

Supporting information

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Effect of O-substitution in imidazole based Zn(II) dual fluorescent probes in the light of arsenate detection in potable water: A combined experimental and theoretical approach

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MASS

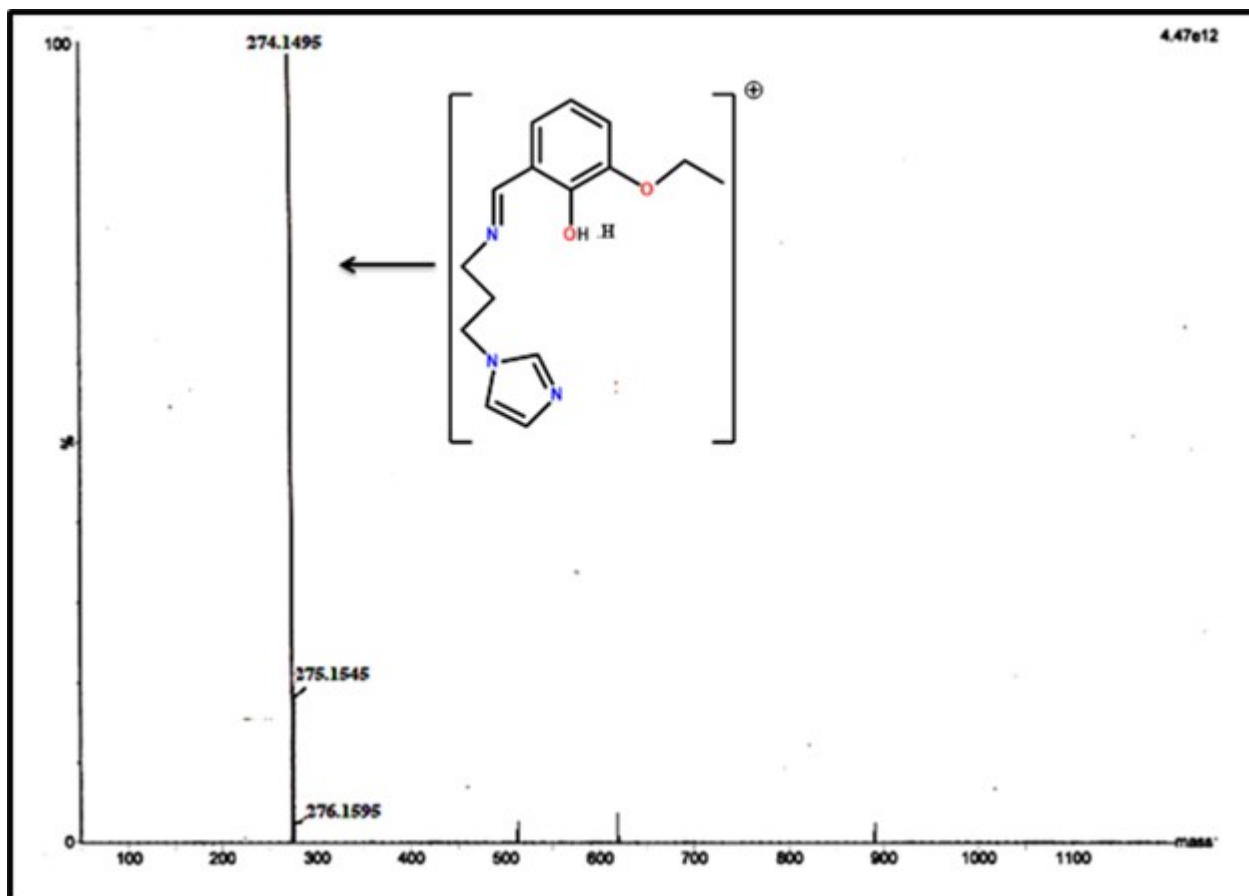


Fig. S1. ESI-MS spectrum of C1

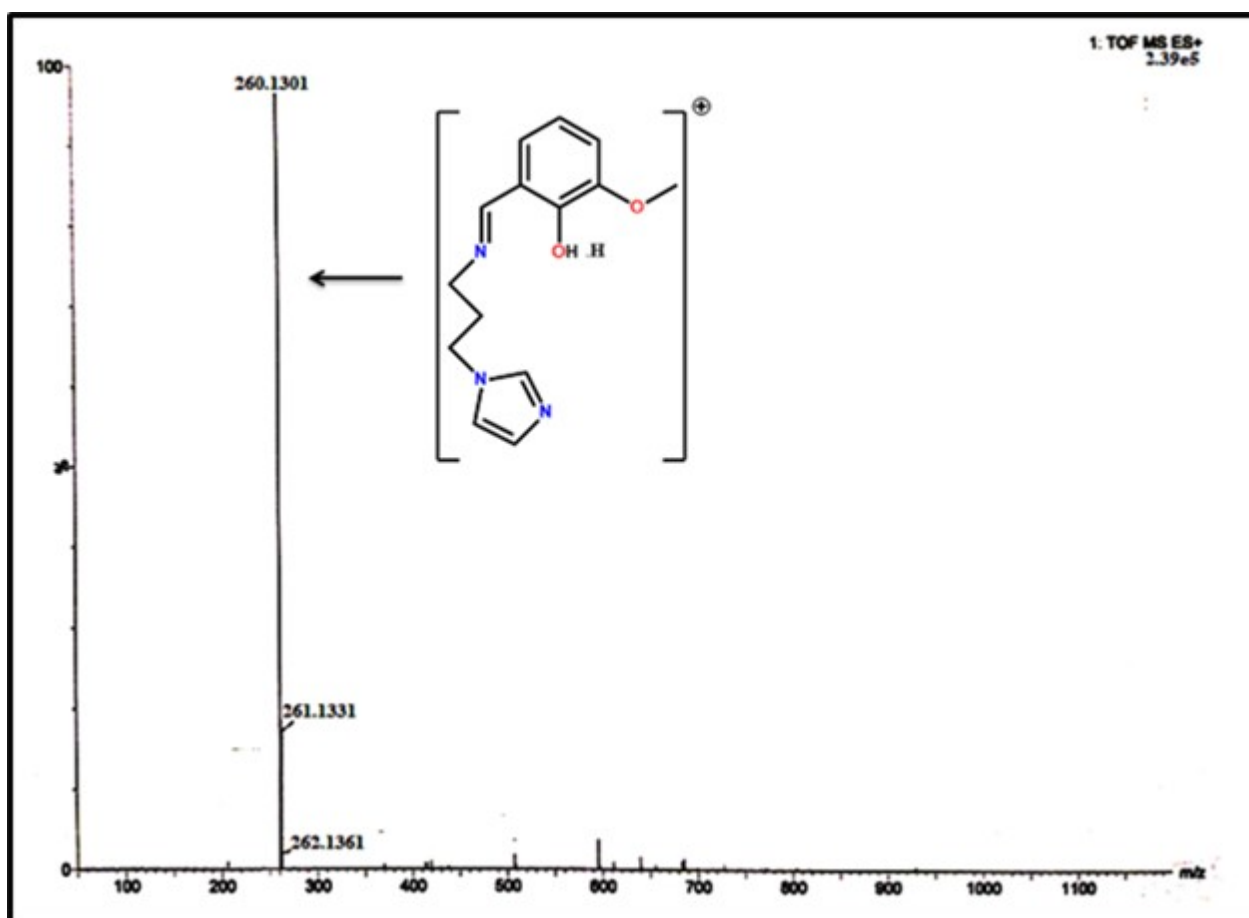


Fig. S2. ESI-MS spectrum of C2

NMR

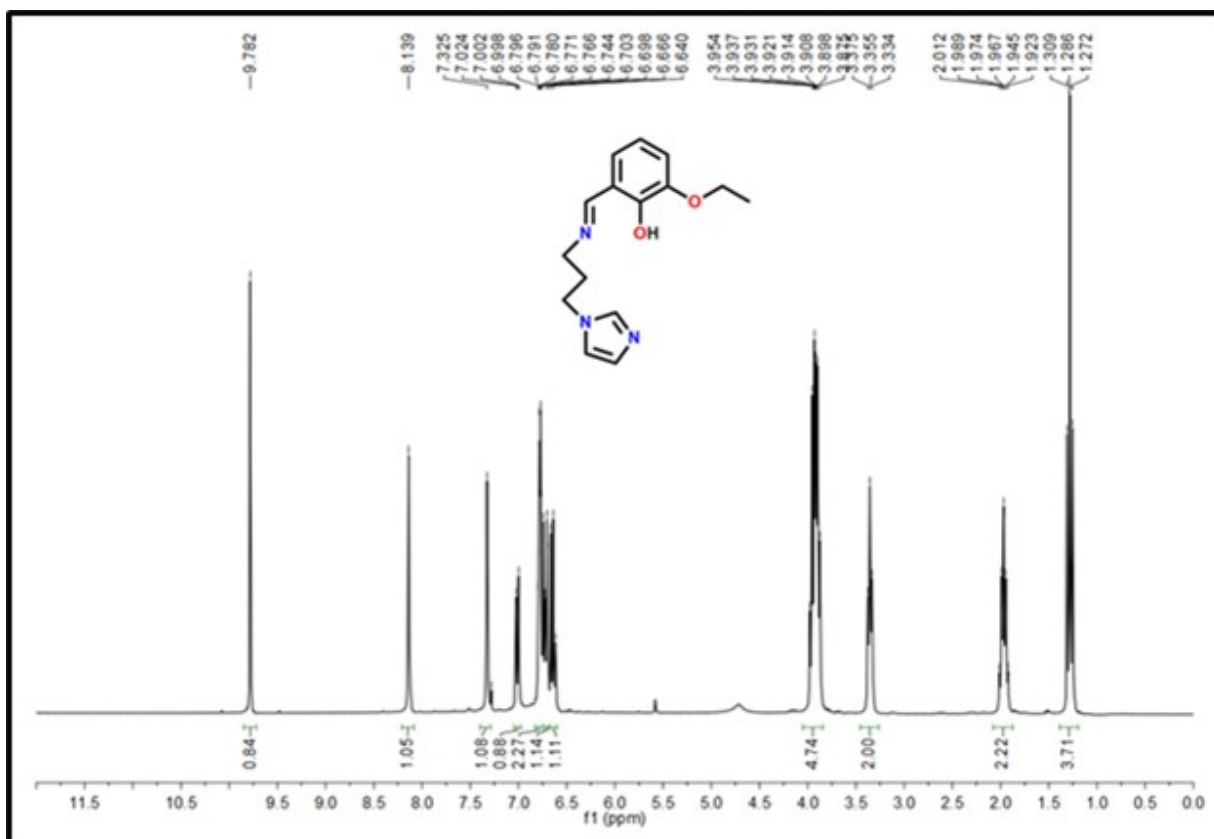


Fig. S3. NMR spectra of C1

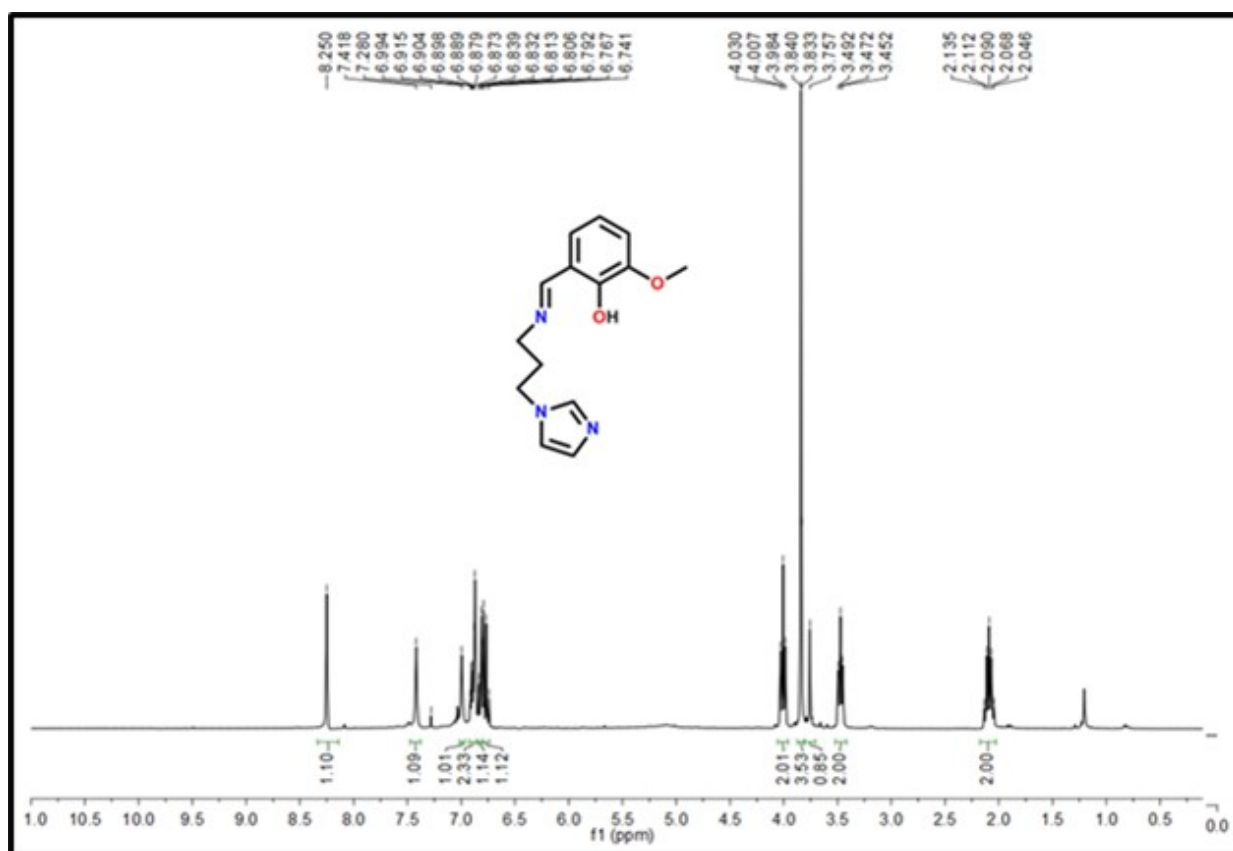


Fig. S4. NMR spectra of C2

FT-IR

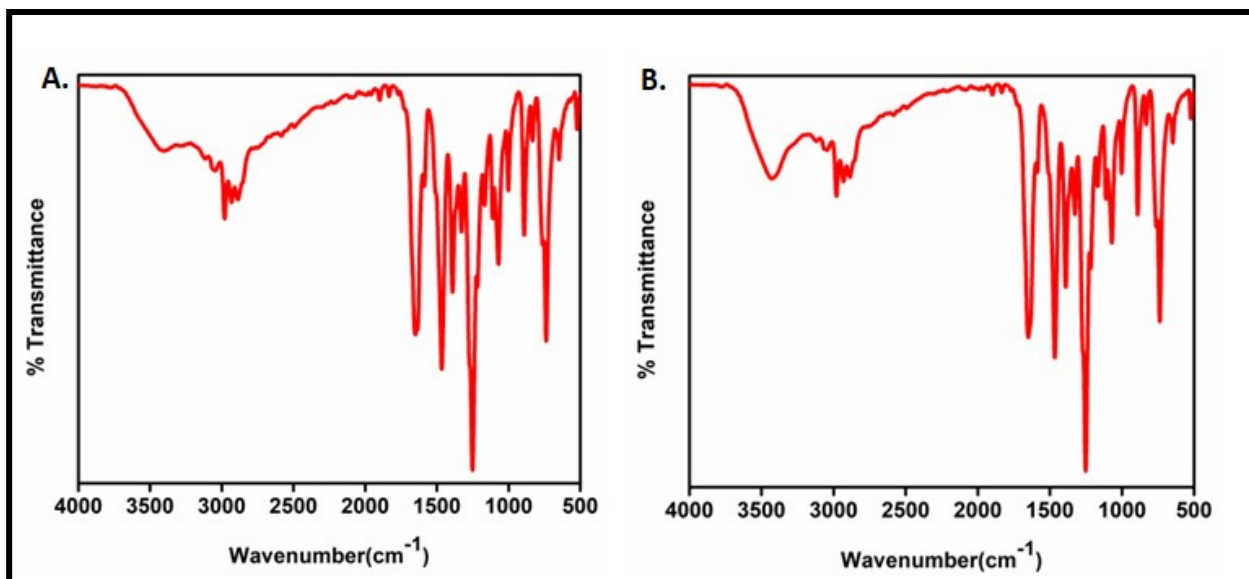


Fig. S5. FT-IR spectrum of (A) ligand C1 (B) ligand C2

UV-Vis

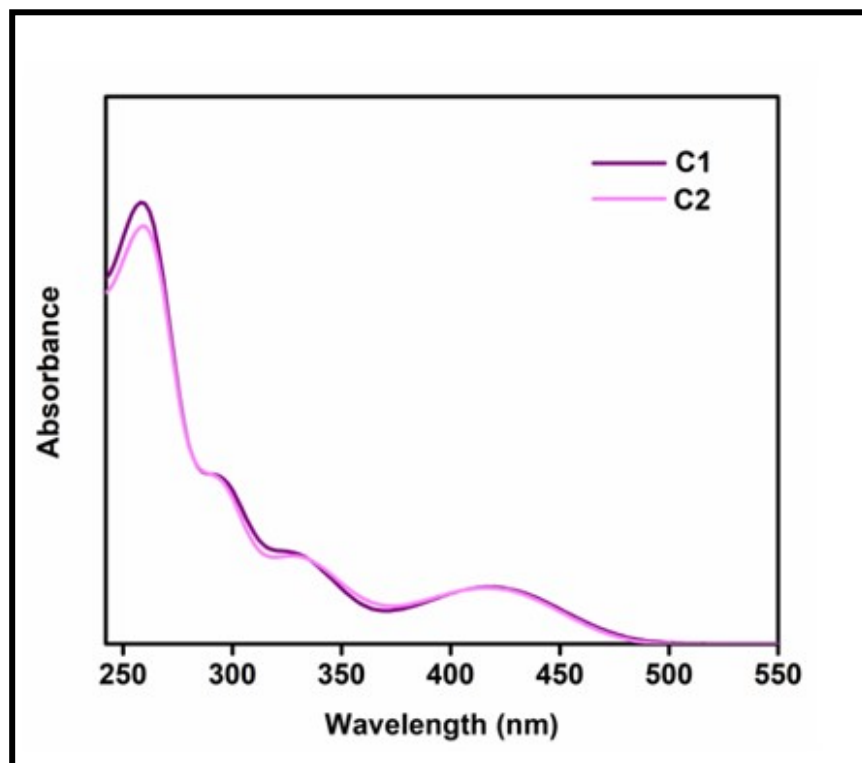


Fig. S6. UV-Vis spectra of ligands C1 and C2

Table S1. Coordination bond lengths (Å) and angles (°) for complex **D1**

I1-Zn1	2.5605(3)
Zn1-O1	1.9251(15)
Zn1-N1	2.0007(18)
Zn1-N3	2.0196(18)
O1-Zn1-N1	96.59(7)
O1- Zn1-N3	104.19(7)
N1-Zn1- N3	112.45(7)
O1-Zn1-I1	118.06(5)
N1-Zn1-I1	116.38(5)
N3-Zn1-I1	108.34(5)
C7- N1- Zn1	120.85(14)
C10- N1- Zn1	121.05(14)
C6- O1- Zn1	124.60(13)
C15- N3- Zn1	125.01(14)
C14-N3- Zn1	128.88(15)

Table S2. Coordination bond lengths (Å) and angles (°) for complex **D2**

I1- Zn1	2.5506(14)
O1- Zn1	1.910(6)
N1- Zn1	1.988(8)
N3- Zn1	1.994(8)
O1- Zn1- N1	96.9(3)
O1- Zn1- N3	103.8(3)
N1- Zn1- N3	111.8(3)
O1- Zn1- I1	118.2(2)
N1- Zn1- I1	115.6(2)
N3- Zn1- I1	109.6(3)
C7- N1- Zn1	119.3(7)
C10- N1- Zn1	122.0(7)
C6- O1- Zn1	126.0(7)
C15- N3- Zn1	125.5(8)
C14-N3- Zn1	131.1(8)

NMR

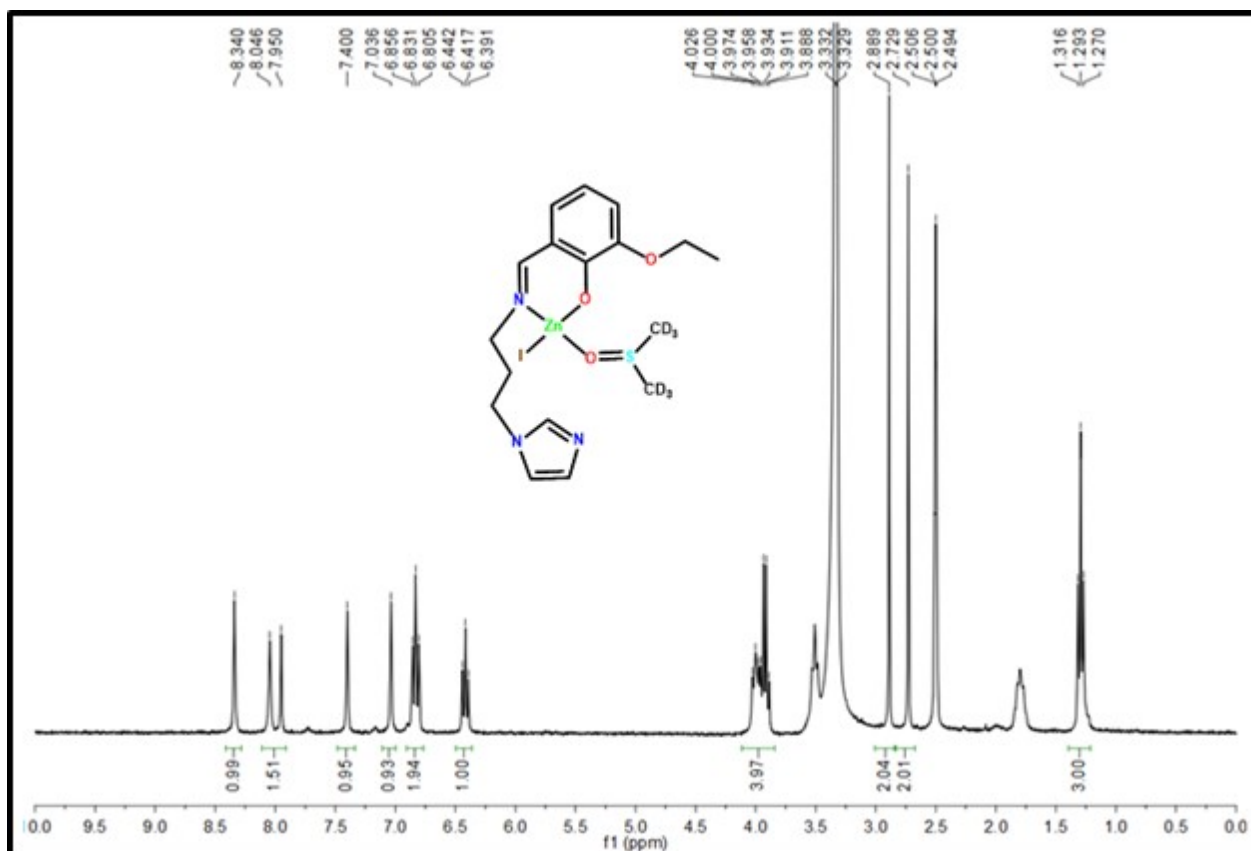


Fig. S7. NMR spectra of **D1**

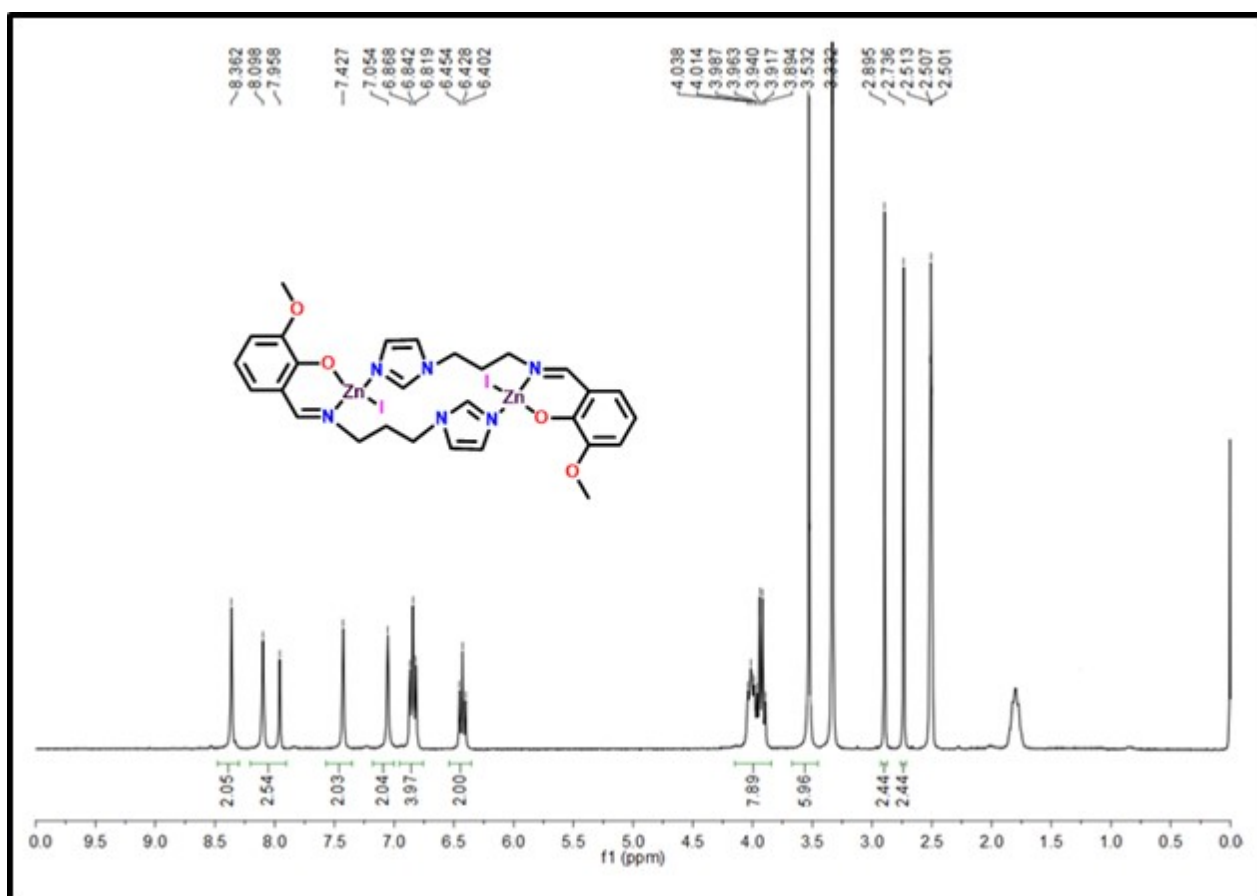


Fig. S8. NMR spectra of **D2**

FT-IR

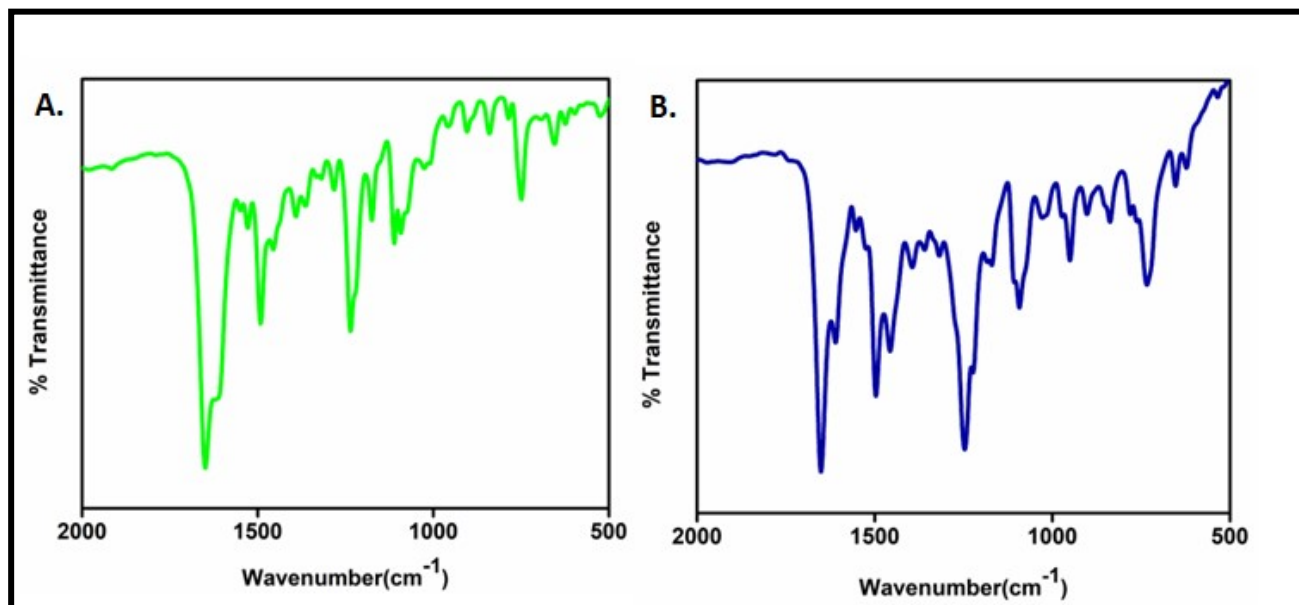


Fig. S9. FT-IR spectrum of complexes (A) D1 and (B) D2

UV-VIS

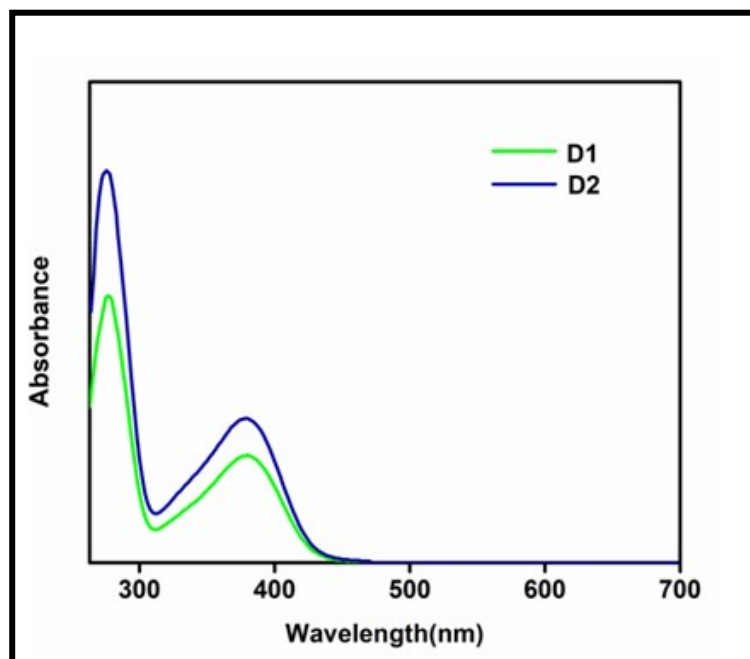


Fig. S10. UV-Vis spectra of complexes D1 and D2

MASS

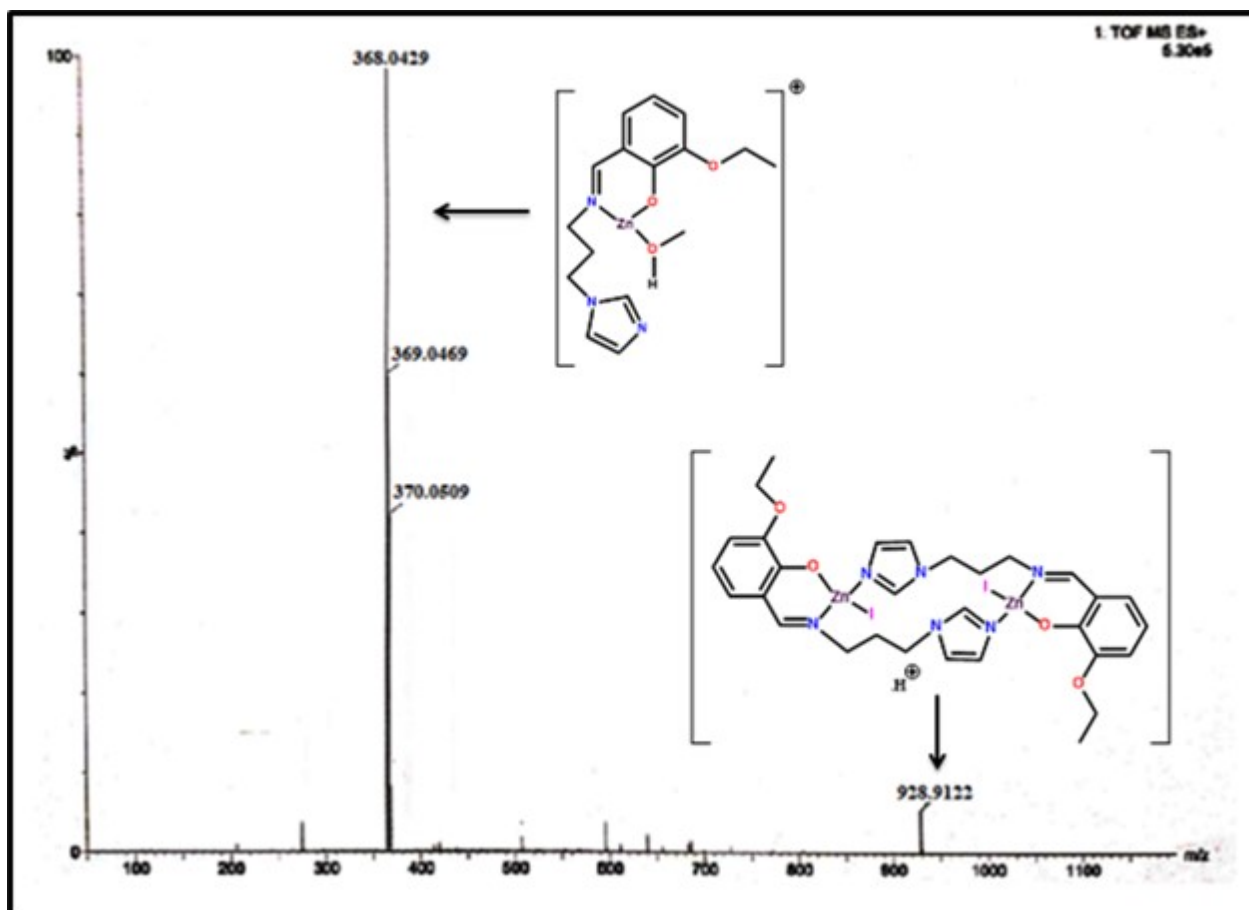


Fig. S11. ESI-MS spectrum of complex D1

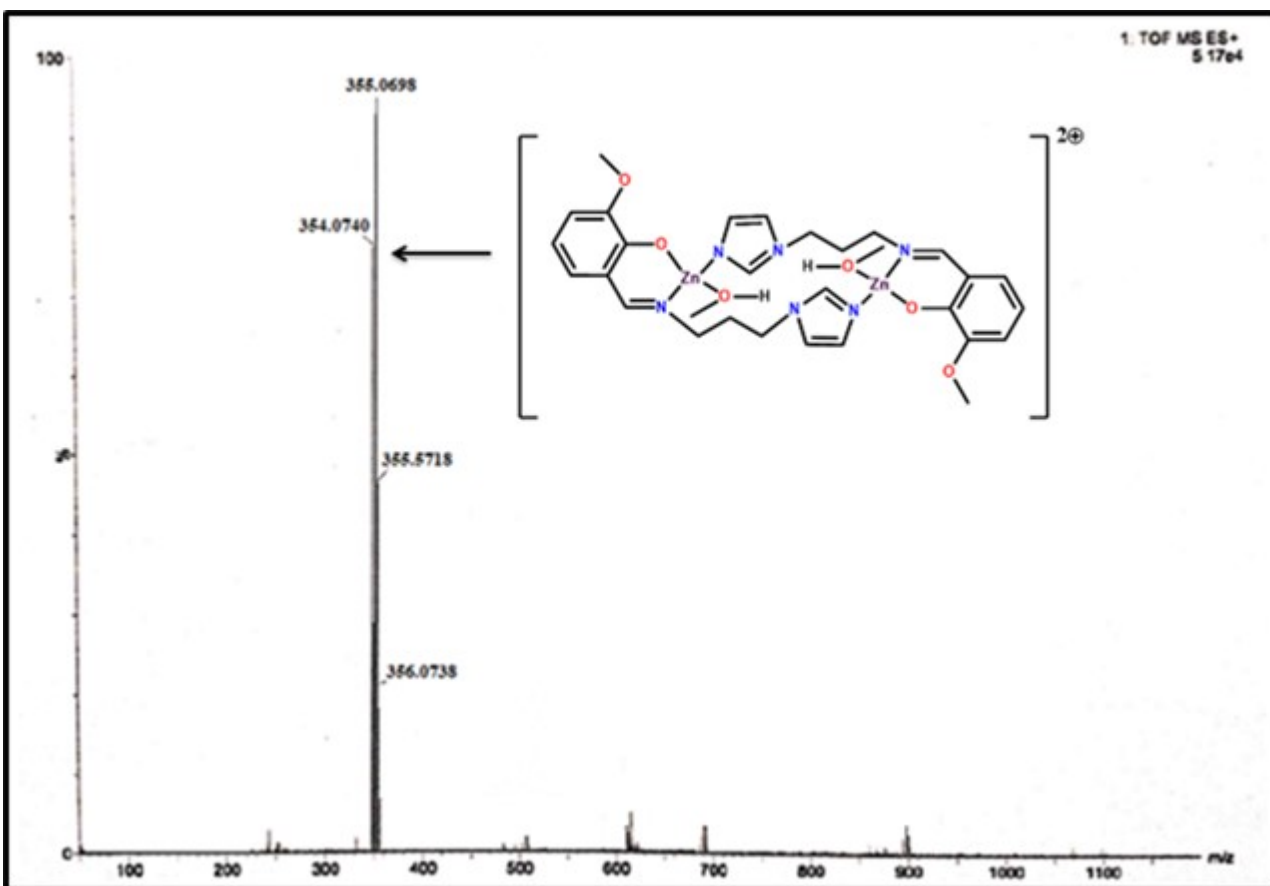


Fig. S12. ESI-MS spectrum of complex **D2**

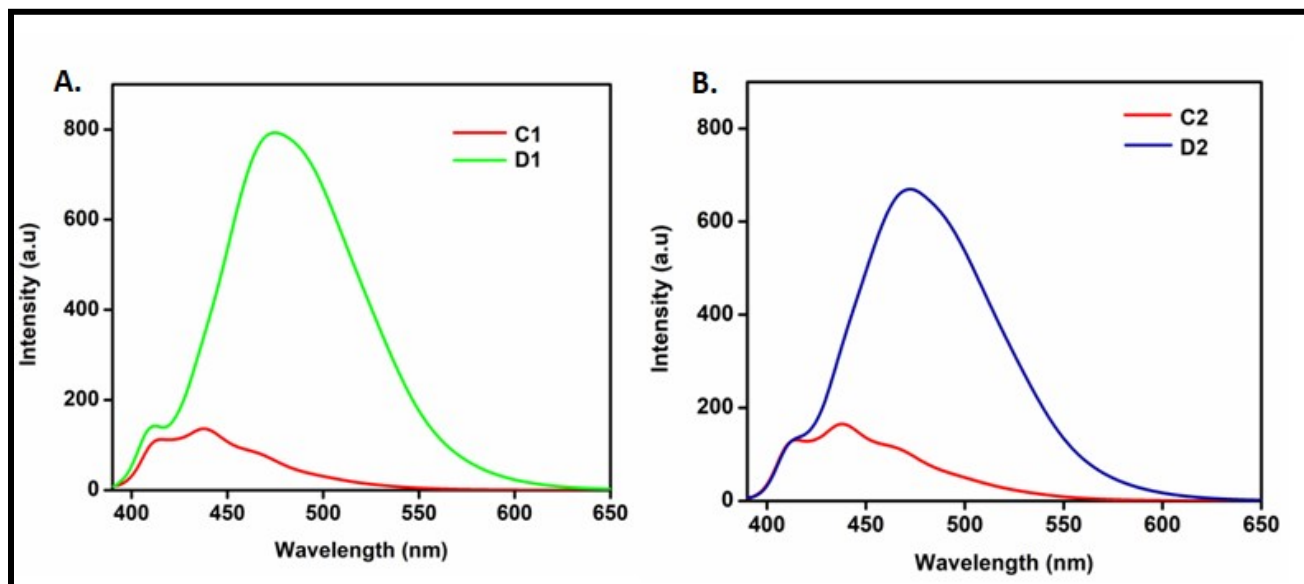


Fig. S13. Emission spectra of 4×10^{-5} (M) concentration of (A) ligands (C1,C2) and (B) complexes (D1 and D2) in 1:1 (v/v) MeOH-H₂O at 298 K within 380-650 nm

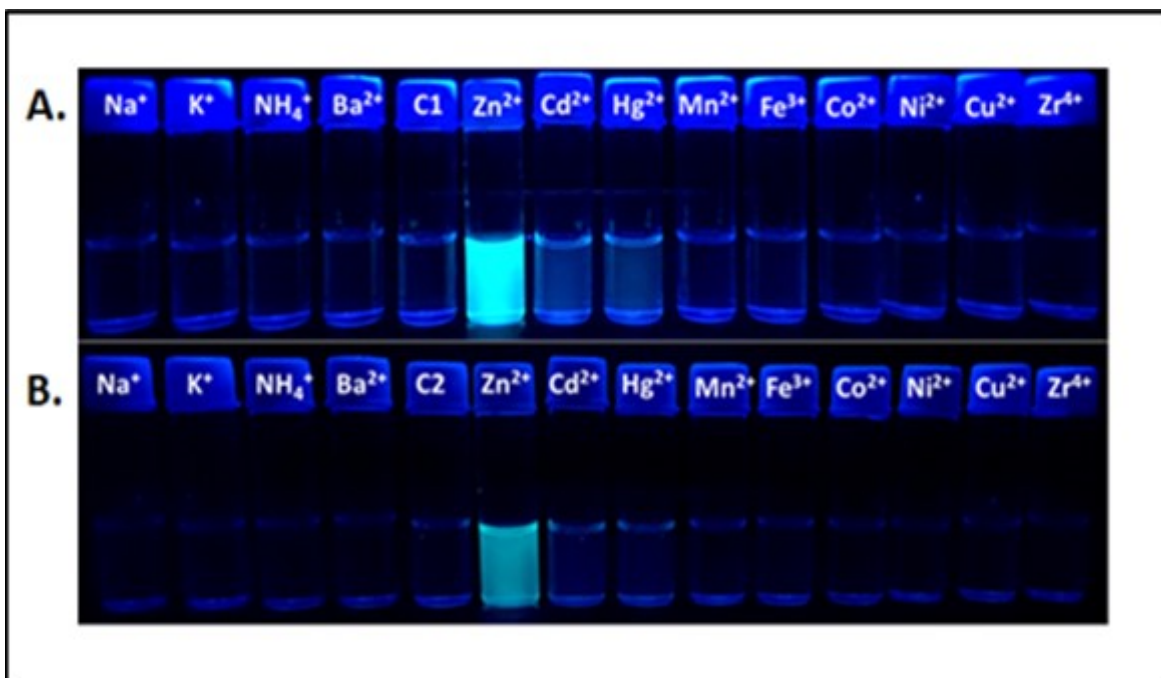


Fig. S14. Naked eye color changes upon addition of different cations (2.4×10^{-6} M) in 1:1 (v/v) MeOH-H₂O solution of (A) C1 and (B) C2 under UV light.

Table S3. Absorption and Emission Maxima (nm) and Quantum Yield of **C1**, **C2** and complexes **D1** and **D2**

Compounds	λ_{max} (abs)	λ_{max} (em)	Quantum Yield (ϕ_f)
C1	420 nm	438 nm	0.019
C2	420 nm	437 nm	0.017
D1	380 nm	474 nm	0.193
D2	379 nm	472 nm	0.048

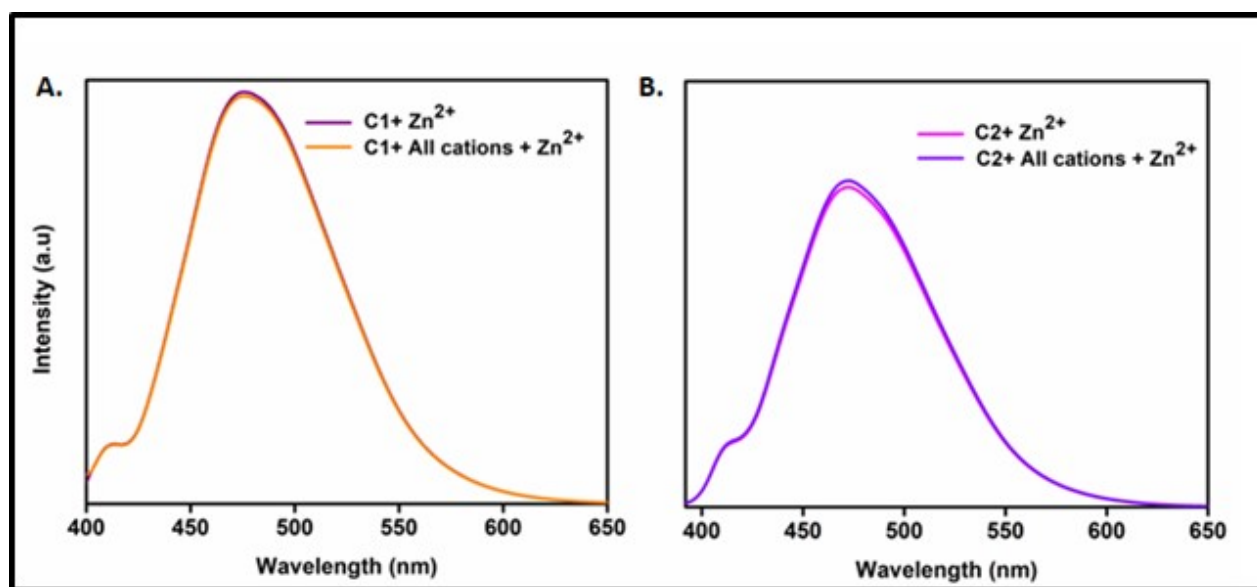


Fig. S15. Non-interference in the fluorescent band of (A) **C1** and (B) **C2** in presence of Zn²⁺ ion in the mixture of all metal ions in 1:1(v/v) MeOH-H₂O medium

Calculation of binding constant for complexes D1 and D2

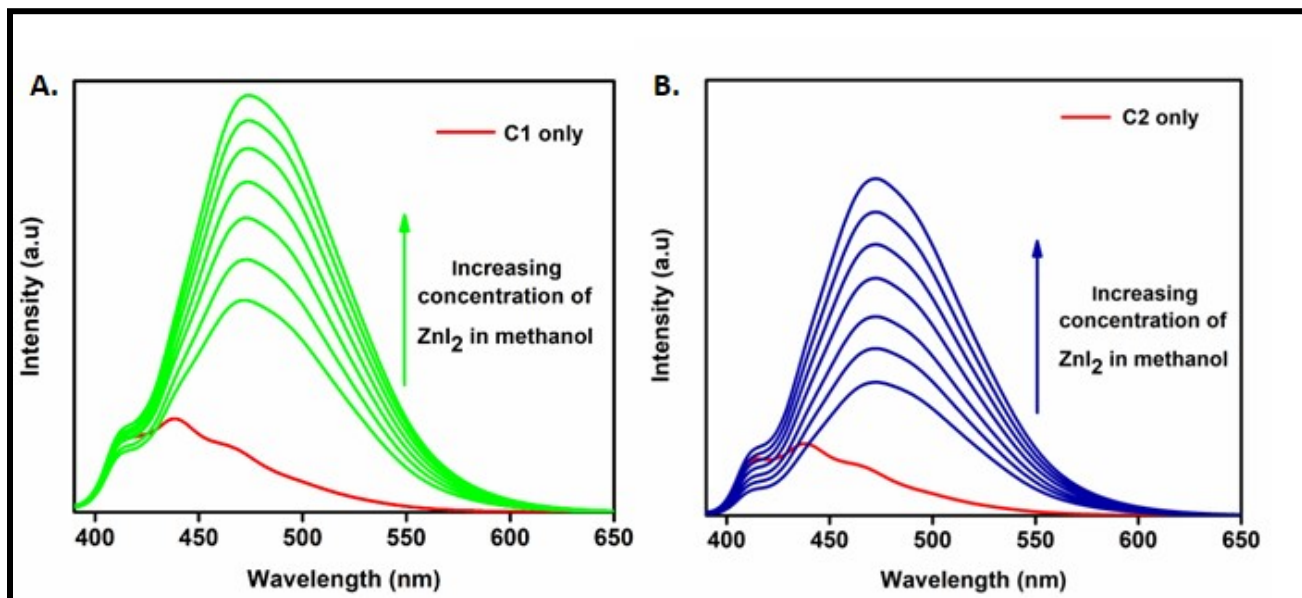


Fig. S16. Modification of emission spectra of (A) C1 (4 × 10⁻⁵ M) upon gradual addition of 2.5 × 10⁻⁶ M ZnI₂ (B) C2 (4 × 10⁻⁵ M) upon gradual addition of 2.5 × 10⁻⁶ M ZnI₂ in 1:1(v/v) MeOH-H₂O medium

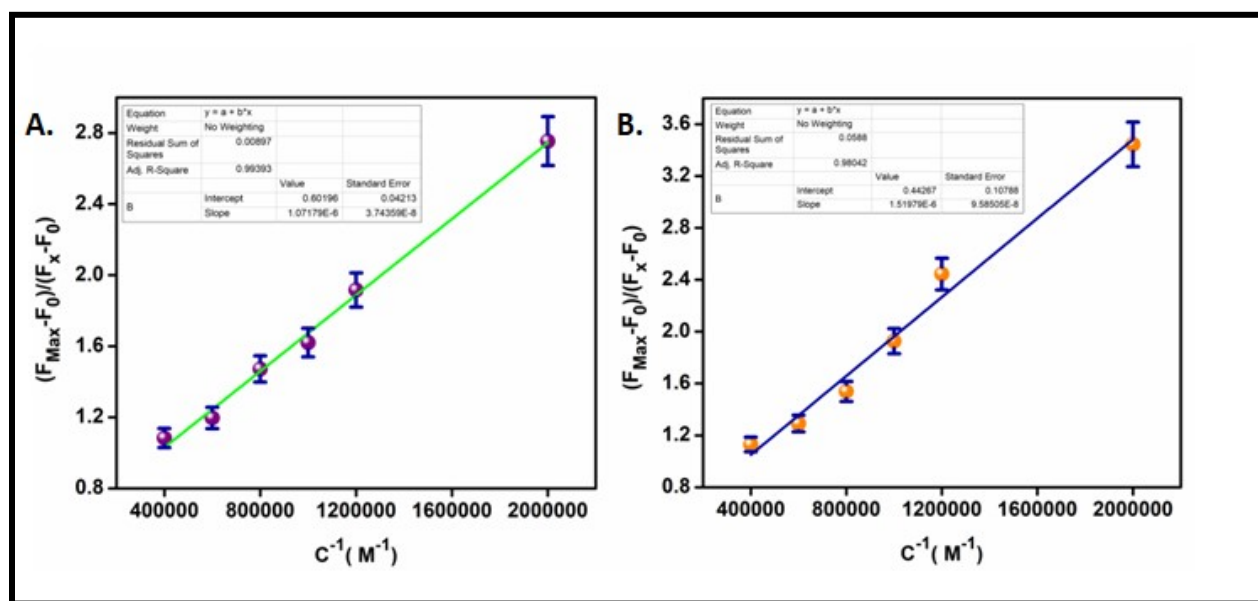


Fig. S17. Determination of binding constant of ligand and metal (A) for D1 and (B) for D2

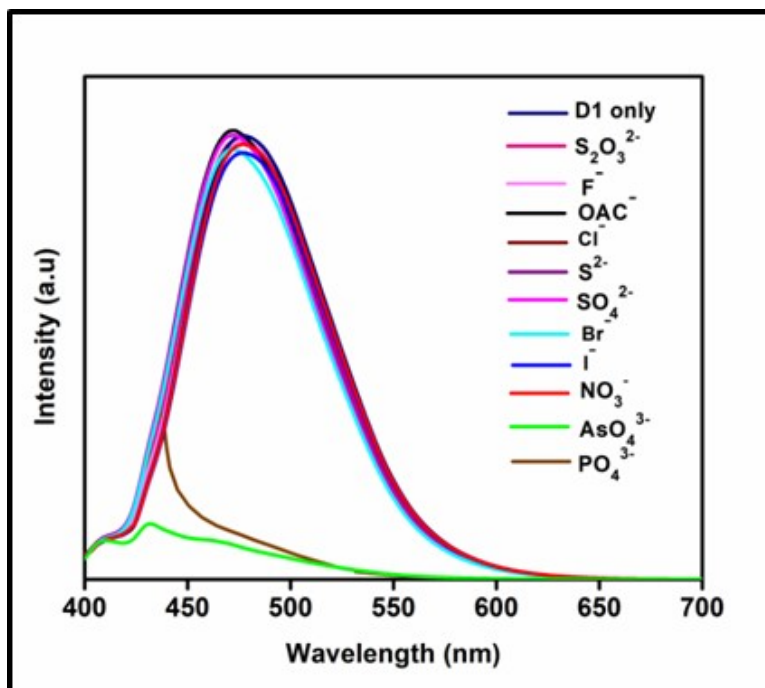


Fig. S18. Luminescence property of complex **D1** in presence of (2.4×10^{-6} M) different anions in 1:1(v/v) MeOH-H₂O medium

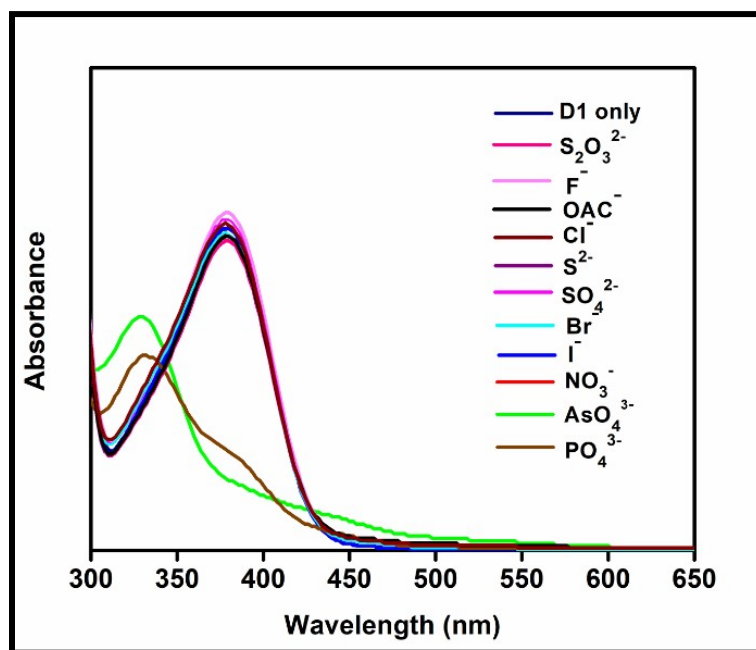


Fig. S19. Change in UV-Vis bands of complex **D1** in presence of (10^{-6} M) different anions in 1:1(v/v) MeOH-H₂O medium

Quenching of luminescence property in presence of AsO_4^{3-} solution

Further studies of photo luminescence property of complexes **D1** and **D2** was done in presence of AsO_4^{3-} solution in 1:1(v/v) MeOH- H_2O solution. To investigate the photo luminescent property we prepared 4 μM solution of **D1**, **D2** and 2.4 μM AsO_4^{3-} solution. Photo Emission intensity was recorded during addition of AsO_4^{3-} solution to **D1** and **D2**.

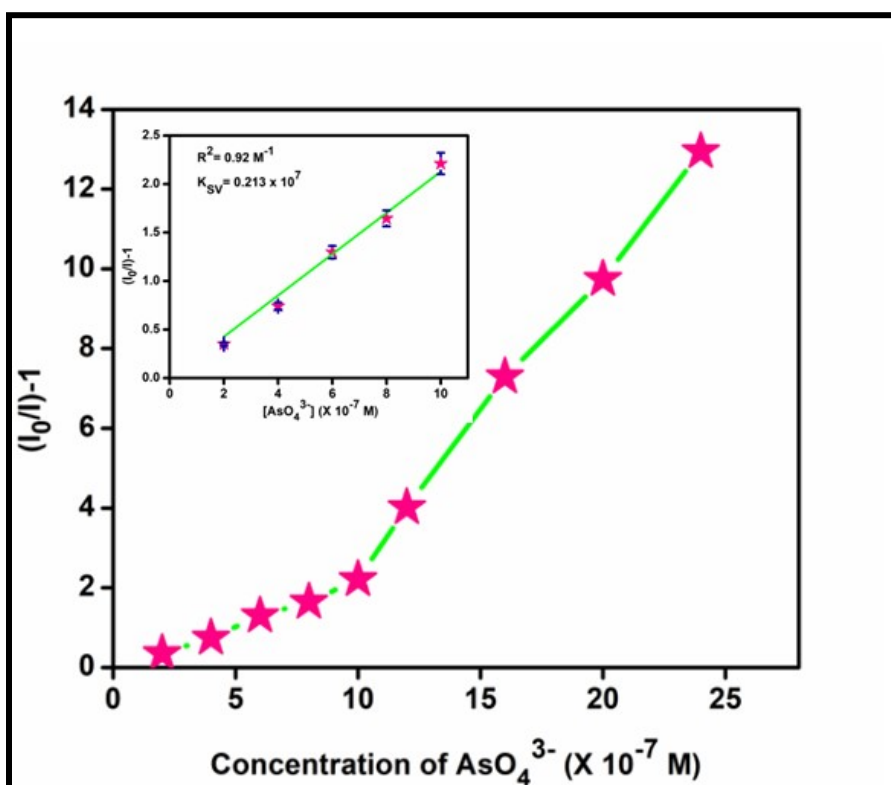


Fig. S20. SV-Plot for addition of AsO_4^{3-} to 1:1(v/v) MeOH- H_2O solution of complex **D1** (Inset: Linear fitting within lower concentration region).

Limit of detection (LOD) calculation in MeOH-H₂O medium

The detection limit of AsO₄³⁻ for both the complex **D1** was calculated using the conventional formula:

$$\text{LOD} = (3\sigma/m)$$

Where, the standard deviation (σ) was calculated via the measurement of five successive fluorescence intensities of **D1** in absence of AsO₄³⁻. The slope (m) obtained by plotting the emission intensity of complexes against the concentration of AsO₄³⁻ added.

Table S4. LOD calculation in MeOH-H₂O solution

Complex	σ	m	LOD ($\times 10^{-7}$ M)	LOD (in ppb)
D1	1.96	11.14	0.527	7.3

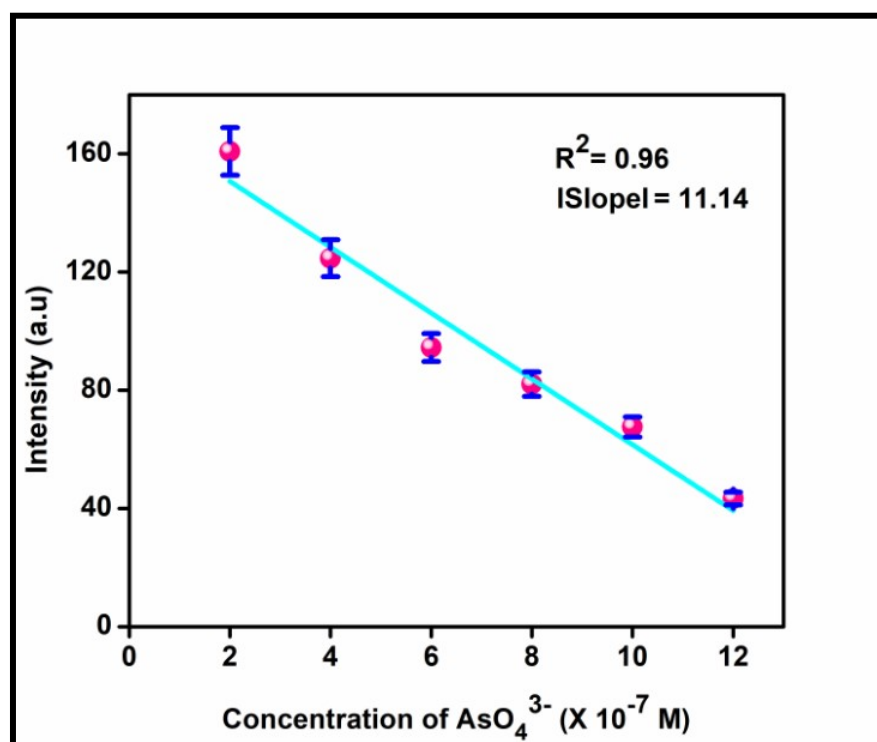


Fig. S21. Intensity vs. AsO₄³⁻ concentration plot for complex **D1** in 1:1(v/v) MeOH-H₂O medium

Luminescence property in presence of AsO_4^{3-} solution in pure aqueous medium

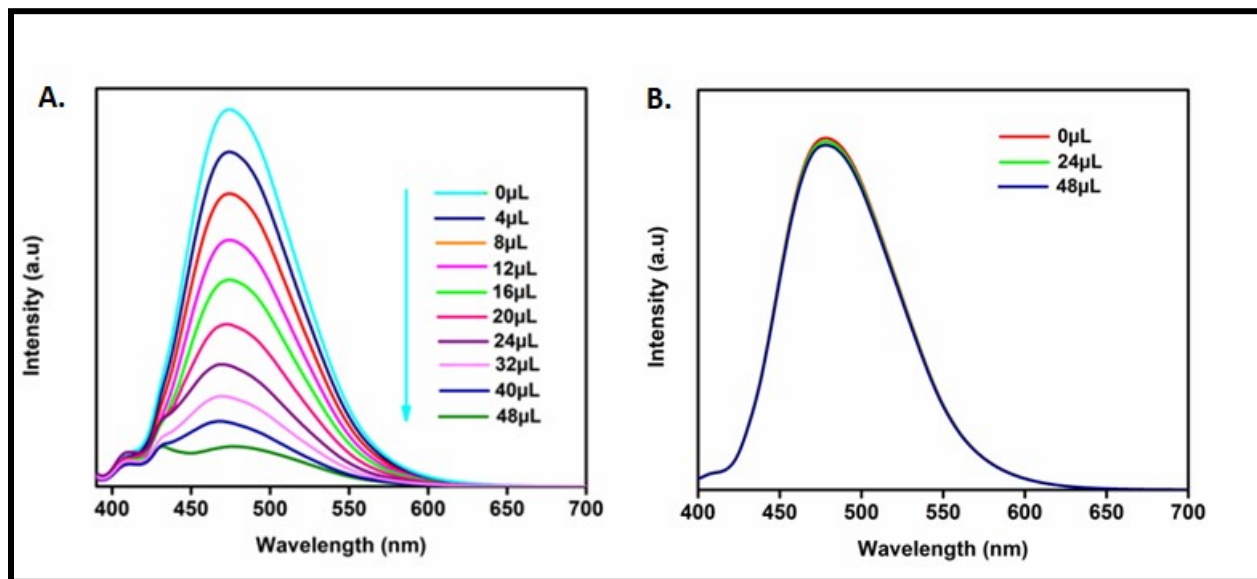


Fig. S22. Fluorescence spectral changes of (A) D1 (B) D2 in presence of AsO_4^{3-} in pure aqueous medium

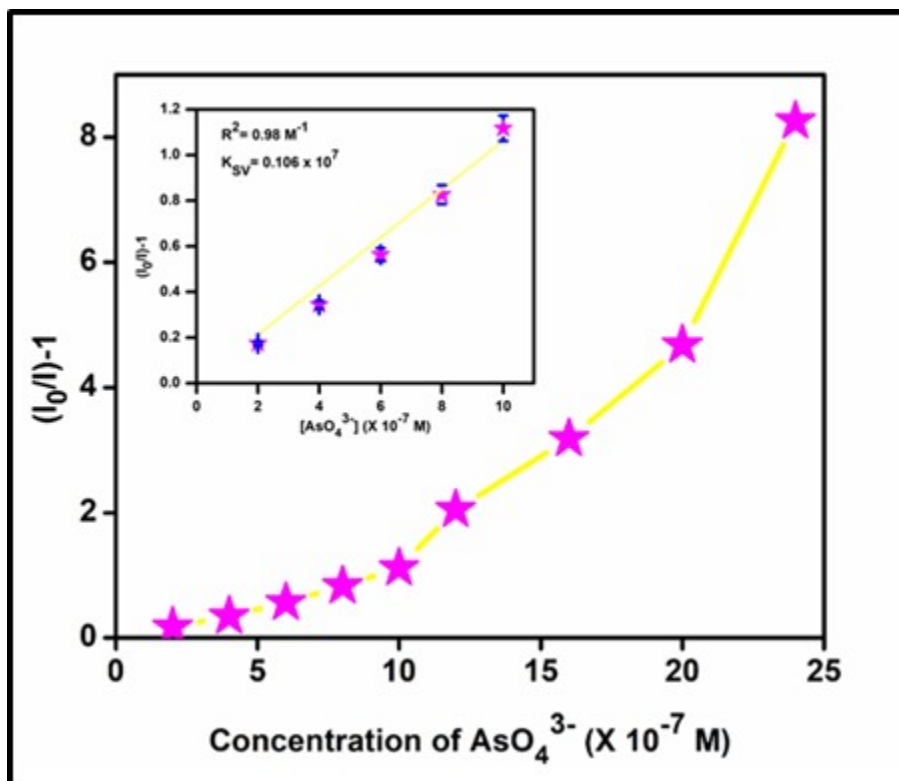


Fig. S23. SV-Plot for addition of AsO_4^{3-} to pure aqueous solution of complex D1 (Inset: Linear fitting within lower concentration region).

Limit of detection (LOD) calculation in pure aqueous medium

Table S5. LOD calculation

complex	σ	m	LOD ($\times 10^{-7}$ M)	LOD (in ppb)
D1	2.21	11.21	0.591	8.2

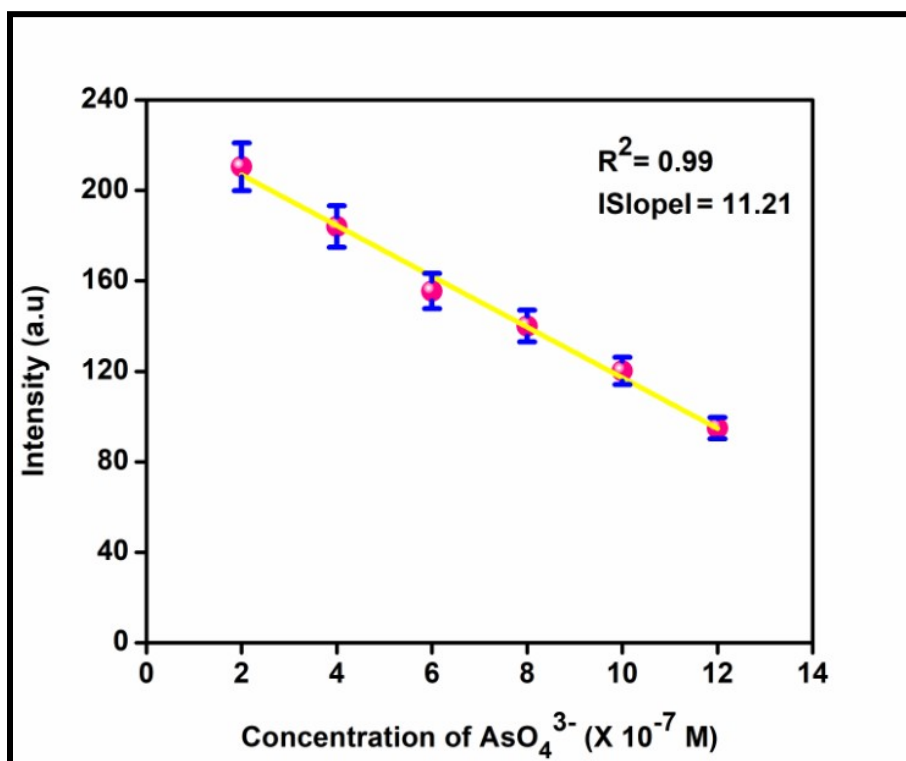


Fig. S24. Intensity vs. AsO₄³⁻ concentration plot for complex **D1** in pure aqueous medium

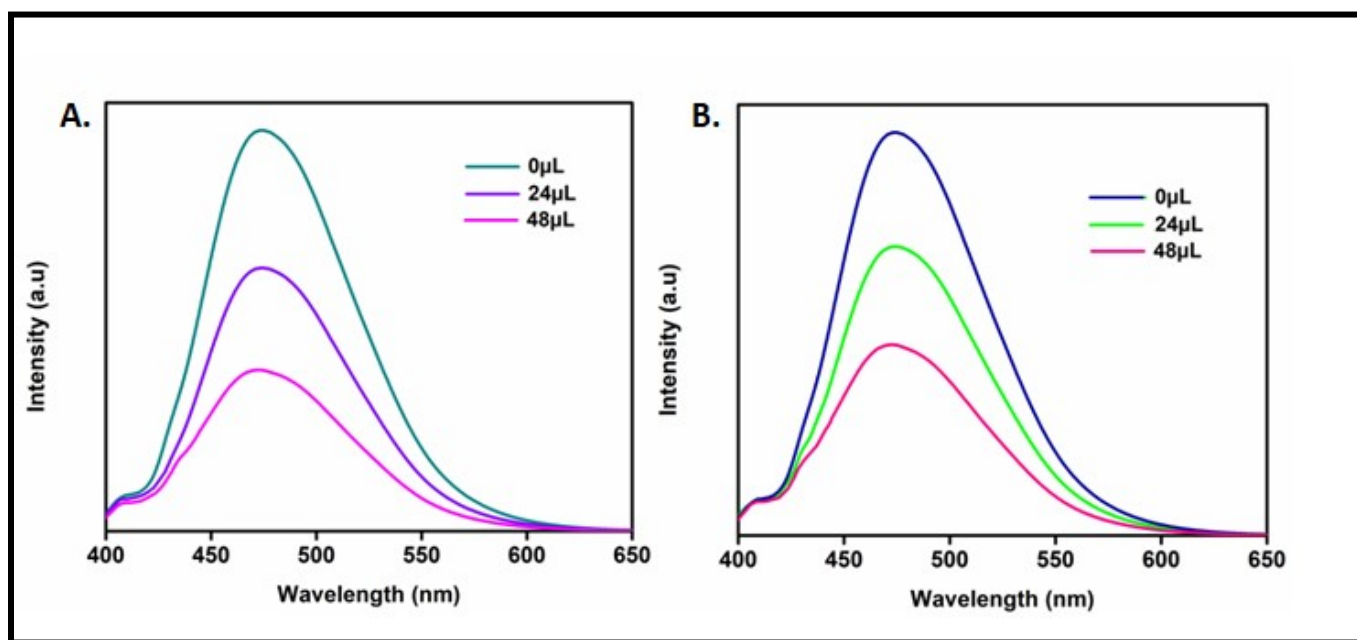


Fig. S25. Fluorescence spectral changes of **D1** in presence of AsO_4^{3-} in (A) tube well water (B) pond water

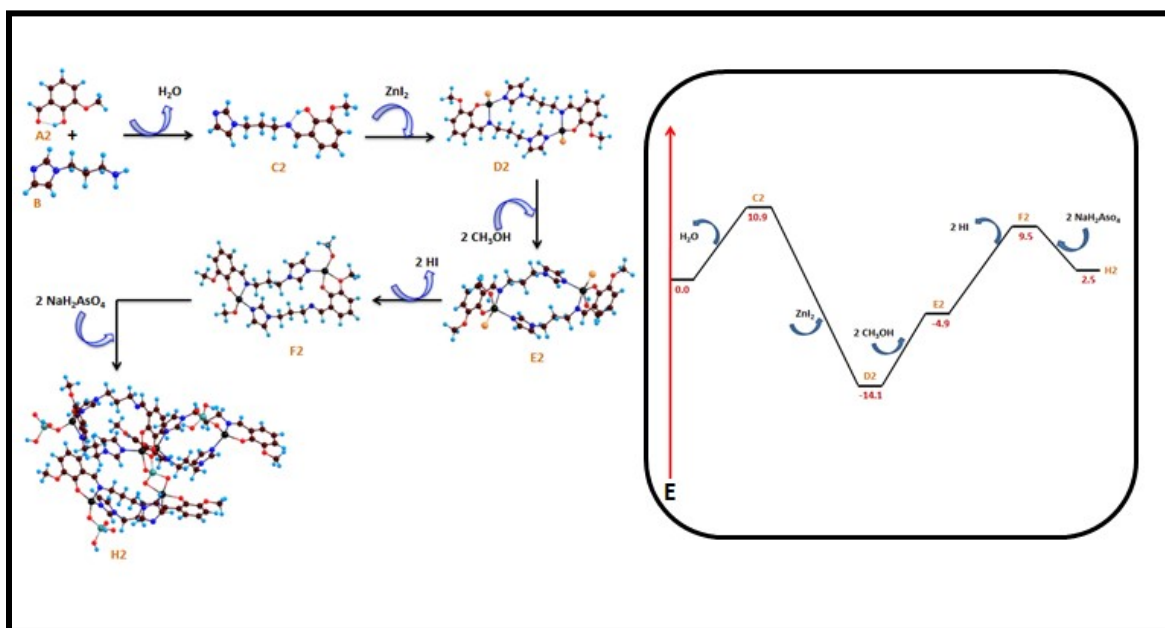


Fig. S26. Mechanism of interaction of **D2** with AsO_4^{3-} in 1:1(v/v) MeOH- H_2O solution (The inset of the above panel shows energy profile diagram of each species involved in the mechanism.

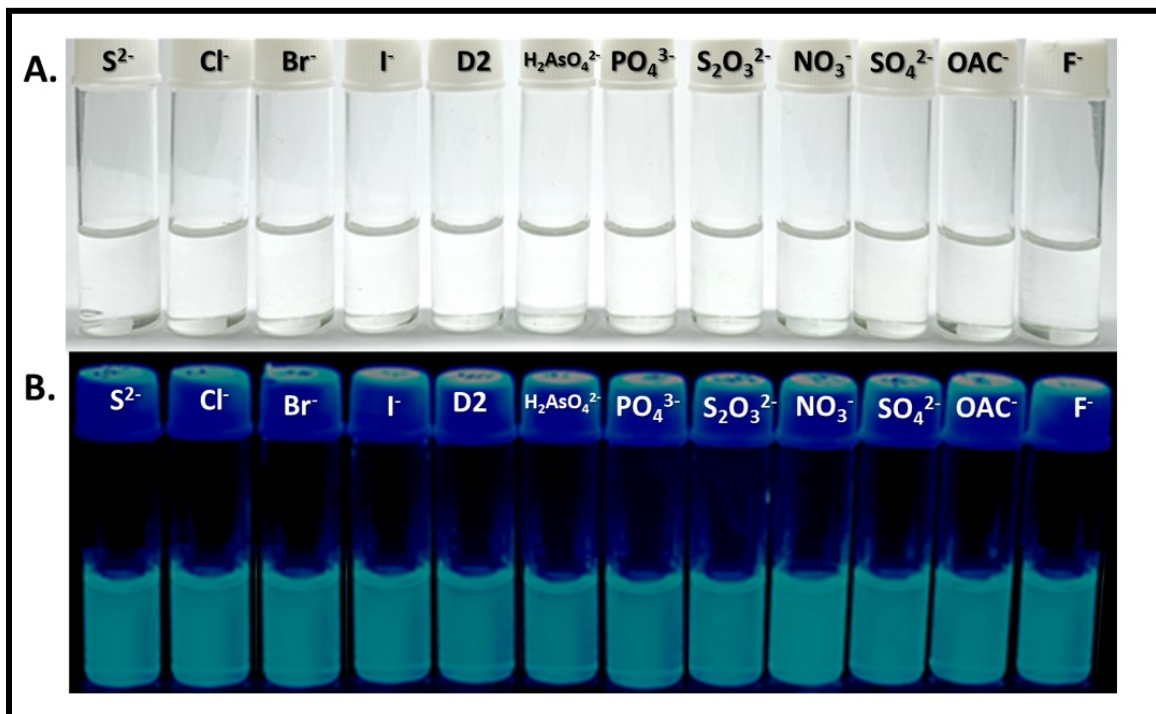


Fig. S27. Naked eye color changes upon addition of different anions ($2.4 \times 10^{-6} \text{M}$) in 1:1(v/v) MeOH-H₂O solution of **D2** under ambient light (**A**) and (**B**) UV light.

Coordinates:

A1

C	1.80818300	1.67752100	-0.00000700
C	1.80240700	0.26421800	0.00000900
C	0.57880200	-0.44497100	0.00000200
C	-0.64232600	0.28070900	-0.00002100
C	-0.60584400	1.67180200	-0.00003700
C	0.61684900	2.37240600	-0.00003000
H	2.76173800	2.19982300	0.00000000
H	-1.53299300	2.23370500	-0.00005600
H	0.60722800	3.45788800	-0.00004200
O	0.51939800	-1.78274800	0.00000900
H	1.45619000	-2.10822700	0.00001600
O	-1.76638500	-0.48259900	-0.00002900
C	-3.03429500	0.17195000	-0.00001200
H	-3.12146800	0.81368700	0.88895200
H	-3.12150300	0.81366600	-0.88898900
C	-4.10397100	-0.90571300	0.00002100
H	-4.01137600	-1.53947200	0.88719600
H	-5.09877700	-0.44728200	0.00003200

H	-4.01140800	-1.53949500	-0.88714100
C	3.05642200	-0.47058200	0.00003900
H	3.97721900	0.14515400	0.00002500
O	3.15170900	-1.70133800	0.00004800

B

C	1.84182600	-1.05656800	-0.22371500
C	1.67053400	1.06187700	0.34264700
C	2.88998500	0.80270100	-0.23241400
N	2.99058300	-0.52472600	-0.58335900
H	1.55904000	-2.09499800	-0.34327700
H	1.22811700	1.96152300	0.74515500
H	3.70387600	1.49402400	-0.40682000
N	0.99733900	-0.14541800	0.35002200
C	-0.36656400	-0.38524900	0.80579600
H	-0.50056700	0.11888800	1.77037200
H	-0.46270800	-1.46057400	0.99231000
C	-1.43068400	0.07712200	-0.19743300
H	-1.29204700	1.14850700	-0.39867300
H	-1.29235500	-0.44275600	-1.15191500
C	-2.85423400	-0.17121900	0.30772300
H	-2.98520100	0.32785000	1.28714500
H	-2.99261700	-1.24564400	0.48722200
N	-3.83018400	0.23559700	-0.70732000
H	-4.77237200	0.01488500	-0.38941500
H	-3.80250900	1.24814600	-0.82312400

H₂O

O	0.00000000	0.00000000	0.11972000
H	0.00000000	0.76156000	-0.47887900
H	0.00000000	-0.76156000	-0.47887900

Cl

C	-2.64660900	-2.48203100	0.55114600
C	-1.85246400	-1.45268500	-0.00119500
C	-2.40551400	-0.16599800	-0.19865900
C	-3.75811600	0.07088600	0.16307300
C	-4.51580800	-0.96274400	0.70612100
C	-3.96053900	-2.24042100	0.90069100

H	-2.20611000	-3.46550900	0.69603100
H	-5.54859100	-0.78729200	0.98480500
H	-4.57350100	-3.02926300	1.32581500
O	-1.70666700	0.85375000	-0.71795400
H	-0.78990400	0.50915300	-0.90808900
O	-4.20021200	1.33755300	-0.06604500
C	-5.54870500	1.65837100	0.26561200
H	-6.23633700	1.00550100	-0.29209200
H	-5.72055100	1.48895400	1.33886400
C	-5.77165800	3.11659800	-0.09598300
H	-5.60041600	3.27769300	-1.16468800
H	-6.79964600	3.41097600	0.14199500
H	-5.08554700	3.76022200	0.46297100
C	-0.47106000	-1.72881600	-0.36371300
H	-0.11968900	-2.75691500	-0.18441100
C	5.75684000	1.25577100	-0.51911800
C	5.50290800	-0.03242300	1.24672700
C	6.38256700	0.98941900	1.50435100
N	6.53710700	1.79044700	0.39512400
H	5.62358800	1.61901600	-1.53051900
H	5.13551700	-0.85049500	1.84905300
H	6.91855600	1.19037900	2.42247400
N	5.10325300	0.14174100	-0.06538400
C	4.13133800	-0.65893700	-0.79765900
H	4.35972200	-1.71845500	-0.63034400
H	4.28541500	-0.46390700	-1.86466600
C	2.67975300	-0.35224600	-0.40517400
H	2.54269000	-0.52617300	0.66887500
H	2.46856400	0.70823500	-0.58421600
C	1.68061900	-1.21225600	-1.19257000
H	1.86680000	-2.28313300	-0.99936600
H	1.83141200	-1.04571400	-2.26882000
N	0.31417600	-0.84484900	-0.86882200

D1

C	6.01471500	-2.77653100	-2.26930500
C	5.47487500	-1.65535100	-1.57051500
C	5.98929700	-1.29683200	-0.27912300
C	7.05213500	-2.11817400	0.25446400
C	7.54301300	-3.19908600	-0.45448600
C	7.02212400	-3.53369600	-1.72762400
H	5.60918700	-3.02176100	-3.24844000
H	8.34083800	-3.80472500	-0.03878800

H	7.42768400	-4.38584600	-2.26410300
O	5.56985400	-0.30348800	0.43711800
O	7.49011800	-1.72184700	1.48119400
C	8.56186600	-2.43799600	2.08229600
H	8.27615700	-3.49106900	2.22798100
H	9.44228600	-2.41975700	1.42240900
C	8.86919200	-1.77136000	3.41278600
H	7.99157400	-1.79471100	4.06650500
H	9.69280100	-2.29122200	3.91462500
H	9.15592500	-0.72628800	3.26061900
C	4.43386500	-0.93443800	-2.24342300
H	4.19477200	-1.32277900	-3.24249900
C	-1.70981200	0.15999600	-1.91193800
C	-1.71366000	2.36321000	-1.87788300
C	-2.81072400	1.89140000	-1.20889600
N	-2.79361800	0.51137900	-1.23124500
H	-1.42016500	-0.86092100	-2.11880700
H	-1.36555600	3.36481700	-2.07950800
H	-3.60983100	2.43590900	-0.72867000
N	-1.02228100	1.25013000	-2.32341700
C	0.27754700	1.23199400	-3.00624800
H	0.50756800	2.26259500	-3.29005900
H	0.17750600	0.64959900	-3.92855400
C	1.37153500	0.65518200	-2.10015600
H	1.39337300	1.22709200	-1.16540500
H	1.11974000	-0.38083700	-1.84032300
C	2.76469200	0.67971800	-2.74332400
H	3.05377200	1.71835400	-2.95064600
H	2.75351300	0.13733500	-3.70131100
N	3.75425100	0.10200200	-1.83568100
C	-7.08164700	0.67225000	3.18597000
C	-6.17597500	0.27087200	2.15977000
C	-6.54975700	0.39748400	0.78043700
C	-7.85802900	0.94288800	0.50257800
C	-8.70535500	1.32185600	1.52835100
C	-8.31705700	1.18650300	2.88222300
H	-6.77305900	0.56050000	4.22309600
H	-9.68548900	1.72764200	1.30266400
H	-9.00234500	1.48923000	3.66786100
O	-5.80038500	0.06911500	-0.22542200
O	-8.14563900	1.03680300	-0.82494800
C	-9.42653300	1.52240000	-1.20868000
H	-10.21358100	0.89056700	-0.77046600
H	-9.57024300	2.54569900	-0.82955700
C	-9.49142300	1.49335900	-2.72659800
H	-9.35049000	0.47323700	-3.09676000
H	-10.46518800	1.85942900	-3.07023600
H	-8.70881100	2.12601600	-3.15705400

C	-4.91632100	-0.25708800	2.60109500
H	-4.80574300	-0.29736900	3.69319900
C	1.82157600	-0.26224700	1.54763000
C	1.23286100	1.18664000	3.09741200
C	2.29463400	1.67773000	2.38889800
N	2.65349700	0.76330200	1.41859200
H	1.82896800	-1.16016100	0.94642000
H	0.66956600	1.59209700	3.92385100
H	2.82115600	2.61493000	2.49347100
N	0.93993500	-0.05183100	2.55316300
C	-0.21479300	-0.89134900	2.88558400
H	-0.28015300	-0.95937300	3.97667600
H	-0.01087000	-1.89734100	2.50632200
C	-1.50900000	-0.33233900	2.28014300
H	-1.68097600	0.68574200	2.65055400
H	-1.38499600	-0.25675100	1.19360100
C	-2.73673400	-1.20243200	2.58751000
H	-2.91383000	-1.24288500	3.67327200
H	-2.55622500	-2.22793700	2.24012800
N	-3.91440400	-0.69103900	1.88978200
Zn	-4.07843700	-0.84029900	-0.20139300
I	-3.20256800	-3.26106800	-0.98003800
Zn	4.22602500	1.03614900	-0.01555800
I	4.44101400	3.68683800	-0.27824700

E1

C	5.61969700	-2.25388400	-2.97872100
C	5.06648200	-1.36032800	-2.01866500
C	5.34056000	-1.53611900	-0.62290200
C	6.21232200	-2.62998100	-0.26367000
C	6.74162600	-3.47022600	-1.22605500
C	6.44214600	-3.28560500	-2.59671900
H	5.38036700	-2.10207900	-4.02911500
H	7.39694400	-4.28560100	-0.93933400
H	6.86471100	-3.96296900	-3.33231200
O	4.84354300	-0.79670900	0.31447000
O	6.45269700	-2.72727500	1.08029300
C	7.27487200	-3.79236800	1.54030900
H	6.84009900	-4.75759300	1.24032300
H	8.27451200	-3.72231600	1.08502600
C	7.36334900	-3.68859700	3.05395000
H	6.36759600	-3.75760300	3.50313800
H	7.98310800	-4.49932000	3.45257200
H	7.80897500	-2.73363600	3.35076000
C	4.18874400	-0.33700600	-2.51340800
H	3.95240000	-0.42509900	-3.58283400
C	-1.61021100	0.49405600	-1.74371100

C	-2.16506700	2.62210200	-1.86642800
C	-3.20081400	1.91055000	-1.32323800
N	-2.83850300	0.57976000	-1.24724700
H	-1.05504800	-0.42830300	-1.82497600
H	-2.04628000	3.67268500	-2.08363400
H	-4.17137100	2.23697100	-0.98187700
N	-1.15611700	1.70929500	-2.12570800
C	0.16419500	1.99903200	-2.70777100
H	0.34403400	3.06989100	-2.57697000
H	0.12943500	1.79423100	-3.78469200
C	1.26831700	1.18649600	-2.02697900
H	1.25898100	1.40562600	-0.95328500
H	1.07277800	0.11389800	-2.14164800
C	2.67024900	1.47640000	-2.58469900
H	2.92432100	2.53069300	-2.43208300
H	2.70322900	1.26262400	-3.66423000
N	3.64346500	0.65286300	-1.86626200
C	-7.01263100	0.19594200	3.30309400
C	-6.07390000	-0.03002700	2.25605800
C	-6.38314100	0.36384000	0.91369900
C	-7.67604600	0.96775100	0.69066600
C	-8.56440000	1.16308800	1.73195600
C	-8.23148400	0.77724700	3.05235900
H	-6.74680800	-0.10670700	4.31377600
H	-9.53227900	1.61662900	1.54760300
H	-8.94444700	0.94384300	3.85385600
O	-5.58040200	0.22661400	-0.08970200
O	-7.90933300	1.30245100	-0.61500400
C	-9.15269500	1.91122700	-0.94135100
H	-9.98303800	1.24376400	-0.66540000
H	-9.27376200	2.84542000	-0.37261500
C	-9.15468700	2.18669000	-2.43589900
H	-9.04378900	1.25533600	-3.00046400
H	-10.09661300	2.66173800	-2.73127500
H	-8.32902000	2.85274300	-2.70566600
C	-4.82316000	-0.62857600	2.63149000
H	-4.71093200	-0.77920600	3.71382100
C	1.95398200	-0.28083600	1.72113700
C	1.04482700	1.16071300	3.11752200
C	2.10028200	1.74760300	2.47715400
N	2.66207800	0.83675200	1.60497100
H	2.14436400	-1.19763800	1.18244800
H	0.35805500	1.53429200	3.86121500
H	2.48636500	2.75294200	2.55691200
N	0.95742800	-0.13113300	2.62508900
C	-0.12992000	-1.07783000	2.89503300
H	-0.19301600	-1.23188600	3.97831100
H	0.14284700	-2.03226400	2.43598400

C	-1.45653700	-0.56299700	2.32191100
H	-1.69688500	0.41388500	2.75926200
H	-1.33000400	-0.41158000	1.24437900
C	-2.63248800	-1.52241400	2.55030200
H	-2.81977900	-1.65177100	3.62725300
H	-2.39171800	-2.50167600	2.12323100
N	-3.82870500	-1.00646900	1.87974300
Zn	-3.94812300	-0.93383600	-0.24145600
I	-1.96210800	-3.09871900	-0.85015200
Zn	4.19741900	1.10293600	0.14111800
I	3.92510100	4.02619400	0.01702600
O	-5.15156500	-2.25362000	-1.43304900
C	-6.16314100	-1.86265100	-2.37743400
H	-5.71760300	-1.59818700	-3.34356700
H	-6.88429700	-2.67600100	-2.51209900
H	-6.65321800	-0.98982300	-1.94668800
H	-4.57291700	-2.95808200	-1.78366600
O	6.16789800	1.67837500	0.80803200
H	6.17281400	2.65001300	0.90539600
C	6.96653600	1.02919700	1.81129100
H	8.02574700	1.26205200	1.65660700
H	6.66256100	1.33960100	2.81815100
H	6.79366100	-0.03972200	1.68811700

F1

C	-6.03619600	-2.16779900	-2.66586300
C	-5.50774800	-1.57733300	-1.48038300
C	-6.01792600	-0.31902200	-1.01171900
C	-7.06696300	0.29182800	-1.79895500
C	-7.54971400	-0.31400000	-2.94404600
C	-7.03191300	-1.55561300	-3.38487500
H	-5.63064700	-3.12285900	-2.99343300
H	-8.33761600	0.15903300	-3.52039100
H	-7.42889400	-2.01145100	-4.28675600
O	-5.61095100	0.30095900	0.04701300
O	-7.50438900	1.48344100	-1.30097500
C	-8.55000900	2.15852700	-1.98581500
H	-8.24039700	2.38702700	-3.01736100
H	-9.44138500	1.51512900	-2.04155800
C	-8.85273000	3.43462000	-1.21768500
H	-7.96494700	4.07298500	-1.16845500
H	-9.65736200	3.99136600	-1.71082300
H	-9.16410300	3.20151500	-0.19472300
C	-4.47098900	-2.31503400	-0.81468500
H	-4.21610200	-3.26771800	-1.30055500
C	1.54678000	-1.78856200	0.23913700

C	1.90675600	-2.55616400	2.27395500
C	2.96846500	-1.78802400	1.87675000
N	2.73016100	-1.30997800	0.60626000
H	1.10195100	-1.56529300	-0.72167900
H	1.70779000	-3.09830100	3.18578700
H	3.87629600	-1.55159500	2.41197400
N	1.00580400	-2.54638400	1.22209000
C	-0.29786000	-3.22043100	1.18033500
H	-0.51118900	-3.56214400	2.19764600
H	-0.21944800	-4.10995400	0.54383700
C	-1.40707900	-2.28684200	0.68601400
H	-1.40392000	-1.37501600	1.29258100
H	-1.20913100	-1.98576500	-0.34957300
C	-2.79879200	-2.93447100	0.75012200
H	-3.03419800	-3.18843500	1.79190000
H	-2.81140500	-3.86843500	0.16572000
N	-3.81595600	-2.00546000	0.26664000
C	7.38768100	2.64352800	0.56786100
C	6.28188500	1.87058200	0.10696600
C	6.48900900	0.53606200	-0.38154600
C	7.84904500	0.04456900	-0.37714900
C	8.89278300	0.82664000	0.08287400
C	8.66390900	2.13857800	0.56102400
H	7.19915400	3.65315900	0.92708500
H	9.90572600	0.43882300	0.08105600
H	9.50068400	2.73357700	0.91388500
O	5.55964300	-0.25064400	-0.82130600
O	7.97677100	-1.22670000	-0.85284600
C	9.27514000	-1.80211800	-0.90340000
H	9.93566700	-1.18695300	-1.53329900
H	9.71330800	-1.83368700	0.10601500
C	9.13432700	-3.20320600	-1.47515300
H	8.70264100	-3.16581000	-2.48014800
H	10.11492800	-3.68857600	-1.53295600
H	8.47974900	-3.81171800	-0.84327400
C	5.00137000	2.52232300	0.13501300
H	5.03757200	3.56790200	0.47269500
C	-1.85012400	1.68984800	0.51434000
C	-1.12307200	2.35811400	2.48470200
C	-2.19914000	1.52973600	2.65015900
N	-2.64353600	1.11728100	1.40770100
H	-1.91914600	1.57759000	-0.55840200
H	-0.50014600	2.88416200	3.19208500
H	-2.70870700	1.17733700	3.53608600
N	-0.91146500	2.45796800	1.11913400
C	0.21708200	3.12902600	0.46992200
H	0.41397900	4.05244200	1.02528400
H	-0.09951400	3.41667800	-0.53787600

C	1.45751000	2.22853100	0.41918600
H	1.68944000	1.87367600	1.43097000
H	1.23928900	1.35313500	-0.20464300
C	2.68366900	2.93831200	-0.16672400
H	2.91649500	3.85355800	0.40157200
H	2.45869900	3.24566200	-1.19827600
N	3.83866100	2.04135800	-0.19357200
Zn	3.62070000	0.02897600	-0.82646000
Zn	-4.29007300	-0.27134700	1.38917600
O	2.13523800	-0.12215500	-2.02497600
C	2.07830200	0.35726700	-3.33190900
H	2.69795600	-0.22504600	-4.04037300
H	1.04359600	0.31518500	-3.71963600
H	2.40307000	1.41354300	-3.43342800
O	-4.33211900	-0.50329800	3.26922300
C	-5.36614300	-1.04944200	4.02486900
H	-5.02110000	-1.27594000	5.05110300
H	-6.23616200	-0.37245600	4.13342800
H	-5.76441600	-2.00170000	3.61868100

G1

C	3.01101700	-2.82835100	0.27982900
C	2.07209100	-1.78924900	0.00567600
C	2.49908300	-0.42191900	0.01354500
C	3.88671900	-0.16053200	0.30325100
C	4.76434300	-1.19894000	0.56322800
C	4.32543000	-2.54310000	0.55165100
H	2.66363100	-3.85871300	0.26902900
H	5.80570900	-0.98920100	0.78078400
H	5.03450800	-3.33835500	0.75907900
O	1.72551700	0.59942900	-0.22050600
O	4.21426200	1.15913800	0.29399300
C	5.55907700	1.52810200	0.58336300
H	5.84030800	1.16246000	1.58222600
H	6.23979100	1.06556000	-0.14690000
C	5.64236100	3.04366400	0.51763600
H	4.96436400	3.49766500	1.24693300
H	6.66350900	3.37457300	0.73637400
H	5.36543400	3.40136900	-0.47890100
C	0.72915700	-2.21836300	-0.26765300
H	0.59874900	-3.30710600	-0.23489400
C	-5.86330200	-0.52921900	0.47783700
C	-4.43936200	1.10917600	0.86327300
C	-5.59050500	1.27114500	1.59472500
N	-6.47724500	0.24528600	1.34759800
H	-6.26463200	-1.43778200	0.04580500

H	-3.52814000	1.67966800	0.75315600
H	-5.83811200	2.07350400	2.27726400
N	-4.62471800	-0.05448900	0.13947200
C	-3.63422600	-0.68079100	-0.72463400
H	-3.01473400	0.12351500	-1.13368100
H	-4.15840700	-1.16757900	-1.55587500
C	-2.77664800	-1.71631300	0.02781400
H	-2.40270900	-1.27471800	0.95928000
H	-3.41405700	-2.55849400	0.32263000
C	-1.58711100	-2.24856500	-0.79787700
H	-1.81765500	-2.17487800	-1.87013200
H	-1.42617500	-3.31297300	-0.58176900
N	-0.33555300	-1.51425900	-0.54533400
Zn	-0.15646000	0.53307300	-0.57944300
O	-1.56255300	1.71404600	-0.82084600
C	-1.46609700	3.07198900	-1.17827200
H	-1.24519000	3.21096900	-2.25040300
H	-2.42663500	3.57088200	-0.97834000
H	-0.69309400	3.61836700	-0.61199800

H1

As	-0.20744300	0.62786400	-2.40197000
O	-0.64486300	0.35868700	-3.94989900
O	1.48650700	0.63277300	-1.92992700
O	-0.69790800	2.06517700	-1.56917800
O	-0.66751500	-0.54006100	-1.18612300
C	1.98325200	2.08095000	4.14410700
C	1.66725000	2.01224300	2.76153000
C	0.30533000	2.01350500	2.34546900
C	-0.69731400	2.20509900	3.34530900
C	-0.35078900	2.26861000	4.69021500
C	0.99377000	2.19348100	5.09457400
H	3.02836800	2.04930600	4.44152700
H	-1.11995400	2.38077300	5.44489000
H	1.24041000	2.23835000	6.15073400
O	-0.05862900	1.87027400	1.07907600
O	-1.96982100	2.34104400	2.87058300
C	-2.98515200	2.70474100	3.80960800
H	-3.14829200	1.87716300	4.51397200
H	-2.64728800	3.57940900	4.38313400
C	-4.26135500	3.02735900	3.05472100
H	-4.63862400	2.14566800	2.53199900
H	-5.02786100	3.36389700	3.76200700
H	-4.08744400	3.82626100	2.32655200
C	2.80689500	1.95515700	1.86966200
H	3.76154700	1.80408100	2.38935400

C	2.83586100	5.31864000	-0.02864200
C	1.81864900	4.32505100	-1.70508600
C	0.90879200	4.96091900	-0.87149000
N	1.55544400	5.57091200	0.17201200
H	3.64462500	5.63490600	0.61735600
H	1.70285800	3.86143500	-2.67543700
H	-0.16540200	5.00708400	-0.98770000
N	3.06261500	4.58321500	-1.15104300
C	4.32810400	3.97241500	-1.56388100
H	5.10922500	4.40111200	-0.92715000
C	4.31238400	2.44079400	-1.46002000
H	3.53487500	2.02037500	-2.10943200
H	5.26695100	2.08044000	-1.86374700
C	4.16764800	1.84781700	-0.05555600
H	4.96156200	2.23220300	0.60361100
H	4.29626800	0.76322700	-0.13636600
N	2.85385800	2.07659600	0.58111500
Zn	1.11331200	2.21702300	-0.54868800
H	4.54034500	4.27763000	-2.59474700
C	-5.95175600	-0.73199500	1.55513600
C	-4.65887000	-0.28717100	1.15279700
C	-3.48451700	-0.86185300	1.74441500
C	-3.69514400	-1.87961700	2.74991300
C	-4.96686600	-2.28490500	3.10952900
C	-6.10956800	-1.70852800	2.50699900
H	-6.82309200	-0.28294900	1.08353200
H	-5.10327900	-3.05457900	3.86151100
H	-7.09869600	-2.04621600	2.80037800
O	-2.27013700	-0.53239500	1.45088600
O	-2.53739400	-2.37825200	3.28132700
C	-2.63387300	-3.35113500	4.31163400
H	-3.22014400	-2.95163200	5.15322100
H	-3.15630200	-4.24639400	3.94043800
C	-1.22160600	-3.69474900	4.75634000
H	-0.70776100	-2.80259900	5.12738200
H	-1.24787400	-4.44327600	5.55609100
H	-0.64156000	-4.09884000	3.92036900
C	-4.63365900	0.77680700	0.18420500
H	-5.63276700	1.14480400	-0.08447200
C	-5.90363500	-0.73828400	-2.77335400
C	-3.84244100	-0.84178700	-3.54856900
C	-4.33253900	-2.09335100	-3.25844700
N	-5.61915700	-2.02307000	-2.77311300
H	-6.84496500	-0.29811800	-2.46822300
H	-2.88862400	-0.49793800	-3.92821800
H	-3.83069300	-3.04479200	-3.37793000
N	-4.86441800	0.03100700	-3.22454100
C	-4.88921800	1.47253900	-3.45283200

H	-5.87364800	1.83035100	-3.12843500
C	-3.77282400	2.27078800	-2.76489200
H	-2.79929900	1.83317200	-2.99466900
H	-3.76936000	3.26380700	-3.23510400
C	-3.90948200	2.51391900	-1.25173300
H	-4.92112000	2.89471600	-1.03849100
H	-3.20053400	3.30428700	-0.98540500
N	-3.62025100	1.37016300	-0.37545700
Zn	-1.65647700	0.80975200	0.12685600
H	-4.82623600	1.64940100	-4.53377200
C	3.55827000	-4.23147300	2.12294700
C	2.89962200	-3.30270900	1.27216300
C	3.61925800	-2.20497900	0.70382200
C	5.03097600	-2.14347900	0.98942600
C	5.64039700	-3.07105000	1.81729600
C	4.90034200	-4.12189700	2.39925700
H	2.97615300	-5.04508500	2.55041700
H	6.70236600	-3.00083700	2.02552000
H	5.39765000	-4.83501600	3.04936200
O	3.08765900	-1.27678300	-0.03825300
O	5.69433800	-1.11190600	0.37455800
C	7.11493000	-1.10102500	0.44197700
H	7.44556200	-0.94676000	1.48067000
H	7.50994100	-2.07094400	0.10752300
C	7.62297300	0.01827300	-0.45216100
H	7.25613900	0.99095400	-0.10733800
H	8.71825100	0.04149400	-0.43989400
H	7.28980200	-0.13469600	-1.48361400
C	1.50477300	-3.56399000	1.02127100
H	1.10920600	-4.41892800	1.58704000
C	1.91900600	-4.54326500	-2.35106500
C	0.92457400	-2.75279400	-3.15289000
C	2.30236000	-2.63516900	-3.22286800
N	2.91287900	-3.75989000	-2.71908600
H	2.02605600	-5.51471100	-1.88600000
H	0.13280500	-2.12702400	-3.54346300
H	2.87230200	-1.81257900	-3.63325200
N	0.69277500	-3.99611100	-2.59020200
C	-0.60225300	-4.52787200	-2.15501300
H	-0.40604700	-5.50913000	-1.70862200
C	-1.33522300	-3.60070600	-1.17634300
H	-1.46743300	-2.61347100	-1.62636700
H	-2.34372900	-4.00789400	-1.02895600
C	-0.71163500	-3.43324900	0.21692400
H	-0.76645100	-4.38586500	0.76764600
H	-1.31110500	-2.69797700	0.76525300
N	0.68214500	-2.95550300	0.22429800
Zn	1.30984700	-1.27270200	-0.90279500

H	-1.22582900	-4.69191300	-3.04160500
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A2

C	-1.01050800	1.83439900	-0.00009500
C	-1.31031300	0.45324500	-0.00011300
C	-0.26911000	-0.50399100	-0.00006200
C	1.07932100	-0.05819900	0.00001800
C	1.34488500	1.30727400	0.00003400
C	0.30270600	2.25577300	-0.00002800
H	-1.82869800	2.55037600	-0.00013300
H	2.37172700	1.65557800	0.00009000
H	0.54661300	3.31351000	-0.00001600
O	-0.49970700	-1.82267500	-0.00011200
H	-1.48465400	-1.93908500	-0.00023100
O	2.01304400	-1.04661600	0.00006600
C	3.37983000	-0.67038200	0.00011200
H	3.63883300	-0.08890300	-0.89497100
H	3.63877600	-0.08890800	0.89521600
C	-2.69354000	0.00645000	-0.00017900
H	-3.45979200	0.80626800	0.00011000
O	-3.05172700	-1.17476600	0.00025600
H	3.94469600	-1.60380100	0.00012800

C2

C	-3.16328400	-2.03416600	0.59324500
C	-2.28371700	-1.08931800	0.01999700
C	-2.72853600	0.23142400	-0.22100900
C	-4.06025200	0.58636800	0.12031400
C	-4.90431500	-0.36548600	0.68394800
C	-4.45659000	-1.67763100	0.92119000
H	-2.80468500	-3.04519400	0.77087800
H	-5.92194500	-0.09870400	0.94615200
H	-5.13499700	-2.40161900	1.36191900
O	-1.94571500	1.17507600	-0.76287900
H	-1.05893900	0.75154300	-0.93571400
O	-4.39676700	1.87844000	-0.14836200
C	-5.71052900	2.30173100	0.17088500
H	-6.46654300	1.73273600	-0.38746100
H	-5.91520500	2.21126200	1.24649900
C	-0.92667500	-1.48750400	-0.32114800
H	-0.66103400	-2.53444800	-0.10710100
C	5.51595600	1.00186700	-0.55250100
C	5.16076800	-0.18977600	1.26301300
C	6.11486400	0.77219500	1.48350300
N	6.33242100	1.51293900	0.34339600

H	5.41288600	1.33245400	-1.57853300
H	4.73089400	-0.95219600	1.89621100
H	6.66238400	0.96959800	2.39556900
N	4.77862300	-0.03999800	-0.05733900
C	3.75022500	-0.79389100	-0.76150100
H	3.89686100	-1.85993900	-0.55006800
H	3.92111900	-0.65490800	-1.83473000
C	2.32552800	-0.36151500	-0.38920600
H	2.17272400	-0.48297700	0.68993500
H	2.19783300	0.70449700	-0.60952500
C	1.26448400	-1.17089600	-1.14866300
H	1.36598400	-2.24490200	-0.91435600
H	1.43006600	-1.05756700	-2.22965800
N	-0.06982500	-0.68591100	-0.84656200
H	-5.76363200	3.35261100	-0.11896300

D2

C	6.36249800	2.96941700	1.83037700
C	5.71170500	1.86203200	1.20872300
C	6.10884100	1.43664100	-0.10365100
C	7.16892300	2.18339000	-0.74115800
C	7.77186700	3.25189900	-0.10396600
C	7.36813900	3.65063400	1.19317900
H	6.04397400	3.26568100	2.82745300
H	8.57002800	3.79886000	-0.59435300
H	7.86060800	4.49176900	1.67108400
O	5.58207900	0.44780400	-0.75148600
O	7.49120900	1.72996400	-1.98438000
C	8.54580100	2.37600100	-2.67091900
H	8.31858800	3.43435000	-2.86310700
H	9.49176500	2.30995400	-2.11548300
C	4.66594100	1.23751500	1.96384000
H	4.49133800	1.69422100	2.94775000
C	-1.81575000	0.06630800	1.76685000
C	-1.24905600	1.87137600	2.89358700
C	-2.37487500	2.12351100	2.16010500
N	-2.72014400	0.98703100	1.45540800
H	-1.79611900	-0.94958900	1.39884200
H	-0.67328800	2.49082600	3.56416200
H	-2.95634700	3.02955500	2.07367100
N	-0.90107100	0.55654900	2.63724300
C	0.34769200	-0.09168500	3.05070200
H	0.19370500	-1.17441400	3.01667100
H	0.53419200	0.17977500	4.09486800
C	1.51112000	0.33689500	2.14576200
H	1.31303600	-0.00850800	1.12406800
H	1.54875400	1.43291800	2.10827500

C	2.88227200	-0.18834700	2.59836100
H	2.87765900	-1.28400700	2.65006400
H	3.11251400	0.18901600	3.60631800
N	3.91288000	0.22040300	1.64399900
C	-6.38432000	-2.96608300	-1.82051200
C	-5.72924000	-1.85892800	-1.20295500
C	-6.12865400	-1.42345500	0.10542300
C	-7.19562800	-2.16007700	0.74327100
C	-7.80226600	-3.22898800	0.11027700
C	-7.39609800	-3.63779600	-1.18296200
H	-6.06403800	-3.26996500	-2.81473000
H	-8.60528500	-3.76848800	0.60097300
H	-7.89167400	-4.47891100	-1.65768000
O	-5.59871500	-0.43380300	0.74935600
O	-7.51999400	-1.69736500	1.98251900
C	-8.58039600	-2.33370300	2.66918600
H	-9.52410500	-2.26593900	2.11012300
H	-8.35947600	-3.39208600	2.86838800
C	-4.67820900	-1.24415900	-1.95874300
H	-4.50540800	-1.70546100	-2.94080500
C	1.81264000	-0.08255000	-1.76504500
C	1.24132400	-1.89579700	-2.87631500
C	2.36824300	-2.14365100	-2.14306500
N	2.71632800	-1.00209700	-1.44804600
H	1.79536200	0.93632600	-1.40521600
H	0.66353000	-2.51967100	-3.54101900
H	2.94929200	-3.04943300	-2.05101100
N	0.89566300	-0.57847700	-2.62975100
C	-0.35230100	0.06854900	-3.04738900
H	-0.53885500	-0.20894200	-4.08996800
H	-0.19720600	1.15128800	-3.01975500
C	-1.51650300	-0.35328700	-2.14030300
H	-1.55503500	-1.44902300	-2.09564200
H	-1.31874900	-0.00114000	-1.12084100
C	-2.88670500	0.17011400	-2.59762800
H	-3.11634200	-0.21385500	-3.60322000
H	-2.88089500	1.26540500	-2.65663500
N	-3.91886300	-0.23088200	-1.64167700
Zn	-4.35397500	0.90718600	0.06829400
Zn	4.35587000	-0.90968900	-0.06933700
H	-8.68505100	-1.80332200	3.61763000
H	8.64999800	1.85178900	-3.62283900
I	-4.80421700	3.46547300	-0.56261600
I	4.84203700	-3.46394600	0.55025300
E2			
C	-5.36401300	4.16704100	-0.81950800

C	-5.12101400	2.77279500	-0.63621800
C	-5.88832500	2.02246400	0.31551700
C	-6.88403700	2.75091500	1.07196300
C	-7.08437900	4.10337200	0.86831100
C	-6.32104400	4.82070900	-0.08599100
H	-4.76907400	4.70626400	-1.55403200
H	-7.83825100	4.63345100	1.44050200
H	-6.50249400	5.88185100	-0.22643900
O	-5.74937900	0.75911000	0.53784400
O	-7.56824500	1.98253000	1.96190200
C	-8.58600100	2.59903200	2.72620300
H	-8.18650000	3.39882300	3.36623100
H	-9.37653900	3.01671200	2.08686600
C	-4.08832600	2.18756100	-1.43542400
H	-3.61094600	2.89593000	-2.12938000
C	2.14003800	0.56387200	-1.36386400
C	1.61573100	2.63348500	-1.90156800
C	2.73534400	2.63199000	-1.11657500
N	3.05052000	1.33131800	-0.77842400
H	2.10826700	-0.51499000	-1.32196600
H	1.06322300	3.43675800	-2.36463600
H	3.35621800	3.45471800	-0.79453500
N	1.24593700	1.30859700	-2.05836600
C	0.00787900	0.83465000	-2.68316800
H	0.13754800	-0.22564400	-2.92096300
H	-0.11786300	1.36898900	-3.63088500
C	-1.19378300	1.05776500	-1.75422000
H	-1.04392700	0.47771500	-0.83756500
H	-1.21996400	2.11468700	-1.46017600
C	-2.54786700	0.68374900	-2.37641900
H	-2.57483200	-0.37918200	-2.63526200
H	-2.68351200	1.24749800	-3.31318100
N	-3.65346700	0.95628200	-1.44688500
C	5.36274900	-4.16731600	0.82020900
C	5.12042600	-2.77296400	0.63688200
C	5.88862100	-2.02288400	-0.31432600
C	6.88455700	-2.75163000	-1.07015700
C	7.08419400	-4.10420400	-0.86653000
C	6.31995800	-4.82131500	0.08720500
H	4.76715000	-4.70636500	1.55432600
H	7.83821400	-4.63453500	-1.43829300
H	6.50086400	-5.88255100	0.22764600
O	5.75036000	-0.75942500	-0.53661200
O	7.56970000	-1.98342800	-1.95952300
C	8.58767000	-2.60028400	-2.72326100
H	9.37762200	-3.01838200	-2.08347200
H	8.18822000	-3.39982300	-3.36363300
C	4.08759500	-2.18735200	1.43567300

H	3.60986100	-2.89551700	2.12959100
C	-2.14028700	-0.56377600	1.36335500
C	-1.61637900	-2.63312900	1.90246000
C	-2.73593900	-2.63192700	1.11736800
N	-3.05079300	-1.33145700	0.77826500
H	-2.10829900	0.51504200	1.32066200
H	-1.06411100	-3.43618500	2.36619000
H	-3.35688500	-3.45476400	0.79572100
N	-1.24637200	-1.30819500	2.05840500
C	-0.00835000	-0.83388700	2.68301000
H	0.11733800	-1.36761800	3.63107700
H	-0.13804000	0.22655600	2.92012000
C	1.19337500	-1.05758600	1.75428100
H	1.21966600	-2.11472800	1.46104100
H	1.04353100	-0.47827100	0.83715100
C	2.54741500	-0.68296600	2.37621000
H	2.68320100	-1.24599600	3.31337400
H	2.57423000	0.38015300	2.63433700
N	3.65304000	-0.95597900	1.44683400
Zn	4.72857900	0.64099000	0.39621700
Zn	-4.72864800	-0.64129300	-0.39653500
H	9.01048500	-1.81314600	-3.35019100
H	-9.00808600	1.81178700	3.35349400
O	-4.99733400	-1.38365200	-2.53120700
O	5.00156500	1.38186300	2.53038000
C	-5.88679100	-0.68976300	-3.42126800
H	-5.50158400	0.32465000	-3.53423800
H	-5.90468300	-1.18269000	-4.39961900
H	-6.90212600	-0.64799900	-3.01106500
C	5.89097600	0.68690400	3.41961200
H	6.90629100	0.64545800	3.00933600
H	5.90896500	1.17875700	4.39850700
H	5.50567100	-0.32759700	3.53149400
H	-5.42322600	-2.23407800	-2.27937300
H	5.42781100	2.23212300	2.27851500
I	6.30585600	3.02220300	-0.00231800
I	-6.30692600	-3.02089400	0.00085800

F2

C	-5.51209800	-3.50252000	-0.49127400
C	-5.17099900	-2.16157300	-0.14452200
C	-5.90823100	-1.06112500	-0.70305100
C	-6.97278600	-1.39382800	-1.62521600
C	-7.26663600	-2.70726400	-1.93858900
C	-6.53261500	-3.77488100	-1.36676600
H	-4.93934800	-4.31398200	-0.04685100
H	-8.07127400	-2.93594200	-2.62937900

H	-6.78551600	-4.79806500	-1.62723500
O	-5.68972200	0.18549700	-0.44628500
O	-7.62603000	-0.30592000	-2.12452500
C	-8.69496000	-0.53251000	-3.02091000
H	-8.36090800	-1.05144800	-3.93100700
H	-9.50029800	-1.11781300	-2.55462500
C	-4.07365600	-1.99958400	0.76479700
H	-3.63331600	-2.94735600	1.10836400
C	2.33073100	-1.24573600	1.02451200
C	1.58711500	-3.14598300	1.86361200
C	2.76324900	-3.36683200	1.20256000
N	3.21893300	-2.17307400	0.68475000
H	2.40617500	-0.20137900	0.75215900
H	0.92788600	-3.80698000	2.40550100
H	3.31363100	-4.28607100	1.06745700
N	1.32277500	-1.79122900	1.74740000
C	0.13714700	-1.11761500	2.28764200
H	0.41110200	-0.08348700	2.51457400
H	-0.09158200	-1.60485000	3.24158700
C	-1.08104600	-1.17603800	1.34905500
H	-1.00476800	-0.39675500	0.58194400
H	-1.08964600	-2.13906800	0.82405100
C	-2.40398400	-1.01590000	2.12108900
H	-2.37684500	-0.11603300	2.74647500
H	-2.52795800	-1.87564300	2.79848800
N	-3.55038600	-0.89641900	1.22001700
C	6.52840500	3.24018000	-0.11495000
C	5.44793400	2.41665500	-0.50001600
C	5.54534300	1.00388800	-0.32697800
C	6.75832100	0.51565500	0.25422800
C	7.80356800	1.33893800	0.62934000
C	7.68974200	2.72656000	0.43808000
H	6.43424500	4.31399300	-0.26473200
H	8.70308000	0.91973200	1.07012700
H	8.50649200	3.38168900	0.72432800
O	4.59759800	0.16745200	-0.66479600
O	6.77273700	-0.86974500	0.41667500
C	8.02745200	-1.56527200	0.40106700
H	8.67873400	-1.14618900	-0.37274800
H	8.51577300	-1.49175900	1.37915900
C	4.27732400	3.07776800	-1.07319500
H	4.39599500	4.17394400	-1.16897500
C	-2.30631800	2.41024000	-0.90676100
C	-1.95236300	4.26727500	0.22427900
C	-2.94697500	3.54612800	0.82704900
N	-3.15627100	2.38432600	0.10853000
H	-2.21001800	1.65075300	-1.66986800
H	-1.49747500	5.21540600	0.46783300

H	-3.53743000	3.73196700	1.71310900
N	-1.55531500	3.53798000	-0.88416500
C	-0.38470300	3.80373500	-1.72399600
H	-0.27696400	4.88948100	-1.81142100
H	-0.59412200	3.41537700	-2.72633700
C	0.87250300	3.15435700	-1.13593600
H	1.03846000	3.53761000	-0.12129000
H	0.70551400	2.07460300	-1.04284500
C	2.14134400	3.36501700	-1.97294500
H	2.41460200	4.43808000	-1.99239000
H	1.93926300	3.06276600	-3.01197300
N	3.18948400	2.51525500	-1.44624500
Zn	4.96612500	-1.74449500	-0.45429400
Zn	-4.52275400	0.96515900	0.93888400
H	7.78121800	-2.59993100	0.15941000
H	-9.07717900	0.45440300	-3.28958500
O	-4.84584900	1.96204600	2.51663200
O	5.81675500	-3.25807900	-1.15294200
C	-5.83848800	1.74156500	3.46737200
H	-5.88662900	0.69429200	3.83010800
H	-5.66512100	2.36684700	4.36288300
H	-6.85572500	1.99149100	3.10732100
C	5.25627800	-4.24778400	-1.95858500
H	5.10238000	-3.92041400	-3.00481900
H	5.92024300	-5.12892100	-2.00214600
H	4.27417200	-4.61924000	-1.60042200

H2

C	-8.03731100	-1.65072900	4.10312700
C	-7.87814600	-2.37771800	2.88896200
C	-8.38827600	-3.71306600	2.77987400
C	-9.04536300	-4.25780700	3.94320700
C	-9.17692000	-3.52004200	5.10665000
C	-8.66999400	-2.20383200	5.19096000
H	-7.65075700	-0.63520200	4.14984300
H	-9.67596600	-3.94746800	5.96980800
H	-8.78976200	-1.64060200	6.11150100
O	-8.29688600	-4.46701100	1.72453900
O	-9.50455800	-5.53305500	3.77327800
C	-10.18612100	-6.13691800	4.85322100
H	-9.54204200	-6.23664500	5.73907700
H	-11.08749000	-5.57309600	5.13343000
C	-7.20414000	-1.67649000	1.82251100
H	-6.87537700	-0.66103700	2.07576300
C	-2.11503600	-0.65454000	-2.19504600
C	-2.71840500	-2.64332700	-2.93104000

C	-1.35547200	-2.58304400	-2.84124600
N	-0.98843700	-1.33142800	-2.38400100
H	-2.20732500	0.34388100	-1.79267800
H	-3.38991000	-3.42846300	-3.24386100
H	-0.61516100	-3.34047000	-3.04444300
N	-3.18889100	-1.40872300	-2.51712600
C	-4.57535700	-1.07797400	-2.18082900
H	-5.23596900	-1.37967700	-2.99904700
H	-4.62194100	0.00587900	-2.07263800
C	-4.98564100	-1.75864800	-0.86656700
H	-5.11048700	-2.83267000	-1.04861600
H	-4.18365400	-1.64041000	-0.13013600
C	-6.29183800	-1.17274700	-0.31612600
H	-6.98365600	-1.00843300	-1.14986000
H	-6.08885600	-0.21274500	0.17577100
N	-6.94222600	-2.09647000	0.62033400
C	3.85698000	-5.18106300	-2.37826500
C	2.66326000	-4.70299100	-1.78777100
C	2.37671100	-3.30397600	-1.82085300
C	3.29395700	-2.47813500	-2.54555700
C	4.46715200	-2.95885300	-3.09407800
C	4.76382700	-4.33499000	-2.99264900
H	4.06241000	-6.24930700	-2.33525000
H	5.15782900	-2.29253700	-3.60051100
H	5.70017100	-4.71445400	-3.39207500
O	1.32410300	-2.76430100	-1.27551800
O	2.86360100	-1.15893300	-2.62427900
C	3.61101500	-0.22462900	-3.40313900
H	4.61096600	-0.08889900	-2.97909500
H	3.69544000	-0.56980500	-4.44012900
C	1.72233200	-5.68188000	-1.24825100
H	1.93925300	-6.72622300	-1.54503100
C	-4.89770800	-5.69878400	0.22779200
C	-4.63978000	-6.62960000	-1.75012100
C	-5.81076000	-5.92130000	-1.72478100
N	-5.96205500	-5.34203300	-0.48059400
H	-4.69587100	-5.40917500	1.24907700
H	-4.17010800	-7.21951900	-2.52226300
H	-6.55626700	-5.77740900	-2.49175500
N	-4.06851000	-6.48341200	-0.49841200
C	-2.74183800	-6.96262800	-0.08673400
H	-2.64589000	-8.00325600	-0.41457600
H	-2.72565300	-6.96327600	1.00788600
C	-1.61896000	-6.08296700	-0.64760600
H	-1.64484600	-6.10438100	-1.74414500
H	-1.79185400	-5.04225000	-0.35299400
C	-0.21130300	-6.48371100	-0.16772900
H	0.07711200	-7.46789100	-0.58585100

H	-0.22811800	-6.58644200	0.92879900
N	0.70203100	-5.41729900	-0.51702800
Zn	0.89625900	-0.84056400	-1.58072200
Zn	-7.53283000	-3.98578800	-0.00265500
H	3.04496100	0.70544800	-3.34862500
H	-10.47748700	-7.13126800	4.50807400
C	3.12395300	7.49712000	4.10524800
C	2.74021200	6.45365600	3.21665500
C	3.71886500	5.54754300	2.69656800
C	5.08797800	5.77410100	3.10037100
C	5.42723000	6.81304500	3.94708400
C	4.43798800	7.68372500	4.46069200
H	2.35188100	8.15750800	4.49506700
H	6.46234800	6.97086100	4.23089300
H	4.72668800	8.48777400	5.13053600
O	3.44728400	4.54624100	1.92566400
O	5.98233000	4.88512500	2.56491200
C	7.35497000	5.07759600	2.84896000
H	7.70549900	6.05911400	2.50138400
H	7.56661200	4.98541100	3.92388000
C	1.33710300	6.34671400	2.92067100
H	0.71353300	7.01097700	3.53715400
C	-4.02237600	5.61447900	-0.00185300
C	-4.22967900	5.54568700	2.19360000
C	-4.93151400	4.51182300	1.64318400
N	-4.79576300	4.56528800	0.26900100
H	-3.72838400	5.91819700	-0.99968200
H	-4.07199200	5.84201700	3.21894900
H	-5.44737200	3.69519700	2.12530700
N	-3.65340700	6.23697600	1.13976400
C	-2.65534100	7.30056400	1.24510900
H	-2.76897800	7.75176900	2.23561800
H	-2.89638100	8.07077900	0.50518100
C	-1.21443500	6.80550000	1.03690200
H	-1.11247400	6.41845100	0.01679700
H	-0.56258800	7.68635400	1.11912400
C	-0.74677100	5.73789300	2.04658500
H	-1.19423900	4.76820800	1.81686000
H	-1.09081100	6.02489000	3.05224800
N	0.72075300	5.59561500	2.05463400
C	-5.93036200	4.89818700	-5.96836700
C	-5.01750800	5.04273800	-4.90339700
C	-5.16397800	4.23590400	-3.73857500
C	-6.28798700	3.35430900	-3.70335500
C	-7.18753700	3.24017400	-4.74764100
C	-7.00225400	4.02293600	-5.90093600
H	-5.78353200	5.50362400	-6.86069400
H	-8.01941900	2.54633500	-4.69364400

H	-7.69772800	3.93120700	-6.72911700
O	-4.31459600	4.25181500	-2.74193600
O	-6.37584600	2.61706000	-2.51304100
C	-7.54616600	1.81040100	-2.28986900
H	-8.44627900	2.42476200	-2.39418100
H	-7.58146500	0.95801900	-2.97472600
C	-3.90426300	5.98040400	-5.06619600
H	-3.67173300	6.23327700	-6.11785300
C	1.34344200	6.36356000	-1.57297800
C	2.18183600	5.40084200	-3.36263700
C	2.56227600	4.71075400	-2.24445400
N	2.02506800	5.32076700	-1.12575100
H	0.79042900	7.06160200	-0.96368700
H	2.37221900	5.23443100	-4.41190300
H	3.14781200	3.81058900	-2.14683700
N	1.40842300	6.46171600	-2.92353300
C	0.47722800	7.25351600	-3.73634100
H	0.96114500	7.48015400	-4.69129000
H	0.31153500	8.20480700	-3.21840100
C	-0.83682300	6.47736000	-3.90474300
H	-0.66633400	5.59543000	-4.53321200
H	-1.12999900	6.09178200	-2.92201800
C	-2.04221200	7.26587700	-4.44521800
H	-1.93560000	7.46586400	-5.52774400
H	-2.10308200	8.23865600	-3.93357900
N	-3.22059300	6.48852600	-4.11155000
Zn	-4.68876300	3.10166800	-1.22431100
Zn	1.83839500	4.22902500	0.75455100
H	-7.46694300	1.44527000	-1.26609300
H	7.88916700	4.29385000	2.30766700
C	-0.33198500	1.29903600	6.48832300
C	0.04865400	0.84859800	5.19031300
C	-0.90198900	0.16271900	4.37302600
C	-2.21489800	-0.04904900	4.91810700
C	-2.55008100	0.41004000	6.17983000
C	-1.59920500	1.08701000	6.97534000
H	0.40520500	1.82627100	7.08966700
H	-3.55006700	0.25040800	6.56764200
H	-1.88001100	1.43866400	7.96343900
O	-0.67019900	-0.27768000	3.16428800
O	-3.04328900	-0.72749600	4.08078800
C	-4.41407100	-0.83694800	4.43622900
H	-4.54053100	-1.38836800	5.37770200
H	-4.87707200	0.15316800	4.50469400
C	1.38617500	1.18718200	4.77690000
H	1.92464400	1.81095100	5.50320700
C	7.13958900	0.18671200	0.80821200
C	5.83598400	1.57112300	-0.31970000

C	6.66725700	0.91468700	-1.18585600
N	7.47864600	0.05306600	-0.47177400
H	7.56778400	-0.38403600	1.62129500
H	5.00922800	2.25447800	-0.45989800
H	6.74549600	0.98517500	-2.26016800
N	6.15727700	1.10417200	0.94336600
C	5.49827100	1.52468100	2.18540100
H	5.34260500	2.60540900	2.12515600
H	6.19501000	1.32670000	3.00703000
C	4.15953200	0.80886400	2.39626300
H	3.59048300	0.88400800	1.46522900
H	4.32908700	-0.25343000	2.61279600
C	3.35711300	1.48218600	3.51061600
H	3.23198300	2.53797500	3.23964300
H	3.90589400	1.44938500	4.46485300
N	2.02274400	0.87341400	3.68631700
C	11.62504100	-4.17906400	2.16172200
C	10.31691500	-3.70575400	1.94000400
C	10.03614400	-2.92764500	0.78182200
C	11.13998400	-2.62571200	-0.07164500
C	12.42778100	-3.06505900	0.17883700
C	12.67296700	-3.86051700	1.31124200
H	11.80999300	-4.79895400	3.03684400
H	13.24301800	-2.81160100	-0.49095000
H	13.67744500	-4.22170900	1.50822200
O	8.83247200	-2.51589300	0.46594200
O	10.77704500	-1.84915400	-1.17753900
C	11.71040400	-1.69715400	-2.25243300
H	12.54576500	-1.05903100	-1.94322200
H	12.08512000	-2.67633700	-2.56786700
C	9.26333500	-4.08194300	2.88959400
H	9.43817800	-5.03606900	3.42136500
C	2.86098000	-2.50259200	3.52678400
C	2.81204100	-4.30942300	2.27529400
C	1.91187400	-3.39920600	1.79004700
N	1.95688000	-2.26647300	2.58293000
H	3.14435600	-1.81634100	4.31145400
H	3.09048900	-5.29088800	1.92480600
H	1.28022700	-3.47916900	0.91447200
N	3.40580800	-3.73139600	3.38478500
C	4.61712700	-4.19158700	4.07158900
H	4.52032700	-5.26516300	4.26156900
H	4.64759000	-3.68914900	5.04476700
C	5.86250800	-3.85776100	3.23908300
H	5.90828300	-4.50713900	2.35733000
H	5.76226900	-2.83517400	2.85837600
C	7.19787000	-3.93009400	3.99572800
H	7.41367100	-4.96080900	4.33493100

H	7.13182200	-3.29696900	4.89476500
N	8.21542400	-3.38788800	3.11762600
Zn	8.59874000	-1.53575900	-1.18531500
Zn	1.08703600	-0.37151200	2.27310300
H	11.16065900	-1.23782400	-3.07385100
H	-4.88534200	-1.39397200	3.62754000
As	1.27216300	1.69121400	-0.34436300
O	2.73781200	2.49251800	-0.08397800
O	0.22981700	2.80802400	0.42094900
O	1.19815000	0.09888000	0.37787300
O	0.95319800	1.18501900	-1.92174900
O	-3.70567100	1.57671800	-0.57086900
O	8.17373100	-1.49925400	-3.06141300
O	-8.45778100	-4.02379700	-1.74699500
As	-9.03628200	-2.69332500	-2.61307400
As	8.34540000	-2.62727800	-4.28813200
As	-3.36562600	1.37641500	1.09139500
O	-2.18927200	2.58917100	1.55558700
O	-2.46280200	-0.12665300	1.06103100
O	-4.68680800	1.41386100	2.05531000
H	-2.01307100	-0.28354600	1.93273900
H	-1.31963100	2.53280800	1.05144900
O	-9.99760200	-3.48768700	-3.87634900
O	-10.34586700	-1.93908800	-1.69226600
O	-7.99019900	-1.55550900	-3.12230400
O	7.03254600	-2.25504600	-5.42645400
O	8.42735400	-4.22426400	-3.98915100
O	9.74689900	-1.96767100	-5.15537400
H	-9.71746600	-4.41894700	-3.90189400
H	-11.11613700	-2.53271800	-1.70717900
H	6.51655500	-3.07082500	-5.55134000
H	9.98890100	-2.57115300	-5.87832300

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