Jean-Didier MarÃ©chal

List of Publications by Year
in descending order

127 papers	3,418 citations	109321 35 h-index	206112 48 g-index
140 all docs	140 docs citations	140 times ranked	3964 citing authors

#	Article	IF	Citations
1	Successes and Challenges in Multiscale Modelling of Artificial Metalloenzymes: the Case Study of POP-Rh2 Cyclopropanase. Faraday Discussions, 2022, , .	3.2	1
2	Controlling oncogenic KRAS signaling pathways with a Palladium-responsive peptide. Communications Chemistry, 2022, 5, .	4.5	1
3	Influence of Association on Binding of Disaccharides to YKL-39 and hHyal-1 Enzymes. International Journal of Molecular Sciences, 2022, 23, 7705.	4.1	0
4	Dynamic Stereoselection of Peptide Helicates and Their Selective Labeling of DNA Replication Foci in Cells**. Angewandte Chemie, 2021, 133, 8941-8948.	2.0	7
5	Dynamic Stereoselection of Peptide Helicates and Their Selective Labeling of DNA Replication Foci in Cells**. Angewandte Chemie - International Edition, 2021, 60, 8859-8866.	13.8	29
6	BioMetAll: Identifying Metal-Binding Sites in Proteins from Backbone Preorganization. Journal of Chemical Information and Modeling, 2021, 61, 311-323.	5.4	25
7	Copper(II) N,N,O-Chelating Complexes as Potential Anticancer Agents. Inorganic Chemistry, 2021, 60, 2939-2952.	4.0	30
8	Hybrid Cyclobutane/Proline-Containing Peptidomimetics: The Conformational Constraint Influences Their Cell-Penetration Ability. International Journal of Molecular Sciences, 2021, 22, 5092.	4.1	5
9	Inhibition of the Human Hsc70 System by Small Ligands as a Potential Anticancer Approach. Cancers, 2021, 13, 2936.	3.7	7
10	Stereoselective Self-Assembly of DNA Binding Helicates Directed by the Viral Î²-Annulus Trimeric Peptide Motif. Bioconjugate Chemistry, 2021, 32, 1564-1569.	3.6	3
11	Design and evolution of chimeric streptavidin for protein-enabled dual gold catalysis. Nature Catalysis, 2021, 4, 643-653.	34.4	32
12	Origin of the Rate Acceleration in the Câ^'C Reductive Elimination from Pt(IV)â€complex in a [Ga₄L₆]^{12â^'} Supramolecular Metallocage. Chemistry - A European Journal, 2021, 27, 15973-15980.	3.3	9
13	Modeling Kinetics and Thermodynamics of Guest Encapsulation into the [M4L6]12â€“ Supramolecular Organometallic Cage. Journal of Chemical Information and Modeling, 2021, 61, 4370-4381.	5.4	10
14	Impact of Cu(<scp>ii</scp>) and Al(<scp>iii</scp>) on the conformational landscape of amyloidÎ²₁₋₄₂. Physical Chemistry Chemical Physics, 2021, 23, 13023-13032.	2.8	7
15	Integrated experimental/computational approaches to characterize the systems formed by vanadium with proteins and enzymes. Inorganic Chemistry Frontiers, 2021, 8, 1951-1974.	6.0	24
16	Quantitative prediction of electronic absorption spectra of copper(II)â€“bioligand systems: Validation and applications. Journal of Inorganic Biochemistry, 2020, 204, 110953.	3.5	27
17	Investigating Potential Inhibitory Effect of Uncaria tomentosa (Catâ€™s Claw) against the Main Protease 3CLpro of SARS-CoV-2 by Molecular Modeling. Evidence-based Complementary and Alternative Medicine, 2020, 2020, 1-14.	1.2	21
18	Chiral Cyclobutane-Containing Cell-Penetrating Peptides as Selective Vectors for Anti-Leishmania Drug Delivery Systems. International Journal of Molecular Sciences, 2020, 21, 7502.	4.1	4

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19	Cofactor Binding Dynamics Influence the Catalytic Activity and Selectivity of an Artificial Metalloenzyme. ACS Catalysis, 2020, 10, 11783-11790.	11.2	24
20	Biospeciation of Potential Vanadium Drugs of Acetylacetonate in the Presence of Proteins. Frontiers in Chemistry, 2020, 8, 345.	3.6	11
21	Stepwise Oxidations in a Cofacial Copper(II) Porphyrin Dimer: Throughâ€Space Spinâ€Coupling and Interplay between Metal and Radical Spins. Chemistry - A European Journal, 2020, 26, 7869-7880.	3.3	15
22	Molecular Modeling for Artificial Metalloenzyme Design and Optimization. Accounts of Chemical Research, 2020, 53, 896-905.	15.6	29
23	An Artificial Hemoprotein with Inducible Peroxidaseâ€and Monooxygenaseâ€Like Activities. Chemistry - A European Journal, 2020, 26, 14929-14937.	3.3	9
24	Reaction Rate Inside the Cavity of [Ga₄L₆]^{12â^'} Supramolecular Metallocage is Regulated by the Encapsulated Solvent. Chemistry - A European Journal, 2020, 26, 6988-6992.	3.3	18
25	Unveiling V^{IV}O²⁺ Binding Modes to Human Serum Albumins by an Integrated Spectroscopicâ€“Computational Approach. Chemistry - A European Journal, 2020, 26, 11316-11326.	3.3	23
26	Differential response to Cadmium exposure by expression of a two and a three-domain metallothionein isoform in the land winkle Pomatias elegans: Valuating the marine heritage of a land snail. Science of the Total Environment, 2019, 648, 561-571.	8.0	15
27	Microsolvation and Encapsulation Effects on Supramolecular Catalysis: Câ€“C Reductive Elimination inside [Ga₄L₆]^{12â€“} Metallocage. Journal of the American Chemical Society, 2019, 141, 13114-13123.	13.7	40
28	GPathFinder: Identification of Ligand-Binding Pathways by a Multi-Objective Genetic Algorithm. International Journal of Molecular Sciences, 2019, 20, 3155.	4.1	14
29	Computational insight into the interaction of oxaliplatin with insulin. Metallomics, 2019, 11, 765-773.	2.4	10
30	Interaction of Vanadium(IV) Species with Ubiquitin: A Combined Instrumental and Computational Approach. Inorganic Chemistry, 2019, 58, 8064-8078.	4.0	28
31	Effect of secondary interactions, steric hindrance and electric charge on the interaction of V^{IV}O species with proteins. New Journal of Chemistry, 2019, 43, 17647-17660.	2.8	22
32	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. Nature Communications, 2019, 10, 2222.	12.8	20
33	Integrated ESI-MS/EPR/computational characterization of the binding of metal species to proteins: vanadium drugâ€“myoglobin application. Inorganic Chemistry Frontiers, 2019, 6, 1561-1578.	6.0	24
34	Studying the reactivity of â€œoldâ€•Cu(II) complexes for â€œnovelâ€•anticancer purposes. Journal of Inorganic Biochemistry, 2019, 195, 51-60.	3.5	11
35	The Effect of Cofactor Binding on the Conformational Plasticity of the Biological Receptors in Artificial Metalloenzymes: The Case Study of LmrR. Frontiers in Chemistry, 2019, 7, 211.	3.6	9
36	Simple Coordination Geometry Descriptors Allow to Accurately Predict Metal-Binding Sites in Proteins. ACS Omega, 2019, 4, 3726-3731.	3.5	20

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37	Functionalized Artificial Bidomain Proteins Based on an Î±-Solenoid Protein Repeat Scaffold: A New Class of Artificial Dielsâ€“Alderases. ACS Omega, 2019, 4, 4437-4447.	3.5	21
38	Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and into the Context of an Artificial Metallohydratase. ACS Catalysis, 2019, 9, 4616-4626.	11.2	10
39	Validation and Applications of Proteinâ€“Ligand Docking Approaches Improved for Metalloligands with Multiple Vacant Sites. Inorganic Chemistry, 2019, 58, 294-306.	4.0	35
40	GARLEEK: Adding an extra flavor to ONIOM. Journal of Computational Chemistry, 2019, 40, 381-386.	3.3	6
41	Defective AMH signaling disrupts GnRH neuron development and function and contributes to hypogonadotropic hypogonadism. ELife, 2019, 8, .	6.0	49
42	ESIgen: Electronic Supporting Information Generator for Computational Chemistry Publications. Journal of Chemical Information and Modeling, 2018, 58, 561-564.	5.4	19
43	Decoding Surface Interaction of V^{IV}O Metallodrug Candidates with Lysozyme. Inorganic Chemistry, 2018, 57, 4456-4469.	4.0	28
44	PyChimera: use UCSF Chimera modules in any Python 2.7 project. Bioinformatics, 2018, 34, 1784-1785.	4.1	18
45	Directed Evolution of an Artificial Imine Reductase. Angewandte Chemie - International Edition, 2018, 57, 1863-1868.	13.8	47
46	Directed Evolution of an Artificial Imine Reductase. Angewandte Chemie, 2018, 130, 1881-1886.	2.0	8
47	An Artificial Heme Enzyme for Cyclopropanation Reactions. Angewandte Chemie, 2018, 130, 7911-7915.	2.0	26
48	An Artificial Heme Enzyme for Cyclopropanation Reactions. Angewandte Chemie - International Edition, 2018, 57, 7785-7789.	13.8	98
49	Prediction of the interaction of metallic moieties with proteins: An update for proteinâ€ligand docking techniques. Journal of Computational Chemistry, 2018, 39, 42-51.	3.3	54
50	DFT Protocol for EPR Prediction of Paramagnetic Cu(II) Complexes and Application to Protein Binding Sites. Magnetochemistry, 2018, 4, 55.	2.4	30
51	Directed Self-Assembly of Trimeric DNA-Bindingchiral Miniprotein Helicates. Frontiers in Chemistry, 2018, 6, 520.	3.6	11
52	Accurate prediction of vertical electronic transitions of Ni(II) coordination compounds via time dependent density functional theory. International Journal of Quantum Chemistry, 2018, 118, e25655.	2.0	16
53	Bioelectrochemical monitoring of soluble guanylate cyclase inhibition by the natural Î²-carboline canthin-6-one. Journal of Molecular Structure, 2017, 1134, 661-667.	3.6	3
54	Elucidating the 3D structures of Al(<scp>iii</scp>)â€“AlÎ² complexes: a template free strategy based on the pre-organization hypothesis. Chemical Science, 2017, 8, 5041-5049.	7.4	21

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55	GaudiMM: A modular multiâ€•objective platform for molecular modeling. Journal of Computational Chemistry, 2017, 38, 2118-2126.	3.3	37
56	Elucidation of Binding Site and Chiral Specificity of Oxidovanadium Drugs with Lysozyme through Theoretical Calculations. Inorganic Chemistry, 2017, 56, 12938-12951.	4.0	40
57	Design of an enantioselective artificial metallo-hydratase enzyme containing an unnatural metal-binding amino acid. Chemical Science, 2017, 8, 7228-7235.	7.4	69
58	New Insights into the Reactivity of Cisplatin with Free and Restrained Nucleophiles: Microsolvation Effects and Base Selectivity in Cisplatinâ€“DNA Interactions. ChemPhysChem, 2016, 17, 3932-3947.	2.1	10
59	Computational insight into the catalytic implication of head/tail-first orientation of arachidonic acid in human 5-lipoxygenase: consequences for the positional specificity of oxygenation. Physical Chemistry Chemical Physics, 2016, 18, 23017-23035.	2.8	22
60	Artificial Metalloenzymes with the Neocarzinostatin Scaffold: Toward a Biocatalyst for the Dielsâ€“Alder Reaction. ChemBioChem, 2016, 17, 433-440.	2.6	36
61	The folding of a metallopeptide. Dalton Transactions, 2016, 45, 881-885.	3.3	9
62	Chapter 15. Enzyme Design. RSC Theoretical and Computational Chemistry Series, 2016, , 481-521.	0.7	1
63	Modeling Cu2+-AÎ² complexes from computational approaches. AIP Advances, 2015, 5, 092402.	1.3	17
64	Toward the Computational Design of Artificial Metalloenzymes: From Proteinâ€“Ligand Docking to Multiscale Approaches. ACS Catalysis, 2015, 5, 2469-2480.	11.2	51
65	Synthesis of Novel Nucleoside Analogues Built on a Bicyclo[4.1.0]heptane Scaffold. Journal of Organic Chemistry, 2015, 80, 9495-9505.	3.2	11
66	From â€œhemoabzymesâ€• to â€œhemozymesâ€: towards new biocatalysts for selective oxidations. Chemical Communications, 2015, 51, 2476-2494.	4.1	54
67	Various strategies for obtaining oxidative artificial hemoproteins with a catalytic oxidative activity: from "Hemoabzymes" to "Hemozymes"?. Journal of Porphyrins and Phthalocyanines, 2014, 18, 1063-1092.	0.8	7
68	Computational simulations of copper complexes relevant to Alzheimer's disease. , 2014, , .		0
69	Direct interaction of natural and synthetic catechins with signal transducer activator of transcription 1 affects both its phosphorylation and activity. FEBS Journal, 2014, 281, 724-738.	4.7	14
70	Monitoring lactoferrin iron levels by fluorescence resonance energy transfer: a combined chemical and computational study. Journal of Biological Inorganic Chemistry, 2014, 19, 439-447.	2.6	15
71	Unravelling novel synergies between organometallic and biological partners: a quantum mechanics/molecular mechanics study of an artificial metalloenzyme. Journal of the Royal Society Interface, 2014, 11, 20140090.	3.4	10
72	Structural, Kinetic, and Docking Studies of Artificial Imine Reductases Based on Biotinâ€“Streptavidin Technology: An Induced Lock-and-Key Hypothesis. Journal of the American Chemical Society, 2014, 136, 15676-15683.	13.7	75

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73	3D Structures and Redox Potentials of Cu²⁺â€“AÎ²(1â€“16) Complexes at Different pH: A Computational Study. Journal of Physical Chemistry B, 2014, 118, 4840-4850.	2.6	30
74	Computational Insights on an Artificial Imine Reductase Based on the Biotinâ€“Streptavidin Technology. ACS Catalysis, 2014, 4, 833-842.	11.2	27
75	Understanding the interaction of an antitumoral platinum(II) 7-azaindolate complex with proteins and DNA. BioMetals, 2014, 27, 1159-1177.	4.1	8
76	Neocarzinostatin-based hybrid biocatalysts for oxidation reactions. Dalton Transactions, 2014, 43, 8344-8354.	3.3	32
77	Neocarzinostatin-based hybrid biocatalysts with a RNase like activity. Bioorganic and Medicinal Chemistry, 2014, 22, 5678-5686.	3.0	10
78	Programmed stereoselective assembly of DNA-binding helical metallopeptides. Chemical Communications, 2014, 50, 11097-11100.	4.1	30
79	Assessing protein-ligand docking for the binding of organometallic compounds to proteins. Journal of Computational Chemistry, 2014, 35, 192-198.	3.3	22
80	Crystal structure of c5321: a protective antigen present in uropathogenic Escherichia coli strains displaying an SLR fold. BMC Structural Biology, 2013, 13, 19.	2.3	17
81	Synthesis, Antiviral Evaluation, and Computational Studies of Cyclobutane and Cyclobutene <scp>L</scp>â€Nucleoside Analogues. European Journal of Organic Chemistry, 2013, 2013, 7761-7775.	2.4	7
82	Computational insights on the possibility of tri-coordinated cisplatinated adducts with protein models. Journal of Inorganic Biochemistry, 2012, 117, 230-236.	3.5	4
83	Crystal Structure of Two Anti-Porphyrin Antibodies with Peroxidase Activity. PLoS ONE, 2012, 7, e51128.	2.5	11
84	Metal Complexation of a <scp>D</scp>â€Riboseâ€Based Ligand Decoded by Experimental and Theoretical Studies. European Journal of Inorganic Chemistry, 2012, 2012, 3308-3319.	2.0	4
85	Stereoselective Formation of Chiral Metallopeptides. Chemistry - A European Journal, 2012, 18, 7030-7035.	3.3	30
86	Synthesis, Antiâ€HIV Activity Studies, and inâ€…silico Rationalization of Cyclobutaneâ€Fused Nucleosides. ChemMedChem, 2012, 7, 1044-1056.	3.2	7
87	Incorporation of Manganese Complexes into Xylanase: New Artificial Metalloenzymes for Enantioselective Epoxidation. ChemBioChem, 2012, 13, 240-251.	2.6	72
88	What can molecular modelling bring to the design of artificial inorganic cofactors?. Faraday Discussions, 2011, 148, 137-159.	3.2	26
89	Three Dimensional Models of Cu²⁺-AÎ²(1â€“16) Complexes from Computational Approaches. Journal of the American Chemical Society, 2011, 133, 15008-15014.	13.7	61
90	Receptor Flexibility in Ligand Docking and Virtual Screening. , 2011, , 99-117.		2

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91	In Silico Analysis of the Apolipoprotein E and the Amyloid Î² Peptide Interaction: Misfolding Induced by Frustration of the Salt Bridge Network. PLoS Computational Biology, 2010, 6, e1000663.	3.2	38
92	Insights into the Mechanism of Binding of Arachidonic Acid to Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2010, 114, 7037-7046.	2.6	30
93	Consensus modes, a robust description of protein collective motions from multiple-minima normal mode analysisâ€"application to the HIV-1 protease. Physical Chemistry Chemical Physics, 2010, 12, 2850.	2.8	31
94	Natural mutations of the anti-Mullerian hormone type II receptor found in persistent Mullerian duct syndrome affect ligand binding, signal transduction and cellular transport. Human Molecular Genetics, 2009, 18, 3002-3013.	2.9	49
95	Targeting STAT1 by myricetin and delphinidin provides efficient protection of the heart from ischemia/reperfusionâ€induced injury. FEBS Letters, 2009, 583, 531-541.	2.8	80
96	Selective oxidation of aromatic sulfide catalyzed by an artificial metalloenzyme: new activity of hemozymes. Organic and Biomolecular Chemistry, 2009, 7, 3208.	2.8	66
97	Use of normal modes for structural modeling of proteins: the case study of rat heme oxygenase 1. European Biophysics Journal, 2008, 37, 1157-1165.	2.2	11
98	How Do Azoles Inhibit Cytochrome P450 Enzymes? A Density Functional Study. Journal of Physical Chemistry A, 2008, 112, 12911-12918.	2.5	76
99	Insights into drug metabolism by cytochromes P450 from modelling studies of CYP2D6â€drug interactions. British Journal of Pharmacology, 2008, 153, S82-9.	5.4	42
100	Insight into the apoptosis-inducing action of Î±-bisabolol towards malignant tumor cells: Involvement of lipid rafts and Bid. Archives of Biochemistry and Biophysics, 2008, 476, 113-123.	3.0	57
101	Hemozymes Peroxidase Activity Of Artificial Hemoproteins Constructed From theStreptomyces lividansXylanase A and Iron(III)-Carboxy-Substituted Porphyrins. Bioconjugate Chemistry, 2008, 19, 899-910.	3.6	43
102	Multiple Substrate Binding by Cytochrome P450 3A4: Estimation of the Number of Bound Substrate Molecules. Drug Metabolism and Disposition, 2008, 36, 2136-2144.	3.3	50
103	Factors affecting imine coordination in (iminoterpyridine)MX2(M = Fe, Co, Ni, Zn): synthesis, structures, DFT calculations and ethylene oligomerisation studies. New Journal of Chemistry, 2007, 31, 75-85.	2.8	30
104	Filling a Hole in Cytochrome P450 BM3 Improves Substrate Binding and Catalytic Efficiency. Journal of Molecular Biology, 2007, 373, 633-651.	4.2	71
105	Mono- vs. bi-metallic assembly on a bulky bis(imino)terpyridine framework: a combined experimental and theoretical study. Dalton Transactions, 2006, , 2350-2361.	3.3	29
106	Design, synthesis and biological activity of new CDK4-specific inhibitors, based on fascaplysin. Organic and Biomolecular Chemistry, 2006, 4, 787.	2.8	42
107	IN SILICO PREDICTION OF DRUG BINDING TO CYP2D6: IDENTIFICATION OF A NEW METABOLITE OF METOCLOPRAMIDE. Drug Metabolism and Disposition, 2006, 34, 1386-1392.	3.3	41
108	Normal mode analysis as a prerequisite for drug design: Application to matrix metalloproteinases inhibitors. FEBS Letters, 2006, 580, 5130-5136.	2.8	58

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109	CA224, a non-planar analogue of fascaplysin, inhibits Cdk4 but not Cdk2 and arrests cells at G0/G1 inhibiting pRB phosphorylation. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 4272-4278.	2.2	27
110	Inhibition of cancer cell growth by cyclin dependent kinase 4 inhibitors synthesized based on the structure of fascaplysin. Bioorganic Chemistry, 2006, 34, 287-297.	4.1	18
111	A DFT study on the relative affinity for oxygen of the Î± and Î² subunits of hemoglobin. Journal of Computational Chemistry, 2006, 27, 1446-1453.	3.3	10
112	Insights into Drug Metabolism from Modelling Studies of Cytochrome P450-Drug Interactions. Current Topics in Medicinal Chemistry, 2006, 6, 1619-1626.	2.1	6
113	IN SILICO AND IN VITRO SCREENING FOR INHIBITION OF CYTOCHROME P450 CYP3A4 BY COMEDICATIONS COMMONLY USED BY PATIENTS WITH CANCER. Drug Metabolism and Disposition, 2006, 34, 534-538.	3.3	58
114	The design and synthesis of novel 3-[2-indol-1-yl-ethyl]-1H-indole derivatives as selective inhibitors of CDK4. Tetrahedron Letters, 2005, 46, 1423-1425.	1.4	44
115	The Design and Synthesis of Novel 3-[2-Indol-1-yl-ethyl]-1H-indole Derivatives as Selective Inhibitors of CDK4.. ChemInform, 2005, 36, no.	0.0	0
116	Why Is Quinidine an Inhibitor of Cytochrome P450 2D6?. Journal of Biological Chemistry, 2005, 280, 38617-38624.	3.4	63
117	Internal cavities and ligand passageways in human hemoglobin characterized by molecular dynamics simulations. Biochimica Et Biophysica Acta - General Subjects, 2005, 1724, 385-393.	2.4	26
118	Progress in cytochrome P450 active site modeling. Archives of Biochemistry and Biophysics, 2005, 433, 361-368.	3.0	26
119	Flexible N,N,N-chelates as supports for iron and cobalt chloride complexes; synthesis, structures, DFT calculations and ethylene oligomerisation studies. Dalton Transactions, 2004, , 3231-3240.	3.3	38
120	Validation of Model of Cytochrome P450 2D6:â€‰ An in Silico Tool for Predicting Metabolism and Inhibition. Journal of Medicinal Chemistry, 2004, 47, 5340-5346.	6.4	78
121	New fascaplysin-based CDK4-specific inhibitors: design, synthesis and biological activity. Chemical Communications, 2004, , 1696-1697.	4.1	29
122	Phe120 contributes to the regiospecificity of cytochrome P450 2D6: mutation leads to the formation of a novel dextromethorphan metabolite. Biochemical Journal, 2004, 380, 353-360.	3.7	69
123	Ab initio calculations predict a very low barrier for the rotation of the axial ligand in Fe(P)(Im). Chemical Physics Letters, 2002, 353, 379-382.	2.6	10
124	Theoretical modeling of the heme group with a hybrid QM/MM method. Journal of Computational Chemistry, 2000, 21, 282-294.	3.3	39
125	Amine conformational change and spin conversion induced by metal-assisted ligand oxidation: from the seven-coordinate iron(II)â€“TPAA complex to the two oxidized iron(II)â€“(py)3tren isomers. Characterization, crystal structures, and density functional study. Inorganica Chimica Acta, 2000, 297, 338-350.	2.4	59
126	Theoretical modeling of the heme group with a hybrid QM/MM method. Journal of Computational Chemistry, 2000, 21, 282.	3.3	1

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127	Selective recognition of A/T-rich DNA 3-way junctions with a three-fold symmetric tripeptide. Chemical Communications, 0, , .	4.1	5