ДОДАТКИ ДО ДИСЕРТАЦІЇ

АНАЛІЗ І ПРОГНОЗУВАННЯ ВЛАСТИВОСТЕЙ МОЛЕКУЛЯРНИХ НАНООБ'ЄКТІВ МЕТОДАМИ ХЕМОІНФОРМАТИКИ,

що подається на здобуття наукового ступеня доктора філософії

СТЕЛЬМАХ СЕРГІЙ ІГОРОВИЧ

ДОДАТОК А

СПИСОК ПУБЛІКАЦІЙ ЗДОБУВАЧА

1. Kuz'min V., Ognichenko L., Sizochenko N., Chapkin V., **Stelmakh S.**, Shyrykalova A., Leszczynski J. Combining Features of Metal Oxide Nanoparticles: Nano-QSAR for Cytotoxicity. *International Journal of Quantitative Structure-Property Relationships*. 2019. Vol. 4, № 1. P. 28-40.

Особистий внесок здобувача: проведено розрахунок дескрипторів, проведено побудову, оптимізацію та валідацію моделей.

2. Kuz'min V., Artemenko A., Ognichenko L., Hromov A., Kosinskaya A., **Stelmakh S.**, Sessions Z., Muratov E. Simplex representation of molecular structure as universal QSAR/QSPR tool. *Structural Chemistry*. 2021. Vol. 32, № 5. P. 1365–1392.

Особистий внесок здобувача: брав участь у написанні розділу огляду, присвяченого моделюванню наночастинок.

3. **Стельмах С. І.**, Кузьмін В. Є., Огніченко Л. М. QSPR моделі для прогнозу дзета-потенціалів наночастинок оксидів. *Вісник ОНУ*. 2021. Том 26, № 2(78), С. 89–100.

Особистий внесок здобувача: проведено розрахунок дескрипторів, проведено побудову, оптимізацію та валідацію моделей. Сумісно зі співавторами проведено інтерпретацію та обговорення результатів.

4. Ognichenko L., Shyrykalova A., **Stelmakh S.**, Tinkov O., Kuz'min V. The importance of Effects of Structural Factors Interaction for Metal Oxides Nanoparticles in QSAR Models for Cytotoxicity. *Nanoscience & Nanotechnologies* : book of

abstracts of 15th International Conference, Thessaloniki, 3-6 July 2018. Thessaloniki, Greece, 2018. P. 203.

Особистий внесок здобувача: проведено побудову, оптимізацію та валідацію моделей.

5. **Stelmakh S.**, Ognichenko L., Kuz'min V. Nano-QSPR for zeta potential of metal oxides. *Chemistry, Physics and Technology of Surface* : proceedings of Ukrainian Conference with International participation dedicated to 90th birthday of Aleksey Chuiko, Academician of NAS of Ukraine, Kyiv 21-22 October 2020. Kyiv, Ukraine, 2020. P. 171.

Особистий внесок здобувача: проведено розрахунок дескрипторів, проведено побудову, оптимізацію та валідацію моделей. Сумісно зі співавторами проведено інтерпретацію та обговорення результатів.

6. **Stelmakh S.**, Kuz'min V. QSPR vs Molecular Docking. Adducts of [60] fullerene as potential HIV-1 PR inhibitors. *Science, Innovation, Quality* : book of Papers of 1st International Scientific-Practical Conference, Berdyansk 17-18 December 2020. Berdyansk, Ukraine, 2020. P. 122.

Особистий внесок здобувача: проведено розрахунок дескрипторів, проведено побудову, оптимізацію та валідацію моделей. Сумісно зі співавторами проведено інтерпретацію та обговорення результатів.

ДОДАТОК Б

СПИСОК РОЗРАХОВАНИХ ПАРАМЕТРІВ У СИСТЕМІ ДЕСКРИПТОРНОГО ОПИСУ НАНООКСИДІВ

Cnk(att)/A	Cnk(groups)/J,J,P,P	Cnk(spdf)/A	Wigner-Seitz radius*size in H2O	Wigner-Seitz radius*F-surface molecules
Cnk(att)/A,A	Cnk(groups)/J,P	Cnk(spdf)/A,B	n -number of molecules in a nanocluster *size in H2O	n -number of molecules in a nanocluster*F- surface molecules
Cnk(att)/A,A,A	Cnk(groups)/J,P,P	Cnk(spdf)/B	F- surface molecules*size in H2O	F- surface molecules*F-surface molecules
Cnk(att)/A,A,A,C	Cnk(groups)/J,P,P,P	Cnk(spdf)/B,B	sv*size in H2O	sv*F- surface molecules
Cnk(att)/A,A,C	Cnk(groups)/K	Cnk(spdf)/B,B,B	electronegativity Met*size in H2O	electronegativity Met *F-surface molecules
Cnk(att)/A,A,C,C	Cnk(groups)/K,P	Cnk(spdf)/B,B,B,B	atom radius*size in H2O	atom radius*F- surface molecules
Cnk(att)/A,C	Cnk(groups)/L	Cnk(spdf)/B,B,B,C	ion radius by Bokij*size in H2O	ion radius by Bokij*F-surface molecules
Cnk(att)/A,C,C	Cnk(groups)/L,P	Cnk(spdf)/B,B,B,D	1ci-covalent index*size in H2O	1ci-covalent index*F-surface molecules
Cnk(att)/A,C,C,C	Cnk(groups)/M	Cnk(spdf)/B,B,C	2ci-covalent index*size in H2O	2ci-covalent index*F-surface molecules
Cnk(att)/B	Cnk(groups)/M,M	Cnk(spdf)/B,B,C,C	z -ion charge*size in H2O	z -ion charge*F- surface molecules
Cnk(att)/B,B	Cnk(groups)/M,M,P	Cnk(spdf)/B,B,D	cpp1*size in H2O	cpp1*F- surface molecules
Cnk(att)/B,B,C	Cnk(groups)/M,M,P,P	Cnk(spdf)/B,B,D,D	cpp2*size in H2O	cpp2*F- surface molecules
Cnk(att)/B,B,C,C	Cnk(groups)/M,P	Cnk(spdf)/B,C	potential ioniz.*size in H2O	potential ioniz.*F- surface molecules
Cnk(att)/B,C	Cnk(groups)/M,P,P	Cnk(spdf)/B,C,C	S H2O*size in H2O	S H2O*F- surface molecules
Cnk(att)/B,C,C	Cnk(groups)/M,P,P,P	Cnk(spdf)/B,C,C,C	V H2O*size in H2O	V H2O*F- surface molecules
Cnk(att)/B,C,C,C	Cnk(groups)/N	Cnk(spdf)/B,D	R H2O*size in H2O	R H2O*F- surface molecules
Cnk(att)/C	Cnk(groups)/N,P	Cnk(spdf)/B,D,D	nominal size*molecular mass	nominal size*sv

Cnk(att)/C,C	Cnk(groups)/N,P,P	Cnk(spdf)/C	size in H2O*molecular mass	size in H2O*sv
Cnk(att)/C,C,C	Cnk(groups)/O	Cnk(spdf)/C,C	molecular mass*molecular mass	molecular mass*sv
Cnk(att)/C,C,C,C	Cnk(groups)/O,O	Cnk(spdf)/C,C,C	mass density*molecular mass	mass density*sv
Cnk(att)/C,C,C,F	Cnk(groups)/O,O,P	Cnk(spdf)/D	Wigner-Seitz radius*molecular mass	Wigner-Seitz radius*sv
Cnk(att)/C,C,C,G	Cnk(groups)/O,O,P,P	Cnk(spdf)/D,D	n -number of molecules in a nanocluster *molecular mass	n -number of molecules in a nanocluster *sv
Cnk(att)/C,C,F	Cnk(groups)/O,P	Cnk(step-okisl)/A	F- surface molecules*molecular mass	F- surface molecules*sv
Cnk(att)/C,C,F,F	Cnk(groups)/O,P,P	Cnk(step-okisl)/A,A	sv*molecular mass	sv*sv
Cnk(att)/C,C,G	Cnk(groups)/O,P,P,P	Cnk(step-okisl)/A,A,A	electronegativity Met *molecular mass	electronegativity Met *sv
Cnk(att)/C,C,G,G	Cnk(groups)/P	Cnk(step-okisl)/A,A,A,A	atom radius*molecular mass	atom radius*sv
Cnk(att)/C,F	Cnk(groups)/P,P	Cnk(step-okisl)/A,A,A,B	ion radius by Bokij*molecular mass	ion radius by Bokij*sv
Cnk(att)/C,F,F	Cnk(groups)/P,P,P	Cnk(step-okisl)/A,A,A,C	1ci-covalent index*molecular mass	1ci-covalent index*sv
Cnk(att)/C,G	Cnk(groups)/P,P,P,P	Cnk(step-okisl)/A,A,A,E	2ci-covalent index*molecular mass	2ci-covalent index*sv
Cnk(att)/C,G,G	Cnk(ion-b)/A	Cnk(step-okisl)/A,A,B	z -ion charge*molecular mass	z -ion charge*sv
Cnk(att)/F	Cnk(ion-b)/A,A	Cnk(step-okisl)/A,A,B,C	cpp1*molecular mass	cpp1*sv
Cnk(att)/F,F	Cnk(ion-b)/A,A,A	Cnk(step-okisl)/A,A,C	cpp2*molecular mass	cpp2*sv
Cnk(att)/G	Cnk(ion-b)/A,A,A,A	Cnk(step-okisl)/A,A,C,C	potential ioniz.*molecular mass	potential ioniz.*sv
Cnk(att)/G,G	Cnk(ion-b)/A,A,A,B	Cnk(step-okisl)/A,A,D	S H2O*molecular mass	S H2O*sv
Cnk(en)/A	Cnk(ion-b)/A,A,B	Cnk(step-okisl)/A,A,E	V H2O*molecular mass	V H2O*sv
Cnk(en)/A,A	Cnk(ion-b)/A,A,B,B	Cnk(step-okisl)/A,B	R H2O*molecular mass	R H2O*sv
Cnk(en)/A,A,A	Cnk(ion-b)/A,B	Cnk(step-okisl)/A,B,C	nominal size*mass density	nominal size*electronegativity Met
Cnk(en)/A,A,A,D	Cnk(ion-b)/A,B,B	Cnk(step-okisl)/A,B,C,C	size in H2O*mass density	size in H2O*electronegativity Met

Cnk(en)/A,A,D	Cnk(ion-b)/B	Cnk(step-okisl)/A,C	molecular mass*mass density	molecular mass*electronegativity Met
Cnk(en)/A,A,D,D	Cnk(ion-b)/B,B	Cnk(step-okisl)/A,C,C	mass density*mass density	mass density*electronegativity Met
Cnk(en)/A,D	Cnk(ion-b)/B,B,B	Cnk(step-okisl)/A,D	Wigner-Seitz radius*mass density	Wigner-Seitz radius*electronegativity Met
Cnk(en)/A,D,D	Cnk(ion-b)/B,B,B,B	Cnk(step-okisl)/A,E	n -number of molecules in a nanocluster *mass density	n -number of molecules in a nanocluster *electronegativity Met
Cnk(en)/A,D,D,D	Cnk(ion-b)/B,B,B,C	Cnk(step-okisl)/B	F- surface molecules*mass density	F- surface molecules*electronegativity Met
Cnk(en)/B	Cnk(ion-b)/B,B,C	Cnk(step-okisl)/B,C	sv*mass density	sv*electronegativity Met
Cnk(en)/B,D	Cnk(ion-b)/B,B,C,C	Cnk(step-okisl)/B,C,C	electronegativity Met *mass density	electronegativity Met *electronegativity Met
Cnk(en)/B,D,D	Cnk(ion-b)/B,C	Cnk(step-okisl)/C	atom radius*mass density	atom radius*electronegativity Met
Cnk(en)/B,D,D,D	Cnk(ion-b)/B,C,C	Cnk(step-okisl)/C,C	ion radius by Bokij*mass density	ion radius by Bokij*electronegativity Met
Cnk(en)/D	Cnk(ion-b)/B,C,C,C	Cnk(step-okisl)/D	1ci-covalent index*mass density	1ci-covalent index*electronegativity Met
Cnk(en)/D,D	Cnk(ion-b)/C	Cnk(step-okisl)/E	2ci-covalent index*mass density	2ci-covalent index*electronegativity Met
Cnk(en)/D,D,D	Cnk(ion-b)/C,C	Cnk(zar-nucl)/A	z -ion charge*mass density	z -ion charge*electronegativity Met
Cnk(en)/D,D,D,D	Cnk(ion-b)/C,C,C	Cnk(zar-nucl)/A,A	cpp1*mass density	cpp1*electronegativity Met
Cnk(groups)/B	Cnk(rep)/A	Cnk(zar-nucl)/A,A,A	cpp2*mass density	cpp2*electronegativity Met

Cnk(groups)/B,P	Cnk(rep)/A,A	Cnk(zar-nucl)/A,A,A,A	potential ioniz.*mass density	potential ioniz.*electronegativity Met
Cnk(groups)/C	Cnk(rep)/A,A,A	Cnk(zar-nucl)/A,A,A,B	S H2O*mass density	S H2O*electronegativity Met
Cnk(groups)/C,C	Cnk(rep)/A,A,A,D	Cnk(zar-nucl)/A,A,A,C	V H2O*mass density	V H2O*electronegativity Met
Cnk(groups)/C,C,P	Cnk(rep)/A,A,D	Cnk(zar-nucl)/A,A,A,D	R H2O*mass density	R H2O*electronegativity Met
Cnk(groups)/C,C,P,P	Cnk(rep)/A,A,D,D	Cnk(zar-nucl)/A,A,B	nominal size*Wigner-Seitz radius	nominal size*atom radius
Cnk(groups)/C,P	Cnk(rep)/A,D	Cnk(zar-nucl)/A,A,B,B	size in H2O*Wigner-Seitz radius	size in H2O*atom radius
Cnk(groups)/C,P,P	Cnk(rep)/A,D,D	Cnk(zar-nucl)/A,A,C	molecular mass*Wigner-Seitz radius	molecular mass*atom radius
Cnk(groups)/C,P,P,P	Cnk(rep)/A,D,D,D	Cnk(zar-nucl)/A,A,C,C	mass density*Wigner-Seitz radius	mass density*atom radius
Cnk(groups)/D	Cnk(rep)/B	Cnk(zar-nucl)/A,A,D	Wigner-Seitz radius*Wigner-Seitz radius	Wigner-Seitz radius*atom radius
Cnk(groups)/D,P	Cnk(rep)/B,D	Cnk(zar-nucl)/A,A,D,D	n -number of molecules in a nanocluster *Wigner-Seitz radius	n -number of molecules in a nanocluster*atom radius
Cnk(groups)/D,P,P	Cnk(rep)/C	Cnk(zar-nucl)/A,B	F- surface molecules*Wigner-Seitz radius	F- surface molecules*atom radius
Cnk(groups)/F	Cnk(rep)/C,C	Cnk(zar-nucl)/A,B,B	sv*Wigner-Seitz radius	sv*atom radius
Cnk(groups)/F,F	Cnk(rep)/C,C,D	Cnk(zar-nucl)/A,B,B,B	electronegativity Met *Wigner-Seitz radius	electronegativity Met *atom radius
Cnk(groups)/F,F,P	Cnk(rep)/C,C,D,D	Cnk(zar-nucl)/A,C	atom radius*Wigner-Seitz radius	atom radius*atom radius
Cnk(groups)/F,F,P,P	Cnk(rep)/C,D	Cnk(zar-nucl)/A,C,C	ion radius by Bokij*Wigner-Seitz radius	ion radius by Bokij*atom radius
Cnk(groups)/F,P	Cnk(rep)/C,D,D	Cnk(zar-nucl)/A,D	1ci-covalent index*Wigner-Seitz radius	1ci-covalent index*atom radius
Cnk(groups)/F,P,P	Cnk(rep)/C,D,D,D	Cnk(zar-nucl)/A,D,D	2ci-covalent index*Wigner-Seitz radius	2ci-covalent index*atom radius
Cnk(groups)/F,P,P,P	Cnk(rep)/D	Cnk(zar-nucl)/B	z -ion charge*Wigner-Seitz radius	z -ion charge*atom radius
Cnk(groups)/G	Cnk(rep)/D,D	Cnk(zar-nucl)/B,B	cpp1*Wigner-Seitz radius	cpp1*atom radius
Cnk(groups)/G,G	Cnk(rep)/D,D,D	Cnk(zar-nucl)/B,B,B	cpp2*Wigner-Seitz radius	cpp2*atom radius
Cnk(groups)/G,G,G	Cnk(rep)/D,D,D,D	Cnk(zar-nucl)/C	potential ioniz.*Wigner-Seitz radius	potential ioniz.*atom radius

Cnk(groups)/G,G,G,P	Cnk(rep)/D,D,D,E	Cnk(zar-nucl)/C,C	S H2O*Wigner-Seitz radius	S H2O*atom radius
Cnk(groups)/G,G,P	Cnk(rep)/D,D,E	Cnk(zar-nucl)/D	V H2O*Wigner-Seitz radius	V H2O*atom radius
Cnk(groups)/G,G,P,P	Cnk(rep)/D,D,E,E	Cnk(zar-nucl)/D,D	R H2O*Wigner-Seitz radius	R H2O*atom radius
Cnk(groups)/G,P	Cnk(rep)/D,E	nominal size*nominal size	nominal size*n -number of molecules in a nanocluster	nominal size*ion radius by Bokij
Cnk(groups)/G,P,P	Cnk(rep)/D,E,E	size in H2O*nominal size	size in H2O*n -number of molecules in a nanocluster	size in H2O*ion radius by Bokij
Cnk(groups)/G,P,P,P	Cnk(rep)/E	molecular mass*nominal size	molecular mass*n -number of molecules in a nanocluster	molecular mass*ion radius by Bokij
Cnk(groups)/H	Cnk(rep)/E,E	mass density*nominal size	mass density*n -number of molecules in a nanocluster	mass density*ion radius by Bokij
Cnk(groups)/H,H	Cnk(rf)/A	Wigner-Seitz radius*nominal size	Wigner-Seitz radius*n -number of molecules in a nanocluster	Wigner-Seitz radius*ion radius by Bokij
Cnk(groups)/H,H,H	Cnk(rf)/A,A	n -number of molecules in a nanocluster*nominal size	n -number of molecules in a nanocluster *n -number of molecules in a nanocluster	n -number of molecules in a nanocluster *ion radius by Bokij
Cnk(groups)/H,H,H,P	Cnk(rf)/A,A,C	F- surface molecules*nominal size	F- surface molecules*n -number of molecules in a nanocluster	F- surface molecules*ion radius by Bokij
Cnk(groups)/H,H,P	Cnk(rf)/A,A,C,C	sv*nominal size	sv*n -number of molecules in a nanocluster	sv*ion radius by Bokij
Cnk(groups)/H,H,P,P	Cnk(rf)/A,C	electronegativity Met*nominal size	electronegativity Met *n -number of molecules in a nanocluster	electronegativity Met *ion radius by Bokij
Cnk(groups)/H,P	Cnk(rf)/A,C,C	atom radius*nominal size	atom radius*n -number of molecules in a nanocluster	atom radius*ion radius by Bokij
Cnk(groups)/H,P,P	Cnk(rf)/A,C,C,C	ion radius by Bokij*nominal size	ion radius by Bokij*n -number of molecules in a nanocluster	ion radius by Bokij*ion radius by Bokij
Cnk(groups)/H,P,P,P	Cnk(rf)/B	1ci-covalent index*nominal size	1ci-covalent index*n -number of molecules in a nanocluster	1ci-covalent index*ion radius by Bokij
Cnk(groups)/I	Cnk(rf)/B,B	2ci-covalent index*nominal size	2ci-covalent index*n -number of molecules in a nanocluster	2ci-covalent index*ion radius by Bokij
Cnk(groups)/I,I	Cnk(rf)/B,B,B	z -ion charge*nominal size	z -ion charge*n -number of molecules in a nanocluster	z -ion charge*ion radius by Bokij

Cnk(groups)/I,I,I	Cnk(rf)/B,B,B,C	cpp1*nominal size	cpp1*n -number of molecules in a nanocluster	cpp1*ion radius by Bokij
Cnk(groups)/I,I,I,P	Cnk(rf)/B,B,C	cpp2*nominal size	cpp2*n -number of molecules in a nanocluster	cpp2*ion radius by Bokij
Cnk(groups)/I,I,P	Cnk(rf)/B,B,C,C	potential ioniz.*nominal size	potential ioniz.*n -number of molecules in a nanocluster	potential ioniz.*ion radius by Bokij
Cnk(groups)/I,I,P,P	Cnk(rf)/B,C	S H2O*nominal size	S H2O*n -number of molecules in a nanocluster	S H2O*ion radius by Bokij
Cnk(groups)/I,P	Cnk(rf)/B,C,C	V H2O*nominal size	V H2O*n -number of molecules in a nanocluster	V H2O*ion radius by Bokij
Cnk(groups)/I,P,P	Cnk(rf)/B,C,C,C	R H2O*nominal size	R H2O*n -number of molecules in a nanocluster	R H2O*ion radius by Bokij
Cnk(groups)/I,P,P,P	Cnk(rf)/C	nominal size*size in H2O	nominal size*F- surface molecules	nominal size*1ci-covalent index
Cnk(groups)/J	Cnk(rf)/C,C	size in H2O*size in H2O	size in H2O*F- surface molecules	size in H2O*1ci-covalent index
Cnk(groups)/J,J	Cnk(rf)/C,C,C	molecular mass*size in H2O	molecular mass*F- surface molecules	molecular mass*1ci-covalent index
Cnk(groups)/J,J,P	Cnk(rf)/C,C,C,C	mass density*size in H2O	mass density*F- surface molecules	mass density*1ci-covalent index

Wigner-Seitz radius*1ci-covalent index	cpp1*z -ion charge	Wigner-Seitz radius*potential ioniz.	cpp1*V H2O
n -number of molecules in a nanocluster*1ci-covalent index	cpp2*z -ion charge	n -number of molecules in a nanocluster *potential ioniz.	cpp2*V H2O
F- surface molecules**1ci-covalent index	potential ioniz.*z -ion charge	F- surface molecules*potential ioniz.	potential ioniz.*V H2O
sv*1ci-covalent index	S H2O*z -ion charge	sv*potential ioniz.	S H2O*V H2O
electronegativity Met *1ci-covalent index	V H2O*z -ion charge	electronegativity Met *potential ioniz.	V H2O*V H2O
atom radius*1ci-covalent index	R H2O*z -ion charge	atom radius*potential ioniz.	R H2O*V H2O

ion radius by Bokij*1ci-covalent index	nominal size*cpp1	ion radius by Bokij*potential ioniz.	nominal size*R H2O
1ci-covalent index*1ci-covalent index	size in H2O*cpp1	1ci-covalent index*potential ioniz.	size in H2O*R H2O
2ci-covalent index*1ci-covalent index	molecular mass*cpp1	2ci-covalent index*potential ioniz.	molecular mass*R H2O
z -ion charge*1ci-covalent index	mass density*cpp1	z -ion charge*potential ioniz.	mass density*R H2O
cpp1*1ci-covalent index	Wigner-Seitz radius*cpp1	cpp1*potential ioniz.	Wigner-Seitz radius*R H2O
cpp2*1ci-covalent index	n -number of molecules in a nanocluster *cpp1	cpp2*potential ioniz.	n -number of molecules in a nanocluster *R H2O
potential ioniz.*1ci-covalent index	F- surface molecules*cpp1	potential ioniz.*potential ioniz.	F- surface molecules*R H2O
S H2O*1ci-covalent index	sv*cpp1	S H2O*potential ioniz.	sv*R H2O
V H2O*1ci-covalent index	electronegativity Met *cpp1	V H2O*potential ioniz.	electronegativity Met *R H2O
R H2O*1ci-covalent index	atom radius*cpp1	R H2O*potential ioniz.	atom radius*R H2O
nominal size*2ci-covalent index	ion radius by Bokij*cpp1	nominal size*S H2O	ion radius by Bokij*R H2O
size in H2O*2ci-covalent index	1ci-covalent index*cpp1	size in H2O*S H2O	1ci-covalent index*R H2O
molecular mass*2ci-covalent index	2ci-covalent index*cpp1	molecular mass*S H2O	2ci-covalent index*R H2O
mass density*2ci-covalent index	z -ion charge*cpp1	mass density*S H2O	z -ion charge*R H2O
Wigner-Seitz radius*2ci-covalent index	cpp1*cpp1	Wigner-Seitz radius*S H2O	cpp1*R H2O
n -number of molecules in a nanocluster *2ci-covalent index	cpp2*cpp1	n -number of molecules in a nanocluster *S H2O	cpp2*R H2O
F- surface molecules*2ci-covalent index	potential ioniz.*cpp1	F- surface molecules*S H2O	potential ioniz.*R H2O

sv*2ci-covalent index	S H2O*cpp1	sv*S H2O	S H2O*R H2O
electronegativity Met *2ci-covalent index	V H2O*cpp1	electronegativity Met *S H2O	V H2O*R H2O
atom radius*2ci-covalent index	R H2O*cpp1	atom radius*S H2O	R H2O*R H2O
ion radius by Bokij*2ci-covalent index	nominal size*cpp2	ion radius by Bokij*S H2O	nominal size
1ci-covalent index*2ci-covalent index	size in H2O*cpp2	1ci-covalent index*S H2O	size in H2O
2ci-covalent index*2ci-covalent index	molecular mass*cpp2	2ci-covalent index*S H2O	molecular mass
z -ion charge*2ci-covalent index	mass density*cpp2	z -ion charge*S H2O	mass density
cpp1*2ci-covalent index	Wigner-Seitz radius*cpp2	cpp1*S H2O	Wigner-Seitz radius
cpp2*2ci-covalent index	n -number of molecules in a nanocluster *cpp2	cpp2*S H2O	n -number of molecules in a nanocluster
potential ioniz.*2ci-covalent index	F- surface molecules*cpp2	potential ioniz.*S H2O	F- surface molecules
S H2O*2ci-covalent index	sv*cpp2	S H2O*S H2O	sv
V H2O*2ci-covalent index	electronegativity Met *cpp2	V H2O*S H2O	electronegativity Met
R H2O*2ci-covalent index	atom radius*cpp2	R H2O*S H2O	atom radius
nominal size*z -ion charge	ion radius by Bokij*cpp2	nominal size*V H2O	ion radius by Bokij
size in H2O*z -ion charge	1ci-covalent index*cpp2	size in H2O*V H2O	1ci-covalent index
molecular mass*z -ion charge	2ci-covalent index*cpp2	molecular mass*V H2O	2ci-covalent index
mass density*z -ion charge	z -ion charge*cpp2	mass density*V H2O	z -ion charge
Wigner-Seitz radius*z -ion charge	cpp1*cpp2	Wigner-Seitz radius*V H2O	cpp1

n -number of molecules in a nanocluster *z -ion charge	cpp2*cpp2	n -number of molecules in a nanocluster*V H2O	cpp2
F- surface molecules*z -ion charge	potential ioniz.*cpp2	F- surface molecules*V H2O	potential ioniz.
sv*z -ion charge	S H2O*cpp2	sv*V H2O	S H2O
electronegativity Met *z -ion charge	V H2O*cpp2	electronegativity Met *V H2O	V H2O
atom radius*z -ion charge	R H2O*cpp2	atom radius*V H2O	R H2O
ion radius by Bokij*z -ion charge	nominal size*potential ioniz.	ion radius by Bokij*V H2O	
1ci-covalent index*z -ion charge	size in H2O*potential ioniz.	1ci-covalent index*V H2O	
2ci-covalent index*z -ion charge	molecular mass*potential ioniz.	2ci-covalent index*V H2O	
z -ion charge*z -ion charge	mass density*potential ioniz.	z -ion charge*V H2O	

ДОДАТОК В

СТАТИСТИЧНІ ХАРАКТЕРИСТИКИ МОДЕЛІ (ζ-ПОТЕНЦІАЛ)

							Y-scrambling	
	Model	R2	Q2	R2(test)	A	N	R2	Q2
f1	1gen.dat	0.887	0.786	0.815	3	44	0.255	0.088
f2	2gen.dat	0.862	0.777	0.886	2	50	0.281	0.057
f3	3gen.dat	0.905	0.854	0.672	3	49	0.287	0.118
f4	4gen.dat	0.875	0.808	0.878	3	43	0.316	0.141
f5	5gen.dat	0.908	0.821	0.805	3	50	0.303	0.112
Consensus		**0.8874**		**0.8112**				

Використані дескриптори:

дескриптор	внесок (%)	дескриптор	внесок (%)	дескриптор	внесок (%)
Cnk(groups)/K,P	7.820428	Cnk(groups)/D,P	0.461088	potential ioniz.*F-surface molecules	0.240071
Cnk(att)/B	7.291867	Cnk(rf)/A,C	0.452382	2ci-covalent index*ion radius by Bokij	0.236233
Cnk(rep)/C	5.570152	potential ioniz.*z -ion charge	0.445771	Cnk(zar-nucl)/B	0.234323
Cnk(groups)/J,P	5.514716	Cnk(step-okisl)/C,C	0.444605	Cnk(rep)/A,D	0.233968
Cnk(groups)/C,P,P	5.105057	Cnk(spdf)/C	0.438806	Cnk(spdf)/B	0.217619
ion radius by Bokij*ion radius by Bokij	4.771832	electronegativity Met *electronegativity Met	0.438468	Cnk(step-okisl)/A,A,C	0.176638
Cnk(rf)/A,C,C,C	4.063792	Cnk(att)/G	0.411164	potential ioniz.*1ci-covalent index	0.161405
ion radius by Bokij*F-surface molecules	3.492322	1ci-covalent index*Wigner-Seitz radius	0.38883	Cnk(zar-nucl)/A	0.160137
Cnk(att)/C,C,C,C	3.104556	Cnk(step-okisl)/A,B	0.379684	atom radius*Wigner-Seitz radius	0.138227

potential ioniz.	2.901308	Cnk(rep)/A	0.352329	ion radius by Bokij*potential ioniz.	0.132681
Cnk(step-okisl)/E	2.588759	Cnk(spdf)/B,B,B,C	0.33544	Cnk(ion-b)/B,B	0.129317
Cnk(ion-b)/A	1.808292	Wigner-Seitz radius*mass density	0.293225	Cnk(rep)/D,E	0.127153
Cnk(rep)/B,D	1.790134	electronegativity Met *2ci-covalent index	0.290198	2ci-covalent index*potential ioniz.	0.119579
F- surface molecules*Wigner-Seitz radius	1.659346	nominal size*F- surface molecules	0.262066	z -ion charge*1ci-covalent index	0.116451
Cnk(groups)/N,P,P	1.567004	Cnk(step-okisl)/A,A,A	0.260342	Cnk(att)/A	0.095217
Cnk(ion-b)/A,A	1.528288	atom radius*2ci-covalent index	0.250806	sv*1ci-covalent index	0.082841
Cnk(step-okisl)/D	1.455438	atom radius*z -ion charge	0.853013	1ci-covalent index*1ci-covalent index	0.063839
mass density*ion radius by Bokij	1.369435	Cnk(att)/C,G,G	0.849665	mass density*1ci-covalent index	0.052494
Wigner-Seitz radius*z -ion charge	1.257126	2ci-covalent index*Wigner-Seitz radius	0.849023	mass density*potential ioniz.	0.030651
mass density	1.249941	F- surface molecules*mass density	0.841635	cpp2*potential ioniz.	0.025833
Wigner-Seitz radius*potential ioniz.	1.240237	Cnk(ion-b)/B	0.78444	nominal size*1ci-covalent index	0.023753
Cnk(att)/C	1.211783	Cnk(ion-b)/A,B	0.756832	2ci-covalent index*mass density	0.02328
atom radius*atom radius	1.179965	Cnk(step-okisl)/B	0.731371	nominal size*cpp2	0.00585
z -ion charge*ion radius by Bokij	1.176517	electronegativity Met *potential ioniz.	0.62508	molecular mass*F-surface molecules	0.00235
Cnk(ion-b)/A,A,B,B	1.137074	Cnk(zar-nucl)/A,A,C,C	0.621479	z -ion charge*molecular mass	0.001471
potential ioniz.*atom radius	1.101148	ion radius by Bokij*cpp1	0.596678	F- surface molecules*sv	0.001167
Cnk(rf)/A	1.095518	Cnk(groups)/P	0.569323	molecular mass*sv	0.000862

atom radius*mass density	1.012372	ion radius by Bokij*Wigner-Seitz radius	0.561242	cpp1*molecular mass	0.000828
Cnk(att)/C,C,C	0.938136	F- surface molecules*z -ion charge	0.55852	1ci-covalent index*molecular mass	0.000693
Cnk(groups)/H	0.934501	Cnk(rep)/D	0.50496	molecular mass*potential ioniz.	0.000592
Cnk(zar-nucl)/A,A,A	0.924121	1ci-covalent index*F-surface molecules	0.48895	molecular mass*nominal size	0.000321
Cnk(zar-nucl)/C	0.89964	Cnk(rep)/D,D,D	0.488696	size in H2O*1ci-covalent index	0.000169
F- surface molecules*atom radius	0.886825	Cnk(rf)/B	0.468679	R H2O*cpp2	0.000118
Cnk(spdf)/B,C	0.461291				

ДОДАТОК Г

СТАТИСТИЧНІ ХАРАКТЕРИСТИКИ МОДЕЛІ (Енергія E_g)

fold--1	**fold--2**	**fold--3**	**fold--4**	**fold--5**
A=2	A=2	A=2	A=2	A=2
Cases count=32	Cases count=31	Cases count=31	Cases count=31	Cases count=31
Var count(N)=17	Var count(N)=18	Var count(N)=22	Var count(N)=33	Var count(N)=27
R2=0.829	R2=0.815	R2=0.803	R2=0.823	R2=0.865
Q2(LOO)=0.670	Q2(LOO)=0.742	Q2(LOO)=0.724	Q2(LOO)=0.727	Q2(LOO)=0.747
S(cv)=0.557	S(cv)=0.448	S(cv)=0.492	S(cv)=0.485	S(cv)=0.462
R2(test)=0.614	R2(test)=0.764	R2(test)=0.744	R2(test)=0.727	R2(test)=0.682

дескриптор	внесок (%)	дескриптор	внесок (%)	дескриптор	внесок (%)	дескриптор	внесок (%)	дескриптор	внесок (%)
Cnk(att)/A,C	16.09	Cnk(att)/A	10.03	Cnk(att)/A	8.51	Cnk(att)/A	7.46	Cnk(att)/G	6.86
Cnk(att)/G	14.17	Cnk(ion-b)/A,A	9.82	Cnk(rep)/A	8.08	Cnk(en)/A,D,D,D	6.34	Cnk(spdf)/B,B	6.67
Cnk(en)/B,B	10.66	Cnk(ion-b)/C,C,C	9.57	Cnk(ion-b)/A,A	7.82	Cnk(att)/A,C	5.99	Cnk(rep)/D,D,D	6.5
Cnk(ion-b)/A	8.24	Cnk(en)/A,D,D	8.63	Cnk(spdf)/B,C	7.38	Cnk(ion-b)/C,C,C,D	5.97	Cnk(att)/A	6.48
Cnk(ox1)/B,B	8.03	Cnk(ion-b)/A,B	8.29	Cnk(att)/A,C	7.09	Cnk(att)/G	4.89	Cnk(spdf)/B,B,B	6.02
Cnk(rep)/B,D,D	7.73	Cnk(att)/A,C	6.35	Cnk(spdf)/B,C,C	6.34	Cnk(ion-b)/A,A,B	4.81	Cnk(en)/A,A,D	5.97
Cnk(ion-b)/D,D	6.17	Cnk(spdf)/B,B	6.1	ci-2	6.03	Cnk(ion-b)/A,A	4.74	Cnk(att)/A,A	5.84

Cnk(ox1)/C,D,D	4.61	n*ci	6.1	Cnk(spdf)/B	5.88	Cnk(groups)/H	4.63	Cnk(ion-b)/C	5.18
Cnk(en)/A,A,D	4.25	Cnk(spdf)/C,C	5.39	ion radius Bokij	5.73	Cnk(en)/A	4.51	Cnk(ion-b)/C,D,D	5.09
Cnk(en)/A,D,D	3.98	Cnk(rep)/D,D	5.01	Cnk(en)/A,A,D	5.43	Cnk(en)/B	4.22	Cnk(en)/A,D	4.72
Cnk(rep)/D,D	3.96	Cnk(rep)/A	4.84	Cnk(ion-b)/C	5.1	Cnk(att)/C,C,G	4.07	Cnk(ion-b)/A,A	4.52
Cnk(en)/A,D	3.85	Cnk(att)/A,C,C	4.22	Cnk(en)/A,D,D	5.06	Cnk(rep)/A	3.96	Cnk(att)/A,C	4.4
n*cpp-2	3.26	Cnk(groups)/N	3.91	Cnk(ion-b)/C,C,C,D	3.27	Cnk(ion-b)/C	3.84	Cnk(en)/A	3.71
Cnk(ion-b)/B,B,B	2.32	Cnk(zar)/A,A	3.22	Cnk(zar)/A	2.96	Cnk(en)/B,D,D	3.39	Cnk(groups)/H,P	3.58
Cnk(r612)/B	1.14	Cnk(groups)/L	2.95	F*ci	2.89	Cnk(groups)/N,P,P	3.34	Cnk(en)/B,B	3.53
Cnk(ion-b)/B	0.97	Cnk(groups)/F,P	2.4	Cnk(groups)/N,P,P	2.85	Cnk(spdf)/B,B,B,B	3.17	nominal size*ci-2	3.45
Cnk(stok)/A,A,F	0.57	F*ci-2	1.83	Cnk(ox1)/C,D	2.83	Cnk(zar)/A,A,A,A	2.59	Cnk(stok)/A,I	3.09
		Cnk(rep)/A,D	1.35	Cnk(groups)/G,G,P,P	2.42	nominal size*ci-2	2.48	Cnk(ox1)/C	2.62
				Cnk(att)/C	2.32	Cnk(rep)/B,D,D	2.32	Cnk(groups)/G,P,P	2.07
				Cnk(rep)/D,D,D	0.75	n*cpp-2	2.3	Cnk(rep)/A,D	1.96
				Cnk(ox1)/D,D	0.72	Cnk(rep)/D,D	2.3	nominal size*ion radius Bokij	1.69
				Cnk(att)/C,C	0.56	Cnk(rep)/A,A,D	2.24	nominal size*electronegativity	1.59
						Cnk(zar)/A	1.74	Cnk(spdf)/B,C,C	1.31
						Cnk(stok)/A,A,F,F	1.45	nominal size*z	1.19

nominal size*cpp	1.44	Cnk(rep)/A,D,D,D	0.82
nominal size*electronegativity	1.17	nominal size*molecular mass	0.63
mass density	0.88	Cnk(en)/B,D	0.51
cpp	0.76		
Cnk(ion-b)/B,B,B	0.75		
Cnk(ion-b)/B,C	0.7		
Cnk(rep)/D,D,D	0.7		
Cnk(groups)/F,F,P,P	0.59		
nominal size*z	0.27		