LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052314.D
Acq On : 8 Feb 2022 11:51
Operator : CG/JU
Sample : N1381-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DB-05(20-22)-02-01-22

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-BG020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052314.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.761	379	387	399	rBV	420147	696093	9.59%	4.125%
2	7.371	654	661	674	rBV	440882	788663	10.86%	4.673%
3	8.228	799	807	813	rBV2	120936	211681	2.92%	1.254%
4	9.397	1000	1006	1021	rVB	301051	542618	7.47%	3.215%
5	11.066	1280	1290	1301	rBV	166565	351604	4.84%	2.083%
6	13.333	1672	1676	1681	rVB5	98300	157928	2.18%	0.936%
7	13.492	1697	1703	1709	rBV	758369	1229289	16.93%	7.284%
8	13.668	1729	1733	1742	rVB3	180758	344196	4.74%	2.040%
9	14.302	1836	1841	1846	rBV	548454	872289	12.01%	5.169%
10	14.625	1890	1896	1900	rBV4	324963	677193	9.33%	4.013%
11	14.708	1906	1910	1916	rVB	786051	1248776	17.20%	7.400%
12	14.849	1930	1934	1936	rBV3	259316	399234	5.50%	2.366%
13	15.536	2048	2051	2055	rVB3	235666	303308	4.18%	1.797%
14	15.671	2070	2074	2080	rVB	680909	975039	13.43%	5.778%
15	16.364	2189	2192	2197	rBV2	558501	817345	11.26%	4.843%
16	21.663	3088	3094	3102	rVB	4182364	7260400	100.00%	43.023%

Sum of corrected areas: 16875656

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
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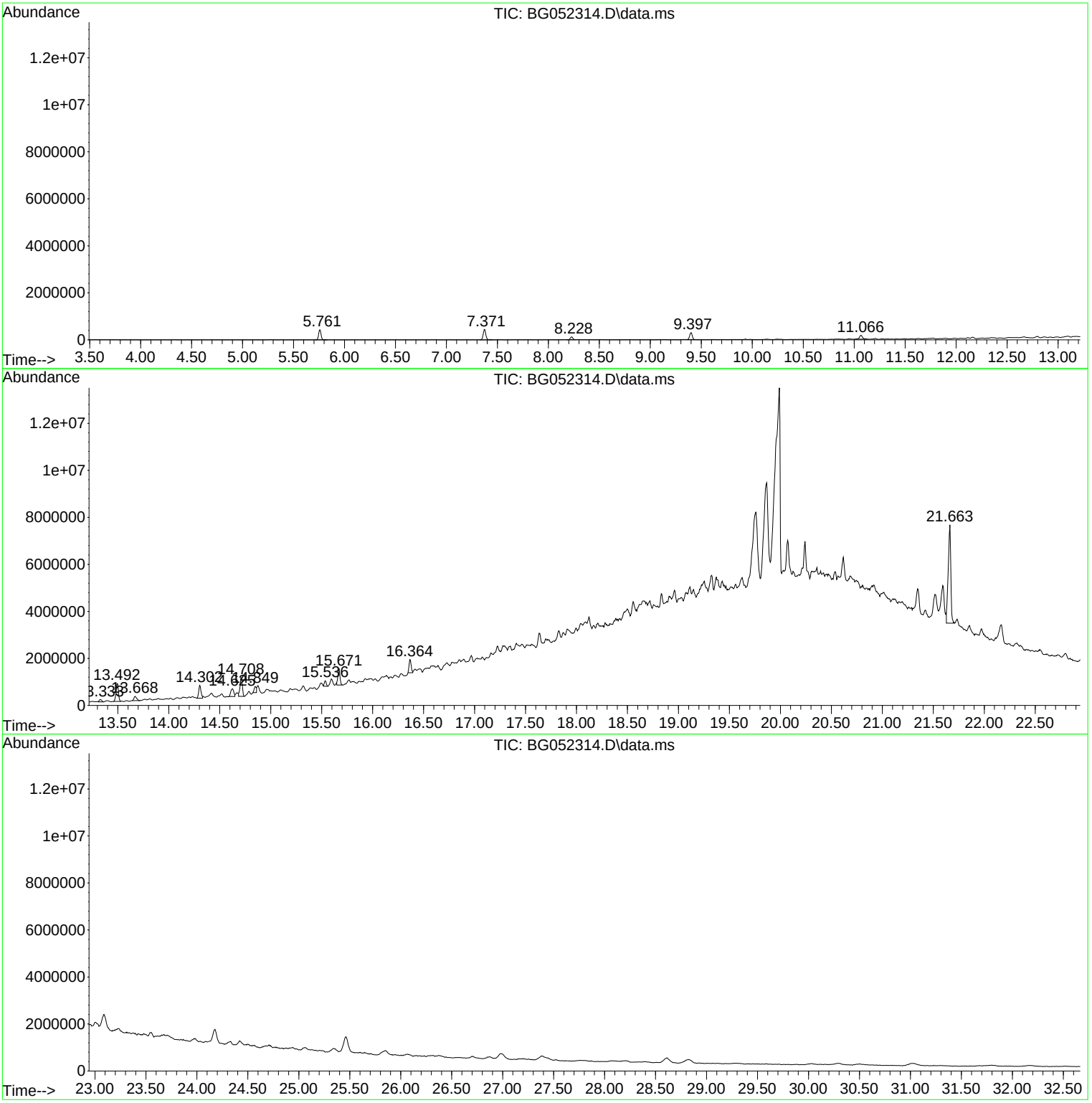
Operator : CG/JU
Sample : N1381-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DB-05(20-22)-02-01-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052314.D
Acq On : 8 Feb 2022 11:51
Operator : CG/JU
Sample : N1381-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DB-05(20-22)-02-01-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

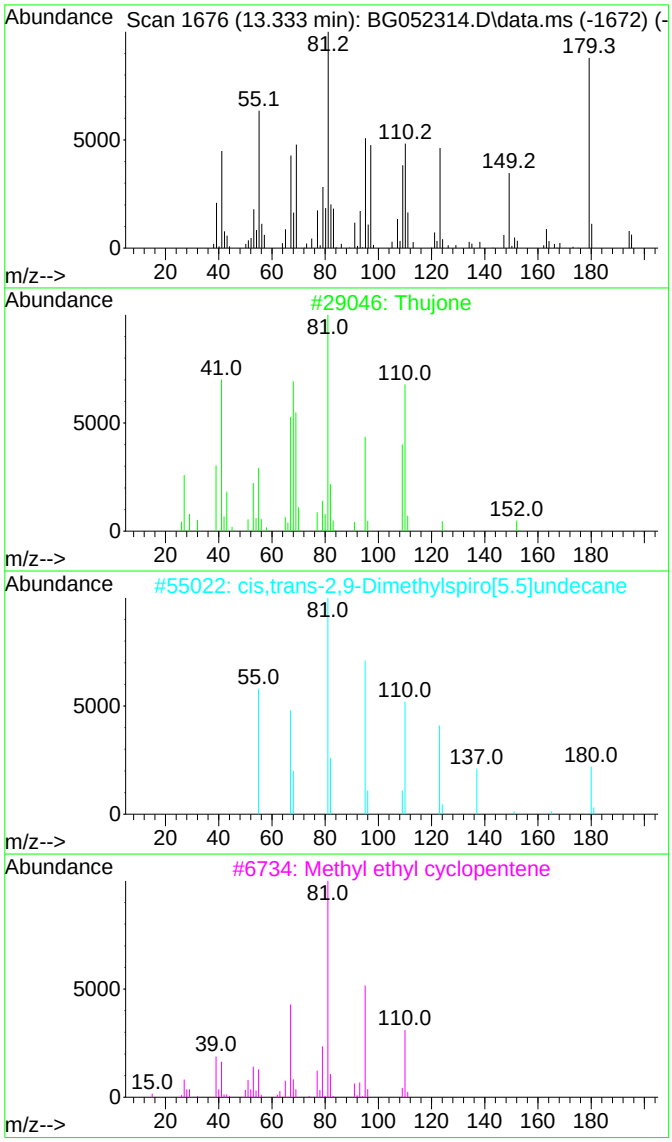
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

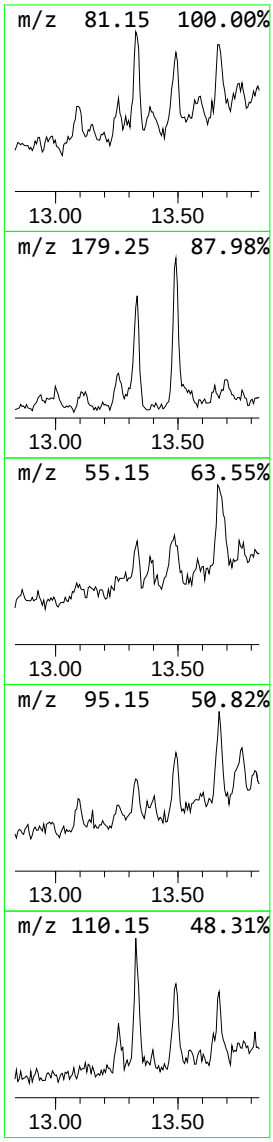
****

Peak Number 1 Thujone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	7.91 ng	157928	Acenaphthene-d10	14.878

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thujone	152	C10H16O	000546-80-5	50
2	cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	50
3	Methyl ethyl cyclopentene	110	C8H14	019780-56-4	41
4	3-Heptyne, 5-methyl-	110	C8H14	061228-09-9	38
5	Cyclohexane, ethylidene-	110	C8H14	001003-64-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052314.D
Acq On : 8 Feb 2022 11:51
Operator : CG/JU
Sample : N1381-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DB-05(20-22)-02-01-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.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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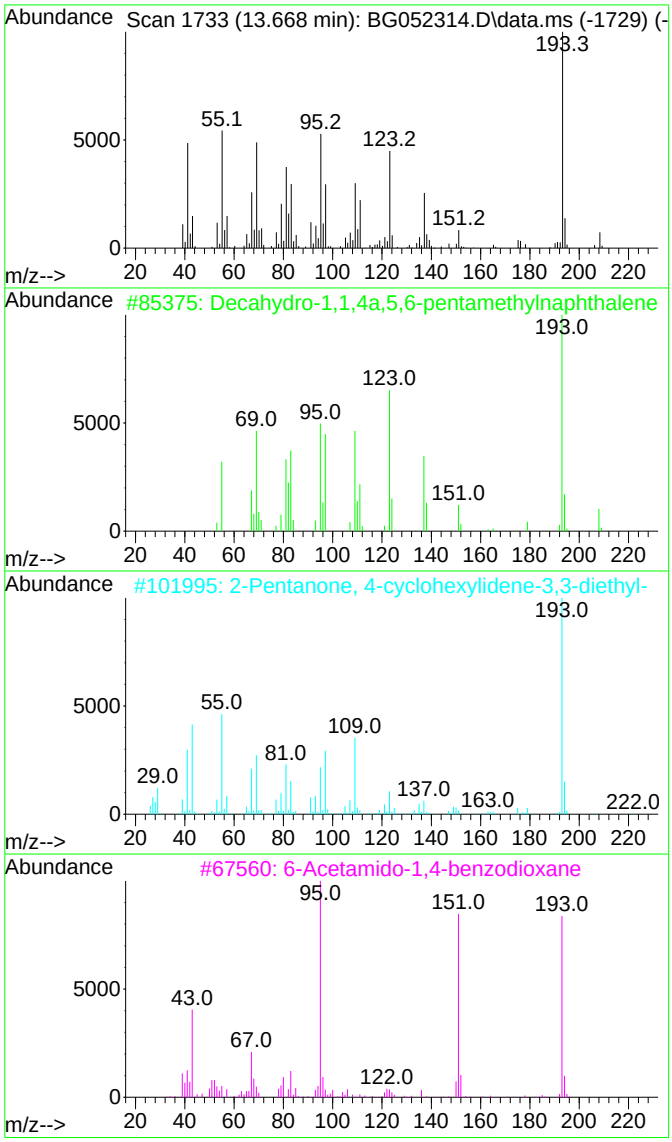
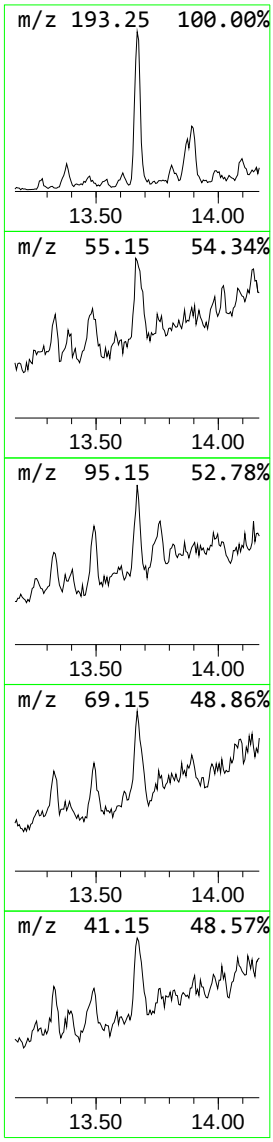
Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.668	17.24 ng	344196	Acenaphthene-d10	14.878

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	92
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	46
3	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	38
4	2-Anthracenamine	193	C14H11N	000613-13-8	38
5	benzoxazole, 5,6-dimethoxy-2-met...	193	C10H11NO3	1000395-98-9	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052314.D
Acq On : 8 Feb 2022 11:51
Operator : CG/JU
Sample : N1381-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DB-05(20-22)-02-01-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.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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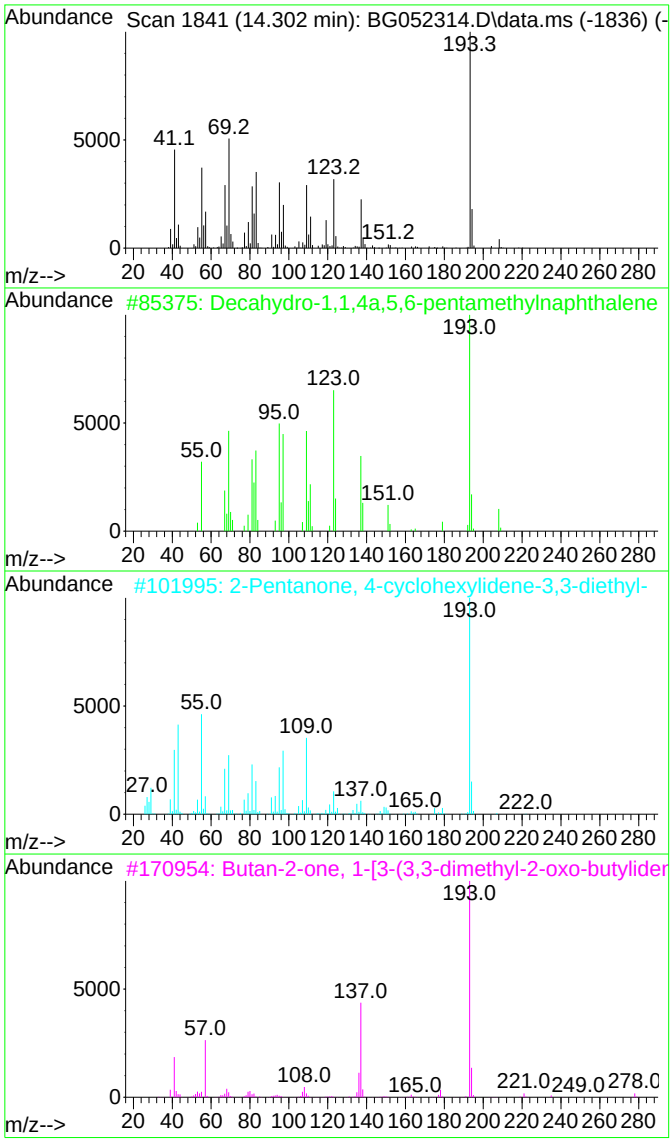
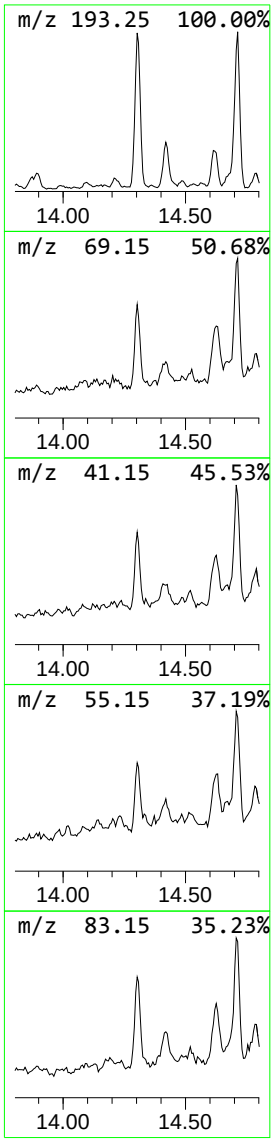
Peak Number 3 unknown14.302 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.302	43.70 ng	872289	Acenaphthene-d10	14.878

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	45
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	42
3	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	38
4	1-Anthracenamine	193	C14H11N	000610-49-1	38
5	2-Anthracenamine	193	C14H11N	000613-13-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052314.D
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Operator : CG/JU
Sample : N1381-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DB-05(20-22)-02-01-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

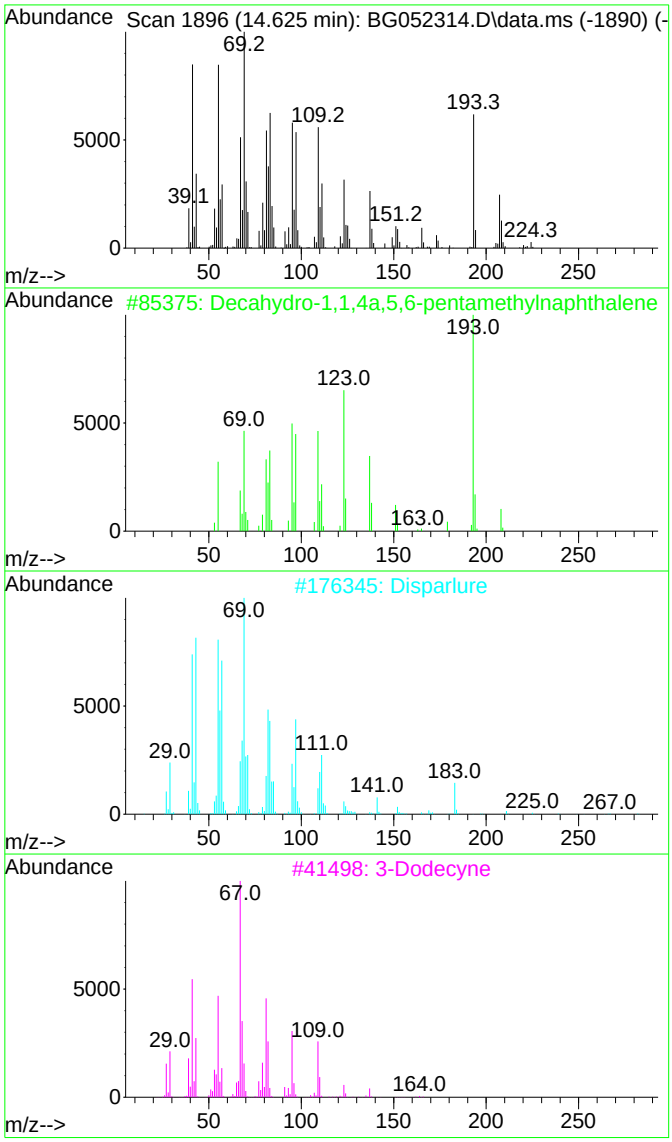
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

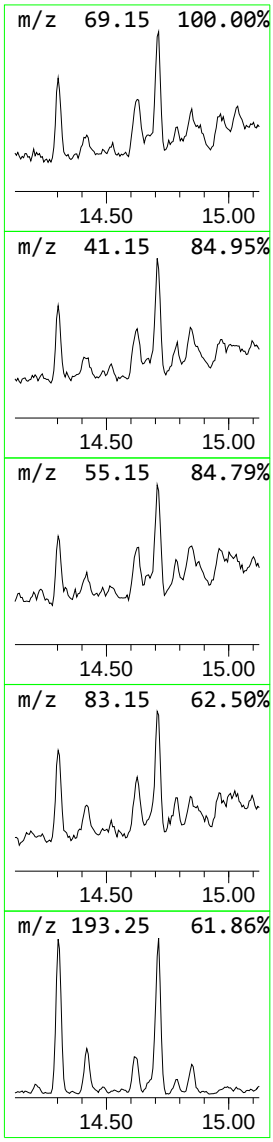
****

Peak Number 4 unknown14.626 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.626	33.92 ng	677193	Acenaphthene-d10	14.878

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	55
2	Disparlure	282	C19H38O	029804-22-6	38
3	3-Dodecyne	166	C12H22	006790-27-8	35
4	1-Dodecanol	186	C12H26O	000112-53-8	30
5	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052314.D
Acq On : 8 Feb 2022 11:51
Operator : CG/JU
Sample : N1381-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DB-05(20-22)-02-01-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

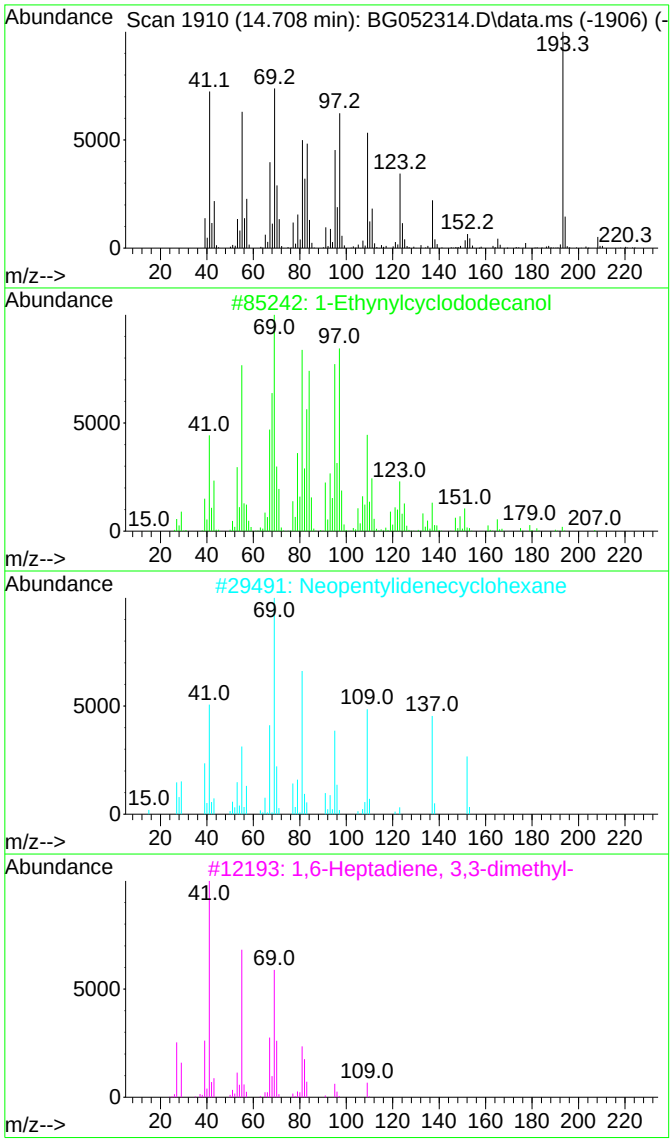
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

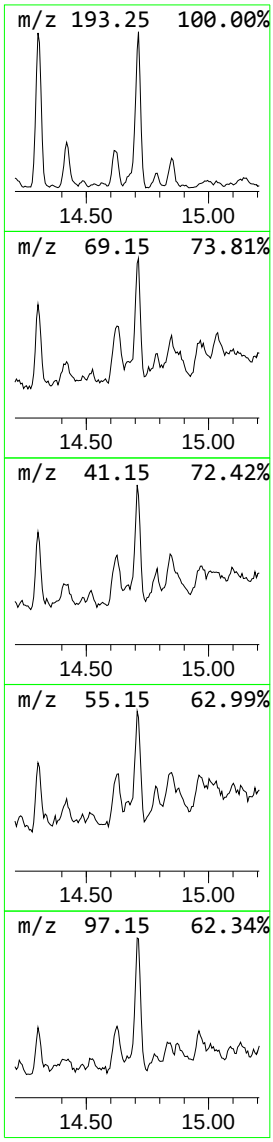
****

Peak Number 5 1-Ethynylcyclododecanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.708	62.56 ng	1248780	Acenaphthene-d10	14.878

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethynylcyclododecanol	208	C14H24O	1000484-40-4	50
2	Neopentylidenecyclohexane	152	C11H20	039546-80-0	41
3	1,6-Heptadiene, 3,3-dimethyl-	124	C9H16	068701-61-1	30
4	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30
5	Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052314.D
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Operator : CG/JU
Sample : N1381-01
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DB-05(20-22)-02-01-22

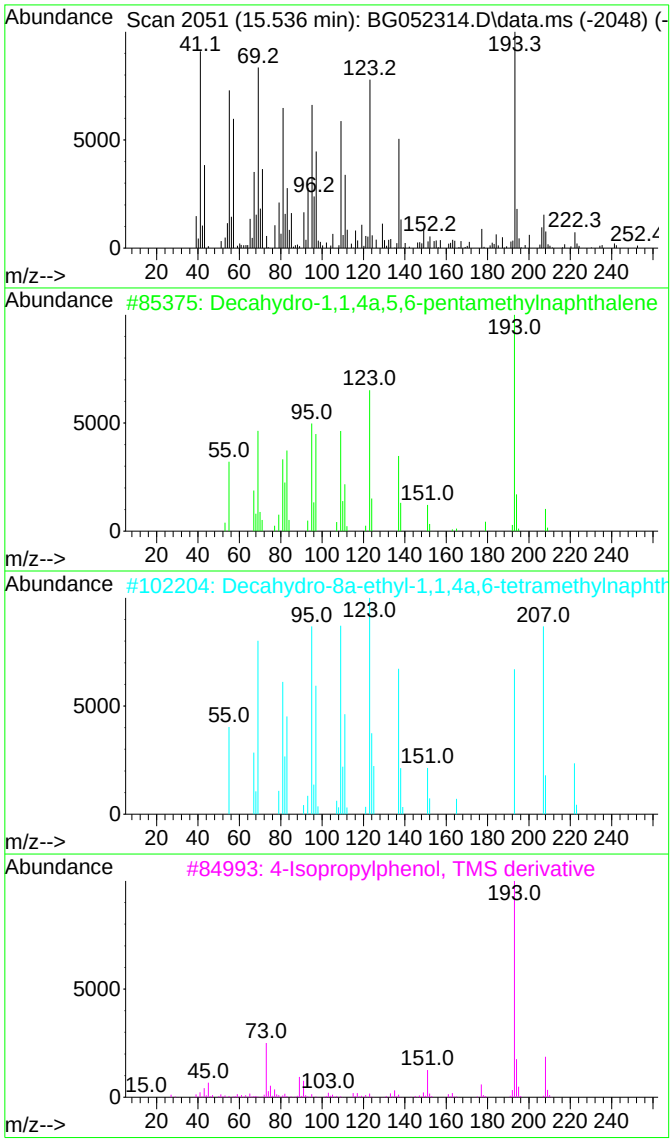
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

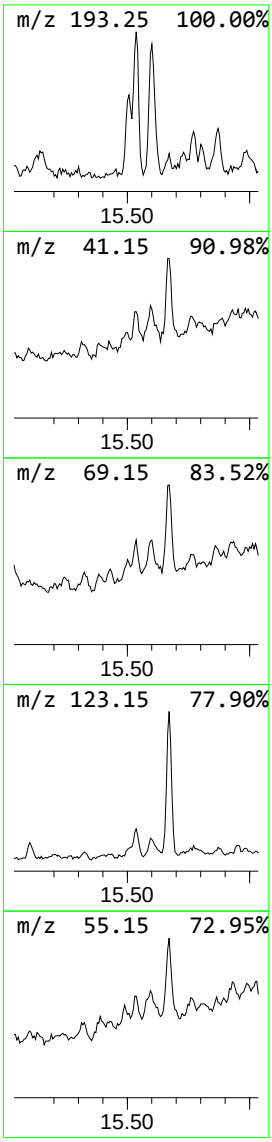
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.536	15.19 ng	303308	Acenaphthene-d10	14.878

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	90
2	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	83
3	4-Isopropylphenol, TMS derivative	208	C12H20OSi	1000373-17-4	25
4	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	18
5	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	15





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Instrument :
BNA_G
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DB-05(20-22)-02-01-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

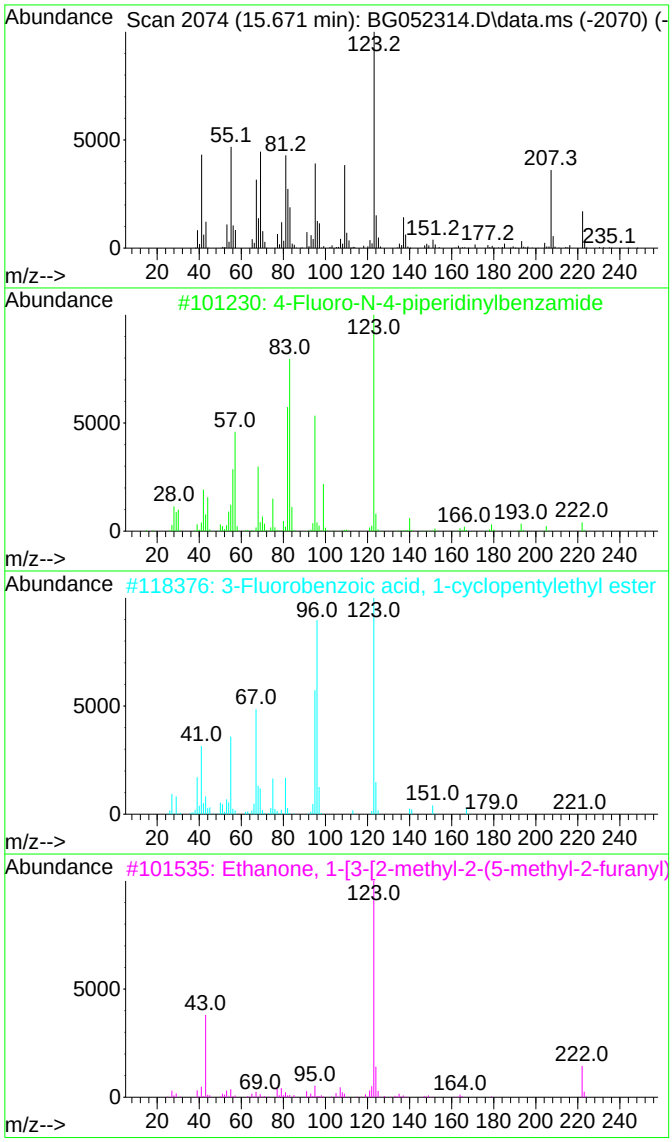
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

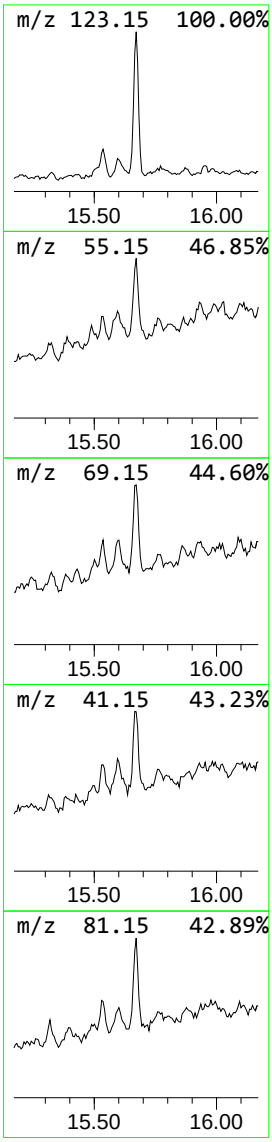
****

Peak Number 7 unknown15.671 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.671	48.85 ng	975039	Acenaphthene-d10	14.878

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluoro-N-4-piperidinylbenzamide	222	C12H15FN2O	075484-39-8	47
2	3-Fluorobenzoic acid, 1-cyclopen...	236	C14H17FO2	1000279-04-7	47
3	Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	46
4	2-Amino-4-acetamino anisole	180	C9H12N2O2	006375-47-9	43
5	2-Fluorobenzoic acid, oct-3-en-2...	250	C15H19FO2	1000299-16-5	43





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DB-05(20-22)-02-01-22

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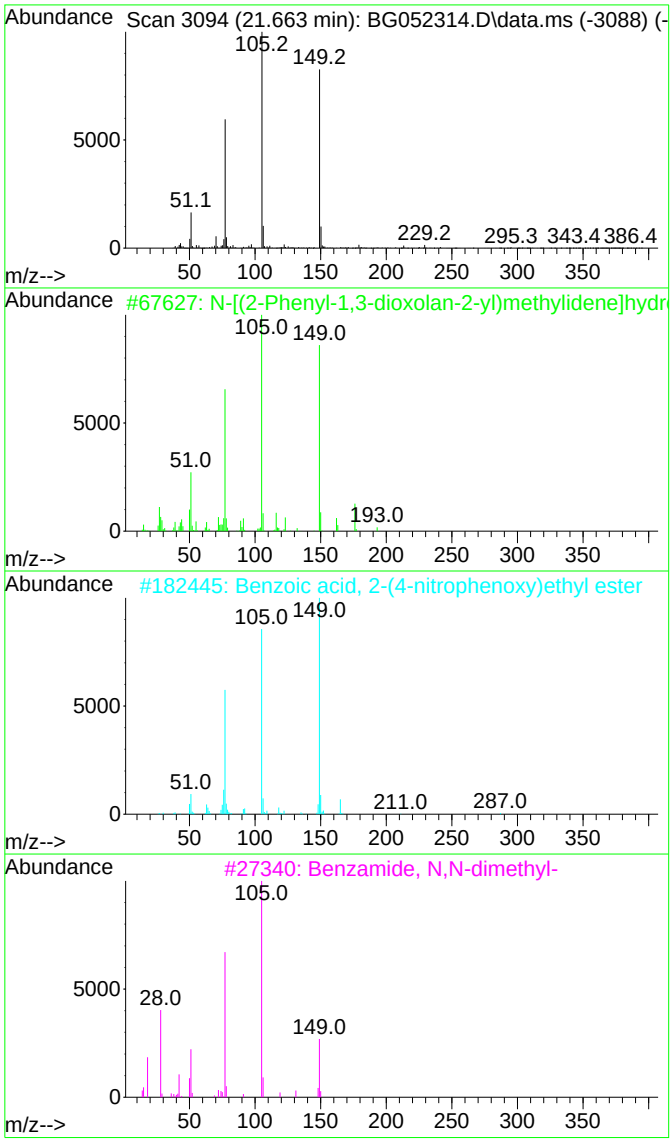
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

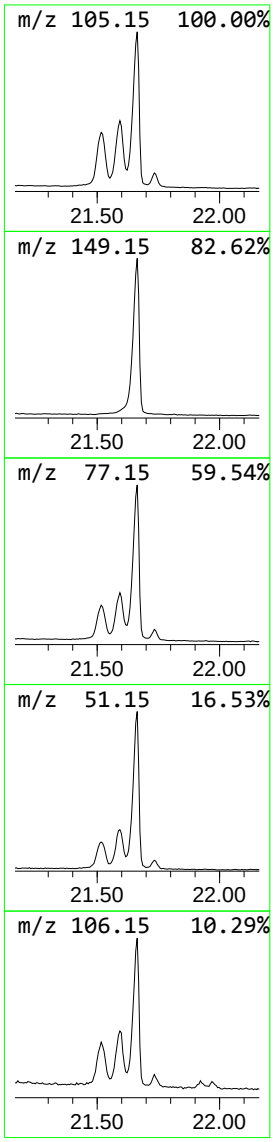
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 N-[(2-Phenyl-1,3-dioxolan-2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.663	20.00 ng	7260400	Chrysene-d12	21.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	83
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
3	Benzamide, N,N-dimethyl-	149	C9H11NO	000611-74-5	78
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
5	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020822\
Data File : BG052314.D
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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
Thujone	13.333	7.9	ng	157928	3	14.878	399234	20.0
Decahydro-1,1,4...	13.668	17.2	ng	344196	3	14.878	399234	20.0
unknown14.302	14.302	43.7	ng	872289	3	14.878	399234	20.0
unknown14.626	14.626	33.9	ng	677193	3	14.878	399234	20.0
1-Ethynylcyclod...	14.708	62.6	ng	1248780	3	14.878	399234	20.0
Decahydro-8a-et...	15.536	15.2	ng	303308	3	14.878	399234	20.0
unknown15.671	15.671	48.9	ng	975039	3	14.878	399234	20.0
N-[(2-Phenyl-1,...	21.663	20.0	ng	7260400	5	21.974	7260400	20.0