Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

One-step preparation of novel 1-(N-indolyl)-1,3-butadienes by base-catalysed isomerization of alkynes as an access to 5-(N-indolyl)-naphthoquinones

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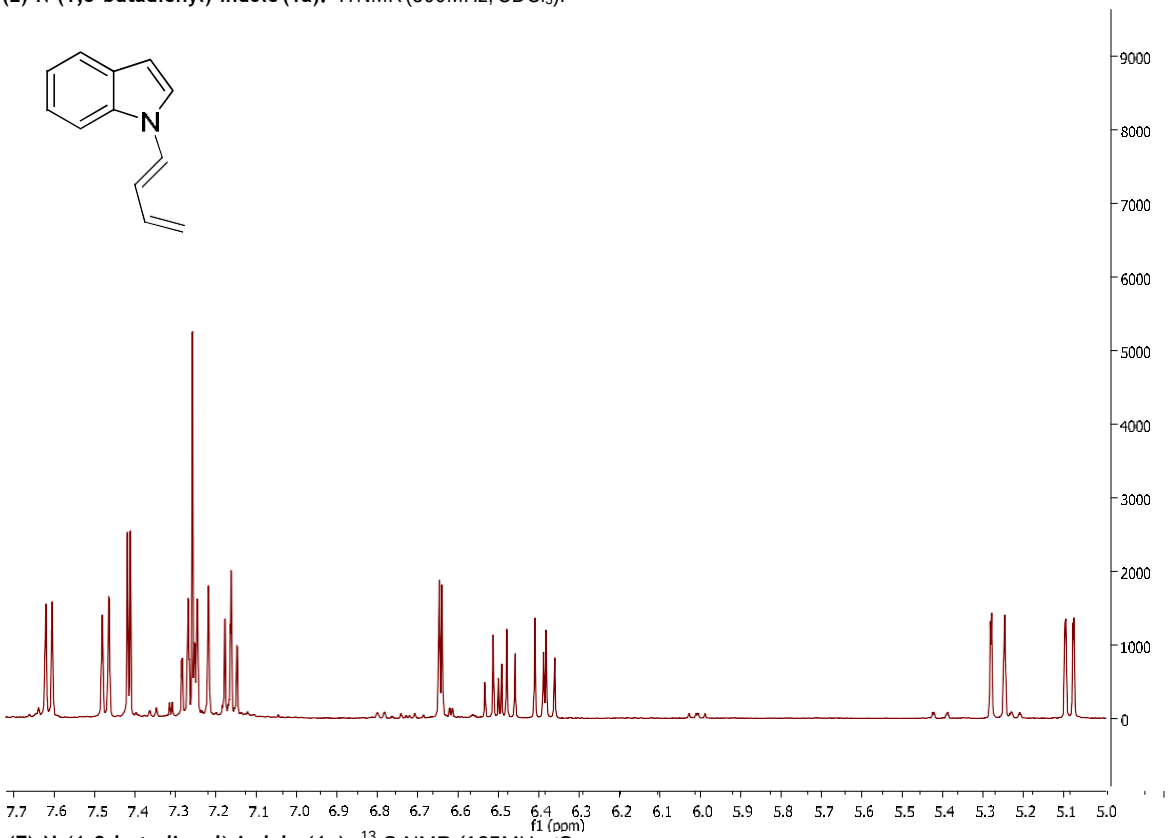
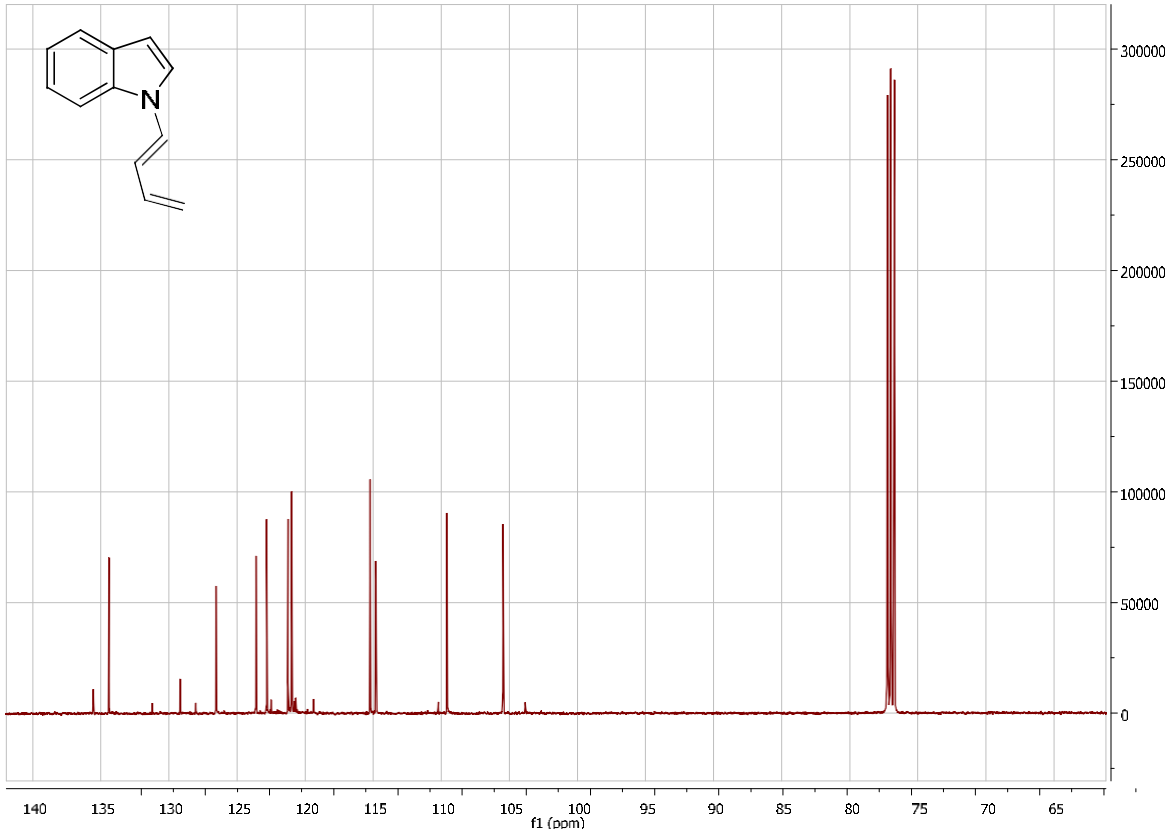
d CEQUINOR (CONICET-CCT-La Plata, UNLP), Bvd 120 N1465, 1900 La Plata, Argentina.

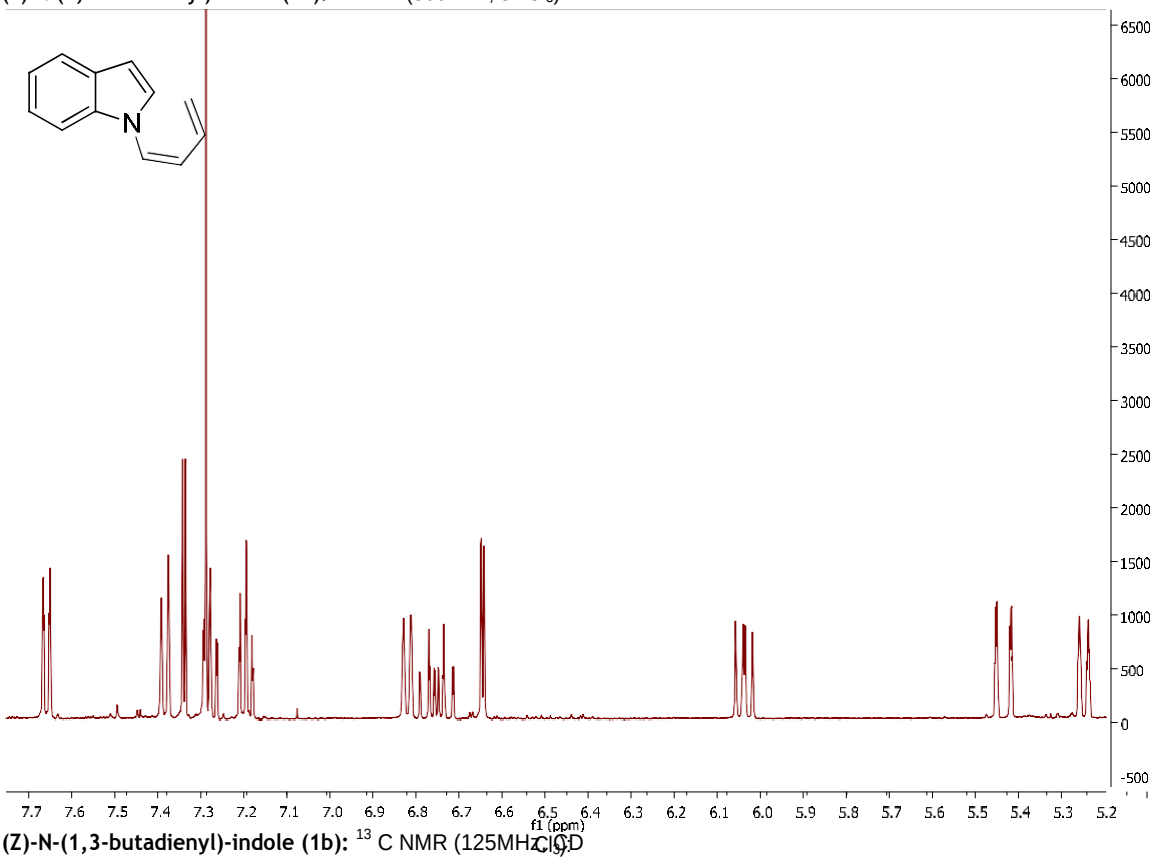
(E)-N-(1,3-butadienyl)-indole (1a): ^{1}H NMR (500MHz, $CDCl_3$):



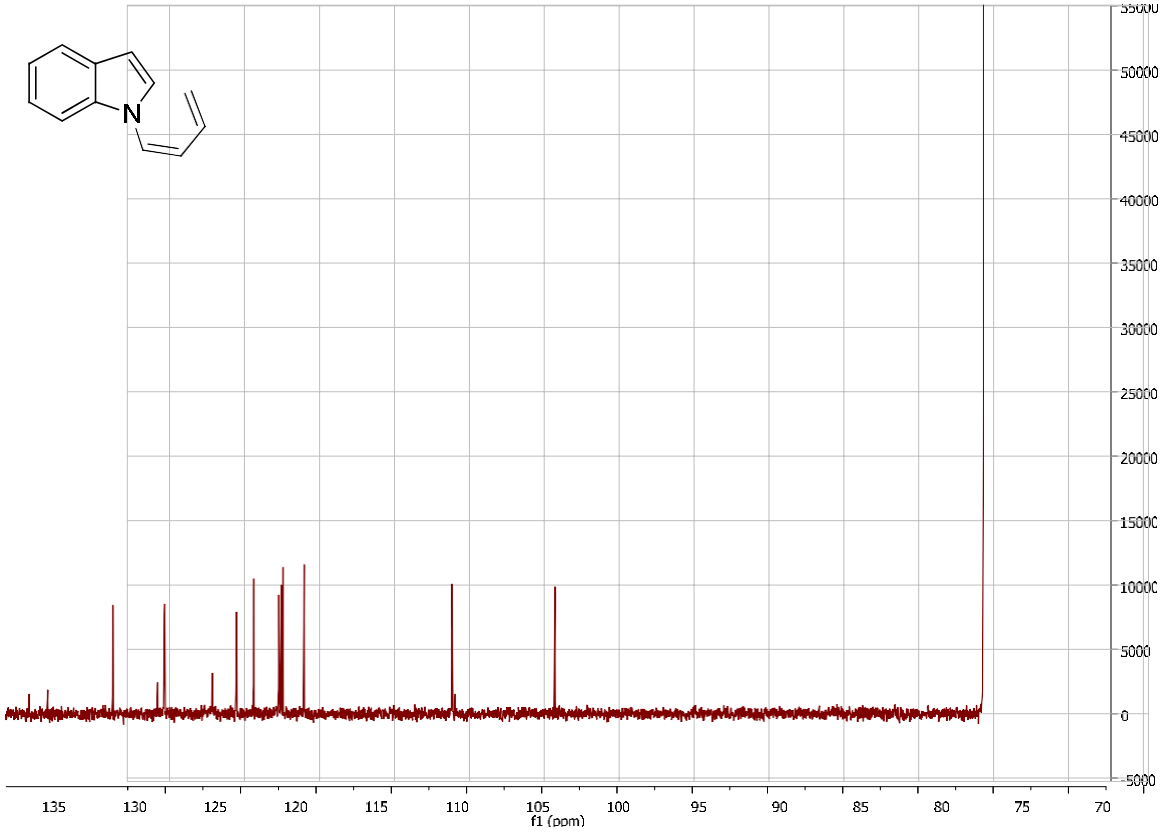
(E)-N-(1,3-butadienyl)-indole (1a): ^{13}C NMR (125MHz, $CDCl_3$):



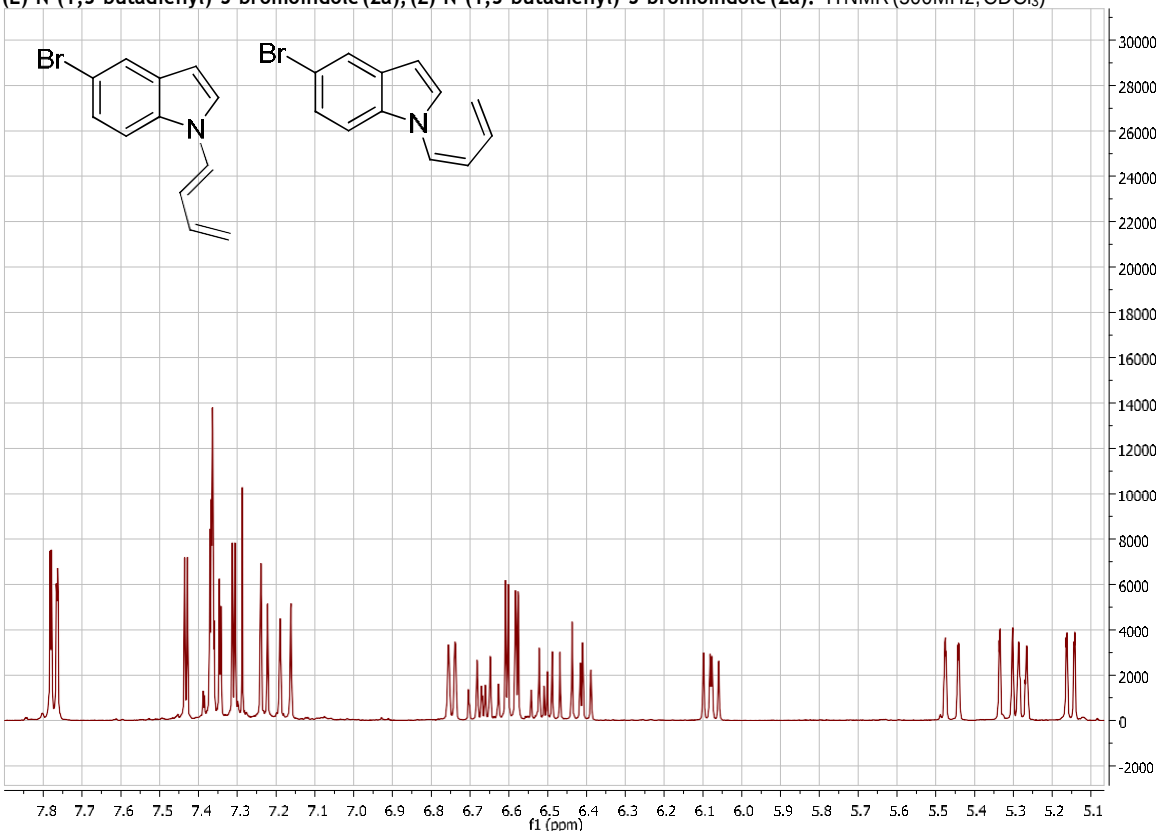
(Z)-N-(1,3-butadienyl)-indole (1b): ^{1}H NMR (500MHz, $CDCl_3$):



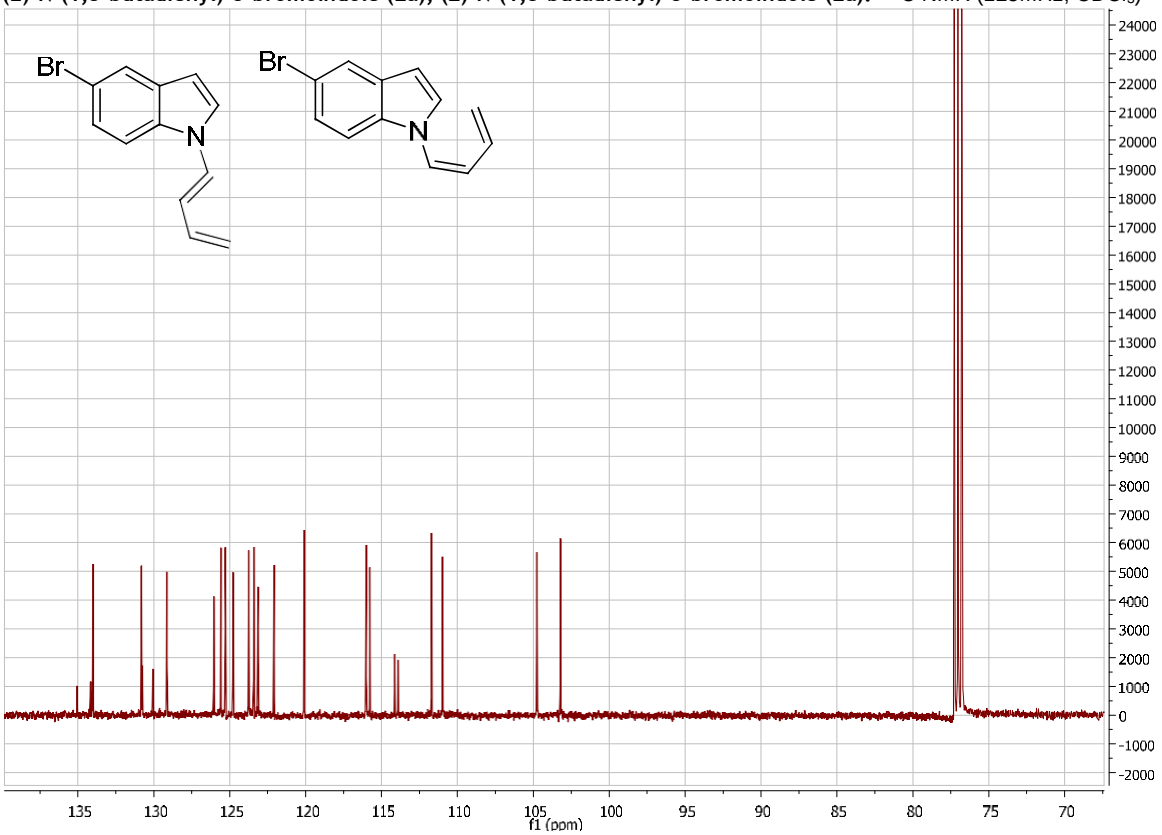
(Z)-N-(1,3-butadienyl)-indole (1b): ^{13}C NMR (125MHz, $CDCl_3$):



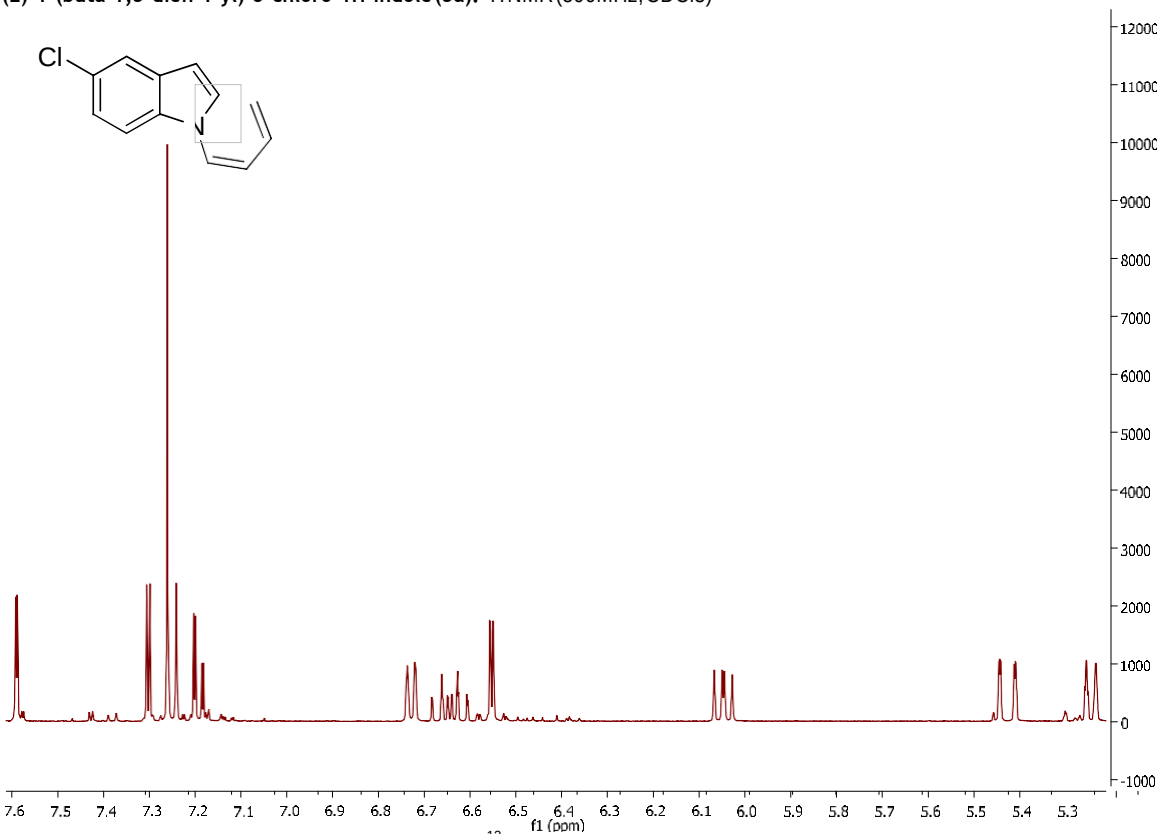
(E)-N-(1,3-butadienyl)-5-bromoindole (2a); (Z)-N-(1,3-butadienyl)-5-bromoindole (2a): ^{1}H NMR (500MHz, $CDCl_3$)



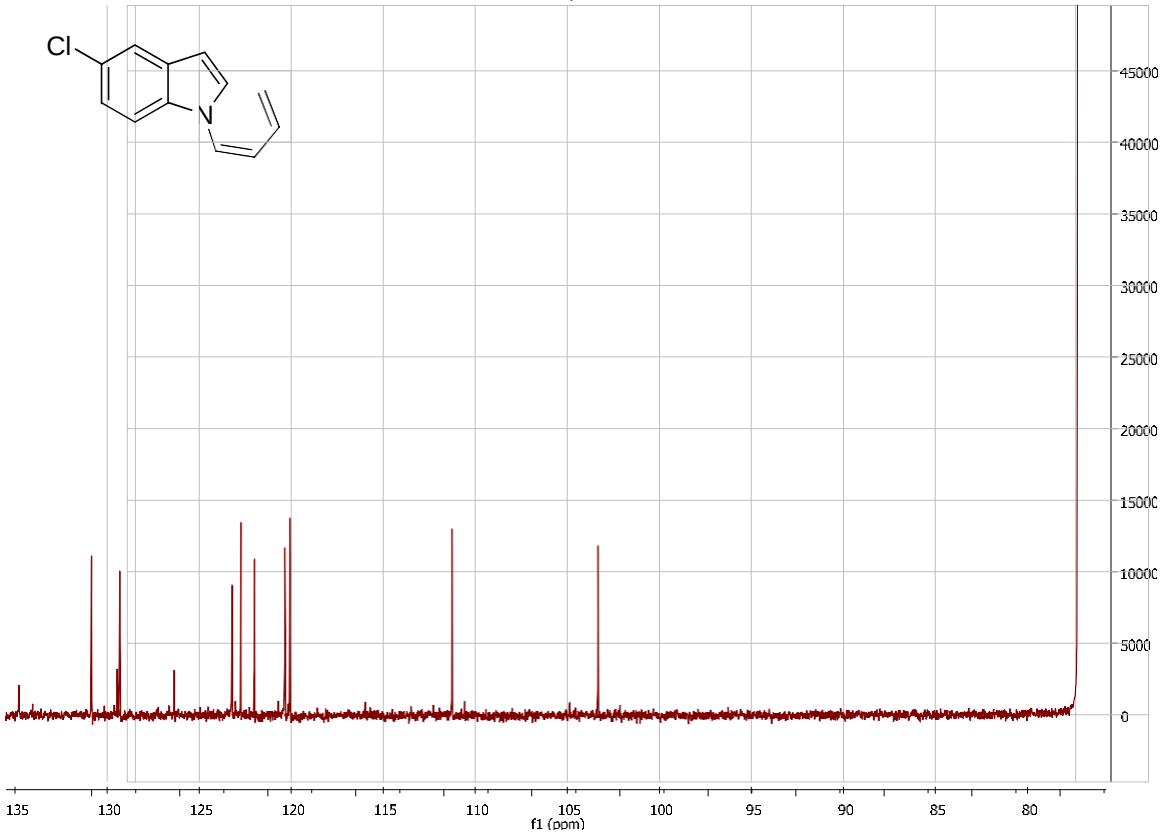
(E)-N-(1,3-butadienyl)-5-bromoindole (2a); (Z)-N-(1,3-butadienyl)-5-bromoindole (2a): ^{13}C NMR (125MHz, $CDCl_3$)



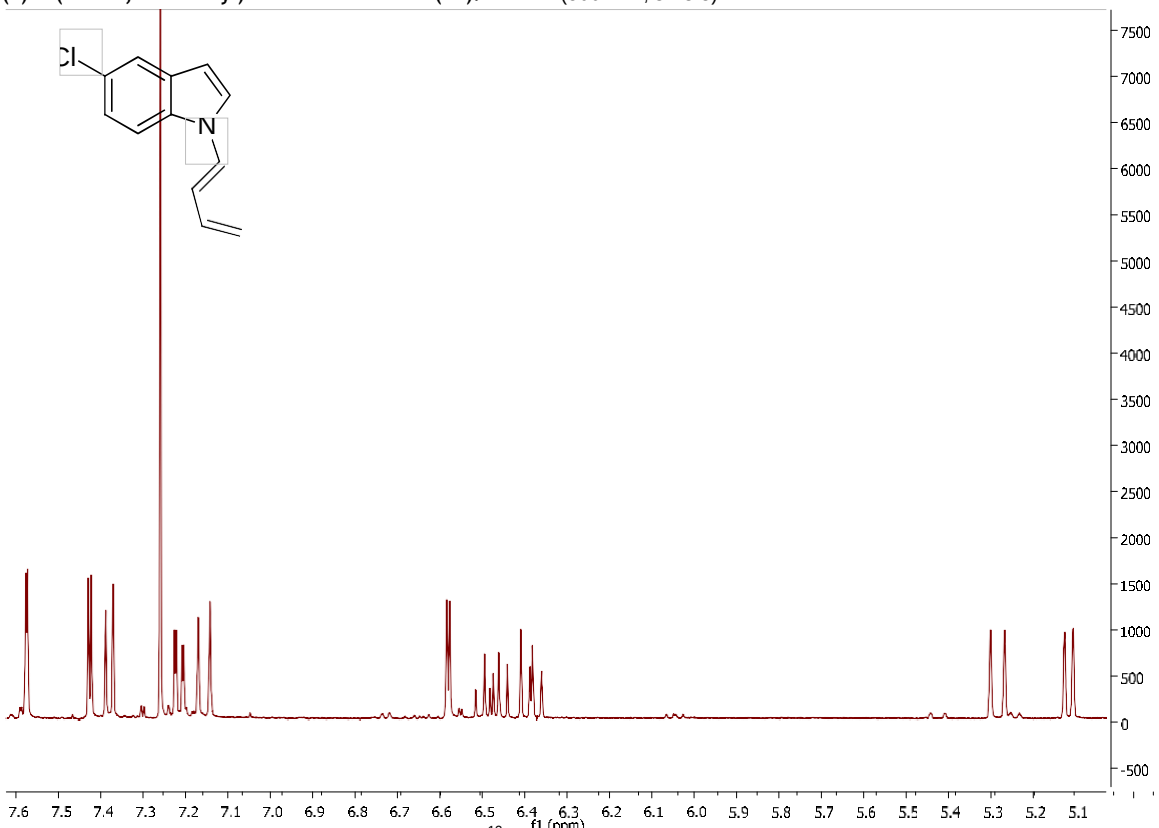
(E)-1-(buta-1,3-dien-1-yl)-5-chloro-1H-indole (3a): ^{1}H NMR (500MHz, CDCl3)



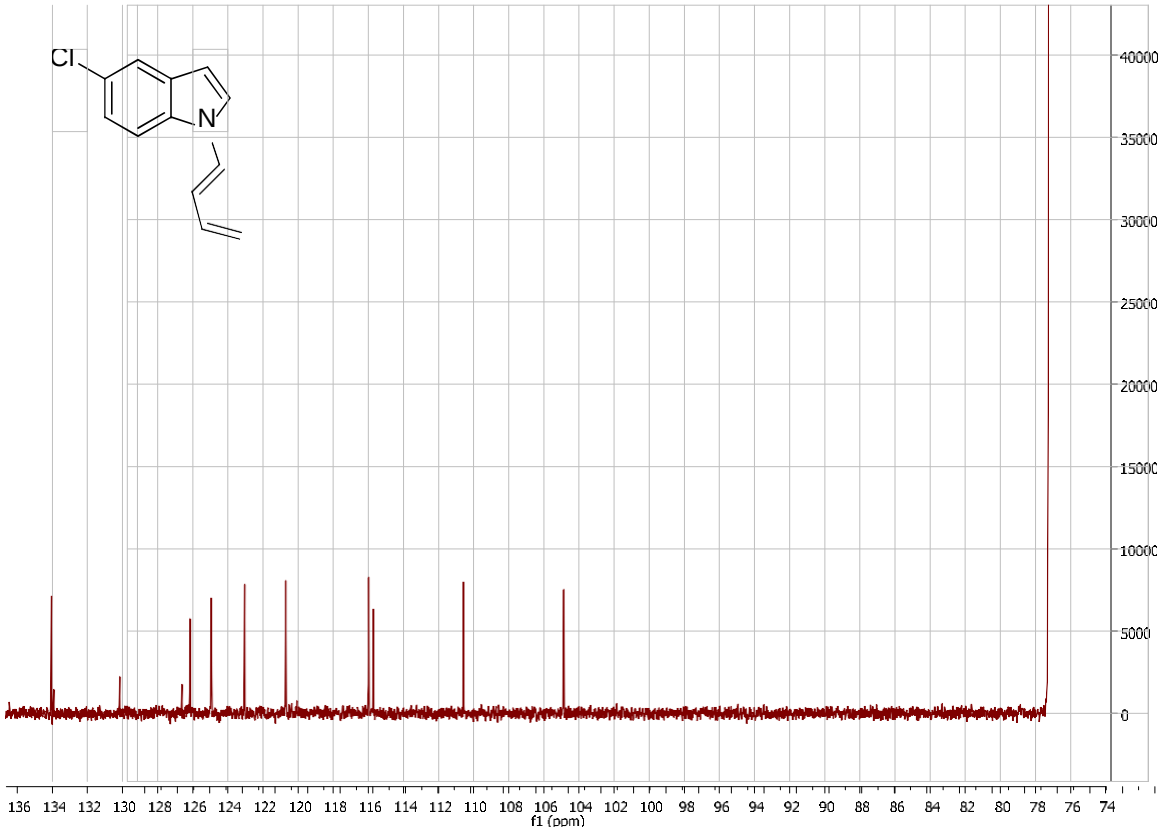
(E)-1-(buta-1,3-dien-1-yl)-5-chloro-1H-indole (3a): ^{13}C NMR (125MHz, CDCl3)



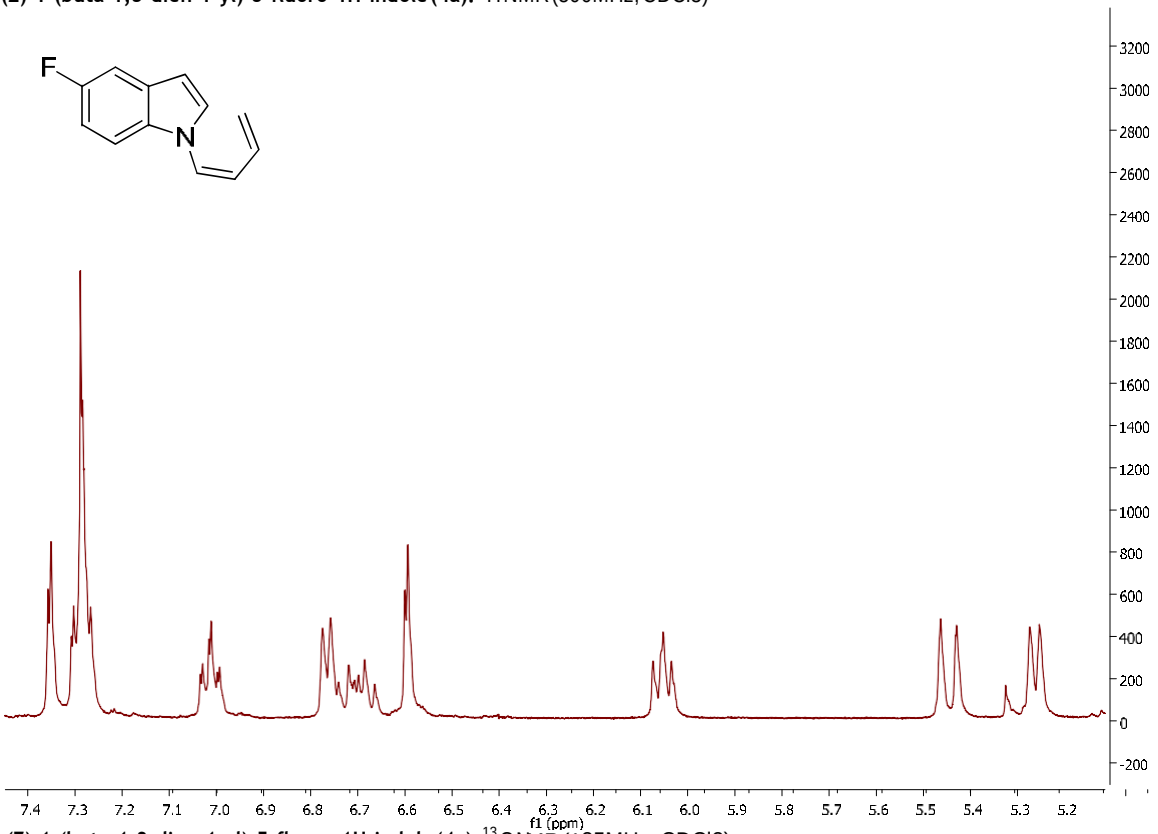
(E)-1-(buta-1,3-dien-1-yl)-5-chloro-1H-indole (3b): ^{1}H NMR (500MHz, CDCl3)



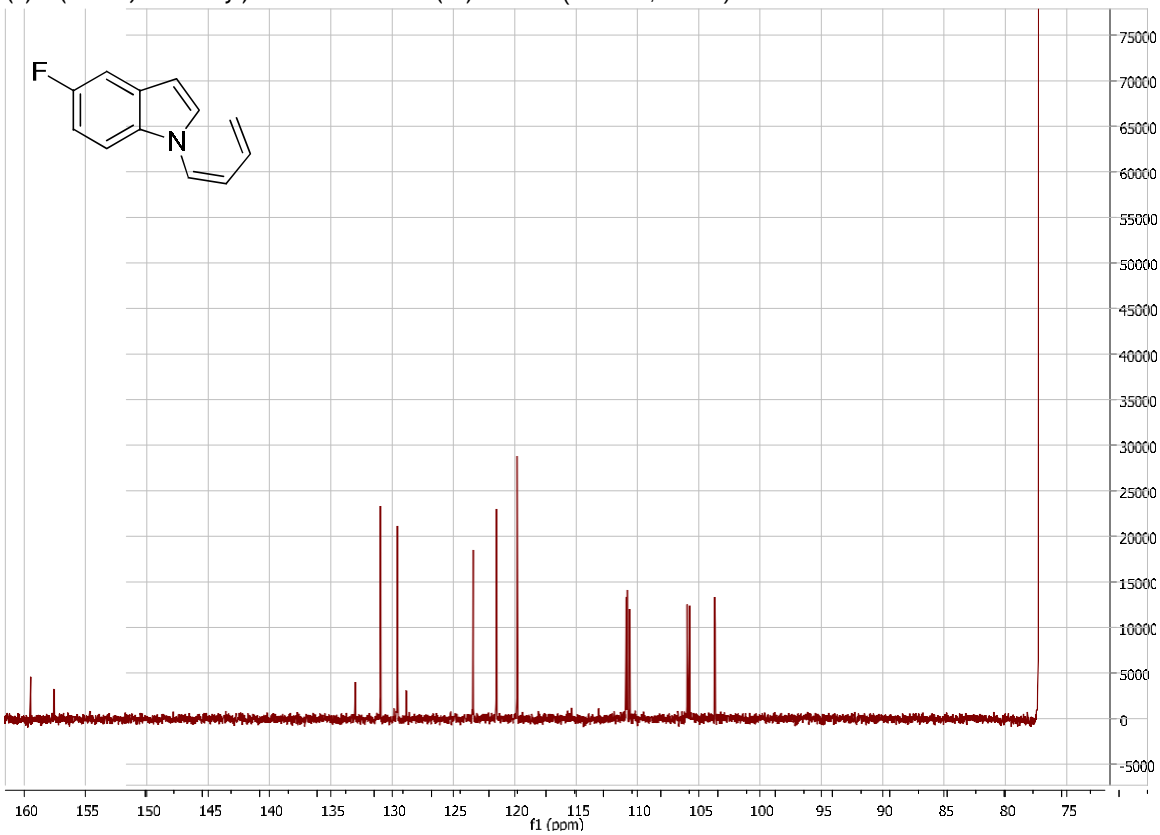
(E)-1-(buta-1,3-dien-1-yl)-5-chloro-1H-indole (3b): ^{13}C NMR (125MHz, CDCl3)



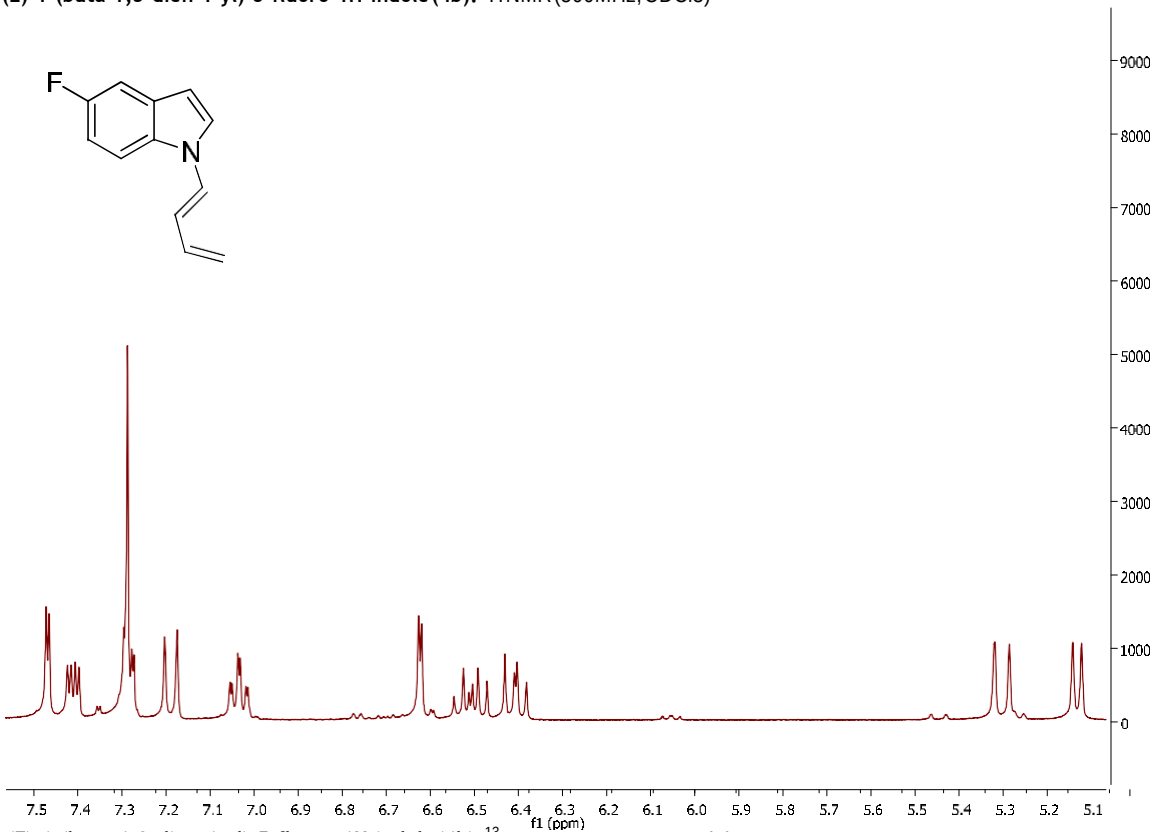
(Z)-1-(buta-1,3-dien-1-yl)-5-fluoro-1H-indole (4a): ^{1}H NMR (500MHz, CDCl3)



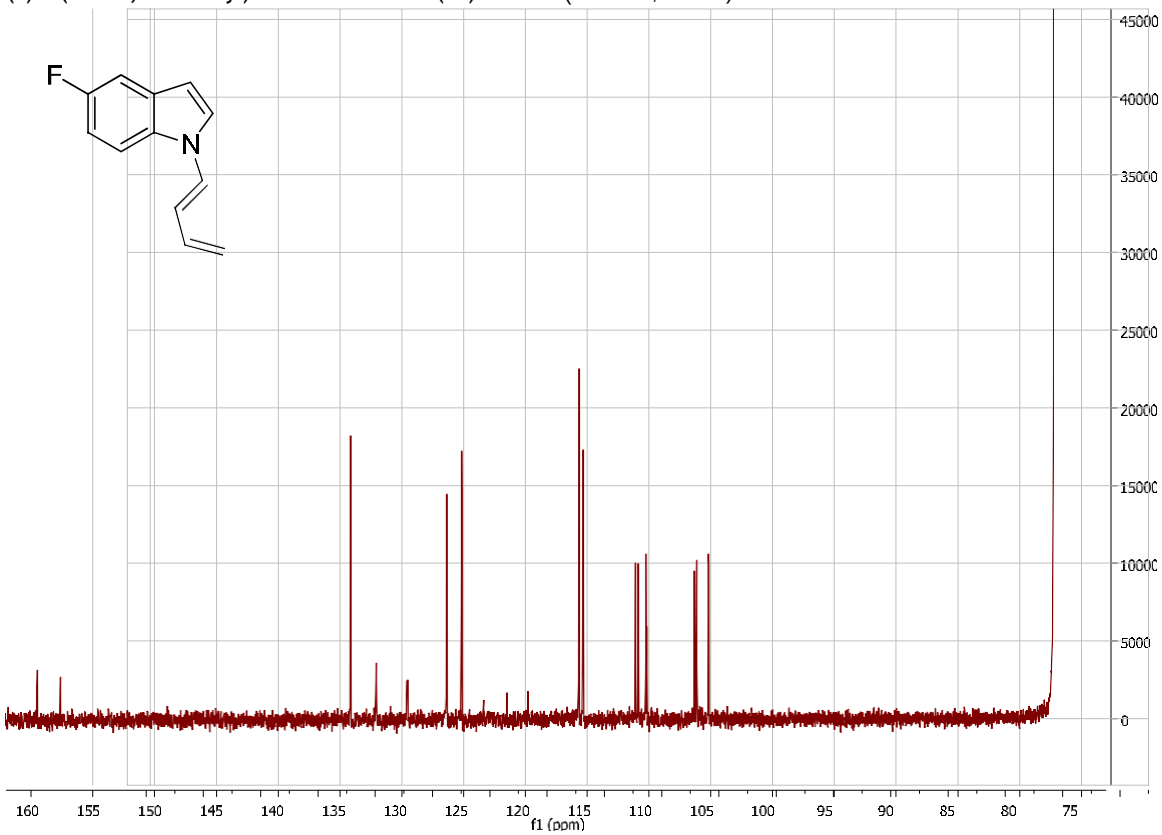
(Z)-1-(buta-1,3-dien-1-yl)-5-fluoro-1H-indole (4a): ^{13}C NMR (125MHz, CDCl3)



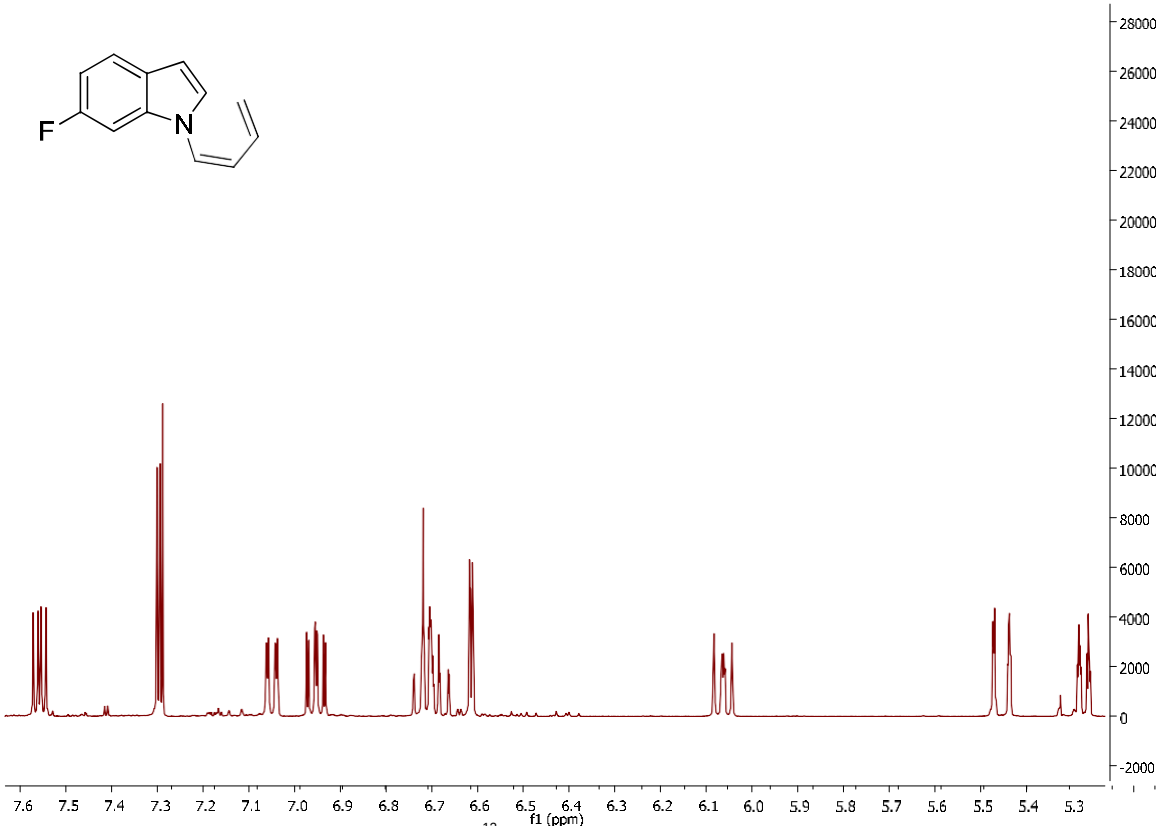
(E)-1-(buta-1,3-dien-1-yl)-5-fluoro-1H-indole (4b): ^{1}H NMR (500MHz, CDCl3)



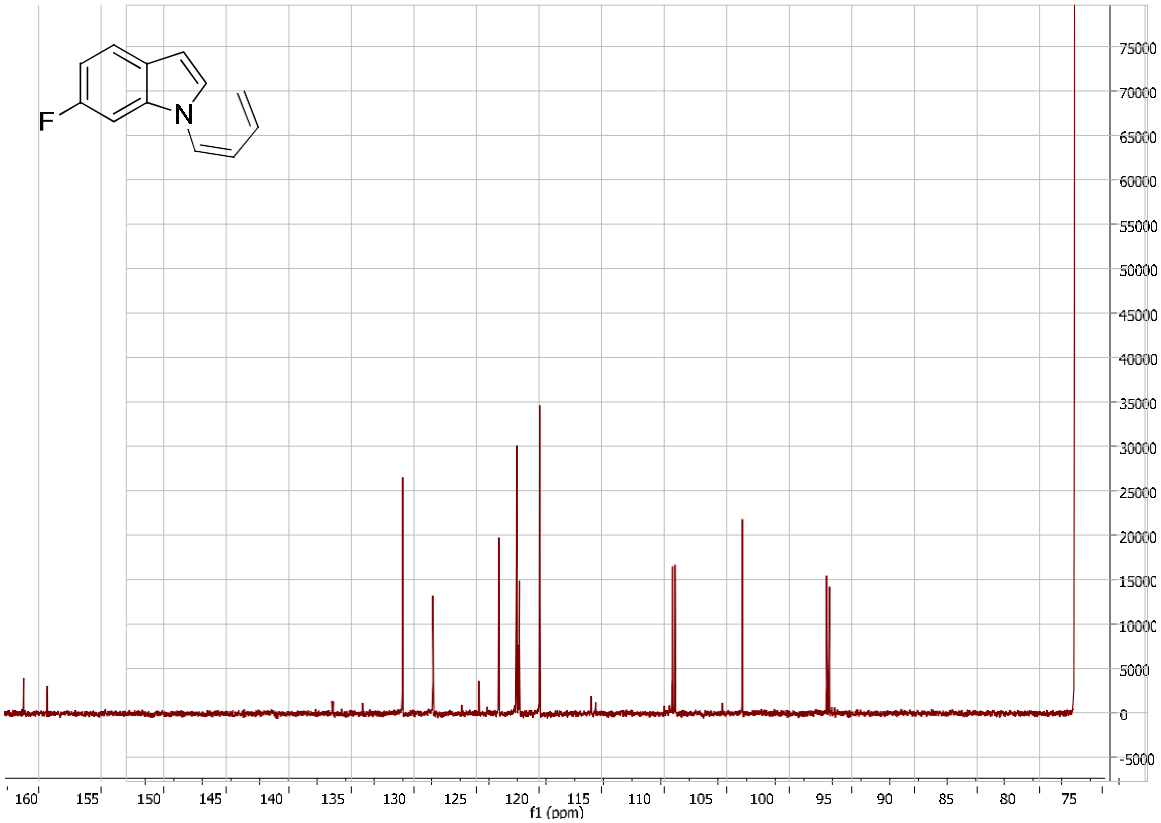
(E)-1-(buta-1,3-dien-1-yl)-5-fluoro-1H-indole (4b): ^{13}C NMR (125MHz, CDCl3)



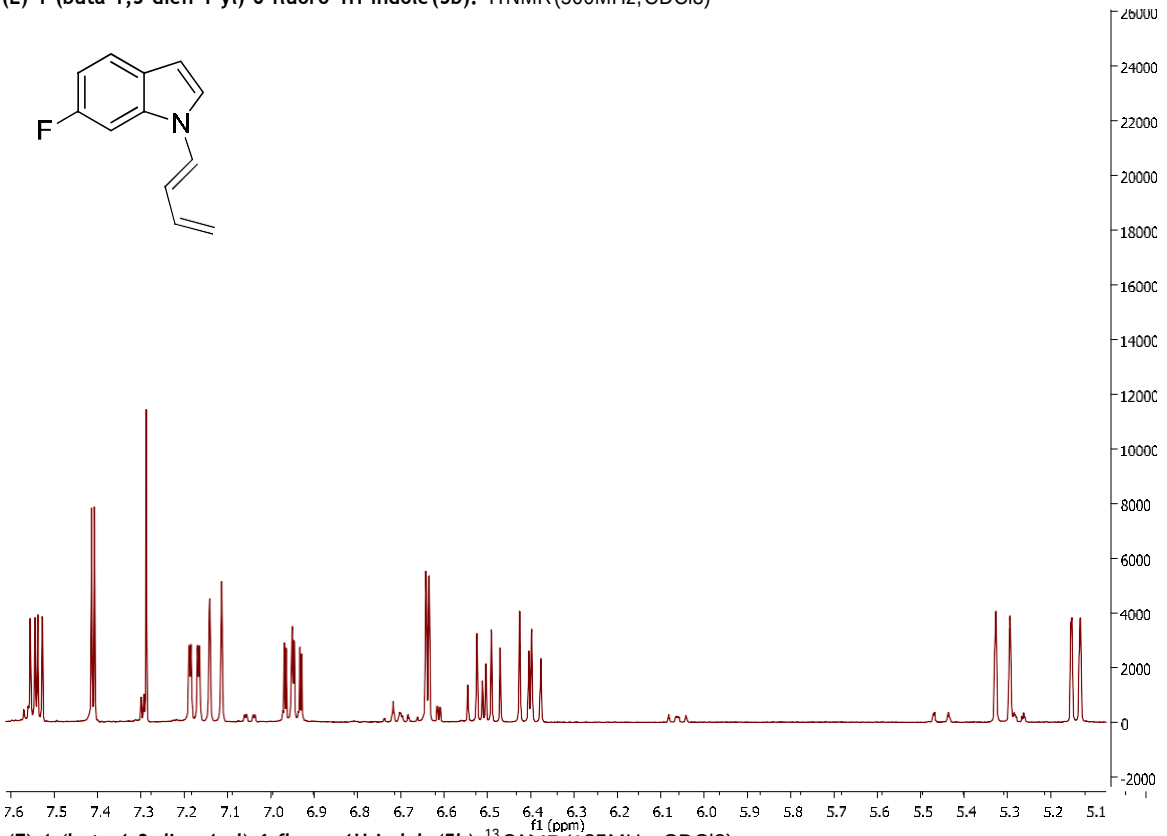
(Z)-1-(buta-1,3-dien-1-yl)-6-fluoro-1H-indole (5a): ^{1}H NMR (500MHz, CDCl3)



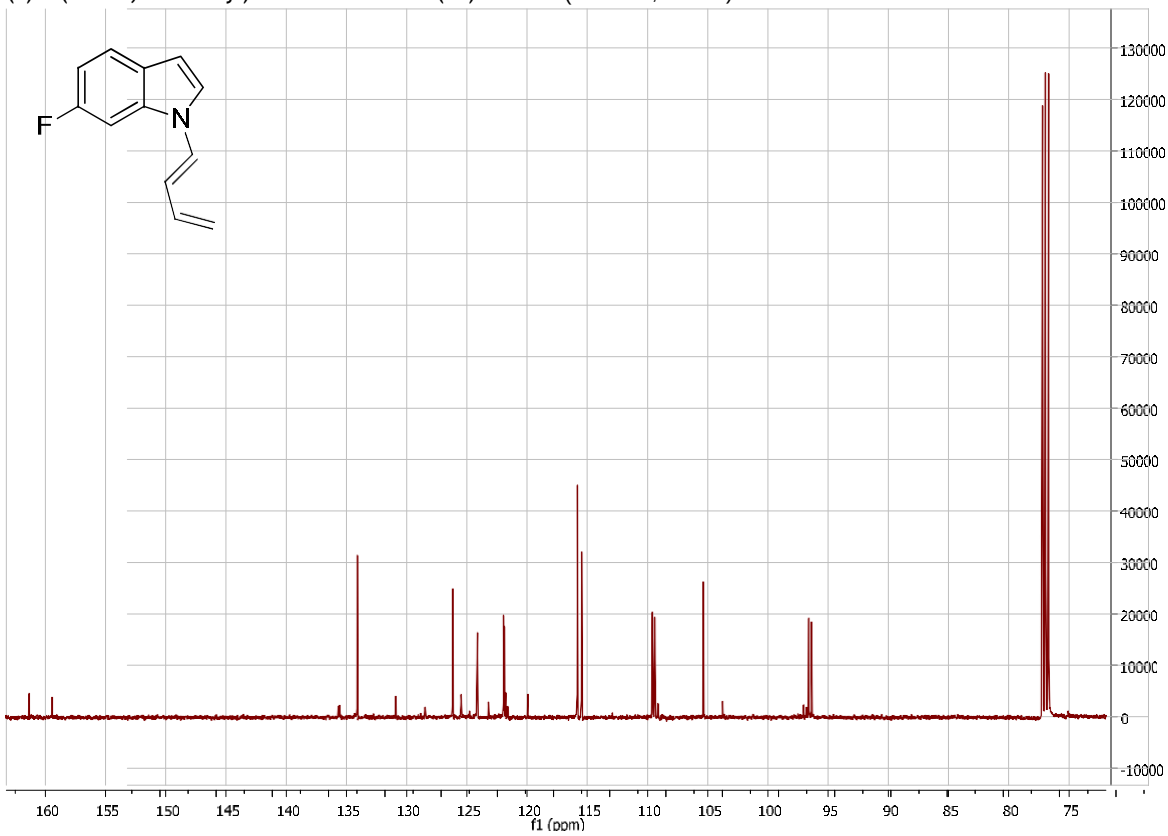
(Z)-1-(buta-1,3-dien-1-yl)-6-fluoro-1H-indole (5a): ^{13}C NMR (125MHz, CDCl3)



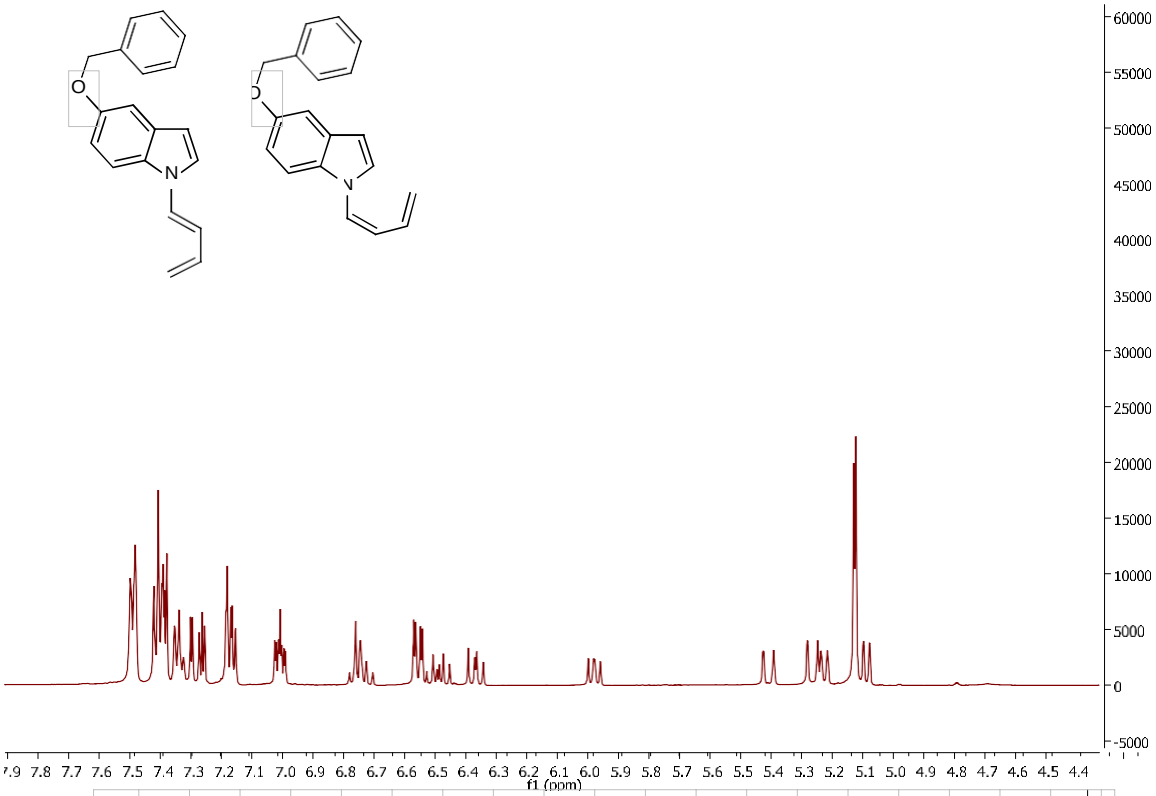
(E)-1-(buta-1,3-dien-1-yl)-6-fluoro-1H-indole (5b): ^{1}H NMR (500MHz, CDCl3)

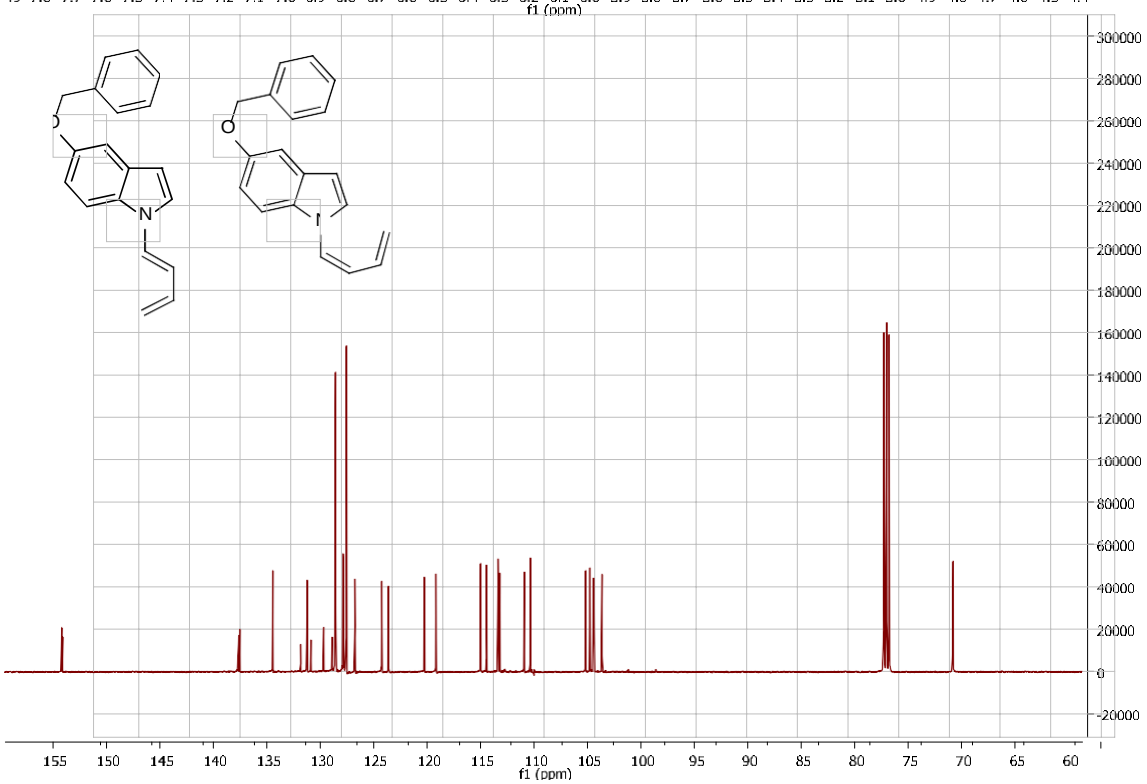


(E)-1-(buta-1,3-dien-1-yl)-6-fluoro-1H-indole (5b): ^{13}C NMR (125MHz, CDCl3)

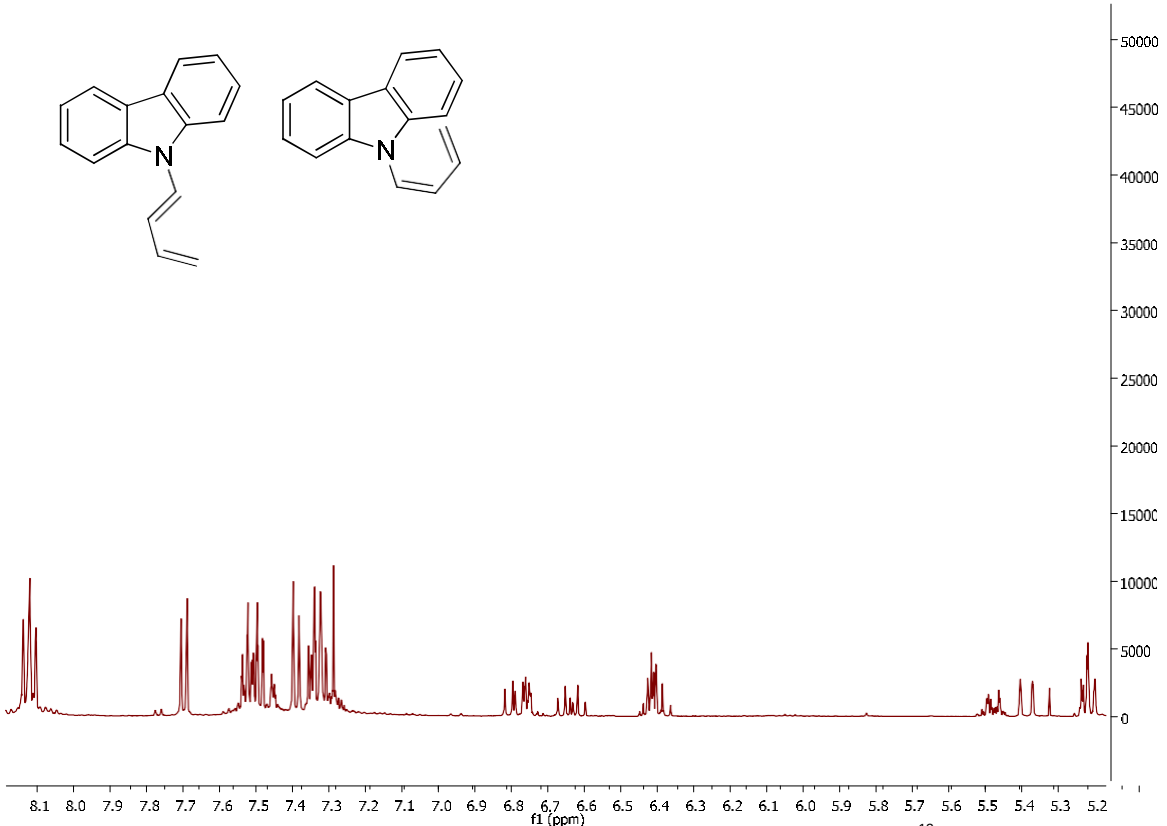


(E)-5-(benzyloxy)-1-(buta-1,3-dien-1-yl)-1H-indole (6a); **(Z)-5-(benzyloxy)-1-(buta-1,3-dien-1-yl)-1H-indole (6b)** ^{1}H NMR (500MHz, CDCl3) and ^{13}C NMR (125MHz, CDCl3)

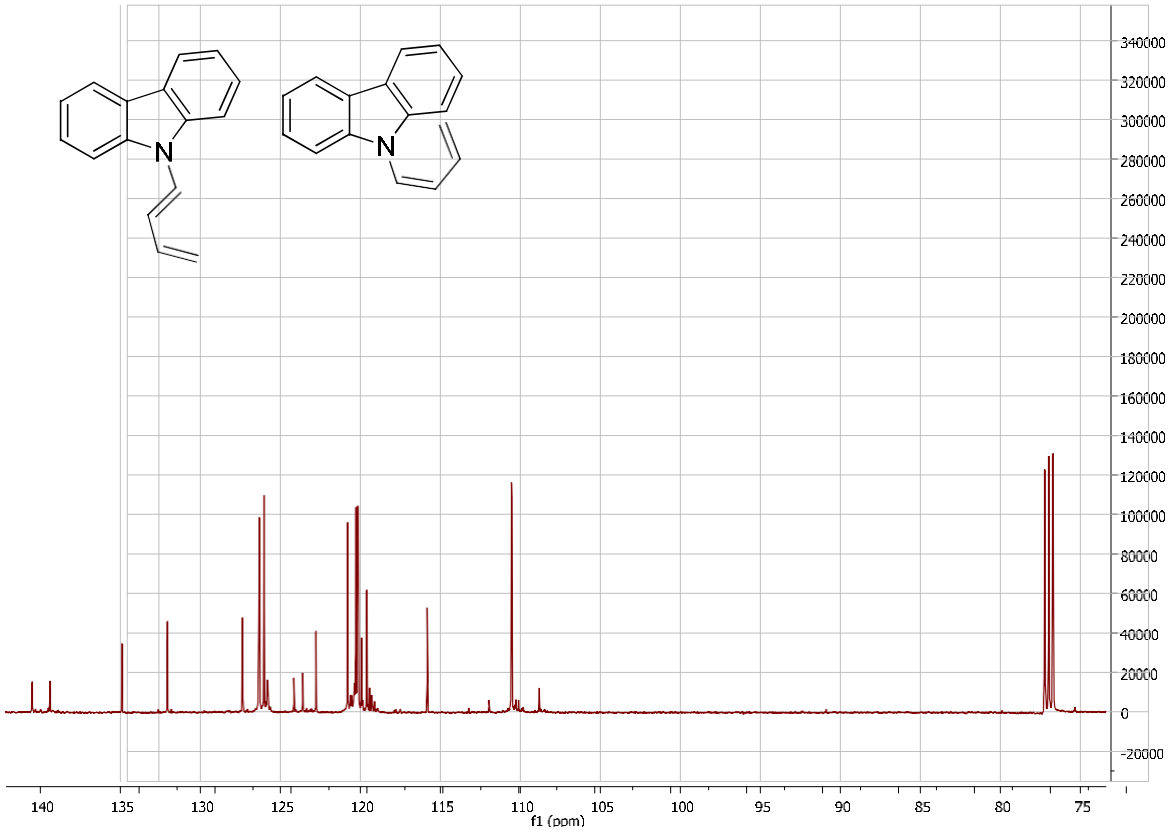




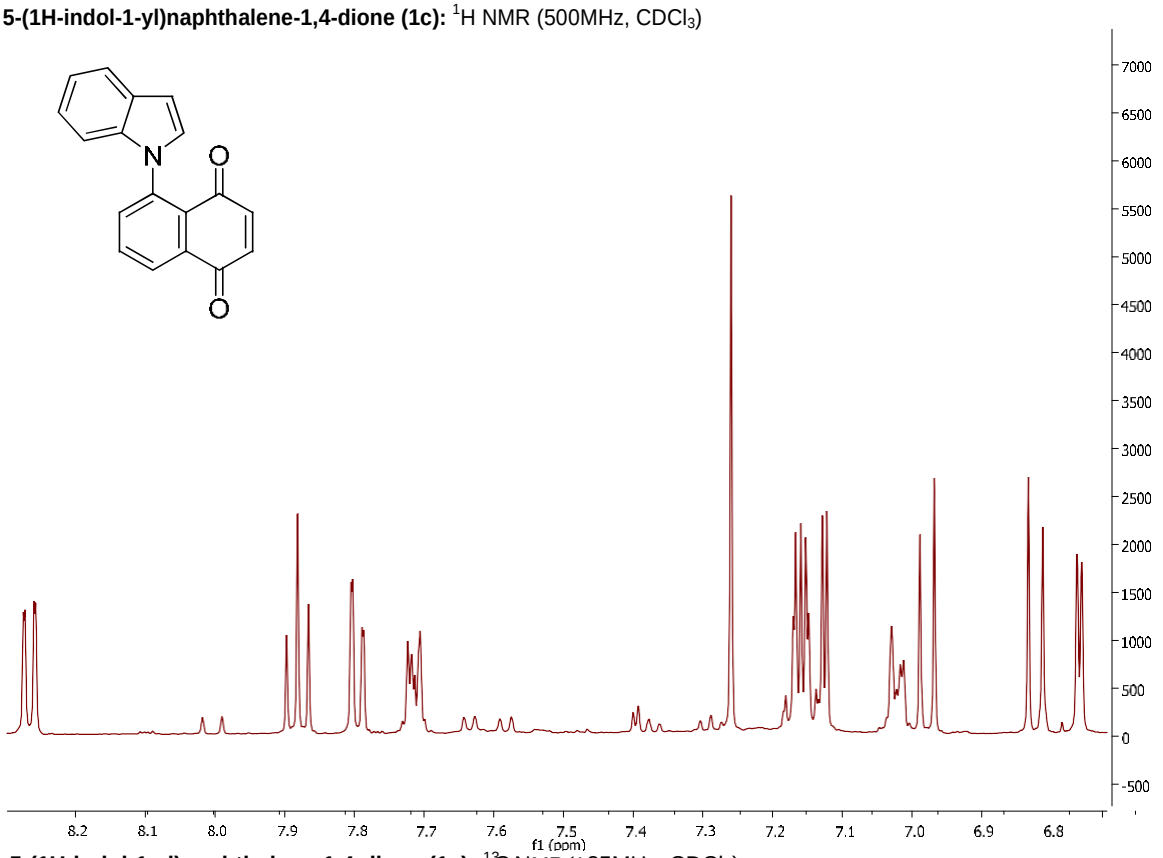
(E)-9-(buta-1,3-dien-1-yl)-9H-carbazole (7a); (Z)-9-(buta-1,3-dien-1-yl)-9H-carbazole (7b): ^{1}H NMR (500MHz, CDCl3)



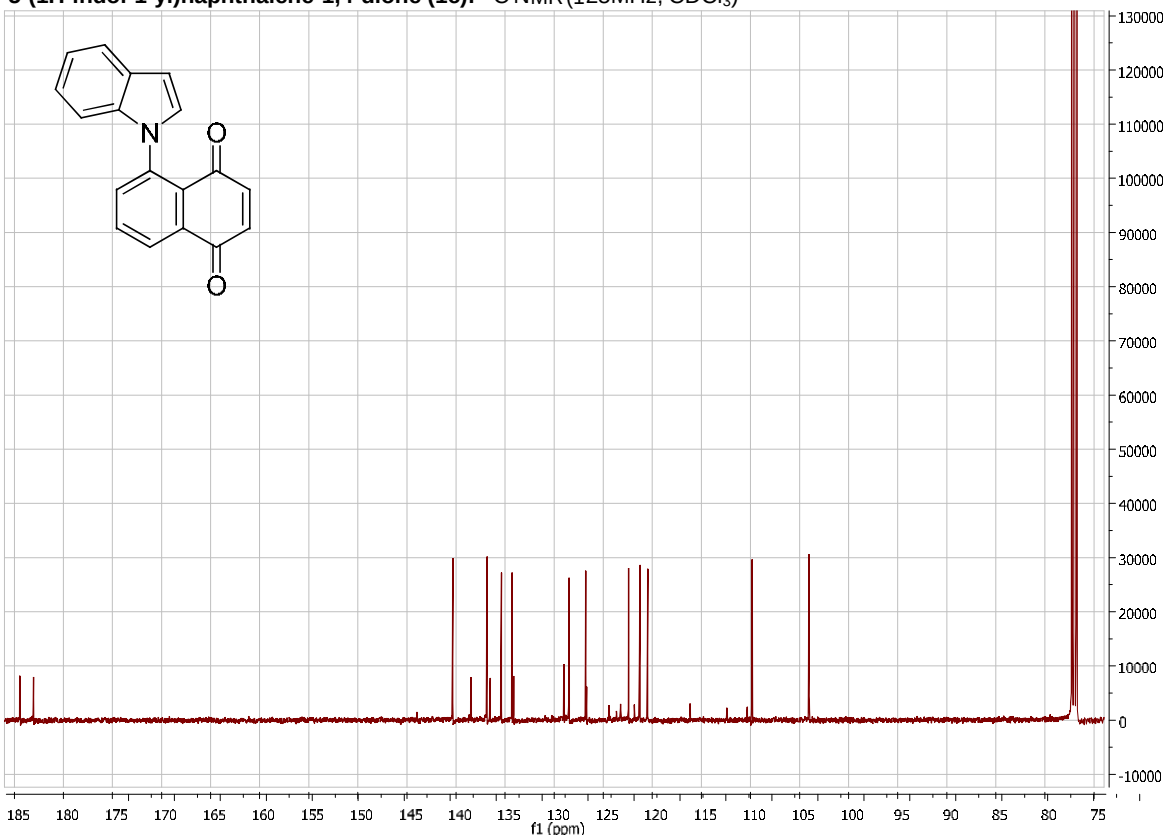
(E)-9-(buta-1,3-dien-1-yl)-9H-carbazole (6a); (Z)-9-(buta-1,3-dien-1-yl)-9H-carbazole (6b) ^{13}C NMR(125MHz, CDCl3)



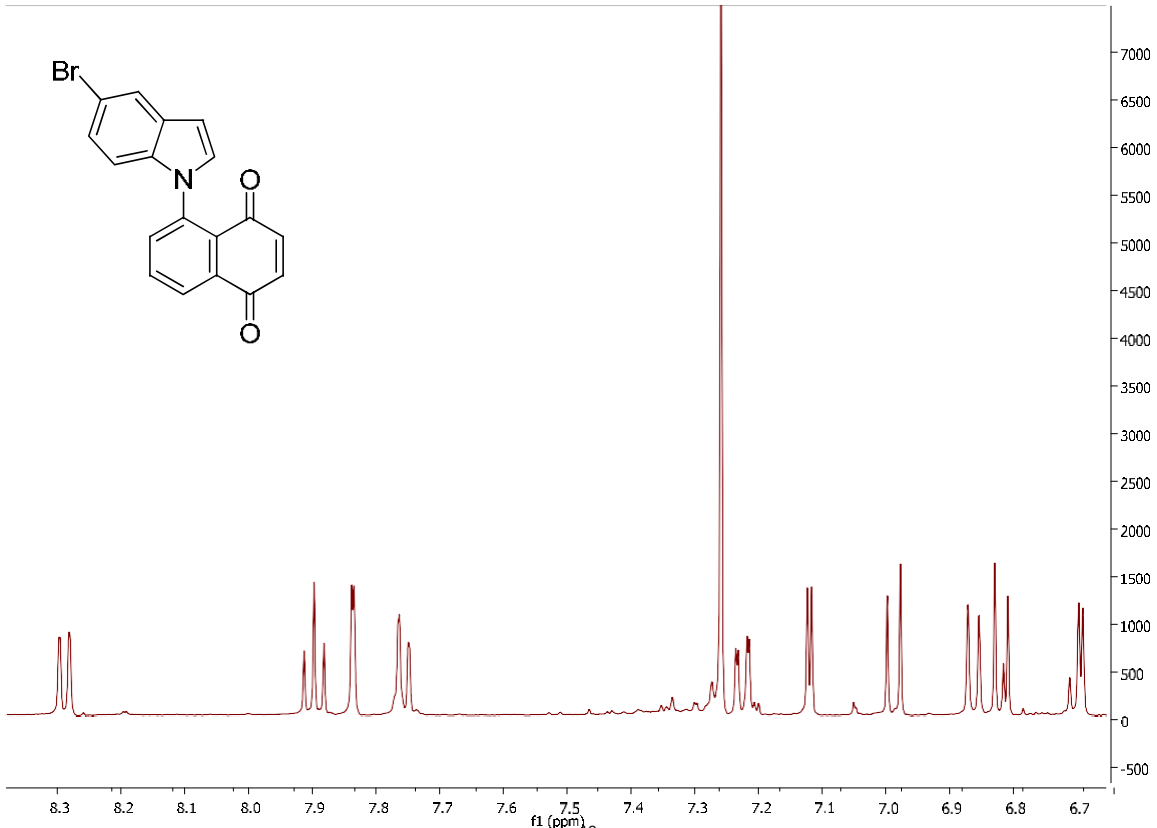
5-(1H-indol-1-yl)naphthalene-1,4-dione (1c): ^{1}H NMR (500MHz, $CDCl_3$)



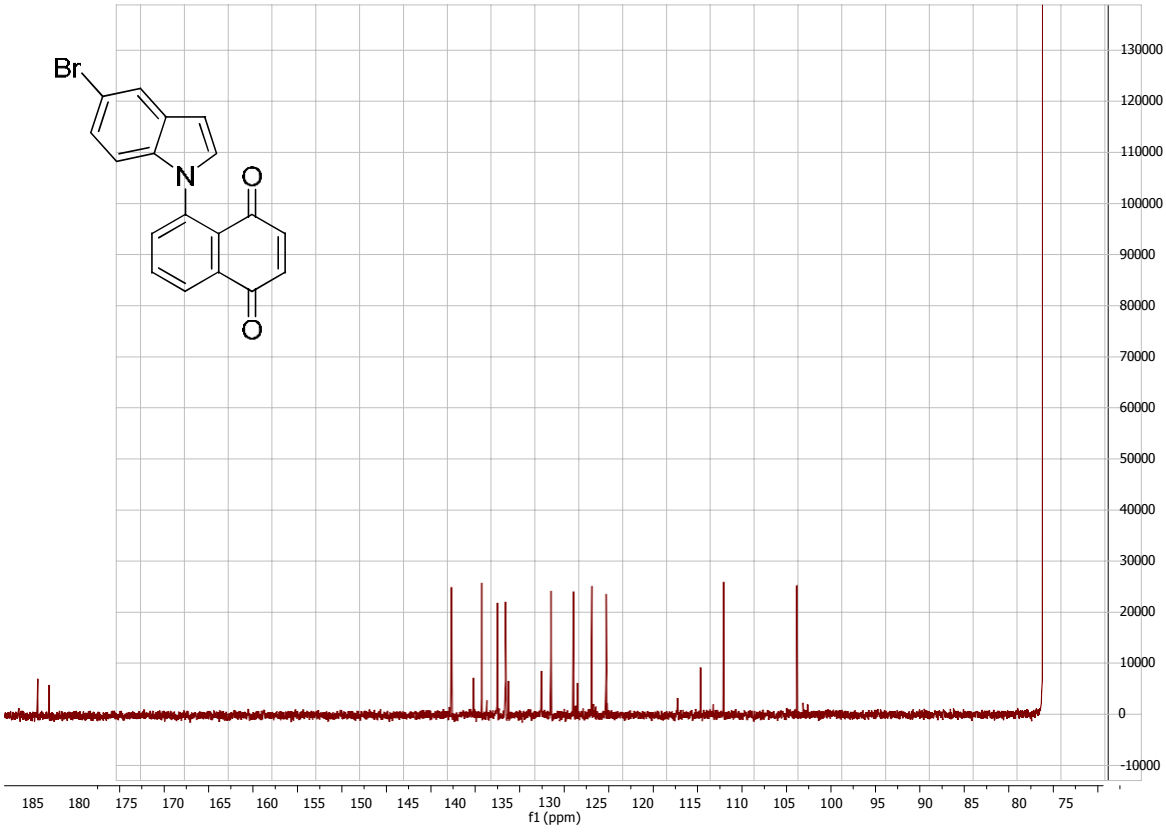
5-(1H-indol-1-yl)naphthalene-1,4-dione (1c): ^{13}C NMR (125MHz, $CDCl_3$)



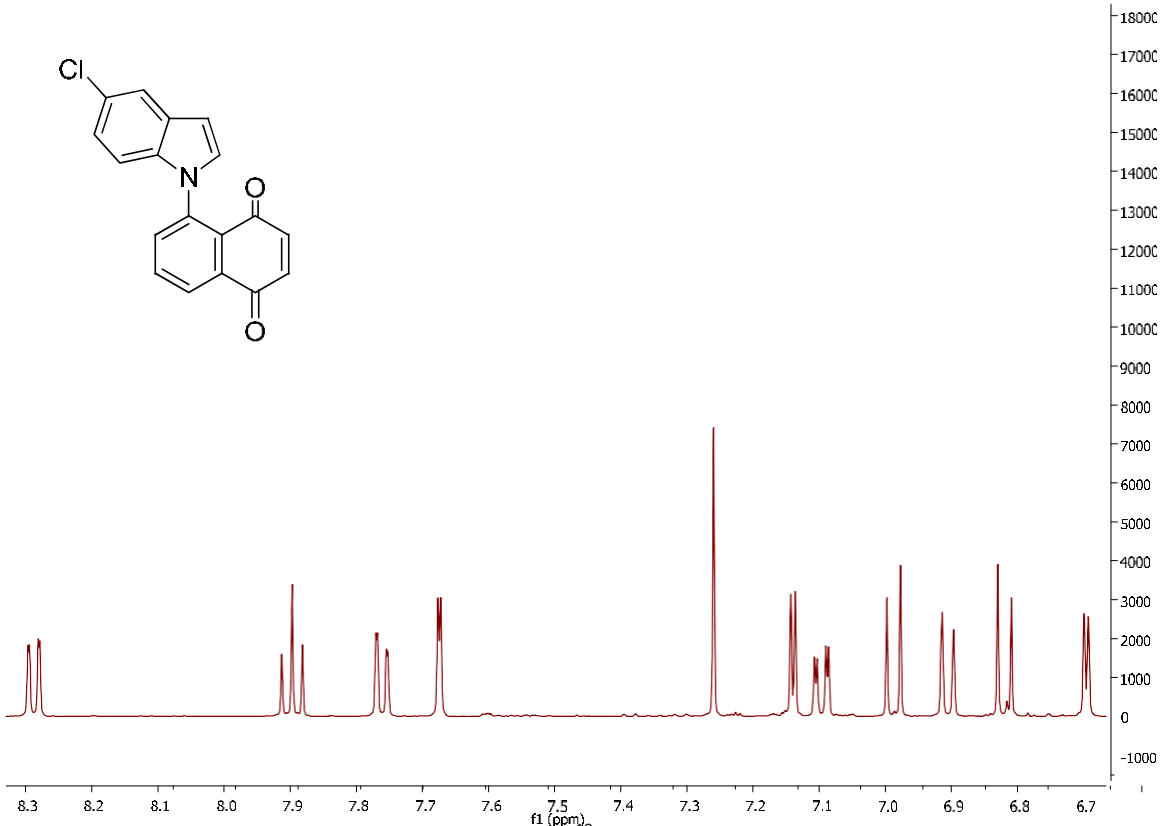
5-(5-bromo-1H-indol-1-yl)naphthalene-1,4-dione (2c): ^{1}H NMR (500MHz, $CDCl_3$)



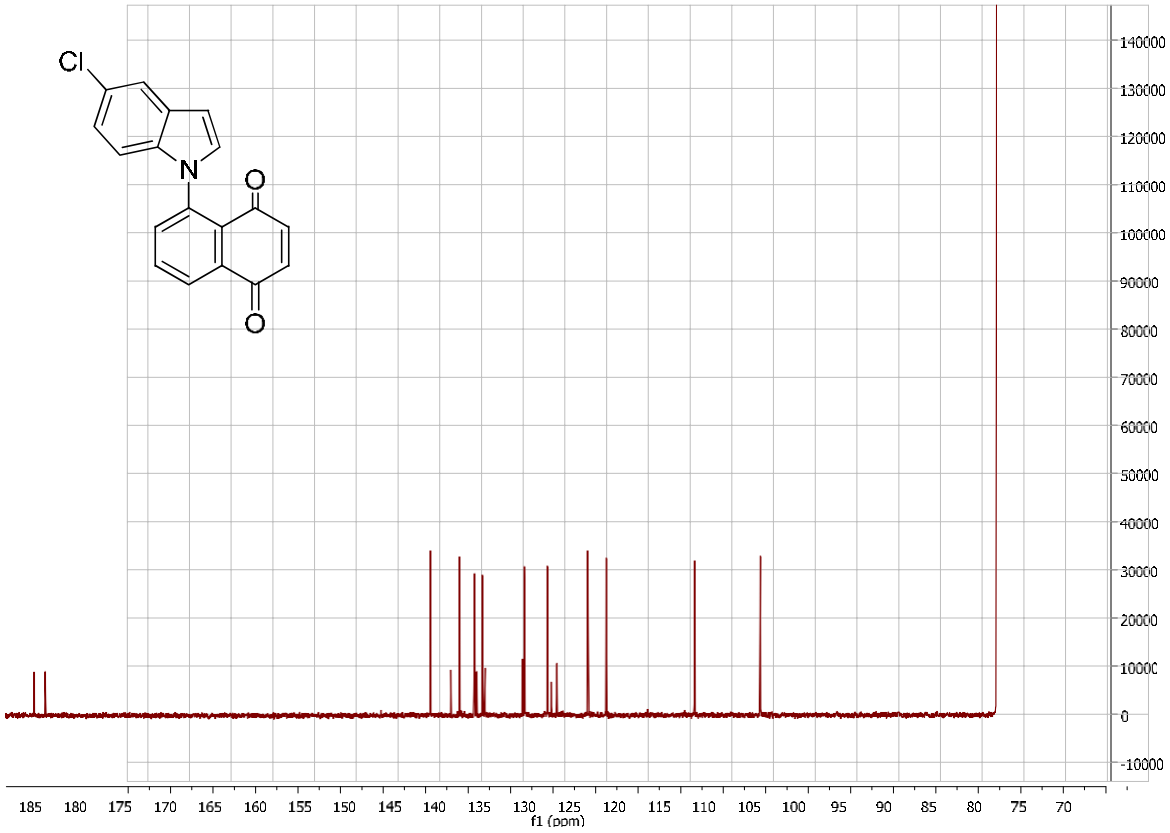
5-(5-bromo-1H-indol-1-yl)naphthalene-1,4-dione (2c): ^{13}C NMR (125MHz, $CDCl_3$)



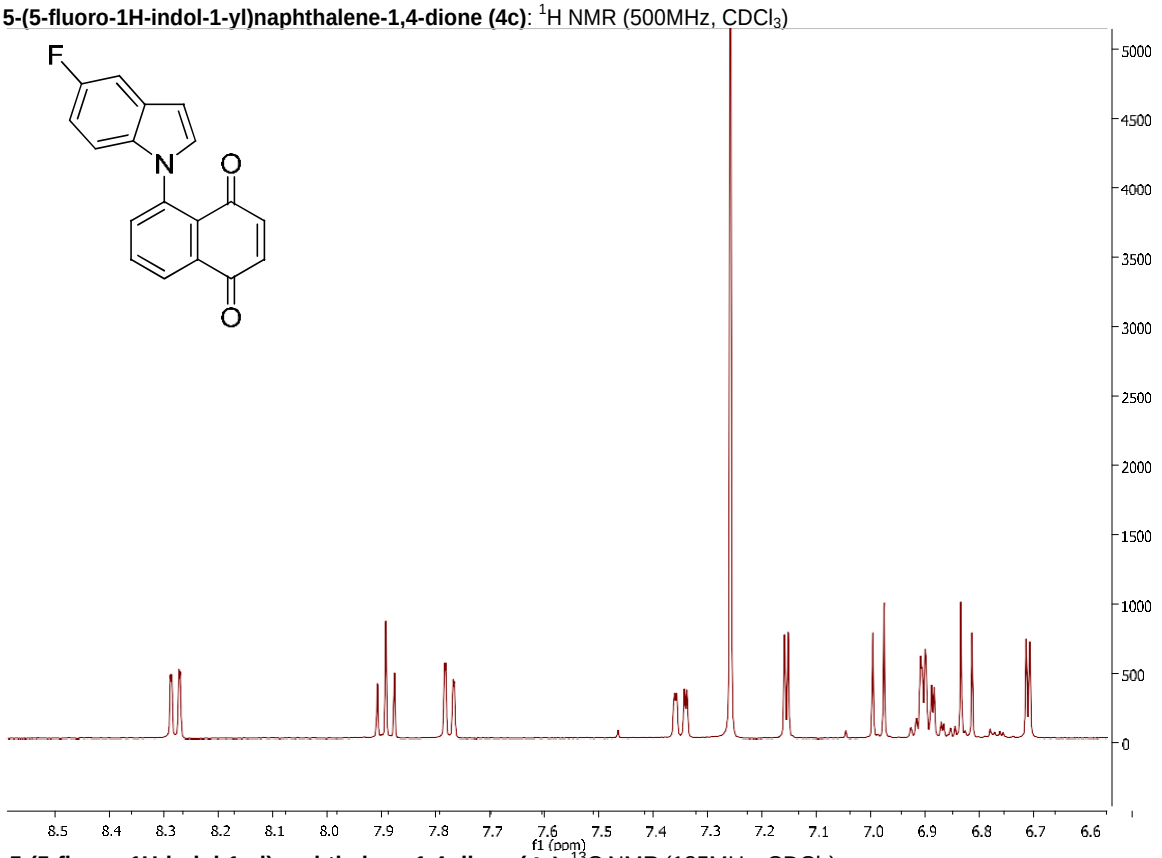
5-(5-chloro-1H-indol-1-yl)naphthalene-1,4-dione (3c): ^{1}H NMR (500MHz, $CDCl_3$)



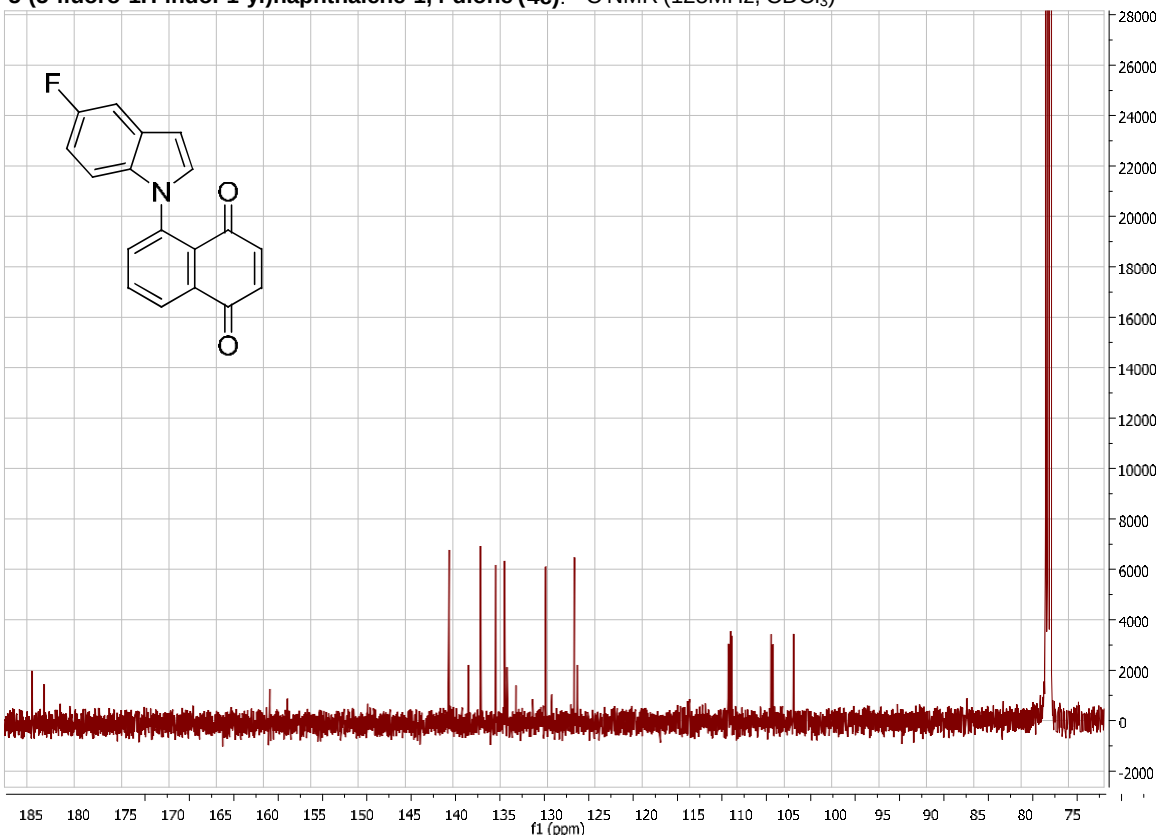
5-(5-chloro-1H-indol-1-yl)naphthalene-1,4-dione (3c): ^{13}C NMR (125MHz, $CDCl_3$)



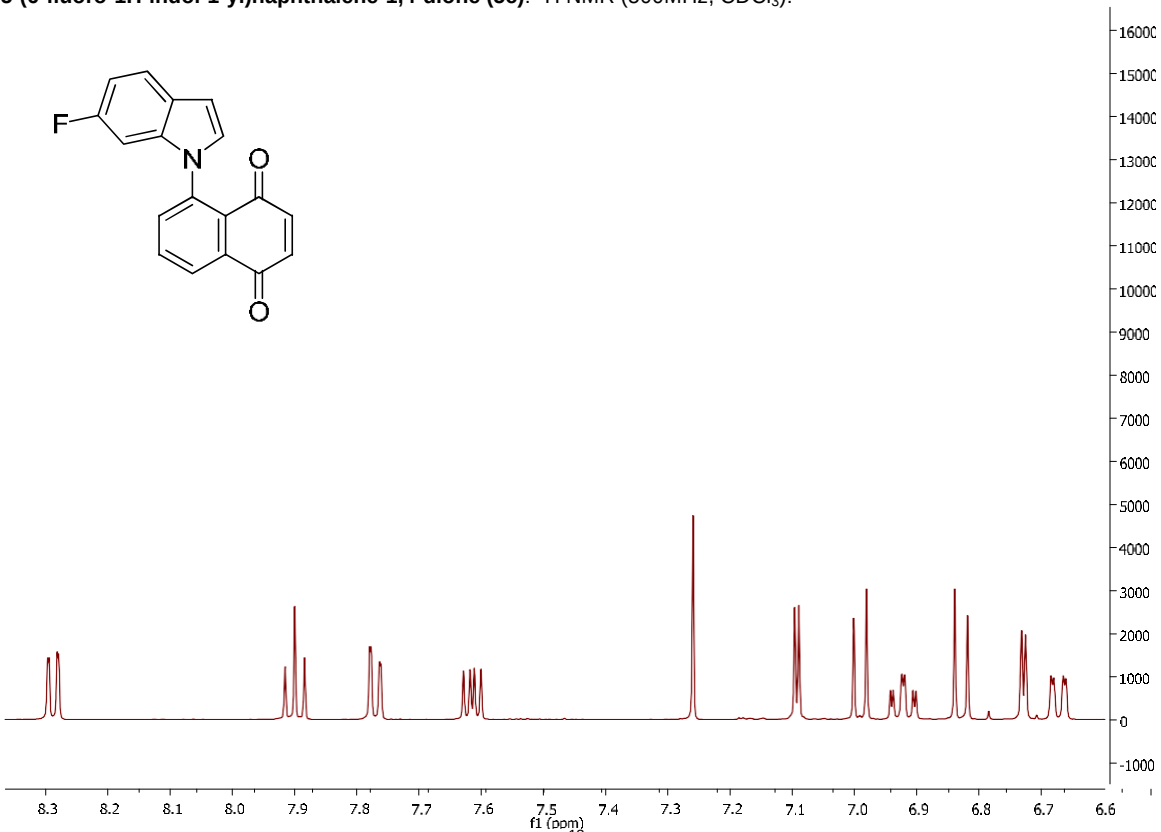
5-(5-fluoro-1H-indol-1-yl)naphthalene-1,4-dione (4c): ^{1}H NMR (500MHz, $CDCl_3$)



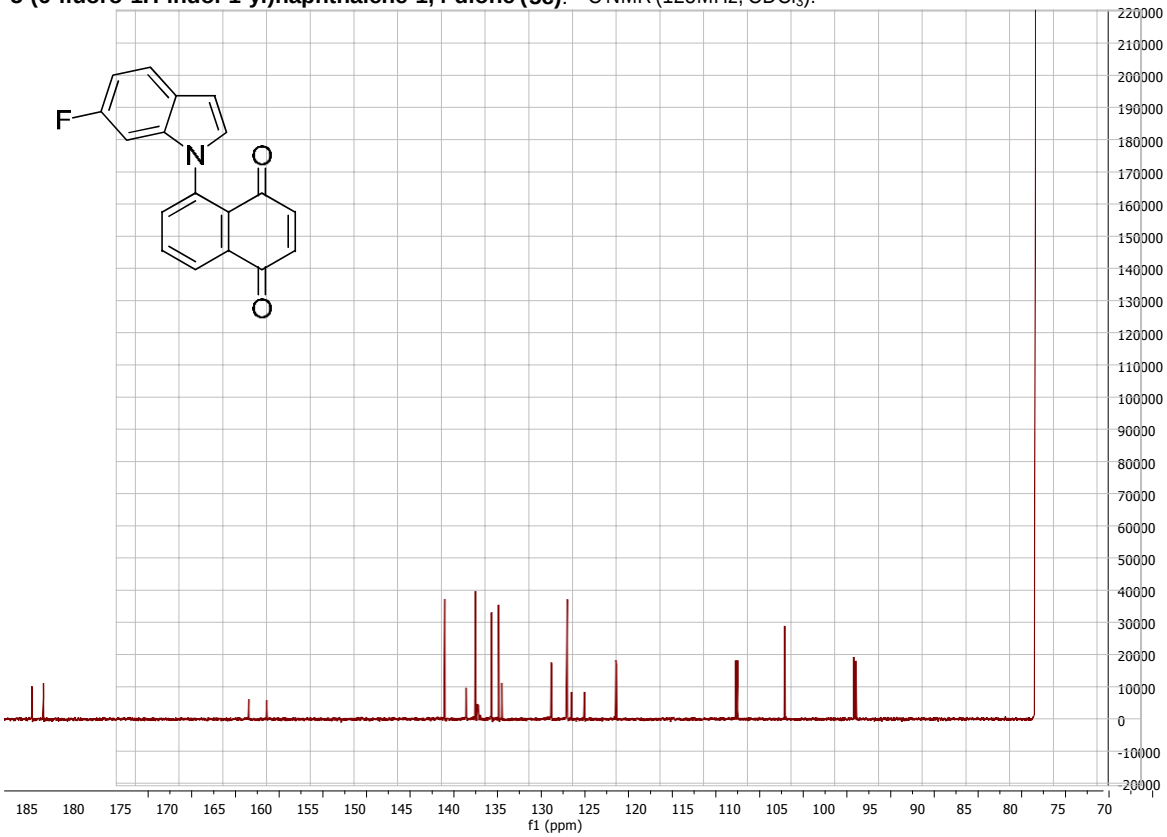
5-(5-fluoro-1H-indol-1-yl)naphthalene-1,4-dione (4c): ^{13}C NMR (125MHz, $CDCl_3$)



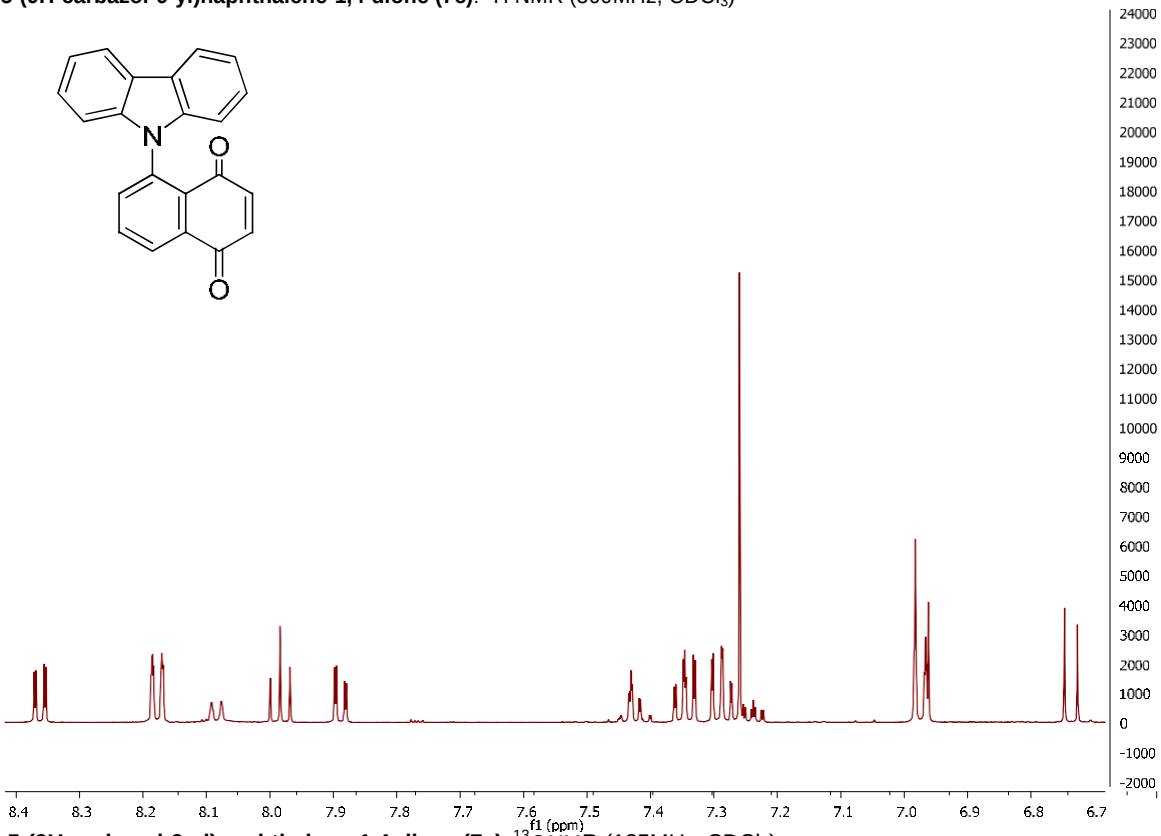
5-(6-fluoro-1H-indol-1-yl)naphthalene-1,4-dione (5c): ^{1}H NMR (500MHz, $CDCl_3$):



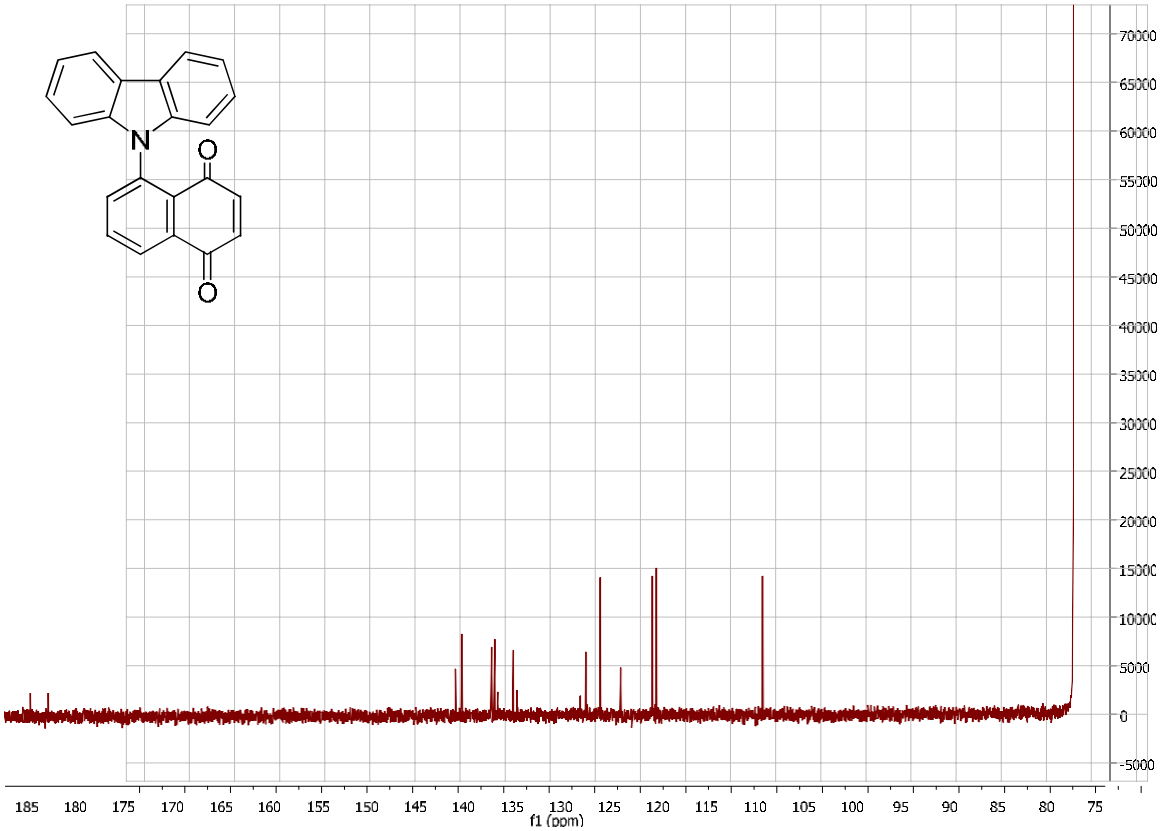
5-(6-fluoro-1H-indol-1-yl)naphthalene-1,4-dione (5c): ^{13}C NMR (125MHz, $CDCl_3$):



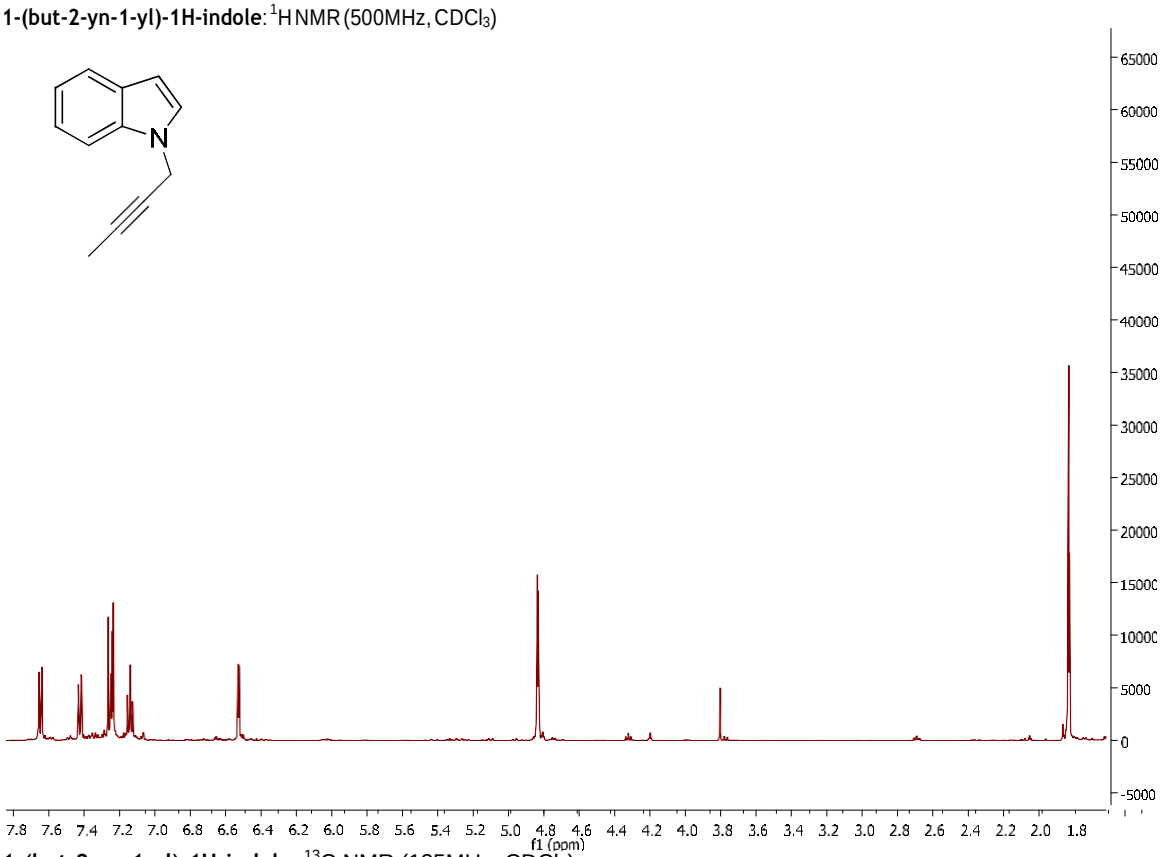
5-(9H-carbazol-9-yl)naphthalene-1,4-dione (7c): ^{1}H NMR (500MHz, $CDCl_3$)



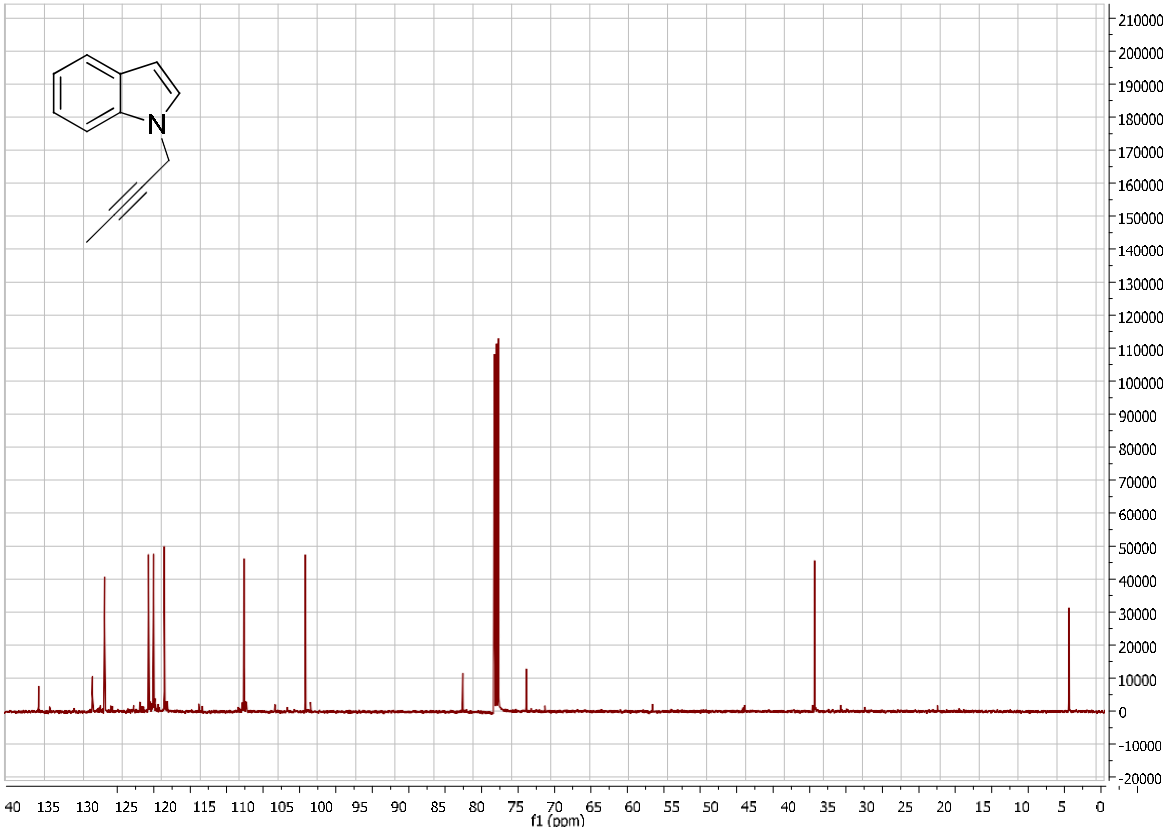
5-(9H-carbazol-9-yl)naphthalene-1,4-dione (7c): ^{13}CNMR (125MHz, $CDCl_3$)



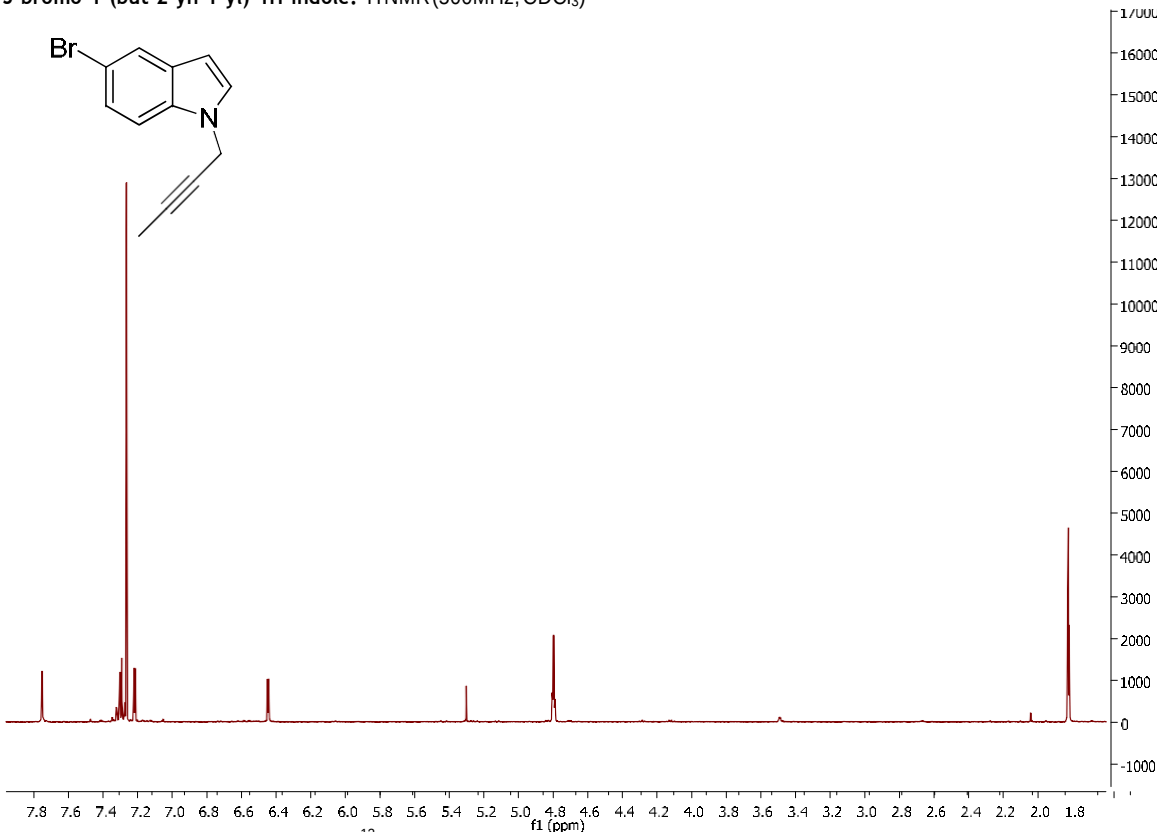
1-(but-2-yn-1-yl)-1H-indole: ^{1}H NMR (500MHz, $CDCl_3$)



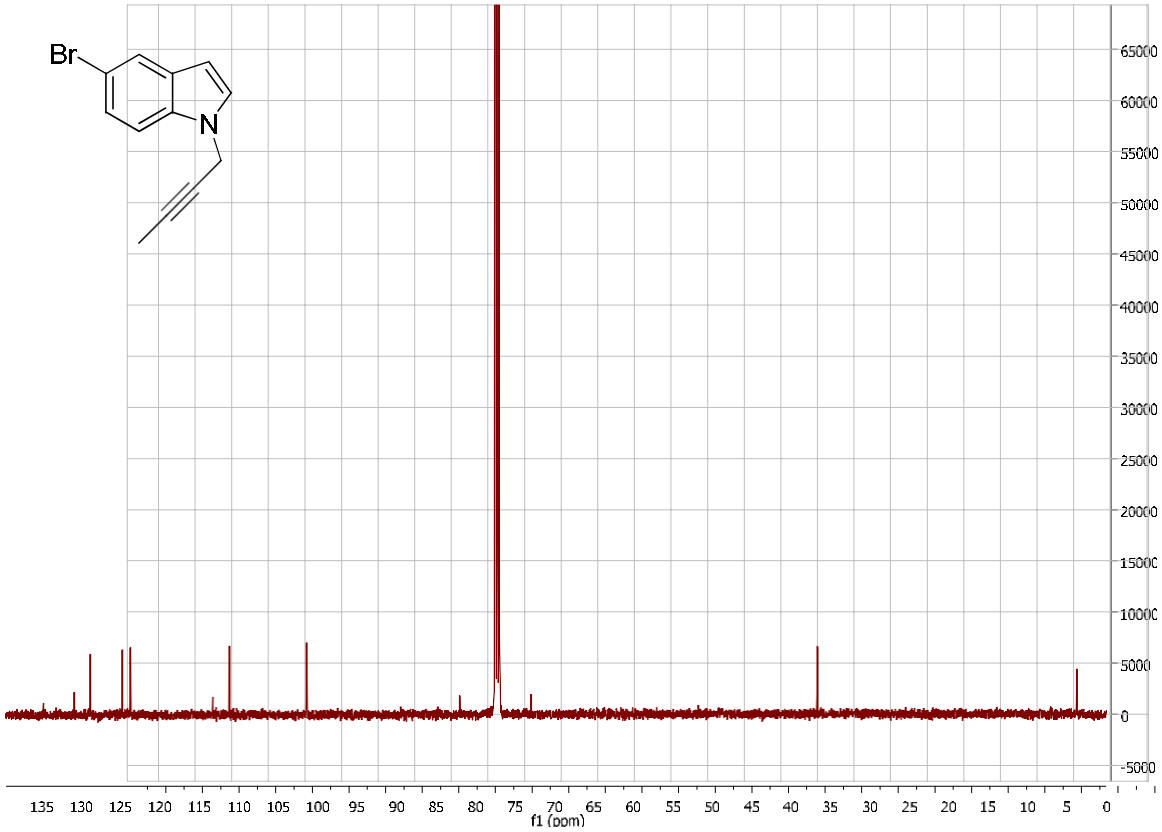
1-(but-2-yn-1-yl)-1H-indole: ^{13}C NMR (125MHz, $CDCl_3$)



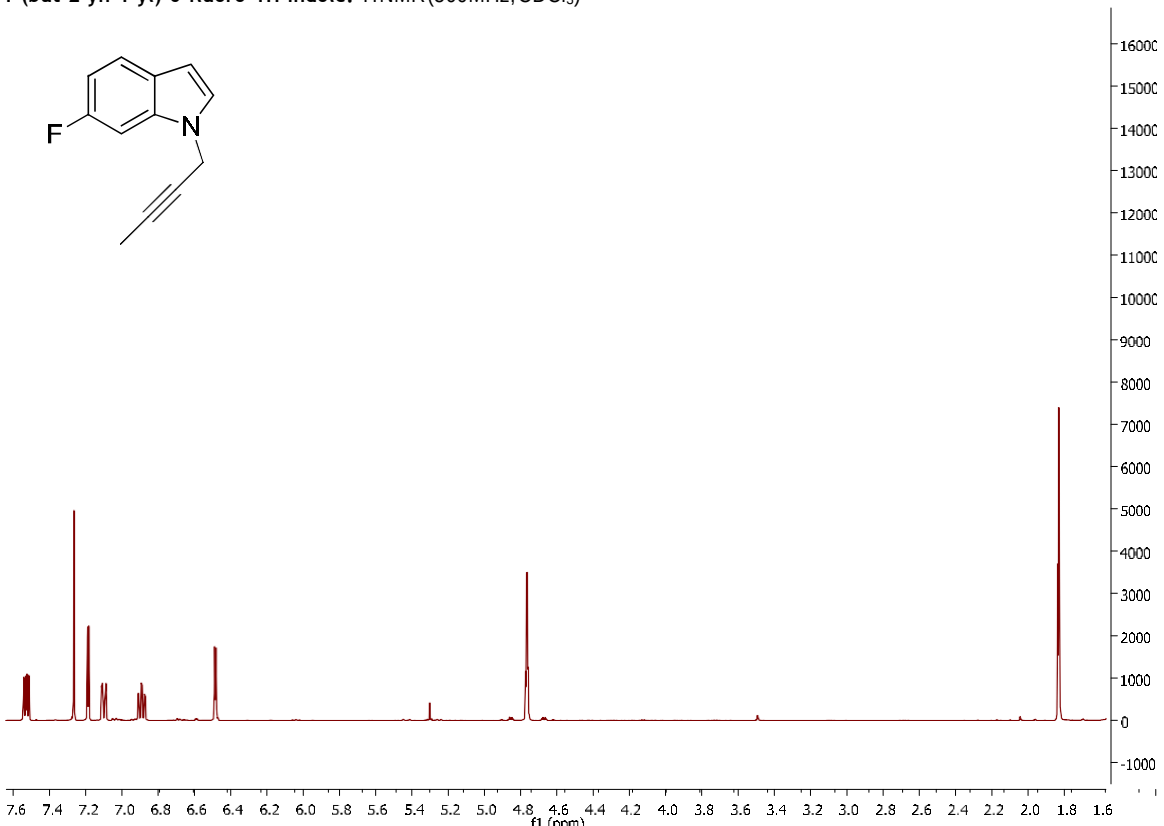
5-bromo-1-(but-2-yn-1-yl)-1H-indole: ^{1}H NMR (500MHz, $CDCl_3$)



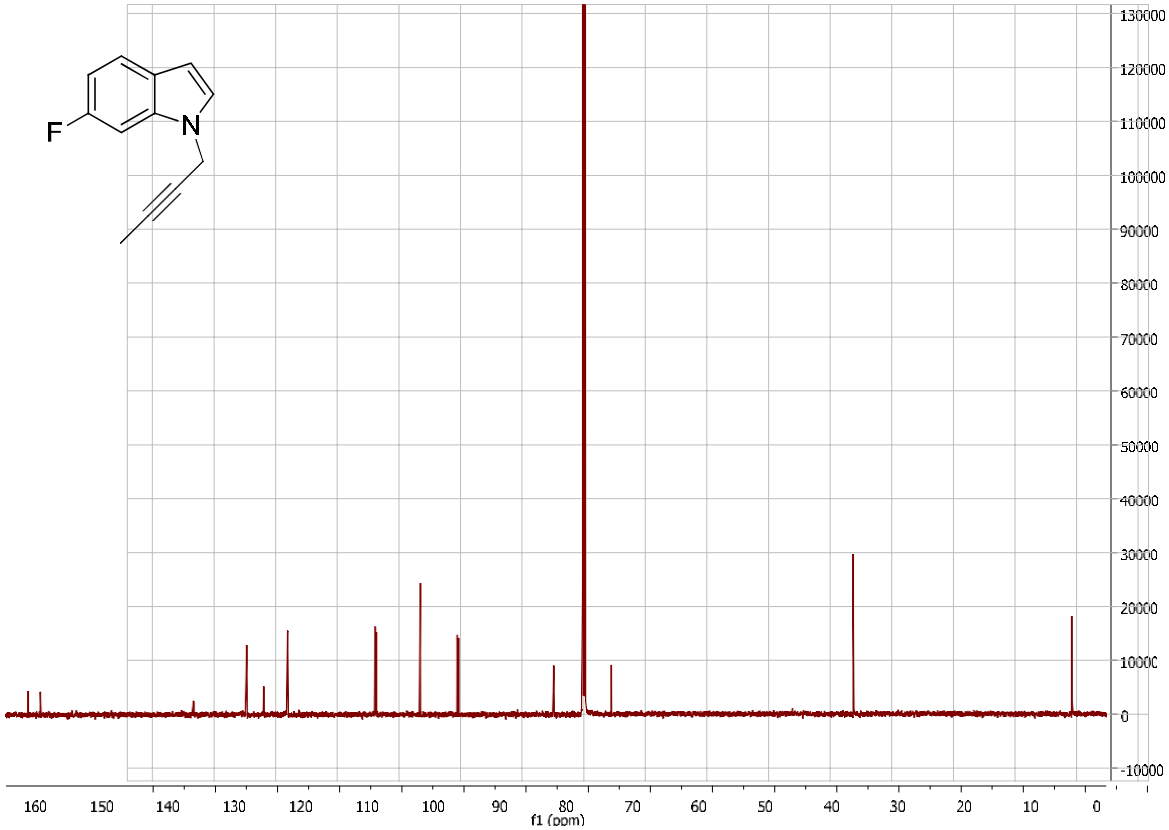
5-bromo-1-(but-2-yn-1-yl)-1H-indole: ^{13}C NMR (125MHz, $CDCl_3$)



1-(but-2-yn-1-yl)-6-fluoro-1H-indole: ^{1}HNMR (500MHz, $CDCl_3$)



1-(but-2-yn-1-yl)-6-fluoro-1H-indole: ^{13}C NMR (125MHz, $CDCl_3$)



Geometric parameters of the lowest-energy conformers of the molecules studied in the present work. Distances (r) are in angstroms and dihedral angles (t) are in degrees.

	7	8	9	10	11	12	1a, 1b
$r(C_{1'}\text{-}C_{2'})$	1.534	1.492	1.505	1.489	1.457	1.352	1.341
$r(C_{2'}\text{-}C_{3'})$	1.452	1.342	1.301	1.275	1.202	1.429	1.443
$r(C_{3'}\text{-}C_{4'})$	1.203	1.277	1.300	1.341	1.448	1.337	1.337
$r(N\text{-}C_{1'})$	1.441	1.474	1.447	1.460	1.447	1.414	1.383
$r(C_2\text{-}N)$	1.372	1.366	1.370	1.366	1.371	1.373	1.382
$r(C_{7a}\text{-}N)$	1.373	1.370	1.372	1.367	1.370	1.375	1.385
$t(C_2\text{-}N\text{-}C_{1'}\text{-}C_{2'})$	-86.80	-39.05	93.8	117.18	-113.80	-5.35	10.82
$t(N\text{-}C_{1'}\text{-}C_{2'}\text{-}C_{3'})$	-169.14	98.42	110.91	164.59	-144.90	167.69	-179.05
$t(C_{1'}\text{-}C_{2'}\text{-}C_{3'}\text{-}C_{4'})$						75.20	-178.79

Energy diagram for the C5 alkyne isomerization. Species are numbered in analogy with those in C4.