Table 1 Main bond length, bond angle, and dihedral angle of SF dug, original B12N12 nanocages, doped nanocages MB11N12 and encapsulated nanocages MB12N12. Where R(4,6) and R(6,6) are quadrilateral-hexagonal B-N bonds and hexagonal-hexagonal B-N bonds, where A(4,4) and A(6,6) are quadrilateral and hexagonal angles.

Systems	Bond length (Å)	Bond angle (º)	Dihedral angle (º)
SF	R(C-C) 1.51	A(S-C-H) 109.47	D(H-C-S-O) -0.01
	R(C-H) 1.07	A(C-S-O) 109.47	D(H-C-S-C) 179.97
	R(C-S) 1.78	A(C-S-C) 140.99	D(S-C-C-C) 179.99
	R(C-H) 1.12	A(C-N=C) 120.00	D(C-C-N=C) 179.98
	R(N=C) 1.29	A(N=C=S) 00.00	D(H-C-N=C) 58.61
	R(C=S) 1.56	A(H-C-H) 108.21	
	R(S=O) 1.67	A(C-C-C) 111.20	
B12N12	R(4,6) 1.49	A(4,4)-(B-N-B) 80.63	D(4,4)-(N-B-N-B) 12.02
	R(6,6) 1.44	A(4,4)-(N-B-N) 98.13	D(6,6)-(N-B-N-B) 24.61
		A(6,6)-(B-N-B) 111.71	D(4,6)-(N-B-N-B) 121.18
		A(6,6)-(N-B-N) 125.51	
BeB11N12	R(4,6) 1.47	A(4,4)-(B-N-B) 79.80	D(4,6)-(N-B-N-B) 121.18
	R(6,6) 1.45	A(4,4)-(N-B-N) 99.38	D(6,6)-(B-N-B-N) 24.88
	R(4,6)-(Be-N) 1.69	A(6,6)-(B-N-B) 110.21	D(4,4)-(B-N-B-N) 11.75
	R(6,6)-(Be-N) 1.58	A(6,6)-(N-B-N) 125.84	D(4,6)-(B-N-B-N) 112.47
		A(4,4)-(N-Be-N) 83.38	D(4,6)-(B-N-Be-N) 7.08
		A(6,6)-(N-Be-N) 120.29	D(4,6)-(N-B-N-Be) -125.56
MgB11N12	R(4,6) 1.47	A(4,4)-(B-N-B) 80.39	D(4,4)-(N-B-N-B) 12.38
	R(6,6) 1.46	A(4,4)-(N-B-N) 98.81	D(6,6)-(B-N-B-N) 26.33
	R(4,6)-(Mg-N) 2.07	A(6,6)-(B-N-B) 108.25	D(4,6)-(B-N-B-N) 134.25
	R(6,6)-(Mg-N) 1.96	A(6,6)-(N-B-N) 123.65	D(4,4)-(N-Mg-N-B) 1.05
		A(4,4)-(N-Mg-N) 69.21	D(6,6)-(B-N-Mg-N) 9.93
		A(6,6)-(N-Mg-N) 106.56	
CaB11N12	R(4,6) 1.48	A(4,4)-(B-N-B) 77.46	D(4,4)-(N-B-N-B) 13.53
	R(6,6) 1.44	A(4,4)-(N-B-N) 100.14	D(6,6)-(B-N-B-N) 24.69
	R(4,6)-(Ca-N) 2.33	A(6,6)-(B-N-B) 114.47	D(4,6)-(B-N-B-N) 135.13
	R(6,6)-(Ca-N) 2.20	A(6,6)-(N-B-N) 120.45	D(4,4)-(N-Ca-N-B) -4.11
		A(4,4)-(N-Ca-N) 60.71	D(6,6)-(B-N-Ca-N) 19.63
		A(6,6)-(N-Ca-N) 90.26	
BeB12N12	R(4,6) 1.49	A(4,4)-(B-N-B) 91.55	D(4,4)-(N-B-N-B) 12.06
	R(6,6) 1.45	A(4,4)-(N-B-N) 93.32	D(6,6)-(B-N-B-N) 25.04
	R(4,6)’ 1.66	A(4,4)-(B-N-B)’ 91.49	D(4,6)-(B-N-B-N) 135.56
	R(6,6)’ 1.59	A(4,4)-(N-B-N)’ 82.33	
	Be-B 1.69	A(6,6)-(B-N-B) 111.34	
	Be-N 1.60	A(6,6)-(N-B-N) 125.38	
		A(6,6)-(B-N-B)’ 126.92	
		A(6,6)-(N-B-N)’ 101.65	
MgB12N12	R(4,6) 1.51	A(4,4)-(B-N-B) 85.43	D(6,6)-(N-B-N-B) 11.82
	R(6,6) 1.44	A(4,4)-(N-B-N) 94.42	D(4,4)-(N-B-N-B) 4.67

	Mg-B	2.26	A(6,6)-(B-N-B)	116.72	D(4,6)-(B-N-B-N)	127.47
	Mg-N	2.36	A(6,6)-(N-B-N)	122.06		
	R(4,6)	1.50	A(4,4)-(B-N-B)	83.46	D(6,6)-(N-B-N-B)	12.42
CaB12N12	R(6,6)	1.45	A(4,4)-(N-B-N)	95.55	D(4,4)-(N-B-N-B)	5.21
	Ca-B	2.29	A(6,6)-(B-N-B)	117.65	D(4,6)-(B-N-B-N)	126.31
	Ca-N	2.37	A(6,6)-(N-B-N)	122.45		

Fig. 1 NBO charge distribution of SF drug, nanocages and complexes

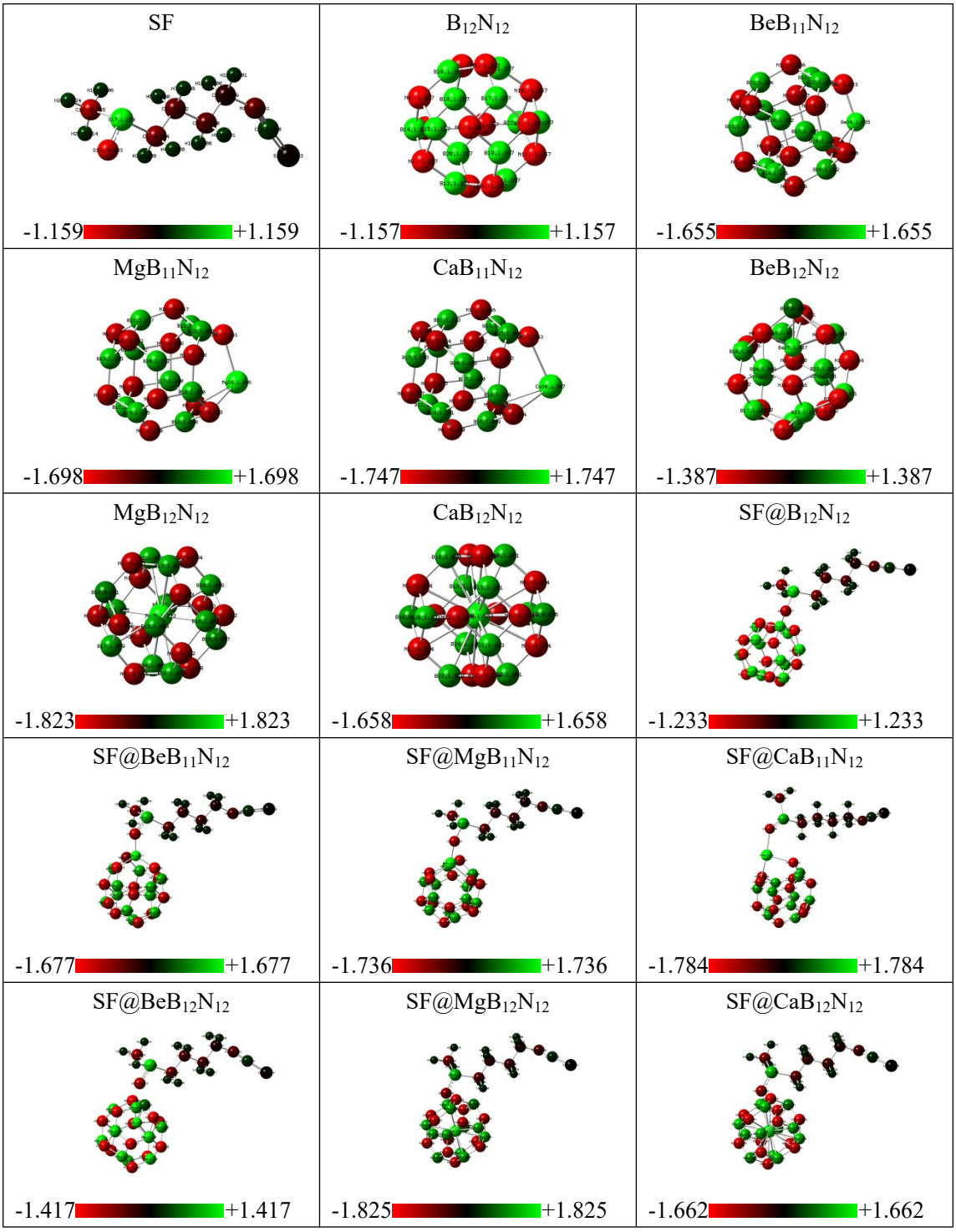
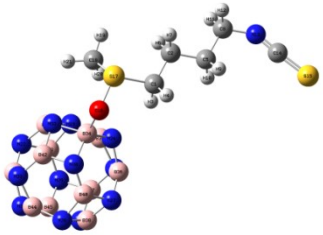
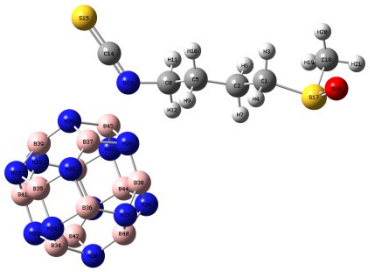
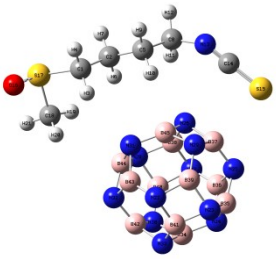
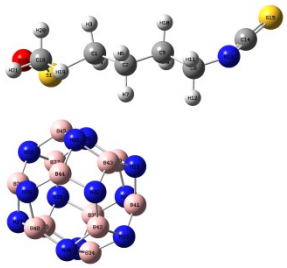
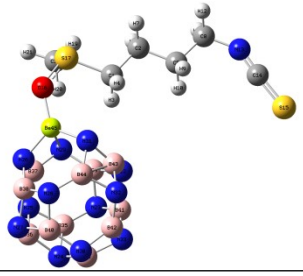
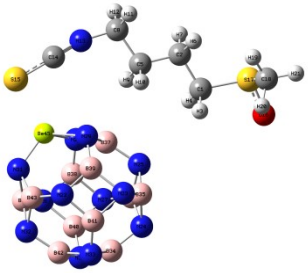
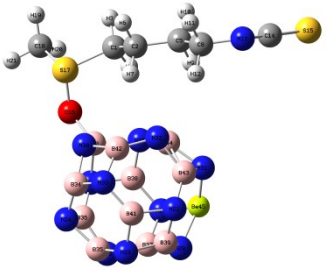
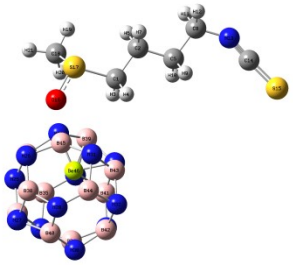
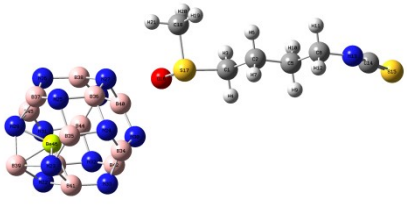
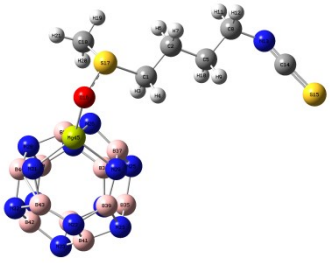
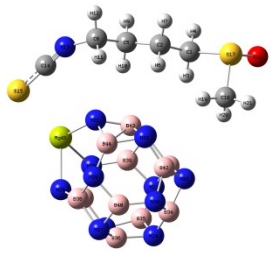
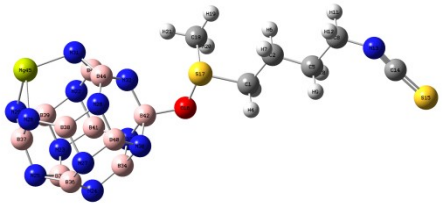
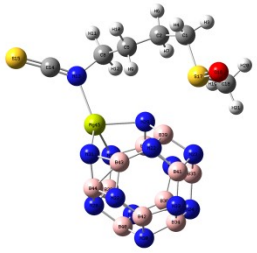
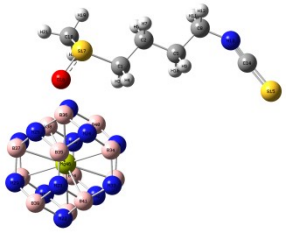
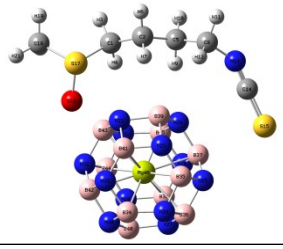
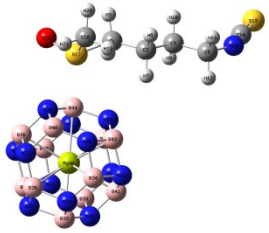
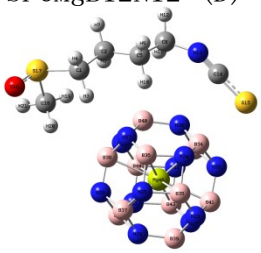
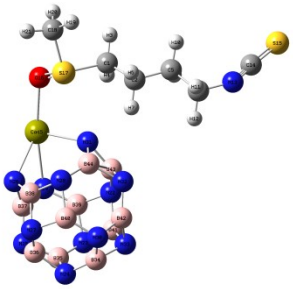
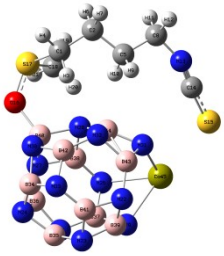
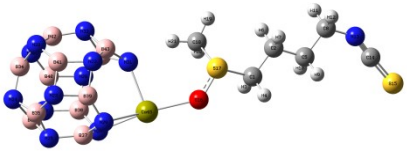


Fig. 2 The structures of complexes formed by sulforaphane adsorption on B12N12, MB11N12 and MB12N12 nanocages

SF@B12N12 (A)	SF@B12N12 (B)
	
SF@B12N12 (C)	SF@B12N12 (D)
	
SF@BeB11N12 (A)	SF@BeB11N12 (B)
	
SF@BeB11N12 (C)	SF@BeB12N12 (A)
	
SF@BeB12N12 (B)	SF@MgB11N12 (A)
	
SF@MgB11N12 (B)	SF@MgB11N12 (C)

	
SF@MgB11N12 (D)	SF@MgB12N12 (A)
	
SF@MgB12N12 (B)	SF@MgB12N12 (C)
	
SF@MgB12N12 (D)	SF@CaB11N12 (A)
	
SF@CaB11N12 (B)	SF@CaB11N12 (C)
	
SF@CaB11N12 (D)	SF@CaB12N12 (A)

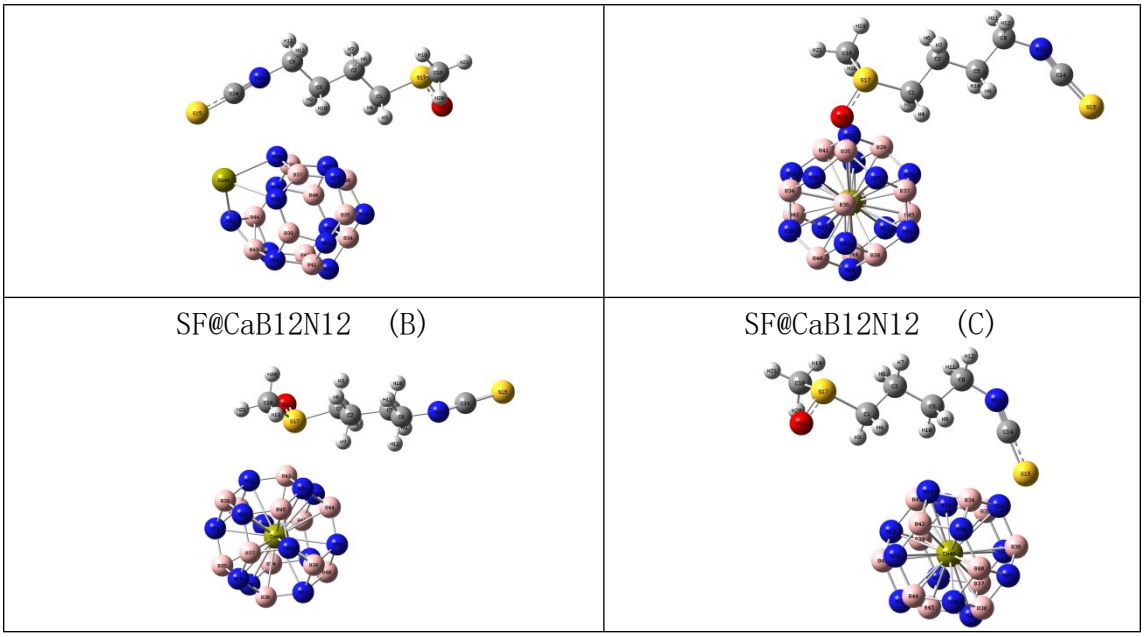


Table 2 The Adsorption energy of complexes formed by sulforaphane adsorbed on B12N12, MB11N12 and MB12N12 nanocages

Complexes	Adsorption energy(kcal/mol)	Complexes	Adsorption energy(kcal/mol)
SF@B12N12 (A)	-58.00	SF@MgB11N12 (D)	-34.59
SF@B12N12 (B)	-32.70	SF@MgB12N12 (A)	-33.78
SF@B12N12 (C)	-13.39	SF@MgB12N12 (B)	-21.61
SF@B12N12 (D)	-28.26	SF@MgB12N12 (C)	-15.23
SF@BeB11N12 (A)	-66.14	SF@MgB12N12 (D)	-18.32
SF@BeB11N12 (B)	-27.65	SF@CaB11N12 (A)	-44.13
SF@BeB11N12 (C)	-63.19	SF@CaB11N12 (B)	-44.06
SF@BeB12N12 (A)	-22.32	SF@CaB11N12 (C)	-29.70
SF@BeB12N12 (B)	-14.89	SF@CaB11N12 (D)	-39.93
SF@MgB11N12 (A)	-51.43	SF@CaB12N12 (A)	-38.34
SF@MgB11N12 (B)	-39.67	SF@CaB12N12 (B)	-16.32
SF@MgB11N12 (C)	-50.86	SF@CaB12N12 (C)	-10.55

The different combining modes between drug and nanocage were considered to confirmed the lowest isomer of the studied comolexes. We have considered different combining modes between drug and nanocages, in which drugs adsorbed on B12N12 nanocages have four structures: structure (A) was through O atom adsorbed on B atom of nanocages, structure (B) was through N atom on cyanide group adsorbed on B atom of nanocages, structure (C) was through S atom on cyanide group adsorbed on B atom of nanocages, and structure (D) was through S atom on sulfuryl group

adsorbed on B atom of nanocages. The adsorption energies were -58.00, -32.70, -13.39, and -28.26 kcal/mol, respectively. The adsorption on BeB11N12 nanocages have three structures: structure (A) was through O atoma dsorbed on the Be atom of nanocages, structure (B) was through S atom on cyanide group adsorbed on the Be atom of nanocages, and structure (C) was through O atoma dsorbed on the B atom of nanocages. The adsorption energy is -66.14, -27.65 and -63.19 kcal/mol, respectively. There are two kinds of structures of drugs absorbed on BeB12N12 nanocages: structure (A) was O atom absobed on the B atom near Be atom of nanocages and structure (B) was O atom absobed on B atom far from Be atom of nanocages. The adsorption energies are -22.32 and -14.89 kcal/mol, respectively. There are four kinds of adsorption structures of drugs adsorbed on MgB11N12 nanocages: structure (A) was O atom adsorbed on Mg atom of nanocages,structure (B) was S atom on the cyanide group adsorbed on Mg atom of nanocages, structure (C) was O atom adsorbed on B atom of nanocages, and structure (D) was N atom on the cyanide group adsorbed on Mg atom of nanocages. The adsorption energies were -51.43, -39.67, -50.86, and -34.59 kcal/mol, respectively. There are four kinds of adsorption structures on MgB12N12 nanocages: structure (A) was O atom adsorbed on B atom of nanocages, structure (B) was O atom and S atom(on cyanide group) adsorbed on B atom of nanocages, structure (C) was S atom on the thionyl group adsorbed B atom of nanocages, and structure (D) was S atom on the cyanide group adsorbed on B atom of nanocage. The adsorption energies are -33.78, -21.61, -15.23, and -18.32 kcal/mol, respectively. There are four kinds of adsorption structures on CaB11N12 nanocages: structure (A) was O atom adsorbed on Ca atom of nanocages, structure (B) was O atom and S atom(on cyanide group) adsorbed on Ca atom of nanocages, structure (C) was O atoms adsorbated on Ca atoms of nanocage, and structure (D) was S atoms on cyanide group absorbed on Ca atoms of nanocage, and the adsorption energies are -44.13, -44.06, -29.70, and -39.93 kcal/mol, respectively. There are three kinds of adsorption structures on CaB11N12 nanocages: structure (A) was O atom adsorbed on B atom of nanocages, structure (B) was S atom on sulfuryl group adsorbed on B atom of nanocages, and structure (C) was S atom on cyanide group adsorbed on B atom of

nanocages. The adsorption energies are -38.34 and -16.32 and -10.55,kcal/mol, respectively. Among the complexes obtained, the complexes formed by O atom (on drugs) adsorbed to Be, Mg, Ca and B atoms (on nanocages) had the highest adsorption energy, indicating that their structures were the most stable.

In conclusion, among the obtained complexes, the complexes formed by sulforaphanin adsorbed to Be, Mg, Ca, and B atoms on the nanocages through the O atom on the sulfuryl group have the largest adsorption energy, indicating that its structure is the most stable. Therefore, through analytical screening, we separately selected type A of all the above structures as the research object.