Daichi Hayakawa

List of Publications by Year
in descending order

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22	236	933447	996975
papers	citations	10 h-index	15 g-index

22	22	22	344
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Folded-chain structure of cellulose II suggested by molecular dynamics simulation. Carbohydrate Research, 2013, 379, 30-37.	2.3	29
2	In Silico Screening Identified Novel Small-molecule Antagonists of PAC1 Receptor. Journal of Pharmacology and Experimental Therapeutics, 2018, 365, 1-8.	2.5	25
3	Evaluation of hydrogen bond networks in cellulose Iβ and II crystals using density functional theory and Carâ€“Parrinello molecular dynamics. Carbohydrate Research, 2017, 449, 103-113.	2.3	24
4	Computational study to evaluate the birefringence of uniaxially oriented film of cellulose triacetate. Carbohydrate Research, 2015, 402, 146-151.	2.3	17
5	DFT study of the influence of acetyl groups of cellulose acetate on its intrinsic birefringence and wavelength dependence. Carbohydrate Polymers, 2019, 207, 122-130.	10.2	14
6	Molecular dynamics simulation of the dissolution process of a cellulose triacetate-II nano-sized crystal in DMSO. Carbohydrate Research, 2011, 346, 2940-2947.	2.3	13
7	Molecular dynamics simulation of dissociation behavior of various crystalline celluloses treated with hot-compressed water. Cellulose, 2014, 21, 3203-3215.	4.9	13
8	Essential structure of orexin 1 receptor antagonist YNT-707, Part I: Role of the 4,5-epoxy ring for binding with orexin 1 receptor. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4176-4179.	2.2	13
9	Essential structure of orexin 1 receptor antagonist YNT-707, Part II: Drastic effect of the 14-hydroxy group on the orexin 1 receptor antagonistic activity. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 774-777.	2.2	12
10	Synthesis of a novel and potent small-molecule antagonist of PAC1 receptor for the treatment of neuropathic pain. European Journal of Medicinal Chemistry, 2020, 186, 111902.	5.5	12
11	Multi-step virtual screening to develop selective DYRK1A inhibitors. Journal of Molecular Graphics and Modelling, 2017, 72, 229-239.	2.4	10
12	A molecular interaction field describing nonconventional intermolecular interactions and its application to proteinâ€“ligand interaction prediction. Journal of Molecular Graphics and Modelling, 2020, 96, 107515.	2.4	10
13	Design, synthesis, and evaluation of novel inhibitors for wild-type human serine racemase. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 441-445.	2.2	9
14	Essential structure of orexin 1 receptor antagonist YNT-707, part III: Role of the 14-hydroxy and the 3-methoxy groups in antagonistic activity toward the orexin 1 receptor in YNT-707 derivatives lacking the 4,5-epoxy ring. Bioorganic and Medicinal Chemistry, 2019, 27, 1747-1758.	3.0	9
15	Formal Syntheses of (â˜)-Lepadiformines A, C, and (â˜)-Fasicularin. Journal of Organic Chemistry, 2019, 84, 5222-5229.	3.2	9
16	Effects of N-Substituents on the Functional Activities of Naltrindole Derivatives for the Î´ Opioid Receptor: Synthesis and Evaluation of Sulfonamide Derivatives. Molecules, 2020, 25, 3792.	3.8	6
17	Investigation of the structure and interaction of cellulose triacetate I crystal using ab initio calculations. Carbohydrate Research, 2014, 388, 61-66.	2.3	5
18	Ab initio studies on the structure of and atomic interactions in cellulose IIII crystals. Carbohydrate Research, 2015, 417, 72-77.	2.3	5

#	Article	IF	Citations
19	Ab initio studies of the crystal structure of cellulose triacetate I. Materials Research Society Symposia Proceedings, 2012, 1470, 21.	0.1	1
20	Ab initio studies of the structure and the interaction of cellulose IIII crystal. Materials Research Society Symposia Proceedings, 2013, 1554, 1.	0.1	0
21	Computational Study of Optical Properties of Cellulose Triacetate Film. Materials Research Society Symposia Proceedings, 2013, 1524, 301.	0.1	0
22	In silico analyses of the effects of a point mutation and a pharmacological chaperone on the thermal fluctuation of phenylalanine hydroxylase. Biophysical Chemistry, 2017, 228, 47-54.	2.8	0