Electronic supplementary information (ESI)

Theoretical study of allopurinol drug sensing by carbon and boron nitride nanostructures: A DFT, QTAIM, RDG, NBO and PCM insight

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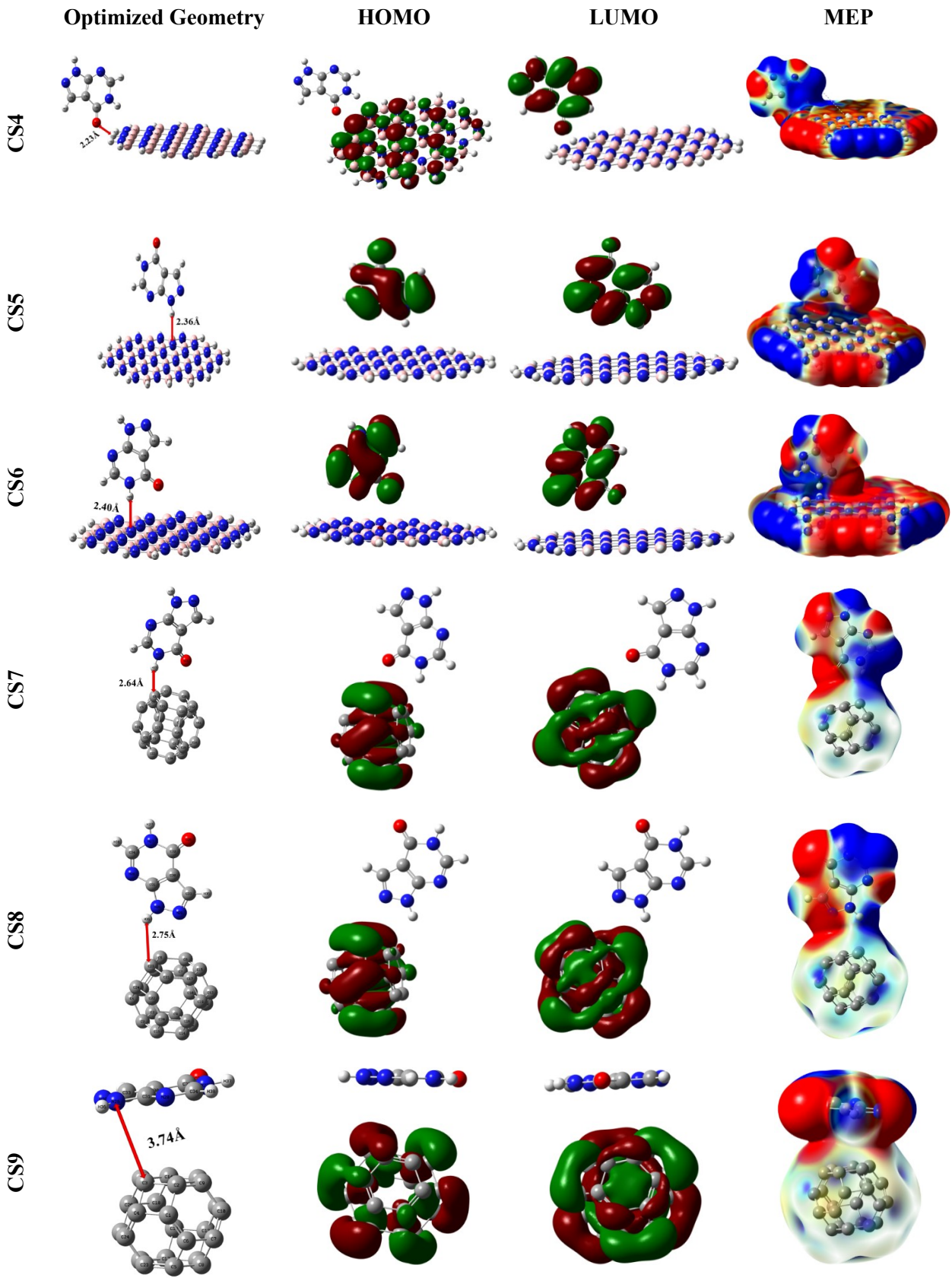

Optimized Geometry
HOMO
LUMO
MEP
CS4
CS5
CS6
CS7
CS8
CS9
2.23Å
2.36Å
2.40Å
2.64Å
2.75Å
3.74Å

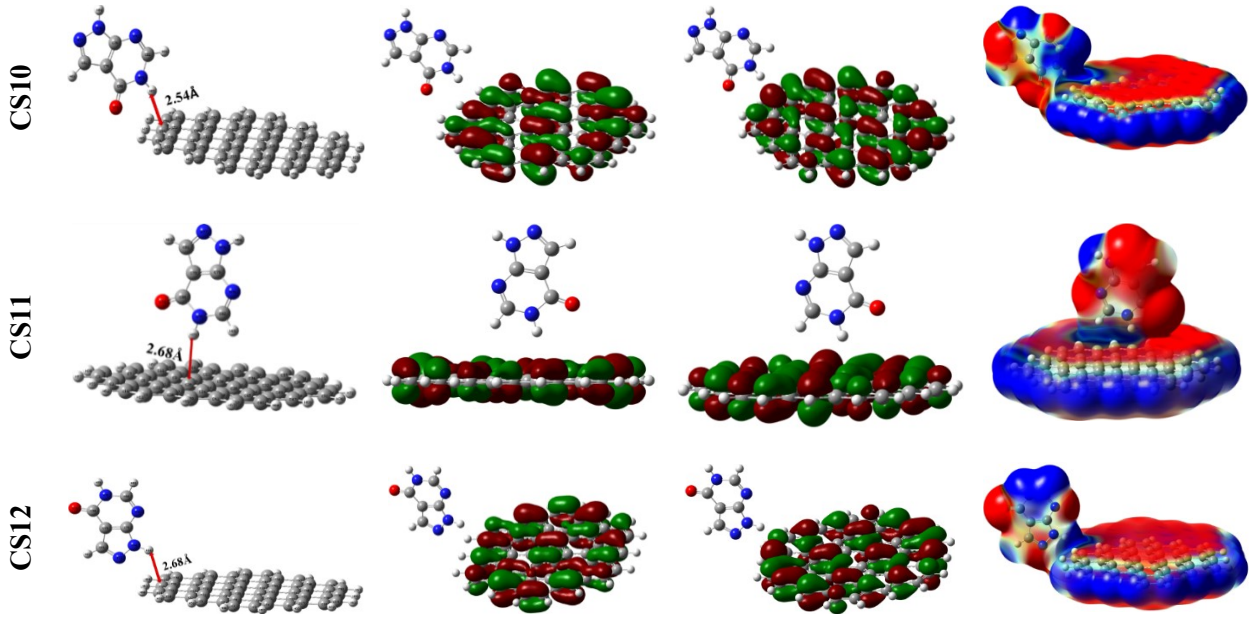
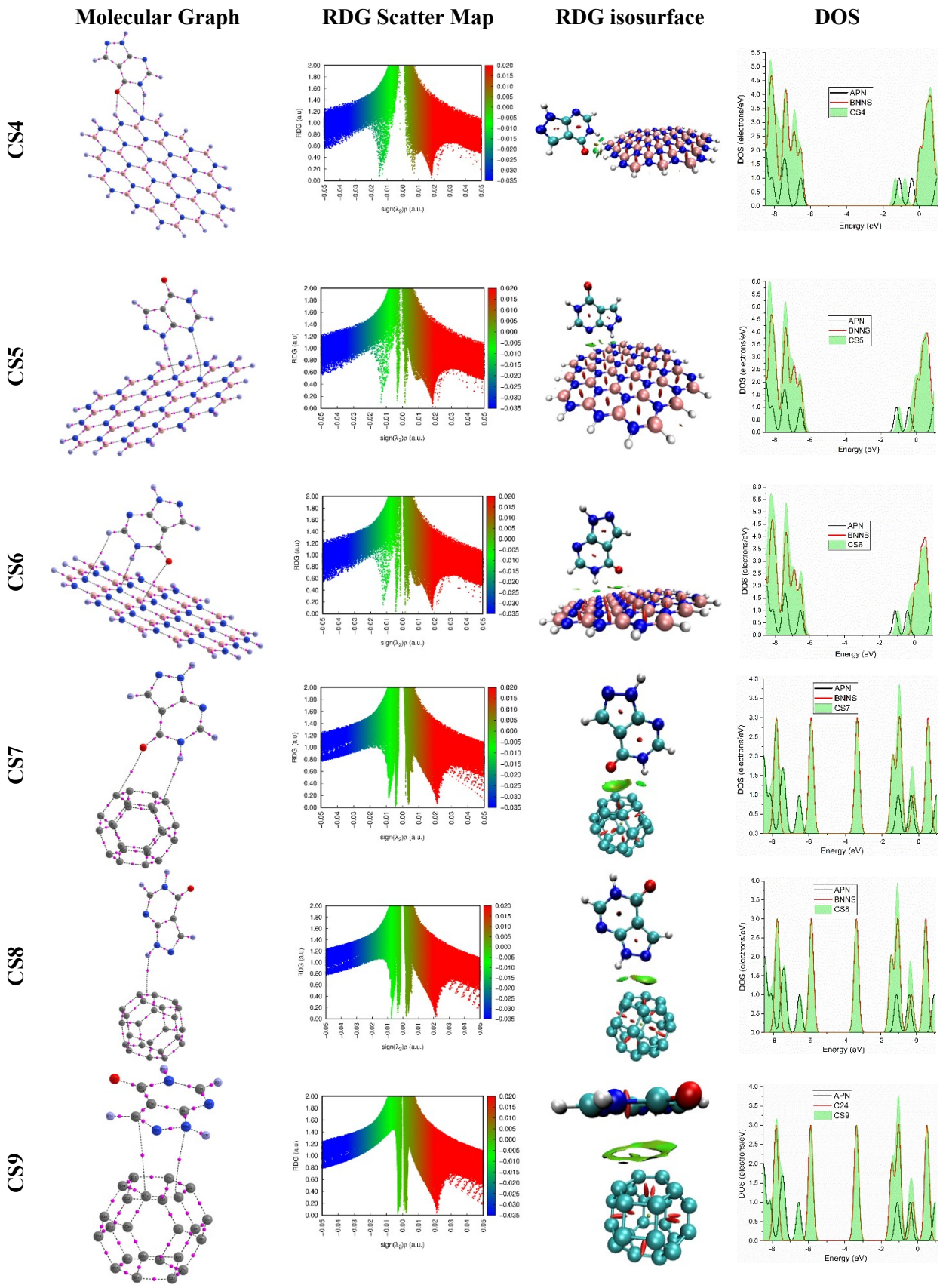


Fig. S1: Optimized geometries, HOMO, LUMO and MEP of CS4-CS12 structures. The MEP surfaces are defined by 0.0004 electron/bohr^3 contour of the electronic density. The Red to blue (- 0.01 a.u. to 0.01 a.u.) colour scheme for MEP surface by indicating the electron rich to electron deficient or partially negative charge to partially positive charge region of the surface respectively.


Molecular Graph
RDG Scatter Map
RDG isosurface
DOS
CS4
CS5
CS6
CS7
CS8
CS9
RDG (a.u)
sign(λ2)ρ (a.u.)
DOS (electrons/eV)
Energy (eV)
APN
BNNS
CS4
CS5
CS6
CS7
CS8
C24
CS9

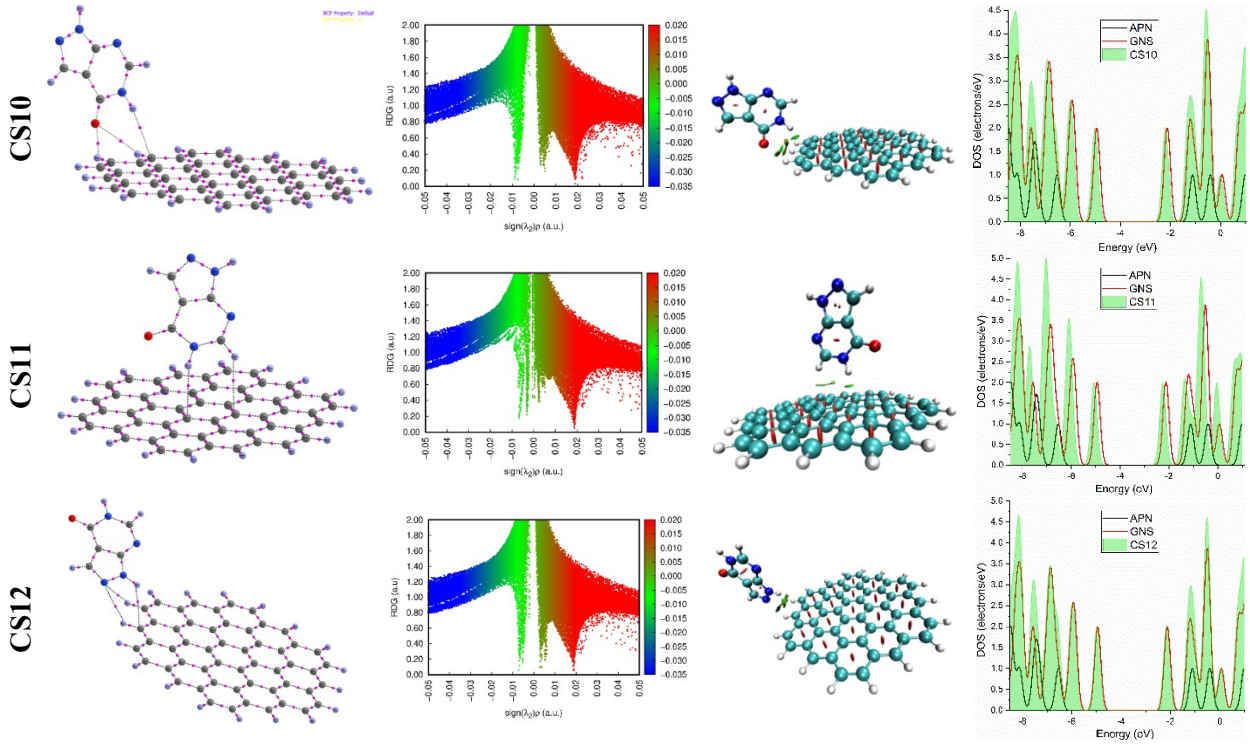


Fig. S2: The molecular graphs, RDG Scatter Map, RDG isosurface and DOS of CS4 – CS12 structures.

Table S1: Structural properties of APN drug molecule.

Interatomic distance in Angstrom				Angle in Degree			
Interacting Atoms	**Our Investigation**	**B3LYP/ 6-311+(d,p)**	**HF**	**Involved Atoms**	**Our Investigation**	**B3LYP/ 6-311+(d,p)**	**HF**
O1-C8	1.22	1.22	1.20	∠N5-N2-C7	112.7	112.5	112.2
				∠N5-N2-H12	120.0	120	120.4
N2-N5-	1.36	1.36	1.35	∠C7-N2-H12	127.3	127.5	120.3
N2-C7	1.35	1.35	1.33	∠C8-N3-C10	125.8	125.7	125.4
				∠C8-N3-H13	114.6	114.9	115.3
N2-H12	1.01	1.01	0.99	∠C10-N3-H13	119.6	119.4	119.3
N3-C8	1.43	1.43	1.41	∠C7-N4-C10	112.4	112.7	112.5
				∠N2-N5-C9	105.3	105.6	106.1
N3-C10	1.37	1.37	1.36	∠C7-C6-C8	119.2	119.1	119.3
N3-H13	1.01	1.01	1.00	∠C7-C6-C9	104.8	104.8	104.3
				∠C8-C6-C9	136.0	136.1	136.4
N4-C7	1.37	1.37	1.37	∠N2-C7-N4	126.0	125.1	126
N4-C10	1.31	1.30	1.28	∠N2-C7-C6	106.0	106	106.6
				∠N4-C7-C6	128.1	127.9	127.4
N5-C9	1.33	1.32	1.30	∠O1-C8-N3	120.3	120.3	120.3
C6-C7	1.40	1.4	1.39	∠O1-C8-C6	130.1	129.9	129.9
				∠N3-C8-C6	109.6	109.8	109.8
C6-C8	1.44	1.44	1.44	∠N5-C9-C6	111.3	111	110.8
C6-C9	1.42	1.42	1.42	∠N5-C9-H11	120.2	120.2	120.8
				∠C6-C9-H11	128.5	128.7	128.4
C9-H11	1.08	1.08	1.07	∠N3-C10-N4	125.0	124.9	125.6
				∠N3-C10-H14	115.7	115.8	115.3
C10-H14	1.09	1.09	1.08	∠N4-C10-H14	119.3	119.4	119.1

Table S2: The values of fractional number of charge transfer (ΔN), the change in individual energy of the donor molecule ($\Delta E_{B(A)}$), the change in individual energy of the acceptor molecule ($\Delta E_{A(B)}$) and total stabilization energy of conjugated structure ($\Delta E_{SE(AB)}$).

Systems	ΔN	$\Delta E_{A(B)}$**(eV)**	$\Delta E_{B(A)}$**(eV)**	$\Delta E_{SE(AB)}$**(eV)**
APN-BNNC	-0.08	0.30	-0.32	-0.02
APN-BNNS	0.09	-0.33	0.31	-0.02
APN-CNC	-0.20	0.82	-0.90	-0.08
APN-GNS	0.07	-0.26	0.25	-0.01