

Supplementary Information

Synthesis, Cytotoxicity and Molecular Docking Studies of the 9-Substituted 5-Styryltetrazolo[1,5-*c*]quinazoline Derivatives

Malose J. Mphahlele ^{1,*}, Samantha Gildenhuys ² and Nishal Parbhoo ²

¹ Department of Chemistry, University of South Africa, Private Bag X06, Florida 1710, South Africa

² Department of Life & Consumer Sciences, University of South Africa, Private Bag X06, Florida 1710, South Africa; gildes@unisa.ac.za (S.G.); parbhn1@unisa.ac.za (N.P.)

* Correspondence: mphahmj@unisa.ac.za; Tel.: +27-11-670-6301

S1. ¹H-NMR and ¹³C-NMR spectra of compounds **2–5**.

S2. Cytotoxicity and dose response curves of Melphalan and compounds **3–5** against HeLa cells.

S3. Cytotoxicity and dose response curves of Melphalan and compounds **3–5** against MCF-7 cells.

S4. Spread sheet for statistical analysis which contains p values for each test.

S1: ^1H NMR and ^{13}C NMR spectra of compounds 2–5

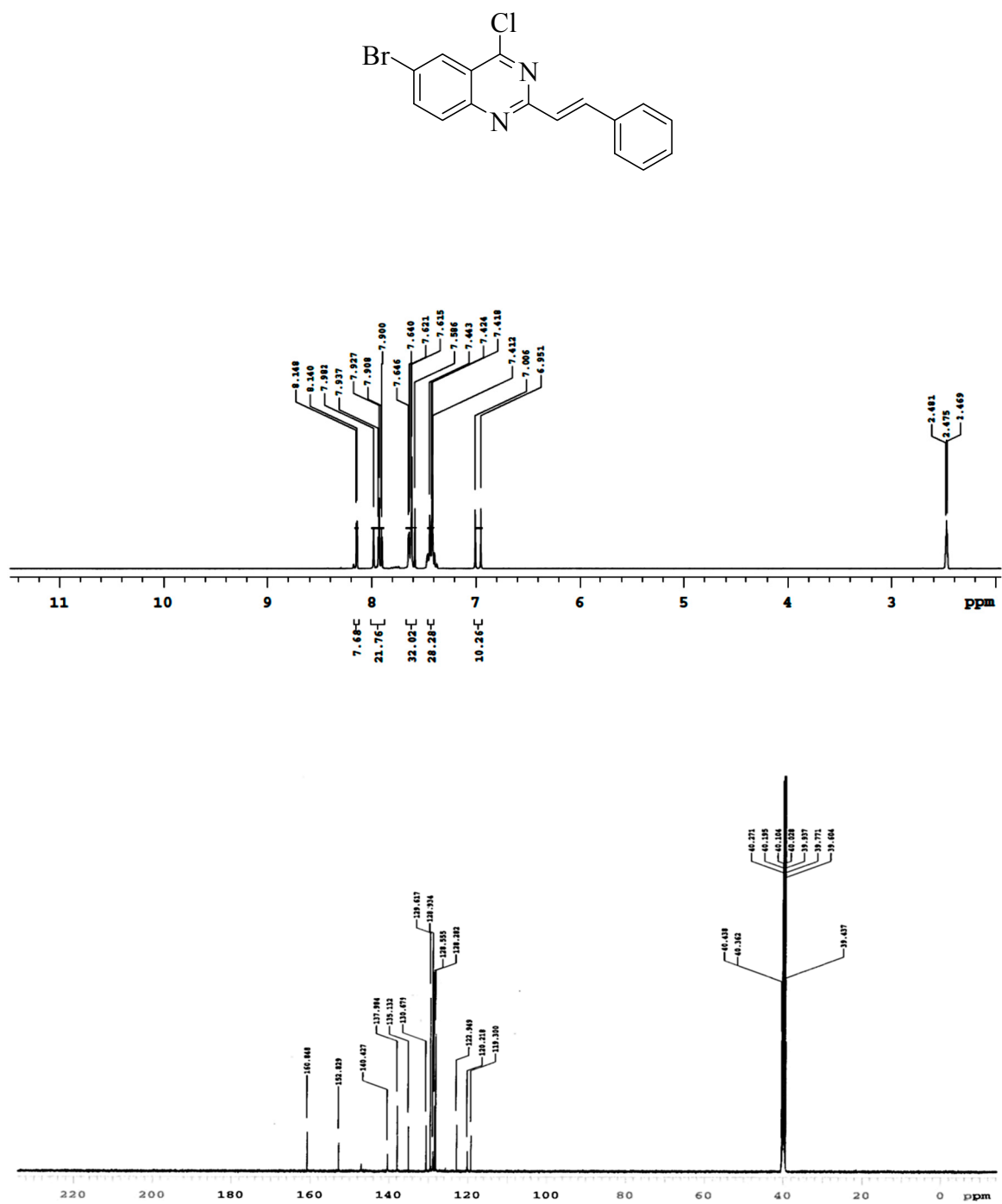


Figure S-1.1: ^1H NMR and ^{13}C NMR spectra of **2a** in DMSO- d_6 at 300 MHz and 75 MHz, respectively

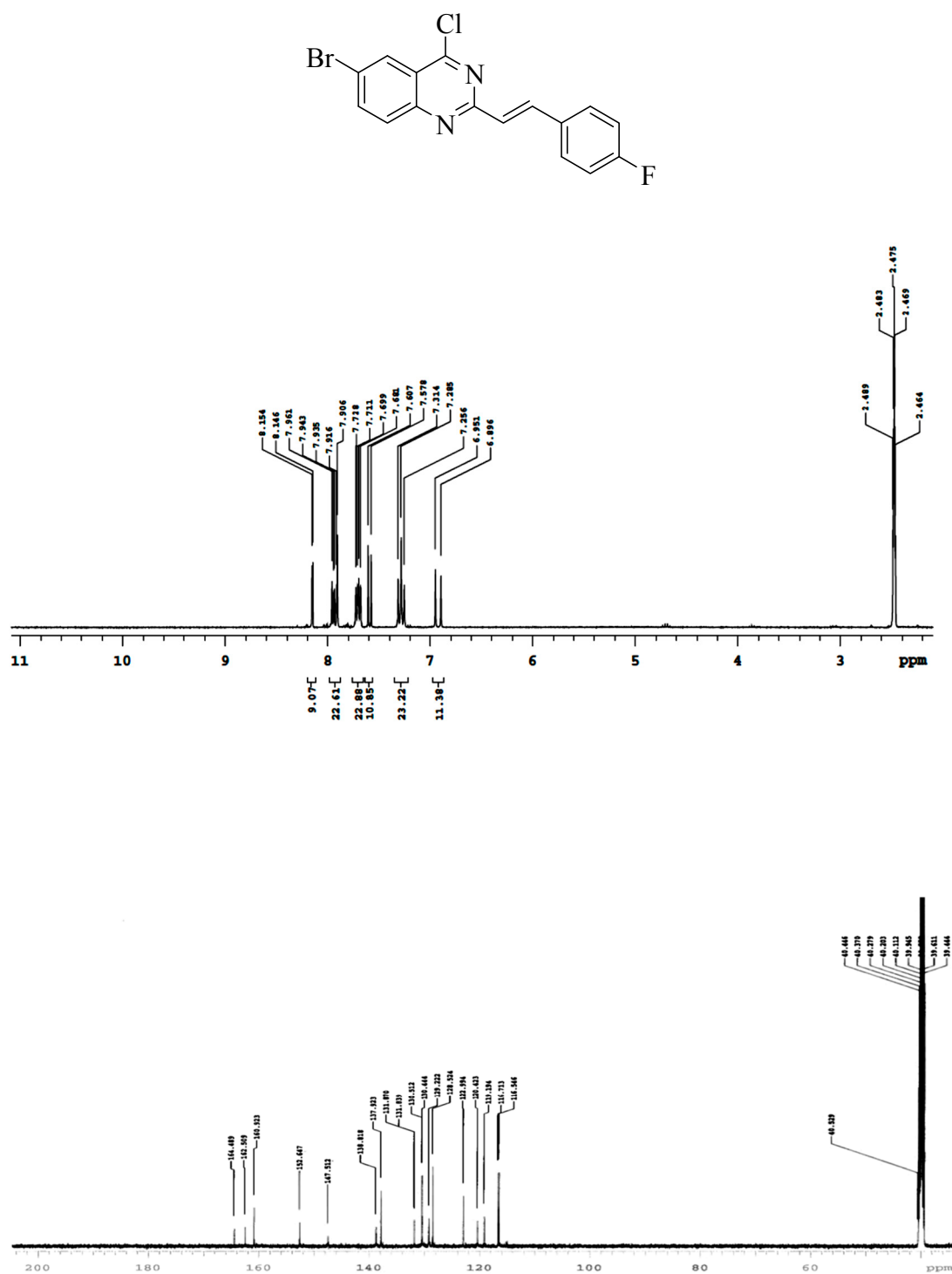


Figure S-1.2: ¹H NMR and ¹³C NMR spectra of **2b** in DMSO-*d*₆ at 300 MHz and 75 MHz, respectively

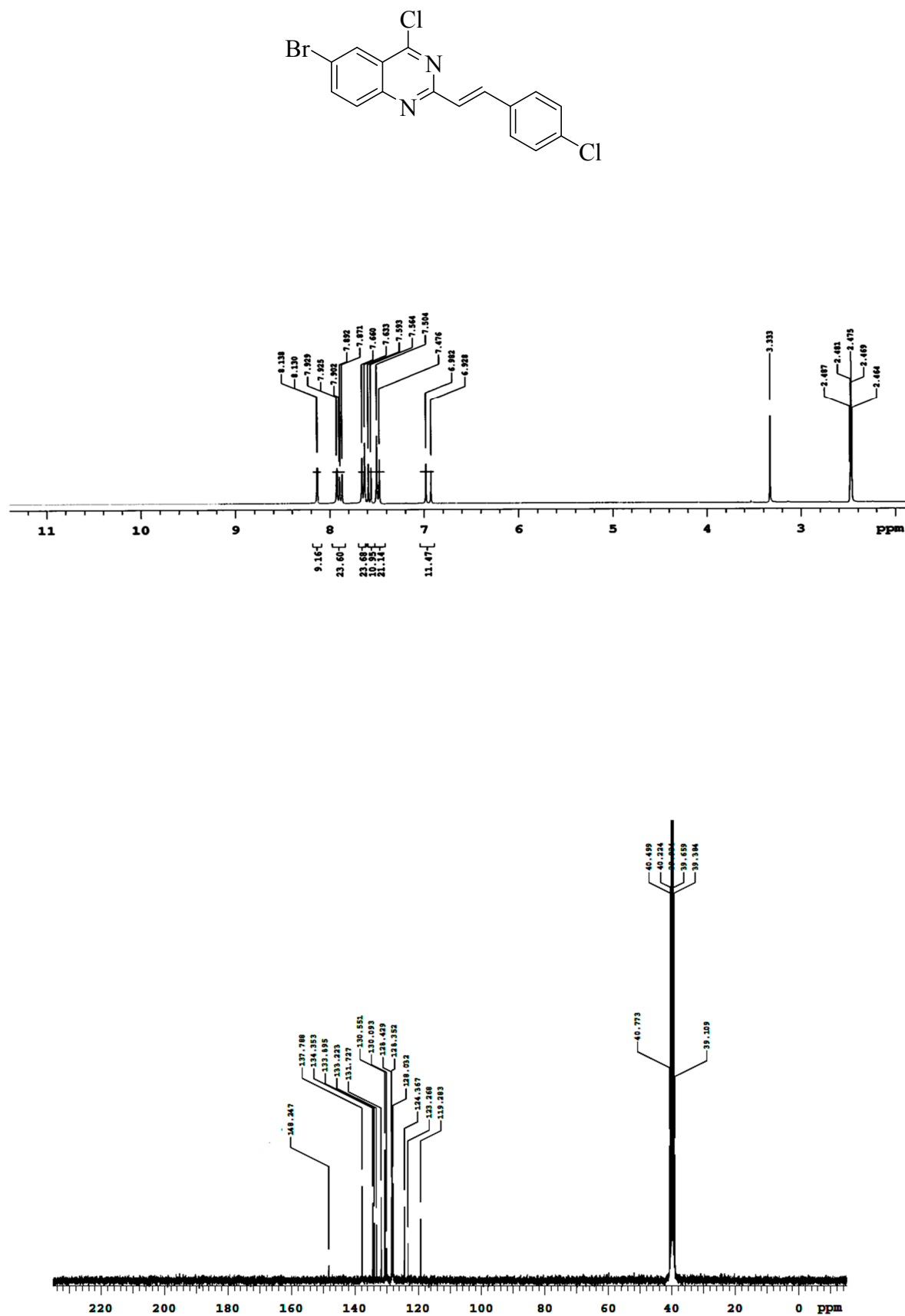


Figure S-1.3: ¹H NMR and ¹³C NMR spectra of **2c** in DMSO-*d*₆ at 300 and 75 MHz, respectively

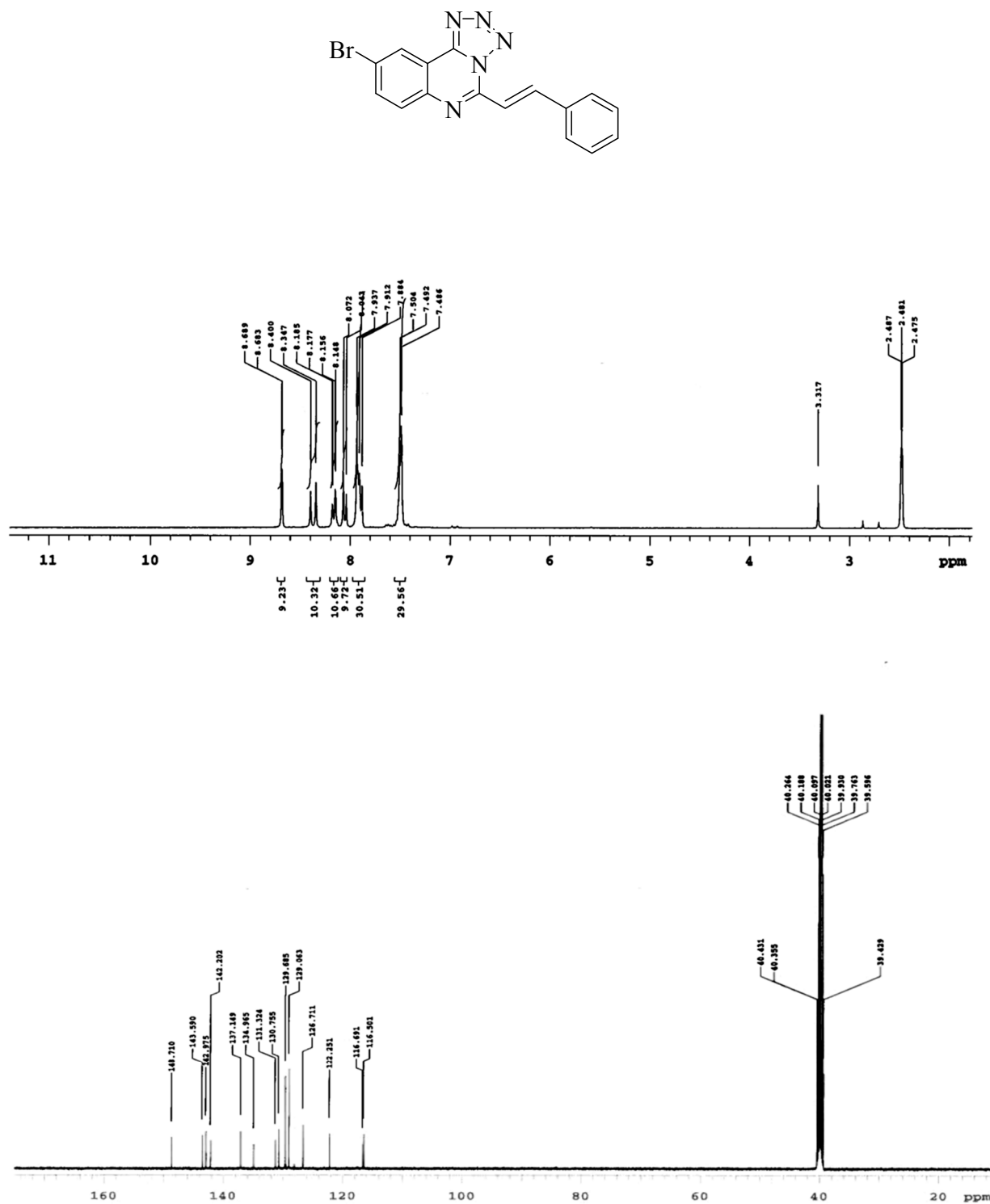


Figure S-1.4: ¹H NMR and ¹³C NMR spectra of **3a** in DMSO-*d*₆ at 300 MHz and 75 MHz, respectively

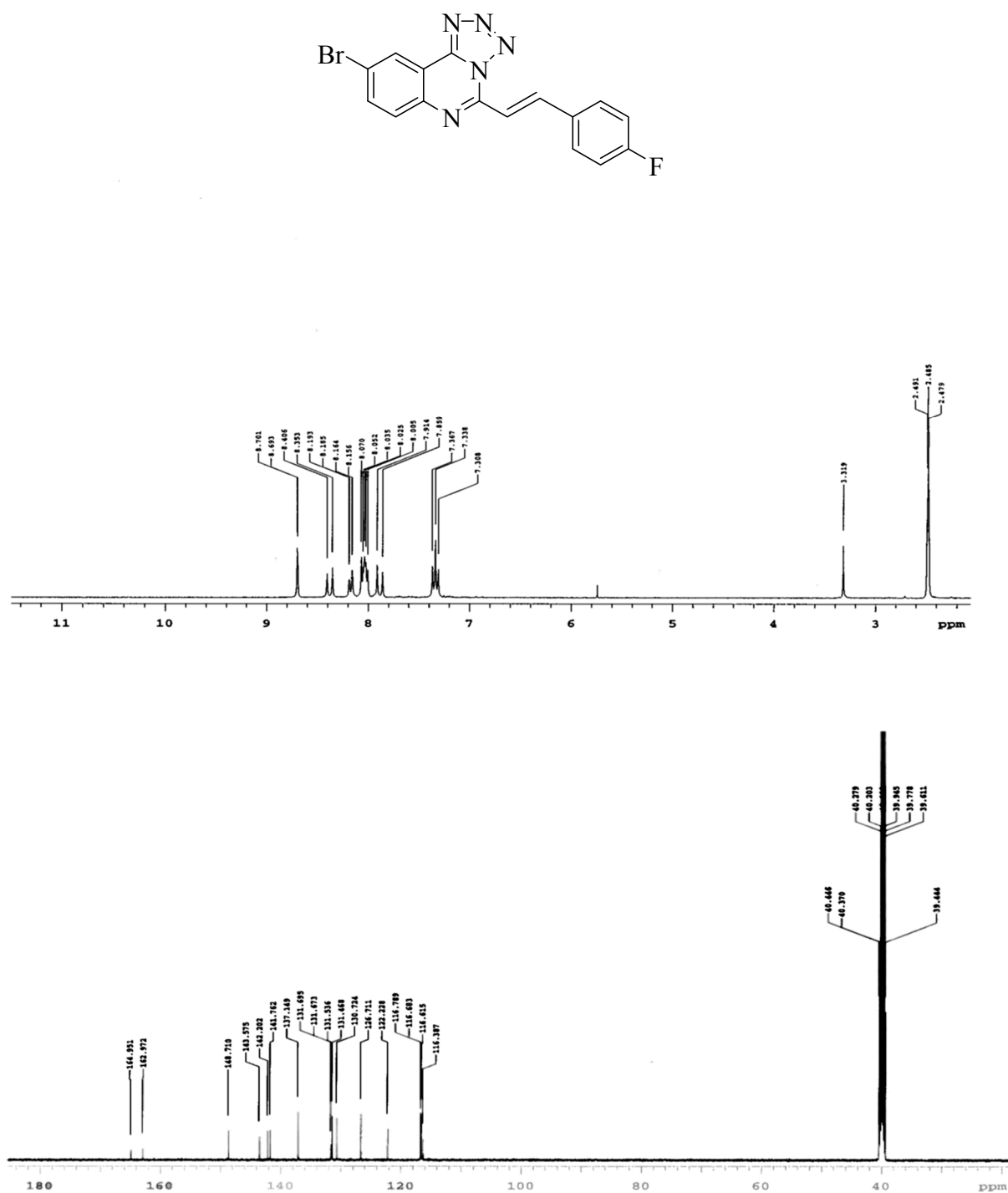


Figure S-1.5: ¹H NMR and ¹³C NMR spectra of **3b** in DMSO-*d*₆ at 300 MHz and 75 MHz, respectively

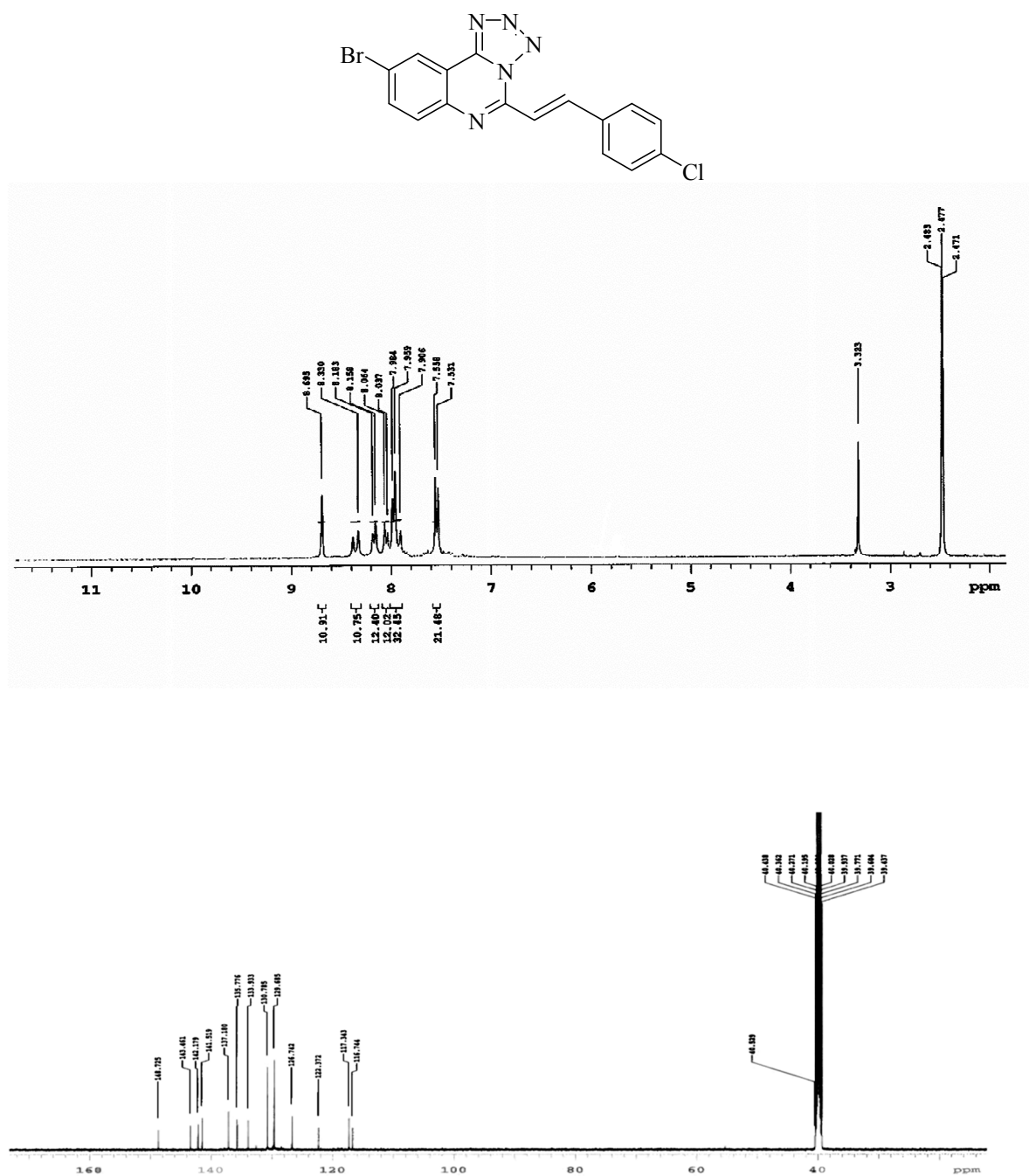


Figure S-1.6: ¹H NMR and ¹³C NMR spectra of **3c** in DMSO-*d*₆ at 300 MHz and 75 MHz, respectively

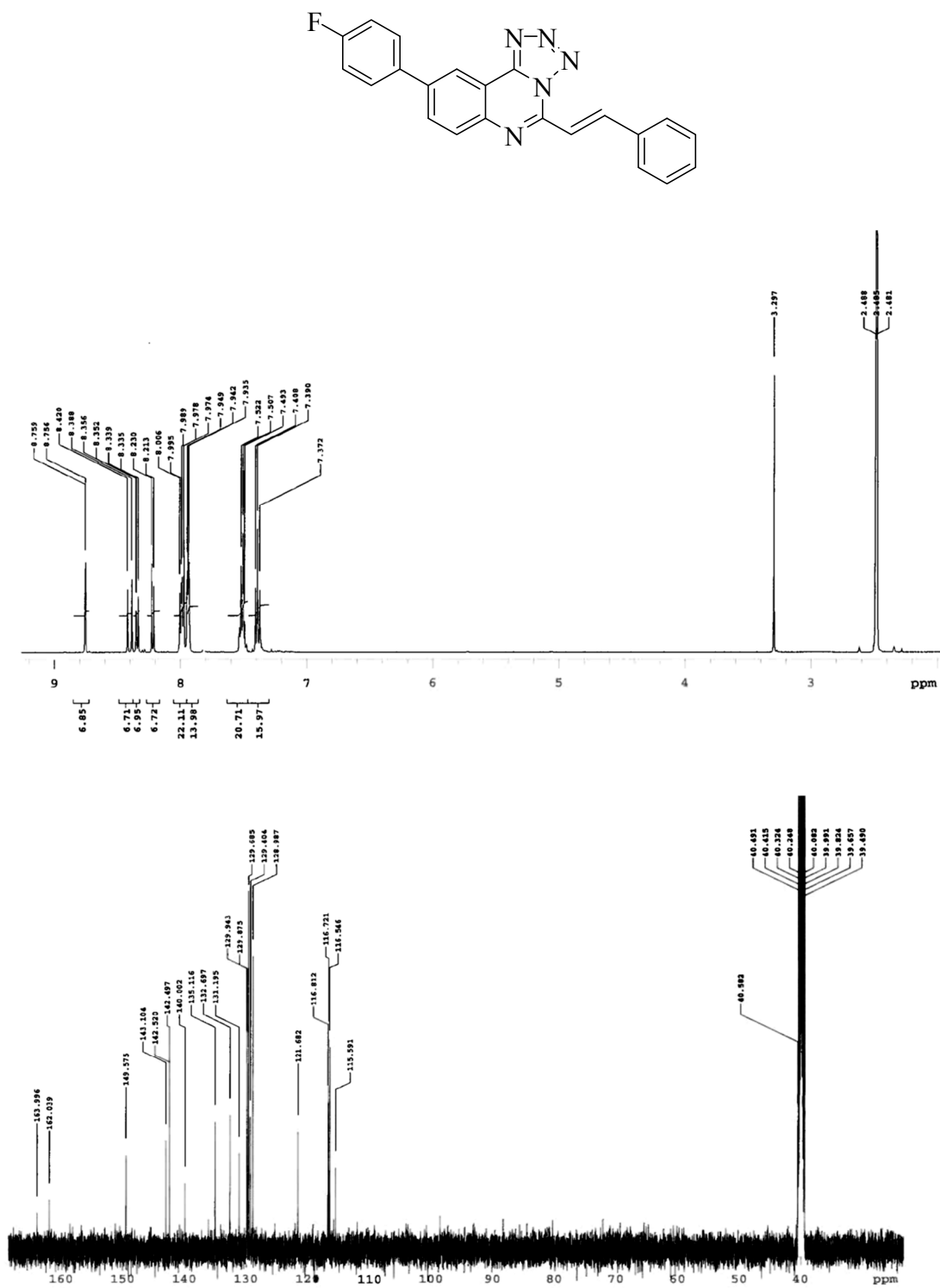


Figure S-1.7: ^1H NMR spectrum of **4a** in $\text{DMSO}-d_6$ at 500 and 125 MHz, respectively

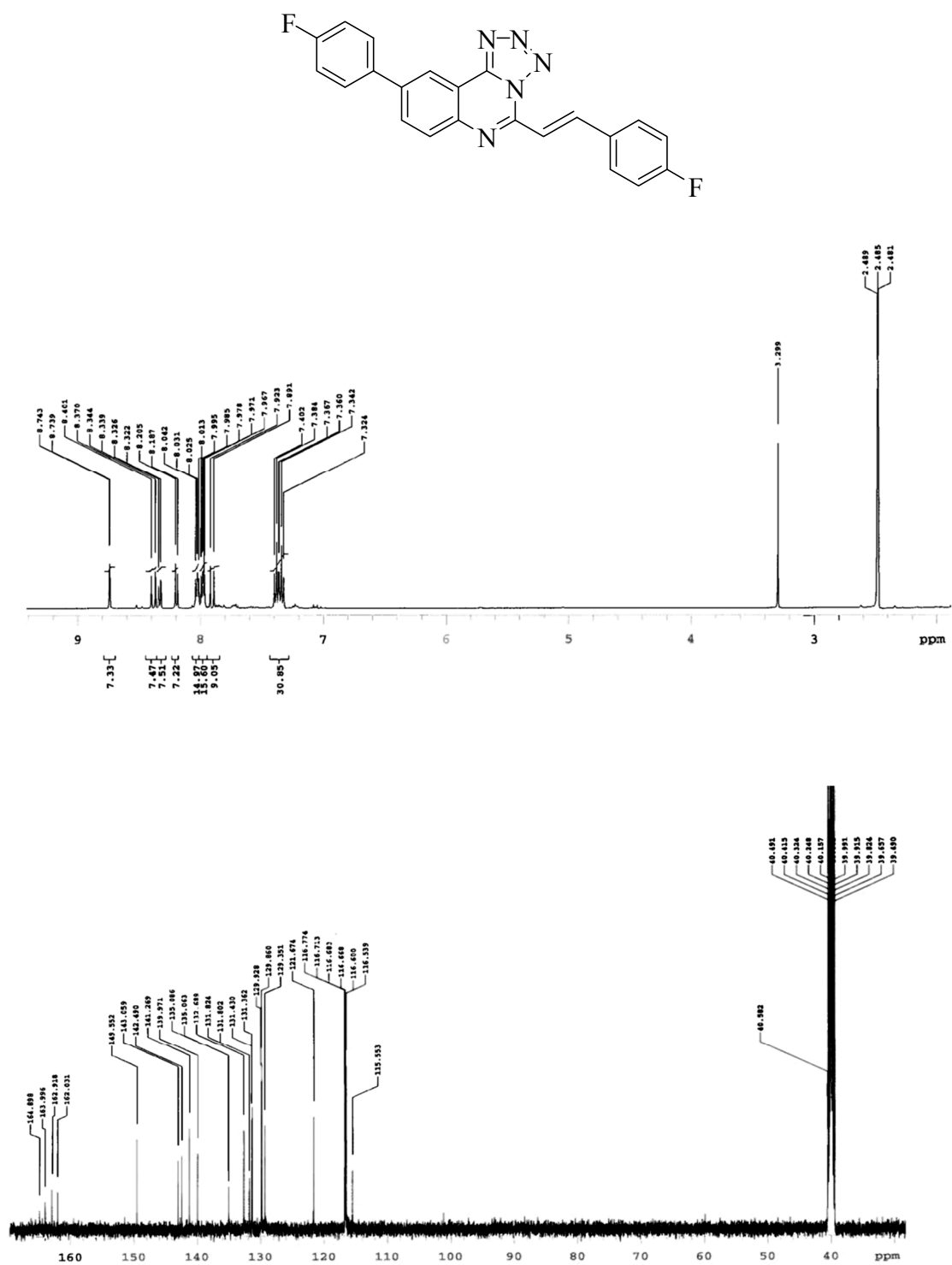


Figure S-1.8: ^1H NMR and ^{13}C NMR spectra of **4b** in $\text{DMSO}-d_6$ at 500 MHz and 125 MHz, respectively

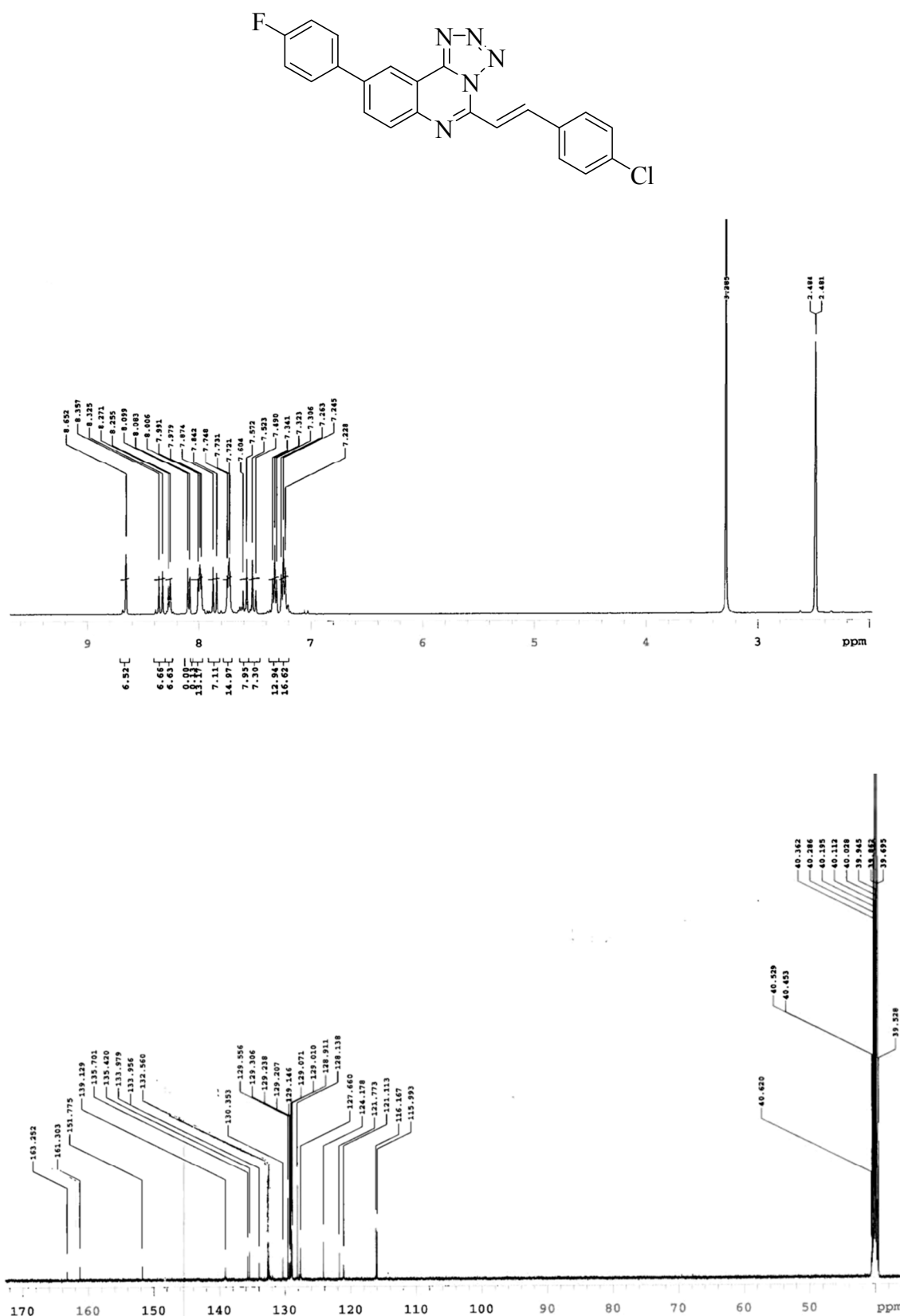


Figure S-1.9: ¹H NMR and ¹³C NMR spectra of **4c** in DMSO-*d*₆ at 500 and 125 MHz, respectively

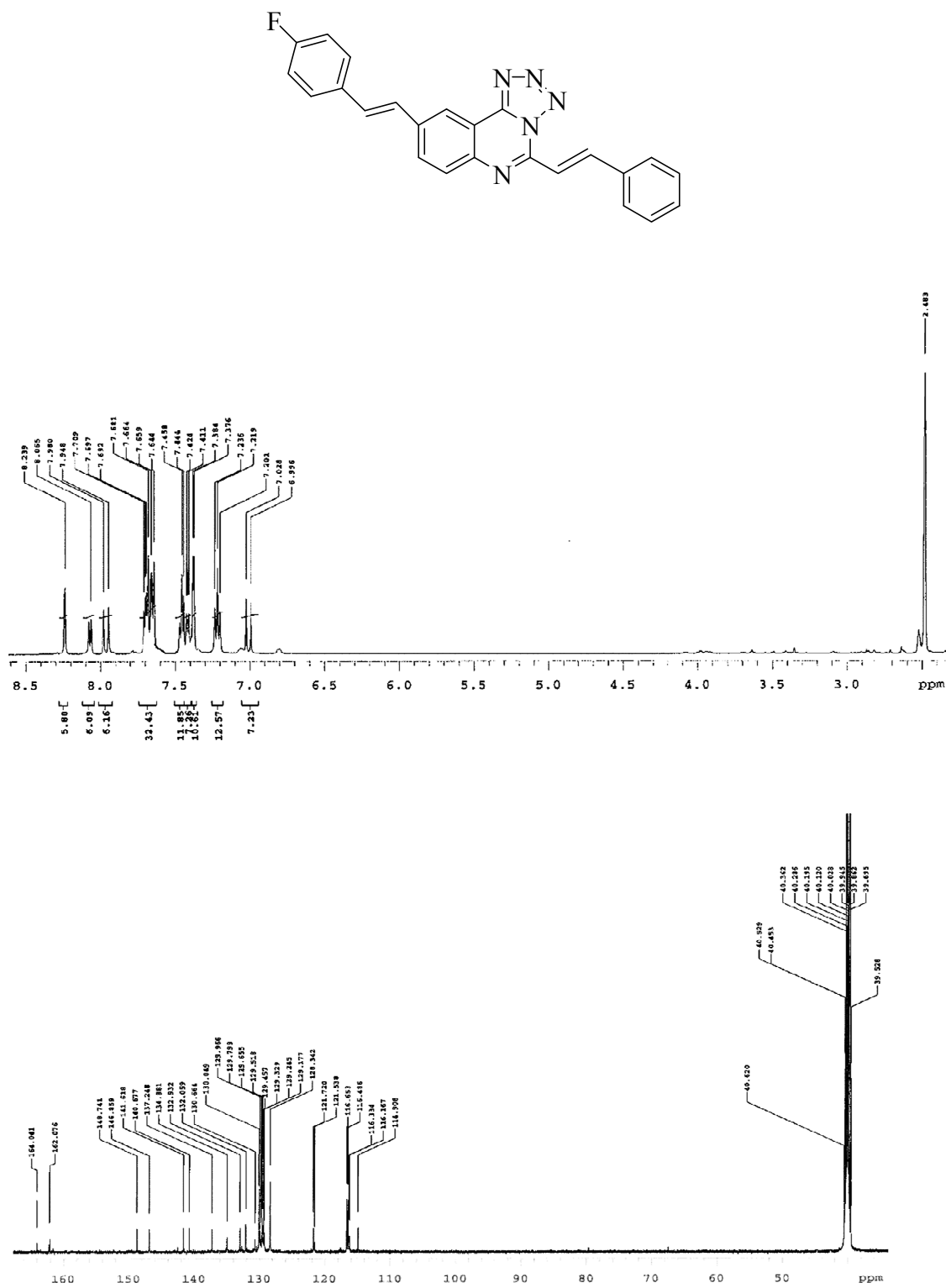


Figure S-1.10: ^1H NMR and ^{13}C NMR spectra of **4d** in $\text{DMSO}-d_6$ at 500 and 125 MHz, respectively

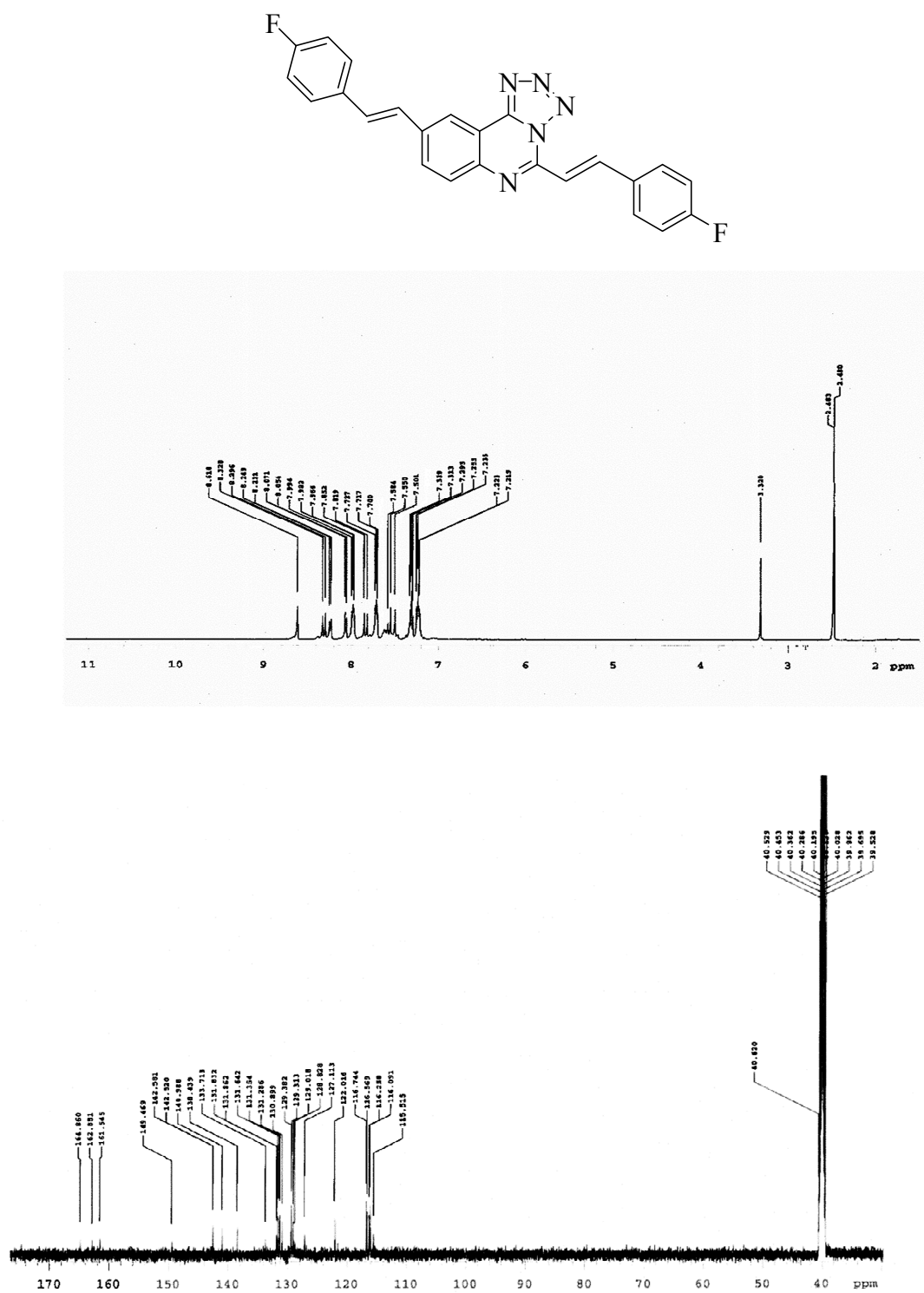


Figure S-1.11: ^1H NMR and ^{13}C NMR spectra of **4e** in $\text{DMSO-}d_6$ at 300 and 75 MHz, respectively

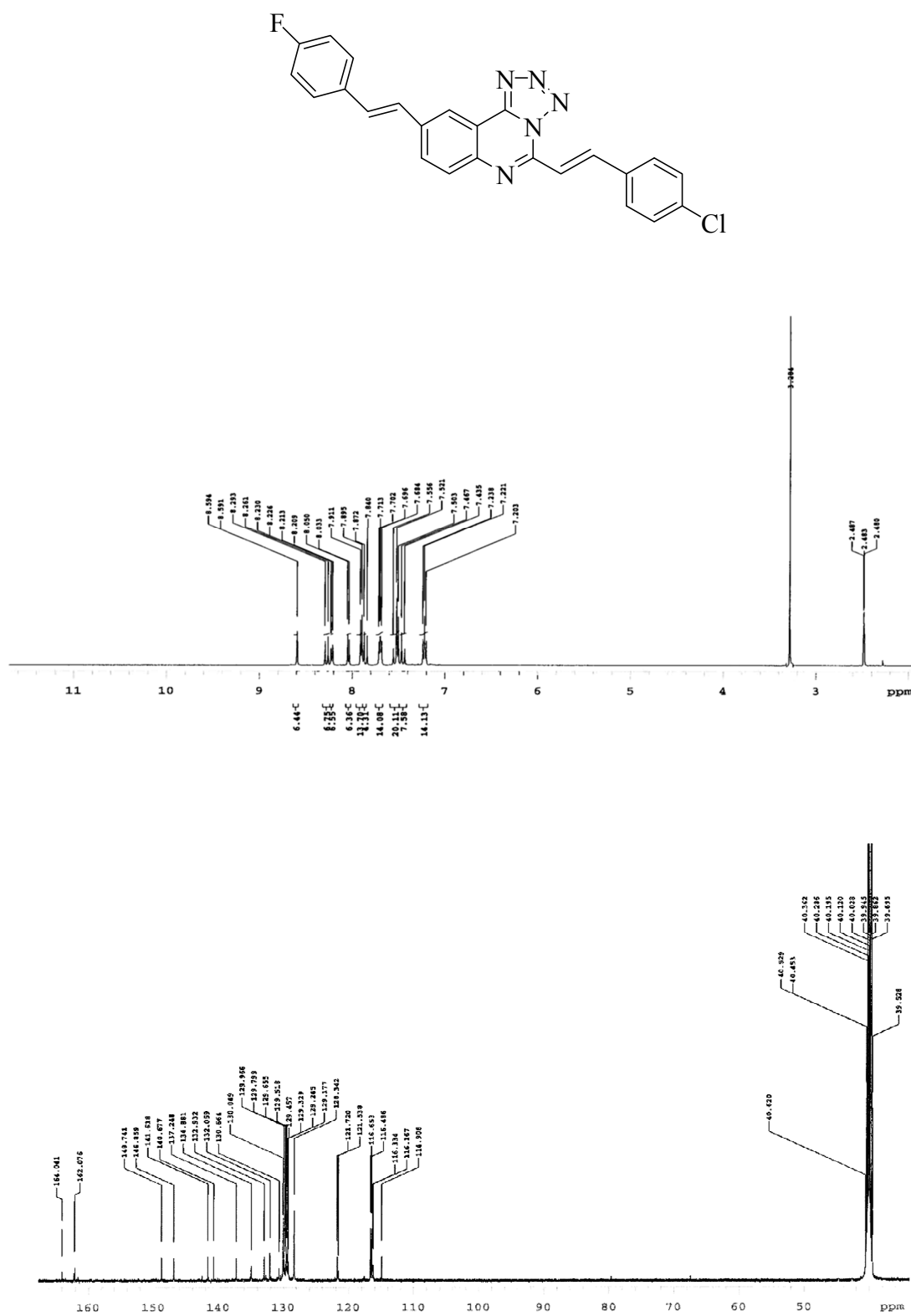


Figure S-1.12: ^1H NMR and ^{13}C NMR spectra of **4f** in $\text{DMSO-}d_6$ at 500 and 125 MHz, respectively

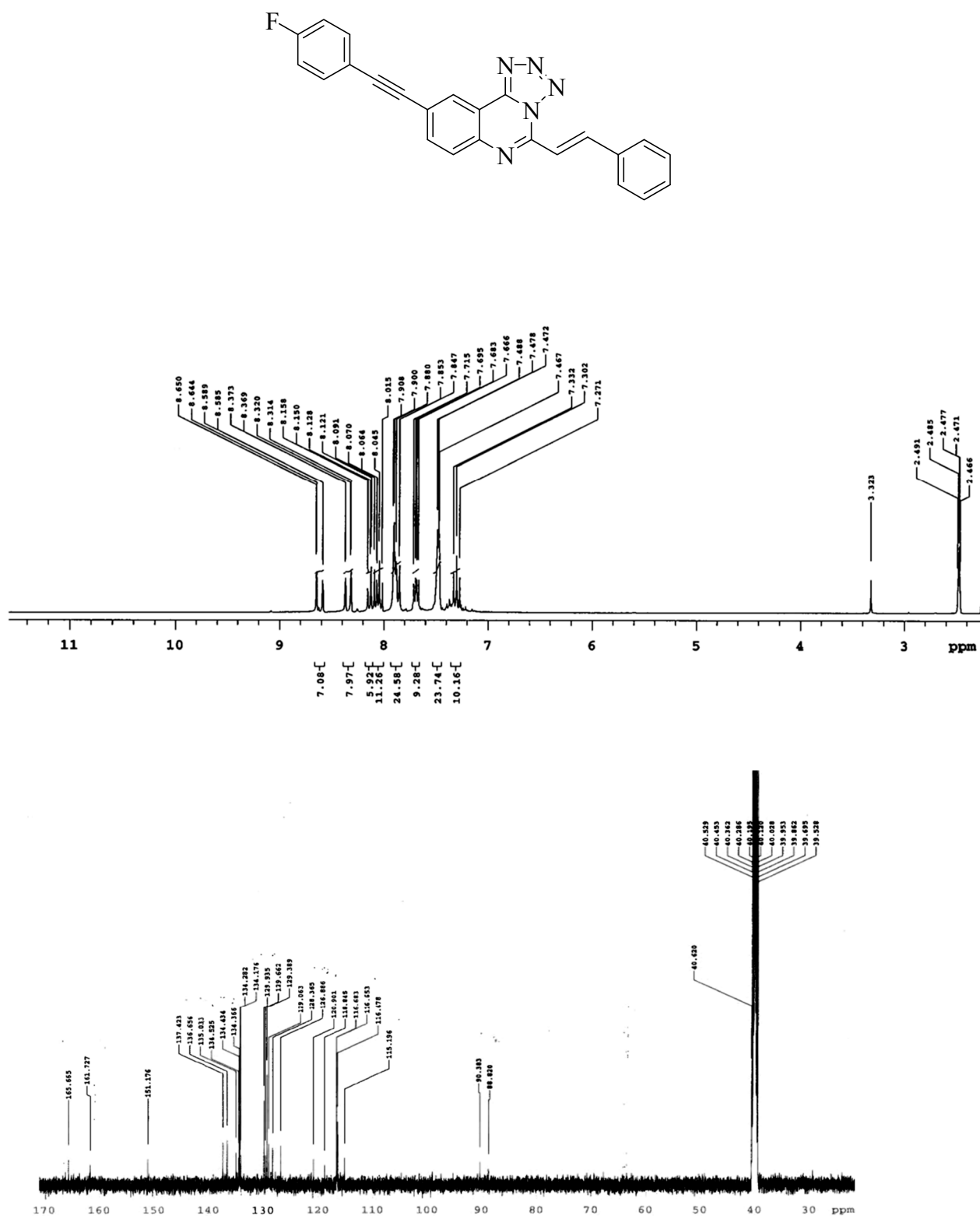


Figure S-1.13: ¹H NMR and ¹³C NMR spectra of **5a** in DMSO-*d*₆ at 500 and 125 MHz, respectively

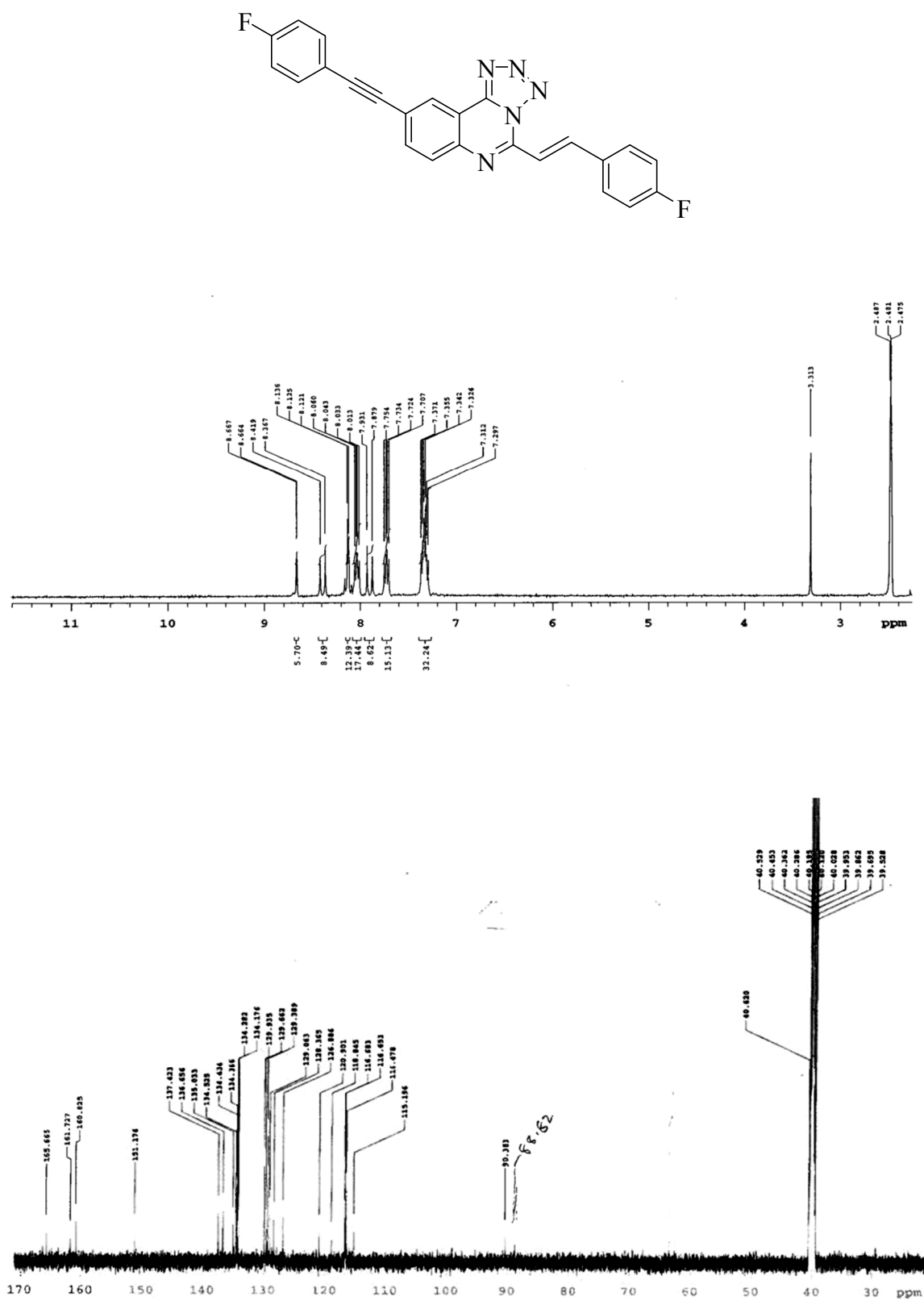


Figure S-1.14: ^1H NMR and ^{13}C NMR spectra of **5b** in $\text{DMSO-}d_6$ at 300 and 75 MHz, respectively

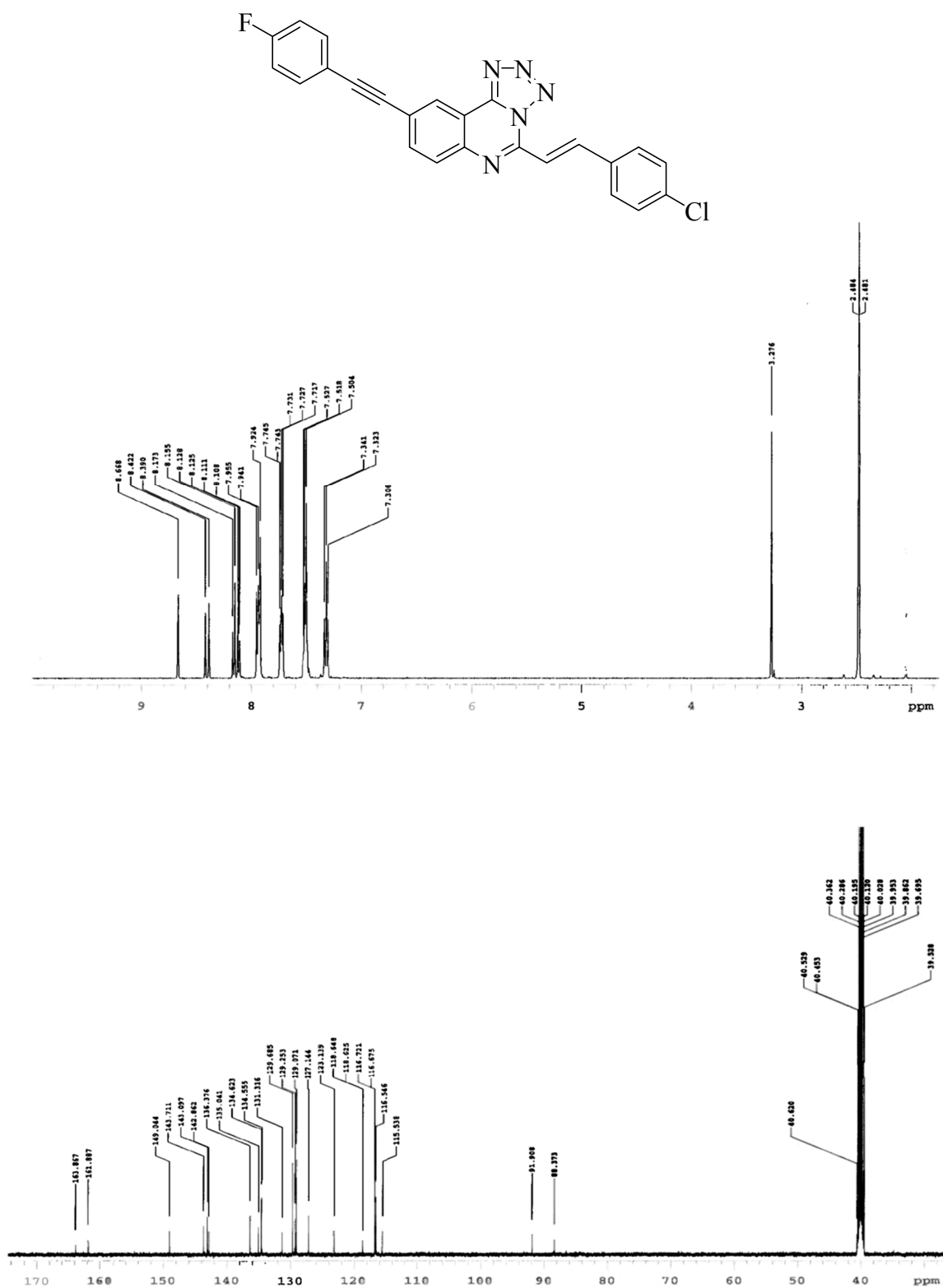


Figure S-1.15: ^1H NMR and ^{13}C NMR spectra of **5c** in $\text{DMSO-}d_6$ at 500 and 125 MHz, respectively

S2: Cytotoxicity and dose response curves of Melphalan and compounds 3–5 against HeLa cells

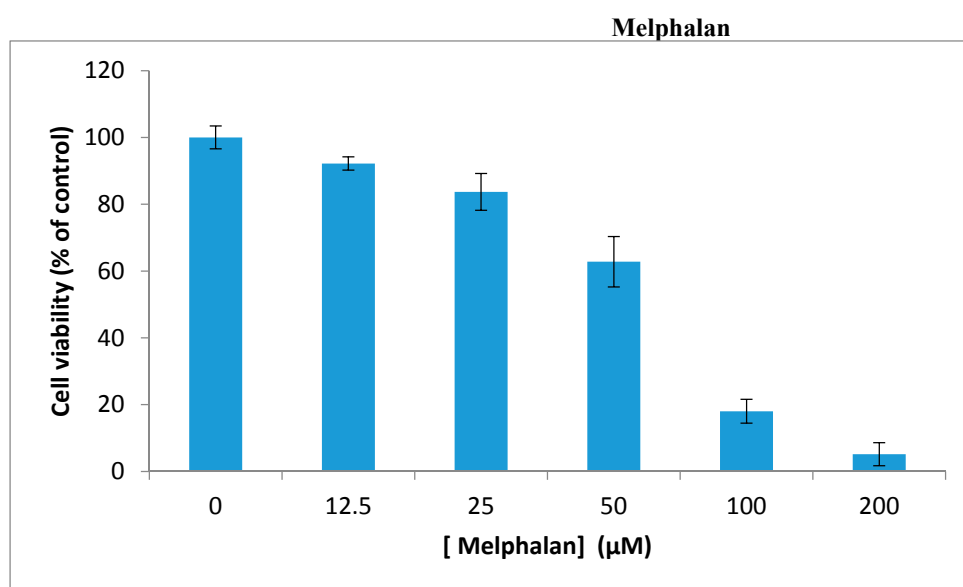
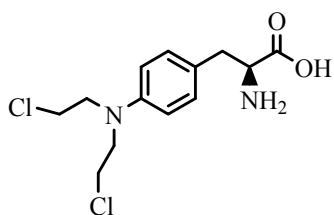


Figure S-2.1: Cytotoxicity of **Melphalan** against HeLa cells

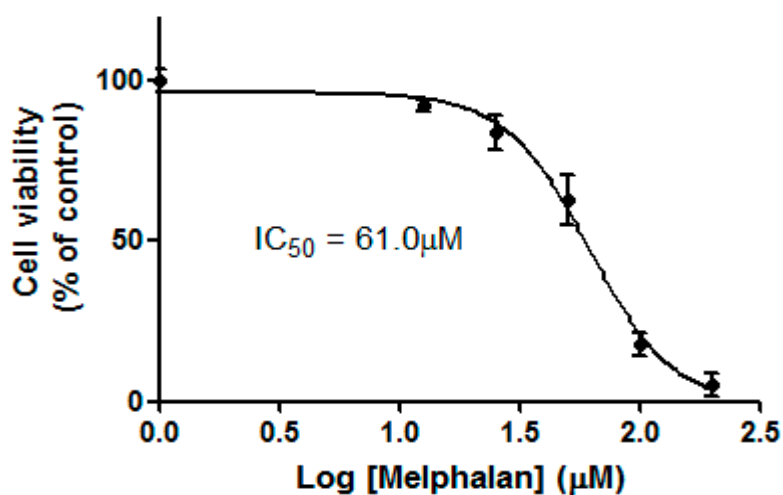
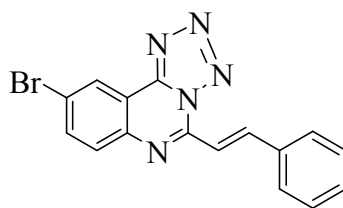


Figure S-2.2: Dose response curve of **Melphalan** against HeLa cells



3a

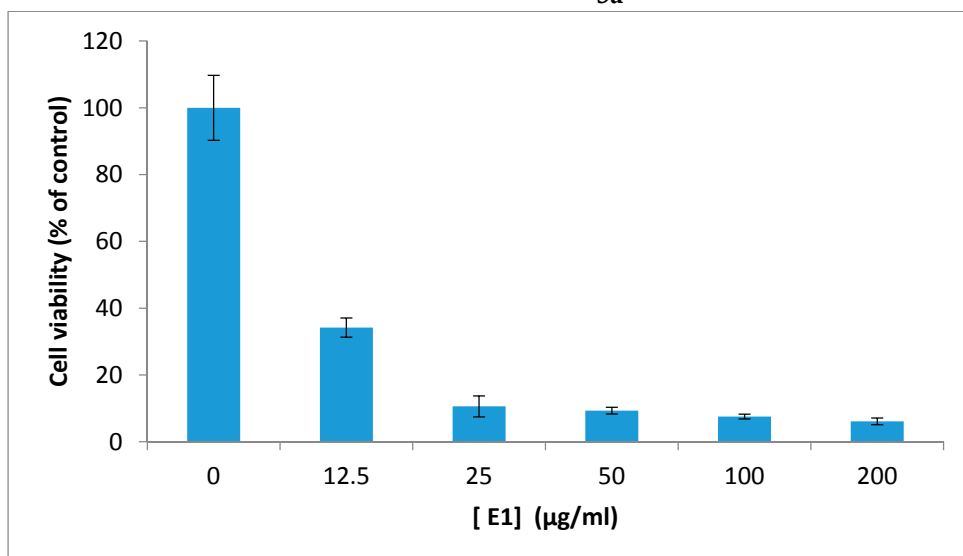


Figure S-2.3: Cytotoxicity of **3a** against HeLa cells

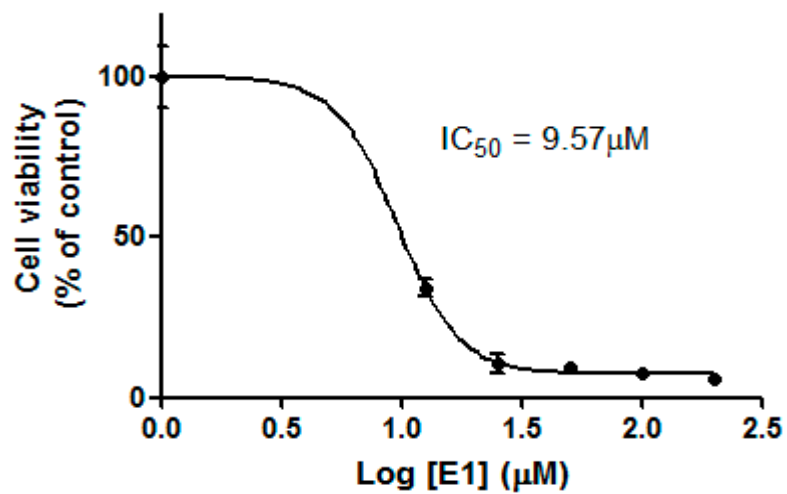
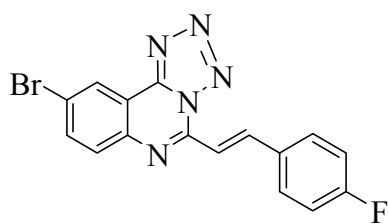


Figure S-2.4: Dose response curve of **3a** against HeLa cells



3b

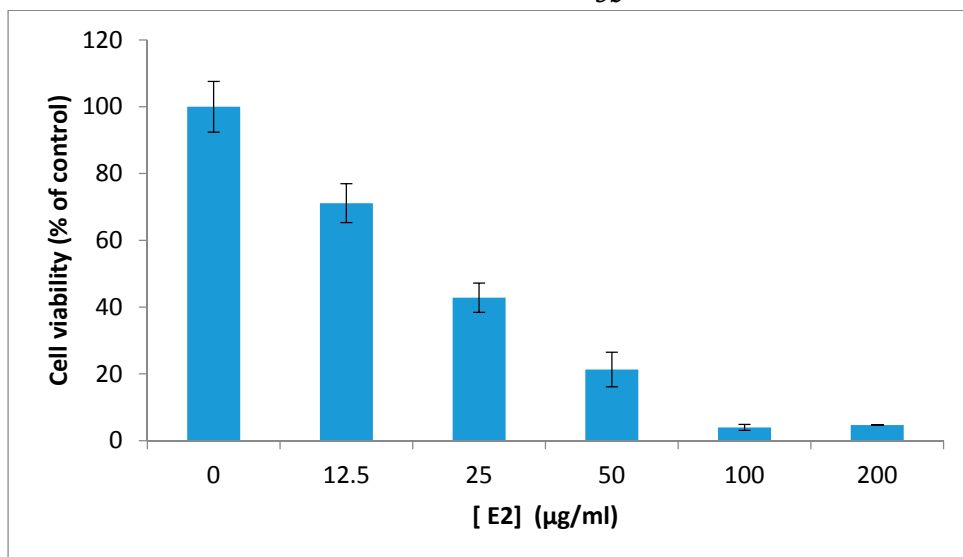


Figure S-2.5: Cytotoxicity of **3b** against HeLa cells

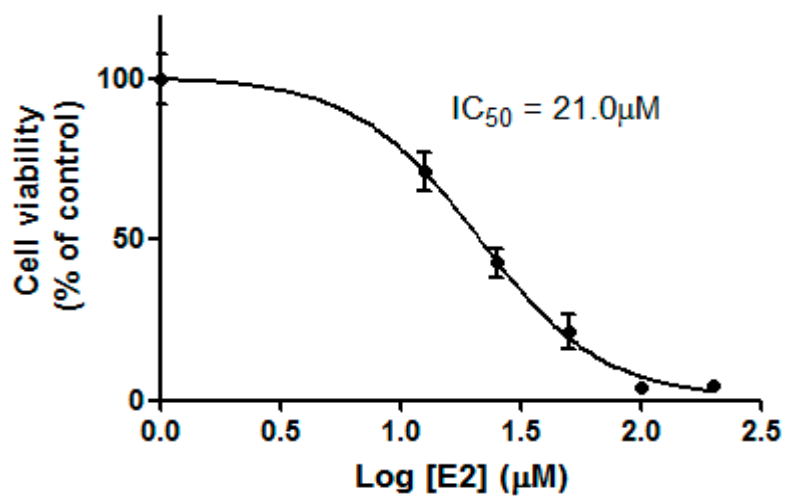


Figure S-2.6: Dose response curve of **3b** against HeLa cells

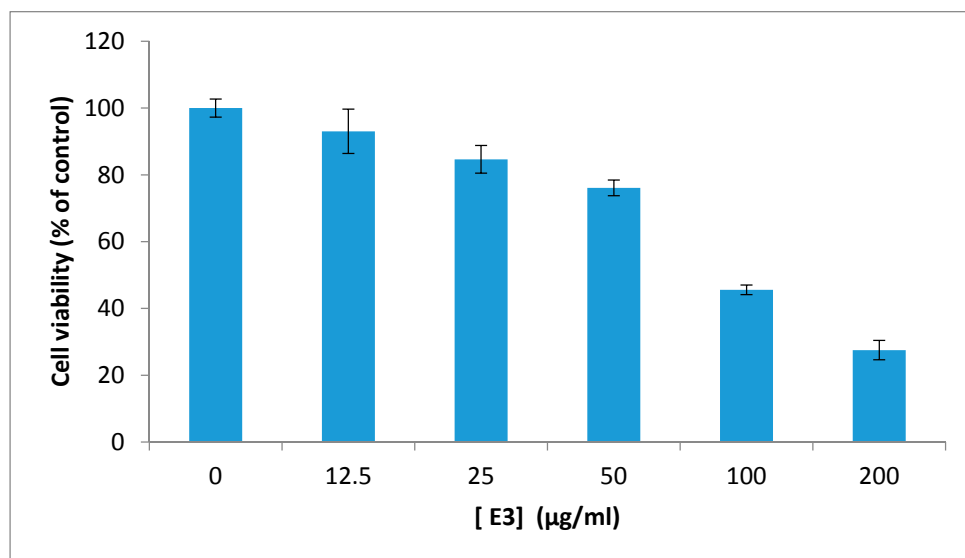
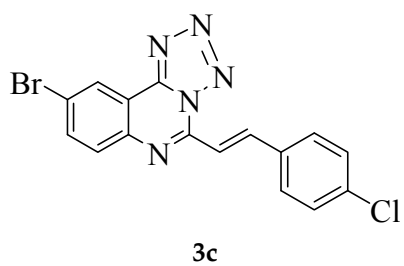


Figure S-2.7: Cytotoxicity of **3c** against HeLa cells

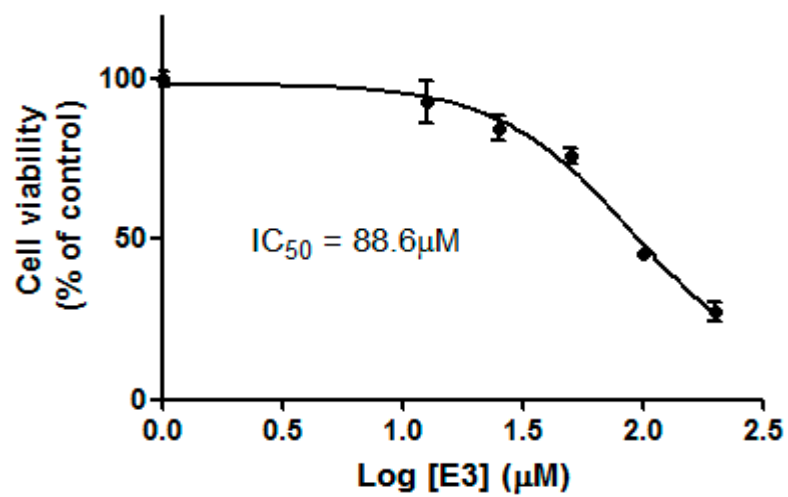
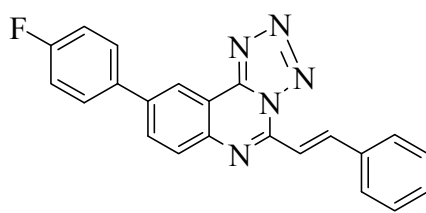


Figure S-2.8: Dose response curve of **3c** against HeLa cells



4a

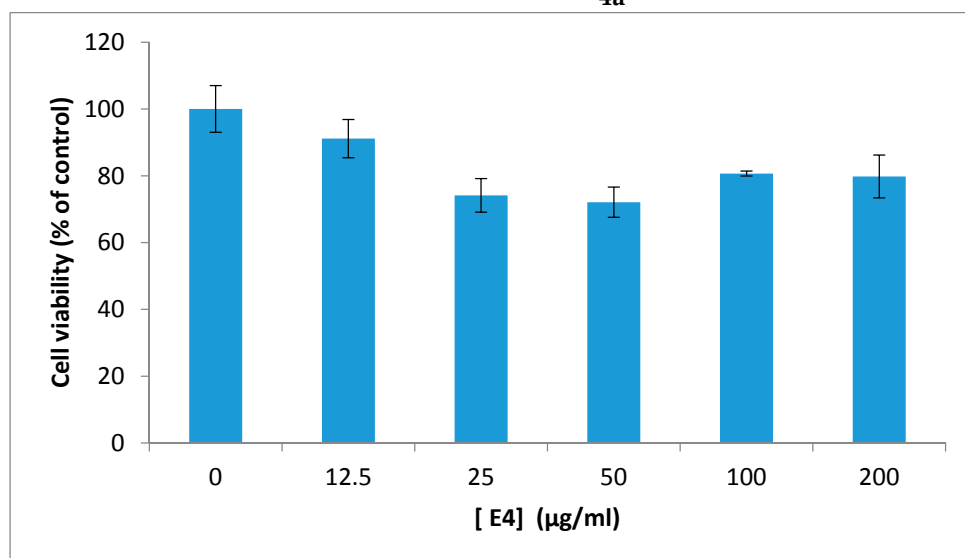
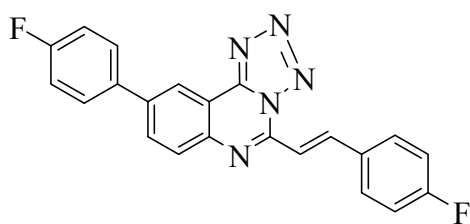


Figure S-2.9: Cytotoxicity of **4a** against HeLa cells



4b

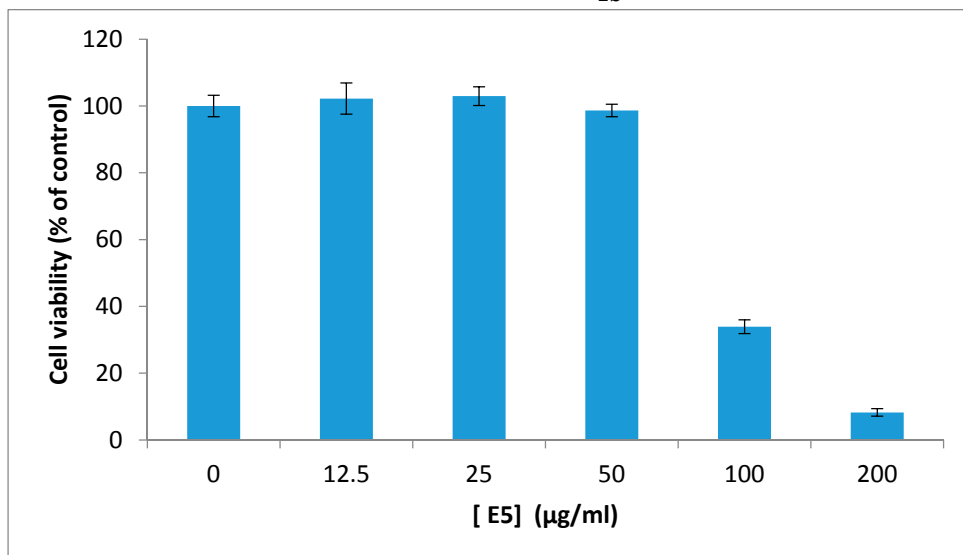


Figure S-2.10: Cytotoxicity of **4b** against HeLa cells

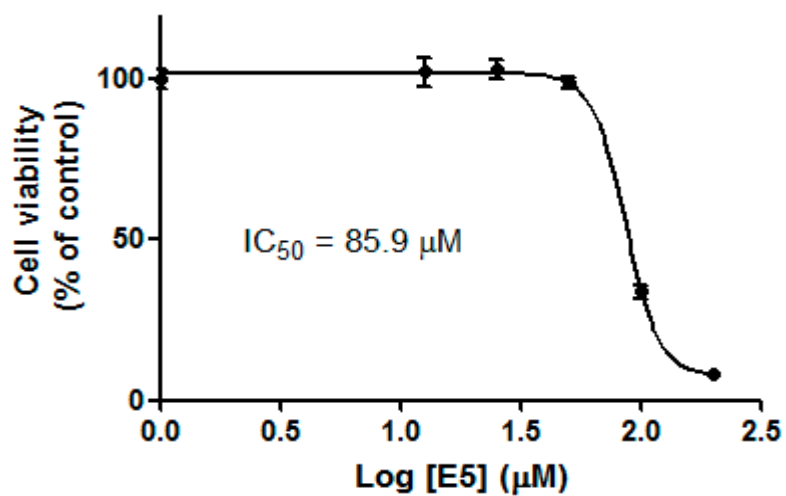
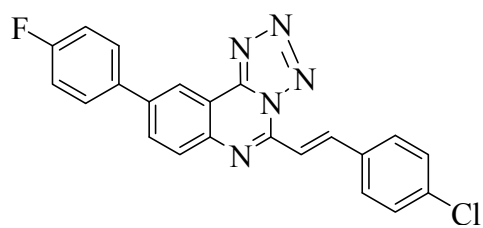


Figure S-2.11: Dose response curve of **4b** against HeLa cells



4c

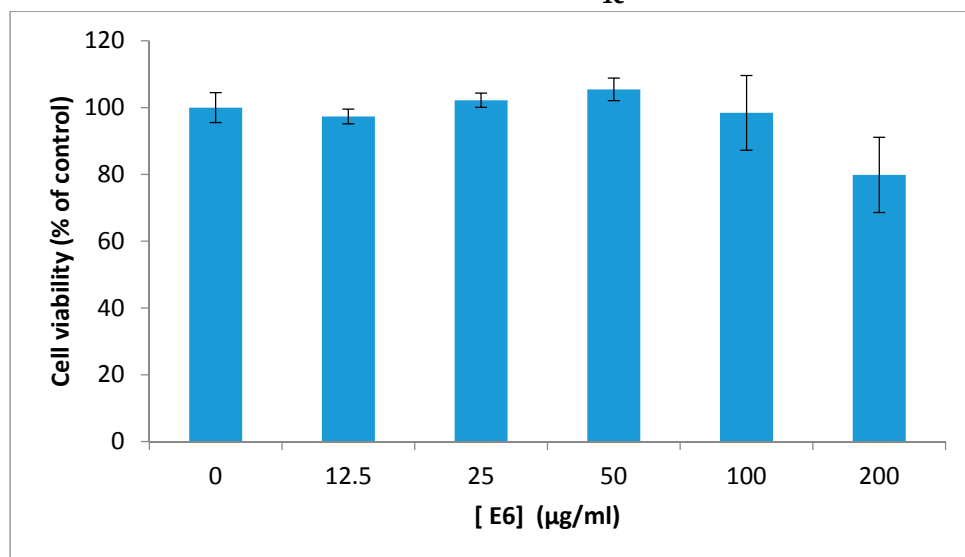
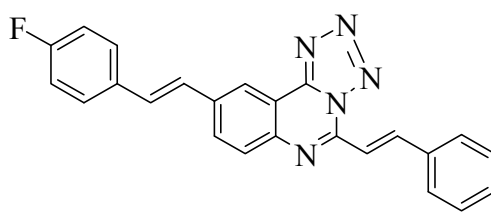


Figure S-2.12: Cytotoxicity of **4c** against HeLa cells



4d

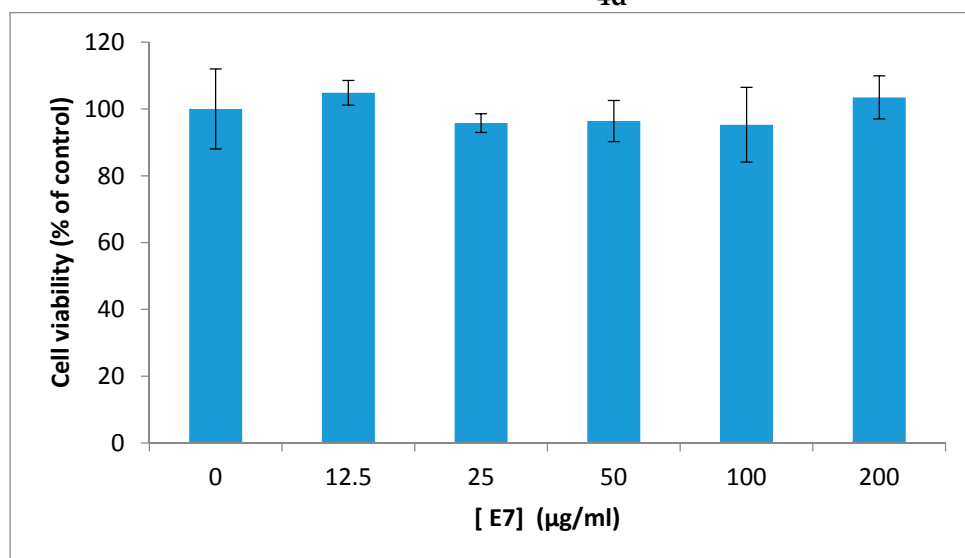
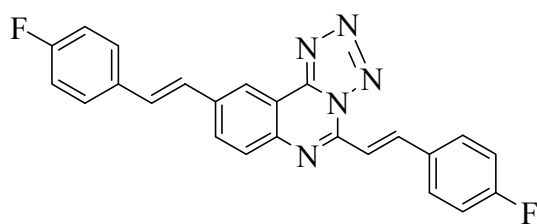


Figure S-2.13: Cytotoxicity of **4d** against HeLa cells



4e

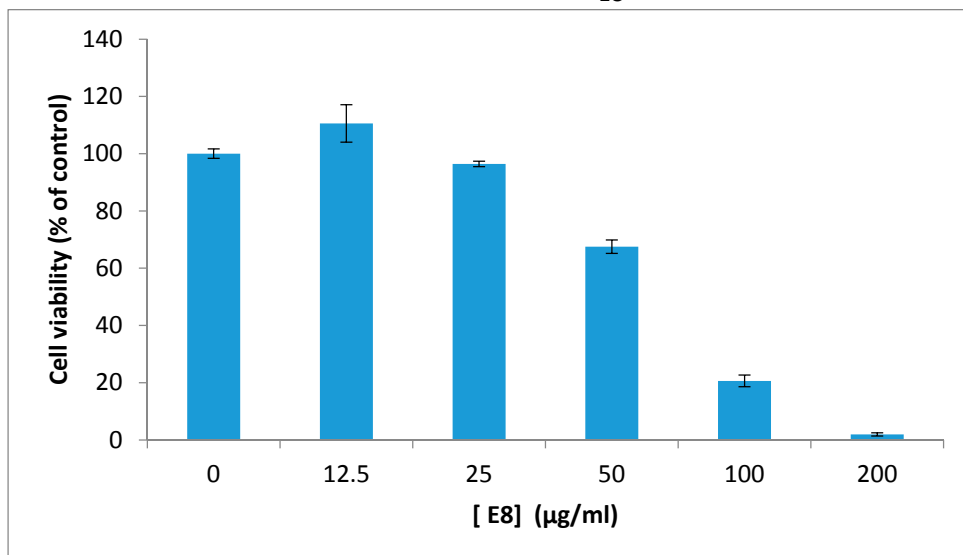


Figure S-2.14: Cytotoxicity of **4e** against HeLa cells

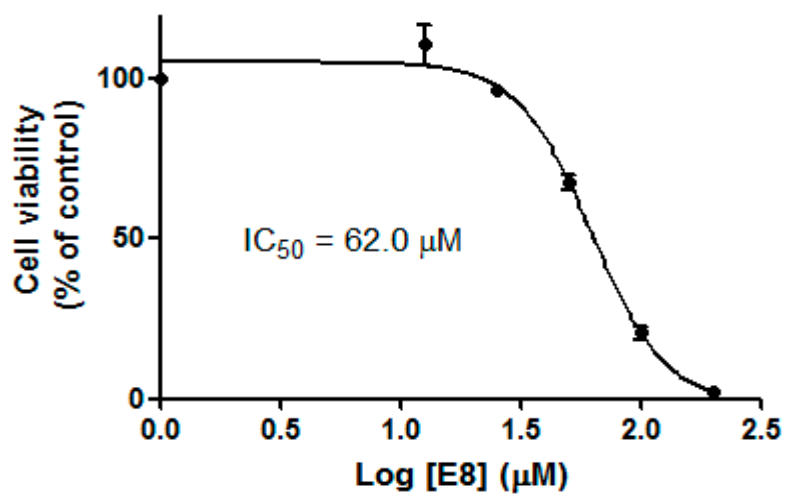
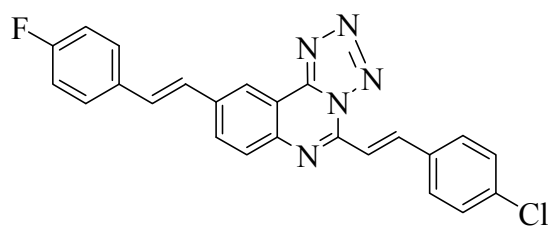


Figure S-2.15: Dose response curve of **4e** against HeLa cells



4f

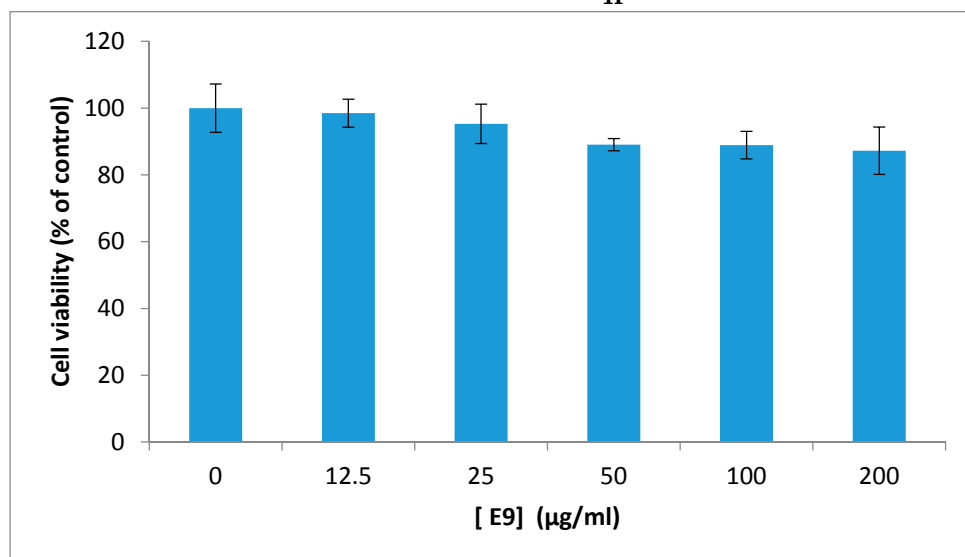
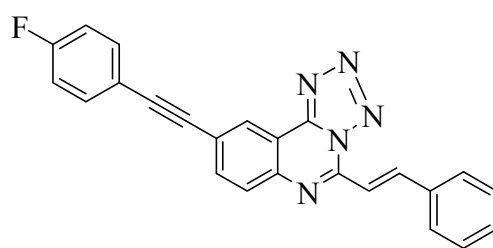


Figure S-2.16: Cytotoxicity of **4f** against HeLa cells



5a

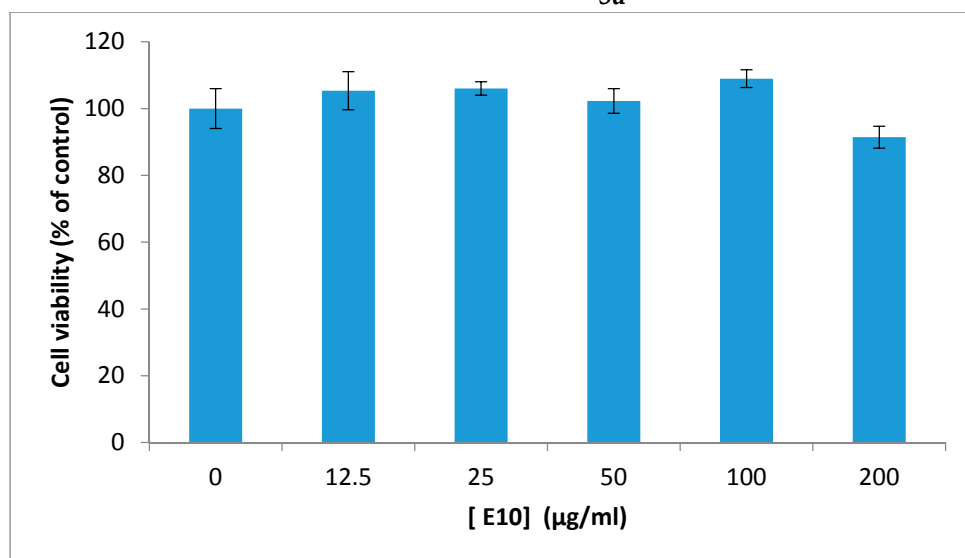


Figure S-2.17: Cytotoxicity of **5a** against HeLa cells

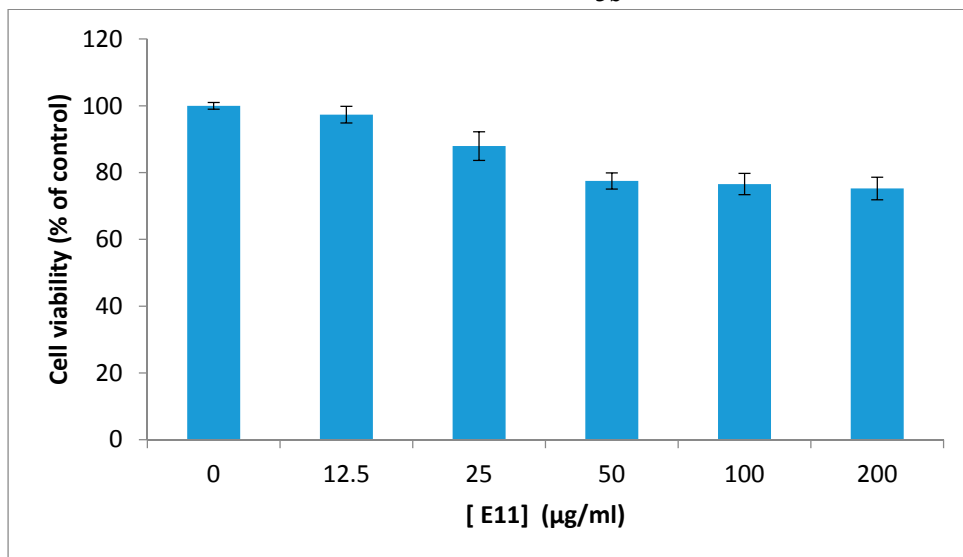
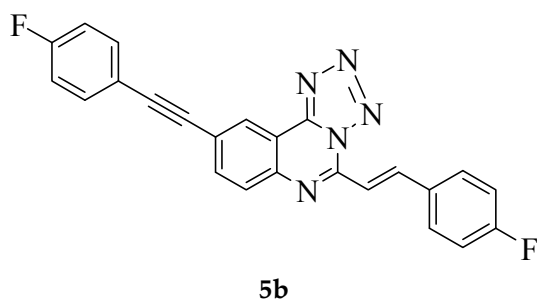
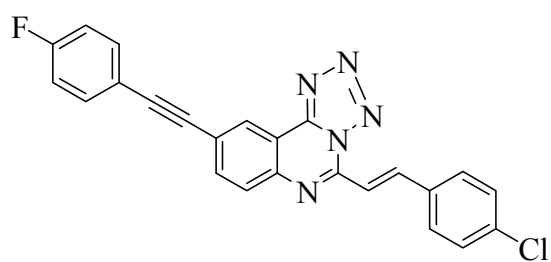


Figure S-2.18: Cytotoxicity of **5b** against HeLa cells



5c

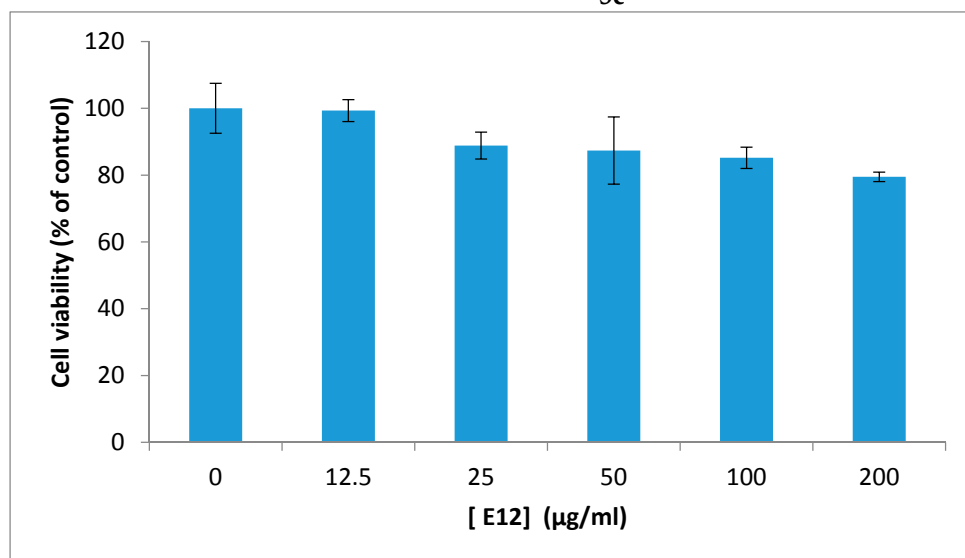


Figure S-2.19: Cytotoxicity of **5c** against HeLa cells

S3: Cytotoxicity and dose response of Melphalan and compounds 3–5 curves against MCF7 cells

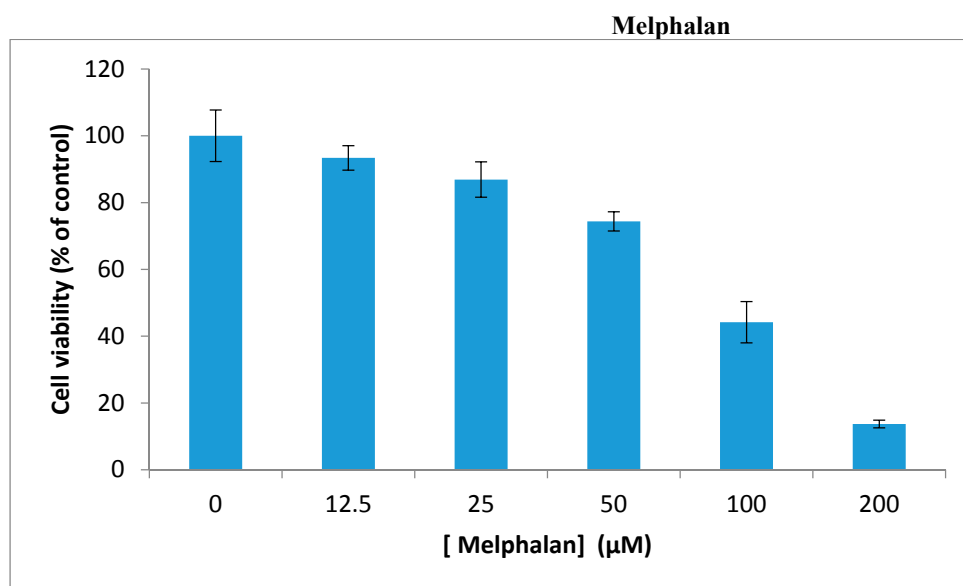
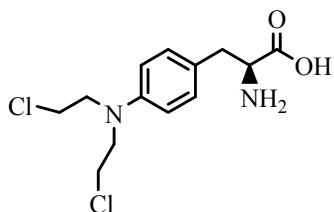


Figure S-3.1: Cytotoxicity of **Melphalan** against MCF-7 cells

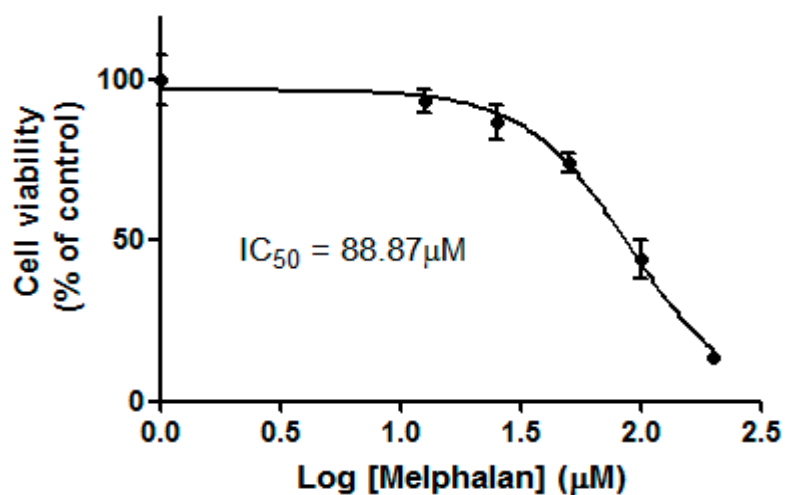


Figure S-3.2: Dose response curve of **Melphalan** against MCF-7 cells

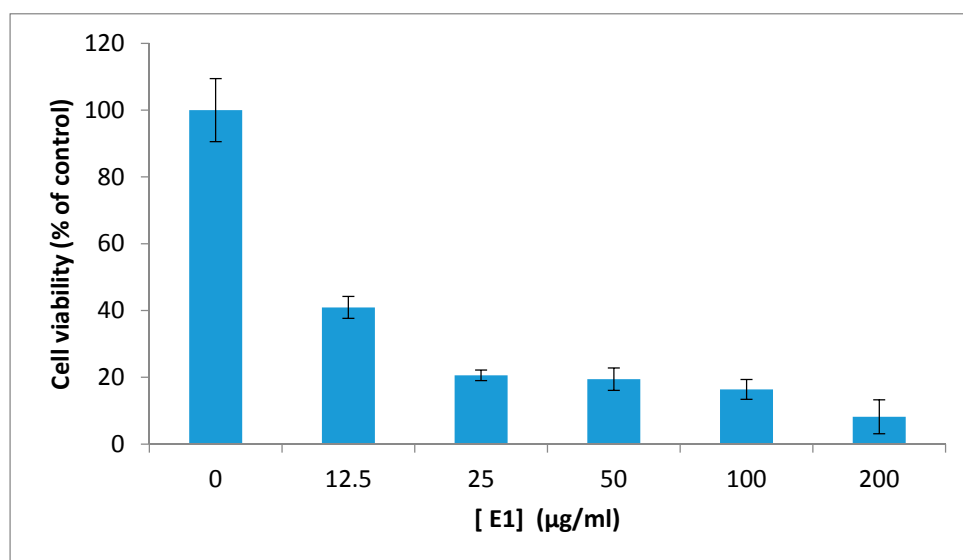
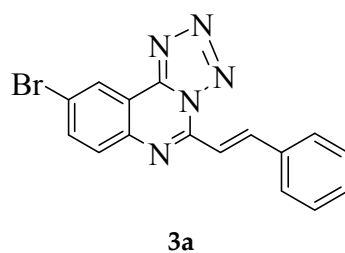


Figure S-3.3: Cytotoxicity of **3a** against MCF-7 cells

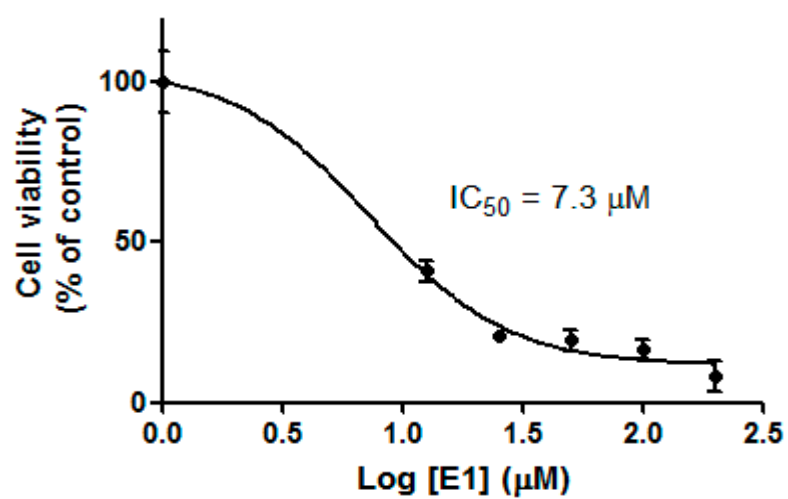
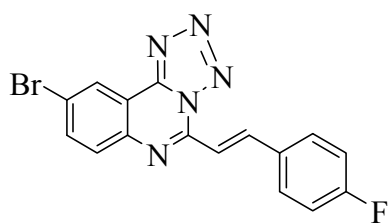


Figure S-3.4: Dose response curve of **3a** against MCF-7 cells



3b

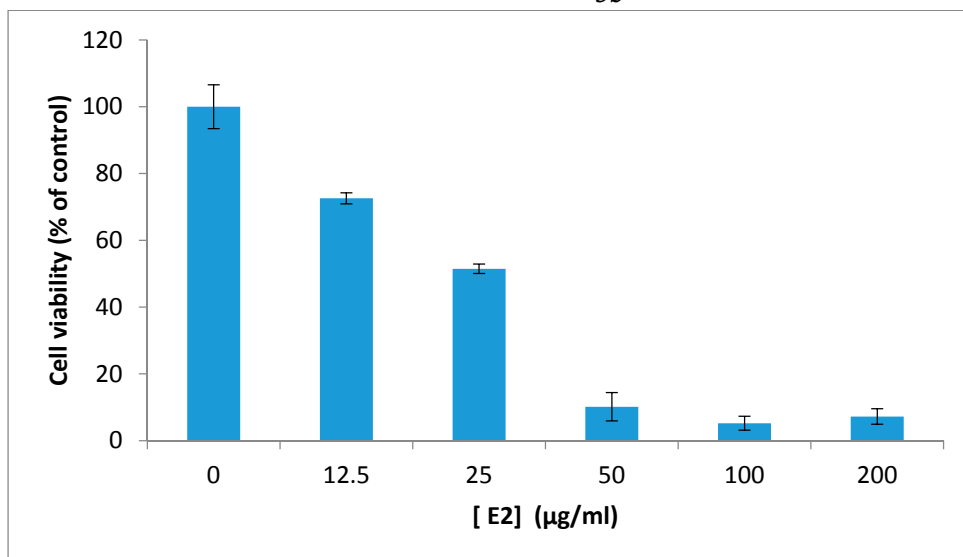


Figure S-3.5: Cytotoxicity of **3b** against MCF-7 cells

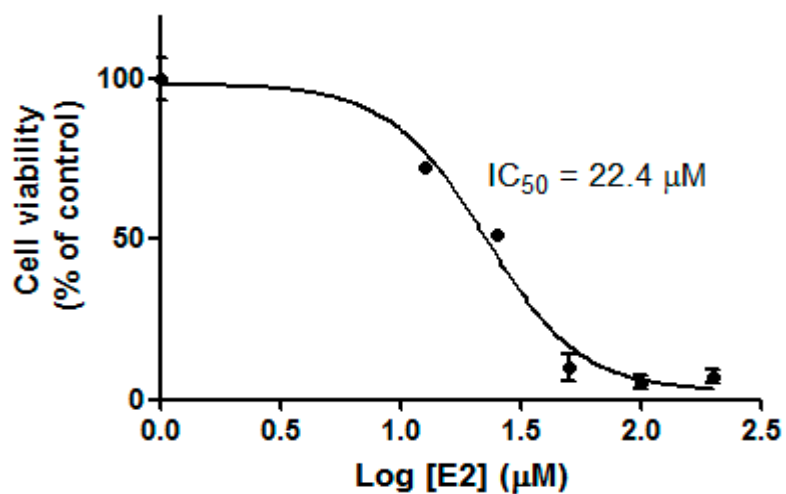


Figure S-3.6: Dose response curve of **3b** against MCF-7 cells

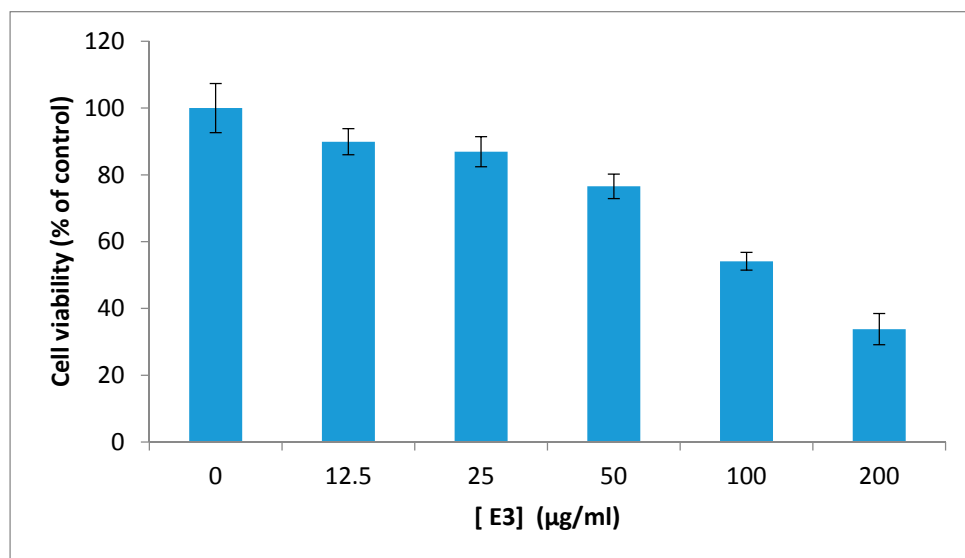
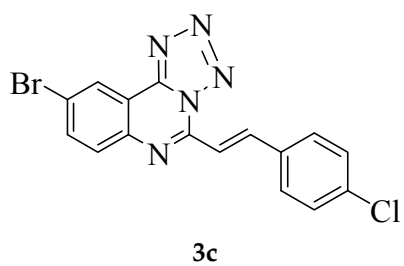


Figure S-3.7: Cytotoxicity of **3c** against MCF-7 cells

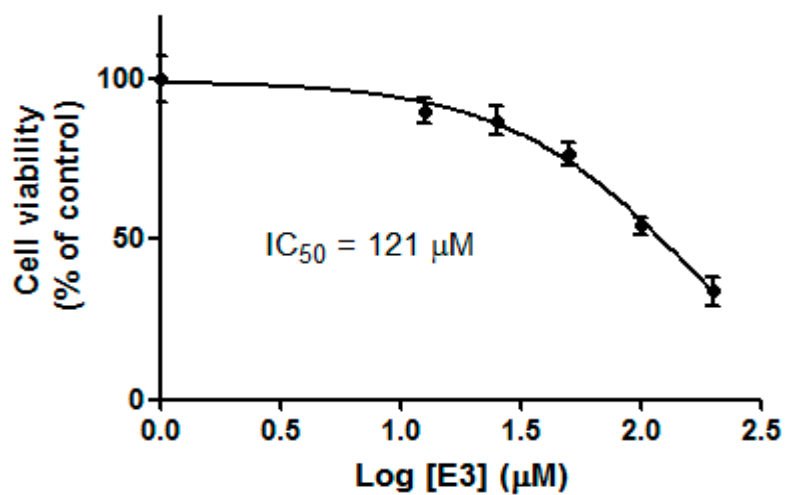
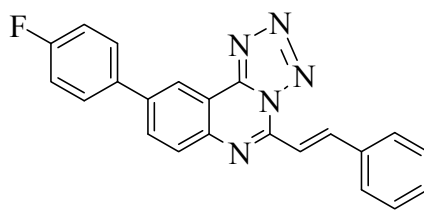


Figure S-3.8: Dose response curve of **3c** against MCF-7 cells



4a

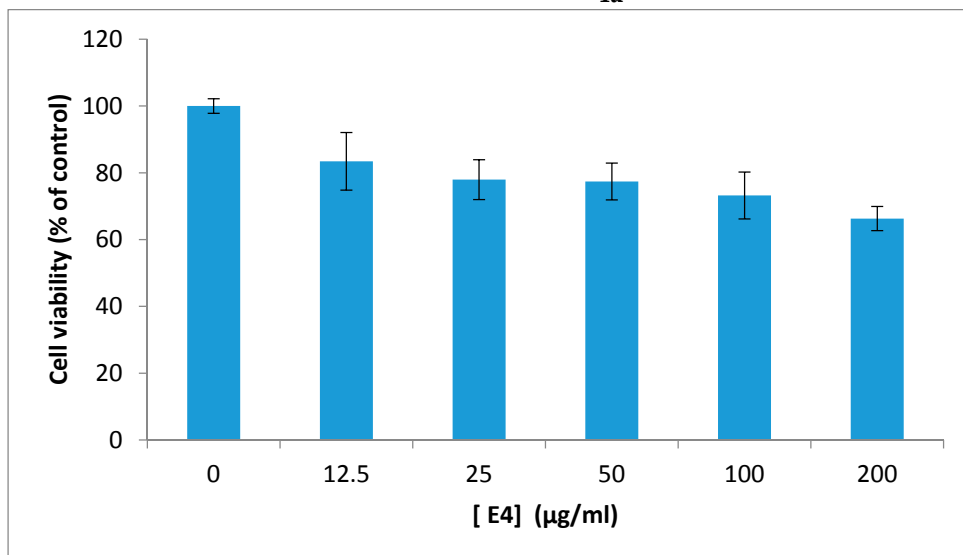


Figure S-3.9: Cytotoxicity of **4a** against MCF-7 cells

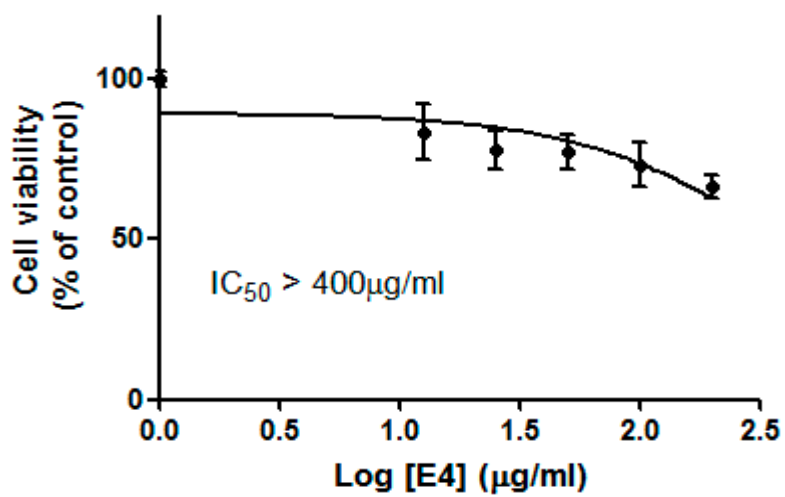
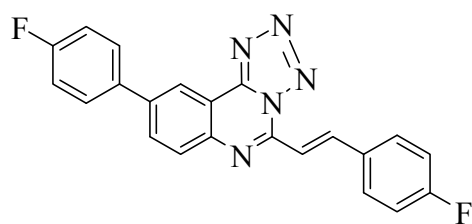


Figure S-3.10: Dose response curve of **4a** against MCF-7 cells



4b

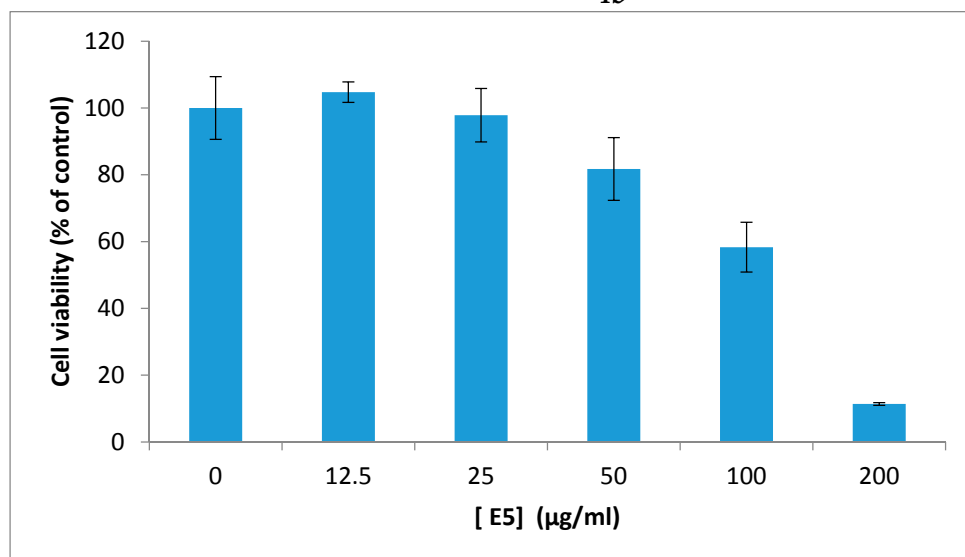
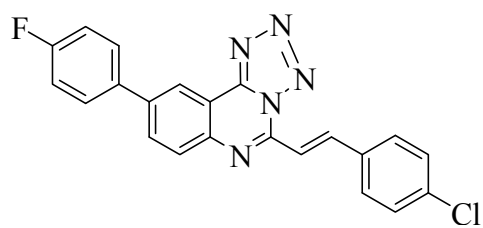


Figure S-3.11: Cytotoxicity of **4b** against MCF-7 cells



4c

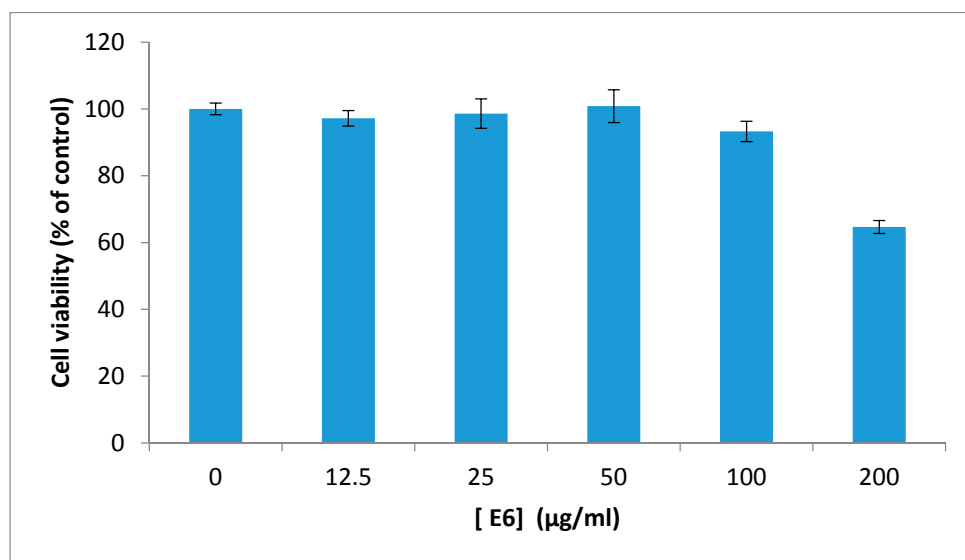
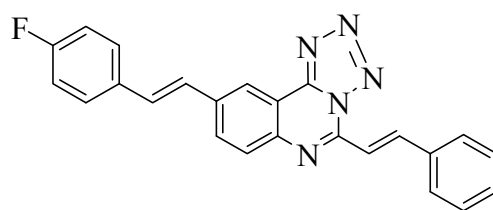


Figure S-3.12: Cytotoxicity of **4c** against MCF-7 cells



4d

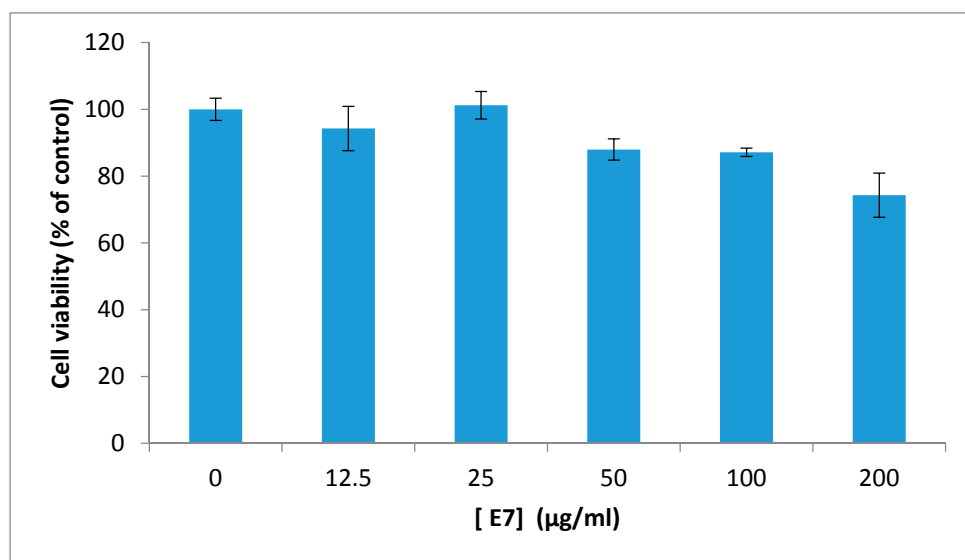
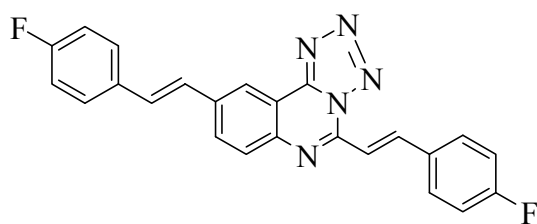


Figure S-3.13: Cytotoxicity of **4e** against MCF-7 cells



4e

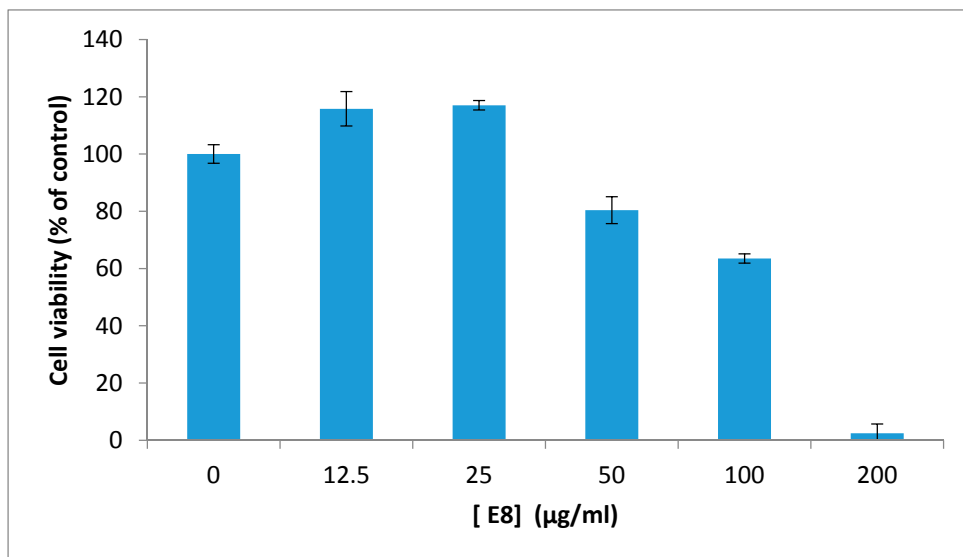


Figure S-3.14: Cytotoxicity of 4e against MCF-7 cells

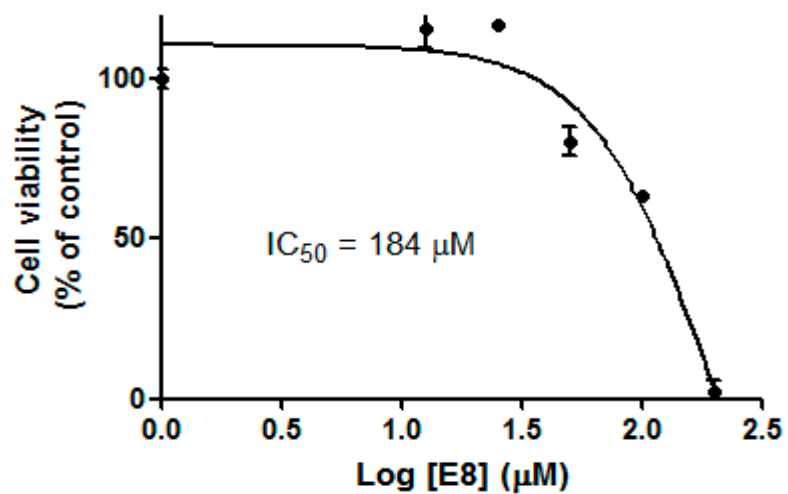
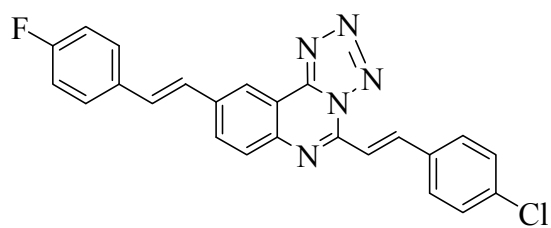


Figure S-3.15: Dose response curve of 4e against MCF-7 cells



4f

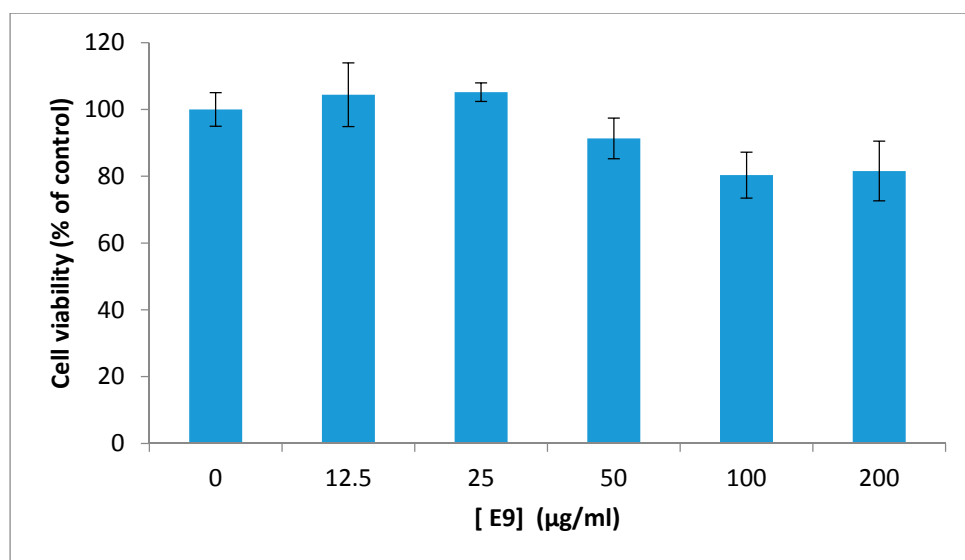
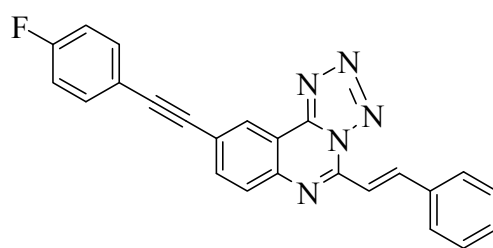


Figure S-3.16: Cytotoxicity of **4f** against MCF-7 cells



5a

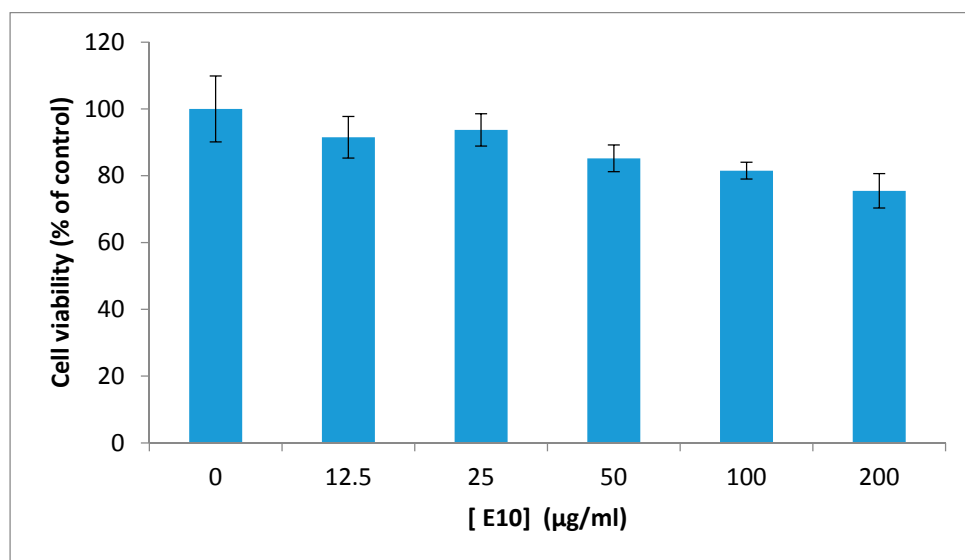


Figure S-3.17: Cytotoxicity of **5a** against MCF-7 cells

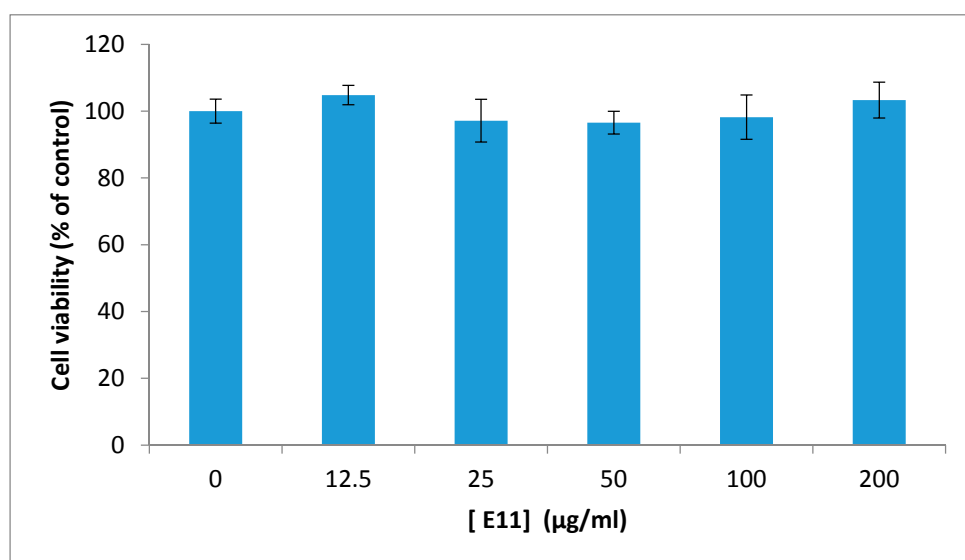
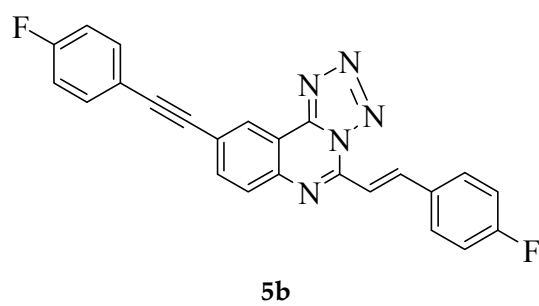


Figure S-3.18: Cytotoxicity of 5b against HeLa cells

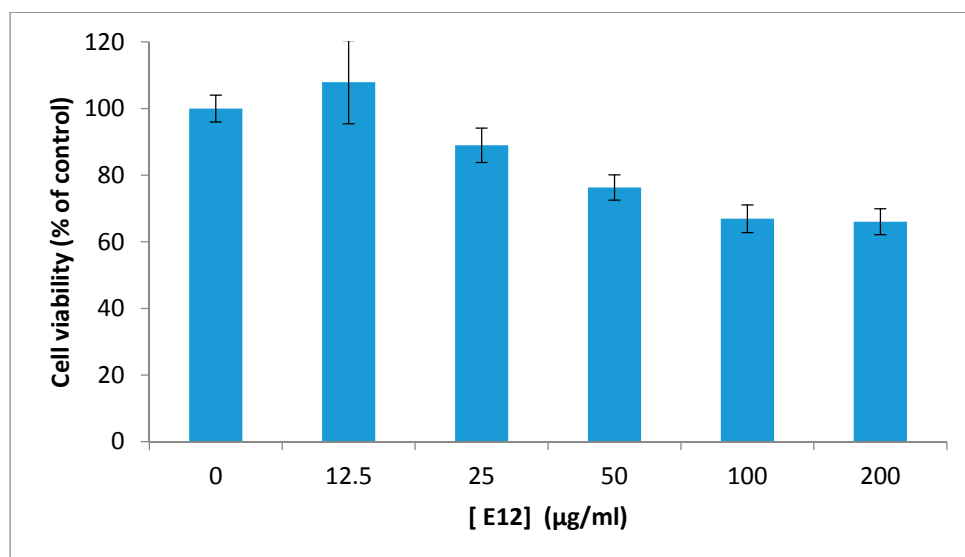
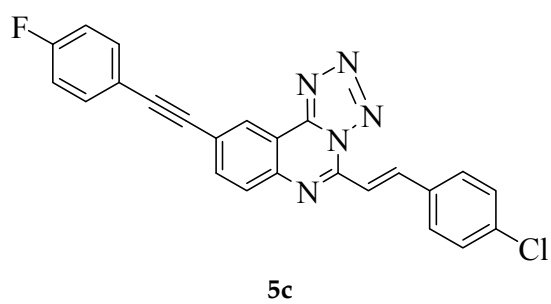


Figure S-3.19: Cytotoxicity of 5c against HeLa cells

S4: Spread sheet for statistical analysis which contains p values for each test

Compound number	Sample Code
3a	E1
3b	E2
3c	E3
4a	E4
4b	E5
4c	E6
4d	E7
4e	E8
4f	E9
5a	E10
5b	E11
5c	E12



UNISA Screening
HeLa and MCF7.xlsx