

CURRICULUM VITAE

Personal information

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Date of birth 12 August, 1976
Nationality Chinese
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Education

09/2002-08/2005 **Ph.D in Applied Chemistry, Beijing Institute of Technology,**
Quantum Chemistry Study on High-energy Density Material
(HEDM) Molecules
09/1999-07/2002 **M.S. in Physical Chemistry, Northeast Normal University,**
Theoretical Study of the Electronic Spectrum Property of Organic
Metal Complex with 2-(2-hydroxyphenyl) pyridine Ligand
09/1995-07/1999 **B.S. in Chemistry Education, Northeast Normal University**

Work Experience

11/2013-11/2014 **Visiting Scholar, UC Davis, CA, USA**
Modeling and Screening based on Insect Olfactory Receptor
09/2007- **Scientific Staff and Teacher, China Agricultural University,**
Computer-aided Pesticide Molecular Design and Discovery
09/2005-07/2007 **Postdoctor, Drug Design and Discovery Center (DDDC),**
Shanghai Institute of Materia Medica (SIMM), Chinese
Academy of Sciences (CAS),
Computer-aided Drug Design on GPCR family β -AR2

Research interests

- (1) Novel pesticide molecular design and discovery based on macromolecular target
 - (2) Biology and molecular biology studies on insect target protein
 - (3) Molecular modeling technology and computational chemistry
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Software

Sybyl, Catalyst, Dock, Autodock, Discovery Studio, Gromacs, Gaussian
Linux/Unix, Windows, Mac,

Scientific Research Project

- (1) Novel pesticide design based on insect target nAChR supported by Natural
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Publications

- (1) Shaohua Liu, Wei Peng, Yanyan Qu, Hongyue Li, Dunlun Song, **Hongxia Duan**, Xinling Yang, Synthesis, insecticidal activity and molecular docking study of clothianidin analogous with hydrazide group, *Chin. Chem. Lett.*, 2014, 25, 1017-1020.
 - (2) CHEN Wen-Ya, WANG Shan-Shan, LI Dong-Ling, PENG Wei, ZHAO Jing-Fu, **DUAN Hong-Xia***, Structure Activity Relationship Studies on Novel Acylpiperidine Compounds Based on Insect OBP1, *CHEMICAL JOURNAL OF CHINESE UNIVERSITIES*, 2013, 12, 2798-2805.
 - (3) **Hongxia Duan***, Dongling Li, Hongchen Liu, Desheng Liang, Xinling Yang, Computational insight into novel molecular recognition mechanism of different bioactive GAs and the *Arabidopsis* receptor GID1A, *Journal of Molecular Modeling*, 2013, 19(10), 4613-4624.
 - (4) **Hongxia Duan***, Weiwei Zhang, Jin Zhao, Desheng Liang, Xinling Yang, Shuhui Jin, A novel halogen bond and a better-known hydrogen bond cooperation of neonicotinoid and insect nicotinic acetylcholine receptor recognition, *J Mol Model*, 2012, V18, 3867-3875.
 - (5) **DUAN Hong-Xia***, YANG Xin-Ling, WANG Dao-Quan, NING Jun, MEI Xiang-Dong, ZHANG Jian, A novel pharmacophore model derived from a class of capsid protein enterovirus 71 inhibitors, *Chinese J. Struct. Chem.* 2012, 31, 1159-1169.
 - (6) Wangcang Su, Yihui Zhou, Yongqiang Ma, Lei Wang, Zheng Zhang, Changhui Rui, **Hongxia Duan**, and Zhaohai Qin, N'-Nitro-2-hydrocarbylidene hydrazinecarboximidamides: Design, synthesis, crystal Structure, insecticidal activity, and structure-activity relationships, *J. Agric. Food Chem.* 2012, 60, 5028-5034.
 - (7) HUANG ChuSheng, LIU HongXing, SHI JianCheng, LIN Sen, **DUAN HongXia**, Total syntheses of 5,7-Dihydroxy-3-isopentenylflavone and 5-hydroxy-3-isopentenylflavone natural compounds, *Chem. J. Chin. Uni.*, 2012, 33, 1978-1983.
 - (8) Zhou Yi-Hui, **Duan Hong-Xia***, Fu Bin, Ma Yong-Qiang, Du Feng-Pei, Wang Ming-An, Qin Zhao-Hai "3D-QSAR study of rocaglamide analogues" *Chem. J. Chin. Uni.*, 2011, 32, 1088-1093.
 - (9) **DUAN HongXia**, WANG Rui Gang, ZHANG JianJun, DONG YanHong, LIANG XiaoMei, WU JingPing, WANG DaoQuan, "QSAR of macrolactone derivatives with herbicidal activity" *Acta Phys. Chim. Sin.*, 2010, 26 (4) 1065-1074.
 - (10) **Duan, Hongxia*** Liang, Desheng Yang, Xinling, "3D quantitative structure-property relationship study on *cis*-neonicotinoid derivatives" *ACTA CHIMICA SINICA*, 2010, 68 (7), 595-602.
 - (11) Hanqing Zhao, Huiqi Jia, **Hongxia Duan**, Jianjun Zhang, Daoquan Wang and Xiaomei Liang, Synthesis of two tetrasaccharides related to the O-Antigen from *Azospirillum brasilense* S17 and *Azospirillum lipoferum* SR65, *Journal of Carbohydrate Chemistry*, 2010, 29, 1-15.
 - (12) **Hongxia Duan**, Zhen Gong, Jiagao Cheng, Weiliang Zhu, Kaixian Chen, Hualiang Jiang "Induction of an aromatic six-membered nitrogen ring via cation- π interaction" *J. Phys. Chem. A*, 2006, 110, 12236-12240.
 - (13) **Hongxia Duan***, Qianshu Li "A series of novel aromatic compounds with a planar N₆ ring" *Chem. Phys. Lett.*, 2006, 432, 331-335.
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- (14) **Hongxia Duan**, Qian Shu Li. "Structure, stability and chemical bonding character of covalent boron azides $BX(N_3)_2$ (X=F, Cl, Br) " *J. Mol. Struct: (Theochem)* 2006, 759, 171-176.
- (15) Qianshu Li, **Hongxia Duan**. "Density functional theoretical study of a series of binary azides $M(N_3)_n$ (n=3,4) ", *J. Phys. Chem. A*, 2005, 109, 9089-9094.
- (16) Qianshu Li, **Hongxia Duan**. "A theoretical studies of the structures and stabilities of N_4O_2 isomers" *Molecular Physics*, 2005, 103(2-3), 249-256.
- (17) Yan Luo, Jun Lin, **Hongxia Duan**, Jie Zhang, Cuikun Lin, "Self-directed assembly of photoactive perylenediimide-bridged silsesquioxane into superlong tubular structure", *Chem. Mater.*, 2005, 17, 2234-2236.
- (18) **Hongxia Duan**, Zhong Ming Su. "Spin coupling rules for the diradicals of the 2,2'-bipyridine and its derivatives" *Synthetic Metals*, 2003,137, 1351-1352.
- (19) **Hongxia Duan**, Zhong Min Su. "Theoretical study of the electronic spectrum property of 2-(2-hydroxyphenyl) pyridine using Time-dependence density functional theory method" *Chemical Research in Chinese Universities*, 2003, 19(2), 196-200.
- (20) Y. Liao, Y. G. Chen, Z. M. Su, Y. H. Kan, **H. X. Duan**, D.X. Zhu, TD-DFT study on electronic spectrum property for Bepp2 and its related complexes, *Synthetic Metals*, 2003,137, 1093-1094.
- (21) Z.M.Su, L.H.Hu, Y.Q.Qiu, S.L.Sun, **H.X.Duan**. "Theoretical chemical study on NLO properties of polypyridinopyridine and its derivatives" *Synthetic Metals*, 2001, 119, 577-578.
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Conferences

- (1) **H. X. Duan***, S. S. Wang, Y. F. Sun, P. Pelosi, X. L. Yang, Rational design of novel (E)- β -farnesene analogous with a Cl substitution based on insect OBP7 crystal structure, *13th IUPAC INTERNATIONAL CONGRESS OF PESTICIDE CHEMISTRY at 248th ACS National Meeting*, 2014.8.10-14, San Francisco, CA.
- (2) D. L. Li, W. Peng, S .S. Wang, **H. X. Duan*** and W. M. Tan, Virtual Screening and Biorational Design of Novel GA Functional Analogues based on *Arabidopsis* Receptor *GID1A*, *the 21st Conference of the International Plant Growth Substances Association (IPGSA)*", *Abstract*, 2013.6.18-2013.6.22, Shanghai, P85.
- (3) D. L. Li, **H. X. Duan***, H. C. Liu, D. S. Liang, X. L. Yang, Novel molecular recognition mechanism between different bioactive GA molecules and *Arabidopsis* receptor *GID1A*, *4th International Symposium on Pesticides and Environmental Safety & 5th Pan Pacific Conference on Pesticide Science & 8th International Workshop on Crop Protection Chemistry and Regulatory Harmonization*, 4th ISPES-V-3-009, p344. **Oral Presentation**, 2012.9.15-9.20, Beijing, China
- (4) W. Peng, W. W. Zhang, S. Sun, **H. X. Duan***, X. L. Yang, 3D-QSAR analysis and molecular docking studies of novel $\alpha 7$ nAChR antagonists, 4th ISPES-V-2-031, p326. **Poster**, 2012.9.15-9.20, Beijing, China
- (5) S. Sun, W. W. Zhang, W. Peng, **H. X. Duan***, The binding mode study between dinotefuran analogues and insect target nAChR by molecular docking method, 4th ISPES-V-5-008, p388. **Poster**, 2012.9.15-9.20, Beijing, China
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