

CERM Publications
(June 2025)

1. Tino AS, Quagliata M, Schiavina M, Pacini L, Papini AM, Felli IC, Pierattelli R. Revealing the Potential of a Chimaera: a Peptide-Peptide Nucleic Acid Molecule Designed To Interact with the SARS-CoV-2 Nucleocapsid Protein. **Angew Chem Int Ed Engl.** 2025 Mar 10;64(11):e202420134. doi: 10.1002/anie.202420134. Epub 2025 Feb 14. (IF 16.1)
2. Cosottini L, Giachetti A, Guerri A, Martinez-Castillo A, Geri A, Zineddu S, Abrescia NGA, Messori L, Turano P, Rosato A. Structural Insight Into a Human H Ferritin@Gold-Monocarbene Adduct: Auophilicity Revealed in a Biological Context. **Angew Chem Int Ed Engl.** 2025 Apr 18:e202503778. doi: 10.1002/anie.202503778. Epub ahead of print. PMID: 40249912. (IF 16.1)
3. Sherry L, Bahar MW, Porta C, Fox H, Grehan K, Nasta V, Duyvesteyn HME, De Colibus L, Marsian J, Murdoch I, Ponndorf D, Kim SR, Shah S, Carlyle S, Swanson JJ, Matthews S, Nicol C, Lomonosoff GP, Macadam AJ, Fry EE, Stuart DI, Stonehouse NJ, Rowlands DJ. Recombinant expression systems for production of stabilised virus-like particles as next-generation polio vaccines. **Nat Commun.** 2025 Jan 18;16(1):831. doi: 10.1038/s41467-025-56118-z (IF 14.7)
4. Bracaglia L, Olivetti S, Felli IC, Pierattelli R. Decoding Order and Disorder in Proteins by NMR Spectroscopy. **J Am Chem Soc.** 2025 Apr 13. doi: 10.1021/jacs.4c14959. Online ahead of print. (IF 14.4)
5. Russomanno P, Zizza P, Cerofolini L, D'Aria F, Iachettini S, Di Vito S, Biroccio A, Amato J, Fragai M, Pagano B. Expanding the Functions of KHSRP Protein: Insights into DNA G-Quadruplex Binding. **Adv Sci (Weinh).** 2025 Feb;12(8):e2410086. doi: 10.1002/advs.202410086. Epub 2025 Jan 6. (IF 14.3)
6. Di Carluccio C, Padilla-Cortés L, Tiemblo-Martín M, Gheorghita GR, Oliva R, Cerofolini L, Masi AA, Abreu C, Tseng HK, Molinaro A, Del Vecchio P, Vaněk O, Lin CC, Marchetti R, Fragai M, Silipo A. Insights into Siglec-7 Binding to Gangliosides: NMR Protein Assignment and the Impact of Ligand Flexibility. **Adv Sci (Weinh).** 2025 Apr 26:e2415782. doi: 10.1002/advs.202415782. Epub ahead of print. PMID: 40285643. (IF 14.3)
7. Viola G, Trivellato D, Laitaoja M, Jänis J, Felli IC, D'Onofrio M, Mollica L, Giachin G, Assfalg M. Conformational signatures induced by ubiquitin modification in the amyloid-forming tau repeat

domain. **Proc Natl Acad Sci U S A**. 2025 Apr 15;122(15):e2425831122. doi: 10.1073/pnas.2425831122. Epub 2025 Apr 8. (IF 9.4)

8. Di Carluccio C, Gerpe Amor T, Lenza MP, Masi AA, Abreu C, Longo V, Albano F, Nieto-Fabregat F, Salvatore P, Falco G, Santana-Medero D, Fragai M, van Kooyk Y, Molinaro A, Valdes-Balbin Y, Vaněk O, Verež-Bencomo V, Marchetti R, Chiodo F, Silipo A. Molecular Basis of Siglec-7 Recognition by *Neisseria meningitidis* Serogroup Y CPS: Implications for Immune Evasion. **JACS Au**. 2025 Apr 30;5(5):2257-2269. doi: 10.1021/jacsau.5c00214. PMID: 40443894; PMCID: PMC12117448. (IF 8.5)
9. Olivieri G, Dal Cortivo G, Del Conte R, Zanzoni S, Marino V, Dell'Orco D, Cantini F. Structural dynamics of calcium and integrin-binding protein 2 (CIB2) reveal uncommon flexibility and heterogeneous calcium and magnesium loading. **Int J Biol Macromol**. 2025 Jan;286:138003. doi: 10.1016/j.ijbiomac.2024.138003. Epub 2024 Nov 23. (IF 7.7)
10. Rossetto D, Nader S, Kufner CL, Lozano GG, Cerofolini L, Fragai M, Martin-Diaconescu V, Zambelli B, Ciurli S, Guella G, Szabla R, Sassellov DD, Mansy SS. Preferential survival of prebiotic metallopeptides in the presence of ultraviolet light. **Chem Sci**. 2025 May 20. doi: 10.1039/d5sc02170g. Epub ahead of print. PMID: 40438176; PMCID: PMC12108965. (IF 7.6)
11. Pesce E, Sodini A, Palmieri E, Valensin S, Tinti C, Rossi M, De Rosa A, Fragai M, Papi F, Cordiglieri C, Berti F, Grifantini R, Micoli F, Nativi C. GMMA decorated with mucin 1 Tn/STn mimetics elicit specific antibodies response and inhibit tumor growth. **NPJ Vaccines**. 2025 Apr 15;10(1):71. doi: 10.1038/s41541-025-01127-8. (IF 6.9)
12. Bruno F, Fiorucci L, Vignoli A, Meyer K, Maiwald M, Ravera E. pyIHM: Indirect Hard Modeling, in Python. **Anal Chem**. 2025 Mar 4;97(8):4598-4605. doi: 10.1021/acs.analchem.4c06484. Epub 2025 Feb 24. (IF 6.7)
13. Vignoli A, Luchinat C, Segata N, Renzi D, Tenori L, Calabrò AS. Serum metabolomics and lipoproteomics discriminate celiac disease and non-celiac gluten sensitivity patients. **Clin Nutr**. 2025 Feb; 45:31-35. doi: 10.1016/j.clnu.2024.12.016. Epub 2024 Dec 19. (IF 6.6)
14. Vignoli A, Bellomo G, Paoletti FP, Luchinat C, Tenori L, Parnetti L. Studying Alzheimer's disease through an integrative serum metabolomic and lipoproteomic approach. **J Transl Med**. 2025 Jan 27;23(1):119. doi: 10.1186/s12967-025-06148-4. (IF 6.1)

15. Vignoli A, Sticchi E, Piccardi B, Palumbo V, Sarti C, Sodero A, Arba F, Fainardi E, Gori AM, Giusti B, Kura A, Tenori L, Baldereschi M. Predicting reperfusion injury and functional status after stroke using blood biomarkers: the STROKELABED study. **J Transl Med.** 2025 Apr 30;23(1):491. doi: 10.1186/s12967-025-06498-z. PMID: 40307929; PMCID: PMC12042387. (IF 6.1)
16. Lang L, Fiorucci L, Parigi G, Luchinat C, Ravera E. Theory of Field-Dependent NMR Shifts in Paramagnetic Molecules. **J Chem Theory Comput.** 2025 May 27. doi: 10.1021/acs.jctc.5c00433. Epub ahead of print. PMID: 40424483. (IF 5.7)
17. Ciofalo C, Laveglia V, Andreini C, Rosato A. Benchmarking Zinc-Binding Site Predictors: A Comparative Analysis of Structure-Based Approaches. **J Chem Inf Model.** 2025 May 26;65(10):5205-5215. doi: 10.1021/acs.jcim.5c00549. Epub 2025 May 15. PMID: 40371807; PMCID: PMC12117554. (IF 5.6)
18. Rynes J, Istvankova E, Dzurov Krafcikova M, Luchinat E, Barbieri L, Banci L, Kamarytova K, Loja T, Fafilek B, Rico-Llanos G, Krejci P, Macurek L, Foldynova-Trantirkova S, Trantirek L. Protein structure and interactions elucidated with in-cell NMR for different cell cycle phases and in 3D human tissue models. **Commun Biol.** 2025 Feb 7;8(1):194. doi: 10.1038/s42003-025-07607-w. (IF 5.2)
19. Pérez-Ropero G, Dolcemascolo R, Pérez-Ràfols A, Andersson K, Danielson UH, Rodrigo G, Buijs J. Regulatory Effects of RNA-Protein Interactions Revealed by Reporter Assays of Bacteria Grown on Solid Media. **Biosensors** (Basel). 2025 Mar 8;15(3):175. doi: 10.3390/bios15030175. (IF 4.9)
20. Querci L, Burgassi L, Ciofi-Baffoni S, Schiavina M, Piccioli M. Optimized ¹³C Relaxation-Filtered Nuclear Magnetic Resonance: Harnessing Optimal Control Pulses and Ultra-High Magnetic Fields for Metalloprotein Structural Elucidation. **Int J Mol Sci.** 2025 Apr 19;26(8):3870. doi: 10.3390/ijms26083870. PMID: 40332551; PMCID: PMC12027794. (IF 4.9)
21. Querci L, Fiorucci L, Grifagni D, Costantini P, Ravera E, Ciofi-Baffoni S, Piccioli M. Shedding Light on the Electron Delocalization Pathway at the [Fe₂S₂]²⁺ Cluster of FDX2. **Inorg Chem.** 2025 Apr 7;64(13):6698-6712. doi: 10.1021/acs.inorgchem.5c00420. Epub 2025 Mar 23. (IF 4.3)
22. Tagliaferro G, Davighi MG, Clemente F, Turchi F, Schiavina M, Matassini C, Goti A, Morrone A, Pierattelli R, Cardona F, Felli IC. Evidence of α -Synuclein/Glucocerebrosidase Dual Targeting by

Iminosugar Derivatives. **ACS Chem Neurosci**. 2025 Apr 2;16(7):1251-1257. doi: 10.1021/acscchemneuro.4c00618. Epub 2025 Mar 13. (IF 4.1)

23. Pujols J, Fornt-Suñé M, Gil-García M, Bartolomé-Nafría A, Canals F, Cerofolini L, Teilum K, Banci L, Esperante SA, Ventura S. MIA40 circumvents the folding constraints imposed by TRIAP1 function. **J Biol Chem**. 2025 Mar;301(3):108268. doi: 10.1016/j.jbc.2025.108268. Epub 2025 Feb 3. (IF 4.0)

24. Ghini V, Tristán AI, Di Paco G, Massai L, Mannelli M, Gamberi T, Fernández I, Rosato A, Turano P, Messori L. Novel NMR-Based Approach to Reveal the 'Metabolic Fingerprint' of Cytotoxic Gold Drugs in Cancer Cells. **J Proteome Res**. 2025 Feb 7;24(2):813-823. doi: 10.1021/acs.jproteome.4c00904. Epub 2025 Jan 6. (IF 3.8)

25. Andreini C. Twenty years in metalloprotein bioinformatics: A short history of a long journey. **J Inorg Biochem**. 2025 May; 266:112854. doi: 10.1016/j.jinorgbio.2025.112854. Epub 2025 Feb 11. (IF 3.8)

26. Ghini V, Pecchioli V, Celli T, Boccia N, Bertini L, Veneziani F, Vannucchi V, Turano P. Metabolomic and lipoproteomic differences and similarities between COVID-19 and other types of pneumonia. **Sci Rep**. 2025 Mar 3;15(1):7507. doi: 10.1038/s41598-025-91965-2. (IF 3.8)

27. Fiorucci L, Ravera E., Not Just Another Crystal Field Software, **J Comput Chem**, 2025, 46, e70063. doi: 10.1002/jcc.70063 (IF 3.4)

28. Provinciali G., Consoli N.A., Caliendo R., Mangini V., Barba L., Giannini C., Tuci G., Giambastiani G., Lelli M., Rossin A. Ammonia Borane and Hydrazine Bis(borane) Confined within Zirconium Bithiazole and Bipyridyl Metal-Organic Frameworks as Chemical Hydrogen Storage Materials, **Journal of Physical Chemistry C**. 2025 129 (13), pp. 6094 – 6108, doi: 10.1021/acs.jpcc.5c00187 (IF 3.3)

29. Kubrak A, Pejanovic R, Kamau K, Kruk D, Ferrage F, Parigi G. Field-dependent relaxation profiles of biomolecular systems. **Phys Chem Chem Phys**. 2025 Jan 22;27(4):1756-1771. doi: 10.1039/d4cp04306e. (IF 2.9)

30. Santambrogio C, Toccafondi M, Donnici L, Pesce E, De Francesco R, Grifantini R, Ponzini E, Milanesi F, Fragai M, Nativi C, Roelens S, Grandori R, Francesconi O. Biomimetic Recognition of SARS-CoV-2 Receptor-Binding Domain N-Glycans by an Antiviral Synthetic Receptor. **Chembiochem**. 2025 Feb 21:e202500106. doi: 10.1002/cbic.202500106. Epub ahead of print. (IF 2.6)
31. Rodella MA, Schneider R, Kümmerle R, Felli IC, Pierattelli R. ¹⁵N-detected TROSY for ¹H-¹⁵N heteronuclear correlation to study intrinsically disordered proteins: strategies to increase spectral quality.. **J Biomol NMR**. 2025 Mar;79(1):15-24. doi: 10.1007/s10858-024-00453-8. Epub 2025 Jan 22. (IF 2.4)
32. Malanho da Silva J, Lanuza J, Bruno F, Calderone V, Ravera E. The structure of His15 acetamide-modified hen egg-white lysozyme: a nice surprise from an old friend. **Acta Crystallogr F Struct Biol Commun**. 2025 Feb 1;81(Pt 2):41-46. doi: 10.1107/S2053230X2500010X. Epub 2025 Jan 13. (IF 1.1)
33. Basoglu A, Bicici RO, Di Cesare F, Baspinar N, Tenori L, Ider M, Gulersoy E. NMR-based-Metabolomics Evaluation in Dogs Infected with Canine Parvovirus: A New Approach for Biomarker/s. **Vet Ital**. 2025 Mar 5;61(1). doi: 10.12834/VetIt.3578.29616.2. (IF 0.5)