Andrea Amadei

List of Publications by Year
in descending order

133 papers	6,121 citations	147566 31 h-index	76769 74 g-index
135 all docs	135 docs citations	135 times ranked	5499 citing authors

#	Article	IF	Citations
1	A general statistical mechanical model for fluid system thermodynamics: Application to sub- and super-critical water. Journal of Chemical Physics, 2022, 156, 044506.	1.2	3
2	Theoretical-computational modelling of the L-alanine CD spectrum in water. Computational and Theoretical Chemistry, 2022, 1209, 113591.	1.1	3
3	Theoretical-computational modelling of the vibrational relaxation of small inorganic species in condensed phase. Results in Chemistry, 2022, 4, 100305.	0.9	2
4	Theoretical Modeling of Redox Potentials of Biomolecules. Molecules, 2022, 27, 1077.	1.7	9
5	Computational Modeling of the Thermodynamics of the Mesophilic and Thermophilic Mutants of Trp-Cage Miniprotein. ACS Omega, 2022, 7, 13448-13454.	1.6	3
6	IR spectroscopy of condensed phase systems: Can the environment induce vibrational mode coupling?. Chemical Physics Letters, 2021, 763, 138168.	1.2	6
7	Theoretical Characterization of the Reduction Potentials of Nucleic Acids in Solution. Journal of Chemical Theory and Computation, 2021, 17, 1301-1307.	2.3	13
8	Segregation on the nanoscale coupled to liquid water polyamorphism in supercooled aqueous ionic-liquid solution. Journal of Chemical Physics, 2021, 155, 104502.	1.2	3
9	Stationary and Time-Dependent Carbon Monoxide Stretching Mode Features in Carboxy Myoglobin: A Theoreticalâ€“Computational Reappraisal. Journal of Physical Chemistry B, 2021, 125, 13624-13634.	1.2	6
10	Fully Atomistic Multiscale Approach for pK_a Prediction. Journal of Physical Chemistry B, 2020, 124, 4712-4722.	1.2	10
11	Length-scale dependence of protein hydration-shell density. Physical Chemistry Chemical Physics, 2020, 22, 7340-7347.	1.3	5
12	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. Physical Chemistry Chemical Physics, 2020, 22, 3008-3016.	1.3	10
13	Evolutionary Modes in Protein Observable Space: The Case of Thioredoxins. Journal of Molecular Evolution, 2019, 87, 175-183.	0.8	1
14	Modelling vibrational relaxation in complex molecular systems. Physical Chemistry Chemical Physics, 2019, 21, 20003-20017.	1.3	6
15	The self-association equilibria of doxorubicin at high concentration and ionic strength characterized by fluorescence spectroscopy and molecular dynamics simulations. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2019, 577, 517-522.	2.3	16
16	Interpretation of Experimental Soret Bands of Porphyrins in Flexible Covalent Cages and in Their Related Ag(I) Fixed Complexes. Journal of Physical Chemistry C, 2019, 123, 13094-13103.	1.5	17
17	Theoreticalâ€“computational modelling of the temperature dependence of the foldingâ€“unfolding thermodynamics and kinetics: the case of a Trp-cage. Physical Chemistry Chemical Physics, 2019, 21, 23162-23168.	1.3	4
18	Density discriminates between thermophilic and mesophilic proteins. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3265-3273.	2.0	10

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19	On the nature of solvatochromic effect: The riboflavin absorption spectrum as a case study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 192, 451-457.	2.0	8
20	A quantitative connection of experimental and simulated folding landscapes by vibrational spectroscopy. Chemical Science, 2018, 9, 9002-9011.	3.7	20
21	Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory. Physical Chemistry Chemical Physics, 2018, 20, 24369-24378.	1.3	49
22	Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. Journal of Computational Chemistry, 2018, 39, 1747-1756.	1.5	17
23	Theoretical-computational modeling of charge transfer and intersystem crossing reactions in complex chemical systems. RSC Advances, 2018, 8, 27900-27918.	1.7	9
24	Theoretical modeling of the absorption spectrum of aqueous riboflavin. Chemical Physics Letters, 2017, 669, 119-124.	1.2	37
25	Flexible and Comprehensive Implementation of MD-PMM Approach in a General and Robust Code. Journal of Chemical Theory and Computation, 2017, 13, 5506-5514.	2.3	15
26	Parallel folding pathways of Fip35 WW domain explained by infrared spectra and their computer simulation. FEBS Letters, 2017, 591, 3265-3275.	1.3	12
27	Alternative Electron-Transfer Channels Ensure Ultrafast Deactivation of Light-Induced Excited States in Riboflavin Binding Protein. Journal of Physical Chemistry Letters, 2017, 8, 3321-3327.	2.1	21
28	Photoinduced electron transfer in a dichromophoric peptide: a numerical experiment. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	14
29	Photoexcitation and relaxation kinetics of molecular systems in solution: towards a complete in silico model. Physical Chemistry Chemical Physics, 2016, 18, 28919-28931.	1.3	19
30	In silico characterization of bimolecular electron transfer reactions: The ferroceneâ€“ferrocenium reaction as a test case. International Journal of Quantum Chemistry, 2016, 116, 1723-1730.	1.0	9
31	The unfolding effects on the protein hydration shell and partial molar volume: a computational study. Physical Chemistry Chemical Physics, 2016, 18, 28175-28182.	1.3	15
32	Theoretical-computational characterization of the temperature-dependent folding thermodynamics of aÎ²-hairpin peptide. Chemical Physics Letters, 2016, 659, 247-251.	1.2	1
33	Extending the essential dynamics analysis to investigate molecular properties: application to the redox potential of proteins. Physical Chemistry Chemical Physics, 2016, 18, 18450-18459.	1.3	18
34	The Perfect Enzyme : Revisiting the Modelling of Initial Proton Transfer in Triosephosphate Isomerase. Theoretical Biology Forum, 2016, 109, 13-36.	0.2	0
35	Essential dynamics for the study of microstructures in liquids. Journal of Computational Chemistry, 2015, 36, 399-407.	1.5	16
36	Monitoring the Folding Kinetics of a Î²-Hairpin by Time-Resolved IR Spectroscopy in Silico. Journal of Physical Chemistry B, 2015, 119, 4849-4856.	1.2	11

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37	Theoretical calculation of the pyrene emission properties in different solvents. Chemical Physics Letters, 2015, 639, 17-22.	1.2	12
38	A few key residues determine the high redox potential shift in azurin mutants. Organic and Biomolecular Chemistry, 2015, 13, 11003-11013.	1.5	35
39	In silico characterization of protein partial molecular volumes and hydration shells. Physical Chemistry Chemical Physics, 2015, 17, 31270-31277.	1.3	35
40	Molecular mechanisms of activation in CDK2. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1929-1935.	2.0	13
41	Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: Explicit treatment of the vibronic transitions. Journal of Chemical Physics, 2014, 140, 164104.	1.2	42
42	Inclusion of cybotactic effect in the theoretical modeling of absorption spectra of liquid-state systems with perturbed matrix method and molecular dynamics simulations: the UVâ€“Vis absorption spectrum of para-nitroaniline as a case study. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	5
43	How the Reorganization Free Energy Affects the Reduction Potential of Structurally Homologous Cytochromes. Journal of Physical Chemistry Letters, 2014, 5, 1534-1540.	2.1	19
44	Theoretical-computational modeling of photo-induced charge separation spectra and charge recombination kinetics in solution. Physical Chemistry Chemical Physics, 2014, 16, 20624-20638.	1.3	15
45	Unambiguous Assignment of Reduction Potentials in Diheme Cytochromes. Journal of Physical Chemistry B, 2014, 118, 7554-7560.	1.2	20
46	On the Nature of DNA Hyperchromic Effect. Journal of Physical Chemistry B, 2013, 117, 8697-8704.	1.2	44
47	A theoretical study on the spectral and electrochemical properties of Ferrocene in different solvents. Inorganica Chimica Acta, 2013, 407, 82-90.	1.2	4
48	Simulation of the Amide I Infrared Spectrum in Photoinduced Peptide Folding/Unfolding Transitions. Journal of Physical Chemistry B, 2013, 117, 12383-12390.	1.2	17
49	Toward a Realistic Modeling of the Photophysics of Molecular Building Blocks for Energy Harvesting: The Charge-Transfer State in 4,7-Dithien-2-yl-2,1,3-benzothiadiazole As a Case Study. Journal of Physical Chemistry C, 2013, 117, 13785-13797.	1.5	13
50	Modeling triplet flavin-indole electron transfer and interradical dipolar interaction: a perturbative approach. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	14
51	Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: The vertical transition approximation. Journal of Chemical Physics, 2013, 139, 114102.	1.2	36
52	A general statistical mechanical approach for modeling redox thermodynamics: the reaction and reorganization free energies. RSC Advances, 2013, 3, 19657.	1.7	16
53	Effect of High Exogenous Electric Pulses on Protein Conformation: Myoglobin as a Case Study. Journal of Physical Chemistry B, 2013, 117, 2273-2279.	1.2	85
54	Thermal and environmental effects on Oligothiophene low-energy singlet electronic excitations in dilute solution: a theoretical and experimental study. Highlights in Theoretical Chemistry, 2013, , 185-198.	0.0	0

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55	A Theoretical Reappraisal of Polylysine in the Investigation of Secondary Structure Sensitivity of Infrared Spectra. Journal of Physical Chemistry B, 2012, 116, 3353-3360.	1.2	19
56	A general theoretical model for electron transfer reactions in complex systems. Physical Chemistry Chemical Physics, 2012, 14, 1360-1370.	1.3	35
57	Essential dynamics: foundation and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 762-770.	6.2	99
58	The Reversible Opening of Water Channels in Cytochrome c Modulates the Heme Iron Reduction Potential. Journal of the American Chemical Society, 2012, 134, 13670-13678.	6.6	71
59	Thermal and environmental effects on Oligothiophene low-energy singlet electronic excitations in dilute solution: a theoretical and experimental study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	7
60	Theoretical modeling of the spectroscopic absorption properties of luciferin and oxyluciferin: A critical comparison with recent experimental studies. Chemical Physics, 2012, 392, 205-214.	0.9	18
61	Effects of local electric fields on the redox free energy of single stranded DNA. Chemical Communications, 2011, 47, 2646-2648.	2.2	8
62	The role of water near charged interfaces: Molecular dynamics simulations of biological macromolecules in presence of high intense electric fields. , 2011, , .		0
63	Kinetics of Carbon Monoxide Migration and Binding in Solvated Neuroglobin As Revealed by Molecular Dynamics Simulations and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2011, 115, 2436-2446.	1.2	17
64	New Insight into the IR-Spectra/Structure Relationship in Amyloid Fibrils: A Theoretical Study on a Prion Peptide. Journal of the American Chemical Society, 2011, 133, 11414-11417.	6.6	28
65	Analysis of Infrared Spectra of Î²-Hairpin Peptides As Derived from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 11872-11878.	1.2	11
66	Modeling of Chemical Reactions in Micelle: Water-Mediated Ketoâ€“Enol Interconversion As a Case Study. Journal of Physical Chemistry B, 2011, 115, 8102-8111.	1.2	23
67	Modeling quantum vibrational excitations in condensed-phase molecular systems. Theoretical Chemistry Accounts, 2011, 129, 31-43.	0.5	26
68	The effects of the L29F mutation on the ligand migration kinetics in crystallized myoglobin as revealed by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 867-879.	1.5	4
69	Entropyâ€“energy balance in base catalyzed ketoâ€enol interconversion: A joint theoretical and experimental investigation. International Journal of Quantum Chemistry, 2011, 111, 1293-1305.	1.0	7
70	Modeling electromagnetic field effects in a biochemical reaction: Understanding reactivity inhibition due to the magnetic field. , 2011, , .		0
71	Characterization of Electronic Properties in Complex Molecular Systems: Modeling of a Micropolarity Probe. Journal of Physical Chemistry B, 2010, 114, 1915-1924.	1.2	17
72	Theoretical-computational modelling of infrared spectra in peptides and proteins: a new frontier for combined theoretical-experimental investigations. Current Opinion in Structural Biology, 2010, 20, 155-161.	2.6	35

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73	On the origin of IR spectral changes upon protein folding. Chemical Physics Letters, 2010, 488, 213-218.	1.2	30
74	Free-Energy Profile for CO Binding to Separated Chains of Human and Trematomus newnesi Hemoglobin: Insights from Molecular Dynamics Simulations and Perturbed Matrix Method. Journal of Physical Chemistry B, 2010, 114, 7002-7008.	1.2	7
75	A fast redox-induced switching mechanism in a conformationally controllable molecular thread in solution. Physical Chemistry Chemical Physics, 2010, 12, 4552.	1.3	8
76	Theoretical characterization of electronic states in interacting chemical systems. Journal of Chemical Physics, 2009, 130, 084109.	1.2	66
77	Structural, thermodynamic, and kinetic properties of Gramicidin analogue GS6 studied by molecular dynamics simulations and statistical mechanics. Biopolymers, 2009, 91, 1154-1160.	1.2	1
78	What can we learn by comparing experimental and theoretical-computational X-ray scattering data?. Journal of Molecular Liquids, 2009, 144, 9-12.	2.3	3
79	Kinetics of Carbon Monoxide Migration and Binding in Solvated Myoglobin as Revealed by Molecular Dynamics Simulations and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2009, 113, 16346-16353.	1.2	17
80	Charge transfer equilibria of aqueous single stranded DNA. Physical Chemistry Chemical Physics, 2009, 11, 10614.	1.3	7
81	Intramolecular charge transfer in Ï€-conjugated oligomers: a theoretical study on the effect of temperature and oxidation state. Theoretical Chemistry Accounts, 2008, 119, 469-476.	0.5	7
82	The Kinetics of Ligand Migration in Crystallized Myoglobin as Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 4277-4281.	0.2	31
83	Solvent Electrostriction-Driven Peptide Folding Revealed by Quasi-Gaussian Entropy Theory and Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 11155-11163.	1.2	9
84	Can a synthetic thread act as an electrochemically switchable molecular device?. Chemical Communications, 2008, , 3399.	2.2	14
85	Protein Folding Pathways Revealed by Essential Dynamics Sampling. Journal of Chemical Theory and Computation, 2008, 4, 1940-1948.	2.3	13
86	Theoretical Modeling of Enzyme Reactions:â€‰ The Thermodynamics of Formation of Compound 0 in Horseradish Peroxidase. Journal of Physical Chemistry B, 2008, 112, 3184-3192.	1.2	24
87	Theoretical characterization of temperature and density dependence of liquid water electronic excitation energy: Comparison with recent experimental data. Journal of Chemical Physics, 2008, 128, 021103.	1.2	22
88	Mixed Quantum-Classical Methods for Molecular Simulations of Biochemical Reactions With Microwave Fields: The Case Study of Myoglobin. IEEE Transactions on Microwave Theory and Techniques, 2008, 56, 2511-2519.	2.9	36
89	Statistical Mechanical Modeling of Chemical Reactions in Condensed Phase Systems. Challenges and Advances in Computational Chemistry and Physics, 2008, , 191-213.	0.6	9
90	Dehydration-driven solvent exposure of hydrophobic surfaces as a driving force in peptide folding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 15230-15235.	3.3	72

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91	Theoretical Characterization of Carbon Monoxide Vibrational Spectrum in Sperm Whale Myoglobin Distal Pocket. Biophysical Journal, 2007, 92, 3442-3447.	0.2	23
92	Theoretical study of intramolecular charge transfer in Ï€-conjugated oligomers. Chemical Physics Letters, 2007, 434, 194-199.	1.2	12
93	Statistical mechanical modelling of chemical reactions in complex systems: the kinetics of the Haem carbon monoxide bindingâ€“unbinding reaction in Myoglobin. Theoretical Chemistry Accounts, 2007, 117, 637-647.	0.5	28
94	Myoglobin as a Case Study for Molecular Simulations in the Presence of a Microwave Electromagnetic Field. , 2006, , .		7
95	Theoretical modeling of the valence UV spectra of 1,2,3-triazine and uracil in solution. Physical Chemistry Chemical Physics, 2006, 8, 1385.	1.3	39
96	On the Effect of a Point Mutation on the Reactivity of CuZn Superoxide Dismutase:Â A Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 7538-7544.	1.2	16
97	Theoretical modeling of chemical reactions in complex environments: the intramolecular proton transfer in aqueous malonaldehyde. Journal of Physical Organic Chemistry, 2006, 19, 518-530.	0.9	28
98	Aggregation of small peptides studied by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2006, 65, 914-921.	1.5	19
99	On the importance of configurational sampling in theoretical calculation of electronic properties of complex molecular systems: Acetone in water. Chemical Physics Letters, 2006, 424, 289-294.	1.2	5
100	Theoretical Characterisation of the Electronic Excitation in Liquid Water. ChemPhysChem, 2005, 6, 53-58.	1.0	31
101	Conformational and Electronic Properties of a Microperoxidase in Aqueous Solution: A Computational Study. ChemPhysChem, 2005, 6, 681-689.	1.0	6
102	Molecular dynamics simulation of the aggregation of the core-recognition motif of the islet amyloid polypeptide in explicit water. Proteins: Structure, Function and Bioinformatics, 2005, 59, 519-527.	1.5	49
103	Thermodynamic and kinetic characterization of a Î²-hairpin peptide in solution: An extended phase space sampling by molecular dynamics simulations in explicit water. Proteins: Structure, Function and Bioinformatics, 2005, 59, 510-518.	1.5	49
104	Ground and excited electronic state thermodynamics of aqueous carbon monoxide: A theoretical study. Journal of Chemical Physics, 2005, 122, 124507.	1.2	6
105	A mean field approach for molecular simulations of fluid systems. Journal of Chemical Physics, 2005, 122, 154109.	1.2	46
106	Characterization of liquid behaviour by means of local density fluctuations. Journal of Molecular Liquids, 2005, 117, 17-21.	2.3	2
107	Theoretical Characterization of Î±-Helix and Î²-Hairpin Folding Kinetics. Journal of the American Chemical Society, 2005, 127, 14825-14832.	6.6	43
108	Molecular Dynamics Simulation of Sperm Whale Myoglobin: Effects of Mutations and Trapped CO on the Structure and Dynamics of Cavities. Biophysical Journal, 2005, 89, 465-474.	0.2	93

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109	Theoretical modeling of vibroelectronic quantum states in complex molecular systems: Solvated carbon monoxide, a test case. Journal of Chemical Physics, 2005, 122, 124506.	1.2	34
110	On the use of the quasi-Gaussian entropy theory in the study of simulated dilute solutions. Journal of Chemical Physics, 2004, 120, 5226-5234.	1.2	9
111	Conformational fluctuations and electronic properties in myoglobin. Journal of Computational Chemistry, 2004, 25, 974-984.	1.5	35
112	Theoretical Modeling of Enzyme Reaction Chemistry:Â The Electron Transfer of the Reduction Mechanism in CuZn Superoxide Dismutase. Journal of Physical Chemistry B, 2004, 108, 16255-16260.	1.2	31
113	A Theoretical Model for the Folding/Unfolding Thermodynamics of Single-Domain Proteins, Based on the Quasi-Gaussian Entropy Theory. Journal of Physical Chemistry B, 2004, 108, 5756-5762.	1.2	9
114	A DFT Study of the Low-Lying Singlet Excited States of the All-Trans Peridinin in vacuo. Journal of Physical Chemistry A, 2004, 108, 6763-6770.	1.1	21
115	Extended Molecular Dynamics Simulation of the Carbon Monoxide Migration in Sperm Whale Myoglobin. Biophysical Journal, 2004, 86, 3855-3862.	0.2	129
116	Structural rearrangements of the two domains of Azotobacter vinelandii rhodanese upon sulfane sulfur release: essential molecular dynamics, NMR relaxation and deuterium exchange on the uniformly labeled protein. International Journal of Biological Macromolecules, 2003, 33, 193-201.	3.6	7
117	The Effect of Protein Conformational Flexibility on the Electronic Properties of a Chromophore. Biophysical Journal, 2003, 84, 2805-2813.	0.2	36
118	Molecular Dynamics Simulation of Protein Folding by Essential Dynamics Sampling: Folding Landscape of Horse Heart Cytochrome c. Biophysical Journal, 2003, 85, 2865-2871.	0.2	67
119	Coherent dynamics in a butane molecule. Physical Review E, 2002, 66, 020901.	0.8	2
120	Statistical Mechanics and Thermodynamics of Simulated Ionic Solutions. Journal of Physical Chemistry B, 2002, 106, 11843-11848.	1.2	18
121	Extension of the perturbed matrix method: application to a water molecule. Chemical Physics Letters, 2002, 365, 450-456.	1.2	51
122	On the Use of the Quasi-Gaussian Entropy Theory in Systems of Polyatomic Flexible Molecules. Journal of Physical Chemistry B, 2001, 105, 1834-1844.	1.2	8
123	A molecular dynamics study of the 41â€56 Î²â€hairpin from B1 domain of protein G. Protein Science, 1999, 8, 2130-2143.	3.1	109
124	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 1999, 36, 419-424.	1.5	277
125	Mechanics and dynamics of B1 domain of protein G: Role of packing and surface hydrophobic residues. Protein Science, 1999, 8, 147-160.	3.1	46
126	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. , 1999, 36, 419.		1

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127	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. , 1999, 36, 419.		8
128	Identification of functional and unfolding motions of cutinase as obtained from molecular dynamics computer simulations. , 1998, 33, 253-264.		40
129	Essential degrees of freedom of proteins. Molecular Engineering, 1995, 5, 71-79.	0.2	5
130	Essential dynamics of proteins. Proteins: Structure, Function and Bioinformatics, 1993, 17, 412-425.	1.5	2,927
131	The conformation of constitutive DNA interaction sites for eukaryotic DNA topoisomerase I on intrinsically curved DNAs. Biochimica Et Biophysica Acta Gene Regulatory Mechanisms, 1991, 1129, 73-82.	2.4	28
132	In vitropreferential topoisomerization of bent DNA. Nucleic Acids Research, 1989, 17, 8463-8474.	6.5	63
133	On the catalytic role of structural fluctuations in enzyme reactions: computational evidence on the formation of compound 0 in horseradish peroxidase. Faraday Discussions, 0, 145, 107-119.	1.6	5