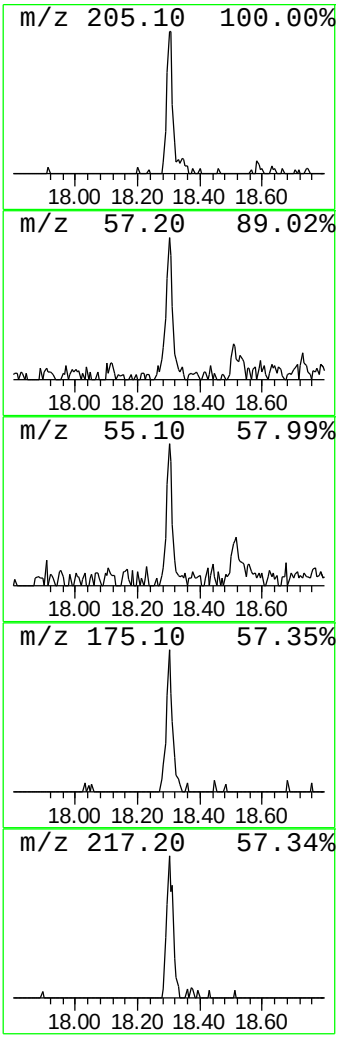
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.86 ng	125578	Phenanthrene-d10	17.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	93
2	Ethanone, 1-(9-anthracenyl)-	220	C16H12O	000784-04-3	38
3	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	35
4	Thiophene, 2-(4-nitrophenyl)-	205	C10H7NO2S	059156-21-7	30
5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	30





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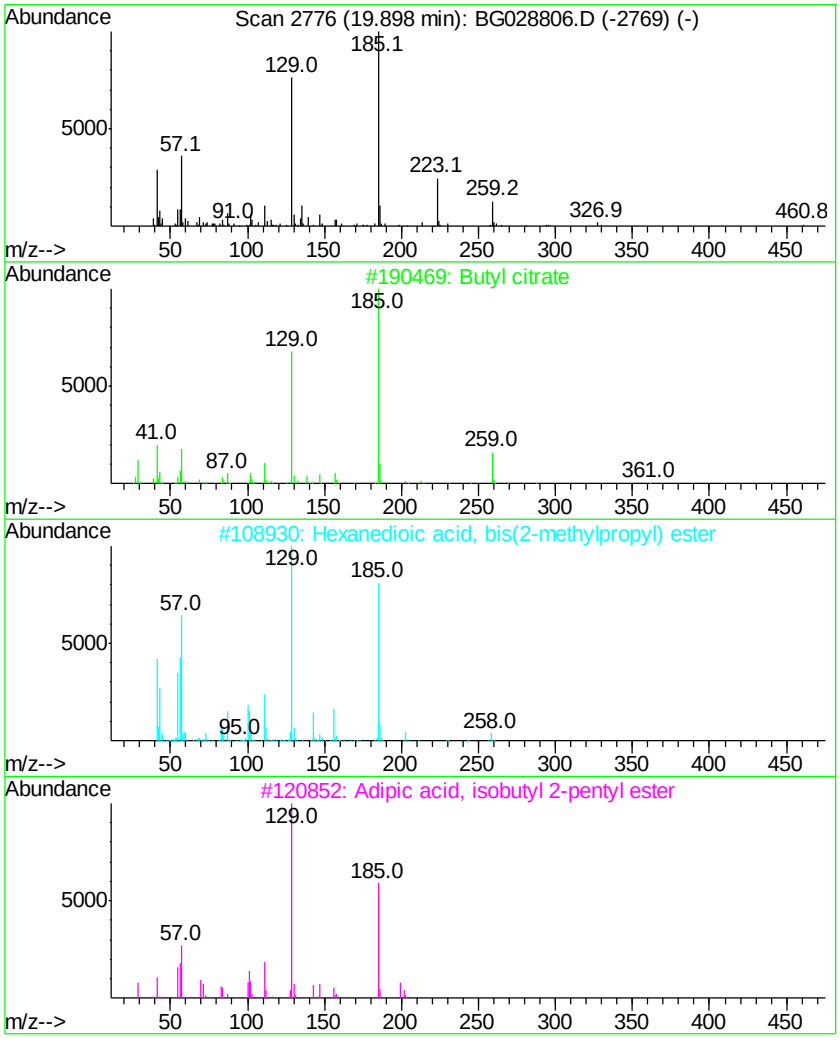
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

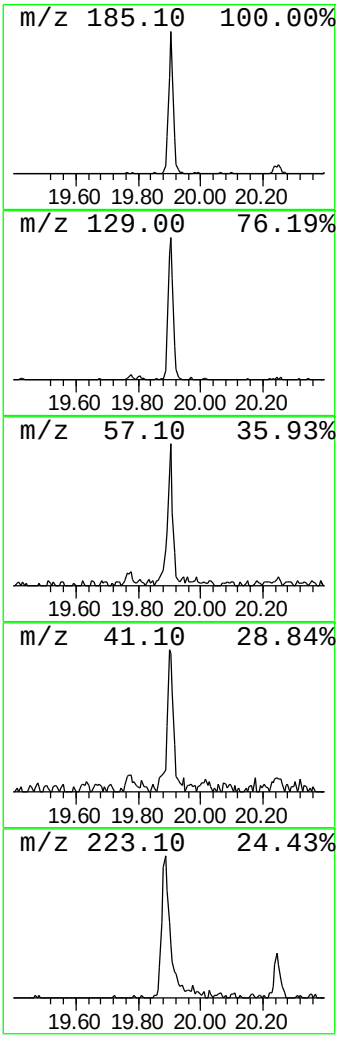
****

Peak Number 8 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	4.18 ng	160488	Chrysene-d12	21.98

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	64
3	Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	50
4	Adipic acid, isobutyl 3-pentyl e...	272	C15H28O4	1000324-60-4	45
5	Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	45





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
unknown5.39	5.39	3.9	ng	38589	1	8.29	200129	20.0
unknown7.82	7.82	86.4	ng	864347	1	8.29	200129	20.0
Phenol, 3-(1,1-di...	14.41	2.4	ng	53319	3	14.90	438600	20.0
unknown15.29	15.29	7.0	ng	153746	3	14.90	438600	20.0
Propanoic acid, 2...	15.67	13.7	ng	299834	3	14.90	438600	20.0
7,9-Di-tert-butyl...	18.30	3.9	ng	125578	4	17.66	650497	20.0
Butyl citrate	19.90	4.2	ng	160488	5	21.98	767851	20.0