Supplementary Information

An Amidothiourea as potential receptor for organic bases by resonance assisted low barrier hydrogen bond formation: Structure and hirshfeld surface analysis

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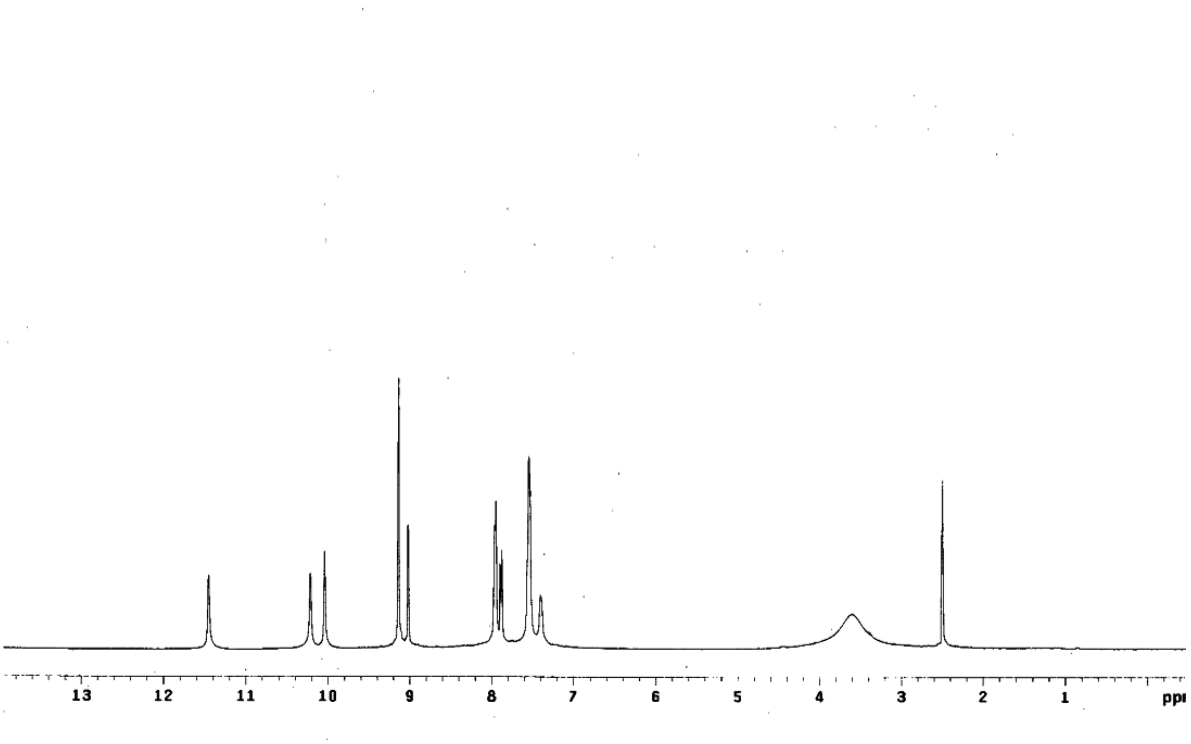

Fig. S1 ^{1}H-NMR spectrum of receptor **L** in d_6-DMSO at 298K.

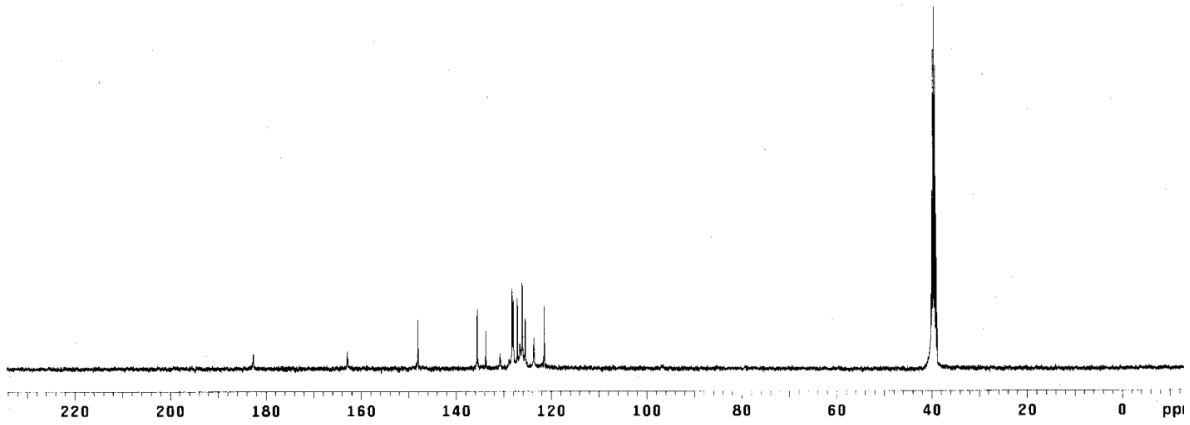

Fig. S2 ^{13}C-NMR spectrum of receptor **L** in d_6-DMSO at 298K.

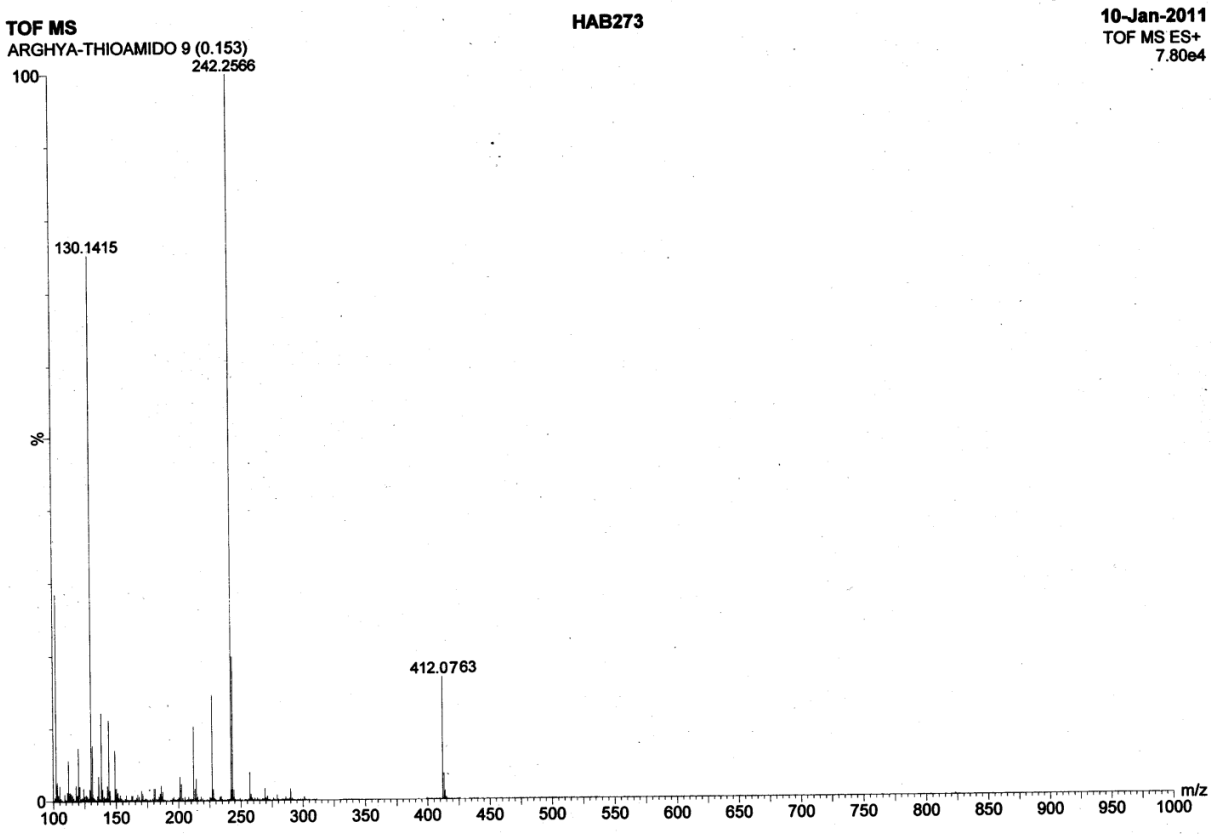

Fig. S3 ESI-Mass spectrum of receptor **L** in acetonitrile**.**

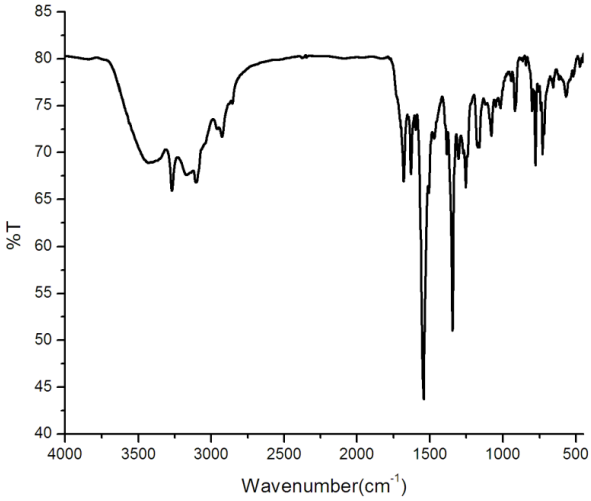

Fig.S4 IR spectrum of receptor **L**.

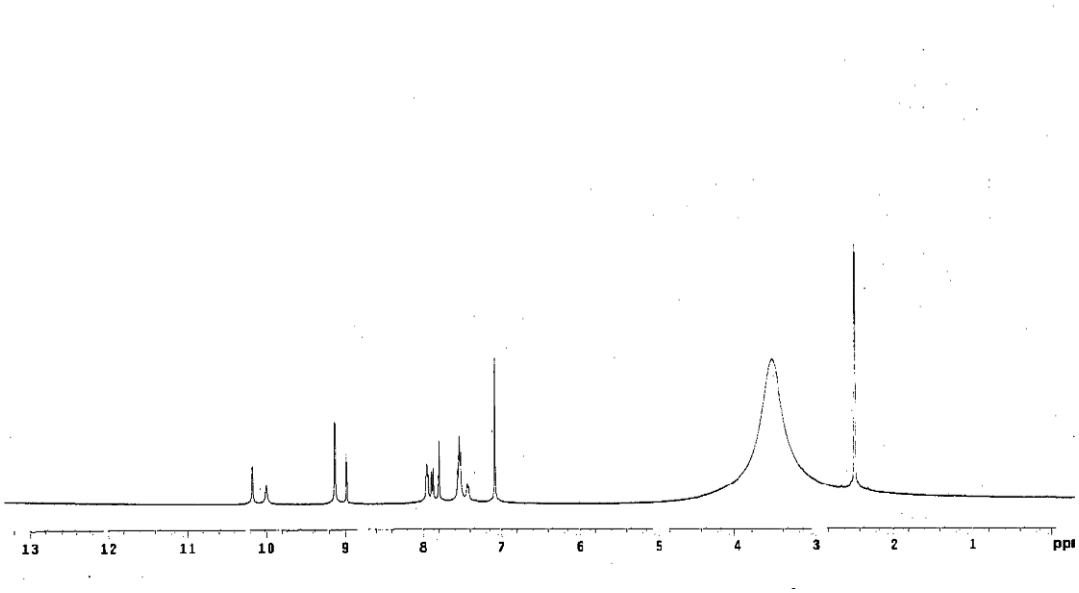

Fig. S5 ^{1}H-NMR spectrum of complex 1 in d_6-DMSO.

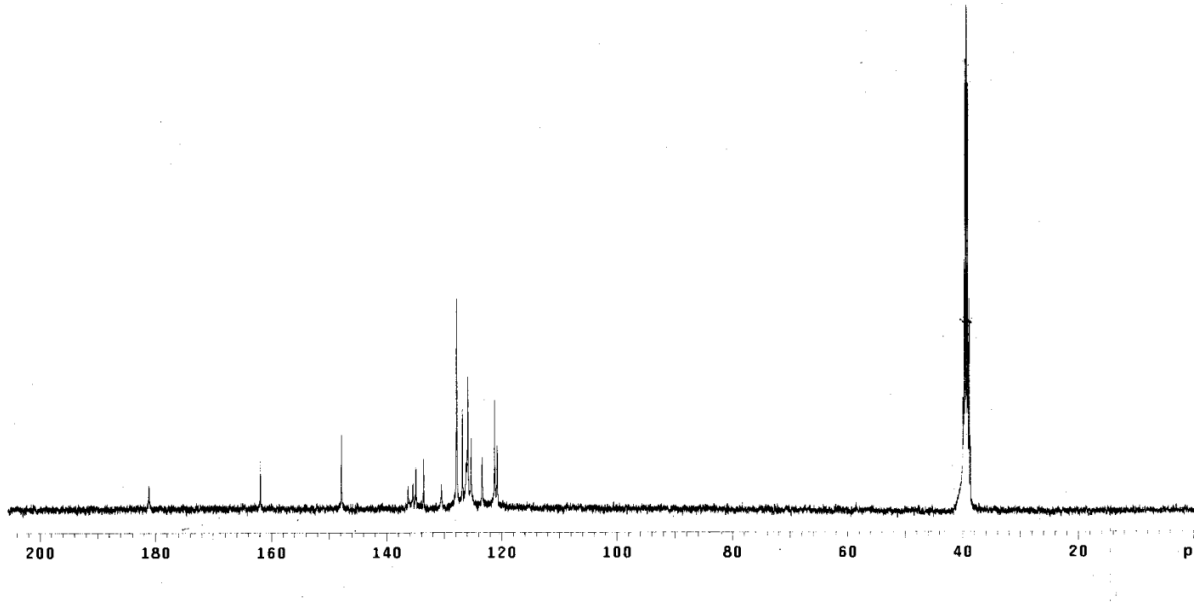

Fig. S6 ^{13}C-NMR spectrum of complex 1 in d_6-DMSO.

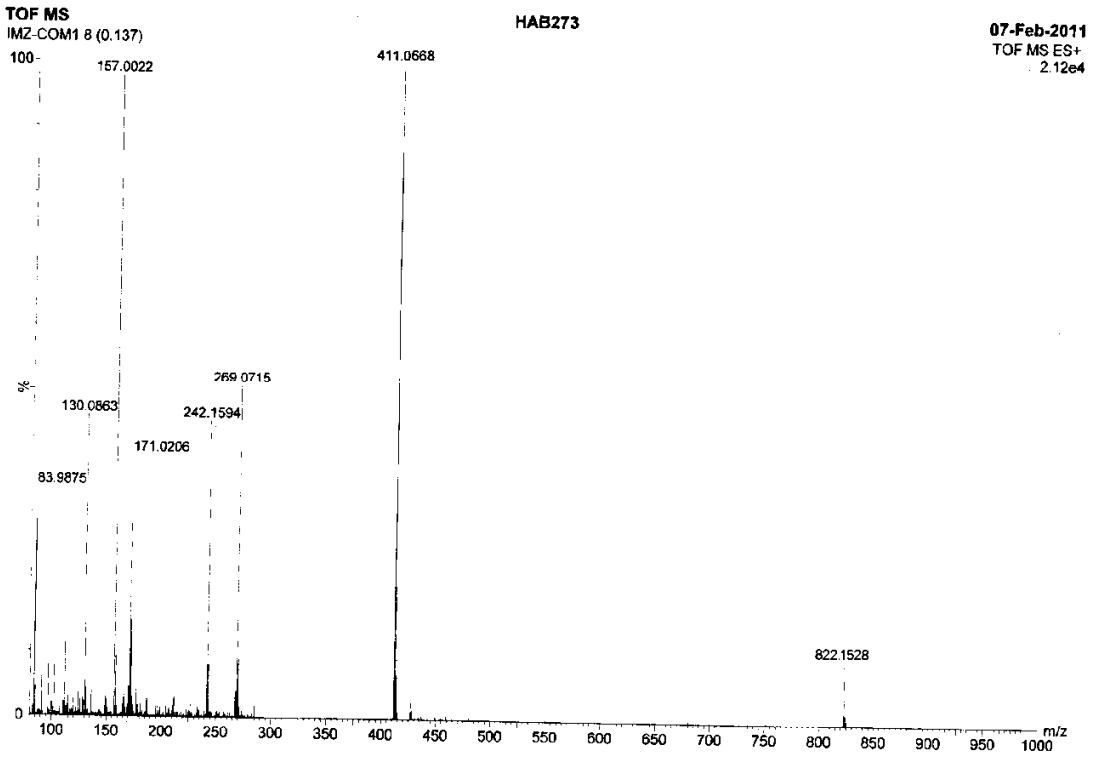

Fig. S7 ESI−Mass spectrum of complex 1.

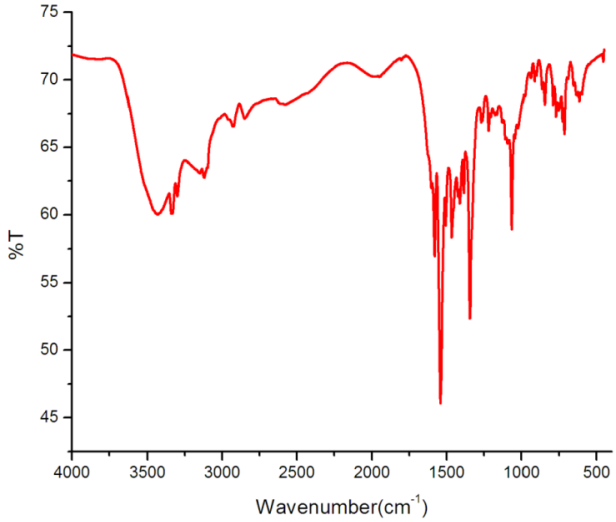

Fig. S8 IR spectrum of complex 1.

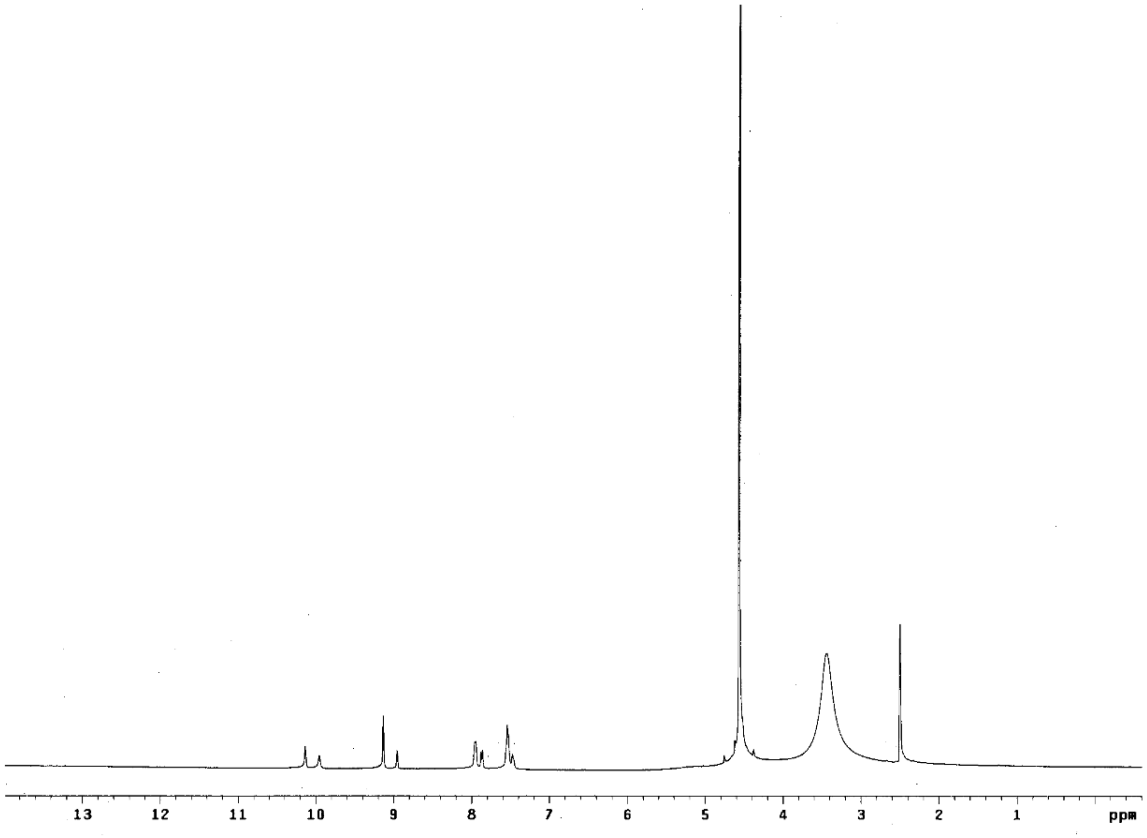

Fig. S9 ^{1}H-NMR spectrum of complex 2 in d_6-DMSO

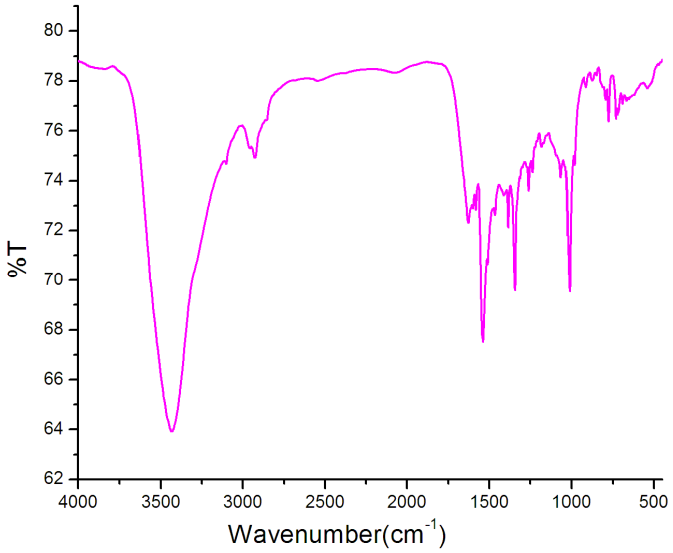

Fig. S10 IR spectrum of complex 2.

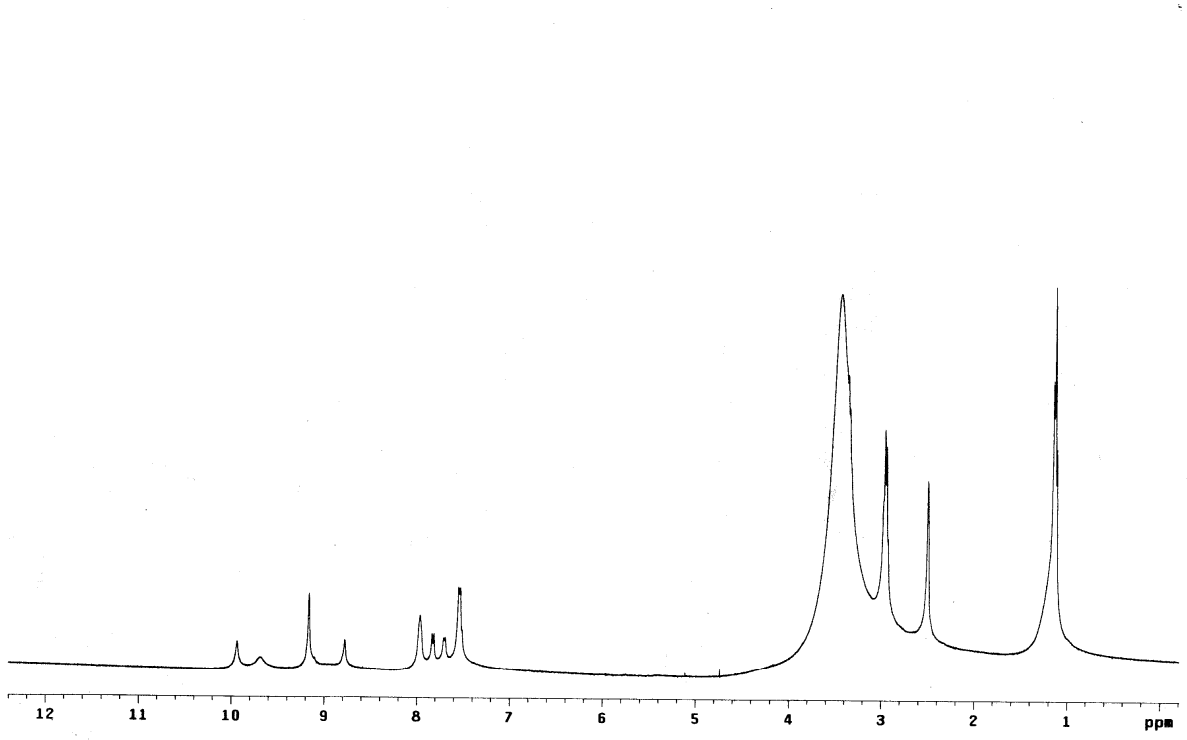

Fig. S11 ^{1}H-NMR spectrum of complex 3 in d_6-DMSO

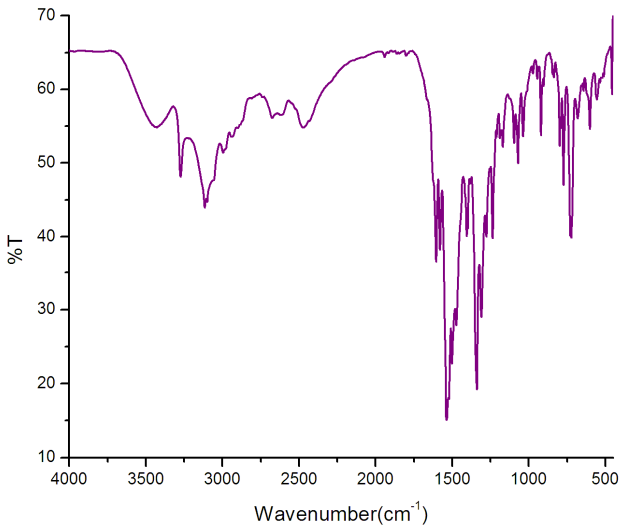

Fig. S12 IR spectrum of complex 3.

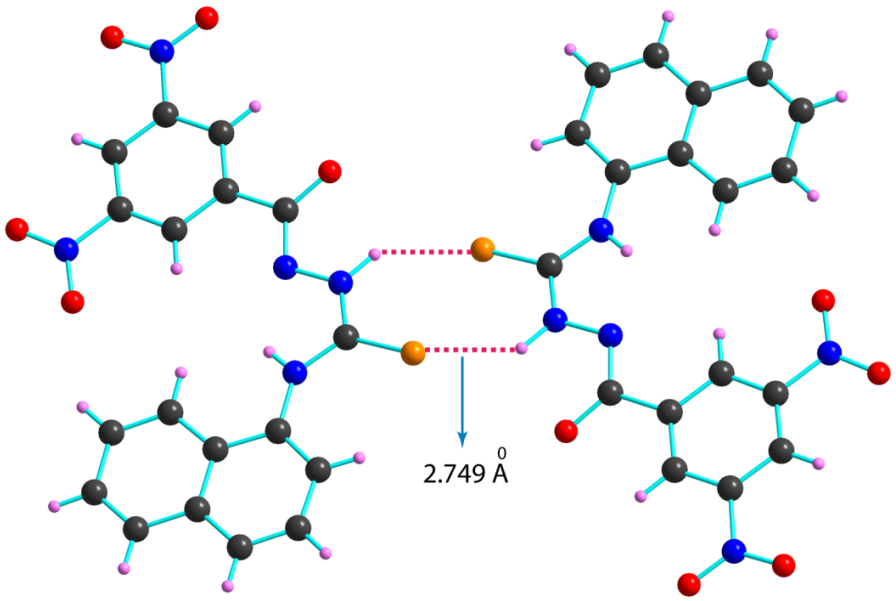

Fig. S13 Intermolecular dimeric hydrogen bonding interaction between two receptors in complex 1.

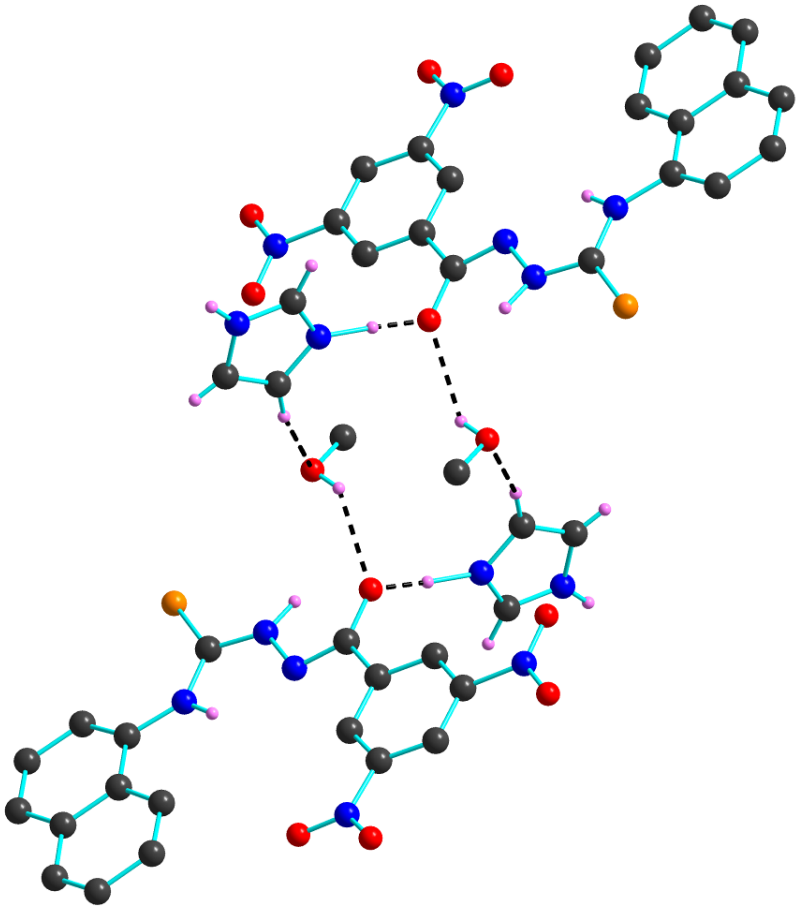

Fig. S14 Intermolecular methanol bridge dimeric hydrogen bonding interaction in the crystal structure of the complex 1.

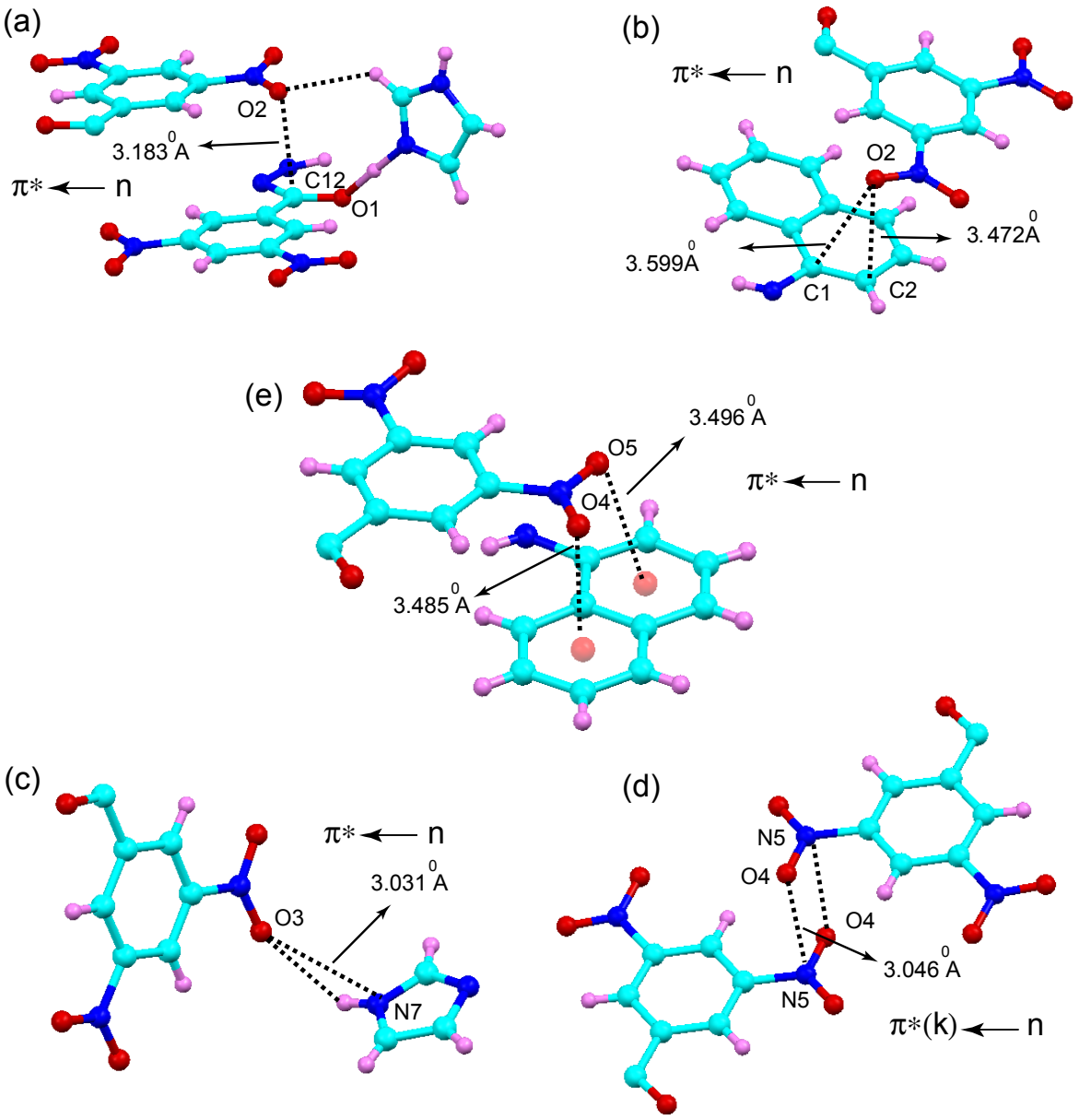

Fig. S15. Showing different electron donor acceptor (EDA) interactions (charge transfer interaction) involving the nitro groups, present in complex 1.

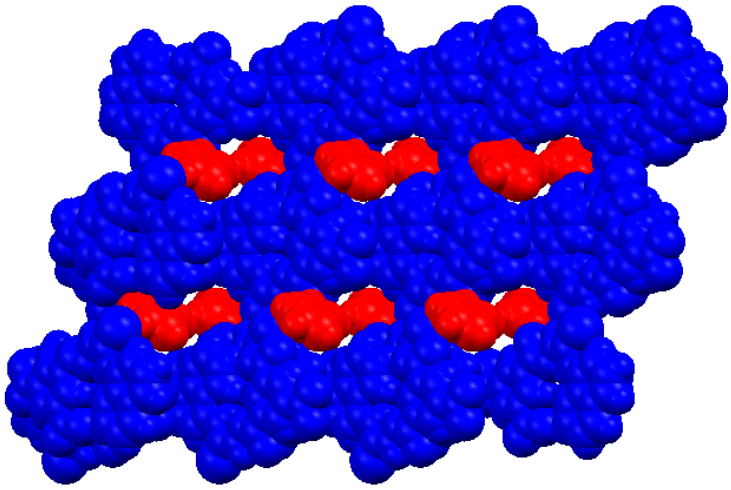

Fig. S16. A perspective view in spacefill model of the crystal packing along 'a' axis without solvent molecules. (blue = receptor, red = imidazole).

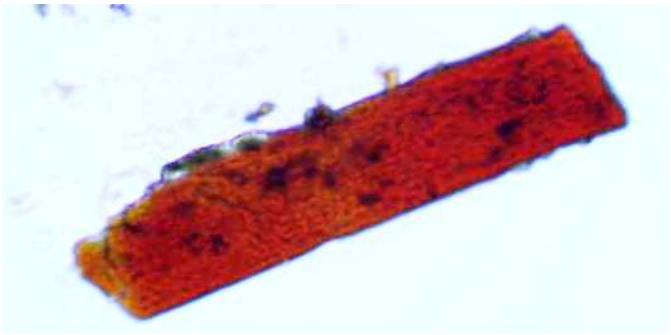

Fig. S17 Optical micrograph image of the single crystal of complex 1.

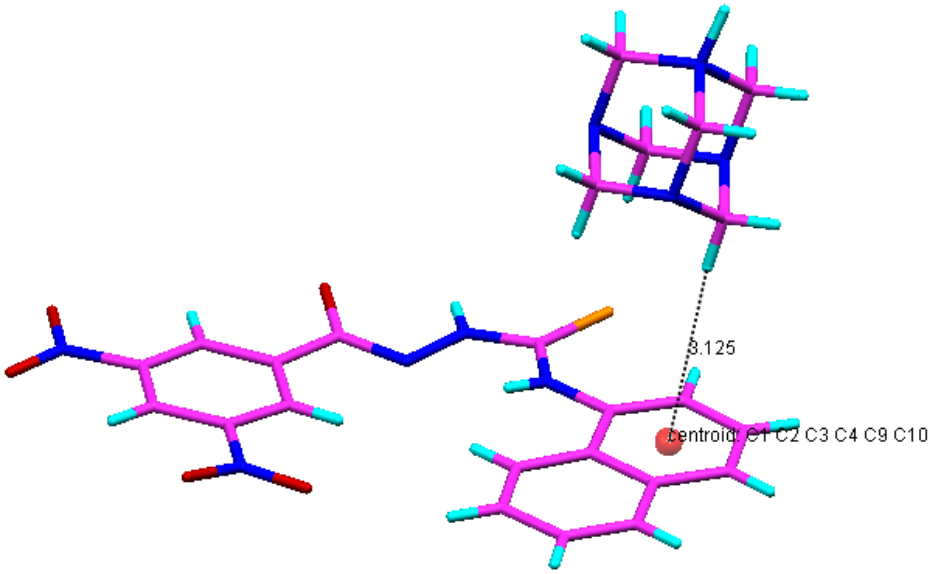

Fig. S18 Showing C−H···π interaction between napthyl ring of the receptor **L** and C−H hydrogen of hexamine guest in complex 2.

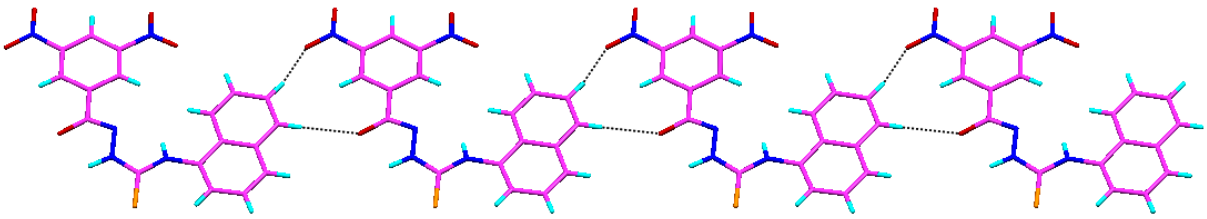

Fig. S19 Showing the formation of hydrogen bonding chain polymeric network among the deprotonated receptors in complex 2. View along 'a' axis.

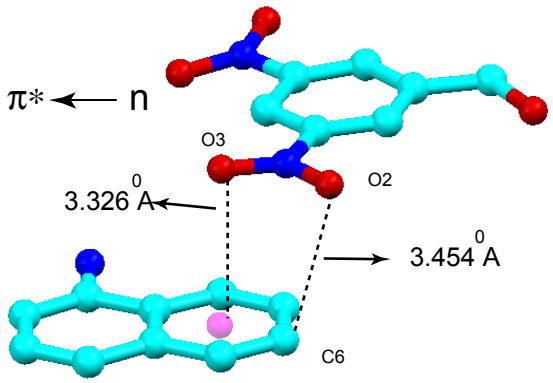

Fig. S20 Showing lone pair····π interaction involving the oxygen atoms of the nitro group and π electron cloud of the napthyl ring in complex 2.

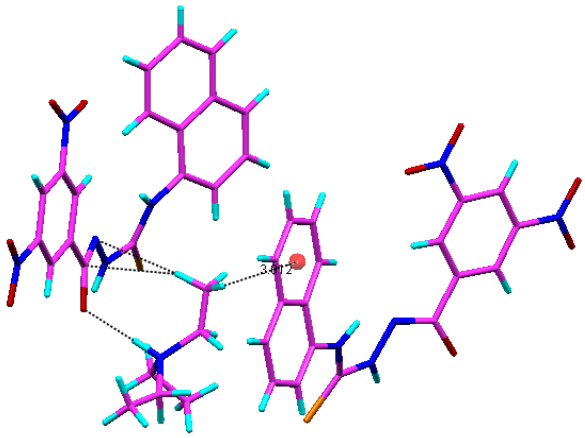

Fig. S21 Showing C−H····π interaction between napthyl ring of the receptor **L** and C−H hydrogen of triethyl amine guest in complex 3.

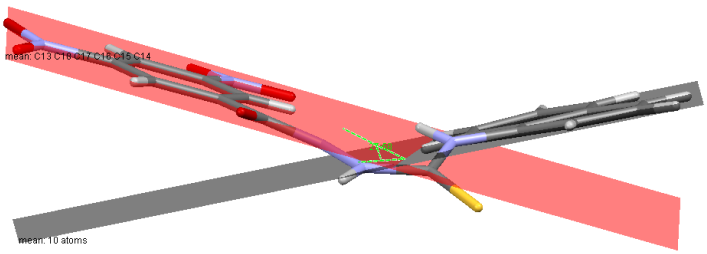

Fig. S22 Showing the receptor in complex 3 is not planer, the dinitro phenyl ring is twisted slightly relative to the napthyl ring, the angle between the planes of the two rings is 27.54°.

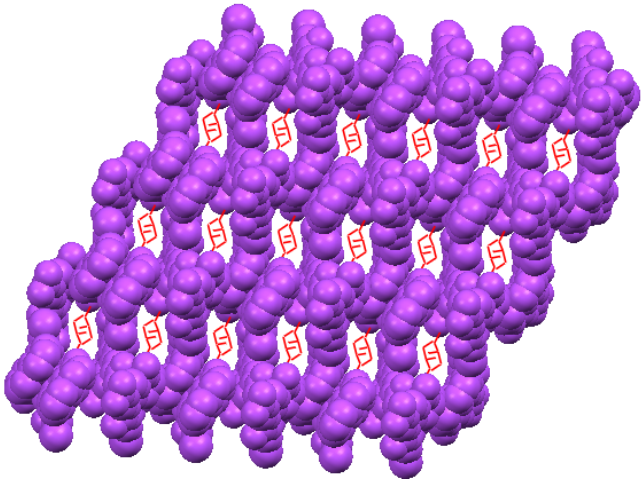

Fig. S23 Packing diagram of the complex 3 along crystallographic 'b' axis. ((violet = receptor (spacefill), red = triethyl amine (wireframe)).

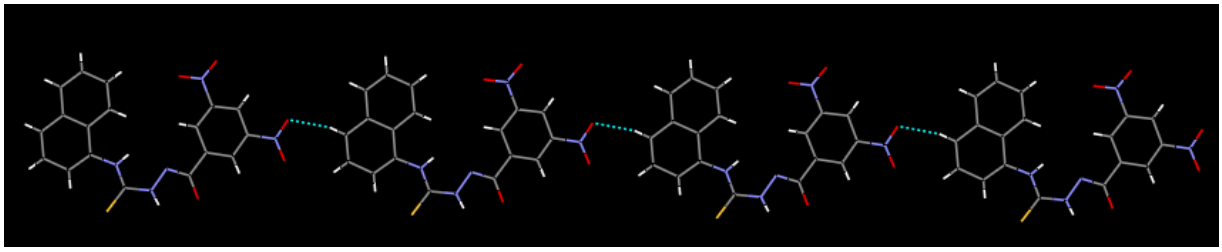

Fig. S24 Showing the formation of hydrogen bonding chain polymeric network among the deprotonated receptors in complex 3. View along 'c' axis.

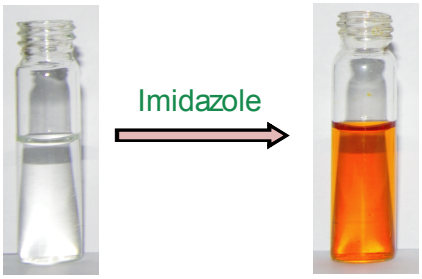

Fig. S25 Color changes observed with the addition of imidazole guest to the CH_3CN solution of receptor **L** (1.6×10^{-3} M).

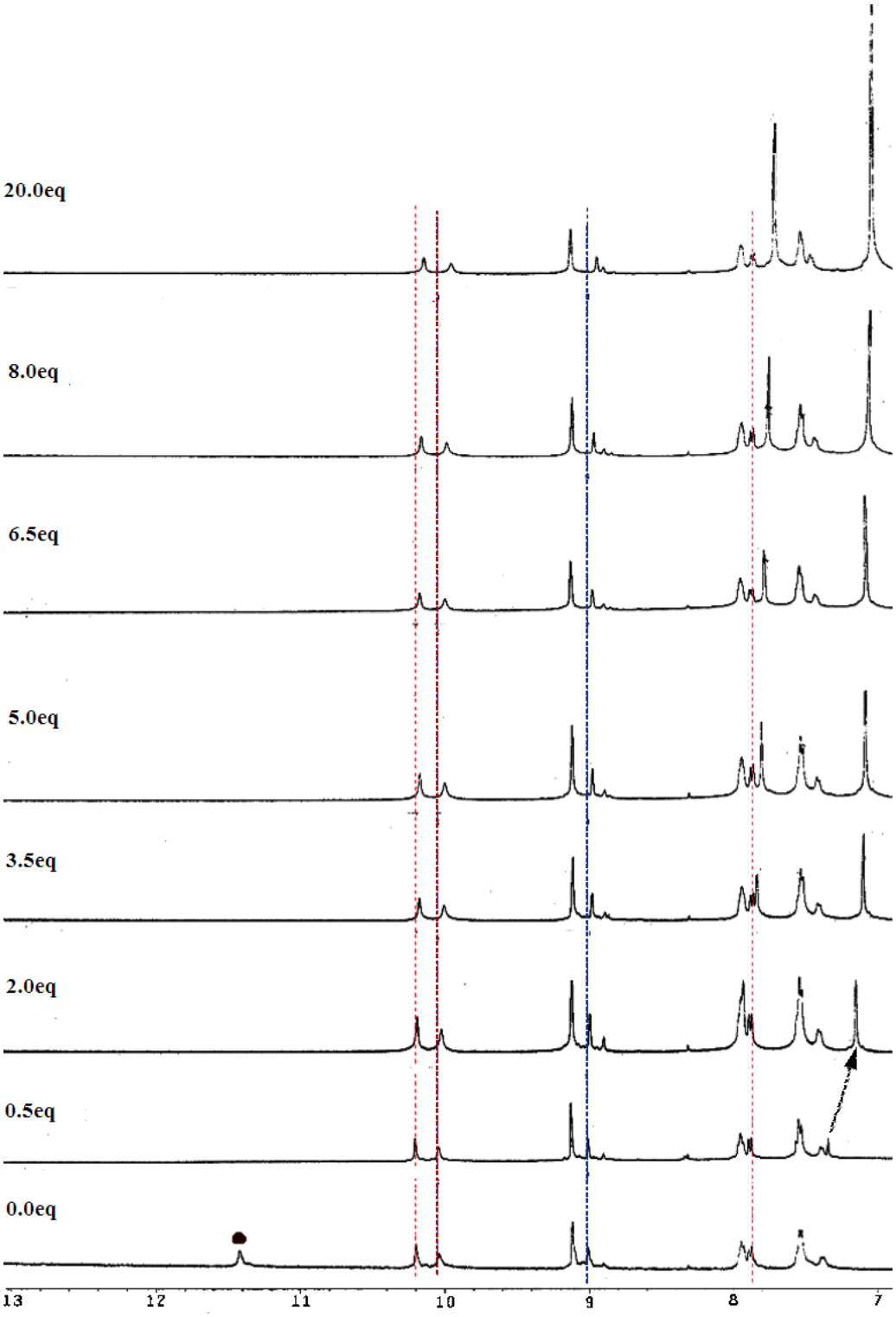

Fig. S26 Stack plot of the ^{1}H-NMR spectra of receptor **L** in the presence of increasing amounts of imidazole recorded in d_6-DMSO.

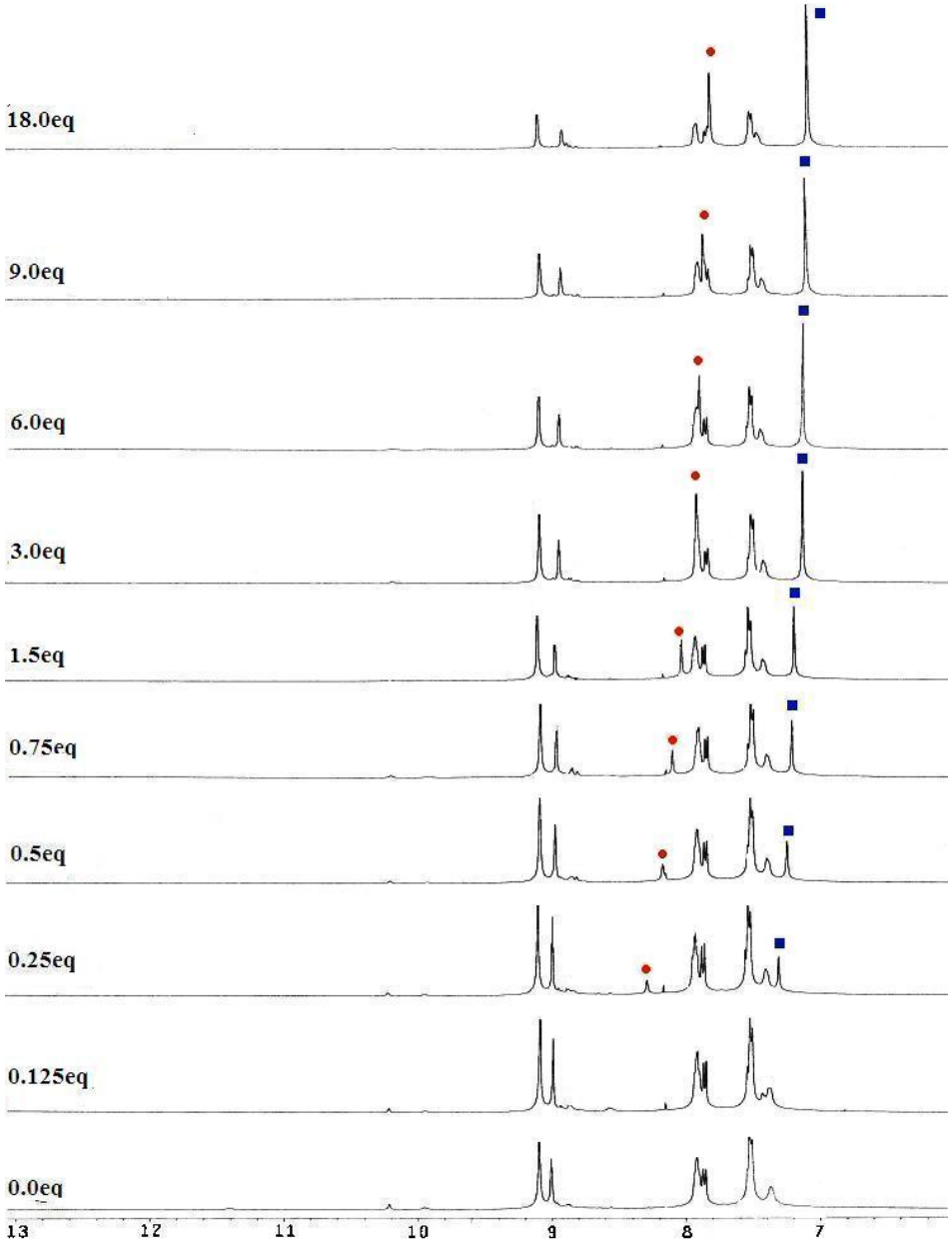

Fig. S27 Stack plot of the ^{1}H-NMR spectra of receptor **L** in the presence of increasing amounts of imidazole recorded in d_6-DMSO:D_2O mixture (9:1).

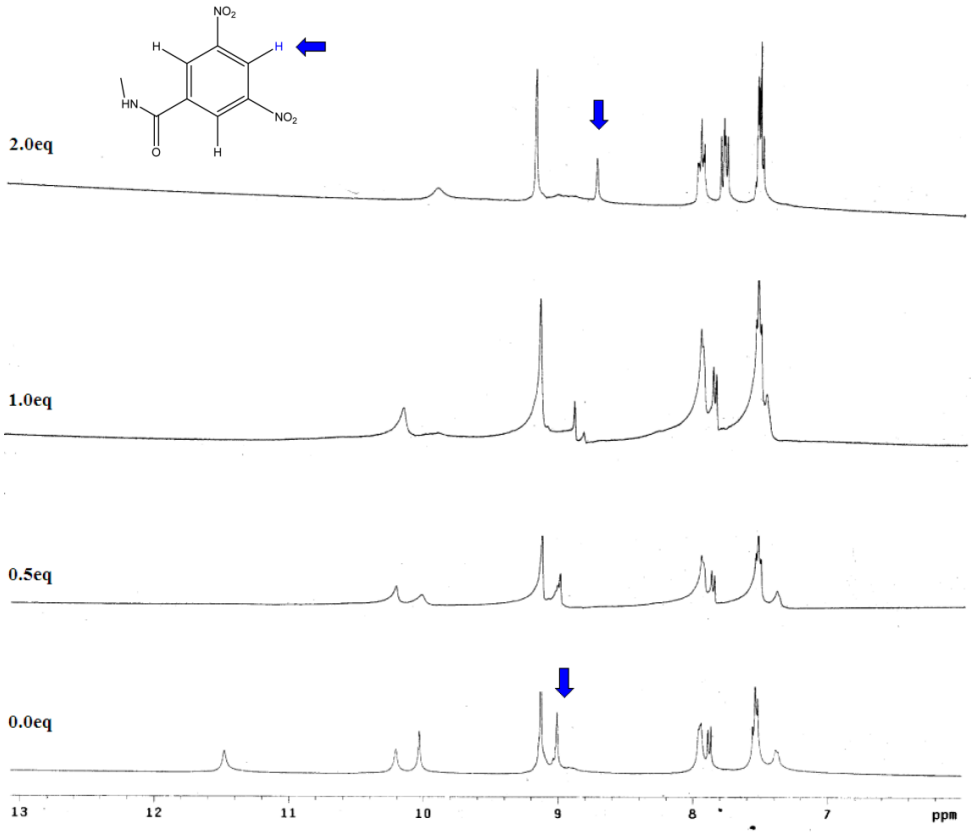

Fig. S28 Stack plot of the ^{1}H-NMR spectra of receptor **L** in the presence of increasing amounts of TBAOH (tetrabutylammonium hydroxide) recorded in d_6-DMSO.

Table S1 C−N bond length comparison table of the receptor in complexes (1−3).

Atoms	Distances		
	Complex1	Complex2	Complex3
C1−N1	1.405(5)	1.413(4)	1.403(6)
C11−N1	1.356(4)	1.359(4)	1.357(6)
C11−N2	1.343(4)	1.350(4)	1.347(6)
C12−N3	1.309(4)	1.304(4)	1.303(6)
C15−N4	1.459(5)	1.483(5)	1.482(8)
C17−N5	1.485(6)	1.488(5)	1.470(7)

Table S2 Hydrogen bonding parameters for complex 1−3.

Atoms	$d_{D\text{-}H}$ (Å)	$d_{H\cdots A}$ (Å)	$d_{D\cdots A}$ (Å)	<D−H···A(°)
Complex-1				
N(6)−H(6N)····O1	1.05	1.58	2.622(4)	177
C(21) –H(21)····O6	0.930	2.706	3.585(7)	158.0
C(19) –H(19)····O2	0.929	2.589	3.237(5)	127.1
N(7) –H(7N)····O3	0.860	2.511	3.031(6)	119.8
N(7) –H(7N)····S1	0.860	2.819	3.454(5)	132.5
N2−H(2N)····S1	0.981	2.742	3.567(3)	139.4
O6−H(6O)····O1	0.820	2.213	2.803(3)	129.1
C4−H(4)····O4	0.929	2.580	3.410(5)	149.0
Complex-2				
N(6)−H(6N)····O1	1.089	1.574	2.651(3)	169.1
C(21)−H(21B)····O6	0.971	2.563	3.284(4)	131.1
C(23)−H(23A)····O6	0.970	2.640	3.344(4)	129.7
O(6) −H(2O) ····N8	0.941	1.964	2.884(4)	165.2
C(19)−H(19A)····O2	0.970	2.653	3.615(5)	171.0
C(22)−H(22A)····O3	0.970	2.631	3.533(5)	154.8
C(23)−H(23B)····O3	0.970	2.701	3.586(5)	151.8
N2−H(2N) ····O6	1.000	2.064	3.040(4)	164.9
C5−H(5) ····O1	0.930	2.553	3.442(4)	160.3
C6−H(6) ····O2	0.931	2.589	3.459(6)	155.7
Complex3				
N(6)−H(6N)····O1	1.04	1.74	2.757(6)	164.9
C(24)−H(24B)····N3	0.961	2.720	3.634(7)	159.0
N(2)−H(2N) ····O1	0.860	2.154	2.896(4)	144.3
C4−H(4) ····O4	0.929	2.579	3.433(5)	153.0

Table S3. Summary of the various contact contributions to the receptor Hirshfeld surface area in complexes (1−3).

	Complex1	Complex2	Complex3
S····H	7.5	7.0	8.4
O····H	23.4	25.7	28.7
N····H	4.8	4.5	5.3
H····H	19.6	26.8	25.7
C····H	22.1	14.2	18.3
C····C	4.4	6.5	4.9
S····O	1.0	1.0	1.3
O····O	0.4	0.4	1.4
O····N	2.3	2.0	0.9
O····C	8.9	7.1	3.3
N····C	4.5	4.1	1.7
S····N	0.0	0.8	0.0