

Supplementary Materials: Article Synthesis and Biological Activities of Ethyl 2-(2-pyridylacetate) Derivatives Containing Thiourea, 1,2,4-triazole, Thiadiazole and Oxadiazole Moieties

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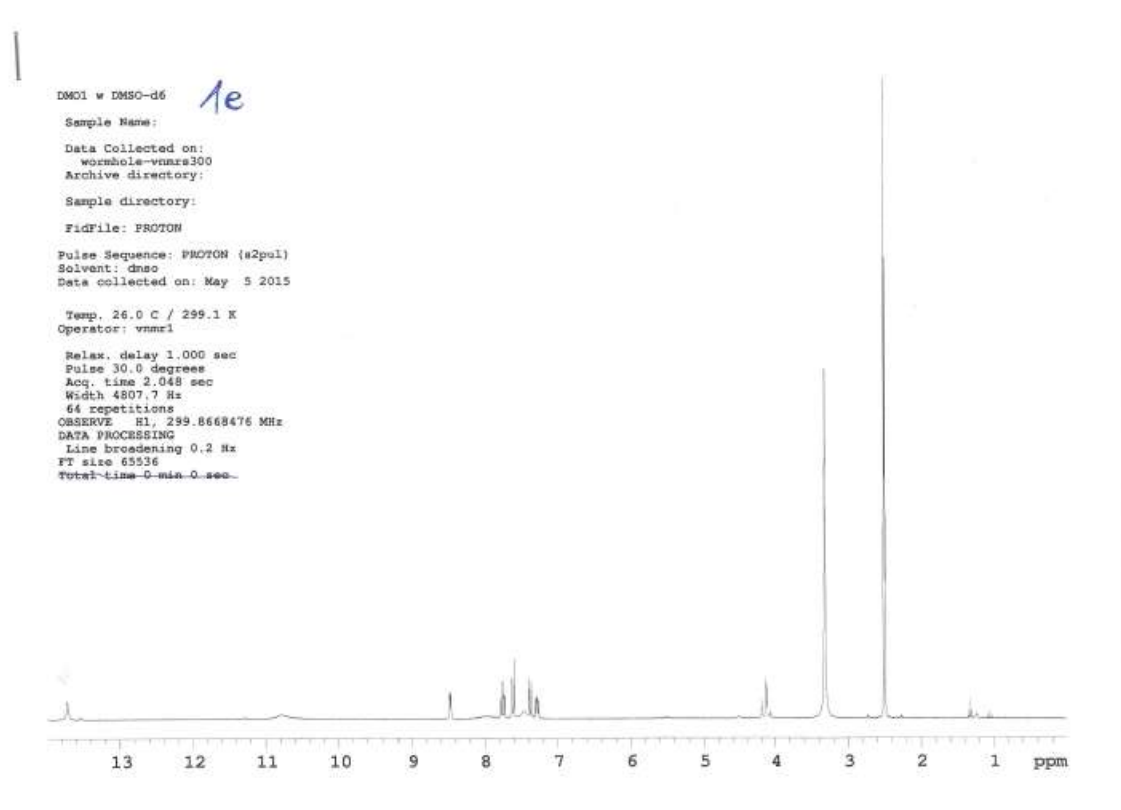


Figure S1. ¹H-NMR-1e-Sample.

DMO2 1H w DMSO

2e

Sample Name:

Data Collected on:
wormhole-vnmrs300

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: May 15 2015

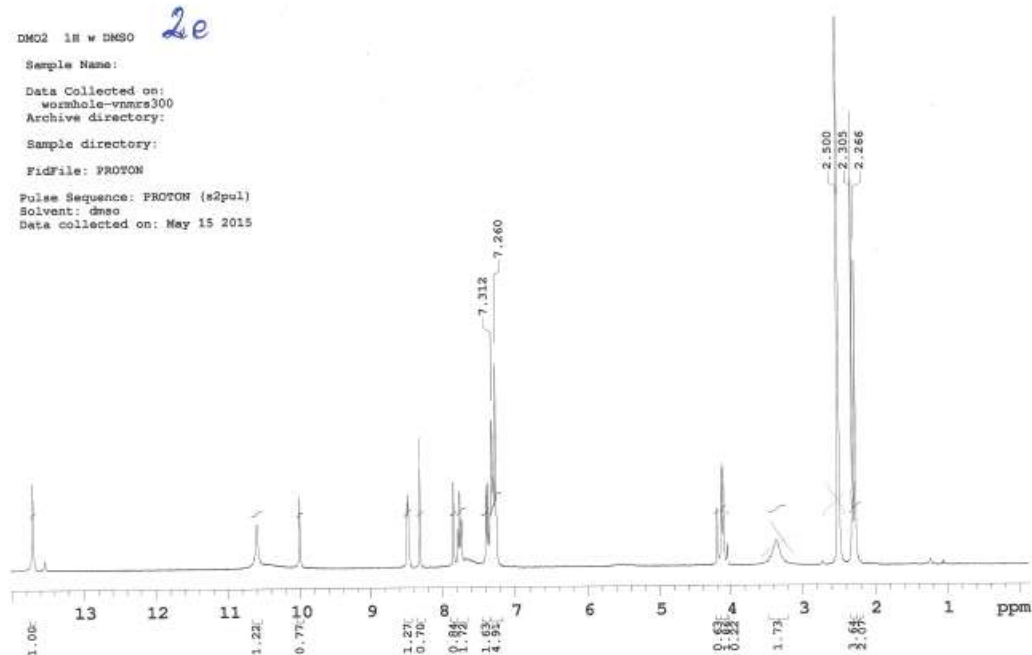


Figure S2. ¹H-NMR-2e-Sample.

NSS2 w DMSO

3e

Sample Name:

Data Collected on:
wormhole-vnmrs300

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: Mar 23 2015

Temp. 26.0 C / 299.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 2.048 sec
Width 4807.7 Hz
64 repetitions

OBSERVE H1, 299.8668481 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min 0.000

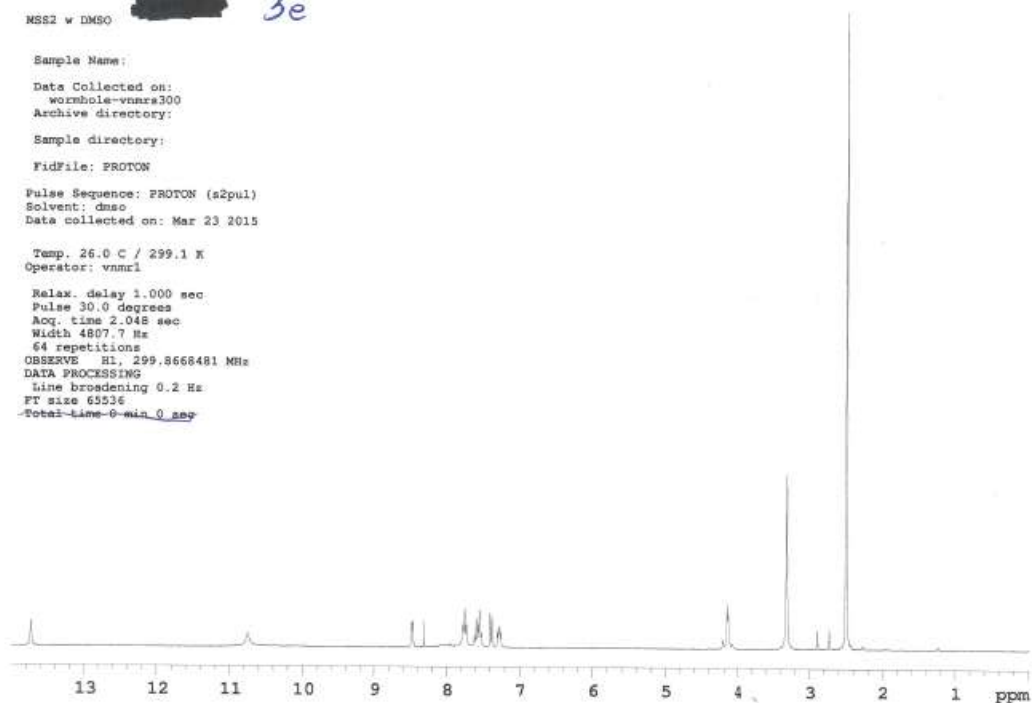


Figure S3. ¹H-NMR-3e-Sample.

DMO4 w DMSO-d6

Sample Name:

Data Collected on:
wormhole-vnmr300

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: May 12 2015

Temp. 26.0 C / 299.1 K

Operator: vnmr1

Relax. delay 1.000 sec

Pulse 30.0 degrees

Acq. time 2.048 sec

Width 4807.7 Hz

64 repetitions

OBSERVE H1, 299.8668478 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min 0 sec

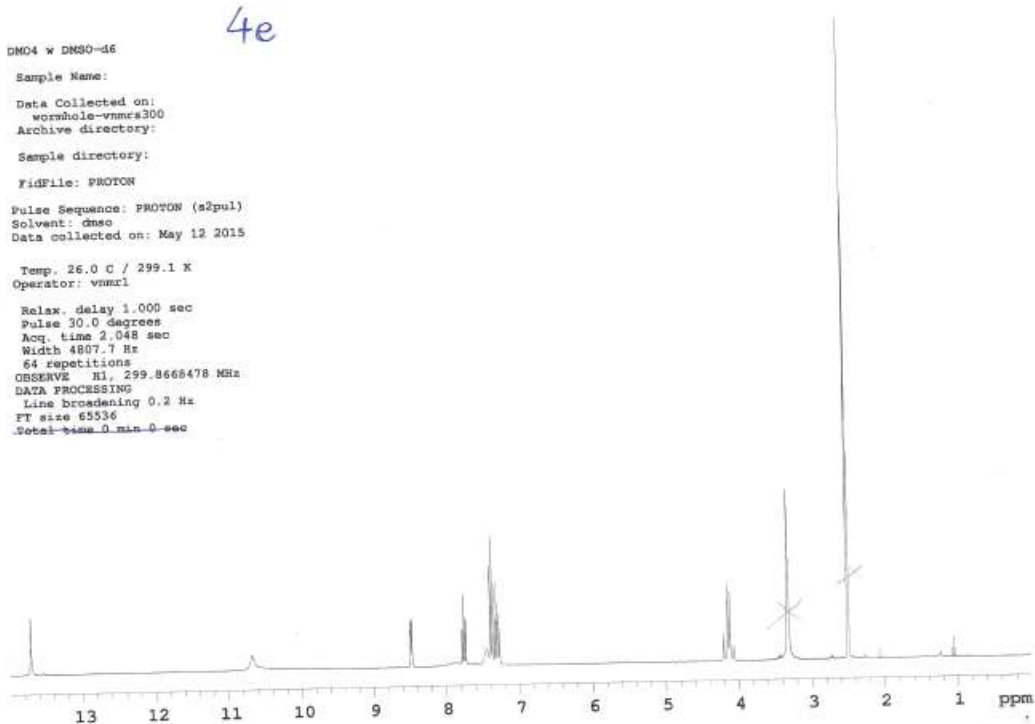


Figure S4. ¹H-NMR-4e-Sample.

MSS-1 w DMSO

Sample Name:

Data Collected on:
wormhole-vnmr300

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: dmsc

Data collected on: Apr 8 2015

Temp. 26.0 C / 299.1 K

Operator: vnmr1

Relax. delay 1.000 sec

Pulse 30.0 degrees

Acq. time 2.048 sec

Width 4807.7 Hz

64 repetitions

OBSERVE H1, 299.8668479 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min 0 sec

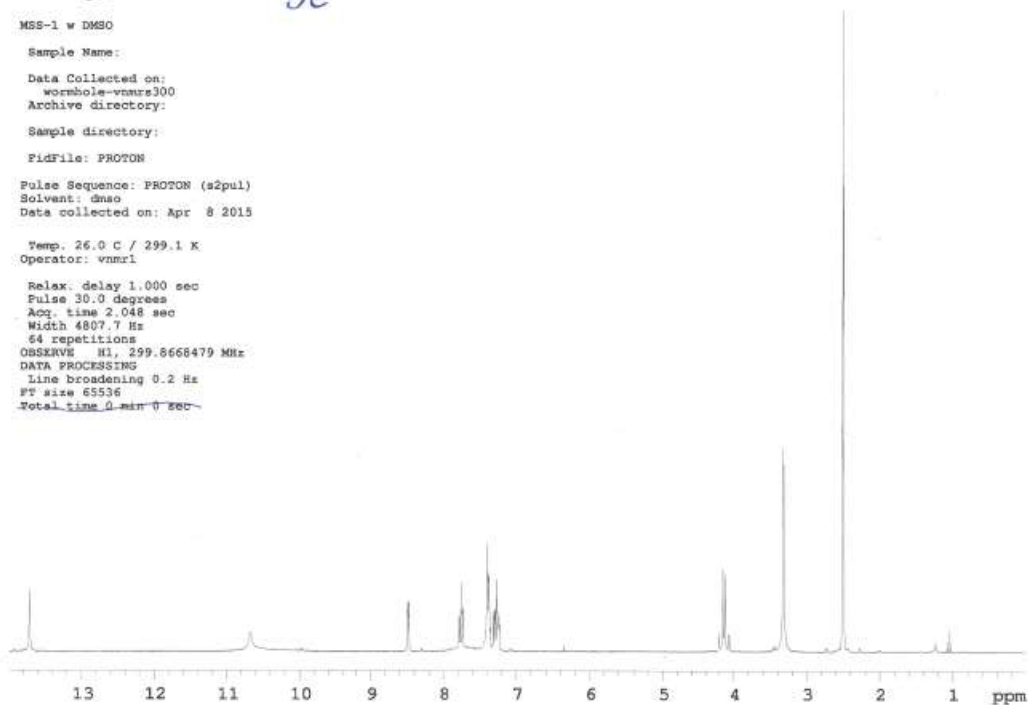


Figure S5. ¹H-NMR-5e-Sample.

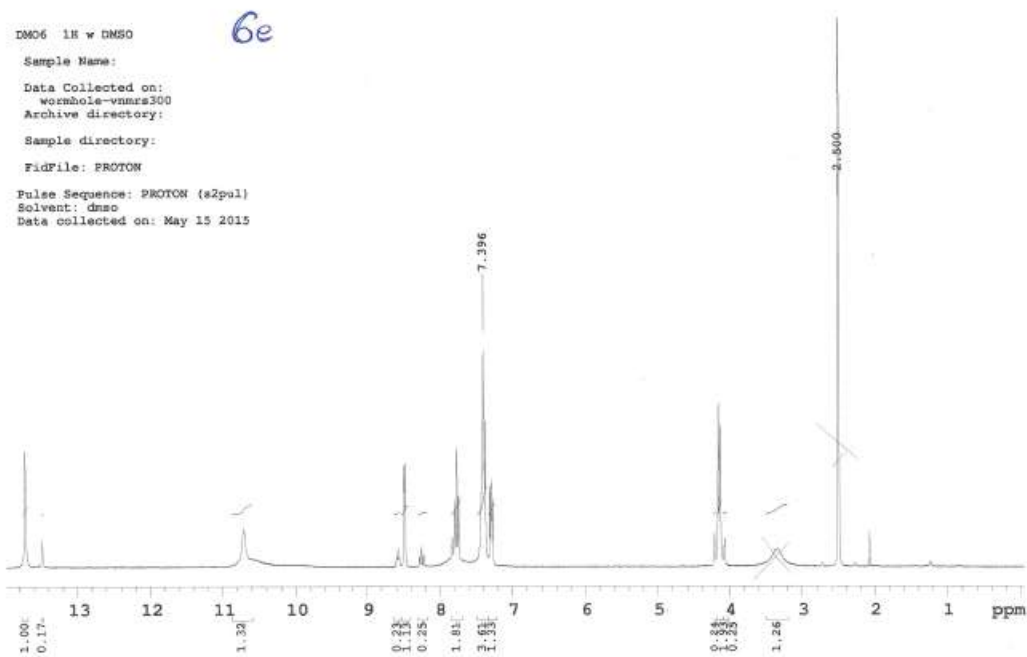


Figure S6. ¹H-NMR-6e-Sample.

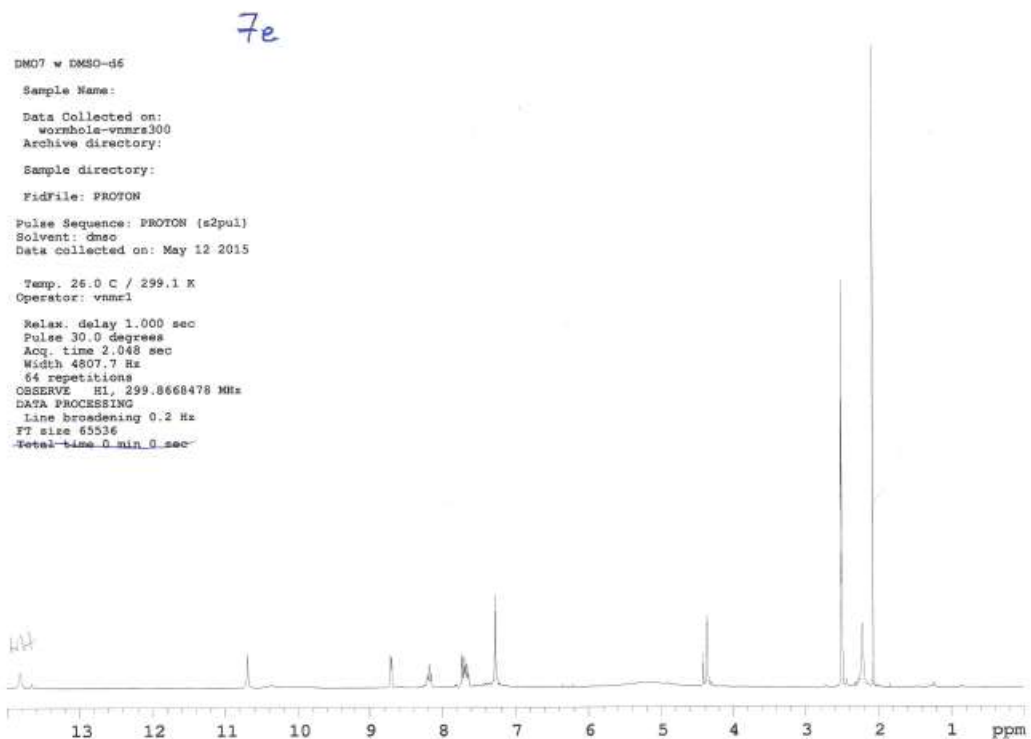


Figure S7. ¹H-NMR-7e-Sample.

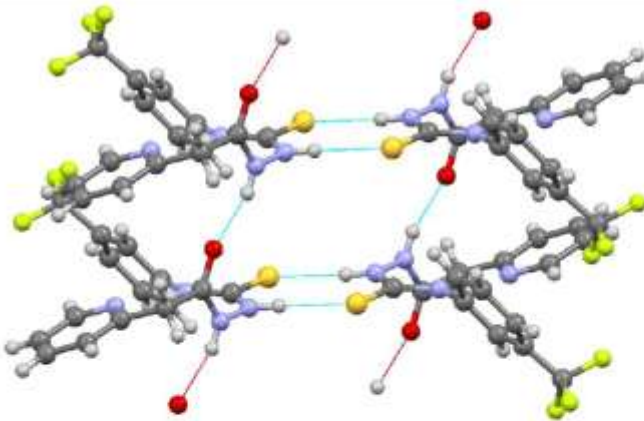
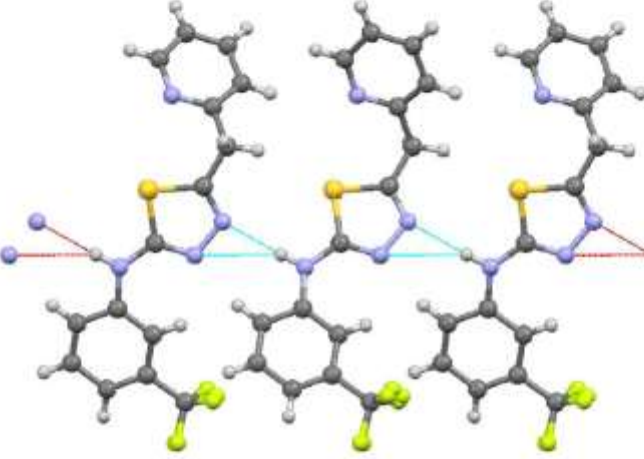
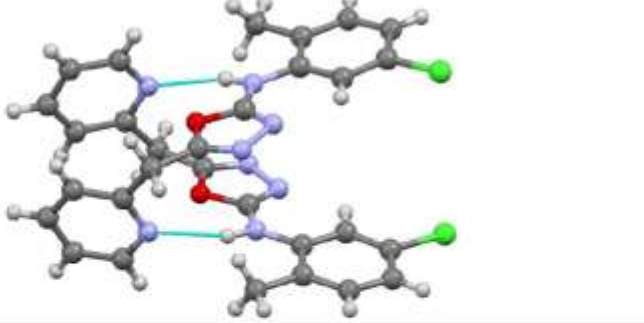
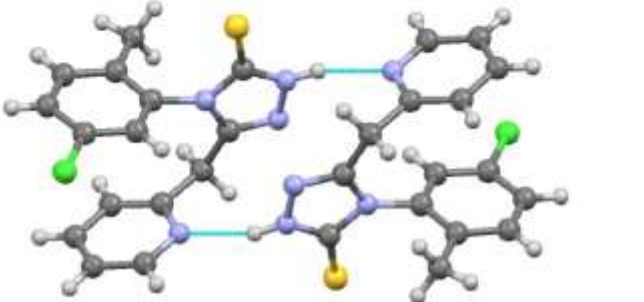
	2-(pyridin-2-ylacetyl)-N-[3-(trifluoromethyl)phenyl]hydrazinecarbothioamide (3) Hydrogen bonds: NH...S (thiourea...thiourea) stabilize dimers NH...O (amide...amide) form chains Resulting association: tape with hydrophobic groups oriented outside
	5-(pyridin-2-ylmethyl)-N-[3-(trifluoromethyl)phenyl]-1,3,4-thiadiazol-2-amine (3b) NH...N hydrogen bonds join molecules into chains
	N-(2-chloro-5-methylphenyl)-5-(pyridin-2-ylmethyl)-1,3,4-oxadiazol-2-amine (7f) NH...N hydrogen bonds (amine...pyridyl) form dimer with crystallographic symmetry of two-fold axis
	4-(5-chloro-2-methylphenyl)-5-(pyridin-2-ylmethyl)-2,4-dihydro-3H-1,2,4-triazole-3-thione (7a) NH...N (triazole...pyridyl) centrosymmetric dimer

Figure S8. Intermolecular hydrogen bonds.