

# Supplementary Materials: Comparative Interactions of Dihydroquinazolin Derivatives with Human Serum Albumin Observed via Multiple Spectroscopy

Yi Wang <sup>1,2</sup>, Meiqing Zhu <sup>1</sup>, Jia Liu <sup>1,3</sup>, Risong Na <sup>1,3</sup>, Feng Liu <sup>2</sup>, Xiangwei Wu <sup>1</sup>, Shisuo Fan <sup>1</sup>, Zhen Wang <sup>1</sup>, Dandan Pan <sup>1</sup>, Jun Tang <sup>1</sup>, Qing X. Li <sup>4</sup>, Rimaohua <sup>1,\*</sup> and Shangzhong Liu <sup>2,\*</sup>

<sup>1</sup> Department of Science of Pesticides, School of Resources and Environment, Anhui Agricultural University, No. 130 Changjiang West Road, Hefei 230036, China; wangyi@ahau.edu.cn (Y.W.); zhumeiqing@ahau.edu.cn (M.Z.); ljia198346@163.com (J.L.); risongna@163.com (R.N.); wxw@ahau.edu.cn (X.W.); fanshisuo@ahau.edu.cn (S.F.); zwang@ahau.edu.cn (Z.W.); dandanpan@ahau.edu.cn (D.P.); tangjun@ahau.edu.cn (J.T.)

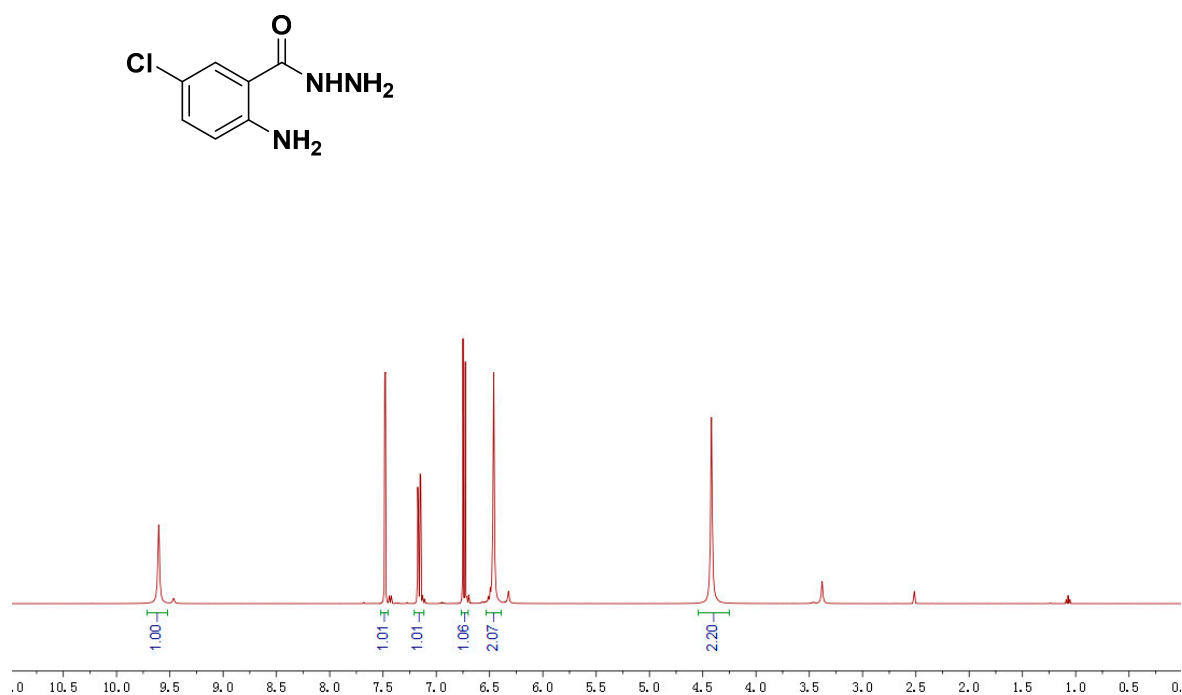
<sup>2</sup> Department of Applied Chemistry, China Agricultural University, No. 2 Yuanmingyuan West Road, Beijing 100193, China; caulf0527@163.com

<sup>3</sup> Collaborative Innovation Center of Henan Grain Crops, National Key Laboratory of Wheat and Maize Crop Science, College of Plant Protection, Henan Agricultural University, Wenhua Road NO. 95, Zhengzhou 450002, China

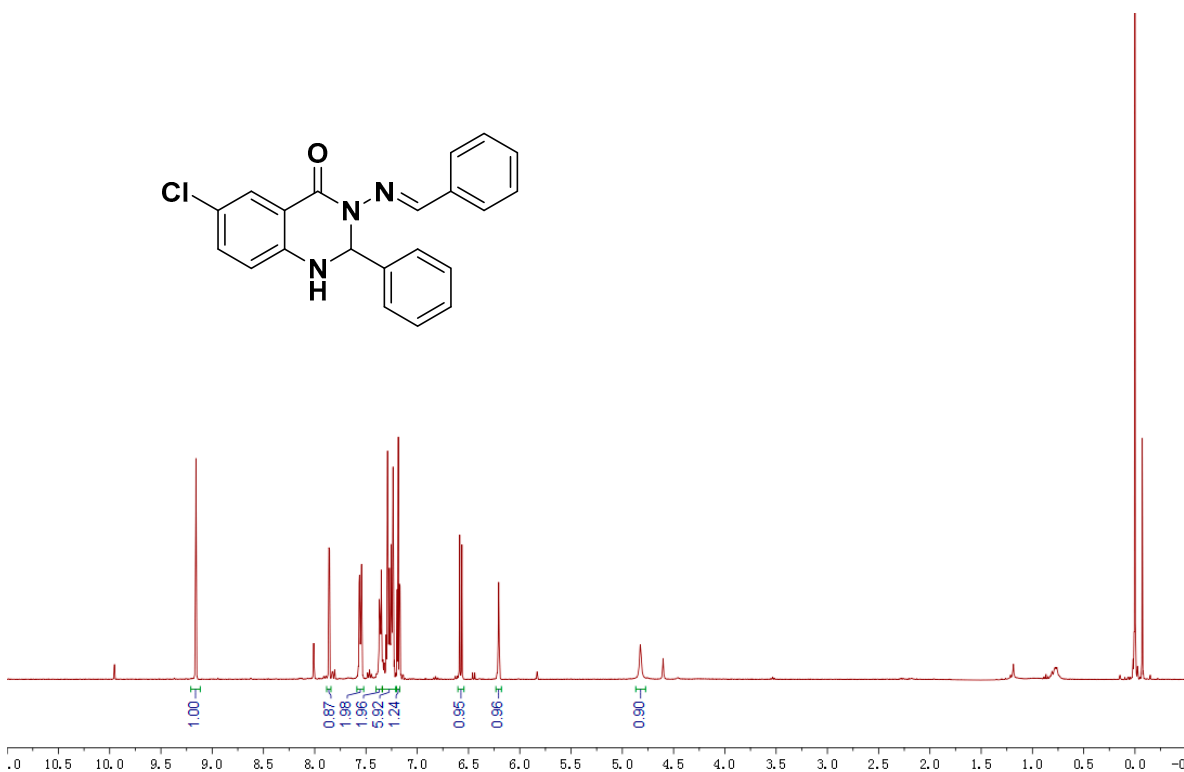
<sup>4</sup> Department of Molecular Biosciences and Bioengineering, University of Hawaii at Manoa, Honolulu, HI 96822, USA; qingl@hawaii.edu (Q.X.L.)

\* Correspondence: rimaohua@ahau.edu.cn (R.H.); shangzho@cau.edu.cn (S.L.); Tel./Fax: +86-0551-6578-6320 (R.H.); +86-010-6273-1010 (S.L.)

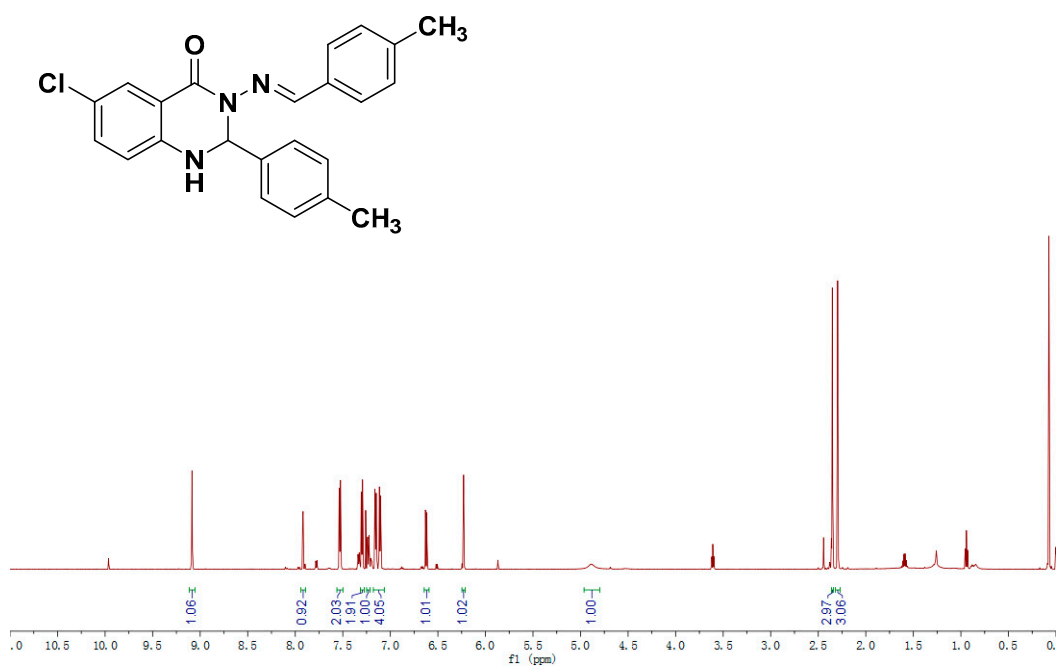
Table of contents	Page No.
1. <sup>1</sup> H NMR spectrum of intermediates compounds.....	2-5
2. <sup>1</sup> H & <sup>13</sup> C NMR spectrum of target compound.....	6-11



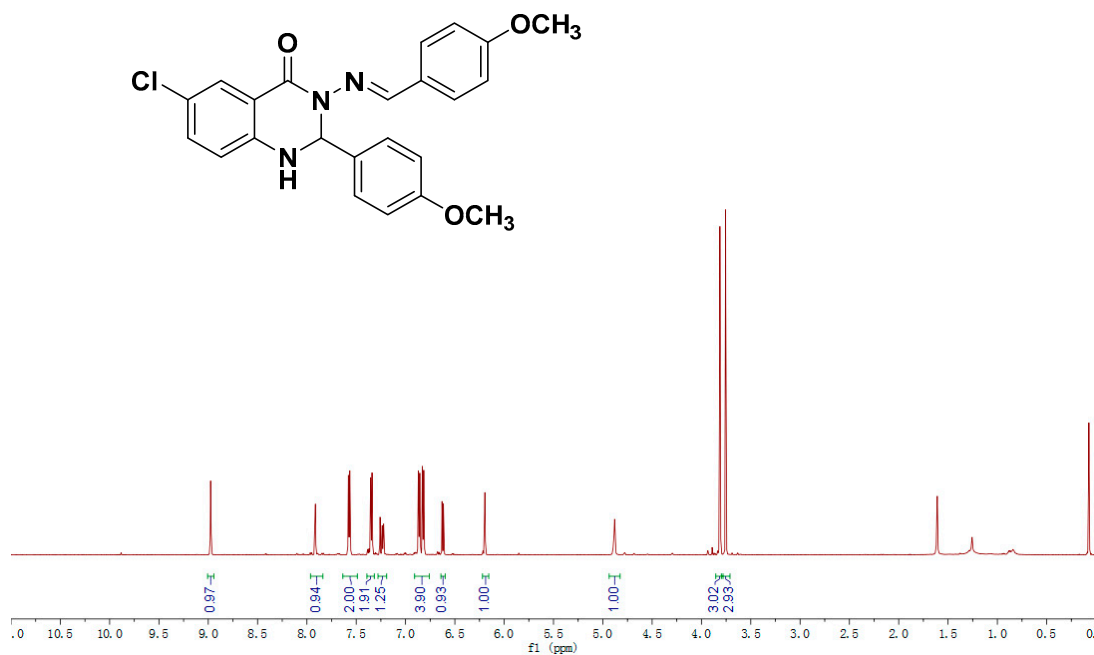
**Spectrum 1.1: <sup>1</sup>H NMR spectrum of 2-Amino-5-chlorobenzohydrazide (1).**



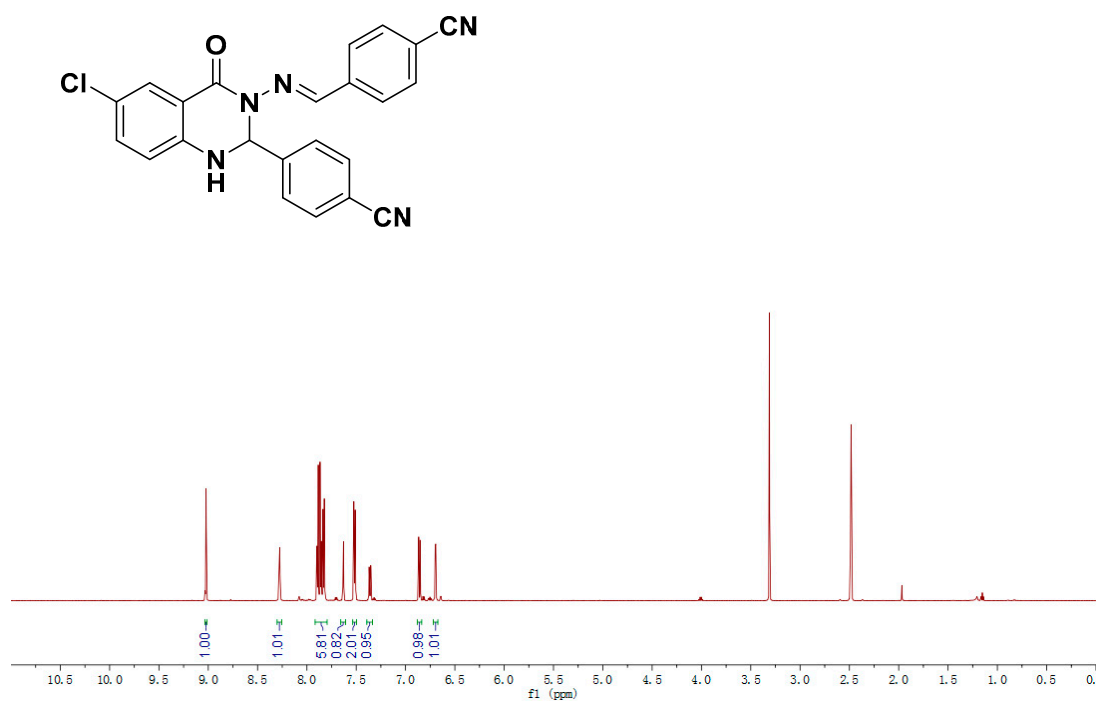
**Spectrum 1.2: <sup>1</sup>H NMR spectrum of 3-(Benzylideneamino)-6-chloro-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (2a).**



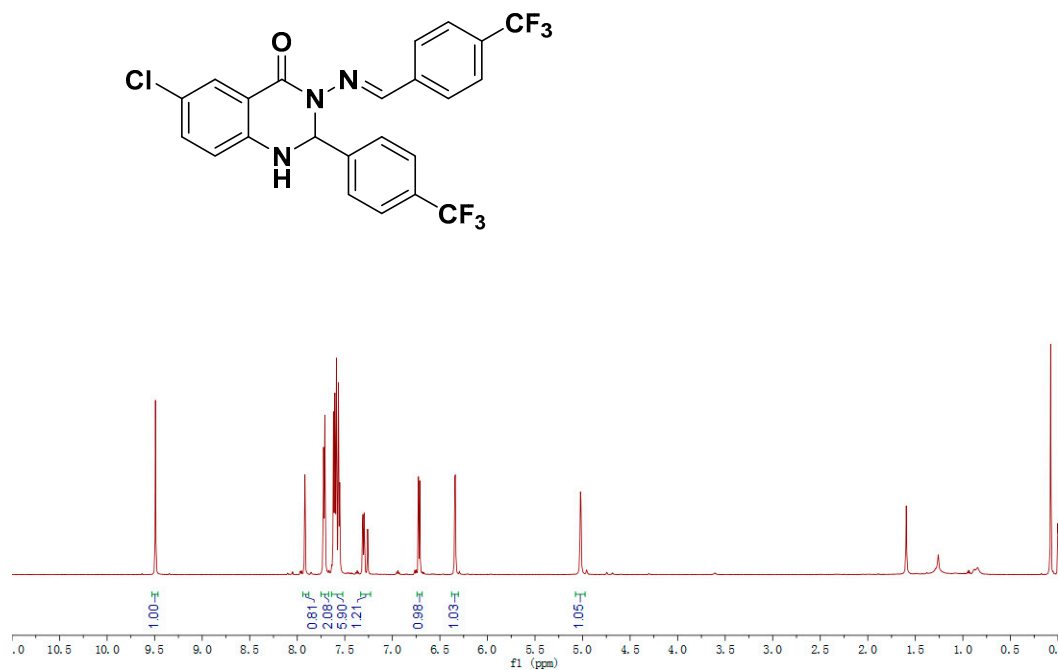
**Spectrum 1.3: <sup>1</sup>H NMR spectrum of 6-chloro-3-((4-methylbenzylidene)amino)-2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one (2b).**



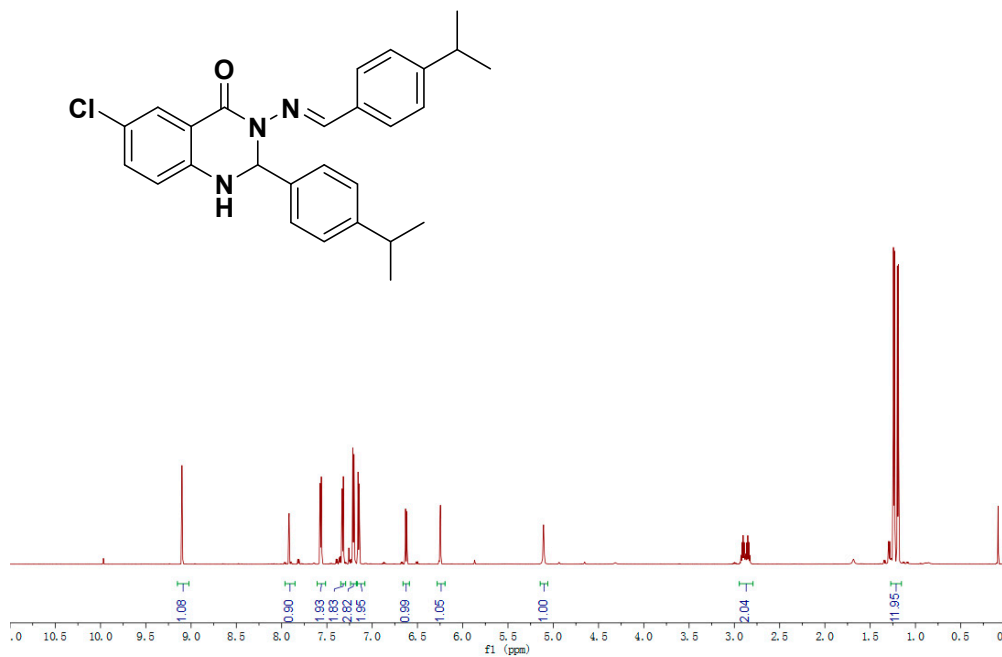
**Spectrum 1.4: <sup>1</sup>H NMR spectrum of 6-chloro-3-((4-methoxybenzylidene)amino)-2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (2c).**



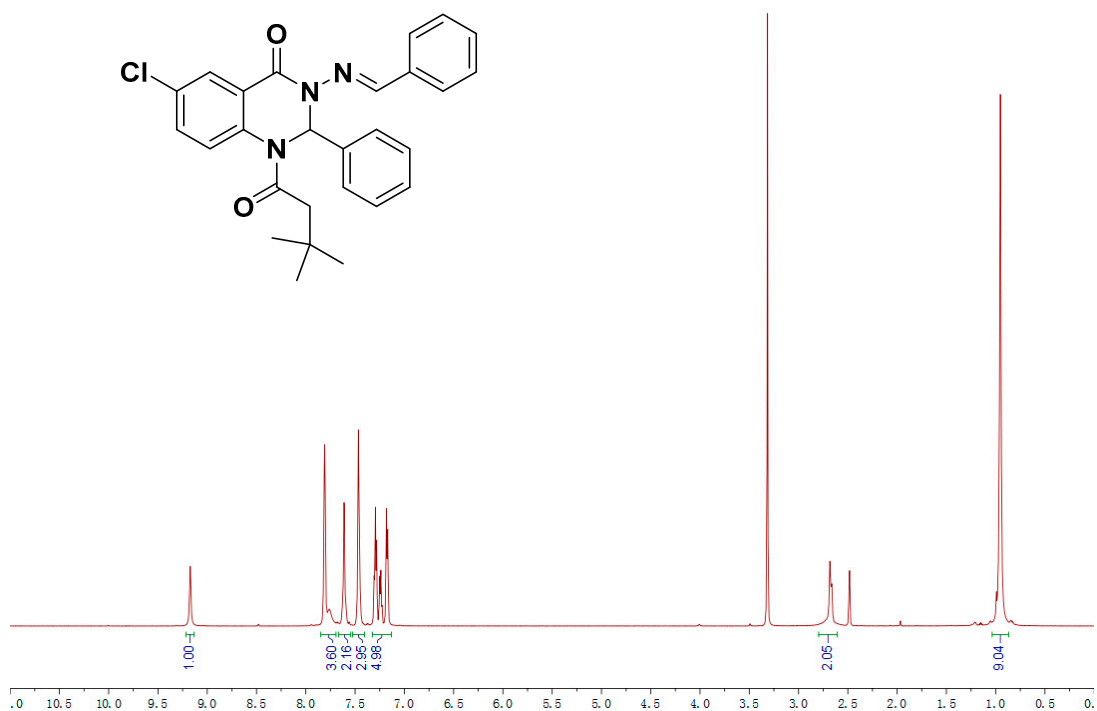
**Spectrum 1.5: <sup>1</sup>H NMR spectrum of 4-(((6-chloro-2-(4-cyanophenyl)-4-oxo-1,4-dihydroquinazolin-3(2H)-yl)imino)methyl)benzonitrile (2d).**



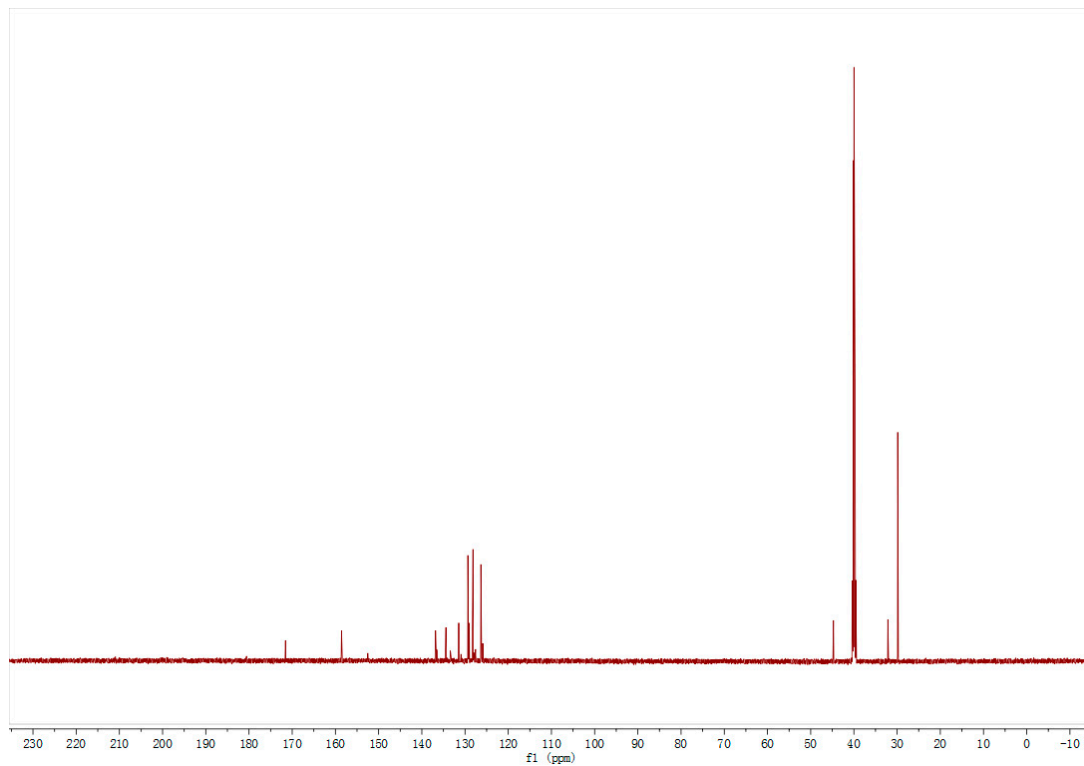
**Spectrum 1.6: <sup>1</sup>H NMR spectrum of 6-chloro-3-(((4-(trifluoromethyl)benzylidene)amino)-2-(4-(trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1H)-one (2e).**



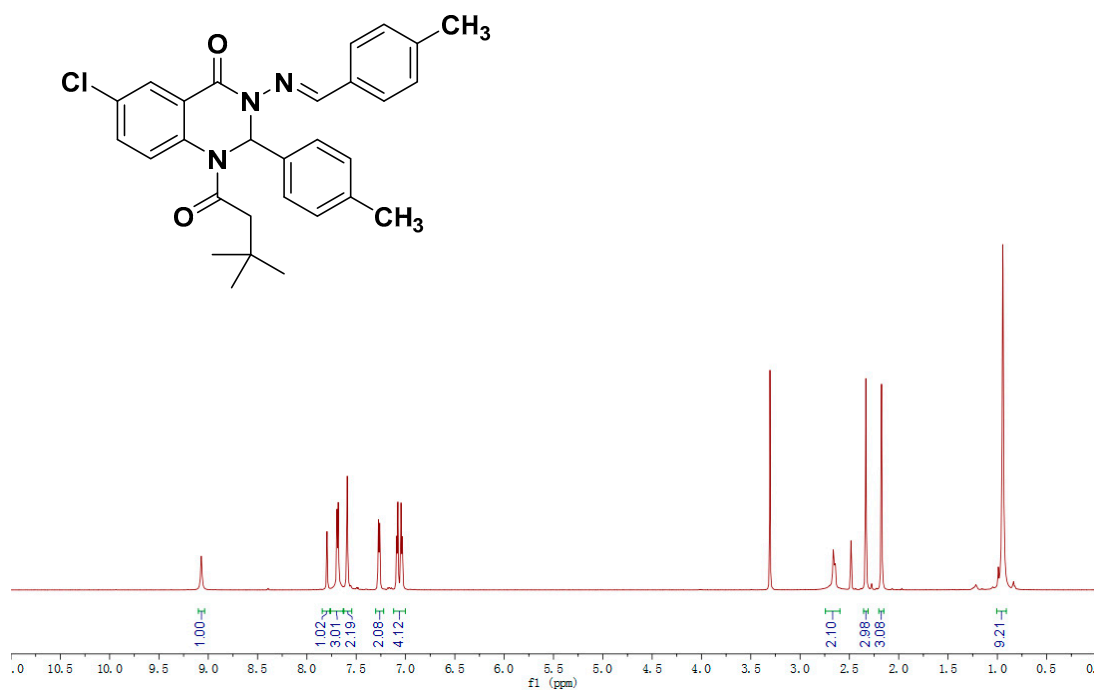
**Spectrum 1.7: <sup>1</sup>H NMR spectrum of 6-chloro-3-((4-isopropylbenzylidene)amino)-2-(4-isopropylphenyl)-2,3-dihydroquinazolin-4(1H)-one (2f).**



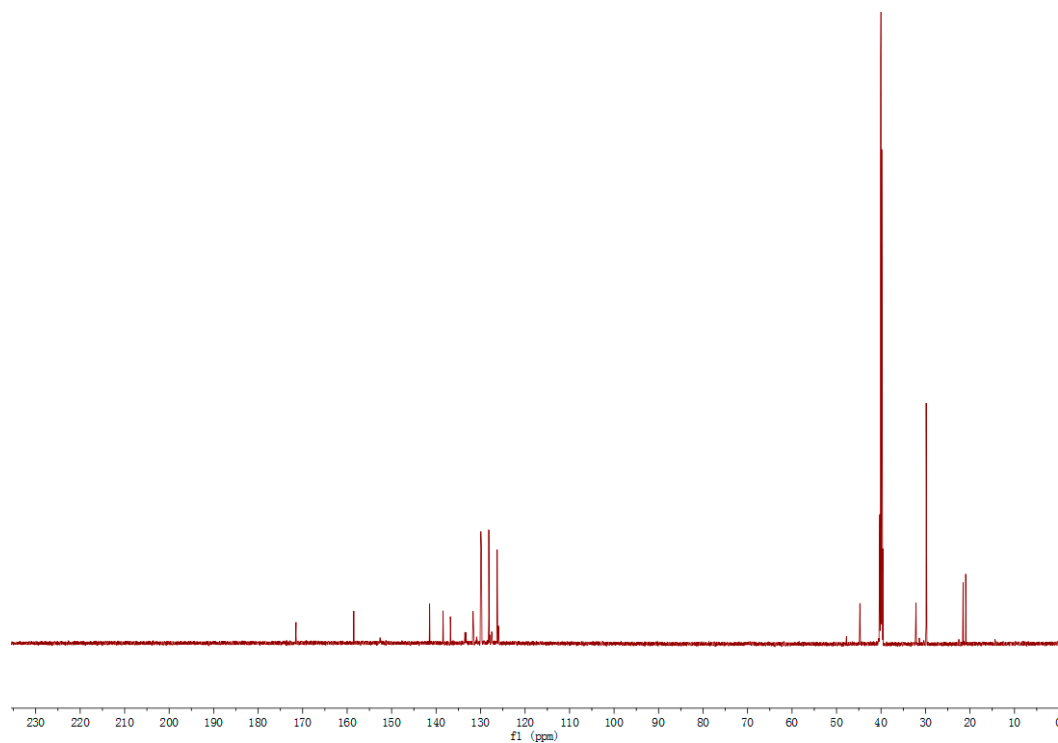
**Spectrum 2.1:  $^1\text{H}$  NMR spectrum of 3-(Benzylideneamino)-6-chloro-1-(3,3-dimethylbutanoyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3a)**



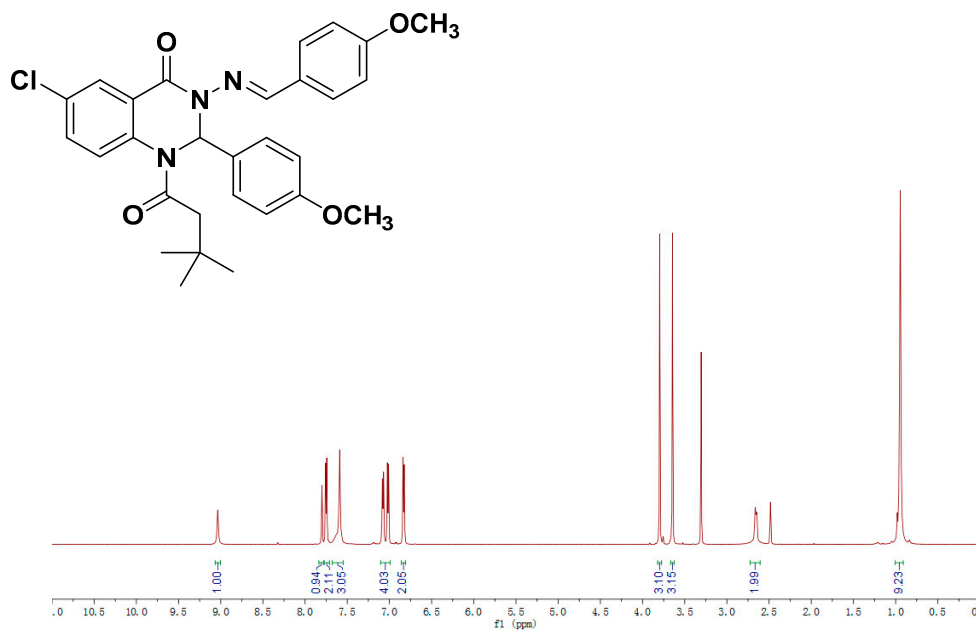
**Spectrum 2.2:  $^{13}\text{C}$  NMR spectrum of 3-(Benzylideneamino)-6-chloro-1-(3,3-dimethylbutanoyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3a).**



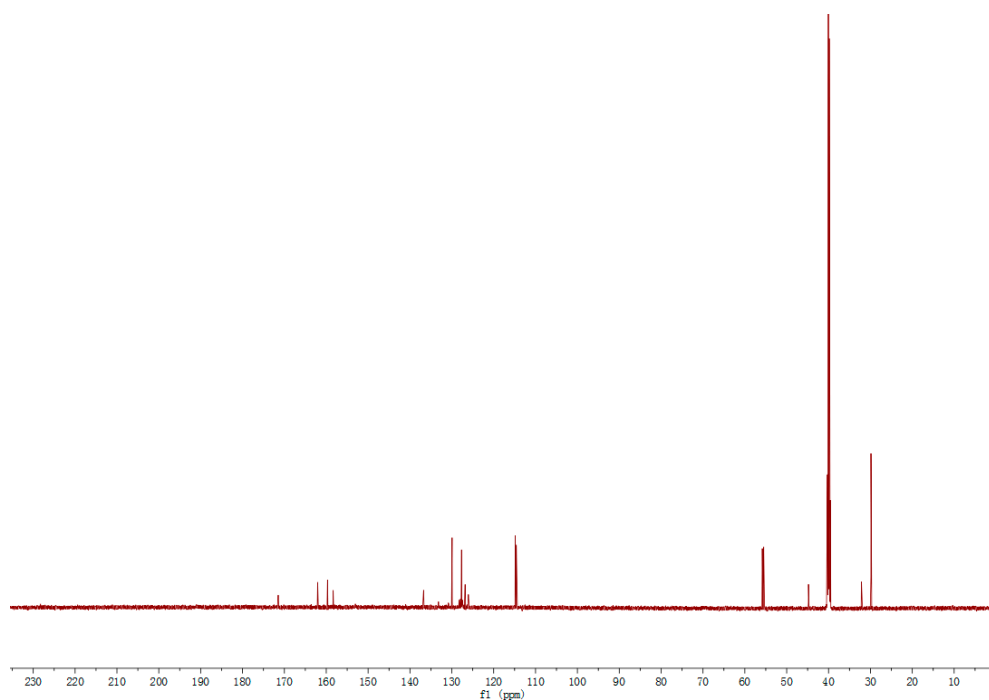
**Spectrum 2.3:  $^1\text{H}$  NMR spectrum of 6-chloro-1-(3,3-dimethylbutanoyl)-3-((4-methylbenzylidene)amino)-2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one (3b)**



**Spectrum 2.4:  $^{13}\text{C}$  NMR spectrum of 6-chloro-1-(3,3-dimethylbutanoyl)-3-((4-methylbenzylidene)amino)-2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one (3b)**

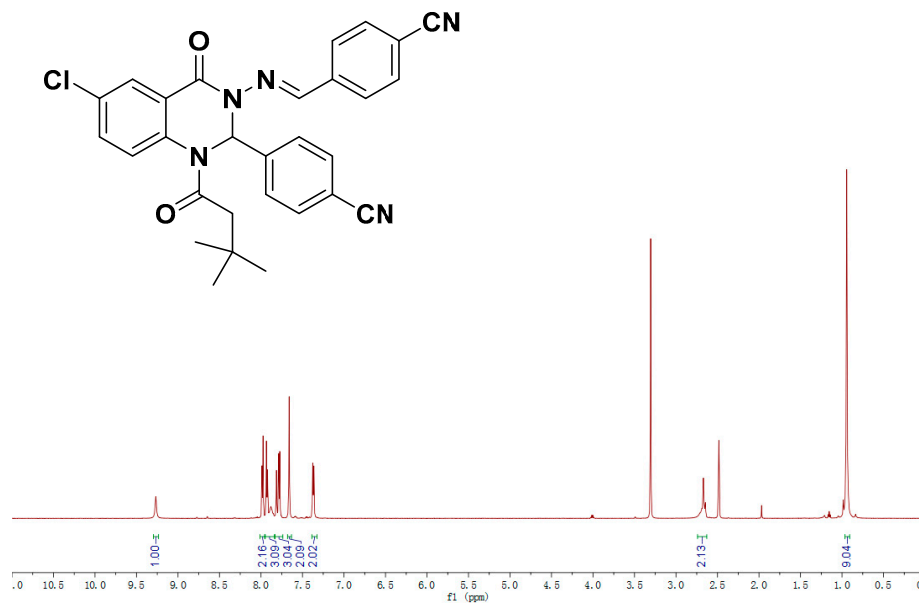


**Spectrum 2.5:  $^1\text{H}$  NMR spectrum of 6-chloro-1-(3,3-dimethylbutanoyl)-3-((4-methoxybenzylidene)amino)-2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3c)**

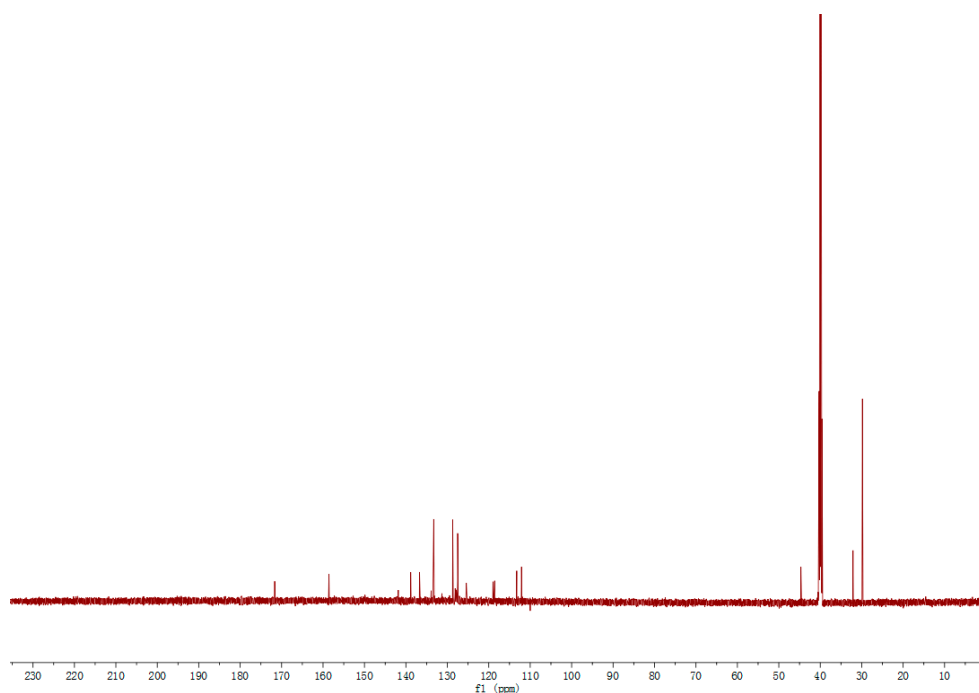


**Spectrum 2.6:  $^{13}\text{C}$  NMR spectrum of 6-chloro-1-(3,3-dimethylbutanoyl)-3-((4-methoxybenzylidene)amino)-2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3c)**

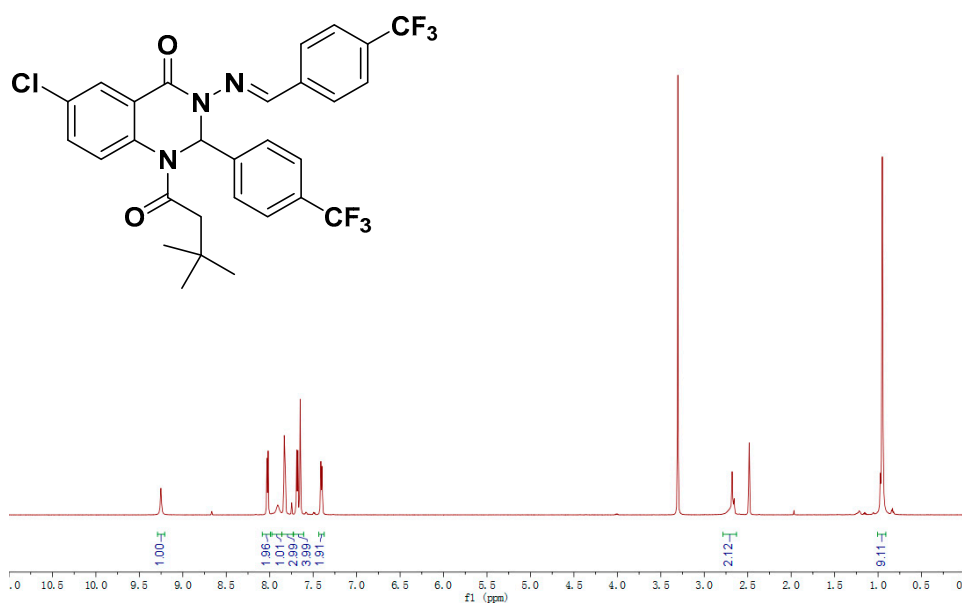




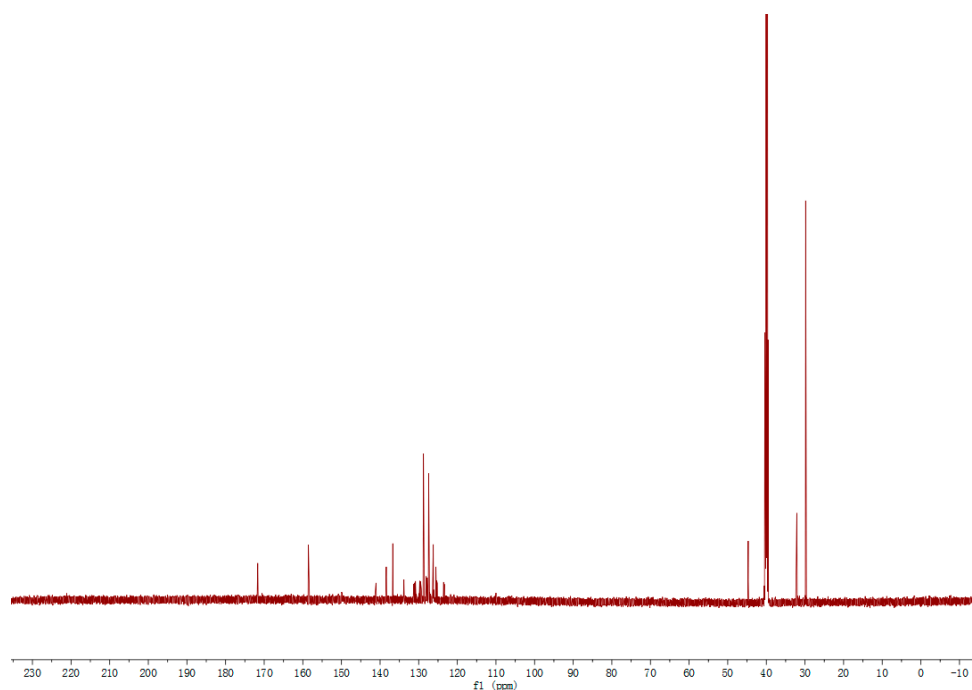
**Spectrum 2.7:  $^1\text{H}$  NMR spectrum of 4-(((6-chloro-2-(4-cyanophenyl)-1-(3,3-dimethylbutanoyl)-4-oxo-1,4-dihydroquinazolin-3(2H)-yl)imino)methyl)benzonitrile (3d)**



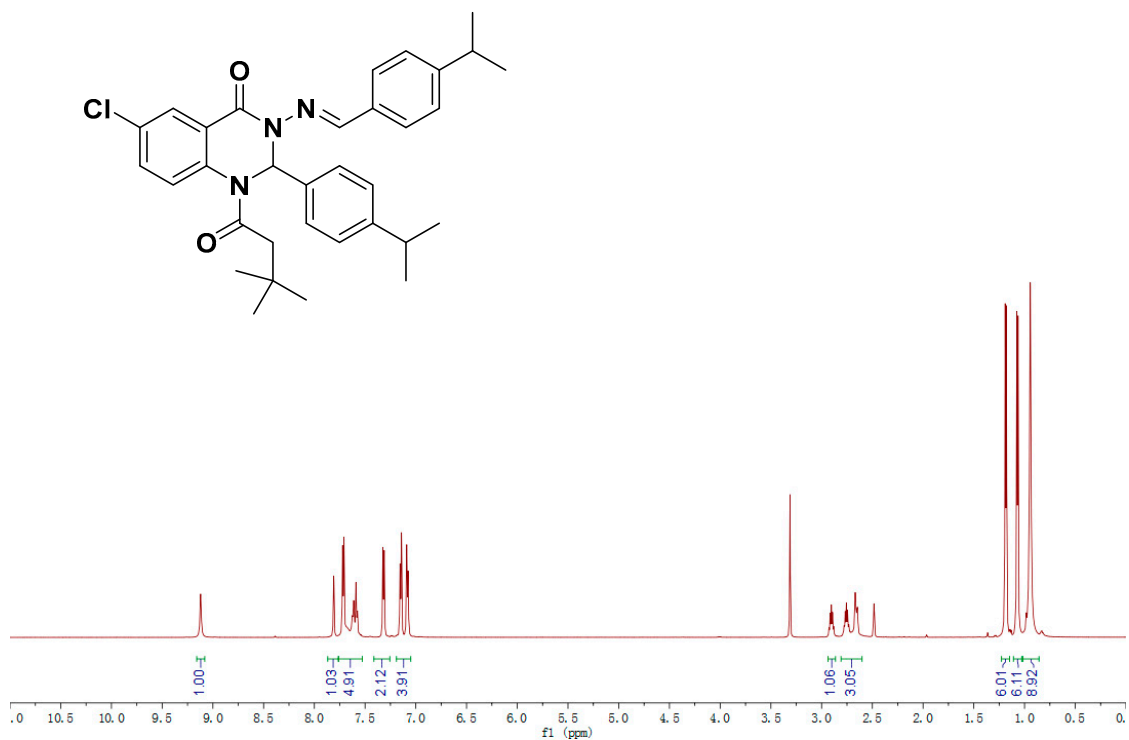
**Spectrum 2.8:  $^{13}\text{C}$  NMR spectrum of 4-(((6-chloro-2-(4-cyanophenyl)-1-(3,3-dimethylbutanoyl)-4-oxo-1,4-dihydroquinazolin-3(2H)-yl)imino)methyl)benzonitrile (3d)**



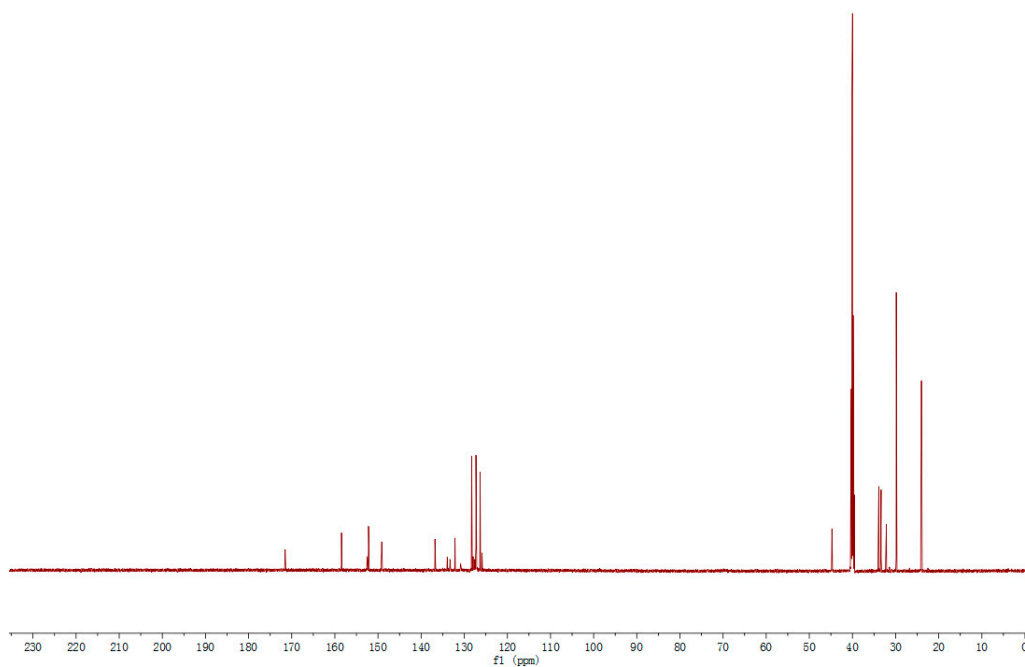
**Spectrum 2.9:  $^1\text{H}$  NMR spectrum of 6-chloro-1-(3,3-dimethylbutanoyl)-3-((4-(trifluoromethyl)benzylidene)amino)-2-(4-(trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1H)-one (3e)**



**Spectrum 2.10:  $^{13}\text{C}$  NMR spectrum of 6-chloro-1-(3,3-dimethylbutanoyl)-3-((4-(trifluoromethyl)benzylidene)amino)-2-(4-(trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1H)-one (3e)**



**Spectrum 2.11:**  $^1\text{H}$  NMR spectrum of 6-chloro-1-(3,3-dimethylbutanoyl)-3-((4-isopropylbenzylidene)amino)-2-(4-isopropylphenyl)-2,3-dihydroquinazolin-4(1H)-one (3f)



**Spectrum 2.12:**  $^{13}\text{C}$  NMR spectrum of 6-chloro-1-(3,3-dimethylbutanoyl)-3-((4-isopropylbenzylidene)amino)-2-(4-isopropylphenyl)-2,3-dihydroquinazolin-4(1H)-one (3f)