

## Supporting Information

### **A Regenerative Dual-Functional Platform Combining Dendritic Silica and Anthraquinone Amide: Advancing Seawater Lithium Detection and Recovery with Biosensing Capabilities†**

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**Materials:**

All the chemicals and reagents utilized in chemical processing and synthetic procedures were of analytical grade. Dry solvents were employed in the chemical synthesis without additional purification steps. TMOS (Tetramethylorthosilicate), hydrazine hydrate, 1,8-dihydroxyanthraquinone, ethylbromoacetate, HEPES buffer, (3-Chloropropyl)triethoxysilane (3-CPTES), urea, potassium carbonate, and BDAC (Benzyl dimethyl dodecyl ammonium chloride) were purchased from Merck (Sigma-Aldrich) & TCI chemical private Ltd. Milli Q water, HCl, NaOH, methanol, chloroform, dimethyl formamide, and chloride salts of all cations and potassium salts of anions were procured from Spectrochem Pvt. Ltd.

**Instrumentation:** The following instruments were utilized for various analyses: The Shimadzu UV 3101PC spectrophotometer and Edinburgh Instruments model Xe-900 captured absorption and fluorescence emission spectra in an aqueous dispersion medium using a 380 nm excitation source. Structural characterization involved obtaining FT-IR spectra using a PerkinElmer GX spectrophotometer with KBr pellets. Surface area measurements were carried out using the Micromeritics 3 FLEX instrument after activating the sample at 55 °C for 1 hour. For surface morphology analysis scanning electron microscopy (SEM-Leo series 1420 VP) equipped with INCA and transmission electron microscopy (TEM) using an electron microscope JEOL-JEM 2100 was used. Lacey carbon-coated grids were used for both techniques. X-ray photoelectron spectroscopy Thermo Fisher Nexsa spectrophotometer with monochromated Al K $\alpha$  radiation at 1486.6 eV was used to analyse the surface and the chemical state. The metal ions concentration was determined using an ICP-MS Thermo Fisher iCAP Qnova series instrument;

samples were preferentially filtered through Thermo Fisher syringe filters (0.24  $\mu\text{m}$ ). Thermal stability was investigated by TGA analysis using a Mettler-Toledo (TGA/SDTA 851E) instrument in the presence of air, with a heating rate of 10  $^{\circ}\text{C}/\text{min}$ . A Rigaku MiniFlex-II (FD 41521) powder diffractometer from Japan was used to record Powder X-ray diffraction profiles at a scan rate of 1 $^{\circ}$  per minute. Fluorescence lifetime measurements were conducted using TSPC experiments on an Edinburgh Instruments OB 920 fluorescence spectrophotometer equipped with a pulse diode laser (Laser-EPLED-380 nm) as the excitation source.

**Batch adsorption studies:** The lithium extraction potential of the material was evaluated by batch adsorption studies. Typically, 5 mg of the material was treated in LiCl aqueous solution of varying concentrations (5 to 100 ppm) and shaken until equilibrium was achieved (2 h). Following the treatment, the filtrates in the sample tubes underwent centrifugation, followed by filtration through a Thermo Fisher syringe filter. The concentration of lithium was then determined using ICP-MS. The equation  $Q_e = (C_i - C_e) V/W$  can be used to find the equilibrium adsorption capacity ( $Q_e$ ) in this case.  $C_i$  and  $C_e$  represent the initial and final concentrations of  $\text{Li}^+$  ions,  $V$  stands for volume in liters, and  $W$  is the mass of the adsorbent in grams. The Langmuir model can be expressed in the usual linear equation form of  $C_e/q_e = 1/K_L q_m + C_e/q_m$  to describe the adsorption isotherm. Here,  $q_e$  represents the equilibrium adsorption;  $q_m$  is the maximum adsorption capacity in  $\text{mg L}^{-1}$ ; and  $C_e$  is the equilibrium metal ion concentration reached prior to any adsorption, while  $K_L$  is the Langmuir adsorption constant in  $\text{L mg}^{-1}$ . For Freundlich adsorption isotherm model, the model described by the equation:  $\ln q_e = \ln K_F + 1/n \ln C_e$ , was employed whereby  $K_F$  ( $\text{L g}^{-1}$ ),  $n$  are Freundlich constants.

**Photophysical studies:** For UV–Visible and fluorescence investigations, a 2 mL suspension of MDNS@DAAH material (0.2 mg per 2 mL, suspended in an aqueous medium) was mixed with various analyte aqueous buffer solutions individually and vigorously shaken using a

vortex shaker for 1 minute. This agitation process was repeated after each spectrophotometric/fluorescence reading. UV–Vis spectra were recorded within the range of 200 to 800 nm, while fluorescence spectra were recorded within the range of 400–680 nm with an excitation wavelength of 390 nm. To determine the limit of detection (LOD), solutions containing analytes in concentrations ranging from 0 to 130  $\mu\text{M}$  were incrementally added to the MDNS@DAAH suspension (0.2 mg per 2 mL), and fluorescent intensity was monitored. The slope (S) of the graph showing fluorescence intensity against increasing analyte concentration was calculated. The standard deviation (SD) was obtained from three blank measurements. The LOD and LOQ were computed using the  $3\sigma$  and  $10\sigma$  formulas, respectively.

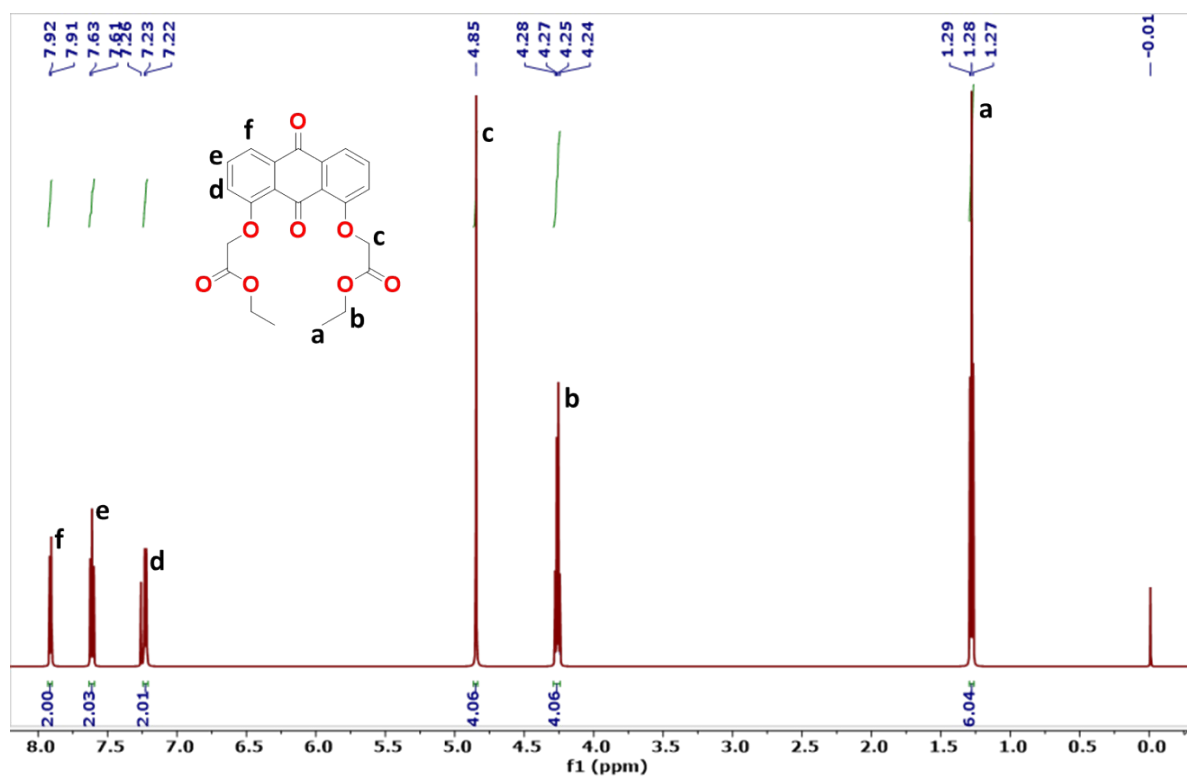
***Biosensing-Fluorescence Imaging Studies:*** A batch of *A. salina* cysts was taken from the freezer and left to hatch overnight in a vigorously aerated vessel exposed to intense visible light. The following day, the hatched cysts developed into *Artemia* larvae (nauplii), which were then used for the biosensing experiments. Approximately 30 *Artemia* nauplii were placed in 10 mL of seawater, to which 100  $\mu\text{L}$  of the suspended MDNS@DAAH aqueous solution (prepared from a 10 mg/10 mL stock solution) was added and allowed to incubate for 2 hours and fluorescence imaging were carried out. The treated *Artemia* nauplii were subsequently exposed to a 10 mL brine solution containing 100  $\mu\text{L}$  of 100  $\mu\text{M}$  of  $\text{Li}^+$  ions. Following this, some organisms from the tube were transferred onto a glass slide and examined under a BX53 OLYMPUS microscope equipped with both bright and fluorescent filters.

***Toxicity Studies:*** Mature *Artemia* nauplii (approximately 30 individuals  $\pm$  3) that had hatched were randomly chosen using a sterile glass dropper and transferred into test tubes containing 10 mL of sterile seawater. In one set of experiments, 100  $\mu\text{L}$  of material suspension (prepared

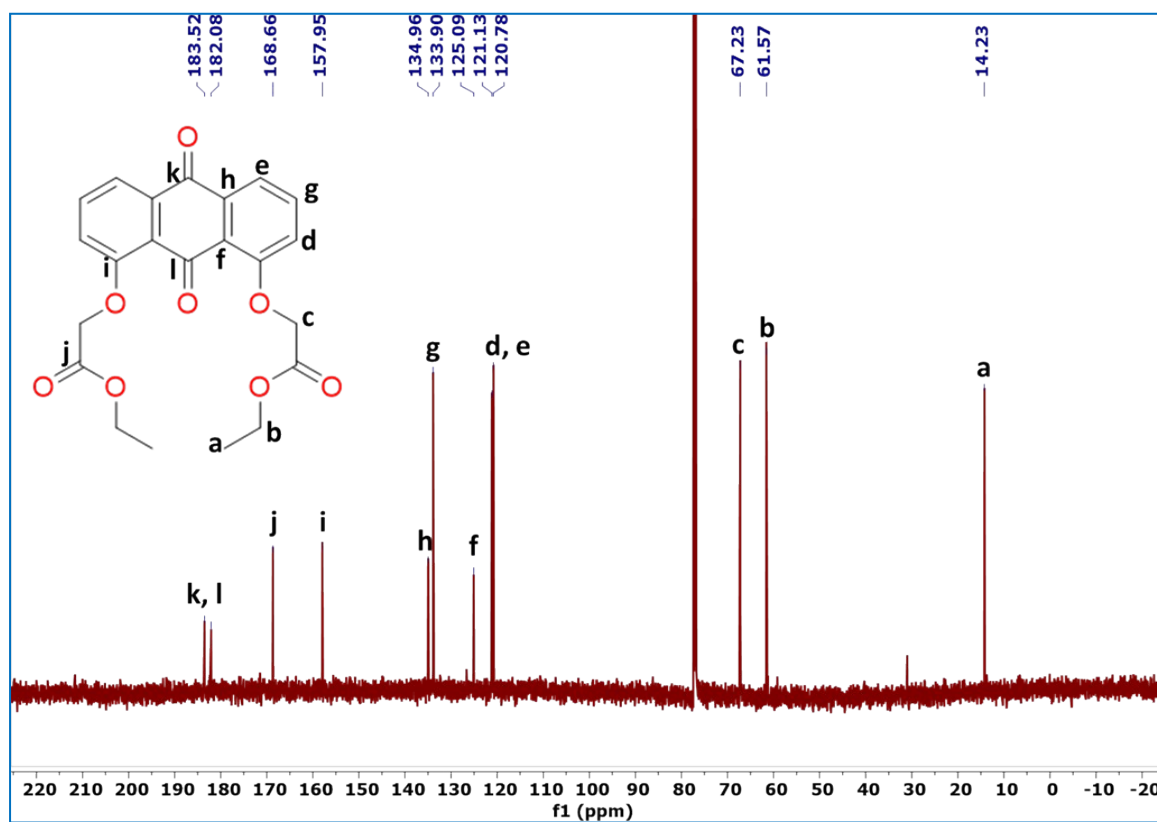
at 10 mg/10 mL) was added to the test tubes and placed under light at room temperature, with the number of live *Artemia* recorded after 6, 12, and 24 hours. Similar experiments were conducted separately, with 100  $\mu\text{L}$  of metal ions only (at  $100 \times 10^{-6} \text{ M Li}^+$ ) in 10 mL of sterile seawater, and in the presence of both material and metal ions. All experiments were conducted in triplicate using  $30 \pm 3$  *Artemia* under identical conditions, and the percentage of mortality was calculated considering the standard deviations using the formula: mortality percentage = (observed mortality – control mortality)/(total number of *Artemia* – control mortality)  $\times 100$ . (Table S6†)

### **Lithium extraction studies from sea bittern.**

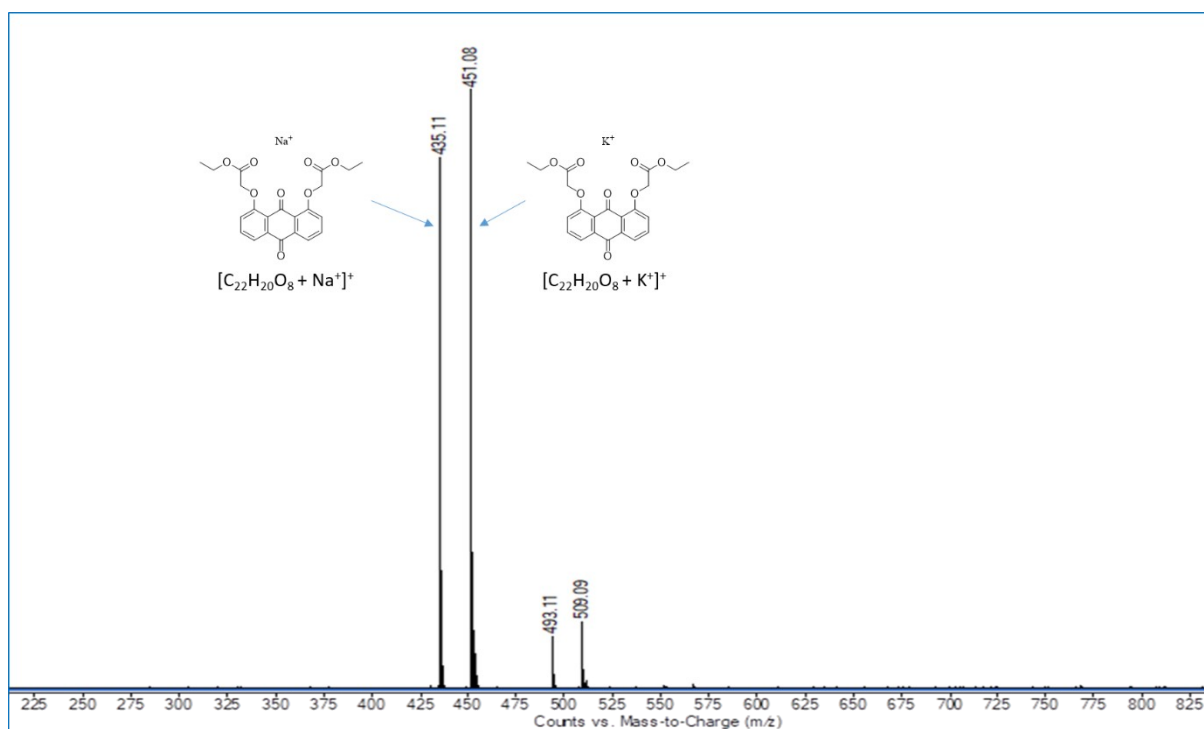
The lithium adsorption experiment from sea bittern was scaled up, using 4 L of sea bittern with a density of 33.13 °Bé (Specific Gravity 1.296). The bittern was filtered and treated with 0.5 g of the material in a 5-liter flask, then stirred overnight (~12 h). The resulting suspension was centrifuged in batches, and the lithium-adsorbed material was recovered. The material was then washed three times with Milli-Q water before lithium stripping. It was then treated with 10 mL of 0.5 N HCl, stirred for 1 hour, centrifuged, and washed with Milli-Q water. The aqueous part was collected in a conical flask and heated on a hot plate to reduce the volume to 5 mL. A saturated  $\text{Na}_2\text{CO}_3$  solution (~ 1.5 g in 5 mL) was added to the heated solution near boiling, resulting in the precipitation of  $\text{Li}_2\text{CO}_3$ , which was then hot filtered. The obtained  $\text{Li}_2\text{CO}_3$  (~ 80 mg) was dried and characterized using powder XRD, with a purity of ~ 98% assessed through ICP-MS analysis.



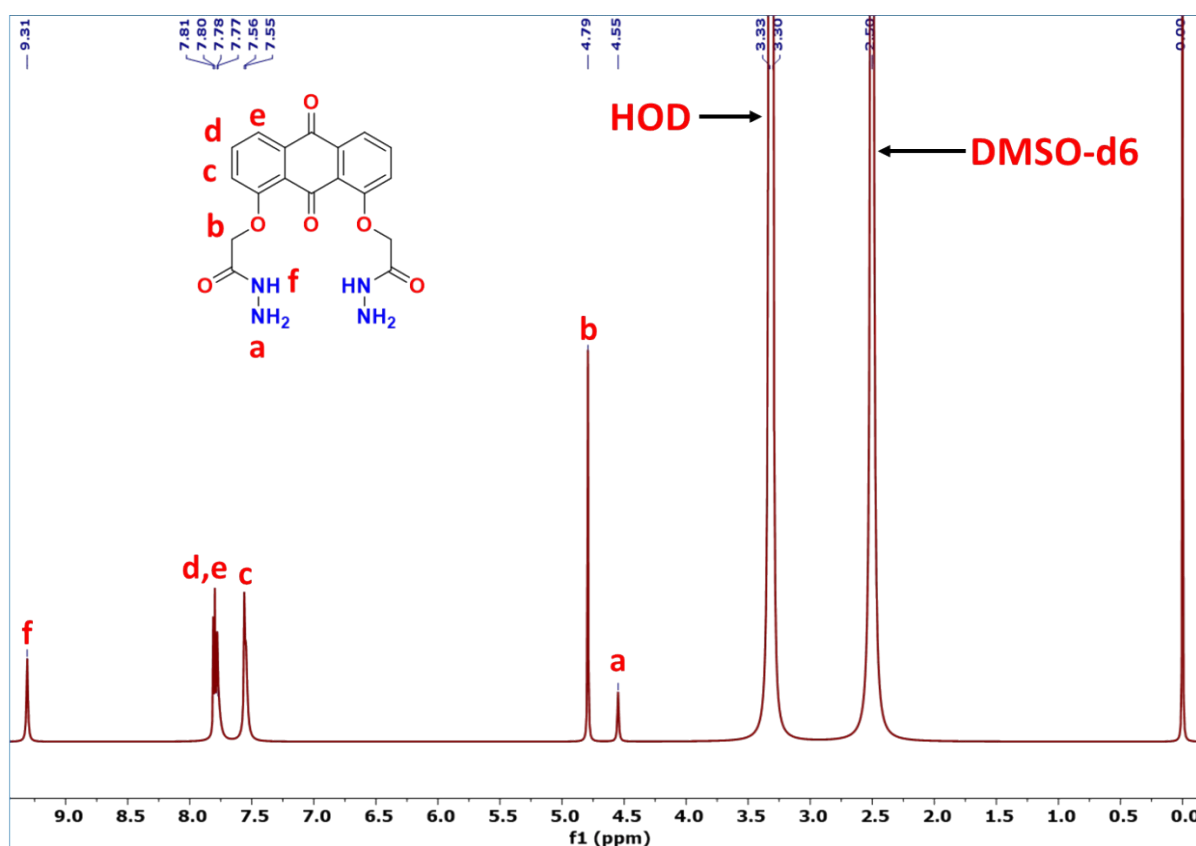
**Fig. S1** <sup>1</sup>H NMR of 2,2'-((9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)bis(oxy)diacetate) at 600 MHz in CDCl<sub>3</sub> solvent.



**Fig. S2** <sup>13</sup>C NMR of 2,2'-((9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)bis(oxy)diacetate) at 600 MHz in CDCl<sub>3</sub> solvent.



**Fig. S3** LC-MS of 2,2'-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)bis(oxy)diacetate).



**Fig. S4**  $^1\text{H}$  NMR of DAAH at 600 MHz in  $\text{DMSO-d}_6$  solvent.

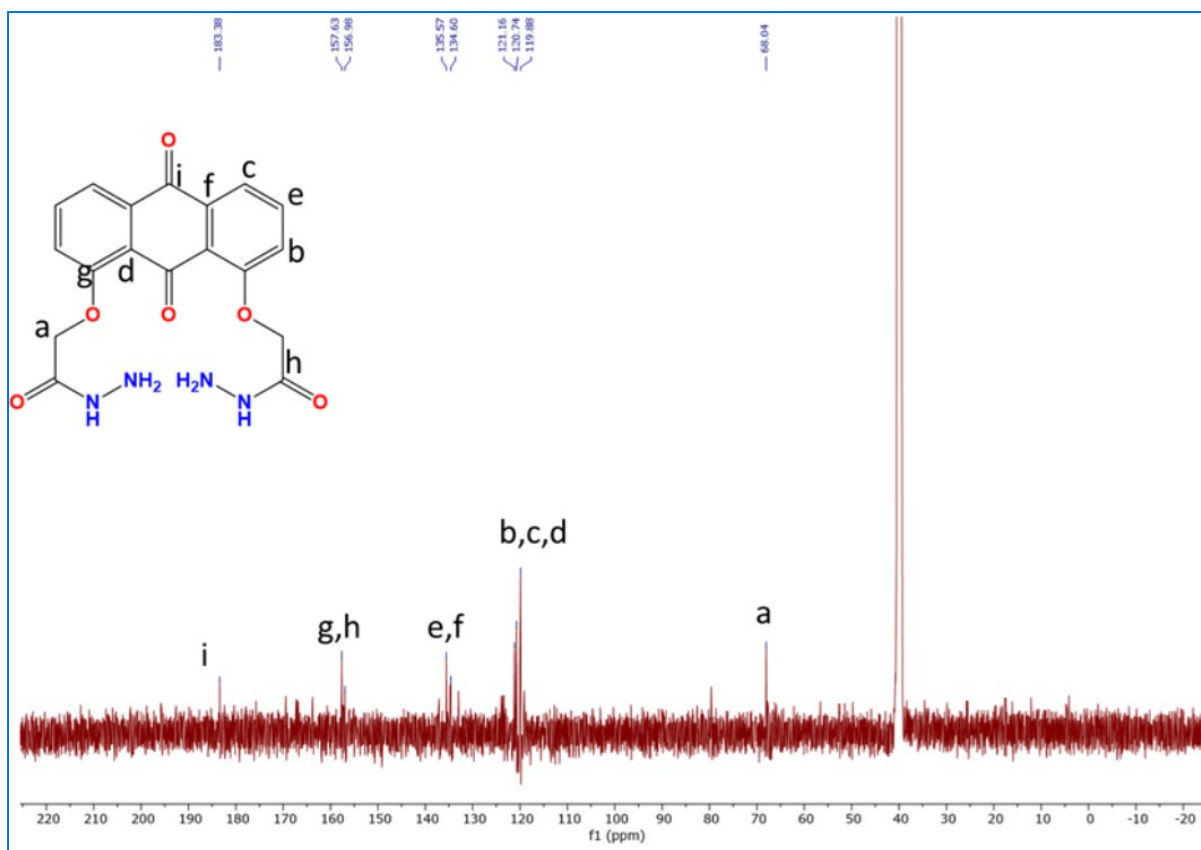


Fig. S5  $^{13}\text{C}$  NMR of DAAH at 600 MHz in DMSO- $d_6$  Solvent.

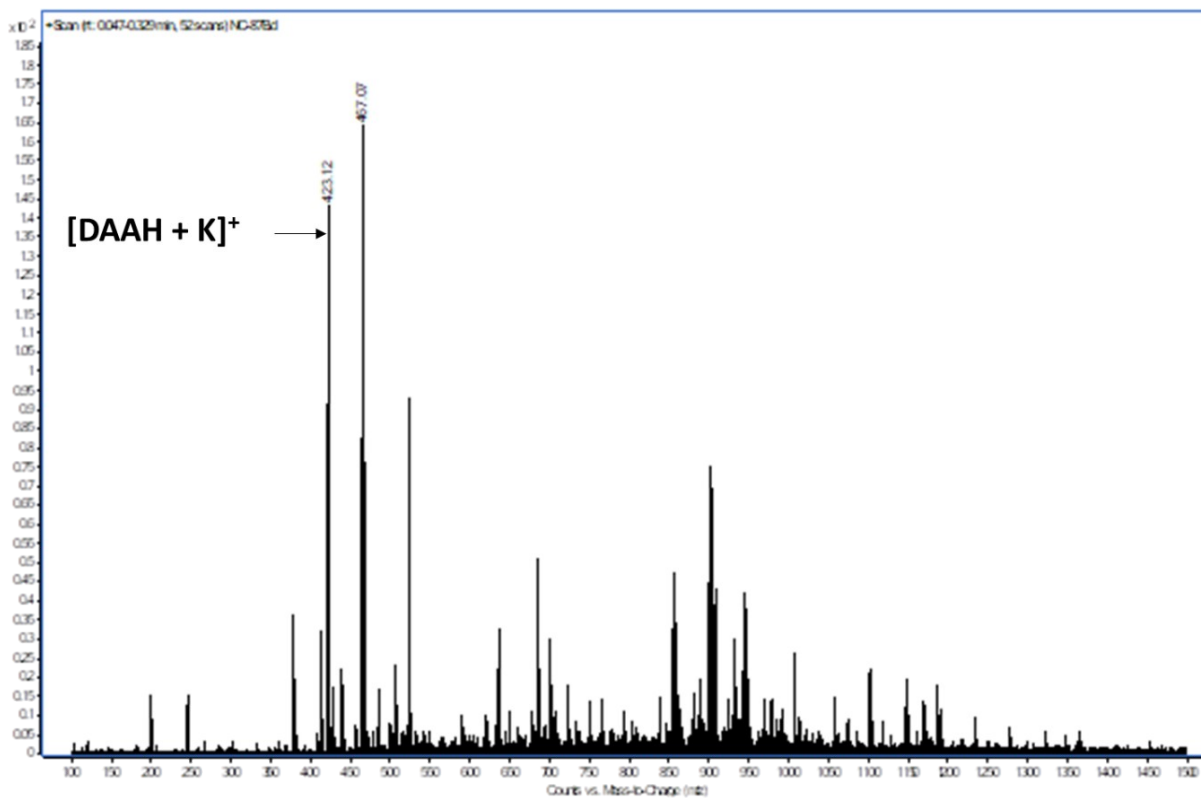
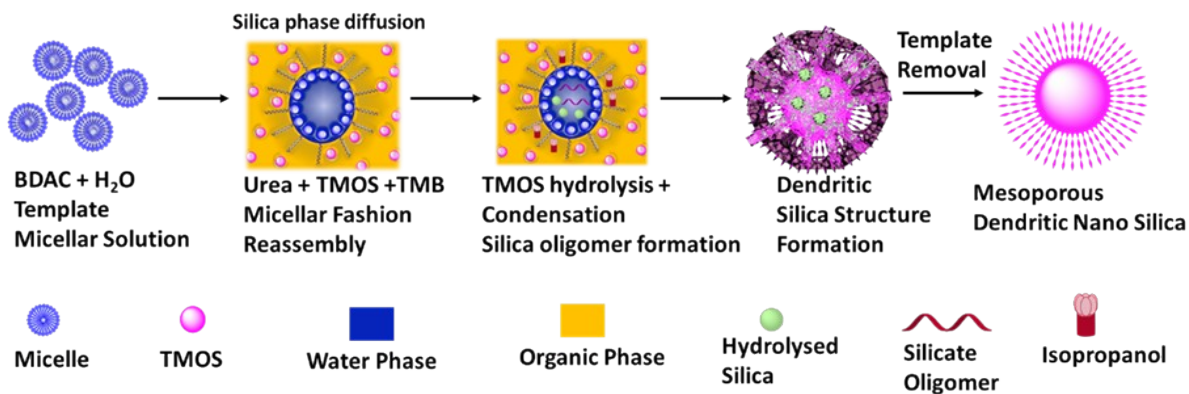
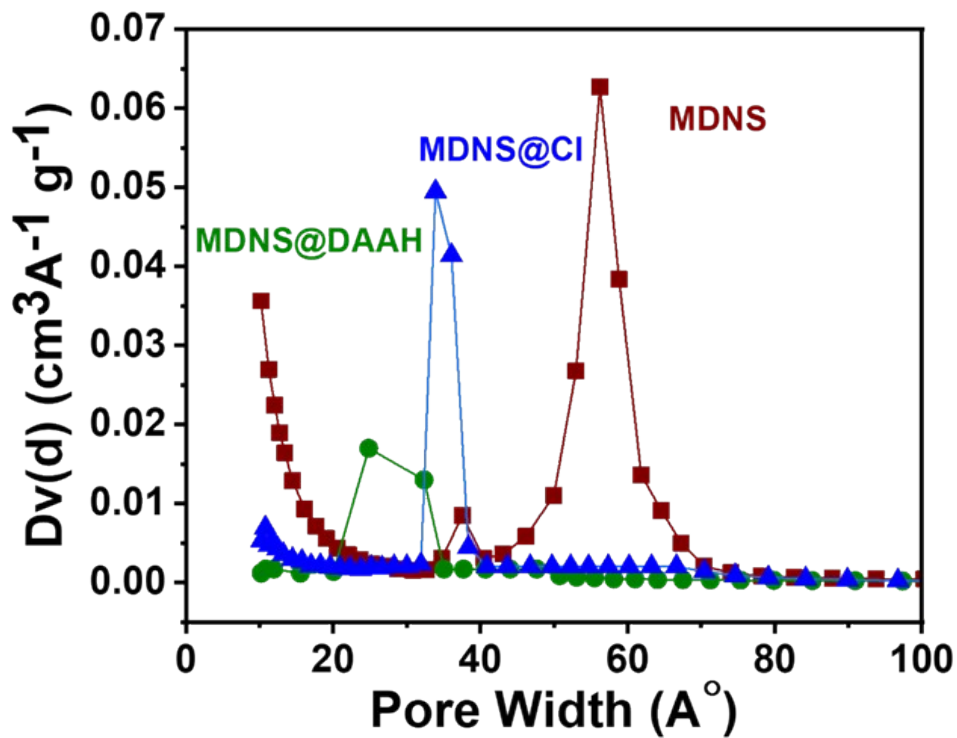


Fig. S6 LC-MS spectrum of DAAH.





**Fig. S7** The schematic representation of the proposed formation of mesoporous dendritic nano-silica.



**Fig. S8** The pore size distribution of the synthesized materials.

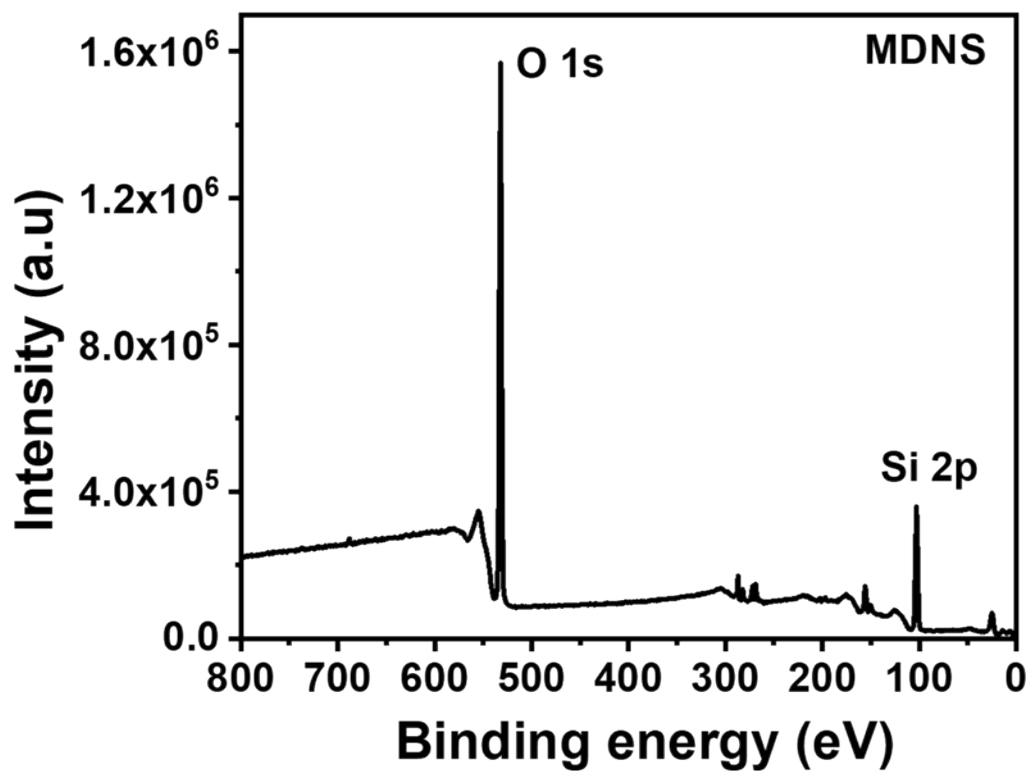


Fig. S9 The Full scan XPS spectra of the synthesized mesoporous dendritic Nano silica (MDNS).

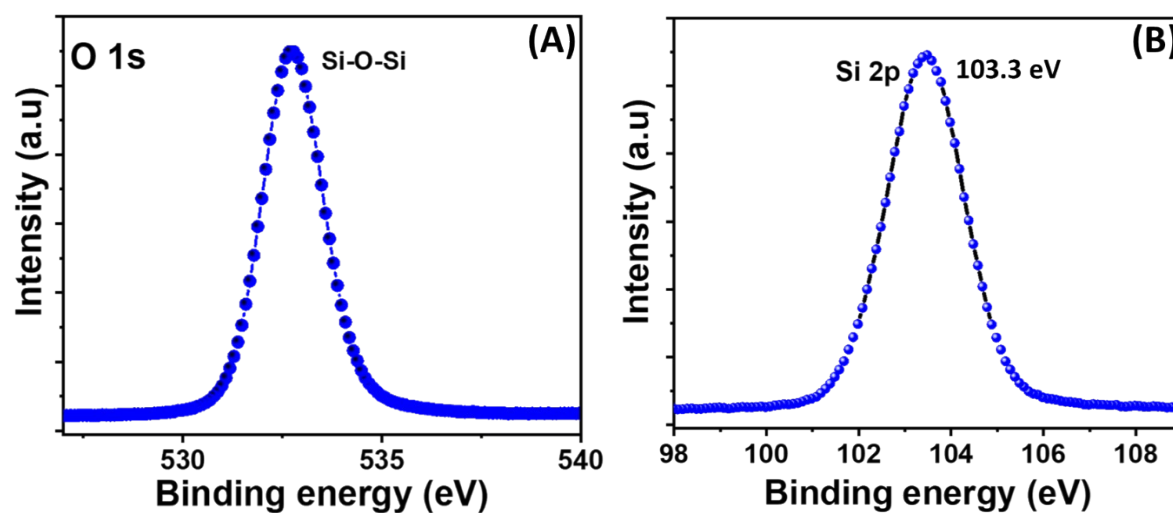


Fig. S10 (A, B) The O 1s and Si-2p XPS spectra of the intermediate material MDNS@Cl.

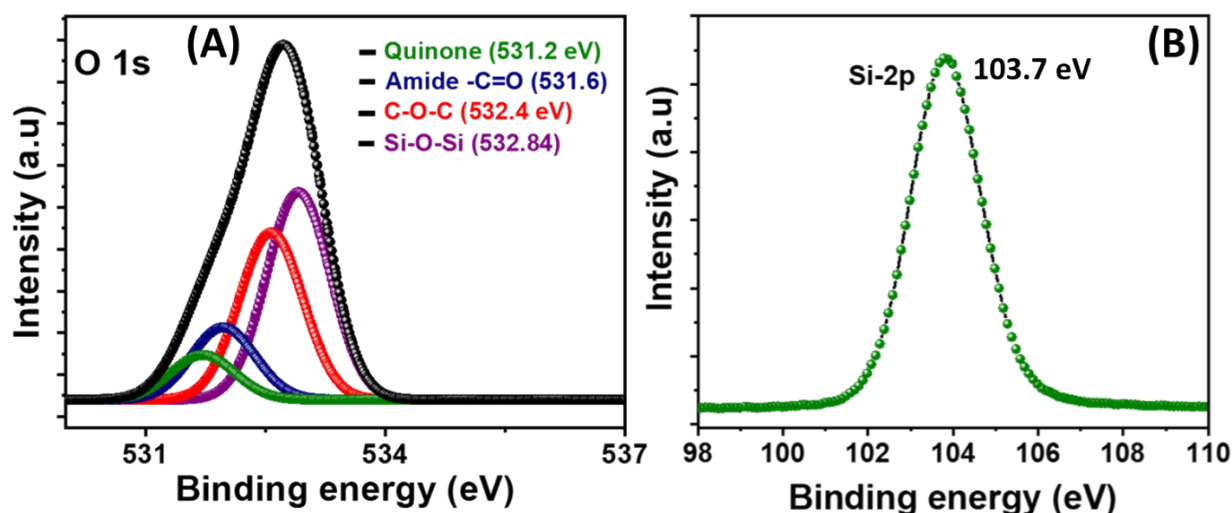


Fig. S11 (A, B) The O 1s and Si-2p XPS spectra of the final material MDNS@DAAH.

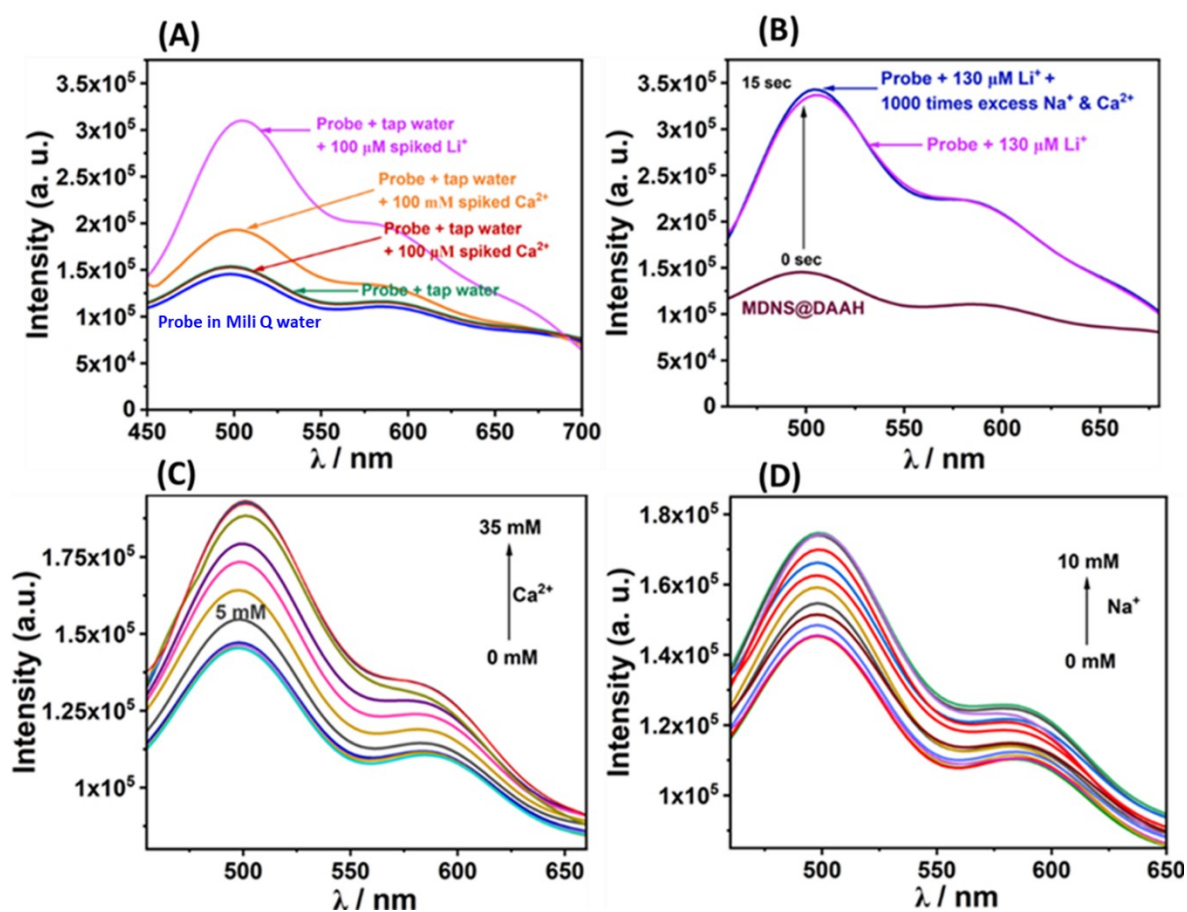
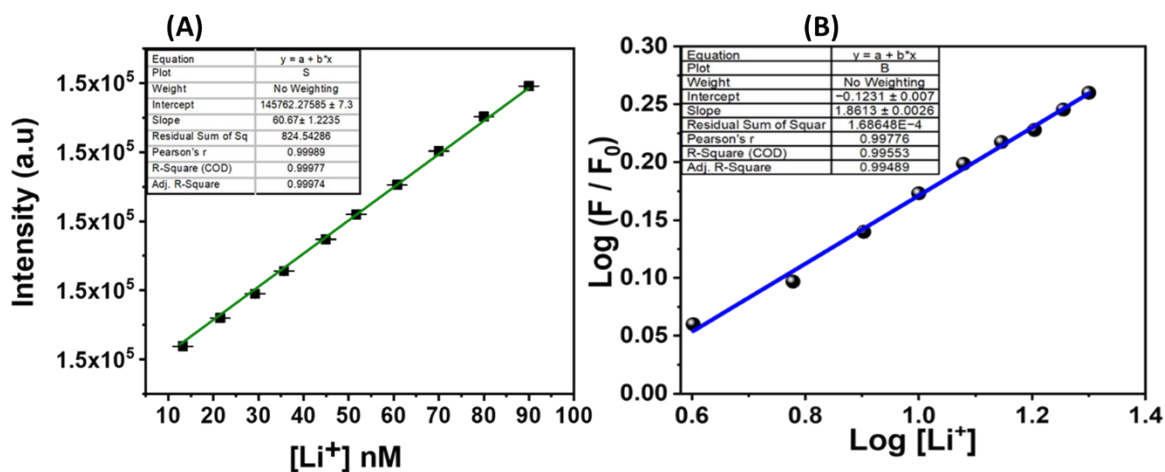


Fig. S12 (A, B) The Fluorescence interference and response behaviour of the material towards  $\text{Li}^+$  ions in tap water and pure aqueous solution. (C, D) The fluorescence titration with the  $\text{Ca}^{2+}$  and  $\text{Na}^+$  ions at saturation concentration.



**Fig. S13** The Linear range plot (A) and the Scatchard plot (B) of the material towards  $\text{Li}^+$  ions.

### Computational methodology:

The conformational search was performed using the *Spartan'08* software to get the lowest energy conformation.<sup>1</sup> The resulting geometries were optimized at B3LYP functional<sup>2</sup> with Grimme's third-generation dispersion<sup>3</sup> and using Ahlrich's double zeta basis set with a polarization function Def2-SVP.<sup>4</sup> All geometry optimization calculations were performed with the Gaussian09 program.<sup>5</sup> The geometries were optimized in the presence of the Truhlar and co-workers' SMD solvation model with water as solvent.<sup>6</sup> Harmonic vibration frequency calculations were performed for all geometries to confirm the minima on their potential energy surface. The average binding energy and Gibbs free energy of the  $\text{LiH}_2\text{O}$  and  $\text{LiCl}$  binding were calculated with the following equation,

$$\Delta E \text{ or } \Delta G = \frac{E \text{ or } G_{\text{complex}} - (E \text{ or } G_{\text{comp}} + nE \text{ or } G_{\text{Li} + \text{H}_2\text{O}/\text{Cl}})}{n}$$

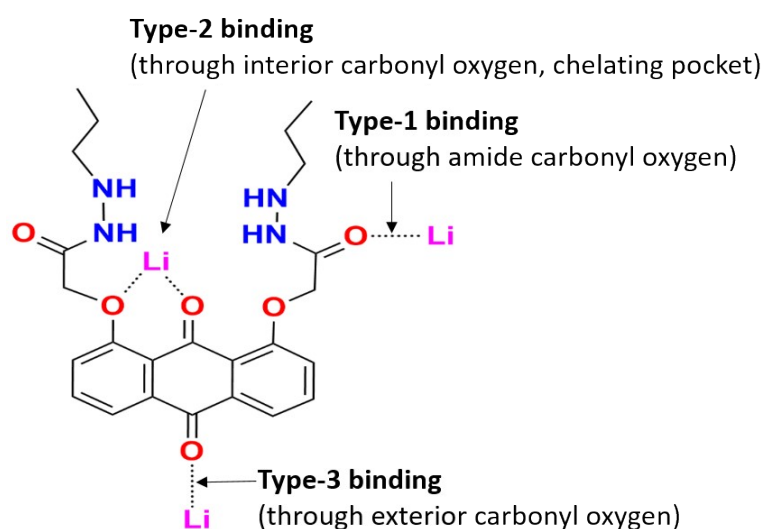
Where in binding energy calculations  $E_{\text{complex}}$  is the electronic energy of the complex, the  $E_{\text{comp}}$  is the electronic energy of the individual compound, the  $E_{\text{Li}+\text{H}_2\text{O}/\text{Cl}}$  is the sum of the electronic energy of the  $\text{Li}^+$  ion and  $\text{H}_2\text{O}$  or  $\text{Cl}^-$  and  $n$  is number of  $\text{Li}^+$  ion,  $\text{H}_2\text{O}$  or  $\text{Cl}^-$  bound to the complex.

In the case of binding Gibbs free energy calculations,  $G_{\text{complex}}$  is the free energy of the complex,  $G_{\text{comp}}$  is the free energy of the individual compound, the  $G_{\text{Li}+\text{H}_2\text{O}/\text{Cl}}$  is the sum of the electronic

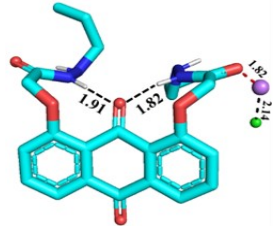
energy of the  $\text{Li}^+$  ion and  $\text{H}_2\text{O}$  or  $\text{Cl}^-$  and  $n$  is number of  $\text{Li}^+$  ion,  $\text{H}_2\text{O}$  or  $\text{Cl}^-$  bound to the complex.

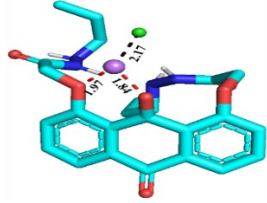
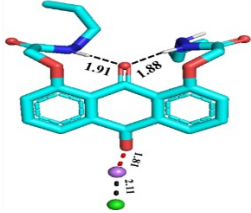
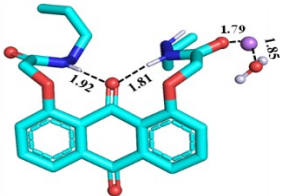
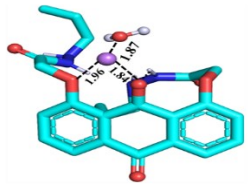
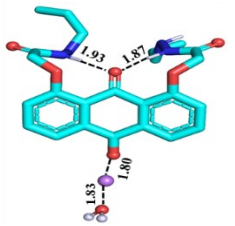
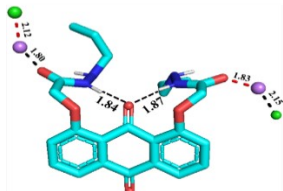
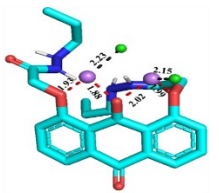
The frontier molecular orbitals (FMOs) were examined for the optimized geometries at a similar level of theory. The HOMO-LUMO band gaps were calculated using the following equation,

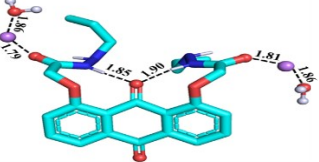
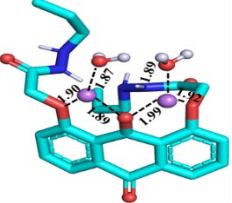
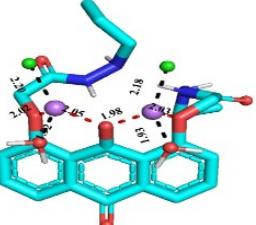
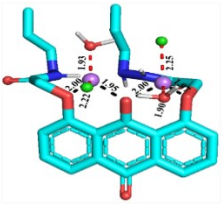
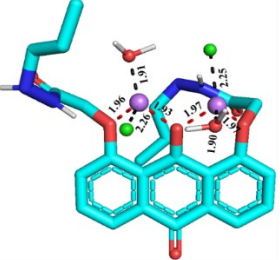
$$\Delta E = E_{LUMO} - E_{HOMO}$$



**Table S1.** The average binding energies ( $\Delta E$ ) and Gibbs free energies ( $\Delta G$ ) in kcal/mol for various probable lithium complexes.

Entries	Complexes	$\Delta E$	$\Delta G$
1	DAAH@1Li@1Cl-Type1 	-26.0	-14.2
2	DAAH@1Li@1Cl-Type2	-34.5	-21.0

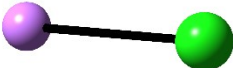


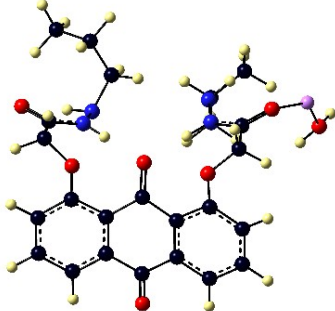
			
3	DAAH@1Li@1Cl-Type3 	-18.1	-9.2
4	DAAH@1Li@1H2O-Type1 	-49.3	-30.3
5	DAAH@1Li@1H2O-Type2 	-56.5	-33.5
6	DAAH@1Li@1H2O-Type3 	-41.8	-23.4
7	DAAH@2Li@2Cl-Type1 	-24.7	-14.1
8	DAAH@2Li@2Cl-Type2 	-34.0	-20.9
9	DAAH@2Li@2H2O-Type-1	-47.8	-27.6

			
10	DAAH@2Li@2H <sub>2</sub> O-Type-2	-53.9	-30.5
			
11	DAAH@2Li@2Cl@2H <sub>2</sub> O-Type2- mode1 [syn(arms)-syn(LiCl)]	-49.0	-25.9
			
12	DAAH@2Li@2Cl@2H <sub>2</sub> O-Type2- mode2 [syn(arms)-anti(LiCl)]	-55.4	-30.8
			
13	DAAH@2Li@2Cl@2H <sub>2</sub> O-Type2- mode3 [anti(arms)-anti(LiCl)]	-57.0	-32.1
			
14	DAAH@2Li@4H <sub>2</sub> O-Type2-mode1 (syn)	-75.2	-40.8





C	0.70874300	-4.32746000	-0.14982200
C	0.40659000	-3.04675300	-0.63795800
H	-5.91275000	1.02038400	0.54317700
H	-5.08951800	-1.04241400	1.70887500
H	-4.55686400	2.06416900	-1.23280400
H	0.14922600	-5.92097400	1.18375400
H	1.57625300	-4.86284200	-0.53516600
O	-0.11491500	-0.18665600	-0.88628200
O	-3.45186300	-2.82304700	2.21317500
O	1.13573500	-2.46327400	-1.63103900
O	-2.17582000	1.15406500	-2.08013400
C	2.54825600	-2.63480600	-1.66895300
H	2.87127200	-2.24212200	-2.64446200
H	2.85998200	-3.68801500	-1.61319700
C	-2.18817000	2.54464000	-2.38440800
C	3.28804500	-1.86302000	-0.57853800
C	-1.35569300	3.36825700	-1.40982200
C	3.54440400	1.27043100	0.59011600
H	2.65309900	1.79276700	0.21101500
H	3.85150100	1.80123100	1.50620500
C	4.66893300	1.33191500	-0.44756900
H	4.76251300	2.38243800	-0.77410000
H	4.36796200	0.76121800	-1.34419900
C	6.01806800	0.83024700	0.06588100
H	6.34222300	1.40043000	0.95321300
H	5.96858400	-0.23382300	0.34425200
H	6.80217700	0.93153500	-0.70199300
C	0.22357100	2.95167200	1.50341500
H	-0.83931800	3.13923500	1.75862700
H	0.39195500	1.86654700	1.59702400
C	1.13450500	3.69997000	2.47121800
H	2.18545600	3.46371700	2.23271500
H	0.94537000	3.29609900	3.48001100
C	0.92868300	5.21592500	2.48272100
H	1.20233900	5.67842400	1.51970200
H	-0.12354600	5.47331000	2.69155400
H	1.55107200	5.69280900	3.25671400
O	4.43673300	-2.19490200	-0.25692100
O	-1.53431900	4.58888100	-1.29773200
N	2.61207300	-0.84280700	-0.03180700
N	3.11492000	-0.06899400	1.02666000
N	-0.38971700	2.69129000	-0.77291100
N	0.50232800	3.32079600	0.10600400
H	-0.26221100	1.68189200	-0.90826800
H	0.34970400	4.32378400	-0.02135000
H	1.65937800	-0.61815400	-0.33731800
H	3.90893800	-0.58688500	1.40816700
H	-3.19778800	2.97637700	-2.42742500
H	-1.74465900	2.63646600	-3.38705800
<b>LiCl</b>			

<p>Electronic Energy (EE) = -467.693901 Hartree  EE + Thermal Free Energy Correction = -467.713434 Hartree</p> <table border="0"> <tr> <td>Li</td> <td>0.00000000</td> <td>0.00000000</td> <td>-1.78143200</td> </tr> <tr> <td>Cl</td> <td>0.00000000</td> <td>0.00000000</td> <td>0.31437000</td> </tr> </table>	Li	0.00000000	0.00000000	-1.78143200	Cl	0.00000000	0.00000000	0.31437000																																																																																	
Li	0.00000000	0.00000000	-1.78143200																																																																																						
Cl	0.00000000	0.00000000	0.31437000																																																																																						
<p><b>Li<sup>+</sup></b></p> <p>Electronic Energy (EE) = -7.424990 Hartree  EE + Thermal Free Energy Correction = -7.437738 Hartree</p> <table border="0"> <tr> <td>Li</td> <td>0.00000000</td> <td>0.00000000</td> <td>0.00000000</td> </tr> </table>	Li	0.00000000	0.00000000	0.00000000																																																																																					
Li	0.00000000	0.00000000	0.00000000																																																																																						
<p><b>H2O</b></p> <p>Electronic Energy (EE) = -76.369891 Hartree  EE + Thermal Free Energy Correction = -76.366570 Hartree</p> <table border="0"> <tr> <td>O</td> <td>0.00000000</td> <td>0.00000000</td> <td>0.12156400</td> </tr> <tr> <td>H</td> <td>0.00000000</td> <td>0.75465500</td> <td>-0.48625700</td> </tr> <tr> <td>H</td> <td>0.00000000</td> <td>-0.75465500</td> <td>-0.48625700</td> </tr> </table>	O	0.00000000	0.00000000	0.12156400	H	0.00000000	0.75465500	-0.48625700	H	0.00000000	-0.75465500	-0.48625700																																																																													
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H	0.00000000	-0.75465500	-0.48625700																																																																																						
<p><b>DAAH@1Li@1H2O-Type1</b></p> <p>Electronic Energy (EE) = -1684.550358 Hartree  EE + Thermal Free Energy Correction = -1684.088585 Hartree</p> <table border="0"> <tr><td>C</td><td>-2.30855300</td><td>-4.37040200</td><td>0.20077800</td></tr> <tr><td>C</td><td>-1.11402700</td><td>-4.39804900</td><td>0.92144100</td></tr> <tr><td>C</td><td>-0.11032200</td><td>-3.47087600</td><td>0.63103800</td></tr> <tr><td>C</td><td>-0.30591900</td><td>-2.47578400</td><td>-0.35724900</td></tr> <tr><td>C</td><td>-1.50901000</td><td>-2.48587400</td><td>-1.10247500</td></tr> <tr><td>C</td><td>-2.50164700</td><td>-3.43442100</td><td>-0.81381900</td></tr> <tr><td>C</td><td>1.17624400</td><td>-3.55592200</td><td>1.38040500</td></tr> <tr><td>C</td><td>0.71832900</td><td>-1.40950200</td><td>-0.51249600</td></tr> <tr><td>C</td><td>2.10596300</td><td>-1.72456500</td><td>-0.08556800</td></tr> <tr><td>C</td><td>2.31290200</td><td>-2.72211900</td><td>0.89699600</td></tr> <tr><td>C</td><td>3.58185600</td><td>-2.94025300</td><td>1.43902300</td></tr> <tr><td>H</td><td>3.70807800</td><td>-3.70072300</td><td>2.21026500</td></tr> <tr><td>C</td><td>4.66616600</td><td>-2.19057200</td><td>0.98041200</td></tr> <tr><td>C</td><td>4.49418700</td><td>-1.23401600</td><td>-0.01877800</td></tr> <tr><td>C</td><td>3.22237500</td><td>-0.99664300</td><td>-0.56256100</td></tr> <tr><td>H</td><td>-3.09377400</td><td>-5.09885500</td><td>0.41398400</td></tr> <tr><td>H</td><td>-0.94435100</td><td>-5.13910400</td><td>1.70293500</td></tr> <tr><td>H</td><td>-3.42173600</td><td>-3.45703000</td><td>-1.39720100</td></tr> <tr><td>H</td><td>5.66294400</td><td>-2.35999500</td><td>1.39345200</td></tr> <tr><td>H</td><td>5.35588000</td><td>-0.67942500</td><td>-0.38976900</td></tr> <tr><td>O</td><td>0.41695100</td><td>-0.27837800</td><td>-0.90425700</td></tr> <tr><td>O</td><td>1.30892100</td><td>-4.32208900</td><td>2.32842200</td></tr> </table>	C	-2.30855300	-4.37040200	0.20077800	C	-1.11402700	-4.39804900	0.92144100	C	-0.11032200	-3.47087600	0.63103800	C	-0.30591900	-2.47578400	-0.35724900	C	-1.50901000	-2.48587400	-1.10247500	C	-2.50164700	-3.43442100	-0.81381900	C	1.17624400	-3.55592200	1.38040500	C	0.71832900	-1.40950200	-0.51249600	C	2.10596300	-1.72456500	-0.08556800	C	2.31290200	-2.72211900	0.89699600	C	3.58185600	-2.94025300	1.43902300	H	3.70807800	-3.70072300	2.21026500	C	4.66616600	-2.19057200	0.98041200	C	4.49418700	-1.23401600	-0.01877800	C	3.22237500	-0.99664300	-0.56256100	H	-3.09377400	-5.09885500	0.41398400	H	-0.94435100	-5.13910400	1.70293500	H	-3.42173600	-3.45703000	-1.39720100	H	5.66294400	-2.35999500	1.39345200	H	5.35588000	-0.67942500	-0.38976900	O	0.41695100	-0.27837800	-0.90425700	O	1.30892100	-4.32208900	2.32842200	
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O	0.41695100	-0.27837800	-0.90425700																																																																																						
O	1.30892100	-4.32208900	2.32842200																																																																																						

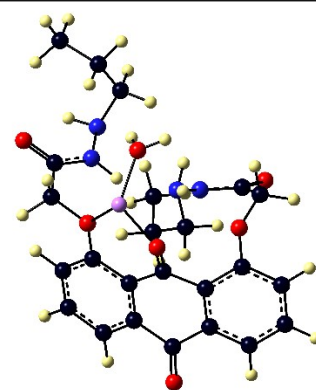
O	3.02605300	-0.12840200	-1.59415100
O	-1.61951200	-1.61623600	-2.14942600
C	3.77800700	1.07874100	-1.65562700
H	3.55319600	1.51953400	-2.63814900
H	4.86432800	0.91686800	-1.60133200
C	-2.87648200	-1.04646700	-2.48352400
C	3.39409000	2.08974300	-0.57694100
C	-3.23318700	0.13593100	-1.60102900
C	0.74676900	3.77460100	0.55420700
H	-0.11210300	3.27197700	0.08394500
H	0.36661300	4.24987600	1.47344100
C	1.30672100	4.84572000	-0.38516400
H	0.45472900	5.44819100	-0.74624400
H	1.73452200	4.35750600	-1.27869600
C	2.34390100	5.76187800	0.26396700
H	1.91929200	6.28494500	1.13780100
H	3.22427500	5.19393500	0.60178000
H	2.70129900	6.52762300	-0.44353300
C	-2.42308100	1.54152000	1.26187100
H	-3.19116800	0.77037100	1.47414800
H	-1.44481000	1.10618300	1.52126200
C	-2.68181400	2.78319800	2.11009500
H	-1.87407700	3.51379000	1.93779200
H	-2.60603100	2.47683100	3.16676000
C	-4.04202100	3.43936700	1.86524800
H	-4.12717600	3.84879800	0.84432200
H	-4.86258400	2.71789100	2.00436100
H	-4.20539200	4.27721600	2.56152700
O	4.19671100	2.96745000	-0.23761400
O	-4.41687400	0.54302300	-1.56626700
N	2.16417400	1.94199600	-0.06005200
N	1.67534100	2.72234100	1.00005600
N	-2.23096600	0.72732200	-0.96381900
N	-2.39078600	1.86863900	-0.17404700
H	-1.27179100	0.35396900	-1.03286500
H	-3.26679800	2.30988200	-0.45780000
H	1.55481600	1.17898300	-0.37155000
H	2.48969500	3.13876700	1.45600300
H	-3.71086500	-1.76066500	-2.44976200
H	-2.79067100	-0.68631100	-3.51997600
Li	-5.79460100	0.92748700	-0.48965100
O	-6.17498200	0.61587700	1.29667400
H	-6.71852000	1.21756000	1.83027900
H	-5.43519000	0.37550200	1.87826100

**DAAH@1Li@1H<sub>2</sub>O-Type2**

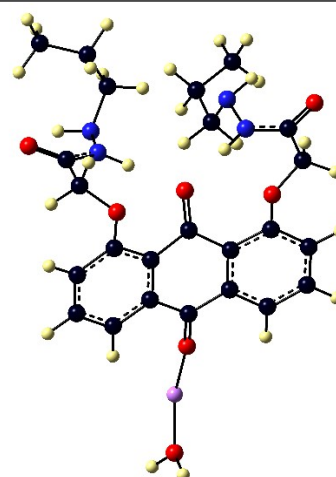
Electronic Energy (EE) = -1684.561873 Hartree

EE + Thermal Free Energy Correction = -1684.093689 Hartree

C	5.15026800	-1.49102900	0.25744600
C	4.95444300	-0.11096600	0.35068500
C	3.78649400	0.45627600	-0.16202200
C	2.82290200	-0.33930800	-0.82486800
C	3.01036400	-1.74093900	-0.86509900
C	4.17486100	-2.30168900	-0.32075900
C	3.51491700	1.89844600	0.08599700
C	1.63632000	0.30763000	-1.42752800
C	1.18303200	1.59137900	-0.84606200
C	2.10917800	2.36842000	-0.10568400
C	1.72929100	3.57202000	0.48712700
H	2.46847200	4.15299500	1.03894300
C	0.40285500	3.99415900	0.39301900
C	-0.53173400	3.24614200	-0.31913200
C	-0.14913600	2.06410100	-0.96999800
H	6.06000500	-1.94369500	0.65742200
H	5.68735100	0.53108800	0.84075400
H	4.30970400	-3.38365100	-0.36181400
H	0.08315800	4.91443000	0.88602500
H	-1.56421200	3.58772600	-0.35707800
O	1.04549200	-0.23468000	-2.36916100
O	4.38225000	2.65080600	0.51251800
O	-1.04360400	1.32566200	-1.69848100
O	2.04048800	-2.55021500	-1.39782800
C	-2.40916500	1.74154300	-1.84259400
H	-2.76728600	1.28503500	-2.77734800
H	-2.49759700	2.82902800	-1.96662800
C	1.47524700	-3.53003600	-0.51772500
C	-3.36365900	1.27534000	-0.75396600
C	0.76940500	-2.88656100	0.68073500
C	-4.14340600	-1.43726900	0.95633300
H	-3.22986700	-2.04273100	0.84015900
H	-4.63588200	-1.78366200	1.88014700
C	-5.07488300	-1.66195000	-0.23967900
H	-5.16732000	-2.75210000	-0.38709400
H	-4.60175900	-1.27087600	-1.15787500
C	-6.46285600	-1.04794000	-0.06363200
H	-6.96227700	-1.44851700	0.83482600
H	-6.40692800	0.04677400	0.03857100
H	-7.10838900	-1.26363400	-0.93024500
C	0.44062200	-0.22924100	2.14741500
H	0.93464100	-0.92640000	2.84830000
H	1.21832400	0.15960100	1.47824800
C	-0.19600700	0.92593600	2.91285200
H	-0.64766800	1.62643900	2.18937600



H	0.62156100	1.47596200	3.40931300
C	-1.23209600	0.49554800	3.95122800
H	-2.10061300	0.01235000	3.47666200
H	-0.79778400	-0.21480200	4.67519000
H	-1.60975600	1.36251100	4.51701000
O	-4.53710700	1.65703200	-0.82070500
O	0.88275100	-3.33188600	1.82019700
N	-2.89149200	0.45170200	0.19390400
N	-3.71339900	-0.05230200	1.21546500
N	0.03981400	-1.79170100	0.36739900
N	-0.54568800	-0.93546900	1.30438200
H	-0.12143700	-1.56101700	-0.60809000
H	-1.18519700	-1.47919000	1.88915400
H	-1.89947900	0.18952300	0.31052700
H	-4.52140400	0.56896900	1.28637700
H	2.22565700	-4.23319800	-0.12772400
H	0.74771600	-4.08975500	-1.12377600
Li	-0.70978800	-0.18632700	-2.90446800
O	-1.80879400	-1.57780900	-2.31217700
H	-2.36470700	-1.45781300	-1.52472700
H	-1.53767200	-2.50938900	-2.28868500
<b>DAAH@1Li@1H<sub>2</sub>O-Type3</b>			
Electronic Energy (EE) = -1684.538404 Hartree			
EE + Thermal Free Energy Correction = -1684.077587 Hartree			
C	-3.32958200	3.45577400	-0.33328400
C	-3.73834000	2.23051600	0.19530300
C	-2.97760400	1.08444500	-0.05379600
C	-1.77909500	1.15325200	-0.80859000
C	-1.40720300	2.39502300	-1.37566800
C	-2.18367300	3.53862300	-1.11980800
C	-3.45109400	-0.21117300	0.48089300
C	-0.91417500	-0.05318600	-0.89547700
C	-1.55961800	-1.37722300	-0.68804600
C	-2.76561600	-1.45078300	0.05323200
C	-3.32328500	-2.68590600	0.39690100
H	-4.24276800	-2.71940500	0.98124200
C	-2.69948200	-3.86342800	-0.01846800
C	-1.53566500	-3.81491000	-0.78166200
C	-0.96172000	-2.58033100	-1.13041000
H	-3.91924900	4.35594700	-0.14803100
H	-4.64651100	2.15273500	0.79303200
H	-1.89944700	4.49582300	-1.55591200
H	-3.13141000	-4.83208600	0.24114600
H	-1.07678000	-4.74178500	-1.12483100
O	0.30584900	0.03959500	-1.04723100
O	-4.42876000	-0.25545200	1.23559200
O	0.12204700	-2.49551000	-1.94802300



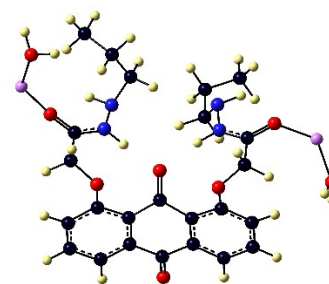
O	-0.35123500	2.41618000	-2.23075600
C	1.15666000	-3.47039100	-1.86461900
H	1.80713100	-3.28684200	-2.73240600
H	0.78737600	-4.50346100	-1.93505000
C	0.48351800	3.56621200	-2.32895300
C	2.00287300	-3.35242200	-0.59926700
C	1.50943700	3.64404900	-1.20559500
C	3.89526400	-1.12010600	1.01775700
H	3.62073900	-0.15243300	0.57196500
H	4.27034700	-0.90242700	2.03122400
C	4.99851600	-1.78290900	0.18824200
H	5.77585600	-1.02087300	0.00346400
H	4.59447700	-2.05058600	-0.80418700
C	5.62849600	-3.00836500	0.84954800
H	6.05705000	-2.75154200	1.83331400
H	4.88801900	-3.80891000	1.00076700
H	6.43875900	-3.42443200	0.22912500
C	2.12960600	2.11405800	1.72772700
H	1.31105200	2.83261800	1.93555900
H	1.67559900	1.11065900	1.68360100
C	3.16329400	2.16811600	2.84858600
H	3.95742500	1.42982800	2.64614900
H	2.66281400	1.83981100	3.77493400
C	3.77889600	3.55167200	3.06660200
H	4.36338600	3.88952200	2.19459500
H	2.99988100	4.30843600	3.26000100
H	4.46391400	3.54761000	3.92951300
O	2.64319100	-4.32874700	-0.19042300
O	2.09812600	4.70661800	-0.96054000
N	1.99071600	-2.14905400	-0.00645200
N	2.64945300	-1.88320700	1.20536400
N	1.76693000	2.48459900	-0.58632800
N	2.74265100	2.37895700	0.41549900
H	1.27820800	1.61921200	-0.84184100
H	3.21126800	3.28776000	0.43218600
H	1.42370800	-1.38473600	-0.38666600
H	2.85319900	-2.79146100	1.62732400
H	-0.07384200	4.51260200	-2.35529000
H	1.01967400	3.46896000	-3.28463200
Li	-5.82473100	-0.64823800	2.30199200
O	-7.58932300	-0.91507500	2.72539600
H	-7.87815100	-1.49988500	3.44402100
H	-8.28737700	-0.97951000	2.05413100

**DAAH@2Li@2H<sub>2</sub>O-Type-1**

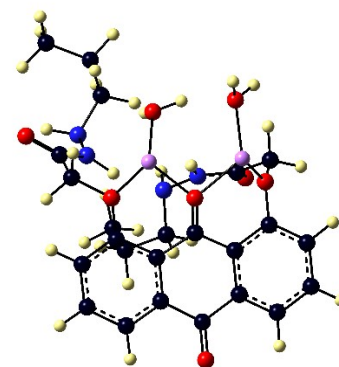
Electronic Energy (EE)= -1768.418994 Hartree

EE + Thermal Free Energy Correction = -1767.932665 Hartree

C	4.78471500	1.49482600	0.17416800
C	3.96957800	2.44528000	0.79009900
C	2.60078800	2.46833400	0.50915200
C	2.03045600	1.52599000	-0.37875800
C	2.88481300	0.62360100	-1.05363800
C	4.25457200	0.59492000	-0.75051900
C	1.75143800	3.50397300	1.16250700
C	0.55109300	1.42698300	-0.47040800
C	-0.23985800	2.63695700	-0.12883800
C	0.33093600	3.61417500	0.72250900
C	-0.42645000	4.69606500	1.17736800
H	0.03367500	5.42232800	1.84794300
C	-1.75201000	4.83536700	0.76326900
C	-2.32235100	3.90797600	-0.10689800
C	-1.57638000	2.80995700	-0.55986300
H	5.85280300	1.46084900	0.39978800
H	4.38058700	3.16989100	1.49365300
H	4.91184600	-0.12890800	-1.23151400
H	-2.34701600	5.68375900	1.10810800
H	-3.34828900	4.04586000	-0.44796400
O	-0.00079100	0.35234500	-0.72872100
O	2.21688700	4.26892600	1.99986100
O	-2.07302900	1.92726900	-1.47661000
O	2.33287900	-0.14661400	-2.03472100
C	-3.43700000	1.53950000	-1.42565800
H	-3.66371400	1.07451800	-2.39706200
H	-4.12880600	2.38375200	-1.29254300
C	2.85403400	-1.44304200	-2.28232500
C	-3.72762600	0.51089900	-0.34443800
C	2.55255700	-2.40095400	-1.14108600
C	-2.63701700	-2.44543100	0.71955900
H	-1.66951000	-2.50264600	0.19959200
H	-2.54811500	-3.08235100	1.61412800
C	-3.76247000	-2.96405500	-0.18024600
H	-3.42298000	-3.91004500	-0.63609000
H	-3.91261700	-2.26012100	-1.01831000
C	-5.07901900	-3.19560000	0.56101200
H	-4.97241700	-3.99010500	1.31827100
H	-5.41218900	-2.28423100	1.08461300
H	-5.88458300	-3.48702900	-0.13025500
C	0.83226600	-2.25804400	1.83972300
H	1.76270700	-1.72033300	2.11079400
H	0.04879100	-1.49880600	1.68915200
C	0.42631300	-3.20040500	2.96772100
H	-0.49778200	-3.72932600	2.67837300

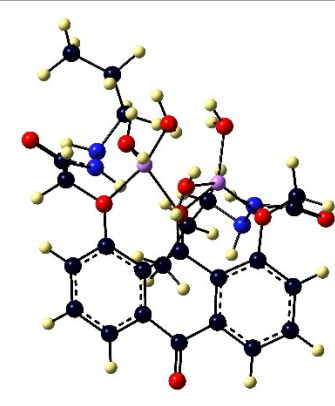


H	0.16869300	-2.57702000	3.84003300
C	1.50749300	-4.20778900	3.36256800
H	1.74321700	-4.90851100	2.54399800
H	2.44285900	-3.69542100	3.64448400
H	1.18640400	-4.81600700	4.22320400
O	-4.91109800	0.29678400	0.00352500
O	3.28857400	-3.39517600	-0.91752400
N	-2.68693800	-0.12081100	0.17950500
N	-2.78125100	-1.06367200	1.21273000
N	1.45126500	-2.15444500	-0.44840500
N	0.99095700	-2.98993000	0.57323300
H	0.87121900	-1.32855500	-0.65617000
H	1.68848300	-3.73102200	0.66879200
H	-1.73358900	0.08009800	-0.15519800
H	-3.69450100	-0.93259500	1.65201400
H	3.93592500	-1.44622600	-2.47730900
H	2.34817700	-1.80411500	-3.19010600
Li	-6.49747200	-0.21850800	-0.65461100
Li	5.08729700	-3.59170300	-1.04810300
O	6.36348400	-2.32867300	-1.53994300
O	-6.78531100	-1.59758800	-1.86944100
H	6.72209800	-1.68455400	-0.90828300
H	6.26454300	-1.83096600	-2.36767600
H	-5.97639200	-2.07168300	-2.12413400
H	-7.41519600	-2.30293000	-1.64892700
<b>DAAH@2Li@2H<sub>2</sub>O-Type-2</b>			
Electronic Energy (EE)= -1768.438617 Hartree			
EE + Thermal Free Energy Correction = -1767.941708 Hartree			
C	5.16072400	1.38961000	-0.72532300
C	5.02916500	0.03634900	-0.40594200
C	3.86110500	-0.42321400	0.20389600
C	2.82146300	0.46911100	0.55522700
C	2.95972400	1.82447500	0.18226900
C	4.12040500	2.27653400	-0.45222600
C	3.67685200	-1.88406900	0.40627800
C	1.63835600	-0.04025800	1.28667600
C	1.27627600	-1.45649200	1.09687400
C	2.27974900	-2.35457400	0.64036800
C	1.99079500	-3.68872700	0.36968600
H	2.79058000	-4.35110200	0.03784800
C	0.67534600	-4.14353100	0.48384200
C	-0.33208600	-3.29104100	0.92296900
C	-0.03920900	-1.96565900	1.27854600
H	6.07064900	1.75525300	-1.20515200
H	5.81698800	-0.67850700	-0.64638200
H	4.20032400	3.33057600	-0.72239800
H	0.42623900	-5.17398900	0.22300200

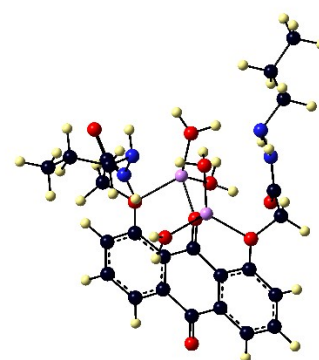




H	-1.35203700	-3.66623800	0.98118900
O	0.97791100	0.73363800	2.01560600
O	4.60595100	-2.67217400	0.29533400
O	-1.00375800	-1.13063500	1.76314400
O	1.93050800	2.71468400	0.42898700
C	-2.34722700	-1.57647200	2.02262300
H	-2.69635200	-1.00826300	2.89767700
H	-2.37886400	-2.63621100	2.30357800
C	1.32216500	3.33680100	-0.72584000
C	-3.35793900	-1.31225300	0.91865600
C	0.64246400	2.31826800	-1.64283100
C	-4.19209600	1.00554100	-1.30595000
H	-3.25926800	1.58488000	-1.39806300
H	-4.74273000	1.14317700	-2.25129100
C	-5.02862300	1.54351500	-0.14026900
H	-5.11082800	2.63651300	-0.27213900
H	-4.48510700	1.39383200	0.80884800
C	-6.42506500	0.93055300	-0.04488500
H	-6.99098400	1.08184500	-0.97976800
H	-6.37497600	-0.15148500	0.15091700
H	-7.00387500	1.38556600	0.77498200
C	0.31965100	-0.68083500	-2.25295500
H	0.88124500	-0.21114200	-3.08066700
H	1.04418200	-0.93460400	-1.46869100
C	-0.37772800	-1.94708100	-2.74185500
H	-0.87657000	-2.43446200	-1.88652100
H	0.40870300	-2.64194400	-3.08180300
C	-1.38322400	-1.71237300	-3.87028900
H	-2.24447100	-1.11995800	-3.52303700
H	-0.91744400	-1.17900700	-4.71627600
H	-1.77882300	-2.66724700	-4.25219500
O	-4.52784600	-1.65351100	1.13035200
O	0.73306200	2.39968700	-2.86390900
N	-2.93864400	-0.70573500	-0.19867200
N	-3.81593600	-0.41804600	-1.25822500
N	-0.04291800	1.34108900	-1.00444000
N	-0.64697100	0.26754500	-1.66437400
H	-0.24123600	1.41791500	-0.01197400
H	-1.25984200	0.64265200	-2.39287800
H	-1.95077700	-0.50304200	-0.43051800
H	-4.64376600	-1.00263800	-1.12776400
H	2.06554500	3.88627600	-1.31774000
H	0.58170900	4.04569400	-0.33066800
Li	-0.77547800	0.50929600	2.69787700
Li	1.21313100	2.69958300	2.20666300
O	-0.25982200	3.87223400	2.35618100
O	-1.97883800	1.74445300	1.96998100
H	-0.56793500	4.22123900	3.20954700
H	-2.30919200	1.55477200	1.07776700
H	-1.57101000	2.63615400	1.92536000

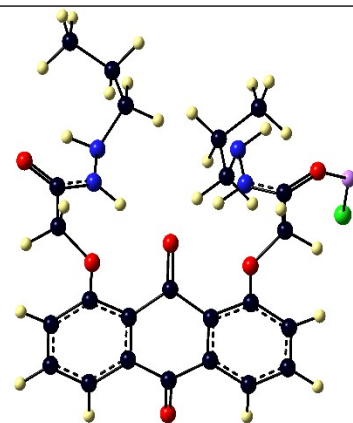
H	-0.29534600	4.63081700	1.74889700	
<b>DAAH@2Li@4H<sub>2</sub>O-Type2-model (syn)</b>				
Electronic Energy (EE) = -1921.246268 Hartree				
EE + Thermal Free Energy Correction = -1920.707818 Hartree				
C	-5.49185000	0.15659300	-0.44159600	
C	-4.86701600	1.38477600	-0.22977000	
C	-3.53411900	1.42939400	0.18189000	
C	-2.78958900	0.24554100	0.41605200	
C	-3.43951700	-0.99045600	0.15213400	
C	-4.77386700	-1.02287400	-0.26702900	
C	-2.89667800	2.76435800	0.31658000	
C	-1.38556400	0.33154300	0.89544300	
C	-0.70246400	1.64113900	0.91962100	
C	-1.43675900	2.81888400	0.60745500	
C	-0.83295800	4.07387600	0.58471300	
H	-1.43518600	4.94832500	0.33967100	
C	0.52663400	4.19303500	0.86849600	
C	1.27137800	3.06946600	1.20430100	
C	0.67503500	1.79982200	1.25312100	
H	-6.53664400	0.11518500	-0.75540900	
H	-5.40020500	2.32193500	-0.39026100	
H	-5.24819900	-1.98803700	-0.44741100	
H	1.01547500	5.16839700	0.83152100	
H	2.33159200	3.18766400	1.41767700	
O	-0.80088700	-0.70637100	1.26609200	
O	-3.54608100	3.79208300	0.16464400	
O	1.41728200	0.70820000	1.59872500	
O	-2.76588500	-2.18778200	0.27369400	
C	2.76908400	0.84005800	2.06754800	
H	2.96034500	-0.05957600	2.67047600	
H	2.88965700	1.70679300	2.73137400	
C	-2.73319900	-3.03520300	-0.90205500	
C	3.82601300	0.87194700	0.97112600	
C	-2.24464200	-2.25334100	-2.12731500	
C	4.46320400	-0.63435000	-1.92754400	
H	3.48367300	-1.01784300	-2.25454800	
H	5.07020600	-0.51393900	-2.83960200	
C	5.13191600	-1.63834700	-0.98516900	
H	5.06572400	-2.63255900	-1.46002000	
H	4.54442300	-1.70676600	-0.05283100	
C	6.59032100	-1.31443800	-0.66370800	
H	7.19800400	-1.26651500	-1.58320500	
H	6.68068400	-0.34753700	-0.14519000	
H	7.03394500	-2.08089200	-0.00794900	
C	0.65960600	-0.21124200	-2.62331800	
H	0.98235000	-0.19361000	-1.56167200	
H	1.15804700	-1.07203300	-3.09597000	

C	1.09538500	1.09105000	-3.28659000
H	0.74425800	1.09826100	-4.33257000
H	2.19661400	1.08581400	-3.31907700
C	0.62684100	2.35011500	-2.55346500
H	-0.47169000	2.43440800	-2.51510200
H	0.99928400	2.35885100	-1.51705600
H	1.00235300	3.25848000	-3.05029100
O	5.01027500	1.00268800	1.29055900
O	-2.82249800	-2.32884400	-3.20726700
N	3.39282000	0.73938200	-0.29199400
N	4.24465700	0.72698900	-1.40541000
N	-1.17660200	-1.46969300	-1.86308700
N	-0.78699700	-0.41728200	-2.70043500
H	-0.76665800	-1.50168300	-0.92832900
H	-1.26009100	0.42137900	-2.35097700
H	2.40217800	0.67986900	-0.50644100
H	5.12788800	1.14013900	-1.09996000
H	-3.72388300	-3.45069900	-1.12608800
H	-2.04182500	-3.85145000	-0.65257700
Li	1.01661300	-1.18410400	1.61410000
Li	-1.52828900	-2.50693600	1.71950400
O	1.06649600	-1.92130700	3.36510200
H	1.48395200	-2.79326400	3.44576100
O	-0.26069400	-3.78957400	1.11621700
H	0.20278100	-4.24980000	1.83431000
H	0.46610900	-3.39944800	0.58460800
H	0.14058900	-2.07086500	3.66006400
O	-1.67336500	-2.37662000	3.62167600
H	-2.14086500	-1.61324800	3.99970400
O	1.86106400	-2.21689900	0.23414800
H	1.95986100	-1.85358800	-0.66067900
H	-1.91869900	-3.12776800	4.18685900
H	2.69301600	-2.68969800	0.40259600
<b>DAAH@2Li@4H<sub>2</sub>O-Type2-mode2 (anti)</b>			
Electronic Energy (EE) = -1921.260486 Hartree			
EE + Thermal Free Energy Correction = -1920.720399 Hartree			
C	-2.50356100	3.23058100	-3.14462400
C	-3.54255200	2.68313500	-2.38993200
C	-3.25672400	1.77107200	-1.37430300
C	-1.92245700	1.37998300	-1.09185800
C	-0.87952000	1.97019200	-1.86112200
C	-1.18154000	2.88164700	-2.88294400
C	-4.39620600	1.23255700	-0.57866900
C	-1.64525100	0.41938700	-0.00591100
C	-2.75463500	-0.05711900	0.85023600
C	-4.09043400	0.32134800	0.55918100
C	-5.15847400	-0.16885100	1.31224200

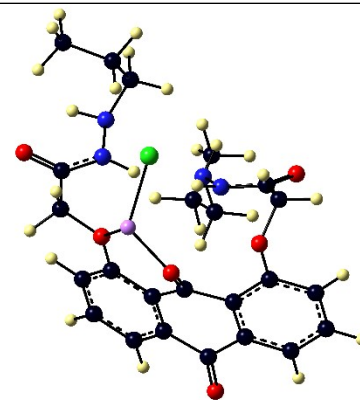


H	-6.17211600	0.13884200	1.05459800
C	-4.92163900	-1.03650100	2.38003800
C	-3.61991600	-1.42185200	2.68768400
C	-2.54226400	-0.95187000	1.92821200
H	-2.72261400	3.93497600	-3.94970000
H	-4.58020000	2.95718100	-2.58053500
H	-0.38062600	3.30575200	-3.48778200
H	-5.75345900	-1.40869900	2.98146900
H	-3.41995800	-2.08724300	3.52922200
O	-5.55191100	1.53809000	-0.84841900
O	-1.27013000	-1.32801500	2.30328600
O	0.41032200	1.61610700	-1.60209200
C	-0.92897600	-2.72939500	2.25630600
H	-1.79951500	-3.35211700	2.50612700
H	-0.14661500	-2.88554900	3.00890400
C	1.50368600	2.45661500	-1.99959400
C	-0.47319700	-3.08731500	0.84721700
C	2.69003100	2.20187100	-1.07467900
C	2.22191400	-4.91105000	-0.52606600
H	2.98843300	-4.83962000	0.26308400
H	1.58228700	-5.78138400	-0.29022700
C	2.88118800	-5.07644000	-1.88969900
H	3.50718700	-4.19035700	-2.09262100
H	2.09655200	-5.09141900	-2.66714200
C	3.72011200	-6.34976700	-1.97352100
H	4.52424400	-6.34776100	-1.21900700
H	3.10279500	-7.24691300	-1.80080100
H	4.18924400	-6.45203800	-2.96455700
O	-1.25697000	-3.02695600	-0.11421700
O	3.84149700	2.17672300	-1.51400300
N	0.81424200	-3.43864300	0.73646800
N	1.43708700	-3.66519300	-0.50230100
N	2.38478600	2.03594100	0.22505500
N	3.35784500	1.69180700	1.18024400
H	1.22116100	3.51832500	-1.91715200
H	1.80959400	2.23630300	-3.03166900
Li	0.29303700	-0.09743500	1.99478700
Li	0.72416900	-0.34934100	-1.29307500
C	3.75942600	2.82817700	2.02915100
H	4.44642100	2.41390700	2.78504200
H	2.86041600	3.17068300	2.56836400
C	4.41709000	3.99618000	1.29588600
H	5.30677500	3.62554400	0.75810200
H	3.72370000	4.38034400	0.52834000
C	4.80521100	5.12330700	2.25072200
H	5.52607900	4.77570800	3.00972600
H	5.26834300	5.96427000	1.71068200
H	3.92310400	5.51387900	2.78555400
H	1.42281900	1.99979500	0.56701400
H	4.16827200	1.35434900	0.65196400

O	-0.48876300	0.00256800	0.18640700
O	2.10256200	-0.65874900	1.92002800
H	2.23938300	-0.97789000	0.99998000
O	2.36398500	-1.15139000	-0.81792000
H	2.23439900	-2.14842000	-0.82574600
H	3.26466100	-0.96309700	-1.12161000
H	2.62734100	0.18778200	1.89246900
O	-0.45499100	-1.50006300	-2.27302600
H	-0.84995300	-2.08512500	-1.58504100
O	0.23021900	1.78349300	2.29814600
H	0.71394100	2.30622000	2.95658400
H	-0.03947300	-2.11497400	-2.89702400
H	-0.53018800	2.33035400	2.04507800
H	1.45459900	-3.31015300	1.51913700
H	0.68920200	-3.70832900	-1.20145200
<b>DAAH@1Li@1Cl-Type1</b>			
Electronic Energy (EE) = -2068.412211 Hartree			
EE + Thermal Free Energy Correction = -2067.971980 Hartree			
C	3.29917700	-3.34547500	0.37551400
C	2.25839700	-3.75077600	-0.46047800
C	0.99649600	-3.16603100	-0.32735000
C	0.76946000	-2.13890800	0.62035600
C	1.82343700	-1.77451000	1.49045700
C	3.08315300	-2.37671600	1.35422800
C	-0.10890300	-3.65342100	-1.20115000
C	-0.53127400	-1.41841300	0.59659400
C	-1.70362500	-2.13973000	0.03762300
C	-1.48915900	-3.17935200	-0.89859900
C	-2.56364300	-3.77775700	-1.56112000
H	-2.36863800	-4.56280000	-2.29211500
C	-3.86636900	-3.36826200	-1.27269300
C	-4.10433600	-2.37656600	-0.32259400
C	-3.03325100	-1.76160800	0.34391900
H	4.28745700	-3.80062000	0.28135000
H	2.40908400	-4.52495400	-1.21330500
H	3.89521400	-2.10186100	2.02694600
H	-4.71209500	-3.83604900	-1.78133600
H	-5.12913900	-2.09172700	-0.08554500
O	-0.61885900	-0.23760000	0.94633800
O	0.10347800	-4.45558200	-2.10392000
O	-3.22096800	-0.85646000	1.34399000
O	1.55021700	-0.89036400	2.49587500
C	-4.30403900	0.06354600	1.28962100
H	-4.37762300	0.50186200	2.29597900
H	-5.26999100	-0.41131700	1.06451600
C	2.54714500	0.04274900	2.89323400
C	-4.08980500	1.20052300	0.29495800



C	2.76395800	1.12010800	1.84358700
C	-1.73098700	3.47711200	-0.49364100
H	-0.78218800	3.07868600	-0.10271100
H	-1.46705800	4.13257500	-1.33983800
C	-2.44569100	4.28666700	0.59101800
H	-1.71217300	4.99577400	1.01309500
H	-2.72730900	3.61060300	1.41799100
C	-3.67440500	5.04871500	0.09457100
H	-3.40869300	5.74063100	-0.72296600
H	-4.44696700	4.36024800	-0.28129000
H	-4.13013900	5.64366200	0.90253100
C	1.71160600	1.77276100	-1.27256400
H	2.57369000	1.09194300	-1.41015600
H	0.79059700	1.17278900	-1.34832300
C	1.72177100	2.84895400	-2.35427200
H	0.83152700	3.49061600	-2.23601500
H	1.61076400	2.33610100	-3.32464700
C	2.99256100	3.70240700	-2.37400600
H	3.08494600	4.32303700	-1.46638200
H	3.89158000	3.06723100	-2.43620000
H	2.99086400	4.39182100	-3.23368500
O	-5.05530500	1.88037900	-0.08020900
O	3.85827500	1.73042600	1.77591800
N	-2.82807000	1.38696800	-0.11491900
N	-2.47358700	2.34721500	-1.07730600
N	1.72289300	1.39186100	1.06922700
N	1.72923700	2.37321500	0.07535800
H	0.85055100	0.84881300	1.15354600
H	2.57623700	2.92751400	0.21151800
H	-2.06404500	0.80103500	0.23789400
H	-3.35108600	2.67519600	-1.48619700
H	3.51847400	-0.41944800	3.11790500
H	2.17625400	0.51191900	3.81667900
Li	5.16423000	1.67478800	0.50895100
Cl	5.47347900	0.89088600	-1.45410800
<b>DAAH@1Li@1Cl-Type2</b>			
Electronic Energy (EE) = -2068.425835 Hartree			
EE + Thermal Free Energy Correction = -2067.982896 Hartree			
C	5.13077500	-1.36992700	0.56251000
C	4.92648000	0.01249600	0.57188400
C	3.79671800	0.54841500	-0.05011500
C	2.88664100	-0.28718500	-0.73717500
C	3.09159400	-1.68552200	-0.71687500
C	4.20897400	-2.21465900	-0.05504000
C	3.51035700	2.00330100	0.08915400
C	1.72536800	0.31514300	-1.42676600
C	1.22117600	1.60702000	-0.90726200

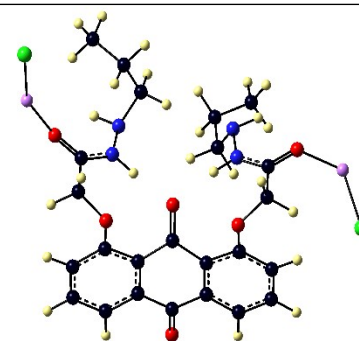


C	2.11426700	2.45050900	-0.20311400
C	1.69833800	3.69252000	0.27809600
H	2.41128600	4.32791100	0.80425900
C	0.37000300	4.08409800	0.10759400
C	-0.53871300	3.25818800	-0.55335300
C	-0.12073800	2.02759000	-1.08134500
H	6.00684900	-1.79619300	1.05591800
H	5.62182900	0.68158800	1.08039300
H	4.34920100	-3.29682700	-0.03794500
H	0.02597300	5.04153400	0.50407500
H	-1.57389200	3.58262200	-0.64762100
O	1.20985900	-0.24656700	-2.39811800
O	4.35300800	2.78583400	0.51131800
O	-0.98432100	1.18566400	-1.72567400
O	2.17541500	-2.51601600	-1.30507200
C	-2.35324500	1.55767700	-1.92376100
H	-2.74073500	0.86309900	-2.68427500
H	-2.43584700	2.57627800	-2.32701900
C	1.51161100	-3.44972600	-0.44124800
C	-3.27755600	1.42072300	-0.72320100
C	0.85077200	-2.74441100	0.74671000
C	-4.12665900	-0.96356400	1.53182300
H	-3.24016000	-1.54356800	1.83070100
H	-4.82531700	-0.99803500	2.38375200
C	-4.76106600	-1.61118900	0.29779500
H	-4.92680000	-2.67585400	0.53959300
H	-4.03260500	-1.59857200	-0.53208500
C	-6.07830700	-0.97082100	-0.13896300
H	-6.82124200	-0.98995800	0.67696100
H	-5.93453500	0.07856000	-0.43796100
H	-6.51421000	-1.50366800	-0.99963000
C	0.30722500	-0.03884300	2.09729100
H	1.07620800	-0.62644000	2.63073500
H	0.82635800	0.59034900	1.36495800
C	-0.45428500	0.84031600	3.08499600
H	-1.17786000	1.46242400	2.53223400
H	0.27733900	1.53283300	3.53433600
C	-1.17169800	0.06670400	4.19281400
H	-1.97826500	-0.57166400	3.79671300
H	-0.46938500	-0.58213600	4.74287800
H	-1.63332700	0.75422600	4.91951900
O	-4.38473900	1.97986100	-0.78519500
O	1.07892500	-3.07119900	1.91084400
N	-2.87926400	0.66952500	0.30563400
N	-3.72089000	0.44922800	1.41301400
N	0.04664200	-1.71339200	0.39751800
N	-0.60863100	-0.91988900	1.34858200
H	-0.35249100	-1.68842800	-0.54934000
H	-1.08793900	-1.54196000	2.00497200
H	-1.95447400	0.21577400	0.39551000

H	-4.54283500	1.03558400	1.25479300	
H	2.19895300	-4.21262000	-0.04665700	
H	0.74605200	-3.93148900	-1.06681900	
Li	-0.56537700	-0.36352700	-2.87369400	
Cl	-1.75649200	-2.10157800	-2.33144800	
<b>DAAH@1Li@1Cl-Type3</b>				
Electronic Energy (EE) = -2068.399708 Hartree				
EE + Thermal Free Energy Correction = -2067.963992 Hartree				
C	-2.90746900	3.53575500	-0.69751100	
C	-3.38462800	2.33595500	-0.16813300	
C	-2.65115200	1.16052300	-0.35392600	
C	-1.41210400	1.17505800	-1.04225900	
C	-0.96778500	2.39160400	-1.61112800	
C	-1.71868100	3.56479100	-1.42285900	
C	-3.19606000	-0.10808100	0.17898200	
C	-0.58221300	-0.05894100	-1.05337500	
C	-1.28110100	-1.35773300	-0.86035800	
C	-2.53249600	-1.37761000	-0.19485600	
C	-3.15318800	-2.58714400	0.12997700	
H	-4.10850300	-2.57998000	0.65446600	
C	-2.54693800	-3.79200300	-0.22897400	
C	-1.33455000	-3.79623100	-0.91445800	
C	-0.69635700	-2.58794000	-1.24178700	
H	-3.47584700	4.45816300	-0.56177200	
H	-4.32479800	2.29987200	0.38229800	
H	-1.37903600	4.50271900	-1.86132800	
H	-3.02947100	-4.74067000	0.01492100	
H	-0.88803300	-4.74427700	-1.21325900	
O	0.64694800	-0.00441600	-1.13323900	
O	-4.20772400	-0.10420200	0.88691600	
O	0.44467800	-2.55422000	-1.98240100	
O	0.14163100	2.36321800	-2.39795300	
C	1.44612800	-3.54864200	-1.79455700	
H	2.16368500	-3.40781400	-2.61636700	
H	1.05917300	-4.57556300	-1.86269100	
C	1.02671000	3.47999200	-2.42817400	
C	2.20211500	-3.41358300	-0.47506300	
C	1.86205400	3.59784700	-1.15765200	
C	3.98055800	-1.11732700	1.20780100	
H	3.69537000	-0.14454100	0.77904600	
H	4.31851100	-0.91514900	2.23746700	
C	5.12430000	-1.73317100	0.39743900	
H	5.89134500	-0.95111700	0.25902900	
H	4.75802900	-1.98118000	-0.61477900	
C	5.75714900	-2.96525700	1.04329100	
H	6.15032000	-2.72954700	2.04697100	
H	5.02700600	-3.78241900	1.14847700	



H	6.59406500	-3.34834600	0.43713200
C	1.97301200	2.21523100	1.86132100
H	1.24190900	3.04631800	1.93236300
H	1.39383800	1.28565900	1.74005900
C	2.80829200	2.13967600	3.13517700
H	3.47392000	1.26154600	3.07732900
H	2.11627400	1.95216000	3.97340100
C	3.62889200	3.39830300	3.42190900
H	4.40333900	3.57006500	2.65569600
H	2.98687000	4.29495600	3.45597600
H	4.14697500	3.31937500	4.39104700
O	2.80242000	-4.38870900	-0.00443200
O	2.37485500	4.67565700	-0.82964700
N	2.16051600	-2.20115600	0.09524700
N	2.75002900	-1.91742600	1.33864700
N	2.04725800	2.44535600	-0.49726000
N	2.82224400	2.36152100	0.66689400
H	1.61770700	1.57137900	-0.81947500
H	3.34220500	3.24012700	0.72110900
H	1.63852800	-1.43399900	-0.34054900
H	2.96209600	-2.82137500	1.76598000
H	0.51679300	4.43851100	-2.59906000
H	1.69983100	3.30237400	-3.27977700
Li	-5.65935300	-0.51997900	1.88651800
Cl	-7.75081000	-0.63826100	2.14783100
<b>DAAH@2Li@2Cl-Type1</b>			
Electronic Energy (EE)= -2536.143626 Hartree			
EE + Thermal Free Energy Correction = -2535.707656 Hartree			
C	4.81619800	1.59259900	0.08692200
C	4.00506200	2.56346700	0.67609800
C	2.63043900	2.56032300	0.42564300
C	2.05012300	1.56979100	-0.40319400
C	2.89885700	0.63800500	-1.04613300
C	4.27693100	0.64015000	-0.77778800
C	1.78682100	3.61623500	1.05287100
C	0.57028700	1.46354500	-0.46518400
C	-0.22152200	2.68331900	-0.16114500
C	0.35557400	3.69576100	0.64262900
C	-0.40455200	4.78519900	1.07480800
H	0.06134600	5.54017200	1.70873700
C	-1.74040300	4.89414200	0.68558900
C	-2.31730300	3.93183000	-0.14169100
C	-1.56684900	2.82899400	-0.57488200
H	5.88982600	1.58032100	0.28811500
H	4.42371600	3.32507600	1.33469200
H	4.93858800	-0.09869700	-1.23695700
H	-2.33889800	5.74629800	1.01484100
H	-3.35162600	4.04612000	-0.46566900



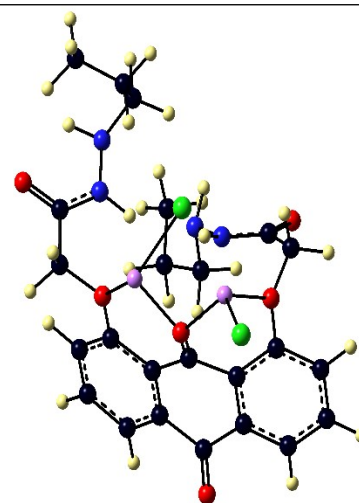
O	0.01435300	0.37899000	-0.66830500
O	2.26346800	4.42078200	1.84615600
O	-2.06686000	1.91392300	-1.45659400
O	2.33509700	-0.20124100	-1.96233300
C	-3.42628100	1.51599700	-1.37659700
H	-3.65252400	0.99652100	-2.32004500
H	-4.12626500	2.35956800	-1.28652000
C	2.85651800	-1.51714600	-2.10963400
C	-3.70262400	0.54760300	-0.23752000
C	2.57845700	-2.37081600	-0.88115100
C	-2.56361400	-2.32215300	1.01959900
H	-1.57628000	-2.40739600	0.54146800
H	-2.50363600	-2.89586300	1.95856400
C	-3.65497700	-2.90499700	0.11753400
H	-3.29553400	-3.87348800	-0.27123900
H	-3.78187400	-2.25469100	-0.76587900
C	-4.99638200	-3.10077500	0.82455100
H	-4.92866400	-3.88488900	1.59707200
H	-5.32482600	-2.17378400	1.32349400
H	-5.78812600	-3.37366400	0.11019900
C	0.97059300	-1.87687300	2.09781600
H	1.93007300	-1.34714000	2.26379600
H	0.21200800	-1.11088900	1.87286600
C	0.57153200	-2.64238700	3.35395300
H	-0.39364700	-3.14720500	3.17745100
H	0.39346800	-1.89710100	4.14723500
C	1.61416800	-3.65529900	3.82960600
H	1.76250700	-4.47163200	3.10299400
H	2.59234500	-3.17255500	3.99426900
H	1.30567600	-4.12170900	4.77884200
O	-4.88275700	0.34192800	0.12606400
O	3.32734400	-3.33043800	-0.57029800
N	-2.65338400	-0.04000200	0.32082100
N	-2.73617200	-0.91213700	1.41563100
N	1.48110300	-2.06726500	-0.20310800
N	1.05481200	-2.76838400	0.92936000
H	0.89447300	-1.26861200	-0.48439000
H	1.74664500	-3.50469600	1.08602100
H	-1.70384000	0.13939900	-0.03587300
H	-3.65635700	-0.76994400	1.83652000
H	3.93668500	-1.53660500	-2.32198900
H	2.33194600	-1.95443700	-2.97212500
Li	-6.42838800	-0.27983800	-0.56989700
Li	5.12855300	-3.50683700	-0.83524500
Cl	-7.36470500	-1.69608900	-1.84935600
Cl	6.51942900	-2.16300400	-1.78556800

**DAAH@2Li@2Cl-Type2**

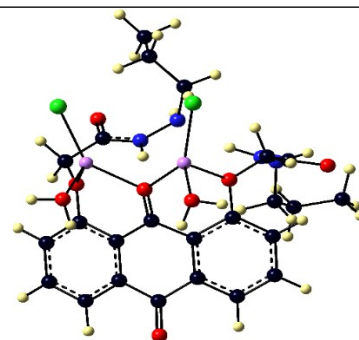
Electronic Energy (EE)= -2536.173073 Hartree

EE + Thermal Free Energy Correction = -2535.729381 Hartree

C	5.05435000	0.08566800	-1.44968200
C	4.76399400	-1.06923700	-0.71957700
C	3.59477700	-1.13269100	0.04120400
C	2.72599000	-0.02082800	0.12513000
C	3.00647800	1.11476400	-0.66519200
C	4.16751000	1.16224800	-1.44346500
C	3.21702000	-2.41538000	0.69418300
C	1.56258900	-0.07764500	1.03494700
C	0.98735000	-1.40082300	1.33674100
C	1.80150800	-2.54905400	1.15495600
C	1.29789300	-3.83046700	1.36827100
H	1.95367300	-4.69116200	1.23551700
C	-0.04651400	-3.99103700	1.70752300
C	-0.87151100	-2.88341100	1.88448600
C	-0.35989600	-1.58523200	1.74339000
H	5.96658300	0.14199900	-2.04701800
H	5.42482000	-1.93645800	-0.75051700
H	4.36793300	2.05366100	-2.04001600
H	-0.46592600	-4.99159800	1.83020300
H	-1.92121100	-3.04040200	2.12485800
O	1.10083800	0.97154900	1.51493300
O	4.00115800	-3.35229300	0.77028800
O	-1.14631900	-0.48354600	1.95021400
O	2.11597700	2.16741500	-0.70336600
C	-2.49094200	-0.61408900	2.44142300
H	-2.69024500	0.29302900	3.03289900
H	-2.59279900	-1.46279400	3.12894700
C	1.50097900	2.43454500	-1.98103300
C	-3.58060800	-0.67258700	1.38388700
C	0.65629100	1.25365000	-2.46804700
C	-4.31637200	0.77321800	-1.61388900
H	-3.39778500	0.90823000	-2.20707800
H	-5.13885200	0.64795100	-2.33705500
C	-4.55262400	2.01956000	-0.75613700
H	-4.55802200	2.88628400	-1.44029800
H	-3.68728500	2.17194900	-0.08847600
C	-5.85000300	1.99053800	0.05074600
H	-6.72623300	1.86256500	-0.60788700
H	-5.85287100	1.16394300	0.77755000
H	-5.98828500	2.92783700	0.61364400
C	-0.20626400	-1.65112500	-1.97564400
H	0.34343700	-1.61624600	-2.93338800
H	0.54085700	-1.73051000	-1.17643900
C	-1.12803500	-2.86632500	-1.94598900
H	-1.61805800	-2.92230700	-0.95919500



H	-0.48796500	-3.76120400	-2.02720700
C	-2.18014400	-2.88115300	-3.05626300
H	-2.90301000	-2.05787200	-2.93965900
H	-1.71184900	-2.78651400	-4.05078000
H	-2.75577500	-3.82072400	-3.04431000
O	-4.74723600	-0.82275200	1.77848200
O	0.73093300	0.84076100	-3.62245900
N	-3.24007400	-0.50690400	0.10245100
N	-4.21487100	-0.51939600	-0.91271100
N	-0.14085200	0.71055000	-1.51852600
N	-0.95869200	-0.40172600	-1.74999700
H	-0.35641200	1.25899800	-0.68246300
H	-1.54699700	-0.20451700	-2.56413400
H	-2.27079400	-0.49629400	-0.25967300
H	-5.09832200	-0.73701100	-0.44713200
H	2.25197300	2.65991300	-2.75015100
H	0.86353700	3.31576500	-1.82247700
Li	-0.65083800	1.38120700	2.06897800
Li	1.40199500	2.91069700	0.99948500
Cl	-0.97620300	3.11489400	0.69610100
Cl	2.66550400	4.20171700	2.18162100
<b>DAAH@2Li@2Cl@2H<sub>2</sub>O-Type2-model</b> <b>[syn(arms)-syn(LiCl)]</b>			
Electronic Energy (EE) = -2688.960957 Hartree EE + Thermal Free Energy Correction = -2688.478348 Hartree			
C	-3.25764600	2.89383800	1.50975400
C	-2.37345500	3.74425600	0.84321000
C	-1.11504000	3.27293800	0.47232600
C	-0.69900800	1.95902100	0.80589900
C	-1.61117400	1.11099000	1.48971500
C	-2.89124500	1.58589700	1.81865400
C	-0.22509100	4.17549700	-0.31383600
C	0.65985700	1.52138800	0.43822300
C	1.34172200	2.23344100	-0.66257100
C	0.94335400	3.55211300	-0.99424300
C	1.61024700	4.27499500	-1.98333300
H	1.28980000	5.29394200	-2.20266100
C	2.66454200	3.68356900	-2.68502100
C	3.05309700	2.37694100	-2.40054300
C	2.40167800	1.64905800	-1.39514100
H	-4.25238300	3.24775900	1.78841400
H	-2.65644300	4.76578600	0.58824800
H	-3.61170300	0.93805200	2.31417800
H	3.19021500	4.24550200	-3.45980700
H	3.87909700	1.91489900	-2.94325000
O	1.22511500	0.58295500	1.03727600
O	-0.48540500	5.36436000	-0.45155800
O	2.80175700	0.38083600	-1.08938800



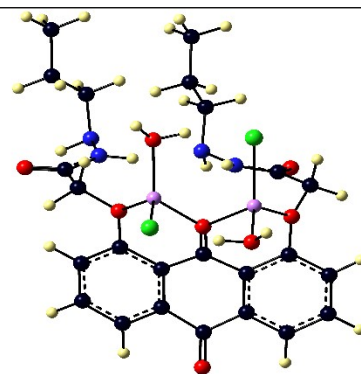
O	-1.20849200	-0.15295200	1.78919700
C	2.97669700	-0.59943000	-2.12171900
H	3.92838900	-1.11219100	-1.92528800
H	3.00235100	-0.13801700	-3.11810700
C	-2.17810900	-1.14752600	2.16573300
C	1.89159900	-1.66608600	-2.12291900
C	-3.20306100	-1.39576000	1.06311600
C	0.21734200	-3.56601400	0.04199000
H	0.31769800	-3.03629600	1.00238700
H	-0.69911200	-4.17648800	0.10414400
C	1.43957400	-4.46101900	-0.17065200
H	1.55837600	-5.05750900	0.75126500
H	2.34378000	-3.82982200	-0.23100000
C	1.33952400	-5.39209900	-1.37727400
H	0.45298700	-6.04527600	-1.30497100
H	1.26724400	-4.82343400	-2.31664000
H	2.22720000	-6.04101200	-1.45420100
C	-3.86576600	-0.48443600	-1.89532500
H	-4.28484300	0.21818400	-1.14706500
H	-2.93019400	-0.03540800	-2.26505500
C	-4.84910400	-0.65844700	-3.04790600
H	-4.40889100	-1.33999100	-3.79680100
H	-4.95934600	0.32148500	-3.54220200
C	-6.22686100	-1.17071800	-2.62311200
H	-6.18253900	-2.19676800	-2.22128800
H	-6.66724200	-0.52553500	-1.84406800
H	-6.92296200	-1.18965100	-3.47696700
O	1.89402600	-2.51269100	-3.02222900
O	-4.41528300	-1.40779400	1.30847900
N	0.97751200	-1.61479700	-1.14076300
N	-0.05866100	-2.54817000	-0.99503000
N	-2.68958000	-1.59466300	-0.16263000
N	-3.52241500	-1.77741800	-1.27743500
H	-1.68164000	-1.76642000	-0.33931000
H	-4.37963600	-2.21010200	-0.92691000
H	1.02238800	-0.90544200	-0.41627200
H	-0.19424600	-2.98567400	-1.90932100
H	-2.70407600	-0.86072000	3.08661200
H	-1.57866300	-2.04533400	2.37243000
Li	3.18492300	-0.01892400	0.86085000
Li	0.60107100	-0.24842700	2.71984500
Cl	4.33625100	-1.88612800	0.70062500
Cl	0.87055400	-2.27675600	3.48620700
O	0.49600500	1.29613900	3.88655900
H	-0.35720200	1.33231200	4.34820500
H	0.54001500	2.14541400	3.41914900
O	3.94418400	1.58688400	1.58699500
H	3.48282300	2.40339300	1.33696400
H	4.86981700	1.75444700	1.34916400

**DAAH@2Li@2Cl@2H<sub>2</sub>O-Type2-model**  
**[syn(arms)-anti(LiCl)]**

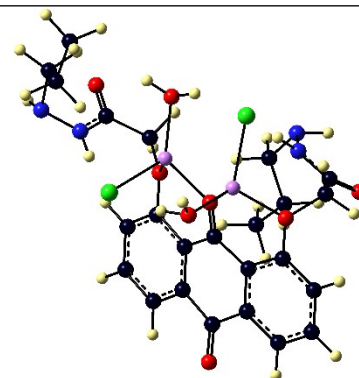
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EE + Thermal Free Energy Correction = -2688.494198 Hartree

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C	1.86683600	-4.18106300	-0.72517600
C	2.25112400	-2.85138600	-0.55766200
C	1.39842500	-1.90784400	0.07498300
C	0.13200700	-2.36124300	0.53862400
C	-0.25517900	-3.69502000	0.32689600
C	3.59788600	-2.45591000	-1.05995200
C	1.86531000	-0.51617500	0.24835900
C	3.02749500	-0.05561600	-0.55414100
C	3.90649100	-1.00439400	-1.13238000
C	5.05717500	-0.60357100	-1.81434600
H	5.71497300	-1.36610200	-2.23256300
C	5.34502000	0.75416500	-1.96088500
C	4.47504900	1.70708100	-1.43736500
C	3.32487800	1.31304200	-0.74461400
H	0.28630100	-5.62723500	-0.43810100
H	2.55561400	-4.87797800	-1.20248100
H	-1.23350500	-4.04751000	0.64759100
H	6.24634300	1.07310500	-2.48818600
H	4.67962500	2.77296900	-1.55131600
O	4.40045700	-3.29662000	-1.44790700
O	2.49379400	2.29057000	-0.24274500
O	-0.69121500	-1.48020500	1.17330200
C	1.83001700	3.12742800	-1.21162200
H	2.53377300	3.48917300	-1.97272800
H	1.42344900	3.97457400	-0.64248800
C	-2.00009200	-1.90283700	1.58297900
C	0.68725900	2.40649000	-1.92808500
C	-2.97847600	-2.15990300	0.44208500
C	-2.39319400	1.95248000	-1.88311000
H	-2.06568500	2.82146500	-2.48350000
H	-3.11239600	1.39100100	-2.49817500
C	-3.05119700	2.41859900	-0.58848200
H	-2.30865400	2.96211500	0.02032400
H	-3.34325900	1.53401800	0.00158900
C	-4.26546300	3.30787000	-0.84417200
H	-3.98583800	4.21843400	-1.40044600
H	-5.03108200	2.77996300	-1.43738000
H	-4.73543300	3.62448000	0.10048000
O	0.55475500	2.47698800	-3.15098900
O	-3.78873700	-3.08921500	0.53277400
N	-0.14047600	1.69964600	-1.12974800
N	-1.26731100	1.03119500	-1.62896100
N	-2.91786900	-1.31923500	-0.60322900



N	-3.76977300	-1.47326200	-1.71147000
H	-0.07498900	1.78294400	-0.11765600
H	-0.98255400	0.60198400	-2.51147000
H	-2.39411800	-1.07062400	2.17988100
H	-1.95017500	-2.79766500	2.21766900
Li	1.91745700	2.08631200	1.63372400
Li	-0.06069800	-0.03096600	2.39807400
C	-4.99631000	-0.66106100	-1.62745800
H	-5.59086000	-0.93487300	-2.51442100
H	-4.72028700	0.39572500	-1.75700700
C	-5.85172900	-0.80163900	-0.36668800
H	-6.15394300	-1.85494900	-0.24364800
H	-5.24319100	-0.54508800	0.51771100
C	-7.07949200	0.10650300	-0.41634100
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H	-7.69144800	0.00537200	0.49415000
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H	-2.20670000	-0.57734600	-0.69062600
H	-4.03194300	-2.46112400	-1.73009700
O	1.32919400	0.25149200	1.06504500
Cl	0.17369600	3.50728100	1.79222100
Cl	1.05861200	-0.21938800	4.31328400
O	3.12485600	1.65800000	3.03345600
H	3.31844600	2.37573900	3.65607000
O	-1.61203500	1.11620900	2.31234700
H	-2.11263900	1.19455100	3.13902300
H	-1.19733500	2.00654200	2.18404800
H	2.56983100	1.02108900	3.55762800
<b>DAAH@2Li@2Cl@2H<sub>2</sub>O-Type2-mode3</b> <b>[anti(arms)-anti(LiCl)]</b>			
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C	5.33830600	-0.23475100	-1.72747100
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C	3.45658400	1.23262400	-1.33825300
C	2.62535200	0.13239300	-1.00519000
C	3.20391600	-1.16094200	-1.04258100
C	4.54672700	-1.33129900	-1.40135800
C	2.92946400	2.62325600	-1.30822900
C	1.20297400	0.36300500	-0.64816600
C	0.74307600	1.74442300	-0.38425500
C	1.56520600	2.84043200	-0.75227000
C	1.13893800	4.15792400	-0.58237300
H	1.79855100	4.97109800	-0.88496700
C	-0.11611800	4.41653500	-0.03196500
C	-0.93405900	3.36455700	0.36825700
C	-0.51319400	2.03620500	0.21301200
H	6.38104500	-0.38479200	-2.01430200



H	5.39516600	1.92110400	-1.95279100
H	4.95861400	-2.34058400	-1.43638600
H	-0.46338300	5.44444500	0.09024000
H	-1.91504900	3.57496600	0.79321500
O	3.61257500	3.56606200	-1.69179600
O	-1.29638300	1.00991600	0.65106200
O	2.45353400	-2.27833300	-0.75544900
C	-2.18845700	1.19020500	1.75930700
H	-1.87840200	2.03429800	2.39069500
H	-2.11640100	0.27225700	2.35874400
C	2.91839100	-3.14477000	0.30472000
C	-3.65434500	1.34275900	1.39192900
C	2.76464200	-2.46064700	1.66397500
C	-5.97139300	-0.00755400	-0.14538200
H	-5.67217500	-0.47333100	0.81333700
H	-7.05878700	0.16276300	-0.08933100
C	-5.65236900	-0.94845900	-1.30336500
H	-4.56476100	-0.95149400	-1.48519000
H	-6.10799300	-0.54639200	-2.22514900
C	-6.13915700	-2.37261900	-1.04499900
H	-5.64458600	-2.80624600	-0.15826600
H	-7.22707600	-2.40405300	-0.86344600
H	-5.92343100	-3.03291800	-1.90022000
O	-4.47472200	1.47339000	2.30439200
O	3.74516500	-2.19590800	2.36681300
N	-3.99568400	1.30815400	0.08860300
N	-5.34576700	1.31883800	-0.30400800
N	1.49388800	-2.18325200	2.00938100
N	1.14935400	-1.57783300	3.22617200
H	-3.31199000	1.16621500	-0.66025000
H	-5.81638700	1.97520400	0.32058400
H	3.97275300	-3.41473800	0.16742300
H	2.29091200	-4.04300600	0.24110400
Li	-1.51591900	-0.61294100	-0.43418800
Li	0.59174600	-2.39813100	-1.37733800
C	1.02370900	-0.11507000	3.13138900
H	0.60793000	0.21958000	4.09620200
H	0.26415400	0.10230000	2.36718300
C	2.30179800	0.66989000	2.82506200
H	3.08985300	0.36369400	3.53444300
H	2.66900200	0.39729700	1.82201500
C	2.08156700	2.17977200	2.90662600
H	1.81674600	2.48872200	3.93196100
H	2.98617300	2.73508600	2.61199300
H	1.26370500	2.50473100	2.24445900
H	0.72118000	-2.57339300	1.45778200
H	1.89181600	-1.81031300	3.89006800
O	0.40520400	-0.58781800	-0.61188500
Cl	-2.19692700	0.08261300	-2.47349200
Cl	-0.51736200	-3.83842900	-0.04442000



O	-2.58940100	-1.71427100	0.70161100
H	-3.49663400	-1.85632500	0.38909000
O	0.05153700	-1.98478400	-3.15305600
H	-0.36756600	-2.70644300	-3.64730900
H	-0.65819300	-1.30038900	-3.07474300
H	-2.12830800	-2.57643800	0.56835000

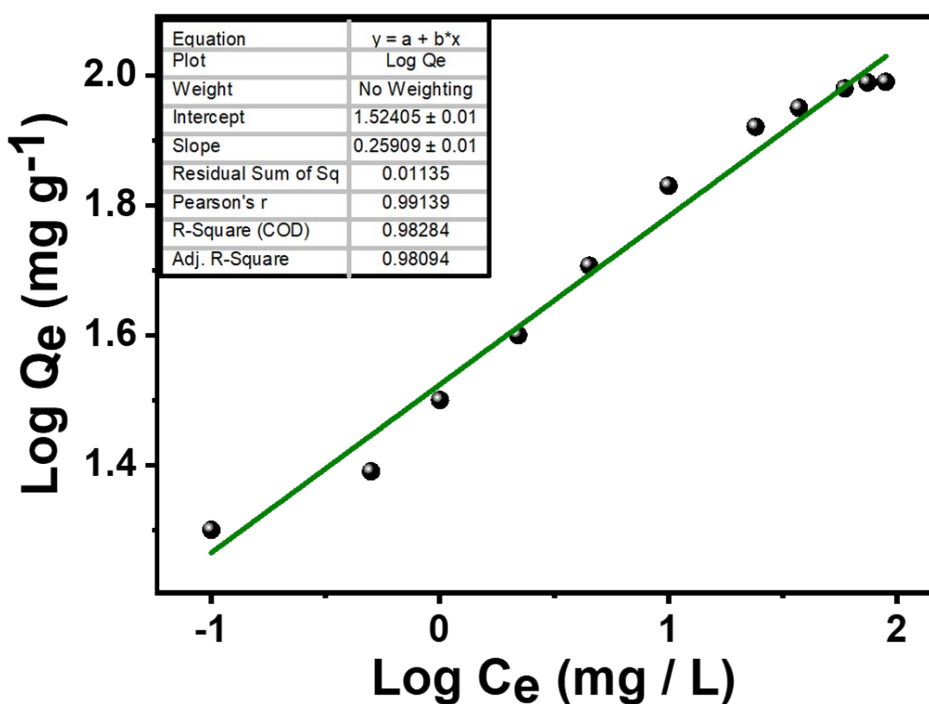


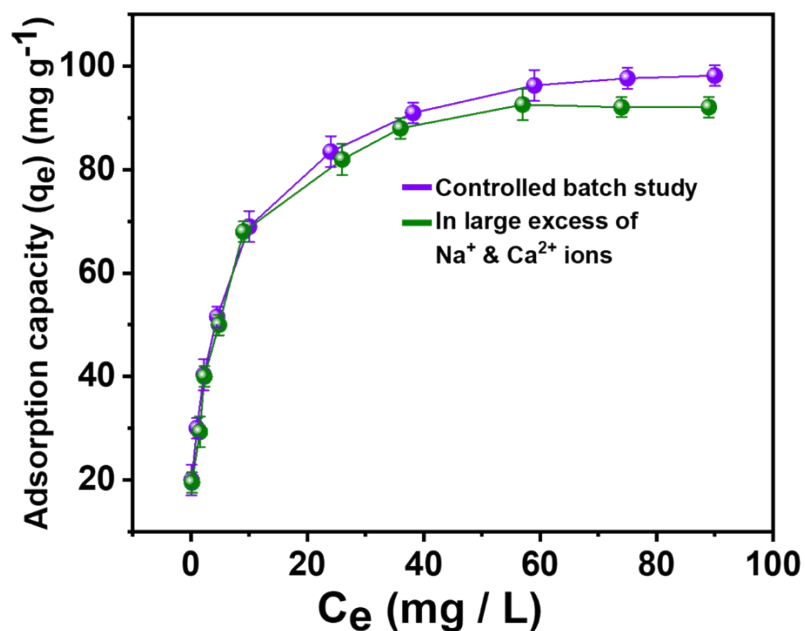
Fig. S14 The Freundlich isotherm plot of the material towards the Li<sup>+</sup> ions.

Table S3. Langmuir and Freundlich adsorption parameters for Li<sup>+</sup> at 25 °C.

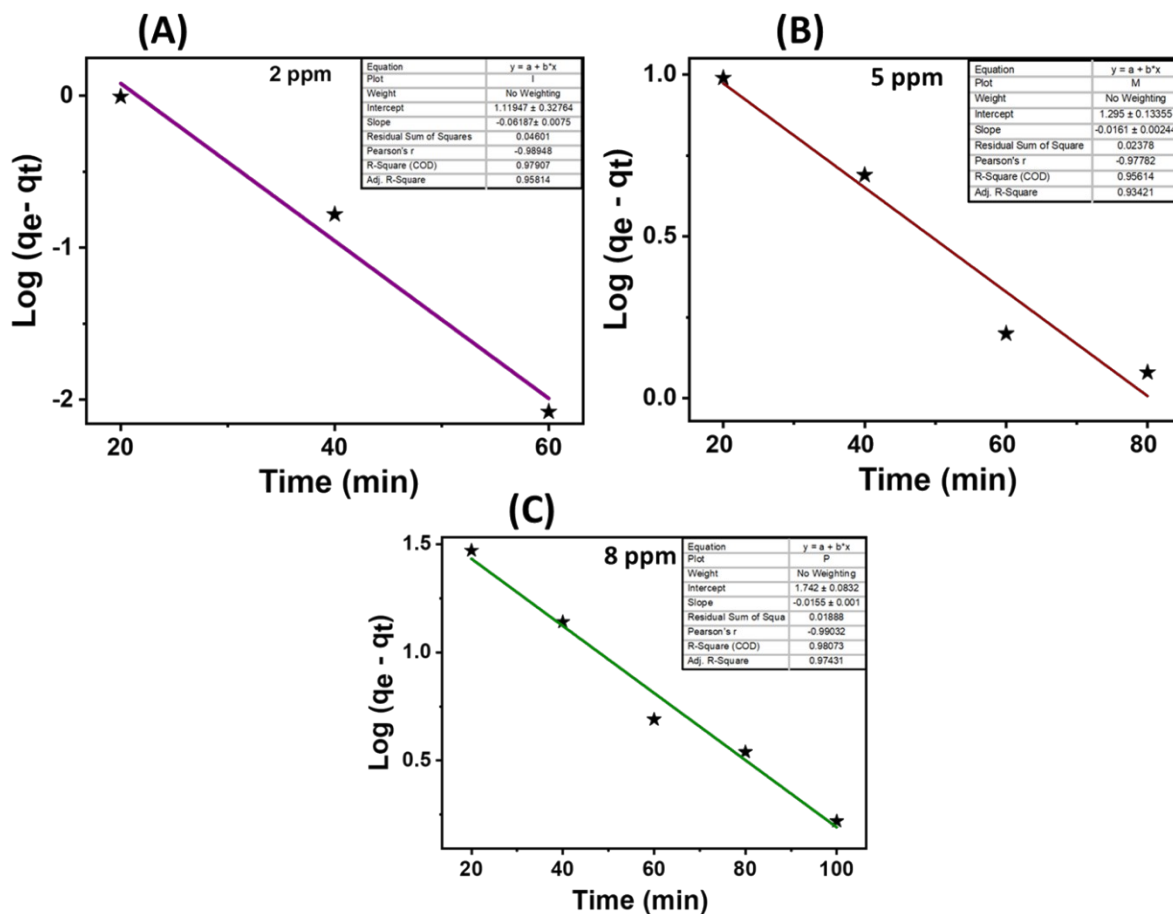
Analytes	Experimental	Langmuir Linear Isotherm			Freundlich adsorption Isotherm		
		q <sub>m</sub> (mg g <sup>-1</sup> )	K <sub>L</sub> (L g <sup>-1</sup> )	R <sup>2</sup>	K <sub>f</sub>	n	R <sup>2</sup>
Li <sup>+</sup>	97.8	100.80	0.33	0.9982	33.42	3.86	0.98284

**Table S4.** The competitive adsorption results from ICP-MS analysis.

S. No.	Metal ions	Initial Concentration ( $C_i$ )	Final Concentration ( $C_f$ )	% Extraction Efficiency
1	$\text{Ca}^{2+}$	31.23	30.05	3.78
2	$\text{Mg}^{2+}$	30.35	29.95	Negligible
3	$\text{Sr}^{2+}$	28.64	28.45	Negligible
4	$\text{Li}^+$	29.75	2.27	92.34
5	$\text{Na}^+$	32.68	32.08	Negligible
6	$\text{K}^+$	31.49	31.16	Negligible
7	$\text{Cs}^+$	29.86	29.34	Negligible
8	$\text{Co}^{2+}$	30.27	29.98	Negligible
9	$\text{Mn}^{2+}$	30.38	30.01	Negligible
10	$\text{Ni}^{2+}$	29.17	29.06	Negligible
11	$\text{Cu}^{2+}$	29.73	29.26	Negligible
12	$\text{Fe}^{2+}$	29.54	29.02	Negligible
13	$\text{Zn}^{2+}$	29.33	28.94	Negligible
14	$\text{Cd}^{2+}$	30.41	30.19	Negligible
15	$\text{Hg}^{2+}$	29.15	28.96	Negligible
16	$\text{Cr}^{3+}$	28.98	28.84	Negligible



**Fig. S15** The equilibrium adsorption capacity plot ( $q_e$ ) (batch study) towards  $\text{Li}^+$  ions in controlled mode and in the presence of large excess (1000 times) of  $\text{Na}^+$  and  $\text{Ca}^{2+}$  ions.



**Fig. S16 (A-C)** The Pseudo first-order rate kinetics model of the material towards specific concentrations ( $\text{Li}^+$ ).

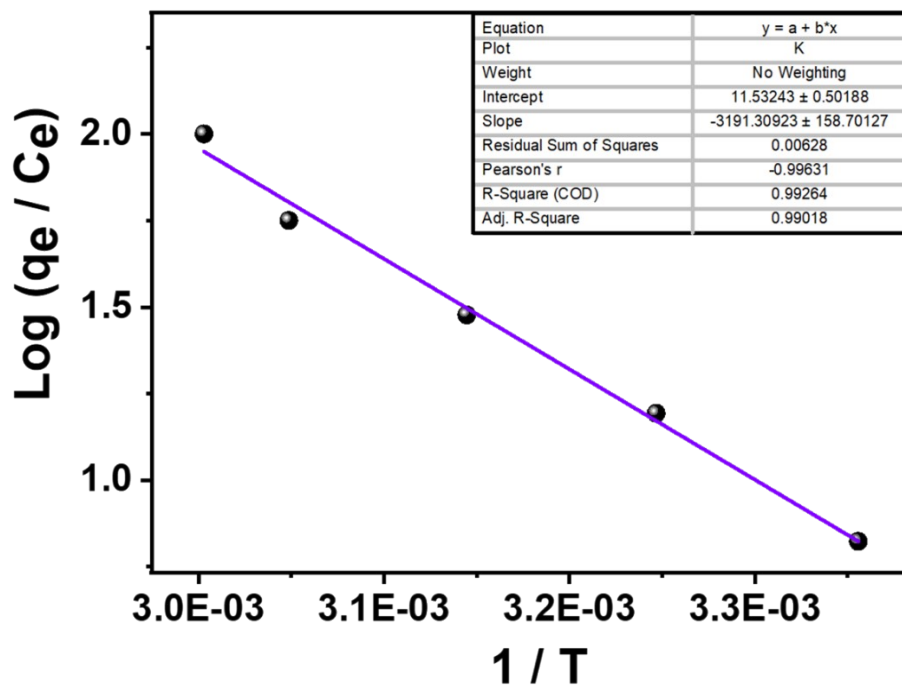


Fig. S17 The Gibbs energy plot of the material towards the  $\text{Li}^+$  ions.

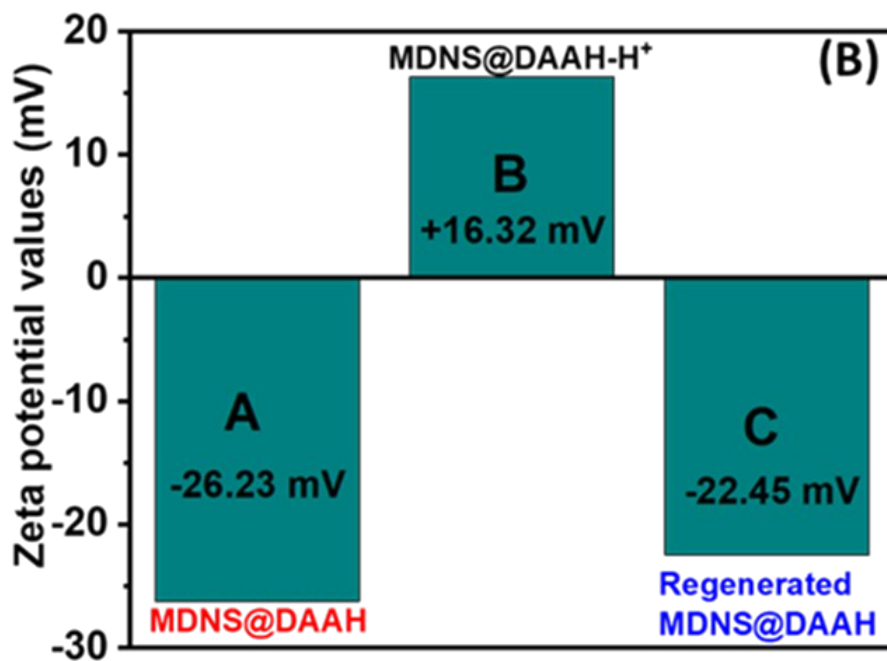
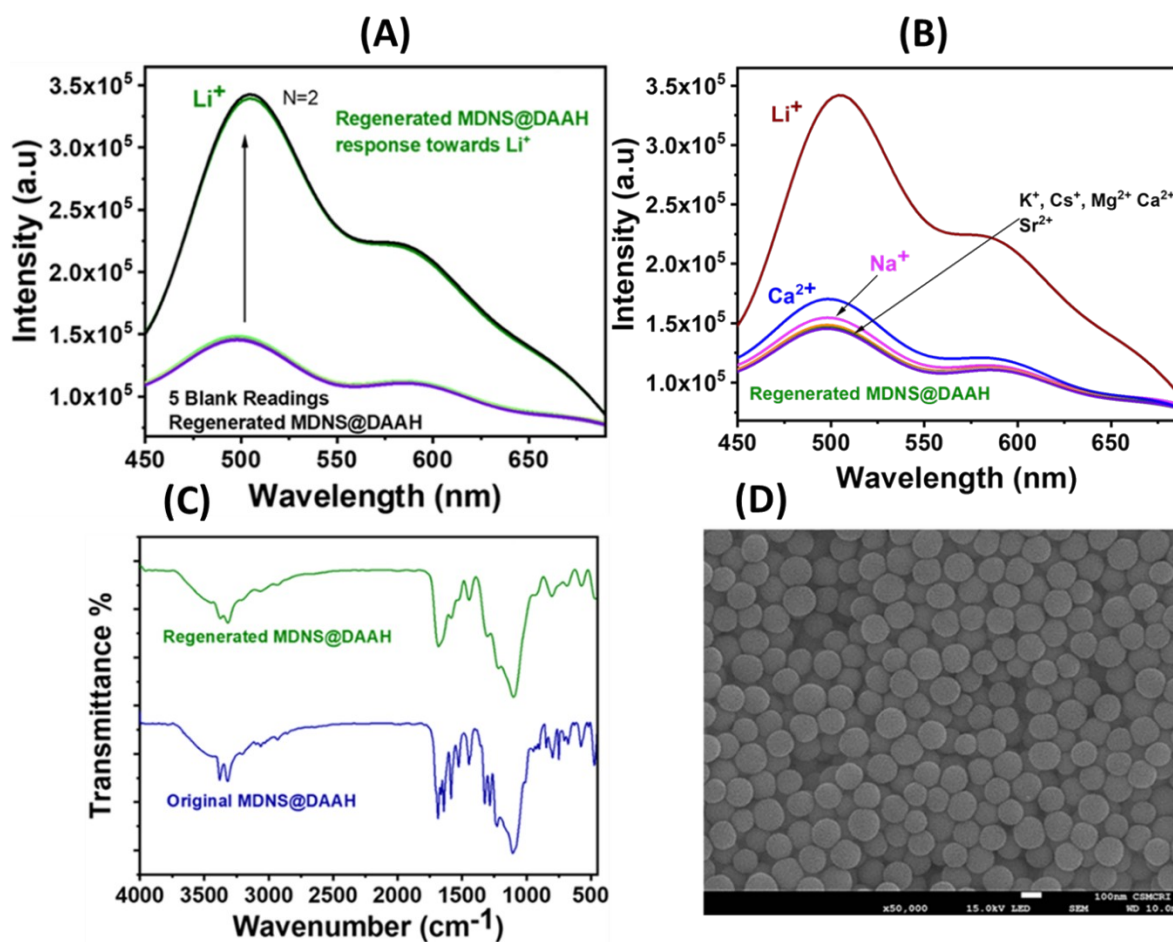


Fig. S18 Zeta potential measurement during acid-base treatment.



**Fig. S19** (A) The optical response (Fluorescence) & (B) selectivity studies (C) functionality FT-IR, and (D) SEM morphology of the regenerated material MDNS@DAAH.

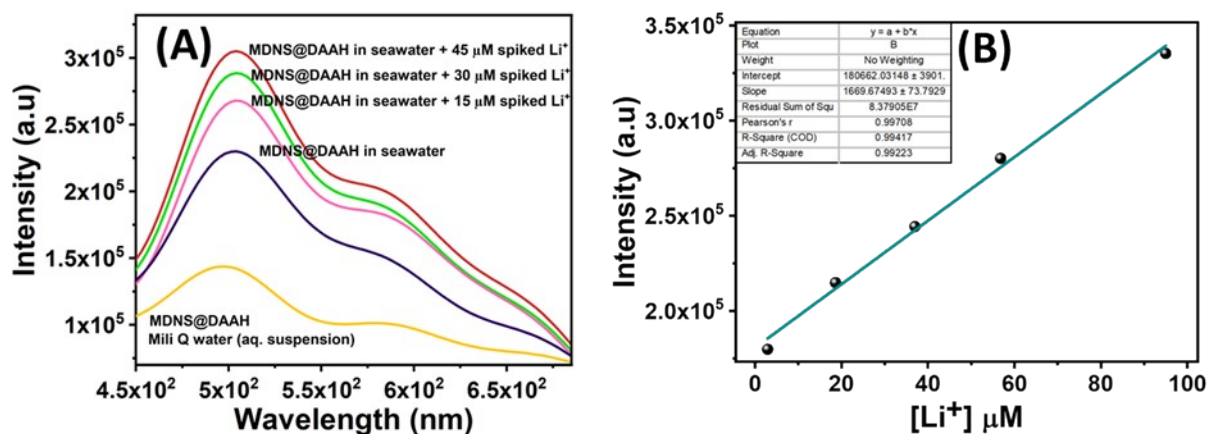
**Table S5.** The comparison of sensing and adsorption parameters with literature reports.

S.No.	Material Type	Sensing Studies/Type	L.O.D.	Adsorption Capacity ( $Q_e$ )	Adsorption from seawater	Ref
1	Ionophore	Yes/ Turn off	–	–	–	[6]
2	Aza crown substituted naphthalene diimide	Yes/ Turn off	5.0 $\mu\text{M}$	–	–	[11]
3	Aza crown naphthalene derivative	Yes/ excimer	21.0 $\mu\text{M}$	–	–	[10]
4	Spiropyran crown ether isomerisation	Yes/ Turn On	4.6 $\mu\text{M}$	–	–	[9]

5	pH independent fluorescent chemosensor	Yes/ Turn off	0.6 mM	–	–	[12]
6	Fluorescent copolymer aggregate sensor	Yes/ Turn off	0.45 $\mu$ M	–	–	[13]
7	Ruthenium based metallacrown complex	Yes/ Turn On	-	–	–	[14]
8	Aminoethyl benzo crown functionalized polymer brushes	No/	-	4.22 mg / g	–	[25]
9	Allyloxy methylol crown ether functionalized polymer brush	No/	-	4.43 mg / g	–	[26]
10	HMO immobilised alpha- alumina beads	No	-	21.7 mg / g	Yes 8.87 mg/g	[27]
11	Carbon decorated with MnO <sub>2</sub> nanocomposites	No	–	88.5 mg / g	–	[29]
12	Functionalized Dendritic Nano Silica	Yes/ Turn-on	4.9 nM	97.8 mg / g	Yes	This Work

**Table S6.** The mortality percentage of *Artemia salina* with MDNS@DAAH with respect to time

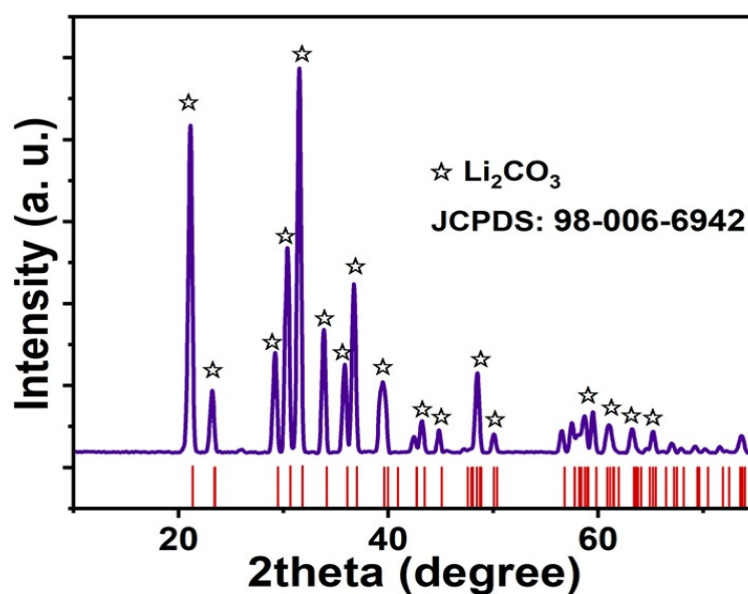
S.No	Experiment	0 hr	6 hr	12 hr	24 hr
1.	Control Experiment	0	0	0	3
2.	MDNS@DAAH	0	0	3	5
3.	Li <sup>+</sup>	0	3	5	10
4.	MDNS@DAAH + Li <sup>+</sup>	0	4	7	14



**Fig. S20** (A) Fluorescence emission of material with seawater and spiked samples and (B) The calibration plot of material with  $\text{Li}^+$  from fluorescence titration experiment.

**Table S7.** Quantification of  $\text{Li}^+$  ions probe materials in seawater sample.

Analyte	Proposed ( $\mu\text{M}$ )	Spiked ( $\mu\text{M}$ )	found	Recovery %	RSD	N=2
$\text{Li}^+$	28.81	15 $\mu\text{M}$	45.21	106.23 %	2.87	2
		30 $\mu\text{M}$	59.93	101.90 %	1.45	2
		45 $\mu\text{M}$	75.38	102.13 %	1.03	2



**Fig. S21** The PXRD profile of the precipitated  $\text{Li}_2\text{CO}_3$  from sea bittern.

## References:

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