SUPPLEMENTARY DATA

Regioselective Synthesis, Structural Investigation and Binding Behavior of 6-Aroyl-7-aryl-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidines with BSA using Various Spectroscopic and *In Silico* Methods

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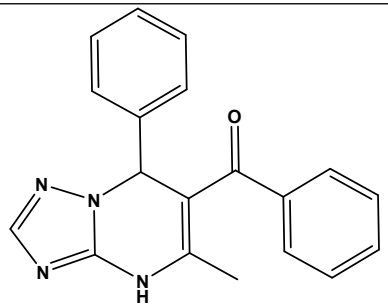
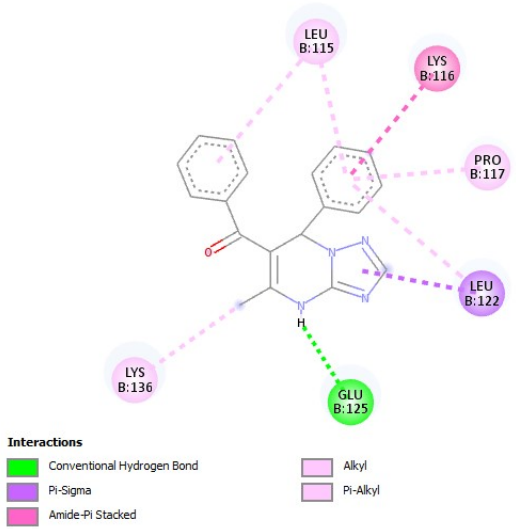
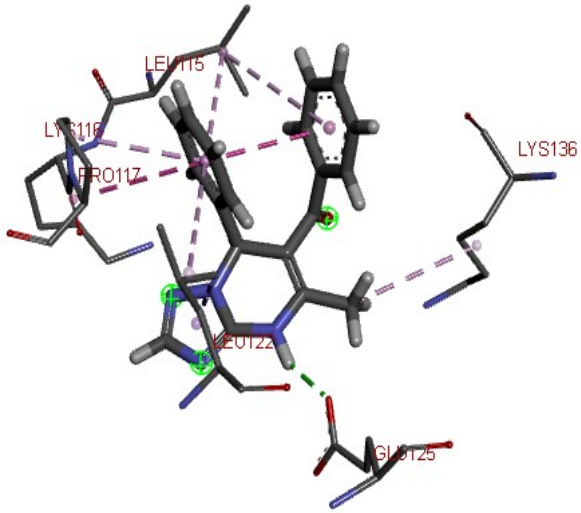
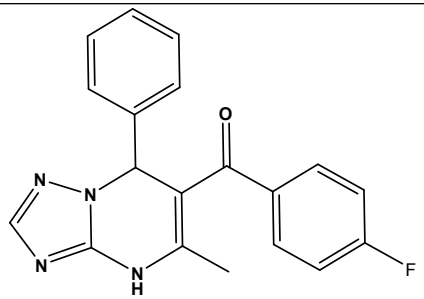
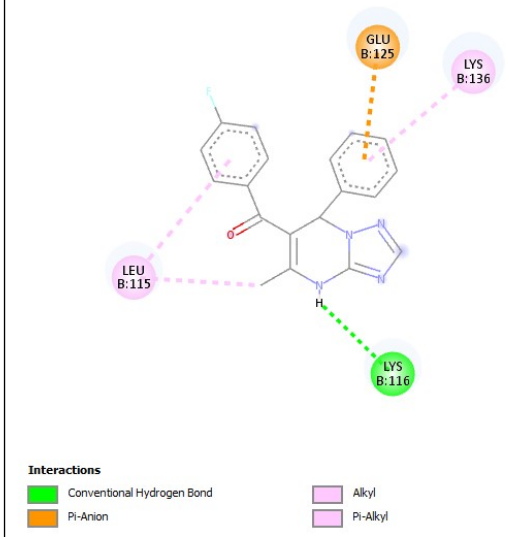
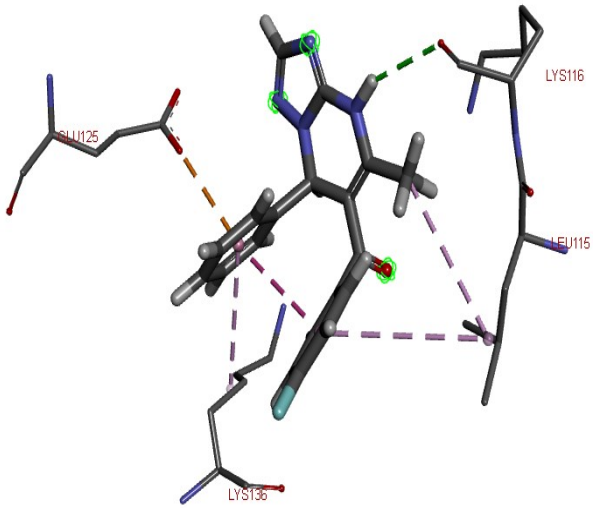
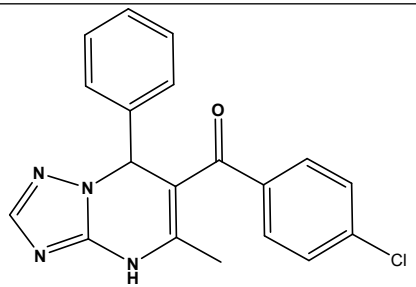
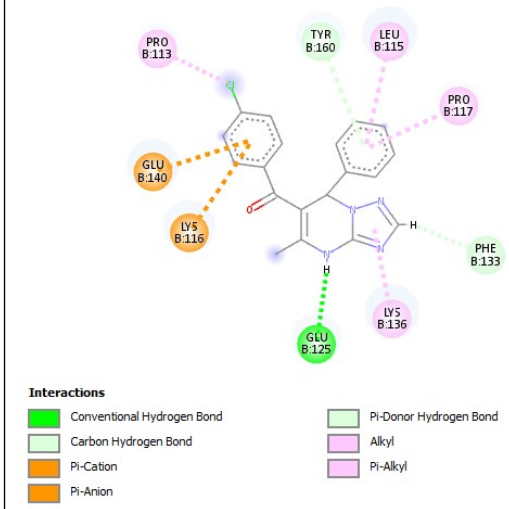
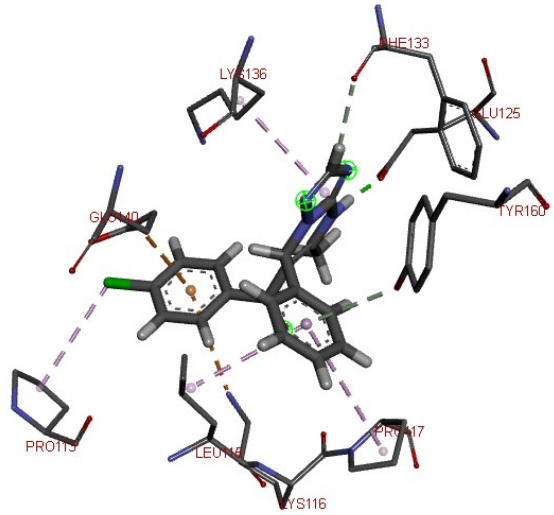
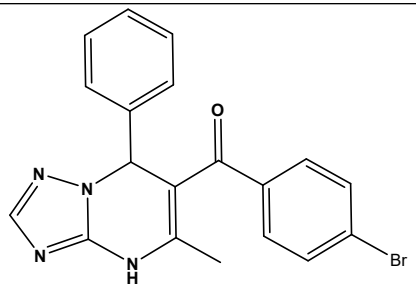
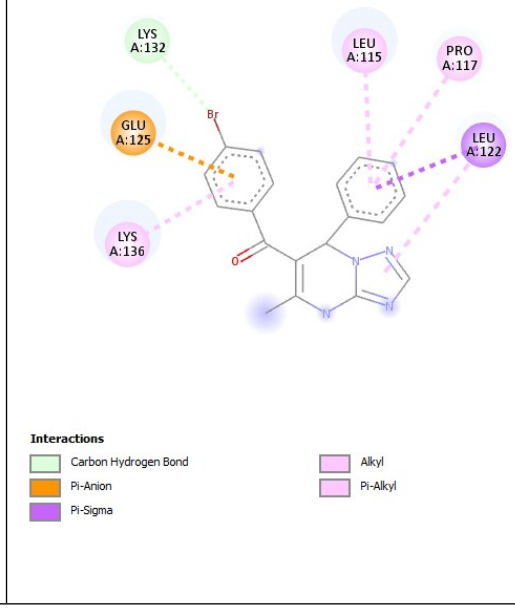
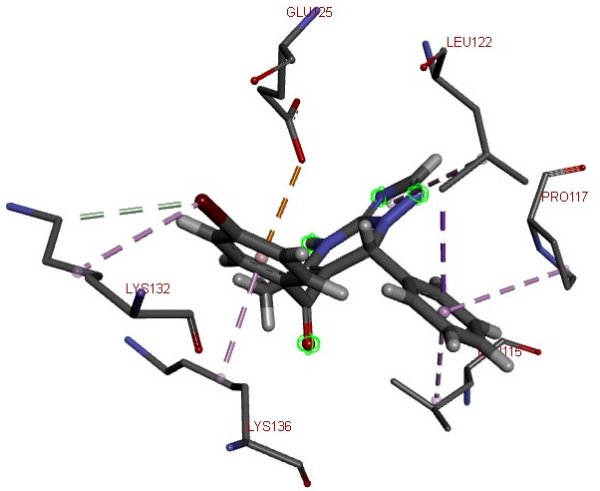
Table S1. 2D and 3D diagram showing of the interaction of ligands **5a-u**, PBZ and IBP with BSA protein.

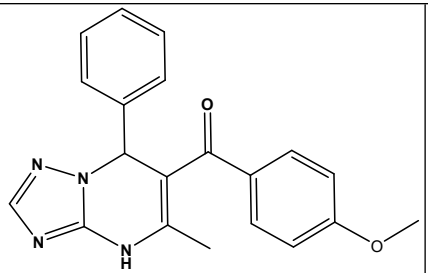
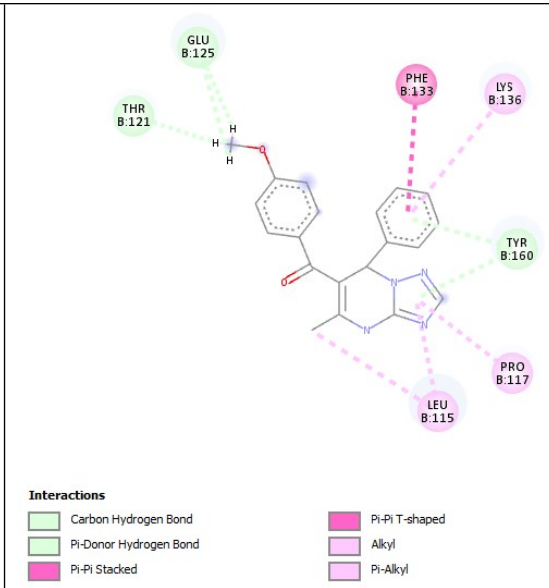
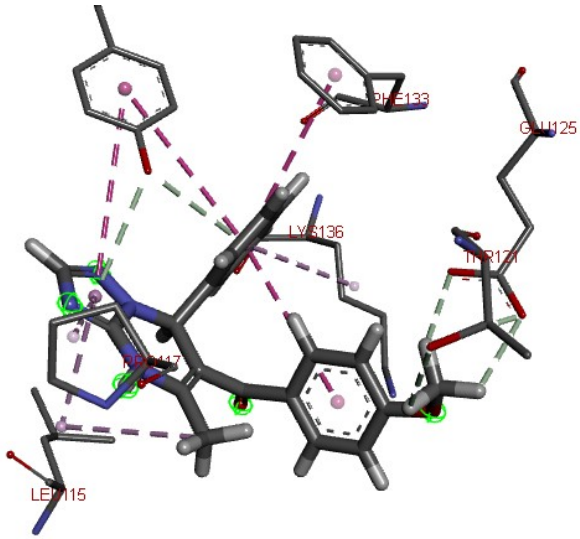
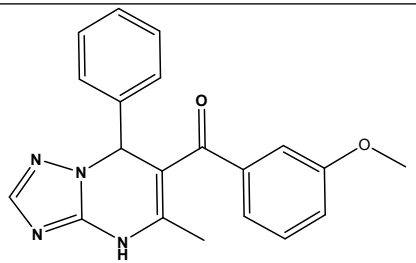
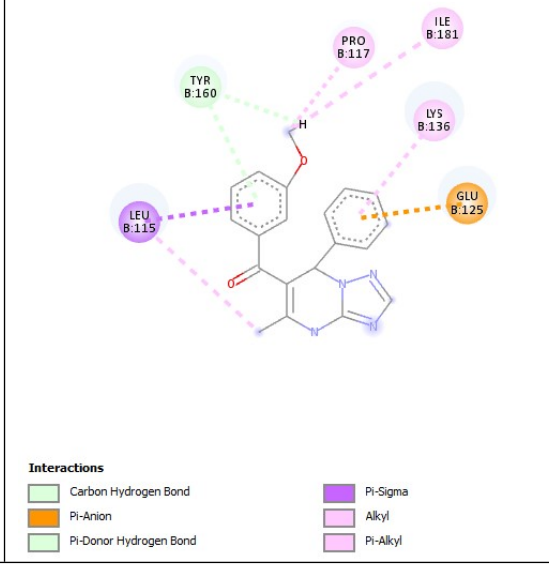
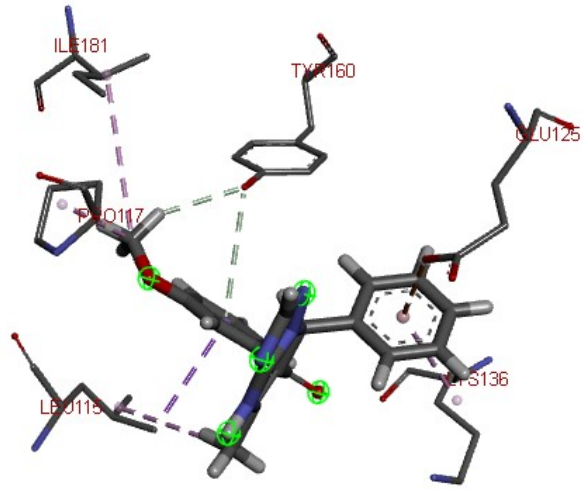
S. no.	Compound	Dock Score/ Binding Energy	2D	3D
1.		-7.4		

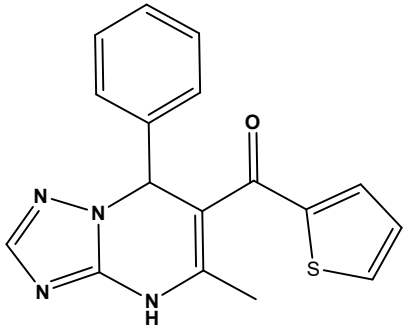
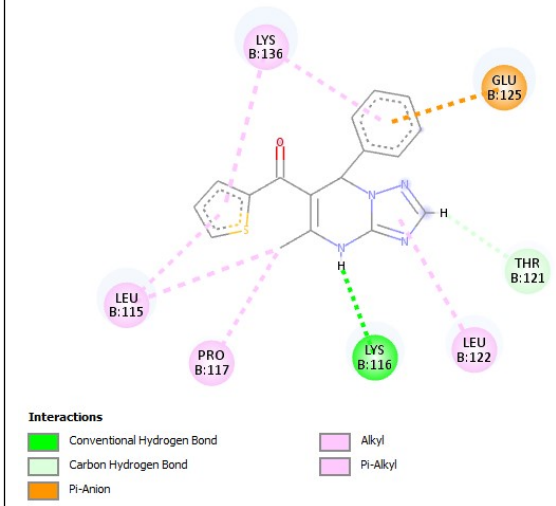
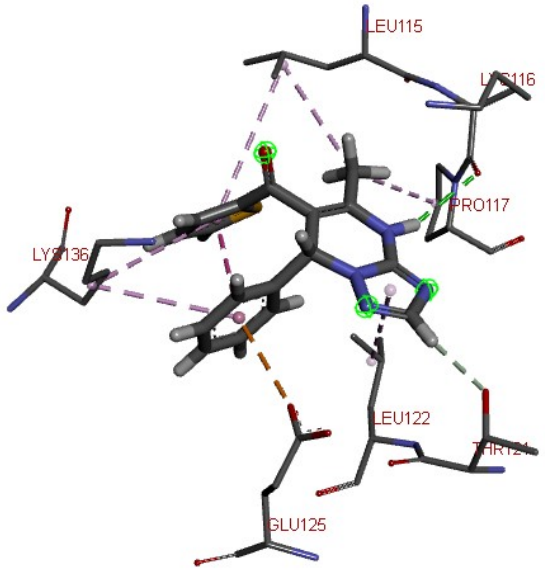
2.		-7.6	 GLU B:125 LYS B:136 LEU B:115 LYS B:116 Interactions Conventional Hydrogen Bond Alkyl Pi-Anion Pi-Alkyl	 LYS116 GLU125 LEU115 LYS136
3.		-7.9	 PRO B:113 TYR B:160 LEU B:115 PRO B:117 GLU B:140 LYS B:116 PHE B:133 LYS B:136 GLU B:125 Interactions Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Cation Pi-Anion Pi-Donor Hydrogen Bond Alkyl Pi-Alkyl	 PHE133 LYS136 GLU125 TYR160 PRO117 LYS116

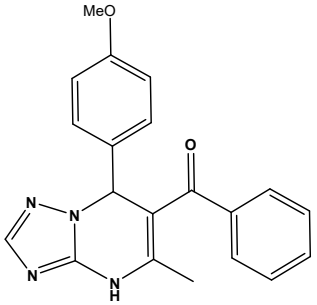
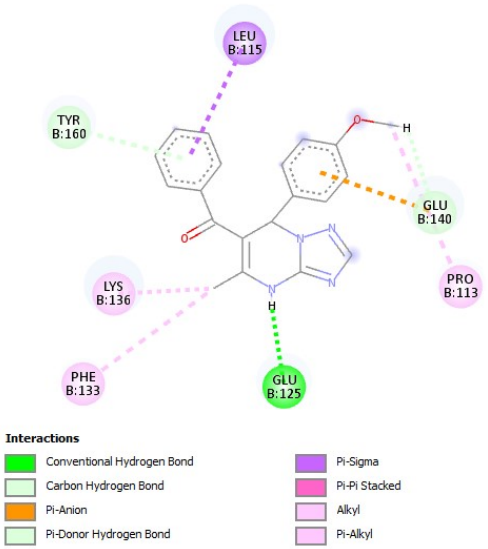
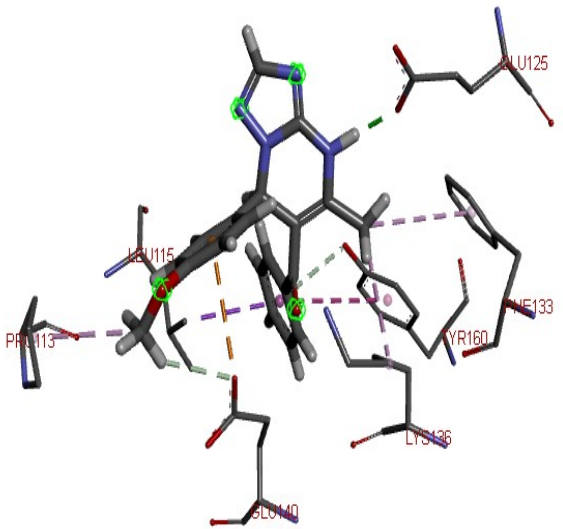
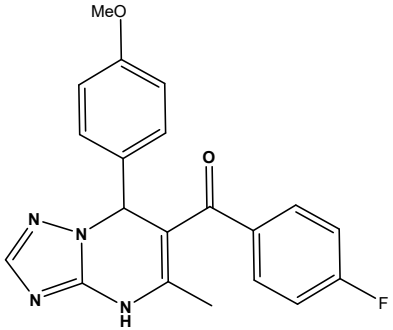
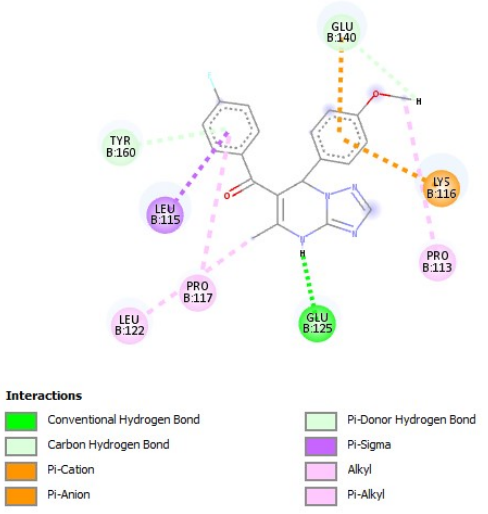
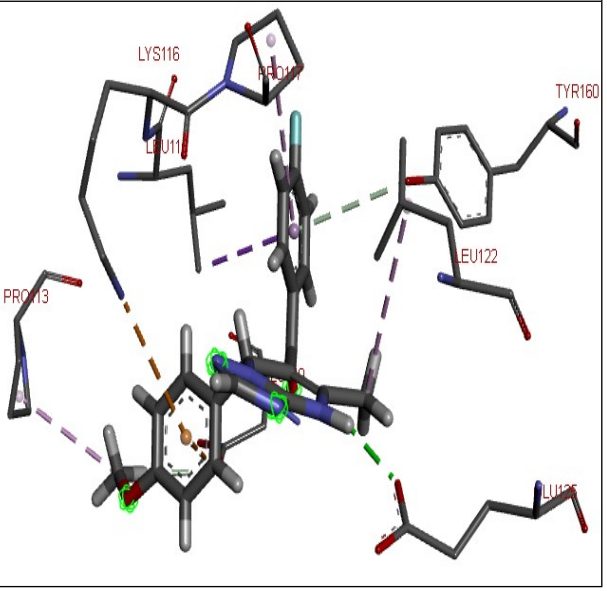
4.		-7.9		

LYS A:132
LEU A:115
PRO A:117
GLU A:125
LEU A:122
LYS A:136
Br
Interactions
Carbon Hydrogen Bond
Pi-Anion
Pi-Sigma
Alkyl
Pi-Alkyl

GLU125
LEU122
PRO117
LYS132
LYS136

5.		-7.4	 GLU B:125 PHE B:133 LYS B:136 THR B:121 TYR B:160 PRO B:117 LEU B:115 Interactions Carbon Hydrogen Bond Pi-Donor Hydrogen Bond Pi-Pi Stacked Pi-Pi T-shaped Alkyl Pi-Alkyl	 PHE133 GLU125 LYS136 LEU115
6.		-7.9	 PRO B:117 ILE B:181 TYR B:160 LYS B:136 LEU B:115 GLU B:125 Interactions Carbon Hydrogen Bond Pi-Anion Pi-Donor Hydrogen Bond Pi-Sigma Alkyl Pi-Alkyl	 ILE181 TYR160 GLU125 LYS136

7.		-7.1	 LYS B:136 GLU B:125 THR B:121 LEU B:115 PRO B:117 LYS B:116 LEU B:122 Interactions Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Anion Alkyl Pi-Alkyl	 LEU115 PRO117 LEU122 GLU125

8.		-7.4		
9.		-7.3		

LEU B:115
TYR B:160
GLU B:140
LYS B:136
PRO B:113
PHE B:133
GLU B:125
Interactions
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Anion
Pi-Donor Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Alkyl
Pi-Alkyl

GLU B:140
TYR B:160
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Interactions
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Carbon Hydrogen Bond
Pi-Cation
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Pi-Sigma
Alkyl
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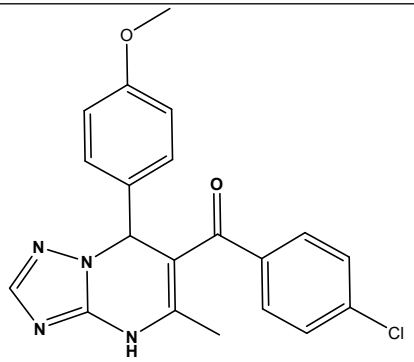
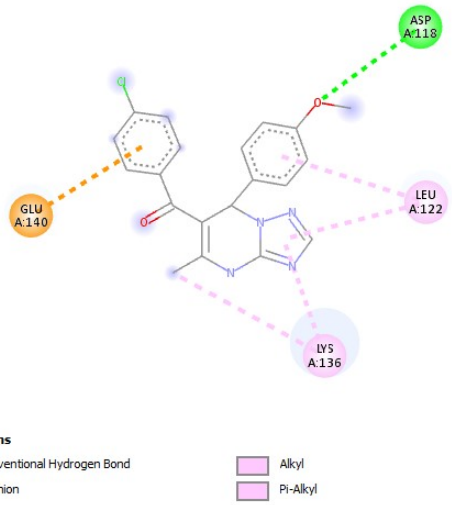
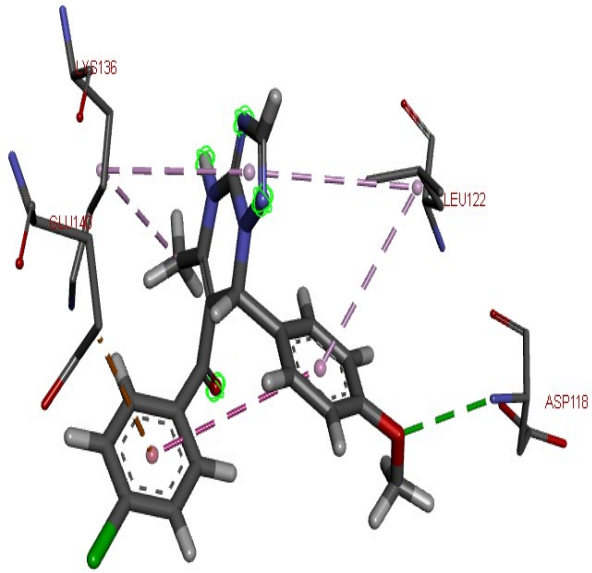
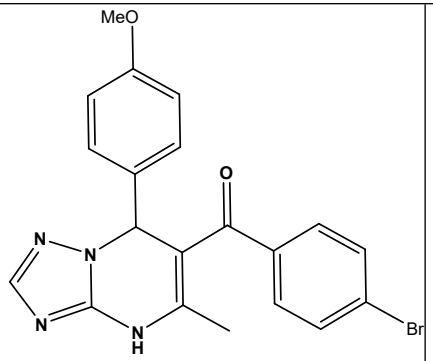
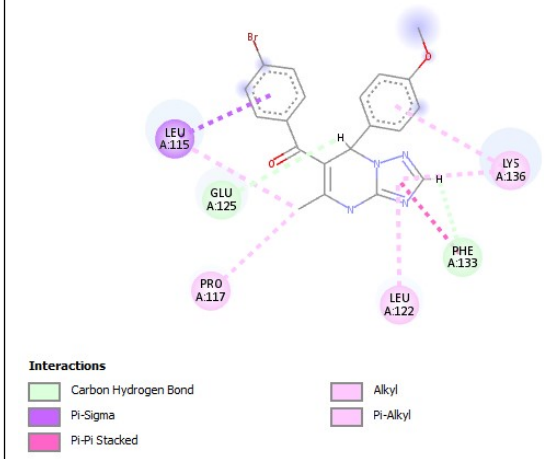
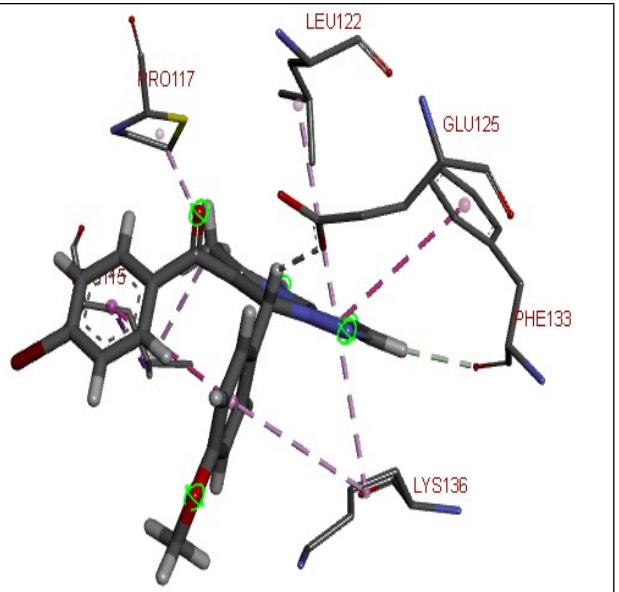
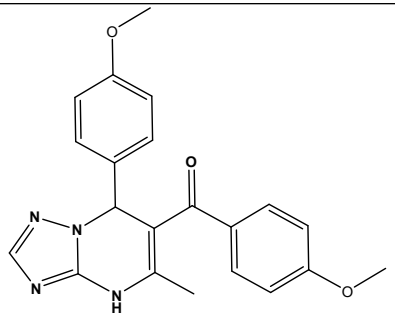
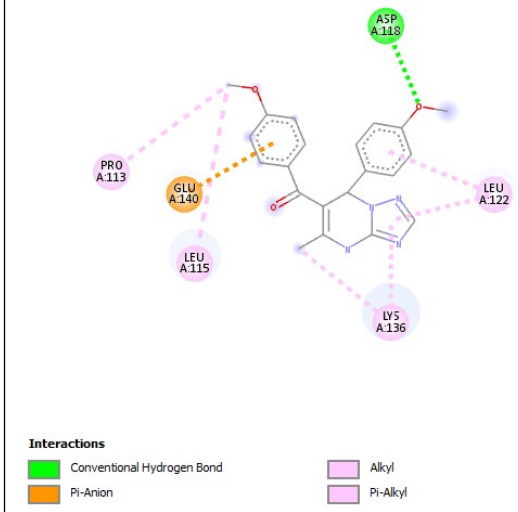
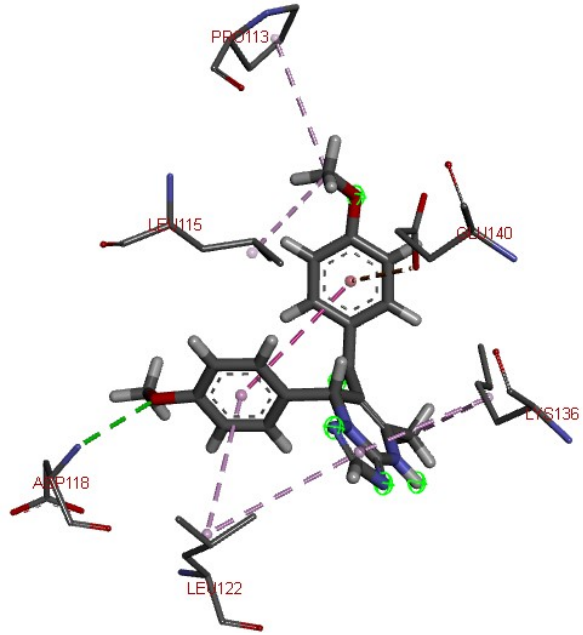
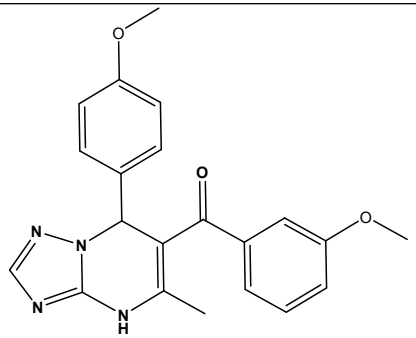
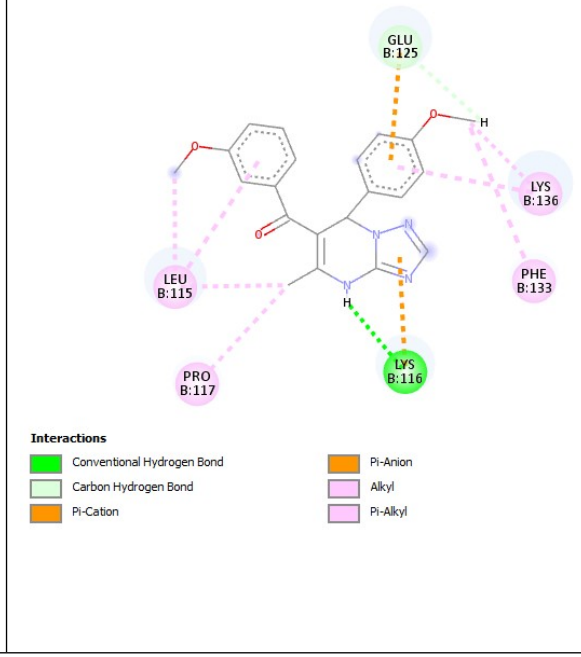
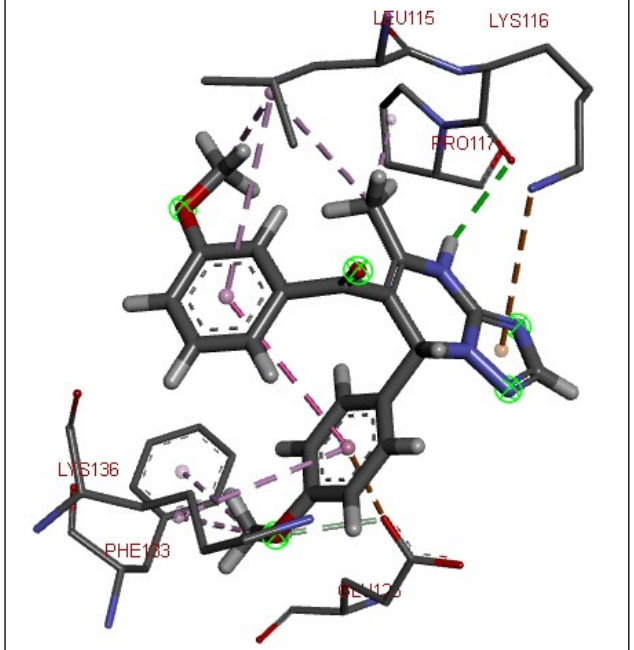
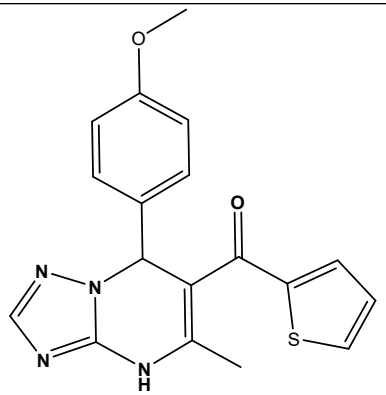
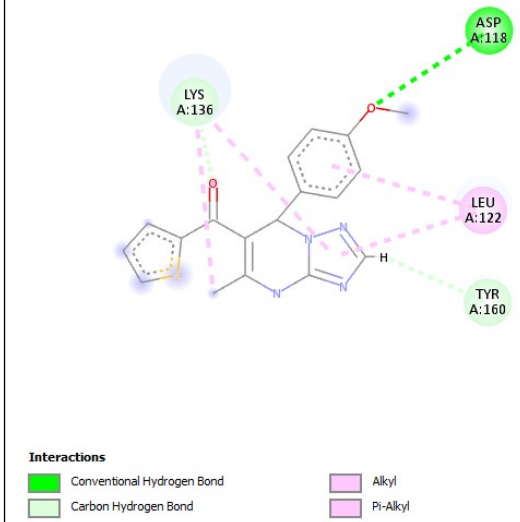
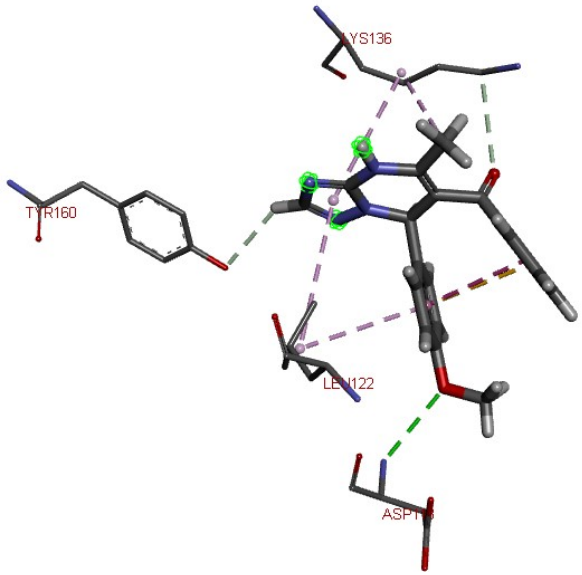
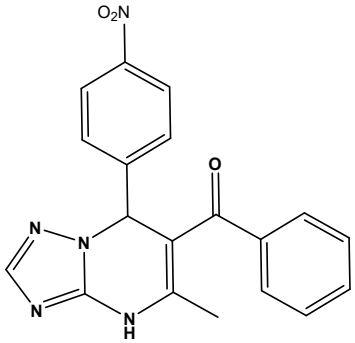
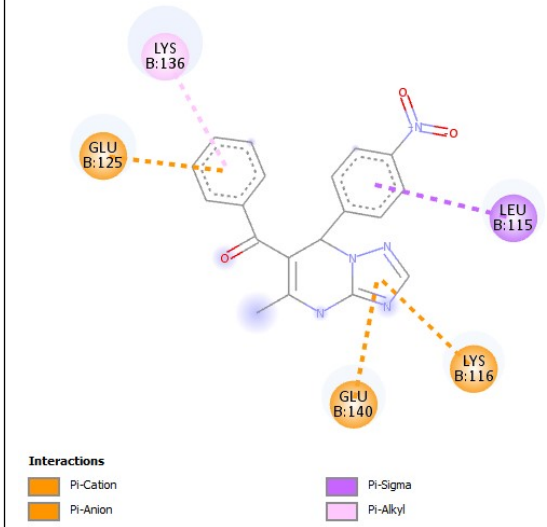
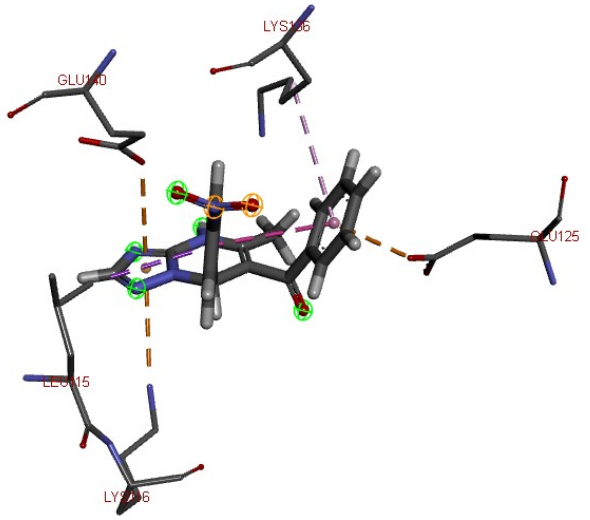
10.		-6.4	 ASP A:118 GLU A:140 LEU A:122 LYS A:136 Interactions Conventional Hydrogen Bond Alkyl Pi-Anion Pi-Alkyl	 LYS136 GLU140 LEU122 ASP118

11.	 MeO O N N N N H Br	-6.5	 Br O H N N H N LEU A:115 GLU A:125 PRO A:117 LEU A:122 PHE A:133 LYS A:136 Interactions Carbon Hydrogen Bond Pi-Sigma Pi-Pi Stacked Alkyl Pi-Alkyl	 LEU122 GLU125 PHE133 LYS136

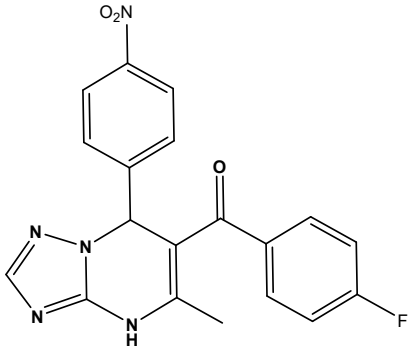
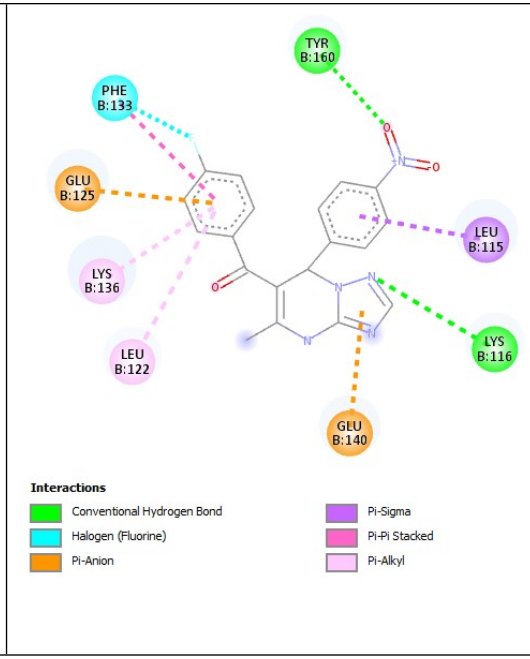
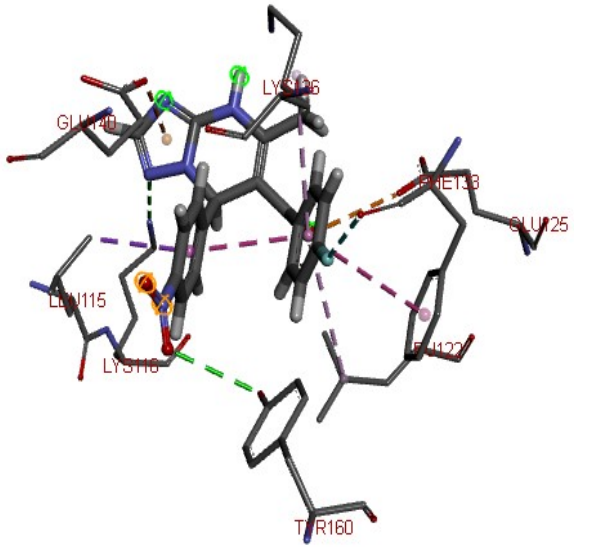
12.		-6.4	 ASP A:118 PRO A:113 GLU A:140 LEU A:122 LEU A:115 LYS A:136 Interactions Conventional Hydrogen Bond Alkyl Pi-Anion Pi-Alkyl	 PRO113 LEU115 GLU140 LYS136 ASP118 LEU122

13.		-7.0	 GLU B:125 LYS B:136 PHE B:133 LEU B:115 PRO B:117 LYS B:116 Interactions Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Cation Pi-Anion Alkyl Pi-Alkyl	 LEU115 LYS116 PRO117 LYS136 PHE133

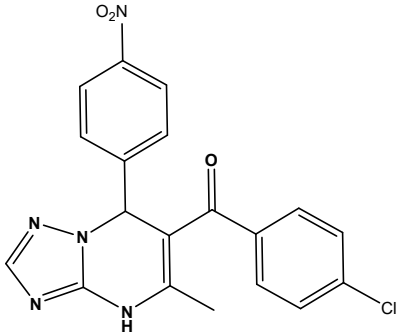
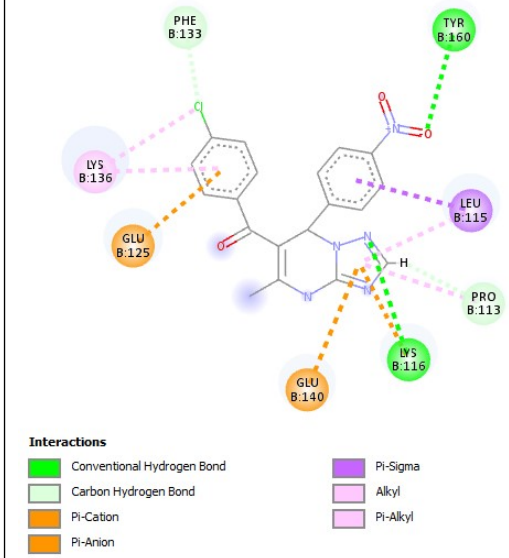
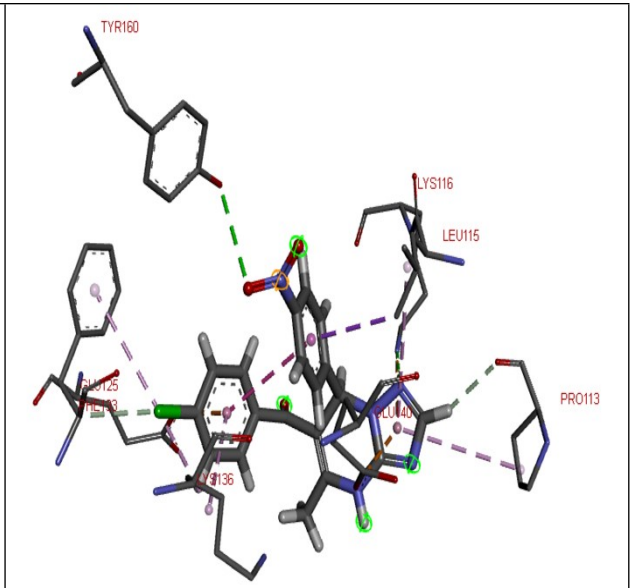
14.		-6.0	 ASP A:118 LYS A:136 LEU A:122 TYR A:160 Interactions Conventional Hydrogen Bond Carbon Hydrogen Bond Alkyl Pi-Alkyl	 LYS136 TYR160 LEU122

15.		-6.4		

LYS B:136
GLU B:125
LEU B:115
LYS B:116
GLU B:140
Interactions
Pi-Cation
Pi-Anion
Pi-Sigma
Pi-Alkyl

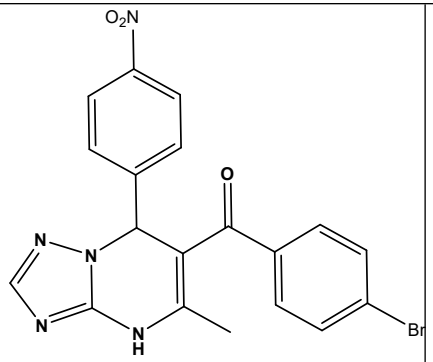
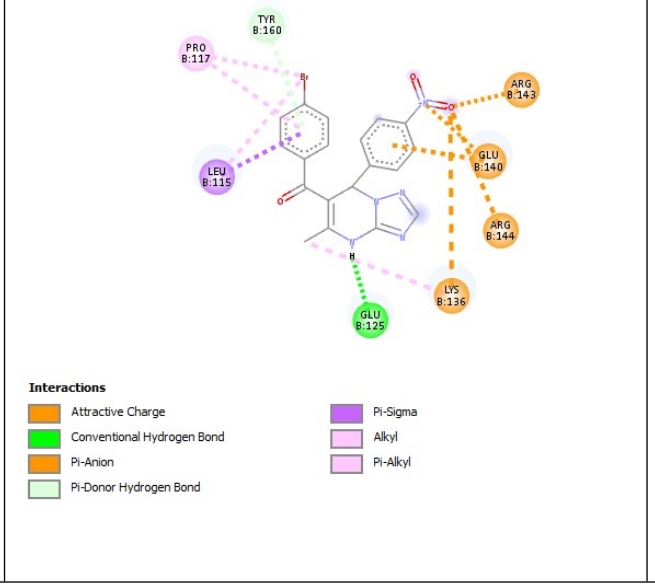
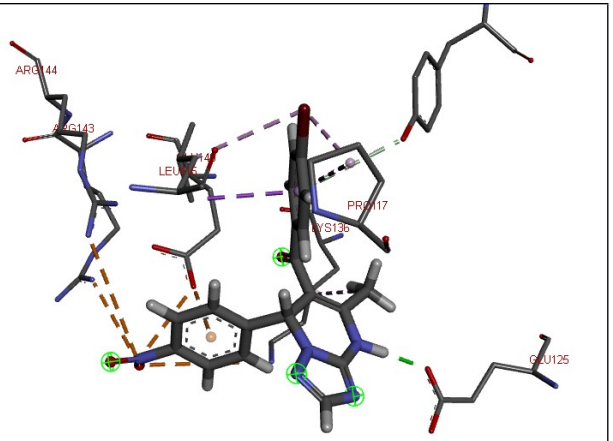
16.		-7.5		

TYR B:160
PHE B:133
GLU B:125
LYS B:136
LEU B:122
LEU B:115
LYS B:116
GLU B:140
Interactions
Conventional Hydrogen Bond
Halogen (Fluorine)
Pi-Anion
Pi-Sigma
Pi-Pi Stacked
Pi-Alkyl
GLU140
LYS136
PHE133
GLU125
LEU115
LYS116
TYR160

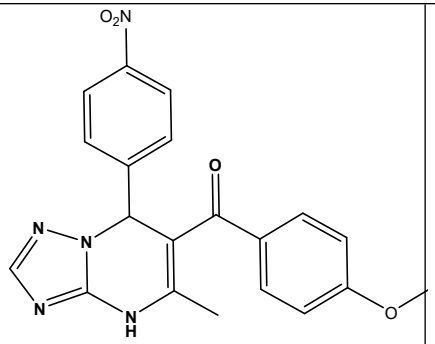
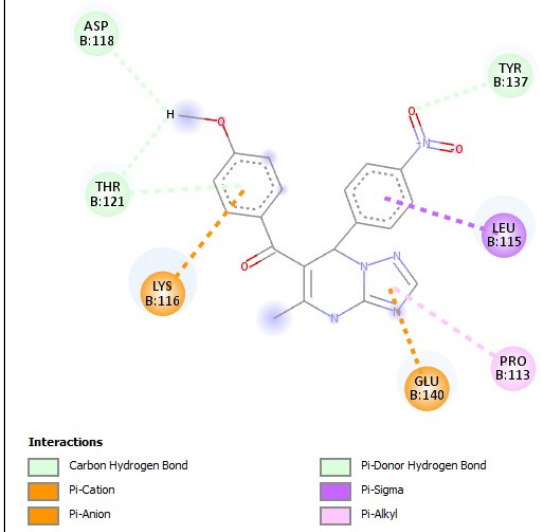
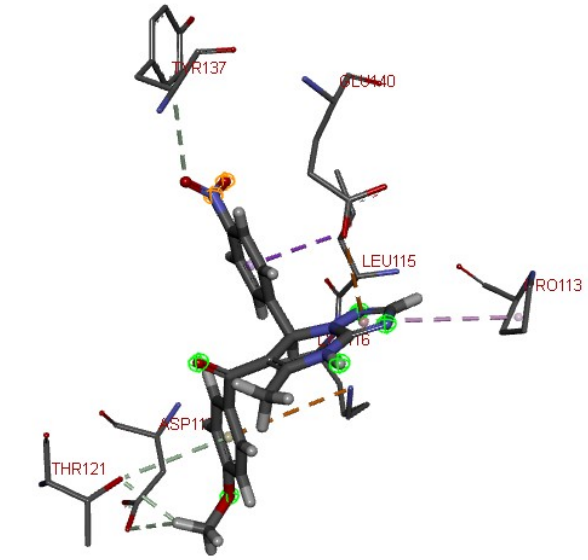
17.		-6.6		

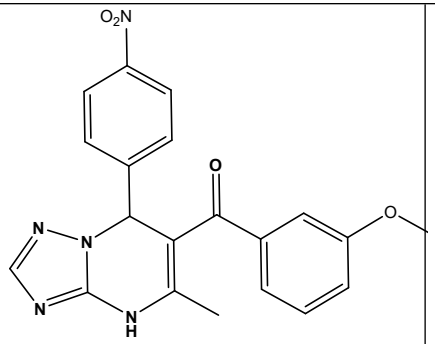
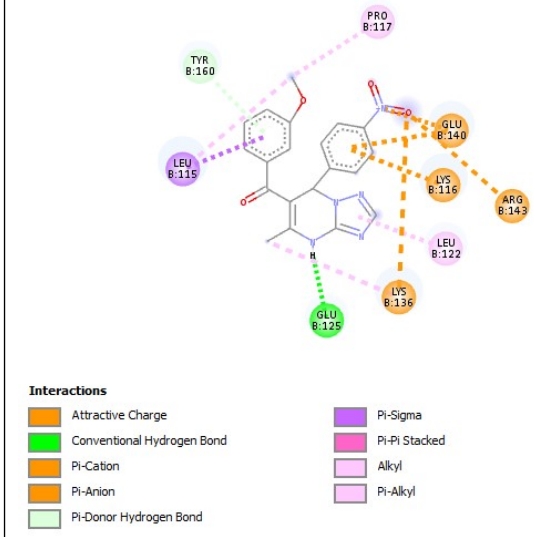
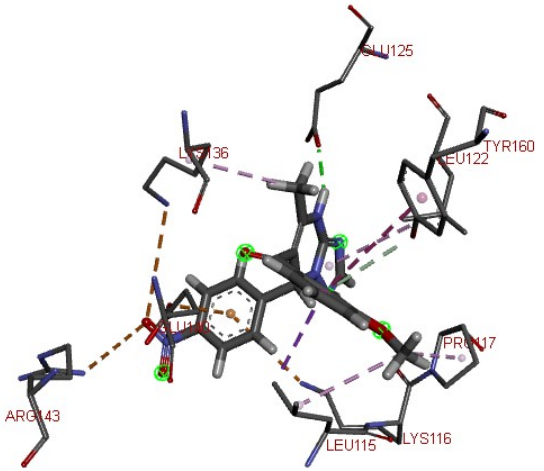
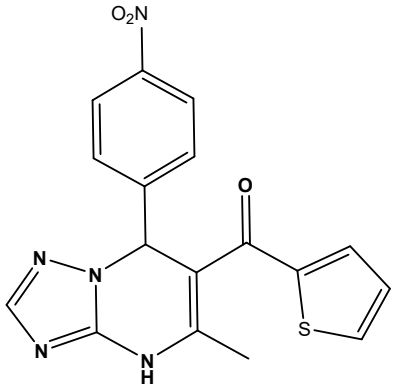
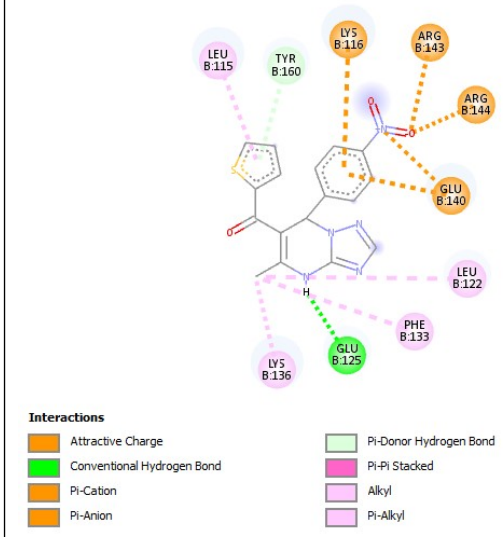
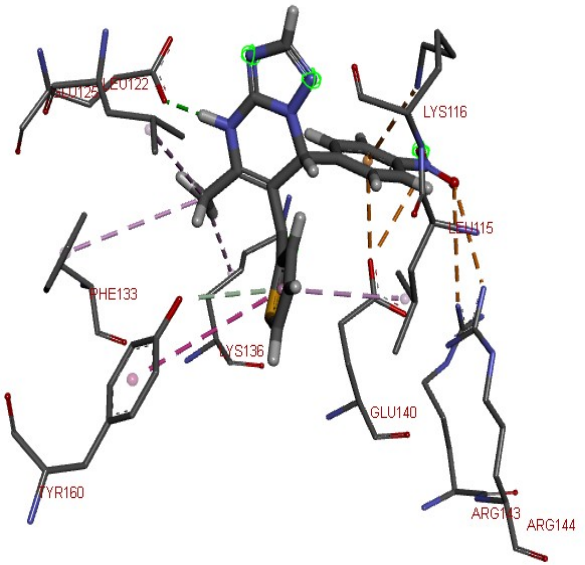
PHE B:133
TYR B:160
LYS B:136
LEU B:115
GLU B:125
PRO B:113
LYS B:116
GLU B:140
Interactions
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Cation
Pi-Anion
Pi-Sigma
Alkyl
Pi-Alkyl

TYR160
LYS116
LEU115
PRO113

18.		-7.3		

TYR B:160
PRO B:117
ARG B:143
LEU B:115
GLU B:140
ARG B:144
LYS B:136
GLU B:125
Interactions
Attractive Charge
Conventional Hydrogen Bond
Pi-Anion
Pi-Donor Hydrogen Bond
Pi-Sigma
Alkyl
Pi-Alkyl
ARG144
ARG143
LEU115
PRO117
LYS136
GLU125

19.		-6.2	 ASP B:118 TYR B:137 THR B:121 LEU B:115 LYS B:116 PRO B:113 GLU B:140 Interactions Carbon Hydrogen Bond Pi-Donor Hydrogen Bond Pi-Cation Pi-Sigma Pi-Anion Pi-Alkyl	 TYR137 LEU115 PRO113 THR121

20.		-7.4		
21.		-6.5		

PRO B:117
TYR B:160
LEU B:115
GLU B:140
LYS B:116
ARG B:143
LEU B:122
LYS B:136
GLU B:125
Interactions
Attractive Charge
Conventional Hydrogen Bond
Pi-Cation
Pi-Anion
Pi-Donor Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Alkyl
Pi-Alkyl
GLU125
TYR160
LEU122
PRO117
ARG143
LEU115
LYS116

LEU B:115
TYR B:160
LYS B:116
ARG B:143
ARG B:144
GLU B:140
LEU B:122
PHE B:133
GLU B:125
LYS B:136
Interactions
Attractive Charge
Conventional Hydrogen Bond
Pi-Cation
Pi-Anion
Pi-Donor Hydrogen Bond
Pi-Pi Stacked
Alkyl
Pi-Alkyl
LEU122
LYS116
LEU115
PHE133
LYS136
GLU140
TYR160
ARG143
ARG144

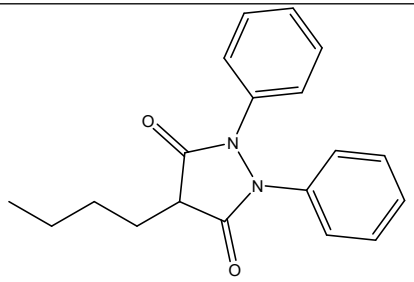
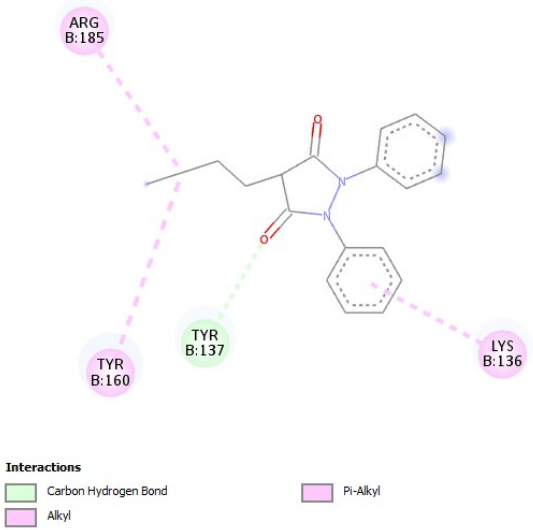
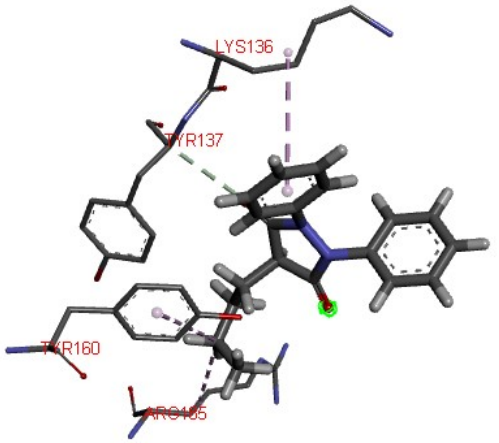
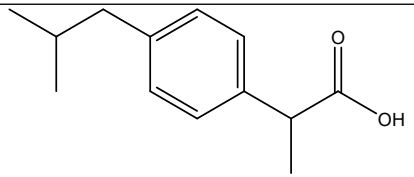
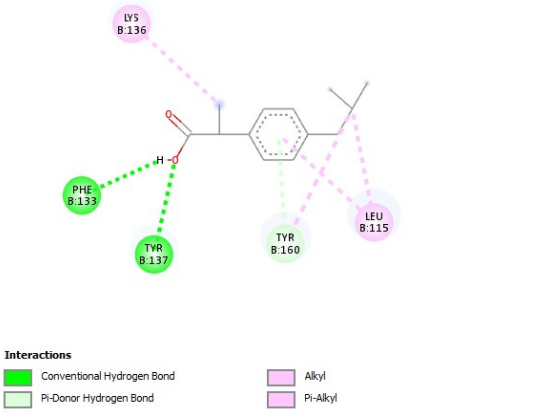
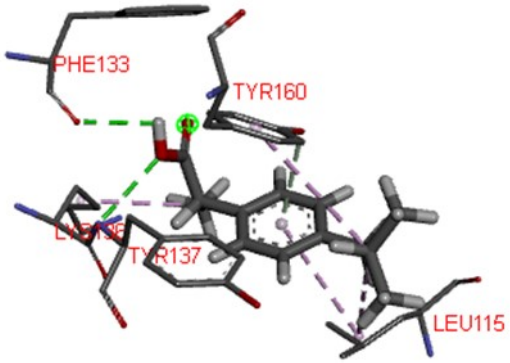
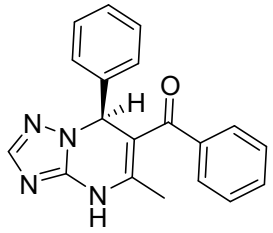
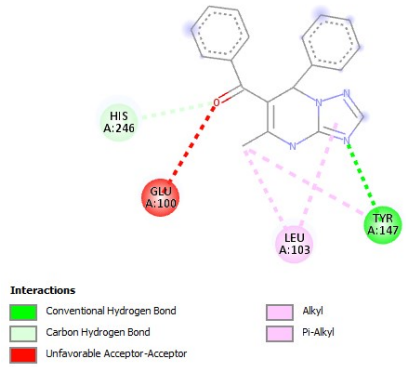
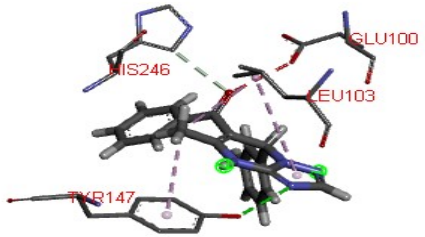
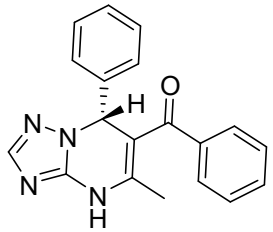
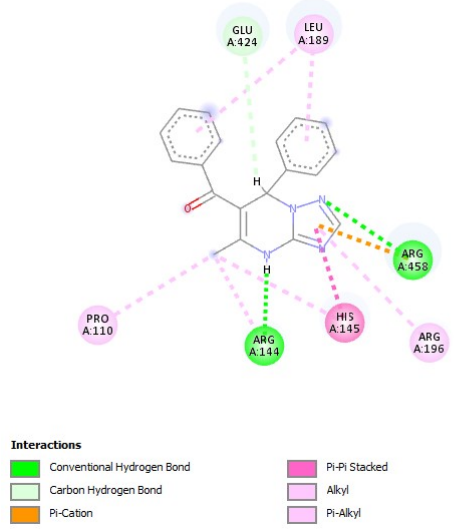
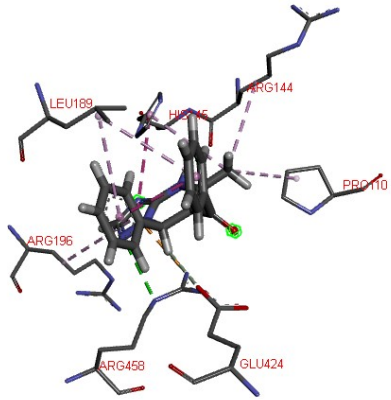
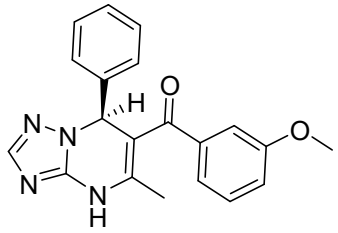
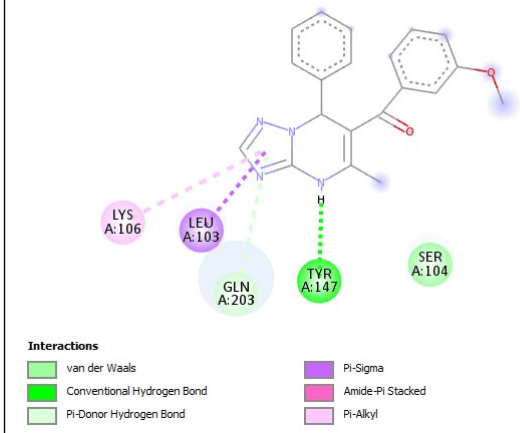
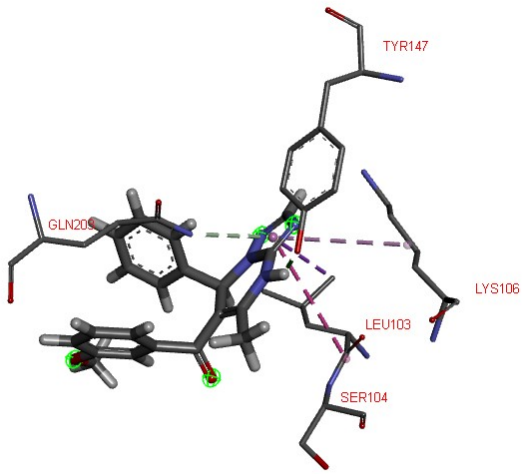
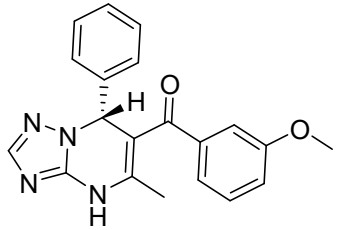
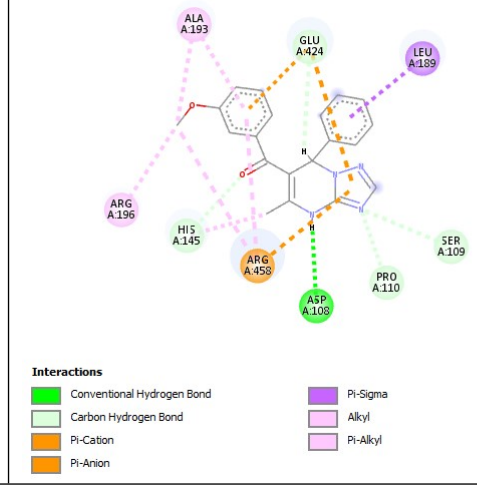
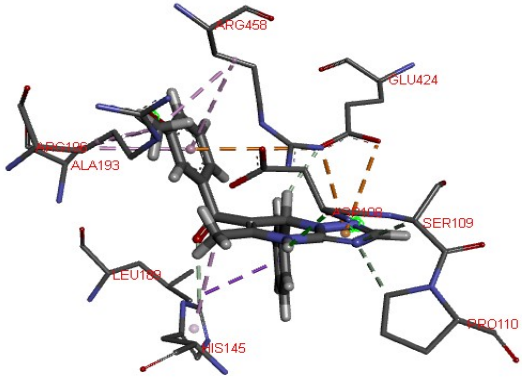
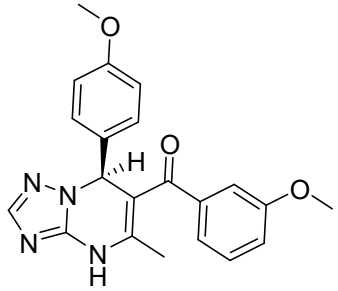
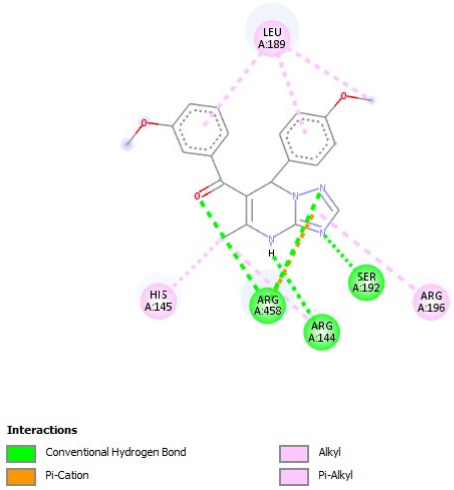
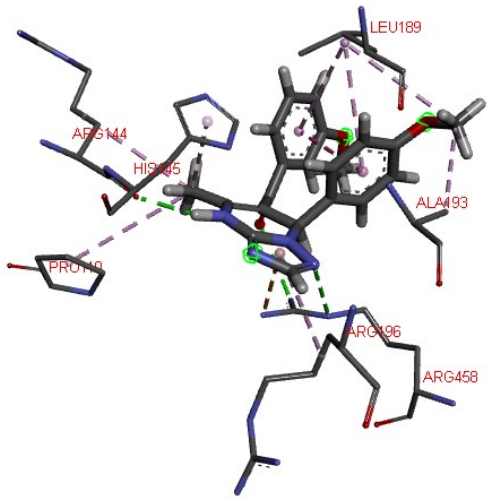
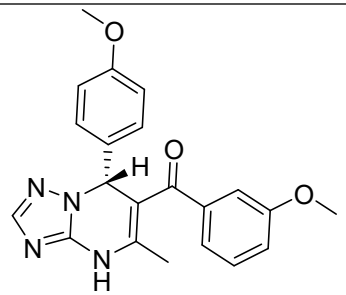
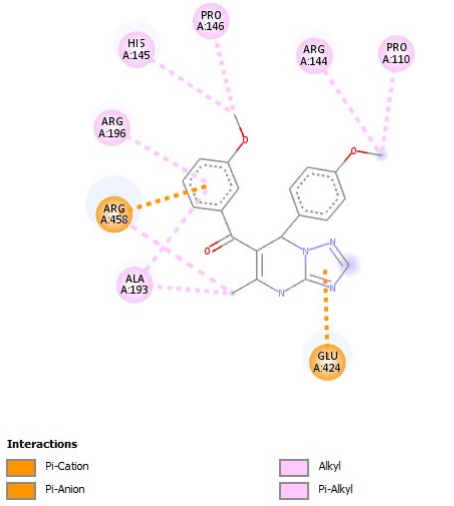
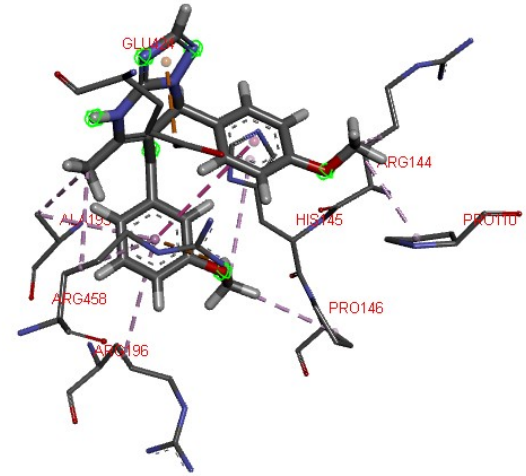
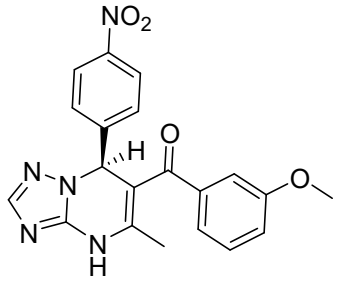
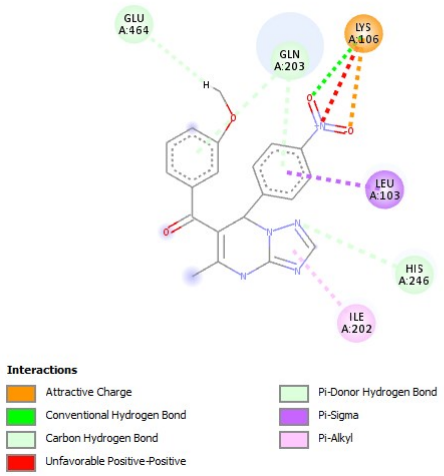
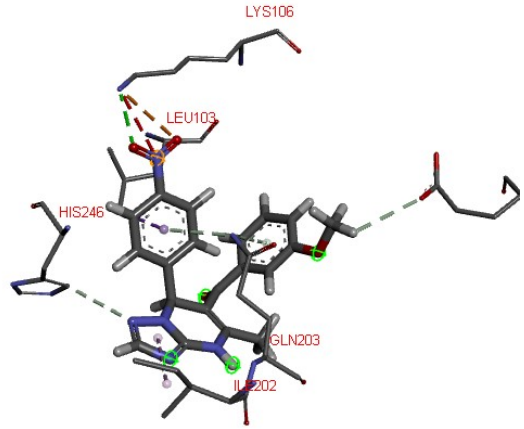
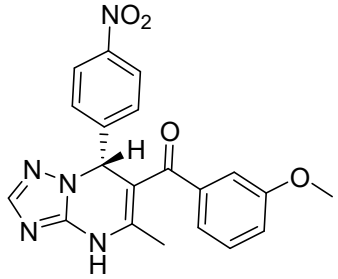
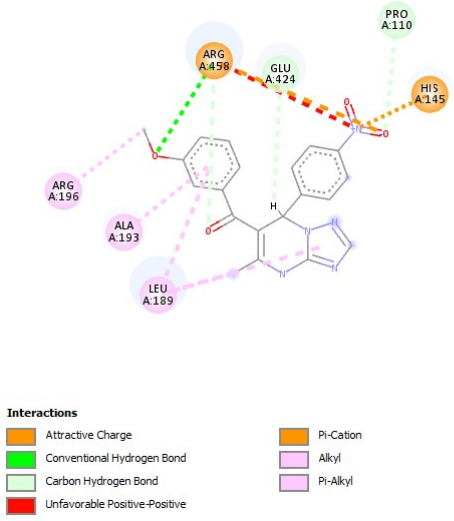
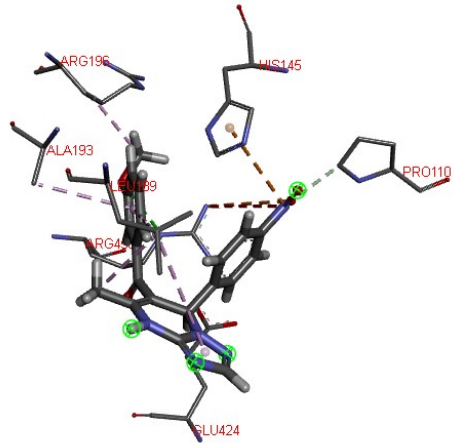
22.		-8.1	 ARG B:185 TYR B:160 TYR B:137 LYS B:136 Interactions Carbon Hydrogen Bond Alkyl Pi-Alkyl	 LYS136 TYR137 TYR160
23.		-6.6	 LYS B:136 PHE B:133 TYR B:137 TYR B:160 LEU B:115 Interactions Conventional Hydrogen Bond Pi-Donor Hydrogen Bond Alkyl Pi-Alkyl	 PHE133 TYR160 TYR137 LEU115

Table S2. 2D and 3D diagram showing of the interaction of *R*- and *S*-enantiomers of compounds (**5a**, **5f**, **5m**, and **5t**) with BSA protein.

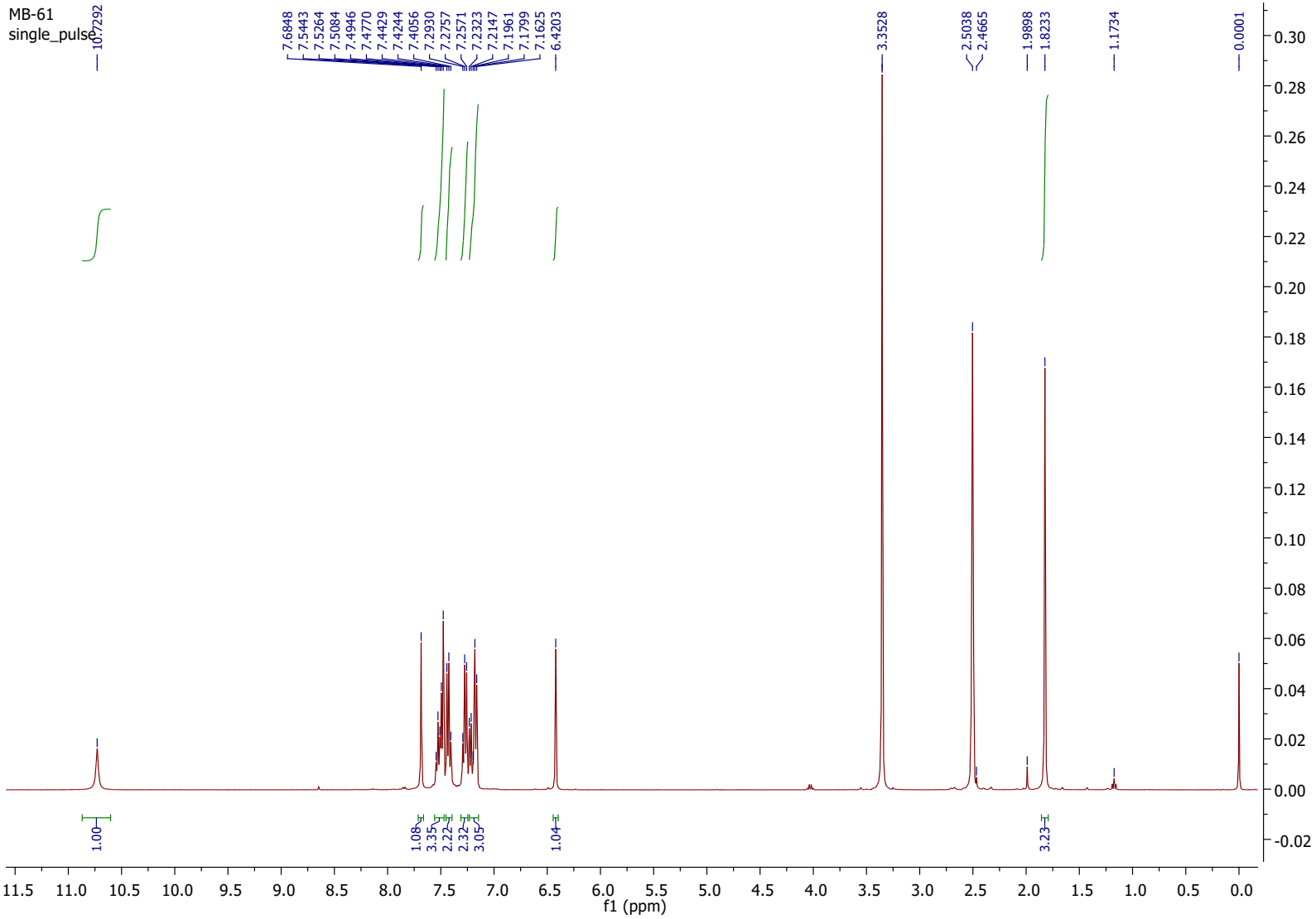
S. no.	Compound	Dock Score/ Binding Energy	2D	3D
1.	 (*S*)-(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(phenyl)methanone	-2.3		
2.	 (*R*)-(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(phenyl)methanone	-7.1		

3.	 (*S*)-(3-methoxyphenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone	-4.5		
4.	 (*R*)-(3-methoxyphenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone	-6.8		

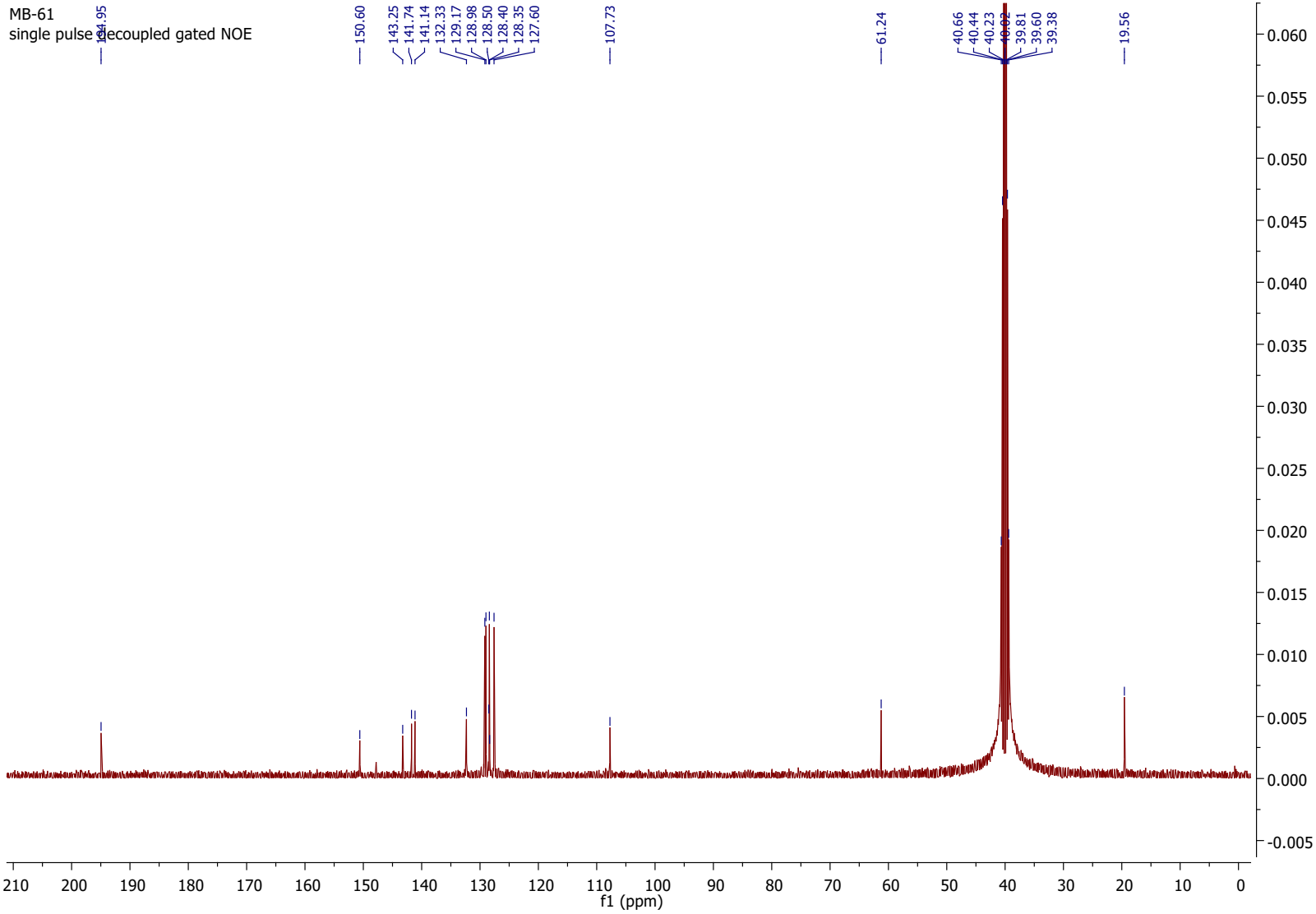
5.	 (*S*)-(3-methoxyphenyl)(7-(4-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone	-5.4		
6.	 (*R*)-(3-methoxyphenyl)(7-(4-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone	-6.0		

7.	 (*S*)-(3-methoxyphenyl)(5-methyl-7-(4-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone	-5.1		
8.	 (*R*)-(3-methoxyphenyl)(5-methyl-7-(4-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone	-5.8		

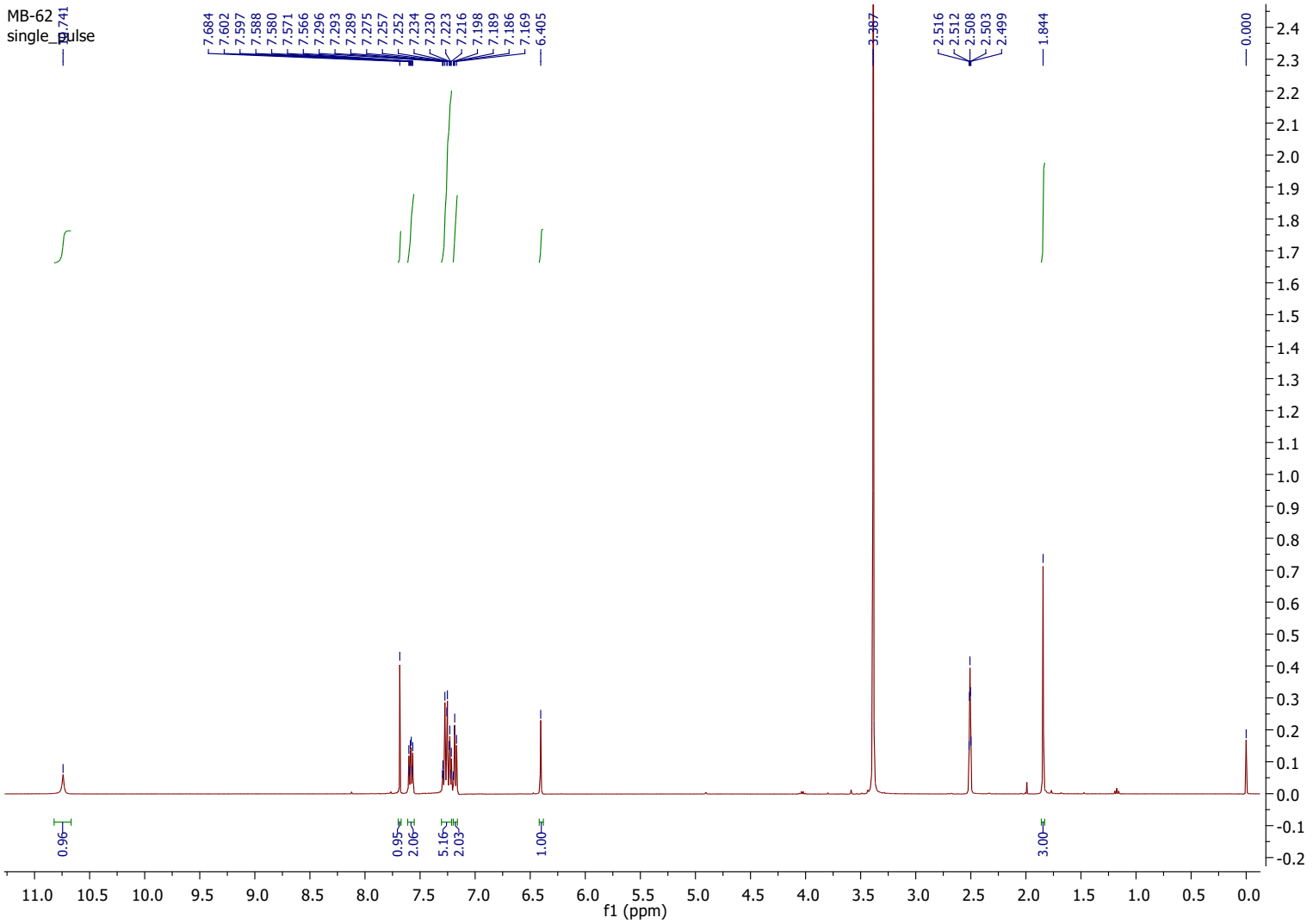
^{1}H NMR of (5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(phenyl)methanone (5a)



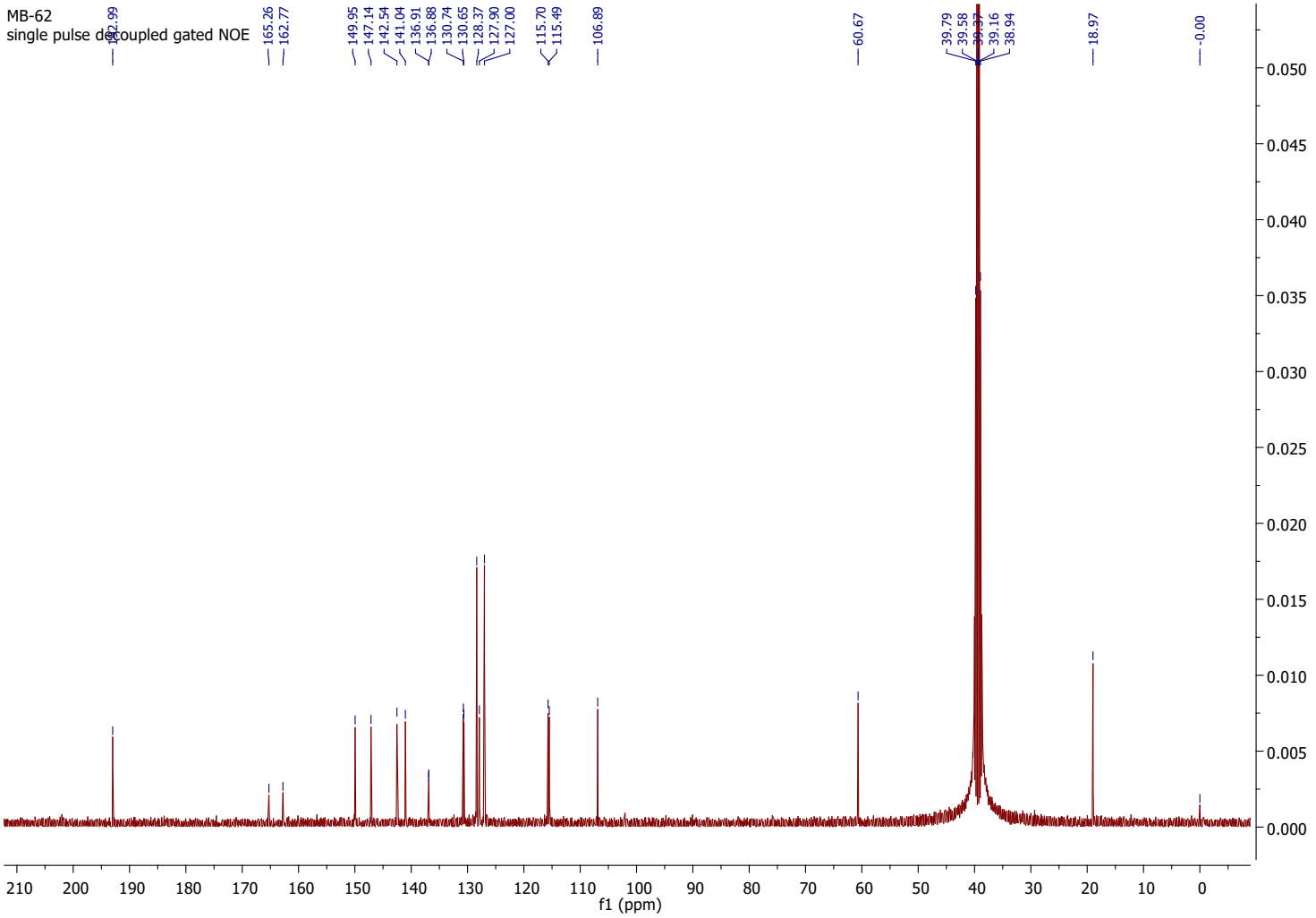
^{13}C NMR of (5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(phenyl)methanone (5a)



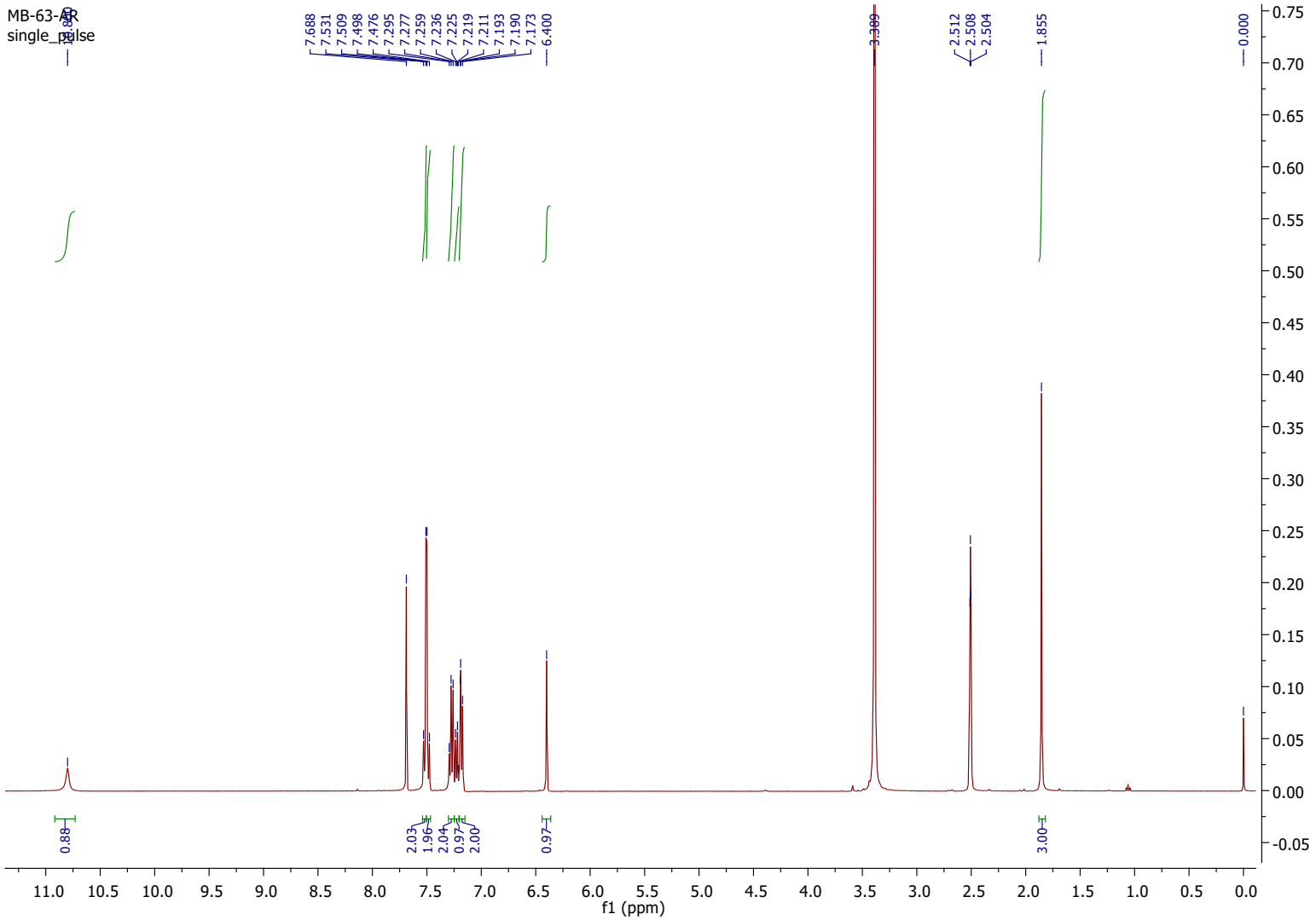
^{1}H NMR of (4"-Fluorophenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5b)



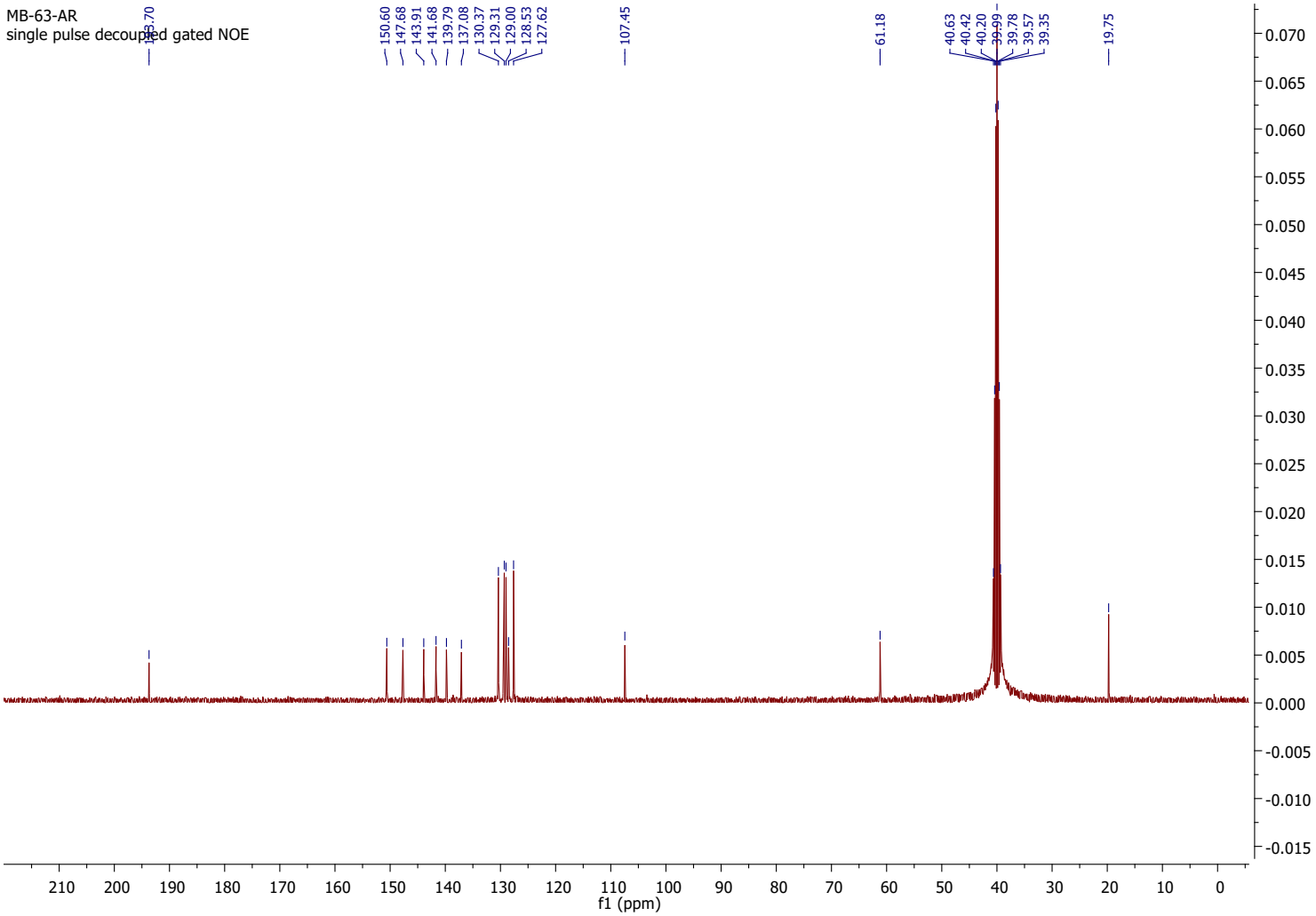
^{13}C NMR of (4''-Fluorophenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5b)



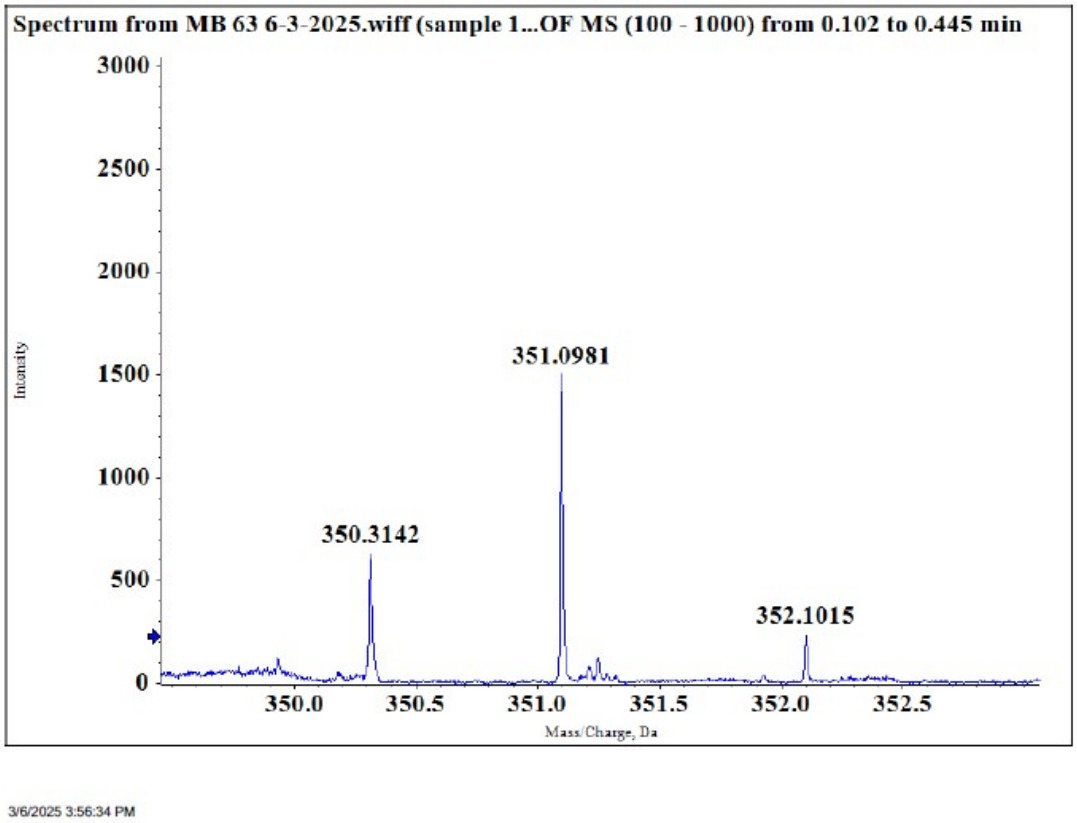
^{1}H NMR of (4"-Chlorophenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5c)



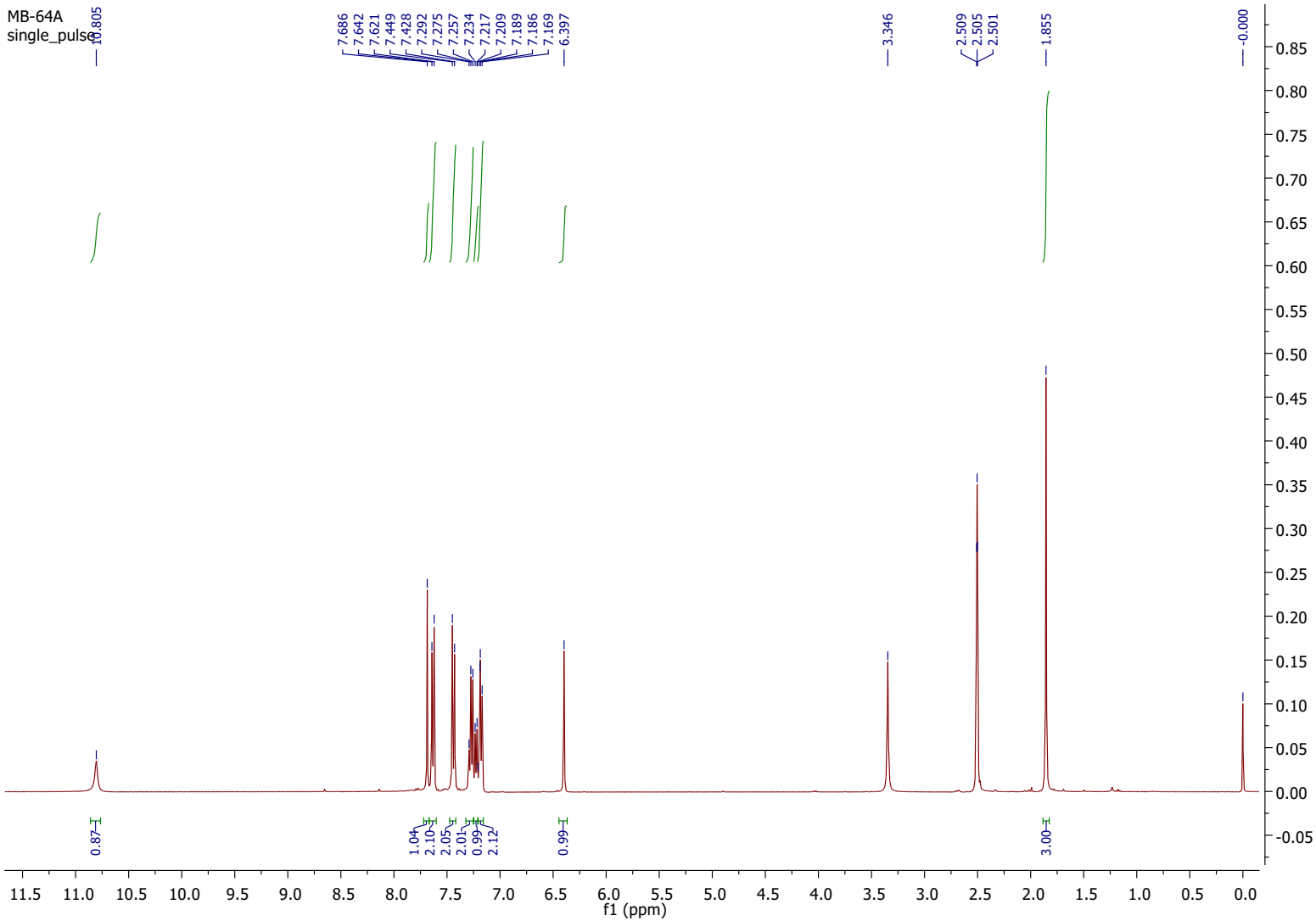
^{13}C NMR of (4''-Chlorophenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5c)



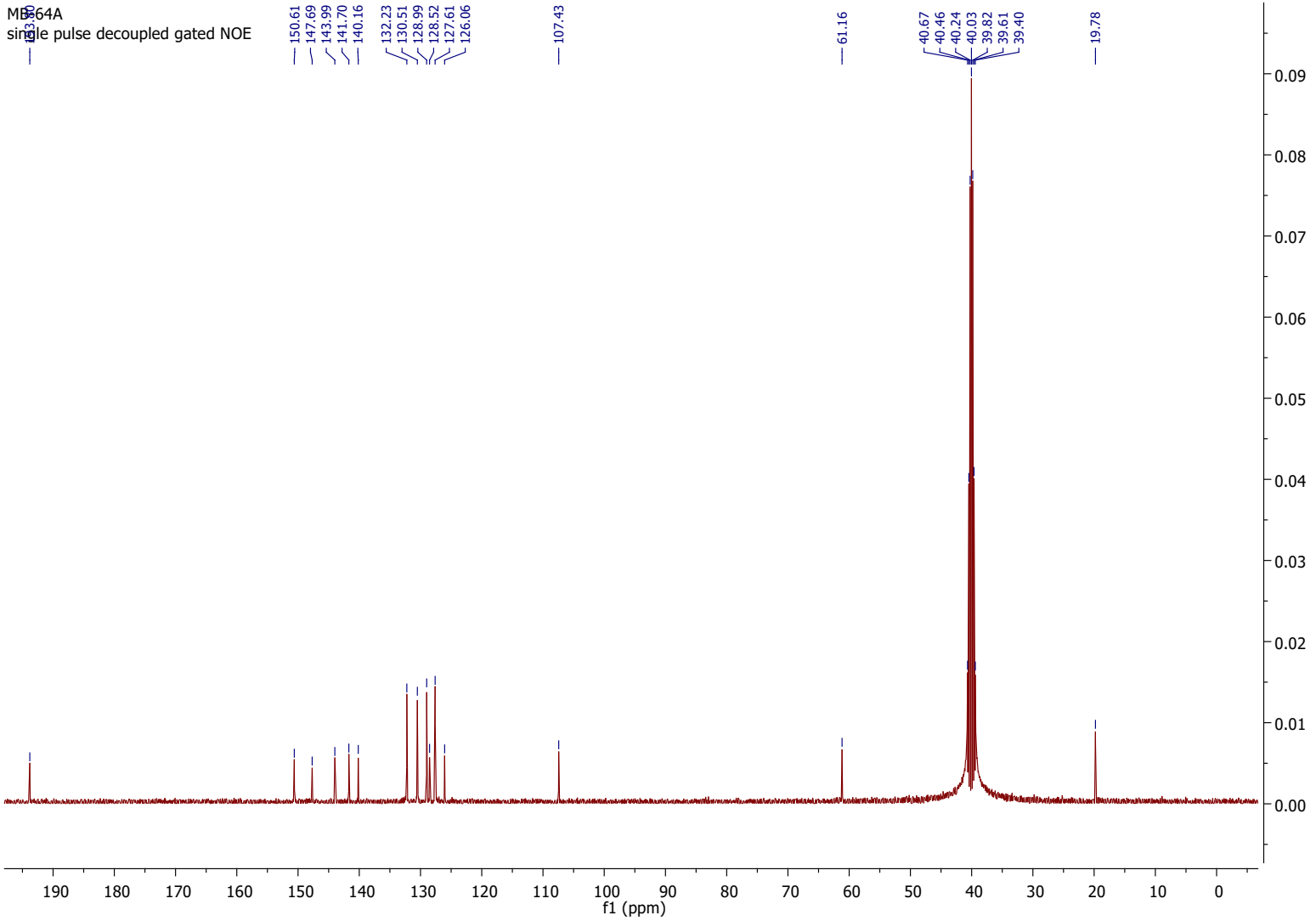
HRMS of (4''-Chlorophenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5c)



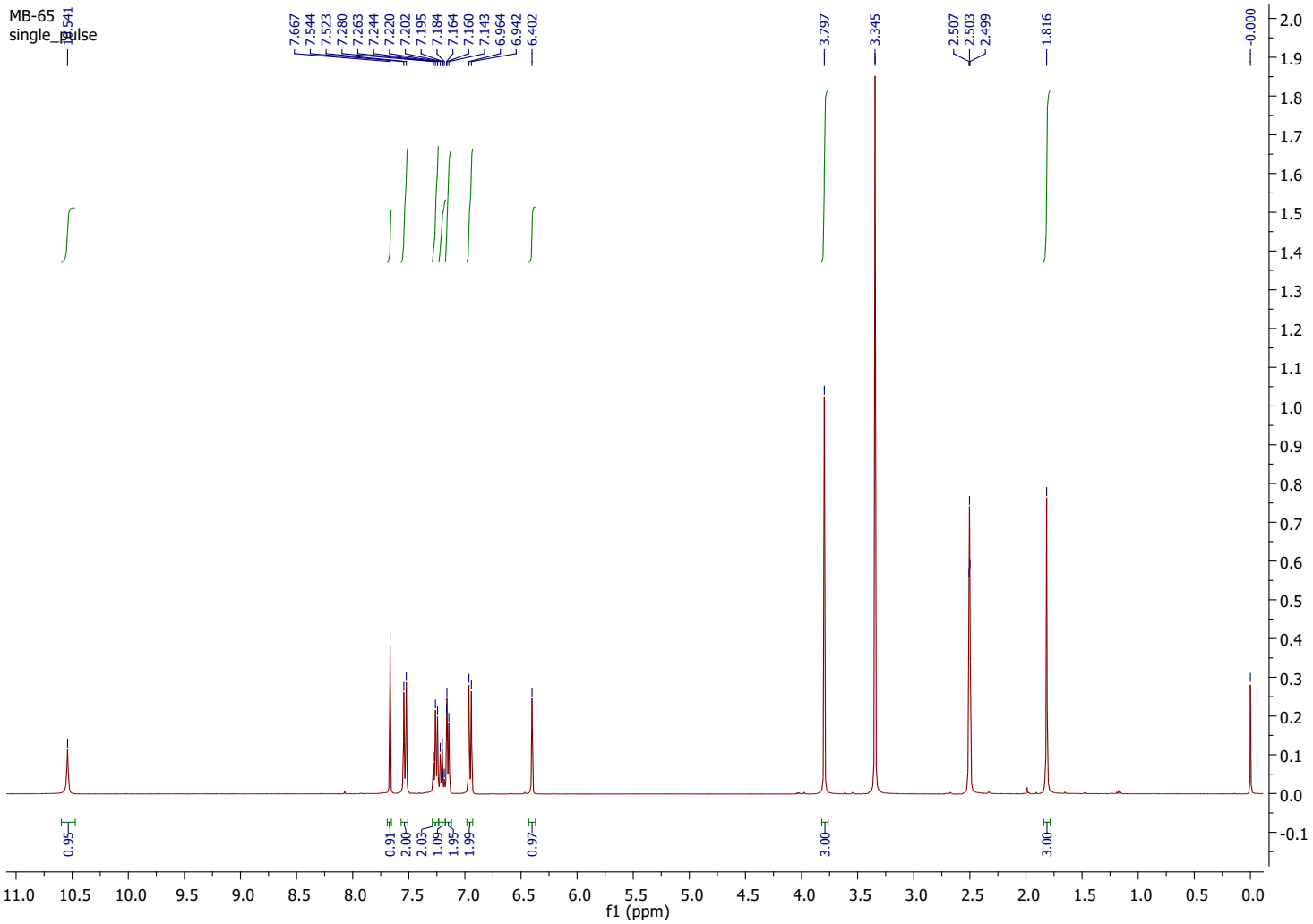
^{1}H NMR of (4''-Bromophenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5d)



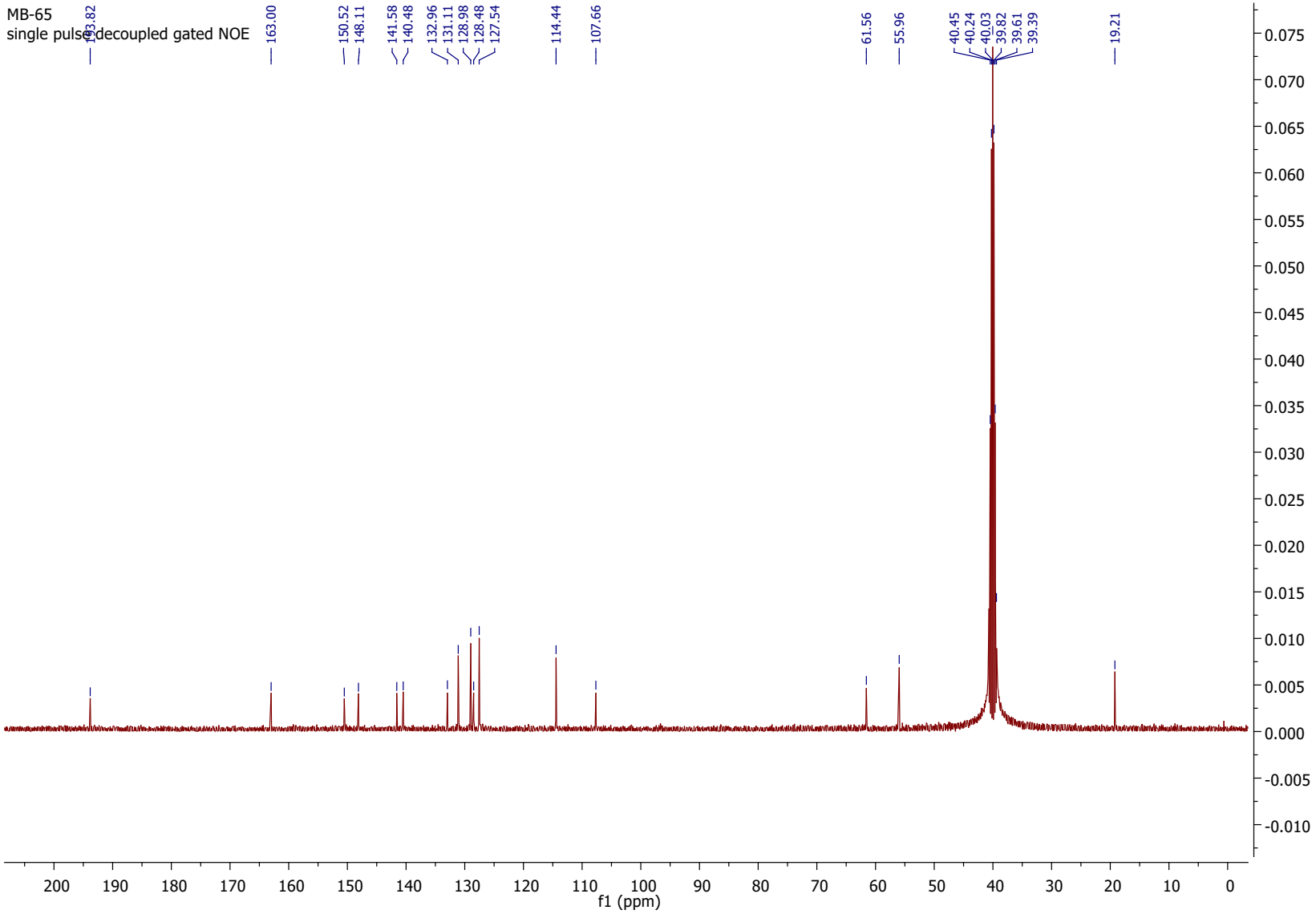
^{13}C NMR of (4"-Bromophenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5d)



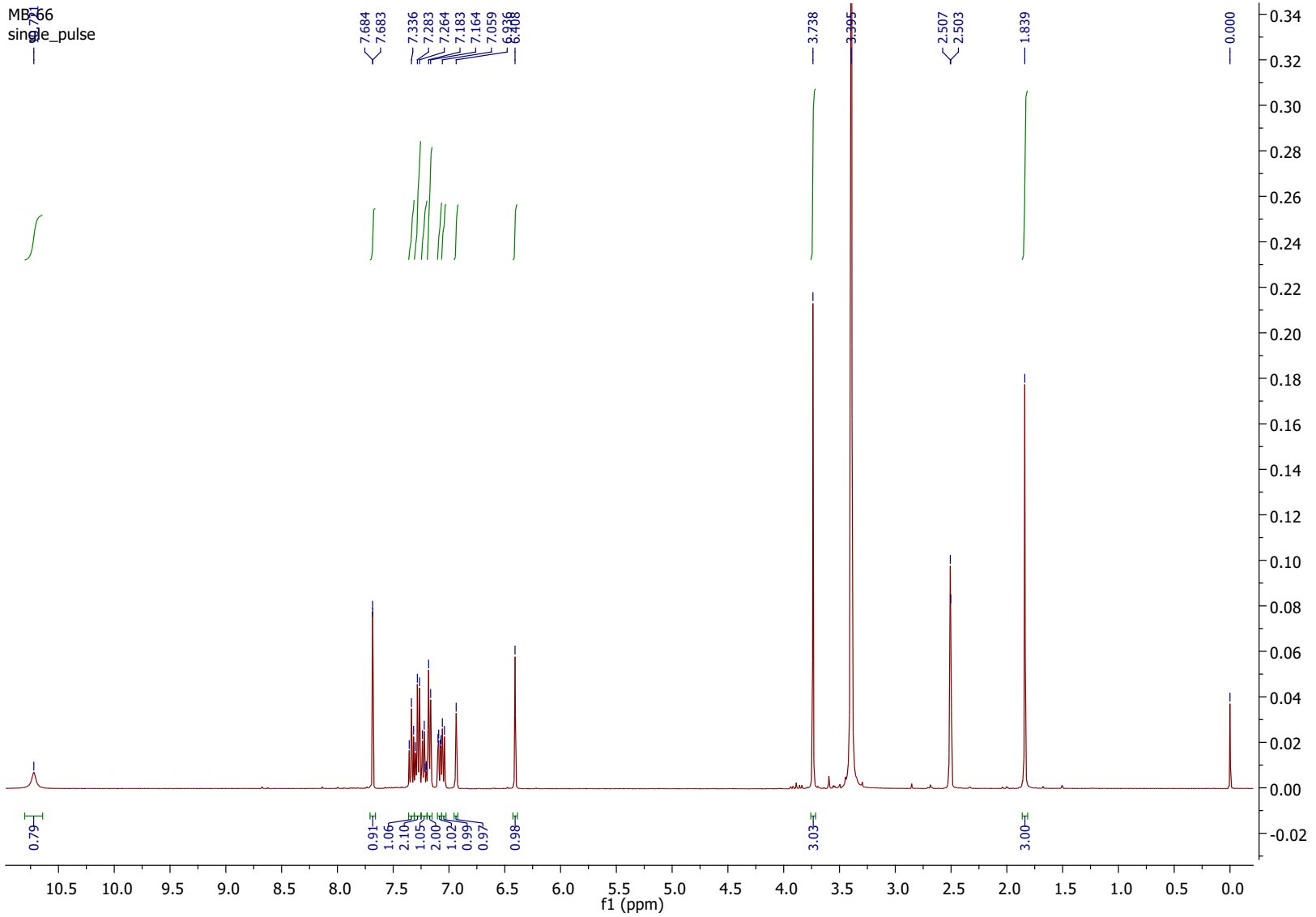
^{1}H NMR of (4"-Methoxyphenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5e)



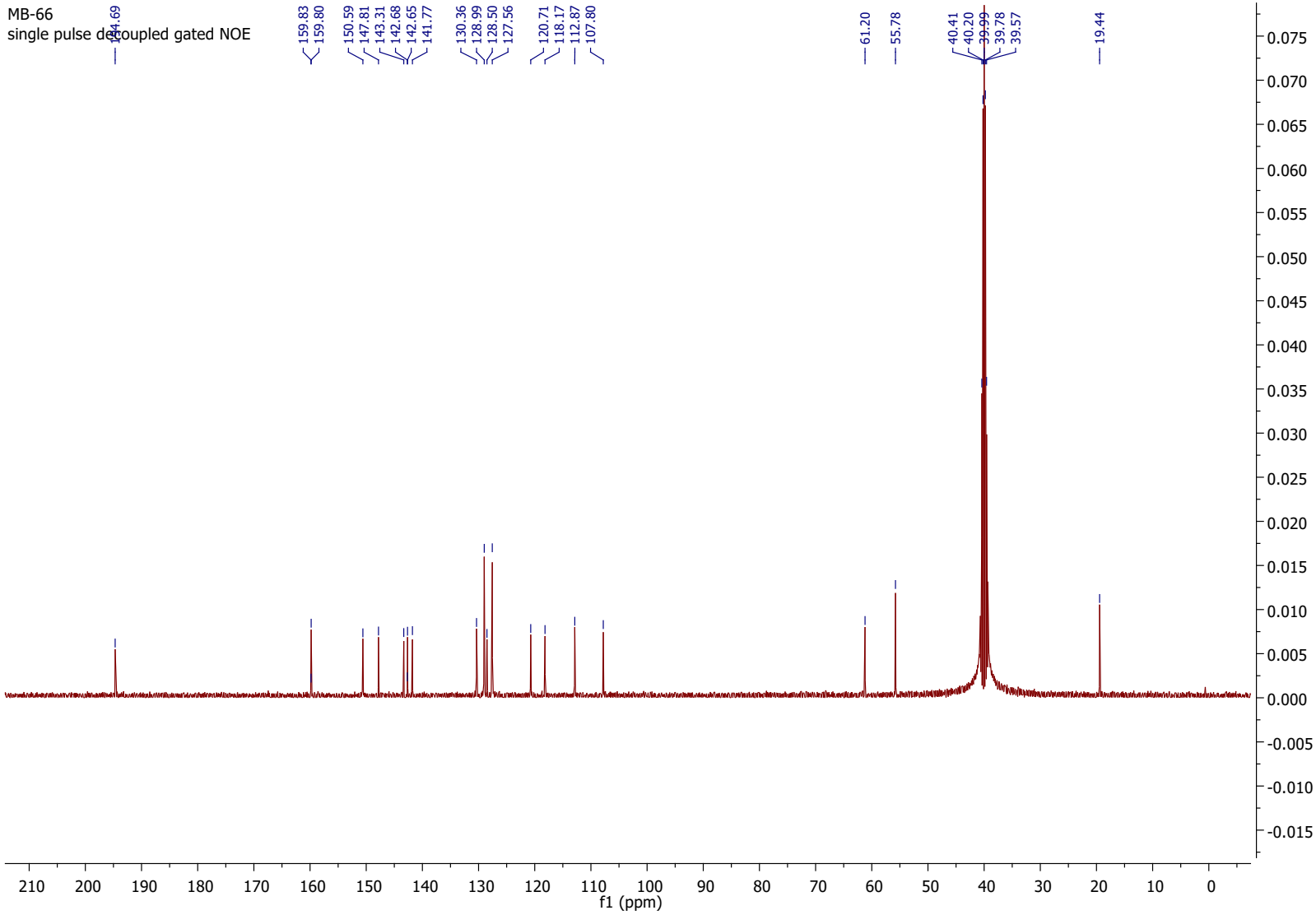
^{13}C NMR of (4''-Methoxyphenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5e)



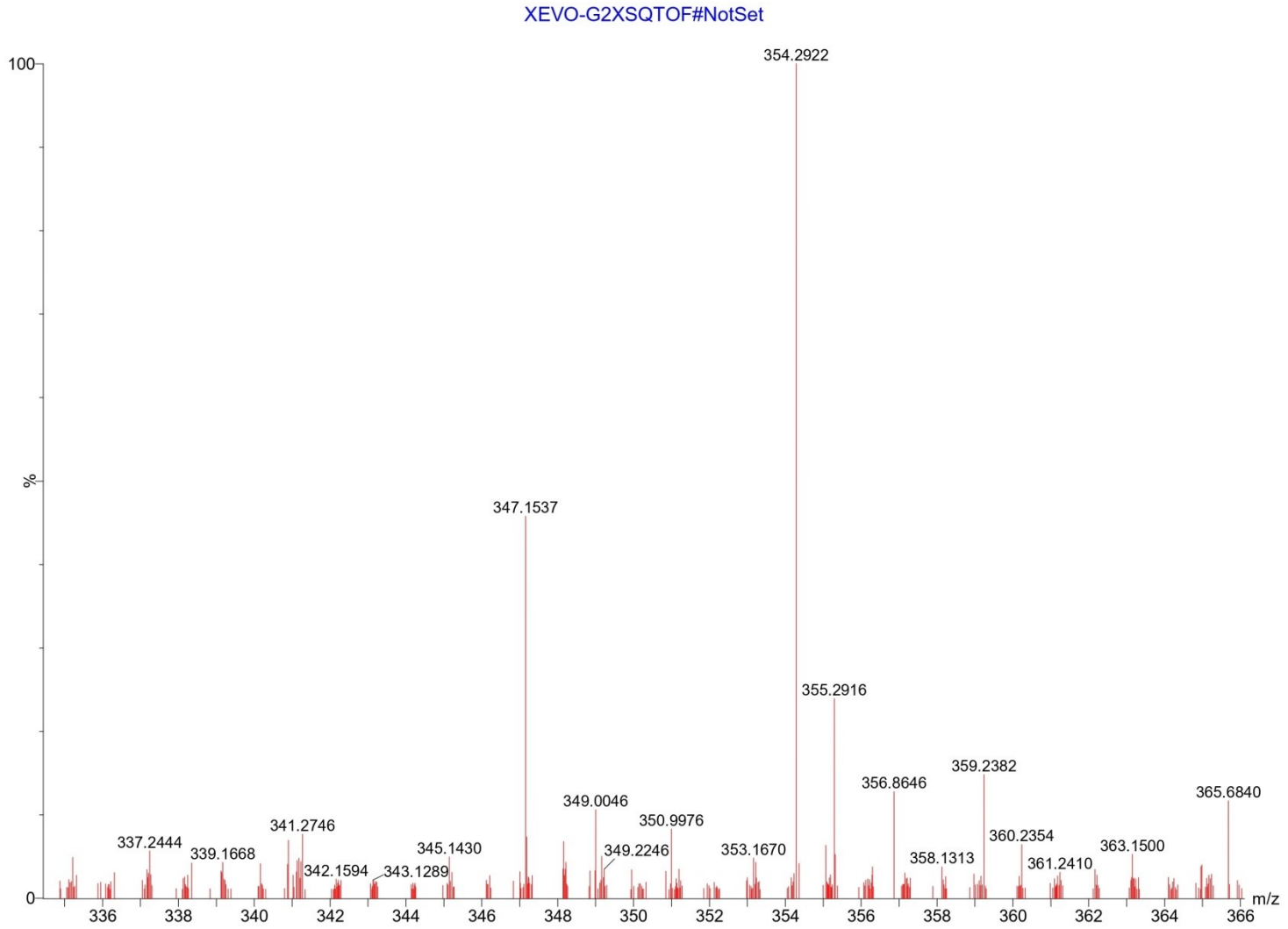
^{1}H NMR of (3"-Methoxyphenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5f)



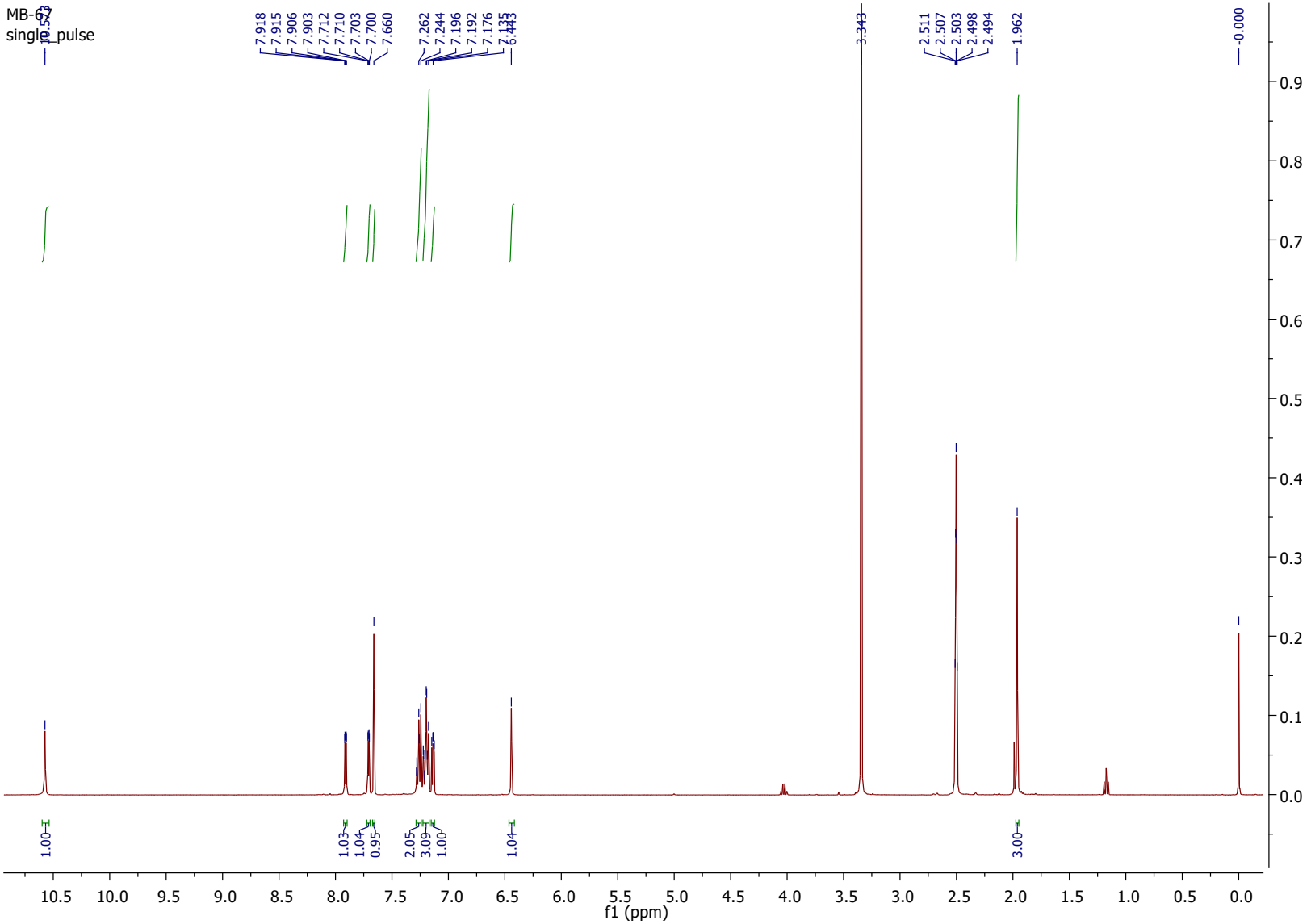
^{13}C NMR of (3''-Methoxyphenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5f)



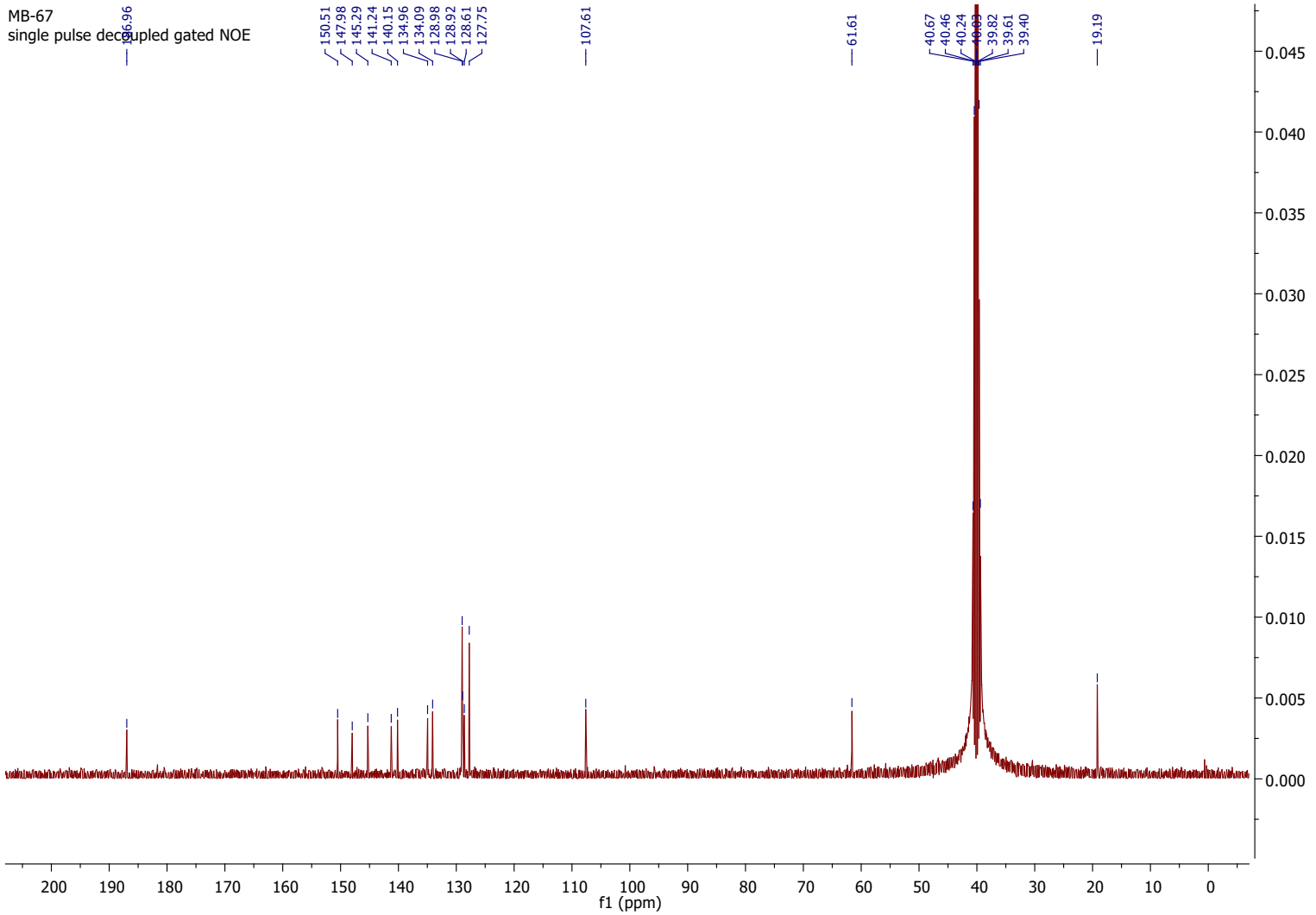
HRMS of (3''-Methoxyphenyl)(5-methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5f)



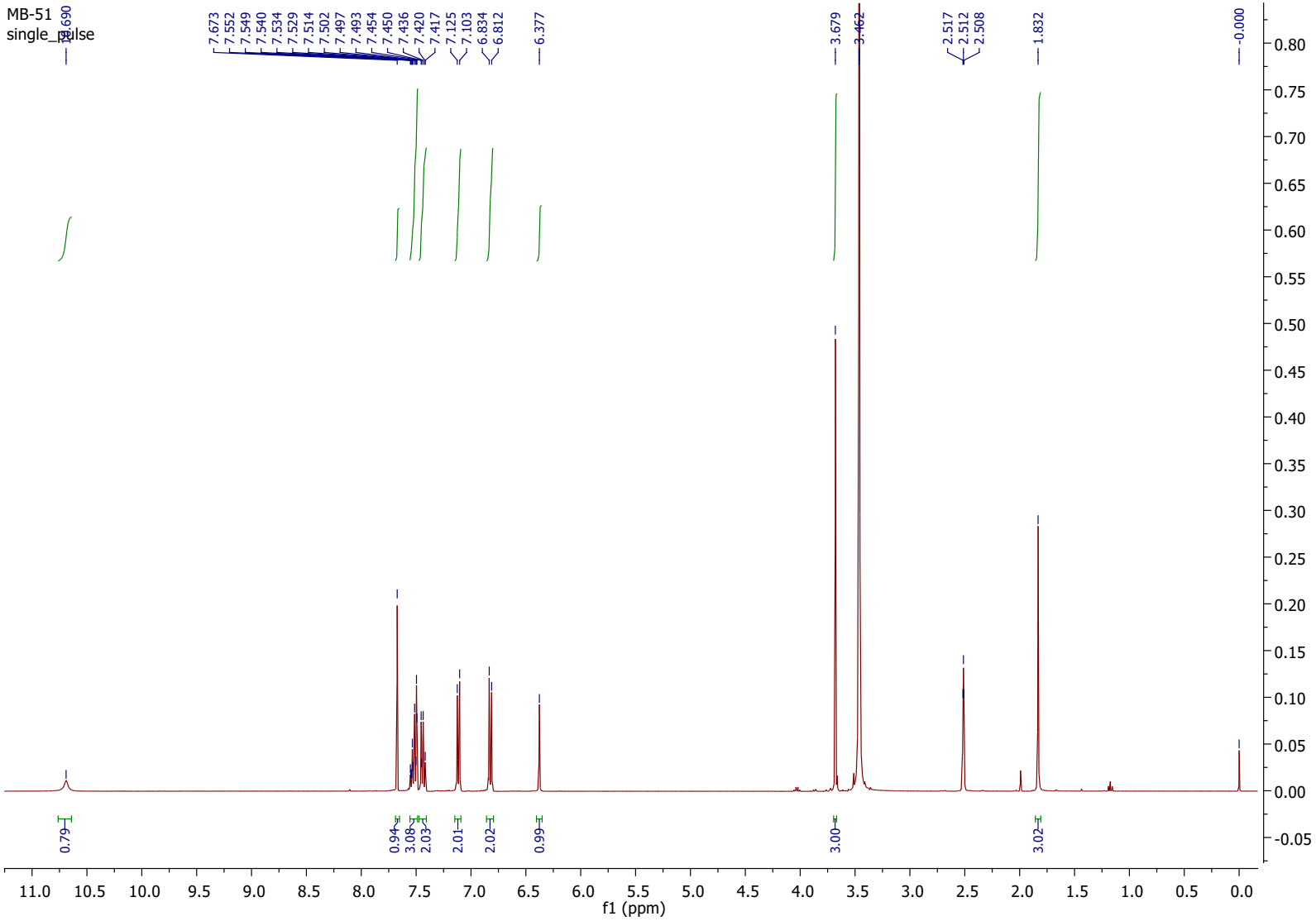
^{1}H NMR of (5-Methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(thiophen-2''-yl)methanone (5g)



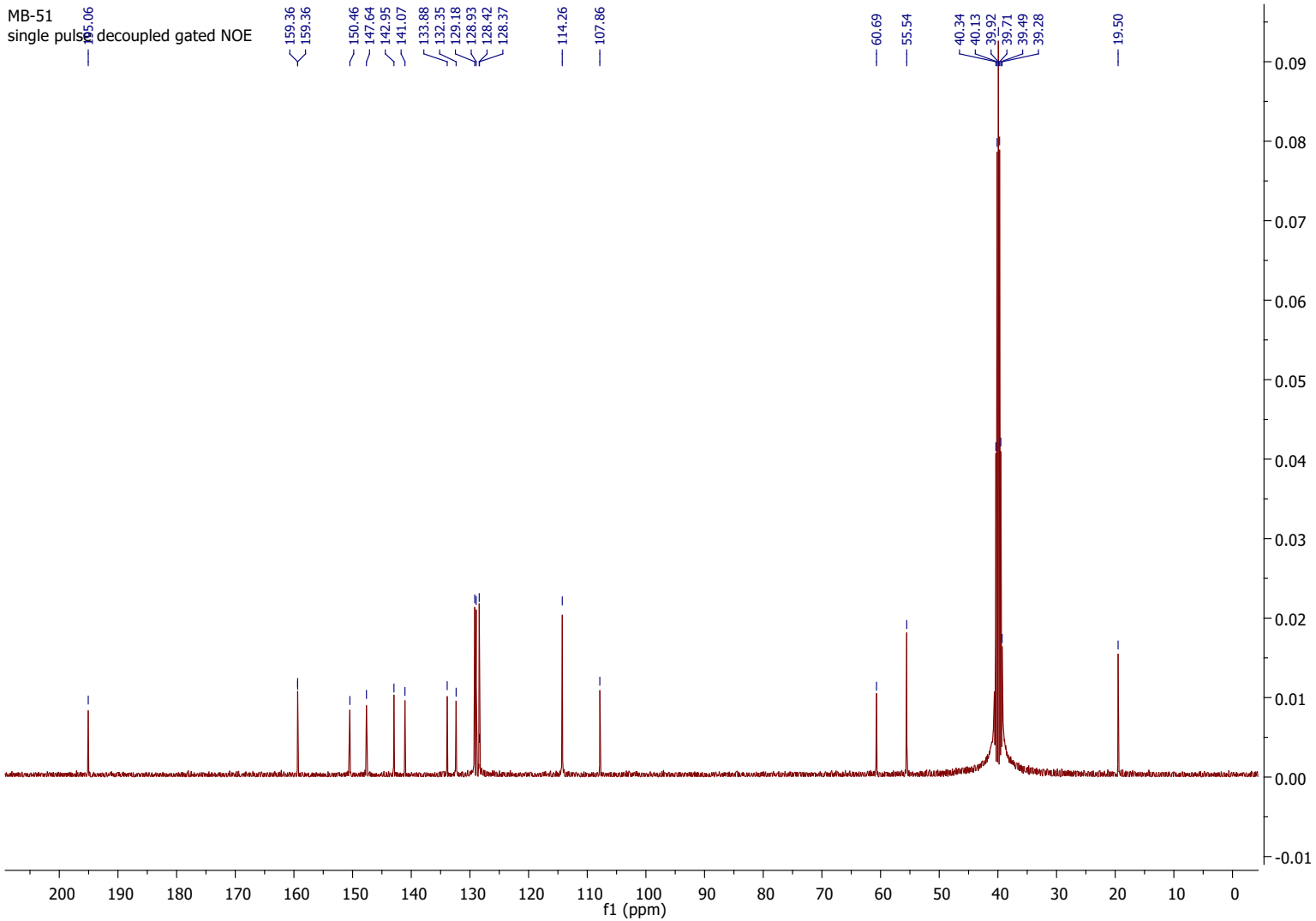
^{13}C NMR of (5-Methyl-7-phenyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(thiophen-2''-yl)methanone (5g)



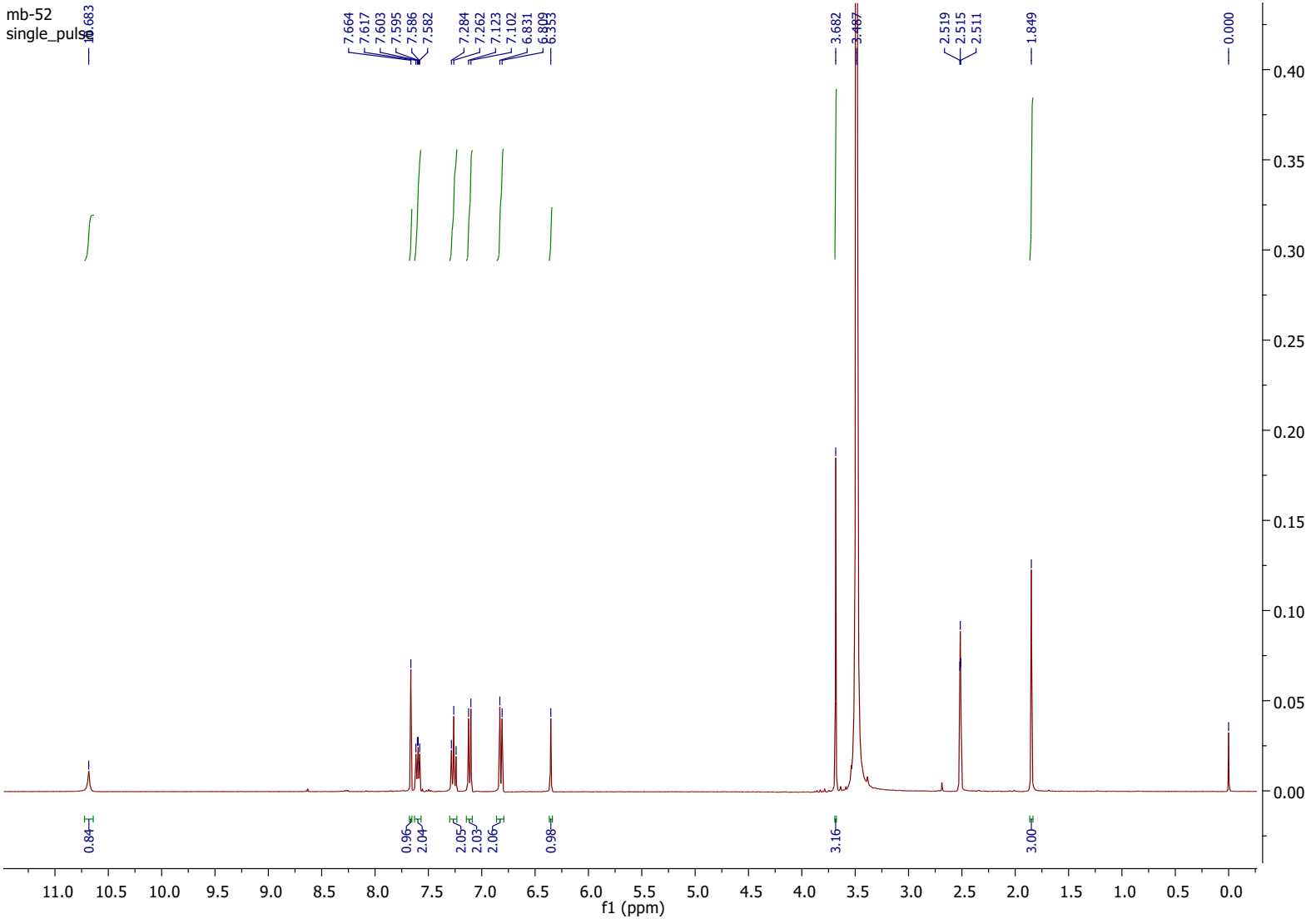
^{1}H NMR of (7-(4'-Methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl) (phenyl)methanone (5h)



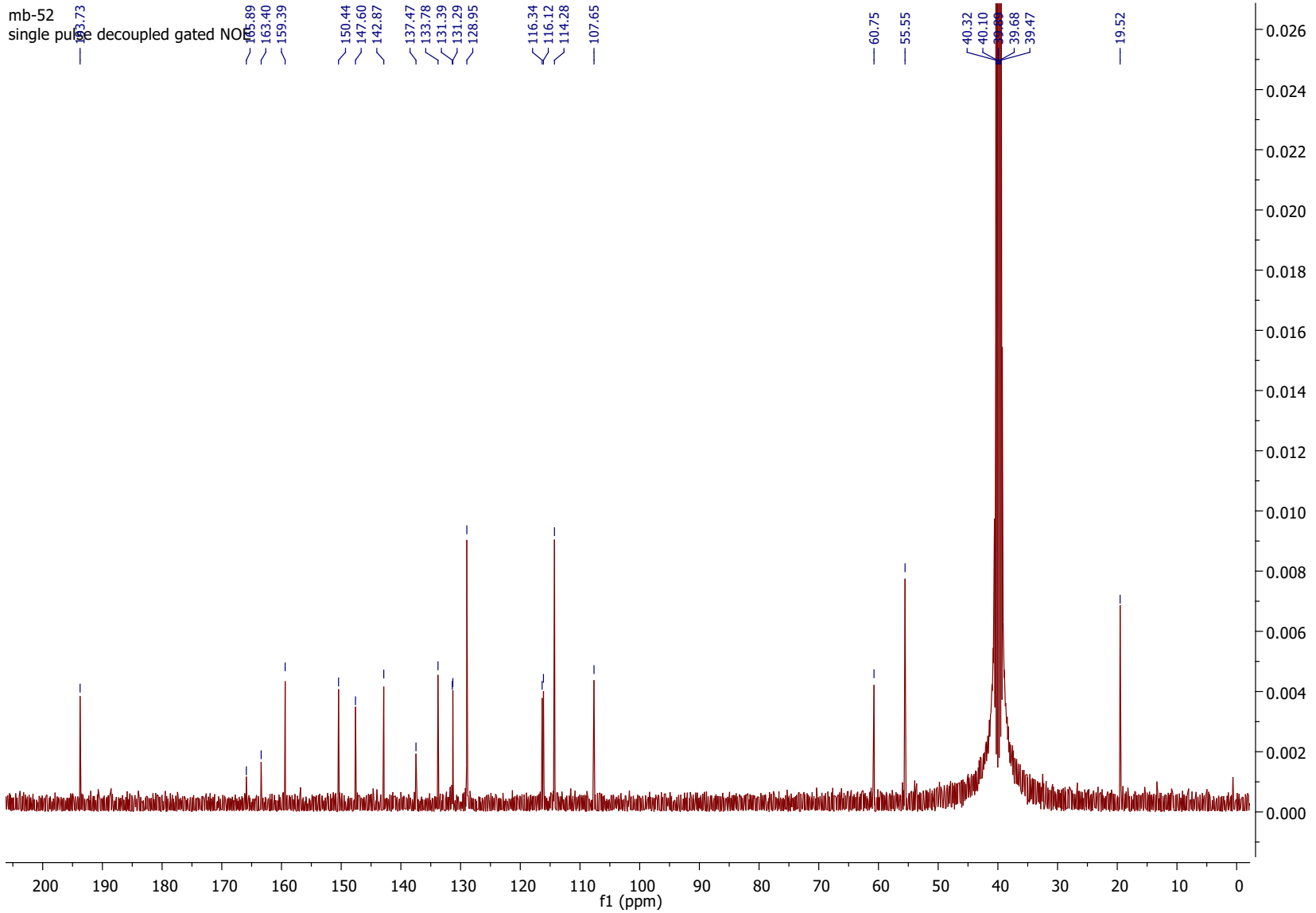
^{13}C NMR of (7-(4'-Methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl) (phenyl)methanone (5h)



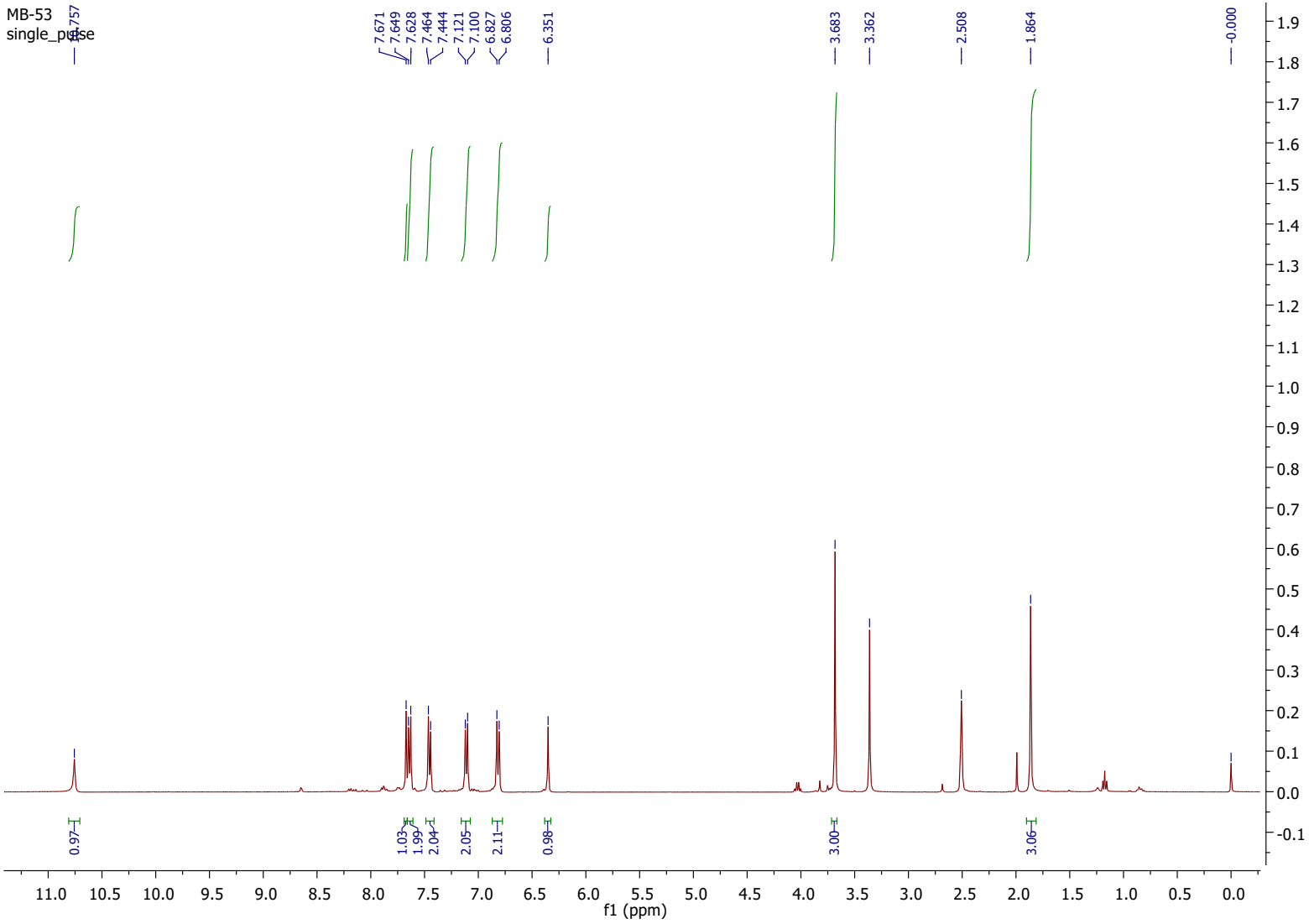
^{1}H NMR of (4"-Fluorophenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5i)



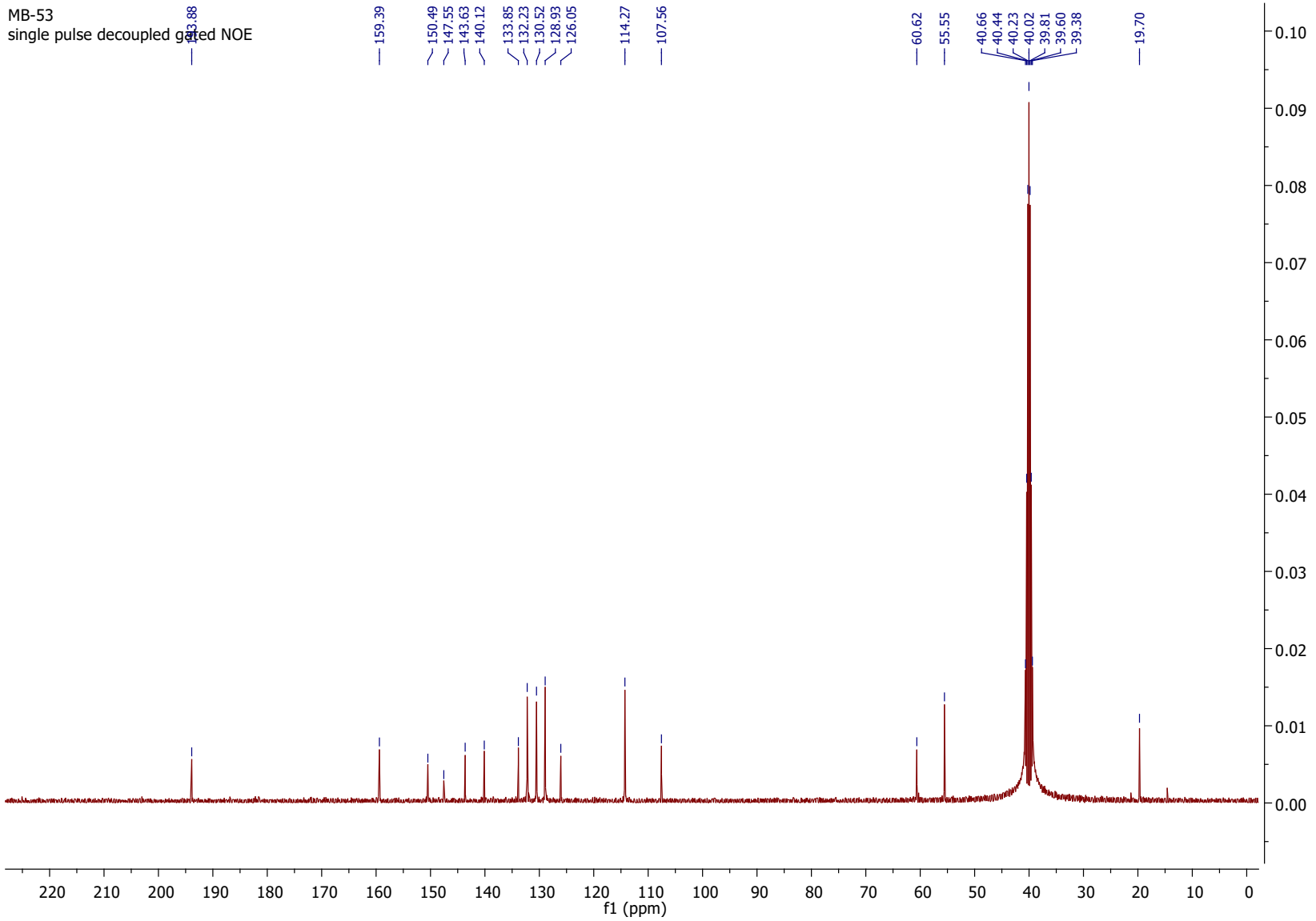
^{13}C NMR of (4''-Fluorophenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5i)



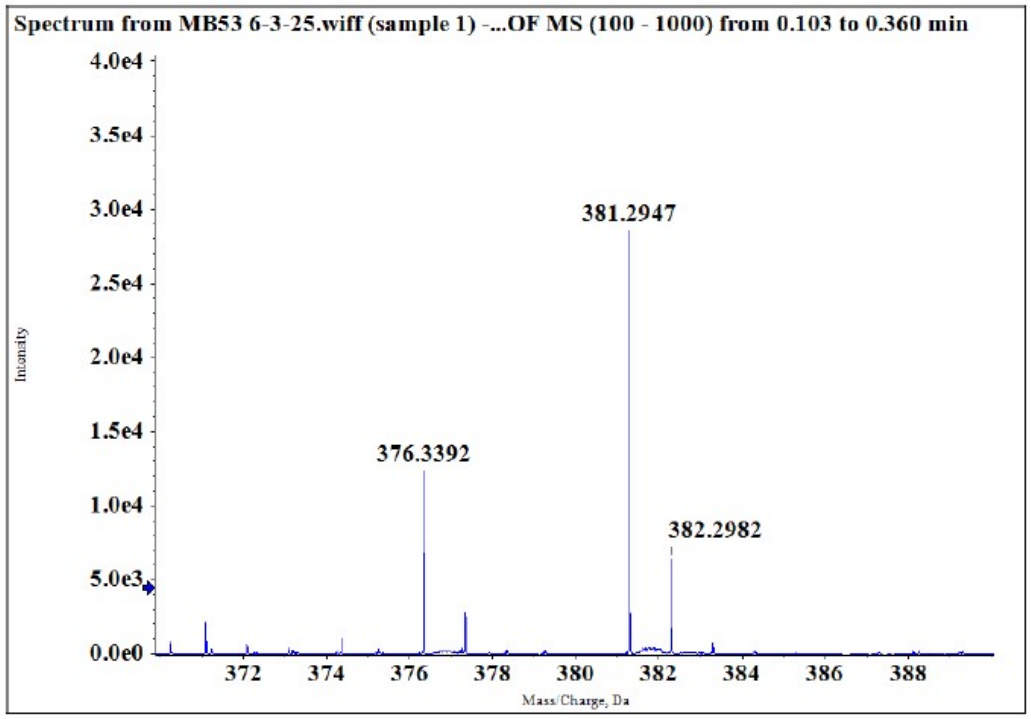
^{1}H NMR of (4''-Chlorophenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5j)



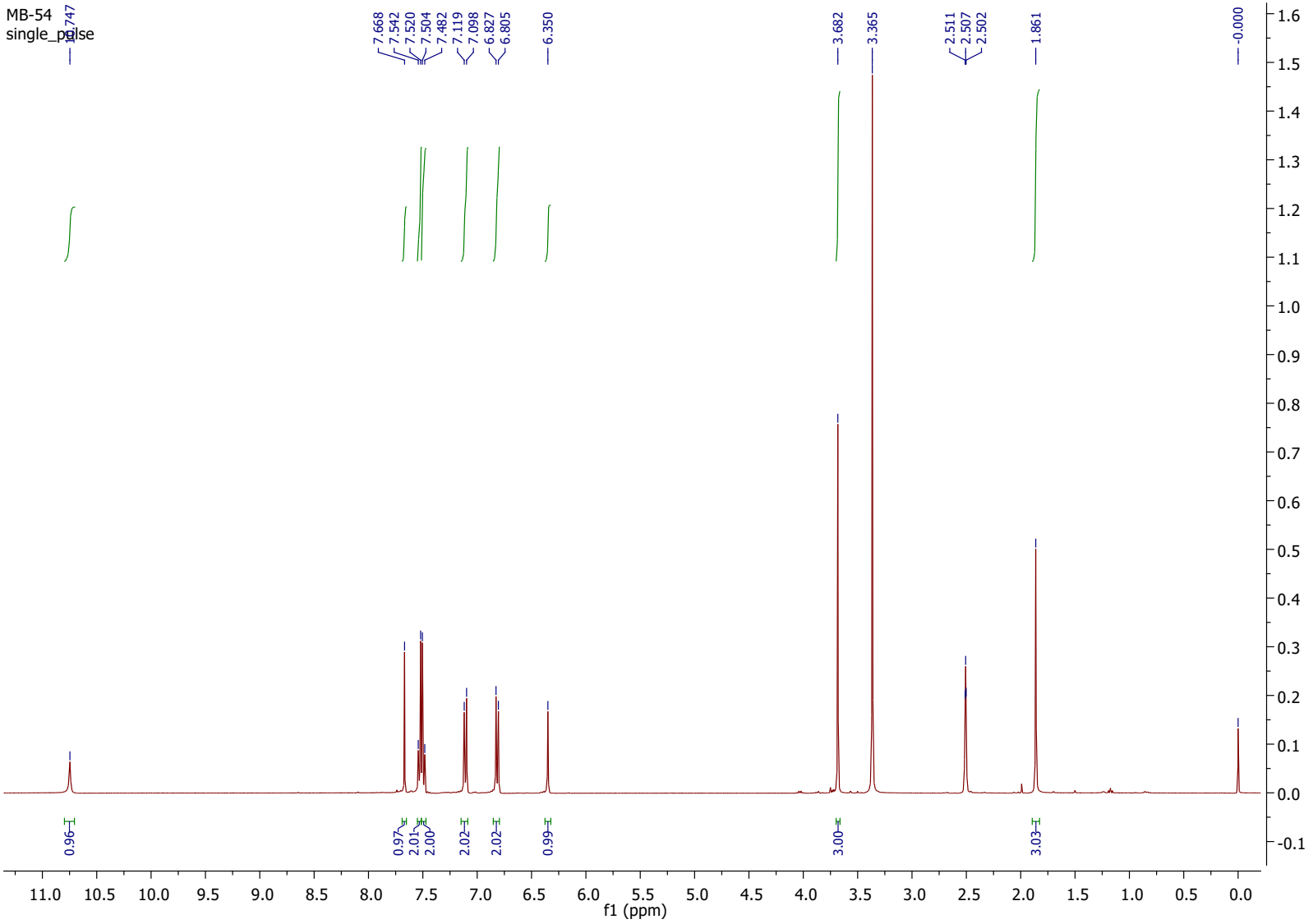
^{13}C NMR of (4''-Chlorophenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5j)



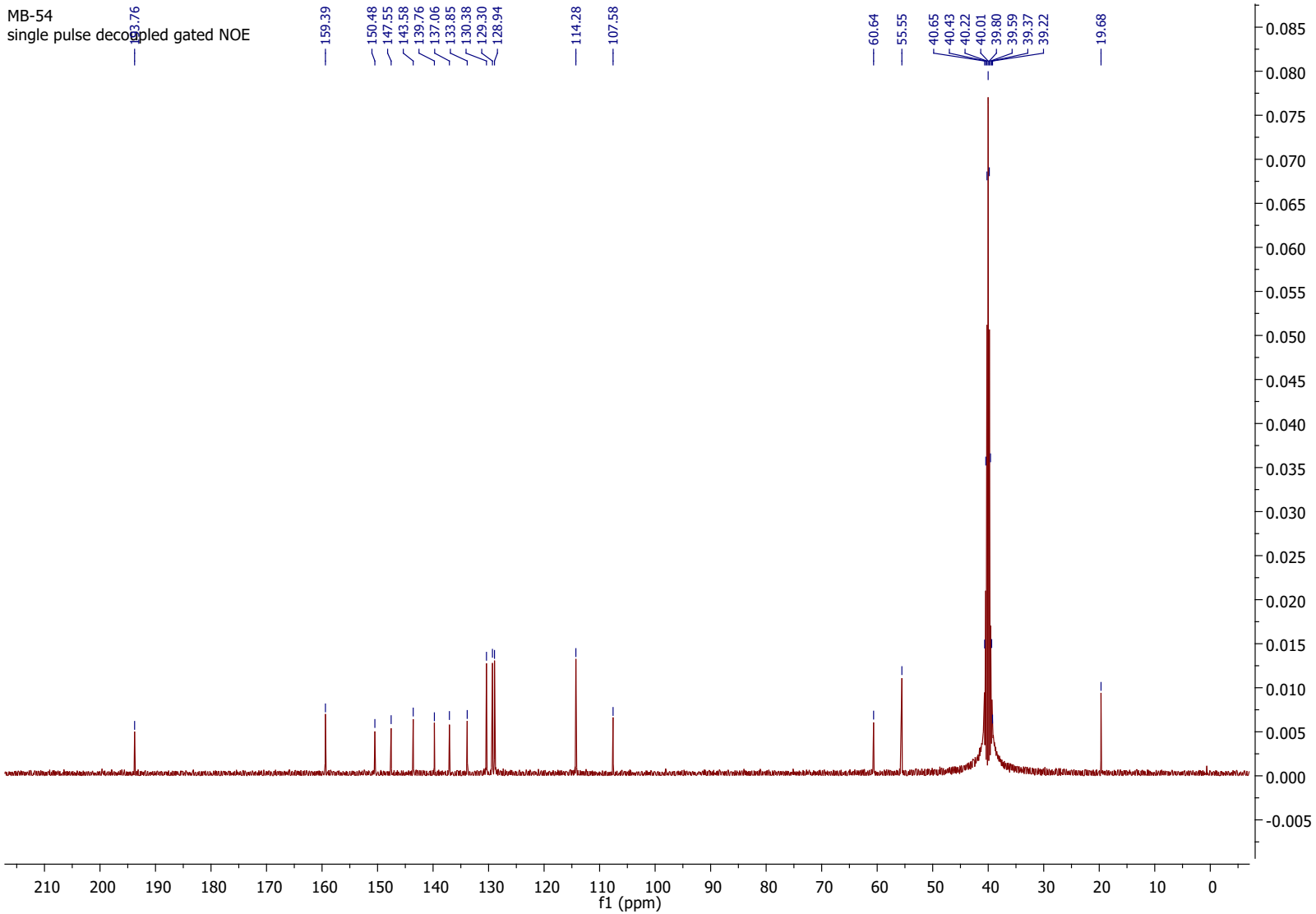
HRMS of (4''-Chlorophenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5j)



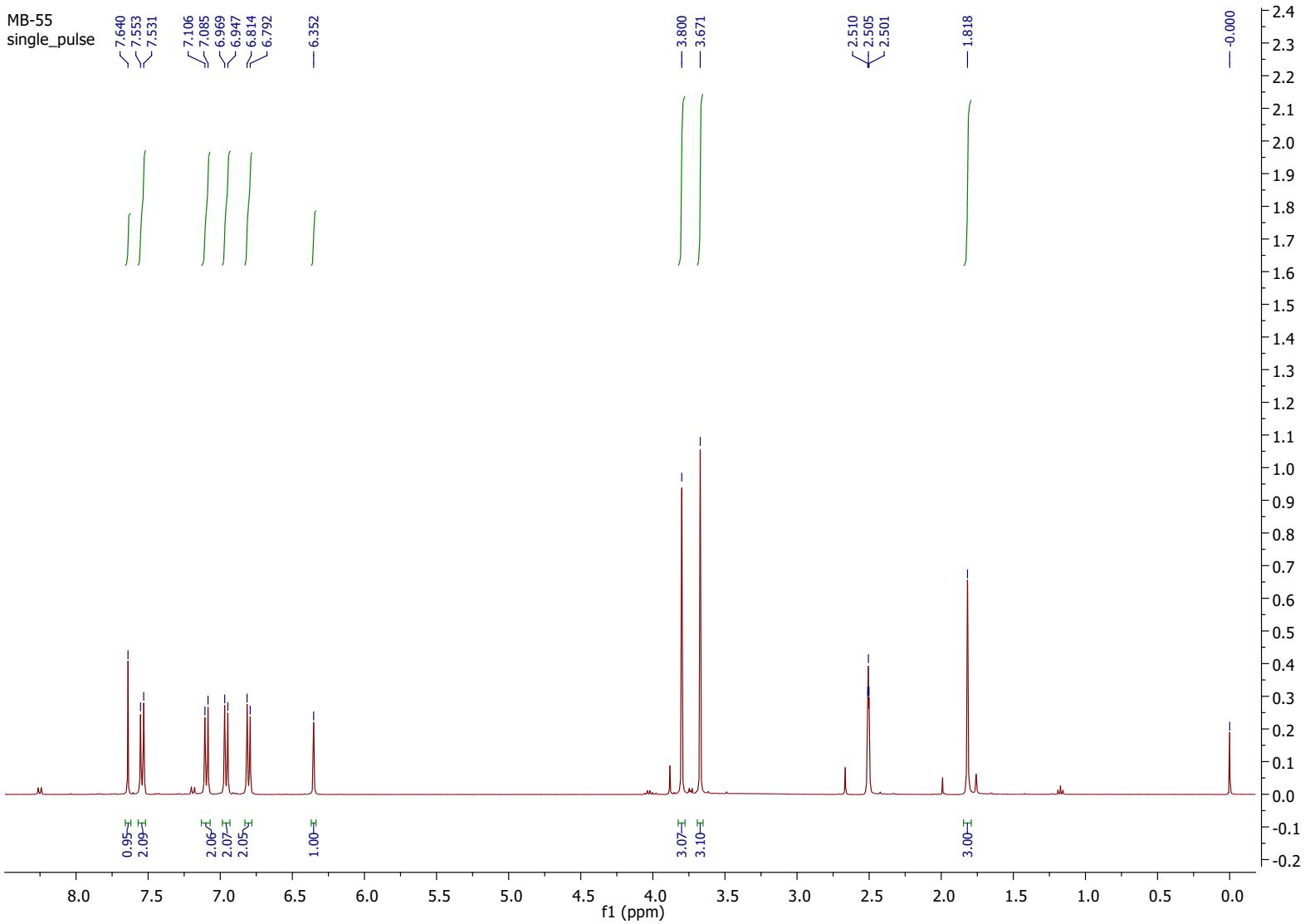
^{1}H NMR of (4''-Bromophenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5k)



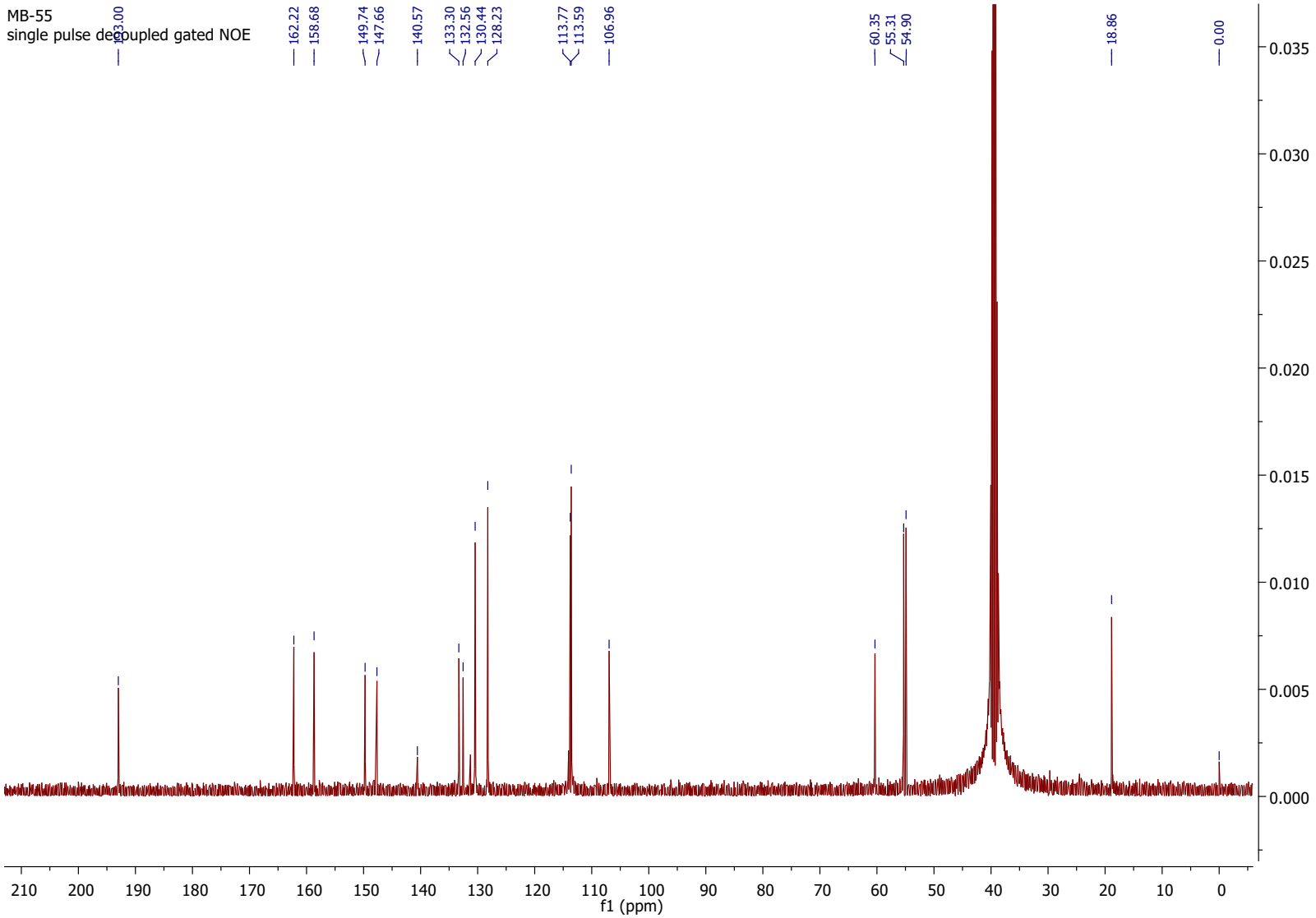
^{13}C NMR of (4''-Bromophenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5k)



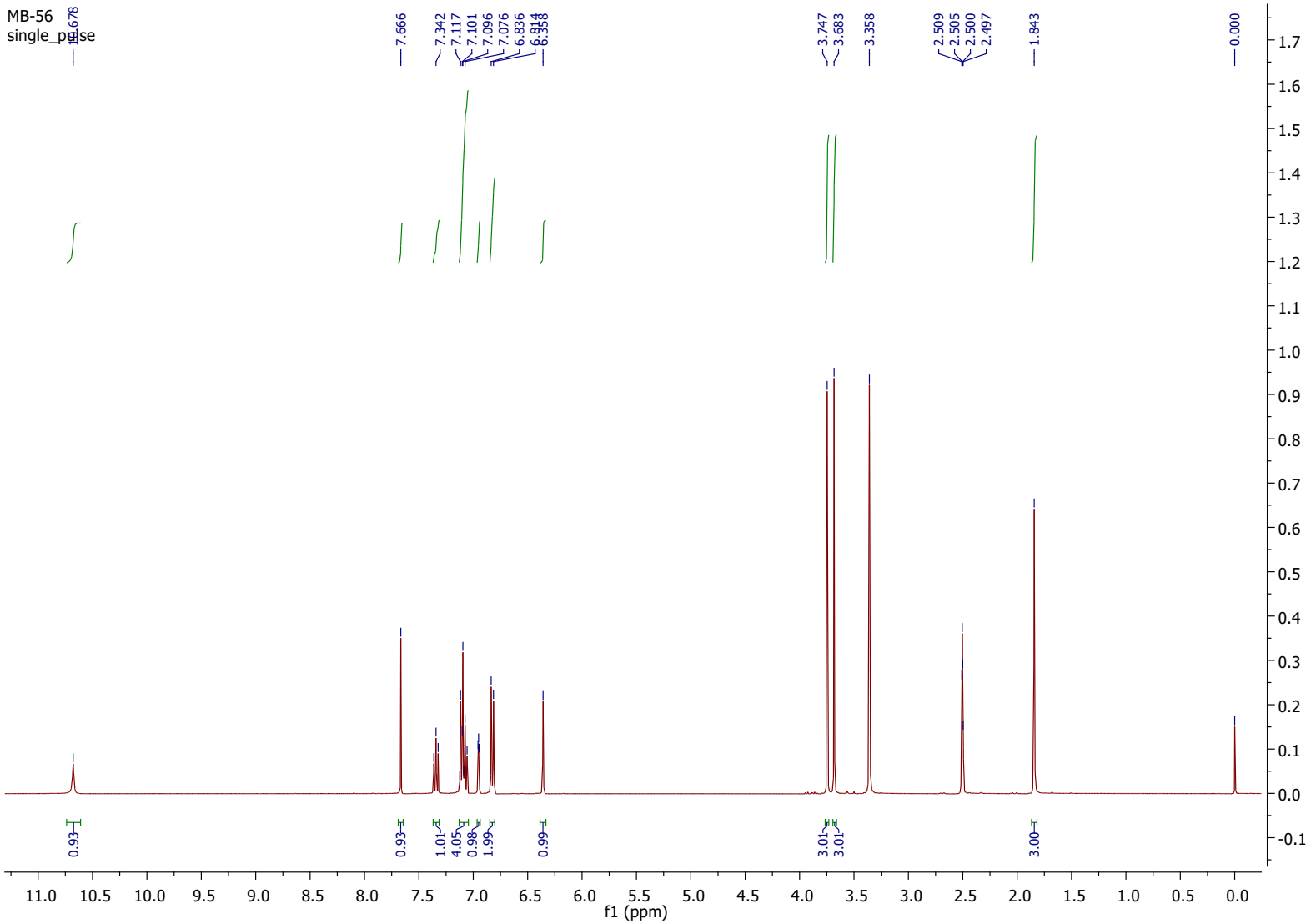
^{1}H NMR of (4''-Methoxyphenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5l)



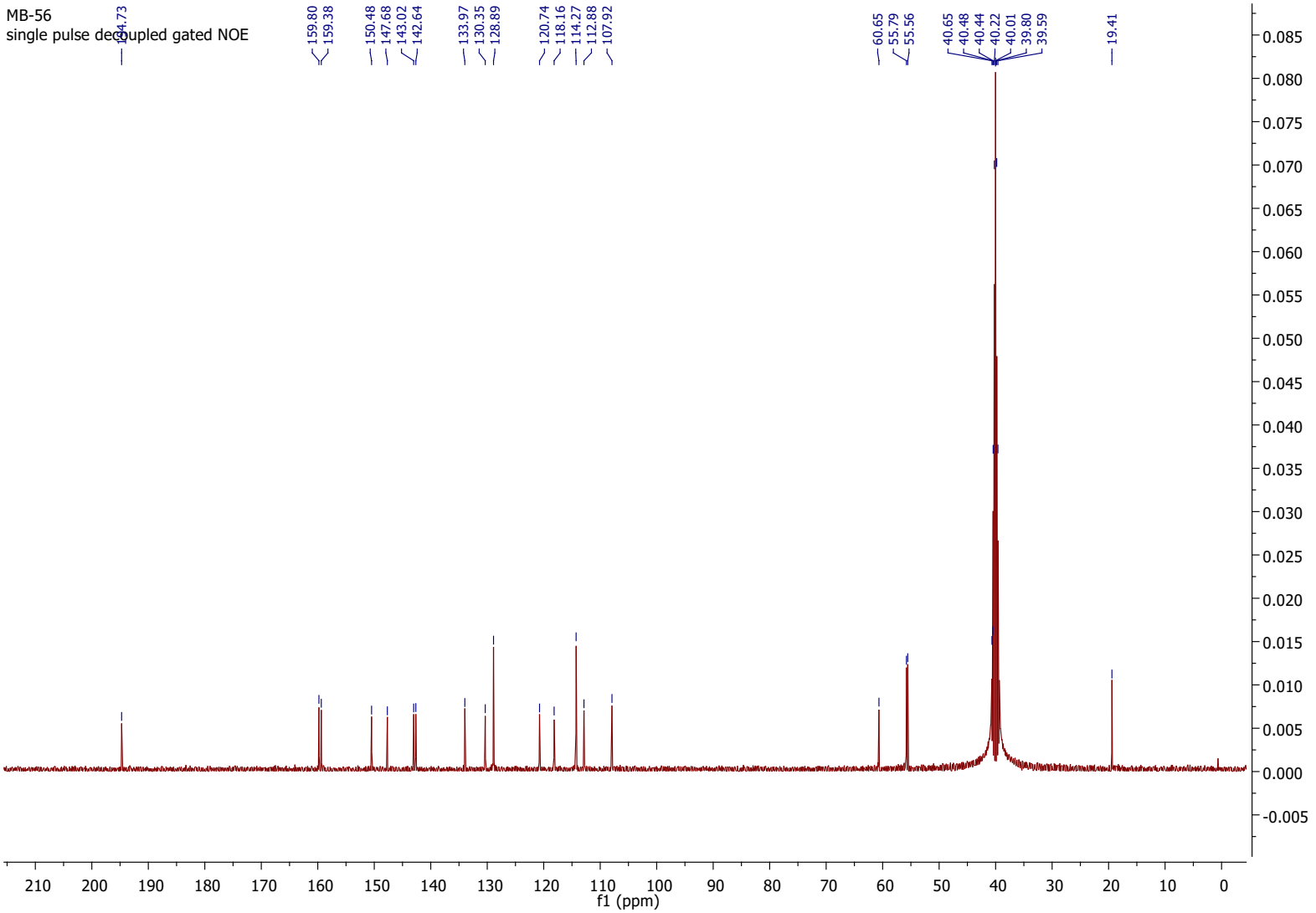
^{13}C NMR of (4''-Methoxyphenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5l)



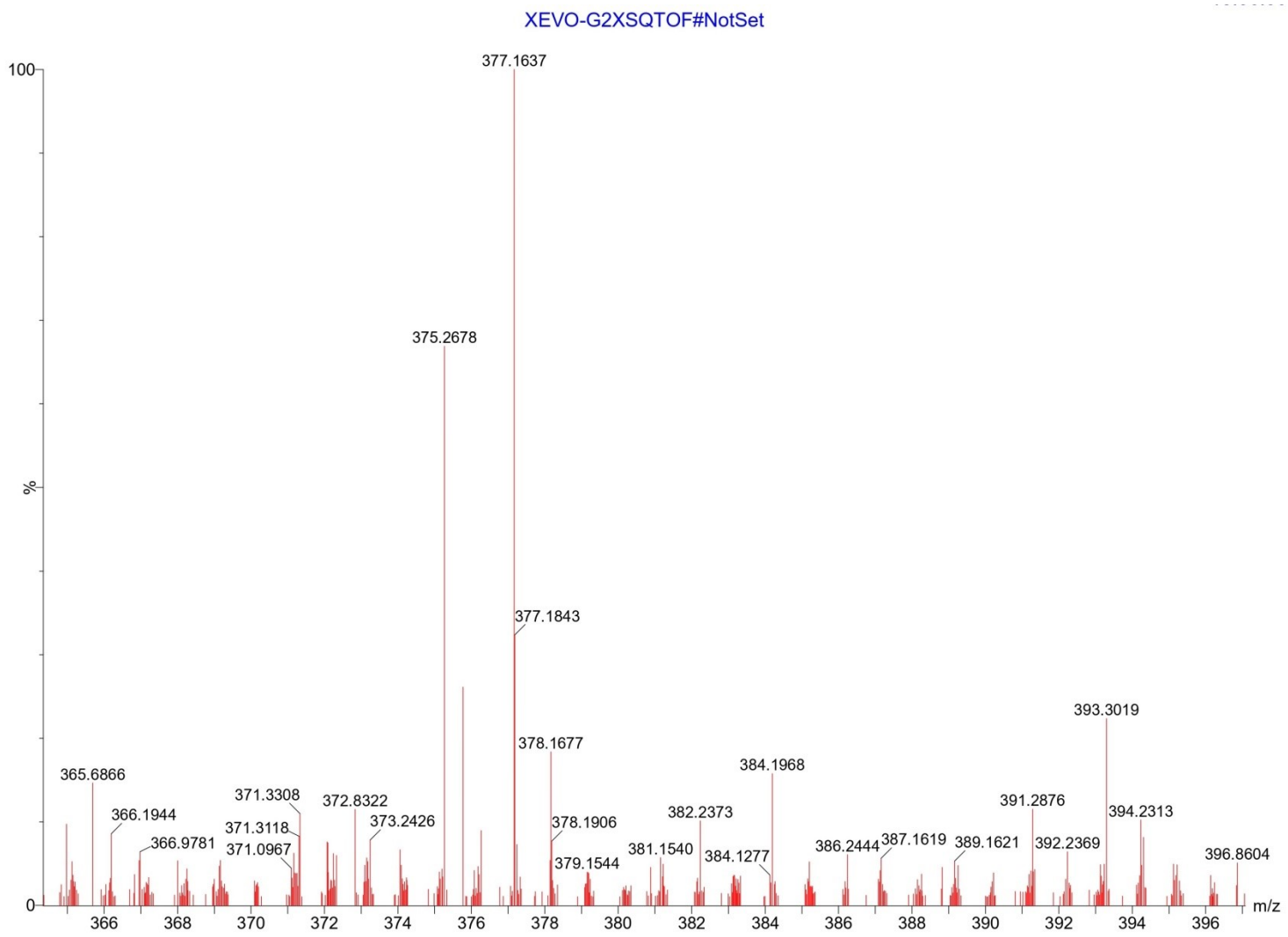
^{1}H NMR of (3"-Methoxyphenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5m)



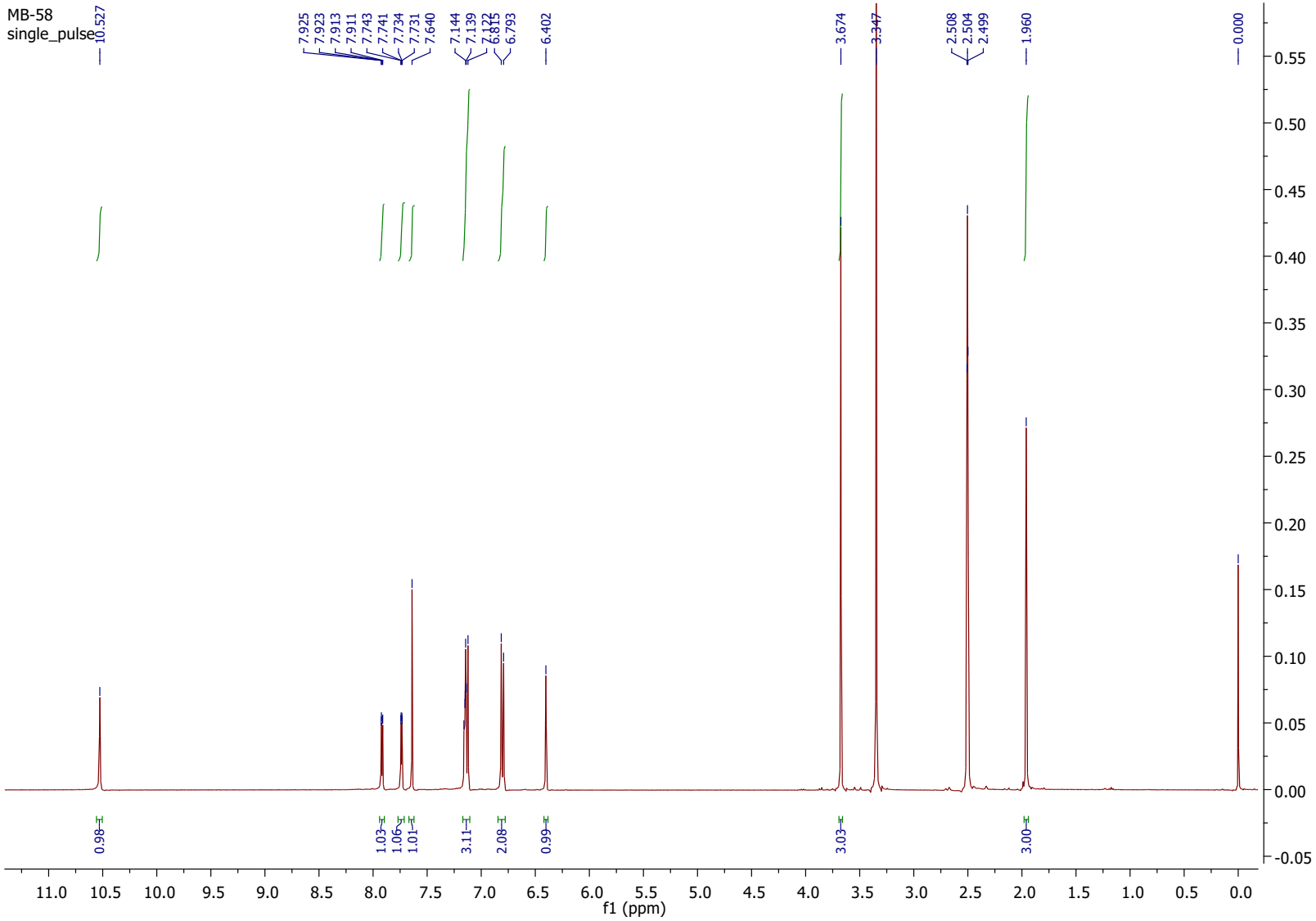
^{13}C NMR of (3''-Methoxyphenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5m)



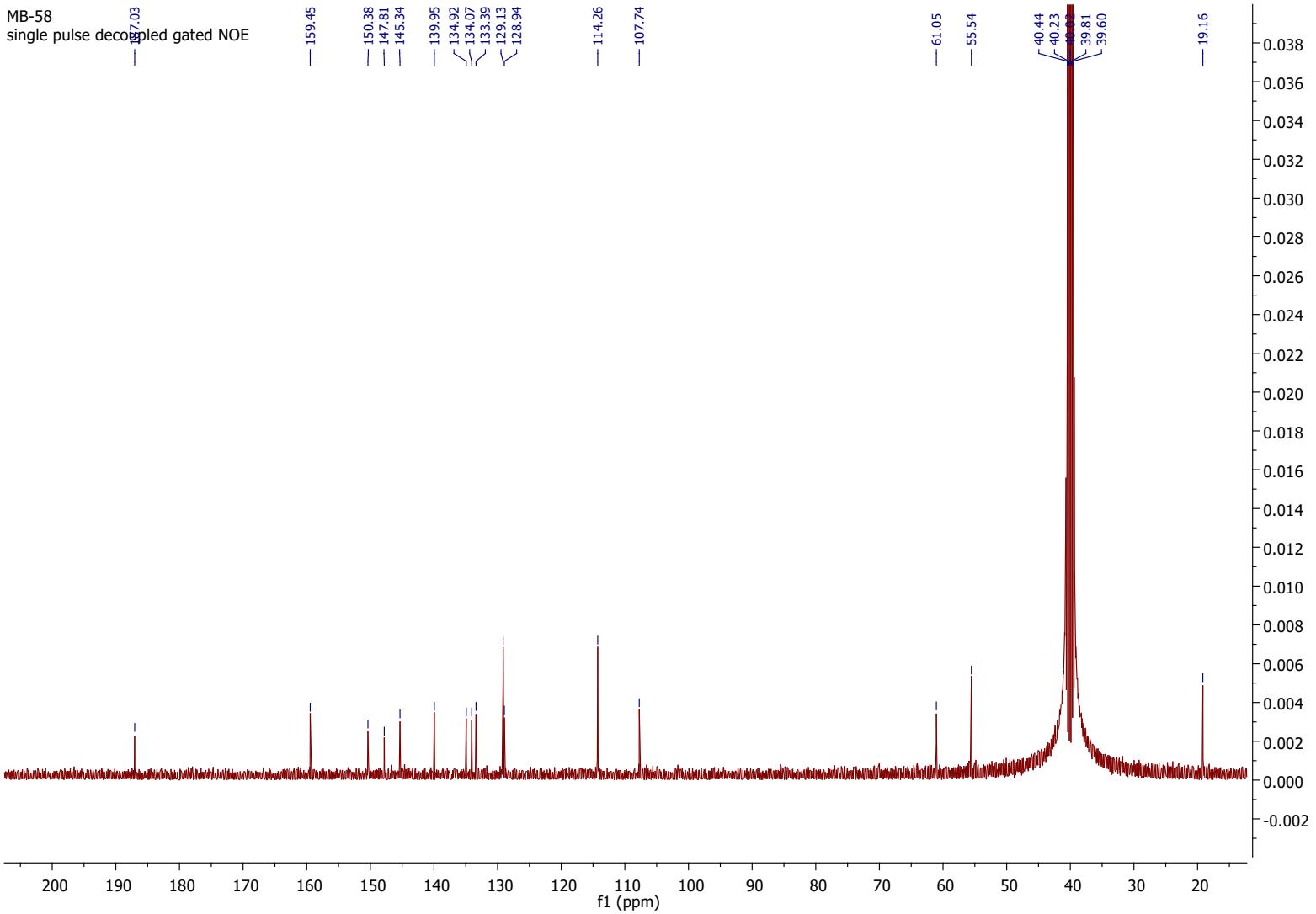
HRMS of (3''-Methoxyphenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5m)



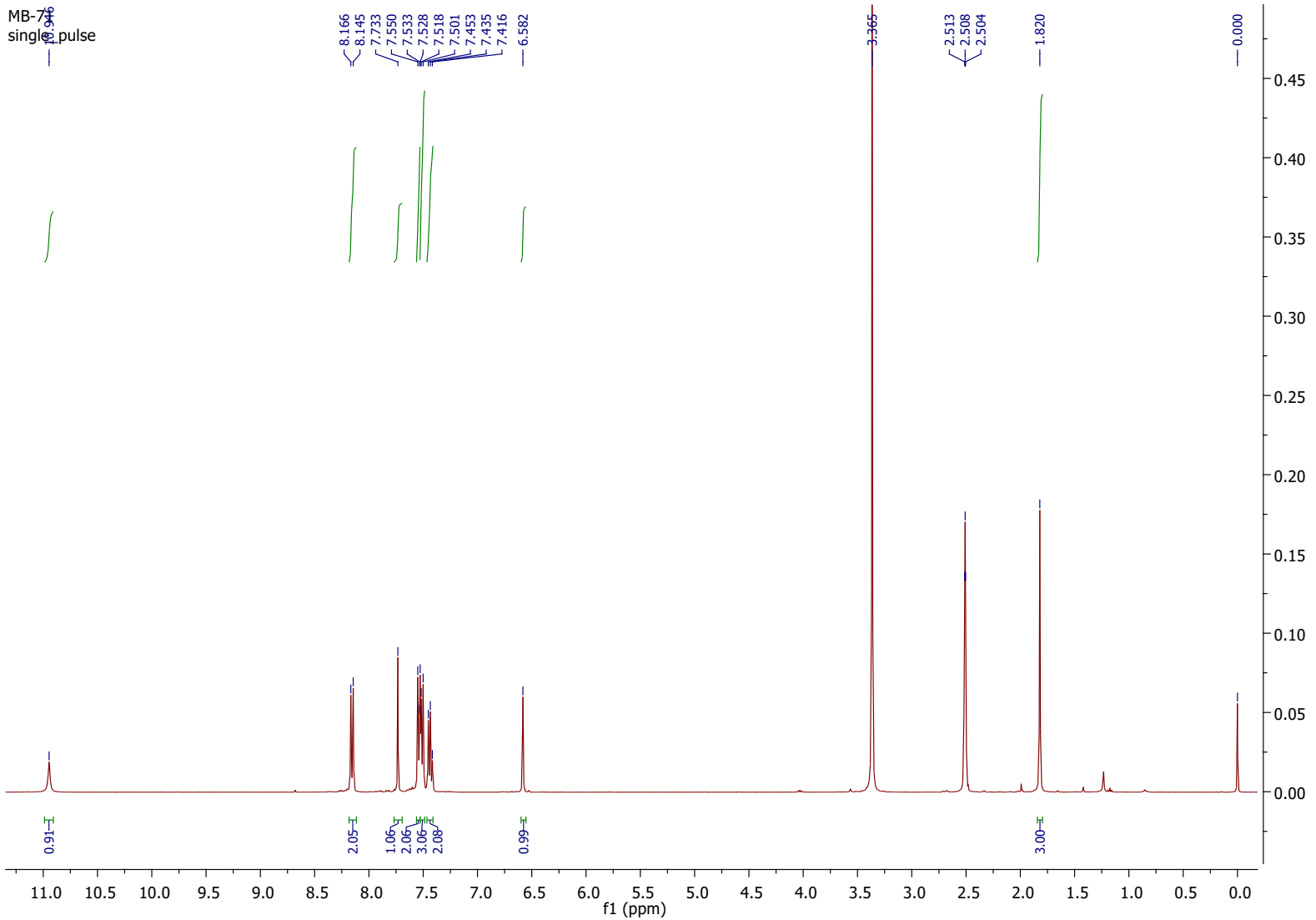
^{1}H NMR of (7-(4'-Methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(thiophen-2''-yl)methanone (5n)



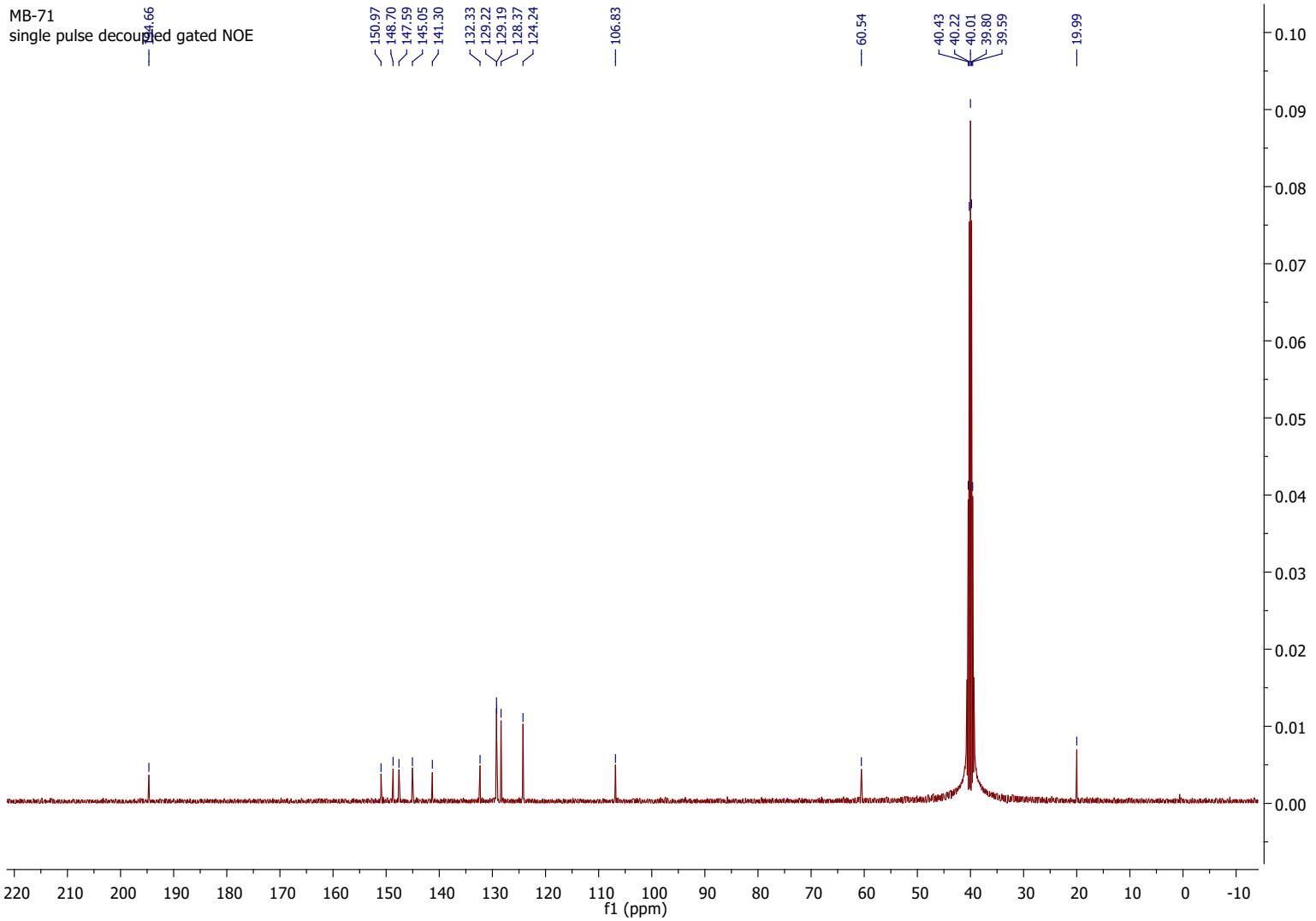
^{13}C NMR of (7-(4'-Methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(thiophen-2''-yl)methanone (5n)



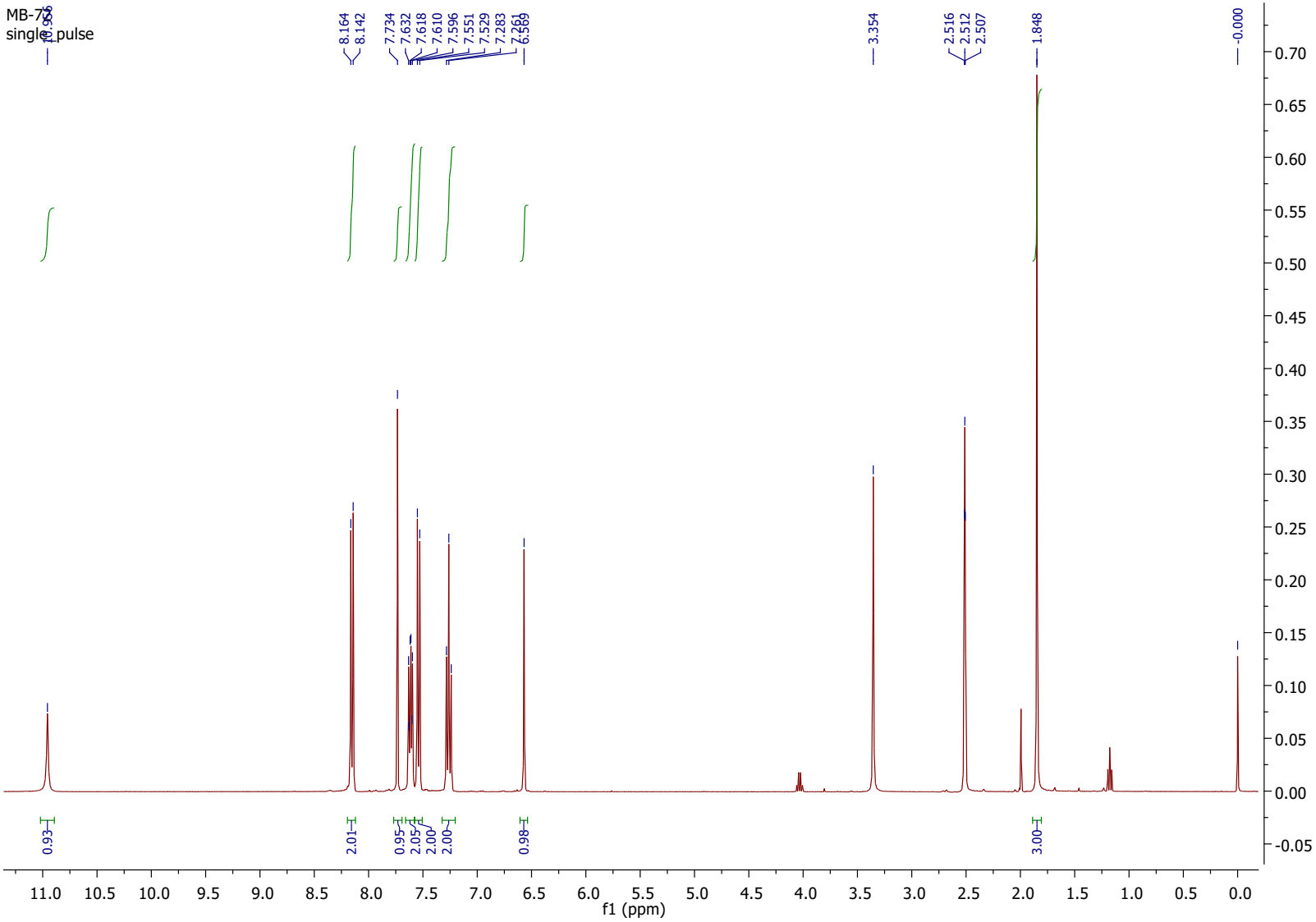
^{1}H NMR of (5-Methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(phenyl)methanone (5o)



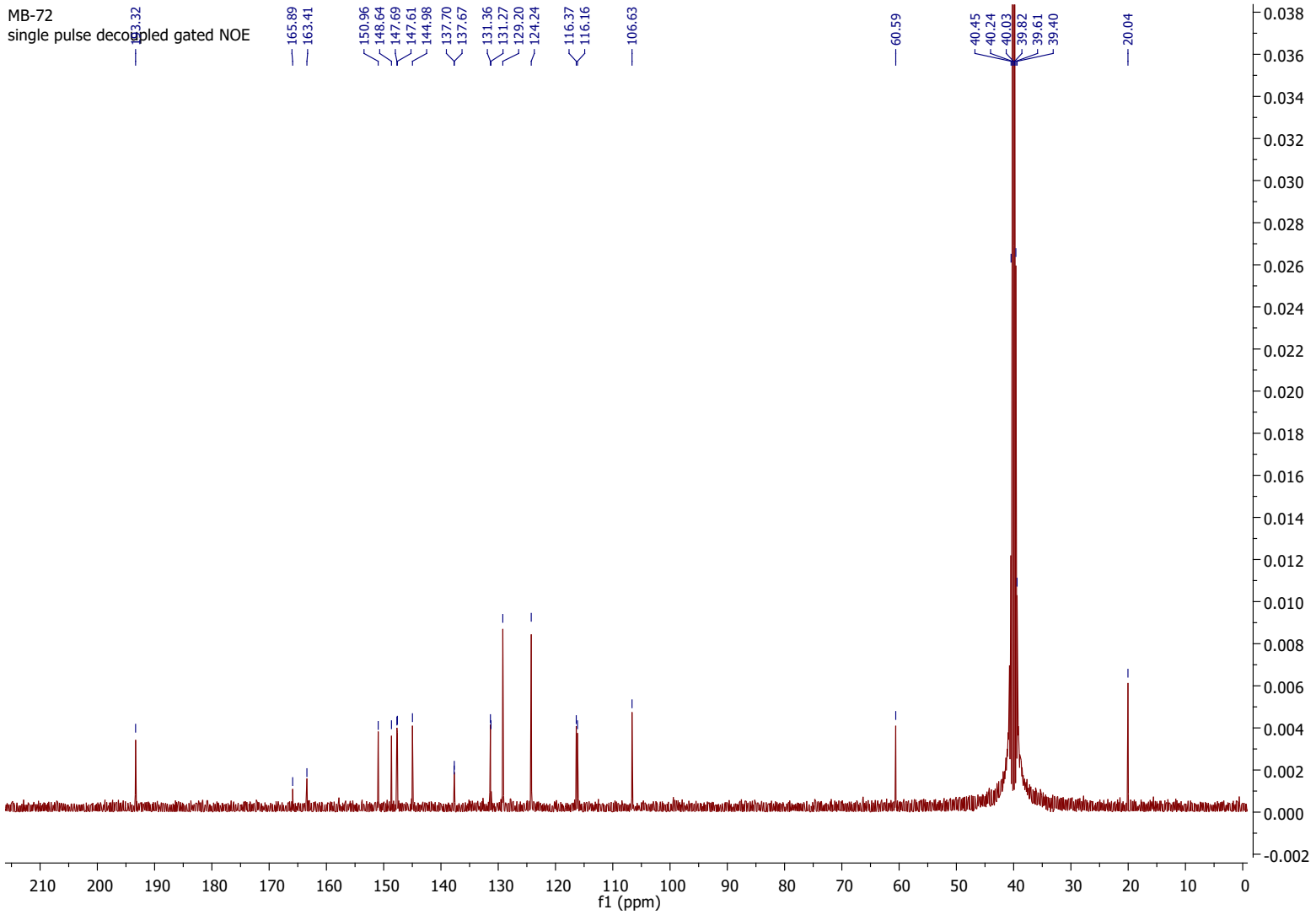
^{13}C NMR of (5-Methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(phenyl)methanone (5o)



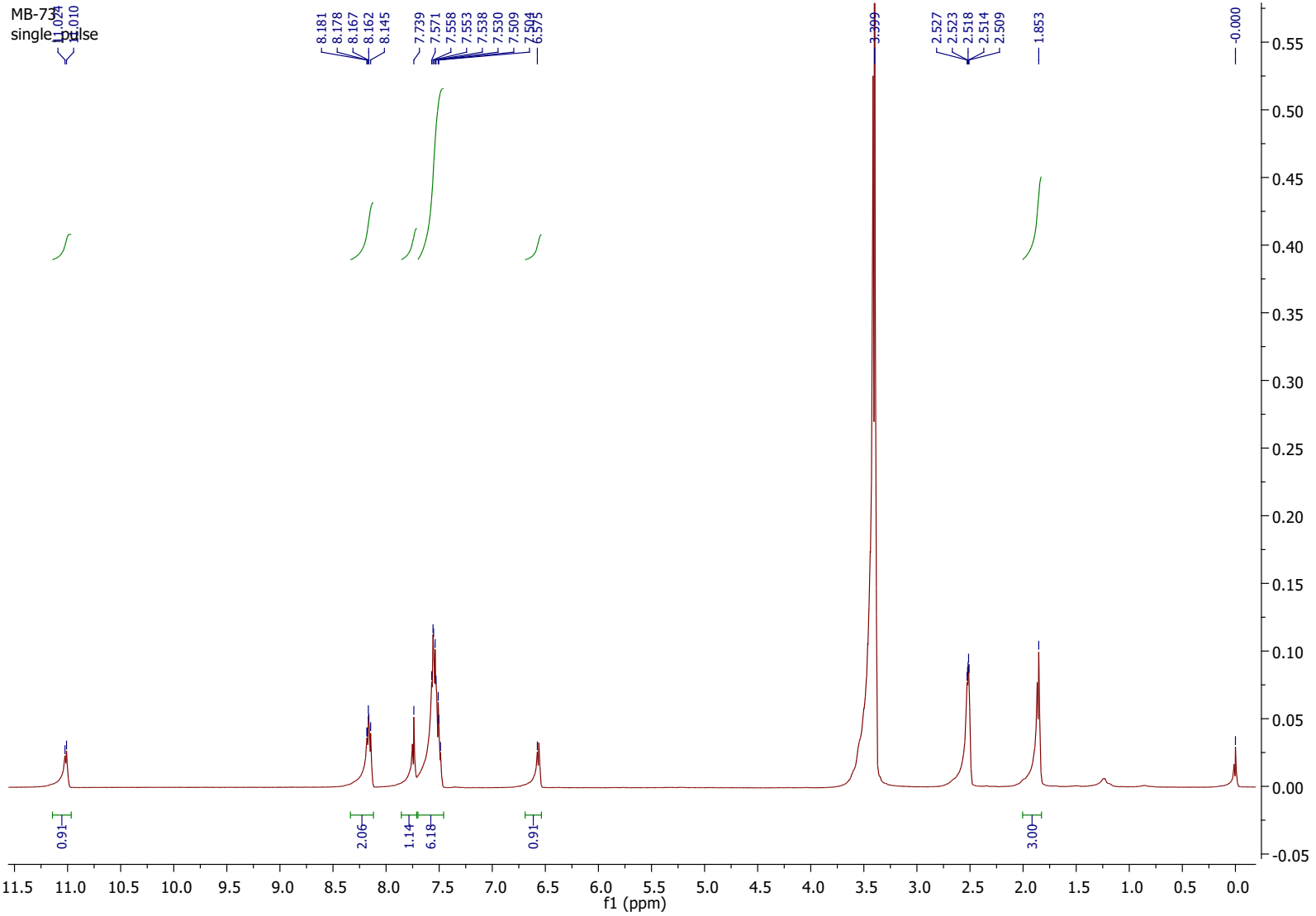
^{1}H NMR of (4''-Fluorophenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5p)



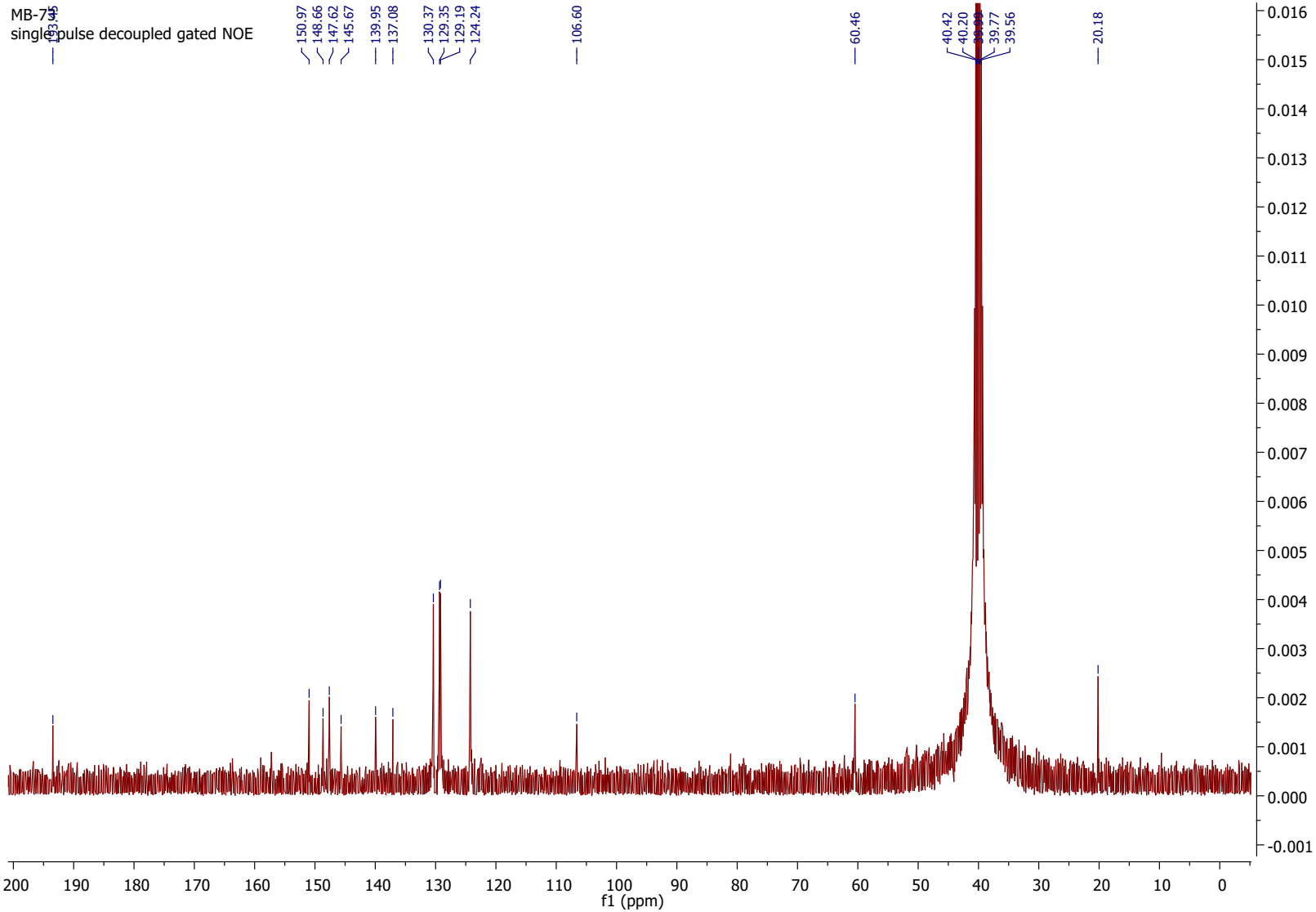
^{13}C NMR of (4''-Fluorophenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5p)



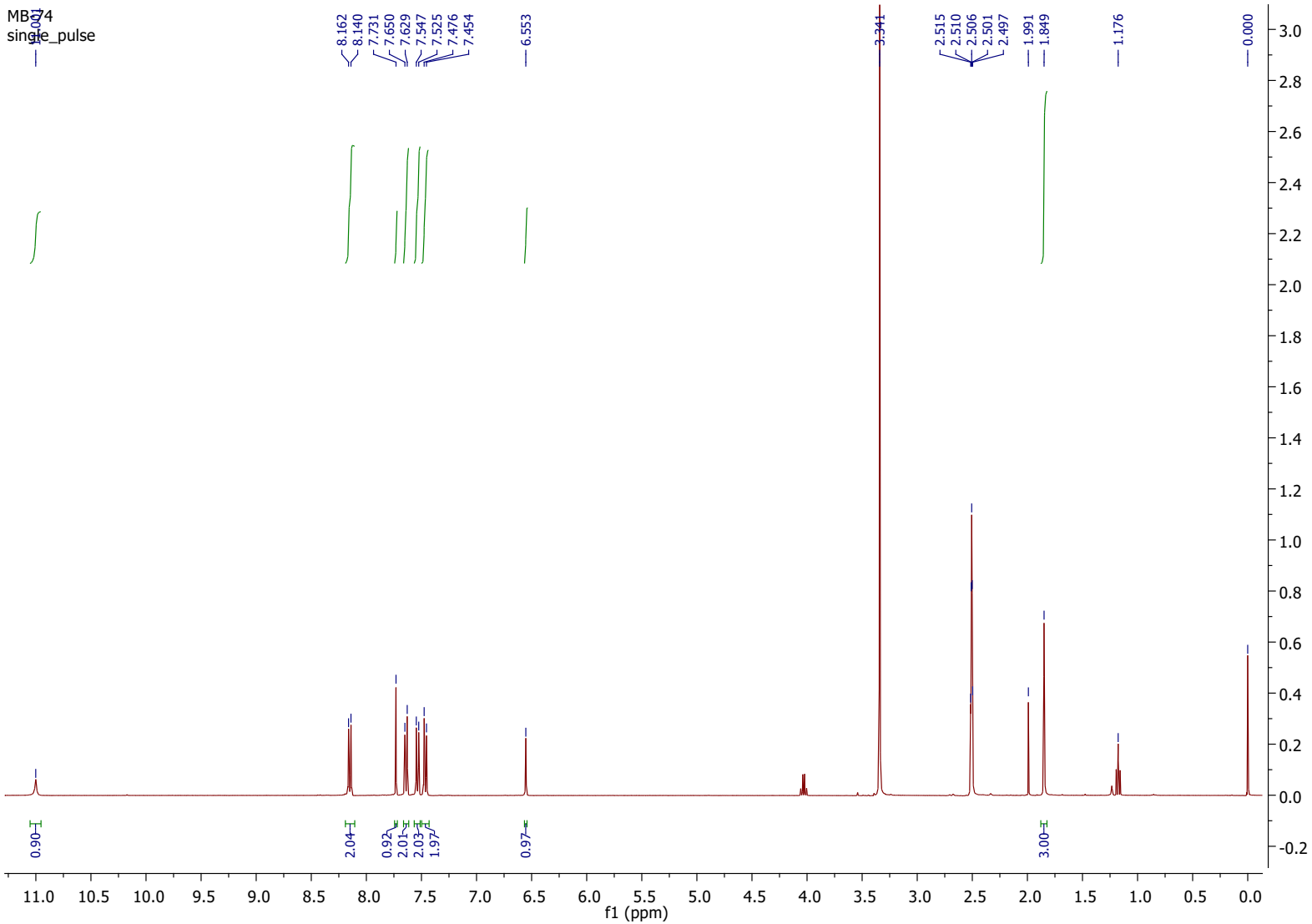
^{13}C NMR of (4''-Chlorophenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5q)



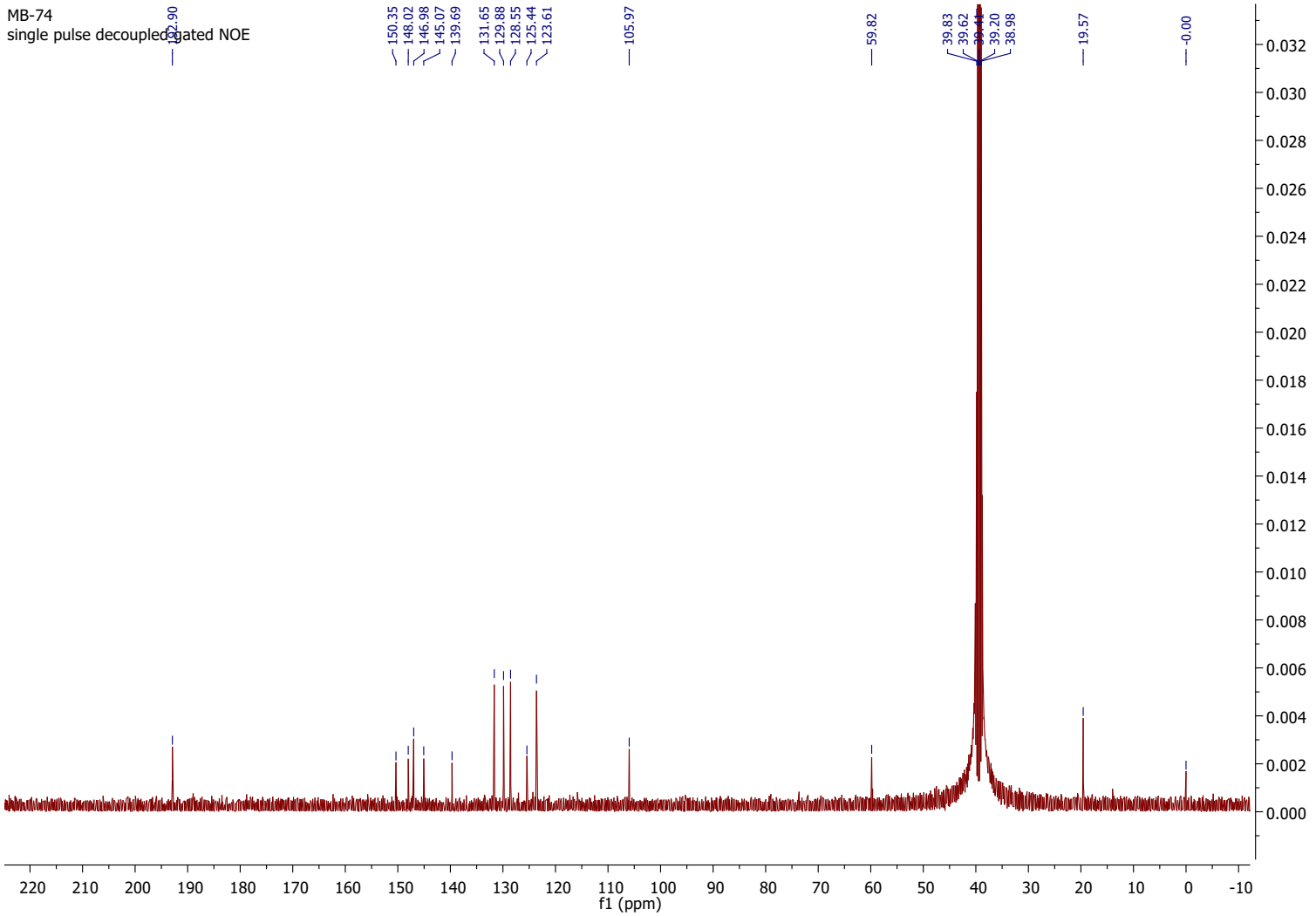
^{13}C NMR of (4''-Chlorophenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5q)



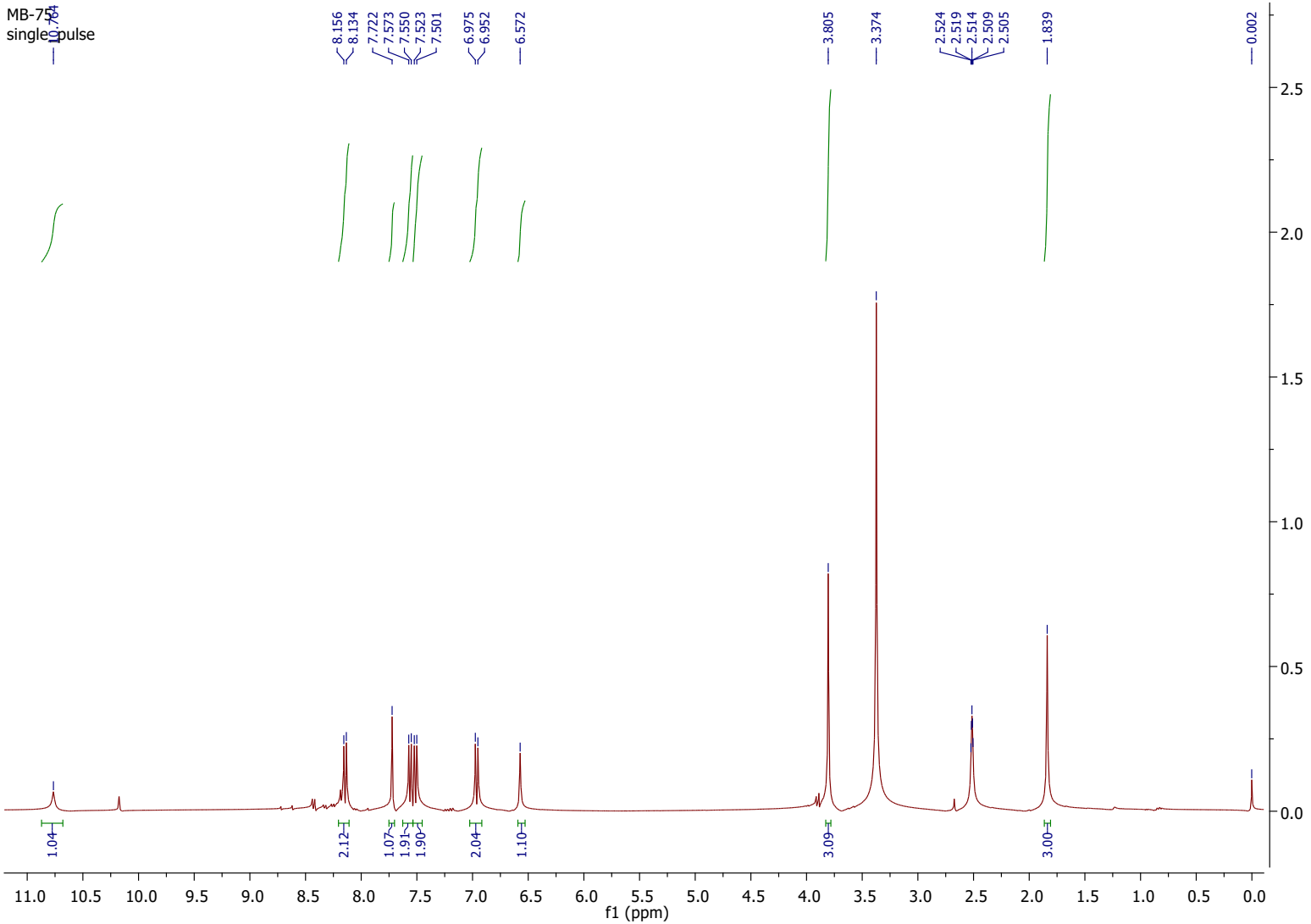
^{1}H NMR of (4"-Bromophenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5r)



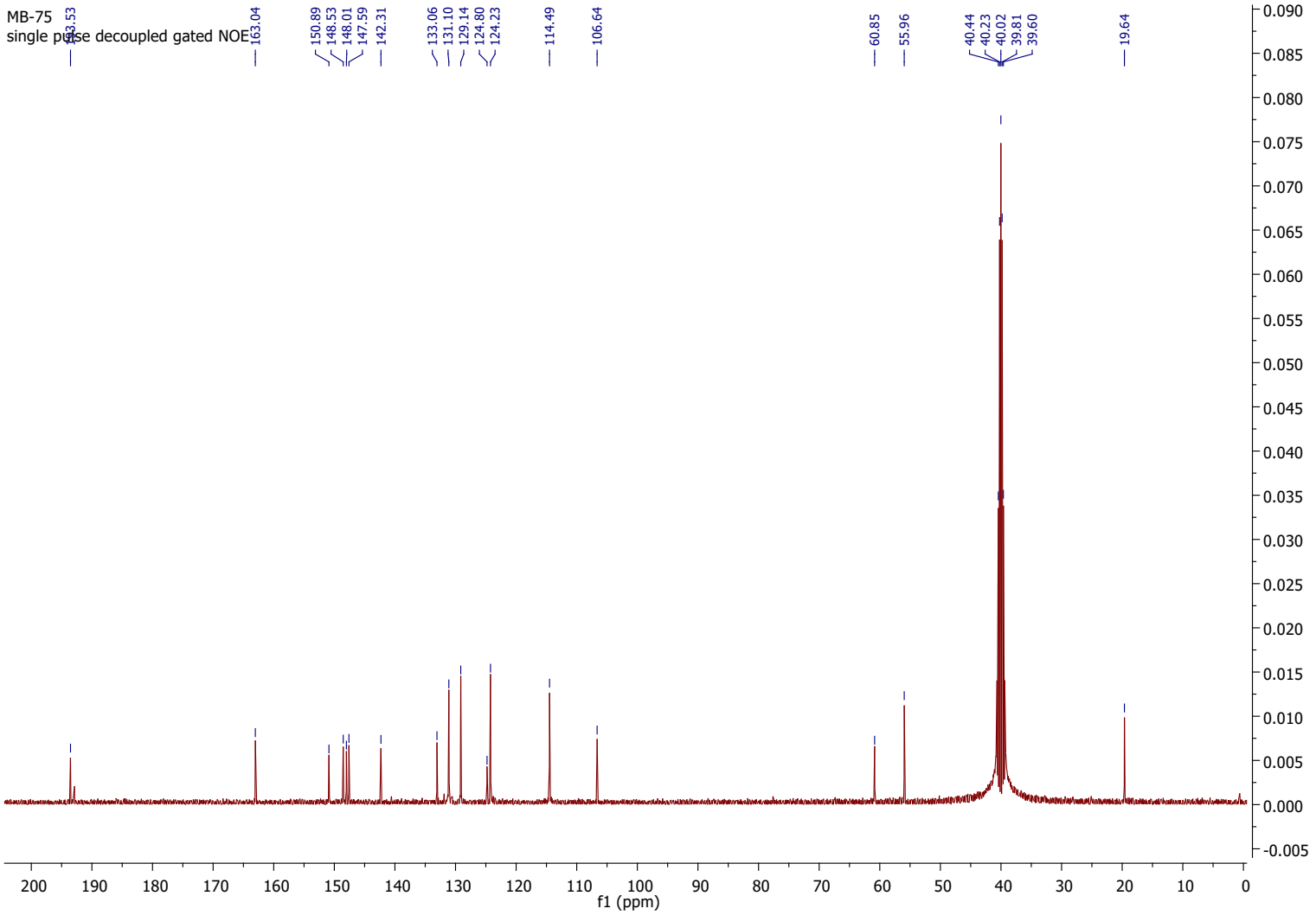
^{13}C NMR of (4"-Bromophenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5r)



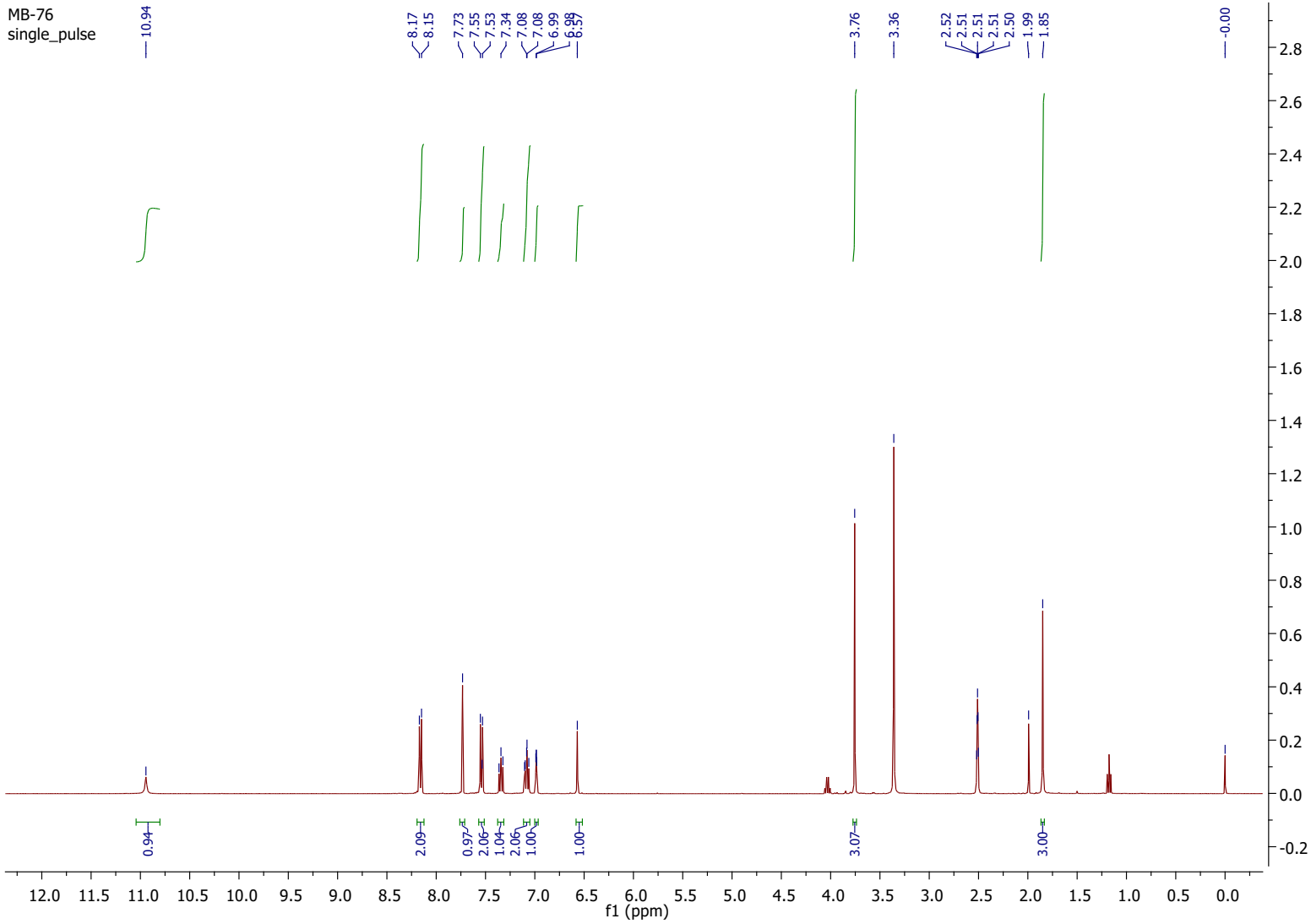
^{1}H NMR of (4''-Methoxyphenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5s)



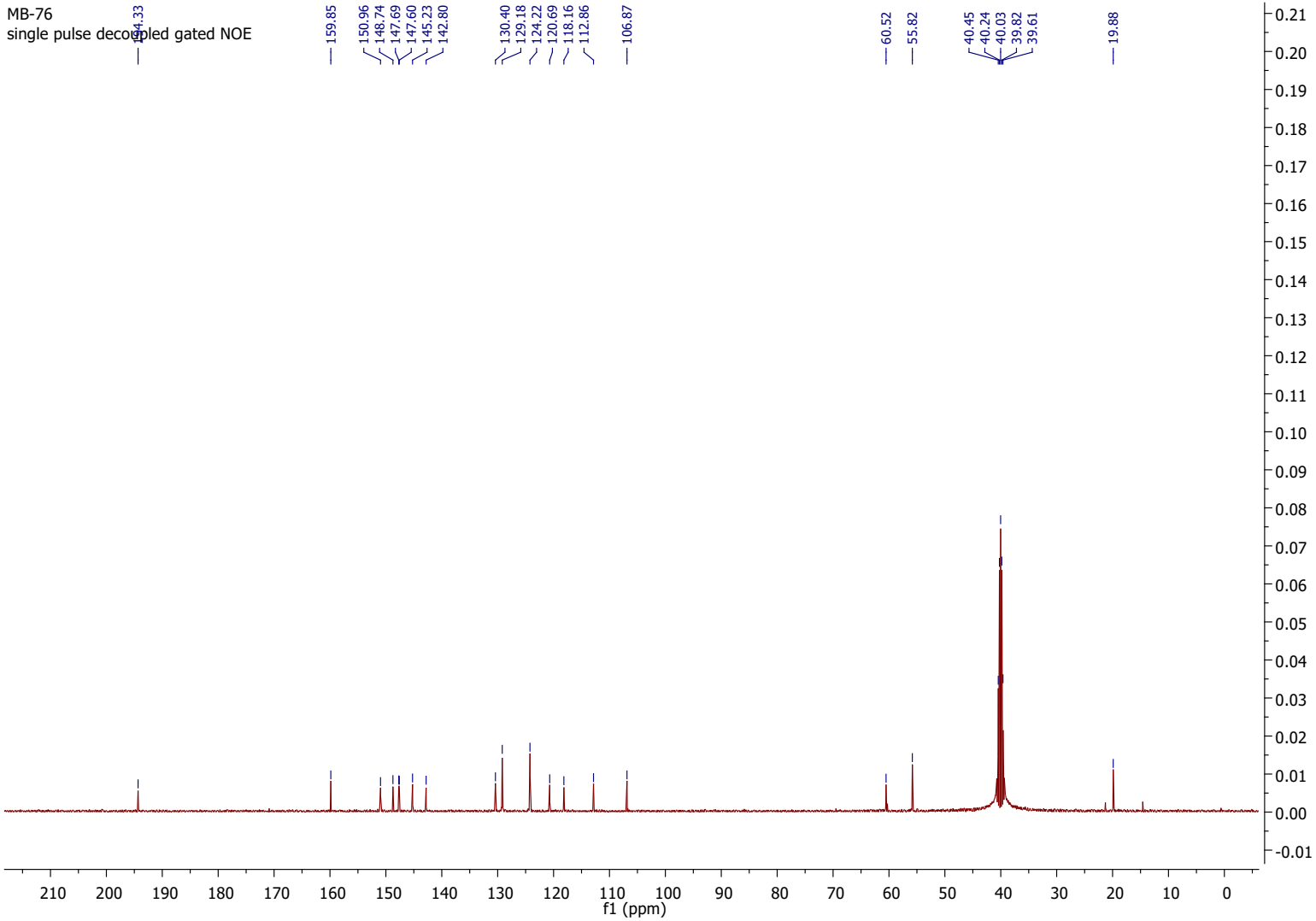
^{13}C NMR of (4"-Methoxyphenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5s)



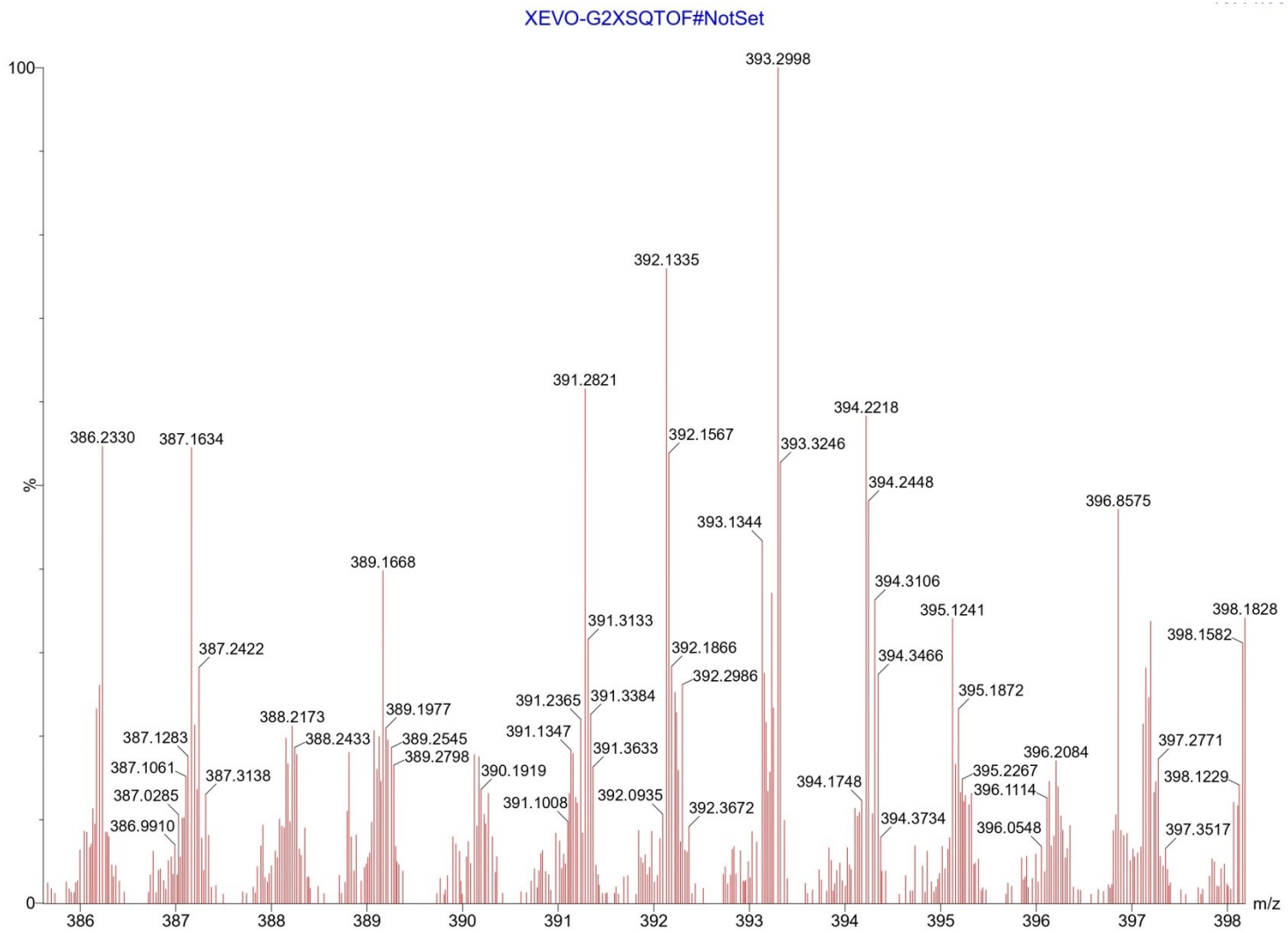
^{1}H NMR of (3"-Methoxyphenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5t)



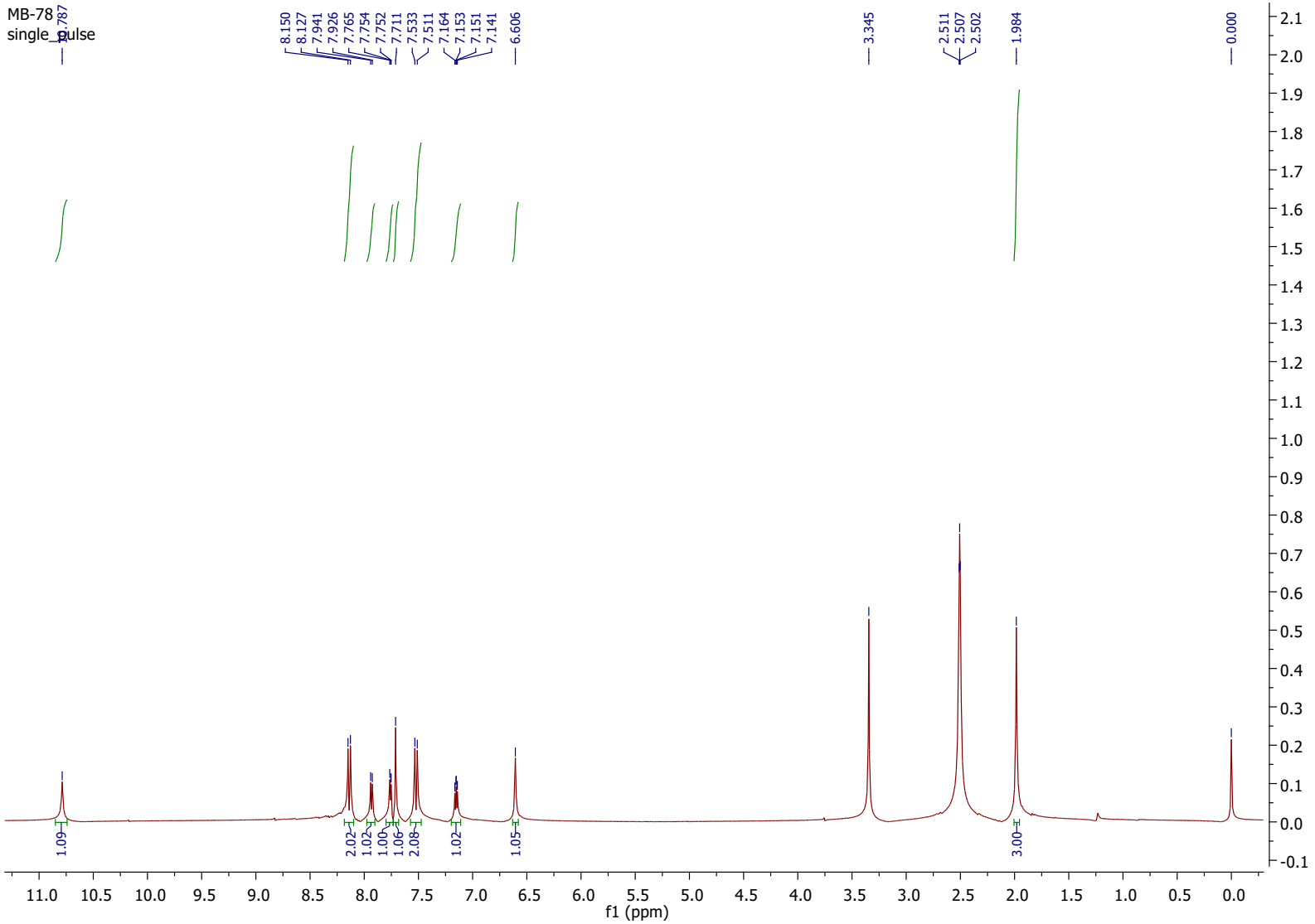
^{13}C NMR of (3''-Methoxyphenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5t)



HRMS of (3''-Methoxyphenyl)(5-methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5t)



^{1}H NMR of 5-Methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(thiophen-2''-yl)methanone (5u)



^{13}C NMR of 5-Methyl-7-(4'-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)(thiophen-2''-yl)methanone (5u)

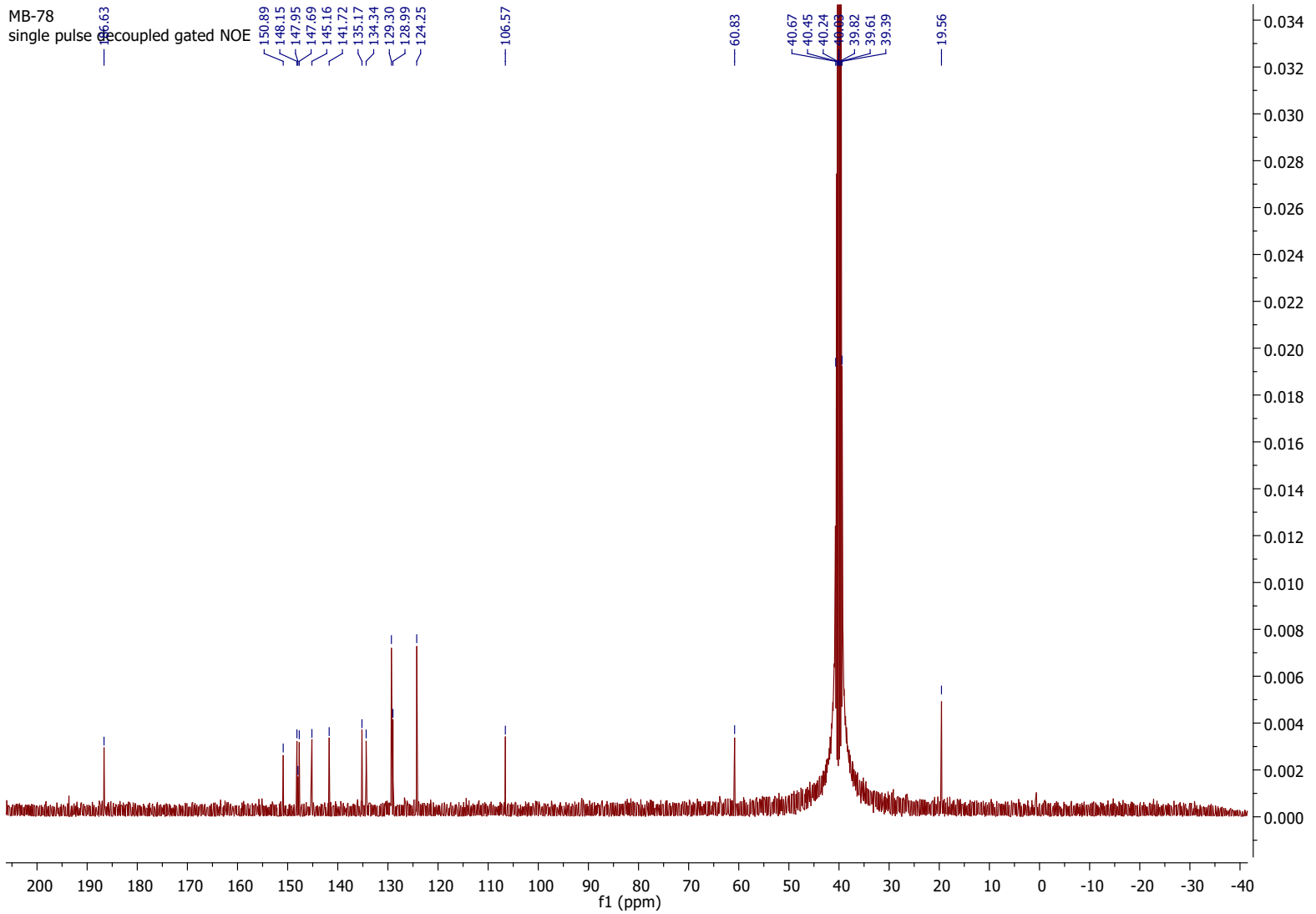


Fig. S1. ^{1}H-^{13}C HMBC NMR of (4"-Methoxyphenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5l)

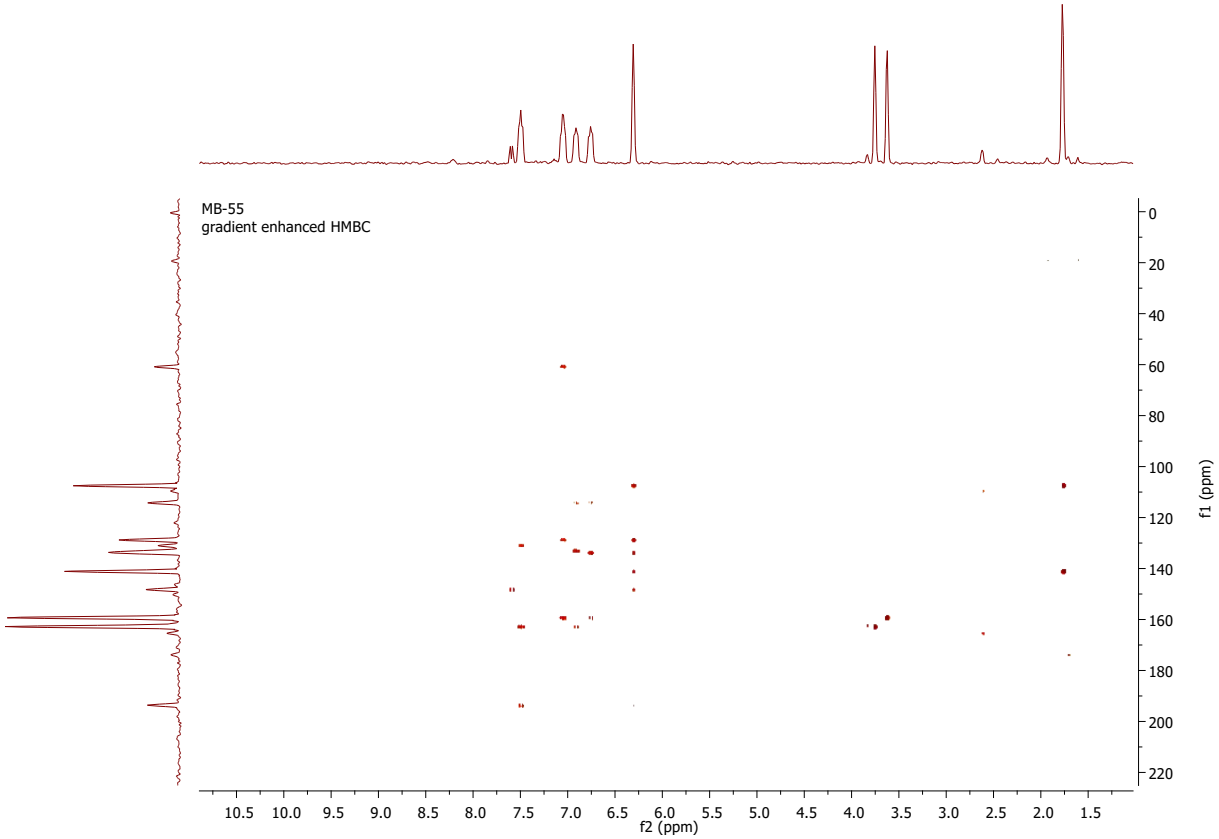


Fig. S2. ^{1}H-^{13}C HSQC NMR of (4''-Methoxyphenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5l)

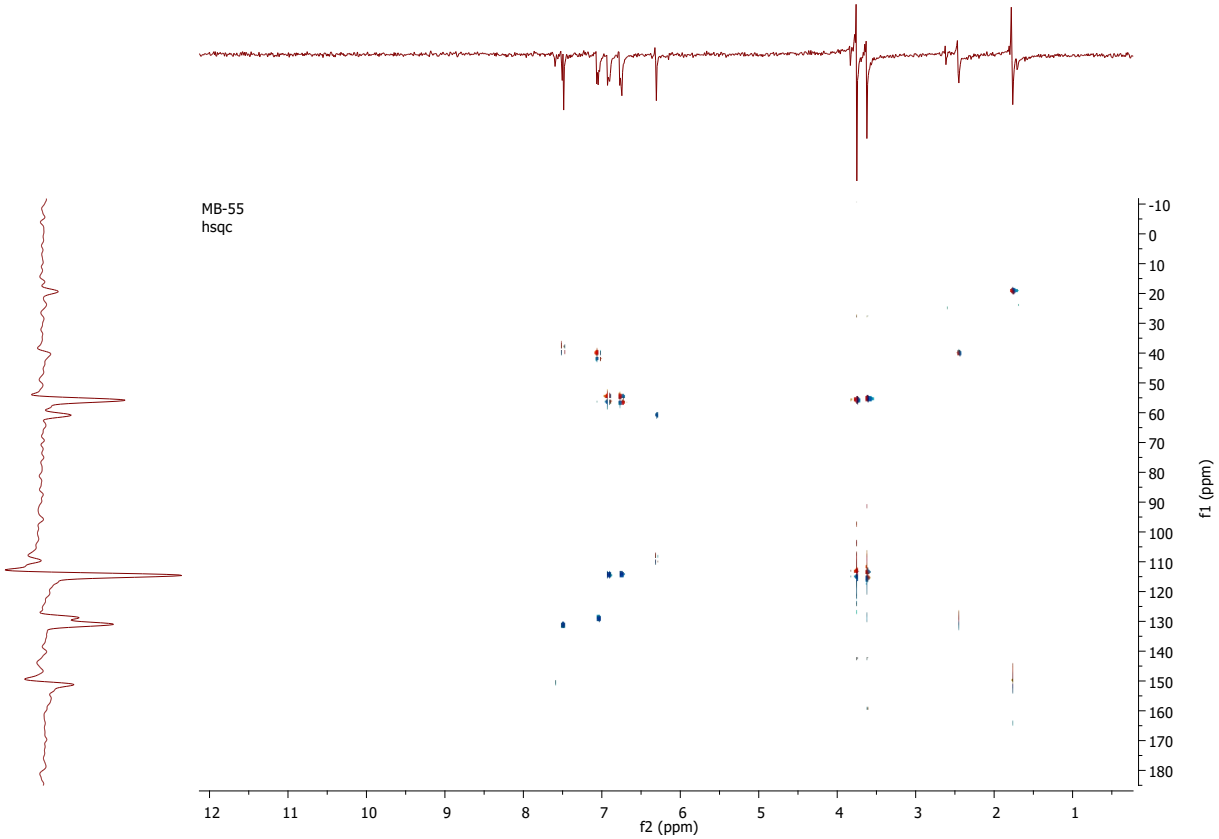


Fig. S3. ^{1}H-^{15}N HMBC NMR of (4''-Methoxyphenyl)(7-(4'-methoxyphenyl)-5-methyl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidin-6-yl)methanone (5l)