Electronic Supplementary Material (ESI) for RSC Advances
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Supplementary Information

8(E)-4-[{2-(2,4-dinitrophenyl)hydrazono}benzene-1,3-diol] as a solvatochromic Schiff base and chromogenic signaling of water content by its deprotonated form in acetonitrile

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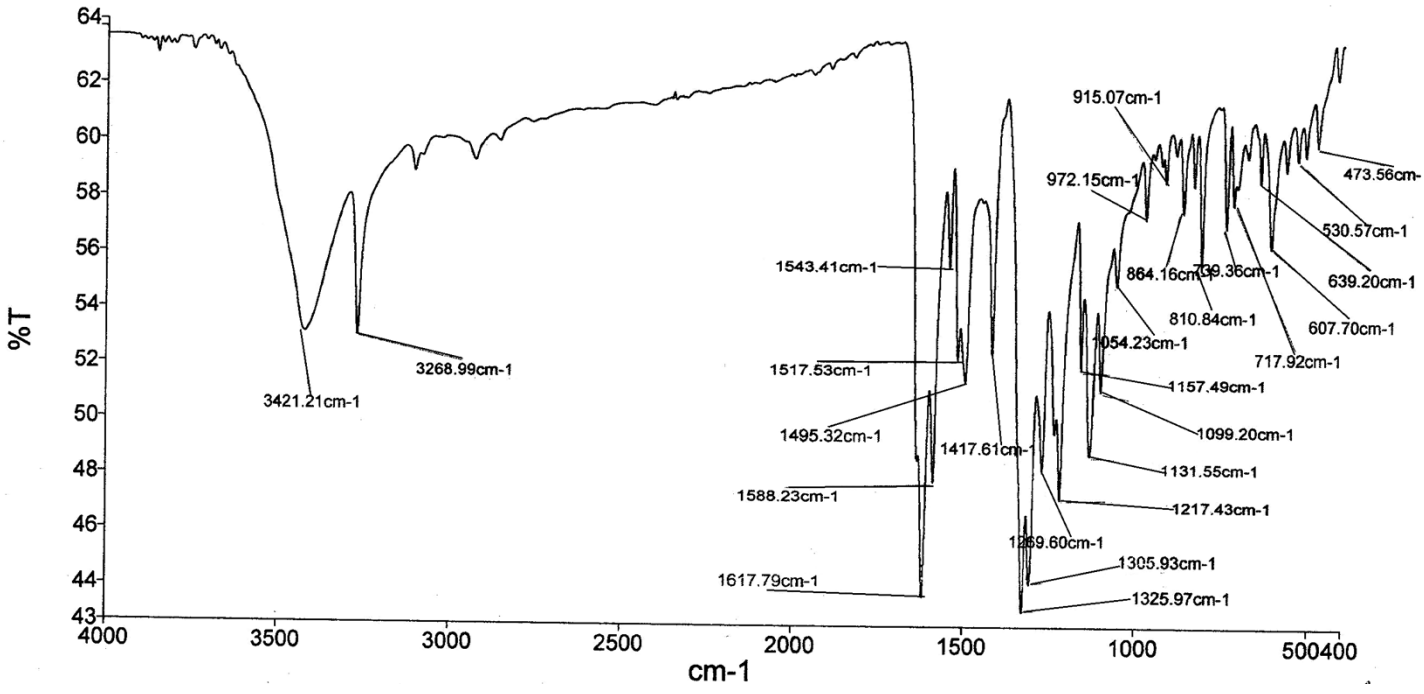

Fig. 1 IR spectra of DBH.

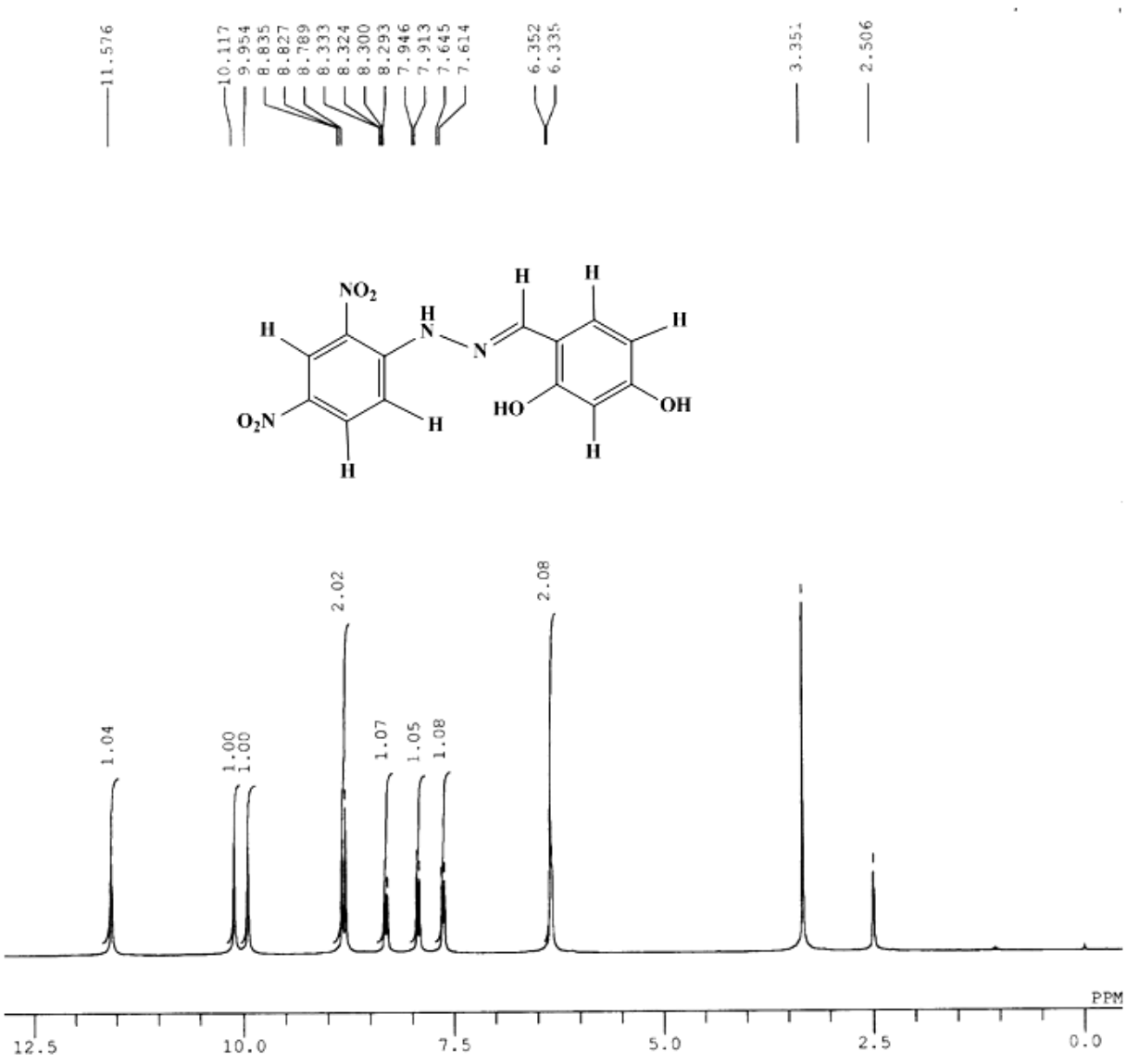

Fig. 2 ^{1}H NMR spectra of DBH.

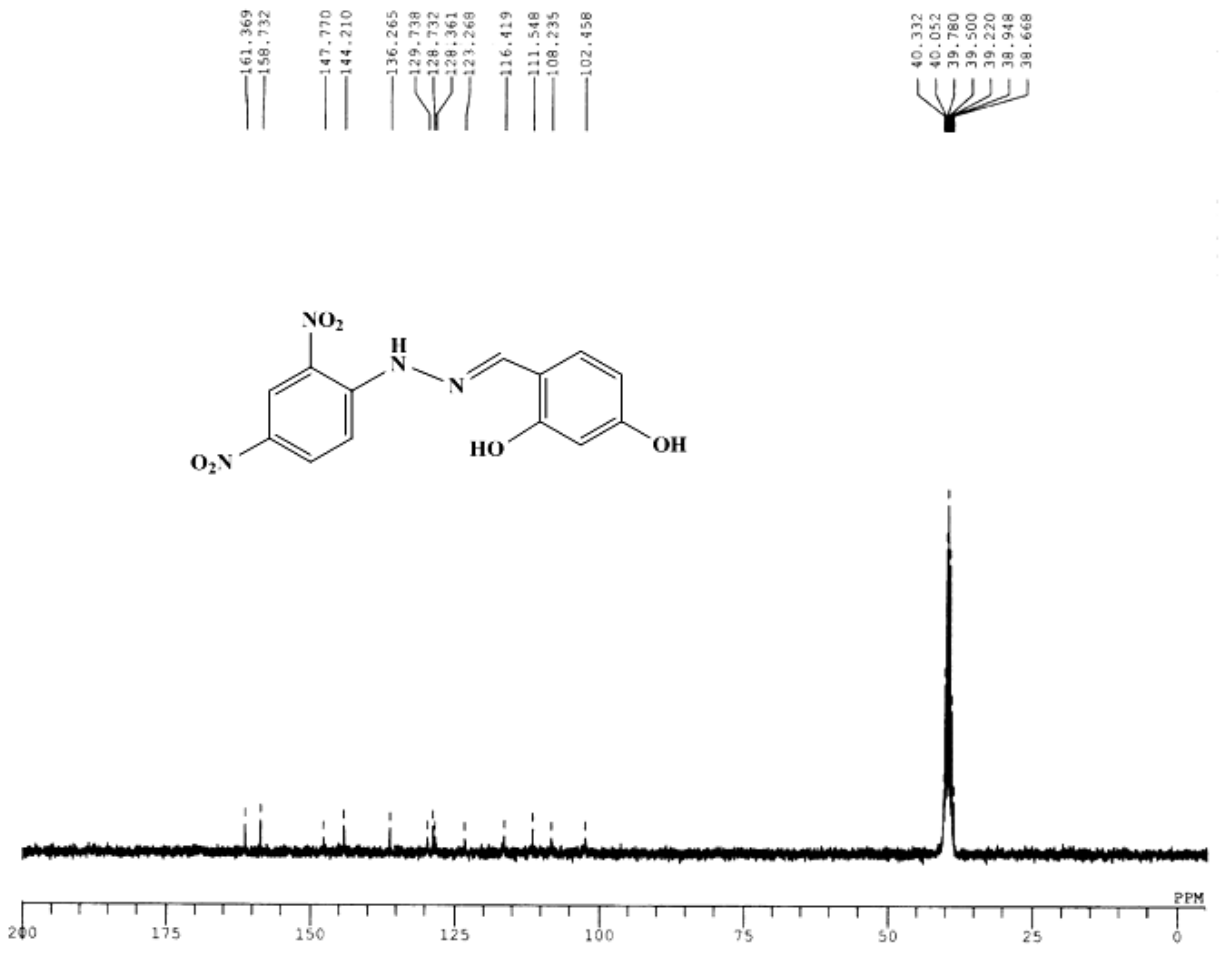

Fig. 3 ^{13}C NMR spectra of DBH.

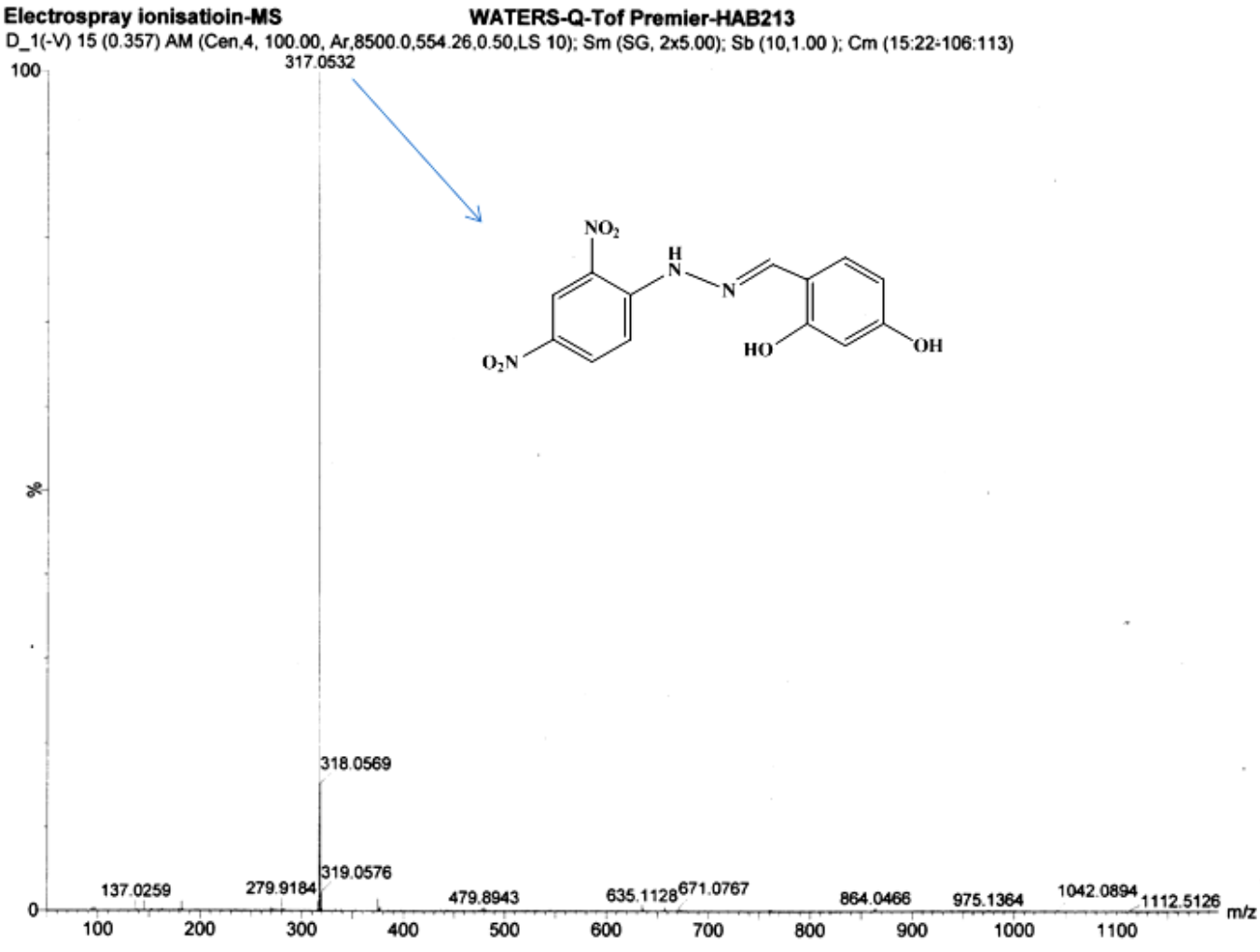

Fig. 4 ESI-MS spectra of DBH.

Empirical Formula	$C_{15}\ H_{16}\ N_4\ O_7\ S$
Formula weight	396.38
Temp, K	293(2)
λ (Å)	0.71073
Crystal system	Monoclinic
Space group	p21/c
a (Å)	19.299
b (Å)	6.620
c (Å)	14.534
α = γ (º)	90.00
β	102.77
V (Å^3)	1811.0
Z	4
D_{calc} (mg/m^3)	1.454
μ (mm^{-1})	0.225
F(000)	824
Crystal size (mm)	0.25×0.24×0.23
θ range for data collection (º)	3.26 - 29.23
No. of reflections collected	7741
No. of independent reflections (R_{int})	4127 (0.0403)
Number of data/restraints/parameters	4127 / 0 / 246
Goodness-of-fit on F^2	0.994
R_1, wR_2 [a,b][(I>2σ(I))]	0.0694, 0.1293
R_1, wR_2[a,b] (all data)	0.1691, 0.1758
Largest difference in peak and hole (e.Å^{-3})	0.582 and -0.283

Table 1 Crystallographic data of DBH.

Bond distances (Å)		Bond angles (°)	
O1-C2	1.358(4)	C7-N1-N2	113.9(3)
O2-C4	1.345(4)	C8-N2-N1	121.4(3)
O3-N3	1.239(4)	O4-N3-O3	121.1(3)
O4-N3	1.223(4)	O4-N3-C9	119.3(3)
O5-N4	1.212(4)	O3-N3-C9	119.6(3)
O6-N4	1.230(4)	O5-N4-O6	123.4(3)
N1-C7	1.291(4)	O5-N4-C11	118.9(3)
N1-N2	1.386(4)	O6-N4-C11	117.7(3)
N2-C8	1.342(4)	N1-C7-C1	124.0(3)
N3-C9	1.442(4)	C6-C1-C2	117.2(3)
N4-C11	1.461(4)	C6-C1-C7	119.2(3)
C7-C1	1.430(4)	C2-C1-C7	123.6(3)
C1-C6	1.404(4)	O1-C2-C1	121.5(3)
C1-C2	1.405(4)	N2-C8-C9	122.8(3)
S1-O7	1.511(3)	N2-C8-C13	121.2(3)
S1-C14	1.755(5)	O7-S1-C14	104.8(2)
S1-C15	1.765(4)	O7-S1-C15	105.2(2)

Table 2 Selected bond distances (Å) and bond angles (°) for DBH.

D−H···A	D−H	H···A	D···A	< (DHA)
N(2)−H(1)···O(3)	0.86	1.96	2.604 (4)	131
O(1)−H(2)···N(1)	0.82	1.99	2.708 (4)	146
O(2)−H(3)···S(1)	0.82	2.80	3.516 (3)	146

Table 3 Hydrogen bond parameters [Å and ˚] in DBH.

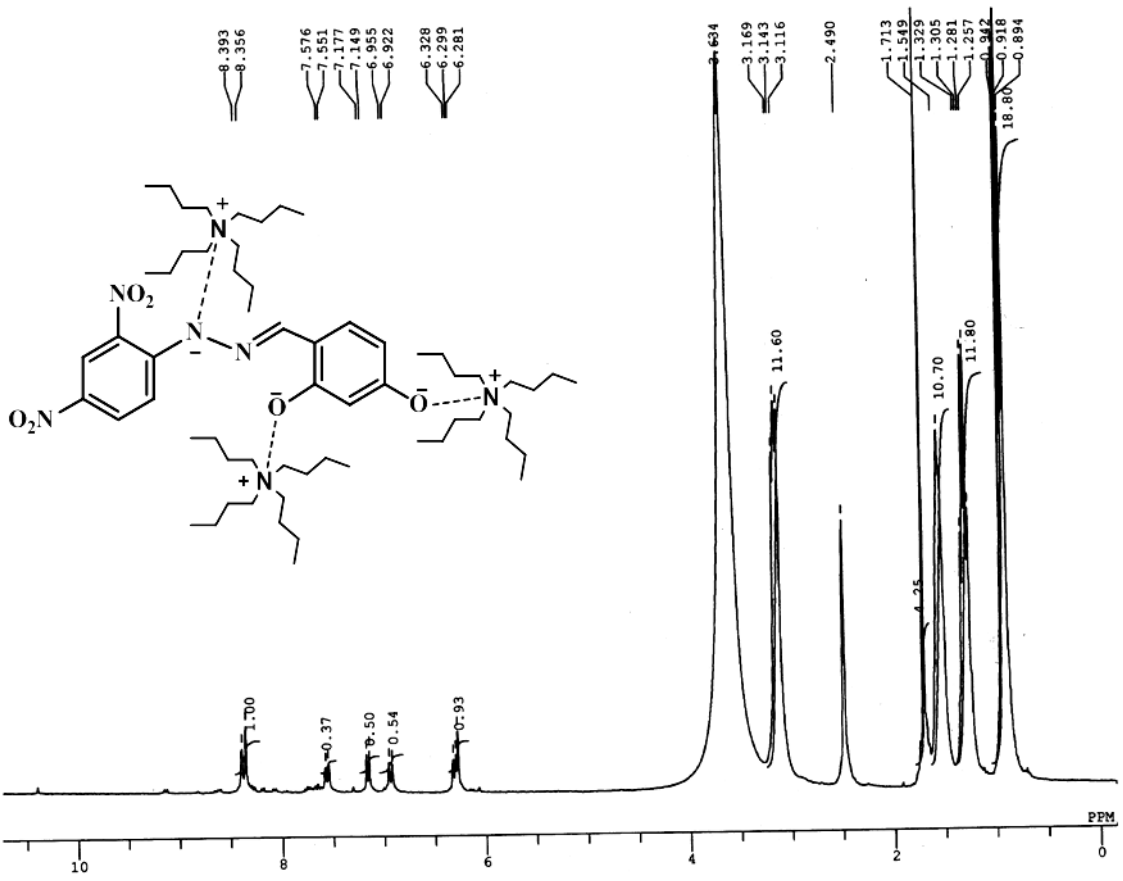

Fig. 5 ^{1}H NMR spectra of tetrabutylammonium salt of DBH.

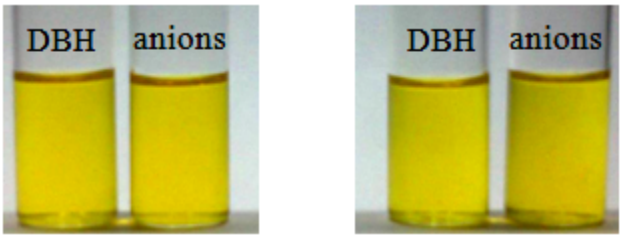

Fig. 6 Color changes of DBH (50 μM) in ethanol (left) and methanol (right) upon addition of 1equivalent of tetrabutylammonium salts of iodide, bromide, fluoride and acetate.

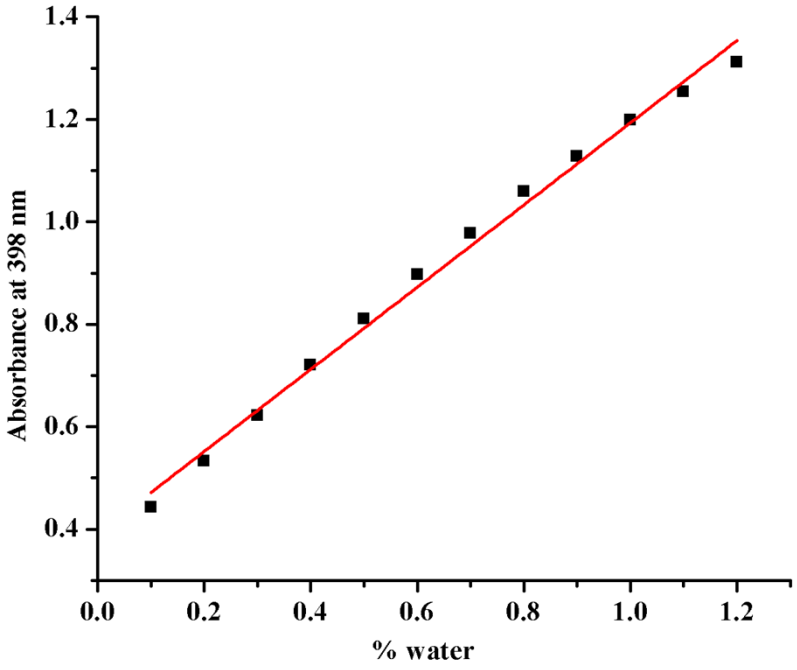

Fig. 7 Absorbance of deprotonated DBH (50 μM DBH + 10 equivalents acetate ions) at 398 nm in acetonitrile as a function of the % water ($R^2 = 0.9929$, linear range = 0.1-1.2%).