Electronic Supplementary Information

A versatile chemosensor for detection of Al^{3+} and Picric acid (PA) in aqueous solution

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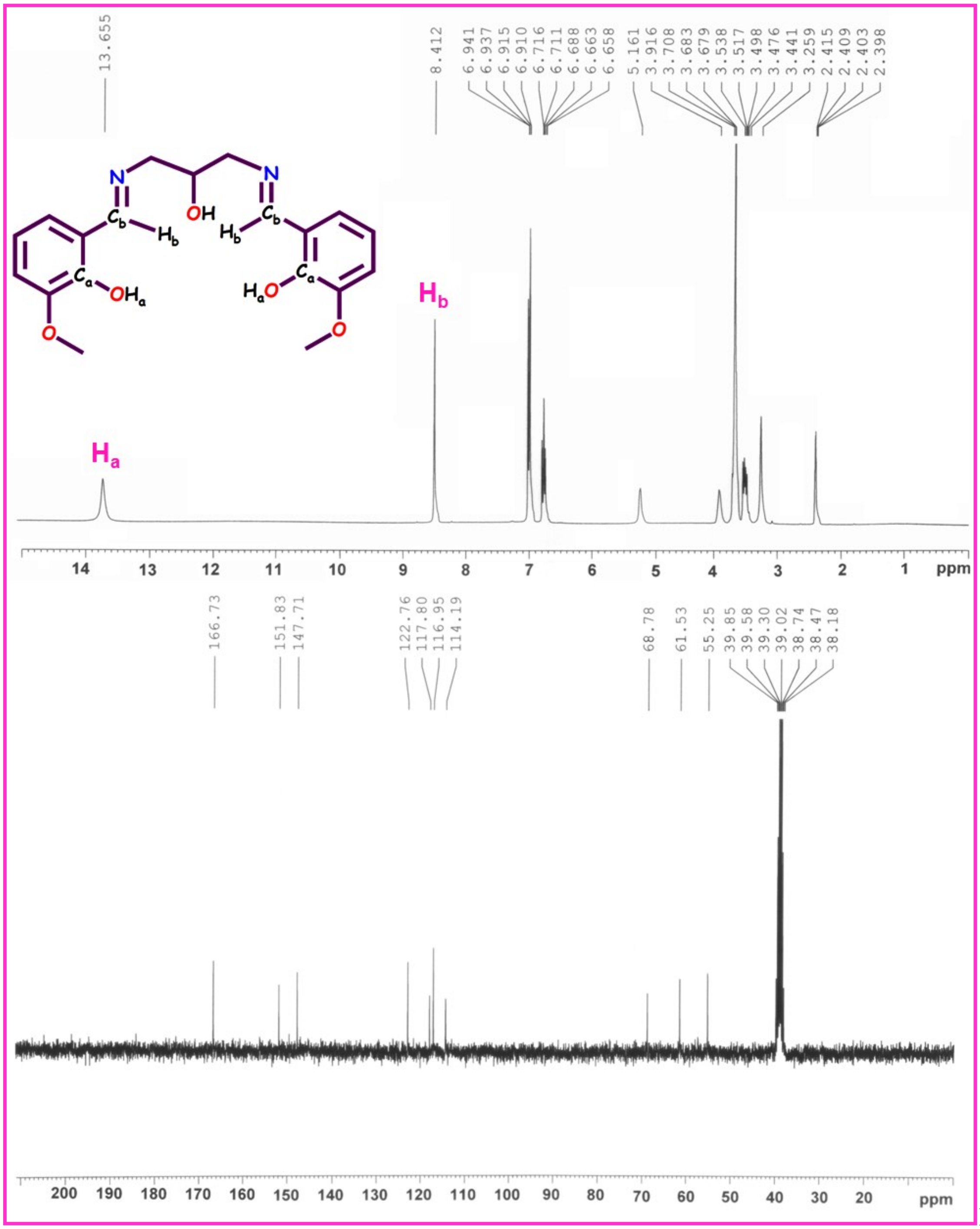
Cartesian coordinates of the enol, Keto and Keto-enol tautomers and the complexes **1** and **2**

1. Characterization and Structural Data.

^{1}H and ^{13}C-NMR spectra: H_2Vm were dissolved in d_6–DMSO and recorded with TMS as internal standard on a Bruker, AV 300 Supercon Digital NMR system.

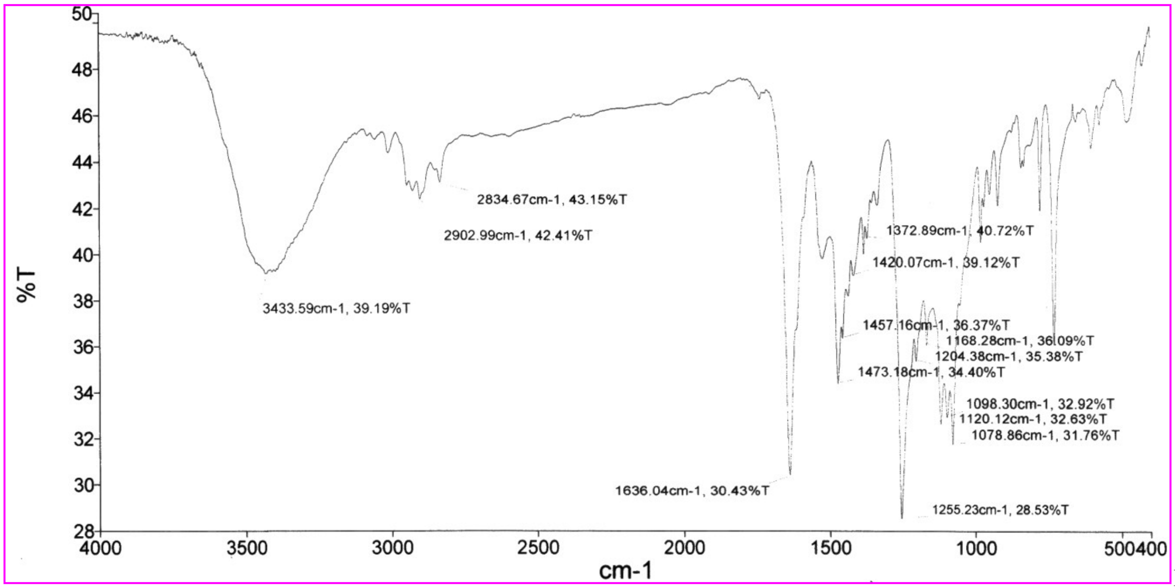


H_2Vm

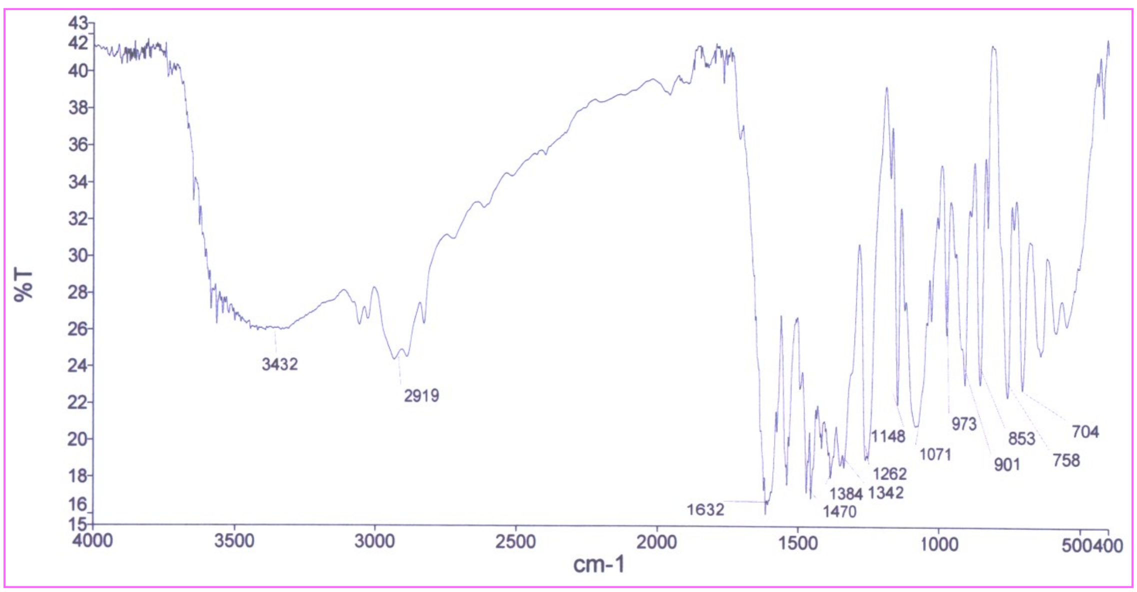
Figure S1. ^{1}H and ^{13}C-NMR spectrum of chemosensor **H_2Vm**.

1. Characterization and Structural Data.

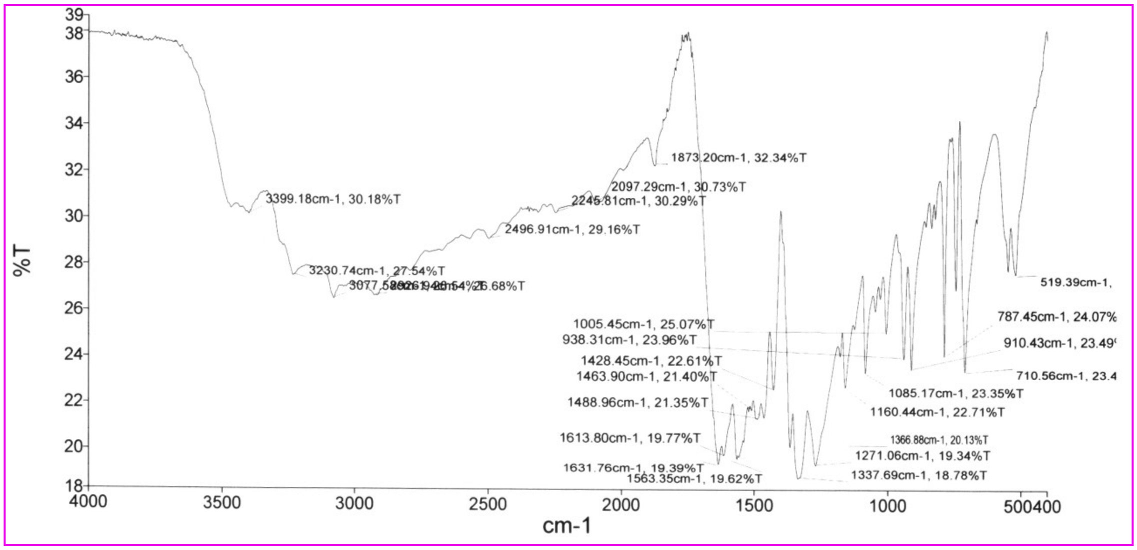
FT−IR spectroscopy: Fourier transform infrared (FT-IR) spectra were recorded with a Perkin−Elmer RXI FT-IR spectrophotometer using the reflectance technique (4000−400 cm^{-1}). Samples were prepared as KBr disks.



H_2Vm



complex**1**



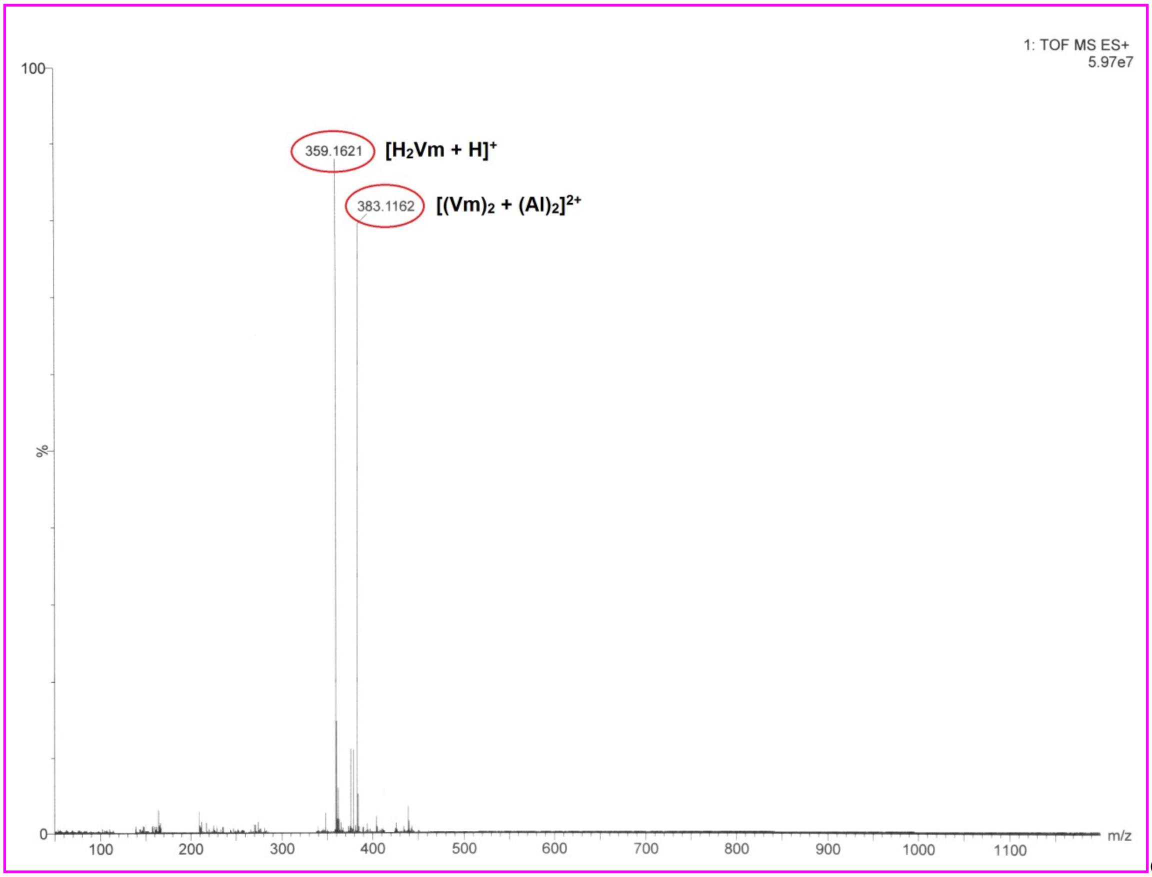
complex**2**

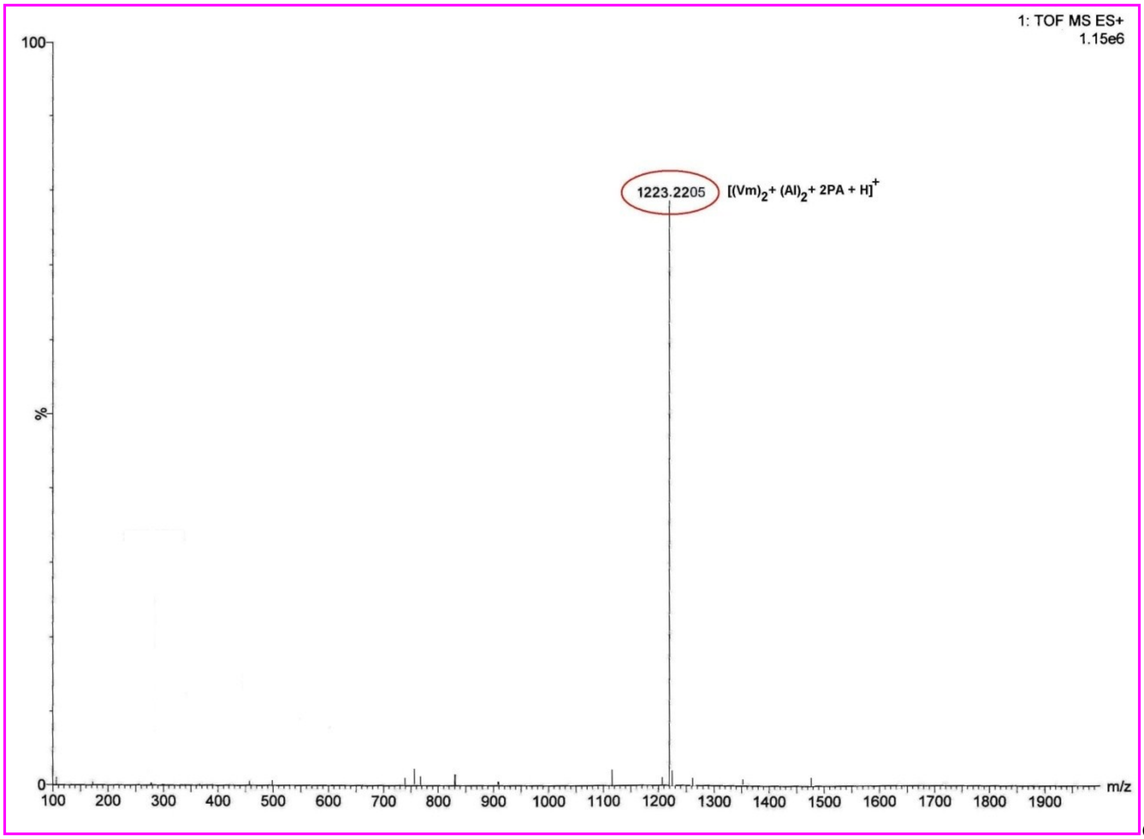
Figure S2. FT−IR Spectrum of **H_2Vm**, [**Al_2-Vm_2**] complex **1** and [**Al_2-Vm_2**].PA complex **2**.

1. Characterization and Structural Data.

Electrospray ionization mass spectra (HR–ESI–MS) were recorded on Qtof Micro YA263 mass spectrometer dissolving the samples in LC–MS quality MeOH.

H_2Vm


1: TOF MS ES+
5.97e7
359.1621
[H2Vm + H]+
383.1162
[(Vm)2 + (Al)2]2+
100
%
0
100
200
300
400
500
600
700
800
900
1000
1100
m/z
Complex1



Complex2

Figure S3. ESI–MS of ligand (**H_2Vm**), [**Al_2-Vm_2**] complex **1** and [**Al_2-Vm_2**]. PA complex **2**.

1. Characterization and Structural Data.

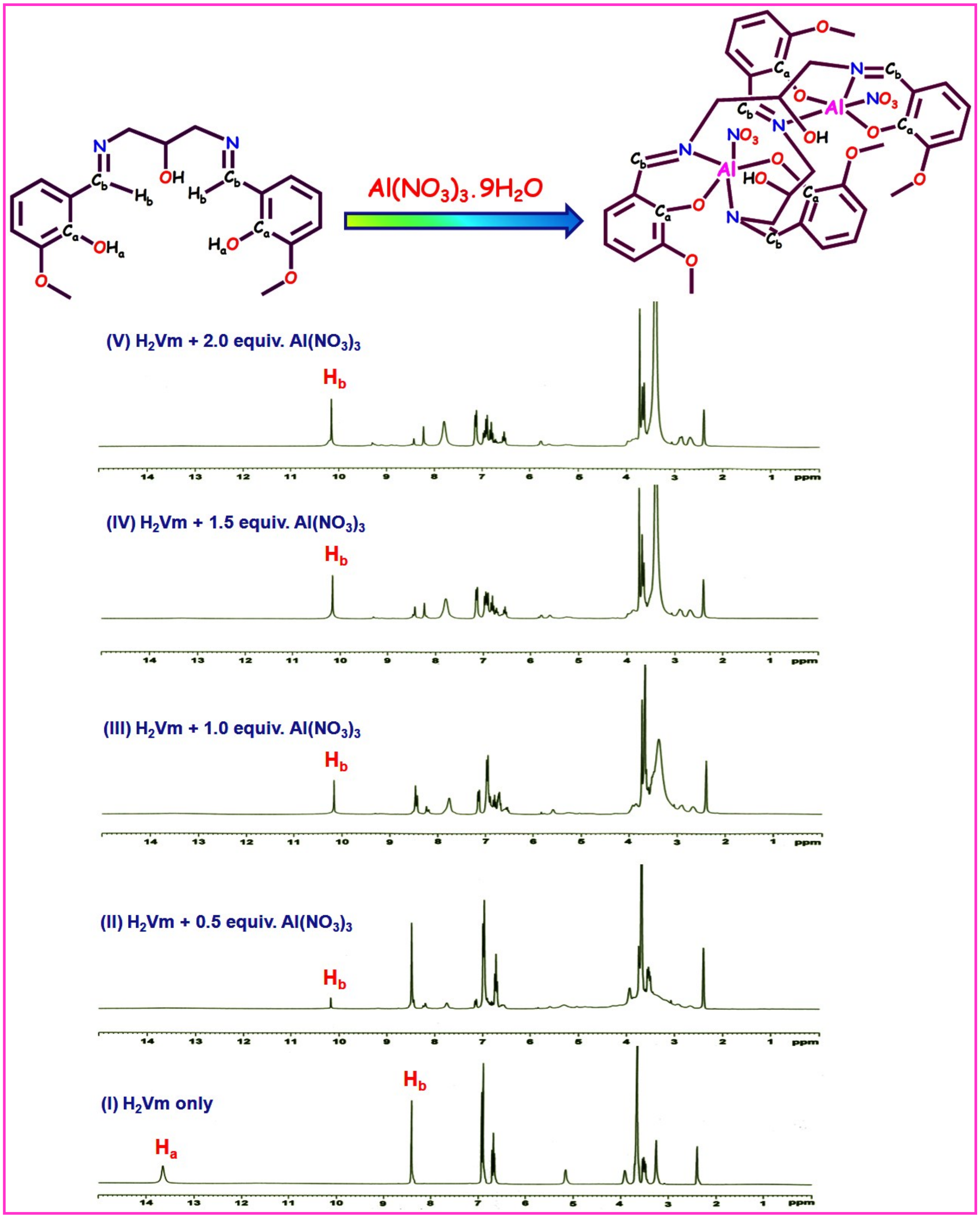


Figure S4. ^{1}H−NMR titration of **H_2Vm** with $Al(NO_3)_3.9H_2O$ in DMSO−d_6 solution.

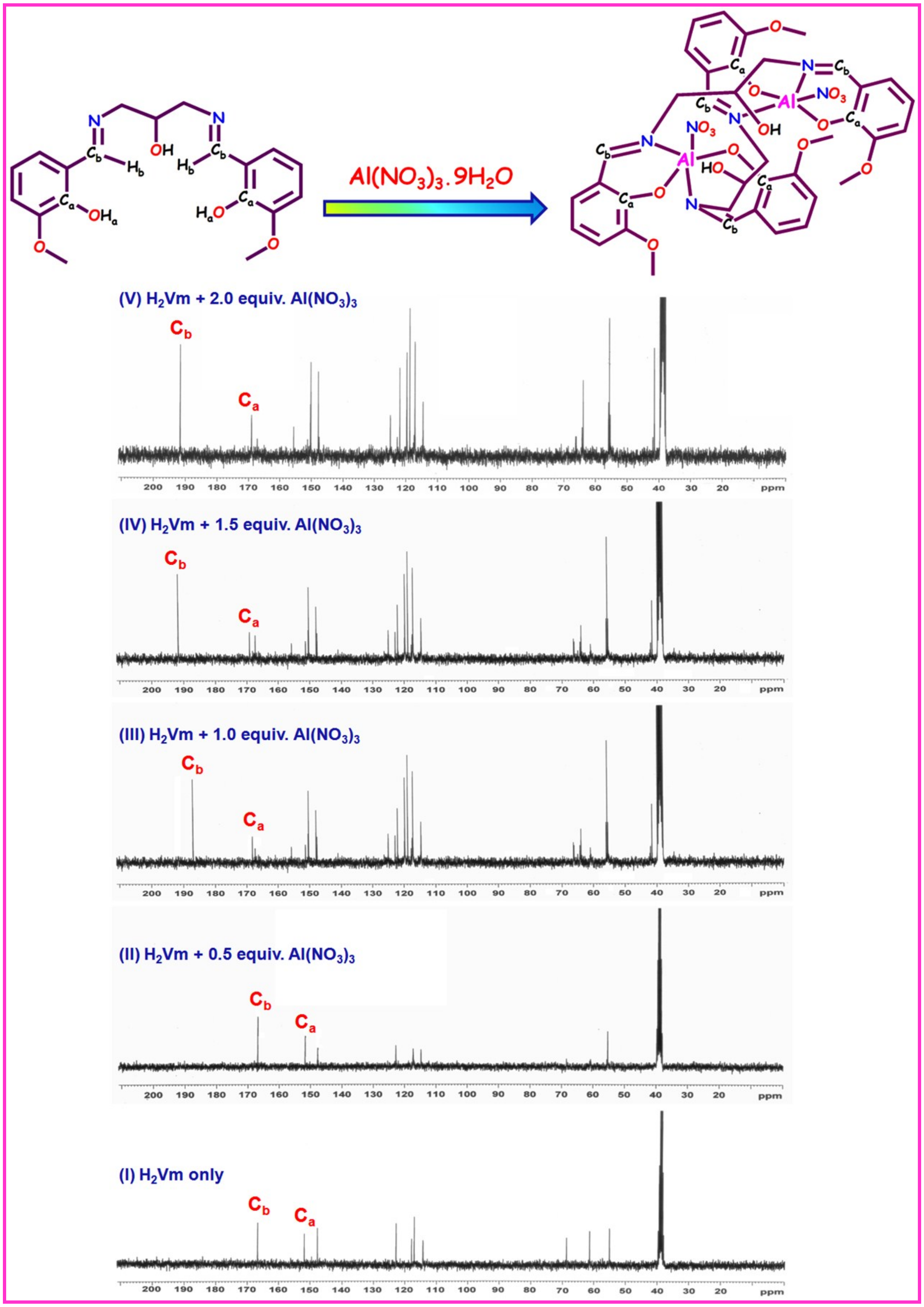


Figure S5. ^{13}C−NMR titration of $\mathbf{H_2Vm}$ with $Al(NO_3)_3.9H_2O$ in DMSO−d_6 solution.

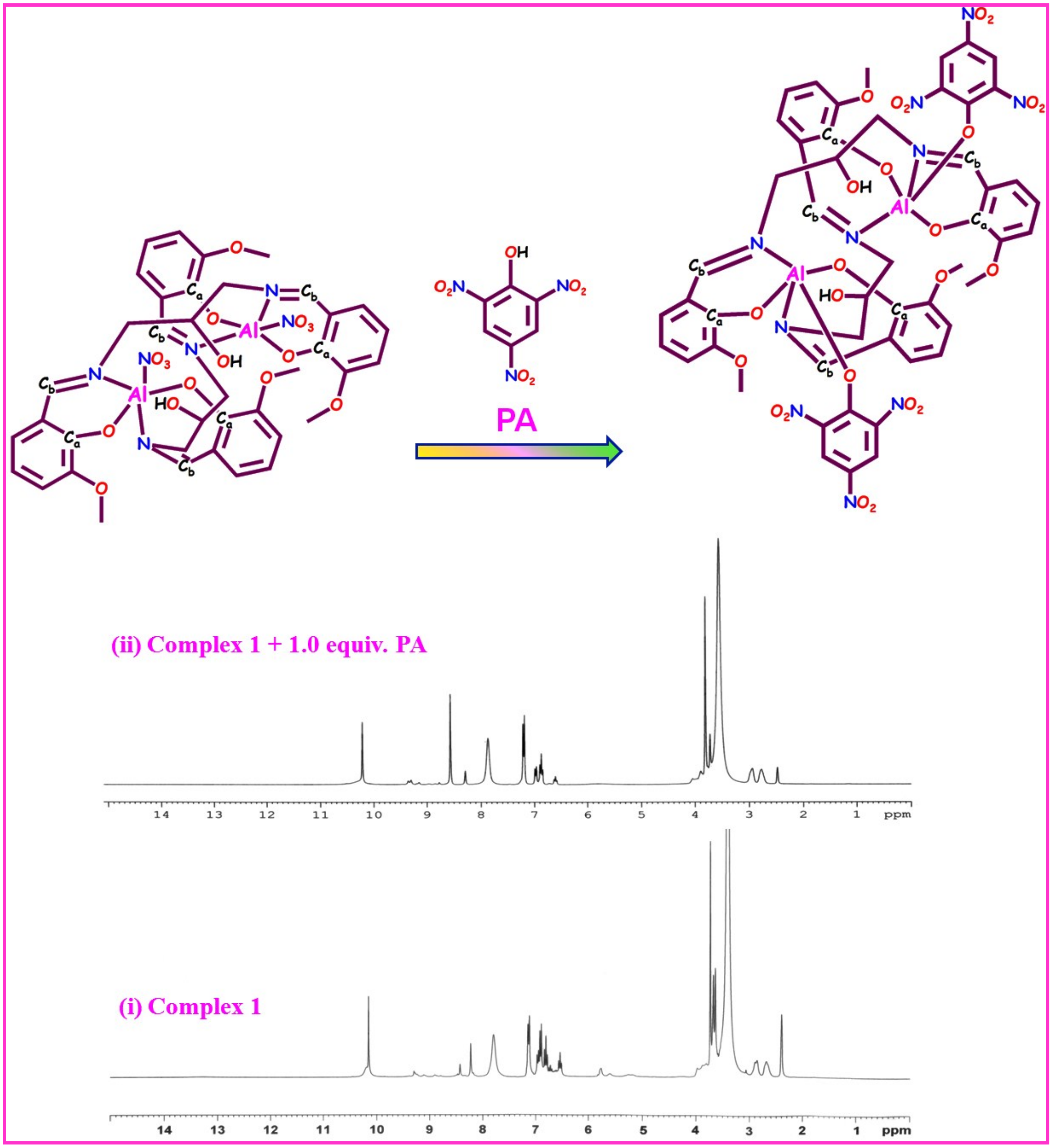


Figure S6. ^{1}H−NMR titration of complex **1** with Picric acid (PA) in DMSO−d_6 solution.

1. Characterization and Structural Data.

Table S1. ^{1}H and ^{13}C-NMR shift data of NMR titration experiment of **H_2Vm**.

^{1}H						
Proton label	**Free H_2Vm (ppm) (A)**	**H_2Vm + 0.5 equiv. $Al(NO_3)_3.9H_2O$(ppm) (B)**	**H_2Vm + 1.0 equiv. $Al(NO_3)_3.9H_2O$(ppm) (C)**	**H_2Vm + 1.5 equiv. $Al(NO_3)_3.9H_2O$(ppm) (D)**	**H_2Vm + 2.0 equiv. $Al(NO_3)_3.9H_2O$(ppm) (E)**	**Shift (E−A) (ppm)**
H_a	13.655	-	-	-	-	-
H_b	8.412	10.161	10.164	10.170	10.176	1.764 **downfield**
^{13}C						
C_a	151.83	151.97	168.89	169.06	169.09	17.26 **downfield**
C_b	166.73	166.96	187.56	191.63	191.67	24.94 **downfield**

2. Photophysical Characterization.

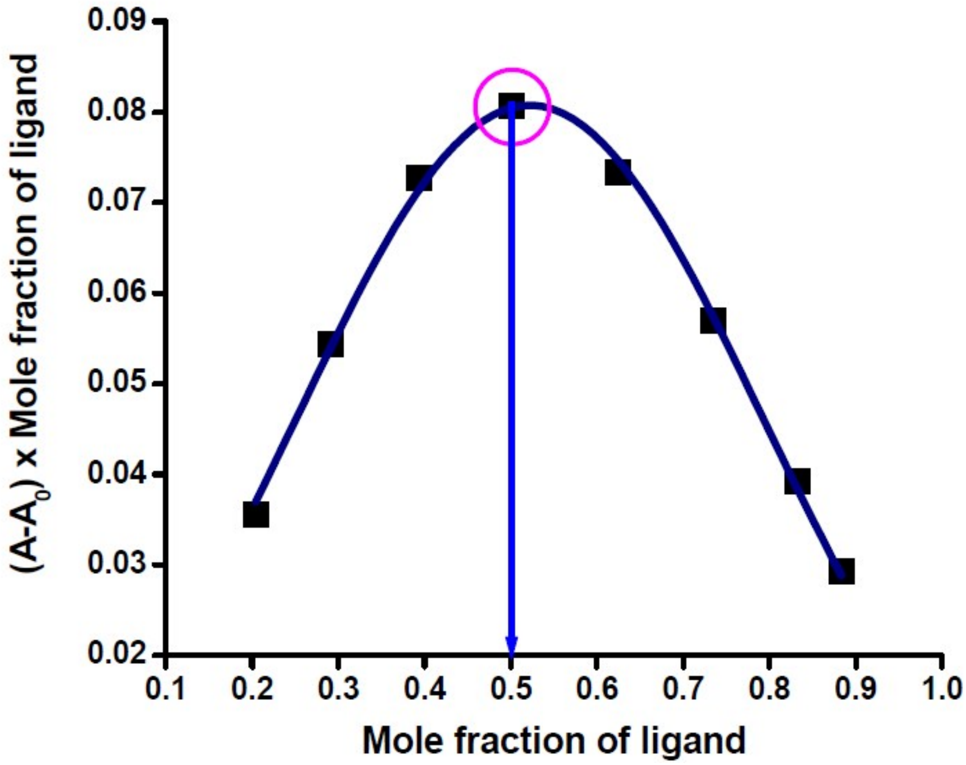


Figure S7. Job′s plot for the identification of (1:1) complex stoichiometry between **H_2Vm** and Al^{3+} using absorbance values at 368 nm.

2. Photophysical Characterization.

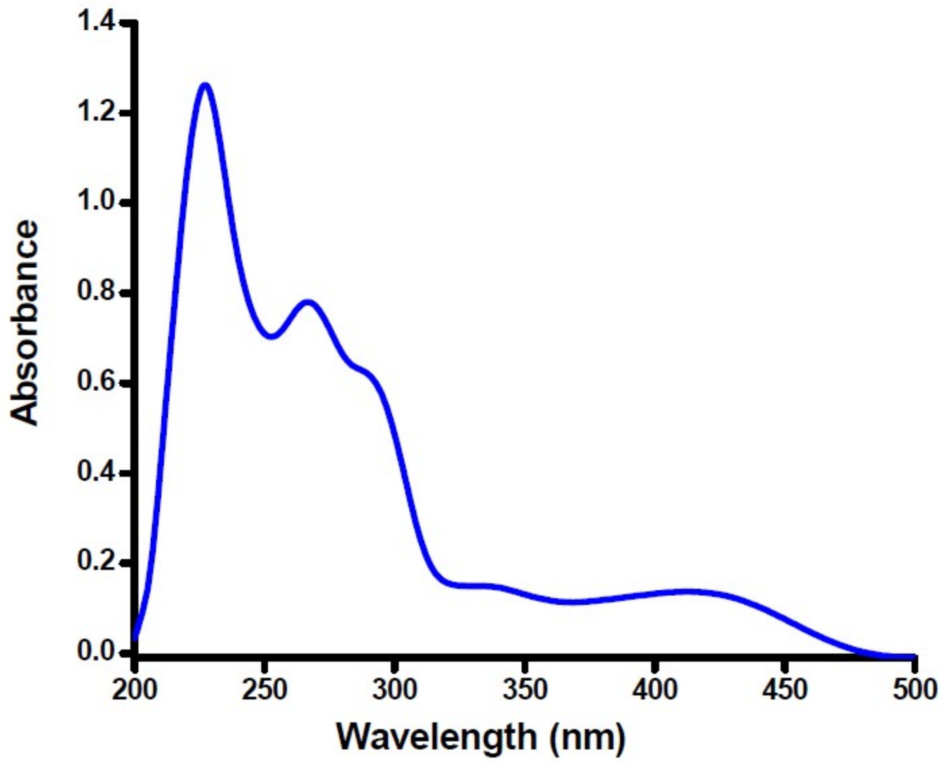


Figure S8. Absorbance spectra of $\mathbf{H_2Vm}$ in methanol solution.

2. Photophysical Characterization.

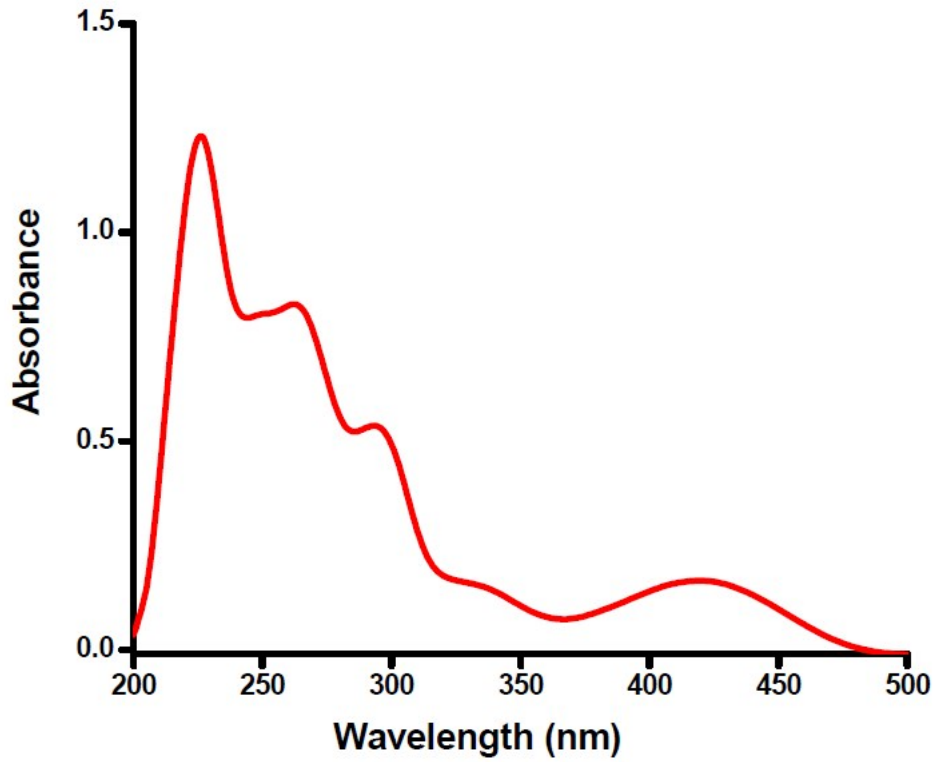


Figure S9. Absorbance spectra of $\mathbf{H_2Vm}$ in HEPES buffer (pH = 7.4) solution.

2. Photophysical Characterization.

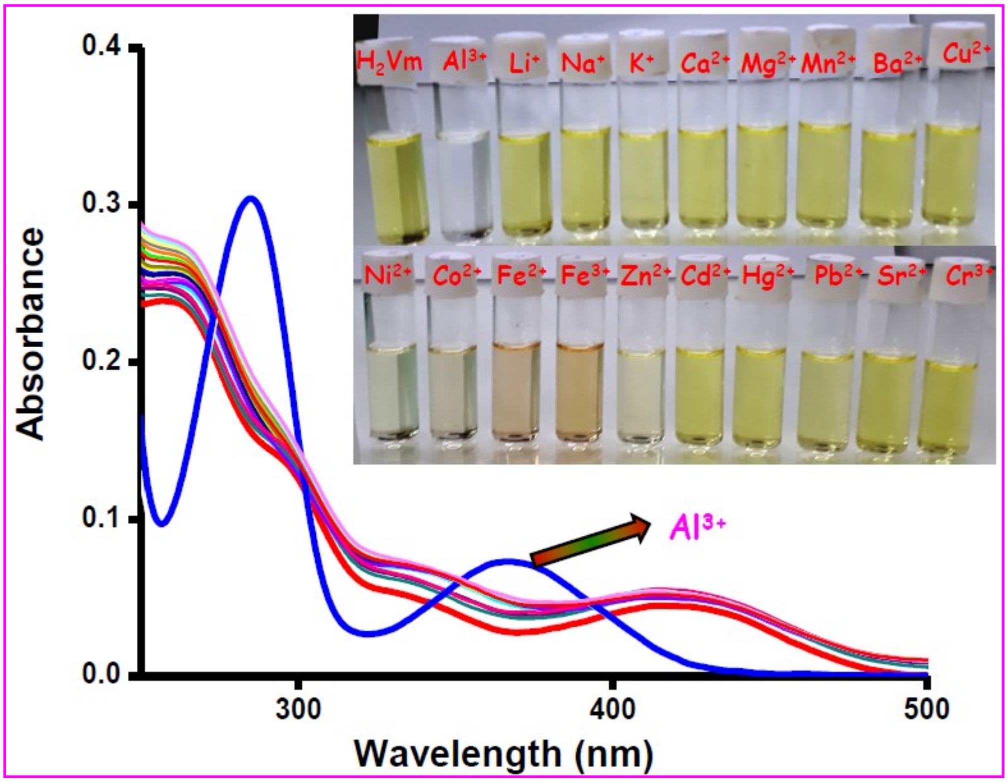


Figure S10. Absorbance spectra of $\mathbf{H_2Vm}$ (5×10^{-7} M) in HEPES buffer (pH = 7.4) solution in the presence different metal ions like Al^{3+}, Li^{+}, Na^{+}, K^{+}, Ca^{2+}, Mg^{2+}, Mn^{2+}, Ba^{2+}, Cu^{2+}, Ni^{2+}, Co^{2+},Fe^{2+}, Fe^{3+}, Zn^{2+}, Cd^{2+}, Hg^{2+}, Pb^{2+}, Sr^{2+} and Cr^{3+}. **Inset:** Visual color change observed with addition of different metal ions to $\mathbf{H_2Vm}$ solution.

2. Photophysical Characterization.

The binding constant (K) determined by the Benesi−Hildebrand expression was found to be 5.23 × 10^5 M^{-1}.

$$\frac{1}{(A - A_0)} = \frac{1}{\{K(A_{max} - A_0)[C]\}} + \frac{1}{(A_{max} - A_0)}$$

Where A_0 is the absorbance of free ligand, A is the observed absorbance at that particular wavelength in the presence of a certain concentration of the metal ion *[C]*, A_{max} is the maximum absorbance value of the complex formed. K is the association constant (M^{-1}) and was determined from the slope of the linear plot and *[C]* is the concentration of the Al^{3+} ion added during titration studies. The goodness of the linear fit of the B–H plot of $1/(A - A_0)$ *vs.* $1/[Al^{3+}]$ for 1:1 complex formation confirms the binding stoichiometry between **H_2Vm** and Al^{3+}.

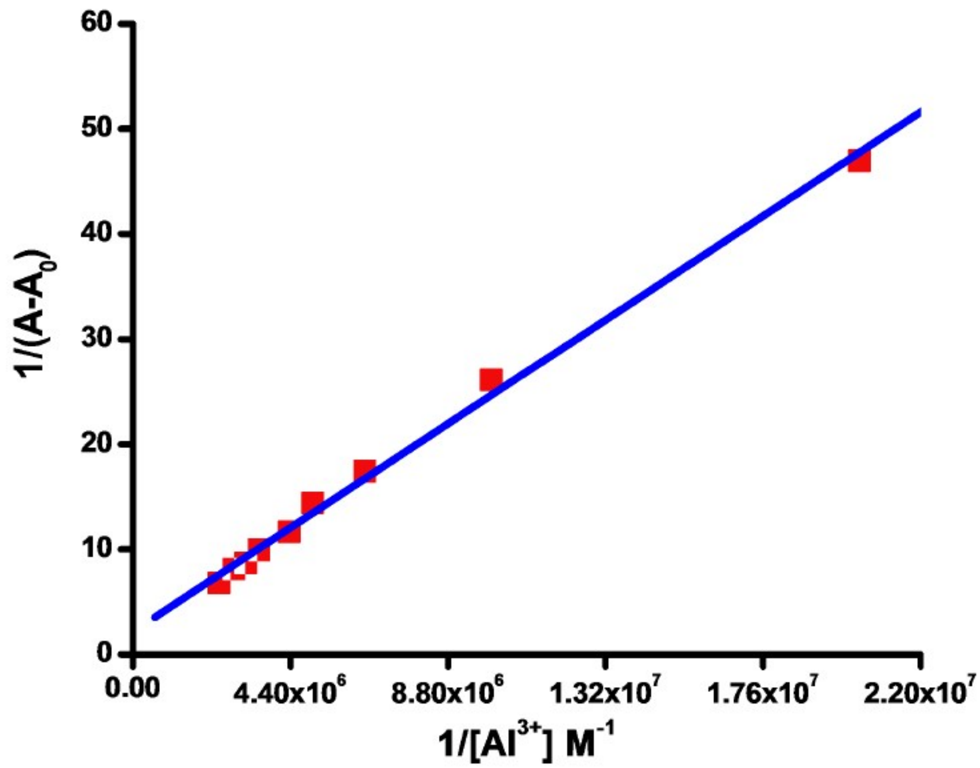


Figure S11. Benesi-Hildebrand plot of absorbance titration curve of **H_2Vm** and [Al^{3+}].

2. Photophysical Characterization.

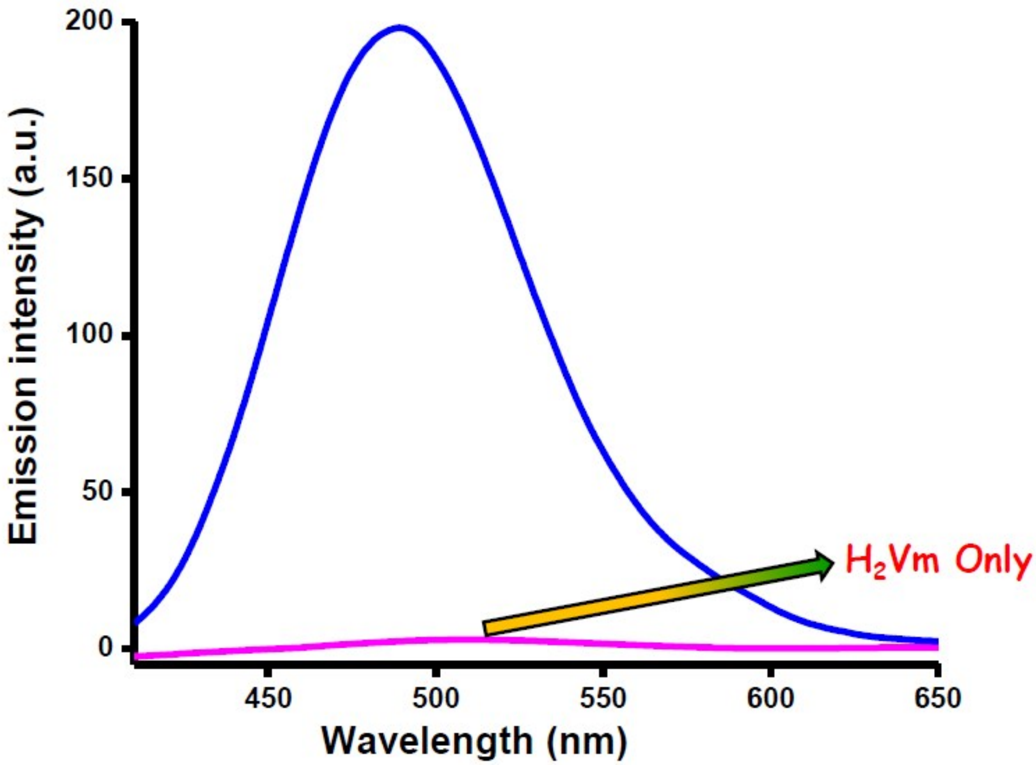


Figure S12. Emission spectra of **H_2Vm** in the presence of [Al^{3+}] in HEPES buffer (pH = 7.4) solution (λ_{ex}= 400 nm, λ_{em}= 488 nm).

2. Photophysical Characterization.

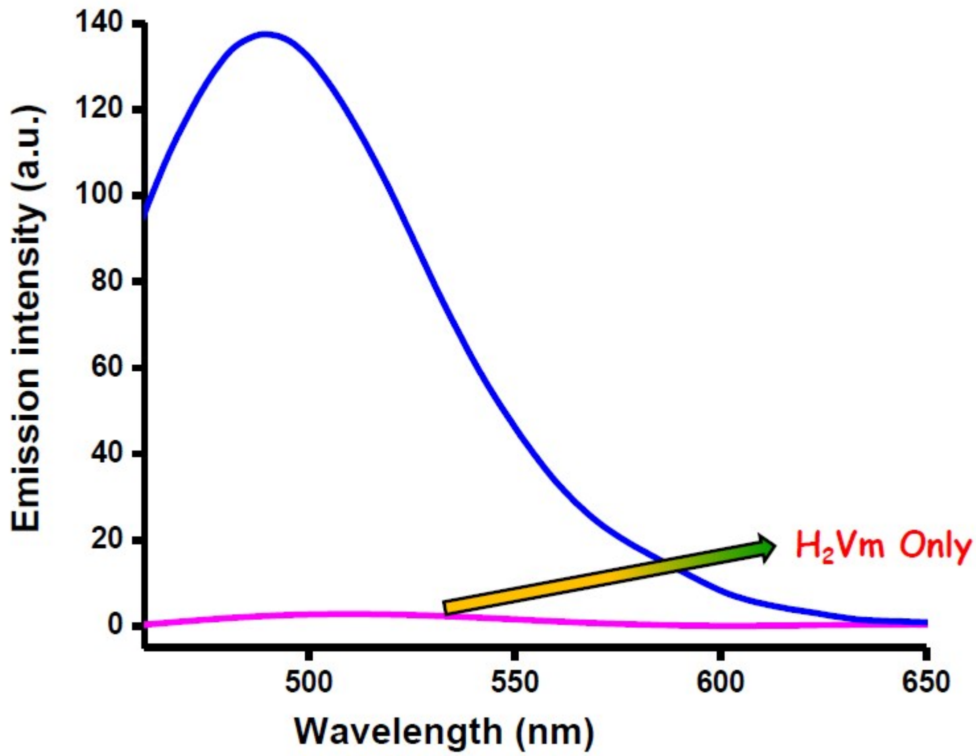


Figure S13. Emission spectra of $\mathbf{H_2Vm}$ in the presence of [Al^{3+}] in HEPES buffer (pH = 7.4) solution (λ_{ex}= 450 nm, λ_{em}= 488 nm).

2. Photophysical Characterization.

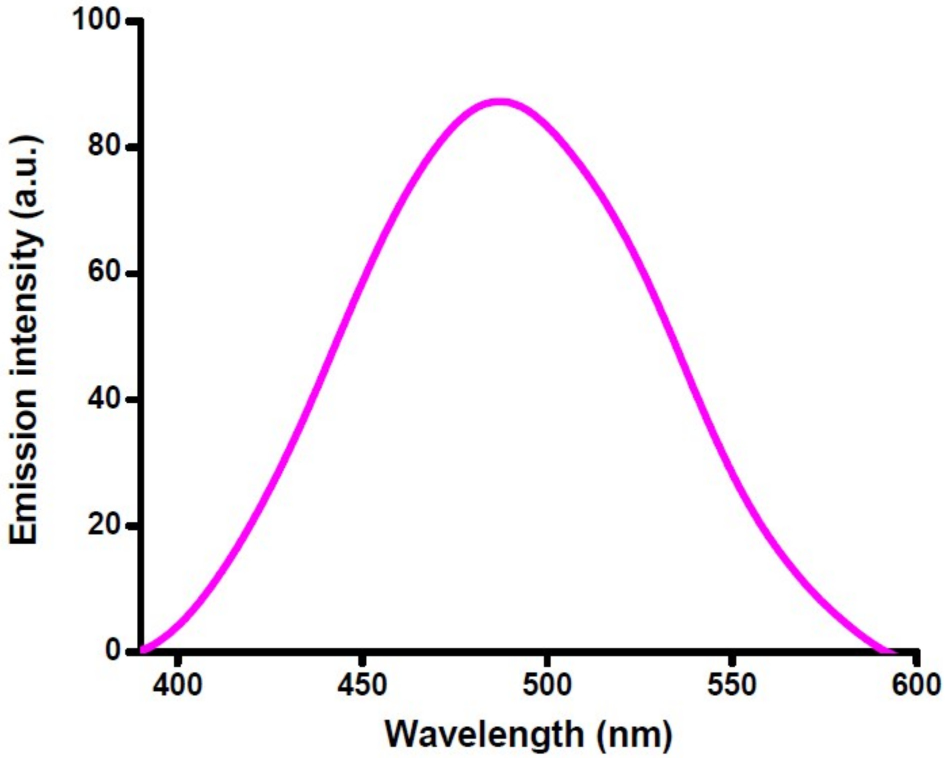


Figure S14. Emission spectra of $\mathbf{H_2Vm}$ in methanol solution.

2. Photophysical Characterization.

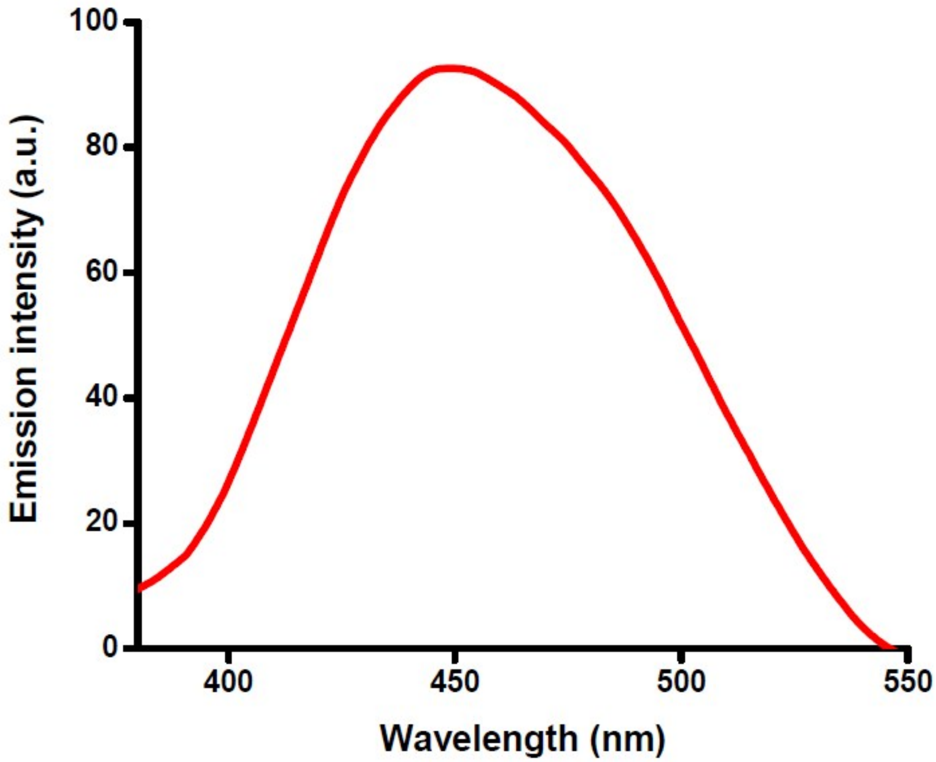


Figure S15. Emission spectra of $\mathbf{H_2Vm}$ in HEPES buffer (pH = 7.4) solution.

2. Photophysical Characterization.

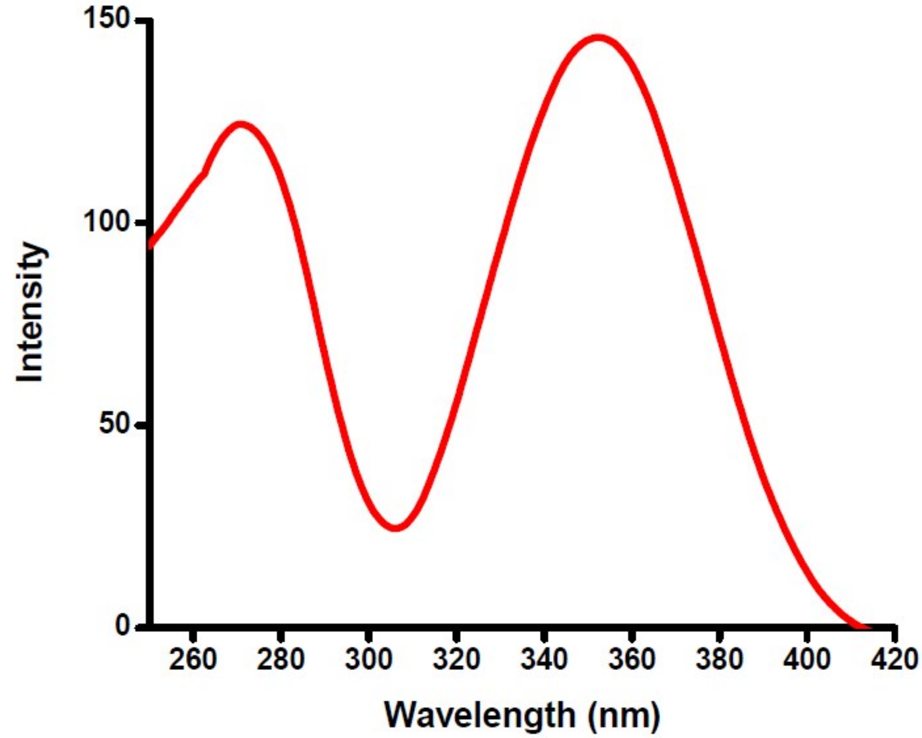


Figure S16. Excitation spectra of $\mathbf{H_2Vm}$ in methanol solution.

2. Photophysical Characterization.

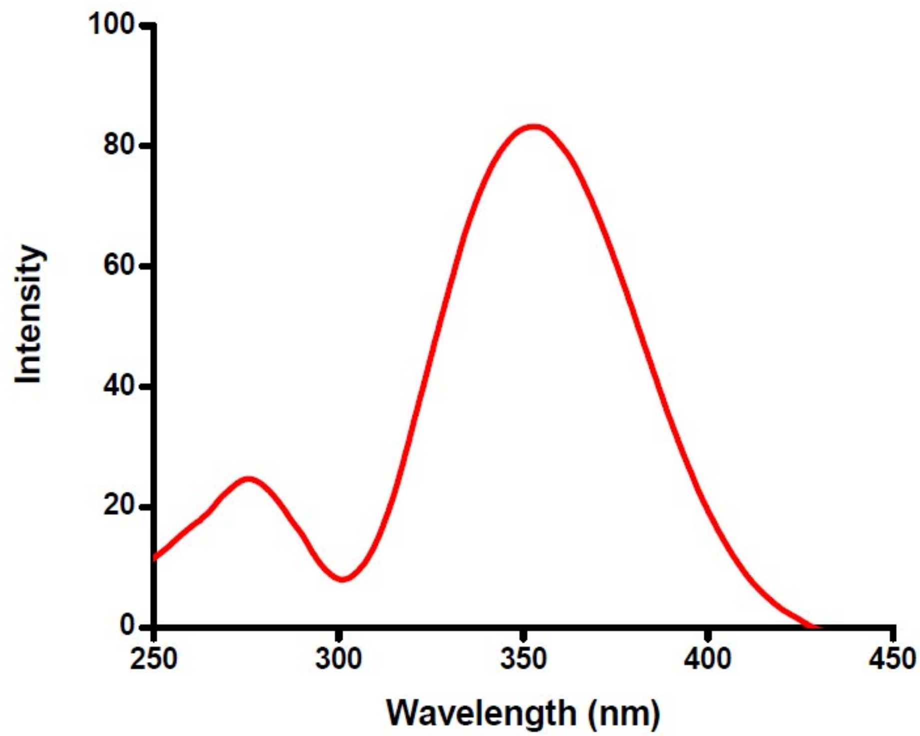


Figure S17. Excitation spectra of $\mathbf{H_2Vm}$ in HEPES buffer (pH = 7.4) solution.

2. Photophysical Characterization.

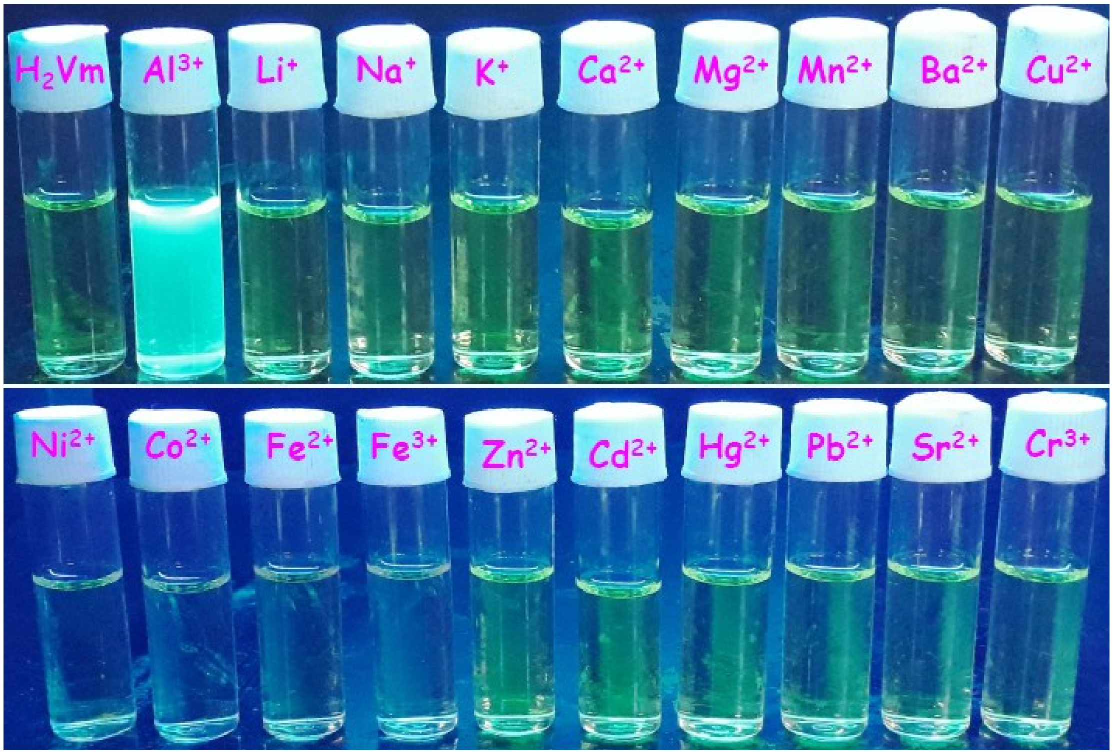


Figure S18. Visual color change observed with addition of different metal ions to **H_2Vm** as seen under UV light (λ = 365 nm).

2. Photophysical Characterization.

According to the linear Benesi–Hildebrand expression, the measured fluorescence intensity $(F - F_0)/(F_x - F_0)$ at 488 nm varied as a function of $1/[Al^{3+}]$ in a linear relationship, which indicates the formation of 1 : 1 stoichiometry between Al^{3+} and **H_2Vm** in the complex.

$$\frac{1}{F_X - F_0} = \frac{1}{F_{max} - F_0} + \frac{1}{K[C]}\left(\frac{1}{F_{max} - F_0}\right)$$

where F_0, F_x and F_{max} are the emission intensities of organic moiety considered in the absence of Al^{3+} ions, at an intermediate Al^{3+} concentration and at a concentration of complete interaction, respectively, K is the binding constant and $[C]$ is the concentration of Al^{3+} ions.

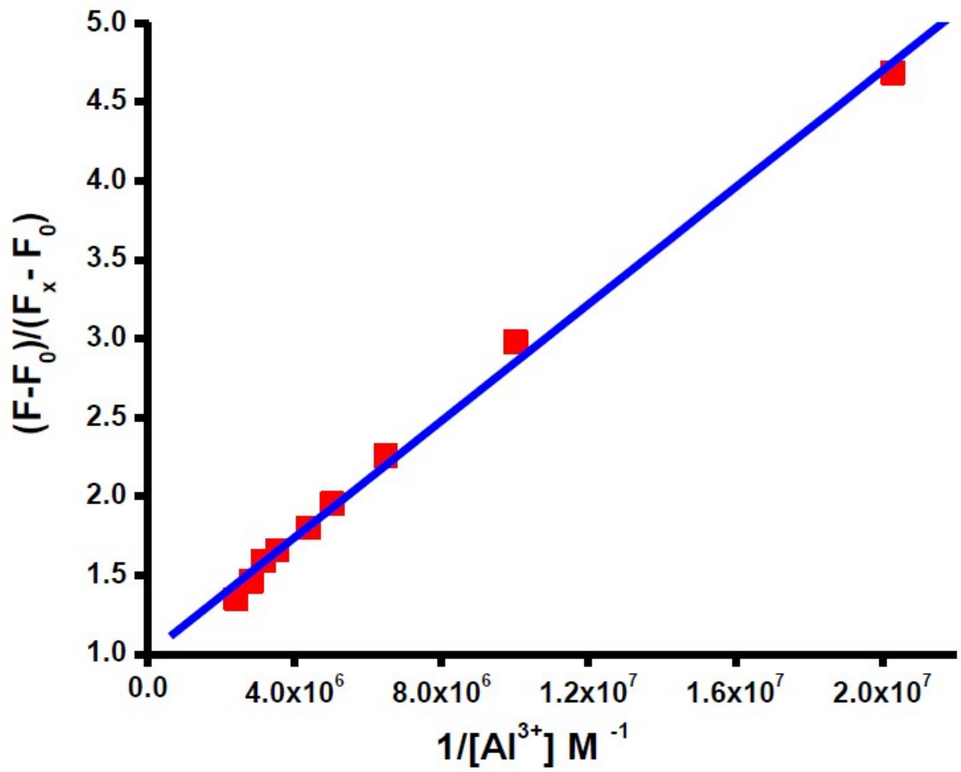


Figure S19. Benesi-Hildebrand plot $[(F\text{-}F_0)/(F_x\text{-}F_0)]$ vs. $1/[Al^{3+}]$ for complexation between **H_2Vm** and Al^{3+} derived from emission titration curve.

2. Photophysical Characterization.

Detection limit calculation in emission spectroscopy.

The limit of detection (**LOD**) of **Al_2-Vm_2** was measured on the basis of fluorescence titration measurement. The detection limit was calculated using the following equation:

$$LOD = K \times \frac{\sigma}{S}$$

where K = 2 or 3 (we take 3 in this case), 'σ' is the standard deviation of the blank solution and 'S' is the slope between the ratio of emission intensity *versus* [Al^{3+}].

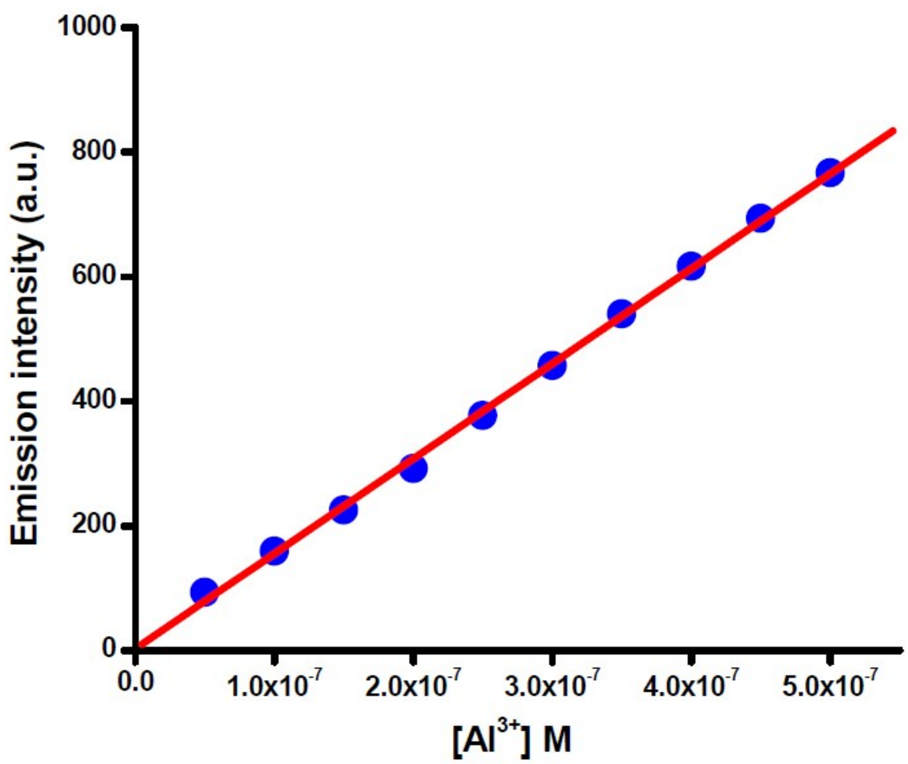


Figure S20. The limit of detection (LOD) of **H_2Vm** for Al^{3+} fluorescence responses (λ_{em}= 488 nm) as a function of Al^{3+} concentration.

2. Photophysical Characterization.

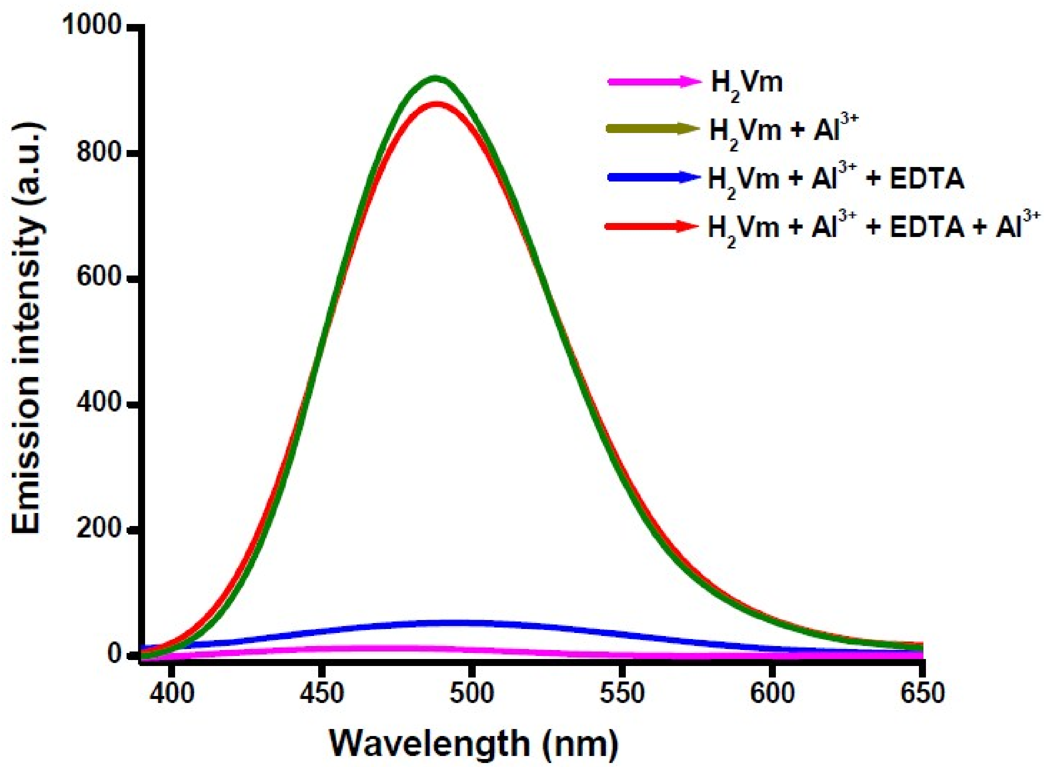


Figure S21. Fluorescence emission spectra of $\mathbf{H_2Vm}$ in the presence of Al^{3+} ion followed by addition of EDTA.

2. Photophysical Characterization.

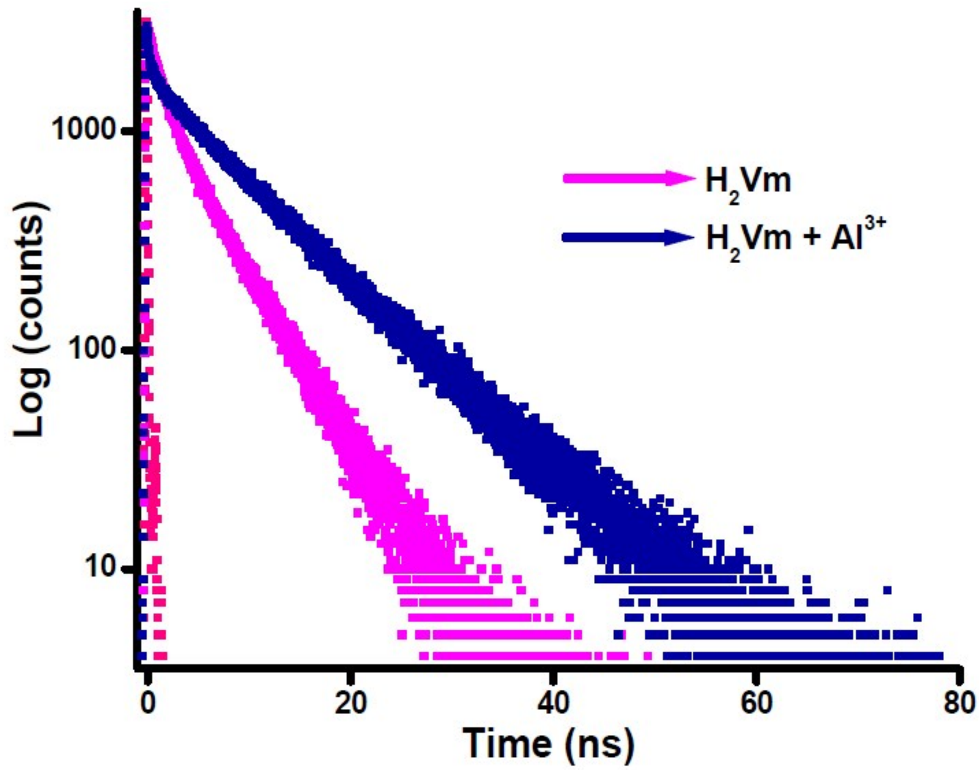


Figure S22. Time–resolved fluorescence decay of **H_2Vm** in the absence and presence of added Al^{3+} solution at 375 nm.

2. Photophysical Characterization.

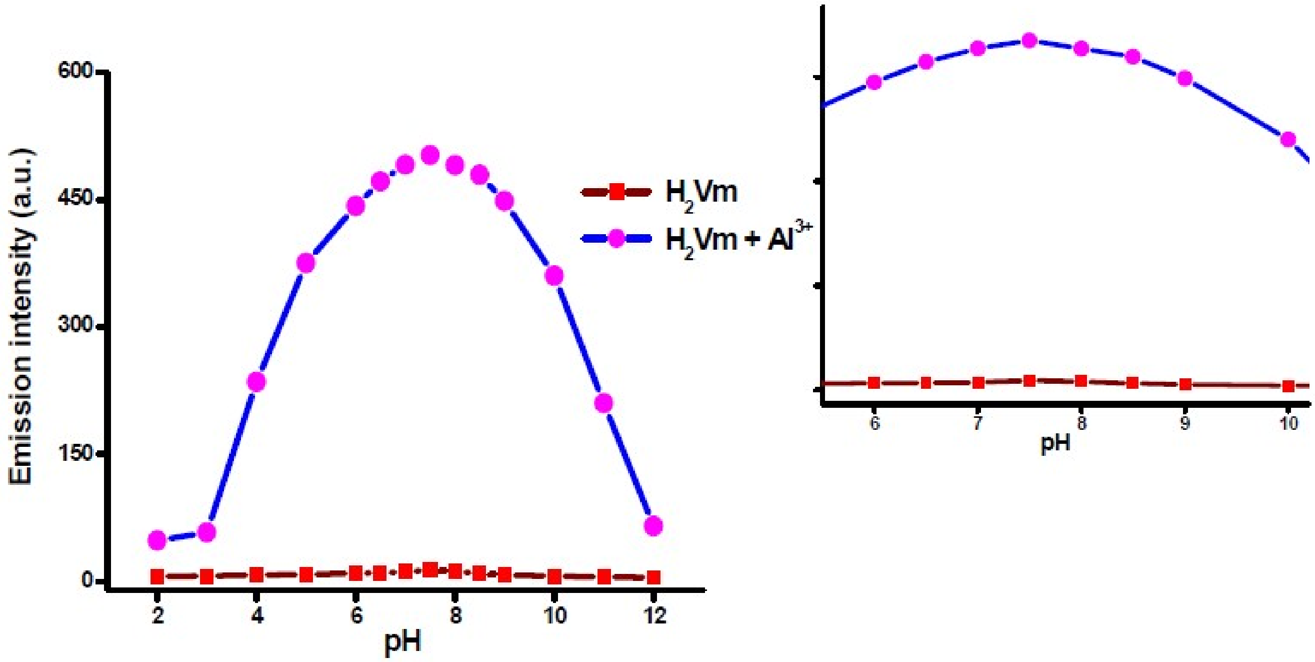


Figure S23. Emission intensity of probe $\mathbf{H_2Vm}$ (5×10^{-7} M) in absence and in presence of Al^{3+} as a function of pH values in aqueous solution at 488 nm. **Inset:** pH plot of zoomed graphic of $\mathbf{H_2Vm}$ and in presence of Al^{3+}.

2. Photophysical Characterization.

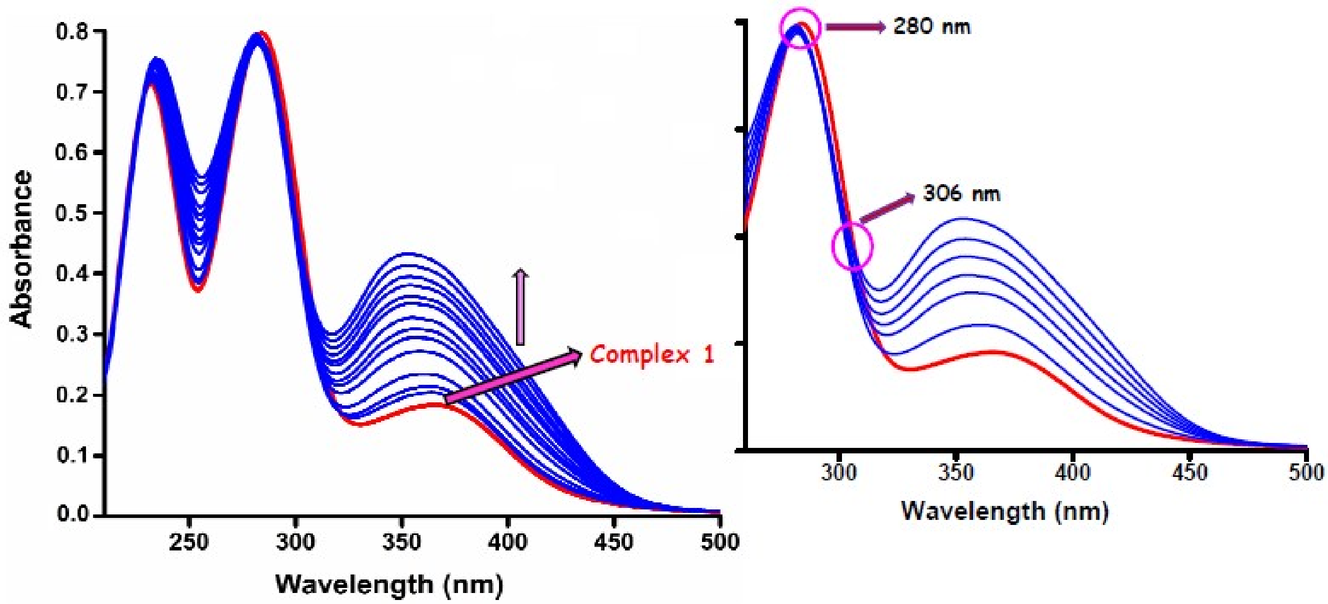


Figure S24. UV-vis spectra of complex **1** (5×10^{-7} M) in HEPES buffer (pH = 7.4) solution in the presence of various concentration of **PA** (0, 0.5, 1, 1.5, 2, 2.5, 3, 4, 5, 6, 7, 8, 9 and 10) $\times10^{-7}$ M. **Inset:** UV-vis spectra of zoomed graphic of complex **1**.

2. Photophysical Characterization.

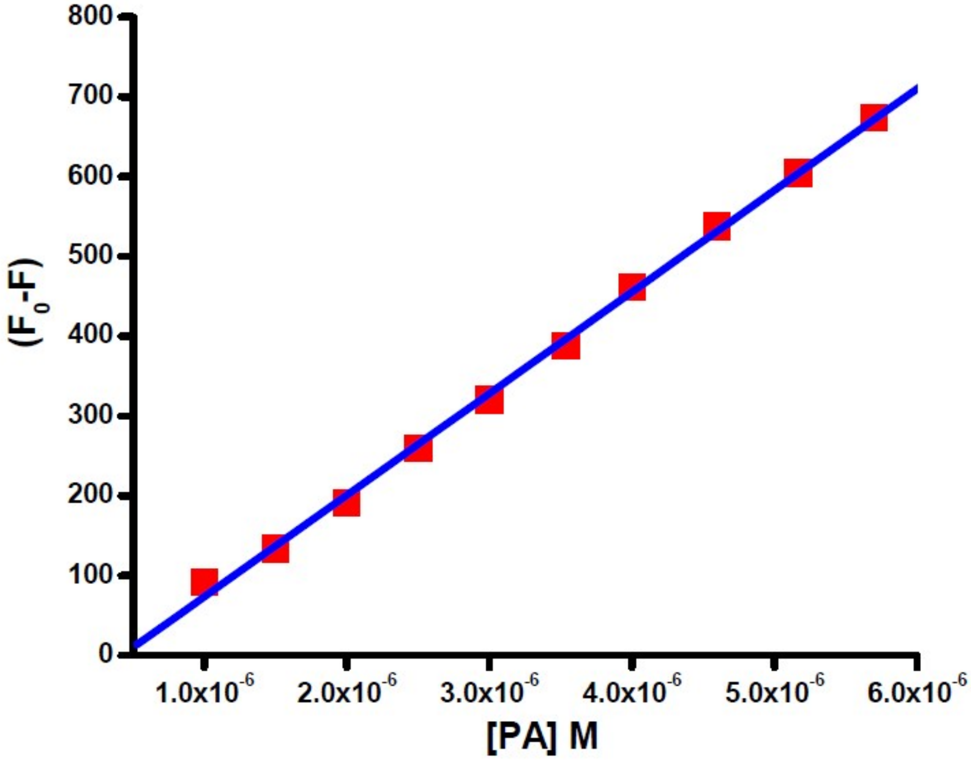


Figure S25. The limit of detection (LOD) of complex **1** for **PA** fluorescence responses (λ_{em}= 484 nm) as a function of **PA** concentration.

2. Photophysical Characterization.

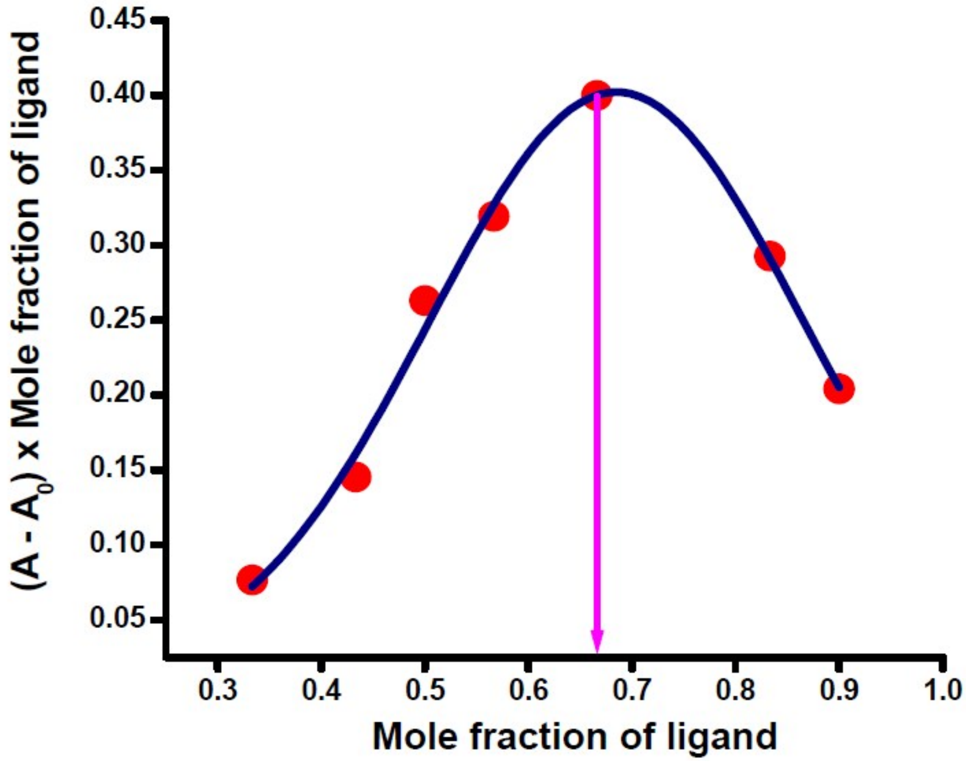


Figure S26. Job′s plot for the identification of complex **1-**PA (1:2) complex stoichiometry using absorbance values at 364 nm.

2. Photophysical Characterization.

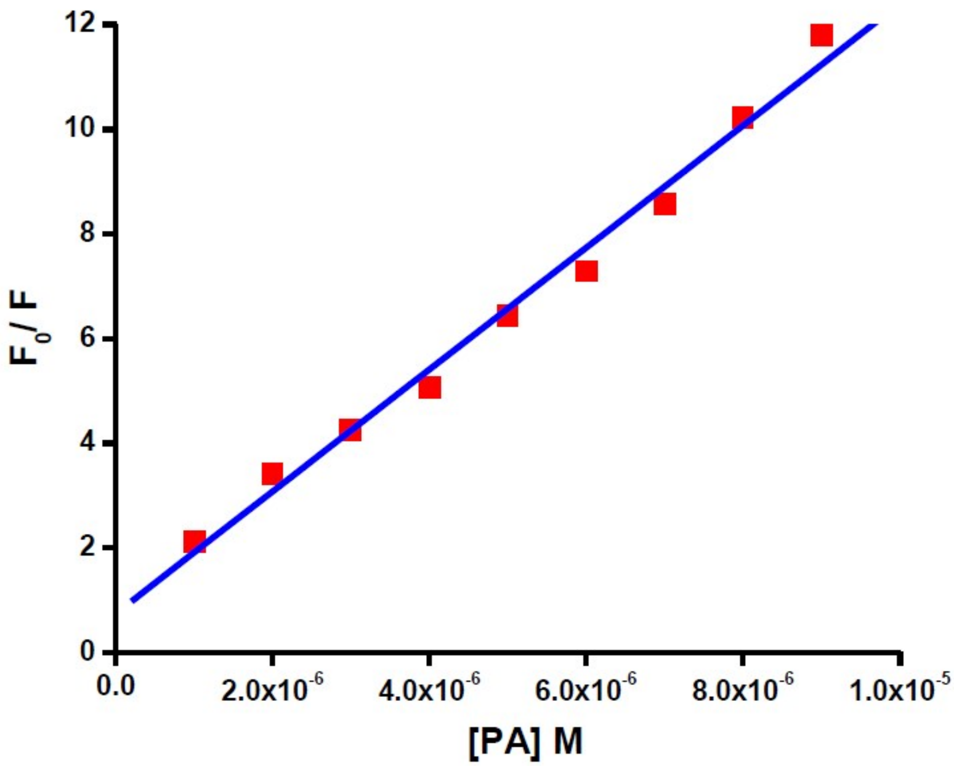


Figure S27. Stern–Volmer plot of fluorescence quenching for complexation between complex **1** and **PA** derived from emission titration curve.

2. Photophysical Characterization.

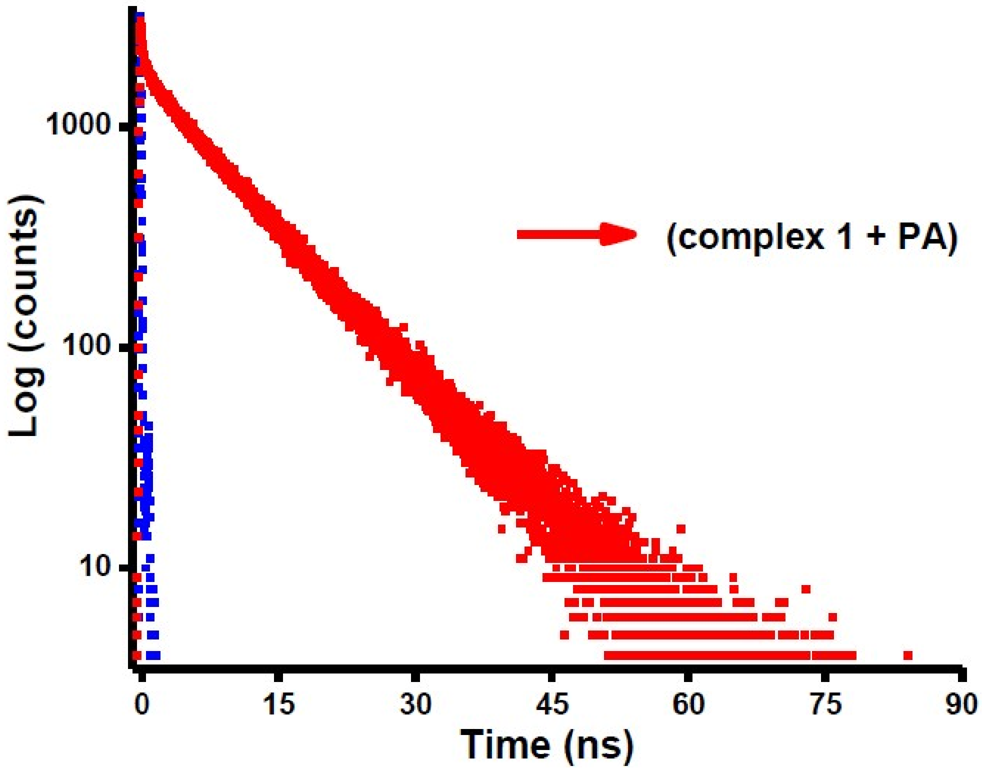


Figure S28. Time–resolved fluorescence decay of complex **1** with PA in solution at 375 nm.

Table S2. Fluorescence lifetime measurement of chemosensor **H_2Vm**, complex **1** and complex **2** in aqueous solution.

	φ_f	τ_{av}(ns)	K_r($\times10^9$) (S^{-1})	K_{nr}($\times10^9$) (S^{-1})	χ2
H_2Vm	0.036	0.074	0.486	13.027	1.010
H_2Vm + Al^{3+} (complex 1)	0.511	0.579	0.883	0.845	1.028
Al_2-Vm_2 complex + PA (complex 2)	0.095	0.528	0.179	1.714	1.019

2. Photophysical Characterization.

Table S3. Stability constant was compared with complexation properties of the other metal ions.

Different metal ions	Stability constant from absorption data (M^{-1})	Stability constant from fluorescence data (M^{-1})
Al^{3+}	5.23×10^5	4.19×10^5
Li^+	1.021×10^4	1.104×10^4
Na^+	1.137×10^4	1.149×10^4
K^+	1.276×10^4	1.257×10^4
Ca^{2+}	1.314×10^4	1.379×10^4
Mg^{2+}	1.576×10^4	1.681×10^4
Mn^{2+}	1.823×10^4	1.885×10^4
Ba^{2+}	1.199×10^4	1.205×10^4
Cu^{2+}	1.079×10^4	1.104×10^4
Fe^{2+}	1.753×10^4	1.767×10^4
Zn^{2+}	2.803×10^4	2.911×10^4
Cd^{2+}	2.158×10^4	2.219×10^4
Hg^{2+}	1.812×10^4	1.915×10^4
Ni^{2+}	1.865×10^4	1.891×10^4
Pb^{2+}	1.943×10^4	1.939×10^4
Sr^{2+}	1.087×10^4	1.109×10^4
Co^{2+}	1.342×10^4	1.351×10^4
Cr^{3+}	1.265×10^4	1.278×10^4

3. Theoretical Data.

Table S4. Selected parameters for the vertical excitation (UV-vis absorption) of **H_2Vm** (bis-keto form), electronic excitation energy (eV) and oscillator strength (*f*), and composition of the low-lying excited state of **H_2Vm**; calculation of the S_0–S_n energy gaps based on optimized ground-state geometries (UV-vis absorption, H_2O used as solvent). Only those transitions that contribute higher than 10% are given

Process	Electronic transitions	Composition	Excitation energy	Oscillator strength (f)	contribution	λ_{exp} (nm)
Absorption	$S_0 \rightarrow S_1$	HOMO → LUMO HOMO-1 → LUMO	3.0108 eV (412 nm)	0.1111	87% 13%	420

Table S5. Selected parameters for the vertical excitation (UV-vis absorptions) and the emission of **Al_2-Vm_2**, electronic excitation energies (eV) and oscillator strengths (*f*) and contributions of the lowest lying excited state; calculation of the S_0–S_n energy gap is based on optimized ground-state geometries (UV-vis absorption) (H_2O used as solvent).

Process	Electronic transitions[1]	Composition	Excitation energy	Oscillator strength (f)	contri-bution	λ_{exp} (nm)
Absorption	$S_0 \rightarrow S_8$	HOMO–3 → LUMO HOMO–2 → LUMO+1 HOMO–1 → LUMO+2	3.4147 eV (363 nm)	0.0822	36% 36% 28%	368

[1]$S_0 \rightarrow S_1$ f = 0.0001; $S_0 \rightarrow S_2$ f = 0.0005; $S_0 \rightarrow S_3$ f = 0.0000; $S_0 \rightarrow S_4$ f = 0.0003; $S_0 \rightarrow S_5$ f = 0.0007; $S_0 \rightarrow S_6$ f = 0.0005; $S_0 \rightarrow S_7$ f = 0.0003.

3. Theoretical Data.

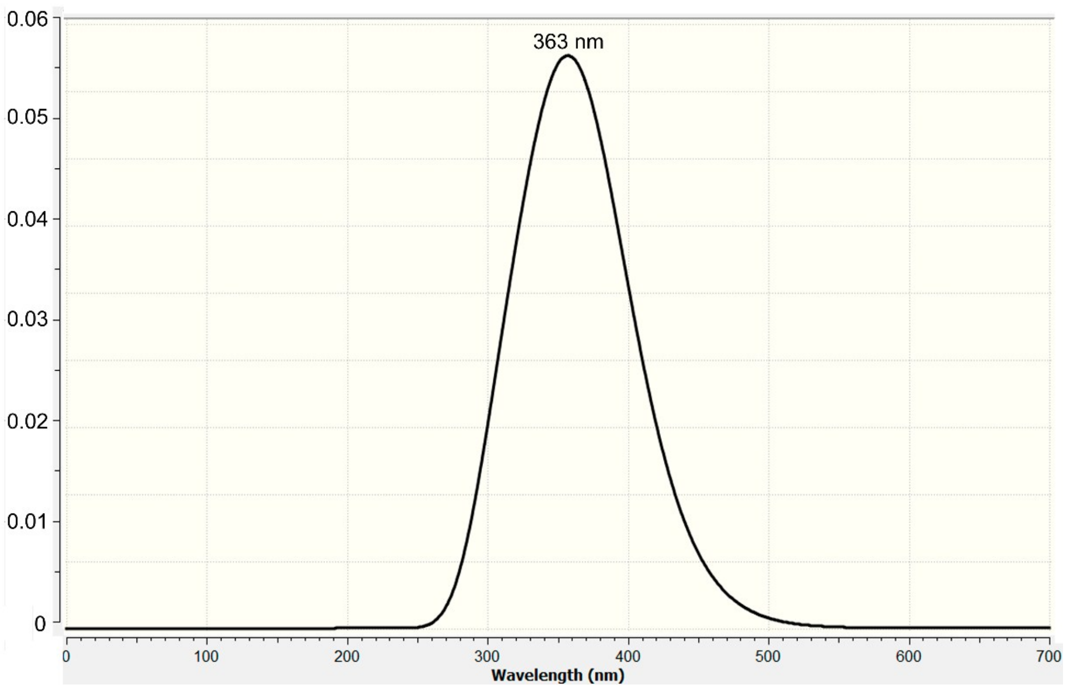


Figure S29. Theoretical UV-vis spectrum of **Al_2-Vm_2**.

4. Cell study.

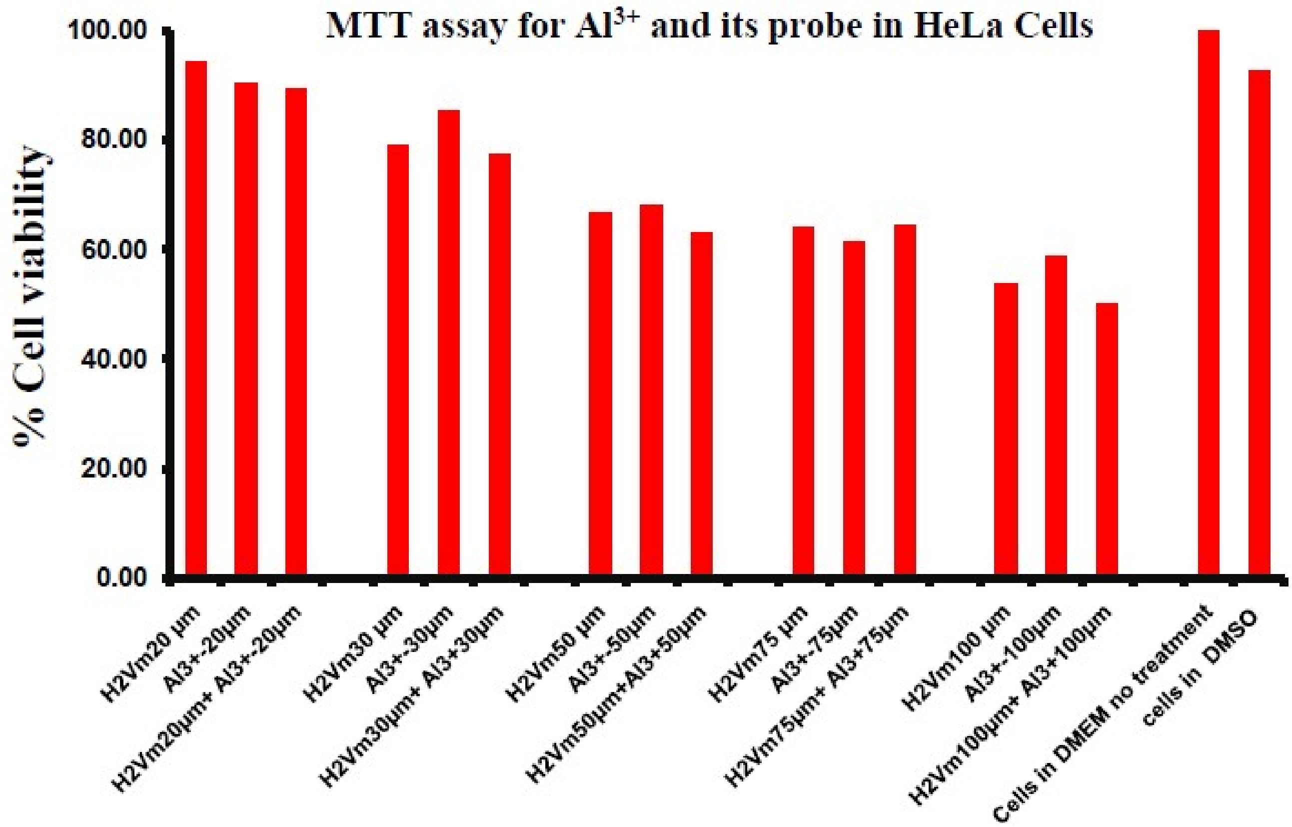


Figure S30. Percentage (%) cell viability of Hela cells treated with different concentrations of **H_2Vm** for 24 hours determined by MTT assay.

5. Cartesian Coordinates.

Enol

C	1.70649300	-1.12030300	5.47524000
C	0.97424100	-0.31509500	4.57345700
C	-0.35273500	0.06388600	4.88641100
C	-0.92779300	-0.37196200	6.10961600
C	-0.18242200	-1.16366200	6.98042000
C	1.13657300	-1.53967800	6.66377300
H	2.72504900	-1.40402100	5.22008600
H	-0.61707800	-1.49839300	7.91587100
H	1.69762100	-2.15781800	7.35851100
O	-1.10423900	0.82373200	4.07546200
H	-0.56156600	1.03699400	3.26600900
O	-2.20724300	0.04232200	6.32644100
C	1.59982200	0.11878600	3.33213400
H	2.63074400	-0.23136600	3.16026200
N	1.00653800	0.86882400	2.47355600
C	-2.85332800	-0.36439700	7.52305500
H	-2.32846100	0.01402900	8.41083200
H	-3.85333800	0.07054300	7.48012900
H	-2.93289300	-1.45834700	7.58319100
C	1.70247200	1.25290900	1.26336100
H	2.69504900	0.77358500	1.19738300
H	1.86589800	2.34199400	1.29107200
C	0.88459100	0.91790400	0.00000000
C	1.70649300	-1.12030300	-5.47524000
C	0.97424100	-0.31509500	-4.57345700
C	-0.35273500	0.06388600	-4.88641100
C	-0.92779300	-0.37196200	-6.10961600
C	-0.18242200	-1.16366200	-6.98042000
C	1.13657300	-1.53967800	-6.66377300
H	2.72504900	-1.40402100	-5.22008600
H	-0.61707800	-1.49839300	-7.91587100
H	1.69762100	-2.15781800	-7.35851100
O	-1.10423900	0.82373200	-4.07546200
H	-0.56156600	1.03699400	-3.26600900
O	-2.20724300	0.04232200	-6.32644100
C	1.59982200	0.11878600	-3.33213400
H	2.63074400	-0.23136600	-3.16026200
N	1.00653800	0.86882400	-2.47355600
C	-2.85332800	-0.36439700	-7.52305500
H	-2.93289300	-1.45834700	-7.58319100
H	-3.85333800	0.07054300	-7.48012900
H	-2.32846100	0.01402900	-8.41083200
C	1.70247200	1.25290900	-1.26336100
H	1.86589800	2.34199400	-1.29107200
H	2.69504900	0.77358500	-1.19738300

H	0.65448400	-0.15342200	0.00000000
O	-0.38551900	1.55120600	0.00000000
H	-0.26762800	2.51575100	0.00000000

Keto

C	1.74319400	-1.03868300	5.62238300
C	1.00073200	-0.29309700	4.64566600
C	-0.39063300	0.09094600	4.88735600
C	-0.95573700	-0.33082000	6.17334600
C	-0.20302400	-1.04601400	7.07424100
C	1.15698700	-1.40426500	6.80009600
H	2.77627800	-1.30642300	5.40736500
H	-0.63270400	-1.35475500	8.02199000
H	1.71044400	-1.96906400	7.54464900
O	-1.06588600	0.74551200	4.05034600
O	-2.24759500	0.05265300	6.34890900
C	1.61567500	0.08983900	3.45101100
H	2.66156700	-0.17247700	3.28412100
N	1.01615900	0.76969100	2.47647700
C	-2.89565600	-0.31598500	7.55507100
H	-2.39207900	0.11994600	8.42926800
H	-3.90901300	0.08297100	7.48208600
H	-2.93871600	-1.40829700	7.66759200
C	1.66798500	1.22426600	1.26573800
H	2.69313000	0.83373900	1.25285600
H	1.73834000	2.32392800	1.27705100
C	0.91648500	0.77762100	0.00000000
C	1.74319400	-1.03868300	-5.62238300
C	1.00073200	-0.29309700	-4.64566600
C	-0.39063300	0.09094600	-4.88735600
C	-0.95573700	-0.33082000	-6.17334600
C	-0.20302400	-1.04601400	-7.07424100
C	1.15698700	-1.40426500	-6.80009600
H	2.77627800	-1.30642300	-5.40736500
H	-0.63270400	-1.35475500	-8.02199000
H	1.71044400	-1.96906400	-7.54464900
O	-1.06588600	0.74551200	-4.05034600
O	-2.24759500	0.05265300	-6.34890900
C	1.61567500	0.08983900	-3.45101100
H	2.66156700	-0.17247700	-3.28412100
N	1.01615900	0.76969100	-2.47647700
C	-2.89565600	-0.31598500	-7.55507100
H	-2.93871600	-1.40829700	-7.66759200
H	-3.90901300	0.08297100	-7.48208600
H	-2.39207900	0.11994600	-8.42926800
C	1.66798500	1.22426600	-1.26573800
H	1.73834000	2.32392800	-1.27705100
H	2.69313000	0.83373900	-1.25285600
H	0.82997200	-0.31409200	0.00000000

O	-0.42786100	1.23725800	0.00000000
H	-0.45202100	2.20964600	0.00000000
H	0.02337300	0.99048600	2.67779100
H	0.02337300	0.99048600	-2.67779100

Keto-enol

C	5.56533200	-1.75001200	0.96656900
C	4.62897900	-0.97929000	0.23962900
C	4.91608800	0.37223800	-0.06526400
C	6.14760200	0.93423000	0.36363800
C	7.05196300	0.15093800	1.07724800
C	6.76143900	-1.19272800	1.38028400
H	5.33037800	-2.78719200	1.19452300
H	7.99397500	0.57484600	1.40722800
H	7.48246300	-1.78249500	1.93856200
O	4.07174300	1.16038700	-0.74849600
O	6.33671900	2.23870800	0.02323300
C	3.38083300	-1.59247800	-0.18850000
H	3.23478500	-2.64528100	0.10246300
N	2.48521700	-0.96844400	-0.86867100
C	7.53958800	2.87417500	0.43036300
H	8.41942400	2.38563400	-0.00983400
H	7.47046500	3.89868200	0.06103300
H	7.63516400	2.88559800	1.52447000
C	1.27418200	-1.66414800	-1.25023700
H	1.24391800	-2.68848000	-0.83863000
H	1.26062400	-1.75527900	-2.34848700
C	0.01109200	-0.90426500	-0.80916200
C	-5.57138900	-1.71399800	1.13701800
C	-4.61776000	-0.99168900	0.34421500
C	-4.88432200	0.37821100	-0.09493900
C	-6.17182000	0.94284100	0.32439400
C	-7.05084800	0.20993100	1.08597800
C	-6.75197000	-1.12939800	1.49740800
H	-5.33718800	-2.73177100	1.44474200
H	-7.99953300	0.64005800	1.39147300
H	-7.47924700	-1.66859100	2.09750700
O	-4.06788700	1.03574600	-0.79119600
O	-6.37263000	2.21537900	-0.11076600
C	-3.42052200	-1.60913300	-0.03113100
H	-3.23874800	-2.64035900	0.27579700
N	-2.46285200	-1.03485100	-0.75218100
C	-7.58219600	2.86070500	0.24867800
H	-7.67927700	2.94959200	1.33987300
H	-7.53134200	3.85696600	-0.19461400
H	-8.45570300	2.32628700	-0.15073800
C	-1.25140700	-1.69803200	-1.19236200
H	-1.28025200	-1.82234500	-2.28606800
H	-1.22143700	-2.70015200	-0.74713400

H	0.03038200	-0.77227200	0.27853700
O	-0.05137200	0.41606500	-1.33061300
H	0.19109700	0.41241700	-2.27144600
H	-2.66923200	-0.05594900	-1.01929500
H	3.26095300	0.62427200	-0.96425800

Complex 1

C	2.29593100	-2.60401500	-2.00944800
C	3.33757800	-3.01267200	-2.88150800
H	3.11885600	-3.15585500	-3.93692000
C	4.60622300	-3.22671500	-2.38820400
H	5.40619000	-3.55366700	-3.04535700
C	4.87996400	-3.01510800	-1.01912500
H	5.88669300	-3.17867900	-0.64994300
C	3.88036400	-2.60417500	-0.14882500
C	2.55028600	-2.41787200	-0.63049200
C	1.01640300	-2.23799500	-2.55073400
H	0.95440500	-2.22024200	-3.64393200
C	-1.18078900	-1.37968600	-2.66083400
H	-2.07143200	-1.93884600	-2.37668600
H	-0.99352400	-1.52421900	-3.73321100
C	-1.47214100	0.10994900	-2.41020400
C	-0.32076900	1.08368600	-2.76320600
H	0.16895000	0.75068000	-3.68817000
H	-0.78492800	2.05002000	-2.96983200
C	1.93182700	1.06792800	-2.06396300
H	2.09523400	0.61616800	-3.04680100
C	3.13359800	1.29822100	-1.30977200
C	4.36776100	0.87607700	-1.85594200
H	4.37493700	0.41694700	-2.84120400
C	5.54433000	1.01681100	-1.14418900
H	6.48909400	0.69209400	-1.56774200
C	5.50210700	1.56619900	0.14944500
H	6.40404200	1.65827400	0.74808200
C	4.30506800	1.98609000	0.70690000
C	3.09025700	1.89675100	-0.02320900
C	4.03239600	3.79988100	2.23895900
H	3.03848400	4.08156300	1.88276400
H	4.79715900	4.40029100	1.73220500
H	4.10127000	3.95688900	3.31746600
C	-2.63464500	2.40199500	-0.08938100
C	-3.81950200	2.63416800	-0.83684800
C	-5.06790100	2.47311200	-0.25789700
H	-5.94361400	2.66552700	-0.87141400
C	-5.19812300	2.05197000	1.07744100
H	-6.18281100	1.93120400	1.51702000
C	-4.06016200	1.77254000	1.81017900
H	-4.14098500	1.40619300	2.83038300
C	-2.77454600	1.92864100	1.24188500

C	-1.62734400	1.55404100	2.02138700
H	-1.85996500	1.21656300	3.03574700
C	0.59778000	1.23502700	2.73454800
H	0.06279800	1.06944600	3.67944300
H	1.22422500	2.11958000	2.86613100
C	1.56011200	0.05122700	2.47034100
C	1.02047200	-1.33837800	2.85097900
H	1.80972100	-2.05543100	2.62511300
H	0.82063200	-1.35285900	3.93106200
C	-1.28689500	-1.83282700	2.80245600
H	-1.21193400	-1.74355300	3.89179800
C	-2.61542100	-2.01612100	2.28754000
C	-3.69954400	-2.20152400	3.18370100
H	-3.49547300	-2.31883100	4.24519800
C	-4.99094500	-2.23851800	2.70476200
H	-5.82560900	-2.39791900	3.38052700
C	-5.24287500	-2.06175600	1.32656500
H	-6.26683900	-2.08426000	0.96966300
C	-4.20047400	-1.86122600	0.43228000
C	-2.85271000	-1.86989900	0.90067100
C	-5.62581000	-1.54071900	-1.45455100
H	-5.47502600	-1.30169800	-2.50815700
H	-6.19505900	-0.73413000	-0.97335800
H	-6.18263800	-2.48303600	-1.36474700
C	5.34443400	-2.34090300	1.71864800
H	5.99252000	-1.64134300	1.17451900
H	5.79564700	-3.34224800	1.70358400
H	5.23079000	-2.00435200	2.75014200
C	-3.24748700	4.23692500	-2.51514700
H	-3.29563700	4.31090100	-3.60363000
H	-2.21760500	4.37328200	-2.17622200
H	-3.89455100	5.00077800	-2.06786000
N	-0.03870000	-1.87949600	-1.87976600
N	0.70388400	1.32692000	-1.71984600
N	-0.37525200	1.56672900	1.66666900
N	-0.19403300	-1.70691400	2.10732800
O	-1.87997700	-1.69460300	0.03497100
O	-4.32431200	-1.65099900	-0.90290000
O	1.61855000	-2.03484400	0.21193000
O	4.03375200	-2.34994400	1.17723200
O	1.97694600	2.31828100	0.52414100
O	4.28357900	2.39955800	2.02670500
O	-1.46787600	2.58266500	-0.65727600
O	-3.73380300	2.92391400	-2.18632800
H	1.83177600	0.02613400	1.41378600
H	-1.74347400	0.22600600	-1.35993200
O	2.70590800	0.21944000	3.29553500
H	3.22771500	0.96474700	2.93899000

O	-2.57143800	0.40109900	-3.26386400
H	-2.96055800	1.24921400	-2.97433100
Al	0.25731300	2.48167700	-0.06887500
Al	-0.17238700	-2.26655300	0.12143700
O	0.14358900	4.27192400	0.89343600
O	-0.25395200	-4.08412800	0.39774000
N	-1.01315700	-4.91056600	-0.35085700
O	-1.53810400	-4.44649800	-1.36400100
O	-1.10471200	-6.05896200	0.04086000
N	0.48290100	4.91921700	-0.17124800
O	0.59588800	6.11929600	-0.22213500
O	0.68772900	4.13305300	-1.17538300

Complex 2

C	-2.08921000	2.57751600	2.05799600
C	-2.41270300	3.69169500	2.85044800
H	-2.64083900	3.55595000	3.89020300
C	-2.44210500	4.93446000	2.29169500
H	-2.69902600	5.79132100	2.88029900
C	-2.13426900	5.09648500	0.93092600
H	-2.15646700	6.07898600	0.50830300
C	-1.81046900	4.02384700	0.15223300
C	-1.79920000	2.73325100	0.71313500
C	-1.96130900	1.26280300	2.65267000
H	-1.98155600	1.24672100	3.73291100
C	-1.46964100	-1.05280700	2.82996800
H	-2.12918100	-1.84802300	2.53081400
H	-1.59222200	-0.83657700	3.88622200
C	-0.05096700	-1.55052800	2.56328800
C	1.10567000	-0.58939300	2.88563100
H	0.93656400	-0.11576500	3.84724600
H	1.98891100	-1.19937200	2.96068800
C	1.42628000	1.68659900	2.30385700
H	1.20034500	1.84843700	3.34569300
C	1.70619500	2.89745300	1.57562800
C	1.70916700	4.12654400	2.24776100
H	1.54881200	4.14700600	3.30816300
C	1.90382800	5.28970900	1.55769900
H	1.90728100	6.23303100	2.06280200
C	2.08693500	5.23818300	0.17192800
H	2.22750800	6.14002600	-0.38861600
C	2.07741100	4.04845500	-0.49601800
C	1.90323700	2.84430500	0.20244800
C	3.56517000	3.69695800	-2.36610600
H	3.88900200	2.74583300	-1.97596500
H	4.25377800	4.47387900	-2.06446400
H	3.49125100	3.66551800	-3.44121500
C	1.83605900	-2.86846400	-0.17284400
C	1.98092500	-4.07637800	0.52581600

C	1.96318600	-5.26600900	-0.14213500
H	2.08176000	-6.17091000	0.41856600
C	1.78059600	-5.31322000	-1.52812800
H	1.76240400	-6.25636900	-2.03324000
C	1.61427200	-4.14579600	-2.21840900
H	1.45476600	-4.16248400	-3.27900500
C	1.63948500	-2.91696700	-1.54626200
C	1.38910200	-1.69985600	-2.27481400
H	1.16067600	-1.85633300	-3.31692500
C	1.12298900	0.58305800	-2.85694400
H	0.94392200	0.11353800	-3.81877000
H	2.02046700	1.17202600	-2.93092000
C	-0.01103800	1.57122100	-2.53599100
C	-1.44073700	1.10710800	-2.80440000
H	-2.08169200	1.91766900	-2.50603400
H	-1.56710300	0.89381600	-3.86080500
C	-1.98711900	-1.19625300	-2.62773200
H	-2.00566900	-1.17971400	-3.70799600
C	-2.14672600	-2.50757400	-2.03323200
C	-2.49545600	-3.61382200	-2.82609200
H	-2.71906400	-3.47274600	-3.86612100
C	-2.55485100	-4.85553900	-2.26739300
H	-2.83120300	-5.70610800	-2.85632000
C	-2.25257600	-5.02476300	-0.90625300
H	-2.29846200	-6.00646000	-0.48367200
C	-1.90450200	-3.96005200	-0.12715300
C	-1.86210400	-2.67008900	-0.68802200
C	-1.50333000	-5.23213900	1.93261900
H	-1.16579200	-4.93832700	2.91046200
H	-0.79574100	-5.91553700	1.47881300
H	-2.47245600	-5.71142300	1.99618200
C	-1.37689400	5.28608500	-1.90703200
H	-0.65392900	5.95260300	-1.45235800
H	-2.33436400	5.78810000	-1.97176500
H	-1.04519600	4.98437600	-2.88446900
C	3.47429300	-3.76005600	2.39771300
H	3.39983100	-3.72686500	3.47273300
H	3.82094900	-2.81684200	2.00797900
H	4.14474300	-4.55301200	2.09689600
N	-1.77772200	0.16388800	2.02859600
N	1.40654500	0.47969400	1.86828700
N	1.39732000	-0.49281500	-1.83925100
N	-1.77841100	-0.10196800	-2.00342000
O	-1.54628500	-1.64179900	0.07664400
O	-1.58086700	-3.99984000	1.19906600
O	-1.50680300	1.69778400	-0.05116200
O	-1.48437600	4.05596800	-1.17359100
O	1.89710000	1.69810000	-0.43860900

O	2.21855600	4.00701000	-1.87846700
O	1.85619100	-1.72242400	0.46822200
O	2.12133000	-4.03825600	1.90843600
H	0.04724900	1.88406500	-1.52675700
H	0.00114800	-1.86467500	1.55412100
O	0.19512500	2.68528000	-3.43535300
H	0.80757500	3.30084300	-2.99789900
O	0.12776100	-2.66912800	3.46288400
H	0.72604700	-3.29897600	3.02616400
Al	2.05573200	-0.01427500	0.01491500
Al	-2.07508100	0.03446500	0.01240800
O	3.96559900	-0.03681000	0.01607400
O	-3.98494700	0.05699900	0.01124900
C	7.31252700	-0.34067900	-1.20902500
C	8.02847400	-0.02953800	-0.05270200
C	7.35002900	0.26389100	1.13002100
C	5.95495000	0.24741800	1.15647500
C	5.23923400	-0.06319400	0.00027200
C	5.91805300	-0.35765300	-1.18248300
H	7.84762000	-0.57242800	-2.14128500
H	7.91428900	0.50853200	2.04164500
C	-5.35891400	0.01626900	-0.03081800
C	-6.05142500	-0.38974000	1.11026000
C	-7.44611300	-0.39697800	1.11411700
C	-8.14893700	0.00305600	-0.02308500
C	-7.45652600	0.40940600	-1.16369200
C	-6.06140800	0.41564900	-1.16771900
H	-7.99202500	-0.71758300	2.01327700
H	-8.01014600	0.72474300	-2.06009700
N	5.24017300	0.55680800	2.40318000
O	4.04108000	0.53435500	2.39373400
O	5.88465500	0.81932500	3.37997900
N	9.49810900	-0.01276900	-0.08085400
O	10.08482200	0.25843700	0.92941100
O	10.05172500	-0.27096400	-1.11296400
N	5.16348700	-0.68522400	-2.40077100
O	3.96544700	-0.69135500	-2.34524500
O	5.77604000	-0.93326500	-3.40160200
N	-9.61891000	-0.00461000	-0.01867800
O	-10.19403300	0.34477400	-1.01144400
O	-10.18438000	-0.35994400	0.97751000
N	-5.31067700	-0.81154600	2.30787000
O	-5.93460200	-1.15500600	3.27284200
O	-4.11198100	-0.79537600	2.27215600
N	-5.33196200	0.84370300	-2.37004200
O	-5.96495400	1.18119800	-3.33120600
O	-4.13297000	0.83834800	-2.34179000