









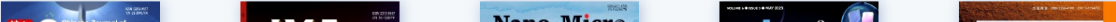


در نشانی: <https://ar.oversea.cnki.net/> جستجو را آغاز کنید:

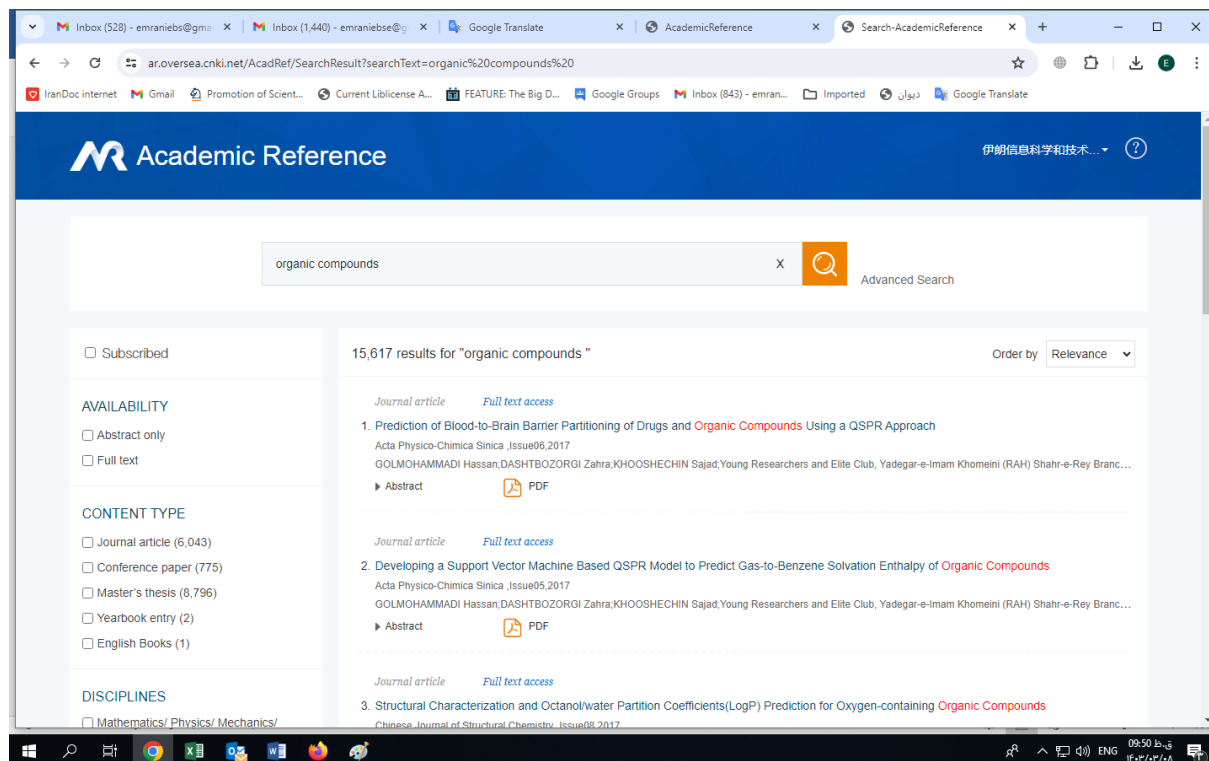
Subjects

 Mathematics/ Physics/ Mechanics/ Astronomy	 Chemistry/ Metallurgy/ Environment/ Mine Industry	 Architecture/ Energy/ Traffic/ Electromechanics, etc	 Literature/ History/ Philosophy	 Electronic Technology & Information Science
 Agriculture	 Politics/ Military Affairs/ Law	 Education & Social Sciences	 Medicine & Public Health	 Economics & Management

English Journals
Original English Journals published in China



• جستجو روی ترکیبات آلی شیمیایی Organic Compounds



The screenshot shows a search results page on the Academic Reference website. The search term is "organic compounds", and there are 15,617 results. The results are sorted by Relevance. The first three results are listed below:

- 1. Prediction of Blood-to-Brain Barrier Partitioning of Drugs and Organic Compounds Using a QSPR Approach**
Acta Physico-Chimica Sinica ,Issue06,2017
GOLMOHAMMADI Hassan,DASHTBOZORGI Zahra,KHOOSHECHIN Sajad;Young Researchers and Elite Club, Yadegar-e-Imam Khomeini (RAH) Shahr-e-Rey Branch...
Abstract PDF
- 2. Developing a Support Vector Machine Based QSPR Model to Predict Gas-to-Benzene Solvation Enthalpy of Organic Compounds**
Acta Physico-Chimica Sinica ,Issue05,2017
GOLMOHAMMADI Hassan,DASHTBOZORGI Zahra,KHOOSHECHIN Sajad;Young Researchers and Elite Club, Yadegar-e-Imam Khomeini (RAH) Shahr-e-Rey Branch...
Abstract PDF
- 3. Structural Characterization and Octanol/water Partition Coefficients(LogP) Prediction for Oxygen-containing Organic Compounds**
Chinese Journal of Structural Chemistry, Issue08,2017

صفحه چکیده و منابع

Acta Physico-Chimica Sinica
Issue 06, 2017, Pages 1160-1170

Downloads: 27 Cites: 1

Prediction of Blood-to-Brain Barrier Partitioning of Drugs and Organic Compounds Using a QSPR Approach

GOLMOHAMMADI Hassan, DASHTBOZORGI Zahra, KHOOSHECHIN Sajad, Young Researchers and Elite Club, Yadegar-e-Imam Khomeini (RAH) Shahr-e-Rey Branch, Islamic Azad University, Young Researchers and Elite Club, Central Tehran Branch, Islamic Azad University, Young Researchers and Elite Club, Yadegar-e-Imam Khomeini (RAH) Shahr-e-Rey Branch, Islamic Azad University, Young Researchers and Elite Club, Central Tehran Branch, Islamic Azad University;
DOI: CNKI:SUN:WLHX.0.2017-06-016

Keywords
Quantitative structure-activity relationship, Blood-to-brain barrier partitioning, Drug, Enhanced replacement method, Support vector machine

Abstract
The purpose of this study was to develop a quantitative structure-property relationship (QSPR) model based on the enhanced replacement method (ERM) and support vector machine (SVM) to predict the blood-to-brain barrier partitioning behavior (log BB) of various drugs and organic compounds. Different molecular descriptors were calculated using a dragon package to represent the molecular structures of the compounds studied. The enhanced replacement method (ERM) was used to select the variables and construct the SVM model. The correlation coefficient, R^2 , between experimental results and predicted log BB was 0.878 and 0.986, respectively. The results obtained demonstrated that, for all compounds, the log BB values estimated by SVM agreed with the experimental data, demonstrating that SVM is an effective method for model development, and can be used as a powerful chemometric tool in QSPR studies.

References
(1) Goldstein G.W., Betz A.L. *Sci Am* 1986; 255, 74. doi: 10.1038/scientificamerican0986-74

روی تمام متن کلید بزیند

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物理化学学报 (Wuli Huaxue Xuebao)
Acta Phys.-Chim. Sin. 2017, 33 (6), 1160-1170 June

[Article] doi: 10.3866/PKU.WHXB201704051 www.whxb.pku.edu.cn

Prediction of Blood-to-Brain Barrier Partitioning of Drugs and Organic Compounds Using a QSPR Approach

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¹Young Researchers and Elite Club, Yadegar-e-Imam Khomeini (RAH) Shahr-e-Rey Branch, Islamic Azad University, Tehran, Iran;
²Young Researchers and Elite Club, Central Tehran Branch, Islamic Azad University, Tehran, Iran

Abstract: The purpose of this study was to develop a quantitative structure-property relationship (QSPR) model based on the enhanced replacement method (ERM) and support vector machine (SVM) to predict the blood-to-brain barrier partitioning behavior (logBB) of various drugs and organic compounds. Different molecular descriptors were calculated using a dragon package to represent the molecular structures of the compounds studied. The enhanced replacement method (ERM) was used to select the variables and construct the SVM model. The correlation coefficient, R^2 , between experimental results and predicted logBB was 0.878 and 0.986, respectively. The results obtained demonstrated that, for all compounds, the logBB values estimated by SVM agreed with the experimental data, demonstrating that SVM is an effective method for model development, and can be used as a powerful chemometric tool in QSPR studies.

Key Words: Quantitative structure-activity relationship; Blood-to-brain barrier partitioning; Drug; Enhanced replacement method; Support vector machine

1 Introduction

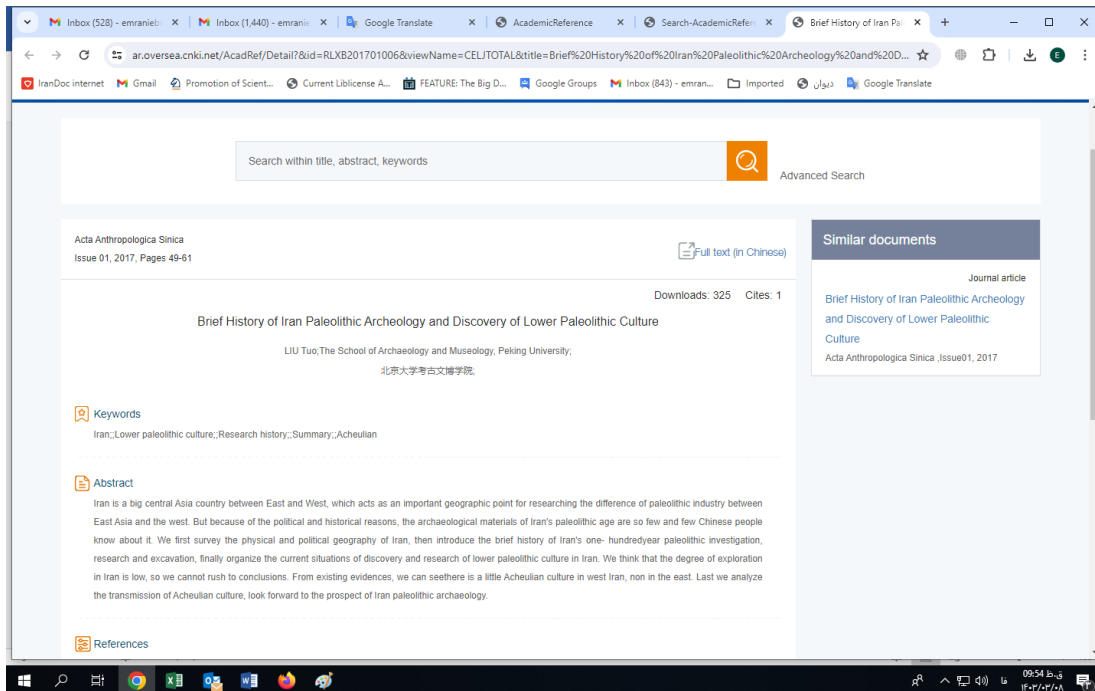
The blood-brain (BB) distribution of a molecule is an important feature to assess the suitability of a molecule as a drug for the central nervous system (CNS)¹⁻³. The blood-brain barrier (BBB) separates the brain from the blood stream and limits the transport of many substances from the systemic libraries. Therefore, rapid and accurate computational methods for screening large chemical databases or virtual libraries are desirable to assist the experimental drug discovery process. Quantitative structure-property relationships (QSPR) studies have been established to be a proficient computational tool in understanding the correlation between the structure of

جستجو از گروه F تاریخ، فلسفه و ادبیات روی تاریخ ایران جستجو انجام شد:

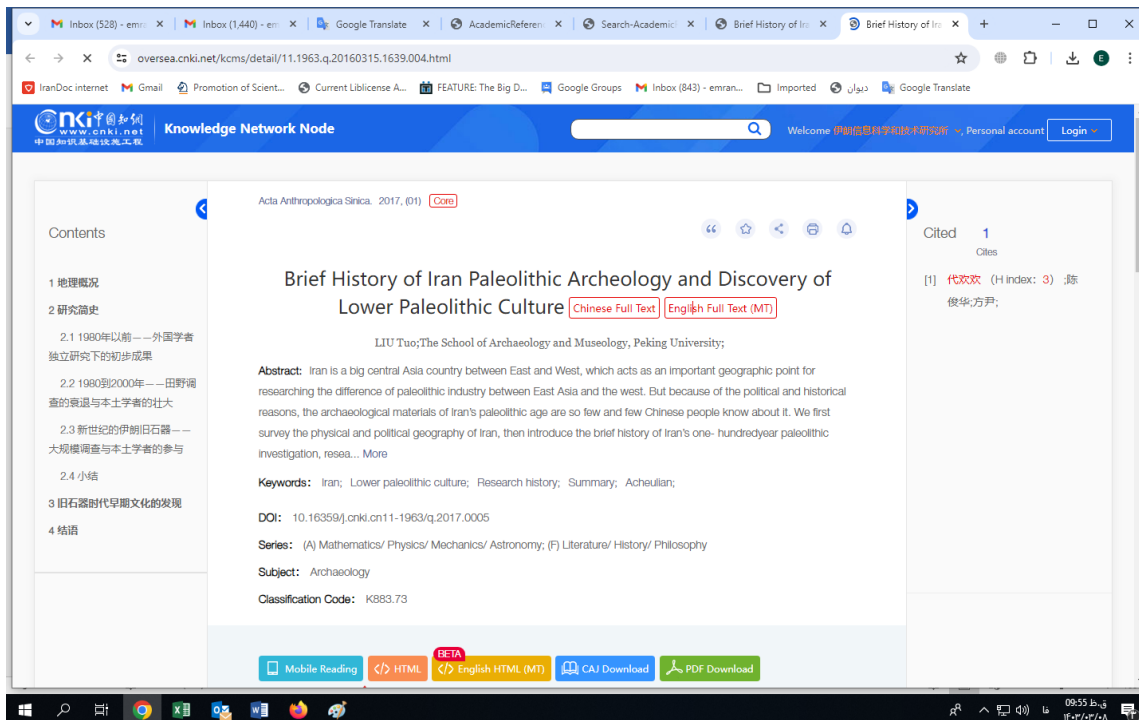
The screenshot shows the Academic Reference website interface. The search bar contains "History of iran" and the search results are for "organic compounds", showing 15,617 results. The left sidebar includes filters for AVAILABILITY (Abstract only, Full text), CONTENT TYPE (Journal article, Conference paper, Master's thesis, Yearbook entry, English Books), and DISCIPLINES (Mathematics, Physics, Mechanics, etc.). The main results list three journal articles with titles like "Prediction of Blood-to-Brain Barrier Partitioning of Drugs and Organic Compounds Using a QSPR Approach".

• روی عنوان کلید بزنید. صفحه چکیده و منابع می آید

The screenshot shows the Academic Reference website interface with the search bar containing "History of iran". The search results are for "History of iran", showing 4 results. The left sidebar filters are similar to the previous screenshot. The main results list three journal articles with titles like "Brief History of Iran Paleolithic Archeology and Discovery of Lower Paleolithic Culture".



● روی تمام متن زیر صفحه به رنگ سبز کلید بزیند



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11871.11; :A; : 1000-3193(2017)01-0049-13

Brief History of Iran Paleolithic Archeology and Discovery of Lower Paleolithic Culture

LIU Tuo

The School of Archaeology and Museology, Peking University, Beijing 100871

Abstract: Iran is a big central Asia country between East and West, which acts as an important geographic point for researching the difference of paleolithic industry between East Asia and the west. But because of the political and historical reasons, the archaeological materials of Iran's paleolithic age are so few and few Chinese people know about it. We first survey the physical and political geography of Iran, then introduce the brief history of Iran's one- hundred-year paleolithic investigation, research and excavation, finally organize the current situations of discovery and research of lower paleolithic culture in Iran. We think that the degree of exploration in Iran is low, so we cannot rush to conclusions. From existing evidences, we can see

: 2015-06-19; : 2015-10-13
: (11&ZD120)
: Email: liutuo228@163.com

Citation: Liu T. Brief History of Iran Paleolithic Archeology and Discovery of Lower Paleolithic Culture[J]. Acta Anthropologica Sinica, 2017, 36(1): 49-61

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