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Corrigendum to "Synthesis of 3-Methoxy-6- [(2, 4, 6-trimethyl--phenylamino)-methyl]-phenol Schiff base characterized by spectral, in-silco and in-vitro studies" [Heliyon Volume 8, Issue 8, August 2022, Article e10070]

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In the original published version of this article, references [24] and [46] contained formatting errors. References [30] and [33] are also duplicates:

[24] A.U. Rahman, M.I. Choudhary, W.J. Thomsen, Bioassay Techniques for Drug Development, Harwood Academic Publishers, Netherlands, 2001, pp. 13–22.

[25] M. Montazerozohori, S. Zahedi, A. Naghiha, M. MontazerZohour, Synthesis of some new antibacterial active cadmium and mercury complexes of 4-(3-(2-(4-(dimethyl aminophenyl allylidene aminopropyl-imino)prop-1-ethyl)-N,N-dimethyl benzene amine, Chem. Speciat. Bioavailability 26 (4) (2014) 240–248.

[26] R.J. Gonzalez, J.B. Tarloff, Evaluation of hepatic sub cellular Fractions for alamar blue and MTT reductase activity, Toxicol. Vitro 15 (2001) 257–259.

[27] G.M. Morris, R. Huey, W. Lindstrom, Autodock4 and AutoDockTools4: automated docking with selective receptor flexibility, J. Comput. Chem. 16 (2009) 2785–2791.

[28] H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Bhat, H. Weissig, I.N. Shindyalov, P.E. Bourne, The protein data bank, Nucleic Acids Res. 28 (2000) 235–242.

[29] Peter W. Rose, The RCSB protein data bank: integrative view of protein, gene and 3D structural information, Nucleic Acids Res. 45 (2017) 271–281.

[30] W.L. DeLano, The PyMOL Molecular Graphics System, DeLano Scientific, San Carlos, CA, 2002.

[31] K. Schoning-Stierand, K. Diedrich, R. F € €ahrrolfes, Proteins plus interactive analysis of protein–ligand binding interfaces, Nucleic Acids Res. 48 (2020) 48–53.

[32] A.C. Wallace, R.A. Laskowski, J.M. Thornton, LIGPLOT: a program to generate schematic diagrams of protein-ligand interactions,

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https://doi.org/10.1016/j.heliyon.2025.e43175

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Protein Eng. 8 (1995) 127–134.

[33] W.L. DeLano, The PyMOL Molecular Graphics System, DeLano Scientific, San Carlos, CA, 2009, p. 700.

[34] A.Z. Gavezzotti, Calculation of lattice energies of organic crystals: the PIXEL integration method in comparison with more traditional methods, Kristallogr. Cryst.Mater. 220 (2005) 499.

[35] A. Gavezzotti. Molecular Aggregation. Structure analysis and molecular simulation of crystals and liquids, Oxford University Press, 2007.

[36] A. Gavezzotti, Efficient computer modeling of organic materials. The atom–atom, Coulomb–London–Pauli (AA-CLP) model for intermolecular electrostaticpolarization, dispersion and repulsion energies, New J. Chem. 35 (2011) 1360–1368.

[37] A. Gavezzotti, The "sceptical chymist": intermolecular doubts and paradoxes, CrystEngComm 15 (2013) 4027–4035.

[38] P. Politzer, F. Abu-Awwad, A comparative analysis of Hartree-Fock and Kohn-Sham orbital energies, Theor. Chem. Acc. 99 (1998) 83.

[39] R.S. Mulliken, A new electroaffinity scale; together with data on valence states and on valence ionization potentials and electron affinities, J. Chem. Phys. 2 (1934) 782.

[40] R.G. Pearson, Absolute electronegativity and hardness: applications to organic chemistry, J. Org. Chem. 54 (1989) 1423.

[41] R.G. Pearson, Chemical Hardness-Applications from Molecules to Solids, John Wiley–VCH, Weinheim, 1997.

[42] N.E.H. Belkafouf, F. Triki-Baara, A. Altomare, R. Rizzi, A. Chouaih, A. Djafri, F. Hamzaoui, Synthesis, PXRD structural determination, Hirshfeld surface analysis and DFT/TD-DFT investigation of 3N-ethyl-2N'-(2-ethylphenylimino) thiazolidin4-one, J. Mol. Struct. 1189 (2019) 8–20.

[43] J. Padmanabhan, R. Parthasarathi, V. Subramanian, P.K. Chattaraj, Electrophilicitybased charge transfer descriptor, J. Phys. Chem. 111 (2007) 1358.

[44] N. Hattori, Enhanced microbial biomass assay using mutant luciferase resistant to benzalkonium chloride, Anal. Biochem. 319 (2003) 287–295.

[45] G. Bhabha, D. Ekiert, M. Jennewein, Divergent evolution of protein conformational dynamics in dihydrofolate reductase, NatStruct. Mol. Biol. 20 (2013) 1243–1249.

[46] Q. Xiayang, A. Cheryl Janson, Ward W. Smith, Martha Head, John lonsdale, alex K konstantinidis, refined structures of ˆI2 -ketoacyl-acyl carrier protein synthase III11Edited by I. A. Wilson, J. Mol. Biol. 307 (2001) 341–356.

[47] C. Davies, R.J. Heath, S.W. White, C.O. Rock, The 1.8 A crystal structure and activesite architecture of beta-ketoacyl-acyl carrier protein synthase III (FabH) from escherichia coli, Structure 15 (2000) 185–195.

References [24] and [46] have now been updated to the correct versions. Reference [33] has been removed. The reference list has been renumbered accordingly. The intext citations have been updated to reflect this change. The correct version of the reference list can be found below:

[24] ***Atta-ur-Rahman., M.Iqbal Choudhary., W.J. Thomsen, Bioassay Techniques for Drug Development, first ed., Harwood Academic, Netherlands, 2001***.

[25] M. Montazerozohori, S. Zahedi, A. Naghiha, M. MontazerZohour, Synthesis of some new antibacterial active cadmium and mercury complexes of 4-(3-(2-(4-(dimethyl aminophenyl allylidene aminopropyl-imino)prop-1-ethyl)-N,N-dimethyl benzene amine, Chem. Speciat. Bioavailability 26 (4) (2014) 240–248.

[26] R.J. Gonzalez, J.B. Tarloff, Evaluation of hepatic sub cellular Fractions for alamar blue and MTT reductase activity, Toxicol. Vitro 15 (2001) 257–259.

[27] G.M. Morris, R. Huey, W. Lindstrom, Autodock4 and AutoDockTools4: automated docking with selective receptor flexibility, J. Comput. Chem. 16 (2009) 2785–2791.

[28] H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Bhat, H. Weissig, I.N. Shindyalov, P.E. Bourne, The protein data bank, Nucleic Acids Res. 28 (2000) 235–242.

[29] Peter W. Rose, The RCSB protein data bank: integrative view of protein, gene and 3D structural information, Nucleic Acids Res. 45 (2017) 271–281.

[30] W.L. DeLano, The PyMOL Molecular Graphics System, DeLano Scientific, San Carlos, CA, 2002.

[31] K. Schoning-Stierand, K. Diedrich, R. F € €ahrrolfes, Proteins plus interactive analysis of protein–ligand binding interfaces, Nucleic Acids Res. 48 (2020) 48–53.

[32] A.C. Wallace, R.A. Laskowski, J.M. Thornton, LIGPLOT: a program to generate schematic diagrams of protein-ligand interactions, Protein Eng. 8 (1995) 127–134.

[33] A.Z. Gavezzotti, Calculation of lattice energies of organic crystals: the PIXEL integration method in comparison with more traditional methods, Kristallogr. Cryst.Mater. 220 (2005) 499.

[34] A. Gavezzotti. Molecular Aggregation. Structure analysis and molecular simulation of crystals and liquids, Oxford University Press, 2007.

[35] A. Gavezzotti, Efficient computer modeling of organic materials. The atom–atom, Coulomb–London–Pauli (AA-CLP) model for intermolecular electrostaticpolarization, dispersion and repulsion energies, New J. Chem. 35 (2011) 1360–1368.

[36] A. Gavezzotti, The "sceptical chymist": intermolecular doubts and paradoxes, CrystEngComm 15 (2013) 4027–4035.

[37] P. Politzer, F. Abu-Awwad, A comparative analysis of Hartree-Fock and Kohn-Sham orbital energies, Theor. Chem. Acc. 99 (1998) 83.

[38] R.S. Mulliken, A new electroaffinity scale; together with data on valence states and on valence ionization potentials and electron affinities, J. Chem. Phys. 2 (1934) 782.

[39] R.G. Pearson, Absolute electronegativity and hardness: applications to organic chemistry, J. Org. Chem. 54 (1989) 1423.

[40] R.G. Pearson, Chemical Hardness-Applications from Molecules to Solids, John Wiley–VCH, Weinheim, 1997.

[41] N.E.H. Belkafouf, F. Triki-Baara, A. Altomare, R. Rizzi, A. Chouaih, A. Djafri, F. Hamzaoui, Synthesis, PXRD structural determination, Hirshfeld surface analysis and DFT/TD-DFT investigation of 3N-ethyl-2N'-(2-ethylphenylimino) thiazolidin4-one, J. Mol. Struct. 1189 (2019) 8–20.

[42] J. Padmanabhan, R. Parthasarathi, V. Subramanian, P.K. Chattaraj, Electrophilicitybased charge transfer descriptor, J. Phys. Chem. 111 (2007) 1358.

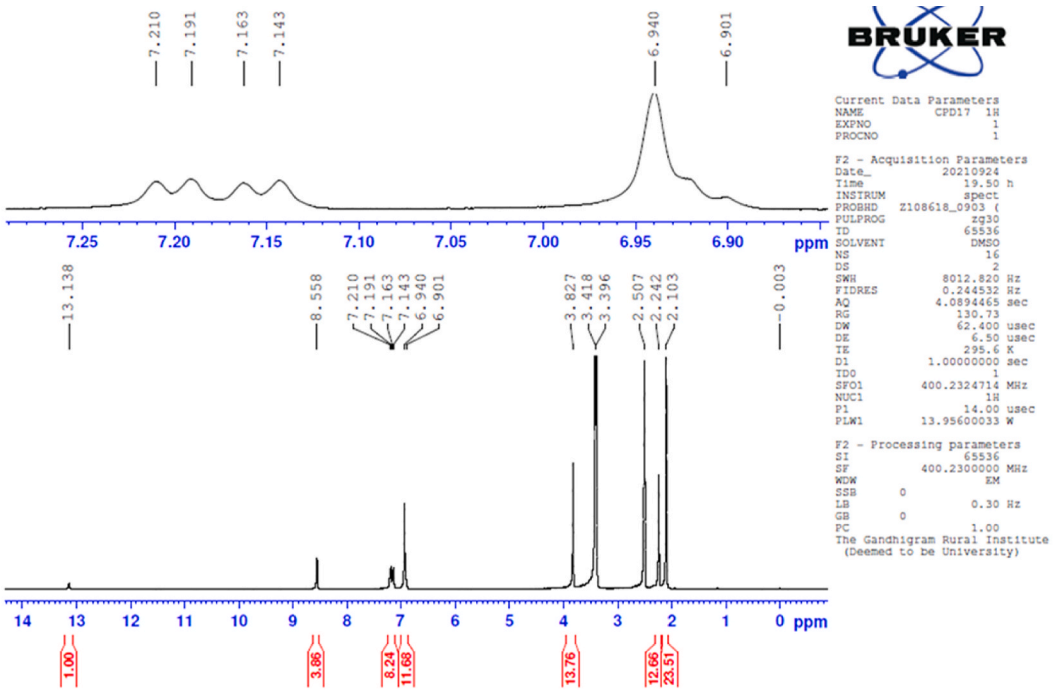
[43] N. Hattori, Enhanced microbial biomass assay using mutant luciferase resistant to benzalkonium chloride, Anal. Biochem. 319 (2003) 287–295.

[44] G. Bhabha, D. Ekiert, M. Jennewein, Divergent evolution of protein conformational dynamics in dihydrofolate reductase, NatStruct. Mol. Biol. 20 (2013) 1243–1249.

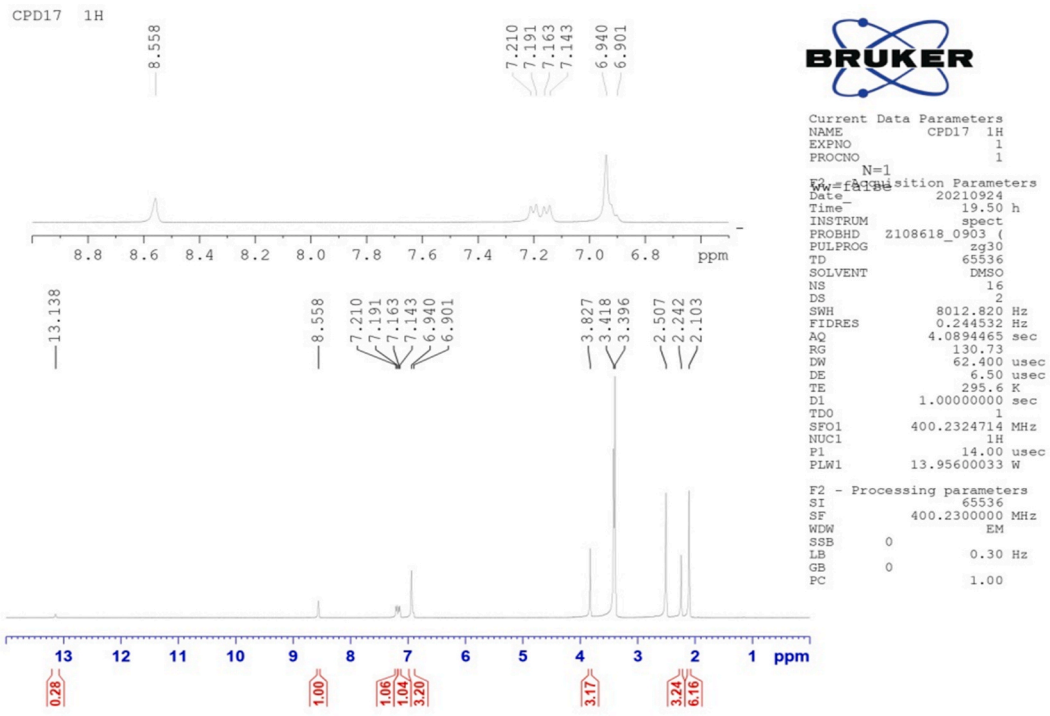
[45] Qiu, X., Janson, C.A., Smith, W.W., Head, M., Lonsdale, J., Konstantinidis, A.K., 2001. Refined structures of β-ketoacyl-acyl carrier protein synthase III. Journal of Molecular Biology 307, 341–356. https://doi.org/10.1006/jmbi.2000.4457.

[46] C. Davies, R.J. Heath, S.W. White, C.O. Rock, The 1.8 A crystal structure and activesite architecture of beta-ketoacyl-acyl carrier protein synthase III (FabH) from escherichia coli, Structure 15 (2000) 185–195.

Figure S3in the Supplementary data was also incorrectly included:



The correct version **of Fig S3** can be found below:



The authors apologize for the errors. Both the HTML and PDF versions of the article have been updated to correct the errors.

Declaration of competing interest

The authors declare no conflict of interest.