

Supplementary Material

Synthesis and *in vitro* Leishmania promastigote growth inhibition efficacy of novel 4(3*H*)-quinazolinone derivatives

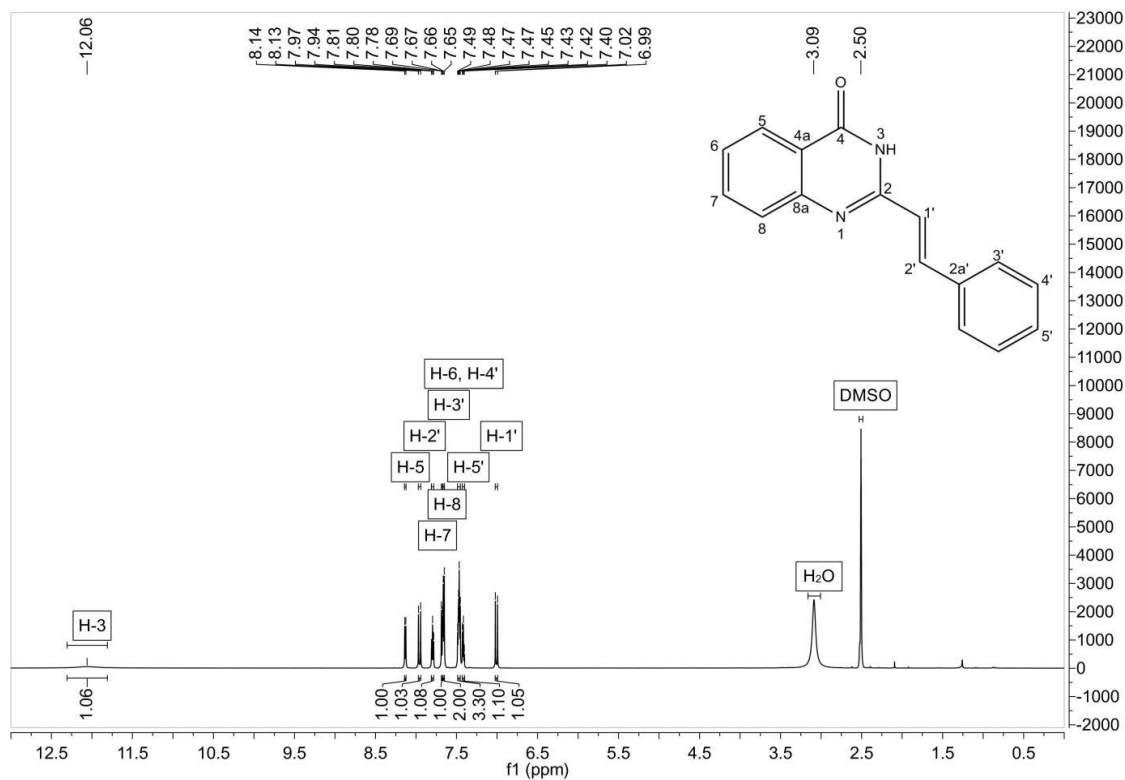
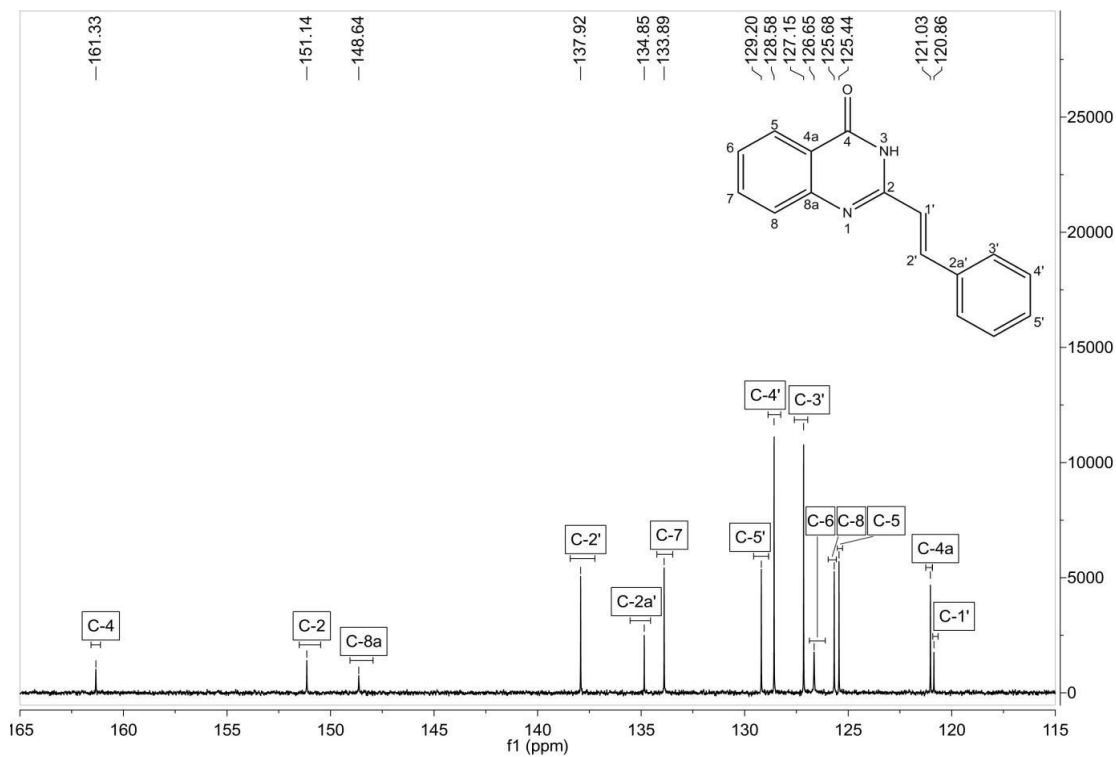
Greg L. Ralph,^a Nonkululeko H. Zuma,^a Janine Aucamp,^b and David D. N'Da^{*a}

^a *Pharmaceutical Chemistry, School of Pharmacy, North-West University, Private Bag X6001, Potchefstroom, 2520, South Africa*

^b *Centre of Excellence for Pharmaceutical Sciences, North-West University, Potchefstroom 2520, South Africa*
Email: david.nda@nwu.ac.za

Table of Contents

S1. ¹ H-NMR and ¹³ C-NMR of 2-styrylquinazolin-4(3 <i>H</i>)-one (1a)	S2
S2. HRMS and IR of 2-styrylquinazolin-4(3 <i>H</i>)-one (1a).....	S3
S3. ¹ H-NMR and ¹³ C-NMR of 2-(4-methoxystyryl)quinazolin-4(3 <i>H</i>)-one (1b)	S4
S4. HRMS and IR of 2-(4-methoxystyryl)quinazolin-4(3 <i>H</i>)-one (1b)	S5
S5. ¹ H-NMR and ¹³ C-NMR of 3-(prop-2-yn-1-yl)-2-styrylquinazolin-4(3 <i>H</i>)-one (2a)	S6
S6. HRMS and IR of 3-(prop-2-yn-1-yl)-2-styrylquinazolin-4(3 <i>H</i>)-one (2a)	S7
S7. ¹ H-NMR and ¹³ C-NMR of 2-(4-methoxystyryl)-3-(prop-2-yn-1-yl)-quinazolin-4(3 <i>H</i>)-one (2b).....	S8
S8. HRMS and IR of 2-(4-methoxystyryl)-3-(prop-2-yn-1-yl)-quinazolin-4(3 <i>H</i>)-one (2b)	S9
S9. ¹ H-NMR, ¹³ C-NMR, HRMS and IR of substituted 3-(benzyltriazolylmethyl)-2-styryl quinazolinones (4a-j) ..	S10

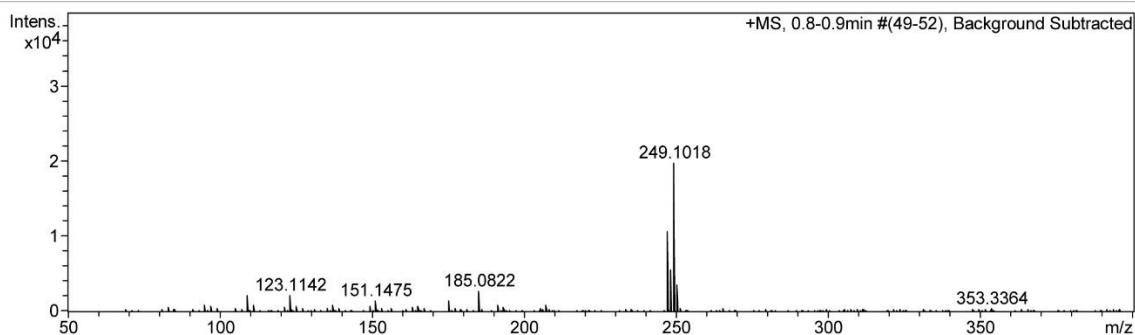
S1. (E)-2-Styrylquinazolin-4(3H)-one (**1a**)¹H-NMR in DMSO-d₆¹³C-NMR in DMSO-d₆

S2. HRMS and IR of 2-styrylquinazolin-4(3H)-one (**1a**)

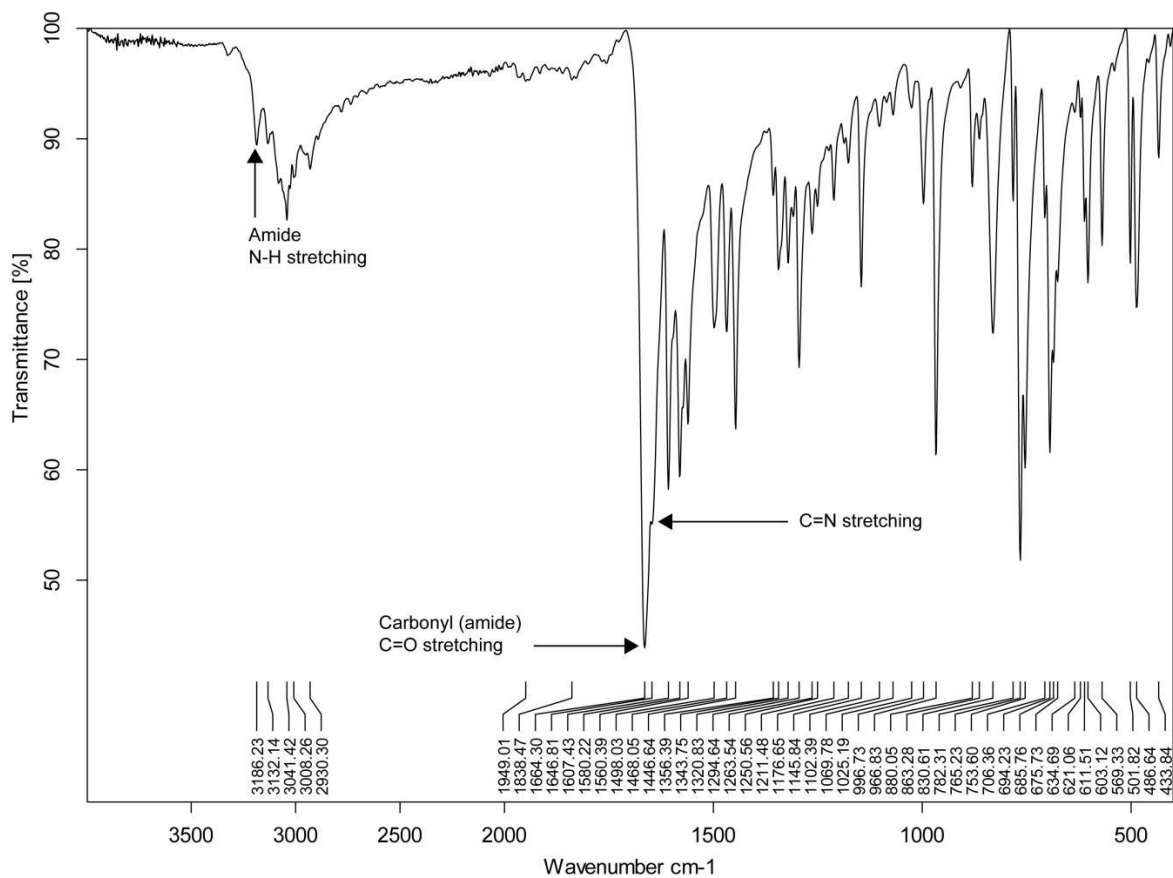
HRMS

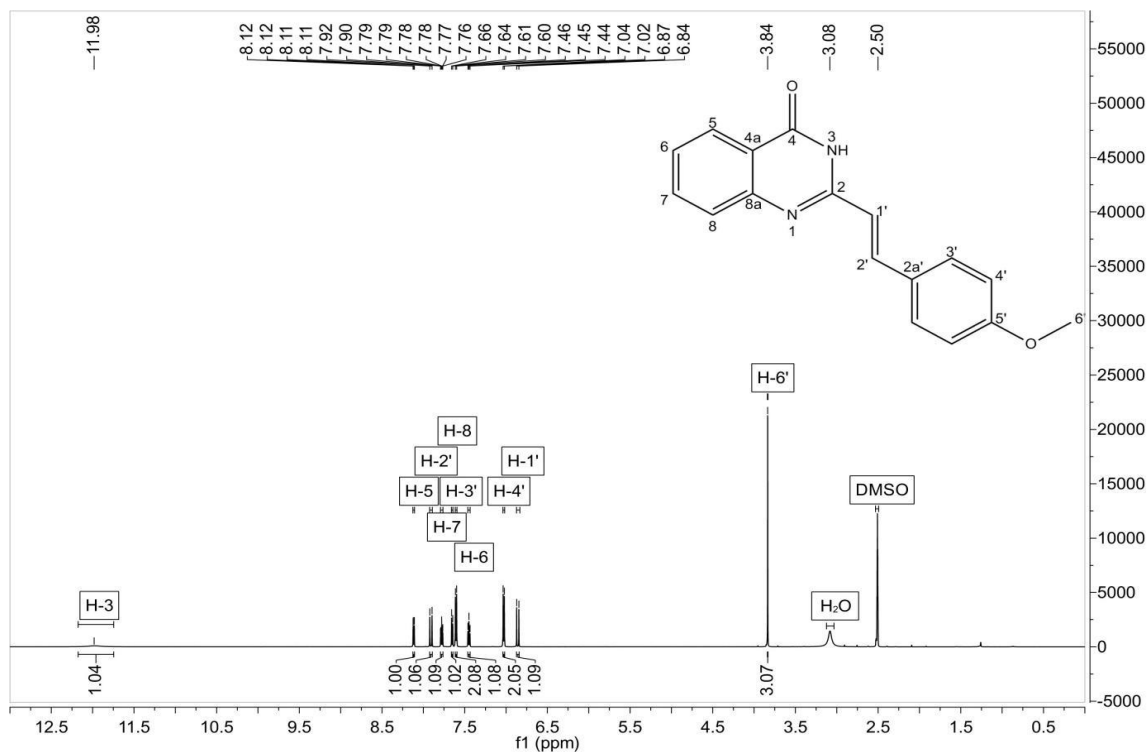
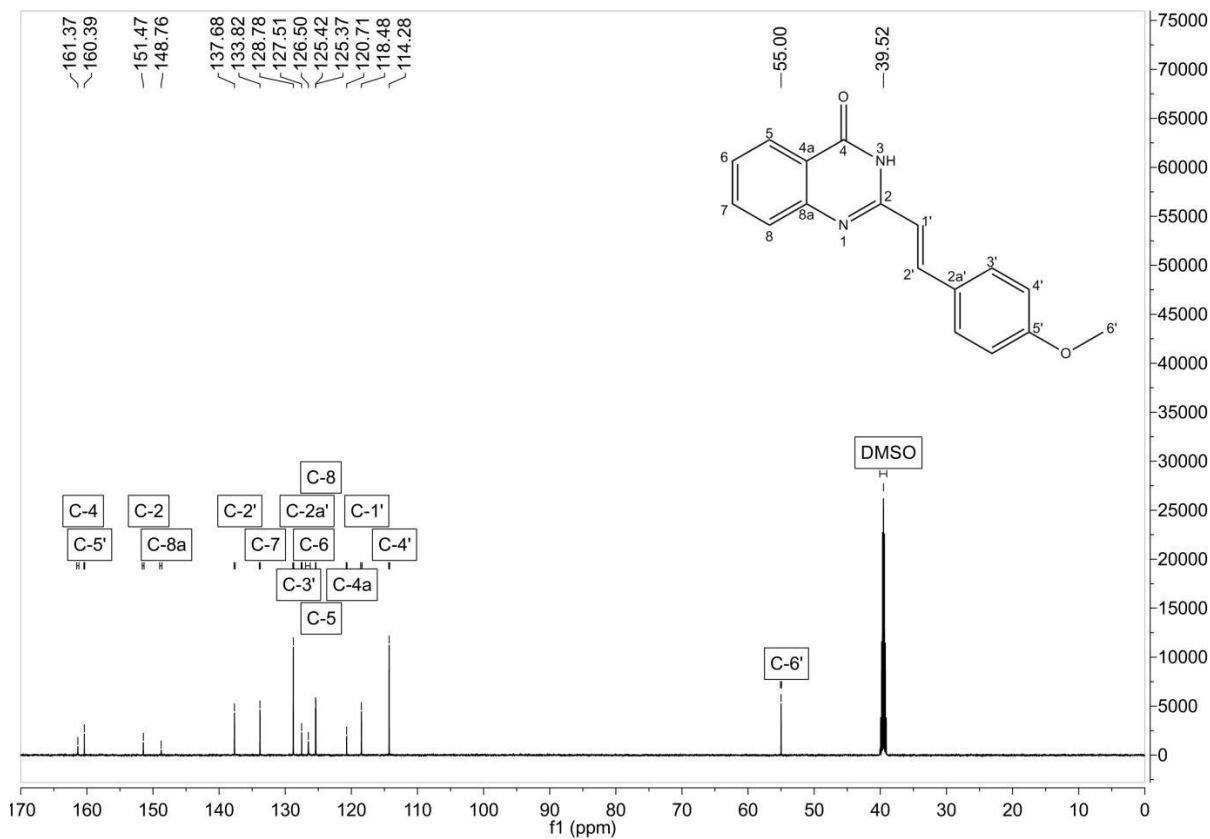
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



IR



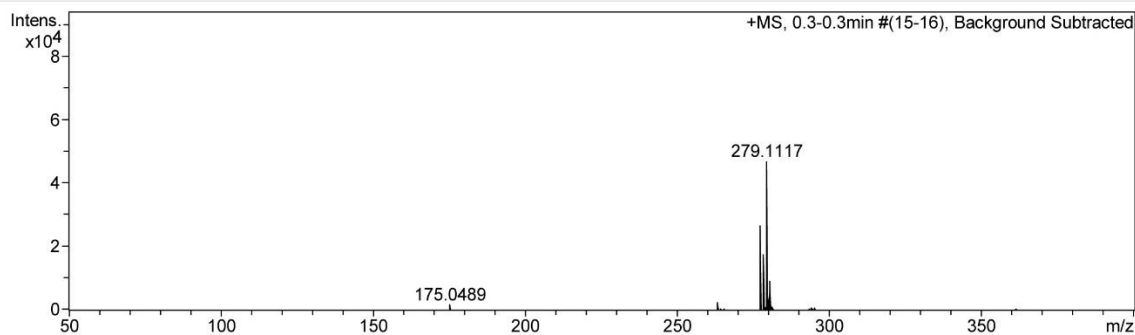
S3. (*E*)-2-(4-Methoxystyryl)-quinazolin-4(3*H*)-one (**1b**)¹H-NMR in DMSO-d₆¹³C-NMR in DMSO-d₆

S4. HRMS and IR of 2-(4-methoxystyryl)quinazolin-4(3H)-one (**1b**)

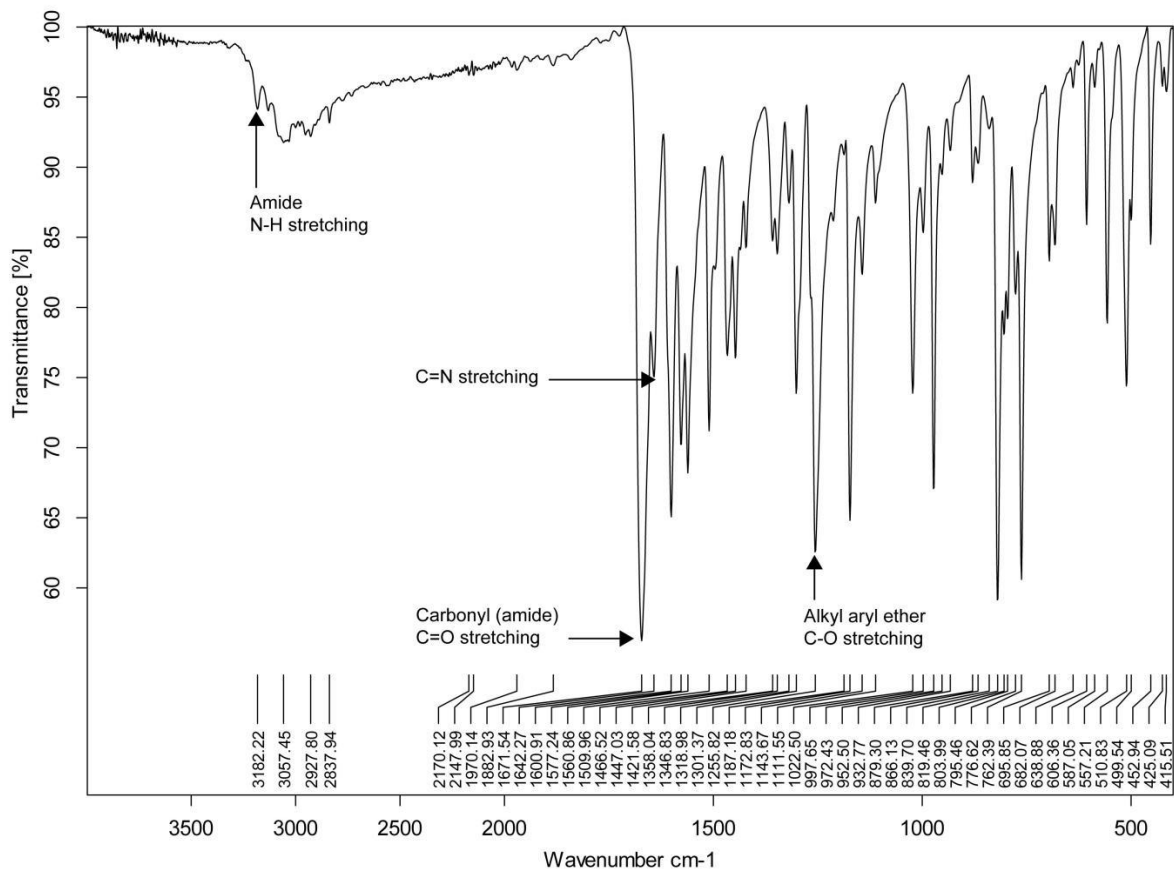
HRMS

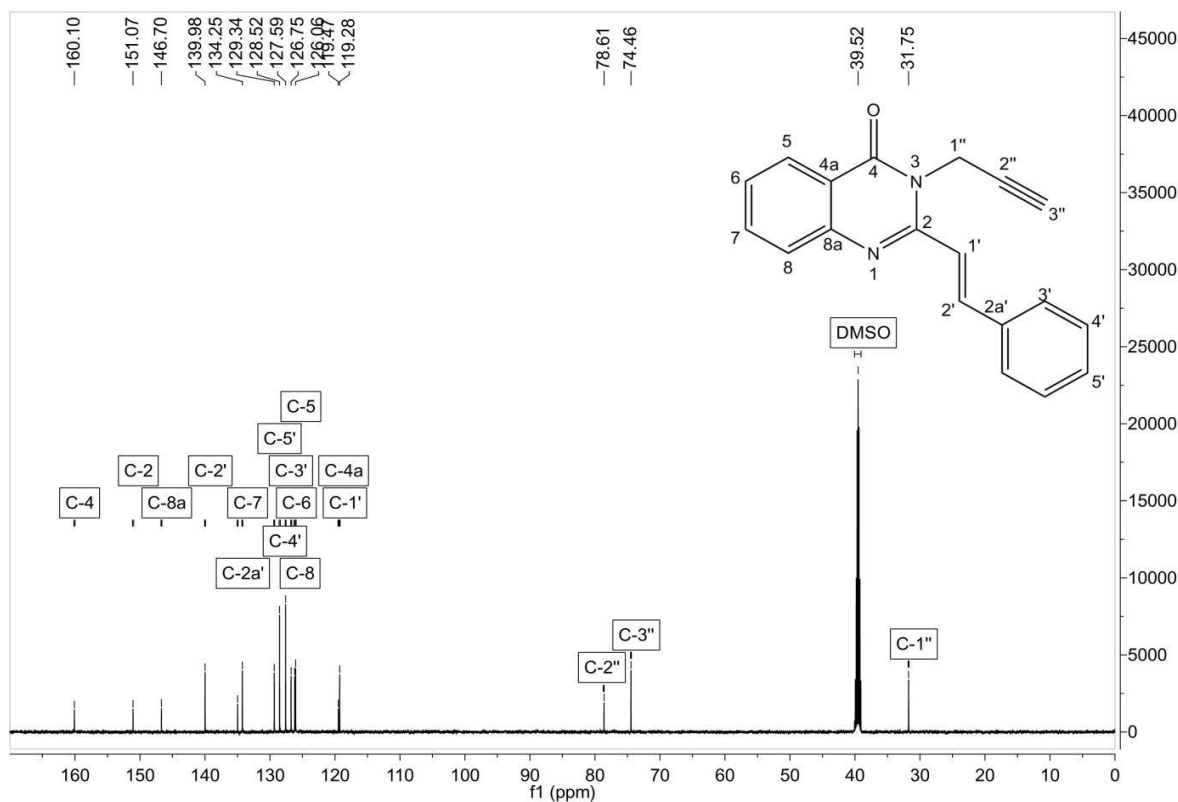
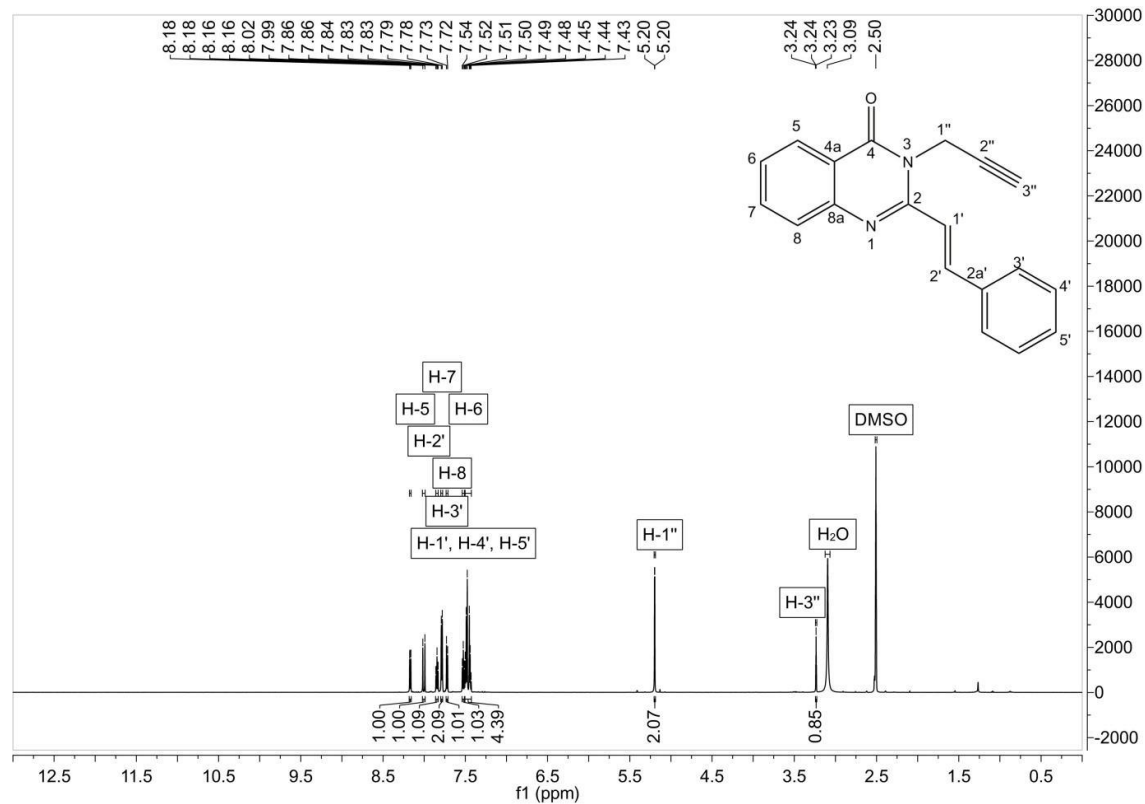
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



IR



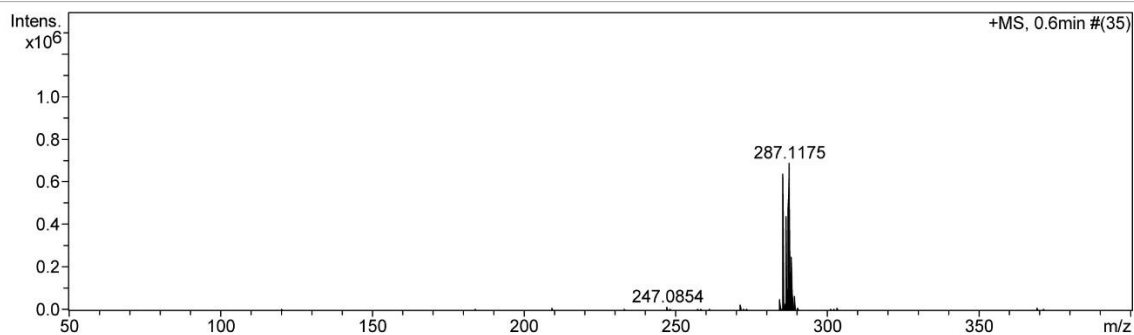
¹H-NMR in DMSO-d₆

S6. HRMS and IR of 3-(prop-2-yn-1-yl)-2-styrylquinazolin-4(3H)-one (**2a**)

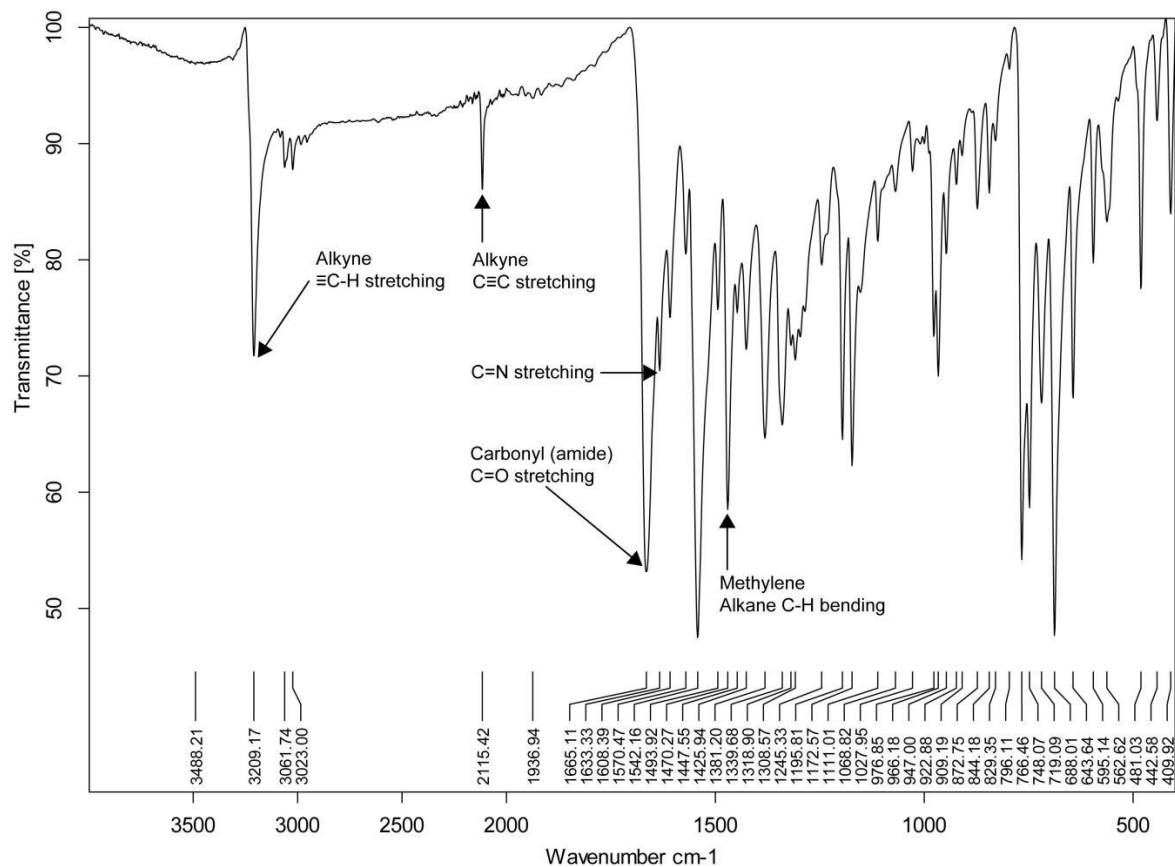
HRMS

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

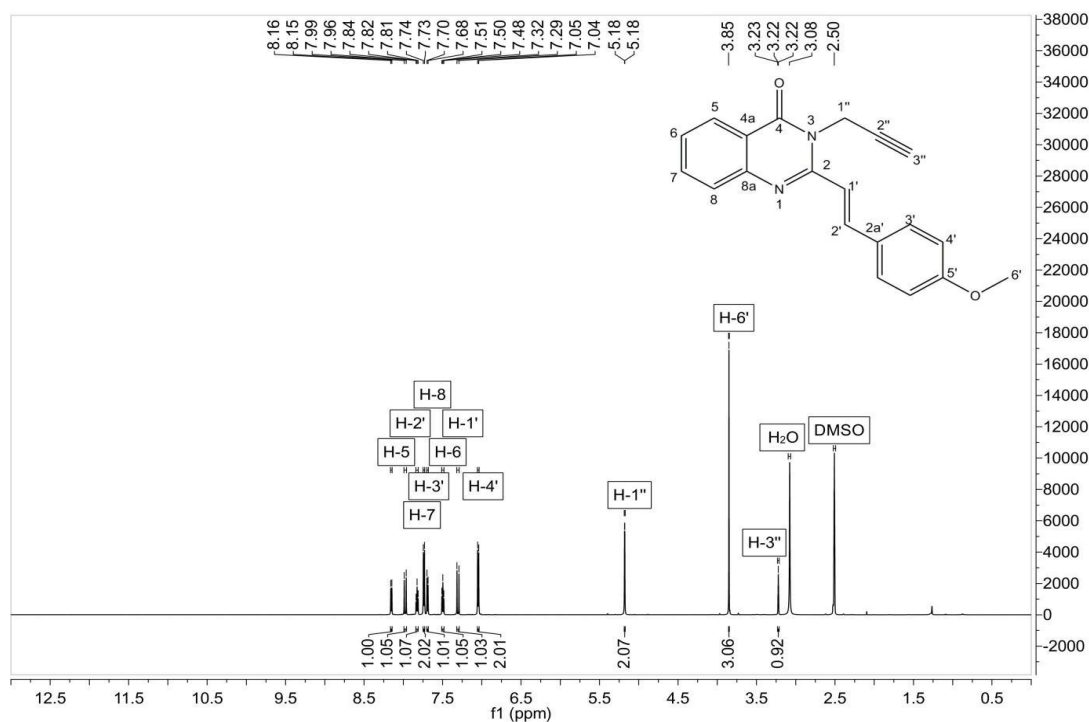


IR

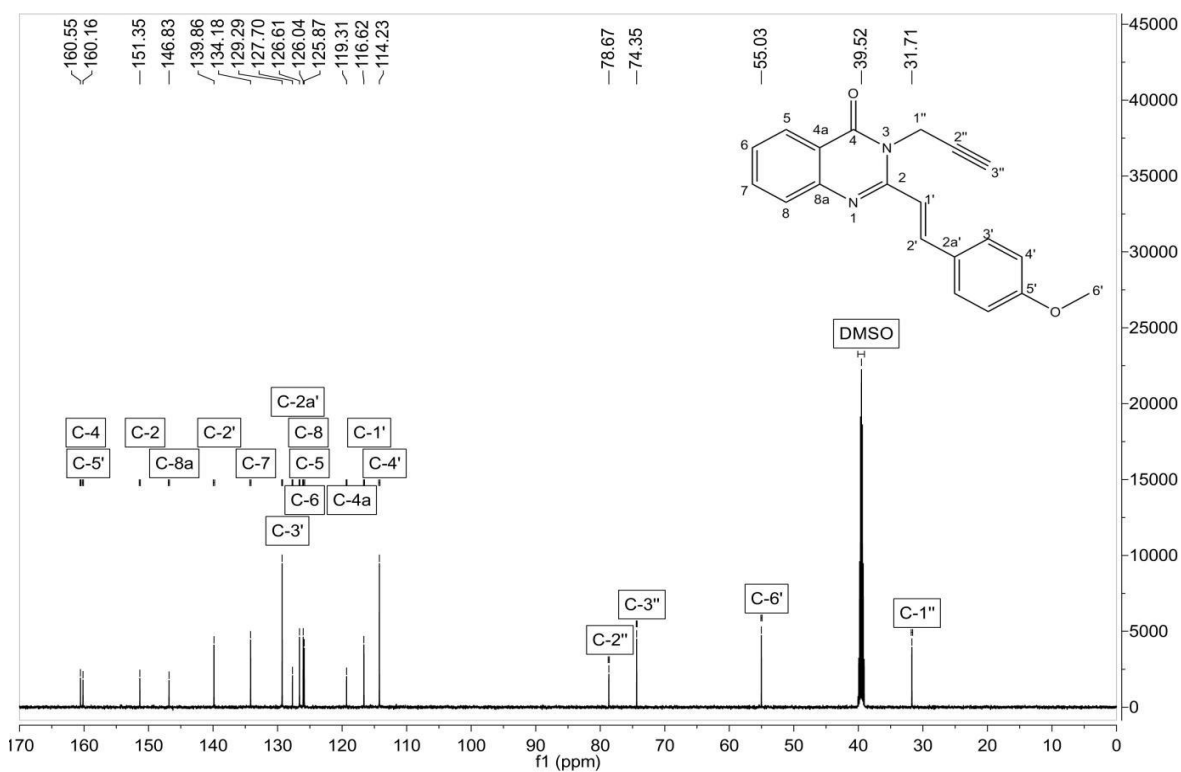


S7. ^1H -NMR and ^{13}C -NMR of 2-(4-methoxystyryl)-3-(prop-2-yn-1-yl)-quinazolin-4(3H)-one (2b)

^1H -NMR in DMSO-d_6



^{13}C -NMR in DMSO-d_6

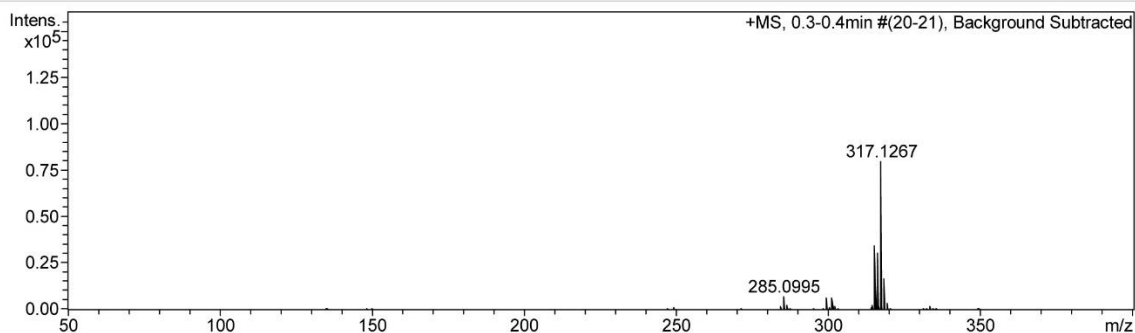


S8. HRMS and IR of 2-(4-methoxystyryl)-3-(prop-2-yn-1-yl)-quinazolin-4(3H)-one (**2b**)

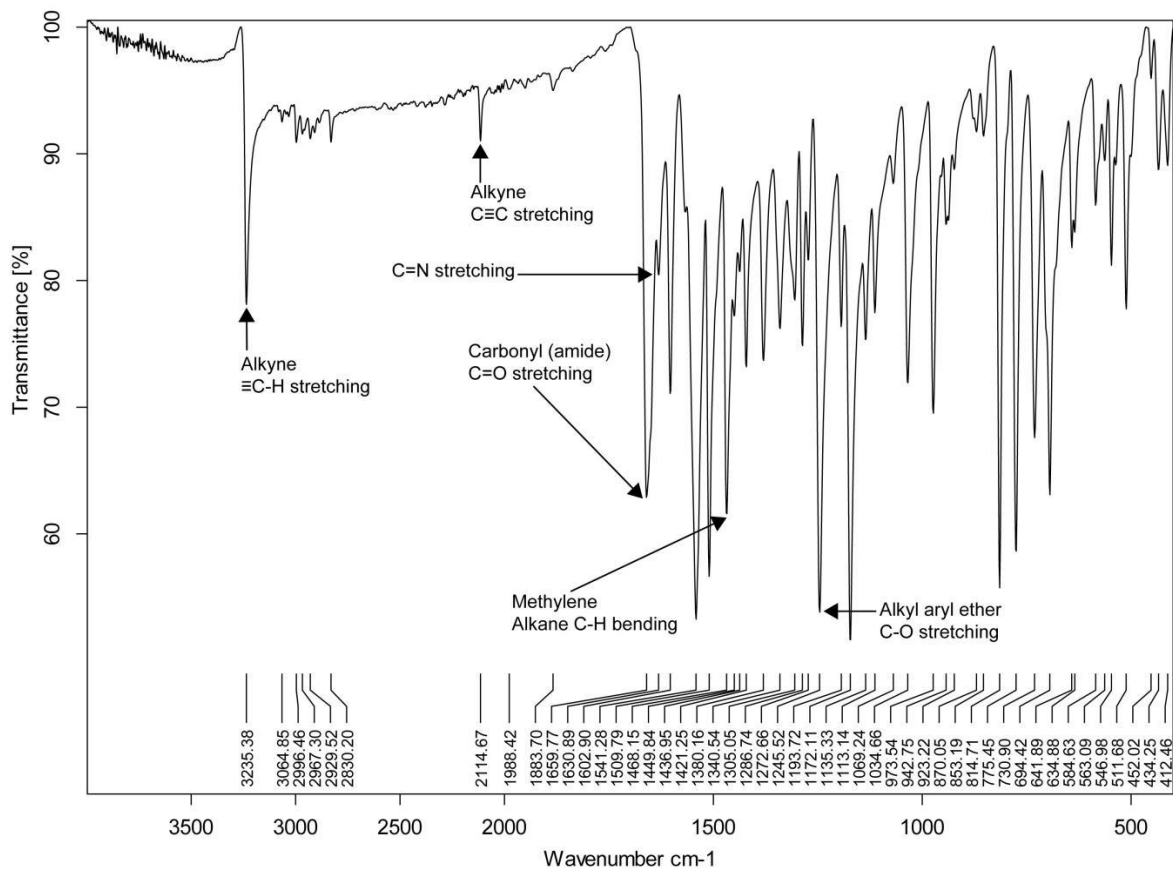
HRMS

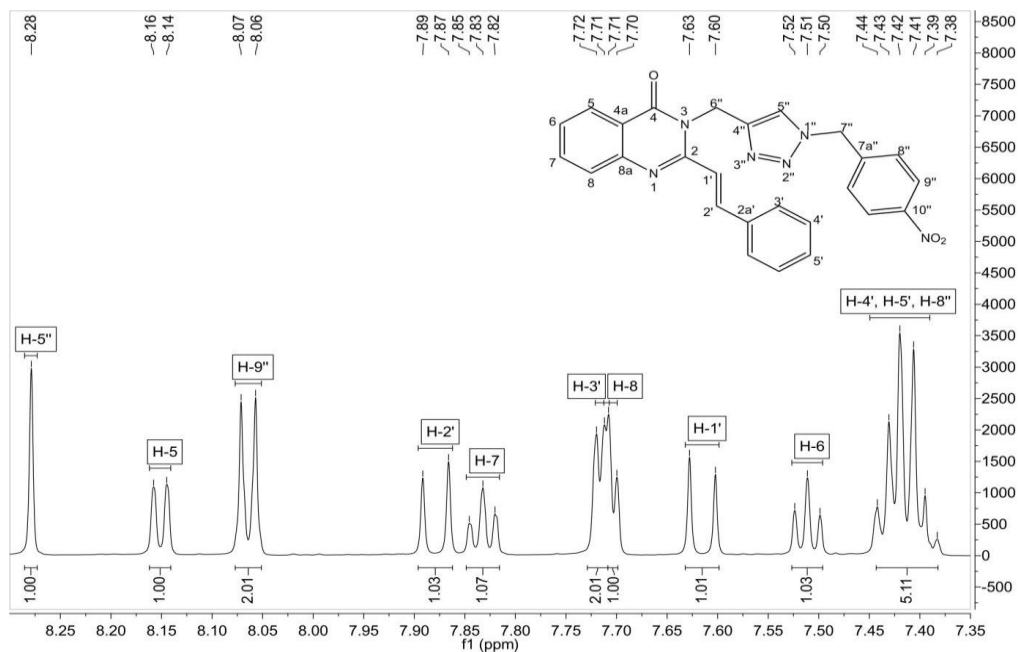
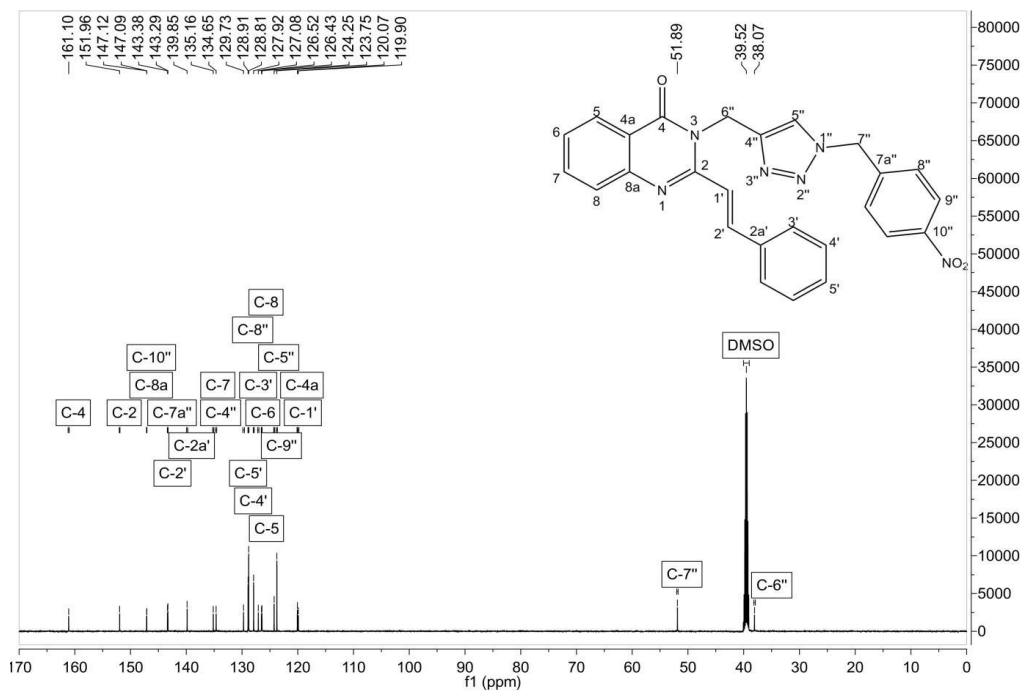
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



IR

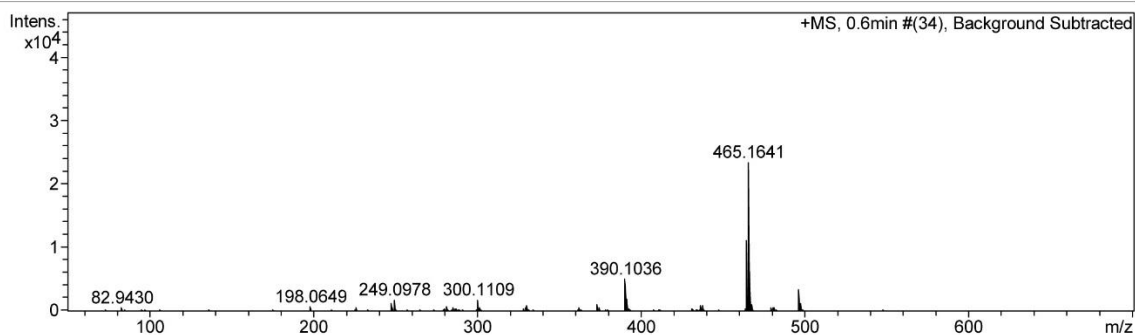


S9. (E)-3-[[1-(4-Nitrobenzyl)-1H-1,2,3-triazol-4-yl]methyl]-2-styrylquinazolin-4(3H)-one **4a**¹H-NMR in DMSO¹³C-NMR in DMSO

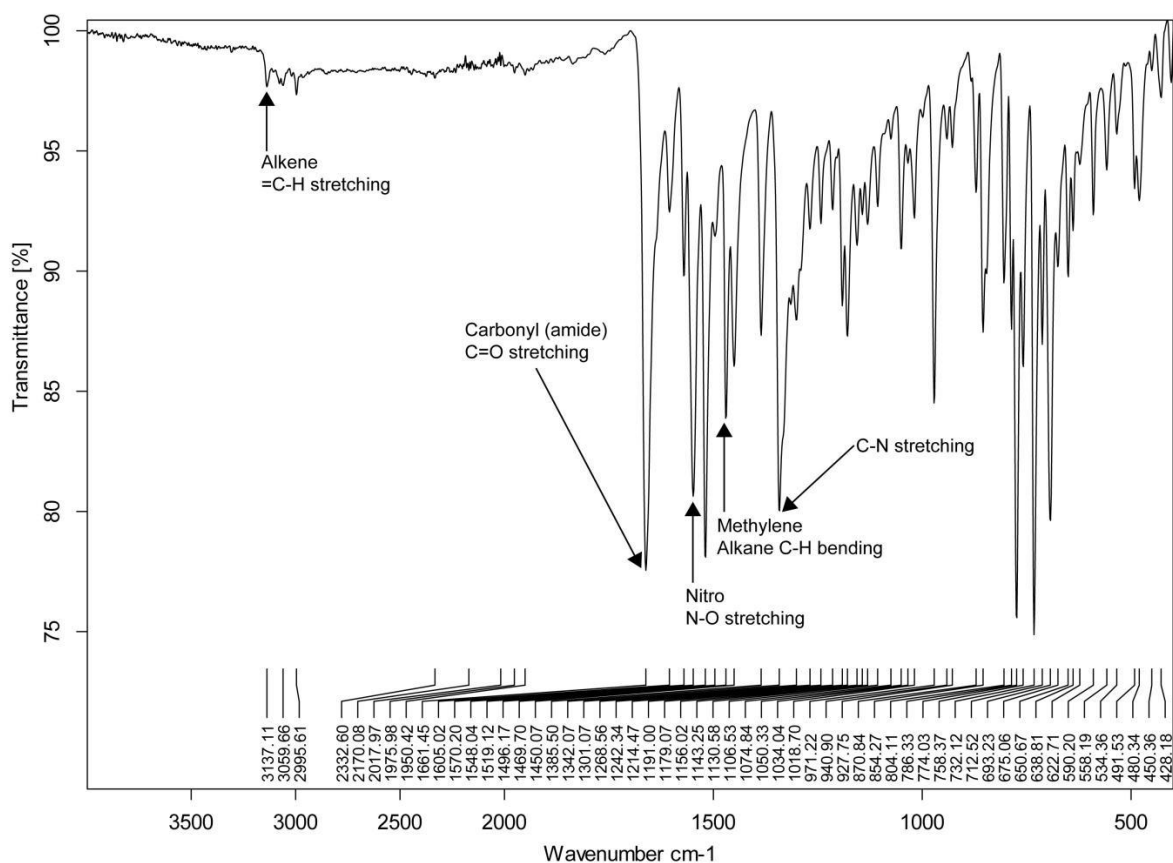
HRMS

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

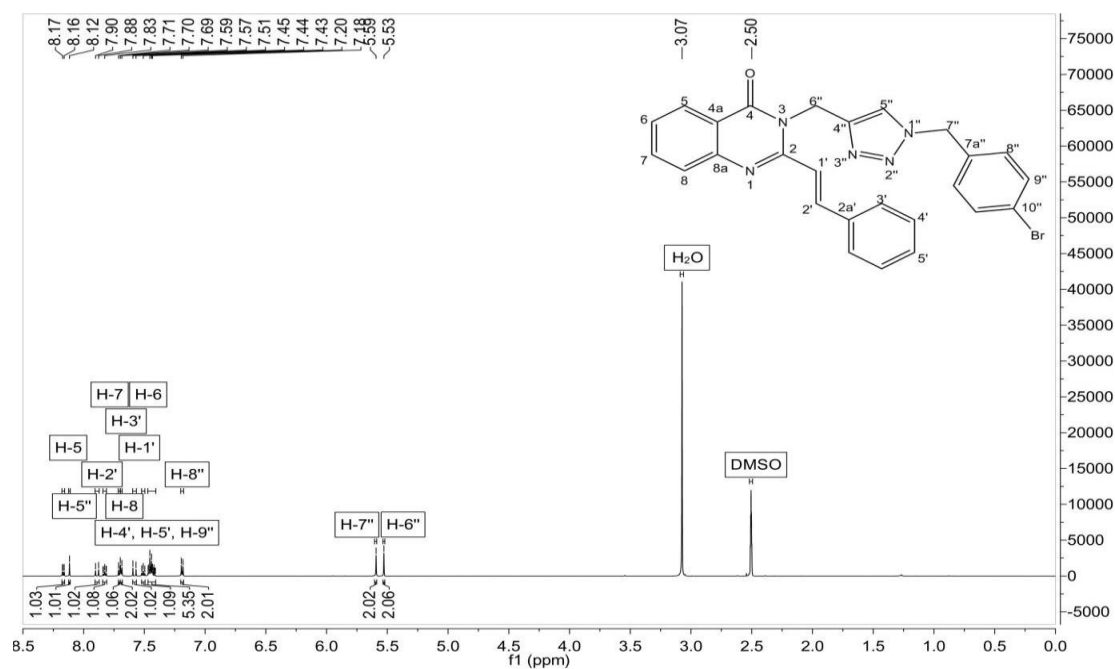


IR

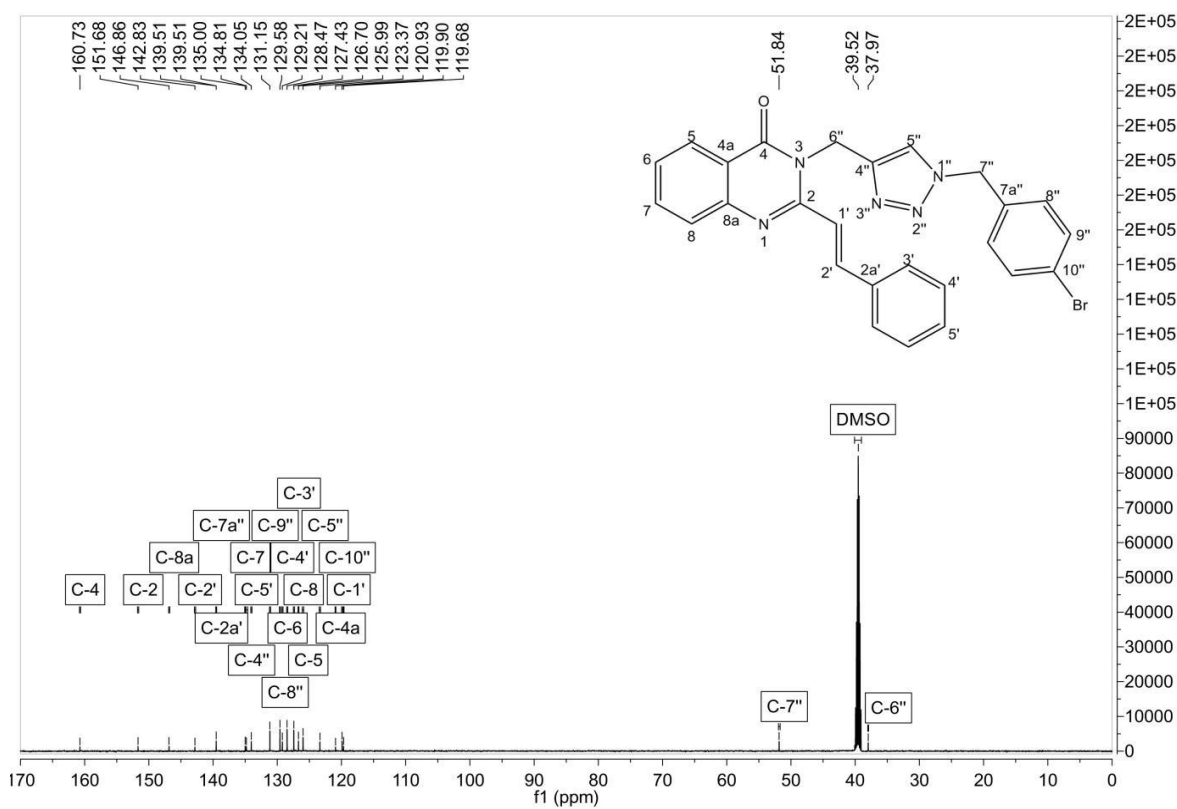


(*E*)-3-{[1-(4-Bromobenzyl)-1*H*-1,2,3-triazol-4-yl]methyl}-2-styrylquinazolin-4(3*H*)-one **4b**

¹H-NMR in DMSO



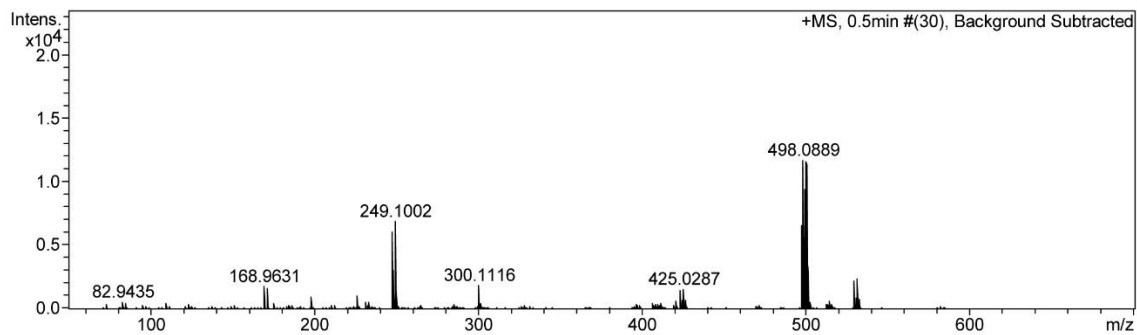
¹³C-NMR in DMSO



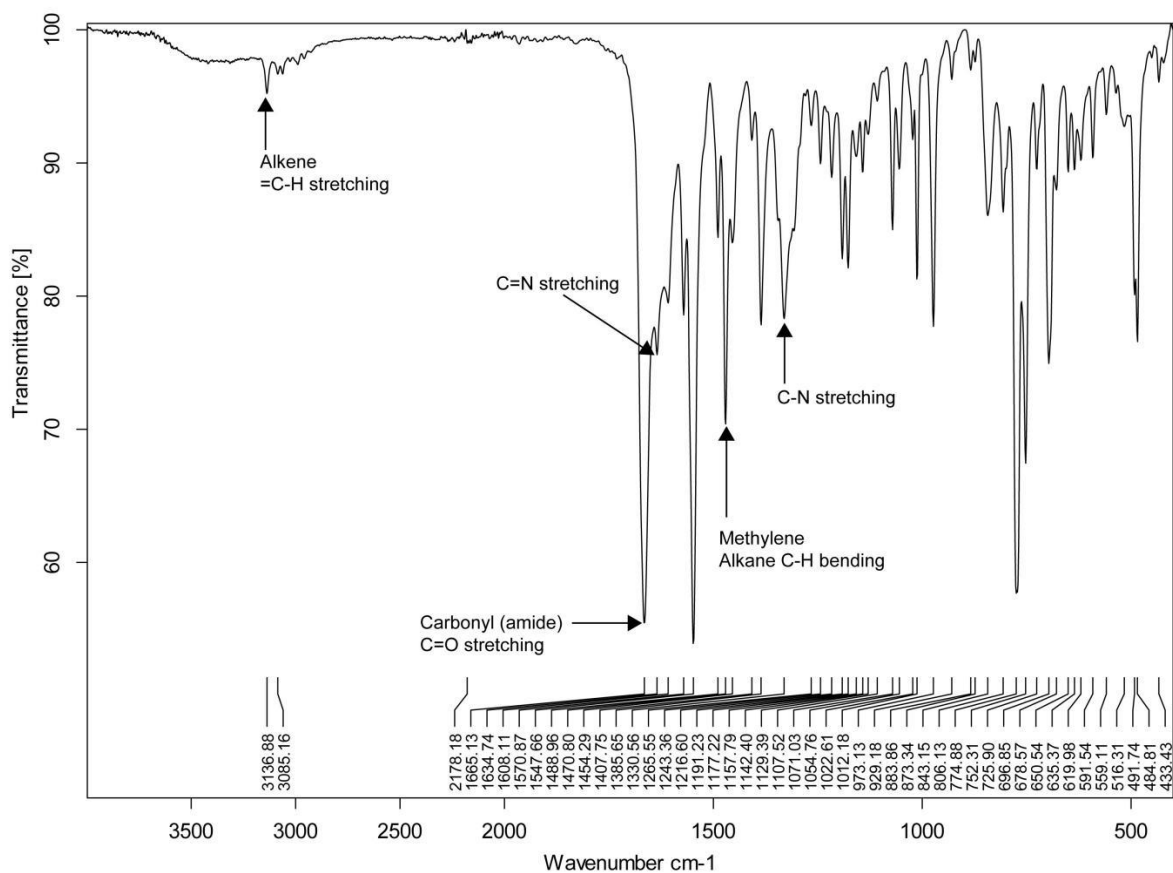
HRMS

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

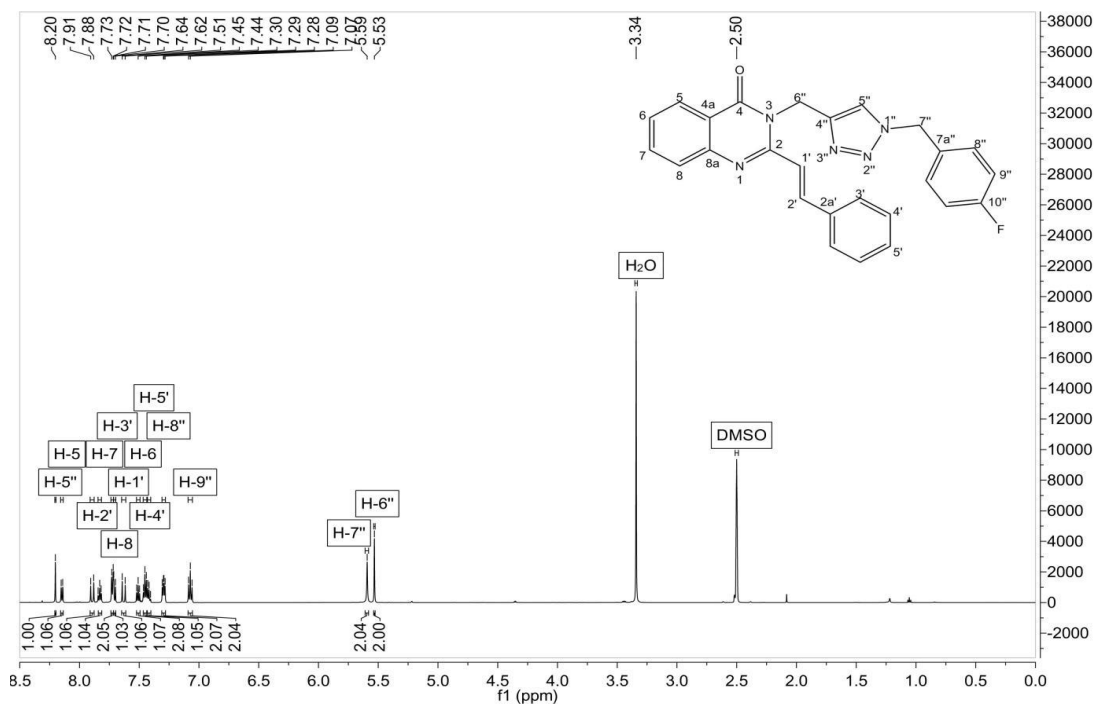


IR

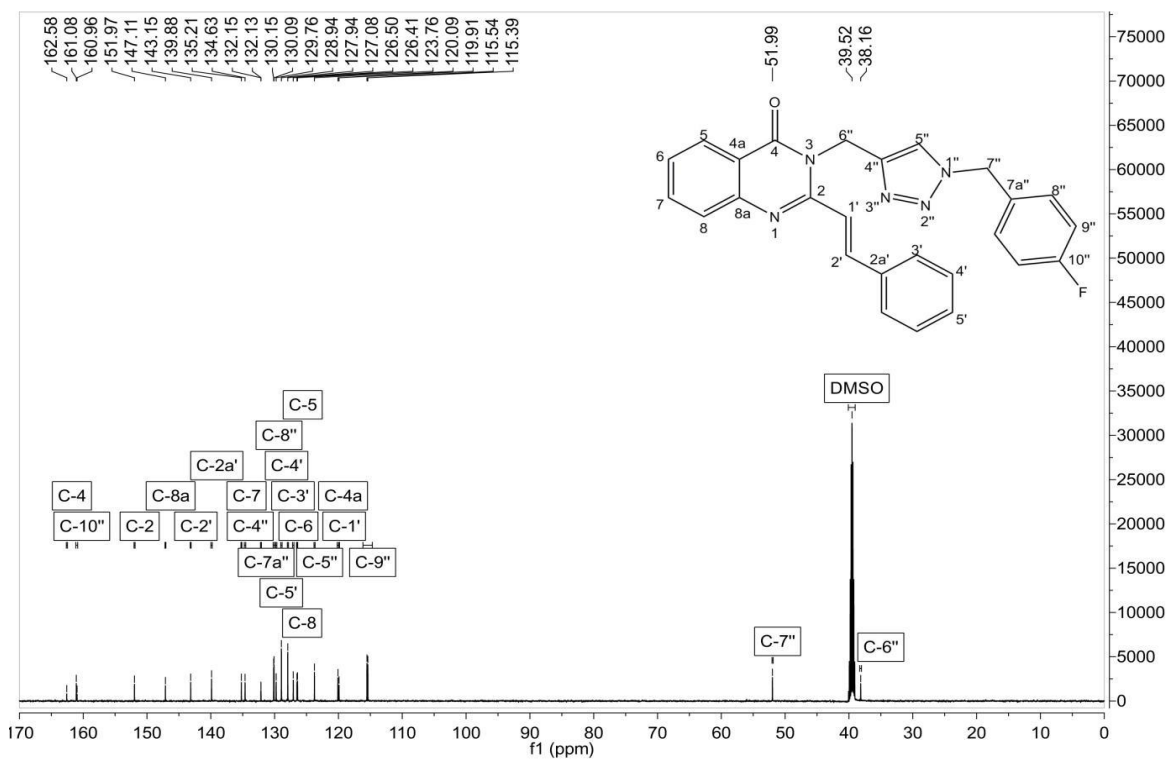


(E)-3-{[1-(4-Fluorobenzyl)-1*H*-1,2,3-triazol-4-yl]methyl}-2-styrylquinazolin-4(3*H*)-one **4c**

¹H-NMR in DMSO



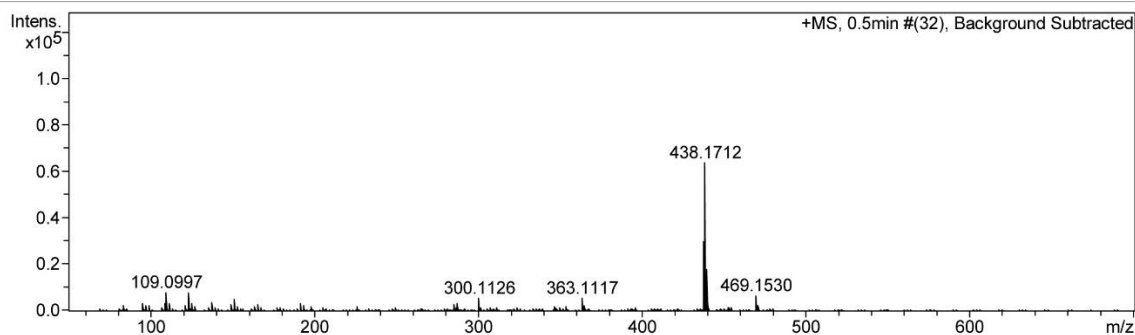
¹³C-NMR in DMSO



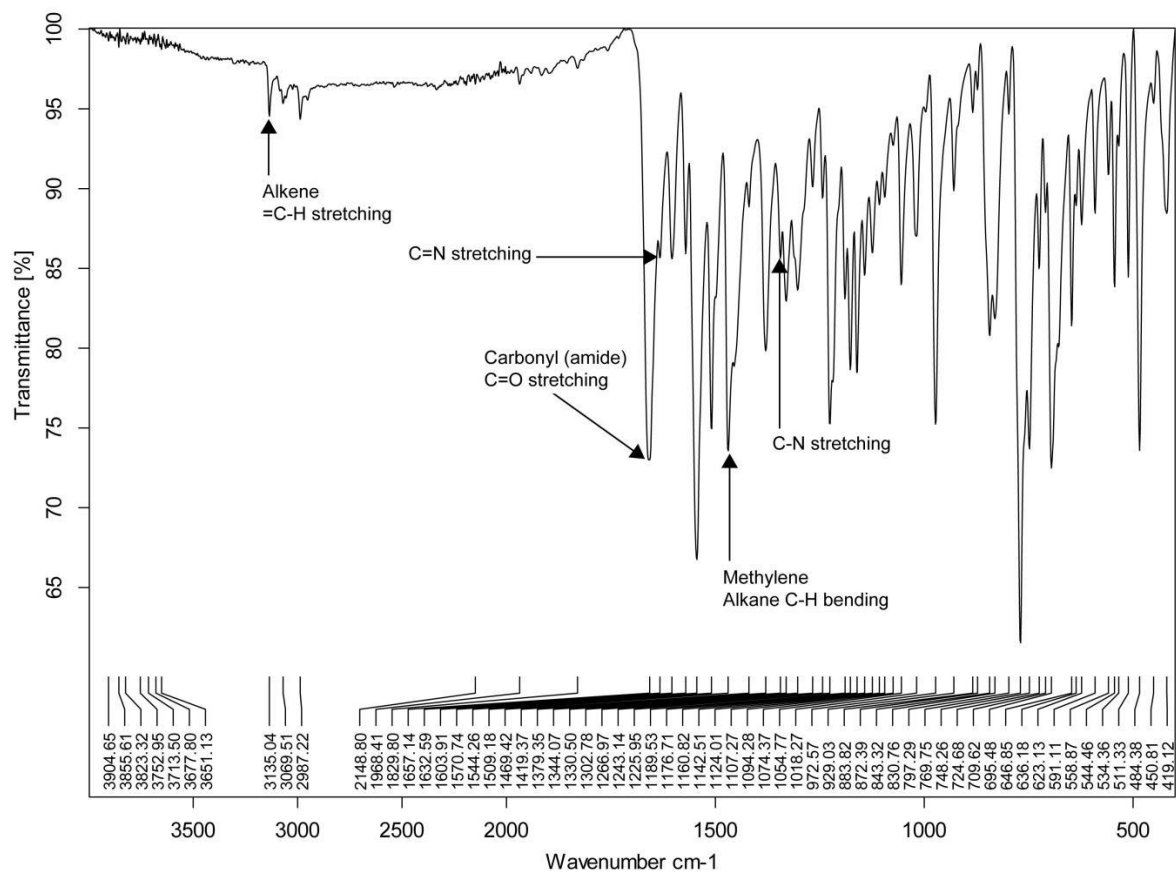
HRMS

Acquisition Parameter

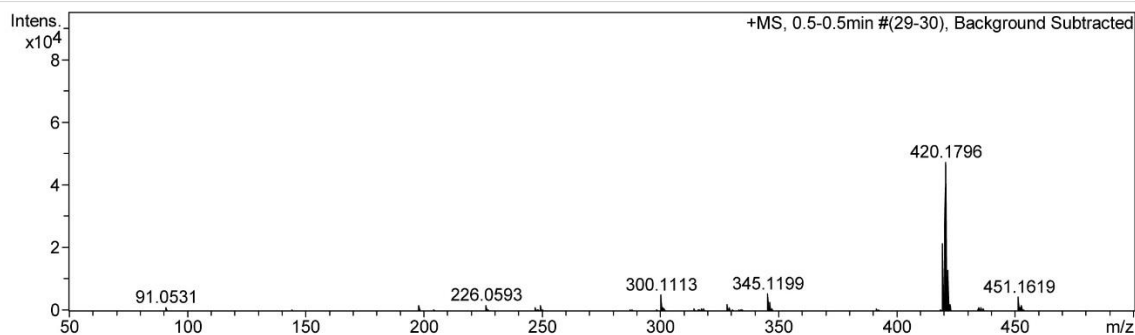
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



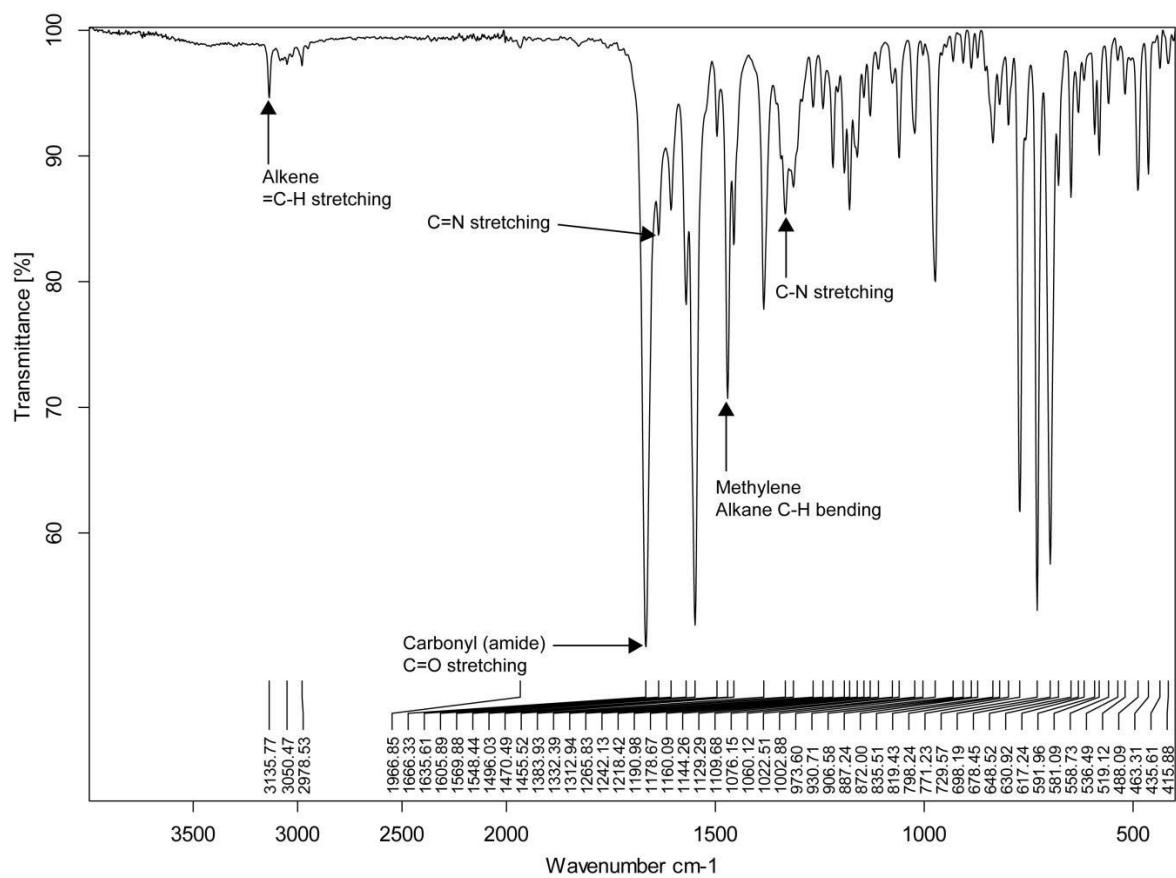
IR



¹H-NMR in DMSO

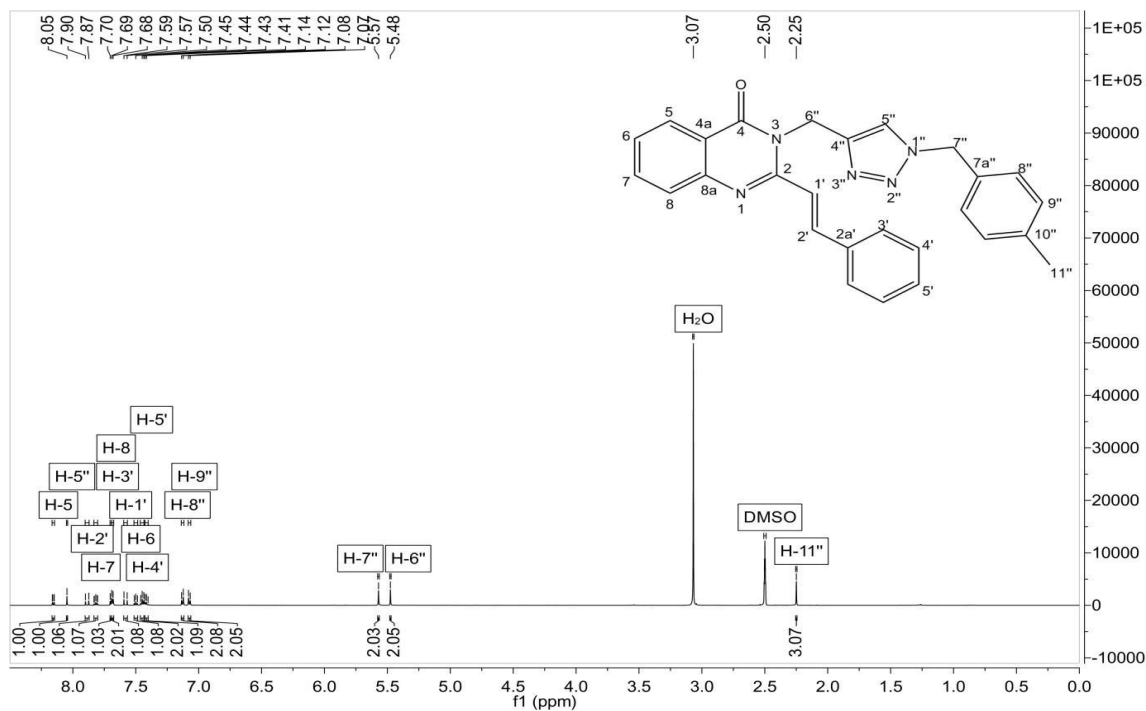


IR

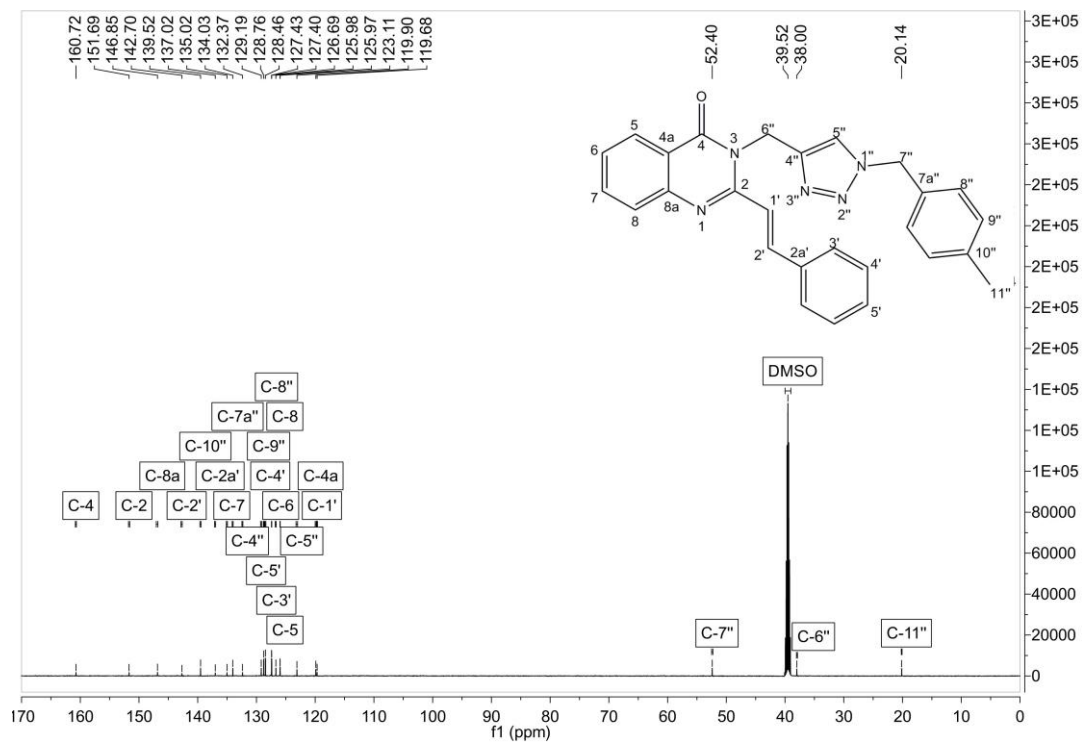


(*E*)-3-[[1-(4-Methylbenzyl)-1*H*-1,2,3-triazol-4-yl]methyl]-2-styrylquinazolin-4(3*H*)-one **4e**

¹H-NMR in DMSO



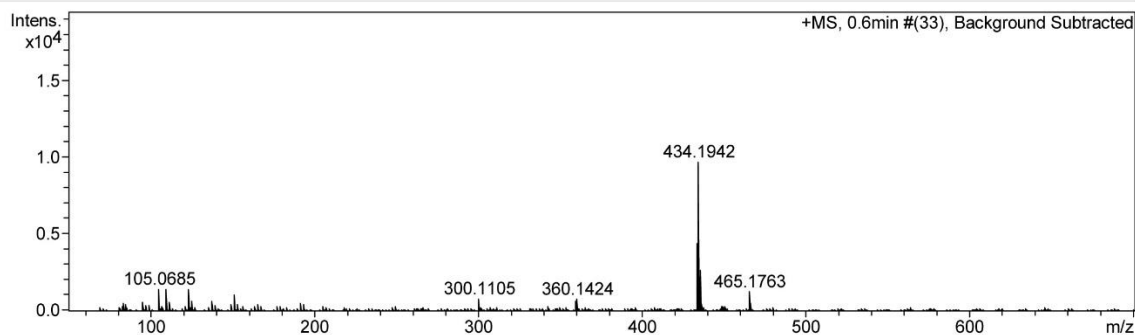
¹³C-NMR in DMSO



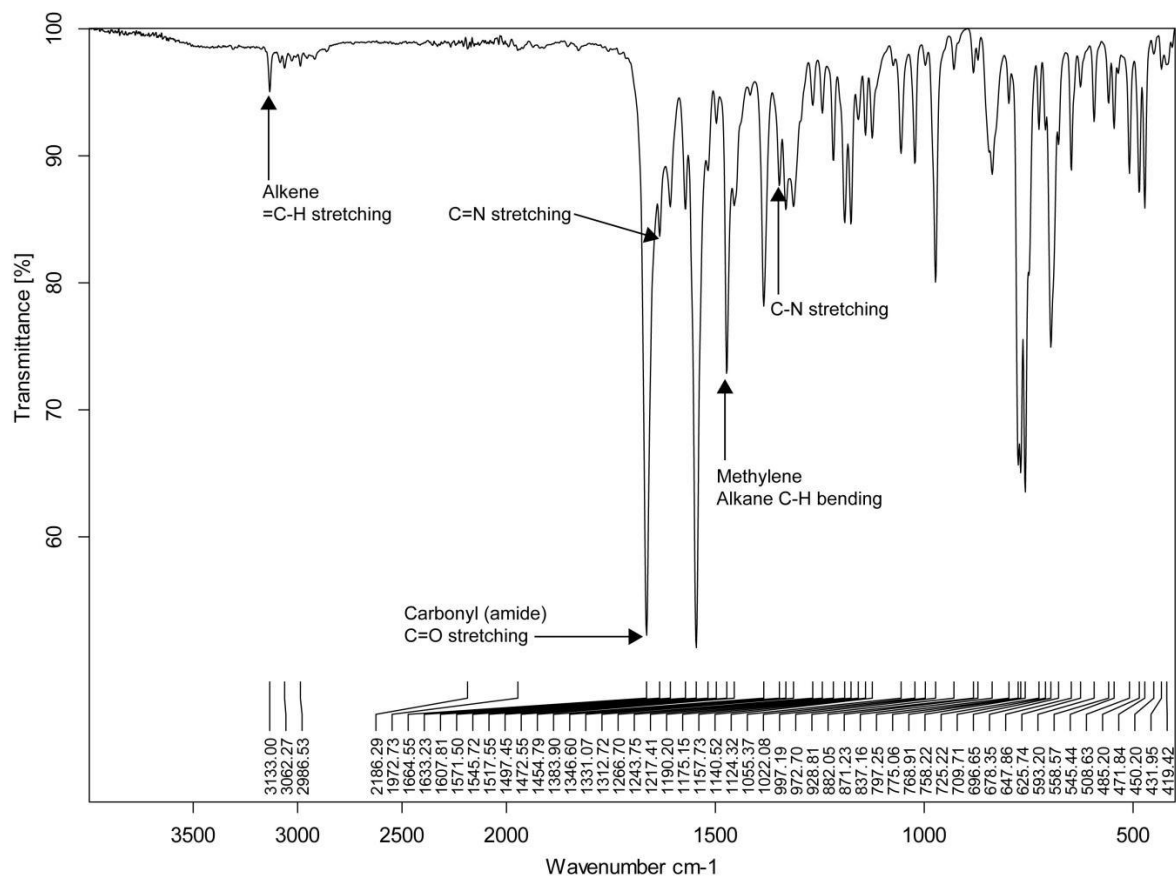
HRMS

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

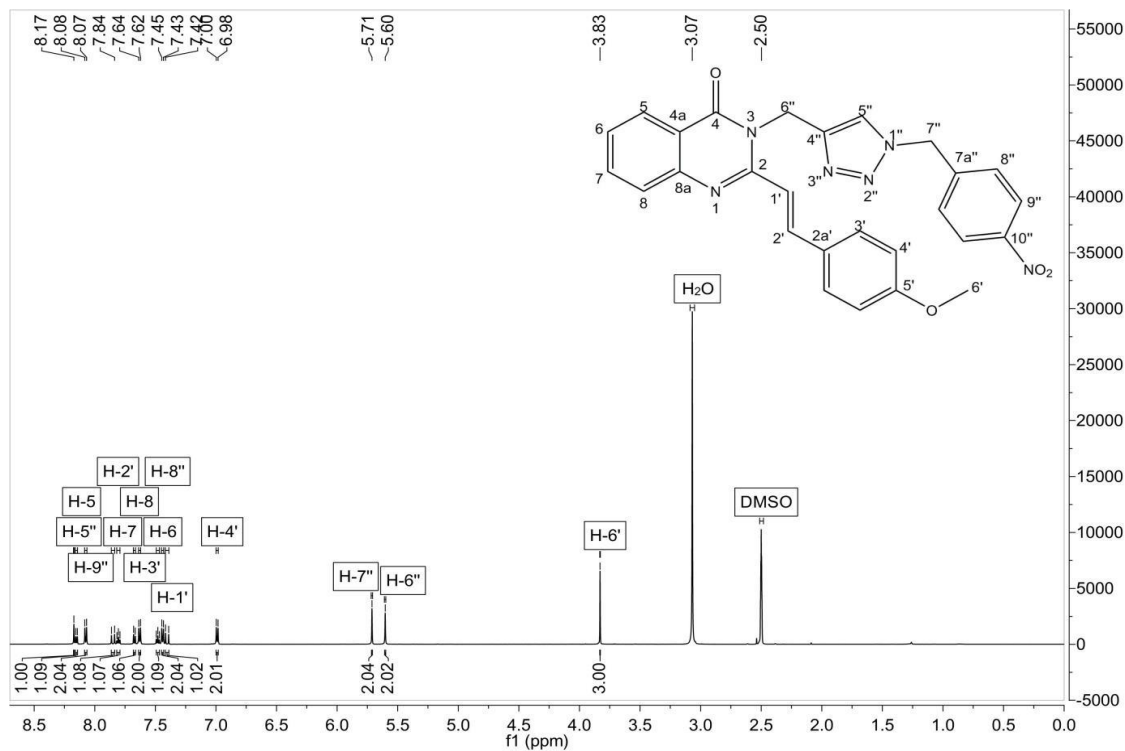


IR

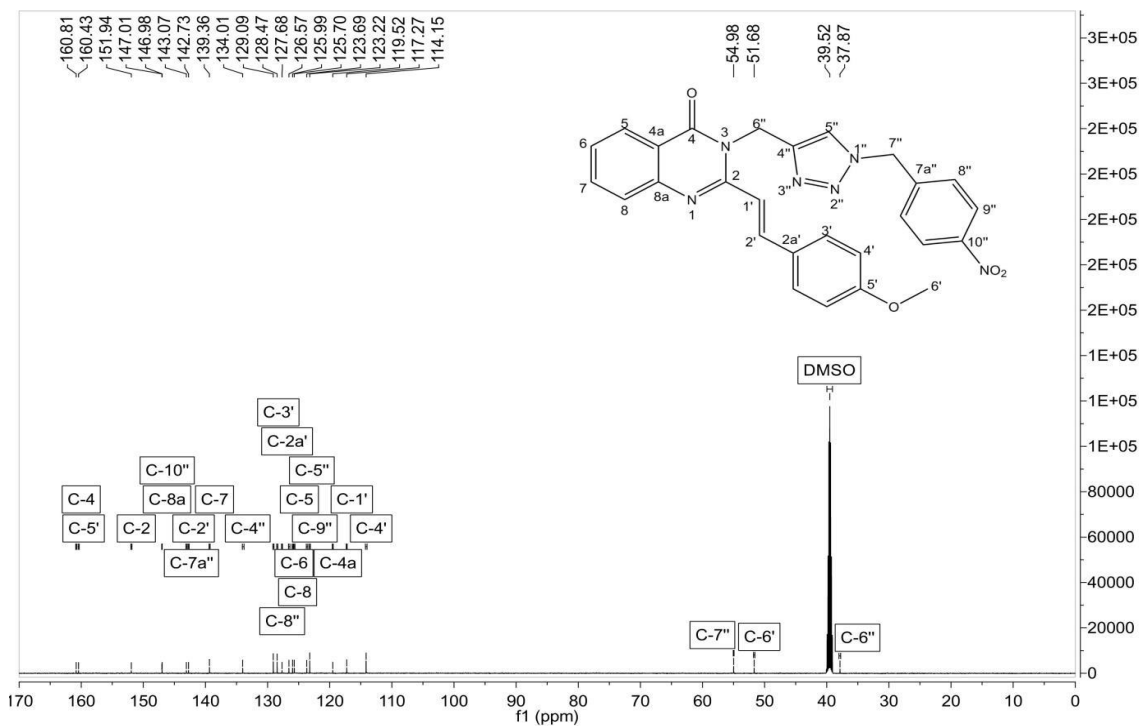


(*E*)-2-(4-Methoxy-styryl)-3-[[1-(4-nitrobenzyl)-1*H*-1,2,3-triazol-4-yl]-methyl]-quinazolin-4(3*H*)-one **4f**

¹H-NMR in DMSO



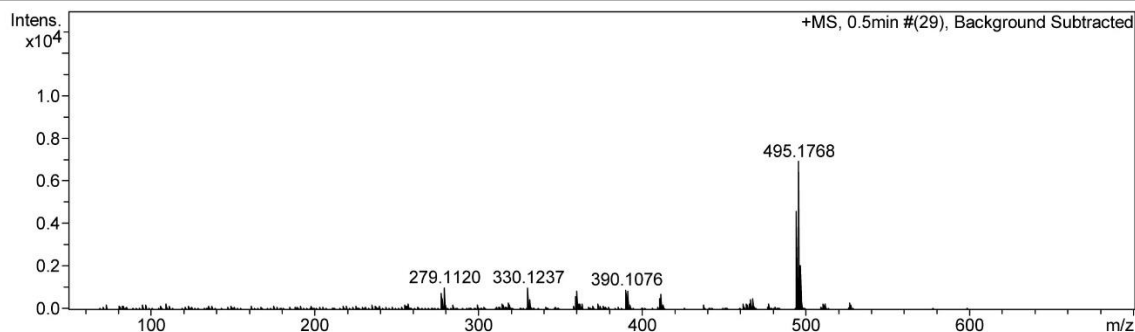
¹³C-NMR in DMSO



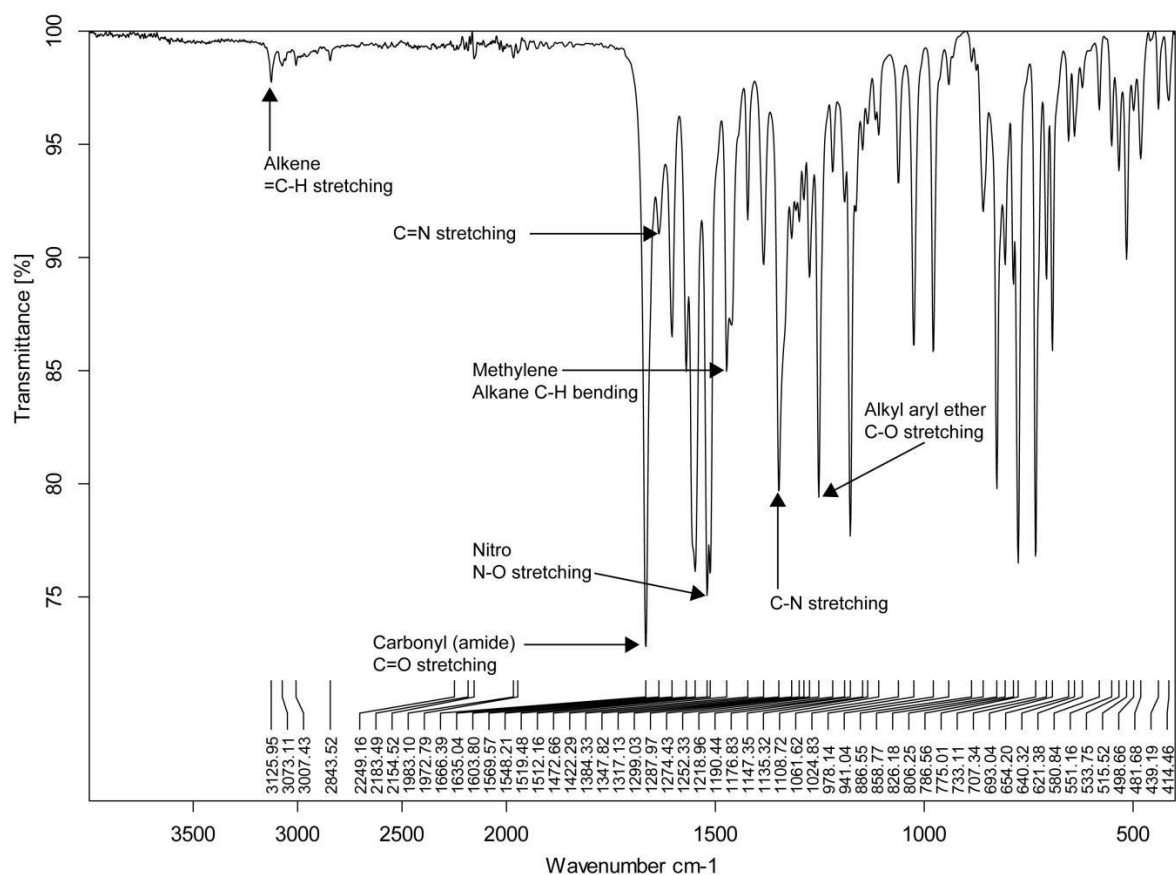
HRMS

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

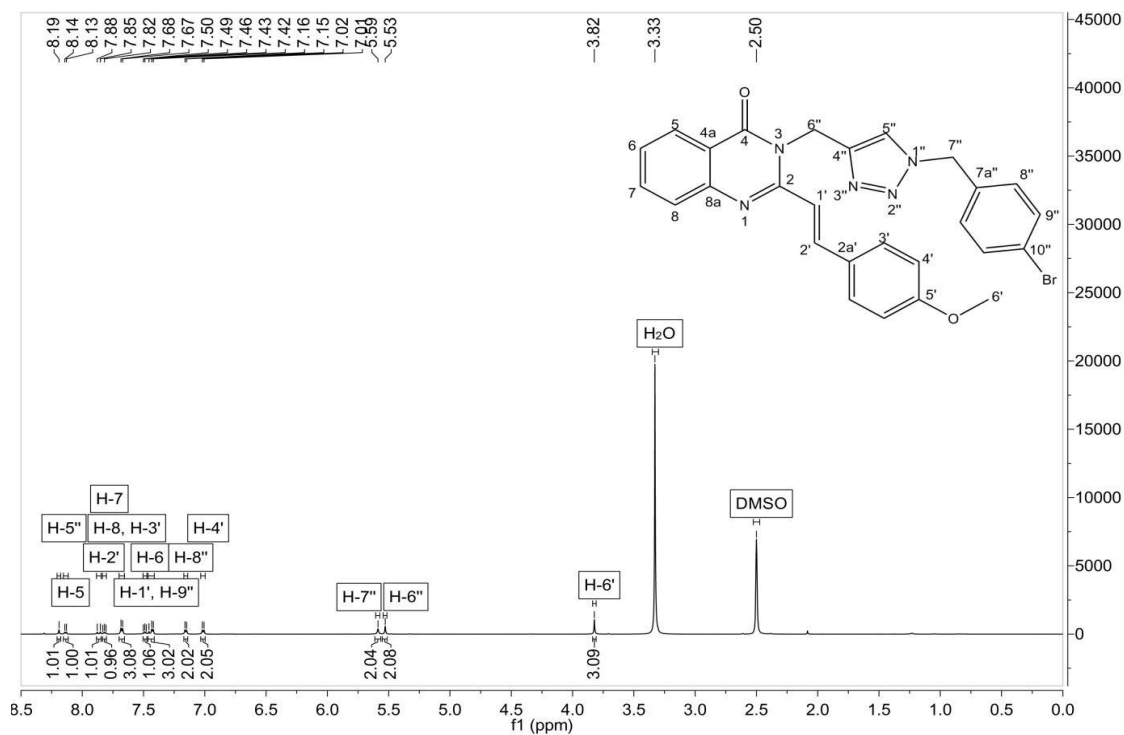


IR

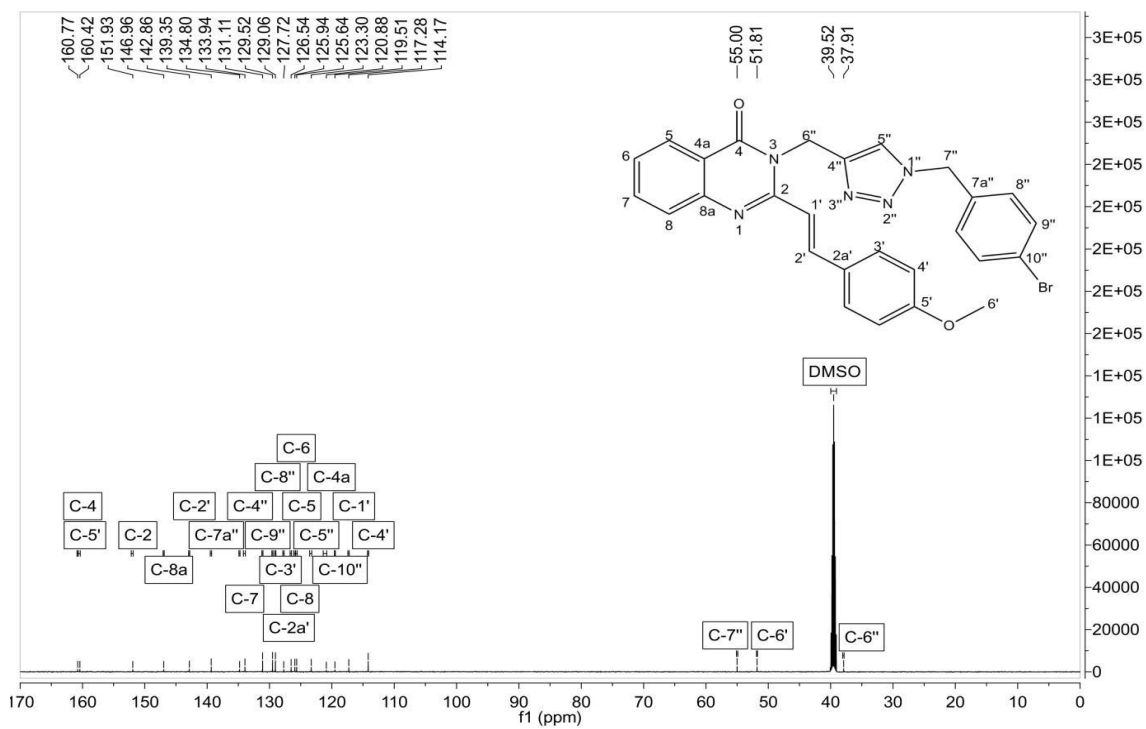


(*E*)-3-[[1-(4-Bromobenzyl)-1*H*-1,2,3-triazol-4-yl]methyl]-2-(4-methoxy styryl)-quinazolin-4(3*H*)-one **4g**

¹H-NMR in DMSO



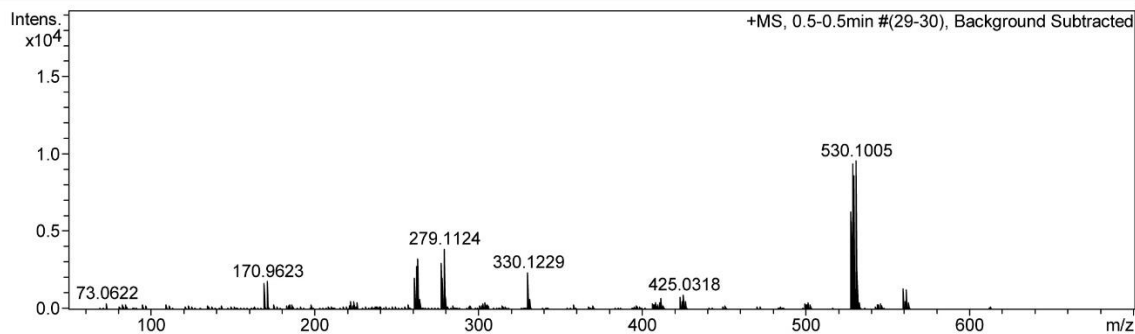
¹³C-NMR in DMSO



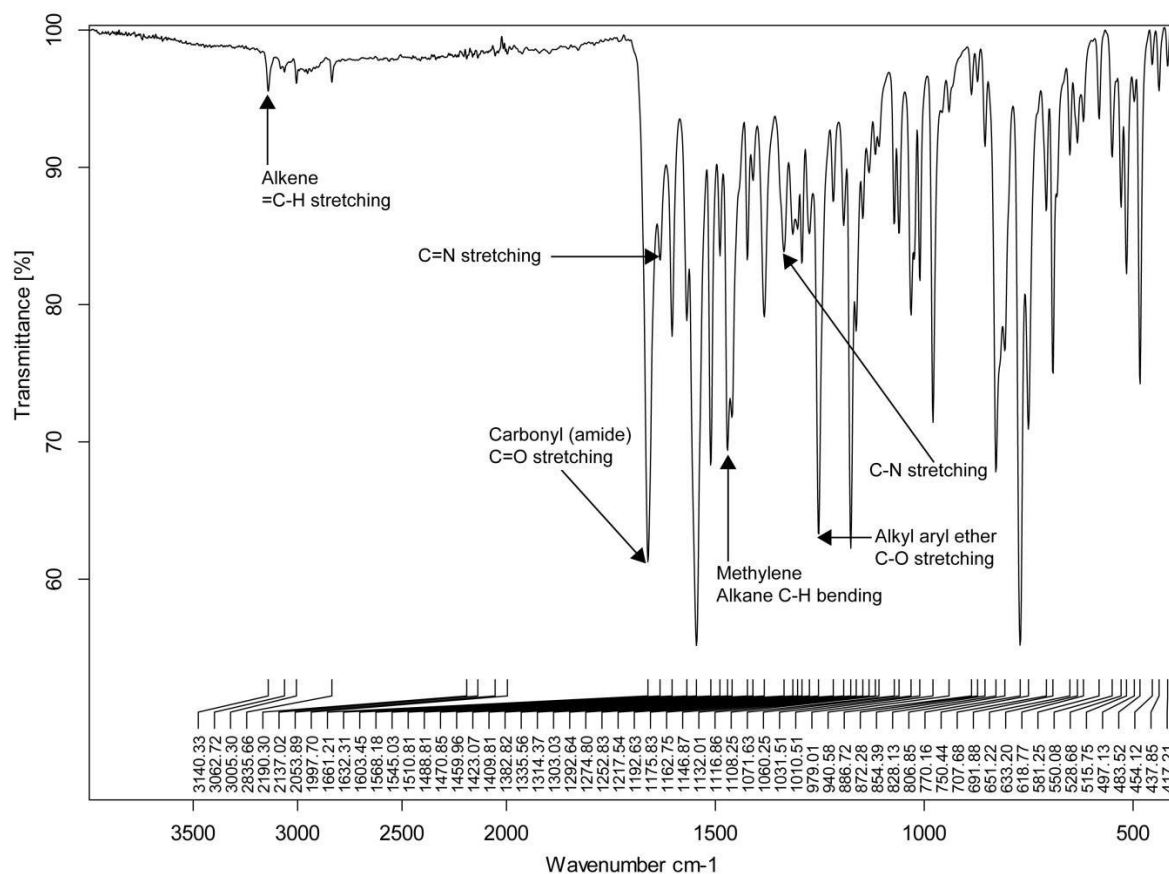
HRMS

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

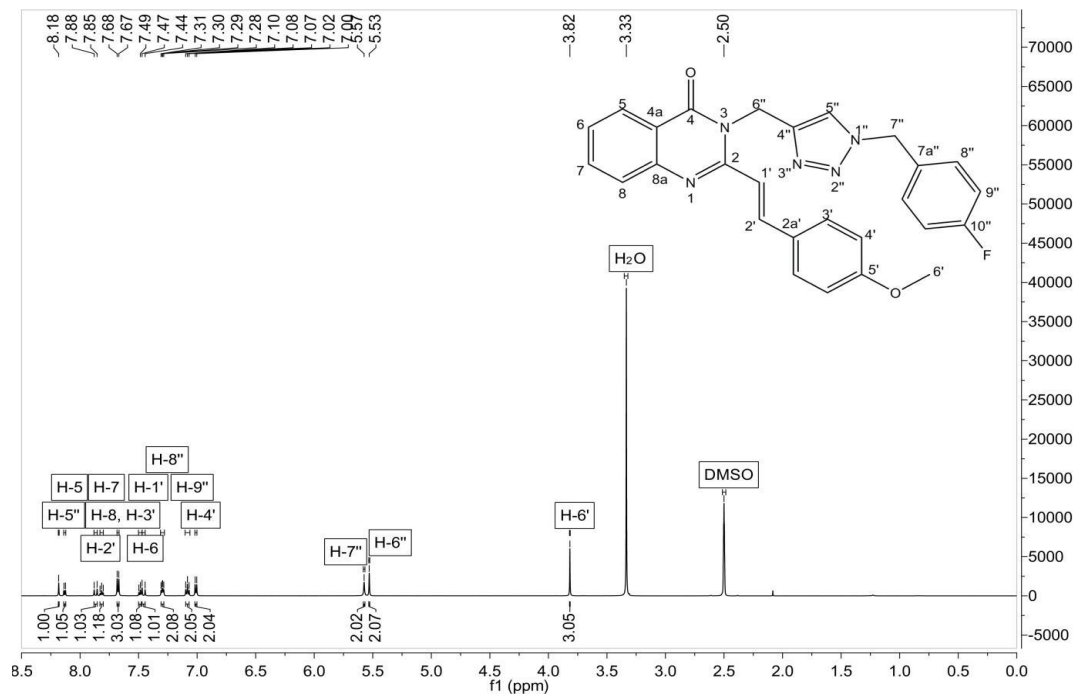


IR

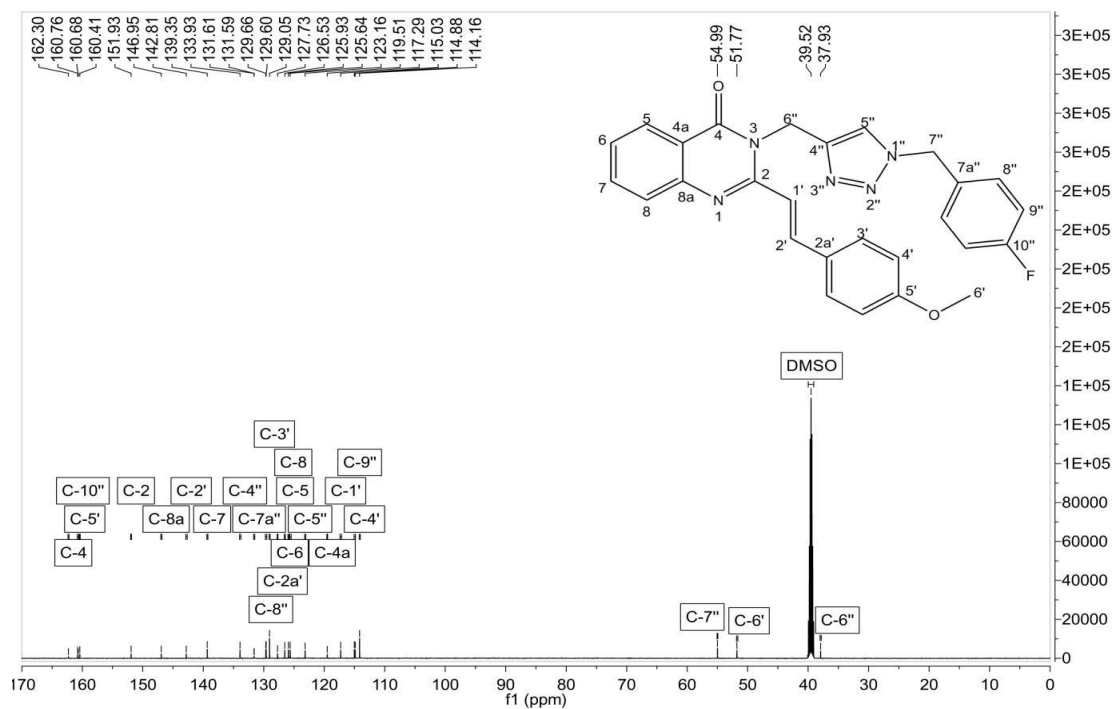


(*E*)-3-([1-(4-Fluorobenzyl)-1*H*-1,2,3-triazol-4-yl]methyl)-2-(4-methoxystyryl)-quinazolin-4(3*H*)-one **4h**

¹H-NMR in DMSO



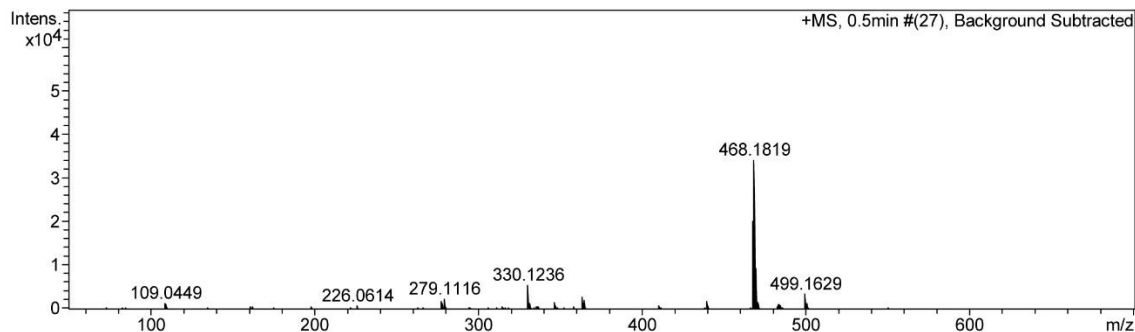
¹³C-NMR in DMSO



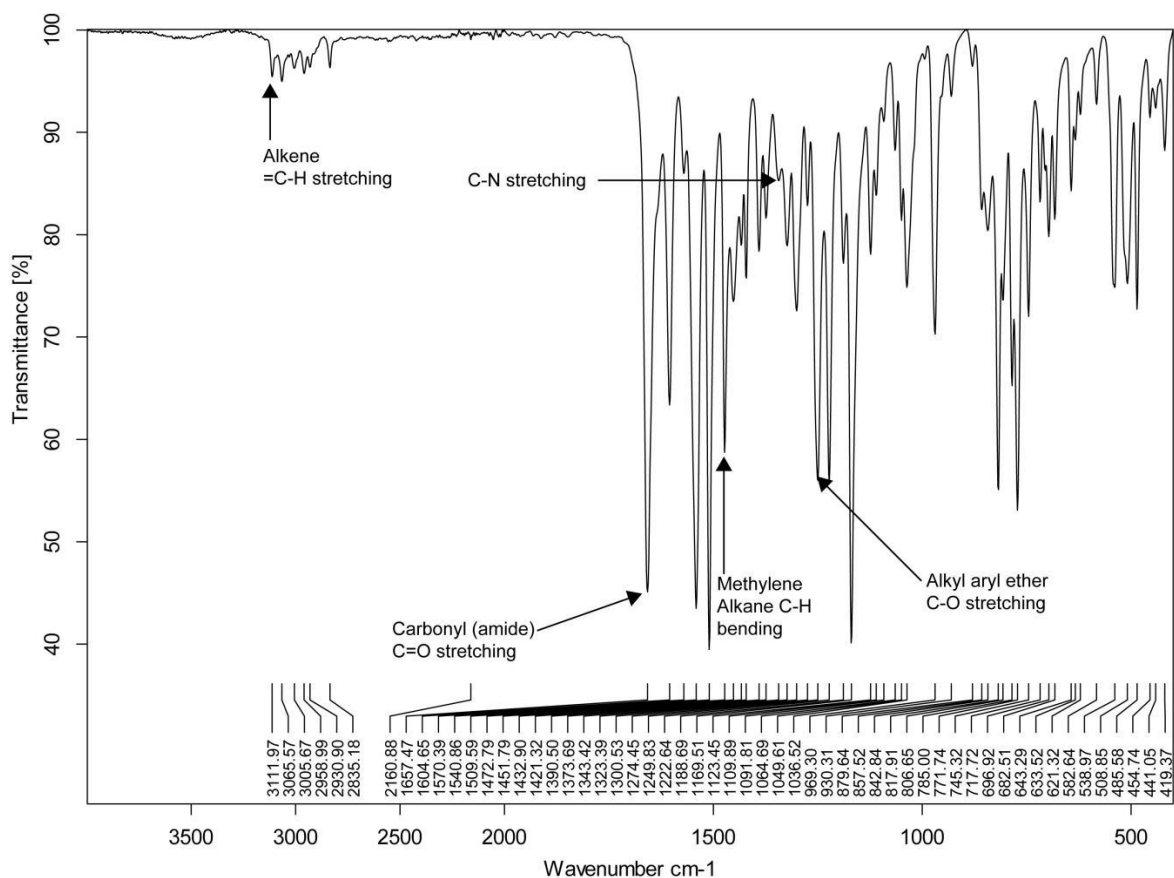
HRMS

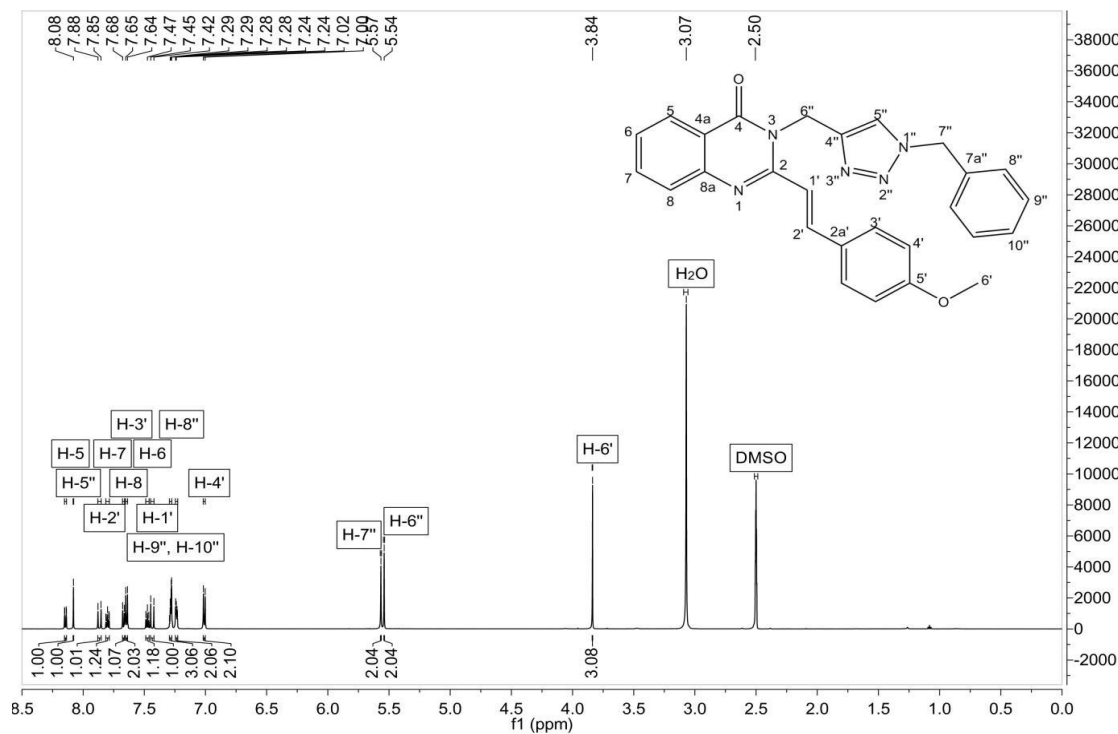
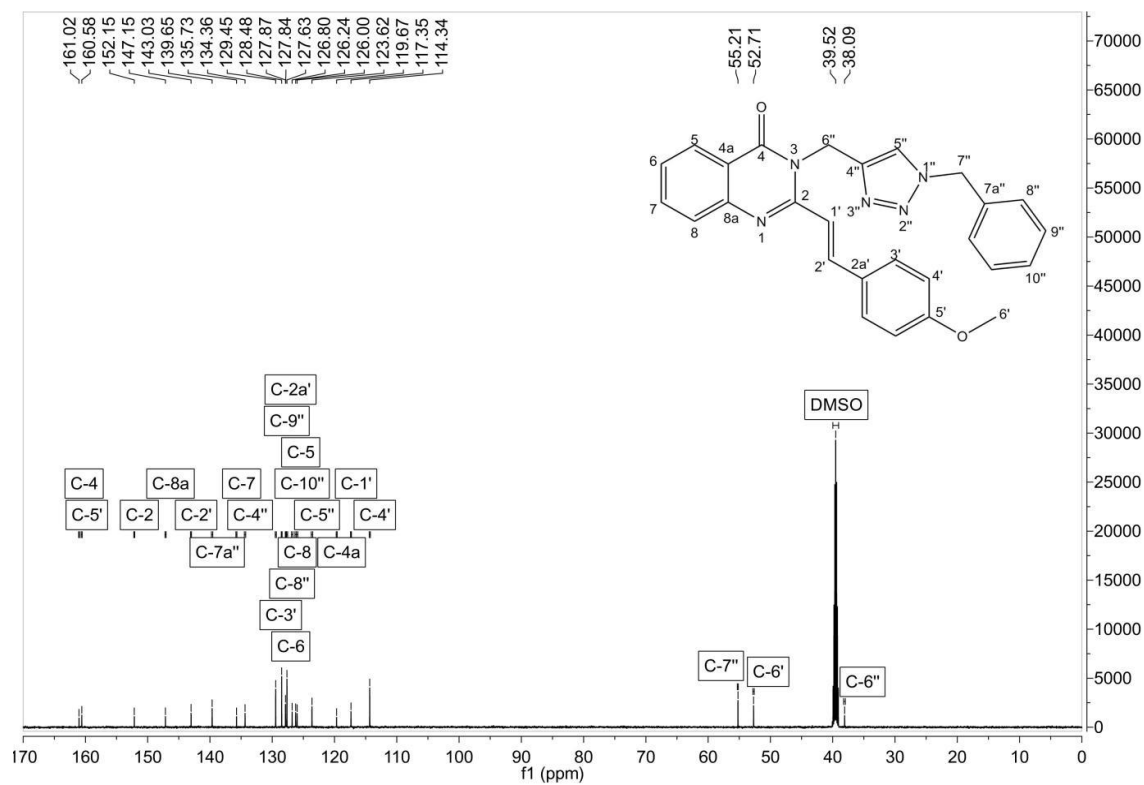
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



IR

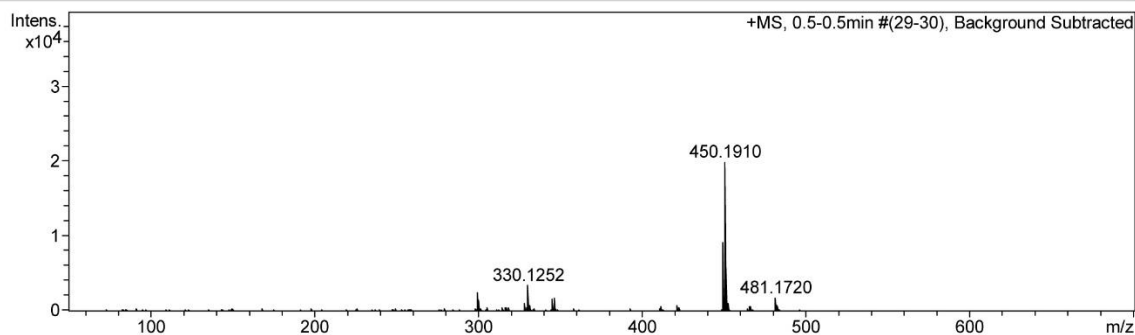


(E)-3-{[1-Benzyl-1*H*-1,2,3-triazol-4-yl]methyl}-2-(4-methoxystyryl)quinazolin-4(3*H*)-one **4i**¹H-NMR in DMSO¹³C-NMR in DMSO

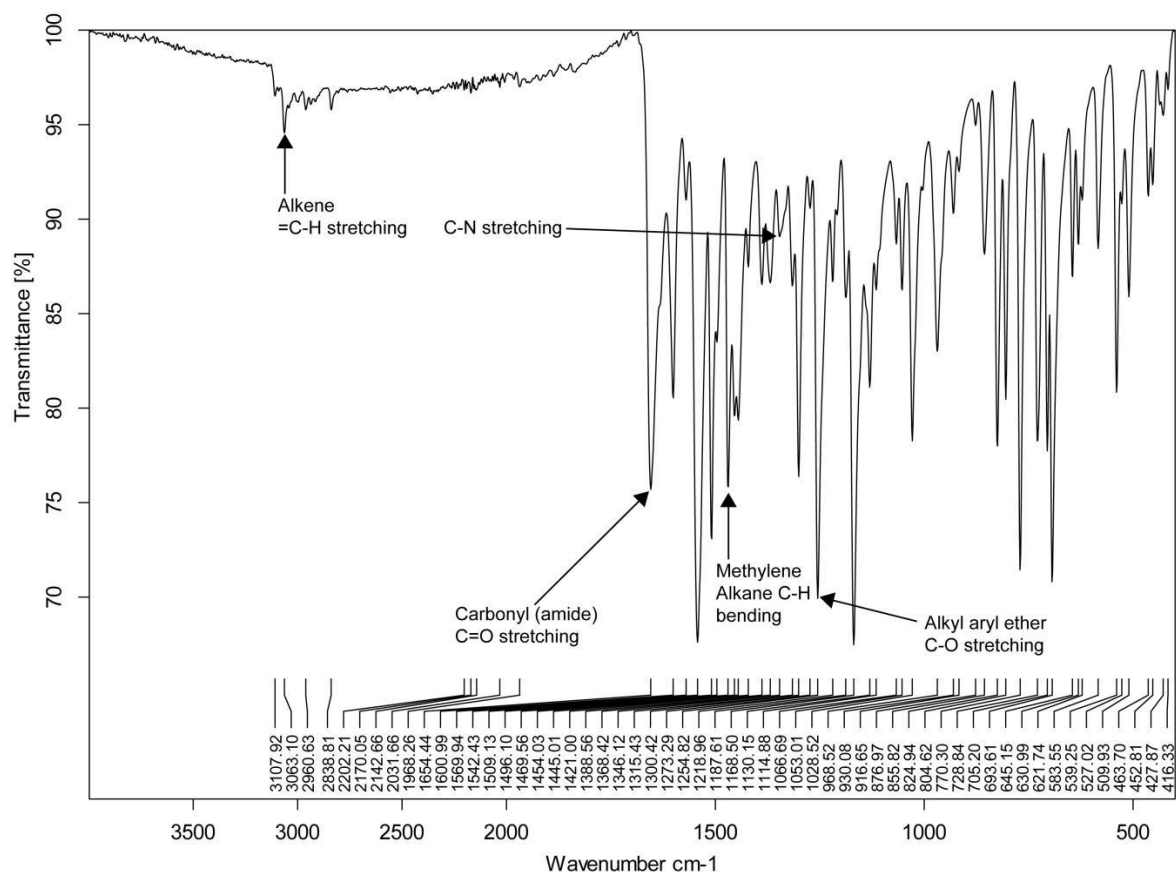
HRMS

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

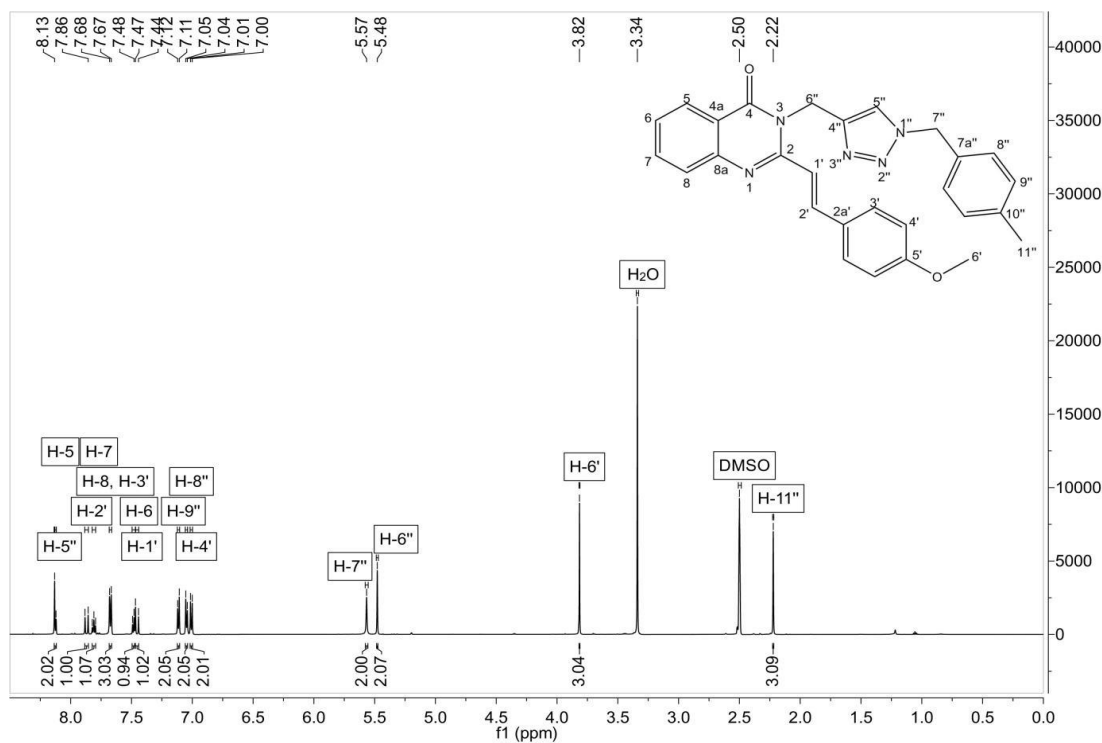


IR

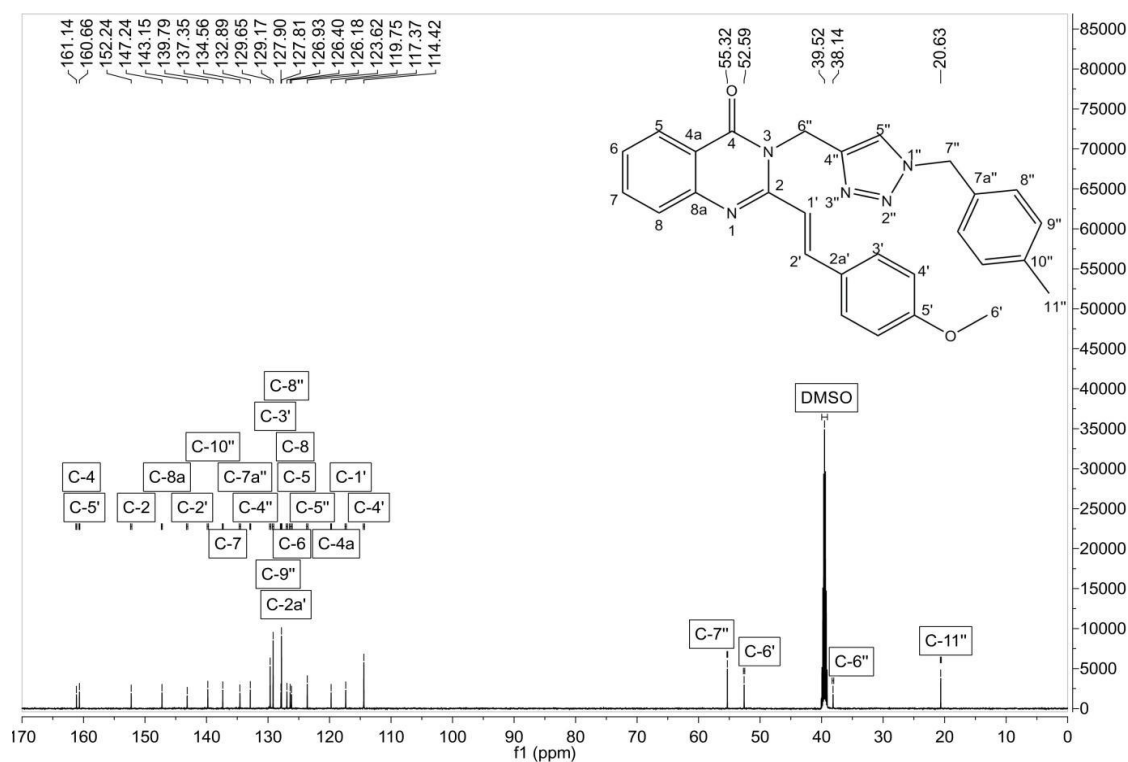


(*E*)-2-(4-Methoxystyryl)-3-([1-(4-methylbenzyl)-1*H*-1,2,3-triazol-4-yl]-methyl)-quinazolin-4(3*H*)-one **4j**

¹H-NMR in DMSO



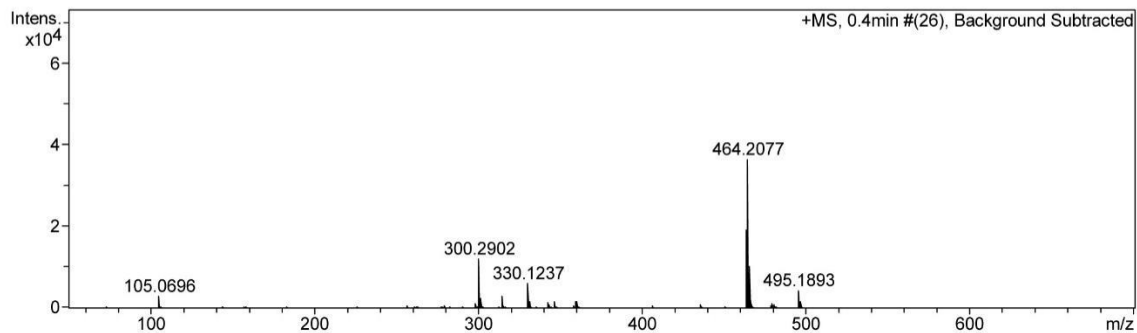
¹³C-NMR in DMSO



HRMS

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



IR

