COSMO-RS based prediction for alpha-linolenic acid (ALA) extraction from microalgae biomass using room temperature ionic liquids (RTILs)

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Abstract

One of the essential fatty acids with therapeutic impacts on human health is known to be omega-3 polyunsaturated fatty acids (PUFA). More lately, ionic liquids (ILs) have received significant attention among scientists in overcoming the disadvantages of traditional solvents in biomass lipid extraction. However, the large pool of cations and anions possibly accessible will lead to a growing number of innovatively synthesized ILs. Nevertheless, the exhaustive measurement of all these systems is economically impractical. The conductive screening model for real solvents (COSMO-RS) is considered a precious approach with the availability of a few models to predict the characteristics of ILs. This work introduces the estimate of capacity values at infinite dilution for a range of ILs using COSMO-RS software as part of solid-liquid extraction. This favorable outcome presented that the capacity values of the IL molecules are extremely dependent on both anions and cations. Among the combinations of cation/anion tested, short alkyl chain cations coupled with inorganic anions were found to be most efficient and therefore superior in the extraction method. Sulphate-, chloride-, and bromide-based ILs were found to have higher extraction capacities in contrast with the remainders, while propanoate revealed an extraordinary capacity when combined with ethyl-based cations. Eventually, the predicted results from COSMO-RS were validated through the experimentally calculated extraction yield of alpha-linolenic acid (ALA) compound from Nannochloropsis sp. microalgae.

Marine Drugs Open Access
Volume 18, Issue 2, 12 February 2020, Article number 108

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SciVal Topic Prominence

Topic: Activity Coefficients | 1-Nitropropane | Ternary Systems
Prominence percentile: 97.929

Chemistry database information

Substances

View all substances (18)

Author keywords
Indexed keywords

EMTREE drug terms: bromide, chloride, ionic liquid, linolenic acid, sulfate, anion, cation, ion, ionic liquid, linolenic acid

EMTREE medical terms: Article, biomass, dilution, extraction, microalgae, nonhuman, prediction, room temperature, software, validation process, chemical structure, chemistry, molecular model, temperature, thermodynamics

MeSH: alpha-Linolenic Acid, Anions, Cations, Computational Chemistry, Ionic Liquids, Ions, Microalgae, Models, Molecular, Molecular Structure, Temperature, Thermodynamics

Chemicals and CAS Registry Numbers:
- bromide, 24959-67-9; chloride, 16887-00-6; linolenic acid, 1955-33-5, 463-40-1; sulfate, 14808-79-8;
- alpha-Linolenic Acid; Anions; Cations; Ionic Liquids; Ions

Funding details

Funding sponsor | Funding number | Acronym
--- | --- | ---
Universiti Putra Malaysia |  |  
Universidad Politécnica de Madrid |  | UPM

Funding text #1
Funding: This research was funded by “Matching grant” with grant number 9300432 and the APC was funded by Research Management Centre (RMC)-University Putra Malaysia (UPM).

Funding text #2
Acknowledgments: The authors would like to acknowledge the Centre of Research in Ionic Liquids (CORIL), Universiti Teknologi Petronas (UTP) for providing the required research facilities and to access COSMO-RS software as the main research platform in this work. This research was supported by the Department of Chemical

ISSN: 16603397
CODEN: MDARE
Source Type: Journal
Original language: English

DOI: 10.3390/md18020108
PubMed ID: 32059424
Document Type: Article
Publisher: MDPI AG

References (60)

1. Duc, D., Vigne, S., Pot, C.

  Oxysterols in autoimmunity (Open Access)

  (2019) International Journal of Molecular Sciences, 20 (18), art. no. 4522. Cited 3 times.
  https://www.mdpi.com/1422-0067/20/18/4522/pdf
  doi: 10.3390/ijms20184522

View at Publisher
2. Lauritano, C., Ianora, A.  
Marine organisms with anti-diabetes properties  (Open Access)  
(2016) Marine Drugs, 14 (12), art. no. 220. Cited 28 times.  
http://www.mdpi.com/1660-3397/14/12/220/pdf  
doi: 10.3390/md14120220  
View at Publisher

3. Ryckebosch, E., Bruneel, C., Muylaert, K., Foubert, I.  
Microalgae as an alternative source of omega-3 long chain polyunsaturated fatty acids  
(2012) Lipid Technology, 24 (6), pp. 128-130. Cited 84 times.  
doi: 10.1002/lite.201200197  
View at Publisher

4. Sinn, N., Milte, C.M., Street, S.J., Buckley, J.D., Coates, A.M., Petkov, J., Howe, P.R.C.  
Effects of n-3 fatty acids, EPA v. DHA, on depressive symptoms, quality of life, memory and executive function in older adults with mild cognitive impairment: A 6-month randomised controlled trial  (Open Access)  
(2012) British Journal of Nutrition, 107 (11), pp. 1682-1693. Cited 169 times.  
http://journals.cambridge.org/BJN  
doi: 10.1017/S0007114511004788  
View at Publisher

5. Domenichiello, A.F., Kitson, A.P., Bazinet, R.P.  
Is docosahexaenoic acid synthesis from α-linolenic acid sufficient to supply the adult brain?  (Open Access)  
(2015) Progress in Lipid Research, 59, pp. 54-66. Cited 97 times.  
www.elsevier.com/locate/plipres  
doi: 10.1016/j.plipres.2015.04.002  
View at Publisher

6. Lemahieu, C., Bruneel, C., Ryckebosch, E., Muylaert, K., Buyse, J., Foubert, I.  
Impact of different omega-3 polyunsaturated fatty acid (n-3 PUFA) sources (flaxseed, Isochrysis galbana, fish oil and DHA Gold) on n-3 LC-PUFA enrichment (efficiency) in the egg yolk  
(2015) Journal of Functional Foods, Part B 19, pp. 821-827. Cited 40 times.  
http://www.elsevier.com/wps/find/journaldescription.cws_home/717426/description#description  
doi: 10.1016/j.jff.2015.04.021  
View at Publisher

7. Gibson, R.A., Muhlhausler, B., Makrides, M.  
Conversion of linoleic acid and alpha-linolenic acid to long-chain polyunsaturated fatty acids (LCPUFAs), with a focus on pregnancy, lactation and the first 2 years of life  
(2011) Maternal and Child Nutrition, 7 (SUPPL. 2), pp. 17-26. Cited 138 times.  
doi: 10.1111/j.1740-8709.2011.00299.x  
View at Publisher

8. Kartikasari, L.R., Hughes, R.J., Geier, M.S., Makrides, M., Gibson, R.A.  
Dietary alpha-linolenic acid enhances omega-3 long chain polyunsaturated fatty acid levels in chicken tissues  
(2012) Prostaglandins Leukotrienes and Essential Fatty Acids, 87 (4-5), pp. 103-109. Cited 44 times.  
doi: 10.1016/j.plefa.2012.07.005  
View at Publisher
1. Liu, J., Sun, Z., Gerken, H. Recent advances in microalgal biotechnology omega-3 polyunsaturated fatty acids from algae (2015) Biotechnol. Adv., 8, pp. 709-727.

2. Handayania, N.A., Ariyantib, D. Potential production of polyunsaturated fatty acids from microalgae (2012) Int. J. Sci. Eng., 1, pp. 13-16. Cited 9 times.

3. Abedi, E., Sahari, M.A. Long-chain polyunsaturated fatty acid sources and evaluation of their nutritional and functional properties (Open Access) (2014) Food Science and Nutrition, 2 (5), pp. 443-463. Cited 192 times. online library.wiley.com/journal/10.1002/%28ISSN%292048-7177 doi: 10.1002/fnsr.3.121 View at Publisher

4. Shahidi, F., Ambigaipalan, P. Omega-3 Polyunsaturated Fatty Acids and Their Health Benefits (2018) Annual Review of Food Science and Technology, 9, pp. 345-381. Cited 88 times. http://www.annualreviews.org/journal/food doi: 10.1146/annurev-food-111317-095850 View at Publisher

5. Lee, J.-Y., Yoo, C., Jun, S.-Y., Ahn, C.-Y., Oh, H.-M. Comparison of several methods for effective lipid extraction from microalgae (2010) Bioresource Technology, 101 (1 SUPPL.), pp. S75-S77. Cited 790 times. http://www.journals.elsevier.com/bioresource-technology/ doi: 10.1016/j.biortech.2009.03.058 View at Publisher

6. Patel, A., Arora, N., Sartaj, K., Pruthi, V., Pruthi, P.A. Sustainable biodiesel production from oleaginous yeasts utilizing hydrolysates of various non-edible lignocellulosic biomasses (2016) Renewable and Sustainable Energy Reviews, 62, pp. 836-855. Cited 74 times. doi: 10.1016/j.rser.2016.05.014 View at Publisher

7. Xu, D.-P., Li, Y., Meng, X., Zhou, T., Zhou, Y., Zheng, J., Zhang, J.-J., (...), Li, H.-B. Natural antioxidants in foods and medicinal plants: Extraction, assessment and resources (Open Access) (2017) International Journal of Molecular Sciences, 18 (1), art. no. 96. Cited 179 times. http://www.mdpi.com/1422-0067/18/1/96/pdf doi: 10.3390/ijms18010096 View at Publisher

8. Mercer, P., Armenta, R.E. Developments in oil extraction from microalgae (2011) European Journal of Lipid Science and Technology, 113 (5), pp. 539-547. Cited 283 times. doi: 10.1002/elt.201000455 View at Publisher
Ahn, D.-G., Cho, C.-G., Jeong, S.-H., Lee, D.-G. 
Design of photobioreactor for mass production of microalgae 
(2011) *J. Korean Soc. Precis. Eng.*, 28, pp. 140-153. Cited 2 times.

Schneider, W.F., Brennecke, J.F., Maginn, E.J., Mindrup, E., Gurkan, B., Price, E., Goodrich, B.  
(2019) *Ionic Liquids Comprising Heteraromatic Anions*. Cited 2 times.

Lei, Z., Chen, B., Koo, Y.-M., MacFarlane, D.R.  
(2017) *Introduction: Ionic Liquids*. Cited 5 times. 
ACS Publications: Washington, DC, USA

Dai, Y., Van Spronsen, J., Witkamp, G.-J., Verpoorte, R., Choi, Y.H.  
Ionic liquids and deep eutectic solvents in natural products research: Mixtures of solids as extraction solvents  
(2013) *Journal of Natural Products*, 76 (11), pp. 2162-2173. Cited 198 times. 
doi: 10.1021/np400051w

Saki, K., Bahmani, M., Rafeian-Kopaei, M.  
The effect of most important medicinal plants on two important psychiatric disorders (anxiety and depression)—a review  
(Open Access)  
(2014) *Asian Pacific Journal of Tropical Medicine*, 7 (51), pp. S34-S42. Cited 138 times. 
http://www.elsevier.com/wps/find/journaldescription.authors/722894/description#description 
doi: 10.1016/S1995-7645(14)60201-7

Kim, Y.-H., Park, S., Kim, M.H., Choi, Y.-K., Yang, Y.-H., Kim, H.J., Kim, H., (...), Lee, S.H.  
Ultrasound-assisted extraction of lipids from Chlorella vulgaris using [Bmim][MeSO_4]  
(2013) *Biomass and Bioenergy*, 56, pp. 99-103. Cited 51 times. 
doi: 10.1016/j.biombioe.2013.04.022

Motlagh, S.R., Harun, M.R., Biak, D.R.A., Hussain, S.A., Wilfreda, C.D., Krishnan, S.  
Screening of long chain imidazolium base ionic liquids for EPA and DHA extraction from microalgae using COSMO-RS model  
(2019) *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences*, 58 (1), pp. 23-29. 
http://www.akademiabaru.com/doc/ARFMTSV58_N1_P23_29.pdf

Kim, Y.-H., Choi, Y.-K., Park, J., Lee, S., Yang, Y.-H., Kim, H.J., Park, T.-J., (...), Lee, S.H.  
Ionic liquid-mediated extraction of lipids from algal biomass  
(2012) *Bioresource Technology*, 109, pp. 312-315. Cited 126 times. 
doi: 10.1016/j.biortech.2011.04.064

Choi, S.-A., Oh, Y.-K., Jeong, M.-J., Kim, S.W., Lee, J.-S., Park, J.-Y.  
Effects of ionic liquid mixtures on lipid extraction from Chlorella vulgaris  
(2014) *Renewable Energy*, 65, pp. 169-174. Cited 71 times. 
doi: 10.1016/j.renene.2013.08.015
Prediction of selective extraction of cresols from aqueous solutions by ionic liquids using theoretical approach

(2011) *Separation Science and Technology*, 46 (13), pp. 2075-2087. Cited 9 times.
doi: 10.1080/01496395.2011.589421

Cyano-containing ionic liquids for the extraction of aromatic hydrocarbons from an aromatic/aliphatic mixture

(2012) *Science China Chemistry*, 55 (8), pp. 1488-1499. Cited 58 times.
doi: 10.1007/s11426-012-4630-x

An overview of the performance of the COSMO-RS approach in predicting the activity coefficients of molecular solutes in ionic liquids and derived properties at infinite dilution

(2017) *Physical Chemistry Chemical Physics*, 19 (19), pp. 11835-11850. Cited 34 times.
doi: 10.1039/c7cp00226b

Activity coefficients at infinite dilution measurements for organic solutes and water in the ionic liquid 4-methyl-N-butyl-pyridinium bis(trifluoromethylsulfonyl)-imide

(2009) *Journal of Chemical Thermodynamics*, 41 (12), pp. 1350-1355. Cited 83 times.
doi: 10.1016/j.jct.2009.06.011

Screening of suitable ionic liquids as green solvents for extraction of eicosapentaenoic acid (EPA) from microalgal biomass using COSMO-RS model (Open Access)

(2019) *Molecules*, 24 (4), art. no. 713. Cited 9 times.
doi: 10.3390/molecules24040713

Quantum chemical based screening of ionic liquids for the extraction of phenol from aqueous solution

(2010) *Industrial and Engineering Chemistry Research*, 49 (6), pp. 2916-2925. Cited 28 times.
doi: 10.1021/ie901684q

Imidazolium-based ionic liquids with inorganic anions in the extraction of salidroside and tyrosol from *Rhodiola*: The role of cations and anions on the extraction mechanism

(2019) *Journal of Molecular Liquids*, 275, pp. 136-145. Cited 9 times.
doi: 10.1016/j.molliq.2018.11.009
40. Hawker, R.R., Haines, R.S., Harper, J.B. (2014) Targets in Heterocyclic Systems, 18, pp. 141-213. Cited 15 times.
   https://www.soc.chim.it/sites/default/files/ths/18/chapter_6.pdf

41. Du, F.-Y., Xiao, X.-H., Luo, X.-J., Li, G.-K. (2009) Talanta, 78 (3), pp. 1177-1184. doi: 10.1016/j.talanta.2009.01.040

42. Xu, W., Chu, K., Li, H., Zhang, Y., Zheng, H., Chen, R., Chen, L. (2012) Molecules, 17 (12), pp. 14323-14335. doi: 10.3390/molecules171214323

43. Kilulya, K.F., Msagati, T.A.M., Mamba, B.B. (2014) Chromatographia, 77 (5-6), pp. 479-486. doi: 10.1007/s10337-014-2632-x

44. Severa, G., Kumar, G., Troung, M., Young, G., Cooney, M.J. (2013) Separation and Purification Technology, 116, pp. 265-270. doi: 10.1016/j.seppur.2013.06.001

45. Kim, Y.-H., Park, S., Kim, M.H., Choi, Y.-K., Yang, Y.-H., Kim, H.J., Kim, H., (...), Lee, S.H. (2013) Biomass and Bioenergy, 56, pp. 99-103. doi: 10.1016/j.biombioe.2013.04.022

46. Praveenkumar, R., Lee, K., Lee, J., Oh, Y.-K. (2015) Green Chemistry, 17 (2), pp. 1226-1234. doi: 10.1039/c4gc01413h
47 Cheong, L.-Z., Guo, Z., Yang, Z., Chua, S.-C., Xu, X.
Extraction and enrichment of n-3 polyunsaturated fatty acids and ethyl esters through reversible π-π Complexation with aromatic rings containing ionic liquids
(2011) *Journal of Agricultural and Food Chemistry*, 59 (16), pp. 8961-8967. Cited 21 times.
doi: 10.1021/jf202043w
View at Publisher

48 Zhang, Q.-G., Wang, N.-N., Yu, Z.-W.
The hydrogen bonding interactions between the ionic liquid 1-Ethyl-3-methylimidazolium ethyl sulfate and water
(2010) *Journal of Physical Chemistry B*, 114 (14), pp. 4747-4754. Cited 182 times.
http://pubs.acs.org/journal/jpckf
doi: 10.1021/jp100498
View at Publisher

49 Mu, X., Jiang, N., Liu, C., Zhang, D.
New Insight into the Formation Mechanism of Imidazolium-Based Ionic Liquids from N-Alkyl Imidazoles and Halogenated Hydrocarbons: A Polar Microenvironment Induced and Autopromoted Process
(2017) *Journal of Physical Chemistry A*, 121 (5), pp. 1133-1139. Cited 8 times.
http://pubs.acs.org/jpca
doi: 10.1021/acs.jpca.6b11610
View at Publisher

50 Kim, Y.-H., Choi, Y.-K., Park, J., Lee, S., Yang, Y.-H., Kim, H.J., Park, T.-J., (...), Lee, S.H.
Ionic liquid-mediated extraction of lipids from algal biomass
(2012) *Bioresource Technology*, 109, pp. 312-315. Cited 126 times.
doi: 10.1016/j.biortech.2011.04.064
View at Publisher

51 Olkiewicz, M., Plechkova, N.V., Earle, M.J., Fabregat, A., Stüber, F., Fortuny, A., Font, J., (...), Bengoa, C.
Biodiesel production from sewage sludge lipids catalysed by Brønsted acidic ionic liquids
(2016) *Applied Catalysis B: Environmental*, 181, pp. 738-746. Cited 52 times.
www.elsevier.com/locate/apcata
doi: 10.1016/j.apcatb.2015.08.039
View at Publisher

52 Miazek, K., Kratky, L., Sulec, R., Jirout, T., Aguedo, M., Richel, A., Goffin, D.
Effect of organic solvents on microalgae growth, metabolism and industrial bioproduct extraction: A review (Open Access)
(2017) *International Journal of Molecular Sciences*, 18 (7), art. no. 1429. Cited 26 times.
http://www.mdpi.com/1422-0067/18/7/1429/pdf
doi: 10.3390/ijms18071429
View at Publisher

53 Zhou, W., Wang, Z., Alam, M.A., Xu, J., Zhu, S., Yuan, Z., Huo, S., (...), Ma, L.
Repeated utilization of ionic liquid to extract lipid from algal biomass (Open Access)
(2019) *International Journal of Polymer Science*, 2019, art. no. 9209210. Cited 7 times.
http://www.hindawi.com/journals/ijps/
doi: 10.1155/2019/9209210
View at Publisher
