Supplementary information

Interactions between β-cyclodextrin as a carrier for anti-cancer drug delivery: A molecular dynamics simulation study

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Table S1: The components of each simulated system in this study

	Components \ Systems	Number of Drug molecule	Number of βCD molecule	Number of Water molecule
1	βCD + 5-Fu + Water	1	1	4000
2	5-Fu + Water	1	0	4000
3	βCD + Ald + Water	1	1	4000
4	Ald + Water	1	0	4000
5	βCD + TMZ + Water	1	1	4000
6	TMZ + Water	1	0	4000
7	βCD + Water	0	1	4000

Table S2: Number of water molecules in different spheres inside β-CD

Distance (nm) / System	0-0.5	0.5-0.8	0.8-0.9	0.9-1.0	0-1.0 (Total)
β-CD + 5-FU + water	3.620 (±0.247)	20.269 (±0.001)	23.175 (±0.021)	47.115 (±0.000)	94.179 (±0.225)
β-CD + Ald + water	2.476 (±0.089)	18.461 (±0.005)	23.262 (±0.038)	46.870 (±0.009)	91.069 (±0.047)
β-CD + TMZ + water	1.404 (±0.025)	19.131 (±0.006)	23.509 (±0.002)	46.416 (±0.005)	90.460 (±0.026)
β-CD + water (reference)	9.728 (±0.012)	20.481 (±0.004)	22.659 (±0.004)	47.385 (±0.006)	100.253 (±0.026)

Figure S1a

(5-Fu in βCD at 20 ns)
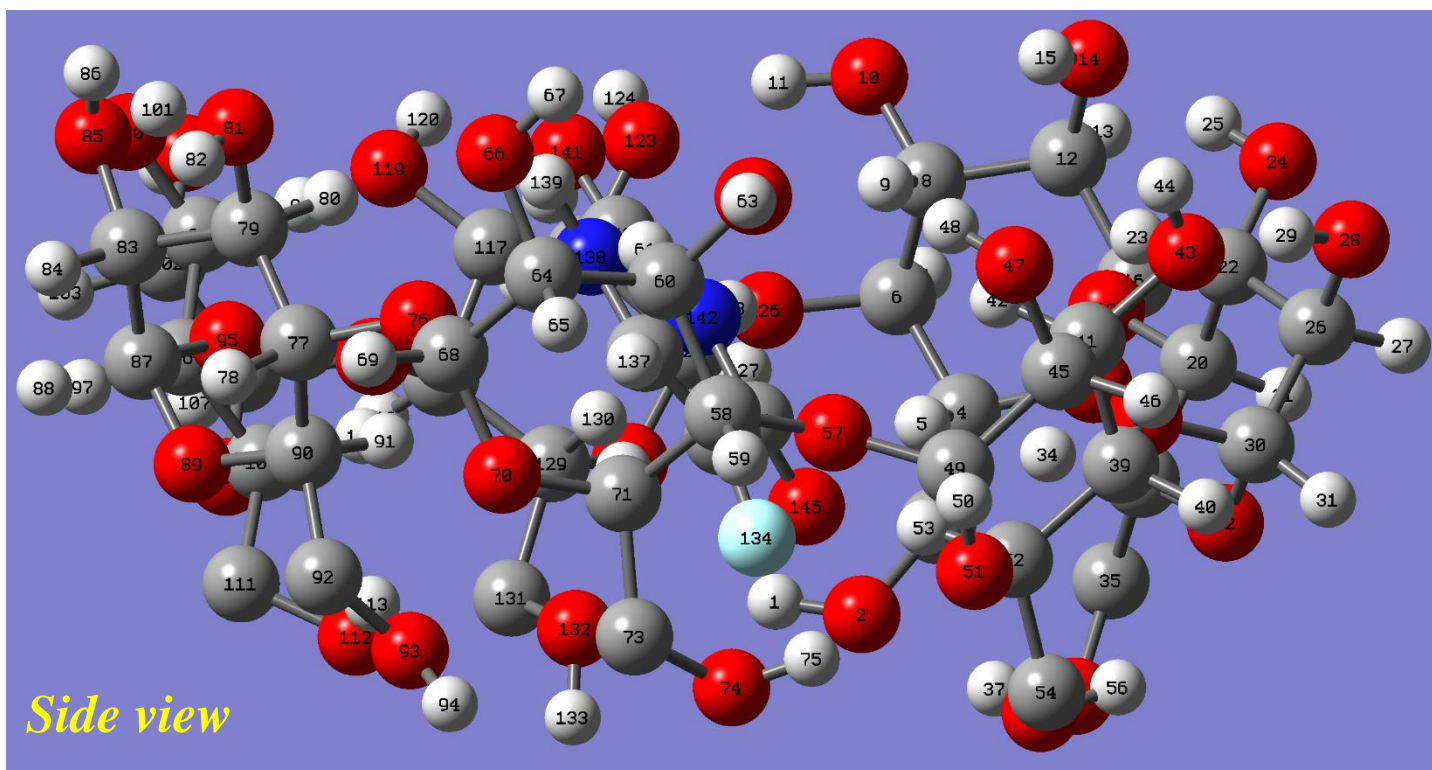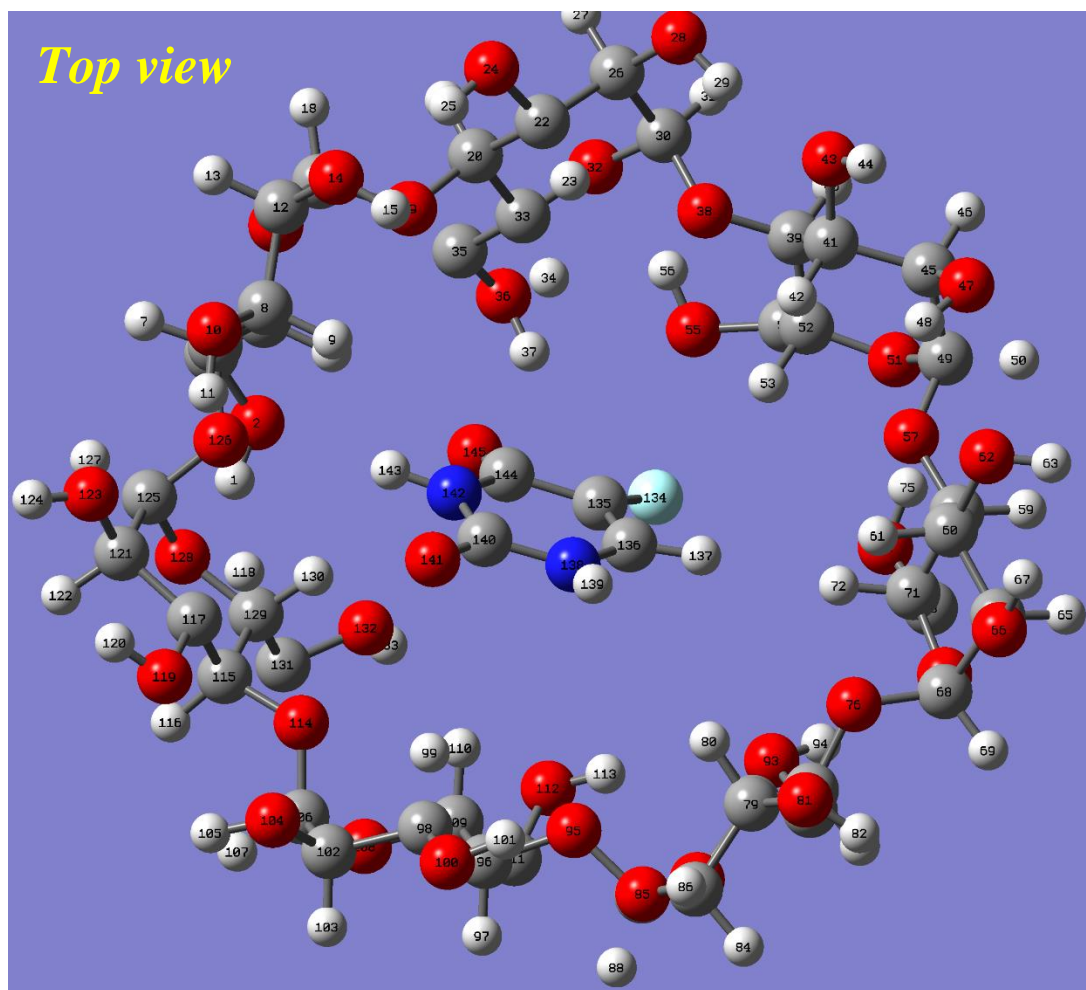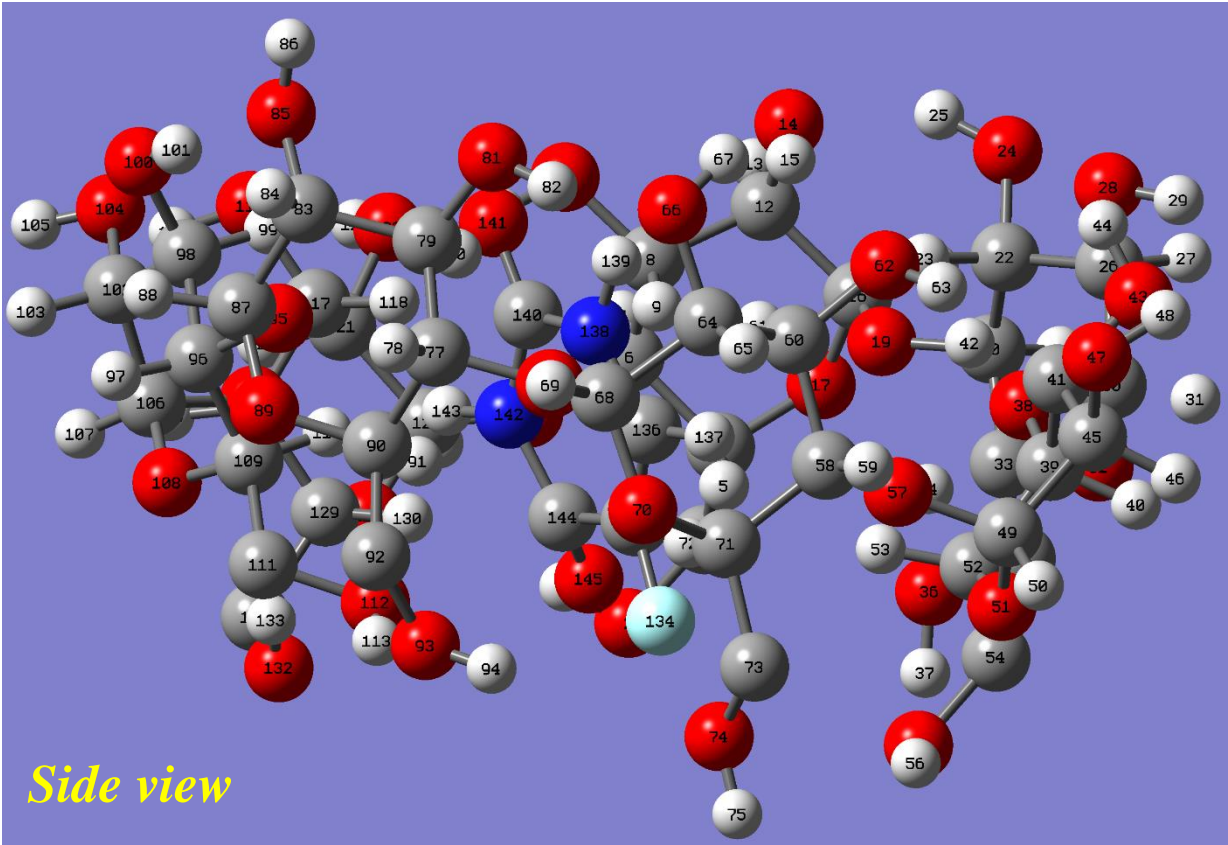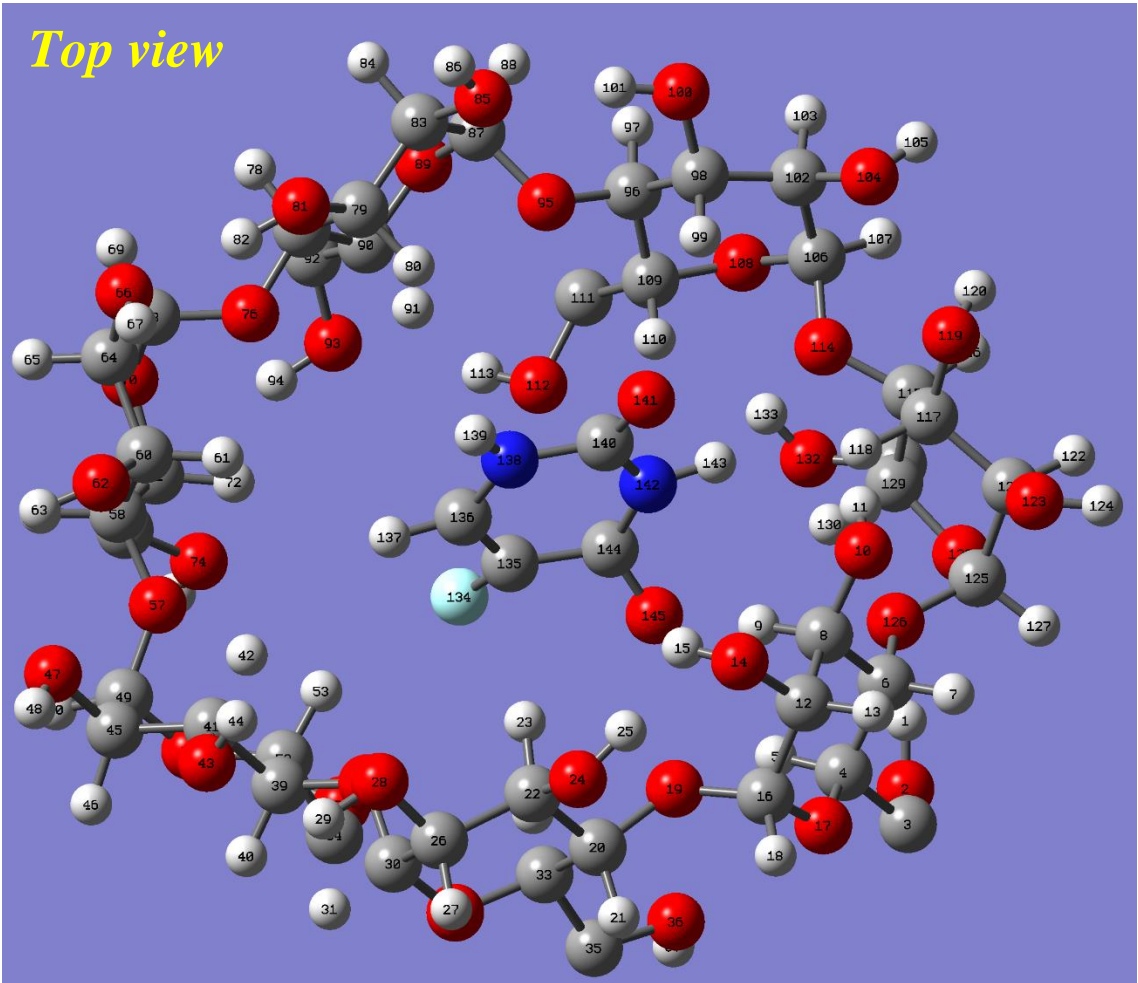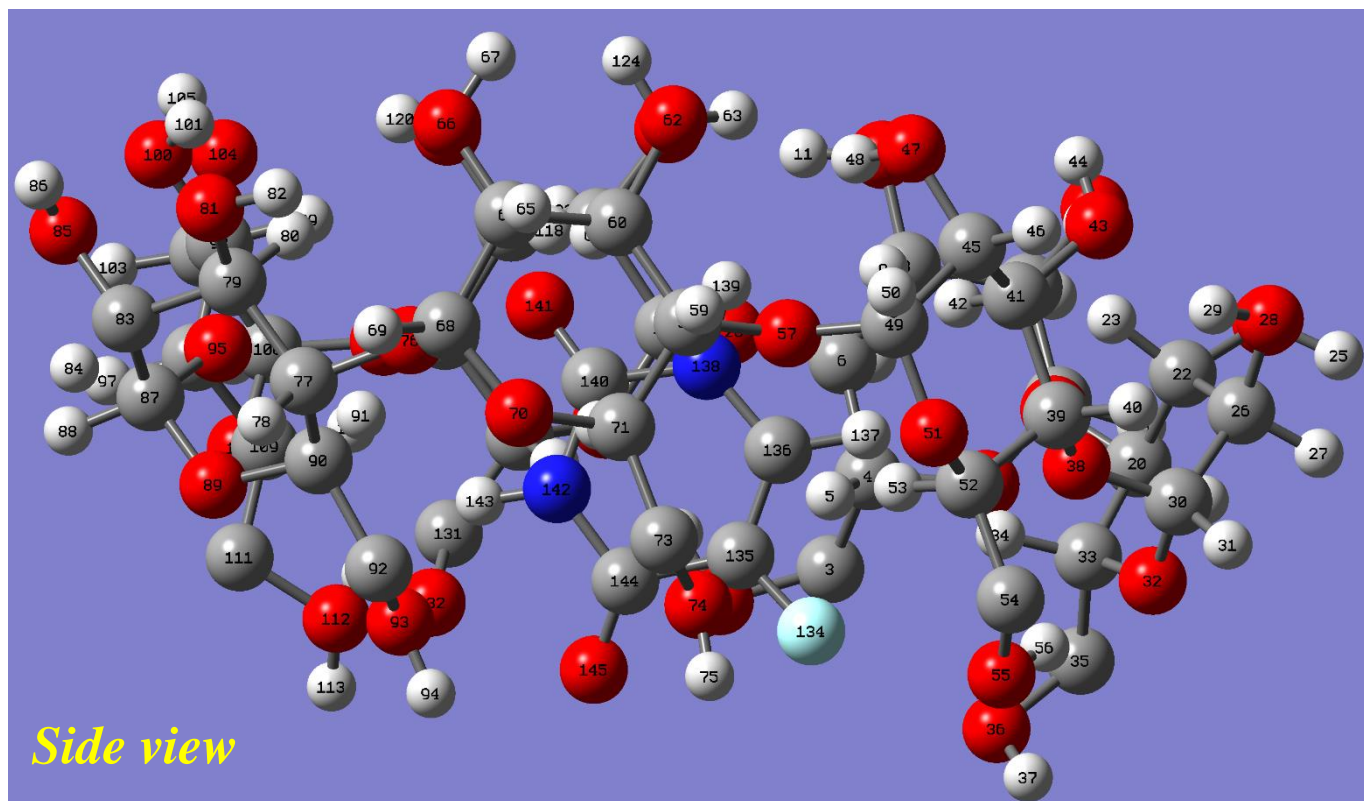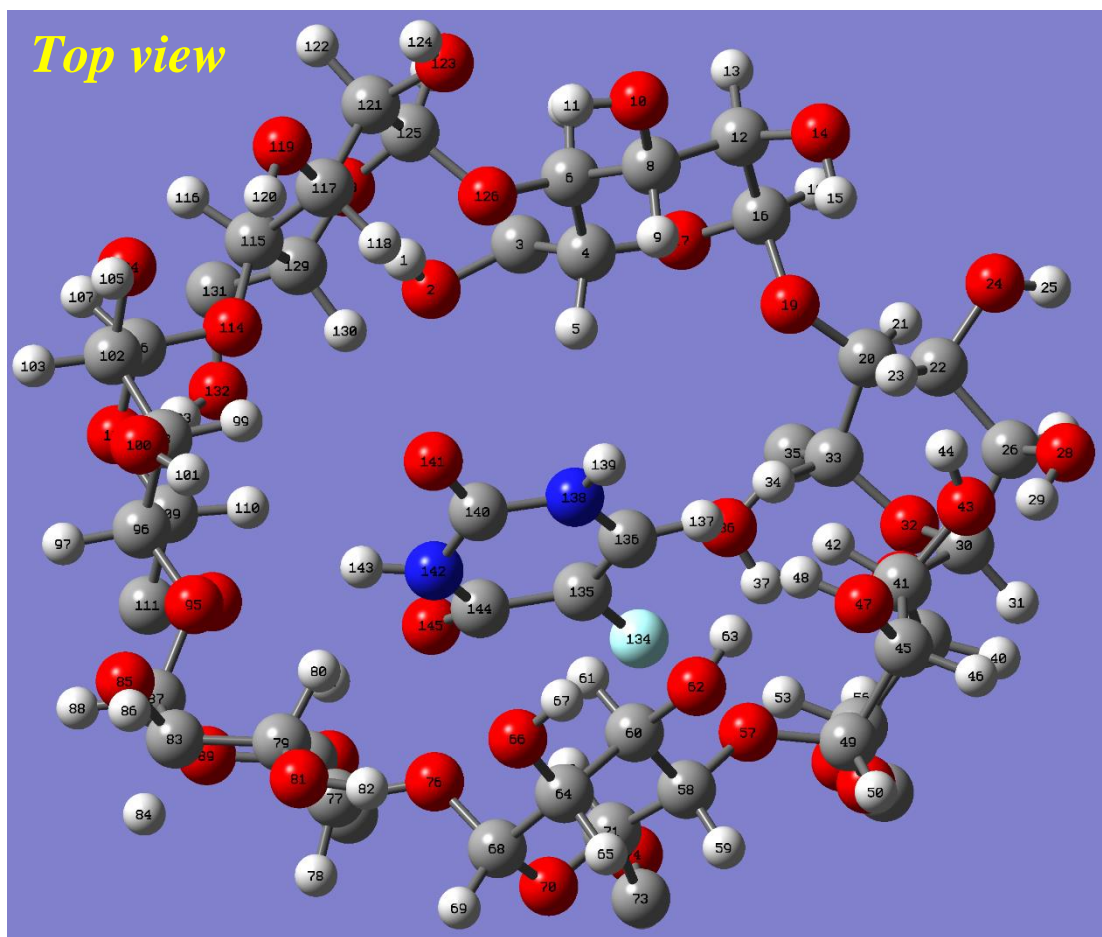
Top view

Side view

Figure S1a

(5-Fu in βCD at 60 ns)

Top view

Side view

Figure S1a

(5-Fu in βCD at 100 ns)

Top view

Side view

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Figure S1b

(Ald in βCD at 20 ns)

Top view

Side view

Figure S1b

(Ald in βCD at 60 ns)

Top view

Side view

Figure S1b

(Ald in βCD at 100 ns)

Top view
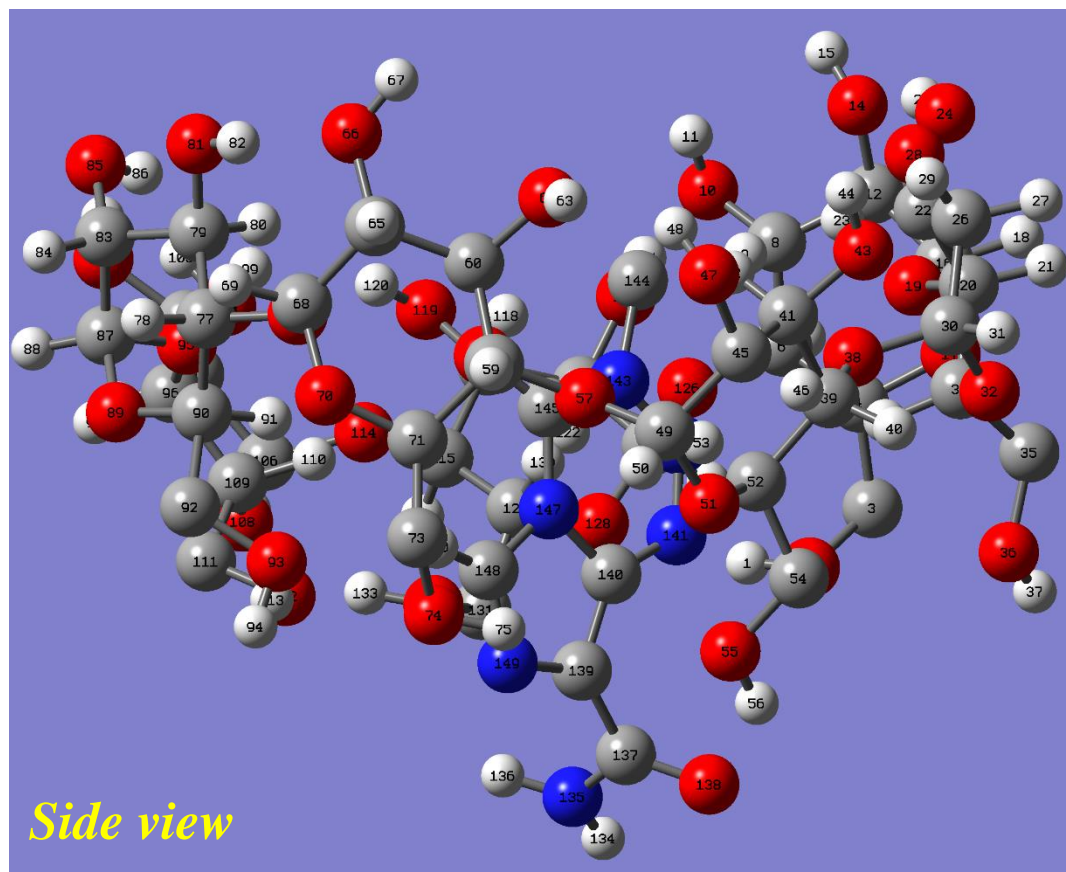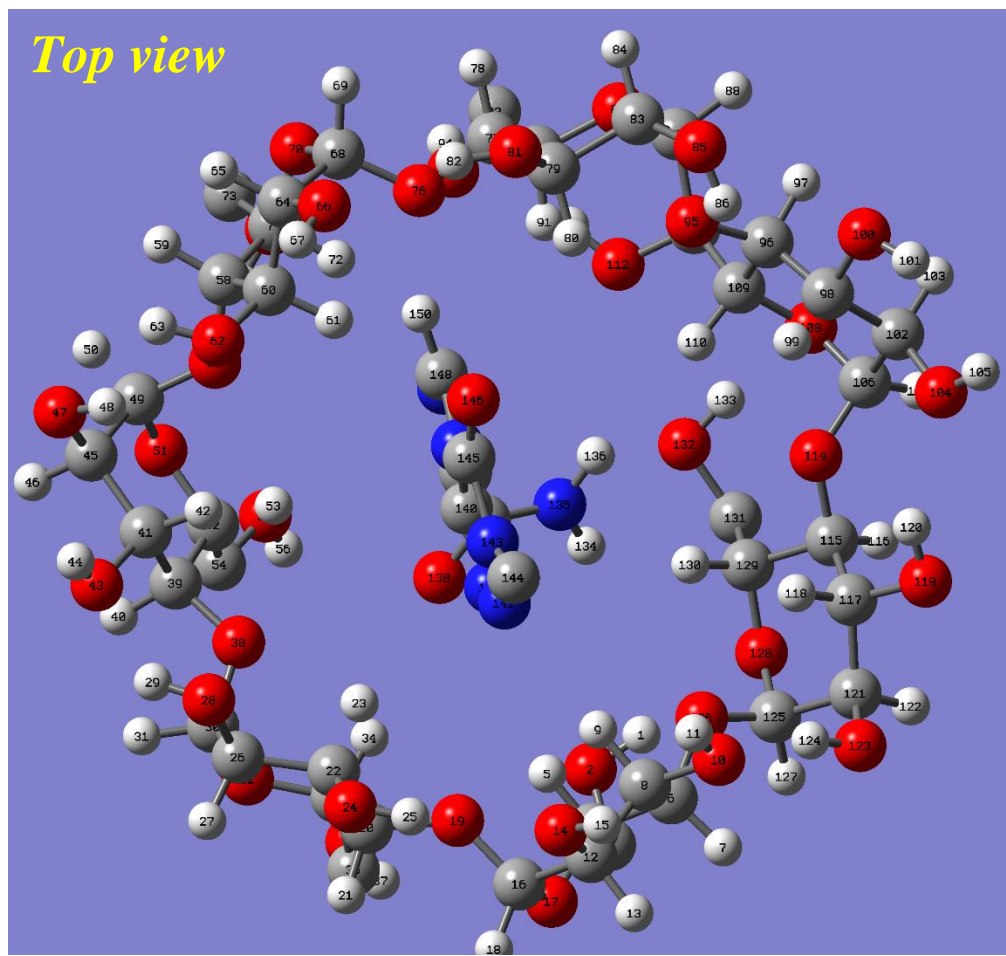

Side view

Figure S1c

(TMZ in βCD at 20 ns)
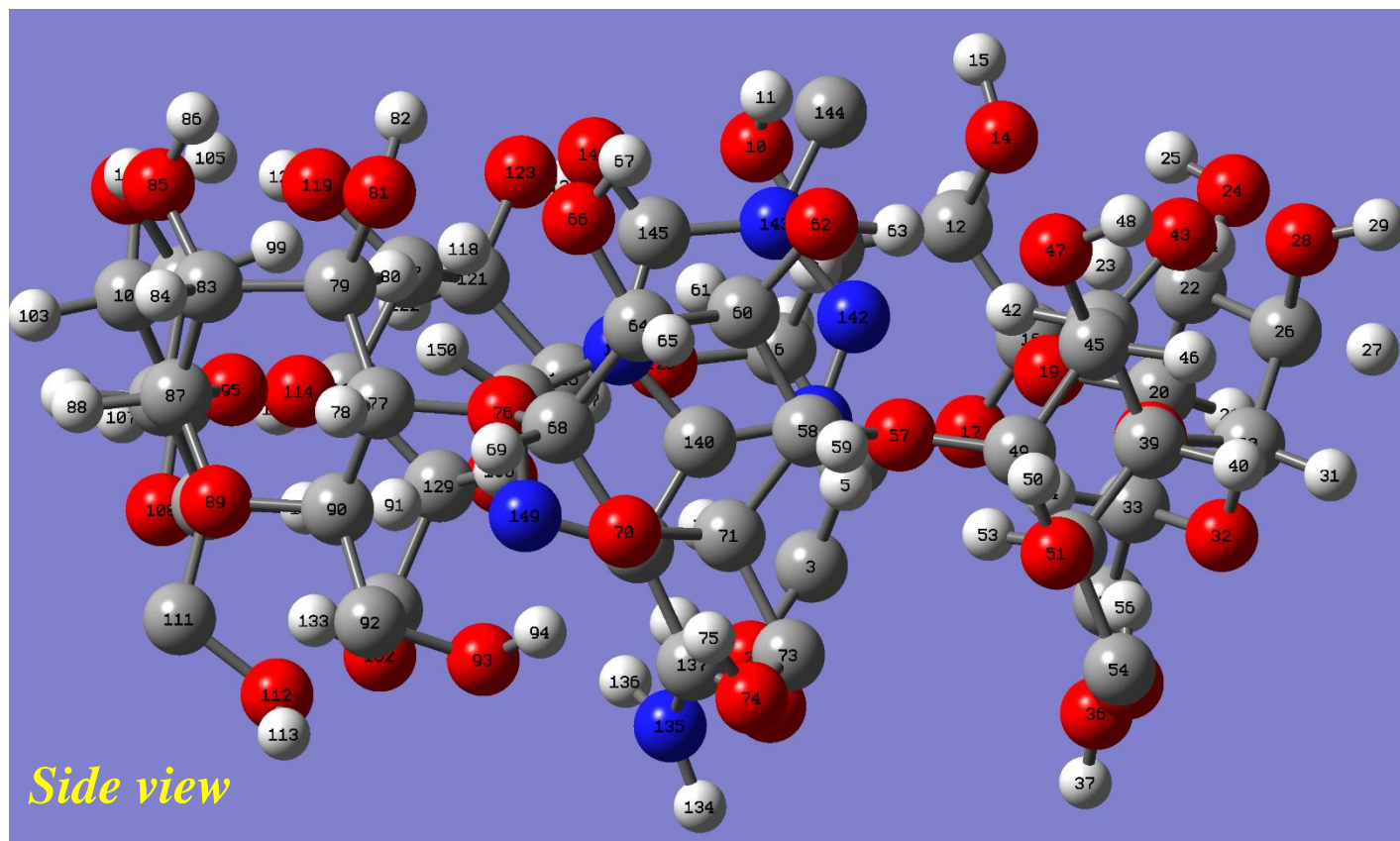
Top view

Side view

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Figure S1c

(TMZ in βCD at 60 ns)

Top view

Side view

Figure S1c

(TMZ in βCD at 100 ns)

Top view

Side view
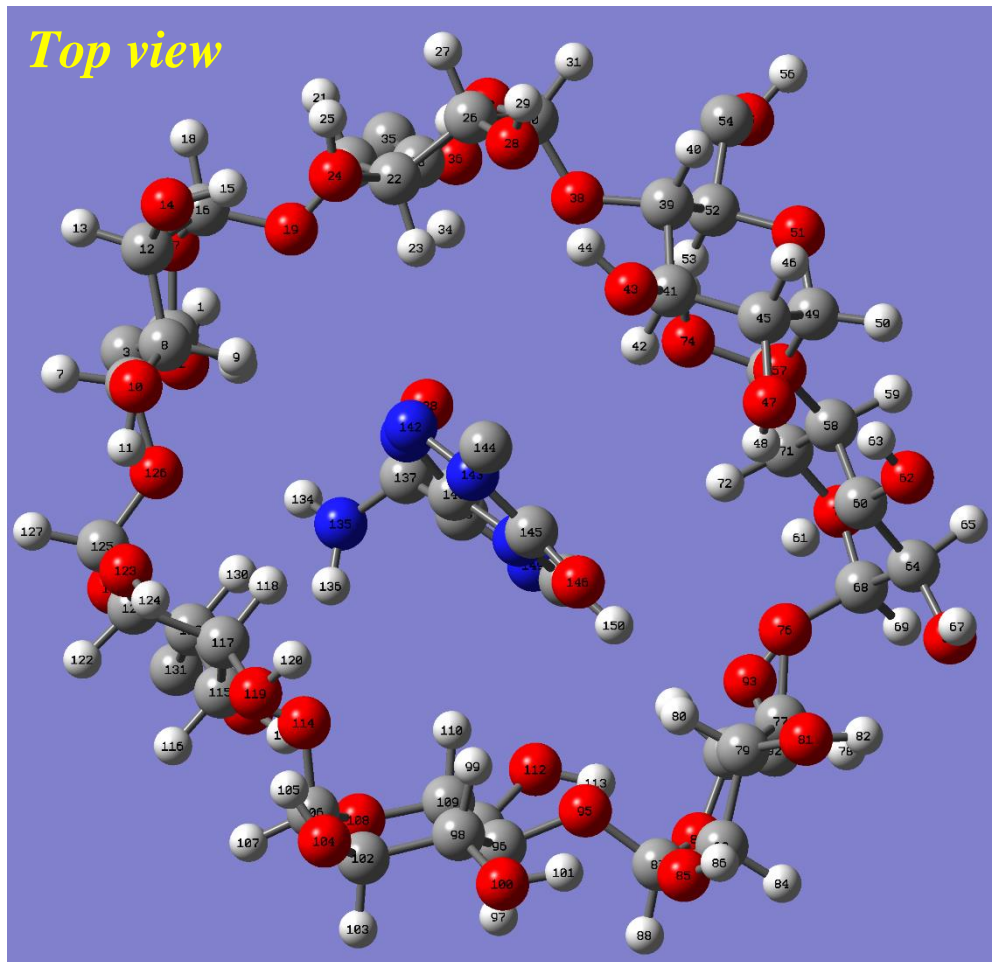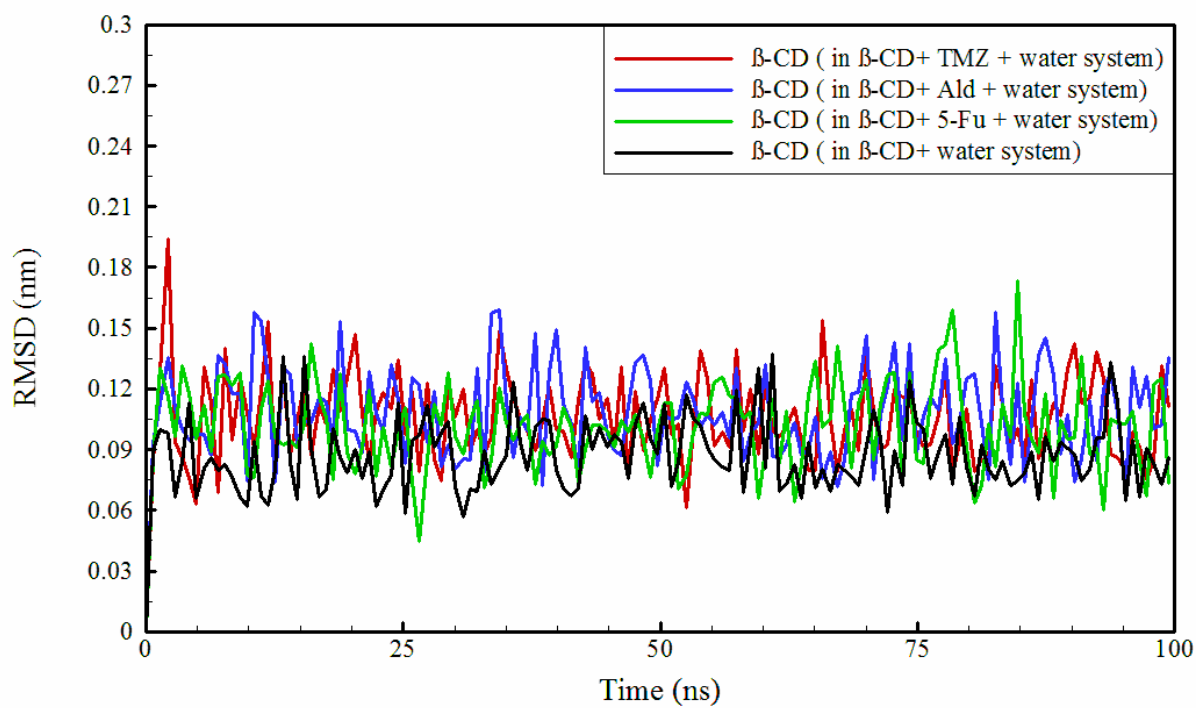
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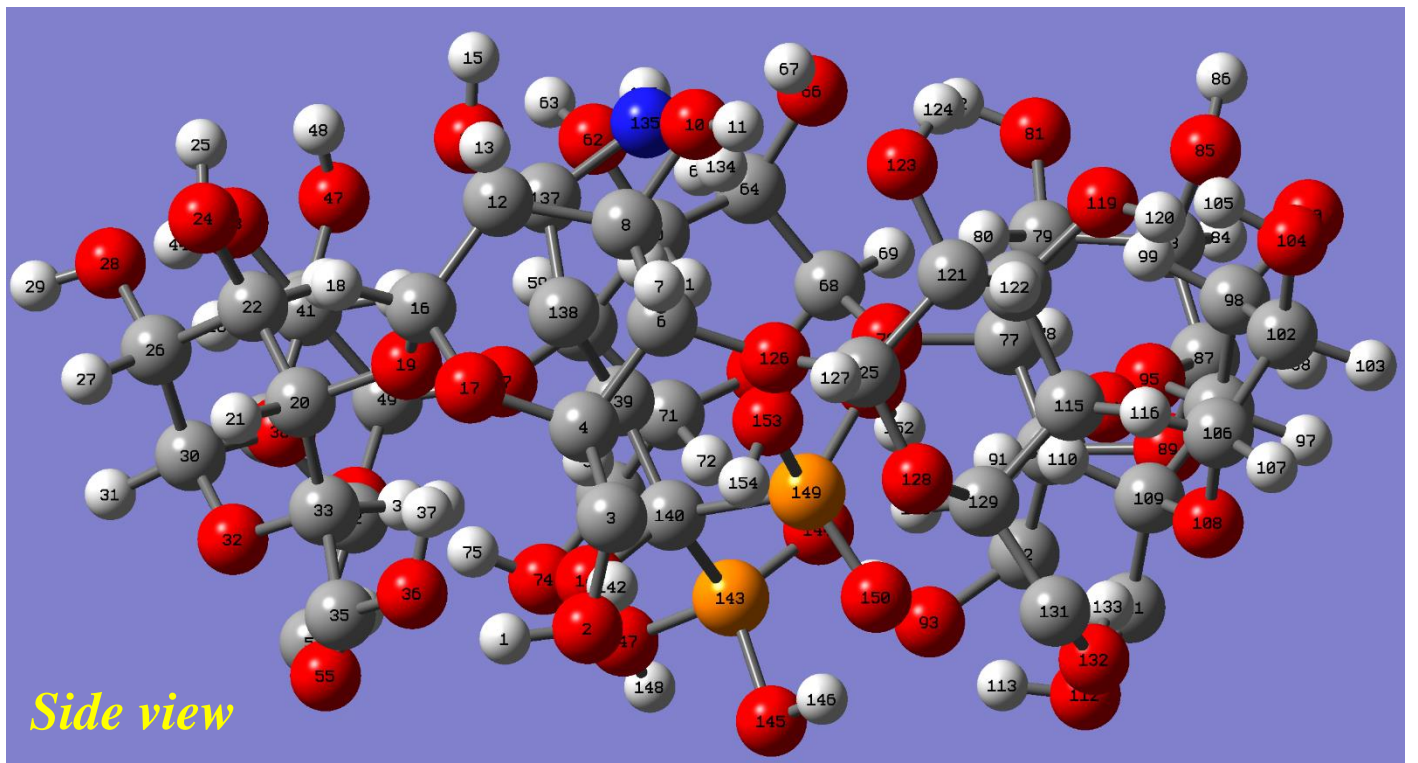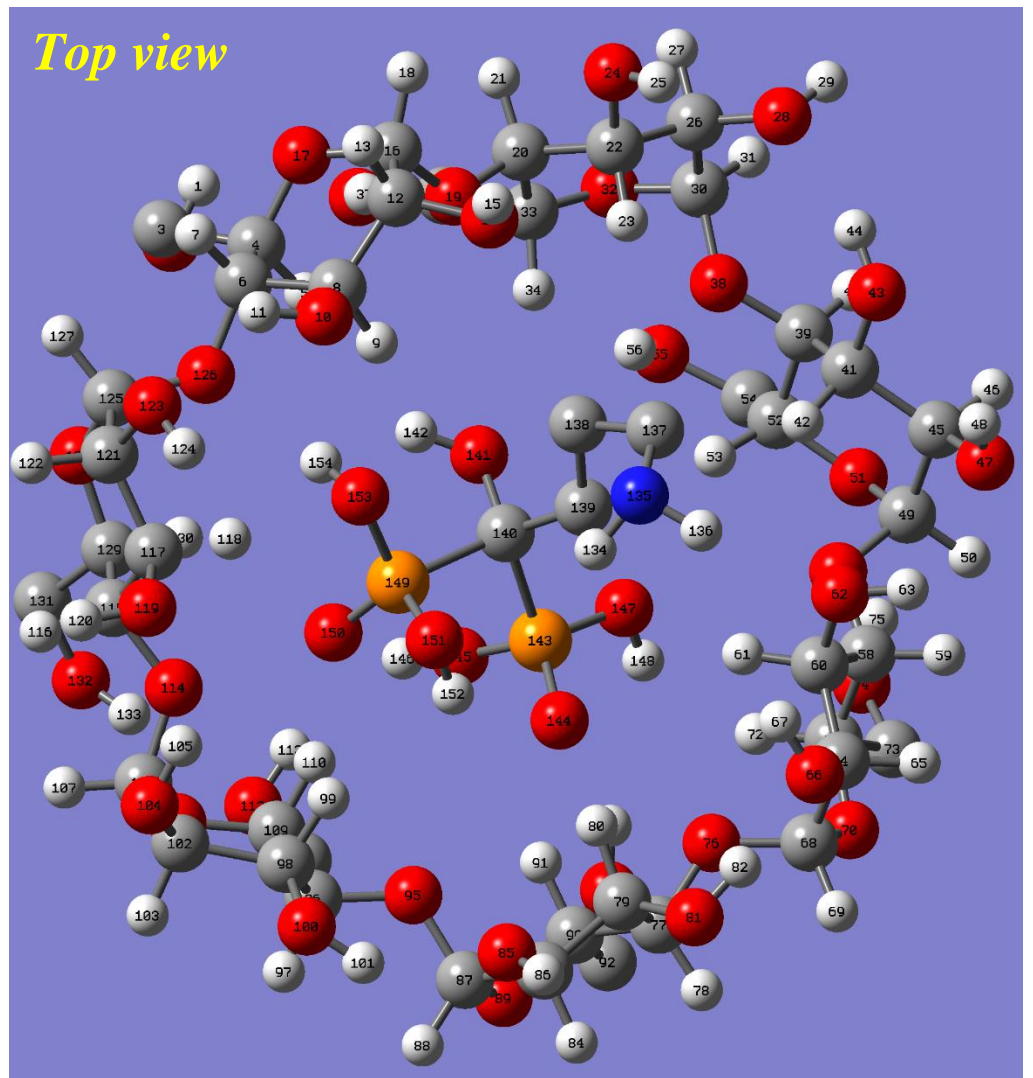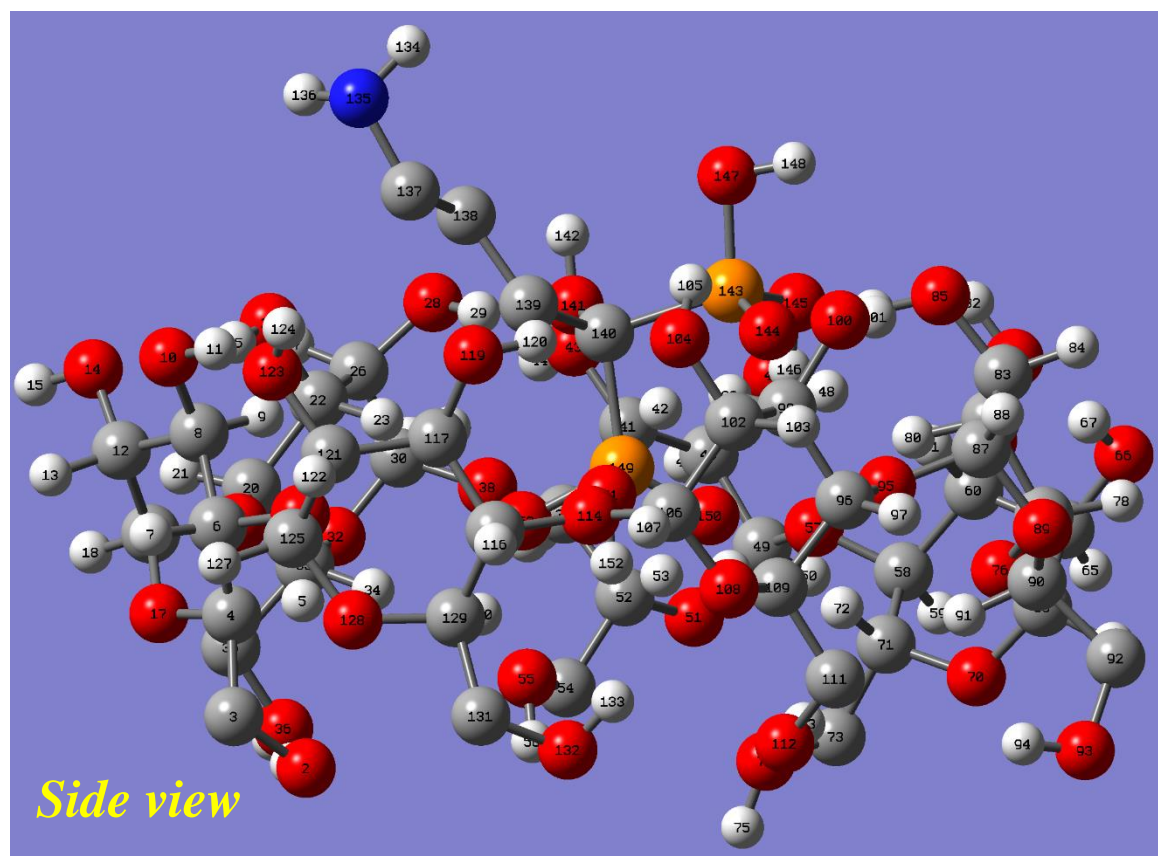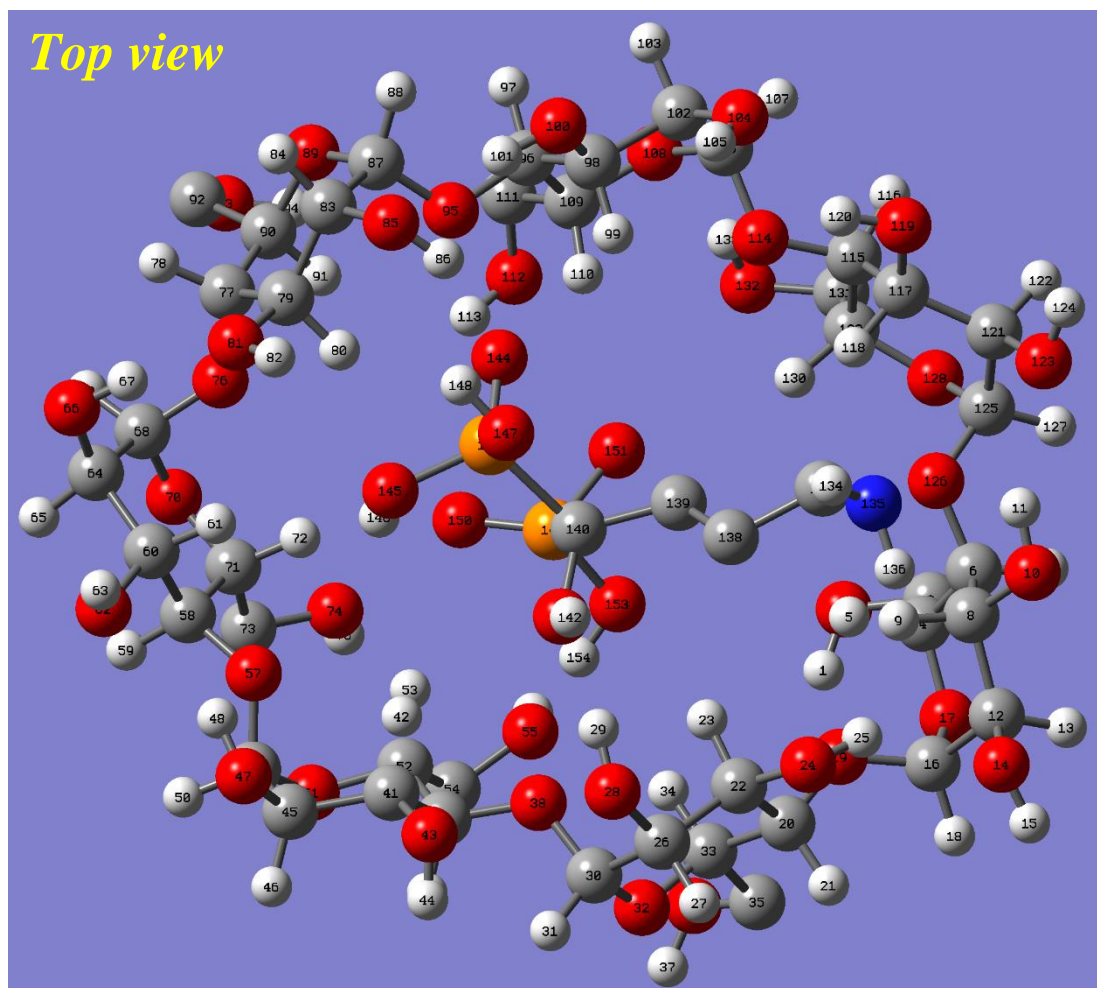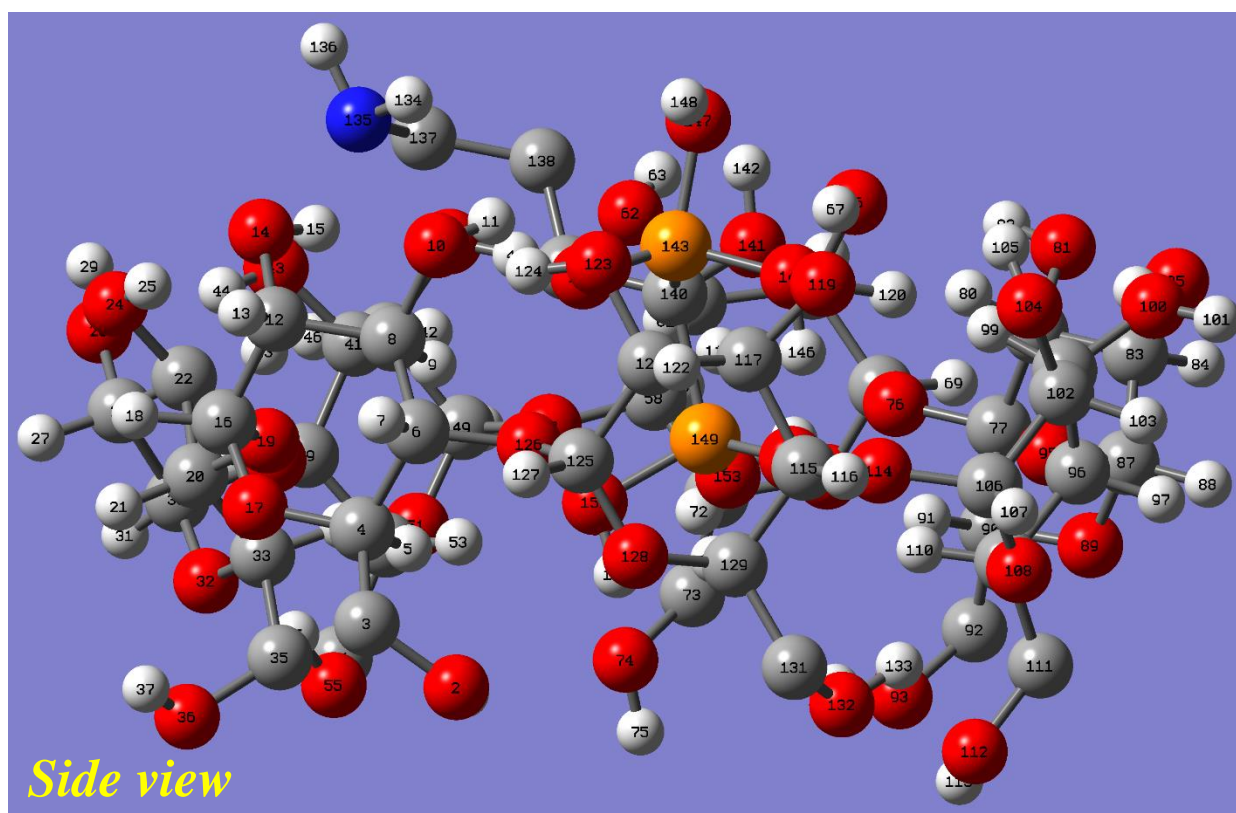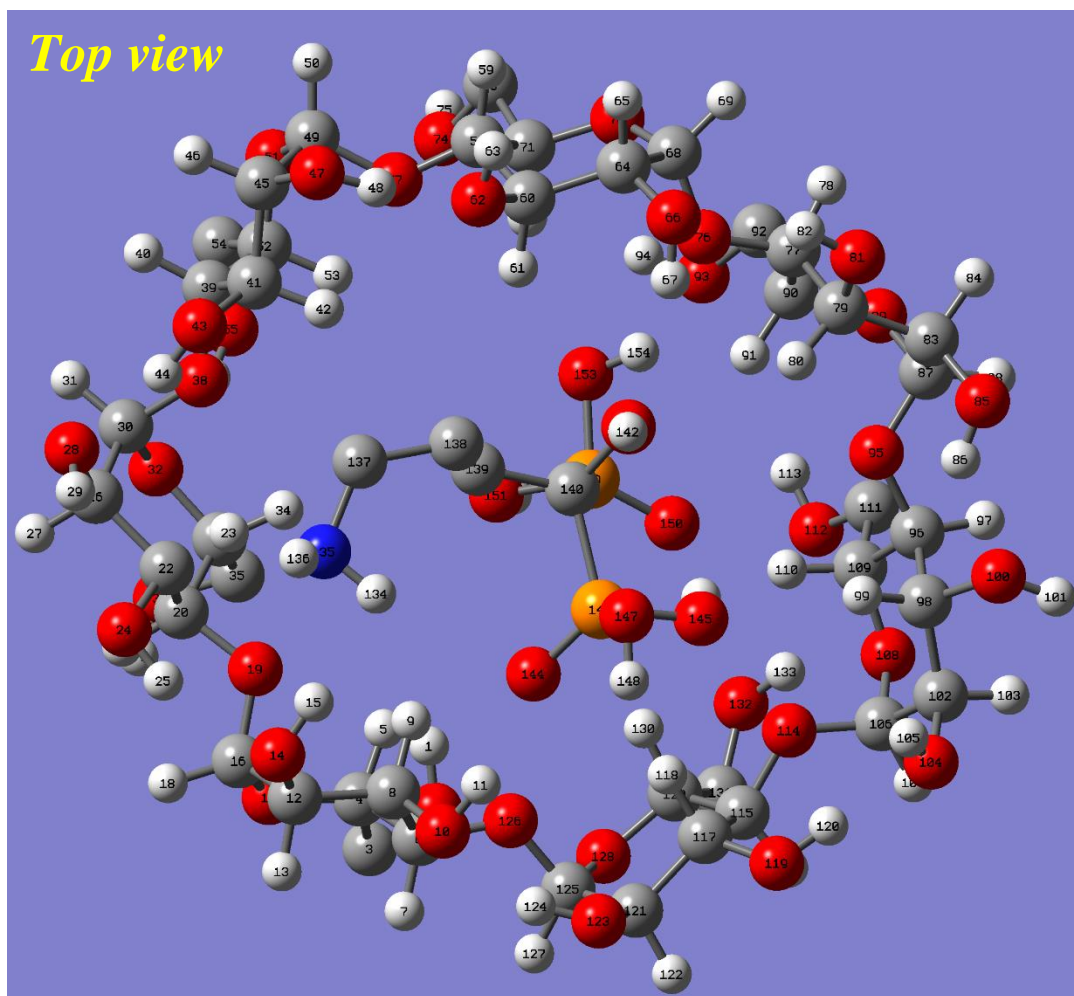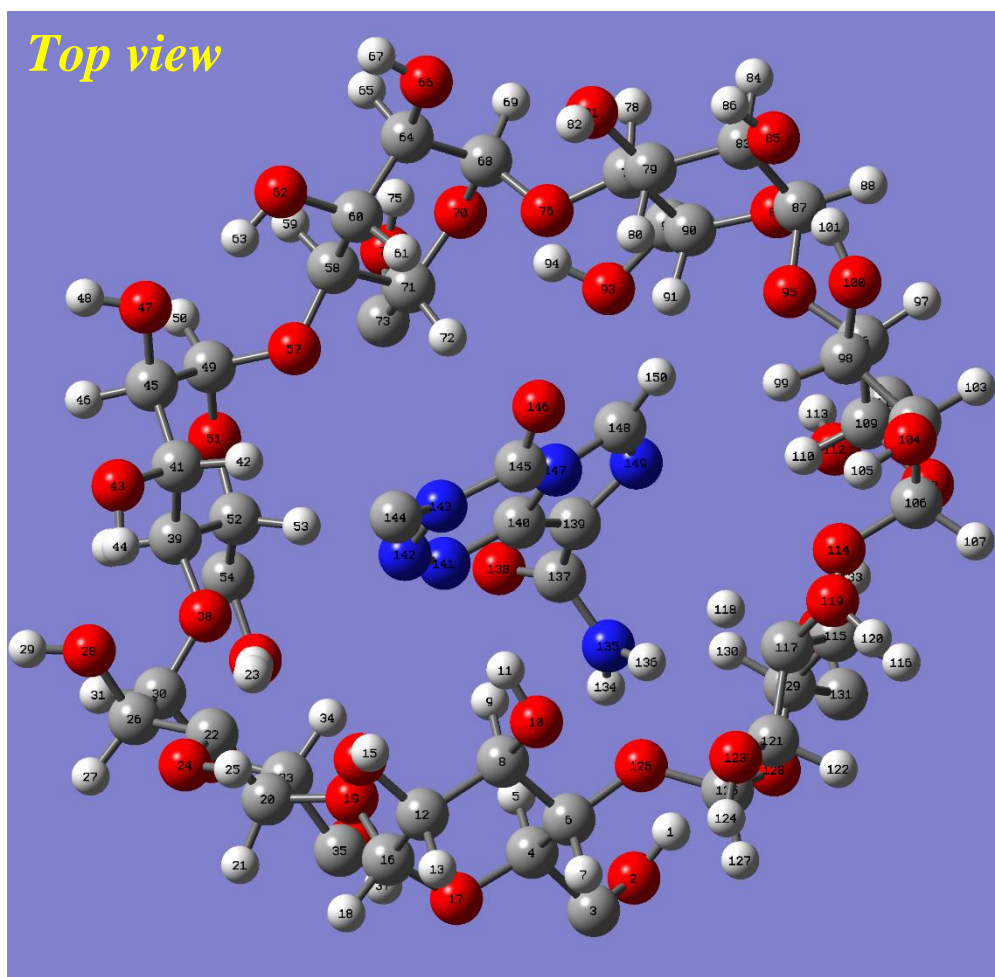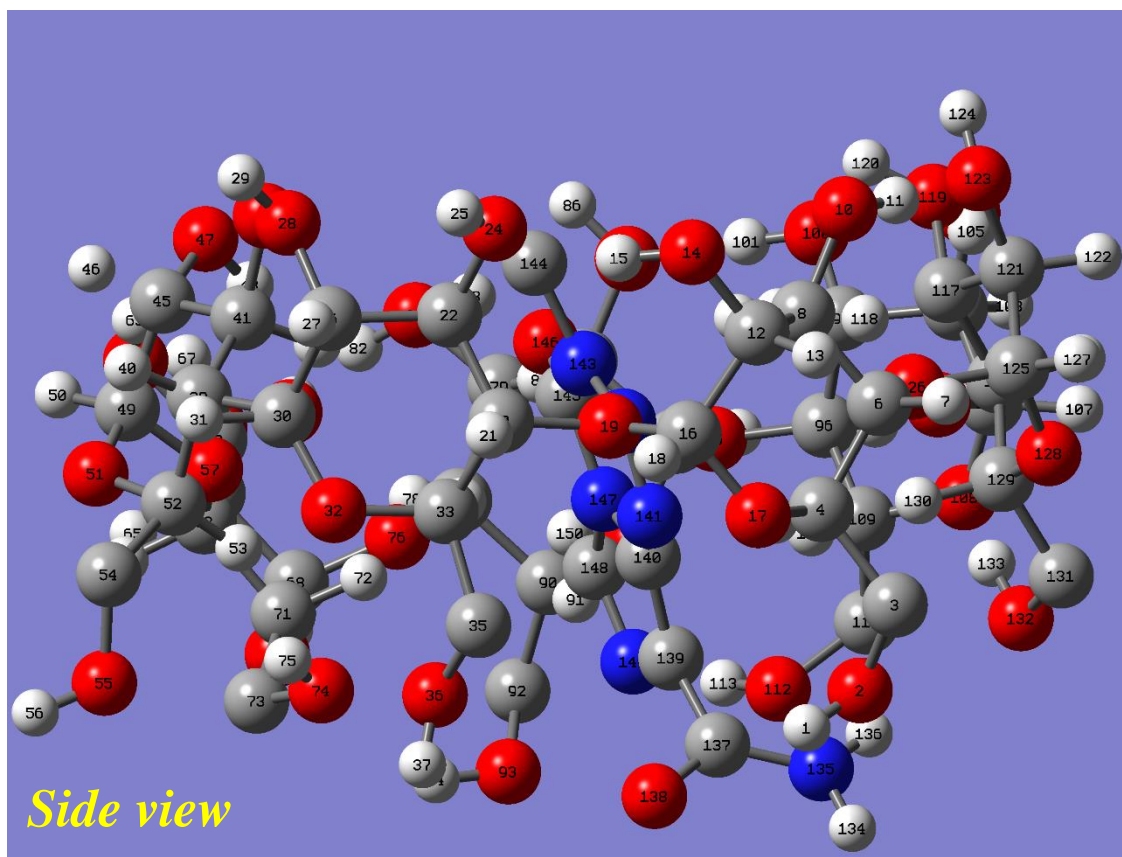
Figure S2: The Root mean square deviation of β-CD in different simulated and reference
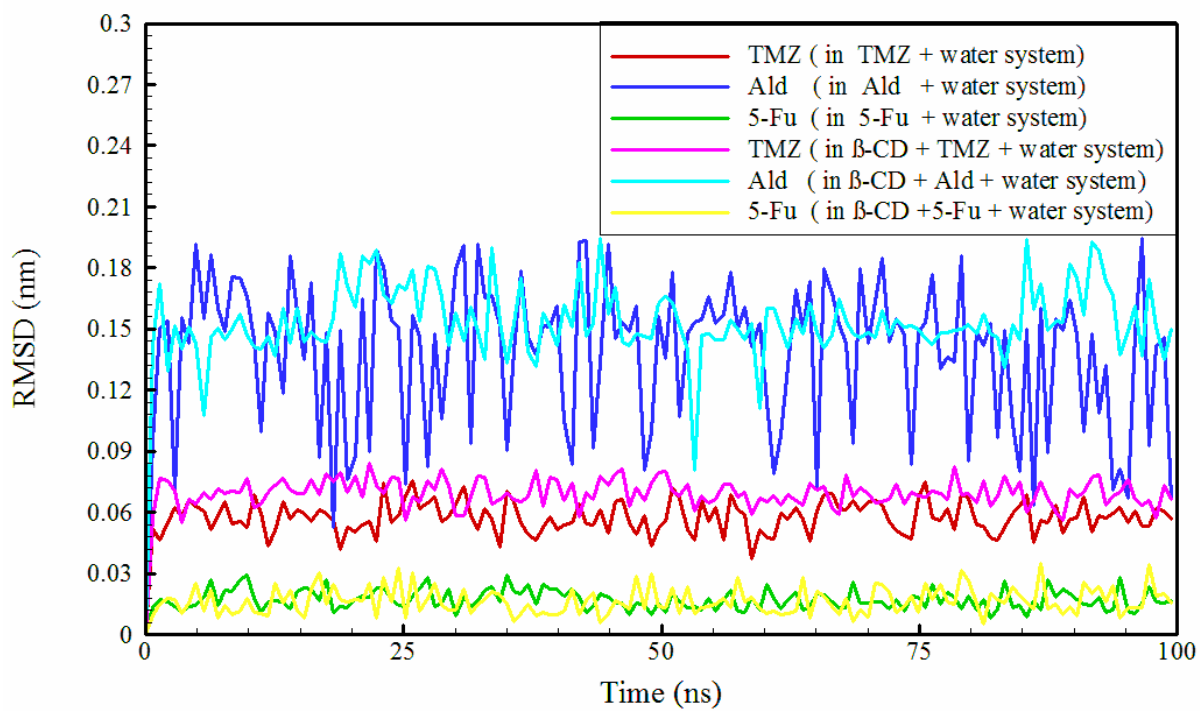
Figure S3: The Root mean square deviation of drugs in different simulated and reference systems