The supplementary materials for

On the potential of WSi_{12} superatom as a drug carrier: A DFT study

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1. Tables

Table S1 Crucial geometric parameters and the HOMO-LUMO gap (in eV) of WSi_{12} calculated by using different methods in conjunction with the Aug-cc-pvDZ basis set for main group atoms and LANL2DZ for W atom.

Methods	W-Si (in Å)	Si_T-Si_T (in Å)	Si_L-Si_L (in Å)	Gap
B3PW91-D3(BJ)	**2.670**	**2.378**	**2.428**	**2.76**
B3LYP-D3(BJ)	2.694	2.396	2.456	2.73
HSE06	2.668	2.378	2.418	2.35

Table S2 Crucial geometric parameters (in Å) as well as the HOMO-LUMO gap (in eV) and binding energy per atom (E_b, in eV) of WSi_{12} calculated by using B3PW91-D3(BJ) method in conjunction with different basis sets for the main group atoms and LANL2DZ for W atom.

Basis set	W-Si	Si_T-Si_T	Si_L-Si_L	Gap	E_b[a]
6-31G(d)	2.656	2.365	2.415	2.74	5.43
6-31+G(d)	2.656	2.365	2.416	2.74	5.40
Aug-cc-pVDZ	2.670	2.378	2.428	2.76	5.44
6-311+G(d)	**2.654**	**2.363**	**2.418**	**2.76**	**5.44**
6-311+G(3df)	2.647	2.359	2.402	2.76	5.53

[a]E_b is calculated by using the formula $E_b = \frac{E(W) + 12E(Si) - E(WSi_{12})}{13}$.

Table S3 Crucial geometric parameters (in Å) as well as the HOMO-LUMO gap (in eV) and binding energy per atom (E_b, in eV) of WSi_{12} calculated by using B3PW91-D3(BJ) method in conjunction with 6-311+G(d) basis set for main group atoms and different basis sets for W atom.

Basis set	W-Si	Si_T-Si_T	Si_L-Si_L	Gap	E_b[a]
LANL2DZ	**2.654**	**2.363**	**2.418**	**2.76**	**5.44**
SDD	2.659	2.368	2.419	2.76	5.39
Def2-TZVP	2.659	2.367	2.419	2.79	5.41
Aug-cc-pVDZ-pp	2.655	2.365	2.413	2.83	5.47

[a]E_b is calculated by using the formula $E_b = \frac{E(W) + 12E(Si) - E(WSi_{12})}{13}$.

Table S4 The proton binding energies (E_b', in kcal/mol) for the nitrogen and sulfur atoms of 6-TG.

Binding sites	E_b'
S1	152.89
N1	120.26
N2	139.48
N3	152.23
N4	122.66
N5	**163.14**

2. Figures

Fig. S1 ESP diagrams of the studied 5-Fu, 5-ASA, INH, 6-TG, and TMZ drugs.

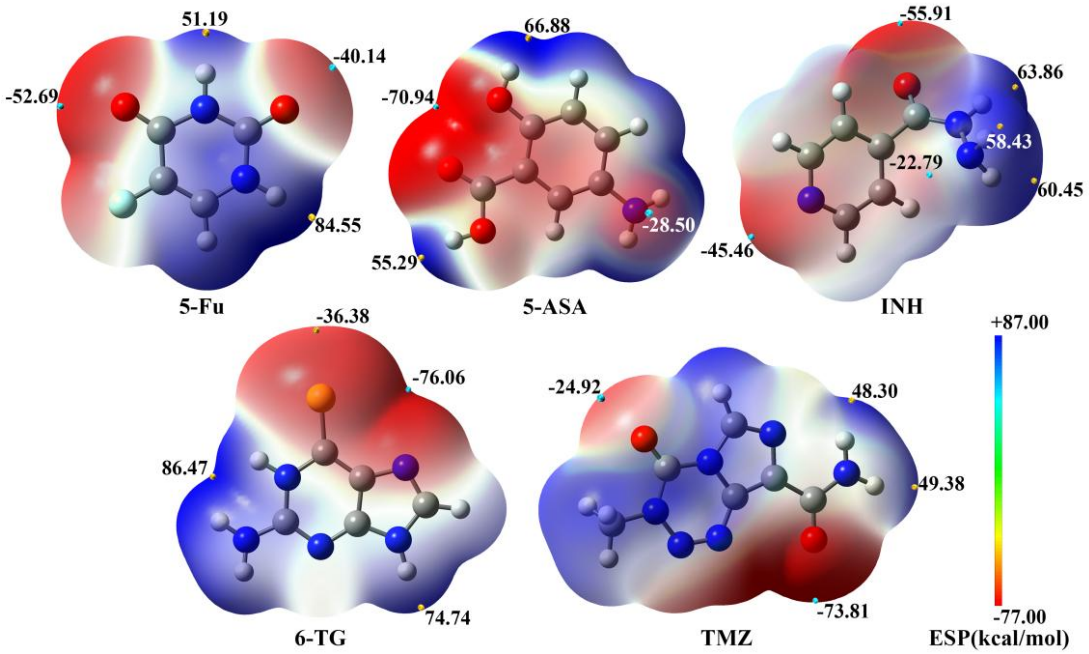


Fig. S2 ALIE diagrams of 5-ASA and INH, where cyan balls represent the minimum points.

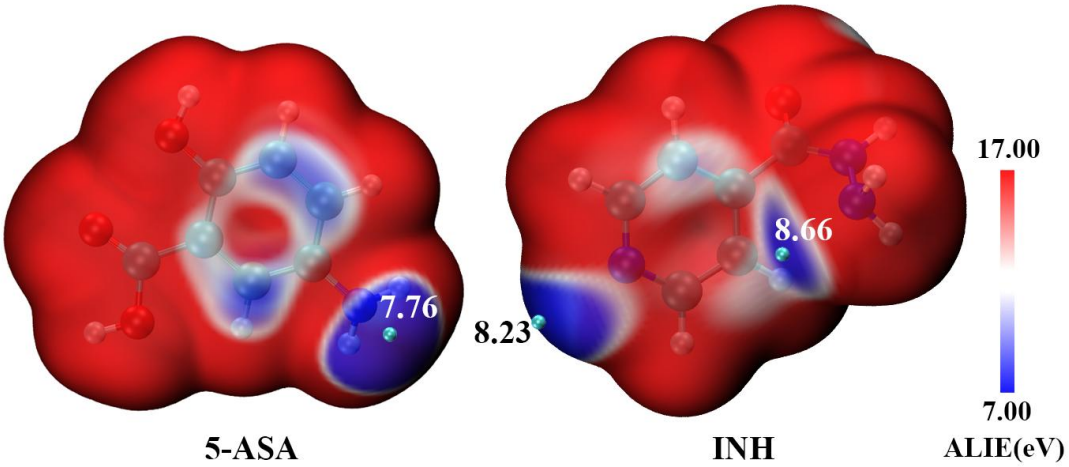


Fig. S3 The HOMO and LUMO orbitals of Drug@WSi_{12} (Drug = 5-Fu, 5-ASA, INH, and 6-TG) and WSi_{12} (Isovalue = 0.02 a.u.).

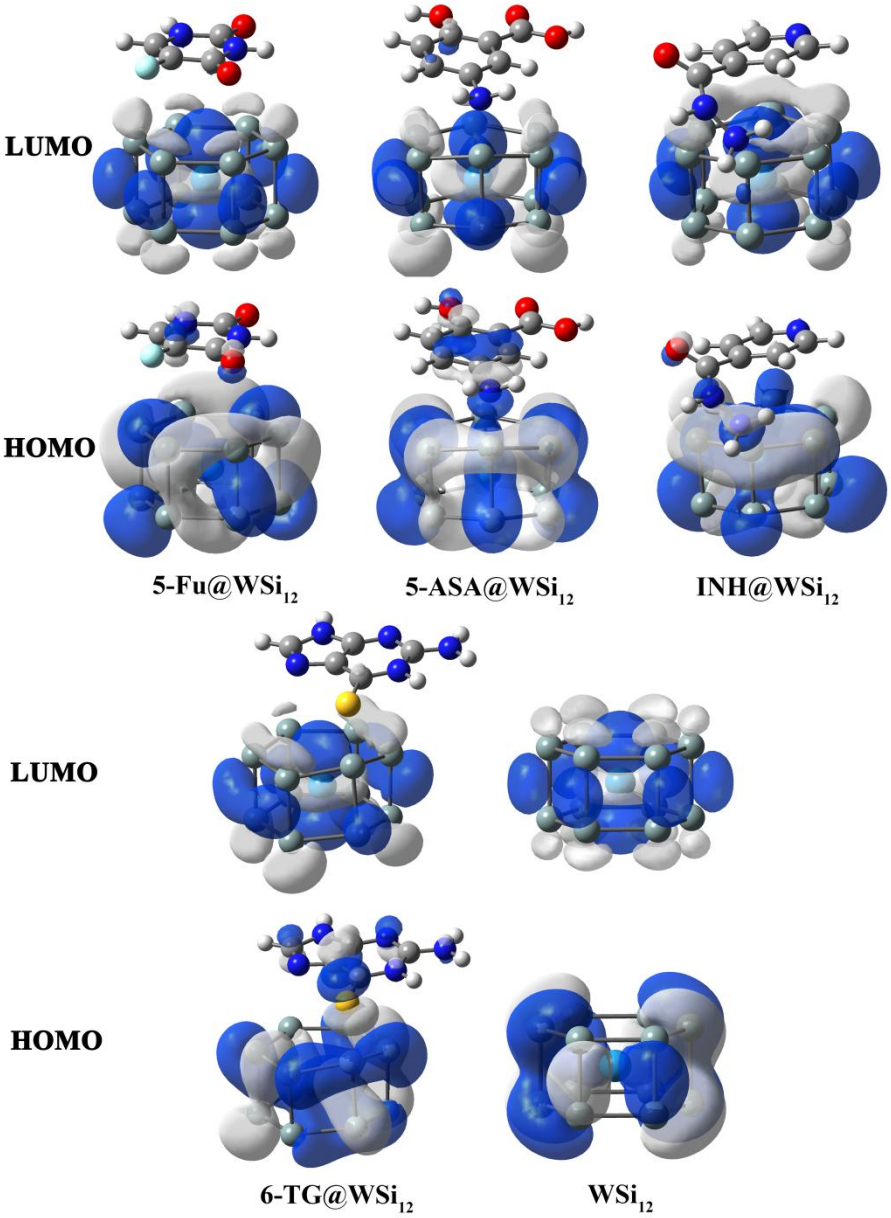


Fig. S4 Projected density of state (PDOS) plots of WSi_{12}, drugs, and Drug@WSi_{12} (Drug = 5-Fu, 5-ASA, INH, and 6-TG) complexes.

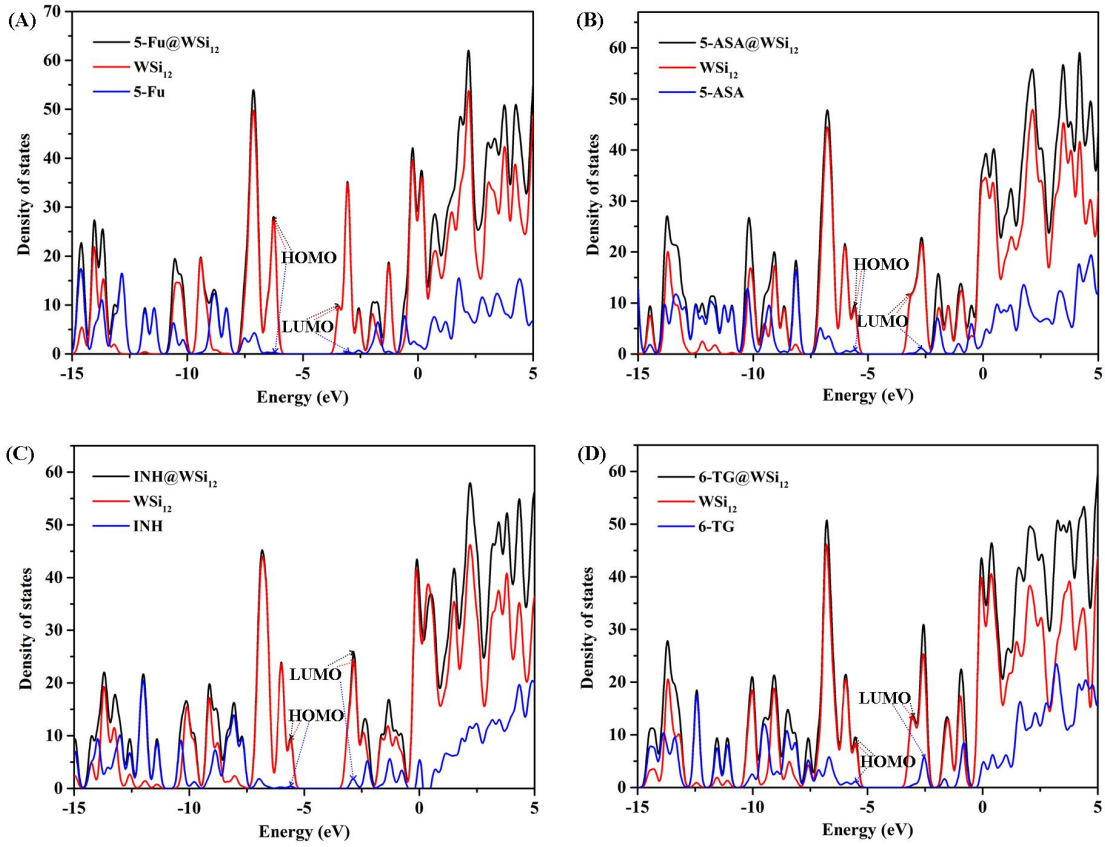


Fig. S5 Infrared (IR) spectra of (A) 5-ASA, WSi_{12}, and 5-ASA@WSi_{12}; (B) INH, WSi_{12}, and INH@WSi_{12}; (C) 6-TG, WSi_{12}, and 6-TG@WSi_{12}.

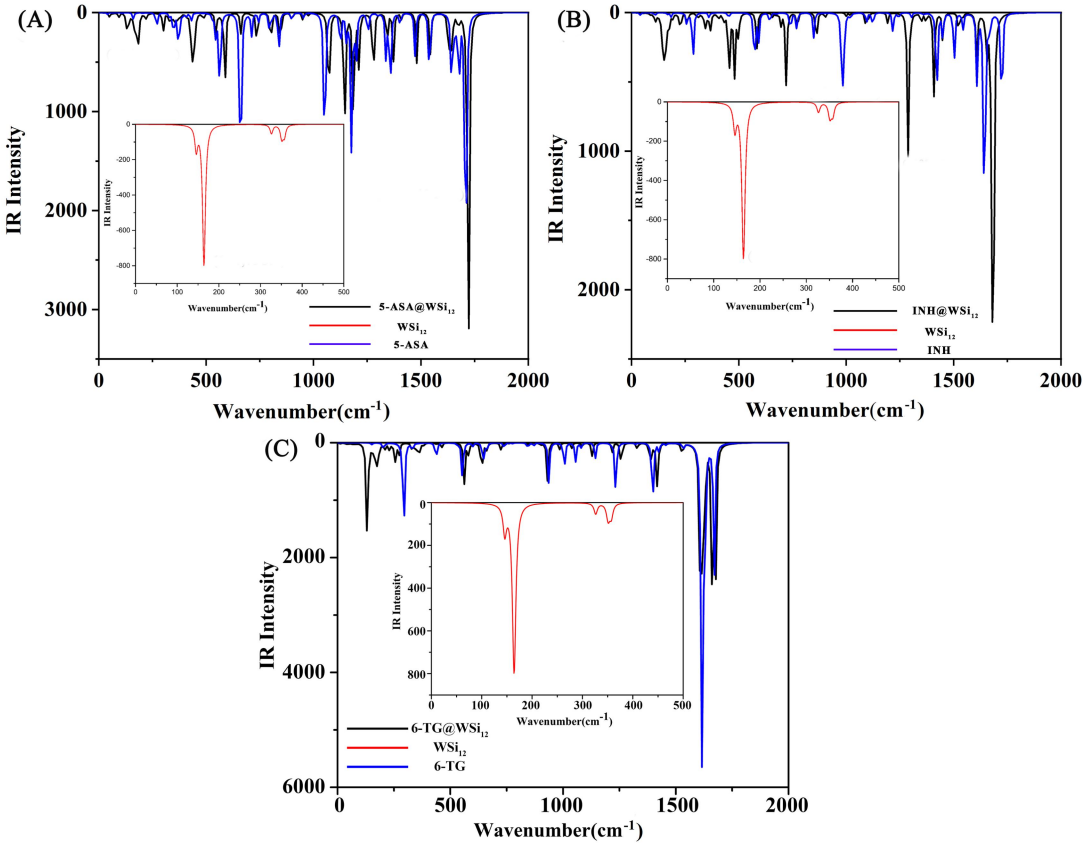


Fig. S6 UV-VIS-NIR spectra of (A) 5-ASA, WSi_{12}, and 5-ASA@WSi_{12}; (B) INH, WSi_{12}, and INH@WSi_{12}; (C) 6-TG, WSi_{12}, and 6-TG@WSi_{12}.

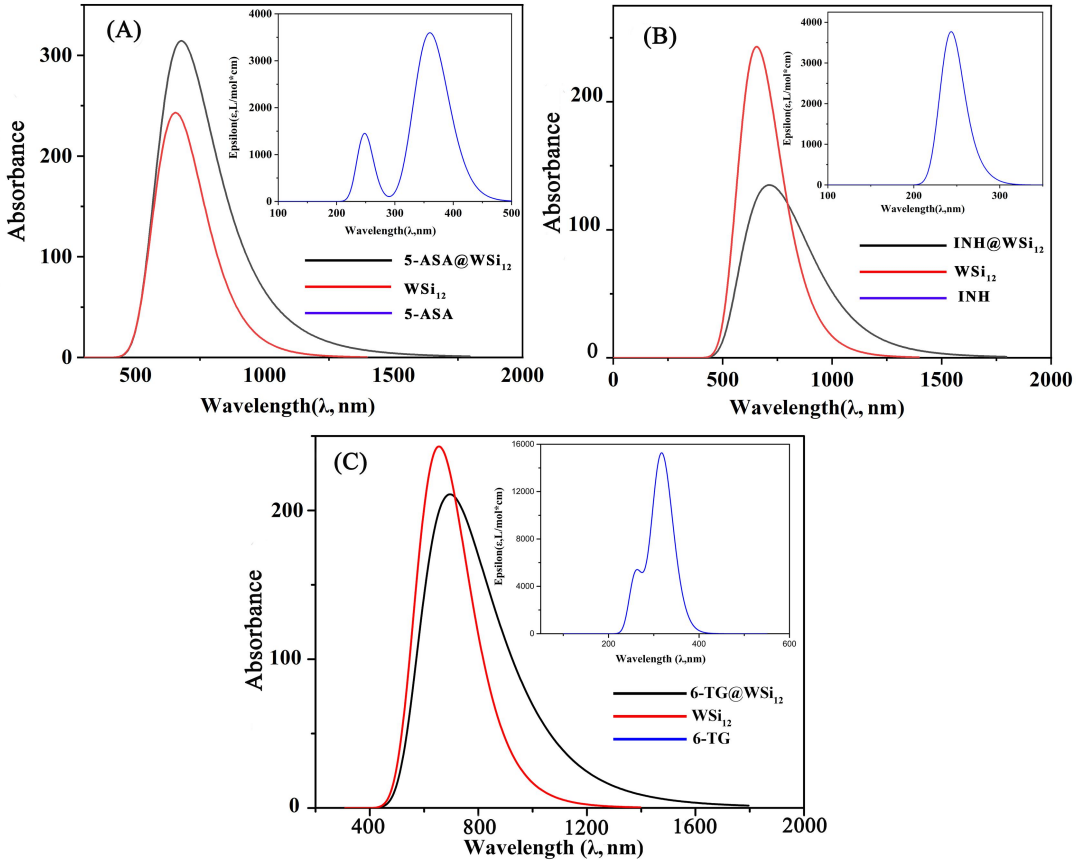


Fig. S7 The correlation between E_{ad} values and the maximum positive ESP values of $W_nSi_{6(n+1)}$ (n = 1, 2, 4, and 6).

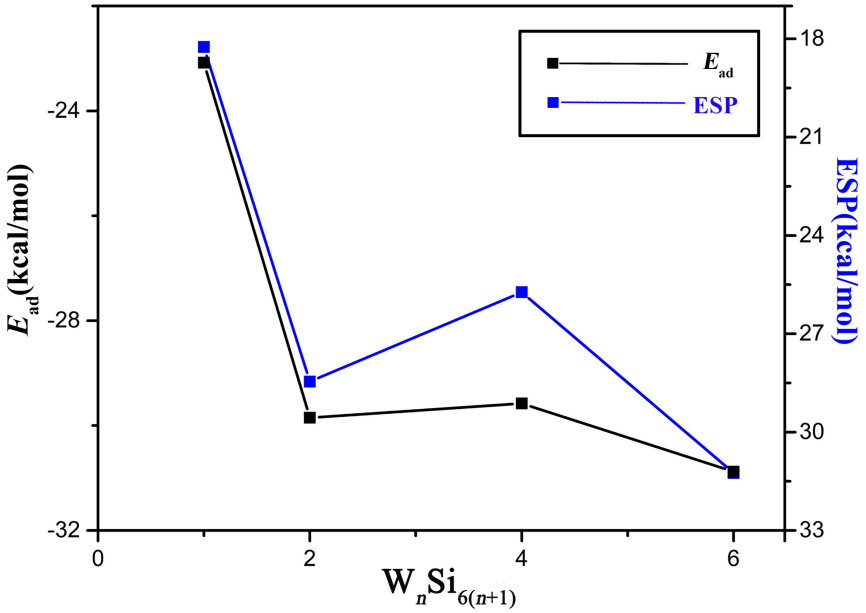
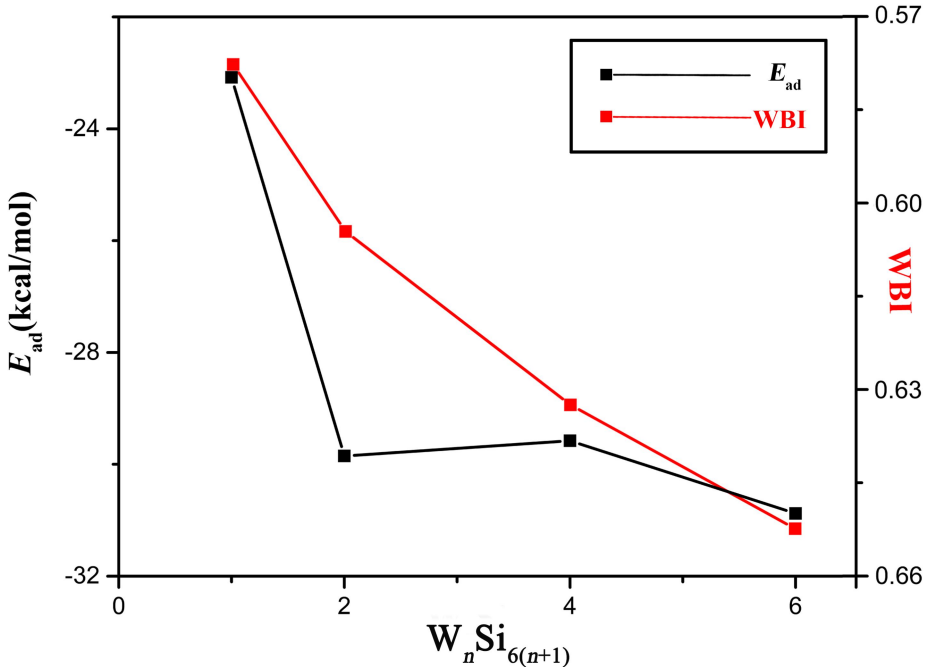


Fig. S8 Correlation between the E_{ad} values and the WBI values of S-Si bonds of 6-TG@$W_nSi_{6(n+1)}$ (n = 1, 2, 4, and 6).



3. Cartesian coordinates

WSi_{12}

Si	2.04518419	-1.18078764	1.21018258
Si	0.00000000	-2.36157528	1.21018258
Si	-2.04518419	-1.18078764	1.21018258
Si	-2.04518419	1.18078764	1.21018258
Si	-0.00000000	2.36157528	1.21018258
Si	2.04518419	1.18078764	1.21018258
Si	2.04518419	-1.18078764	-1.21018258
Si	-0.00000000	-2.36157528	-1.21018258
Si	-2.04518419	-1.18078764	-1.21018258
Si	-2.04518419	1.18078764	-1.21018258
Si	0.00000000	2.36157528	-1.21018258
Si	2.04518419	1.18078764	-1.21018258
W	-0.00000000	-0.00000000	0.00000000

5-Fu@WSi_{12}

Si	2.27294000	2.22224000	0.51887900
Si	2.46861700	1.34503100	-1.66553600
Si	2.38140800	-0.98279300	-2.01374400
Si	2.06787500	-2.44049700	-0.18098400
Si	1.85719100	-1.56168300	2.00249300
Si	1.94988500	0.77425200	2.35207400
Si	-0.12398500	2.38657500	0.22668600
Si	0.06616000	1.50072900	-1.94982300
Si	-0.01750400	-0.84005100	-2.30458800
Si	-0.32747600	-2.30698600	-0.47243000
Si	-0.53703100	-1.41678100	1.71436800
Si	-0.45202900	0.91958800	2.05357600
W	0.95863000	-0.02799200	0.02599300
C	-3.66413300	-1.48039800	-0.28669500
N	-3.45794200	-0.44676000	-1.17504000
C	-3.34715400	0.91534300	-0.88753100
C	-3.52266900	1.21693700	0.51524400
C	-3.73553400	0.23662500	1.42901900
N	-3.79179100	-1.07523400	1.02455400
H	-3.87592000	0.43260500	2.49003600
O	-3.71888500	-2.66246300	-0.63064600
H	-3.36668500	-0.71338000	-2.15577700
H	-3.94878300	-1.80101200	1.71672300
O	-3.12184800	1.74302600	-1.77523100
F	-3.48760800	2.51132100	0.87357500

5-ASA@WSi_{12}

Si	1.40576800	-0.75148700	2.38435100
Si	0.34836100	-2.22623700	0.90316100
Si	-0.53452300	-1.66841000	-1.19521900
Si	-1.02882800	0.62472100	-1.48806400
Si	-0.34136900	2.22529400	0.12221200
Si	0.86854700	1.53830600	2.05598900
Si	3.44014900	-0.50577900	1.14486000
Si	2.58669600	-2.14850000	-0.32503000
Si	1.57534900	-1.37872100	-2.31645900
Si	1.05275900	0.91054500	-2.66772800
Si	1.76707500	2.48994000	-1.05495100
Si	2.94785700	1.80468800	0.88220700
W	1.20591500	0.09125500	-0.14980900
C	-4.44134500	-0.54172300	-0.52230600
C	-4.21587700	-1.91974700	-0.60368000
C	-3.27456700	-2.53532100	0.19932000
C	-2.54248100	-1.77108600	1.12064800
C	-2.76180500	-0.40990300	1.21728300
C	-3.70529800	0.23174800	0.40261200
H	-4.78670200	-2.50910200	-1.32277500
H	-3.09722100	-3.60652400	0.11316700
H	-2.18827000	0.17512400	1.93195900
N	-1.48894500	-2.37774800	1.88190000
H	-1.39678300	-1.93814800	2.80116800
H	-1.66837100	-3.36972100	2.03443800
O	-5.35676300	0.05694000	-1.31184000
H	-5.79227200	-0.60636900	-1.87615400
C	-3.88003900	1.69050400	0.51806800
O	-4.45602600	2.40216900	-0.29234100
O	-3.31174400	2.19373400	1.63113600
H	-3.39299900	3.16550900	1.61637100

INH@WSi_{12}

Si	-1.17467000	-0.78976800	-0.03918000
Si	-0.70137800	1.30101700	0.92973600
Si	1.35855100	1.67096200	1.99353700
Si	2.96758200	-0.05311700	2.08516600
Si	2.51799500	-2.16621400	1.12286000
Si	0.43469300	-2.51602400	0.04928200
Si	-0.20038900	-0.05579300	-2.13116800
Si	0.22489100	2.06862600	-1.15440600
Si	2.30174000	2.44502800	-0.08603600
Si	3.93735000	0.72931700	0.00635900
Si	3.47074900	-1.38164800	-0.96838700

Si	1.39686600	-1.79638700	-2.05774400
W	1.39476700	-0.04760500	-0.03952100
C	-5.19747600	-1.50904500	1.88868500
C	-4.45260500	-0.37761900	1.56178700
C	-4.68589100	0.24645400	0.33461000
C	-5.68658500	-0.27252600	-0.49863400
C	-6.39000800	-1.39535300	-0.05610500
N	-6.15296800	-2.02040300	1.10139200
H	-5.02349600	-2.02318500	2.83270100
H	-3.71026800	0.02543600	2.24300500
H	-5.91676400	0.16527000	-1.45483700
H	-7.17697700	-1.81943400	-0.67594100
C	-3.87122800	1.47215200	0.03927600
O	-3.47895900	2.19418500	0.95230500
N	-3.51741700	1.75564700	-1.24363700
H	-2.85812500	2.52833800	-1.31554800
N	-3.70727200	0.89175000	-2.31896100
H	-4.02938100	1.42154700	-3.11762900
H	-2.82541700	0.43148000	-2.55263800

6-TG@WSi_{12}

Si	-4.04479400	1.15916900	0.14766500
Si	-3.95554200	-0.89989200	-1.09290000
Si	-1.89539600	-1.45920000	-2.11864100
Si	0.03138200	-0.11220200	-2.03505800
Si	-0.21899100	1.97562800	-0.93341000
Si	-2.20153800	2.71401400	0.15320400
Si	-3.24173200	0.05982600	2.19516100
Si	-3.04578500	-1.94785100	0.93045700
Si	-1.06434100	-2.58237500	-0.17969300
Si	0.76424100	-1.16335900	-0.01329700
Si	0.64307300	0.92023200	1.04722900
Si	-1.36531600	1.53070200	2.13220300
W	-1.72388300	0.08230400	0.00520300
N	6.98271300	0.56669300	0.71706300
C	7.03500900	-0.62062100	1.42847000
H	7.89945100	-0.88409600	2.02183400
N	5.96308100	-1.34437300	1.29679000
C	5.15338000	-0.61377800	0.45501000
C	3.87515900	-0.85225500	-0.04827700
N	3.42956300	0.13575300	-0.88859700
H	2.51053100	-0.00828100	-1.31716500
C	4.08213600	1.31001300	-1.14632900
N	3.44413600	2.18804200	-1.94582700

H	2.43196800	2.15841300	-2.00191600
H	3.86641100	3.09977200	-2.01658500
N	5.28687400	1.57311300	-0.67711500
C	5.77757900	0.59446500	0.08356900
H	7.68342800	1.29049700	0.67938200
S	2.88861000	-2.20087500	0.30235700

TMZ@WSi_{12}

Si	-0.08128000	2.18057700	0.85307200
Si	0.41727600	1.60493100	-1.36592100
Si	0.39353700	-0.68329000	-1.99130100
Si	-0.23232700	-2.35451700	-0.41550300
Si	-0.78174400	-1.70769900	1.80118200
Si	-0.71133400	0.57092400	2.41894700
Si	-2.39979000	2.44056400	0.19048200
Si	-1.88993100	1.78656200	-2.01498700
Si	-1.92422800	-0.48711100	-2.66460600
Si	-2.54890500	-2.12185300	-1.05893700
Si	-3.11039500	-1.48710200	1.15794300
Si	-3.02681000	0.79451100	1.75178100
W	-1.33582000	0.01907700	-0.12451700
C	0.69486542	-5.77615174	-2.07725789
N	0.77899683	-4.91657939	-0.99642171
N	-0.41914207	-3.17608101	-1.86114620
C	-0.54179251	-3.89283272	-3.00900837
O	1.17545837	-6.87553592	-2.12777806
N	-0.00784449	-5.17230410	-3.12367659
N	0.22177877	-3.67127698	-0.89353919
C	1.47592954	-5.38071940	0.19307308
H	0.98593404	-6.27461171	0.58127043
H	2.51376462	-5.60998784	-0.05023814
H	1.42013558	-4.58006085	0.92601562
C	-0.26579613	-5.61932117	-4.39055090
N	-0.90626396	-4.70681460	-5.07890183
H	0.03749868	-6.59834925	-4.72740894
C	-1.10020366	-3.63137009	-4.25002738
C	-1.81733603	-2.42116485	-4.68114985
O	-2.15346563	-1.54572584	-3.87989965
N	-2.09393488	-2.37681855	-5.99376570
H	-2.64229030	-1.61331872	-6.35386629
H	-1.85076539	-3.15237761	-6.59047700