„Tarnowskie Colloquia Naukowe. Tarnow Scientific Colloquia"

WYTYCZNE DLA AUTORÓW

Nauki ścisłe

Tytuł (Title)

Komentarz [R1]: @Header should be inserted the type of submitted article, here is the list of available types: Original Research, Review, Clinical case study, Perspective, Communication.

Title should be specific, descriptive, concise, and comprehensible to readers outside the field and not longer than 250 characters.

Given-name Surname1[a,*], Given-name Surname2[b]

[a]*Affiliation, Address, City and Postal Code, Country*

[a]*Affiliation, Address, City and Postal Code, Country*

[*]Corresponding author: r_kurczab@pwsztar.edu.pl

Streszczenie (Abstract)

The objective of this template is to enable you in an easy way to style your article attractively in a similar style. This section should contain no more than **300 words.**

Słowa kluczowe (key words):

Wstęp (Introduction)

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Materiały i Metody (Materials and Methods)

All **apparatus** used should be described; commercially available instruments are referred to by their stock numbers (for example, Perkin-Elmer 457 or Varian HA-100 spectrometers). The accuracy of primary measurements should be stated.

Podtytuł 1

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Podtytuł 2

Using the 'Object' option and selecting the '**Microsoft Equation 3.0'**, you can create equations in the Word® equation plug-in editor, or if the MathType™ equation editor is installed on your computer, in the **MathType™** equation editor. Example equation:

$$\Delta G_{bind} = \Delta E_{MM} + \Delta G_{sol} + \Delta G_{SA} \quad (1)$$

Komentarz [R2]: All equations should be numbered.

Wyniki i Dyskusja (Results and Discussion)

For **tabular summations** that do not deserve to be presented as a table, lists are often used. Lists may be either numbered or bulleted. Below you see examples of both.

1. The first entry in this list
2. The second entry
   2.1. A subentry
3. The last entry
   - A bulleted list item
   - Another one

Ensure that all **tables, figures and schemes** are cited in the text in numerical order. Trade names should have an initial capital letter, and trademark protection should be acknowledged in the standard fashion, using the superscripted characters for trademarks and registered trademarks respectively. All measurements and **data should be given in SI units** where possible, or other internationally accepted units. **Abbreviation**s should be used consistently throughout the text, and all nonstandard abbreviations should be defined on first usage.

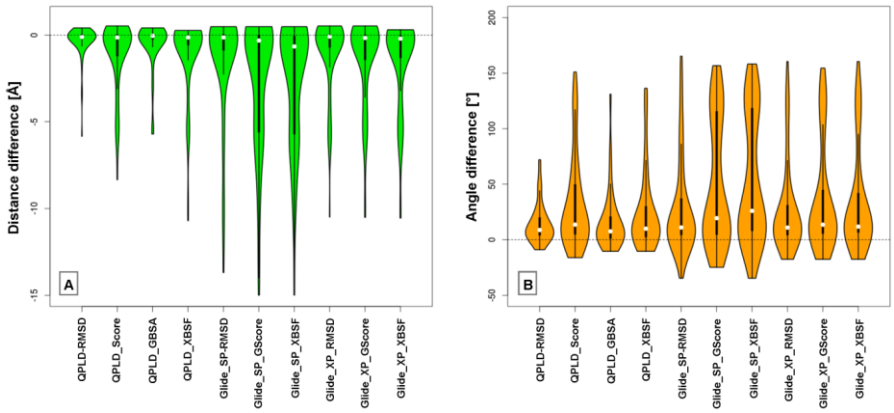
Below, the example table and figure with captions are attached.

Tabela 1. (Table 1.) General description of the used set of X-ray ligand–protein complexes with halogen bonding (XB).

Halogen[a]	No. of complexes	XB angle range [°]	XB distance range [Å]	Crystal resolution range [Å]

Cl	39	141 - 176	2.67 – 3.67	1.00 – 2.90
Br	32	159 – 176	2.34 – 3.69	1.10 – 2.92
I	35	148 - 178	2.83 – 3.76	1.25 – 2.90

[a]This is the format for table footnotes.



Rysunek 1. (Figure 1.) Violin plots showing the difference in halogen bonding distance (A) and σ-hole angle (B) calculated between the best pose predicted by the given scoring method and the crystallographic geometry.

Komentarz [R3]: Figure File Requirements:
- **File format**: tiff or png,
- **Resolution**: 300 – 600 dpi,
- **Text within Figures**: Arial, Times font only in 8-12 poin,
- **Captions**: in the manuscript, not in the figure file.

Podsumowanie (Conclusions)

Podziękowania (Acknowledgments)

The study was supported by the National Science Center Grant No DEC-2014…….

Literatura (References)

Komentarz [R4]: The citation style: for article (1), software (2), book (3), online resources (4), patents (5), disertations and thesis (6), material presented at meeting (7). EndNote style attached, for Mendeley Reference Manager users, the citing style *RSC Advances* should be used.

1. K. Wichapong, A. Rohe, C. Platzer, I. Slynko, F. Erdmann, M. Schmidt and W. Sippl, *J. Chem. Inf. Model.*, 2014, **54**, 881–893.
2. F. James, AIM2000, version 1.0, University of Applied Sciences, Bielefeld, Germany, 2000.
3. L. H. Hartwell, L. Hood, M. L. Goldberg, A. E. Reynolds and L. M. Silver, Genetics: From Genes to Genomes, McGrawHill, New York, 4th edn., 2011, ch. 6, pp. 162–198.
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5. US Pat., US20100120727A1, 2010.
6. A. McMillen, MBA Dissertation, University of Bath, 2010.
7. H. C. Freeman, Proceedings of the 21st International Conference on Coordination Chemistry, Toulouse, 1980.

Informacje dodatkowe (Supplementary information)

Supplementary material that may be helpful in the review process should be prepared and provided as have been shown below.

Rysunek S1. The comparison of atomic partial charges assigned by OPLS3 force field.

Plik S1. The list of PDB ID codes including halogenated ligand–protein complexes used.

Tabela S1. The comparison of median, 95% confidence interval (CI) and standard deviation (SD) calculated for differences between estimated halogen bonding geometry (XB distance and angle) by the given docking/scoring procedure and crystallographic structure.

		XB distance [Å]			XB angle [°]		
		Median	95% CI	SD	Median	95% CI	SD
QPLD	RMSD	-0.11	-0.52; -0.11	0.90	8.8	10.58; 18.68	17.84
	GScore	-0.14	-1.52; -0.63	1.96	13.63	23.39; 42.22	41.49
	GBSA	-0.05	-0.81; -0.20	1.35	7.58	10.55; 22.88	27.16
	XBSF	-0.13	-1.51; -0.52	2.19	9.99	16.91; 33.38	36.28
Glide_SP	RMSD	-0.14	-2.18; -0.76	3.13	11.06	18.89; 38.12	42.36
	GScore	-0.32	-3.38; -1.72	3.66	19.44	37.42; 62.51	55.27
	XBSF	-0.66	-3.46; -1.87	3.50	25.99	41.36; 66.74	55.89
Glide_XP	RMSD	-0.09	-1.50; -0.53	2.15	10.97	18.67; 36.94	40.23
	GScore	-0.21	-2.05; -0.91	2.51	13.59	26.32; 48.26	48.31
	XBSF	-0.17	-1.93; -0.82	2.45	11.81	24.01; 44.69	45.55