

# Accuracy of determination of self-diffusion coefficients in studies of porphyrin-based complexes by 2D DOSY

Khodov I.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

## Abstract

© ISUCT Publishing. Influence of chemical exchange processes on the accuracy of determination of self-diffusion complexes of porphyrin-nickel complexes was shown. A method of estimating the inaccuracy of the self-diffusion coefficients for an inverted porphyrin complex was proposed. The values obtained using two different approaches to recording DOSY spectra, STE and CPMG, were compared. Allowing for exchange was shown to be important for accurate diffusion measurements and correct interpretation of results obtained in studied of molecular-level processes.

<http://dx.doi.org/10.6060/mhc170200k>

## Keywords

2D DOSY, Chemical exchange, J-modulation, N-confused porphyrins, NMR, Self-diffusion coefficients

## References

- [1] Khodov I.A., Nikiforov M.Y., Alper G.A., Blokhin D.S., Efimov S.V., Klochkov V.V., Georgi N. J. Mol. Struct. 2013, 1035, 358-362.
- [2] Khodov I.A., Efimov S.V., Klochkov V.V., Alper G.A., Batista de Carvalho L.A.E. Eur. J. Pharm. Sci. 2014, 65C, 65-73.
- [3] Khodov I.A., Efimov S.V., Klochkov V.V., Batista de Carvalho L.A.E., Kiselev M.G. J. Mol. Struct. 2016, 1106, 373-381.
- [4] Khodov I.A., Efimov S.V., Nikiforov M.Y., Klochkov V.V., Georgi N. J. Pharm. Sci. 2014, 103, 392-394.
- [5] Kalmykov P.A., Khodov I.A., Klochkov V.V., Klyuev M.V. Russ. Chem. Bull. 2017, 66, 70-75.
- [6] Efimov S., Zgadzay Y., Klochkov V. Appl. Magn. Reson. 2014, 45, 1225-1235.
- [7] Efimov S.V., Karataeva F.K., Aganov A.V., Berger S., Klochkov V.V. J. Mol. Struct. 2013, 1036, 298-304.
- [8] Bikmullin A.G., Alimova F.K., Aganov A.V., Klochkov V.V., Usachev K.S. Res. J. Pharm. Biol. Chem. Sci. 2015, 6, 25-31.
- [9] Usachev K.S., Efimov S.V., Kolosova O.A., Klochkova E.A., Aganov A.V., Klochkov V.V. J. Biomol. NMR 2015, 62, 71-79.
- [10] Usachev K.S., Filippov A.V., Khairutdinov B.I., Antzutkin O.N., Klochkov V.V. J. Mol. Struct. 2014, 1076, 518-523.
- [11] Ksenofontov A.A., Guseva G.B., Antina E.V., Khodov I.A., Vyugin A.I. Sens. Actuators, B Chem. 2017, 251, 858-868.
- [12] Maltceva O., Mamardashvili G., Khodov I., Lazovskiy D., Khodova V., Krest'yaninov M., Mamardashvili N., Dehaen W. Supramol. Chem. 2017, 29, 360-369.
- [13] Khodov I.A., Alper G.A., Mamardashvili G.M., Mamardashvili N.Z. J. Mol. Struct. 2015, 1099, 174-180.

- [14] Bichan N.G., Tyulyaeva E.Y., Khodov I.A., Lomova T.N. *J. Mol. Struct.* 2014, 1061, 82-89.
- [15] Khodov I.A., Nikiforov M.Y., Alper G.A., Mamardashvili G.M., Mamardashvili N.Z., Koifman O.I. *J. Mol. Struct.* 2014, 1081, 426-430.
- [16] Ballester P., Claudel M., Durot S., Kocher L., Schoepff L., Heitz V. *Chem. Eur. J.* 2015, 21, 15339-15348.
- [17] Malyasova A.S., Kokareva E.A., Tarakanov P.A., Aleksandriiskii V.V., Khelevina O.G., Koifman O.I. *Russ. J. Org. Chem.* 2014, 49, 1812-1818.
- [18] Marchand G., Roy H., Mendive-Tapia D., Jacquemin D. *Phys. Chem. Chem. Phys.* 2015, 17, 5290-5297.
- [19] Paul A.K., Karunakaran S.C., Joseph J., Ramaiah D. *Photochem. Photobiol.* 2015, 91, 1348-1355.
- [20] Renney C.M., Fukuhara G., Inoue Y., Davis A.P. *Chem. Commun.* 2015, 51, 9551-9554.
- [21] Watarai H., Kurahashi Y. *Anal. Chem.* 2016, 88, 4619-4623.
- [22] Xie J., Chen X., Huang Z., Zuo T. *J. Mol. Model.* 2015, 21, 140.
- [23] Yang J., Wang Z., Hu K., Li Y., Feng J., Shi J., Gu J. *ACS Appl. Mater. Interfaces* 2015, 7, 11956-11964.
- [24] Zhao T., Wang Y.-L., Zhu L.-N., Huo Y.-F., Wang Y.-J., Kong D.-M. *RSC Adv.* 2015, 5, 47709-47717.
- [25] Babailov S.P. *Macroheterocycles* 2010, 3, 218-221.
- [26] Brotherhood P.R., Luck I.J., Crossley M.J. *Magn. Reson. Chem.* 2009, 47, 257-262.
- [27] Volov A.N., Zamilatskov I.A., Mikhel I.S., Erzina D.R., Ponomarev G.V., Koifman O.I., Tsivadze A.Y. *Macroheterocycles* 2014, 7, 256-261.
- [28] Stolypko A.L., Belykh D.V. *Macroheterocycles* 2015, 8, 389-393.
- [29] Belykh D.V., Stolypko A.L. *Macroheterocycles* 2017, 10, 51-56.
- [30] Stolypko A.L., Belykh D.V., Startseva O.M. *Macroheterocycles* 2015, 8, 47-49.
- [31] Durot S., Taesch J., Heitz V. *Chem. Rev.* 2014, 114, 8542-8578.
- [32] Oliva A.I., Gómez K., González G., Ballester P. *New J. Chem.* 2008, 32, 2159-2163.
- [33] Watanabe H., Kamatani Y., Tamiaki H. *Chem. - An Asian J.* 2017, 12, 759-767.
- [34] Chiba Y., Liu M., Tachibana Y., Fujihara T., Tsuji Y., Terao J. *Chem. - An Asian J.* 2017, 12, 1900-1904.
- [35] Ikawa Y., Takeda M., Suzuki M., Osuka A., Furuta H. *Chem. Commun.* 2010, 46, 5689-5691.
- [36] Ishizuka T., Yamasaki H., Osuka A., Furuta H. *Tetrahedron* 2007, 63, 5137-5147.
- [37] Krasnikov S.A., Sergeeva N.N., Brzhezinskaya M.M., Preobrajenski A.B., Sergeeva Y.N., Vinogradov N., Cafolla A.A., Senge M.O., Vinogradov A.S. *J. Phys. Condens. Matter* 2008, 20, 235207.
- [38] Thomas A.P., Saneesh Babu P.S., Asha Nair S., Ramakrishnan S., Ramaiah D., Chandrashekar T.K., Srinivasan A., Radhakrishna Pillai M. *J. Med. Chem.* 2012, 55, 5110-5120.
- [39] Xie Y.S., Yamaguchi K., Toganoh M., Uno H., Suzuki M., Mori S., Saito S., Osuka A., Furuta H. *Angew. Chem. Int. Ed.* 2009, 48, 5496-5499.
- [40] Zhu X., Wong W.-K., Lo W.-K., Wong W.-Y. *Chem. Commun.* 2005, 1022-1024.
- [41] Harvey J.D., Ziegler C.J. *Chem. Commun. (Camb.)* 2002, 2, 1942-1943.
- [42] Khodov I.A., Maltceva O.V., Klochkov V.V., Koifman O.I., Mamardashvili N.Z. *New J. Chem.* 2017, 41, 7932-7937.
- [43] Srinivasan A., Furuta H., Osuka A. *Chem. Commun.* 2001, 1666-1667.
- [44] Furuta H., Asano T., Ogawa T. *J. Am. Chem. Soc.* 1994, 116, 767-768.
- [45] Furuta H., Maeda H., Osuka A. *J. Org. Chem.* 2001, 66, 8563-8572.
- [46] Ishikawa Y., Yoshida I., Akaiwa K., Koguchi E., Sasaki T., Furuta H. *Chem. Lett.* 1997, 26, 453-454.
- [47] Aguilar J.A., Adams R.W., Nilsson M., Morris G.A. *J. Magn. Reson.* 2014, 238, 16-19.
- [48] Pelta M.D., Morris G.A., Stchedroff M.J., Hammond S.J. *Magn. Reson. Chem.* 2002, 40, S147-S152.
- [49] Botana A., Aguilar J.A., Nilsson M., Morris G.A. *J. Magn. Reson.* 2011, 208, 270-278.
- [50] Johnson C.S. *J. Magn. Reson. Ser. A* 1993, 102, 214-218.
- [51] Cabrera E.J., Berger S., Bräuer P., Kärger J. *J. Magn. Reson.* 2002, 157, 124-131.
- [52] Chen A., Shapiro M. *J. Am. Chem. Soc.* 1999, 121, 5338-5339.
- [53] Zhang X., Li C.-G., Ye C.-H., Liu M.-L. *Anal. Chem.* 2001, 73, 3528-3534.
- [54] Aguilar J.A., Nilsson M., Bodenhausen G., Morris G.A. *Chem. Commun.* 2012, 48, 811-813.
- [55] Cabrera E.J., Berger S. *Magn. Reson. Chem.* 2002, 40, S122- S127.