**Supplementary data**

**The drug delivery appraisal of Cu and Ni decorated B12N12 nanocage for an 8-hydroxyquinoline drug: A DFT and TD-DFT computational study**

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| **F:\final opted\AD\AD-b\AD-B\AD-b--BOND-f.jpg** | | **F:\final opted\AD\AD-b\AD-B\AD-b--f.jpg** | |
| **A-b** | | **A-a** | |
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| **A-d** | | **A-c** | |
| **F:\final opted\BD\BD-b\BD-b\BD-B- bond-F.jpg** | **F:\final opted\BD\BD-a\BD-a\BD-A-BOND-F.jpg** | |
| **B-b** | **B-a** | |
| **F:\final opted\BD\BD-d\BD-d\BD-d-F.jpg** | **F:\final opted\BD\BD-c\BD-c\BD-C-bond-F.jpg** | |
| **B-d** | **B-c** | |

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| **F:\final opted\CD\CD-b\CD-b\CD-B-f.jpg** | **F:\final opted\CD\CD-a\CD-a\CD-A-F-jpg.jpg** |
| **C-b** | **C-a** |
| **F:\final opted\CD\CD-d\CD-d\CD-D-F.jpg** | **F:\final opted\CD\CD-c\CD-c\CD-C-f-jpg.jpg** |
| **C-d** | **C-c** |

**Figure S1.** Optimized structuresof 8-HQ on the surface of the pristine and Cu&Ni functionalized B12N12

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| E:\final opted\Model A\A\BOND-J.jpg |
| (A)B12N12 |

|  |  |
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| F:\final opted\Model C\C\C-BOND-J.jpg | F:\final opted\Model B\B\B-BOND-J.jpg |
| (C)B12N12-Ni | (B)B12N12-Cu |

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| **F:\final opted\AD\AD-a\AD-a\AD-BOND-j.jpg** |
| **A-a** |

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| **F:\final opted\AD\AD-C\AD-C\AD-d-bond-j.jpg** | **F:\final opted\AD\AD-C\AD-C\AD-c-BOND-j.jpg** | **F:\final opted\AD\AD-a\AD-a\AD-B-bond-j.jpg** |
| **A-d** | **A-c** | **A-b** |

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| **F:\final opted\BD\BD-b\BD-b\BD-b-bond-j-jpg.jpg** | | **F:\final opted\BD\BD-a\BD-a\BD-A-bond-2-j.jpg** |
| **B-b** | | **B-a** |
| **F:\final opted\BD\BD-d\BD-d\BD-D-BOND -J-.jpg** | | **F:\final opted\BD\BD-c\BD-c\BD-C-bond-j-.jpg** |
| **B-d** | | **B-c** |
| ***F:\final opted\CD\CD-b\CD-b\CD-B-bond-j-.jpg*** | | ***F:\final opted\CD\CD-a\CD-a\CD-A-j-jpg.jpg*** | | |
| **C -b** | | **C-a** | | |
| **F:\final opted\CD\CD-d\CD-d\CD-D-bond-j.jpg** | | **F:\final opted\CD\CD-c\CD-c\CD-C-bond-j-jpg.jpg** | | |
| **C -d** | | **C -c** | | |

**Figure S2.** The bond lengthof 8-HQ on the surface of the pristine and Cu&Ni functionalized B12N12.

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| D:\optimized\final opted\AD\AD-b\AD-B-FREQ\AD-B-FREQ1_ir.jpg | D:\optimized\final opted\AD\AD-a\AD-a-freq\AD-A-FREQ_ir.jpg |
| **A-b** | **A-a** |

|  |  |
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| D:\optimized\final opted\BD\BD-b\BD-b-FREQ\BD-B-FREQ 1_ir.jpg | D:\optimized\final opted\BD\BD-a\BD-a-FREQ\BD-A-FREQ 1_ir.jpg |
| B-b | B-a |

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| D:\optimized\final opted\CD\CD-b\CD-b-FREQ\CD-B-FREQ1_ir.jpg | D:\optimized\final opted\CD\CD-a\CD-a-FREQ\CD-A-FREQ1_ir.jpg |
| C-b | C-a |

**Figure S3.** The IR plots of 8-HQ on the surface of the pristine and Cu&Ni functionalized B12N12