Electronic Supplementary Material (ESI) for RSC Advances.

Naphthoquinone based chemosensors for transition metal ions: Experiment and Theory

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Supplementary Material

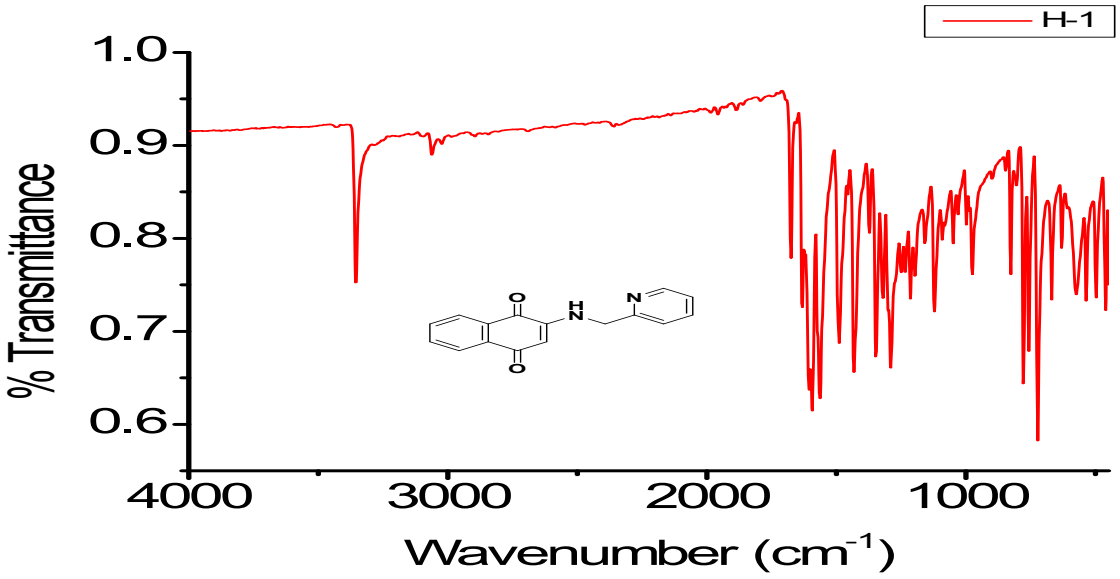


Fig. S-1 a) FT-IR spectrum of **H-1** in region 4000 cm^{-1} to 400 cm^{-1}.

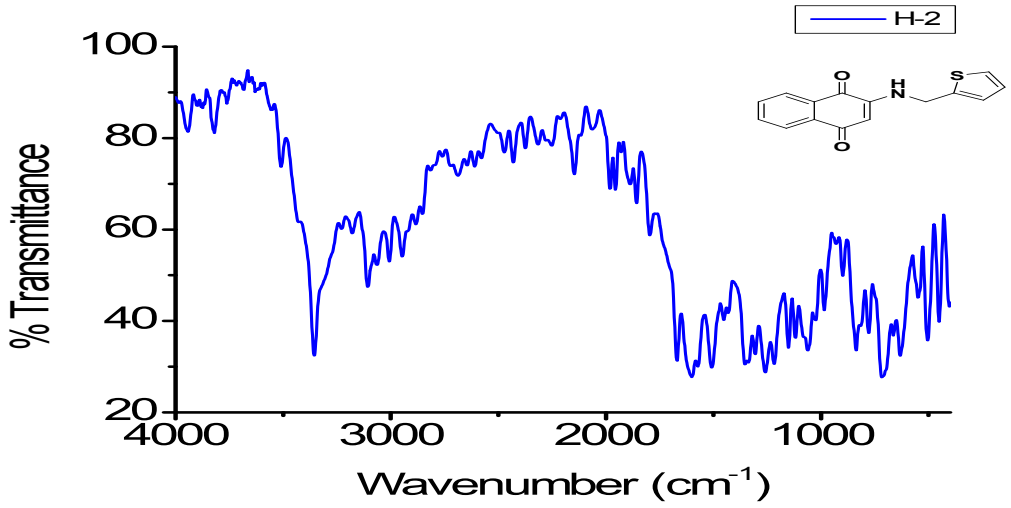


Fig. S-1 b) FT-IR spectrum of **H-2** in region 4000 cm^{-1} to 400 cm^{-1}

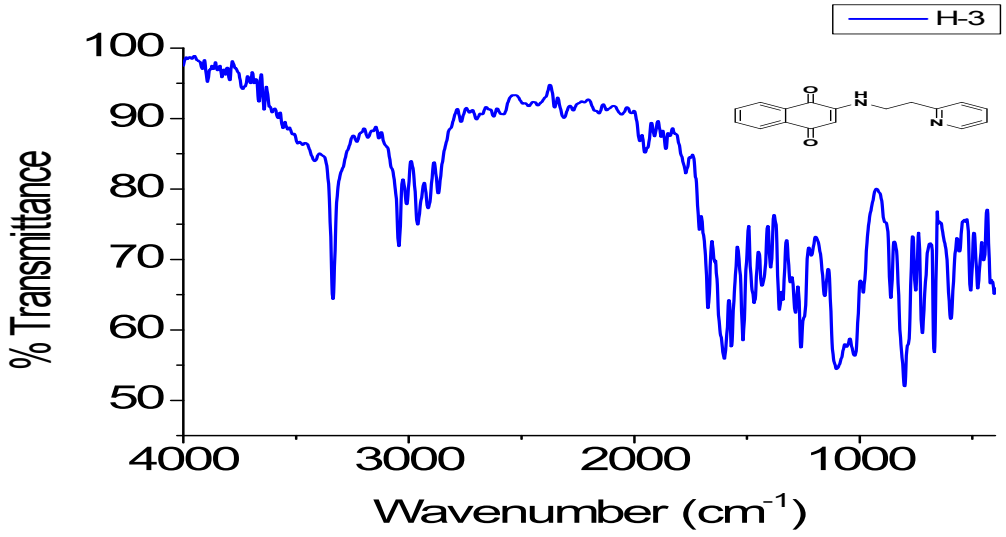


Fig. S-1 c) FT-IR spectrum of **H-3** in region 4000 cm^{-1} to 400 cm^{-1}

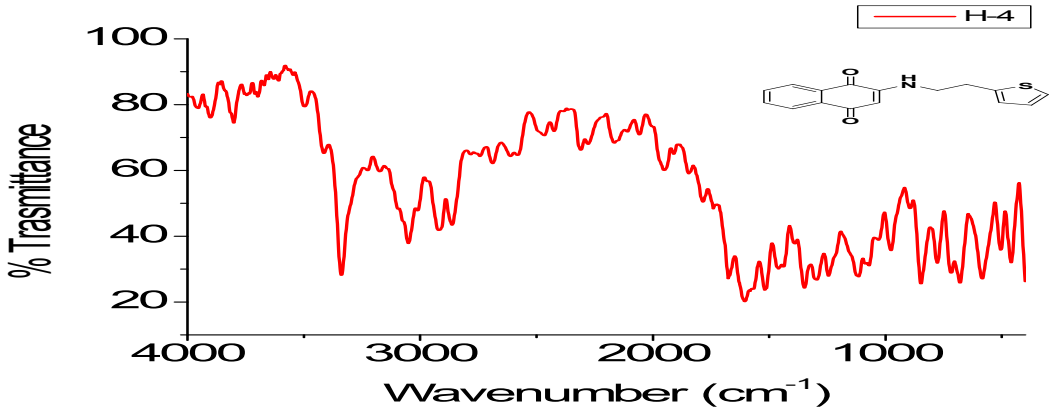
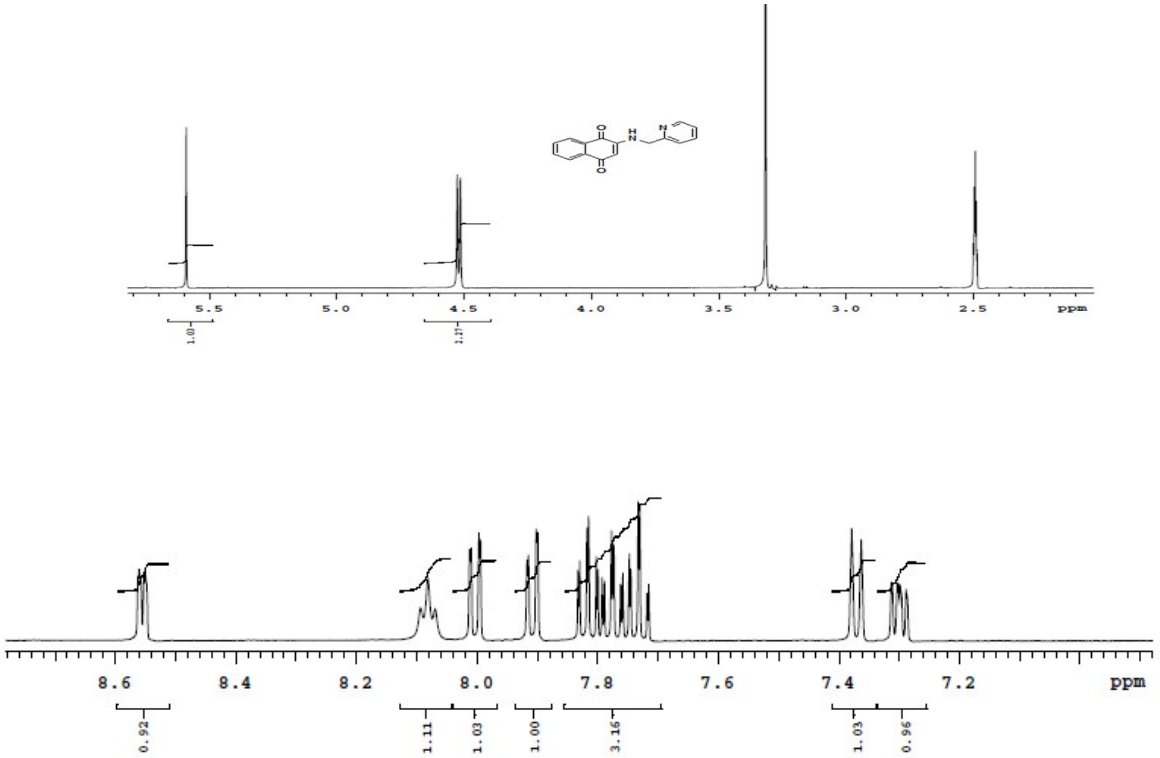


Fig. S-1 d) FT-IR spectrum of **H-4** in region 4000 cm^{-1} to 400 cm^{-1}

a)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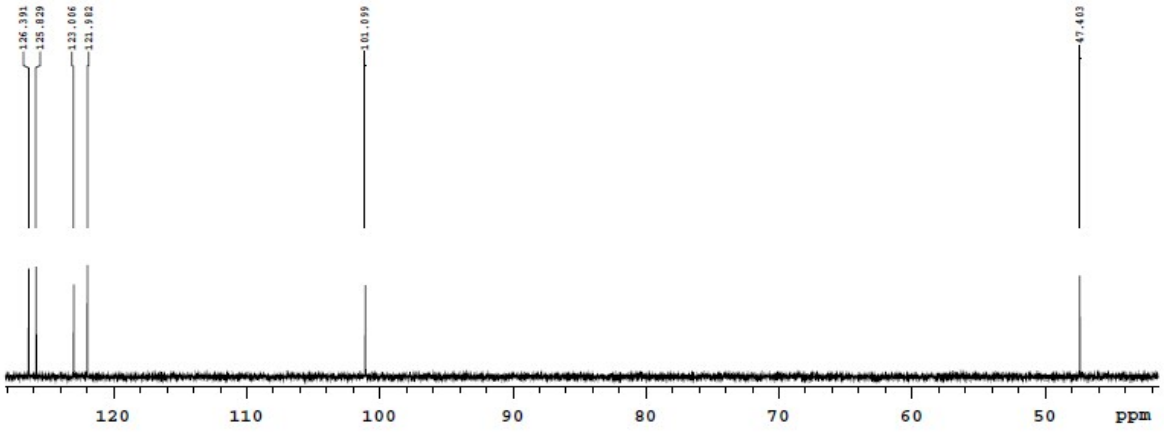
5.0
4.5
4.0
3.5
3.0
2.5
ppm
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm
0.92
1.11
1.03
1.00
3.16
1.03
0.96

b)


126.391
125.829
123.066
121.982
101.099
47.403
120
110
100
90
80
70
60
50
ppm

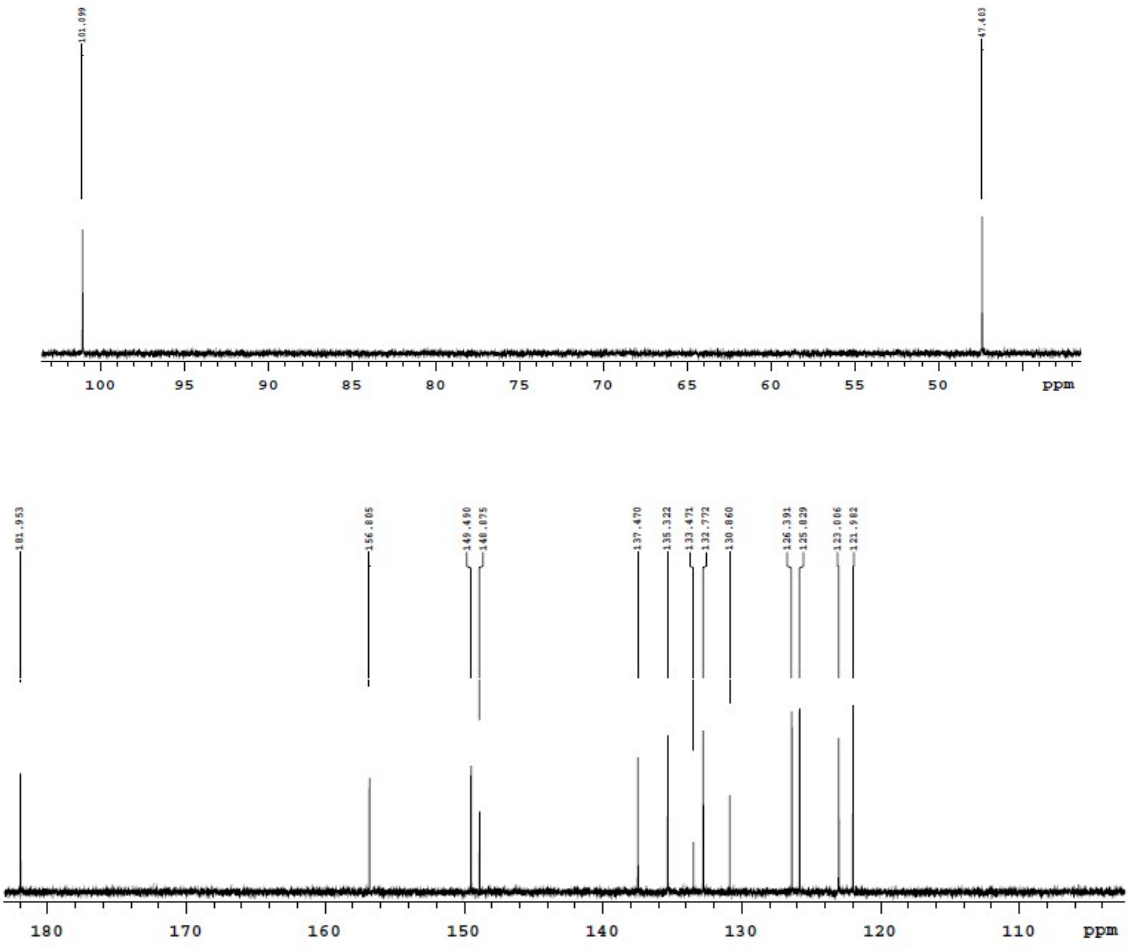
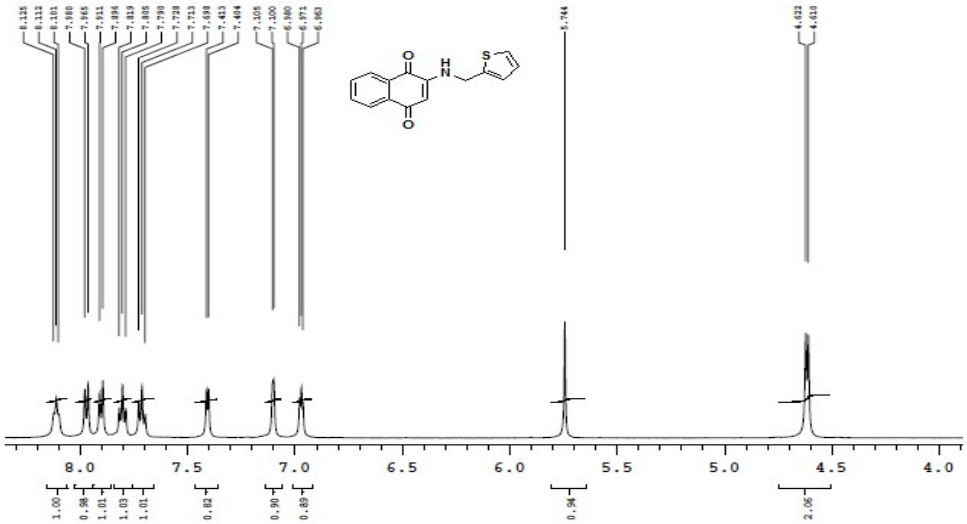


Fig. S2 a) ^{1}H and b) ^{13}C NMR spectra of **H-1** in DMSO-d_6 solvent.

a)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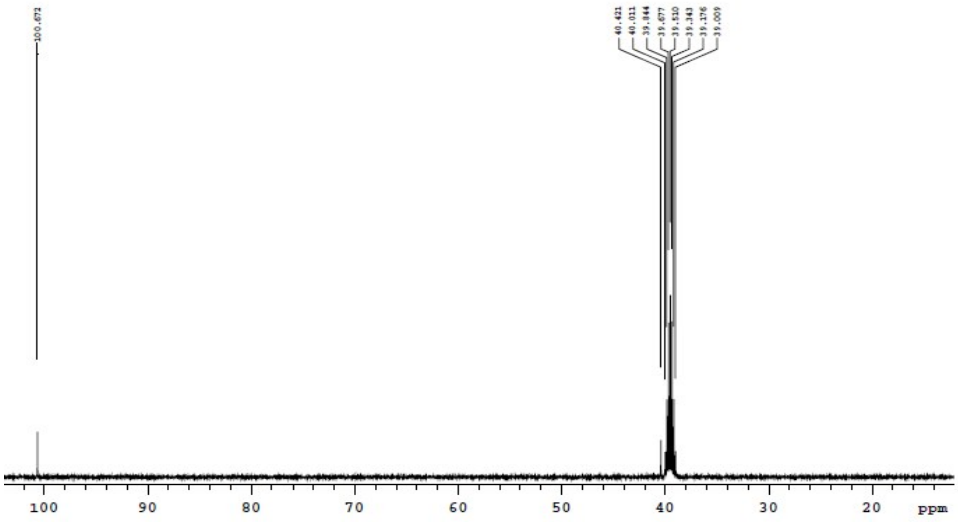
8.112
8.101
7.980
7.965
7.931
7.896
7.819
7.805
7.790
7.738
7.713
7.698
7.413
7.404
7.105
7.100
6.980
6.971
6.963
5.744
4.633
4.610
O
H
N
S
O
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
1.00
0.98
1.01
1.03
1.01
0.82
0.90
0.89
0.94
2.06

b)


100.672
40.421
40.011
39.844
39.677
39.510
39.343
39.176
39.009
100
90
80
70
60
50
40
30
20
ppm

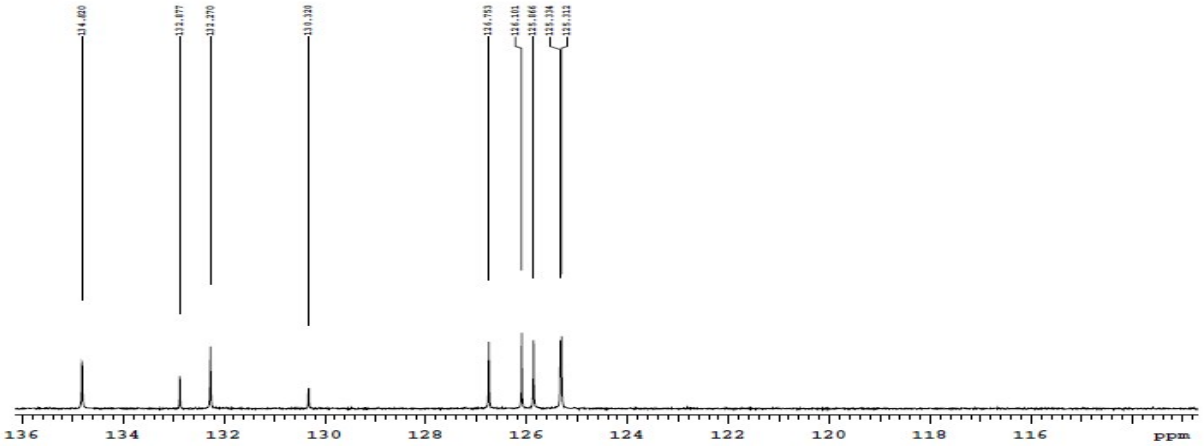
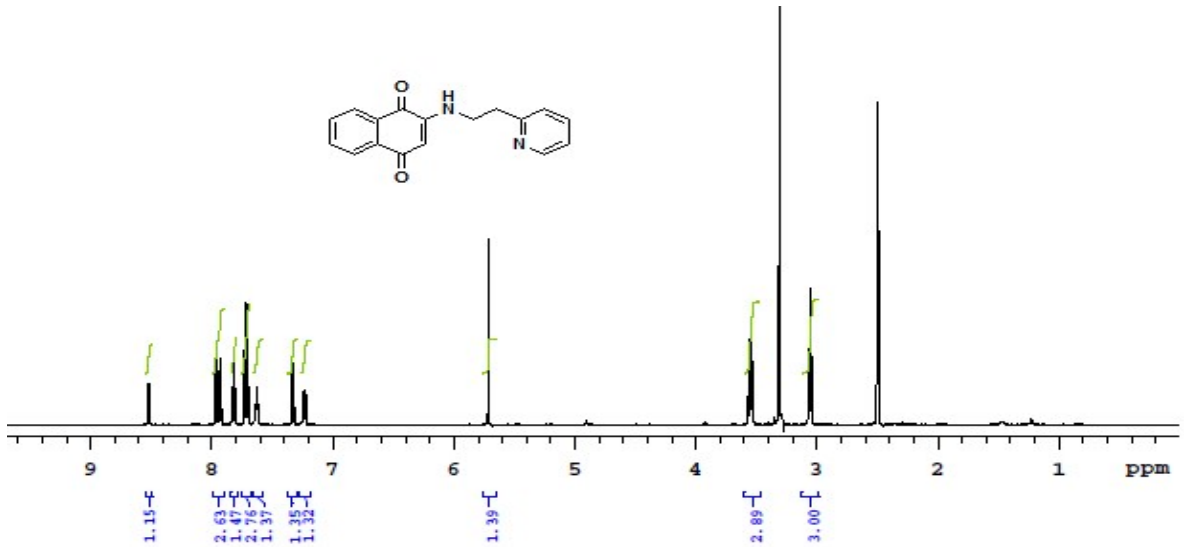


Fig. S3 a)^{1}H, b) ^{13}C NMR spectra of **H-2** in DMSO-d_6 solvent

a)



b)

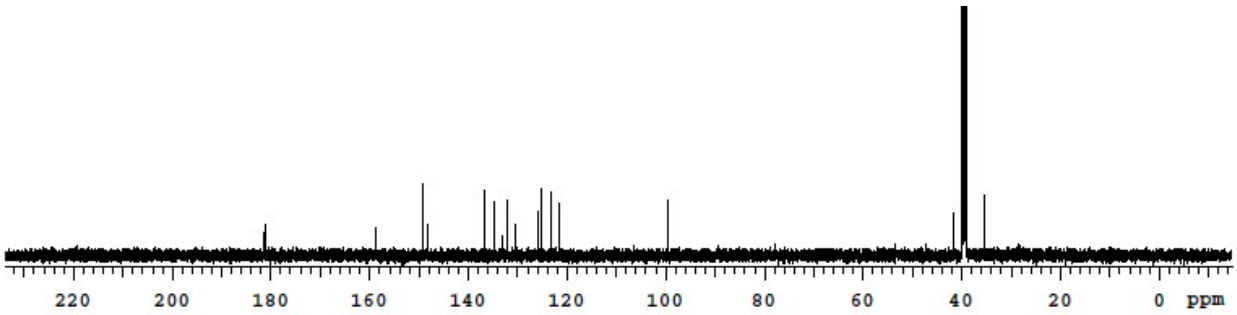
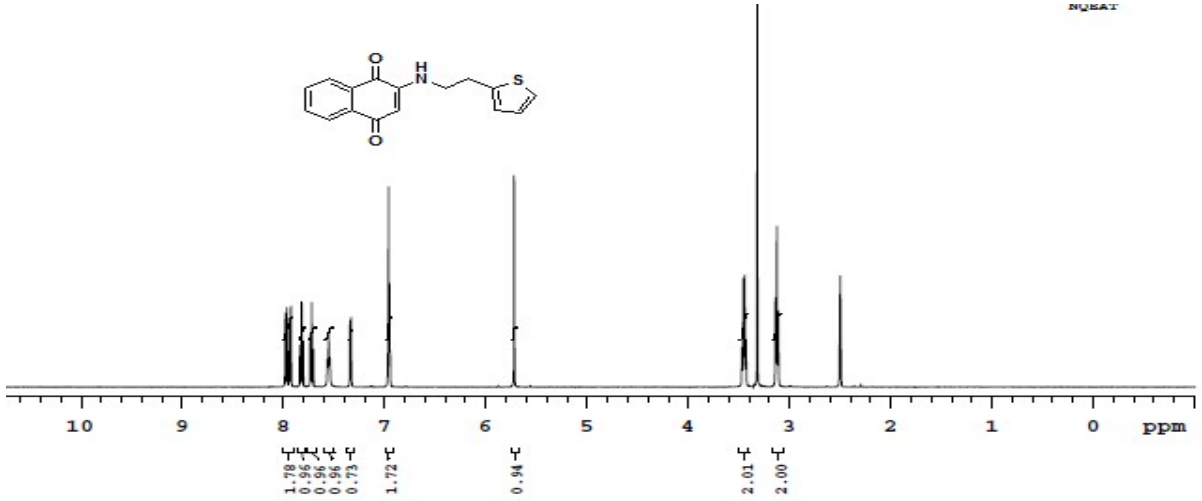


Fig.S4 a) ^{1}H and b) ^{13}C NMR spectra of **H-3** in DMSO-d_6.

a)



b)

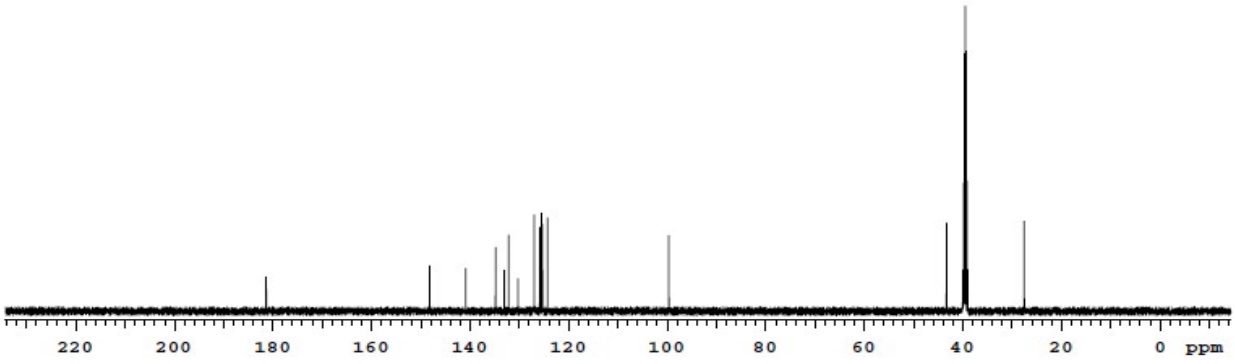
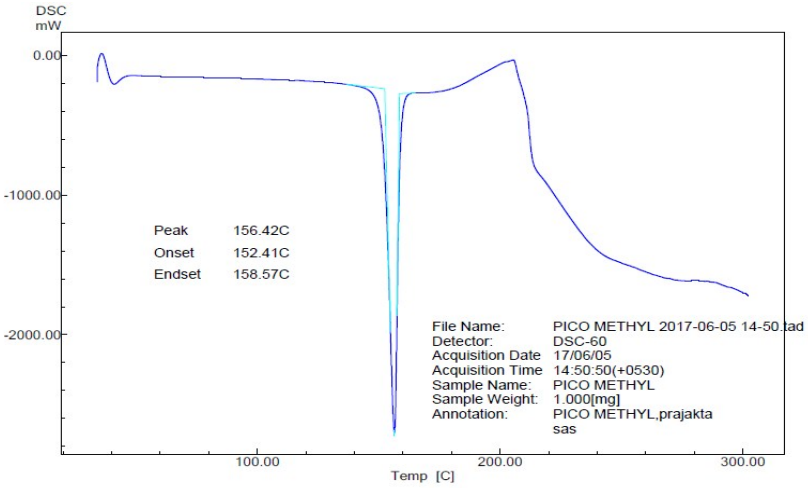
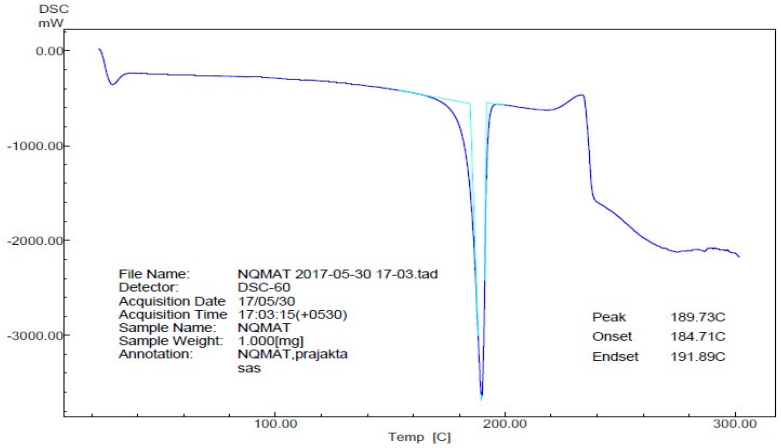


Fig. S5 a) ^{1}H and b) ^{13}C NMR spectra of **H-4** in DMSO-d_6 solvent.

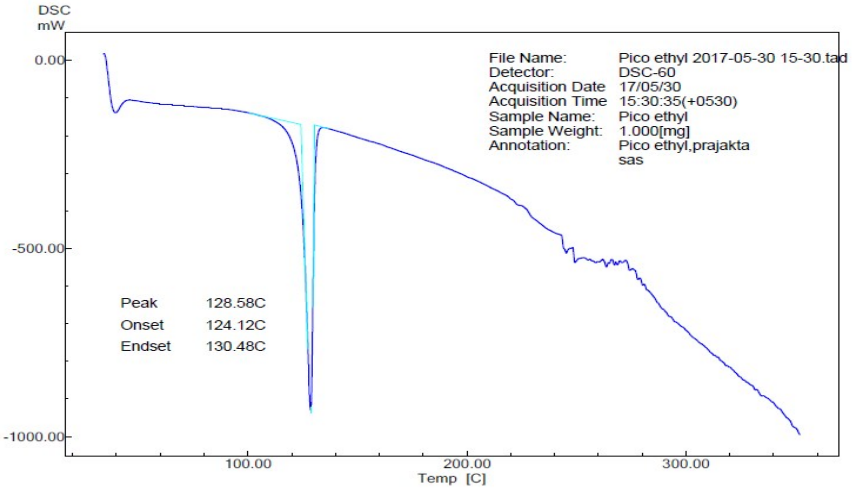
H-1


DSC
mW
0.00
-1000.00
-2000.00
Peak 156.42C
Onset 152.41C
Endset 158.57C
File Name: PICO METHYL 2017-06-05 14-50.tad
Detector: DSC-60
Acquisition Date 17/06/05
Acquisition Time 14:50:50(+0530)
Sample Name: PICO METHYL
Sample Weight: 1.000[mg]
Annotation: PICO METHYL,prajakta sas
100.00
200.00
300.00
Temp [C]

H-2


DSC
mW
0.00
-1000.00
-2000.00
-3000.00
File Name: NQMAT 2017-05-30 17-03.tad
Detector: DSC-60
Acquisition Date 17/05/30
Acquisition Time 17:03:15(+0530)
Sample Name: NQMAT
Sample Weight: 1.000[mg]
Annotation: NQMAT,prajakta sas
Peak 189.73C
Onset 184.71C
Endset 191.89C
100.00
200.00
300.00
Temp [C]

H-3



H-4

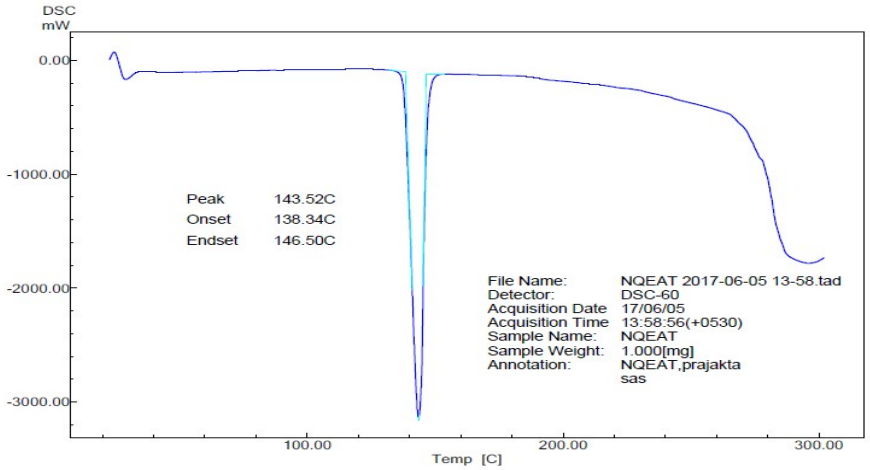


Fig. S6 DSC plot of H-1, H-2, H-3 and H-4

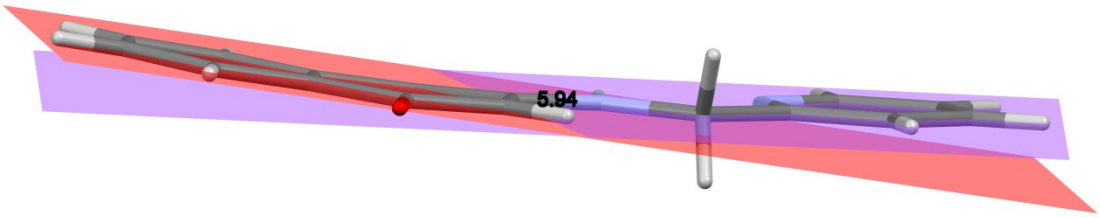
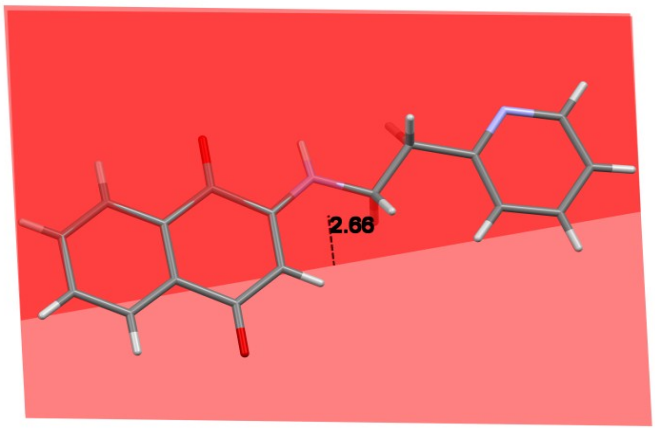


Fig. S7 Figure showing planarity of naphthoquinone and pyridyl ring of chemosensor H-1

a)



b)

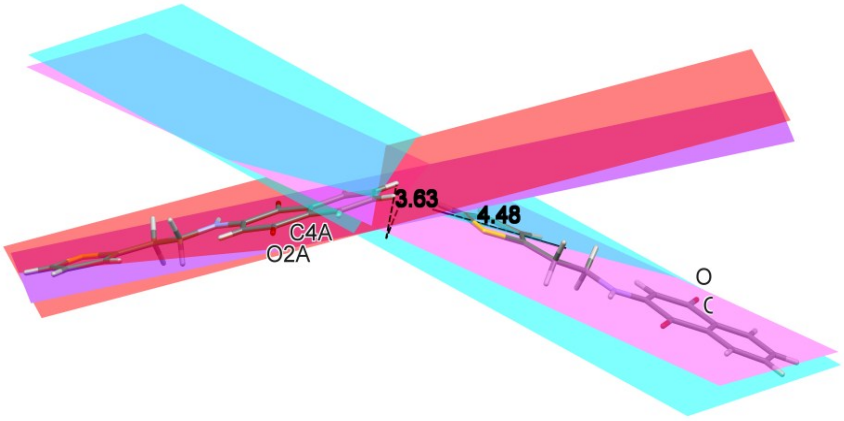


Fig. S8 Figure showing planarity of naphthoquinone and pyridyl ring of H-3 (a) and H-4 (b)

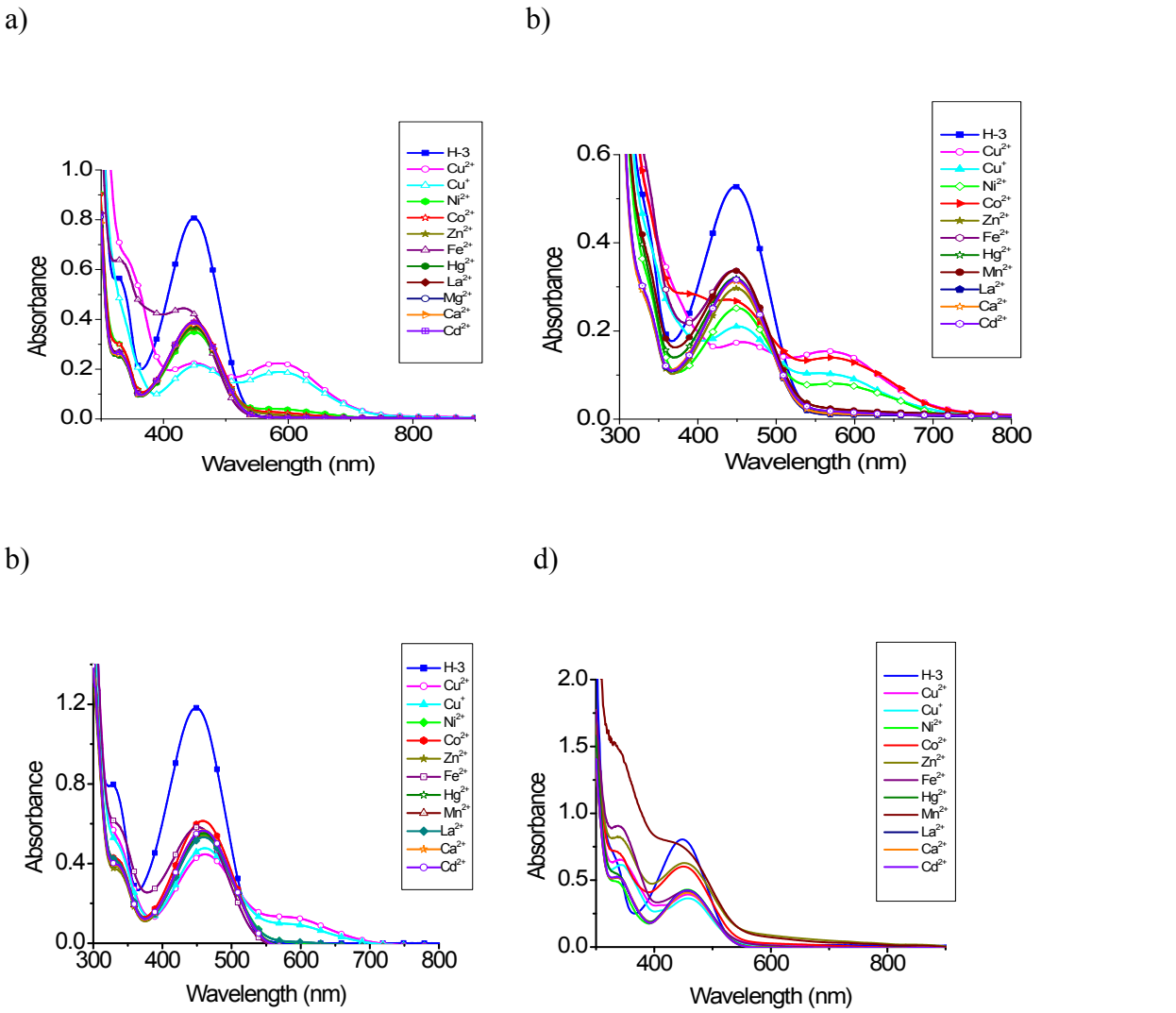
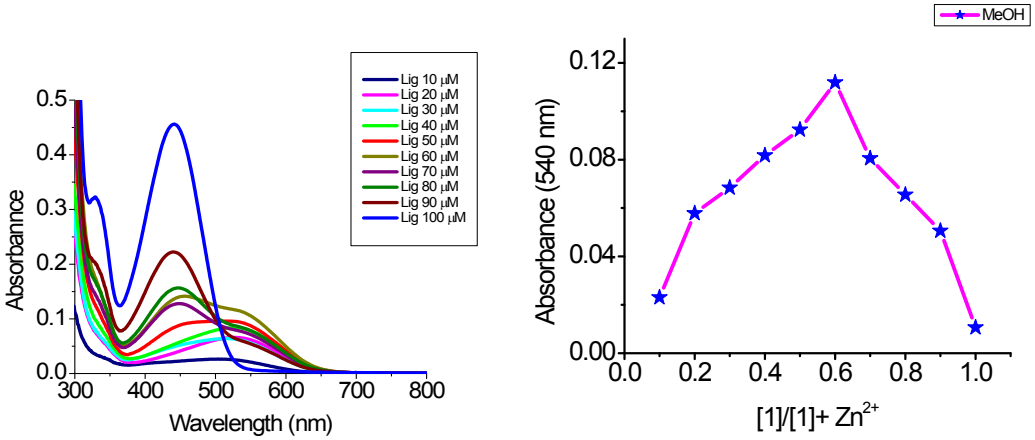
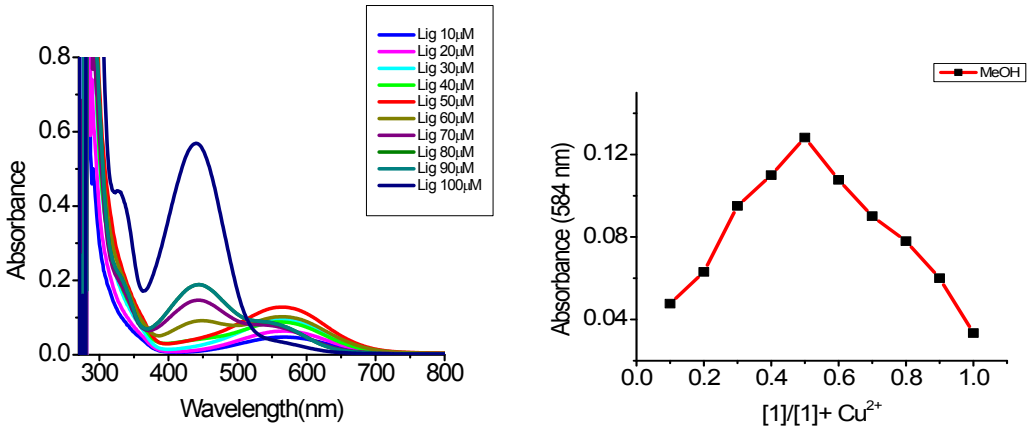


Fig. S9 a) UV-Visible spectra of H-3 in presence of various metal ions in methanol. b) UV-Visible spectra of H-3 in presence of various metal ions in methanol-triethylamine. c) UV-Visible spectra of H-3 in presence of various metal ions in methanol: water media. d) UV-Visual spectra of H-3 in presence of various metal ions in methanol-TEA-water

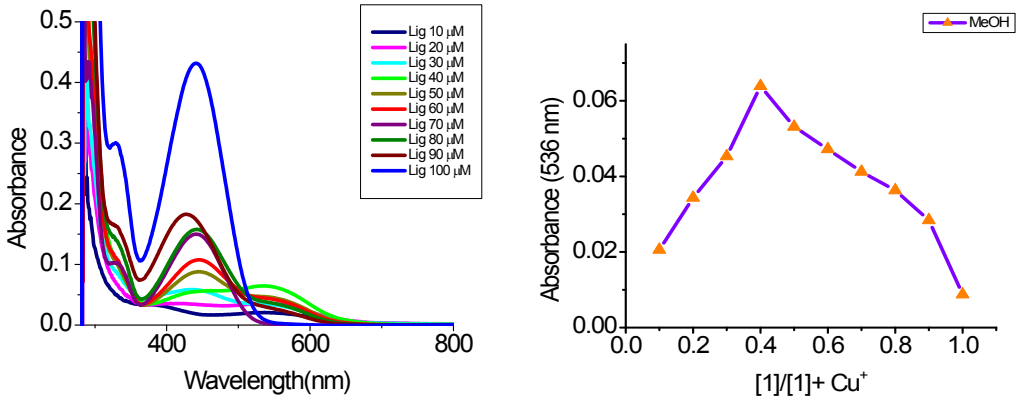
Zn^{2+}


Absorbance
Wavelength (nm)
Lig 10 μM
Lig 20 μM
Lig 30 μM
Lig 40 μM
Lig 50 μM
Lig 60 μM
Lig 70 μM
Lig 80 μM
Lig 90 μM
Lig 100 μM
MeOH
Absorbance (540 nm)
[1]/[1]+ Zn2+

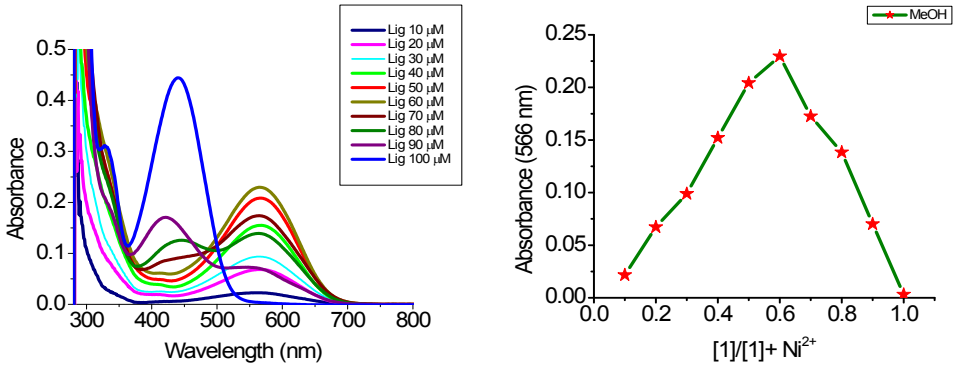
Cu^{2+}


Absorbance
Wavelength(nm)
Lig 10μM
Lig 20μM
Lig 30μM
Lig 40μM
Lig 50μM
Lig 60μM
Lig 70μM
Lig 80μM
Lig 90μM
Lig 100μM
MeOH
Absorbance (584 nm)
[1]/[1]+ Cu2+

Cu^{+}


Absorbance
Wavelength(nm)
Lig 10 μM
Lig 20 μM
Lig 30 μM
Lig 40 μM
Lig 50 μM
Lig 60 μM
Lig 70 μM
Lig 80 μM
Lig 90 μM
Lig 100 μM
MeOH
Absorbance (536 nm)
[1]/[1]+ Cu+

Ni^{2+}



Co^{2+}

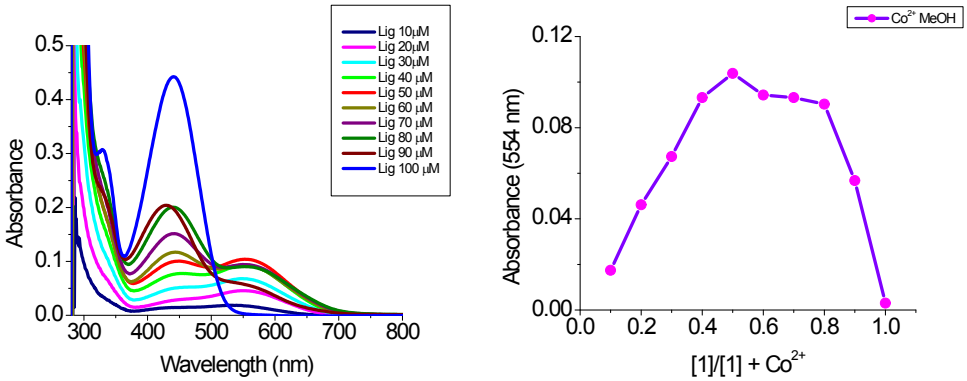
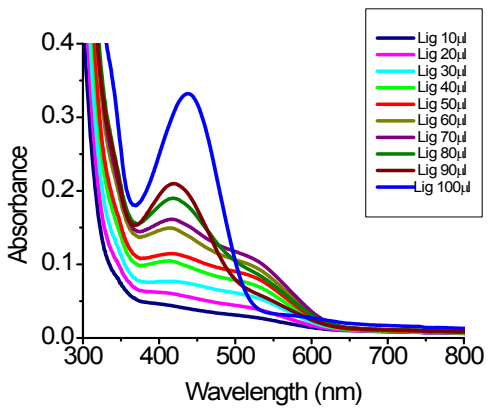
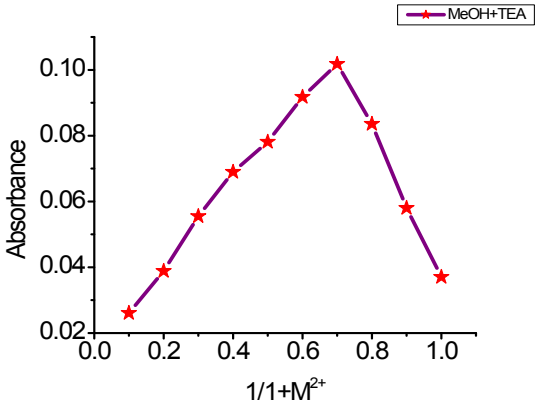


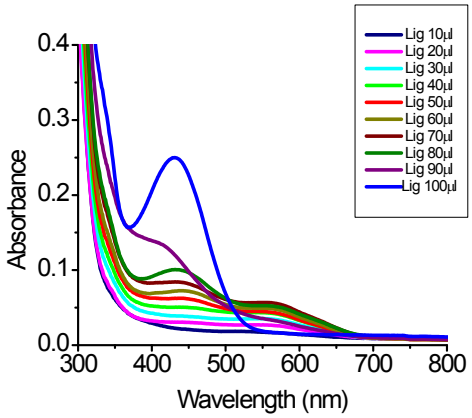
Fig. S10 Job's plot experiment for H-1 and Cu^{2+}, Cu^{+}, Ni^{2+}, Co^{2+} and Zn^{2+} in methanol.

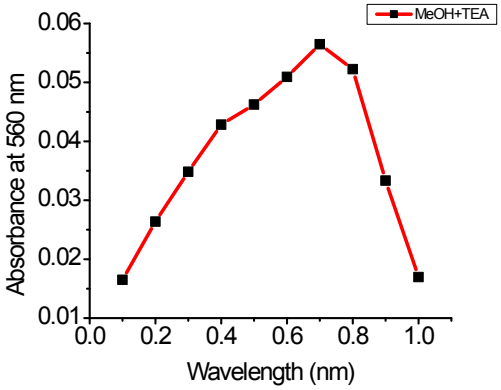
Zn^{2+}


Lig 10µl
Lig 20µl
Lig 30µl
Lig 40µl
Lig 50µl
Lig 60µl
Lig 70µl
Lig 80µl
Lig 90µl
Lig 100µl
Absorbance
Wavelength (nm)

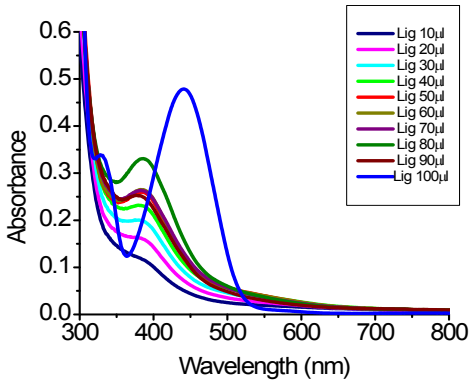

MeOH+TEA
Absorbance
1/1+M2+

Ni^{2+}


Lig 10µl
Lig 20µl
Lig 30µl
Lig 40µl
Lig 50µl
Lig 60µl
Lig 70µl
Lig 80µl
Lig 90µl
Lig 100µl
Absorbance
Wavelength (nm)


MeOH+TEA
Absorbance at 560 nm
Wavelength (nm)

Co^{2+}


Lig 10µl
Lig 20µl
Lig 30µl
Lig 40µl
Lig 50µl
Lig 60µl
Lig 70µl
Lig 80µl
Lig 90µl
Lig 100µl
Absorbance
Wavelength (nm)

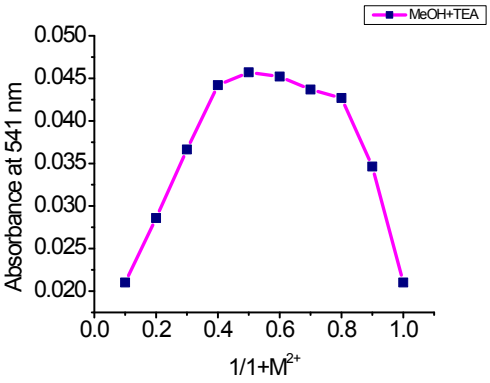

MeOH+TEA
Absorbance at 541 nm
1/1+M2+

Fig. S11 Job's plot experiment for H-1 and Zn^{2+}, $Ni^{2+}$and Co^{2+}in methanol + TEA mixture.

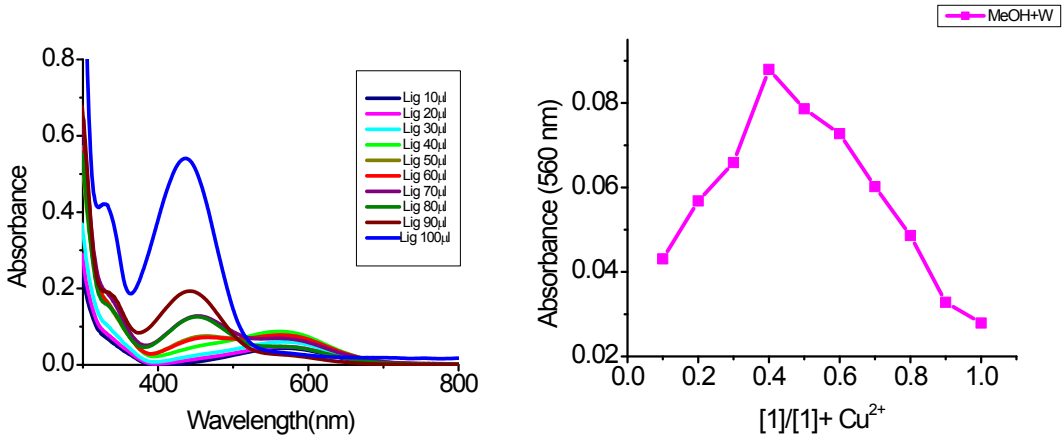


Fig S12 Job's plot experiment for H-1 and Cu^{2+} in methanol: water mixture

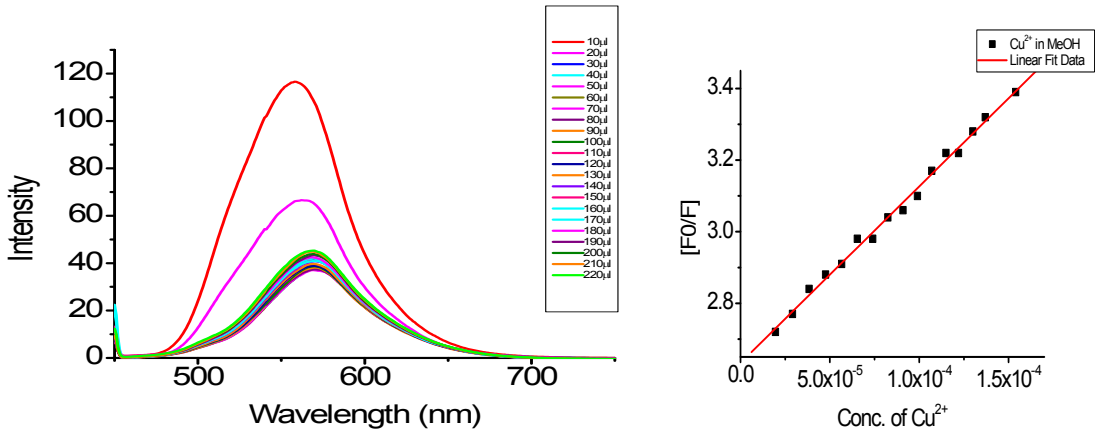


Fig. S13 a) Association constant experiment of Cu^{2+} in methanol with H-1

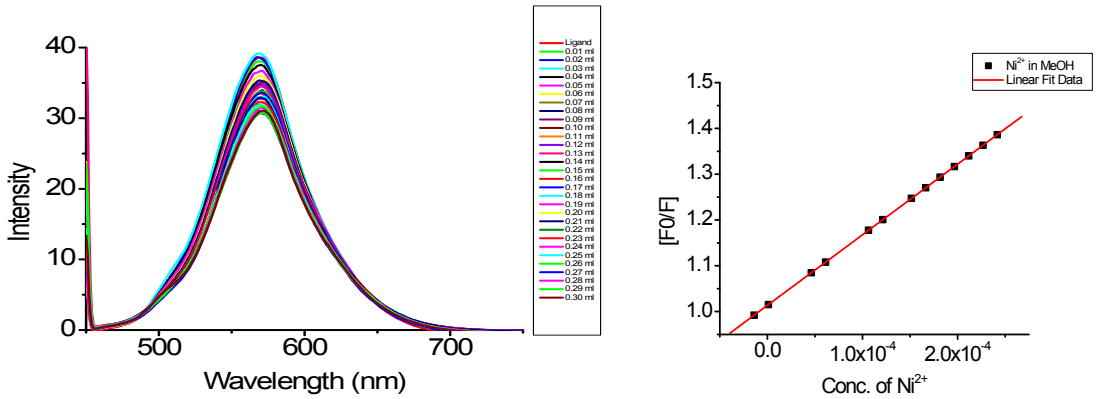
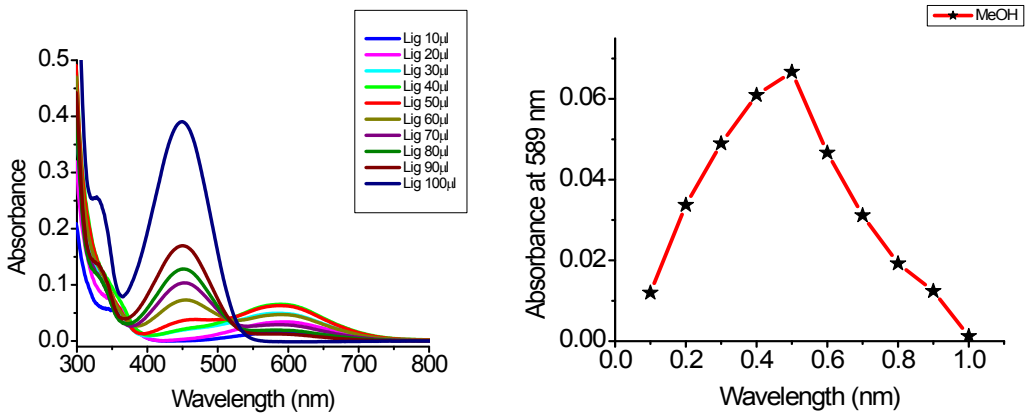


Fig. S13 b) Association constant experiment of Ni^{2+} in methanol with H-1

Cu^{2+}



Ni^{2+}

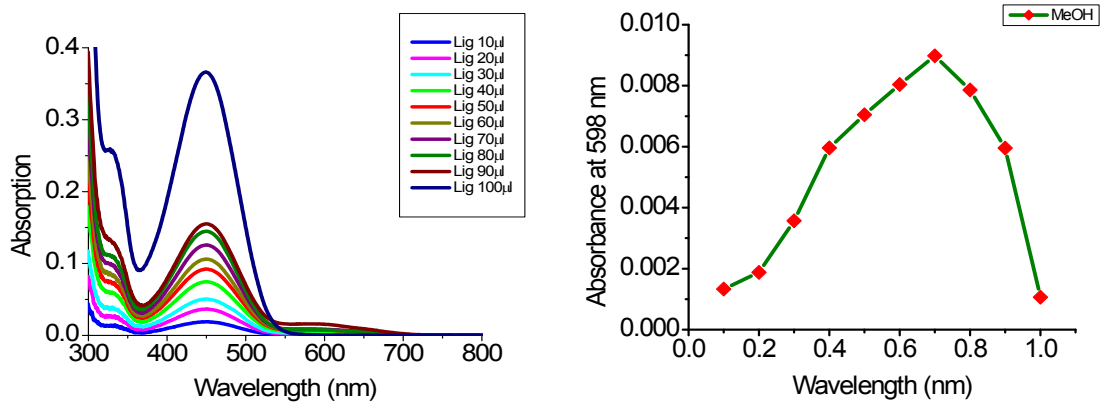
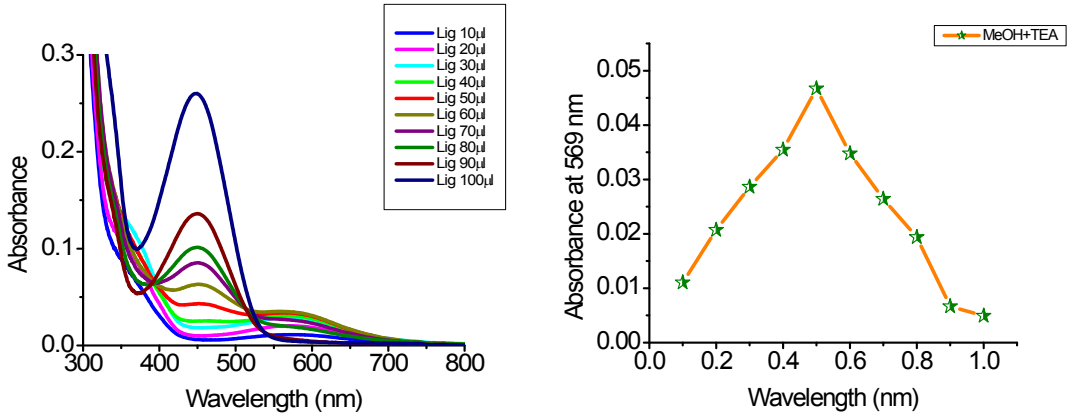
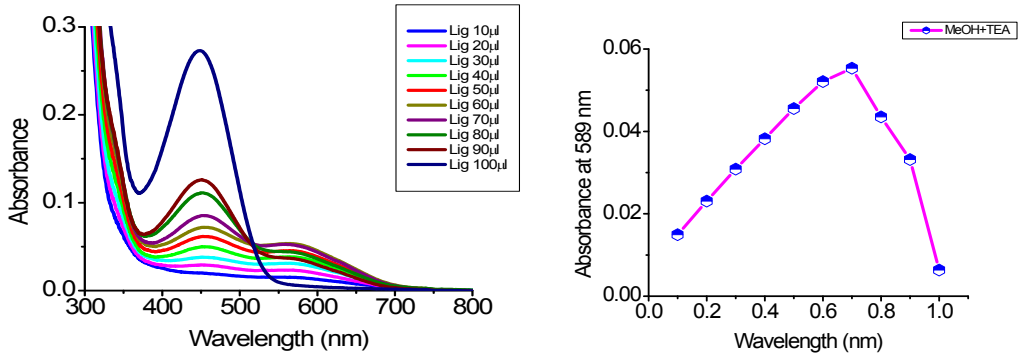


Fig.S14 Job's plot experiment for H-3 and Cu^{2+} and Ni^{2+} in methanol.

Cu^{2+}



Ni^{2+}



Co^{2+}

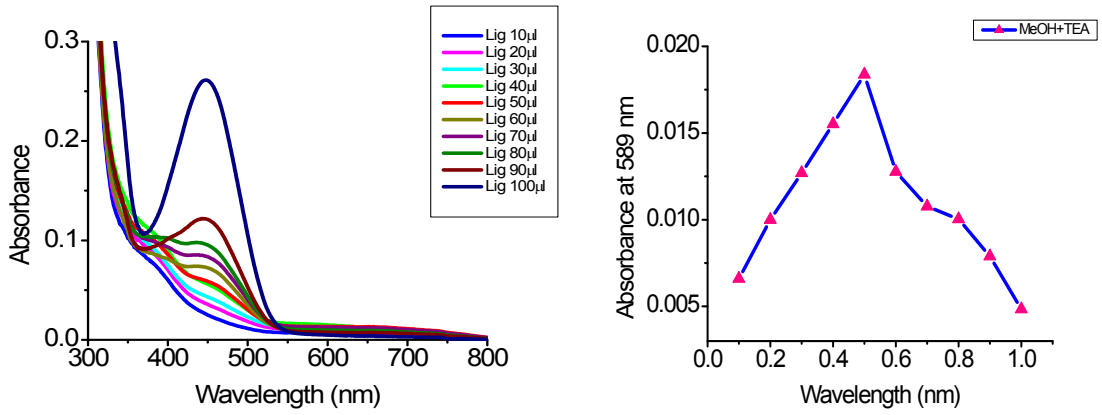
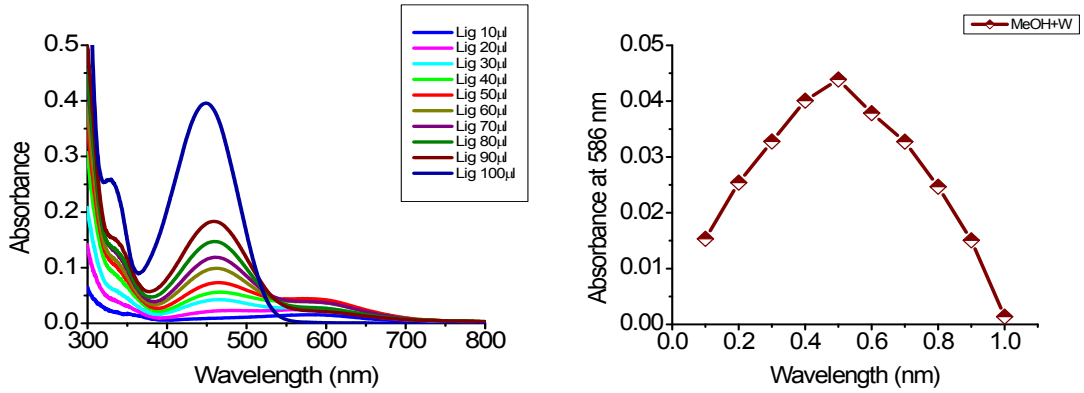


Fig. S15 Job's plot experiment for H-3 and Cu^{2+}, Ni^{2+} and Co^{2+} in methanol:triethylamine

Cu^{2+}



Cu^{+}

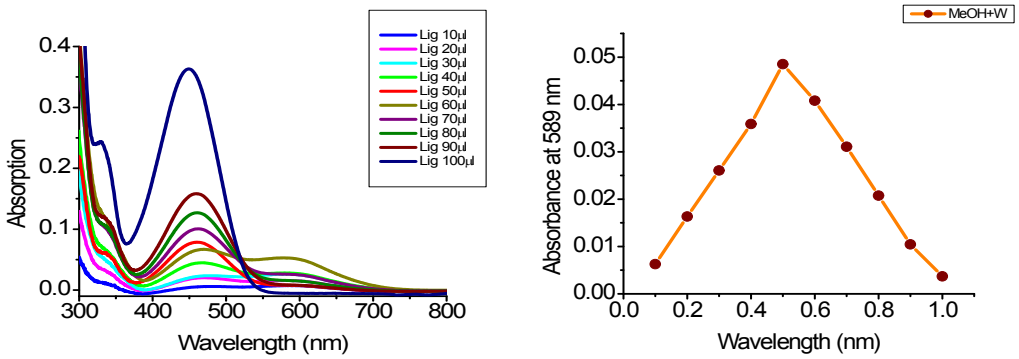


Fig.S16 Job's plot experiment for H-3 and $Cu^{2+}$and Cu^{+} in methanol :water.

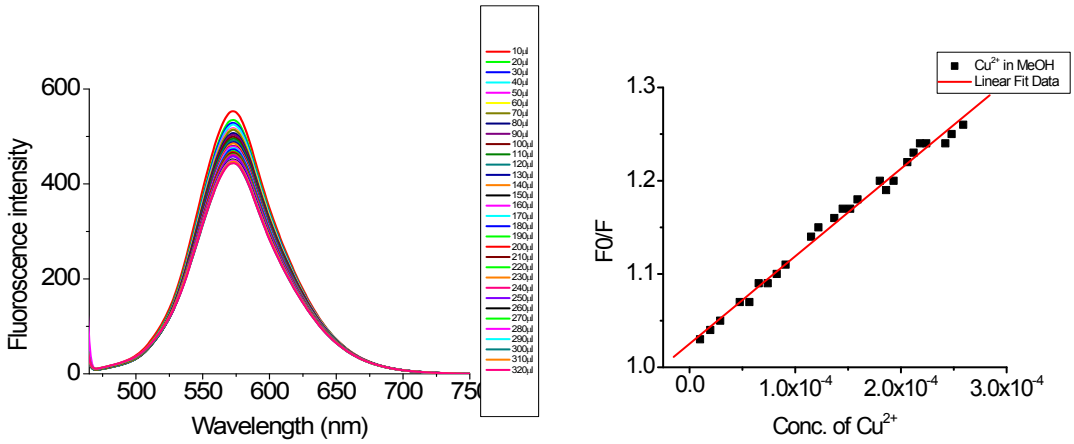


Fig. S17 a) Cu^{2+} in methanol association constant graph for H-3

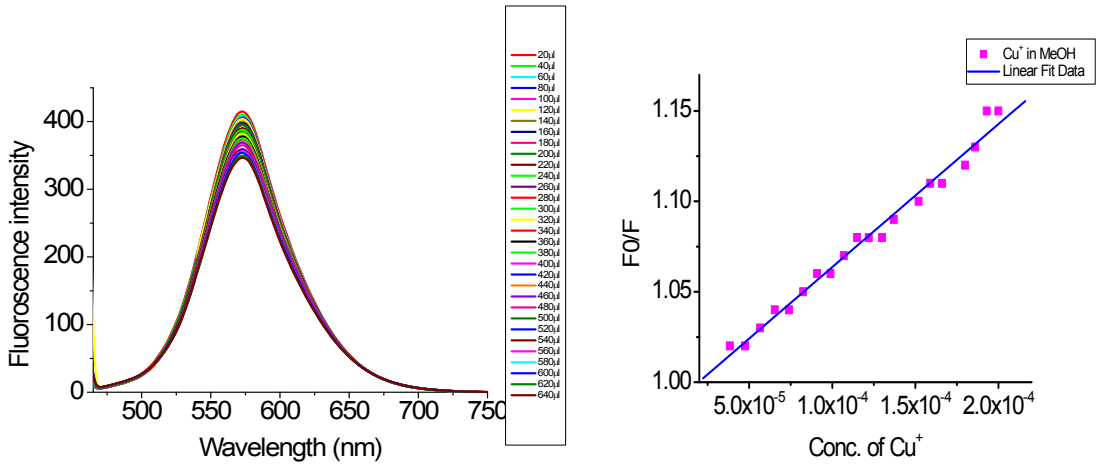


Fig. S17 b) Cu^{+} in methanol association constant graph for H-3.

Fig. S18 Color changes observed to Chemosensor H-3 and metal ions (1×10^{-4} M) in methanol

a) b)

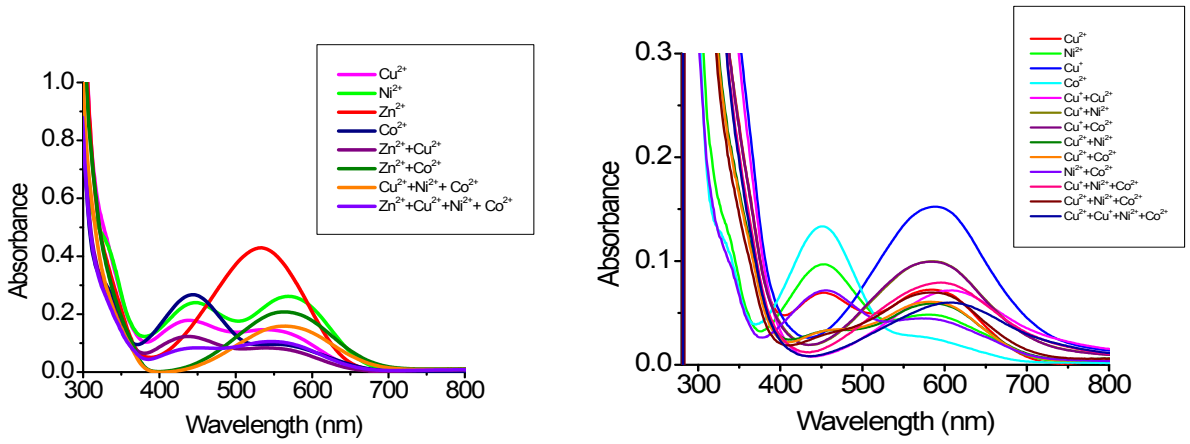
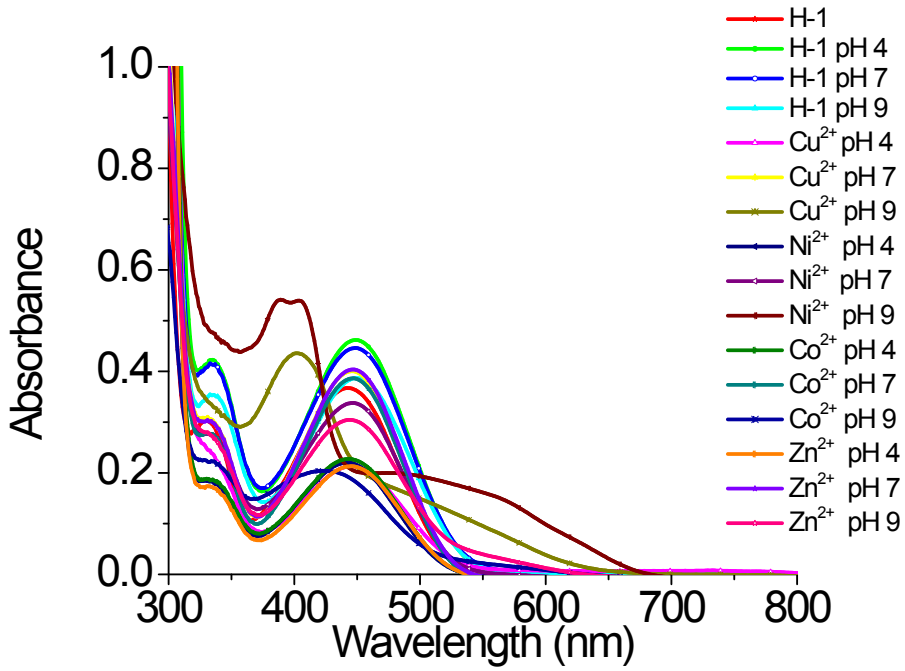


Fig. S19 (a)UV-visible of competitive binding of selected metal ions with chemosensor H-1 in methanol. b) UV-visible of competitive binding of selected metal ions with chemosensor H-3 in methanol.

a)



b)

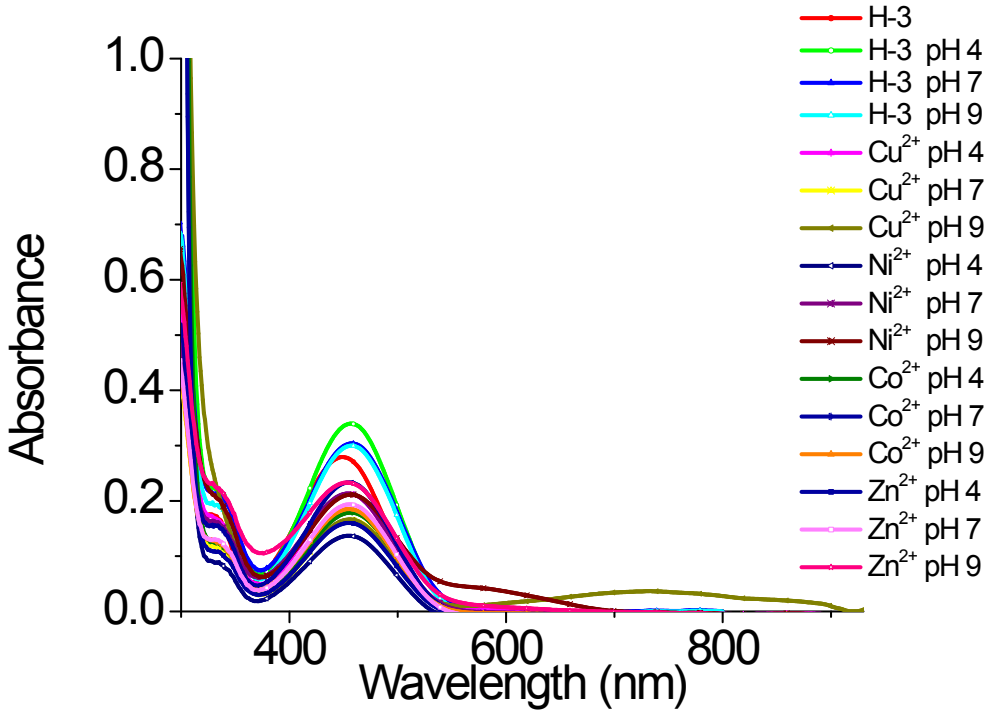


Fig.S20 pH dependent binding studies for metal ions Zn^{2+}, Cu^{2+} and Ni^{2+} of ligands a) H-1 and b) H-3.

a) b)

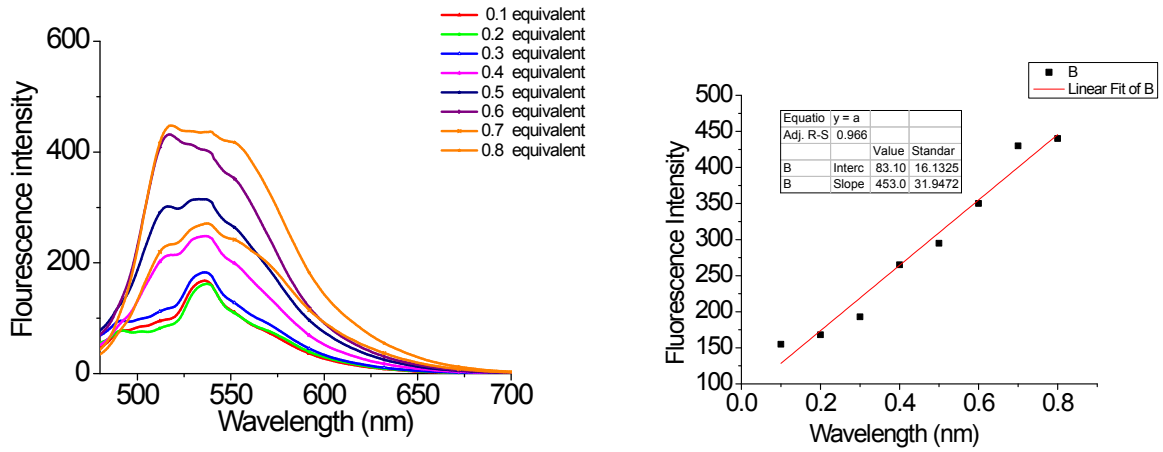


Fig. S21 a) Fluorescence spectra of H-1 with an increasing concentration of Cu^{2+} **b**) plot of the intensity at 462 nm for mixture of the H-1 and Cu^{2+} in methanol.

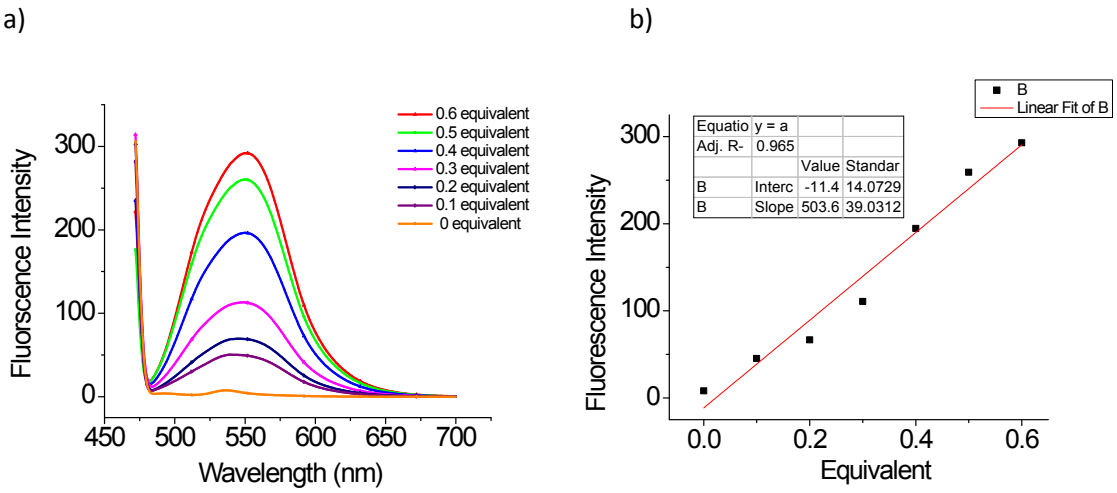


Fig.S22 a) Fluorescence spectra of H-3 with an increasing concentration of Cu^{2+} **b**) plot of the intensity at 462 nm for mixture of the H-3 and Cu^{2+} in methanol.

Table S1 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for H-1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7394(1)	2411(1)	1286(1)	18(1)
O(2)	-552(1)	-987(1)	1100(1)	21(1)
N(1)	5129(2)	2262(1)	348(1)	14(1)
N(2)	7423(2)	3942(1)	-325(1)	15(1)
C(1)	5682(2)	1543(1)	1246(1)	13(1)
C(2)	4232(2)	1457(1)	738(1)	13(1)
C(3)	2166(2)	627(1)	702(1)	15(1)
C(4)	1326(2)	-257(1)	1132(1)	14(1)
C(5)	2128(2)	-1236(1)	2044(1)	16(1)
C(6)	3545(2)	-1334(1)	2501(1)	19(1)
C(7)	5642(2)	-484(1)	2552(1)	20(1)
C(8)	6321(2)	472(1)	2146(1)	17(1)
C(9)	4916(2)	558(1)	1684(1)	13(1)
C(10)	2814(2)	-299(1)	1631(1)	13(1)
C(11)	3973(2)	2359(1)	-167(1)	14(1)
C(12)	5417(2)	3325(1)	-528(1)	13(1)
C(13)	4634(2)	3536(1)	-1048(1)	15(1)
C(14)	6012(2)	4421(1)	-1368(1)	15(1)
C(15)	8097(2)	5071(1)	-1163(1)	15(1)
C(16)	8724(2)	4801(1)	-642(1)	16(1)

Table S2 Bond lengths [Å] and angles [°] for H-1.

O(1)-C(1)	1.2196(13)
O(2)-C(4)	1.2342(13)
N(1)-C(2)	1.3354(13)
N(1)-C(11)	1.4455(13)
N(1)-H(1)	0.8800
N(2)-C(12)	1.3359(13)
N(2)-C(16)	1.3442(14)
C(1)-C(9)	1.4841(14)
C(1)-C(2)	1.5066(14)
C(2)-C(3)	1.3694(14)
C(3)-C(4)	1.4363(15)
C(3)-H(3)	0.9500
C(4)-C(10)	1.4994(15)
C(5)-C(6)	1.3894(16)
C(5)-C(10)	1.3948(15)
C(5)-H(5)	0.9500
C(6)-C(7)	1.3943(16)
C(6)-H(6)	0.9500
C(7)-C(8)	1.3882(16)
C(7)-H(7)	0.9500
C(8)-C(9)	1.3975(15)
C(8)-H(8)	0.9500
C(9)-C(10)	1.3999(14)
C(11)-C(12)	1.5120(14)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.3960(14)
C(13)-C(14)	1.3870(15)
C(13)-H(13)	0.9500
C(14)-C(15)	1.3873(15)
C(14)-H(14)	0.9500
C(15)-C(16)	1.3842(15)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500

C(2)-N(1)-C(11)	122.70(9)
C(2)-N(1)-H(1)	118.6
C(11)-N(1)-H(1)	118.6
C(12)-N(2)-C(16)	117.60(9)
O(1)-C(1)-C(9)	122.66(10)
O(1)-C(1)-C(2)	120.01(9)
C(9)-C(1)-C(2)	117.32(9)
N(1)-C(2)-C(3)	125.01(10)
N(1)-C(2)-C(1)	114.23(9)
C(3)-C(2)-C(1)	120.76(9)
C(2)-C(3)-C(4)	122.46(10)
C(2)-C(3)-H(3)	118.8
C(4)-C(3)-H(3)	118.8
O(2)-C(4)-C(3)	122.29(10)
O(2)-C(4)-C(10)	119.50(10)
C(3)-C(4)-C(10)	118.21(9)
C(6)-C(5)-C(10)	120.03(10)
C(6)-C(5)-H(5)	120.0
C(10)-C(5)-H(5)	120.0
C(5)-C(6)-C(7)	120.26(10)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	120.15(10)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(7)-C(8)-C(9)	119.77(10)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	120.1
C(8)-C(9)-C(10)	120.15(10)
C(8)-C(9)-C(1)	119.65(9)
C(10)-C(9)-C(1)	120.19(9)
C(5)-C(10)-C(9)	119.63(10)
C(5)-C(10)-C(4)	119.61(9)
C(9)-C(10)-C(4)	120.73(9)
N(1)-C(11)-C(12)	110.78(8)

N(1)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11A)	109.5
N(1)-C(11)-H(11B)	109.5
C(12)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
N(2)-C(12)-C(13)	123.01(9)
N(2)-C(12)-C(11)	117.02(9)
C(13)-C(12)-C(11)	119.97(9)
C(14)-C(13)-C(12)	118.36(9)
C(14)-C(13)-H(13)	120.8
C(12)-C(13)-H(13)	120.8
C(13)-C(14)-C(15)	119.26(10)
C(13)-C(14)-H(14)	120.4
C(15)-C(14)-H(14)	120.4
C(16)-C(15)-C(14)	118.20(10)
C(16)-C(15)-H(15)	120.9
C(14)-C(15)-H(15)	120.9
N(2)-C(16)-C(15)	123.55(10)
N(2)-C(16)-H(16)	118.2
C(15)-C(16)-H(16)	118.2

Symmetry transformations used to generate equivalent atoms:

Table S3 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for H-1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	16(1)	19(1)	19(1)	2(1)	-2(1)	-6(1)
O(2)	19(1)	23(1)	20(1)	0(1)	0(1)	-10(1)
N(1)	14(1)	16(1)	13(1)	2(1)	-1(1)	-5(1)
N(2)	14(1)	17(1)	14(1)	0(1)	0(1)	-2(1)
C(1)	13(1)	12(1)	14(1)	-1(1)	1(1)	0(1)
C(2)	14(1)	11(1)	13(1)	0(1)	1(1)	0(1)
C(3)	17(1)	16(1)	13(1)	0(1)	-1(1)	-3(1)
C(4)	14(1)	13(1)	16(1)	-2(1)	1(1)	-3(1)
C(5)	17(1)	16(1)	16(1)	-1(1)	5(1)	-2(1)
C(6)	22(1)	20(1)	15(1)	3(1)	5(1)	0(1)
C(7)	21(1)	26(1)	13(1)	2(1)	0(1)	1(1)
C(8)	14(1)	20(1)	16(1)	0(1)	0(1)	-1(1)
C(9)	13(1)	13(1)	12(1)	-1(1)	2(1)	1(1)
C(10)	14(1)	12(1)	13(1)	-2(1)	3(1)	0(1)
C(11)	14(1)	16(1)	12(1)	1(1)	-1(1)	-3(1)
C(12)	13(1)	11(1)	14(1)	-1(1)	1(1)	0(1)
C(13)	14(1)	15(1)	14(1)	-1(1)	-1(1)	-2(1)
C(14)	18(1)	16(1)	12(1)	0(1)	-1(1)	0(1)
C(15)	15(1)	16(1)	15(1)	1(1)	3(1)	-2(1)
C(16)	13(1)	18(1)	16(1)	0(1)	-1(1)	-4(1)

Table S4 Torsion angles [°] for H-1.

C(11)-N(1)-C(2)-C(3)	0.57(17)
C(11)-N(1)-C(2)-C(1)	-178.42(9)
O(1)-C(1)-C(2)-N(1)	6.24(14)
C(9)-C(1)-C(2)-N(1)	-174.47(9)
O(1)-C(1)-C(2)-C(3)	-172.80(10)
C(9)-C(1)-C(2)-C(3)	6.50(14)
N(1)-C(2)-C(3)-C(4)	178.05(10)
C(1)-C(2)-C(3)-C(4)	-3.02(16)
C(2)-C(3)-C(4)-O(2)	179.07(10)
C(2)-C(3)-C(4)-C(10)	-1.61(16)
C(10)-C(5)-C(6)-C(7)	0.79(17)
C(5)-C(6)-C(7)-C(8)	0.25(18)
C(6)-C(7)-C(8)-C(9)	-1.08(17)
C(7)-C(8)-C(9)-C(10)	0.87(16)
C(7)-C(8)-C(9)-C(1)	-178.20(10)
O(1)-C(1)-C(9)-C(8)	-7.03(16)
C(2)-C(1)-C(9)-C(8)	173.70(9)
O(1)-C(1)-C(9)-C(10)	173.91(10)
C(2)-C(1)-C(9)-C(10)	-5.37(14)
C(6)-C(5)-C(10)-C(9)	-1.00(16)
C(6)-C(5)-C(10)-C(4)	177.30(10)
C(8)-C(9)-C(10)-C(5)	0.17(15)
C(1)-C(9)-C(10)-C(5)	179.23(9)
C(8)-C(9)-C(10)-C(4)	-178.11(9)
C(1)-C(9)-C(10)-C(4)	0.95(15)
O(2)-C(4)-C(10)-C(5)	3.75(15)
C(3)-C(4)-C(10)-C(5)	-175.59(10)
O(2)-C(4)-C(10)-C(9)	-177.97(10)
C(3)-C(4)-C(10)-C(9)	2.69(15)
C(2)-N(1)-C(11)-C(12)	-179.10(9)
C(16)-N(2)-C(12)-C(13)	0.01(16)
C(16)-N(2)-C(12)-C(11)	179.89(9)
N(1)-C(11)-C(12)-N(2)	-1.24(13)
N(1)-C(11)-C(12)-C(13)	178.64(9)

N(2)-C(12)-C(13)-C(14)	0.32(16)
C(11)-C(12)-C(13)-C(14)	-179.56(10)
C(12)-C(13)-C(14)-C(15)	-0.45(16)
C(13)-C(14)-C(15)-C(16)	0.27(16)
C(12)-N(2)-C(16)-C(15)	-0.22(16)
C(14)-C(15)-C(16)-N(2)	0.07(17)

Symmetry transformations used to generate equivalent atoms:

Table S5 Hydrogen bonds for H-1[Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(16)-H(16)...N(2)#1	0.95	2.56	3.3915(14)	146.5
C(15)-H(15)...O(1)#1	0.95	2.58	3.3634(13)	140.2
C(13)-H(13)...O(2)#2	0.95	2.34	3.1655(13)	145.1
C(11)-H(11B)...O(2)#2	0.99	2.66	3.2198(13)	116.1
C(11)-H(11B)...O(2)#2	0.99	2.66	3.2198(13)	116.1
C(13)-H(13)...O(2)#2	0.95	2.34	3.1655(13)	145.1
C(15)-H(15)...O(1)#1	0.95	2.58	3.3634(13)	140.2
C(16)-H(16)...N(2)#1	0.95	2.56	3.3915(14)	146.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z #2 -x,-y,-z

Table S6 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for H-3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1638(2)	-469(1)	5171(2)	12(1)
O(2)	10655(2)	-638(1)	9052(2)	14(1)
N(1)	3473(3)	232(1)	6992(2)	10(1)
N(2)	961(3)	1730(1)	8168(2)	13(1)
C(1)	3669(3)	-519(1)	6063(2)	8(1)
C(2)	4858(3)	-140(1)	7122(2)	9(1)
C(3)	7180(3)	-184(1)	8099(2)	10(1)
C(4)	8572(3)	-594(1)	8171(2)	9(1)
C(5)	8760(3)	-1380(1)	7166(2)	12(1)
C(6)	7746(4)	-1739(1)	6200(2)	14(1)
C(7)	5396(4)	-1703(1)	5199(2)	13(1)
C(8)	4047(3)	-1309(1)	5174(2)	10(1)
C(9)	5059(3)	-947(1)	6140(2)	9(1)
C(10)	7437(3)	-982(1)	7140(2)	9(1)
C(11)	4266(3)	633(1)	7961(2)	9(1)
C(12)	2186(3)	979(1)	7662(2)	9(1)
C(13)	2796(3)	1423(1)	8505(2)	9(1)
C(14)	5065(3)	1514(1)	9548(2)	13(1)
C(15)	5439(4)	1933(1)	10267(2)	15(1)
C(16)	3565(4)	2250(1)	9935(2)	14(1)
C(17)	1372(4)	2131(1)	8876(2)	14(1)

Table S7 Bond lengths [Å] and angles [°] for H-3.

O(1)-C(1)	1.220(2)
O(2)-C(4)	1.237(2)
N(1)-C(2)	1.339(2)
N(1)-C(11)	1.459(2)
N(1)-H(1)	0.8800
N(2)-C(17)	1.335(2)
N(2)-C(13)	1.348(2)
C(1)-C(9)	1.484(2)
C(1)-C(2)	1.504(2)
C(2)-C(3)	1.375(2)
C(3)-C(4)	1.437(2)
C(3)-H(3)	0.9500
C(4)-C(10)	1.503(2)
C(5)-C(6)	1.388(3)
C(5)-C(10)	1.392(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.394(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.387(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.397(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.405(2)
C(11)-C(12)	1.521(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.509(2)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.396(3)
C(14)-C(15)	1.387(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.384(3)
C(15)-H(15)	0.9500

C(16)-C(17)	1.391(3)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500

C(2)-N(1)-C(11)	122.20(15)
C(2)-N(1)-H(1)	118.9
C(11)-N(1)-H(1)	118.9
C(17)-N(2)-C(13)	117.65(16)
O(1)-C(1)-C(9)	122.10(16)
O(1)-C(1)-C(2)	120.19(16)
C(9)-C(1)-C(2)	117.71(15)
N(1)-C(2)-C(3)	124.94(17)
N(1)-C(2)-C(1)	113.90(15)
C(3)-C(2)-C(1)	121.15(16)
C(2)-C(3)-C(4)	121.96(17)
C(2)-C(3)-H(3)	119.0
C(4)-C(3)-H(3)	119.0
O(2)-C(4)-C(3)	122.44(17)
O(2)-C(4)-C(10)	119.09(16)
C(3)-C(4)-C(10)	118.46(15)
C(6)-C(5)-C(10)	120.19(17)
C(6)-C(5)-H(5)	119.9
C(10)-C(5)-H(5)	119.9
C(7)-C(6)-C(5)	120.29(18)
C(7)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(6)-C(7)-C(8)	120.10(18)
C(6)-C(7)-H(7)	120.0
C(8)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	119.90(17)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	120.1
C(8)-C(9)-C(10)	120.01(16)
C(8)-C(9)-C(1)	120.09(16)
C(10)-C(9)-C(1)	119.86(16)
C(5)-C(10)-C(9)	119.51(16)

C(5)-C(10)-C(4)	119.67(16)
C(9)-C(10)-C(4)	120.83(16)
N(1)-C(11)-C(12)	109.42(14)
N(1)-C(11)-H(11A)	109.8
C(12)-C(11)-H(11A)	109.8
N(1)-C(11)-H(11B)	109.8
C(12)-C(11)-H(11B)	109.8
H(11A)-C(11)-H(11B)	108.2
C(13)-C(12)-C(11)	115.53(14)
C(13)-C(12)-H(12A)	108.4
C(11)-C(12)-H(12A)	108.4
C(13)-C(12)-H(12B)	108.4
C(11)-C(12)-H(12B)	108.4
H(12A)-C(12)-H(12B)	107.5
N(2)-C(13)-C(14)	122.24(17)
N(2)-C(13)-C(12)	114.42(15)
C(14)-C(13)-C(12)	123.34(16)
C(15)-C(14)-C(13)	118.86(17)
C(15)-C(14)-H(14)	120.6
C(13)-C(14)-H(14)	120.6
C(16)-C(15)-C(14)	119.42(18)
C(16)-C(15)-H(15)	120.3
C(14)-C(15)-H(15)	120.3
C(15)-C(16)-C(17)	117.75(18)
C(15)-C(16)-H(16)	121.1
C(17)-C(16)-H(16)	121.1
N(2)-C(17)-C(16)	124.07(18)
N(2)-C(17)-H(17)	118.0
C(16)-C(17)-H(17)	118.0

Symmetry transformations used to generate equivalent atoms:

Table S8 Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H-3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	9(1)	12(1)	13(1)	-1(1)	-2(1)	1(1)
O(2)	10(1)	16(1)	13(1)	0(1)	-4(1)	2(1)
N(1)	8(1)	9(1)	12(1)	-1(1)	-2(1)	1(1)
N(2)	12(1)	14(1)	14(1)	-2(1)	0(1)	3(1)
C(1)	8(1)	11(1)	7(1)	2(1)	2(1)	-1(1)
C(2)	9(1)	9(1)	9(1)	0(1)	3(1)	0(1)
C(3)	9(1)	9(1)	10(1)	-1(1)	0(1)	-2(1)
C(4)	10(1)	10(1)	8(1)	2(1)	1(1)	0(1)
C(5)	10(1)	13(1)	13(1)	2(1)	1(1)	1(1)
C(6)	16(1)	10(1)	18(1)	1(1)	4(1)	3(1)
C(7)	15(1)	9(1)	15(1)	-1(1)	2(1)	-4(1)
C(8)	9(1)	11(1)	11(1)	0(1)	1(1)	-3(1)
C(9)	9(1)	9(1)	8(1)	1(1)	2(1)	0(1)
C(10)	9(1)	10(1)	8(1)	2(1)	1(1)	0(1)
C(11)	9(1)	8(1)	10(1)	-1(1)	-2(1)	1(1)
C(12)	7(1)	11(1)	10(1)	-1(1)	0(1)	-1(1)
C(13)	11(1)	9(1)	8(1)	0(1)	3(1)	1(1)
C(14)	10(1)	12(1)	15(1)	-1(1)	0(1)	2(1)
C(15)	12(1)	15(1)	16(1)	-2(1)	-1(1)	-1(1)
C(16)	19(1)	9(1)	14(1)	-2(1)	4(1)	-1(1)
C(17)	16(1)	13(1)	14(1)	-1(1)	1(1)	6(1)

Table S9 Torsion angles [°] for H-3.

C(11)-N(1)-C(2)-C(3)	-2.9(3)
C(11)-N(1)-C(2)-C(1)	178.03(15)
O(1)-C(1)-C(2)-N(1)	1.1(2)
C(9)-C(1)-C(2)-N(1)	-179.38(15)
O(1)-C(1)-C(2)-C(3)	-178.07(17)
C(9)-C(1)-C(2)-C(3)	1.5(2)
N(1)-C(2)-C(3)-C(4)	-179.60(17)
C(1)-C(2)-C(3)-C(4)	-0.6(3)
C(2)-C(3)-C(4)-O(2)	-179.58(17)
C(2)-C(3)-C(4)-C(10)	0.1(3)
C(10)-C(5)-C(6)-C(7)	0.0(3)
C(5)-C(6)-C(7)-C(8)	-0.6(3)
C(6)-C(7)-C(8)-C(9)	0.7(3)
C(7)-C(8)-C(9)-C(10)	-0.2(3)
C(7)-C(8)-C(9)-C(1)	177.43(17)
O(1)-C(1)-C(9)-C(8)	-0.1(3)
C(2)-C(1)-C(9)-C(8)	-179.63(16)
O(1)-C(1)-C(9)-C(10)	177.58(17)
C(2)-C(1)-C(9)-C(10)	-2.0(2)
C(6)-C(5)-C(10)-C(9)	0.5(3)
C(6)-C(5)-C(10)-C(4)	-179.10(17)
C(8)-C(9)-C(10)-C(5)	-0.4(3)
C(1)-C(9)-C(10)-C(5)	-178.06(16)
C(8)-C(9)-C(10)-C(4)	179.21(16)
C(1)-C(9)-C(10)-C(4)	1.6(3)
O(2)-C(4)-C(10)-C(5)	-1.3(3)
C(3)-C(4)-C(10)-C(5)	179.03(17)
O(2)-C(4)-C(10)-C(9)	179.09(17)
C(3)-C(4)-C(10)-C(9)	-0.6(2)
C(2)-N(1)-C(11)-C(12)	-174.53(16)
N(1)-C(11)-C(12)-C(13)	-176.52(15)
C(17)-N(2)-C(13)-C(14)	-0.2(3)
C(17)-N(2)-C(13)-C(12)	179.90(16)
C(11)-C(12)-C(13)-N(2)	177.50(16)

C(11)-C(12)-C(13)-C(14)	-2.4(3)
N(2)-C(13)-C(14)-C(15)	0.3(3)
C(12)-C(13)-C(14)-C(15)	-179.82(17)
C(13)-C(14)-C(15)-C(16)	-0.1(3)
C(14)-C(15)-C(16)-C(17)	-0.2(3)
C(13)-N(2)-C(17)-C(16)	-0.1(3)
C(15)-C(16)-C(17)-N(2)	0.3(3)

Symmetry transformations used to generate equivalent atoms:

Table S10 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for H-4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1A)	5856(3)	3065(2)	3128(1)	19(1)
S(1)	8601(2)	1312(2)	8119(1)	19(1)
O(2A)	15717(7)	4130(4)	5656(1)	17(1)
O(1A)	6728(6)	224(4)	5487(1)	15(1)
N(1)	6517(7)	2964(5)	9776(1)	12(1)
O(1)	8438(6)	4936(4)	10479(1)	14(1)
O(2)	-489(6)	1102(4)	10663(1)	17(1)
C(11A)	9175(9)	2856(6)	4379(2)	12(1)
N(1A)	8420(7)	1942(5)	4781(1)	13(1)
C(13)	6741(9)	1165(6)	8589(2)	13(1)
C(16A)	7988(10)	4270(7)	2804(2)	19(1)
C(13A)	7868(9)	3377(6)	3595(2)	13(1)
C(12A)	7071(9)	2537(6)	4021(2)	13(1)
C(2A)	9878(9)	2127(6)	5156(2)	12(1)
C(3A)	12191(9)	3109(6)	5203(2)	14(1)
C(4A)	13623(9)	3236(6)	5613(2)	13(1)
C(10A)	12579(9)	2283(6)	6005(2)	12(1)
C(5A)	13933(10)	2386(6)	6410(2)	15(1)
C(6A)	12974(10)	1490(7)	6774(2)	17(1)
C(14A)	10008(10)	4351(6)	3496(2)	16(1)
C(15A)	10091(11)	4856(7)	3043(2)	22(1)
C(9A)	10207(9)	1285(6)	5970(2)	12(1)
C(1A)	8743(9)	1130(6)	5540(2)	11(1)
C(8A)	9261(9)	380(6)	6339(2)	14(1)
C(7A)	10642(10)	485(6)	6735(2)	18(1)
C(16)	6365(10)	10(7)	7794(2)	19(1)
C(12)	7640(9)	2123(6)	9018(2)	14(1)
C(11)	5644(9)	1931(6)	9377(2)	12(1)
C(2)	5197(9)	2909(6)	10155(2)	12(1)
C(1)	6395(9)	4044(6)	10534(2)	12(1)

C(9)	5105(9)	4067(6)	10967(2)	11(1)
C(10)	2764(9)	3087(6)	11007(2)	12(1)
C(5)	1531(9)	3131(6)	11413(2)	16(1)
C(6)	2598(10)	4184(7)	11772(2)	18(1)
C(14)	4520(9)	146(6)	8490(2)	16(1)
C(15)	4323(10)	-502(7)	8035(2)	19(1)
C(8)	6181(9)	5112(6)	11327(2)	14(1)
C(7)	4927(10)	5184(6)	11728(2)	19(1)
C(4)	1575(9)	1965(6)	10617(2)	12(1)
C(3)	2899(9)	1966(6)	10203(2)	13(1)

Table S11 Bond lengths [Å] and angles [°] for H-4.

S(1A)-C(16A)	1.725(6)
S(1A)-C(13A)	1.734(5)
S(1)-C(16)	1.727(6)
S(1)-C(13)	1.733(5)
O(2A)-C(4A)	1.246(6)
O(1A)-C(1A)	1.219(6)
N(1)-C(2)	1.343(6)
N(1)-C(11)	1.452(6)
N(1)-H(1)	0.8800
O(1)-C(1)	1.239(6)
O(2)-C(4)	1.234(6)
C(11A)-N(1A)	1.463(6)
C(11A)-C(12A)	1.528(6)
C(11A)-H(11A)	0.9900
C(11A)-H(11B)	0.9900
N(1A)-C(2A)	1.343(6)
N(1A)-H(1A)	0.8800
C(13)-C(14)	1.366(7)
C(13)-C(12)	1.500(7)
C(16A)-C(15A)	1.342(8)
C(16A)-H(16A)	0.9500
C(13A)-C(14A)	1.339(7)
C(13A)-C(12A)	1.500(7)
C(12A)-H(12A)	0.9900
C(12A)-H(12B)	0.9900
C(2A)-C(3A)	1.375(7)
C(2A)-C(1A)	1.510(7)
C(3A)-C(4A)	1.426(7)
C(3A)-H(3A)	0.9500
C(4A)-C(10A)	1.493(7)
C(10A)-C(5A)	1.391(7)
C(10A)-C(9A)	1.405(7)
C(5A)-C(6A)	1.391(7)
C(5A)-H(5A)	0.9500

C(6A)-C(7A)	1.390(8)
C(6A)-H(6A)	0.9500
C(14A)-C(15A)	1.423(7)
C(14A)-H(14A)	0.9500
C(15A)-H(15A)	0.9500
C(9A)-C(8A)	1.403(7)
C(9A)-C(1A)	1.482(7)
C(8A)-C(7A)	1.376(7)
C(8A)-H(8A)	0.9500
C(7A)-H(7A)	0.9500
C(16)-C(15)	1.346(8)
C(16)-H(16)	0.9500
C(12)-C(11)	1.525(7)
C(12)-H(12C)	0.9900
C(12)-H(12D)	0.9900
C(11)-H(11C)	0.9900
C(11)-H(11D)	0.9900
C(2)-C(3)	1.366(7)
C(2)-C(1)	1.497(7)
C(1)-C(9)	1.474(7)
C(9)-C(10)	1.395(7)
C(9)-C(8)	1.397(7)
C(10)-C(5)	1.391(7)
C(10)-C(4)	1.513(7)
C(5)-C(6)	1.396(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.398(8)
C(6)-H(6)	0.9500
C(14)-C(15)	1.429(7)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(8)-C(7)	1.386(7)
C(8)-H(8)	0.9500
C(7)-H(7)	0.9500
C(4)-C(3)	1.434(7)
C(3)-H(3)	0.9500

C(16A)-S(1A)-C(13A)	92.0(3)
C(16)-S(1)-C(13)	92.4(3)
C(2)-N(1)-C(11)	121.9(4)
C(2)-N(1)-H(1)	119.1
C(11)-N(1)-H(1)	119.1
N(1A)-C(11A)-C(12A)	110.1(4)
N(1A)-C(11A)-H(11A)	109.6
C(12A)-C(11A)-H(11A)	109.6
N(1A)-C(11A)-H(11B)	109.6
C(12A)-C(11A)-H(11B)	109.6
H(11A)-C(11A)-H(11B)	108.2
C(2A)-N(1A)-C(11A)	121.2(4)
C(2A)-N(1A)-H(1A)	119.4
C(11A)-N(1A)-H(1A)	119.4
C(14)-C(13)-C(12)	129.6(5)
C(14)-C(13)-S(1)	110.2(4)
C(12)-C(13)-S(1)	120.2(4)
C(15A)-C(16A)-S(1A)	110.8(4)
C(15A)-C(16A)-H(16A)	124.6
S(1A)-C(16A)-H(16A)	124.6
C(14A)-C(13A)-C(12A)	130.6(5)
C(14A)-C(13A)-S(1A)	110.3(4)
C(12A)-C(13A)-S(1A)	119.0(4)
C(13A)-C(12A)-C(11A)	110.9(4)
C(13A)-C(12A)-H(12A)	109.5
C(11A)-C(12A)-H(12A)	109.5
C(13A)-C(12A)-H(12B)	109.5
C(11A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	108.0
N(1A)-C(2A)-C(3A)	125.4(4)
N(1A)-C(2A)-C(1A)	113.5(4)
C(3A)-C(2A)-C(1A)	121.1(4)
C(2A)-C(3A)-C(4A)	121.9(4)
C(2A)-C(3A)-H(3A)	119.1
C(4A)-C(3A)-H(3A)	119.1

O(2A)-C(4A)-C(3A)	121.8(4)
O(2A)-C(4A)-C(10A)	119.0(4)
C(3A)-C(4A)-C(10A)	119.2(4)
C(5A)-C(10A)-C(9A)	119.2(4)
C(5A)-C(10A)-C(4A)	120.4(4)
C(9A)-C(10A)-C(4A)	120.4(4)
C(10A)-C(5A)-C(6A)	120.6(5)
C(10A)-C(5A)-H(5A)	119.7
C(6A)-C(5A)-H(5A)	119.7
C(7A)-C(6A)-C(5A)	119.9(5)
C(7A)-C(6A)-H(6A)	120.0
C(5A)-C(6A)-H(6A)	120.0
C(13A)-C(14A)-C(15A)	113.7(5)
C(13A)-C(14A)-H(14A)	123.1
C(15A)-C(14A)-H(14A)	123.1
C(16A)-C(15A)-C(14A)	113.1(5)
C(16A)-C(15A)-H(15A)	123.5
C(14A)-C(15A)-H(15A)	123.5
C(8A)-C(9A)-C(10A)	119.8(4)
C(8A)-C(9A)-C(1A)	119.9(4)
C(10A)-C(9A)-C(1A)	120.3(4)
O(1A)-C(1A)-C(9A)	122.7(4)
O(1A)-C(1A)-C(2A)	120.1(4)
C(9A)-C(1A)-C(2A)	117.1(4)
C(7A)-C(8A)-C(9A)	120.1(5)
C(7A)-C(8A)-H(8A)	120.0
C(9A)-C(8A)-H(8A)	120.0
C(8A)-C(7A)-C(6A)	120.4(5)
C(8A)-C(7A)-H(7A)	119.8
C(6A)-C(7A)-H(7A)	119.8
C(15)-C(16)-S(1)	111.0(4)
C(15)-C(16)-H(16)	124.5
S(1)-C(16)-H(16)	124.5
C(13)-C(12)-C(11)	111.8(4)
C(13)-C(12)-H(12C)	109.3
C(11)-C(12)-H(12C)	109.3

C(13)-C(12)-H(12D)	109.3
C(11)-C(12)-H(12D)	109.3
H(12C)-C(12)-H(12D)	107.9
N(1)-C(11)-C(12)	110.2(4)
N(1)-C(11)-H(11C)	109.6
C(12)-C(11)-H(11C)	109.6
N(1)-C(11)-H(11D)	109.6
C(12)-C(11)-H(11D)	109.6
H(11C)-C(11)-H(11D)	108.1
N(1)-C(2)-C(3)	125.0(4)
N(1)-C(2)-C(1)	114.6(4)
C(3)-C(2)-C(1)	120.4(4)
O(1)-C(1)-C(9)	121.6(4)
O(1)-C(1)-C(2)	119.5(4)
C(9)-C(1)-C(2)	118.8(4)
C(10)-C(9)-C(8)	120.3(4)
C(10)-C(9)-C(1)	119.5(4)
C(8)-C(9)-C(1)	120.1(4)
C(5)-C(10)-C(9)	119.4(5)
C(5)-C(10)-C(4)	119.9(4)
C(9)-C(10)-C(4)	120.7(4)
C(10)-C(5)-C(6)	120.2(5)
C(10)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	120.2(5)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(13)-C(14)-C(15)	113.0(5)
C(13)-C(14)-H(14)	123.5
C(15)-C(14)-H(14)	123.5
C(16)-C(15)-C(14)	113.4(5)
C(16)-C(15)-H(15)	123.3
C(14)-C(15)-H(15)	123.3
C(7)-C(8)-C(9)	120.2(5)
C(7)-C(8)-H(8)	119.9
C(9)-C(8)-H(8)	119.9

C(8)-C(7)-C(6)	119.6(5)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
O(2)-C(4)-C(3)	122.5(5)
O(2)-C(4)-C(10)	119.4(4)
C(3)-C(4)-C(10)	118.1(4)
C(2)-C(3)-C(4)	122.4(4)
C(2)-C(3)-H(3)	118.8
C(4)-C(3)-H(3)	118.8

Symmetry transformations used to generate equivalent atoms:

Table S12 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for H-4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1A)	16(1)	20(1)	21(1)	2(1)	-5(1)	1(1)
S(1)	14(1)	22(1)	21(1)	-3(1)	5(1)	0(1)
O(2A)	13(2)	12(2)	25(2)	2(1)	0(1)	-4(1)
O(1A)	10(2)	14(2)	21(2)	1(1)	2(1)	-1(1)
N(1)	7(2)	11(2)	17(2)	-1(2)	1(2)	-2(2)
O(1)	8(2)	14(2)	21(2)	1(1)	3(1)	0(1)
O(2)	9(2)	14(2)	27(2)	0(1)	2(1)	-2(1)
C(11A)	8(2)	12(2)	15(2)	2(2)	1(2)	2(2)
N(1A)	7(2)	12(2)	17(2)	1(2)	1(2)	-2(2)
C(13)	12(2)	13(2)	15(2)	2(2)	2(2)	6(2)
C(16A)	22(3)	19(3)	16(2)	5(2)	-2(2)	3(2)
C(13A)	11(2)	12(2)	19(2)	-4(2)	-3(2)	6(2)
C(12A)	7(2)	11(2)	21(3)	1(2)	1(2)	0(2)
C(2A)	13(2)	10(2)	13(2)	2(2)	2(2)	4(2)
C(3A)	15(2)	10(2)	15(2)	1(2)	1(2)	1(2)
C(4A)	9(2)	7(2)	21(3)	-1(2)	4(2)	1(2)
C(10A)	13(2)	5(2)	18(2)	-2(2)	2(2)	1(2)
C(5A)	14(2)	13(2)	18(2)	0(2)	0(2)	3(2)
C(6A)	20(3)	20(3)	13(2)	1(2)	-2(2)	7(2)
C(14A)	13(2)	15(2)	21(3)	2(2)	1(2)	2(2)
C(15A)	24(3)	22(3)	22(3)	4(2)	5(2)	4(2)
C(9A)	12(2)	8(2)	16(2)	0(2)	3(2)	3(2)
C(1A)	8(2)	7(2)	19(2)	-1(2)	3(2)	2(2)
C(8A)	6(2)	12(2)	23(3)	0(2)	1(2)	1(2)
C(7A)	21(3)	15(2)	20(3)	4(2)	7(2)	6(2)
C(16)	17(3)	23(3)	19(3)	-6(2)	-2(2)	7(2)
C(12)	12(2)	10(2)	18(2)	-2(2)	0(2)	1(2)
C(11)	12(2)	8(2)	16(2)	0(2)	-1(2)	1(2)
C(2)	17(2)	8(2)	12(2)	0(2)	-1(2)	6(2)
C(1)	13(2)	6(2)	16(2)	1(2)	0(2)	2(2)
C(9)	14(2)	6(2)	14(2)	4(2)	0(2)	4(2)

C(10)	14(2)	7(2)	17(2)	3(2)	-1(2)	1(2)
C(5)	12(2)	13(2)	23(3)	3(2)	2(2)	0(2)
C(6)	20(3)	20(3)	15(2)	2(2)	4(2)	7(2)
C(14)	12(2)	17(2)	21(3)	0(2)	4(2)	4(2)
C(15)	14(3)	22(3)	21(3)	-4(2)	-4(2)	1(2)
C(8)	12(2)	9(2)	22(3)	5(2)	0(2)	5(2)
C(7)	25(3)	15(2)	18(3)	0(2)	-3(2)	9(2)
C(4)	10(2)	5(2)	19(2)	4(2)	-1(2)	1(2)
C(3)	13(2)	10(2)	15(2)	-1(2)	-1(2)	2(2)

Table S13 Torsion angles [°] for H-4.

C(12A)-C(11A)-N(1A)-C(2A)	-174.7(4)
C(16)-S(1)-C(13)-C(14)	0.3(4)
C(16)-S(1)-C(13)-C(12)	-178.3(4)
C(13A)-S(1A)-C(16A)-C(15A)	0.2(4)
C(16A)-S(1A)-C(13A)-C(14A)	0.2(4)
C(16A)-S(1A)-C(13A)-C(12A)	-178.0(4)
C(14A)-C(13A)-C(12A)-C(11A)	-2.3(7)
S(1A)-C(13A)-C(12A)-C(11A)	175.6(3)
N(1A)-C(11A)-C(12A)-C(13A)	-176.4(4)
C(11A)-N(1A)-C(2A)-C(3A)	-2.2(7)
C(11A)-N(1A)-C(2A)-C(1A)	177.9(4)
N(1A)-C(2A)-C(3A)-C(4A)	-179.9(4)
C(1A)-C(2A)-C(3A)-C(4A)	0.0(7)
C(2A)-C(3A)-C(4A)-O(2A)	-179.8(5)
C(2A)-C(3A)-C(4A)-C(10A)	-0.4(7)
O(2A)-C(4A)-C(10A)-C(5A)	-0.4(7)
C(3A)-C(4A)-C(10A)-C(5A)	-179.9(4)
O(2A)-C(4A)-C(10A)-C(9A)	179.0(4)
C(3A)-C(4A)-C(10A)-C(9A)	-0.4(7)
C(9A)-C(10A)-C(5A)-C(6A)	1.1(7)
C(4A)-C(10A)-C(5A)-C(6A)	-179.5(4)
C(10A)-C(5A)-C(6A)-C(7A)	-0.1(7)
C(12A)-C(13A)-C(14A)-C(15A)	177.4(5)
S(1A)-C(13A)-C(14A)-C(15A)	-0.6(6)
S(1A)-C(16A)-C(15A)-C(14A)	-0.5(6)
C(13A)-C(14A)-C(15A)-C(16A)	0.7(7)
C(5A)-C(10A)-C(9A)-C(8A)	-1.3(7)
C(4A)-C(10A)-C(9A)-C(8A)	179.2(4)
C(5A)-C(10A)-C(9A)-C(1A)	-179.0(4)
C(4A)-C(10A)-C(9A)-C(1A)	1.6(7)
C(8A)-C(9A)-C(1A)-O(1A)	-0.9(7)
C(10A)-C(9A)-C(1A)-O(1A)	176.7(4)
C(8A)-C(9A)-C(1A)-C(2A)	-179.6(4)
C(10A)-C(9A)-C(1A)-C(2A)	-2.0(6)

N(1A)-C(2A)-C(1A)-O(1A)	2.3(6)
C(3A)-C(2A)-C(1A)-O(1A)	-177.6(4)
N(1A)-C(2A)-C(1A)-C(9A)	-178.9(4)
C(3A)-C(2A)-C(1A)-C(9A)	1.2(6)
C(10A)-C(9A)-C(8A)-C(7A)	0.6(7)
C(1A)-C(9A)-C(8A)-C(7A)	178.3(4)
C(9A)-C(8A)-C(7A)-C(6A)	0.3(7)
C(5A)-C(6A)-C(7A)-C(8A)	-0.6(8)
C(13)-S(1)-C(16)-C(15)	-0.1(4)
C(14)-C(13)-C(12)-C(11)	-2.8(7)
S(1)-C(13)-C(12)-C(11)	175.4(3)
C(2)-N(1)-C(11)-C(12)	-174.1(4)
C(13)-C(12)-C(11)-N(1)	-176.2(4)
C(11)-N(1)-C(2)-C(3)	-3.0(7)
C(11)-N(1)-C(2)-C(1)	179.3(4)
N(1)-C(2)-C(1)-O(1)	0.4(6)
C(3)-C(2)-C(1)-O(1)	-177.3(4)
N(1)-C(2)-C(1)-C(9)	-179.5(4)
C(3)-C(2)-C(1)-C(9)	2.7(6)
O(1)-C(1)-C(9)-C(10)	177.6(4)
C(2)-C(1)-C(9)-C(10)	-2.5(6)
O(1)-C(1)-C(9)-C(8)	-0.1(7)
C(2)-C(1)-C(9)-C(8)	179.9(4)
C(8)-C(9)-C(10)-C(5)	-1.4(7)
C(1)-C(9)-C(10)-C(5)	-179.0(4)
C(8)-C(9)-C(10)-C(4)	179.4(4)
C(1)-C(9)-C(10)-C(4)	1.8(6)
C(9)-C(10)-C(5)-C(6)	1.8(7)
C(4)-C(10)-C(5)-C(6)	-179.0(4)
C(10)-C(5)-C(6)-C(7)	-0.9(7)
C(12)-C(13)-C(14)-C(15)	177.9(5)
S(1)-C(13)-C(14)-C(15)	-0.4(6)
S(1)-C(16)-C(15)-C(14)	-0.2(6)
C(13)-C(14)-C(15)-C(16)	0.4(7)
C(10)-C(9)-C(8)-C(7)	0.0(7)
C(1)-C(9)-C(8)-C(7)	177.5(4)

C(9)-C(8)-C(7)-C(6)	1.0(7)
C(5)-C(6)-C(7)-C(8)	-0.6(7)
C(5)-C(10)-C(4)-O(2)	0.3(7)
C(9)-C(10)-C(4)-O(2)	179.5(4)
C(5)-C(10)-C(4)-C(3)	179.6(4)
C(9)-C(10)-C(4)-C(3)	-1.2(6)
N(1)-C(2)-C(3)-C(4)	-179.7(4)
C(1)-C(2)-C(3)-C(4)	-2.2(7)
O(2)-C(4)-C(3)-C(2)	-179.3(4)
C(10)-C(4)-C(3)-C(2)	1.5(7)

Symmetry transformations used to generate equivalent atoms:

Table S14 Hydrogen bonds for H-4 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(3)-H(3)...O(2)#1	0.95	2.65	3.584(6)	168.1
C(14)-H(14)...O(2)#1	0.95	2.50	3.440(6)	168.1
C(12)-H(12D)...O(2)#2	0.99	2.59	3.392(6)	138.0
C(16)-H(16)...S(1A)#3	0.95	2.95	3.681(5)	134.7
C(14A)-H(14A)...O(2A)#4	0.95	2.51	3.445(6)	168.5
C(3A)-H(3A)...O(2A)#4	0.95	2.61	3.545(6)	168.9
C(12A)-H(12B)...O(2A)#5	0.99	2.61	3.405(6)	137.5
N(1A)-H(1A)...O(1A)#3	0.88	2.28	3.120(5)	159.8
N(1)-H(1)...O(1)#6	0.88	2.26	3.105(5)	161.4
C(3)-H(3)...O(2)#1	0.95	2.65	3.584(6)	168.1
C(14)-H(14)...O(2)#1	0.95	2.50	3.440(6)	168.1
C(12)-H(12D)...O(2)#2	0.99	2.59	3.392(6)	138.0
N(1)-H(1)...O(1)#6	0.88	2.26	3.105(5)	161.4
C(3)-H(3)...O(2)#1	0.95	2.65	3.584(6)	168.1
C(14)-H(14)...O(2)#1	0.95	2.50	3.440(6)	168.1
C(12)-H(12D)...O(2)#2	0.99	2.59	3.392(6)	138.0
C(16)-H(16)...S(1A)#3	0.95	2.95	3.681(5)	134.7
C(14A)-H(14A)...O(2A)#4	0.95	2.51	3.445(6)	168.5
C(3A)-H(3A)...O(2A)#4	0.95	2.61	3.545(6)	168.9
C(12A)-H(12B)...O(2A)#5	0.99	2.61	3.405(6)	137.5
N(1A)-H(1A)...O(1A)#3	0.88	2.28	3.120(5)	159.8
N(1)-H(1)...O(1)#6	0.88	2.26	3.105(5)	161.4
C(3)-H(3)...O(2)#1	0.95	2.65	3.584(6)	168.1
C(14)-H(14)...O(2)#1	0.95	2.50	3.440(6)	168.1
C(12)-H(12D)...O(2)#2	0.99	2.59	3.392(6)	138.0
N(1)-H(1)...O(1)#6	0.88	2.26	3.105(5)	161.4
N(1)-H(1)...O(1)#6	0.88	2.26	3.105(5)	161.4
N(1A)-H(1A)...O(1A)#3	0.88	2.28	3.120(5)	159.8
C(12A)-H(12B)...O(2A)#5	0.99	2.61	3.405(6)	137.5
C(3A)-H(3A)...O(2A)#4	0.95	2.61	3.545(6)	168.9
C(14A)-H(14A)...O(2A)#4	0.95	2.51	3.445(6)	168.5
C(16)-H(16)...S(1A)#3	0.95	2.95	3.681(5)	134.7

C(12)-H(12D)...O(2)#2	0.99	2.59	3.392(6)	138.0
C(14)-H(14)...O(2)#1	0.95	2.50	3.440(6)	168.1
C(3)-H(3)...O(2)#1	0.95	2.65	3.584(6)	168.1
N(1)-H(1)...O(1)#6	0.88	2.26	3.105(5)	161.4
N(1A)-H(1A)...O(1A)#3	0.88	2.28	3.120(5)	159.8
C(12A)-H(12B)...O(2A)#5	0.99	2.61	3.405(6)	137.5
C(3A)-H(3A)...O(2A)#4	0.95	2.61	3.545(6)	168.9
C(14A)-H(14A)...O(2A)#4	0.95	2.51	3.445(6)	168.5
C(16)-H(16)...S(1A)#3	0.95	2.95	3.681(5)	134.7
C(12)-H(12D)...O(2)#2	0.99	2.59	3.392(6)	138.0
C(14)-H(14)...O(2)#1	0.95	2.50	3.440(6)	168.1
C(3)-H(3)...O(2)#1	0.95	2.65	3.584(6)	168.1
N(1)-H(1)...O(1)#6	0.88	2.26	3.105(5)	161.4
N(1A)-H(1A)...O(1A)#3	0.88	2.28	3.120(5)	159.8
C(12A)-H(12B)...O(2A)#5	0.99	2.61	3.405(6)	137.5
C(3A)-H(3A)...O(2A)#4	0.95	2.61	3.545(6)	168.9
C(14A)-H(14A)...O(2A)#4	0.95	2.51	3.445(6)	168.5
C(16)-H(16)...S(1A)#3	0.95	2.95	3.681(5)	134.7
C(12)-H(12D)...O(2)#2	0.99	2.59	3.392(6)	138.0
C(14)-H(14)...O(2)#1	0.95	2.50	3.440(6)	168.1
C(3)-H(3)...O(2)#1	0.95	2.65	3.584(6)	168.1

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+2 #2 -x+1,-y,-z+2 #3 -x+1,-y,-z+1

#4 -x+3,-y+1,-z+1 #5 -x+2,-y+1,-z+1 #6 -x+2,-y+1,-z+2