Supporting Information

***Org. Commun.* X:X (2025) XX-XX**

Synthesis and Antidiabetic Assessment of Substituted 2-Benzylidene-1-Indanone Derivatives Using *In Vitro* and *In Silico* Techniques

Selvakumar Sabapathi [1], Babai Mahdi [1,2], Mohamad Hafizi Abu Bakar [3], Andrey A. Mikhaylov [4,5], Mohammad Tasyriq Che Omar [6], Azeana Zahari [7], S. Yaallini Sukumaran [7] and Mohamad Nurul Azmi [1] *

[1]School of Chemical Sciences, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia
[2]Department of Chemistry, Nigerian Army University Biu, Borno State, 1500, Nigeria
[3]School of Industrial Technology, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia
[4]Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry of the Russian Academy of Sciences, 16/10 Miklukho-Maklaya St, Moscow 117997, Russia
[5]Laboratory of Medicinal Substances Chemistry, Institute of Translational Medicine, Pirogov Russian National Research Medical University, Ostrovitianov 1, Moscow, 117997, Russia
[6]School of Distance Education, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia
[7]Department of Chemistry, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia

Table of Contents — **Page**

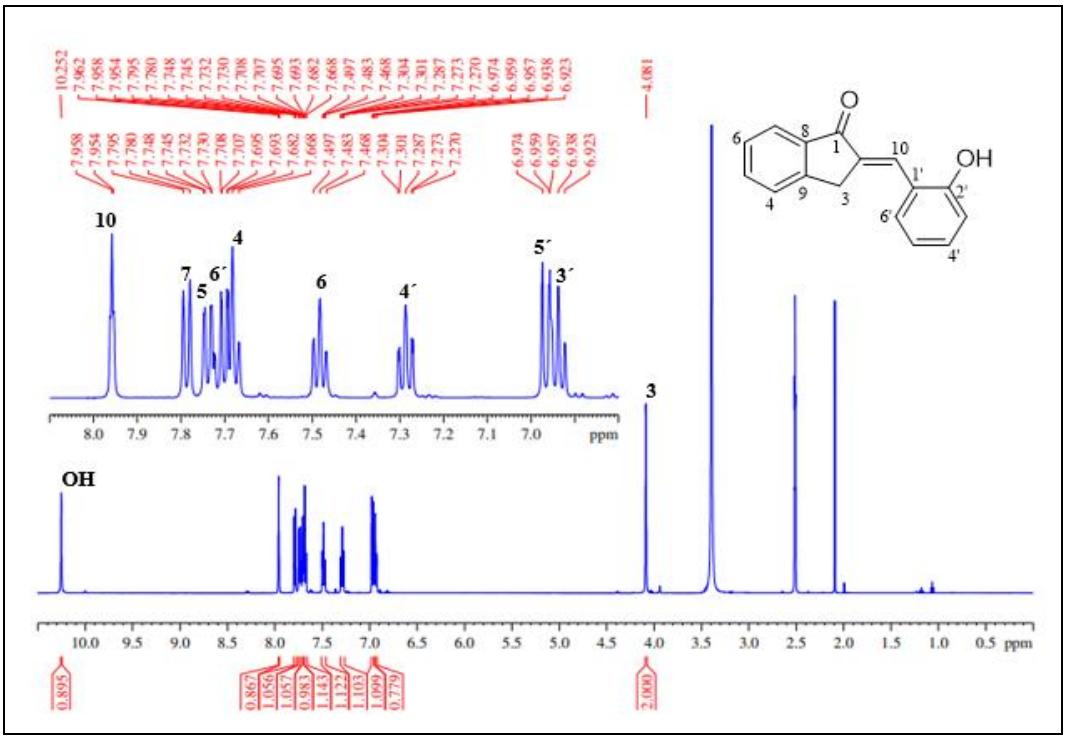

Figure S1: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum **3a**

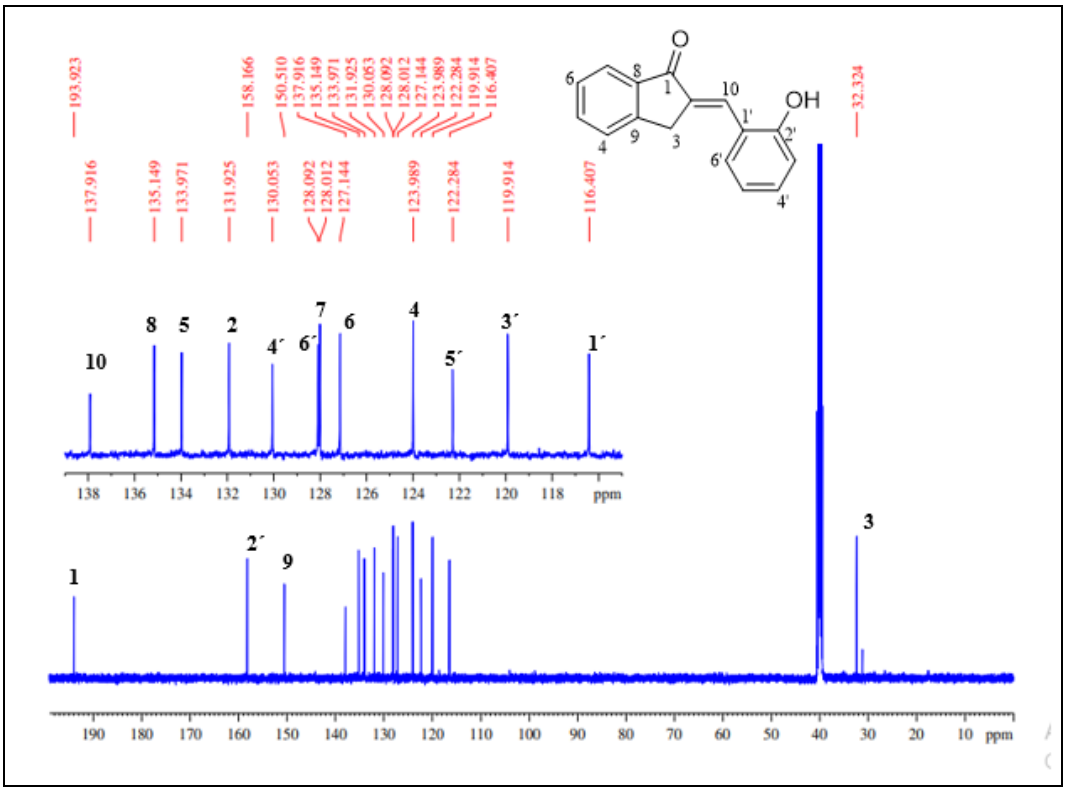

Figure S2: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of **3a**

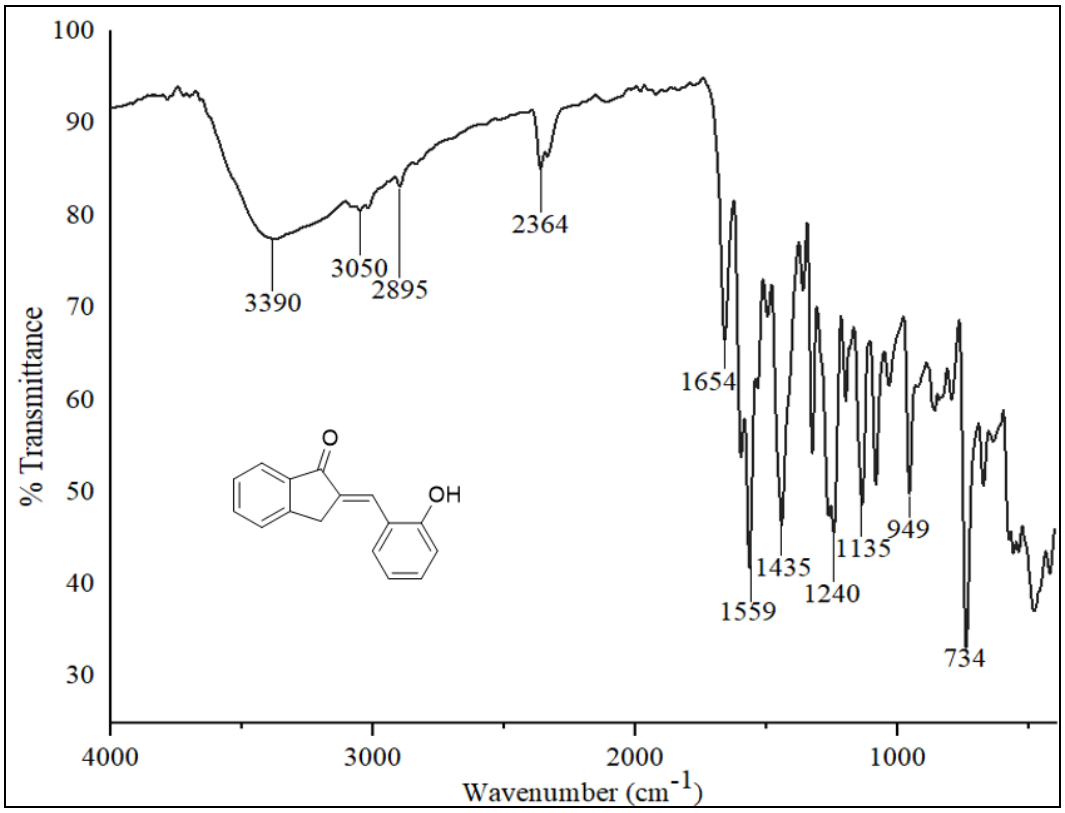

Figure S3: FT-IR Spectrum for compound **3a**

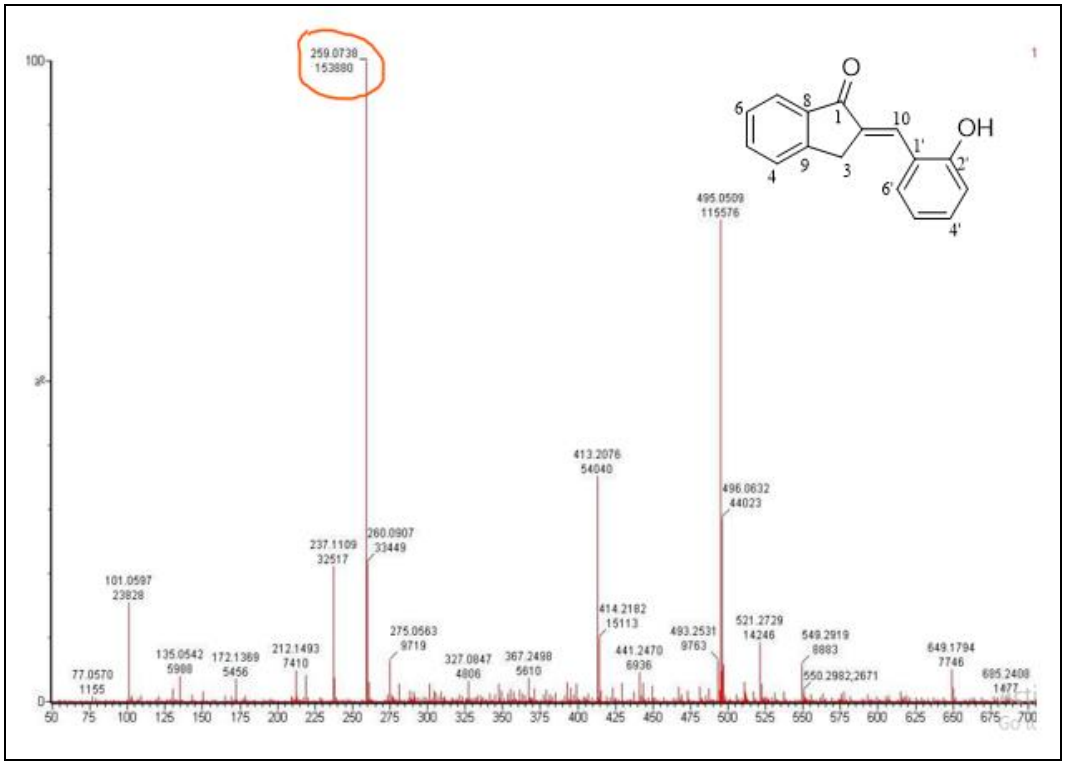

Figure S4: HRMS Spectrum for compound **3a**

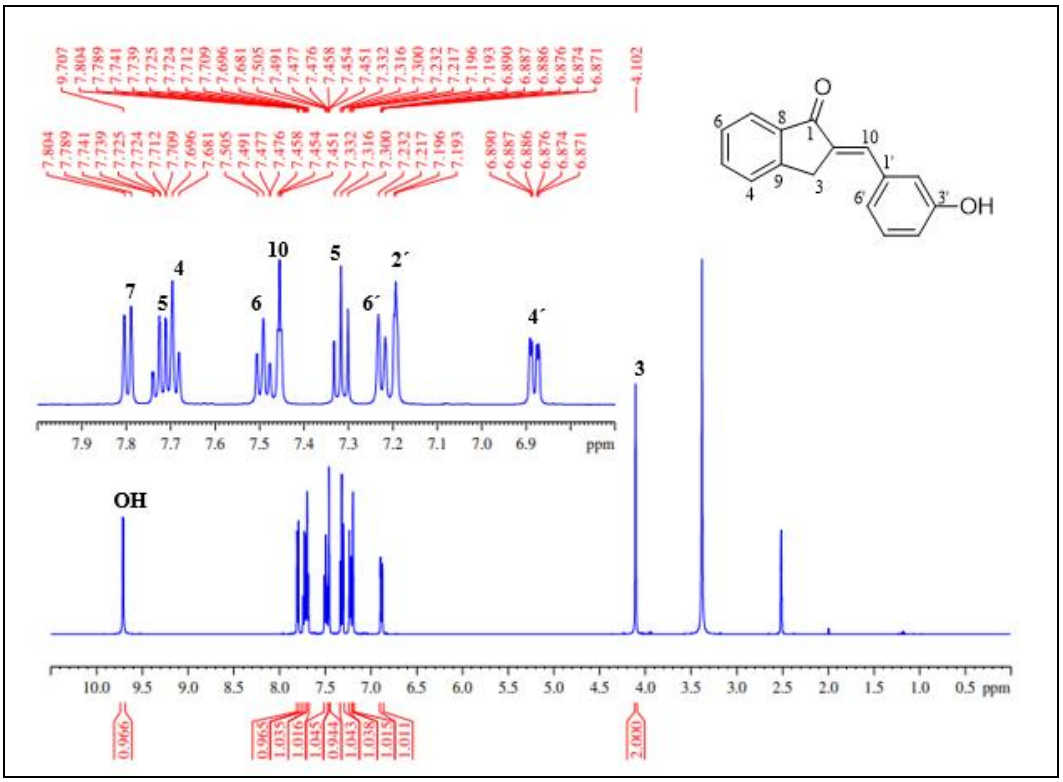

Figure S5: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum of **3b**

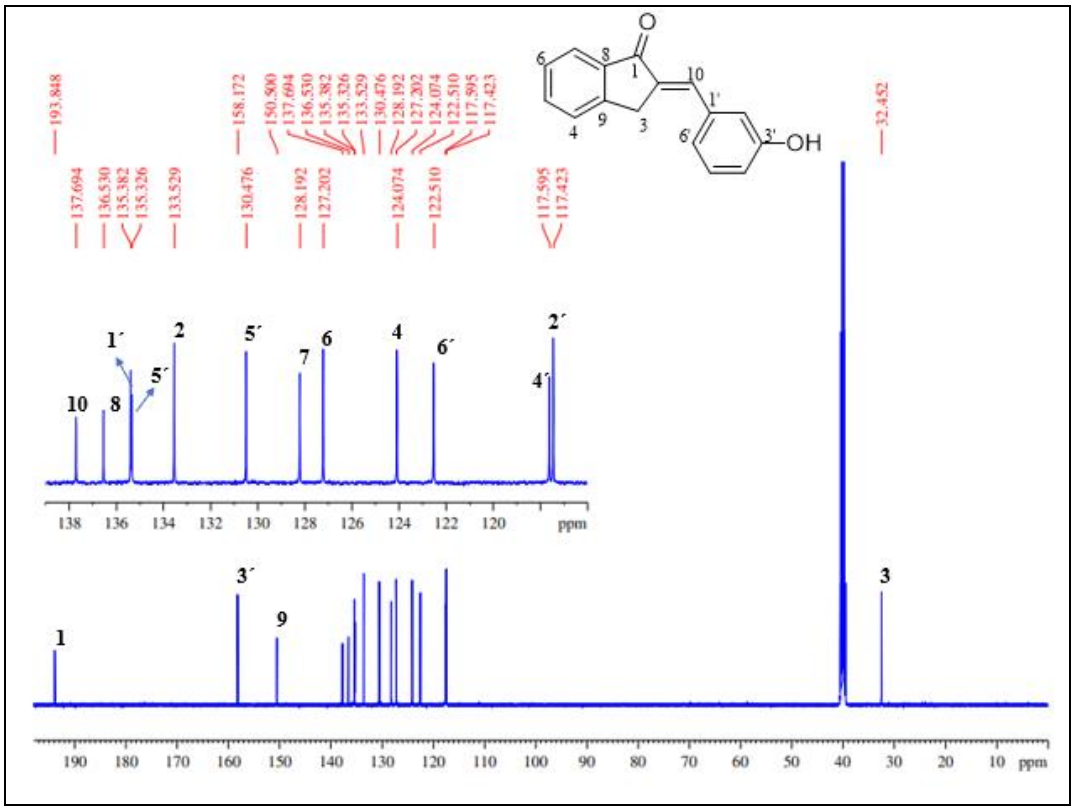

Figure S6: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of **3b**

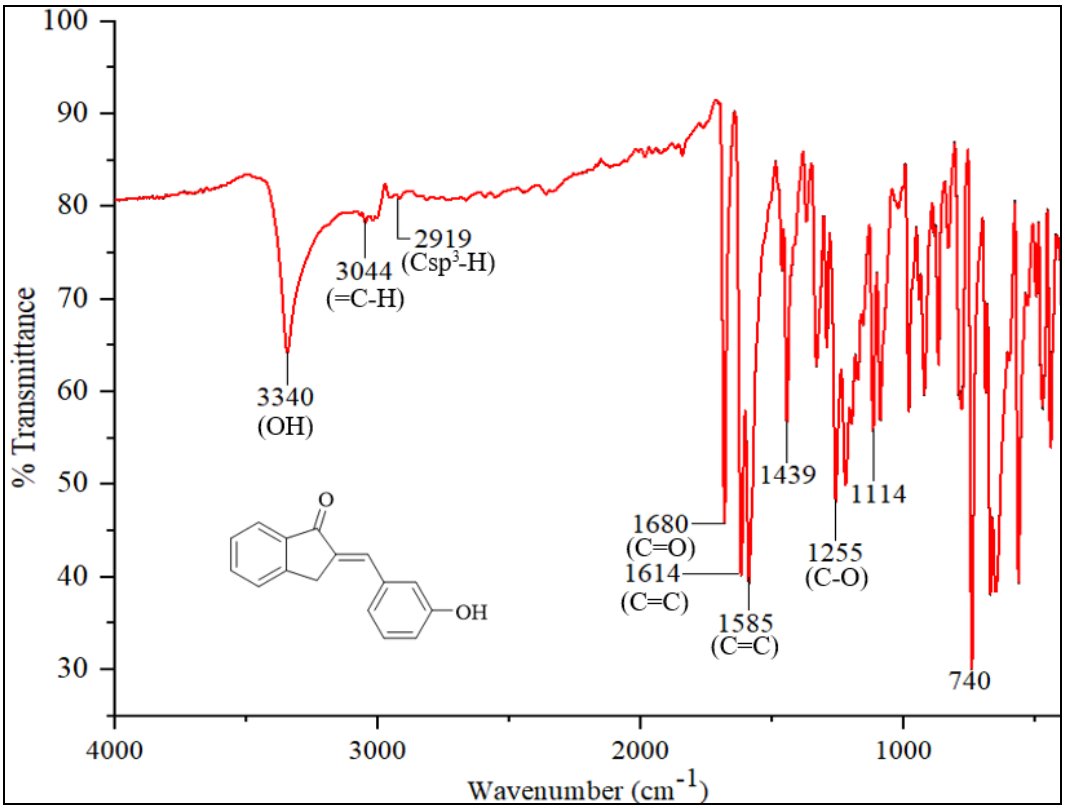

Figure S7: FT-IR Spectrum of **3b**

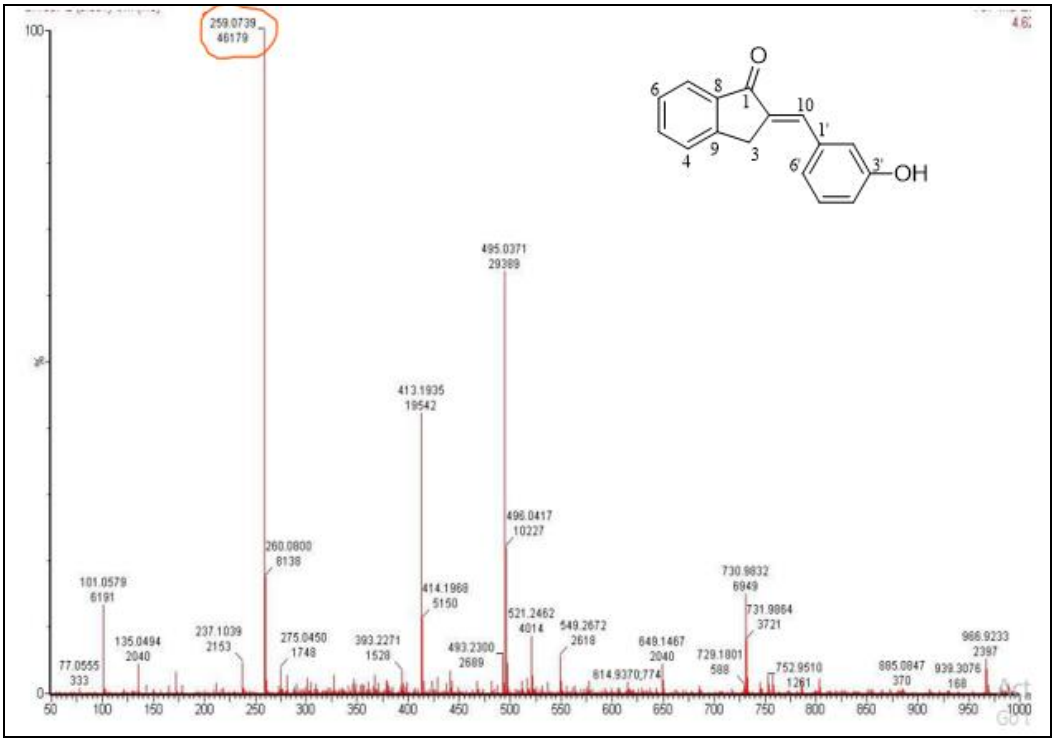

Figure S8: HRMS Spectrum of **3b**

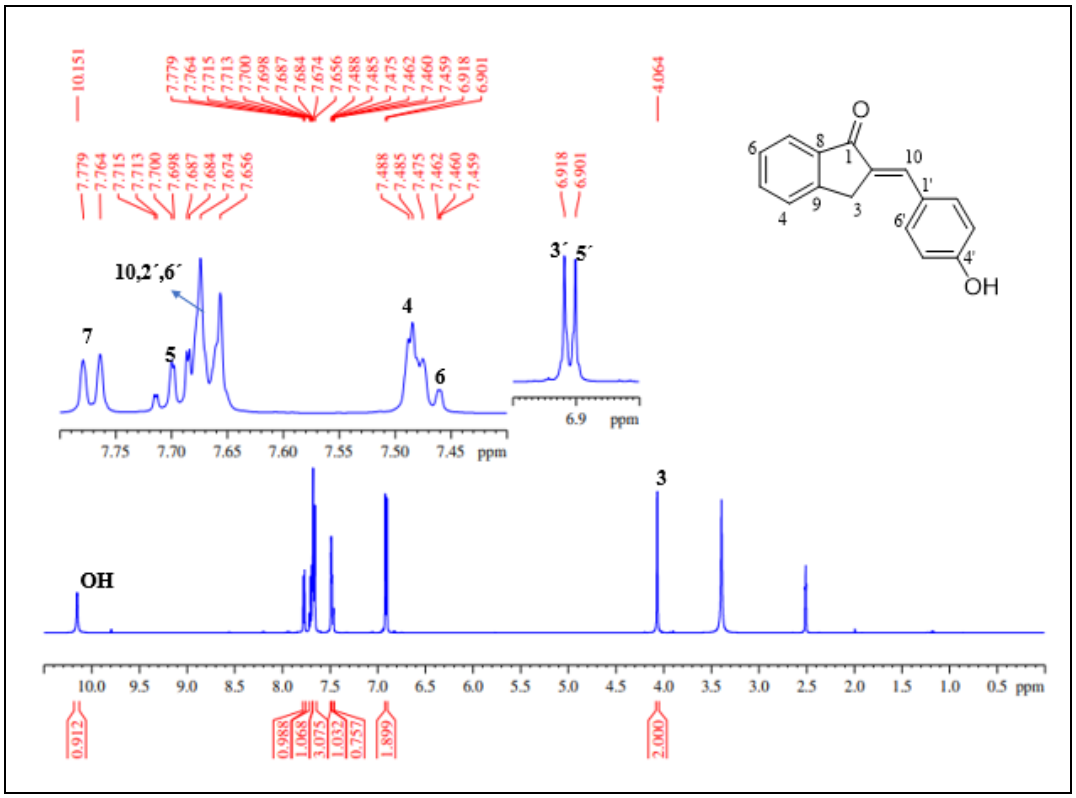

Figure S9: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum **3c**

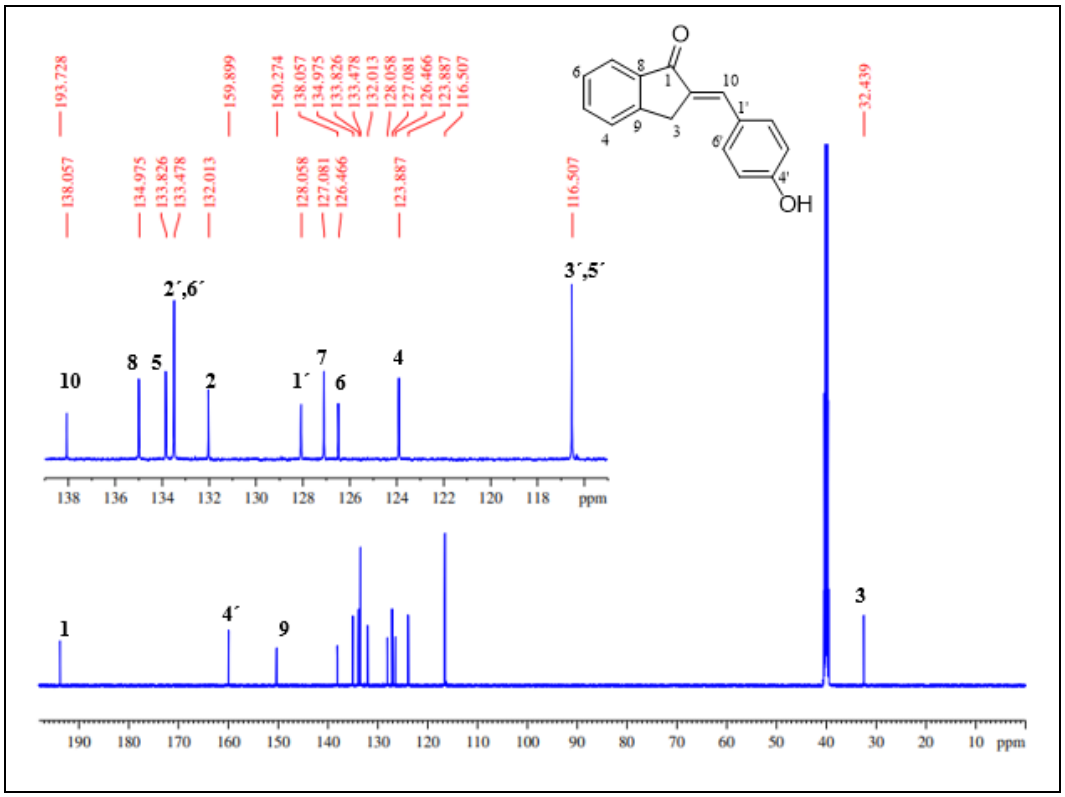

Figure S10: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of **3c**

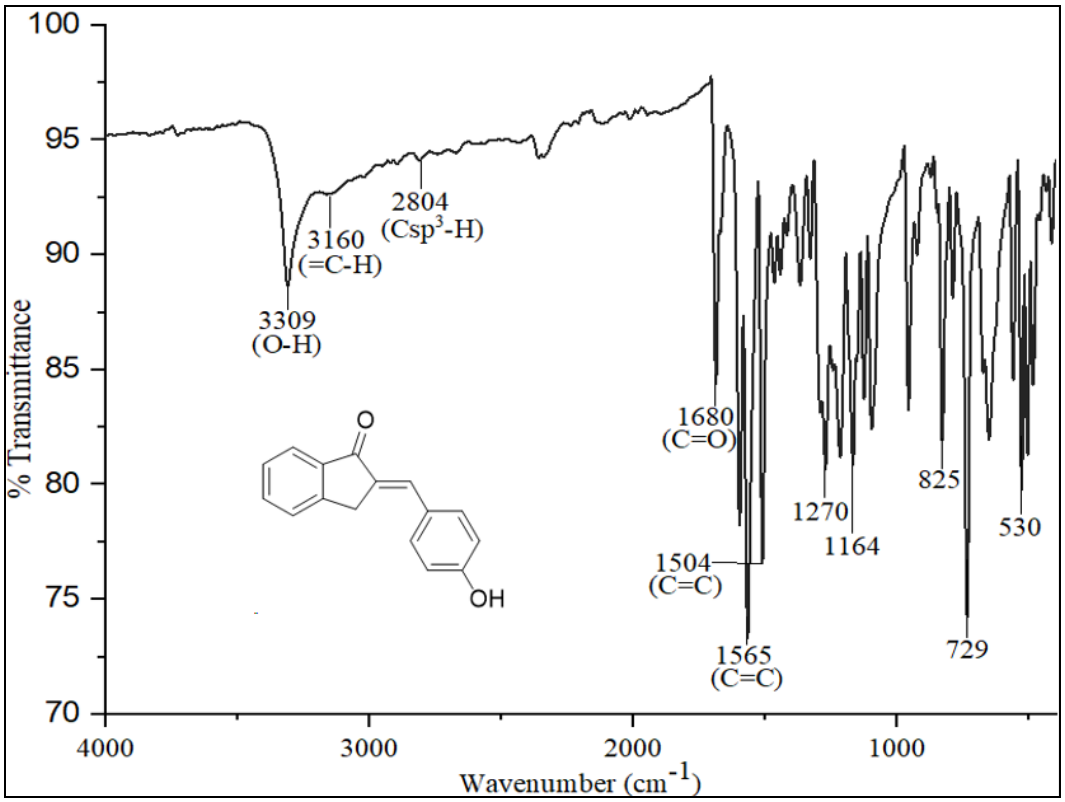

Figure S11: FT-IR Spectrum of **3c**

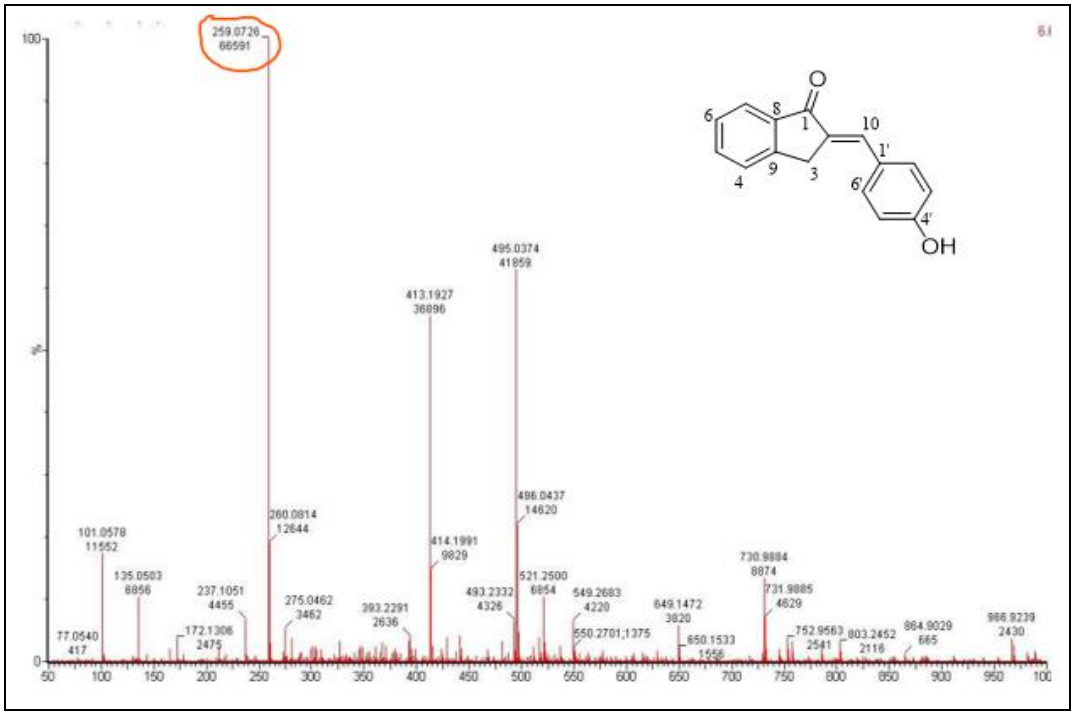

Figure S12: HRMS Spectrum of **3c**

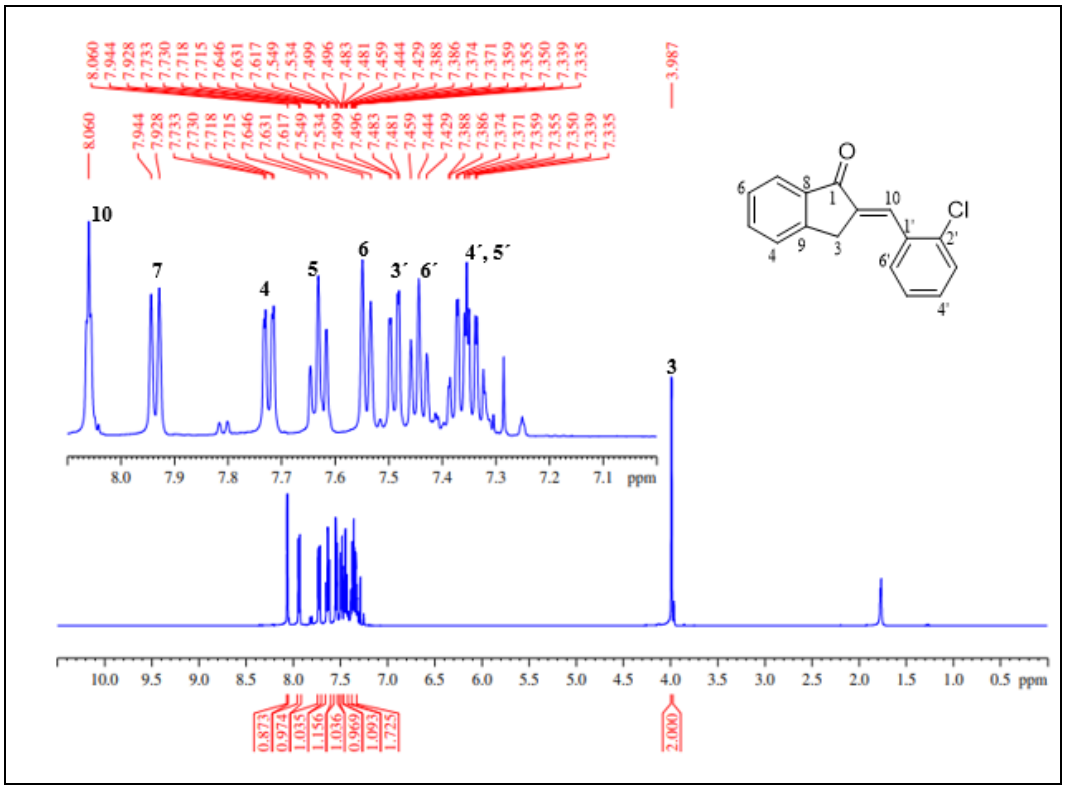

Figure S13: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum **3d**

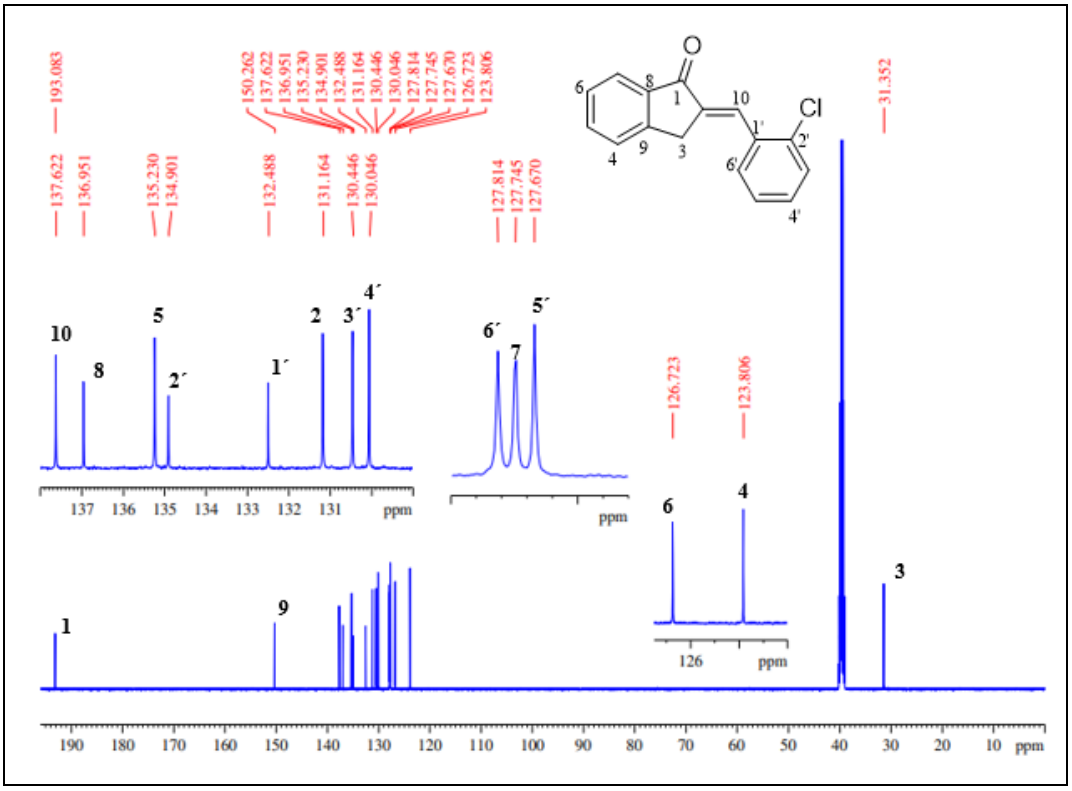

Figure S14: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of **3d**

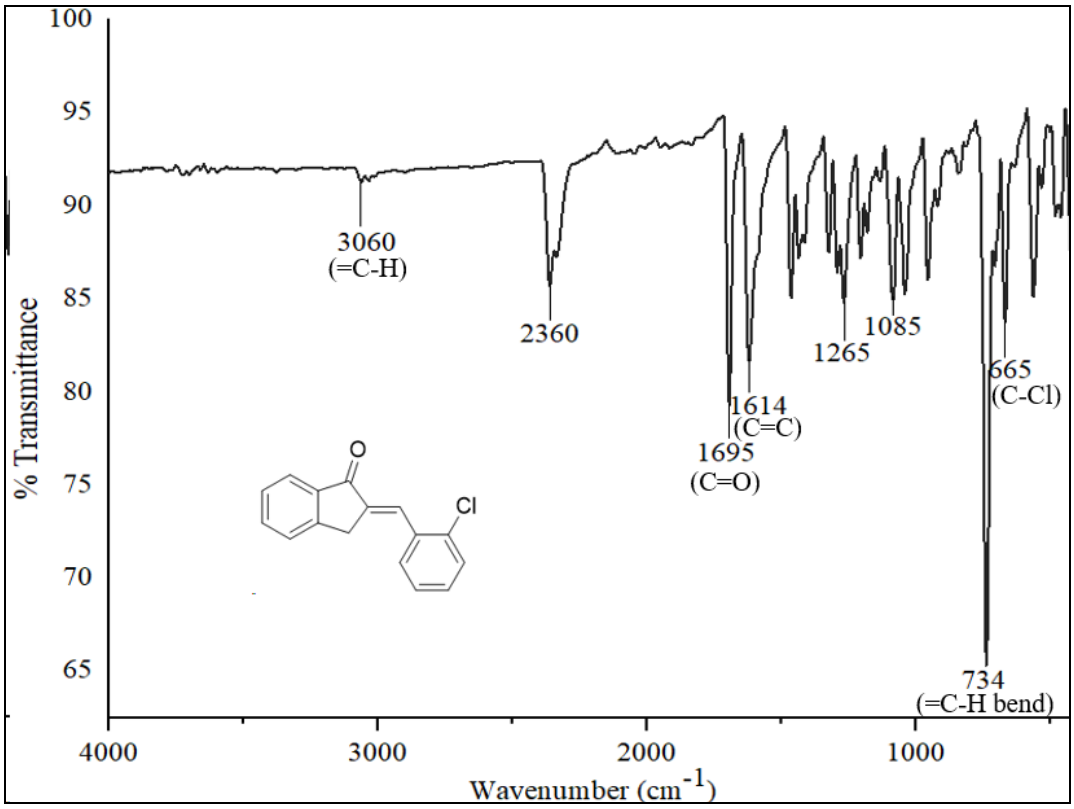

Figure S15: FT-IR Spectrum of **3d**

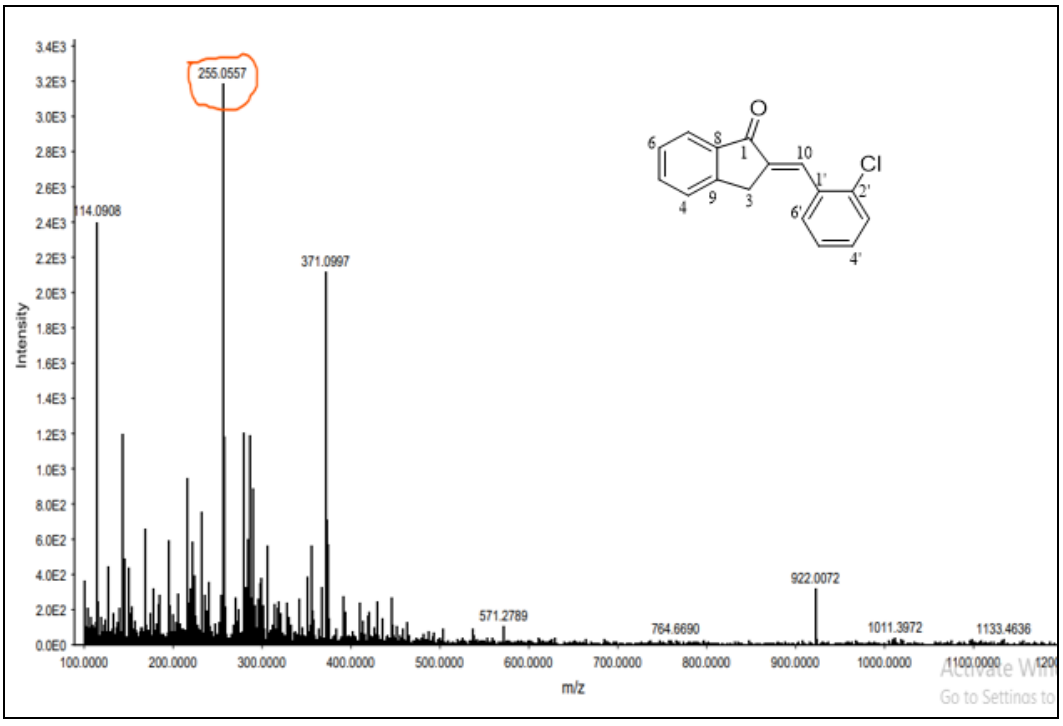

Figure S16: HRMS Spectrum of **3d**

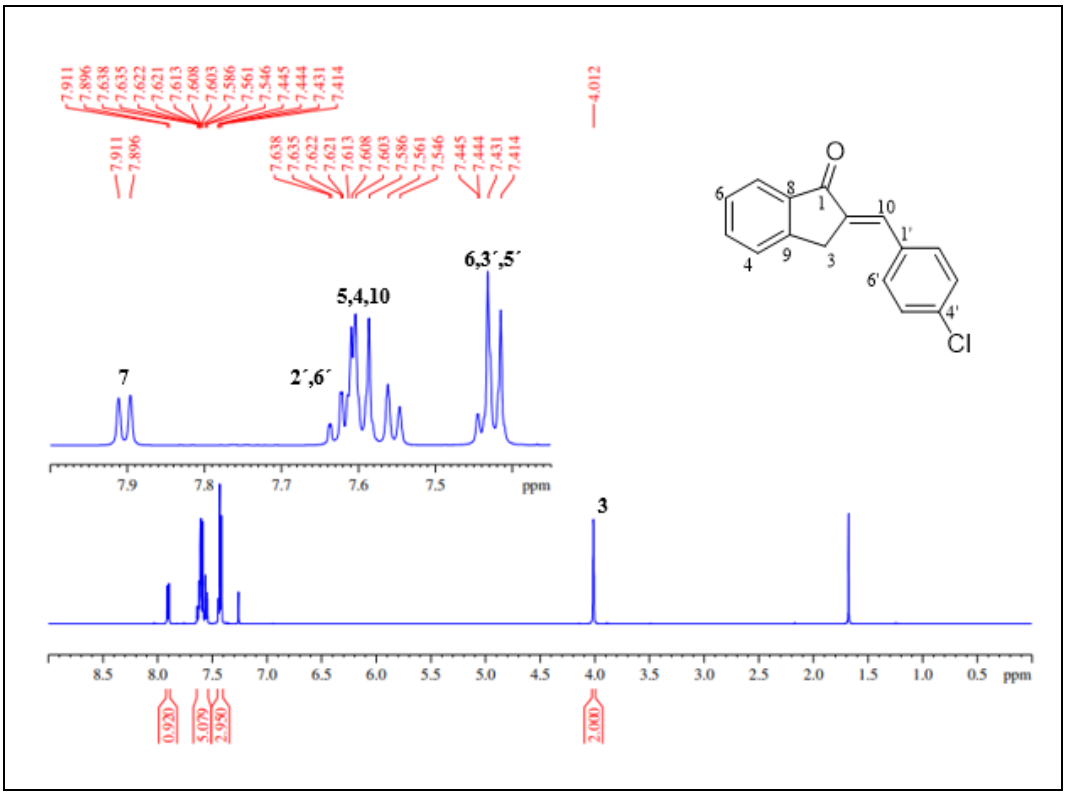

Figure S17: ^{1}H-NMR (500 MHz, DMSO-d_6) Spectrum **3e**

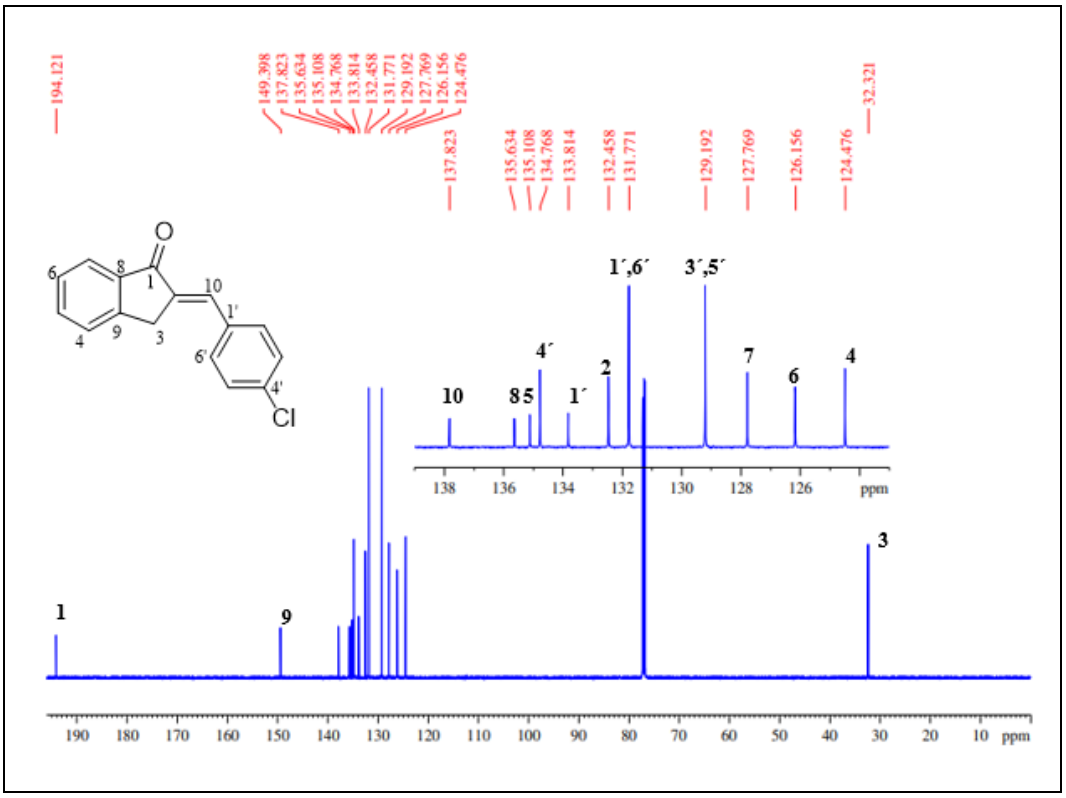

Figure S18: ^{13}C-NMR (125 MHz, DMSO-d_6) Spectrum of **3e**

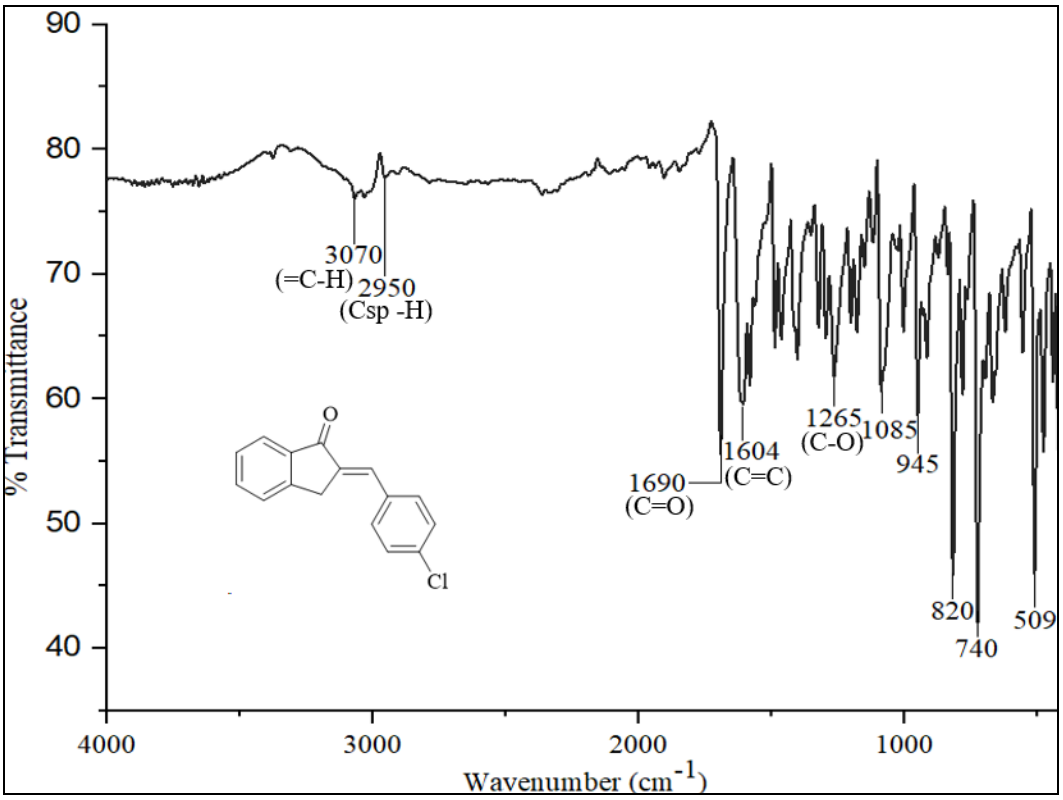

Figure S19: FT-IR Spectrum of **3e**

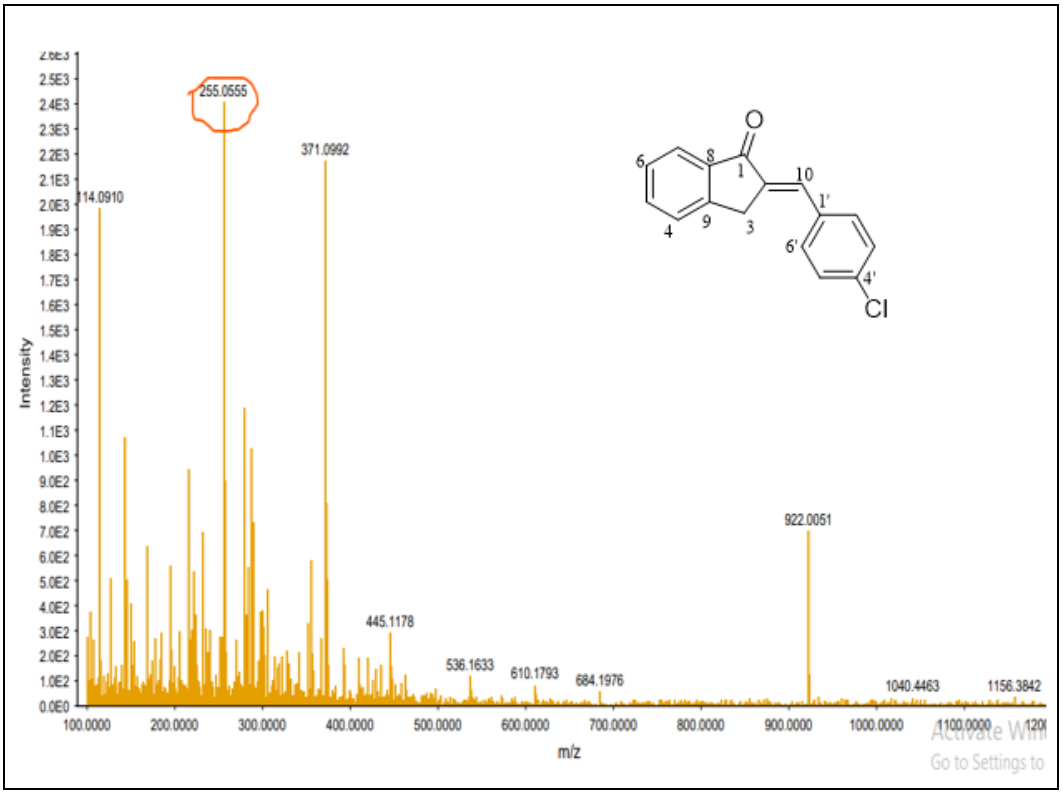

Figure S20: HRMS Spectrum of **3e**

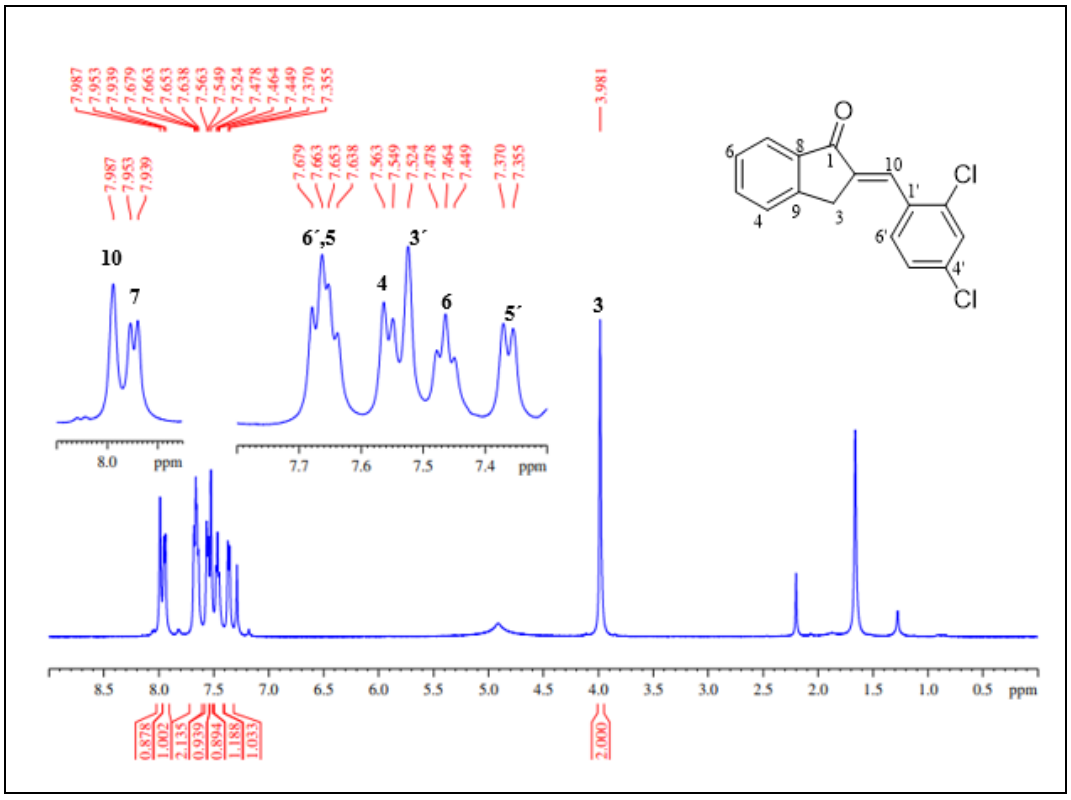

Figure S21: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3f**

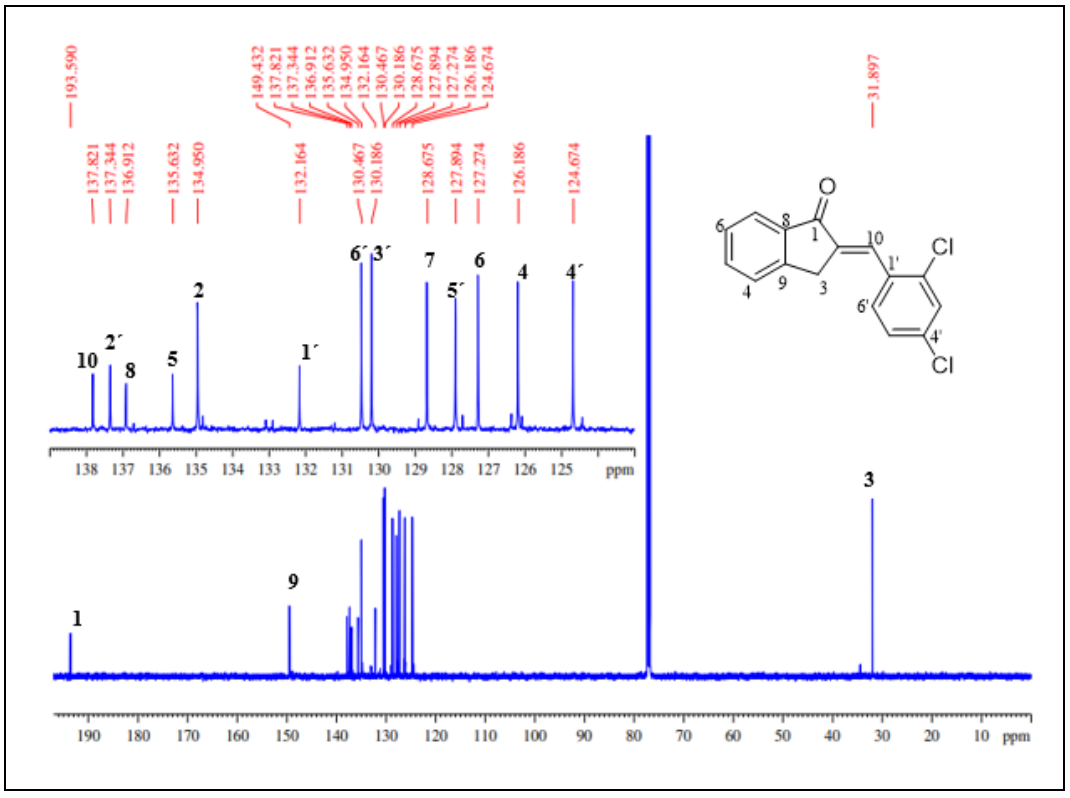

Figure S22: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3f**

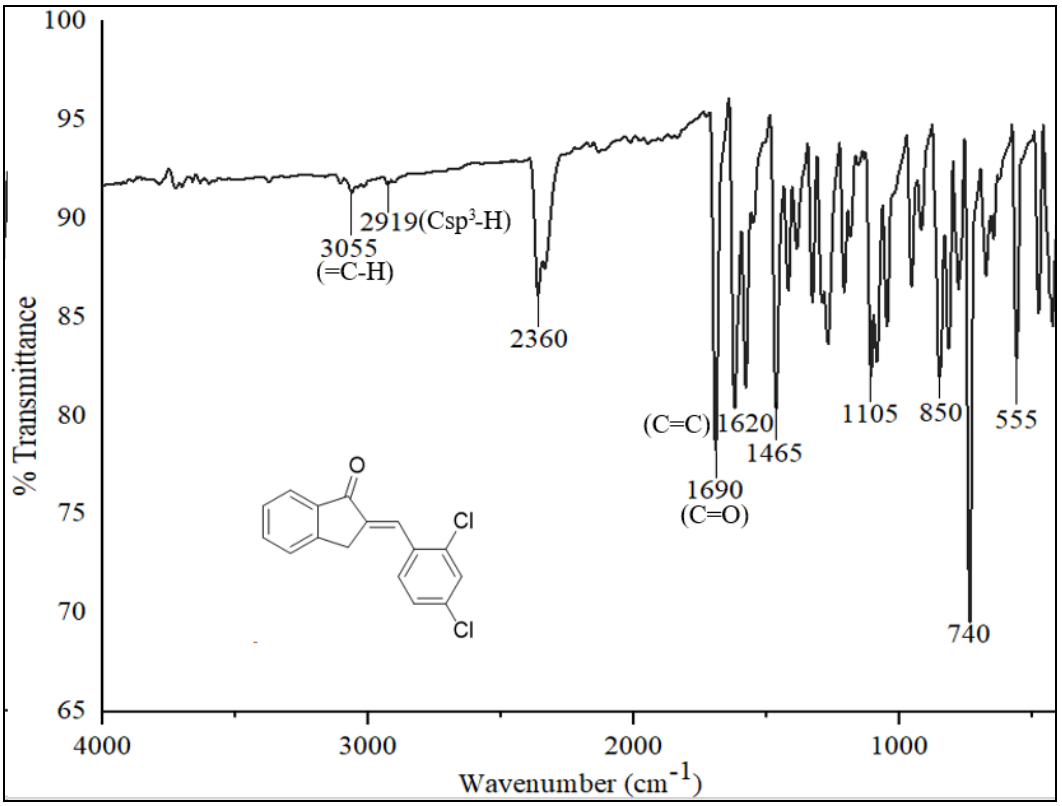

Figure S23: FT-IR Spectrum of **3f**

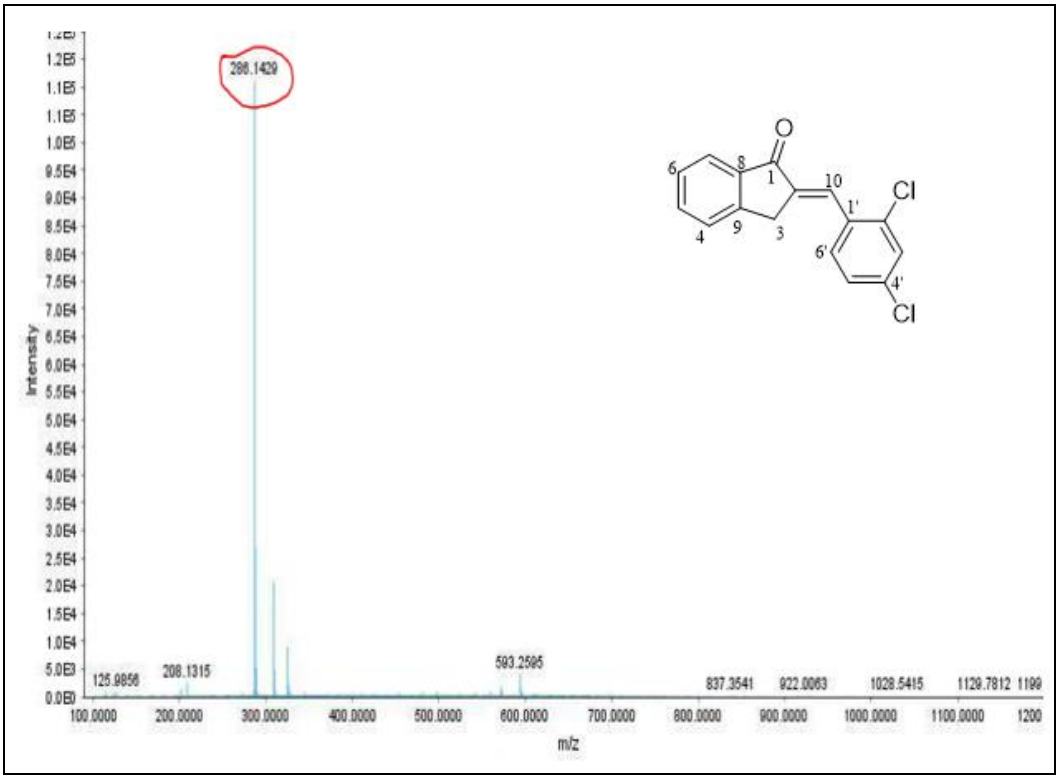

Figure S24: HRMS Spectrum of **3f**

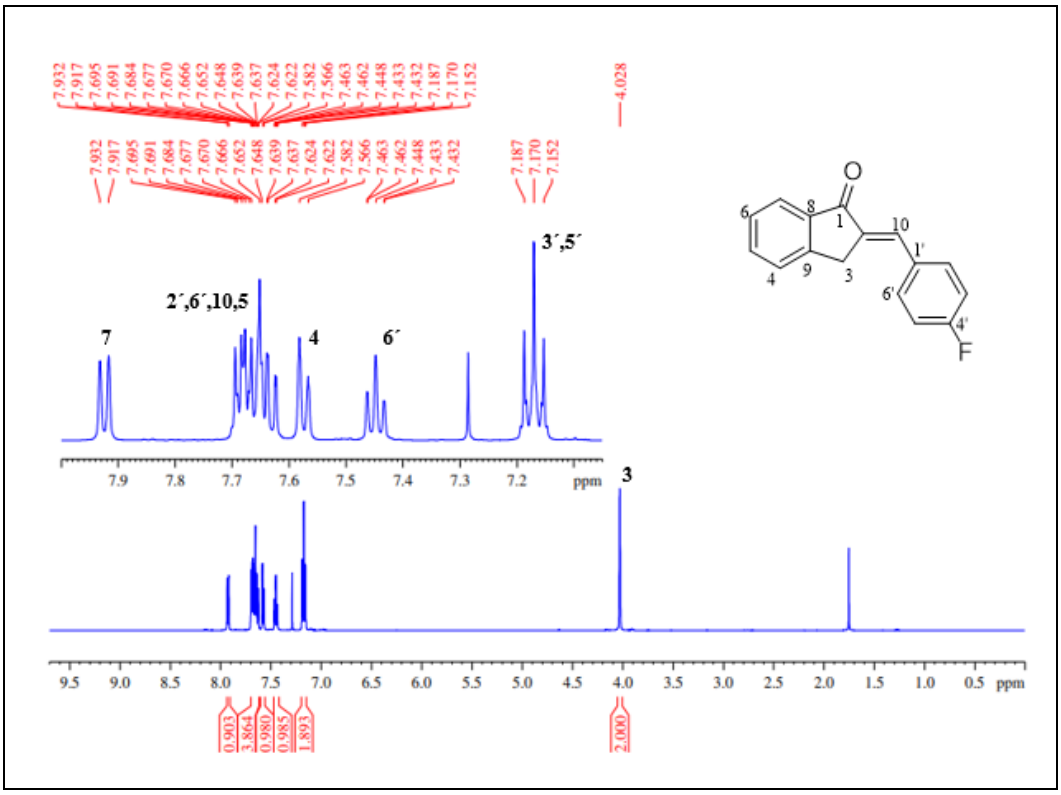

Figure S25: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3g**

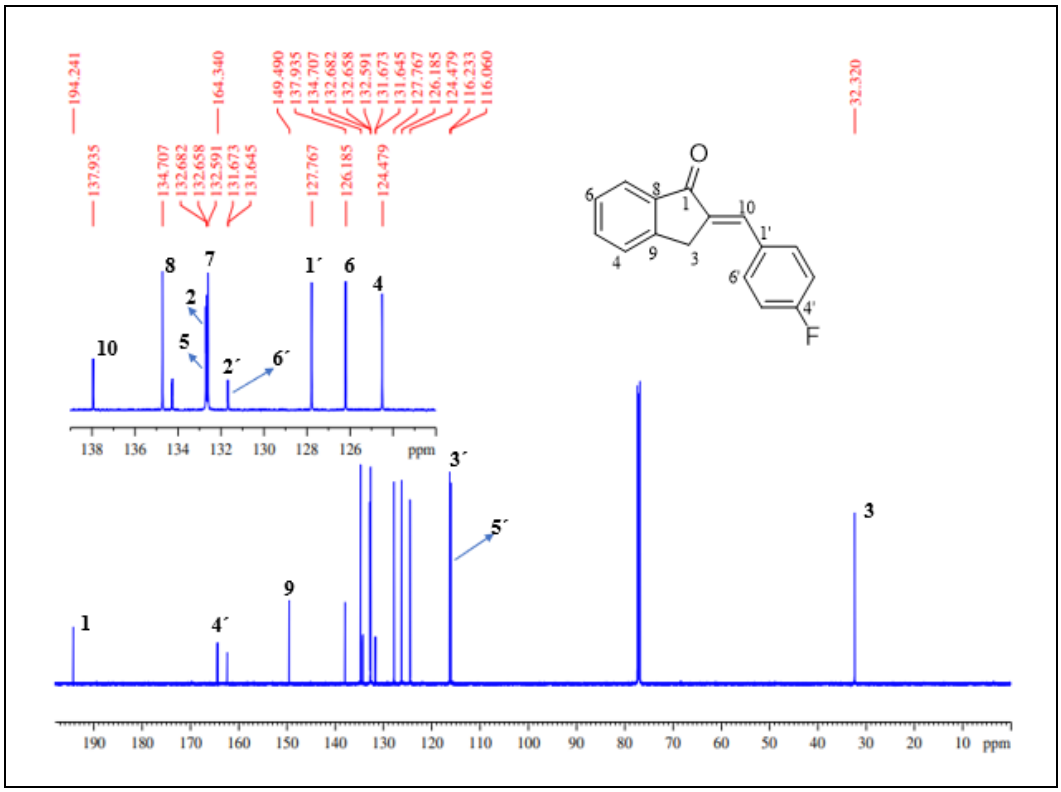

Figure S26: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3g**

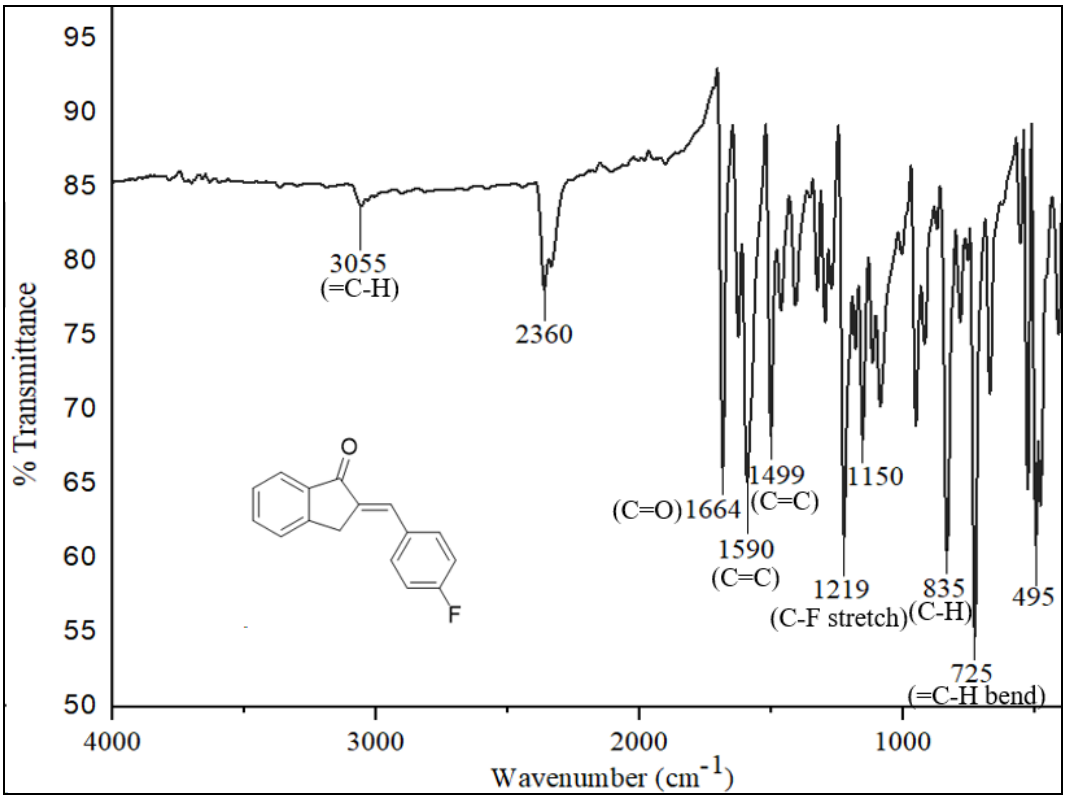

Figure S27: FT-IR Spectrum of **3g**

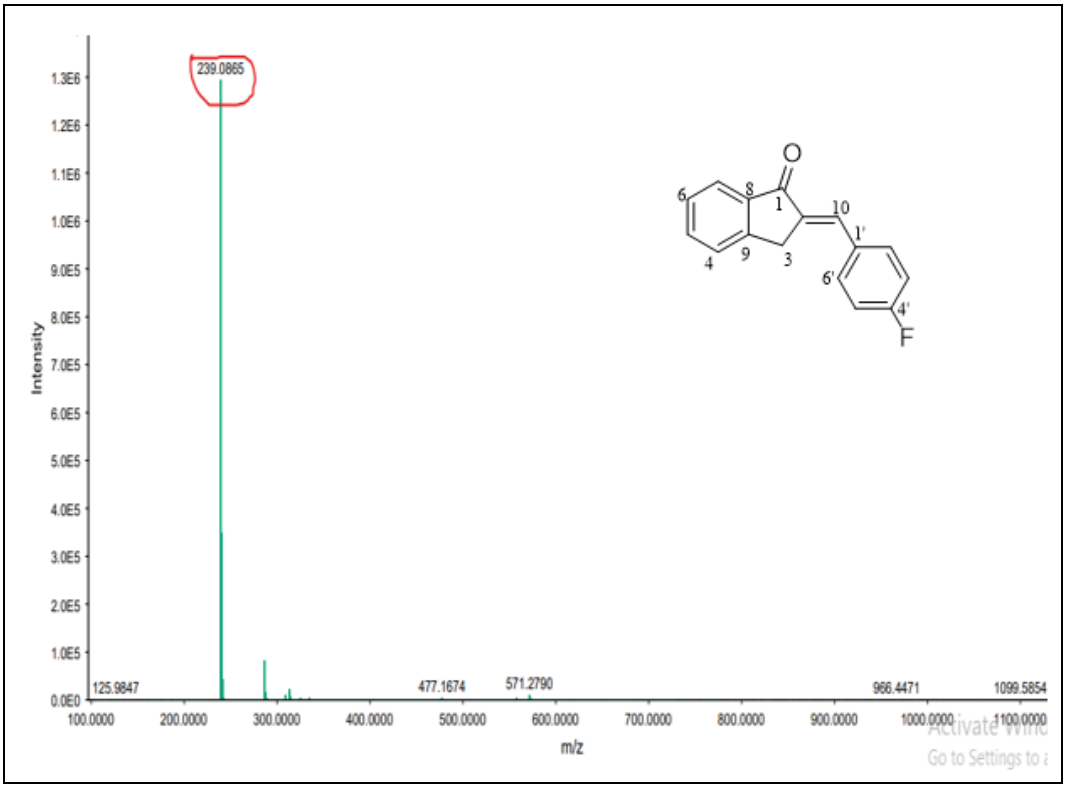

Figure S28: HRMS Spectrum of **3g**

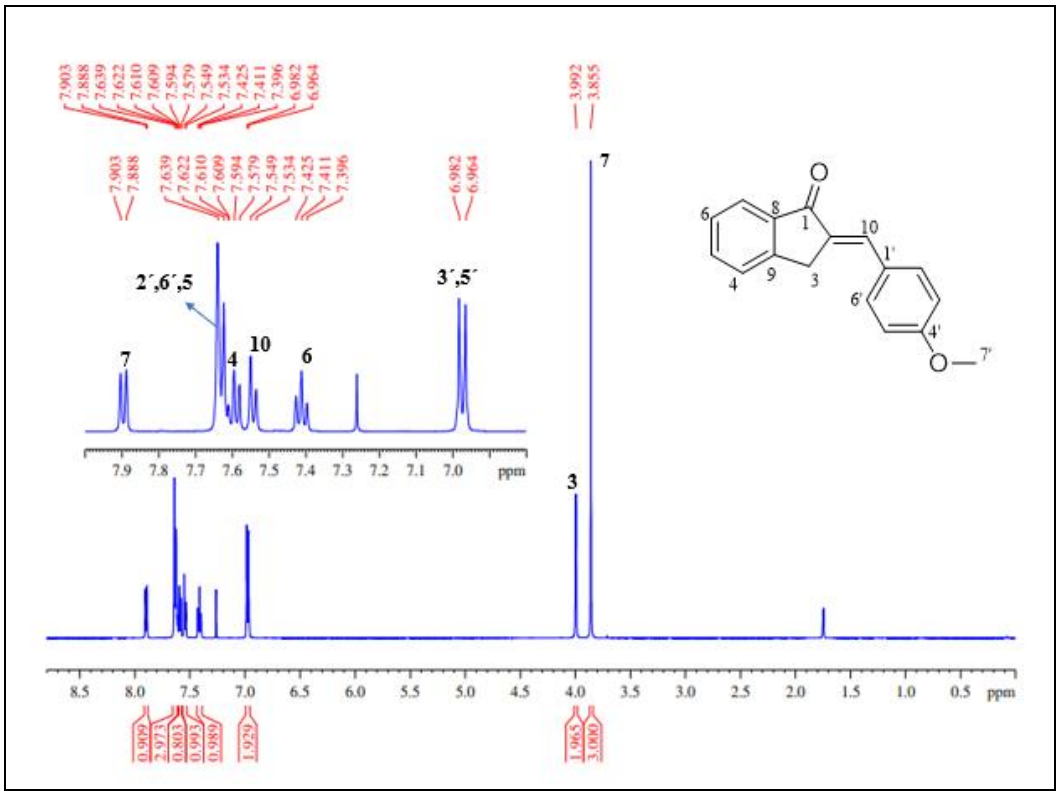

Figure S29: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3h**

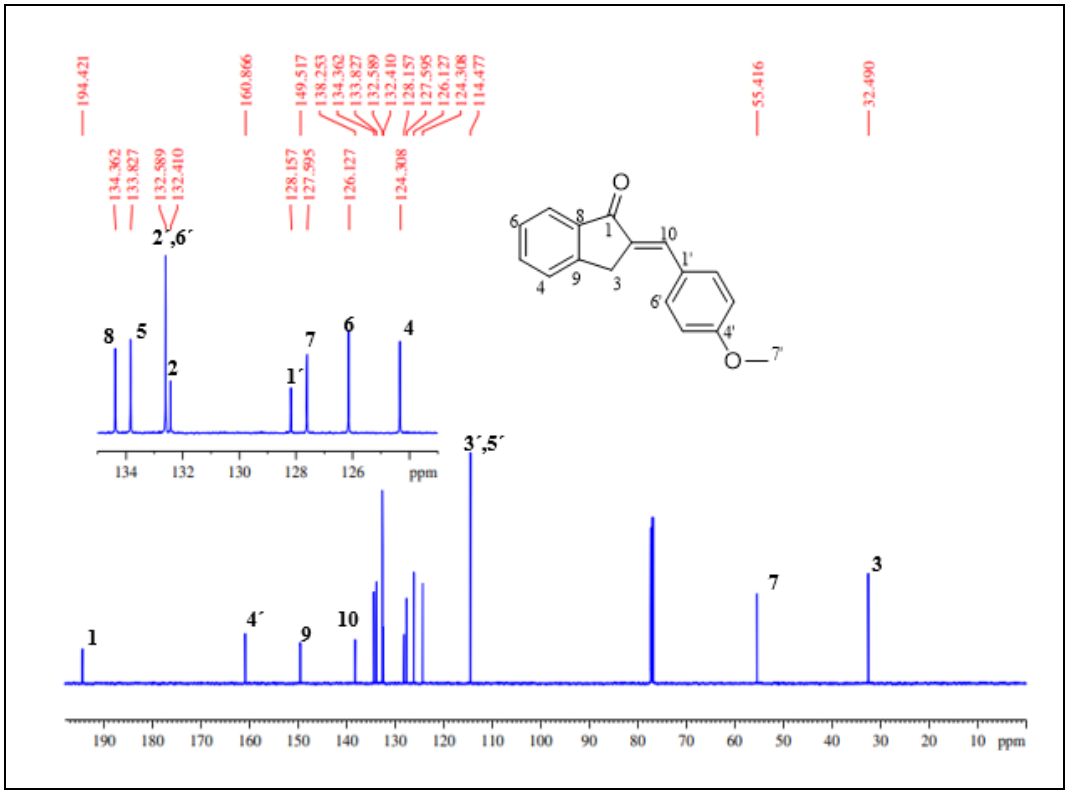

Figure S30: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3h**

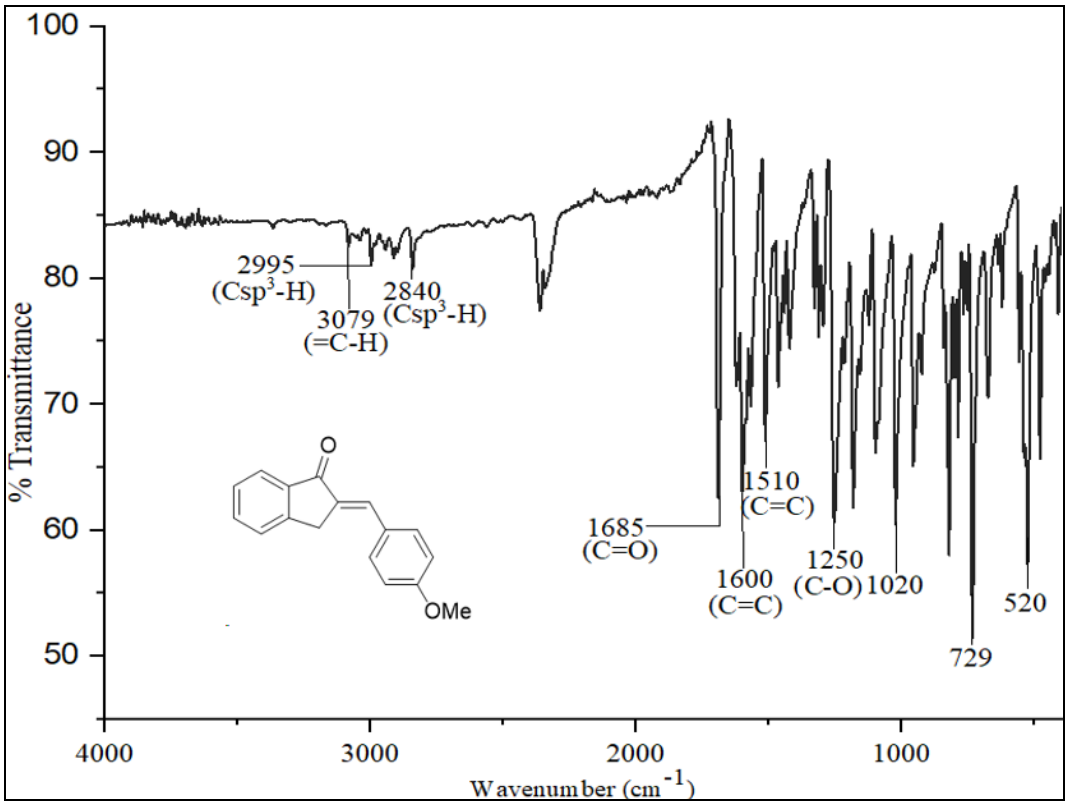

Figure S31: FT-IR Spectrum of **3h**

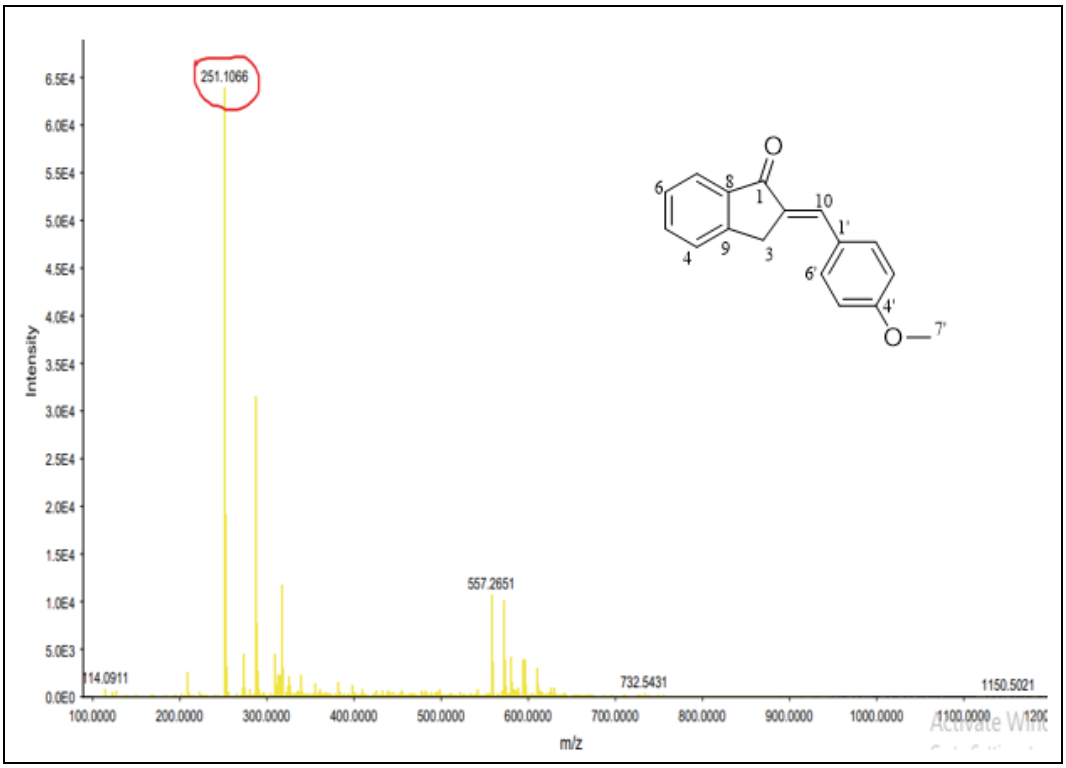

Figure S32: HRMS Spectrum of **3h**

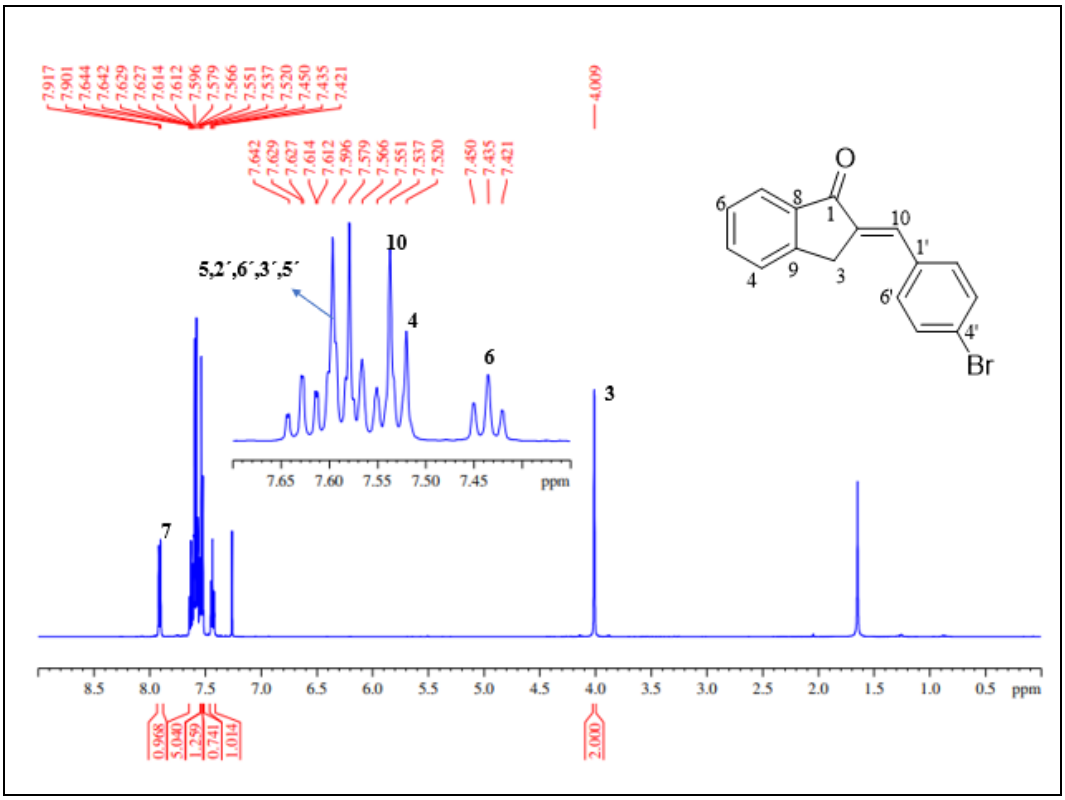

Figure S33: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3i**

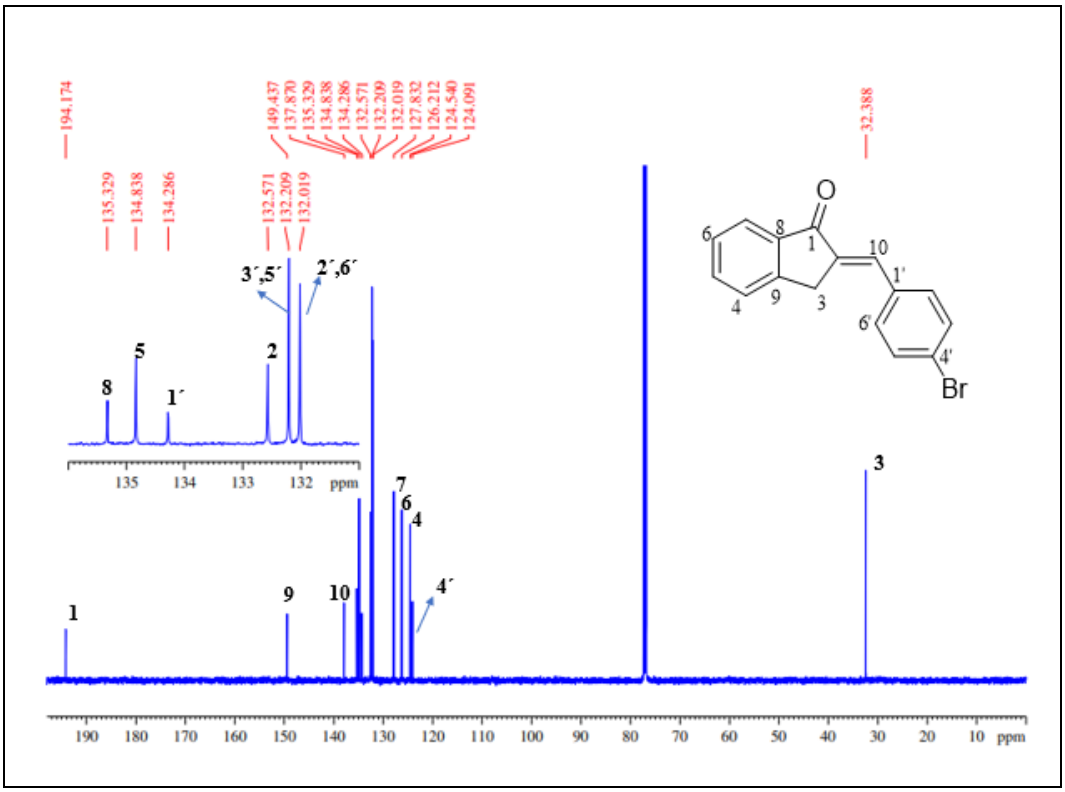

Figure S34: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3i**

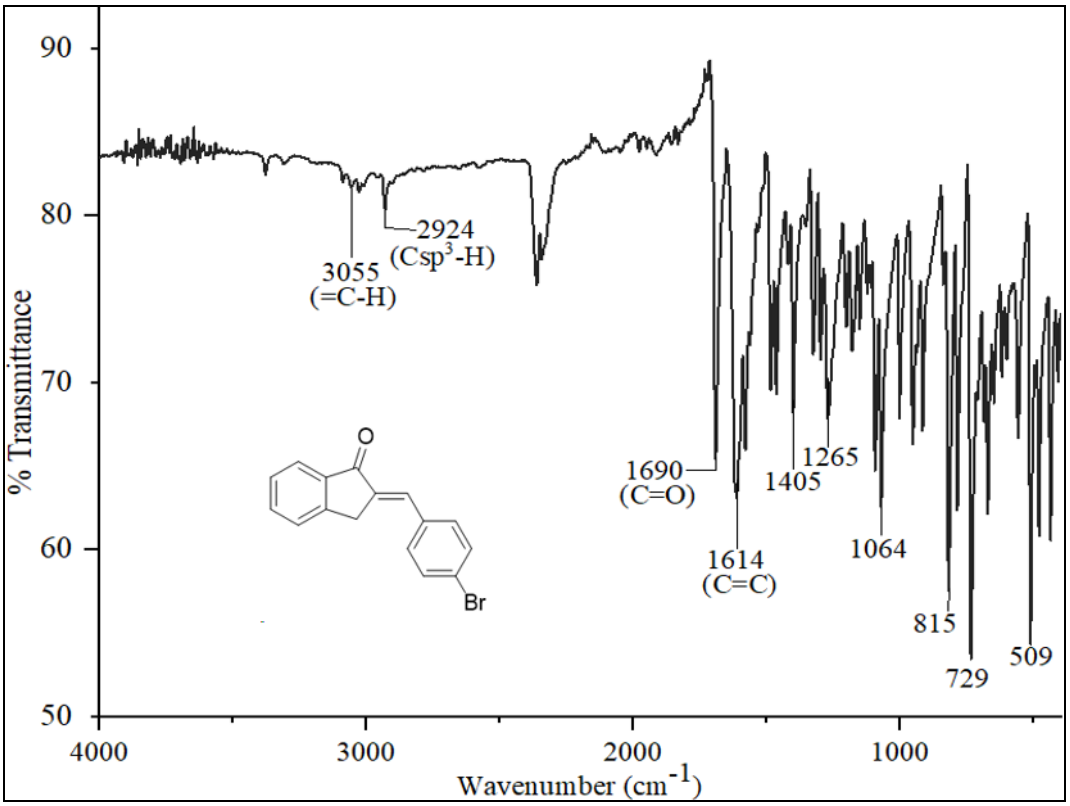

Figure S35: FT-IR Spectrum of **3i**

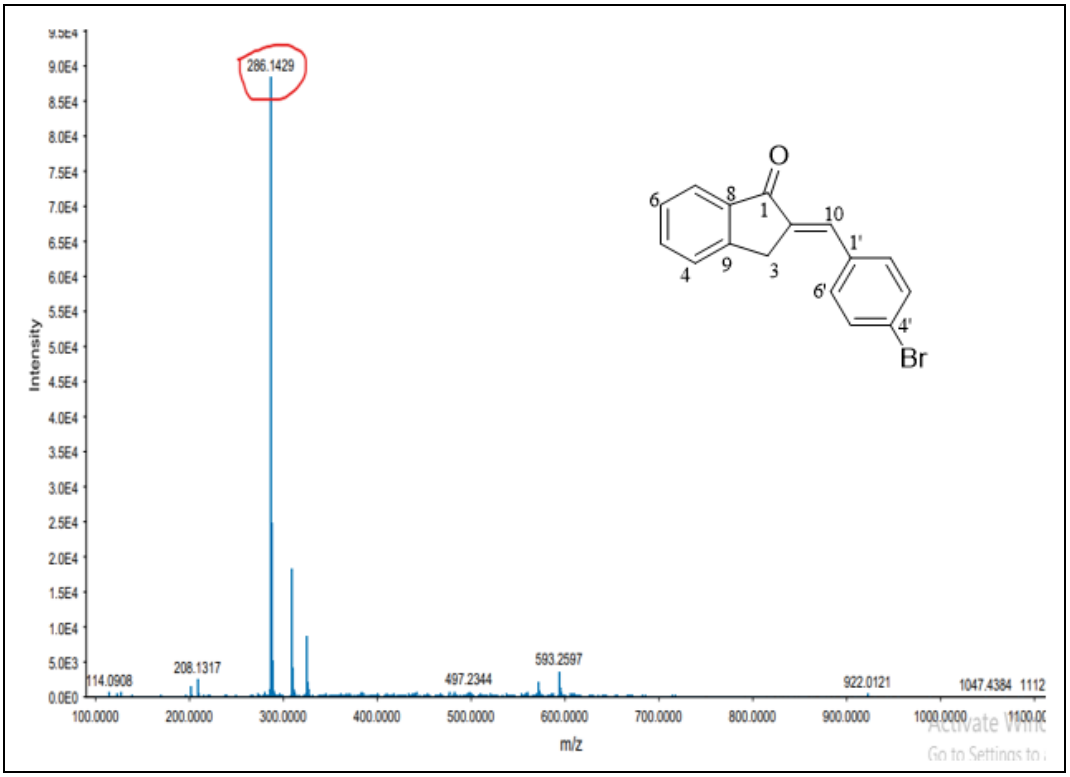

Figure S36: HRMS Spectrum of **3i**

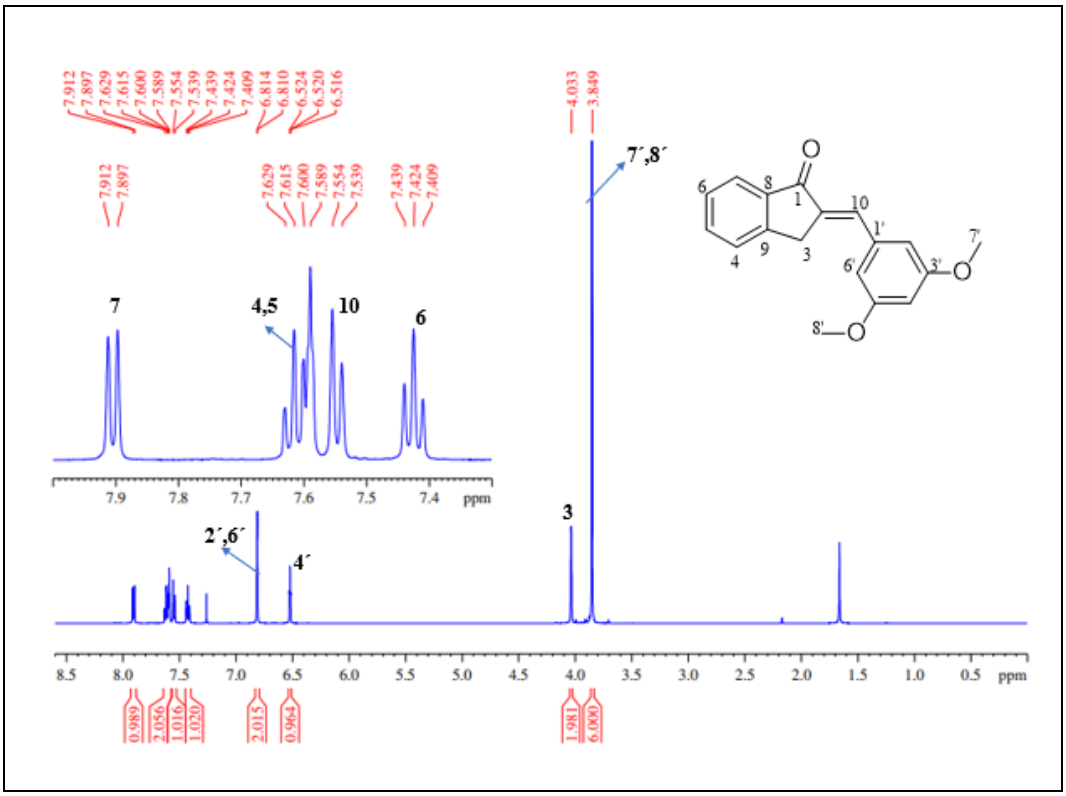

Figure S37: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3j**

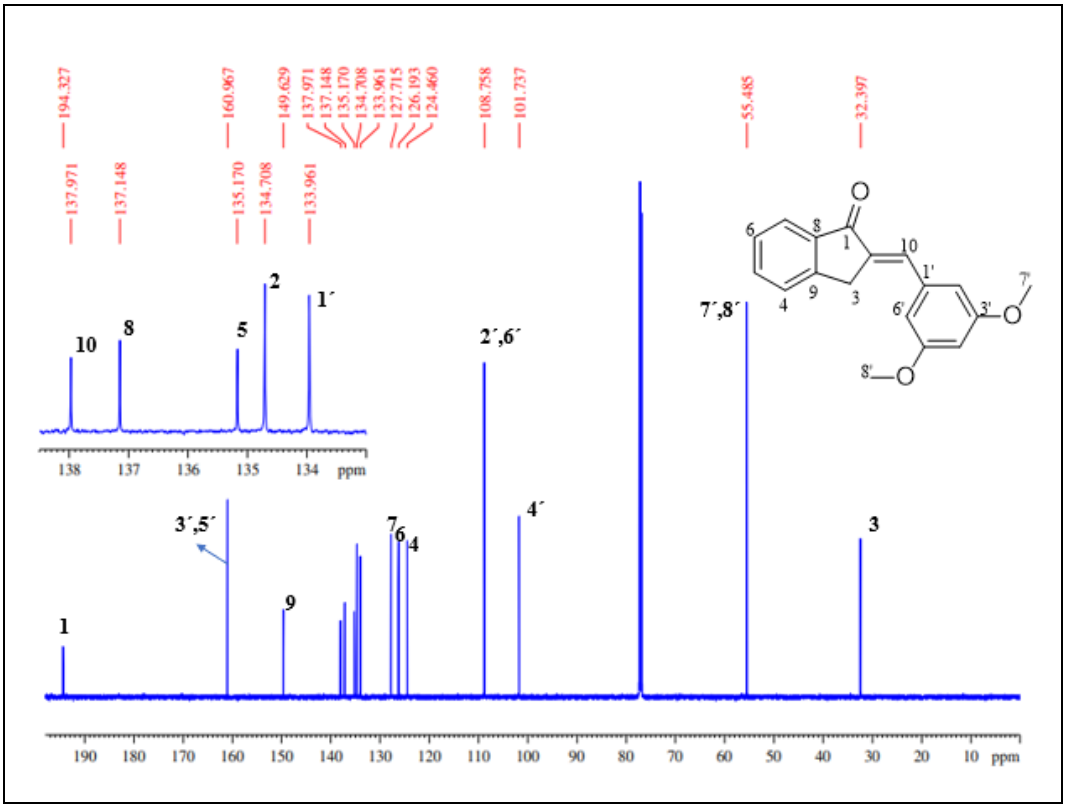

Figure S38: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3j**

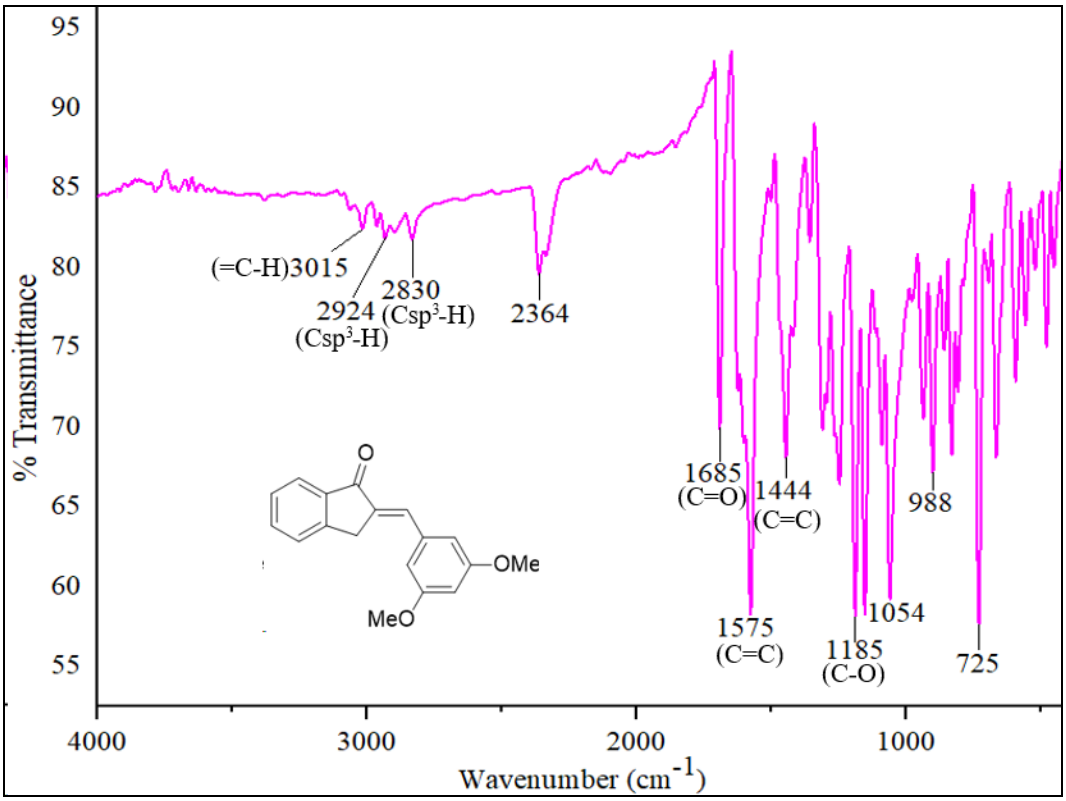

Figure S39: FT-IR Spectrum of **3j**

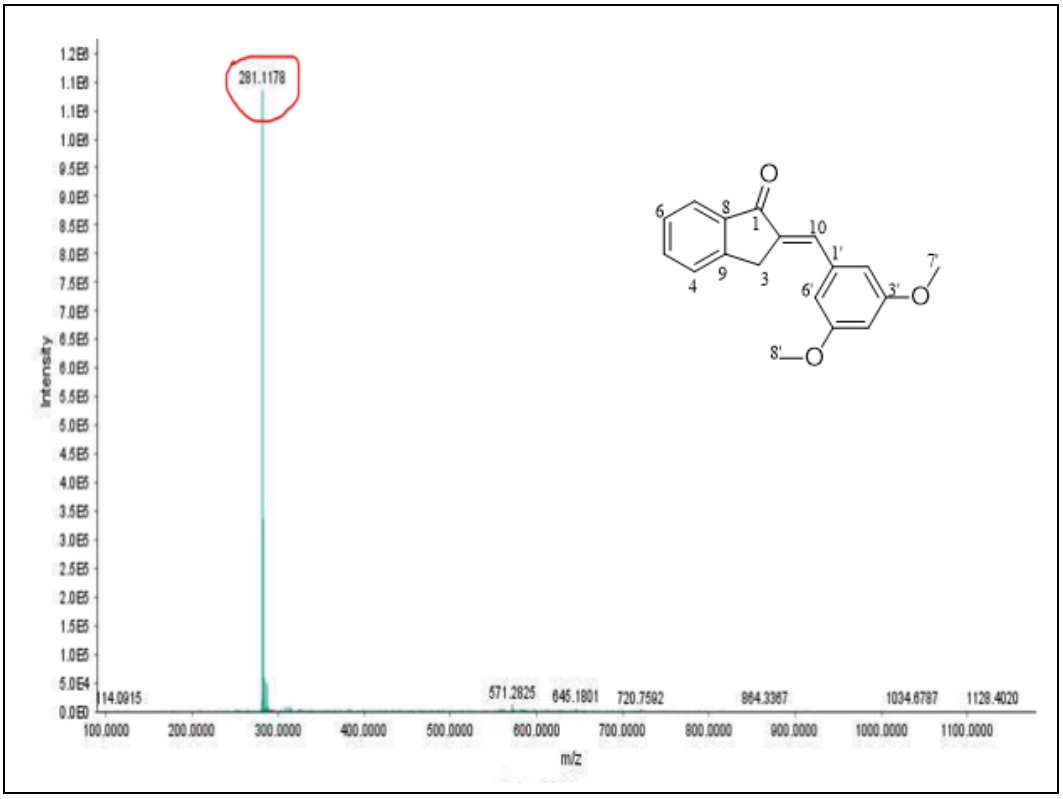

Figure S40: HRMS Spectrum of **3j**

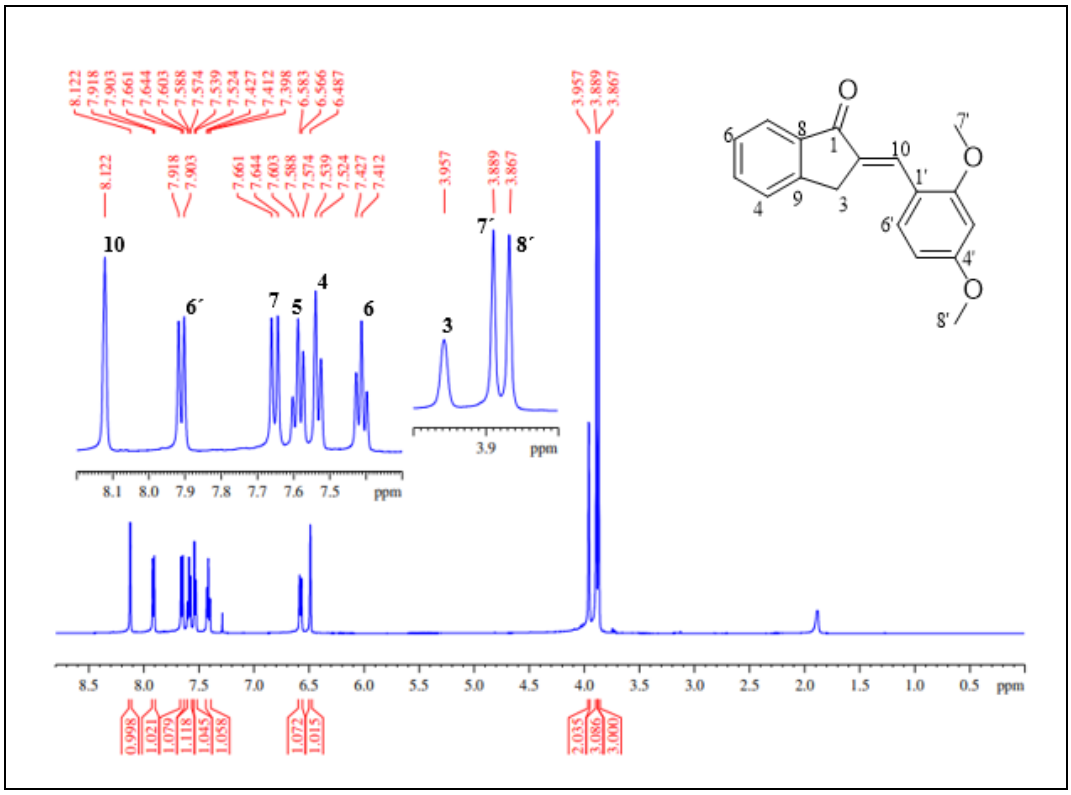

Figure S41: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3k**

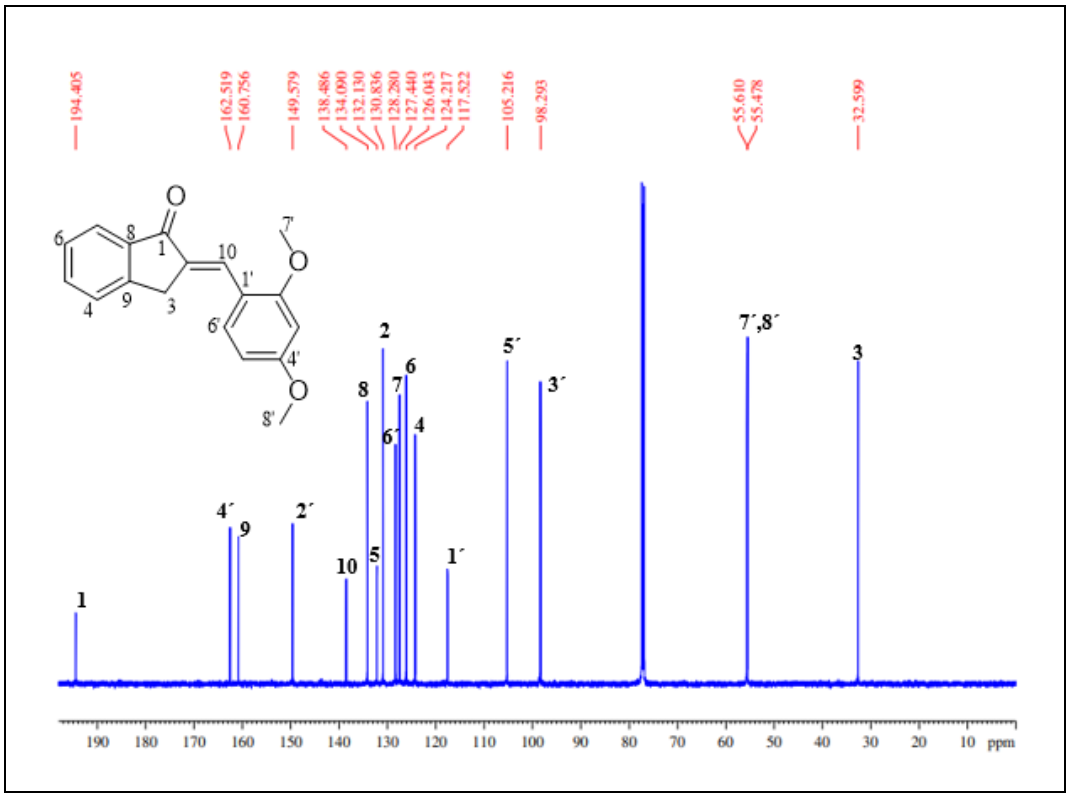

Figure S42: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3k**

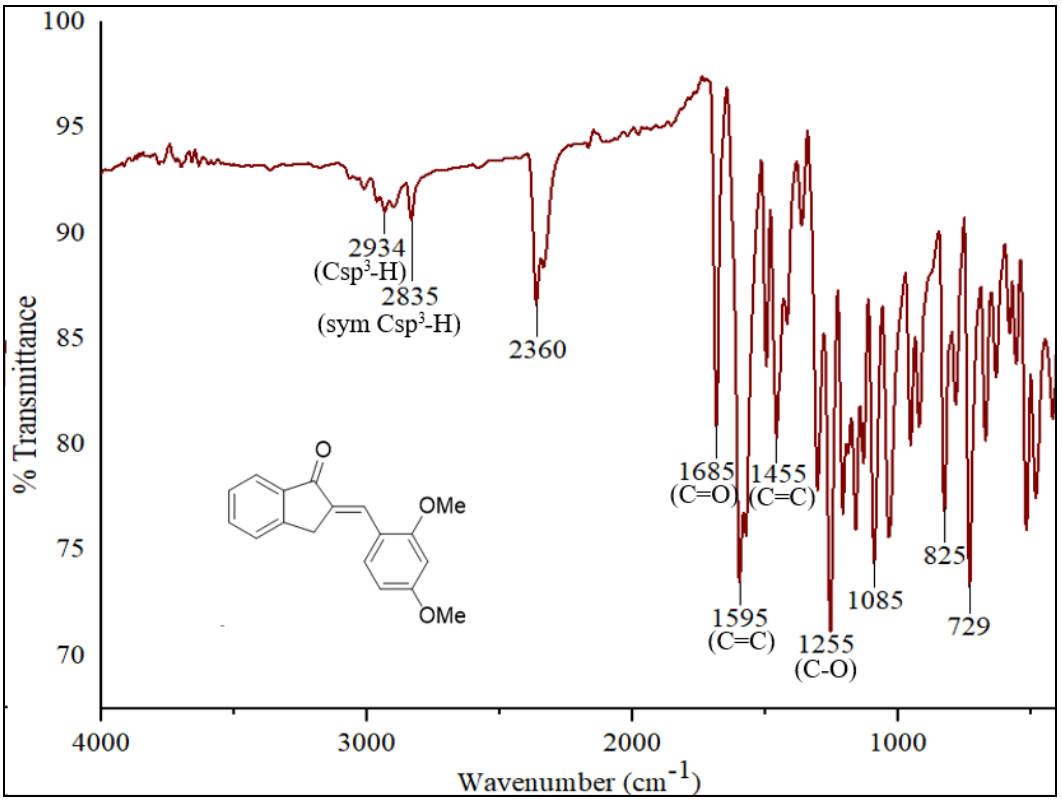

Figure S43: FT-IR Spectrum of **3k**

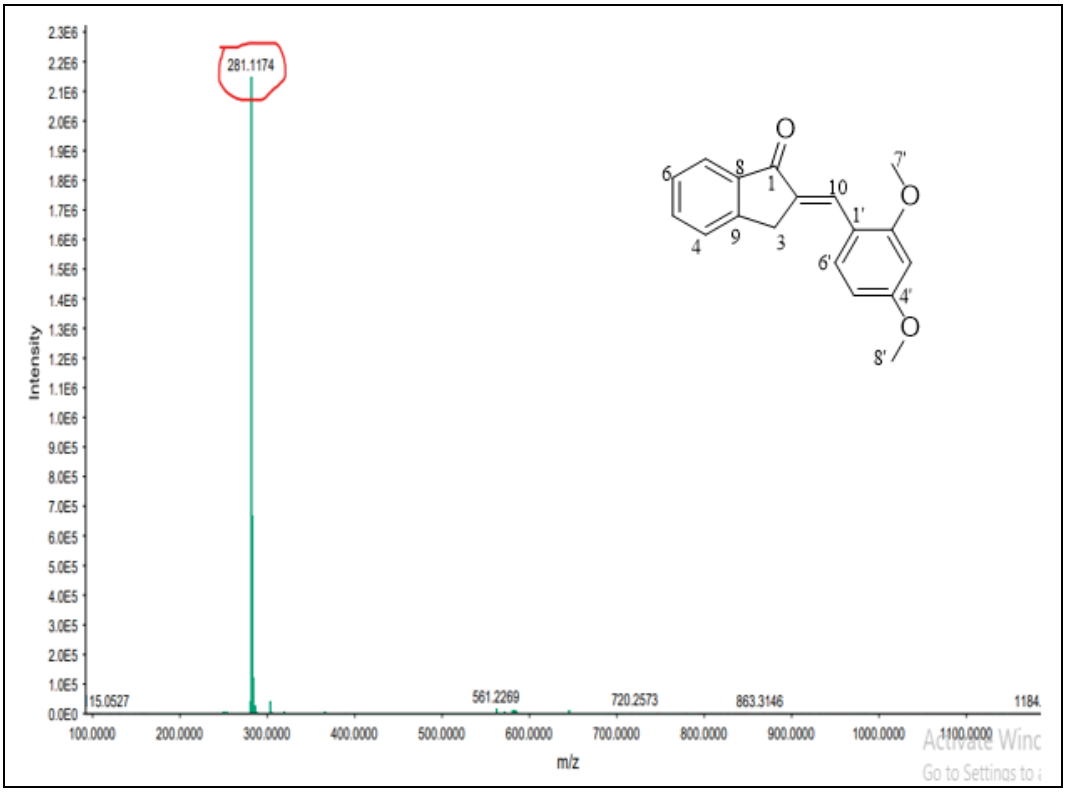

Figure S44: HRMS Spectrum of **3k**

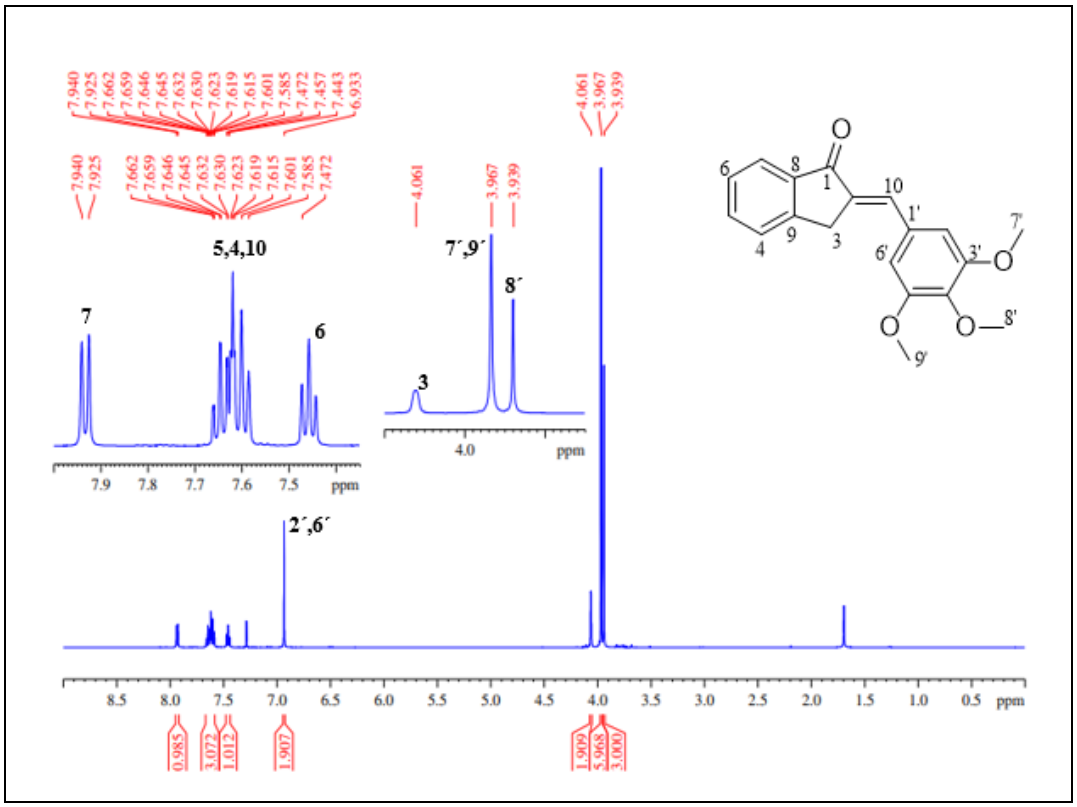

Figure S45: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3l**

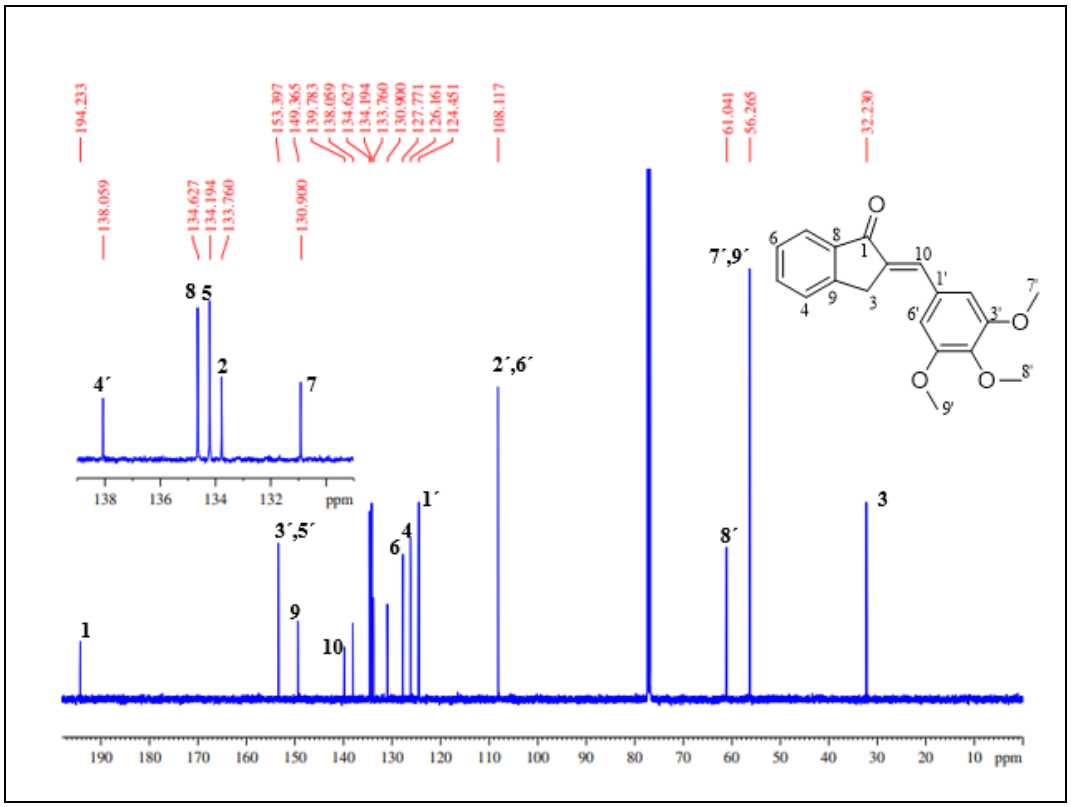

Figure S46: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3l**

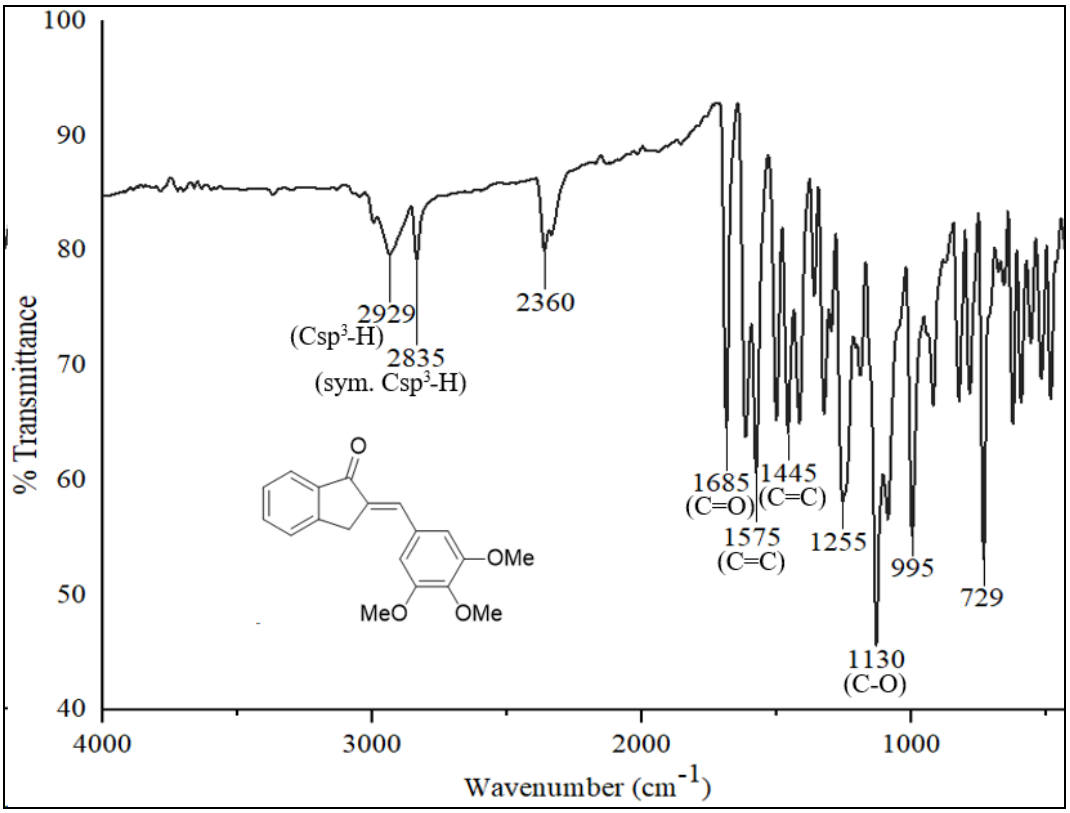

Figure S47: FT-IR Spectrum of **3l**

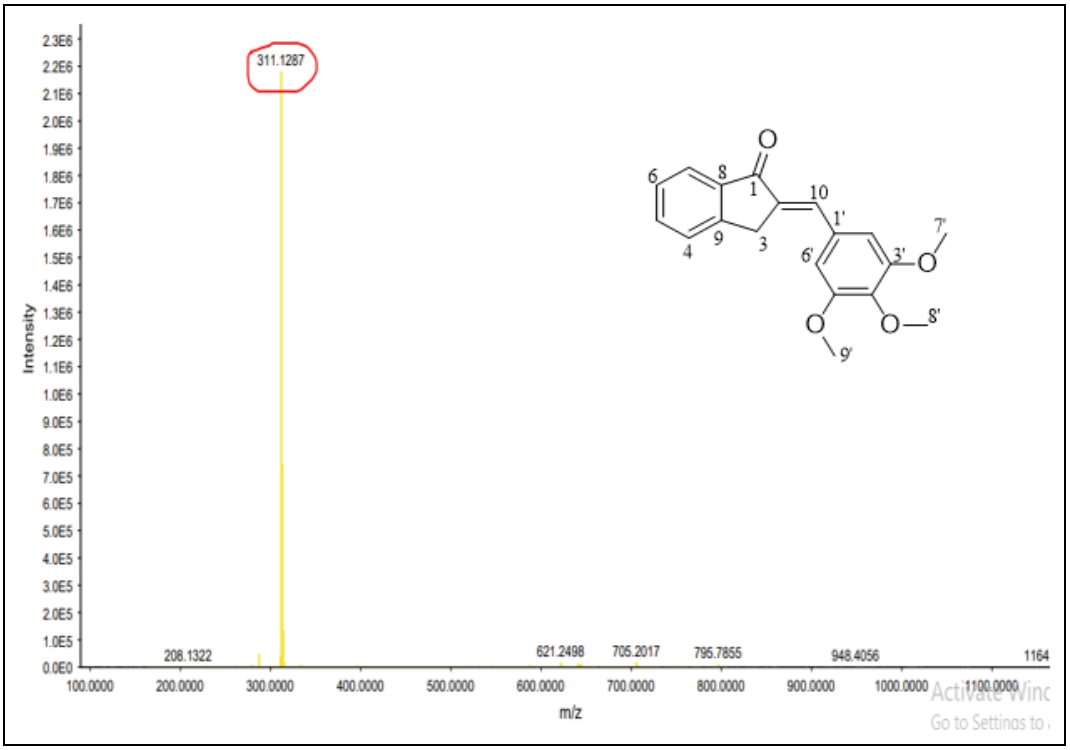

Figure S48: HRMS Spectrum of **3l**

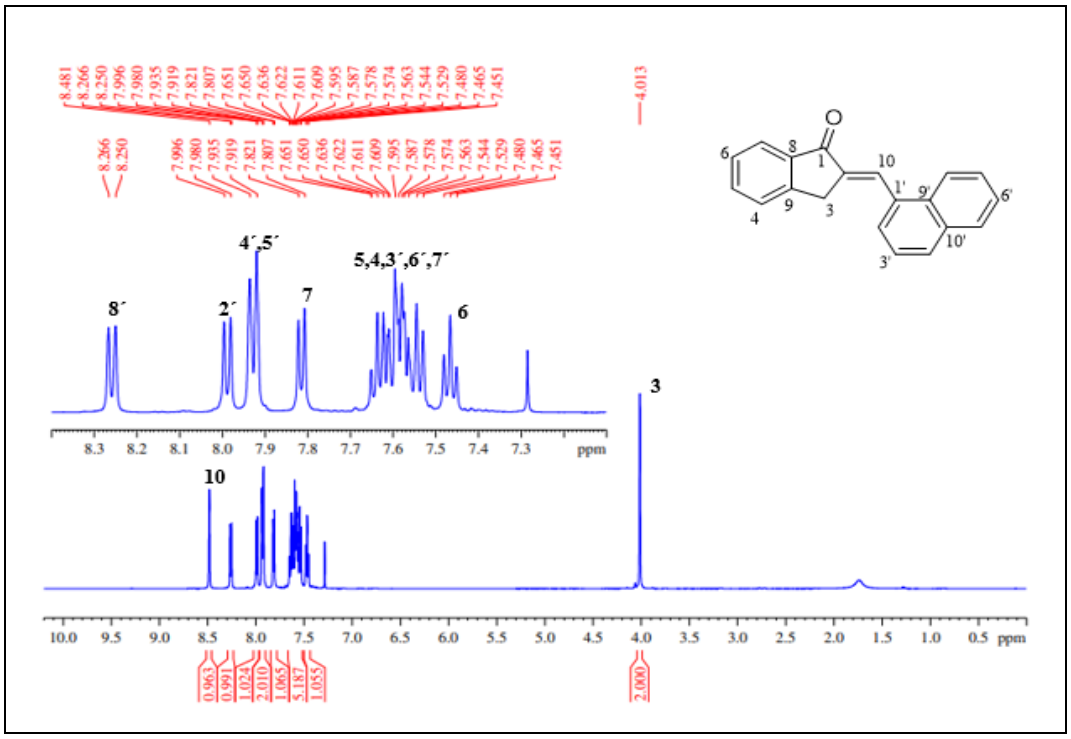

Figure S49: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3m**

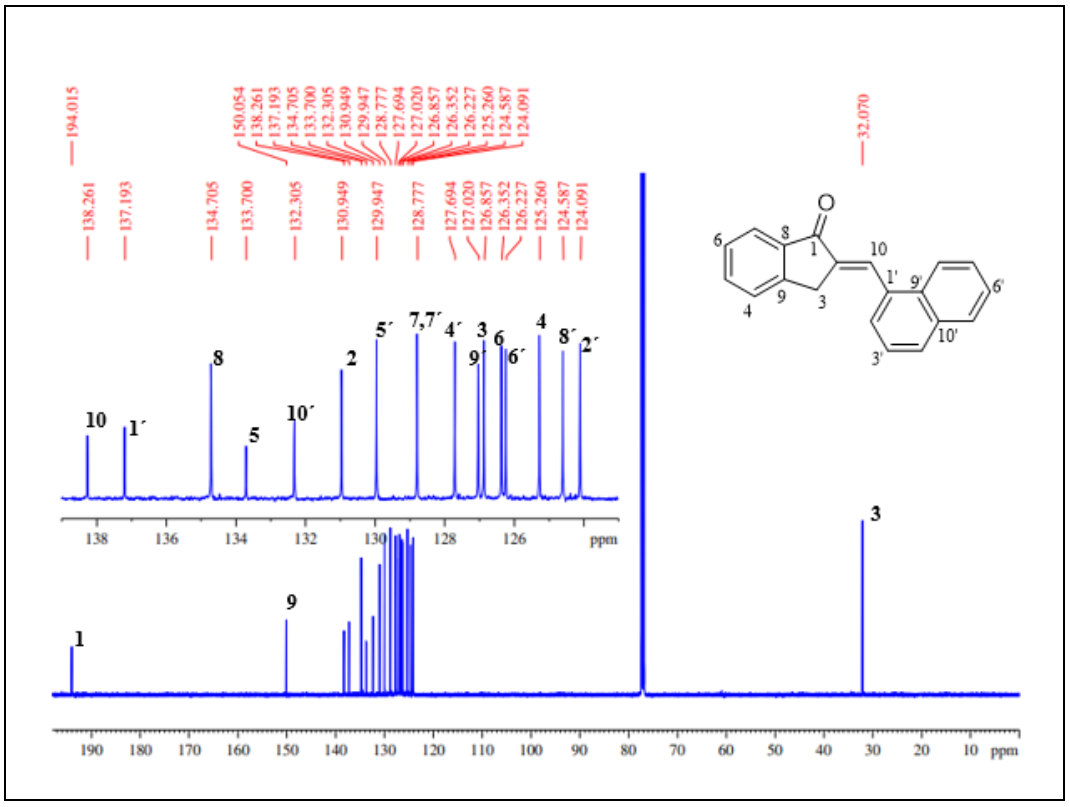

Figure S50: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3m**

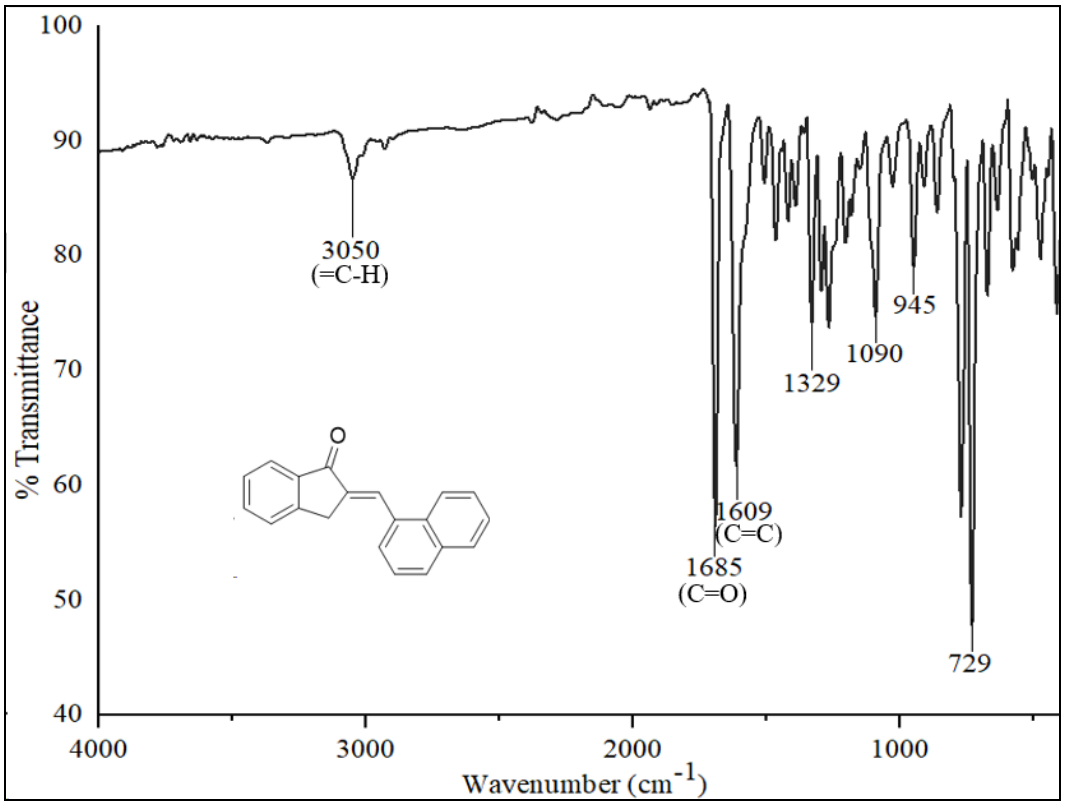

Figure S51: FT-IR Spectrum of **3m**

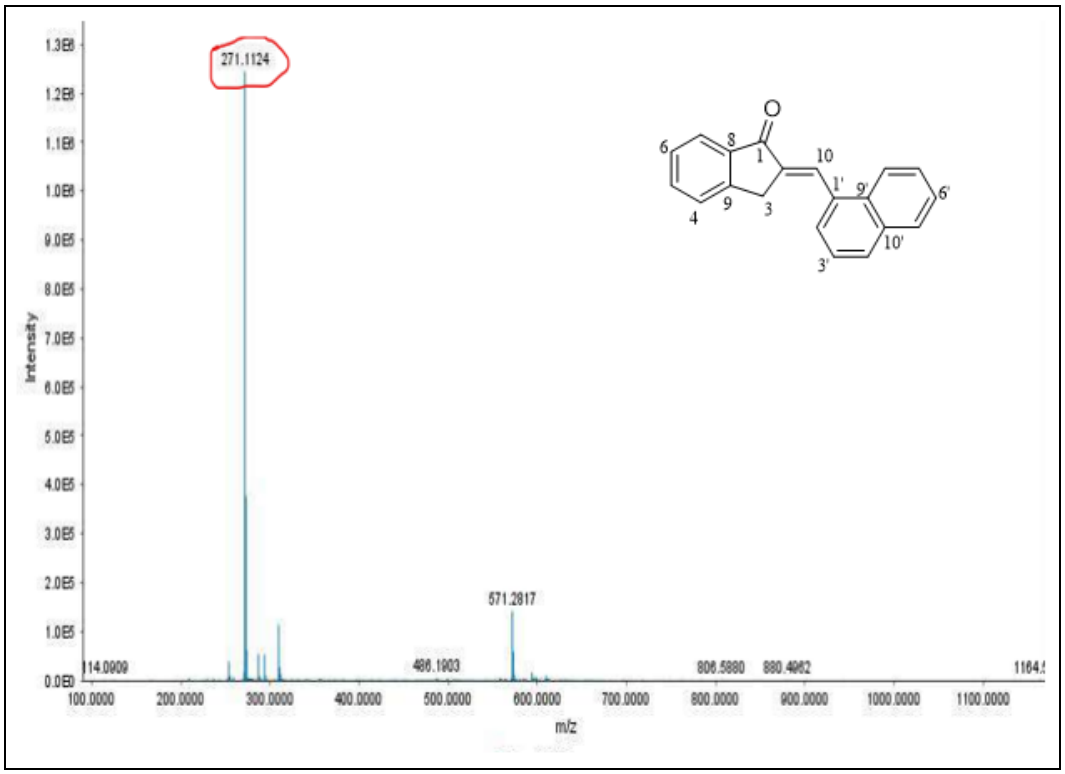

Figure S52: HRMS Spectrum of **3m**

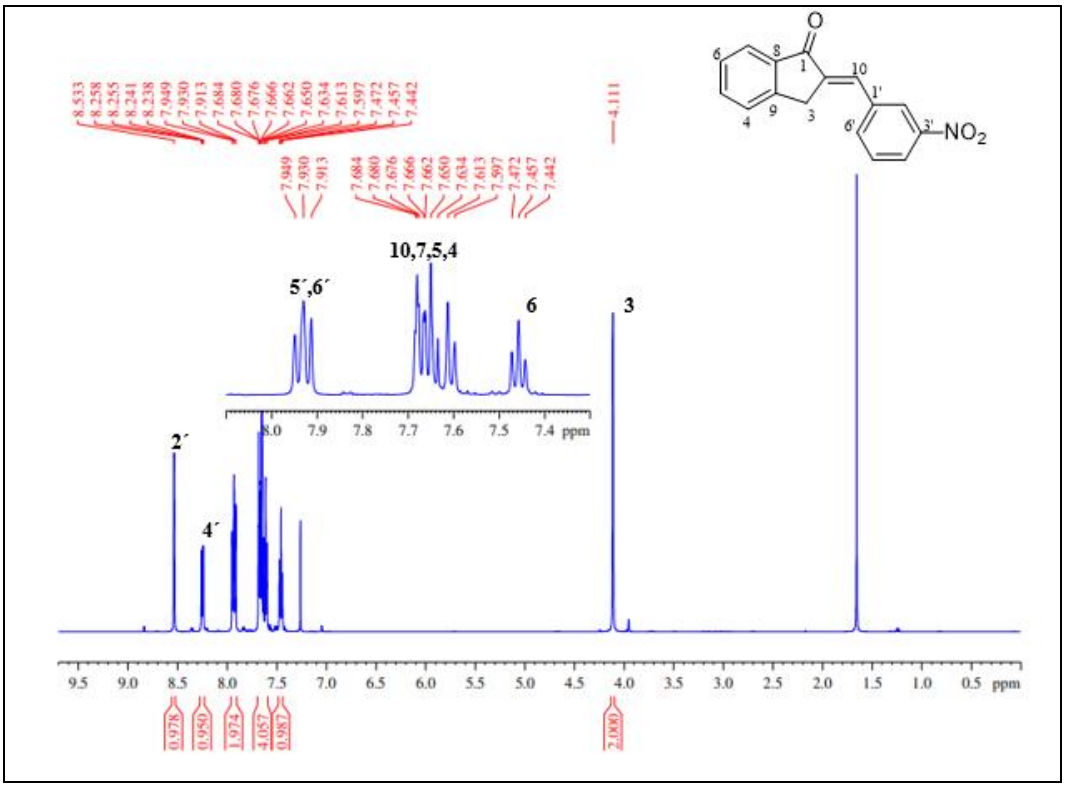

Figure S53: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3n**

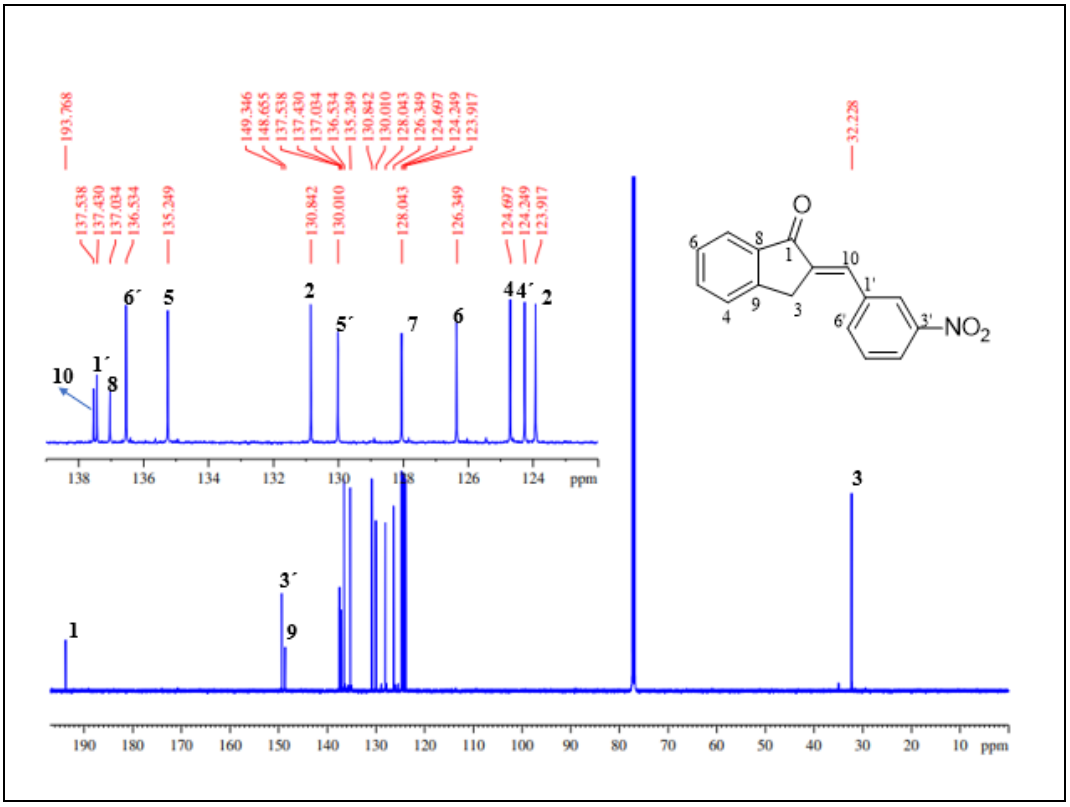

Figure S54: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3n**

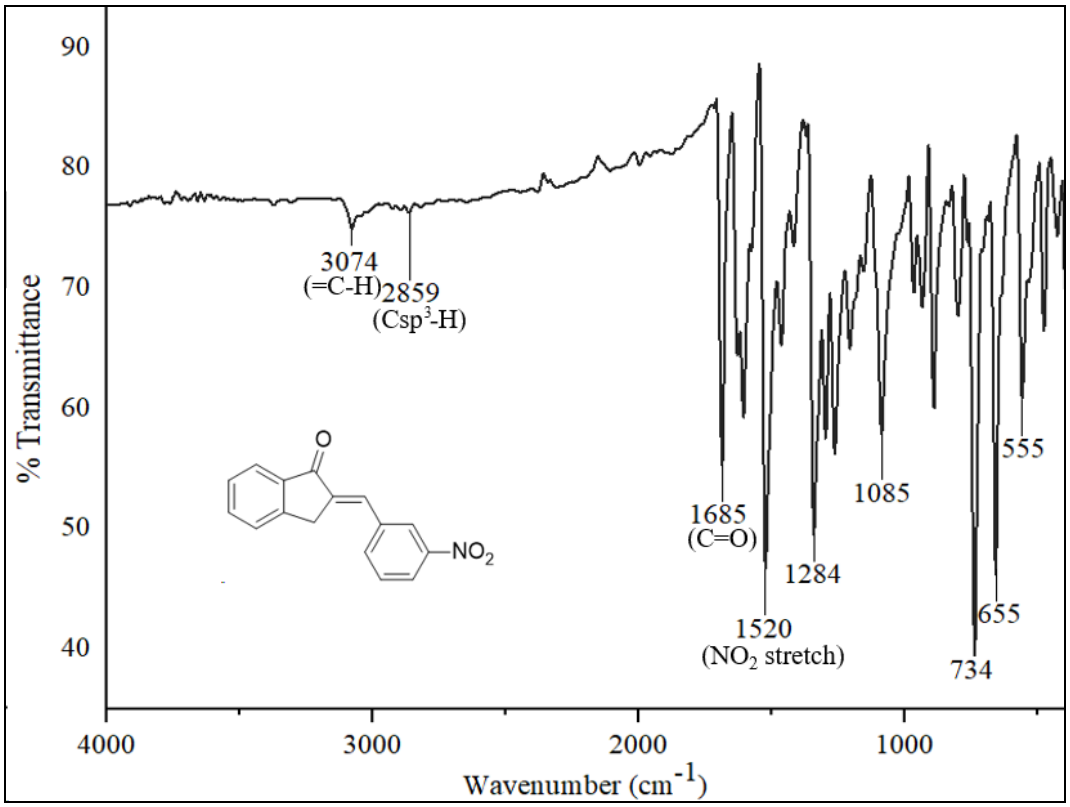

Figure S55: FT-IR Spectrum of **3n**

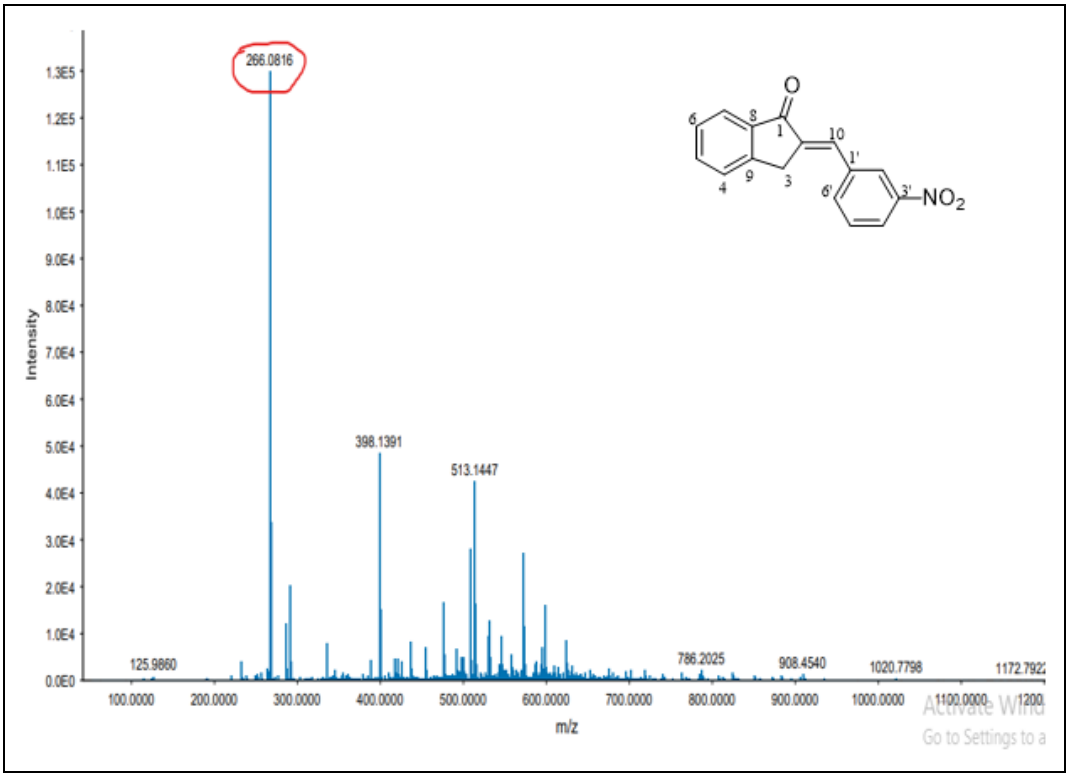

Figure S56: HRMS Spectrum of **3n**

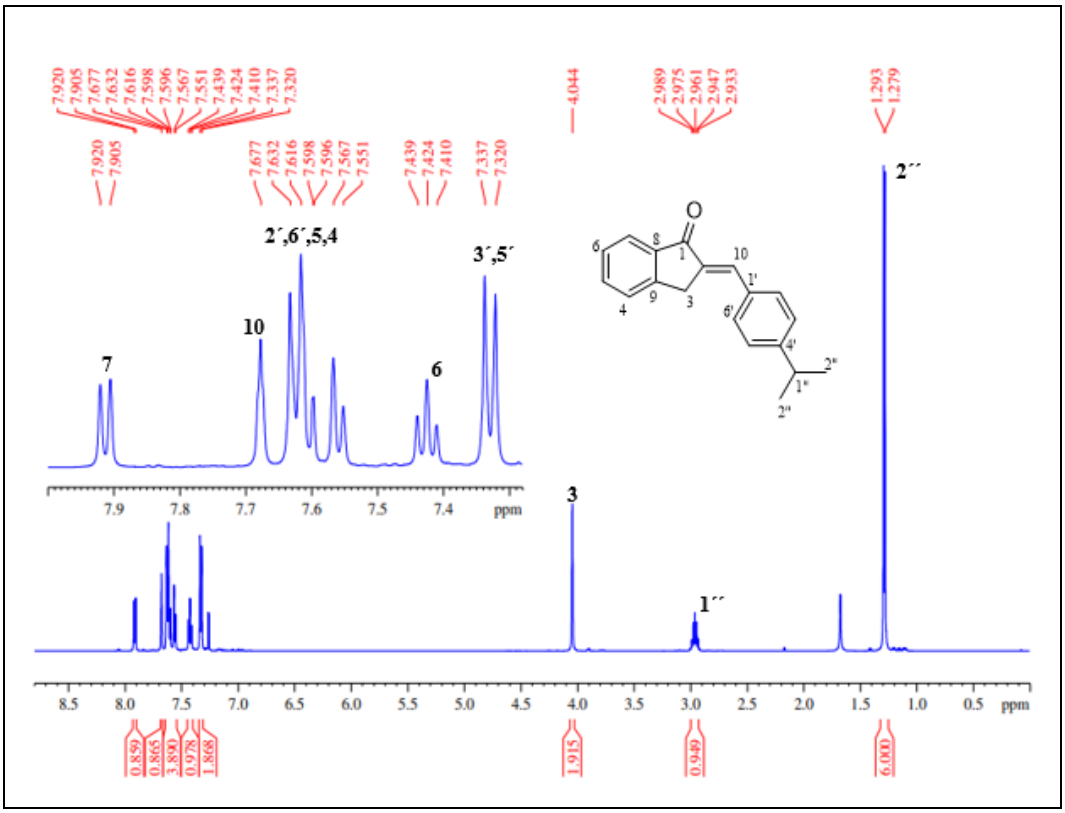

Figure S57: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3o**

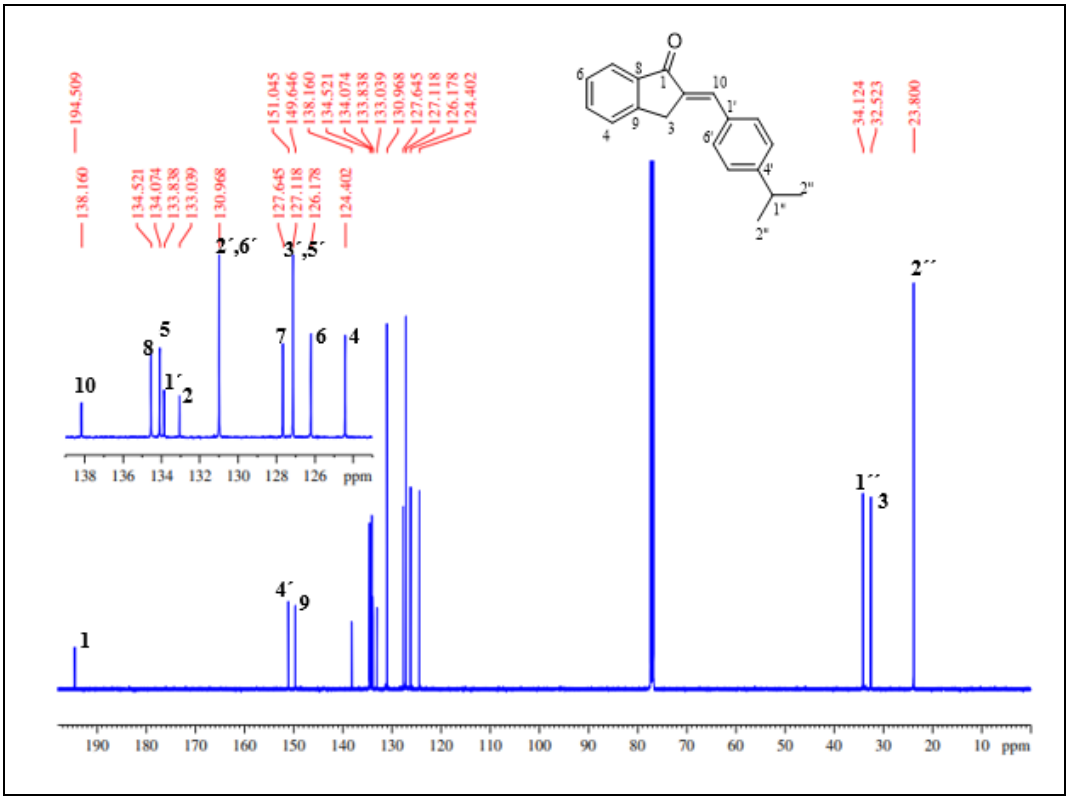

Figure S58: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3o**

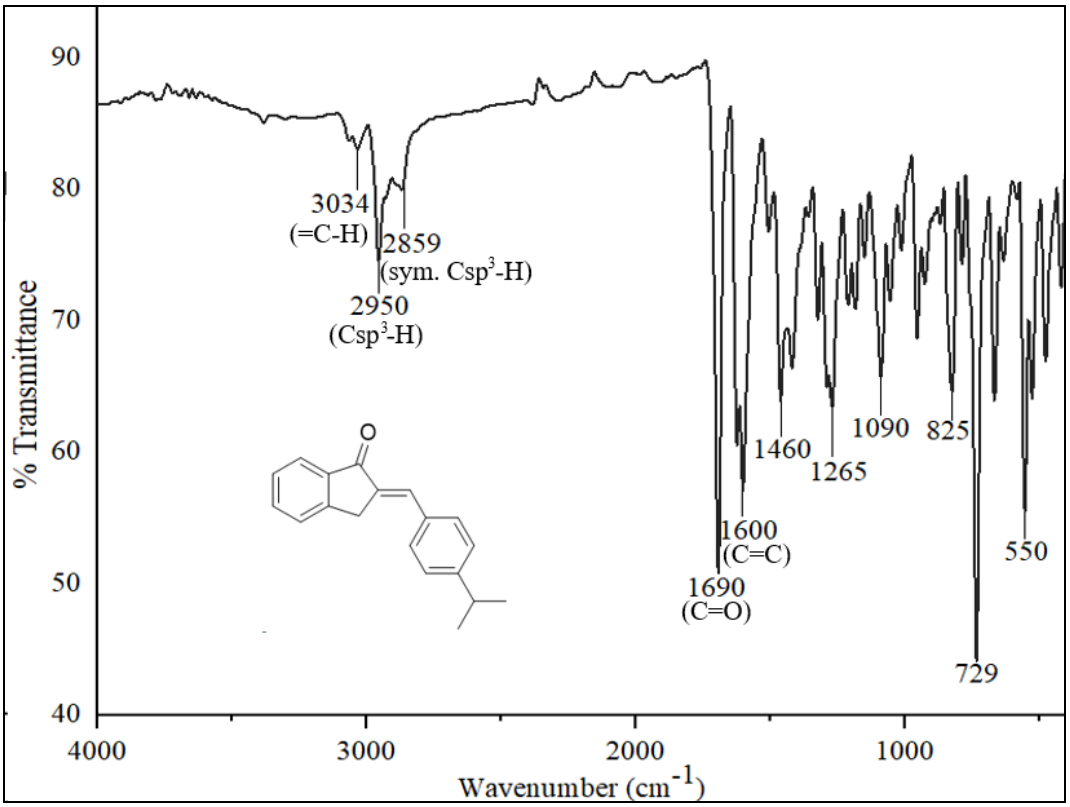

Figure S59: FT-IR Spectrum of **3o**

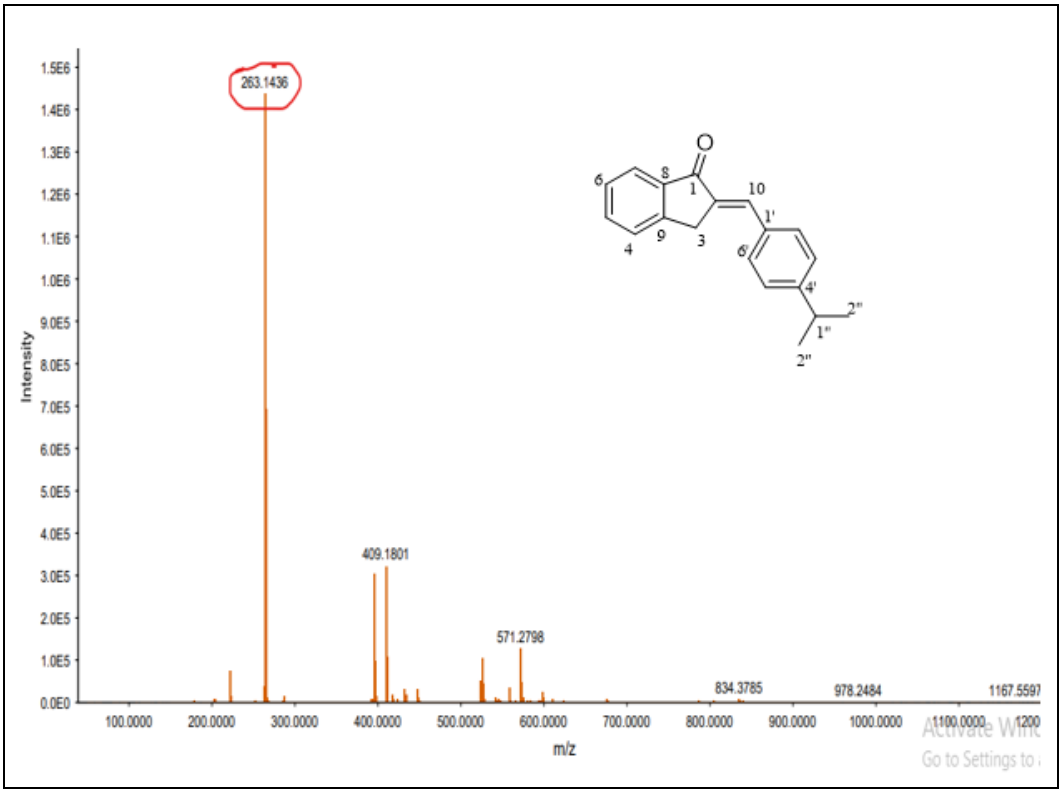

Figure S60: HRMS Spectrum of **3o**

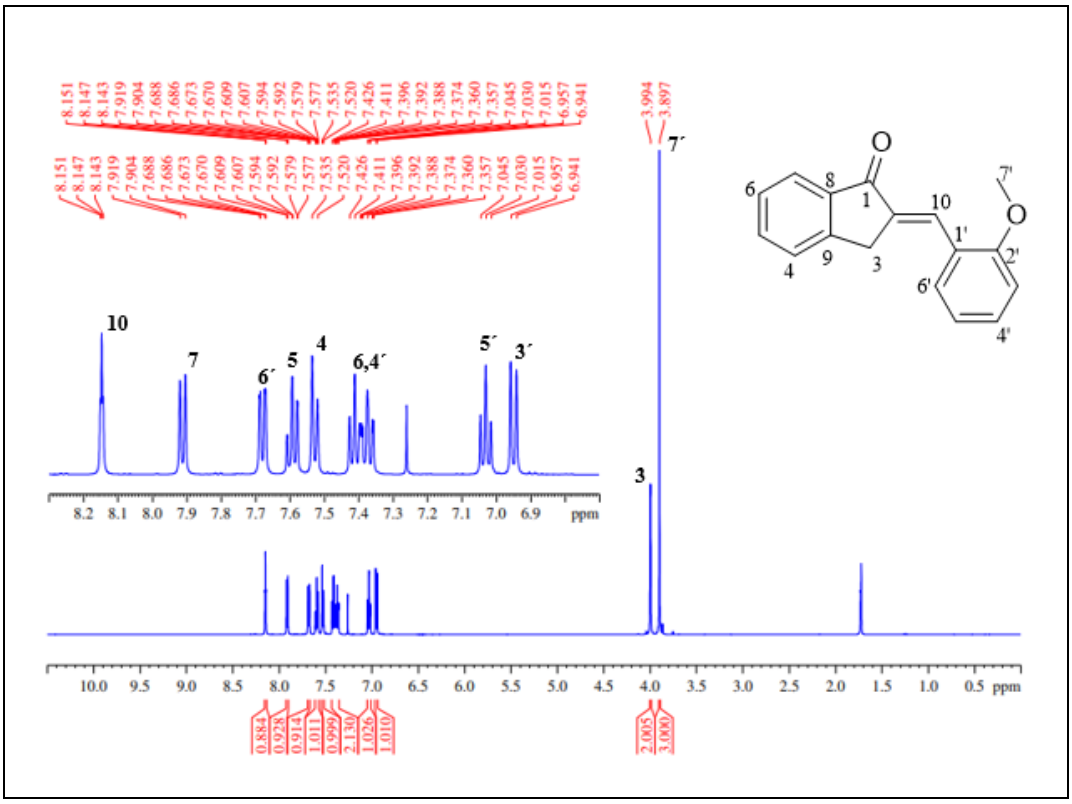

Figure S61: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum **3p**

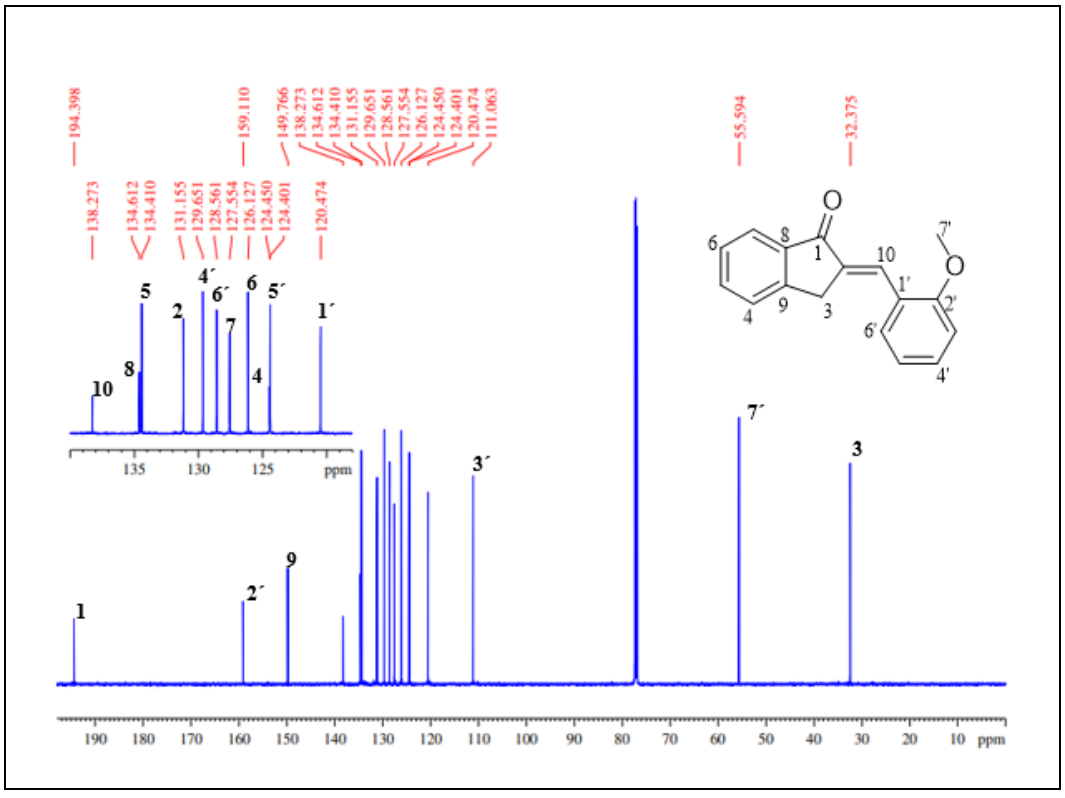

Figure S62: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of **3p**

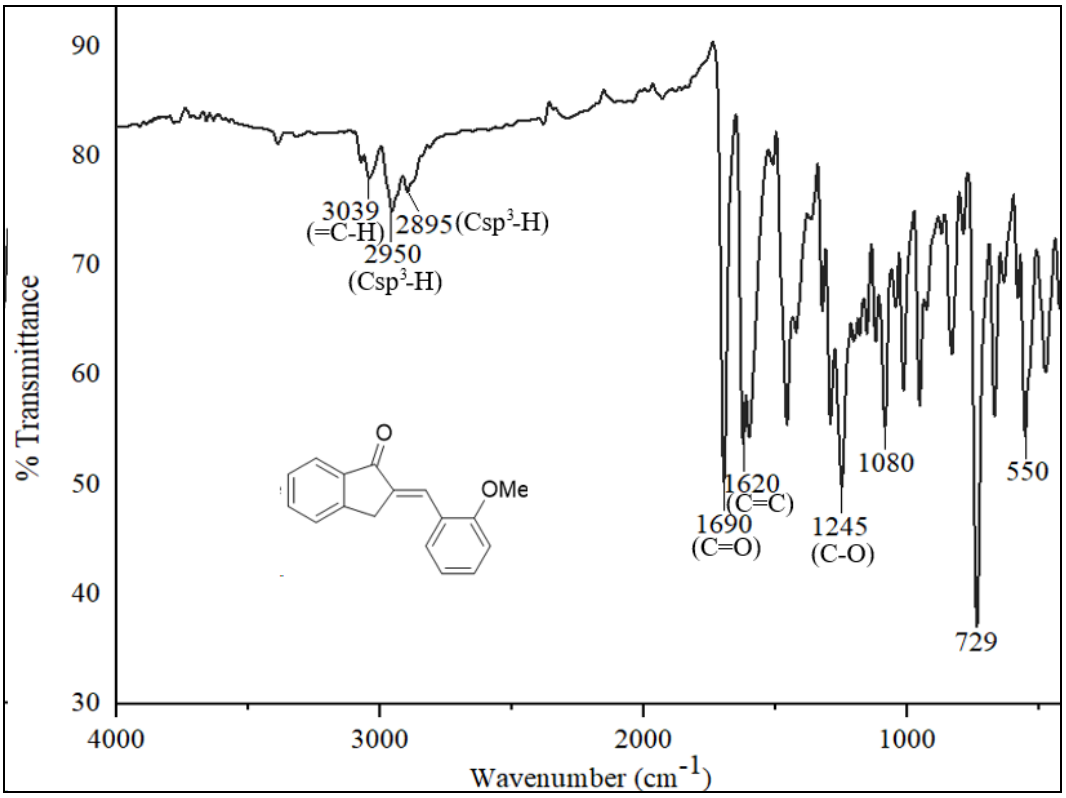

Figure S63: FT-IR Spectrum of **3p**

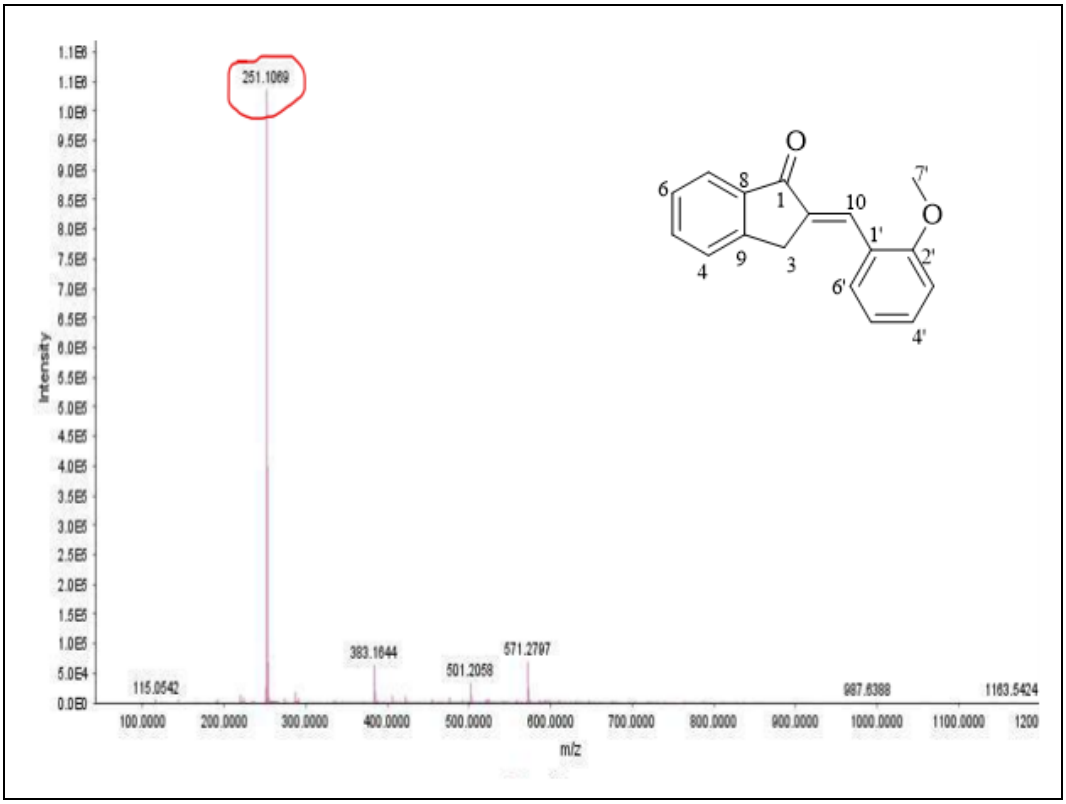

Figure S64: HRMS Spectrum of **3p**

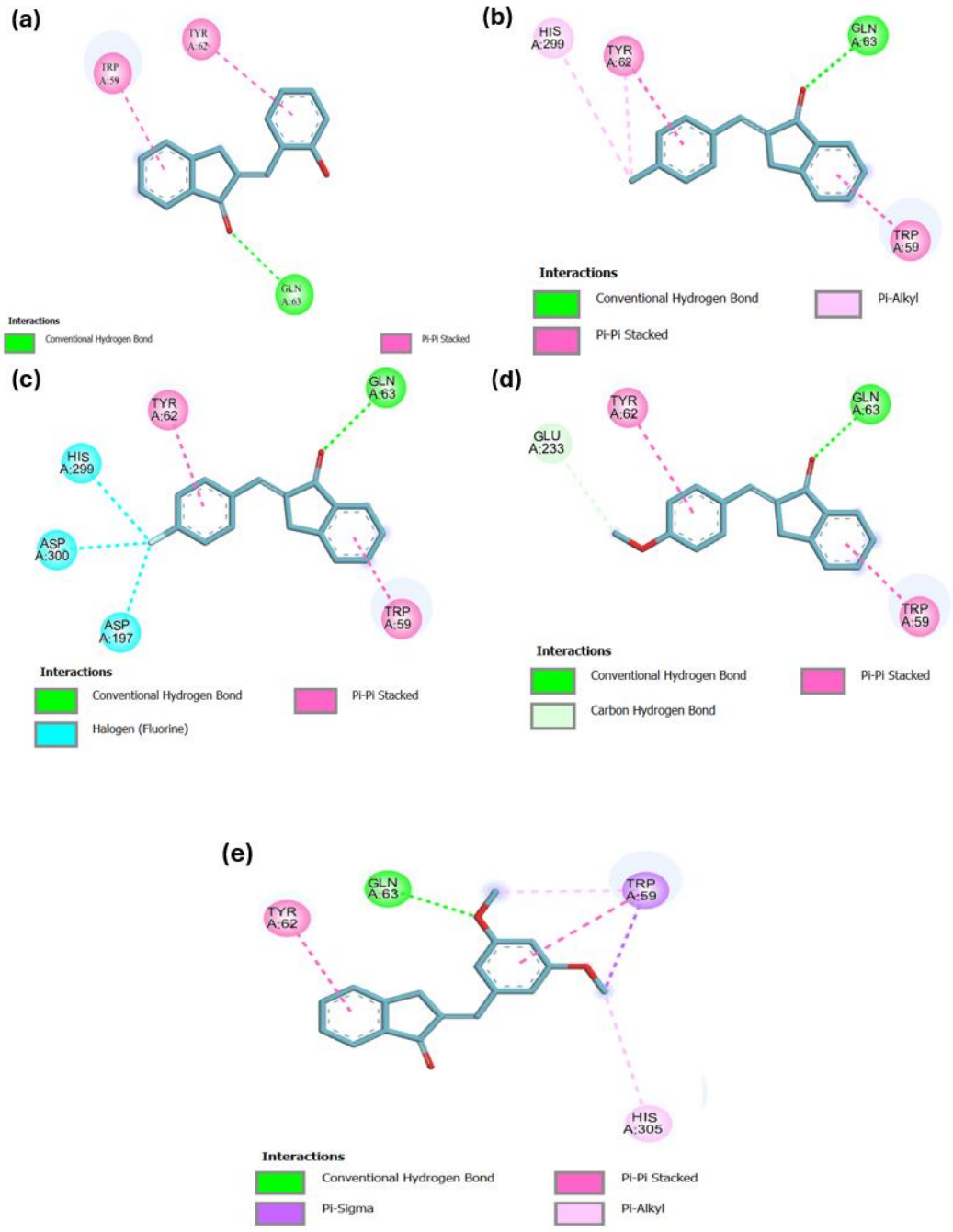

Figure S65: 2D representations of the binding modes of compounds **3a** (a), **3e** (b), **3g** (c), **3h** (d), **3j** (e) to human pancreatic α-amylase (PDB ID: 2QV4).

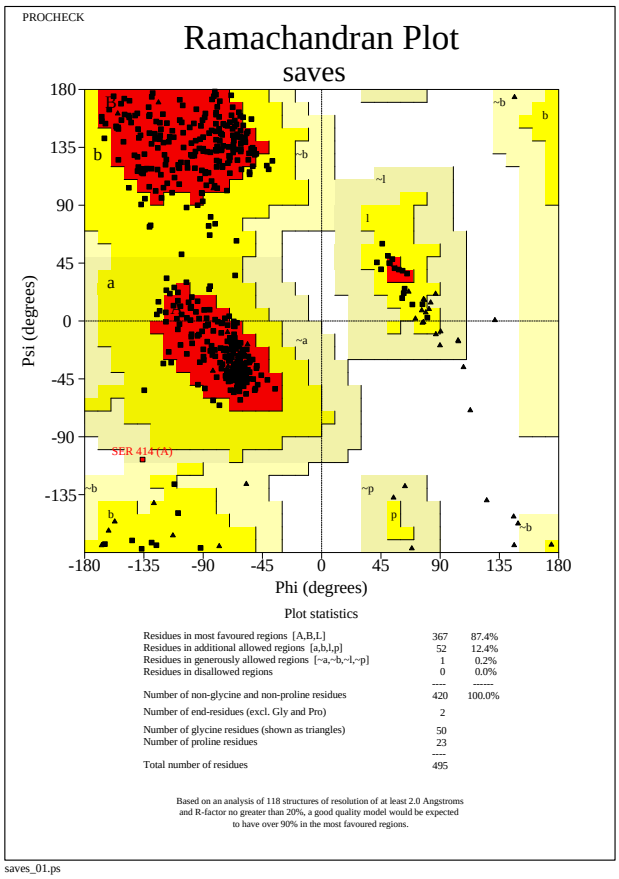

Figure S66. Ramachandran plot of human p pancreatic α-amylase (PDB ID: 2QV4) showing the distribution of phi (φ) and psi (ψ) dihedral angles.