

SUPPORTING INFORMATION

Studies of axially chiral atropisomers of an indole-substituted phthalonitrile

Derivative

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¹H NMR spectrum of compound 1 (DMSO-d₆, 500MHz)

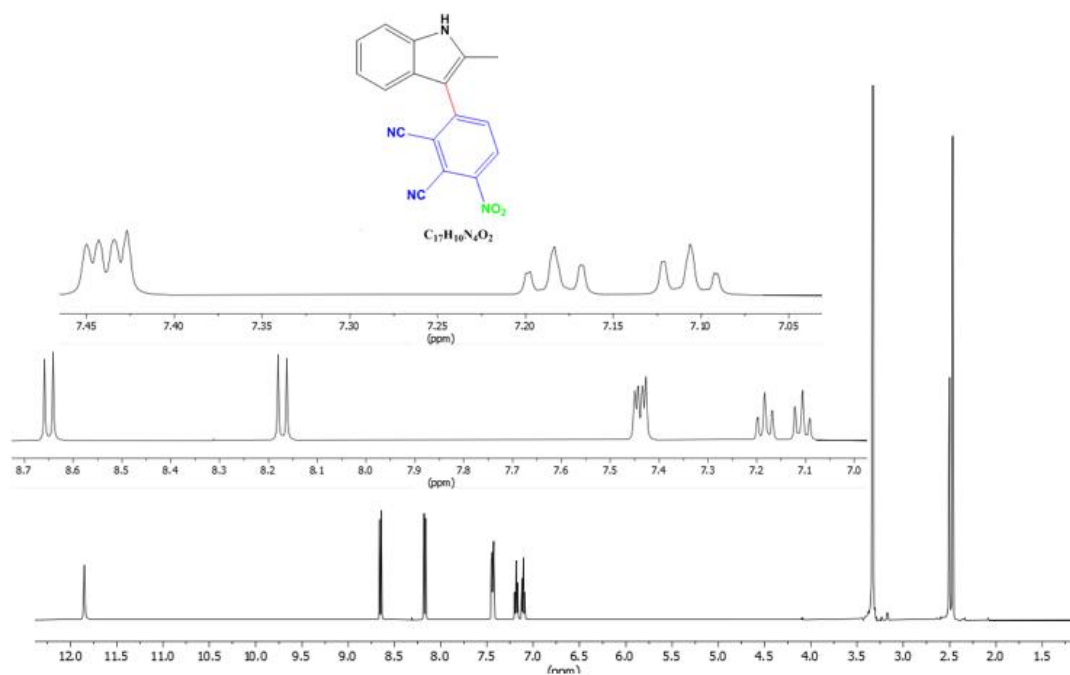


Figure 1: ¹H NMR spectrum of compound 1 (DMSO-d₆, 500MHz)

¹³C NMR spectrum of compound 1 (DMSO-d₆, 500MHz)

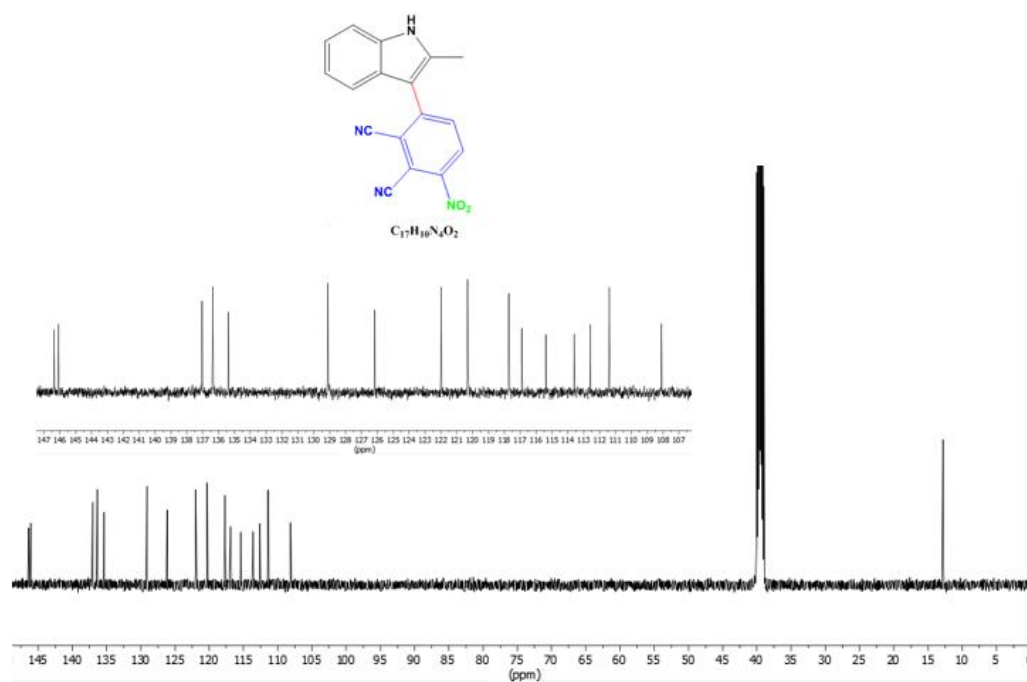


Figure 2: ¹³C NMR spectrum of compound 1 (DMSO-d₆, 500MHz)

Mass spectrum of compound 1



Figure 3: Mass spectrum of compound 1

Table 1. Atomic charge of **1** / B3LYP/6-311+G(d,p)

C 1	-0.306435	C 1
C 2	1.016547	C 2
C 3	-0.853723	C 3
C 4	-0.372516	C 4
C 5	-0.215889	C 5
C 6	-0.558119	C 6
C 7	-0.042428	C 7
C 8	0.710581	C 8
H 9	0.143726	H 9
H 10	0.144263	H 10
H 11	0.146884	H 11
H 12	0.140918	H 12
H 13	0.35258	H 13
N 14	-0.054832	N 14
C 15	-0.734683	C 15
H 16	0.196938	H 16
H 17	0.172886	H 17
H 18	0.171677	H 18
C 19	0.454169	C 19
C 20	2.017888	C 20
C 21	-0.512532	C 21
C 22	1.876063	C 22
C 23	-0.353055	C 23
H 24	0.18143	H 24
C 25	-0.774381	C 25
H 26	0.189427	H 26
C 27	-1.459249	C 27
N 28	-0.211078	N 28
C 29	-0.992569	C 29
N 30	-0.254836	N 30
N 31	-0.143973	H 31
O 32	-0.018756	
O 33	-0.05692	