LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
Data File : BG028808.D
Acq On : 18 Sep 2017 23:38
Operator : SJ/JU
Sample : I5259-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170600-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	5.394	300	307	316	rBV	20697	39272	1.16%	0.272%
2	5.858	378	386	397	rBV	287919	490582	14.52%	3.399%
3	7.439	648	655	665	rBV	202705	386749	11.44%	2.680%
4	7.821	712	720	730	rBV	509172	887459	26.26%	6.149%
5	8.291	792	800	806	rBV	107222	184577	5.46%	1.279%
6	8.614	847	855	864	rBV	428156	770767	22.81%	5.340%
7	9.460	991	999	1011	rBV2	355996	671088	19.86%	4.650%
8	11.111	1272	1280	1289	rBV	136210	263515	7.80%	1.826%
9	13.526	1681	1691	1702	rBV	1132612	1797987	53.21%	12.458%
10	13.772	1725	1733	1740	rBV2	19320	35086	1.04%	0.243%
11	14.348	1824	1831	1837	rBV	22524	38906	1.15%	0.270%
12	14.413	1837	1842	1847	rVB2	56074	79526	2.35%	0.551%
13	14.906	1920	1926	1934	rBV2	248321	423894	12.54%	2.937%
14	15.294	1985	1992	2002	rBV	144110	208794	6.18%	1.447%
15	15.670	2050	2056	2060	rBV	260710	355610	10.52%	2.464%
16	16.399	2173	2180	2193	rBV	1113938	1766622	52.28%	12.240%
17	17.227	2313	2321	2327	rBV	35679	49318	1.46%	0.342%
18	17.586	2377	2382	2387	rBV3	31057	41742	1.24%	0.289%
19	17.656	2387	2394	2404	rVV2	388088	627361	18.57%	4.347%
20	18.302	2495	2504	2511	rBV3	71448	112439	3.33%	0.779%
21	19.883	2767	2773	2774	rVV	34880	42490	1.26%	0.294%
22	19.901	2774	2776	2782	rVB2	44116	60135	1.78%	0.417%
23	20.247	2829	2835	2844	rBV	2564762	3379205	100.00%	23.414%
24	21.411	3027	3033	3039	rBV2	50314	101099	2.99%	0.700%
25	21.563	3056	3059	3074	rVB2	13826	41462	1.23%	0.287%
26	21.980	3122	3130	3138	rBV	396696	749008	22.17%	5.190%
27	23.185	3329	3335	3344	rBV4	32483	90810	2.69%	0.629%
28	25.453	3708	3721	3737	rBV3	225392	737100	21.81%	5.107%

Sum of corrected areas: 14432603

LSC Report - Integrated Chromatogram

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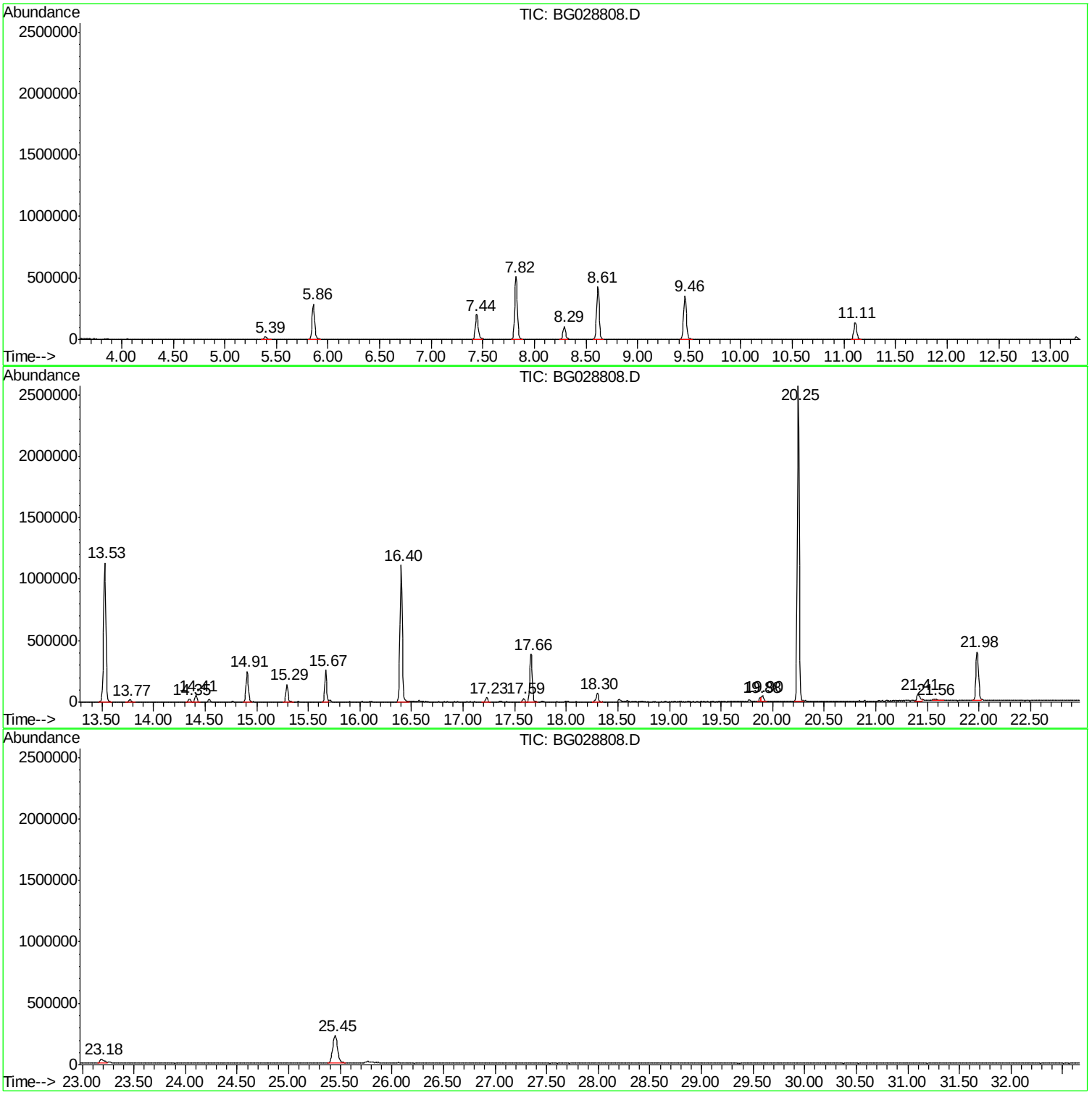
Sample : I5259-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170600-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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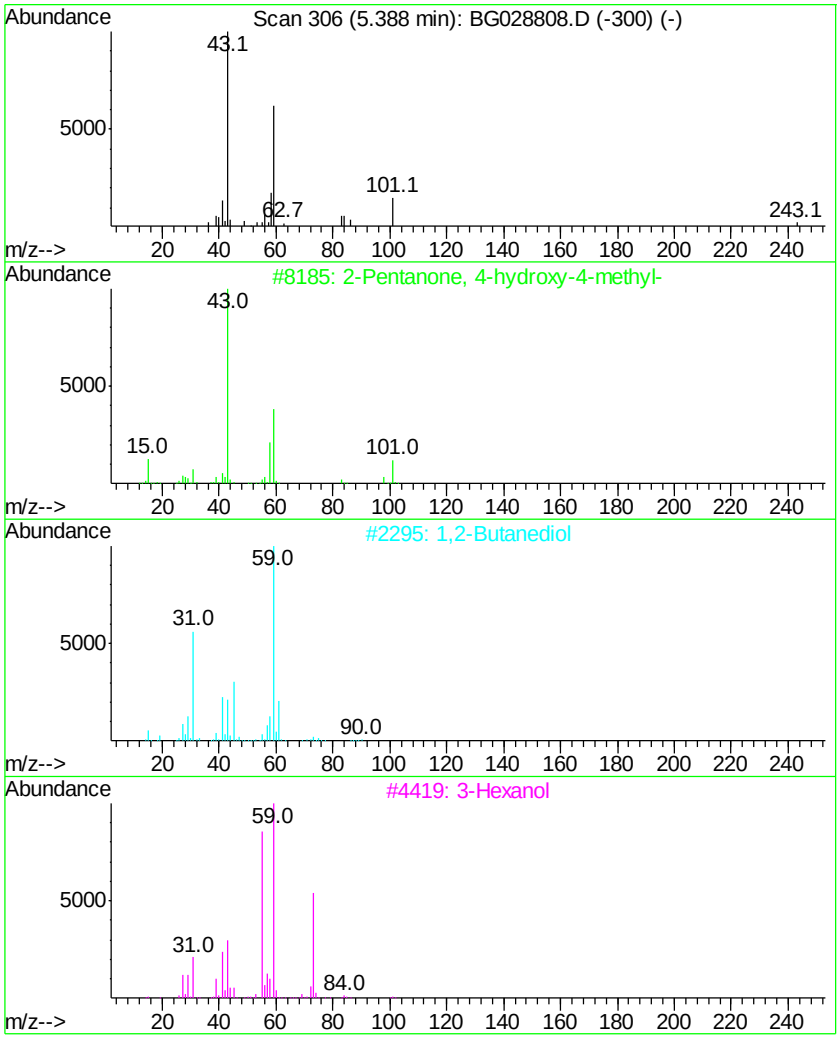
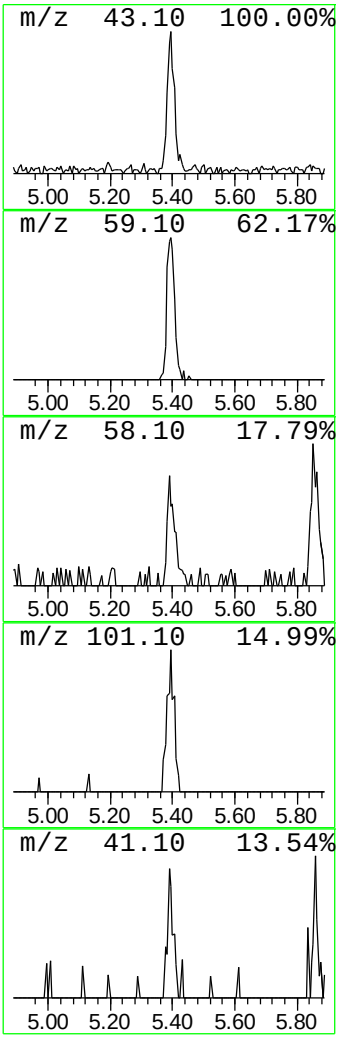
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.39	4.26 ng	39272	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	59
2	1,2-Butanediol	90	C4H10O2	000584-03-2	23
3	3-Hexanol	102	C6H14O	000623-37-0	23
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Instrument : BNA_G
ClientSampleId : 20170600-COMP-A

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

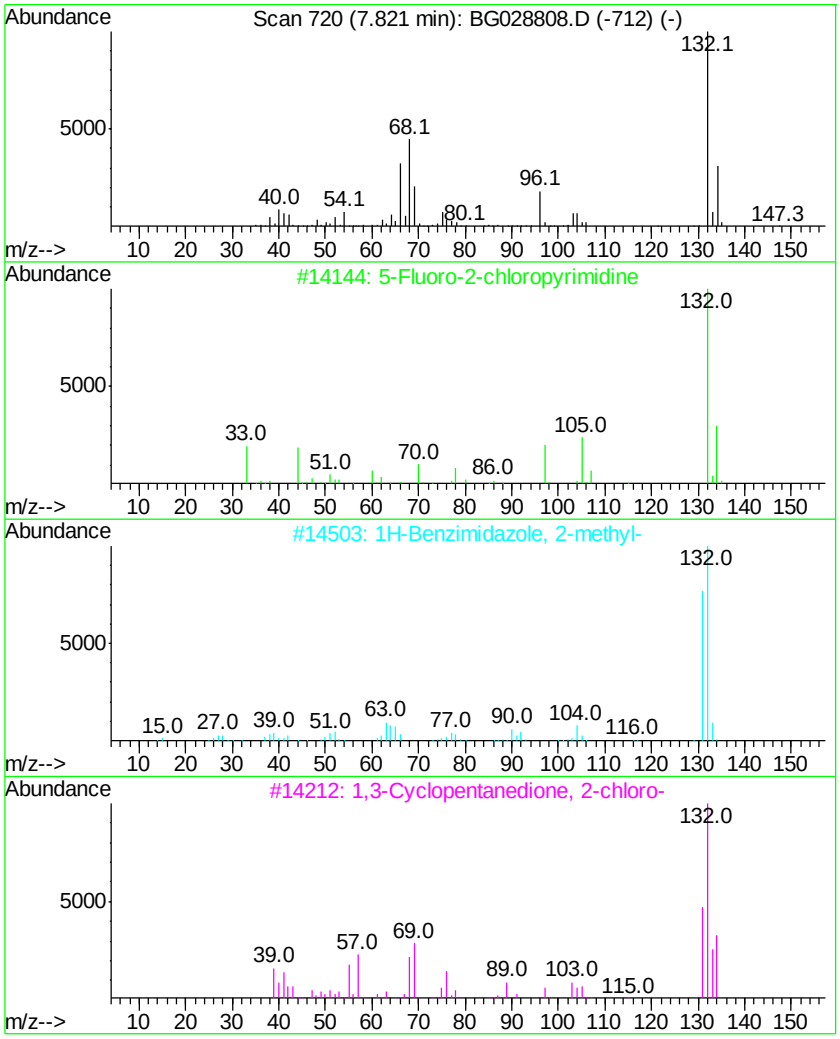
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

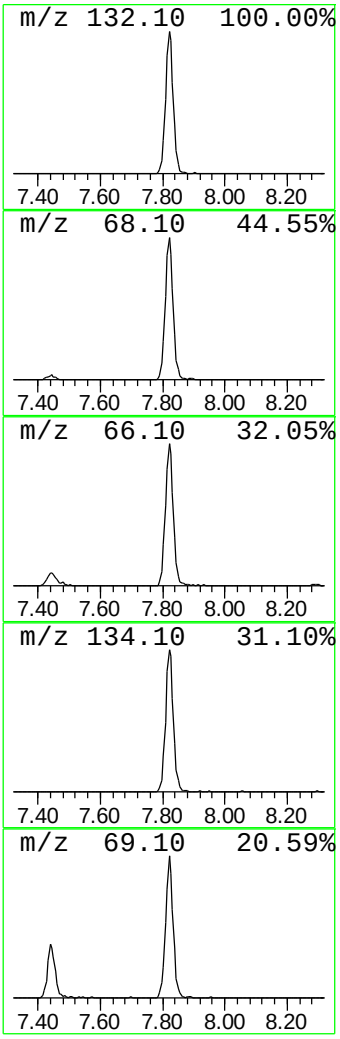
****

Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	96.16 ng	887459	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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Sample : I5259-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170600-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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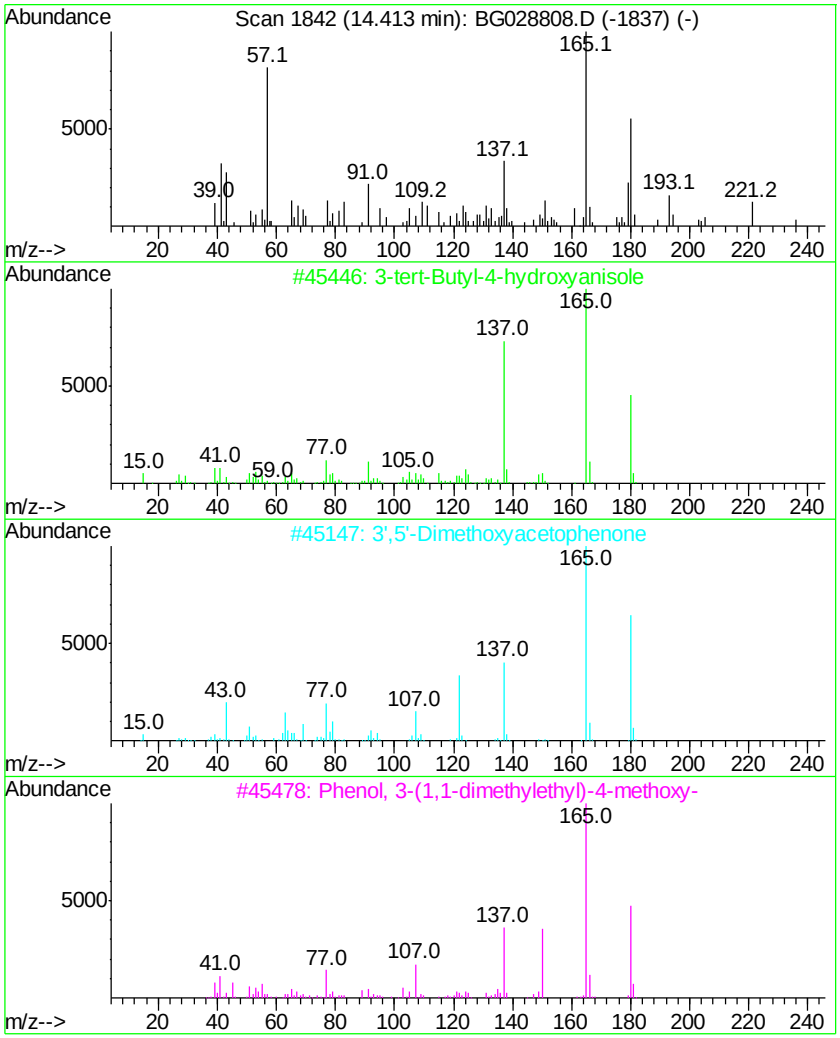
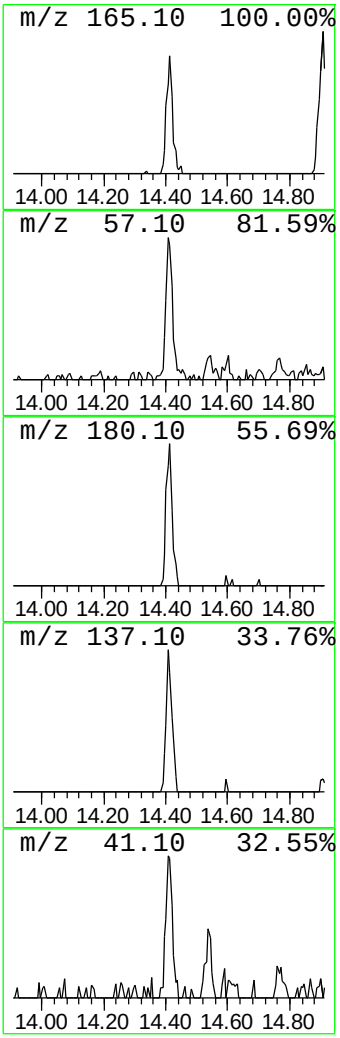
Peak Number 4 3-tert-Butyl-4-hydroxyanisole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	3.75 ng	79526	Acenaphthene-d10	14.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	62
2	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	62
3	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	62
4	2',4'-Dimethoxyacetophenone	180	C10H12O3	000829-20-9	52
5	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	001131-62-0	52





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Operator : SJ/JU
Sample : I5259-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170600-COMP-A

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

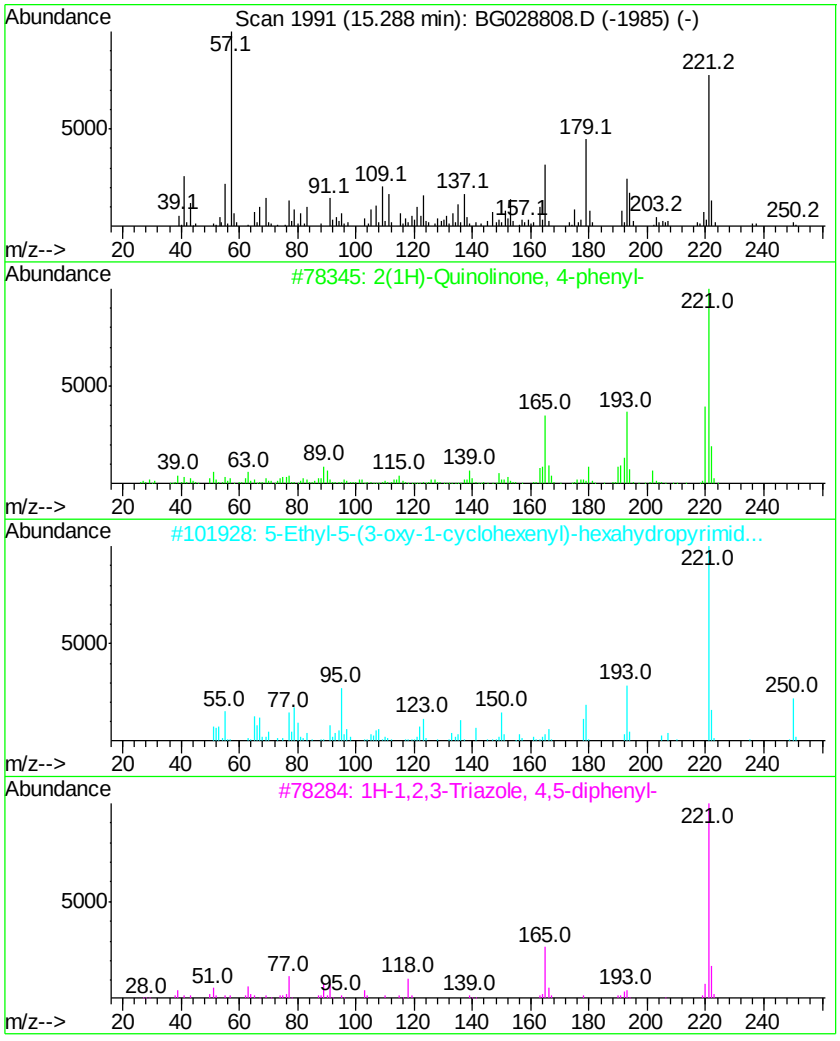
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

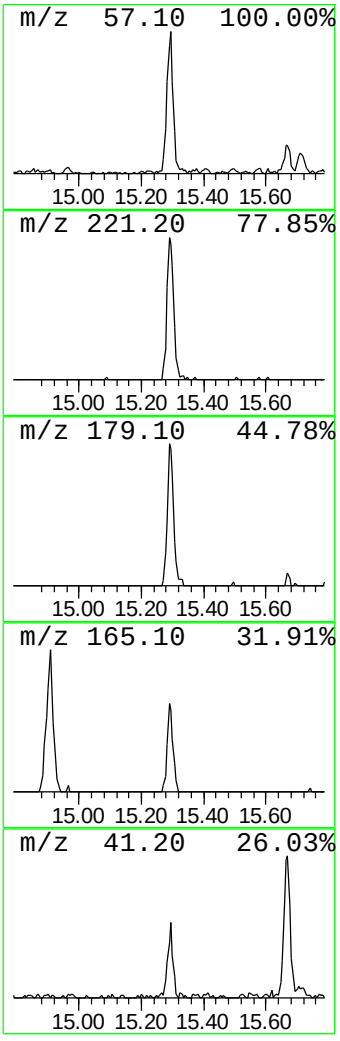
****

Peak Number 5 unknown15.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	9.85 ng	208794	Acenaphthene-d10	14.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2	41
2	5-Ethyl-5-(3-oxy-1-cyclohexenyl)...	250	C12H14N2O4	035305-10-3	35
3	1H-1,2,3-Triazole, 4,5-diphenyl-	221	C14H11N3	005533-73-3	30
4	Oxazole, 4,5-diphenyl-	221	C15H11NO	004675-18-7	27
5	Propynone, 3-(2-aminophenyl)-1-p...	221	C15H11NO	1000311-26-1	25





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ClientSampleId : 20170600-COMP-A

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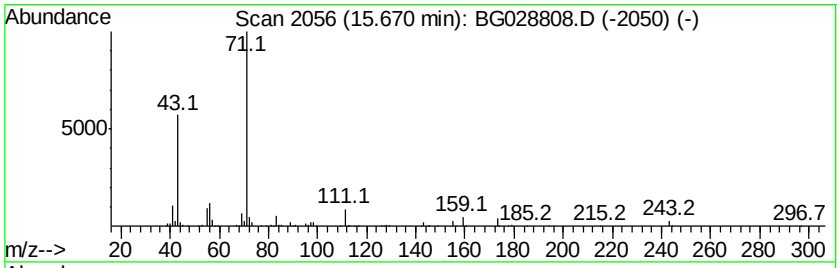
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

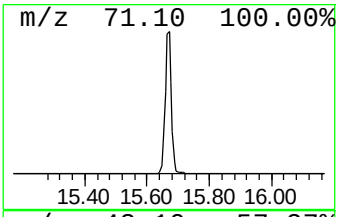
****

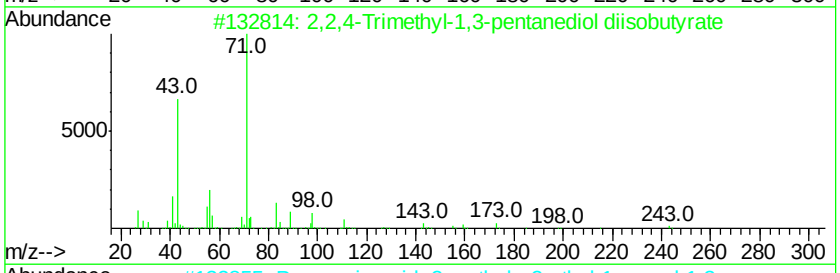
Peak Number 6 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 3

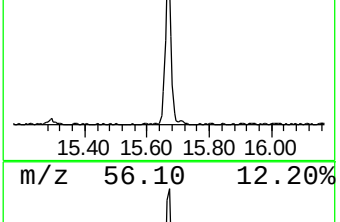
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	16.78 ng	355610	Acenaphthene-d10	14.91

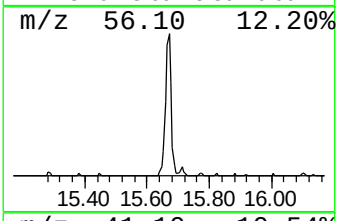
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	56
2	Propanoic acid, 2-methyl-, 2-eth...	286	C16H30O4	074367-30-9	56
3	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	56
4	3-Cyclopentylpropionic acid, 2-t...	226	C13H22O3	1000293-46-9	53
5	Boronic acid, ethyl-, bis(2,2-di...	214	C12H27BO2	067753-47-3	50

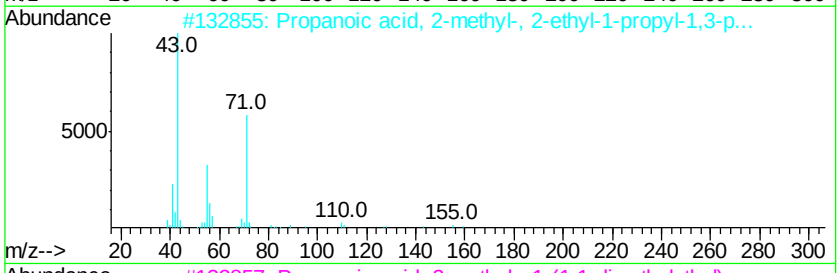


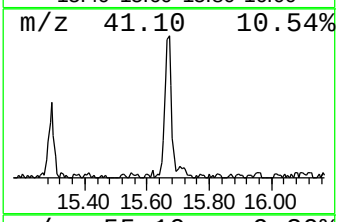


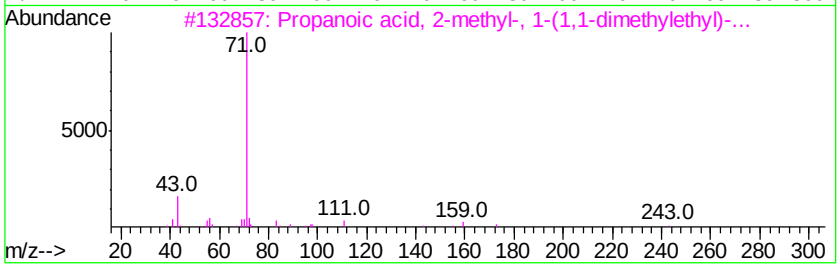


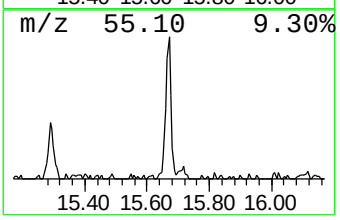












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

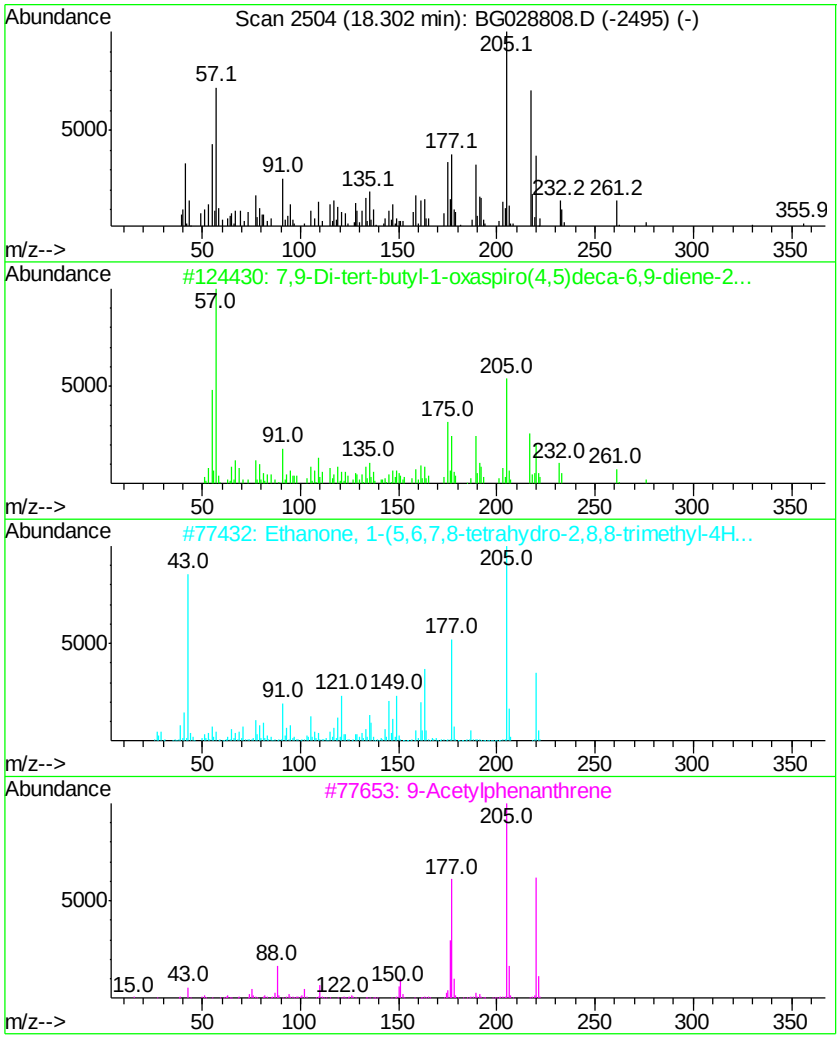
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

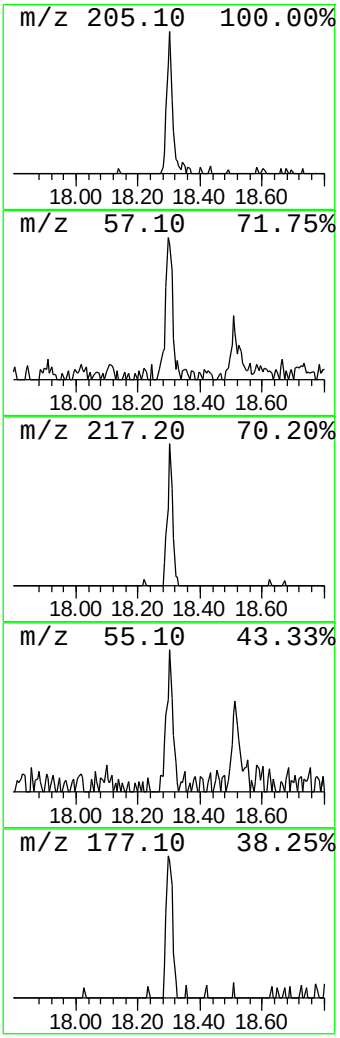
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.58 ng	112439	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-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	60
3	9-Acetylphenanthrene	220	C16H12O	002039-77-2	38
4	2,6-Bis(1,1-dimethylethyl)-4-met...	262	C18H30O	004278-82-4	38
5	2,4-Diamino-6-nitroquinazoline	205	C8H7N5O2	007154-34-9	38





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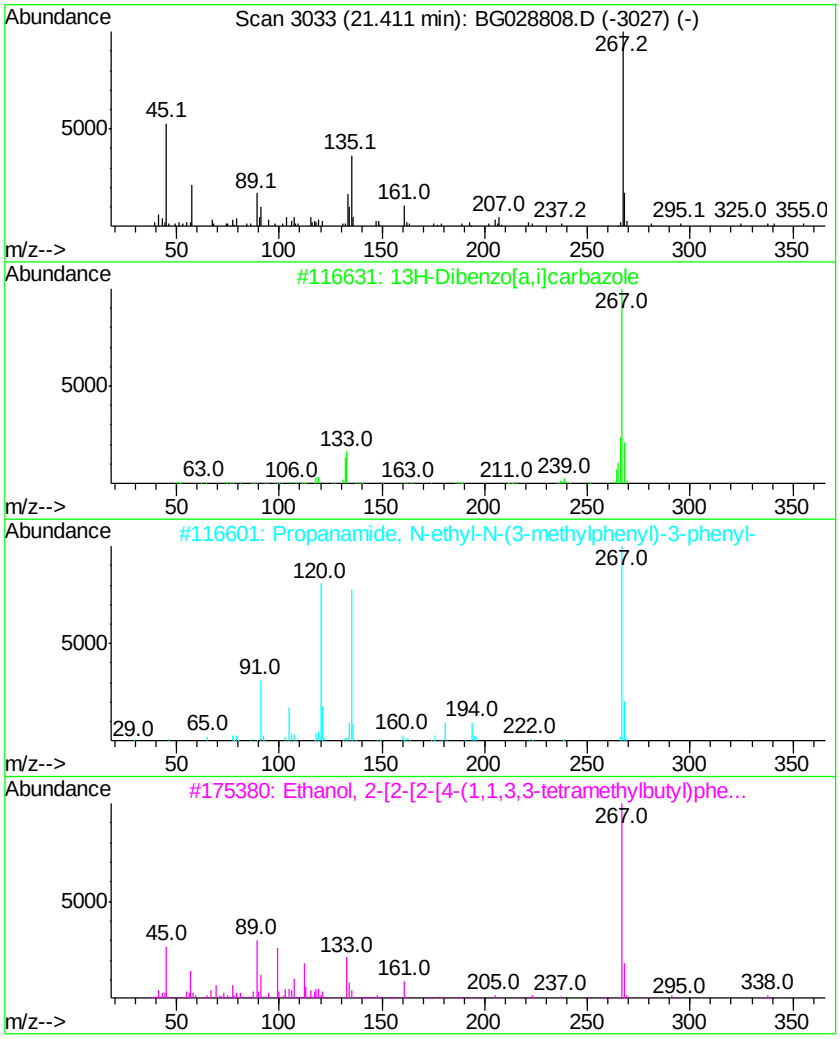
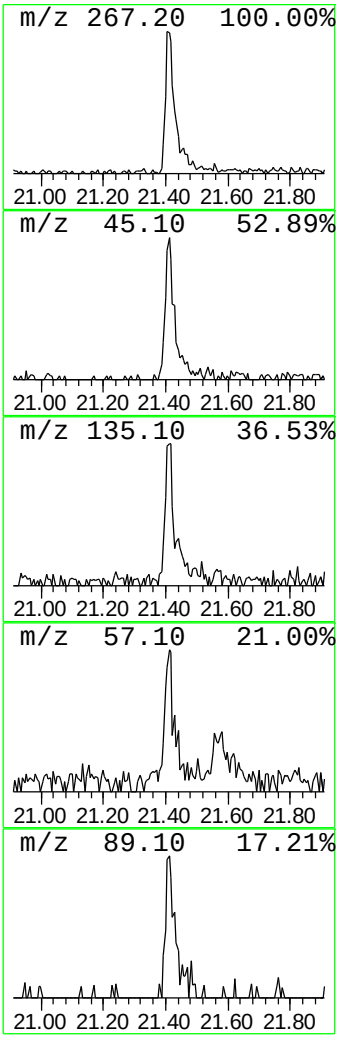
****

Peak Number 8 13H-Dibenzo[a,i]carbazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	2.70 ng	101099	Chrysene-d12	21.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13H-Dibenzo[a,i]carbazole	267	C20H13N	000239-64-5	50
2	Propanamide, N-ethyl-N-(3-methyl...	267	C18H21NO	1000308-21-3	50
3	Ethanol, 2-[2-[2-[4-(1,1,3,3-tet...	338	C20H34O4	002315-62-0	38
4	4,5-Ethylene-8,9-dimethoxy-4,5-d...	267	C17H17NO2	107208-75-3	38
5	7H-Dibenzo(a,g)carbazole	267	C20H13N	000207-84-1	38





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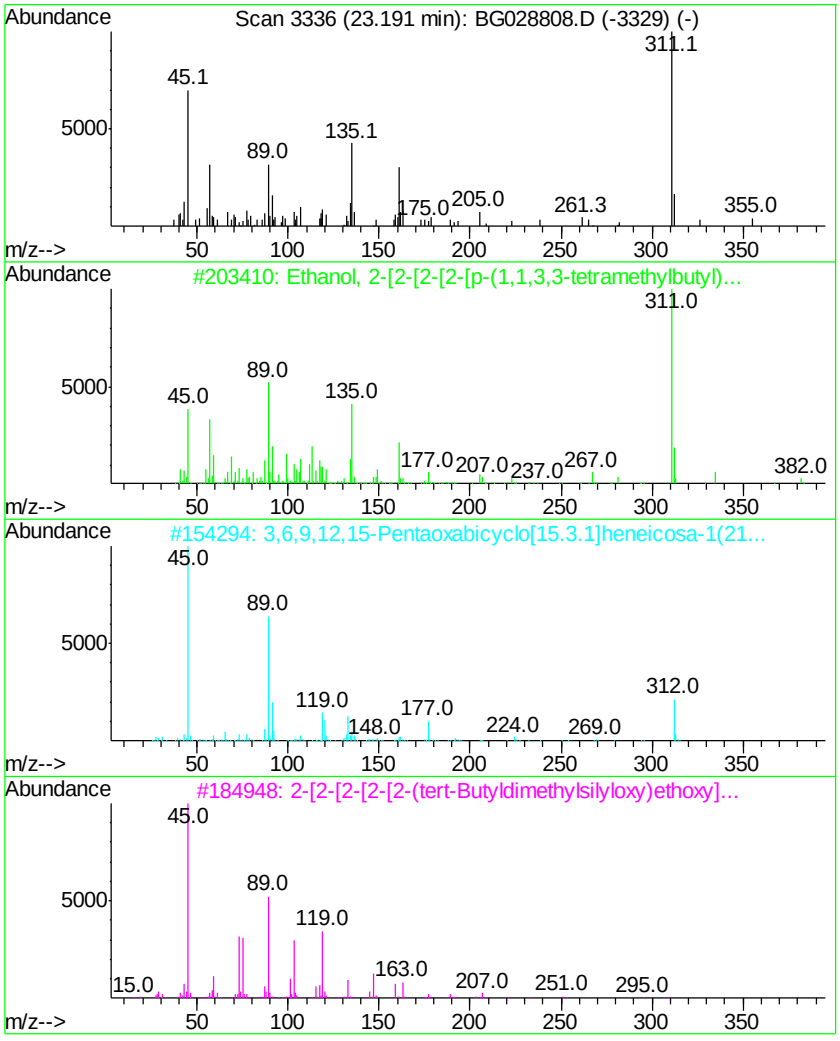
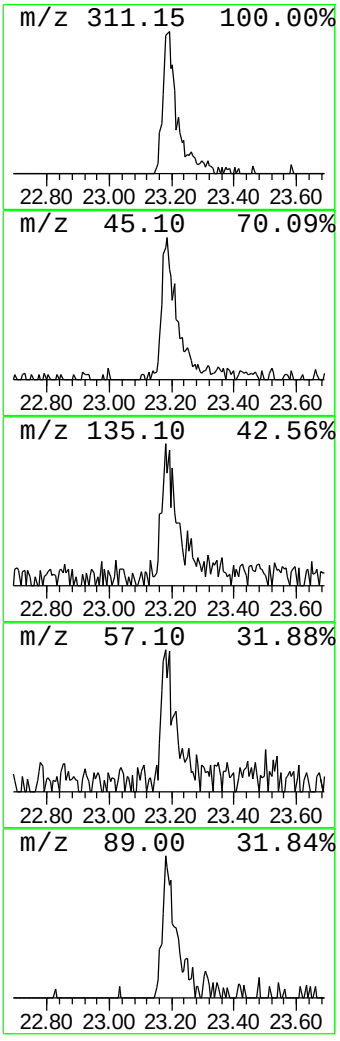
****

Peak Number 9 unknown23.19 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.42 ng	90810	Chrysene-d12	21.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[2-[2-[p-(1,1,3,3-...	382	C22H38O5	002315-63-1	38
2	3,6,9,12,15-Pentaoxabicyclo[15.3...	312	C16H24O6	065112-36-9	38
3	2-[2-[2-[2-(tert-Butyldimethy...	352	C16H36O6Si	1000352-10-3	27
4	5-(2,4-Dimethylphenyl)-3-(5-nitr...	311	C17H13NO5	309293-98-9	23
5	Thebaine	311	C19H21NO3	000115-37-7	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091817\
Data File : BG028808.D
Acq On : 18 Sep 2017 23:38
Operator : SJ/JU
Sample : I5259-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170600-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.39	4.3	ng	39272	1	8.29	184577	20.0
unknown7.82	7.82	96.2	ng	887459	1	8.29	184577	20.0
3-tert-Butyl-4-hy...	14.41	3.8	ng	79526	3	14.91	423894	20.0
unknown15.29	15.29	9.8	ng	208794	3	14.91	423894	20.0
2,2,4-Trimethyl-1...	15.67	16.8	ng	355610	3	14.91	423894	20.0
7,9-Di-tert-butyl...	18.30	3.6	ng	112439	4	17.66	627361	20.0
13H-Dibenzo[a,i]c...	21.41	2.7	ng	101099	5	21.98	749008	20.0
unknown23.19	23.19	2.4	ng	90810	5	21.98	749008	20.0