Supporting Information

Pyridinium Modified β-Cyclodextrin: An Ionic Supramolecular Ligand for Palladium acetate in C-C Coupling Reactions in Water
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Spectrum data for pyridinium modified β-cyclodextrin:
NMR spectrum for N-octyl-pyridine-2-amine(2).
Figure S1. $^1$H-NMR (300 MHz, CDCl$_3$) spectrum of N-octyl-pyridine-2-amine (2).

![Figure S1](image)

Figure S2. $^{13}$C-NMR spectrum (75 MHz, CDCl$_3$) of N-octyl-pyridine-2-amine (2).

![Figure S2](image)

Figure S3. ESI-MS Spectra of N-octyl-pyridine-2-amine (2).

![Figure S3](image)
Figure S4. $^1$H NMR (300 MHz, DMSO-d$_6$) for pyridinium modified $\beta$-cyclodextrin (3).

Figure S5. ESI-MS spectrum for pyridinium modified $\beta$-cyclodextrin (3) (M+1) adduct.
Figure S6. $^{13}$C-NMR spectrum (75 MHz, DMSO-d$_6$) for pyridinium modified β-cyclodextrin (3).

Figure S7. 2D-NOESY NMR spectrum of pyr:β-CD (3) (300 MHz in DMSO-d$_6$).
Figure S8. Elemental analysis of pyr:β-CD (3).

Figure S9. IR spectra for β-CD (blue), Pyr:β-CD (3) (green) and Pd@Pyr:β-CD (wine).
Figure S10. XRF image of Pd@pyr:β-CD complex

Figure S11. $^1$H NMR (300 MHz, DMSO-$_d_6$) for pyr:β-CD (blue) and Pd@pyr:β-CD (red).

Figure S12. Water solubility of a) pyr:β-CD (3) (0.1 mmol in 2mL water), b) N-octyl-pyridine-2-amine (2) and β-cyclodextrin in 2mL water.
Theoretical Calculation

Molecular modeling studies of pyridinium and pyridinium modified β-cyclodextrin

Energy minimization studies

The complexation of pyridinium modified β-cyclodextrin was also confirmed from energy minimization studies. From this studies N-octyl-pyridine-2-amine (2) present in outside the modified β-cyclodextrin cavity (Figure S7 Mode A) which was more favored than that of inclusion of N-octyl-pyridine-2-amine (2) inside the modified β-cyclodextrin (Figure S8. Mode B), because lower complexation energy (Mode A) (ΔE) -64.8600 kcal M$^{-1}$ is preferred more than that of mode B (ΔE) -50.8292 kcal M$^{-1}$.

Table S1: Molecular Modeling Studies of pyridinium modified β-cyclodextrin

<table>
<thead>
<tr>
<th>Mode of Pyridinium</th>
<th>Mode of Inclusion</th>
<th>β-CD as Host (ΔE$^a$ Kcal.M$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-octyl-pyridine-2-amine present in outside the pyridinium modified β-cyclodextrin cavity</td>
<td>Mode A</td>
<td>-64.8600</td>
</tr>
<tr>
<td>N-octyl-pyridine-2-amine present in inside the pyridinium modified β-cyclodextrin cavity</td>
<td>Mode B</td>
<td>-50.8292</td>
</tr>
</tbody>
</table>

Figure S13 Mode A: CVFF optimized inclusion complex of N-octyl-pyridine-2-amine (2) group outside the Pyr:β-CD (3).
**Figure S14** Mode B: CVFF optimized inclusion complex of $N$-octyl-pyridine-2-amine (2) group inside the Pyr-$\beta$-CD (3) cavity.

**Figure S15.** Mode A: CVFF optimized inclusion complex of $N$-octyl-pyridine-2-amine group outside the pyridinium modified $\beta$-cyclodextrin.
**Figure S16.** Mode A: CVFF optimized inclusion complex of $N$-octyl-pyridine-2-amine group inside the pyridinium modified $\beta$-cyclodextrin cavity.

**Figure S17.** CVFF optimized inclusion complex of $\beta$-cyclodextrin with pyridinium; In mode B: with inclusion of $N$-octyl sides for pyridinium in $\beta$-cyclodextrin.

**Figure S18.** CVFF optimized inclusion complex of $\beta$-cyclodextrin with pyridinium; In mode A: with inclusion of pyridine sides for pyridinium in $\beta$-cyclodextrin.
Figure S19. a) UV-Vis absorption spectra for Monotosyl-β-CD (Red), pyridinium modified- β-CD (Blue), N-octyl-pyridine-2-amine (Green), b) UV-DRS spectra for pyridinium modified- β-CD (Red), pyridinium modified- β-CD with Pd(OAc)$_2$ (Green).

Spectroscopic data for compound 4a-r
Figure S20. $^1$H-NMR spectrum for 4a

Figure S21. $^{13}$C-NMR spectrum for 4a

Figure S22. $^1$H-NMR spectrum for 4b
Figure S23. $^{13}$C-NMR spectrum for 4b

Figure S24. $^1$H-NMR spectrum for 4c
Figure S25. $^{13}$C-NMR spectrum for 4c

Figure S26. $^1$H-NMR spectrum for 4d
Figure S27. $^{13}$C-NMR spectrum for 4d

Figure S28. $^1$H-NMR spectrum for 4e
Figure S29. $^{13}$C-NMR spectrum for 4e

Figure S30. $^1$H-NMR spectrum for 4f
**Figure S31.** $^{13}$C-NMR spectrum for 4f

**Figure S32.** $^1$H-NMR spectrum for 4i
Figure S33. $^{13}$C-NMR spectrum for 4i

Figure S34. $^1$H-NMR spectrum for 4i
Figure S35. $^1$H-NMR spectrum for 4K

Figure S36. $^1$H-NMR spectrum for 4l
Figure S37. $^{13}$C-NMR spectrum for 4l

Figure S38. $^1$H-NMR spectrum for 4m
Figure S39. $^{13}$C-NMR spectrum for 4m

Figure S40. $^1$H-NMR spectrum for 4o
Figure S41. $^{13}$C-NMR spectrum for 4o

Spectroscopic data for compound 5a-k

Figure S42. $^1$H-NMR spectrum for 6a
Figure S43. $^1$C-NMR spectrum for 6a

Figure S44. $^1$H-NMR spectrum for 6b
**Figure S45.** $^{13}$C-NMR spectrum for 6b

**Figure S46.** $^1$H-NMR spectrum for 6c
**Figure S47.** $^{13}$C-NMR spectrum for 6c

**Figure S48.** $^1$H-NMR spectrum for 6d
Figure S49. $^{13}$C-NMR spectrum for 6d

Figure S50. $^1$H-NMR spectrum for 6e
Figure S51. $^1$C-NMR spectrum for 6e

Figure S52. $^1$H-NMR spectrum for 6f
Figure S53. $^{13}$C-NMR spectrum for 6f

Figure S54. $^1$H-NMR spectrum for 6g
Figure S55. $^1$H-NMR spectrum for 6h

Figure S56. $^1$H-NMR spectrum for 6i
Figure S57. $^1$H-NMR spectrum for 6j

Figure S58. $^1$H-NMR spectrum for 6k
Figure S59. $^{13}$C-NMR spectrum for 6k