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Supplementary Information

Urazole Decorated Multifunctional Mesoporous Polymer Networks for Efficient Capture of Uranium (VI) from Aqueous Matrices

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Materials and Methods

Materials

Indole-3-carboxaldehyde (97%), 4,4" -methylene bis-phenyl isocyanate (98%), ethyl carbazate (97%, 1,8-diaminooctane (≥98%) were used as purchased from sigma-Aldrich. Tris(2-aminoethyl)amine (>98.0%) and 1,4-diazobicyclo[2.2.2]octane were bought from Tokyo Chemical Industry Pvt Ltd. Salts were bought from Central Drug House (P) Ltd. (CDH). All the solvents were purchased from Sisco Research Laboratories Pvt. Ltd. The stock solution of uranyl was prepared by dissolving of $UO_2(NO_3)_2.6H_2O$ (Sisco Research Laboratories Pvt. Ltd.) in DI water. DMSO-d_6 were used as NMR solvent was purchased from sigma-Aldrich.

Synthesis of 4,4'-(4,4'-Diphenylmethylene)-bistriazolinedione (MDI-bisTAD)

The synthesis of MDI-bisTAD was carried out following a procedure from previous reports.[1,2] Initially, ethyl carbazate (1 g, 9.605 mmol) was dissolved in toluene (7.5 mL) and cooled in an ice bath under an inert atmosphere. To this chilled solution, a toluene solution (5 mL) of 4,4'-methylenebis(phenyl isocyanate) (1.2 g, 4.802 mmol) was added dropwise with constant stirring. The reaction mixture was then stirred at ambient temperature for 3 h, followed by heating at 90 °C for an additional 2 h. Upon cooling, the resulting solid, 4,4'-(4,4'-diphenylmethylene)bis(carbethoxysemicarbazide), was collected by filtration, washed with toluene, and dried under vacuum (yield: 95%). Subsequently, the obtained bis-semicarbazide (1 g, 2.182 mmol) was treated with 5 mL of 4 M aqueous KOH and refluxed for 2 h under inert conditions. After the reaction, the hot mixture was filtered, cooled to room temperature, and acidified to pH 1 using concentrated hydrochloric acid. The precipitated product, 4,4'-(4,4'-diphenylmethylene) bisurazole (MDI-bisurazole), was filtered, washed with distilled water, and dried.

For the final step, MDI-bisurazole (0.8 g, 2.183 mmol), DABCO-Br (2.03 g, 1.288 mmol), and dry dichloromethane (10 mL) were combined in a 50 mL round-bottom flask and stirred under inert atmosphere at room temperature for 5 h. After completion, the mixture was filtered, and the residue was washed with dichloromethane. The pink filtrate was concentrated under reduced pressure to obtain the final product, MDI-bisTAD, as a pink solid (~89% yield). MDI-bis Urazole: ^{1}H NMR (500 MHz, DMSO-d_6 δ(ppm)): 10.44 (2H, s, NH), 7.47-7.33 (8H, m, ArH), 4.02(CH_2), ^{13}C NMR (DMSO d_6, 500MHz): 159.21 (CO), 142.44 (C), 130.39 (C), 129.65 (C), 126.74 (C), 40.07 (C).

Synthesis of Octyl-bisTAD

The synthesis of OCT-bisTAD was carried out following a procedure from previous reports[2,3] To synthesize octyl-bisTAD, diphenyl carbonate (1.0 g, 4.65 mmol) was melted at 85 °C under an inert atmosphere. Ethyl carbazate (1.02 g, 9.81 mmol) was added to the molten diphenyl carbonate, and the reaction mixture was stirred for 1.5 h. Upon completion, the intermediate product, ethyl phenyl hydrazine-1,2-dicarboxylate (EPHD), was precipitated by adding the mixture to cold water. The solid was collected by filtration and dried under vacuum. Next, EPHD (0.25 g, 1.12 mmol) was heated to 90 °C until molten, after which 1,8-diaminooctane (65 mg, 0.56 mmol) was added. The mixture was stirred for 40 minutes at this temperature under an inert atmosphere, followed by further heating to 240 °C for 1.5 h under a gentle flow of argon. The resulting bisurazole derivative was cooled to room temperature, washed with diethyl ether, and dried. For the final step, octyl-bisurazole (0.25 g, 0.80 mmol), DABCO-Br (0.74 g, 0.47 mmol), and dry dichloromethane (7 mL) were placed in a round-bottom flask and stirred at room temperature for 5 h under inert atmosphere. After reaction completion, the mixture was filtered, and the residue was washed with additional dichloromethane. The pink filtrate was concentrated under reduced pressure using a rotary evaporator at a bath temperature not exceeding 30 °C. The resulting product, octyl-bisTAD, was obtained as a pink solid (yield: ~85%). OCT-bis Urazole:^{1}H NMR (500 MHz, DMSO-d_6 δ(ppm)): 9.96 (2H, s, NH), 3.3-3.27 (2H, t, CH_2), 1.5-1.44(2H,q,CH_2), 1.18(4H,q,CH_2) ^{13}C NMR(DMSO d_6, 500MHz): 155.62 (CO), 38.34 (C), 28.91 (C), 27.92 (C), 26.48 (C).

Model Reaction (INTMonomer with Octyl-monoTAD): A model reaction was conducted using INTS monomer (50 mg, 0.0948 mmol) and octyl-monoTAD (27.96 mg, 0.0948 mmol). The monomer was dissolved in a minimal volume of THF and a stoichiometric amount of octyl-monoTAD dissolved in THF was added dropwise to the INTS monomer solution under continuous stirring. The reaction proceeded instantaneously at room temperature, confirmed by the disappearance of the characteristic pink color of the TAD. After completion, the reaction mixture was concentrated under reduced pressure using a rotary evaporator. The adduct rinsed with methanol, and dried under vacuum.

Uranium adsoption: The concentration of uranyl ions ($UO2^{2+}$) remaining in solution after adsorption was determined using the Arsenazo III spectrophotometric method, following a modified protocol reported in the literature.,[4] For the colorimetric assay, 1 mL of the supernatant solution was mixed with 1 mL of Arsenazo III reagent (0.01%w/v) and pH 2-3 was maintained using HCl. The resulting solution was allowed to equilibrate for 2 minutes, and the absorbance was recorded at 652 nm using a UV–Vis spectrophotometer. A clear increase in absorbance at this wavelength corresponded to the formation of the UO_2^{2+}–Arsenazo III complex.

Adsorption Isotherm: In this study, the adsorption performance of the synthesized porous polymer toward uranyl ions in aqueous solution was investigated. Typically, 20mL of uranyl nitrate solution with varying concentrations (ranging from 20 to 200 ppm, pH 6±0.5) was added to a vial containing 4 mg of accurately weighed, freeze-dried porous polymer (INTS-Polymer). The mixture was stirred at 500 rpm at room temperature in a sealed glass vial to prevent evaporation and contamination. After the desired contact time, a 1 mL aliquot was withdrawn from the suspension and immediately centrifuged for a few minutes to separate the solid adsorbent from the solution. The resulting supernatant was analyzed using the Arsenazo III spectrophotometric method to determine the residual uranyl concentration. The equilibrium adsorption capacity (Q_e, mg/g) and adsorption efficiency (%) were calculated using the following equations:

$$\mathbf{Q_e = [(C_o - C_e) \times V]/ M \ldots\ldots\ldots\ldots\ldots\ldots (S1)}$$

$$\mathbf{Adsorption\ efficiency\ (\%) = [(C_o - C_t)/C_o] \times 100 \ldots\ldots\ldots\ldots\ldots\ldots (S2)}$$

Where C_o and C_e (mg L^{-1}) are the initial and equilibrium concentration (after adsorption) of the uranyl ions in the stock solution, C_t is the concentration of the uranyl ions solution at time (t), M (g) is the weight of porous polymers, V is the total volume of iodine solution in litter.

The adsorption behavior of uranyl ions onto the synthesized porous polymer further was examined by fitting the experimental data to both the Langmuir and Freundlich isotherm models. These models help describe the interaction between the uranyl species and the polymeric adsorbent surface under equilibrium conditions.

Langmuir Isotherm Model

The Langmuir model assumes monolayer adsorption onto a homogeneous surface with a finite number of identical sites. The equation governing this model is:

$$\mathbf{Q_e = Q_m K_L C_e/(1+K_L C_e) \text{ ………………....(S3)}}$$

Where Q_e (mg/g) is the amount of uranyl adsorbed at equilibrium, C_e (mg/L) is the equilibrium concentration of uranyl in solution, Q_m (mg/g) represents the theoretical maximum adsorption capacity of the polymer and K_L (mg/L) is the Langmuir constant, which reflects the affinity between the adsorbent and uranyl ions.

Freundlich Isotherm Model

The Freundlich model is an empirical expression applicable to adsorption on heterogeneous surfaces and multilayer adsorption. It is given by:

$$\mathbf{Q_e = K_F C_e^{1/n} \text{ ……………………...(S4)}}$$

Where Q_e(mg/g), C_e(mg/L) and Q_m(mg/g) are as previously defined, K_F is the Freundlich constant indicative of adsorption capacity, and n is a dimensionless factor related to adsorption intensity or surface heterogeneity.

Adsorption Kinetics: To investigate the rate and mechanism of uranyl ion adsorption onto the porous polymer, kinetic studies were conducted using a 20ppm uranyl solution. In a typical experiment, 4 mg of the adsorbent was added to 20 mL of the uranyl solution in a glass vessel and stirred continuously at room temperature of pH 6±0.5. At predetermined time intervals, 1mL aliquots were withdrawn from the mixture, and the adsorbent was separated by filtration. The residual uranyl concentration in the supernatant was measured using the UV–Vis spectrophotometric.

The amount of uranyl adsorbed at any time t, denoted as q_t (mg/g), was calculated using the following equation:

$$\mathbf{q_t = (C_0 - C_t) \times V/m \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(S5)}$$

Where C_0 and C_t (mg/L) are the initial and time-dependent uranyl concentrations, respectively, V is the volume of the solution in liters, and m is the mass of the adsorbent used (g). To understand the adsorption kinetics and rate-controlling mechanism, the experimental data were fitted to two common kinetic models:

Pseudo-First-Order Kinetic Model

$$\mathbf{\ln (q_e - q_t) = \ln q_e - k_1 t \ldots\ldots\ldots\ (S6)}$$

Pseudo-Second-Order Kinetic Model

$$\mathbf{t/q_t = 1/k_2\, q_e^2 + t/q_e \ldots\ldots\ldots\ldots\ldots\ldots(S7)}$$

Where q_e (mg/g) is the equilibrium adsorption capacity, q_t (mg/g) is the adsorption capacity at time t, $k_1(min^{-1})$ and $k_2(g \cdot mg^{-1} \cdot min^{-1})$ are the pseudo-first-order and pseudo-second-order rate constants, respectively. The model fitting was evaluated based on the correlation coefficients (R^2) and comparison between experimental and calculated q_e values.

Effect of pH: To assess the influence of solution pH on the adsorption performance of the synthesized porous polymer toward uranyl ions, a series of experiments were conducted across a pH range of 3 to 9. A aqueous solution of uranyl nitrate was prepared and its pH adjusted using dilute hydrochloric acid or potassium hydroxide. Then, 4 mg of the adsorbent was added to 20 mL of each solution in individual glass vials. The suspensions were magnetically stirred at room temperature. Afterward, the solid adsorbent was removed and the concentration of remaining uranyl ions in the filtrate was determined spectrophotometrically. The equilibrium adsorption capacity (mg/g) was calculated based on the initial and final concentrations using Equation (S1) and Adsoption efficiency was calculated using equation S2.

Influence of Competitive ion: To evaluate the selectivity of the polymer toward uranyl ions in the presence of competing metal ions, a series of binary and mixed-ion adsorption experiments were performed. In a typical experiment, 4 mg of the polymer was added to a binary solution containing 10mL of 20 ppm U(VI) and 10 mL of competing metal ion (1:1

equivalent), such as VO^{2+}, Co^{2+}, Ni^{2+}, Fe^{3+}, Cu^{2+}, Zn^{2+}, Mg^{2+}, Na^{+}, K^{+} and Ca^{2+}. These binary mixtures were stirred at 500 rpm in closed glass vials at room temperature. After equilibration, the mixtures were filtered separate the solid phase. The residual concentration of uranyl in the filtrate was measured using UV–Vis spectroscopy. Additionally, a multi-ion selectivity test was conducted by mixing all competing ions together with uranyl in the same solution to assess the adsorbent's real-world performance. The equilibrium adsorption capacity (mg/g) was calculated based on the initial and final concentrations using Equation (S1) and Adsoption efficiency was calculated using equation S2. The distribution coefficient (K_d, mL/g) is a useful parameter to evaluate the affinity of the adsorbent toward uranyl ions in solution. It was calculated using the following:

$$\mathbf{k_d = (C1 - C2)/C2 \times V/M \;\ldots\ldots\ldots\ldots\ldots\; (S8)}$$

The distribution coefficient values was calculated by the formula used in equation (S8). Herein, K_d is the distribution coefficient, C2 and C1 represents the final and initial concentration, respectively. V represents the volume of the total solution, while M is the weight of the adsorbent.

Adsorption in Simulated sea-water, tap water, river water, lake water, pond water and STP water: Simulated seawater was prepared following a previously reported procedure,[5] using appropriate amounts of salts to produce metal ions to replicate the composition of natural seawater. The pH of the solution was adjusted and maintained at 8 (average seawater pH) throughout the experiment. A series of uranyl solutions with concentrations of 2, 4, 6, 8, and 10 µM were prepared in this medium. To each 20 mL solution, 4 mg of the polymer adsorbent was added, and the mixture was stirred at 500 rpm for 6 hours in a sealed container at room temperature. After equilibrium was reached, the supernatant was separated by filtration, and the residual uranyl concentration was determined.

In addition, Adsorption experiments were performed using various real water matrices, including potable tap water (IIT Patna, India), lake water (Jagdahwa Lake, Kaimur, Bihar, India), river water (Gandak River, Hajipur, Bihar, India), pond water (Bagh Taj Khan Pokhar, Hajipur, Bihar, India), and STP effluent (Saidpur, Patna, Bihar, India). Each 20 mL water sample was spiked with 2 ppm uranyl nitrate and treated following the same procedure described above. The adsorption capacity and removal efficiency were calculated using Equations (S1) and (S2), based on the difference between the initial and final uranyl concentrations.

Uranium uptake in natural sea water: Natural seawater was collected from Puri Beach, Odisha (India) and used without pretreatment (pH = 8.1 ± 0.5). For isotherm studies, uranyl solutions of 2-10 μM were prepared in seawater, and 4 mg of adsorbent was added to 20 mL of each solution and stirred at 500 rpm for 6 h; the supernatant was filtered, and the remaining U(VI) concentration was measured by UV–Vis spectroscopy.

For kinetics, seawater (20 mL) was spiked to 5 ppm U(VI), mixed with 4 mg adsorbent in 20 mL total volume, and aliquots (1 mL) were withdrawn at defined intervals, filtered, and analysed.

To evaluate selectivity, real seawater samples were spiked with U(VI) (5 ppm) and an equimolar (1:1) concentration of a competing metal ion (VO^{2+}, Co^{2+}, Ni^{2+}, Fe^{3+}, Cu^{2+}, Zn^{2+}, Mg^{2+}, Na^{+}, K^{+} and Ca^{2+}). In each binary test, 4 mg of the polymer was added to 20 mL of the U/metal-ion mixture and stirred at 500 rpm at room temperature. After equilibrium, the solution was filtered, and the remaining U(VI) concentration was determined by UV-Vis spectroscopy. A multi-ion experiment was also performed by spiking seawater with U(VI) and all competing ions together at 1:1 equivalence. Adsorption capacity and efficiency were calculated using Equations (S1) and (S2).

For adsorption capacity in natural (without any external controlled addition) seawater, the polymer was dispersed in 1 L of seawater and stirred for 3 days, collected by vacuum filtration, and eluted with 0.1 M HNO_3 followed by DI water; the eluate was analysed by ICP-MS to quantify the adsorbed uranium. The adsorption capacity was calculated using the equation (8):

$$\mathbf{Q = C \times V/M \ \ldots\ldots\ldots\ldots\ldots\ldots.. \ (S8)}$$

where Q (mg g^{-1}) is the adsorption capacity, C (mg L^{-1}) is the uranium concentration in the eluent measured by ICP-MS, V(L) is the volume of the elution solution, and m(g) is the mass of the dried polymer. The protocol was followed as reported in our earlier work.[6, 7]

Dynamic Flow study: A glass column (20 cm in length, 1 cm inner diameter) was packed with 15 mg of the polymer adsorbent, resulting in a uniform bed height of approximately 8 cm. To ensure consistent elution, a syringe pump was used to regulate the flow rate at 0.5 mL/min. The column was initially challenged with 50 mL of an aqueous uranyl solution (20 ppm) prepared in deionized water. The effluent was collected at defined intervals, and the concentration of residual uranyl ions was determined. For dynamic adsorption study of real Sea water sample, U(VI) spiked sample (5ppm) was prepared as described above.

Elution: After adsorption, the saturated adsorbent was carefully removed via vacuum filtration, and subjected to desorption treatments using various eluents: deionized water, 0.1 M HNO_3, 0.1 M NaCl, and 0.1 M Na_2CO_3. In each trial, 15 mg of U(VI)-loaded polymer was dispersed in 20 mL of the respective eluent and stirred continuously at room temperature for 2 hours. After the desorption period, the suspension was filtered using vacuum filtration. After elution, the filtrate was either analyzed directly by UV-Vis spectroscopy or subjected to freeze-drying. The resulting solid was then redissolved to prepare a concentrated solution for further analysis. The elution efficiency (%) was calculated using the following equation:

$$elution\ efficiency\ (\%) = \frac{Ce \times V}{m \times qe} \times 100 \quad \text{................ (S9)}$$

Where Ce is the uranium concentration in the eluent at equilibrium (mg/L), V is the volume of the eluent solution (mL), m is the mass of the U(VI)-loaded adsorbent (mg), qe is the initial adsorption capacity of the polymer (mg/g). The elution–adsorption cycle using 0.1 M Na_2CO_3 followed by 0.1 M HNO_3 and DI was further repeated for five cycles to evaluate reusability.

DFT methodologies: We have utilized the Gaussian[8] 16 to examine the interaction energy between uranyl ions ($UO_2(NO_3)_2$) and functional moieties of the complexes. In this work, the geometries of each possible coordination mode of complexes, with uranyl ions ($UO_2(NO_3)_2$), were optimized at the B3LYP method[9] and 6-311G(d,p)/ECP60MWB-SEG basis set. Here, 6-311G(d,p) was specifically employed for C, H, N, and O atoms.[10] The ECP60MWB-SEG basis set with its corresponding relativistic pseudo-potential was applied for uranium in $UO_2(NO_3)_2$, while the SDD basis set and pseudo-potential were used for vanadium in VO^{2+} and their respective complexes.[11, 12] The interaction energy is calculated as the difference between the sum of the monomers' total energies and the product complex's total energy.[13]

General characterization:

Fourier transform infrared (FT-IR) spectra A Perkin Elmer Spectrum 400 FT-IR with a universal ATR mode accessory was used to obtain (FT-IR) spectra. Sixty scans of FT-IR data covering a wave number range of 500–4000 cm^{-1} are provided.

Nuclear Magnetic Resonance (NMR) Spectroscopy– A Bruker 400 MHZ spectrometer was used for ^{1}H-NMR spectra. DMSO-d_6 was used as an NMR solvent.

Solid state ^{13}C NMR spectra were recorded using Jeol NMR ECZ 500 MHz. Carbon chemical shifts are expressed in parts per million (δ scale).

Thermogravimetric analyses (TGA) were carried out on a Q6OO SDT TA analyzer under an N_2 atmosphere at a heating rate of 10ºC min^{-1} within a temperature range of 30−700°C.

Scanning Electron Microscopy (SEM) Surface morphology measurements were executed with a Gemini – 500 Zeiss (Germany) scanning electron microscope with energy-dispersive X-ray spectroscopy (EDX). Porous polymer samples were freeze-dried before analysis. To avoid charging during SEM analyses, we coated all the porous polymer samples with a thin layer (around 10nm of 1min) of gold by spin coater before analyses.

N_2 adsorption-desorption analyses Using a liquid nitrogen bath at 77 K, N_2 adsorption-desorption measurements were carried out automatically using a Quantachrome Quadrasorb volumetric device. All freeze-dried porous polymer samples were vacuum-exhausted for 10 hours at 125°C before the gas adsorption investigations. Using the Brunauer-Emmett-Teller (BET) model, the surface areas were calculated between P/P_0 values of 0.05 and 0.35. The non-localized density functional theory (NLDFT) and Barrett-Joyner-Halenda (BJH) technique were utilized to compute the pore size distributions.

UV-vis spectra were obtained using Shimadzu UV 2550 Spectrophotometer with a wavelength range of 200-800 nm.

Powder X-ray diffraction (PXRD) Malvern Panalytical Empyrean diffractometer (with λ = 1.5418 Å, Cu Kα radiation) was utilized for powder X-ray diffraction (PXRD) measurement whose Generator voltage 45kV and Tube current 40mA and step size is 0.02630.

Water Contact Angle (WCA) Measurements were carried out in the CA Goniometer RaméHart instrument Model 250, and the contact angle was measured using DROP image Advance CA software.

Inductively coupled plasma mass spectrometry (ICP-MS) Measurements were performed using an Agilent 7850 ICP-MS instrument.

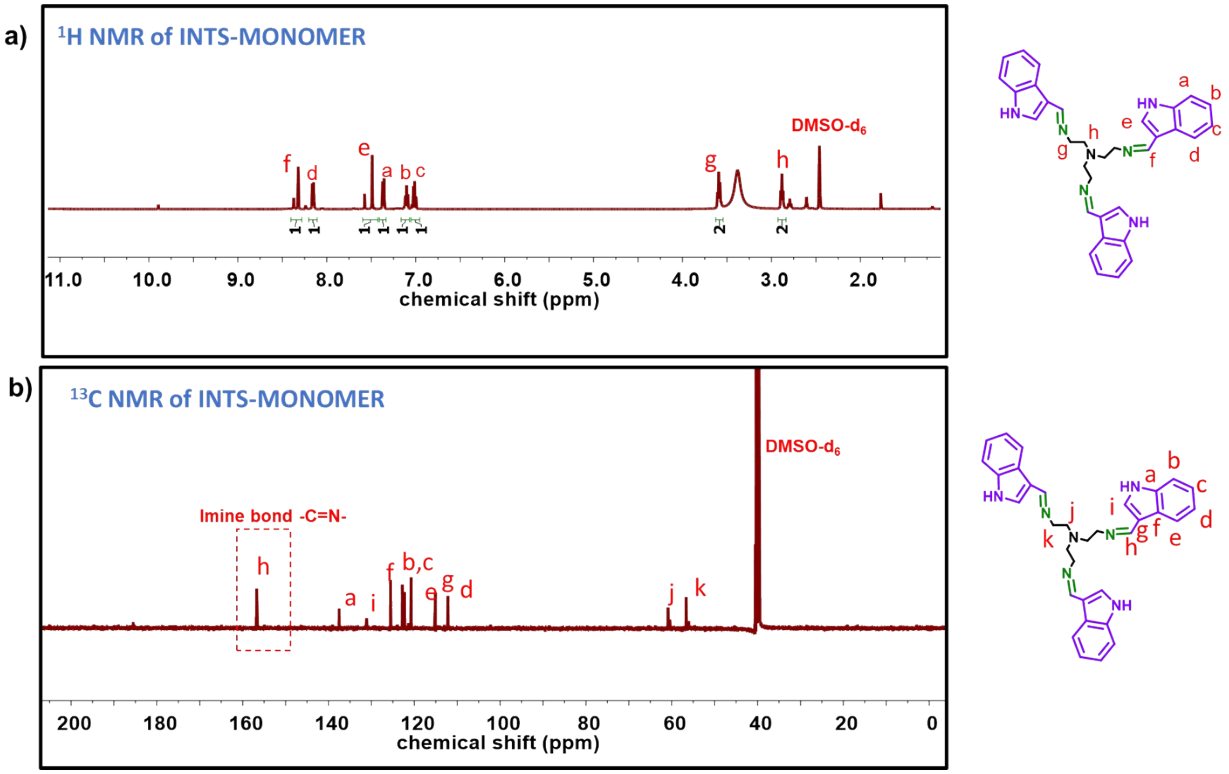


Figure S1: (a) ^{1}H NMR and (b) ^{13}C NMR signals of INTS-monomer.

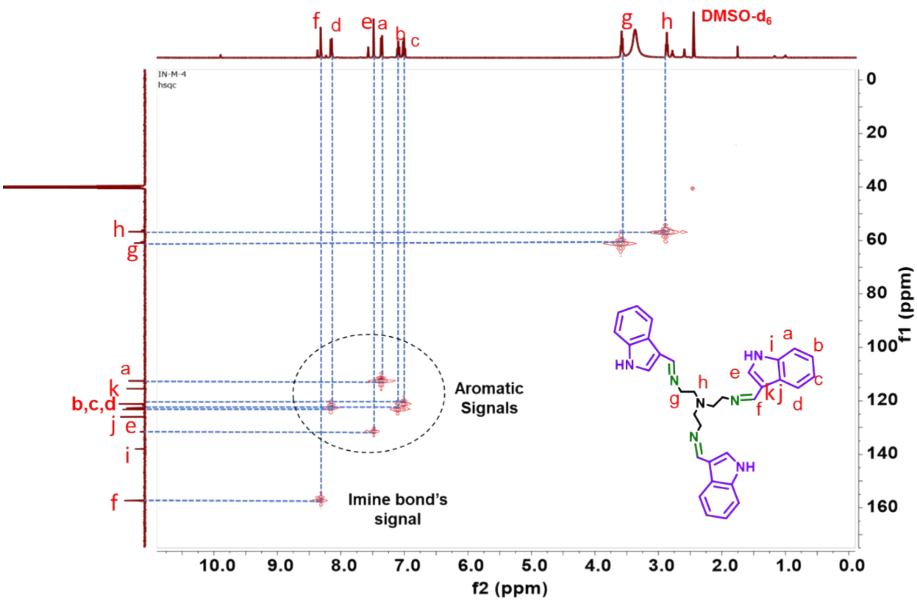


Figure S2: HSQC of INTS-monomer.

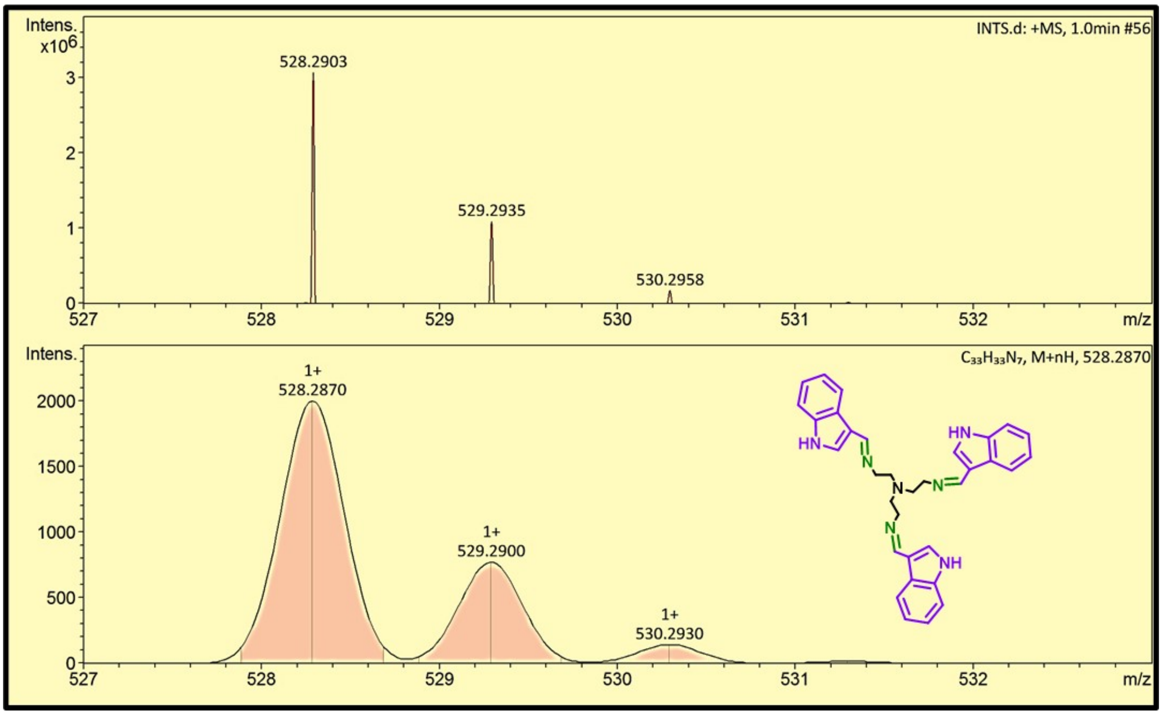
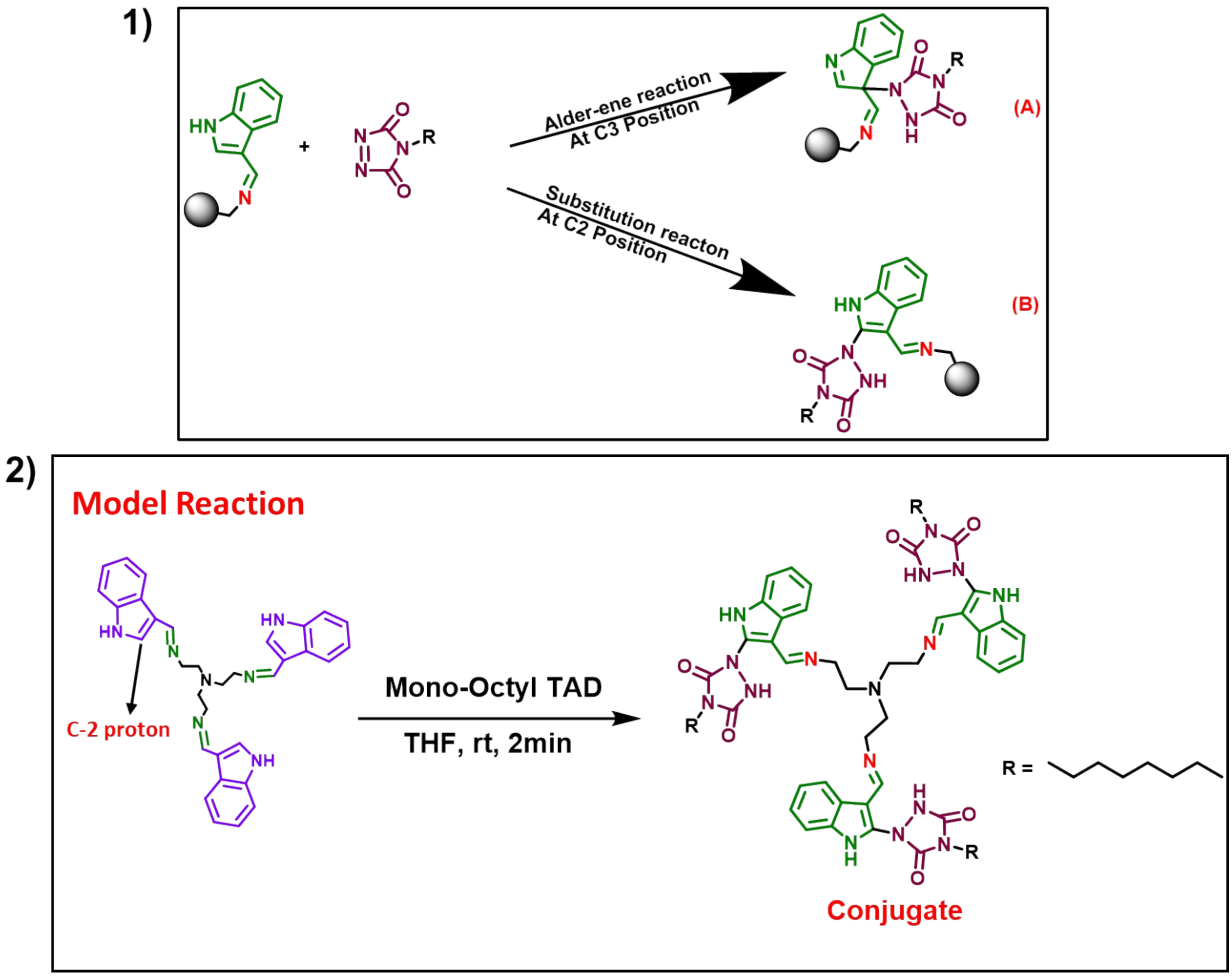


Figure S3: Mass spectrum of INTS-monomer.



Scheme S1: Possible Pathways of TAD-Indole Reaction, **S2:** Model Reaction Between INTS-Monomer and Octyl Mono-TAD

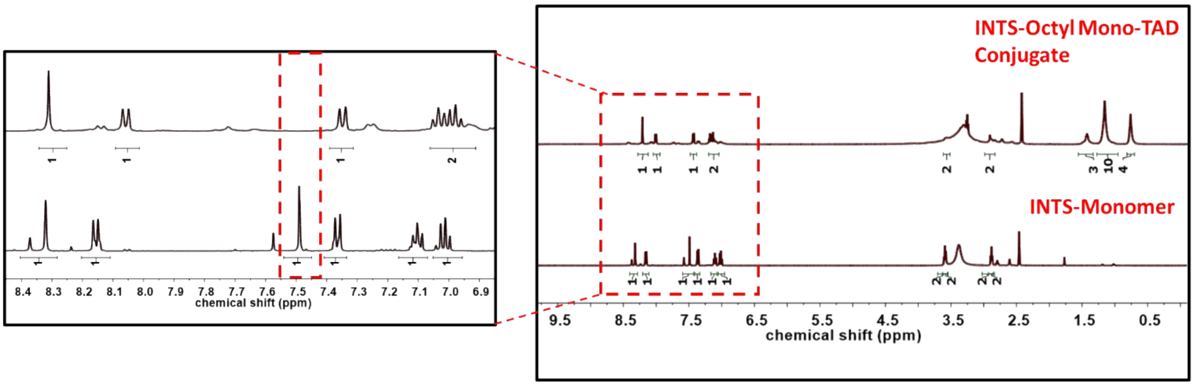


Figure S4: (a) ^{1}H NMR signals of INTS-monomer and INTS-Octyl Mono TAD conjugate.

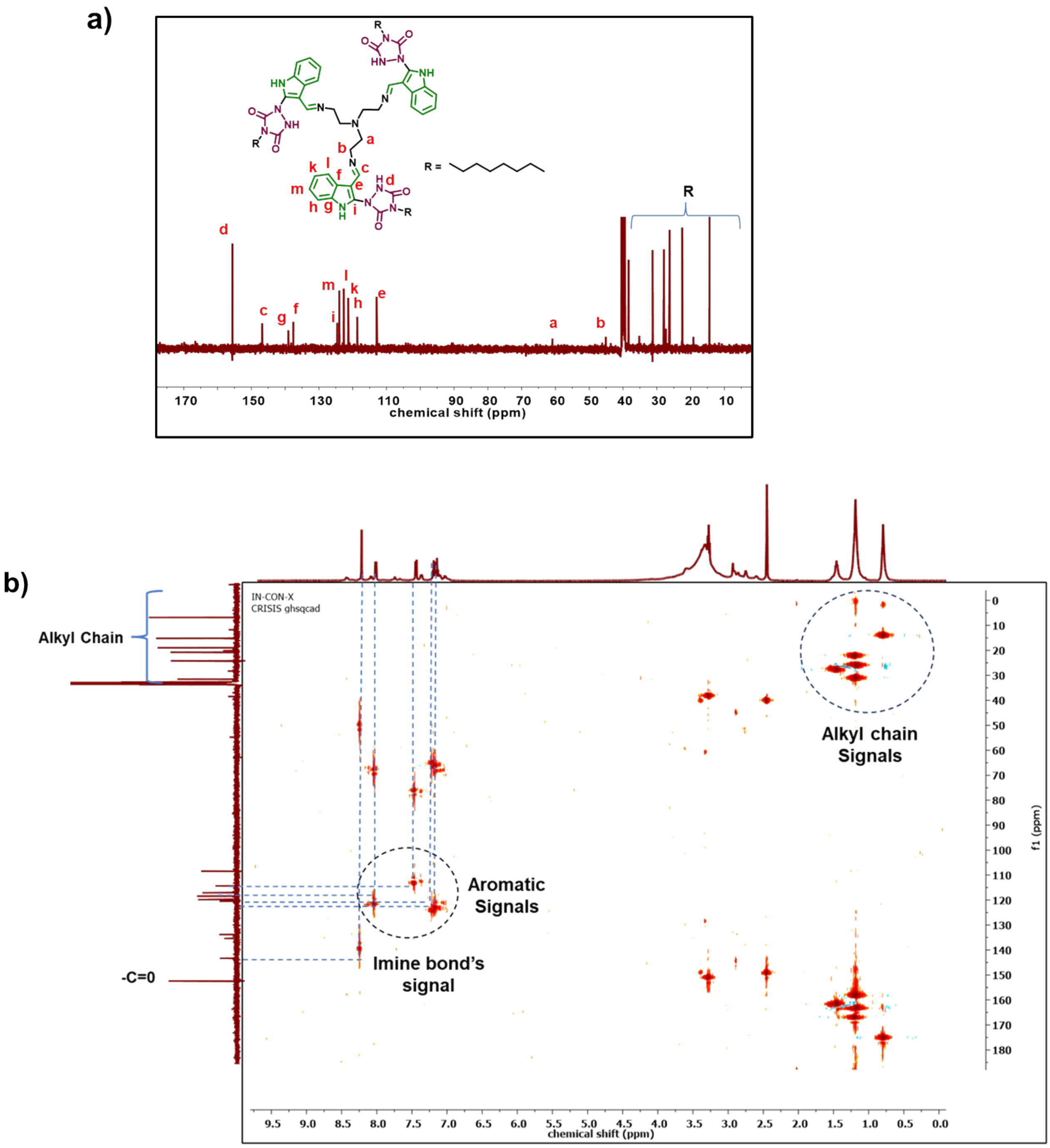


Figure S5: (a) ^{13}C NMR signals b) HSQC of INTS-monomer and Octyl MonoTAD Conjugate.

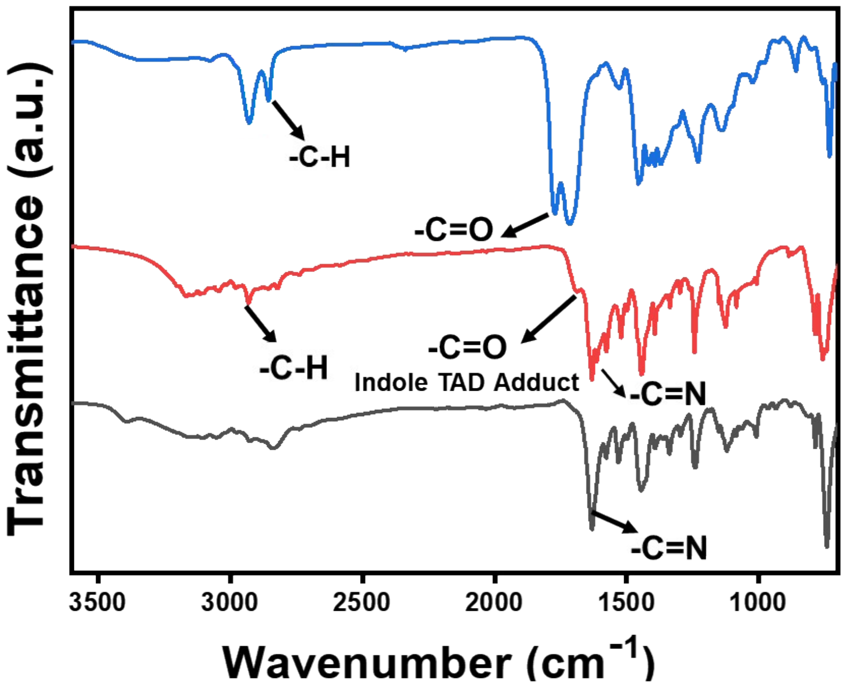
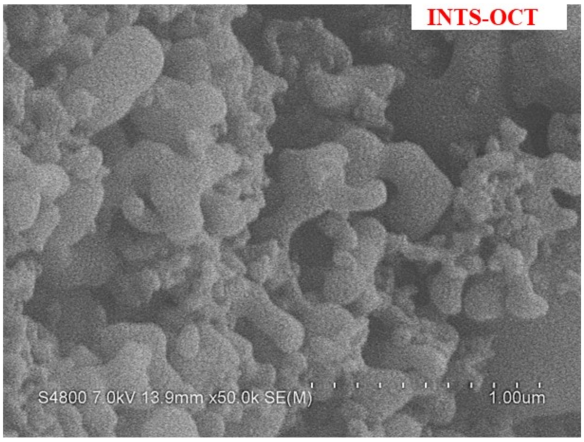


Figure S6: FTIR Analysis of INTS-Monomer, INTS-OCT and Octyl bis-TAD.

a)



b)

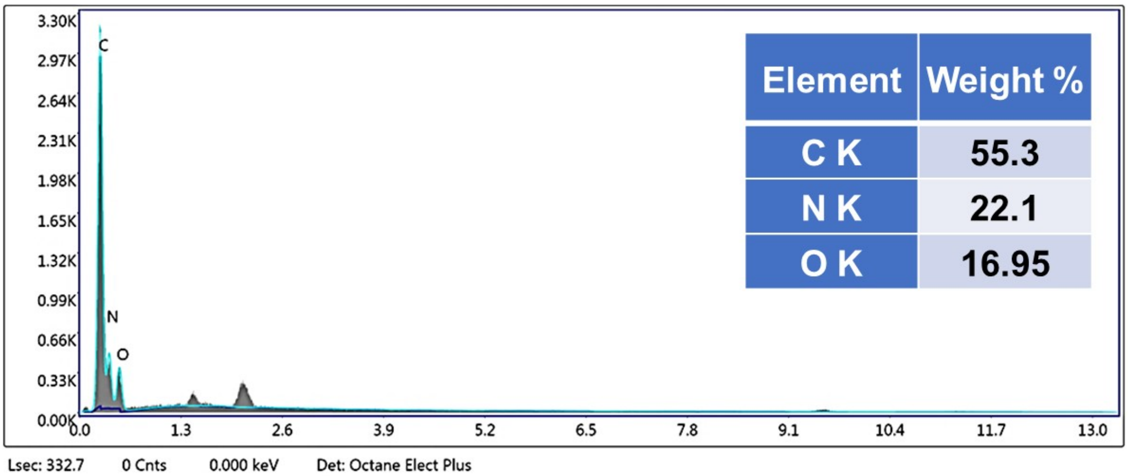


Figure S7: (a) FESEM (b) EDX analysis INTS-OCT.

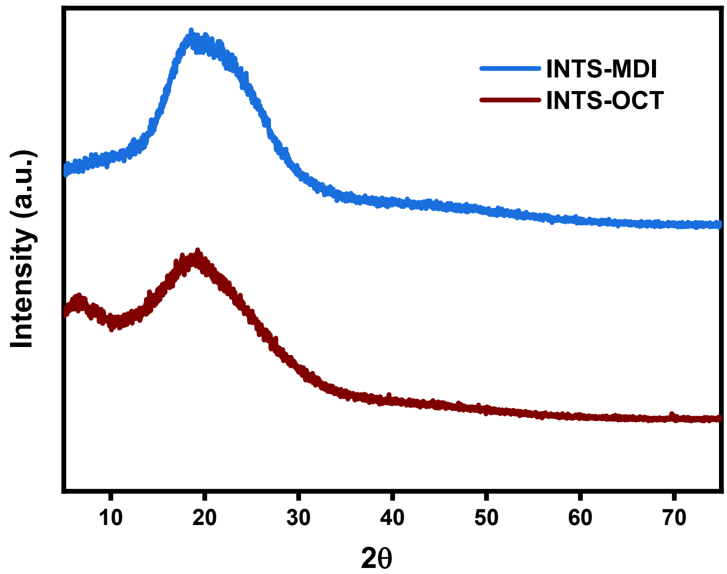


Figure S8: PXRD of INTS-MDI and INTS-OCT.

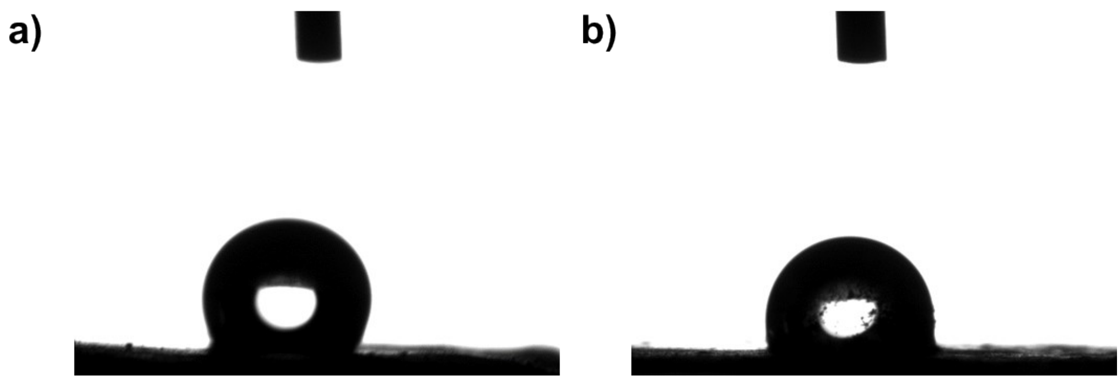


Figure S9: water contact angle analysis of (a) INTS-MDI and (b) INTS-OCT.

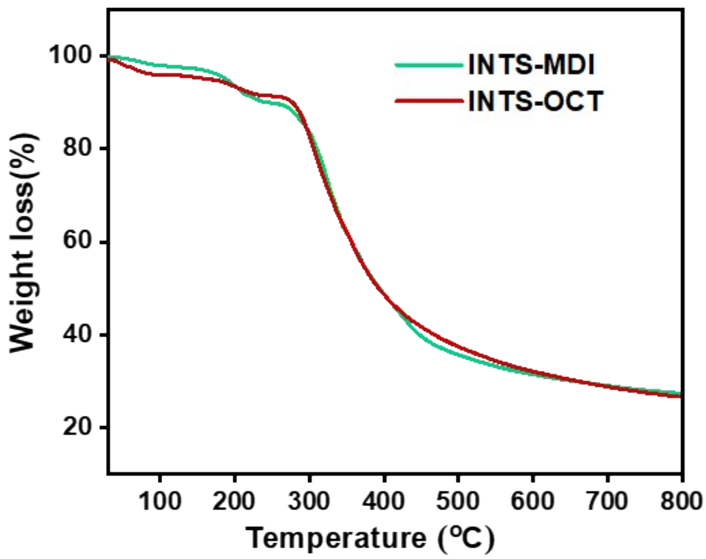


Figure S10: Thermogravimetric analysis of INTS-OCT and INTS-MDI

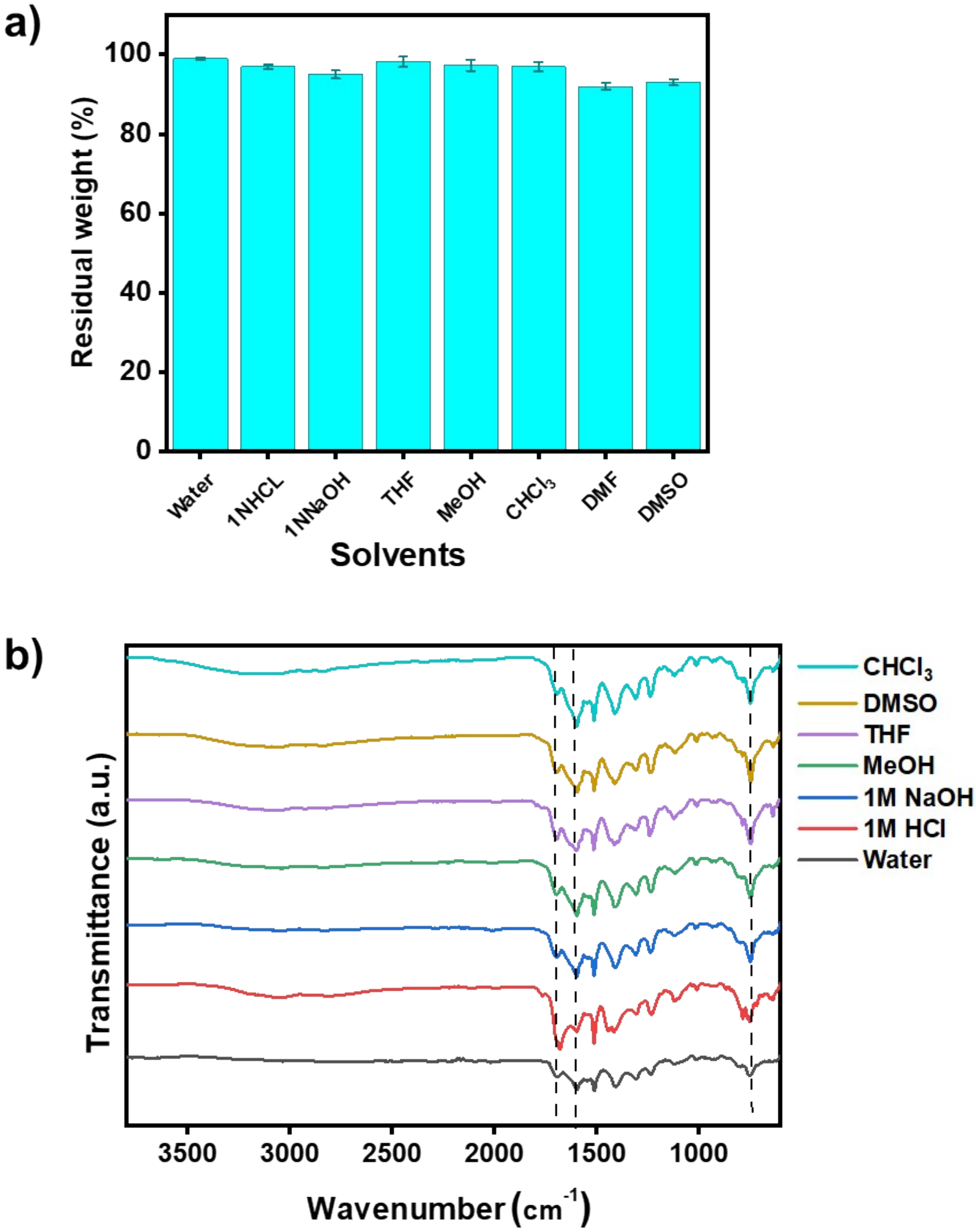


Figure S11: (a) Residual weight percentage plot of INTS-MDI after exposure to different solvents. **(b)** FTIR analysis of INTS after treatment with different protic, aprotic, acidic, and basic solvents.

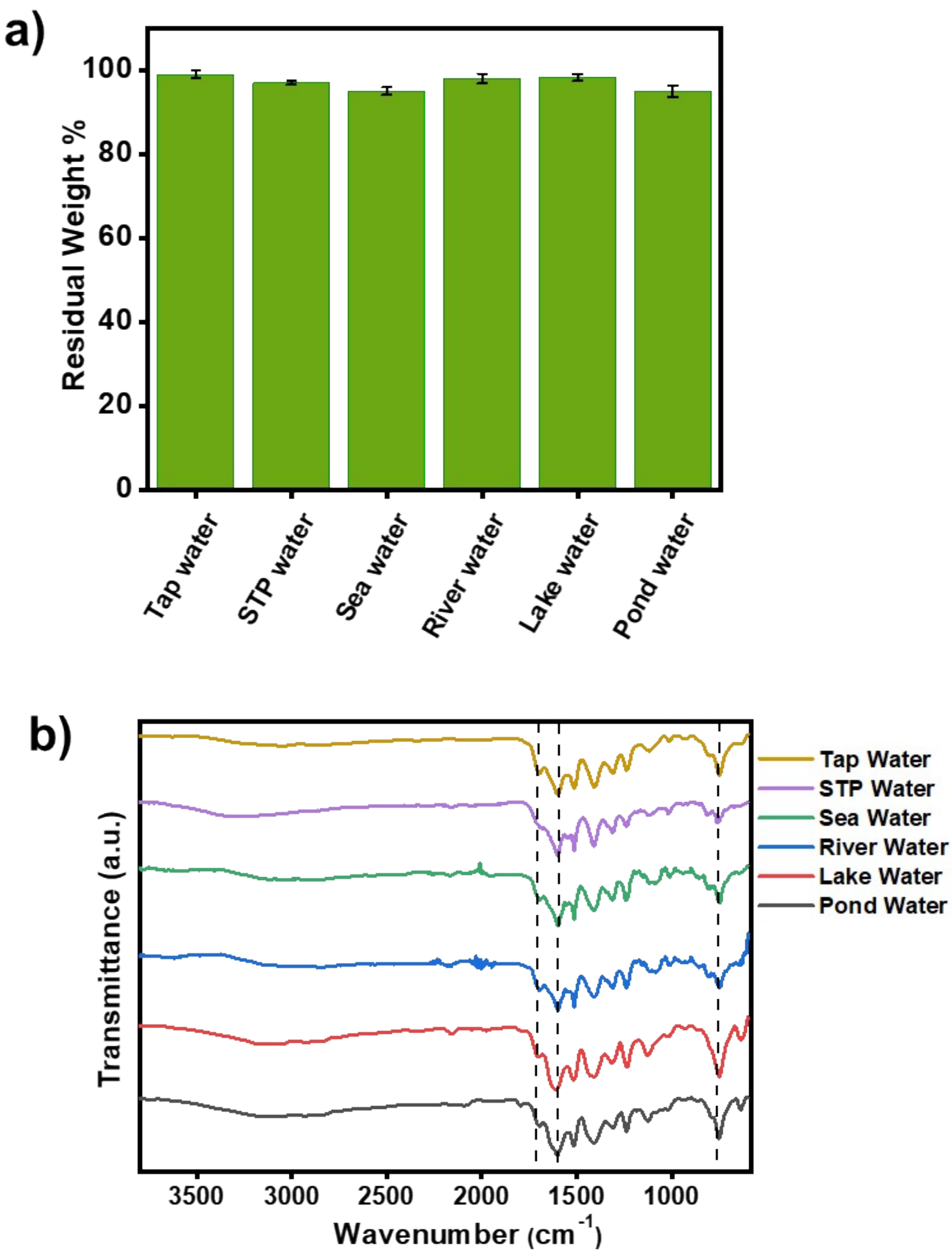


Figure S12: (a) Residual weight percentage plot of INTS-MDI after exposure to different real world water samples. **(b)** FTIR analysis of INTS after treatment with different real world water samples.

Table S1: Elemental analysis (CHNS %) of INTS-MDI and INTS-OCT

Element (%)	INTS-MDI	INTS-OCT
Carbon	61.2	57.25
Hydrogen	5.08	6.48
Nitrogen	19.3	21.2

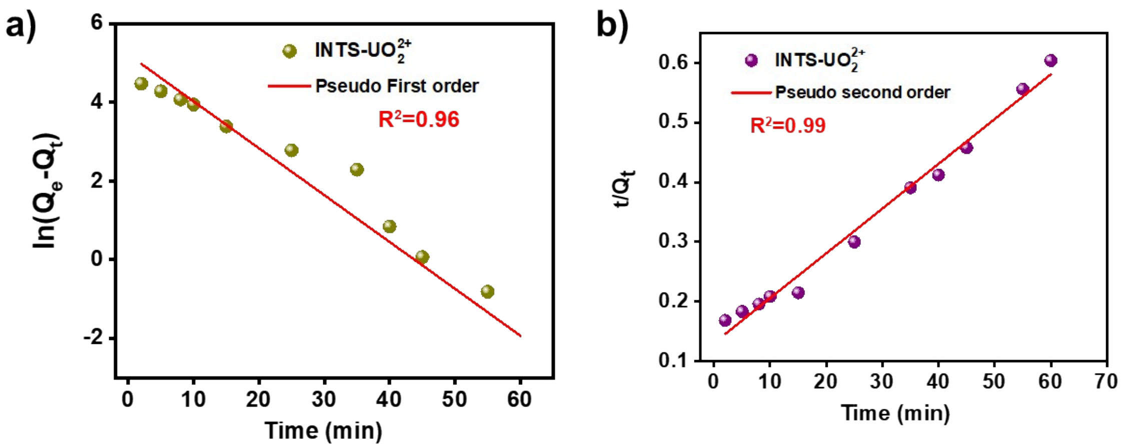


Figure S13: The fitting plot with pseudo-first-order and pseudo-second-order for adsorption of uranyl ion (a and b) by INTS-MDI

Table S2: Adsorption isotherm parameters of the linear pseudo-first-order and pseudo-second-order model for uranyl ion adsorption by INTS-MDI

Model	Parameters	INTS-MDI
Pseudo-first order	Q_e (mg g^{-1})	183
	k_1 (min^{-1})	0.11
	R^2	0.96
Pseudo-second order	Q_e (mg g^{-1})	133.3
	k_2 (g g^{-1} min^{-1})	0.429
	R^2	0.99

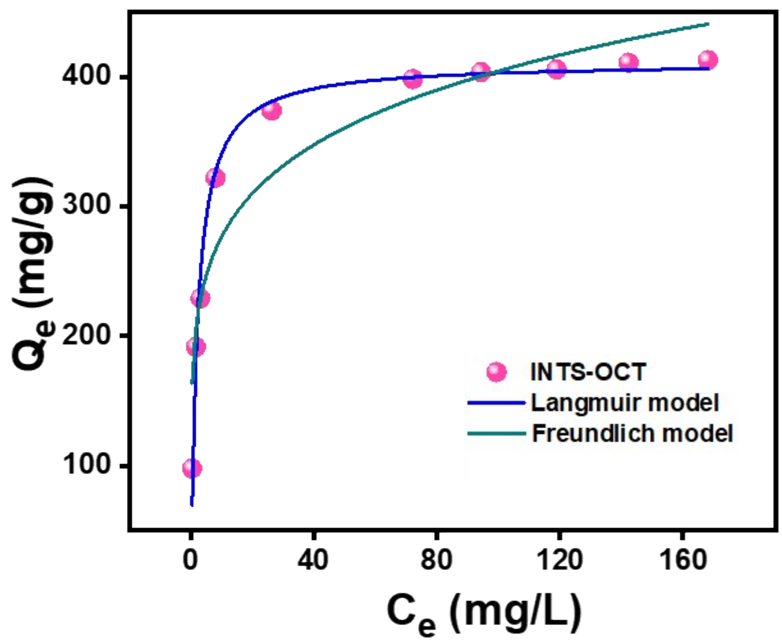


Figure S14: Adsorption isotherm of INTS-OCT fitted with Langmuir model and Freundlich model

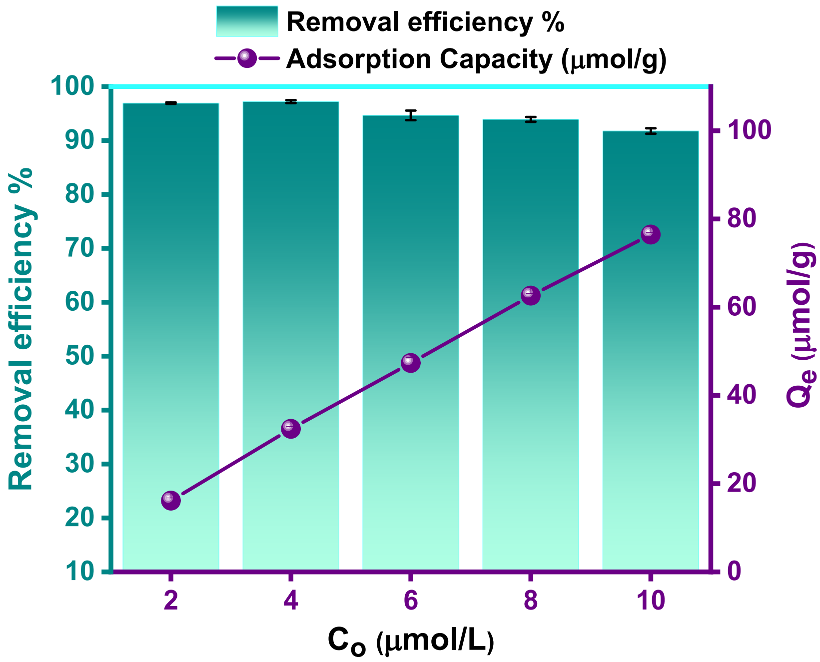


Figure S15: Uranium adsorption from simulated sea-water

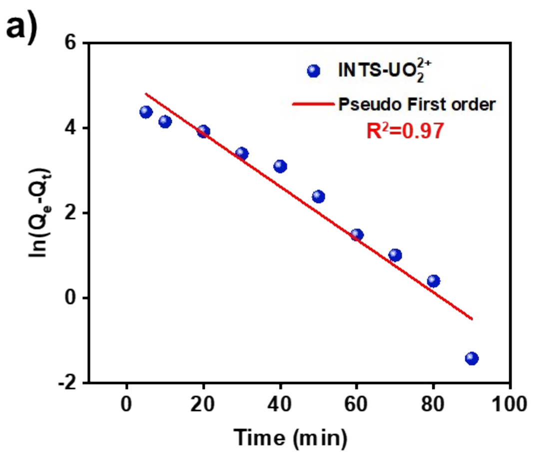


Figure S16: Kinetic fitting plots for uranium adsorption from natural seawater by INTS-MDI: **(a)** pseudo-first-order and **(b)** pseudo-second-order models.

Table S3: Adsorption isotherm parameters of the linear pseudo-first-order and pseudo-second-order model for uranyl ion adsorption from sea water by INTS-MDI

Model	Parameters	INTS
Pseudo-first order	**Q_e (mg g^{-1})**	**165**
	k_1 (min^{-1})	**0.0621**
	R^2	**0.97**
Pseudo-second order	**Q_e (mg g^{-1})**	**135**
	k_2 (g g^{-1} min^{-1})	**0.261**
	R^2	**0.99**

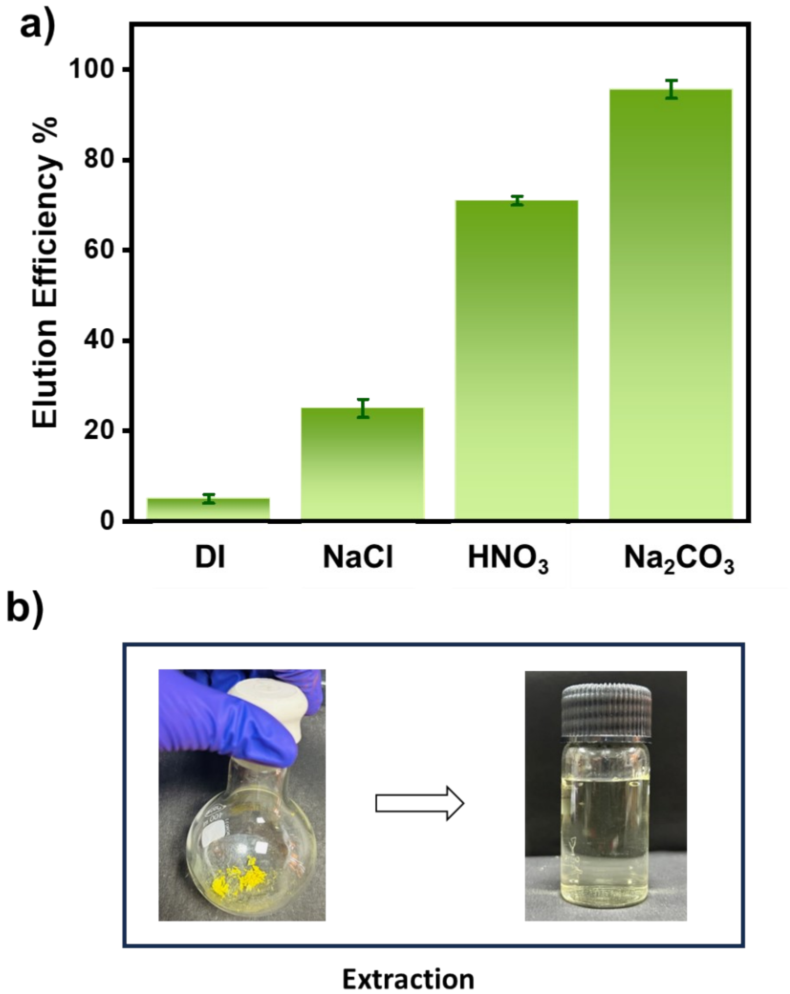


Figure S17: (**a)** Elution efficiency of different eluents **(b)** Photograph showing the recovered solid obtained after freeze-drying the desorbed solution(left) and the resulting concentrated uranyl solution upon re-dissolution in water (right)

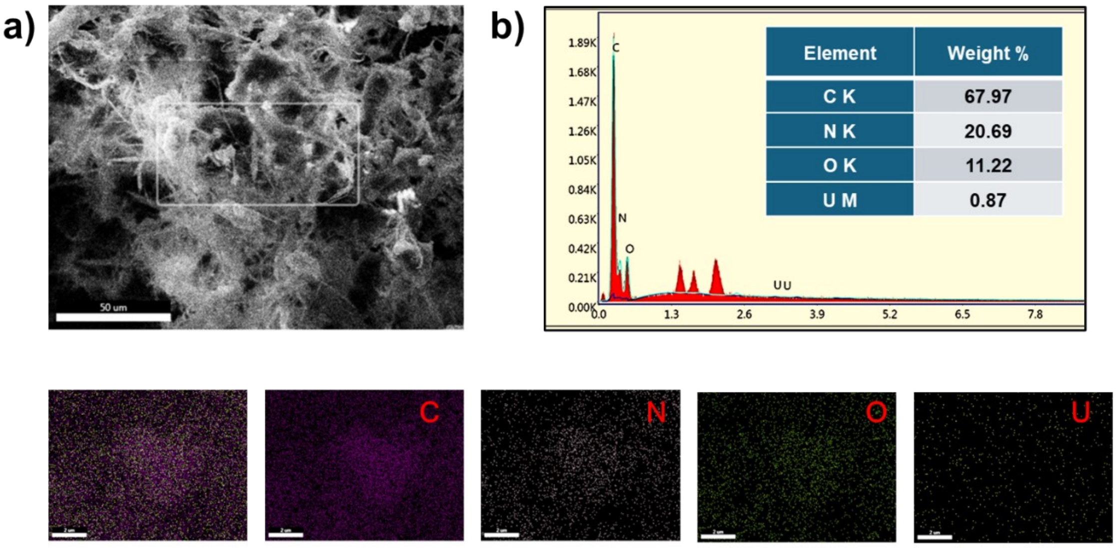


Figure S18: (a)FESEM (b) EDX analysis and Elemental mapping (below) of INTS-MDI after desorption.

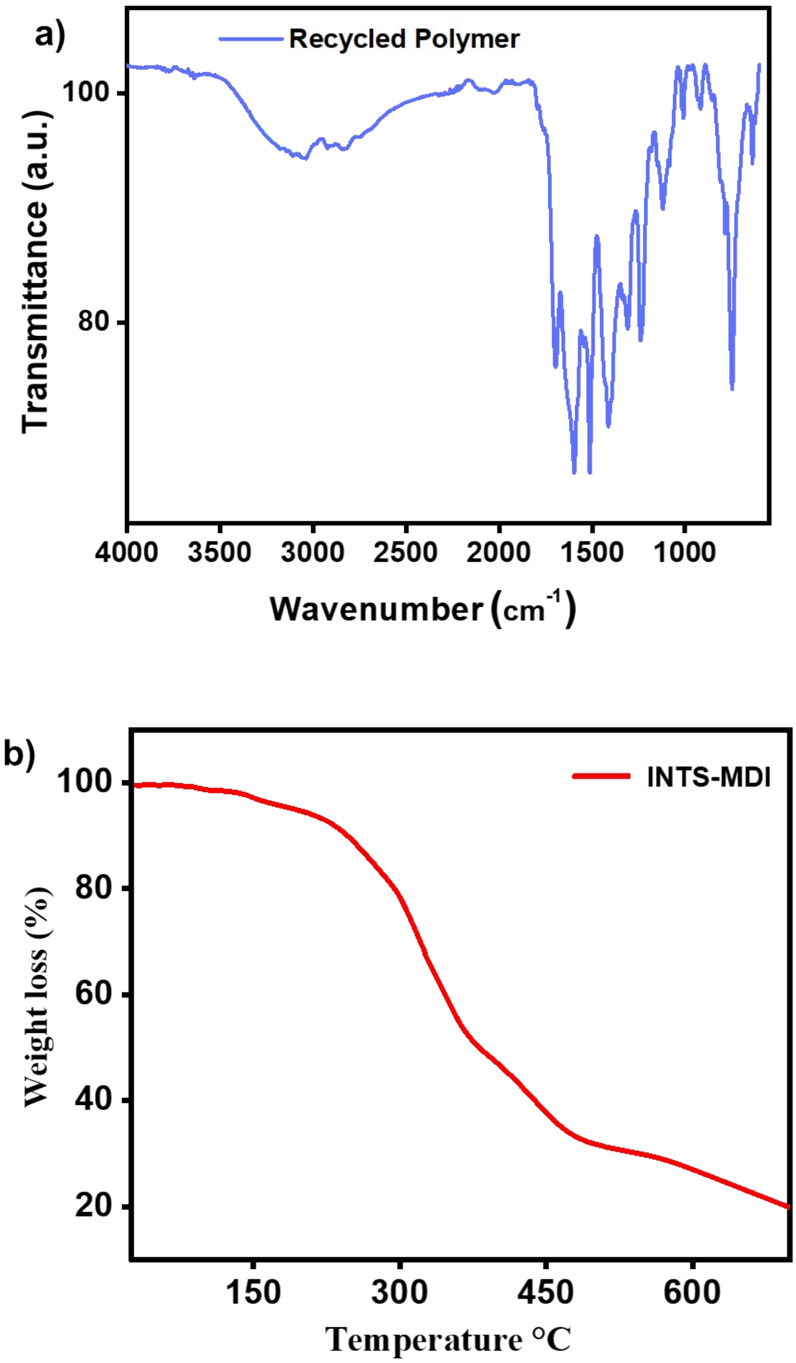


Figure S19: (a) FTIR (b) TGA analysis of recycled INTS-MDI

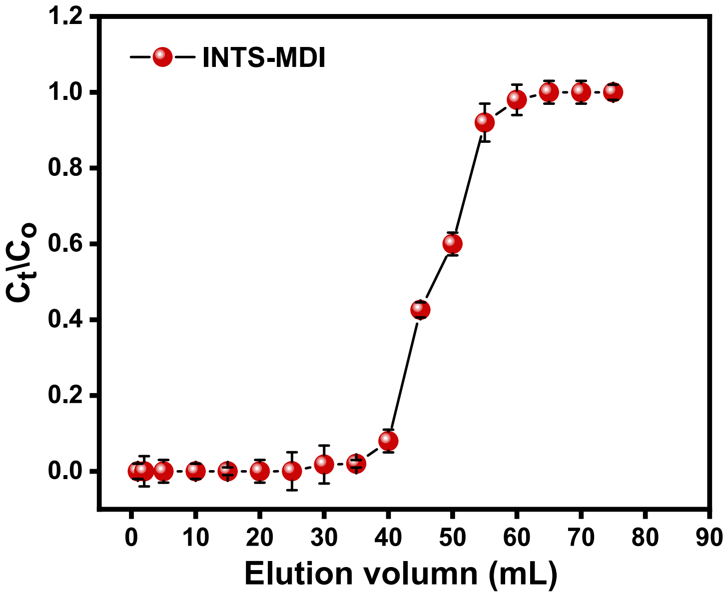


Figure S20: Breakthrough profile of column-based Uranium capture test.

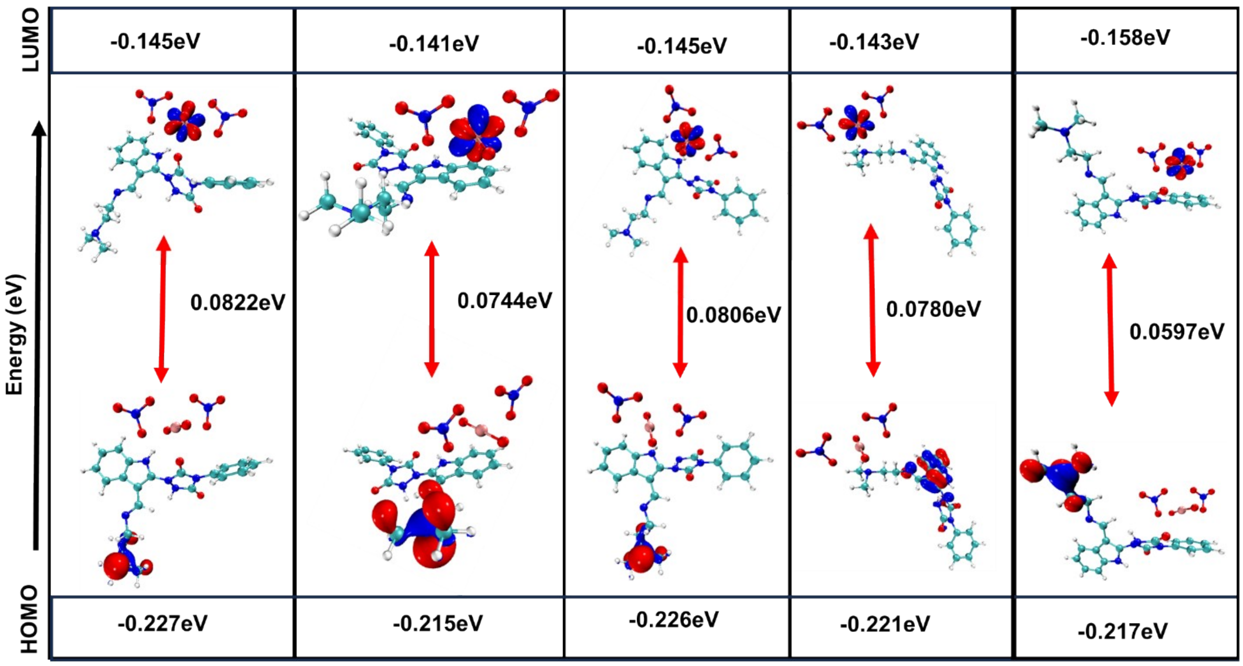


Figure S21: FMO figures of different binding sites of INTS-MDI

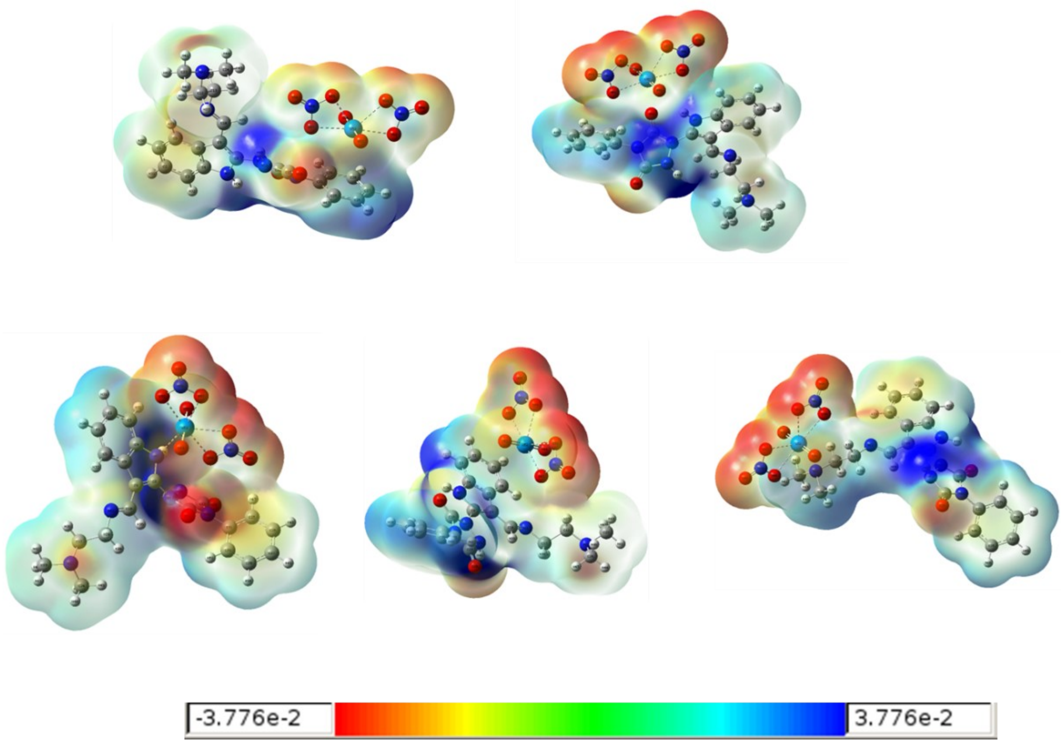


Figure S22: Electrostatic potential map illustrating the charge distribution at different binding sites of INTS-MDI.

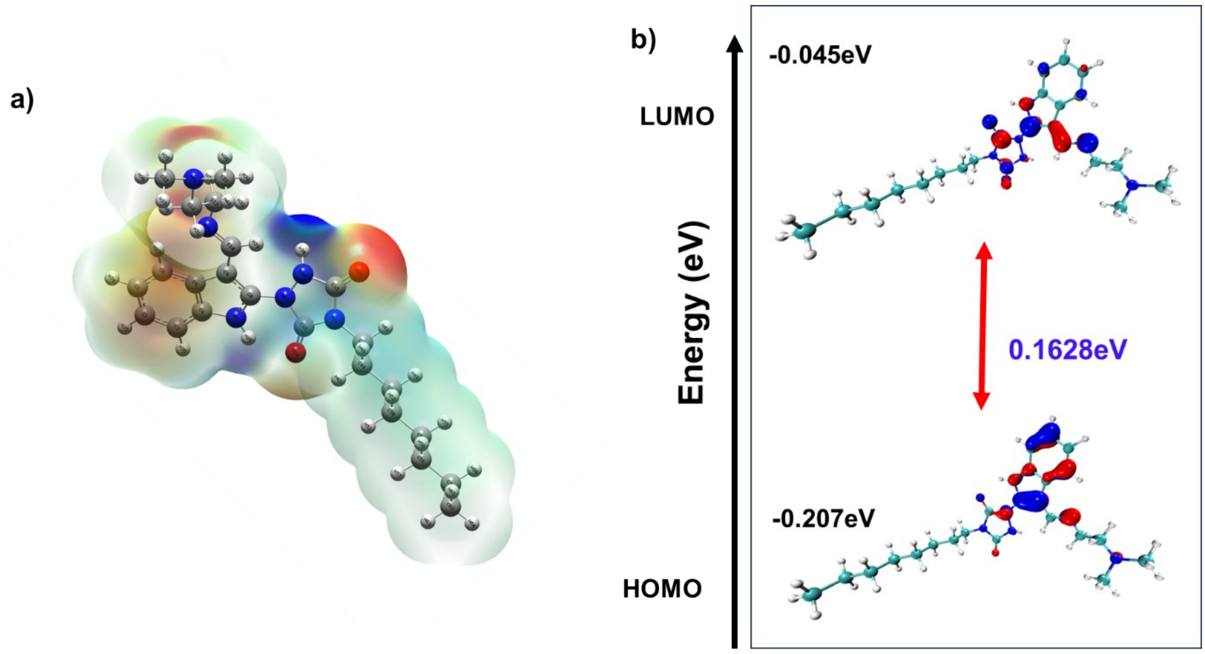


Figure S23: (a) Electrostatic potential map and (b) frontier molecular orbital (FMO) diagram of INTS-OCT.

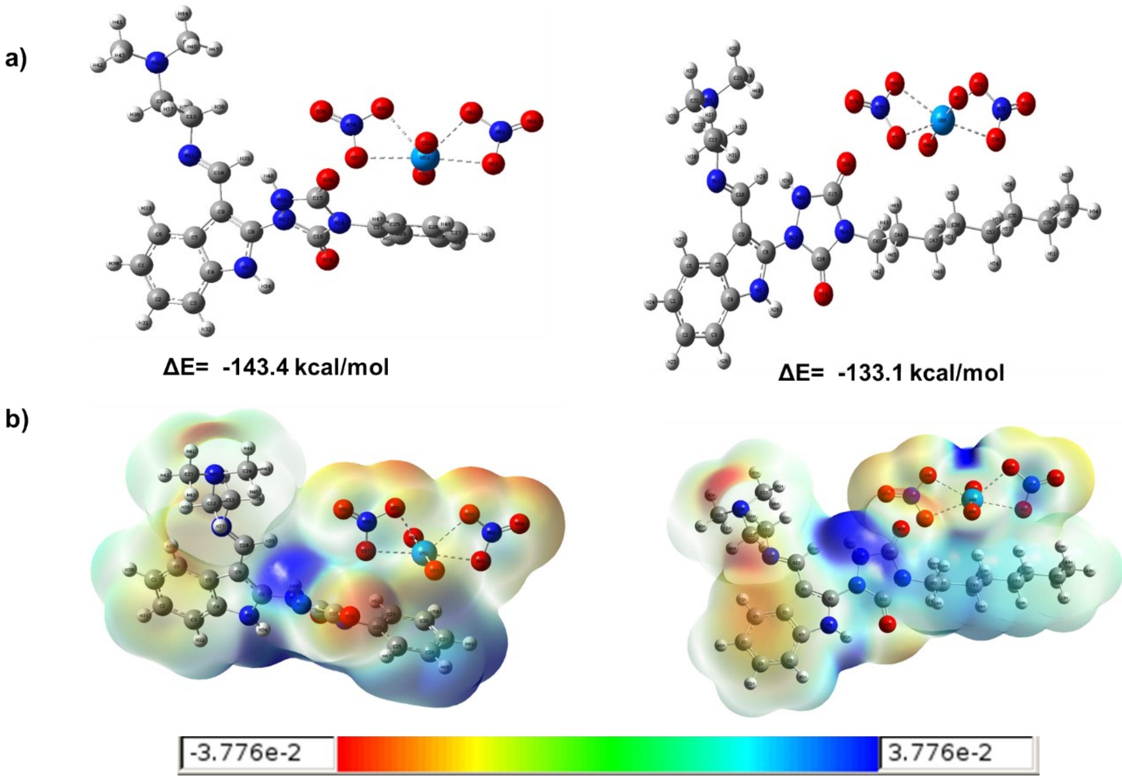


Figure 24: (a) Comparative optimized geometries showing $UO_2(NO_3)_2$ binding at the aromatic site of INTS-MDI and the octyl site of INTS-OCT. (b) Corresponding MEP maps highlighting differences in local electron density around the uranyl coordination region.

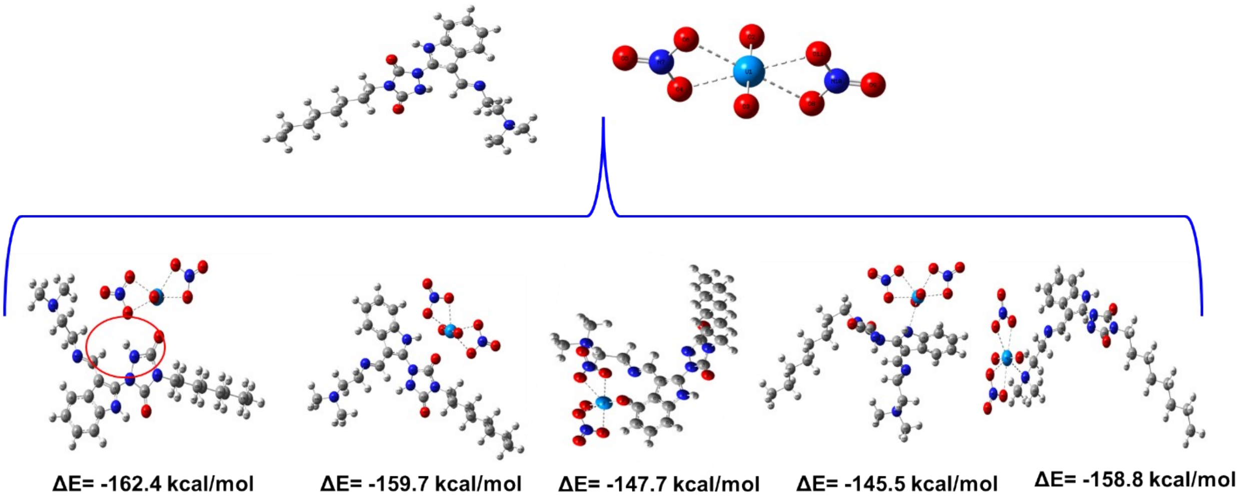


Figure S25: Optimize geometry structures of ($UO_2(NO_3)_2$) with different binding sites of polymer INTS-OCT

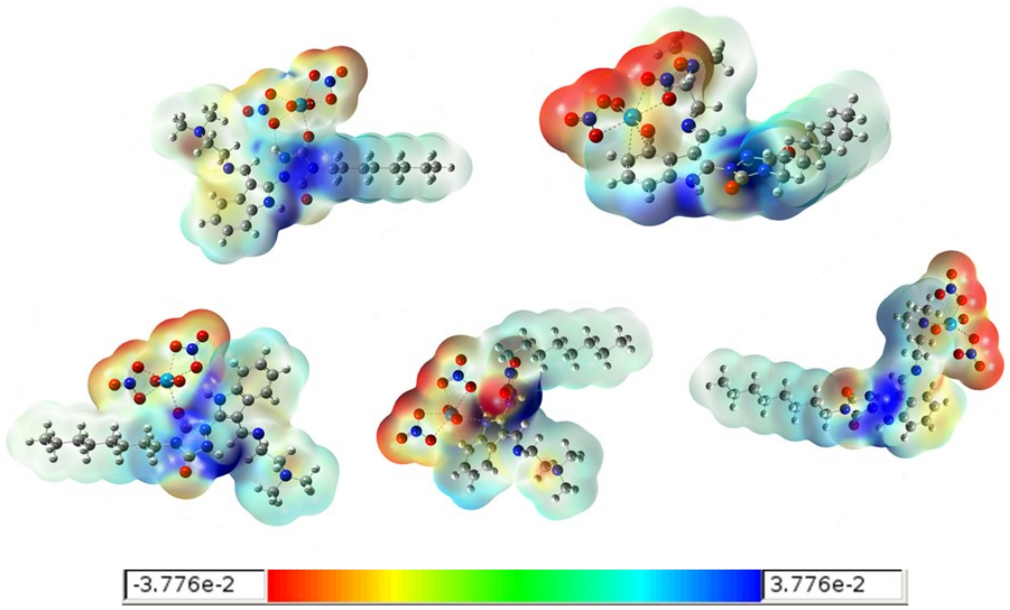


Figure S26: Electrostatic potential map illustrating the charge distribution at different binding sites of INTS-OCT.

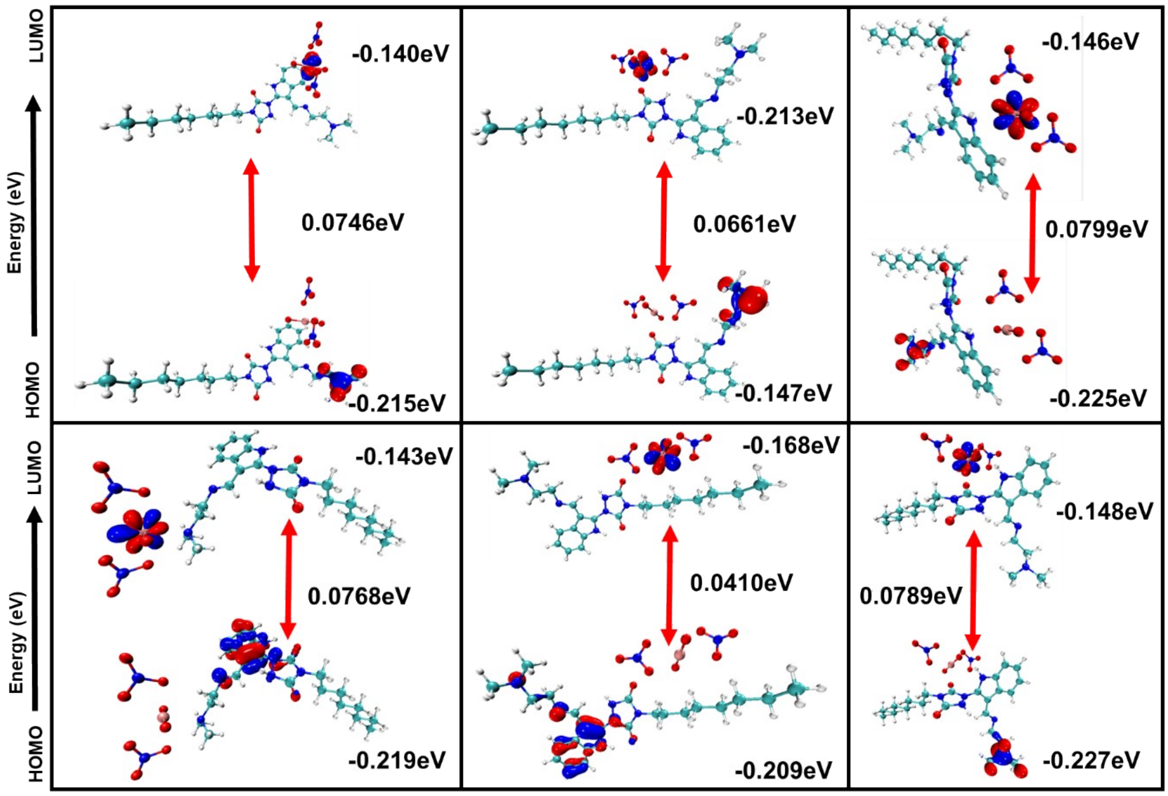


Figure S27: FMO figures of different binding sites of INTS-OCT

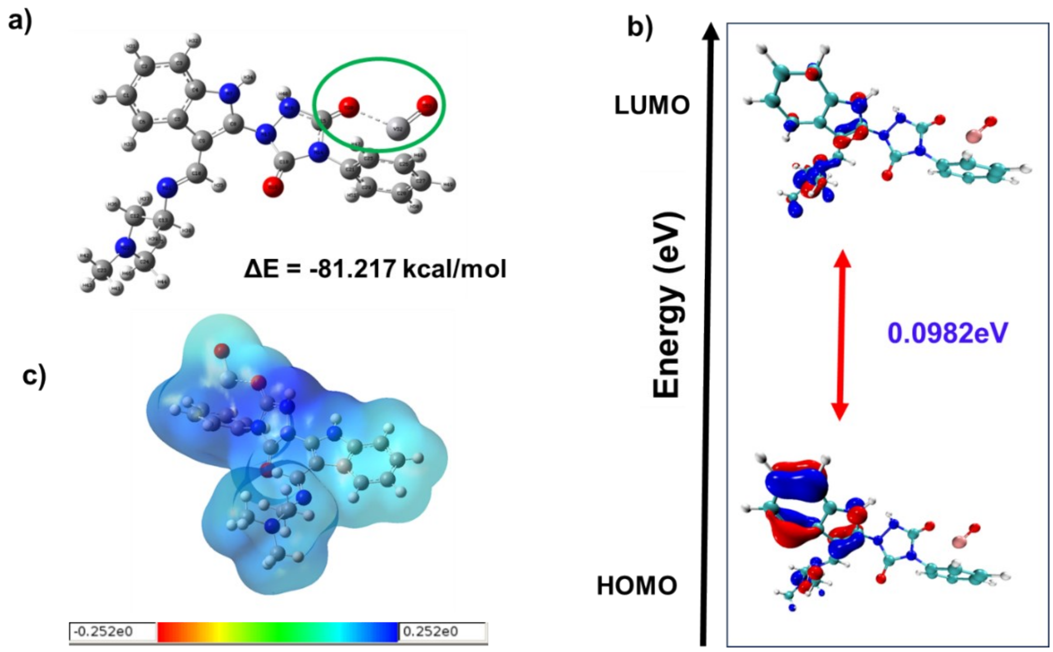


Figure S28: DFT analysis showing the interaction of VO^{2+} ion with INTS-MDI 9A0 Optimized structure with interaction site highlighted, (b) FMO figure and (c) electrostatic potential map illustrating charge distribution.

Table S4: Comparison of adsorption capacity and equilibrium time of U(VI) adsorption by INTS-MDI with other reported materials

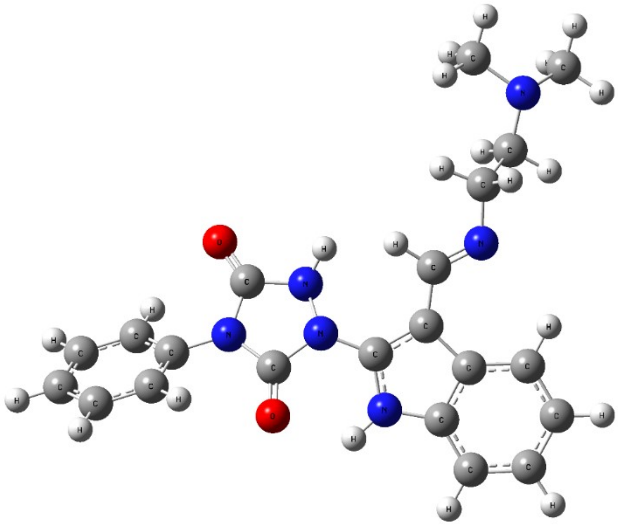
S.No.	Material	pH	Kinetics (Equilibrium time) (min)	Adsorption capacity (mg/g)	Functionality	Ref.
1.	$Mn_{0.5}Ti_{0.5}O_y$	4	150	695.2	Hydroxide	Ref.[14]
2.	IAA-CTSA	6.5	300	847.5	Amide, Indole (cation–π)	Ref.[15]
3.	PEI@MWCNTs	5	120	97.60	Amines	Ref.[16]
4.	ZIF-90-ABOA	8	180	353.4	Amidoxime	Ref.[17]
5.	JUC-505-COOH	5	80	464	Acid (-COOH)	Ref.[18]
6.	AO-OBHSPIMs	6	360	227	Amidoxime	Ref.[19]
7.	PAN-AO/PVA	6	480	320.6	Amidoxime	Ref.[20]
8.	PAGM-1	8	180	196.12	Hydroxyl, carboxyl, and amide	Ref.[21]
9.	CHMBC-PAO	5	720	310.30	Amidoxime	Ref.[22]
10.	$\boldsymbol{\beta}$-CD-g-PAO	6	20	944.75	Amidoxime	Ref.[23]
11.	AO/BB-Cas	5	-	801	Amidoxime	Ref.[24]
12.	HCMP-AO	6	15	450	Amidoxime	Ref.[25]
13.	Fe3O4/P(AA-MMA-DVP)	4.5	-	413.2	Phosphine oxide	Ref.[26]
14.	i-MZIF90(50)	7	120	1489.13	Carboxylate and imine	Ref.[27]
15.	AO-GTA	4	-	875.2	Amidoxime	Ref.[28]
16.	PAA/CS	4	250	289.6	Hydroxyl, carboxyl, and amide	Ref.[29]
17.	CaCO3@aCS/PA	4	150	842.0	CO_3^{2-}andPO_4^{3-}	Ref.[30]
18.	Organic cage (HPOC-α)	7	2160	716.84	Amidoxime	Ref.[31]
19.	tPF AO	6	15	578.9	Amidoxime	Ref.[32]
20.	**INTS-MDI**	**6**	**50**	**956.27**	**Urazole, Imine, Amine, Indole**	**This Work**

Table S5: Comparison of uranium uptake performance of INTS-MDI with previously reported adsorbents in natural seawater (unspiked), including adsorption capacity and extraction time

S.No.	Material	Adsorption capacity (mg/g)	Time (Days)	Ref.
1.	PAGM	1.6	2.5	Ref[21]
2.	UiO-66-AO	2.68	3	Ref[7]
3.	FF-PT	3.22	30	Ref[33]
4.	PAOBS-4	1.04	30	Ref[34]
5.	PLMR	2.14	10	Ref[35]
6.	**INTS-MDI**	**3.5**	**3**	**This work**

Table S6: Cartesian coordinates of the optimized geometries.

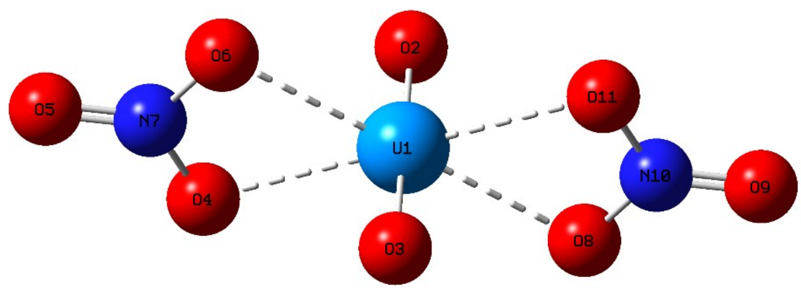
(INTS)



C	3.41314900	2.74028000	-3.08435900
C	4.49552000	1.85543700	-2.93499100
C	4.41161900	0.75351800	-2.09428500
C	3.21140000	0.56304800	-1.41119400
C	2.11313800	1.44546700	-1.53981800
C	2.22236700	2.54909400	-2.39726100
N	2.84275100	-0.44405300	-0.53431900
C	1.57572400	-0.18897100	-0.07651500
C	1.07117200	0.96729300	-0.65489100
C	-0.20248300	1.59559400	-0.36963900
N	-0.64295800	2.61392000	-0.99483600
C	-2.88706600	3.19870300	-1.77183100
C	-1.91490600	3.17719200	-0.58295900
N	0.68705600	-3.00089000	1.90283800
C	-0.58493000	-2.61974300	1.44596300
N	-0.36944200	-1.50450800	0.63235900
N	0.96900800	-1.06384900	0.84075000
C	1.65706200	-2.07637500	1.50457900
O	2.85633900	-2.13950400	1.66622600
O	-1.64961200	-3.12847300	1.67905200
C	0.95389300	-4.17247200	2.68104100

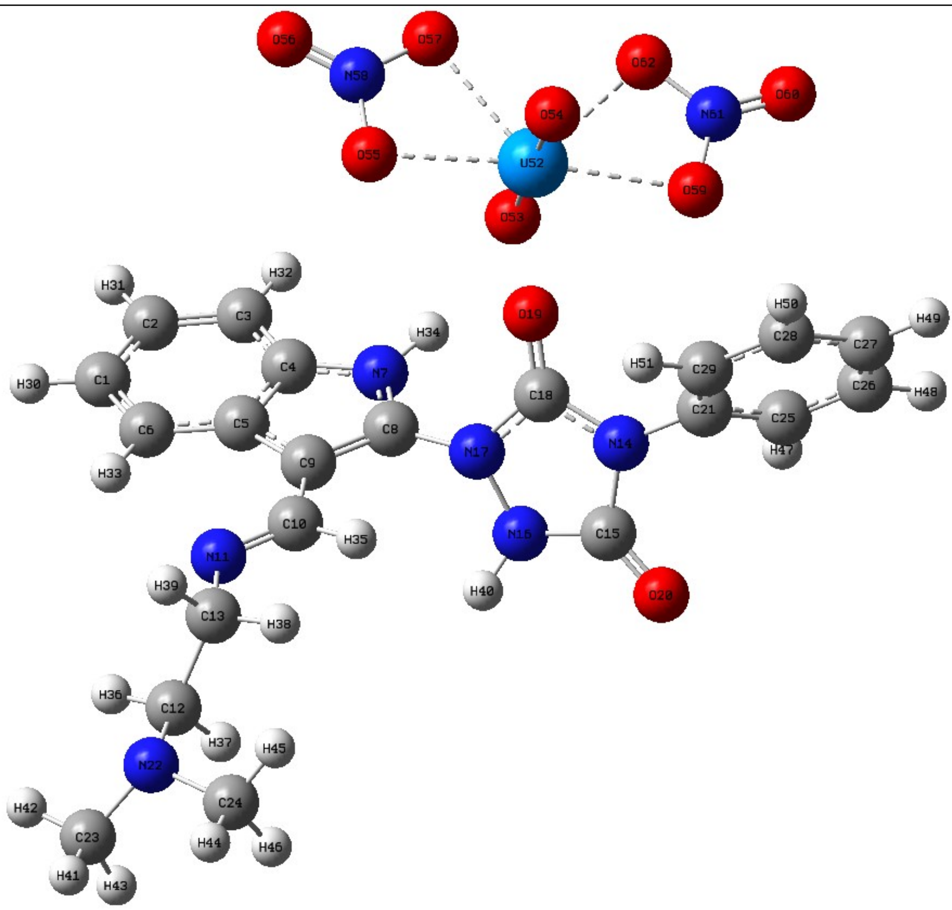
N	-4.10007000	3.96650900	-1.50357200
C	-4.78301600	4.33681500	-2.73673700
C	-5.01102400	3.28663300	-0.59099500
C	0.25723200	-5.35116000	2.41027100
C	0.51211900	-6.48545200	3.17464600
C	1.46168700	-6.45294500	4.19301900
C	2.15512300	-5.27309600	4.45142500
C	1.90170200	-4.12678400	3.70445000
H	3.51378500	3.58951900	-3.75058200
H	5.41105400	2.03404200	-3.48713200
H	5.24269600	0.06732500	-1.97841700
H	1.38604900	3.22559400	-2.50468700
H	3.44871600	-1.12577500	-0.09939700
H	-0.78106100	1.17705700	0.47344600
H	-2.36248600	3.66638800	-2.60821200
H	-3.11342000	2.15911400	-2.07855700
H	-2.34505600	2.63045000	0.27195000
H	-1.75554600	4.21429600	-0.26896500
H	-1.06776800	-0.77609300	0.71962300
H	-5.64226100	4.97122400	-2.50428900
H	-4.10741900	4.90631500	-3.37901900
H	-5.15006800	3.46465900	-3.31047100
H	-5.87832800	3.92273200	-0.39850000
H	-4.52545700	3.09527300	0.36741100
H	-5.37644800	2.32081900	-0.99032500
H	-0.48709400	-5.37351900	1.62698200
H	-0.03419900	-7.39814700	2.96742200
H	1.65944000	-7.34100400	4.78185900
H	2.89605400	-5.23806700	5.24153800
H	2.44606200	-3.21382700	3.89980200

$UO_2(NO_3)_2$



U	-0.20865300	0.96388000	0.00071000
O	-0.20972000	0.96457900	-1.75110300
O	-0.20739200	0.96315600	1.75252100
O	-1.28531200	3.13282300	0.00225600
O	-0.20036100	5.03057700	0.00218500
O	0.87652700	3.12823600	0.00078600
N	-0.20291400	3.84071300	0.00177000
O	-1.29505100	-1.19948500	0.00051200
O	-0.21944700	-3.10258100	-0.00091300
N	-0.21606900	-1.91274200	-0.00043700
O	0.86675400	-1.20552500	-0.00092400

Adduct1



C	3.19695900	2.97828600	-3.12761400
C	4.24179500	2.04126400	-3.25905900
C	4.16803400	0.78945800	-2.67137800
C	3.01139100	0.49490400	-1.94445400
C	1.95389400	1.42629700	-1.79236700
C	2.05518600	2.68762400	-2.40093000
N	2.66475400	-0.66119600	-1.27271400
C	1.44915400	-0.45557600	-0.66180600
C	0.95788900	0.80385600	-0.95651700
C	-0.30192100	1.34128000	-0.47190700
N	-0.74955300	2.48144300	-0.81578500
C	-3.00478600	3.24335600	-1.37817000
C	-2.01129900	2.92444100	-0.25082900
N	0.43771600	-3.22353800	1.35233100
C	-0.54804000	-3.29481600	0.33433500
N	-0.20202000	-2.27908400	-0.55417000

N	0.79841600	-1.47175600	0.06078300
C	1.24603800	-2.13078000	1.16273900
O	2.21905400	-1.80367200	1.86296800
O	-1.46284500	-4.06380900	0.24704800
C	0.52948900	-4.14121700	2.45507400
N	-4.20665700	3.92022400	-0.90177100
C	-4.90995300	4.59179000	-1.98790700
C	-5.10488400	3.03513100	-0.17045000
C	0.59906400	-5.50694200	2.19464700
C	0.68363100	-6.39503500	3.26155100
C	0.70933700	-5.91957800	4.57061100
C	0.64060200	-4.55039700	4.81756400
C	0.54096200	-3.65244800	3.75941500
H	3.29640700	3.94723100	-3.60275500
H	5.12339600	2.30682100	-3.83077400
H	4.97204500	0.06984300	-2.76904300
H	1.25055400	3.40081300	-2.28822600
H	3.29030700	-1.43328500	-1.07576200
H	-0.85322600	0.70369100	0.24026300
H	-2.49345400	3.90450700	-2.08158600
H	-3.24327400	2.31309100	-1.93030200
H	-2.42699200	2.18382000	0.45008700
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H	-0.95237900	-1.76173800	-0.99696300
H	-5.75969500	5.14873800	-1.58530900
H	-4.24254300	5.30371900	-2.47864600
H	-5.29407100	3.89352300	-2.75542100
H	-5.96428400	3.60433400	0.19133000
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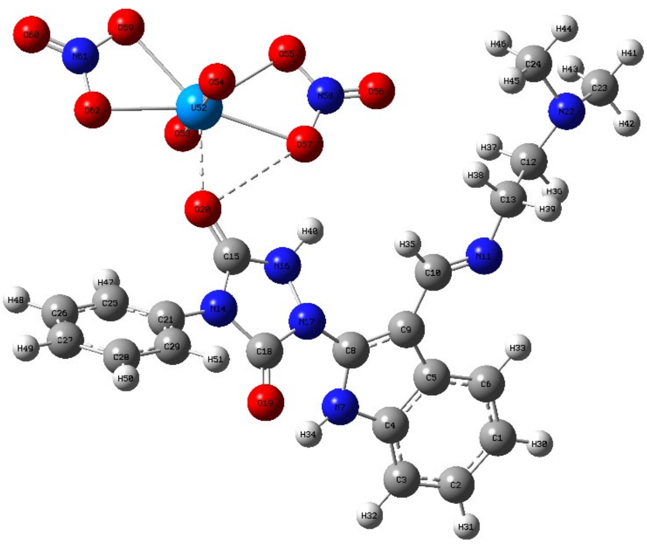
H	-5.48387700	2.20057000	-0.79152600
H	0.58645600	-5.86759900	1.17460700
H	0.74075300	-7.45898500	3.06674600
H	0.78587100	-6.61536800	5.39767600
H	0.66166700	-4.17704200	5.83425500
H	0.48306800	-2.58743800	3.94488800

U	4.60287400	-2.03698200	2.06276500
O	4.56885000	-2.37937200	0.31817700
O	4.56038000	-1.68781500	3.78419300
O	4.82229900	0.34464500	1.56888600
O	6.73192800	1.39073400	1.37070200
O	6.66829500	-0.75142200	1.80036900
N	6.11408700	0.38790400	1.56870400
O	4.10752000	-4.39731200	2.49327400
O	5.63226400	-5.93527800	2.78814100
N	5.33252900	-4.79725700	2.57841700
O	6.19653200	-3.85675400	2.41621200

Adduct2

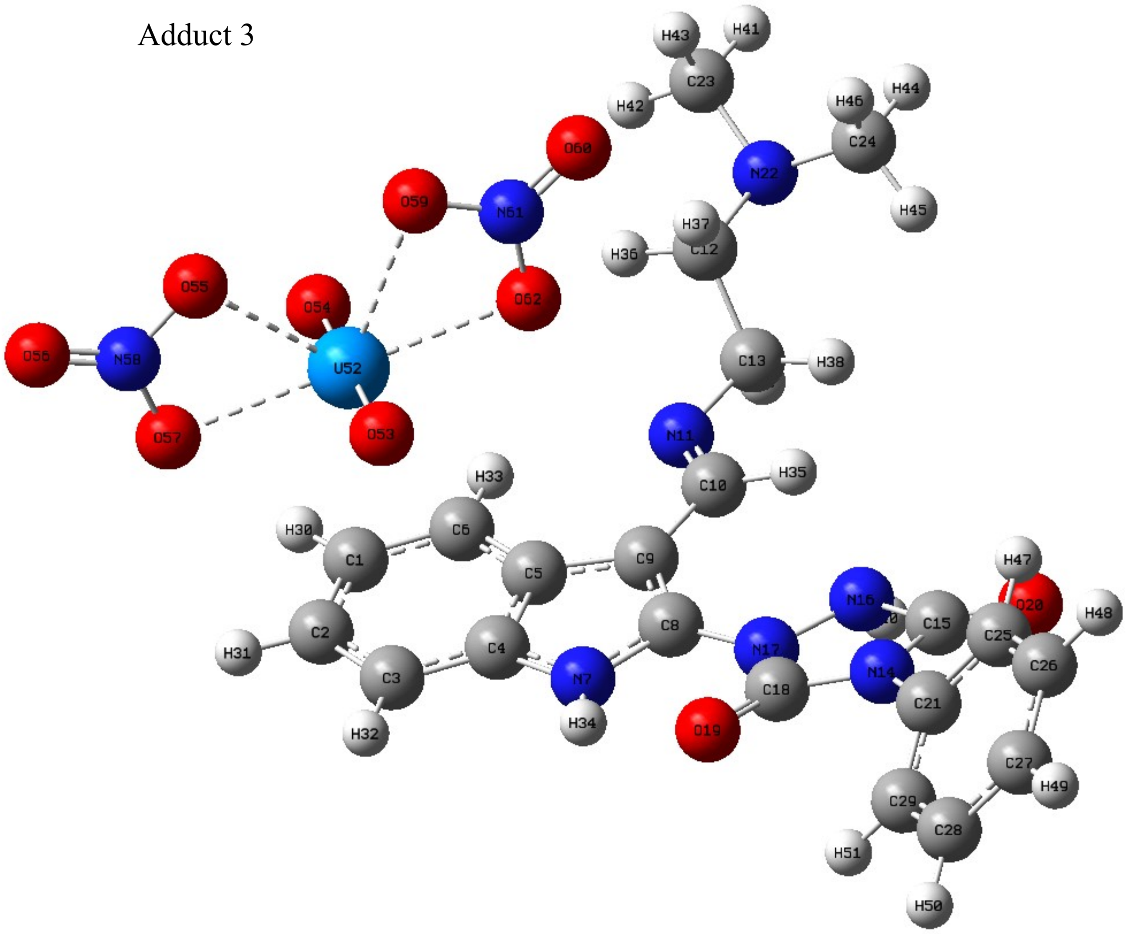


C	3.06083500	2.48838400	-3.32017500
C	4.12569400	1.56867800	-3.29740600
C	4.10690200	0.46617600	-2.45571500
C	2.98797000	0.30917500	-1.63718100
C	1.91182600	1.22855300	-1.63534300
C	1.95384800	2.33240000	-2.50000000
N	2.69123200	-0.69457600	-0.72996100
C	1.49729700	-0.38472700	-0.11891600
C	0.96559200	0.78244400	-0.63562000

C	-0.26400000	1.43084300	-0.20973000
N	-0.70052100	2.49692500	-0.74957900
C	-2.90369300	3.38132700	-1.35068300
C	-1.90872000	3.10191300	-0.21549900
N	0.84543100	-3.04492600	2.15954800
C	-0.40003400	-2.84942700	1.61707100
N	-0.30112800	-1.83631700	0.72383500
N	0.97176300	-1.23718700	0.86993100
C	1.74578200	-2.06987000	1.66730500
O	2.93234000	-1.99614500	1.86678100
O	-1.43081200	-3.48299100	1.89749400
C	1.20506800	-4.09082100	3.07598900
N	-3.98450400	4.27860100	-0.94695100
C	-4.66304800	4.84692500	-2.10470900
C	-4.94279800	3.64655700	-0.04514600
C	0.79828500	-5.39959300	2.82326400
C	1.14273700	-6.40229300	3.72438200
C	1.90028900	-6.10181600	4.85407400
C	2.31129000	-4.79141000	5.08803000
C	1.96042100	-3.77607800	4.20388700
H	3.11133000	3.33679300	-3.99278600
H	4.97594700	1.72228300	-3.95185000
H	4.92393700	-0.24585000	-2.43975000
H	1.13351800	3.03612900	-2.50464100
H	3.35764000	-1.34049900	-0.33246300
H	-0.79420900	0.97182200	0.64127400
H	-2.34456700	3.86481600	-2.15544300
H	-3.28379100	2.42291900	-1.74923900
H	-2.36197200	2.48078800	0.57097400
H	-1.64016100	4.06815300	0.22641100
H	-1.11320100	-1.25280000	0.51719800
H	-5.41477800	5.56742300	-1.77192300
H	-3.94415700	5.37655900	-2.73450700
H	-5.17313500	4.08795400	-2.72769300
H	-5.69882300	4.37840700	0.25006900

H	-4.44592100	3.30229200	0.86344400
H	-5.45655300	2.78117200	-0.50086700
H	0.21388400	-5.63192400	1.94290200
H	0.81856800	-7.41890900	3.53794700
H	2.16955200	-6.88710700	5.55040300
H	2.90236000	-4.55338100	5.96420700
H	2.27857400	-2.75730200	4.37940900
U	-3.78083300	-3.66906200	1.46757500
O	-3.40831800	-4.27011800	-0.14273400
O	-4.14735100	-3.03656600	3.06536700
O	-5.11851600	-1.85656200	0.43775700
O	-4.35712100	0.08214900	-0.21516800
O	-3.04061900	-1.37836400	0.74247300
N	-4.19114300	-0.99055200	0.28971500
O	-5.56453400	-5.32029700	1.68830500
O	-5.29396300	-7.33058200	2.50205700
N	-4.84983500	-6.26273500	2.20337100
O	-3.61087800	-5.94304000	2.36504300

Adduct 3



C	2.64354800	4.35728400	-1.26427000
C	3.89383100	3.70956300	-1.22411800
C	4.03043900	2.45324800	-0.63795200
C	2.88644200	1.85624500	-0.12323200
C	1.60480500	2.47182300	-0.17654000
C	1.49127800	3.74968700	-0.74768500
N	2.73014500	0.63475300	0.49088200
C	1.40106700	0.45345800	0.79259100
C	0.64952900	1.56104600	0.41063800
C	-0.78871600	1.77949500	0.50592100
N	-1.31779700	2.90014700	0.21340900
C	-3.33199100	3.34527500	-1.11117700
C	-2.76567500	3.00681500	0.27722900
N	0.89436300	-2.89318700	1.87125600
C	-0.34406500	-2.33799500	2.22705400
N	-0.27970000	-0.98495700	1.84082400
N	1.05468800	-0.71462000	1.47068700

C	1.77157500	-1.91245700	1.41261000
O	2.91451500	-2.04087900	1.03462400
O	-1.28105800	-2.86977300	2.75336600
C	1.22761100	-4.28121000	2.01204200
N	-4.75593200	3.67469200	-1.06762200
C	-5.16366000	4.44067300	-2.24011400
C	-5.60073800	2.49683400	-0.90288600
C	0.29138400	-5.24662000	1.64312100
C	0.60995800	-6.59310100	1.78750900
C	1.85501500	-6.97392500	2.28258900
C	2.78407000	-6.00065900	2.64224900
C	2.47429400	-4.64988400	2.51642800
H	2.57970700	5.36219200	-1.66733100
H	4.75995900	4.20050600	-1.64912700
H	4.99139800	1.95441300	-0.60539600
H	0.53209700	4.24957600	-0.73926700
H	3.40650300	-0.11473800	0.57000100
H	-1.40575800	0.92420100	0.80501300
H	-2.78940800	4.21926500	-1.47931600
H	-3.11438300	2.51819100	-1.80956800
H	-3.22272300	2.08732700	0.67411500
H	-3.02584000	3.83078400	0.94960000
H	-0.64023100	-0.34624800	2.54356800
H	-6.21408500	4.72728900	-2.14299600
H	-4.57037200	5.35518100	-2.31127300
H	-5.04958900	3.88118800	-3.18710700
H	-6.64672700	2.80474900	-0.83072100
H	-5.35028800	1.96857700	0.01890500
H	-5.50925500	1.78323500	-1.74319000
H	-0.67636600	-4.94885300	1.26368400
H	-0.11838500	-7.34437000	1.50638300
H	2.10008200	-8.02426000	2.38734200
H	3.75492400	-6.28944700	3.02715300
H	3.19693100	-3.89351800	2.78907900
U	1.63150700	3.06798000	-3.73734700

O	2.46025900	1.54100000	-3.46925200
O	0.80917500	4.61052600	-3.92628600
O	2.52948300	3.22307300	-5.99906300
O	4.42201100	4.18441700	-6.51906000
O	3.73519800	4.10809300	-4.44509200
N	3.60939100	3.85774900	-5.70634800
O	-0.03708300	1.95709000	-5.14299900
O	-1.88328000	1.06366100	-4.38760700
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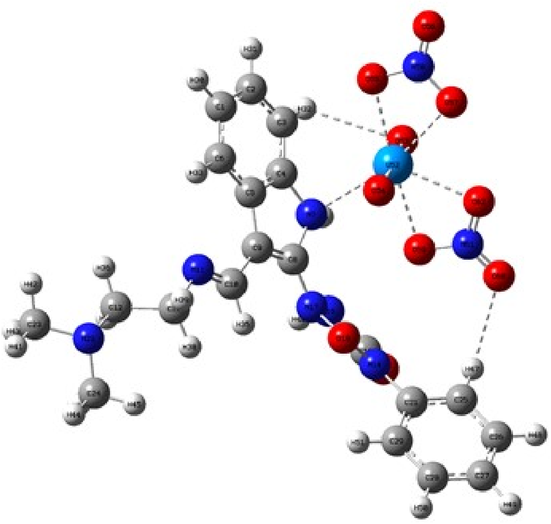
Adduct 4



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C	3.96160600	0.75247400	-3.27105000

C	2.92630800	0.39378600	-2.40757300
C	1.95391000	1.31251100	-1.94905800
C	2.04546300	2.64829200	-2.34416600
N	2.67730400	-0.85145200	-1.78568600
C	1.44039300	-0.72271000	-1.10166500
C	0.99559900	0.57083400	-1.14404100
C	-0.21427600	1.07834800	-0.50815700
N	-0.56959600	2.29400400	-0.62600200
C	-2.76653300	3.30135900	-1.00364400
C	-1.79623000	2.71284900	0.03146700
N	0.83888800	-3.38952200	1.10989800
C	1.02671300	-4.08733100	-0.08344100
N	1.15978900	-3.10427700	-1.09979300
N	0.86560700	-1.84412500	-0.50196900
C	0.78672900	-2.01122800	0.90410700
O	0.67867500	-1.13081300	1.71042800
O	1.04216900	-5.27134900	-0.26748400
C	0.71484600	-4.01213700	2.39620900
N	-3.91365700	3.96583800	-0.39328600
C	-4.57535900	4.86212400	-1.33317300
C	-4.86697400	3.03039400	0.19137400
C	1.65929200	-4.95469900	2.79509300
C	1.52186200	-5.56728400	4.03708700
C	0.46156700	-5.23097800	4.87557700
C	-0.47013500	-4.27783000	4.46971100
C	-0.35207300	-3.66857600	3.22451300
H	3.17209900	4.05562000	-3.50223500
H	4.82229100	2.41478700	-4.31244500
H	4.67357900	0.02715300	-3.64480100
H	1.30963700	3.35740000	-1.99288400
H	2.88189700	-1.73219200	-2.24716500
H	-0.78980500	0.35556400	0.08148000
H	-2.21160600	4.04169800	-1.58493900
H	-3.07497000	2.50578600	-1.70990500
H	-2.25972400	1.88770700	0.59127300

H	-1.54996800	3.50739400	0.74313600
H	0.53434000	-3.30429800	-1.87688500
H	-5.38153700	5.39660600	-0.82452100
H	-3.86325700	5.60216300	-1.70547000
H	-5.01237700	4.33591100	-2.20302300
H	-5.68185800	3.58587900	0.66130600
H	-4.39108900	2.42796800	0.96683800
H	-5.30722300	2.34357800	-0.55706500
H	2.49374000	-5.19042500	2.15015600
H	2.25433100	-6.30125200	4.35127900
H	0.36401200	-5.70642000	5.84464300
H	-1.29380000	-4.00825300	5.12024300
H	-1.07103100	-2.92582500	2.90455200
U	4.99017700	-0.36101500	-0.36074000
O	5.71911000	-1.37847800	-1.60430900
O	4.14216100	0.65598100	0.79102100
O	6.25712400	1.56361000	-1.16992300
O	8.20027200	2.17407900	-0.37463600
O	7.16230200	0.42275600	0.42154000
N	7.26536900	1.43082400	-0.37100000
O	3.84583000	-2.36990400	0.51057200
O	4.70701100	-3.69160100	2.02589200
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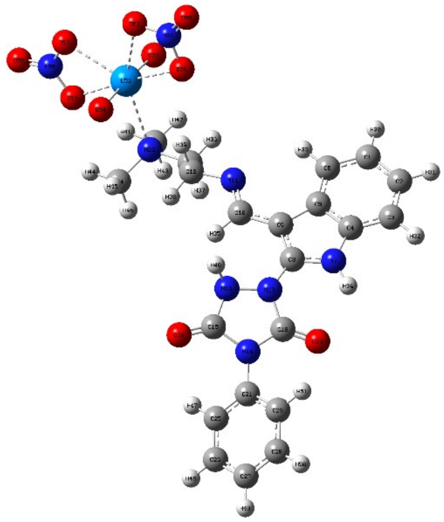
Adduct 5



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C	3.16680800	-0.85605200	-2.44738300
C	2.18589800	0.14659700	-2.61354100
C	2.15745600	0.87422200	-3.81125000
N	2.99977800	-1.40117500	-1.18319100
C	1.92819900	-0.80369600	-0.57751600
C	1.37455200	0.17040700	-1.40816600
C	0.20376700	0.98739000	-1.17004200
N	-0.21613300	1.85480300	-2.01140900
C	-2.39548100	2.48520500	-2.83669300
C	-1.41114400	2.59991900	-1.66481100
N	1.10184100	-2.51911200	2.43379900
C	0.40211600	-1.32331500	2.64031400
N	0.63890300	-0.53982000	1.49333200
N	1.63193400	-1.19315200	0.73363400
C	1.87457800	-2.45414400	1.26890500
O	2.60405600	-3.30166700	0.80474900
O	-0.26715600	-0.99531900	3.58140900
C	1.07520200	-3.63673700	3.33101100
N	-3.64321300	3.29735300	-2.71936700
C	-4.45922400	3.06642600	-3.94246800

C	-4.44516900	2.88331200	-1.53803300
C	-0.13441600	-4.01484500	3.91421100
C	-0.15993800	-5.09321800	4.79280600
C	1.00680200	-5.79830200	5.07864100
C	2.20768600	-5.41572600	4.48615200
C	2.25138400	-4.33055400	3.61603400
H	3.08164500	1.12947200	-5.72488300
H	4.76386100	-0.64633000	-5.39869300
H	4.84377500	-1.94435500	-3.27973900
H	1.41972200	1.65184200	-3.94645600
H	3.44081300	-2.22899400	-0.80630400
H	-0.34000100	0.81265100	-0.23382100
H	-1.87844600	2.79308800	-3.74875900
H	-2.67308300	1.42966300	-2.96603400
H	-1.86799300	2.24496100	-0.72891900
H	-1.12167600	3.64734400	-1.51532300
H	0.87164400	0.42598300	1.70739100
H	-5.36217500	3.67448000	-3.89920300
H	-3.88690800	3.34604700	-4.82590900
H	-4.74229500	2.00886200	-4.01582600
H	-5.38063100	3.44168200	-1.52970300
H	-3.90850800	3.09945400	-0.61699800
H	-4.66858600	1.80966900	-1.58649500
H	-1.03782800	-3.46175600	3.69811900
H	-1.09824500	-5.38272900	5.25100200
H	0.98030000	-6.64076100	5.75972600
H	3.11984100	-5.95913400	4.70280200
H	3.18171300	-4.03818200	3.15022300
U	-3.08551900	5.87976900	-2.57969500
O	-3.11093700	5.90851800	-4.34017700
O	-3.04534900	5.72923600	-0.82466900
O	-5.55152700	5.74202000	-2.53385800
O	-6.86415600	7.48696500	-2.42192000
O	-4.69175300	7.71987900	-2.45782200
N	-5.76726300	7.01554600	-2.46827100

O	-0.64983500	5.81310600	-2.63575000
O	0.64953400	7.56968200	-2.55854900
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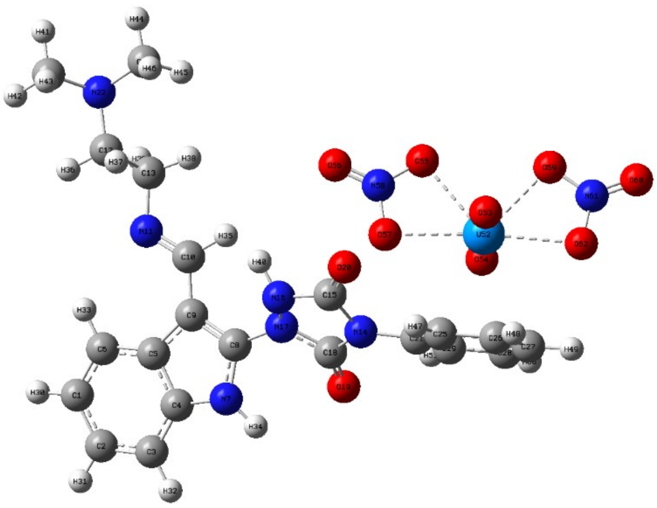
O	-1.52455400	7.78307500	-2.50604600

Adduct 6



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C	4.42837200	0.75574700	-2.65875300
C	3.19020600	0.63289700	-2.02806500
C	2.14717800	1.57296700	-2.21355000
C	2.35068300	2.66030000	-3.07515600
N	2.72934300	-0.34749000	-1.16391000
C	1.46079500	-0.00480700	-0.75699400
C	1.04791700	1.16403900	-1.36818600
C	-0.21229200	1.84166300	-1.12073600
N	-0.59541600	2.86346100	-1.77682200
C	-2.80607500	3.49535200	-2.60967900
C	-1.85557400	3.48231800	-1.40333800
N	0.32188800	-2.56997500	1.43015300
C	-0.84019300	-2.37837700	0.64865200
N	-0.50110800	-1.40438300	-0.28338700
N	0.73583600	-0.82305200	0.12209300
C	1.30881500	-1.62325800	1.08768800
O	2.44081700	-1.54916600	1.51057100

O	-1.89851800	-2.94070500	0.74479200
C	0.37040200	-3.40402300	2.57236700
N	-3.99000900	4.32152800	-2.39443800
C	-4.64776700	4.65037300	-3.65249000
C	-4.93357200	3.72735200	-1.45493800
C	-0.36118200	-4.60059300	2.60014600
C	-0.36004700	-5.38446500	3.74687600
C	0.36798200	-5.00400500	4.87546600
C	1.12940100	-3.83500700	4.83544700
C	1.13178500	-3.02521900	3.69152900
H	3.75333100	3.61680200	-4.37812700
H	5.55241700	1.96860200	-4.01485000
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H	1.55564100	3.37780100	-3.22415900
H	3.30357000	-1.01310500	-0.66861800
H	-0.81577100	1.45016000	-0.28356000
H	-2.24974100	3.90605300	-3.45564500
H	-3.07104000	2.45351300	-2.87763800
H	-2.31500400	2.98180200	-0.53763600
H	-1.66212200	4.52360400	-1.12519100
H	-1.23187800	-0.72868300	-0.47713200
H	-5.48392500	5.32838500	-3.46327500
H	-3.94555100	5.15833300	-4.31757500
H	-5.04339400	3.76291200	-4.18239600
H	-5.77816400	4.40469900	-1.30812600
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H	-5.33122200	2.75508600	-1.80489100
H	-0.94922100	-4.88806000	1.74160100
H	-0.94476200	-6.29605100	3.76292000
H	0.35671000	-5.61492500	5.76933200
H	1.74525800	-3.55472700	5.68308500
H	1.76401500	-2.14933700	3.64380900
U	-1.04606700	-1.69619100	5.32348200
O	-2.34306400	-2.75352100	4.80215100
O	0.31075600	-0.69249600	5.80866600
O	-2.32102700	0.27135500	4.60289700
O	-2.27676100	1.11280300	2.58660900
O	-1.03826400	-0.60948500	3.11045400
N	-1.90371400	0.30882000	3.39125400
O	-2.19418700	-1.22281000	7.40831500
O	-1.96309100	-2.39113700	9.24149300
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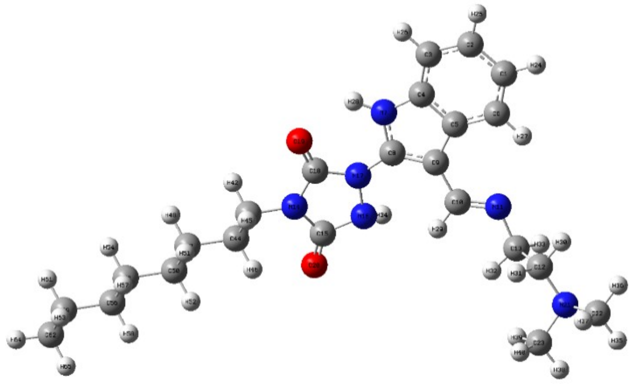
INTS-OCT



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C	2.04277500	2.11298200	-0.21240300
C	2.11920800	3.34233800	-0.88172100
N	2.88973700	0.33103600	0.88683900
C	1.53225100	0.15949900	0.79827300
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C	-2.30555700	2.52918000	-1.10878500
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N	-0.40250600	-1.18242900	1.50855300
N	0.99190700	-0.96714100	1.42987000
C	1.65368700	-2.17615700	1.62478000
O	2.84766000	-2.37822200	1.53971400
O	-1.64078500	-2.99269900	2.30249800
N	-3.87844700	3.01362600	-2.99198200
C	-3.95924600	3.59695500	-4.32477300
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H	5.39273000	1.59937800	0.41762600
H	1.21198400	3.81300600	-1.23247000
H	3.50694300	-0.40576600	1.20027000
H	-1.14236800	0.59794600	0.04171600
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H	-2.11540300	1.81444000	-3.14828700
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H	-0.88586400	-0.48103700	2.06146800
H	-4.99331200	3.87824100	-4.54090500
H	-3.34697700	4.50040700	-4.37294200
H	-3.62073500	2.90904300	-5.12304700

H	-5.78429700	2.15594300	-3.12627700
H	-4.76893500	1.47891000	-1.85563200
H	-4.47245300	1.03011300	-3.55148900
C	0.91790200	-4.49710800	2.26237900
H	1.88795500	-4.53469500	2.76154400
H	0.14528600	-4.79735800	2.97271800
C	0.90644400	-5.40349200	1.02868700
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H	-0.06648500	-5.31612000	0.53328700
C	1.17684000	-6.86828600	1.38887700
H	2.14666000	-6.94501200	1.89667800
H	0.42443600	-7.21055600	2.11065500
C	1.16933500	-7.79938900	0.17106200
H	1.91993700	-7.45469900	-0.55128300
H	0.19964000	-7.72177200	-0.33653100
C	1.44090600	-9.26637400	0.52280100
H	2.41050500	-9.34286300	1.03152400
H	0.69027700	-9.60984800	1.24620100
C	1.43389200	-10.19893300	-0.69353900
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H	0.46440200	-10.12305300	-1.20283000
C	1.70557100	-11.66668000	-0.34428200
H	0.95579100	-12.00970100	0.37893900
H	2.67442300	-11.74274200	0.16409100
C	1.69652500	-12.59100800	-1.56508900
H	2.46002400	-12.29481200	-2.29122500
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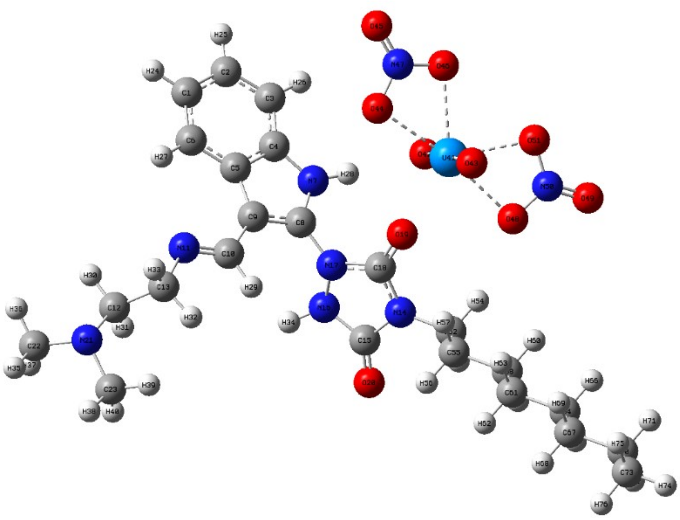
Adduct1’



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C	2.73727026	0.11108555	-1.82018209

C	1.86036777	1.21856149	-1.70433894
C	2.23886757	2.45555211	-2.25030400
N	2.13286995	-0.97777296	-1.22263336
C	0.93050730	-0.56689197	-0.69229718
C	0.70473081	0.76960205	-0.96864864
C	-0.46853036	1.51907108	-0.55289629
N	-0.66883802	2.73259445	-0.87820189
C	-2.69143729	3.92233463	-1.56816856
C	-1.86762625	3.38773454	-0.38704452
N	-0.68040370	-3.17628636	1.11822692
C	-1.57539592	-3.05638958	0.03767444
N	-1.00878824	-2.08277326	-0.78419695
N	0.05269037	-1.46488008	-0.05994064
C	0.28908125	-2.22169575	1.04809039
O	1.23176161	-2.06675435	1.84835125
O	-2.59195952	-3.67082138	-0.14063109
N	-3.78075093	4.79922843	-1.15082221
C	-4.25760387	5.62428154	-2.25406179
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H	3.77976376	3.49517271	-3.30700576
H	5.28576098	1.54974902	-3.47456463
H	4.64404718	-0.64869245	-2.52175589
H	1.57289436	3.30284220	-2.16452275
H	2.58454963	-1.86112380	-1.02197701
H	-1.18226168	0.97497570	0.08874638
H	-2.01165130	4.49608508	-2.20225759
H	-3.05375918	3.07093400	-2.17720933
H	-2.46785927	2.71752302	0.24784235
H	-1.56799073	4.24743230	0.22126320
H	-1.63130289	-1.43743917	-1.25622654
H	-5.01849298	6.31911418	-1.88991250
H	-3.43235071	6.21202781	-2.66224476
H	-4.70205003	5.03486700	-3.07824574
H	-5.64832545	4.78800655	-0.20436283
H	-4.54134345	3.53988408	0.35845378
H	-5.35980966	3.34886220	-1.21087249
U	3.52465447	-2.61213337	2.24210711
O	3.57848551	-3.02878112	0.51589174
O	3.40647700	-2.17894456	3.94047271
O	4.21989186	-0.33744366	1.69342181
O	6.29921633	0.33584454	1.63642666
O	5.80668111	-1.73583788	2.12929964
N	5.49299399	-0.52766303	1.81009249
O	2.46437737	-4.78343870	2.72035061
O	3.56874870	-6.60136235	3.22668436
N	3.55687140	-5.44192489	2.93796876
O	4.61960143	-4.73031797	2.81400574
C	-0.84670609	-4.15727394	2.20400641
H	-1.49157607	-4.93394451	1.79072211
H	0.13078474	-4.59390038	2.41155276

C	-1.46537338	-3.54826897	3.46434145
H	-2.44454729	-3.12481468	3.21507798
H	-0.83426894	-2.72479889	3.81447802
C	-1.61466949	-4.59074822	4.57856866
H	-2.23524323	-5.42120829	4.21943084
H	-0.63074224	-5.01763014	4.80705305
C	-2.22943954	-4.01544895	5.85957269
H	-3.21338504	-3.58761650	5.62888417
H	-1.60950170	-3.18275783	6.21482986
C	-2.37719521	-5.05030241	6.98065830
H	-2.99653628	-5.88357019	6.62471066
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H	-2.37006663	-3.64409778	8.61995675
C	-3.13647631	-5.51052151	9.38745326
H	-2.15264291	-5.93837322	9.61465938
H	-3.75497363	-6.34369288	9.03228130
C	-3.74779351	-4.93042092	10.66593809
H	-3.83872644	-5.69109890	11.44597557
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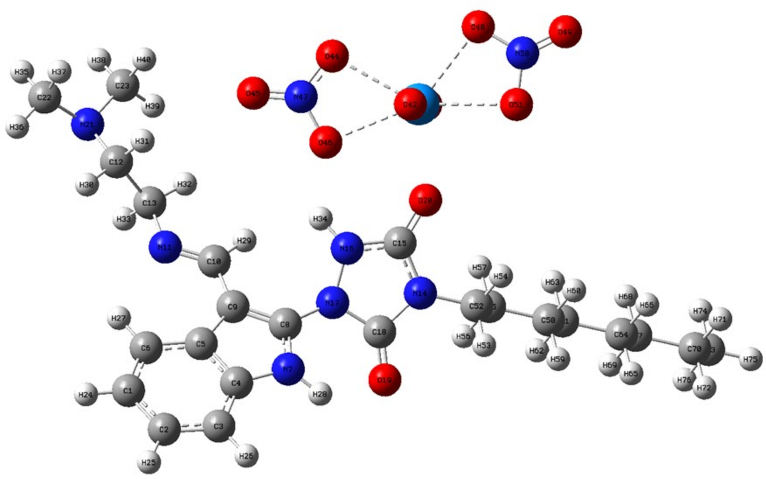
Adduct2'



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C	2.84379900	0.36104500	-2.49285100
C	1.76066200	1.25698700	-2.32983700
C	1.61284000	2.32118500	-3.23170500
N	2.74683500	-0.60649500	-1.50633600
C	1.67674800	-0.29512600	-0.69904000
C	1.02626500	0.83737100	-1.15488300
C	-0.12114500	1.48475500	-0.54015100
N	-0.67701700	2.51340600	-1.04187200
C	-2.96959800	3.33827200	-1.27697100

C	-1.78187500	3.12908600	-0.32663500
N	1.53071000	-2.89432700	1.72075300
C	0.20500900	-2.70521700	1.47013400
N	0.09746000	-1.70428600	0.56034300
N	1.37580700	-1.11625200	0.40407300
C	2.29960700	-1.94558700	1.03109100
O	3.50533500	-1.89432000	0.96467300
O	-0.72924800	-3.34582900	1.98498800
N	-3.96661900	4.26442600	-0.74481800
C	-4.85103600	4.75312800	-1.79468000
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H	2.44860800	3.28070200	-4.95159700
H	4.33410700	1.70775200	-5.18961100
H	4.61481300	-0.19090500	-3.61444400
H	0.78606000	3.00718500	-3.11409800
H	3.49040300	-1.22289600	-1.21141500
H	-0.47379800	1.06447000	0.41648500
H	-2.56955100	3.76514100	-2.19986000
H	-3.40846500	2.35701600	-1.53715700
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H	-0.73428400	-1.11335200	0.54097500
H	-5.53595400	5.49745500	-1.38015300
H	-4.26499400	5.23513000	-2.58093200
H	-5.45953400	3.95419200	-2.25942200
H	-5.42965600	4.45561300	0.73978300
H	-4.07828100	3.41345900	1.18052100
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U	-3.10583800	-3.48050800	2.23780200
O	-3.23480000	-4.15212300	0.61831600
O	-2.97755200	-2.77802500	3.84449900
O	-4.64406700	-1.65814000	1.57192500
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N	-3.77955600	-0.82129900	1.14220400
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O	-4.27999600	-7.05008800	3.86550200
N	-3.93364800	-6.01083800	3.38940400
O	-2.69907600	-5.71370500	3.16416400
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H	3.06931600	-4.19067700	2.15737200
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C	2.24573200	-3.48093400	4.04054900
H	2.88648600	-2.59335800	4.07224500
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C	2.83962800	-4.58347800	4.92451700
H	3.81601700	-4.88443500	4.52444500
H	2.19905900	-5.47280000	4.87644400
C	3.00213300	-4.15594600	6.38782200
H	3.64187100	-3.26575200	6.43527500

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C	3.59349700	-5.25353400	7.27949400
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H	3.70786000	-6.81466000	9.58763700
H	5.32265200	-6.23041200	9.23757800
C	4.50816300	-5.49368000	11.09766400
H	3.54453300	-5.21640200	11.53620900
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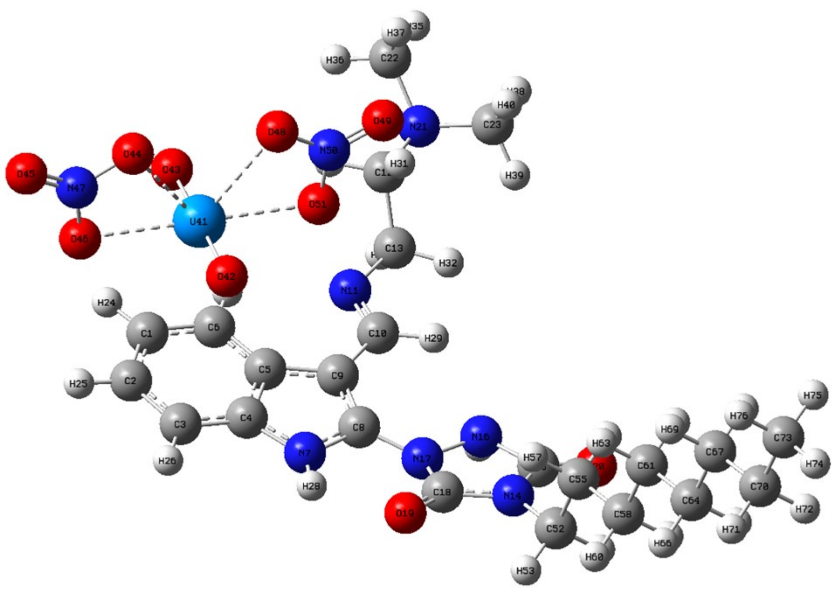
H	5.17136900	-4.62724900	11.18363100

Adduct 3’



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C	1.62075900	2.19991300	-0.30804700
C	1.64529100	3.34192000	-1.12528400
N	2.50866300	0.35314900	0.63433100
C	1.21610200	0.48270600	1.08601700
C	0.61232500	1.61349700	0.54450600
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C	-3.20357400	3.70633900	-0.98638900
C	-2.52193600	3.59197000	0.38677100
N	0.30887800	-2.44926900	2.85224300
C	-0.76165600	-1.63485700	3.20504900

N	-0.52997200	-0.39847900	2.56317800
N	0.77525500	-0.45019900	2.02260000
C	1.26637100	-1.75702300	2.13717800
O	2.31452100	-2.17538900	1.69332800
O	-1.69361100	-1.90014900	3.91526300
N	-4.54007300	4.29248800	-0.89971600
C	-4.97228100	4.83025100	-2.18479600
C	-5.53010600	3.36024700	-0.37190700
H	2.85402000	4.51132400	-2.46824200
H	4.80245900	2.99614200	-2.39427600
H	4.79893600	0.99545900	-0.91525300
H	0.78847600	4.00254900	-1.13802100
H	3.05899000	-0.47849000	0.81184900
H	-1.44784000	1.45824500	1.26034600
H	-2.58275800	4.35931200	-1.60450000
H	-3.21120800	2.71653600	-1.47629200
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H	-5.94315100	5.31914700	-2.06924300
H	-4.25754000	5.57909600	-2.53369900
H	-5.07176600	4.05703200	-2.96912100
H	-6.49630400	3.86344500	-0.28588500
H	-5.24695100	3.02142500	0.62633900
H	-5.66267300	2.46802800	-1.01237400
U	1.23243800	2.08246700	-3.86891200
O	1.91915800	0.52563800	-3.42685300
O	0.56527600	3.66634400	-4.23996700
O	1.81274900	1.73221300	-6.21129200
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O	3.31696200	2.69903200	-5.00393400
N	2.98676300	2.25681900	-6.17235600
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O	-2.54631600	0.50120200	-3.74066900
N	-1.43877700	0.95324000	-3.78047900
O	-0.84707900	1.44889300	-2.74523500
C	0.42750600	-3.86030400	3.23120800
H	1.49017300	-4.05867300	3.38133300
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H	-1.21763700	-4.55445600	2.03053000
H	0.34882300	-4.64131100	1.22719900
C	-0.03207500	-6.27531000	2.59582700
H	-0.53262100	-6.42738600	3.56040500
H	1.02638900	-6.51567800	2.75737900
C	-0.61877300	-7.24477900	1.56321200
H	-1.67662700	-7.00285000	1.40145700
H	-0.11967100	-7.09009400	0.59845300
C	-0.49208000	-8.71741800	1.96911600
H	-0.99051700	-8.87072700	2.93492000

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C	-0.95320400	-11.16193700	1.34166100
H	0.10449500	-11.40234300	1.50413000
H	-1.45093600	-11.31496000	2.30693600
C	-1.54162700	-12.12462900	0.30638200
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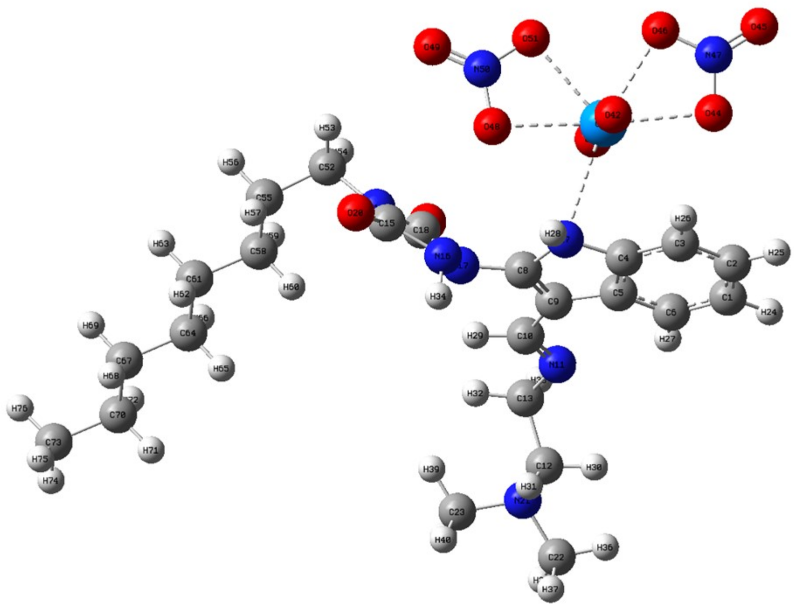
Adduct4’



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C	2.54823800	0.08675300	-2.62621700
C	1.75083600	1.14206000	-2.12429500
C	1.81606900	2.39153500	-2.74285300
N	2.39078000	-1.02335100	-1.76838000
C	1.35528900	-0.69213800	-0.85824700
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C	-0.02590700	1.30757100	-0.21262600
N	-0.34388400	2.51748100	-0.44310500
C	-2.51938600	3.63601000	-0.46578100
C	-1.35739800	3.12834500	0.40085200
N	1.26353900	-2.94324600	1.82061100
C	1.11851700	-3.81653500	0.75799200

N	0.98003200	-3.01225100	-0.40664200
N	0.88578800	-1.65801100	0.03516200
C	1.19500200	-1.61895800	1.42420300
O	1.34460700	-0.62713100	2.08379100
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N	-3.45945900	4.46976600	0.27679100
C	-4.28332700	5.27406300	-0.61694300
C	-4.28901000	3.70550200	1.20058500
H	2.72294100	3.51360900	-4.32748300
H	4.07223300	1.64087400	-5.19003600
H	3.95381900	-0.60383800	-4.13272900
H	1.21396900	3.20426500	-2.36225500
H	2.45018000	-1.97971200	-2.10328700
H	-0.47579100	0.72928200	0.60295800
H	-2.08710600	4.23864100	-1.26823200
H	-3.02033400	2.77368800	-0.94772800
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H	0.16368000	-3.28565400	-0.94818800
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H	-3.64679400	5.89508500	-1.25138200
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H	-4.94331200	4.38521100	1.75137400
H	-3.67128200	3.18110000	1.93140200
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O	4.96968000	-3.04908400	2.19765900
N	4.98765000	-2.31341500	1.25244300
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H	-1.14069000	-2.65038700	3.21890200
C	-1.89149800	-3.61548800	4.99391300
H	-2.25436200	-4.51523800	4.48081900
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C	-3.06421200	-2.65609600	5.22586800
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C	-4.20738100	-3.26989900	6.04175700
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C	-6.51839100	-2.93248100	7.08933300
H	-7.33852800	-2.22435300	7.23575600
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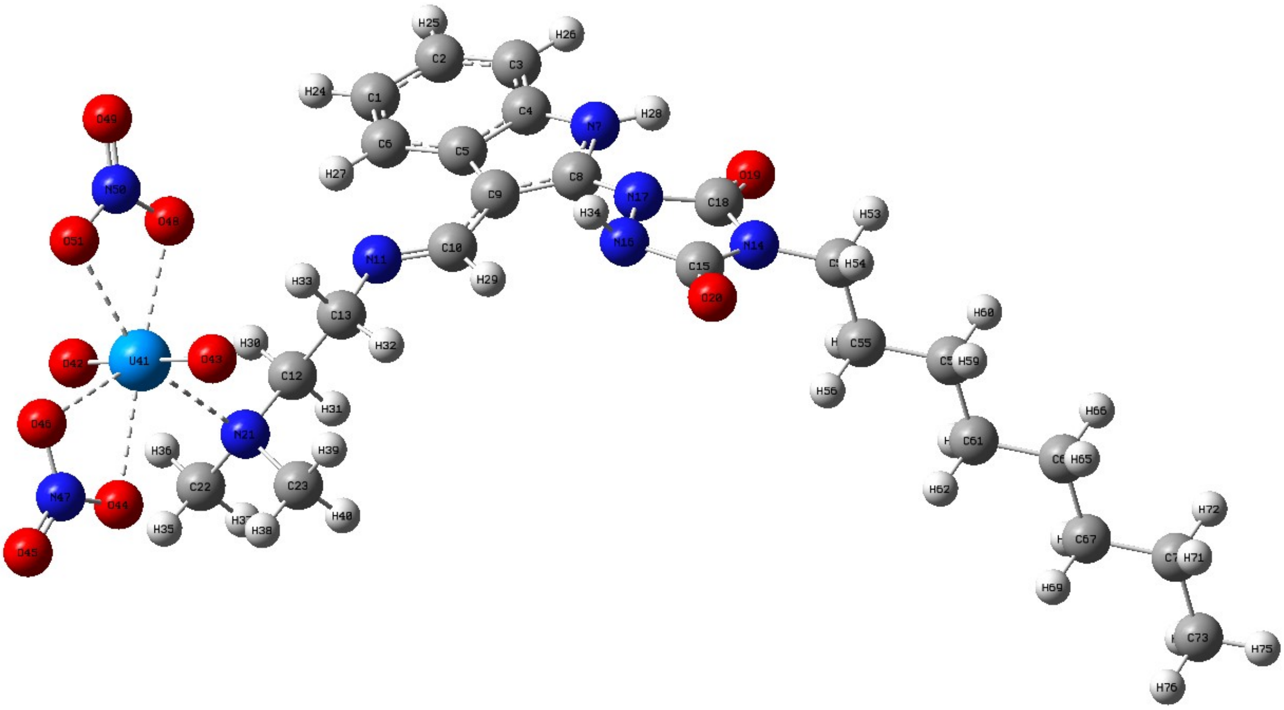
Adduct 5’



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C	2.53195900	-1.38726500	-2.19800900
C	1.67560300	-0.29913100	-2.47744700
C	1.55278900	0.14295200	-3.80173300
N	2.49654400	-1.60793900	-0.82913600
C	1.62167400	-0.72536500	-0.25677700
C	1.07516700	0.12009000	-1.22212700
C	0.07351500	1.14853000	-1.04227400
N	-0.35824100	1.87024500	-2.00667700
C	-2.53353400	2.66065000	-2.69044500
C	-1.37750700	2.85542400	-1.70016200
N	1.05908300	-1.60639900	3.13718200
C	0.55194000	-0.31450500	3.15458900

N	0.70900300	0.17619600	1.83901900
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C	1.64752700	-1.91131800	1.91959900
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C	-4.30769400	3.61046900	-1.27836100
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H	3.65674300	-2.09120400	-5.28757400
H	3.90140200	-2.88885000	-2.94542100
H	0.90988800	0.98147700	-4.02728100
H	2.88664500	-2.38921100	-0.31944000
H	-0.33279100	1.27100700	-0.03101600
H	-2.12539900	2.69640100	-3.70335600
H	-2.95642600	1.65595800	-2.55023200
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H	-0.93302400	3.85017200	-1.82907900
H	1.09621800	1.11497100	1.80161500
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H	-5.15395100	4.29662500	-1.27991000
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N	-0.00228200	6.90478000	-3.61360500
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C	1.03254300	-2.51537700	4.28487400
H	1.93631400	-3.12442000	4.22571100
H	1.08778400	-1.89051500	5.17824600
C	-0.21828000	-3.39736100	4.31314900
H	-1.10496700	-2.75469700	4.33322500
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C	-0.23111700	-4.33747500	5.52340600
H	-0.16821700	-3.74491200	6.44480300
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H	-2.81060500	-7.65497600	5.92736600
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H	-1.87365800	-8.63655800	8.03947800
C	-4.01777500	-8.88904200	8.10923300
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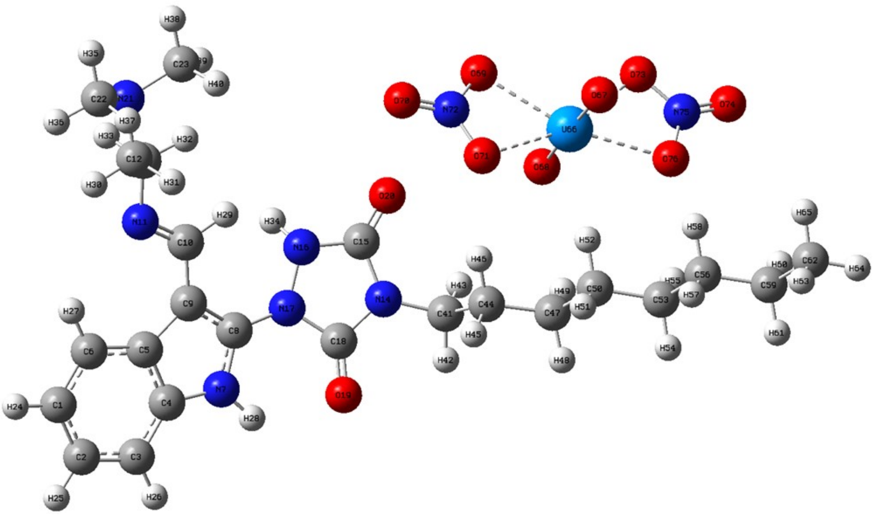
Adduct6’



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C	-1.84164700	0.75633400	1.42170200
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N	-0.98740400	-1.43493900	2.41155500
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C	-7.38884800	-0.30417800	-1.75287900
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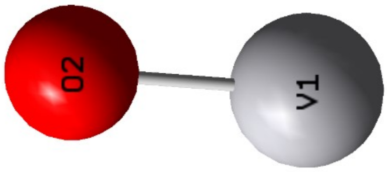			
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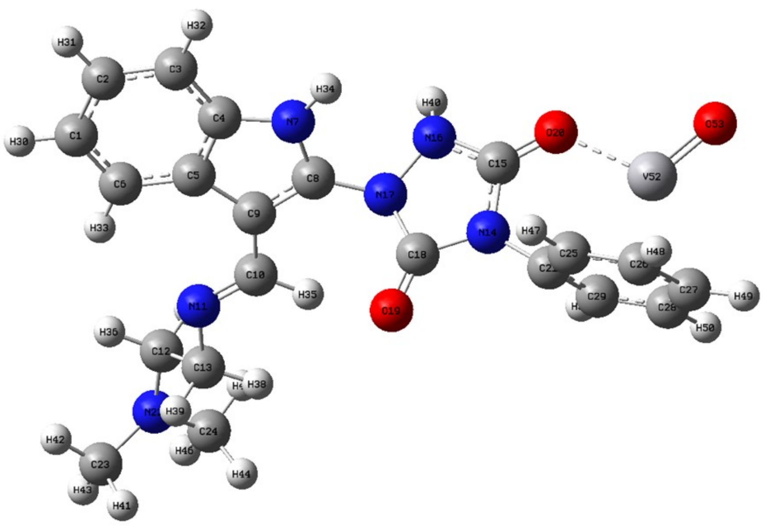			
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