

## Supplementary Material

### **Synthesis and Characterization of Novel Heterocyclic Chalcones from 1-Phenyl-1*H*-pyrazol-3-ol**

Arminas Urbonavičius<sup>1,3</sup>, Graziana Fortunato<sup>1,2</sup>, Emilija Ambrazaitytė<sup>1</sup>, Elena Plytninkienė<sup>1,3</sup>, Aurimas Bieliauskas<sup>3</sup>, Vaida Milišiūnaitė<sup>1,3</sup>, Renzo Luisi<sup>2</sup>, Eglė Arbačiauskienė<sup>1\*</sup>, Sonata Krikštolaitytė<sup>1</sup>, Algirdas Šačkus<sup>1,3\*</sup>

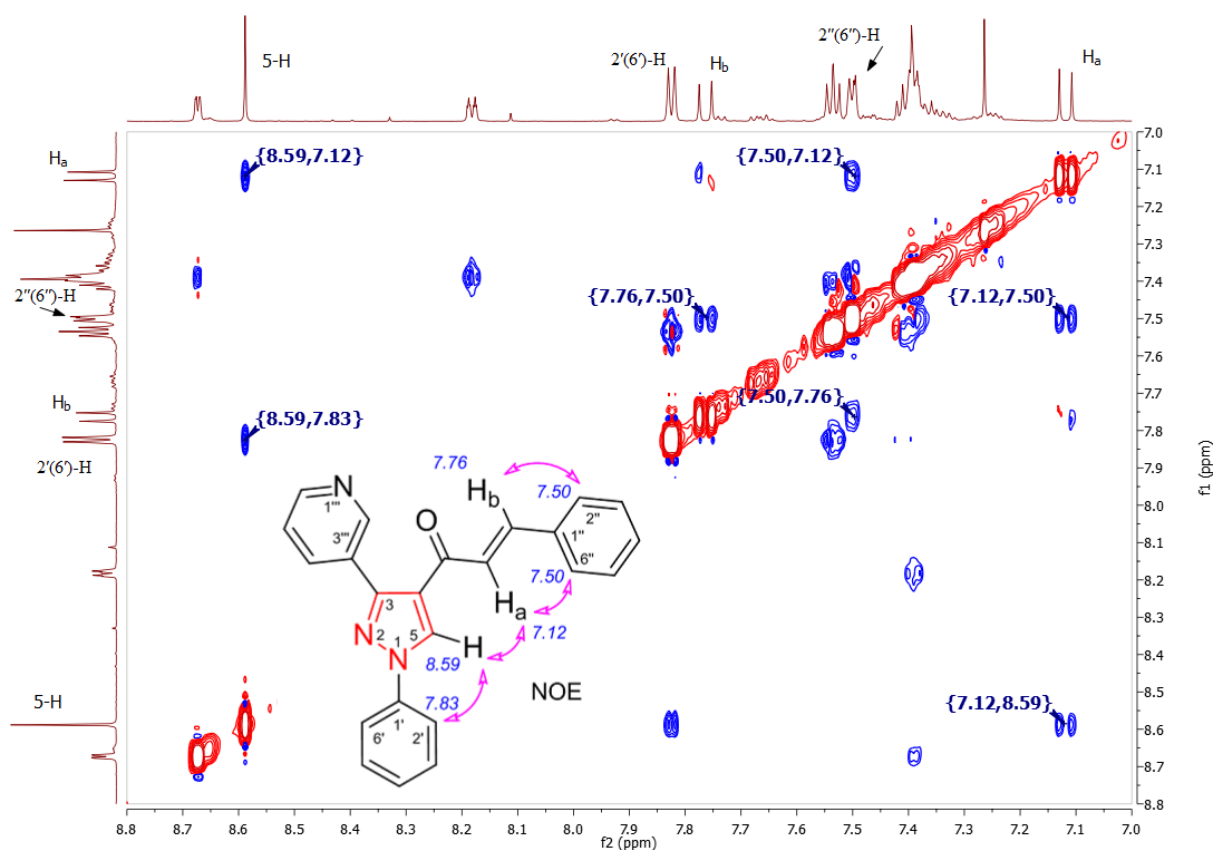
<sup>1</sup>Department of Organic Chemistry, Kaunas University of Technology, Radvilėnų pl. 19, LT-50254 Kaunas, Lithuania

<sup>2</sup>Department of Pharmacy - Drug Sciences, University of Bari "Aldo Moro", Via E. Orabona 4, I- 70125 Bari, Italy

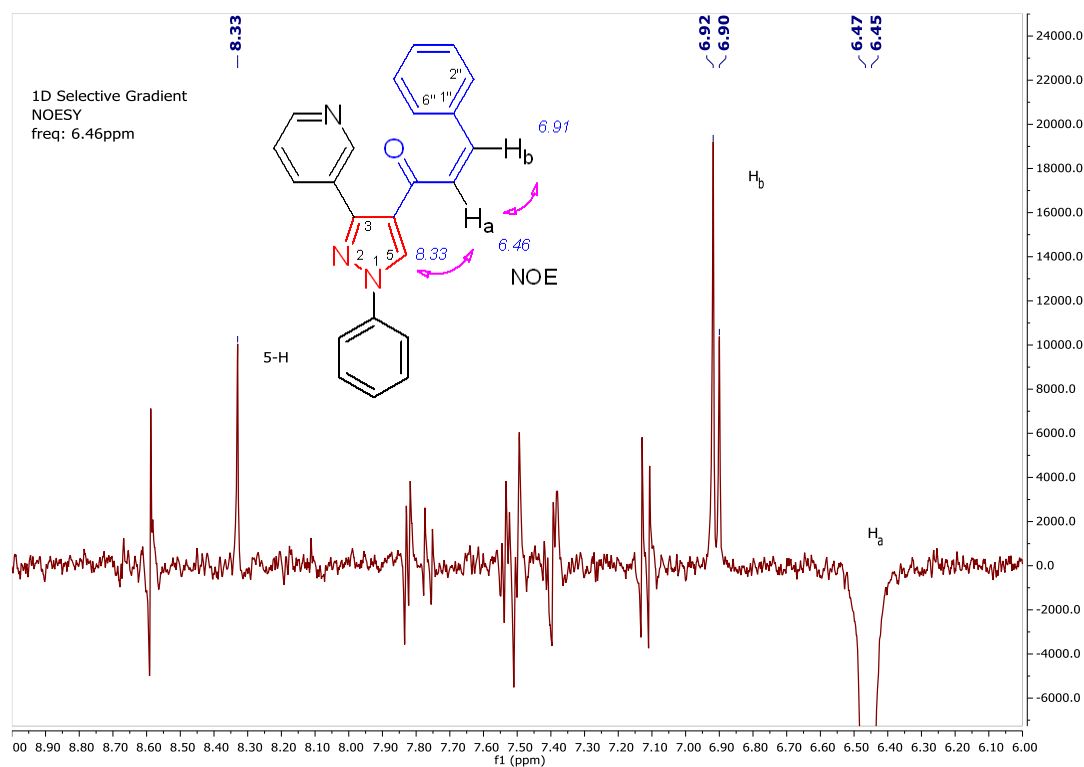
<sup>3</sup>Institute of Synthetic Chemistry, Kaunas University of Technology, K. Baršausko g. 59, LT-51423 Kaunas, Lithuania

\* Corresponding authors

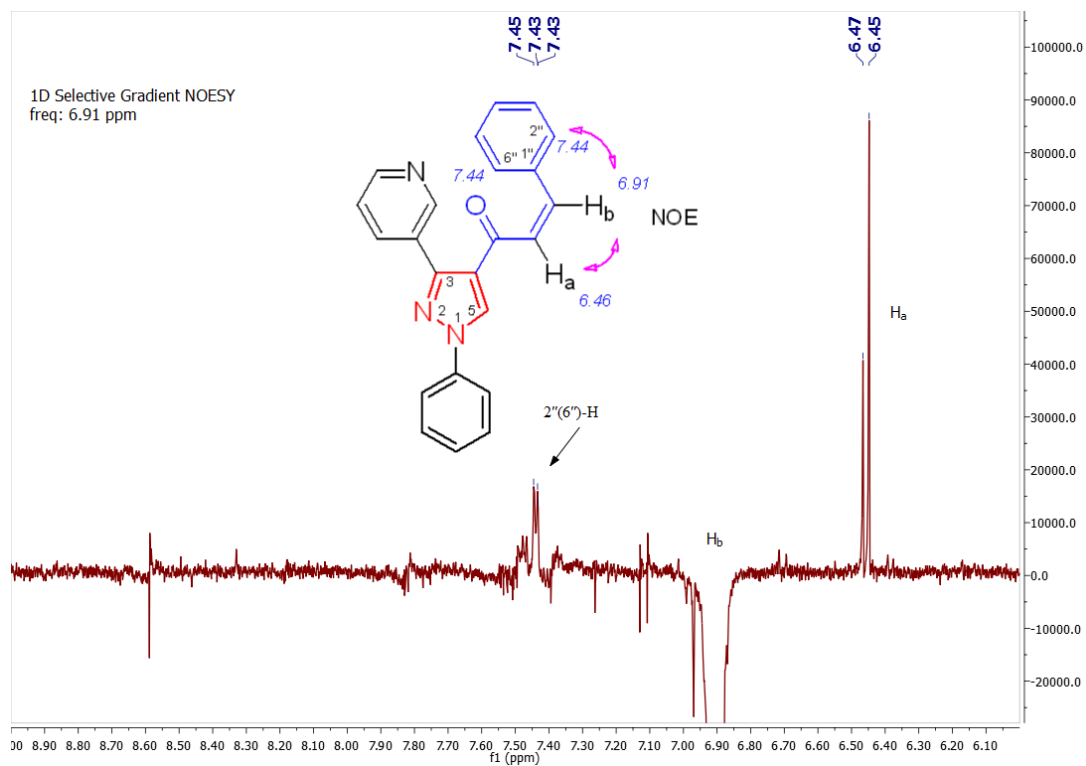
E-mail address: algirdas.sackus@ktu.lt (A. Šačkus), egle.arbaciauskiene@ktu.lt (E. Arbačiauskienė)



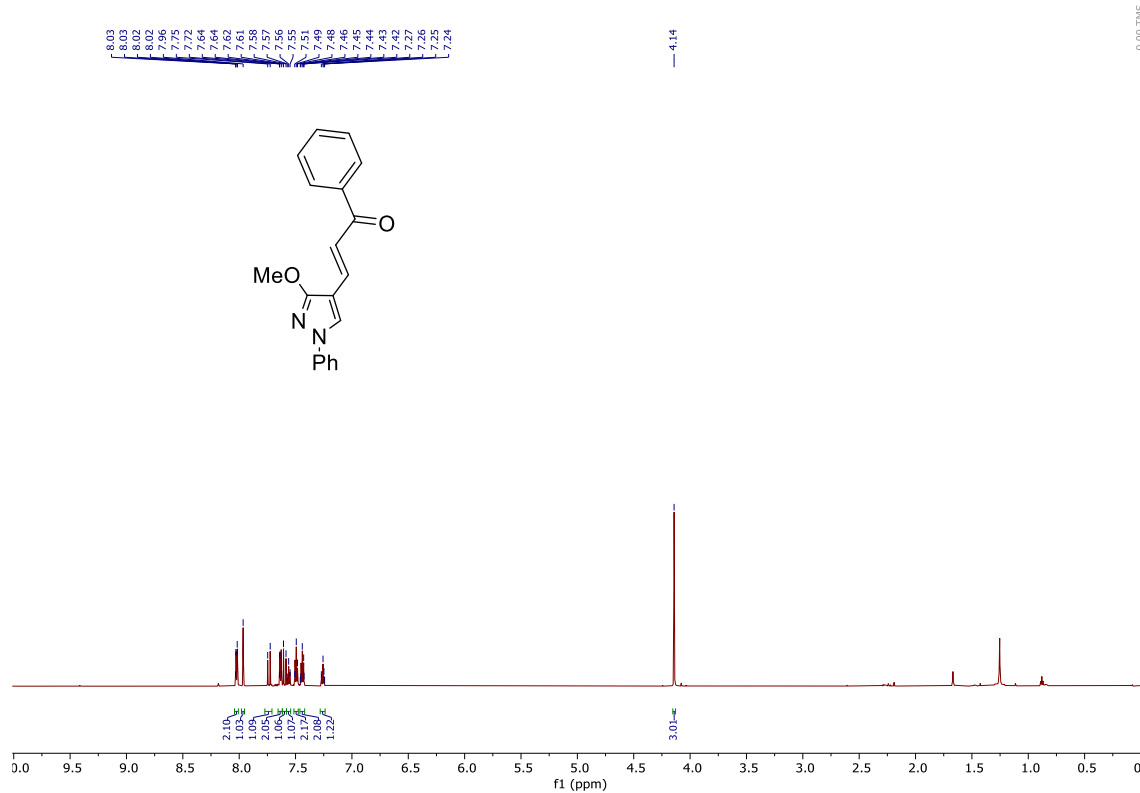
**Figure S1.  $^1\text{H}$ - $^1\text{H}$  NOESY NMR spectrum (*E*-12a, *Z*-13a) (700 MHz,  $\text{CDCl}_3$ )**



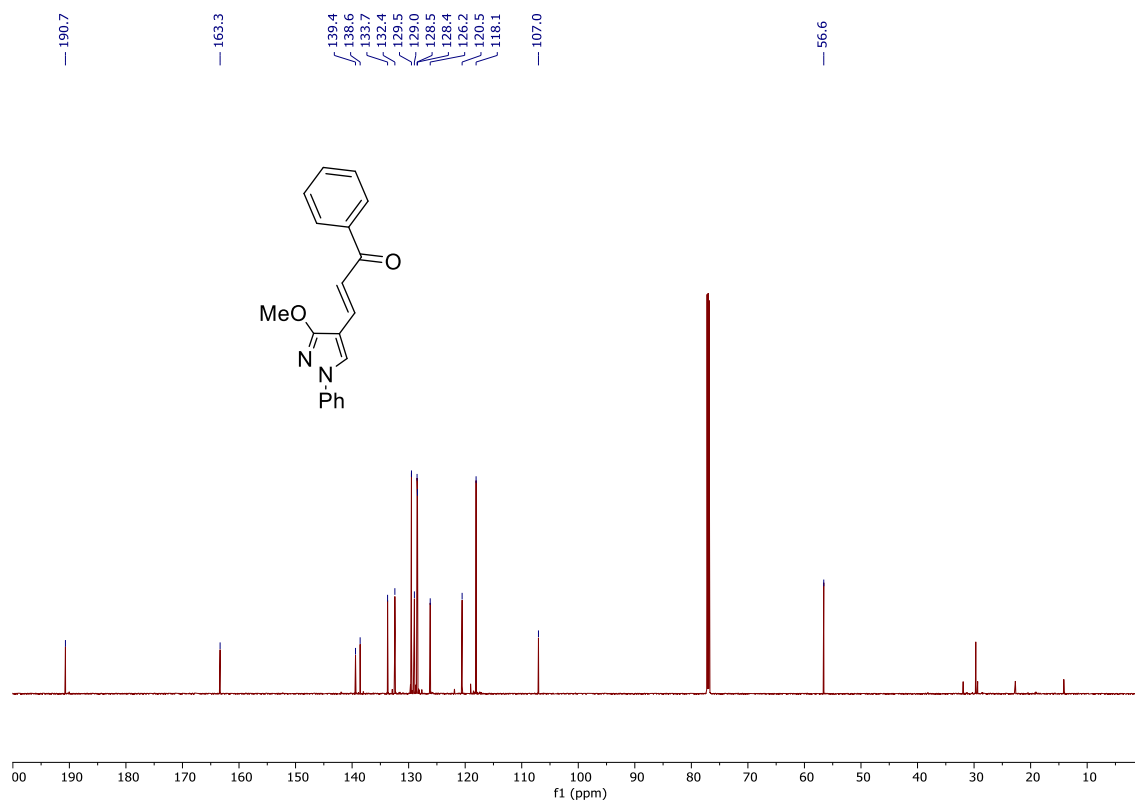
**Figure S2. 1D Selective Gradient NOESY spectrum (*E*-12a, *Z*-13a) (700 MHz,  $\text{CDCl}_3$ )**



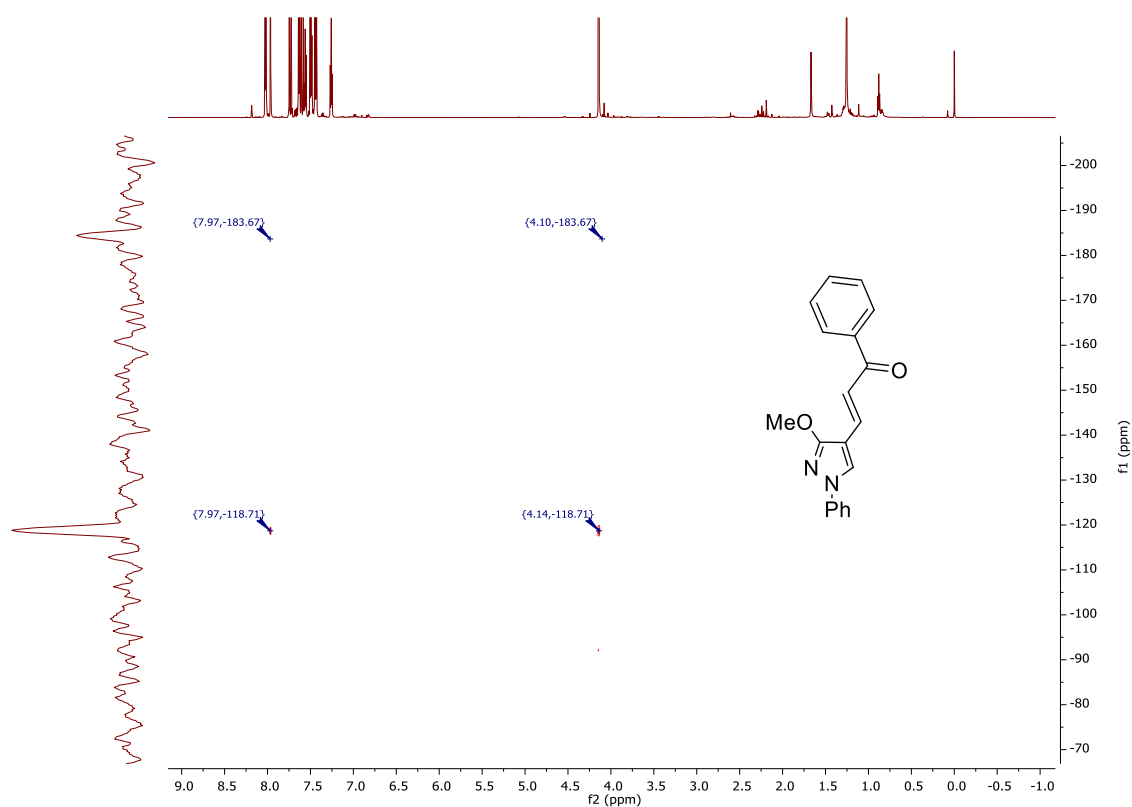
**Figure S3.** 1D Selective Gradient NOESY spectrum (*E*-12a, *Z*-13a) (700 MHz,  $CDCl_3$ )



**Figure S4.** (*2E*)-3-[3-(Methoxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4a).  $^1H$  NMR spectrum (700 MHz,  $CDCl_3$ )



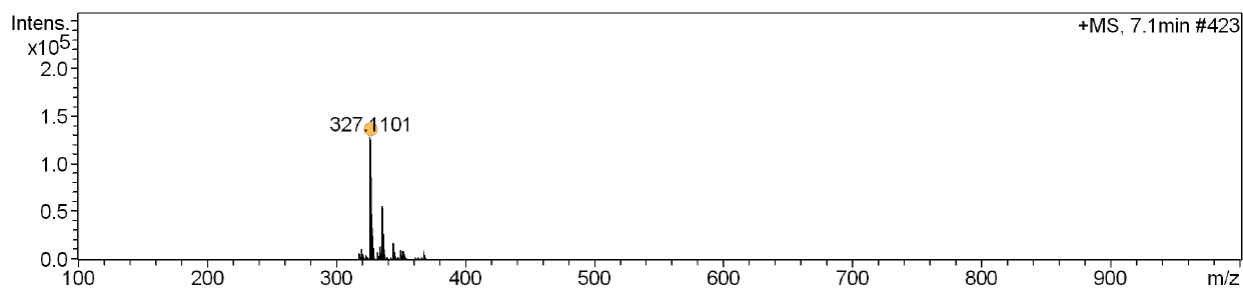
**Figure S5. (2E)-3-[3-(Methoxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4a). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)**



**Figure S6. (2E)-3-[3-(Methoxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4a). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)**

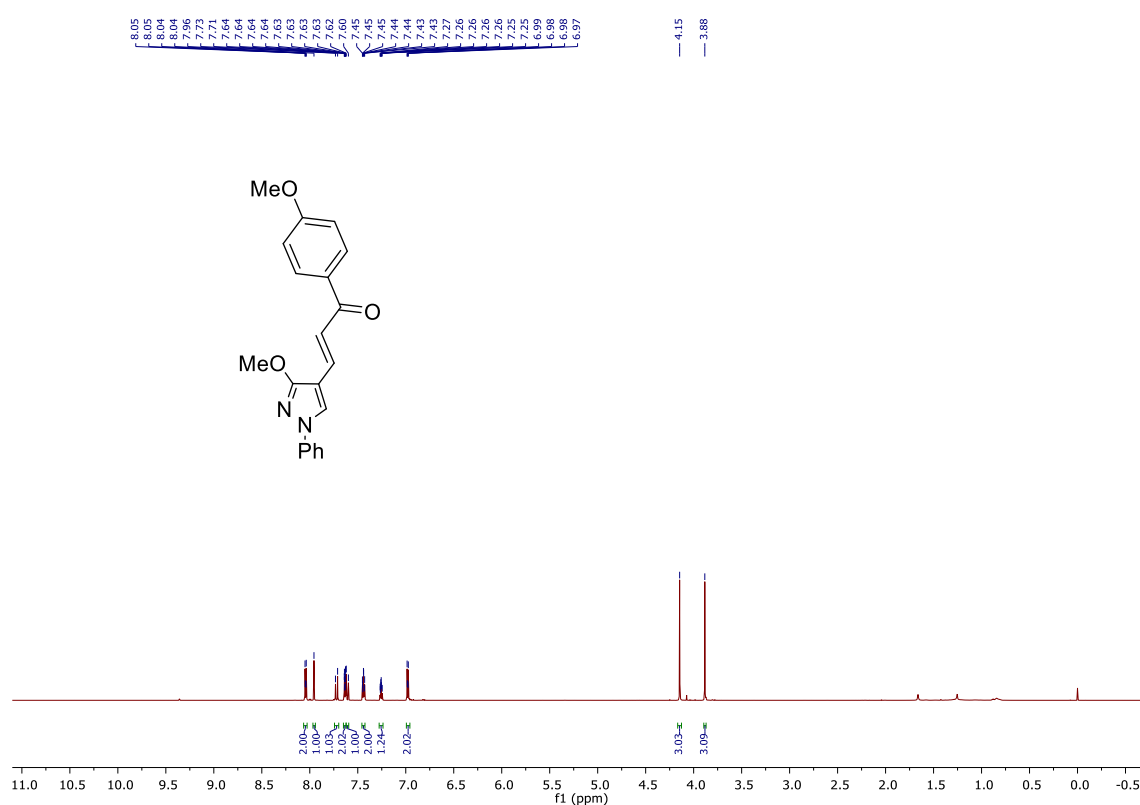


+MS, 7.1min #423

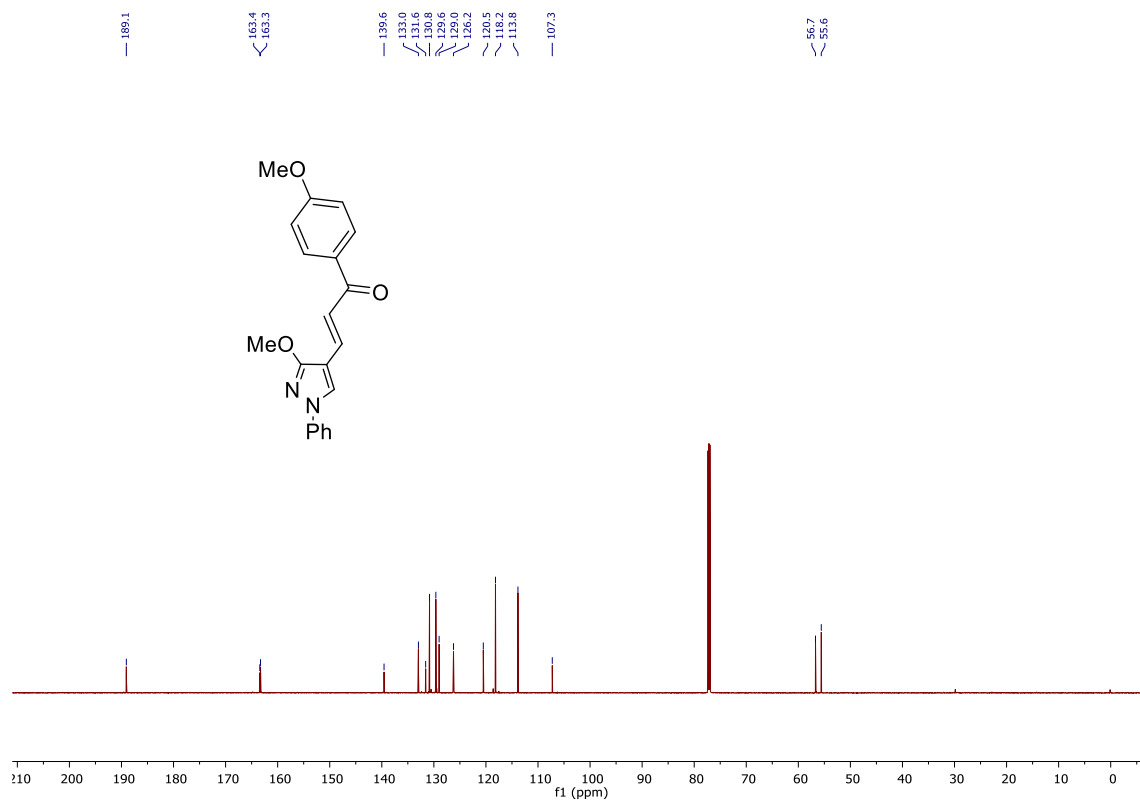


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
327.1101	1	C <sub>19</sub> H <sub>16</sub> N <sub>2</sub> NaO <sub>2</sub>	327.1104	1.0	7.3	2	100.00	12.5	even		ok

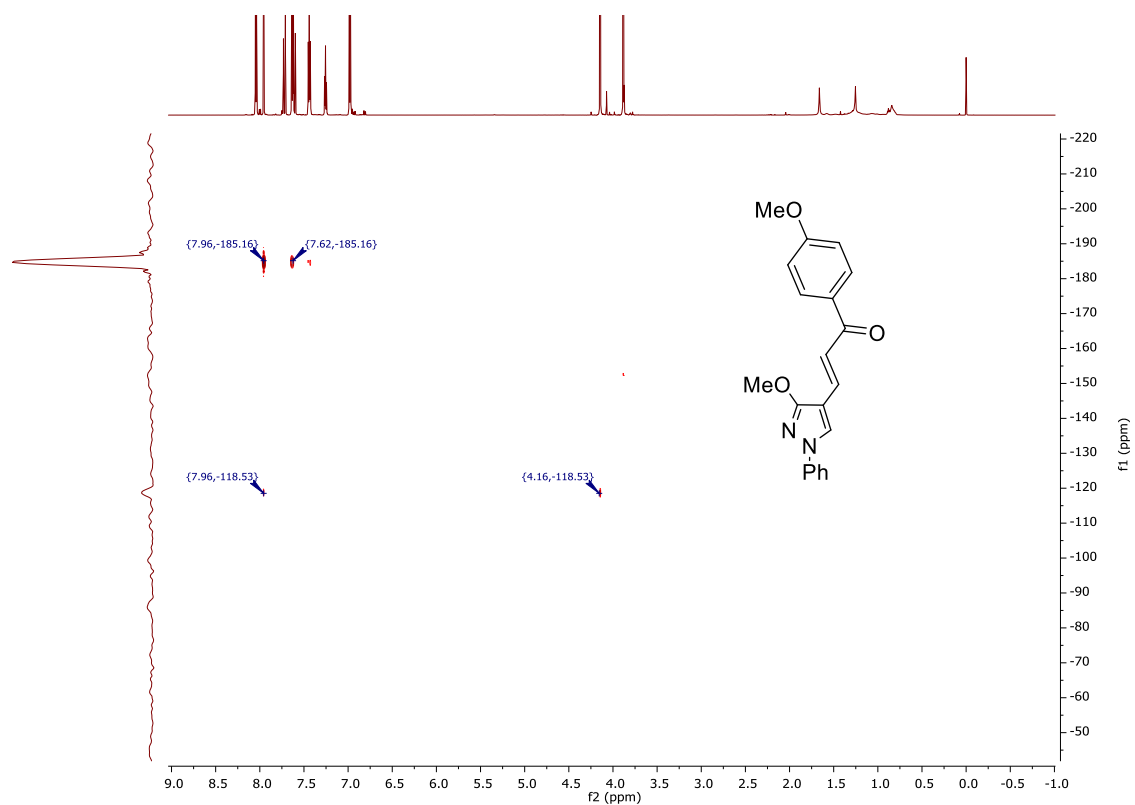
**Figure S7. (2E)-3-[3-(Methoxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4a). HRMS (ESI-TOF).**



**Figure S8. (2E)-1-(4-Methoxyphenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4b). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**

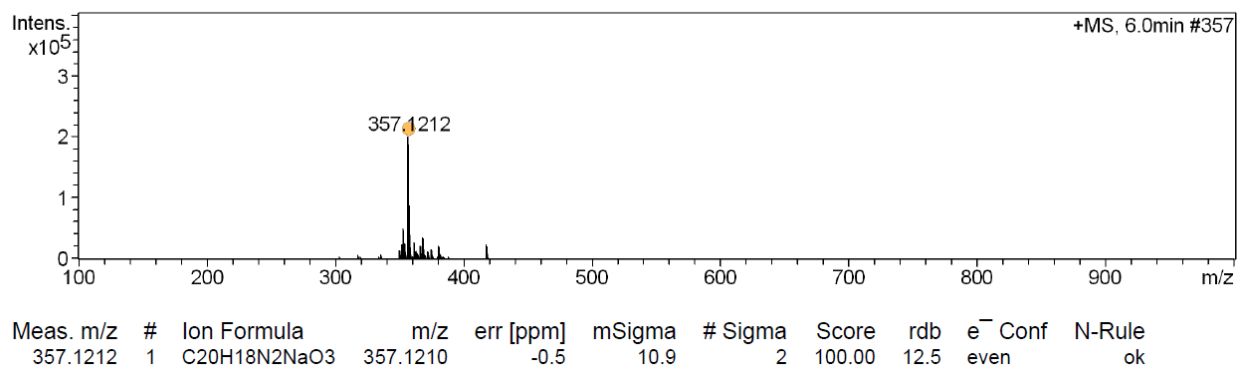


**Figure S9.** (2E)-1-(4-Methoxyphenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4b). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)

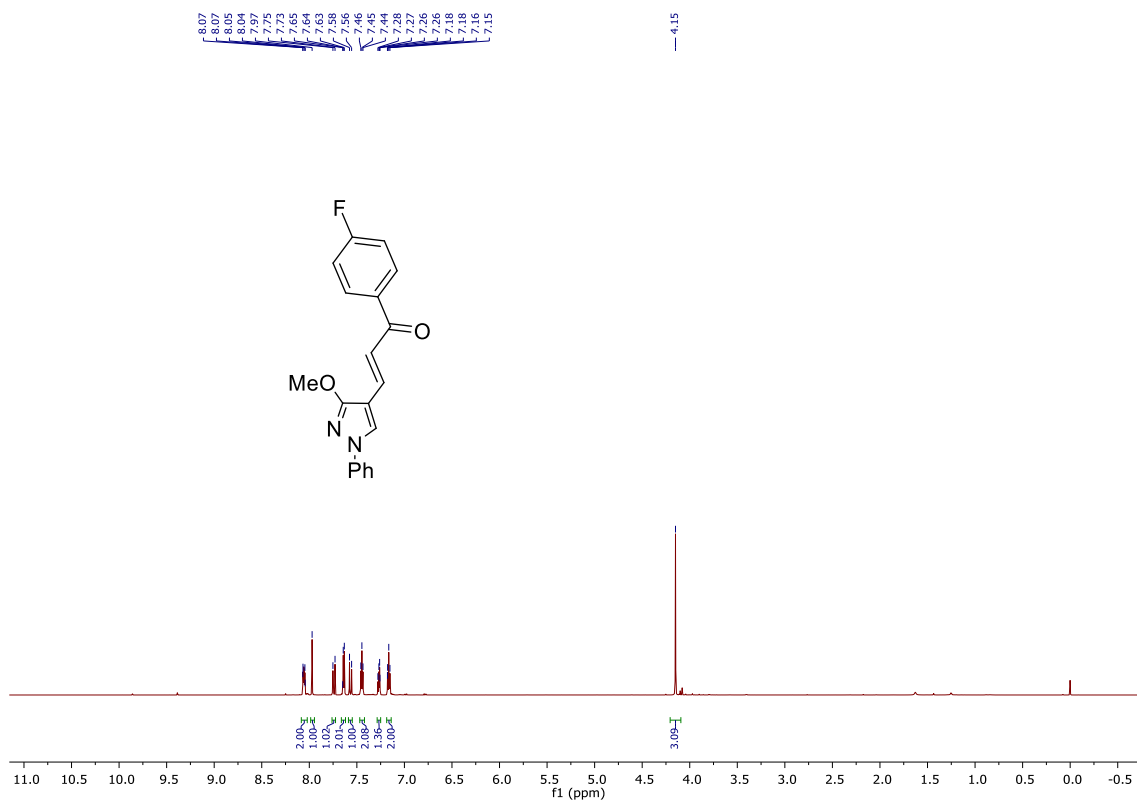


**Figure S10.** (2E)-1-(4-Methoxyphenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4b). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)

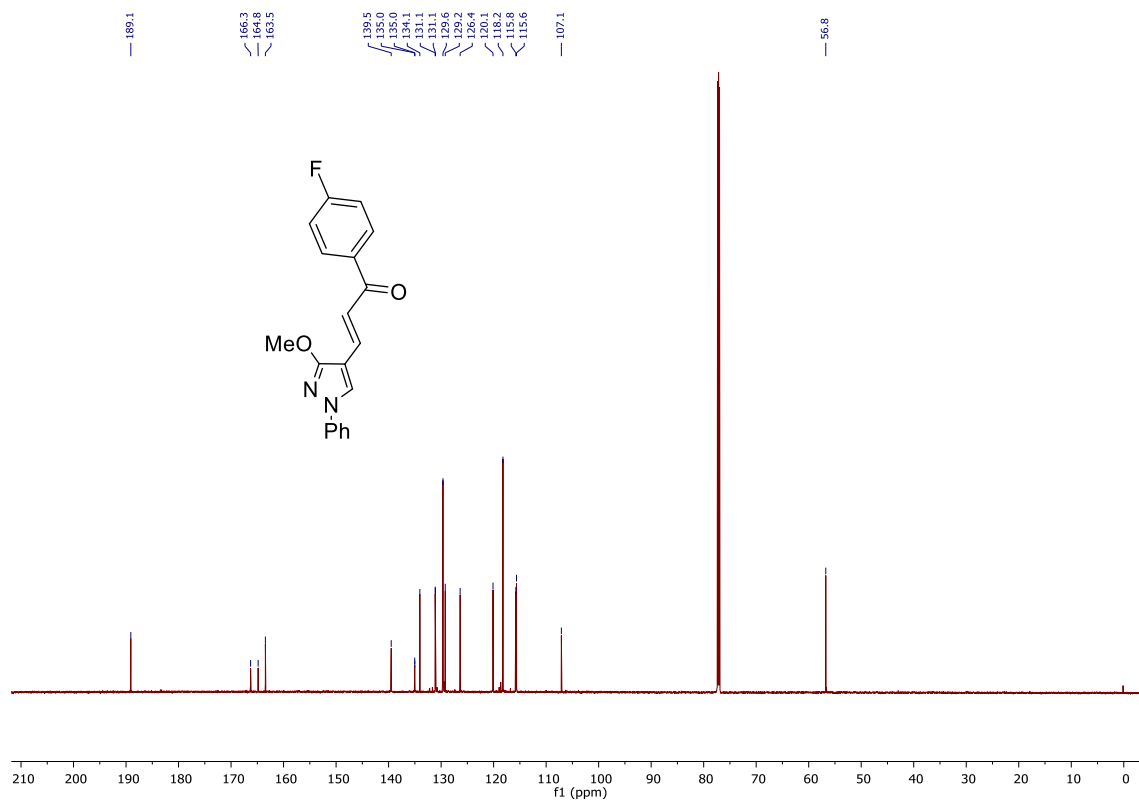
+MS, 6.0min #357



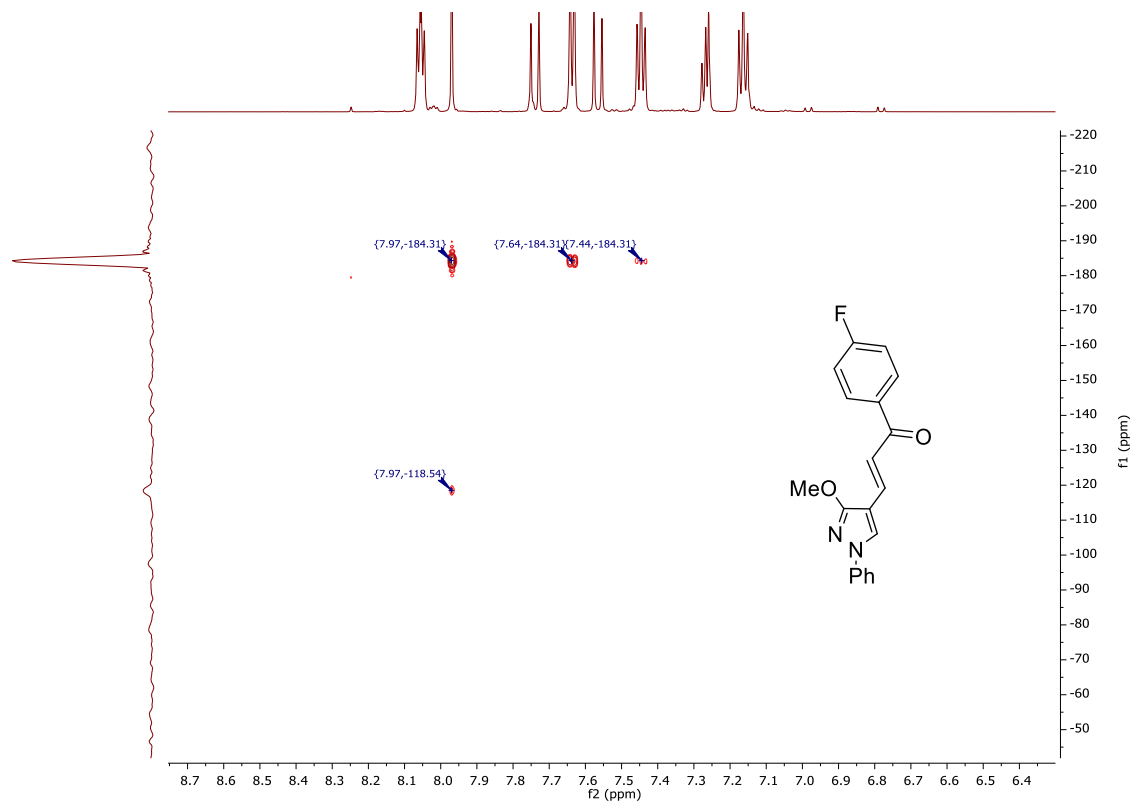
**Figure S11. (2E)-1-(4-Methoxyphenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4b). HRMS (ESI-TOF).**



**Figure S12. (2E)-1-(4-Fluorophenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4c). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**

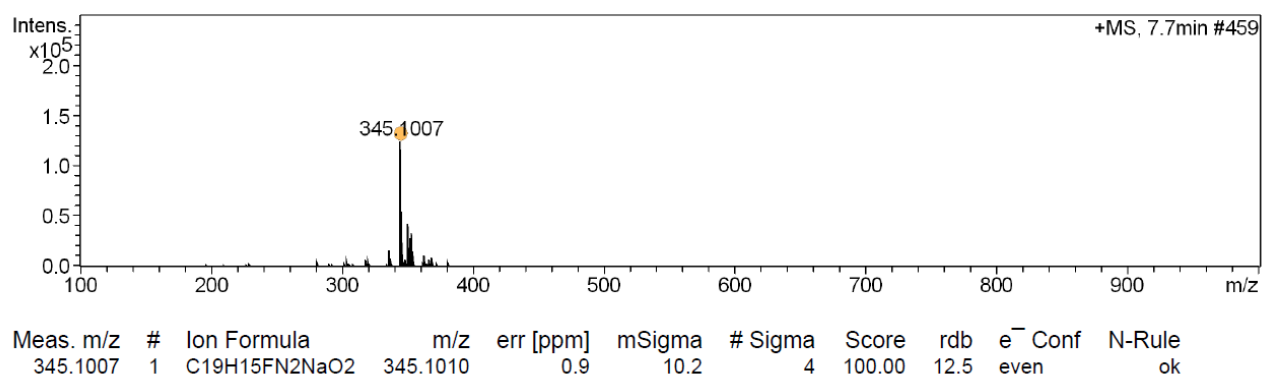


**Figure S13.** (2E)-1-(4-Fluorophenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4c). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)

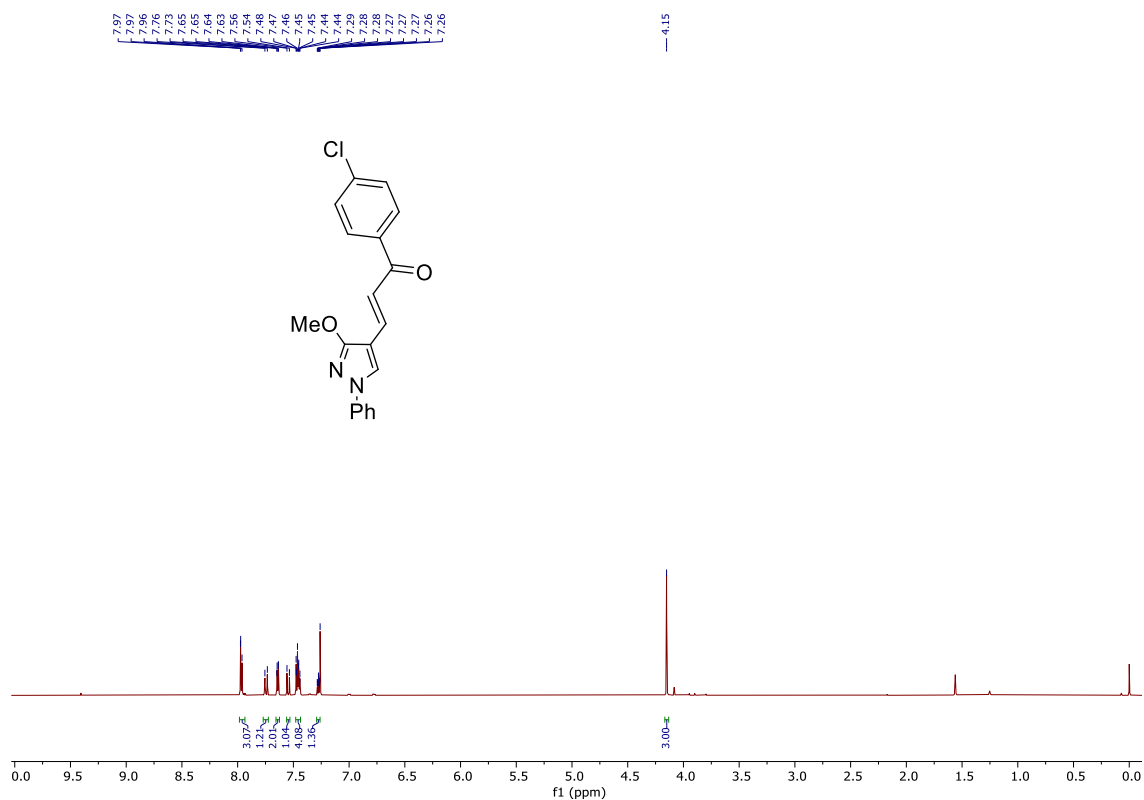


**Figure S14.** (2E)-1-(4-Fluorophenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4c). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)

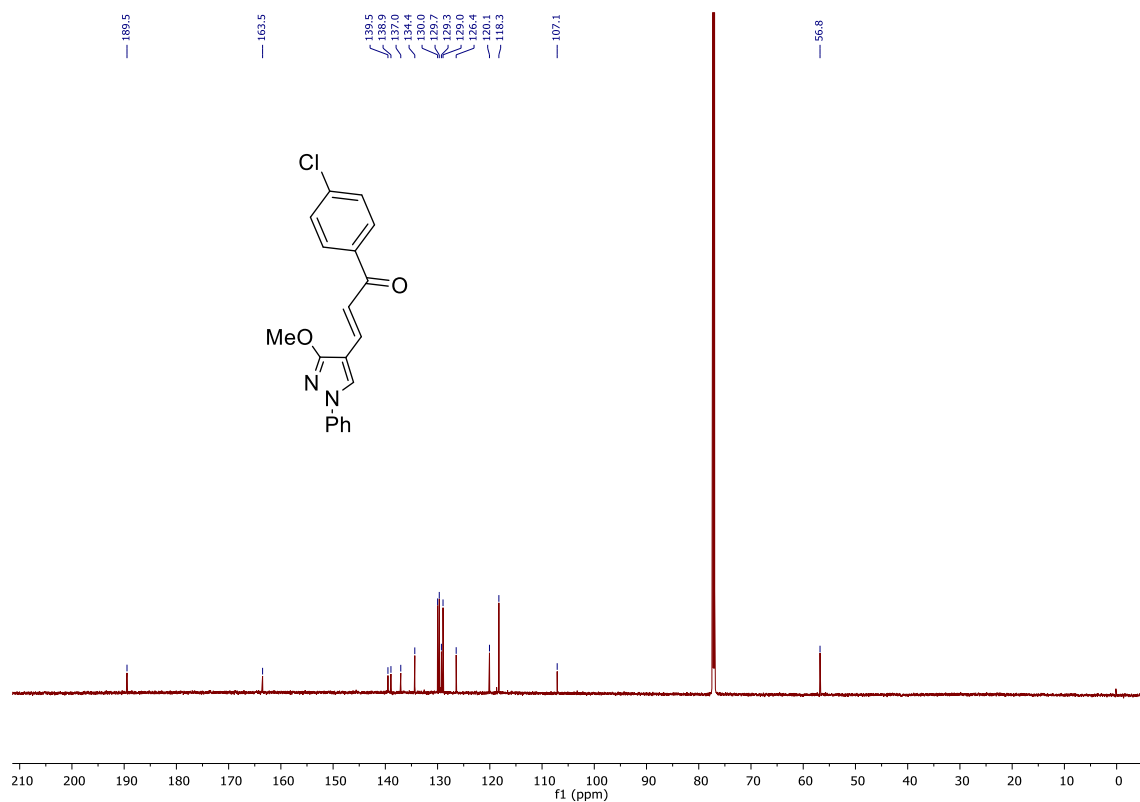
+MS, 7.7min #459



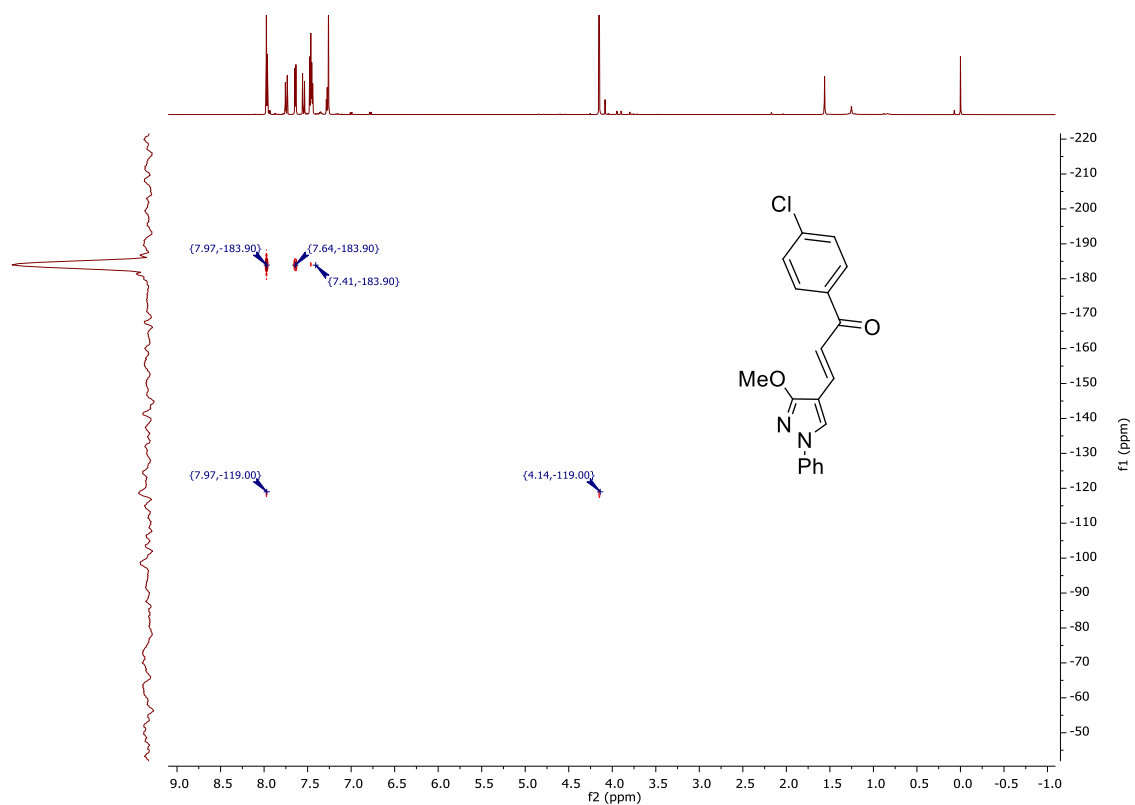
**Figure S15. (2E)-1-(4-Fluorophenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4c). HRMS (ESI-TOF).**



**Figure S16. (2E)-1-(4-Chlorophenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4d). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**

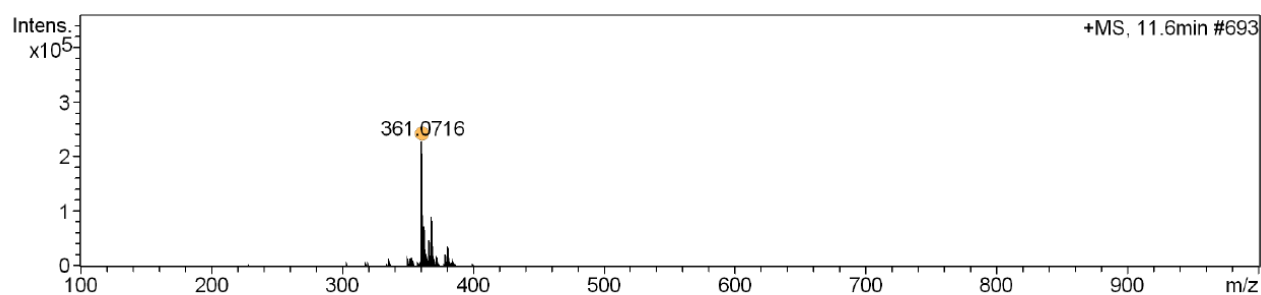


**Figure S17.** (2E)-1-(4-Chlorophenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4d). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



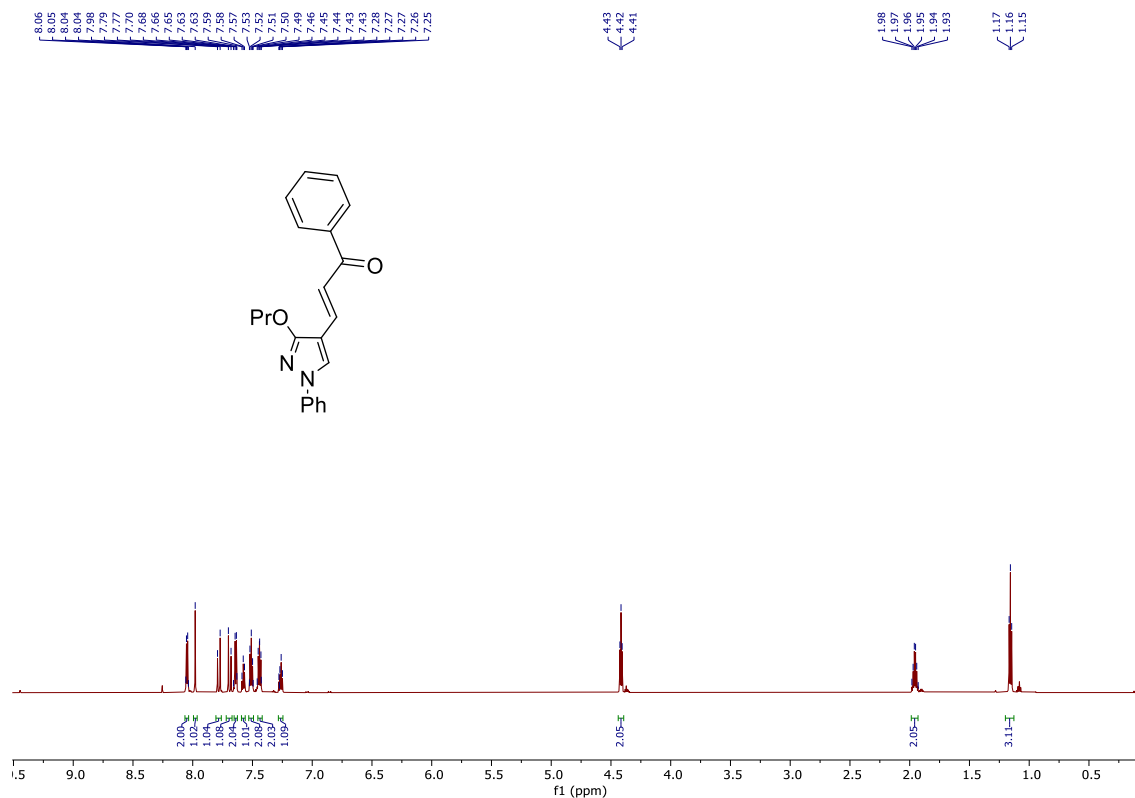
**Figure S18.** (2E)-1-(4-Chlorophenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4d). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)

+MS, 11.6min #693

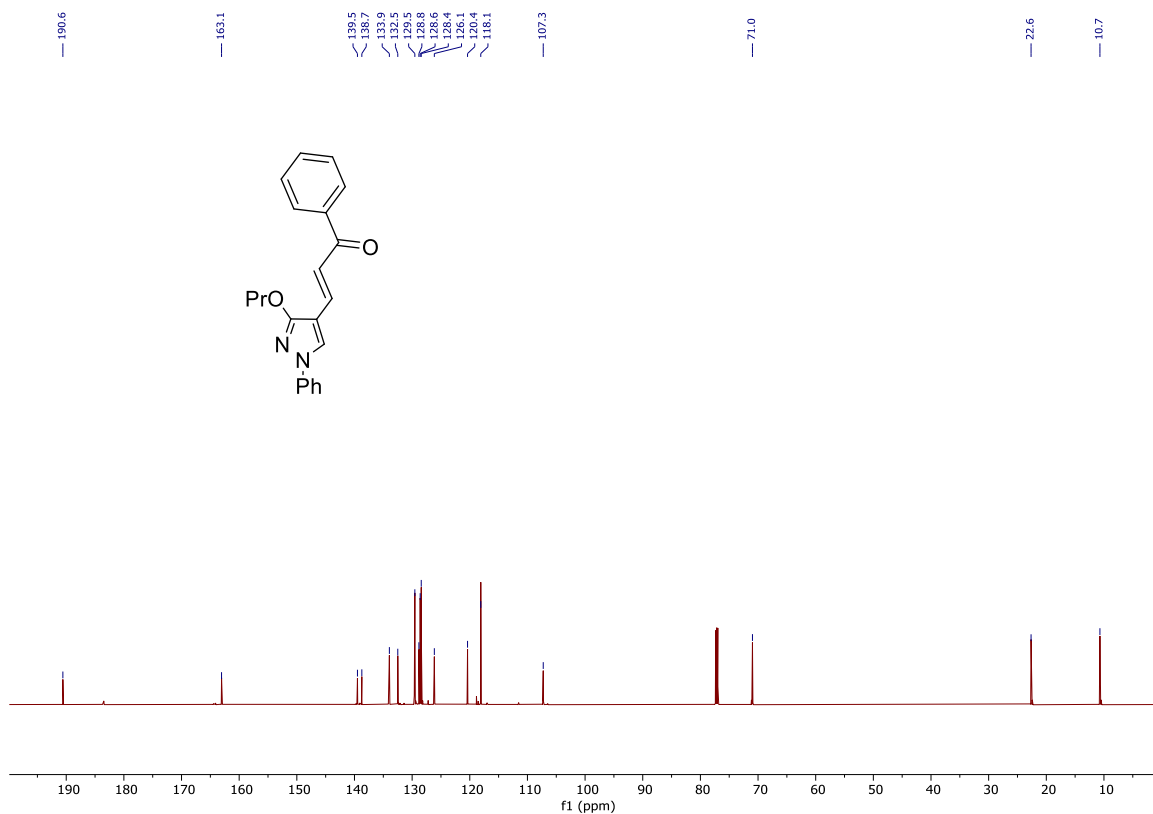


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
361.0716	1	C <sub>19</sub> H <sub>15</sub> ClN <sub>2</sub> NaO <sub>2</sub>	361.0714	0.4	12.0	1	100.00	12.5	even		ok

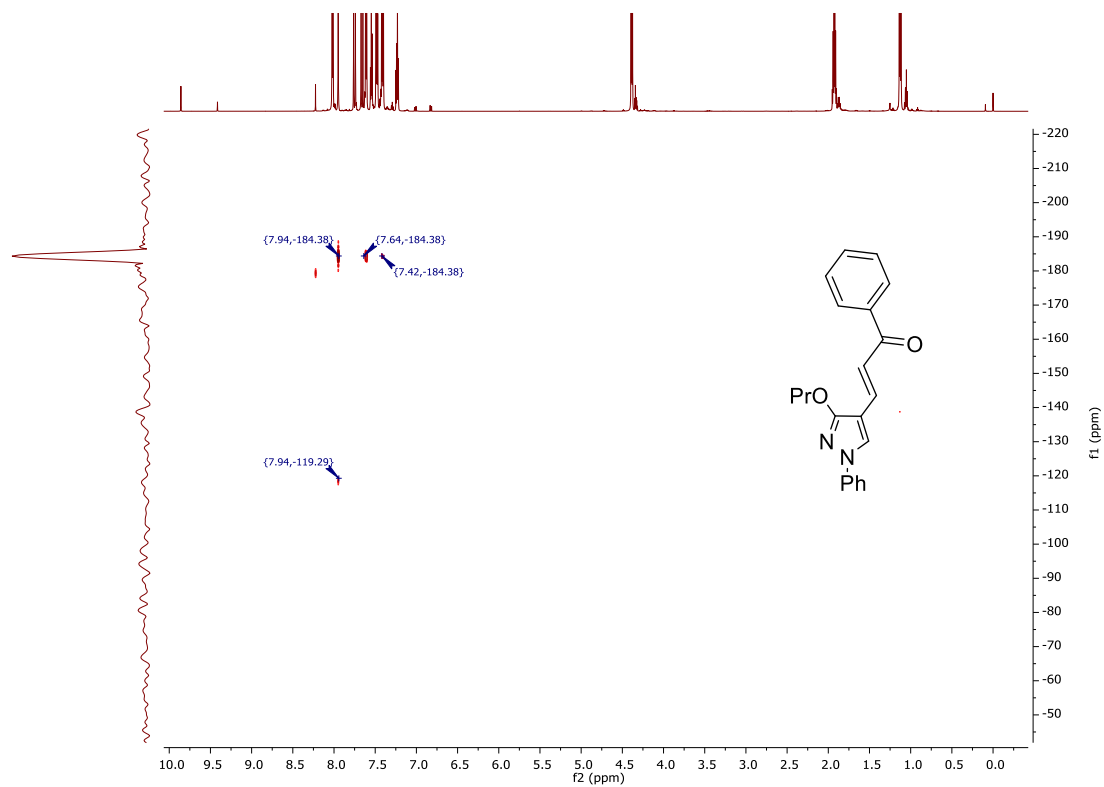
**Figure S19. (2E)-1-(4-Chlorophenyl)-3-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (4d). HRMS (ESI-TOF).**



**Figure S20. (2E)-1-Phenyl-3-(1-phenyl-3-propoxy-1H-pyrazol-4-yl)prop-2-en-1-one (4e). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**



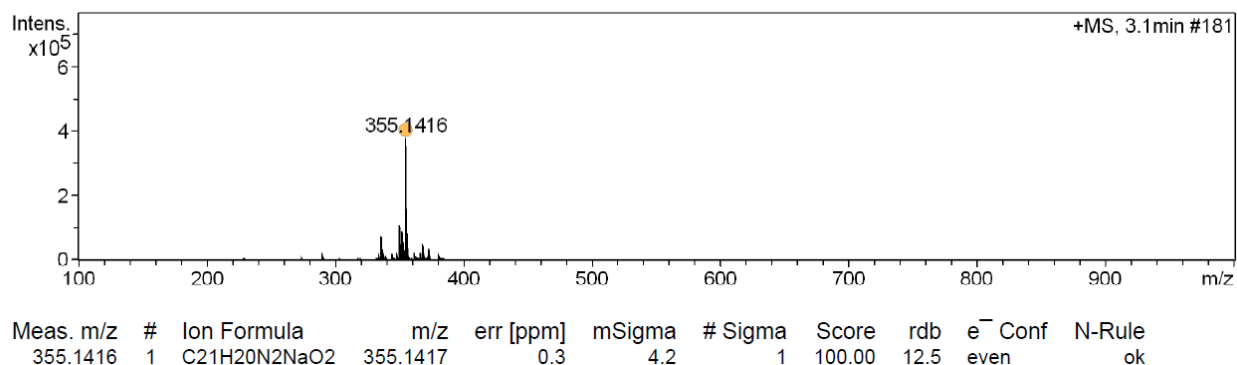
**Figure S21. (2E)-1-Phenyl-3-(1-phenyl-3-propoxy-1H-pyrazol-4-yl)prop-2-en-1-one (4e). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)**



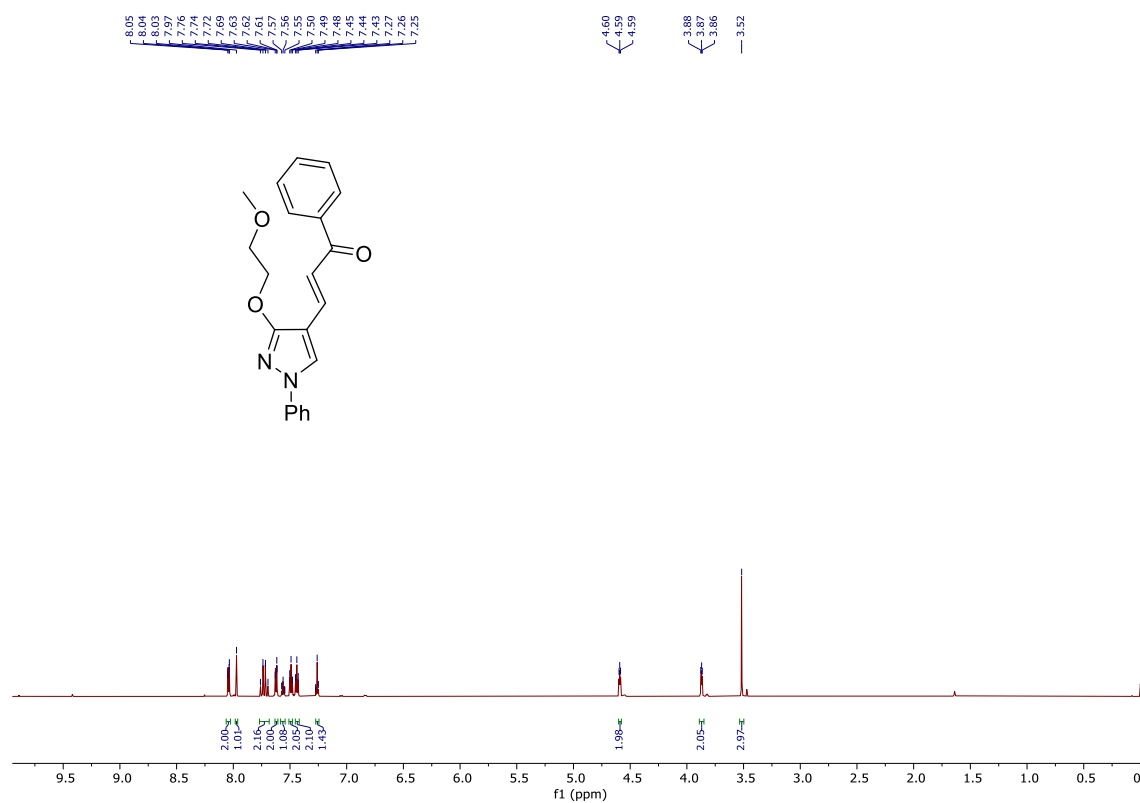
**Figure S22. (2E)-1-Phenyl-3-(1-phenyl-3-propoxy-1H-pyrazol-4-yl)prop-2-en-1-one (4e). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)**



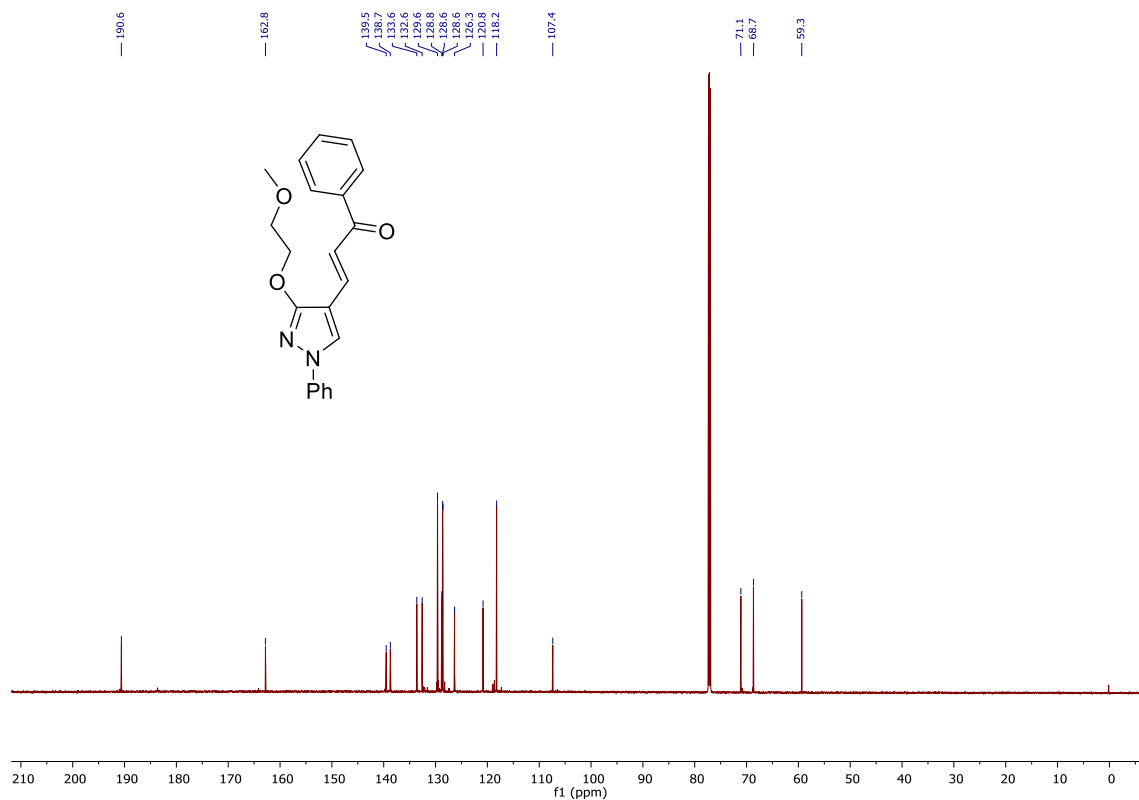
+MS, 3.1min #181



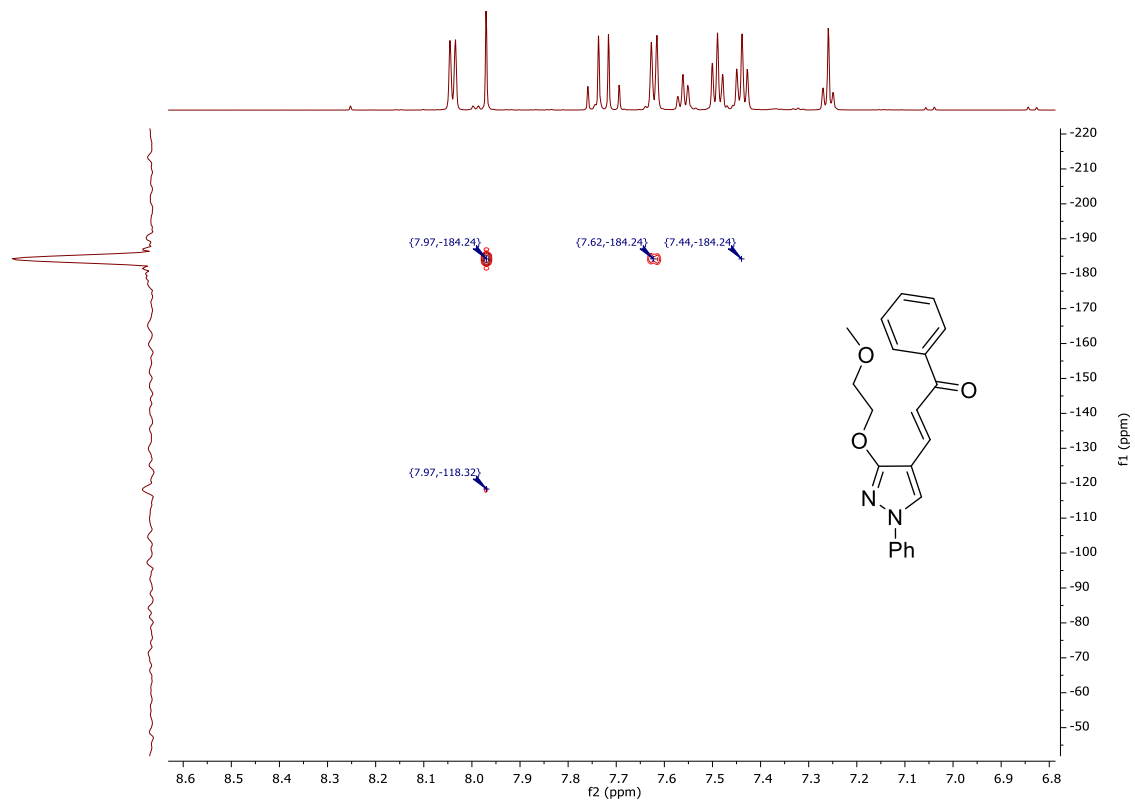
**Figure S23. (2E)-1-Phenyl-3-(1-phenyl-3-propoxy-1H-pyrazol-4-yl)prop-2-en-1-one (4e). HRMS (ESI-TOF).**



**Figure S24. (2E)-3-[3-(2-Methoxyethoxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4f). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**

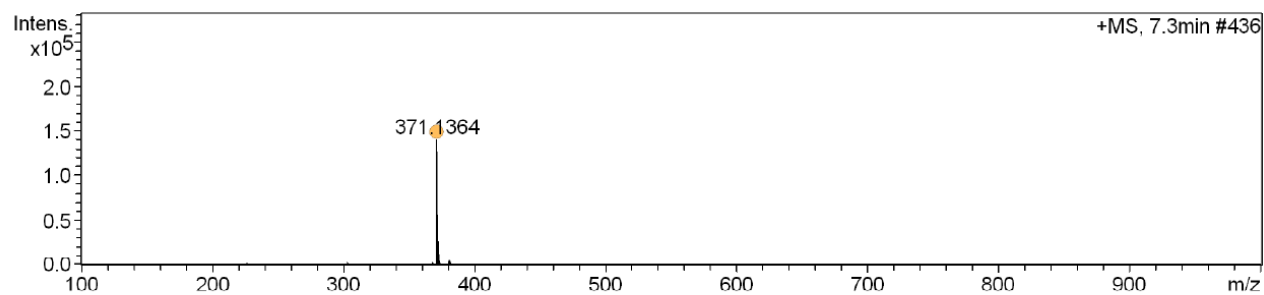


**Figure S25.** (2E)-3-[3-(2-Methoxyethoxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4f). <sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>)



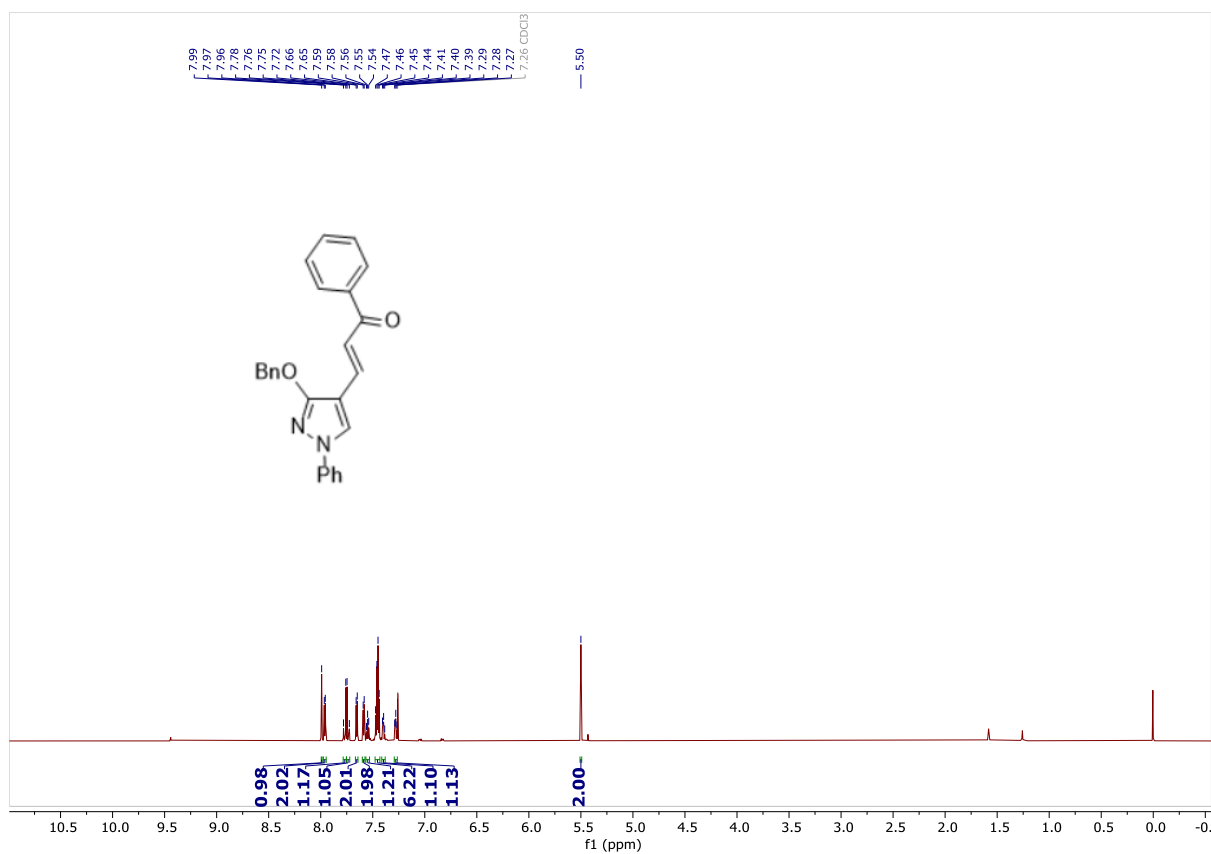
**Figure S26.** (2E)-3-[3-(2-Methoxyethoxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4f). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)

+MS, 7.3min #436

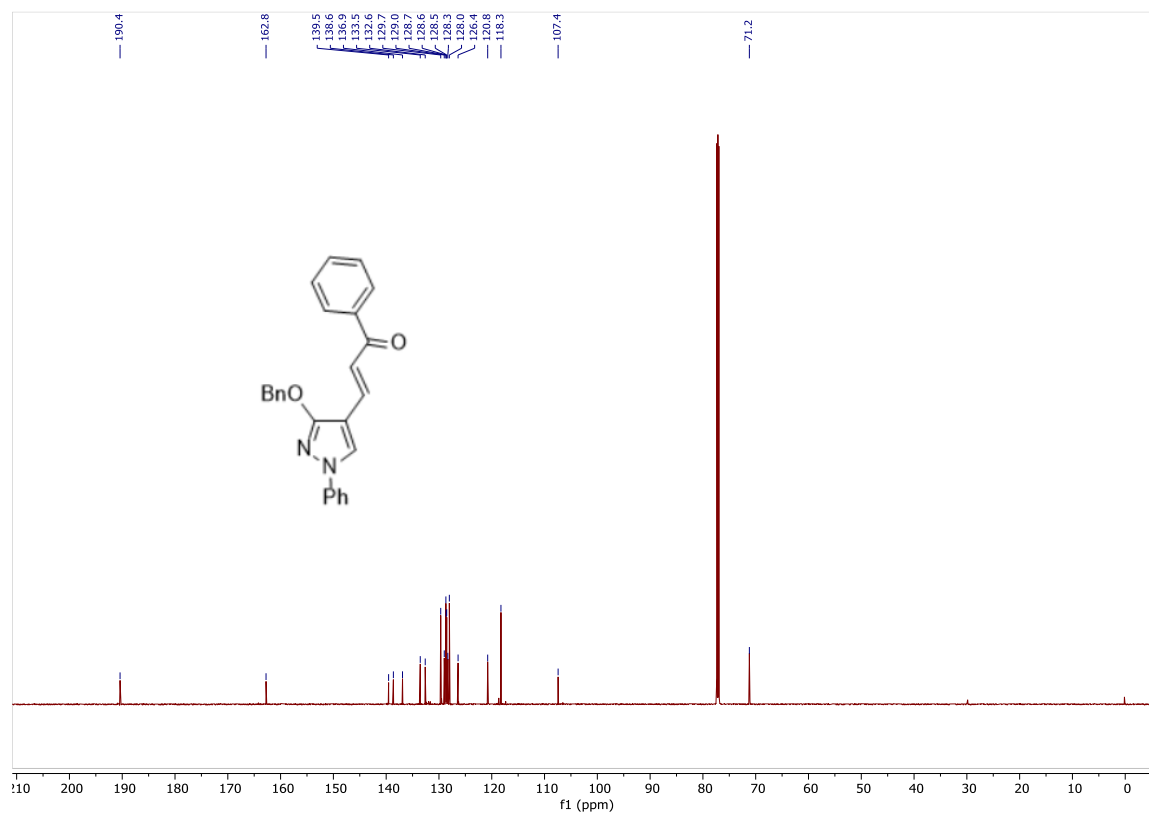


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
371.1364	1	C21H20N2NaO3	371.1366	-0.6	15.7	3	100.00	12.5	even		ok

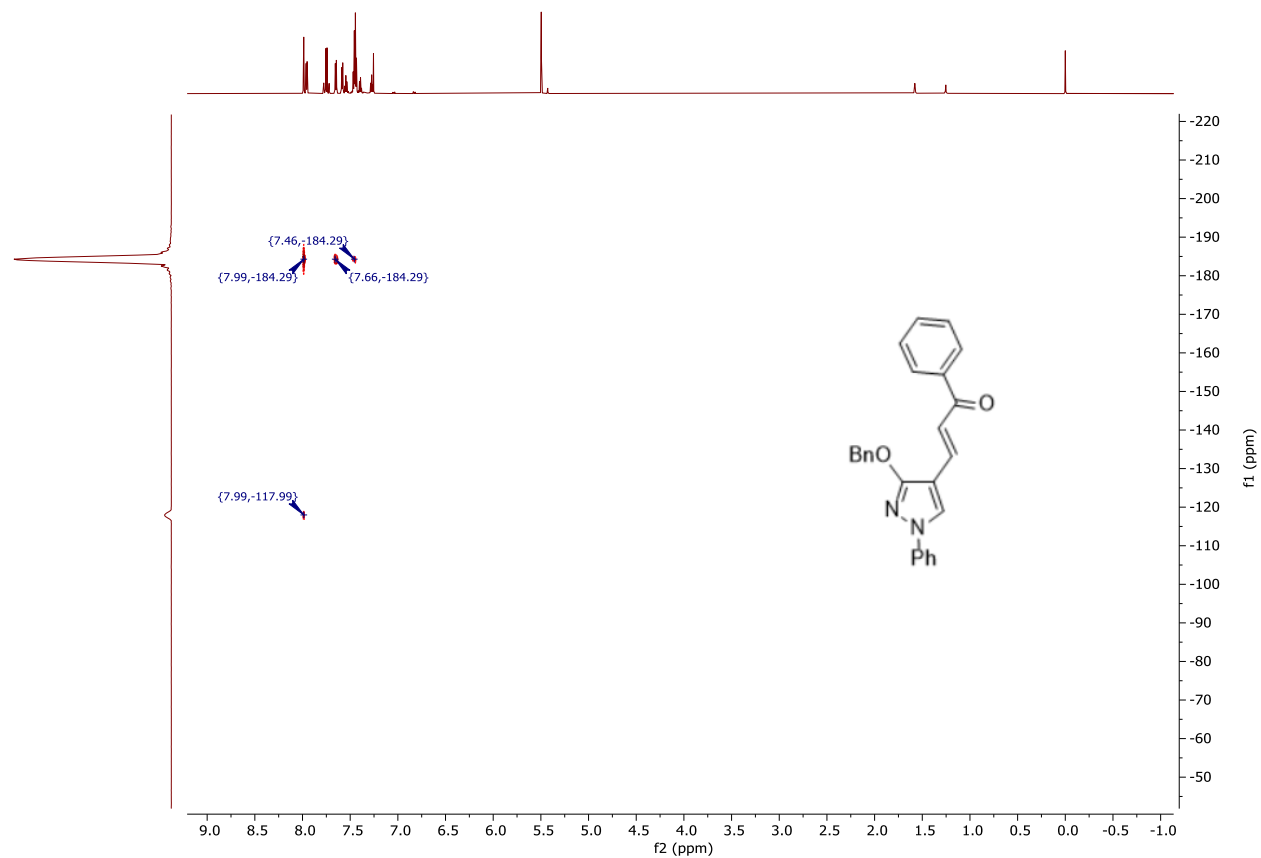
**Figure S27. (2E)-3-[3-(2-Methoxyethoxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4f). HRMS (ESI-TOF).**



**Figure S28. (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4g). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**

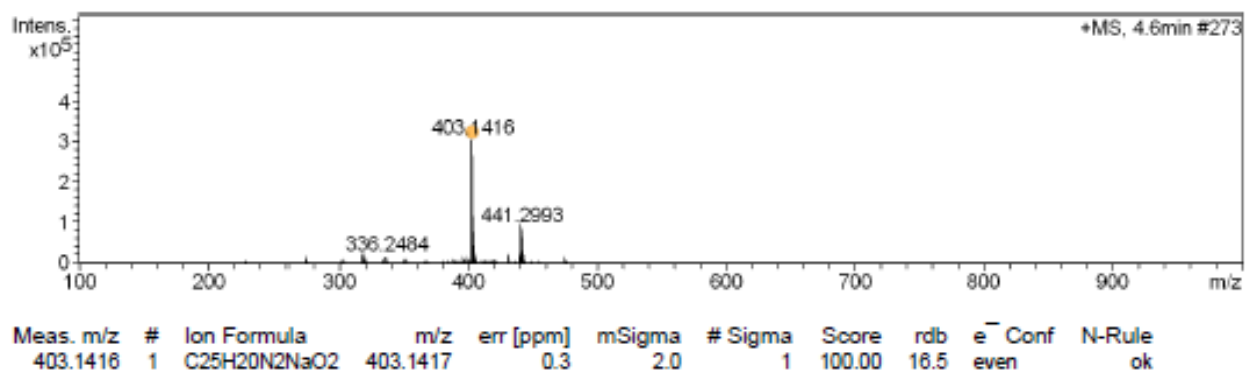


**Figure S29.** (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4g). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)

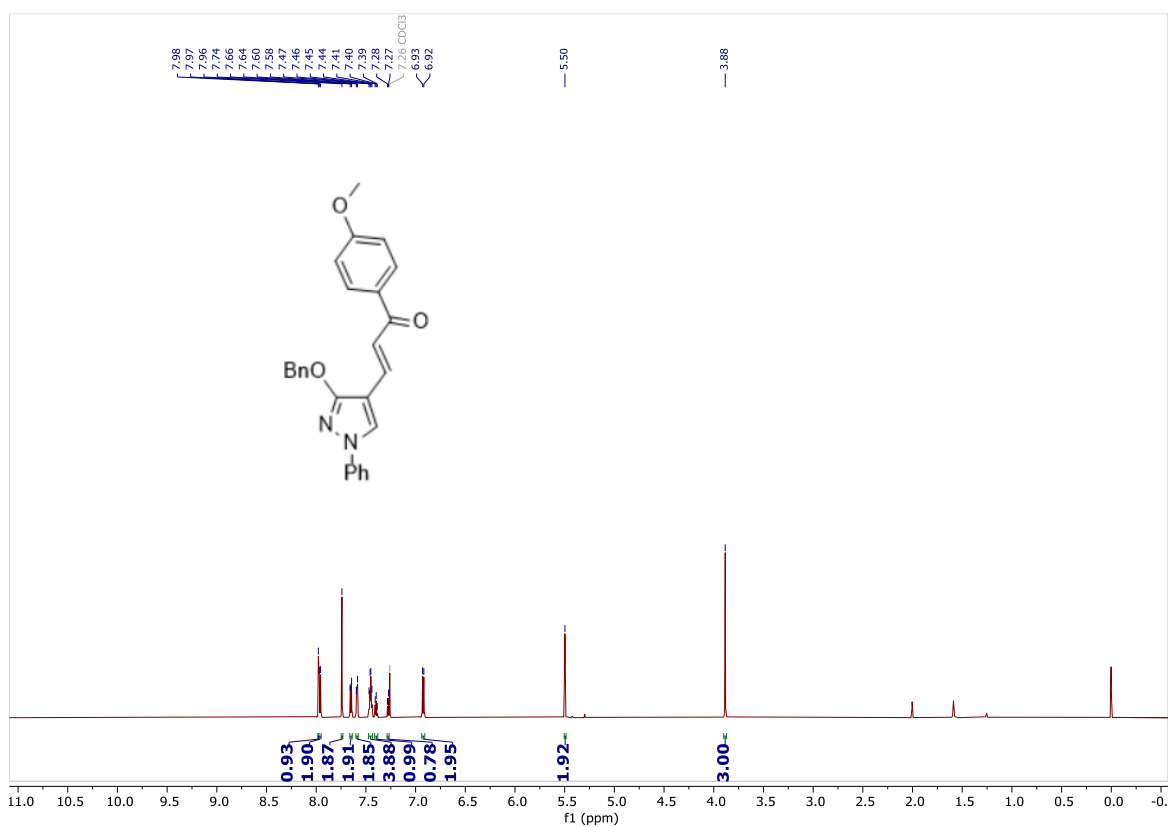


**Figure S30.** (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4g). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)

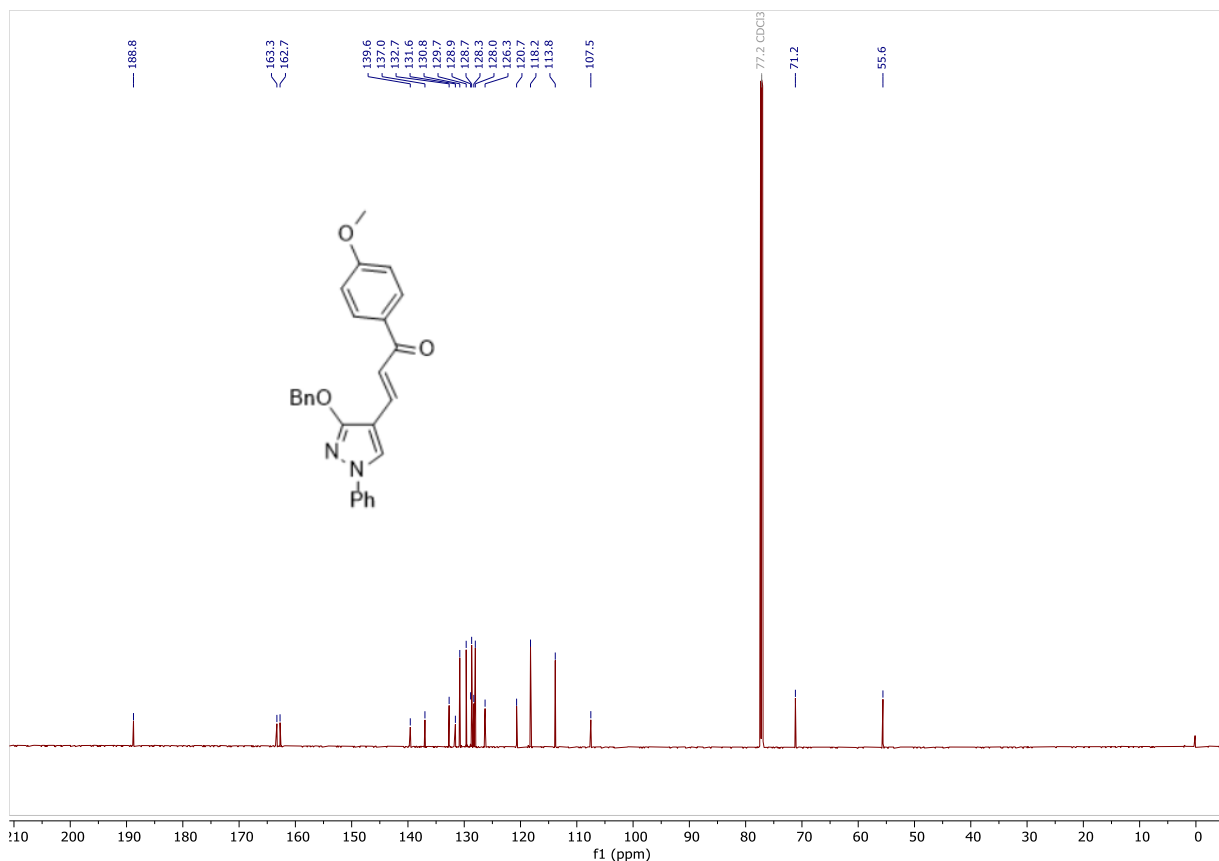
+MS, 4.6min #273



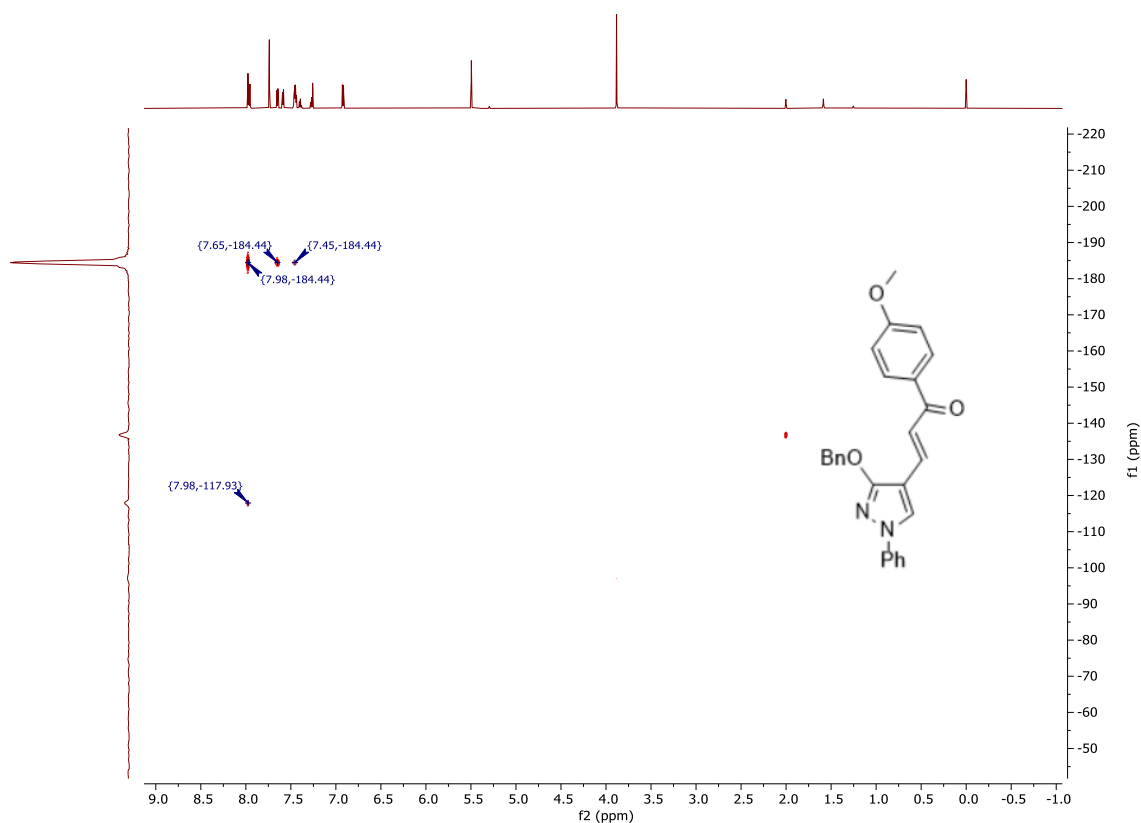
**Figure S31.** (2*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-phenylprop-2-en-1-one (4g). HRMS (ESI-TOF).



**Figure S32.** (2*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-(4-methoxyphenyl)prop-2-en-1-one (4h). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)



**Figure S33.** (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-(4-methoxyphenyl)prop-2-en-1-one (4h). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



**Figure S34.** (E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-(4-methoxyphenyl)prop-2-en-1-one (4h). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)

+MS, 3.9min #236

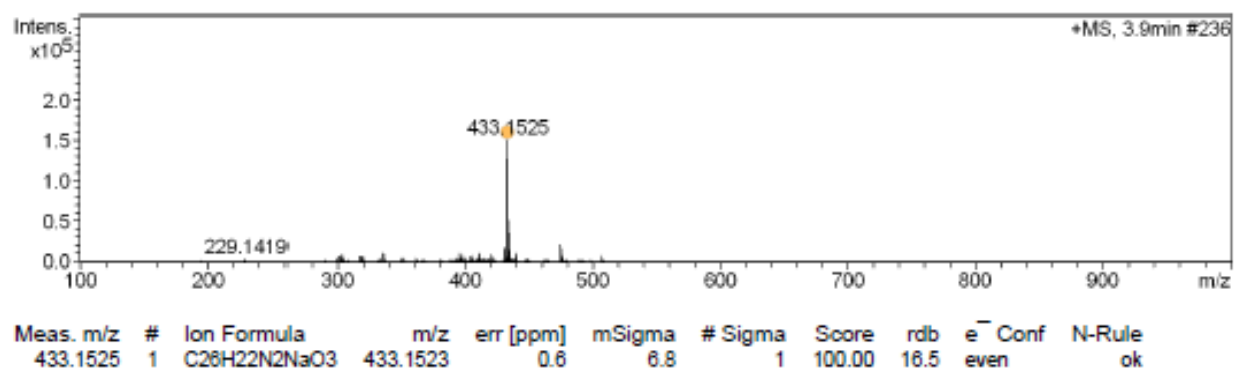


Figure S35. (*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-(4-methoxyphenyl)prop-2-en-1-one (4h). HRMS (ESI-TOF).

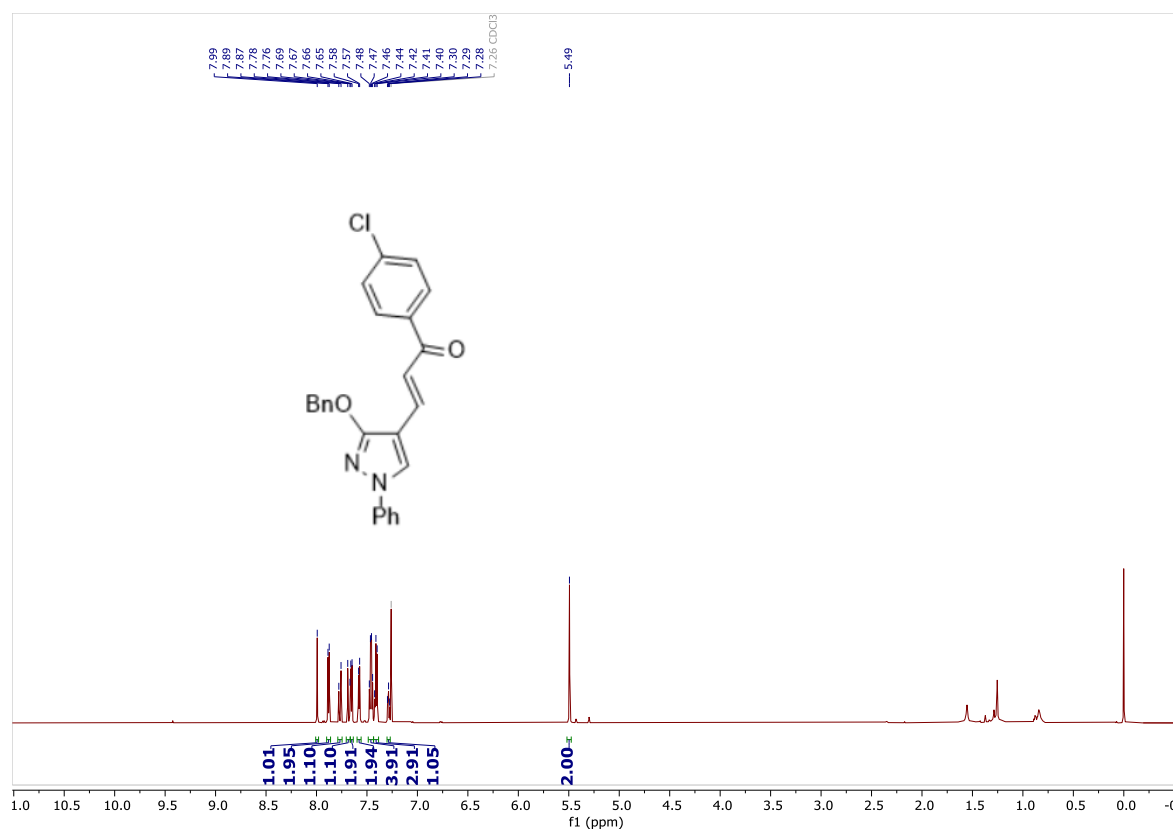
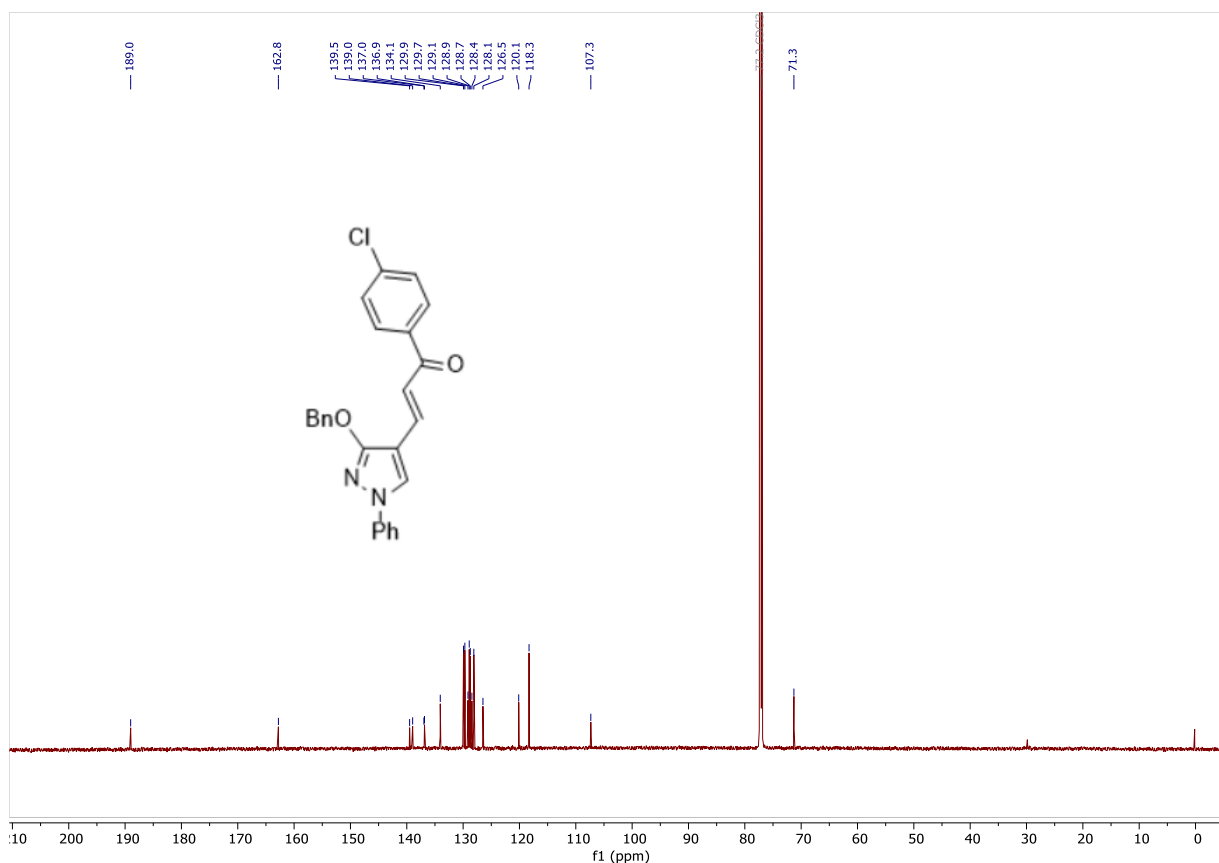
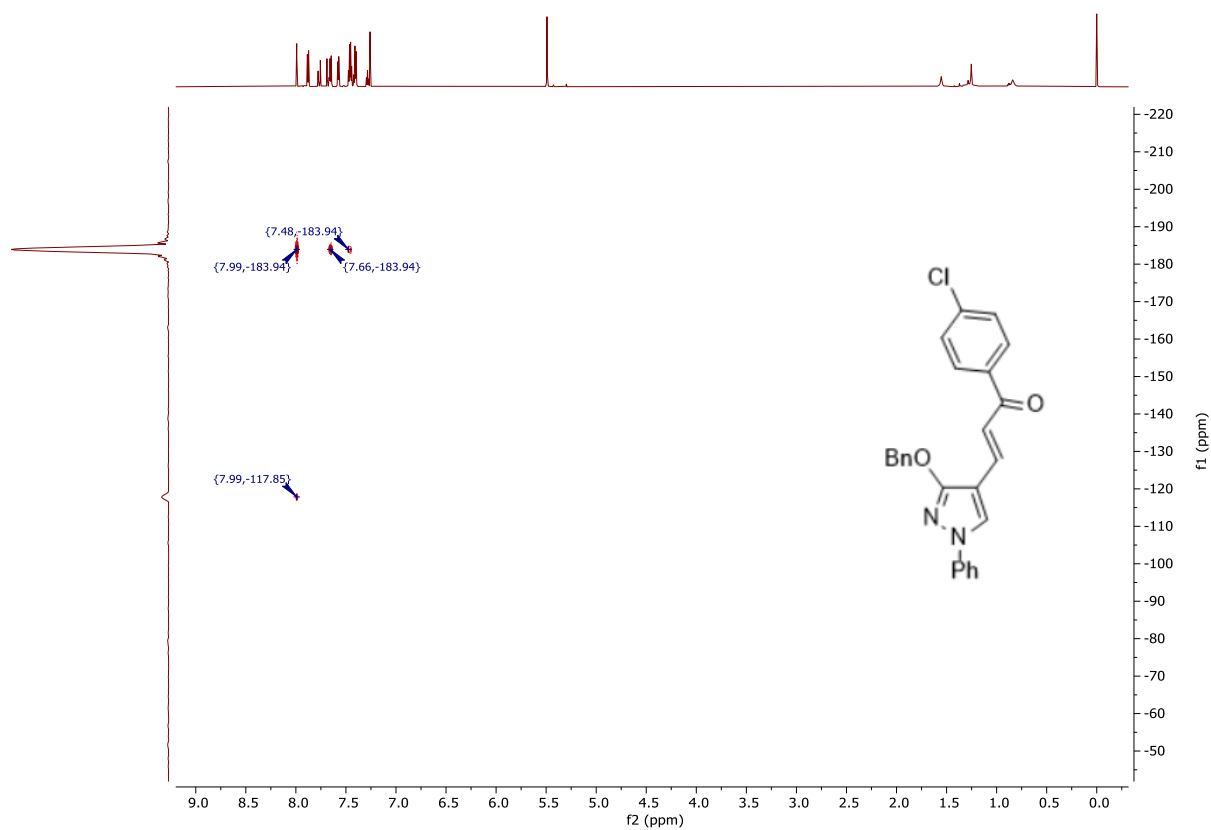


Figure S36. (2*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-(4-chlorophenyl)prop-2-en-1-one (4i). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)



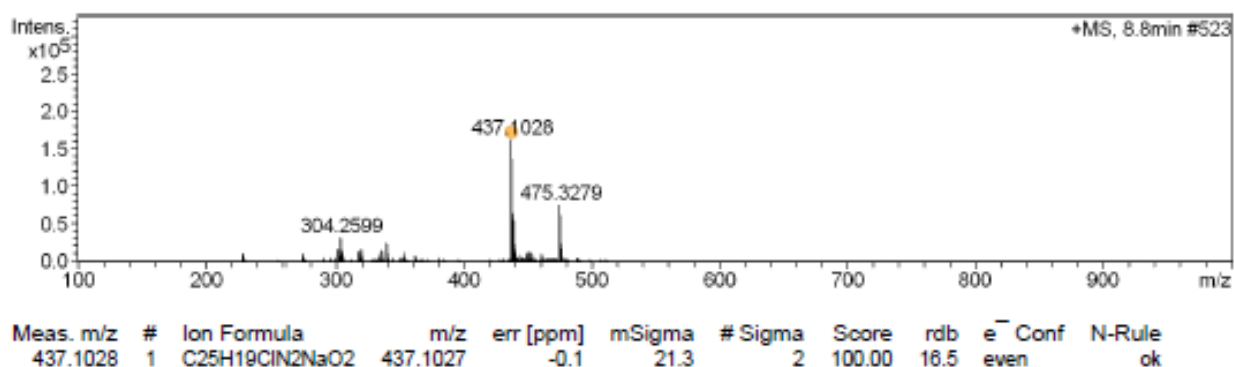
**Figure S37.** (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-(4-chlorophenyl)prop-2-en-1-one (4i). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



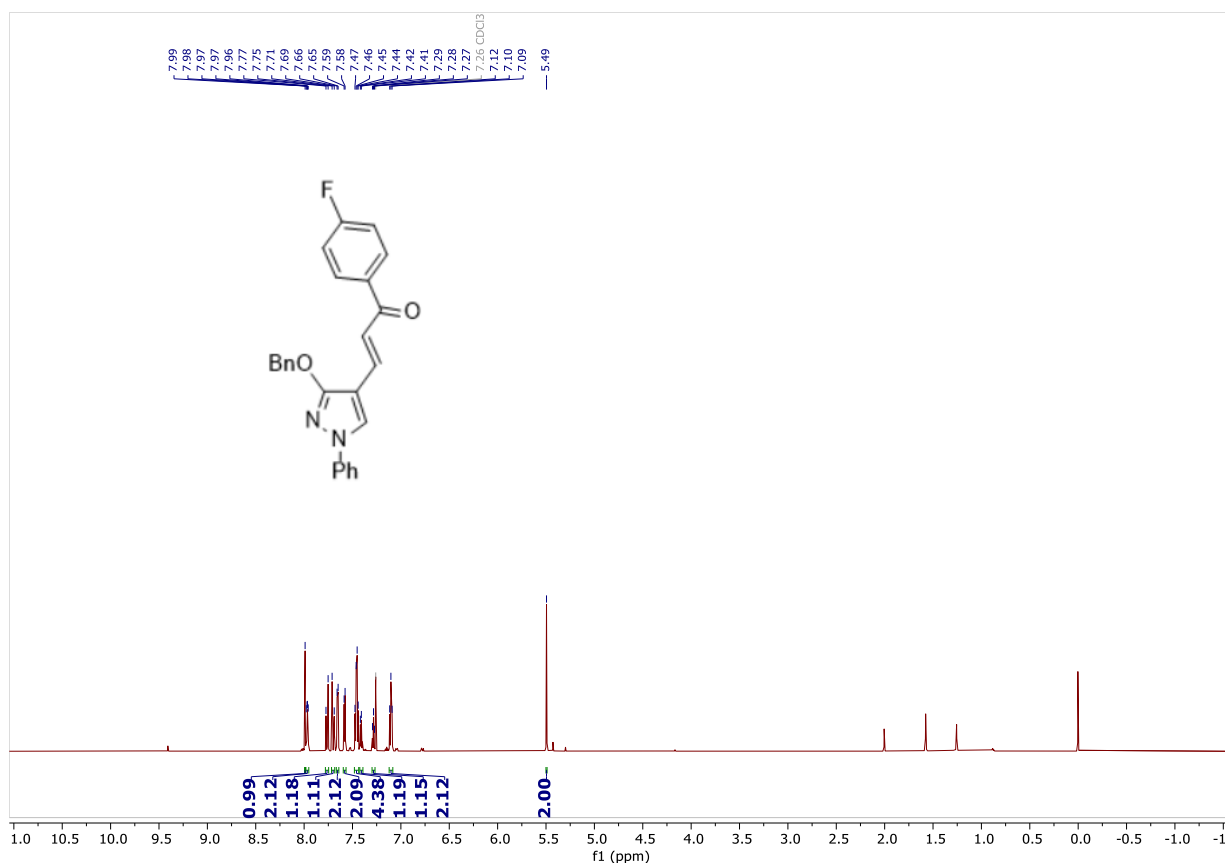
**Figure S38.** (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-(4-chlorophenyl)prop-2-en-1-one (4i). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)



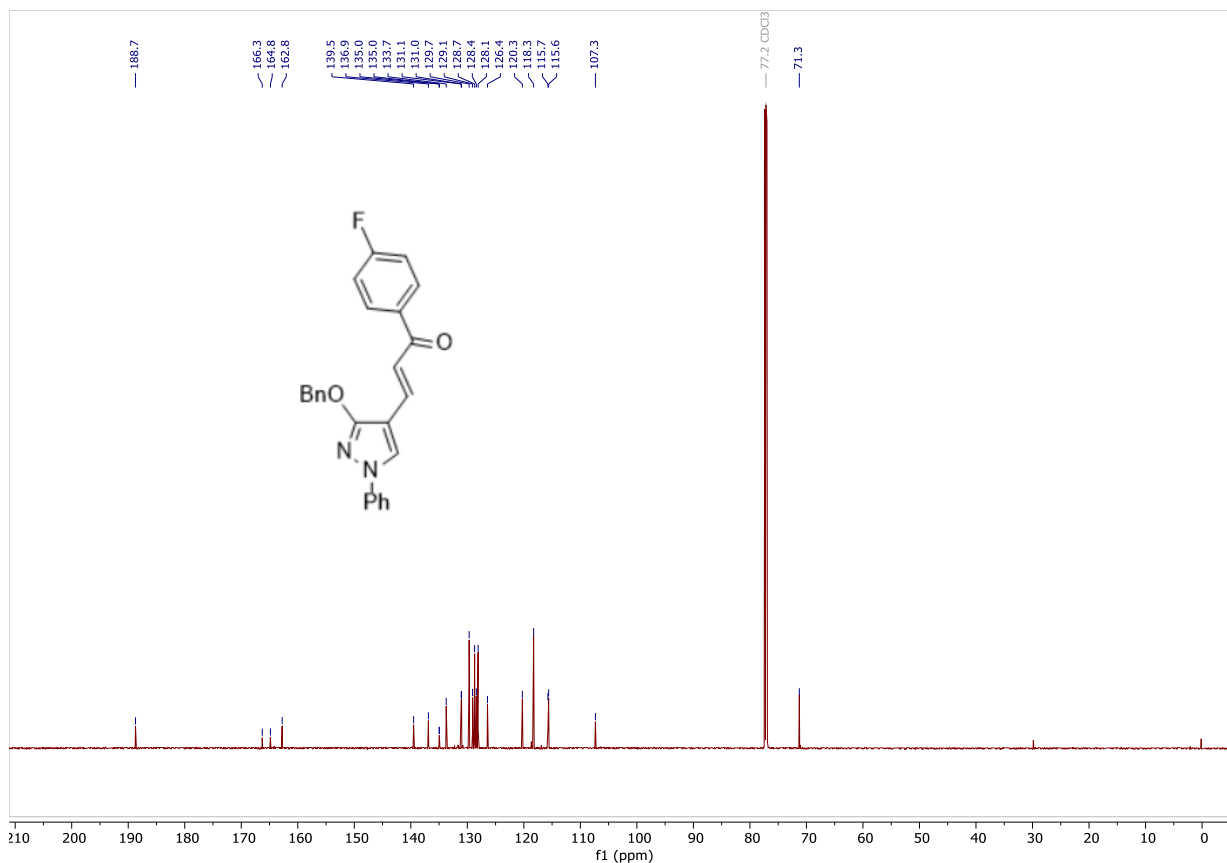
+MS, 8.8min #523



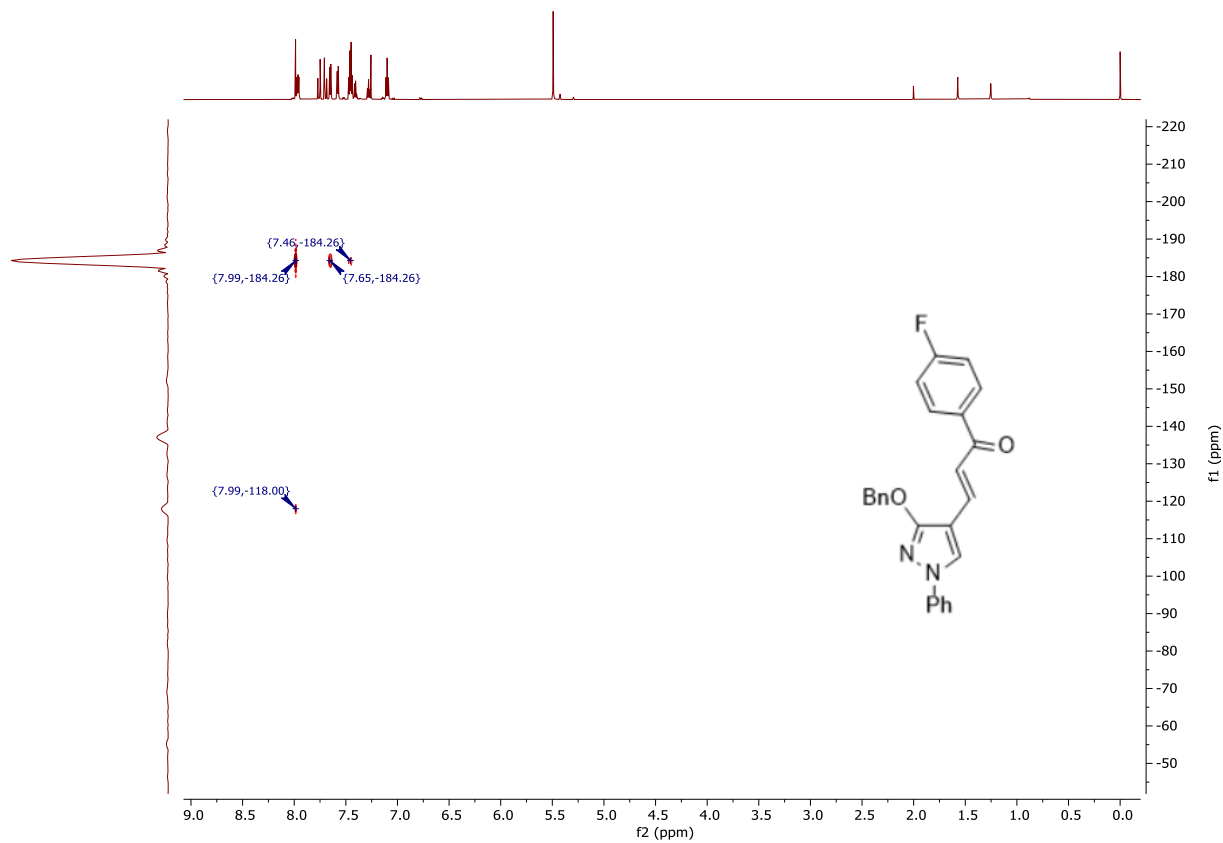
**Figure S39.** (2*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-(4-chlorophenyl)prop-2-en-1-one (4i). HRMS (ESI-TOF).



**Figure S40.** (2*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-(4-fluorophenyl)prop-2-en-1-one (4j). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)

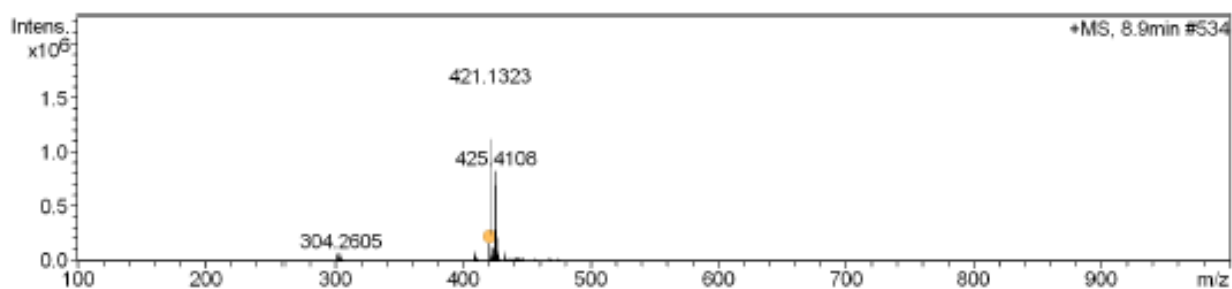


**Figure S41. (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-(4-fluorophenyl)prop-2-en-1-one (4j). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)**



**Figure S42. (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-(4-fluorophenyl)prop-2-en-1-one (4j). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)**

+MS, 8.9min #534



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
421.1323	1	C <sub>25</sub> H <sub>19</sub> FN <sub>2</sub> NaO <sub>2</sub>	421.1323	-0.0	19.1	1	100.00	16.5	even		ok

Figure S43. (2*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-(4-fluorophenyl)prop-2-en-1-one (4j). HRMS (ESI-TOF).

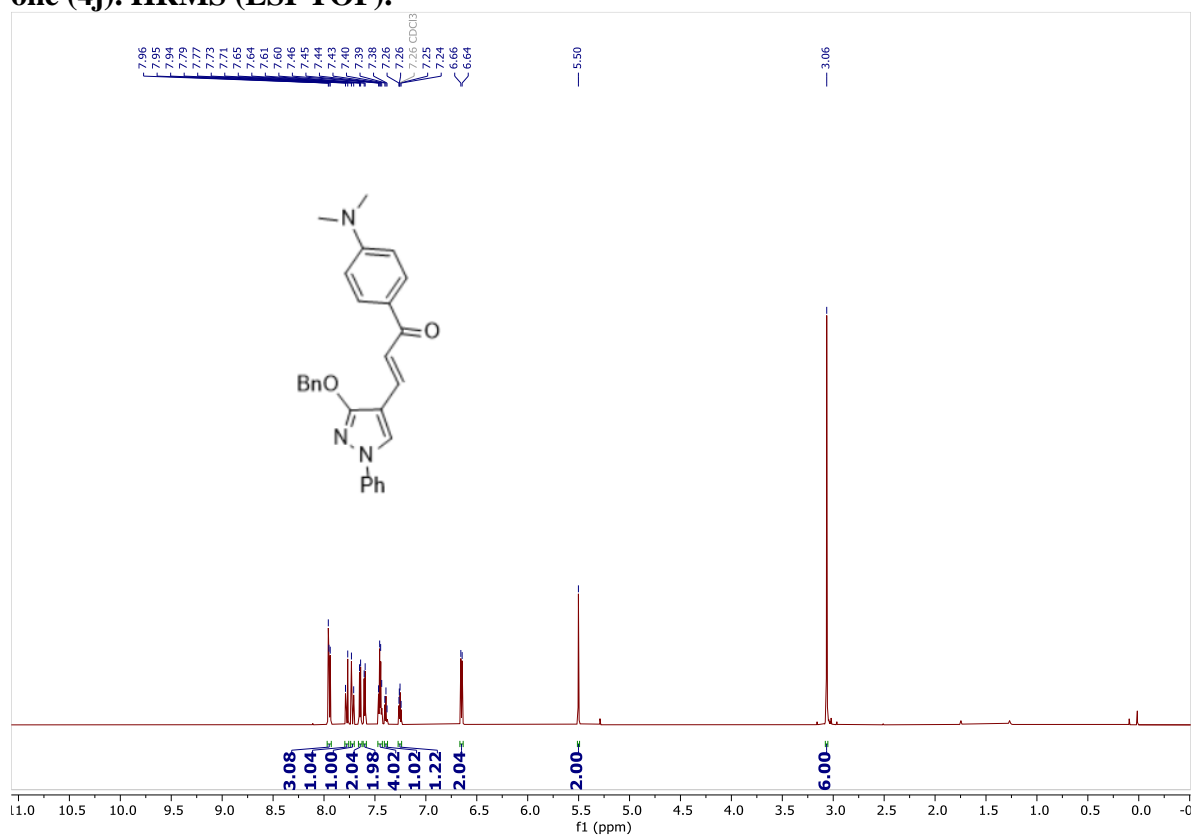
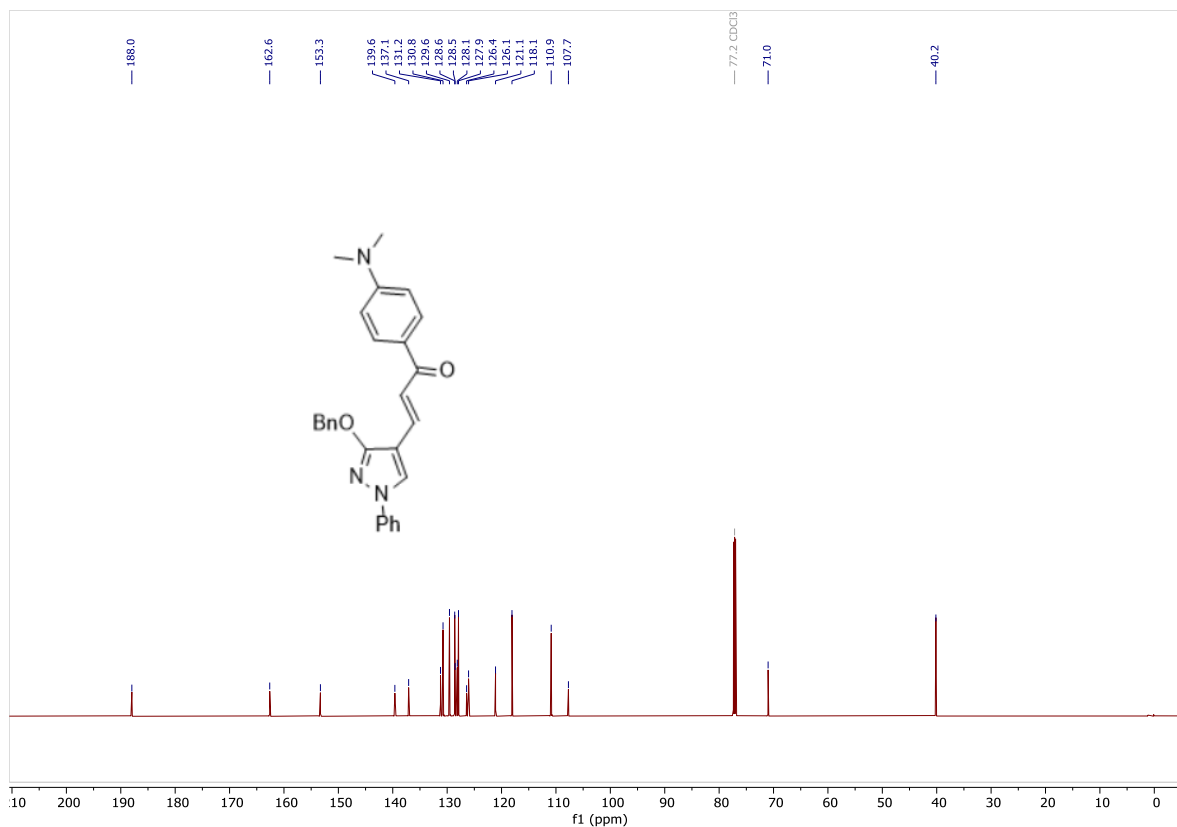
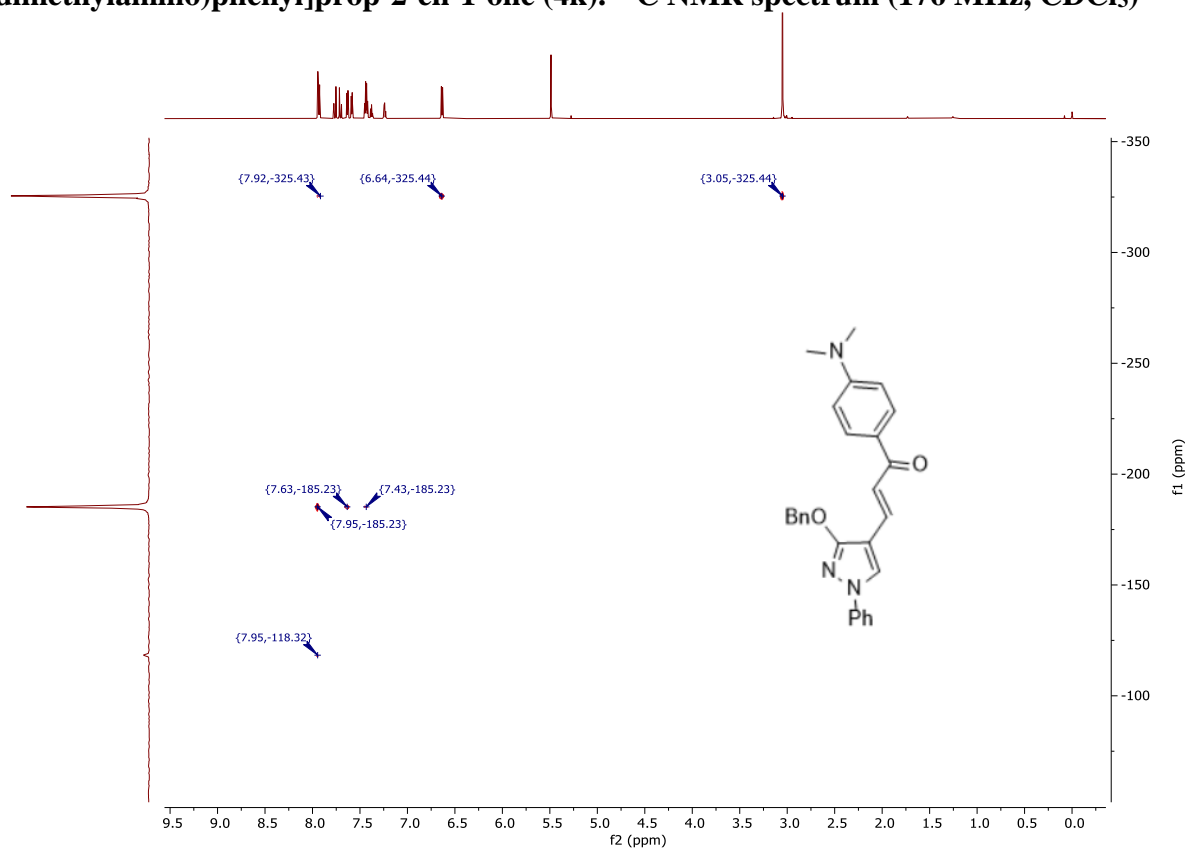


Figure S44. (2*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-[4-(dimethylamino)phenyl]prop-2-en-1-one (4k). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)

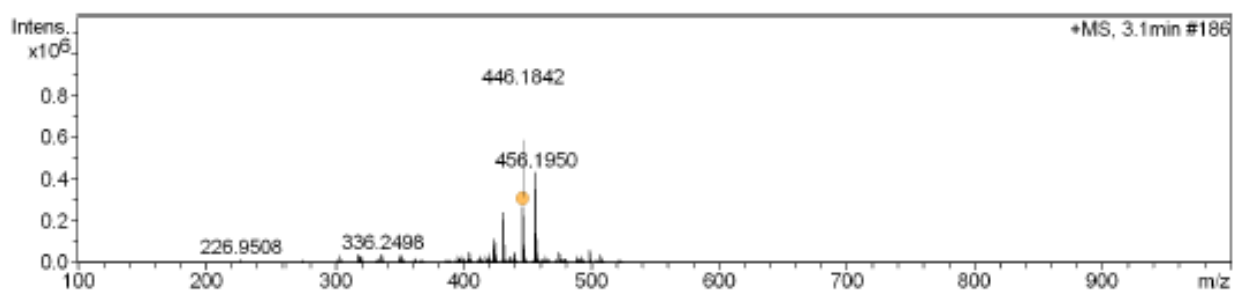


**Figure S45. (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-[4-(dimethylamino)phenyl]prop-2-en-1-one (4k).  $^{13}\text{C}$  NMR spectrum (176 MHz, CDCl<sub>3</sub>)**



**Figure S46. (2E)-3-[3-(Benzyloxy)-1-phenyl-1H-pyrazol-4-yl]-1-[4-(dimethylamino)phenyl]prop-2-en-1-one (4k).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)**

+MS, 3.1min #186



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
446.1842	1	C <sub>27</sub> H <sub>25</sub> N <sub>3</sub> NaO <sub>2</sub>	446.1839	0.7	3.6	1	100.00	16.5	even		ok

Figure S47. (2*E*)-3-[3-(Benzyloxy)-1-phenyl-1*H*-pyrazol-4-yl]-1-[4-(dimethylamino)phenyl]prop-2-en-1-one (4k). HRMS (ESI-TOF).

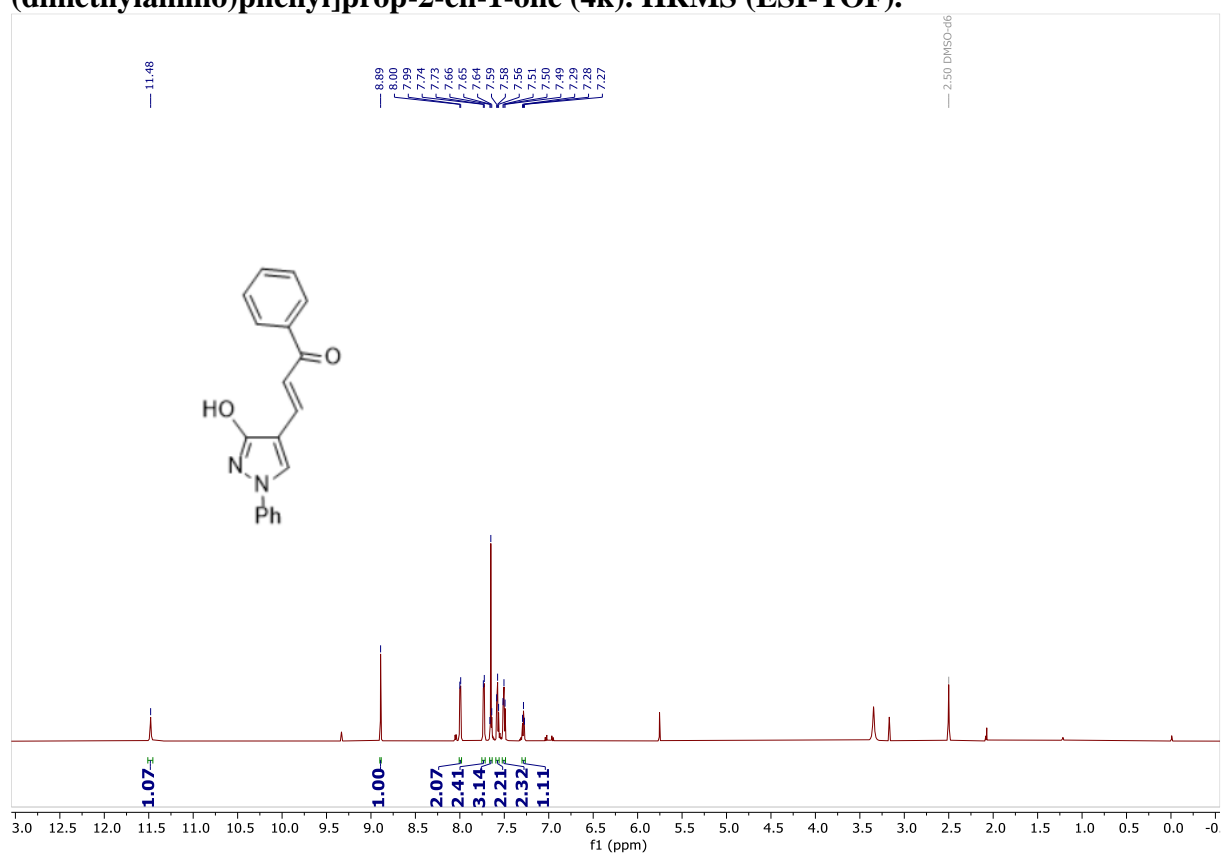
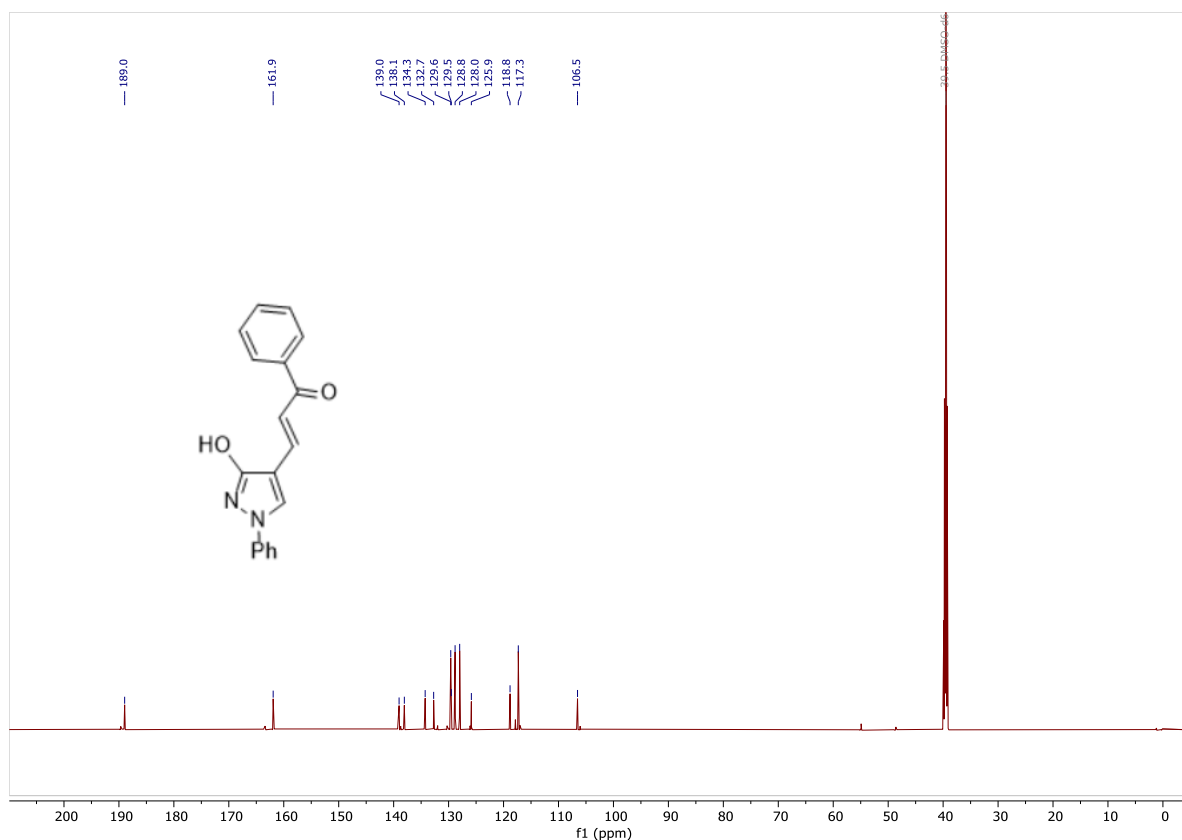
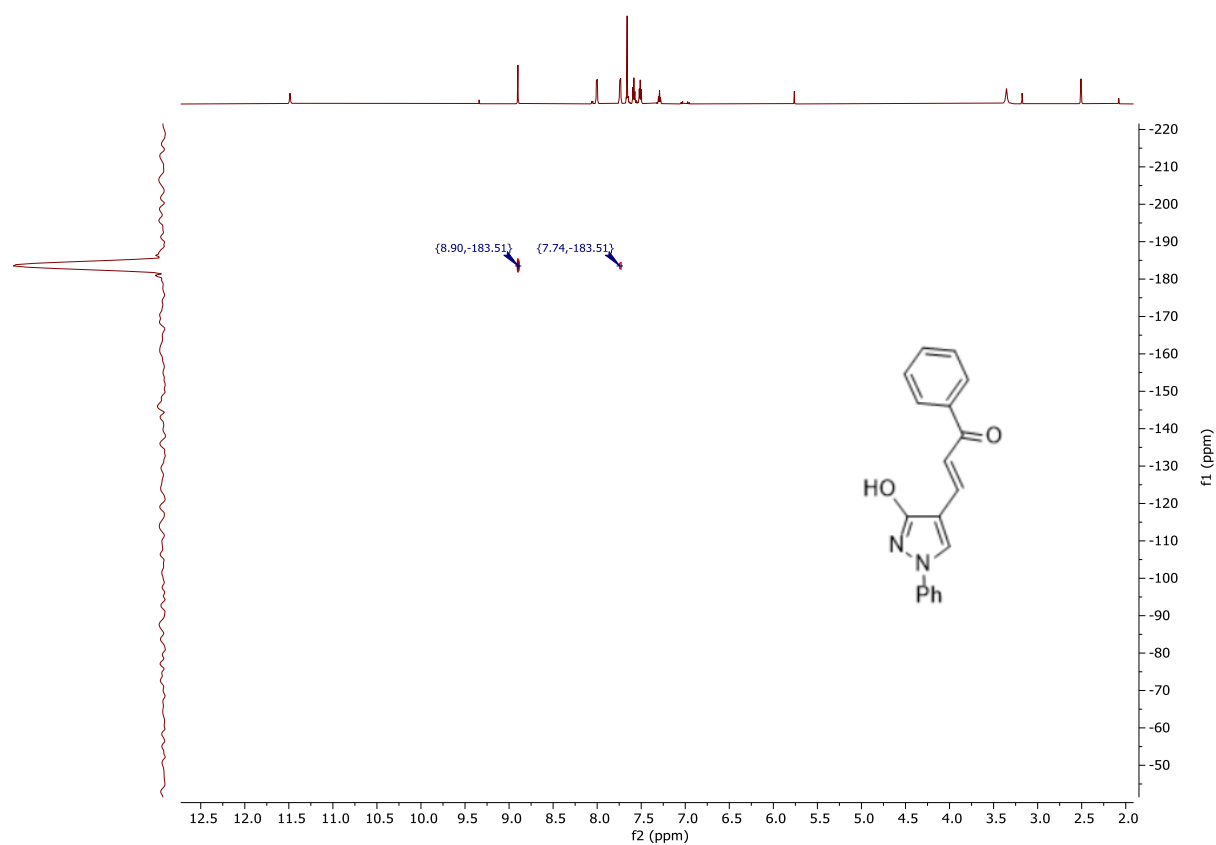


Figure S48. (2*E*)-3-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-1-phenylprop-2-en-1-one (5a). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)



**Figure S49.** (2E)-3-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-1-phenylprop-2-en-1-one (5a). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



**Figure S50.** (2E)-3-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-1-phenylprop-2-en-1-one (5a). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, DMSO-*d*<sub>6</sub>)

+MS, 12.6min #754

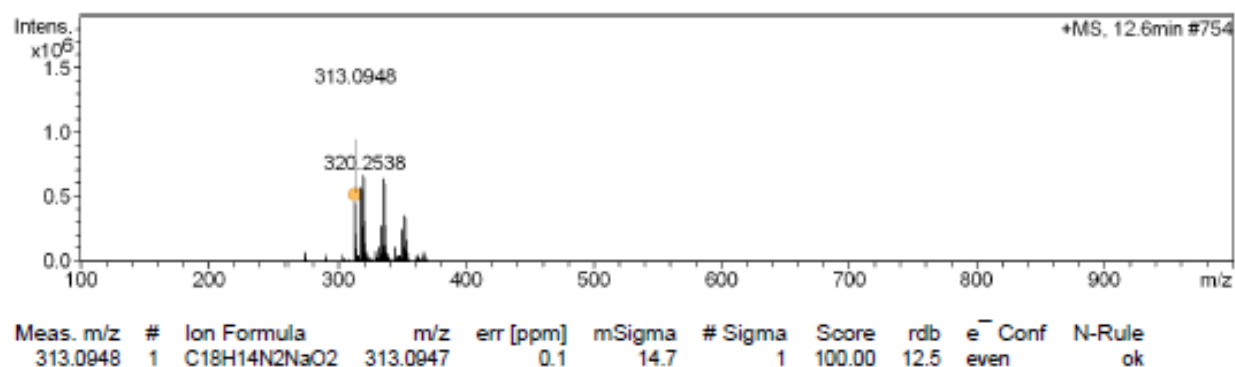


Figure S51. (2*E*)-3-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-1-phenylprop-2-en-1-one (5a). HRMS (ESI-TOF).

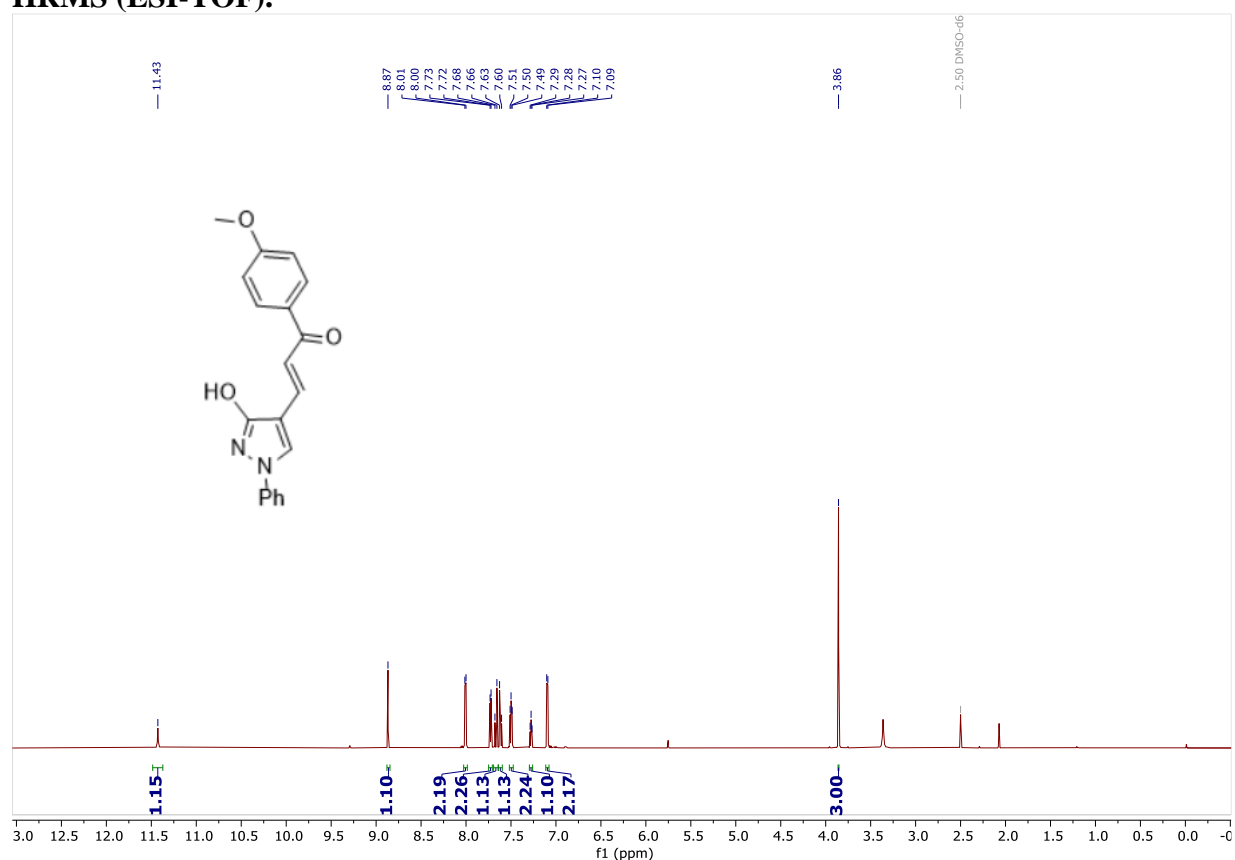
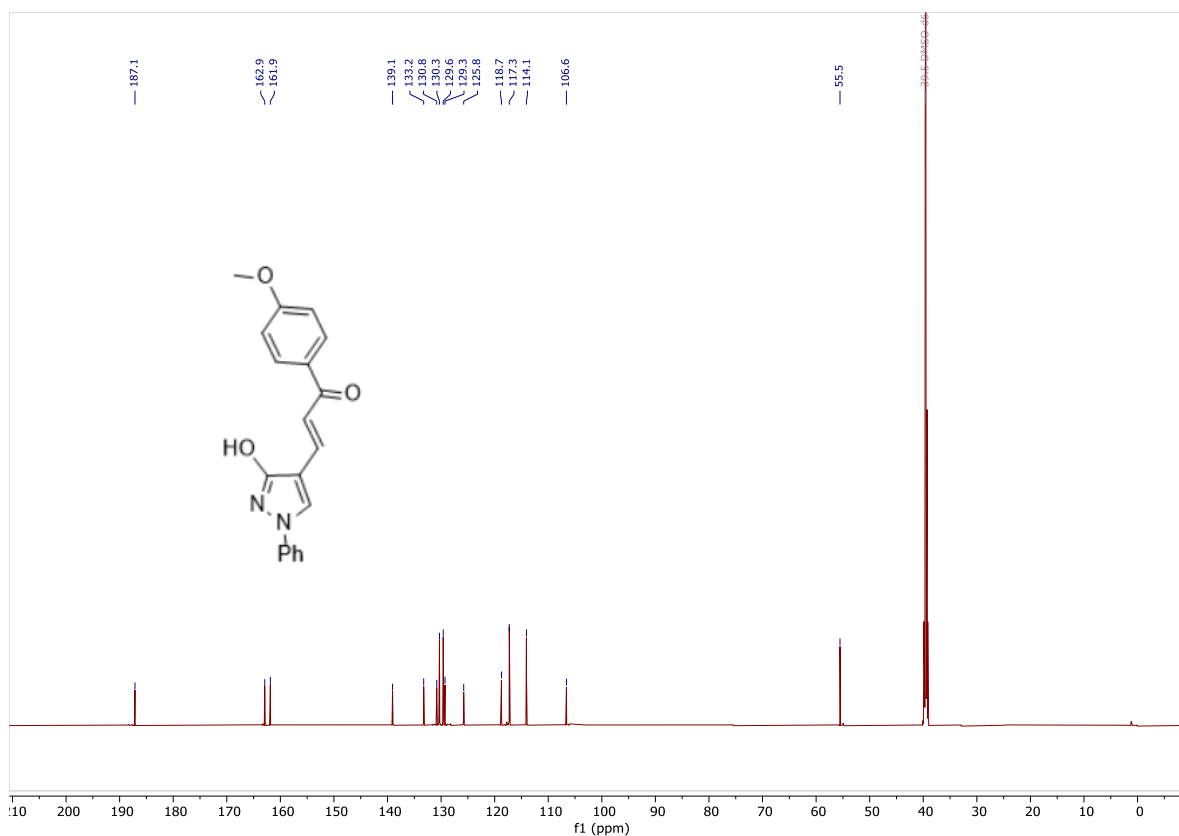
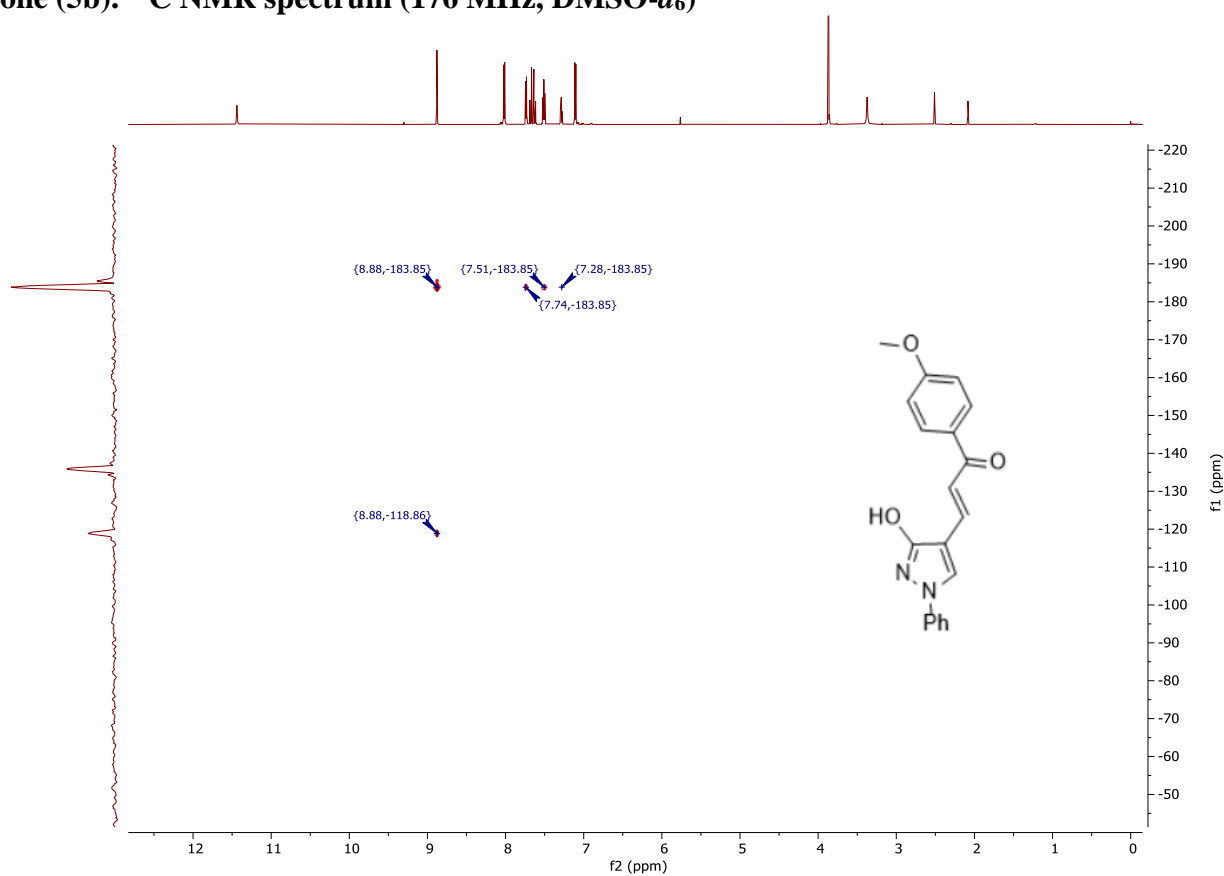


Figure S52. (2*E*)-3-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (5b). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)



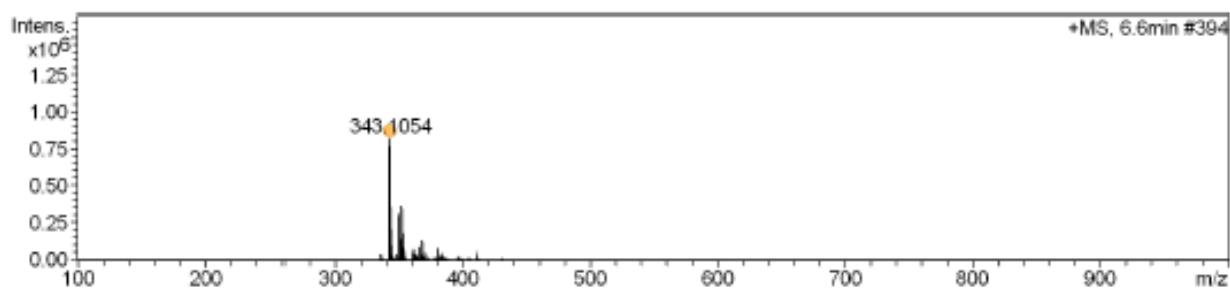
**Figure S53.** (2E)-3-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (5b). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



**Figure S54.** (2E)-3-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (5b). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, DMSO-*d*<sub>6</sub>)



+MS, 6.6min #394



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup>	Conf	N-Rule
343.1054	1	C <sub>19</sub> H <sub>16</sub> N <sub>2</sub> NaO <sub>3</sub>	343.1053	0.3	30.8	2	100.00	12.5	even		ok

Figure S55. (2*E*)-3-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (5b). HRMS (ESI-TOF).

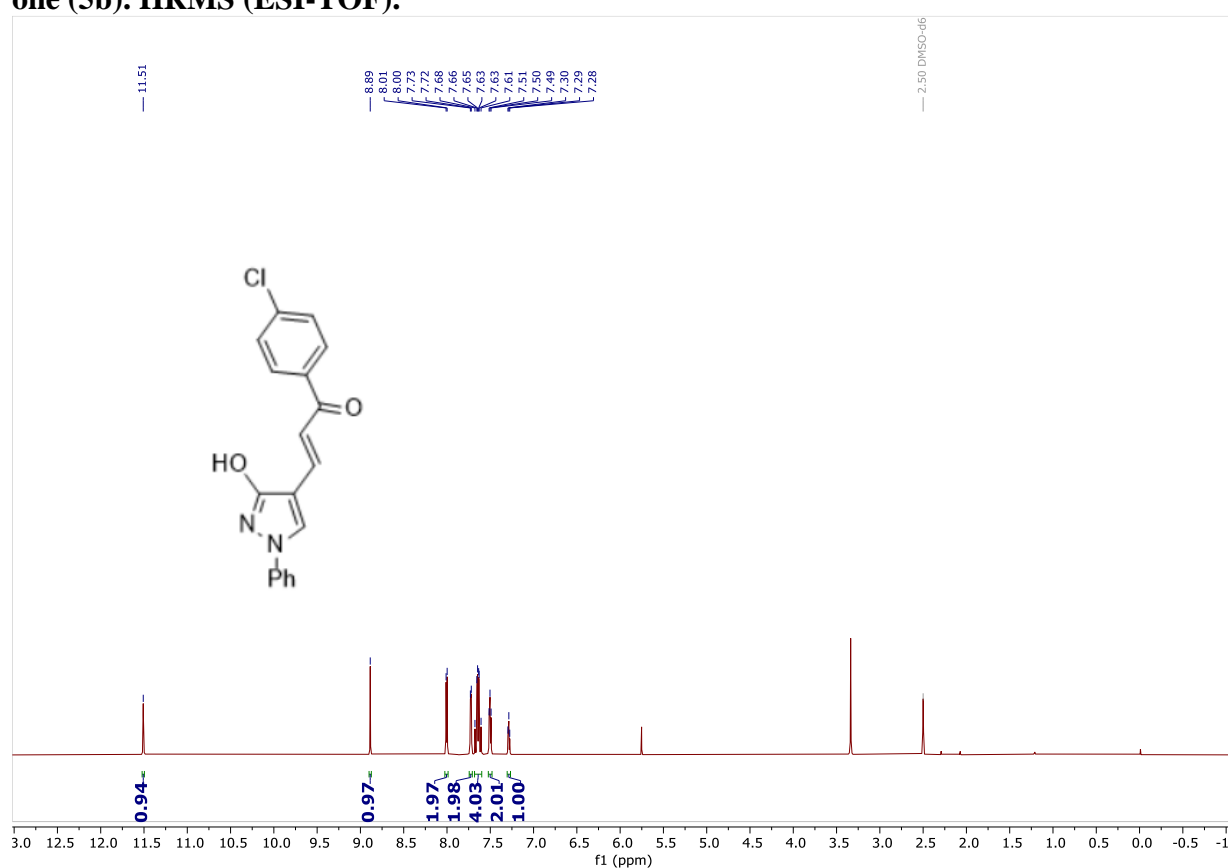
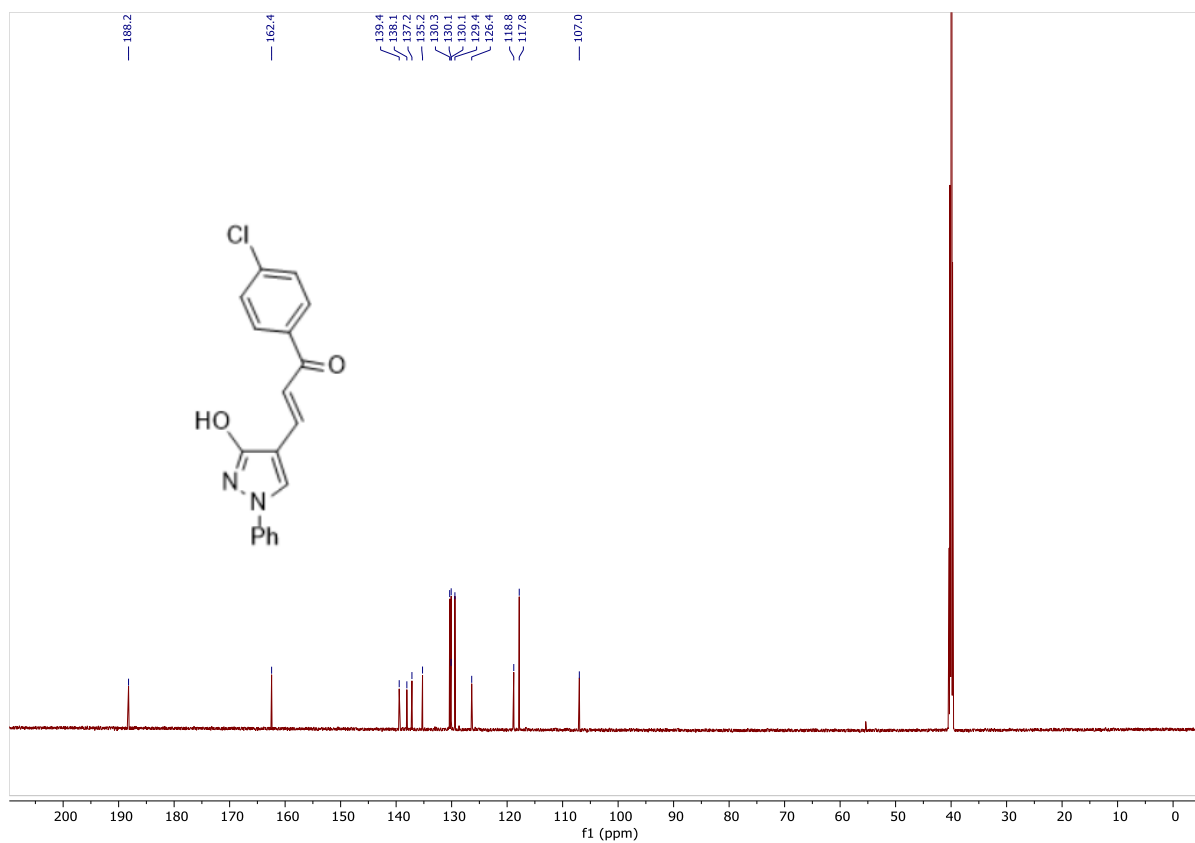
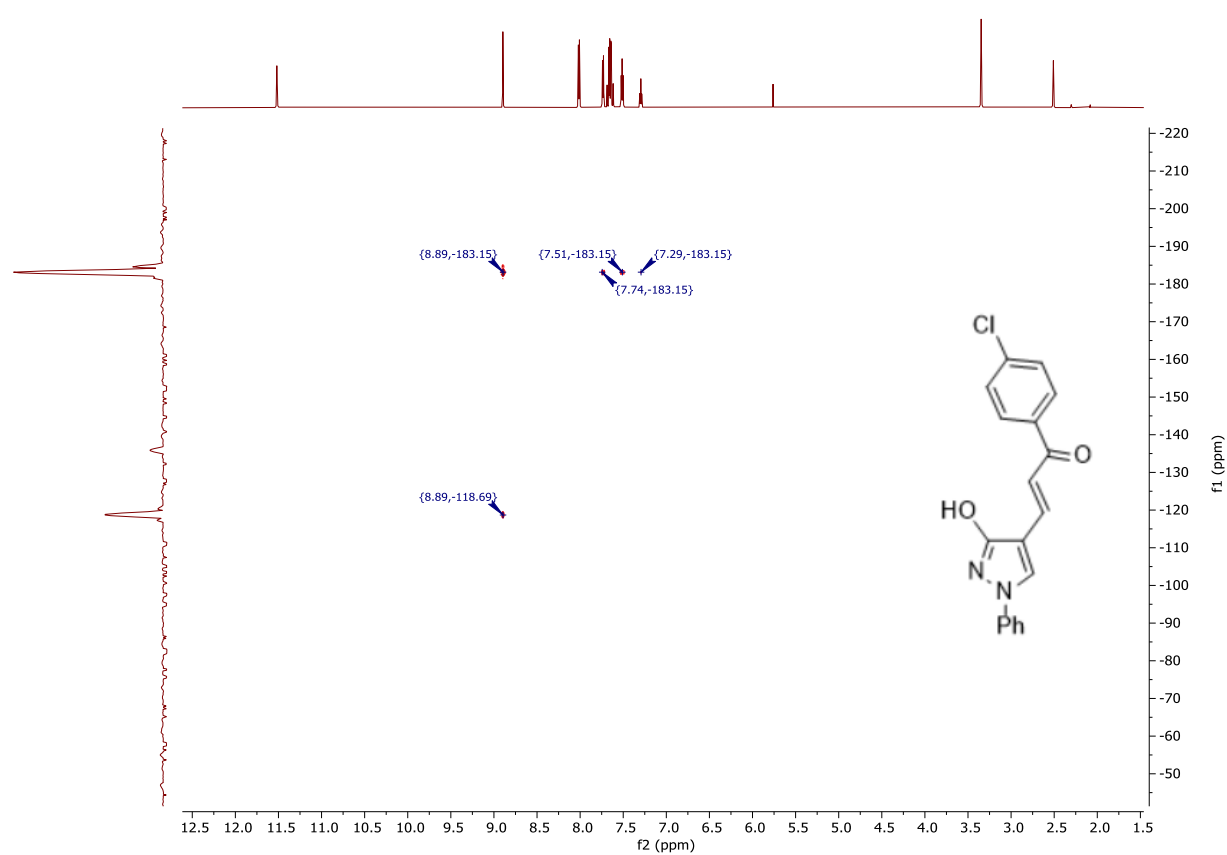


Figure S56. (2*E*)-1-(4-Chlorophenyl)-3-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (5c). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)

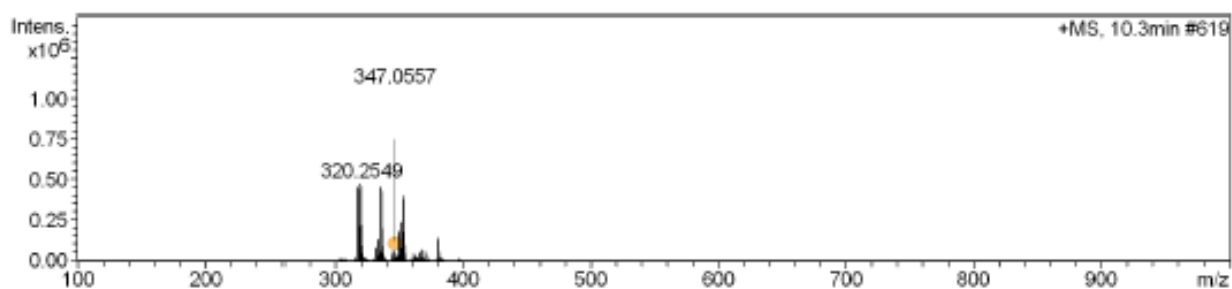


**Figure S57.** (E)-1-(4-Chlorophenyl)-3-(3-hydroxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (5c). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



**Figure S58.** (E)-1-(4-Chlorophenyl)-3-(3-hydroxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (5c). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, DMSO-*d*<sub>6</sub>)

+MS, 10.3min #619



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
347.0557	1	C18H13ClN2NaO2	347.0558	0.1	26.6	1	100.00	12.5	even		ok

Figure S59. (2*E*)-1-(4-Chlorophenyl)-3-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (5c). HRMS (ESI-TOF).

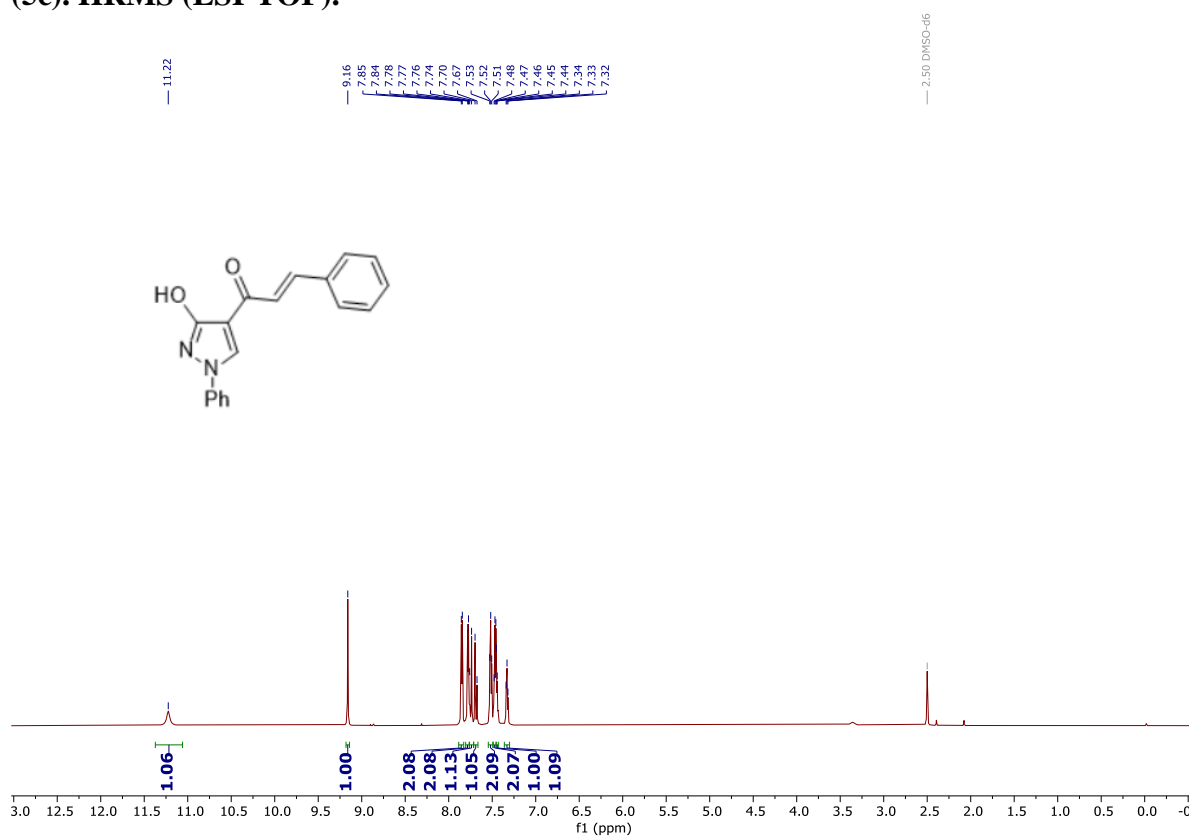
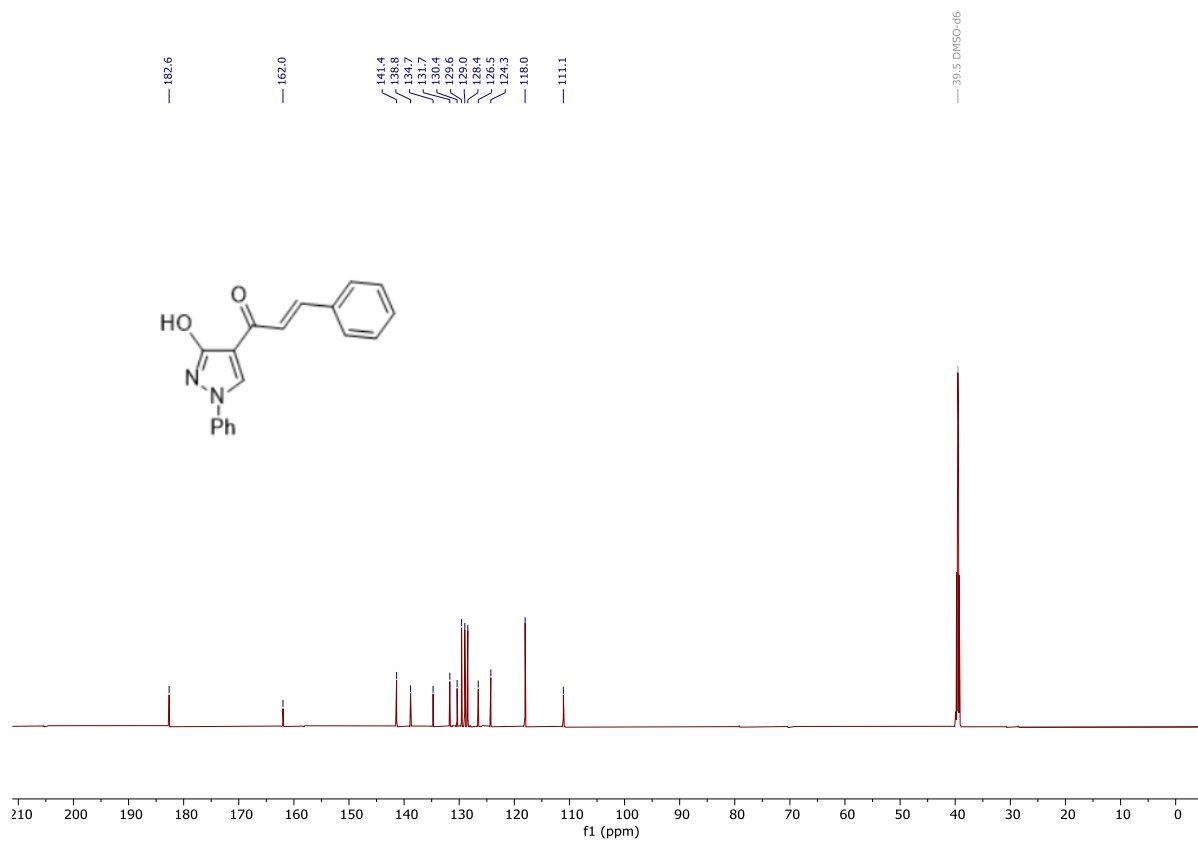
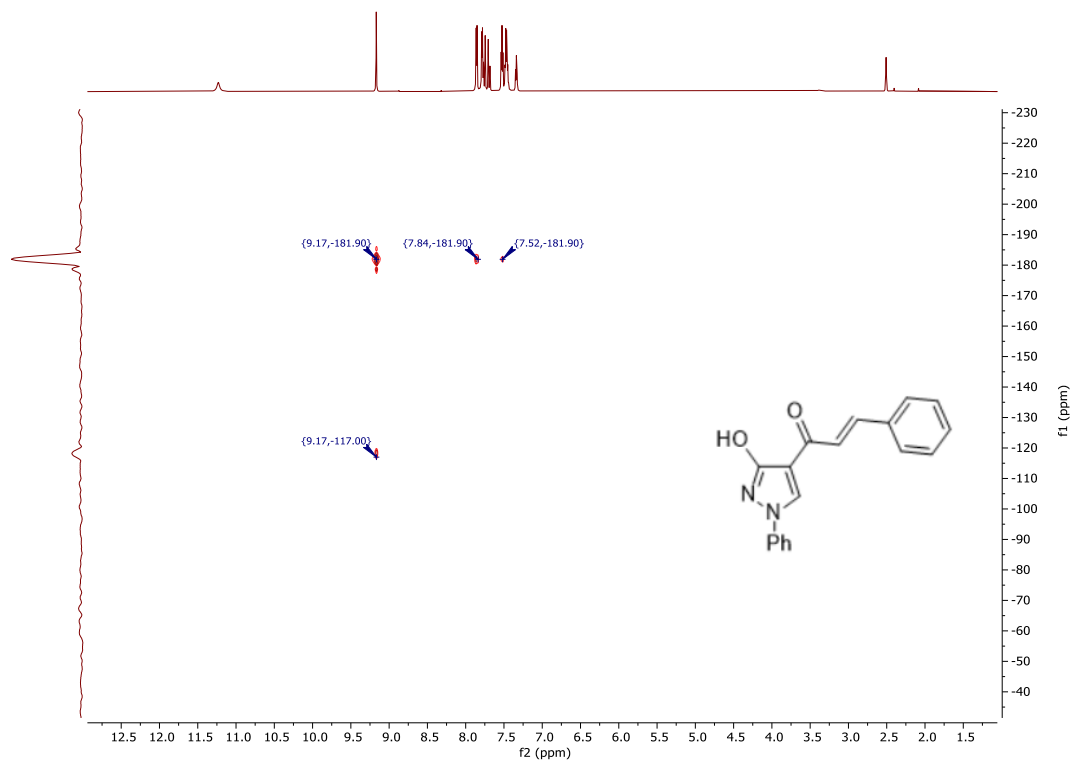


Figure S60. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-phenylprop-2-en-1-one (8a) <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)



**Figure S61.** (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-phenylprop-2-en-1-one (8a). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



**Figure S62.** (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-phenylprop-2-en-1-one (8a). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, DMSO-*d*<sub>6</sub>)

+MS, 8.2min #492

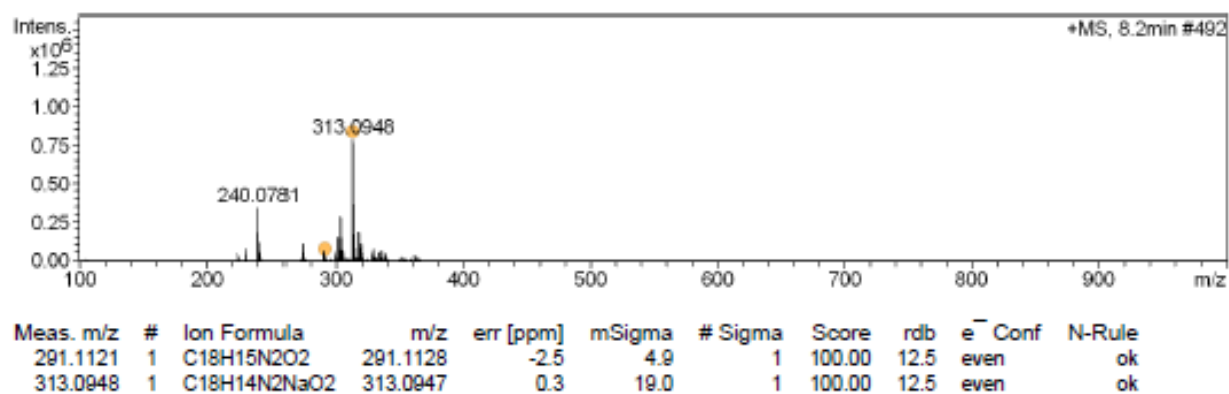


Figure S63. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-phenylprop-2-en-1-one (8a). HRMS (ESI-TOF).

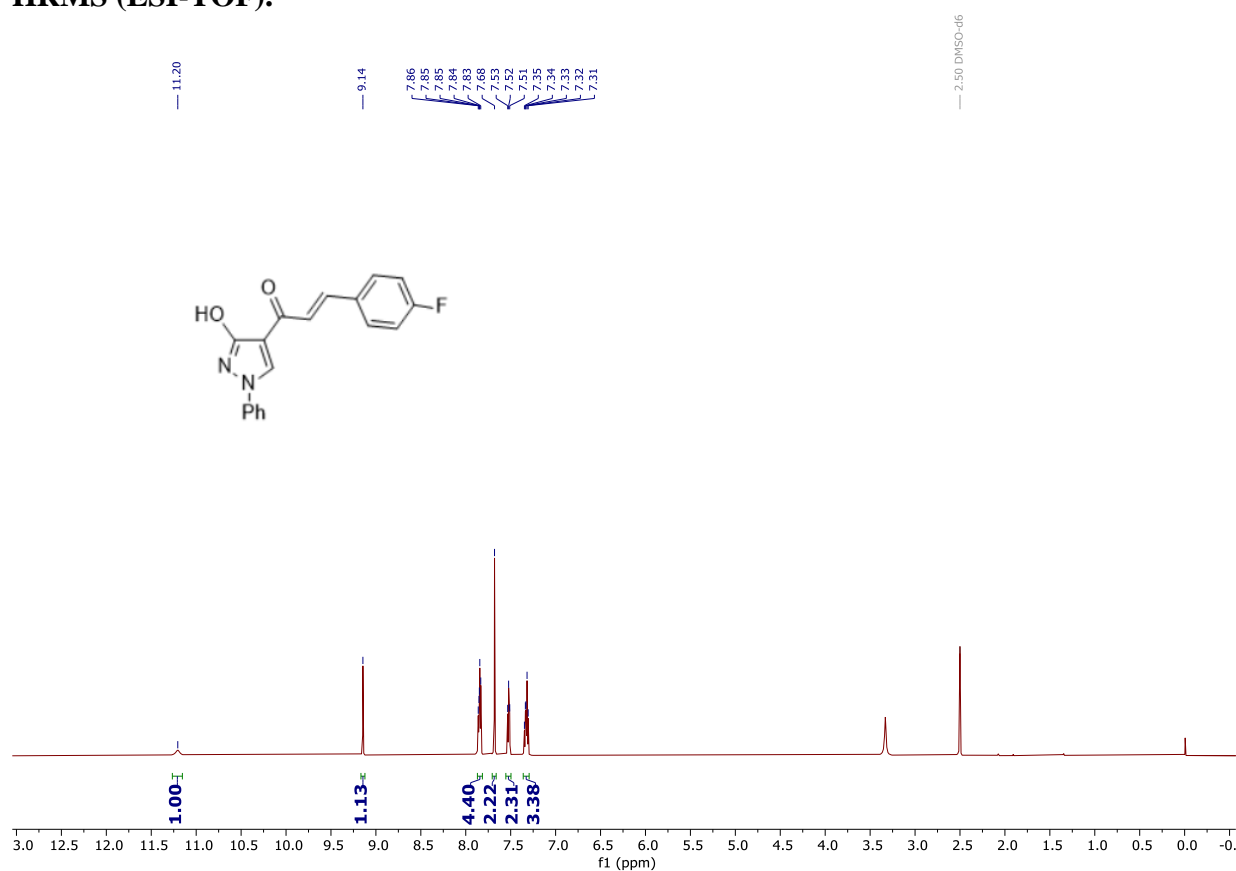
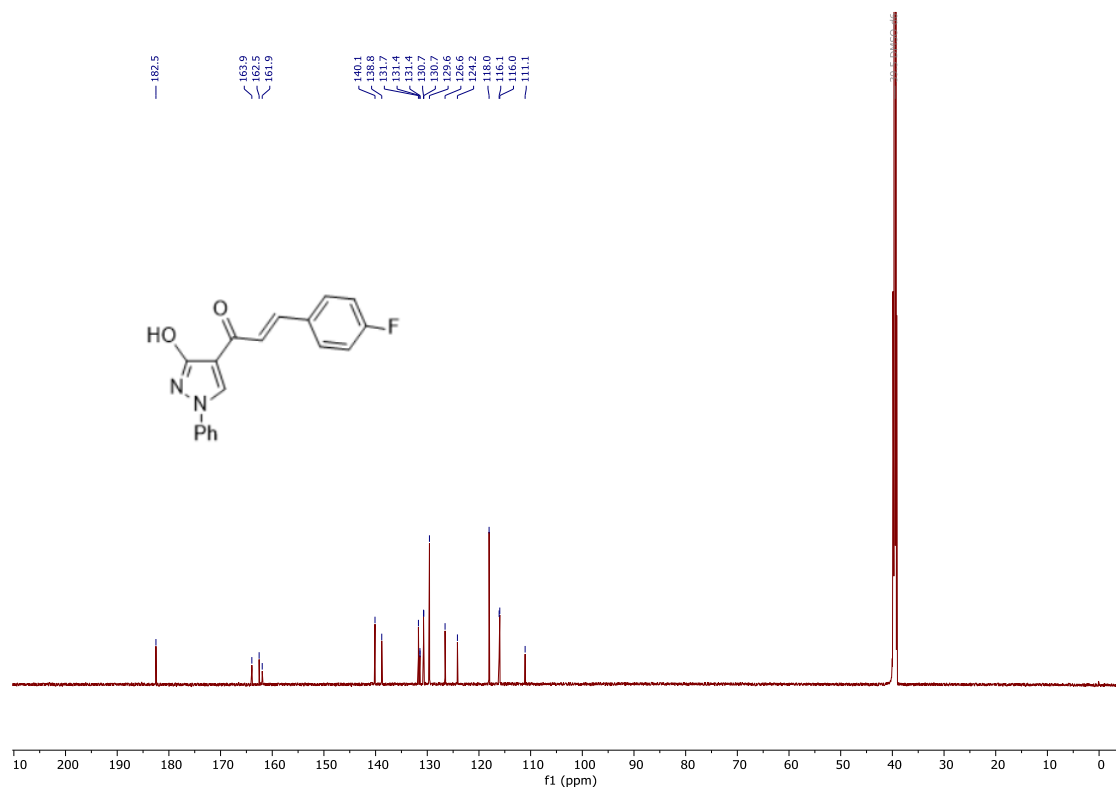
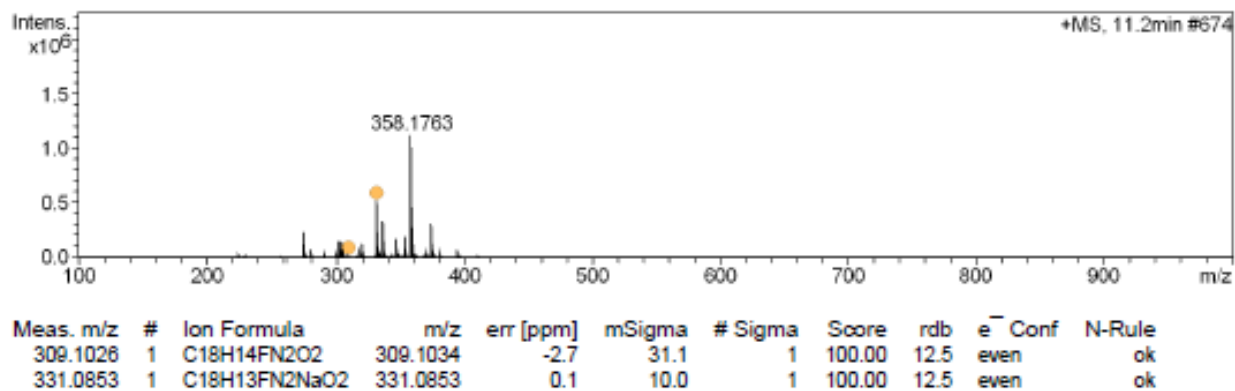


Figure S64. (2*E*)-3-(4-Fluorophenyl)-1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (8b). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)

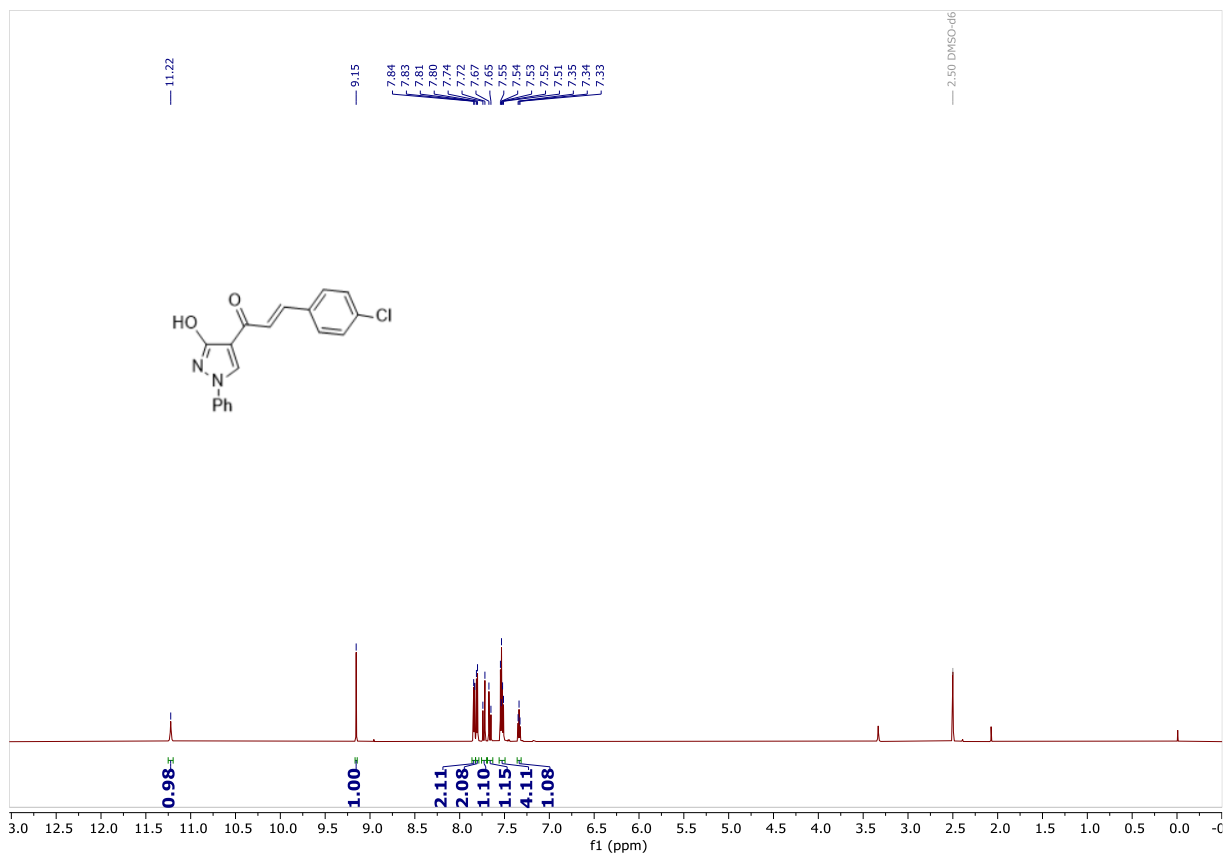


**Figure S65.** (2*E*)-3-(4-Fluorophenyl)-1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (8b). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)

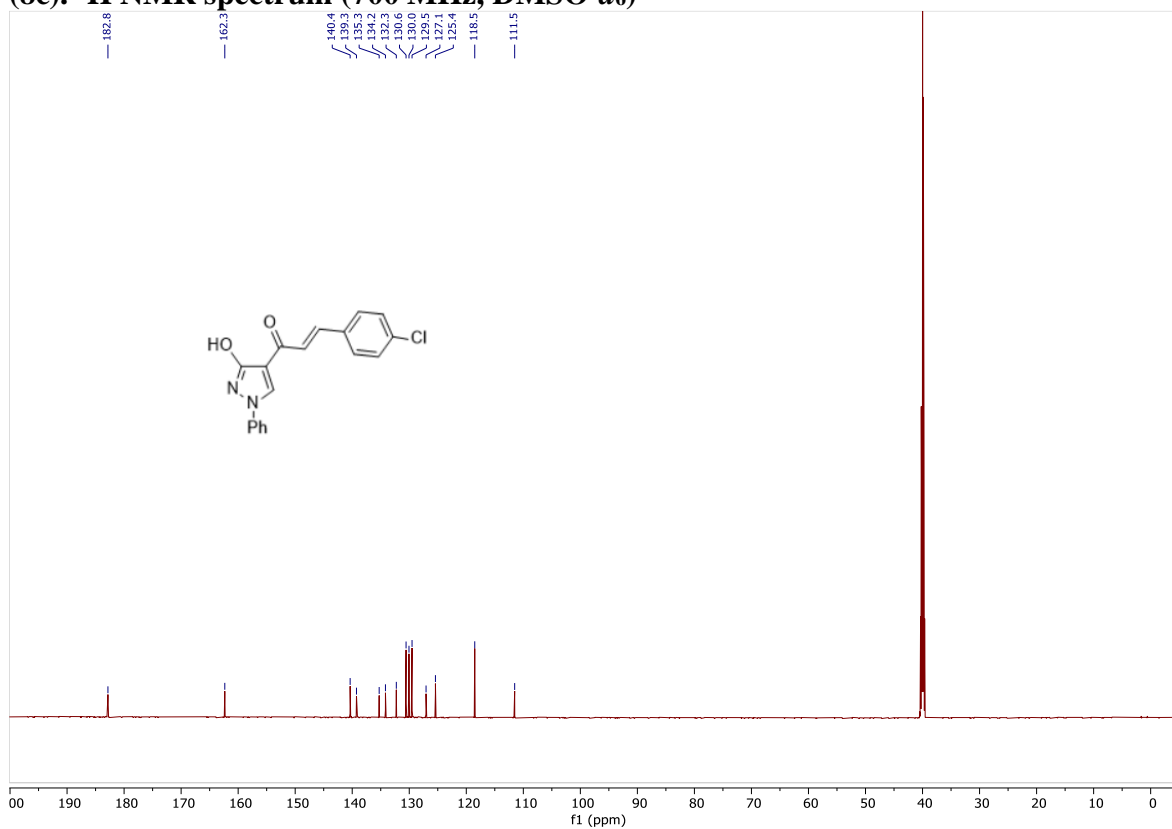
**+MS, 11.2min #674**



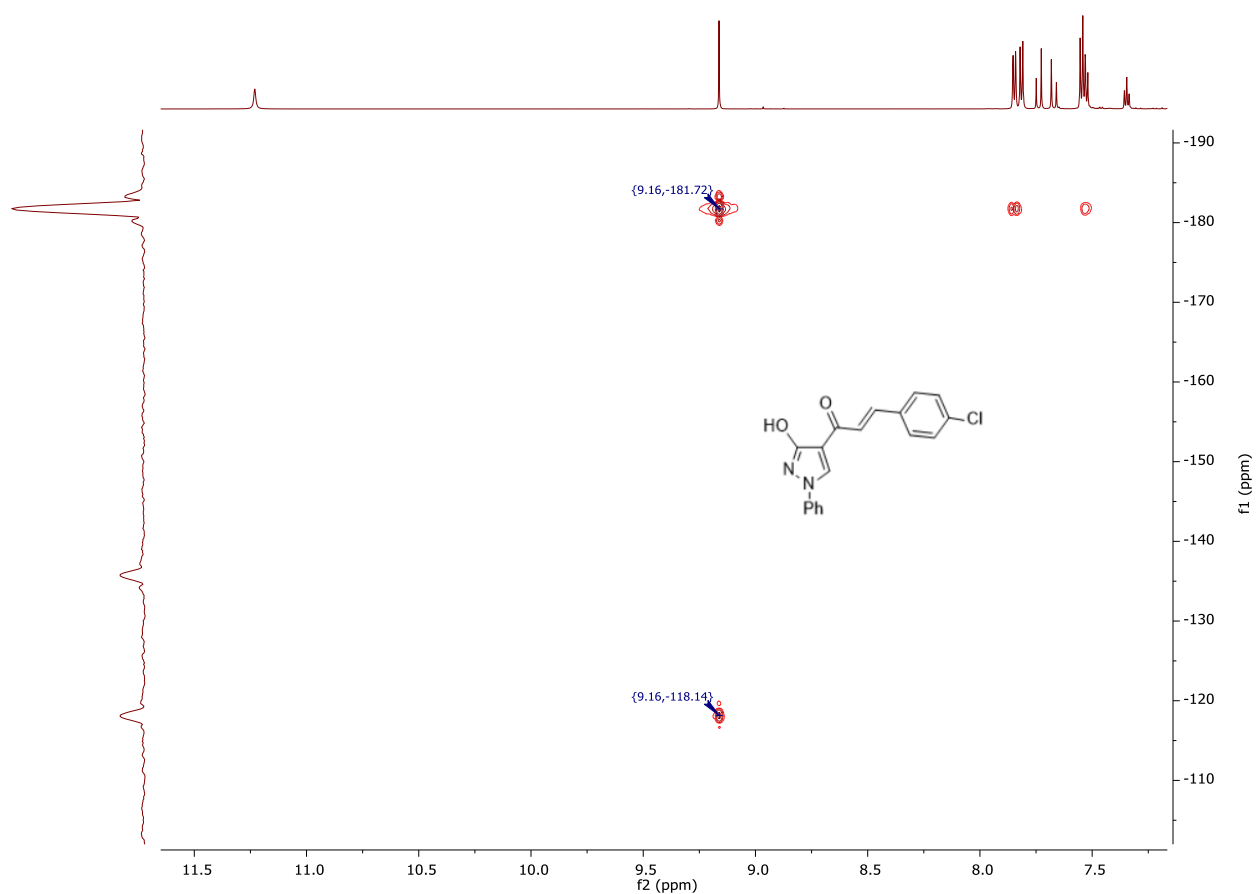
**Figure S66.** (2*E*)-3-(4-Fluorophenyl)-1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (8b). HRMS (ESI-TOF).



**Figure S67.** (2*E*)-3-(4-Chlorophenyl)-1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (8c). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)

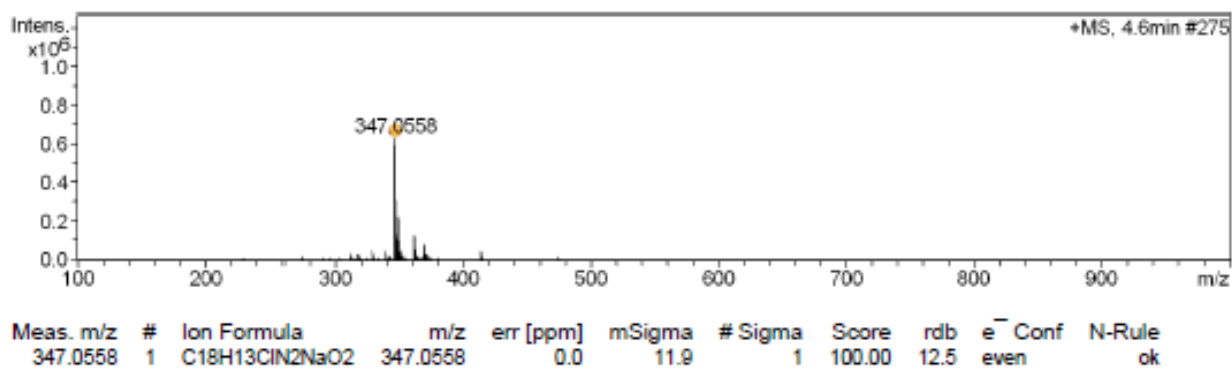


**Figure S68.** (2*E*)-3-(4-Chlorophenyl)-1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (8c). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



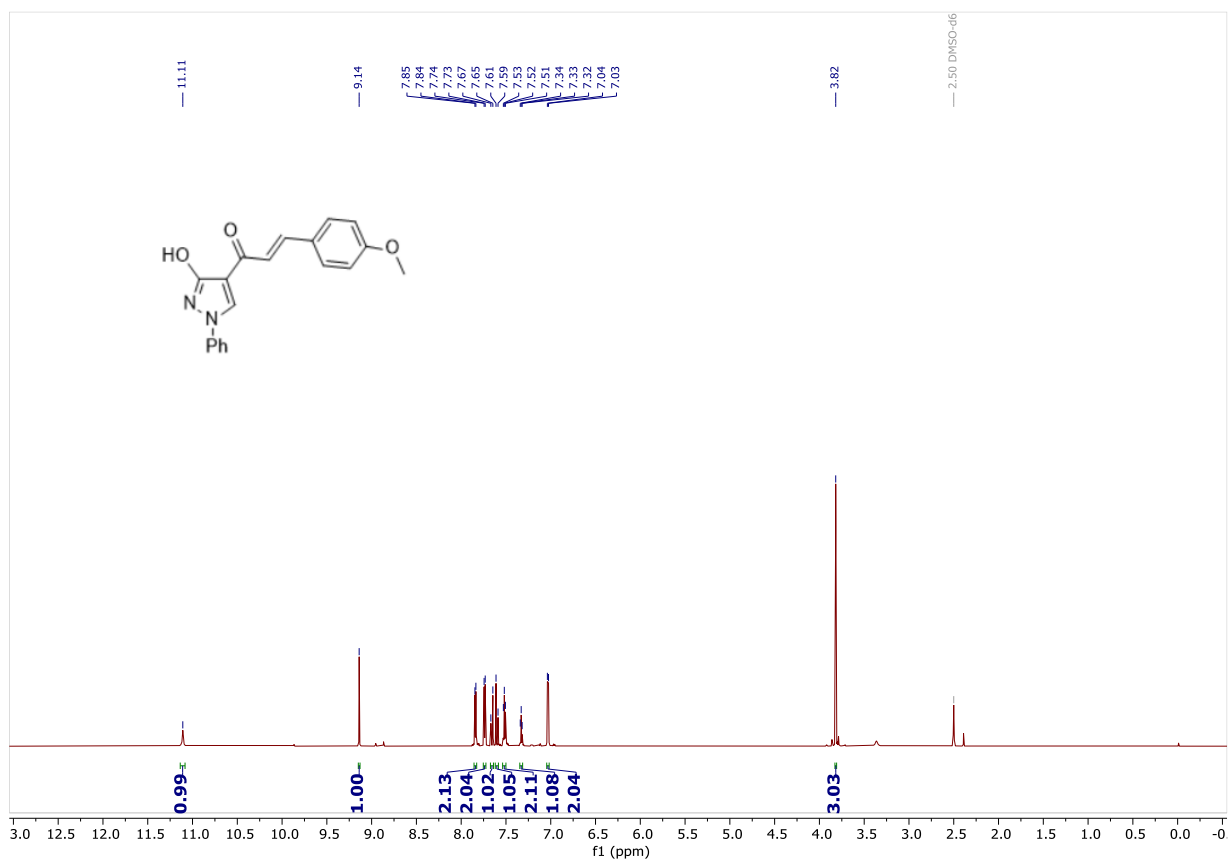
**Figure S69.** (E)-3-(4-Chlorophenyl)-1-(3-hydroxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (8c).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{DMSO}-d_6$ )

**+MS, 4.6min #275**

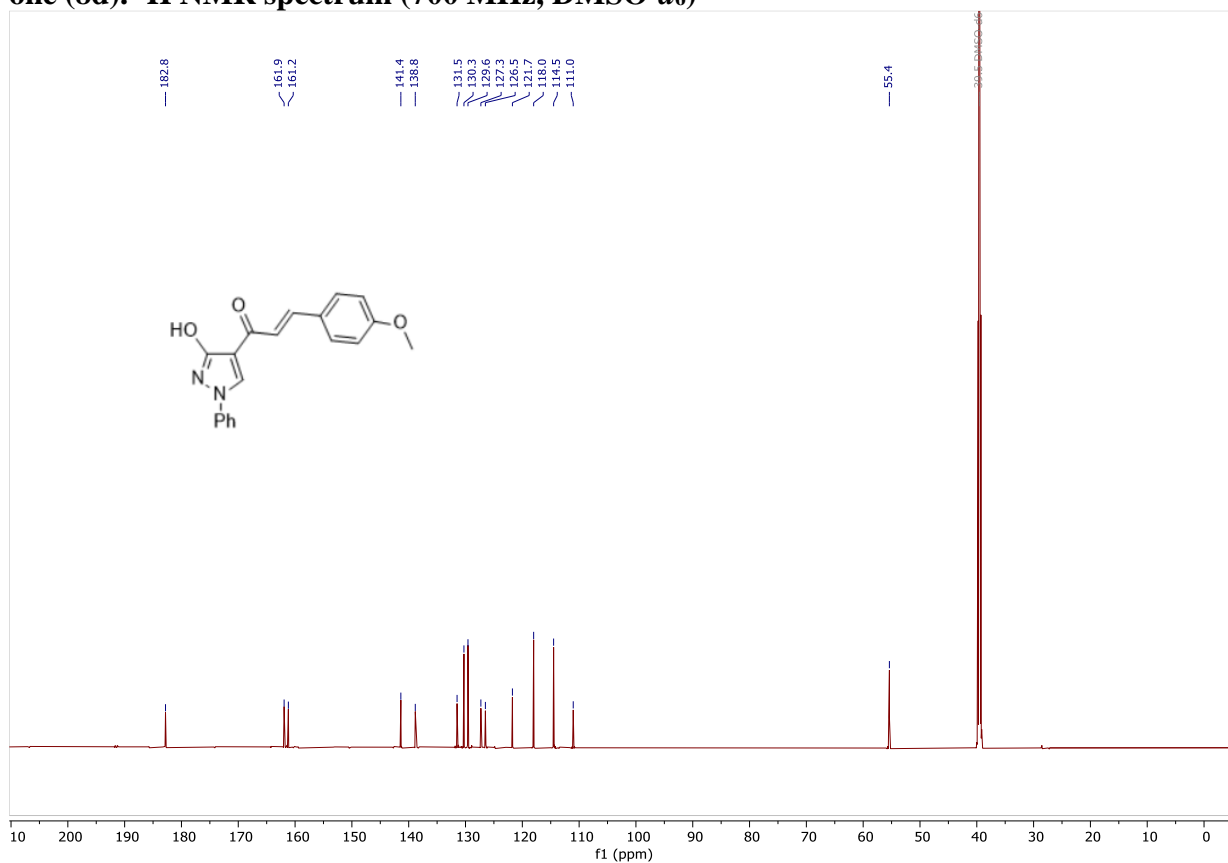


**Figure S70.** (E)-3-(4-Chlorophenyl)-1-(3-hydroxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (8c). HRMS (ESI-TOF).

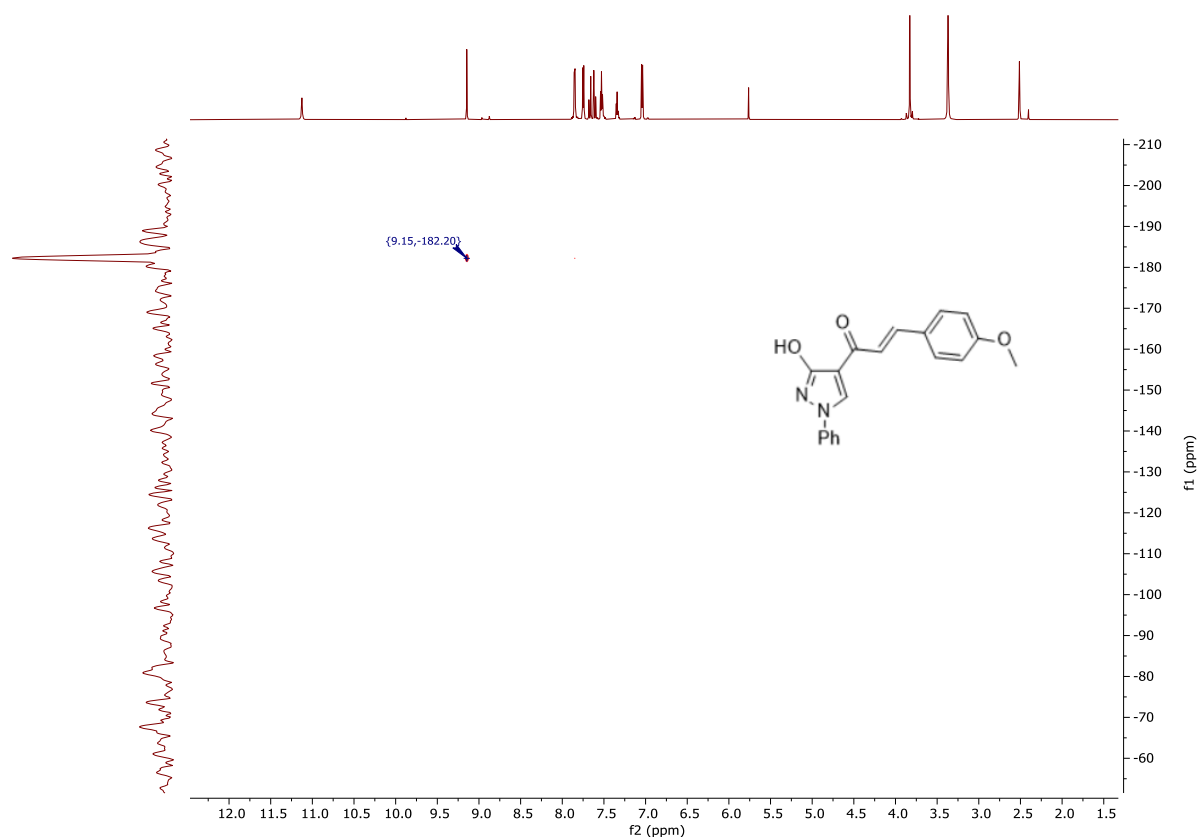




**Figure S71.** (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (8d). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)

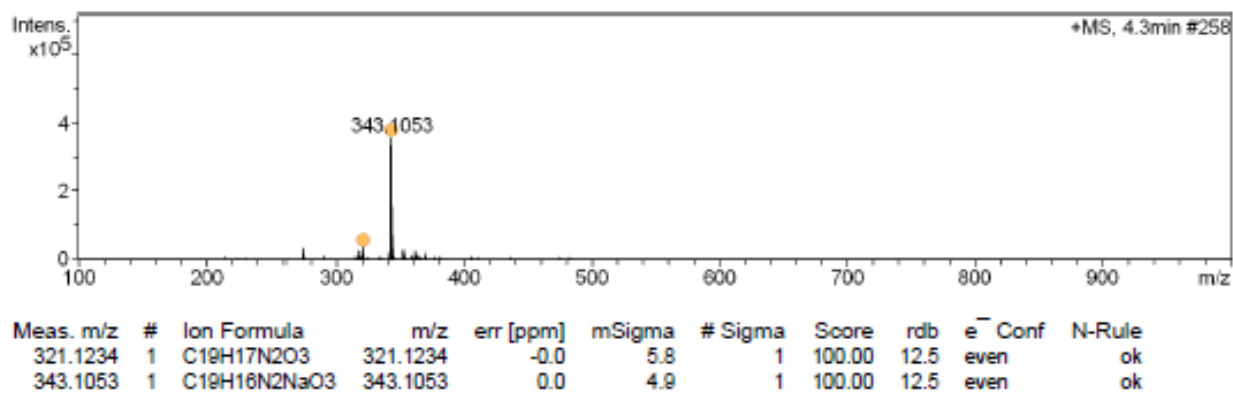


**Figure S72.** (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (8d). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)

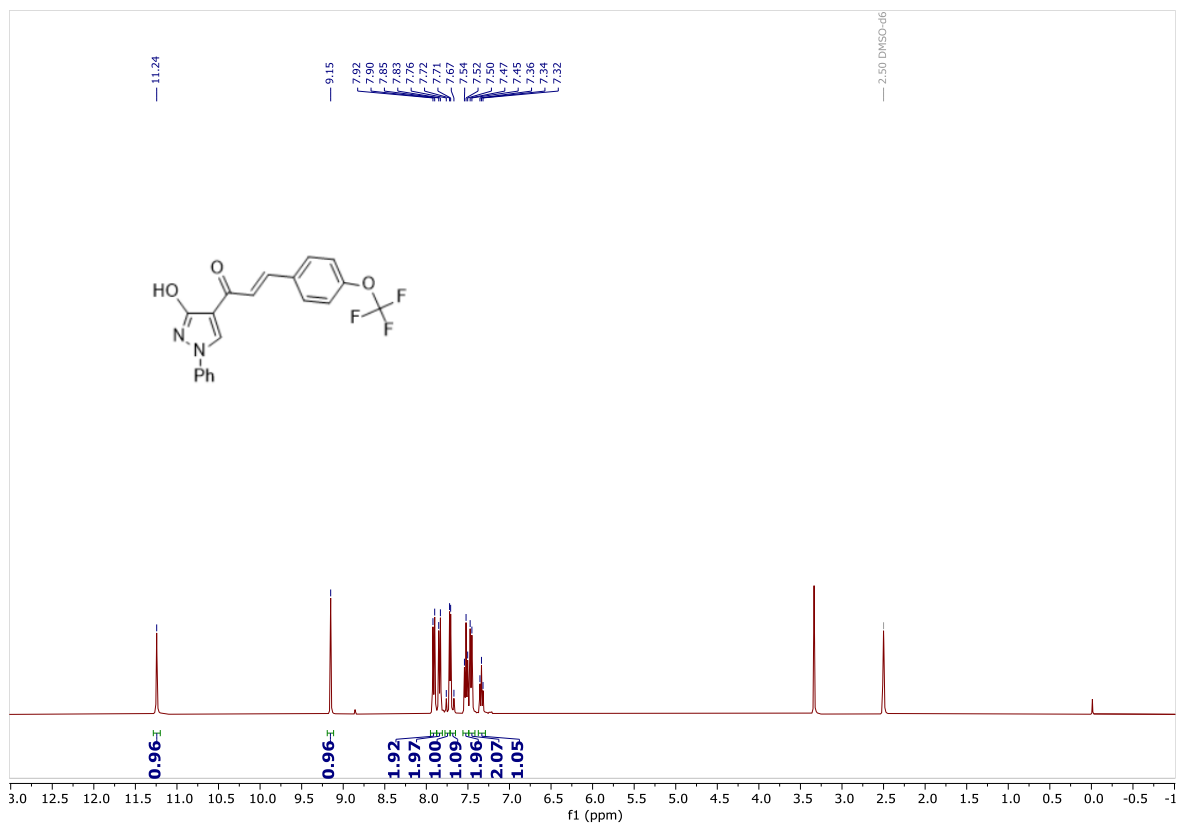


**Figure S73.** (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (8d).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{DMSO}-d_6$ )

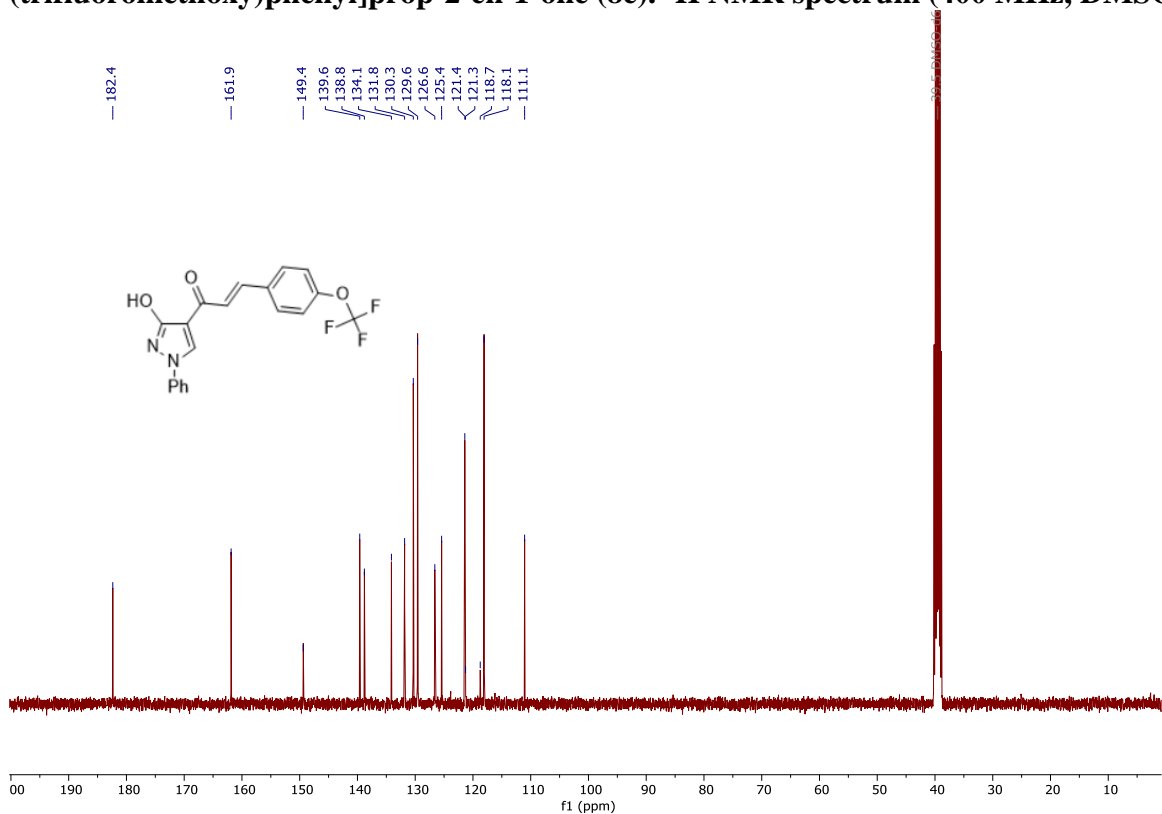
**+MS, 4.3min #258**



**Figure S74.** (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (8d). HRMS (ESI-TOF).



**Figure S75.** (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (8e). <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>)



**Figure S76.** (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (8e). <sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>)

+MS, 4.6min #273

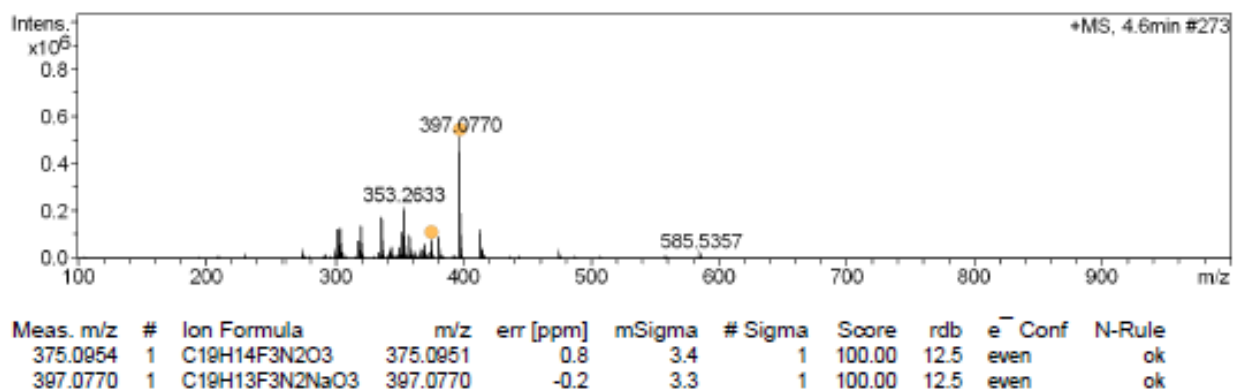


Figure S77. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (8e). HRMS (ESI-TOF).

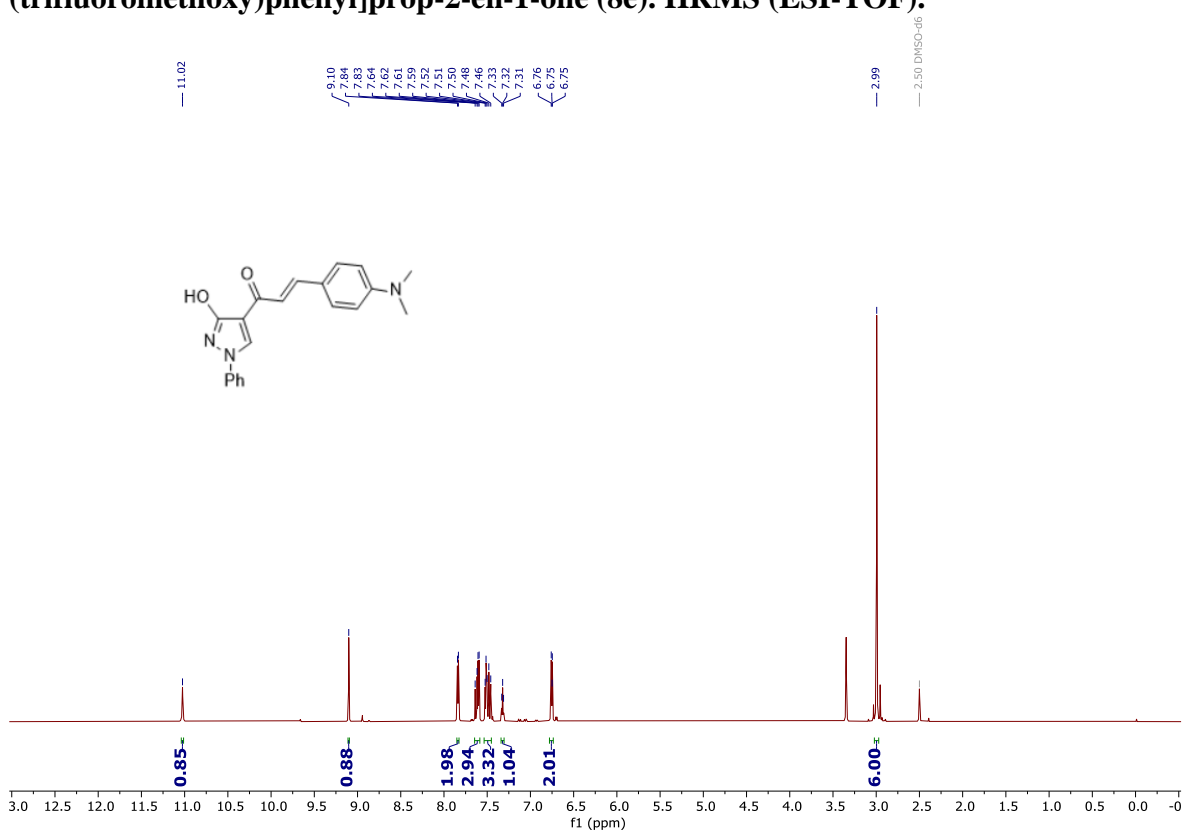
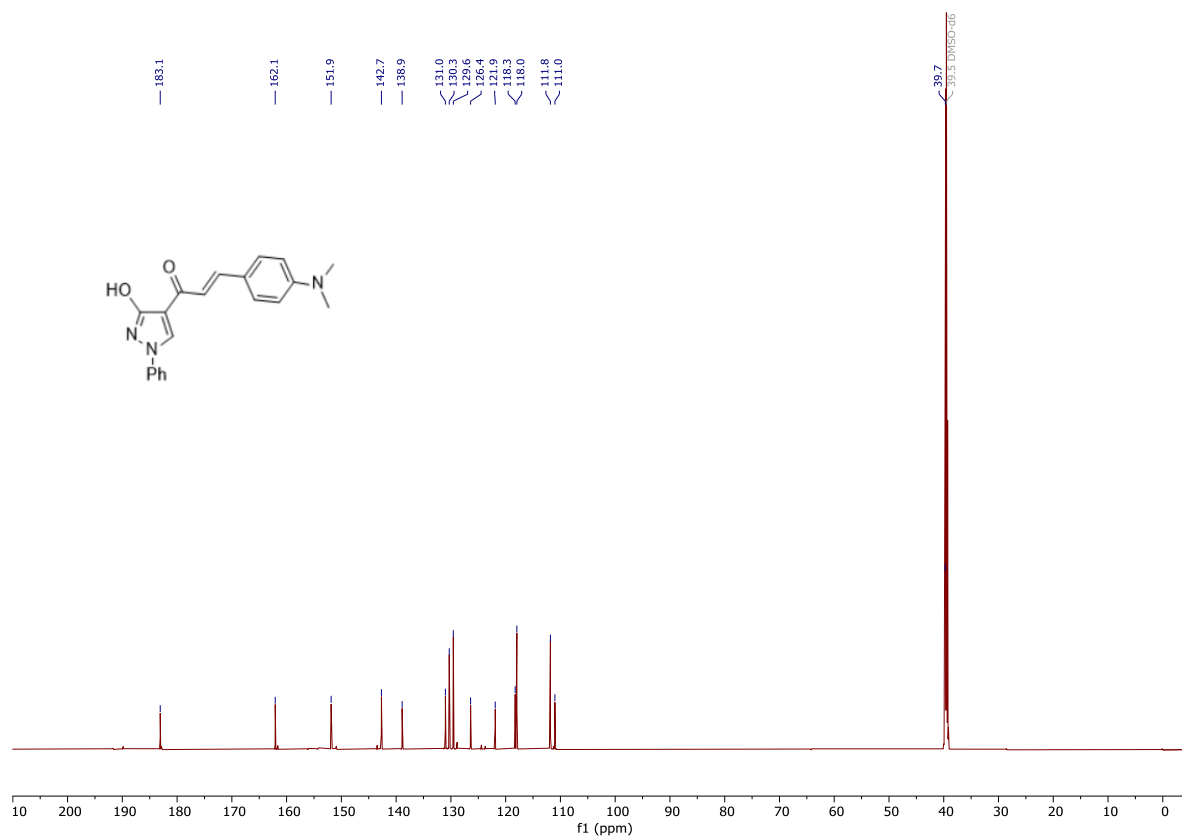
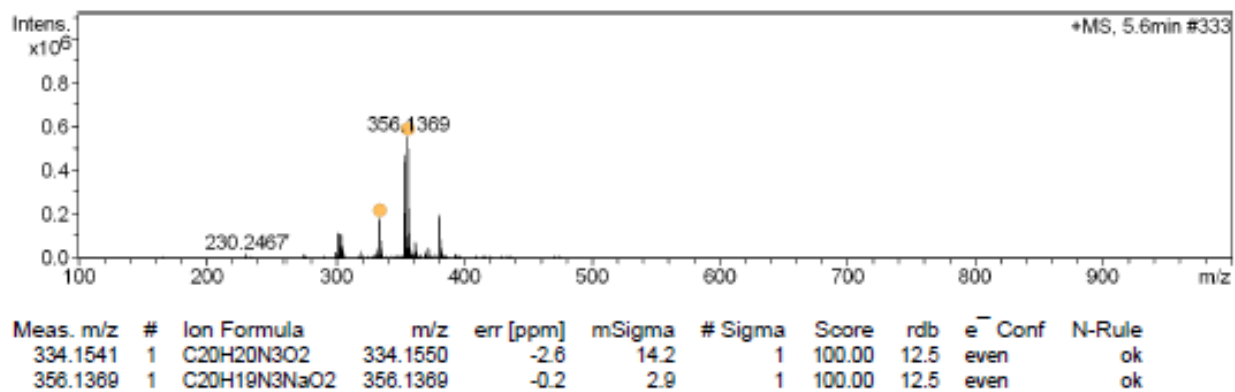


Figure S78. (2*E*)-3-[4-(Dimethylamino)phenyl]-1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (8f). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)

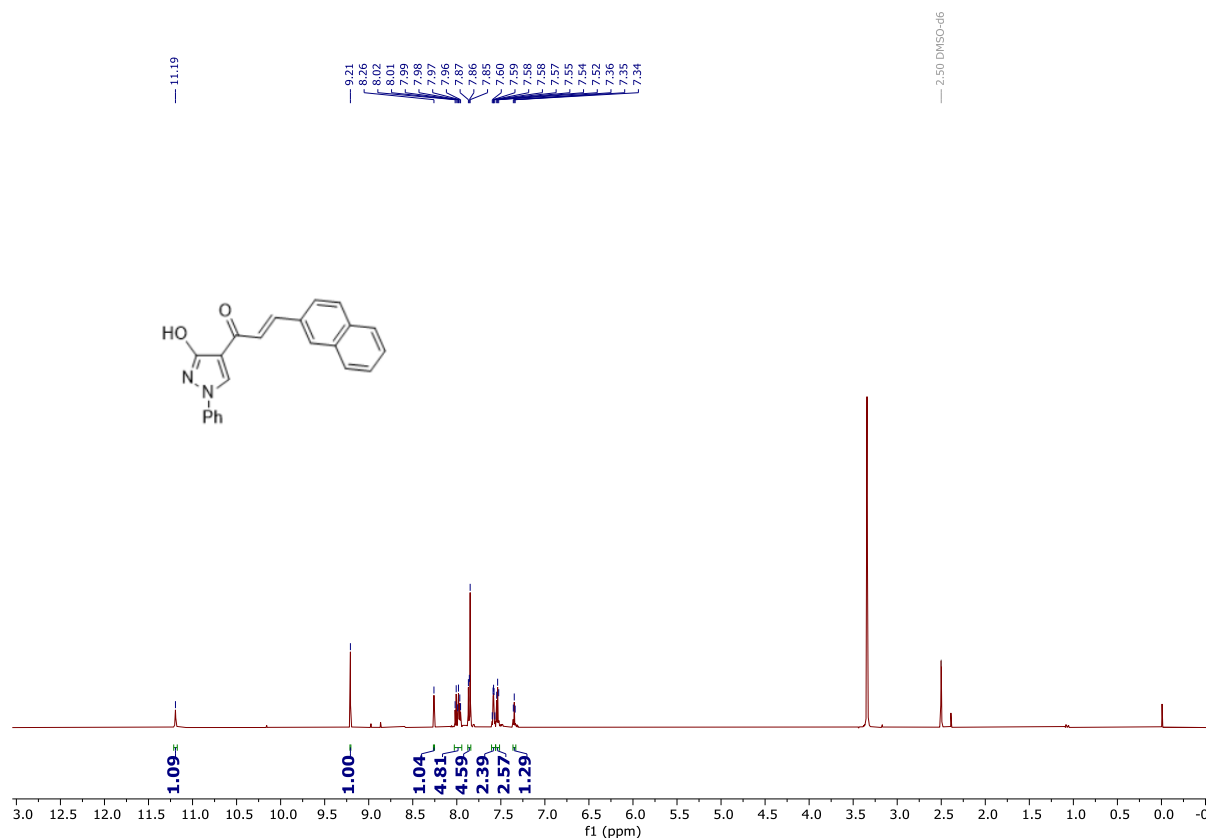


**Figure S79.** (2E)-3-[4-(Dimethylamino)phenyl]-1-(3-hydroxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (8f). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)

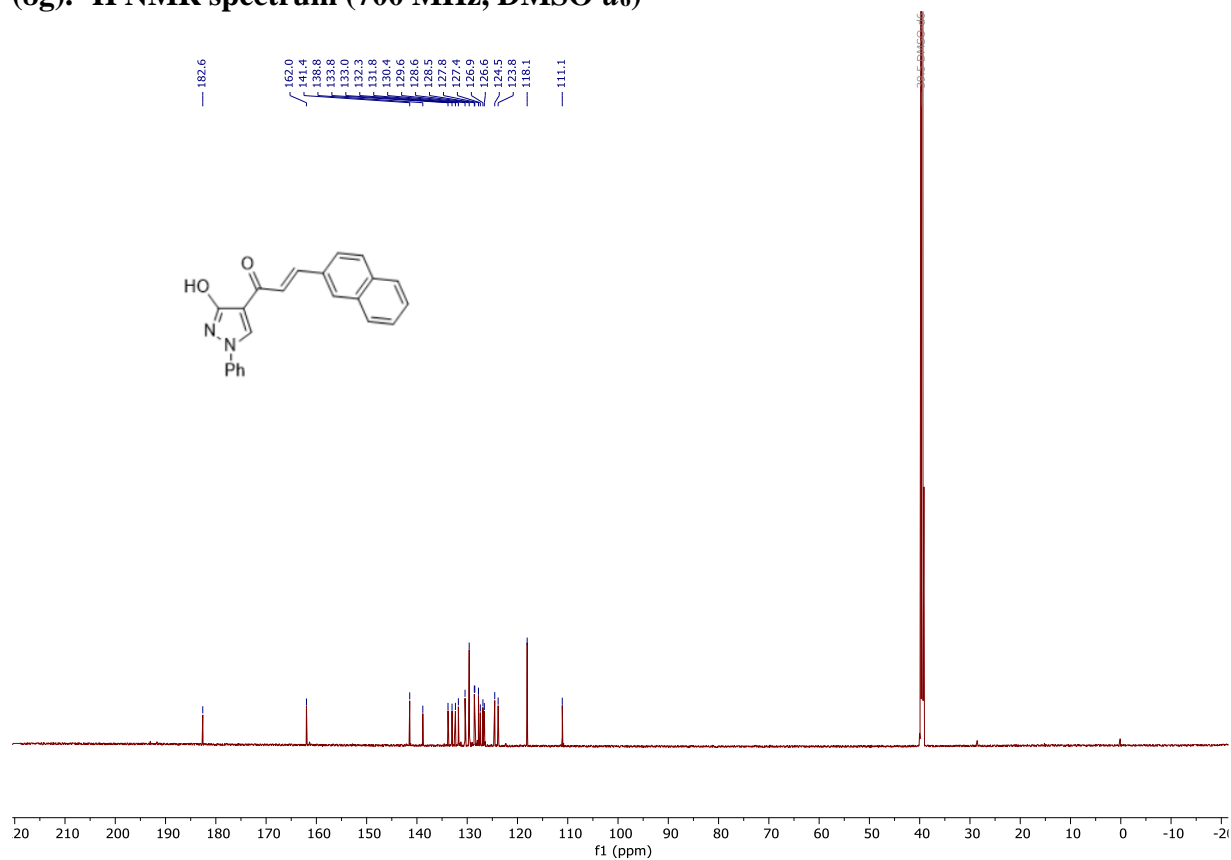
**+MS, 5.6min #333**



**Figure S80.** (2E)-3-[4-(Dimethylamino)phenyl]-1-(3-hydroxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (8f). HRMS (ESI-TOF).



**Figure S81. (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(naphthalen-2-yl)prop-2-en-1-one (8g). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)**



**Figure S82. (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(naphthalen-2-yl)prop-2-en-1-one (8g). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)**

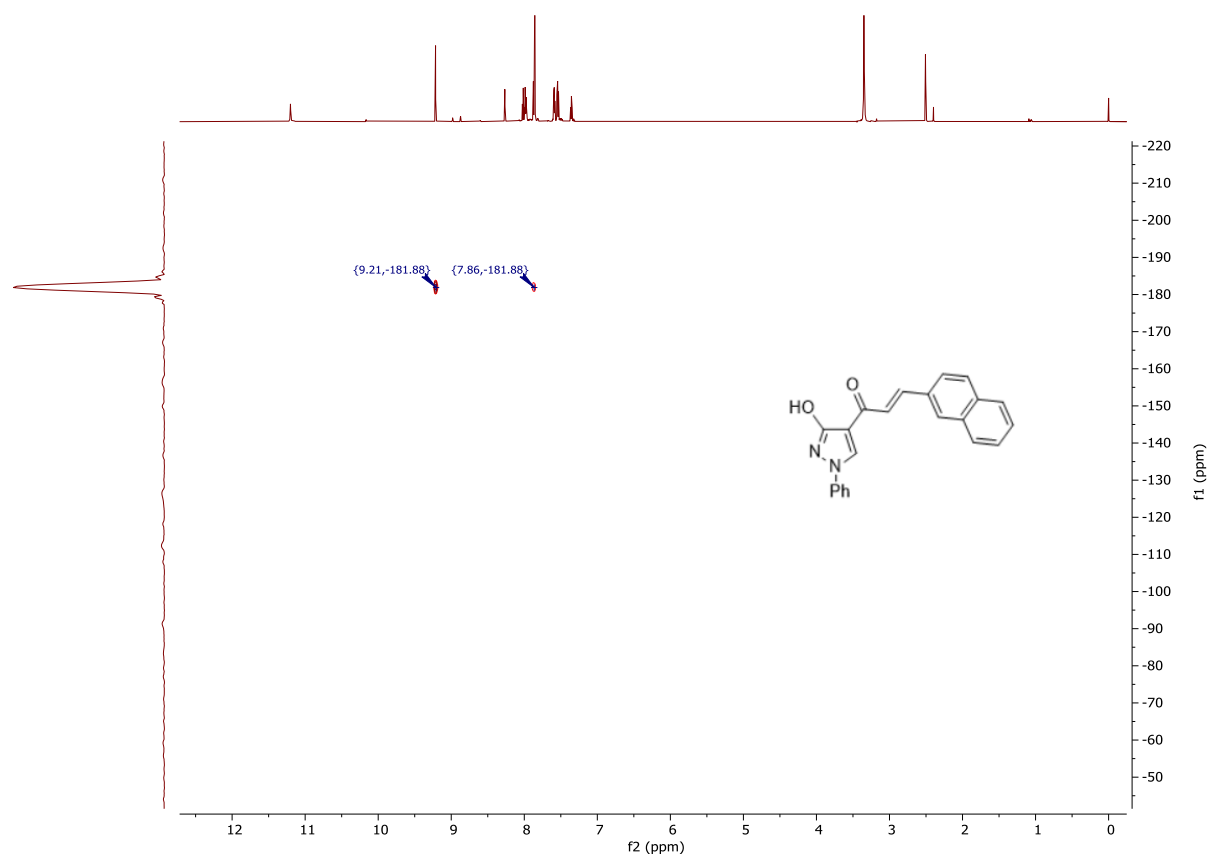
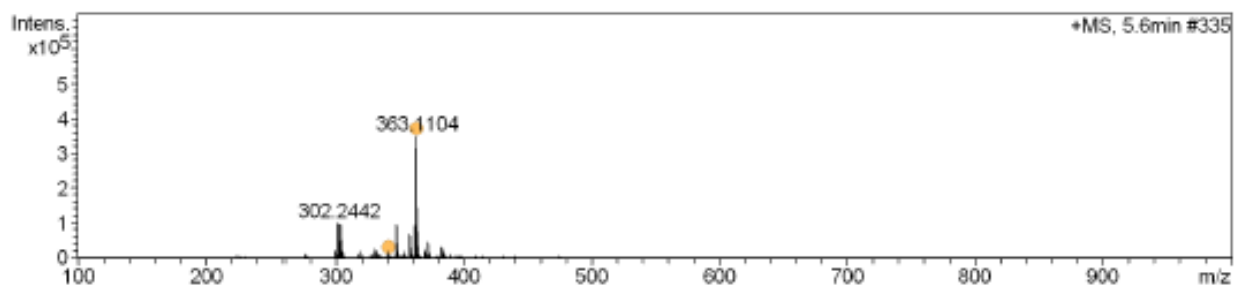


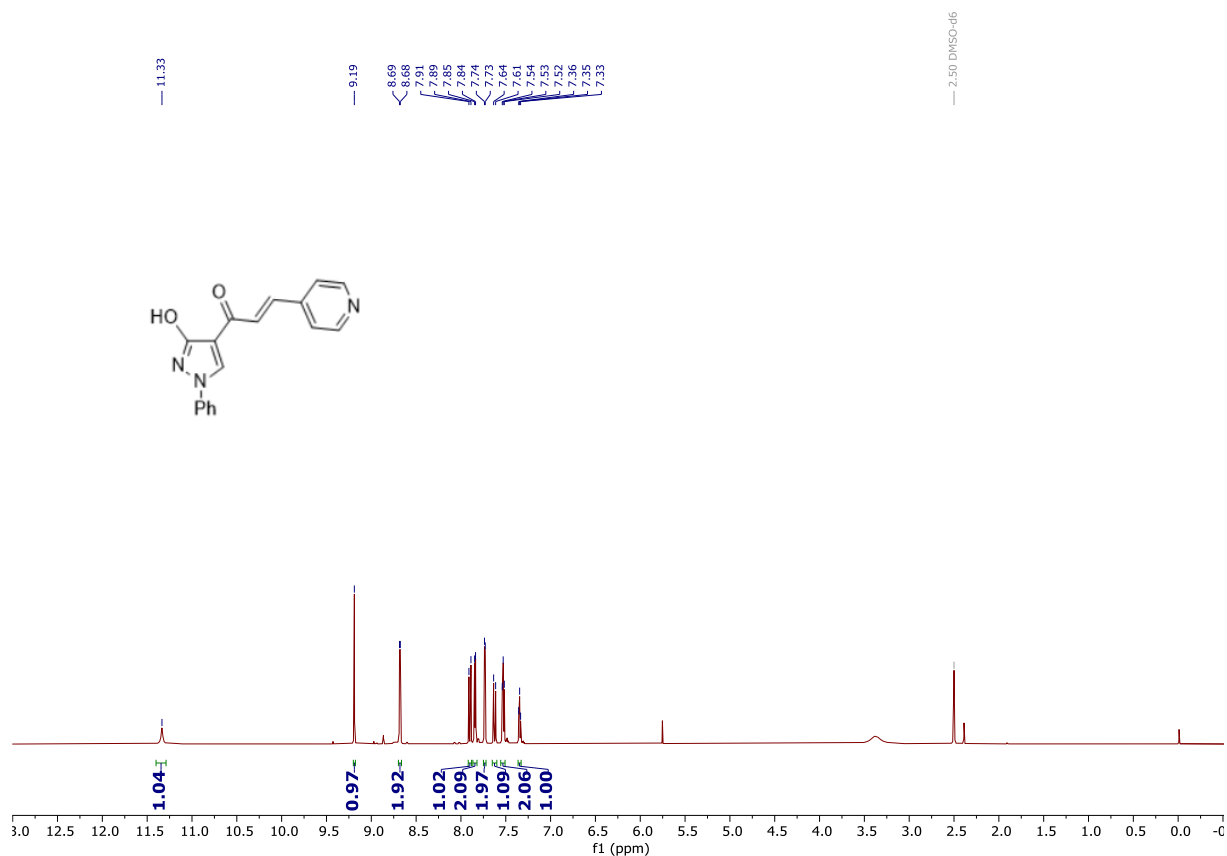
Figure S83. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(naphthalen-2-yl)prop-2-en-1-one (8g).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{DMSO}-d_6$ )

+MS, 5.6min #335



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup>	Conf	N-Rule
341.1282	1	C <sub>22</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	341.1285	0.9	37.1	1	100.00	15.5	even		ok
363.1104	1	C <sub>22</sub> H <sub>16</sub> N <sub>2</sub> NaO <sub>2</sub>	363.1104	-0.1	4.6	1	100.00	15.5	even		ok

Figure S84. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(naphthalen-2-yl)prop-2-en-1-one (8g). HRMS (ESI-TOF).





+MS, 8.0min #479

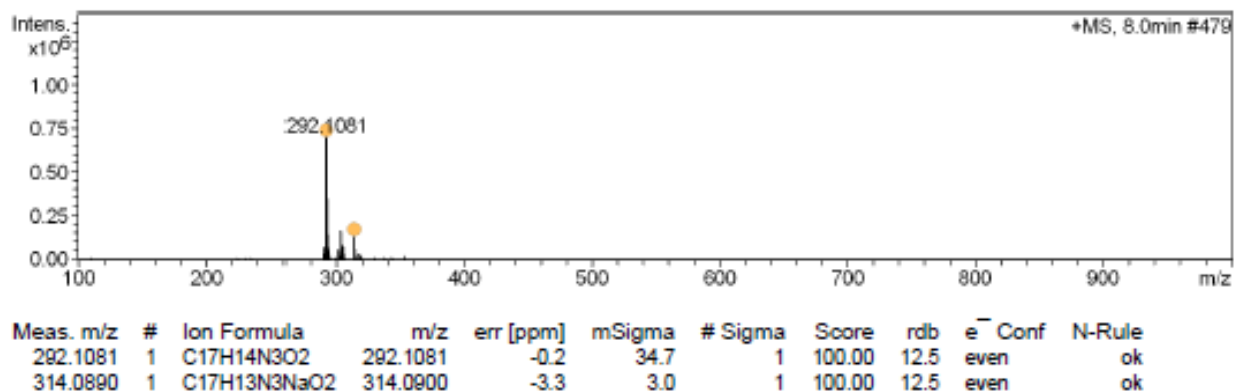


Figure S87. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(pyridin-4-yl)prop-2-en-1-one (8h). HRMS (ESI-TOF).

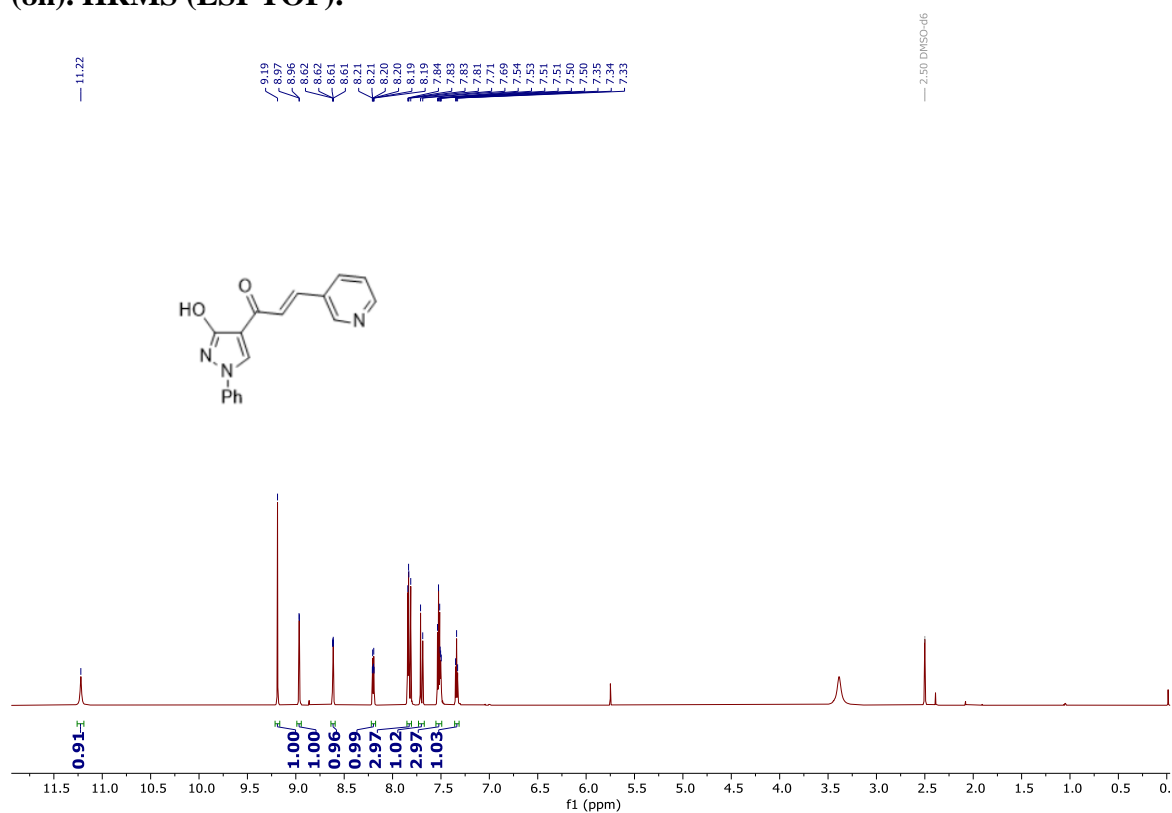
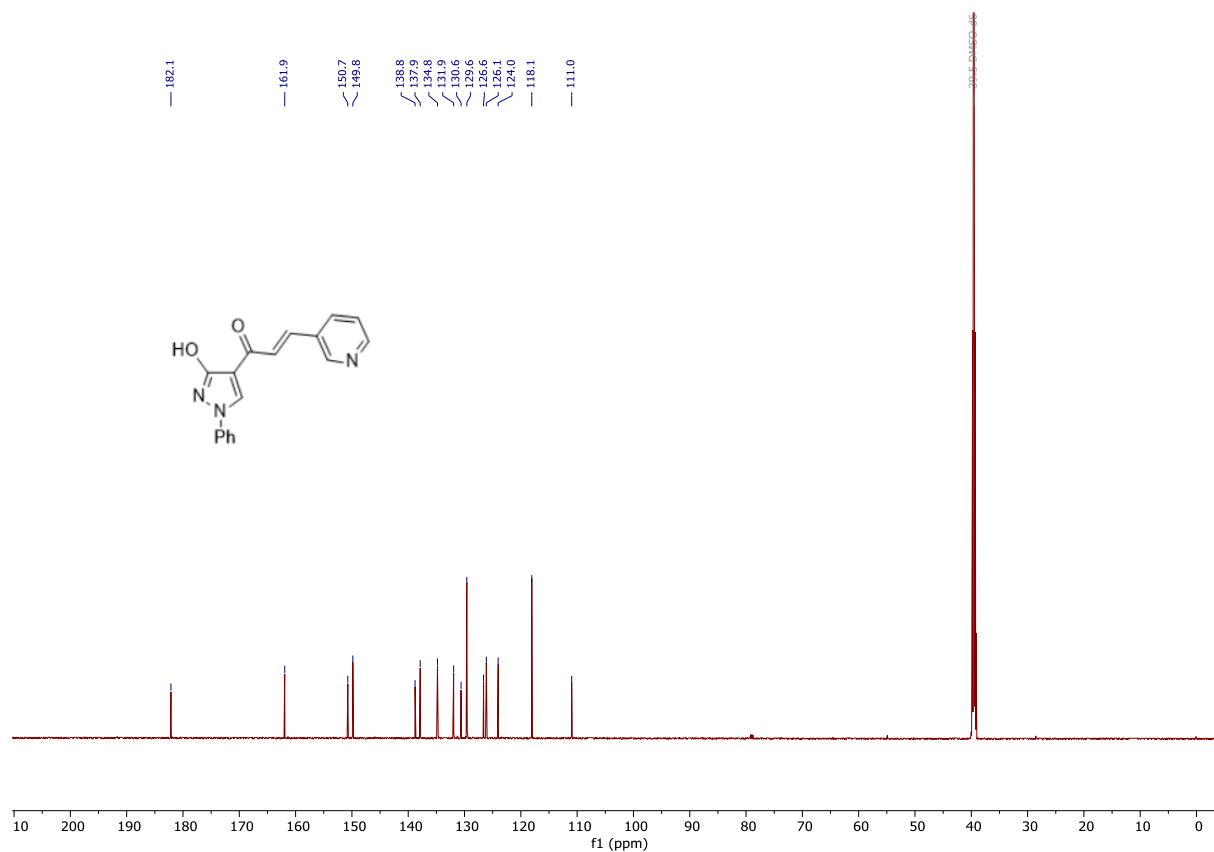
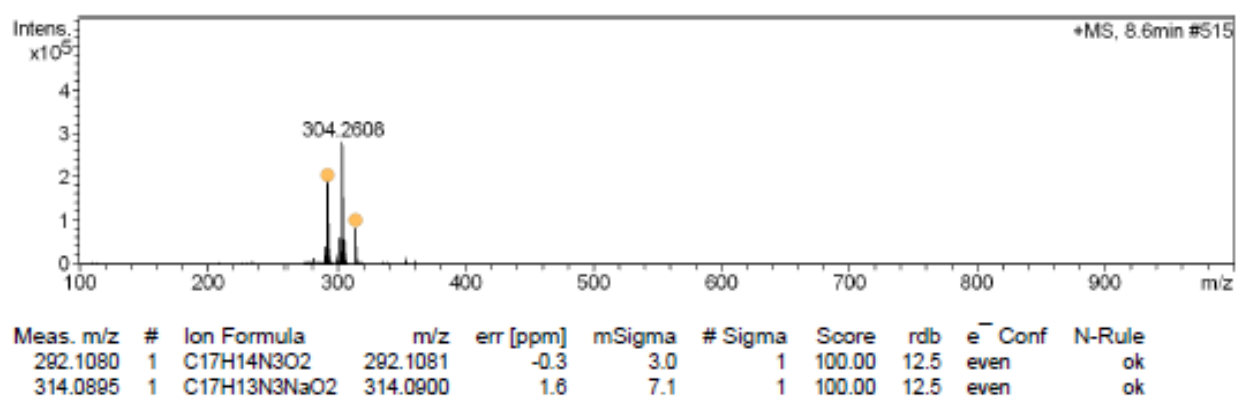


Figure S88. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(pyridin-3-yl)prop-2-en-1-one (8i). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)

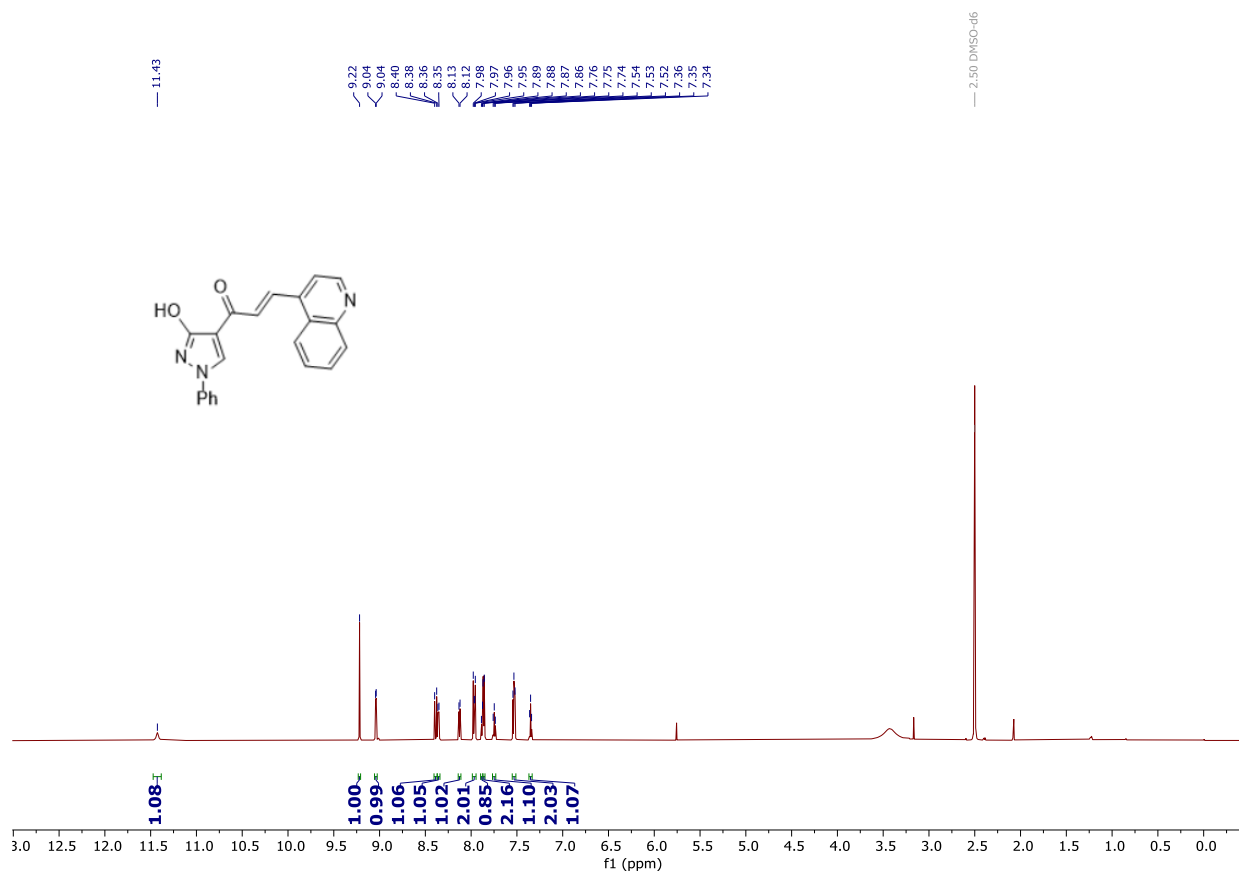


**Figure S89.** (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(pyridin-3-yl)prop-2-en-1-one (8i). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)

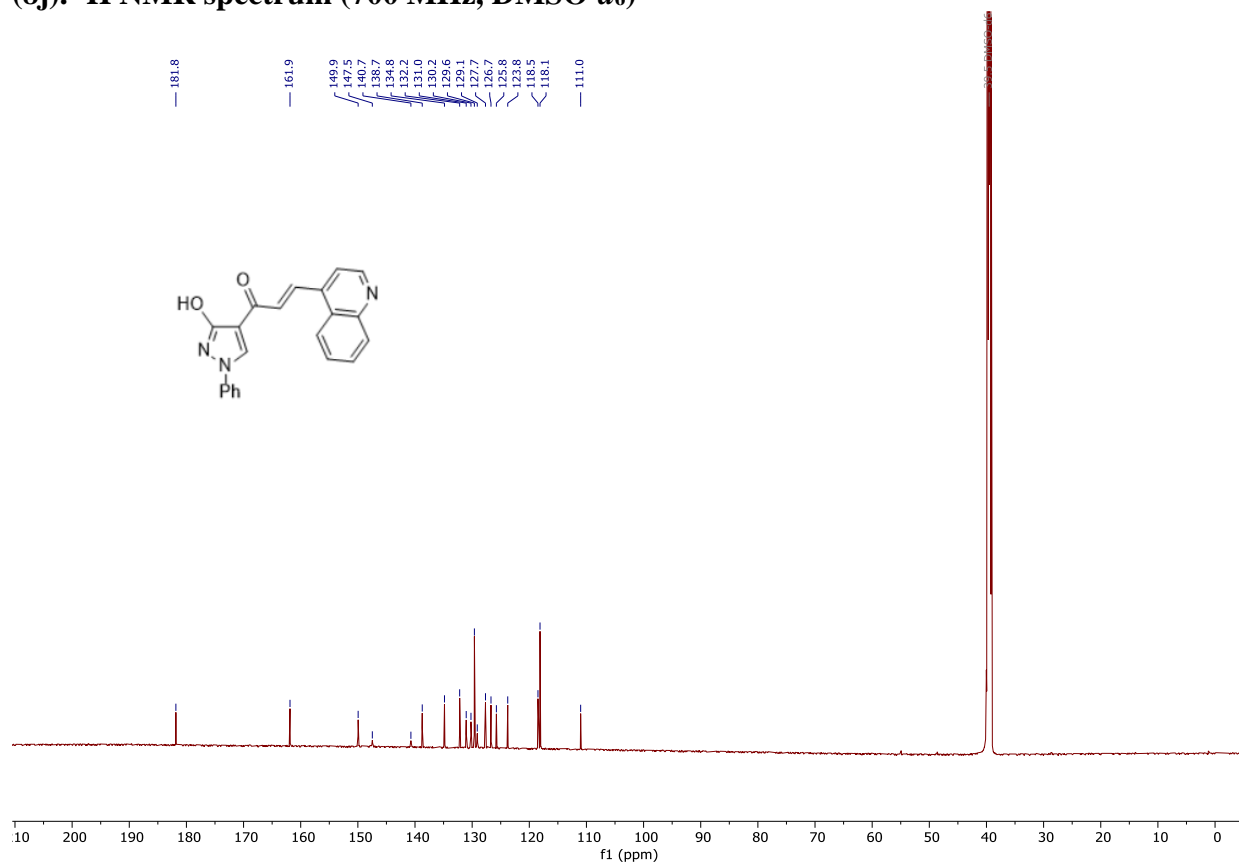
**+MS, 8.6min #515**



**Figure S90.** (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(pyridin-3-yl)prop-2-en-1-one (8i). HRMS (ESI-TOF).



**Figure S91.** (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(quinolin-4-yl)prop-2-en-1-one (8j). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)



**Figure S92.** (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(quinolin-4-yl)prop-2-en-1-one (8j). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)

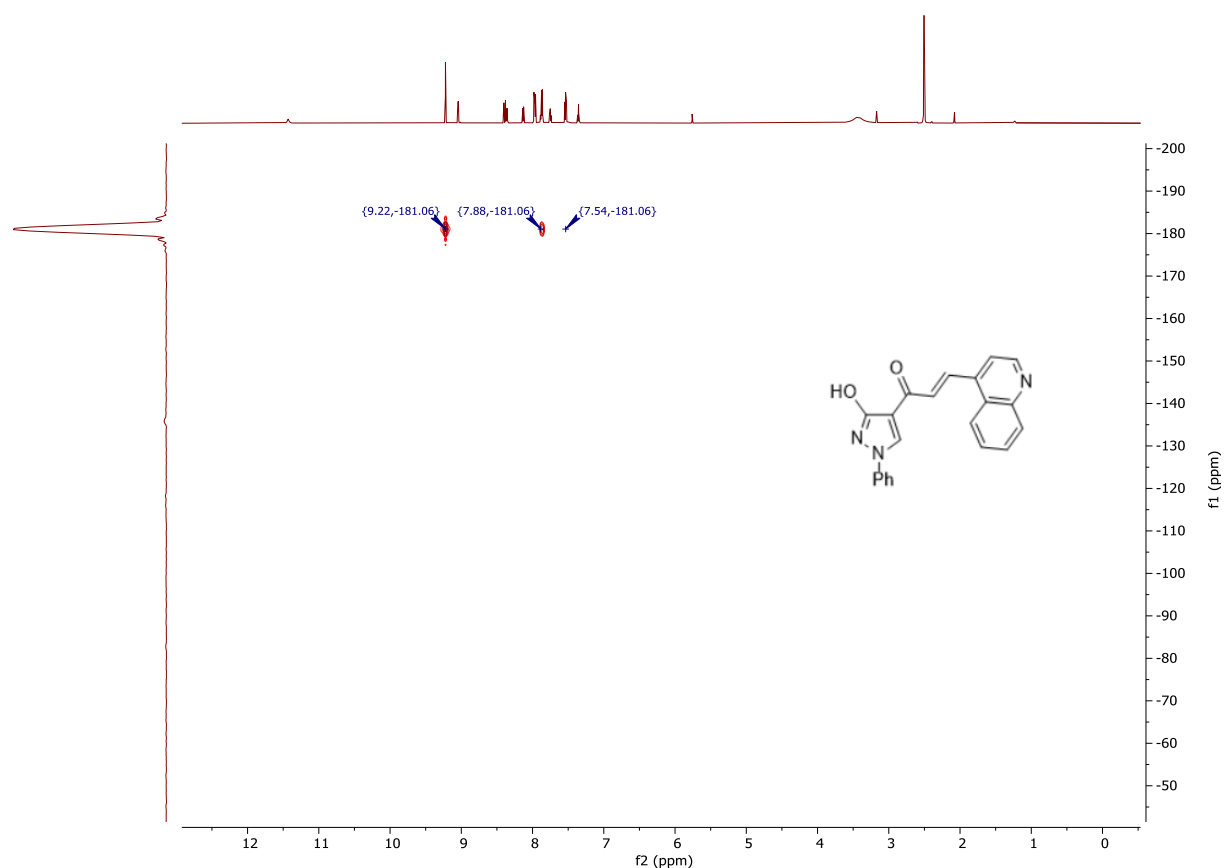


Figure S93. (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(quinolin-4-yl)prop-2-en-1-one (8j).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{DMSO}-d_6$ )

+MS, 3.5min #207

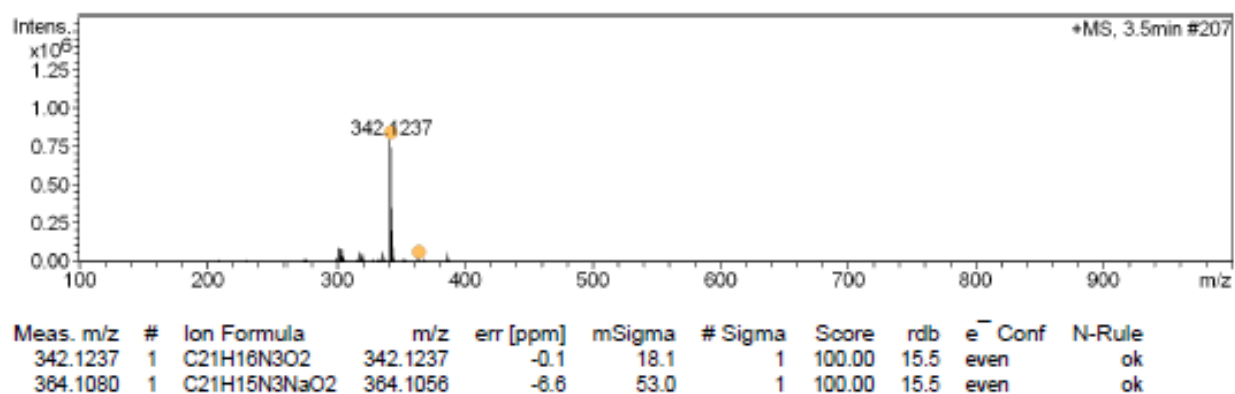
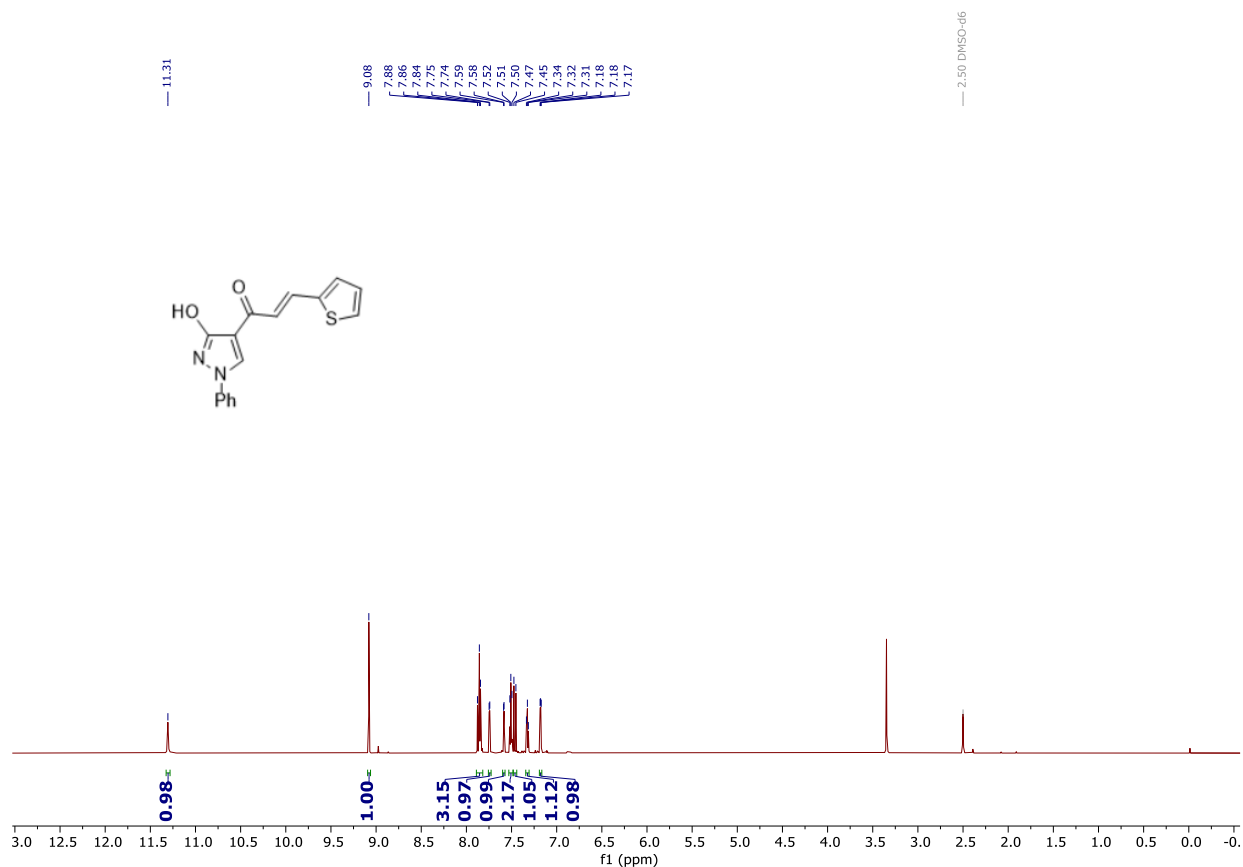
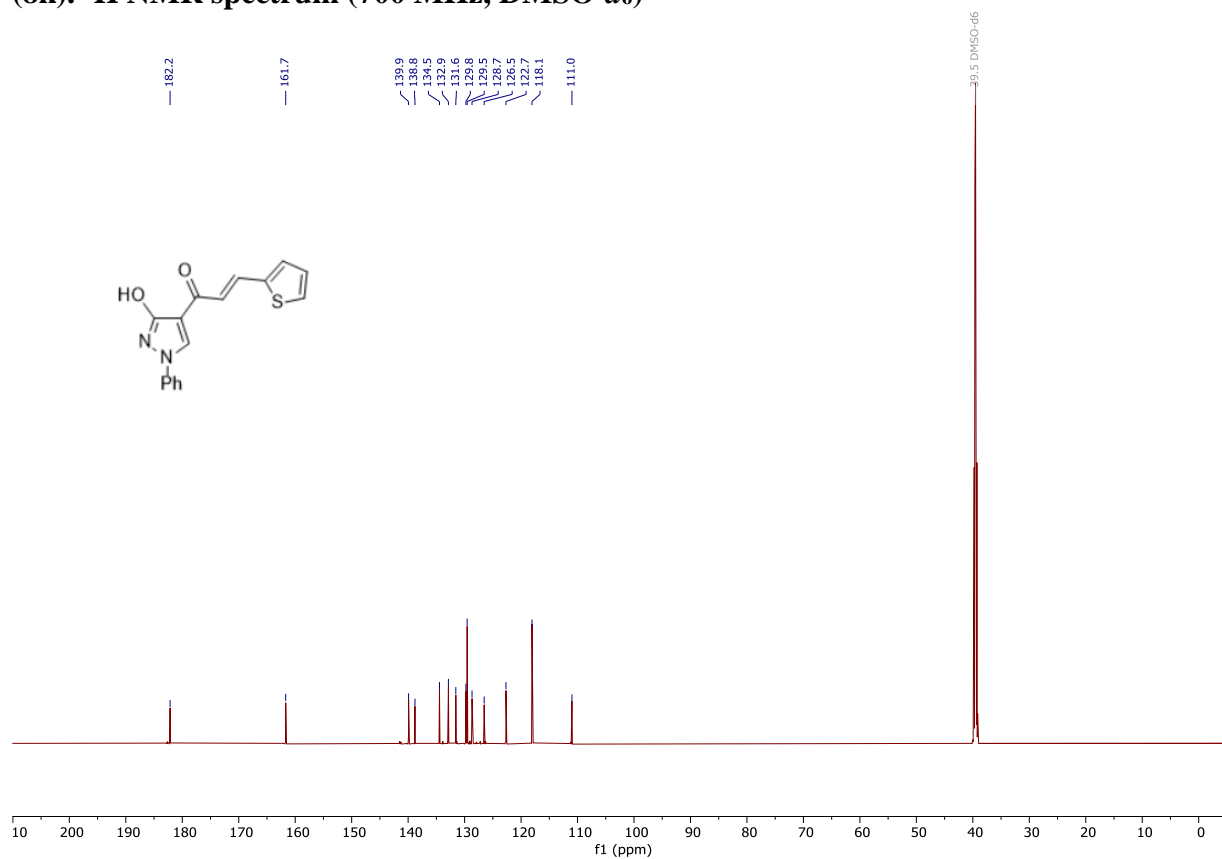


Figure S94. (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(quinolin-4-yl)prop-2-en-1-one (8j). HRMS (ESI-TOF).



**Figure S95. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(thiophen-2-yl)prop-2-en-1-one (8k). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)**



**Figure S96. (2*E*)-1-(3-Hydroxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(thiophen-2-yl)prop-2-en-1-one (8k). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)**

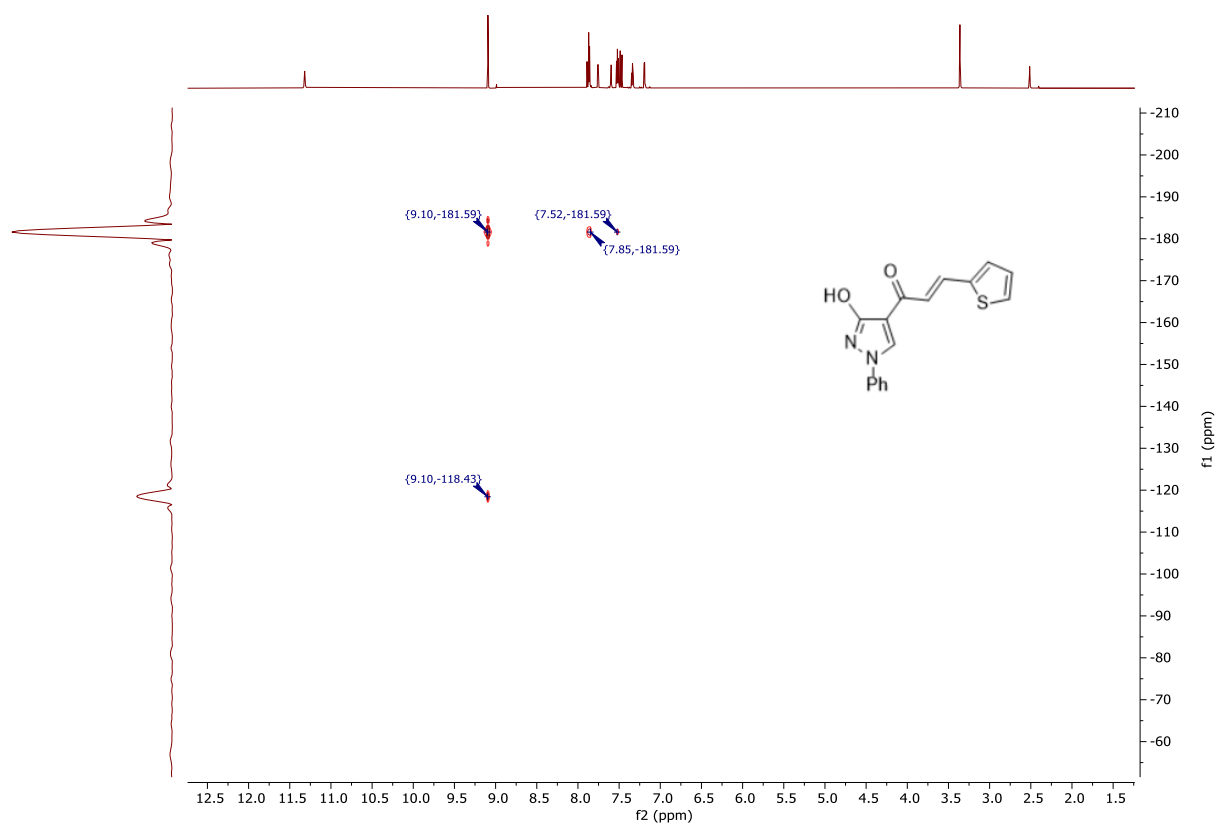
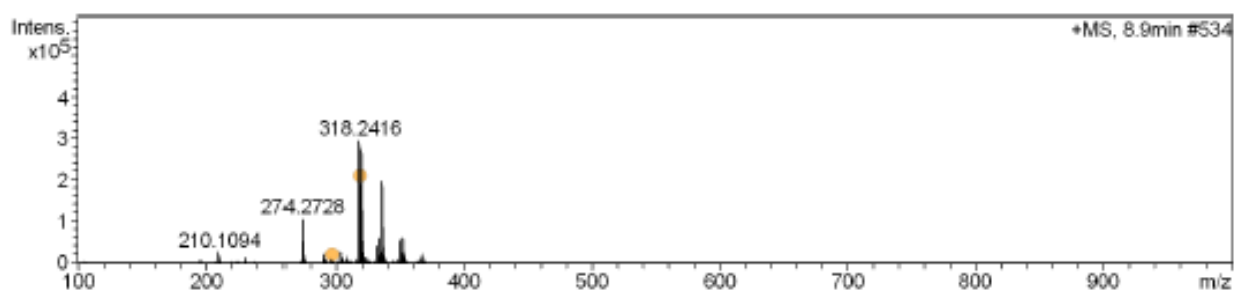


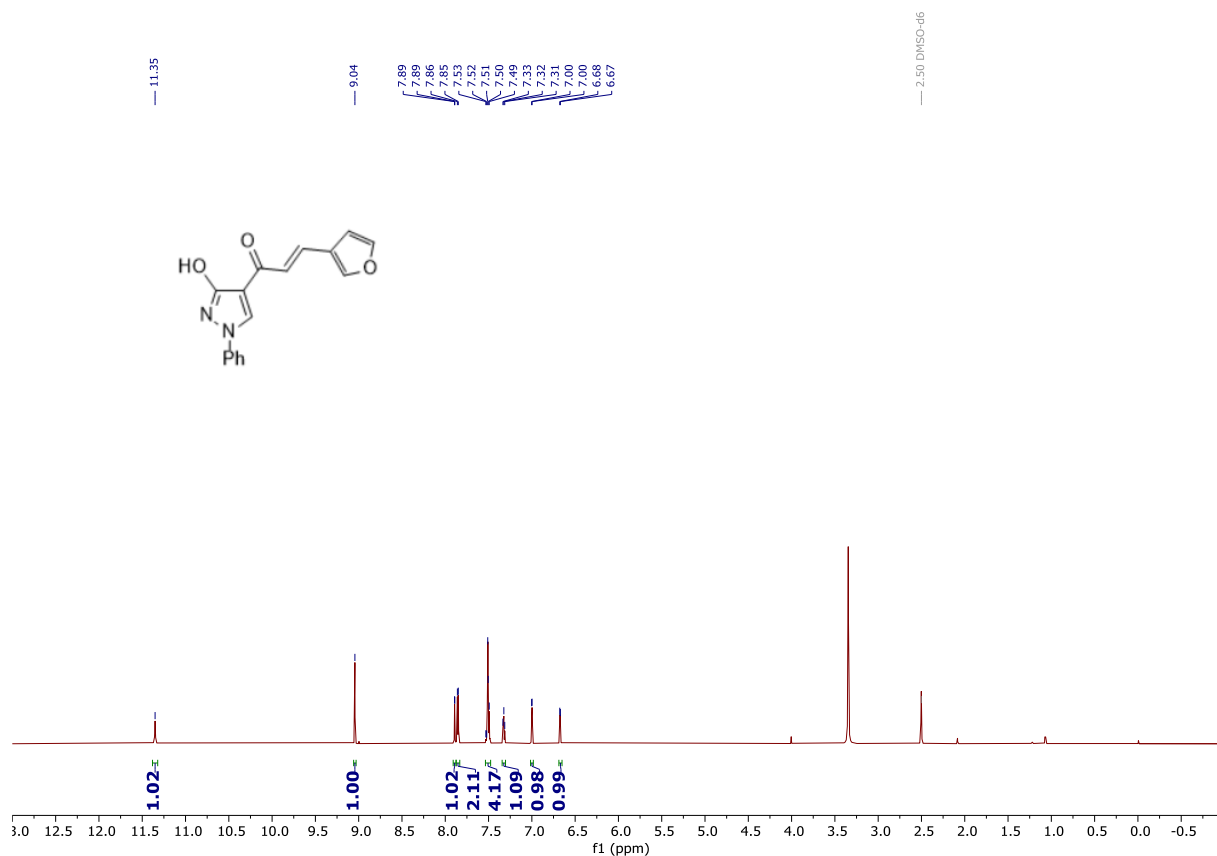
Figure S97. (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(thiophen-2-yl)prop-2-en-1-one (8k).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{DMSO}-d_6$ )

+MS, 8.9min #534

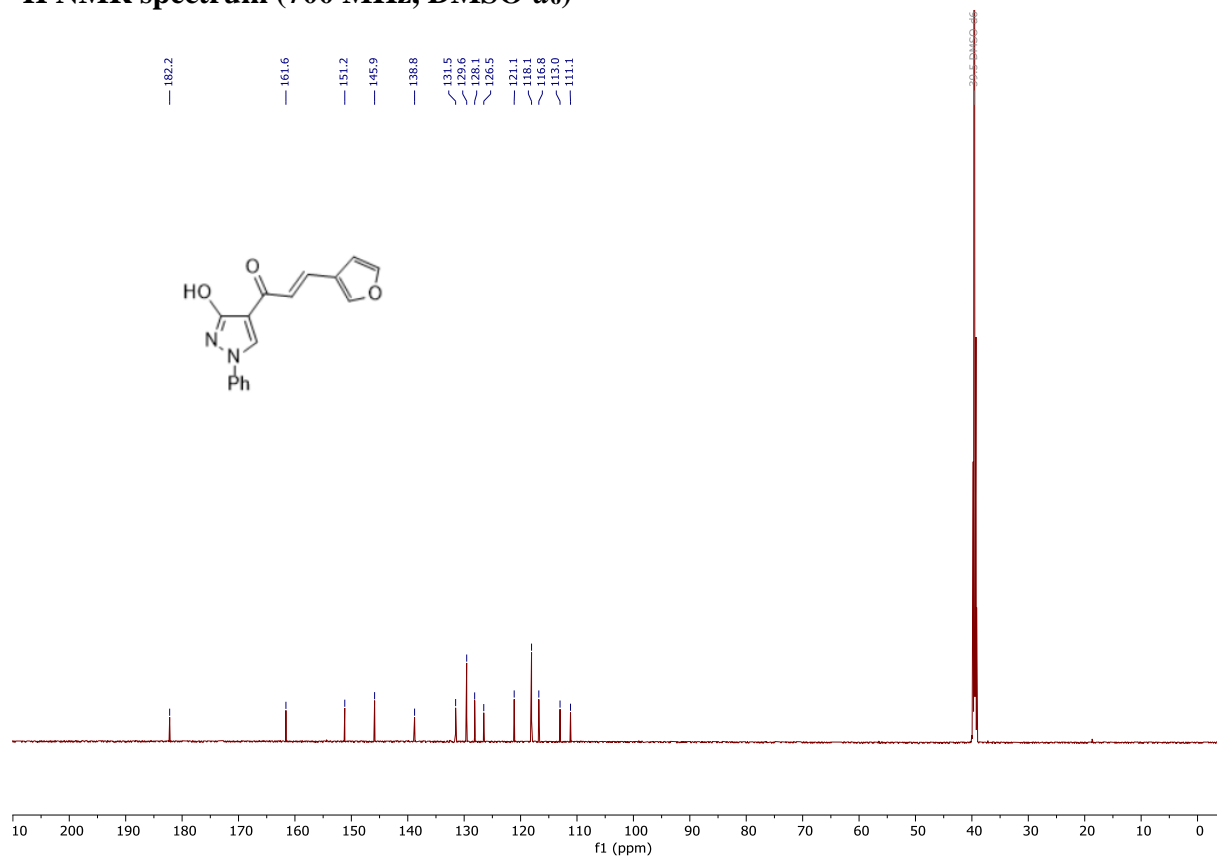


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup>	Conf	N-Rule
297.0683	1	C <sub>16</sub> H <sub>13</sub> N <sub>2</sub> O <sub>2</sub> S	297.0692	-3.0	34.6	1	100.00	11.5	even		ok
319.0512	1	C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> NaO <sub>2</sub> S	319.0512	-0.2	6.8	1	100.00	11.5	even		ok

Figure S98. (2E)-1-(3-Hydroxy-1-phenyl-1H-pyrazol-4-yl)-3-(thiophen-2-yl)prop-2-en-1-one (8k). HRMS (ESI-TOF).



**Figure S99. (2E)-3-(Furan-3-yl)-1-(3-hydroxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (8l). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)**



**Figure S100. (2E)-3-(Furan-3-yl)-1-(3-hydroxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (8l). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)**

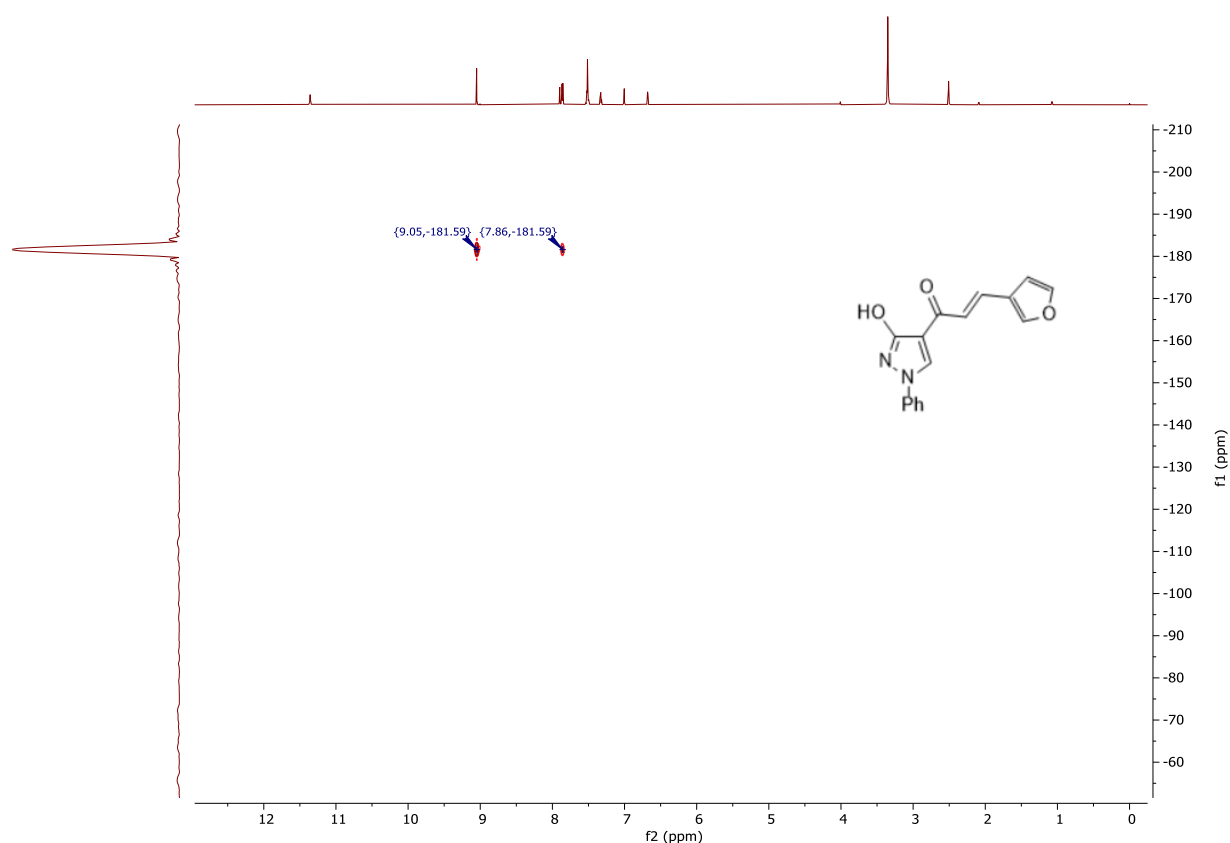


Figure S101. (2*E*)-3-(Furan-3-yl)-1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (8l).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{DMSO}-d_6$ )

+MS, 5.3min #318

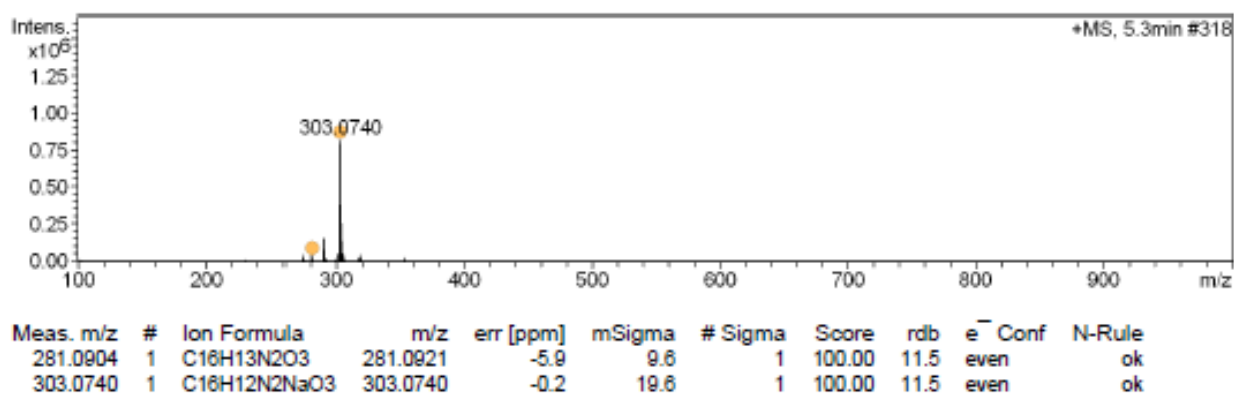
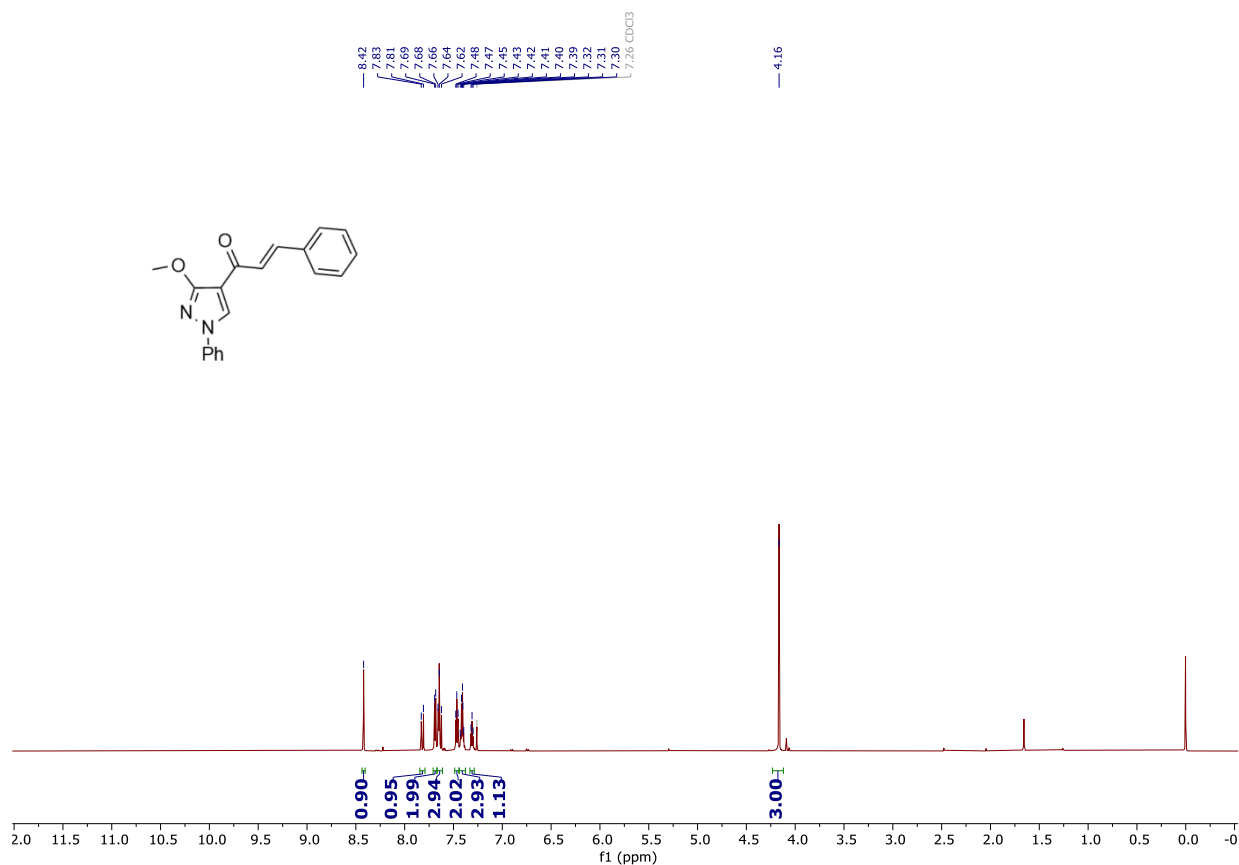
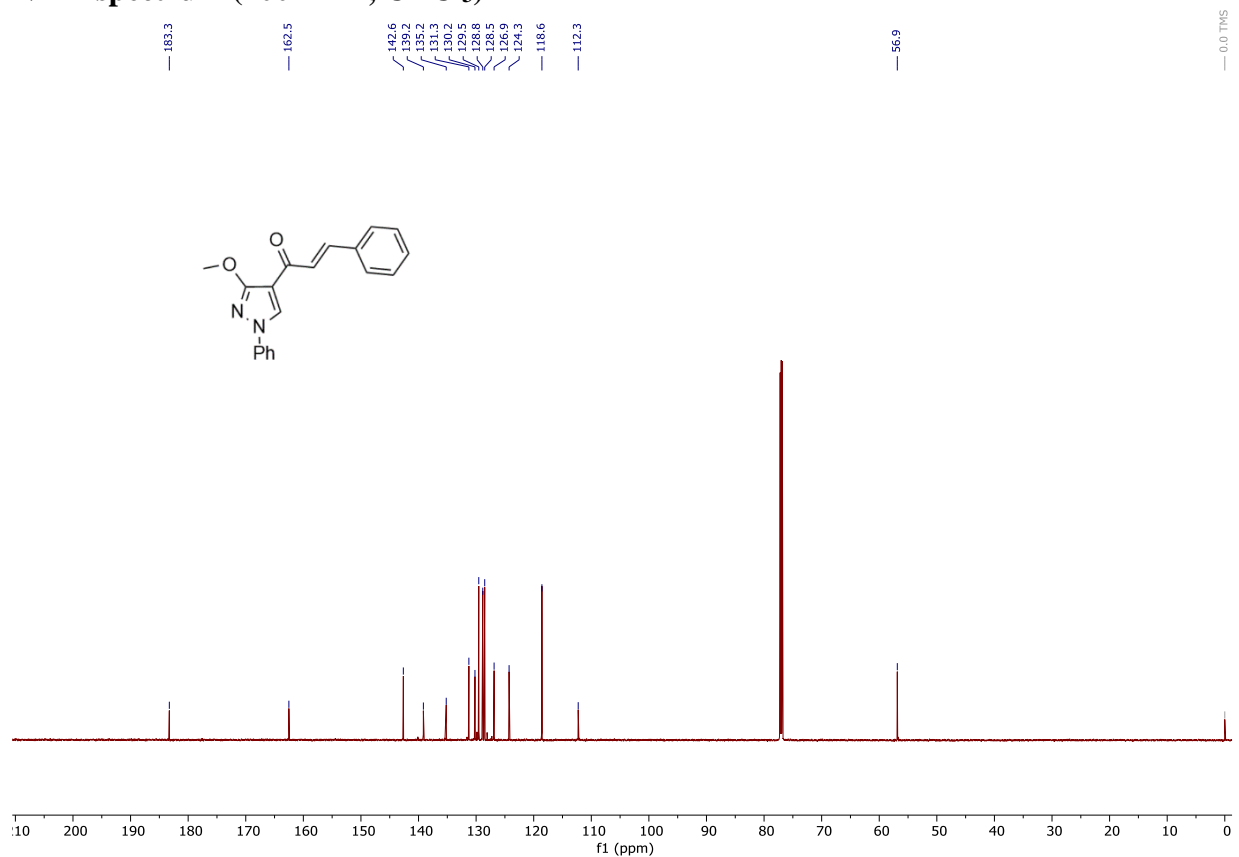


Figure S102. (2*E*)-3-(Furan-3-yl)-1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (8l). HRMS (ESI-TOF).

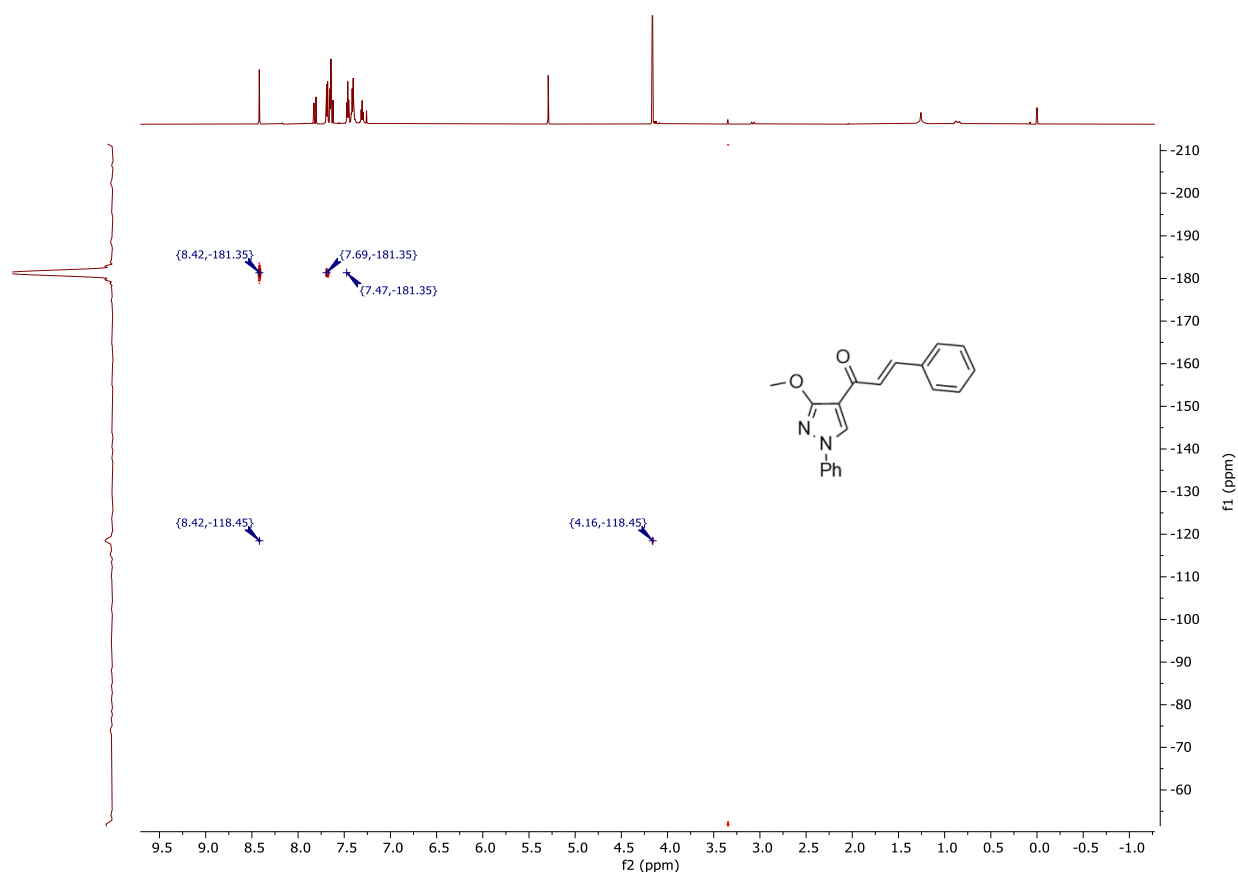




**Figure S103. (2E)-1-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-phenylprop-2-en-1-one (9a). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**

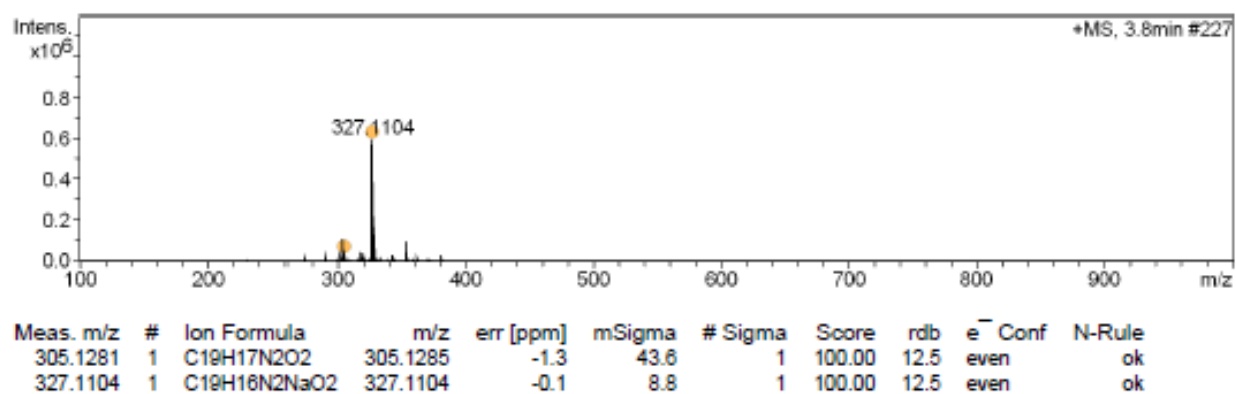


**Figure S104. (2E)-1-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-phenylprop-2-en-1-one (9a). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)**

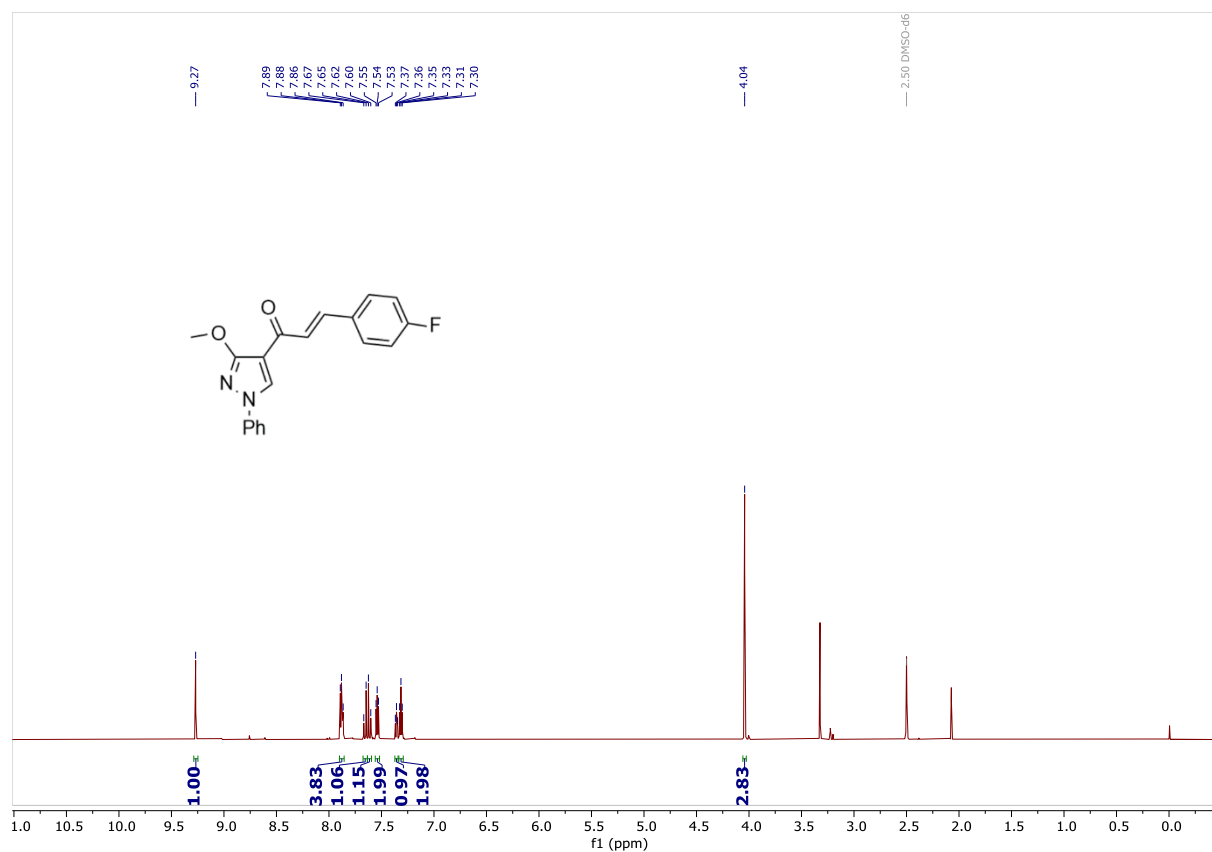


**Figure S105.** (2E)-1-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-phenylprop-2-en-1-one (9a).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

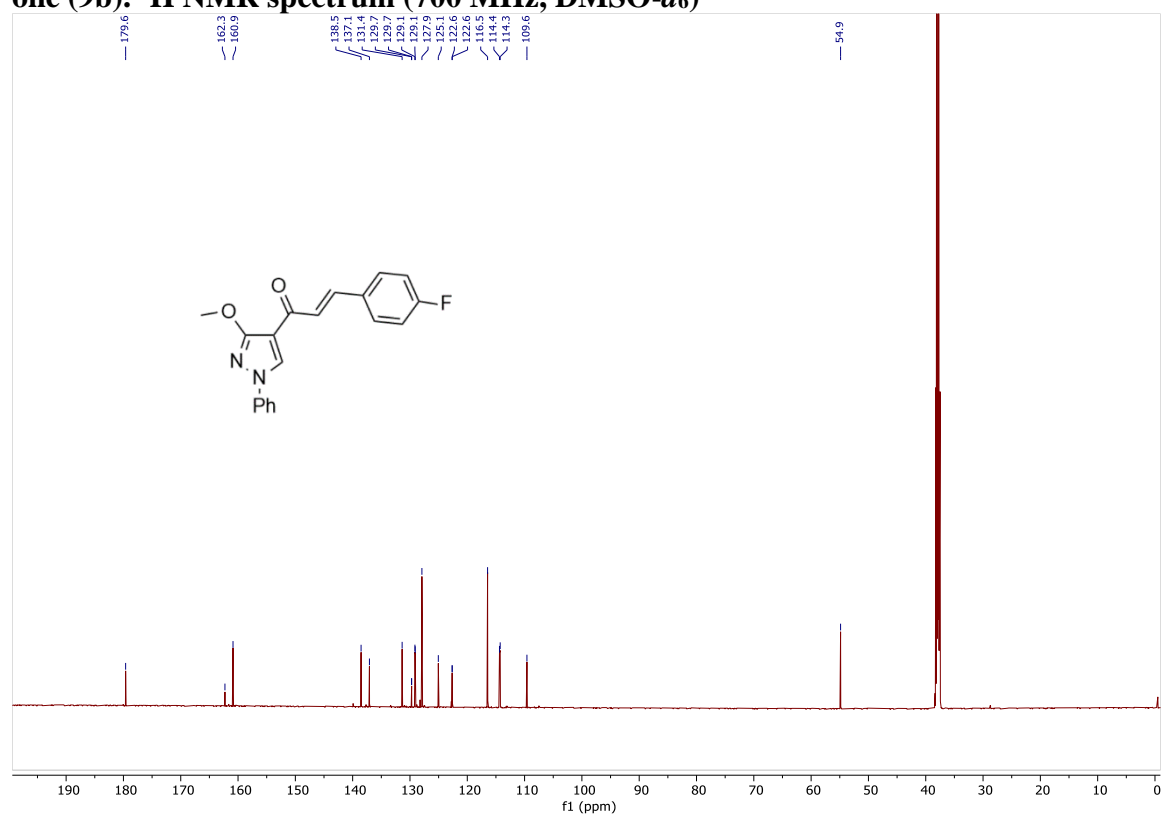
**+MS, 3.8min #227**



**Figure S106.** (2E)-1-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-phenylprop-2-en-1-one (9a). HRMS (ESI-TOF).



**Figure S107.** (2E)-3-(4-Fluorophenyl)-1-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (9b). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)



**Figure S108.** (2E)-3-(4-Fluorophenyl)-1-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (9b). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)

+MS, 5.5min #328

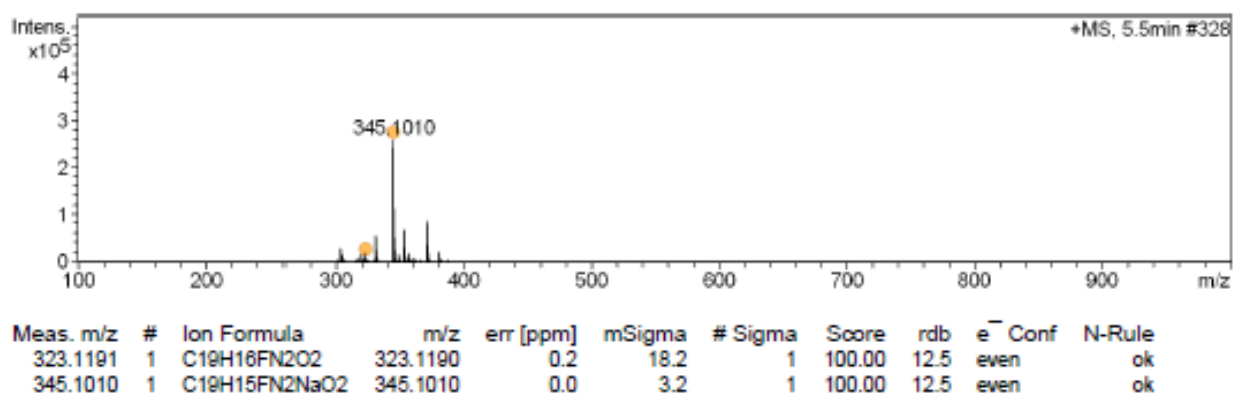


Figure S109. (2*E*)-3-(4-Fluorophenyl)-1-(3-methoxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (9b). HRMS (ESI-TOF).

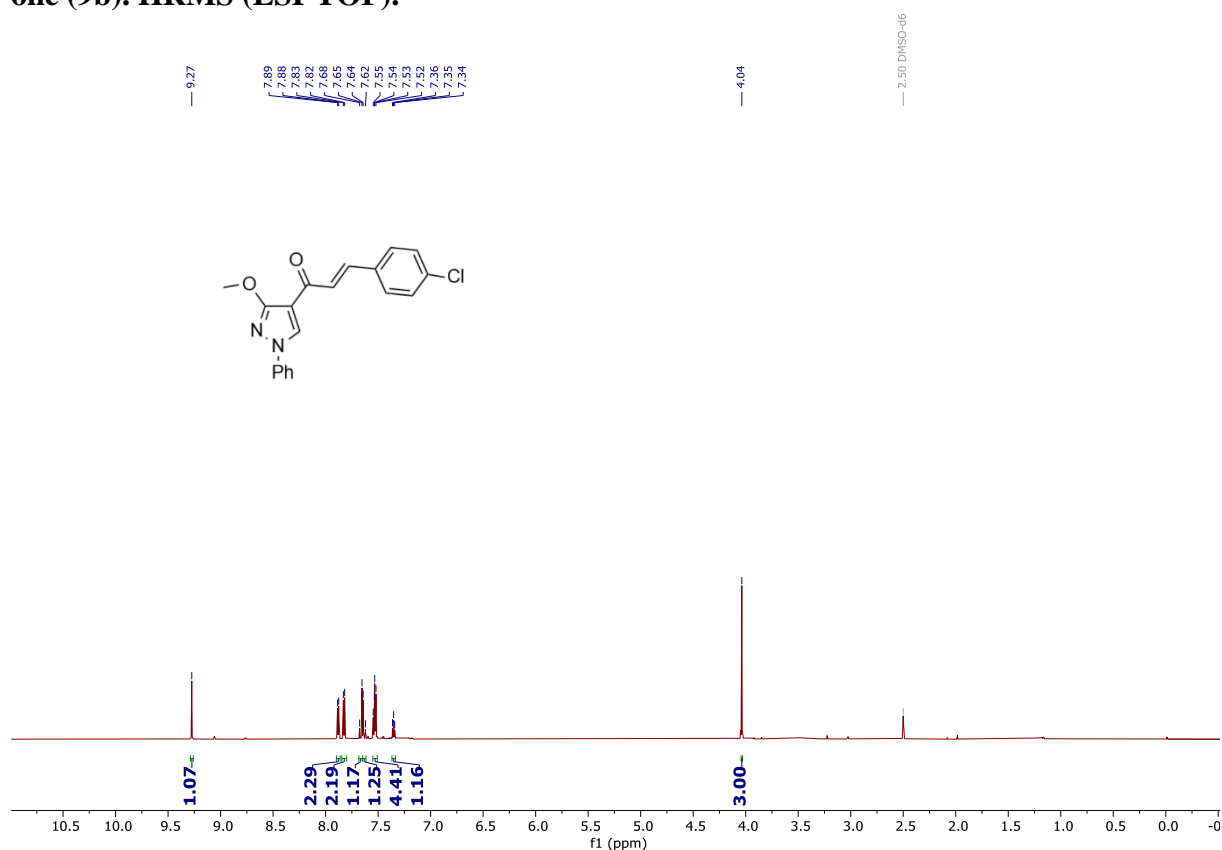
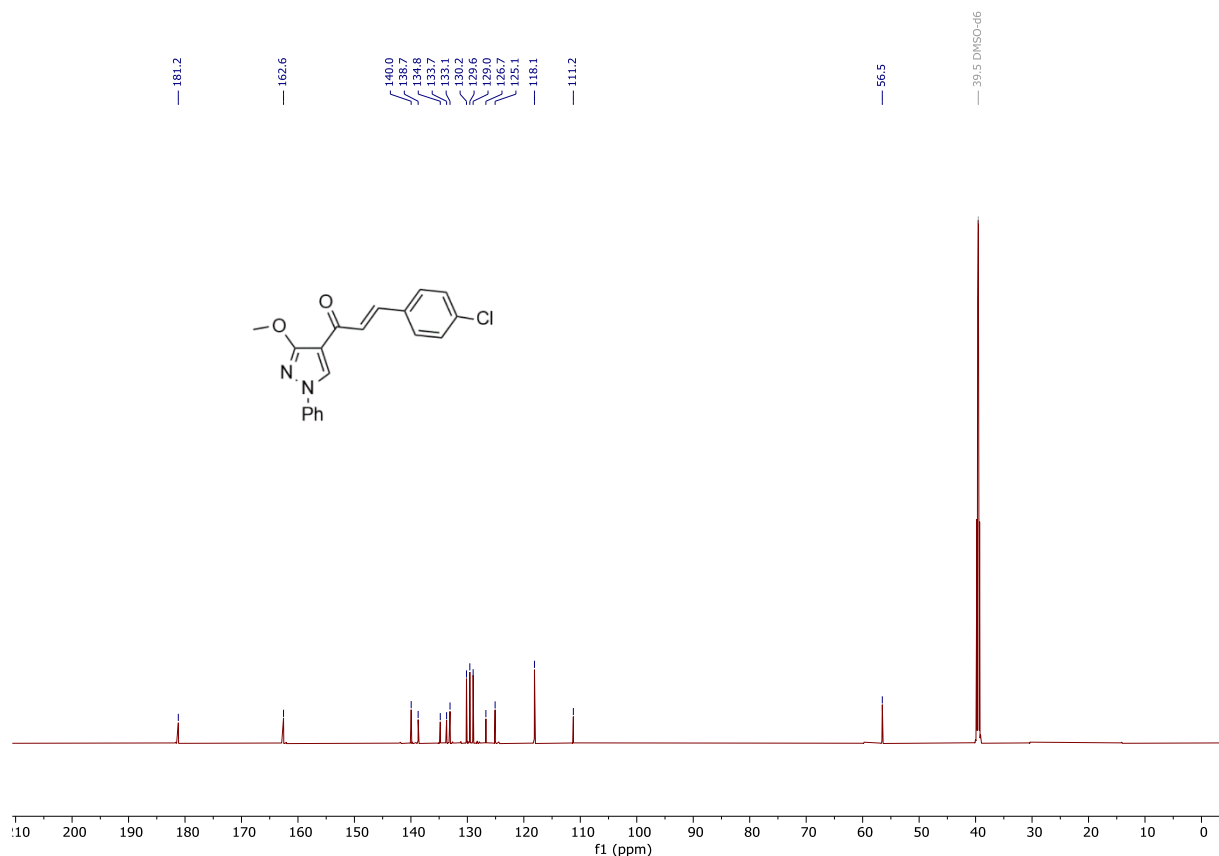
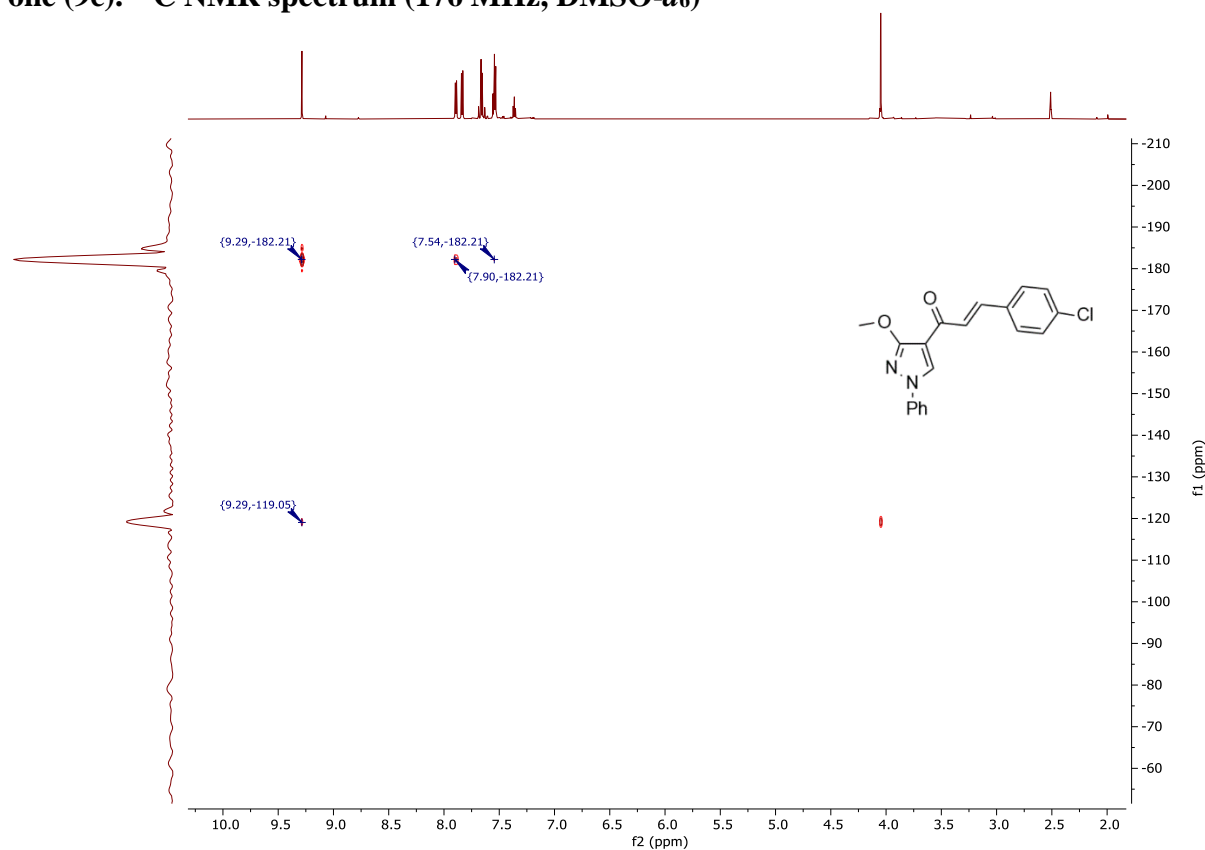


Figure S110. (2*E*)-3-(4-Chlorophenyl)-1-(3-methoxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (9c). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)

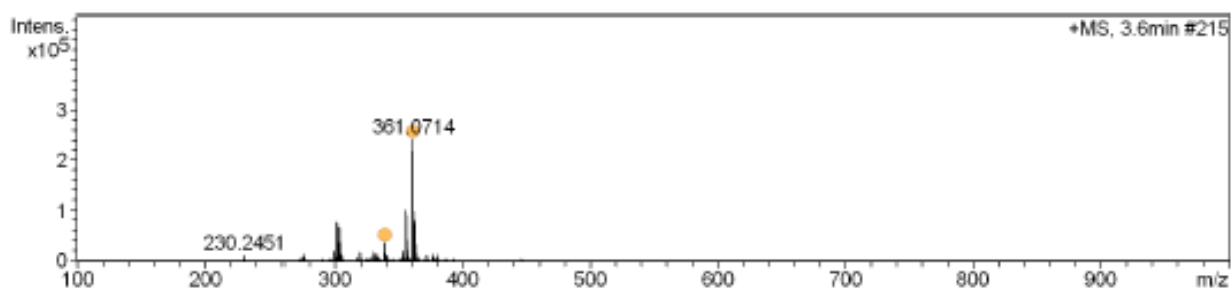


**Figure S111.** (2E)-3-(4-Chlorophenyl)-1-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (9c). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



**Figure S112.** (2E)-3-(4-Chlorophenyl)-1-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (9c). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, DMSO-*d*<sub>6</sub>)

+MS, 3.6min #215



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
339.0892	1	C19H16ClN2O2	339.0895	-1.0	13.6	1	100.00	12.5	even		ok
361.0714	1	C19H15ClN2NaO2	361.0714	-0.0	6.3	1	100.00	12.5	even		ok

Figure S113. (2*E*)-3-(4-Chlorophenyl)-1-(3-methoxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (9c). HRMS (ESI-TOF).

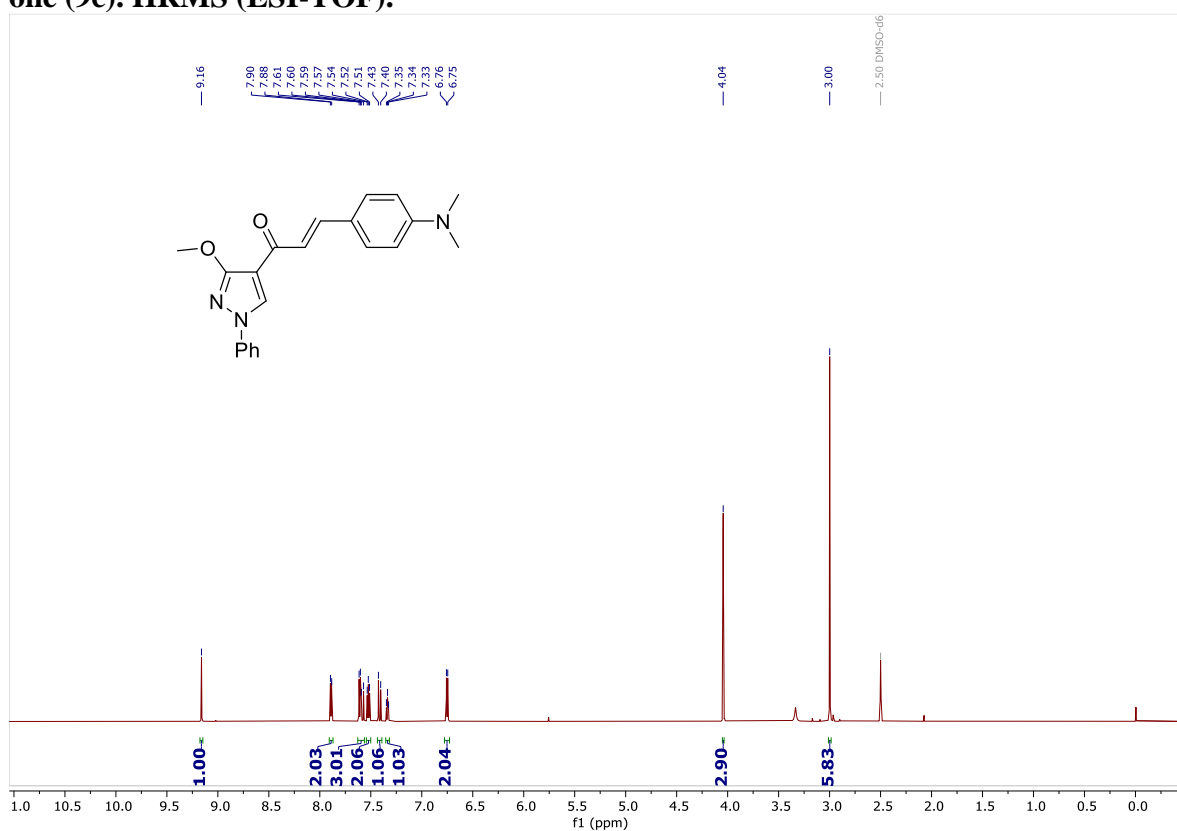
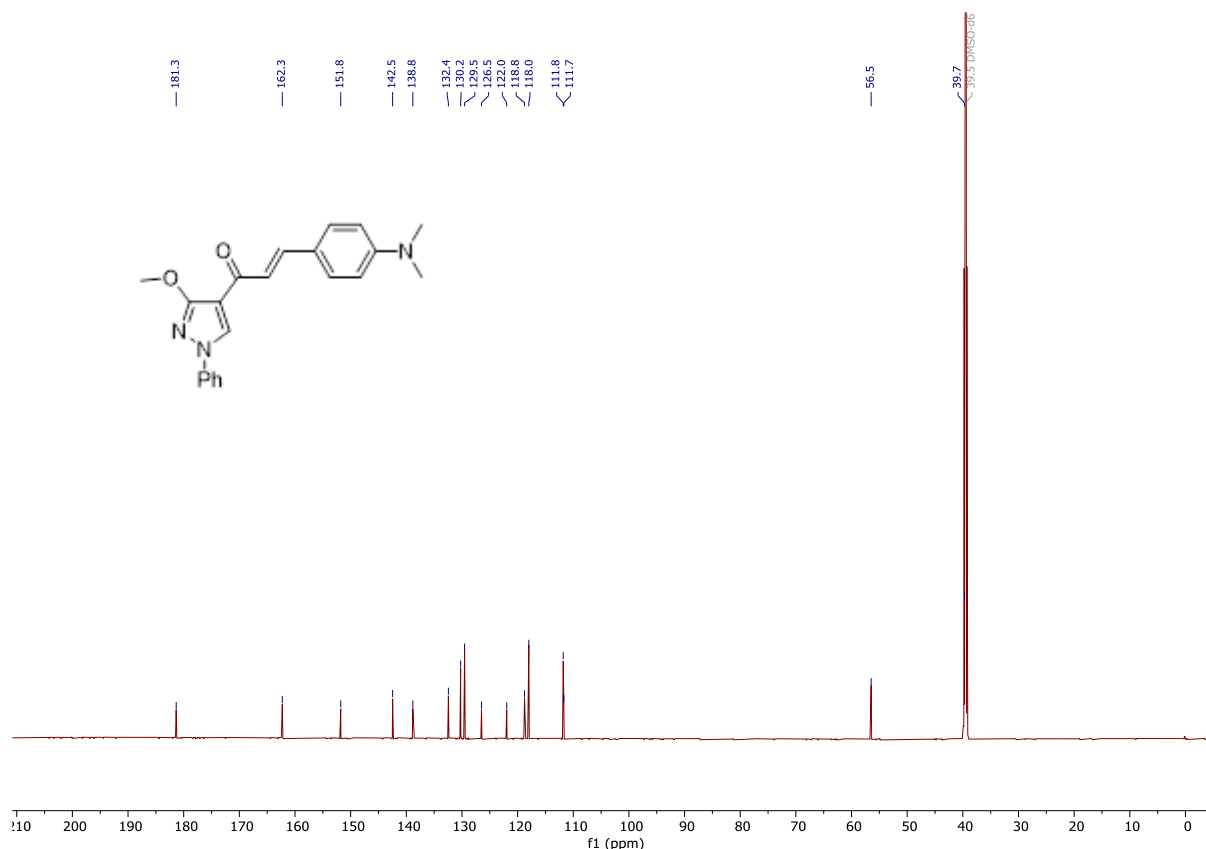
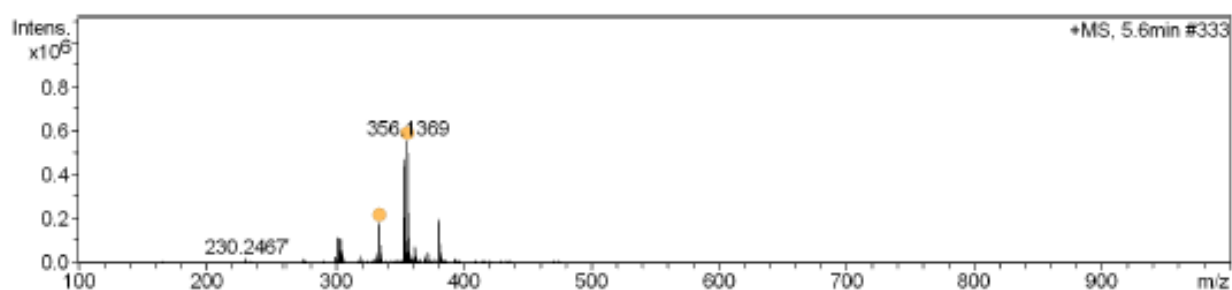


Figure S114. (2*E*)-3-[4-(Dimethylamino)phenyl]-1-(3-methoxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (9d). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)



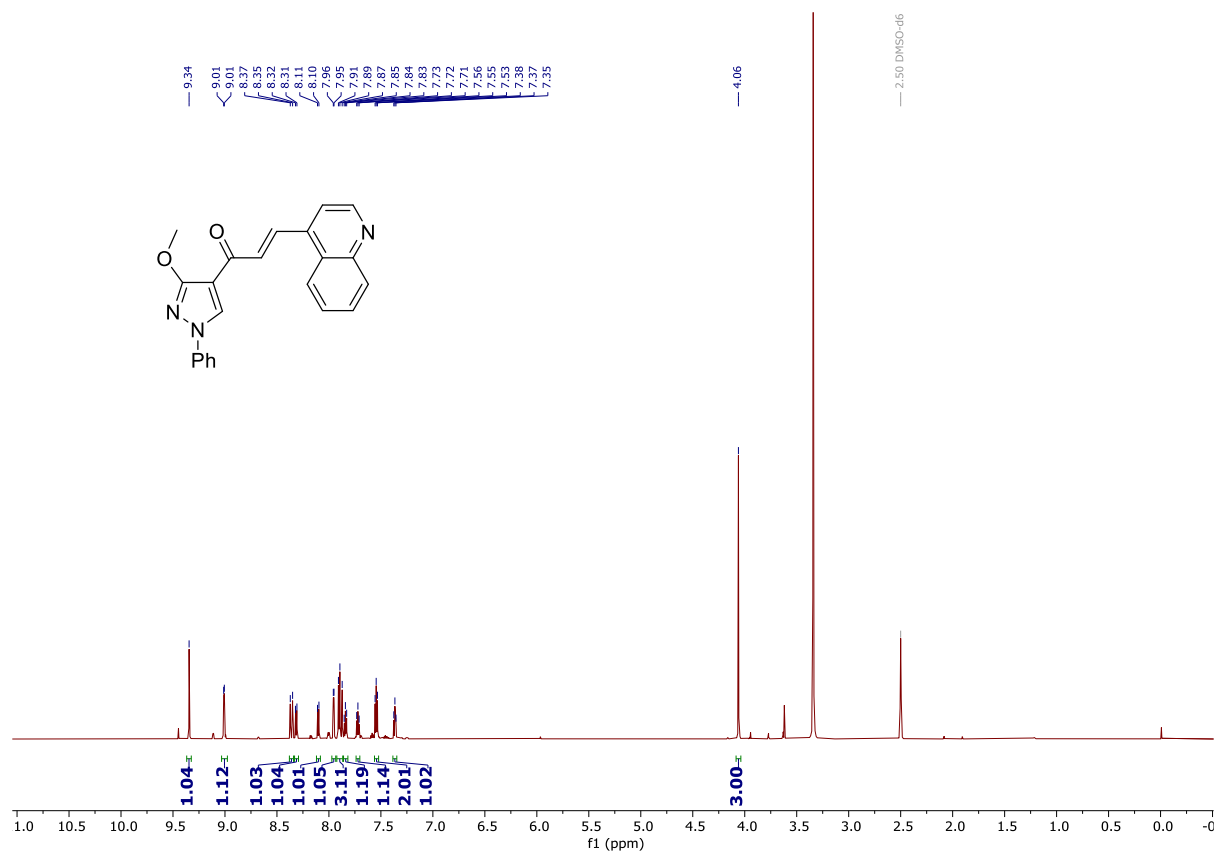
**Figure S115.** (2*E*)-3-[4-(Dimethylamino)phenyl]-1-(3-methoxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (9d). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)

**+MS, 5.6min #333**

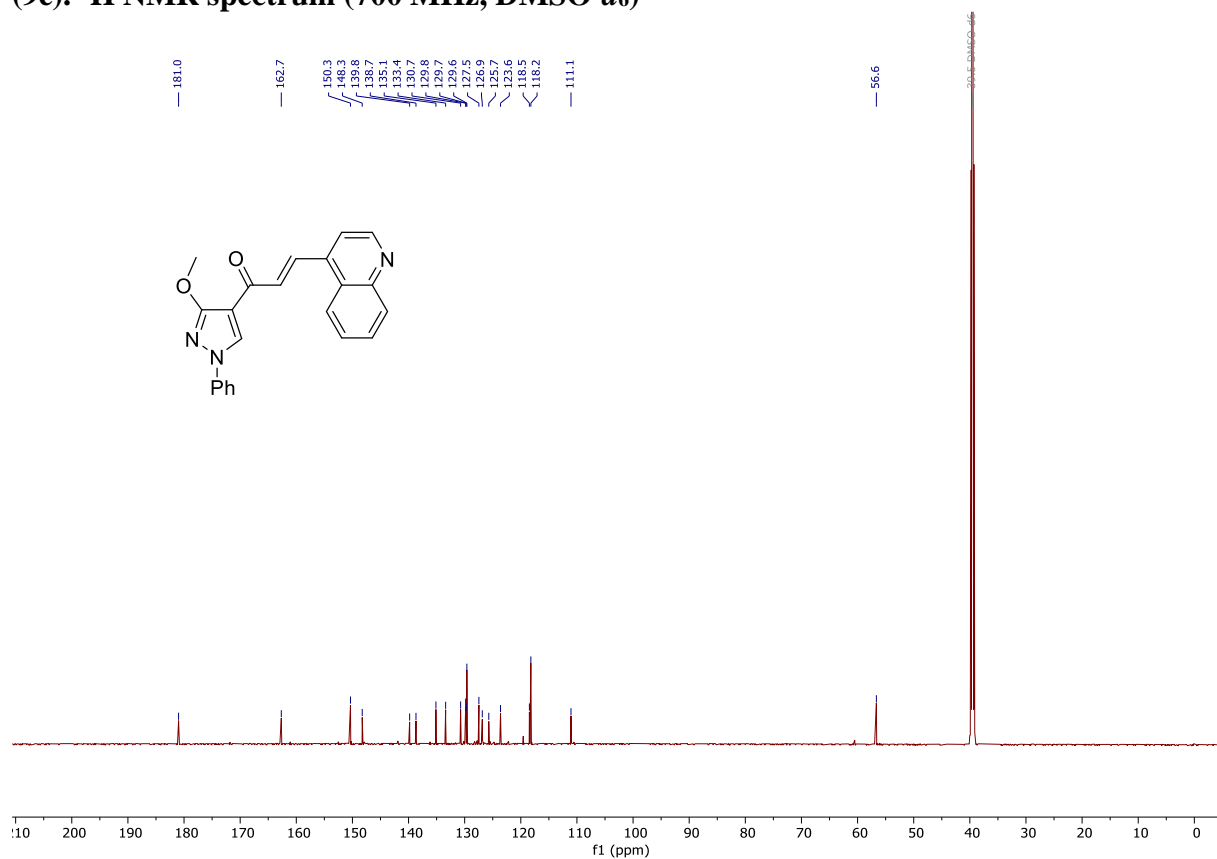


Meas. <i>m/z</i>	#	Ion Formula	<i>m/z</i>	err [ppm]	<i>mSigma</i>	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
334.1541	1	C <sub>20</sub> H <sub>20</sub> N <sub>3</sub> O <sub>2</sub>	334.1550	-2.6	14.2	1	100.00	12.5	even	ok
356.1369	1	C <sub>20</sub> H <sub>19</sub> N <sub>3</sub> NaO <sub>2</sub>	356.1369	-0.2	2.9	1	100.00	12.5	even	ok

**Figure S116.** (2*E*)-3-[4-(Dimethylamino)phenyl]-1-(3-methoxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (9d). HRMS (ESI-TOF).



**Figure S117.** (2E)-1-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-(quinolin-4-yl)prop-2-en-1-one (9e). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)



**Figure S118.** (2E)-1-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-(quinolin-4-yl)prop-2-en-1-one (9e). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



+MS, 5.8min #350

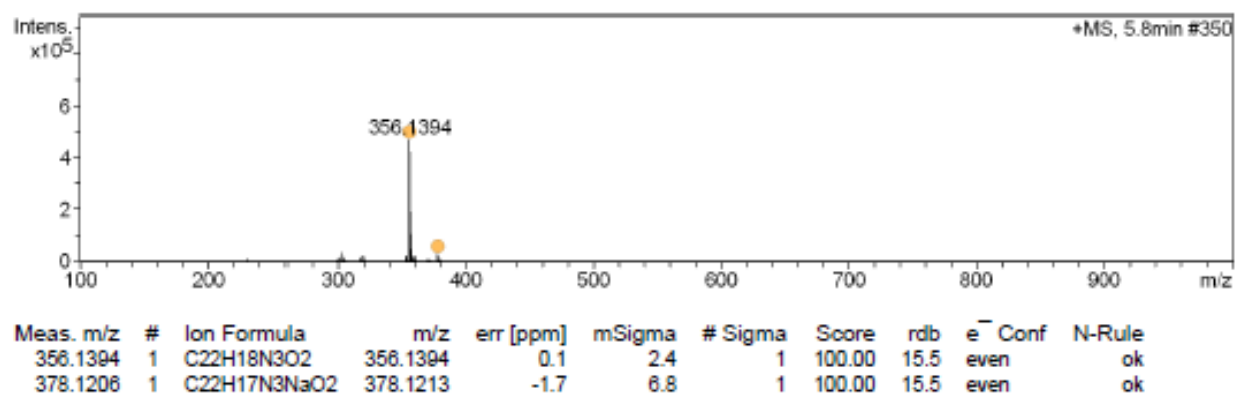


Figure S119. (2*E*)-1-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(quinolin-4-yl)prop-2-en-1-one (9e). HRMS (ESI-TOF).

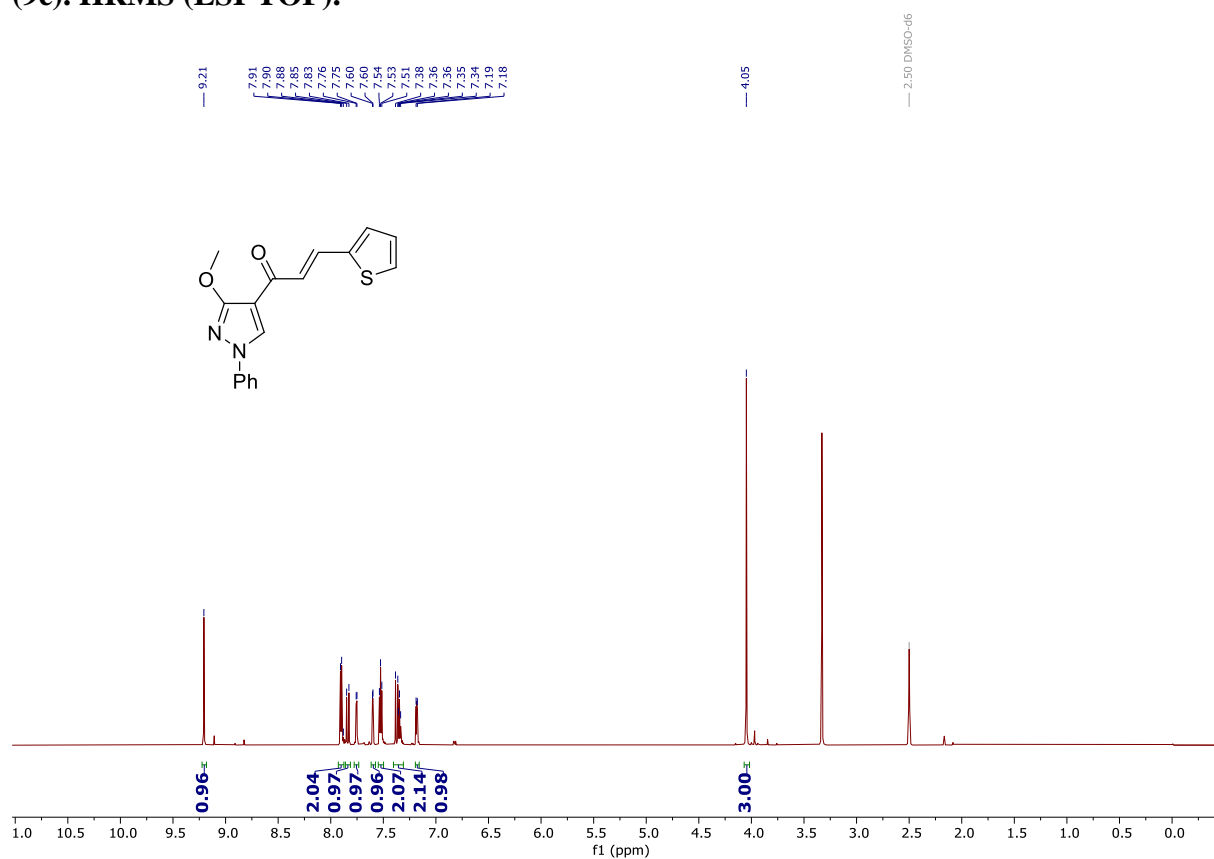
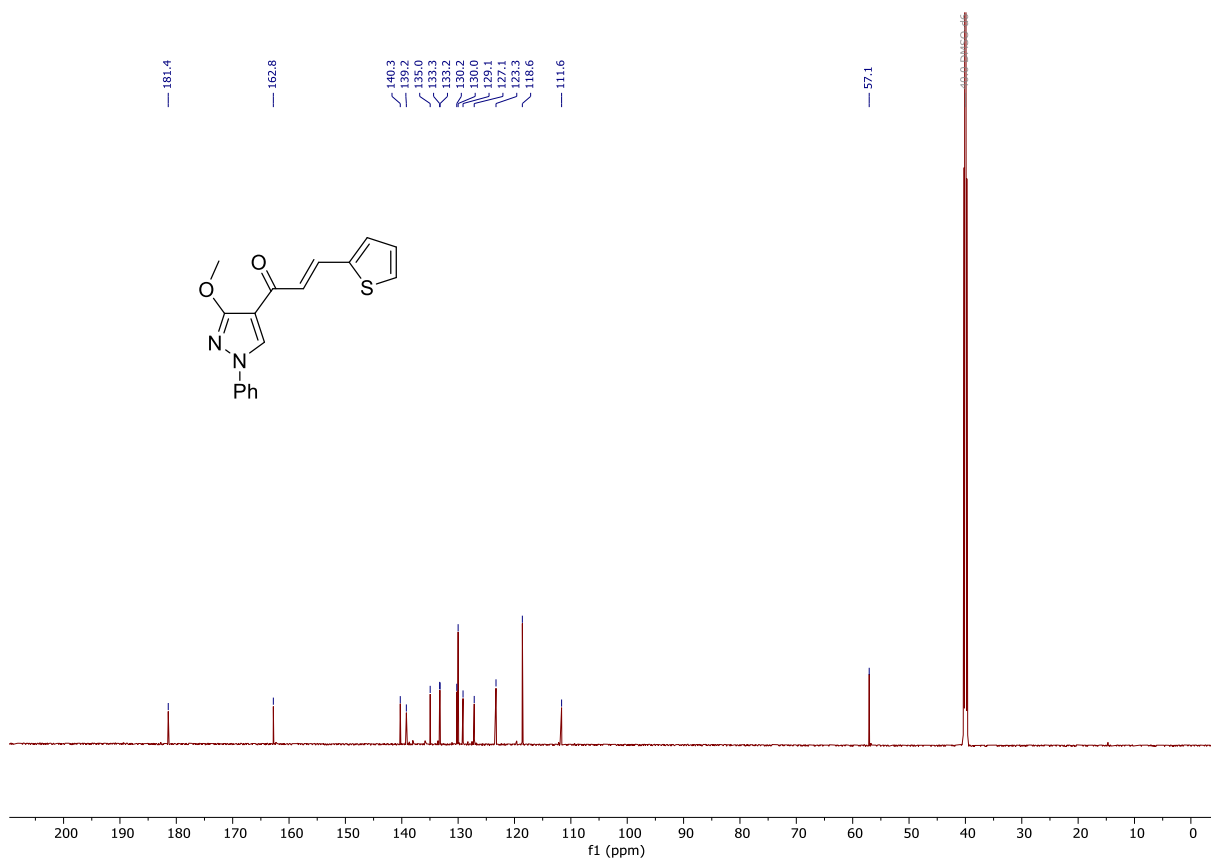
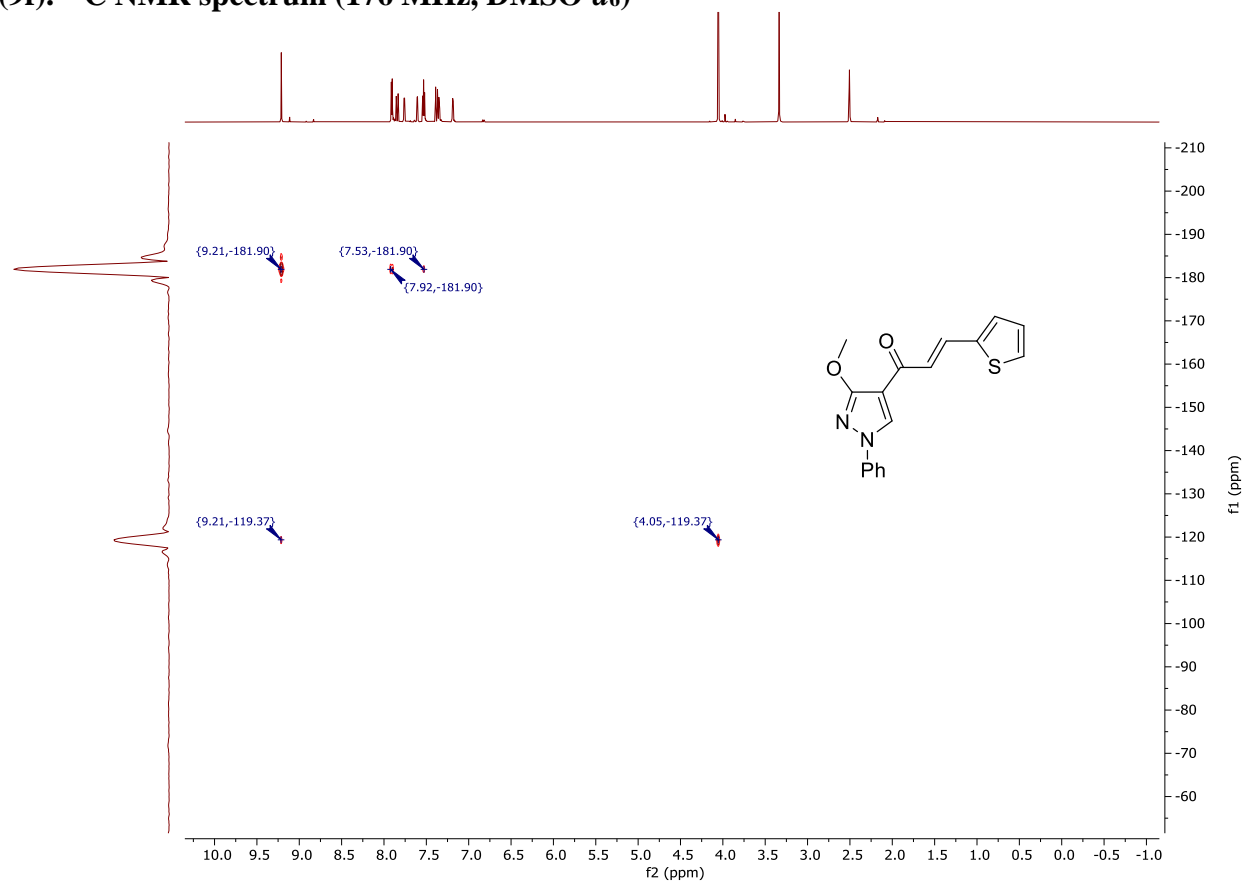


Figure S120. (2*E*)-1-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(thiophen-2-yl)prop-2-en-1-one (9f). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>)



**Figure S121.** (2E)-1-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-(thiophen-2-yl)prop-2-en-1-one (9f). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



**Figure S122.** (2E)-1-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-(thiophen-2-yl)prop-2-en-1-one (9f). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, DMSO-*d*<sub>6</sub>)

+MS, 7.4min #444

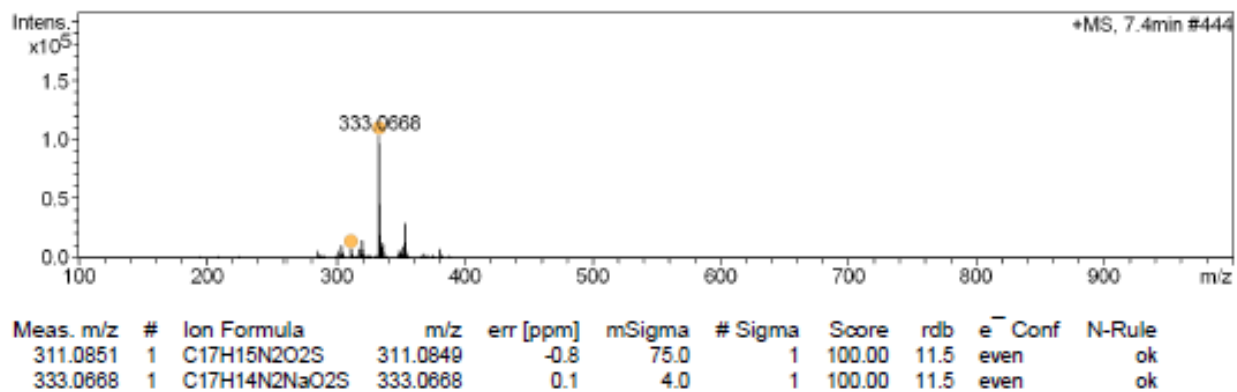


Figure S123. (2*E*)-1-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-3-(thiophen-2-yl)prop-2-en-1-one (9f). HRMS (ESI-TOF).

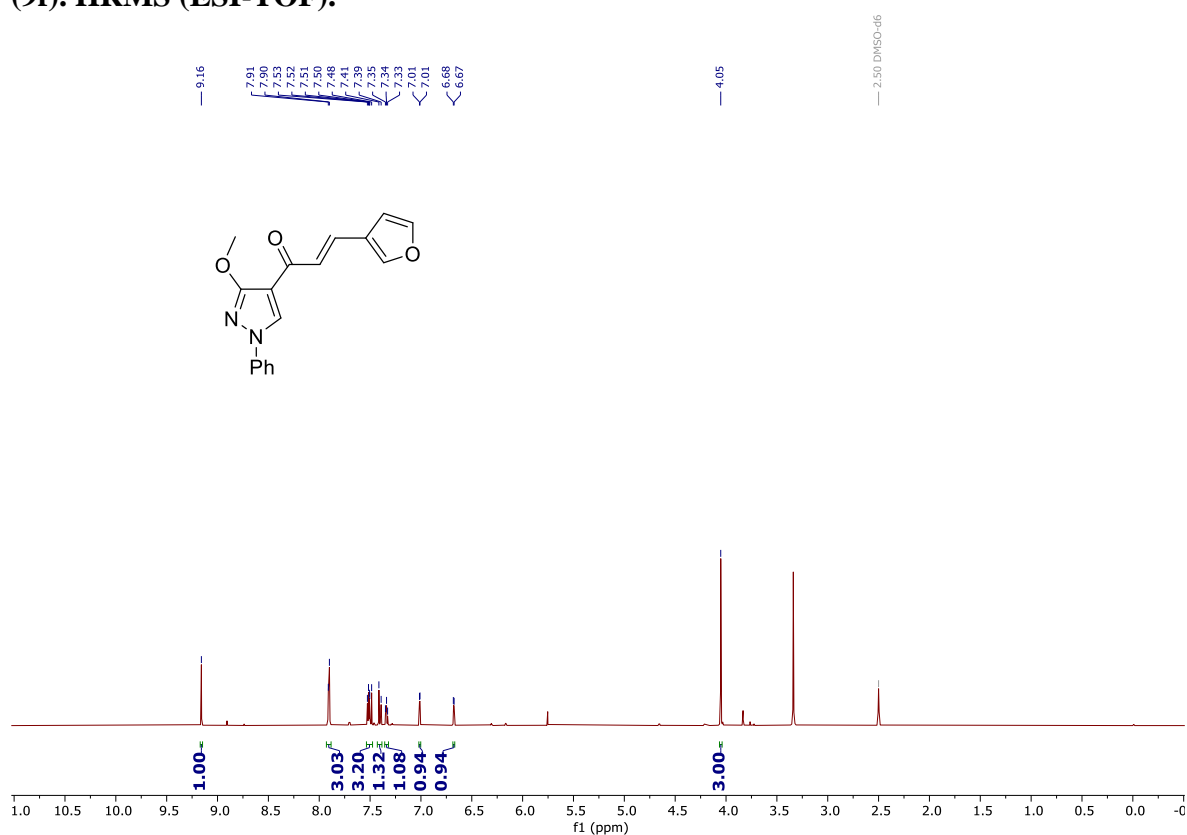
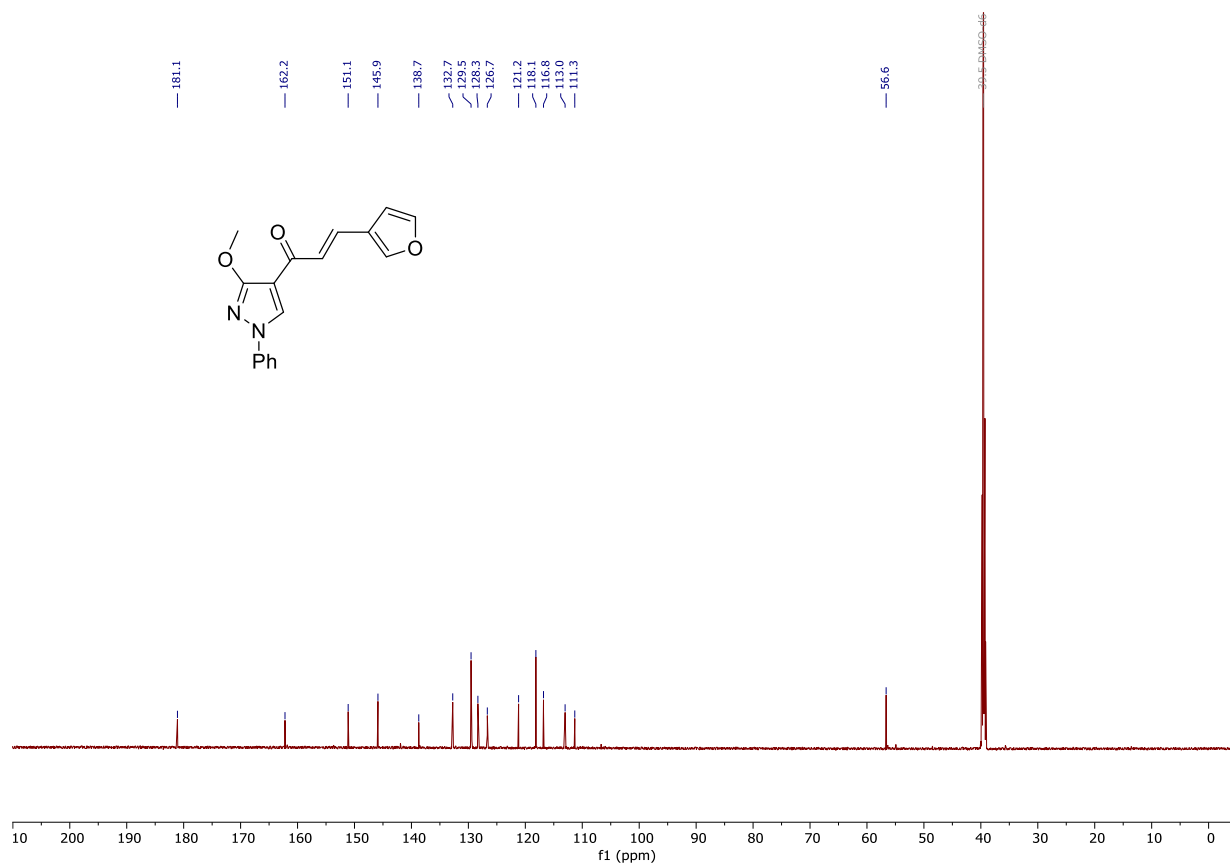
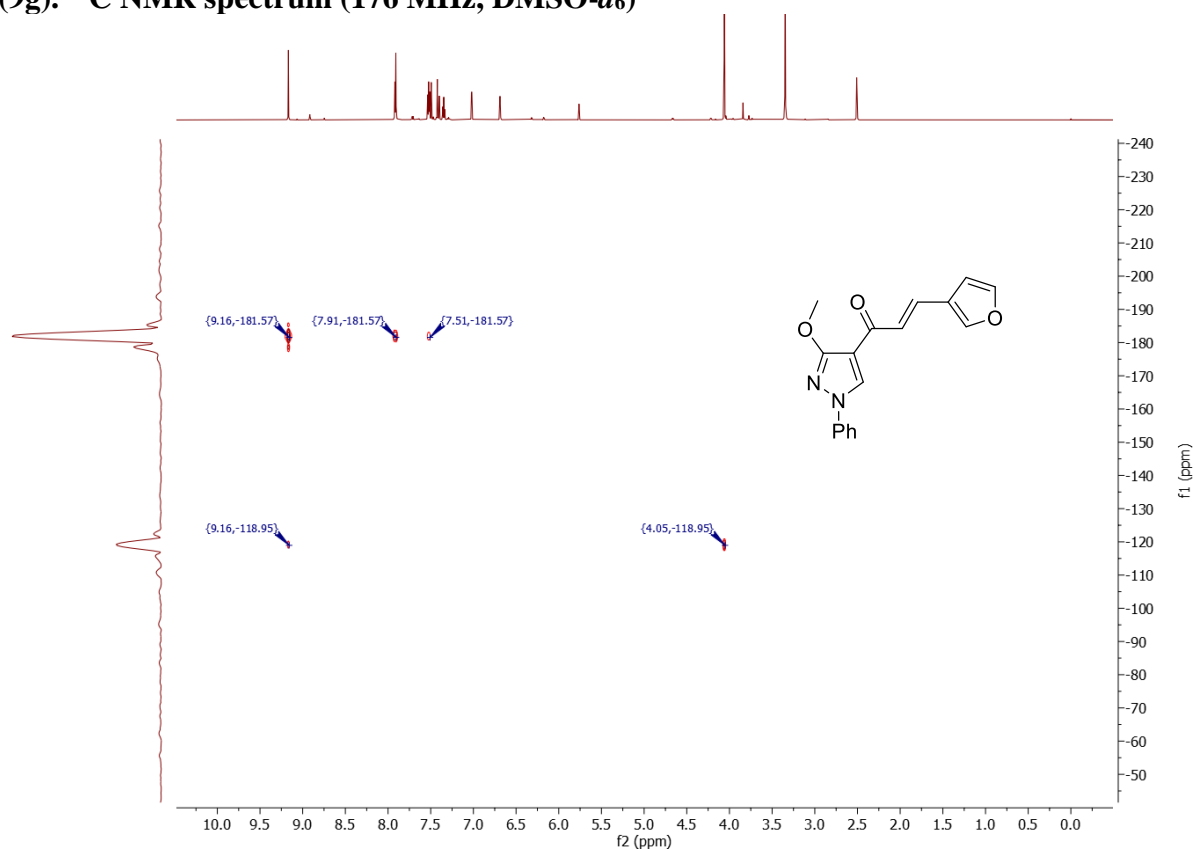


Figure S124. (2*E*)-3-(Furan-3-yl)-1-(3-methoxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (9g). <sup>1</sup>H NMR spectrum (700 MHz, DMSO-*d*<sub>6</sub>):



**Figure S125.** (2E)-3-(Furan-3-yl)-1-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (9g). <sup>13</sup>C NMR spectrum (176 MHz, DMSO-*d*<sub>6</sub>)



**Figure S126.** (2E)-3-(Furan-3-yl)-1-(3-methoxy-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (9g). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, DMSO-*d*<sub>6</sub>)

+MS, 6.6min #398

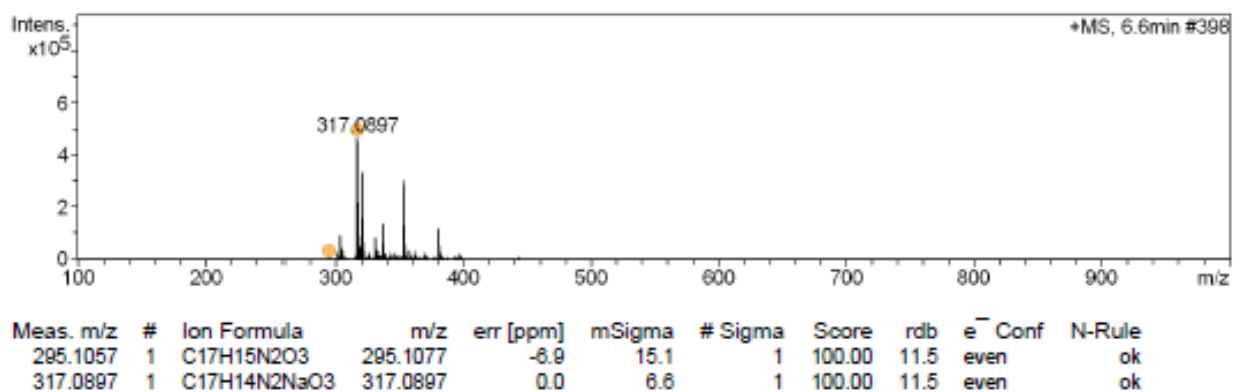


Figure S127. (2*E*)-3-(Furan-3-yl)-1-(3-methoxy-1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one (9g). HRMS (ESI-TOF).

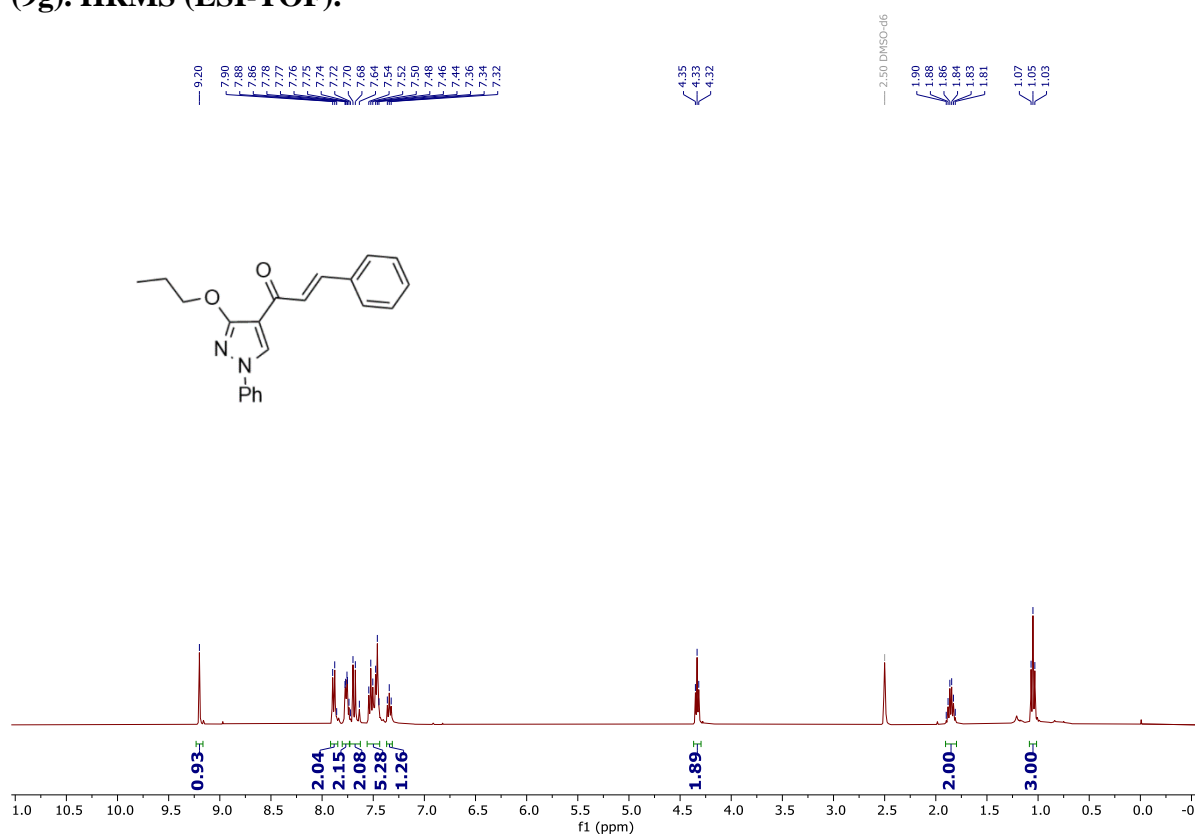


Figure S128. (2*E*)-3-Phenyl-1-(1-phenyl-3-propoxy-1*H*-pyrazol-4-yl)prop-2-en-1-one (9h). <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>)

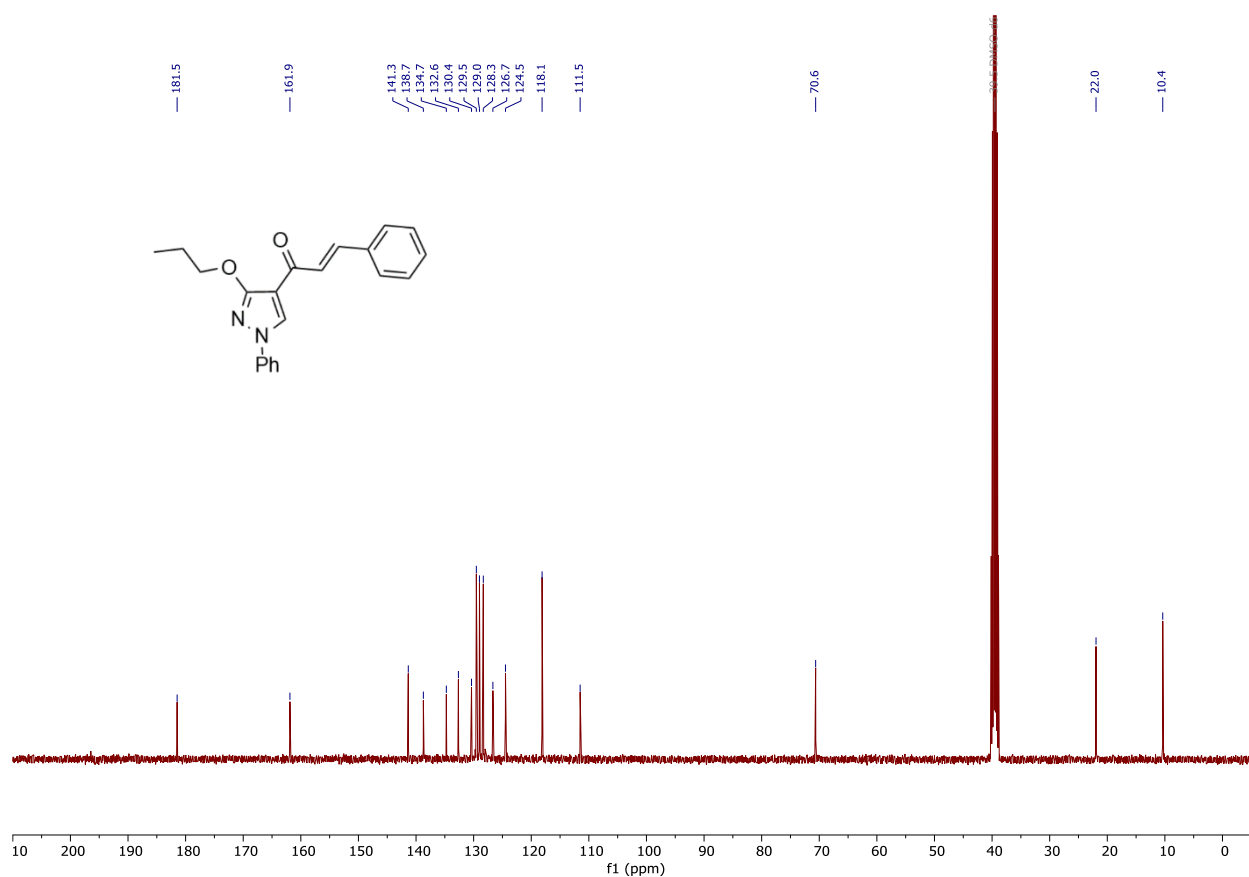
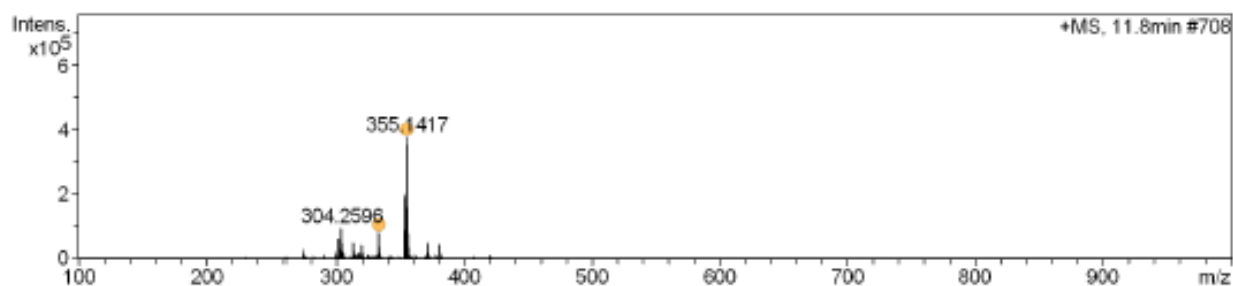


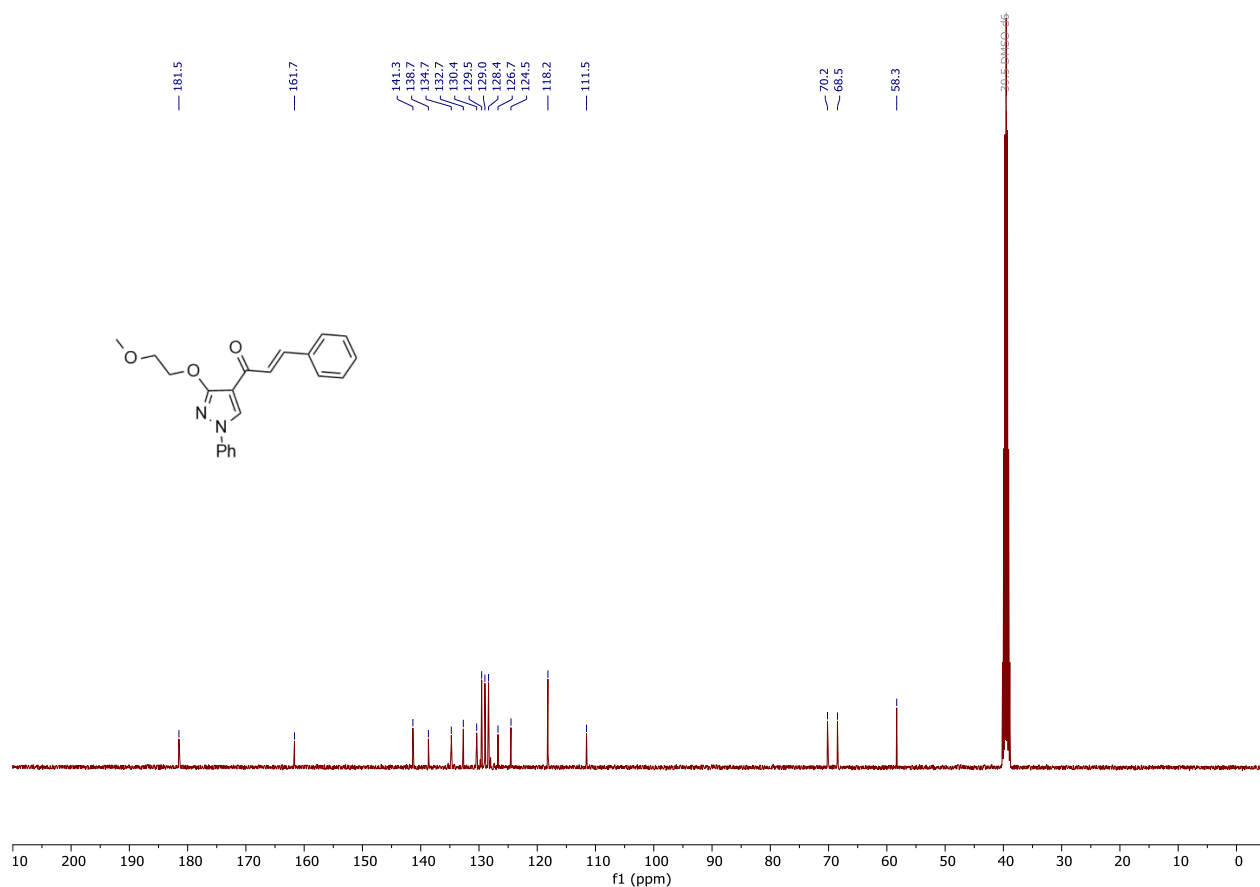
Figure S129. (2E)-3-Phenyl-1-(1-phenyl-3-propoxy-1H-pyrazol-4-yl)prop-2-en-1-one (9h). <sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>)

+MS, 11.8min #708

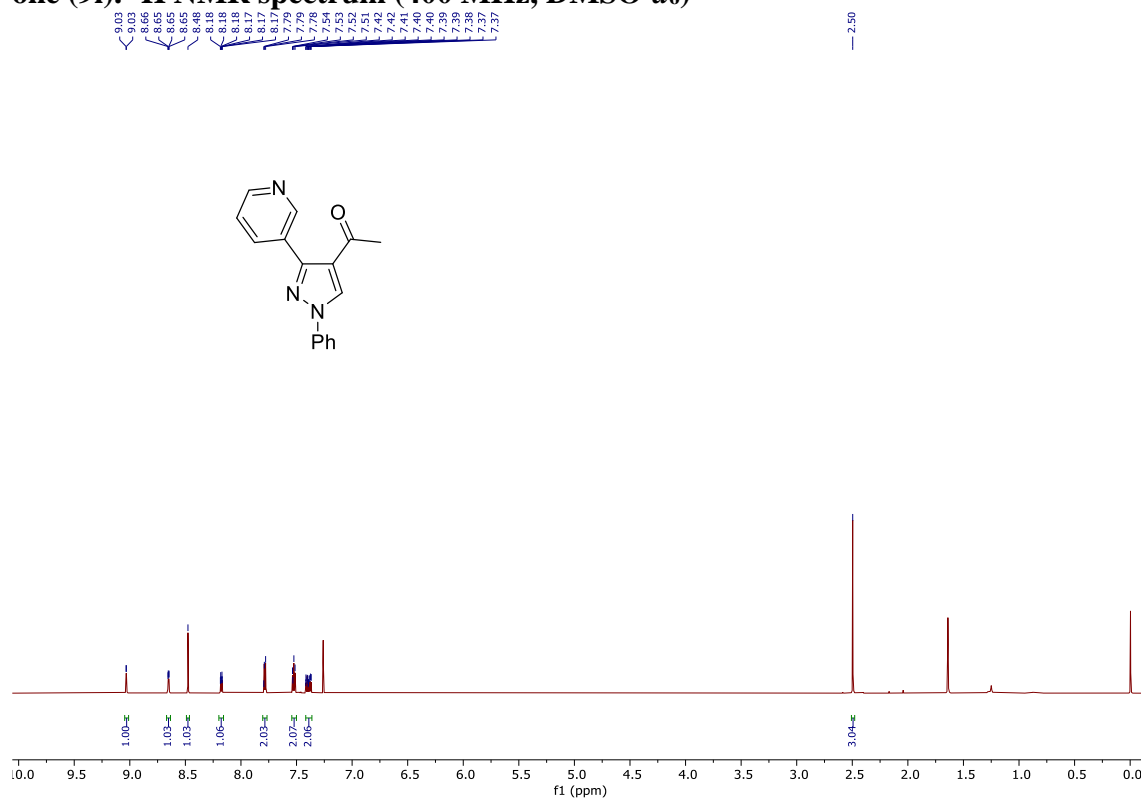


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
333.1591	1	C <sub>21</sub> H <sub>21</sub> N <sub>2</sub> O <sub>2</sub>	333.1598	-2.0	4.0	1	100.00	12.5	even	ok
355.1417	1	C <sub>21</sub> H <sub>20</sub> N <sub>2</sub> NaO <sub>2</sub>	355.1417	-0.0	1.8	1	100.00	12.5	even	ok

Figure S130. (2E)-3-Phenyl-1-(1-phenyl-3-propoxy-1H-pyrazol-4-yl)prop-2-en-1-one (9h). HRMS (ESI-TOF).

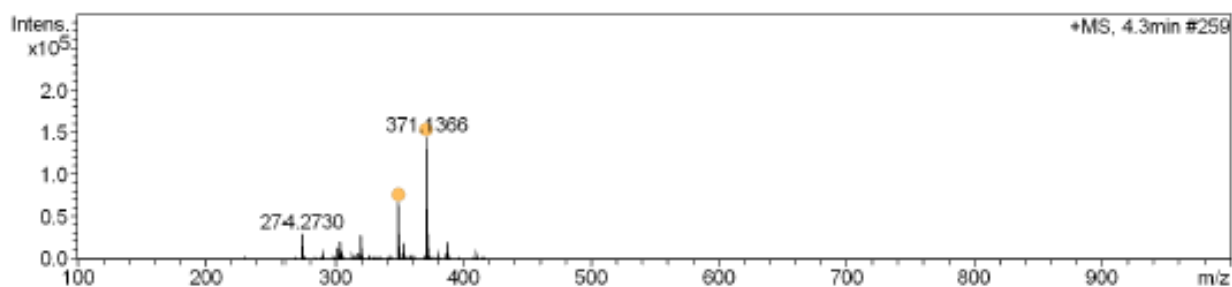


**Figure S131.** (E)-1-[3-(2-Methoxyethoxy)-1-phenyl-1H-pyrazol-4-yl]-3-phenylprop-2-en-1-one (9i). <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>)



**Figure S132.** (E)-1-[3-(2-Methoxyethoxy)-1-phenyl-1H-pyrazol-4-yl]-3-phenylprop-2-en-1-one (9i). <sup>13</sup>C NMR spectrum (101 MHz, DMSO-*d*<sub>6</sub>)

+MS, 4.3min #259



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
349.1550	1	C <sub>21</sub> H <sub>21</sub> N <sub>2</sub> O <sub>3</sub>	349.1547	0.9	0.8	1	100.00	12.5	even	ok
371.1368	1	C <sub>21</sub> H <sub>20</sub> N <sub>2</sub> NaO <sub>3</sub>	371.1366	-0.1	5.0	1	100.00	12.5	even	ok

Figure S133. (2*E*)-1-[3-(2-Methoxyethoxy)-1-phenyl-1*H*-pyrazol-4-yl]-3-phenylprop-2-en-1-one (9i). HRMS (ESI-TOF).

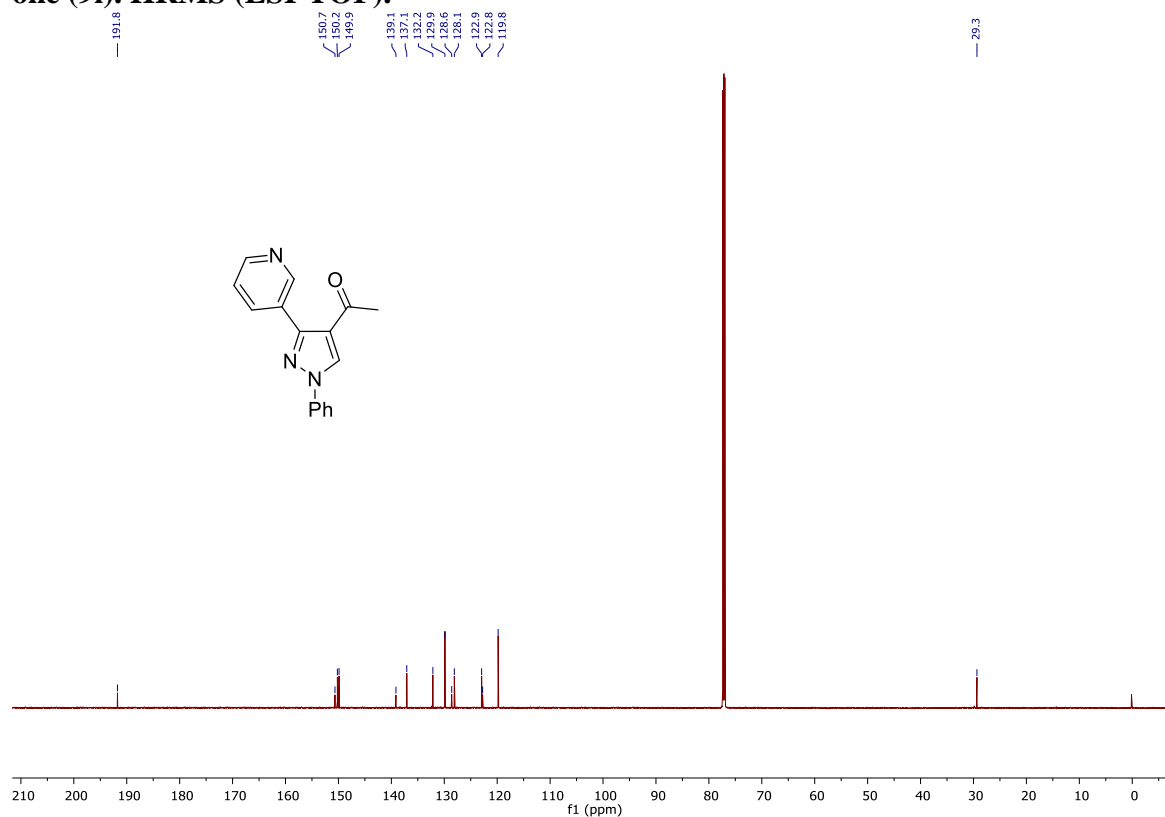
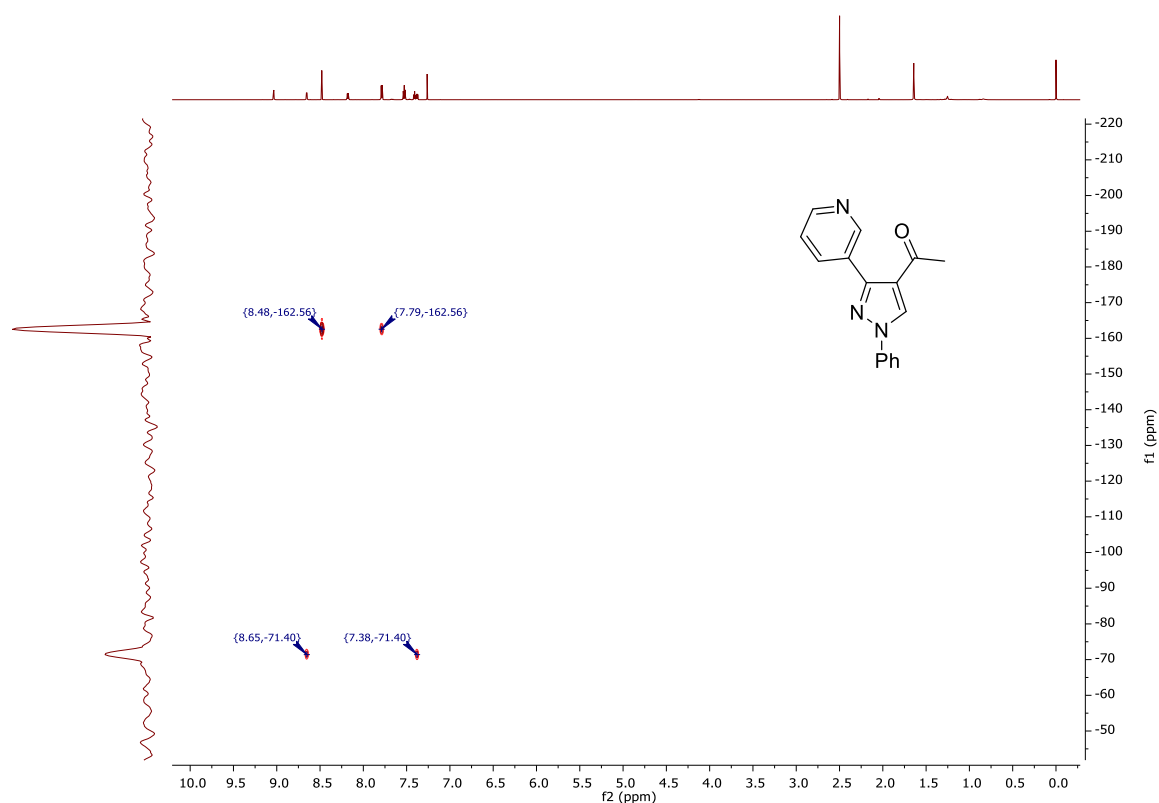


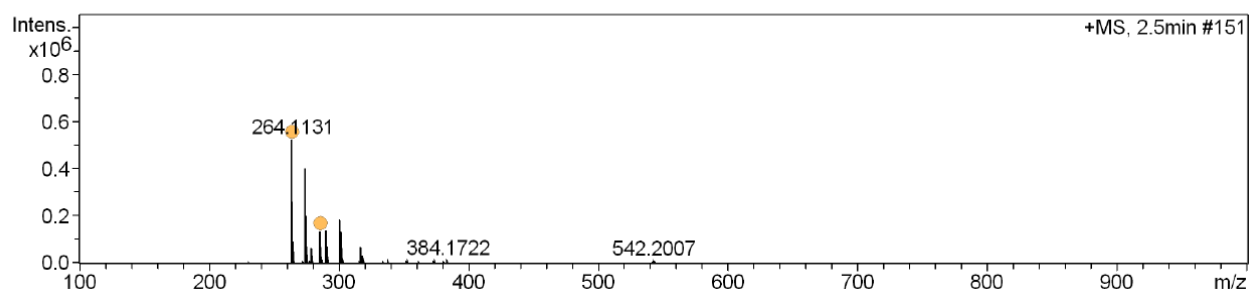
Figure S134. 1-[1-Phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]ethan-1-one (11a). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)





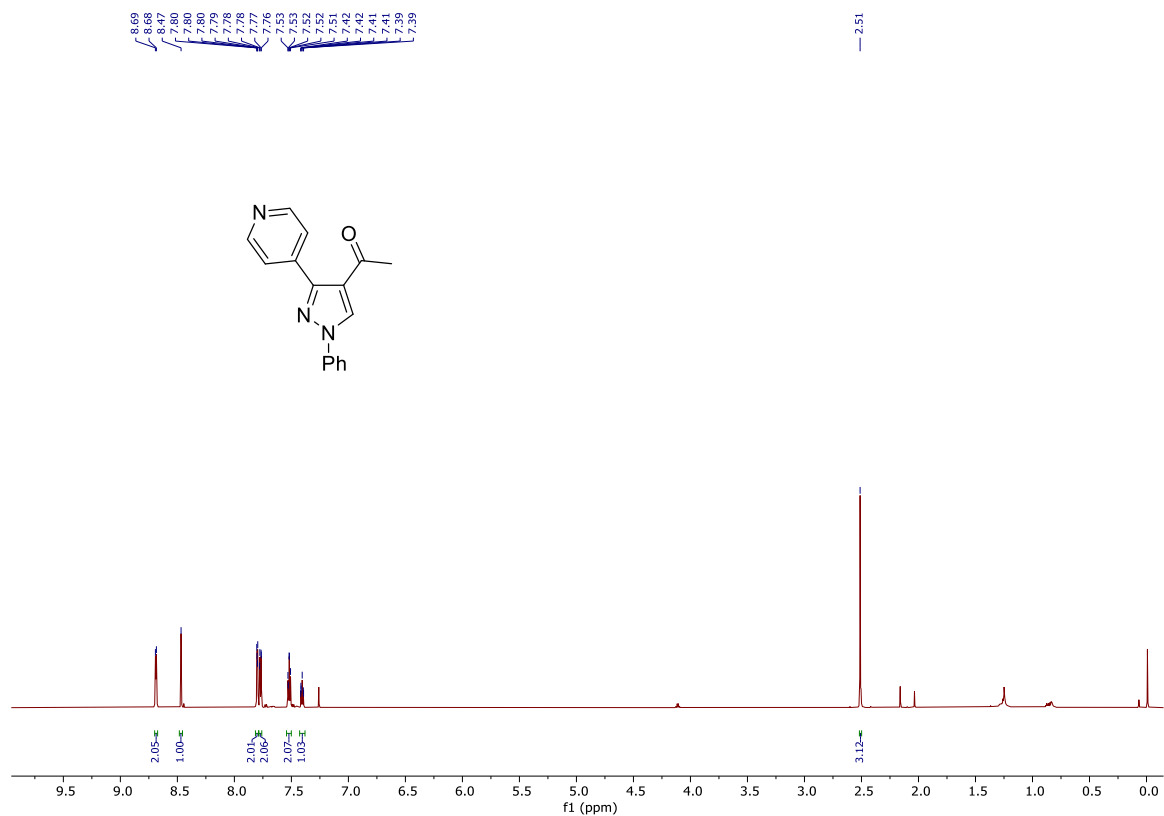
**Figure S135.** 1-[1-Phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]ethan-1-one (11a).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

**+MS, 2.5min #151**

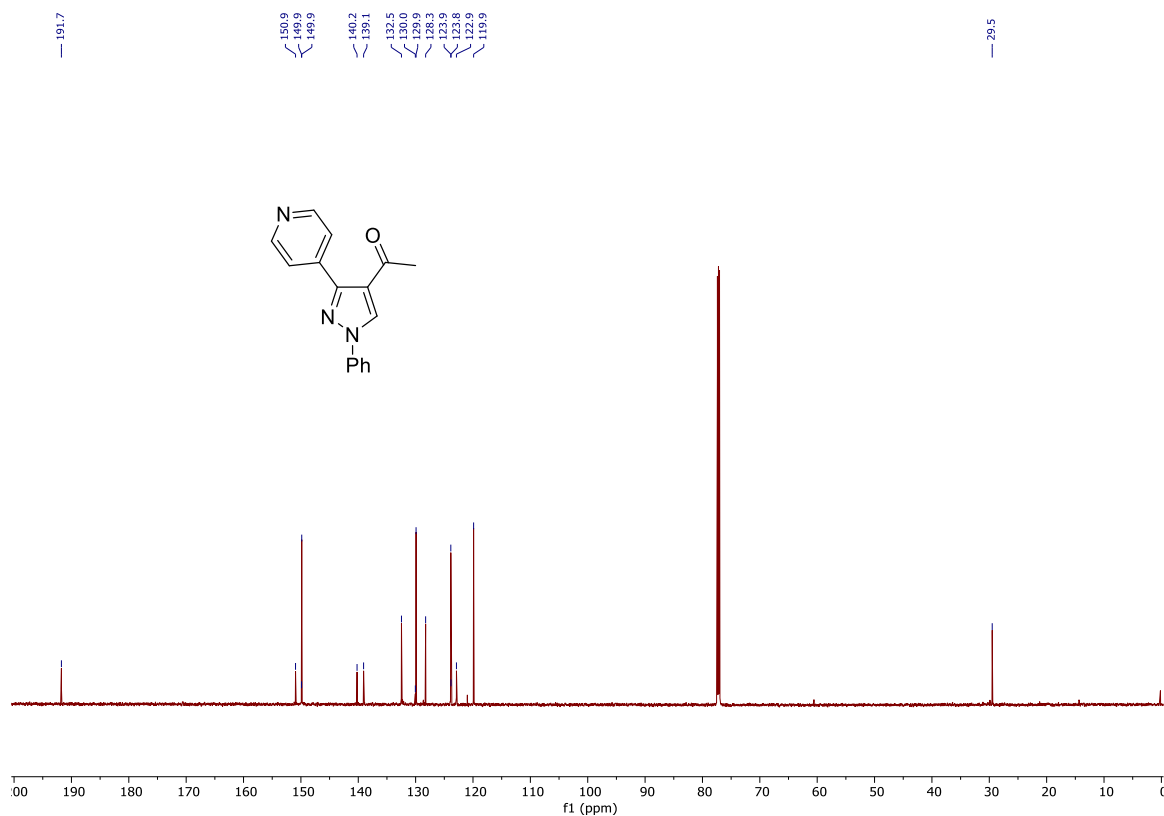


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
264.1131	1	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O	264.1131	-0.2	0.5	1	100.00	11.5	even		ok
286.0948	1	C <sub>16</sub> H <sub>13</sub> N <sub>3</sub> NaO	286.0951	1.1	4.2	1	100.00	11.5	even		ok

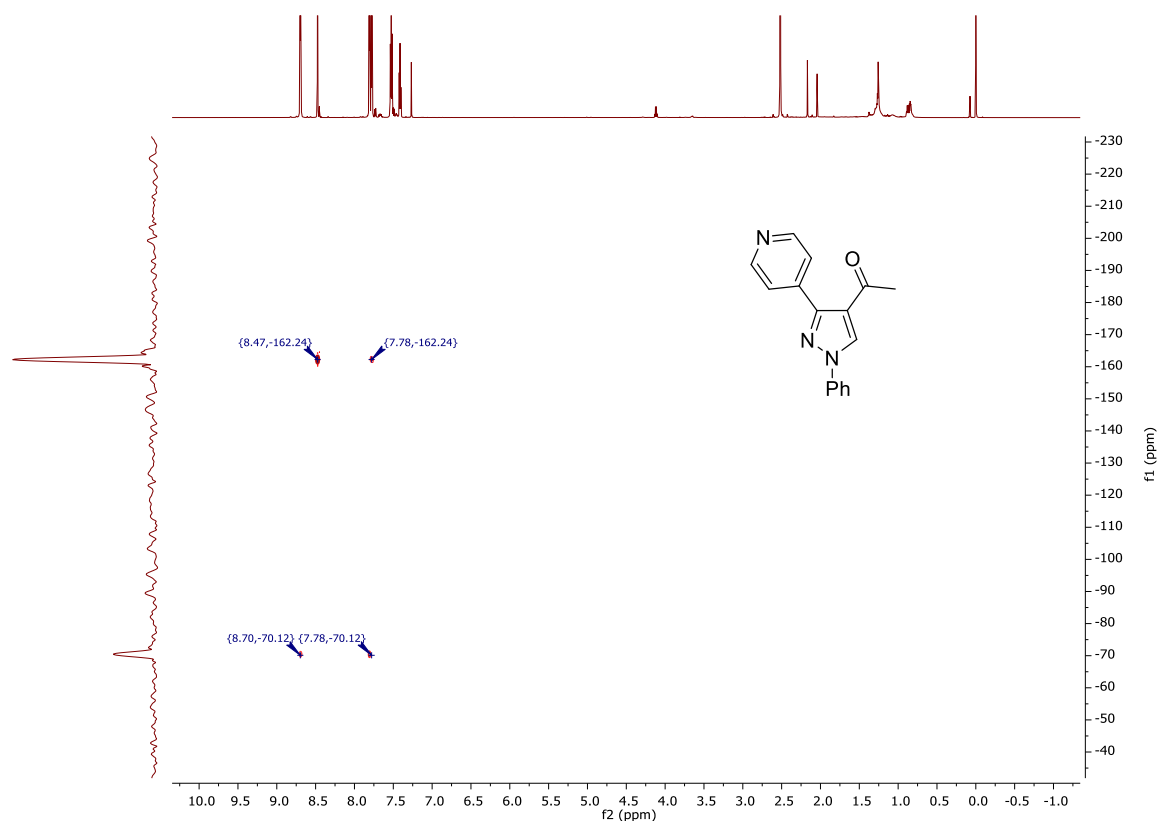
**Figure S136.** 1-[1-Phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]ethan-1-one (11a). HRMS (ESI-TOF).



**Figure S137. 1-[1-Phenyl-3-(pyridin-4-yl)-1H-pyrazol-4-yl]ethan-1-one (11b). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**

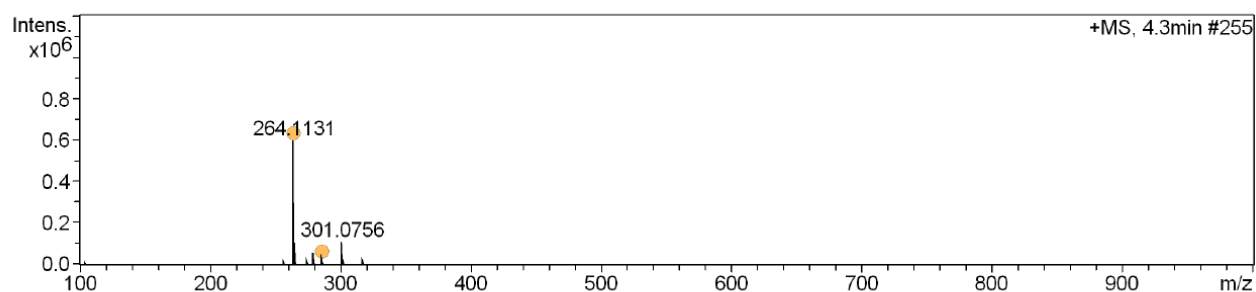


**Figure S138. 1-[1-Phenyl-3-(pyridin-4-yl)-1H-pyrazol-4-yl]ethan-1-one (11b). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)**



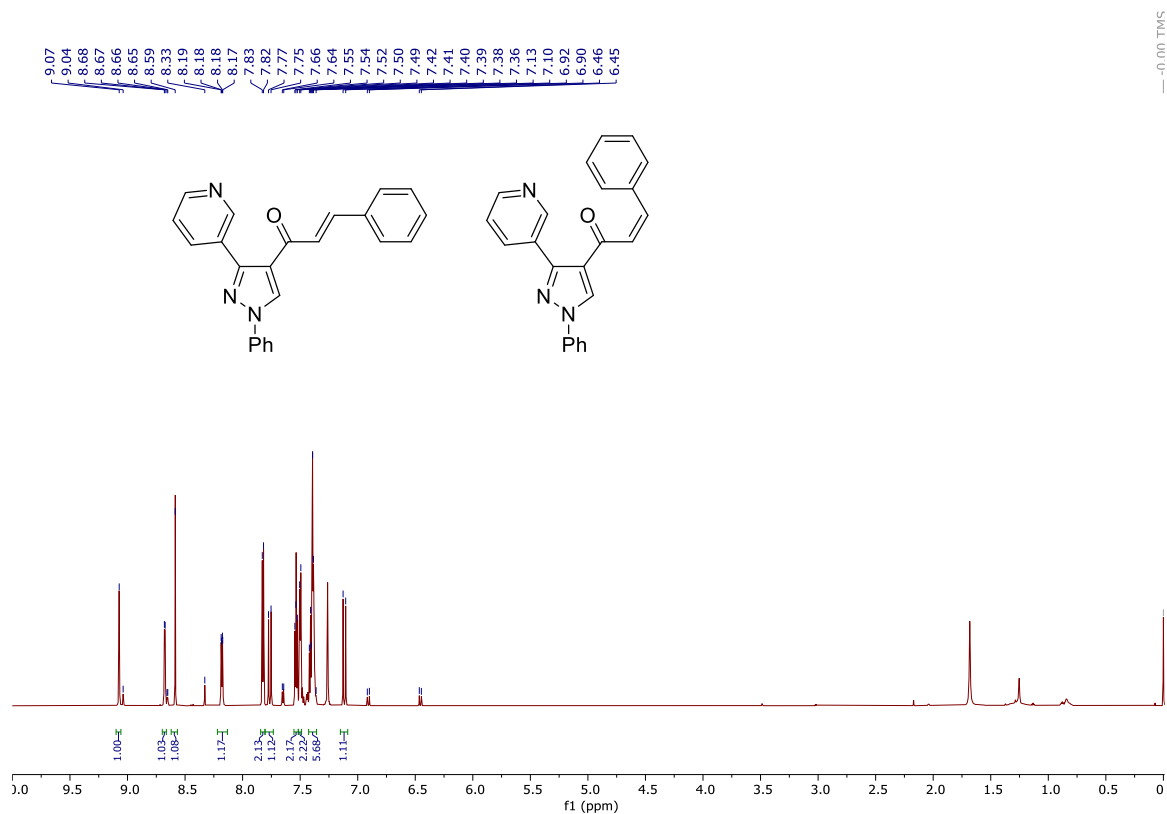
**Figure S139.** 1-[1-Phenyl-3-(pyridin-4-yl)-1*H*-pyrazol-4-yl]ethan-1-one (11b).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

**+MS, 4.3min #255**

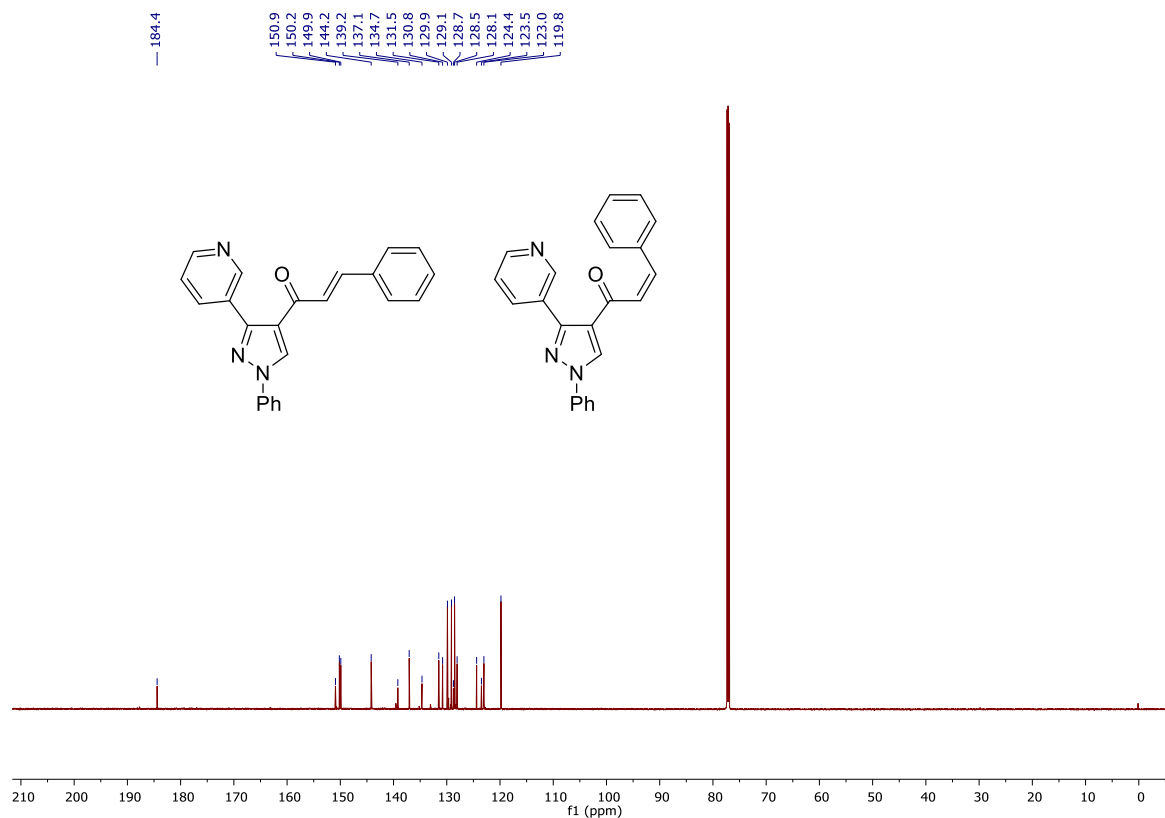


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
264.1131	1	C <sub>16</sub> H <sub>14</sub> N <sub>3</sub> O	264.1131	-0.3	3.0	1	100.00	11.5	even	ok
286.0951	1	C <sub>16</sub> H <sub>13</sub> N <sub>3</sub> NaO	286.0951	0.0	10.7	1	100.00	11.5	even	ok

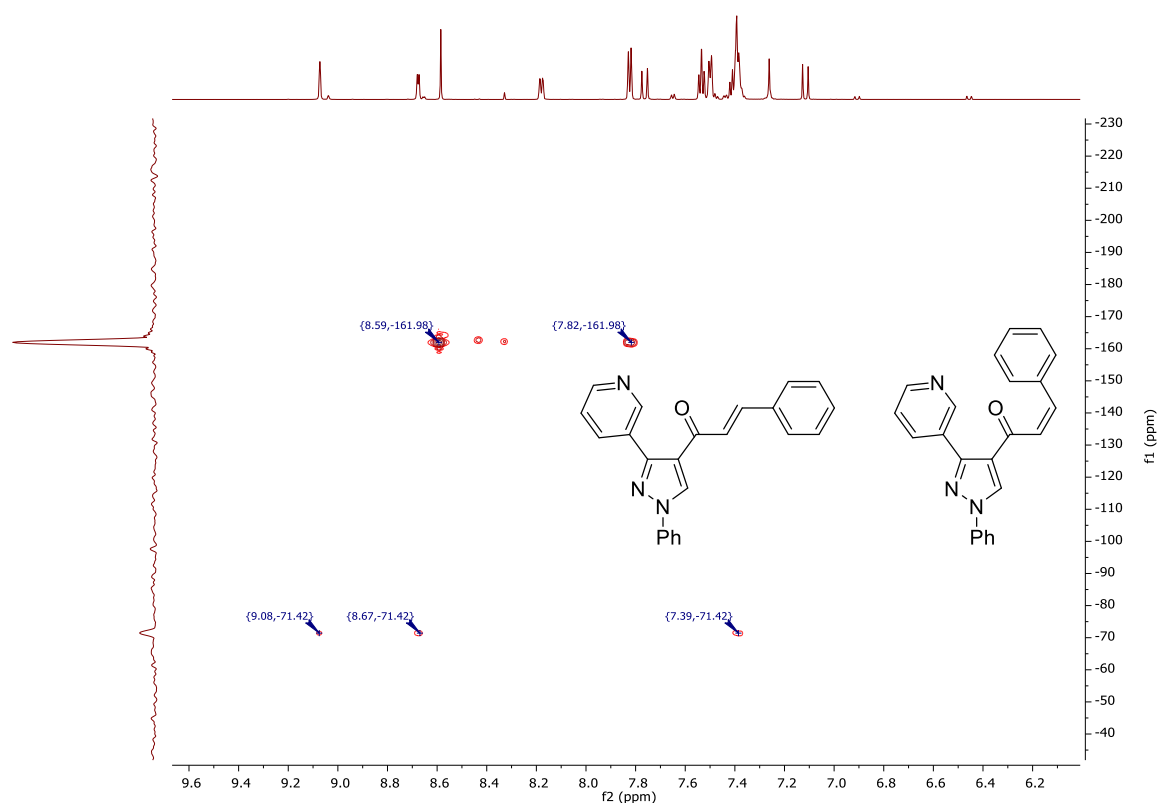
**Figure S140.** 1-[1-Phenyl-3-(pyridin-4-yl)-1*H*-pyrazol-4-yl]ethan-1-one (11b). HRMS (ESI-TOF).



**Figure S141.** (2E/Z)-3-Phenyl-1-[1-phenyl-3-(pyridin-3-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (E-12a, Z-13a). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)

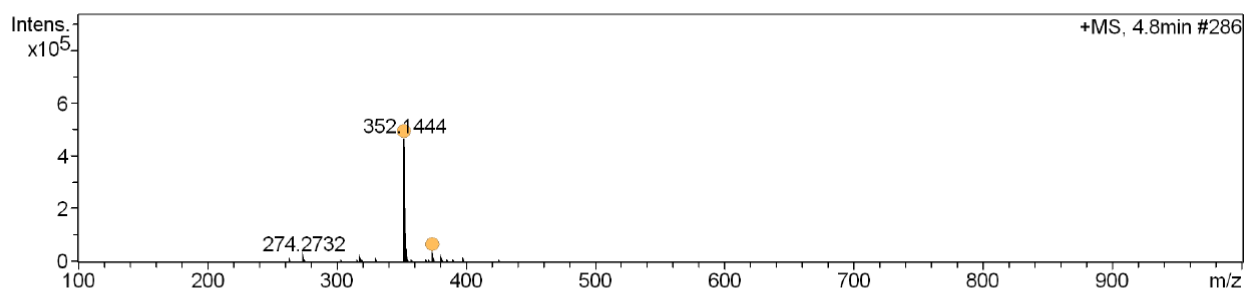


**Figure S142.** (2E/Z)-3-Phenyl-1-[1-phenyl-3-(pyridin-3-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (E-12a, Z-13a). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



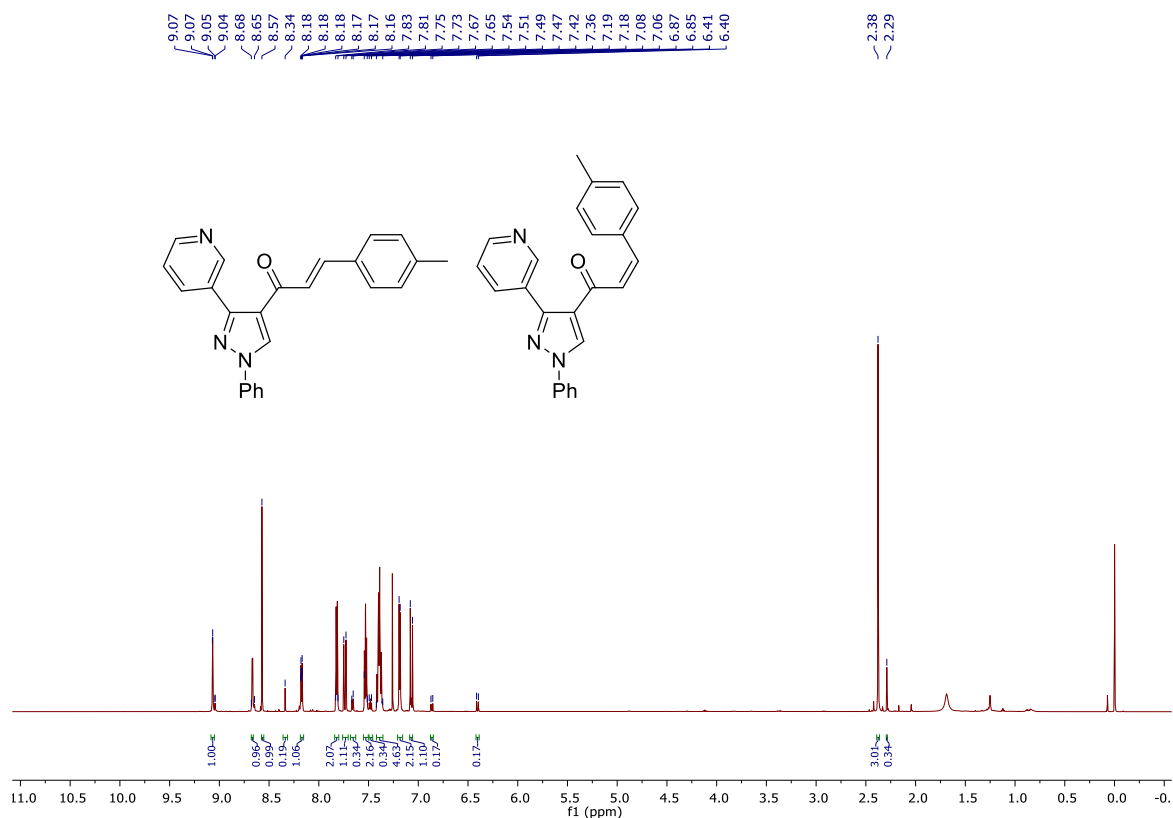
**Figure S143.** (2*E/Z*)-3-Phenyl-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (*E*-12a, *Z*-13a).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

**+MS, 4.8min #286**

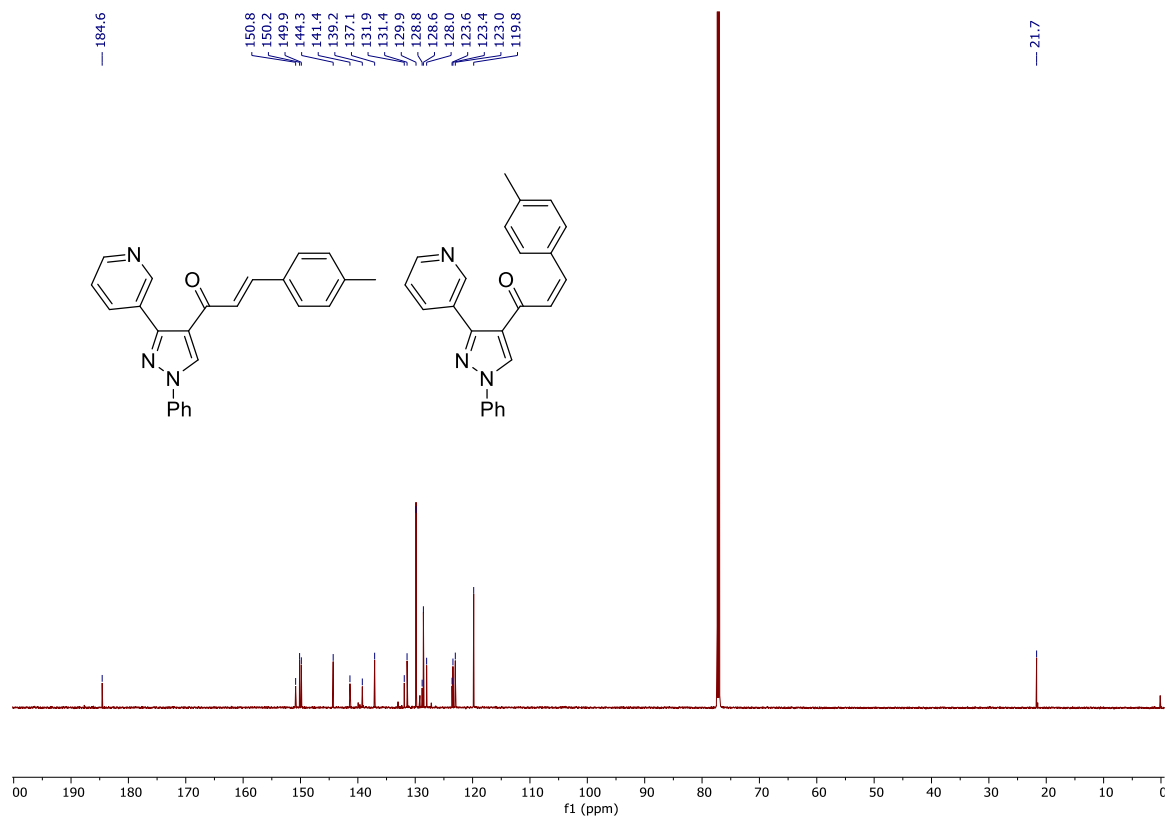


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
352.1444	1	C <sub>23</sub> H <sub>18</sub> N <sub>3</sub> O	352.1444	0.0	5.8	1	100.00	16.5	even	ok
374.1261	1	C <sub>23</sub> H <sub>17</sub> N <sub>3</sub> NaO	374.1264	0.8	5.6	1	100.00	16.5	even	ok

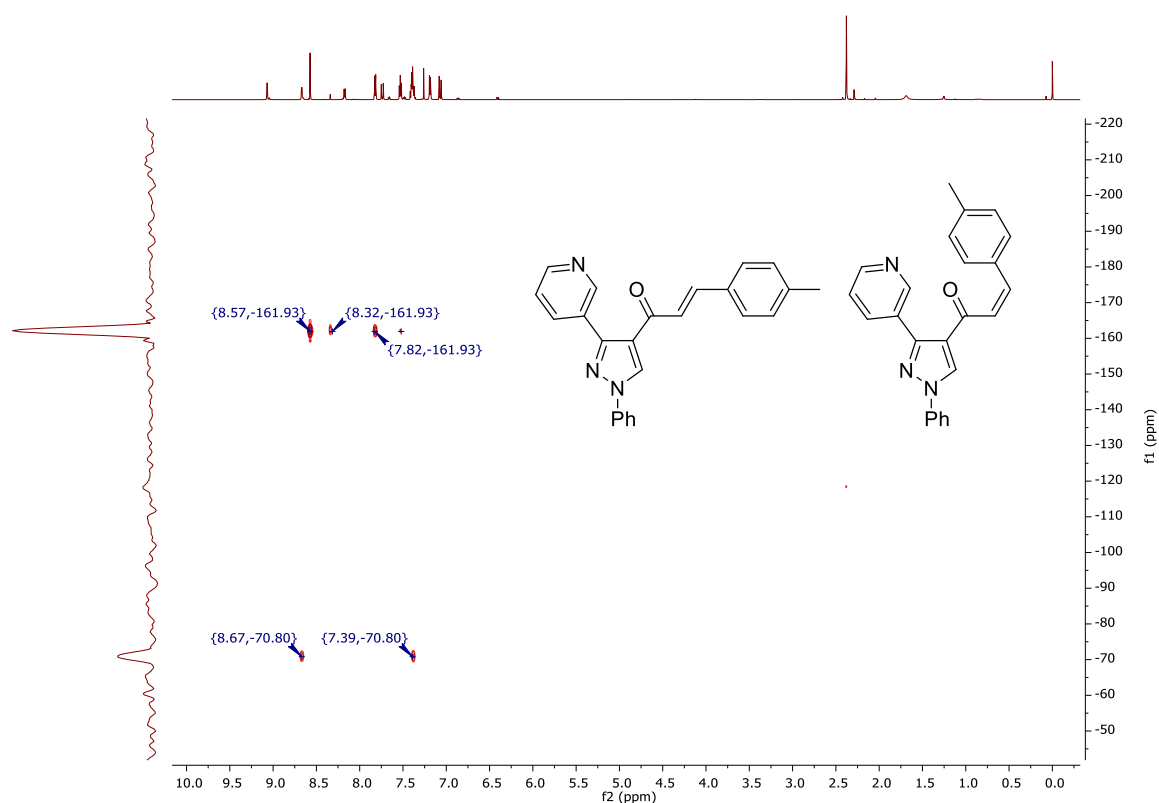
**Figure S144.** (2*E/Z*)-3-Phenyl-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (*E*-12a, *Z*-13a). HRMS (ESI-TOF).



**Figure S145.** (2*E/Z*)-3-(4-Methylphenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-Pyrazol-4-yl]prop-2-en-1-one (E-12b, Z-13b). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)

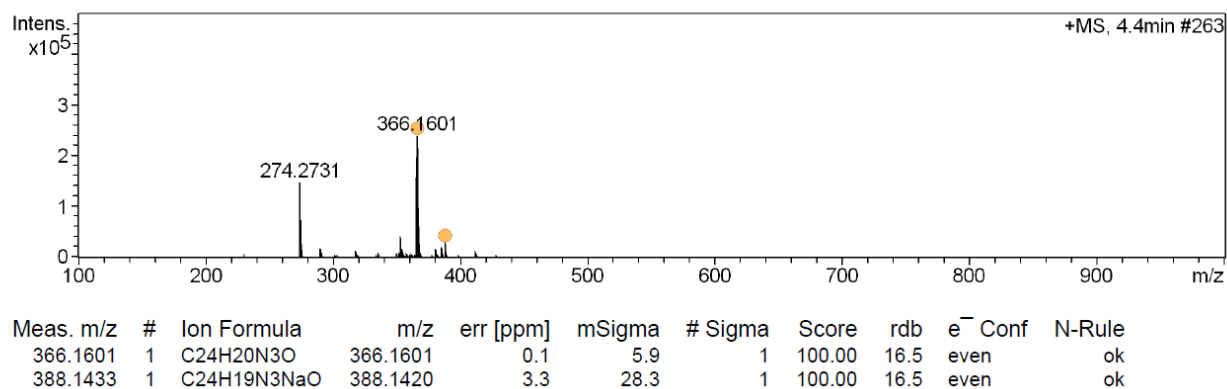


**Figure S146.** (2*E/Z*)-3-(4-Methylphenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-Pyrazol-4-yl]prop-2-en-1-one (E-12b, Z-13b). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)

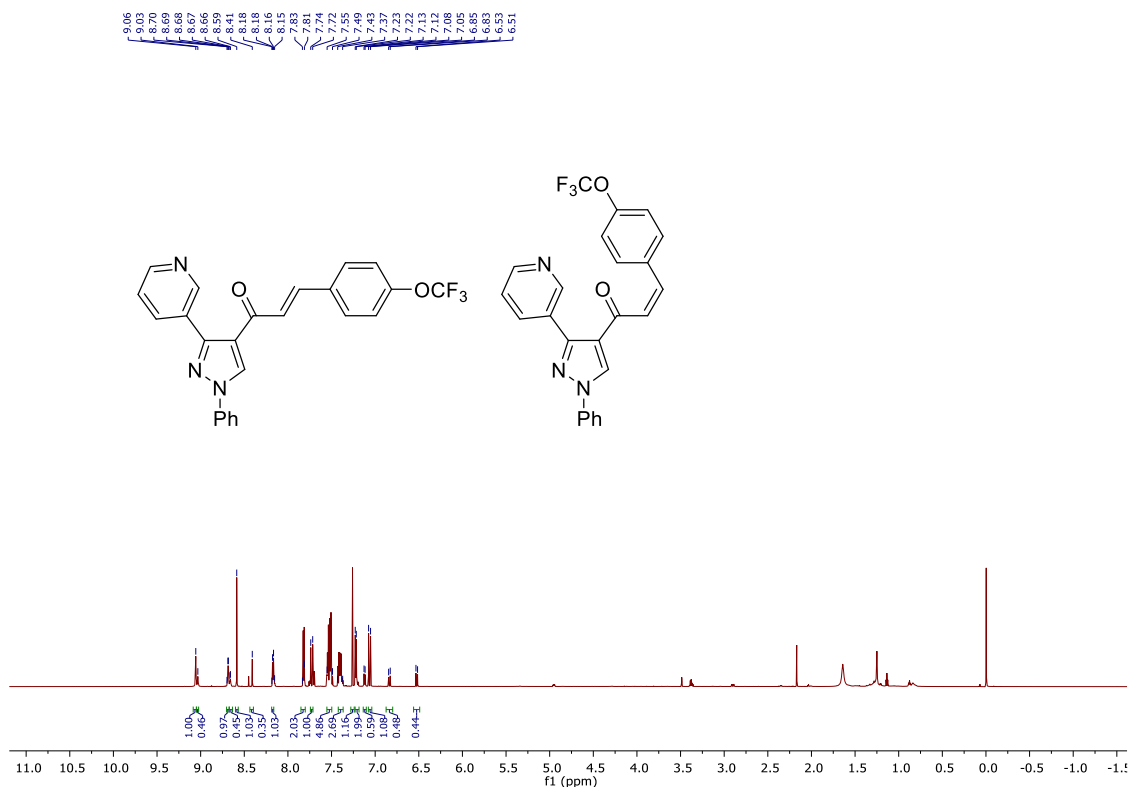


**Figure S147.** (2*E/Z*)-3-(4-Methylphenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-Pyrazol-4-yl]prop-2-en-1-one (*E*-12b, *Z*-13b).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

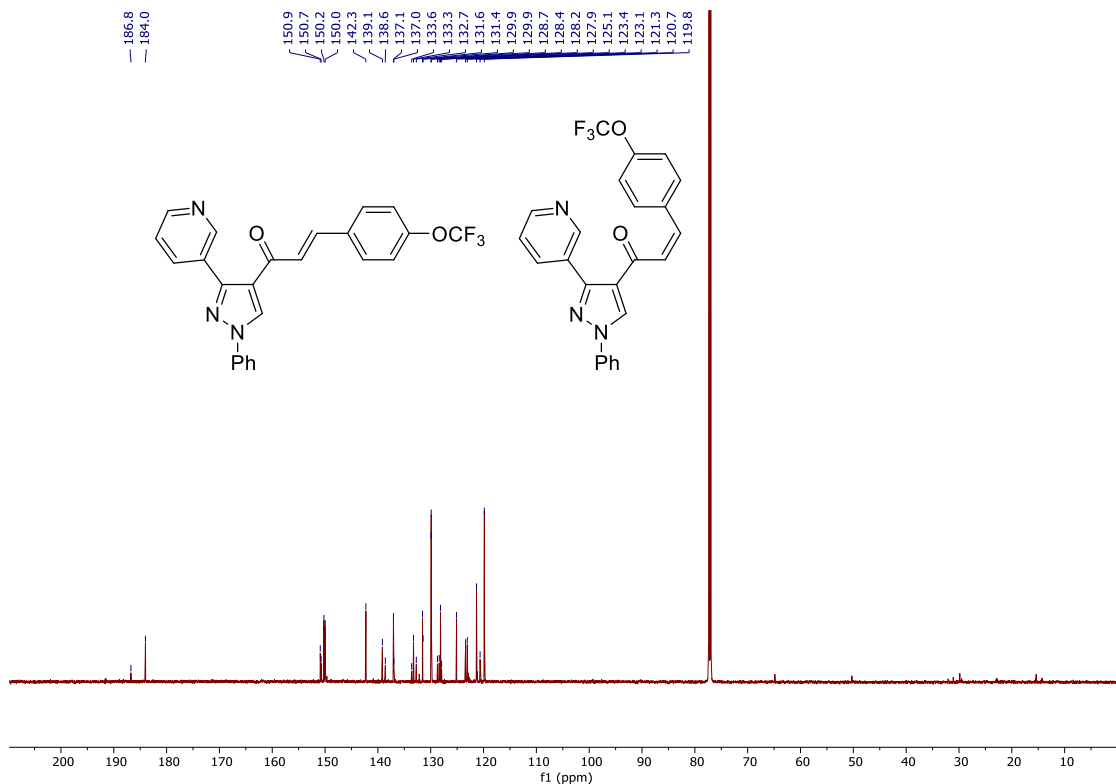
+MS, 4.4min #263



**Figure S148.** (2*E/Z*)-3-(4-Methylphenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-Pyrazol-4-yl]prop-2-en-1-one (*E*-12b, *Z*-13b). HRMS (ESI-TOF).

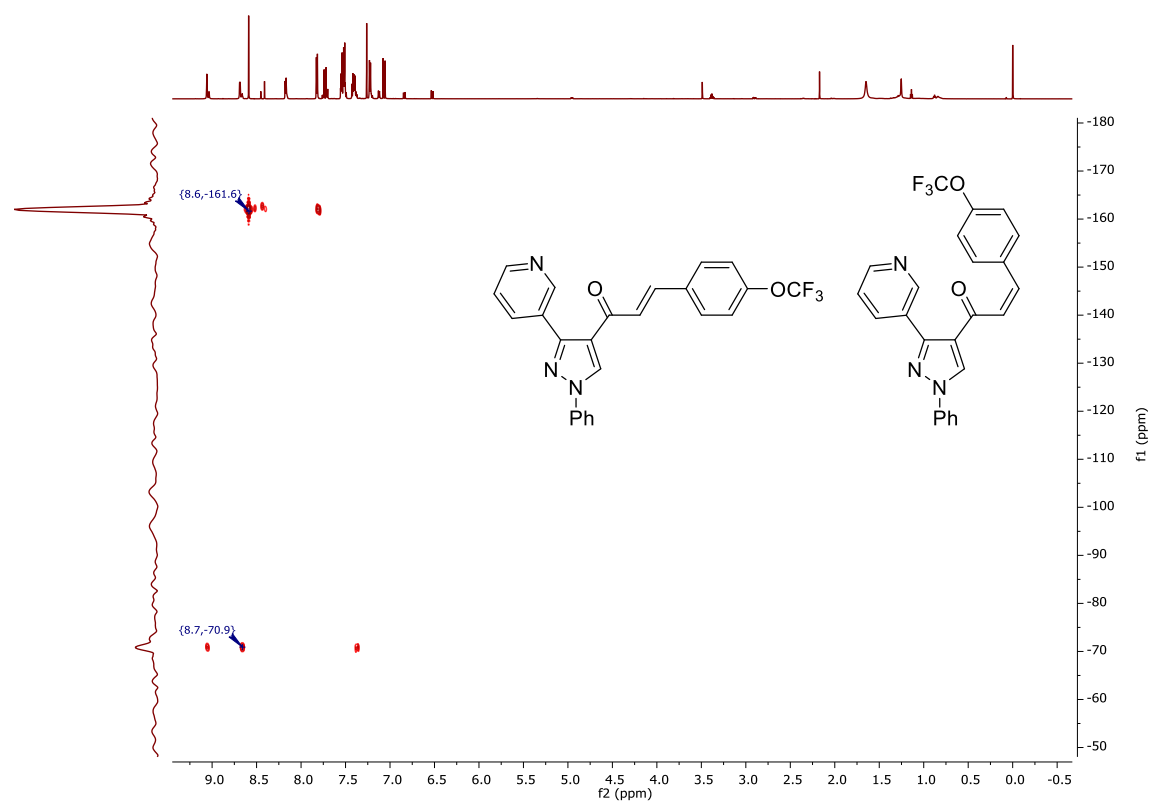


**Figure S149.** (2*E/Z*)-1-[1-Phenyl-3-(pyridine-3-yl)-1*H*-pyrazol-4-yl]-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (*E*-12c, *Z*-13c). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)



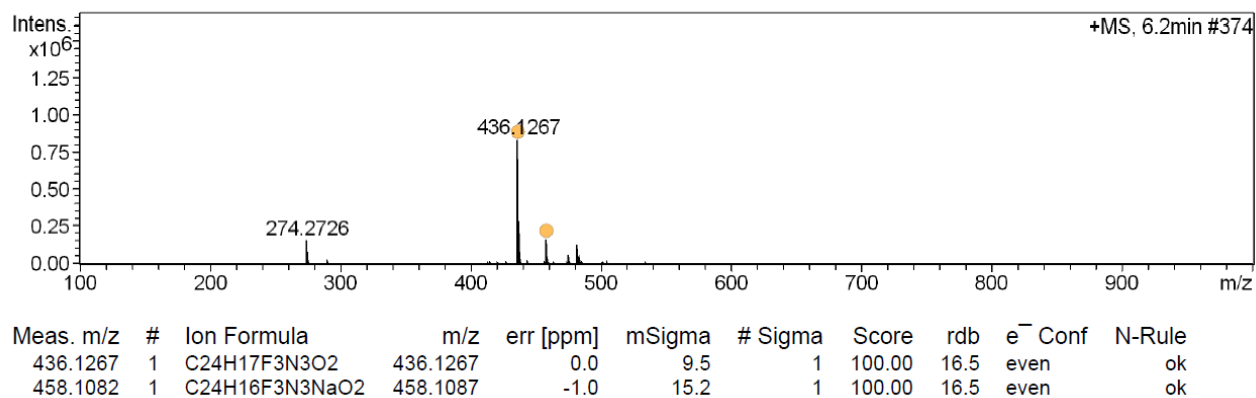
**Figure S150.** (2*E/Z*)-1-[1-Phenyl-3-(pyridine-3-yl)-1*H*-pyrazol-4-yl]-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (*E*-12c, *Z*-13c). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



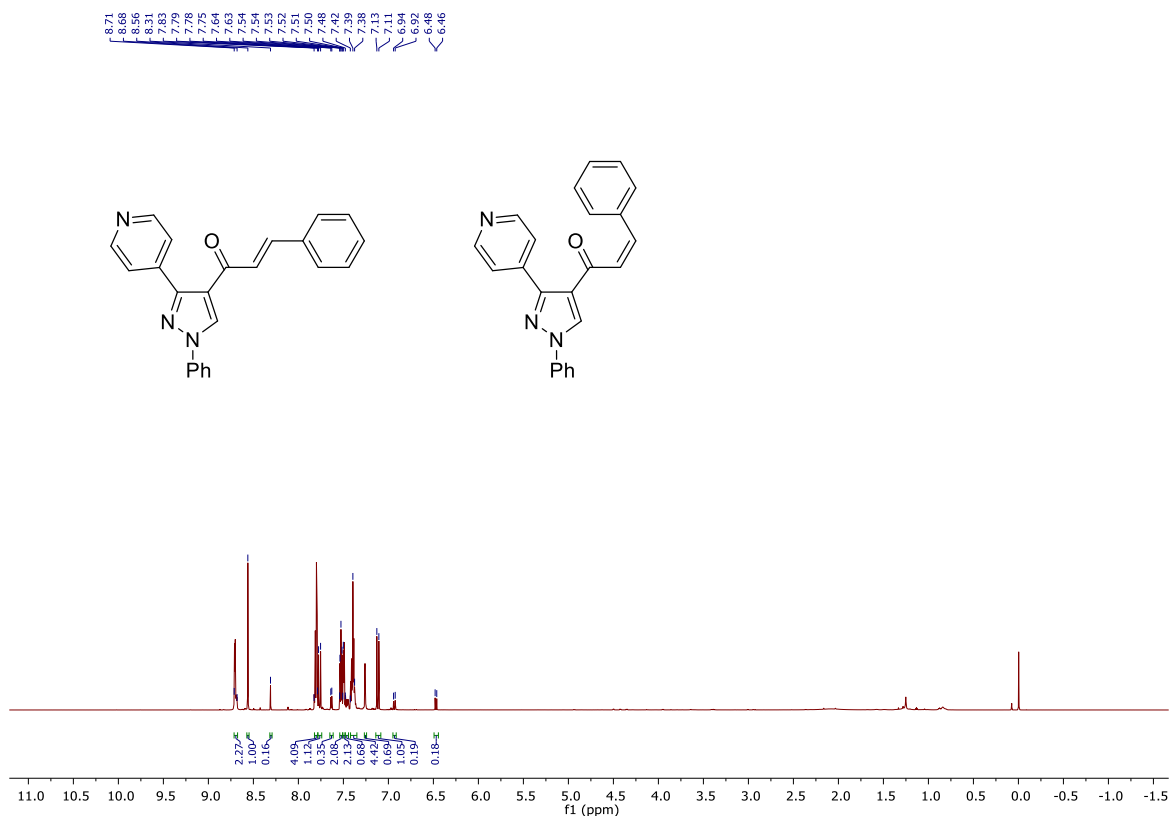


**Figure S151.** (2*E/Z*)-1-[1-Phenyl-3-(pyridine-3-yl)-1*H*-pyrazol-4-yl]-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (*E*-12c, *Z*-13c).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

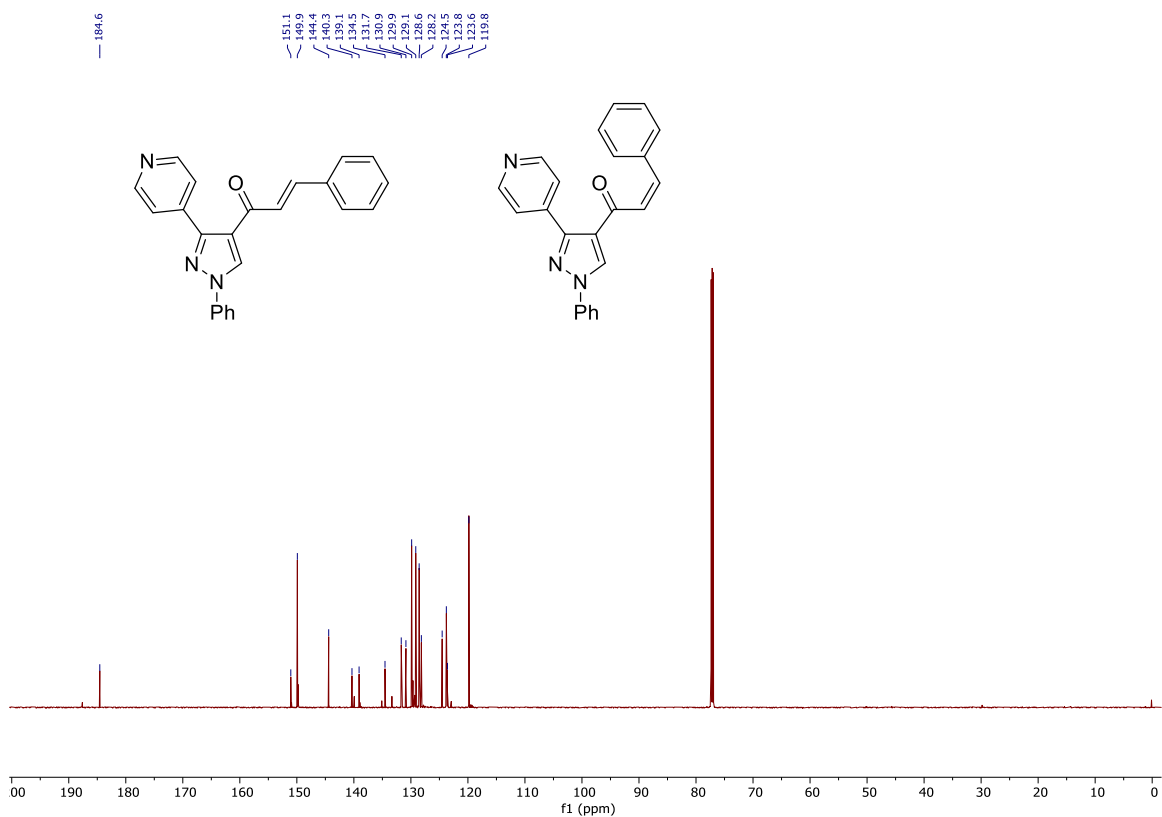
**+MS, 6.2min #374**



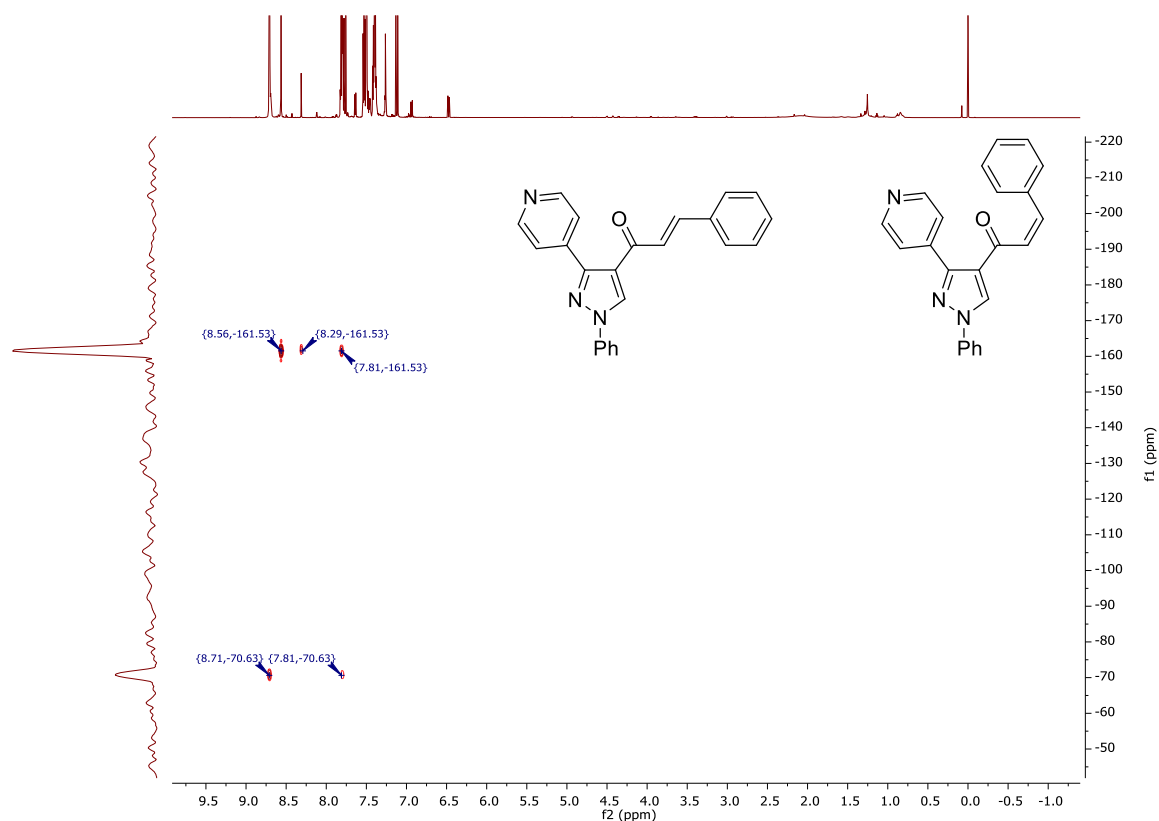
**Figure S152.** (2*E/Z*)-1-[1-Phenyl-3-(pyridine-3-yl)-1*H*-pyrazol-4-yl]-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (*E*-12c, *Z*-13c). HRMS (ESI-TOF).



**Figure S153.** (2*E/Z*)-3-Phenyl-1-[1-phenyl-3-(pyridin-4-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (*E*-12d, *Z*-13d). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)

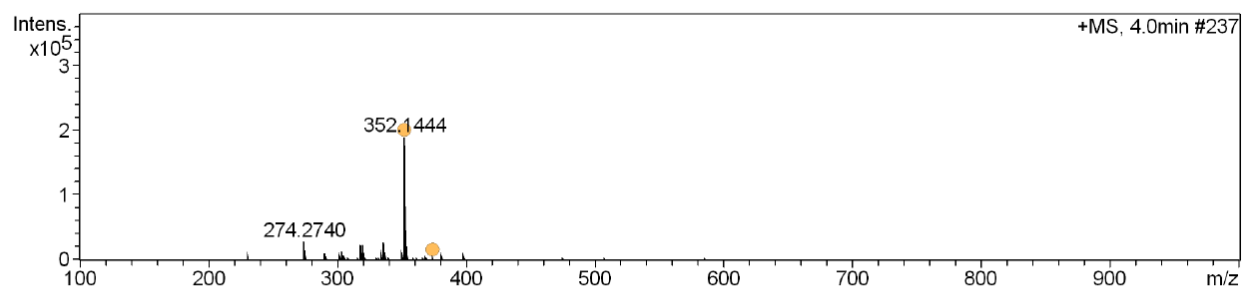


**Figure S154.** (2*E/Z*)-3-Phenyl-1-[1-phenyl-3-(pyridin-4-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (*E*-12d, *Z*-13d). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



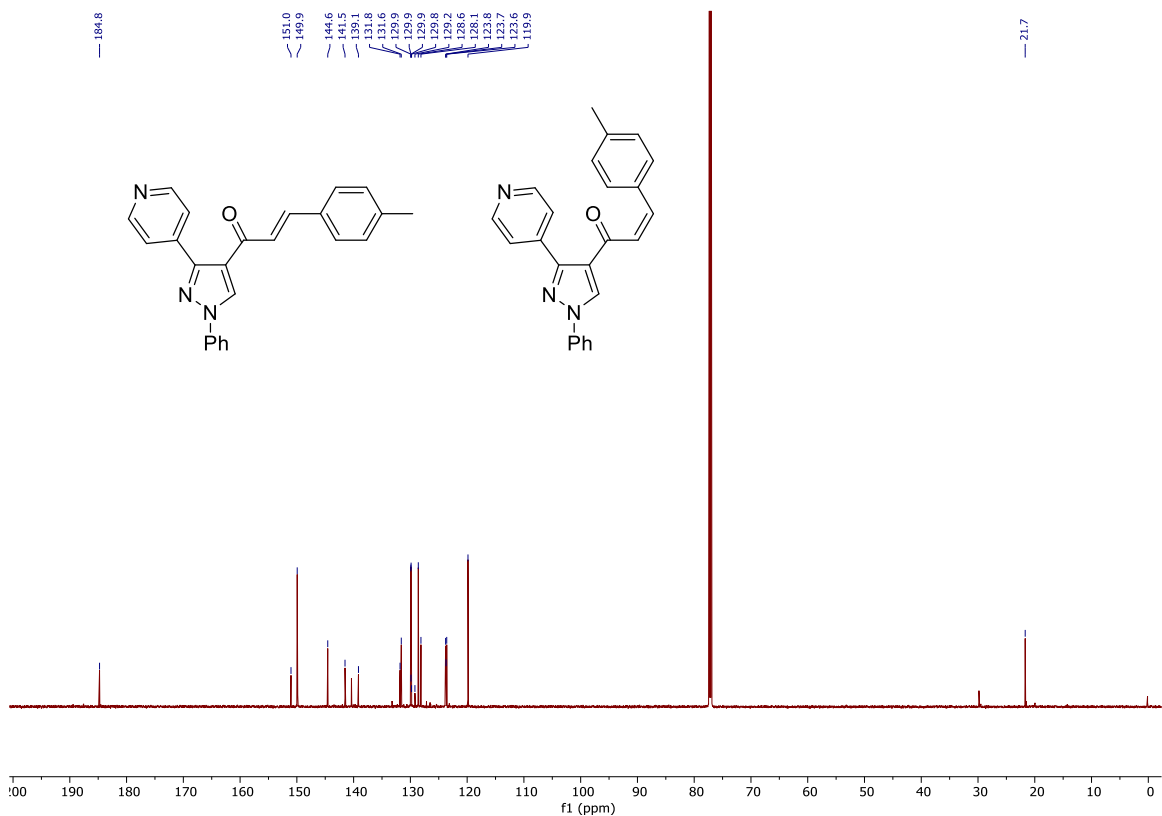
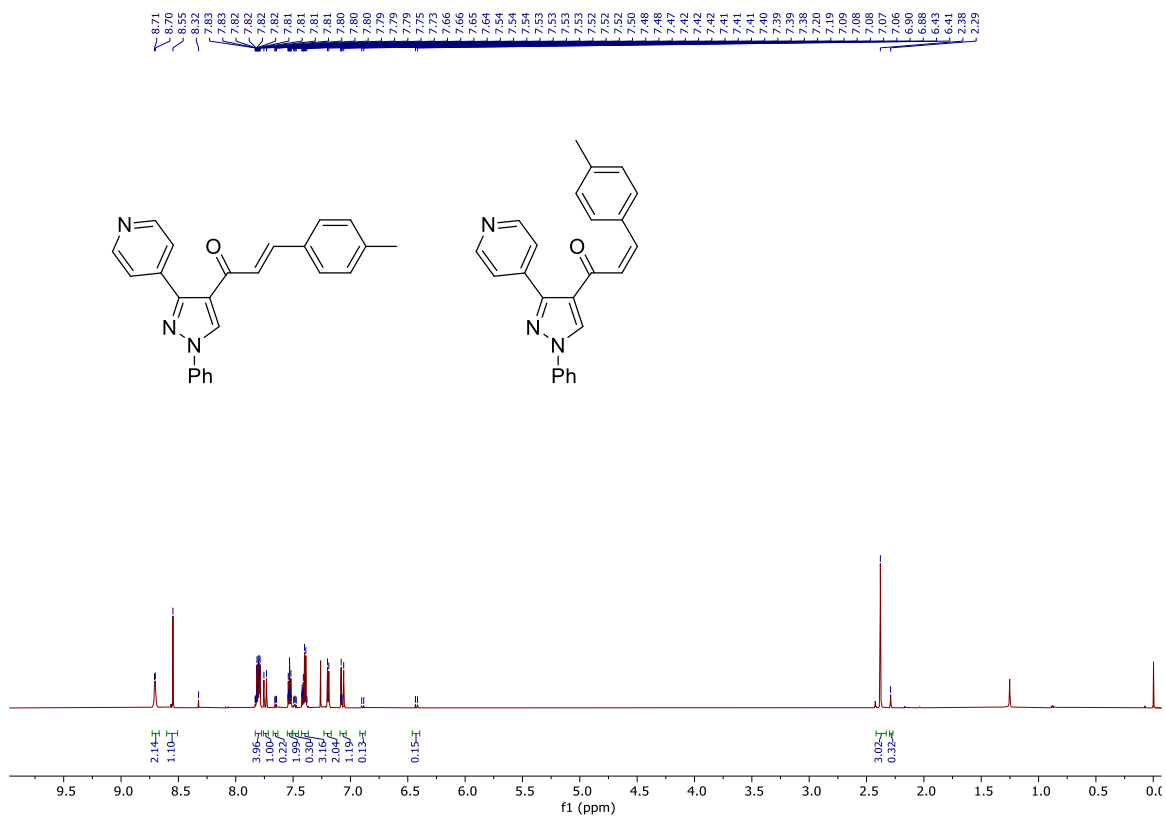
**Figure S155.** (2*E/Z*)-3-Phenyl-1-[1-phenyl-3-(pyridin-4-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (*E*-12d, *Z*-13d).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

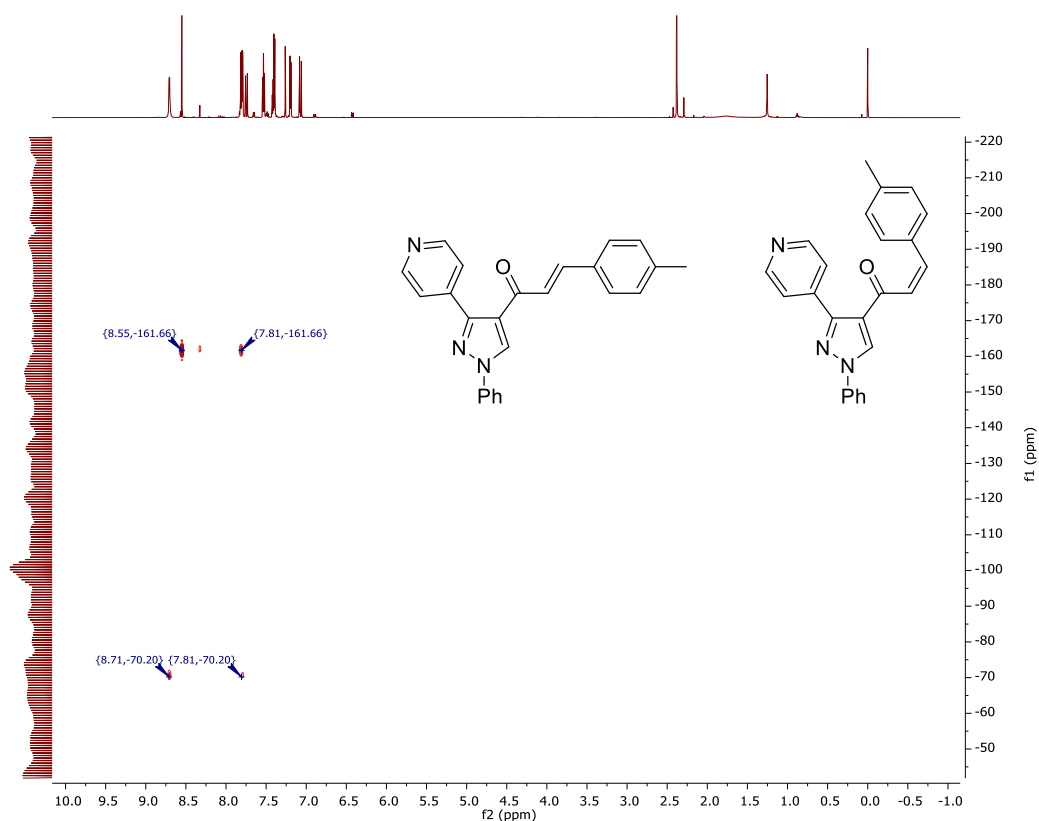
**+MS, 4.0min #237**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
352.1444	1	C <sub>23</sub> H <sub>18</sub> N <sub>3</sub> O	352.1444	-0.1	2.5	1	100.00	16.5	even	ok
374.1266	1	C <sub>23</sub> H <sub>17</sub> N <sub>3</sub> NaO	374.1264	-0.6	18.1	1	100.00	16.5	even	ok

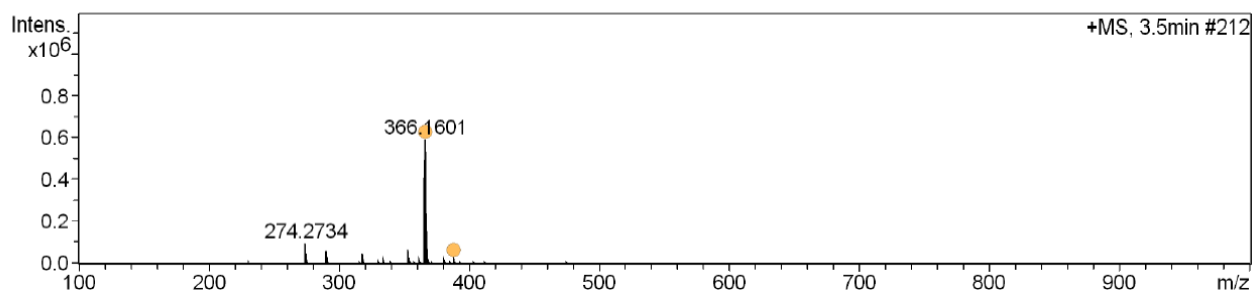
**Figure S156.** (2*E/Z*)-3-Phenyl-1-[1-phenyl-3-(pyridin-4-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (*E*-12d, *Z*-13d). HRMS (ESI-TOF).





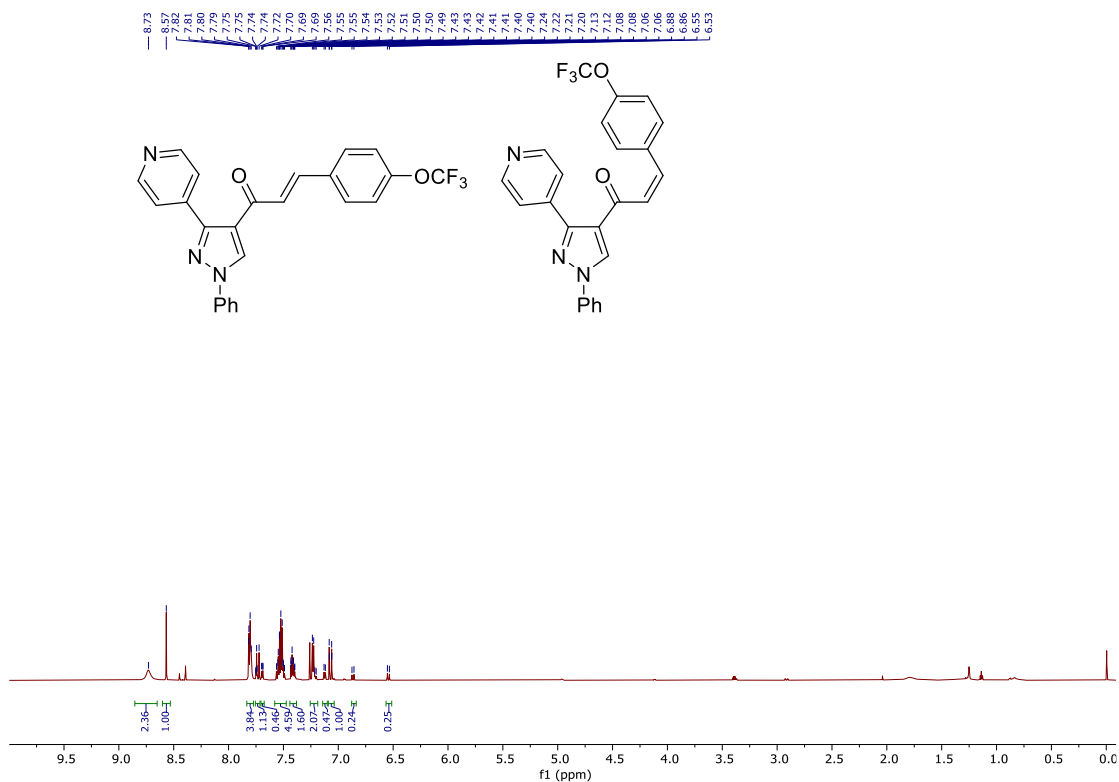
**Figure S159.** (2*E/Z*)-3-(4-Methylphenyl)-1-[1-phenyl-3-(pyridine-4-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (*E*-12e, *Z*-13e).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

+MS, 3.5min #212

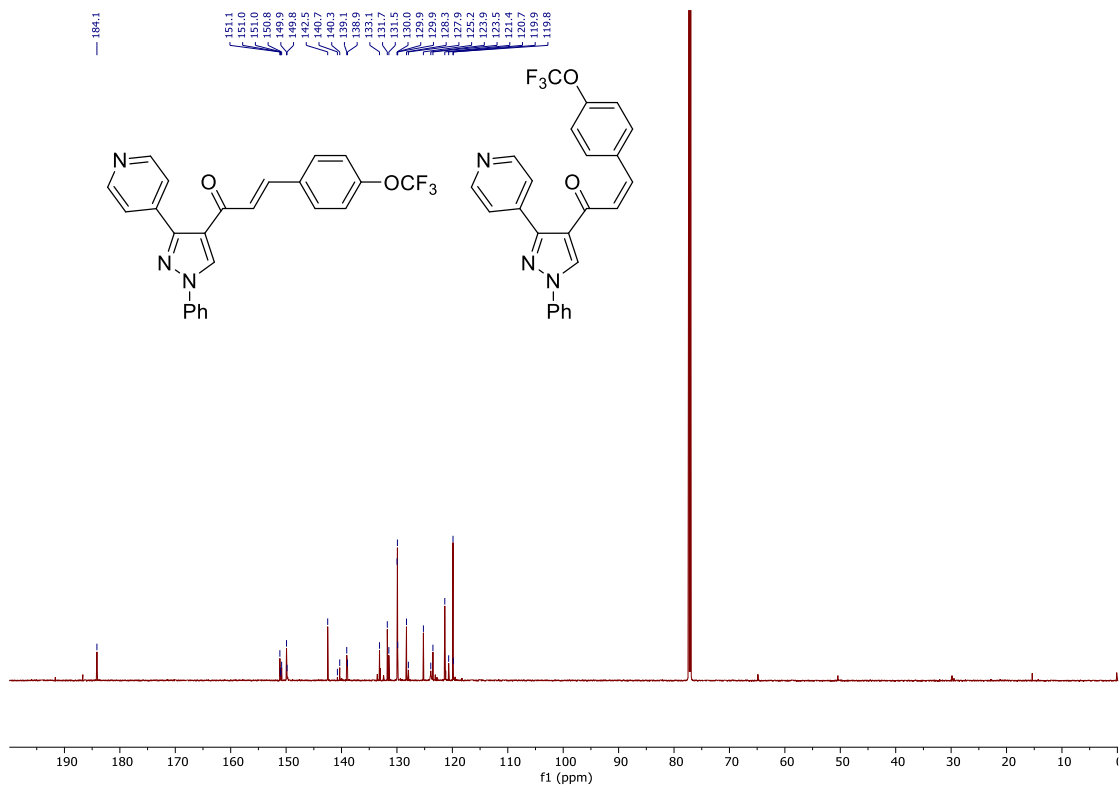


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
366.1601	1	C <sub>24</sub> H <sub>20</sub> N <sub>3</sub> O	366.1601	-0.0	9.5	1	100.00	16.5	even	ok
388.1422	1	C <sub>24</sub> H <sub>19</sub> N <sub>3</sub> NaO	388.1420	-0.4	2.7	1	100.00	16.5	even	ok

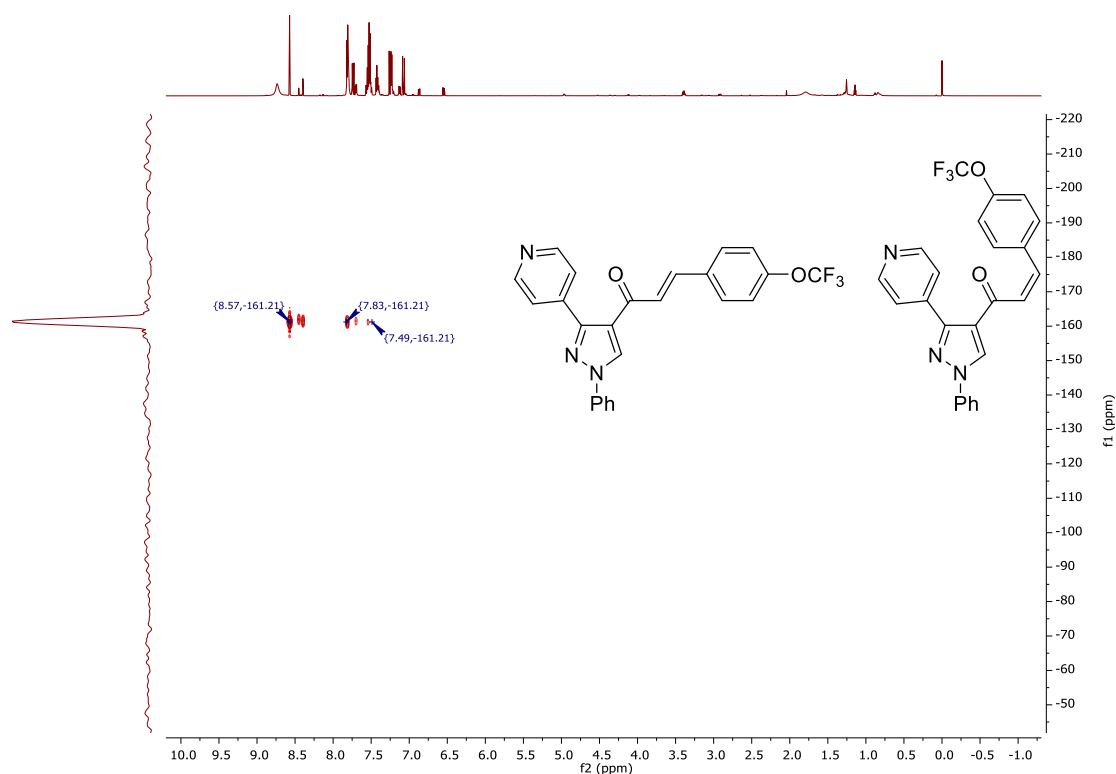
**Figure S160.** (2*E/Z*)-3-(4-Methylphenyl)-1-[1-phenyl-3-(pyridine-4-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (*E*-12e, *Z*-13e). HRMS (ESI-TOF).



**Figure S161.** (2*E/Z*)-1-[1-Phenyl-3-(pyridine-4-yl)-1*H*-pyrazol-4-yl]-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one spectrum (*E*-12f, *Z*-13f). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)

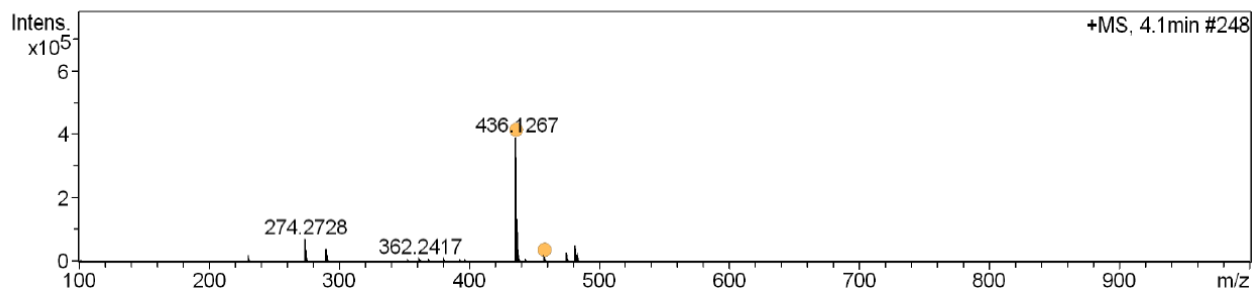


**Figure S162.** (2*E/Z*)-1-[1-Phenyl-3-(pyridine-4-yl)-1*H*-pyrazol-4-yl]-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one spectrum (*E*-12f, *Z*-13f). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



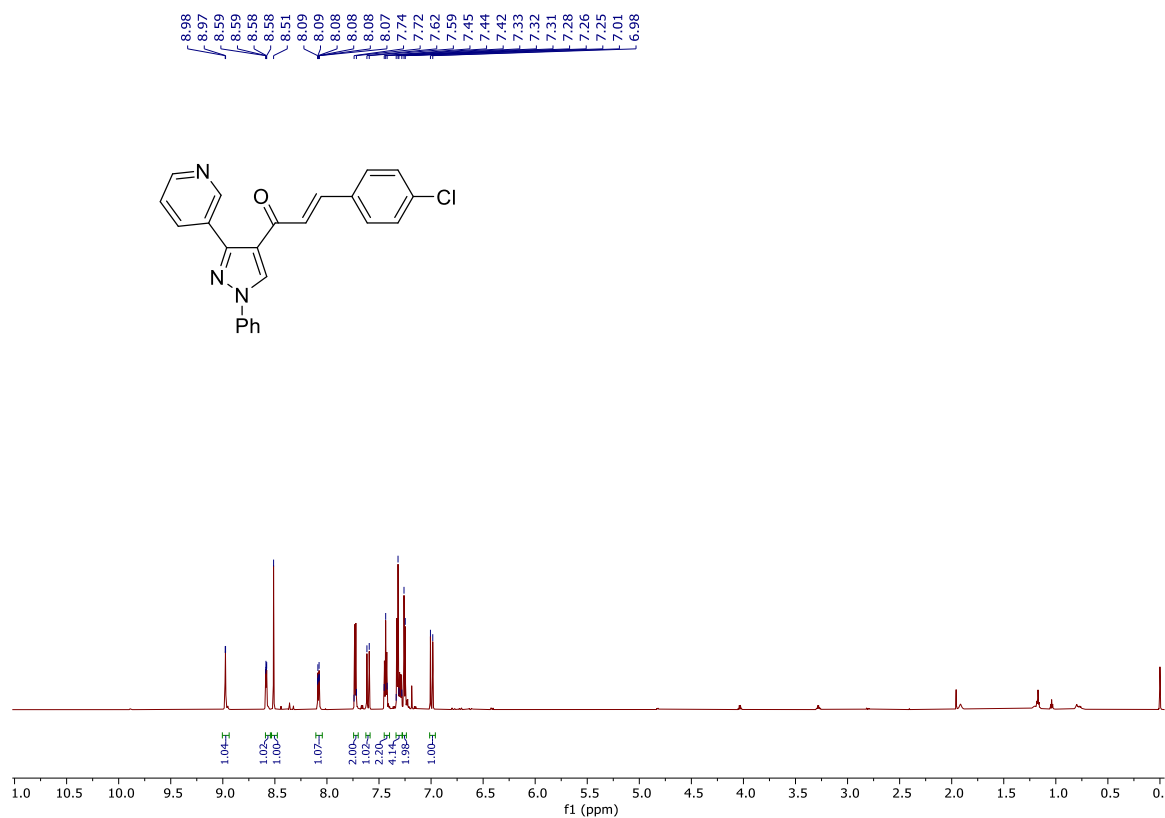
**Figure S163.** (2*E/Z*)-1-[1-Phenyl-3-(pyridine-4-yl)-1*H*-pyrazol-4-yl]-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (*E*-12f, *Z*-13f).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

**+MS, 4.1min #248**

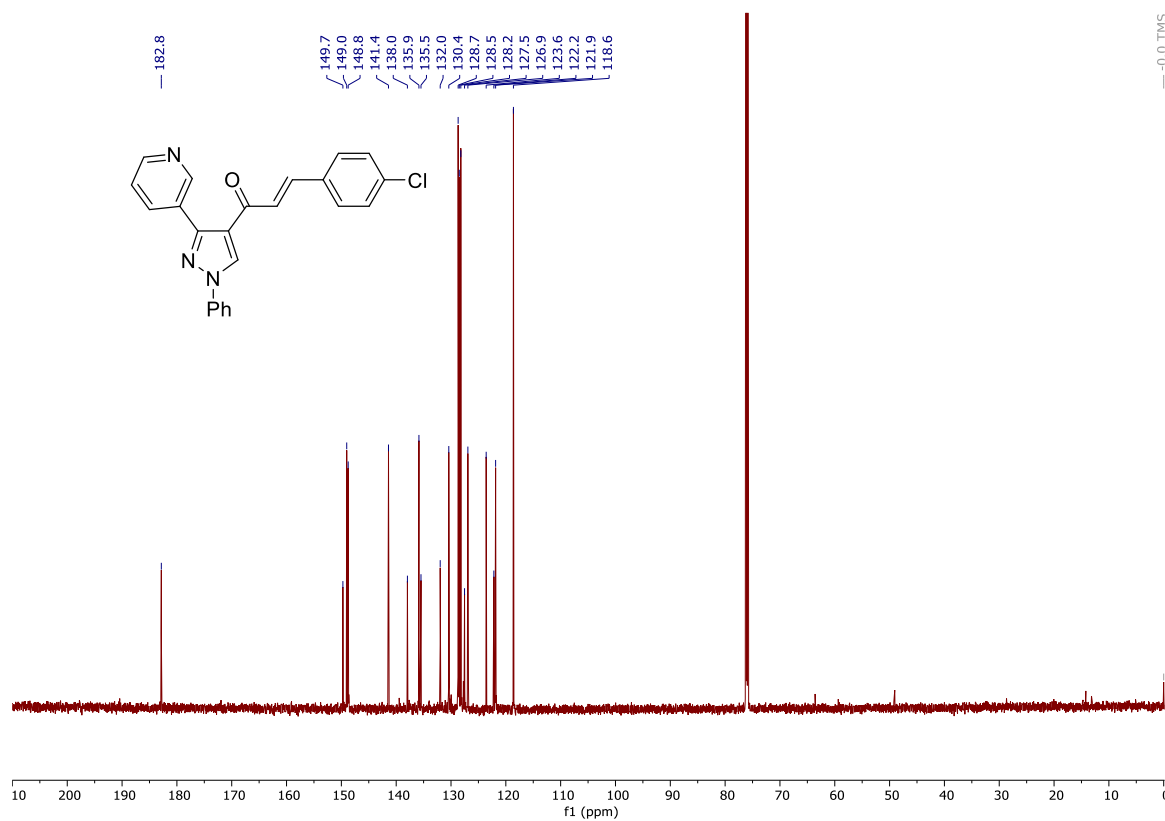


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
436.1267	1	C <sub>24</sub> H <sub>17</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	436.1267	0.0	12.5	1	100.00	16.5	even		ok
458.1083	1	C <sub>24</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> NaO <sub>2</sub>	458.1087	-0.9	35.7	1	100.00	16.5	even		ok

**Figure S164.** (2*E/Z*)-1-[1-Phenyl-3-(pyridine-4-yl)-1*H*-pyrazol-4-yl]-3-[4-(trifluoromethoxy)phenyl]prop-2-en-1-one (*E*-12f, *Z*-13f). HRMS (ESI-TOF).

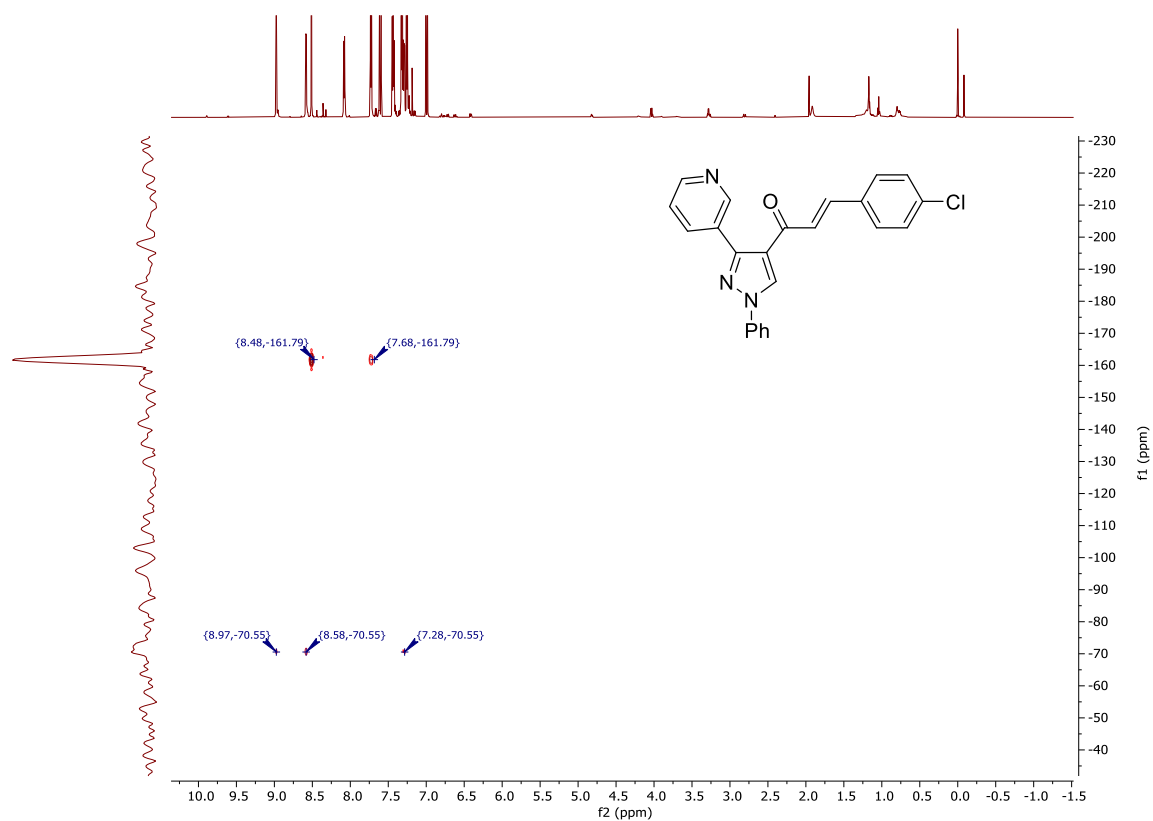


**Figure S165.** (2E)-3-(4-Chlorophenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12g). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)



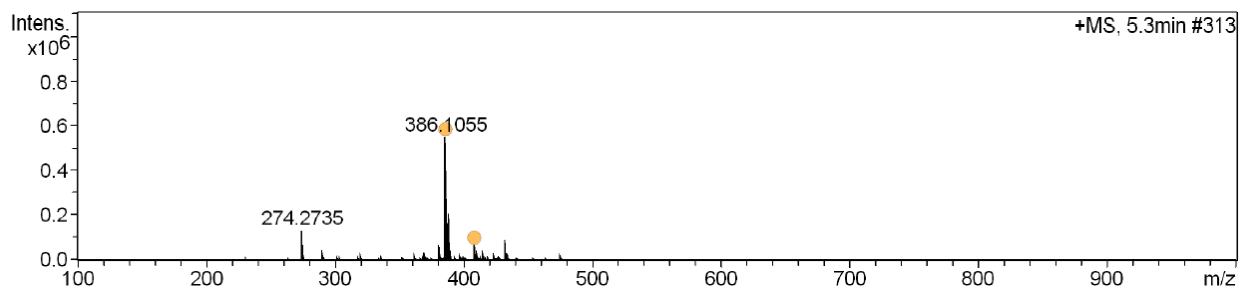
**Figure S166.** (2E)-3-(4-Chlorophenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12g). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)





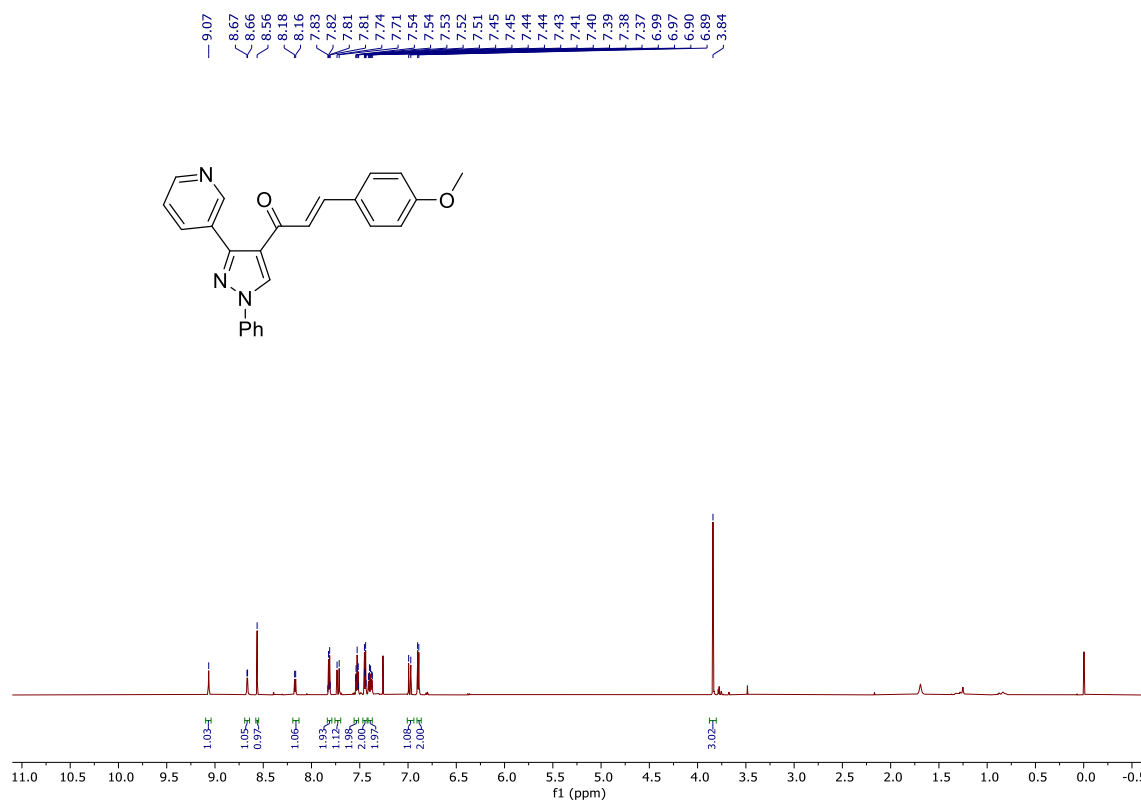
**Figure S167.** (2*E*)-3-(4-Chlorophenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (12g).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

+MS, 5.3min #313

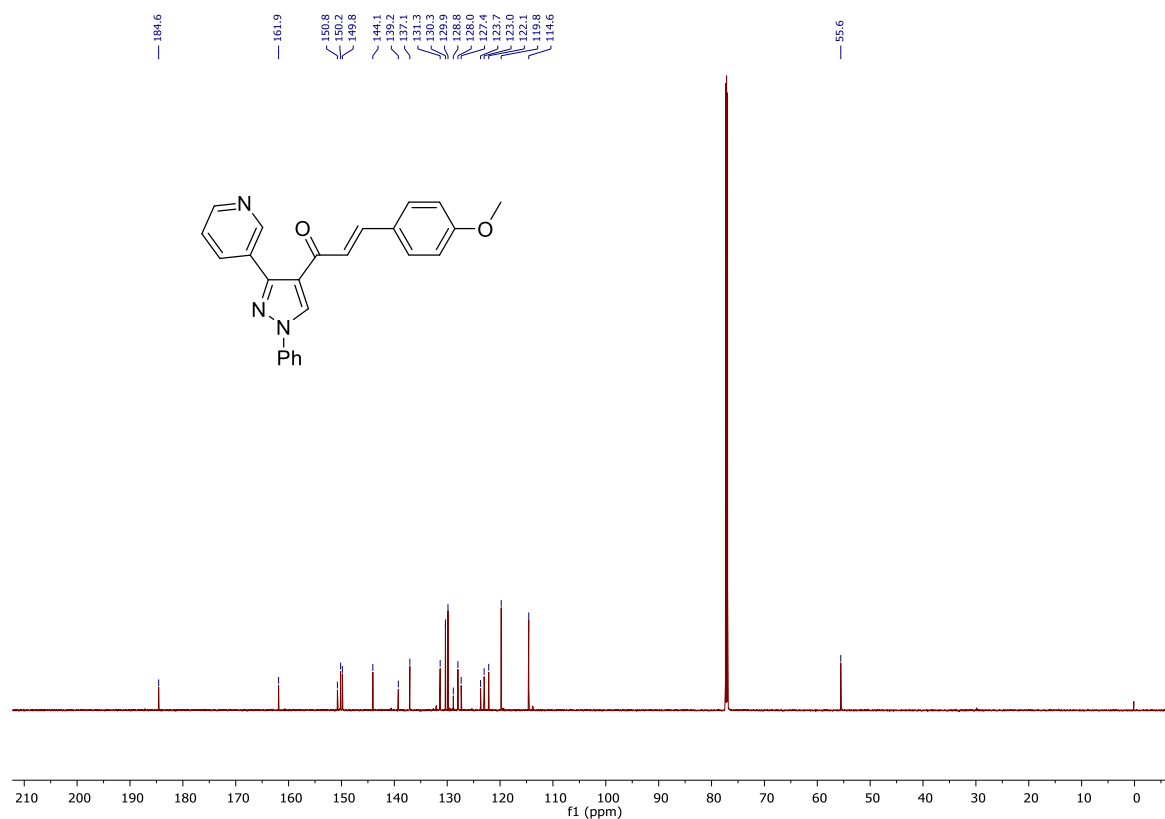


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
386.1055	1	C <sub>23</sub> H <sub>17</sub> ClN <sub>3</sub> O	386.1055	-0.1	14.7	1	100.00	16.5	even	ok
408.0874	1	C <sub>23</sub> H <sub>16</sub> ClN <sub>3</sub> NaO	408.0874	0.1	52.5	1	100.00	16.5	even	ok

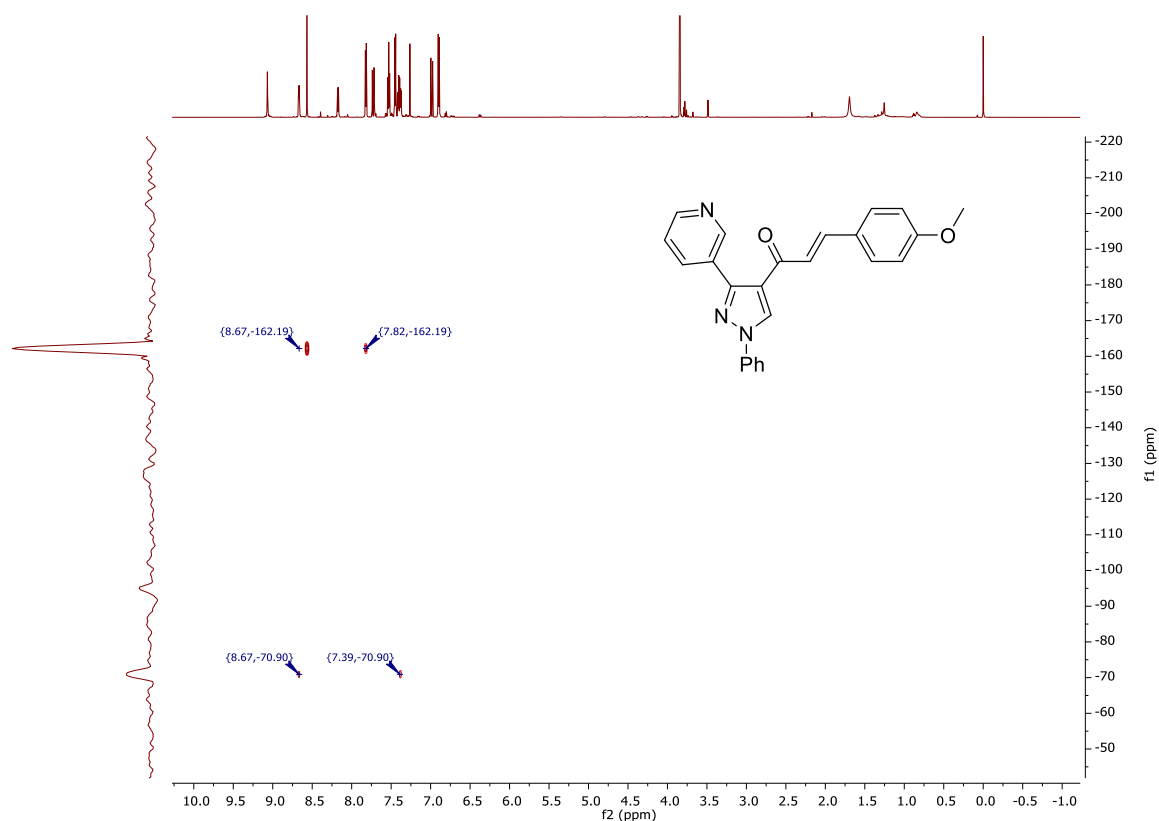
**Figure S168.** (2*E*)-3-(4-Chlorophenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (12g). HRMS (ESI-TOF).



**Figure S169.** (2E)-3-(4-Methoxyphenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12h). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)

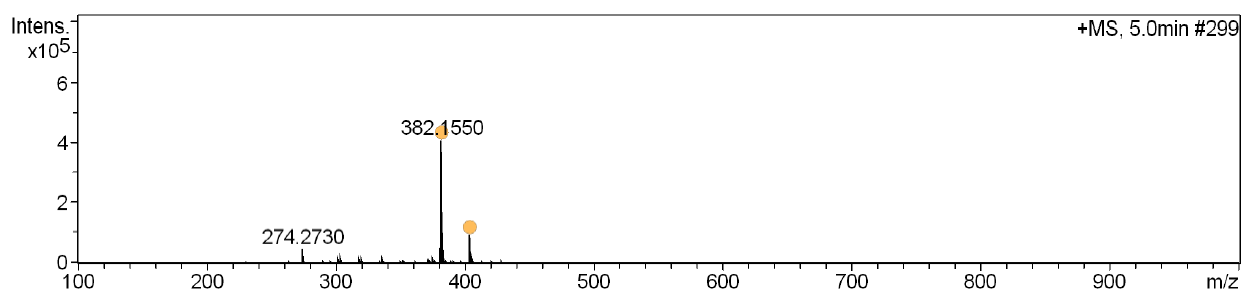


**Figure S170.** (2E)-3-(4-Methoxyphenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12h). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



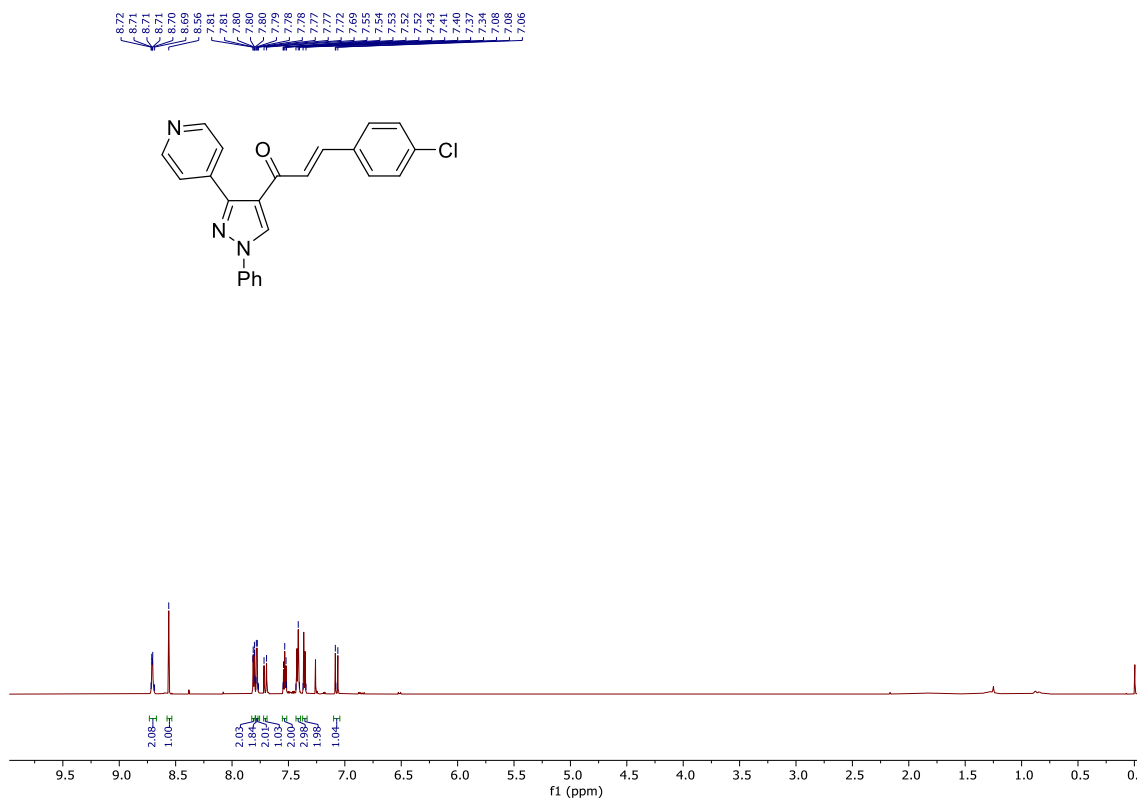
**Figure S171.** (2*E*)-3-(4-Methoxyphenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (12h).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

**+MS, 5.0min #299**

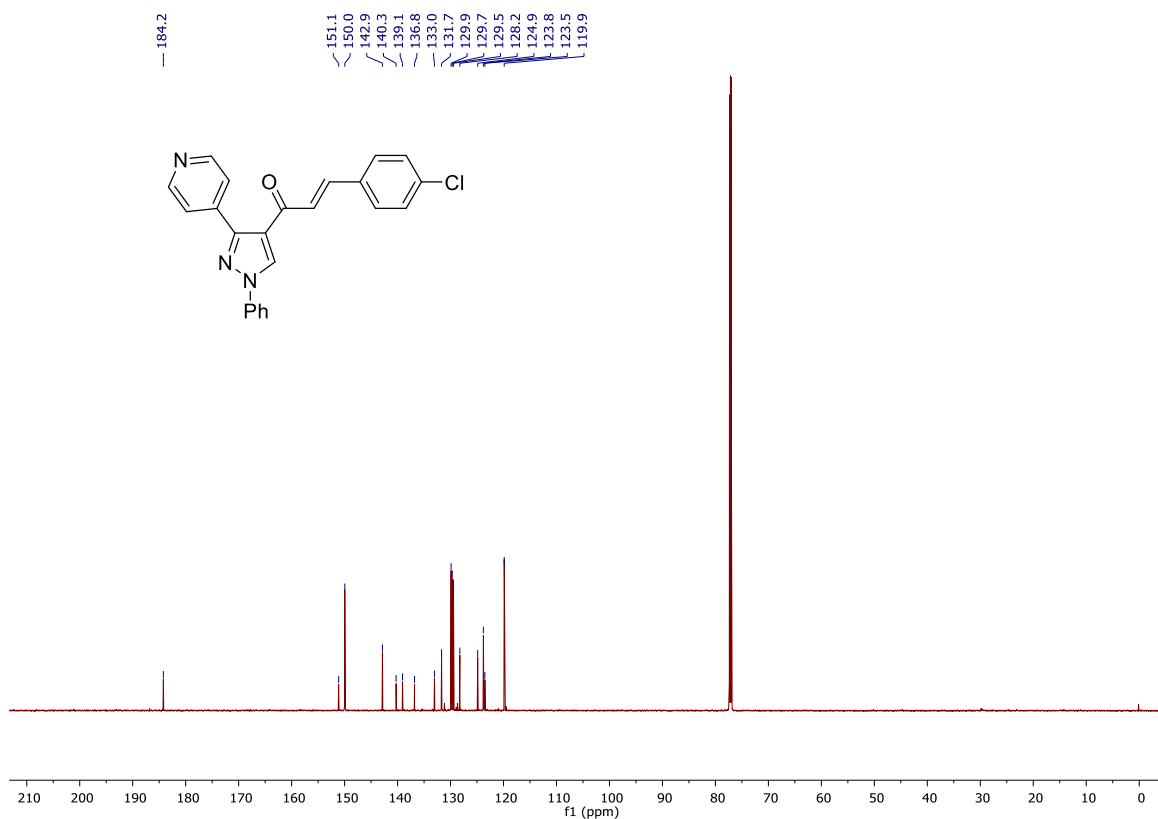


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
382.1550	1	C <sub>24</sub> H <sub>20</sub> N <sub>3</sub> O <sub>2</sub>	382.1550	0.1	3.3	1	100.00	16.5	even	ok
404.1369	1	C <sub>24</sub> H <sub>19</sub> N <sub>3</sub> NaO <sub>2</sub>	404.1369	-0.1	5.7	1	100.00	16.5	even	ok

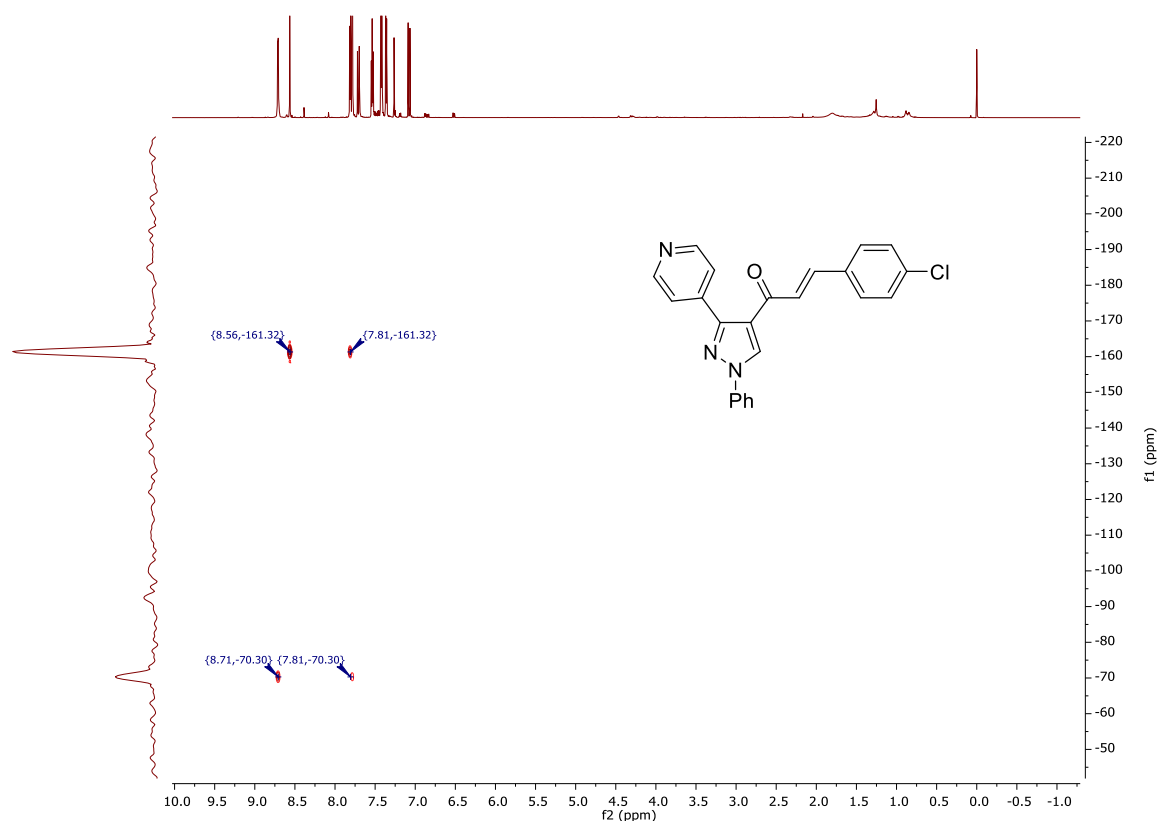
**Figure S172.** (2*E*)-3-(4-Methoxyphenyl)-1-[1-phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (12h). HRMS (ESI-TOF).



**Figure S173. (2E)-3-(4-Chlorophenyl)-1-[1-phenyl-3-(pyridin-4-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12i). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)**

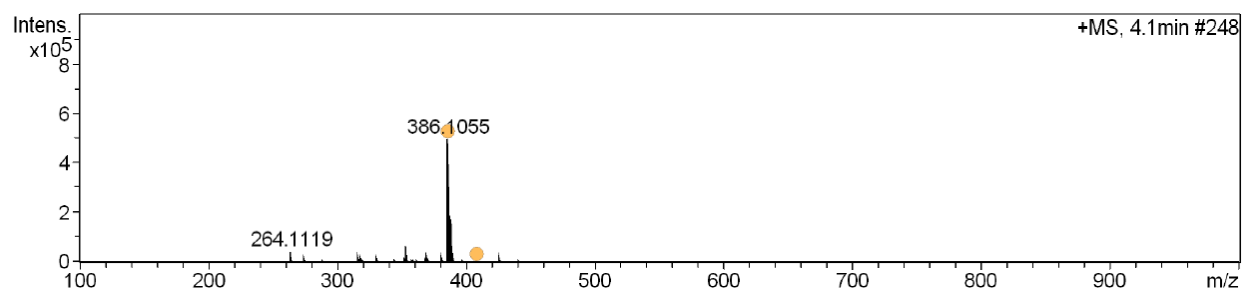


**Figure S174. (2E)-3-(4-Chlorophenyl)-1-[1-phenyl-3-(pyridin-4-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12i). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)**



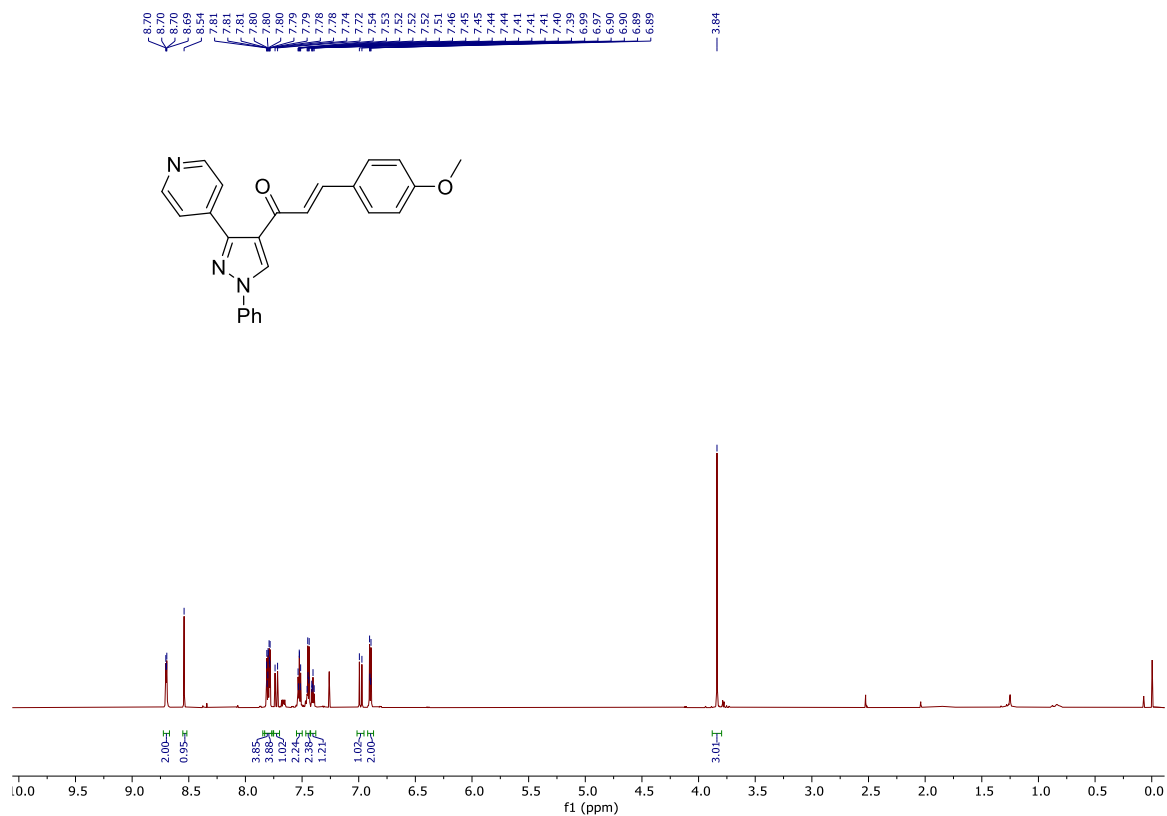
**Figure S175.** (2*E*)-3-(4-Chlorophenyl)-1-[1-phenyl-3-(pyridin-4-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (12i).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

**+MS, 4.1min #248**

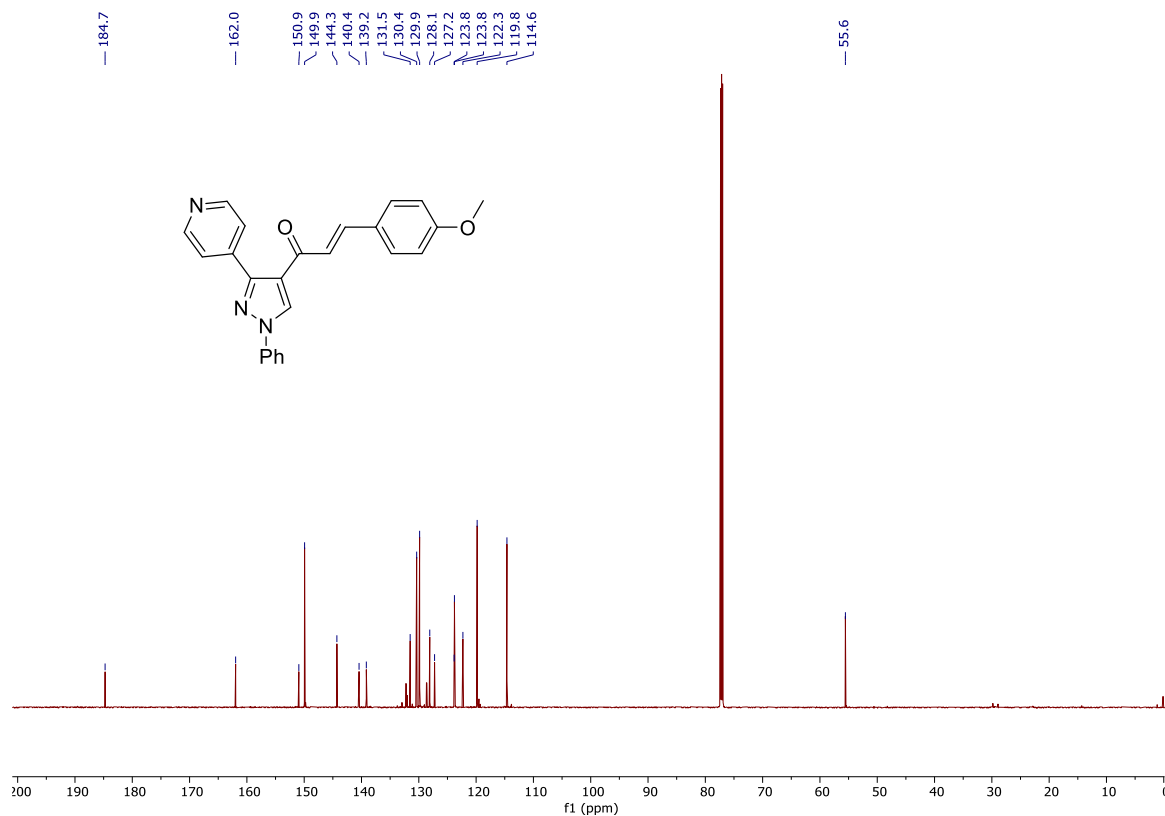


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
386.1055	1	C <sub>23</sub> H <sub>17</sub> ClN <sub>3</sub> O	386.1055	0.2	4.2	1	100.00	16.5	even	ok
408.0864	1	C <sub>23</sub> H <sub>16</sub> ClN <sub>3</sub> NaO	408.0874	2.5	182.6	1	100.00	16.5	even	ok

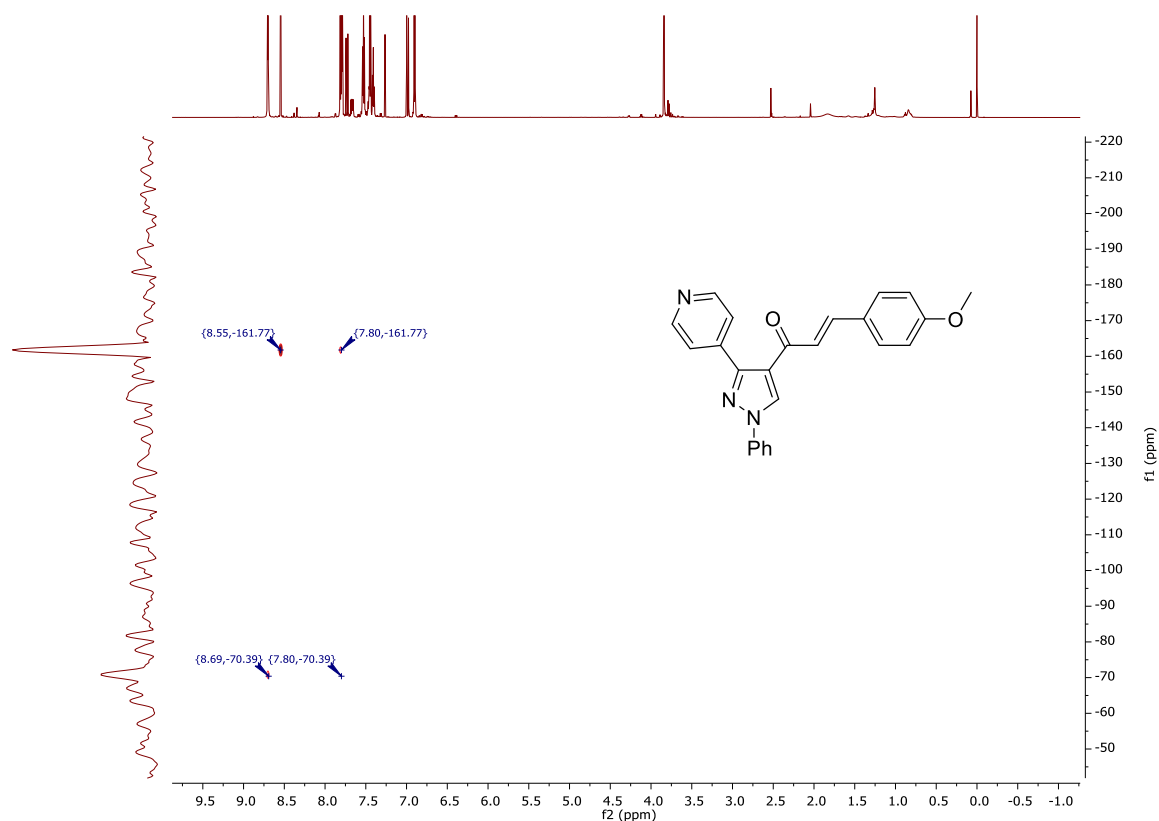
**Figure S176.** (2*E*)-3-(4-Chlorophenyl)-1-[1-phenyl-3-(pyridin-4-yl)-1*H*-pyrazol-4-yl]prop-2-en-1-one (12i). HRMS (ESI-TOF).



**Figure S177.** (2E)-3-(4-Methoxyphenyl)-1-[1-phenyl-3-(pyridin-4-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12j). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)

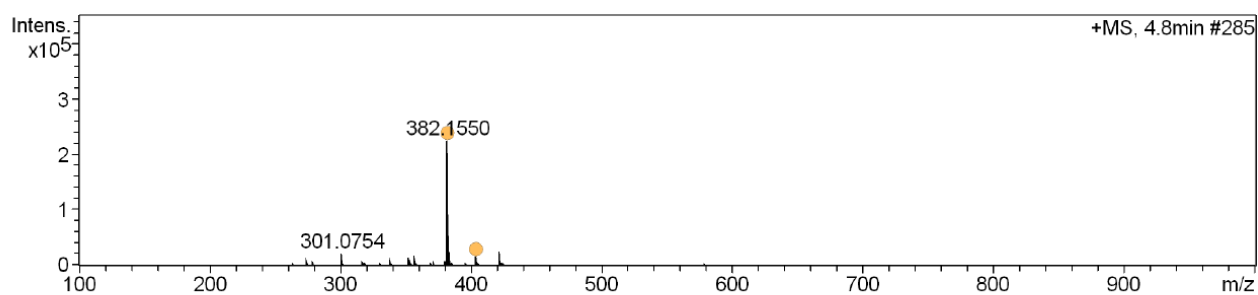


**Figure S178.** (2E)-3-(4-Methoxyphenyl)-1-[1-phenyl-3-(pyridin-4-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12j). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



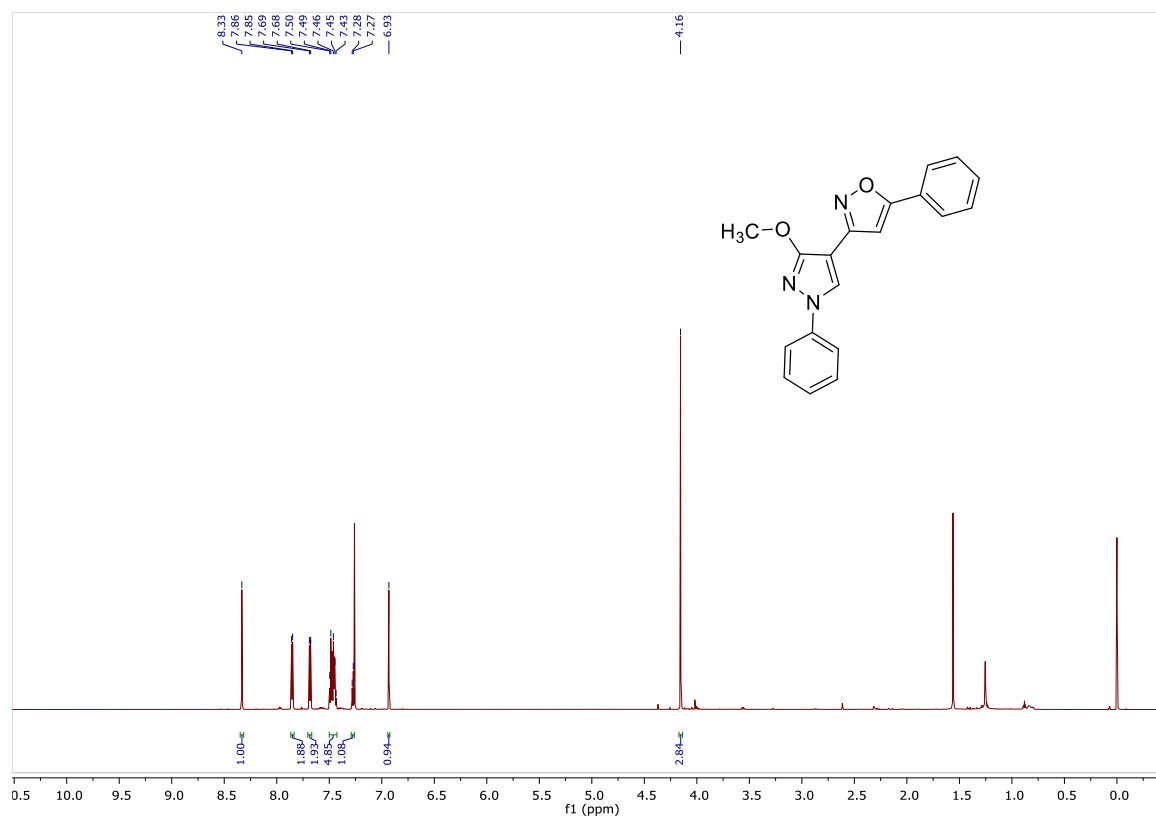
**Figure S179.** (2E)-3-(4-Methoxyphenyl)-1-[1-phenyl-3-(pyridin-4-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12j).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

**+MS, 4.8min #285**

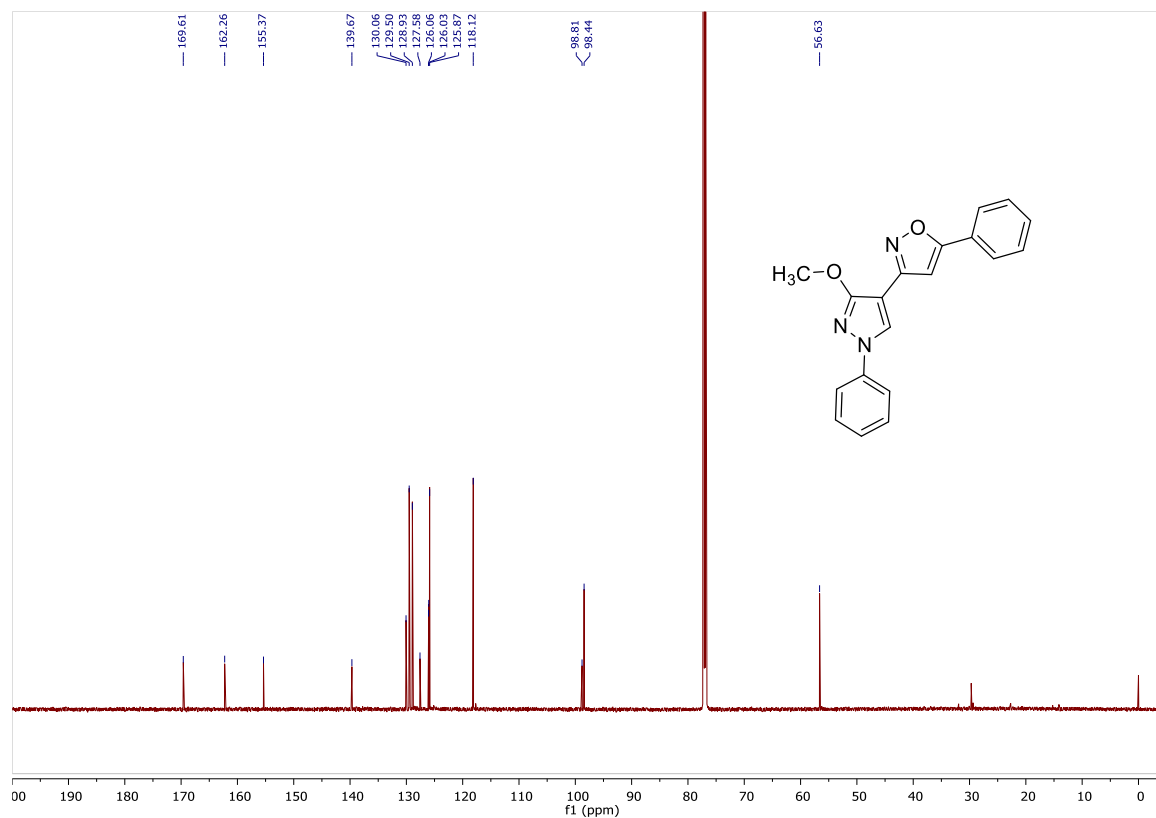


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
382.1550	1	C <sub>24</sub> H <sub>20</sub> N <sub>3</sub> O <sub>2</sub>	382.1550	-0.1	4.9	1	100.00	16.5	even	ok
404.1357	1	C <sub>24</sub> H <sub>19</sub> N <sub>3</sub> NaO <sub>2</sub>	404.1369	3.2	21.2	1	100.00	16.5	even	ok

**Figure S180.** (2E)-3-(4-Methoxyphenyl)-1-[1-phenyl-3-(pyridin-4-yl)-1H-pyrazol-4-yl]prop-2-en-1-one (12j). HRMS (ESI-TOF).



**Figure S181.** 3-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-5-phenyl-1,2-oxazole (14). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)



**Figure S182.** 3-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-5-phenyl-1,2-oxazole (14). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



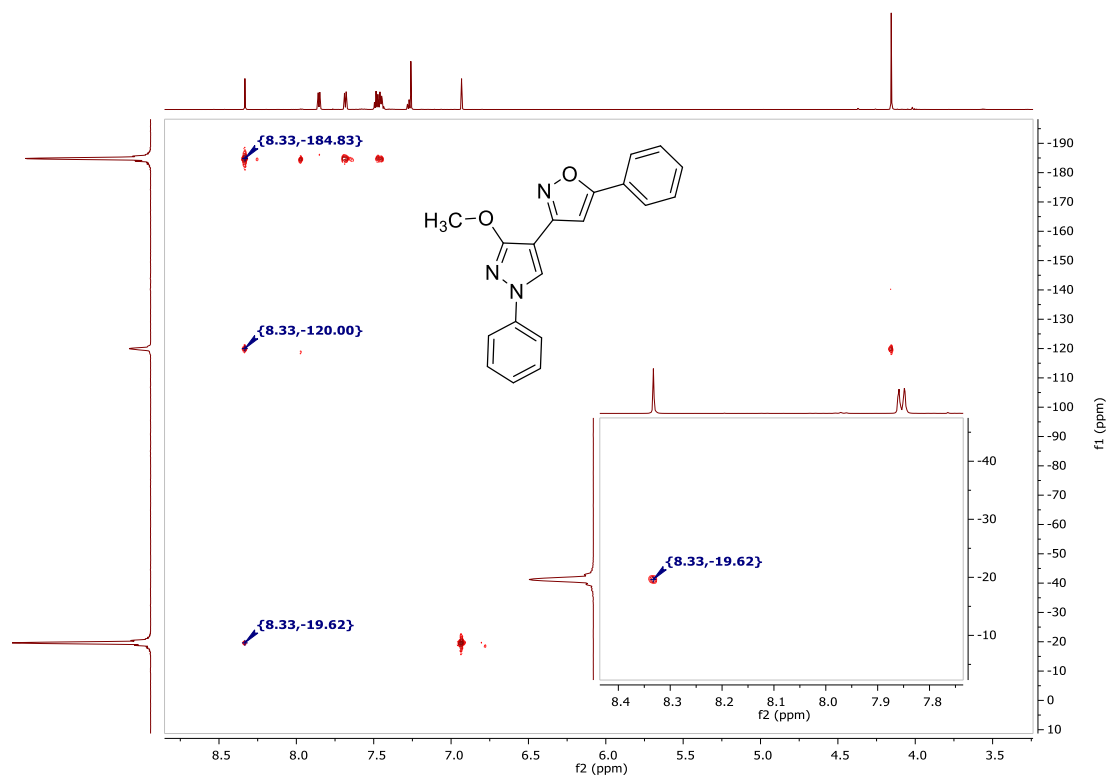
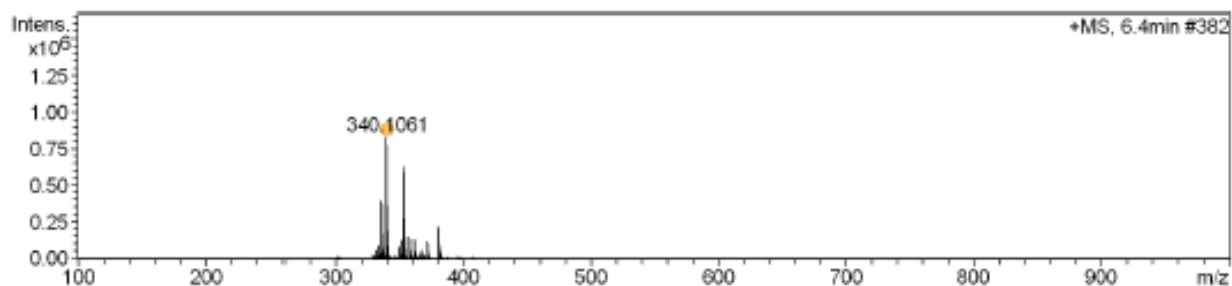


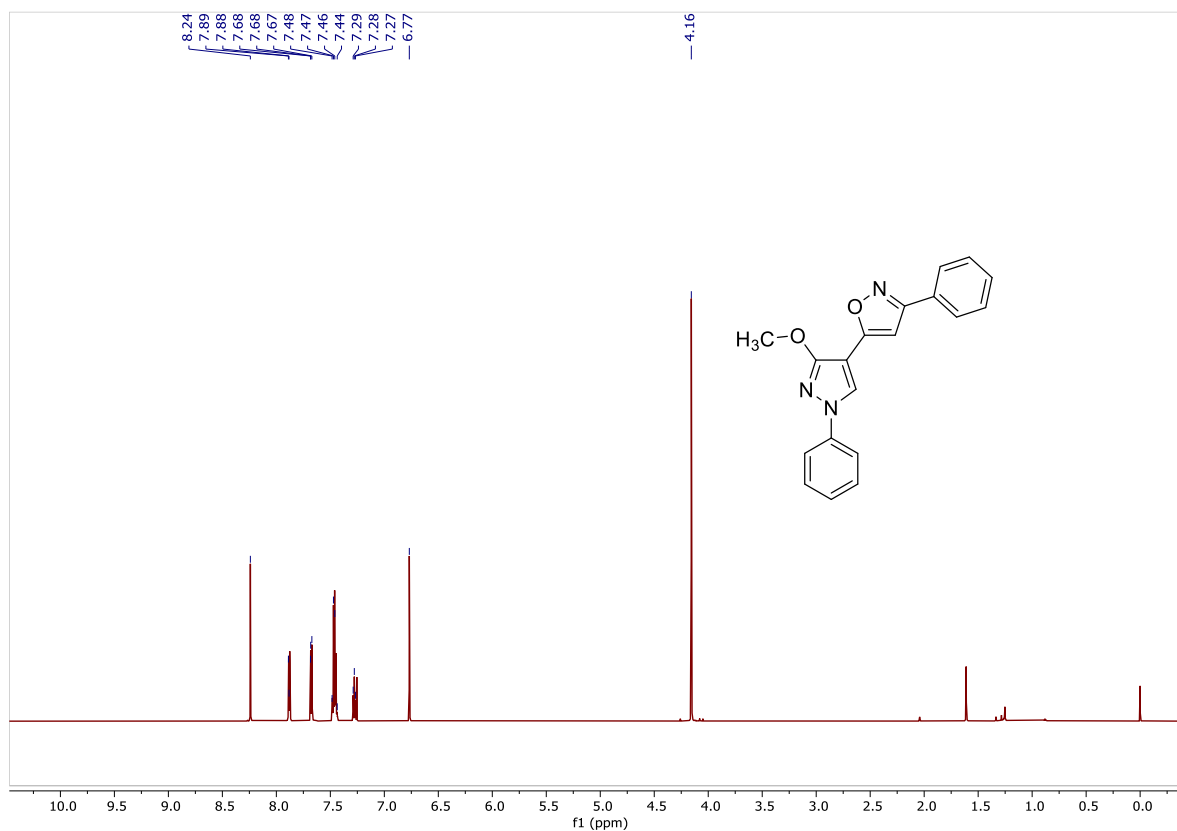
Figure S183. 3-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-5-phenyl-1,2-oxazole (14).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

+MS, 6.4min #382

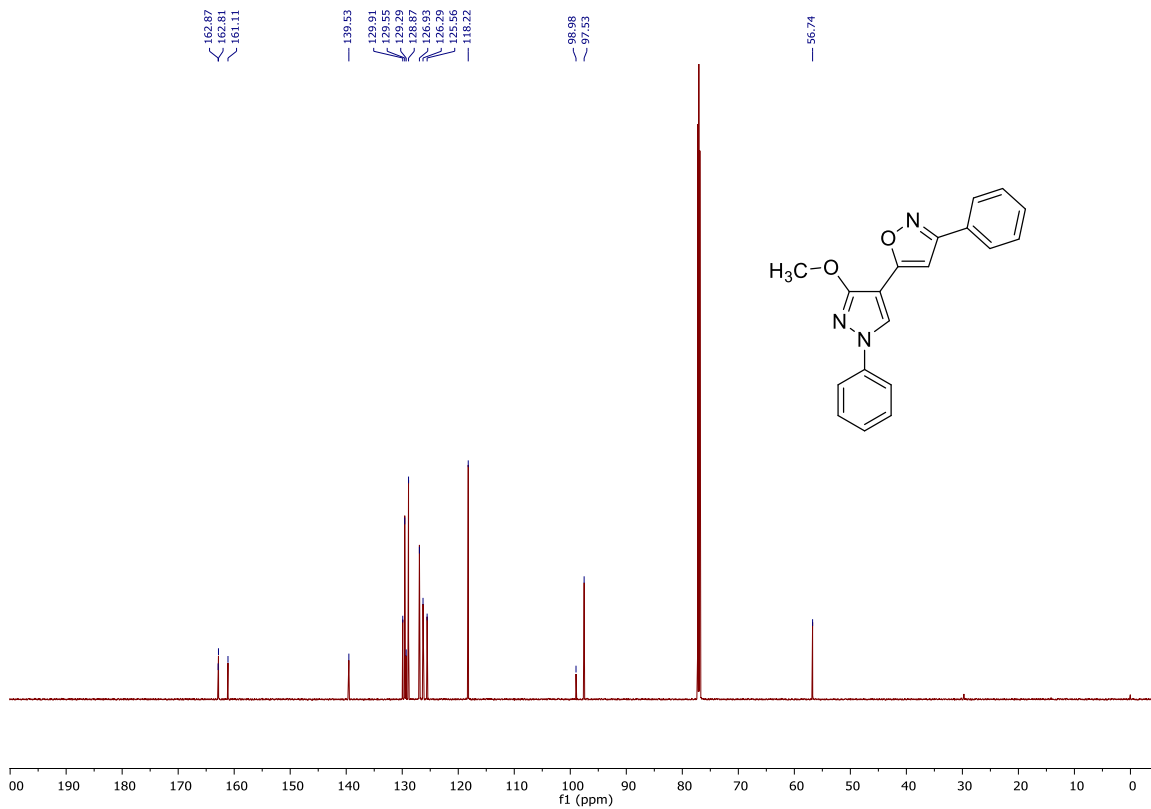


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup>	Conf	N-Rule
340.1061	1	C <sub>19</sub> H <sub>15</sub> N <sub>3</sub> NaO <sub>2</sub>	340.1056	-1.3	17.1	2	100.00	13.5	even		ok

Figure S184. 3-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-5-phenyl-1,2-oxazole (14). HRMS (ESI-TOF).



**Figure S185.** 5-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-phenyl-1,2-oxazole (15). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)



**Figure S186.** 5-(3-Methoxy-1-phenyl-1H-pyrazol-4-yl)-3-phenyl-1,2-oxazole (15). <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)

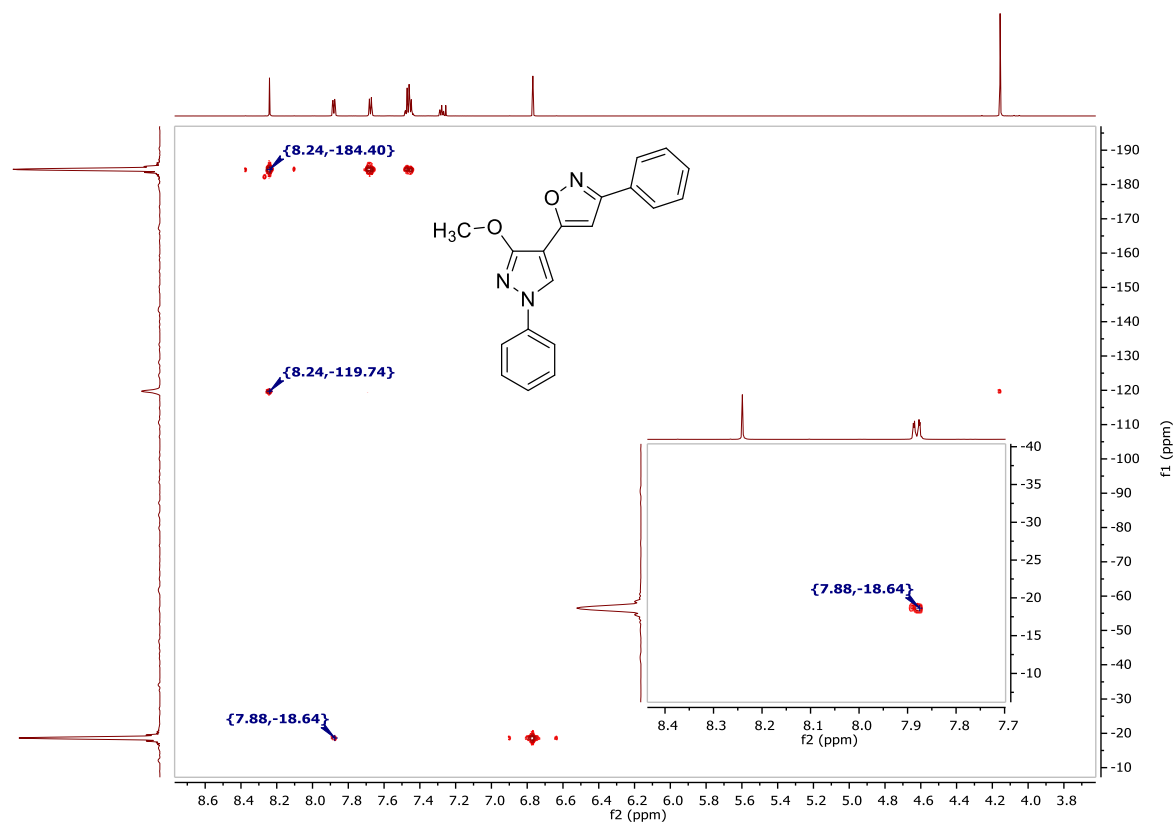


Figure S187. 5-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-3-phenyl-1,2-oxazole (15).  $^1\text{H}$ - $^{15}\text{N}$  HMBC NMR spectrum (71 MHz,  $\text{CDCl}_3$ )

+MS, 4.5min #269

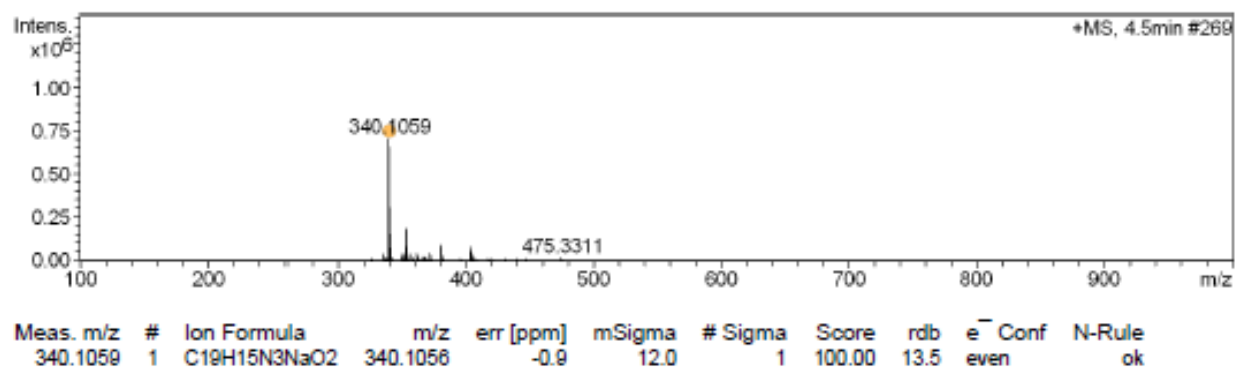
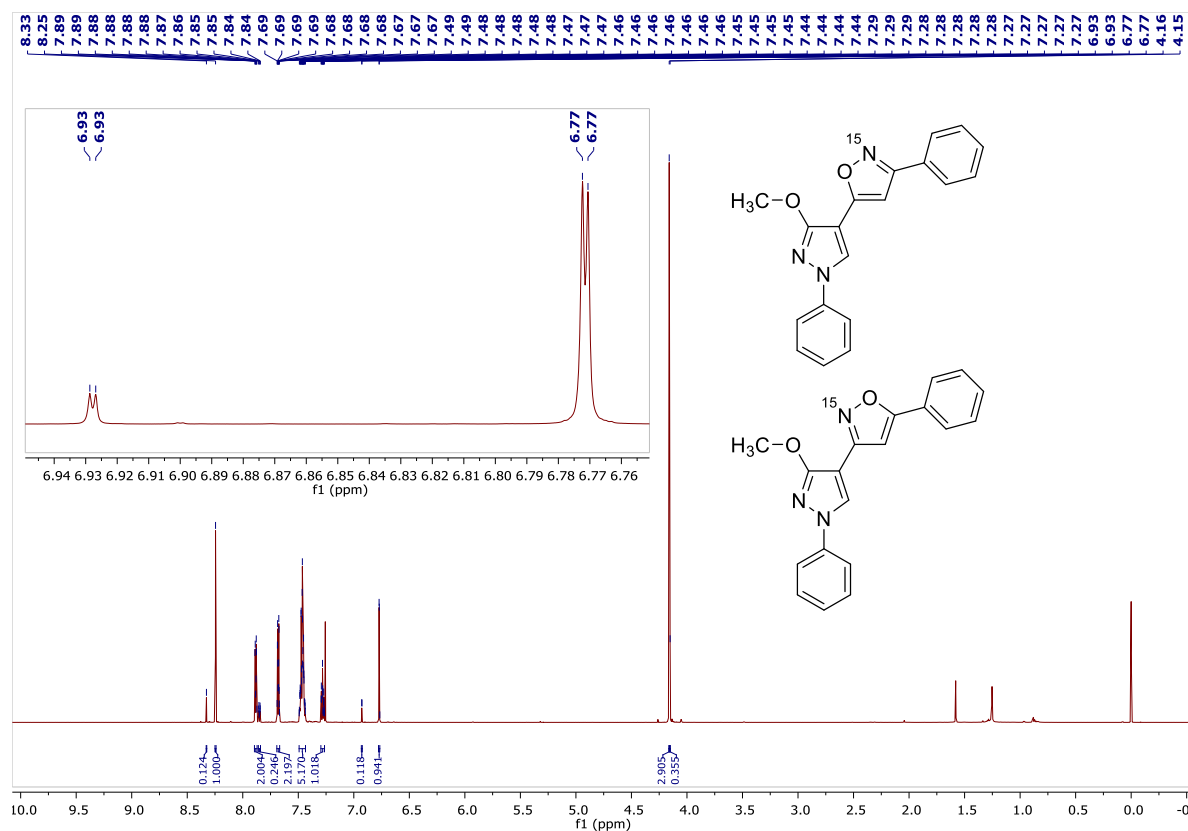
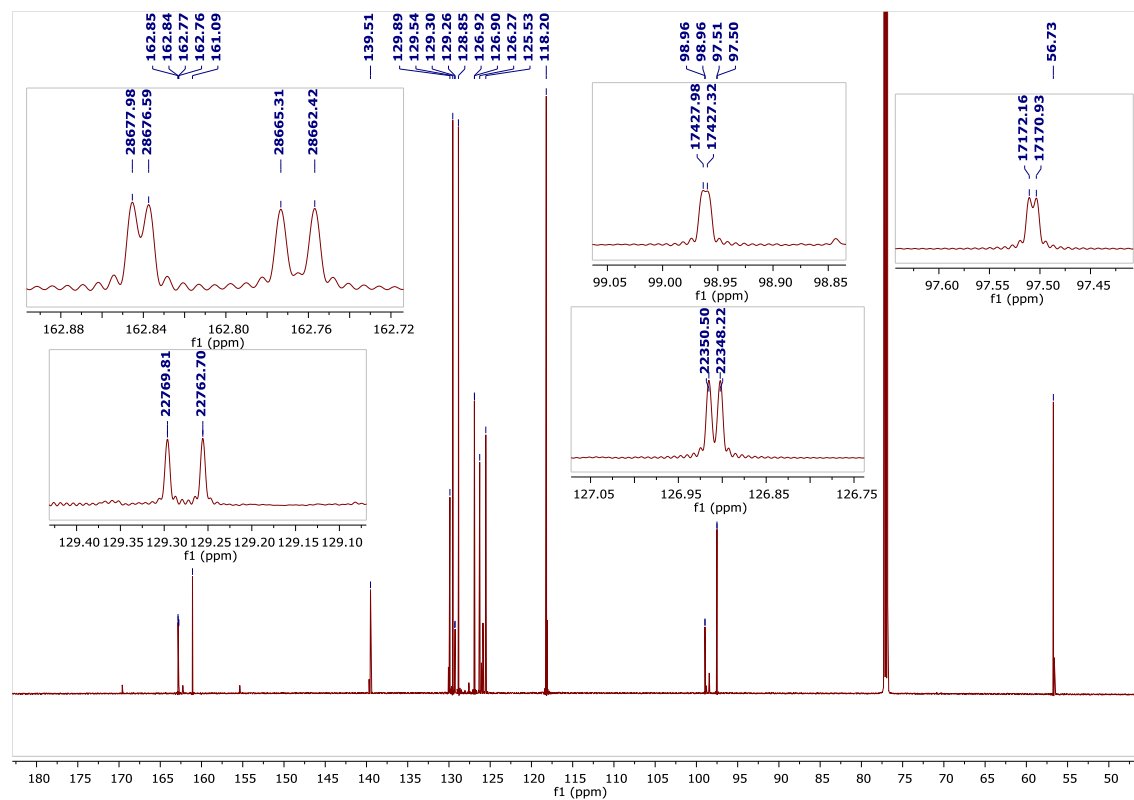


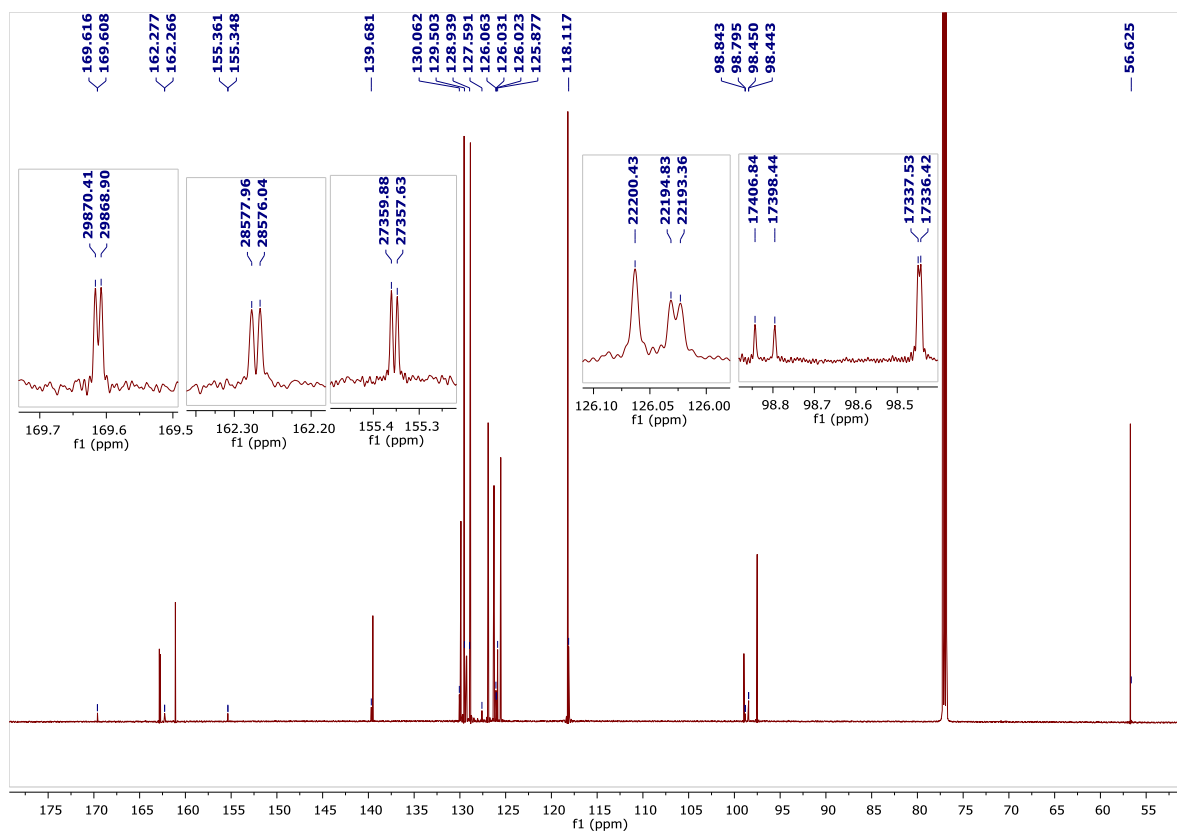
Figure S188. 5-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-3-phenyl-1,2-oxazole (15). HRMS (ESI-TOF).



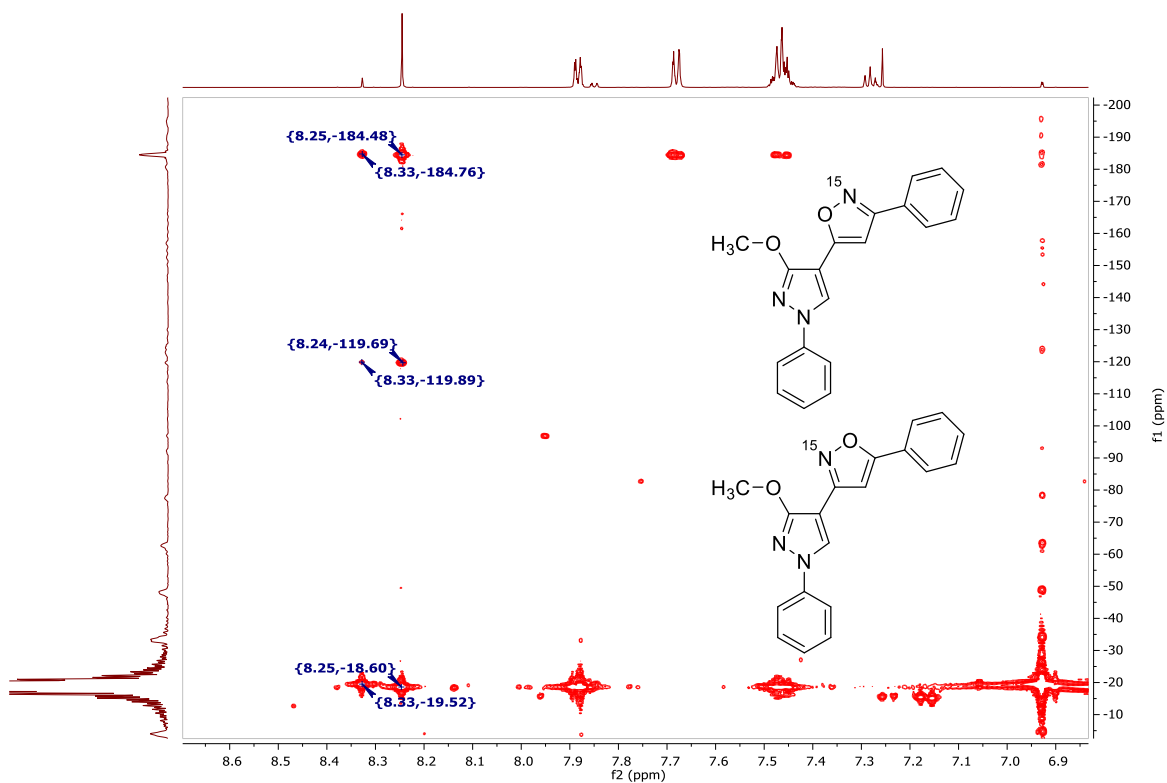
**Figure S189.** 3(5)-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-(5)3-phenyl-<sup>15</sup>N-1,2-oxazole (mixture of 16, 17). <sup>1</sup>H NMR spectrum (700 MHz, CDCl<sub>3</sub>)



**Figure S190.** 3(5)-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-(5)3-phenyl-<sup>15</sup>N-1,2-oxazole (mixture of 16, 17), signals of major regioisomer 16. <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)

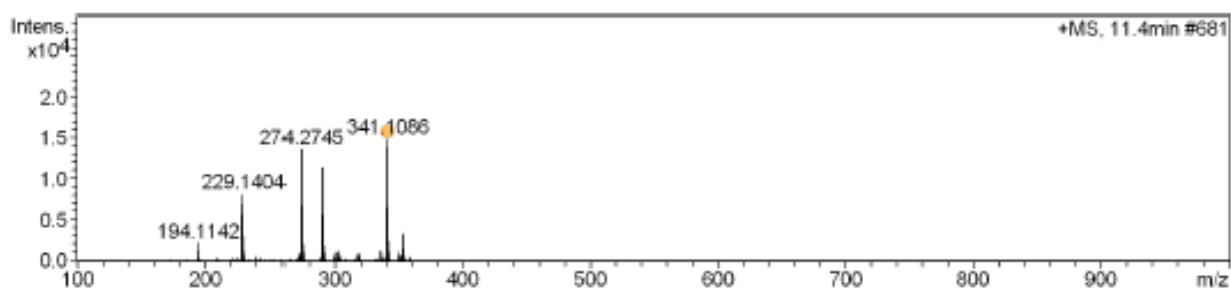


**Figure S191.** 3(5)-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-(5)3-phenyl-<sup>15</sup>N-1,2-oxazole (mixture of 16, 17), signals of minor regioisomer 17. <sup>13</sup>C NMR spectrum (176 MHz, CDCl<sub>3</sub>)



**Figure S192.** 3(5)-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-(5)3-phenyl-<sup>15</sup>N-1,2-oxazole (mixture of 16, 17). <sup>1</sup>H-<sup>15</sup>N HMBC NMR spectrum (71 MHz, CDCl<sub>3</sub>)

+MS, 11.4min #681



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e	Conf	N-Rule
341.1086	1	C <sub>19</sub> H <sub>15</sub> N <sub>3</sub> NaO <sub>2</sub>	340.1056	-0.2	731.9	6	0.00	13.5	even		ok

Figure S193. 3(5)-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-(5)3-phenyl-<sup>15</sup>N-1,2-oxazole (mixture of 16, 17). HRMS (ESI-TOF).

### <Chromatogram>

mAU

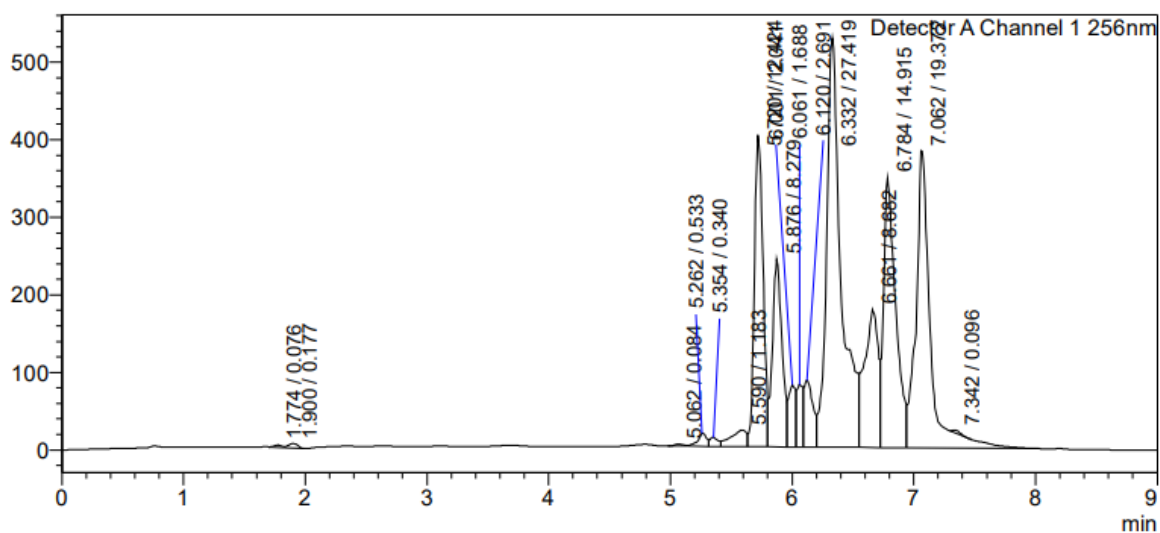
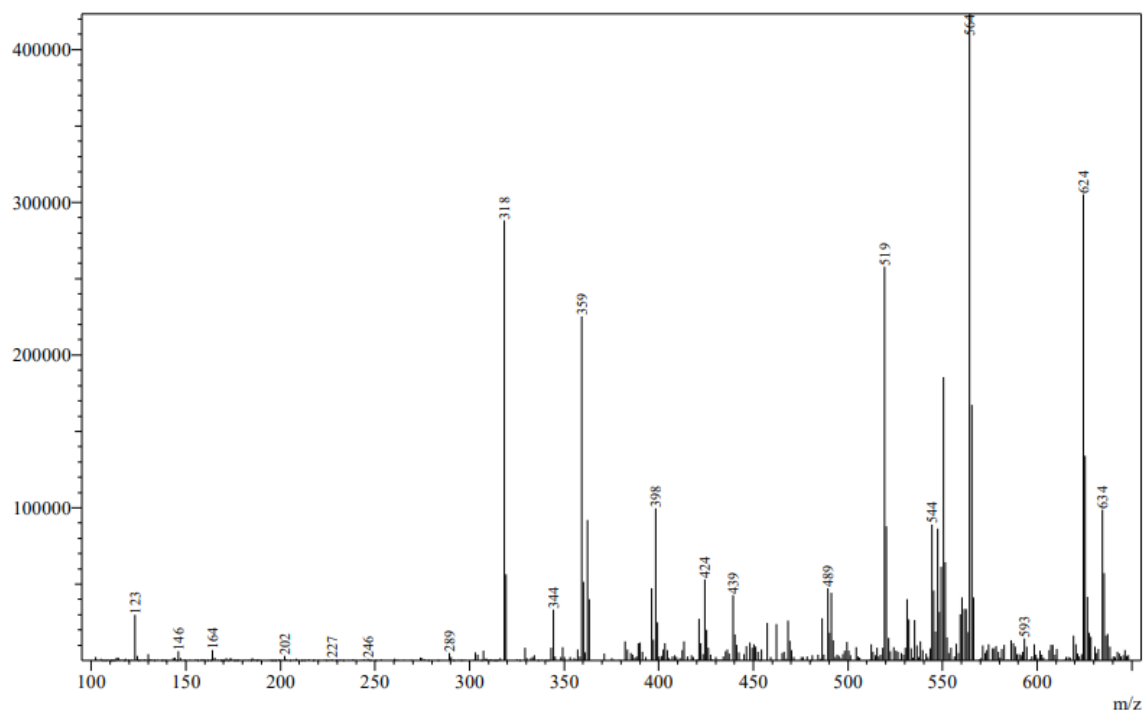


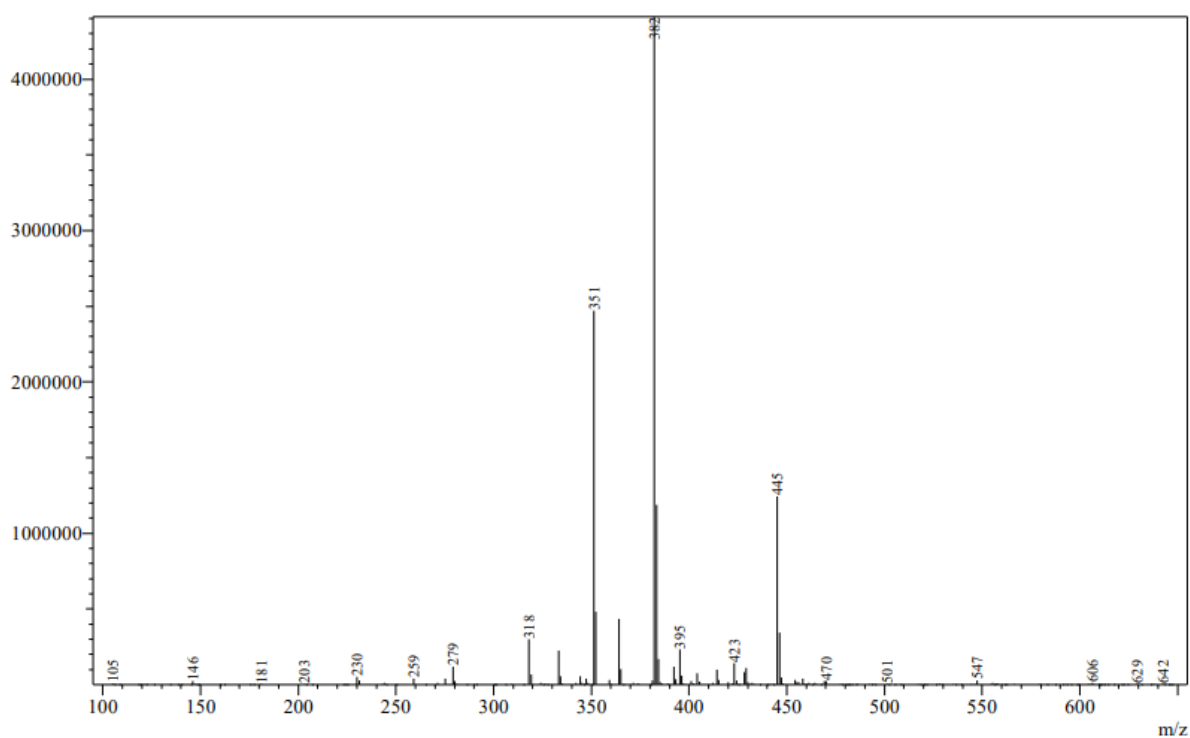
Figure S194. HPLC data of crude reaction mixture of compounds 14,15.

Line#:10 R.Time:7.100(Scan#:1279)  
MassPeaks:384  
Spectrum Mode:Averaged 7.083-7.117(1276-1282) Base Peak:564(423388)  
BG Mode:Calc Segment 1 - Event 1



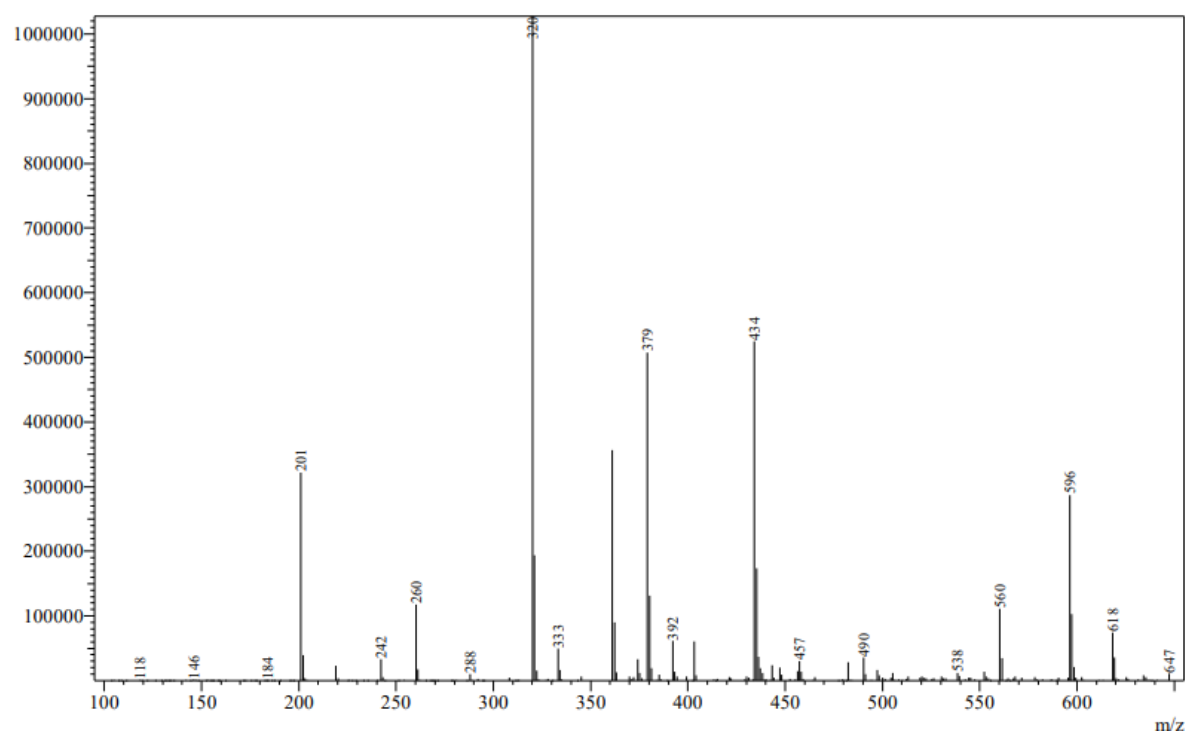
**Figure S195.** MS data of crude reaction mixture of compounds 14,15 (peak retention time 7.1 min.).

Line#:6 R.Time:6.333(Scan#:1141)  
MassPeaks:197  
Spectrum Mode:Averaged 6.317-6.350(1138-1144) Base Peak:382(4412462)  
BG Mode:Calc Segment 1 - Event 1



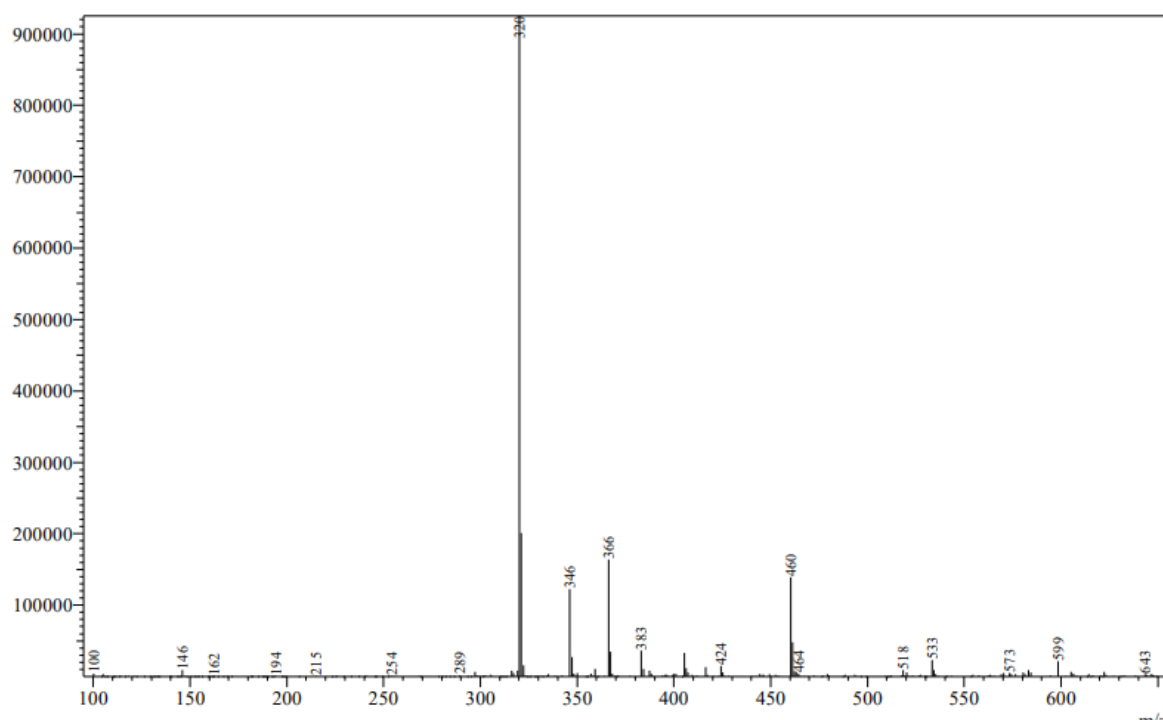
**Figure S196.** MS data of crude reaction mixture of compounds 14,15 (peak retention time 6.3 min.).

Line#:7 R.Time:6.650(Scan#:1198)  
 MassPeaks:224  
 Spectrum Mode:Averaged 6.633-6.667(1195-1201) Base Peak:320(1027526)  
 BG Mode:Calc Segment 1 - Event 1



**Figure S197. MS data of crude reaction mixture of compounds 14,15 (peak retention time 6.6 min.).**

Line#:8 R.Time:6.750(Scan#:1216)  
 MassPeaks:251  
 Spectrum Mode:Averaged 6.733-6.767(1213-1219) Base Peak:320(925279)  
 BG Mode:Calc Segment 1 - Event 1



**Figure S198. MS data of crude reaction mixture of compounds 14,15 (peak retention time 6.7 min.).**