

Supplementary Materials

Synthesis and Antiproliferative Activity of 2,4,6,7-Tetrasubstituted-2*H*-pyrazolo[4,3-*c*]pyridines

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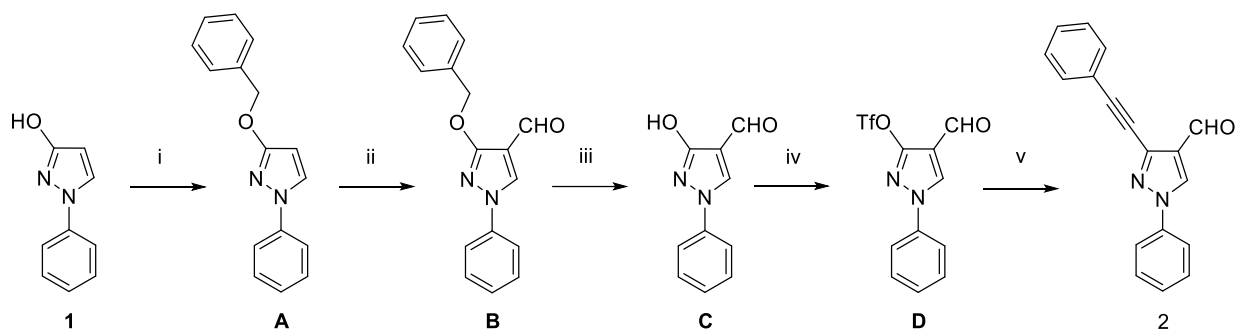
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Scheme S1. Synthesis of 1-phenyl-3-(phenylethynyl)-1*H*-pyrazole-4-carbaldehyde (**2**) by previously published procedures.

Reagents and conditions: i: NaH, BnCl, DMF, argon atmosphere, 60 °C, 1 h; ii: POCl₃, DMF, 0 °C for 10 min to 60 °C for 30 min; iii: TFA, toluene, rt, 24 h; iv: Tf₂O, TEA, DCM, rt, 1 h.

Table S1. Fundamental absorption and fluorescence characteristics of compounds **18-42** in THF ($\lambda_{\text{ex}} = 350$ nm)

Compound	λ_{abs} (nm)	$\varepsilon \times 10^3$ (dm ³ mol ⁻¹ cm ⁻¹)	λ_{em} (nm)	SS (nm)	Φ_f (%)
18	260	30.38	442	130	18.9
	312	13.23			
19	261	34.67	447	136	26.2
	311	16.86			
20	260	35.55	437	126	53.2
	311	16.29			
21	263	31.95	461	151	71.8
	310	15.80			
	351 shoulder	8.07			
22	267	32.04	478	167	56.8
	311	16.09			
	357 shoulder	7.74			
23	265	28.94	467	202	72.7
24	261	36.46	449	138	17.6
	311	17.34			
25	261	29.68	449	139	30.0
	310	15.11			
26	263	38.05	450	140	48.7
	310	17.48			
27	265	31.58	466	117	72.2
	317	14.93			
	349 shoulder	9.31			
28	266	30.31	481	125	62.8
	316	13.14			
	356 shoulder	7.28			
29	264	24.96	465	201	74.8
30	262	32.79	449	137	21.3
	312	14.13			
31	265	35.93	464	199	73.1
32	264	39.45	465	201	64.7
33	263	35.01	449	141	52.2
	308	14.49			
34	260	21.84	453	140	0.9
	313	10.61			
35	260	45.49	445	133	7.0
	312	21.11			
36	262	37.32	455	141	14.2
	314	16.56			
37	266	36.30	470	204	61.7
38	265	41.18	467	202	68.9
39	269	29.03	487	118	39.7
	369	9.84			
40	265	48.93	469	204	83.5
41	265	36.45	467	202	69.9
42	265	42.38	470	205	84.6

Table S2. Fundamental absorption* and fluorescence characteristics of compounds **18-42** in Britton–Robinson buffer at pH 5, 7 and 9 ($\lambda_{\text{ex}} = 360 \text{ nm}$)

Compound	pH = 5			pH = 7			pH = 9		
	$\lambda_{\text{abs}} \text{ (nm)}$	$\lambda_{\text{em}} \text{ (nm)}$	$\Phi_f \text{ (\%)}$	$\lambda_{\text{abs}} \text{ (nm)}$	$\lambda_{\text{em}} \text{ (nm)}$	$\Phi_f \text{ (\%)}$	$\lambda_{\text{abs}} \text{ (nm)}$	$\lambda_{\text{em}} \text{ (nm)}$	$\Phi_f \text{ (\%)}$
18	259	447	40.4	254	439	16.0	253	436	22.1
19	258	455	4.4	253	459	33.4	253	458	34.3
20	261	444	2.0	255	440	6.5	255	439	5.7
21	259	497	12.2	256	458	37.2	256	458	59.9
22	257	507	0.4	256	511	4.3	256	495	7.1
23	259	445	0.1	255	461	0.1	255	469	0.1
24	261	443	81.3	254	442	17.7	254	435	17.7
25	259	486	2.0	253	456	18.2	252	455	43.1
26	262	446	0.4	257	446	6.1	256	440	6.6
27	264	509	17.0	257	459	22.0	258	458	24.0
28	257	499	0.2	256	504	9.6	255	495	14.2
29	262	446	0.3	255	466	0.2	254	454	0.2
30	261	444	77.5	260	438	14.0	262	436	15.3
31	262	511	18.2	269	457	35.3	267	457	37.8
32	257	497	1.3	255	491	13.5	255	485	14.9
33	263	459	35.7	265	449	17.9	266	448	17.4
34	264	438	8.6	266	439	8.7	264	440	10.1
35	267	438	10.1	269	440	9.9	267	438	11.1
36	265	443	15.3	266	441	14.1	265	443	17.6
37	264	443	0.4	254	495	0.1	255	475	0.2
38	269	457	28.9	270	458	35.6	272	458	36.0
39	285	479	26.6	280	481	31.5	277	480	34.3
40	266	493	10.1	269	481	15.0	268	482	17.4
41	271	474	11.6	272	472	17.0	270	470	19.1
42	269	458	18.5	271	459	33.6	270	458	37.5

*In aqueous solution, the absorption bands above 300 nm become extremely broad, and they are manifested as an extended shoulder, for which it is impossible to identify precise maximum position. Nevertheless, for all species, it was possible to use 360 nm as an excitation wavelength in fluorescence experiments in the examined pH range.

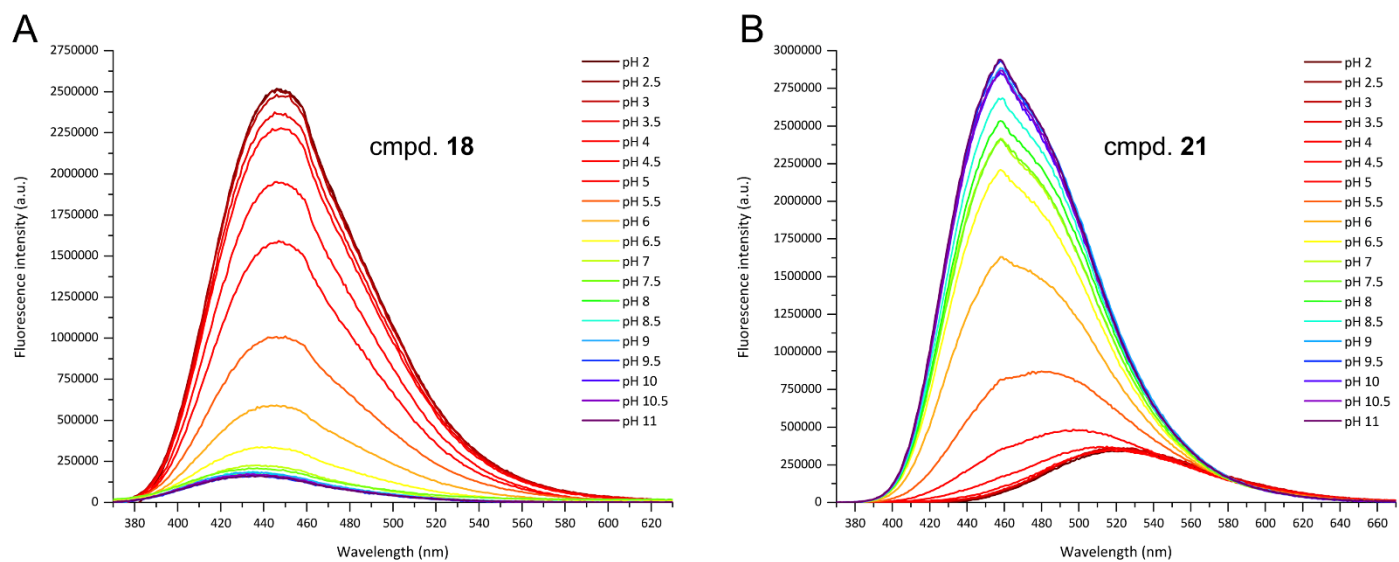


Figure S1. Fluorescence spectra ($\lambda_{\text{ex}} = 360$ nm) and titration profiles for compounds **18** (part A) and **21** (part B) in Britton–Robinson buffer at pH 2–11.

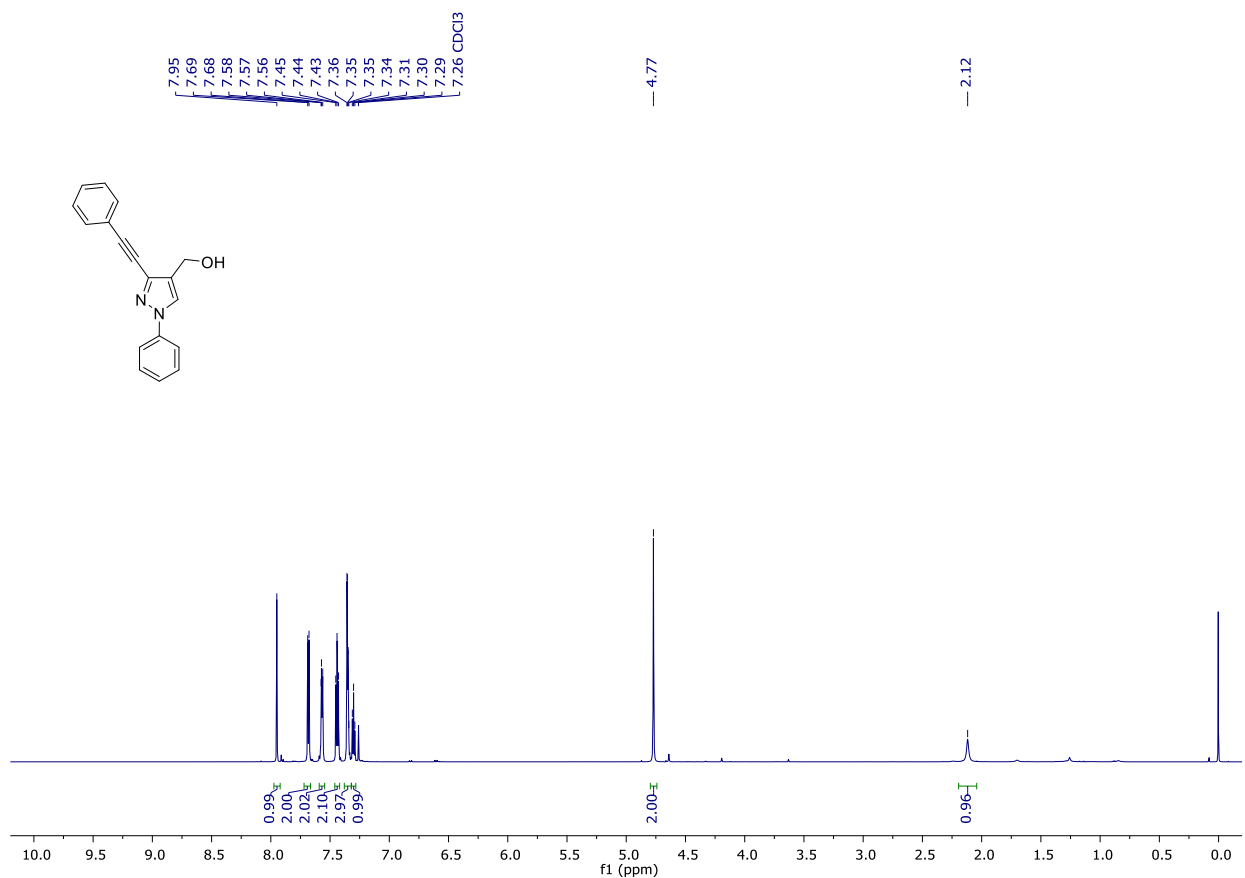


Figure S2. [1-Phenyl-3-(phenylethynyl)-1*H*-pyrazol-4-yl]methanol (**3**). ¹H NMR spectrum (700 MHz, CDCl₃).

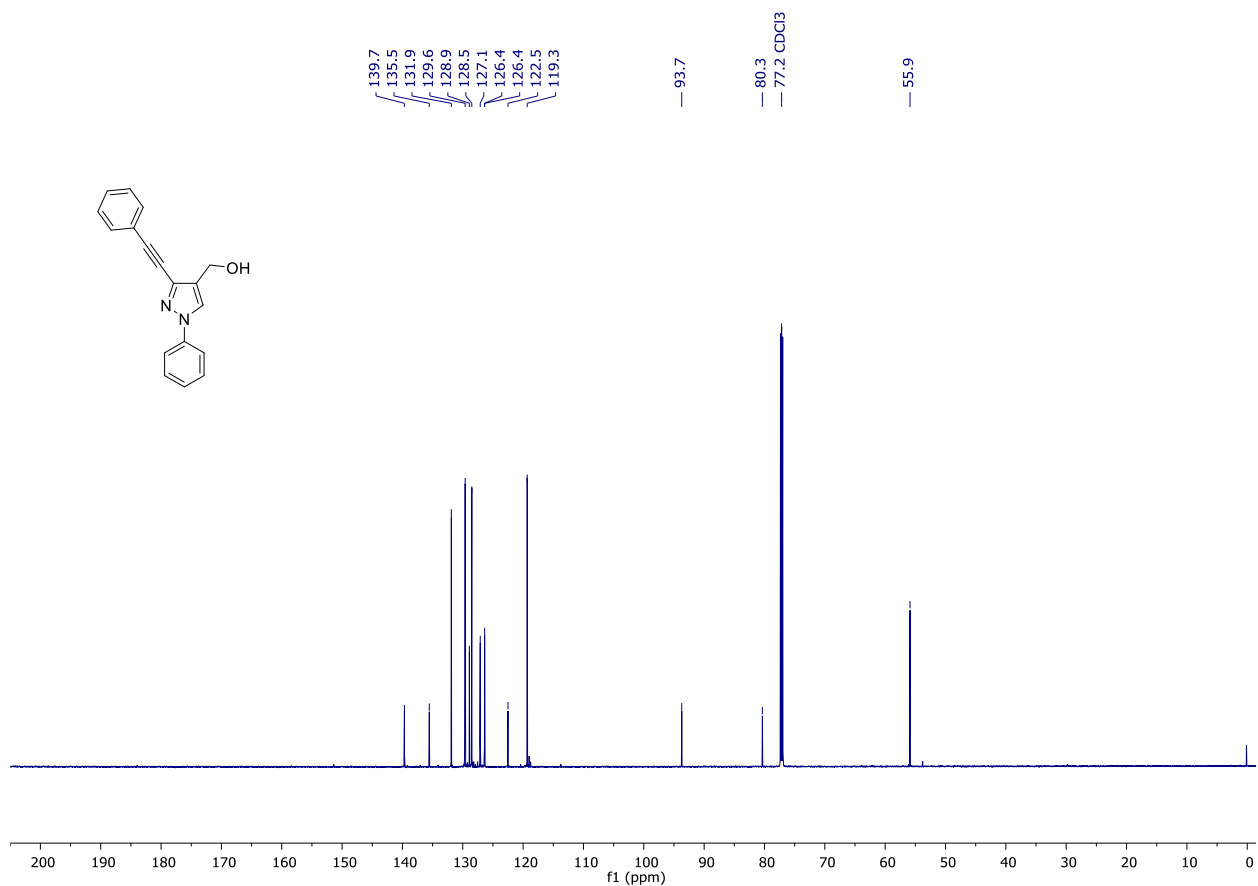


Figure S3. [1-Phenyl-3-(phenylethynyl)-1*H*-pyrazol-4-yl]methanol (**3**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 8.6min #514

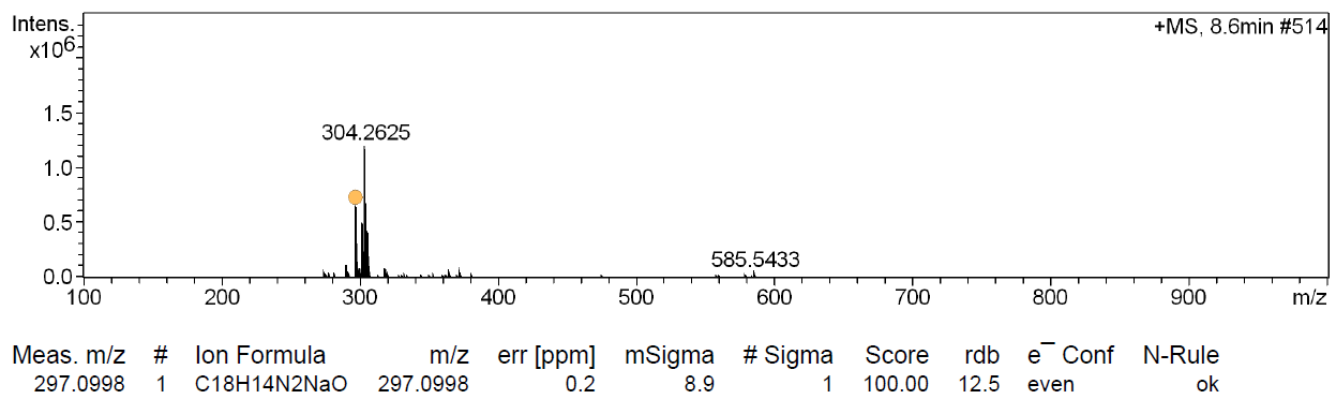


Figure S4. [1-Phenyl-3-(phenylethynyl)-1*H*-pyrazol-4-yl]methanol (**3**). HRMS (ESI-TOF).

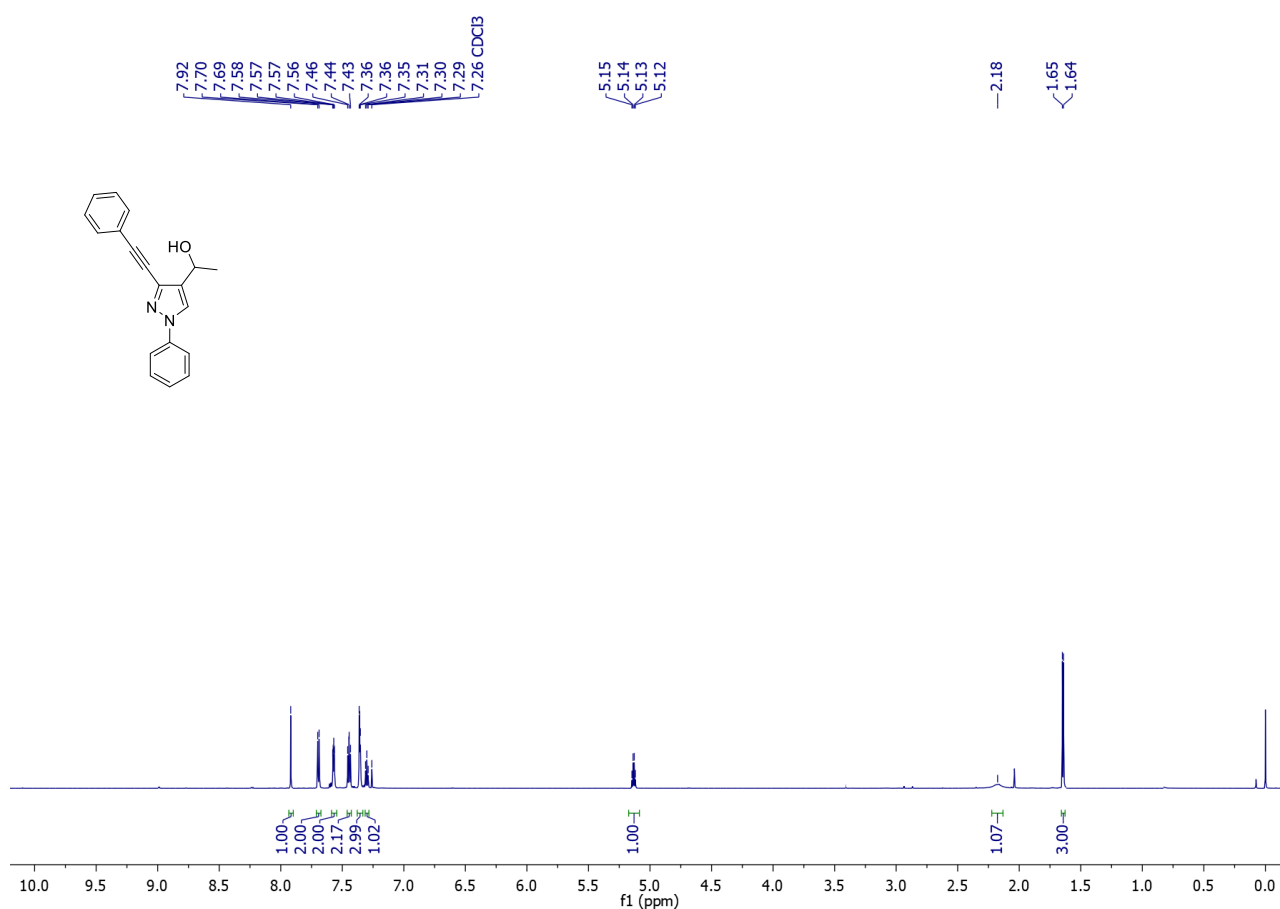


Figure S5. 1-[1-Phenyl-3-(phenylethynyl)-1*H*-pyrazol-4-yl]ethanol-1-ol (**4**). ¹H NMR spectrum (700 MHz, CDCl₃).

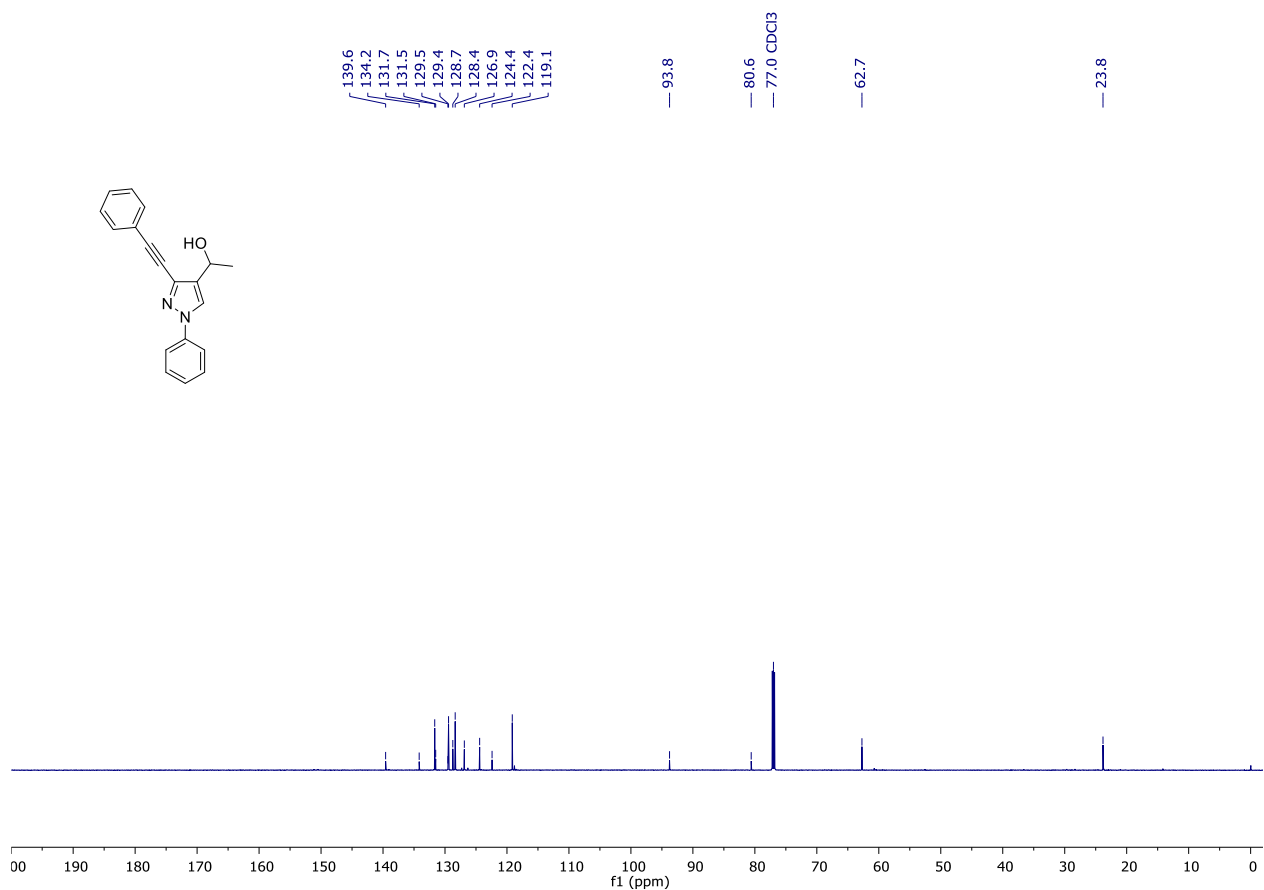


Figure S6. 1-[1-Phenyl-3-(phenylethynyl)-1H-pyrazol-4-yl]ethanol-1-ol (**4**). ¹³C NMR (176 MHz, CDCl₃).

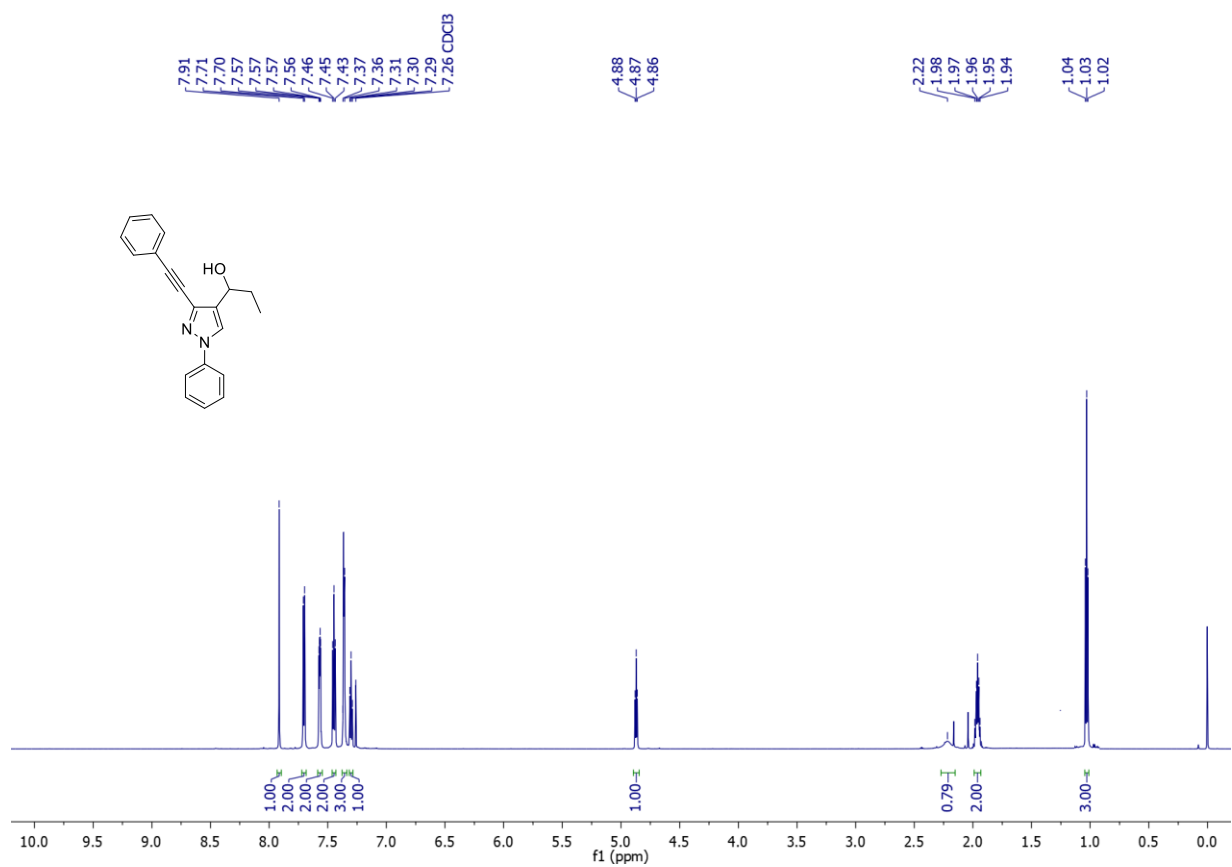


Figure S7. 1-(1-phenyl-3-(phenylethynyl)-1H-pyrazol-4-yl)propan-1-ol (**5**). ¹H NMR spectrum (700 MHz, CDCl₃).

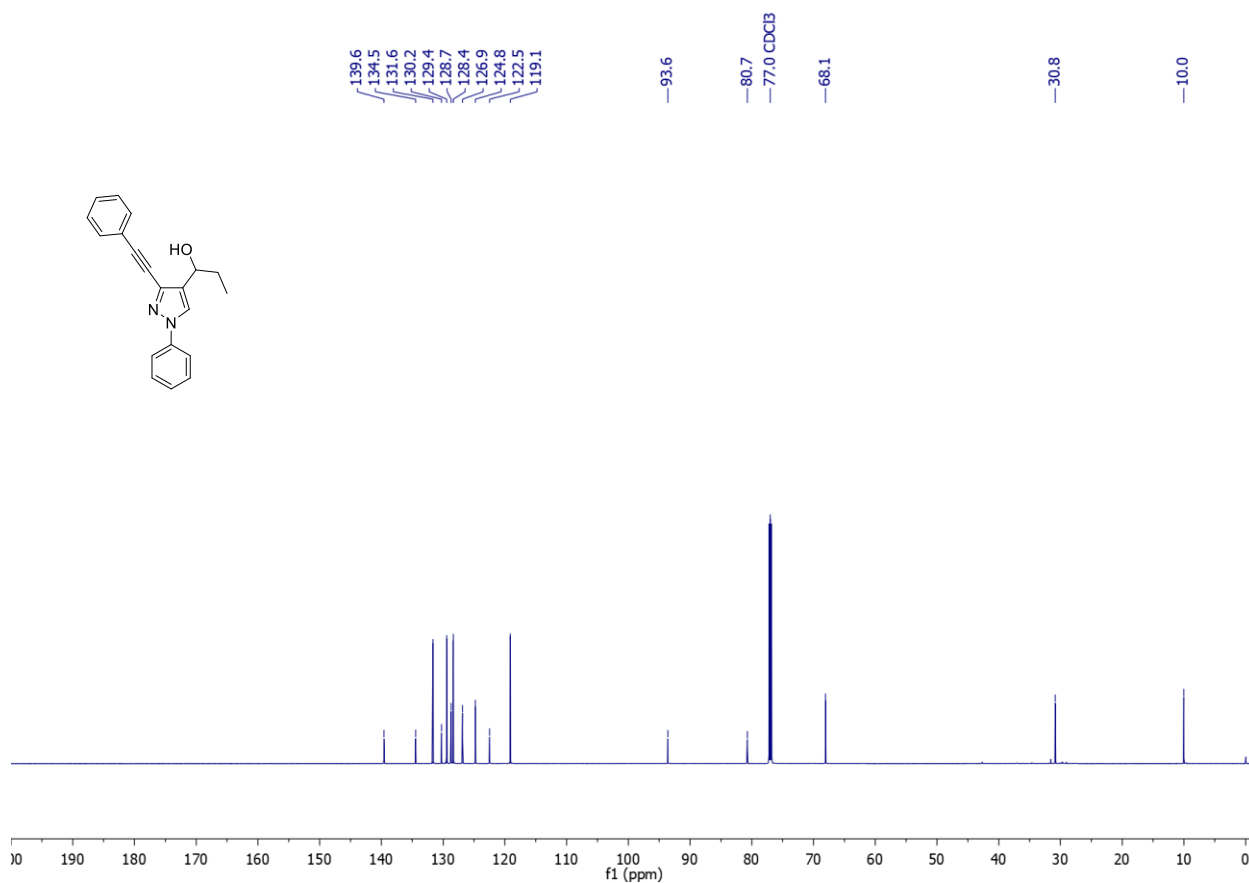
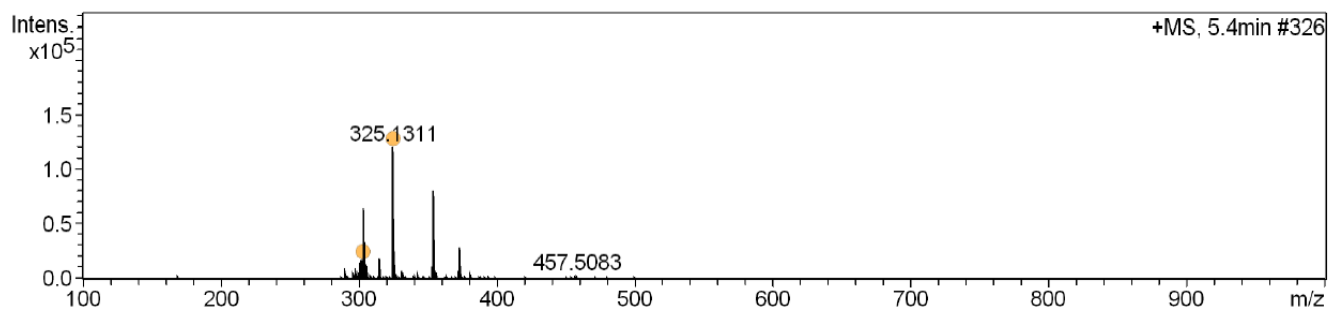


Figure S8. 1-(1-phenyl-3-(phenylethynyl)-1H-pyrazol-4-yl)propan-1-ol (**5**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 5.4min #326



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
303.1491	1	C ₂₀ H ₁₉ N ₂ O	303.1492	-0.2	12.3	1	100.00	12.5	even	ok
325.1311	1	C ₂₀ H ₁₈ N ₂ NaO	325.1311	-0.2	4.5	1	100.00	12.5	even	ok

Figure S9. 1-(1-phenyl-3-(phenylethynyl)-1H-pyrazol-4-yl)propan-1-ol (**5**). HRMS (ESI-TOF).

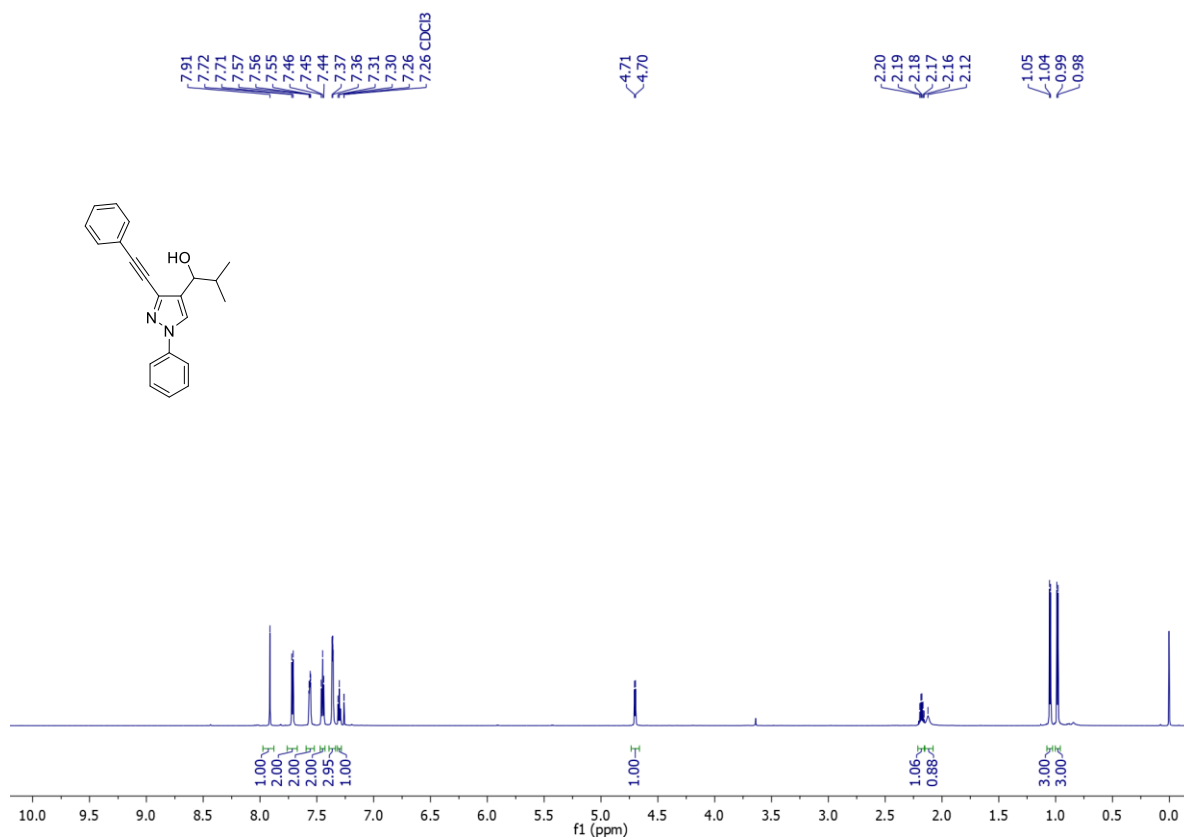


Figure S10. 2-Methyl-1-[1-phenyl-3-(phenylethynyl)-1H-pyrazol-4-yl]propan-1-ol (**6**). ¹H NMR spectrum (700 MHz, CDCl₃).

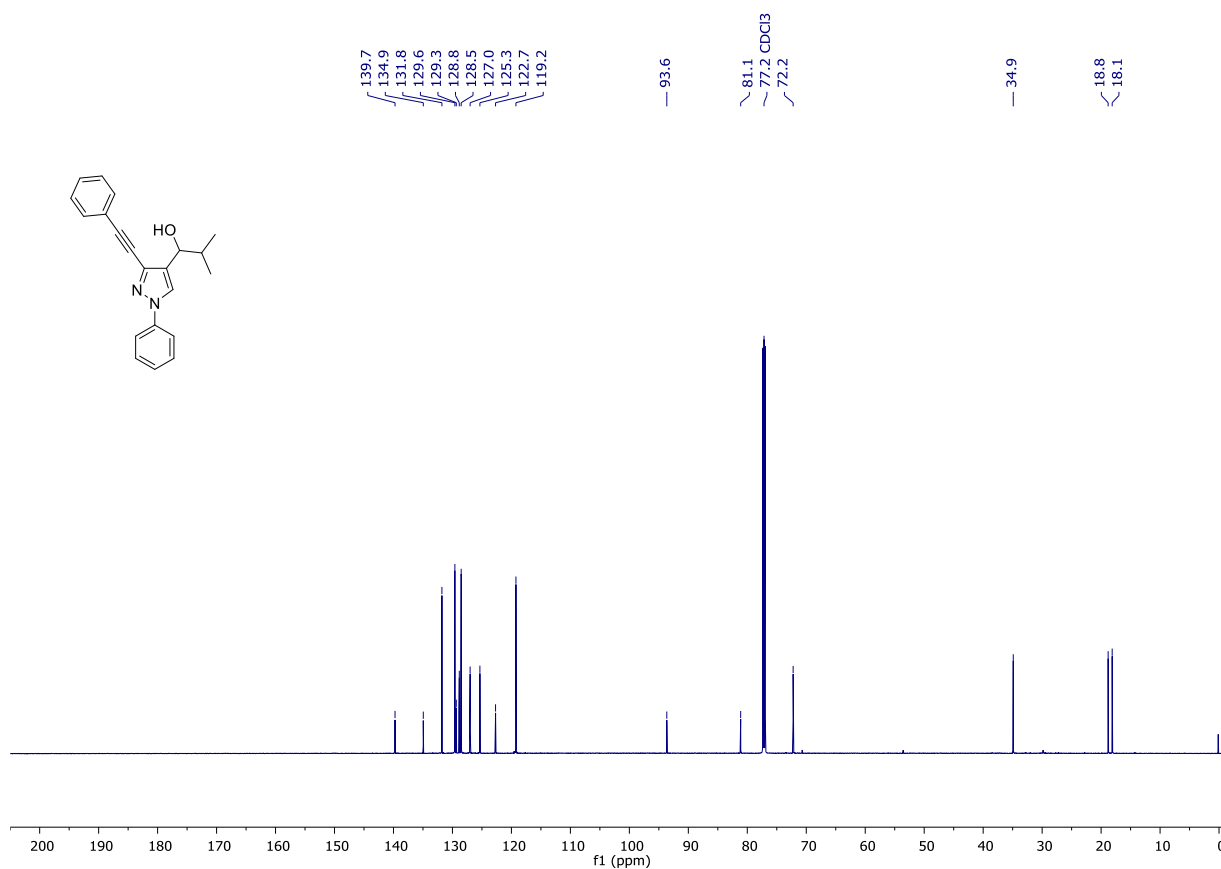


Figure S11. 2-Methyl-1-[1-phenyl-3-(phenylethynyl)-1H-pyrazol-4-yl]propan-1-ol (**6**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 2.5min #150

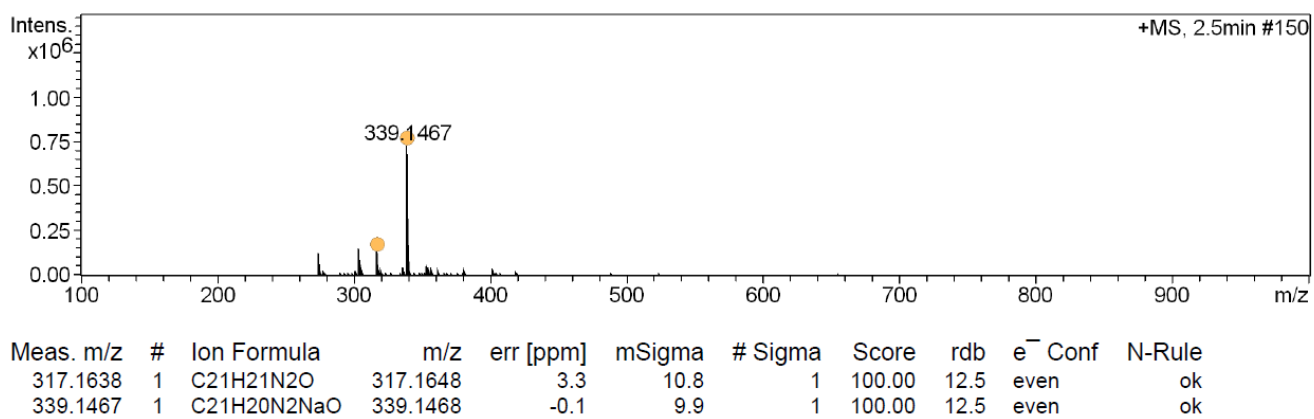


Figure S12. 2-Methyl-1-[1-phenyl-3-(phenylethynyl)-1*H*-pyrazol-4-yl]propan-1-ol (**6**). HRMS (ESI-TOF).

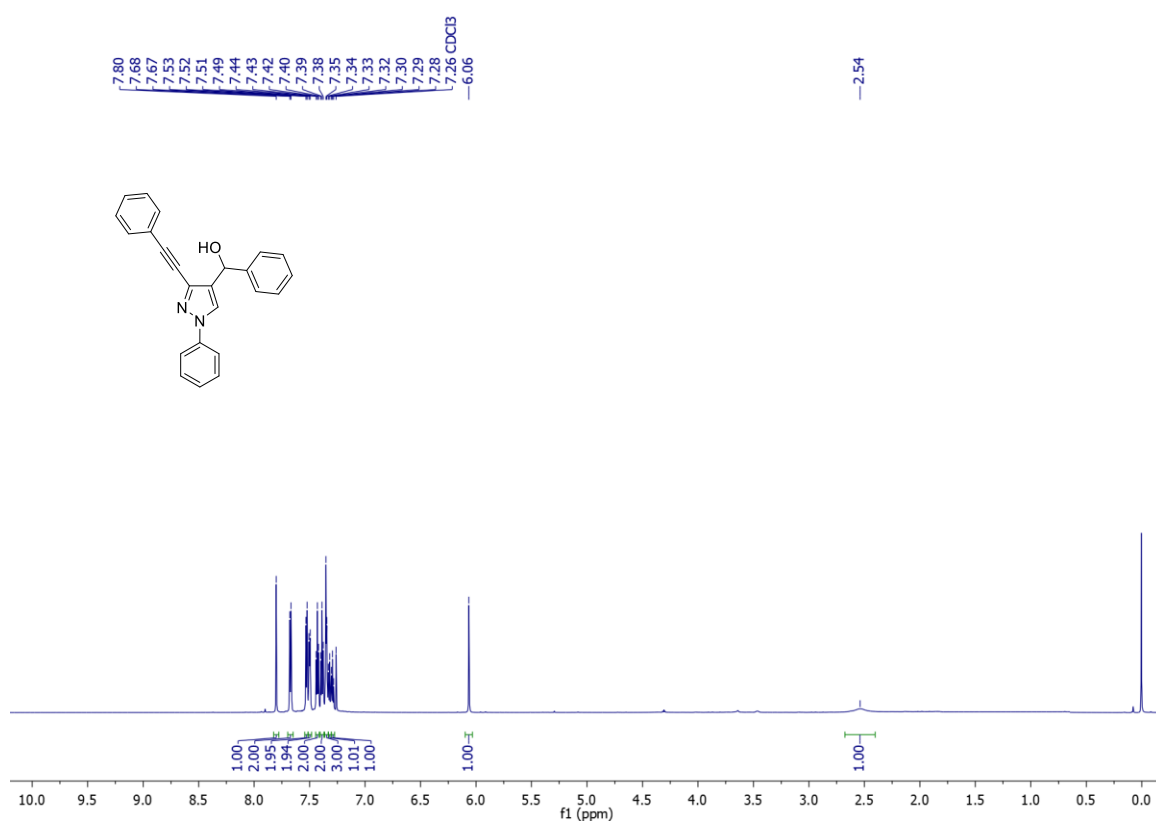


Figure S13. Phenyl(1-phenyl-3-(phenylethynyl)-1*H*-pyrazol-4-yl)methanol (**7**). ¹H NMR spectrum (700 MHz, CDCl₃).

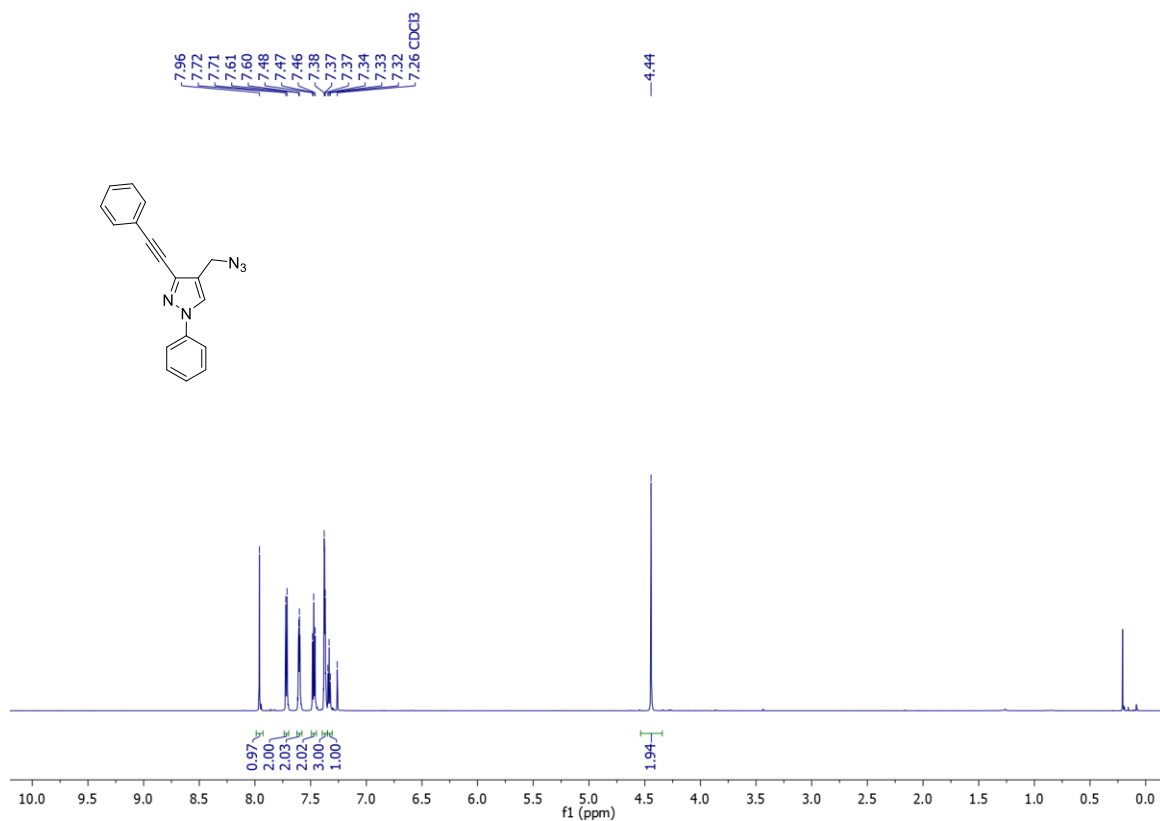


Figure S16. 4-(Azidomethyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**8**). ¹H NMR spectrum (700 MHz, CDCl₃).

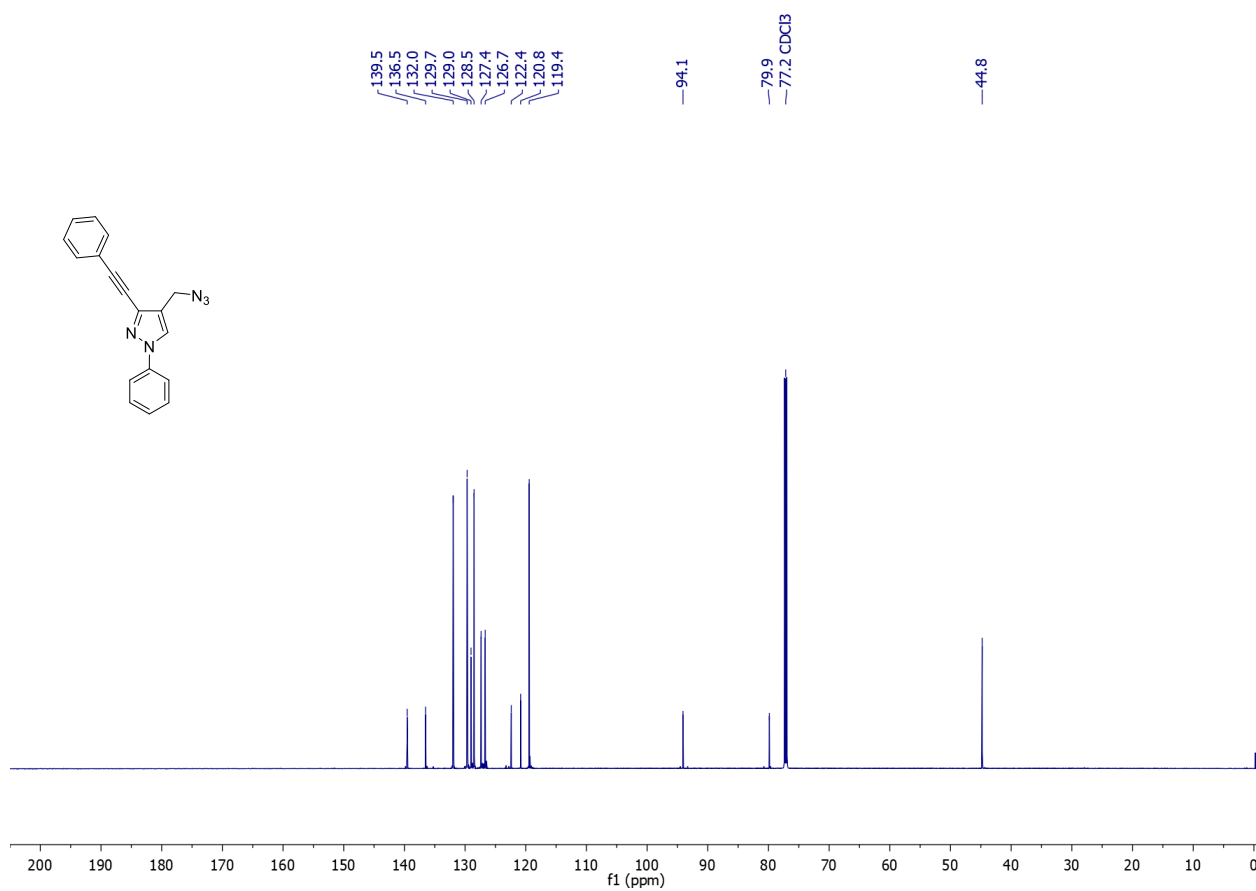


Figure S17. 4-(Azidomethyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**8**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 8.3min #500

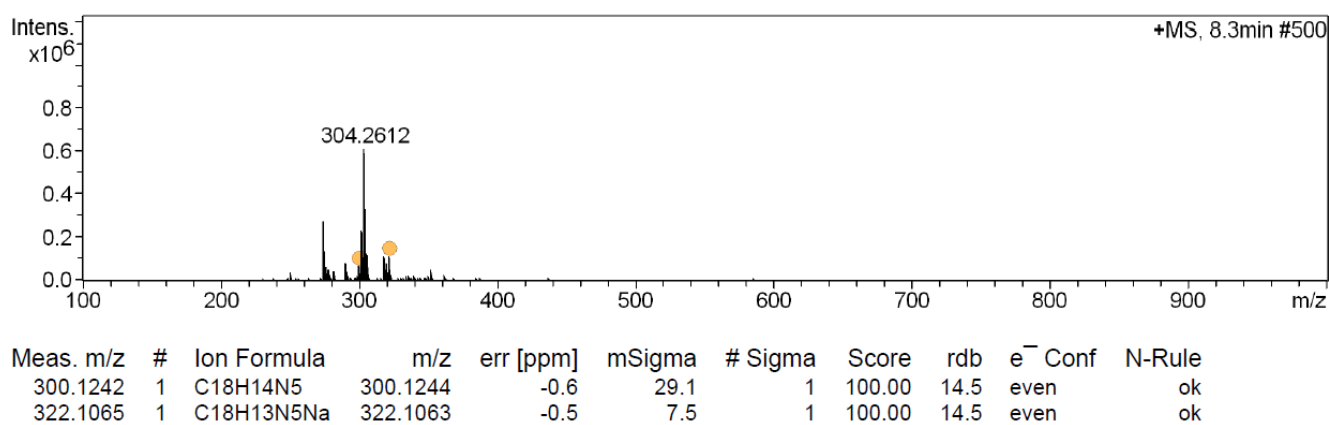


Figure S18. 4-(Azidomethyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**8**). HRMS (ESI-TOF).

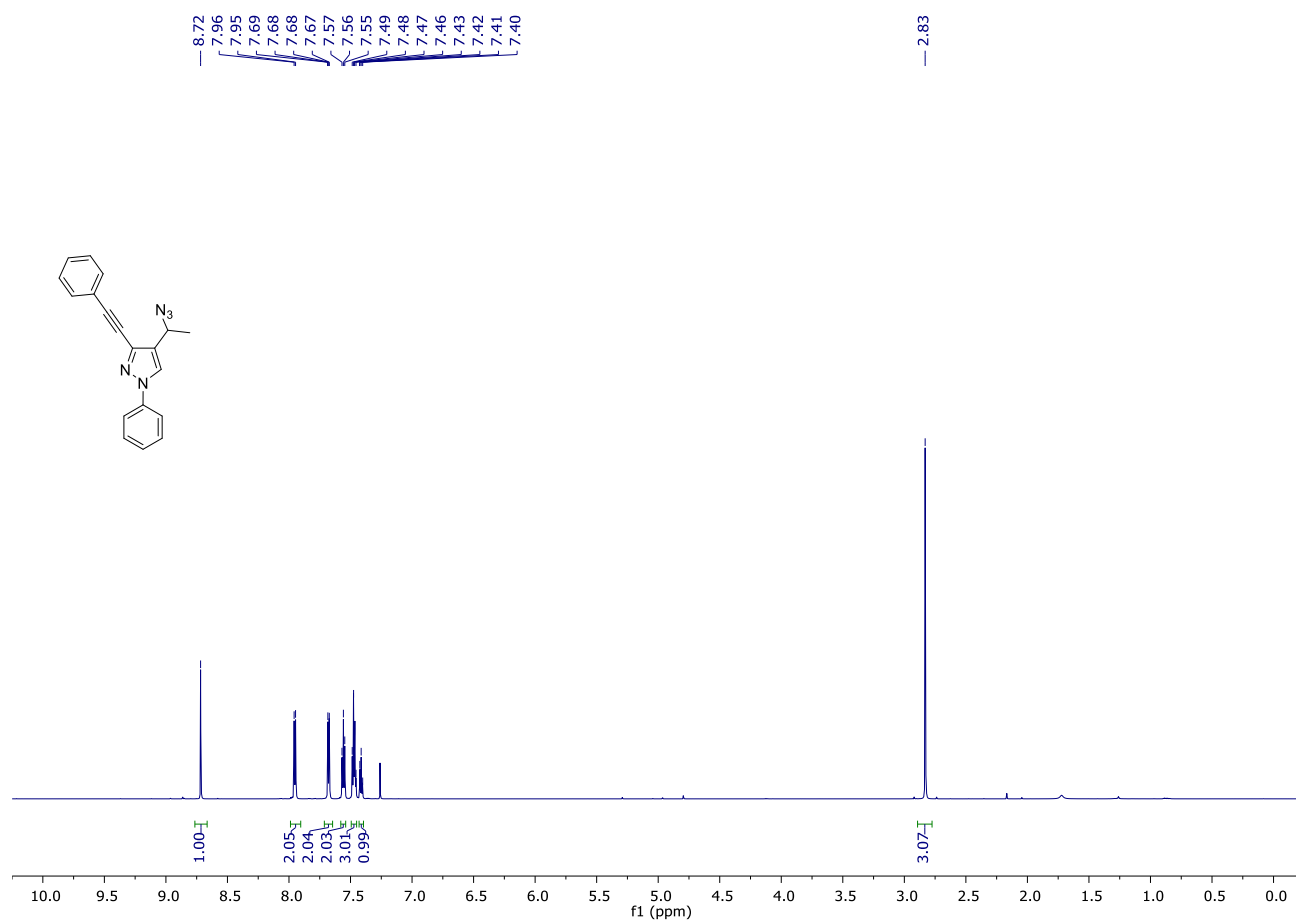


Figure S19. 4-(1-Azidoethyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**9**). ¹H NMR spectrum (700 MHz, CDCl₃).

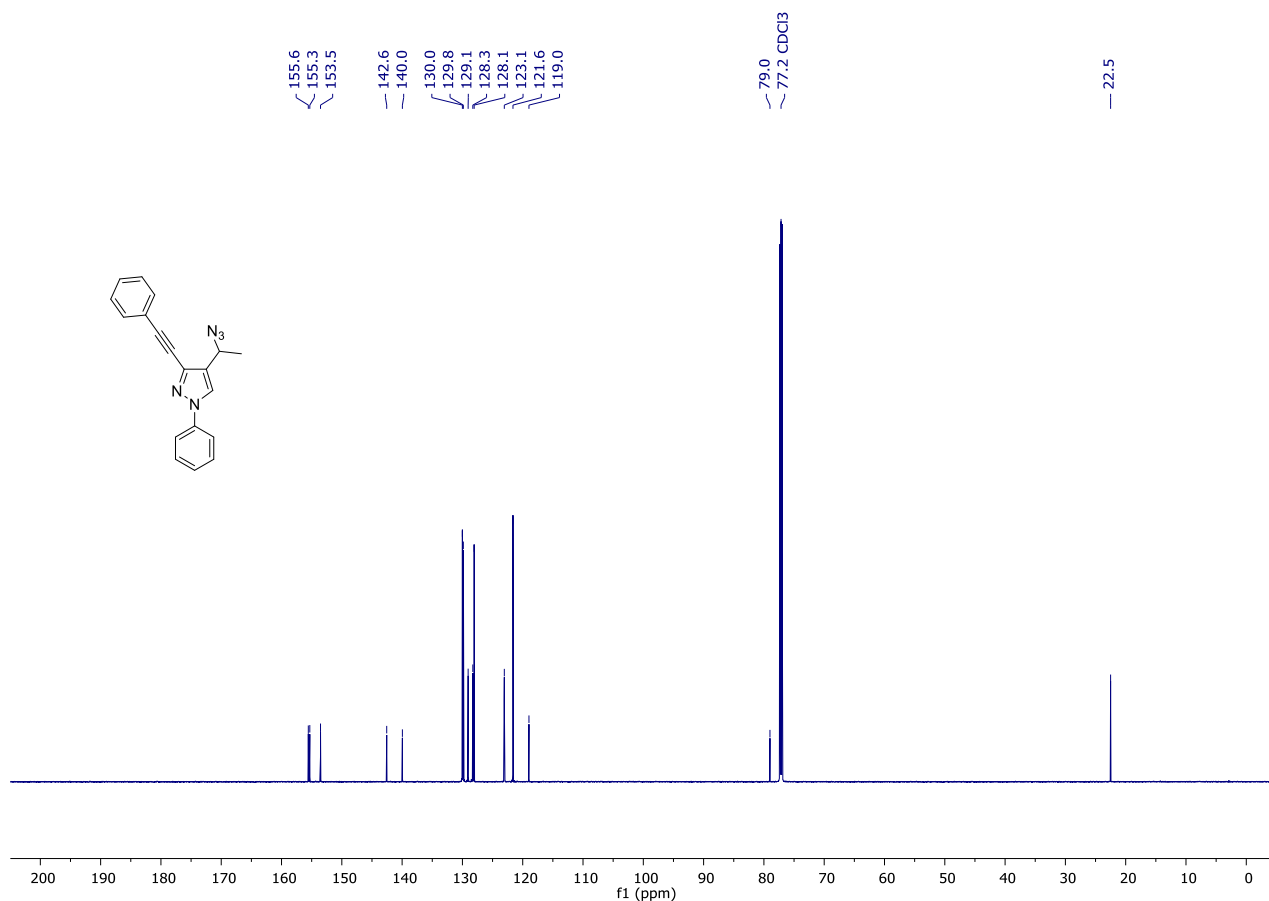
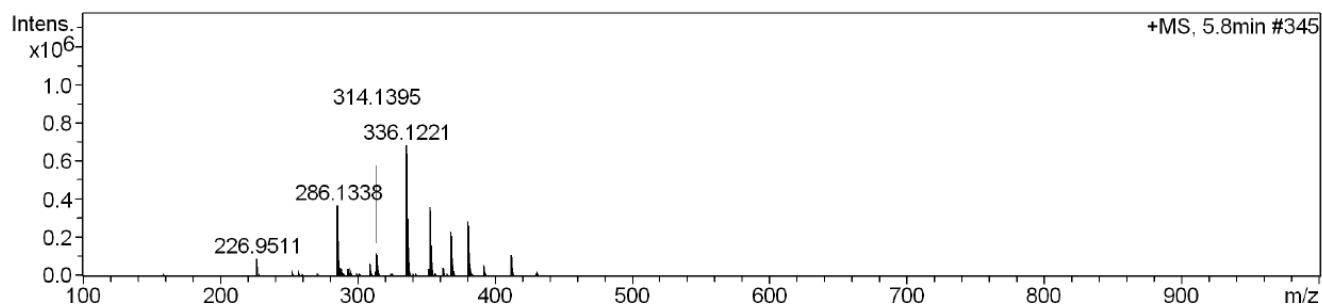


Figure S20. 4-(1-Azidoethyl)-1-phenyl-3-(phenylethynyl)-1H-pyrazole (**9**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 5.8min #345



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
314.1395	1	C ₁₉ H ₁₆ N ₅	314.1400	-1.6	42.0	1	100.00	14.5	even	ok
336.1221	1	C ₁₉ H ₁₅ N ₅ Na	336.1220	-0.4	4.5	1	100.00	14.5	even	ok

Figure S21. 4-(1-Azidoethyl)-1-phenyl-3-(phenylethynyl)-1H-pyrazole (**9**). HRMS (ESI-TOF).

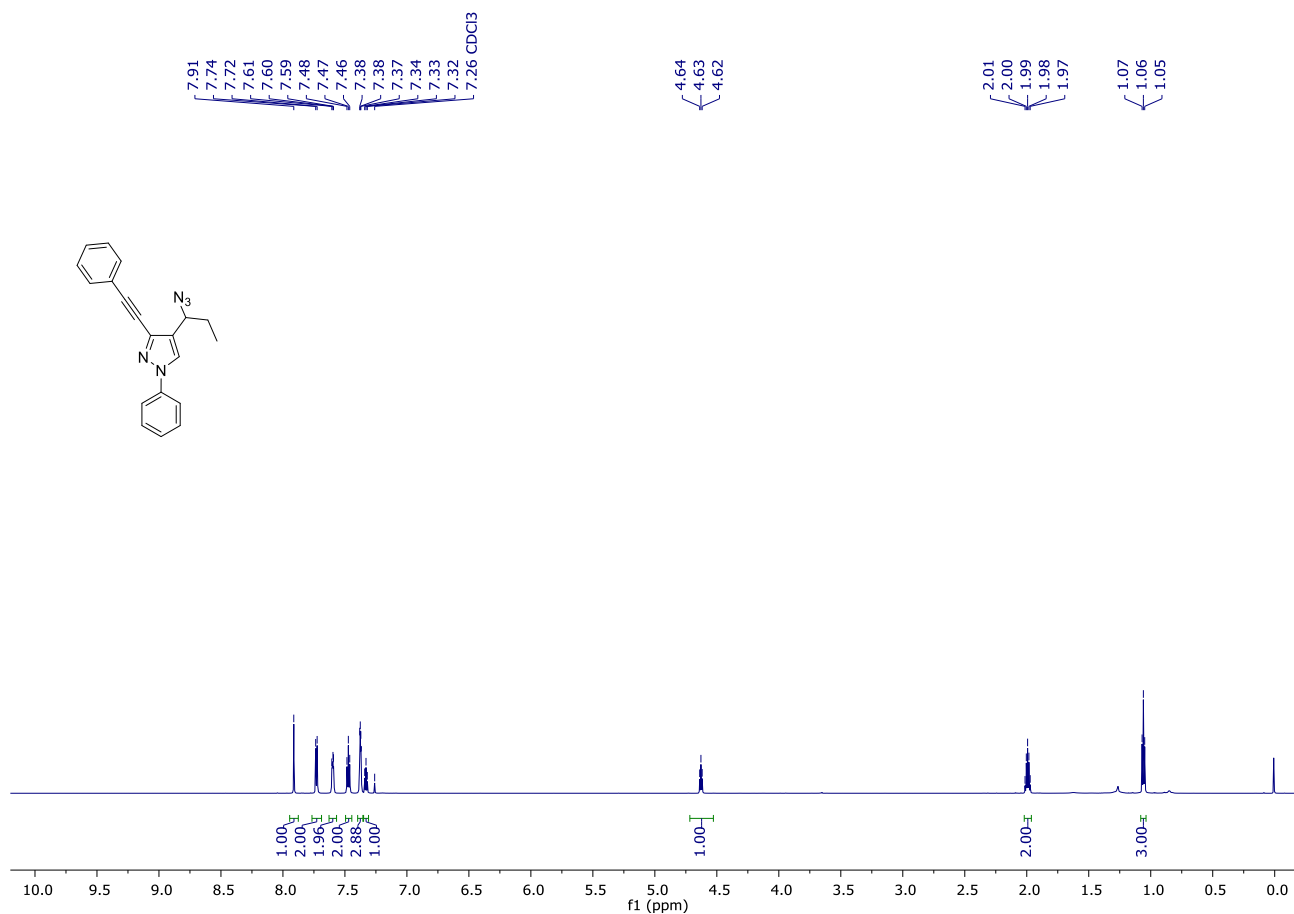


Figure S22. 4-(1-Azidopropyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**10**). ¹H NMR spectrum (700 MHz, CDCl₃).

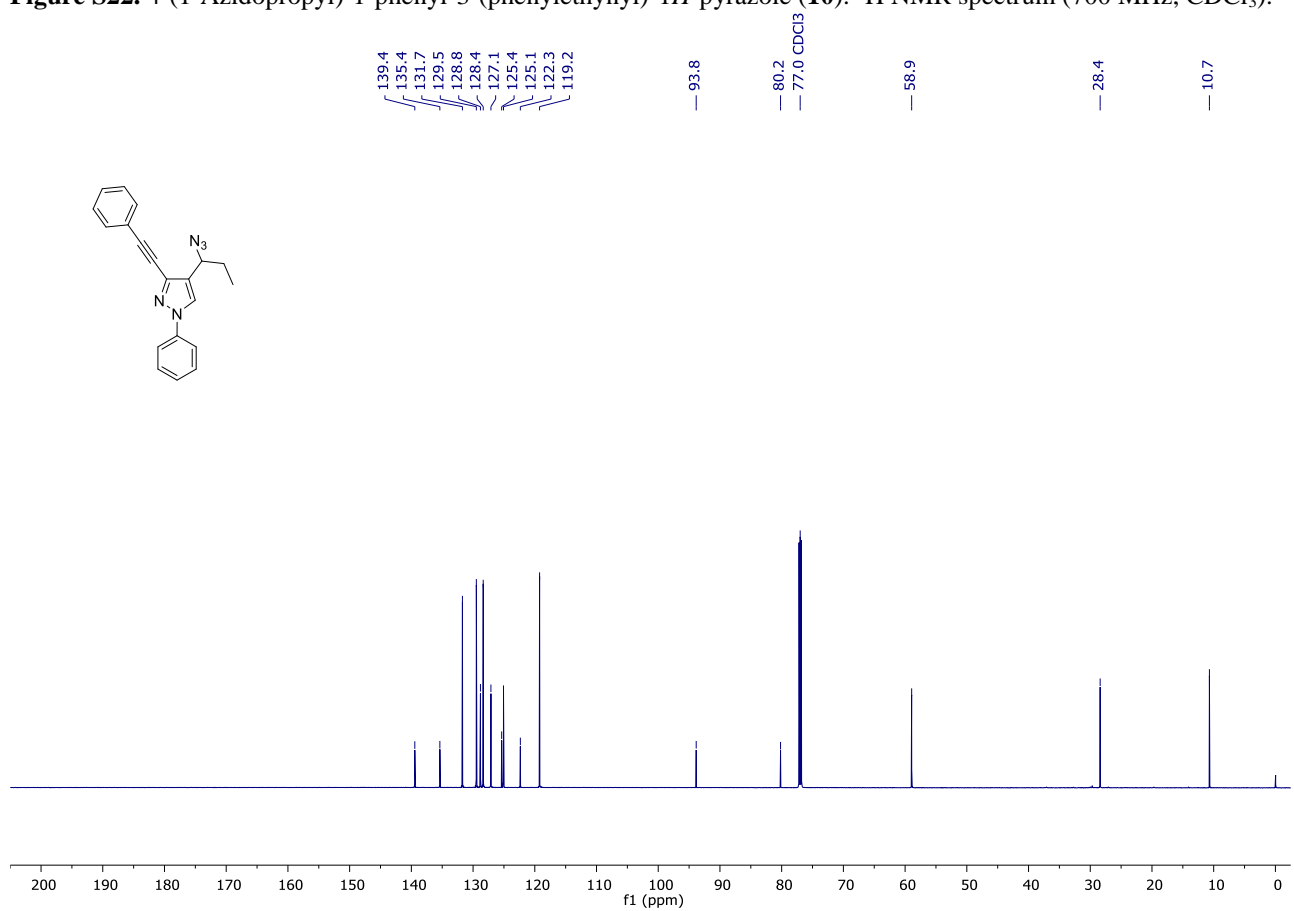


Figure S23. 4-(1-Azidopropyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**10**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 6.0min #358

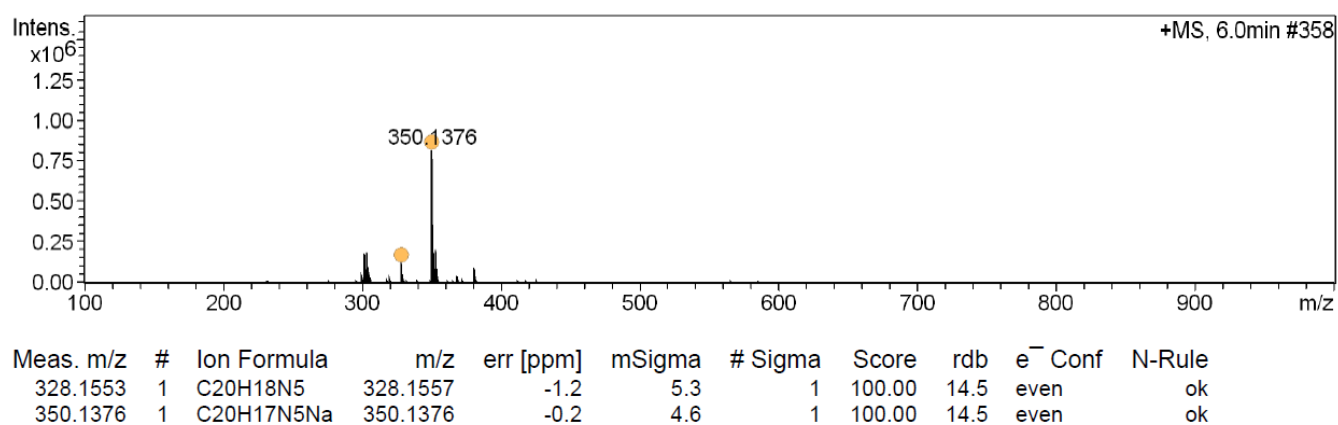


Figure S24. 2,6,7-Triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**18**). HRMS (ESI-TOF).

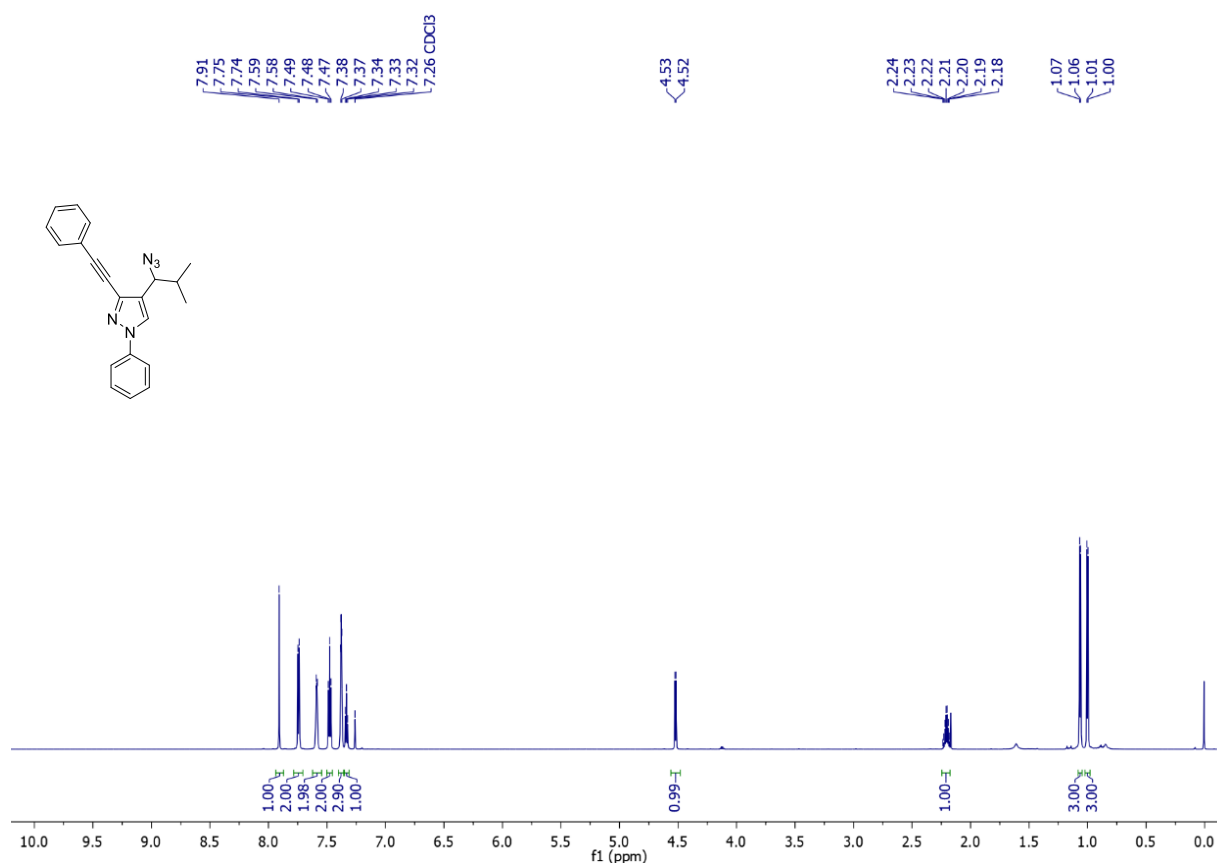


Figure S25. 4-(Azido-2-methylpropyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**11**). ¹H NMR spectrum (700 MHz, CDCl₃).

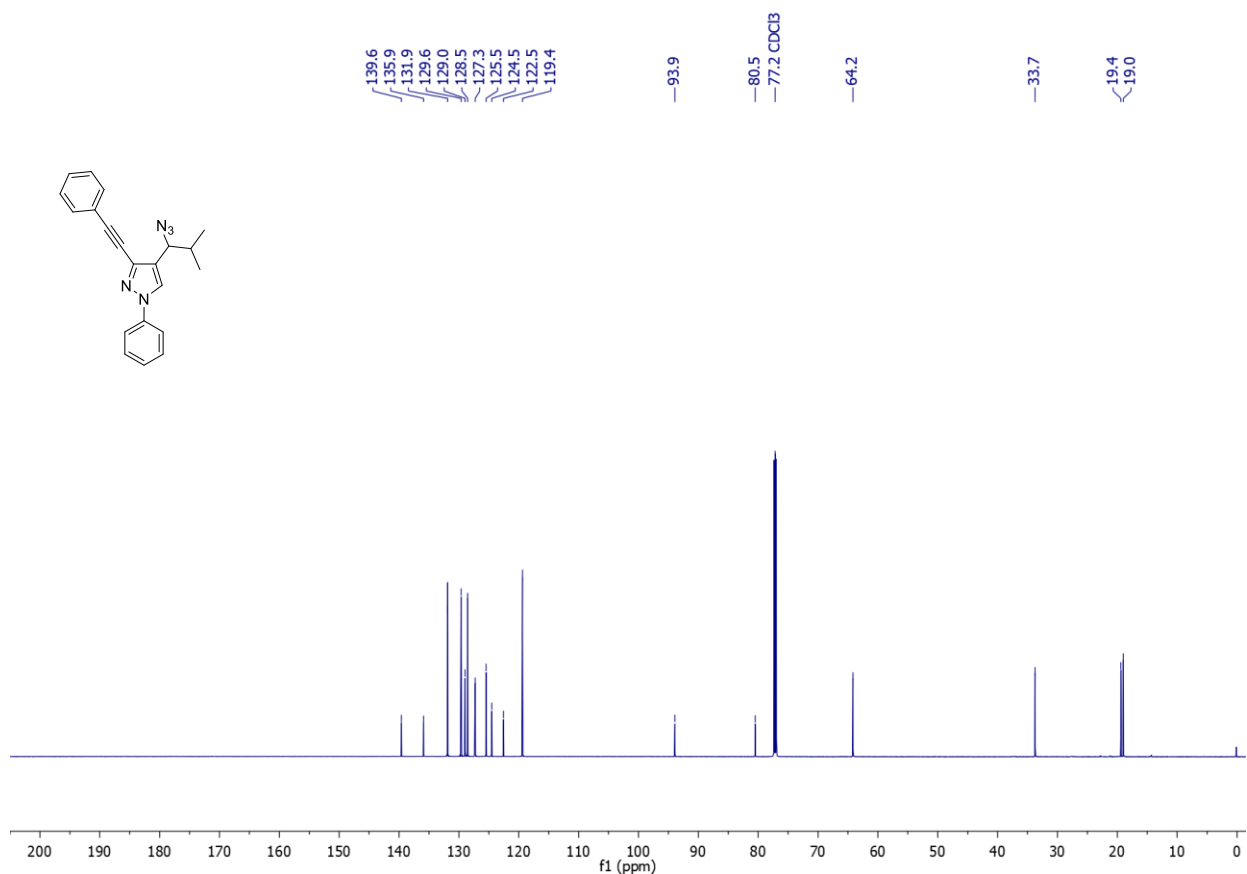


Figure S26. 4-(Azido-2-methylpropyl)-1-phenyl-3-(phenylethynyl)-1H-pyrazole (**11**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 5.3min #318

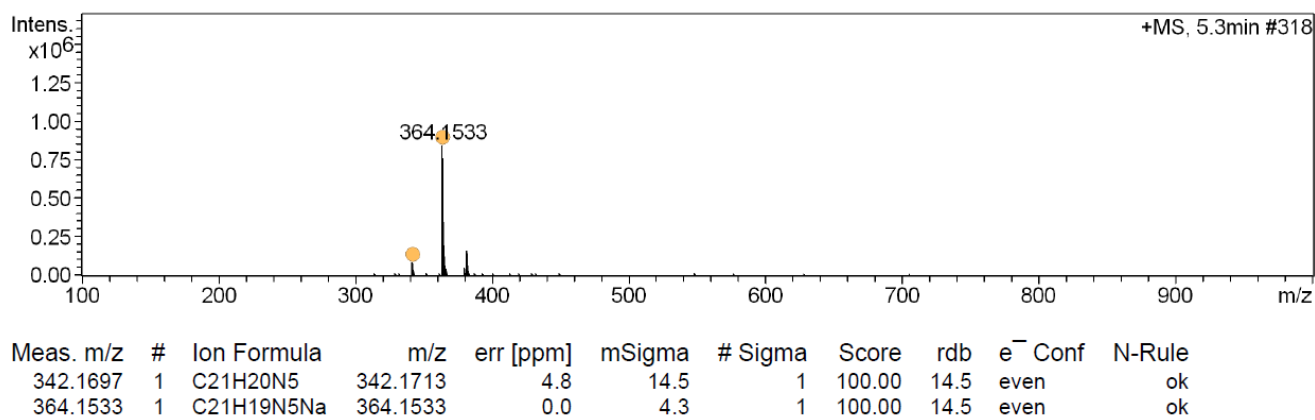


Figure S27. 4-(Azido-2-methylpropyl)-1-phenyl-3-(phenylethynyl)-1H-pyrazole (**11**). HRMS (ESI-TOF).

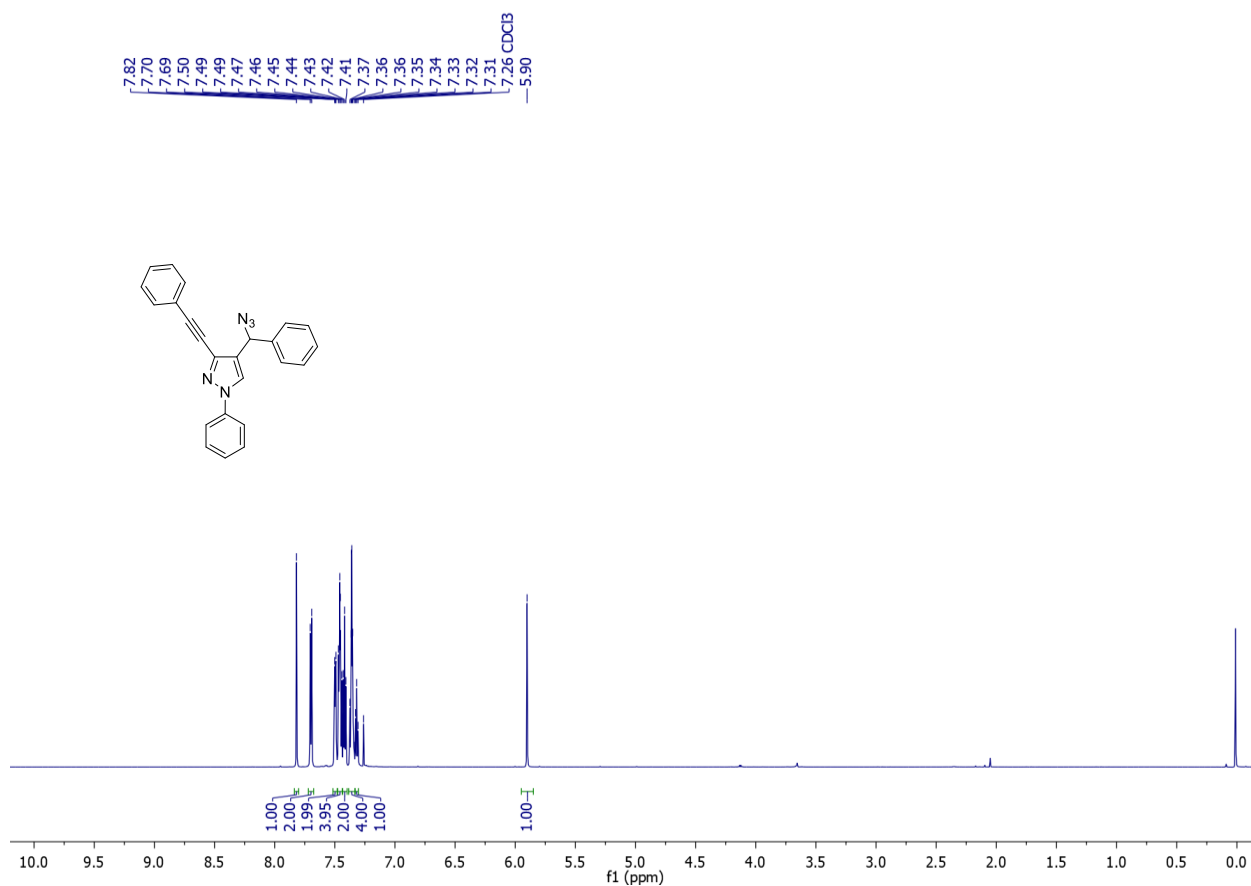


Figure S28. 4-(Azido(phenyl)methyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**12**). ¹H NMR spectrum (700 MHz, CDCl₃).

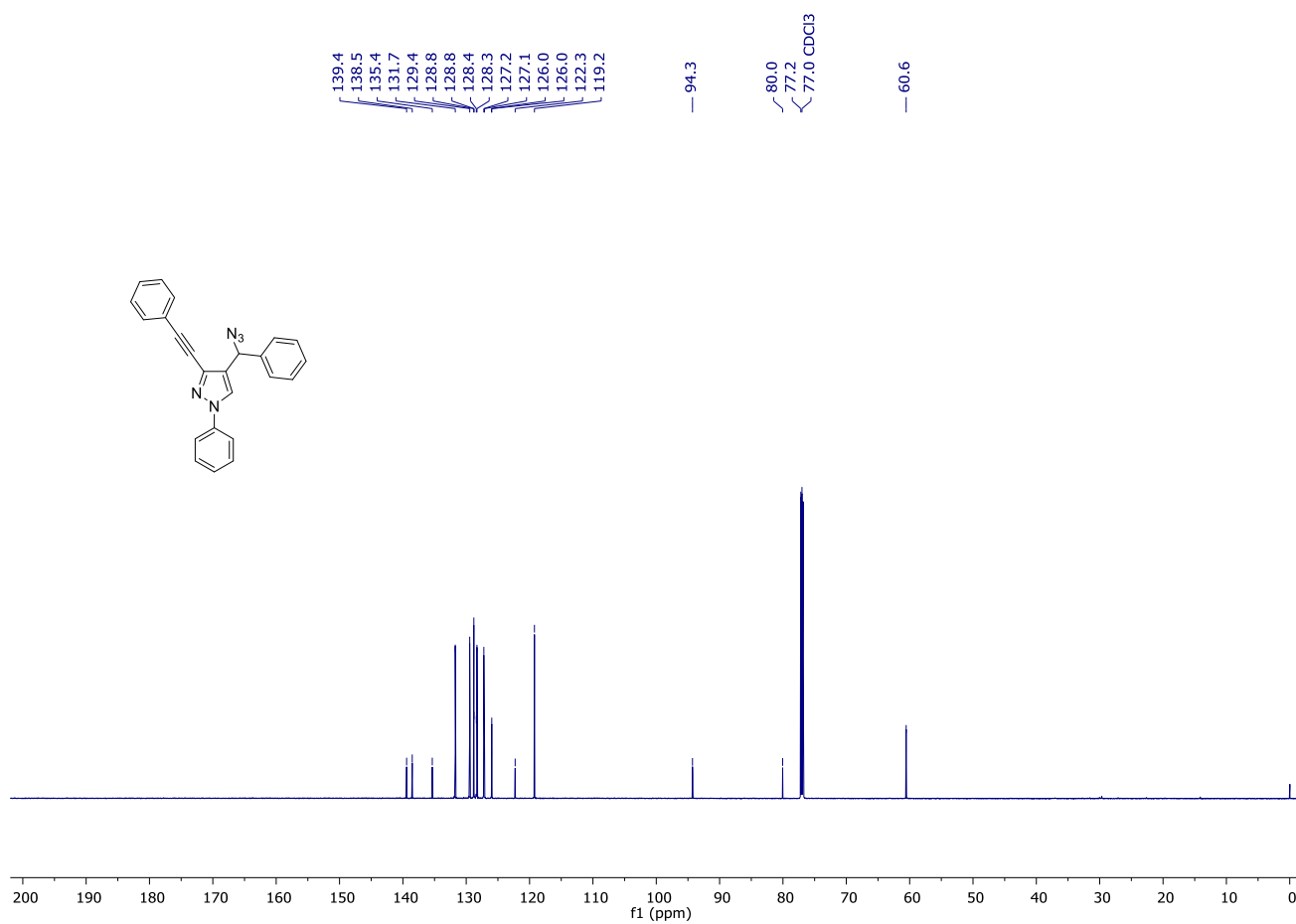


Figure S29. 4-(Azido(phenyl)methyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**12**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 7.6min #457

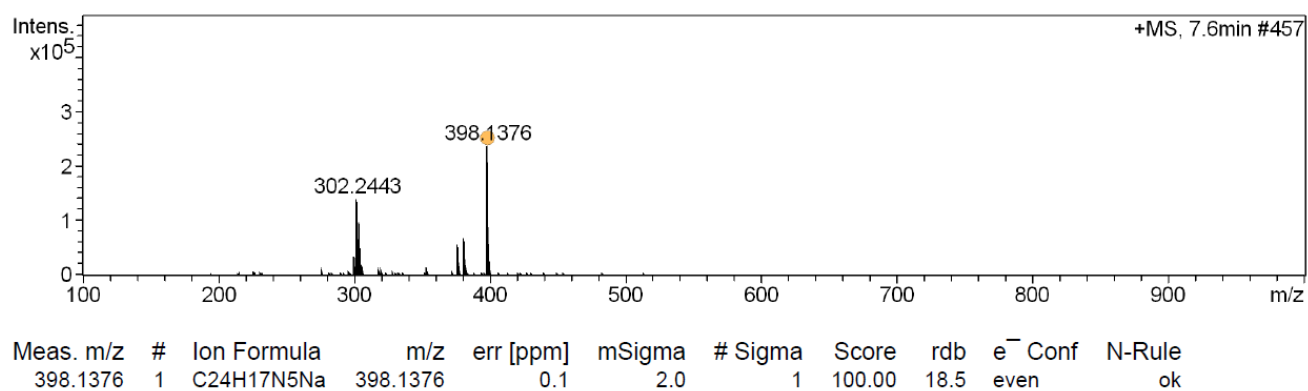


Figure S30. 4-(Azido(phenyl)methyl)-1-phenyl-3-(phenylethynyl)-1*H*-pyrazole (**12**). HRMS (ESI-TOF).

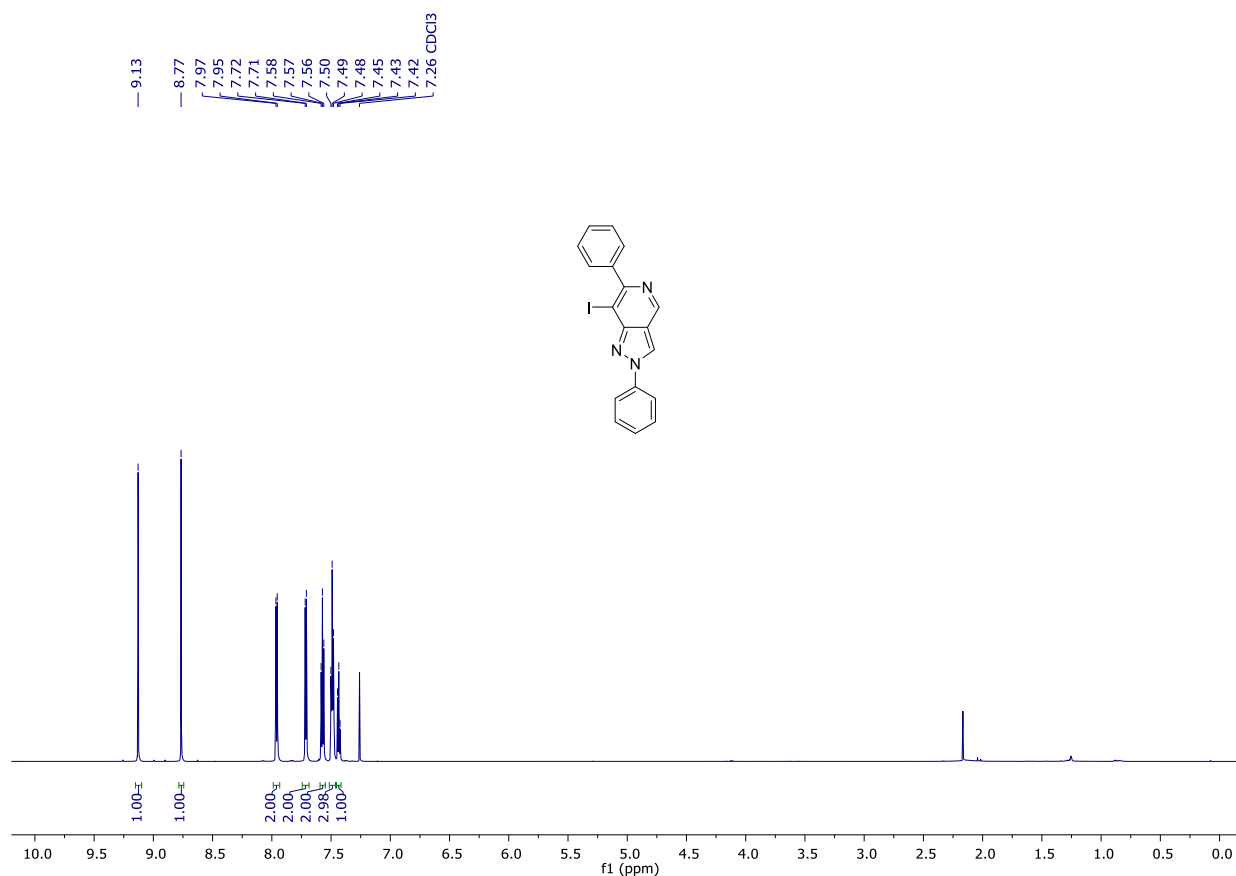


Figure S31. 7-Iodo-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**13**). ¹H NMR spectrum (700 MHz, CDCl₃).

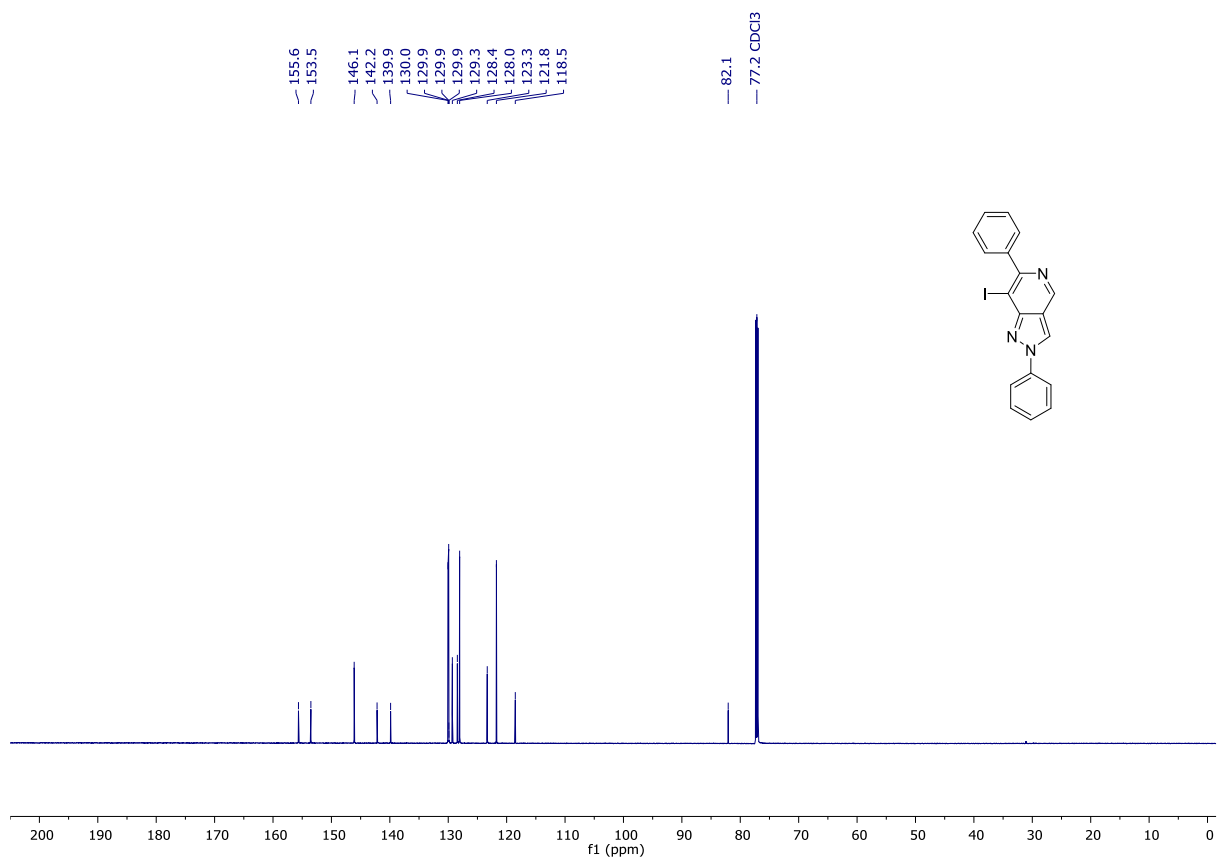


Figure S32. 7-Iodo-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**13**). ¹³C NMR (176 MHz, CDCl₃).

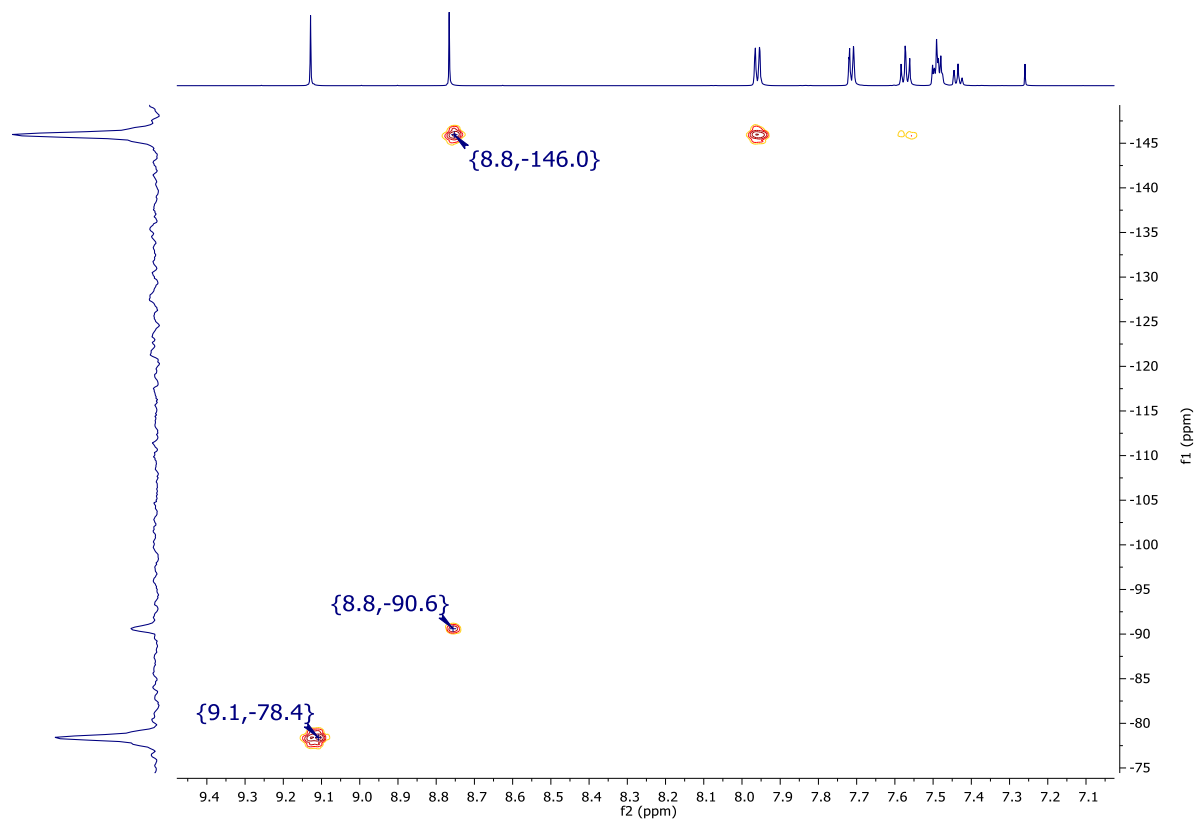


Figure S33. 7-Iodo-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**13**). ¹H-¹⁵N HMBC spectrum (700 MHz, CDCl₃).

+MS, 4.4min #264

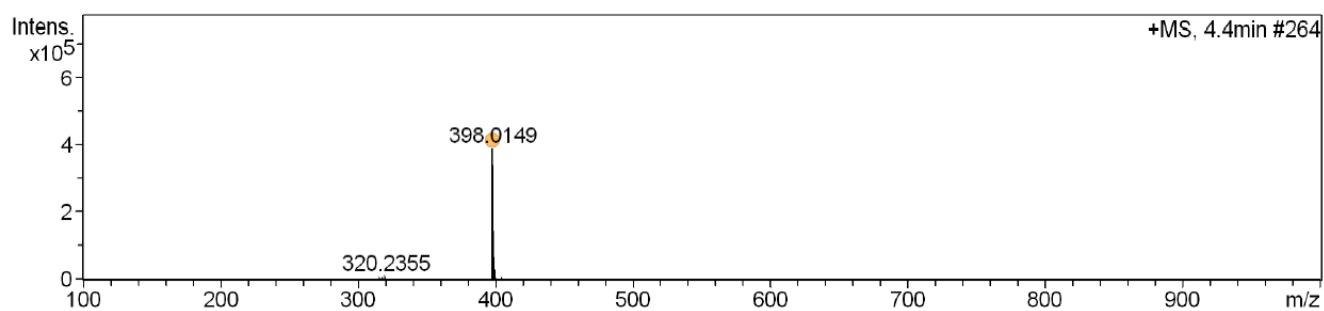


Figure S34. 7-Iodo-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**13**). HRMS (ESI-TOF).

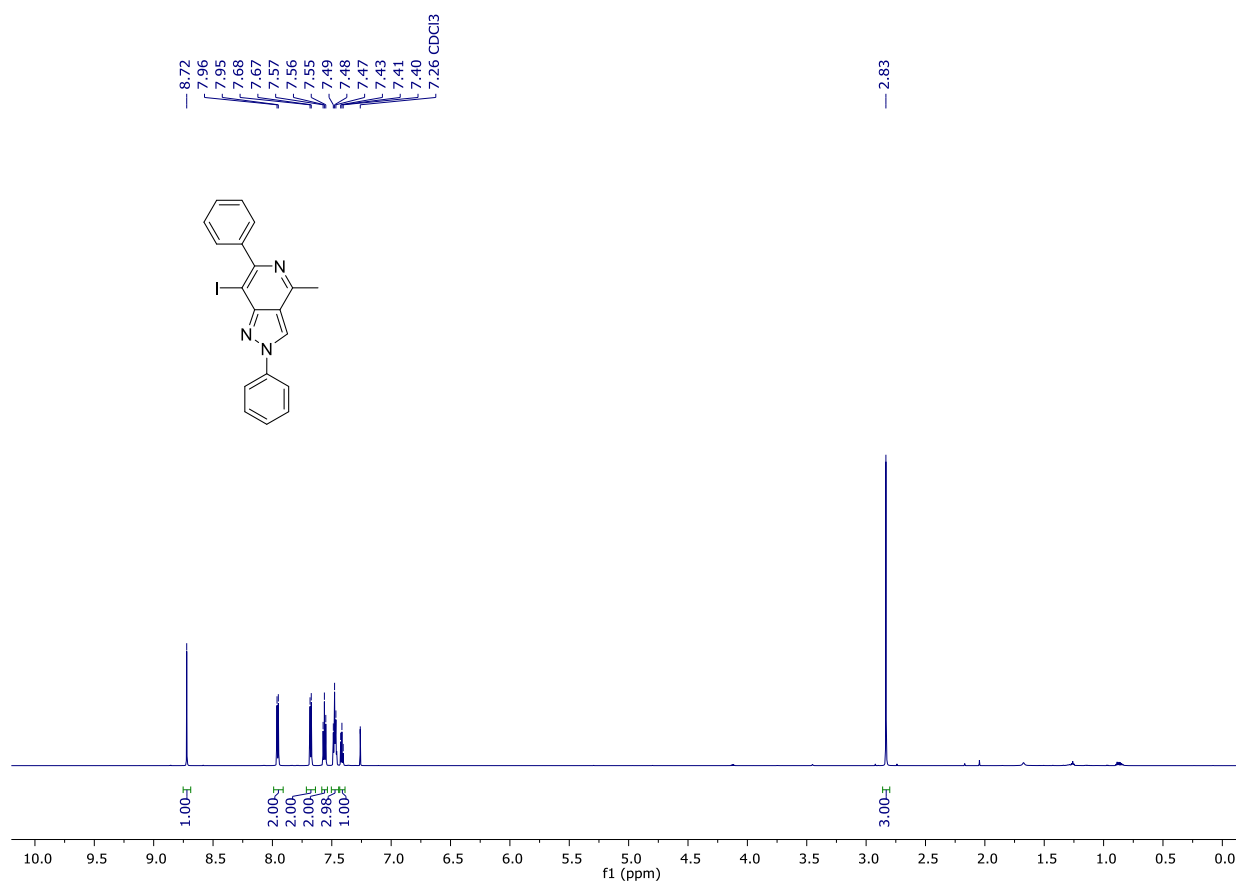


Figure S35. 7-Iodo-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**14**). ¹H NMR spectrum (700 MHz, CDCl₃).

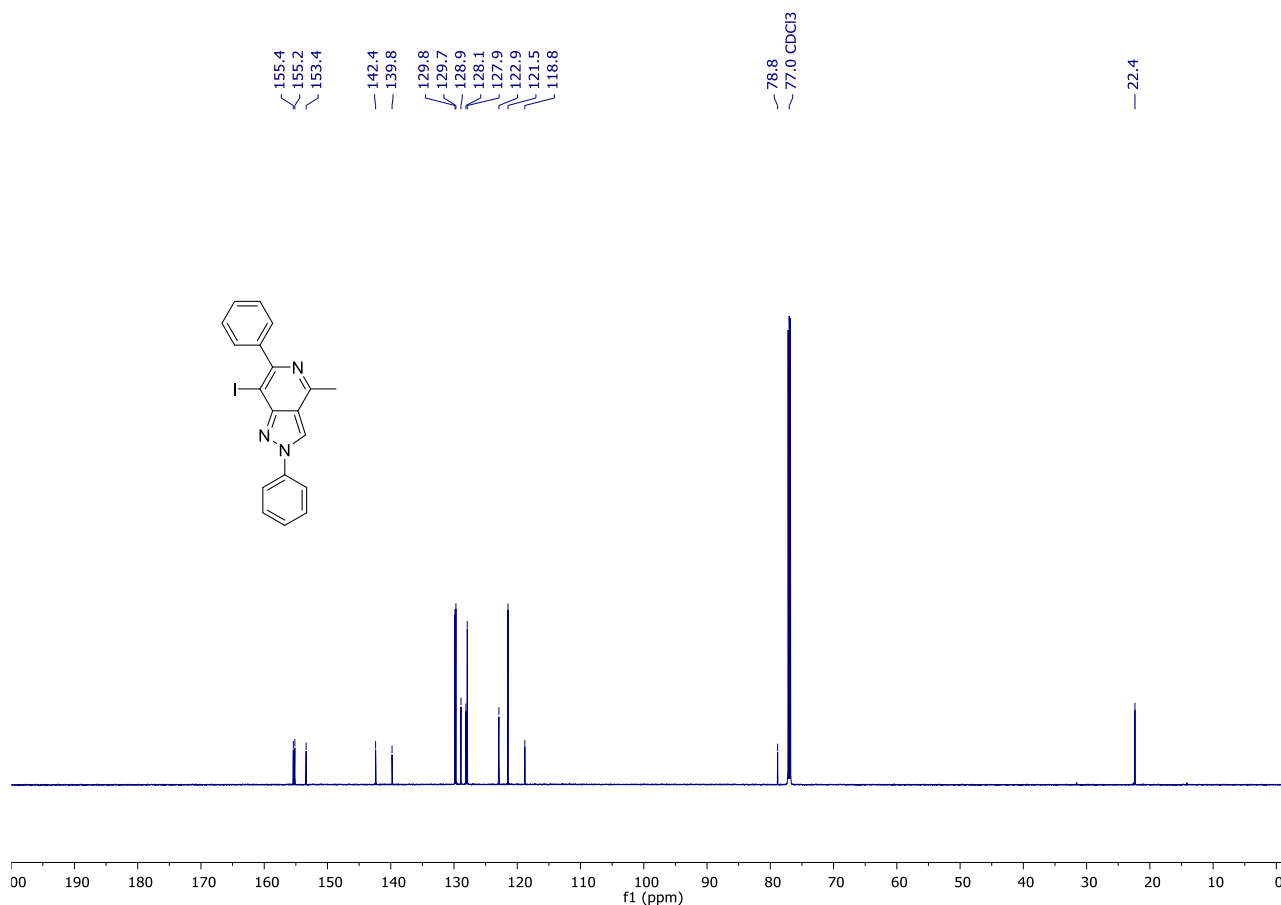


Figure S36. 7-Iodo-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**14**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 4.2min #252

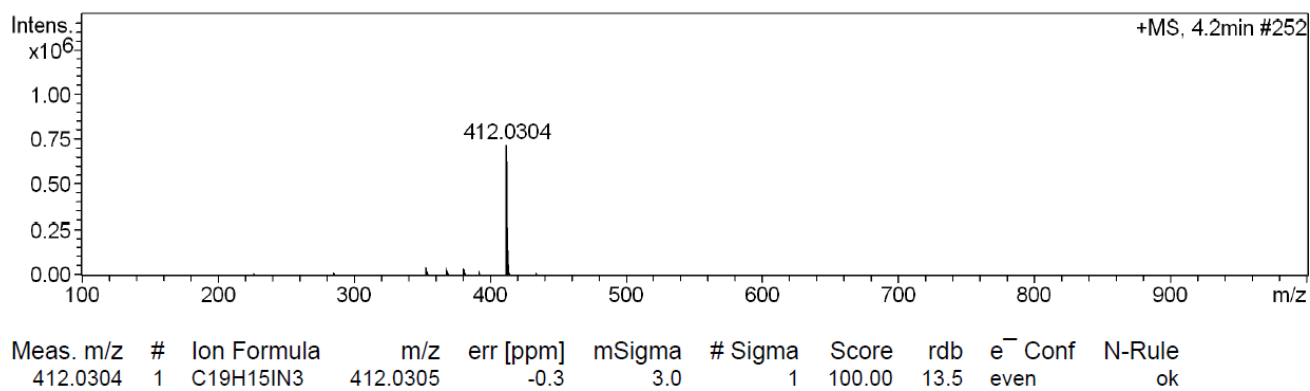


Figure S37. 7-Iodo-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**14**). HRMS (ESI-TOF).

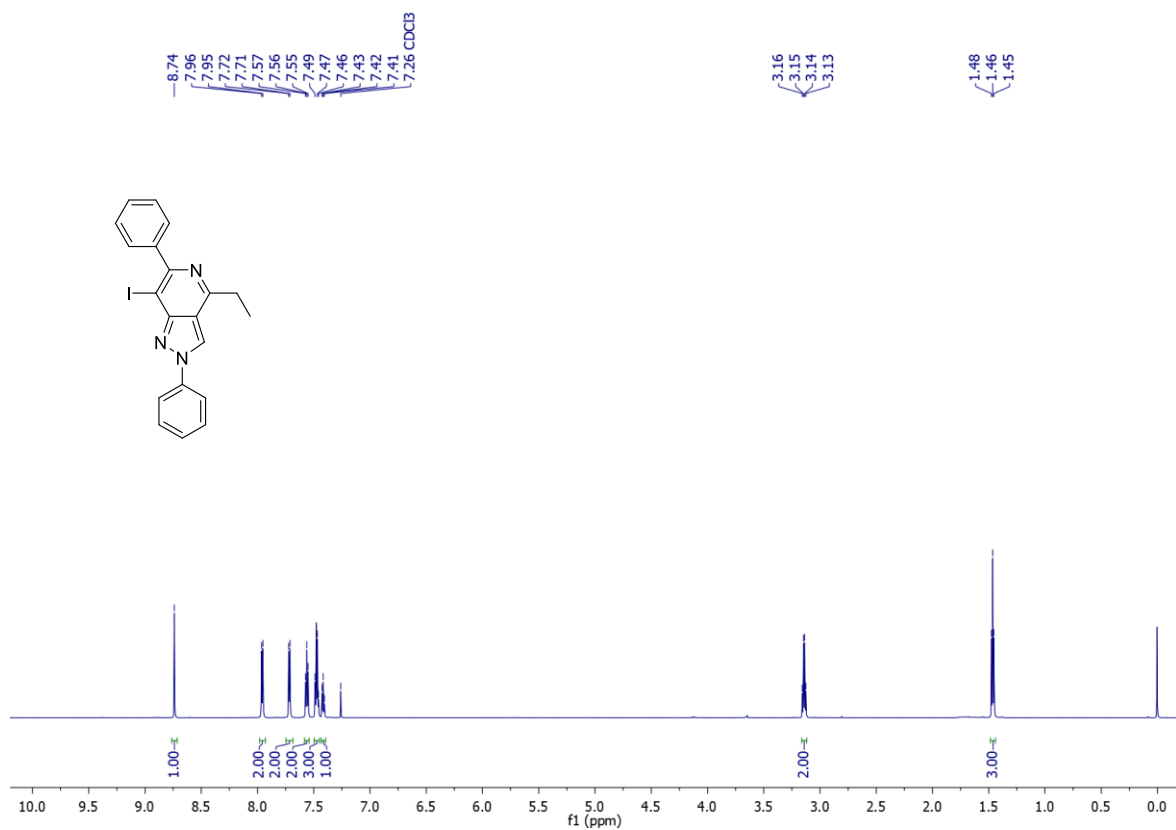


Figure S38. 4-Ethyl-7-iodo-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**15**). ¹H NMR spectrum (700 MHz, CDCl₃).

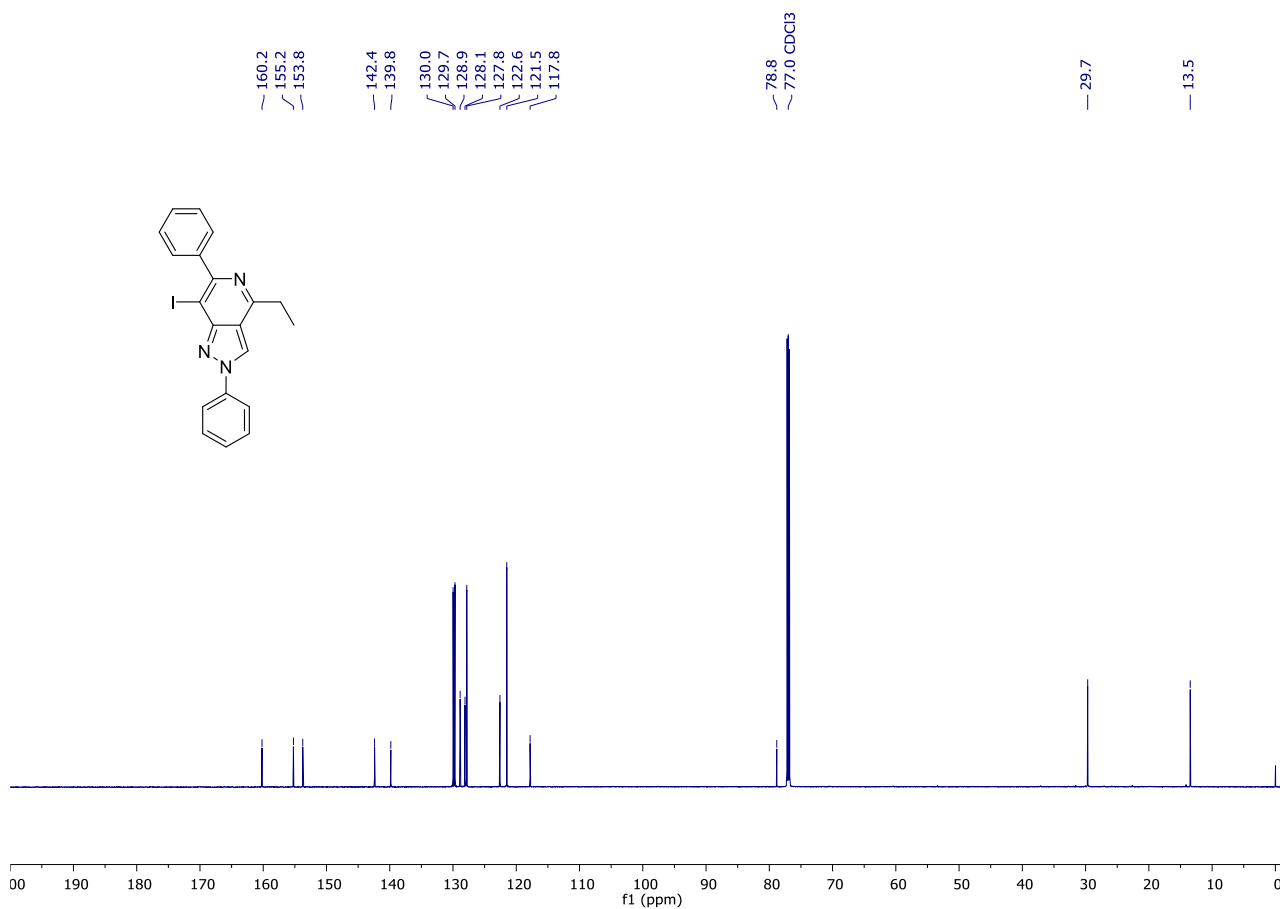


Figure S39. 4-Ethyl-7-iodo-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**15**). ¹³C NMR (176 MHz, CDCl₃).

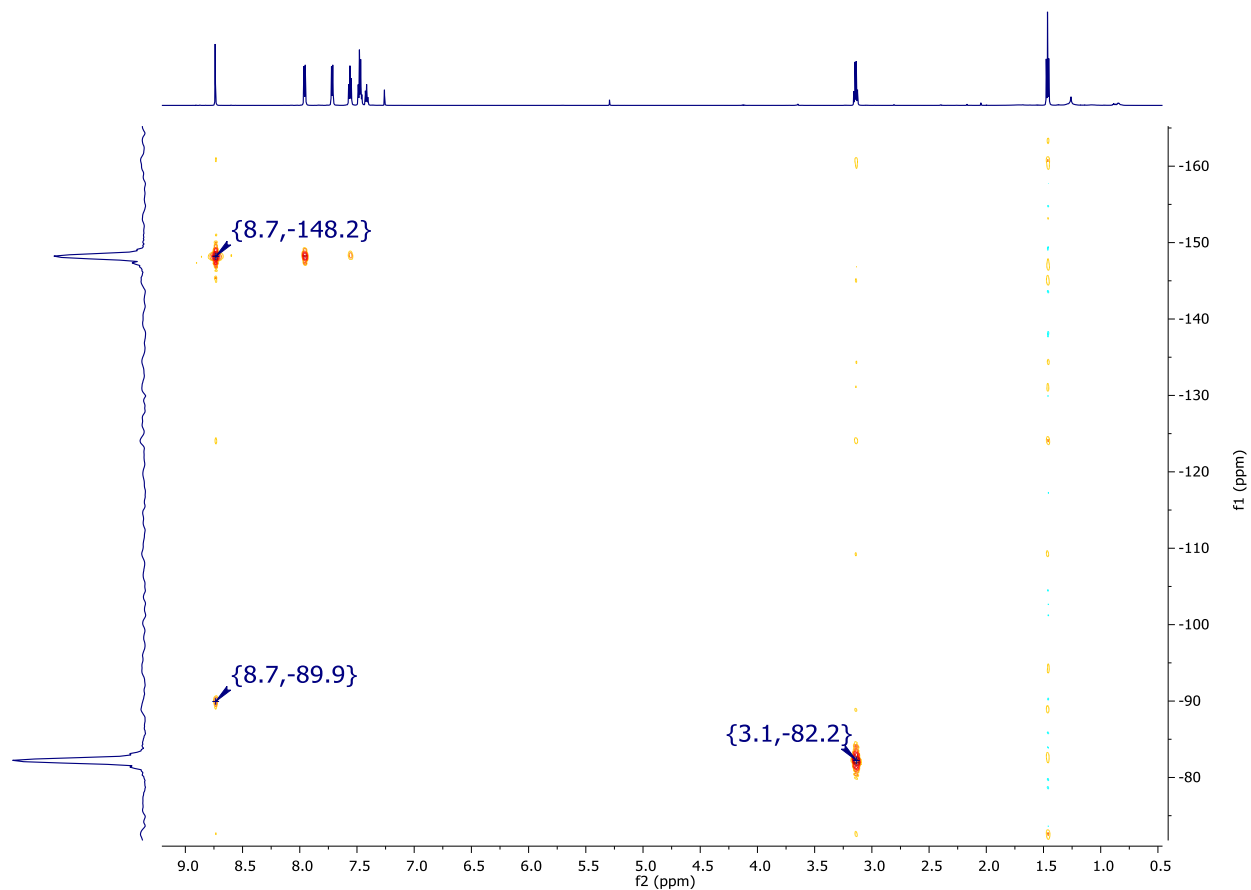
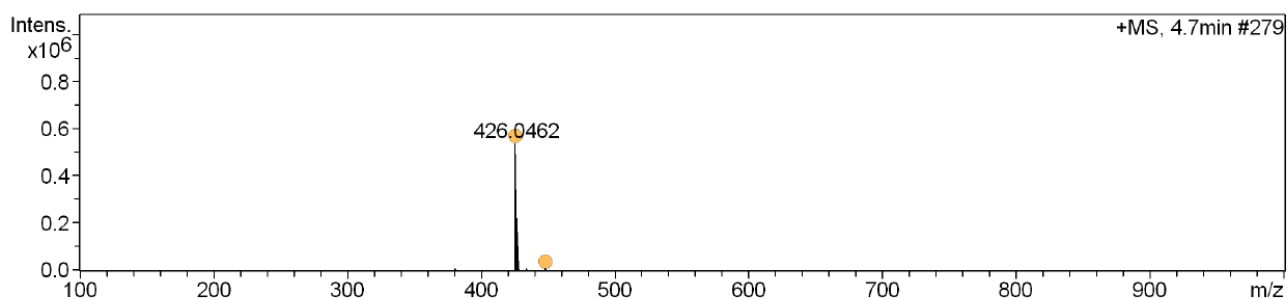


Figure S40. 4-Ethyl-7-iodo-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**15**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3)

+MS, 4.7min #279



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
426.0462	1	C ₂₀ H ₁₇ IN ₃	426.0462	0.0	1.6	1	100.00	13.5	even	ok
448.0274	1	C ₂₀ H ₁₆ IN ₃ Na	448.0281	-1.7	14.6	1	100.00	13.5	even	ok

Figure S41. 4-Ethyl-7-iodo-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**15**). HRMS (ESI-TOF).

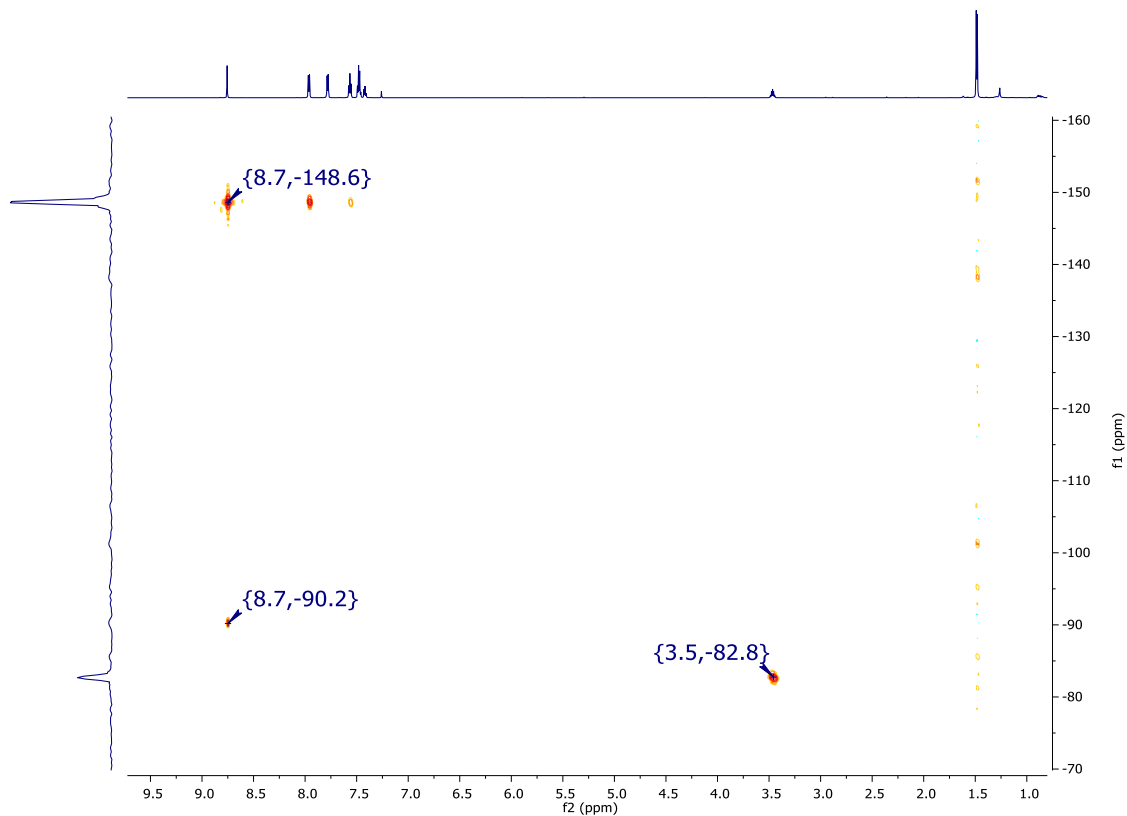


Figure S44. 7-Iodo-4-isopropyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**16**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3)

+MS, 5.8min #347

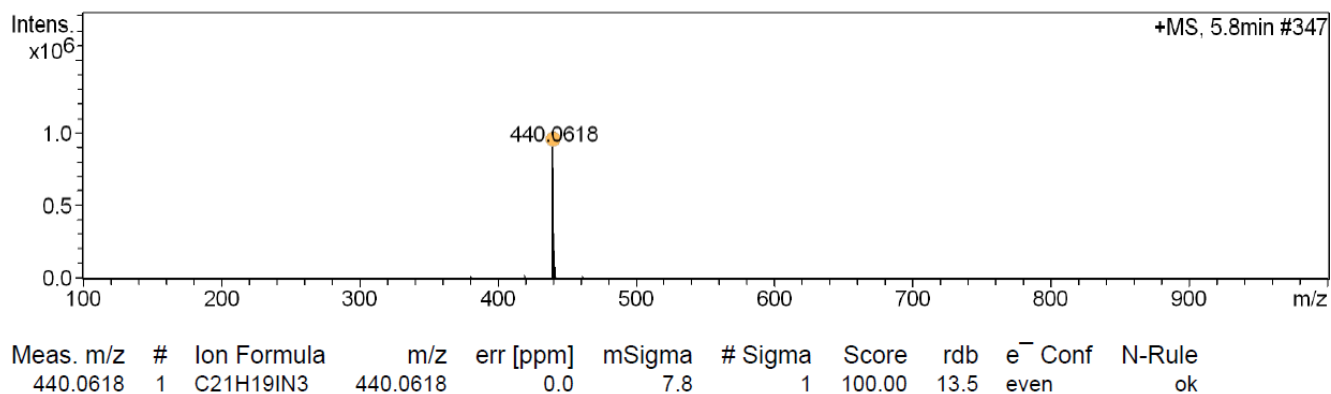


Figure S45. 7-Iodo-4-isopropyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**16**). HRMS (ESI-TOF).

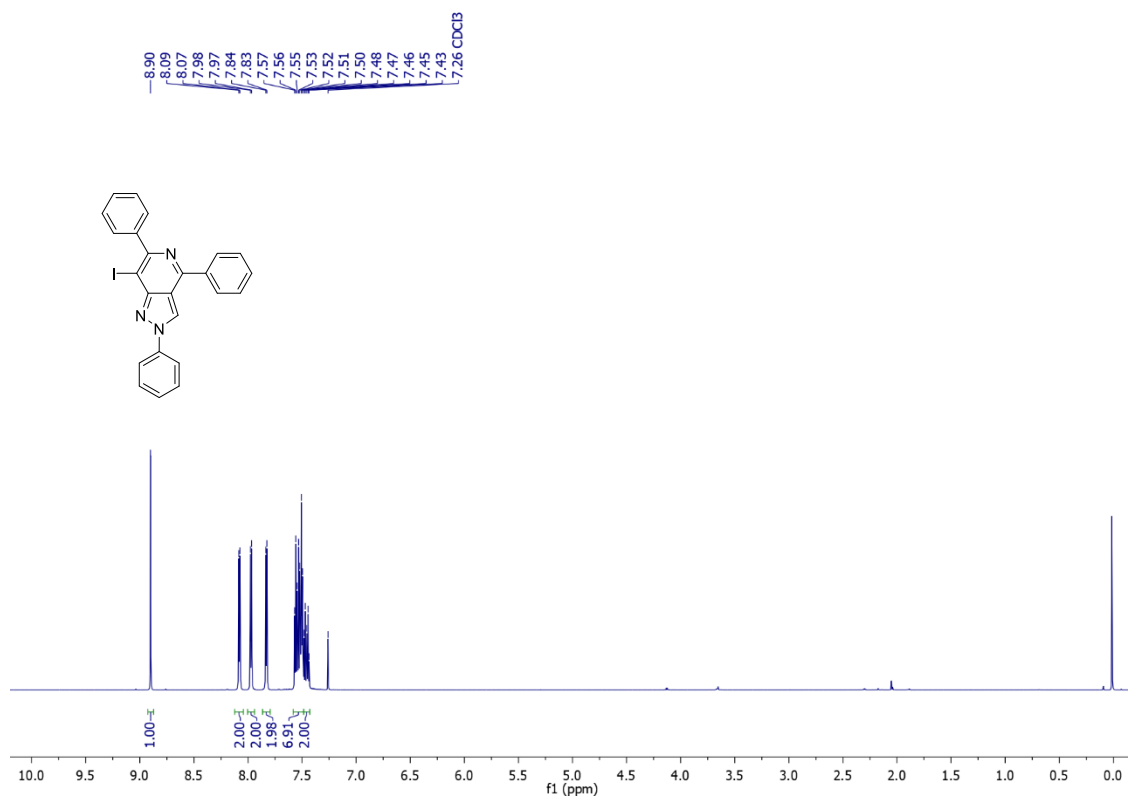


Figure S46. 7-Iodo-2,4,6-triphenyl-2H-pyrazolo[4,3-c]pyridine (**17**). ¹H NMR spectrum (700 MHz, CDCl₃).

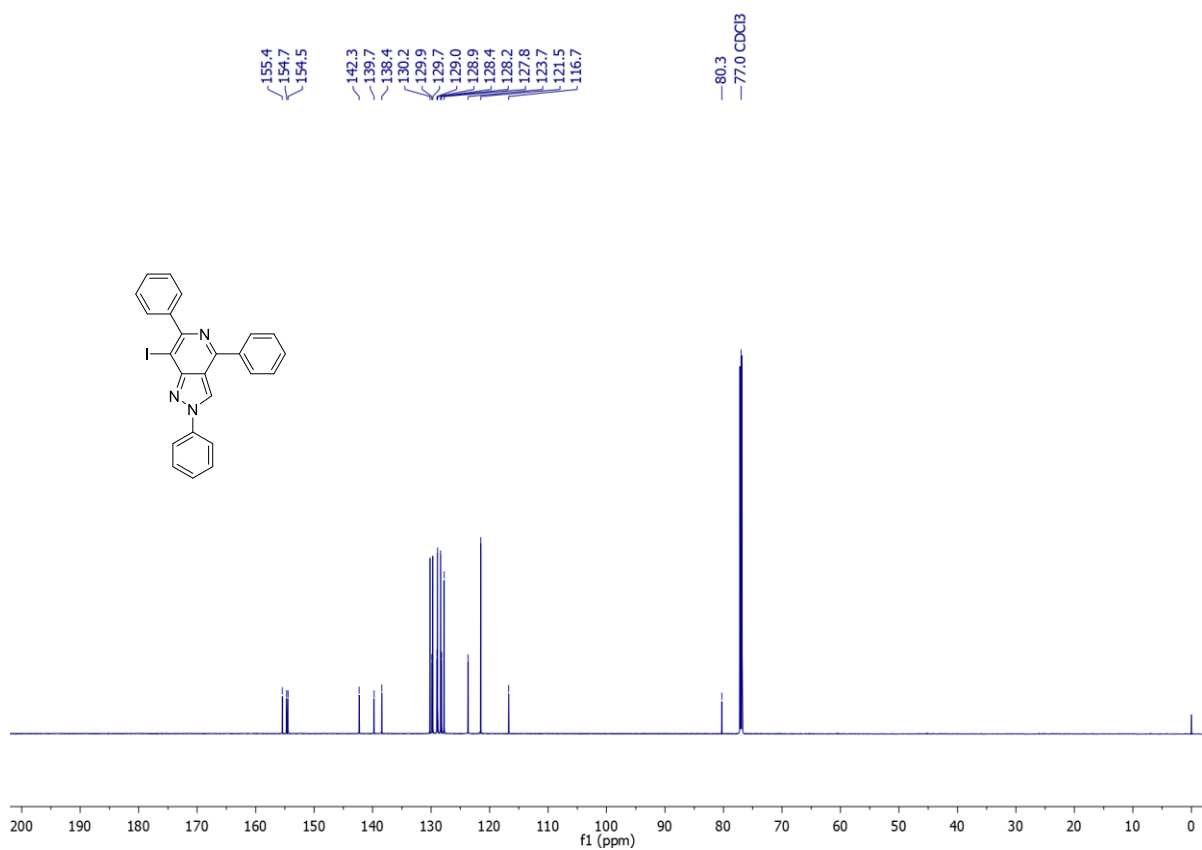


Figure S47. 7-Iodo-2,4,6-triphenyl-2H-pyrazolo[4,3-c]pyridine (**17**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 3.5min #212

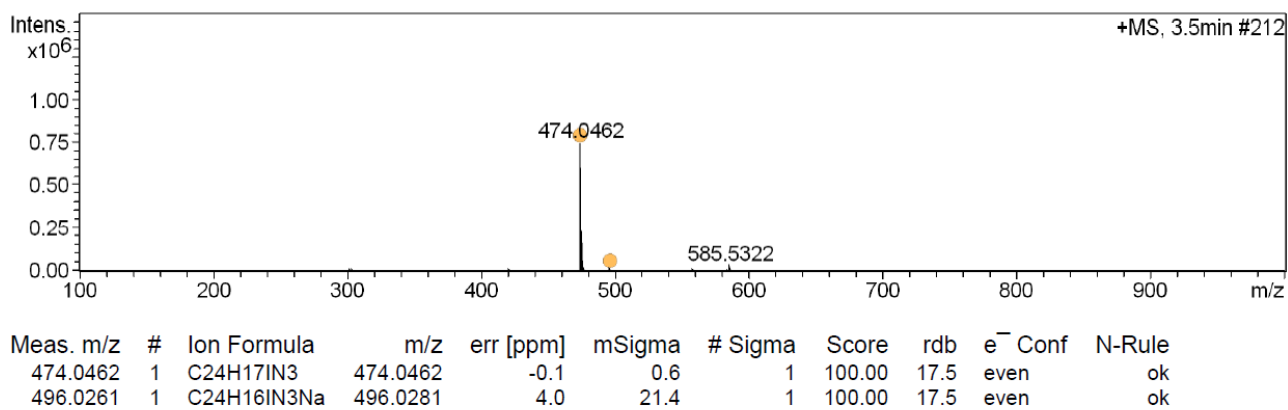


Figure S48. 7-Iodo-2,4,6-triphenyl-2H-pyrazolo[4,3-c]pyridine (**17**). HRMS (ESI-TOF).

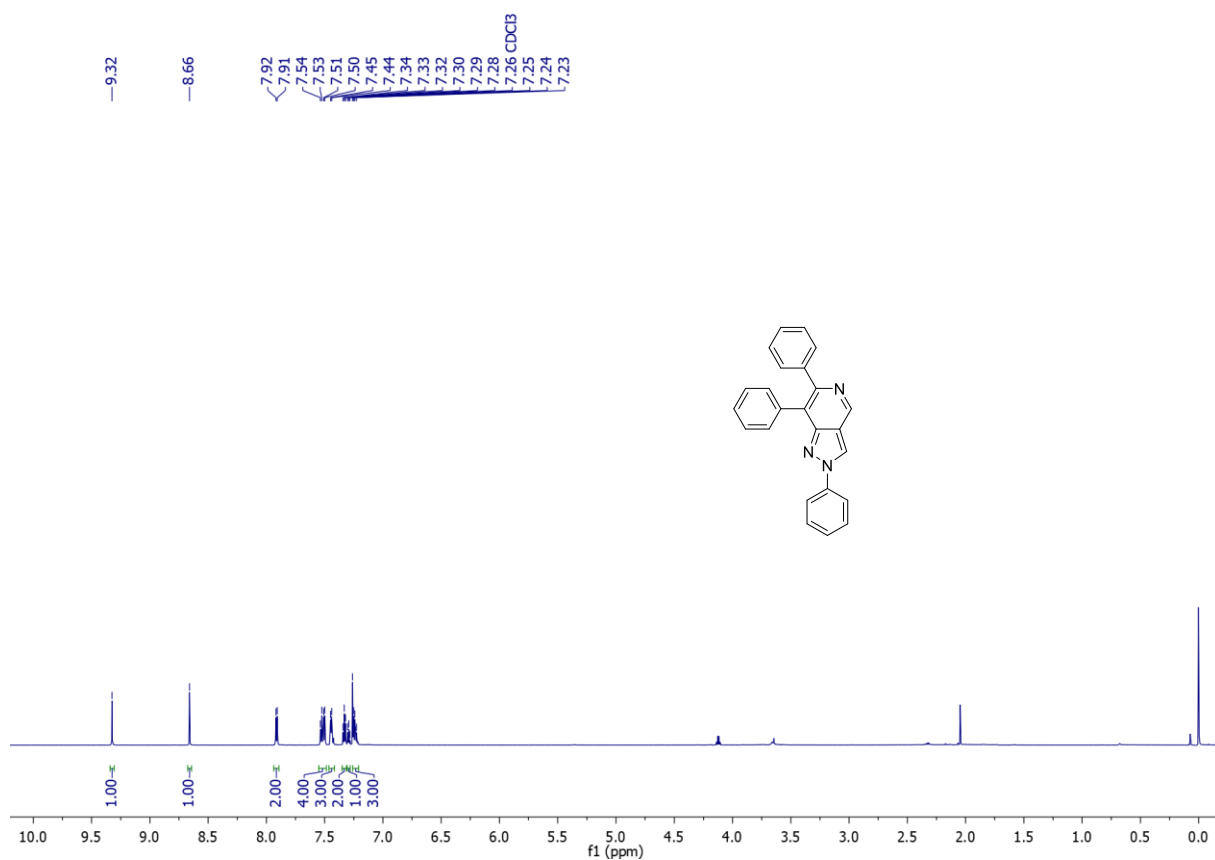


Figure S49. 2,6,7-Triphenyl-2H-pyrazolo[4,3-c]pyridine (**18**). ¹H NMR spectrum (700 MHz, CDCl₃).

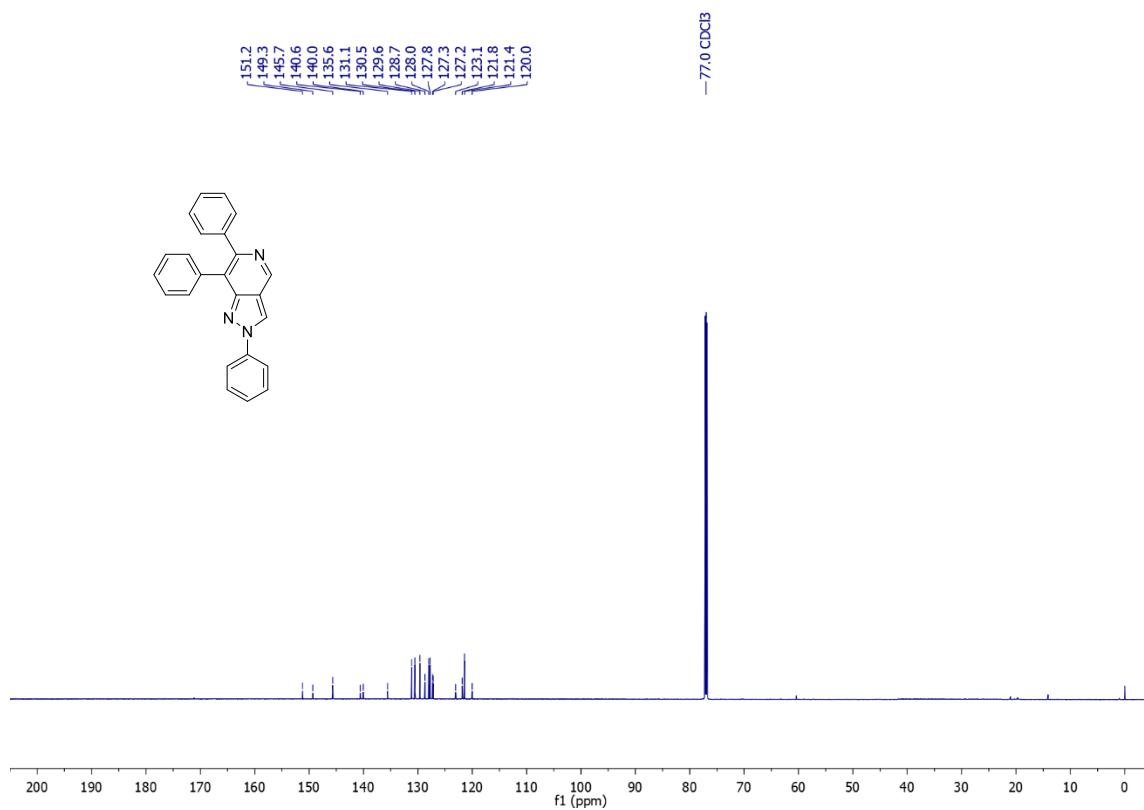


Figure S50. 2,6,7-Triphenyl-2H-pyrazolo[4,3-*c*]pyridine (**18**). ¹³C NMR (176 MHz, CDCl₃).

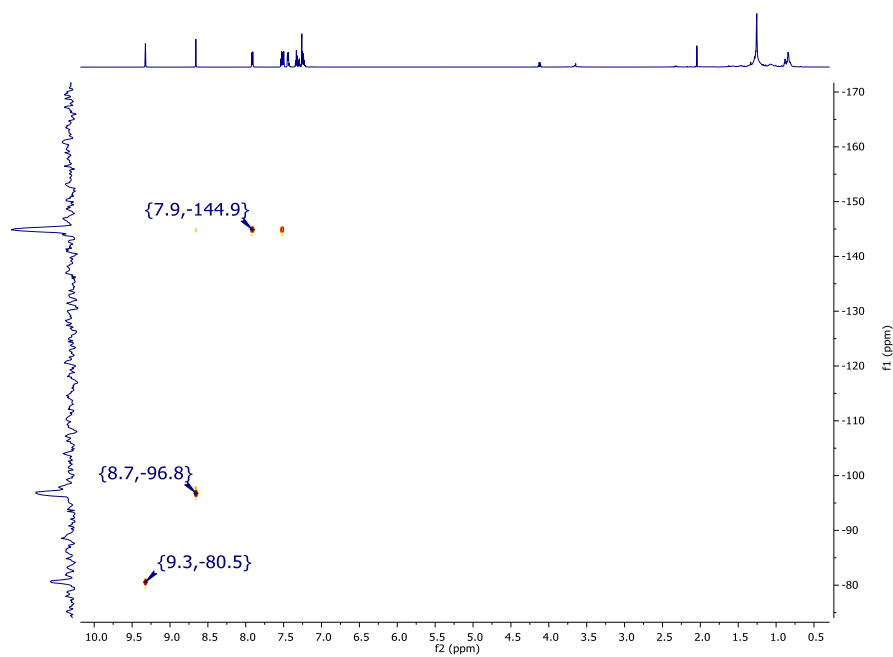


Figure S51. 2,6,7-Triphenyl-2H-pyrazolo[4,3-*c*]pyridine (**18**). ¹H-¹⁵N LR-HSQC spectrum (700 MHz, CDCl₃).

+MS, 7.6min #457

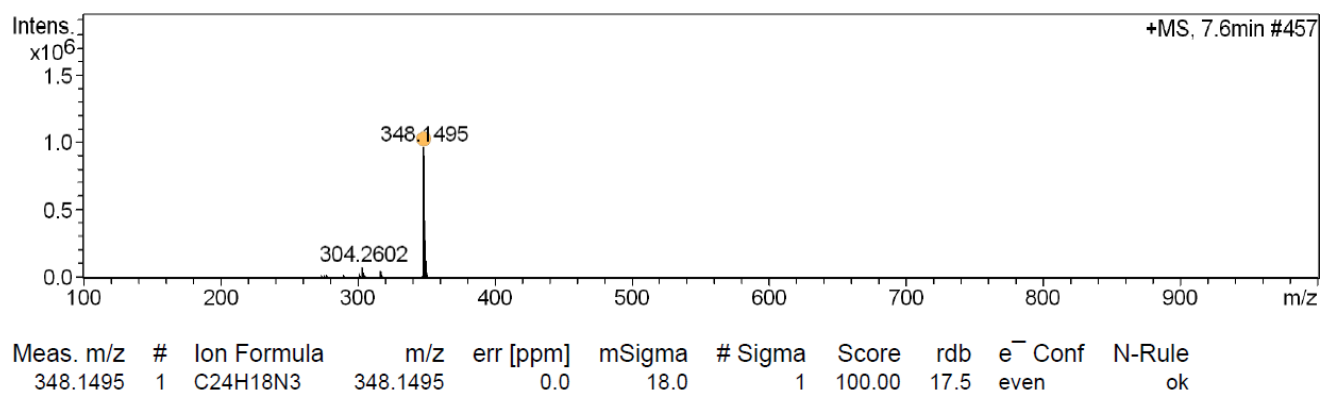


Figure S52. 2,6,7-Triphenyl-2H-pyrazolo[4,3-c]pyridine (**18**). HRMS (ESI-TOF).

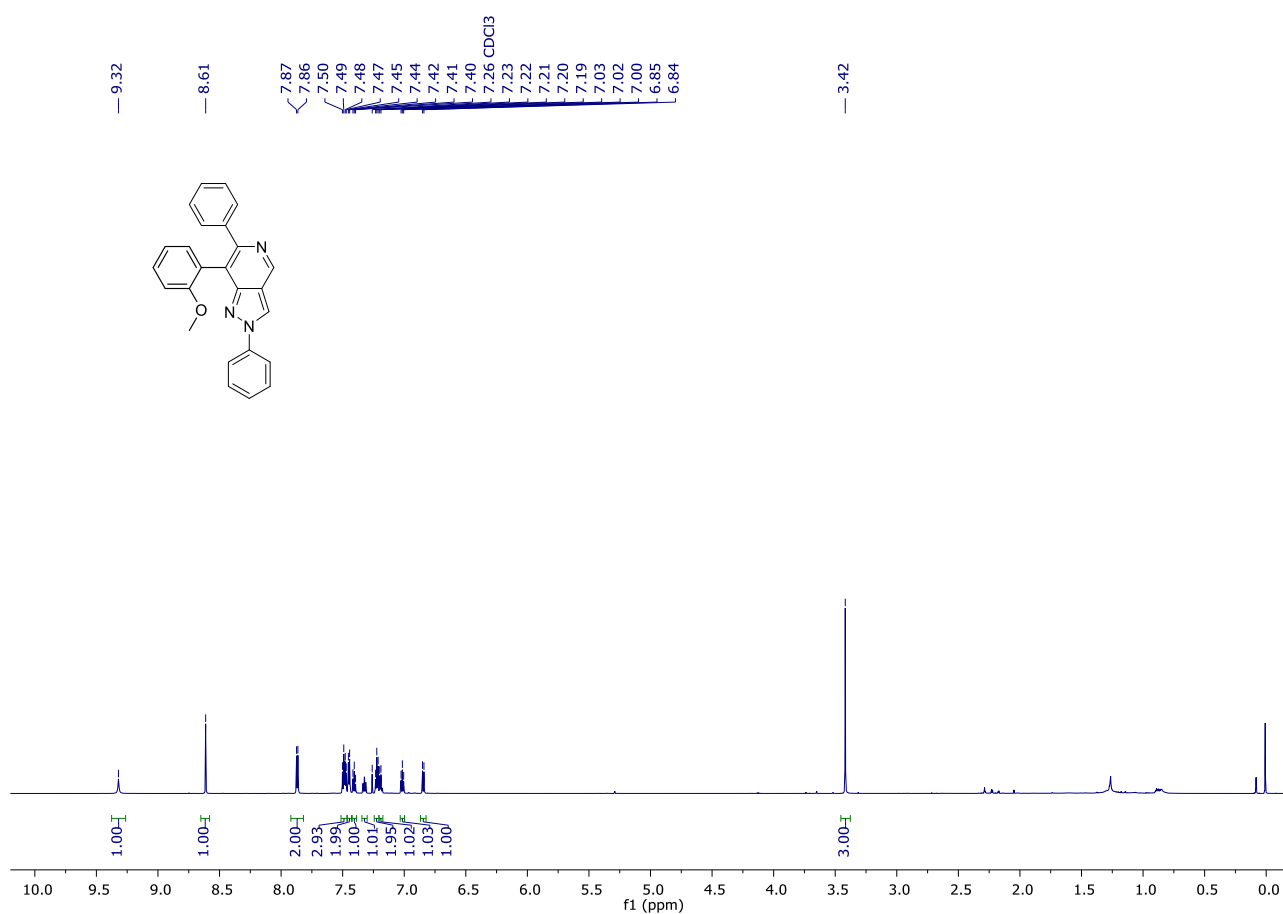


Figure S53. 7-(2-Methoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**19**). ¹H NMR spectrum (700 MHz, CDCl₃).

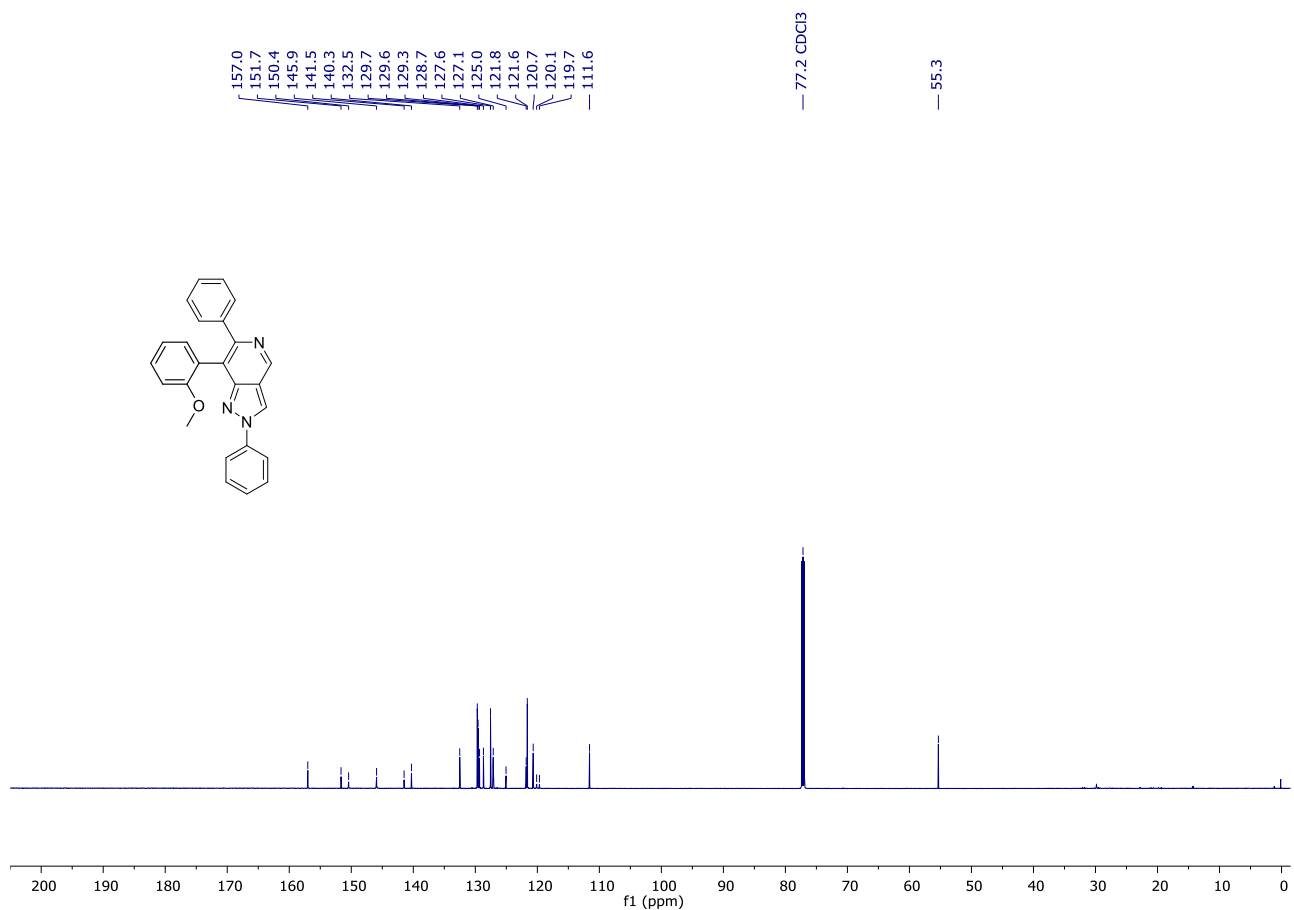


Figure S54. 7-(2-Methoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**19**). ¹³C NMR (176 MHz, CDCl₃).

+MS, 5.2min #309

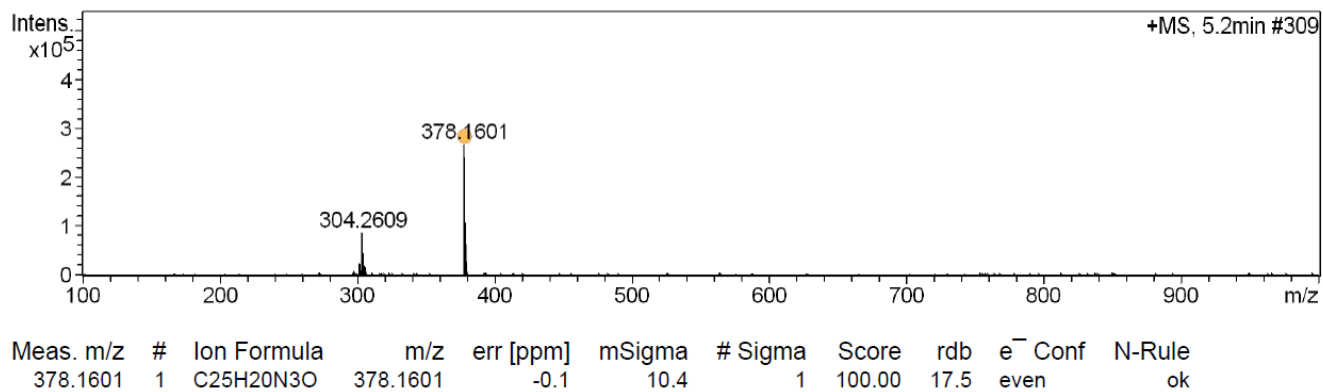


Figure S55. 7-(2-Methoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**19**). HRMS (ESI-TOF).

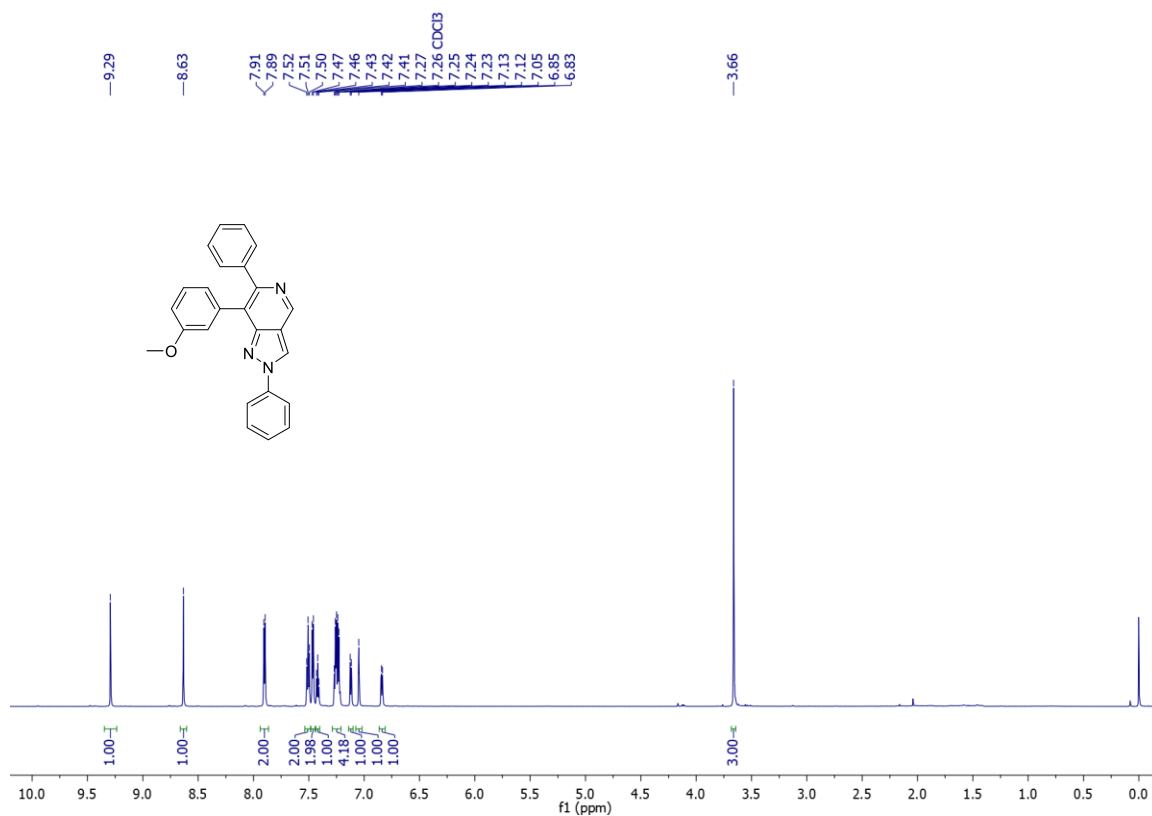


Figure S56. 7-(3-Methoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**20**). ¹H NMR spectrum (700 MHz, CDCl₃).

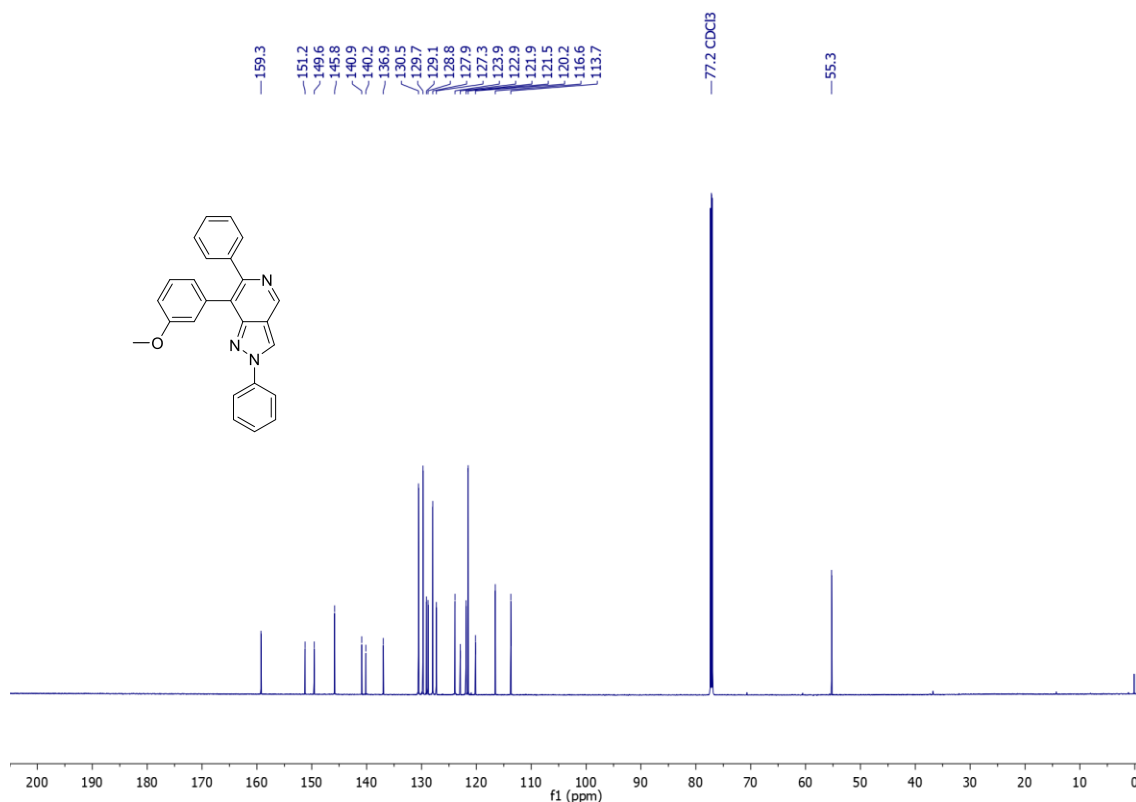


Figure S57. 7-(3-Methoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**20**). ¹³C NMR (176 MHz, CDCl₃).

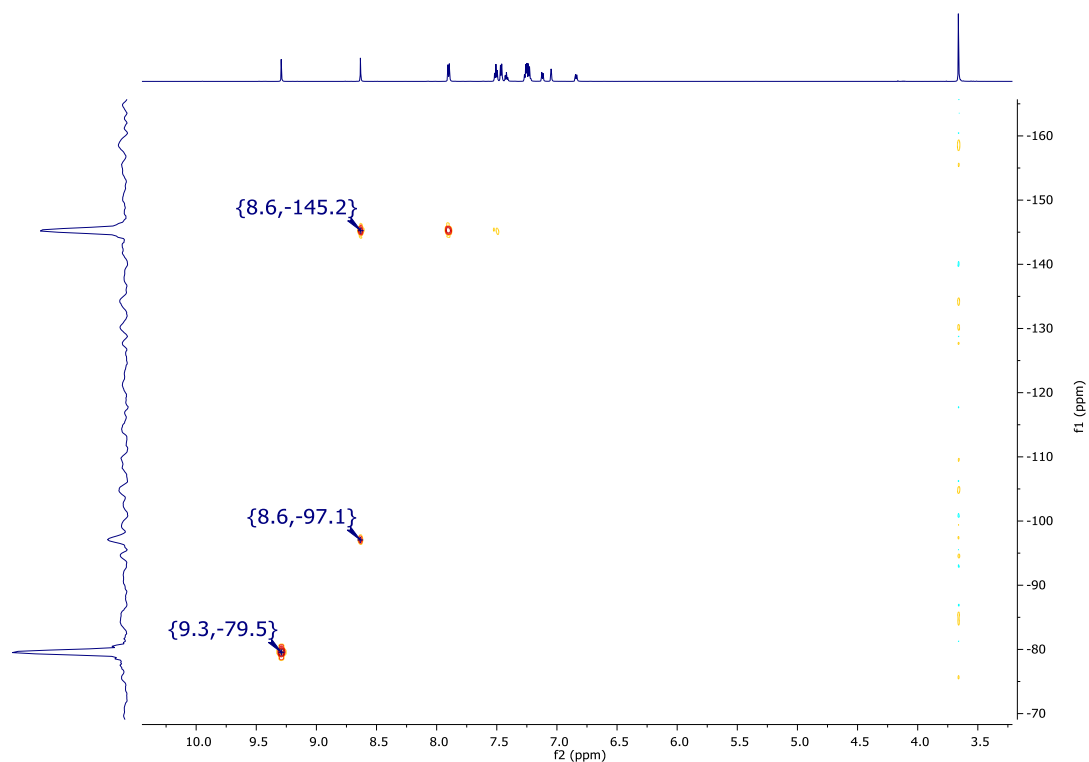


Figure S58. 7-(3-Methoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**20**). ¹H-¹⁵N HMBC spectrum (700 MHz, CDCl₃).

+MS, 3.8min #225

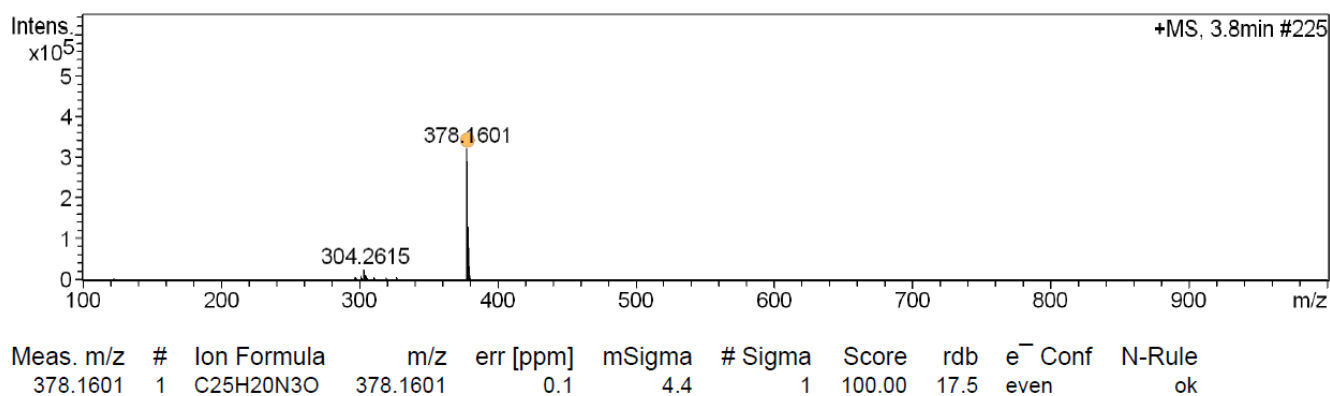


Figure S59. 7-(3-Methoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**20**). HRMS (ESI-TOF).

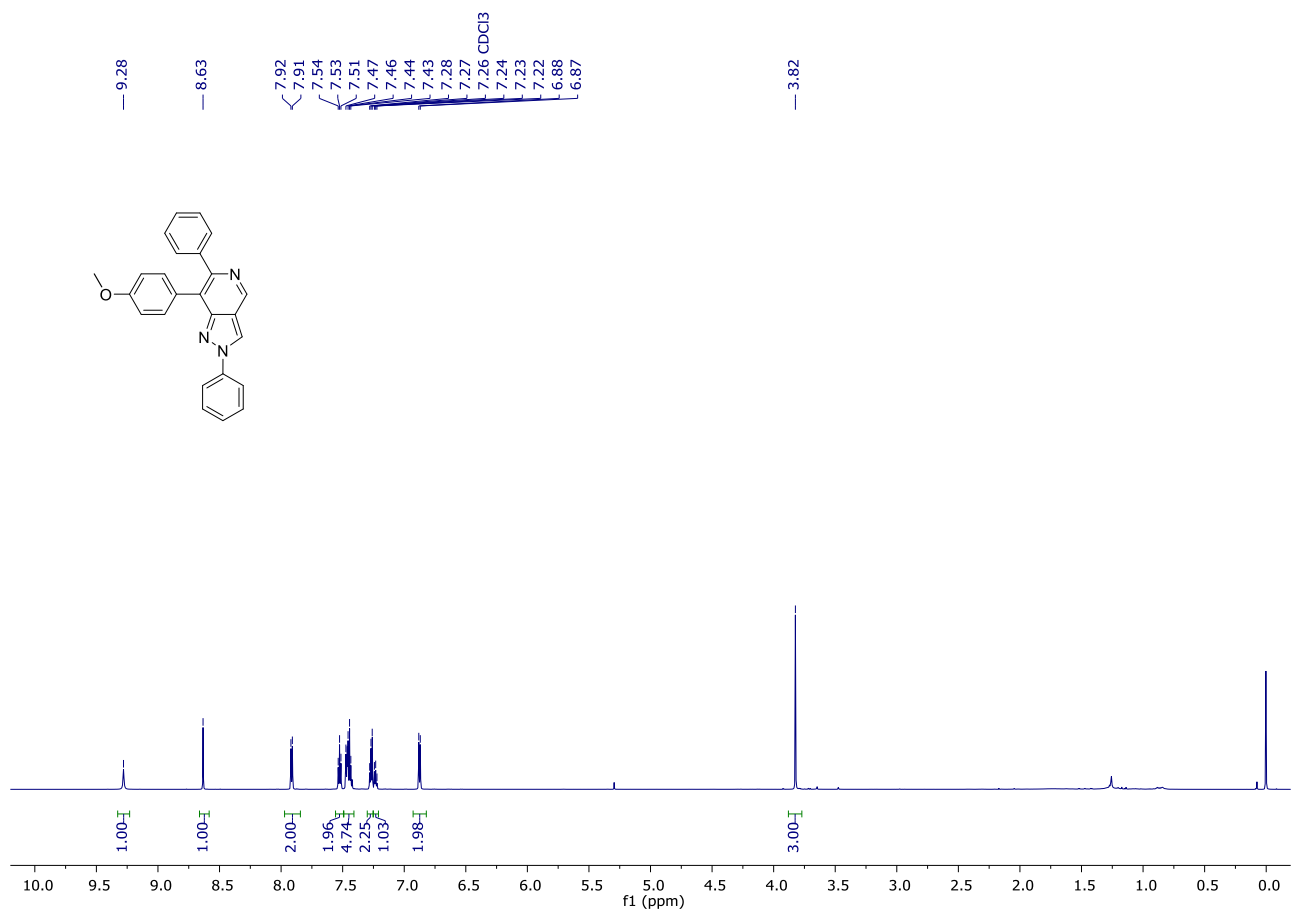


Figure S60. 7-(4-Methoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**21**). ¹H NMR spectrum (700 MHz, CDCl₃).

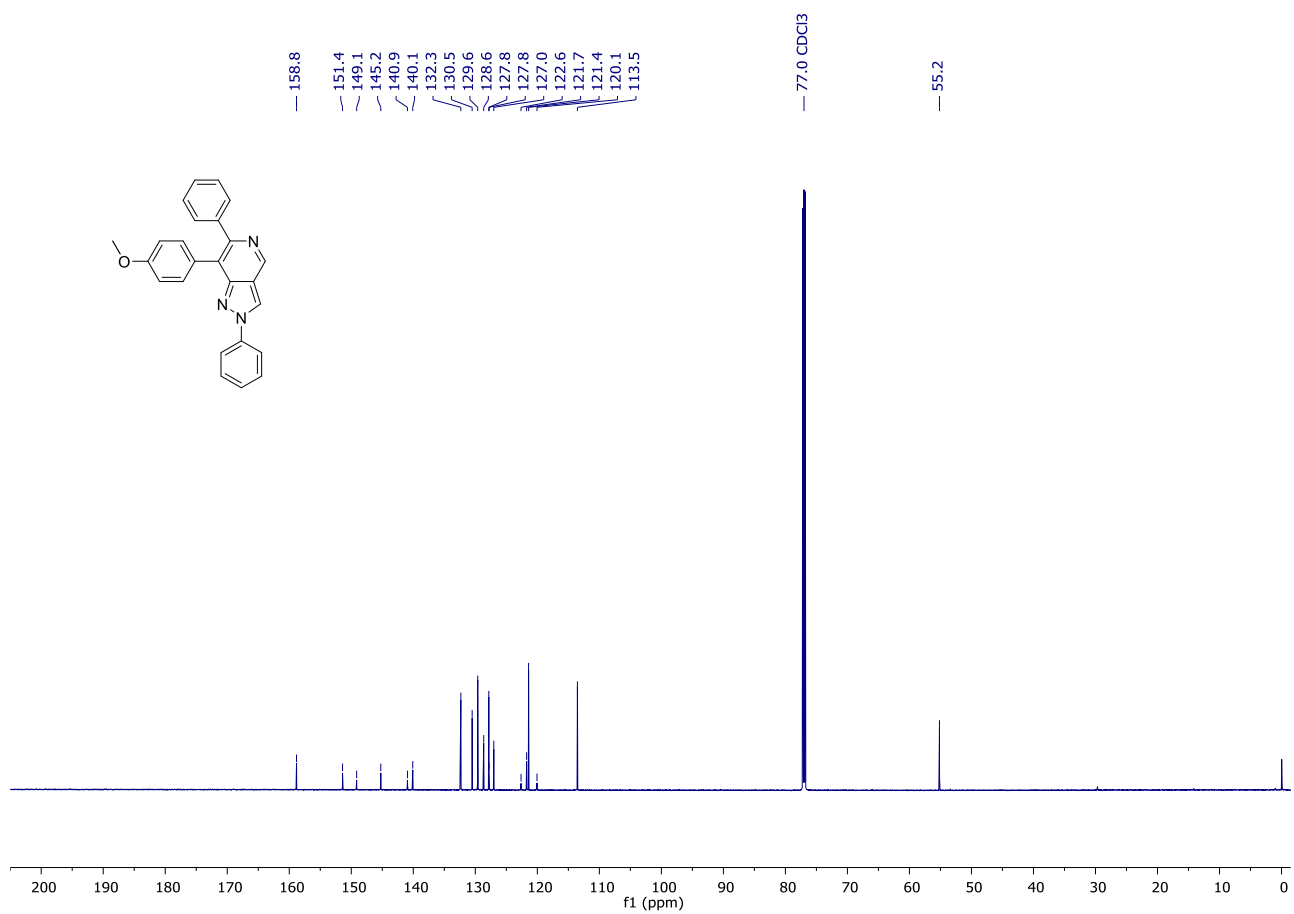


Figure S61. 7-(4-Methoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**21**). ¹³C NMR (176 MHz, CDCl₃).

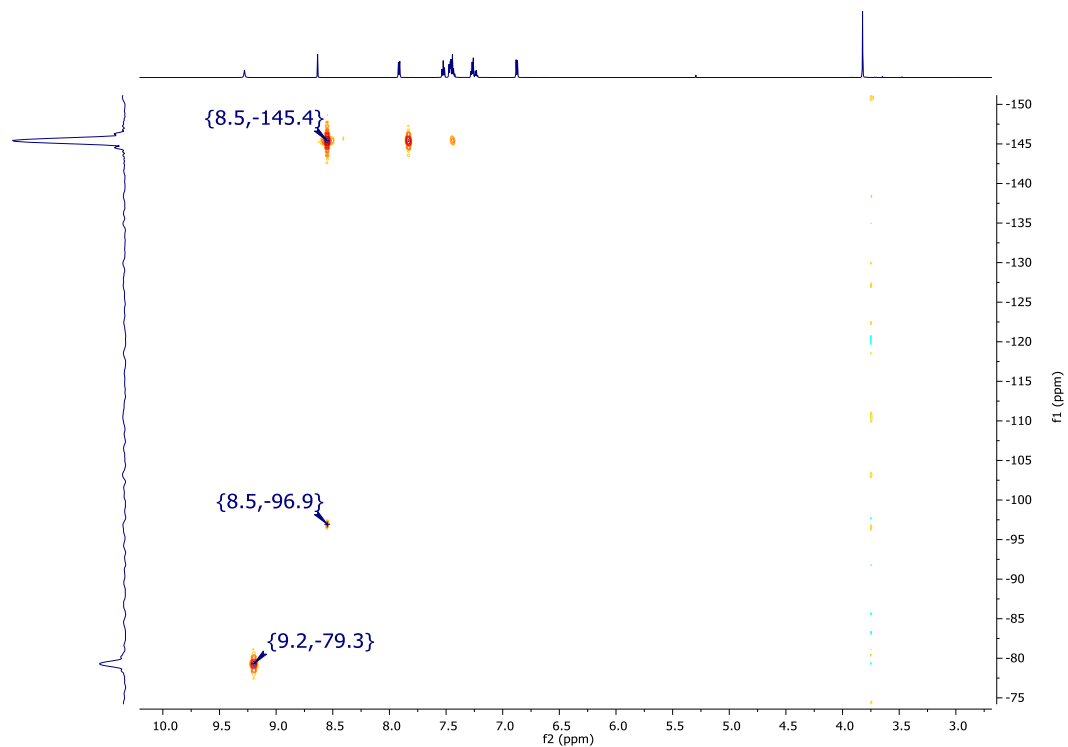
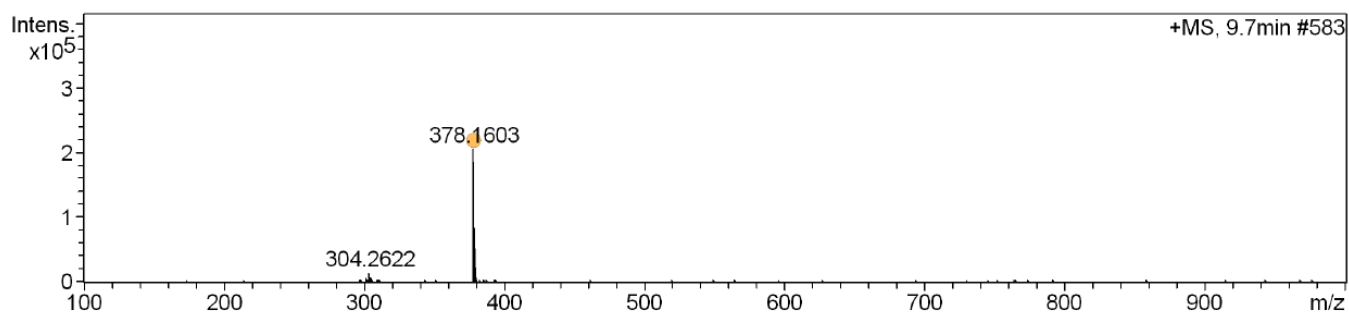


Figure S62. 7-(4-Methoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**21**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 9.7min #583



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e^- Conf	N-Rule
378.1603	1	$\text{C}_{25}\text{H}_{20}\text{N}_3\text{O}$	378.1601	-0.6	1.3	1	100.00	17.5	even	ok

Figure S63. 7-(4-Methoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**21**). HRMS (ESI-TOF).

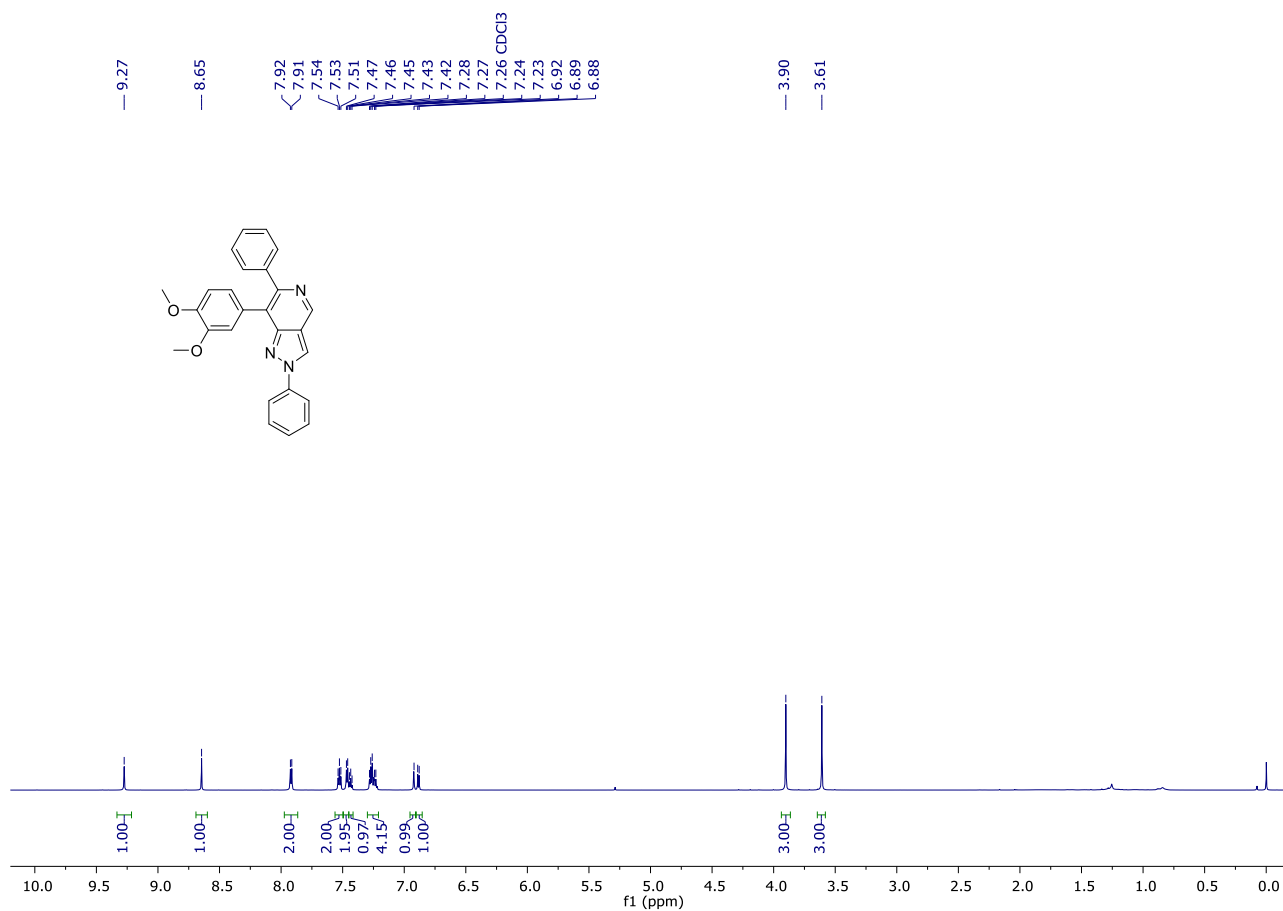


Figure S64. 7-(3,4-Dimethoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**22**). ¹H NMR spectrum (700 MHz, CDCl₃).

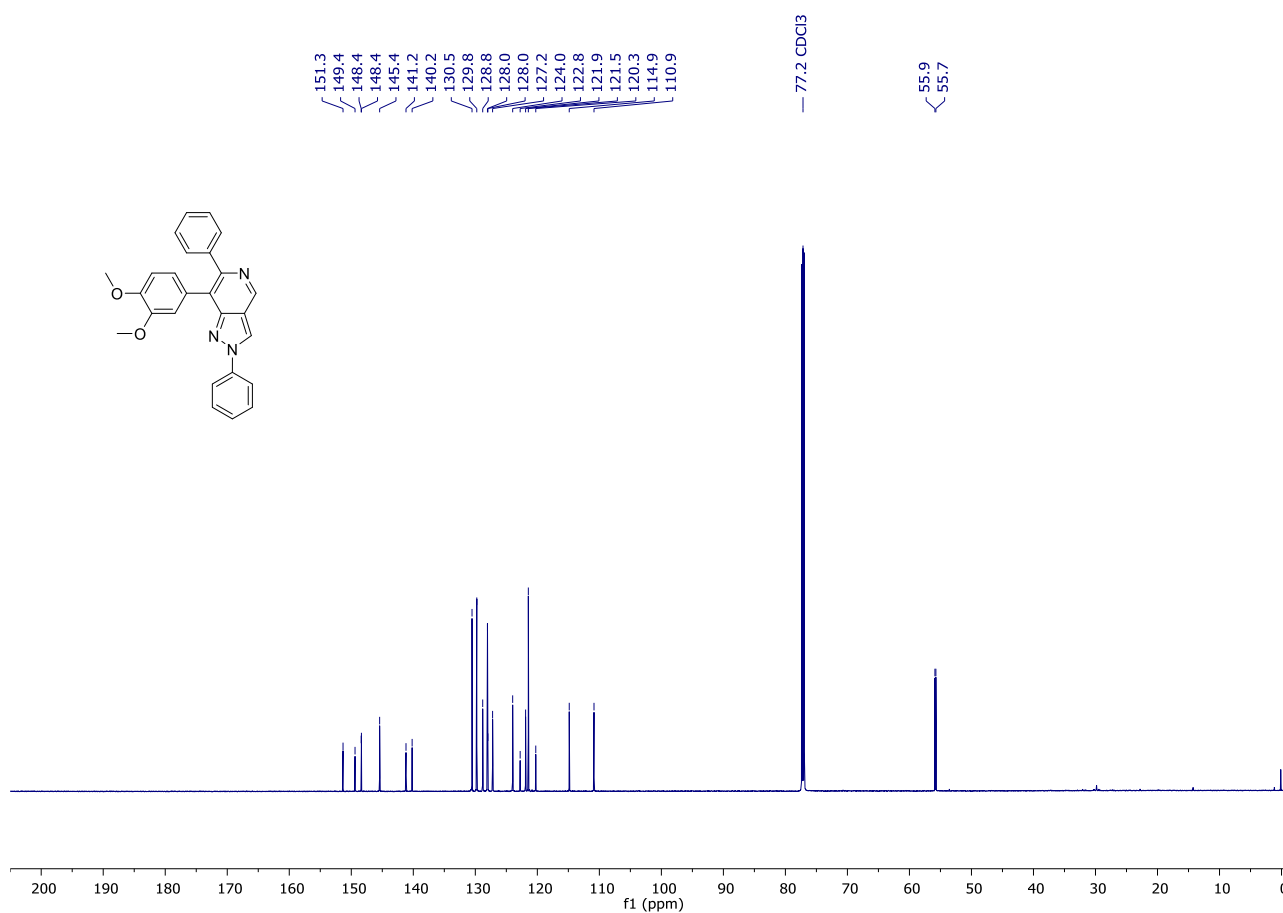


Figure S65. 7-(3,4-Dimethoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**22**). ¹³C NMR (176 MHz, CDCl₃).

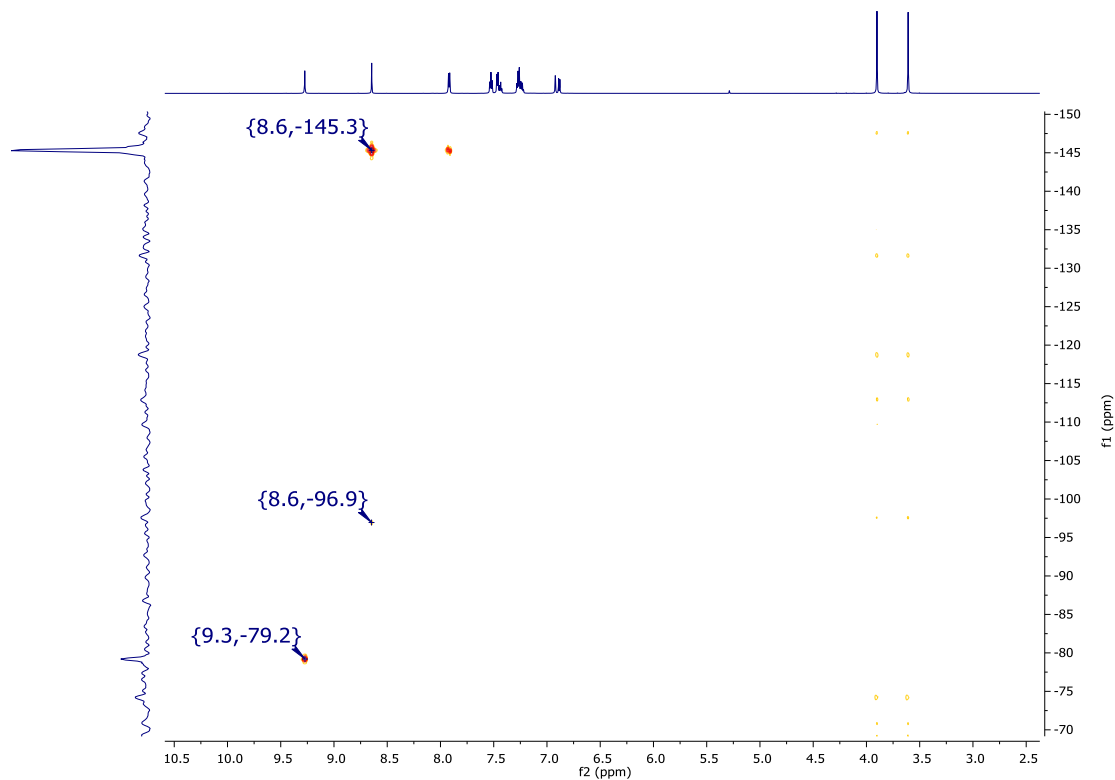


Figure S66. 7-(3,4-Dimethoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**22**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 3.1min #185

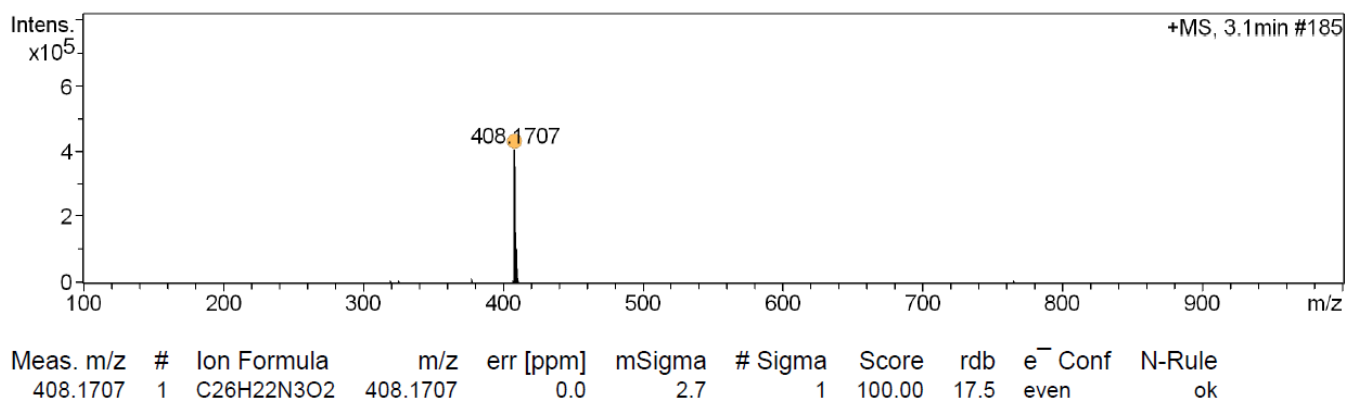


Figure S67. 7-(3,4-Dimethoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**22**). HRMS (ESI-TOF).

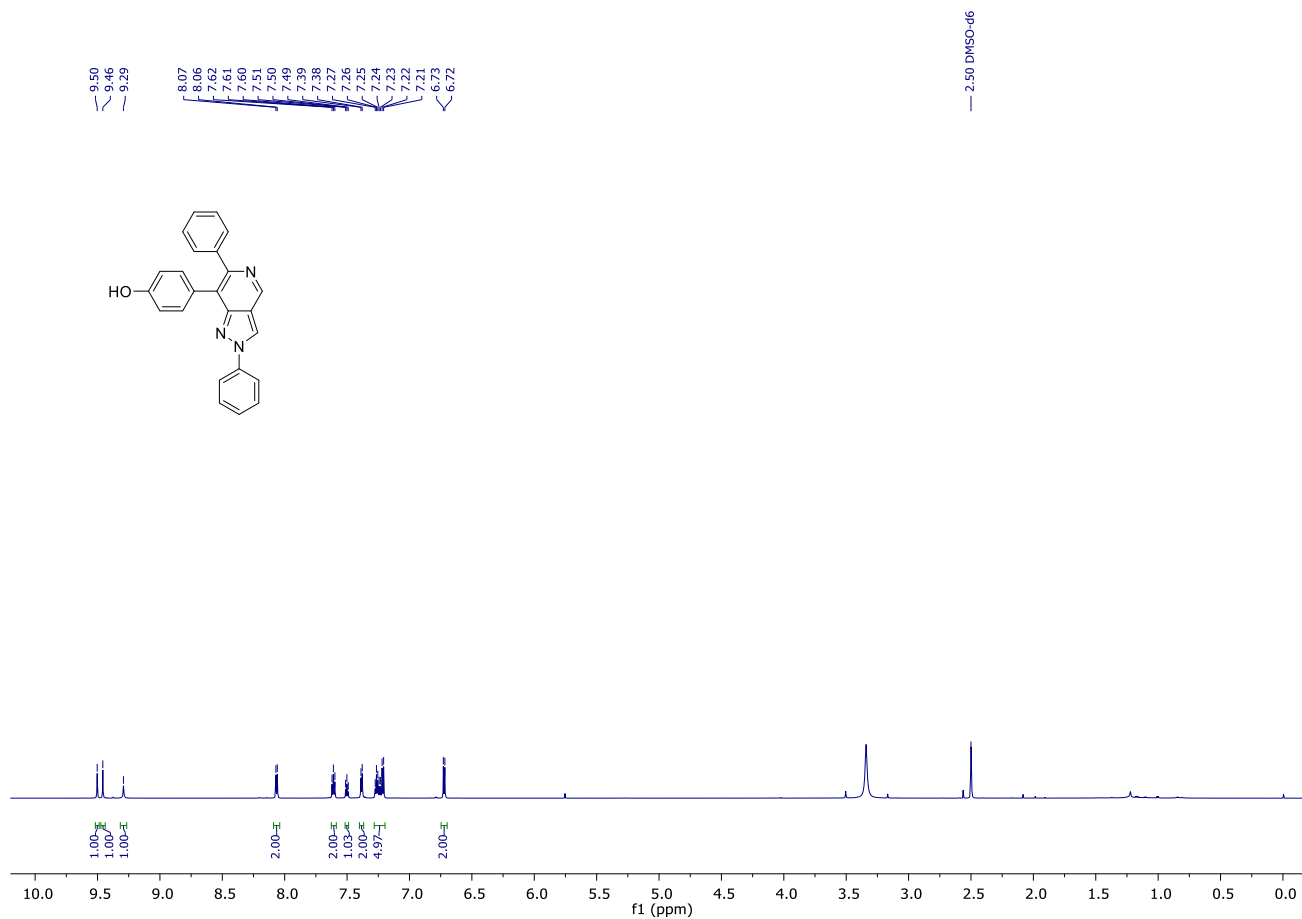


Figure S68. 4-(2,6-Diphenyl-2H-pyrazolo[4,3-*c*]pyridin-7-yl)phenol (**23**). ¹H NMR spectrum (700 MHz, DMSO-*d*₆).

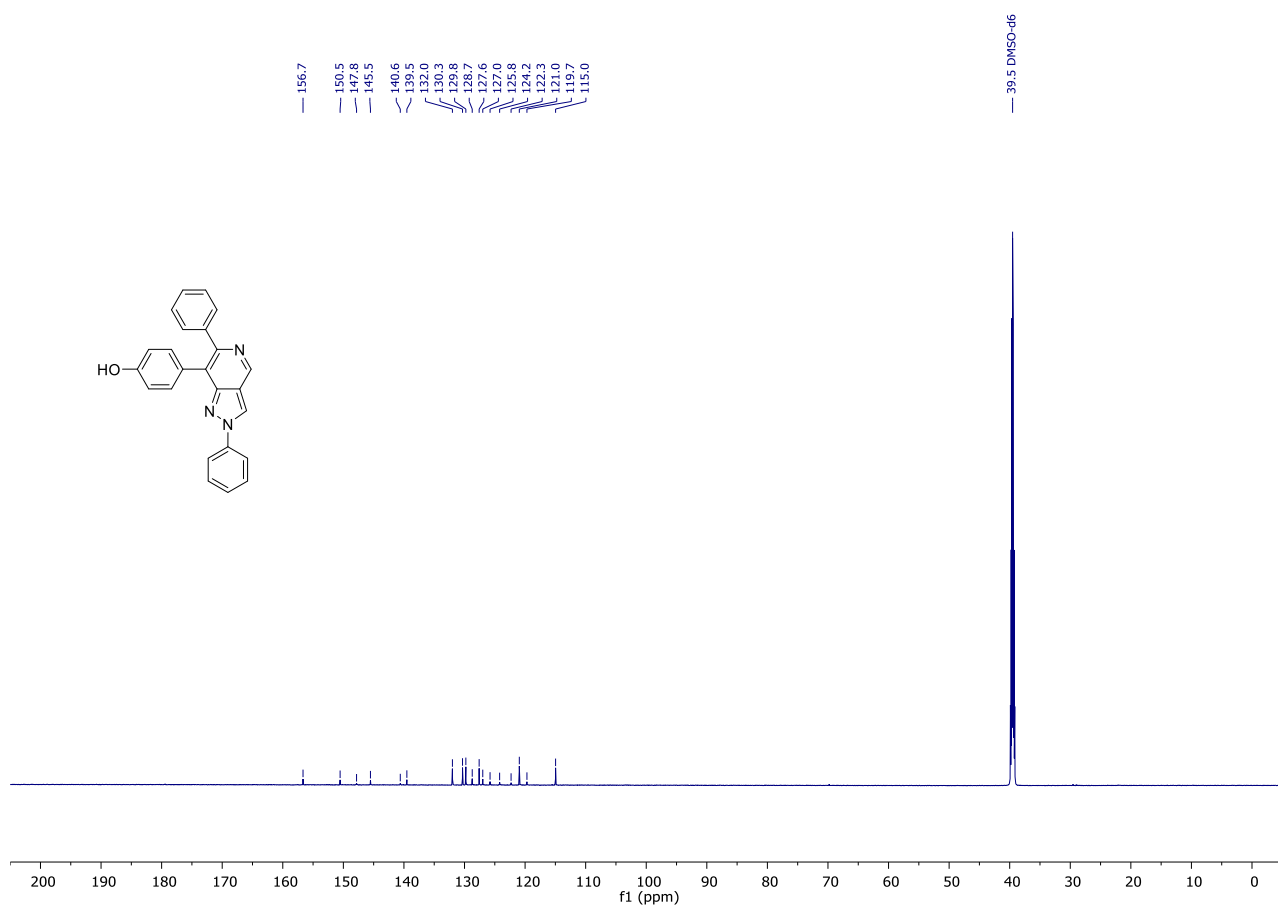


Figure S69. 4-(2,6-Diphenyl-2H-pyrazolo[4,3-*c*]pyridin-7-yl)phenol (**23**). ¹³C NMR (176 MHz, DMSO-*d*₆).

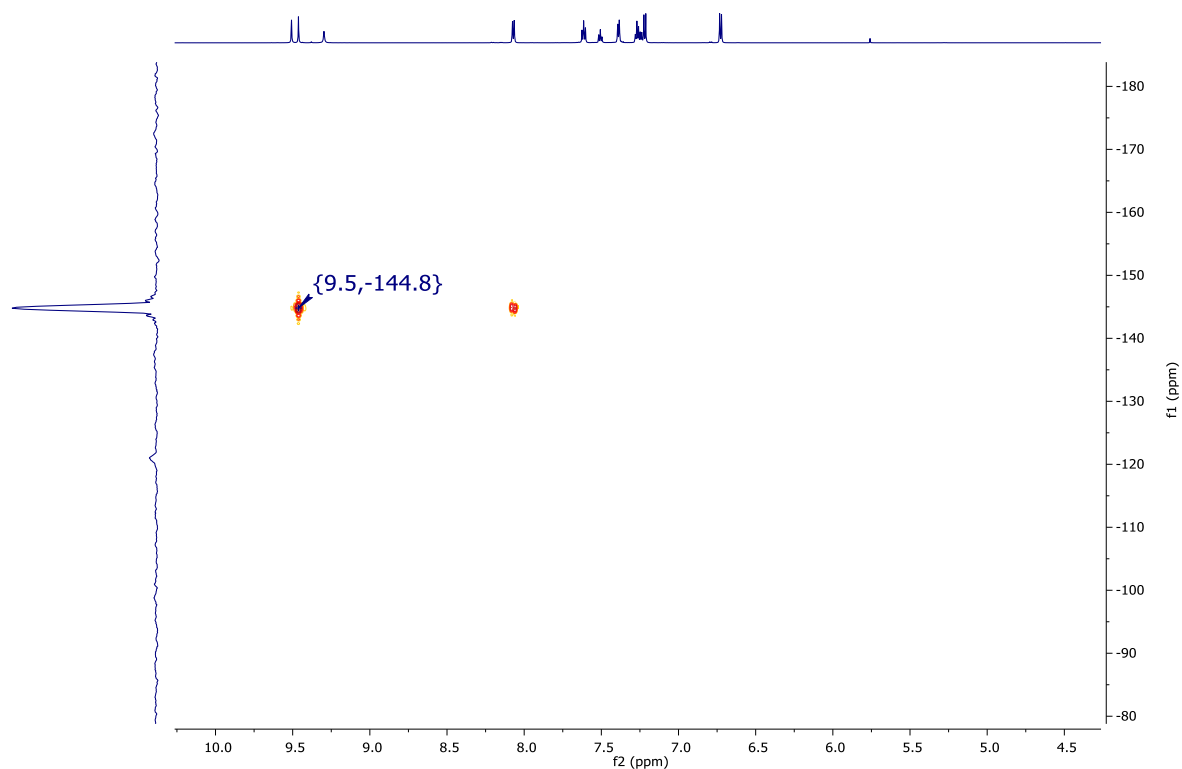
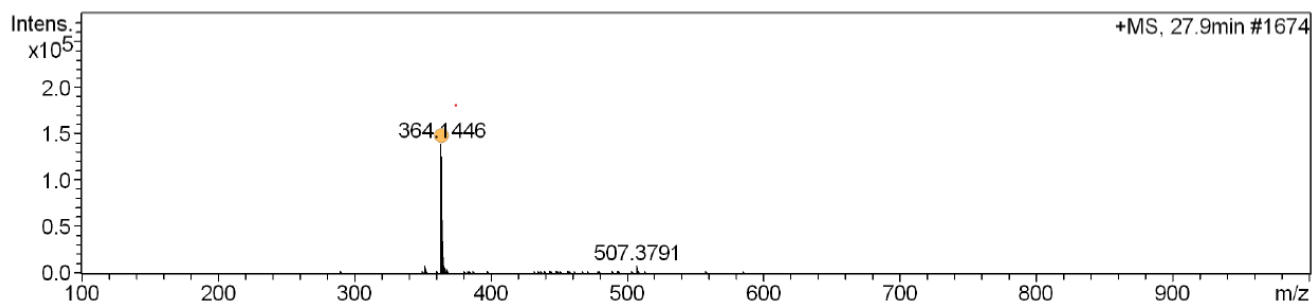


Figure S70. 4-(2,6-Diphenyl-2*H*-pyrazolo[4,3-*c*]pyridin-7-yl)phenol (**23**). ^1H - ^{15}N HMBC spectrum (700 MHz, $\text{DMSO-}d_6$).

+MS, 27.9min #1674



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e^-	Conf	N-Rule
364.1446	1	C ₂₄ H ₁₈ N ₃ O	364.1444	0.4	3.3	1	100.00	17.5	even		ok

Figure S71. 4-(2,6-Diphenyl-2*H*-pyrazolo[4,3-*c*]pyridin-7-yl)phenol (**23**). HRMS (ESI-TOF).

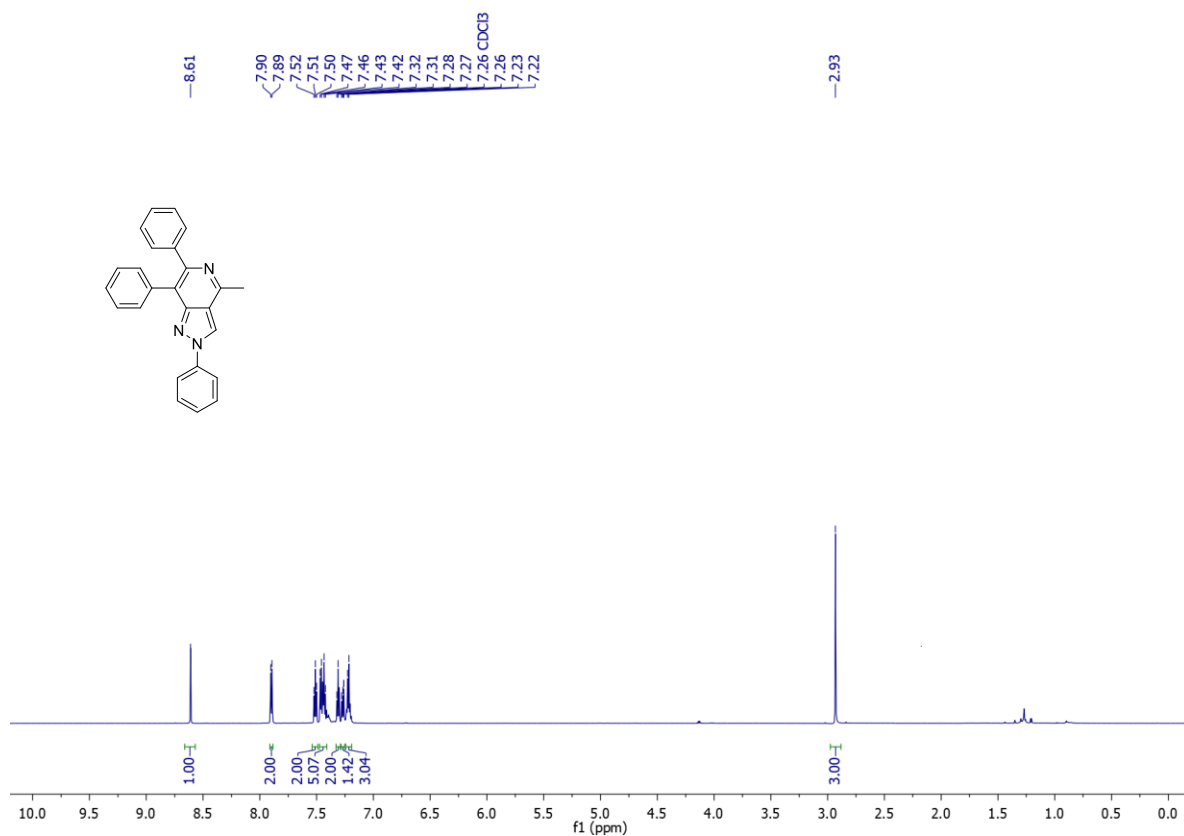


Figure S72. 4-Methyl-2,6,7-triphenyl-2H-pyrazolo[4,3-c]pyridine (**24**). ¹H NMR spectrum (700 MHz, CDCl₃).

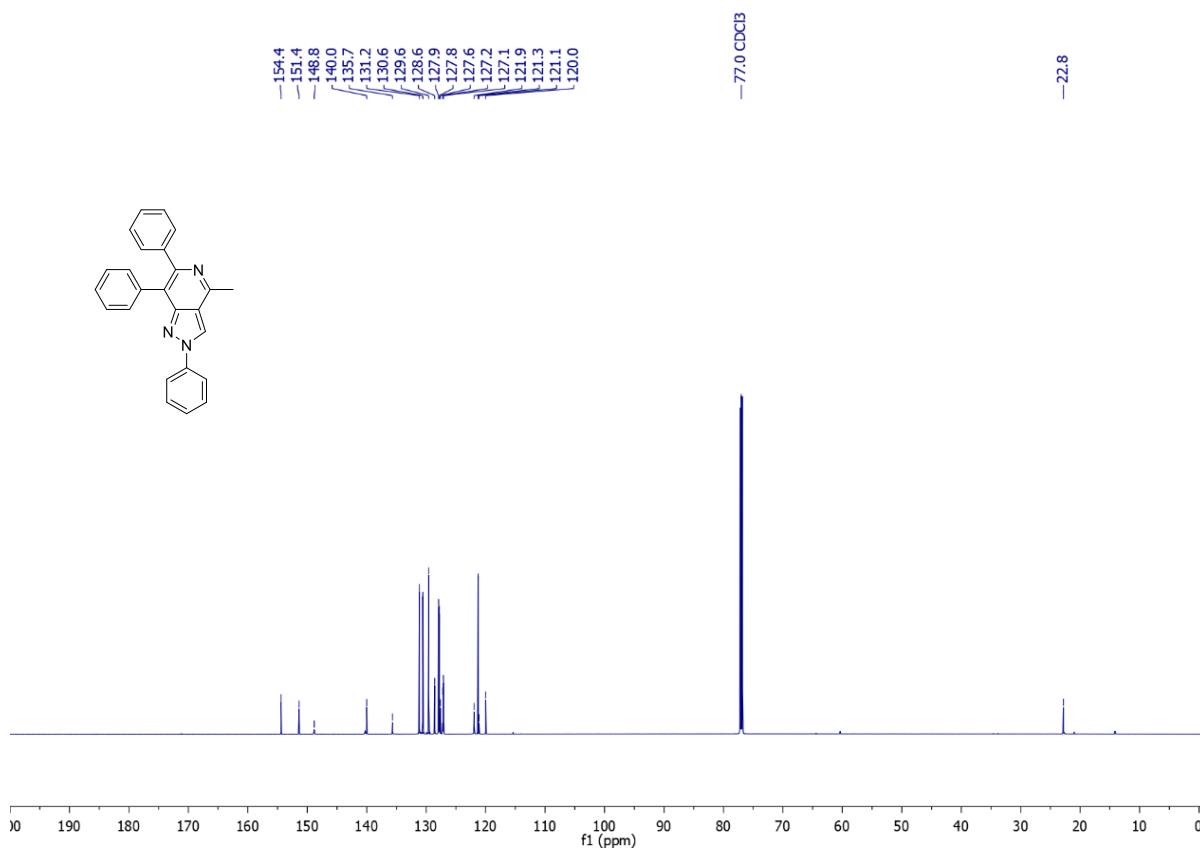


Figure S73. 4-Methyl-2,6,7-triphenyl-2H-pyrazolo[4,3-c]pyridine (**24**). ¹³C NMR (176 MHz, CDCl₃).

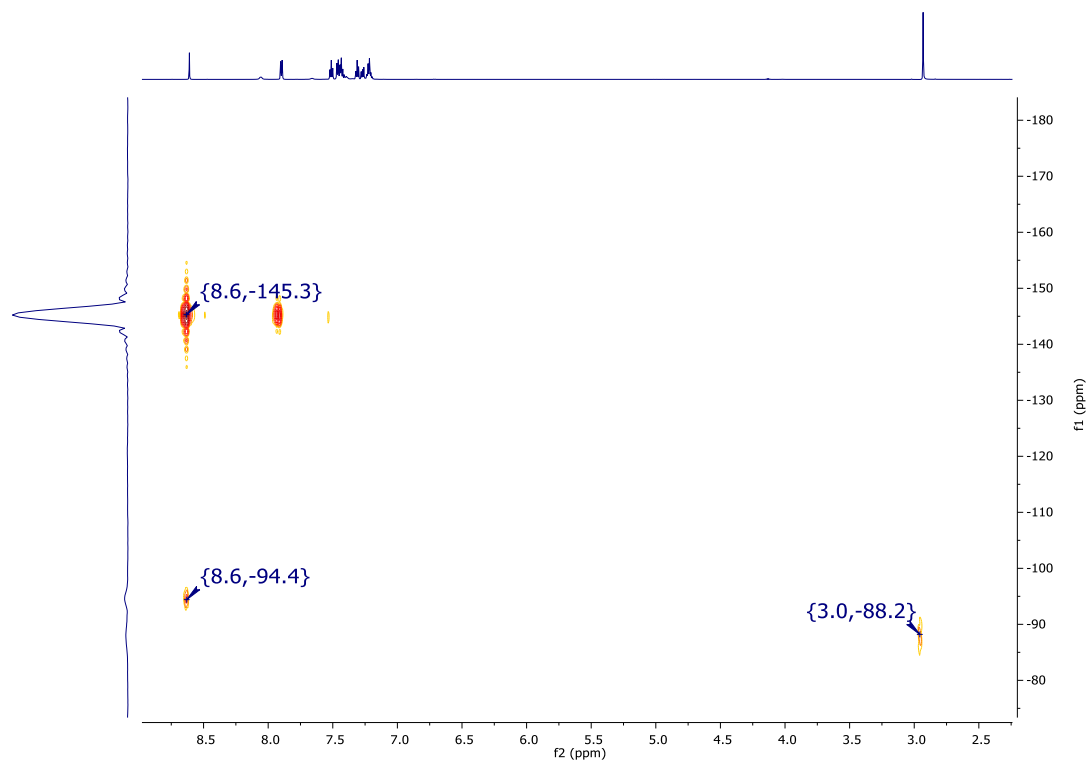
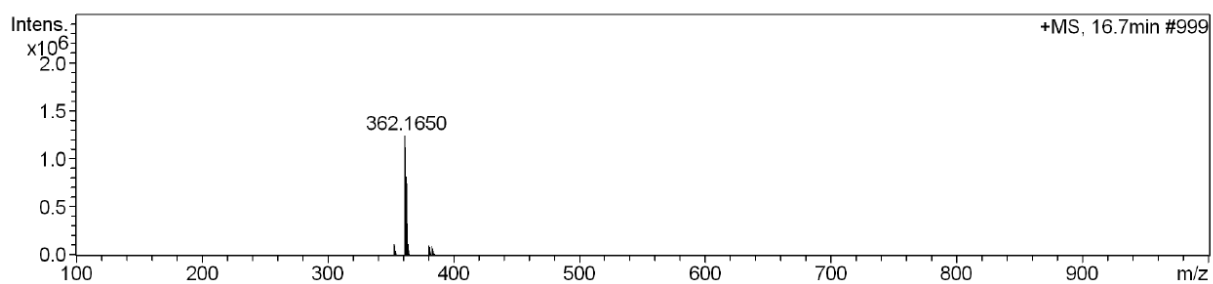


Figure S74. 4-Methyl-2,6,7-triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**24**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 16.7min #999



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e^- Conf	N-Rule
362.1650	1	$\text{C}_{25}\text{H}_{20}\text{N}_3$	362.1652	0.6	218.5	1	100.00	17.5	even	ok

Figure S75. 4-Methyl-2,6,7-triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**24**). HRMS (ESI-TOF).

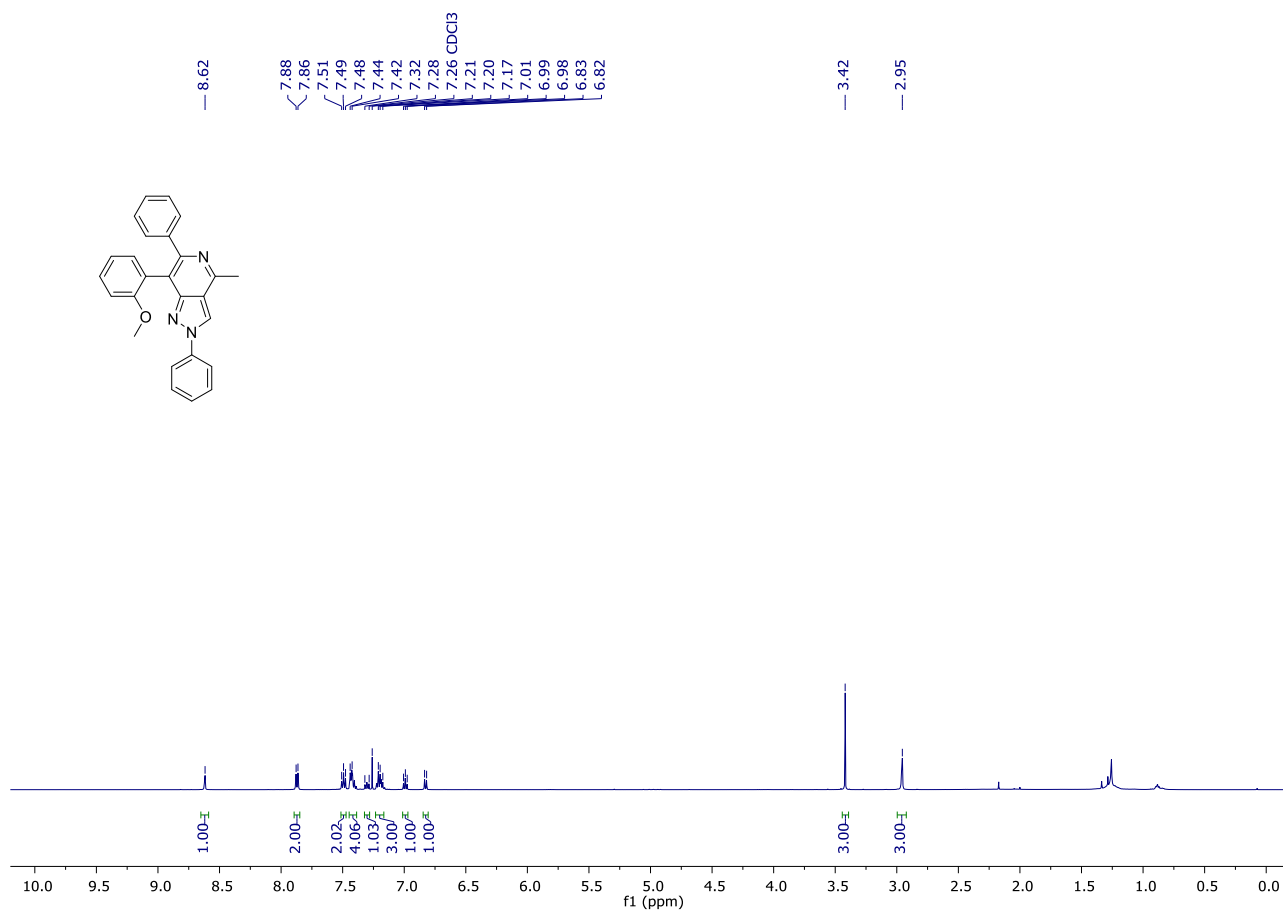


Figure S76. 7-(2-Methoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**25**). ¹H NMR spectrum (500 MHz, CDCl₃).

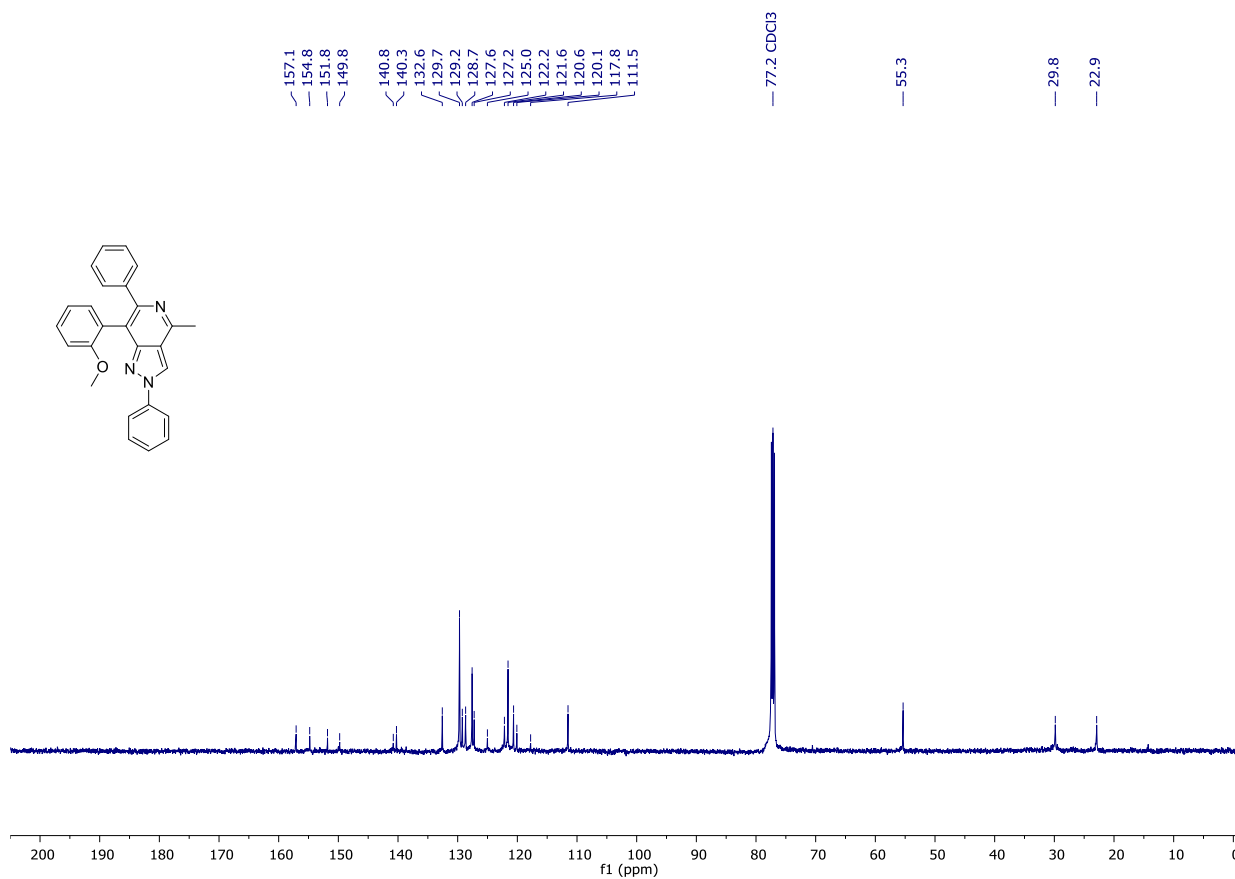
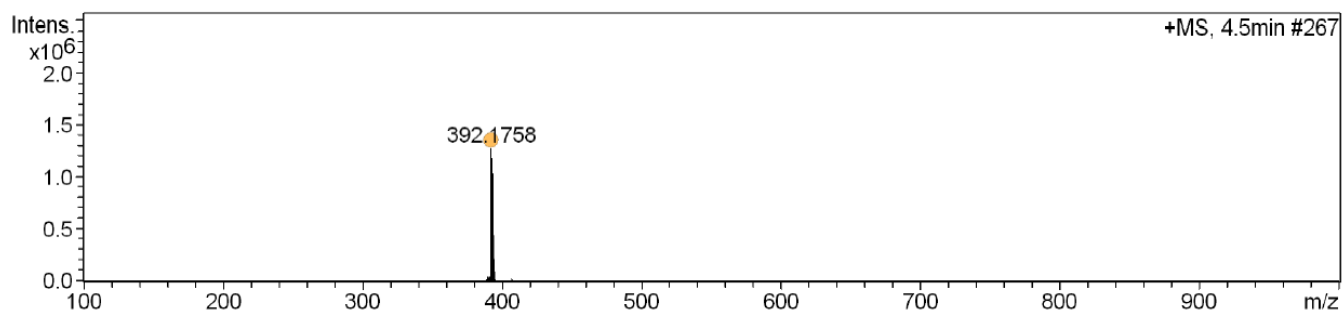


Figure S77. 7-(2-Methoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**25**). ¹³C NMR (126 MHz, CDCl₃).

+MS, 4.5min #267



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e^-	Conf	N-Rule
392.1758	1	C ₂₆ H ₂₂ N ₃ O	392.1757	0.2	325.3	1	100.00	17.5	even		ok

Figure S78. 7-(2-Methoxyphenyl)-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**25**). HRMS (ESI-TOF).

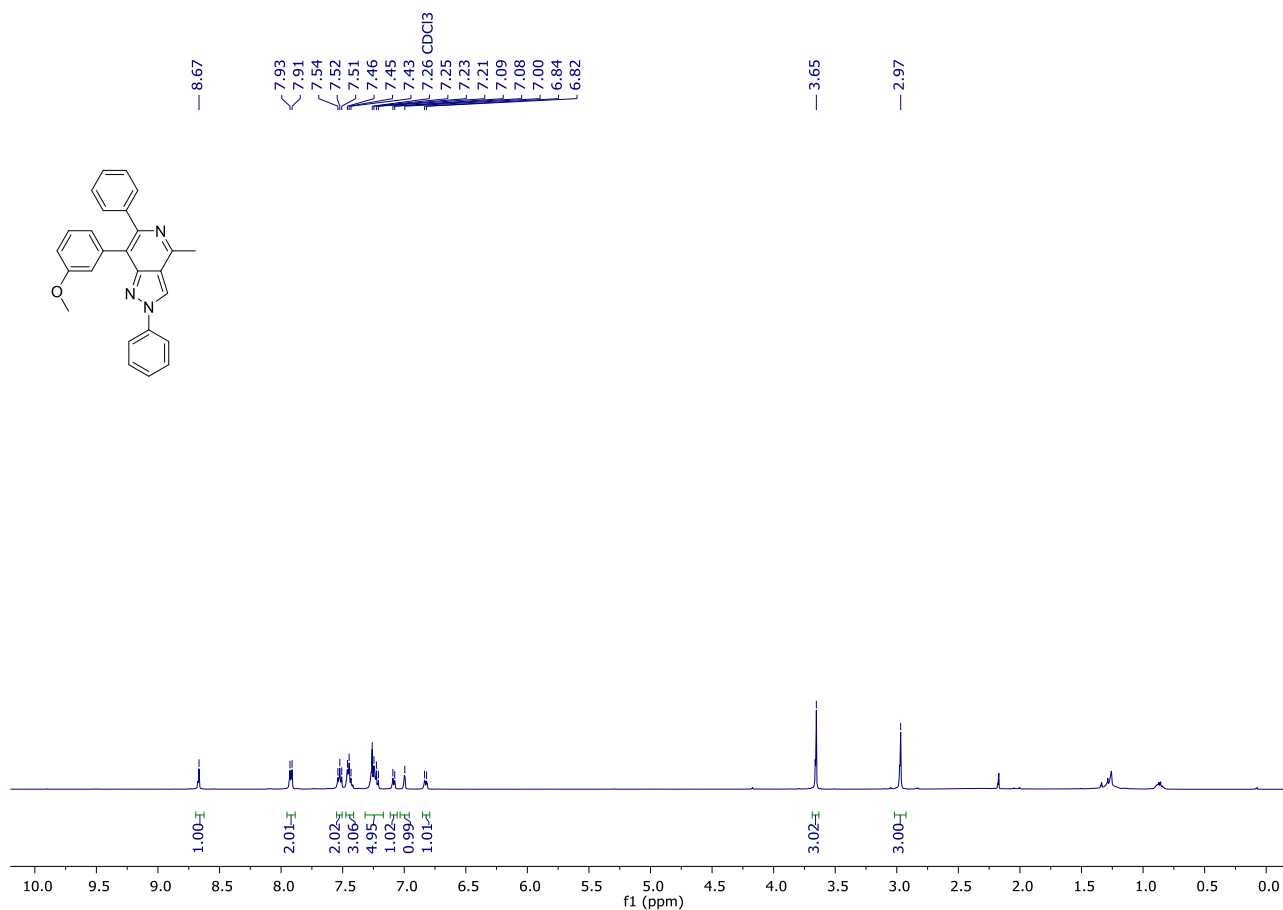


Figure S79. 7-(3-Methoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**26**). ¹H NMR spectrum (500 MHz, CDCl₃).

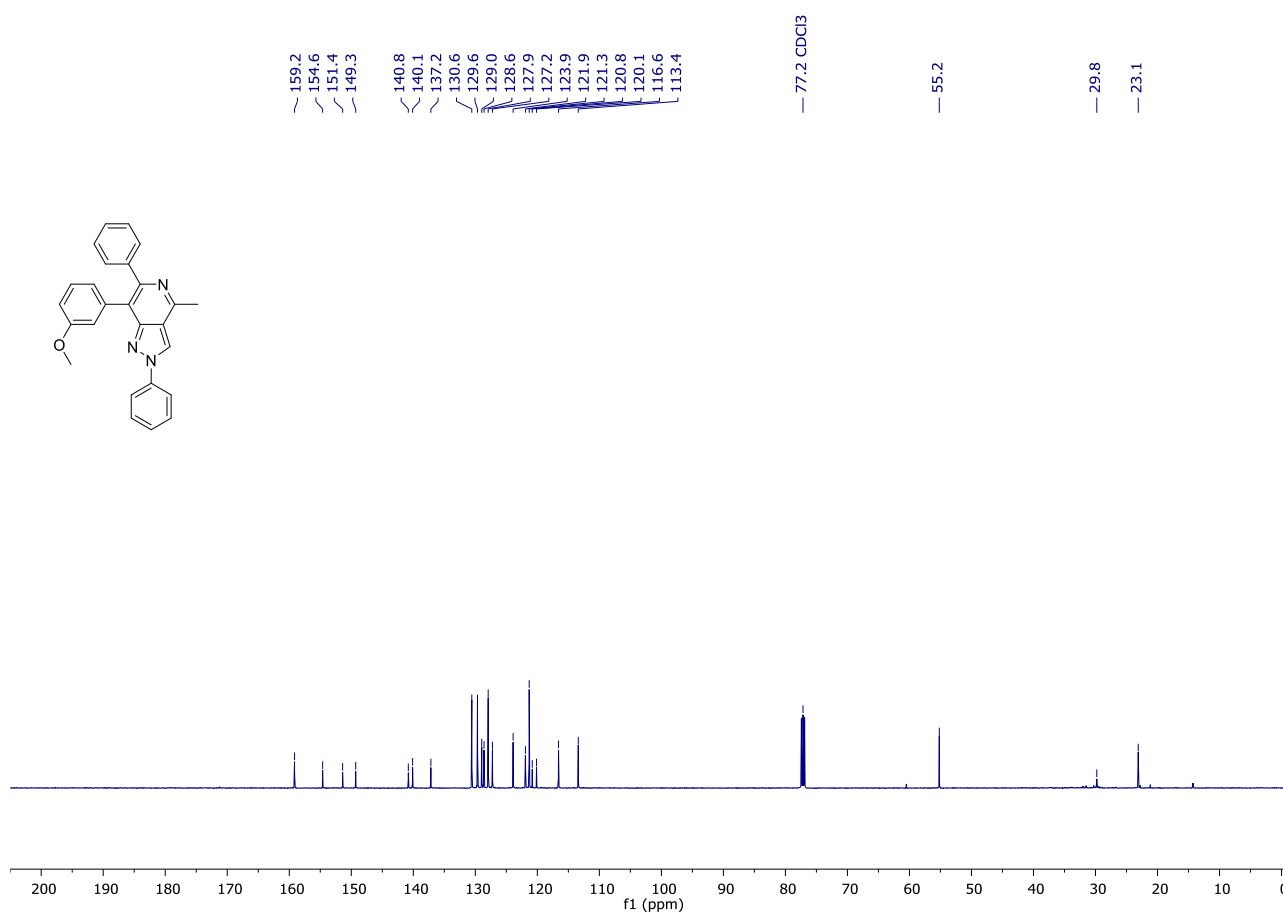


Figure S80. 7-(3-Methoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**26**). ¹³C NMR (126 MHz, CDCl₃).

+MS, 5.8min #348

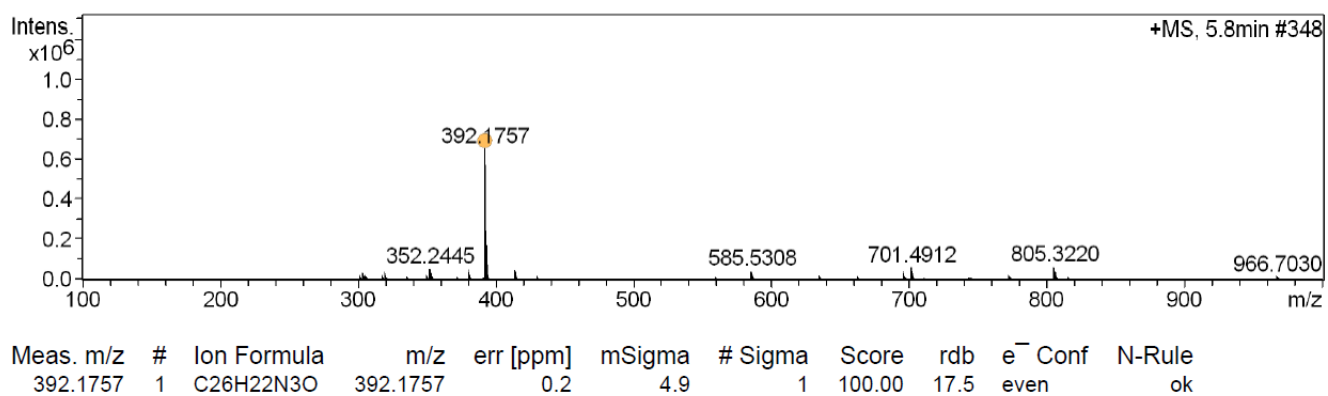


Figure S81. 7-(3-Methoxyphenyl)-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**26**). HRMS (ESI-TOF).

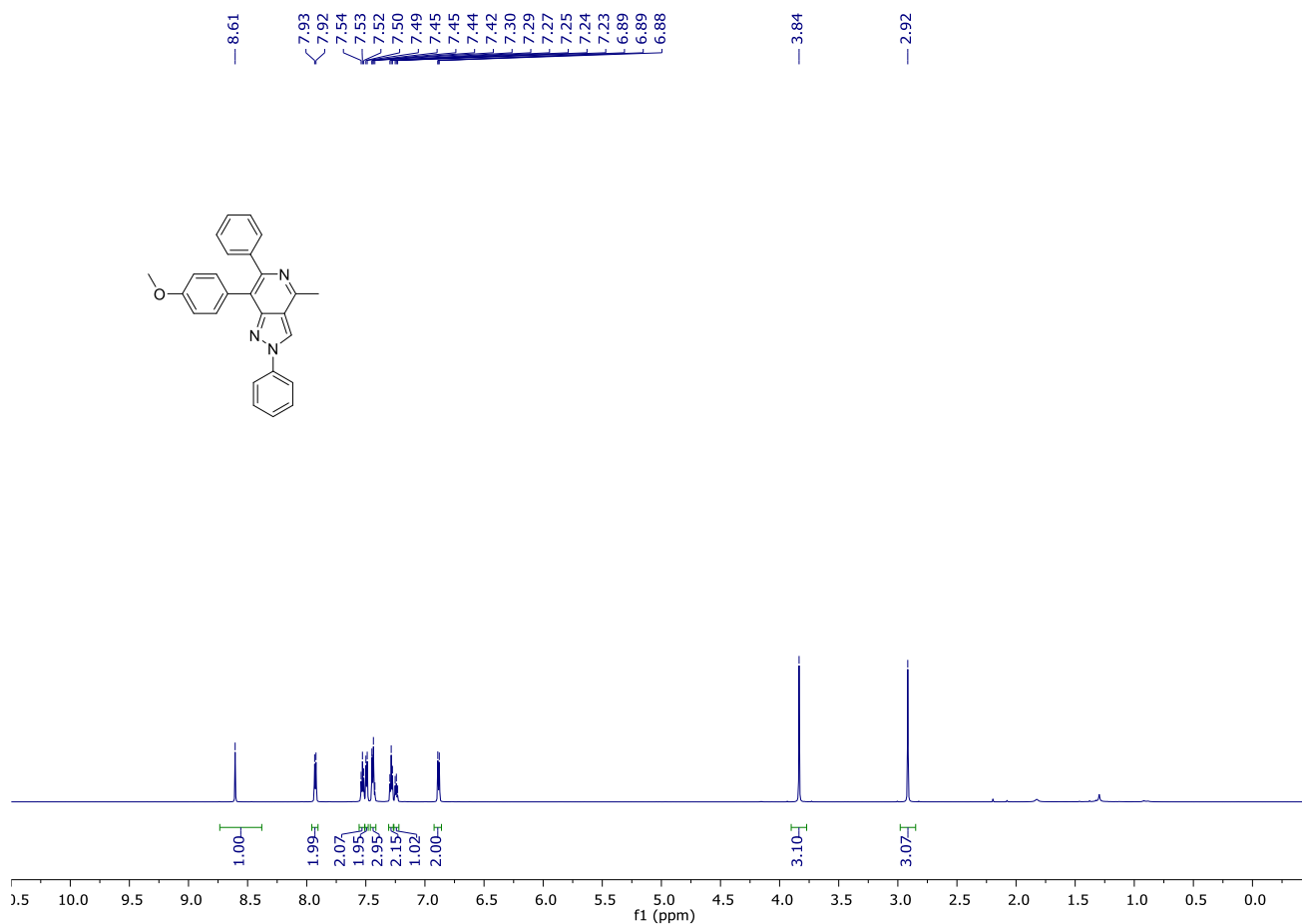


Figure S82. 7-(4-Methoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**27**). ¹H NMR spectrum (700 MHz, CDCl₃).

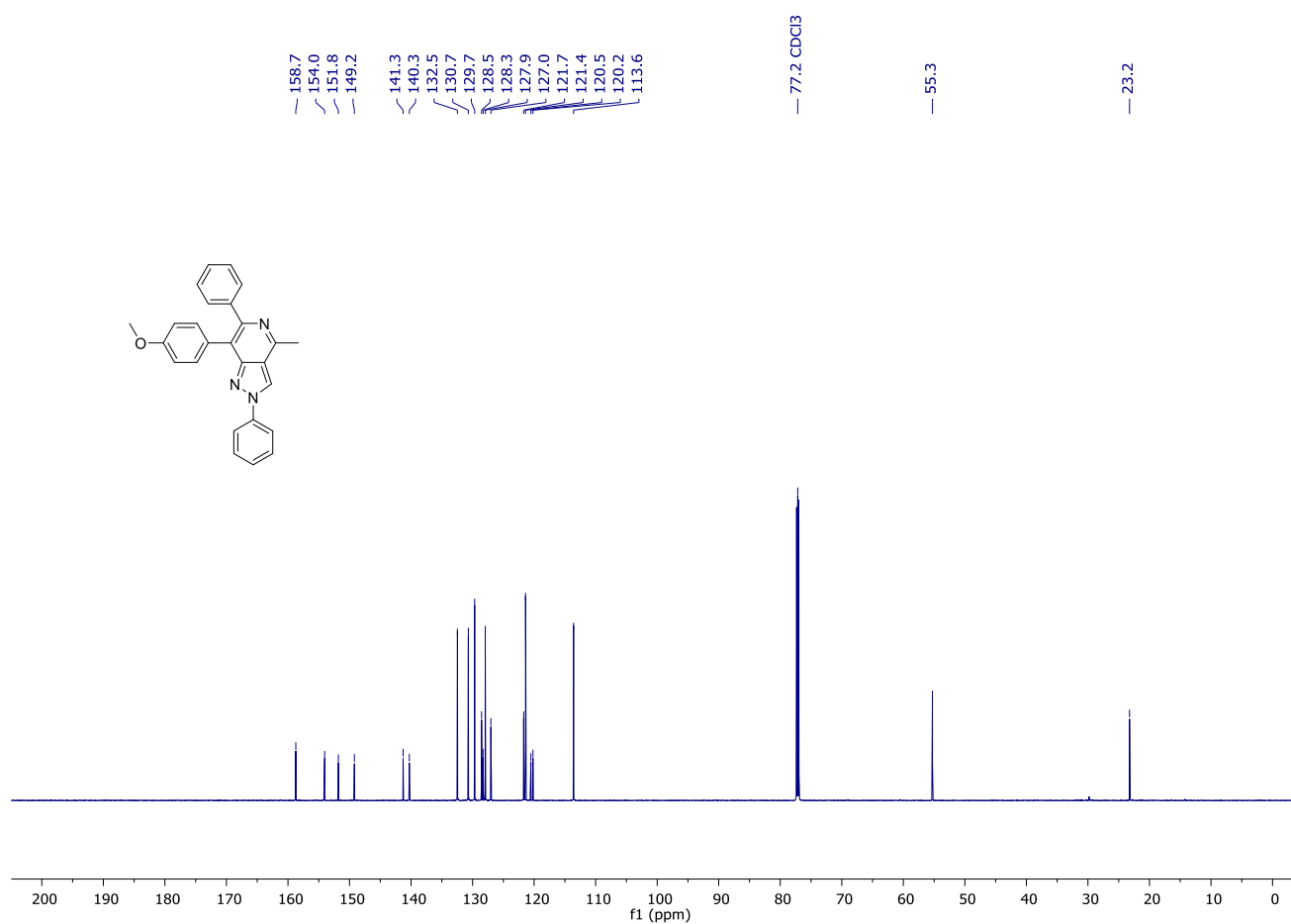


Figure S83. 7-(4-Methoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**27**). ¹³C NMR (176 MHz, CDCl₃).

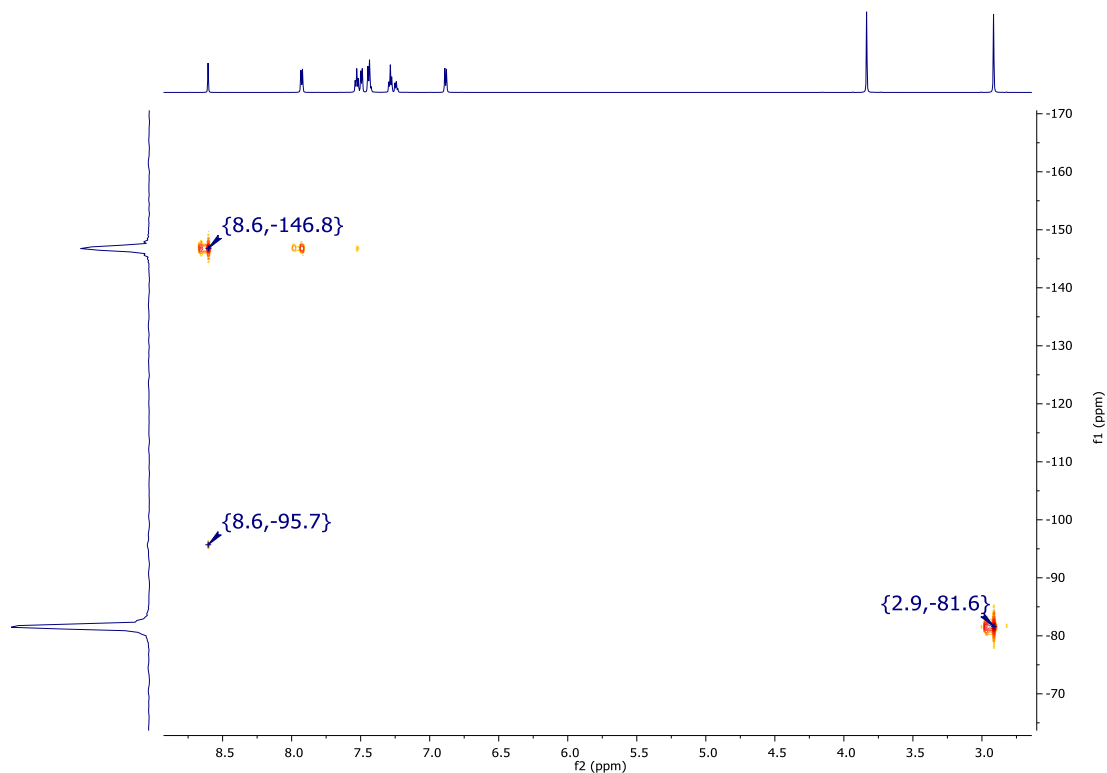
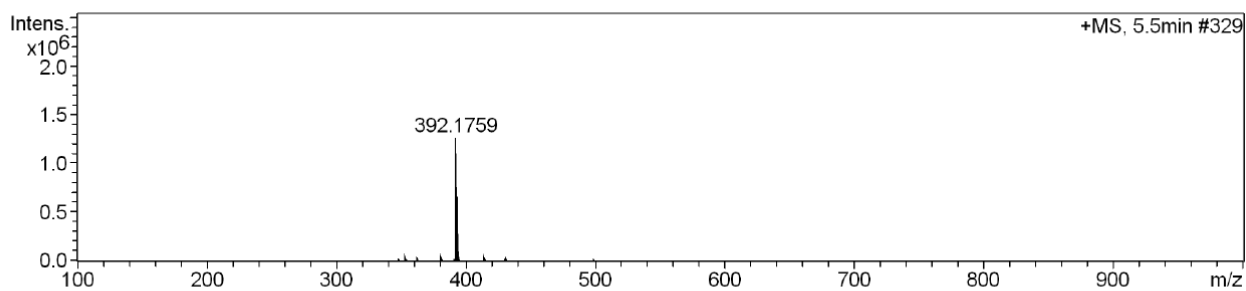


Figure S84. 7-(4-Methoxyphenyl)-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**27**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 5.5min #329



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e^-	Conf	N-Rule
392.1759	1	$\text{C}_{26}\text{H}_{22}\text{N}_3\text{O}$	392.1757	0.4	155.5	1	100.00	17.5	even		ok

Figure S85. 7-(4-Methoxyphenyl)-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**27**). HRMS (ESI-TOF).

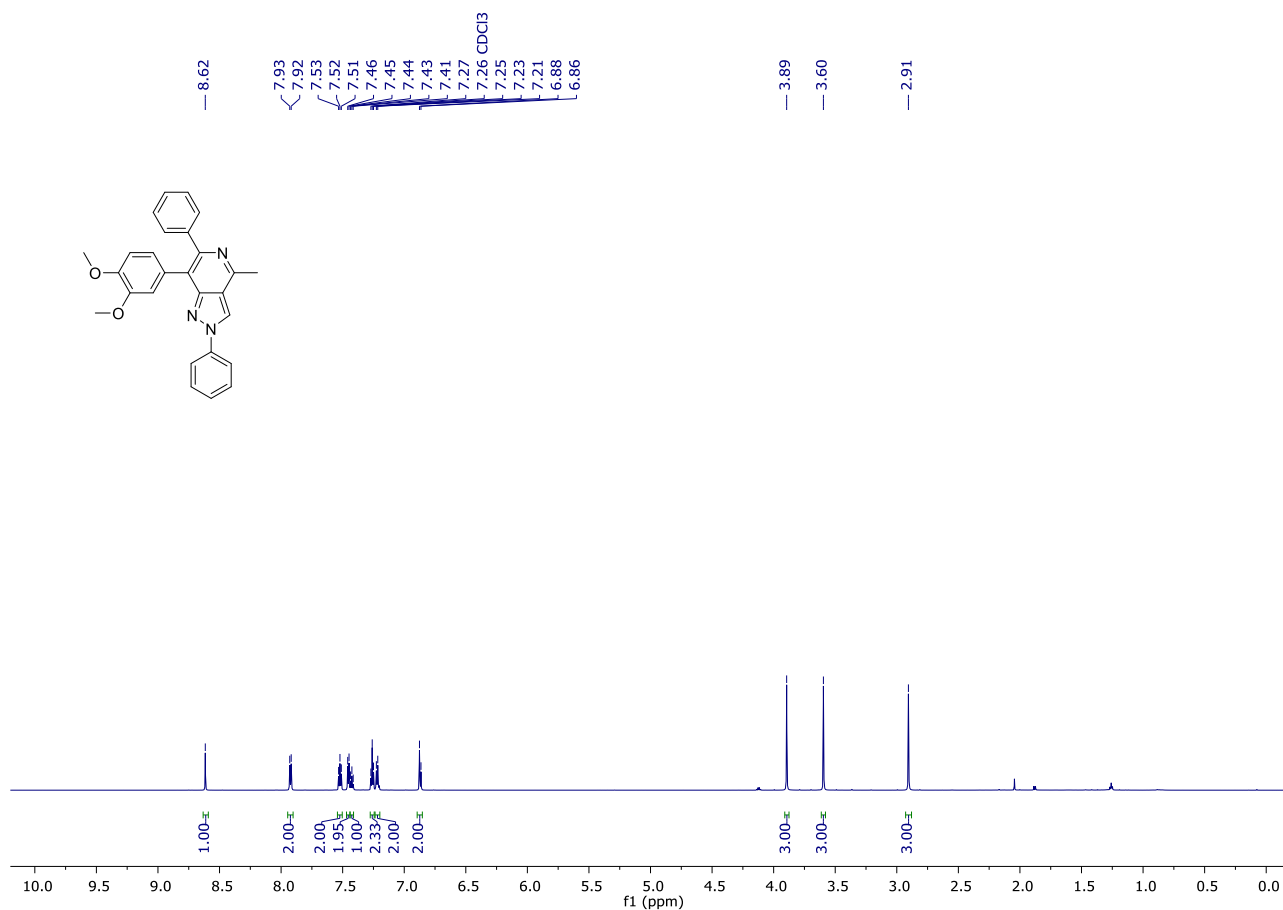


Figure S86. 7-(3,4-Dimethoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**28**). ¹H NMR spectrum (700 MHz, CDCl₃).

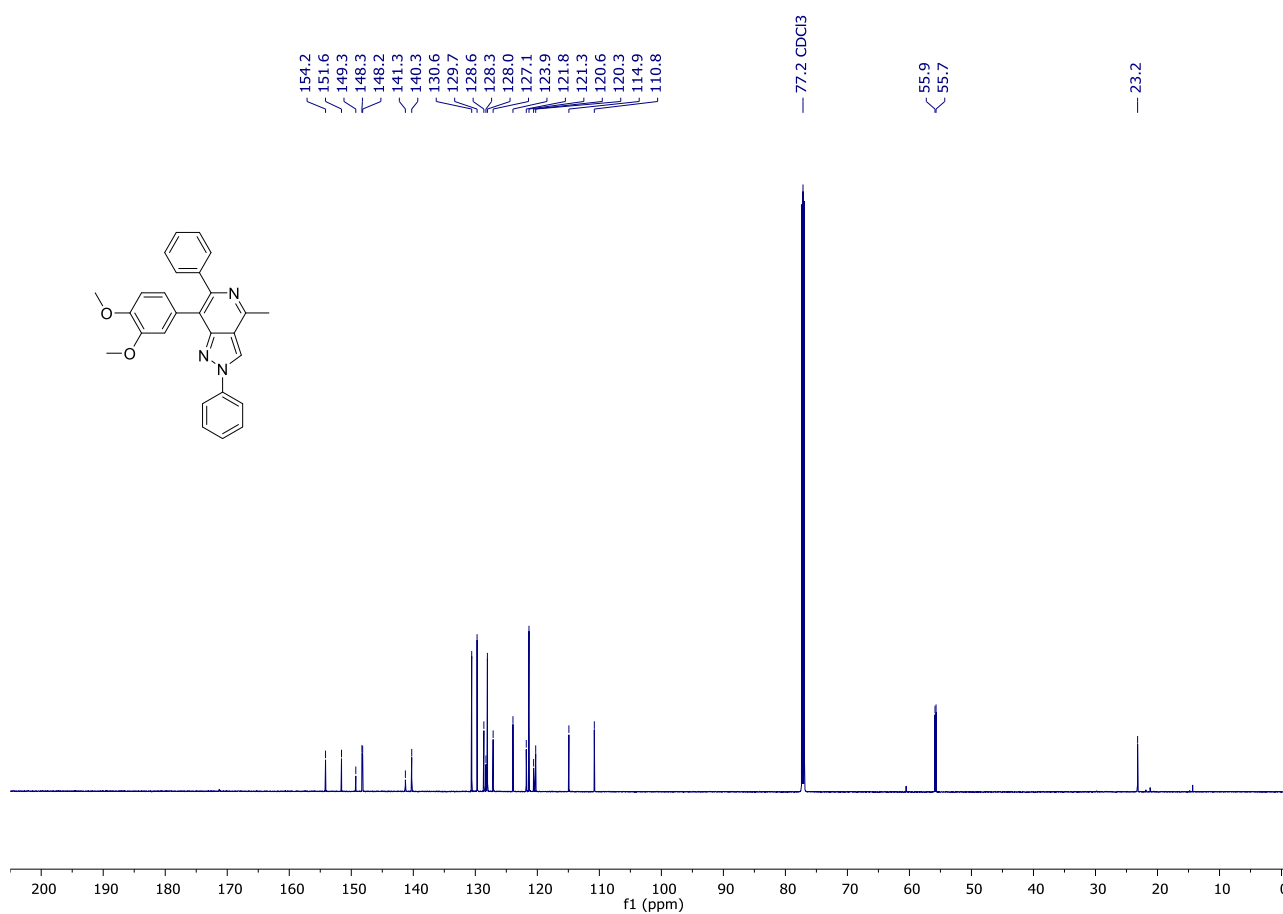


Figure S87. 7-(3,4-Dimethoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**28**). ¹³C NMR (176 MHz, CDCl₃).

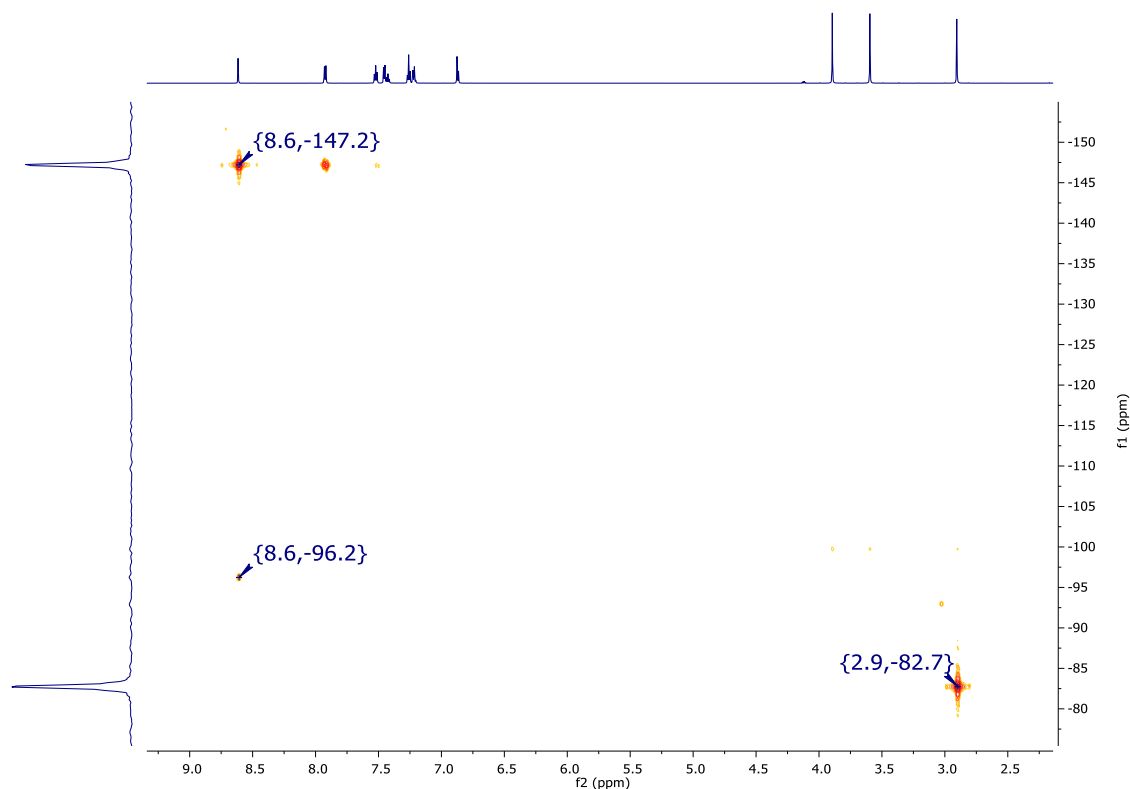
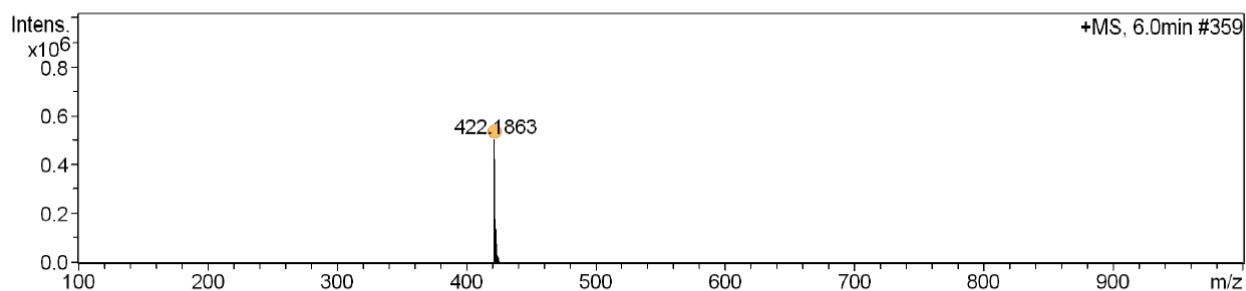


Figure S88. 7-(3,4-Dimethoxyphenyl)-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**28**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 6.0min #359



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
422.1863	1	C ₂₇ H ₂₄ N ₃ O ₂	422.1863	-0.1	2.3	1	100.00	17.5	even	ok

Figure S89. 7-(3,4-Dimethoxyphenyl)-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**28**). HRMS (ESI-TOF).

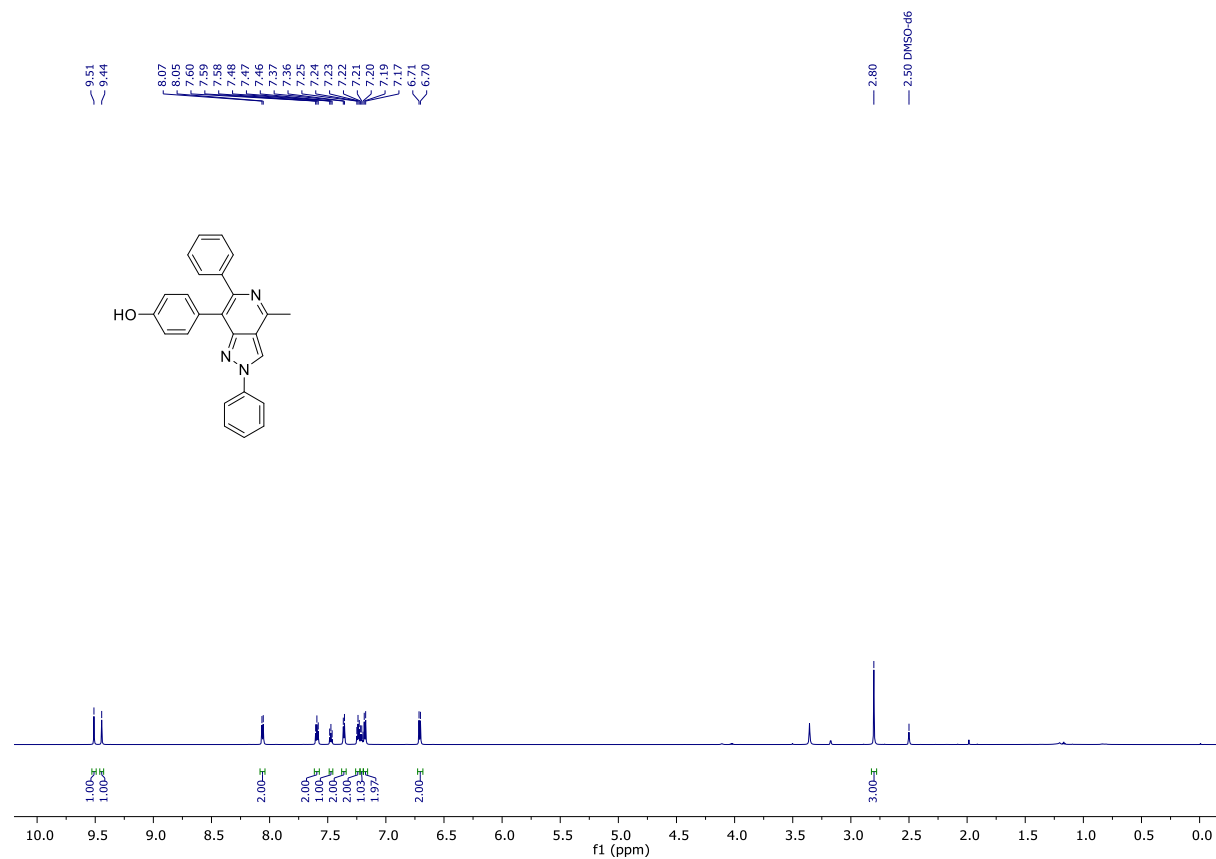


Figure S90. 4-(4-Methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridin-7-yl)phenol (**29**). ¹H NMR spectrum (700 MHz, DMSO-*d*₆).

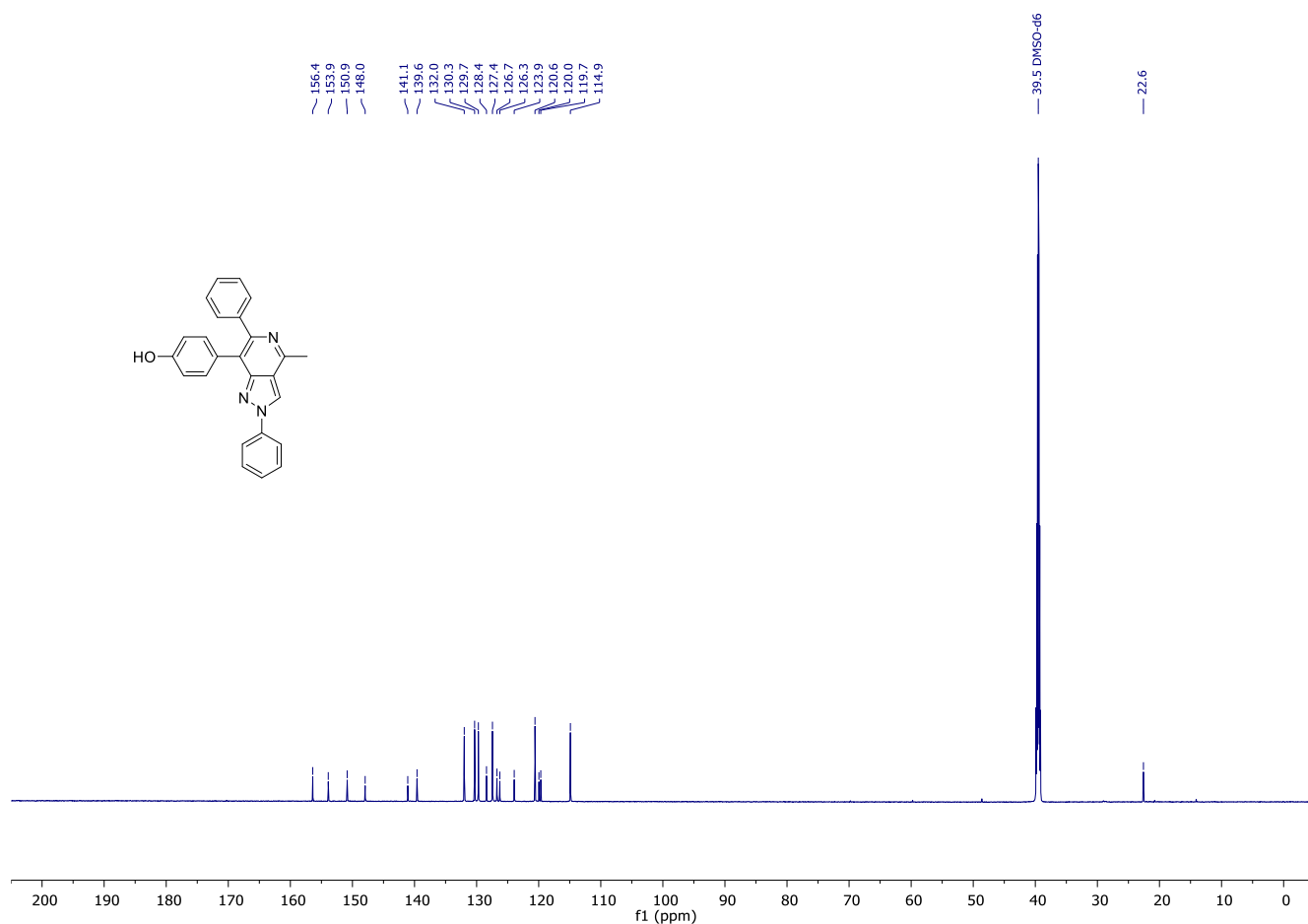


Figure S91. 4-(4-Methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridin-7-yl)phenol (**29**). ¹³C NMR (176 MHz, DMSO-*d*₆).

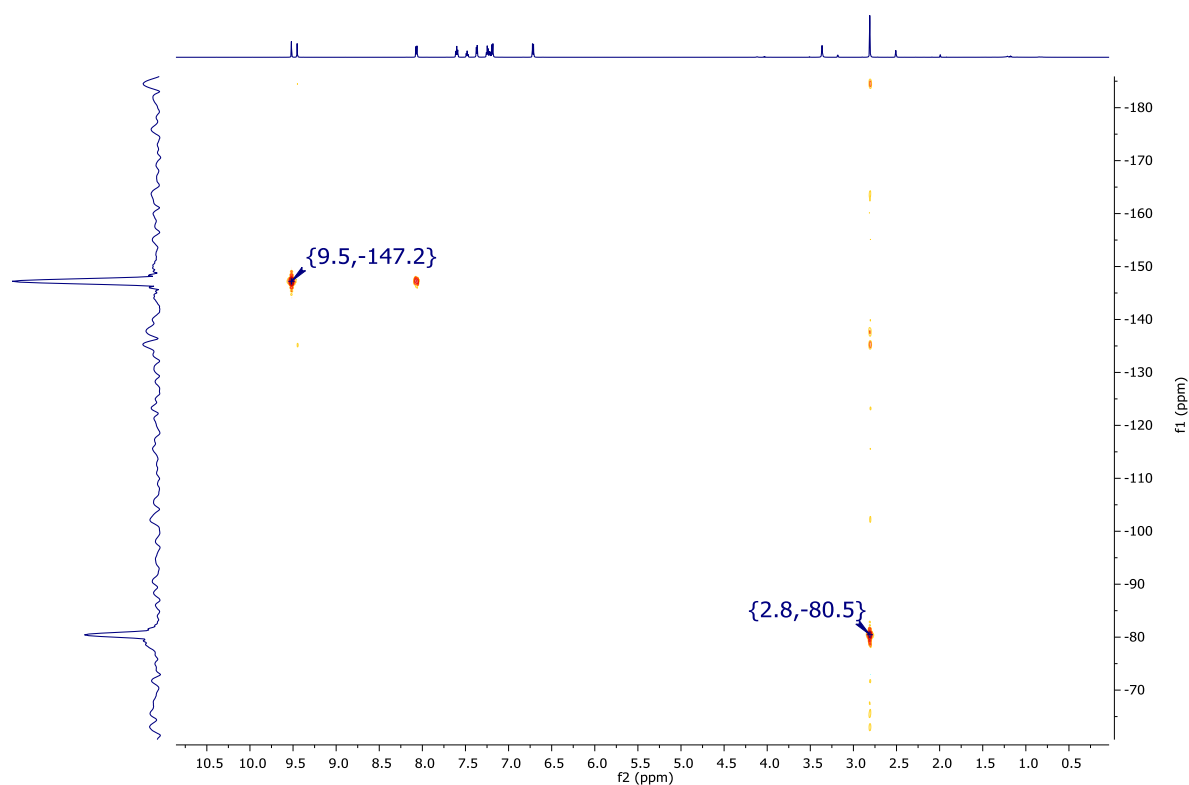
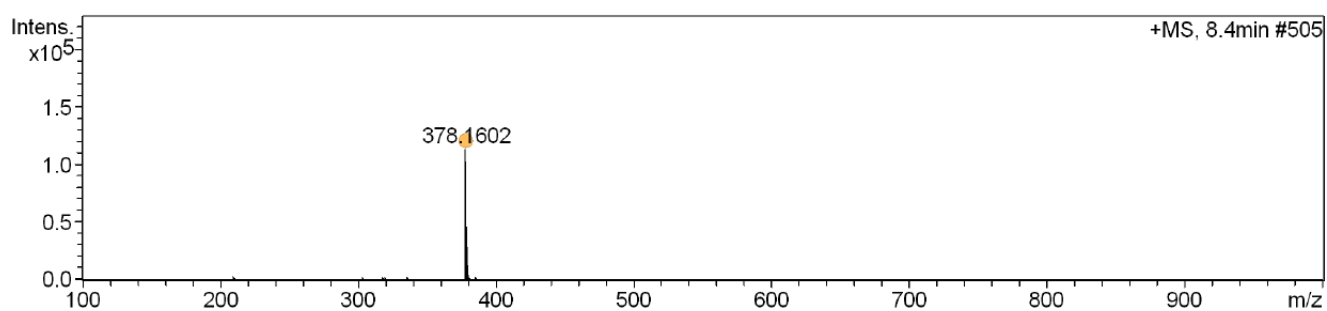


Figure S92. 4-(4-Methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridin-7-yl)phenol (**29**). ^1H - ^{15}N HMBC spectrum (700 MHz, $\text{DMSO-}d_6$).

+MS, 8.4min #505



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻	Conf	N-Rule
378.1602	1	C ₂₅ H ₂₀ N ₃ O	378.1601	-0.4	1.7	1	100.00	17.5	even		ok

Figure S93. 4-(4-Methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridin-7-yl)phenol (**29**). HRMS (ESI-TOF).

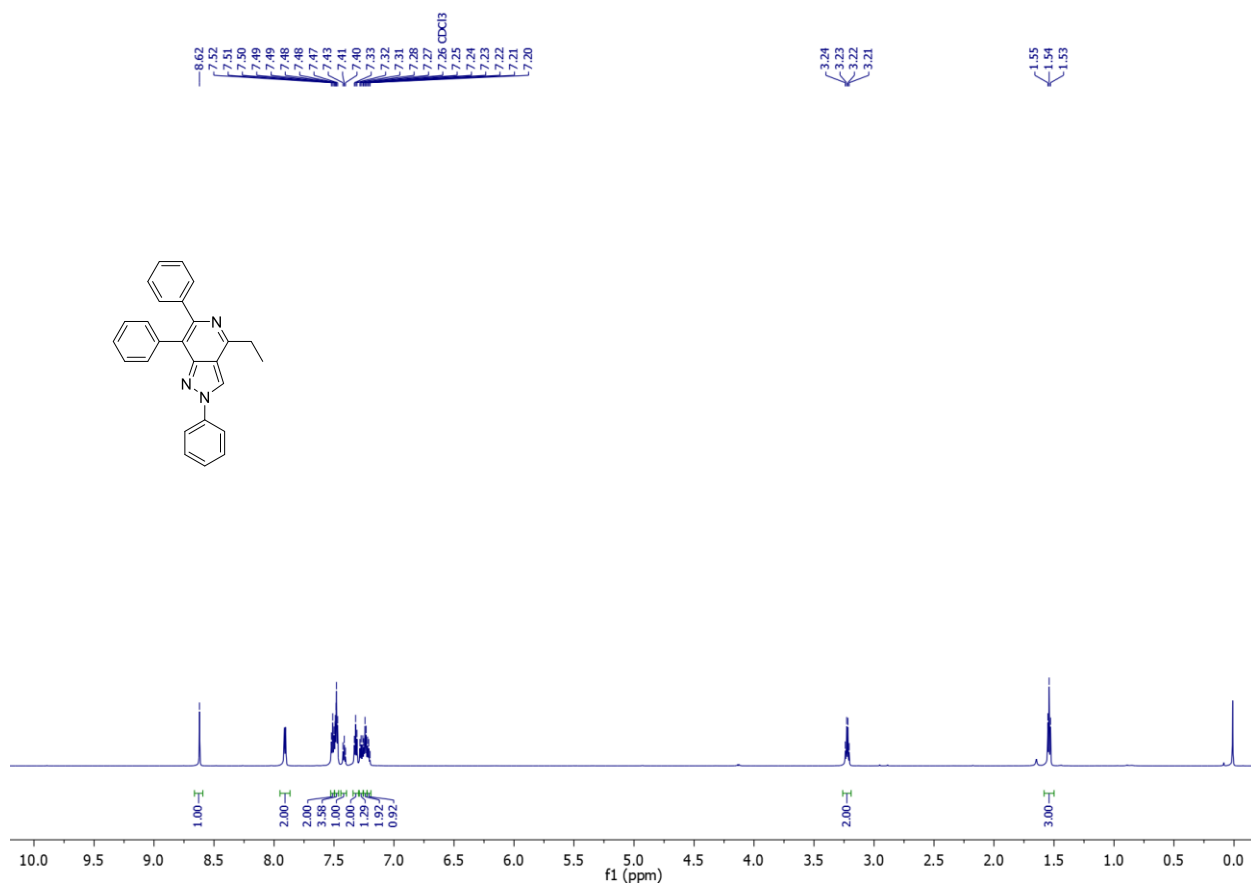


Figure S94. 4-Ethyl-2,6,7-triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**30**). ¹H NMR spectrum (700 MHz, CDCl₃).

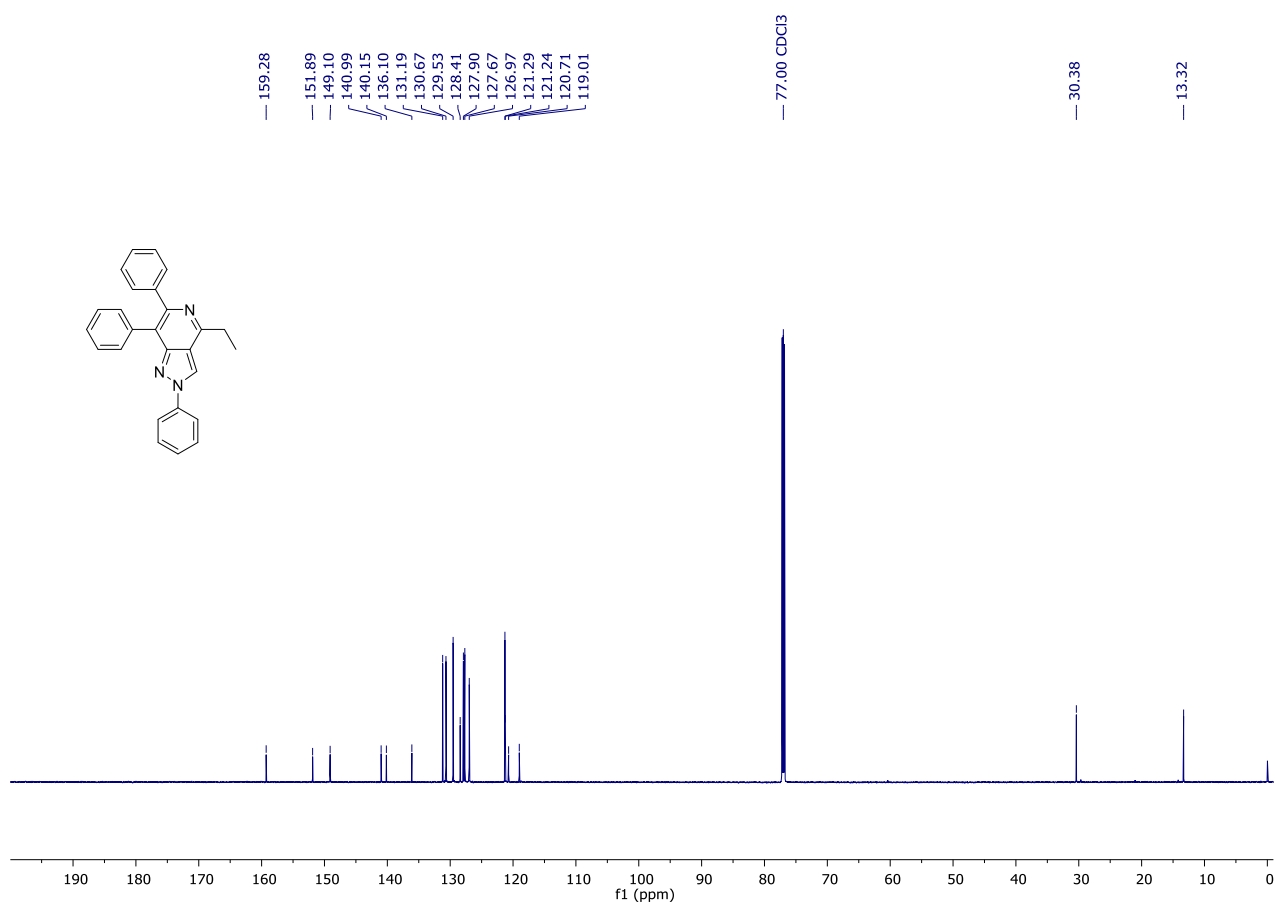


Figure S95. 4-Ethyl-2,6,7-triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**30**). ¹³C NMR (176 MHz, CDCl₃).

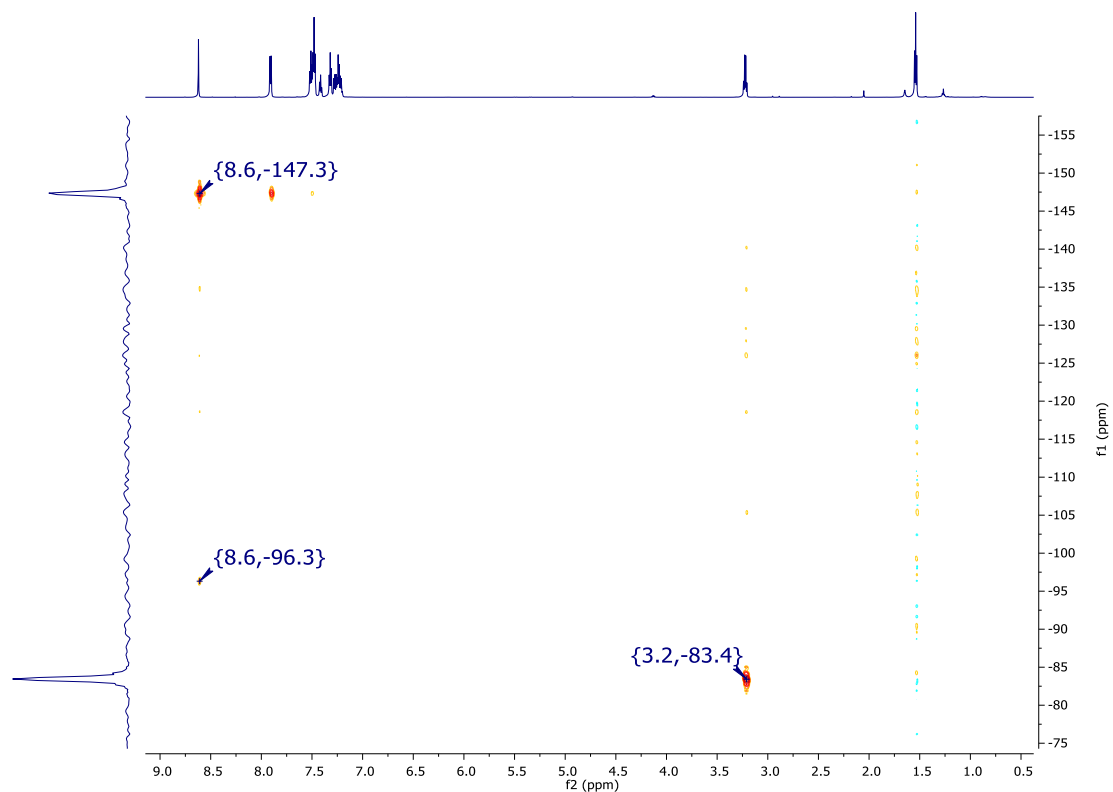
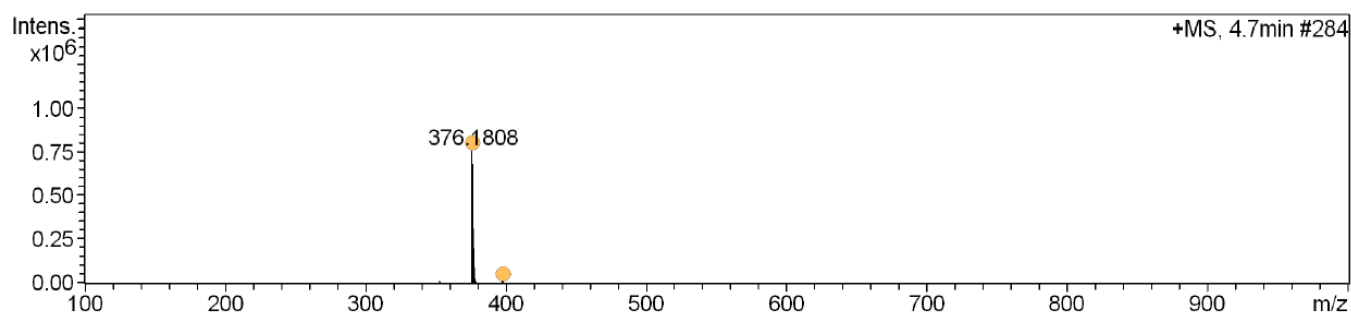


Figure S96. 4-Ethyl-2,6,7-triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**30**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 4.7min #284



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻	Conf	N-Rule
376.1808	1	C ₂₆ H ₂₂ N ₃	376.1808	0.1	2.5	1	100.00	17.5	even		ok
398.1611	1	C ₂₆ H ₂₁ N ₃ Na	398.1628	4.2	33.1	1	100.00	17.5	even		ok

Figure S97. 4-Ethyl-2,6,7-triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**30**). HRMS (ESI-TOF).

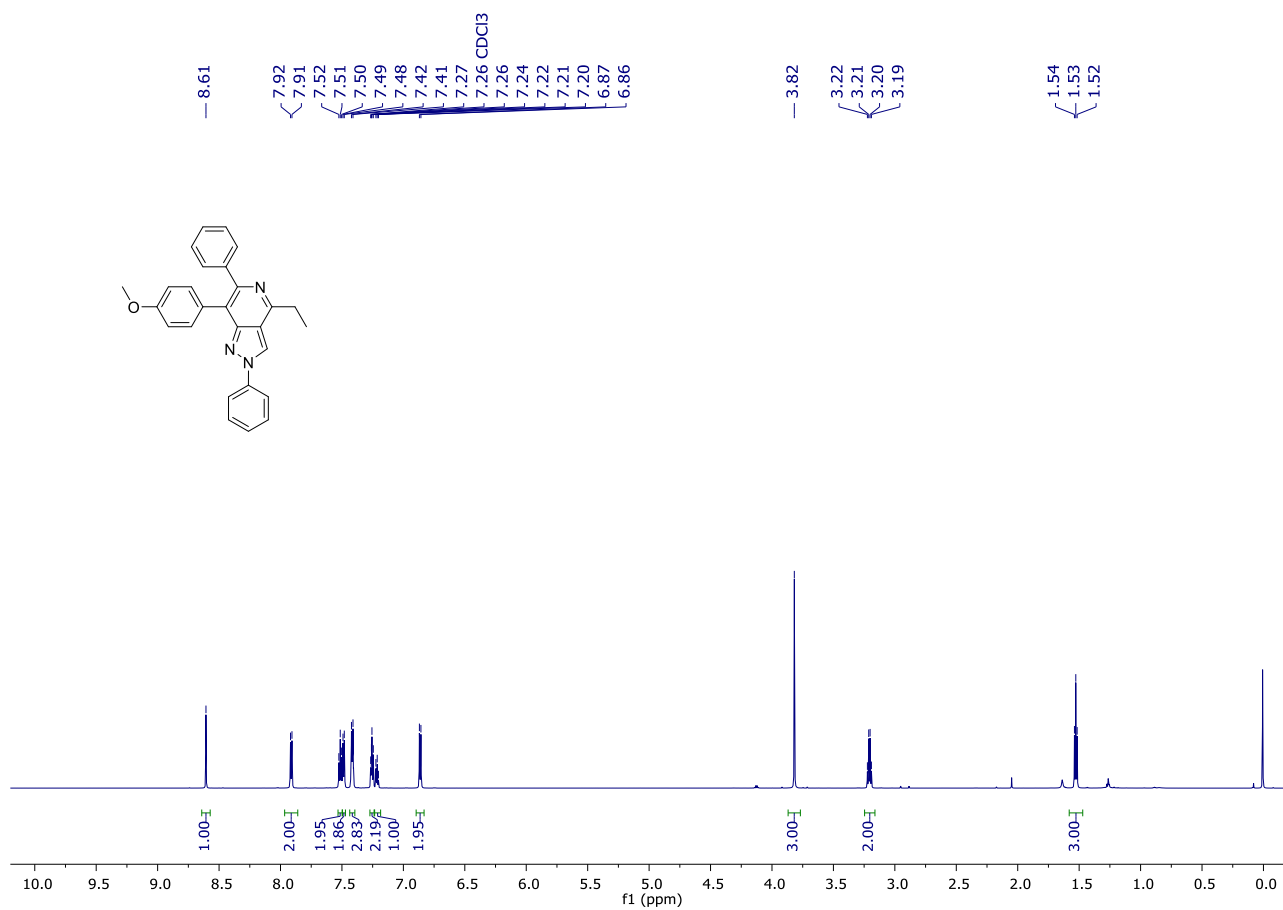


Figure S98. 4-Ethyl-7-(4-methoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**31**). ¹H NMR spectrum (700 MHz, CDCl₃).

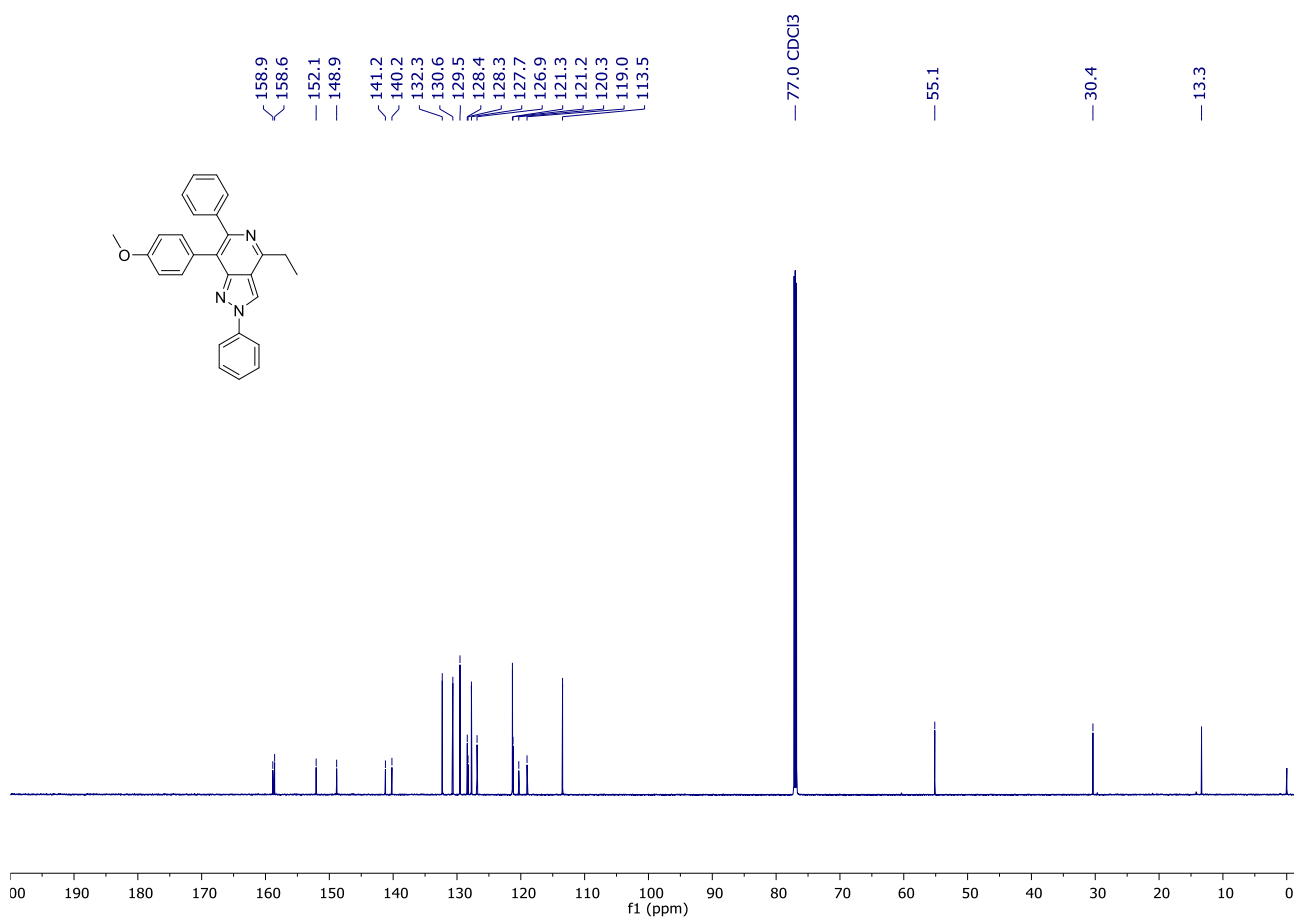


Figure S99. 4-Ethyl-7-(4-methoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**31**). ¹³C NMR (176 MHz, CDCl₃).

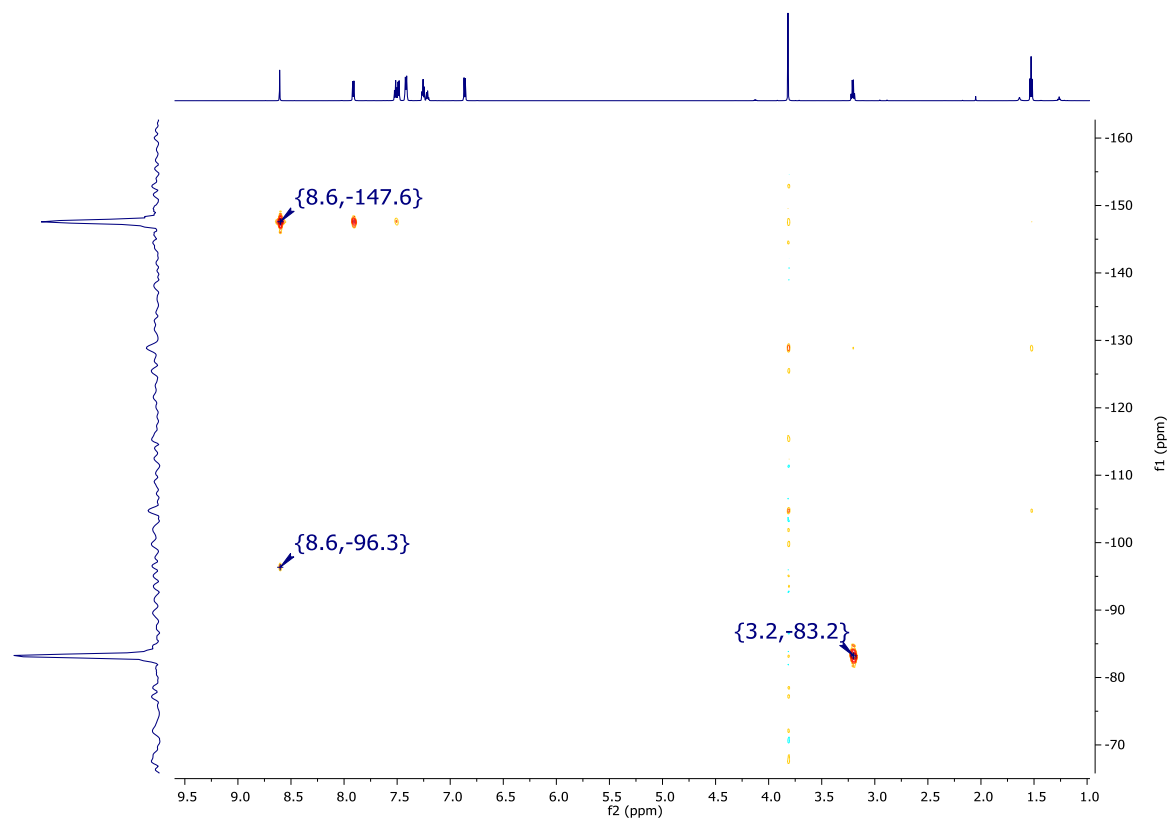
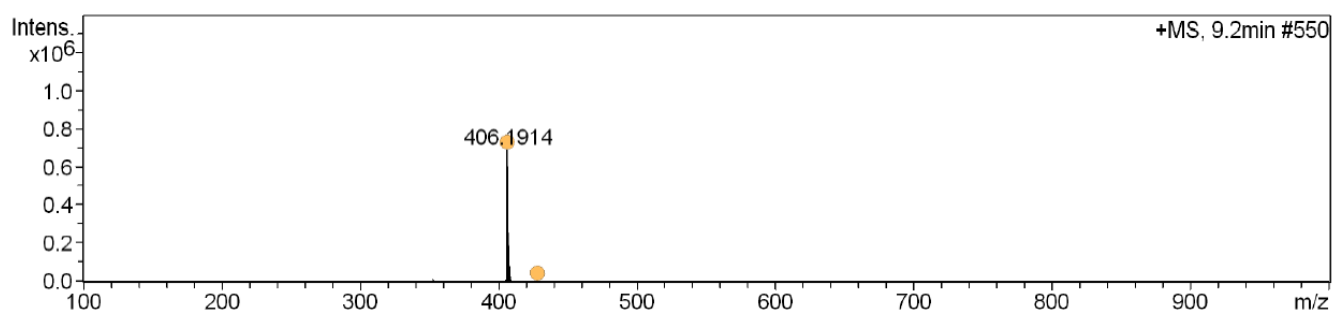


Figure S100. 4-Ethyl-7-(4-methoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**31**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 9.2min #550



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
406.1914	1	C ₂₇ H ₂₄ N ₃ O	406.1914	-0.0	2.1	1	100.00	17.5	even	ok
428.1745	1	C ₂₇ H ₂₃ N ₃ NaO	428.1733	-2.8	25.2	1	100.00	17.5	even	ok

Figure S101. 4-Ethyl-7-(4-methoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**31**). HRMS (ESI-TOF).

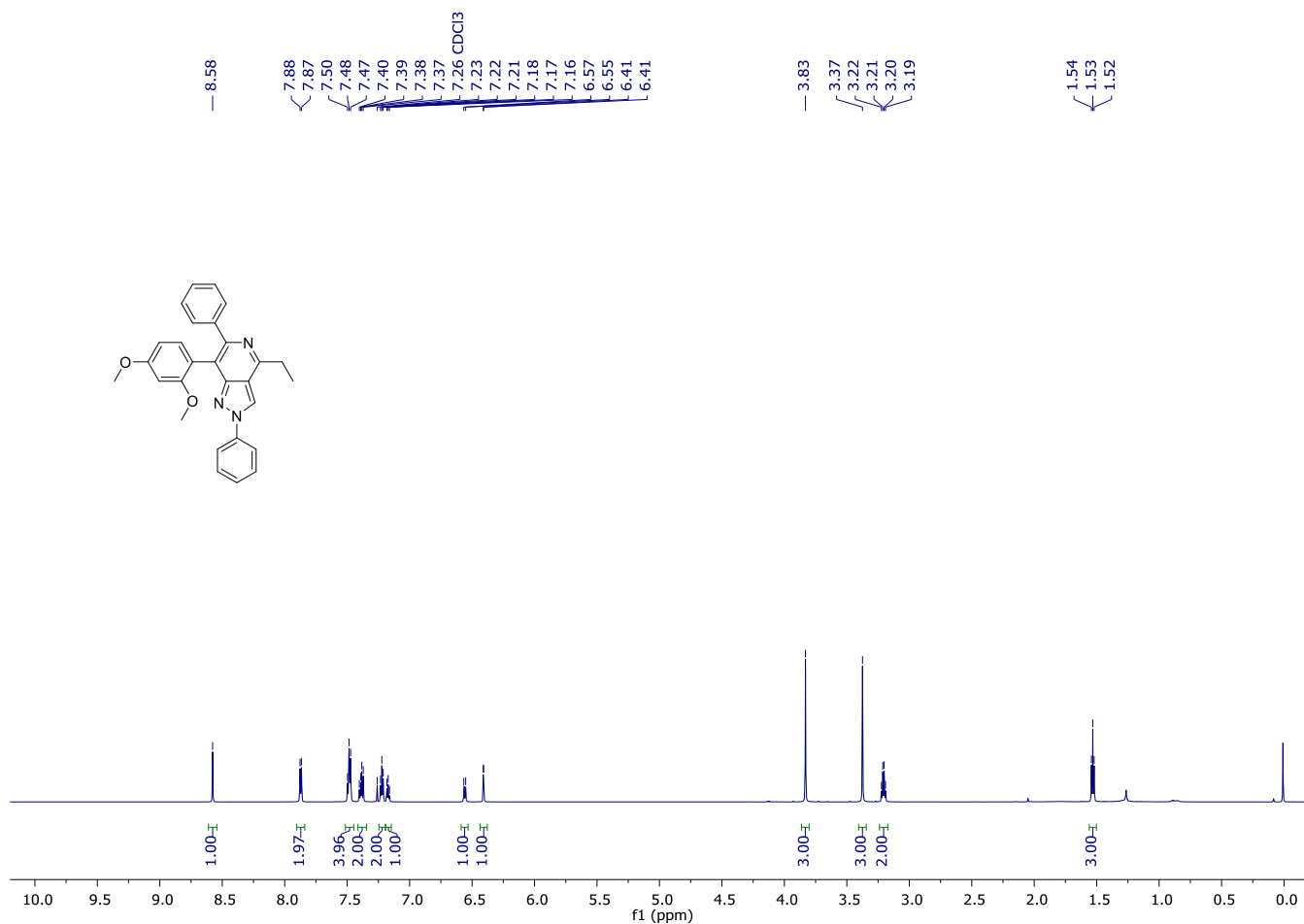


Figure S102. 7-(2,4-Dimethoxyphenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**32**). ¹H NMR spectrum (700 MHz, CDCl₃).

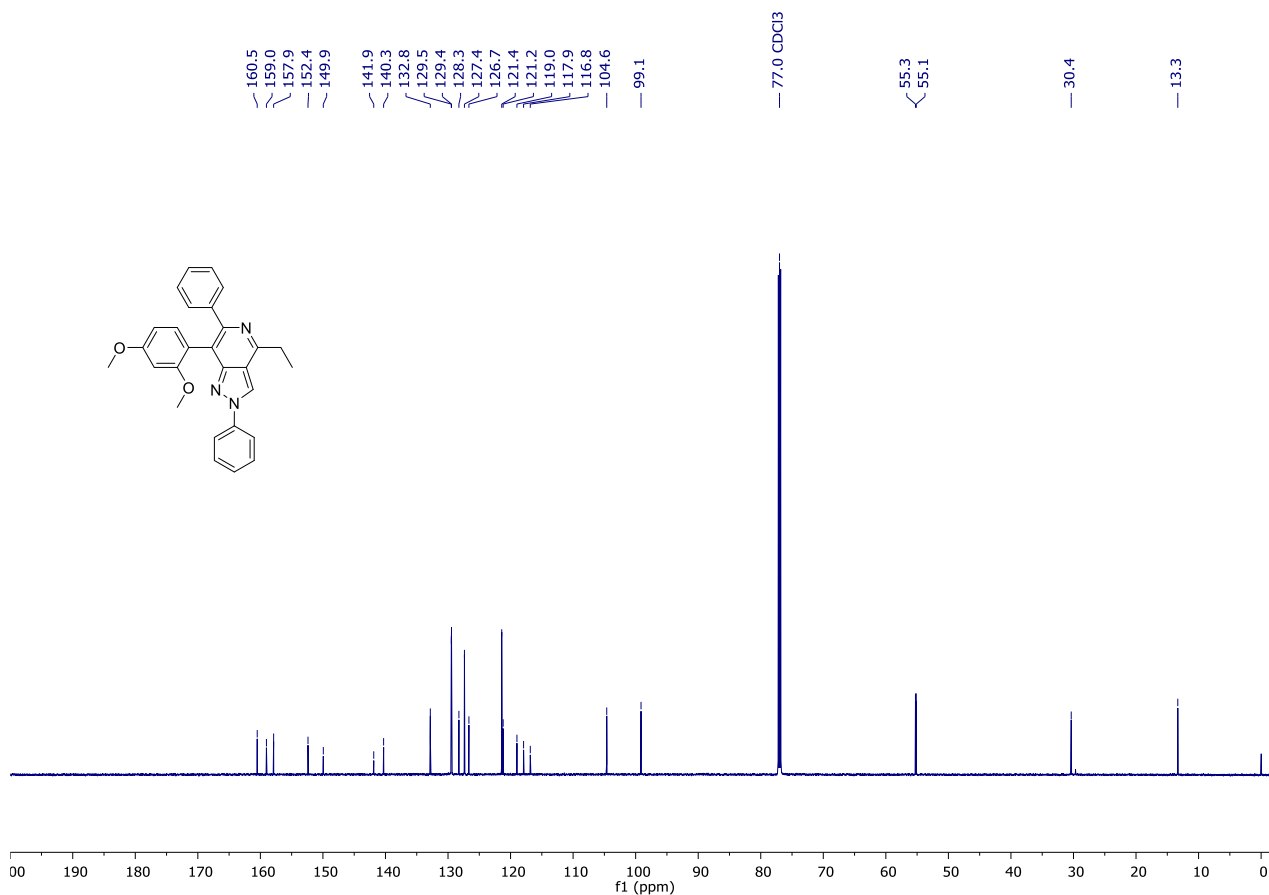


Figure S103. 7-(2,4-Dimethoxyphenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**32**). ¹³C NMR (176 MHz, CDCl₃).

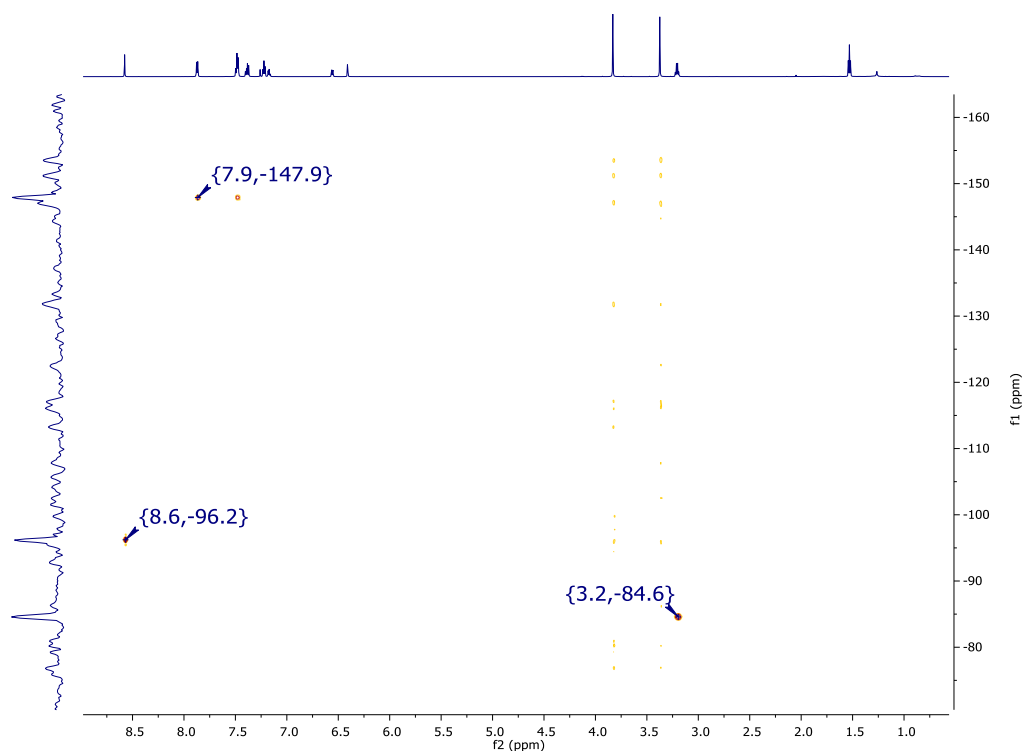
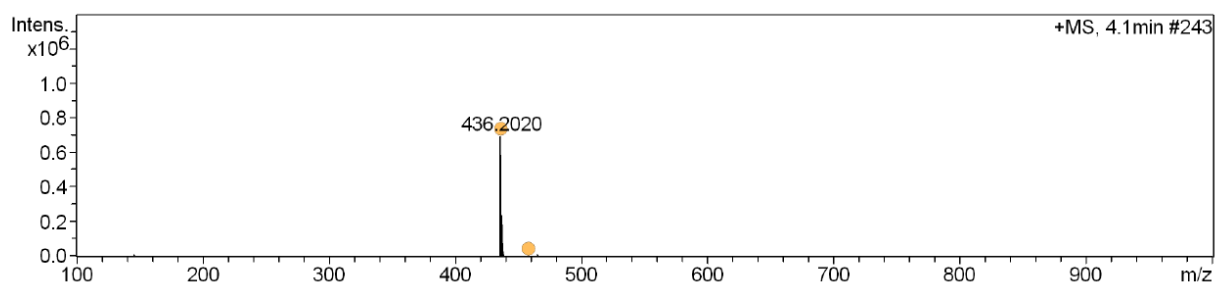


Figure S104. 7-(2,4-Dimethoxyphenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**32**). ^1H - ^{15}N LR HSQMBBC spectrum (700 MHz, CDCl_3).

+MS, 4.1min #243



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻	Conf	N-Rule
436.2020	1	C ₂₈ H ₂₆ N ₃ O ₂	436.2020	-0.2	2.7	1	100.00	17.5	even		ok
458.1873	1	C ₂₈ H ₂₅ N ₃ NaO ₂	458.1839	7.5	98.4	1	100.00	17.5	even		ok

Figure S105. 7-(2,4-Dimethoxyphenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**32**). HRMS (ESI-TOF).

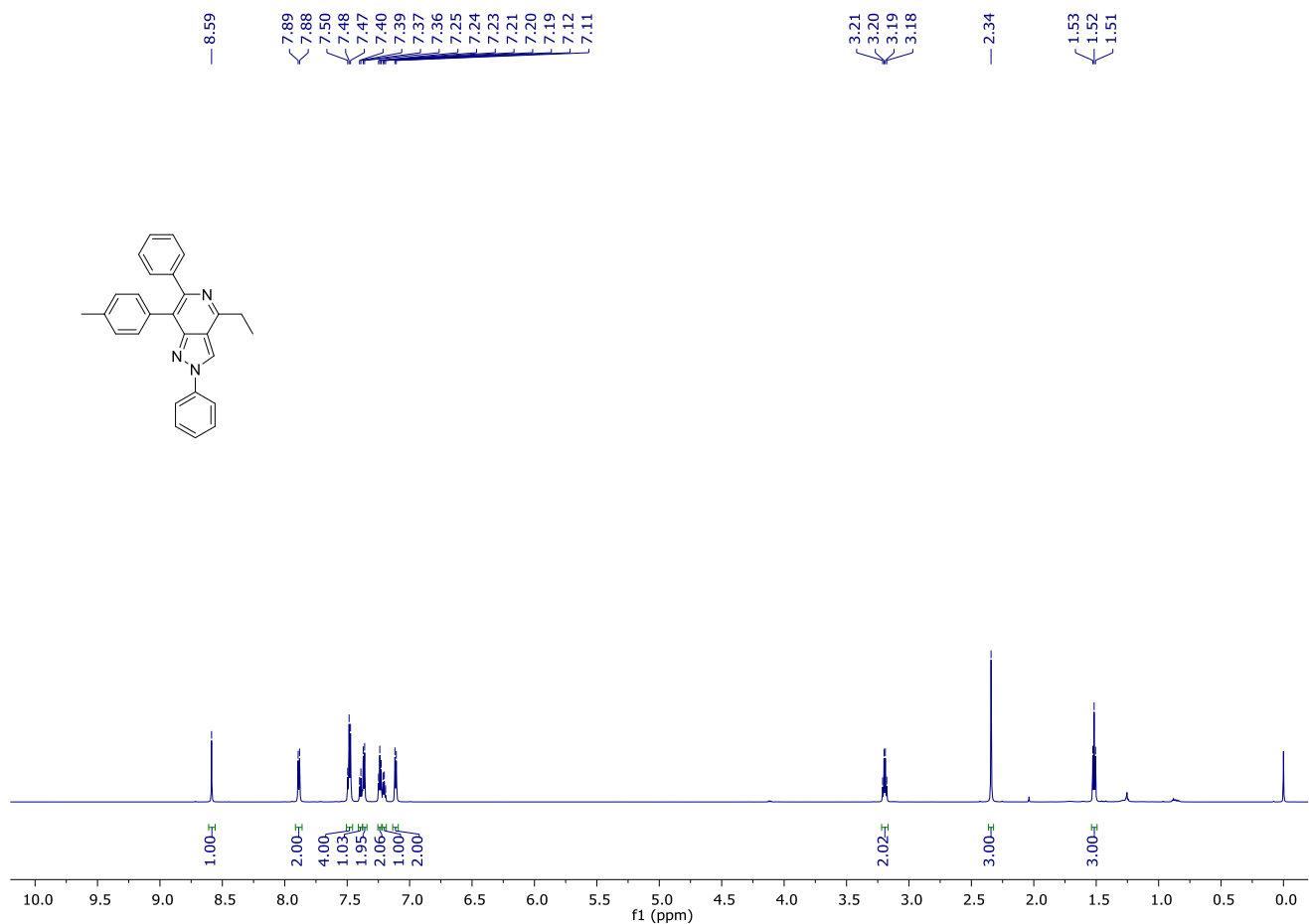


Figure S106. 4-Ethyl-2,6-diphenyl-7-(*p*-tolyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**33**). ¹H NMR spectrum (700 MHz, CDCl₃).

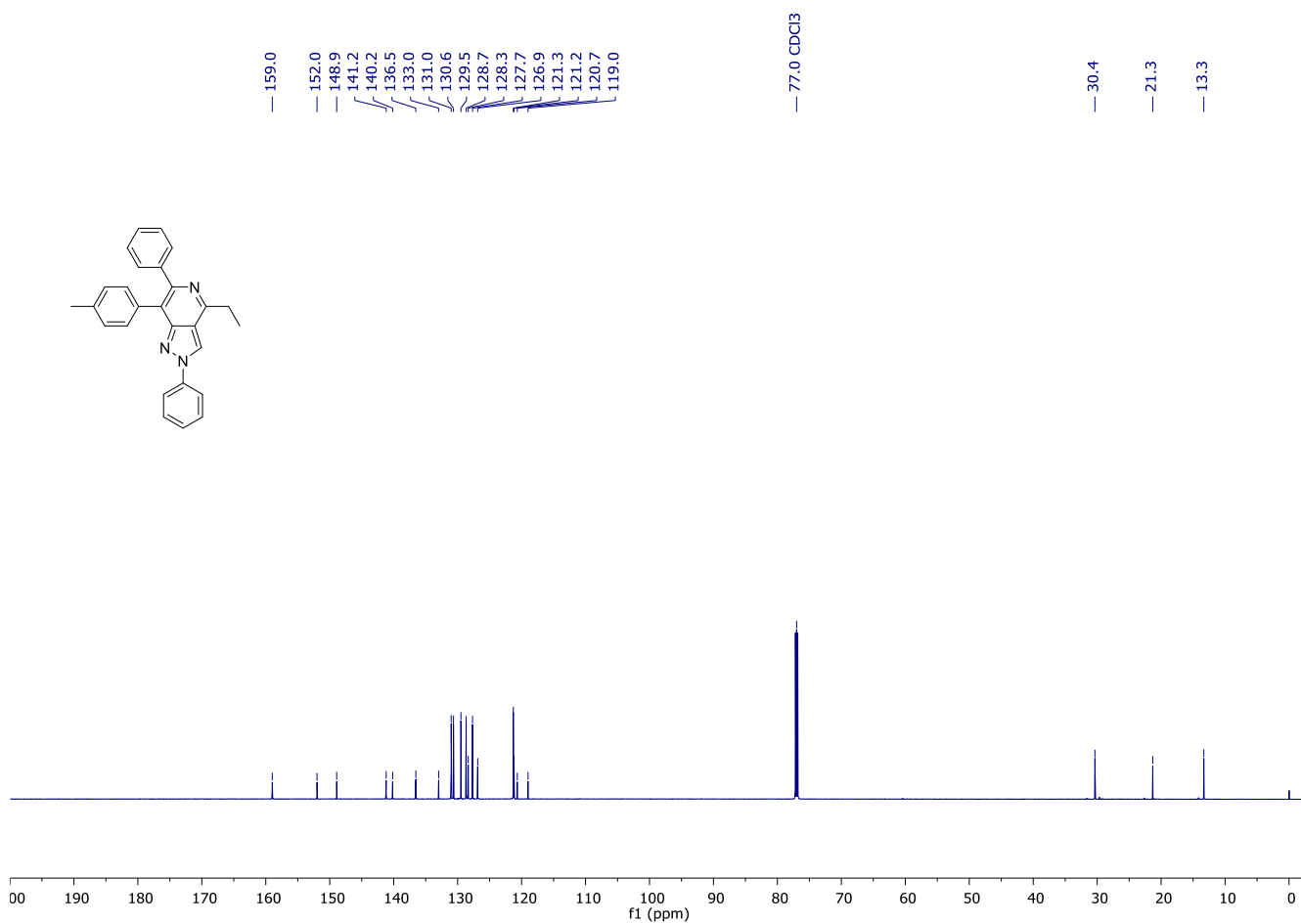


Figure S107. 4-Ethyl-2,6-diphenyl-7-(*p*-tolyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**33**). ¹³C NMR (176 MHz, CDCl₃).

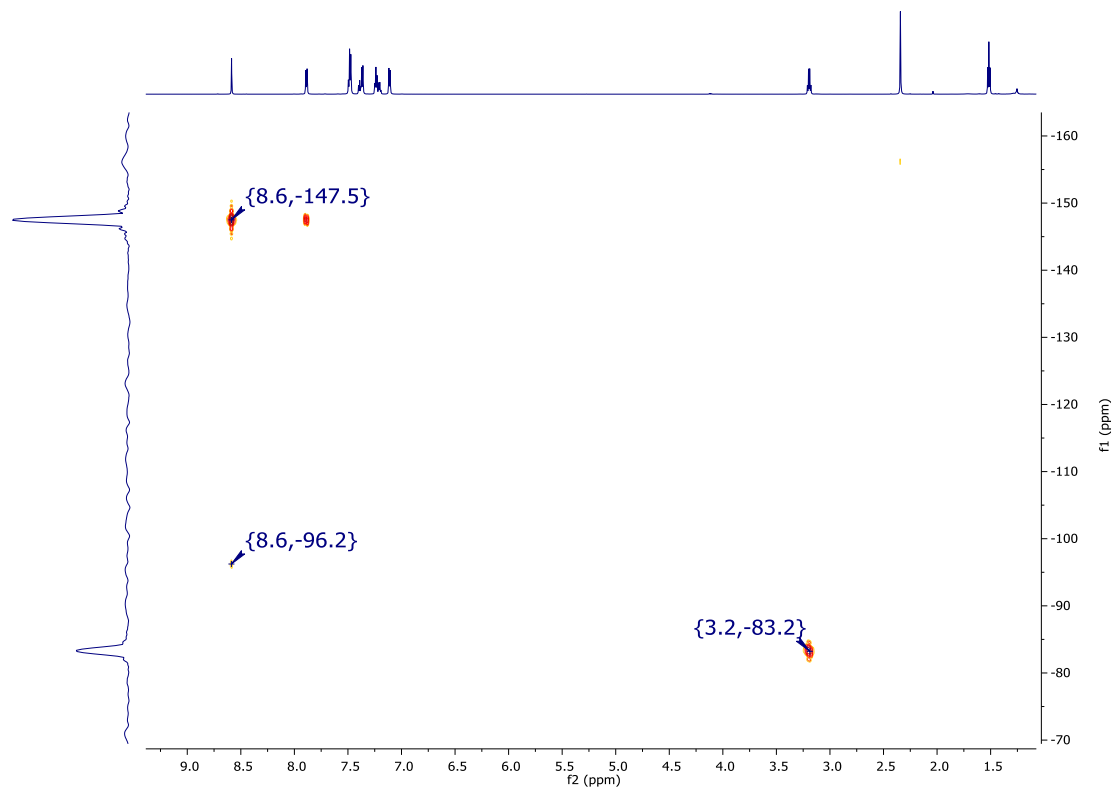
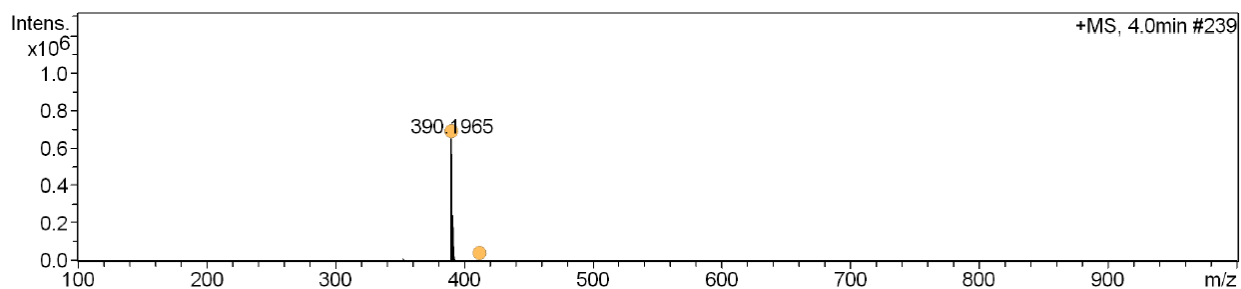


Figure S108. 4-Ethyl-2,6-diphenyl-7-(*p*-tolyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**33**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 4.0min #239



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
390.1965	1	C ₂₇ H ₂₄ N ₃	390.1965	-0.2	3.5	1	100.00	17.5	even	ok
412.1796	1	C ₂₇ H ₂₃ N ₃ Na	412.1784	-2.8	772.2	1	-1.#J	17.5	even	ok

Figure S109. 4-Ethyl-2,6-diphenyl-7-(*p*-tolyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**33**). HRMS (ESI-TOF).

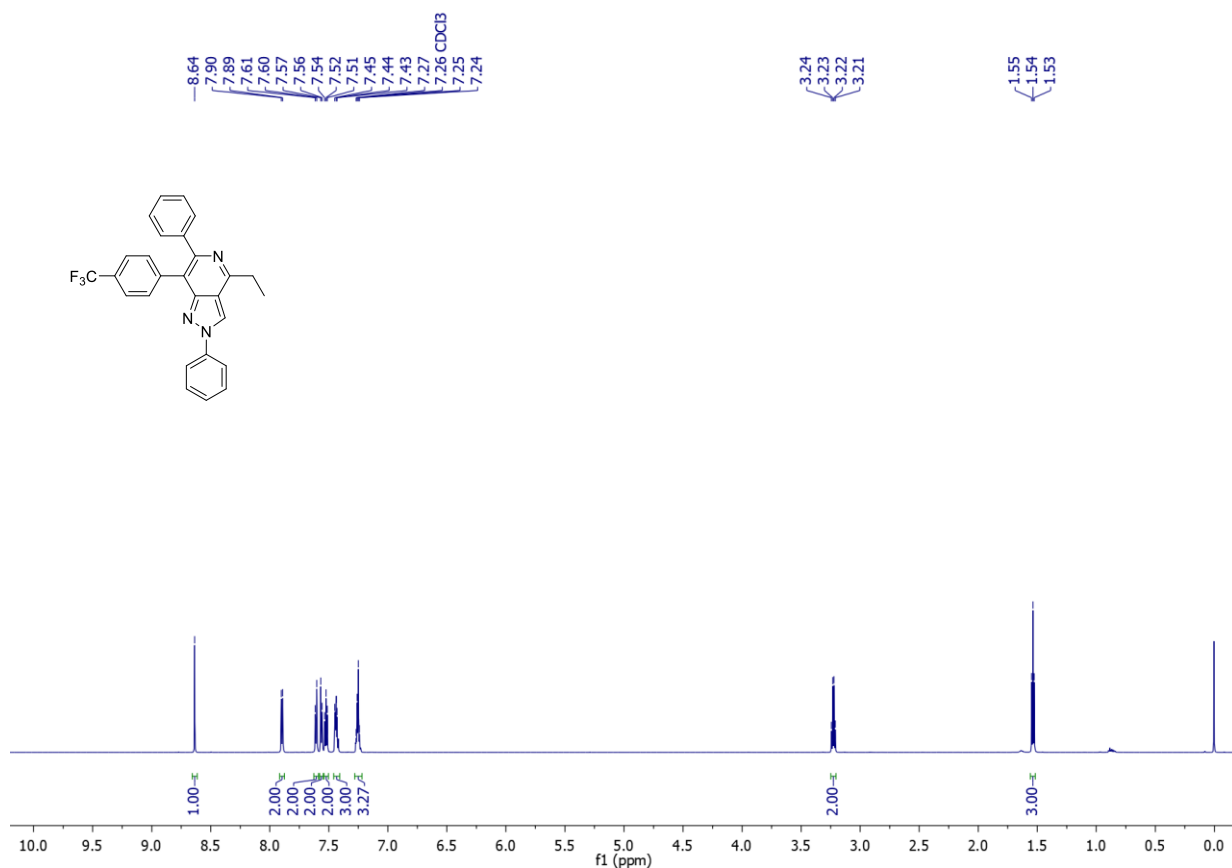


Figure S110. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethyl)phenyl)-2H-pyrazolo[4,3-c]pyridine (**34**). ¹H NMR spectrum (700 MHz, CDCl₃).

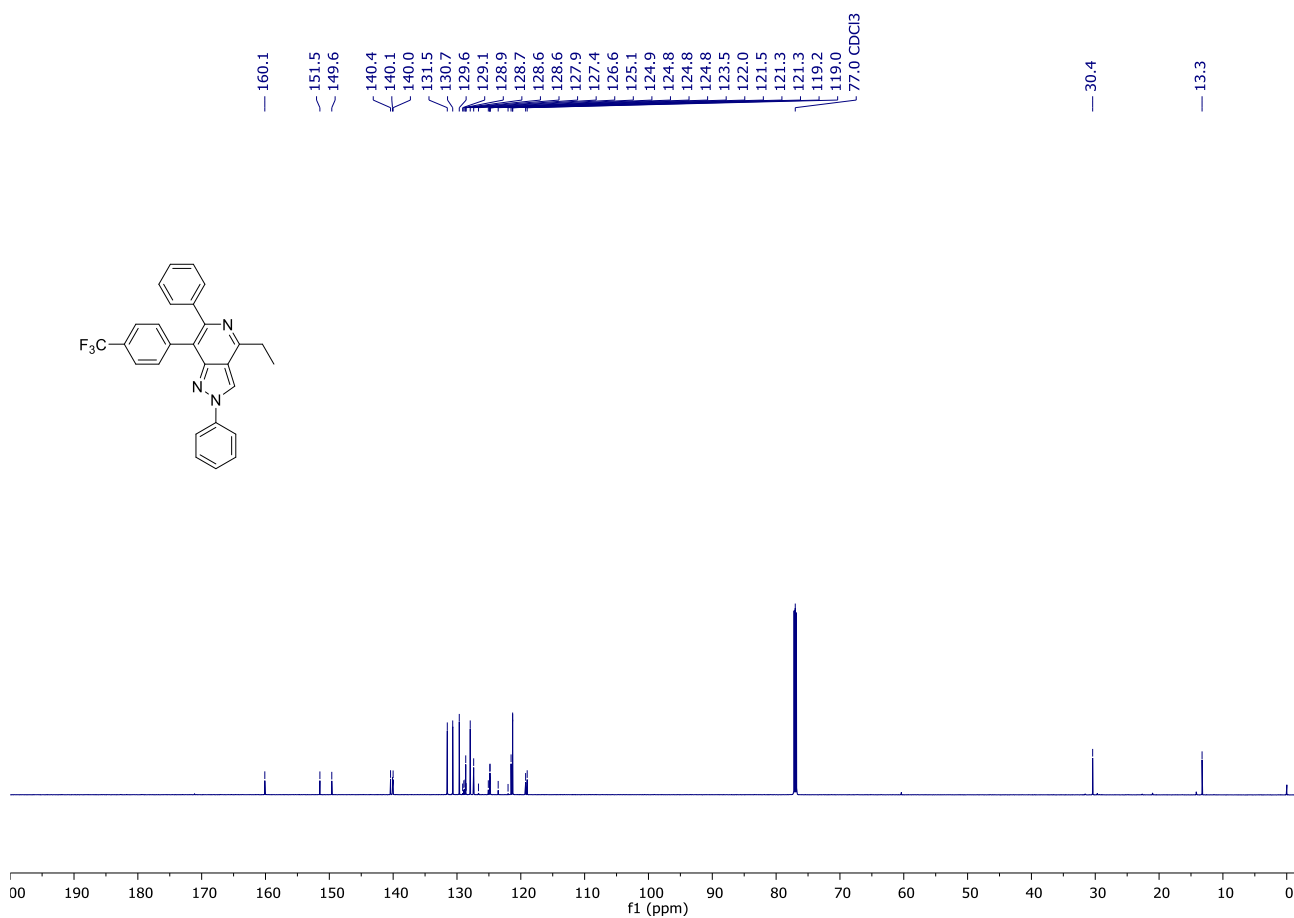


Figure S111. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethyl)phenyl)-2H-pyrazolo[4,3-c]pyridine (**34**). ¹³C NMR (176 MHz, CDCl₃).

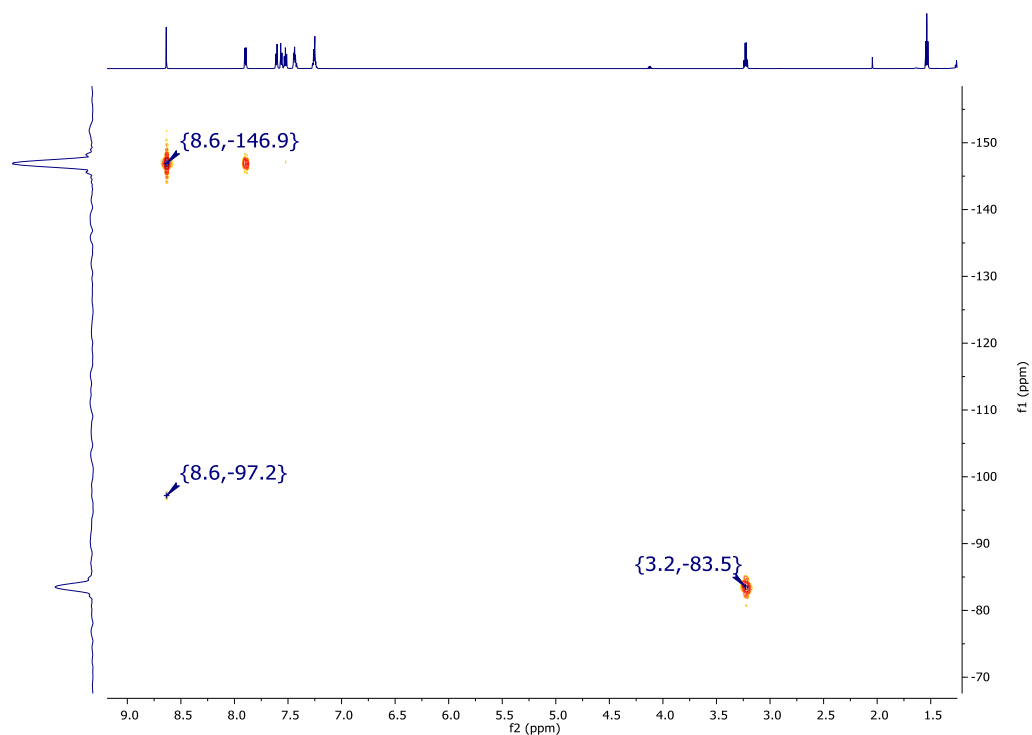


Figure S112. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethyl)phenyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**34**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

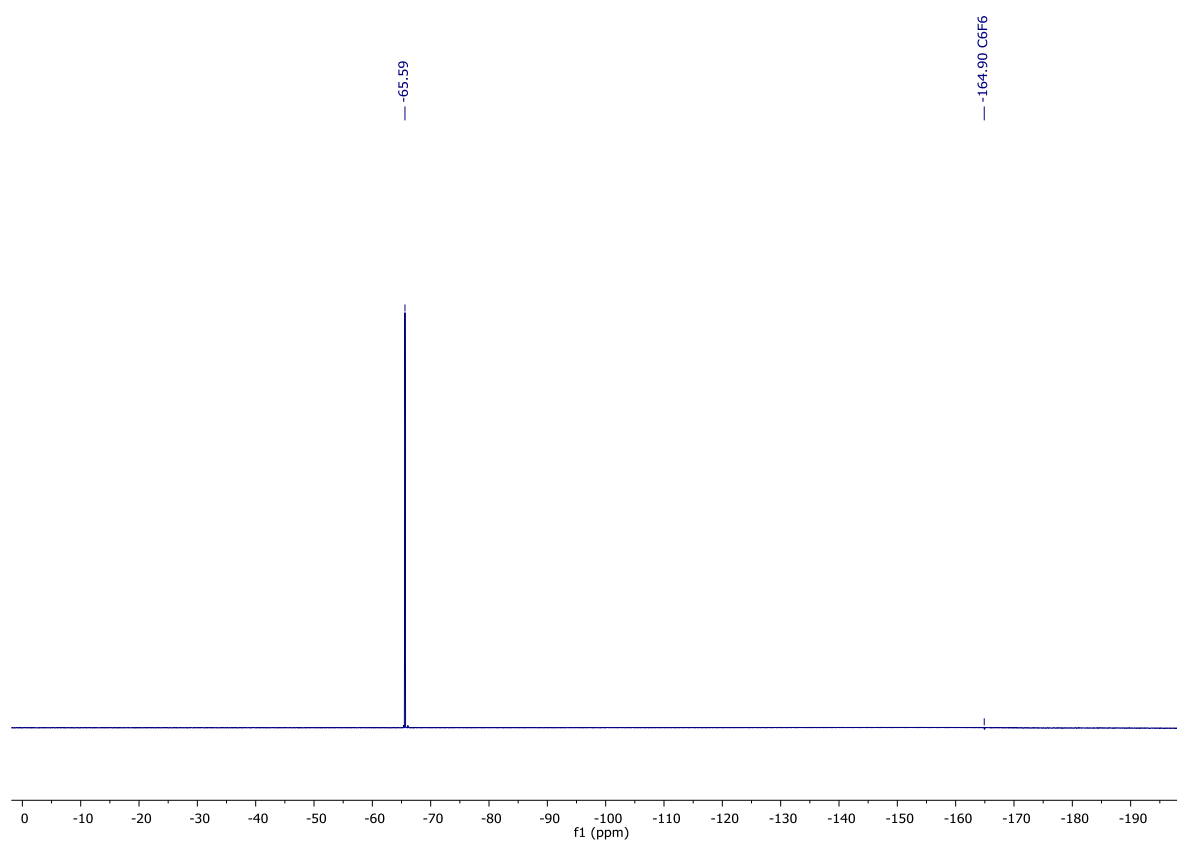


Figure S113. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethyl)phenyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**34**). ^{19}F NMR spectrum (500 MHz, CDCl_3).

+MS, 3.3min #200

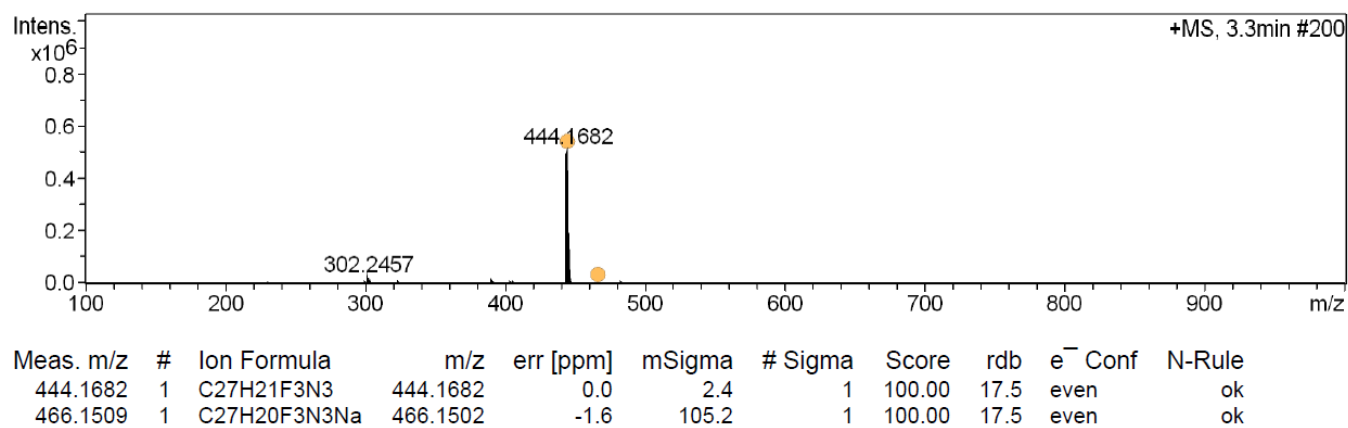


Figure S114. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethyl)phenyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**34**). HRMS (ESI-TOF).

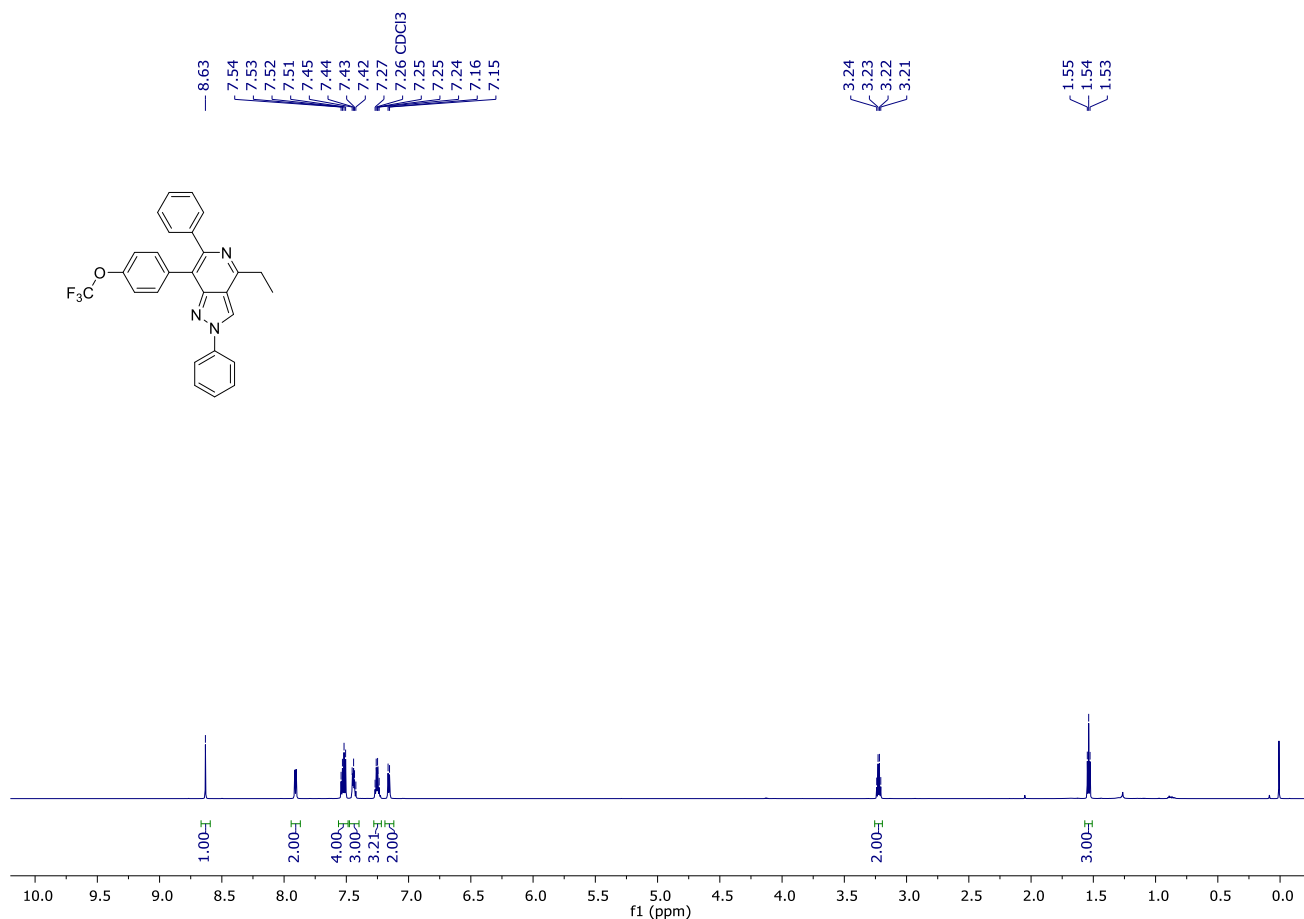


Figure S115. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethoxy)phenyl)-2H-pyrazolo[4,3-c]pyridine (35). ¹H NMR spectrum (700 MHz, CDCl₃).

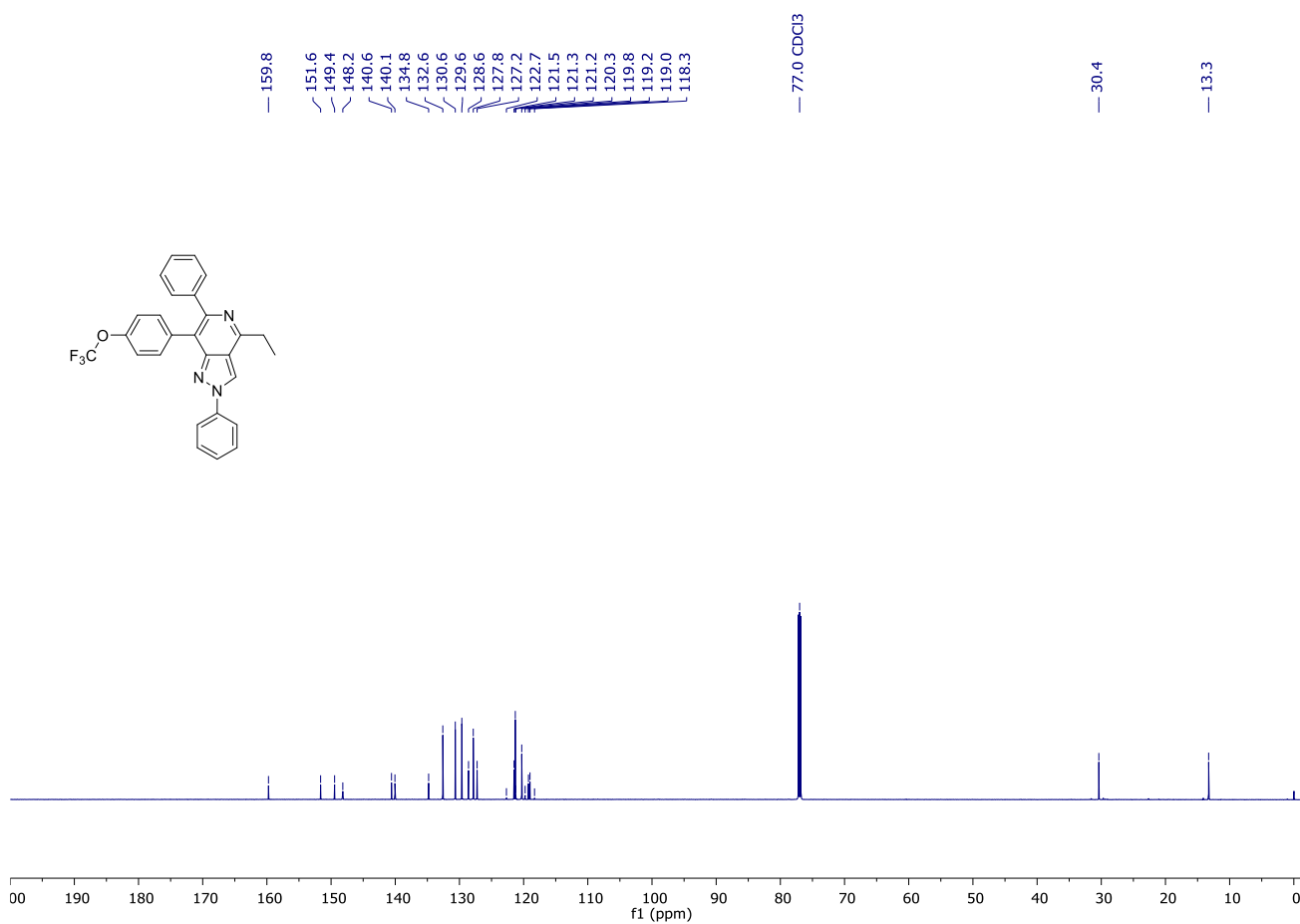


Figure S116. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethoxy)phenyl)-2H-pyrazolo[4,3-c]pyridine (35). ¹³C NMR (176 MHz, CDCl₃).

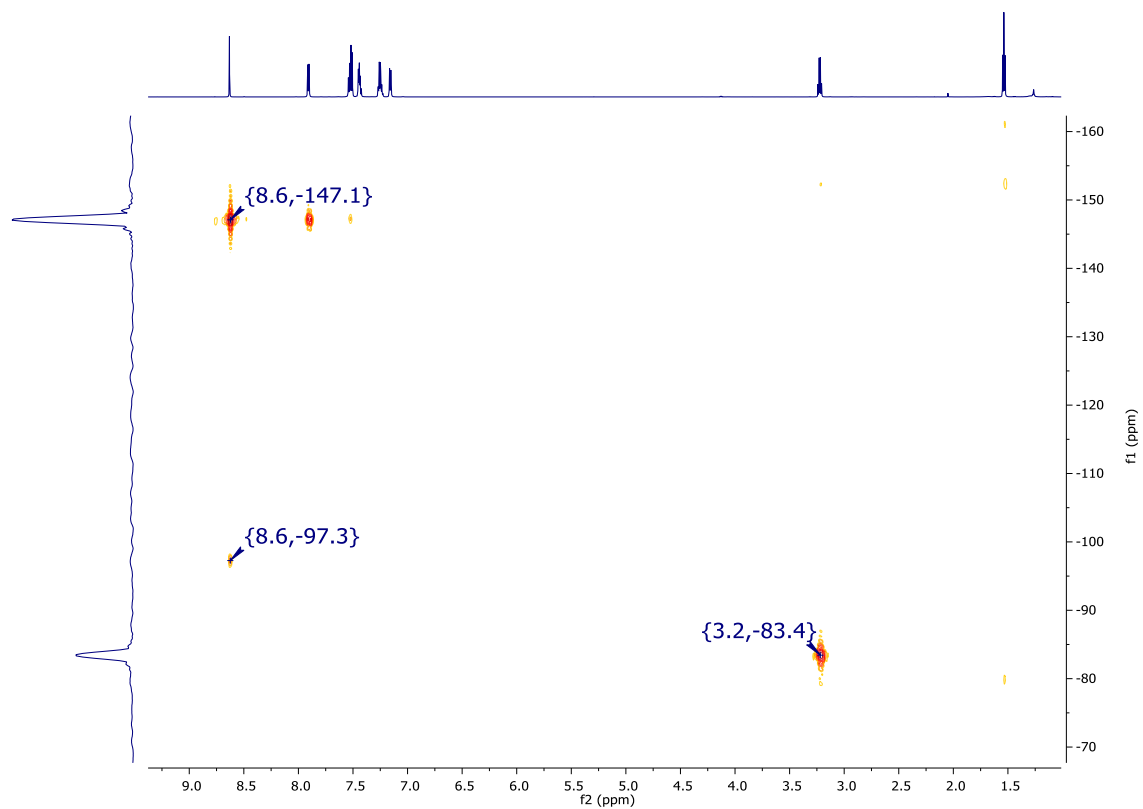


Figure S117. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethoxy)phenyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**35**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

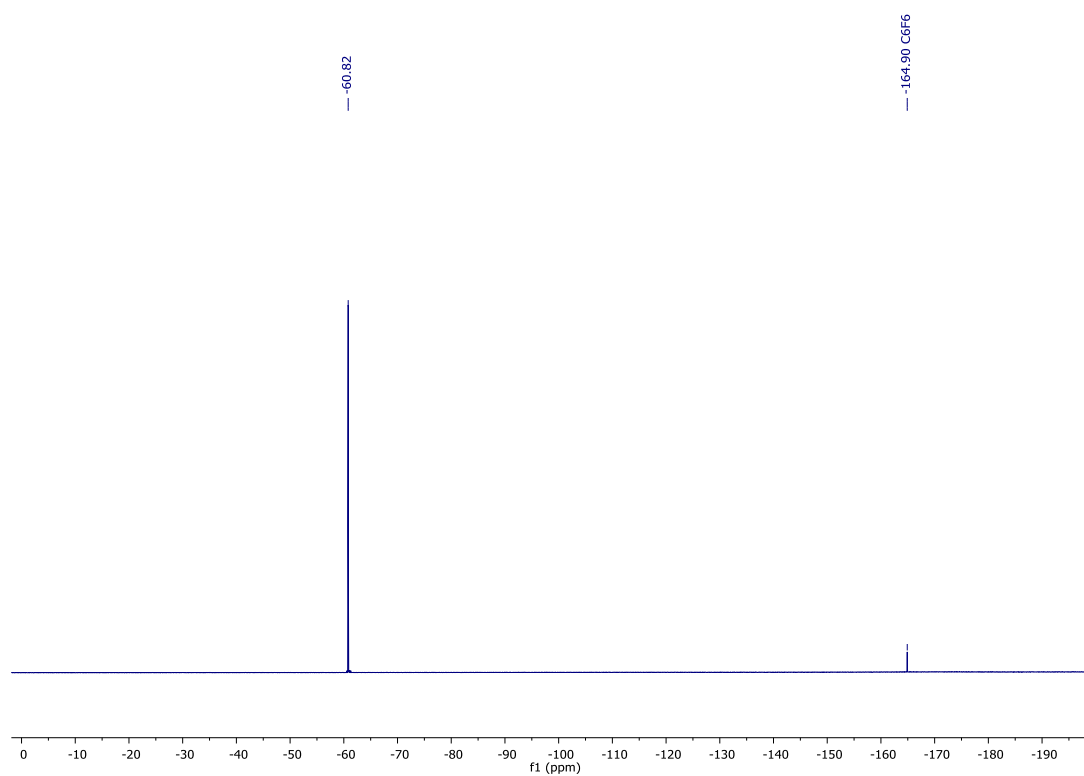
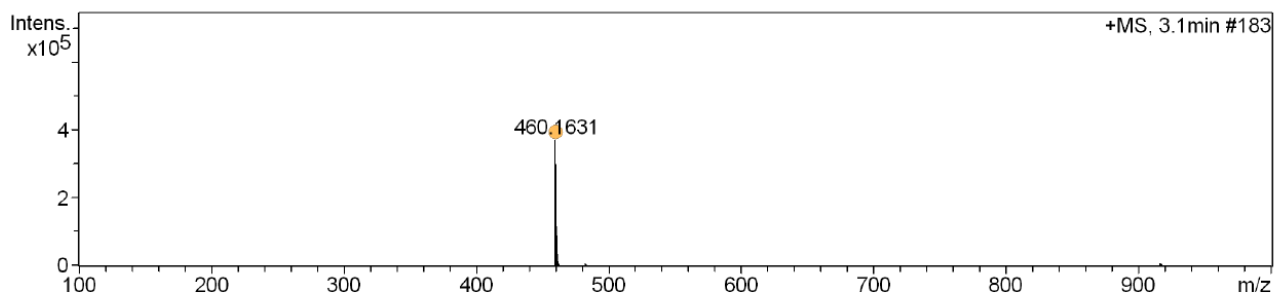


Figure S118. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethoxy)phenyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**35**). ^{19}F NMR spectrum (500 MHz, CDCl_3).

+MS, 3.1min #183



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻	Conf	N-Rule
460.1631	1	C ₂₇ H ₂₁ F ₃ N ₃ O	460.1631	0.1	5.5	1	100.00	17.5	even		ok

Figure S119. 4-Ethyl-2,6-diphenyl-7-(4-(trifluoromethoxy)phenyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**35**). HRMS (ESI-TOF).

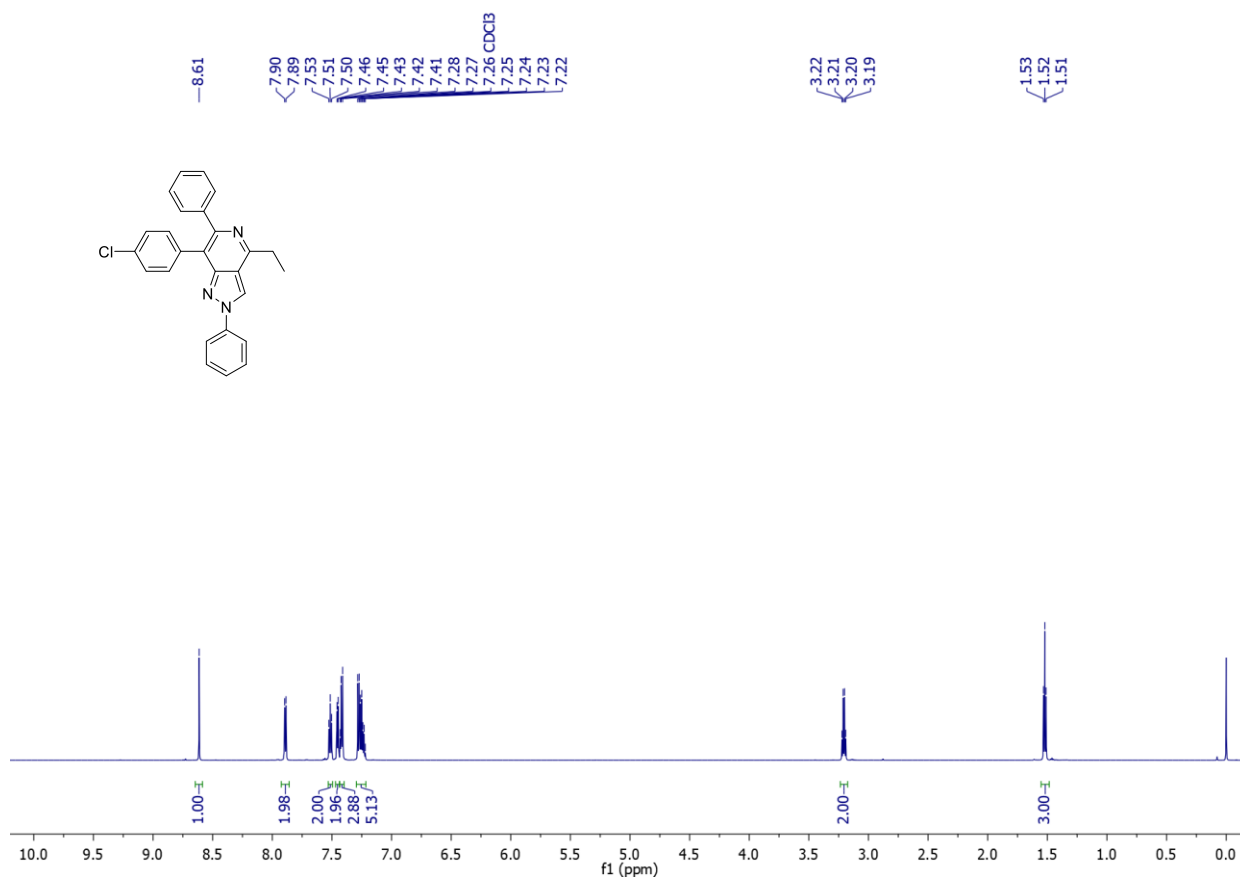


Figure S120. 7-(4-Chlorophenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**36**). ¹H NMR spectrum (700 MHz, CDCl₃).

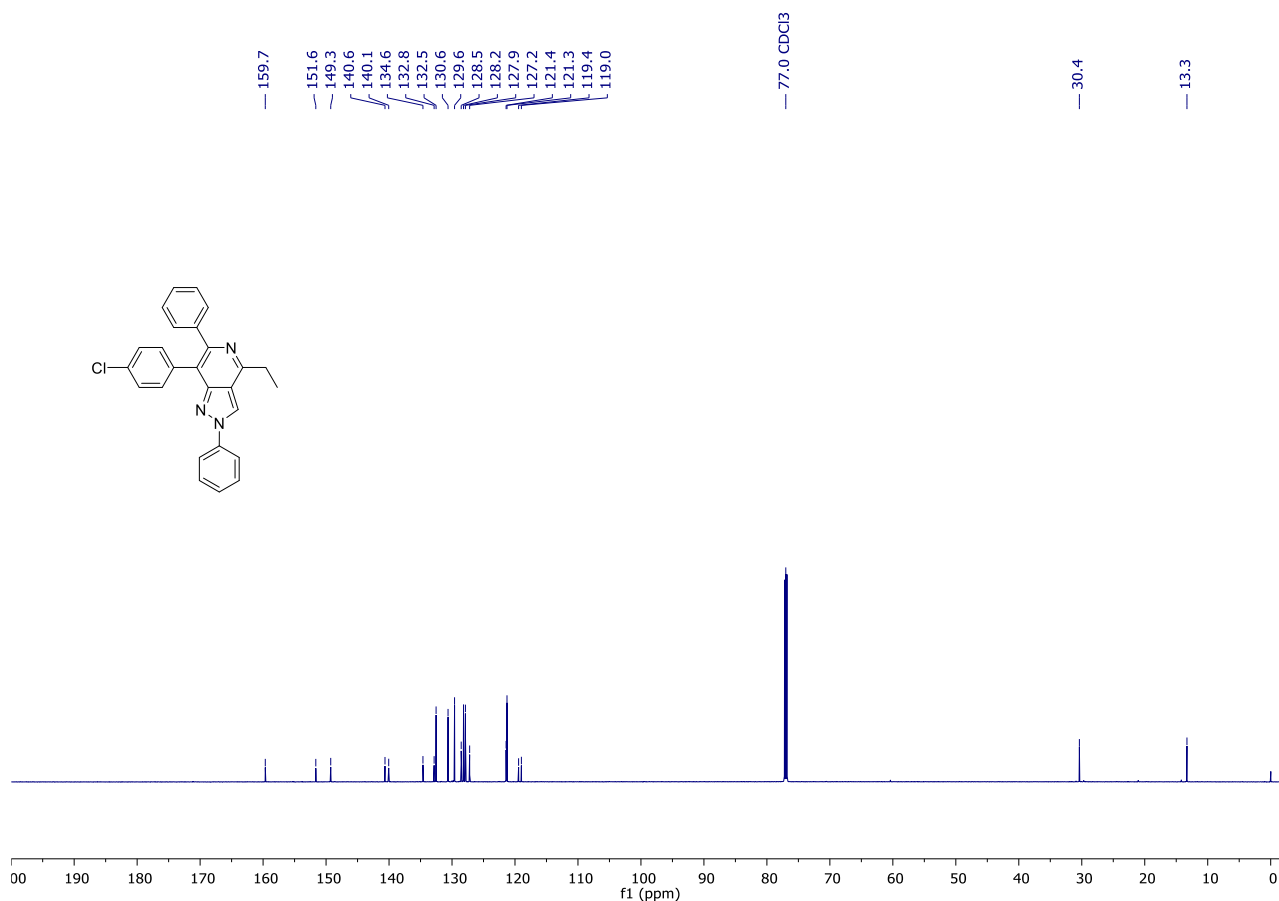


Figure S121. 7-(4-Chlorophenyl)-4-ethyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**36**). ^{13}C NMR (176 MHz, CDCl_3).

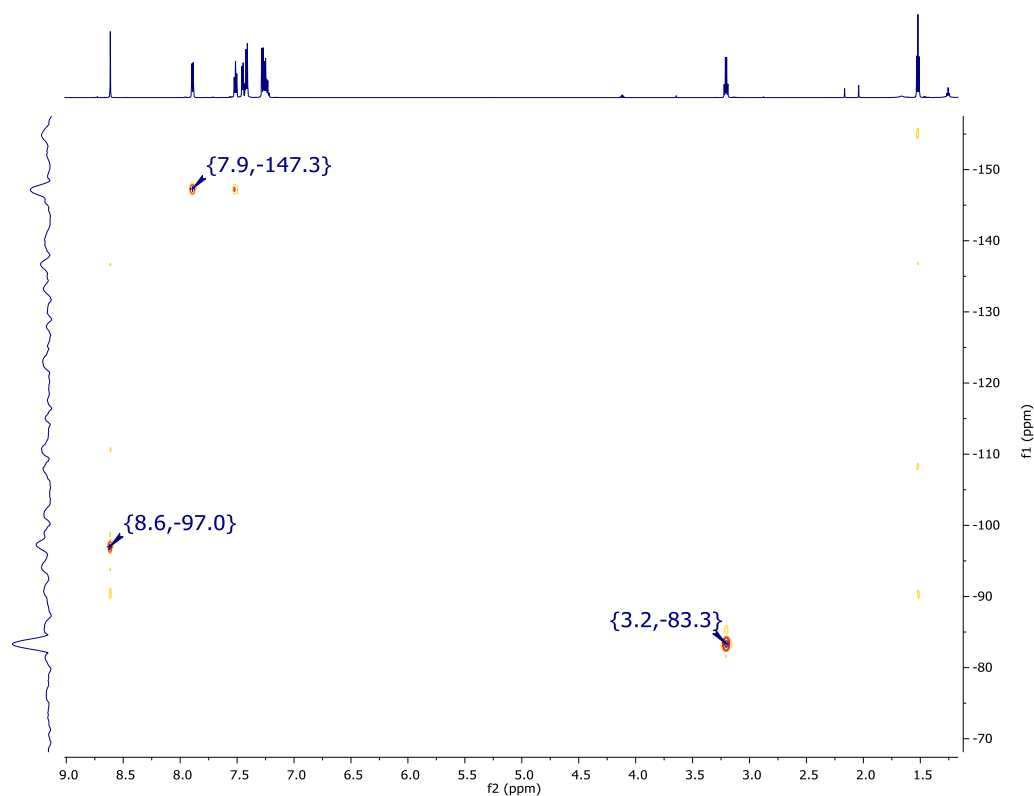


Figure S122. 7-(4-Chlorophenyl)-4-ethyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**36**). ^1H - ^{15}N LR HSQMBC spectrum (700 MHz, CDCl_3).

+MS, 3.0min #181

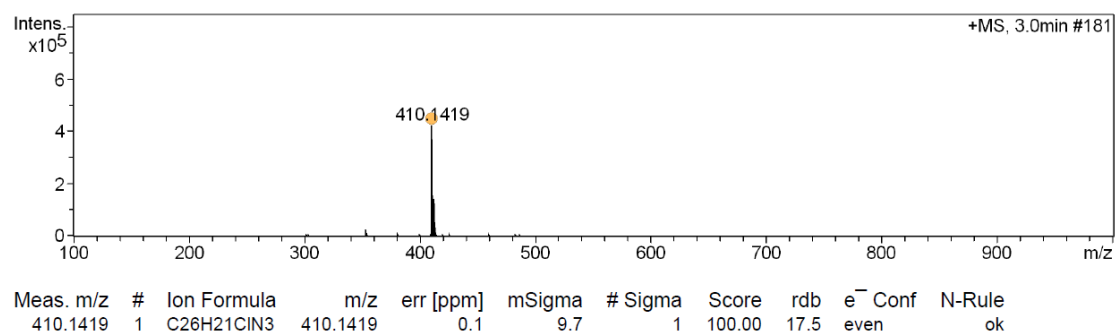


Figure S123. 7-(4-Chlorophenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**36**). HRMS (ESI-TOF).

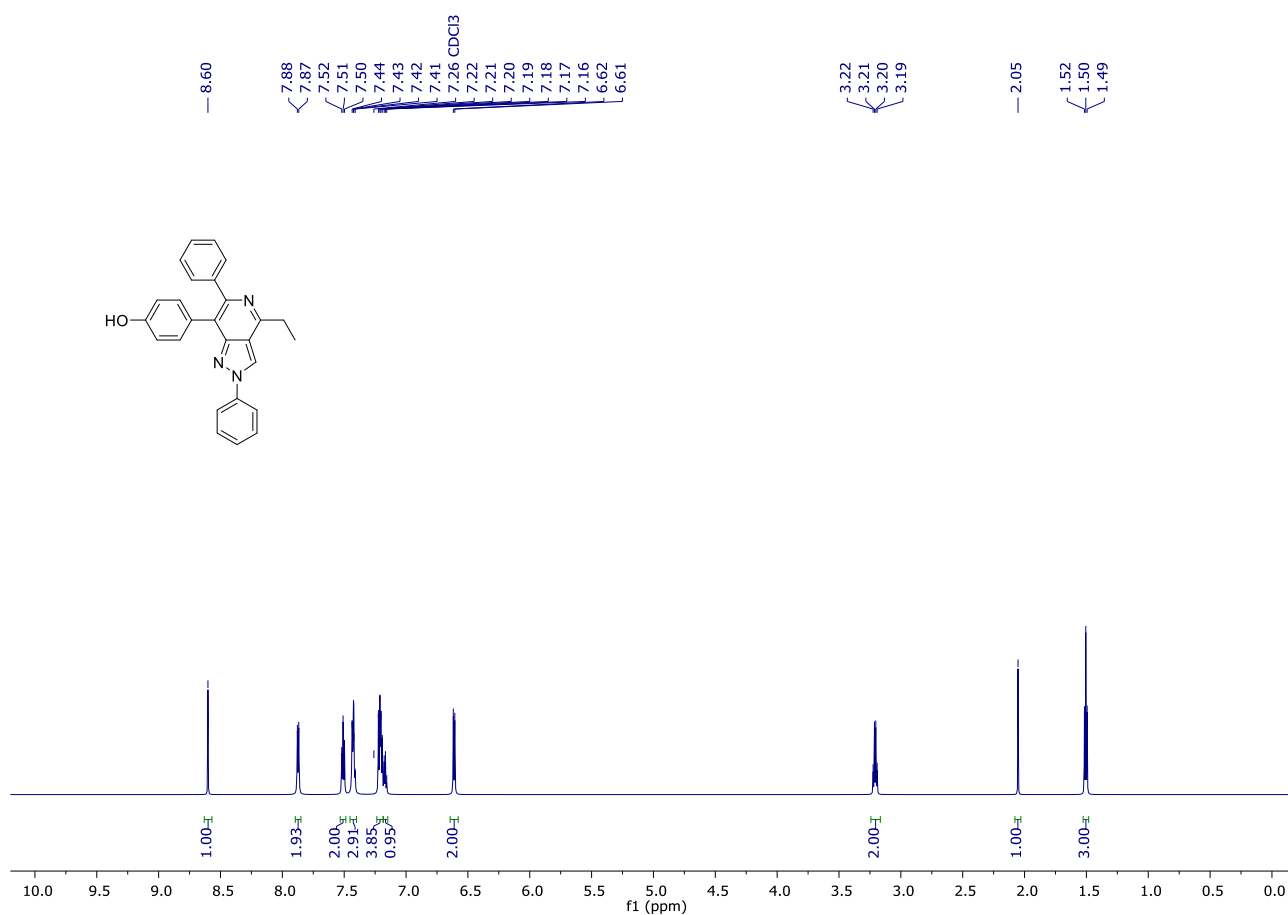


Figure S124. 4-(4-Ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridin-7-yl)phenol (**37**). ¹H NMR spectrum (700 MHz, CDCl₃).

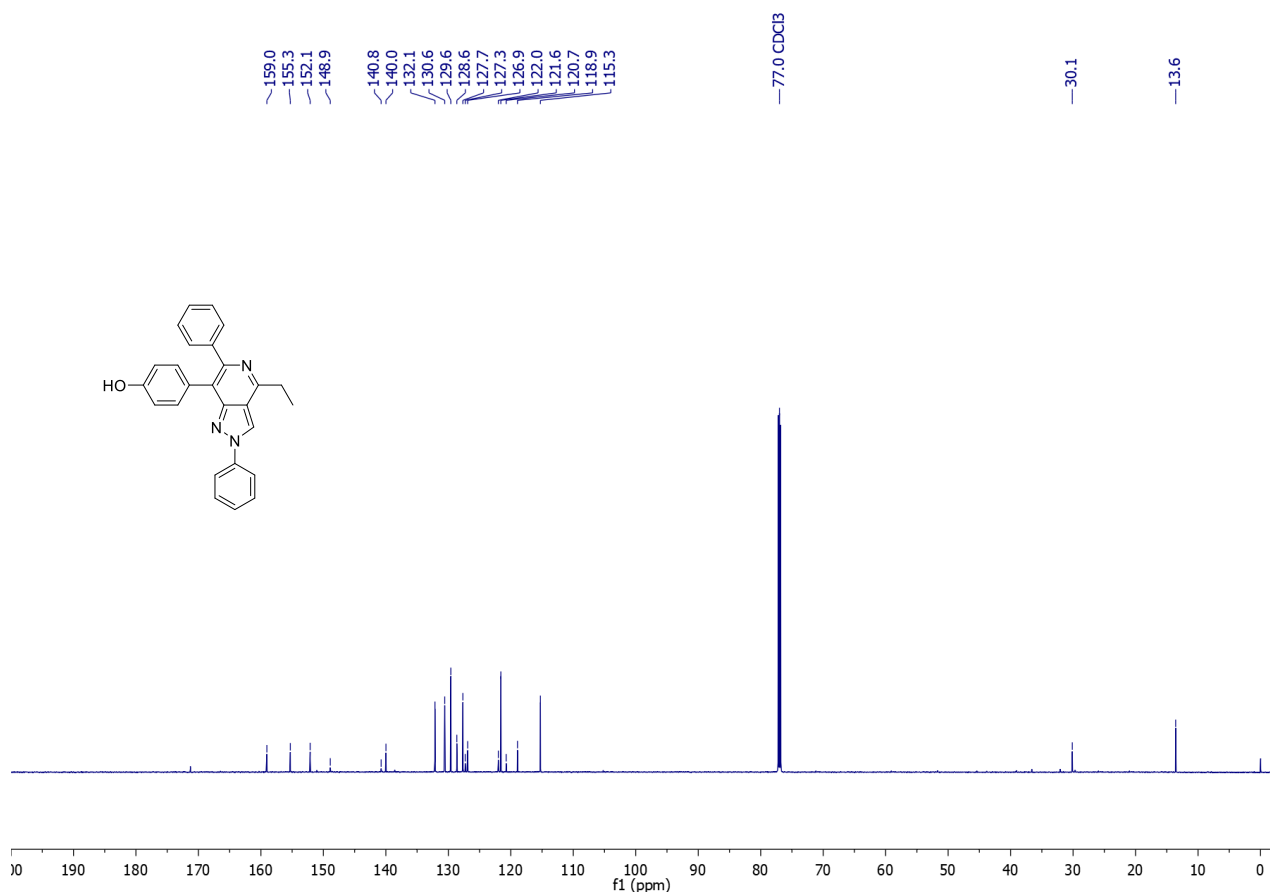


Figure S125. 4-(4-Ethyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridin-7-yl)phenol (37). ¹³C NMR (176 MHz, CDCl₃).

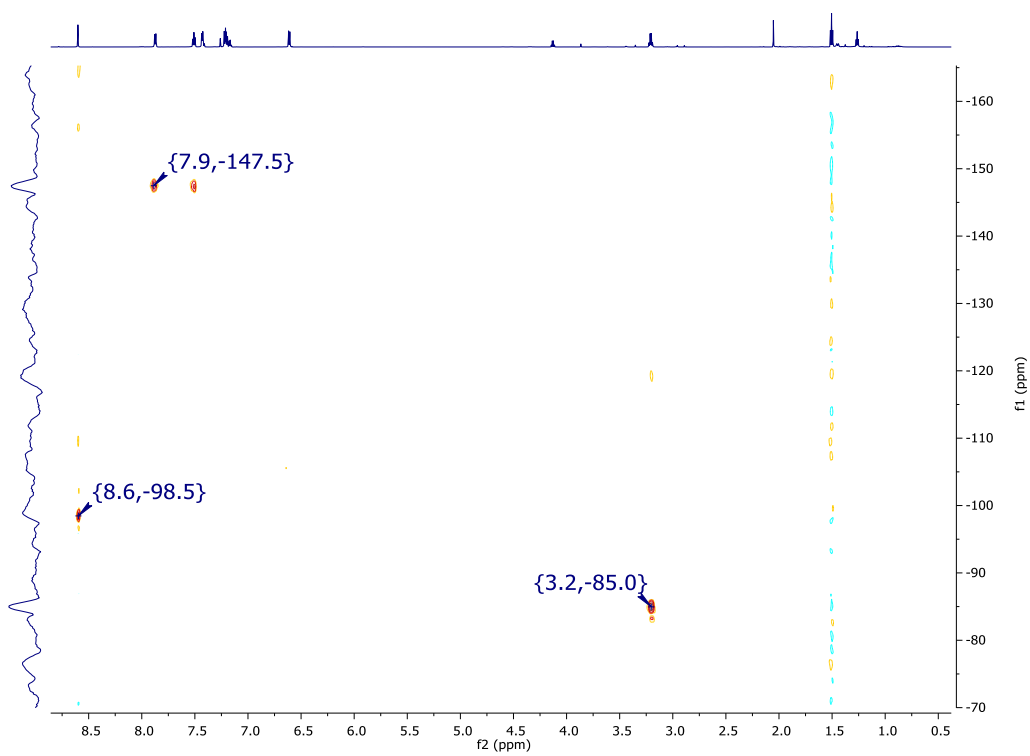
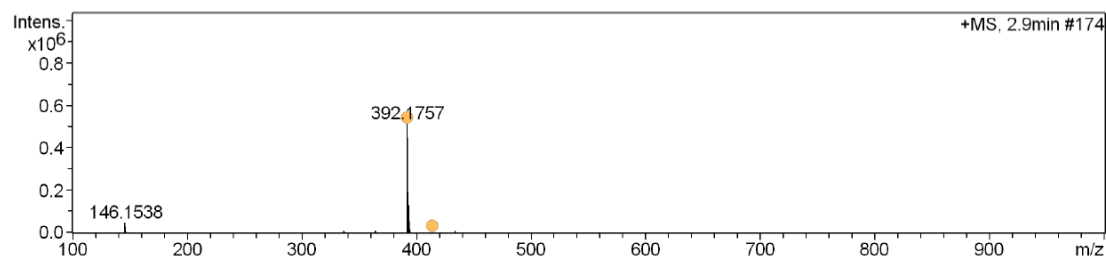


Figure S126. 4-(4-Ethyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridin-7-yl)phenol (37). ¹H-¹⁵N LR HSQMBBC spectrum (700 MHz, CDCl₃).

+MS, 2.9min #174



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
392.1757	1	C ₂₆ H ₂₂ N ₃ O	392.1757	-0.0	3.0	1	100.00	17.5	even	ok
414.1589	1	C ₂₆ H ₂₁ N ₃ NaO	414.1577	-2.8	41.5	1	100.00	17.5	even	ok

Figure S127. 4-(4-Ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridin-7-yl)phenol (**37**). HRMS (ESI-TOF).

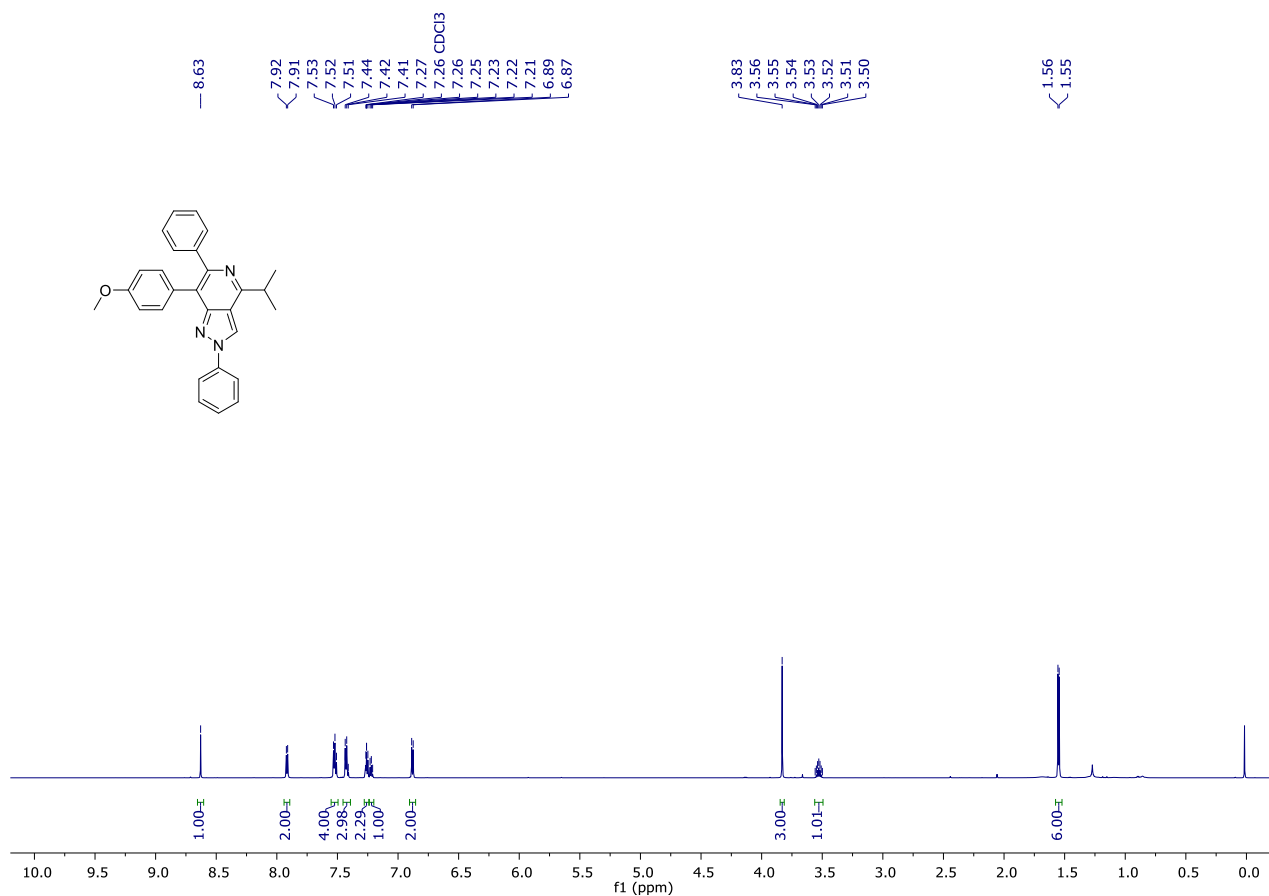


Figure S128. 4-Isopropyl-7-(4-methoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**38**). ¹H NMR spectrum (700 MHz, CDCl₃).

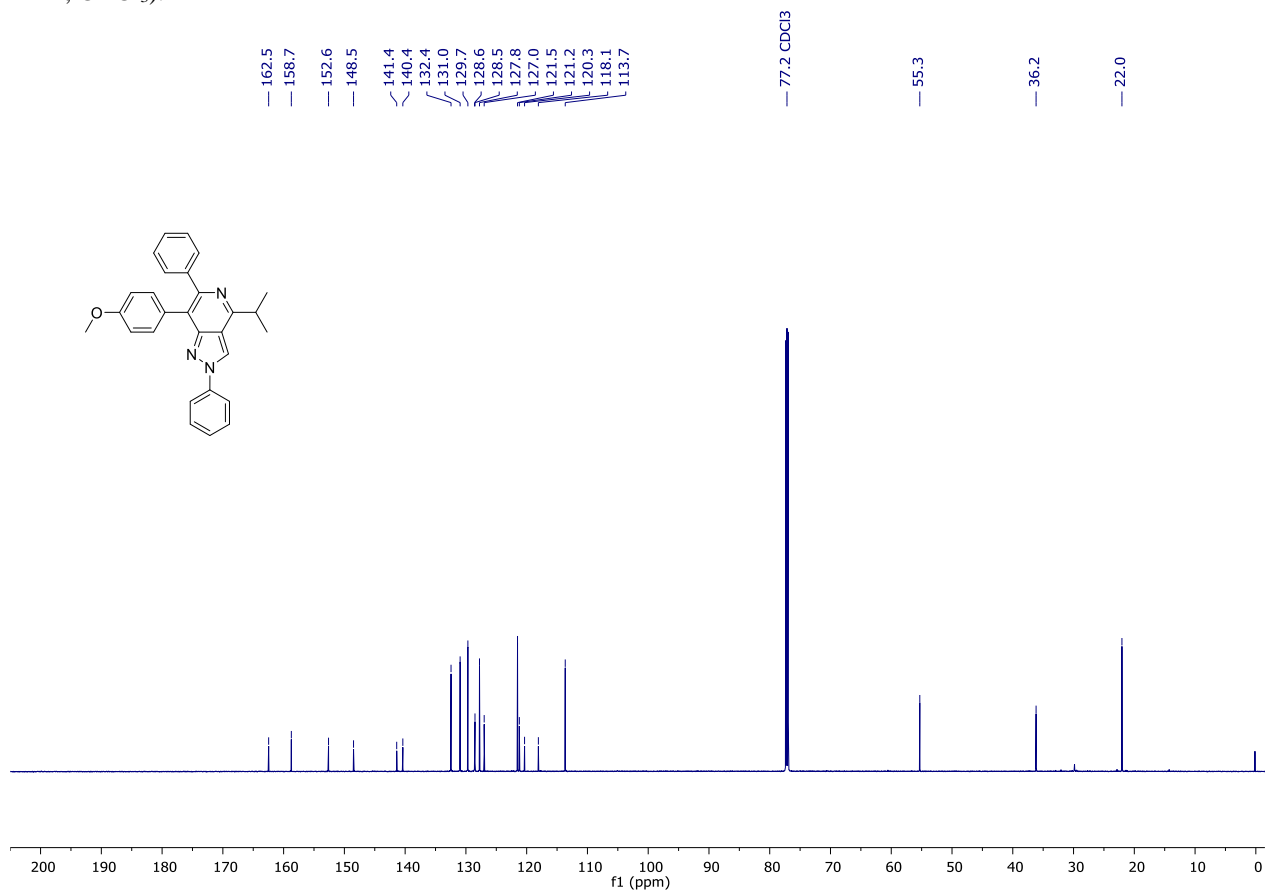


Figure S129. 4-Isopropyl-7-(4-methoxyphenyl)-4-methyl-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**38**). ¹³C NMR (176 MHz, CDCl₃).

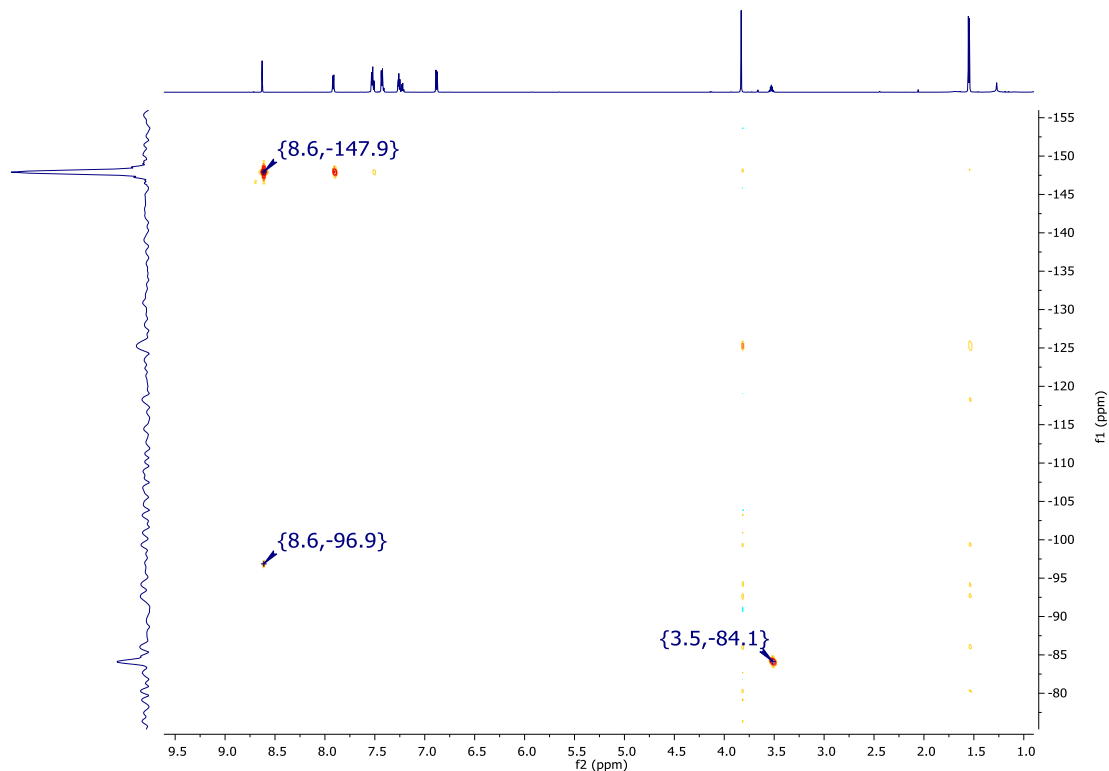
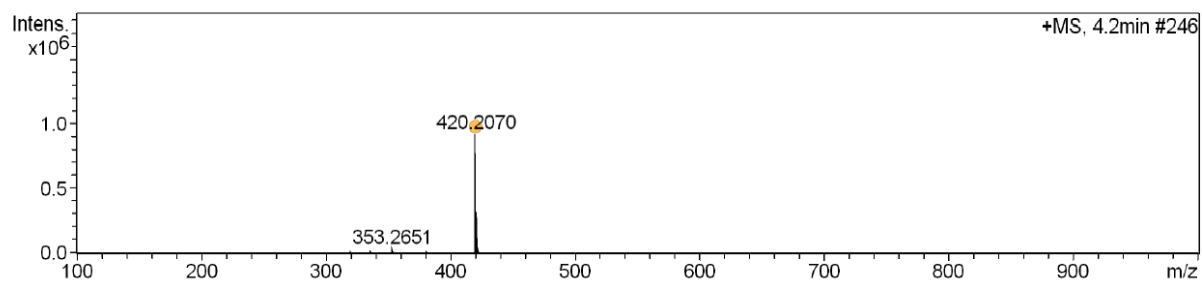


Figure S130. 4-Isopropyl-7-(4-methoxyphenyl)-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**38**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 4.2min #246



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e^-	Conf	N-Rule
420.2070	1	C ₂₈ H ₂₆ N ₃ O	420.2070	-0.0	17.8	1	100.00	17.5	even		ok

Figure S131. 4-Isopropyl-7-(4-methoxyphenyl)-4-methyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**38**). HRMS (ESI-TOF).

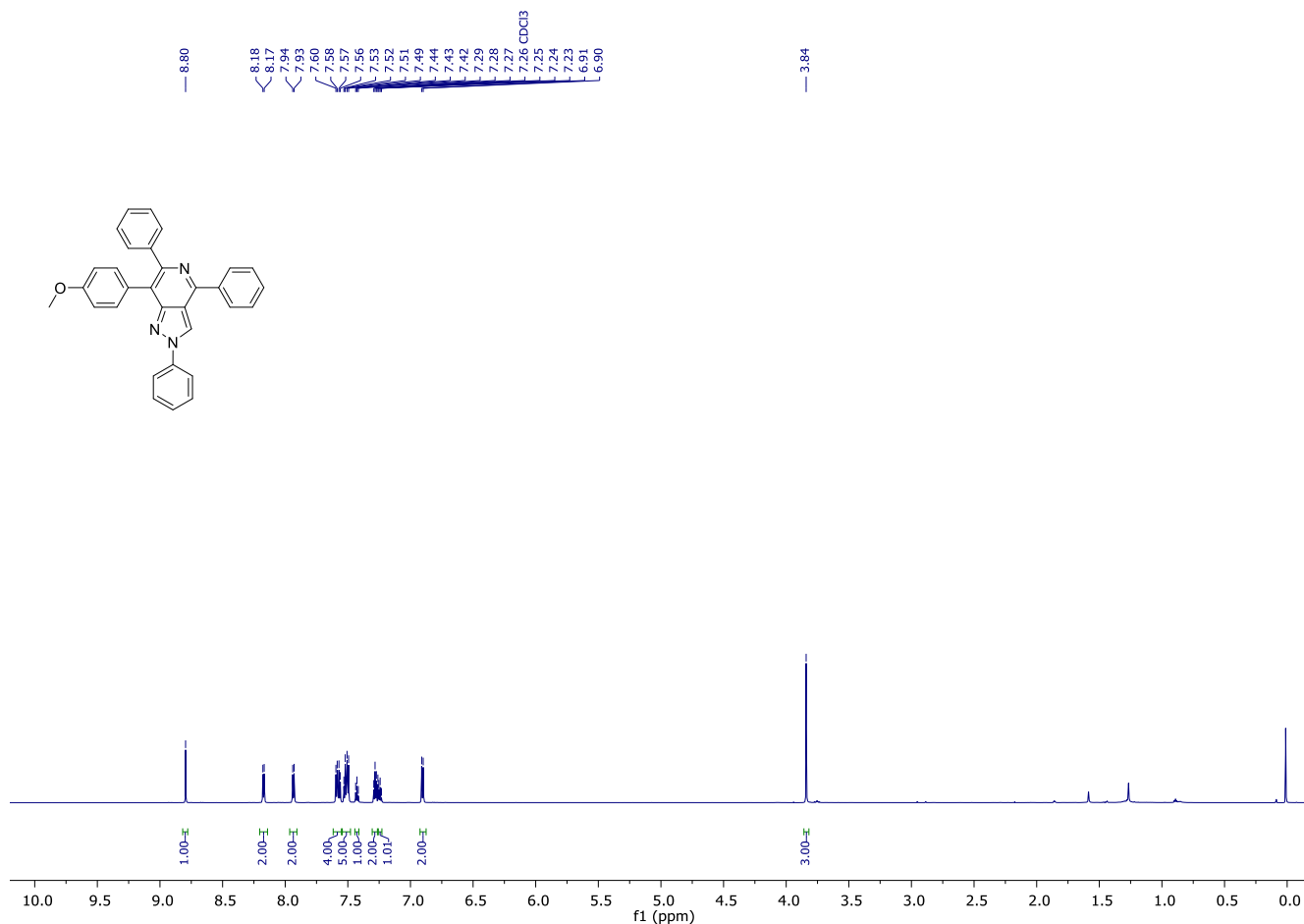


Figure S132. 7-(4-Methoxyphenyl)-2,4,6-triphenyl-2H-pyrazolo[4,3-c]pyridine (**39**). ¹H NMR spectrum (700 MHz, CDCl₃).

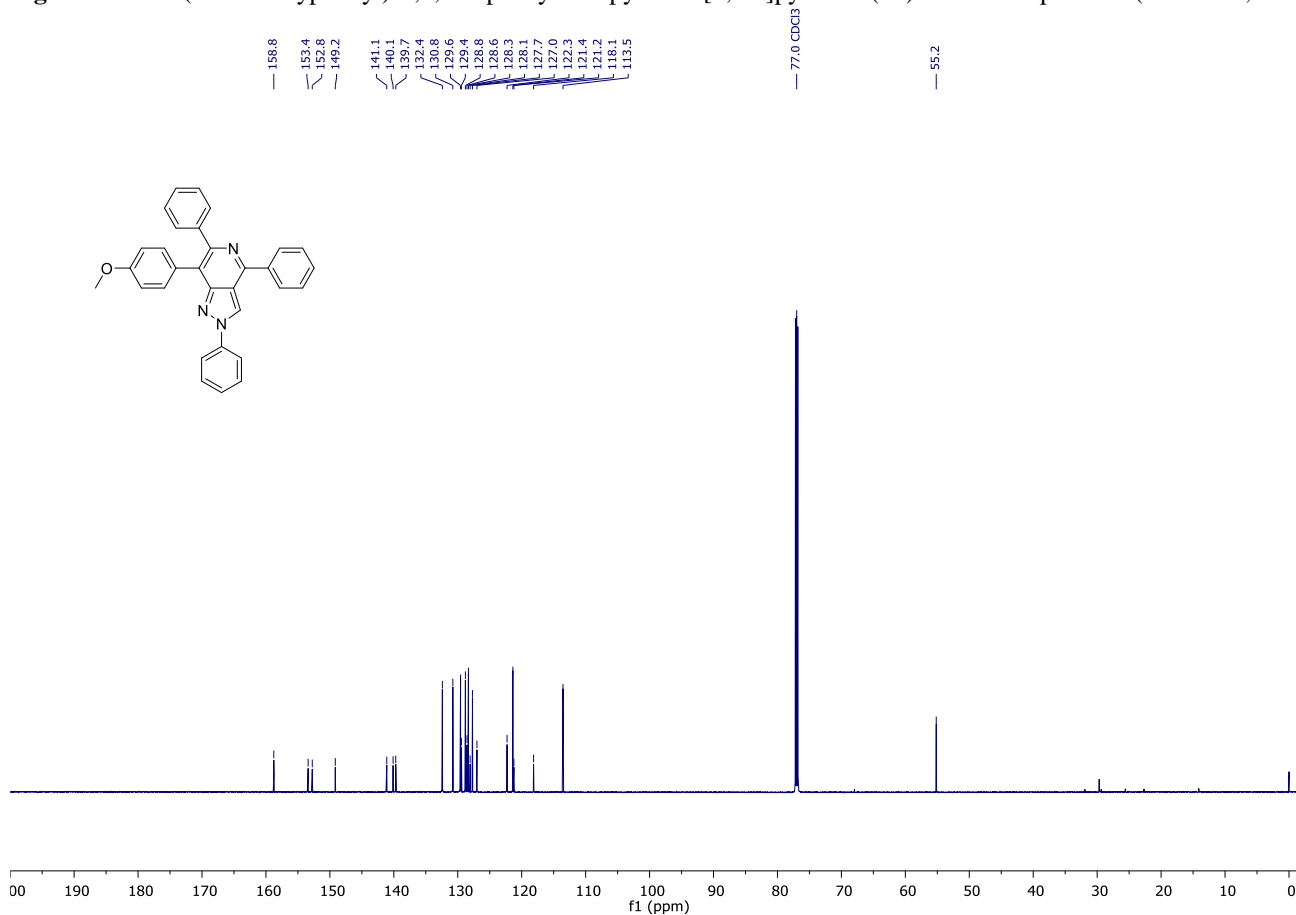


Figure S133. 7-(4-Methoxyphenyl)-2,4,6-triphenyl-2H-pyrazolo[4,3-c]pyridine (**39**). ¹³C NMR (176 MHz, CDCl₃).

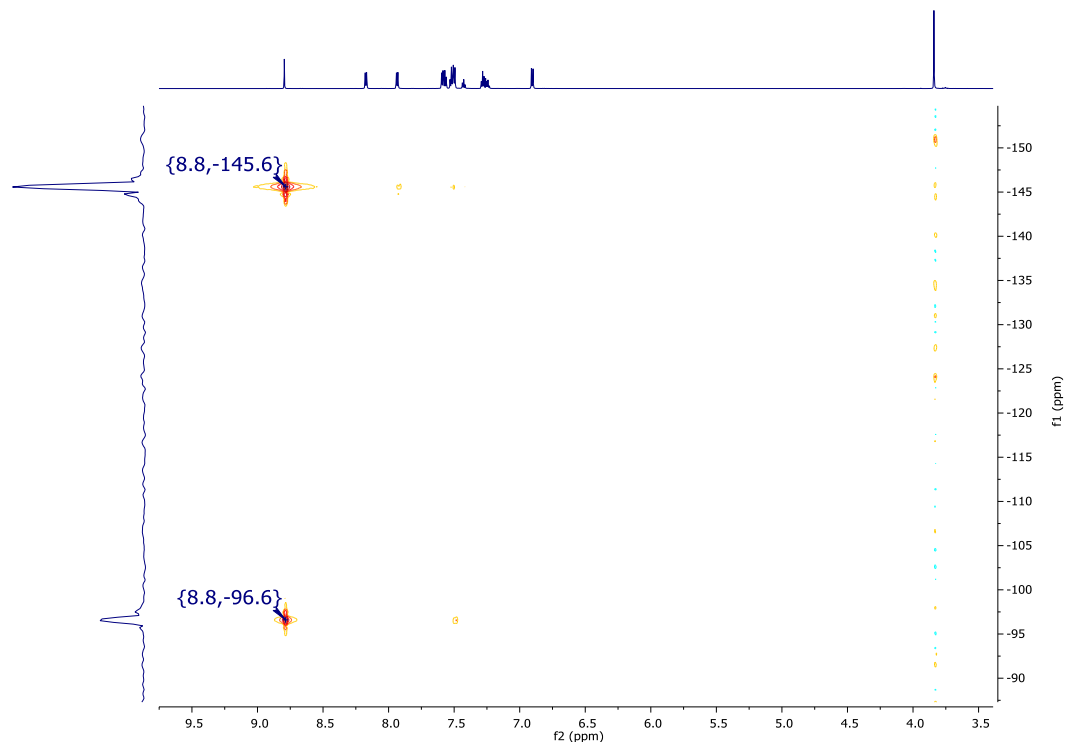
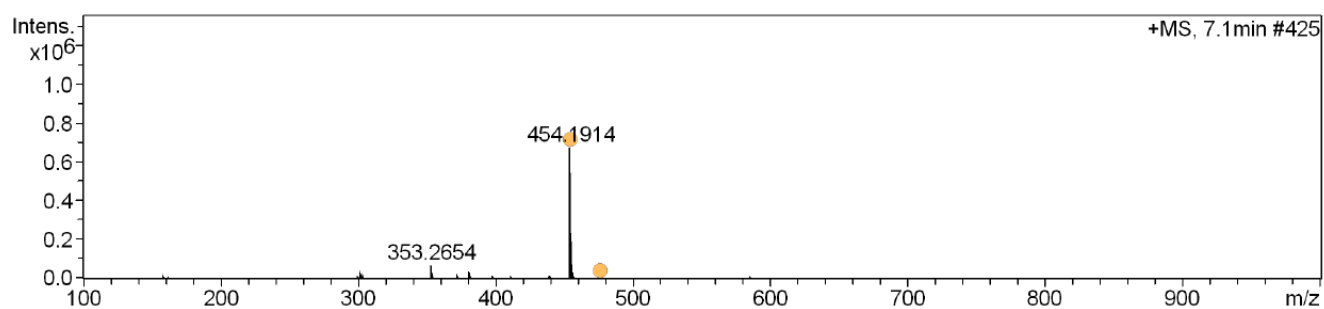


Figure S134. 7-(4-Methoxyphenyl)-2,4,6-triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**39**). ^1H - ^{15}N LR HSQMBBC spectrum (700 MHz, CDCl_3).

+MS, 7.1min #425



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
454.1914	1	C ₃₁ H ₂₄ N ₃ O	454.1914	0.0	1.4	1	100.00	21.5	even	ok
476.1721	1	C ₃₁ H ₂₃ N ₃ NaO	476.1733	2.6	107.0	1	100.00	21.5	even	ok

Figure S135. 7-(4-Methoxyphenyl)-2,4,6-triphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**39**). HRMS (ESI-TOF).

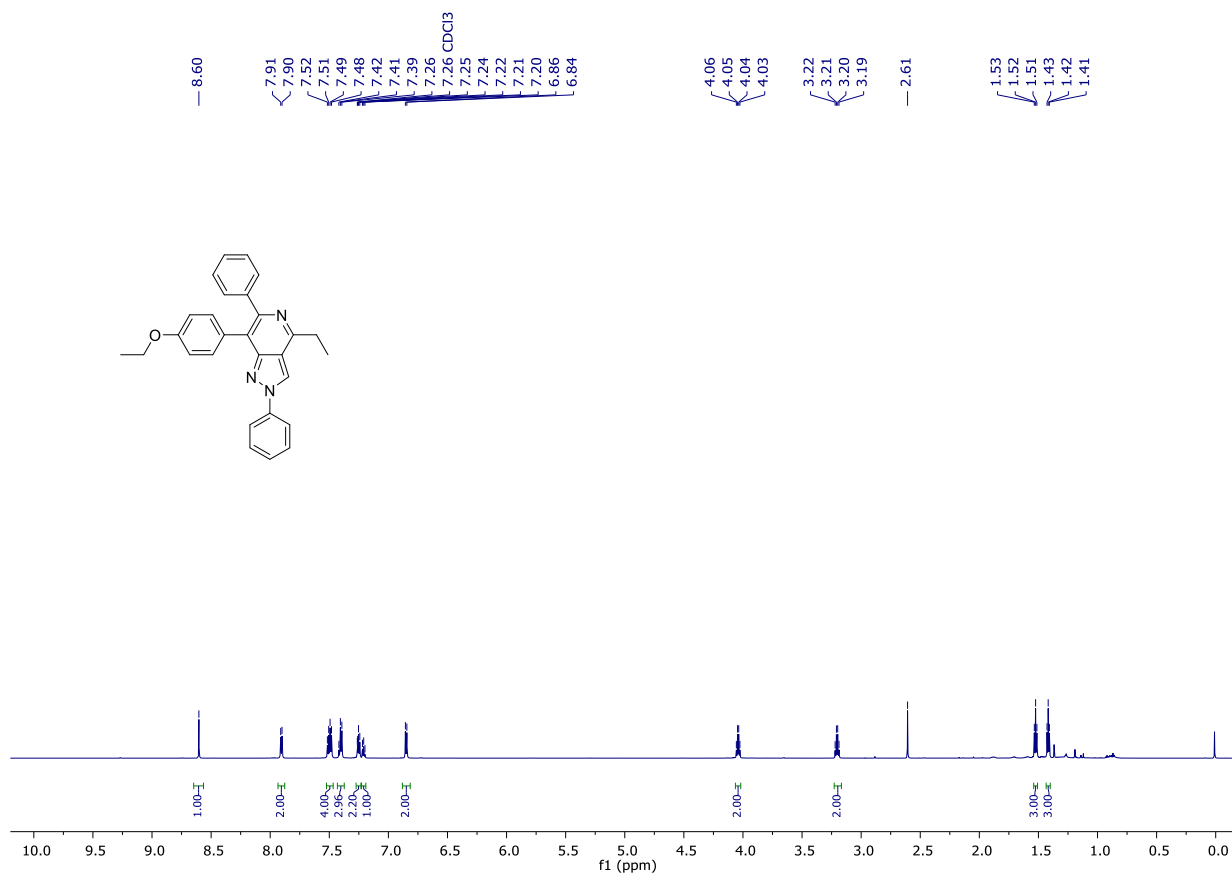


Figure S136. 7-(4-Ethoxyphenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**40**). ¹H NMR spectrum (700 MHz, CDCl₃).

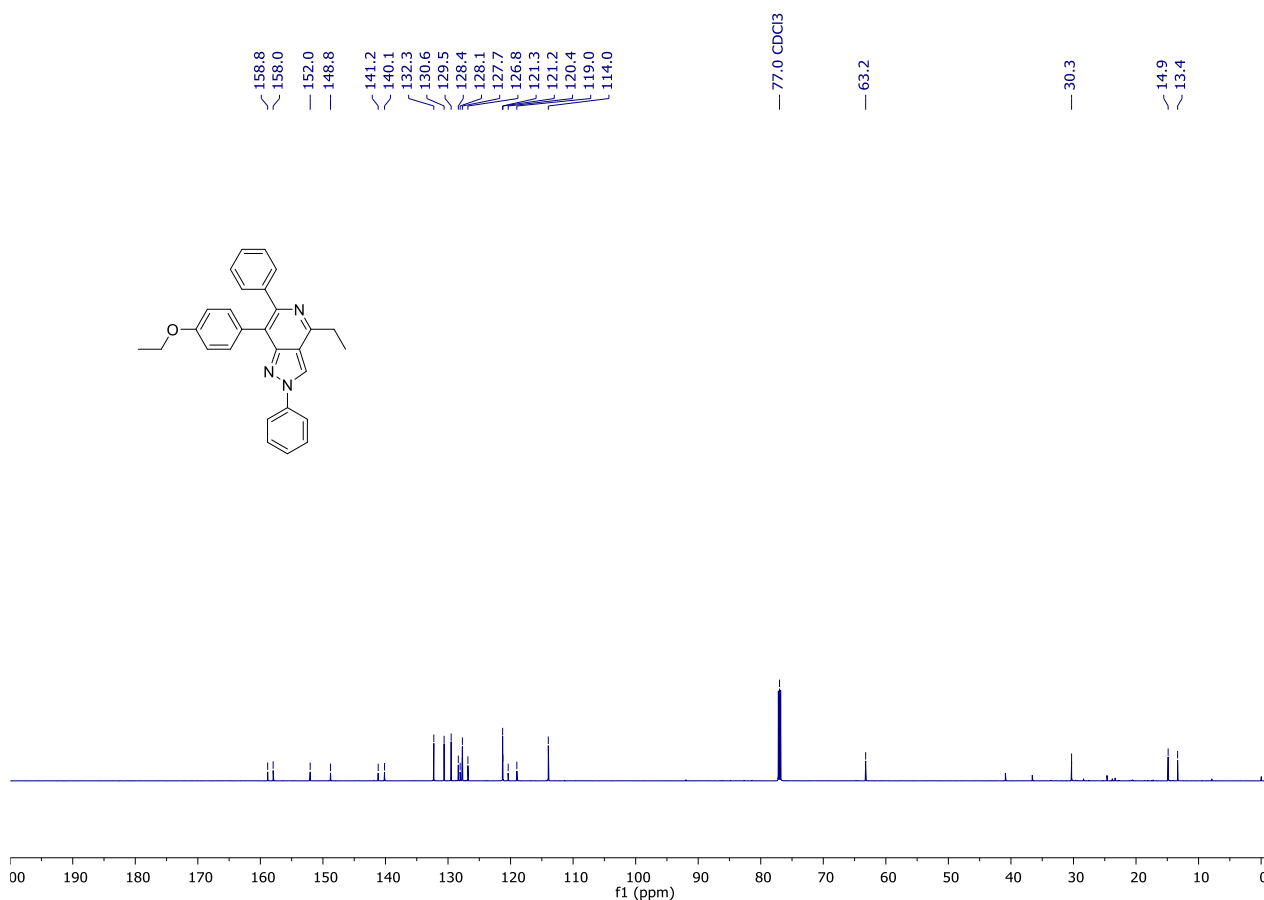


Figure S137. 7-(4-Ethoxyphenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**40**). ¹³C NMR (176 MHz, CDCl₃).

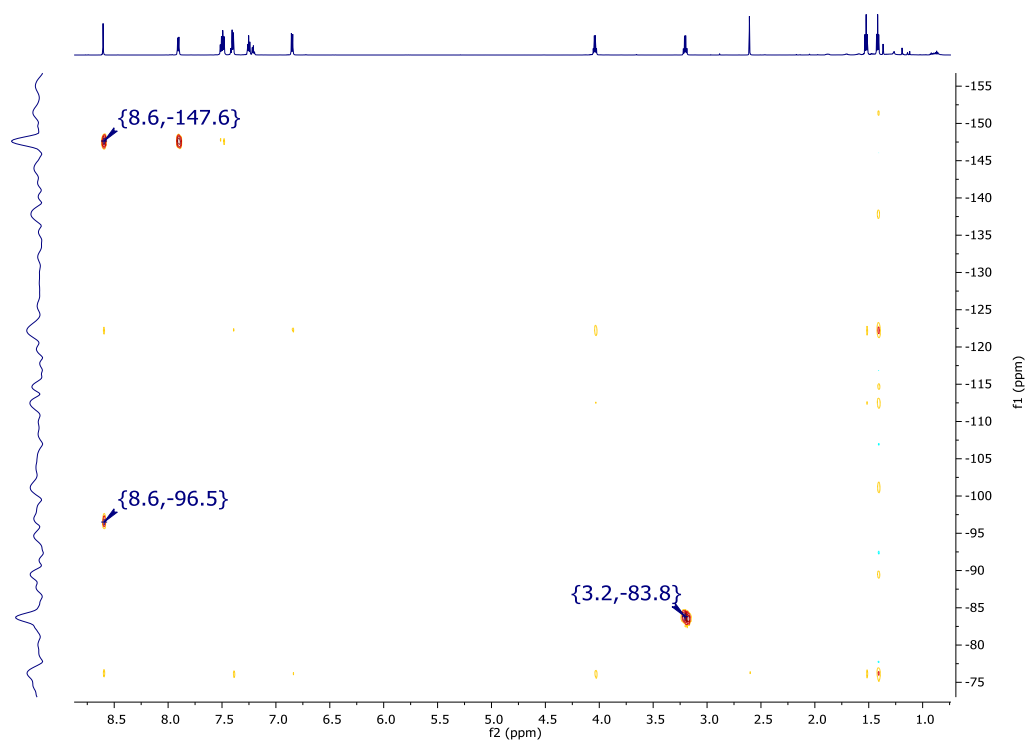
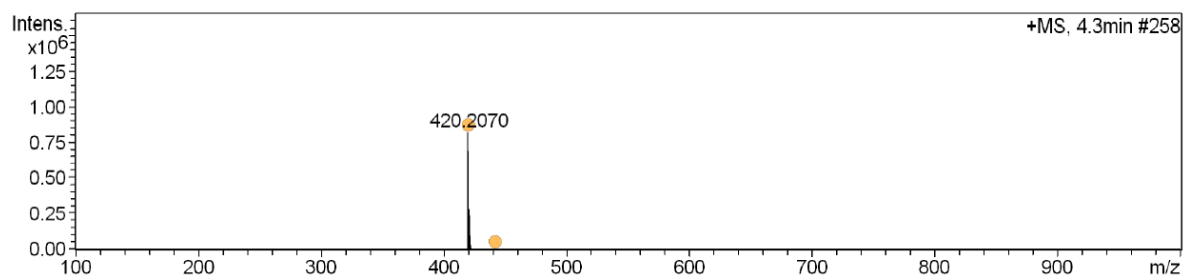


Figure S138. 7-(4-Ethoxyphenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**40**). ^1H - ^{15}N LR HSQMBBC spectrum (700 MHz, CDCl_3).

+MS, 4.3min #258



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻	Conf	N-Rule
420.2070	1	C ₂₈ H ₂₆ N ₃ O	420.2070	-0.1	14.5	1	100.00	17.5	even		ok
442.1894	1	C ₂₈ H ₂₅ N ₃ NaO	442.1890	-1.0	34.0	1	100.00	17.5	even		ok

Figure S139. 7-(4-Ethoxyphenyl)-4-ethyl-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**40**). HRMS (ESI-TOF).

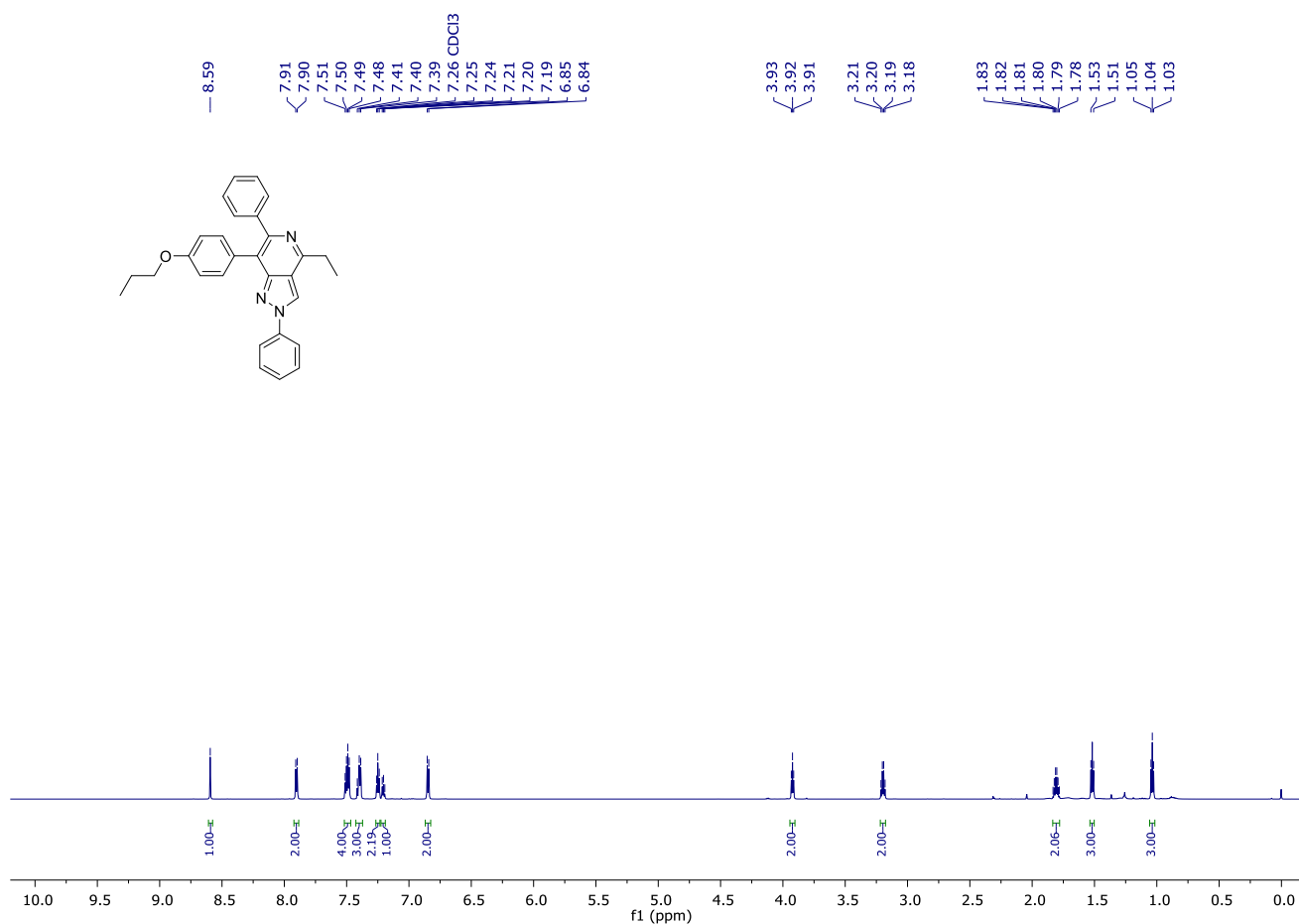


Figure S140. 4-Ethyl-2,6-diphenyl-7-(4-propoxyphenyl)-2H-pyrazolo[4,3-c]pyridine (**41**). ¹H NMR spectrum (700 MHz, CDCl₃).

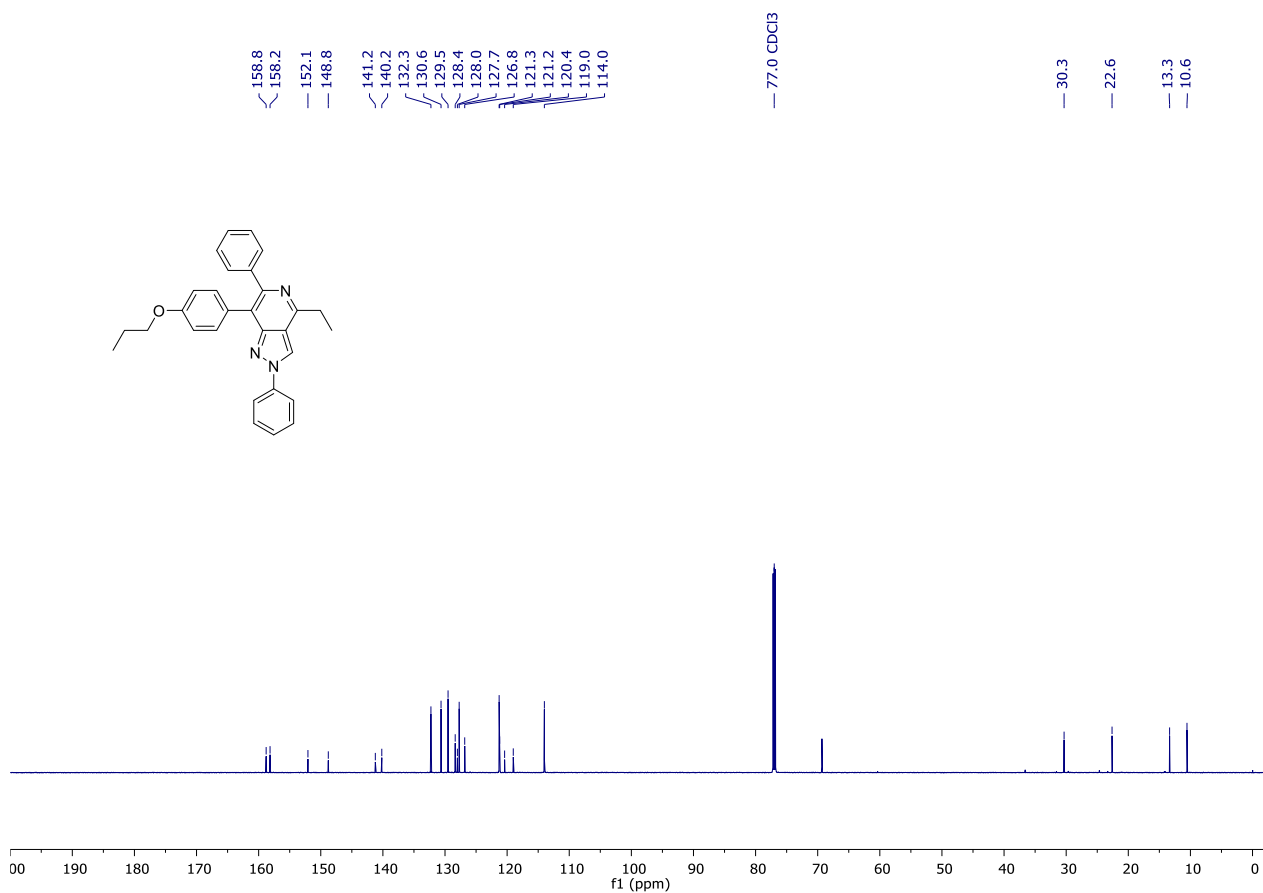


Figure S141. 4-Ethyl-2,6-diphenyl-7-(4-propoxyphenyl)-2H-pyrazolo[4,3-c]pyridine (**41**). ¹³C NMR (176 MHz, CDCl₃).

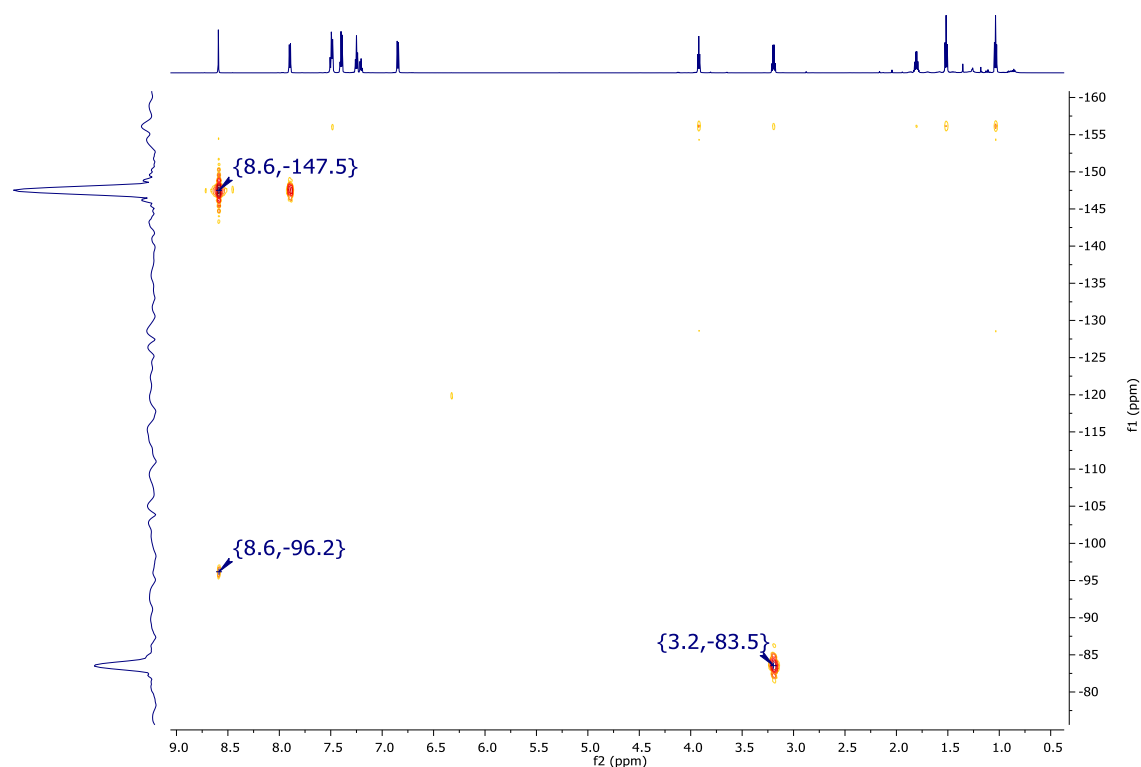
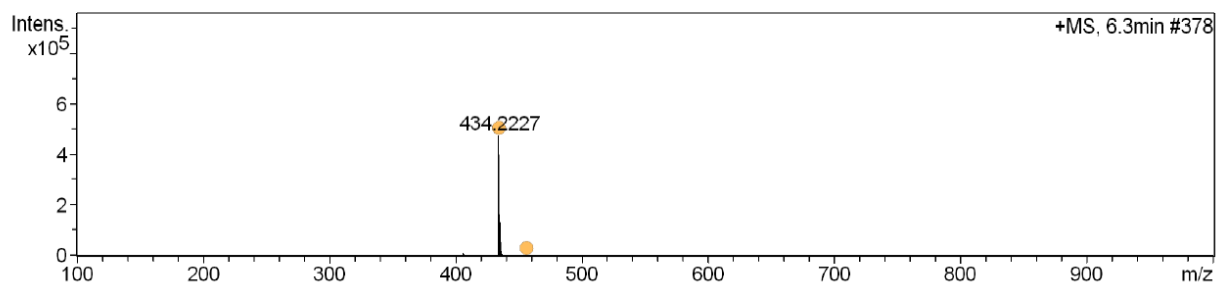


Figure S142. 4-Ethyl-2,6-diphenyl-7-(4-propoxyphenyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**41**). ^1H - ^{15}N HMBC spectrum (700 MHz, CDCl_3).

+MS, 6.3min #378



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e^- Conf	N-Rule
434.2227	1	$\text{C}_{29}\text{H}_{28}\text{N}_3\text{O}$	434.2227	0.1	2.2	1	100.00	17.5	even	ok
456.2041	1	$\text{C}_{29}\text{H}_{27}\text{N}_3\text{NaO}$	456.2046	-1.1	30.0	1	100.00	17.5	even	ok

Figure S143. 4-Ethyl-2,6-diphenyl-7-(4-propoxyphenyl)-2*H*-pyrazolo[4,3-*c*]pyridine (**41**). HRMS (ESI-TOF).

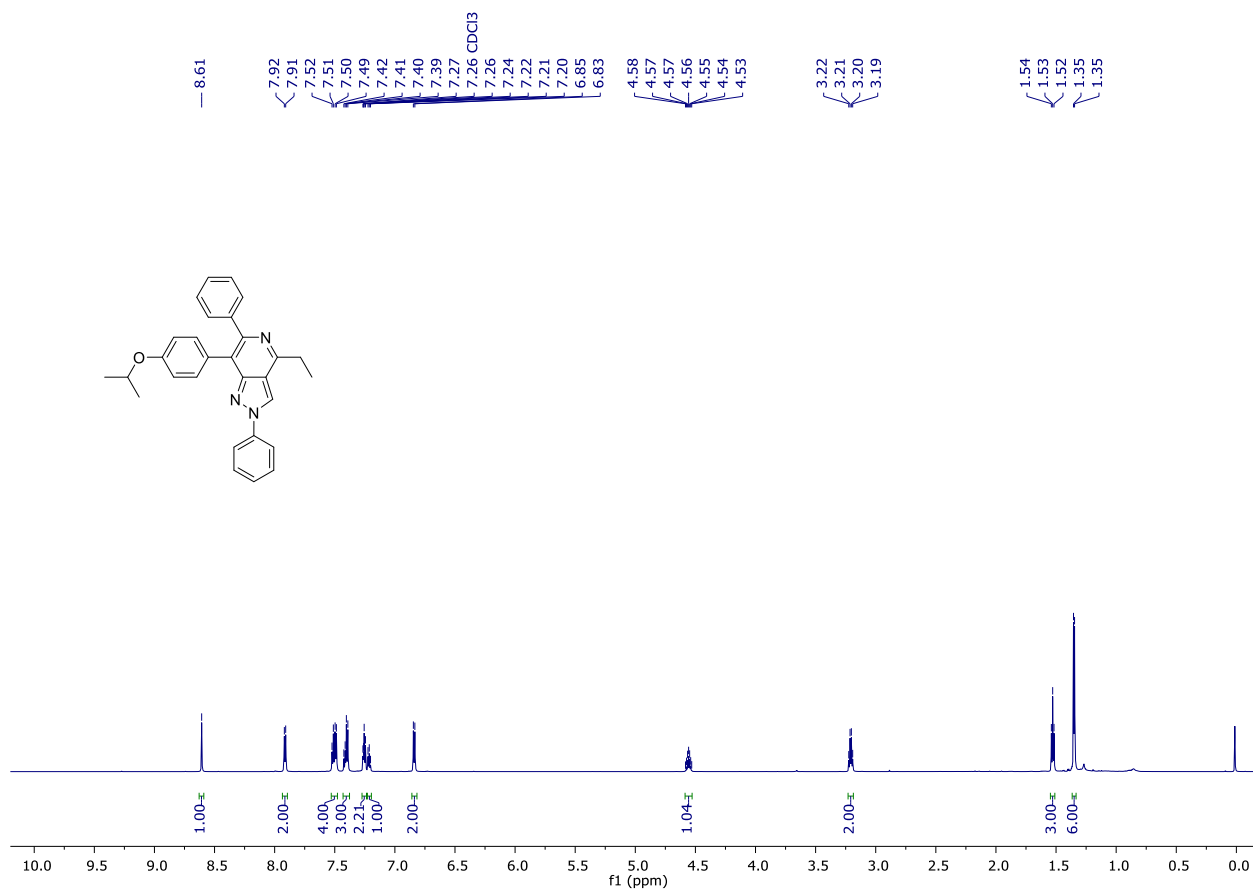


Figure S144. 4-Ethyl-7-(4-isopropoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**42**). ¹H NMR spectrum (700 MHz, CDCl₃).

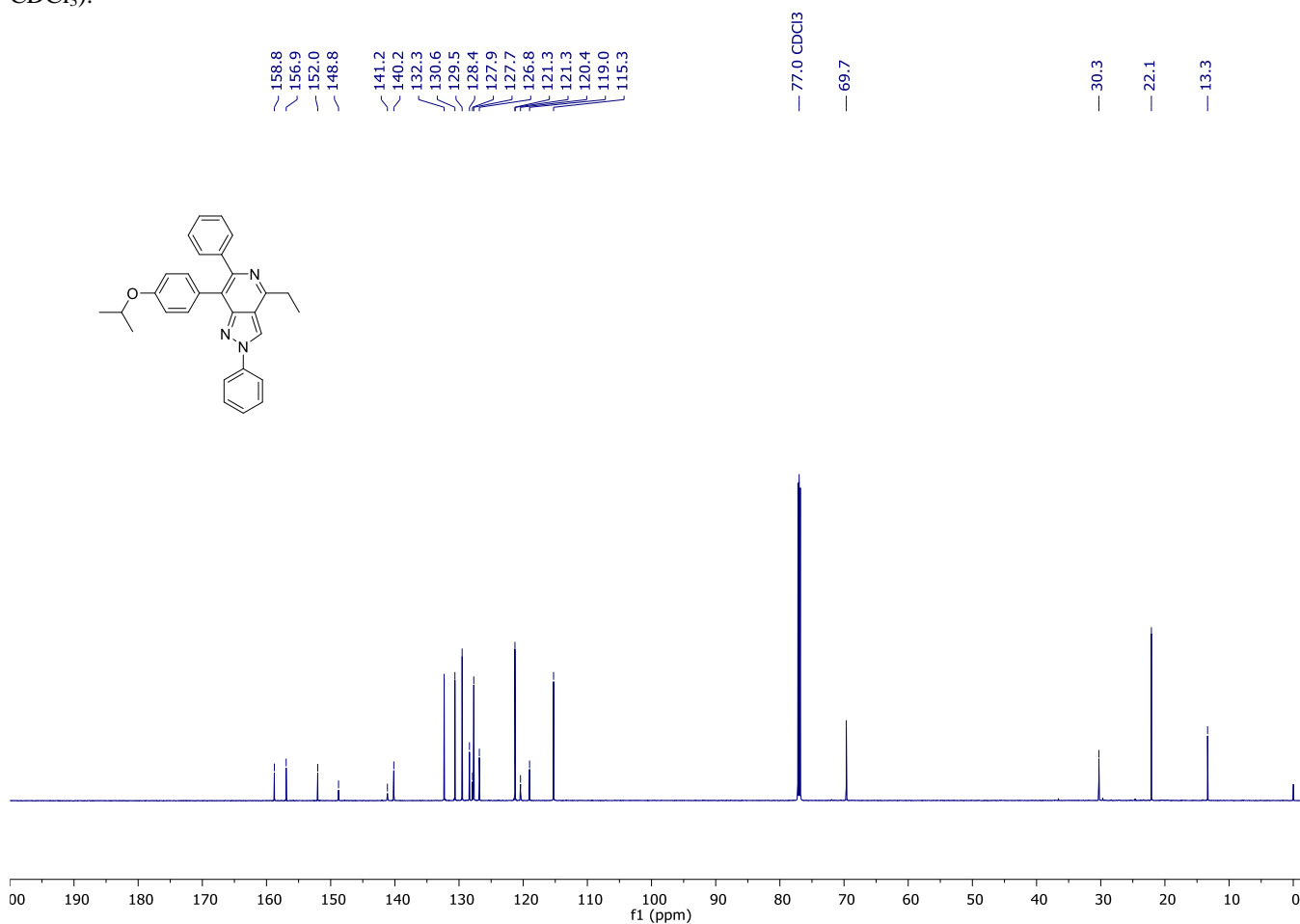


Figure S145. 4-Ethyl-7-(4-isopropoxyphenyl)-2,6-diphenyl-2H-pyrazolo[4,3-c]pyridine (**42**). ¹³C NMR (176 MHz, CDCl₃).

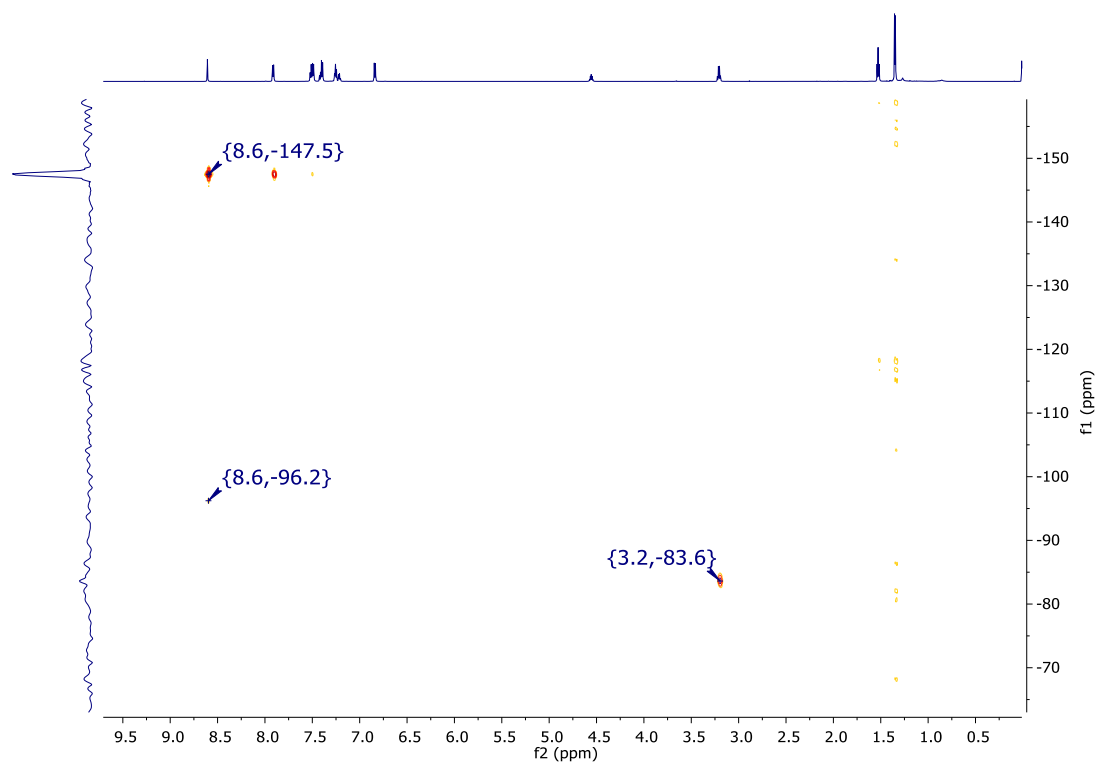
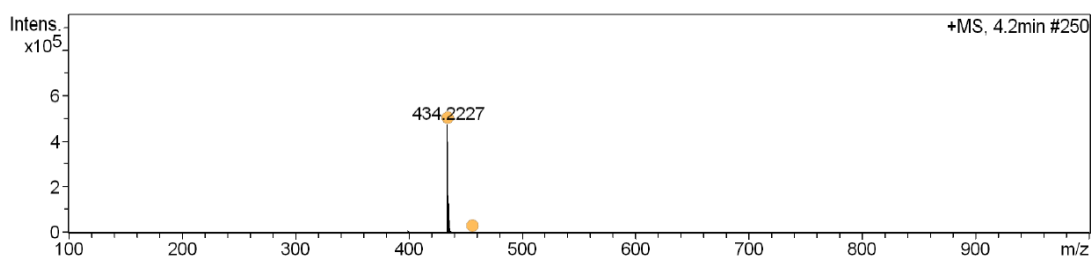


Figure S146. 4-Ethyl-7-(4-isopropoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**42**). ¹H-¹⁵N HMBC spectrum (700 MHz, CDCl₃).

+MS, 4.2min #250



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
434.2227	1	C ₂₉ H ₂₈ N ₃ O	434.2227	0.1	4.5	1	100.00	17.5	even	ok
456.2052	1	C ₂₉ H ₂₇ N ₃ NaO	456.2046	-1.3	31.9	1	100.00	17.5	even	ok

Figure S147. 4-Ethyl-7-(4-isopropoxyphenyl)-2,6-diphenyl-2*H*-pyrazolo[4,3-*c*]pyridine (**42**). HRMS (ESI-TOF).