LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

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-BG102516.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	5.329	418	424	431	rVB	424587	662714	8.76%	1.308%
2	5.799	495	504	512	rVB	956670	1566411	20.70%	3.092%
3	7.403	771	777	791	rVB	616607	1152147	15.22%	2.275%
4	7.791	835	843	853	rBV	1506617	2733760	36.12%	5.397%
5	8.267	918	924	934	rVB	453534	814407	10.76%	1.608%
6	8.596	970	980	988	rBV	1328548	2433160	32.15%	4.803%
7	9.442	1115	1124	1134	rVB	1166845	2175954	28.75%	4.296%
8	9.577	1142	1147	1153	rVB4	53734	87719	1.16%	0.173%
9	11.093	1396	1405	1411	rBV	565895	1038972	13.73%	2.051%
10	11.146	1411	1414	1421	rVB2	70893	110988	1.47%	0.219%
11	11.851	1529	1534	1543	rBV6	48409	119244	1.58%	0.235%
12	12.726	1677	1683	1689	rBV2	85822	152245	2.01%	0.301%
13	12.949	1715	1721	1726	rBV	64242	109441	1.45%	0.216%
14	13.508	1808	1816	1825	rVB	3031299	4753672	62.81%	9.385%
15	13.719	1848	1852	1859	rVB3	54873	96312	1.27%	0.190%
16	14.207	1928	1935	1939	rBV3	48248	89731	1.19%	0.177%
17	14.442	1971	1975	1983	rBV6	39132	79027	1.04%	0.156%
18	14.882	2045	2050	2056	rVB	893744	1386377	18.32%	2.737%
19	14.947	2056	2061	2068	rVB	318389	521081	6.88%	1.029%
20	15.276	2107	2117	2124	rBV	368247	670013	8.85%	1.323%
21	15.922	2220	2227	2233	rVB3	101568	182133	2.41%	0.360%
22	16.210	2273	2276	2281	rVB	64981	102292	1.35%	0.202%
23	16.363	2296	2302	2314	rVB	2919165	4606109	60.86%	9.093%
24	16.898	2386	2393	2398	rBV4	56701	117055	1.55%	0.231%
25	17.280	2450	2458	2465	rVB	889046	1429476	18.89%	2.822%
26	17.444	2481	2486	2493	rVB2	119048	213802	2.82%	0.422%
27	17.626	2510	2517	2520	rBV2	1243728	1983184	26.20%	3.915%
28	17.667	2520	2524	2530	rVV	1942008	2927025	38.67%	5.778%
29	17.732	2530	2535	2536	rVV4	54612	90383	1.19%	0.178%
30	17.755	2536	2539	2544	rVB	132872	183993	2.43%	0.363%
31	18.026	2576	2585	2592	rBV3	137589	264186	3.49%	0.522%
32	18.202	2609	2615	2619	rBV4	61463	82161	1.09%	0.162%
33	18.490	2656	2664	2669	rBV2	106135	208051	2.75%	0.411%
34	18.543	2669	2673	2678	rVB2	119448	176857	2.34%	0.349%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

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-BG102516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.690	2692	2698	2702	rBV5	88114	194072	2.56%	0.383%
36	19.030	2751	2756	2760	rVB2	261759	380365	5.03%	0.751%
37	19.407	2814	2820	2828	rBV	651137	1046624	13.83%	2.066%
38	19.542	2838	2843	2849	rBV	157997	245779	3.25%	0.485%
39	19.659	2858	2863	2869	rVB	580405	876712	11.58%	1.731%
40	19.741	2871	2877	2882	rBV8	63886	126444	1.67%	0.250%
41	19.988	2914	2919	2920	rBV5	60830	86487	1.14%	0.171%
42	20.023	2920	2925	2930	rVV	406249	637633	8.42%	1.259%
43	20.206	2950	2956	2962	rBV	5728947	7568524	100.00%	14.941%
44	21.287	3137	3140	3149	rVB6	41538	79461	1.05%	0.157%
45	21.921	3239	3248	3255	rBV	1603186	3009911	39.77%	5.942%
46	23.637	3533	3540	3549	rVB4	105136	274407	3.63%	0.542%
47	25.352	3819	3832	3845	rBV2	937218	2807990	37.10%	5.543%

Sum of corrected areas: 50654491

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
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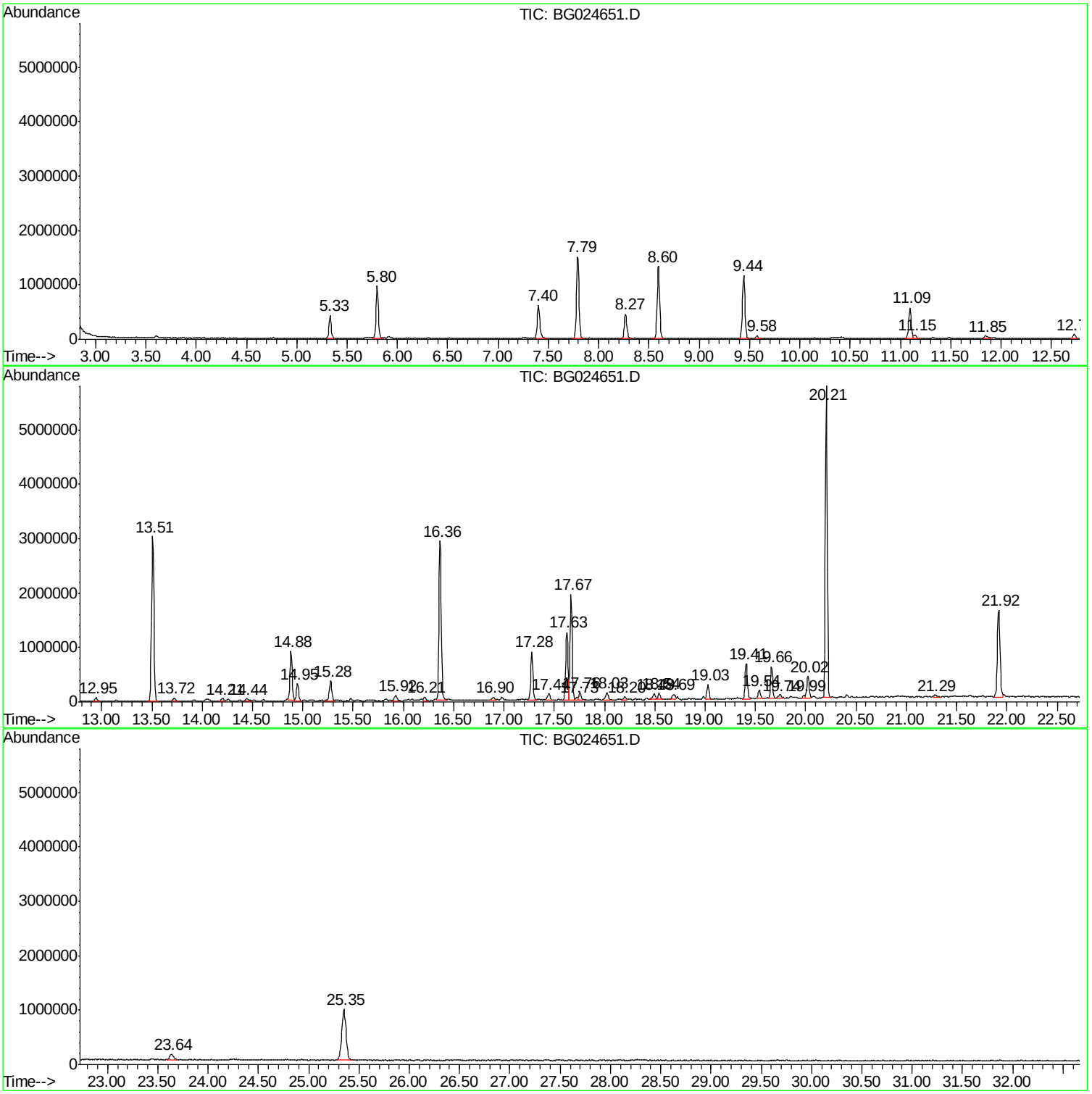
Instrument :
BNA_G
ClientSampleId :
GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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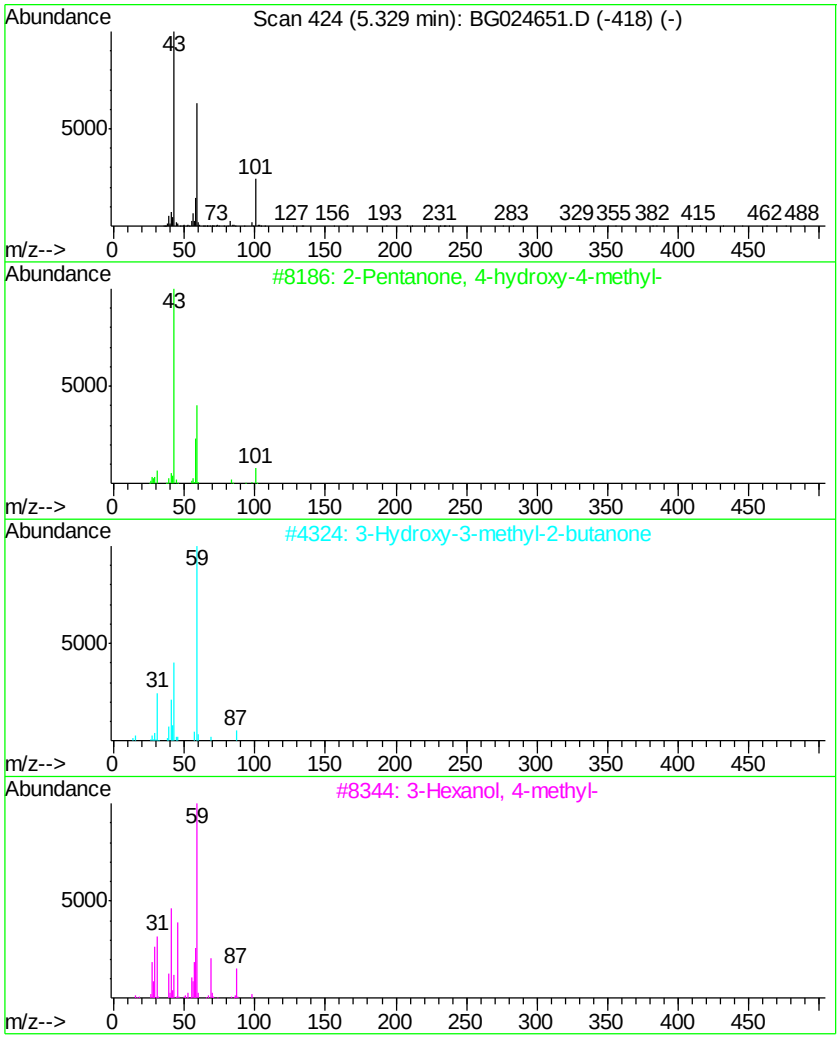
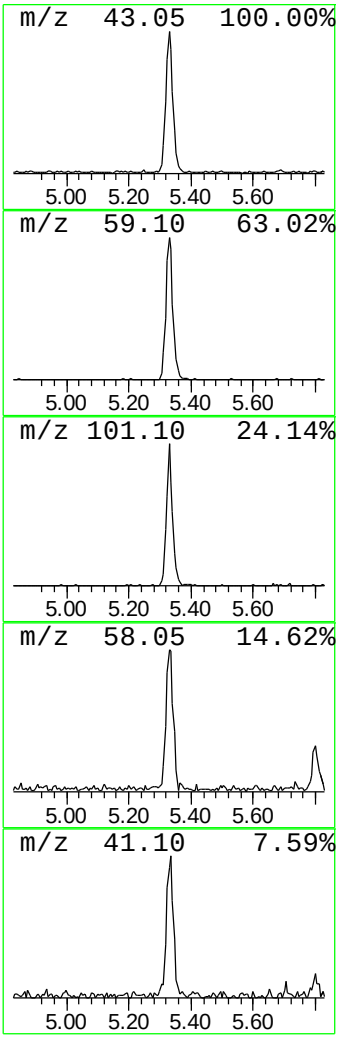
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	16.27 ng	662714	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

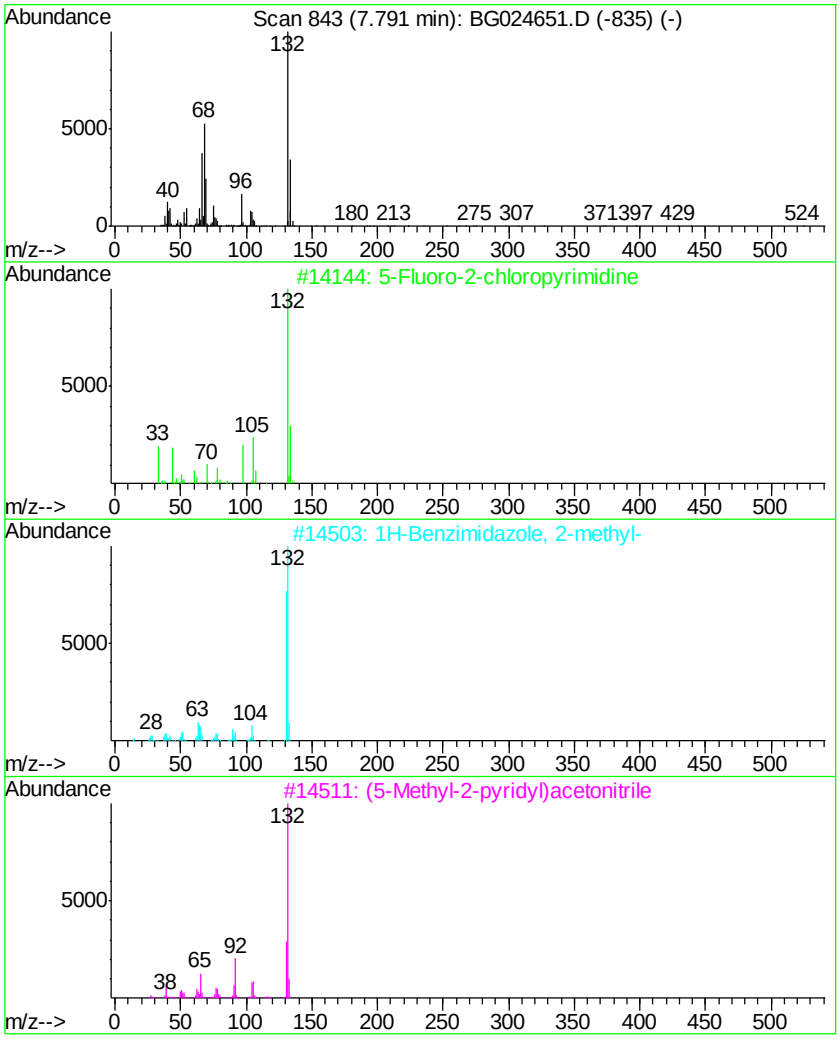
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

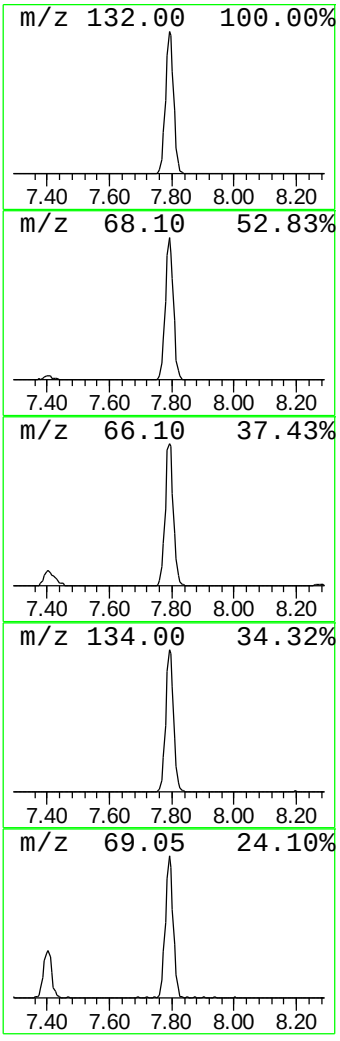
****

Peak Number 2 unknown7.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	67.14 ng	2733760	1,4-Dichlorobenzene-d4	8.27

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	27
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	12





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

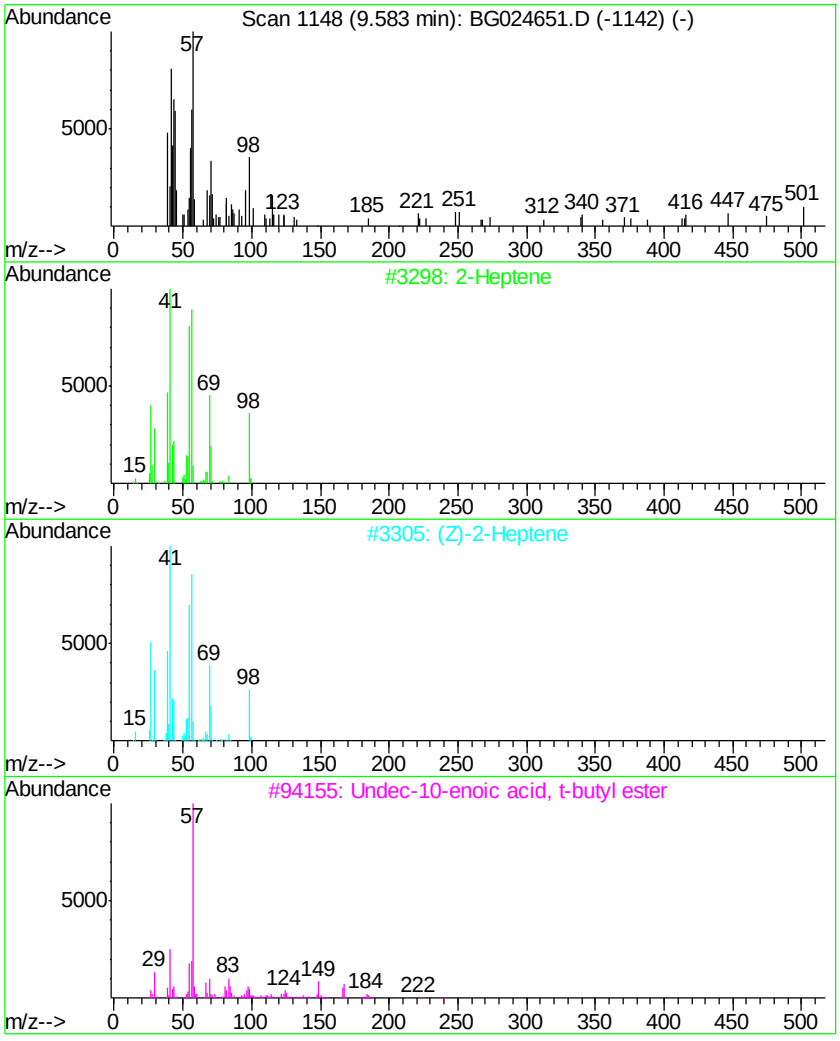
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

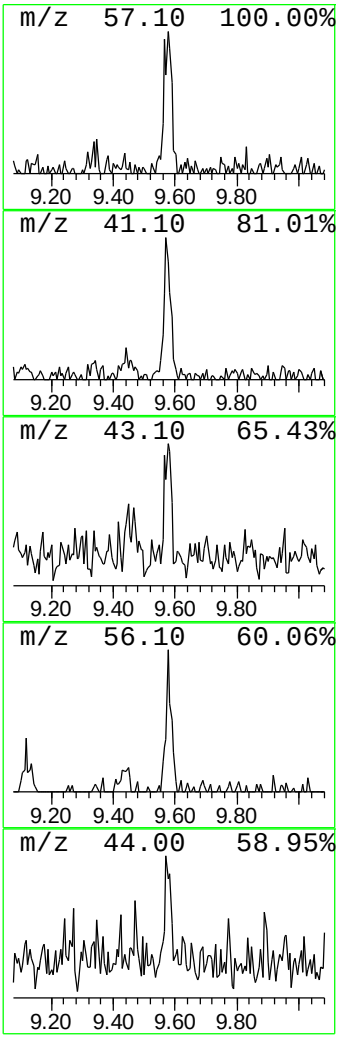
****

Peak Number 4 2-Heptene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.58	2.15 ng	87719	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptene	98	C7H14	000592-77-8	52
2	(Z)-2-Heptene	98	C7H14	006443-92-1	50
3	Undec-10-enoic acid, t-butyl ester	240	C15H28O2	093757-41-6	45
4	1-Heptene	98	C7H14	000592-76-7	43
5	2-Heptene, (E)-	98	C7H14	014686-13-6	40





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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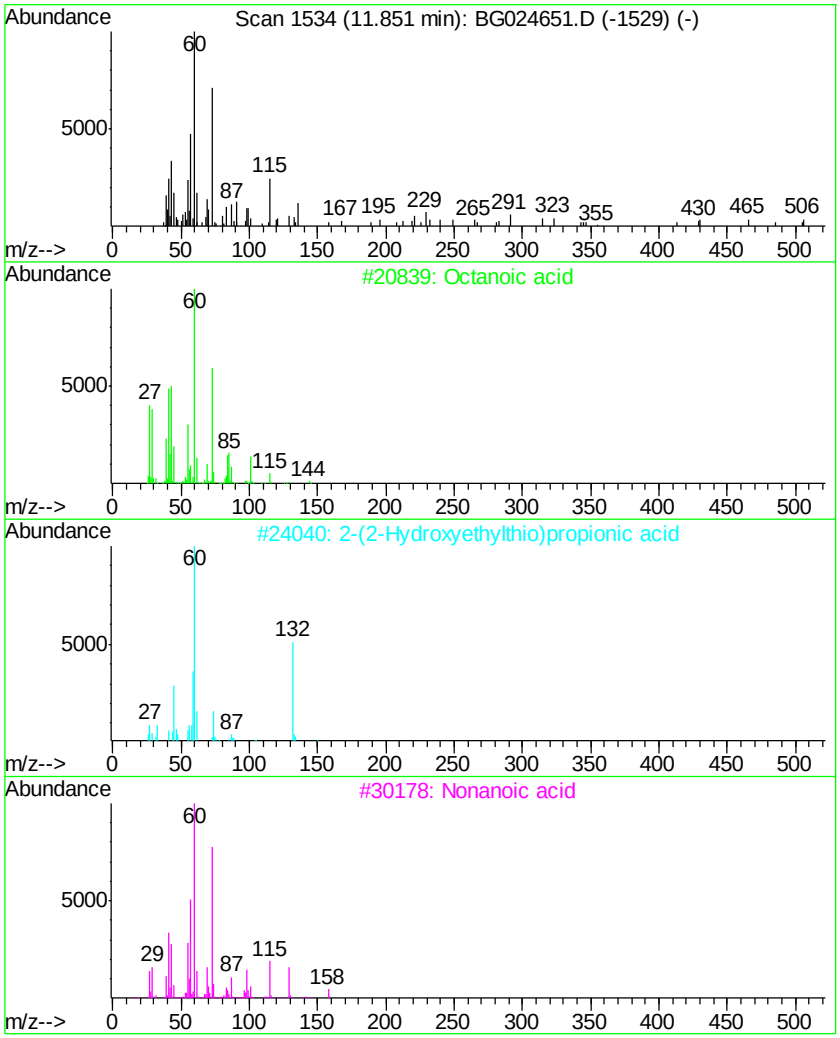
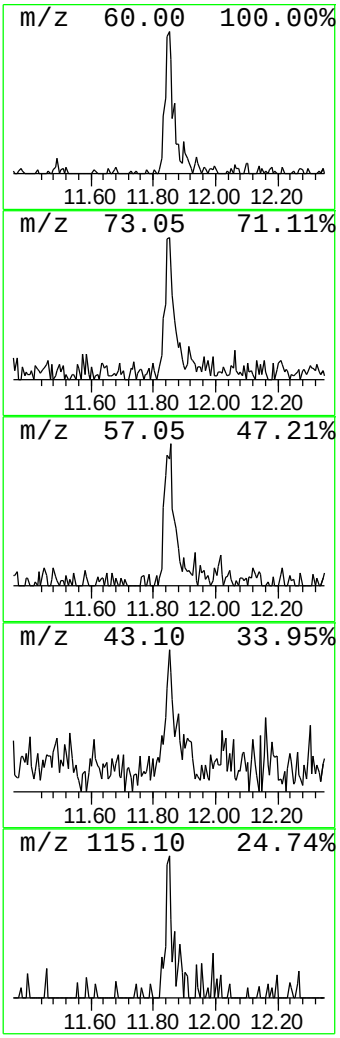
Peak Number 5 Octanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.30 ng	119244	Naphthalene-d8	11.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	53
2	2-(2-Hydroxyethylthio)propionic ...	150	C5H10O3S	209276-28-8	53
3	Nonanoic acid	158	C9H18O2	000112-05-0	53
4	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	42
5	1,3-Oxathiolane, 2,2-dimethyl-	118	C5H10OS	005684-31-1	42





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
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Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

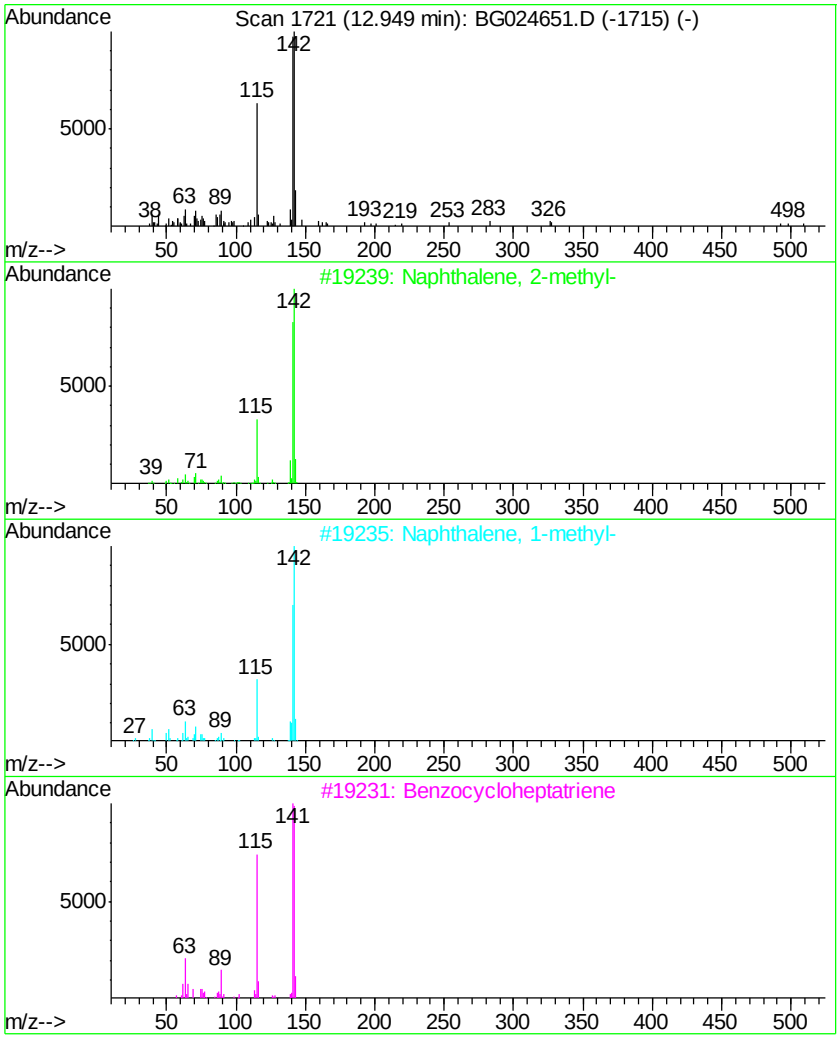
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

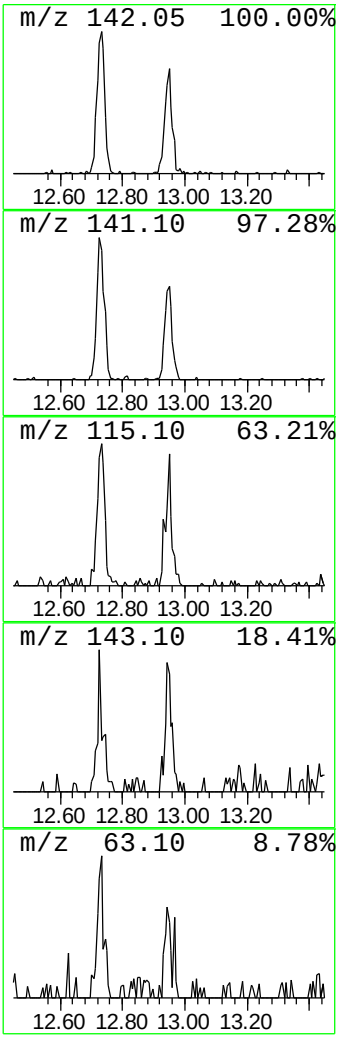
****

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.95	2.11 ng	109441	Naphthalene-d8	11.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	87
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	87
3	Benzocycloheptatriene	142	C11H10	000264-09-5	87
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	86





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Data File : BG024651.D
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Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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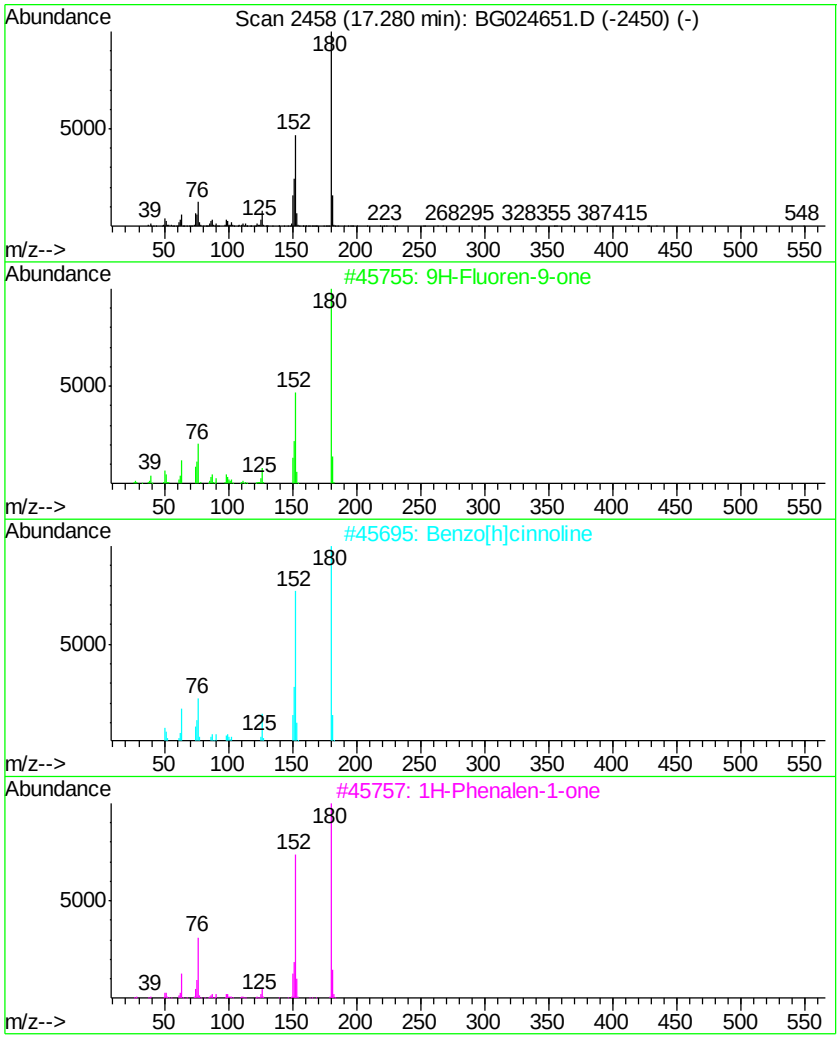
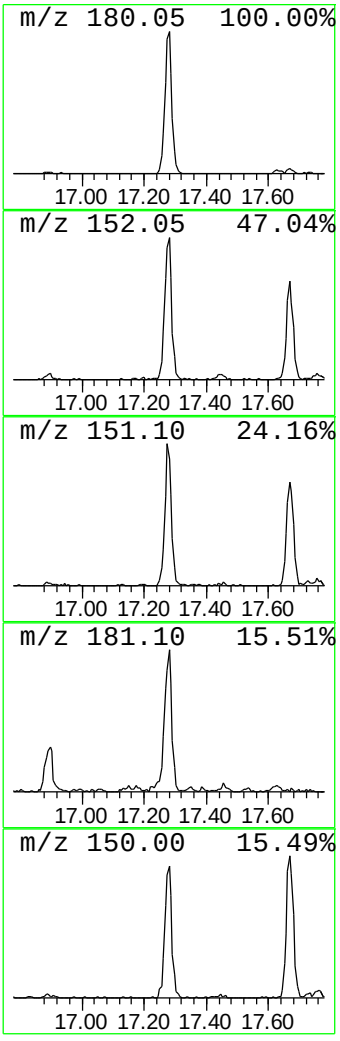
Peak Number 7 9H-Fluoren-9-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	14.42 ng	1429480	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluoren-9-one	180	C13H8O	000486-25-9	94
2	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	91
3	1H-Phenalen-1-one	180	C13H8O	000548-39-0	58
4	2,3-Diazaphenanthrene	180	C12H8N2	000229-72-1	53
5	Benzo(f)quinoxaline	180	C12H8N2	000230-33-1	43





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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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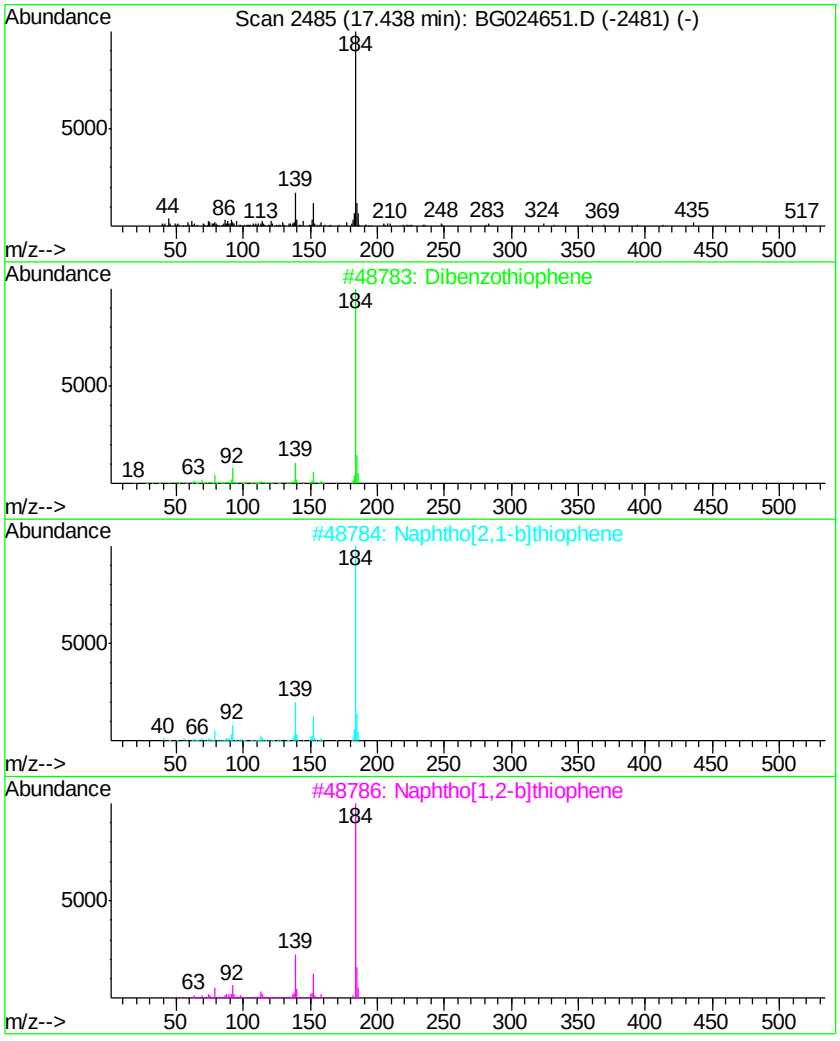
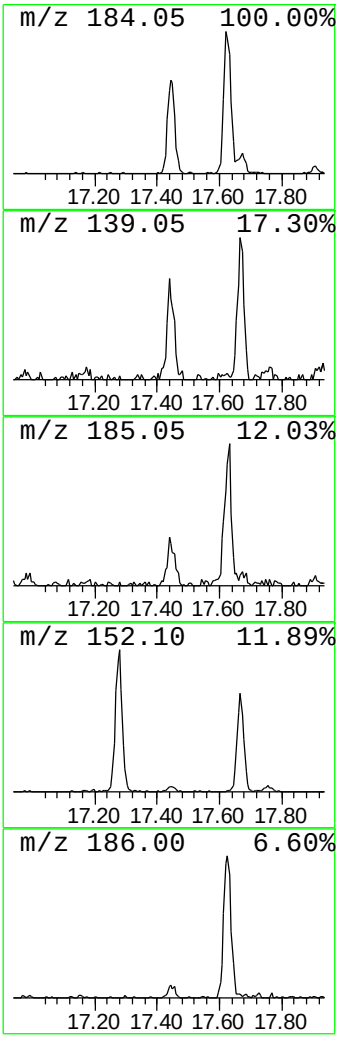
Peak Number 8 Dibenzothiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	2.16 ng	213802	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	83
2	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	81
3	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	72
4	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	64
5	Naphthalene, 2-ethenyl-6-methoxy-	184	C13H12O	063444-51-9	59





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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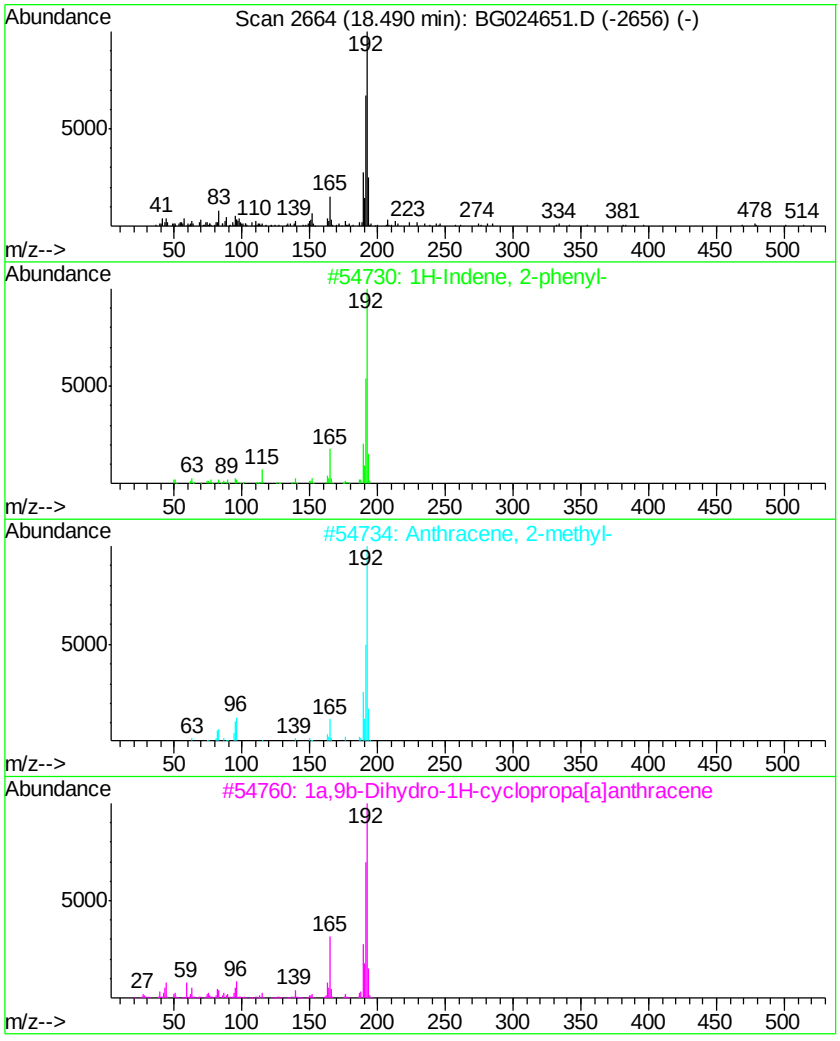
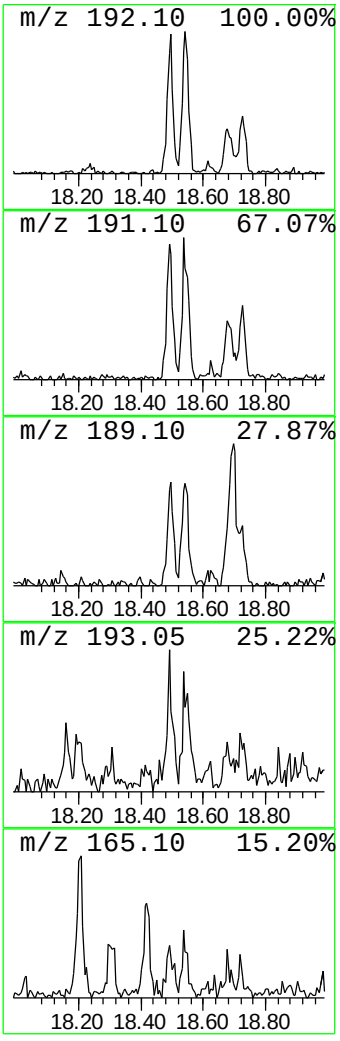
Peak Number 9 1H-Indene, 2-phenyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.49	2.10 ng	208051	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	81
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
3	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	70
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	70
5	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	68





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Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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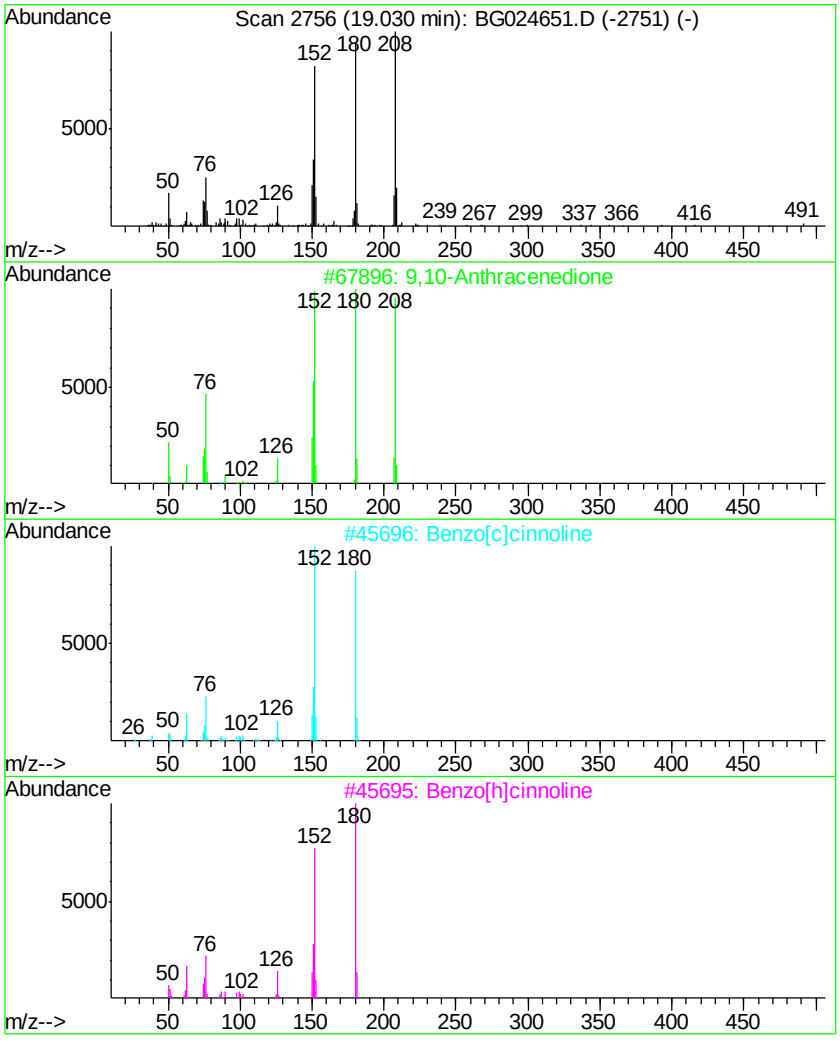
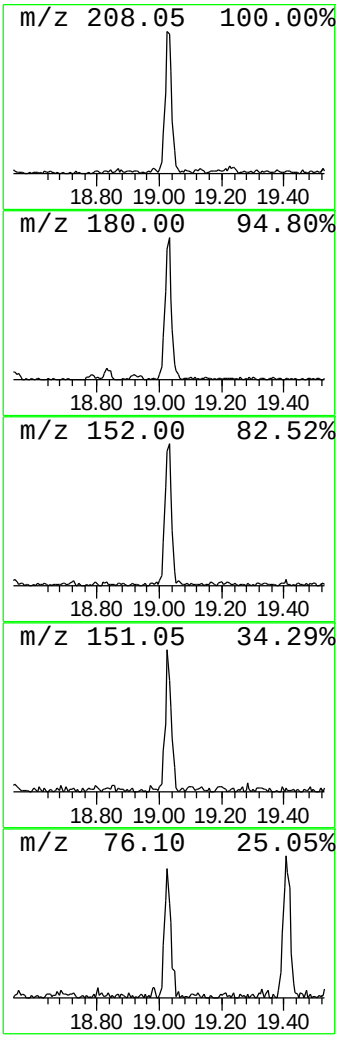
Peak Number 10 9,10-Anthracenedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	3.84 ng	380365	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	97
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	83
3	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	53
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	52
5	9H-Fluoren-9-one	180	C13H8O	000486-25-9	43





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Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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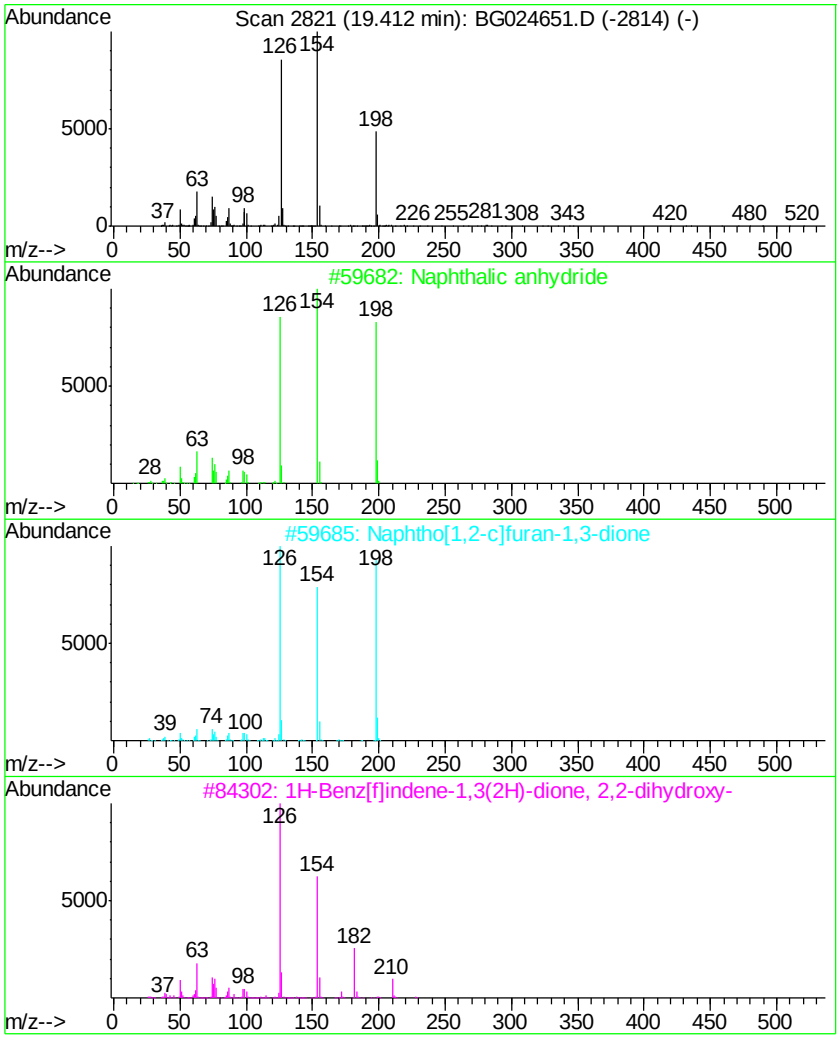
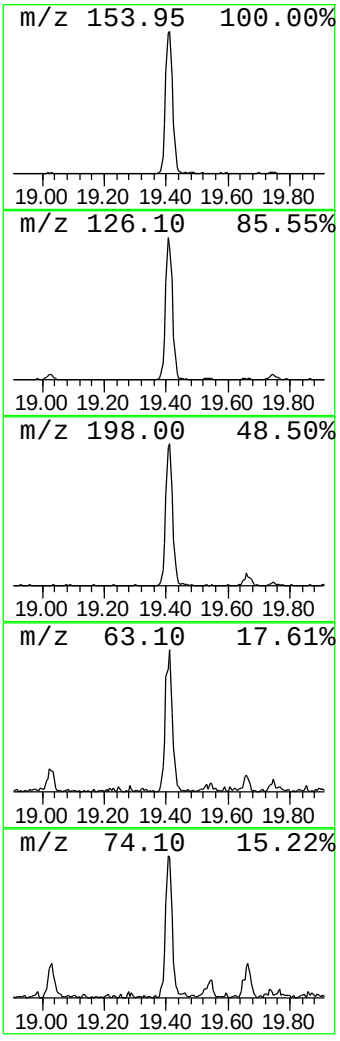
Peak Number 11 Naphthalic anhydride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.41	10.56 ng	1046620	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalic anhydride	198	C12H6O3	000081-84-5	94
2	Naphtho[1,2-c]furan-1,3-dione	198	C12H6O3	005343-99-7	78
3	1H-Benz[f]indene-1,3(2H)-dione, ...	228	C13H8O4	038627-57-5	47
4	Benzoic acid, 5-chloro-2-hydroxy-	172	C7H5ClO3	000321-14-2	42
5	Benzothiazole, 4,5,6,7-tetrahydr...	154	C7H10N2S	002933-29-1	42





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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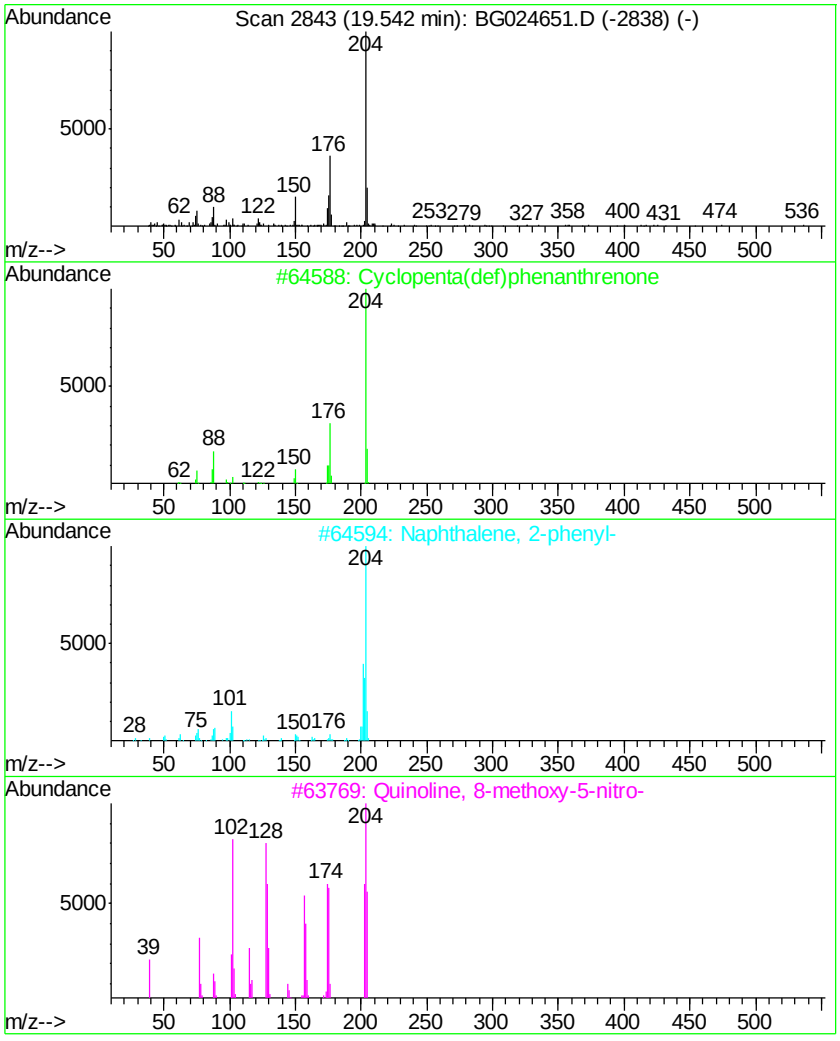
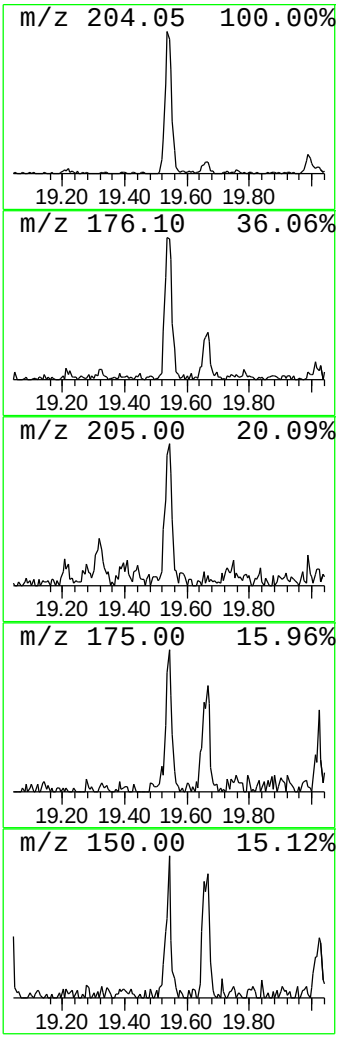
Peak Number 12 Cyclopenta(def)phenanthrenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.54	2.48 ng	245779	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	93
2	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	53
3	Quinoline, 8-methoxy-5-nitro-	204	C10H8N2O3	1000298-88-7	50
4	[1,2,4]Triazolo[5,1-b]quinazolin...	204	C10H12N4O	1000337-56-5	50
5	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024651.D
Acq On : 3 Nov 2016 13:51
Operator : UM/SJ
Sample : H5502-30
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-88-7.6-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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...	5.33	16.3	ng	662714	1	8.27	814407	20.0
unknown7.79	7.79	67.1	ng	2733760	1	8.27	814407	20.0
2-Heptene	9.58	2.1	ng	87719	1	8.27	814407	20.0
Octanoic acid	11.85	2.3	ng	119244	2	11.09	1038970	20.0
Naphthalene, 1-me...	12.95	2.1	ng	109441	2	11.09	1038970	20.0
9H-Fluoren-9-one	17.28	14.4	ng	1429480	4	17.63	1983180	20.0
Dibenzothiophene	17.44	2.2	ng	213802	4	17.63	1983180	20.0
1H-Indene, 2-phenyl-	18.49	2.1	ng	208051	4	17.63	1983180	20.0
9,10-Anthracenedione	19.03	3.8	ng	380365	4	17.63	1983180	20.0
Naphthalic anhydride	19.41	10.6	ng	1046620	4	17.63	1983180	20.0
Cyclopenta(def)ph...	19.54	2.5	ng	245779	4	17.63	1983180	20.0