

SUPPLEMENTARY INFORMATION

Special Section on Transition Metal Catalyzed Synthesis of Medicinally Relevant Molecules

REGULAR ARTICLE

Delineating an alternate convergent synthesis of Brexpiprazole: A novel use of commercial 6,7-dihydrobenzo[*b*]thiophen-4(5*H*)-one as precursor to an efficacious Buchwald-Hartwig amination step

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DR15-BL-062-199 in CDCl3
 1H NMR
 A.R. NO: NA170277
 Sample Name:
 Data Collected on:
 DR15-vms400
 Archive directory:
 Sample directory:
 FidFile: NA170277
 Pulse Sequence: FROGOM (zgpg3)
 Solvent: cdcl3
 Data collected on: Jul 25 2017

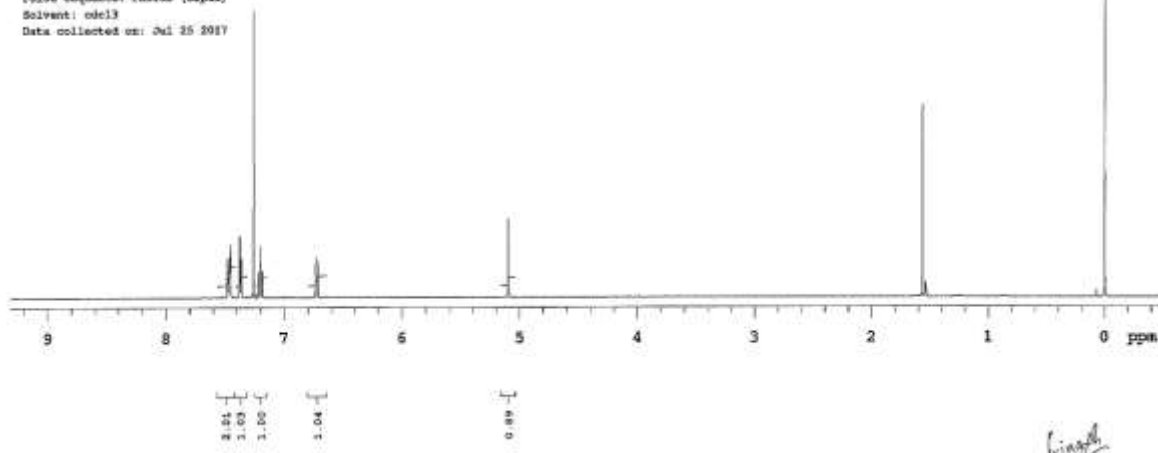
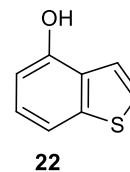


Fig S1: ¹H NMR of 22

DR15-BL-199 in CDCl3
 13C NMR
 A.R. NO: NA170322
 Sample Name:
 Data Collected on:
 DR15-vms400
 Archive directory:
 Sample directory:
 FidFile: NA170322
 Pulse Sequence: GANON (zgpg3)
 Solvent: cdcl3
 Data collected on: Jul 27 2017

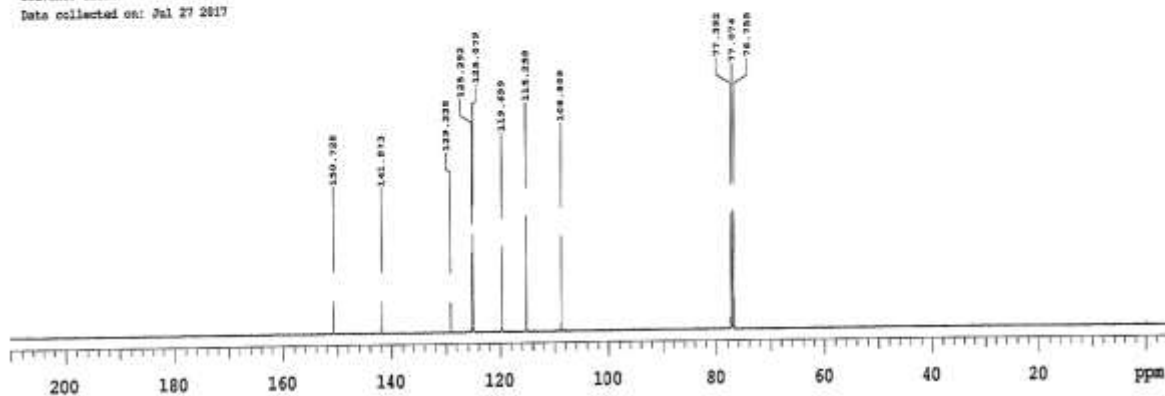
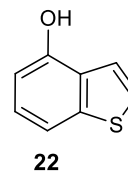


Fig S2: ¹³C NMR of 22

BPL-CPRII-148 in CDCl3
 A.R.NO: MA16R069

Sample Name:

Data Collected on:
 DRILS-vnmrs400
 Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Aug 5 2016

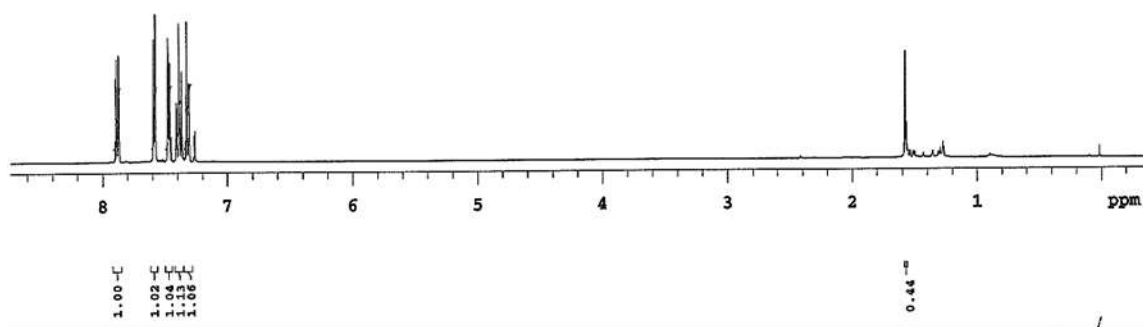
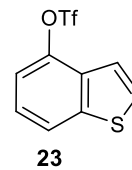


Fig S3: ¹H NMR of 23

DRILS-LMR37-208 in CDCl3
 13C NMR
 A R NO: MA17G092

Sample Name:

Data Collected on:
 DRILS-vnmrs400
 Archive directory:

Sample directory:

FidFile: MA17G092

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jul 10 2017

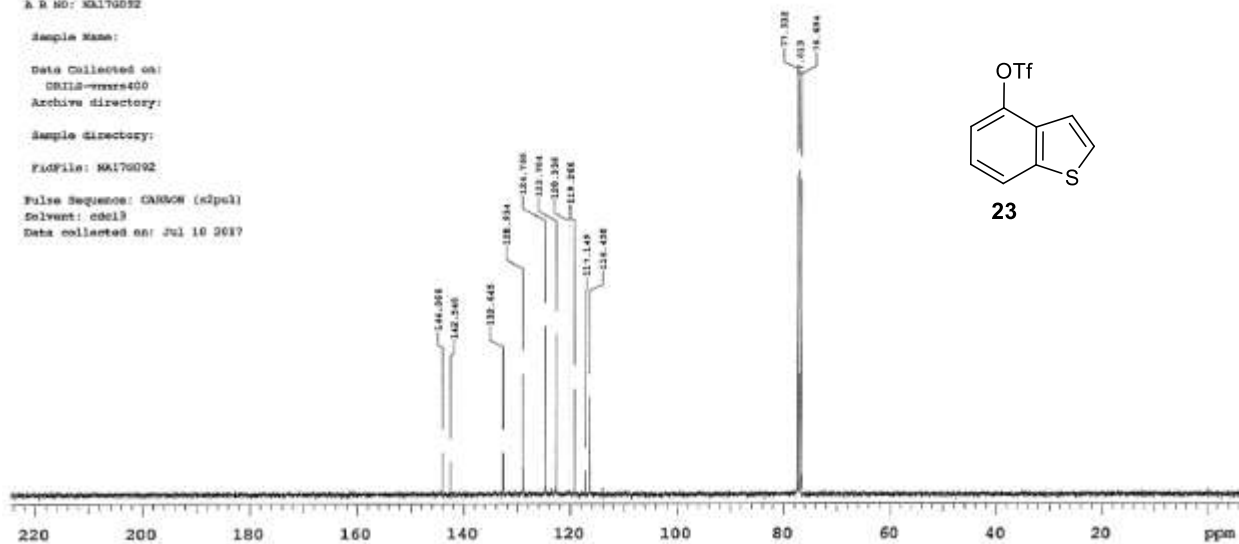
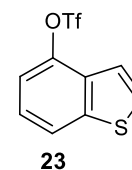


Fig S4: ¹³C NMR of 23

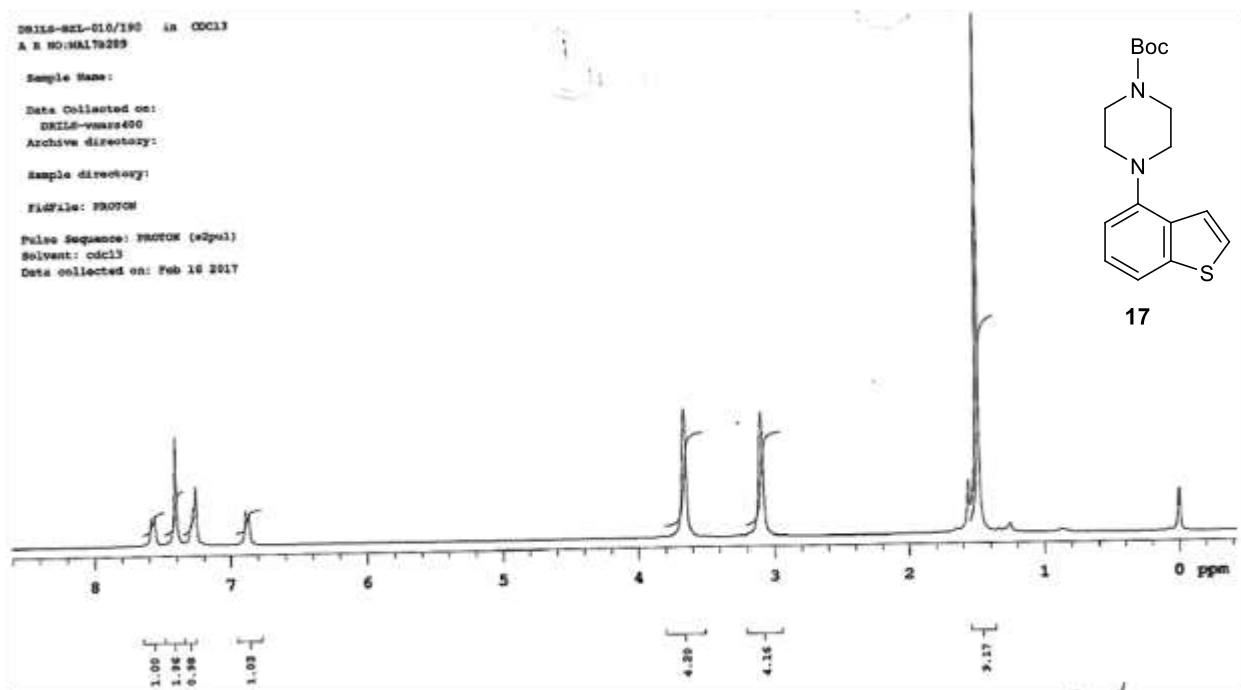


Fig S5: ^1H NMR of 17

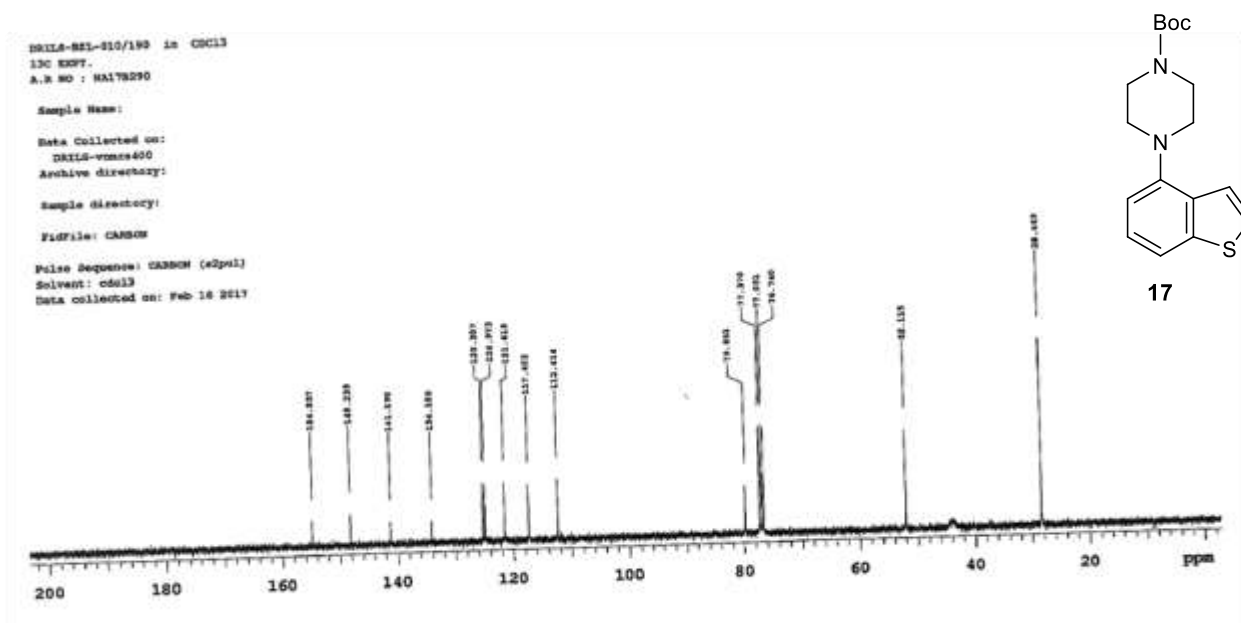


Fig S6: ^{13}C NMR of 17

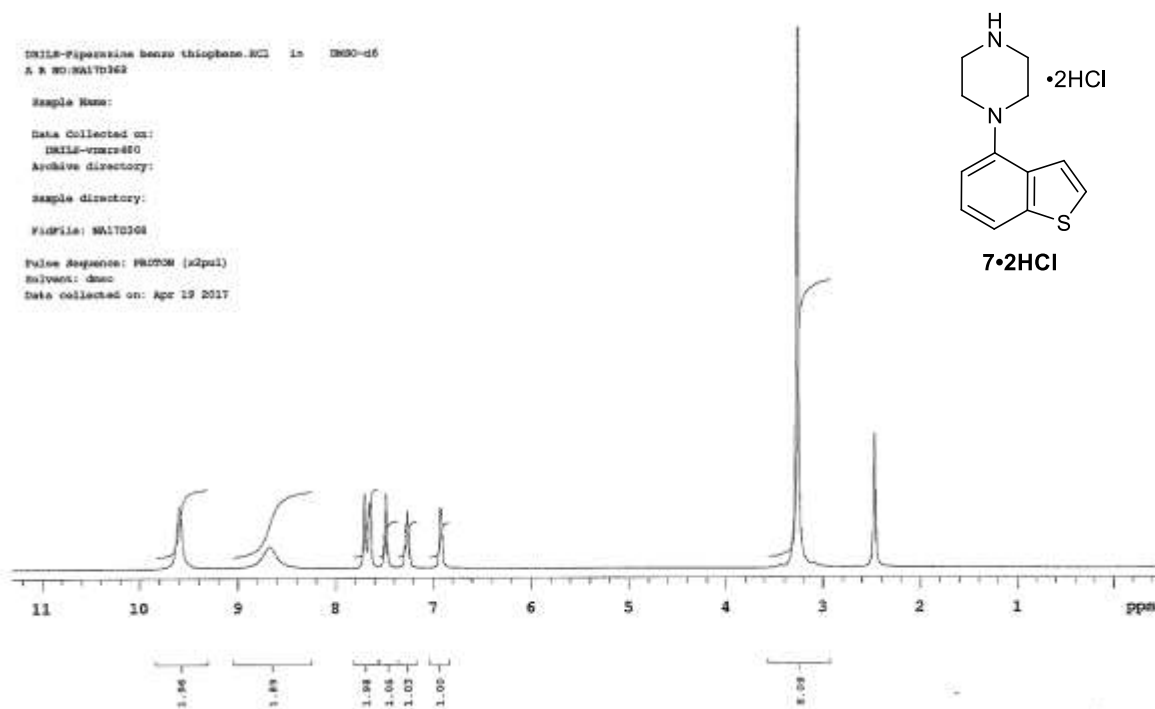


Fig S7: ^1H NMR of 7•2HCl (Table 1, Entry 10)

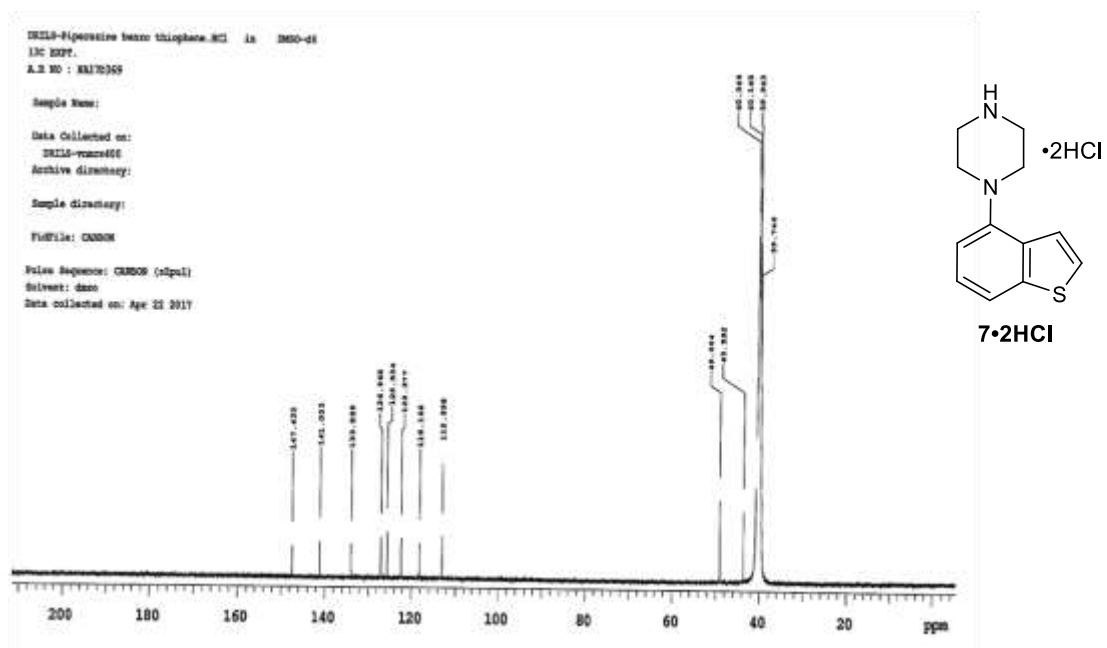


Fig S8: ^{13}C NMR of 7•2HCl (Table 1, Entry 10)

BPL/CPRI/121 in DMSO-d6
A.N.NO: HA16F276

Sample Name:

Date Collected on:
DRHS-vvms400
Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: Jun 29 2016

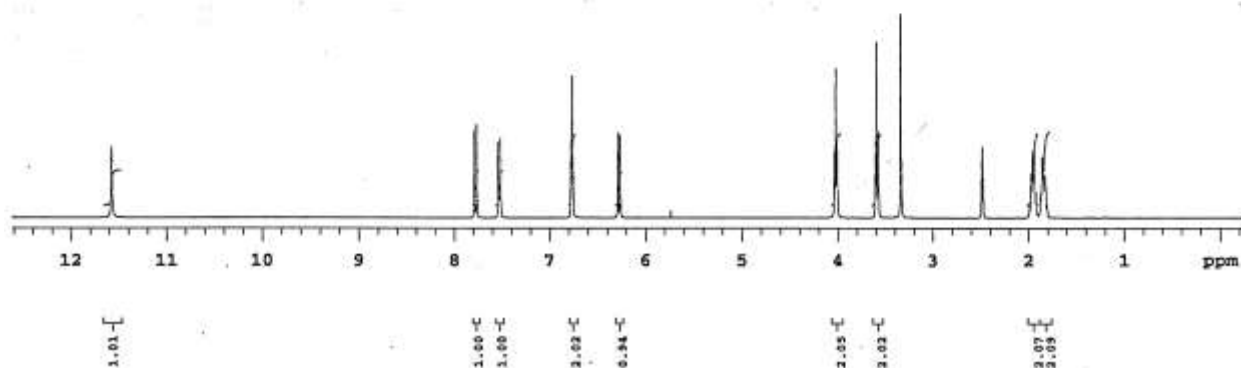
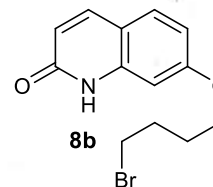


Fig S9: ¹H NMR of 8b

BPL/CPRI/121 in DMSO-d6
13C EXPT
A.N.NO: HA16F277

Sample Name:

Date Collected on:
DRHS-vvms400
Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: dmsd
Data collected on: Jun 29 2016

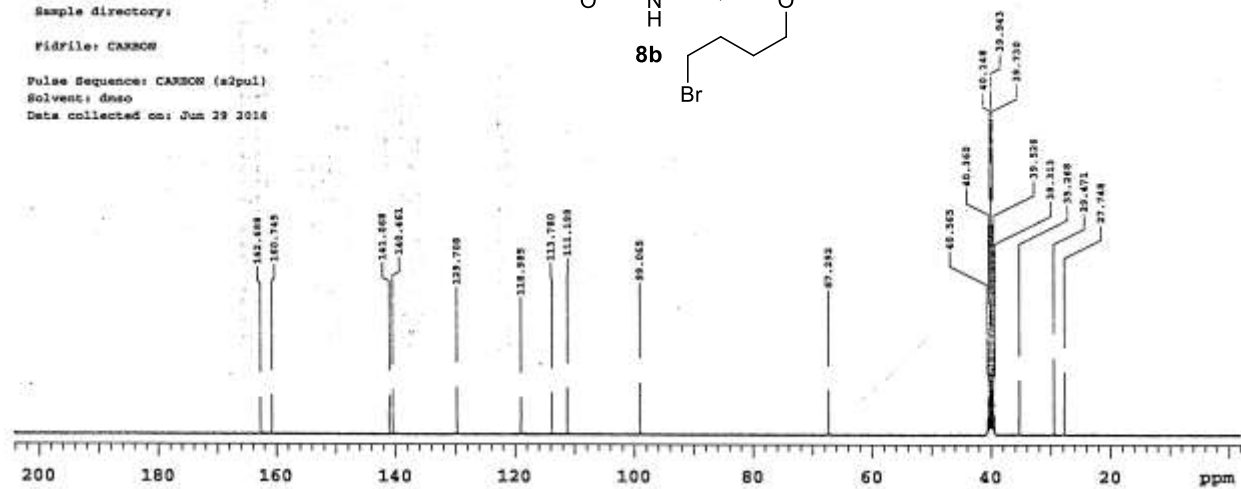
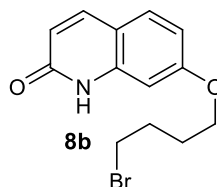


Fig S10: ¹³C NMR of 8b

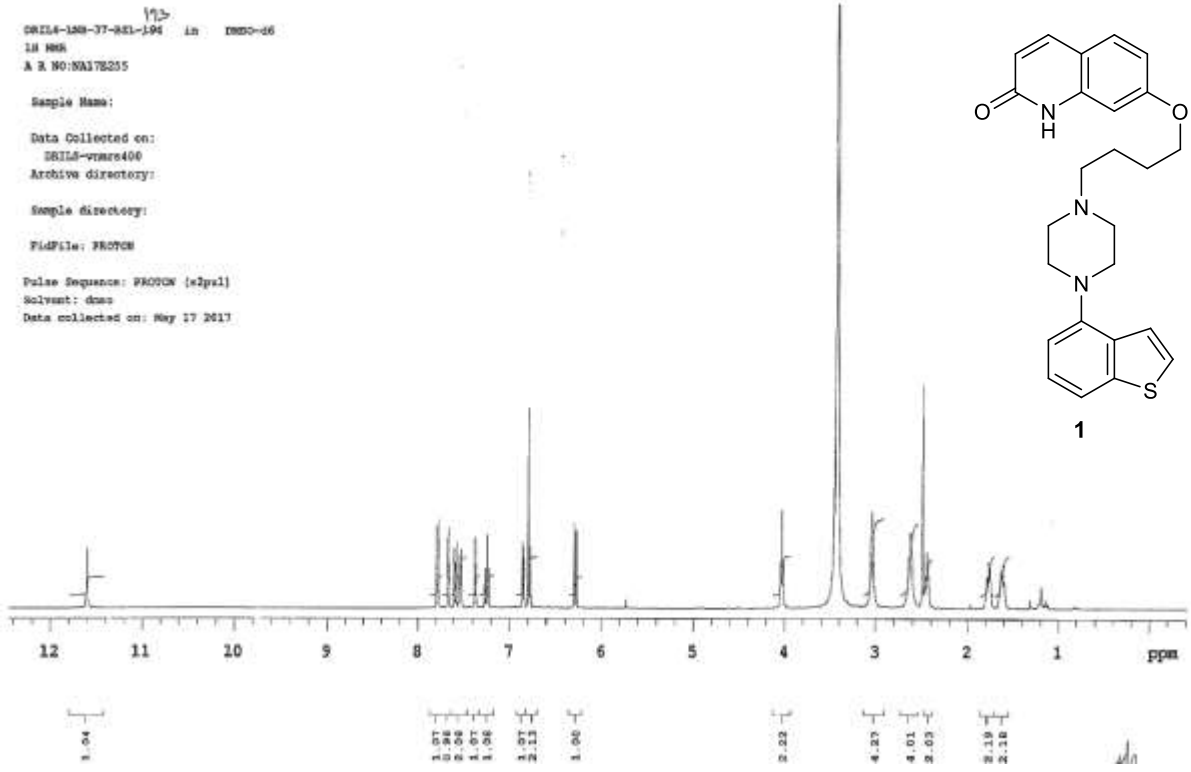


Fig S11: ¹H NMR of 1



Fig S12: ¹³C NMR of 1