Electronic Supplementary Information

In the search of active nanocarriers for delivery of mitomycin C drug

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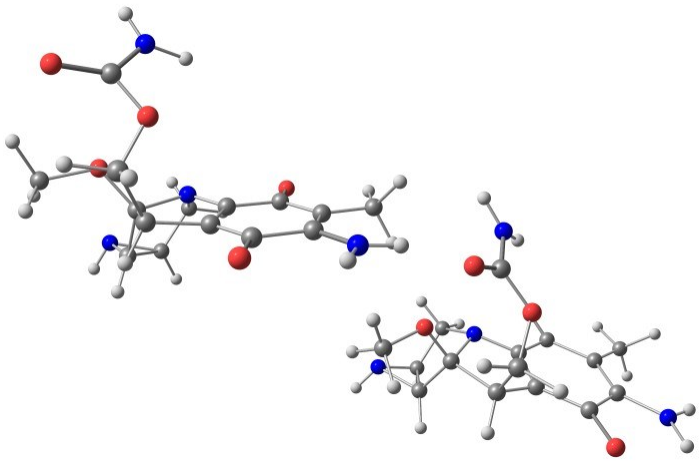
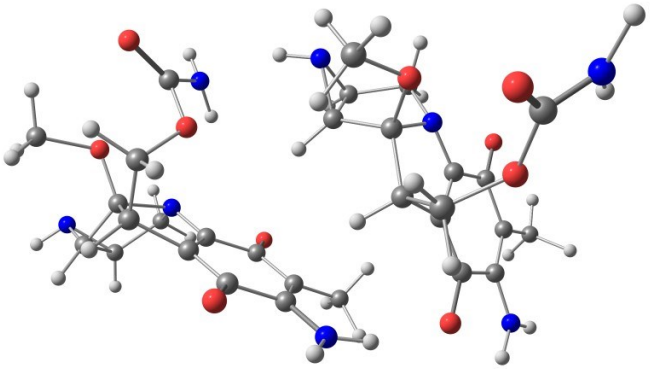
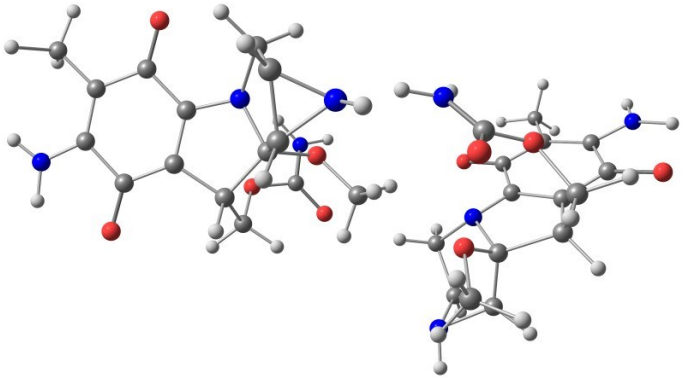


E_{bind}= -10.19 kcal mol^{-1}
E_{int}= -11.12 kcal mol^{-1}



E_{bind} = -12.99 kcal mol^{-1}

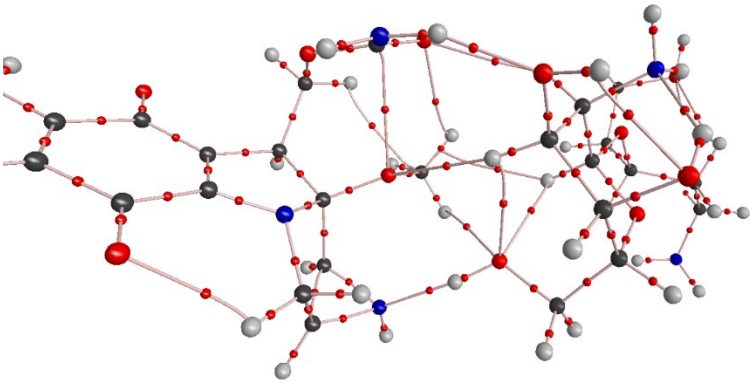
E_{int} = -13.65 kcal mol^{-1}



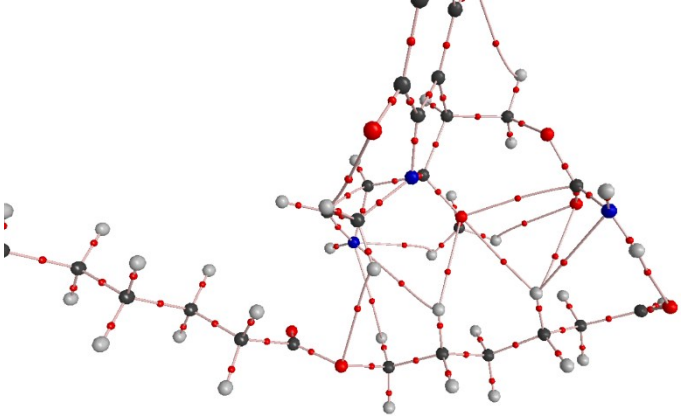
E_{bind} =13.92 kcal mol^{-1}

E_{int} = -14.12 kcal mol^{-1}

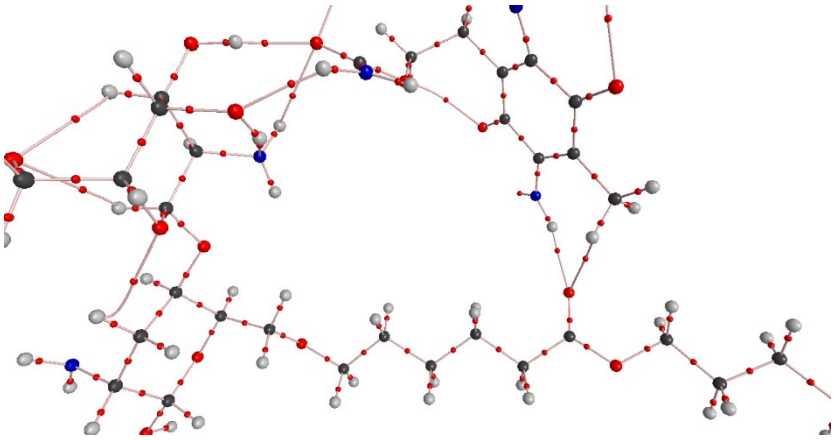
Fig. S1. Stable configurations for the interaction of two MMC molecules together with corresponding binding and interaction energies.



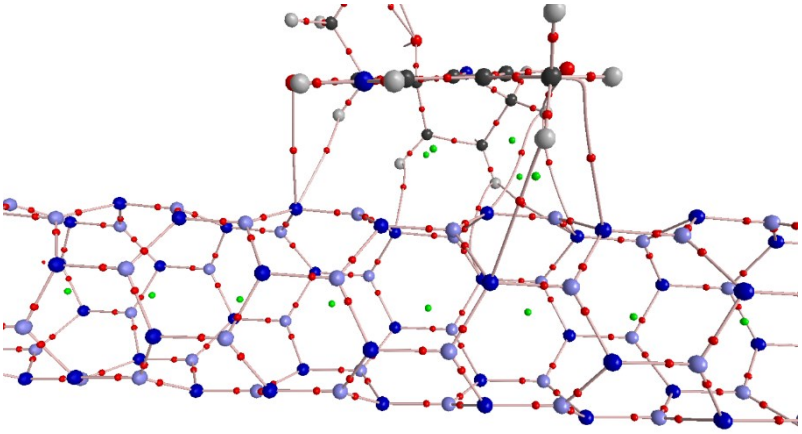
MMC-CS



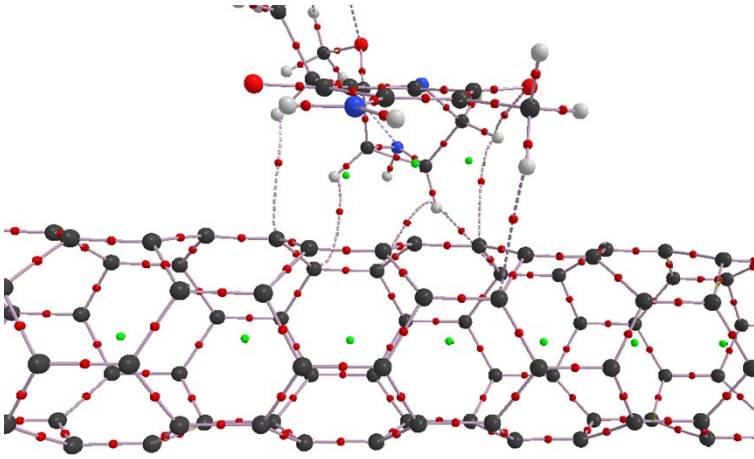
MMC-PCL



MMC-PCL/CS



MMC-BNNT-21



MMC-CNT-21

Fig. S2 QTAIM molecular graphs for the most stable complexes between MMC and carriers. Lines connecting the nuclei are the bond paths and the small red and green dots indicate the positions of the BCPs and CCPs.

Table S1. Condensed nucleophilicity (f^-) and electrophilicity (f^+) for different sites in considered carriers.

Carrier	Site	f^-	f^+
CS	O(3)	0.007	-
	O(7)	0.021	-
	O(8)	0.017	-
	O(11)	0.014	-
	O(15)	0.007	-
	O(18)	0.002	-
	O(19)	0.064	-
	O(21)	0.006	-
	N(10)	0.075	-
	N(22)	0.467	-
	H(31)	-	0.017
	H(40)	-	0.018
	H(41)	-	0.009
	H(43)	-	0.026
	H(44)	-	0.038
	H(45)	-	0.039
	H(46)	-	0.005
PCL	O(7)	0.052	-
	O(8)	0.194	-
	O(15)	0.294	-
	O(37)	0.004	-
	H(36)	-	0.123
	H(38)	-	0.007
	O(7)	0.033	-
	O(8)	0.112	-

PCL/CS	O(15)	0.055	-
	O(16)	0.145	-
	H(17)	-	0.019
	H(26)	-	0.050
	H(27)	-	0.050