LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101421\
Data File : BG050594.D
Acq On : 14 Oct 2021 19:15
Operator : CG/JU
Sample : M4193-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 351

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.797	385	393	408	rBV	639587	1099770	40.77%	7.015%
2	7.401	658	666	678	rBV	651213	1167718	43.29%	7.448%
3	8.258	801	812	823	rBV	191430	332550	12.33%	2.121%
4	9.428	1002	1011	1019	rBV	413745	777874	28.84%	4.961%
5	10.826	1243	1249	1259	rBV	120436	223748	8.29%	1.427%
6	11.079	1285	1292	1300	rVB	243211	451245	16.73%	2.878%
7	13.499	1696	1704	1711	rVB	952419	1540603	57.11%	9.826%
8	14.292	1834	1839	1842	rBV2	135500	209806	7.78%	1.338%
9	14.381	1849	1854	1863	rBV3	166974	314092	11.64%	2.003%
10	14.616	1888	1894	1898	rBV6	112686	248030	9.19%	1.582%
11	14.698	1904	1908	1914	rVB3	214852	346736	12.85%	2.212%
12	14.839	1925	1932	1933	rBV5	141685	256374	9.50%	1.635%
13	14.874	1934	1938	1944	rVB2	390028	656171	24.33%	4.185%
14	15.362	2017	2021	2027	rBV6	141322	351352	13.03%	2.241%
15	15.656	2067	2071	2076	rVB	358722	511189	18.95%	3.260%
16	16.361	2187	2191	2195	rBV3	576067	1025874	38.03%	6.543%
17	16.584	2224	2229	2233	rBV	1791993	2697496	100.00%	17.205%
18	20.227	2846	2849	2854	rVB	1689541	2243104	83.16%	14.307%
19	21.925	3133	3138	3144	rVB2	359458	620255	22.99%	3.956%
20	25.327	3709	3717	3732	rVB2	191133	604305	22.40%	3.854%

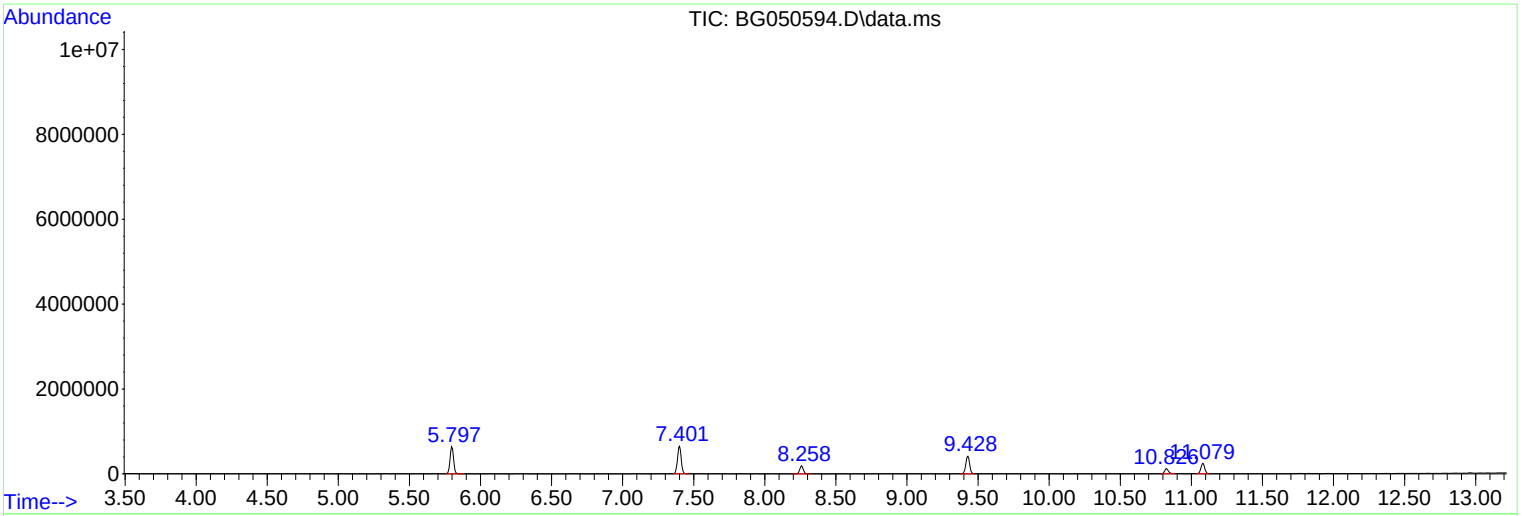
Sum of corrected areas: 15678292

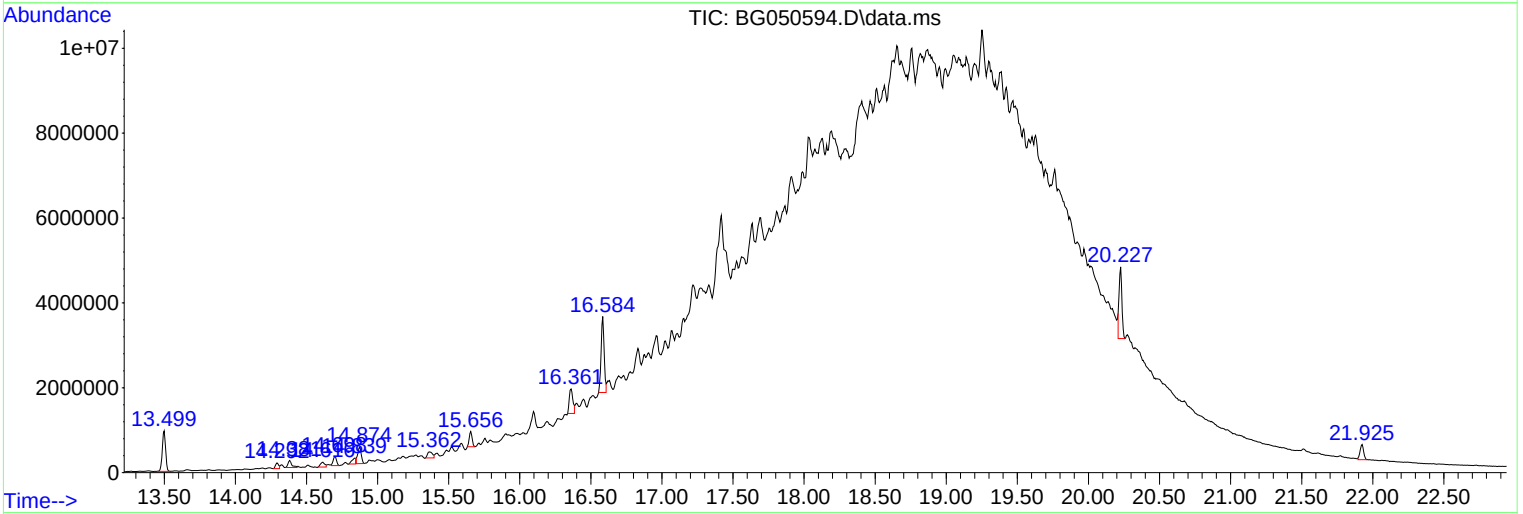
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101421\
Data File : BG050594.D
Acq On : 14 Oct 2021 19:15
Operator : CG/JU
Sample : M4193-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

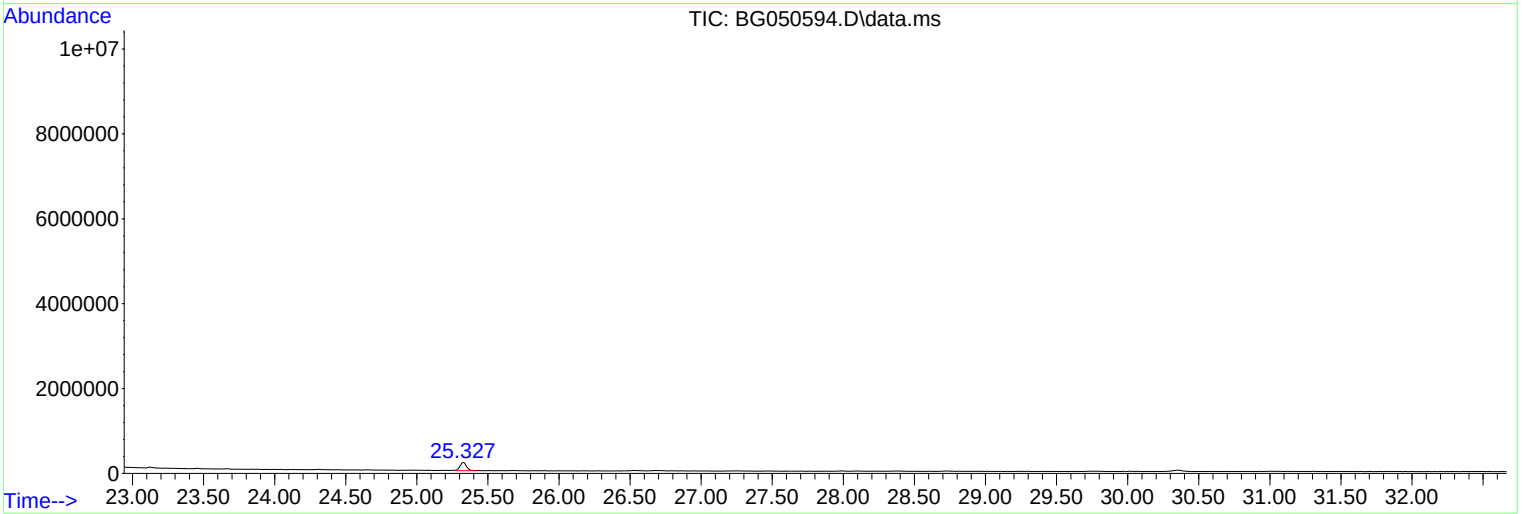
Instrument :
BNA_G
ClientSampleId :
351

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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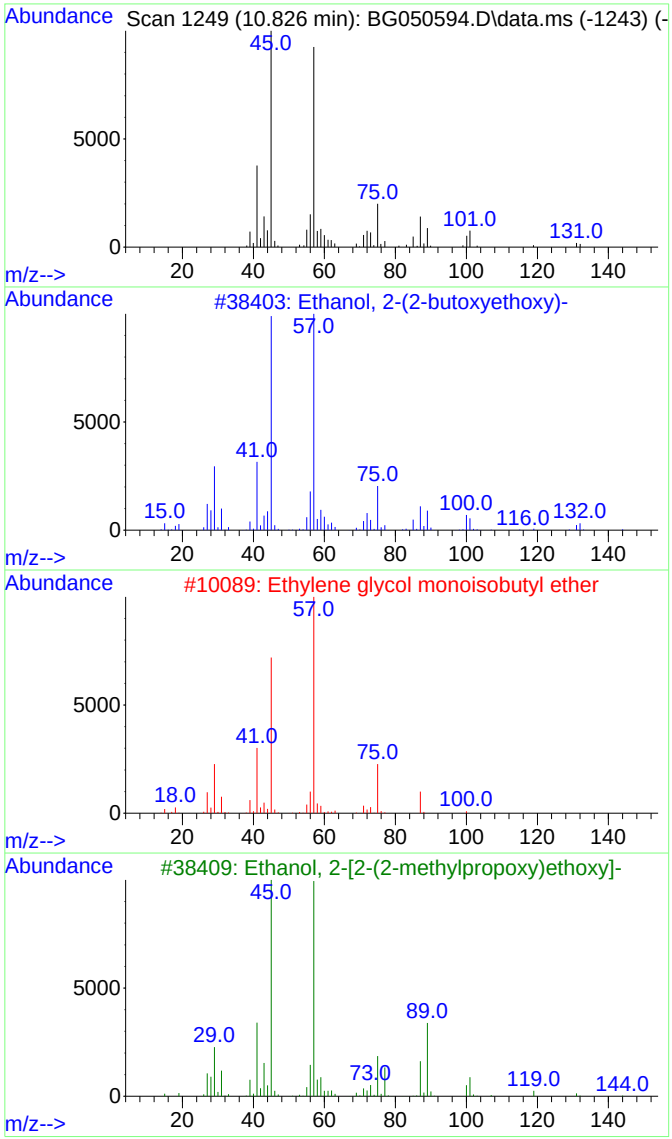
TIC Integration Parameters: LSCINT.P

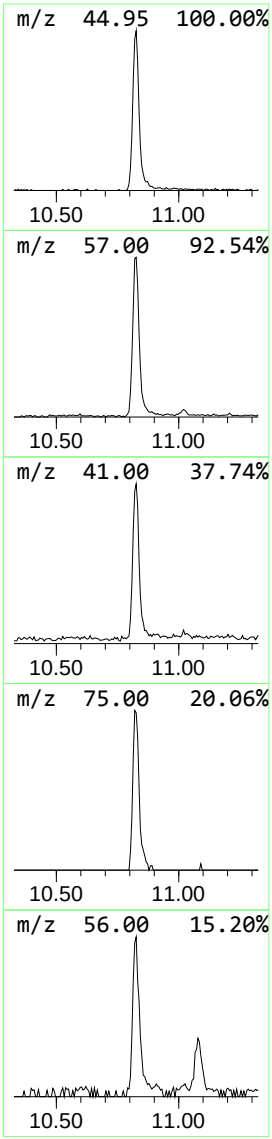
****

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.826	9.92 ng	223748	Naphthalene-d8	11.079

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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Data File : BG050594.D
Acq On : 14 Oct 2021 19:15
Operator : CG/JU
Sample : M4193-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 351

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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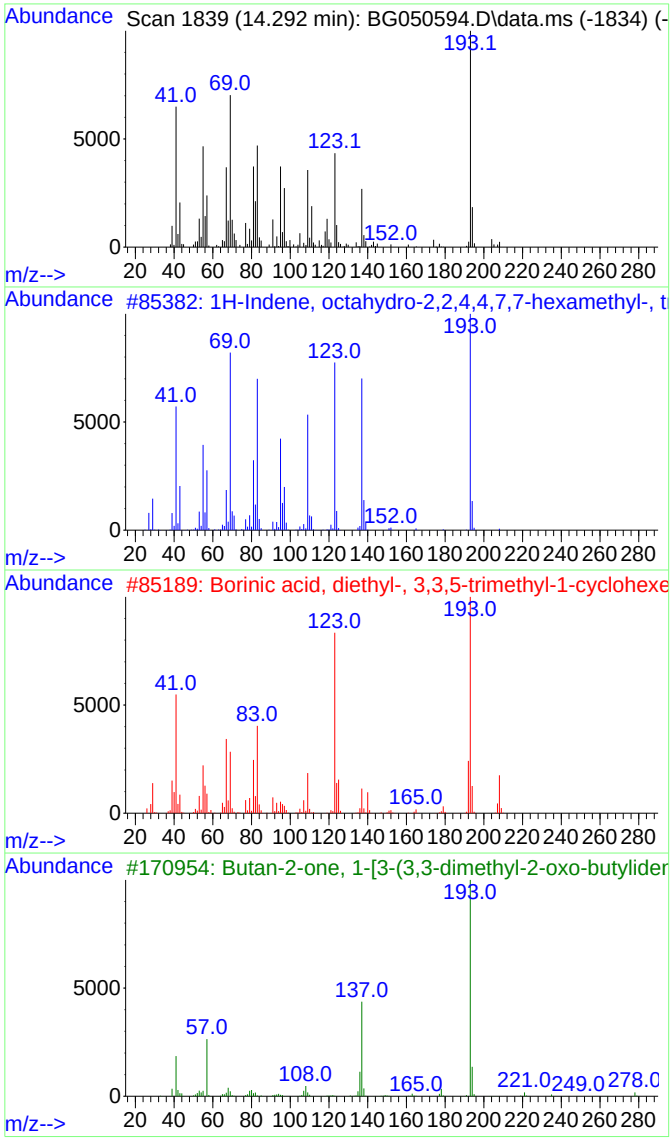
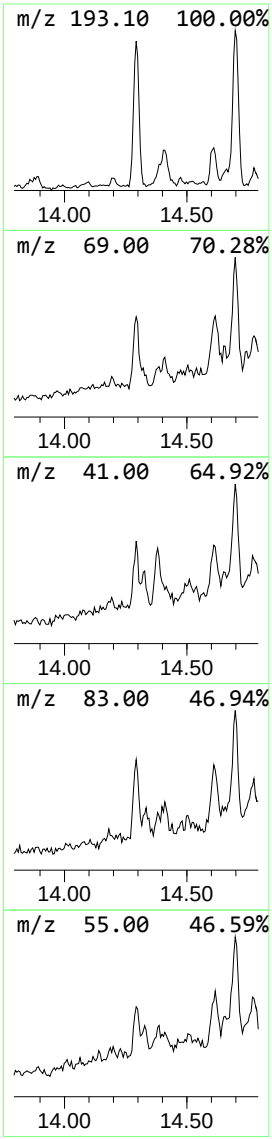
Peak Number 2 1H-Indene, octahydro-2,2,4,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.293	6.39 ng	209806	Acenaphthene-d10	14.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	72
2	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	45
3	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	27
4	2,6-Dodecadiene, 2,6-dimethyl-	194	C14H26	1000164-67-6	27
5	2-Anthracenamine	193	C14H11N	000613-13-8	27





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Acq On : 14 Oct 2021 19:15
Operator : CG/JU
Sample : M4193-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 351

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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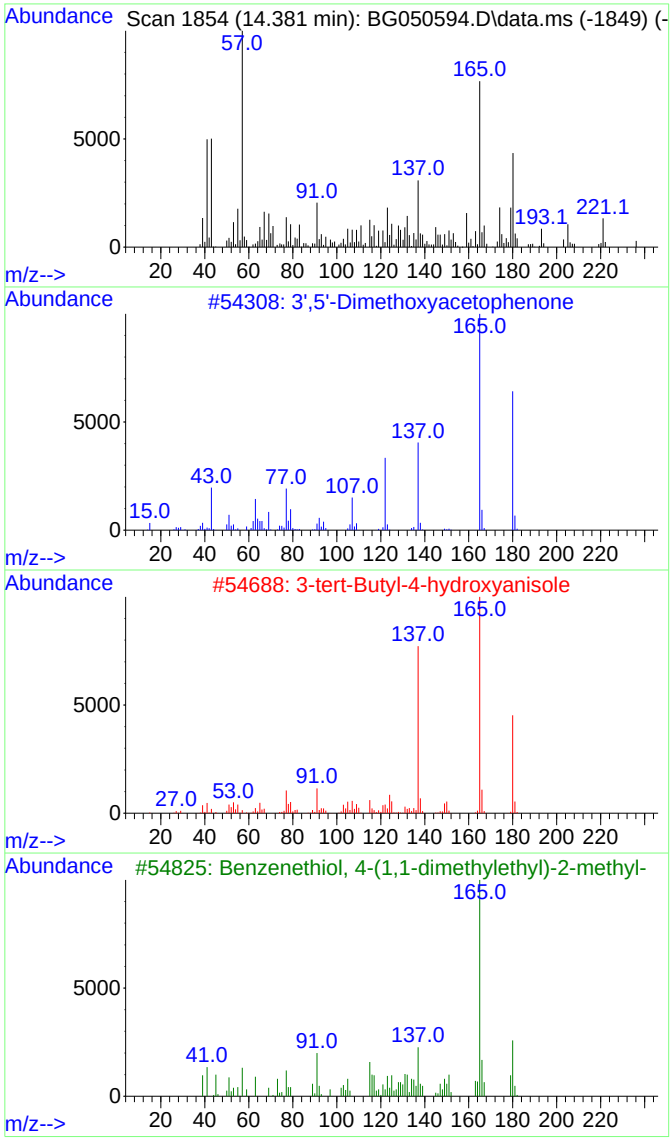
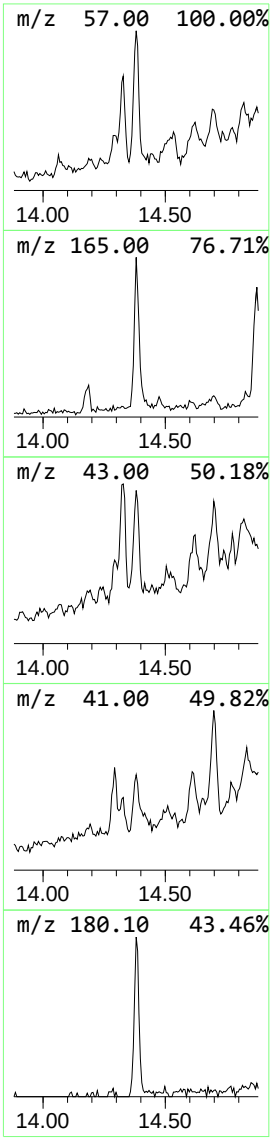
Peak Number 3 3',5'-Dimethoxyacetophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.381	9.57 ng	314092	Acenaphthene-d10	14.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	83
2	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	64
3	Benzenethiol, 4-(1,1-dimethyleth...	180	C11H16S	015570-10-2	52
4	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	001131-62-0	49
5	2',4'-Dimethoxyacetophenone	180	C10H12O3	000829-20-9	49





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Acq On : 14 Oct 2021 19:15
Operator : CG/JU
Sample : M4193-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 351

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

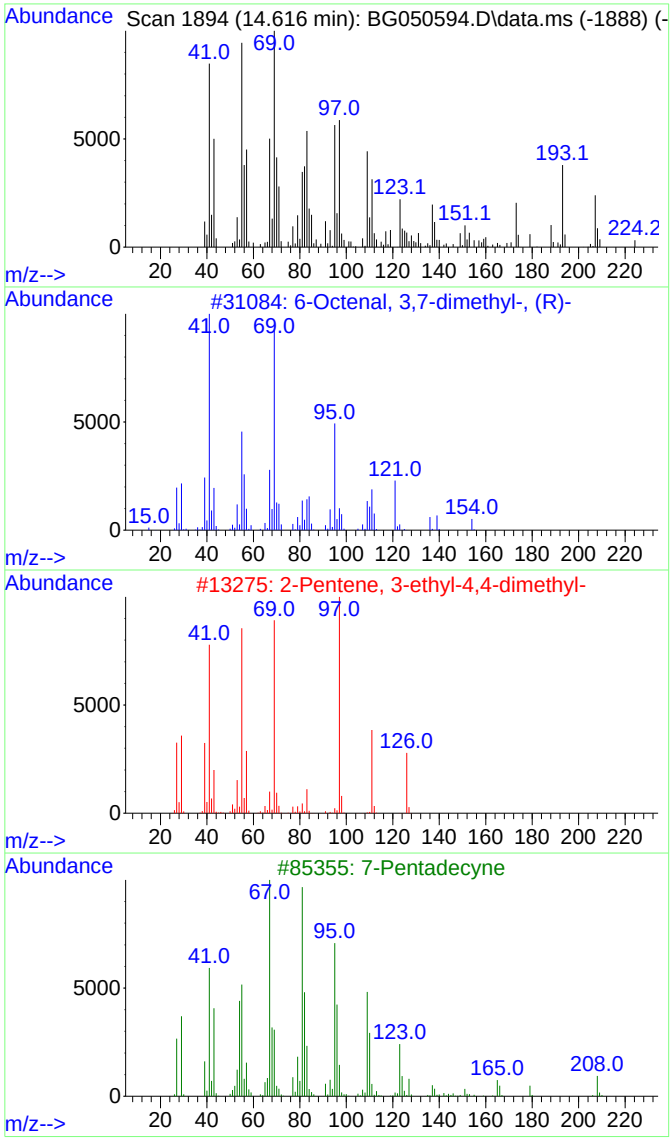
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

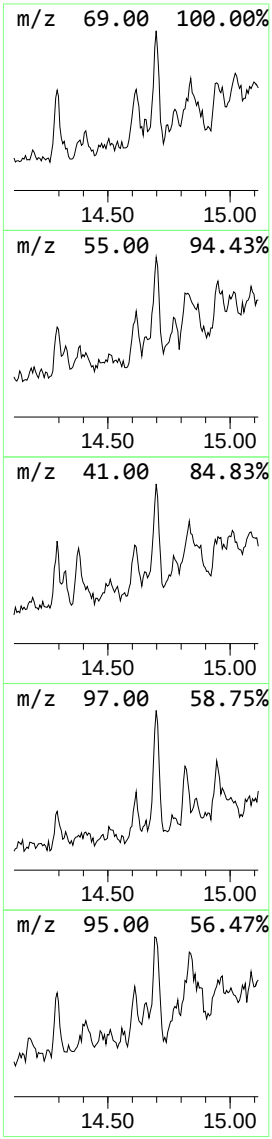
****

Peak Number 4 unknown14.616 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.616	7.56 ng	248030	Acenaphthene-d10	14.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octenal, 3,7-dimethyl-, (R)-	154	C10H18O	002385-77-5	35
2	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	22
3	7-Pentadecyne	208	C15H28	022089-89-0	22
4	Cyclohexane, 1,1'-ethylidenebis-	194	C14H26	002319-61-1	18
5	3-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-8	18





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Data File : BG050594.D
Acq On : 14 Oct 2021 19:15
Operator : CG/JU
Sample : M4193-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 351

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

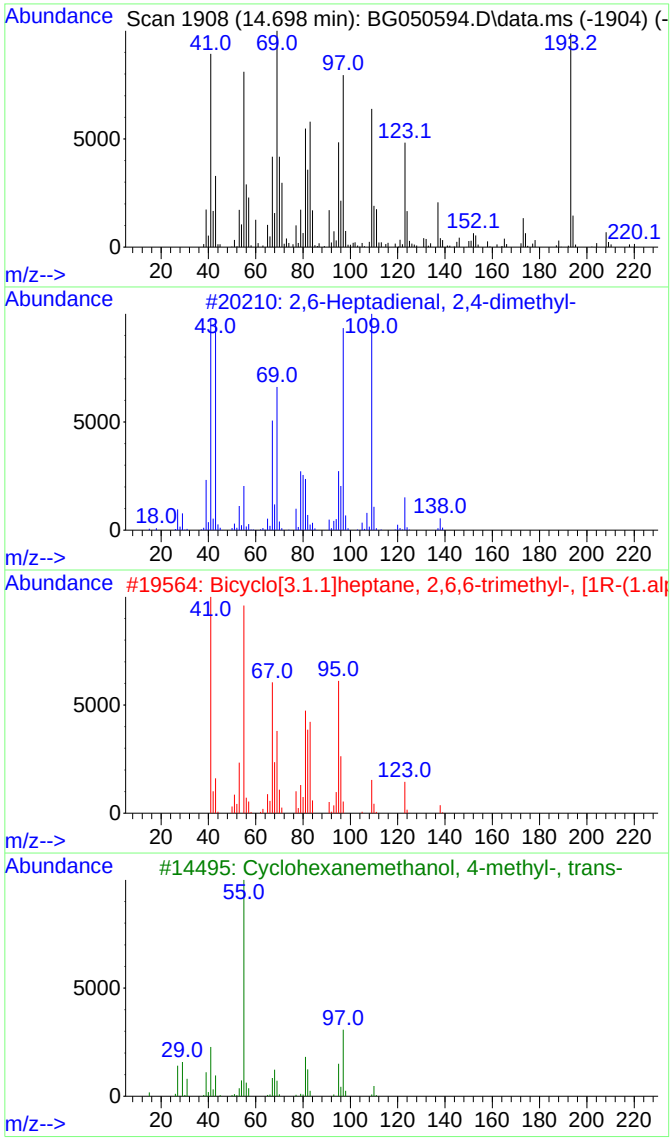
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

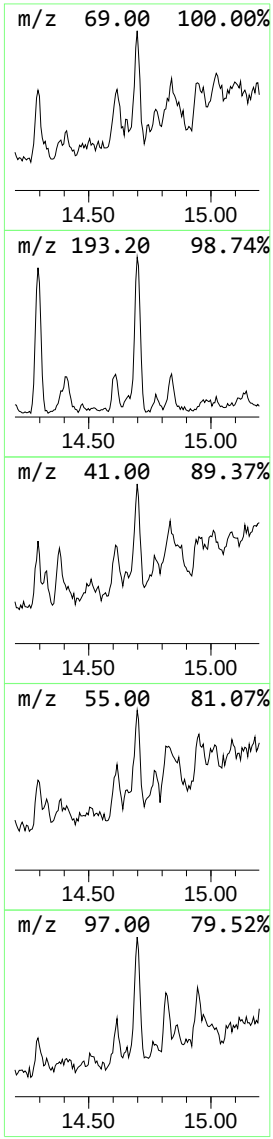
****

Peak Number 5 unknown14.698 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.698	10.57 ng	346736	Acenaphthene-d10	14.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	30
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	25
3	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-49-3	22
4	4-Hexen-3-one, 4,5-dimethyl-	126	C8H14O	017325-90-5	22
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	22





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 351

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

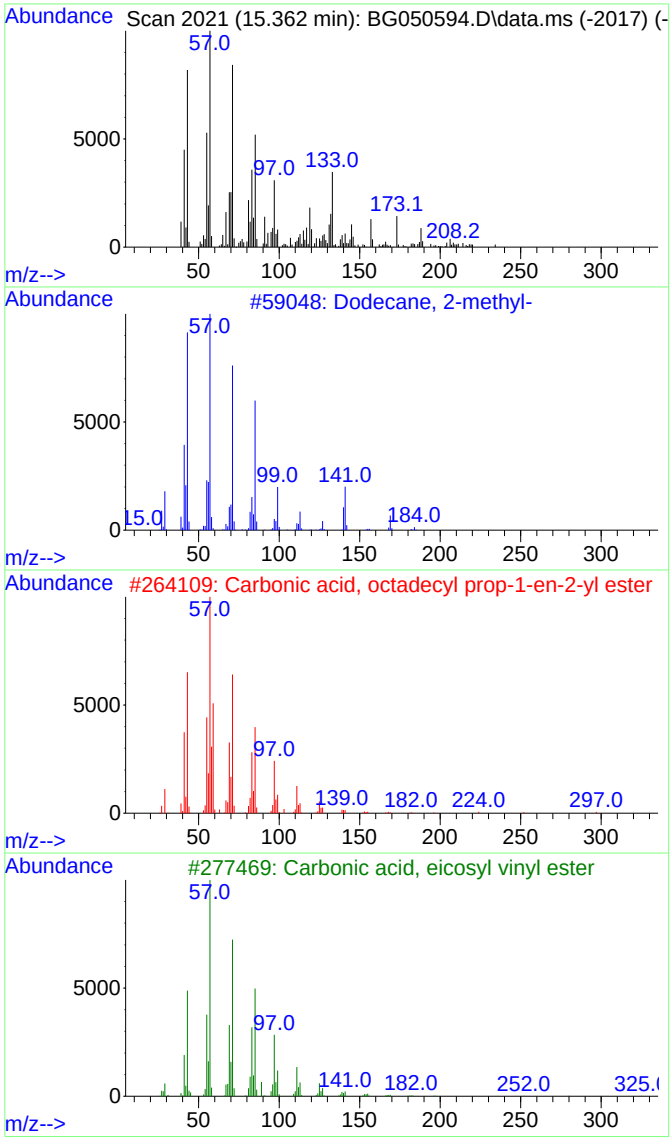
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

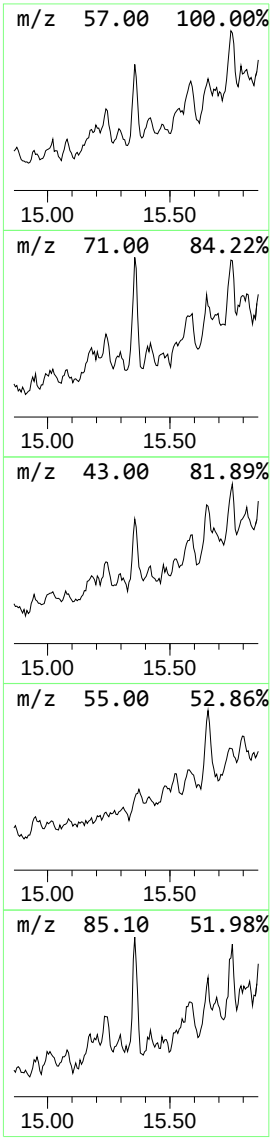
****

Peak Number 6 Dodecane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.362	10.71 ng	351352	Acenaphthene-d10	14.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	60
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	58
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	52
4	Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	46
5	Tetradecane	198	C14H30	000629-59-4	46





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 351

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

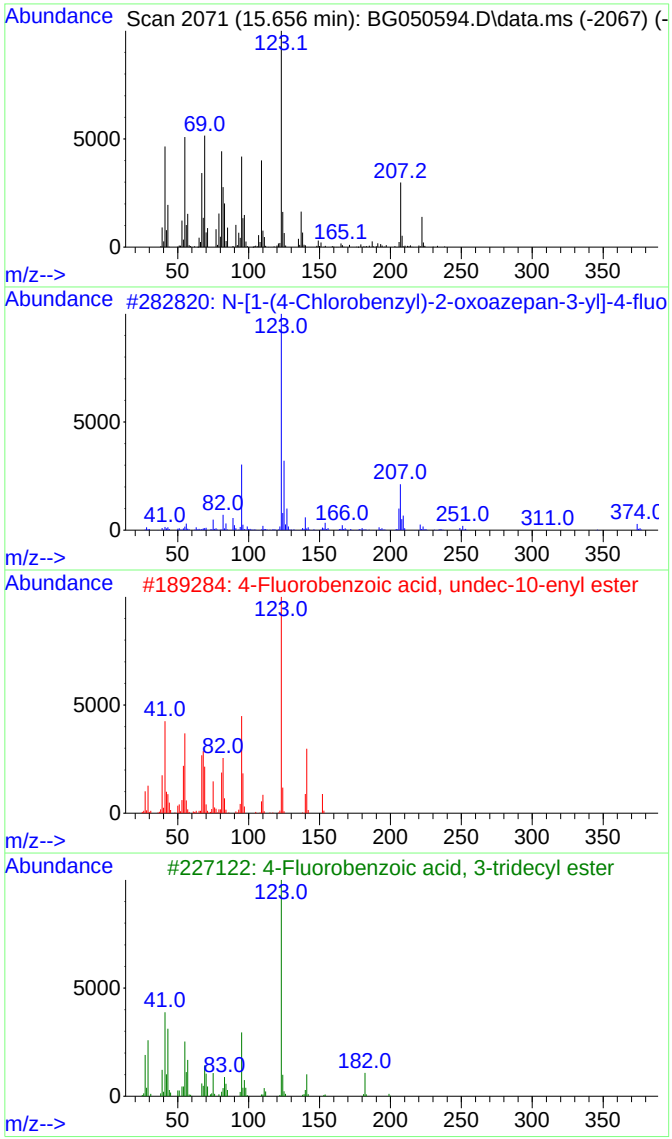
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

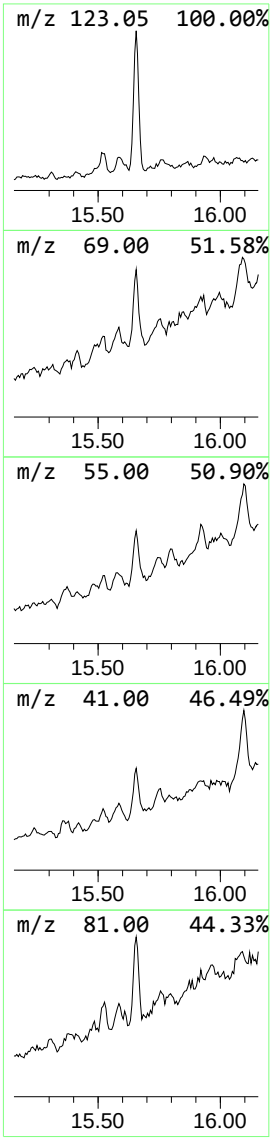
****

Peak Number 7 N-[1-(4-Chlorobenzyl)-2-oxo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.656	15.58 ng	511189	Acenaphthene-d10	14.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[1-(4-Chlorobenzyl)-2-oxoazepa...	374	C20H20ClFN2O2	1000481-70-9	50
2	4-Fluorobenzoic acid, undec-10-e...	292	C18H25FO2	1000279-02-8	47
3	4-Fluorobenzoic acid, 3-tridecyl...	322	C20H31FO2	1000280-67-9	47
4	Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	46
5	2-Fluorobenzoic acid, oct-3-en-2...	250	C15H19FO2	1000299-16-5	43





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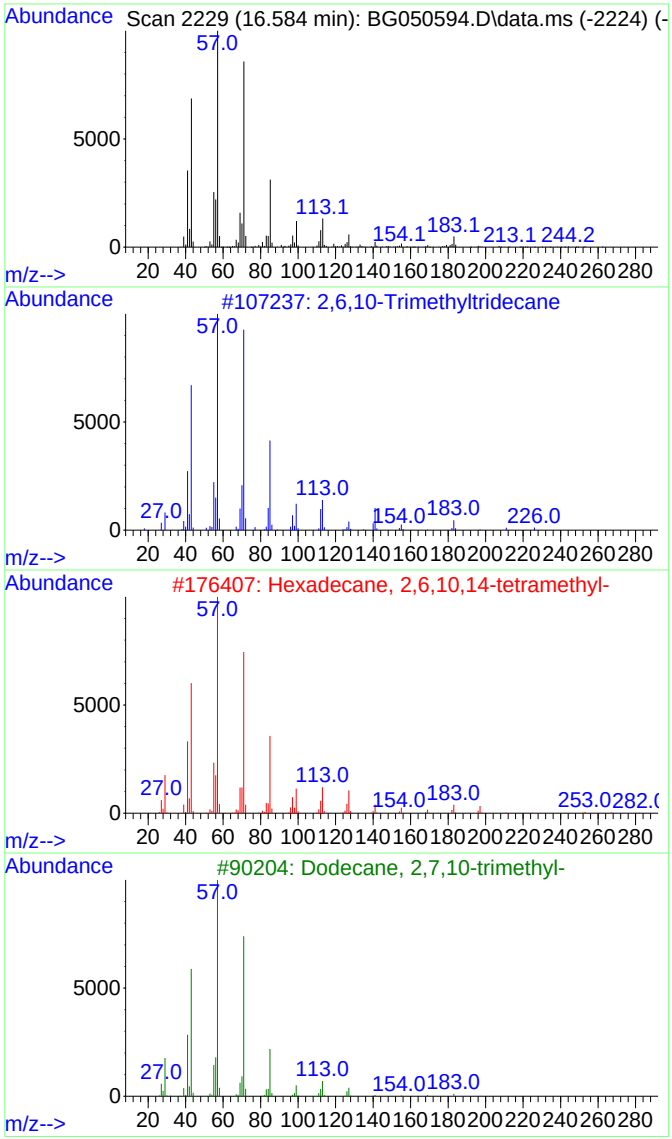
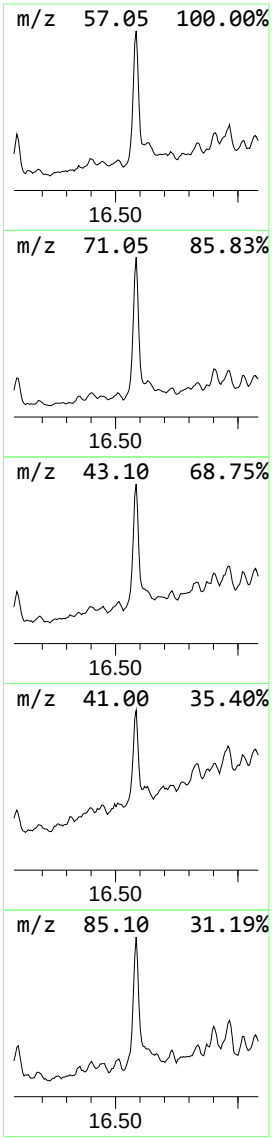
****

Peak Number 8 2,6,10-Trimethyltridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.584	20.00 ng	2697500	Phenanthrene-d10	17.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	90
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4	Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
5	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	80





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.826	9.9	ng	223748	2	11.079	451245	20.0
1H-Indene, octa...	14.293	6.4	ng	209806	3	14.874	656171	20.0
3',5'-Dimethoxy...	14.381	9.6	ng	314092	3	14.874	656171	20.0
unknown14.616	14.616	7.6	ng	248030	3	14.874	656171	20.0
unknown14.698	14.698	10.6	ng	346736	3	14.874	656171	20.0
Dodecane, 2-met...	15.362	10.7	ng	351352	3	14.874	656171	20.0
N-[1-(4-Chlorob...	15.656	15.6	ng	511189	3	14.874	656171	20.0
2,6,10-Trimethy...	16.584	20.0	ng	2697500	4	17.630	2697500	20.0