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

Supplementary Materials

Ultrasensitive fluorescent detection of nitroexplosives by dihydro-oxoisobenzofuranyl-phthalazinone engendered from Cd(II) catalyzed cyclization of azinodimethylidyne-benzoic acid

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1. Experimental

1.1. Reagents: To perform the experiment work we used analytical grade solvents were first dried and then distilled by usual procedures prior to use.[1] Solvents like distilled water, absolute ethanol, diethyl ether, dichloromethane were obtained from HiMedia Chemicals Ltd. The reagents, 2- carboxybenzaldehyde and hydrazine monohydrate were procured from Sigma Aldrich Pvt. Ltd. Metal nitrates like $NaNO_3$, $Ca(NO_3)_2{\cdot}4H_2O$, KNO_3, $Mg(NO_3)_2{\cdot}6H_2O$, $Mn(NO_3)_2{\cdot}4H_2O$, $Fe(NO_3)_2.9H_2O$, $Co(NO_3)_2{\cdot}6H_2O$, $Cu(NO_3)_2{\cdot}3H_2O$, $Ni(NO_3)_2{\cdot}6H_2O$, $Cd(NO_3)_2{\cdot}4H_2O$, $Zn(NO_3)_2{\cdot}6H_2O$, $AgNO_3$, $Pb(NO_3)_2$, $Hg(NO_3)_2.H_2O$, $Gd(NO_3)_3{\cdot}xH_2O$, $Dy(NO_3)_2{\cdot}xH_2O$, $La(NO_3)_2{\cdot}xH_2O$ and $Yb(ac)_3{\cdot}xH_2O$ were used as a source of metal ions which were also obtained from Sigma Aldrich. p-nitrophenol(**1**) *o*-nitrophenol(**2**), *m*-nitrophenol(**3**), 3-Methoxyphenol(**4**), 2-Isopropylphenol(**5**), 2,4,6-Trinitrophenol(**6**), 2,4-Dibromophenol(**7**), 3-Chlorophenol (**8**), 2,4,6-Trichlorophenol(**9**), 2,4-Dichlorophenol(**10**), Quinol(**11**), Phenol(**12**), Resorcinol(**13**), 4-Chloroaniline (**14**), Tertbutylaniline(**15**), 2-Chloroaniline(**16**), 2,4 - Difluoroaniline(**17**) and Aniline(**18**) were used as a source of NAC's amd analytes ions which were procured from Alfa Aesar.

1.2. General methods. The elemental analysis of **1** was acquired on Exeter Analytical Inc. model CE-440 CHN analyzer. FT-IR spectral analysis was obtained from Shimadzu FT-IR spectrometer using KBr pallets (4000–400 cm^{-1}) and electronic absorption spectra were procured from Systronics double beam UV-Vis Spectrophotometer: 2201. ^1H (500 MHz) and ^{13}C (500 MHz) were obtained from Bruker and Jeol delta-2 spectrometers, respectively using DMSOd_6 as a solvent and tertamethylsilane (TMS) as an internal reference material. In NMR the chemical shift values are mentioned in parts per million (ppm). Fluorescence spectra were recorded on Fluorescence spectrophotometer RF-5301.

1.3. Materials and Equipment Melting point was uncorrected. The NMR spectra were performed on a Bruker 400 MHz or 600 MHz spectrometer. The chemical shifts (δ) in 1H NMR were reported relative to tetramethylsilane (Me_4Si) as internal standard (δ 0.0) or proton resonance resulting from incomplete deuteration of NMR solvent: $CDCl_3$ (δ 7.26) or DMSO-d_6 (δ 2.50). Coupling constants (J) are expressed in hertz. 13C NMR spectra were recorded at 100 MHz or 125 MHz, and the chemical shifts (δ) were reported relative to $CDCl_3$ (δ 77.10) or DMSO-d6 (δ40.50). Elemental analysis of carbon, nitrogen and hydrogen was performed using an Elementary Vario EL analyzer. UV-vis spectra were recorded using a SHIMAD2U UV-2550 spectrometer. Emission spectra were recorded using a Hitachi F-4600 fluorescence spectrophotometer. All solvents were purchased from Sinopharm and used without further purification unless otherwise denoted. Tetrahydrofuran, ethanol, and acetonitrile were further dried over calcium hydride, and distilled under high vacuum just before use. All chemicals were purchased from Aladdin, Aldrich, Alfa Aesar and Sinopharm, and were used as received

1.4. **UV−vis and fluorescence Studies.** To perform the absorption and emission spectral studies 10 μM stock solution of **1** was prepared in DMF/H_2O (6: 4, v/v) media. Solutions of metal ions namely Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}, Fe^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Hg^{2+}, Ag^+ and Pb^{2+} and NAC's p-nitrophenol(**1**) *o*-nitrophenol(**2**), *m*-nitrophenol(**3**), 3-Methoxyphenol(**4**), 2-Isopropylphenol(**5**), 2,4,6-Trinitrophenol(**6**), 2,4-Dibromophenol(**7**), 3-Chlorophenol (**8**), 2,4,6-Trichlorophenol(**9**), 2,4-Dichlorophenol(**10**), Quinol(**11**), Phenol(**12**), Resorcinol(**13**), 4-Chloroaniline (**14**), Tertbutylaniline(**15**), 2-Chloroaniline(**16**), 2,4 - Difluoroaniline(**17**) and Aniline(**18**) of concentration 100 μM (for individual addition) and 10 μM (for titration experiments) were prepared from their nitrate salts in double distilled water and their stock solution used as a source of metal ions. A 2.5 mL solution of **1** was taken in a quartz cell with 1 cm optical path length. The fluorescence experiments at rt were recorded with excitation (λ_{ex}) of 1 at 480 nm. In a typical titration, metal ions in fixed fractions were gradually added with the help of micropipette to a solution of 1 followed by thorough mixing.

1.5. **UV-vis titration in organic media** The UV-vis titrations of ligand L with o-NP and PA in organic solvents were carried out by placing 2 mL DMF solution of ligand (1.0×10^{-5} mol•L^{-1}) in a quartz cuvette of 1 cm width. At 25 °C, the dilute solution of o-NP and PA in methanol (1.0×10^{-5} mol•L^{-1}) was added in an incremental fashion. The absorption of additives was deducted through adding the solution of additives into the cuvettes of sample solution and background solvent simultaneously before measurement.

1.6. **Photoluminescence measurements** For fluorescence measurements, **1** were excited at their λ_{max} of UV absorption and their emissions were monitored within the suitable region while keeping 5.0 nm slit width for both source and detector at 400 V voltage.

1.7. **Fluorescence quenching titration with NACs in aqueous media** The fluorescence quenching titrations with different NACs in aqueous media were carried out by placing 2 mL aqueous solution of probe (2) in a quartz cuvette of 1 cm width. Then, the aqueous or methanol solution of several NACs was added in an incremental fashion at 25 °C. Probe (2) was excited at their λ_{max} of UV absorption and their emissions were monitored within the suitable region while keeping 10.0 nm slit width for both source and detector and voltage as 700 V. The fluorescence quenching efficiency (η) for each of NACs was calculated by the following equation:

$$\eta = (F0 - F)/F0 \times 100\%$$

F0 and F are the fluorescence intensities in the absence and presence of NACs, respectively.

1.8. **Calculation of the Stern-Volmer constant** The sensitivity of two polymers toward PA was estimated from the Stern-Volmer constant (KSV). The Stern-Volmer plots were plotted as a function of the PA concentration ([C]) in the following equation:

$$F0/F - 1 = K_{sv} \times [C]$$

Thus, K_{sv} can be calculated from the slope of the linear Stern-Volmer plot obtained at low concentration range of o-NP and PA.

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1.9. Quantum yield measurement

Fluorescence quantum yields (Φ_F) were determined by steady state comparative method using following Equation:

$$\phi_s = \phi_1 \frac{F_S A_1}{F_1 A_S} \left(\frac{n_1}{n_s} \right)^2$$

F_1 and F_S are the areas under the fluorescence curves of the Probe **1** and the reference, respectively. A_1 and A_S are the absorbance of the sample and reference at the excitation wavelength, and n_1 and n_S are the refractive indices of solvents used for the sample and standard, respectively.[2-6]

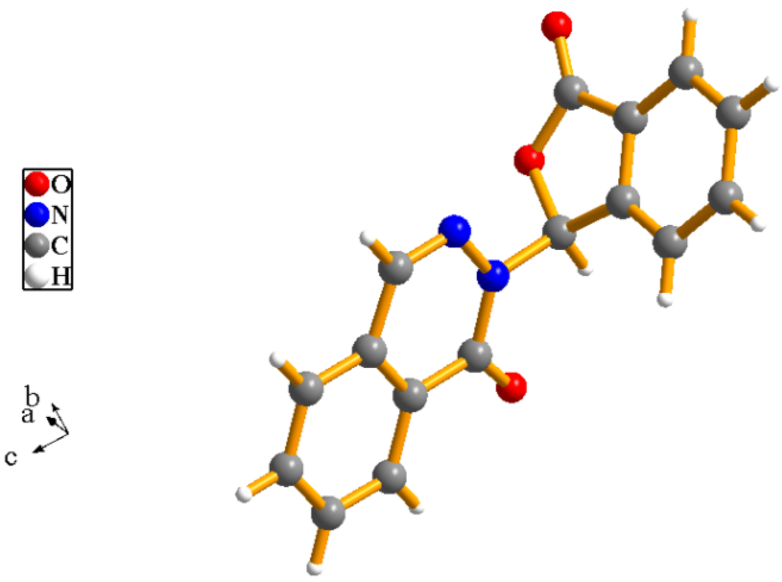
Reference used fluorescein standard yield (Φ_F = 0.79).[7]

Refractive Index of mixed DMF + water (6:4, v/v) = 1.455.

2. Table and Figs

Table S1 Crystal Data and Structure Refinements for **1**

Empirical Formula	$C_{16}H_{10}N_2O_3$
Formula weight	278.26
Crystal system	Triclinic
Space group	P_1
Shape and Color	Block like, colorless
a (Å)	7.222 (3) Å
b (Å)	8.023 (3) Å
c (Å)	11.178 (4) Å
α (°)	80.103 (11)°
β(°)	86.160 (11)°
γ(°)	88.646 (13)°
V (Å^3)	636.5 (4) Å^3
Z	2
Radiation type	Mo Kα
D_{calc}(Mg m^{-3})	1.452 Mg m^{-3}
Mo *Kα* radiation, λ	0.71073 Å
μ(mm^{-1})	0.10 mm^{-1}
F(000)	288
θ	1.9–25.0°
θ_{min}, θ_{max} (°)	25.0°, 1.9°
$h_{min–max}$	−8 8
$k_{min–max}$	−9 9
$l_{min–max}$	−13 13
Dimension	0.36 × 0.28 × 0.22 mm
T	296 K
No. of measured, independent and observed [I > 2σ(I)] reflections	10286, 2236, 1828
T_{min}, T_{max}	0.698, 0.746
(sin θ/λ)max (Å^{-1})	0.595
Data / restraints / parameters	2236/0/190
wR2[I > 2σ (I)]	1828
***R_{int}*,**	0.031
CCDC	
***R*[*F*^{2} > 2σ(*F*^{2})]**	0.040
***wR*(*F*^{2})**	0.142
S	1.11
$(\Delta/\sigma)_{max}$	< 0.001
Δρmax, Δρmin (e Å^{-3})	0.18 e Å^{-3},−0.20 e Å^{-3}
GOF on F^2	1.114



$w = 1/[\sigma^2(F_o^2) + (0.0919P)^2 + 0.0297P]$; where $P = (F_o^2 + 2F_c^2)/3$

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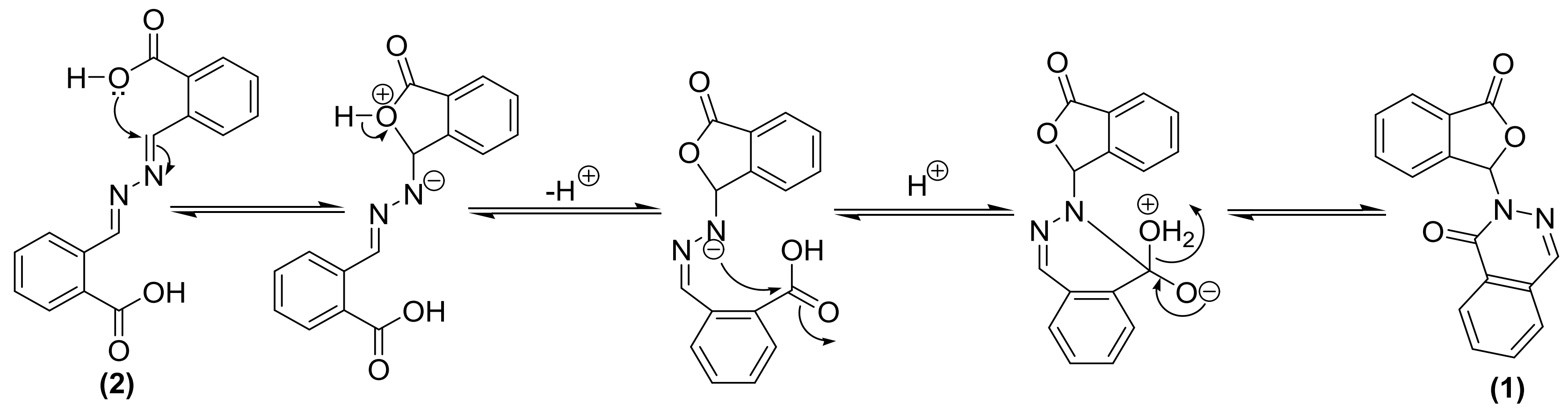
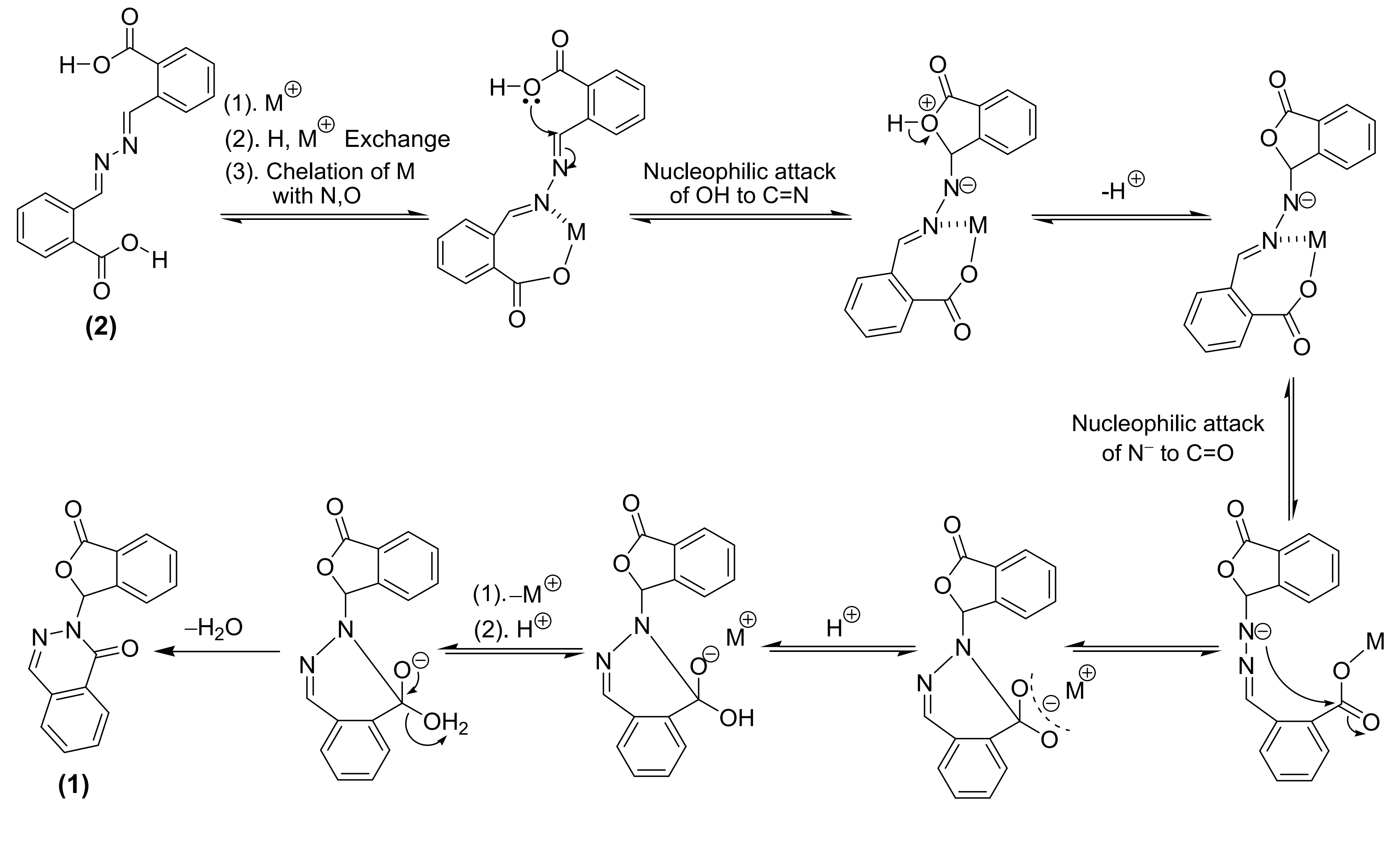
Table S2 Hydrogen-bond geometry (Å,º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O3^{i}	0.93	2.41	3.2935 (19)	158
C4—H4···O1^{ii}	0.93	2.54	3.215 (2)	130

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, *y*−1, *z*.



(a)



(b)

Scheme S1. Proposed Mechanism for (a) Self-cyclization route and (b) metal-catalyzed cyclization, for the formation of **1** from that of **2**.

Crystal structure and weak bonding interaction study

In this work, we chose 2-carboxybenzaldehyde and hydrazine monohydrate as reagents to form **2,2′-(Azinodimethylidyne) bis-benzoic Acid** and Resulting ligand was treated with different metals to form CPs/MOFs due to having carboxylate groups are present in the linker but unexpected heterocyclic product was formed namely **2-(1,3-dihydro-1-oxoisobenzofuran-3-yl)phthalazin-1(2H)-one**. (Özbey et al., 1998). The title compound's molecular structure is depicted in Fig. 1. The C9—C10—C11— N1 and N2—C14—C15—C16 torsion angles are -175.9 (2) and 178.0 (2) degrees, respectively, in the phthalazine system. The C8—C6—C5 O2 torsion angle of the pththalide ring structure is -176.68 (2)°, making this one almost planar. The length of the N1—C8 bond 1.448 (2) shows single bond character, and the associated bond angles reveal that the C8 atom is sp^3 (chiral centre). The phthalazine ring's C16—N2 bond length 1.288 (2) has double bond character and is shorter than that of a homologous compound's azomethine group. The dihedral angle formed by the phthalide and phthalazine ring systems is 87.2 (3) degrees are almost perpendicular to each other. The molecules are linked in the crystal structure by weak C—H---O hydrogen bonding interactions, which create layers parallel to the ab plane. The computed hydrogen bond lengths were 2.41 and 2.54, respectively (Table1, Fig. 2). Furthermore as a non-covalent interaction, hydrogen bonding is very significant in supramolecular chemistry and physics. The application of hydrogen bonding among heterocycle compounds and solvent molecules comprising O or N donors to produce supermolecules has been proven. According to one study, the interaction of 2,6-diacetylpyridine with 1,2-phenylenediamine can lead to formation of benzimidazole group via oxidative dehydrogenation. In anhydrous absolute ethanol, a benzimidazole derivative was also obtained from the reaction of 5-bromo-2-hydroxybenzaldehyde and 1,2-phenylenediamine. In this study, we used 2-carboxybenzaldehyde and hydrazinehydrate as reagents to produce a new product 2,2′−(azinodimethylidyne)bis-benzoic Acid for complex formation with different metals, however various dissimilar metals surprisingly generated a new heterocyclic compound 2−(1,3−dihydro−1−oxoisobenzofuran−3−yl)phthalazin−1(2H)−one at various time intervals, as a result of this effort. The compound was established as a result of this. Which is essential for the detection of 2-Nitrophenol and Picric acid selectively.

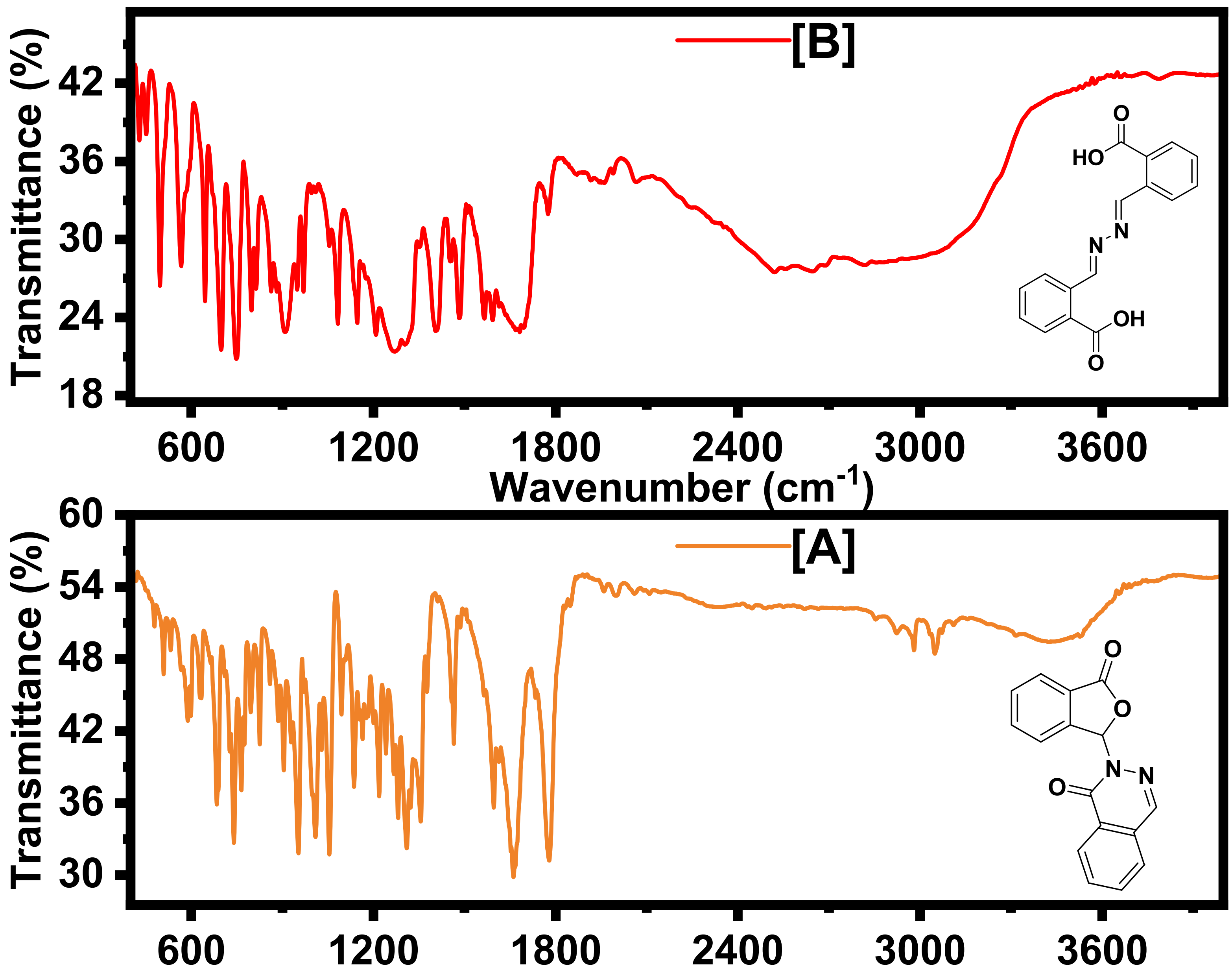


Fig. S1 FTIR Spectra of (B) ADMBA and (A) **1**

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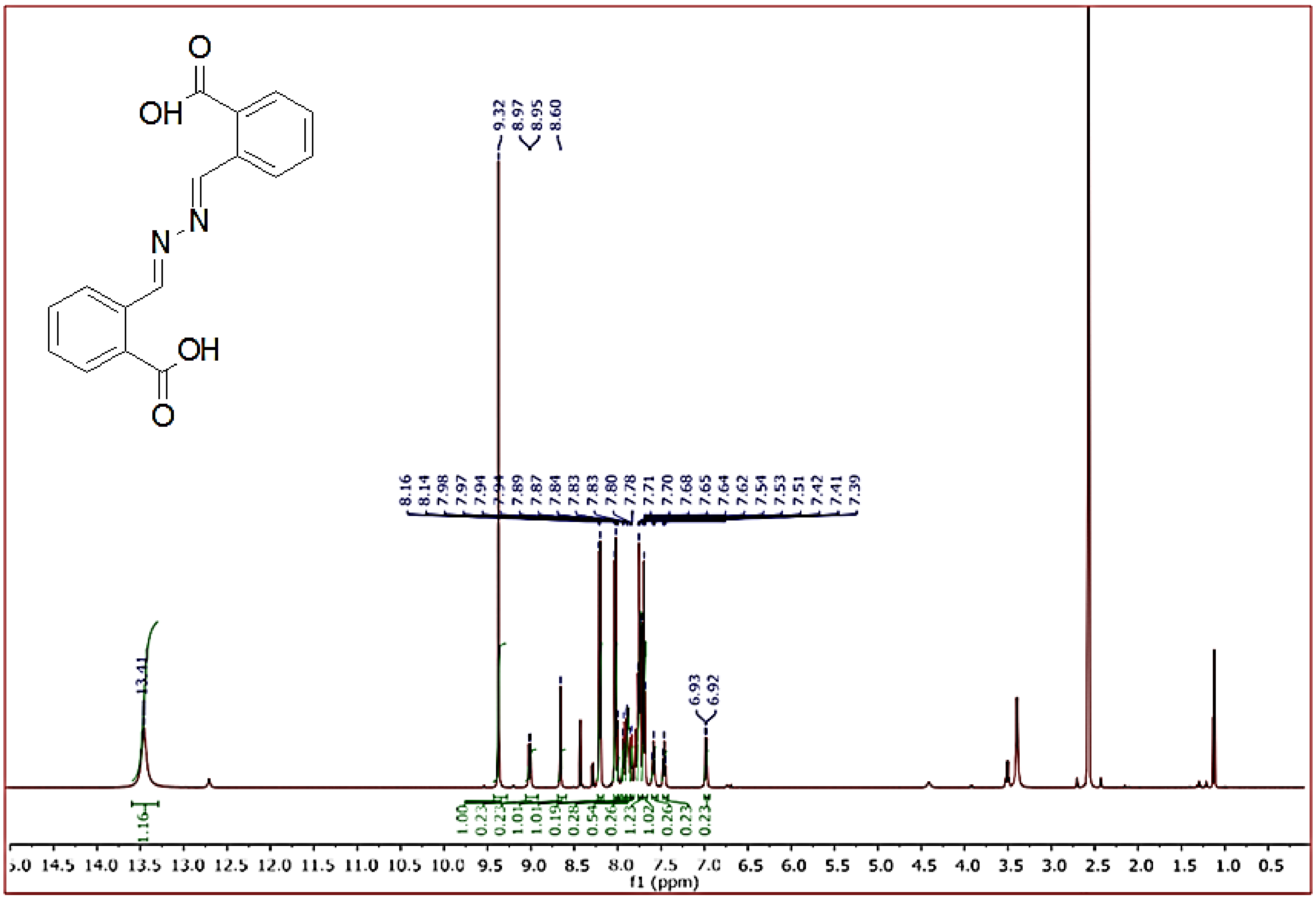

Fig. S2 ^{1}H NMR Spectra of ADMBA

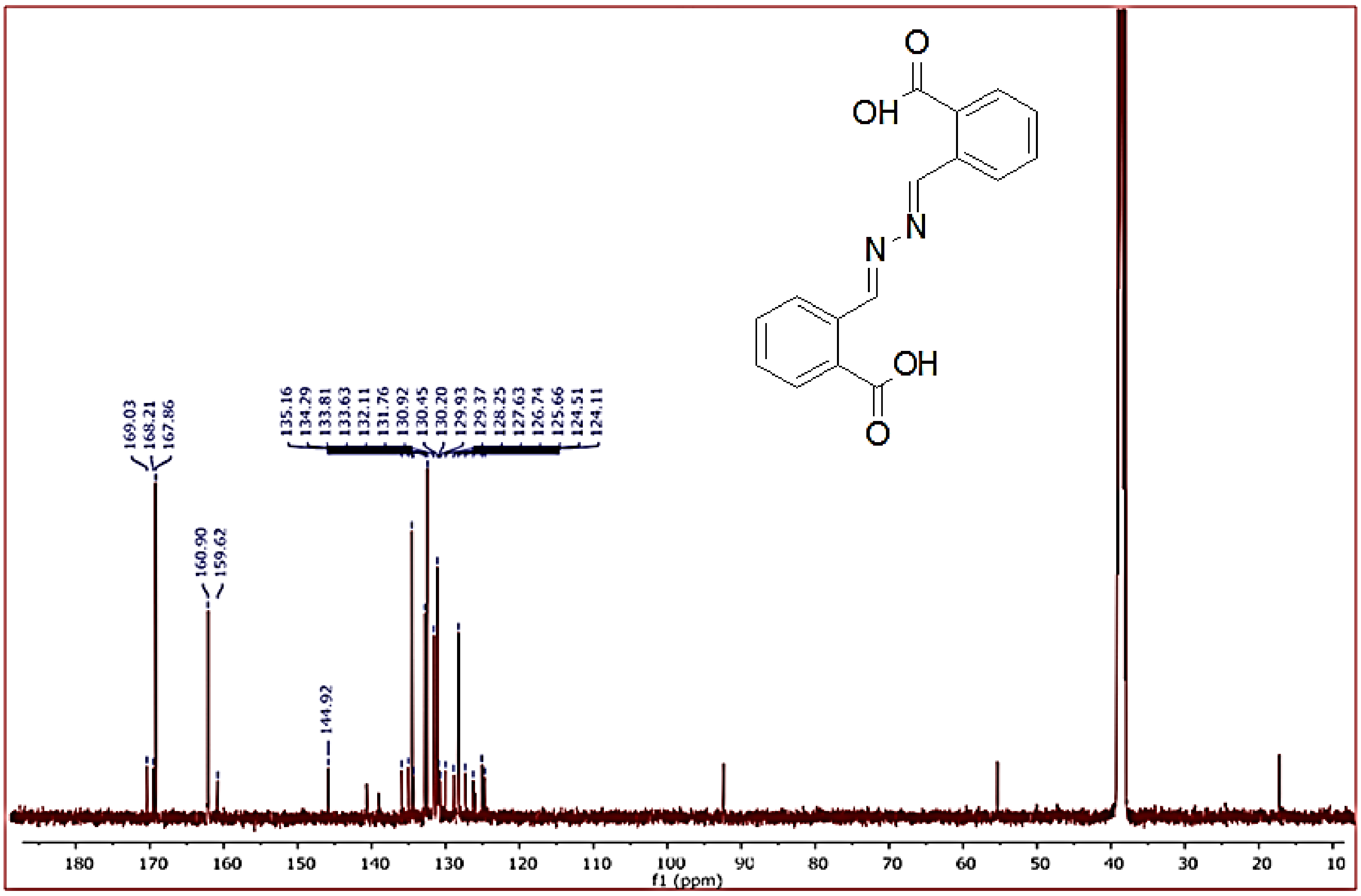

Fig. S3 ^{13}C NMR Spectra of ADMBA

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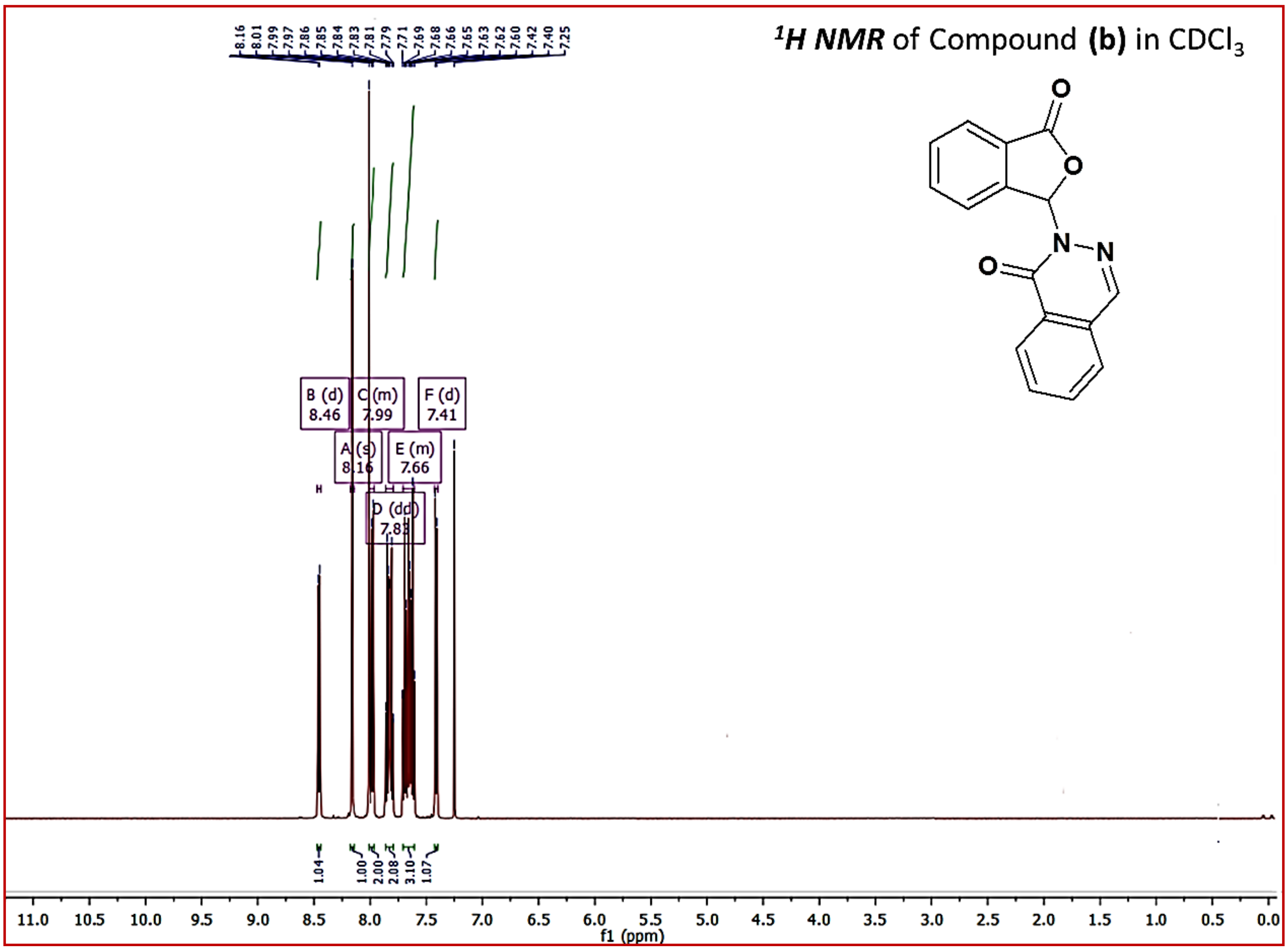

Fig. S4 ^{1}H NMR Spectra of **1**

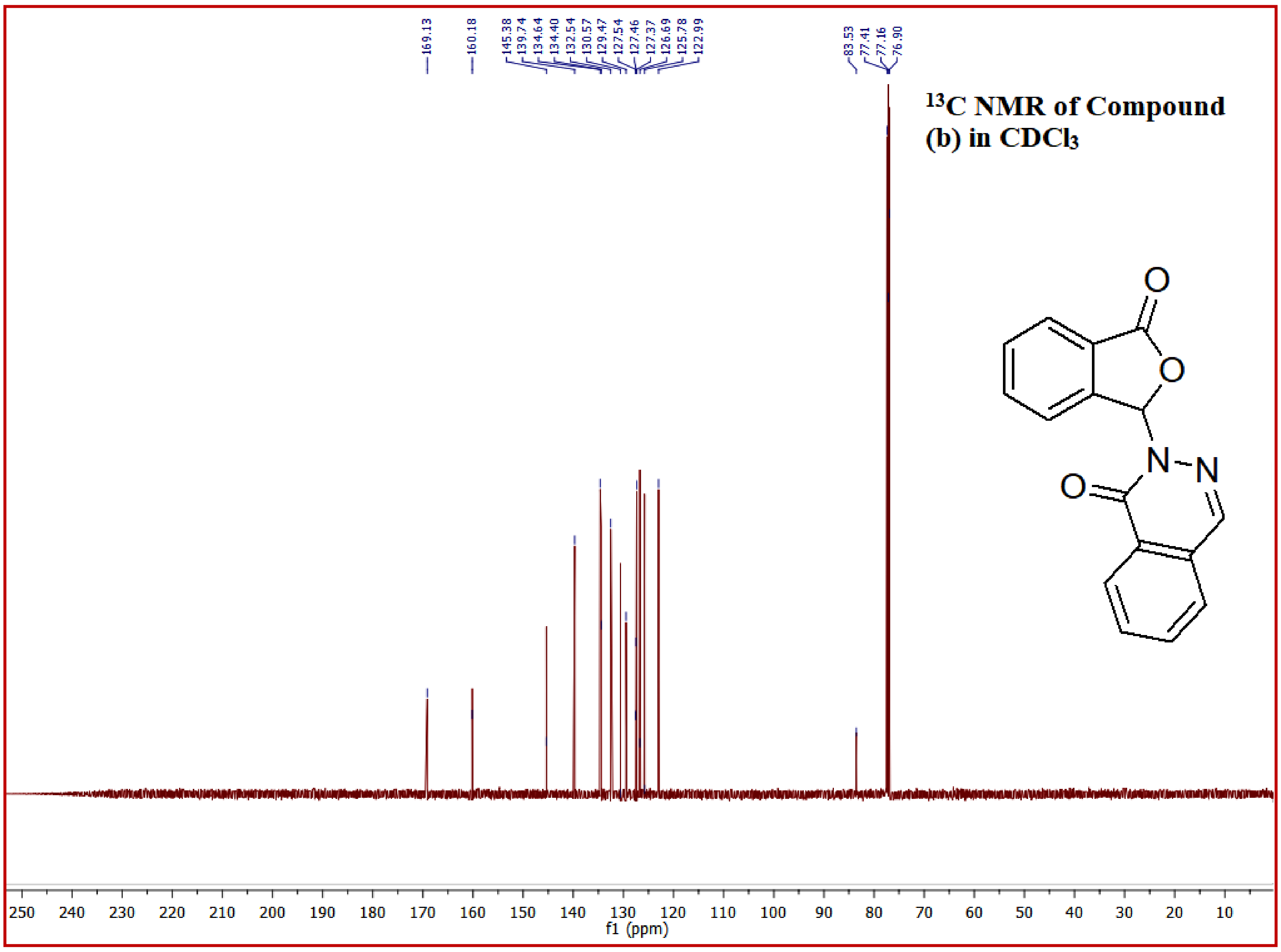

Fig. S5 ^{13}C NMR Spectra of **1**

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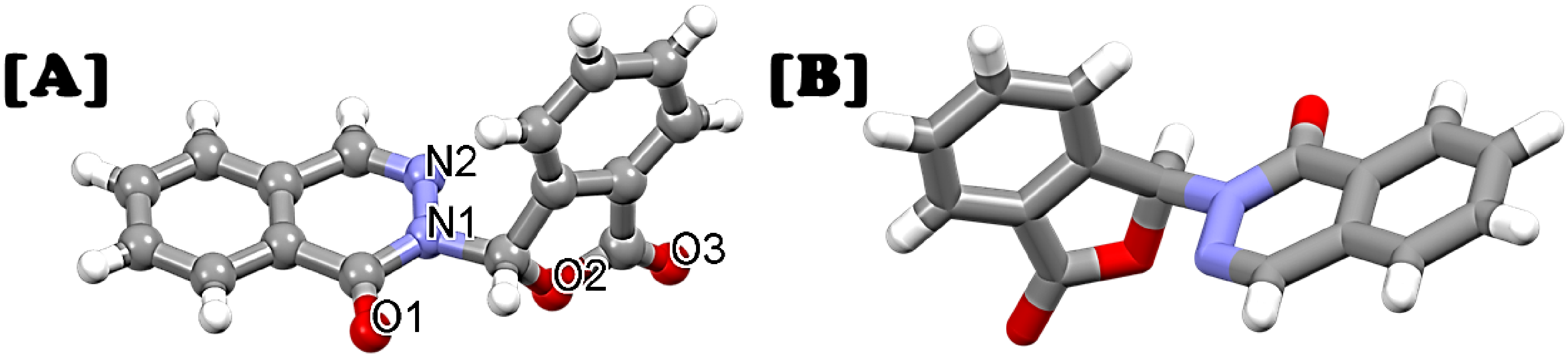

Fig. S6. Asymmetric unit of **1**

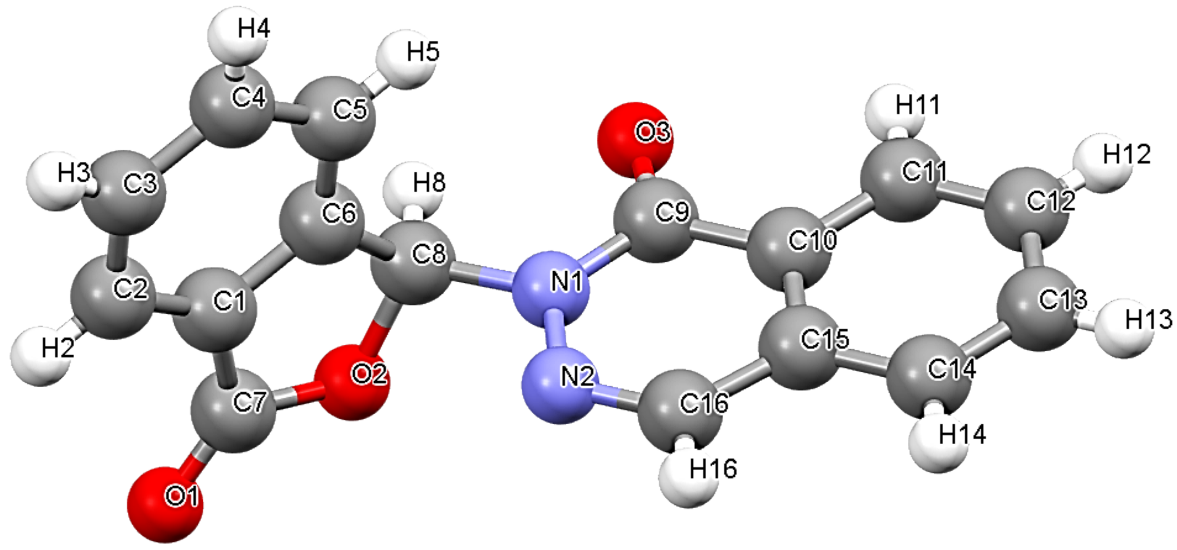

Fig. S7 The molecular structure exhibiting the atom-numbering scheme.

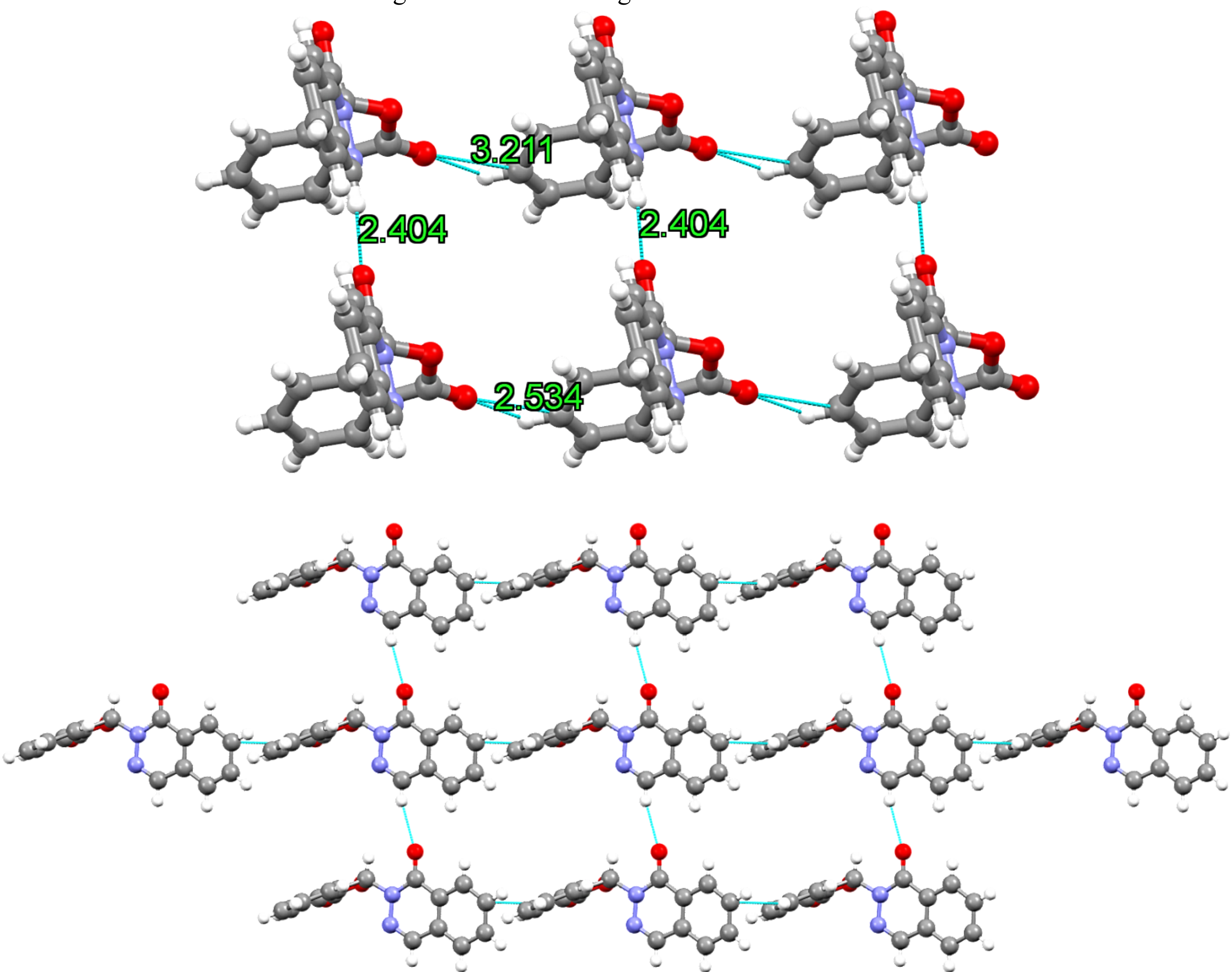

Fig. S8 Supramolecular network view of the title structure. Intermolecular hydrogen bonds are shown as green dotted dashed lines.

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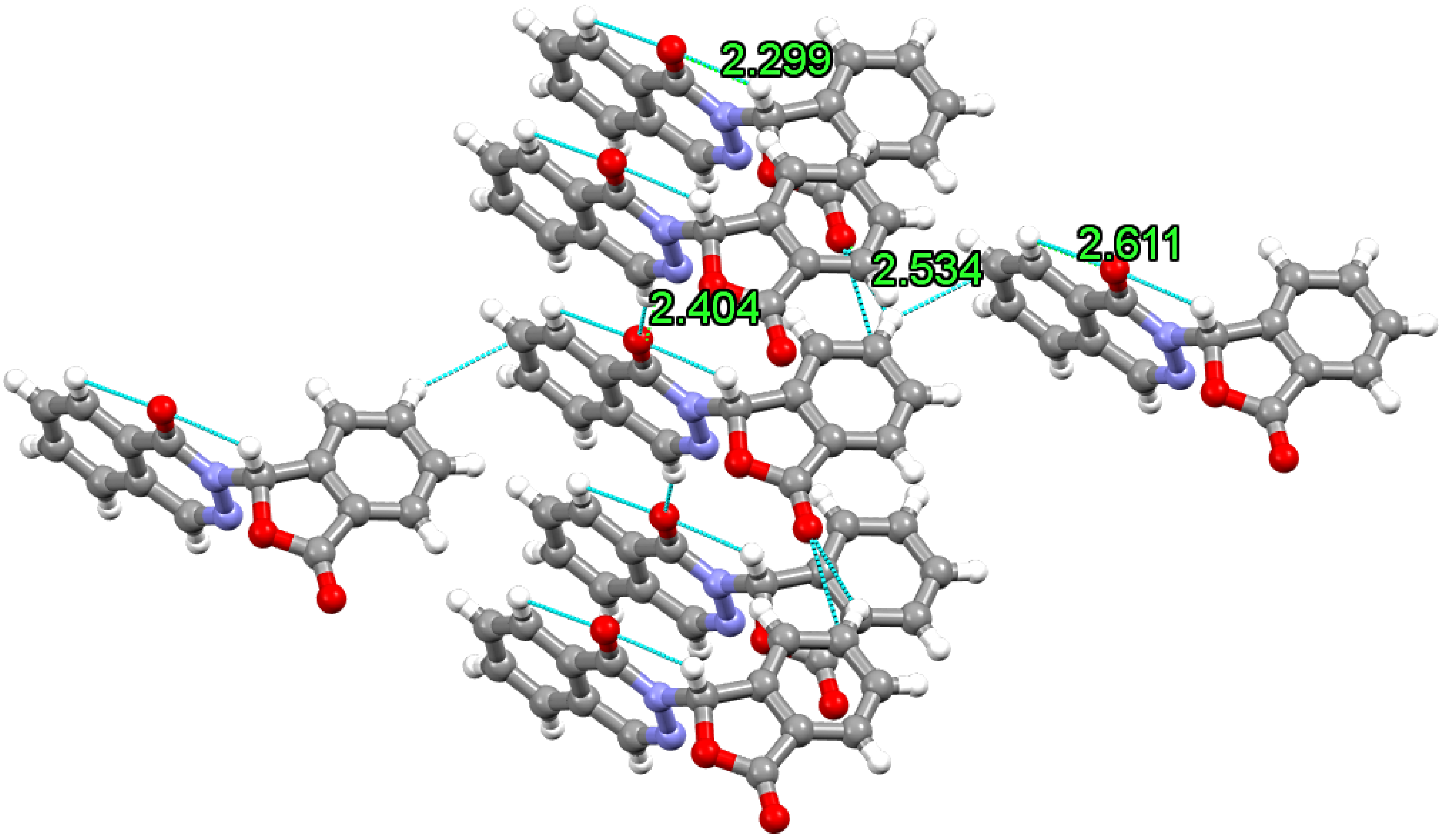

Fig. S9 H−−−O–H hydrogen bonding interactions of the title structure. Intramolecular and intermolecular hydrogen bonds are shown as green dotted dashed lines.

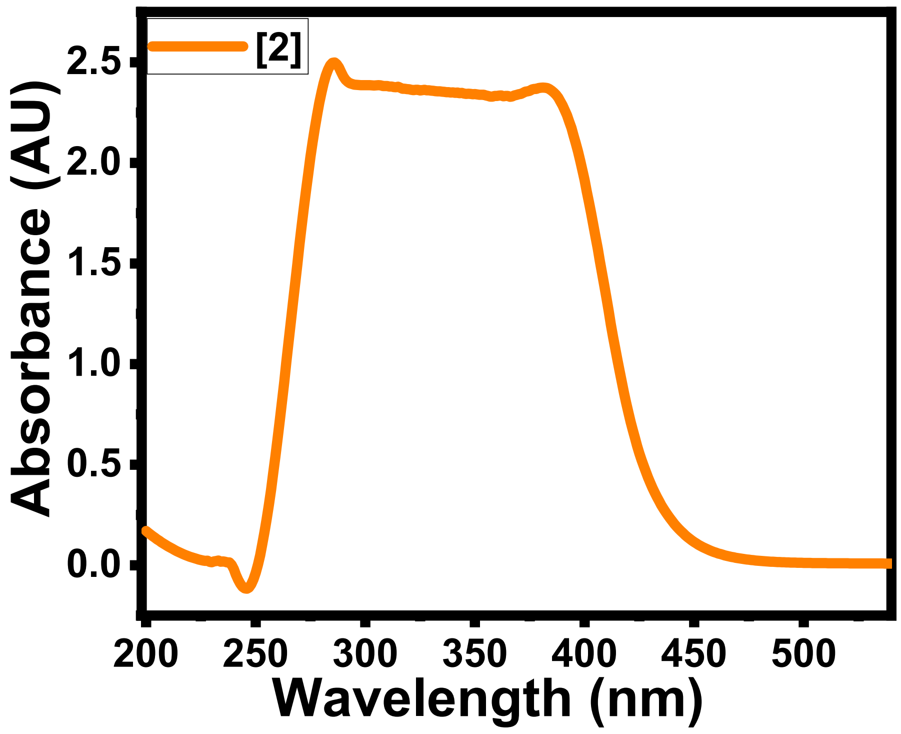

Fig. S10: UV/vis Spectra of the **2**

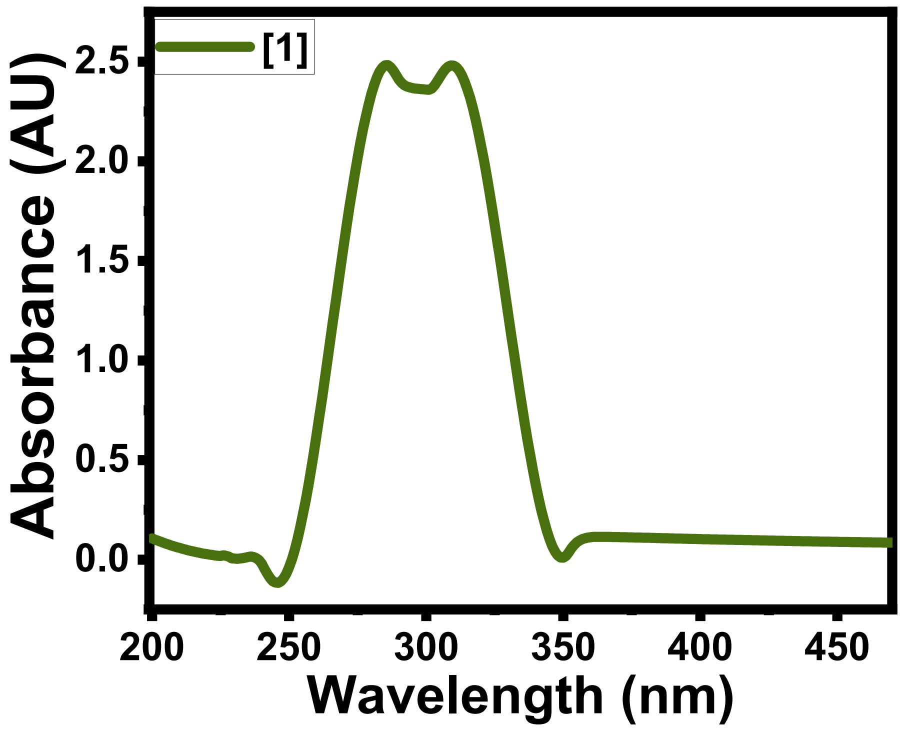

Fig. S11: UV/vis Spectra of the **1**

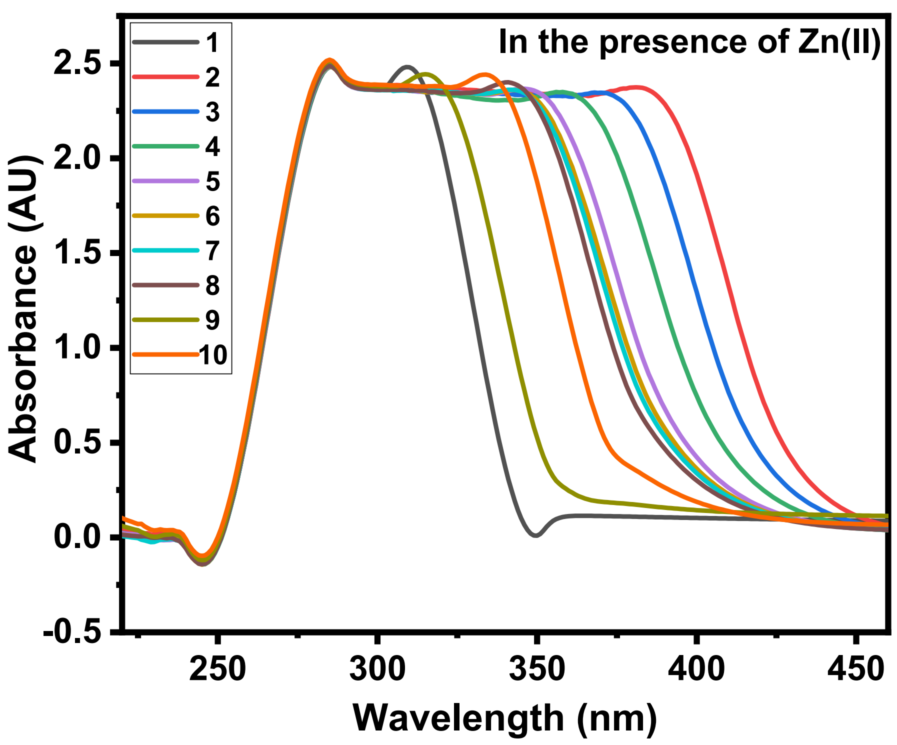

Fig. S12: Reaction Kinetics in the presence of Zn(II) ions in time interval ~ 13 min conversion time required is 1.5 h.

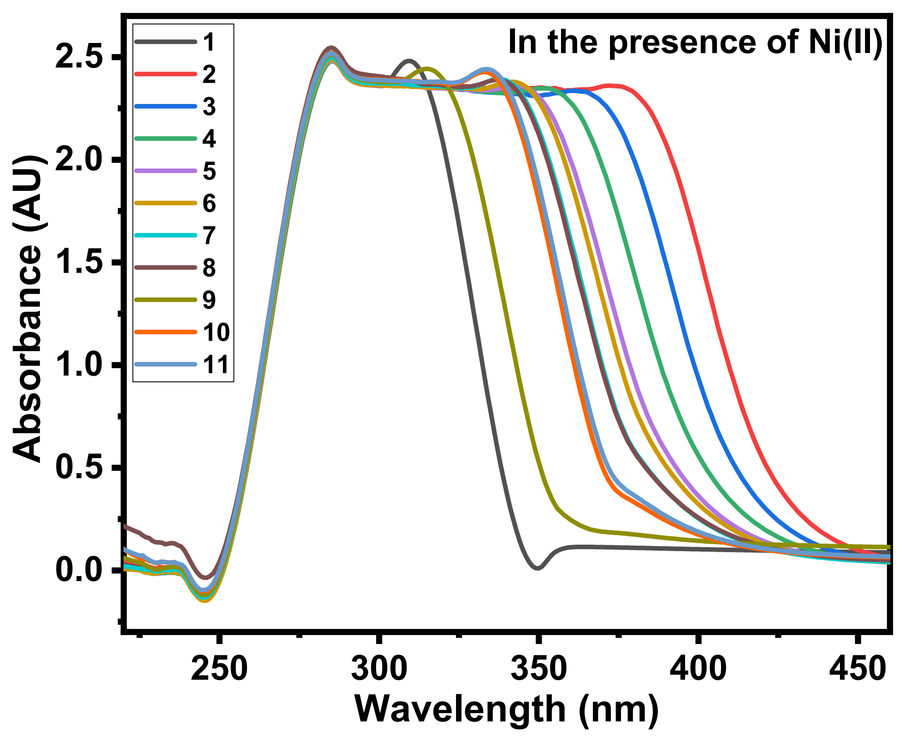

Fig. S13: Reaction Kinetics in the presence of Ni(II) ions in time interval ~ 21 min conversion time required is 2.5 h.

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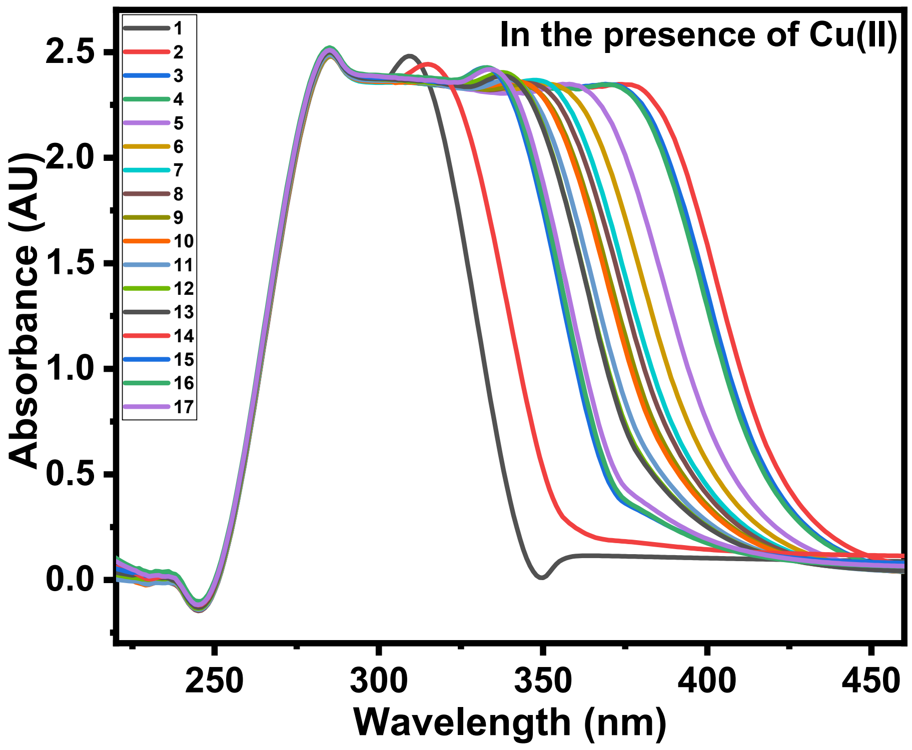

Fig. S14: Reaction Kinetics in the presence of Cu(II) ions in time interval ~ 34 min conversion time required is 4.0 h.

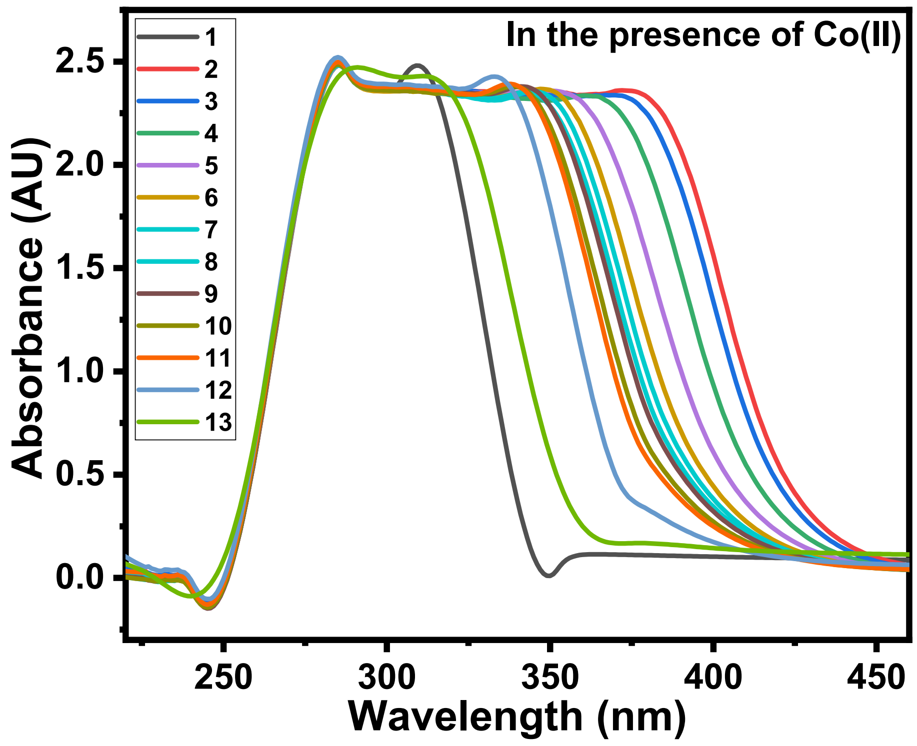

Fig. S15: Reaction Kinetics in the presence of Co(II) ions in time interval ~ 26 min conversion time required is 3.0 h.

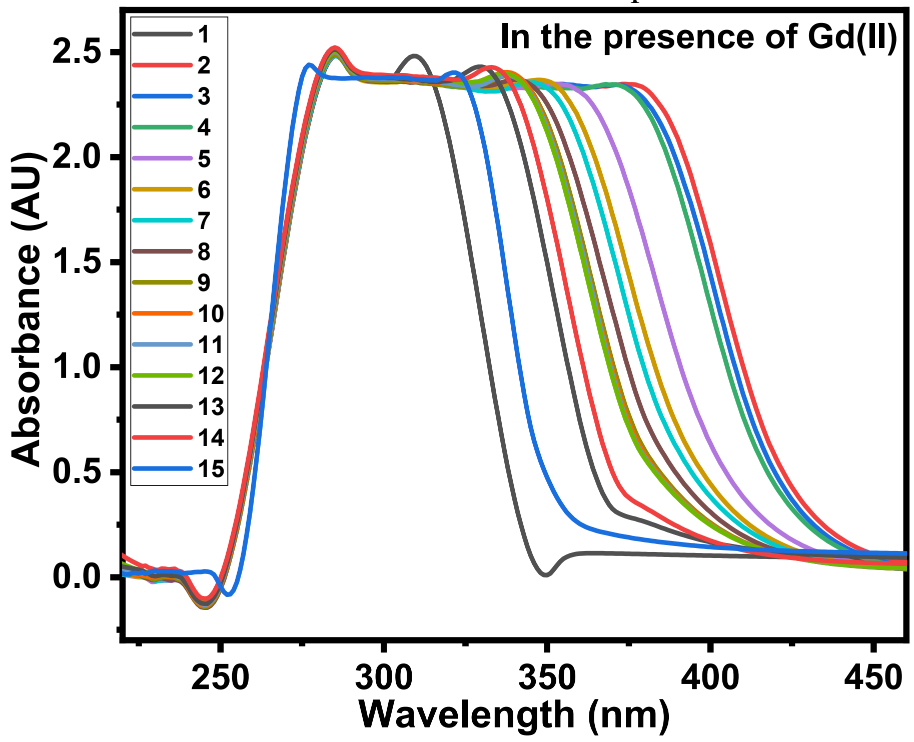

Fig. S16: Reaction Kinetics in the presence of Gd(II) ions in time interval ~ 39 min conversion time required is 4.5 h.

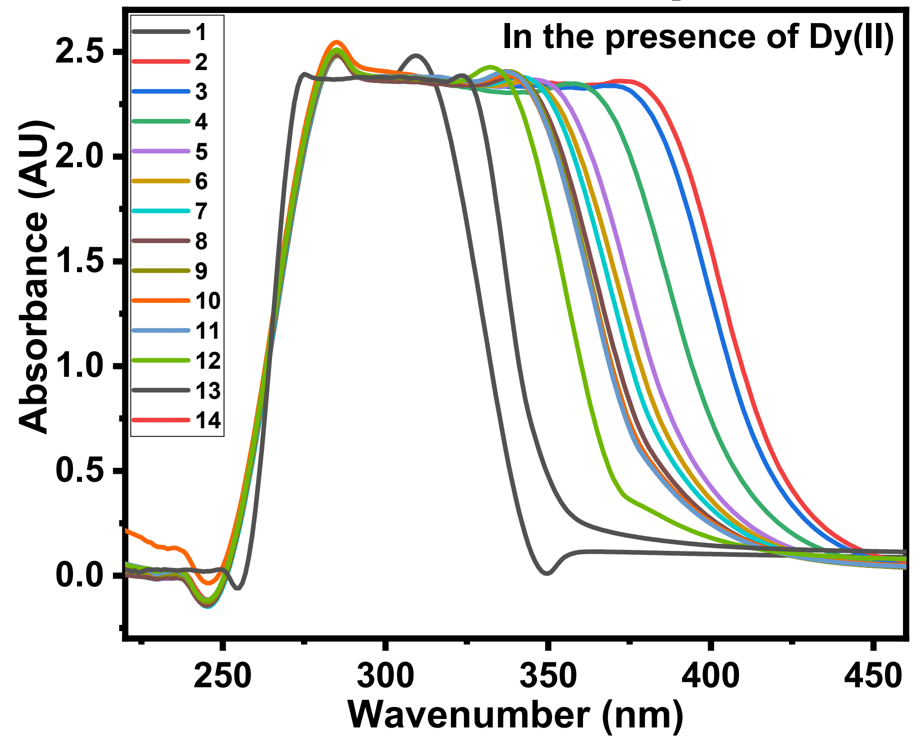

Fig. S17: Reaction Kinetics in the presence of Dy(II) ions in time interval ~ 34 min conversion time required is 4.0 h.

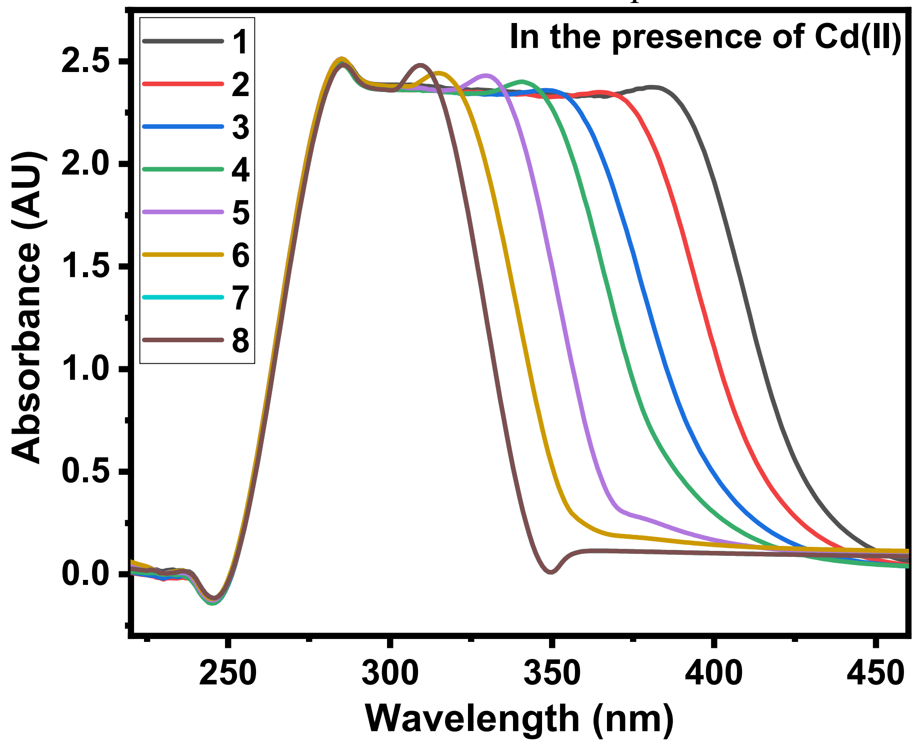

Fig. S18: Reaction Kinetics in the presence of Cd(II) ions in time interval ~ 4 min conversion time required is 0.5 h.

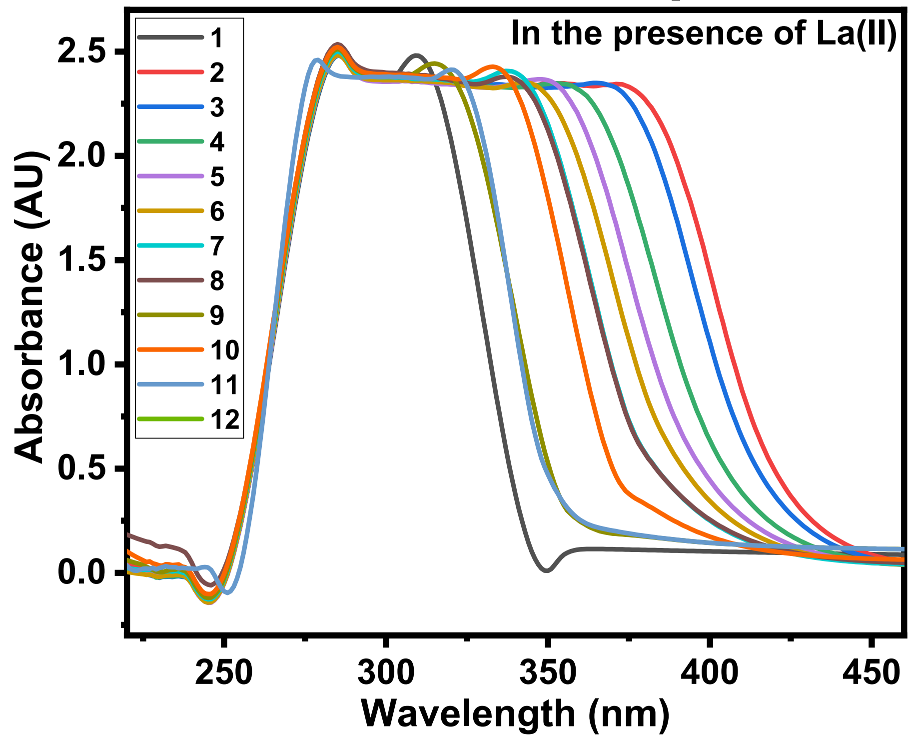

Fig. S19: Reaction Kinetics in the presence of La(II) ions in time interval ~ 34 min conversion time required is 4.0 h.

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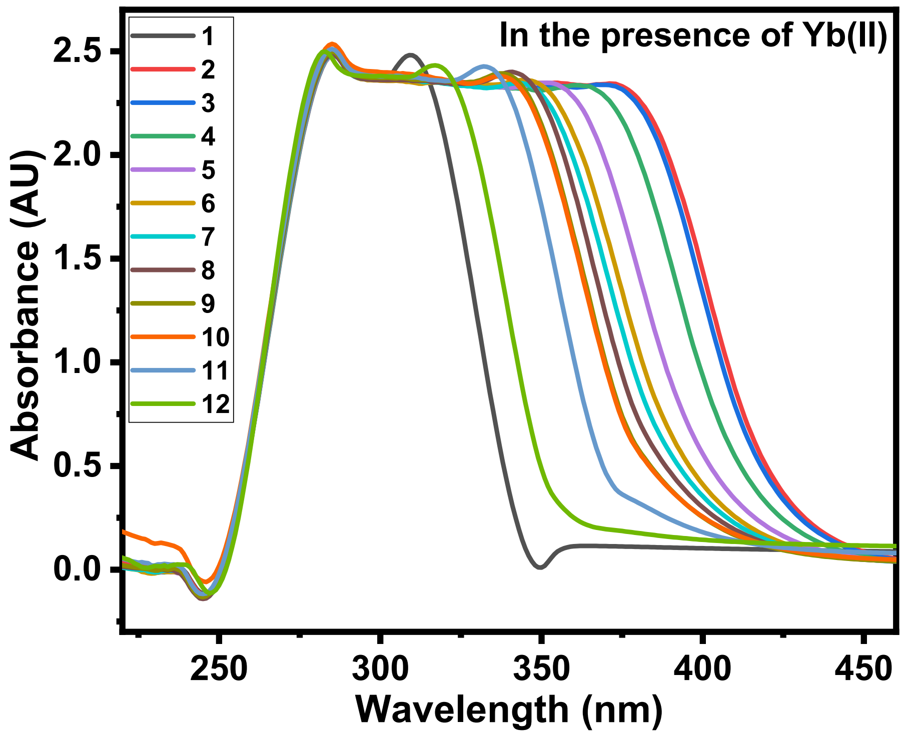

Fig. S20: Reaction Kinetics in the presence of Yb(II) ions in time interval~ 43 min conversion time required is 5.0 h.

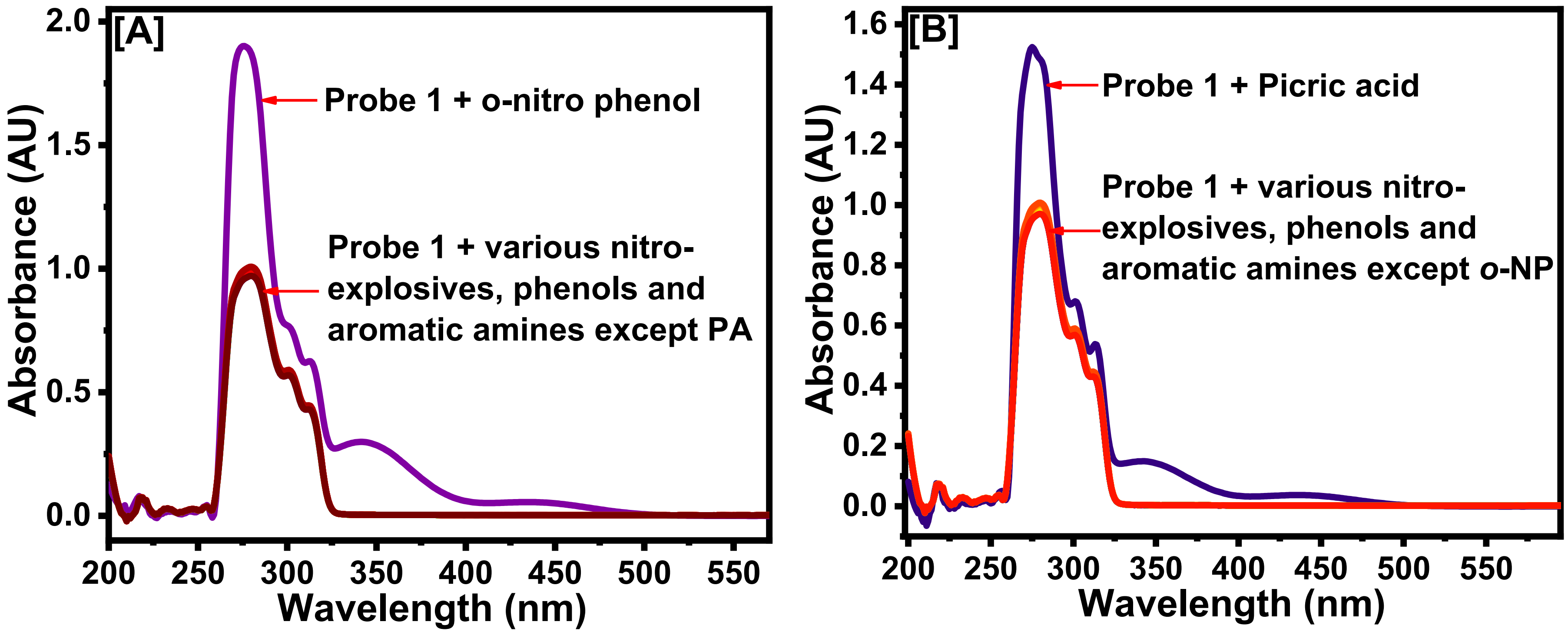

Fig. S21 (A) and (B)UV/vis spectra of **1** in presence of nitroaromatics, phenols and aromatic amines in solvent containing molar ratio (DMF: H_2O; 6:4).

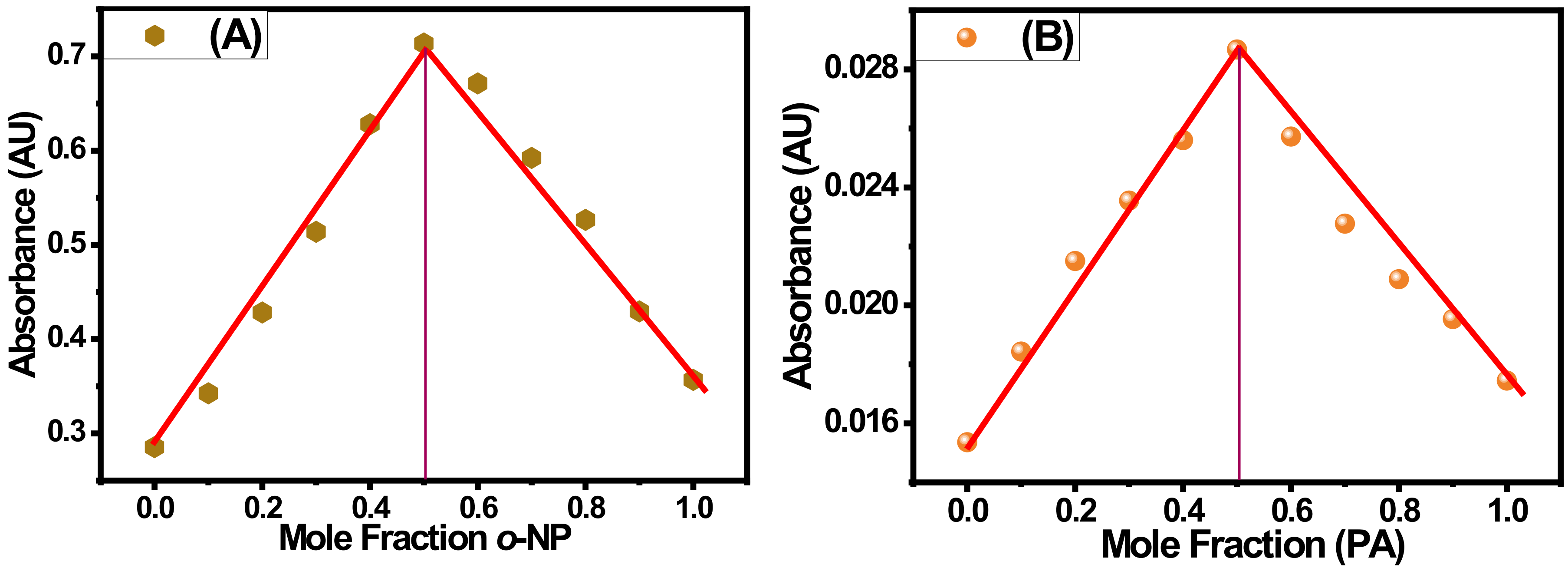

Fig. S22 Job's plot for the binding of **1** with (A) o-NP, and **(B)** with PA at $\lambda_{(ab)}$ 278 nm.

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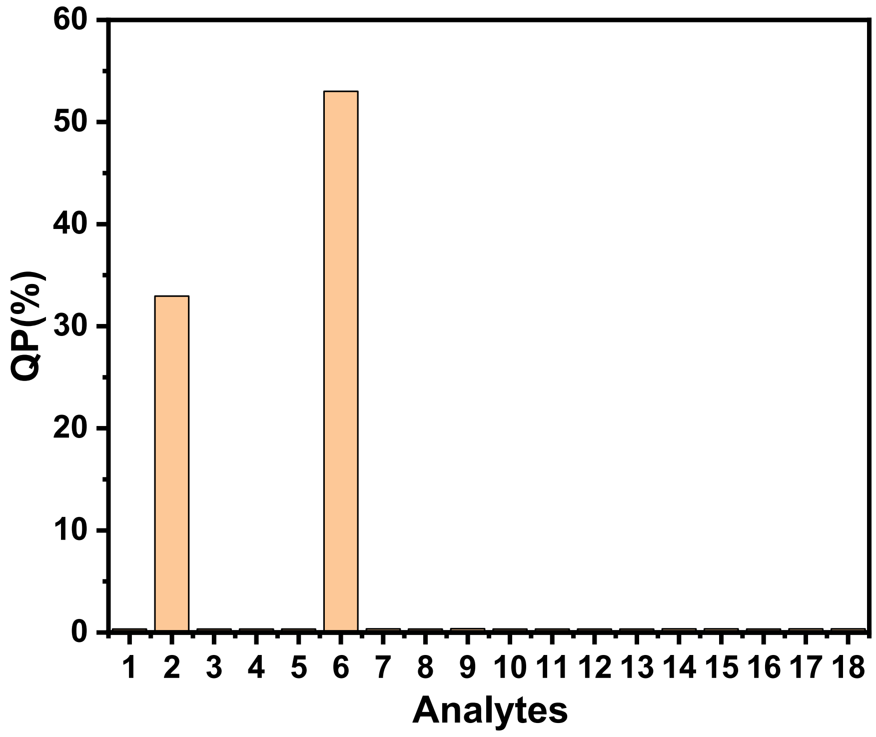

Fig. S23 Fluorescence response of **1** (10 μM) toward various NACs, phenols and aniline derivatives (i.e. p-nitrophenol (**1**) o-nitrophenol (**2**), m-nitrophenol (**3**), 3-Methoxyphenol (**4**), 2-Isopropylphenol (**5**), 2,4,6-Trinitrophenol (**6**), 2,4-Dibromophenol (**7**), 3-Chlorophenol (**8**), 2,4,6-Trichlorophenol (**9**), 2,4-Dichlorophenol (**10**), Quinol (**11**), Phenol (**12**), Resorcinol (**13**), 4-Chloroaniline (**14**), Tertbutylaniline (**15**), 2-Chloroaniline (**16**), 2,4-Difluoroaniline (**17**) and aniline (**18**) (λ_{ex} = 300 nm).

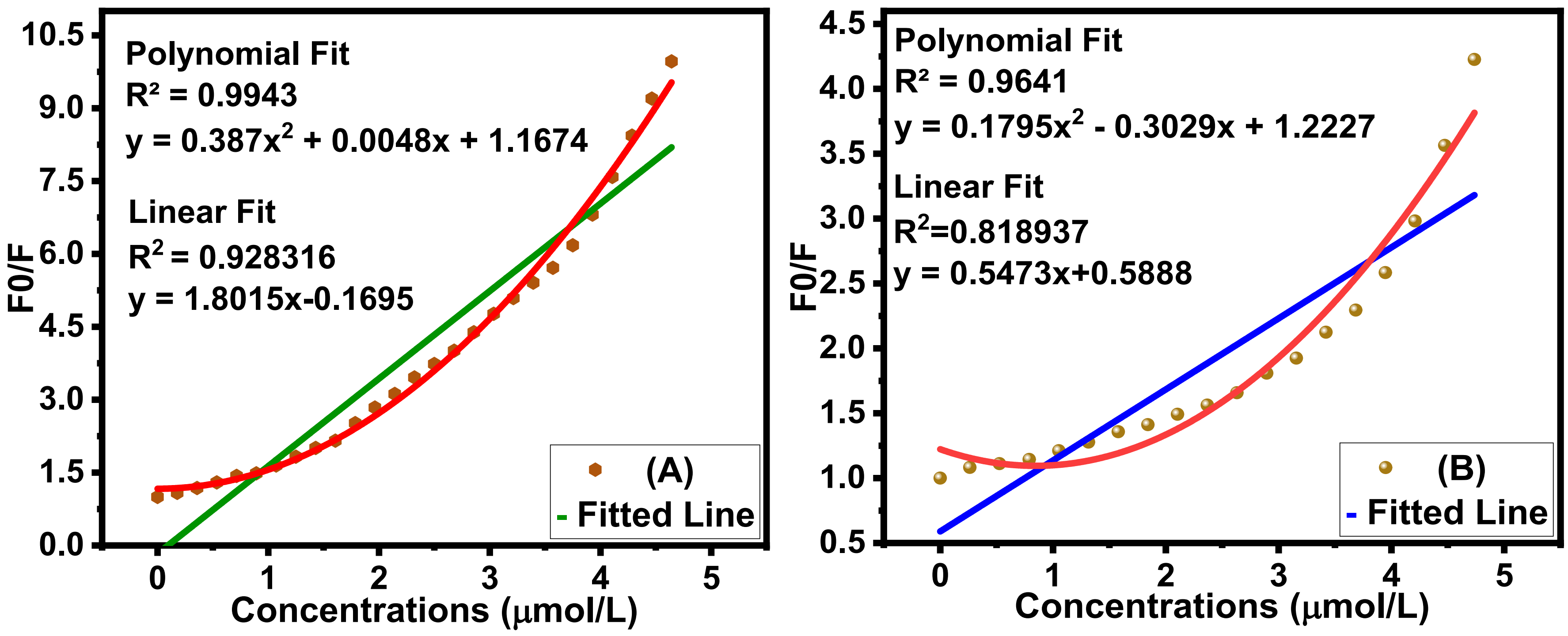

Fig.: S24 Polynomial and Linear Fitted curve of **1** (F_0/F) Vs Concentration (A) by adding successive concentrations of o-NP and **1** (B) by adding successive concentrations of PA.

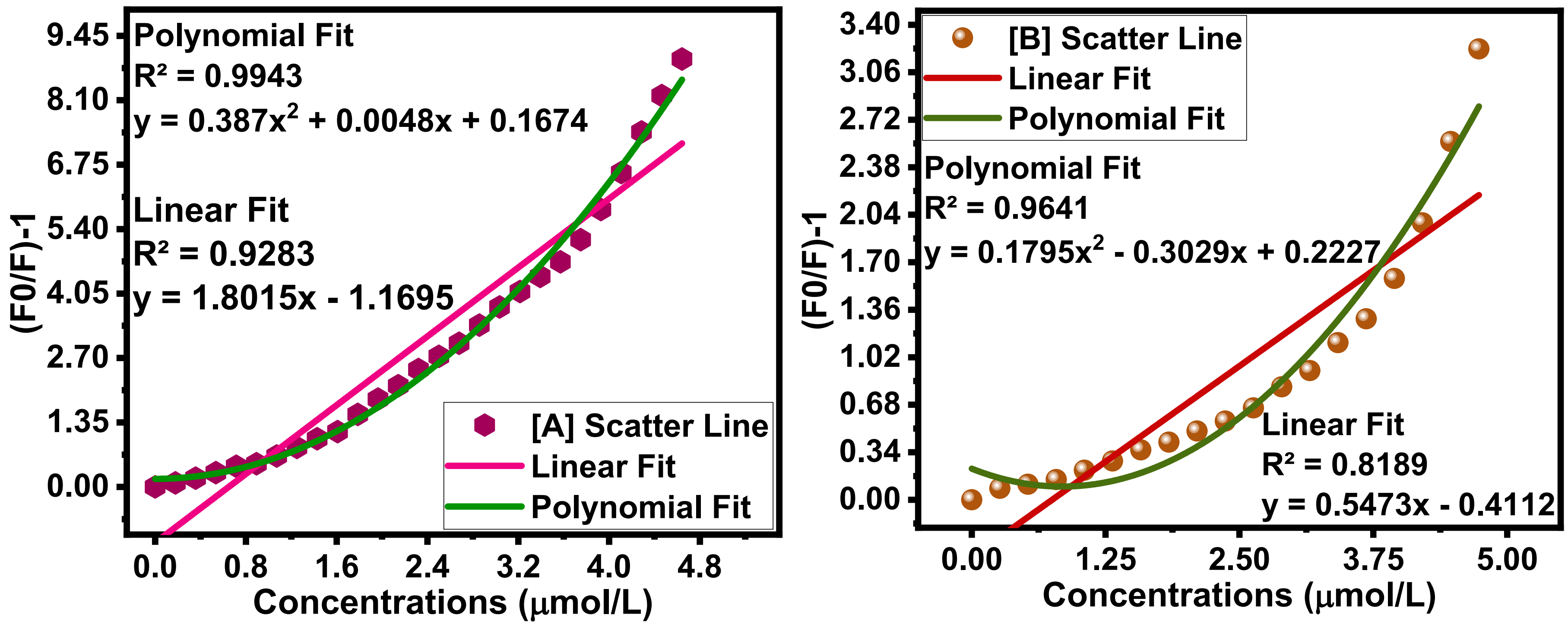

Fig.: S25 Polynomial and Linear Fitted Stern-Volmer curve (F_0/F)-1 Vs Concentration of **1** (A) by adding successive concentrations of o-NP and probe-2 (B) by adding successive concentrations of PA.

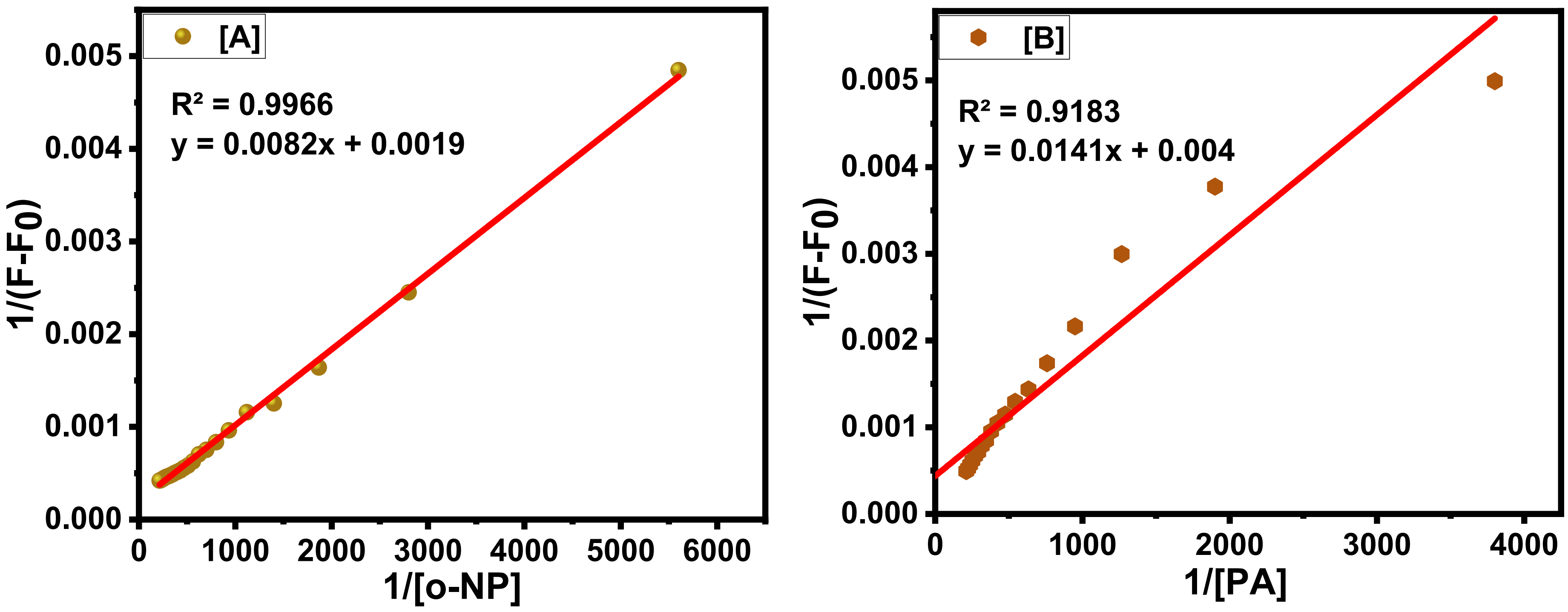

Fig. S26 13 Benesi–Hildebrand plot for binding of **1** with (A) o-NP and (B) PA.

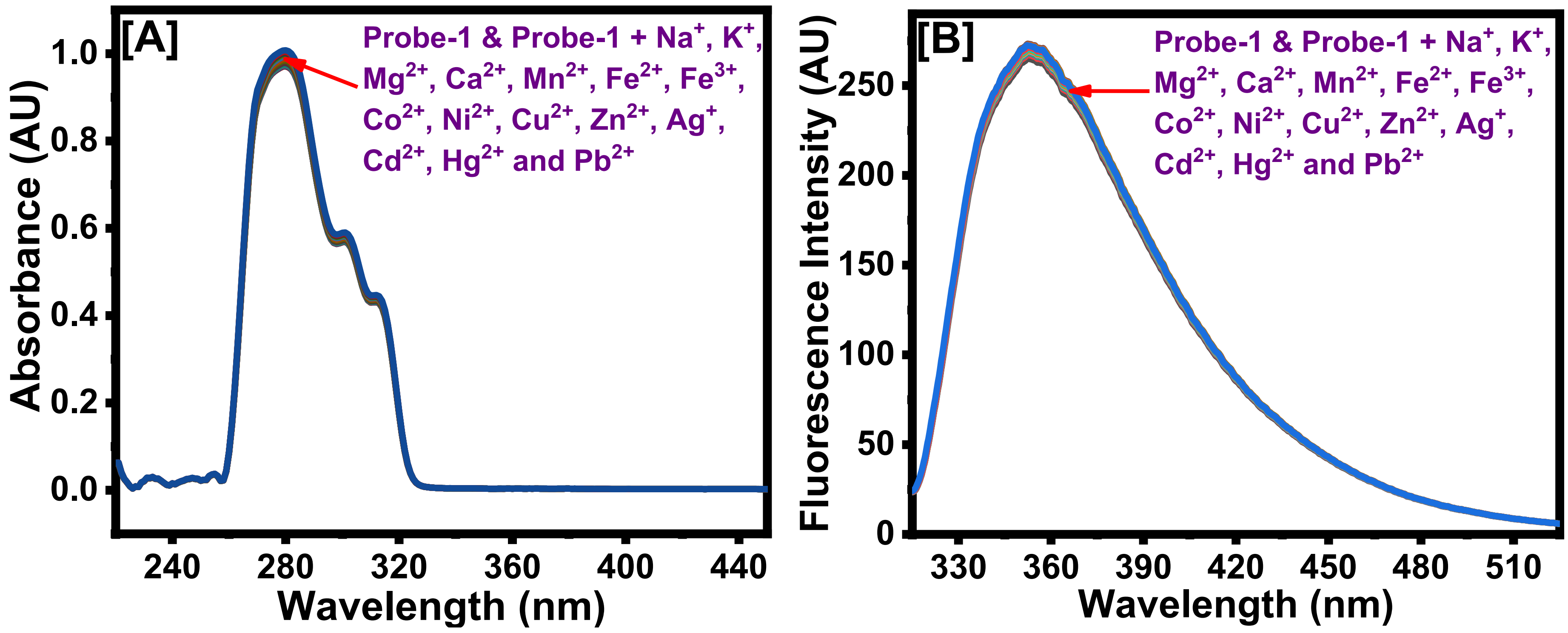

Fig. S27 UV/vis spectra (A) and Fluorescence spectra (B) of Probe **1** in presence of various metal ions in the solvent containing molar ratio (DMF/ H_2O; 6:4 v/v).

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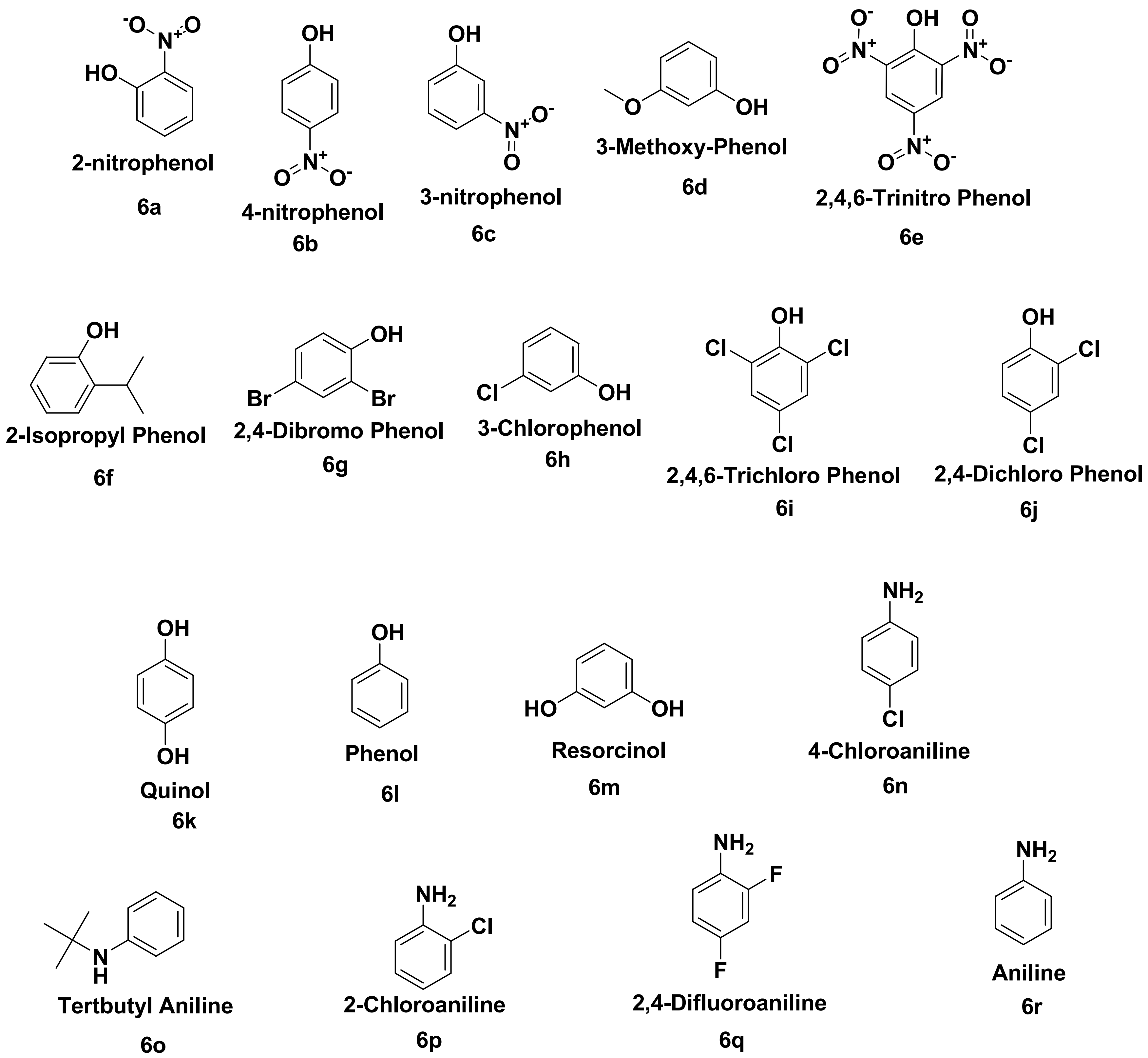

Scheme S1. Guests 6 used in this study

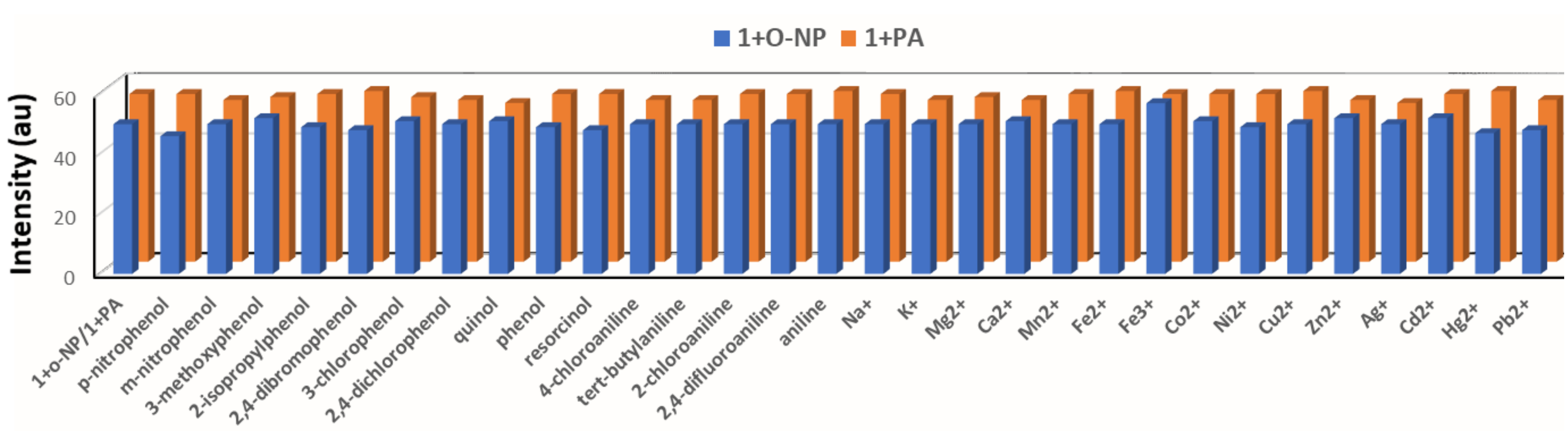

Fig. S28 Bar diagram showing interference of various cations, phenols and amines in binding of 1 with *o*-NP/PA in way (addition of analytes to the solution of 1+*o*-NP+analytes/1+PA+analytes).

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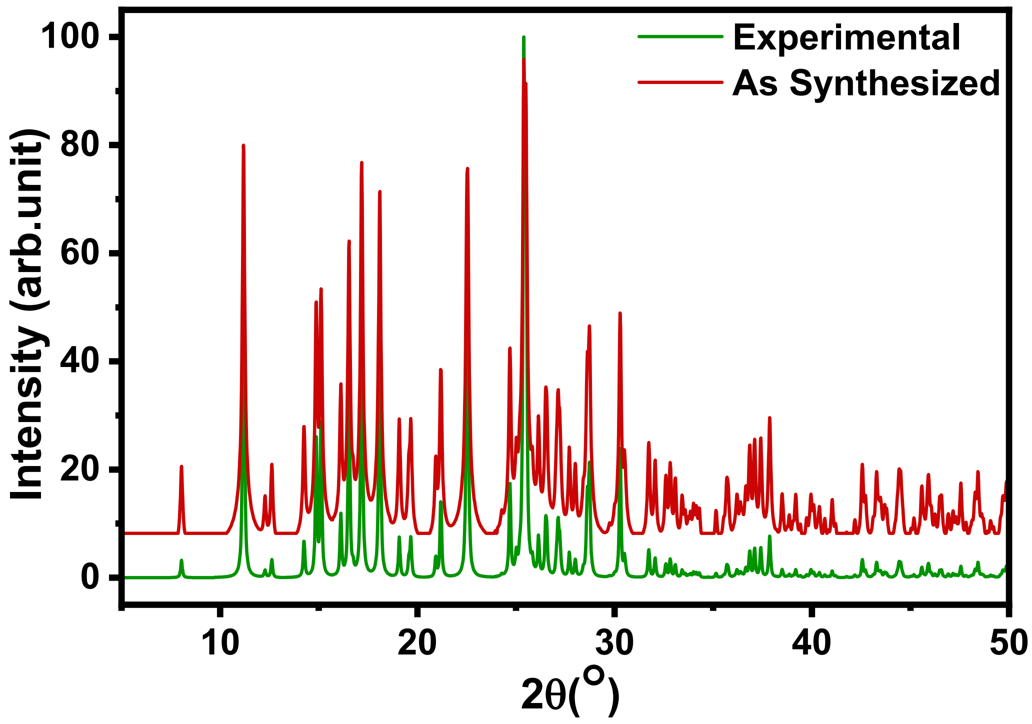


Fig. S29 Experimental PXRD pattern of 1 matching with its simulated PXRD patterns obtained from single crystal-XRD data.

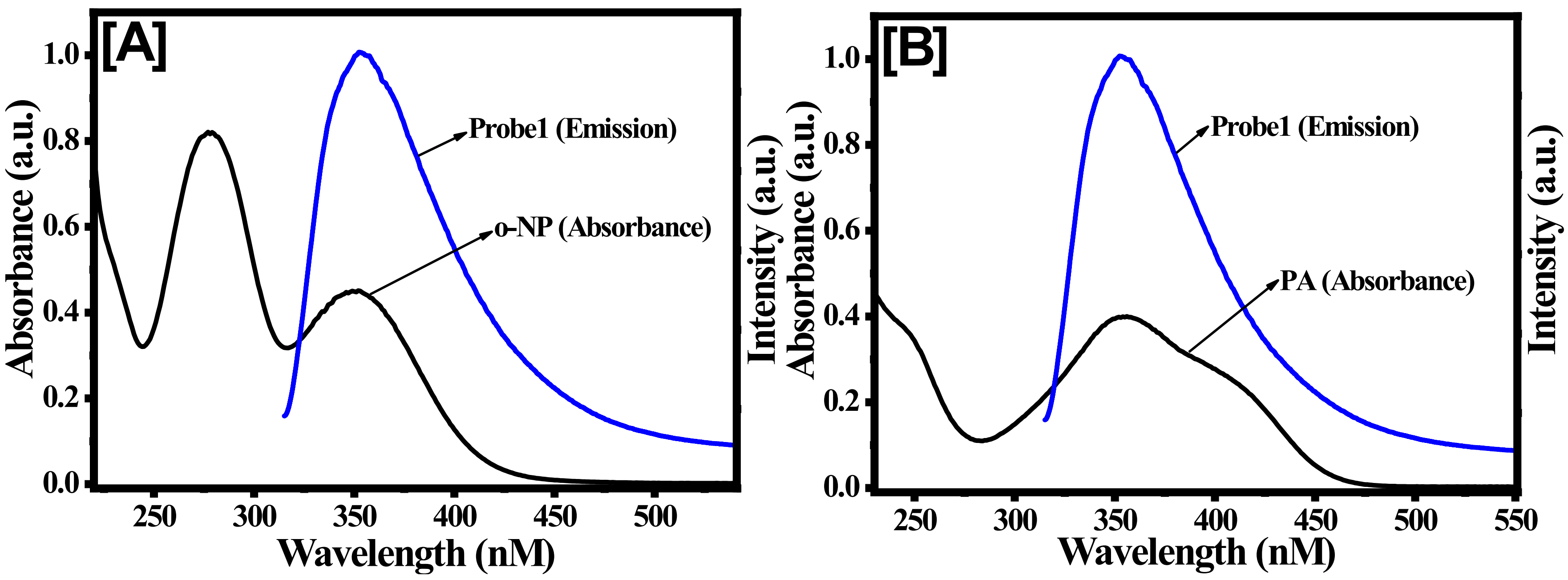


Fig. S30 Absorption spectra of electron deficient nitro-explosives (A) o-NP ; (B) PA and emission spectra of Probe 1

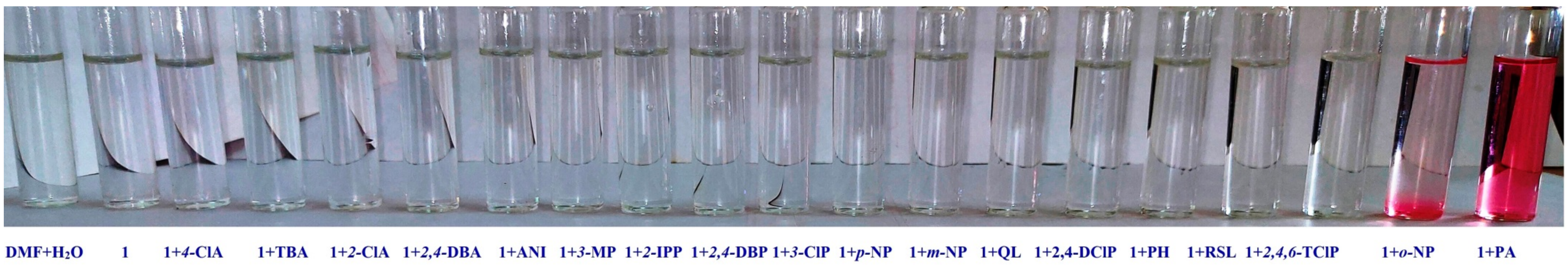
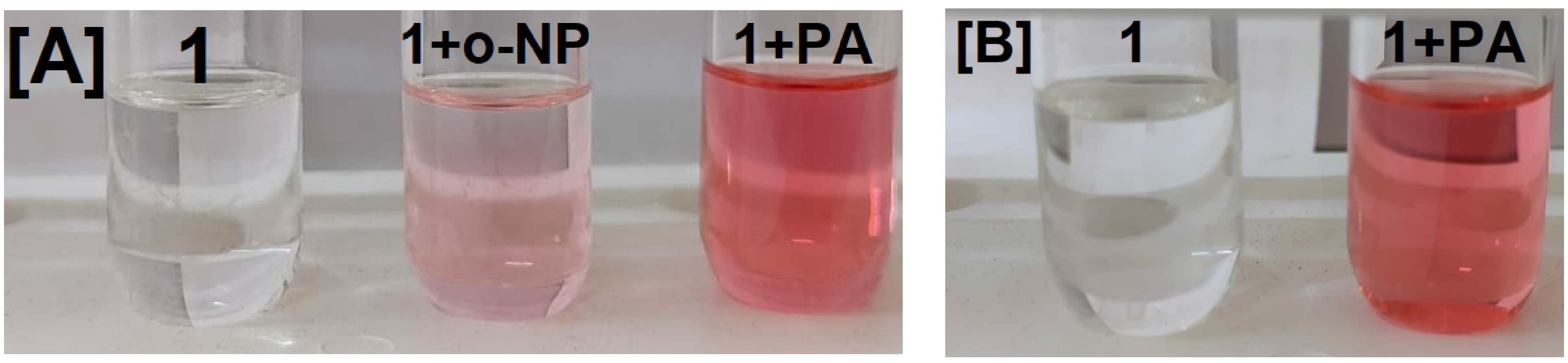


Fig. S31 Picture showing distinct color change from colorless to pink of **1** (10 μM) in presence of various analytes in mixed DMF/H_2O media (6:4, v/v).



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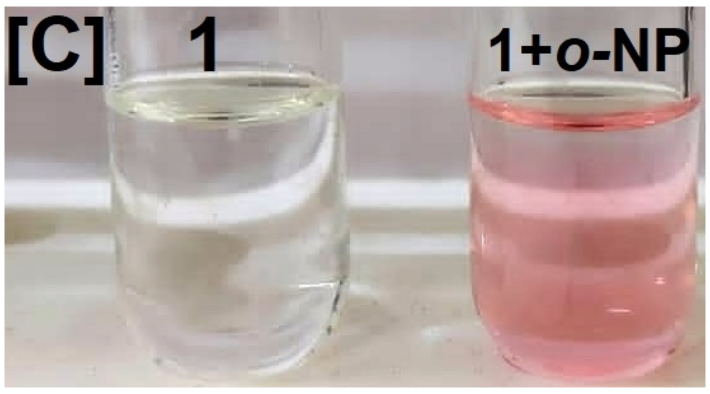

Fig. S32 Picture showing distinct color change from colorless to pink of **1** (10 μM) in presence of Picric Acid and orthonitrophenol in mixed DMF/H_2O media (6:4, v/v).

Table S3 Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.64016 (19)	0.64908 (16)	0.23125 (12)	0.0639 (4)
O1	0.44116 (16)	0.2912 (2)	0.45763 (13)	0.0733 (5)
O3	0.7361 (2)	0.85312 (17)	0.07881 (16)	0.0859 (5)
N2	0.89755 (18)	0.4044 (2)	0.33700 (13)	0.0517 (4)
N1	0.70815 (18)	0.38580 (19)	0.35247 (12)	0.0473 (4)
C15	0.7292 (2)	0.56125 (19)	0.05049 (15)	0.0428 (4)
C10	0.67588 (19)	0.4187 (2)	0.13127 (14)	0.0405 (4)
C11	0.6886 (2)	0.2616 (2)	0.09718 (15)	0.0477 (4)
H11	0.653506	0.164608	0.151506	0.057*
C2	0.7253 (2)	0.2050 (2)	0.54667 (14)	0.0426 (4)
C14	0.7965 (2)	0.5525 (2)	−0.06760 (16)	0.0498 (4)
H14	0.832421	0.649424	−0.121768	0.060*
C13	0.8080 (2)	0.3962 (2)	−0.10159 (16)	0.0527 (5)
H13	0.851843	0.386519	−0.180283	0.063*
C12	0.7553 (2)	0.2528 (2)	−0.02023 (16)	0.0535 (5)
H12	0.764907	0.148018	−0.045175	0.064*
C3	0.6445 (3)	0.1009 (2)	0.64841 (16)	0.0538 (5)
H3	0.516518	0.087069	0.657205	0.065*
C7	0.9170 (2)	0.2251 (2)	0.53299 (15)	0.0435 (4)
C8	0.9928 (2)	0.3292 (2)	0.42413 (16)	0.0513 (5)
H8	1.120774	0.343398	0.415989	0.062*
C1	0.6100 (2)	0.2944 (2)	0.45241 (15)	0.0477 (4)
C9	0.6104 (2)	0.4696 (2)	0.24962 (15)	0.0489 (4)
H9	0.477316	0.447494	0.265084	0.059*
C6	1.0273 (2)	0.1421 (2)	0.62398 (17)	0.0559 (5)
H6	1.155290	0.155816	0.616696	0.067*
C16	0.7064 (3)	0.7063 (2)	0.11389 (18)	0.0576 (5)
C4	0.7556 (3)	0.0189 (2)	0.73568 (17)	0.0594 (5)
H4	0.702531	−0.051842	0.803362	0.071*
C5	0.9457 (3)	0.0407 (2)	0.72359 (17)	0.0612 (5)
H5	1.019063	−0.014169	0.783964	0.073*

Table S4 Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0753 (9)	0.0560 (8)	0.0652 (9)	0.0223 (7)	−0.0187 (7)	−0.0210 (6)

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O1	0.0303 (7)	0.1121 (12)	0.0704 (9)	−0.0017 (7)	−0.0071 (6)	0.0064 (8)
O3	0.1173 (13)	0.0383 (8)	0.1042 (12)	0.0045 (8)	−0.0355 (10)	−0.0080 (7)
N2	0.0313 (7)	0.0721 (10)	0.0505 (8)	0.0000 (6)	−0.0041 (6)	−0.0067 (7)
N1	0.0318 (7)	0.0662 (10)	0.0432 (8)	0.0052 (6)	−0.0057 (5)	−0.0068 (6)
C15	0.0387 (8)	0.0383 (8)	0.0508 (9)	0.0042 (6)	−0.0151 (7)	−0.0016 (7)
C10	0.0315 (7)	0.0459 (9)	0.0433 (9)	0.0026 (6)	−0.0107 (6)	−0.0027 (7)
C11	0.0481 (9)	0.0410 (9)	0.0523 (10)	−0.0034 (7)	−0.0096 (7)	0.0002 (7)
C2	0.0375 (8)	0.0489 (9)	0.0436 (9)	0.0030 (7)	−0.0061 (7)	−0.0131 (7)
C14	0.0441 (9)	0.0497 (10)	0.0508 (10)	−0.0008 (7)	−0.0105 (7)	0.0078 (7)
C13	0.0492 (10)	0.0629 (11)	0.0453 (9)	0.0068 (8)	−0.0075 (7)	−0.0067 (8)
C12	0.0589 (11)	0.0468 (10)	0.0567 (10)	0.0043 (8)	−0.0109 (8)	−0.0119 (8)
C3	0.0472 (9)	0.0571 (11)	0.0568 (11)	−0.0008 (8)	−0.0029 (8)	−0.0088 (8)
C7	0.0362 (8)	0.0509 (9)	0.0465 (9)	0.0047 (7)	−0.0080 (7)	−0.0156 (7)
C8	0.0302 (8)	0.0698 (12)	0.0540 (10)	0.0000 (7)	−0.0063 (7)	−0.0096 (8)
C1	0.0340 (8)	0.0618 (11)	0.0481 (9)	0.0015 (7)	−0.0044 (7)	−0.0112 (8)
C9	0.0389 (8)	0.0592 (11)	0.0488 (10)	0.0086 (7)	−0.0100 (7)	−0.0084 (8)
C6	0.0428 (9)	0.0665 (12)	0.0609 (11)	0.0088 (8)	−0.0169 (8)	−0.0143 (9)
C16	0.0617 (11)	0.0439 (11)	0.0690 (12)	0.0102 (8)	−0.0260 (9)	−0.0073 (8)
C4	0.0664 (12)	0.0541 (11)	0.0557 (11)	0.0029 (9)	−0.0066 (9)	−0.0033 (8)
C5	0.0680 (12)	0.0604 (12)	0.0562 (11)	0.0149 (9)	−0.0209 (9)	−0.0085 (9)

Table S5 Geometric parameters (Å,°)

O2—C16	1.371 (3)	C2—C1	1.465 (2)
O2—C9	1.438 (2)	C14—C13	1.371 (3)
O1—C1	1.218 (2)	C14—H14	0.9300
O3—C16	1.195 (2)	C13—C12	1.382 (3)
N2—C8	1.286 (2)	C13—H13	0.9300
N2—N1	1.3756 (19)	C12—H12	0.9300
N1—C1	1.387 (2)	C3—C4	1.374 (2)
N1—C9	1.447 (2)	C3—H3	0.9300
C15—C10	1.375 (2)	C7—C6	1.401 (2)
C15—C14	1.388 (3)	C7—C8	1.436 (2)
C15—C16	1.464 (3)	C8—H8	0.9300
C10—C11	1.377 (2)	C9—H9	0.9800
C10—C9	1.495 (2)	C6—C5	1.368 (3)
C11—C12	1.380 (3)	C6—H6	0.9300
C11—H11	0.9300	C4—C5	1.383 (3)
C2—C3	1.392 (2)	C4—H4	0.9300
C2—C7	1.393 (2)	C5—H5	0.9300
C16—O2—C9	110.36 (13)	C2—C3—H3	120.3
C8—N2—N1	116.51 (14)	C2—C7—C6	119.22 (16)
N2—N1—C1	126.57 (13)	C2—C7—C8	117.86 (14)
N2—N1—C9	113.50 (13)	C6—C7—C8	122.91 (15)
C1—N1—C9	119.90 (14)	N2—C8—C7	125.06 (15)
C10—C15—C14	121.57 (15)	N2—C8—H8	117.5
C10—C15—C16	107.96 (16)	C7—C8—H8	117.5
C14—C15—C16	130.44 (16)	O1—C1—N1	120.74 (16)
C15—C10—C11	120.65 (15)	O1—C1—C2	124.45 (16)

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C15—C10—C9	108.70 (15)	N1—C1—C2	114.81 (14)
C11—C10—C9	130.64 (15)	O2—C9—N1	110.16 (13)
C10—C11—C12	117.82 (15)	O2—C9—C10	104.54 (13)
C10—C11—H11	121.1	N1—C9—C10	114.04 (13)
C12—C11—H11	121.1	O2—C9—H9	109.3
C3—C2—C7	120.40 (15)	N1—C9—H9	109.3
C3—C2—C1	120.51 (15)	C10—C9—H9	109.3
C7—C2—C1	119.09 (15)	C5—C6—C7	119.66 (17)
C13—C14—C15	117.70 (15)	C5—C6—H6	120.2
C13—C14—H14	121.2	C7—C6—H6	120.2
C15—C14—H14	121.2	O3—C16—O2	121.08 (18)
C14—C13—C12	120.74 (17)	O3—C16—C15	130.6 (2)
C14—C13—H13	119.6	O2—C16—C15	108.35 (15)
C12—C13—H13	119.6	C3—C4—C5	120.46 (18)
C11—C12—C13	121.52 (17)	C3—C4—H4	119.8
C11—C12—H12	119.2	C5—C4—H4	119.8
C13—C12—H12	119.2	C6—C5—C4	120.87 (17)
C4—C3—C2	119.37 (17)	C6—C5—H5	119.6
C4—C3—H3	120.3	C4—C5—H5	119.6

Table S6 Major Peak profiles and its 2θ / (Degree) corresponding with Indexing of (h.k.l.) value of Probe 2.

Sr. No.	2 Theta	D spacing	h	k	l
1	8.039	10.9892	0	0	1
2	11.187	7.9030	0	1	0
3	12.274	7.2052	1	0	0
4	12.621	7.0083	0	1	1
5	14.250	6.2102	1	0	1
6	14.871	5.9525	0	-1	1
7	15.116	5.8564	-1	0	1
8	16.118	5.4946	0	0	2
9	16.533	5.3575	1	1	0
10	16.739	5.2921	-1	1	0
11	17.175	5.1588	1	1	1
12	18.006	4.9224	0	1	2
13	18.094	4.8989	-1	1	1
14	19.083	4.6471	1	-1	1
15	19.568	4.5330	-1	-1	1
16	19.667	4.5103	1	0	2
17	20.932	4.2405	-1	0	2
18	21.171	4.1932	1	1	2
19	21.194	4.1886	0	-1	2
20	22.482	3.9515	0	2	0
21	22.509	3.9469	-1	1	2
22	22.556	3.9387	0	2	1
23	24.102	3.6894	1	-1	2
24	24.279	3.6631	0	0	3
25	24.692	3.6026	2	0	0
26	24.967	3.5636	0	1	3
27	25.017	3.5566	-1	-1	2
28	25.198	3.5314	0	-2	1
29	25.366	3.5084	1	2	1
30	25.398	3.5041	0	2	2
31	25.502	3.4900	2	0	1
32	25.556	3.4828	1	2	0
33	25.827	3.4468	-1	2	0
34	26.142	3.4060	-1	2	1
35	26.503	3.3604	-2	0	1
36	26.563	3.3530	1	0	3
37	27.052	3.2934	2	1	0
38	27.133	3.2839	1	1	3
39	27.220	3.2736	2	1	1
40	27.310	3.2629	-2	1	0
41	27.705	3.2173	1	2	2
42	27.999	3.1842	-1	0	3
43	28.010	3.1830	1	-2	1
44	28.225	3.1592	-1	-2	1

45	28.412	3.1388	-2	1	1
46	28.531	3.1260	0	-1	3
47	28.613	3.1172	2	-1	1
48	28.665	3.1117	-1	1	3
49	28.727	3.1051	2	0	2
50	28.880	3.0891	-1	2	2
51	29.276	3.0481	-2	-1	1
52	29.741	3.0015	2	1	2
53	30.000	2.9762	0	-2	2
54	30.282	2.9491	0	2	3
55	30.504	2.9282	-2	0	2
56	30.579	2.9212	1	-1	3
57	31.690	2.8212	-2	1	2
58	31.737	2.8172	-1	-1	3
59	32.053	2.7901	2	-1	2
60	32.063	2.7892	1	2	3
61	32.224	2.7757	1	-2	2
62	32.566	2.7473	0	0	4
63	32.602	2.7443	0	1	4
64	32.821	2.7265	-1	-2	2
65	33.075	2.7062	2	2	1
66	33.424	2.6787	2	2	0
67	33.458	2.6761	-2	-1	2
68	33.497	2.6731	-1	2	3
69	33.575	2.6671	0	3	1
70	33.735	2.6547	2	0	3
71	33.849	2.6461	-2	2	0
72	34.004	2.6343	0	3	0
73	34.132	2.6248	1	1	4
74	34.143	2.6239	2	1	3
75	34.150	2.6234	1	0	4
76	34.291	2.6129	-2	2	1
77	34.751	2.5794	2	2	2
78	35.147	2.5513	0	3	2
79	35.395	2.5340	2	-2	1
80	35.535	2.5243	1	3	1
81	35.684	2.5141	-1	0	4
82	35.744	2.5100	-2	-2	1
83	35.767	2.5084	-1	1	4
84	36.037	2.4902	-2	0	3
85	36.130	2.4841	1	3	0
86	36.142	2.4833	0	-2	3
87	36.211	2.4787	-1	3	1
88	36.373	2.4680	0	-3	1
89	36.380	2.4676	0	-1	4
90	36.429	2.4644	-1	3	0
91	36.477	2.4612	0	2	4
92	36.621	2.4519	-2	1	3
93	36.659	2.4494	-2	2	2
94	36.851	2.4371	1	3	2
95	37.100	2.4213	2	-1	3
96	37.414	2.4017	3	0	0
97	37.797	2.3783	3	0	1
98	37.822	2.3767	1	2	4
99	37.866	2.3741	-1	3	2
100	37.869	2.3739	1	-2	3
101	37.871	2.3738	1	-1	4
102	38.218	2.3530	2	2	3
103	38.493	2.3368	1	-3	1
104	38.506	2.3361	0	3	3
105	38.562	2.3328	-1	-3	1
106	38.722	2.3236	2	-2	2
107	38.741	2.3225	-1	-2	3
108	38.858	2.3157	-3	0	1
109	38.977	2.3089	3	1	1
110	39.030	2.3059	3	1	0
111	39.044	2.3051	-2	-1	3
112	39.186	2.2971	-1	-1	4
113	39.310	2.2901	-3	1	0
114	39.417	2.2842	-1	2	4
115	39.737	2.2665	-2	-2	2
116	39.884	2.2585	2	1	4
117	39.917	2.2567	1	3	3
118	39.946	2.2551	2	0	4
119	39.964	2.2542	3	0	2
120	40.095	2.2471	3	-1	1
121	40.286	2.2369	-3	1	1
122	40.386	2.2315	0	-3	2
123	40.654	2.2175	0	1	5
124	40.662	2.2171	-2	2	3
125	40.683	2.2159	3	1	2
126	40.837	2.2080	-3	-1	1
127	41.034	2.1978	0	0	5

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128	41.201	2.1893	-1	3	3
129	41.527	2.1729	2	3	1
130	41.765	2.1610	1	1	5
131	41.972	2.1508	-3	0	2
132	42.173	2.1411	1	-3	2
133	42.180	2.1407	1	0	5
134	42.214	2.1391	2	3	0
135	42.524	2.1242	2	3	2
136	42.559	2.1225	3	-1	2
137	42.562	2.1224	-1	-3	2
138	42.607	2.1202	-2	0	4
139	42.708	2.1154	-2	3	1
140	42.722	2.1148	-2	1	4
141	42.737	2.1141	-2	3	0
142	42.923	2.1053	-3	1	2
143	43.111	2.0966	2	2	4
144	43.161	2.0943	0	-2	4
145	43.284	2.0886	2	-1	4
146	43.302	2.0878	0	3	4
147	43.398	2.0834	3	2	1
148	43.472	2.0800	-1	1	5
149	43.485	2.0795	2	-2	3
150	43.533	2.0773	0	2	5
151	43.692	2.0701	3	0	3
152	43.789	2.0657	-1	0	5
153	43.834	2.0637	3	2	0
154	43.979	2.0572	3	1	3
155	44.219	2.0466	-3	-1	2
156	44.315	2.0424	-2	3	2
157	44.342	2.0412	-3	2	0
158	44.399	2.0387	2	-3	1
159	44.431	2.0373	1	3	4
160	44.503	2.0342	1	-2	4
161	44.521	2.0334	-2	-3	1
162	44.543	2.0325	1	2	5
163	44.586	2.0306	3	2	2
164	44.602	2.0299	0	-1	5
165	44.851	2.0192	-3	2	1
166	45.034	2.0115	-2	-2	3
167	45.115	2.0080	2	3	3
168	45.184	2.0051	0	4	1
169	45.431	1.9948	3	-2	1
170	45.577	1.9887	-1	-2	4
171	45.623	1.9869	-2	-1	4
172	45.688	1.9842	0	-3	3
173	45.717	1.9830	1	-1	5
174	45.857	1.9772	-3	-2	1
175	45.894	1.9758	0	4	0
176	45.918	1.9748	-1	3	4
177	45.950	1.9735	-2	2	4
178	46.052	1.9693	0	4	2
179	46.249	1.9614	-1	2	5
180	46.481	1.9521	-3	0	3
181	46.487	1.9519	3	-1	3
182	46.576	1.9484	2	1	5
183	46.690	1.9439	1	4	1
184	46.917	1.9350	-3	2	2
185	46.996	1.9319	-3	1	3
186	46.997	1.9319	2	0	5
187	47.150	1.9260	-1	-1	5
188	47.164	1.9255	1	-3	3
189	47.302	1.9202	3	2	3
190	47.313	1.9198	-1	4	1
191	47.388	1.9169	1	4	2
192	47.426	1.9154	-2	3	3
193	47.531	1.9114	1	4	0
194	47.559	1.9104	2	-3	2
195	47.817	1.9007	-1	-3	3
196	47.850	1.8995	-1	4	0
197	48.033	1.8926	3	-2	2
198	48.125	1.8892	0	-4	1
199	48.265	1.8841	-2	-3	2
200	48.297	1.8829	-1	4	2
201	48.430	1.8780	0	4	3
202	48.607	1.8716	3	1	4
203	48.699	1.8683	3	0	4
204	48.918	1.8604	-3	-1	3
205	49.063	1.8553	0	1	6
206	49.099	1.8540	2	2	5
207	49.102	1.8539	2	3	4
208	49.209	1.8501	0	3	5
209	49.316	1.8464	-3	-2	2
210	49.363	1.8447	2	-2	4

211	49.573	1.8374	1	4	3
212	49.681	1.8336	-2	1	5
213	49.742	1.8315	0	0	6
214	49.851	1.8278	-1	-4	1
215	49.872	1.8271	1	-4	1
216	49.882	1.8267	1	1	6
217	49.929	1.8251	-2	0	5
218	50.091	1.8196	1	3	5
219	50.306	1.8123	2	-1	5
220	50.372	1.8101	3	3	1
221	50.394	1.8094	-3	2	3
222	50.591	1.8028	1	0	6
223	50.635	1.8013	4	0	0
224	50.737	1.7979	-1	4	3
225	50.795	1.7960	4	0	1
226	50.827	1.7950	0	-2	5
227	51.092	1.7863	3	3	2
228	51.105	1.7858	3	3	0
229	51.229	1.7818	0	2	6
230	51.337	1.7783	-2	-2	4
231	51.360	1.7776	3	2	4
232	51.586	1.7703	2	4	1
233	51.625	1.7691	3	-1	4
234	51.657	1.7680	-1	1	6
235	51.698	1.7668	4	1	1
236	51.731	1.7657	0	-4	2
237	51.733	1.7656	-1	3	5
238	51.783	1.7640	-3	3	0
239	51.836	1.7624	-2	3	4
240	51.877	1.7611	1	-2	5
241	51.880	1.7610	4	1	0
242	51.898	1.7604	-3	3	1
243	51.919	1.7597	-4	0	1
244	51.977	1.7579	3	-2	3
245	51.985	1.7577	1	2	6
246	51.992	1.7574	0	-3	4
247	52.010	1.7569	2	-3	3
248	52.096	1.7542	2	4	2
249	52.116	1.7535	-3	0	4
250	52.163	1.7521	0	4	4
251	52.179	1.7516	-4	1	0
252	52.241	1.7496	-2	2	5
253	52.252	1.7493	-3	1	4
254	52.274	1.7486	-1	0	6
255	52.391	1.7450	4	0	2
256	52.507	1.7414	2	4	0
257	52.673	1.7363	4	-1	1
258	52.739	1.7343	-2	4	1
259	52.940	1.7282	4	1	2
260	52.955	1.7277	-2	-1	5
261	53.090	1.7237	3	-3	1
262	53.098	1.7234	-2	4	0
263	53.103	1.7233	-4	1	1
264	53.111	1.7230	1	4	4
265	53.111	1.7230	-1	-2	5
266	53.185	1.7208	0	-1	6
267	53.199	1.7204	1	-3	4
268	53.222	1.7197	-2	-3	3
269	53.225	1.7196	3	3	3
270	53.250	1.7188	-3	-3	1
271	53.254	1.7187	1	-4	2
272	53.428	1.7136	-3	3	2
273	53.476	1.7121	-4	-1	1
274	53.507	1.7112	-1	-4	2
275	53.783	1.7031	-1	2	6
276	53.786	1.7030	-2	4	2
277	54.000	1.6967	2	1	6
278	54.006	1.6966	2	4	3
279	54.007	1.6965	-3	-2	3
280	54.031	1.6958	1	-1	6
281	54.070	1.6947	-1	-3	4
282	54.260	1.6892	2	3	5
283	54.325	1.6873	3	1	5
284	54.490	1.6826	-1	4	4
285	54.558	1.6807	4	-1	2
286	54.575	1.6802	-4	0	2
287	54.694	1.6768	-3	-1	4
288	54.706	1.6765	2	0	6
289	54.738	1.6756	3	0	5
290	54.806	1.6737	-2	-4	1
291	54.845	1.6726	2	-4	1
292	55.089	1.6657	-3	2	4
293	55.282	1.6604	4	2	1

294	55.334	1.6589	4	0	3
295	55.395	1.6572	-4	1	2
296	55.539	1.6533	4	1	3
297	55.570	1.6525	-1	-1	6
298	55.748	1.6476	3	-3	2
299	55.780	1.6467	4	2	0
300	55.957	1.6419	2	2	6
301	55.999	1.6408	0	3	6
302	56.129	1.6373	2	-2	5
303	56.149	1.6368	4	2	2
304	56.186	1.6358	-2	4	3
305	56.292	1.6330	-3	3	3
306	56.348	1.6315	-4	2	0
307	56.402	1.6300	-4	-1	2
308	56.526	1.6268	0	-4	3
309	56.560	1.6258	3	2	5
310	56.659	1.6233	3	3	4
311	56.676	1.6228	1	3	6
312	56.695	1.6223	-3	-3	2
313	56.908	1.6168	-4	2	1
314	57.069	1.6126	0	4	5
315	57.071	1.6125	3	-2	4
316	57.136	1.6108	4	-2	1
317	57.221	1.6086	2	4	4
318	57.331	1.6058	-2	1	6
319	57.341	1.6056	-2	3	5
320	57.419	1.6036	0	5	1
321	57.549	1.6002	2	-3	4
322	57.619	1.5985	-4	-2	1
323	57.741	1.5954	4	-1	3
324	57.761	1.5949	3	-1	5
325	57.832	1.5931	1	4	5
326	57.833	1.5931	1	-4	3
327	57.837	1.5930	0	5	2
328	57.850	1.5926	0	1	7
329	57.872	1.5921	-2	0	6
330	57.895	1.5915	2	-4	2
331	58.012	1.5886	2	-1	6
332	58.331	1.5806	-1	-4	3
333	58.333	1.5806	0	5	0
334	58.339	1.5805	4	2	3
335	58.374	1.5796	-2	-4	2
336	58.445	1.5778	-1	3	6
337	58.453	1.5776	1	1	7
338	58.457	1.5775	-2	-2	5
339	58.477	1.5770	-4	0	3
340	58.489	1.5767	-3	1	5
341	58.660	1.5726	1	5	1
342	58.770	1.5699	0	0	7
343	58.790	1.5694	-4	2	2
344	58.944	1.5657	1	5	2
345	58.950	1.5655	-4	1	3
346	59.054	1.5630	0	-2	6
347	59.114	1.5616	0	-3	5
348	59.196	1.5596	-2	-3	4
349	59.237	1.5586	4	-2	2
350	59.260	1.5581	-1	5	1
351	59.269	1.5578	3	4	1
352	59.353	1.5558	-2	2	6
353	59.377	1.5553	4	1	4
354	59.393	1.5549	-1	4	5
355	59.401	1.5547	1	0	7
356	59.483	1.5528	0	2	7
357	59.492	1.5525	4	0	4
358	59.567	1.5508	0	5	3
359	59.606	1.5498	3	4	2
360	59.639	1.5490	3	-3	3
361	59.689	1.5479	1	5	0
362	59.747	1.5465	-3	-2	4
363	59.796	1.5454	-1	5	2
364	59.831	1.5445	-2	4	4
365	59.878	1.5434	1	-2	6
366	60.029	1.5399	-1	5	0
367	60.042	1.5396	1	2	7
368	60.099	1.5383	1	-3	5
369	60.236	1.5351	3	4	0
370	60.306	1.5335	-1	1	7
371	60.368	1.5321	-3	3	4
372	60.407	1.5312	2	3	6
373	60.529	1.5284	1	5	3
374	60.535	1.5283	-4	-1	3
375	60.539	1.5282	0	-5	1
376	60.720	1.5240	-4	-2	2

Supplementary Materials

377	60.827	1.5216	-3	2	5
378	60.844	1.5212	-3	4	1
379	60.932	1.5193	-2	-1	6
380	60.955	1.5187	3	1	6
381	61.047	1.5167	-3	4	0
382	61.155	1.5142	-1	-3	5
383	61.170	1.5139	-1	0	7
384	61.233	1.5125	4	3	1
385	61.236	1.5124	3	4	3
386	61.254	1.5120	3	3	5
387	61.255	1.5120	-1	-2	6
388	61.300	1.5110	-3	-3	3
389	61.374	1.5094	-3	-1	5
390	61.611	1.5041	2	4	5
391	61.617	1.5040	-1	5	3
392	61.643	1.5034	3	0	6
393	61.743	1.5012	4	3	2
394	61.764	1.5008	4	2	4
395	61.919	1.4974	-4	2	3
396	61.925	1.4972	-3	4	2
397	61.933	1.4971	-1	2	7
398	61.990	1.4958	-1	-5	1
399	62.003	1.4955	4	3	0
400	62.061	1.4943	2	1	7
401	62.075	1.4940	1	-5	1
402	62.099	1.4935	4	-1	4
403	62.128	1.4928	2	-4	3
404	62.172	1.4919	0	-1	7
405	62.348	1.4881	0	-4	4
406	62.471	1.4855	-3	-4	1
407	62.526	1.4843	3	-4	1
408	62.544	1.4839	0	5	4
409	62.569	1.4834	4	-2	3
410	62.740	1.4798	3	2	6
411	62.801	1.4785	-4	3	0
412	62.816	1.4781	1	-1	7
413	62.869	1.4770	2	5	1
414	62.987	1.4745	0	4	6
415	63.009	1.4741	2	0	7
416	63.019	1.4739	2	5	2
417	63.025	1.4737	-4	3	1
418	63.080	1.4726	-2	-4	3
419	63.155	1.4710	3	-2	5
420	63.356	1.4668	1	5	4
421	63.458	1.4647	1	-4	4
422	63.488	1.4641	-4	0	4
423	63.516	1.4635	4	3	3
424	63.548	1.4629	0	3	7
425	63.562	1.4626	2	2	7
426	63.584	1.4621	1	4	6
427	63.641	1.4610	-4	1	4
428	63.658	1.4606	2	-2	6
429	63.787	1.4580	-2	3	6
430	63.837	1.4569	4	-3	1
431	63.959	1.4545	0	-5	2
432	63.980	1.4540	2	5	0
433	64.018	1.4532	-2	5	1
434	64.026	1.4531	2	-3	5
435	64.028	1.4531	-4	-3	1
436	64.053	1.4525	1	3	7
437	64.174	1.4501	-1	-4	4
438	64.252	1.4485	-3	4	3
439	64.325	1.4471	4	1	5
440	64.423	1.4451	2	5	3
441	64.465	1.4443	-1	-1	7
442	64.503	1.4435	-4	3	2
443	64.600	1.4416	-2	4	5
444	64.626	1.4410	5	0	0
445	64.633	1.4409	-2	5	0
446	64.634	1.4409	3	-3	4
447	64.642	1.4407	5	0	1
448	64.653	1.4405	-2	5	2
449	64.660	1.4404	-1	5	4
450	64.730	1.4390	4	0	5
451	64.979	1.4341	-4	-2	3
452	65.232	1.4291	3	-4	2
453	65.305	1.4277	-1	4	6
454	65.328	1.4272	1	-5	2
455	65.385	1.4261	5	1	1
456	65.487	1.4242	-1	-5	2
457	65.529	1.4234	-3	3	5
458	65.576	1.4224	-3	1	6
459	65.615	1.4217	-2	1	7

460	65.663	1.4208	5	1	0
461	65.746	1.4192	-4	-1	4
462	65.850	1.4172	-5	0	1
463	65.898	1.4163	5	0	2
464	65.901	1.4162	-3	-4	2
465	65.943	1.4154	-1	3	7
466	65.986	1.4146	-5	1	0
467	66.044	1.4135	-3	0	6
468	66.057	1.4133	-2	-3	5
469	66.102	1.4124	4	-3	2
470	66.196	1.4106	-4	2	4
471	66.294	1.4088	5	-1	1
472	66.304	1.4086	-2	-2	6
473	66.315	1.4084	-2	-5	1
474	66.319	1.4083	4	2	5
475	66.342	1.4079	5	1	2
476	66.349	1.4077	2	-1	7
477	66.403	1.4067	-3	-2	5
478	66.407	1.4066	-2	0	7
479	66.479	1.4053	2	-5	1
480	66.496	1.4050	4	3	4
481	66.518	1.4046	-2	5	3
482	66.674	1.4017	0	5	5
483	66.886	1.3977	3	3	6
484	66.907	1.3973	-5	1	1
485	66.940	1.3967	-3	-3	4
486	66.968	1.3962	0	-3	6
487	67.040	1.3949	2	5	4
488	67.055	1.3946	2	4	6
489	67.083	1.3941	0	1	8
490	67.168	1.3926	-5	-1	1
491	67.191	1.3921	-4	3	3
492	67.201	1.3919	-2	2	7
493	67.244	1.3912	-4	-3	2
494	67.341	1.3894	1	5	5
495	67.424	1.3879	2	3	7
496	67.426	1.3878	2	-4	4
497	67.484	1.3868	-3	2	6
498	67.512	1.3863	4	-1	5
499	67.519	1.3862	1	1	8
500	67.757	1.3819	-3	4	4
501	67.770	1.3816	1	-3	6
502	67.823	1.3807	5	-1	2
503	67.842	1.3803	0	-2	7
504	68.112	1.3755	3	4	5
505	68.218	1.3736	0	0	8
506	68.280	1.3726	-5	0	2
507	68.301	1.3722	0	2	8
508	68.358	1.3712	5	0	3
509	68.398	1.3705	3	1	7
510	68.485	1.3689	5	2	1
511	68.490	1.3689	1	-2	7
512	68.497	1.3687	0	-5	3
513	68.508	1.3685	5	1	3
514	68.683	1.3655	1	0	8
515	68.703	1.3651	1	2	8
516	68.810	1.3633	-2	-4	4
517	68.841	1.3627	-1	5	5
518	68.864	1.3623	-3	-1	6
519	68.996	1.3600	-1	-3	6
520	69.033	1.3594	-5	1	2
521	69.043	1.3592	5	2	0
522	69.084	1.3585	0	-4	5
523	69.090	1.3584	3	-4	3
524	69.135	1.3577	5	2	2
525	69.208	1.3564	4	4	1
526	69.332	1.3543	3	0	7
527	69.356	1.3539	-4	1	5
528	69.469	1.3519	-1	1	8
529	69.495	1.3515	-4	0	5
530	69.506	1.3513	2	-5	2
531	69.535	1.3508	4	-3	3
532	69.537	1.3508	-2	-1	7
533	69.563	1.3503	-2	5	4
534	69.672	1.3485	-5	2	0
535	69.704	1.3480	1	-5	3
536	69.744	1.3473	3	5	1
537	69.769	1.3469	3	5	2
538	69.796	1.3464	3	2	7
539	69.811	1.3461	0	4	7
540	69.814	1.3461	-2	-5	2
541	69.860	1.3453	-5	-1	2
542	70.006	1.3429	-1	-2	7

543	70.022	1.3426	1	-4	5
544	70.091	1.3415	-1	-5	3
545	70.130	1.3408	3	-2	6
546	70.216	1.3394	4	4	0
547	70.257	1.3387	5	-2	1
548	70.263	1.3386	1	4	7
549	70.276	1.3384	4	1	6
550	70.286	1.3382	-5	2	1
551	70.295	1.3381	-4	-2	4
552	70.386	1.3365	-2	4	6
553	70.479	1.3350	0	6	1
554	70.534	1.3341	5	-1	3
555	70.555	1.3338	-1	0	8
556	70.570	1.3335	0	6	2
557	70.608	1.3329	4	3	5
558	70.628	1.3326	3	-3	5
559	70.700	1.3314	-1	2	8
560	70.792	1.3299	4	4	3
561	70.796	1.3298	-5	-2	1
562	70.804	1.3297	2	5	5
563	70.915	1.3279	3	5	0
564	70.936	1.3275	-1	-4	5
565	70.947	1.3274	4	0	6
566	70.977	1.3269	5	2	3
567	70.989	1.3267	3	5	3
568	71.022	1.3261	-4	3	4
569	71.087	1.3251	-2	3	7
570	71.143	1.3242	-4	4	1
571	71.214	1.3230	-4	4	0
572	71.355	1.3208	2	-3	6
573	71.379	1.3204	-3	5	1
574	71.528	1.3180	-4	2	5
575	71.536	1.3179	1	6	2
576	71.561	1.3175	1	6	1
577	71.578	1.3172	-4	-3	3
578	71.580	1.3172	0	6	0
579	71.655	1.3160	0	-1	8
580	71.676	1.3156	-3	3	6
581	71.817	1.3134	0	3	8
582	71.831	1.3132	5	1	4
583	71.847	1.3129	-3	5	0
584	71.849	1.3129	0	6	3
585	71.858	1.3127	-5	0	3
586	71.869	1.3126	0	5	6
587	71.912	1.3119	2	-2	7
588	71.924	1.3117	2	0	8
589	71.940	1.3115	-4	-1	5
590	71.965	1.3111	5	0	4
591	72.027	1.3101	5	-2	2
592	72.086	1.3092	-5	2	2
593	72.097	1.3090	-3	5	2
594	72.134	1.3084	-1	4	7
595	72.140	1.3083	1	-1	8
596	72.164	1.3079	-1	6	1
597	72.179	1.3077	1	3	8
598	72.258	1.3065	-4	4	2
599	72.314	1.3056	-5	1	3
600	72.361	1.3049	-3	4	5
601	72.369	1.3047	-1	6	2
602	72.399	1.3043	1	5	6
603	72.403	1.3042	-4	-4	1
604	72.470	1.3032	4	-4	1
605	72.536	1.3021	4	-2	5
606	72.693	1.2997	1	6	3
607	72.770	1.2985	1	6	0
608	73.140	1.2929	-1	6	0
609	73.196	1.2920	3	4	6
610	73.258	1.2911	-3	-5	1
611	73.350	1.2897	4	4	4
612	73.380	1.2892	3	5	4
613	73.462	1.2880	-3	1	7
614	73.465	1.2879	2	4	7
615	73.467	1.2879	3	3	7
616	73.493	1.2875	3	-5	1
617	73.530	1.2870	-3	-3	5
618	73.652	1.2851	2	-5	3
619	73.684	1.2847	-5	-1	3
620	73.704	1.2844	2	-4	5
621	73.707	1.2843	-5	-2	2
622	73.726	1.2840	-2	5	5
623	73.745	1.2838	-2	-3	6
624	73.750	1.2837	-1	6	3
625	73.801	1.2829	5	3	1

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626	73.850	1.2822	0	-6	1
627	73.895	1.2815	4	-1	6
628	73.911	1.2813	-3	-2	6
629	73.914	1.2812	-1	-1	8
630	73.975	1.2803	5	2	4
631	73.987	1.2802	-3	5	3
632	74.027	1.2796	3	-4	4
633	74.068	1.2790	4	-3	4
634	74.071	1.2789	0	-5	4
635	74.081	1.2788	-1	5	6
636	74.153	1.2777	5	3	2
637	74.185	1.2772	-3	0	7
638	74.197	1.2770	-1	3	8
639	74.292	1.2756	0	6	4
640	74.374	1.2745	5	-1	4
641	74.409	1.2739	-2	-5	3
642	74.538	1.2720	-4	4	3
643	74.556	1.2718	-2	1	8
644	74.619	1.2709	5	3	0
645	74.872	1.2672	-2	-2	7
646	74.888	1.2670	4	-4	2
647	74.949	1.2661	5	-2	3
648	75.003	1.2653	-3	2	7
649	75.012	1.2652	1	6	4
650	75.036	1.2648	-5	2	3
651	75.127	1.2635	1	-5	4
652	75.139	1.2634	-1	-6	1
653	75.223	1.2622	2	6	2
654	75.266	1.2615	2	3	8
655	75.278	1.2614	1	-6	1
656	75.350	1.2603	2	-1	8
657	75.362	1.2602	2	6	1
658	75.491	1.2583	-2	-4	5
659	75.533	1.2577	-5	3	0
660	75.553	1.2575	0	-3	7
661	75.582	1.2571	-2	0	8
662	75.649	1.2561	2	5	6
663	75.670	1.2558	5	3	3
664	75.728	1.2550	-4	-4	2
665	75.730	1.2550	-1	-5	4
666	75.783	1.2542	-2	2	8
667	75.783	1.2542	4	3	6
668	75.853	1.2532	-5	3	1
669	75.930	1.2522	-4	3	5
670	76.021	1.2509	-3	-4	4
671	76.027	1.2508	-4	1	6
672	76.202	1.2484	1	-3	7
673	76.247	1.2477	2	6	3
674	76.254	1.2476	5	1	5
675	76.283	1.2472	-1	6	4
676	76.286	1.2472	3	-5	2
677	76.375	1.2460	5	-3	1
678	76.436	1.2451	-4	0	6
679	76.526	1.2439	-5	0	4
680	76.543	1.2436	-2	6	1
681	76.595	1.2429	-5	-3	1
682	76.600	1.2429	-4	-2	5
683	76.634	1.2424	3	1	8
684	76.660	1.2420	5	0	5
685	76.661	1.2420	2	6	0
686	76.689	1.2416	0	-4	6
687	76.697	1.2415	-5	1	4
688	76.732	1.2411	-3	-5	2
689	76.856	1.2394	-2	6	2
690	76.879	1.2390	0	1	9
691	76.900	1.2388	3	5	5
692	76.964	1.2379	-4	-3	4
693	77.017	1.2372	-3	5	4
694	77.032	1.2370	4	4	5
695	77.129	1.2357	-2	4	7
696	77.149	1.2354	-3	-1	7
697	77.170	1.2351	4	1	7
698	77.180	1.2350	1	1	9
699	77.251	1.2340	0	-6	2
700	77.266	1.2338	0	-2	8
701	77.329	1.2330	-5	3	2
702	77.386	1.2322	-2	6	0
703	77.478	1.2310	1	-4	6
704	77.504	1.2306	0	4	8
705	77.564	1.2298	3	-3	6
706	77.598	1.2294	-1	-3	7
707	77.700	1.2280	3	2	8
708	77.731	1.2276	-5	-2	3

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709	77.761	1.2272	0	2	9
710	77.769	1.2271	1	-2	8
711	77.802	1.2266	3	0	8
712	77.826	1.2263	1	4	8
713	77.854	1.2260	-4	2	6
714	77.861	1.2259	0	6	5
715	77.947	1.2247	-4	4	4
716	77.962	1.2245	3	-2	7
717	78.004	1.2240	-3	4	6
718	78.030	1.2236	1	2	9
719	78.067	1.2231	0	5	7
720	78.082	1.2229	5	2	5
721	78.091	1.2228	4	0	7
722	78.228	1.2210	0	0	9
723	78.321	1.2198	-2	6	3
724	78.366	1.2192	5	-3	2
725	78.429	1.2184	4	-4	3
726	78.458	1.2180	1	6	5
727	78.470	1.2179	1	5	7
728	78.476	1.2178	4	2	7
729	78.547	1.2169	1	-6	2
730	78.557	1.2167	1	0	9
731	78.583	1.2164	-1	-4	6
732	78.585	1.2164	-5	-1	4
733	78.634	1.2157	-1	-6	2
734	78.762	1.2141	-3	3	7
735	78.831	1.2132	-2	-1	8
736	78.861	1.2128	2	-5	4
737	78.919	1.2121	4	5	2
738	78.952	1.2116	-2	5	6
739	78.981	1.2113	5	-2	4
740	79.007	1.2109	4	5	1
741	79.027	1.2107	4	-2	6
742	79.071	1.2101	-4	-1	6
743	79.095	1.2098	-5	2	4
744	79.102	1.2097	-2	-6	1
745	79.229	1.2081	-2	3	8
746	79.257	1.2077	-1	1	9
747	79.291	1.2073	5	-1	5
748	79.295	1.2073	3	4	7
749	79.375	1.2062	2	-6	1
750	79.440	1.2054	-1	-2	8
751	79.527	1.2043	2	-3	7
752	79.646	1.2028	4	-3	5
753	79.701	1.2021	-5	-3	2
754	79.703	1.2021	6	0	1
755	79.800	1.2009	6	0	0
756	79.855	1.2002	-1	4	8
757	79.935	1.1992	-1	6	5
758	79.942	1.1991	-5	3	3
759	79.977	1.1987	4	5	3
760	79.990	1.1985	3	-4	5
761	80.048	1.1978	-2	-5	4
762	80.150	1.1965	-4	-4	3
763	80.150	1.1965	2	1	9
764	80.161	1.1964	-1	2	9
765	80.192	1.1960	3	-5	3
766	80.240	1.1954	4	5	0
767	80.332	1.1943	-1	5	7
768	80.358	1.1939	6	1	1
769	80.565	1.1914	-1	0	9
770	80.638	1.1905	0	-5	5
771	80.725	1.1894	6	1	0
772	80.749	1.1891	6	0	2
773	80.812	1.1884	2	4	8
774	80.852	1.1879	0	3	9
775	80.920	1.1871	-2	6	4
776	80.928	1.1870	2	-4	6
777	80.934	1.1869	2	-2	8
778	80.962	1.1865	2	2	9
779	80.973	1.1864	3	3	8
780	81.039	1.1856	-6	0	1
781	81.044	1.1855	-3	-3	6
782	81.083	1.1851	-6	1	0
783	81.089	1.1850	1	3	9
784	81.094	1.1849	-4	5	1
785	81.131	1.1845	6	1	2
786	81.153	1.1842	-3	5	5
787	81.174	1.1840	3	-1	8
788	81.187	1.1838	5	4	1
789	81.220	1.1834	4	-1	7
790	81.257	1.1830	6	-1	1
791	81.259	1.1830	5	4	2

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792	81.297	1.1825	-3	-5	3
793	81.433	1.1809	-4	5	0
794	81.483	1.1803	5	-3	3
795	81.508	1.1800	3	6	2
796	81.510	1.1799	3	5	6
797	81.531	1.1797	2	5	7
798	81.544	1.1795	2	0	9
799	81.558	1.1794	1	-5	5
800	81.711	1.1775	2	6	5
801	81.734	1.1773	5	1	6
802	81.746	1.1771	0	-6	3
803	81.755	1.1770	3	6	1
804	81.777	1.1768	0	-1	9
805	81.800	1.1765	4	4	6
806	81.874	1.1756	-4	3	6
807	81.894	1.1754	-4	5	2
808	81.981	1.1744	4	3	7
809	82.048	1.1736	-6	1	1
810	82.102	1.1729	5	3	5
811	82.133	1.1726	1	-1	9
812	82.140	1.1725	-5	1	5
813	82.169	1.1721	4	5	4
814	82.174	1.1721	-3	1	8
815	82.231	1.1714	-6	-1	1
816	82.242	1.1713	-5	0	5
817	82.253	1.1712	5	4	0
818	82.280	1.1708	-2	-3	7
819	82.282	1.1708	-3	-2	7
820	82.368	1.1698	-1	-5	5
821	82.399	1.1695	3	6	3
822	82.403	1.1694	5	0	6
823	82.451	1.1688	-4	4	5
824	82.469	1.1686	5	4	3
825	82.488	1.1684	2	-6	2
826	82.520	1.1680	0	6	6
827	82.569	1.1675	6	-1	2
828	82.604	1.1671	-3	-4	5
829	82.605	1.1671	-4	-5	1
830	82.660	1.1664	-2	-6	2
831	82.830	1.1645	-5	-2	4
832	82.907	1.1636	4	-5	1
833	82.914	1.1635	1	-6	3
834	82.929	1.1633	6	0	3
835	83.039	1.1621	6	1	3
836	83.063	1.1618	4	-4	4
837	83.111	1.1612	-2	-4	6
838	83.137	1.1609	3	6	0
839	83.143	1.1609	-3	0	8
840	83.209	1.1601	6	2	1
841	83.221	1.1600	-1	-6	3
842	83.261	1.1595	-1	3	9
843	83.262	1.1595	5	2	6
844	83.370	1.1583	-4	-3	5
845	83.399	1.1580	-3	2	8
846	83.408	1.1579	-6	0	2
847	83.440	1.1575	-5	4	0
848	83.483	1.1570	-5	4	1
849	83.487	1.1570	-3	6	1
850	83.643	1.1552	-4	1	7
851	83.669	1.1549	-5	3	4
852	83.709	1.1545	6	2	2
853	83.827	1.1531	-4	5	3
854	83.843	1.1529	6	2	0
855	83.878	1.1526	-4	-2	6
856	83.904	1.1523	-3	6	2
857	83.911	1.1522	-5	-3	3
858	83.967	1.1516	2	3	9
859	84.062	1.1505	-1	-1	9
860	84.092	1.1502	5	-2	5
861	84.143	1.1496	-6	1	2
862	84.203	1.1489	-3	6	0
863	84.238	1.1486	-2	-2	8
864	84.256	1.1483	-2	1	9
865	84.311	1.1477	-4	0	7
866	84.421	1.1465	3	6	4
867	84.449	1.1462	-5	-4	1
868	84.530	1.1453	5	-4	1
869	84.536	1.1453	-5	-1	5
870	84.549	1.1451	0	7	2
871	84.554	1.1451	-6	2	0
872	84.633	1.1442	-2	6	5
873	84.657	1.1439	-5	4	2
874	84.663	1.1439	-3	4	7

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875	84.678	1.1437	-1	6	6
876	84.732	1.1431	0	7	1
877	84.807	1.1423	5	4	4
878	84.826	1.1421	-2	4	8
879	84.862	1.1417	-6	-1	2
880	84.946	1.1408	0	-3	8
881	84.995	1.1402	6	-2	1
882	85.007	1.1401	6	-1	3
883	85.010	1.1401	4	1	8
884	85.110	1.1390	2	-5	5
885	85.123	1.1389	2	-1	9
886	85.162	1.1384	-4	2	7
887	85.179	1.1382	-2	2	9
888	85.183	1.1382	3	-5	4
889	85.191	1.1381	0	-4	7
890	85.217	1.1378	-2	5	7
891	85.243	1.1376	-6	2	1
892	85.257	1.1374	0	5	8
893	85.260	1.1374	5	-1	6
894	85.339	1.1365	6	2	3
895	85.437	1.1355	1	7	2
896	85.449	1.1353	3	-3	7
897	85.451	1.1353	-3	6	3
898	85.468	1.1351	1	-3	8
899	85.481	1.1350	4	5	5
900	85.497	1.1348	0	7	3
901	85.508	1.1347	4	-5	2
902	85.520	1.1346	-2	0	9
903	85.543	1.1343	1	5	8
904	85.607	1.1337	-6	-2	1
905	85.644	1.1333	-4	-4	4
906	85.645	1.1332	-3	-6	1
907	85.705	1.1326	5	-3	4
908	85.727	1.1324	3	1	9
909	85.730	1.1323	1	7	1
910	85.853	1.1310	1	-4	7
911	86.022	1.1292	4	2	8
912	86.045	1.1290	0	7	0
913	86.048	1.1290	3	-6	1
914	86.069	1.1287	6	1	4
915	86.087	1.1286	-4	-5	2
916	86.102	1.1284	0	4	9
917	86.107	1.1283	2	6	6
918	86.181	1.1276	4	0	8
919	86.227	1.1271	6	0	4
920	86.257	1.1268	4	-3	6
921	86.273	1.1266	1	7	3
922	86.290	1.1264	-1	7	2
923	86.296	1.1264	-3	-1	8
924	86.307	1.1262	1	4	9
925	86.363	1.1257	-1	7	1
926	86.372	1.1256	-3	5	6
927	86.402	1.1253	3	4	8
928	86.500	1.1242	3	2	9
929	86.508	1.1241	4	-2	7
930	86.565	1.1236	6	-2	2
931	86.700	1.1221	3	-2	8
932	86.707	1.1221	2	-6	3
933	86.719	1.1219	-2	-5	5
934	86.746	1.1217	5	-4	2
935	86.805	1.1211	-3	3	8
936	86.881	1.1203	-4	5	4
937	86.894	1.1201	-6	0	3
938	86.937	1.1197	-3	-5	4
939	86.958	1.1195	-5	4	3
940	86.968	1.1194	5	3	6
941	86.973	1.1193	3	-4	6
942	87.051	1.1185	-1	-3	8
943	87.060	1.1184	-6	2	2
944	87.135	1.1177	3	0	9
945	87.150	1.1175	1	7	0
946	87.156	1.1174	-1	-4	7
947	87.162	1.1174	-4	-1	7
948	87.194	1.1171	3	5	7
949	87.318	1.1158	-2	-6	3
950	87.319	1.1158	0	-6	4
951	87.346	1.1155	-1	7	3
952	87.358	1.1154	-6	1	3
953	87.423	1.1147	0	1	10
954	87.477	1.1142	0	-2	9
955	87.563	1.1133	3	6	5
956	87.563	1.1133	-1	7	0
957	87.571	1.1132	0	7	4

958	87.596	1.1130	-1	5	8
959	87.607	1.1129	1	1	10
960	87.638	1.1125	4	4	7
961	87.764	1.1113	-5	-4	2
962	87.858	1.1103	1	-2	9
963	88.016	1.1087	0	2	10
964	88.035	1.1085	-4	4	6
965	88.092	1.1080	6	2	4
966	88.122	1.1077	-3	6	4
967	88.170	1.1072	1	2	10
968	88.210	1.1068	0	-5	6
969	88.224	1.1067	6	3	1
970	88.236	1.1065	1	7	4
971	88.257	1.1063	0	6	7
972	88.263	1.1063	5	4	5
973	88.266	1.1062	5	1	7
974	88.281	1.1061	-2	3	9
975	88.368	1.1052	1	-6	4
976	88.451	1.1044	2	5	8
977	88.482	1.1041	0	-7	1
978	88.493	1.1040	-6	-2	2
979	88.495	1.1040	-5	3	5
980	88.520	1.1037	-1	4	9
981	88.564	1.1033	6	-1	4
982	88.610	1.1028	-6	-1	3
983	88.613	1.1028	2	-3	8
984	88.622	1.1027	1	6	7
985	88.640	1.1025	-5	1	6
986	88.778	1.1012	4	-4	5
987	88.858	1.1004	-4	3	7
988	88.892	1.1001	-1	-6	4
989	88.945	1.0995	2	7	2
990	88.960	1.0994	-2	-1	9
991	88.999	1.0990	-5	-2	5
992	89.008	1.0989	-5	0	6
993	89.009	1.0989	1	-5	6
994	89.009	1.0989	0	0	10
995	89.015	1.0989	3	-6	2
996	89.122	1.0978	6	3	0
997	89.134	1.0977	2	4	9
998	89.135	1.0977	2	-4	7
999	89.196	1.0971	5	0	7
1000	89.212	1.0969	4	3	8
1001	89.214	1.0969	-5	-3	4
1002	89.221	1.0968	1	0	10
1003	89.226	1.0968	4	-5	3
1004	89.258	1.0965	6	-2	3
1005	89.271	1.0964	-3	-6	2
1006	89.347	1.0956	2	7	1
1007	89.450	1.0946	-2	6	6
1008	89.451	1.0946	3	3	9
1009	89.514	1.0940	5	2	7
1010	89.526	1.0939	-1	7	4
1011	89.529	1.0939	4	-1	8
1012	89.531	1.0939	-3	-3	7
1013	89.670	1.0925	2	7	3
1014	89.696	1.0923	-1	-7	1
1015	89.716	1.0921	-1	-2	9
1016	89.860	1.0907	-1	1	10
1017	89.889	1.0904	1	-7	1
1018	90.000	1.0894	-6	2	3

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