Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Photochromic and molecular switching behaviour of new Schiff base-containing hydantoin ring: Synthesis, characterization and crystal structure

Petar T. Todorov,[a*] Petia N. Peneva,[a] Stela I. Georgieva,[b] Rusi I. Rusew,[c] Boris L. Shivachev,[c] Anton H. Georgiev,[a]

[a]*Department of Organic Chemistry, University of Chemical Technology and Metallurgy, 1756 Sofia, Bulgaria, e-mail: pepi_37@abv.bg*

[b]*Department of Analytical Chemistry, University of Chemical Technology and Metallurgy, 1756 Sofia, Bulgaria.*

[c]*Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria.*

IR-spectrum

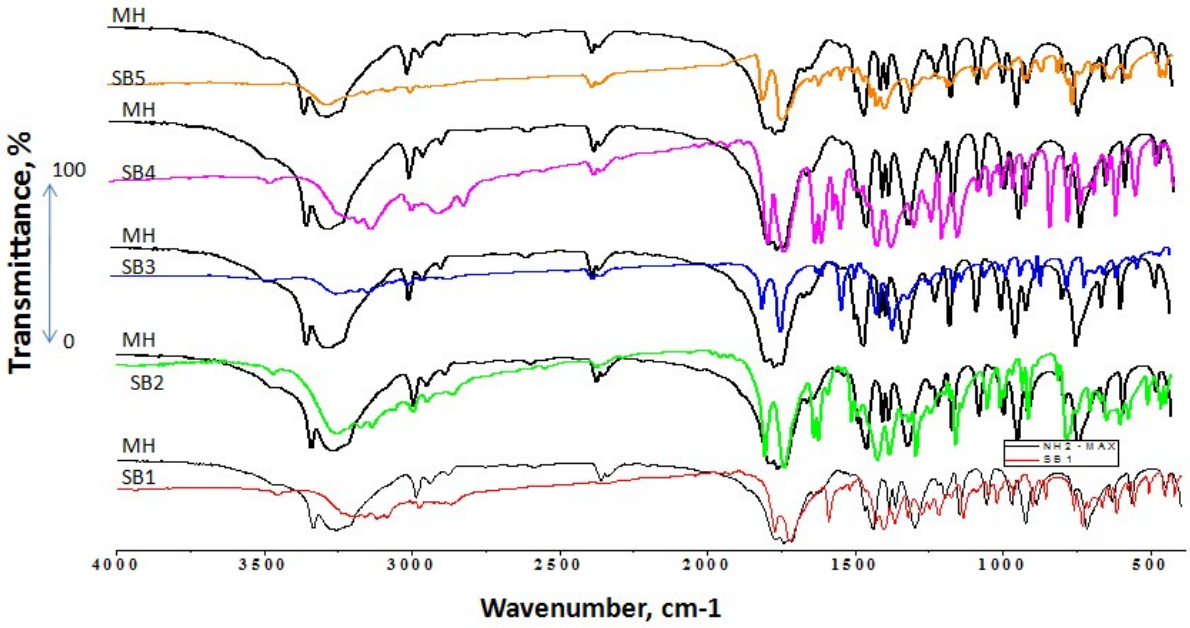


Fig.S1 IR-spectrum of synthesis 3-amino-5,5'-dimethylhydantoin Schiff bases (SB1, SB2, SB3, SB4 and SB5) and free ligand 3-amino-5,5'-dimethylhydantoin (MH).

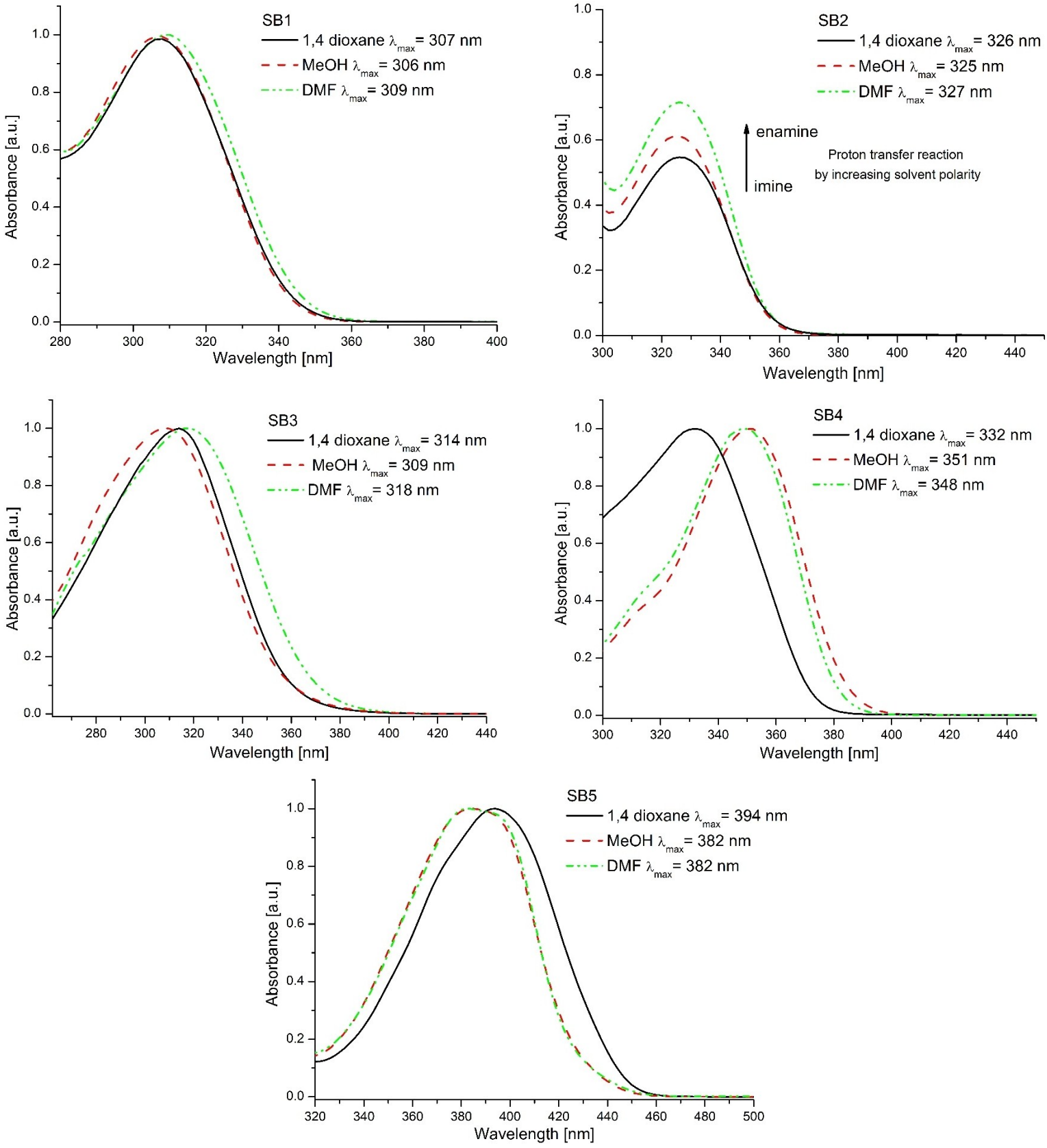


Fig. S2 Normalized UV-VIS spectra of the SB's in 1,4-dioxane, MeOH and DMF solutions.

Electrochemistry

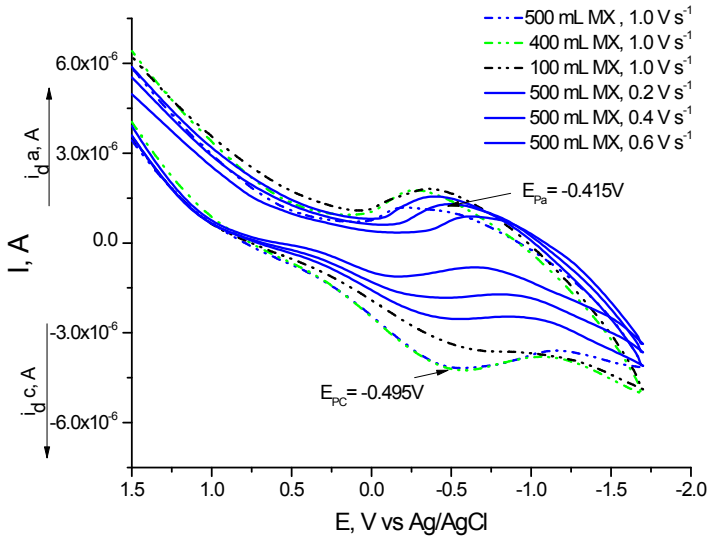
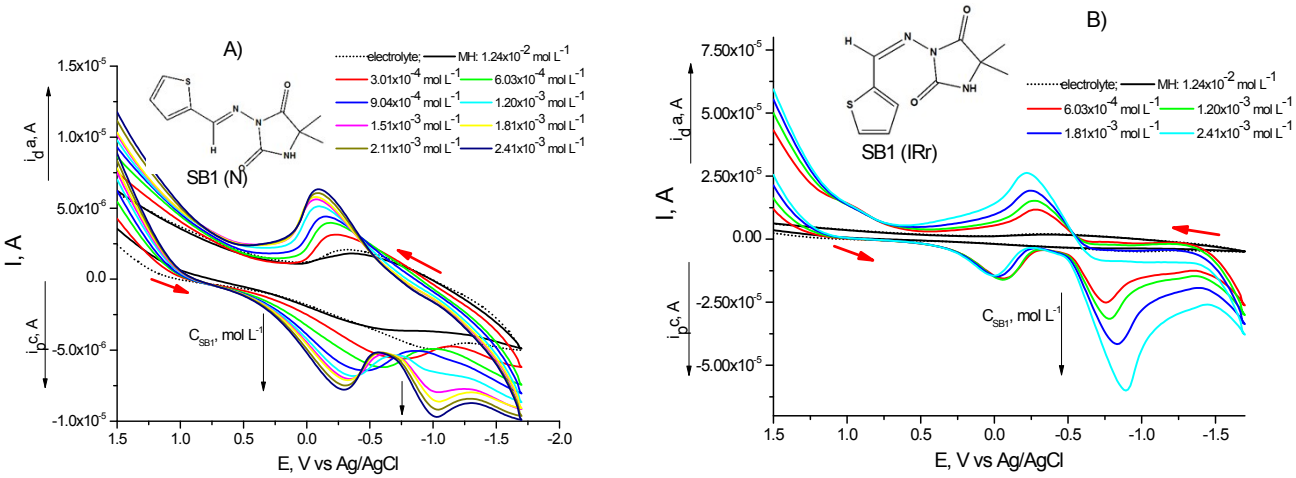
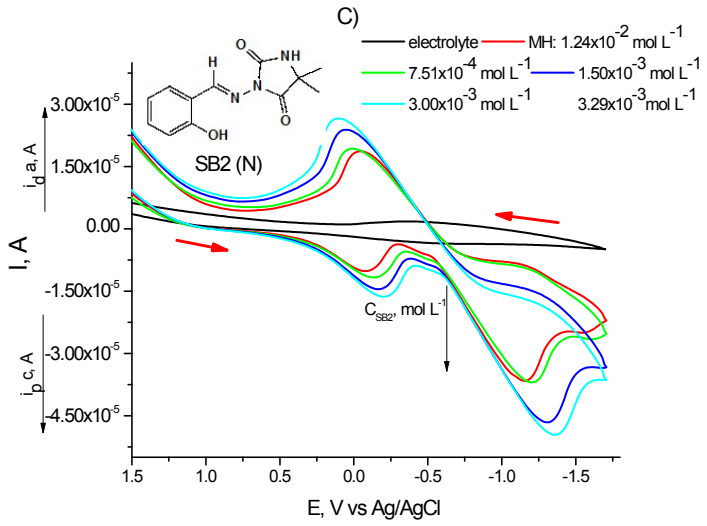
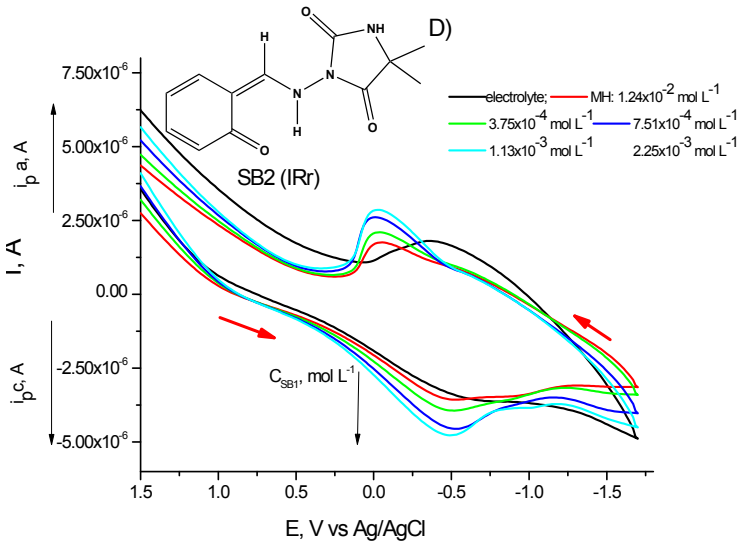
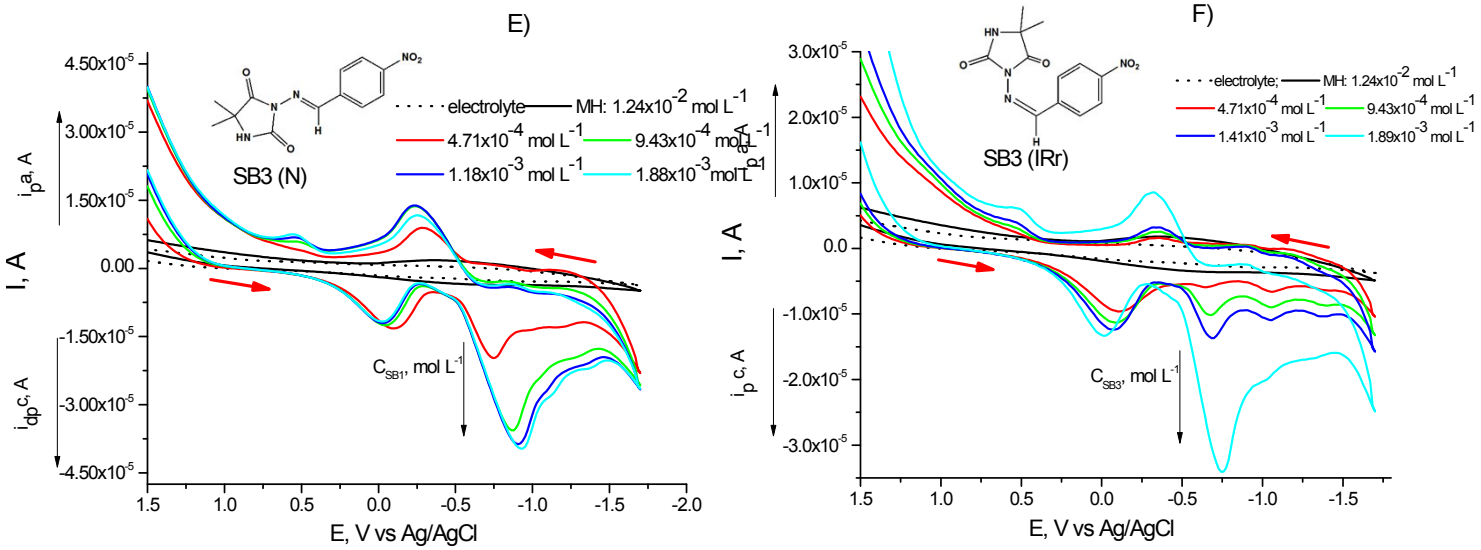


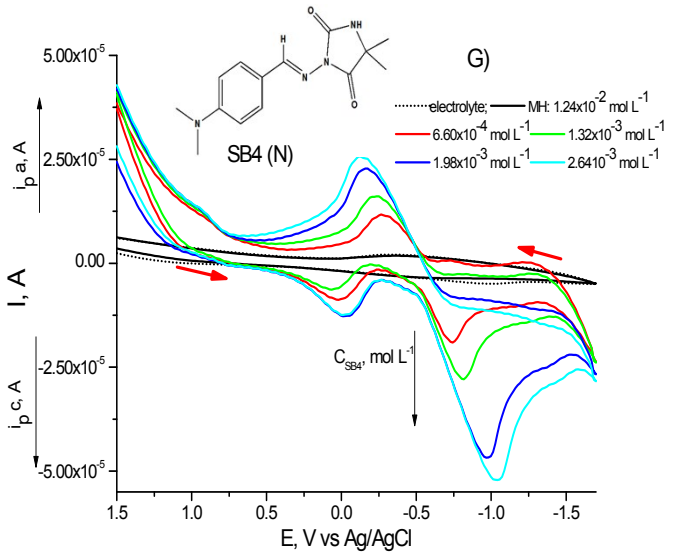
Fig. S3 Cvs of free 3-amino-5,5'-dimethylhydantoin (MH) (0.0868mol L^{-1}) at different volumes and scan rate.

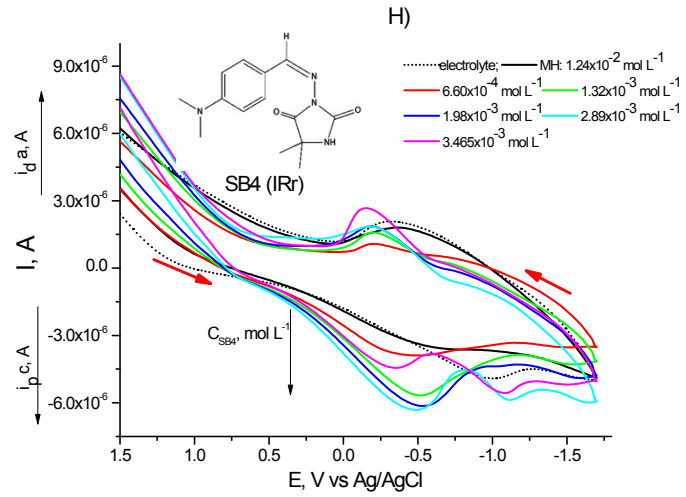



C)
electrolyte
MH: 1.24x10-2 mol L-1
7.51x10-4 mol L-1
1.50x10-3 mol L-1
3.00x10-3 mol L-1
3.29x10-3mol L-1
SB2 (N)
3.00x10-5
1.50x10-5
0.00
-1.50x10-5
-3.00x10-5
-4.50x10-5
id a, A
ip c, A
I, A
CSB2, mol L-1
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
E, V vs Ag/AgCl


D)
electrolyte;
MH: 1.24x10-2 mol L-1
3.75x10-4 mol L-1
7.51x10-4 mol L-1
1.13x10-3 mol L-1
2.25x10-3 mol L-1
SB2 (IRr)
7.50x10-6
5.00x10-6
2.50x10-6
0.00
-2.50x10-6
-5.00x10-6
ip a, A
ipc, A
I, A
CSB1, mol L-1
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
E, V vs Ag/AgCl


E)
SB3 (N)
electrolyte
MH: 1.24x10-2 mol L-1
4.71x10-4 mol L-1
9.43x10-4 mol L-1
1.18x10-3 mol L-1
1.88x10-3 mol L-1
I, A
ipa, A
ipc, A
CSB1, mol L-1
E, V vs Ag/AgCl
F)
SB3 (IRr)
electrolyte;
MH: 1.24x10-2 mol L-1
4.71x10-4 mol L-1
9.43x10-4 mol L-1
1.41x10-3 mol L-1
1.89x10-3 mol L-1
I, A
ipc, A
CSB3, mol L-1
E, V vs Ag/AgCl


G)
SB4 (N)
electrolyte; MH: 1.24x10-2 mol L-1
6.60x10-4 mol L-1
1.32x10-3 mol L-1
1.98x10-3 mol L-1
2.6410-3 mol L-1
5.00x10-5
2.50x10-5
0.00
-2.50x10-5
-5.00x10-5
ip a, A
ip c, A
I, A
CSB4, mol L-1
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
E, V vs Ag/AgCl


H)
SB4 (IRr)
electrolyte; MH: 1.24x10-2 mol L-1
6.60x10-4 mol L-1
1.32x10-3 mol L-1
1.98x10-3 mol L-1
2.89x10-3 mol L-1
3.465x10-3 mol L-1
9.0x10-6
6.0x10-6
3.0x10-6
0.0
-3.0x10-6
-6.0x10-6
id a, A
ip c, A
I, A
CSB4, mol L-1
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
E, V vs Ag/AgCl

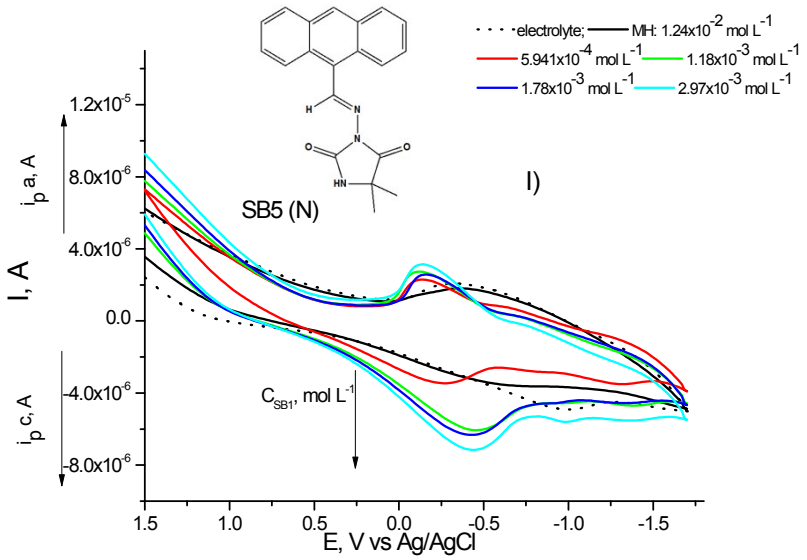


Fig. S4 Cyclic voltammograms of 3-amino-5,5'-dimethylhydantoin Schiff bases from A) to I) before (SB(N)) and after (SB(IRr)) UV illumination with λ = 365 nm at scan rate 100 mV s^{-1} and different concentrations.

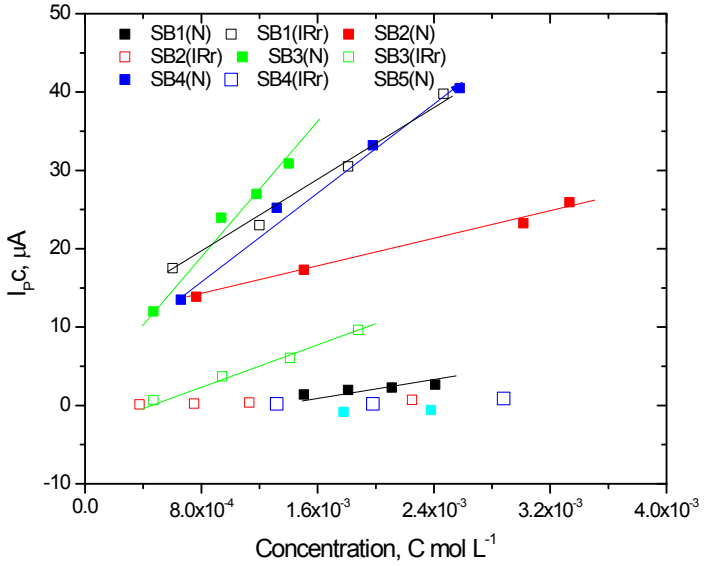


Fig.S5 CVs of Ipc vs. different concentrations of 3-amino-5,5'-dimethylhydantoin Schiff bases before (SB(N)) and after (SB(IRr)) UV illumination with λ = 365 nm and scan rate 100 mV s^{-1}

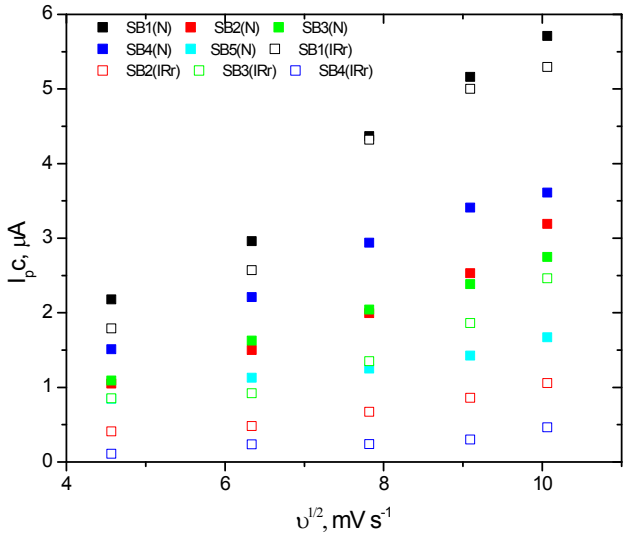


Fig. S6 Plot of cathodic peak high, I_{pc} µA *vs.* scan rate, $\vee^{1/2}$ mV s^{-1} in rang from 20 to 100 mV s^{-1}

NMR-spectrum

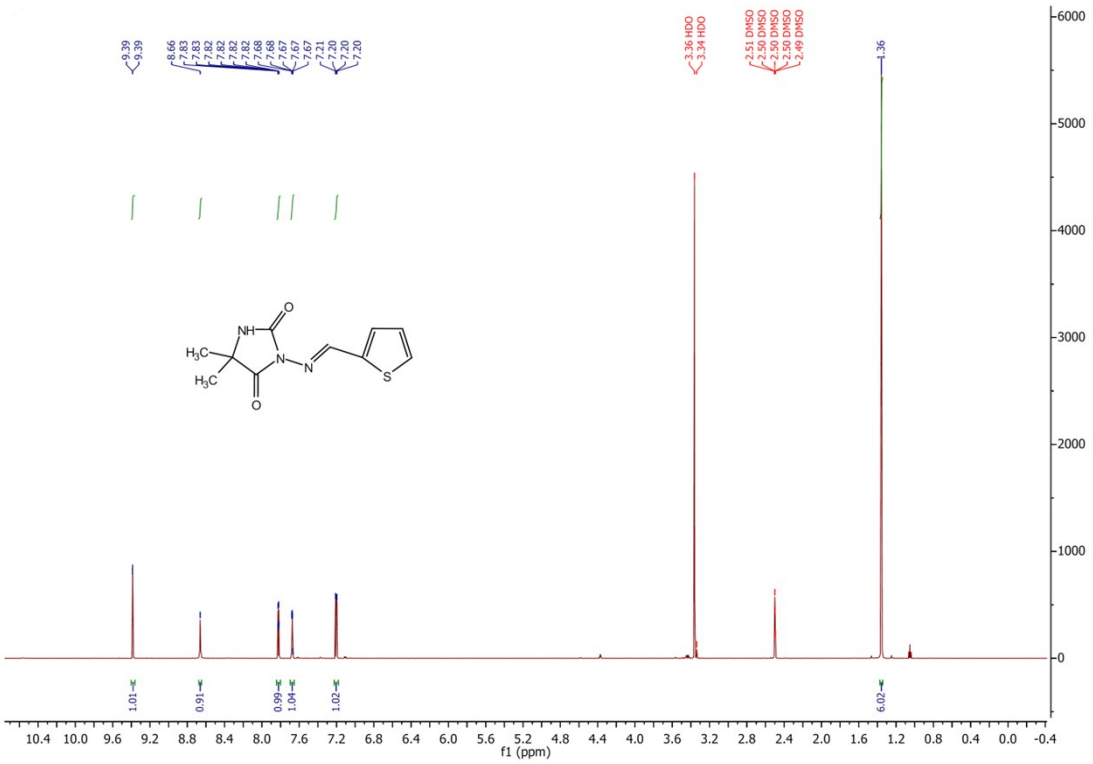


Fig. S7 1HNMR spectrum of **SB1**

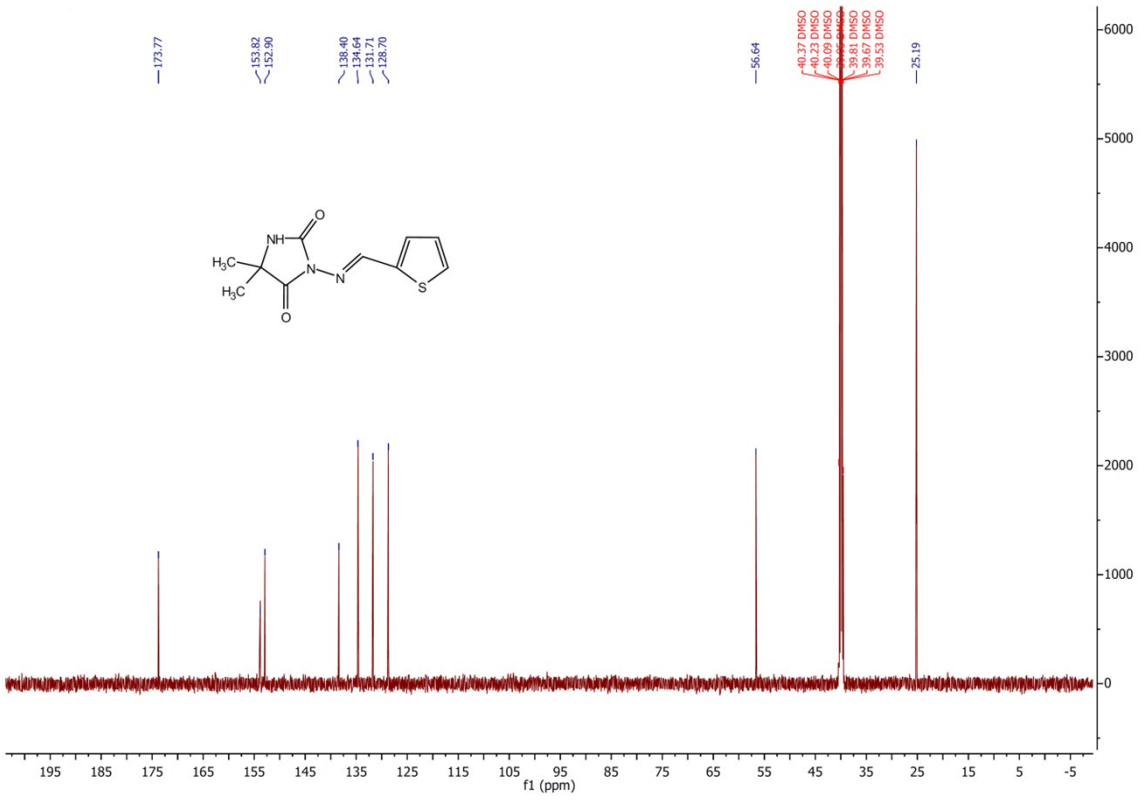


Fig. S8 13CNMR spectrum of **SB1**

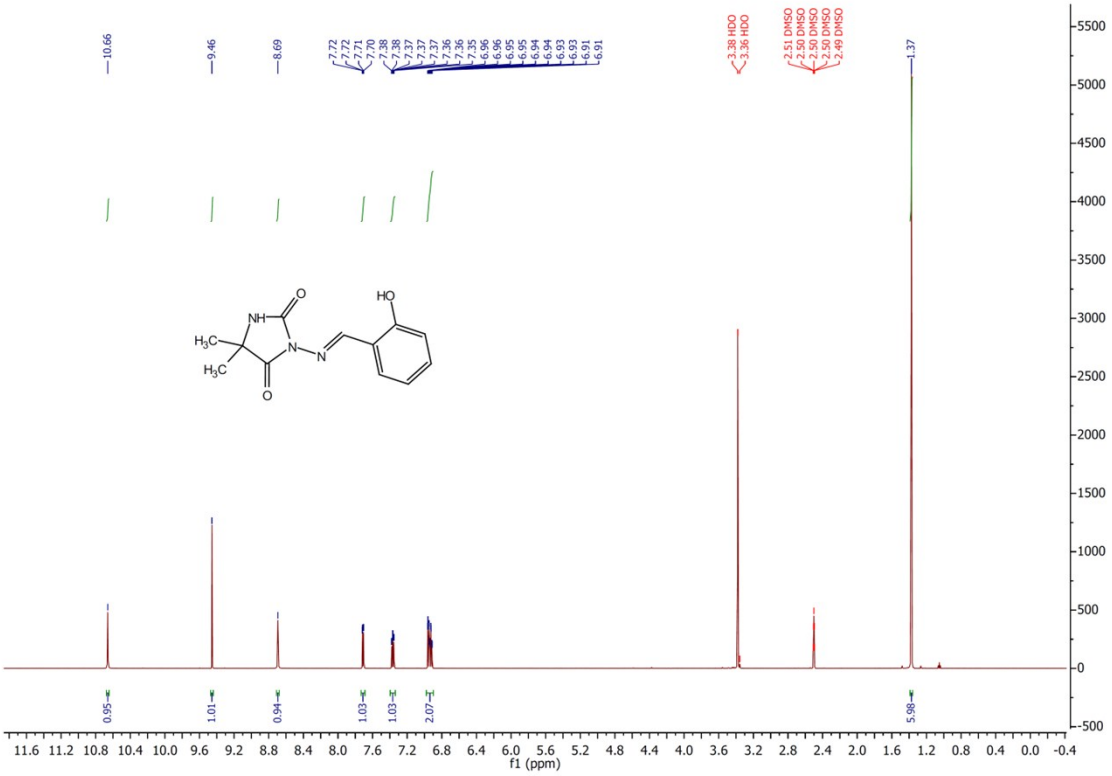


Fig. S9 1HNMR spectrum of **SB2**

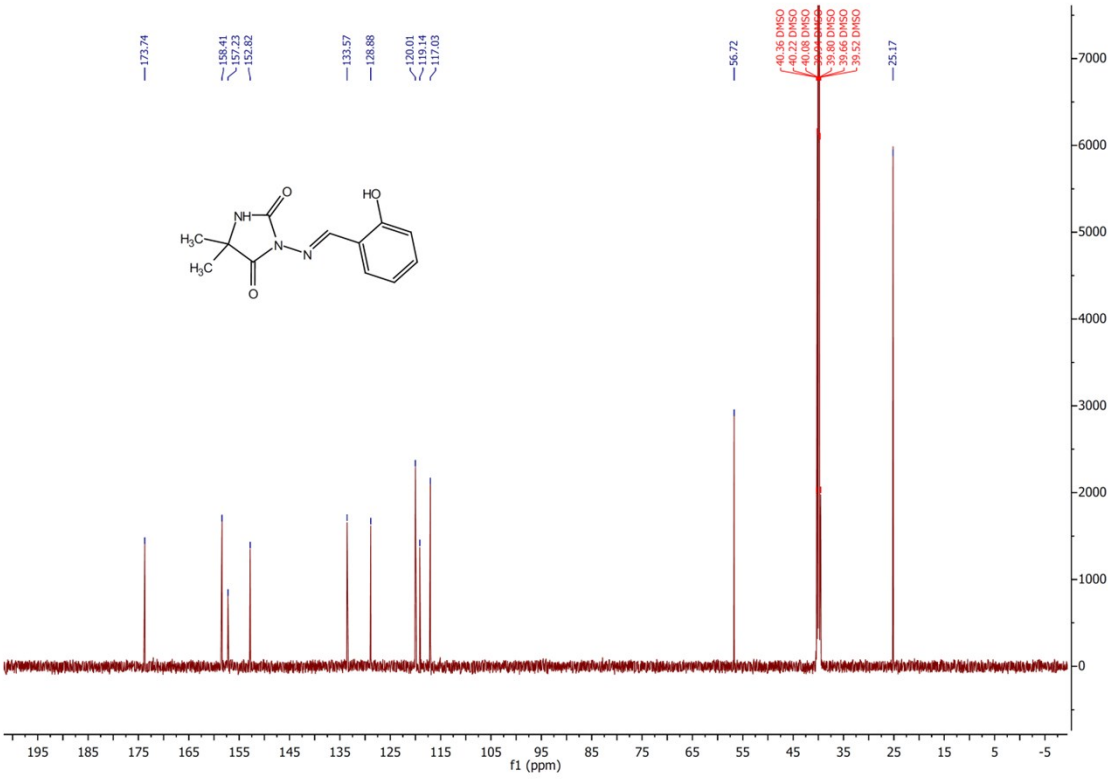


Fig. S10 13CNMR spectrum of **SB2**

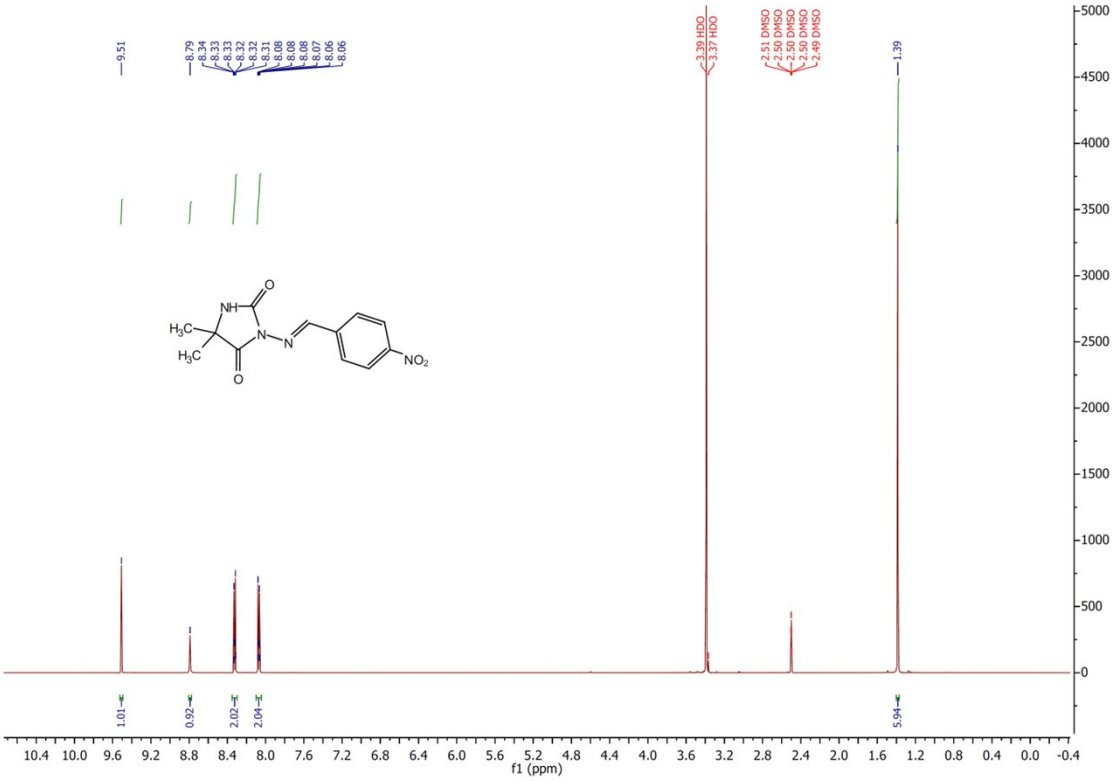


Fig. S11 1HNMR spectrum of **SB3**

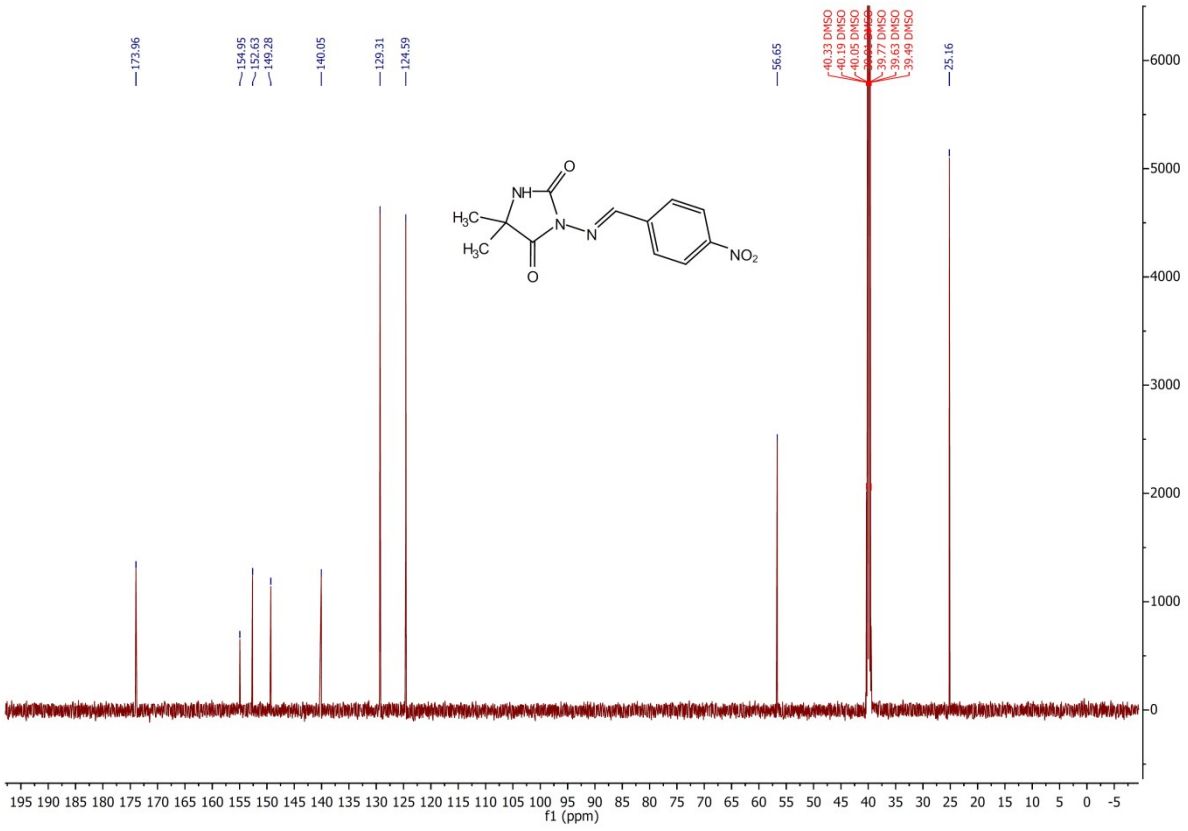


Fig. S12 13CNMR spectrum of **SB3**

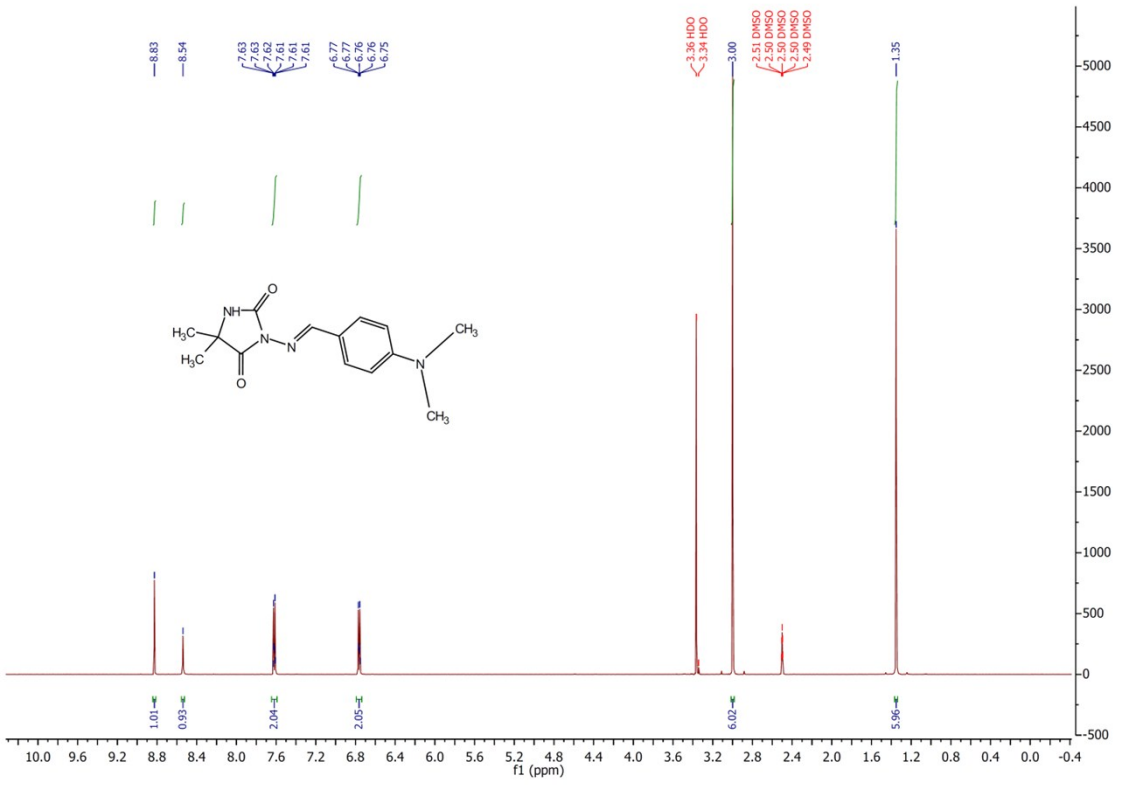


Fig. S13 1HNMR spectrum of **SB4**

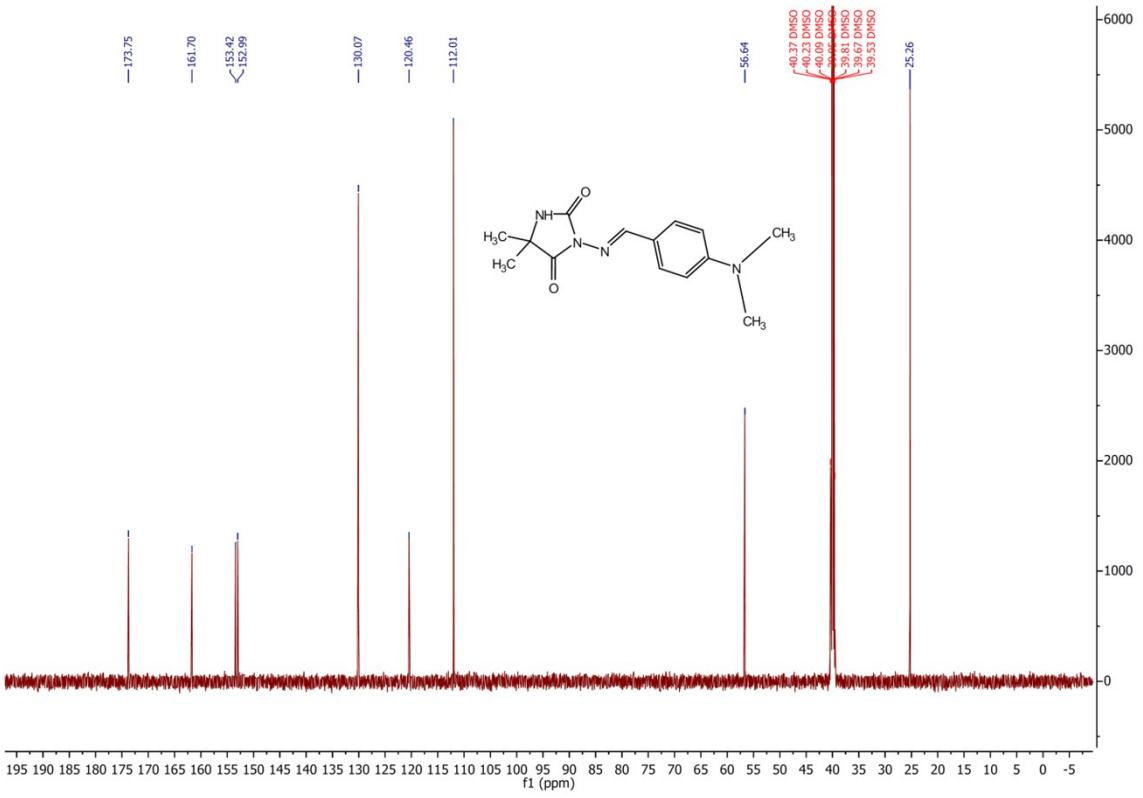


Fig. S14 13CNMR spectrum of **SB4**

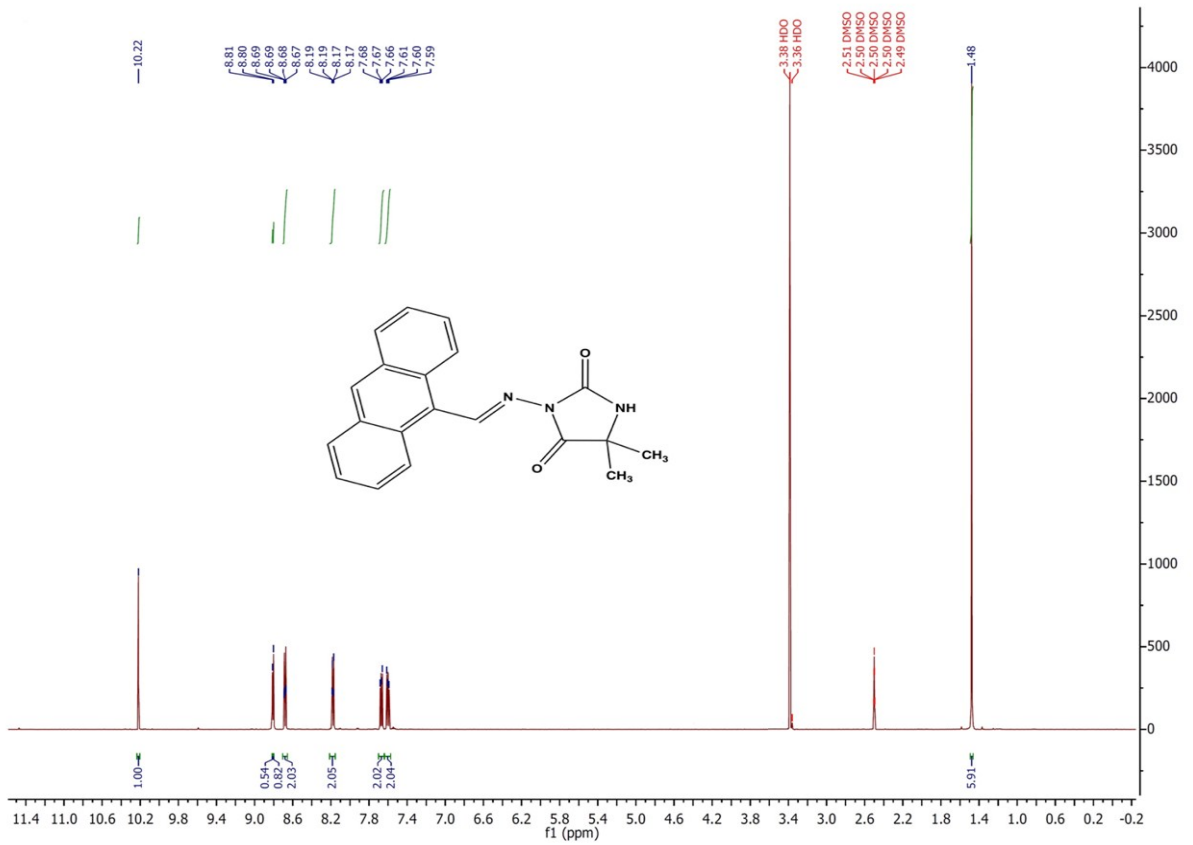


Fig. S15 1HNMR spectrum of **SB5**

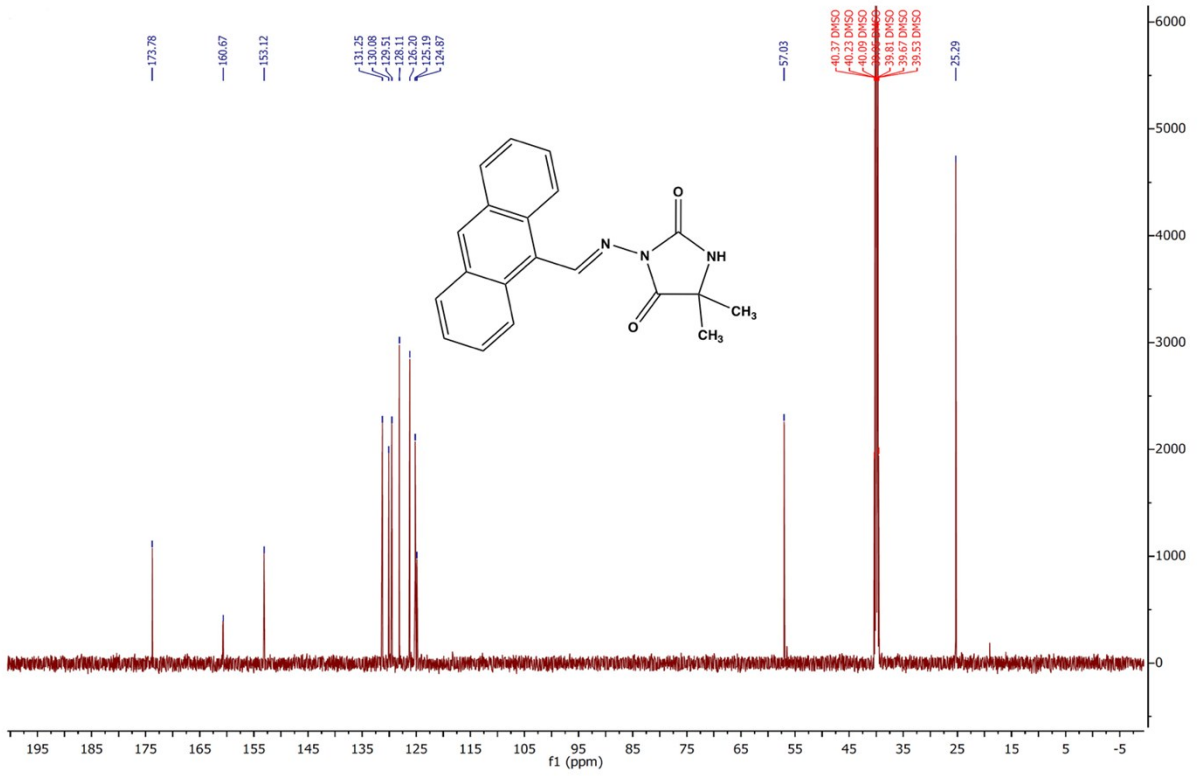


Fig. S16 13CNMR spectrum of **SB5**

X-ray Diffraction

Table S1 Bond lengths, angles and torsion angles for compounds **SB1-3** and **SB5**.

Structure	S459 – **SB1**	S453 – **SB2**	S467 – **SB3**	S458 – **SB5**
Bonds	**Å**	**Å**		**Å**
N1—C3	1.4542 (19)	1.461 (2)	1.470 (3)	1.452 (5)
N1—C5	1.3342 (18)	1.325 (2)	1.332 (3)	1.343 (5)
N2—C4	1.3847 (18)	1.376 (2)	1.383 (3)	1.365 (4)
N2—C5	1.4113 (18)	1.423 (2)	1.424 (3)	1.422 (4)
N3—N2	1.3936 (16)	1.380 (2)	1.389 (3)	1.392 (4)
N3—C6	1.278 (2)	1.283 (2)	1.281 (3)	1.263 (4)
O4—C4	1.2029 (19)	1.212 (2)	1.216 (3)	1.217 (4)
O5—C5	1.2184 (17)	1.217 (2)	1.224 (3)	1.198 (4)
O8—C8	–	1.350 (2)	–	–
N4—O1	–	–	1.225 (3)	–
N4—O2	–	–	1.221 (3)	–
S1—C7	1.7166 (17)	–	–	–
S1—C8	1.708 (2)	–	–	–
Angles	°	°		°
N3—N2—C5	117.59 (11)	117.92 (14)	117.89 (19)	119.0 (3)
C6—N3—N2	116.23 (13)	119.56 (15)	117.9 (2)	115.6 (3)
C4—N2—N3	128.87 (12)	130.37 (14)	130.0 (2)	128.4 (3)
O4—C4—N2	126.66 (14)	126.77 (17)	127.0 (3)	126.1 (3)
O5—C5—N1	129.05 (14)	129.70 (17)	129.1 (3)	129.7 (4)
O5—C5—N2	124.00 (13)	123.81 (17)	124.1 (2)	124.8 (3)
O8—C8—C7	–	122.30 (18)	–	–
C8—S1—C7	90.98 (10)	–		–
C6—C7—S1	123.05 (12)	–		–
O2—N4—O1	–	–	122.5 (2)	–
Torsion angles	°	°		°
N3—N2—C4—O4	−12.6 (3)	−10.4 (3)	−10.0 (5)	8.4 (6)
N3—N2—C5—O5	15.6 (2)	8.1 (3)	8.0 (4)	−8.9 (5)
C6—C7—C8—O8	–	−1.6 (3)	–	–
N2—N3—C6—C7	−175.22 (13)	−176.37 (15)	−176.5 (2)	177.4 (3)
C8—C7—C6—N3	–	–	0.8 (4)	32.6 (5)
C20—C7—C6—N3	–	–	–	−150.6 (3)
S1—C7—C6—N3	0.0 (2)	–	–	–
S1—C7—C10—C9	−0.5 (2)	–	–	–
O2—N4—C10—C11	–	–	–10.2 (4)	–
O1—N4—C10—C9	–	–	9.8 (4)	–

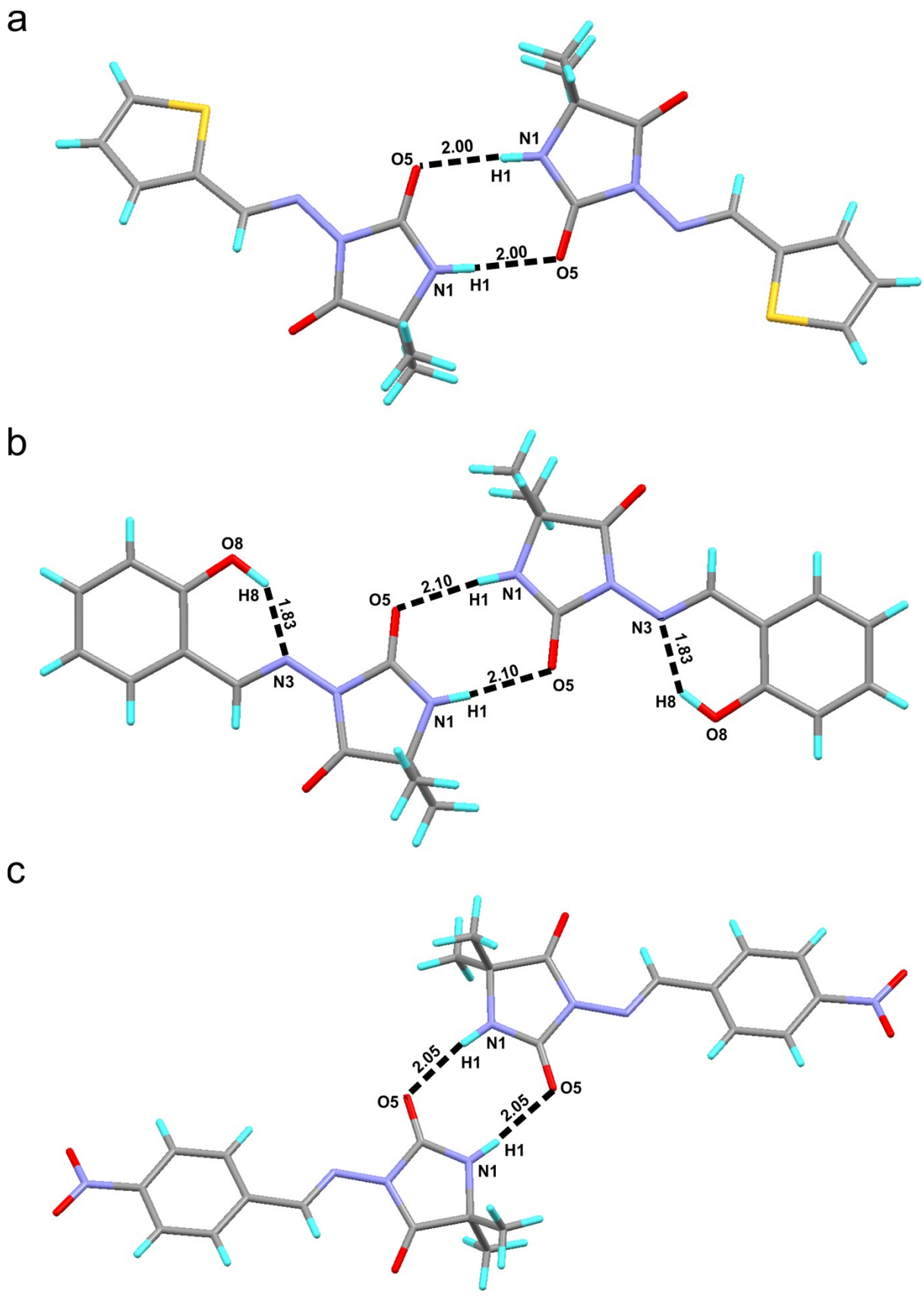


Fig. SX3 Observed N-H…O interactions in a) **SB1**, b) **SB2** and c) **SB3**.

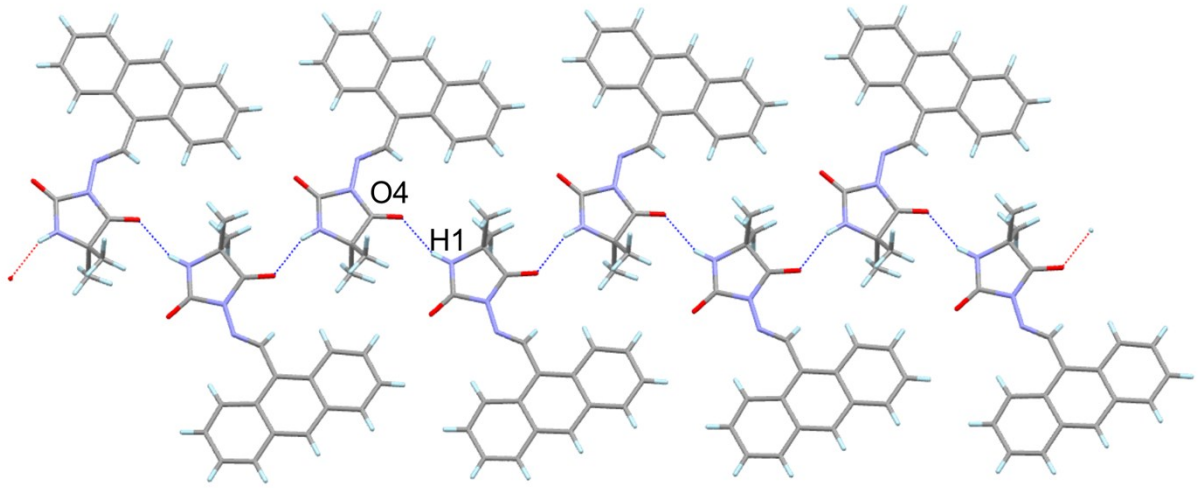
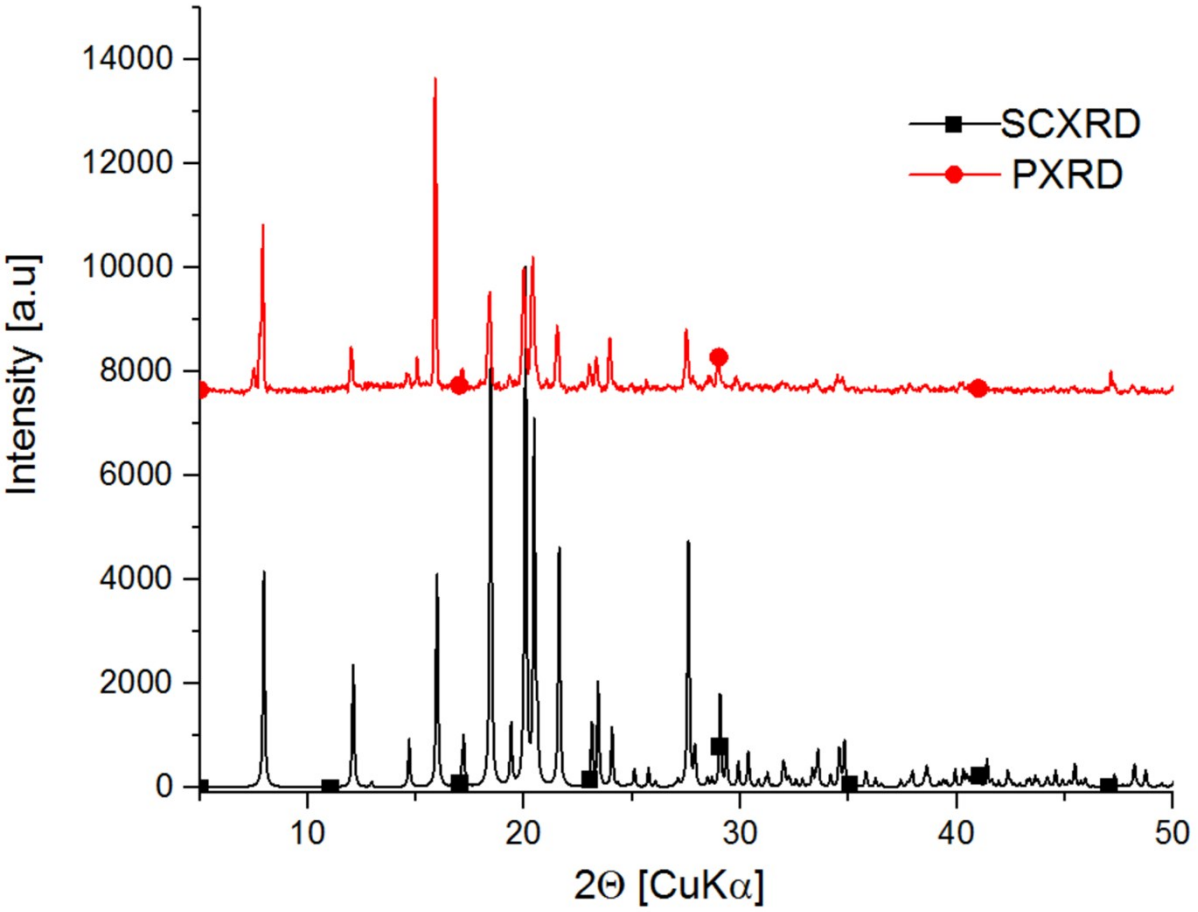


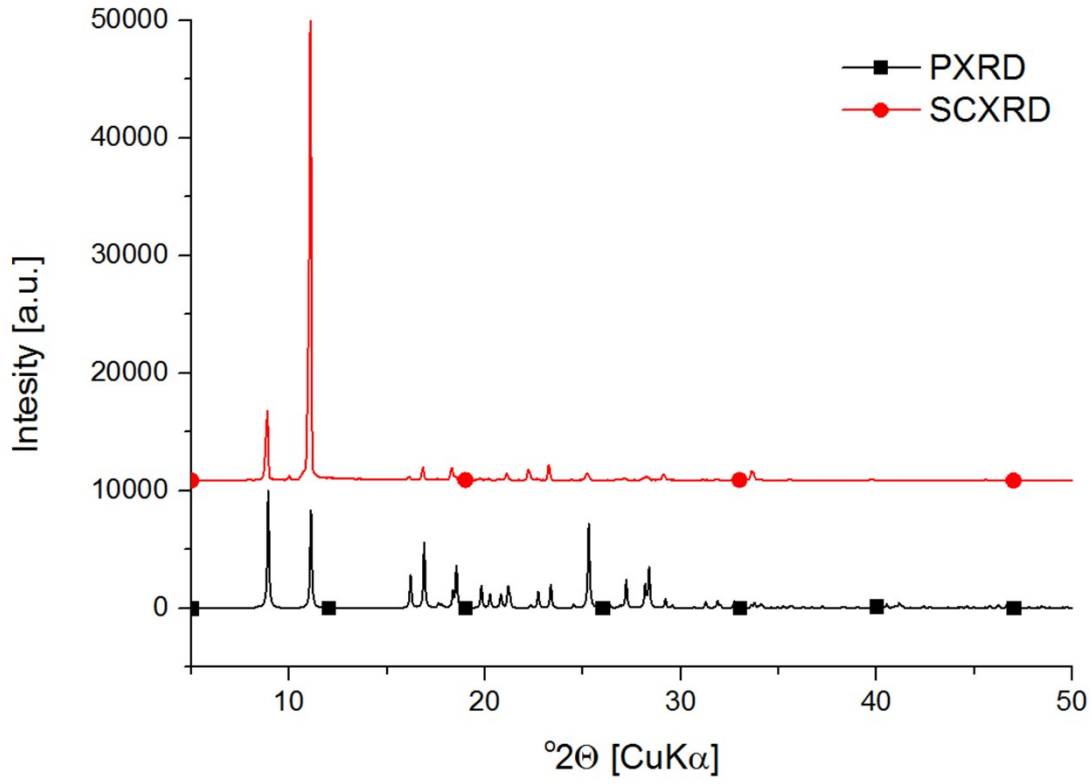
Fig. SX4 Observed N-H…O interactions in **SB5**.

Powder diffraction data

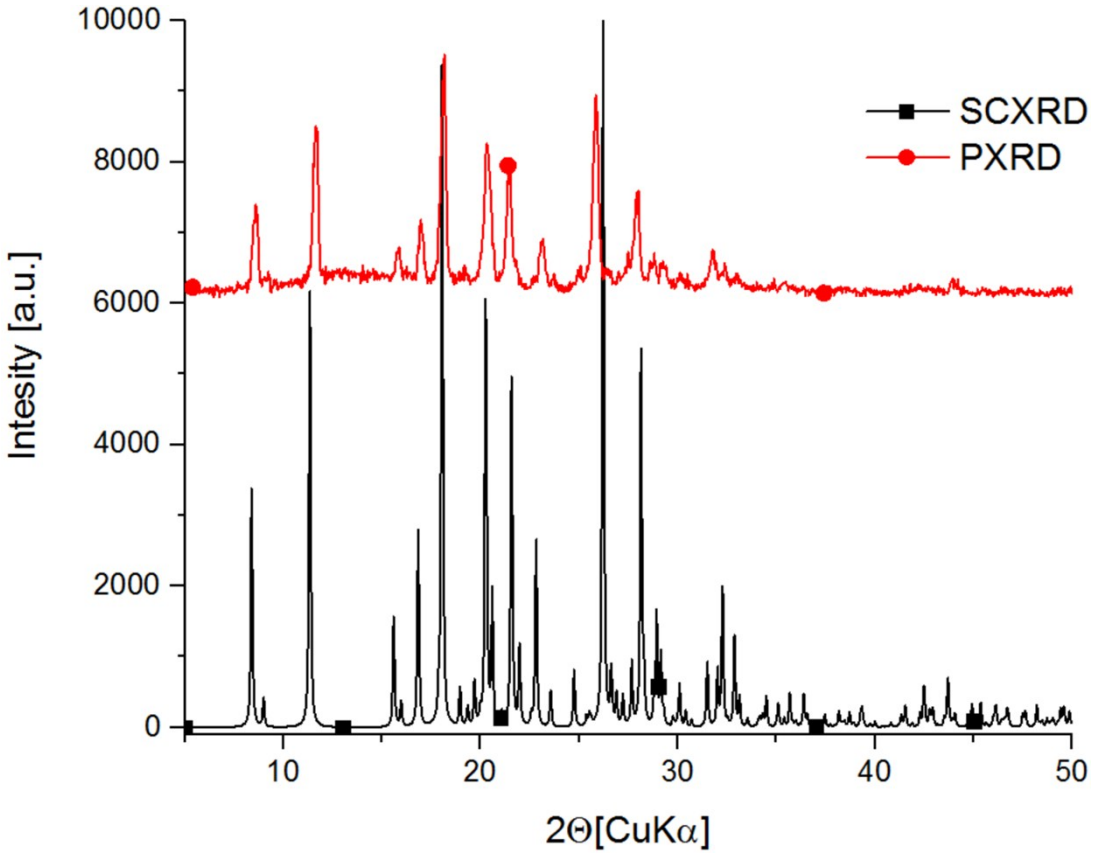
SB2



SB2


PXRD
SCXRD
Intesity [a.u.]
°2Θ [CuKα]
50000
40000
30000
20000
10000
0
10
20
30
40
50

SB3


SCXRD
PXRD
Intesity [a.u.]
2Θ[CuKα]
10000
8000
6000
4000
2000
0
10
20
30
40
50

SB5

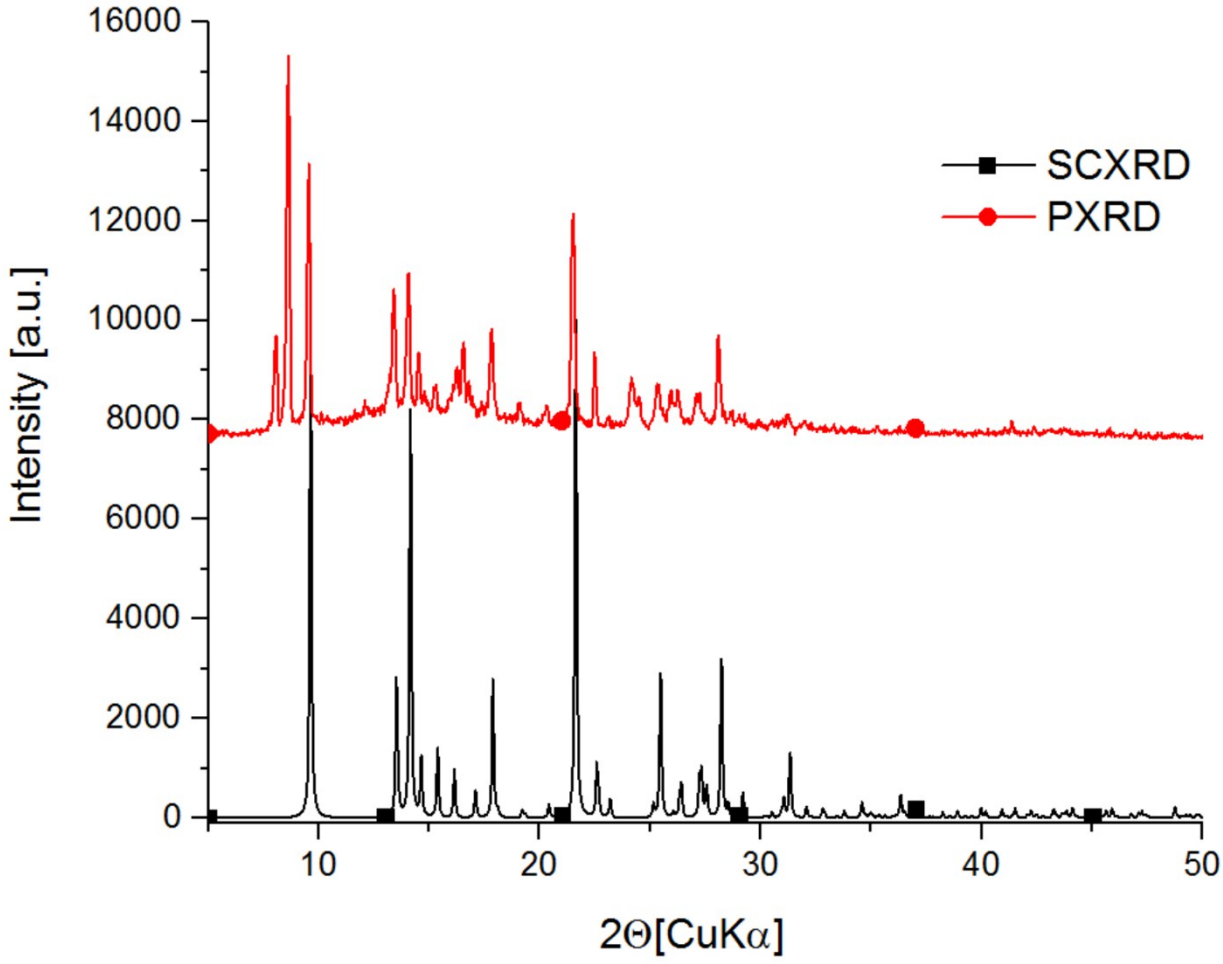


Fig. SX5 Estimation of the purity of the compounds by comparison of powder diffraction data and those generated from single crystal structure. For SB5 in addition the observed structure crystal of a supposed polymorph is present. Peaks observed in the diffractogram cannot be related those of the starting compounds.