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| # | Paper | IF | Citations |
|------|--|------|-----------|
| 1553 | Protein Dynamics and Contact Topology Reveal ProteinDNA Binding Orientation. | | |
| 1552 | Erratum: The role of dynamic conformational ensembles in biomolecular recognition. <i>Nature Chemical Biology</i> , 2009 , 5, 954-954 | 11.7 | 20 |
| 1551 | How do transcription factors select specific binding sites in the genome?. 2009 , 16, 1118-20 | | 39 |
| 1550 | During transitions proteins make fleeting bonds. 2009 , 139, 1049-51 | | 10 |
| 1549 | The structural basis of pregnane X receptor binding promiscuity. 2009 , 48, 11572-81 | | 61 |
| 1548 | Excited protein states of human tear lipocalin for low- and high-affinity ligand binding revealed by functional AB loop motion. 2010 , 149, 47-57 | | 9 |
| 1547 | Designing ensembles in conformational and sequence space to characterize and engineer proteins. 2010 , 20, 377-84 | | 22 |
| 1546 | Ubiquitin--molecular mechanisms for recognition of different structures. 2010 , 20, 367-76 | | 30 |
| 1545 | Structural dynamics in DNA damage signaling and repair. 2010 , 20, 283-94 | | 41 |
| 1544 | A single mutation promotes amyloidogenicity through a highly promiscuous dimer interface. 2010 , 18, 563-70 | | 35 |
| 1543 | The meandering of disordered proteins in conformational space. 2010 , 18, 416-9 | | 13 |
| 1542 | Free state conformational sampling of the SAM-I riboswitch aptamer domain. 2010 , 18, 787-97 | | 142 |
| 1541 | Drug discovery and mutant p53. 2010 , 20, 542-55 | | 51 |
| 1540 | Induced fit, conformational selection and independent dynamic segments: an extended view of binding events. 2010 , 35, 539-46 | | 617 |
| 1539 | Mechanisms of transcription factor selectivity. 2010 , 26, 75-83 | | 109 |
| 1538 | Amyloid assemblies: protein legos at a crossroads in bottom-up synthetic biology. 2010 , 11, 2347-57 | | 26 |
| 1537 | RNA Dynamics by Design: Biasing Ensembles Towards the Ligand-Bound State. 2010 , 122, 5867-5869 | | 1 |

| | | |
|------|---|----------|
| 1536 | RNA dynamics by design: biasing ensembles towards the ligand-bound state. 2010 , 49, 5731-3 | 40 |
| 1535 | In Pursuit of Fully Flexible Protein-Ligand Docking: Modeling the Bilateral Mechanism of Binding. 2010 , 29, 164-73 | 17 |
| 1534 | Enzyme dynamics point to stepwise conformational selection in catalysis. 2010 , 14, 652-9 | 169 |
| 1533 | Enzymatic activity in disordered states of proteins. 2010 , 14, 671-5 | 17 |
| 1532 | Beyond directed evolution--semi-rational protein engineering and design. 2010 , 21, 734-43 | 308 |
| 1531 | Comparison of current docking tools for the simulation of inhibitor binding by the transmembrane domain of the sarco/endoplasmic reticulum calcium ATPase. 2010 , 150, 88-97 | 31 |
| 1530 | Assessing the native state conformational distribution of ubiquitin by peptide acidity. 2010 , 153, 70-82 | 8 |
| 1529 | FiberDock: Flexible induced-fit backbone refinement in molecular docking. 2010 , 78, 1503-19 | 144 |
| 1528 | Intermodule cooperativity in the structure and dynamics of consecutive complement control modules in human C1r: structural biology. 2010 , 277, 3986-98 | 5 |
| 1527 | NMR backbone dynamics studies of human PED/PEA-15 outline protein functional sites. 2010 , 277, 4229-40 | 9 |
| 1526 | A DNA-promoted amyloid proteinopathy in Escherichia coli. 2010 , 77, 1456-69 | 39 |
| 1525 | Dynamics connect substrate recognition to catalysis in protein kinase A. <i>Nature Chemical Biology</i> , 2010 , 6, 821-8 | 11.7 155 |
| 1524 | Mutational effects and the evolution of new protein functions. 2010 , 11, 572-82 | 291 |
| 1523 | A selection fit mechanism in BMP receptor IA as a possible source for BMP ligand-receptor promiscuity. 2010 , 5, e13049 | 9 |
| 1522 | A novel p53 phosphorylation site within the MDM2 ubiquitination signal: I. phosphorylation at SER269 in vivo is linked to inactivation of p53 function. 2010 , 285, 37762-72 | 21 |
| 1521 | Two-dimensional NMR and all-atom molecular dynamics of cytochrome P450 CYP119 reveal hidden conformational substates. 2010 , 285, 9594-9603 | 39 |
| 1520 | Entropic mechanism of large fluctuation in allosteric transition. 2010 , 107, 7775-80 | 48 |
| 1519 | Molecular dynamics simulations show that conformational selection governs the binding preferences of imatinib for several tyrosine kinases. 2010 , 285, 13807-15 | 65 |

| | | |
|------|--|-----|
| 1518 | Synergistic allostery, a sophisticated regulatory network for the control of aromatic amino acid biosynthesis in <i>Mycobacterium tuberculosis</i> . 2010 , 285, 30567-76 | 50 |
| 1517 | Regulation of response regulator autophosphorylation through interdomain contacts. 2010 , 285, 32325-35 | 48 |
| 1516 | SwarmDock and the use of normal modes in protein-protein docking. 2010 , 11, 3623-48 | 120 |
| 1515 | Using entropy maximization to understand the determinants of structural dynamics beyond native contact topology. 2010 , 6, e1000816 | 29 |
| 1514 | The role of oligomerization and cooperative regulation in protein function: the case of tryptophan synthase. 2010 , 6, e1000994 | 31 |
| 1513 | Lysine120 interactions with p53 response elements can allosterically direct p53 organization. 2010 , 6, e1000878 | 15 |
| 1512 | Substrate-induced changes in protease active site conformation impact on subsequent reactions with substrates. 2010 , 285, 22950-6 | 13 |
| 1511 | A coordination cage with an adaptable cavity size. 2010 , 132, 14004-5 | 173 |
| 1510 | Polymorphism in Alzheimer Abeta amyloid organization reflects conformational selection in a rugged energy landscape. 2010 , 110, 4820-38 | 239 |
| 1509 | Backbone flexibility controls the activity and specificity of a protein-protein interface: specificity in snake venom metalloproteases. 2010 , 132, 10330-7 | 40 |
| 1508 | Direct renin inhibitors as a new therapy for hypertension. 2010 , 53, 7490-520 | 63 |
| 1507 | Evolvability and single-genotype fluctuation in phenotypic properties: a simple heteropolymer model. 2010 , 98, 2487-96 | 8 |
| 1506 | Anharmonic normal mode analysis of elastic network model improves the modeling of atomic fluctuations in protein crystal structures. 2010 , 98, 3025-34 | 26 |
| 1505 | Rbx1 flexible linker facilitates cullin-RING ligase function before neddylation and after deneddylation. 2010 , 99, 736-44 | 23 |
| 1504 | Role of the conformational versatility of the neurotrophin N-terminal regions in their recognition by Trk receptors. 2010 , 99, 2273-8 | 7 |
| 1503 | A combined molecular dynamics and rapid kinetics approach to identify conserved three-dimensional communication networks in elongation factor Tu. 2010 , 99, 3735-43 | 13 |
| 1502 | Conformational selection in G-proteins: lessons from Ras and Rho. 2010 , 99, L87-9 | 46 |
| 1501 | Dynamics-Based Discovery of Allosteric Inhibitors: Selection of New Ligands for the C-terminal Domain of Hsp90. 2010 , 6, 2978-89 | 70 |

| | | |
|------|---|-----|
| 1500 | Side-chain conformational changes of transcription factor PhoB upon DNA binding: a population-shift mechanism. 2010 , 132, 12653-9 | 11 |
| 1499 | Conformational selection in the recognition of the snurportin importin beta binding domain by importin beta. 2010 , 49, 5042-7 | 16 |
| 1498 | Why does binding of proteins to DNA or proteins to proteins not necessarily spell function?. 2010 , 5, 265-72 | 25 |
| 1497 | Photoinitiated singlet and triplet electron transfer across a redesigned [myoglobin, cytochrome b5] interface. 2010 , 132, 6165-75 | 19 |
| 1496 | Dynamic active-site protection by the <i>M. tuberculosis</i> protein tyrosine phosphatase PtpB lid domain. 2010 , 132, 4772-80 | 26 |
| 1495 | The HN(COCA)HAHB NMR experiment for the stereospecific assignment of Hbeta-protons in non-native states of proteins. 2010 , 132, 918-9 | 5 |
| 1494 | Computational Study of the DNA-Binding Protein <i>Helicobacter pylori</i> NikR: The Role of Ni(2.). 2010 , 6, 3503-15 | 27 |
| 1493 | An adaptable peptide-based porous material. 2010 , 329, 1053-7 | 313 |
| 1492 | Evolutionary optimization of computationally designed enzymes: Kemp eliminases of the KE07 series. 2010 , 396, 1025-42 | 132 |
| 1491 | Molecular dynamics reveal the essential role of linker motions in the function of cullin-RING E3 ligases. 2010 , 396, 1508-23 | 34 |
| 1490 | Many local motions cooperate to produce the adenylate kinase conformational transition. 2010 , 400, 618-31 | 78 |
| 1489 | Computational mapping of anchoring spots on protein surfaces. 2010 , 402, 259-77 | 59 |
| 1488 | Crystal structures of the multidrug binding repressor <i>Corynebacterium glutamicum</i> CgmR in complex with inducers and with an operator. 2010 , 403, 174-84 | 51 |
| 1487 | A rare example of lock-and-key RNA recognition. 2010 , 404, 553-4 | 2 |
| 1486 | Allostery and population shift in drug discovery. 2010 , 10, 715-22 | 163 |
| 1485 | Reaching biological timescales with all-atom molecular dynamics simulations. 2010 , 10, 745-52 | 98 |
| 1484 | Conformational selection in the molten globule state of the nuclear coactivator binding domain of CBP. 2010 , 107, 12535-40 | 135 |
| 1483 | Protein Dynamics as Reported by NMR. 2010 , 35-75 | 13 |

| | | |
|------|---|-----|
| 1482 | Structural basis for cyclic Py-Im polyamide allosteric inhibition of nuclear receptor binding. 2010 , 132, 14521-9 | 79 |
| 1481 | The dynamics of drug-target interactions: drug-target residence time and its impact on efficacy and safety. 2010 , 5, 305-10 | 147 |
| 1480 | Relation between kinetic conversion rates and ANM mode frequencies. 2010 , | |
| 1479 | Differential binding of p53 and nutlin to MDM2 and MDMX: computational studies. 2010 , 9, 1167-81 | 78 |
| 1478 | Small-molecule inhibitors of IL-2/IL-2R: lessons learned and applied. 2011 , 348, 25-59 | 50 |
| 1477 | Substrate recognition and transport behavior analyses of amino acid antiporter with coarse-grained models. 2010 , 6, 2430-8 | 26 |
| 1476 | Biasing conformational ensembles towards bioactive-like conformers for ligand-based drug design. 2010 , 5, 943-59 | 14 |
| 1475 | Conformational variability of organophosphorus hydrolase upon soman and paraoxon binding. 2011 , 115, 15389-98 | 7 |
| 1474 | On the role of electrostatics in protein-protein interactions. 2011 , 8, 035001 | 104 |
| 1473 | Multi-domain conformational selection underlies pre-mRNA splicing regulation by U2AF. 2011 , 475, 408-11 | 156 |
| 1472 | Targeting multiple conformations leads to small molecule inhibitors of the uPAR α PA protein-protein interaction that block cancer cell invasion. 2011 , 6, 1232-43 | 44 |
| 1471 | Conformational flexibility influences degree of hydration of nucleic acid hybrids. 2011 , 115, 13862-72 | 26 |
| 1470 | Millisecond dynamics in glutaredoxin during catalytic turnover is dependent on substrate binding and absent in the resting states. 2011 , 133, 3034-42 | 16 |
| 1469 | Three clusters of conformational states in p450cam reveal a multistep pathway for closing of the substrate access channel. 2011 , 50, 693-703 | 46 |
| 1468 | Exploring weak, transient protein-protein interactions in crowded in vivo environments by in-cell nuclear magnetic resonance spectroscopy. 2011 , 50, 9225-36 | 125 |
| 1467 | Determination of Conformational Equilibria in Proteins Using Residual Dipolar Couplings. 2011 , 7, 4189-4195 | 33 |
| 1466 | Free-energy landscapes of protein domain movements upon ligand binding. 2011 , 115, 7629-36 | 26 |
| 1465 | Induced fit or conformational selection? The role of the semi-closed state in the maltose binding protein. 2011 , 50, 10530-9 | 76 |

| | | |
|------|---|---------|
| 1464 | Self-assembled enzymatic monolayer directly bound to a gold surface: activity and molecular recognition force spectroscopy studies. 2011 , 133, 13284-7 | 7 |
| 1463 | Stochastic ensembles, conformationally adaptive teamwork, and enzymatic detoxification. 2011 , 50, 3866-72 | 7 |
| 1462 | Free energy simulations of a GTPase: GTP and GDP binding to archaeal initiation factor 2. 2011 , 115, 6749-63 | 26 |
| 1461 | On-the-Fly Identification of Conformational Substates from Molecular Dynamics Simulations. 2011 , 7, 778-89 | 12 |
| 1460 | Identification of nucleic acid binding residues in the FCS domain of the polycomb group protein polyhomeotic. 2011 , 50, 4998-5007 | 7 |
| 1459 | The expanding view of protein-protein interactions: complexes involving intrinsically disordered proteins. 2011 , 8, 035003 | 48 |
| 1458 | Toward a predictive understanding of slow methyl group dynamics in proteins. 2011 , 101, 910-5 | 35 |
| 1457 | Hybrid schemes based on quantum mechanics/molecular mechanics simulations goals to success, problems, and perspectives. 2011 , 85, 81-142 | 18 |
| 1456 | Structural studies on the interaction of saccharides and glycomimetics with galectin-1: A 3D perspective using a combined molecular modeling and NMR approach. 2011 , 84, 49-64 | 8 |
| 1455 | Protein-protein interactions: principles, techniques, and their potential role in new drug development. 2011 , 28, 929-38 | 36 |
| 1454 | Computational ligand-based rational design: Role of conformational sampling and force fields in model development. 2011 , 2, 356-370 | 58 |
| 1453 | Mapping unstructured regions and synergistic folding in intrinsically disordered proteins with amide H/D exchange mass spectrometry. 2011 , 50, 8722-32 | 70 |
| 1452 | p38 β activation triggers dynamical changes in allosteric docking sites. 2011 , 50, 1384-95 | 9 |
| 1451 | Markov state model reveals folding and functional dynamics in ultra-long MD trajectories. 2011 , 133, 18413-9 | 129 |
| 1450 | Conformational analysis of a nitroxide side chain in an α -helix with density functional theory. 2011 , 115, 397-405 | 31 |
| 1449 | Transmembrane communication: general principles and lessons from the structure and function of the M2 proton channel, K ⁺ channels, and integrin receptors. 2011 , 80, 211-37 | 32 |
| 1448 | The moderately efficient enzyme: evolutionary and physicochemical trends shaping enzyme parameters. 2011 , 50, 4402-10 | 574 |
| 1447 | Twisted Schiff base intermediates and substrate locale revise transaldolase mechanism. <i>Nature Chemical Biology</i> , 2011 , 7, 678-84 | 11.7 51 |

| | | |
|------|---|----------|
| 1446 | Promiscuity, stability and cold adaptation of a newly isolated acylaminoacyl peptidase. 2011 , 93, 1543-54 | 19 |
| 1445 | Conformational adaptation in drug-target interactions and residence time. 2011 , 3, 1491-501 | 149 |
| 1444 | Computational medicinal chemistry in fragment-based drug discovery: what, how and when. 2011 , 3, 95-134 | 16 |
| 1443 | Discovery of selective bioactive small molecules by targeting an RNA dynamic ensemble. <i>Nature Chemical Biology</i> , 2011 , 7, 553-9 | 11.7 169 |
| 1442 | The dynamic nature of RNA as key to understanding riboswitch mechanisms. 2011 , 44, 1339-48 | 146 |
| 1441 | Structural instability tuning as a regulatory mechanism in protein-protein interactions. 2011 , 44, 734-44 | 28 |
| 1440 | Critical scaffolding regions of the tumor suppressor Axin1 are natively unfolded. 2011 , 405, 773-86 | 46 |
| 1439 | Concerted dynamics link allosteric sites in the PBX homeodomain. 2011 , 405, 819-30 | 23 |
| 1438 | Classification and annotation of the relationship between protein structural change and ligand binding. 2011 , 408, 568-84 | 39 |
| 1437 | Temporal development of protein structure during S100A11 folding and dimerization probed by oxidative labeling and mass spectrometry. 2011 , 409, 669-79 | 19 |
| 1436 | Structure of H/ACA RNP protein Nhp2p reveals cis/trans isomerization of a conserved proline at the RNA and Nop10 binding interface. 2011 , 411, 927-42 | 26 |
| 1435 | Enzyme inhibition by allosteric capture of an inactive conformation. 2011 , 411, 999-1016 | 30 |
| 1434 | cAMP-dependent protein kinase A selects the excited state of the membrane substrate phospholamban. 2011 , 412, 155-64 | 54 |
| 1433 | A hydrogen bond regulates slow motions in ubiquitin by modulating a β -turn flip. 2011 , 411, 1037-48 | 25 |
| 1432 | Excited-state control of protein activity. 2011 , 412, 153-4 | 2 |
| 1431 | Disparate degrees of hypervariable loop flexibility control T-cell receptor cross-reactivity, specificity, and binding mechanism. 2011 , 414, 385-400 | 56 |
| 1430 | Direct visualization reveals dynamics of a transient intermediate during protein assembly. 2011 , 108, 6450-5 | 28 |
| 1429 | Characterizing RNA dynamics at atomic resolution using solution-state NMR spectroscopy. 2011 , 8, 919-31 | 116 |

| | | |
|------|--|-----|
| 1428 | 50th anniversary of the word "allosteric". 2011 , 20, 1119-24 | 60 |
| 1427 | The role of conformational ensembles in ligand recognition in G-protein coupled receptors. 2011 , 133, 13197-204 | 62 |
| 1426 | Hydrogen exchange mass spectrometry of bacteriorhodopsin reveals light-induced changes in the structural dynamics of a biomolecular machine. 2011 , 133, 20237-44 | 16 |
| 1425 | Side-chain conformational changes upon Protein-Protein Association. 2011 , 408, 356-65 | 29 |
| 1424 | Dynamic diagnosis of familial prion diseases supports the β - β loop as a universal interference target. 2011 , 6, e19093 | 51 |
| 1423 | Predicting inactive conformations of protein kinases using active structures: conformational selection of type-II inhibitors. 2011 , 6, e22644 | 20 |
| 1422 | Can enzyme engineering benefit from the modulation of protein motions? Lessons learned from NMR relaxation dispersion experiments. 2011 , 18, 336-43 | 13 |
| 1421 | Gene-specific transcription activation via long-range allosteric shape-shifting. 2011 , 439, 15-25 | 32 |
| 1420 | Conformational selection or induced fit? 50 years of debate resolved. 2011 , 3, 19 | 183 |
| 1419 | Substrate-induced conformational changes in Plasmodium falciparum guanosine monophosphate synthetase. 2011 , 278, 3756-68 | 6 |
| 1418 | Crystal structure of Onconase at 1.1 Å resolution—insights into substrate binding and collective motion. 2011 , 278, 4136-49 | 13 |
| 1417 | Competing allosteric mechanisms modulate substrate binding in a dimeric enzyme. 2011 , 18, 288-94 | 67 |
| 1416 | Transient Hoogsteen base pairs in canonical duplex DNA. 2011 , 470, 498-502 | 233 |
| 1415 | Beyond the random coil: stochastic conformational switching in intrinsically disordered proteins. 2011 , 19, 566-76 | 87 |
| 1414 | A systematic study of the energetics involved in structural changes upon association and connectivity in protein interaction networks. 2011 , 19, 881-9 | 38 |
| 1413 | Relative solvent accessible surface area predicts protein conformational changes upon binding. 2011 , 19, 859-67 | 120 |
| 1412 | Interconversion of two GDP-bound conformations and their selection in an Arf-family small G protein. 2011 , 19, 988-98 | 8 |
| 1411 | Dynamic allostery: linkers are not merely flexible. 2011 , 19, 907-17 | 171 |

| | | |
|------|---|-----|
| 1410 | Protein dynamics and allostery: an NMR view. 2011 , 21, 62-7 | 190 |
| 1409 | Protein folding mechanisms studied by pulsed oxidative labeling and mass spectrometry. 2011 , 21, 634-40 | 18 |
| 1408 | Allostery in pharmacology: thermodynamics, evolution and design. 2011 , 106, 463-73 | 19 |
| 1407 | Structural analysis of heme proteins: implications for design and prediction. 2011 , 11, 13 | 88 |
| 1406 | Hemoglobin allostery: variations on the theme. 2011 , 1807, 1262-72 | 30 |
| 1405 | The importin β binding domain as a master regulator of nucleocytoplasmic transport. 2011 , 1813, 1578-92 | 110 |
| 1404 | Hydrogen exchange mass spectrometry for studying protein structure and dynamics. 2011 , 40, 1224-34 | 555 |
| 1403 | Efficient incorporation of protein flexibility and dynamics into molecular docking simulations. 2011 , 50, 6157-69 | 78 |
| 1402 | On the role of flexibility in protein-ligand interactions: the example of p53 tetramerization domain. 2011 , 6, 1463-9 | 17 |
| 1401 | Flexible organometallic cages: efficient formation by C-H activation-directed multicomponent assembly, isomerization, and host-guest properties. 2011 , 6, 1348-52 | 22 |
| 1400 | Protein-ligand docking. 2011 , 16, 2289-306 | 13 |
| 1399 | Receptor flexibility in small-molecule docking calculations. 2011 , 1, 298-314 | 38 |
| 1398 | Recognition of S-adenosylmethionine by riboswitches. 2011 , 2, 299-311 | 45 |
| 1397 | Understanding biomolecular motion, recognition, and allostery by use of conformational ensembles. 2011 , 40, 1339-55 | 78 |
| 1396 | Topology-based modeling of intrinsically disordered proteins: balancing intrinsic folding and intermolecular interactions. 2011 , 79, 1251-66 | 60 |
| 1395 | Efficient mapping of ligand migration channel networks in dynamic proteins. 2011 , 79, 2475-90 | 18 |
| 1394 | NMR structure and dynamics of recombinant wild type and mutated jerdostatin, a selective inhibitor of integrin $\alpha 1$. 2011 , 79, 2530-42 | 10 |
| 1393 | The structure of human ubiquitin in 2-methyl-2,4-pentanediol: a new conformational switch. 2011 , 20, 630-9 | 37 |

| | | |
|------|--|-----|
| 1392 | NMR reveals novel mechanisms of protein activity regulation. 2011 , 20, 773-82 | 41 |
| 1391 | Allostery turns 50: is the vintage yet attractive?. 2011 , 20, 1097-9 | 7 |
| 1390 | Pre-existing soft modes of motion uniquely defined by native contact topology facilitate ligand binding to proteins. 2011 , 20, 1645-58 | 74 |
| 1389 | Azurin modulates the association of Mdm2 with p53: SPR evidence from interaction of the full-length proteins. 2011 , 24, 707-14 | 25 |
| 1388 | The utility of hydrogen/deuterium exchange mass spectrometry in biopharmaceutical comparability studies. 2011 , 100, 2071-86 | 274 |
| 1387 | Role of protein flexibility in the discovery of new drugs. 2011 , 72, 26-35 | 12 |
| 1386 | A chirality-based metrics for free-energy calculations in biomolecular systems. 2011 , 32, 2627-37 | 20 |
| 1385 | X-ray solution scattering studies of the structural diversity intrinsic to protein ensembles. 2011 , 95, 531-42 | 25 |
| 1384 | From "fluctuation fit" to "conformational selection": evolution, rediscovery, and integration of a concept. 2011 , 33, 30-4 | 27 |
| 1383 | An introduction to NMR-based approaches for measuring protein dynamics. 2011 , 1814, 942-68 | 327 |
| 1382 | Structure determination and dynamics of protein-RNA complexes by NMR spectroscopy. 2011 , 58, 1-61 | 74 |
| 1381 | Modeling loop entropy. 2011 , 487, 99-132 | 16 |
| 1380 | Molecular mechanism of selective recruitment of Syk kinases by the membrane antigen-receptor complex. 2011 , 286, 25872-81 | 12 |
| 1379 | Therapeutic targeting of HCV internal ribosomal entry site RNA. 2011 , 21, 117-28 | 31 |
| 1378 | PPAR δ population shift produces disease-related changes in molecular networks associated with metabolic syndrome. 2011 , 2, e192 | 4 |
| 1377 | Perturbation analyses of intermolecular interactions. 2011 , 84, 026704 | 3 |
| 1376 | Evidence for an allosteric mechanism of substrate release from membrane-transporter accessory binding proteins. 2011 , 108, E1285-92 | 21 |
| 1375 | Molecular sensing by the aptamer domain of the FMN riboswitch: a general model for ligand binding by conformational selection. 2011 , 39, 8586-98 | 73 |

| | | | |
|------|---|------|-----|
| 1374 | Role of dynamics in the autoinhibition and activation of the exchange protein directly activated by cyclic AMP (EPAC). 2011 , 286, 42655-42669 | | 34 |
| 1373 | Dynamic fluctuations lubricate the circadian clock. 2011 , 108, 14377-8 | | |
| 1372 | Mapping allostery through the covariance analysis of NMR chemical shifts. 2011 , 108, 6133-8 | | 173 |
| 1371 | Small angle neutron scattering reveals pH-dependent conformational changes in <i>Trichoderma reesei</i> cellobiohydrolase I: implications for enzymatic activity. 2011 , 286, 32801-9 | | 28 |
| 1370 | Molecular evolution of protein conformational changes revealed by a network of evolutionarily coupled residues. 2011 , 28, 2675-85 | | 37 |
| 1369 | Thermodynamic and kinetic basis for recognition and repair of 8-oxoguanine in DNA by human 8-oxoguanine-DNA glycosylase. 2011 , 39, 4836-50 | | 14 |
| 1368 | Structure and catalysis of acylaminoacyl peptidase: closed and open subunits of a dimer oligopeptidase. 2011 , 286, 1987-98 | | 35 |
| 1367 | A unified view of cystic fibrosis transmembrane conductance regulator (CFTR) gating: combining the allostery of a ligand-gated channel with the enzymatic activity of an ATP-binding cassette (ABC) transporter. 2011 , 286, 12813-9 | | 36 |
| 1366 | Distinct allostery induced in the cyclic GMP-binding, cyclic GMP-specific phosphodiesterase (PDE5) by cyclic GMP, sildenafil, and metal ions. 2011 , 286, 8545-8554 | | 18 |
| 1365 | Tyrosine latching of a regulatory gate affords allosteric control of aromatic amino acid biosynthesis. 2011 , 286, 10216-24 | | 43 |
| 1364 | Broad disorder and the allosteric mechanism of myosin II regulation by phosphorylation. 2011 , 108, 8218-23 | | 15 |
| 1363 | Dynamically committed, uncommitted, and quenched states encoded in protein kinase A revealed by NMR spectroscopy. 2011 , 108, 6969-74 | | 117 |
| 1362 | Protein regulation: the statistical theory of allostery. <i>Nature Chemical Biology</i> , 2011 , 7, 411-2 | 11.7 | 17 |
| 1361 | Huntington's disease: flipping a switch on huntingtin. <i>Nature Chemical Biology</i> , 2011 , 7, 412-4 | 11.7 | 15 |
| 1360 | Conformational capture of the SAM-II riboswitch. <i>Nature Chemical Biology</i> , 2011 , 7, 393-400 | 11.7 | 132 |
| 1359 | RNA folding: a tale of two riboswitches. <i>Nature Chemical Biology</i> , 2011 , 7, 342-3 | 11.7 | 5 |
| 1358 | Conformational sampling and nucleotide-dependent transitions of the GroEL subunit probed by unbiased molecular dynamics simulations. 2011 , 7, e1002004 | | 24 |
| 1357 | Cyclic AMP analog blocks kinase activation by stabilizing inactive conformation: conformational selection highlights a new concept in allosteric inhibitor design. 2011 , 10, M110.004390 | | 58 |

| | | |
|------|---|----|
| 1356 | Trapping conformational states along ligand-binding dynamics of peptide deformylase: the impact of induced fit on enzyme catalysis. 2011 , 9, e1001066 | 26 |
| 1355 | In silico elucidation of the recognition dynamics of ubiquitin. 2011 , 7, e1002035 | 40 |
| 1354 | Anchoring intrinsically disordered proteins to multiple targets: lessons from N-terminus of the p53 protein. 2011 , 12, 1410-30 | 19 |
| 1353 | Accessing a hidden conformation of the maltose binding protein using accelerated molecular dynamics. 2011 , 7, e1002034 | 92 |
| 1352 | Interconversion of functional motions between mesophilic and thermophilic adenylate kinases. 2011 , 7, e1002103 | 18 |
| 1351 | Molecular motions as a drug target: mechanistic simulations of anthrax toxin edema factor function led to the discovery of novel allosteric inhibitors. 2012 , 4, 580-604 | 15 |
| 1350 | Corresponding functional dynamics across the Hsp90 Chaperone family: insights from a multiscale analysis of MD simulations. 2012 , 8, e1002433 | 82 |
| 1349 | A preformed binding interface in the unbound ensemble of an intrinsically disordered protein: evidence from molecular simulations. 2012 , 8, e1002605 | 98 |
| 1348 | The role of flexibility and conformational selection in the binding promiscuity of PDZ domains. 2012 , 8, e1002749 | 56 |
| 1347 | What is the role of motif D in the nucleotide incorporation catalyzed by the RNA-dependent RNA polymerase from poliovirus?. 2012 , 8, e1002851 | 45 |
| 1346 | Macromolecule-assisted de novo protein folding. 2012 , 13, 10368-86 | 7 |
| 1345 | Mechanism of drug efficacy within the EGF receptor revealed by microsecond molecular dynamics simulation. 2012 , 11, 2394-400 | 11 |
| 1344 | Revealing conformational substates of lipidated N-Ras protein by pressure modulation. 2012 , 109, 460-5 | 93 |
| 1343 | Flexibility and binding affinity in protein-ligand, protein-protein and multi-component protein interactions: limitations of current computational approaches. 2012 , 9, 20-33 | 64 |
| 1342 | Composite low affinity interactions dictate recognition of the cyclin-dependent kinase inhibitor Sic1 by the SCFCdc4 ubiquitin ligase. 2012 , 109, 3287-92 | 51 |
| 1341 | Multiple conformations of SAM-II riboswitch detected with SAXS and NMR spectroscopy. 2012 , 40, 3117-30 | 61 |
| 1340 | The Different Ways through Which Specificity Works in Orthosteric and Allosteric Drugs. 2012 , 18, 1311-1316 | 4 |
| 1339 | Monitoring shifts in the conformation equilibrium of the membrane protein cytochrome P450 reductase (POR) in nanodiscs. 2012 , 287, 34596-603 | 54 |

| | | |
|------|--|-----|
| 1338 | Catalytic control of enzymatic fluorine specificity. 2012 , 109, 19667-72 | 26 |
| 1337 | Interdomain dynamics and coactivation of the mRNA decapping enzyme Dcp2 are mediated by a gatekeeper tryptophan. 2012 , 109, 2872-7 | 25 |
| 1336 | A flexible multidomain structure drives the function of the urokinase-type plasminogen activator receptor (uPAR). 2012 , 287, 34304-15 | 40 |
| 1335 | Biophysical and computational fragment-based approaches to targeting protein-protein interactions: applications in structure-guided drug discovery. 2012 , 45, 383-426 | 74 |
| 1334 | PSCDB: a database for protein structural change upon ligand binding. 2012 , 40, D554-8 | 38 |
| 1333 | Resolving two-dimensional kinetics of the integrin β ₃ -fibrinogen interactions using binding-unbinding correlation spectroscopy. 2012 , 287, 35275-35285 | 29 |
| 1332 | Disorder-function relationships for the cell cycle regulatory proteins p21 and p27. 2012 , 393, 259-74 | 60 |
| 1331 | Nucleosome dynamics: HMGB1 relaxes canonical nucleosome structure to facilitate estrogen receptor binding. 2012 , 40, 10161-71 | 30 |
| 1330 | Double electron-electron resonance shows cytochrome P450cam undergoes a conformational change in solution upon binding substrate. 2012 , 109, 12888-93 | 45 |
| 1329 | Structure and mechanism of purine-binding riboswitches. 2012 , 45, 345-81 | 57 |
| 1328 | Structural activation of the transcriptional repressor EthR from Mycobacterium tuberculosis by single amino acid change mimicking natural and synthetic ligands. 2012 , 40, 3018-30 | 22 |
| 1327 | Exploiting substrate recognition for selective inhibition of protein kinases. 2012 , 18, 2914-20 | 10 |
| 1326 | The different ways through which specificity works in orthosteric and allosteric drugs. 2012 , 18, 1311-6 | 74 |
| 1325 | Understanding pre-structured motifs (PreSMos) in intrinsically unfolded proteins. 2012 , 13, 34-54 | 68 |
| 1324 | An inhibitory peptide derived from the β subunit of the epithelial sodium channel (ENaC) shows a helical conformation. 2012 , 29, 761-74 | 8 |
| 1323 | cAMP-dependent allostery and dynamics in Epac: an NMR view. 2012 , 40, 219-23 | 15 |
| 1322 | Kinetic characterization of the critical step in HIV-1 protease maturation. 2012 , 109, 20449-54 | 85 |
| 1321 | Biased agonism of protease-activated receptor 1 by activated protein C caused by noncanonical cleavage at Arg46. 2012 , 120, 5237-46 | 157 |

| | | |
|------|---|-----|
| 1320 | Thumbs down for HIV: domain level rearrangements do occur in the NNRTI-bound HIV-1 reverse transcriptase. 2012 , 134, 12885-8 | 20 |
| 1319 | Local Fluctuations and Conformational Transitions in Proteins. 2012 , 8, 4775-85 | 31 |
| 1318 | Immobilization of proteins for single-molecule fluorescence resonance energy transfer measurements of conformation and dynamics. 2012 , 896, 3-20 | 21 |
| 1317 | Ubiquitin dynamics in complexes reveal molecular recognition mechanisms beyond induced fit and conformational selection. 2012 , 8, e1002704 | 50 |
| 1316 | Ubiquitin chain conformation regulates recognition and activity of interacting proteins. 2012 , 492, 266-70 | 132 |
| 1315 | Real-Time Monitoring of Protein Conformational Dynamics in Solution Using Kinetic Capillary Electrophoresis. 2012 , 124, 12632-12636 | 1 |
| 1314 | Real-time monitoring of protein conformational dynamics in solution using kinetic capillary electrophoresis. 2012 , 51, 12464-8 | 27 |
| 1313 | The binding mechanism, multiple binding modes, and allosteric regulation of <i>Staphylococcus aureus</i> Sortase A probed by molecular dynamics simulations. 2012 , 21, 1858-71 | 28 |
| 1312 | Combining conformational sampling and selection to identify the binding mode of zinc-bound amyloid peptides with bifunctional molecules. 2012 , 26, 963-76 | 11 |
| 1311 | NMR line shapes and multi-state binding equilibria. 2012 , 53, 257-70 | 63 |
| 1310 | Structural and Entropic Allosteric Signal Transduction Strength via Correlated Motions. 2012 , 3, 1722-6 | 17 |
| 1309 | Attributes of short linear motifs. 2012 , 8, 268-81 | 362 |
| 1308 | Assembly of the five-way junction in the ribosomal small subunit using hybrid MD-G ⁻ simulations. 2012 , 116, 6819-31 | 20 |
| 1307 | GTP binding leads to narrowing of the conformer population while preserving the structure of the RNA aptamer: a site-specific time-resolved fluorescence dynamics study. 2012 , 51, 9260-9 | 6 |
| 1306 | FlexE: Using elastic network models to compare models of protein structure. 2012 , 8, 3985-3991 | 19 |
| 1305 | An ensemble view of thrombin allostery. 2012 , 393, 889-98 | 47 |
| 1304 | Ultrafast site-specific fluorescence quenching of 2-aminopurine in a DNA hairpin studied by femtosecond down-conversion. 2012 , 116, 2819-25 | 18 |
| 1303 | Local folding and misfolding in the PBX homeodomain from a three-state analysis of CPMG relaxation dispersion NMR data. 2012 , 116, 10317-29 | 13 |

| | | |
|------|--|-----|
| 1302 | Subtle Monte Carlo Updates in Dense Molecular Systems. 2012 , 8, 695-702 | 21 |
| 1301 | Pseudoknot preorganization of the preQ1 class I riboswitch. 2012 , 134, 11928-31 | 48 |
| 1300 | NMR structure and dynamics of the C-terminal domain from human Rev1 and its complex with Rev1 interacting region of DNA polymerase β 2012 , 51, 5506-20 | 60 |
| 1299 | From Molecular Phylogenetics to Quantum Chemistry: Discovering Enzyme Design Principles through Computation. 2012 , 2, e201209018 | 2 |
| 1298 | Structural characterisation, stability and antibody recognition of chimeric NHBA-GNA1030: an investigational vaccine component against <i>Neisseria meningitidis</i> . 2012 , 30, 1330-42 | 9 |
| 1297 | Paths of long-range communication in the E2 enzymes of family 3: a molecular dynamics investigation. 2012 , 14, 12515-25 | 32 |
| 1296 | Single enzyme studies reveal the existence of discrete functional states for monomeric enzymes and how they are "selected" upon allosteric regulation. 2012 , 134, 9296-302 | 32 |
| 1295 | Functional complexity and regulation through RNA dynamics. 2012 , 482, 322-30 | 229 |
| 1294 | Exploring polymorphisms in B-DNA helical conformations. 2012 , 40, 10668-78 | 68 |
| 1293 | Small heat-shock proteins: paramedics of the cell. 2013 , 328, 69-98 | 95 |
| 1292 | Towards the physical basis of how intrinsic disorder mediates protein function. 2012 , 524, 123-31 | 67 |
| 1291 | Selective molecular recognition in amyloid growth and transmission and cross-species barriers. 2012 , 421, 172-84 | 66 |
| 1290 | Conformational dynamics of a membrane transport protein probed by H/D exchange and covalent labeling: the glycerol facilitator. 2012 , 416, 400-13 | 42 |
| 1289 | Multistate allostery in response regulators: phosphorylation and mutagenesis activate RegA via alternate modes. 2012 , 417, 468-87 | 13 |
| 1288 | Mapping the transition state for DNA bending by IHF. 2012 , 418, 300-15 | 22 |
| 1287 | Catalytic versatility and backups in enzyme active sites: the case of serum paraoxonase 1. 2012 , 418, 181-96 | 122 |
| 1286 | Electrostatically accelerated coupled binding and folding of intrinsically disordered proteins. 2012 , 422, 674-684 | 60 |
| 1285 | Antigen-antibody interface properties: composition, residue interactions, and features of 53 non-redundant structures. 2012 , 1824, 520-32 | 96 |

| | | |
|------|---|-----|
| 1284 | Metal binding sites in amyloid oligomers: Complexes and mechanisms. 2012 , 256, 2245-2252 | 85 |
| 1283 | Time scales of slow motions in ubiquitin explored by heteronuclear double resonance. 2012 , 134, 2481-4 | 28 |
| 1282 | Conformer Selection and Intensified Dynamics During Catalytic Turnover in Chymotrypsin. 2012 , 124, 9804-9807 | 5 |
| 1281 | Conformer selection and intensified dynamics during catalytic turnover in chymotrypsin. 2012 , 51, 9666-9 | 23 |
| 1280 | Modeling loop backbone flexibility in receptor-ligand docking simulations. 2012 , 33, 2504-15 | 14 |
| 1279 | Nucleotide recognition by the initiation factor α IF5B: free energy simulations of a neoclassical GTPase. 2012 , 80, 2742-57 | 5 |
| 1278 | Relationships between kinetic constants and the amino acid composition of enzymes from the yeast <i>Saccharomyces cerevisiae</i> glycolysis pathway. 2012 , 2012, 11 | 4 |
| 1277 | Hot spots and transient pockets: predicting the determinants of small-molecule binding to a protein-protein interface. 2012 , 52, 120-33 | 106 |
| 1276 | Interaction Kinetic Data Generated by Surface Plasmon Resonance Biosensors and the Use of Kinetic Rate Constants in Lead Generation and Optimization. 2012 , 45-70 | |
| 1275 | NMR Methods for the Determination of Protein-Ligand Interactions. 2012 , 71-98 | |
| 1274 | Modeling of the role of conformational dynamics in kinetics of the antigen-antibody interaction in heterogeneous phase. 2012 , 116, 5679-88 | 5 |
| 1273 | Modulation of a ligand's energy landscape and kinetics by the chemical environment. 2012 , 116, 13597-607 | 1 |
| 1272 | Insilico study of the A(2A)R-D (2)R kinetics and interfacial contact surface for heteromerization. 2012 , 43, 1451-64 | 16 |
| 1271 | Fuzziness: linking regulation to protein dynamics. 2012 , 8, 168-77 | 128 |
| 1270 | Structural and dynamic control of T-cell receptor specificity, cross-reactivity, and binding mechanism. 2012 , 250, 10-31 | 58 |
| 1269 | Ligand-receptor interaction platforms and their applications for drug discovery. 2012 , 7, 969-88 | 81 |
| 1268 | Electrostatics of hydrogen exchange for analyzing protein flexibility. 2012 , 831, 369-405 | 2 |
| 1267 | Distinct states of methionyl-tRNA synthetase indicate inhibitor binding by conformational selection. 2012 , 20, 1681-91 | 54 |

| | | |
|------|---|----|
| 1266 | Probing the diverse landscape of protein flexibility and binding. 2012 , 22, 643-50 | 87 |
| 1265 | Chapter 4: Intrinsic Motions of DNA Polymerases Underlie Their Remarkable Specificity and Selectivity and Suggest a Hybrid Substrate Binding Mechanism. 81-110 | 2 |
| 1264 | The different flexibility of c-Src and c-Abl kinases regulates the accessibility of a druggable inactive conformation. 2012 , 134, 2496-9 | 84 |
| 1263 | Dynamic optimization of signal transduction via intrinsic disorder. 2012 , 8, 194-7 | 3 |
| 1262 | Synergistic folding of two intrinsically disordered proteins: searching for conformational selection. 2012 , 8, 198-209 | 47 |
| 1261 | Mechanistic insights into the retaining glucosyl-3-phosphoglycerate synthase from mycobacteria. 2012 , 287, 24649-61 | 16 |
| 1260 | Protein NMR Techniques. 2012 , | 5 |
| 1259 | Bioinspiration. 2012 , | 15 |
| 1258 | Manipulating protein conformations by single-molecule AFM-FRET nanoscopy. 2012 , 6, 1221-9 | 59 |
| 1257 | Mapping molecular flexibility of proteins with site-directed spin labeling: a case study of myoglobin. 2012 , 51, 6568-83 | 48 |
| 1256 | In silico strategies toward enzyme function and dynamics. 2012 , 87, 249-92 | 2 |
| 1255 | Allostery and binding cooperativity of the catalytic subunit of protein kinase A by NMR spectroscopy and molecular dynamics simulations. 2012 , 87, 363-89 | 33 |
| 1254 | Using a combination of computational and experimental techniques to understand the molecular basis for protein allostery. 2012 , 87, 391-413 | 8 |
| 1253 | Kinetic rate constant prediction supports the conformational selection mechanism of protein binding. 2012 , 8, e1002351 | 43 |
| 1252 | Stapled BH3 peptides against MCL-1: mechanism and design using atomistic simulations. 2012 , 7, e43985 | 35 |
| 1251 | Conformational selection underlies recognition of a molybdoenzyme by its dedicated chaperone. 2012 , 7, e49523 | 18 |
| 1250 | Protein Folding, Binding and Energy Landscape: A Synthesis. 2012 , | 10 |
| 1249 | Learning generative models of molecular dynamics. 2012 , 13 Suppl 1, S5 | 5 |

| | | |
|------|--|-----|
| 1248 | Protein dynamics at Eph receptor-ligand interfaces as revealed by crystallography, NMR and MD simulations. 2012 , 5, 2 | 20 |
| 1247 | Minimal ensembles of side chain conformers for modeling protein-protein interactions. 2012 , 80, 591-601 | 25 |
| 1246 | Riboswitch structure in the ligand-free state. 2012 , 3, 369-84 | 51 |
| 1245 | Conformational selection through electrostatics: Free energy simulations of GTP and GDP binding to archaeal initiation factor 2. 2012 , 80, 1264-82 | 8 |
| 1244 | Conformational selection and induced changes along the catalytic cycle of Escherichia coli dihydrofolate reductase. 2012 , 80, 2369-83 | 18 |
| 1243 | Metabolite recognition principles and molecular mechanisms underlying riboswitch function. 2012 , 41, 343-70 | 124 |
| 1242 | Bioinformatics and variability in drug response: a protein structural perspective. 2012 , 9, 1409-37 | 57 |
| 1241 | Photoactivated structural dynamics of fluorescent proteins. 2012 , 40, 531-8 | 19 |
| 1240 | Protein function and allostery: a dynamic relationship. 2012 , 1260, 81-6 | 33 |
| 1239 | Protein activity regulation by conformational entropy. 2012 , 488, 236-40 | 374 |
| 1238 | Interactions via intrinsically disordered regions: what kind of motifs?. 2012 , 64, 513-20 | 62 |
| 1237 | How do dynamic cellular signals travel long distances?. 2012 , 8, 22-6 | 28 |
| 1236 | Quantitative analysis of multisite protein-ligand interactions by NMR: binding of intrinsically disordered p53 transactivation subdomains with the TAZ2 domain of CBP. 2012 , 134, 3792-803 | 104 |
| 1235 | Conformational Selection versus Induced Fit in Kinases: The Case of PI3K- α . 2012 , 124, 666-670 | 3 |
| 1234 | Allostery and the Monod-Wyman-Changeux model after 50 years. 2012 , 41, 103-33 | 265 |
| 1233 | Studying "invisible" excited protein states in slow exchange with a major state conformation. 2012 , 134, 8148-61 | 321 |
| 1232 | Conformational selection and folding-upon-binding of intrinsically disordered protein CP12 regulate photosynthetic enzymes assembly. 2012 , 287, 21372-83 | 48 |
| 1231 | Large-scale motions in the adenylate kinase solution ensemble: coarse-grained simulations and comparison with solution X-ray scattering. 2012 , 396, 84-91 | 26 |

| | | |
|------|---|-----|
| 1230 | Can biochemistry drive drug discovery beyond simple potency measurements?. 2012 , 17, 388-95 | 5 |
| 1229 | Motif switches: decision-making in cell regulation. 2012 , 22, 378-85 | 107 |
| 1228 | Dynamics in multi-domain protein recognition of RNA. 2012 , 22, 287-96 | 82 |
| 1227 | Heteronuclear Adiabatic Relaxation Dispersion (HARD) for quantitative analysis of conformational dynamics in proteins. 2012 , 219, 75-82 | 8 |
| 1226 | Recognition pliability is coupled to structural heterogeneity: a calmodulin intrinsically disordered binding region complex. 2012 , 20, 522-33 | 47 |
| 1225 | Structural and functional analysis of HtrA1 and its subdomains. 2012 , 20, 1040-50 | 65 |
| 1224 | Mutual remodeling and conformation grid: a mediator code?. 2012 , 20, 755-7 | 3 |
| 1223 | Promiscuity in protein-RNA interactions: conformational ensembles facilitate molecular recognition in the spliceosome: conformational diversity in U2AF ₁ facilitates binding to diverse RNA sequences. 2012 , 34, 174-80 | 12 |
| 1222 | Conformational selection versus induced fit in kinases: the case of PI3K- β . 2012 , 51, 642-6 | 15 |
| 1221 | Thermodynamics of allostery paves a way to allosteric drugs. 2013 , 1834, 830-5 | 34 |
| 1220 | Macromolecular symmetric assembly prediction using swarm intelligence dynamic modeling. 2013 , 21, 1097-1106 | 27 |
| 1219 | Disruption of intrinsic motions as a mechanism for enzyme inhibition. 2013 , 105, 494-501 | 2 |
| 1218 | Solution NMR refinement of a metal ion bound protein using metal ion inclusive restrained molecular dynamics methods. 2013 , 56, 125-37 | 19 |
| 1217 | DNA unwinding heterogeneity by RecBCD results from static molecules able to equilibrate. 2013 , 500, 482-5 | 62 |
| 1216 | Mechanisms of anticoagulant and cytoprotective actions of the protein C pathway. 2013 , 11 Suppl 1, 242-53 | 110 |
| 1215 | Cooperative unfolding of compact conformations of the intrinsically disordered protein osteopontin. 2013 , 52, 5167-75 | 61 |
| 1214 | Redox-linked domain movements in the catalytic cycle of cytochrome p450 reductase. 2013 , 21, 1581-9 | 57 |
| 1213 | A single mutation in the core domain of the lac repressor reduces leakiness. 2013 , 12, 67 | 21 |

| | | |
|------|---|-----|
| 1212 | Molecular recognition with boronic acids-applications in chemical biology. 2013 , 6, 161-74 | 65 |
| 1211 | Assembly of hemoglobin from denatured monomeric subunits: heme ligation effects and off-pathway intermediates studied by electrospray mass spectrometry. 2013 , 52, 1717-24 | 7 |
| 1210 | How conformational changes can affect catalysis, inhibition and drug resistance of enzymes with induced-fit binding mechanism such as the HIV-1 protease. 2013 , 1834, 867-73 | 11 |
| 1209 | The time correlation function perspective of NMR relaxation in proteins. 2013 , 139, 084107 | 4 |
| 1208 | Conformational entropy of intrinsically disordered protein. 2013 , 117, 5503-9 | 25 |
| 1207 | Conformational selection is a dominant mechanism of ligand binding. 2013 , 52, 5723-9 | 96 |
| 1206 | Computational design of ligand-binding proteins with high affinity and selectivity. 2013 , 501, 212-216 | 299 |
| 1205 | Regulation of the transient receptor potential channel TRPA1 by its N-terminal ankyrin repeat domain. 2013 , 19, 4689-700 | 25 |
| 1204 | Conformational plasticity of an enzyme during catalysis: intricate coupling between cyclophilin A dynamics and substrate turnover. 2013 , 104, 216-26 | 32 |
| 1203 | NMR-based conformational ensembles explain pH-gated opening and closing of OmpG channel. 2013 , 135, 15101-13 | 28 |
| 1202 | The conformational landscape of an intrinsically disordered DNA-binding domain of a transcription regulator. 2013 , 117, 13842-50 | 19 |
| 1201 | 50 years of allosteric interactions: the twists and turns of the models. 2013 , 14, 819-29 | 114 |
| 1200 | Ribosomally synthesized and post-translationally modified peptide natural products: new insights into the role of leader and core peptides during biosynthesis. 2013 , 19, 7662-77 | 74 |
| 1199 | Ubiquitin: molecular modeling and simulations. 2013 , 46, 29-40 | 15 |
| 1198 | Molecular Chaperones. 2013 , | 12 |
| 1197 | Molecular simulations of a dynamic protein complex: role of salt-bridges and polar interactions in configurational transitions. 2013 , 105, 2412-7 | 24 |
| 1196 | Allosteric regulation of SERCA by phosphorylation-mediated conformational shift of phospholamban. 2013 , 110, 17338-43 | 98 |
| 1195 | Circular dichroism and site-directed spin labeling reveal structural and dynamical features of high-pressure states of myoglobin. 2013 , 110, E4714-22 | 35 |

| | | |
|------|---|-----|
| 1194 | Molecular dynamics simulations indicate an induced-fit mechanism for LSD1/CoREST-H3-histone molecular recognition. 2013 , 6, 15 | 14 |
| 1193 | Role of Water and Ions on the Dynamical Transition of RNA. 2013 , 4, 3325-3329 | 10 |
| 1192 | Fisher information metric for the Langevin equation and least informative models of continuous stochastic dynamics. 2013 , 139, 121931 | 13 |
| 1191 | Rational epitope design for protein targeting. 2013 , 8, 397-404 | 30 |
| 1190 | Structural ensemble of an intrinsically disordered polypeptide. 2013 , 117, 118-24 | 64 |
| 1189 | Biosensors based on nanomechanical systems. 2013 , 42, 1287-311 | 269 |
| 1188 | Microsecond folding experiments and simulations: a match is made. 2013 , 15, 3372-88 | 48 |
| 1187 | Mechanism of flexibility control for ATP access of hepatitis C virus NS3 helicase. 2013 , 31, 129-41 | 3 |
| 1186 | Ligand binding and self-association cooperativity of β -lactoglobulin. 2013 , 26, 67-75 | 45 |
| 1185 | Catalysis-enhancement via rotary fluctuation of F1-ATPase. 2013 , 105, 2385-91 | 21 |
| 1184 | Replica exchange molecular dynamics simulations of an α -type small acid soluble protein (SASP). 2013 , 184, 17-21 | 2 |
| 1183 | The origins of allostery: from personal memories to material for the future. 2013 , 425, 1396-406 | 12 |
| 1182 | Long-range interactions in the β -subunit of tryptophan synthase help to coordinate ligand binding, catalysis, and substrate channeling. 2013 , 425, 1527-45 | 30 |
| 1181 | Side chain dynamics of carboxyl and carbonyl groups in the catalytic function of Escherichia coli ribonuclease H. 2013 , 135, 18024-7 | 12 |
| 1180 | Structures of the excited states of phospholamban and shifts in their populations upon phosphorylation. 2013 , 52, 6684-94 | 20 |
| 1179 | Troubleshooting and deconvoluting label-free cell phenotypic assays in drug discovery. 2013 , 67, 69-81 | 33 |
| 1178 | 'Pathway drug cocktail': targeting Ras signaling based on structural pathways. 2013 , 19, 695-704 | 49 |
| 1177 | Impact of mutations on the allosteric conformational equilibrium. 2013 , 425, 647-61 | 38 |

| | | | |
|------|--|------|-----|
| 1176 | Three sites and you are out: ternary synergistic allostery controls aromatic amino acid biosynthesis in <i>Mycobacterium tuberculosis</i> . 2013 , 425, 1582-92 | | 30 |
| 1175 | Intrinsic dynamics of an extended hydrophobic core in the <i>S. cerevisiae</i> RNase III dsRBD contributes to recognition of specific RNA binding sites. 2013 , 425, 546-62 | | 12 |
| 1174 | Allosteric conformational barcodes direct signaling in the cell. 2013 , 21, 1509-21 | | 43 |
| 1173 | NMR spectroscopy on domain dynamics in biomacromolecules. 2013 , 112, 58-117 | | 14 |
| 1172 | Label-free cell phenotypic assessment of the biased agonism and efficacy of agonists at the endogenous muscarinic M3 receptors. 2013 , 68, 323-33 | | 35 |
| 1171 | Relationships between metabolic fluxes and enzyme amino acid composition. 2013 , 8, 107-120 | | 1 |
| 1170 | Directional selection precedes conformational selection in ubiquitin-UIM binding. 2013 , 52, 3709-11 | | 4 |
| 1169 | Protein charge and mass contribute to the spatio-temporal dynamics of protein-protein interactions in a minimal proteome. 2013 , 13, 1339-51 | | 14 |
| 1168 | Structure of the full-length HCV IRES in solution. 2013 , 4, 1612 | | 63 |
| 1167 | Flexible backbone sampling methods to model and design protein alternative conformations. 2013 , 523, 61-85 | | 36 |
| 1166 | Molecular recognition and ligand association. 2013 , 64, 151-75 | | 145 |
| 1165 | Functionally relevant conformational dynamics of water-soluble proteins. 2013 , 47, 149-160 | | 1 |
| 1164 | A single-molecule dissection of ligand binding to a protein with intrinsic dynamics. <i>Nature Chemical Biology</i> , 2013 , 9, 313-8 | 11.7 | 87 |
| 1163 | Flexibility and reactivity in promiscuous enzymes. 2013 , 14, 285-92 | | 32 |
| 1162 | Allostery in disease and in drug discovery. 2013 , 153, 293-305 | | 447 |
| 1161 | Molecular dynamics simulations with replica-averaged structural restraints generate structural ensembles according to the maximum entropy principle. 2013 , 138, 094112 | | 143 |
| 1160 | Encyclopedia of Biophysics. 2013 , 1385-1394 | | 1 |
| 1159 | RRM-RNA recognition: NMR or crystallography and new findings. 2013 , 23, 100-8 | | 132 |

| | | |
|------|--|---------|
| 1158 | The role of ligands on the equilibria between functional states of a G protein-coupled receptor. 2013 , 135, 9465-74 | 128 |
| 1157 | Organic Stereochemistry. Part 5. 2013 , 96, 747-798 | 17 |
| 1156 | Rapid Conformational Fluctuations of Disordered HIV-1 Fusion Peptide in Solution. 2013 , 9, 2870-4 | 7 |
| 1155 | Stochastic mechano-chemical kinetics of molecular motors: A multidisciplinary enterprise from a physicist's perspective. 2013 , 529, 1-197 | 166 |
| 1154 | Alternative splicing of intrinsically disordered regions and rewiring of protein interactions. 2013 , 23, 443-50 | 134 |
| 1153 | NMR relaxation in proteins with fast internal motions and slow conformational exchange: model-free framework and Markov state simulations. 2013 , 117, 6625-34 | 25 |
| 1152 | Mapping the Native Conformational Ensemble of Proteins from a Combination of Simulations and Experiments: New Insight into the src-SH3 Domain. 2013 , 4, 1943-8 | 12 |
| 1151 | The underappreciated role of allostery in the cellular network. 2013 , 42, 169-89 | 137 |
| 1150 | Organic Stereochemistry. Part 6. 2013 , 96, 1005-1030 | 5 |
| 1149 | The archaeal exosome: identification and quantification of site-specific motions that correlate with cap and RNA binding. 2013 , 52, 8312-6 | 25 |
| 1148 | Ensemble-based characterization of unbound and bound states on protein energy landscape. 2013 , 22, 734-44 | 7 |
| 1147 | Allosteric inhibition through suppression of transient conformational states. <i>Nature Chemical Biology</i> , 2013 , 9, 462-5 | 11.7 82 |
| 1146 | Cooperativity of allosteric receptors. 2013 , 425, 1424-32 | 29 |
| 1145 | Drug-Target Residence Time. 2013 , 287-344 | 4 |
| 1144 | On the Dielectric "Constant" of Proteins: Smooth Dielectric Function for Macromolecular Modeling and Its Implementation in DelPhi. 2013 , 9, 2126-2136 | 322 |
| 1143 | Photo-switched self-assembly of a gemini helical peptide into supramolecular architectures. 2013 , 5, 6270-4 | 24 |
| 1142 | Entropic mechanism of allosteric communication in conformational transitions of dihydrofolate reductase. 2013 , 117, 12864-77 | 11 |
| 1141 | Allostery and folding of the N-terminal receiver domain of protein NtrC. 2013 , 117, 13182-93 | 4 |

| | | |
|------|--|-----|
| 1140 | Characterization of the interdomain motions in hen lysozyme using residual dipolar couplings as replica-averaged structural restraints in molecular dynamics simulations. 2013 , 52, 6480-6 | 29 |
| 1139 | Diversity of allosteric regulation in proteases. 2013 , 8, 19-26 | 40 |
| 1138 | Elucidating the ensemble of functionally-relevant transitions in protein systems with a robotics-inspired method. 2013 , 13 Suppl 1, S8 | 16 |
| 1137 | Recovering a representative conformational ensemble from underdetermined macromolecular structural data. 2013 , 135, 16595-609 | 88 |
| 1136 | A computational analysis of binding modes and conformation changes of MDM2 induced by p53 and inhibitor bindings. 2013 , 27, 965-74 | 61 |
| 1135 | Specialized Dynamical Properties of Promiscuous Residues Revealed by Simulated Conformational Ensembles. 2013 , 9, 5127-5147 | 30 |
| 1134 | RNA/Peptide Binding Driven by Electrostatics-Insight from Bidirectional Pulling Simulations. 2013 , 9, 1720-30 | 44 |
| 1133 | Distal structural elements coordinate a conserved base flipping network. 2013 , 52, 1669-76 | 5 |
| 1132 | Exploring the Dynamic Functional Landscape of Adenylate Kinase Modulated by Substrates. 2013 , 9, 84-95 | 63 |
| 1131 | Ordering a dynamic protein via a small-molecule stabilizer. 2013 , 135, 3363-6 | 61 |
| 1130 | Solution structure and dynamics of human hemoglobin in the carbonmonoxy form. 2013 , 52, 5809-20 | 13 |
| 1129 | Validated Conformational Ensembles Are Key for the Successful Prediction of Protein Complexes. 2013 , 9, 1830-7 | 4 |
| 1128 | Bond elasticity controls molecular recognition specificity in antibody-antigen binding. 2013 , 13, 5197-202 | 2 |
| 1127 | Thumb inhibitor binding eliminates functionally important dynamics in the hepatitis C virus RNA polymerase. 2013 , 81, 40-52 | 35 |
| 1126 | Regulatory R region of the CFTR chloride channel is a dynamic integrator of phospho-dependent intra- and intermolecular interactions. 2013 , 110, E4427-36 | 110 |
| 1125 | An essential serotype recognition pocket on phage P22 tailspike protein forces Salmonella enterica serovar Paratyphi A O-antigen fragments to bind as nonsolution conformers. 2013 , 23, 486-94 | 12 |
| 1124 | Electrostatically accelerated encounter and folding for facile recognition of intrinsically disordered proteins. 2013 , 9, e1003363 | 67 |
| 1123 | Multi-Objective Stochastic Search for Sampling Local Minima in the Protein Energy Surface. 2013 , | 23 |

| | | |
|------|---|----|
| 1122 | Utilizing a dynamical description of IspH to aid in the development of novel antimicrobial drugs. 2013 , 9, e1003395 | 7 |
| 1121 | Capturing cooperative interactions with the PSI-MI format. 2013 , 2013, bat066 | 9 |
| 1120 | "Gate-keeper" residues and active-site rearrangements in DNA polymerase help discriminate non-cognate nucleotides. 2013 , 9, e1003074 | 9 |
| 1119 | A transient helical molecular recognition element in the disordered N-terminus of the Sgs1 helicase is critical for chromosome stability and binding of Top3/Rmi1. 2013 , 41, 10215-27 | 19 |
| 1118 | Calcineurin A versus NS5A-TP2/HD domain containing 2: a case study of site-directed low-frequency random mutagenesis for dissecting target specificity of peptide aptamers. 2013 , 12, 1939-52 | 1 |
| 1117 | Minute time scale prolyl isomerization governs antibody recognition of an intrinsically disordered immunodominant epitope. 2013 , 288, 13110-23 | 13 |
| 1116 | CABS-flex: Server for fast simulation of protein structure fluctuations. 2013 , 41, W427-31 | 98 |
| 1115 | Autoactivation of thrombin precursors. 2013 , 288, 11601-10 | 32 |
| 1114 | PROTEIN DYNAMICS IN PHOSPHORYLATION-MEDIATED ALLOSTERY PROBED BY AMIDE EXCHANGE MASS SPECTROMETRY. 2013 , 09, 19-27 | |
| 1113 | CoDNaS: a database of conformational diversity in the native state of proteins. 2013 , 29, 2512-4 | 26 |
| 1112 | Are nicotinic acetylcholine receptors coupled to G proteins?. 2013 , 35, 1025-34 | 52 |
| 1111 | The concept of allosteric interaction and its consequences for the chemistry of the brain. 2013 , 288, 26969-26986 | 86 |
| 1110 | Signaling through dynamic linkers as revealed by PKA. 2013 , 110, 14231-6 | 84 |
| 1109 | Population shift underlies Ca ²⁺ -induced regulatory transitions in the sodium-calcium exchanger (NCX). 2013 , 288, 23141-9 | 21 |
| 1108 | A mechanism for localized dynamics-driven affinity regulation of the binding of von Willebrand factor to platelet glycoprotein Ib. 2013 , 288, 26658-67 | 17 |
| 1107 | Folding and ligand recognition of the TPP riboswitch aptamer at single-molecule resolution. 2013 , 110, 4188-93 | 93 |
| 1106 | INSIGHTS IN ENZYME FUNCTIONAL DYNAMICS AND ACTIVITY REGULATION BY SINGLE MOLECULE STUDIES. 2013 , 08, 137-160 | 15 |
| 1105 | Stationary distribution of self-organized states and biological information generation. 2013 , 3, 3329 | 1 |

| | | |
|------|---|----|
| 1104 | An adaptable and dynamically porous organic salt traps unique tetrahalide dianions. 2013 , 52, 13444-8 | 60 |
| 1103 | An Adaptable and Dynamically Porous Organic Salt Traps Unique Tetrahalide Dianions. 2013 , 125, 13686-13690 | 20 |
| 1102 | The Archaeal Exosome: Identification and Quantification of Site-Specific Motions That Correlate with Cap and RNA Binding. 2013 , 125, 8470-8474 | 3 |
| 1101 | Directional Selection Precedes Conformational Selection in Ubiquitin-UBIM Binding. 2013 , 125, 3797-3799 | |
| 1100 | Ensemble-based interpretations of NMR structural data to describe protein internal dynamics. 2013 , 18, 10548-67 | 22 |
| 1099 | Progress in molecular imaging in endoscopy and endomicroscopy for cancer imaging. 2013 , 4, 1-22 | 12 |
| 1098 | The catalytic roles of P185 and T188 and substrate-binding loop flexibility in 3 β -hydroxysteroid dehydrogenase/carbonyl reductase from <i>Comamonas testosteroni</i> . 2013 , 8, e63594 | 4 |
| 1097 | Mechanistic insight into the relationship between N-terminal acetylation of β -synuclein and fibril formation rates by NMR and fluorescence. 2013 , 8, e75018 | 34 |
| 1096 | Effect of short- and long-range interactions on trp rotamer populations determined by site-directed tryptophan fluorescence of tear lipocalin. 2013 , 8, e78754 | 2 |
| 1095 | Revealing the properties of plant defensins through dynamics. 2013 , 18, 11311-26 | 16 |
| 1094 | Probing the residual structure in avian prion hexarepeats by CD, NMR and MD techniques. 2013 , 18, 11467-84 | 6 |
| 1093 | Shedding light on protein folding, structural and functional dynamics by single molecule studies. 2014 , 19, 19407-34 | 17 |
| 1092 | Observing single enzyme molecules interconvert between activity states upon heating. 2014 , 9, e86224 | 14 |
| 1091 | Investigating the dynamic aspects of drug-protein recognition through a combination of MD and NMR analyses: implications for the development of protein-protein interaction inhibitors. 2014 , 9, e97153 | 10 |
| 1090 | Insight derived from molecular dynamics simulations into molecular motions, thermodynamics and kinetics of HIV-1 gp120. 2014 , 9, e104714 | 9 |
| 1089 | The folding of the specific DNA recognition subdomain of the sleeping beauty transposase is temperature-dependent and is required for its binding to the transposon DNA. 2014 , 9, e112114 | 2 |
| 1088 | RNA-guided assembly of Rev-RRE nuclear export complexes. 2014 , 3, e03656 | 65 |
| 1087 | NMR approaches in structure-based lead discovery: recent developments and new frontiers for targeting multi-protein complexes. 2014 , 116, 101-12 | 47 |

| | | |
|------|---|----|
| 1086 | Computational enzyme design: transitioning from catalytic proteins to enzymes. 2014 , 27, 87-94 | 54 |
| 1085 | Light-regulated tetracycline binding to the Tet repressor. 2014 , 20, 2508-14 | 9 |
| 1084 | Information transfer by leaky, heterogeneous, protein kinase signaling systems. 2014 , 111, E326-33 | 73 |
| 1083 | Regulation of sporulation initiation by NprR and its signaling peptide NprRB: molecular recognition and conformational changes. 2014 , 98, 9399-412 | 16 |
| 1082 | Molecular dynamics simulations of the Nip7 proteins from the marine deep- and shallow-water <i>Pyrococcus</i> species. 2014 , 14, 23 | 6 |
| 1081 | Understanding the Role of Conformational Dynamics in Protein-Ligand Interactions Using NMR Relaxation Methods. 2014 , 255-266 | 2 |
| 1080 | Evidence of conformational selection driving the formation of ligand binding sites in protein-protein interfaces. 2014 , 10, e1003872 | 19 |
| 1079 | The dynamic conformational landscape of gamma-secretase. 2015 , 128, 589-98 | 51 |
| 1078 | Quantitatively characterizing the ligand binding mechanisms of choline binding protein using Markov state model analysis. 2014 , 10, e1003767 | 55 |
| 1077 | Dynamic conformational change regulates the protein-DNA recognition: an investigation on binding of a Y-family polymerase to its target DNA. 2014 , 10, e1003804 | 42 |
| 1076 | Coupling of lever arm swing and biased Brownian motion in actomyosin. 2014 , 10, e1003552 | 9 |
| 1075 | Competitive and cooperative interactions mediate RNA transfer from herpesvirus saimiri ORF57 to the mammalian export adaptor ALYREF. 2014 , 10, e1003907 | 21 |
| 1074 | Crystal structure of the mouse interleukin-3 receptor: insights into interleukin-3 binding and receptor activation. 2014 , 463, 393-403 | 5 |
| 1073 | Protein flexibility facilitates quaternary structure assembly and evolution. 2014 , 12, e1001870 | 56 |
| 1072 | Relationship between Metabolic Fluxes and Sequence-Derived Properties of Enzymes. 2014 , 2014, 817102 | 1 |
| 1071 | A multiscale hybrid evolutionary algorithm to obtain sample-based representations of multi-basin protein energy landscapes. 2014 , | 13 |
| 1070 | Contribution of protein phosphorylation to binding-induced folding of the SLBP-histone mRNA complex probed by phosphorus-31 NMR. 2014 , 4, 853-7 | 6 |
| 1069 | Characterization of the conformational fluctuations in the Josephin domain of ataxin-3. 2014 , 107, 2932-2940 | 13 |

| | | |
|------|---|-----|
| 1068 | Ligand binding modulates the structural dynamics and compactness of the major birch pollen allergen. 2014 , 107, 2972-2981 | 19 |
| 1067 | Principles of allosteric interactions in cell signaling. 2014 , 136, 17692-701 | 97 |
| 1066 | How Protein Disorder Controls Non-Photochemical Fluorescence Quenching. 2014 , 157-185 | 2 |
| 1065 | Variations on the theme: allosteric control in hemoglobin. 2014 , 281, 633-43 | 11 |
| 1064 | Many-body effect in ion binding to RNA. 2014 , 141, 055101 | 11 |
| 1063 | Iterative Stochastic Elimination for Solving Complex Combinatorial Problems in Drug Discovery. 2014 , 54, 1338-1357 | 12 |
| 1062 | New strategies for integrative dynamic modeling of macromolecular assembly. 2014 , 96, 77-111 | 8 |
| 1061 | Magnetic resonance access to transiently formed protein complexes. 2014 , 3, 115-23 | 5 |
| 1060 | Multi-state targeting machinery govern the fidelity and efficiency of protein localization. 2014 , 805, 385-409 | 2 |
| 1059 | Harnessing allostery: a novel approach to drug discovery. 2014 , 34, 1242-85 | 100 |
| 1058 | Single-molecule pull-down (SiMPull) for new-age biochemistry: methodology and biochemical applications of single-molecule pull-down (SiMPull) for probing biomolecular interactions in crude cell extracts. 2014 , 36, 1109-19 | 16 |
| 1057 | Specificity of a protein-protein interface: local dynamics direct substrate recognition of effector caspases. 2014 , 82, 546-55 | 20 |
| 1056 | Conformational changes in DNA-binding proteins: relationships with precomplex features and contributions to specificity and stability. 2014 , 82, 841-57 | 23 |
| 1055 | Allosteric linkers in cAMP signalling. 2014 , 42, 139-44 | 16 |
| 1054 | Susceptibility to HLA-DM protein is determined by a dynamic conformation of major histocompatibility complex class II molecule bound with peptide. 2014 , 289, 23449-64 | 39 |
| 1053 | Microsecond folding and domain motions of a spider silk protein structural switch. 2014 , 136, 17136-44 | 33 |
| 1052 | Nonequilibrium capture rates induce protein accumulation and enhanced adsorption to solid-state nanopores. 2014 , 8, 12238-49 | 17 |
| 1051 | On the Modeling of Polar Component of Solvation Energy using Smooth Gaussian-Based Dielectric Function. 2014 , 13, | 30 |

| | | |
|------|---|-----|
| 1050 | Photosynthetic Energy Transfer and Charge Separation in Higher Plants. 2014 , 79-118 | 1 |
| 1049 | Biophysics of protein evolution and evolutionary protein biophysics. 2014 , 11, 20140419 | 144 |
| 1048 | Single-molecule characterization of Fen1 and Fen1/PCNA complexes acting on flap substrates. 2014 , 42, 1857-72 | 29 |
| 1047 | Type 1 and Type 2 scenarios in hydrogen exchange mass spectrometry studies on protein-ligand complexes. 2014 , 139, 6078-87 | 30 |
| 1046 | TCR scanning of peptide/MHC through complementary matching of receptor and ligand molecular flexibility. 2014 , 192, 2885-91 | 45 |
| 1045 | Protein conformational populations and functionally relevant substates. 2014 , 47, 149-56 | 68 |
| 1044 | Fine-tuned broad binding capability of human lipocalin-type prostaglandin D synthase for various small lipophilic ligands. 2014 , 588, 962-9 | 12 |
| 1043 | Protein Conformational Dynamics. 2014 , | 9 |
| 1042 | Side-chain control of porosity closure in single- and multiple-peptide-based porous materials by cooperative folding. 2014 , 6, 343-51 | 88 |
| 1041 | Disentangling the low-energy states of the major light-harvesting complex of plants and their role in photoprotection. 2014 , 1837, 1027-38 | 57 |
| 1040 | Measuring similarity between dynamic ensembles of biomolecules. 2014 , 11, 552-4 | 26 |
| 1039 | Out-of-equilibrium biomolecular interactions monitored by picosecond fluorescence in microfluidic droplets. 2014 , 14, 1767-74 | 12 |
| 1038 | Molecular biology: Protein binding cannot subdue a lively RNA. 2014 , 506, 303-4 | 2 |
| 1037 | Protein-guided RNA dynamics during early ribosome assembly. 2014 , 506, 334-8 | 110 |
| 1036 | Essential role of conformational selection in ligand binding. 2014 , 186, 13-21 | 82 |
| 1035 | Multiple conformational selection and induced fit events take place in allosteric propagation. 2014 , 186, 22-30 | 78 |
| 1034 | Exploring the role of receptor flexibility in structure-based drug discovery. 2014 , 186, 31-45 | 105 |
| 1033 | Interplay between conformational selection and induced fit in multidomain protein-ligand binding probed by paramagnetic relaxation enhancement. 2014 , 186, 3-12 | 37 |

| | | |
|------|--|-----|
| 1032 | Enhancing the quality of protein conformation ensembles with relative populations. 2014 , 58, 209-25 | 5 |
| 1031 | The free energy landscape in translational science: how can somatic mutations result in constitutive oncogenic activation?. 2014 , 16, 6332-41 | 34 |
| 1030 | Conformational recognition of an intrinsically disordered protein. 2014 , 106, 1771-9 | 40 |
| 1029 | Advancing simulations of biological materials: applications of coarse-grained models on graphics processing unit hardware. 2014 , 40, 802-820 | 3 |
| 1028 | Protein conformational dynamics dictate the binding affinity for a ligand. 2014 , 5, 3724 | 88 |
| 1027 | Small-angle X-ray scattering- and nuclear magnetic resonance-derived conformational ensemble of the highly flexible antitoxin PaaA2. 2014 , 22, 854-65 | 44 |
| 1026 | Mapping protein conformational heterogeneity under pressure with site-directed spin labeling and double electron-electron resonance. 2014 , 111, E1201-10 | 33 |
| 1025 | PyInteraph: a framework for the analysis of interaction networks in structural ensembles of proteins. 2014 , 54, 1537-51 | 71 |
| 1024 | Discriminating binding mechanisms of an intrinsically disordered protein via a multi-state coarse-grained model. 2014 , 140, 175102 | 36 |
| 1023 | PeptiSite: a structural database of peptide binding sites in 4D. 2014 , 445, 717-23 | 10 |
| 1022 | Disordered proteinaceous machines. 2014 , 114, 6806-43 | 92 |
| 1021 | Describing the Conformational Landscape of Small Organic Molecules through Gaussian Mixtures in Dihedral Space. 2014 , 10, 2557-68 | 10 |
| 1020 | Structural insights into proapoptotic signaling mediated by MTCH2, VDAC2, TOM40 and TOM22. 2014 , 26, 370-82 | 17 |
| 1019 | Contribution of proline to the pre-structuring tendency of transient helical secondary structure elements in intrinsically disordered proteins. 2014 , 1840, 993-1003 | 26 |
| 1018 | Familial Alzheimer A2 V mutation reduces the intrinsic disorder and completely changes the free energy landscape of the A β -28 monomer. 2014 , 118, 501-10 | 56 |
| 1017 | Single molecule insights on conformational selection and induced fit mechanism. 2014 , 186, 46-54 | 37 |
| 1016 | Computing protein dynamics from protein structure with elastic network models. 2014 , 4, 488-503 | 28 |
| 1015 | Interplay between partner and ligand facilitates the folding and binding of an intrinsically disordered protein. 2014 , 111, 15420-5 | 112 |

| | | |
|------|---|----|
| 1014 | Exploration of Conformational Spaces of High-Mannose-Type Oligosaccharides by an NMR-Validated Simulation. 2014 , 126, 11121-11124 | 10 |
| 1013 | RevErb β preferentially deforms DNA by induced fit. 2014 , 15, 643-6 | 7 |
| 1012 | Exploration of conformational spaces of high-mannose-type oligosaccharides by an NMR-validated simulation. 2014 , 53, 10941-4 | 54 |
| 1011 | Lean forward: Genetic analysis of temperature-sensitive mutants unfolds the secrets of oligomeric protein complex assembly. 2014 , 36, 836-46 | 9 |
| 1010 | Understanding the structural dynamics of TCR-pMHC complex interactions. 2014 , 35, 604-612 | 34 |
| 1009 | Compensatory adaptations of structural dynamics in an intrinsically disordered protein complex. 2014 , 53, 3840-3 | 43 |
| 1008 | Deformable nature of various damaged DNA duplexes estimated by an electrochemical analysis on electrodes. 2014 , 50, 11126-8 | 3 |
| 1007 | Maintenance of native-like protein dynamics may not be required for engineering functional proteins. 2014 , 21, 1330-1340 | 26 |
| 1006 | Conformational state distributions and catalytically relevant dynamics of a hinge-bending enzyme studied by single-molecule FRET and a coarse-grained simulation. 2014 , 107, 1913-1923 | 20 |
| 1005 | Enzyme dynamics and engineering: one step at a time. 2014 , 21, 1259-1260 | 6 |
| 1004 | Picosecond-resolved fluorescence studies of substrate and cofactor-binding domain mutants in a thermophilic alcohol dehydrogenase uncover an extended network of communication. 2014 , 136, 14821-33 | 15 |
| 1003 | Linkage and allostery in snRNP protein/RNA complexes. 2014 , 53, 3529-39 | 14 |
| 1002 | Residue-Specific Side-Chain Polymorphisms via Particle Belief Propagation. 2014 , 11, 33-41 | 2 |
| 1001 | Structure-based virtual screening of the nociceptin receptor: hybrid docking and shape-based approaches for improved hit identification. 2014 , 54, 2732-43 | 22 |
| 1000 | Structural basis of valmerins as dual inhibitors of GSK3 β /CDK5. 2014 , 20, 2407 | 20 |
| 999 | Exploring transition pathway and free-energy profile of large-scale protein conformational change by combining normal mode analysis and umbrella sampling molecular dynamics. 2014 , 118, 134-43 | 49 |
| 998 | Conformational Changes and Free Energies in a Proline Isomerase. 2014 , 10, 4169-74 | 32 |
| 997 | Conformational investigation in solution of a fluorinated anti-inflammatory drug by NMR spectroscopy in weakly ordering media. 2014 , 118, 9007-16 | 21 |

| | | |
|-----|--|------|
| 996 | Mapping central Helix linker mediated conformational transition pathway of calmodulin via simple computational approach. 2014 , 118, 9677-85 | 13 |
| 995 | Targeting matrix metalloproteinases: exploring the dynamics of the s1' pocket in the design of selective, small molecule inhibitors. 2014 , 57, 10205-19 | 58 |
| 994 | Mass spectrometry methods for studying structure and dynamics of biological macromolecules. 2014 , 86, 213-32 | 107 |
| 993 | An allosteric modulator of HIV-1 protease shows equipotent inhibition of wild-type and drug-resistant proteases. 2014 , 57, 6468-78 | 17 |
| 992 | Real-time assessment of possible electromagnetic-field-induced changes in protein conformation and thermal stability. 2014 , 35, 470-8 | 0 |
| 991 | Assembly of amyloid peptides in the presence of fibril seeds: one-pot coarse-grained molecular dynamics simulations. 2014 , 118, 9238-46 | 16 |
| 990 | Dual effects of familial Alzheimer's disease mutations (D7H, D7N, and H6R) on amyloid peptide: correlation dynamics and zinc binding. 2014 , 82, 3286-97 | 17 |
| 989 | An overview of recent advances in structural bioinformatics of protein-protein interactions and a guide to their principles. 2014 , 116, 141-50 | 51 |
| 988 | Effects of protein-ligand interactions on hydrogen/deuterium exchange kinetics: canonical and noncanonical scenarios. 2014 , 86, 6715-22 | 36 |
| 987 | Concerted dynamic motions of an FABP4 model and its ligands revealed by microsecond molecular dynamics simulations. 2014 , 53, 6409-17 | 9 |
| 986 | Probing the free energy landscape of the fast-folding gpW protein by relaxation dispersion NMR. 2014 , 136, 7444-51 | 28 |
| 985 | Conformational landscapes for KMSKS loop in tyrosyl-tRNA synthetases. 2014 , 15, 45-61 | 12 |
| 984 | Classification of intrinsically disordered regions and proteins. 2014 , 114, 6589-631 | 1141 |
| 983 | (19)F NMR reveals multiple conformations at the dimer interface of the nonstructural protein 1 effector domain from influenza A virus. 2014 , 22, 515-525 | 30 |
| 982 | Molecular landscape of the interaction between the urease accessory proteins UreE and UreG. 2014 , 1844, 1662-74 | 28 |
| 981 | Mg(2+)-induced conformational changes in the btuB riboswitch from E. coli. 2014 , 20, 36-45 | 13 |
| 980 | Influence of orthosteric ligand binding on the conformational dynamics of the β_2 -adrenergic receptor via essential dynamics sampling simulation. 2014 , 48, 399-413 | 1 |
| 979 | Both protein dynamics and ligand concentration can shift the binding mechanism between conformational selection and induced fit. 2014 , 111, 10197-202 | 61 |

| | | |
|-----|---|----|
| 978 | Molecular kinetics. Ras activation by SOS: allosteric regulation by altered fluctuation dynamics. 2014 , 345, 50-4 | 94 |
| 977 | Active site coupling in PDE:PKA complexes promotes resetting of mammalian cAMP signaling. 2014 , 107, 1426-40 | 21 |
| 976 | Ligand concentration regulates the pathways of coupled protein folding and binding. 2014 , 136, 822-5 | 48 |
| 975 | Elements and modulation of functional dynamics. 2014 , 57, 7819-37 | 14 |
| 974 | Poly(ethylene glycol)-mediated conformational alteration of β -chymotrypsin prevents inactivation of insulin by stabilizing active intermediates. 2014 , 11, 3361-70 | 1 |
| 973 | The pKa value and accessibility of cysteine residues are key determinants for protein substrate discrimination by glutaredoxin. 2014 , 53, 2533-40 | 31 |
| 972 | Coupled folding and binding of the disordered protein PUMA does not require particular residual structure. 2014 , 136, 5197-200 | 81 |
| 971 | Conformational selection in protein binding and function. 2014 , 23, 1508-18 | 70 |
| 970 | Recognition of the HIV capsid by the TRIM5 β restriction factor is mediated by a subset of pre-existing conformations of the TRIM5 β SPRY domain. 2014 , 53, 1466-76 | 18 |
| 969 | Exploiting conformational dynamics in drug discovery: design of C-terminal inhibitors of Hsp90 with improved activities. 2014 , 54, 195-208 | 46 |
| 968 | Toward in silico biomolecular manipulation through static modes: atomic scale characterization of HIV-1 protease flexibility. 2014 , 118, 2821-30 | 2 |
| 967 | Structure-activity relationships of thiostrepton derivatives: implications for rational drug design. 2014 , 28, 1205-15 | 9 |
| 966 | Applying conformational selection theory to improve crossdocking efficiency in 3-phosphoinositide dependent protein kinase-1. 2014 , 82, 436-51 | 1 |
| 965 | The copper(II) and zinc(II) coordination mode of HExxH and HxxEH motif in small peptides: the role of carboxylate location and hydrogen bonding network. 2014 , 130, 92-102 | 16 |
| 964 | Thermodynamic and structural basis for relaxation of specificity in protein-DNA recognition. 2014 , 426, 84-104 | 10 |
| 963 | Mechanism of Folding and Binding of an Intrinsically Disordered Protein As Revealed by ab Initio Simulations. 2014 , 10, 2224-31 | 29 |
| 962 | Transient electrostatic interactions dominate the conformational equilibrium sampled by multidomain splicing factor U2AF65: a combined NMR and SAXS study. 2014 , 136, 7068-76 | 57 |
| 961 | Picosecond-resolved fluorescent probes at functionally distinct tryptophans within a thermophilic alcohol dehydrogenase: relationship of temperature-dependent changes in fluorescence to catalysis. 2014 , 118, 6049-61 | 20 |

| | | |
|-----|---|-----|
| 960 | NMR approaches for structural analysis of multidomain proteins and complexes in solution. 2014 , 80, 26-63 | 130 |
| 959 | Asymmetric perturbations of signalling oligomers. 2014 , 114, 153-69 | 11 |
| 958 | Themes and variations in riboswitch structure and function. 2014 , 1839, 908-918 | 75 |
| 957 | Nuclear Magnetic Resonance of Large Molecules in Natural Products. 2014 , 1-18 | 1 |
| 956 | ABSINTH Implicit Solvation Model and Force Field Paradigm for Use in Simulations of Intrinsically Disordered Proteins. 2014 , 208-231 | |
| 955 | Kompensatorische Anpassungen der strukturellen Dynamik eines intrinsisch unstrukturierten Protein-Komplexes. 2014 , 126, 3919-3922 | 10 |
| 954 | Tuning RNA Flexibility with Helix Length and Junction Sequence. 2015 , 109, 2644-2653 | 14 |
| 953 | Water-Mediated Recognition of Simple Alkyl Chains by Heart-Type Fatty-Acid-Binding Protein. 2015 , 127, 1528-1531 | 3 |
| 952 | The Physical Basis of Ligand Binding. 2015 , 3-43 | 4 |
| 951 | Lessons in Protein Design from Combined Evolution and Conformational Dynamics. 2015 , 5, 14259 | 10 |
| 950 | A Review of Evolutionary Algorithms for Computing Functional Conformations of Protein Molecules. 2015 , 31-64 | 8 |
| 949 | Large-scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. 2015 , 36, 1772-85 | 19 |
| 948 | The tyrosine gate of the bacterial lectin FimH: a conformational analysis by NMR spectroscopy and X-ray crystallography. 2015 , 16, 1235-46 | 34 |
| 947 | Direct Observation of Kinetic Pathways of Biomolecular Recognition. 2015 , 21, 16172-7 | 9 |
| 946 | The role of conformational selection in the molecular recognition of the wild type and mutants XPA67-80 peptides by ERCC1. 2015 , 83, 1341-51 | 2 |
| 945 | Noncognate DNA damage prevents the formation of the active conformation of the Y-family DNA polymerases DinB and DNA polymerase η . 2015 , 282, 2646-60 | 8 |
| 944 | Regulation of integrins in platelets. 2015 , 104, 323-33 | 32 |
| 943 | Mechanostability of the Single-Electron-Transfer Complexes of Anabaena Ferredoxin-NADP(+) Reductase. 2015 , 16, 3161-9 | 3 |

| | | |
|-----|--|-----|
| 942 | Differences in binding behavior of (-)-epigallocatechin gallate to β -lactoglobulin heterodimers (AB) compared to homodimers (A) and (B). 2015 , 28, 656-66 | 18 |
| 941 | Aqueous Molecular Dynamics Simulations of the M. tuberculosis Enoyl-ACP Reductase-NADH System and Its Complex with a Substrate Mimic or Diphenyl Ethers Inhibitors. 2015 , 16, 23695-722 | 13 |
| 940 | On the energy components governing molecular recognition in the framework of continuum approaches. 2015 , 2, 5 | 25 |
| 939 | Integrating atomistic molecular dynamics simulations, experiments, and network analysis to study protein dynamics: strength in unity. 2015 , 2, 28 | 48 |
| 938 | Mapping the Conformation Space of Wildtype and Mutant H-Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. 2015 , 11, e1004470 | 31 |
| 937 | Human Non-neutralizing HIV-1 Envelope Monoclonal Antibodies Limit the Number of Founder Viruses during SHIV Mucosal Infection in Rhesus Macaques. 2015 , 11, e1005042 | 111 |
| 936 | Bridging scales through multiscale modeling: a case study on protein kinase A. 2015 , 6, 250 | 16 |
| 935 | A Database of Force-Field Parameters, Dynamics, and Properties of Antimicrobial Compounds. 2015 , 20, 13997-4021 | 42 |
| 934 | Exploring the potential impact of an expanded genetic code on protein function. 2015 , 112, 6961-6 | 56 |
| 933 | Conformational features of 4-(N)-squalenoyl-gemcitabine in solution: a combined NMR and molecular dynamics investigation. 2015 , 39, 3484-3496 | 3 |
| 932 | Tracking individual membrane proteins and their biochemistry: The power of direct observation. 2015 , 98, 22-30 | 15 |
| 931 | Computing transition paths in multiple-basin proteins with a probabilistic roadmap algorithm guided by structure data. 2015 , | 4 |
| 930 | Coupling of Conformational Transitions in the N-terminal Domain of the 51-kDa FK506-binding Protein (FKBP51) Near Its Site of Interaction with the Steroid Receptor Proteins. 2015 , 290, 15746-15757 | 12 |
| 929 | MESMER: minimal ensemble solutions to multiple experimental restraints. 2015 , 31, 1951-8 | 8 |
| 928 | Evolutionary search strategies for efficient sample-based representations of multiple-basin protein energy landscapes. 2015 , | 4 |
| 927 | Forkhead followed by disordered tail: The intrinsically disordered regions of FOXO3a. 2015 , 3, e1056906 | 10 |
| 926 | Using Pseudocontact Shifts and Residual Dipolar Couplings as Exact NMR Restraints for the Determination of Protein Structural Ensembles. 2015 , 54, 7470-6 | 16 |
| 925 | A pre-structured helix in the intrinsically disordered 4EBP1. 2015 , 11, 366-9 | 11 |

| | | |
|-----|---|-----|
| 924 | Binding affinities controlled by shifting conformational equilibria: opportunities and limitations. 2015 , 108, 2585-2590 | 9 |
| 923 | Markov state models provide insights into dynamic modulation of protein function. 2015 , 48, 414-22 | 172 |
| 922 | Adaptability in protein structures: structural dynamics and implications in ligand design. 2015 , 33, 298-321 | 6 |
| 921 | "Invisible" conformers of an antifungal disulfide protein revealed by constrained cold and heat unfolding, CEST-NMR experiments, and molecular dynamics calculations. 2015 , 21, 5136-44 | 33 |
| 920 | Enhanced Conformational Sampling Using Replica Exchange with Collective-Variable Tempering. 2015 , 11, 1077-85 | 68 |
| 919 | BAX-induced apoptosis can be initiated through a conformational selection mechanism. 2015 , 23, 139-148 | 29 |
| 918 | Independent Metrics for Protein Backbone and Side-Chain Flexibility: Time Scales and Effects of Ligand Binding. 2015 , 11, 851-60 | 23 |
| 917 | Predicted structures for kappa opioid G-protein coupled receptor bound to selective agonists. 2015 , 55, 614-27 | 9 |
| 916 | Distal regulation of heme binding of heme oxygenase-1 mediated by conformational fluctuations. 2015 , 54, 340-8 | 14 |
| 915 | Quantitative biophysical characterization of intrinsically disordered proteins. 2015 , 54, 1314-26 | 42 |
| 914 | Decoding the Mobility and Time Scales of Protein Loops. 2015 , 11, 1308-14 | 29 |
| 913 | Network of long-range concerted chemical shift displacements upon ligand binding to human angiogenin. 2015 , 24, 525-33 | 16 |
| 912 | New look at hemoglobin allostery. 2015 , 115, 1702-24 | 104 |
| 911 | Water-mediated recognition of simple alkyl chains by heart-type fatty-acid-binding protein. 2015 , 54, 1508-11 | 31 |
| 910 | Conformational changes and allosteric communications in human serum albumin due to ligand binding. 2015 , 33, 2192-204 | 9 |
| 909 | Synthetic biology for the directed evolution of protein biocatalysts: navigating sequence space intelligently. 2015 , 44, 1172-239 | 267 |
| 908 | The design of covalent allosteric drugs. 2015 , 55, 249-67 | 76 |
| 907 | Role of indirect readout mechanism in TATA box binding protein-DNA interaction. 2015 , 29, 283-95 | 3 |

| | | |
|-----|--|-----|
| 906 | Impact of stable protein-protein interaction on protein conformational space. 2015 , 31, 149-155 | 3 |
| 905 | Dynamics based pharmacophore models for screening potential inhibitors of mycobacterial cyclopropane synthase. 2015 , 55, 848-60 | 37 |
| 904 | Nanoscale protein domain motion and long-range allostery in signaling proteins- a view from neutron spin echo spectroscopy. 2015 , 7, 165-174 | 9 |
| 903 | Relaxation dispersion NMR spectroscopy for the study of protein allostery. 2015 , 7, 191-200 | 26 |
| 902 | A (15)N CPMG relaxation dispersion experiment more resistant to resonance offset and pulse imperfection. 2015 , 257, 1-7 | 28 |
| 901 | The RAS-Binding Domain of Human BRAF Protein Serine/Threonine Kinase Exhibits Allosteric Conformational Changes upon Binding HRAS. 2015 , 23, 1382-1393 | 24 |
| 900 | Computational evidence to design an appropriate candidate for the treatment of Alzheimer's disease through replacement of the heptamethylene linker of bis(7)tacrine with S-allylcysteine. 2015 , 5, 66840-66851 | 3 |
| 899 | A novel allosteric mechanism on protein-DNA interactions underlying the phosphorylation-dependent regulation of Ets1 target gene expressions. 2015 , 427, 1655-69 | 18 |
| 898 | 3D Structural Fluctuation of IgG1 Antibody Revealed by Individual Particle Electron Tomography. 2015 , 5, 9803 | 69 |
| 897 | Unveiling Inherent Degeneracies in Determining Population-Weighted Ensembles of Interdomain Orientational Distributions Using NMR Residual Dipolar Couplings: Application to RNA Helix Junction Helix Motifs. 2015 , 119, 9614-26 | 8 |
| 896 | Allostery through the computational microscope: cAMP activation of a canonical signalling domain. 2015 , 6, 7588 | 68 |
| 895 | Protein conformational plasticity and complex ligand-binding kinetics explored by atomistic simulations and Markov models. 2015 , 6, 7653 | 252 |
| 894 | Allosteric therapies for lung cancer. 2015 , 34, 303-12 | 10 |
| 893 | FlexAID: Revisiting Docking on Non-Native-Complex Structures. 2015 , 55, 1323-36 | 32 |
| 892 | Microsecond protein dynamics observed at the single-molecule level. 2015 , 6, 7685 | 52 |
| 891 | A Data-Driven Evolutionary Algorithm for Mapping Multibasin Protein Energy Landscapes. 2015 , 22, 844-60 | 21 |
| 890 | Conformational kinetics reveals affinities of protein conformational states. 2015 , 112, 9352-7 | 23 |
| 889 | Fusion of selected regions of mycobacterial antigens for enhancing sensitivity in serodiagnosis of tuberculosis. 2015 , 115, 104-11 | 12 |

| | | |
|-----|---|----|
| 888 | Inhibition and Reversal of Microbial Attachment by an Antibody with Parasteric Activity against the FimH Adhesin of Uropathogenic E. coli. 2015 , 11, e1004857 | 35 |
| 887 | Selectivity by small-molecule inhibitors of protein interactions can be driven by protein surface fluctuations. 2015 , 11, e1004081 | 17 |
| 886 | AnchorDock: Blind and Flexible Anchor-Driven Peptide Docking. 2015 , 23, 929-940 | 49 |
| 885 | Exploring the Alzheimer amyloid- β peptide conformational ensemble: A review of molecular dynamics approaches. 2015 , 69, 86-91 | 49 |
| 884 | Characterization of the flexible lip regions in bacteriophage lambda lysozyme using MD simulations. 2015 , 44, 235-47 | 3 |
| 883 | Computational docking simulations of a DNA-aptamer for argininamide and related ligands. 2015 , 29, 643-54 | 32 |
| 882 | Design of protein switches based on an ensemble model of allostery. 2015 , 6, 6968 | 51 |
| 881 | Protein Flexibility in Drug Discovery: From Theory to Computation. 2015 , 10, 1141-8 | 42 |
| 880 | From protein structure to function via single crystal optical spectroscopy. 2015 , 2, 12 | 9 |
| 879 | AAA+ chaperones and acyldepsipeptides activate the ClpP protease via conformational control. 2015 , 6, 6320 | 78 |
| 878 | Imprints of function on the folding landscape: functional role for an intermediate in a conserved eukaryotic binding protein. 2015 , 17, 11042-52 | 14 |
| 877 | Response of CnrX from <i>Cupriavidus metallidurans</i> CH34 to nickel binding. 2015 , 7, 622-31 | 15 |
| 876 | Combining label-free cell phenotypic profiling with computational approaches for novel drug discovery. 2015 , 10, 331-43 | 17 |
| 875 | Structural disorder of folded proteins: isotope-edited 2D IR spectroscopy and Markov state modeling. 2015 , 108, 1747-1757 | 20 |
| 874 | A Topology Potential-Based Method for Identifying Essential Proteins from PPI Networks. 2015 , 12, 372-83 | 59 |
| 873 | Balancing between affinity and speed in target DNA search by zinc-finger proteins via modulation of dynamic conformational ensemble. 2015 , 112, E5142-9 | 73 |
| 872 | Structure and Dynamics of Intrinsically Disordered Proteins. 2015 , 870, 35-48 | 11 |
| 871 | Toward Focusing Conformational Ensembles on Bioactive Conformations: A Molecular Mechanics/Quantum Mechanics Study. 2015 , 55, 2154-67 | 24 |

| | | |
|-----|---|----|
| 870 | On the analysis and comparison of conformer-specific essential dynamics upon ligand binding to a protein. 2015 , 142, 245101 | 3 |
| 869 | Single-molecule spectroscopy reveals how calmodulin activates NO synthase by controlling its conformational fluctuation dynamics. 2015 , 112, 11835-40 | 34 |
| 868 | Mechanism of cAMP Partial Agonism in Protein Kinase G (PKG). 2015 , 290, 28631-41 | 35 |
| 867 | Ensembles of a small number of conformations with relative populations. 2015 , 63, 341-351 | 2 |
| 866 | Molecular dynamics simulations of the Escherichia coli HPPK apo-enzyme reveal a network of conformational transitions. 2015 , 54, 6734-42 | 11 |
| 865 | Information content of long-range NMR data for the characterization of conformational heterogeneity. 2015 , 62, 353-71 | 17 |
| 864 | Changes in protein structure at the interface accompanying complex formation. 2015 , 2, 643-52 | 14 |
| 863 | Couplings between hierarchical conformational dynamics from multi-time correlation functions and two-dimensional lifetime spectra: Application to adenylate kinase. 2015 , 142, 212404 | 13 |
| 862 | Parallel Allostery by cAMP and PDE Coordinates Activation and Termination Phases in cAMP Signaling. 2015 , 109, 1251-63 | 14 |
| 861 | Structural plasticity in Mycobacterium tuberculosis uracil-DNA glycosylase (MtUng) and its functional implications. 2015 , 71, 1514-27 | 11 |
| 860 | Enhanced molecular mobility of ordinarily structured regions drives polyglutamine disease. 2015 , 290, 24190-200 | 18 |
| 859 | The N-Terminal Peptides of the Three Human Isoforms of the Mitochondrial Voltage-Dependent Anion Channel Have Different Helical Propensities. 2015 , 54, 5646-56 | 16 |
| 858 | Inactive conformation enhances binding function in physiological conditions. 2015 , 112, 9884-9 | 18 |
| 857 | Open challenges in structure-based virtual screening: Receptor modeling, target flexibility consideration and active site water molecules description. 2015 , 583, 105-19 | 78 |
| 856 | Dynamics of the BH3-Only Protein Binding Interface of Bcl-xL. 2015 , 109, 1049-57 | 9 |
| 855 | Structural analysis of the unmutated ancestor of the HIV-1 envelope V2 region antibody CH58 isolated from an RV144 vaccine efficacy trial vaccinee. 2015 , 2, 713-22 | 11 |
| 854 | Measurement of State-Specific Association Constants in Allosteric Sensors through Molecular Stapling and NMR. 2015 , 137, 10777-85 | 28 |
| 853 | Dissecting Protein Configurational Entropy into Conformational and Vibrational Contributions. 2015 , 119, 12623-31 | 19 |

| | | |
|-----|--|-----|
| 852 | A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. 2015 , 55, 2256-74 | 52 |
| 851 | Flexible receptor docking for drug discovery. 2015 , 10, 1189-200 | 46 |
| 850 | Recognition of Damaged DNA for Nucleotide Excision Repair: A Correlated Motion Mechanism with a Mismatched cis-syn Thymine Dimer Lesion. 2015 , 54, 5263-7 | 20 |
| 849 | Sampling of conformational ensemble for virtual screening using molecular dynamics simulations and normal mode analysis. 2015 , 7, 2317-31 | 18 |
| 848 | Domain Motion Enhanced (DoME) Model for Efficient Conformational Sampling of Multidomain Proteins. 2015 , 119, 14584-93 | 8 |
| 847 | Protein Folding: Part II Energy Landscapes and Protein Dynamics. 2015 , 61-94 | 0 |
| 846 | The s2D method: simultaneous sequence-based prediction of the statistical populations of ordered and disordered regions in proteins. 2015 , 427, 982-996 | 60 |
| 845 | Automatic state partitioning for multibody systems (APM): an efficient algorithm for constructing Markov state models to elucidate conformational dynamics of multibody systems. 2015 , 11, 17-27 | 29 |
| 844 | Allostery without a conformational change? Revisiting the paradigm. 2015 , 30, 17-24 | 137 |
| 843 | Tunneling isomerization of small carboxylic acids and their complexes in solid matrixes: a computational insight. 2015 , 119, 2628-35 | 29 |
| 842 | Molecular Modeling of Proteins. 2015 , | 6 |
| 841 | Intrinsic flexibility of NLRP pyrin domains is a key factor in their conformational dynamics, fold stability, and dimerization. 2015 , 24, 174-81 | 20 |
| 840 | Dynamic principle for designing antagonistic/agonistic molecules for EphA4 receptor, the only known ALS modifier. 2015 , 10, 372-8 | 18 |
| 839 | Structural details of light activation of the LOV2-based photoswitch PA-Rac1. 2015 , 10, 502-9 | 17 |
| 838 | Ligand binding to a high-energy partially unfolded protein. 2015 , 24, 129-37 | 8 |
| 837 | Coupled binding-bending-folding: The complex conformational dynamics of protein-DNA binding studied by atomistic molecular dynamics simulations. 2015 , 1850, 1091-1098 | 25 |
| 836 | Evolution of conformational dynamics determines the conversion of a promiscuous generalist into a specialist enzyme. 2015 , 32, 132-43 | 87 |
| 835 | Electrostatic free energies in translational GTPases: Classic allostery and the rest. 2015 , 1850, 1006-1016 | 4 |

| | | |
|-----|---|-----|
| 834 | Soft templates in encapsulation complexes. 2015 , 44, 490-9 | 95 |
| 833 | Paralog-Specific Patterns of Structural Disorder and Phosphorylation in the Vertebrate SH3-SH2-Tyrosine Kinase Protein Family. 2016 , 8, 2806-25 | 5 |
| 832 | High mobility group protein 1: A collaborator in nucleosome dynamics and estrogen-responsive gene expression. 2016 , 7, 206-22 | 7 |
| 831 | Essential Strategies for Revealing Nanoscale Protein Dynamics by Neutron Spin Echo Spectroscopy. 2016 , 566, 253-70 | 5 |
| 830 | Insights into Protein-Ligand Interactions: Mechanisms, Models, and Methods. 2016 , 17, | 504 |
| 829 | Binding Mechanisms of Intrinsically Disordered Proteins: Theory, Simulation, and Experiment. 2016 , 3, 52 | 80 |
| 828 | Investigating the Role of Large-Scale Domain Dynamics in Protein-Protein Interactions. 2016 , 3, 54 | 14 |
| 827 | Extracting Conformational Ensembles of Small Molecules from Molecular Dynamics Simulations: Ampicillin as a Test Case. 2016 , 4, 5 | 13 |
| 826 | Effect of the Solvent Temperatures on Dynamics of Serine Protease Proteinase K. 2016 , 17, 254 | 14 |
| 825 | Coenzyme Q Biosynthesis: Evidence for a Substrate Access Channel in the FAD-Dependent Monooxygenase Coq6. 2016 , 12, e1004690 | 4 |
| 824 | Computational Simulation of the Activation Cycle of G β Subunit in the G Protein Cycle Using an Elastic Network Model. 2016 , 11, e0159528 | 3 |
| 823 | Enhancing backbone sampling in Monte Carlo simulations using internal coordinates normal mode analysis. 2016 , 24, 4855-4866 | 1 |
| 822 | Structure of the NS3 helicase from Zika virus. 2016 , 23, 752-4 | 69 |
| 821 | Correlating Calmodulin Landscapes with Chemical Catalysis in Neuronal Nitric Oxide Synthase using Time-Resolved FRET and a 5-Deazaflavin Thermodynamic Trap. 2016 , 6, 5170-5180 | 13 |
| 820 | Conformational selection underpins recognition of multiple DNA sequences by proteins and consequent functional actions. 2016 , 18, 21618-28 | 0 |
| 819 | Comprehensive analysis of motions in molecular dynamics trajectories of the actin capping protein and its inhibitor complexes. 2016 , 84, 948-56 | 6 |
| 818 | The role of side chain entropy and mutual information for improving the de novo design of Kemp eliminases KE07 and KE70. 2016 , 18, 19386-96 | 19 |
| 817 | Analytical methods for structural ensembles and dynamics of intrinsically disordered proteins. 2016 , 8, 429-439 | 10 |

| | | |
|-----|--|----|
| 816 | Coarse-grained molecular simulations of allosteric cooperativity. 2016 , 144, 105101 | 8 |
| 815 | Residue Geometry Networks: A Rigidity-Based Approach to the Amino Acid Network and Evolutionary Rate Analysis. 2016 , 6, 33213 | 10 |
| 814 | Conformational Dynamics of apo-GlnBP Revealed by Experimental and Computational Analysis. 2016 , 128, 14196-14200 | 3 |
| 813 | Comparing allosteric transitions in the domains of calmodulin through coarse-grained simulations. 2016 , 144, 105102 | 4 |
| 812 | Distinct Dynamic Modes Enable the Engagement of Dissimilar Ligands in a Promiscuous Atypical RNA Recognition Motif. 2016 , 55, 7141-7150 | 20 |
| 811 | Molecular Mechanism for Conformational Dynamics of Ras[GTP Elucidated from In-Situ Structural Transition in Crystal. 2016 , 6, 25931 | 29 |
| 810 | NMR Characterization of Information Flow and Allosteric Communities in the MAP Kinase p38. 2016 , 6, 28655 | 16 |
| 809 | Structural and Dynamic Insights of the Interaction between Tritrpticin and Micelles: An NMR Study. 2016 , 111, 2676-2688 | 17 |
| 808 | Structure of ring-shaped Aβ oligomers determined by conformational selection. 2016 , 6, 21429 | 24 |
| 807 | Multibody cofactor and substrate molecular recognition in the myo-inositol monophosphatase enzyme. 2016 , 6, 30275 | 13 |
| 806 | A Network of Conformational Transitions Revealed by Molecular Dynamics Simulations of the Binary Complex of Escherichia coli 6-Hydroxymethyl-7,8-dihydropterin Pyrophosphokinase with MgATP. 2016 , 55, 6931-6939 | 8 |
| 805 | Visualizing single-stranded nucleic acids in solution. 2017 , 45, e66 | 13 |
| 804 | Microsecond Timescale Dynamics of GDP-Bound Ras Underlies the Formation of Novel Inhibitor-Binding Pockets. 2016 , 128, 15858-15861 | 3 |
| 803 | Vibrational resonance, allostery, and activation in rhodopsin-like G protein-coupled receptors. 2016 , 6, 37290 | 19 |
| 802 | Molecular dynamics simulations elucidate the mode of protein recognition by Skp1 and the F-box domain in the SCF complex. 2016 , 84, 159-71 | 11 |
| 801 | Long-Range Communication between Different Functional Sites in the Picornaviral 3C Protein. 2016 , 24, 509-517 | 6 |
| 800 | Switching between cis and trans anions of 2-(2'-hydroxyphenyl)benzimidazole: a molecular rotation perturbed by chemical stabilization. 2016 , 18, 11081-90 | 13 |
| 799 | Conformational Destabilization of Immunoglobulin G Increases the Low pH Binding Affinity with the Neonatal Fc Receptor. 2016 , 291, 1817-1825 | 29 |

| | | |
|-----|--|-----|
| 798 | Conformation switching of AIM2 PYD domain revealed by NMR relaxation and MD simulation. 2016 , 473, 636-41 | 7 |
| 797 | Noncovalent Interactions by Quantum Monte Carlo. 2016 , 116, 5188-215 | 97 |
| 796 | Emerging Computational Methods for the Rational Discovery of Allosteric Drugs. 2016 , 116, 6370-90 | 140 |
| 795 | Visualizing ensembles in structural biology. 2016 , 67, 44-53 | 18 |
| 794 | Designing an efficient multi-epitope peptide vaccine against <i>Vibrio cholerae</i> via combined immunoinformatics and protein interaction based approaches. 2016 , 62, 82-95 | 96 |
| 793 | Advances in NMR Methods To Map Allosteric Sites: From Models to Translation. 2016 , 116, 6267-304 | 60 |
| 792 | Molecular Dynamics Simulations to Study Structure-Function Relationship in Psychrophilic Enzymes. 2016 , 675-698 | |
| 791 | Biased Allostery. 2016 , 111, 902-8 | 18 |
| 790 | Conformational Dynamics of apo-GlnBP Revealed by Experimental and Computational Analysis. 2016 , 55, 13990-13994 | 26 |
| 789 | Analyzing slowly exchanging protein conformations by ion mobility mass spectrometry: study of the dynamic equilibrium of prolyl oligopeptidase. 2016 , 51, 504-11 | 5 |
| 788 | Pushing the Backbone in Protein-Protein Docking. 2016 , 24, 1821-1829 | 33 |
| 787 | Interferon Beta: From Molecular Level to Therapeutic Effects. 2016 , 326, 343-72 | 33 |
| 786 | An accurately preorganized IRES RNA structure enables eIF4G capture for initiation of viral translation. 2016 , 23, 859-64 | 28 |
| 785 | Exploiting computationally derived out-of-the-box protein conformations for drug design. 2016 , 8, 1887-1897 | 6 |
| 784 | How human IgGs against DNA recognize oligonucleotides and DNA. 2016 , 29, 596-610 | 3 |
| 783 | Conformational Substates of Amyloidogenic hIAPP Revealed by High Pressure NMR Spectroscopy. 2016 , 1, 3239-3243 | 6 |
| 782 | Multilevel Changes in Protein Dynamics upon Complex Formation of the Calcium-Loaded S100A4 with a Nonmuscle Myosin IIA Tail Fragment. 2016 , 17, 1829-1838 | 8 |
| 781 | Dynamic Modulation of DNA Hybridization Using Allosteric DNA Tetrahedral Nanostructures. 2016 , 88, 8043-9 | 37 |

| | | |
|-----|--|----|
| 780 | Biomimetic fabrication of biotinylated peptide nanostructures upon diatom scaffold; a plausible model for sustainable energy. 2016 , 6, 73692-73698 | 21 |
| 779 | A stochastic roadmap method to model protein structural transitions. 2016 , 34, 1705-1733 | 4 |
| 778 | Microsecond Timescale Dynamics of GDP-Bound Ras Underlies the Formation of Novel Inhibitor-Binding Pockets. 2016 , 55, 15629-15632 | 13 |
| 777 | Engineering of the Conformational Dynamics of an Enzyme for Relieving the Product Inhibition. 2016 , 6, 8440-8445 | 30 |
| 776 | Probing conformational and functional substates of calmodulin by high pressure FTIR spectroscopy: influence of Ca binding and the hypervariable region of K-Ras4B. 2016 , 18, 30020-30028 | 17 |
| 775 | Distinct Roles for Conformational Dynamics in Protein-Ligand Interactions. 2016 , 24, 2053-2066 | 20 |
| 774 | Millisecond Hydrogen Exchange. 2016 , 73-91 | 1 |
| 773 | Structural Architecture of Prothrombin in Solution Revealed by Single Molecule Spectroscopy. 2016 , 291, 18107-16 | 17 |
| 772 | Differential utilization of binding loop flexibility in T cell receptor ligand selection and cross-reactivity. 2016 , 6, 25070 | 16 |
| 771 | A Novel EA-based Memetic Approach for Efficiently Mapping Complex Fitness Landscapes. 2016 , | 3 |
| 770 | Production of unstable proteins through the formation of stable core complexes. 2016 , 7, 10932 | 4 |
| 769 | Foldamer-mediated manipulation of a pre-amyloid toxin. 2016 , 7, 11412 | 43 |
| 768 | Mode localization in the cooperative dynamics of protein recognition. 2016 , 145, 015101 | 6 |
| 767 | Sample-based Models of Protein Structural Transitions. 2016 , | 2 |
| 766 | Computing energy landscape maps and structural excursions of proteins. 2016 , 17 Suppl 4, 546 | 8 |
| 765 | Histidine switch controlling pH-dependent protein folding and DNA binding in a transcription factor at the core of synthetic network devices. 2016 , 12, 2417-26 | 14 |
| 764 | Effect of Inactivating Mutations on Peptide Conformational Ensembles: The Plant Polypeptide Hormone Systemin. 2016 , 56, 1267-81 | 2 |
| 763 | Structured and Unstructured Binding of an Intrinsically Disordered Protein as Revealed by Atomistic Simulations. 2016 , 138, 8742-51 | 30 |

| | | |
|-----|---|-----|
| 762 | Elucidation of the conformational dynamics of multi-body systems by construction of Markov state models. 2016 , 18, 30228-30235 | 14 |
| 761 | The principle of conformational signaling. 2016 , 45, 4252-84 | 29 |
| 760 | Conformational Selection in a Protein-Protein Interaction Revealed by Dynamic Pathway Analysis. 2016 , 14, 32-42 | 36 |
| 759 | A Short Practical Guide to the Quantitative Analysis of Engineered Enzymes. 2016 , 27-44 | 1 |
| 758 | Studying Protein-Protein Binding through T-Jump Induced Dissociation: Transient 2D IR Spectroscopy of Insulin Dimer. 2016 , 120, 5134-45 | 37 |
| 757 | Resolution of Site-Specific Conformational Heterogeneity in Proline-Rich Molecular Recognition by Src Homology 3 Domains. 2016 , 138, 1130-3 | 12 |
| 756 | Conformational Heterogeneity of Unbound Proteins Enhances Recognition in Protein-Protein Encounters. 2016 , 12, 3236-49 | 9 |
| 755 | Nanoscale Engineering of Designer Cellulosomes. 2016 , 28, 5619-47 | 35 |
| 754 | Active-Site-Directed Inhibitors of Prolyl Oligopeptidase Abolish Its Conformational Dynamics. 2016 , 17, 913-7 | 11 |
| 753 | Molecular perception of interactions between bis(7)tacrine and cystamine-tacrine dimer with cholinesterases as the promising proposed agents for the treatment of Alzheimer's disease. 2016 , 34, 855-69 | 15 |
| 752 | Role of Molecular Dynamics and Related Methods in Drug Discovery. 2016 , 59, 4035-61 | 505 |
| 751 | Ras Conformational Ensembles, Allostery, and Signaling. 2016 , 116, 6607-65 | 199 |
| 750 | Dynamic conformational ensembles regulate casein kinase-1 isoforms: Insights from molecular dynamics and molecular docking studies. 2016 , 61, 39-46 | 0 |
| 749 | 1,1,2,2-Tetracyanocyclopropane (TCCP) as supramolecular synthon. 2016 , 18, 1693-8 | 45 |
| 748 | A dynamic checkpoint in oxidative lesion discrimination by formamidopyrimidine-DNA glycosylase. 2016 , 44, 683-94 | 15 |
| 747 | Optimization of Conformational Dynamics in an Epistatic Evolutionary Trajectory. 2016 , 33, 1768-76 | 40 |
| 746 | Ancestral Protein Reconstruction Yields Insights into Adaptive Evolution of Binding Specificity in Solute-Binding Proteins. 2016 , 23, 236-245 | 59 |
| 745 | Controlling Allosteric Networks in Proteins. 2016 , 116, 6463-87 | 135 |

| | | |
|-----|---|-----|
| 744 | The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. 2016 , 116, 6391-423 | 213 |
| 743 | A General, Adaptive, Roadmap-Based Algorithm for Protein Motion Computation. 2016 , 15, 158-65 | 6 |
| 742 | Molecular Science of Fluctuations Toward Biological Functions. 2016 , | 3 |
| 741 | Protein Allostery and Conformational Dynamics. 2016 , 116, 6503-15 | 209 |
| 740 | Energetic and flexibility properties captured by long molecular dynamics simulations of a membrane-embedded pMHCII-TCR complex. 2016 , 12, 1350-66 | 7 |
| 739 | Atomistic picture of conformational exchange in a T4 lysozyme cavity mutant: an experiment-guided molecular dynamics study. 2016 , 7, 3602-3613 | 24 |
| 738 | Conformational Rearrangements of Individual Nucleotides during RNA-Ligand Binding Are Rate-Differentiated. 2016 , 138, 3627-30 | 16 |
| 737 | A Flexible Domain-Domain Hinge Promotes an Induced-fit Dominant Mechanism for the Loading of Guide-DNA into Argonaute Protein in <i>Thermus thermophilus</i> . 2016 , 120, 2709-20 | 17 |
| 736 | Ligand-Dependent Conformational Dynamics of Dihydrofolate Reductase. 2016 , 55, 1485-93 | 5 |
| 735 | On the link between conformational changes, ligand binding and heat capacity. 2016 , 1860, 868-878 | 44 |
| 734 | The Role of Conformational Changes in Molecular Recognition. 2016 , 120, 2138-44 | 10 |
| 733 | Remote Control by Inter-Enzyme Allostery: A Novel Paradigm for Regulation of the Shikimate Pathway. 2016 , 428, 1237-1255 | 19 |
| 732 | Conformational Dynamics and Allostery in Pyruvate Kinase. 2016 , 291, 9244-56 | 19 |
| 731 | Allosteric Mechanisms in Chaperonin Machines. 2016 , 116, 6588-606 | 65 |
| 730 | Solution NMR Spectroscopy for the Study of Enzyme Allostery. 2016 , 116, 6323-69 | 79 |
| 729 | Structural disorder: a tool for housekeeping proteins performing tissue-specific interactions. 2016 , 34, 1930-45 | 4 |
| 728 | Using THz Spectroscopy, Evolutionary Network Analysis Methods, and MD Simulation to Map the Evolution of Allosteric Communication Pathways in c-Type Lysozymes. 2016 , 33, 40-61 | 5 |
| 727 | Evolution of magnetization due to asymmetric dimerization: theoretical considerations and application to aberrant oligomers formed by apoSOD1(2SH). 2016 , 18, 5720-8 | 6 |

| | | |
|-----|---|-----|
| 726 | Importance of long-time simulations for rare event sampling in zinc finger proteins. 2016 , 34, 125-34 | 13 |
| 725 | Deciphering the cause of evolutionary variance within intrinsically disordered regions in human proteins. 2017 , 35, 233-249 | 7 |
| 724 | The role of dimer asymmetry and protomer dynamics in enzyme catalysis. 2017 , 355, | 113 |
| 723 | Principles of protein structural ensemble determination. 2017 , 42, 106-116 | 196 |
| 722 | Statistical mechanical model of gas adsorption in porous crystals with dynamic moieties. 2017 , 114, E287-E296 | 29 |
| 721 | Stacking Interactions Induced Selective Conformation of Discrete Aromatic Arrays and Borromean Rings. 2017 , 139, 1653-1660 | 87 |
| 720 | Common Hits Approach: Combining Pharmacophore Modeling and Molecular Dynamics Simulations. 2017 , 57, 365-385 | 47 |
| 719 | Protein-ligand (un)binding kinetics as a new paradigm for drug discovery at the crossroad between experiments and modelling. 2017 , 8, 534-550 | 51 |
| 718 | Designing an efficient multi-epitope oral vaccine against <i>Helicobacter pylori</i> using immunoinformatics and structural vaccinology approaches. 2017 , 13, 699-713 | 64 |
| 717 | Fundamentals of Enzyme Engineering. 2017 , | 3 |
| 716 | Piecing it together: Unraveling the elusive structure-function relationship in single-pass membrane receptors. 2017 , 1859, 1398-1416 | 17 |
| 715 | Predicting Protein Dynamics and Allostery Using Multi-Protein Atomic Distance Constraints. 2017 , 25, 546-558 | 31 |
| 714 | Predicting Allosteric Changes from Conformational Ensembles. 2017 , 25, 393-394 | 1 |
| 713 | Asymmetric configurations in a reengineered homodimer reveal multiple subunit communication pathways in protein allostery. 2017 , 292, 6086-6093 | 5 |
| 712 | An integrated perspective on RNA aptamer ligand-recognition models: clearing muddy waters. 2017 , 19, 6921-6932 | 8 |
| 711 | Altering the allosteric pathway in IGPS suppresses millisecond motions and catalytic activity. 2017 , 114, E3414-E3423 | 40 |
| 710 | Mechanistic Models Fit to Variable Temperature Calorimetric Data Provide Insights into Cooperativity. 2017 , 112, 1328-1338 | 4 |
| 709 | Structural Characterization of the Early Events in the Nucleation-Condensation Mechanism in a Protein Folding Process. 2017 , 139, 6899-6910 | 15 |

| | | |
|-----|---|----|
| 708 | Redox-Sensitive MarR Homologue BifR from Burkholderia thailandensis Regulates Biofilm Formation. 2017 , 56, 2315-2327 | 7 |
| 707 | Systematic Dissociation Pathway Searches Guided by Principal Component Modes. 2017 , 13, 2230-2244 | 7 |
| 706 | Induced Fit Is a Special Case of Conformational Selection. 2017 , 56, 2853-2859 | 29 |
| 705 | Mechanisms of Ubiquitin-Nucleosome Recognition and Regulation of 53BP1 Chromatin Recruitment by RNF168/169 and RAD18. 2017 , 66, 473-487.e9 | 51 |
| 704 | Computational Protein Design. 2017 , | 5 |
| 703 | Ligand Binding Swaps between Soft Internal Modes of β Tubulin and Alters Its Accessible Conformational Space. 2017 , 121, 118-128 | 9 |
| 702 | Computational Tools for Allosteric Drug Discovery: Site Identification and Focus Library Design. 2017 , 1529, 439-446 | 12 |
| 701 | Modeling Binding with Large Conformational Changes: Key Points in Ensemble-Docking Approaches. 2017 , 57, 1563-1578 | 13 |
| 700 | The maximum penalty criterion for ridge regression: application to the calibration of the force constant in elastic network models. 2017 , 9, 627-641 | 12 |
| 699 | Time-dependent inhibition of PHD2. 2017 , 37, | 3 |
| 698 | Induced-Fit Recognition of CCG Trinucleotide Repeats by a Nickel-Chromomycin Complex Resulting in Large-Scale DNA Deformation. 2017 , 56, 8761-8765 | 22 |
| 697 | The transient manifold structure of the p53 extreme C-terminal domain: insight into disorder, recognition, and binding promiscuity by molecular dynamics simulations. 2017 , 19, 21287-21296 | 11 |
| 696 | Allosteric Fine-Tuning of the Binding Pocket Dynamics in the ITK SH2 Domain by a Distal Molecular Switch: An Atomistic Perspective. 2017 , 121, 6131-6138 | 1 |
| 695 | Combined Monte Carlo/torsion-angle molecular dynamics for ensemble modeling of proteins, nucleic acids and carbohydrates. 2017 , 73, 179-190 | 11 |
| 694 | Structures of Large Protein Complexes Determined by Nuclear Magnetic Resonance Spectroscopy. 2017 , 46, 317-336 | 42 |
| 693 | A Network of Conformational Transitions in the Apo Form of NDM-1 Enzyme Revealed by MD Simulation and a Markov State Model. 2017 , 121, 2952-2960 | 6 |
| 692 | Relation between Protein Intrinsic Normal Mode Weights and Pre-Existing Conformer Populations. 2017 , 121, 3686-3700 | 5 |
| 691 | Exploring Binding Mechanisms in Nuclear Hormone Receptors by Monte Carlo and X-ray-derived Motions. 2017 , 112, 1147-1156 | 18 |

| | | |
|-----|--|----|
| 690 | Tuning the Continuum of Structural States in the Native Ensemble of a Regulatory Protein. 2017 , 8, 1683-1687 | 7 |
| 689 | Opposing Intermolecular Tuning of Ca Affinity for Calmodulin by Neurogranin and CaMKII Peptides. 2017 , 112, 1105-1119 | 8 |
| 688 | The Michaelis Complex of Arginine Kinase Samples the Transition State at a Frequency That Matches the Catalytic Rate. 2017 , 139, 4846-4853 | 9 |
| 687 | Dynamic Descriptions of Highly Flexible Molecules from NMR Dipolar Couplings: Physical Basis and Limitations. 2017 , 139, 5011-5014 | 10 |
| 686 | Molecular dynamics simulations elucidate conformational selection and induced fit mechanisms in the binding of PD-1 and PD-L1. 2017 , 13, 892-900 | 18 |
| 685 | Phosphorylation-induced conformational dynamics in an intrinsically disordered protein and potential role in phenotypic heterogeneity. 2017 , 114, E2644-E2653 | 55 |
| 684 | Integration on Ligand and Structure Based Approaches in GPCRs. 2017 , 101-161 | 0 |
| 683 | Integrated structural biology to unravel molecular mechanisms of protein-RNA recognition. 2017 , 118-119, 119-136 | 35 |
| 682 | Multiple Conformations of Gal3 Protein Drive the Galactose-Induced Allosteric Activation of the GAL Genetic Switch of <i>Saccharomyces cerevisiae</i> . 2017 , 429, 158-176 | 2 |
| 681 | Synthesis of a biological active Hairpin peptide by addition of two structural motifs. 2017 , 25, 603-608 | 8 |
| 680 | (S)Pinning down protein interactions by NMR. 2017 , 26, 436-451 | 33 |
| 679 | Modeling Protein Excited-state Structures from "Over-length" Chemical Cross-links. 2017 , 292, 1187-1196 | 30 |
| 678 | Binding Site Configurations Probe the Structure and Dynamics of the Zinc Finger of NEMO (NF- κ B Essential Modulator). 2017 , 56, 623-633 | 14 |
| 677 | Complementary oligonucleotides regulate induced fit ligand binding in duplexed aptamers. 2017 , 8, 2251-2256 | 20 |
| 676 | Energetics and structural characterization of the "DFG-flip" conformational transition of B-RAF kinase: a SITS molecular dynamics study. 2017 , 19, 1257-1267 | 13 |
| 675 | Oxatub[5,6]arene: synthesis, conformational analysis, and the recognition of C60 and C70. 2016 , 53, 336-339 | 26 |
| 674 | Mobile base station with conformational selections for the network maintenance in wireless multihop infrastructure. 2017 , 28, e3130 | 2 |
| 673 | Protein-peptide association kinetics beyond the seconds timescale from atomistic simulations. 2017 , 8, 1095 | 76 |

| | | |
|-----|--|----|
| 672 | Conformational heterogeneity in tails of DNA-binding proteins is augmented by proline containing repeats. 2017 , 13, 2531-2544 | 1 |
| 671 | Using chirality to probe the conformational dynamics and assembly of intrinsically disordered amyloid proteins. 2017 , 7, 12433 | 24 |
| 670 | Synthesis of Naphthyridine Dimers with Conformational Restriction and Binding to DNA and RNA. 2017 , 12, 3077-3087 | 7 |
| 669 | Power of protein/tRNA functional assembly against aberrant aggregation. 2017 , 19, 28014-28027 | |
| 668 | Engineering of the Conformational Dynamics of Lipase To Increase Enantioselectivity. 2017 , 7, 7593-7599 | 21 |
| 667 | Slow molecular recognition by RNA. 2017 , 23, 1745-1753 | 20 |
| 666 | Molecular Simulations of Melittin-Induced Membrane Pores. 2017 , 121, 10209-10214 | 18 |
| 665 | Interplay between the folding mechanism and binding modes in folding coupled to binding processes. 2017 , 19, 28512-28516 | 5 |
| 664 | Cardiotoxins: Functional Role of Local Conformational Changes. 2017 , 57, 2799-2810 | 12 |
| 663 | Membrane Dynamics of β Secretase Provides a Molecular Basis for β Amyloid Binding and Processing. 2017 , 8, 2424-2436 | 34 |
| 662 | Enhanced Sampling of Intrinsic Structural Heterogeneity of the BH3-Only Protein Binding Interface of Bcl-xL. 2017 , 121, 9160-9168 | 13 |
| 661 | Biologically derived metal organic frameworks. 2017 , 349, 102-128 | 70 |
| 660 | Emergence of Alternative Structures in Amyloid Beta 1-42 Monomeric Landscape by N-terminal Hexapeptide Amyloid Inhibitors. 2017 , 7, 9941 | 19 |
| 659 | Direct observation of conformational population shifts in crystalline human hemoglobin. 2017 , 292, 18258-18269 | |
| 658 | Protein phosphorylation and its role in the regulation of Annexin A2 function. 2017 , 1861, 2515-2529 | 53 |
| 657 | Path lumping: An efficient algorithm to identify metastable path channels for conformational dynamics of multi-body systems. 2017 , 147, 044112 | 5 |
| 656 | Investigating Protein Sequence-structure-dynamics Relationships with Bio3D-web. 2017 , | 2 |
| 655 | Calcium-Mediated Control of S100 Proteins: Allosteric Communication via an Agitator/Signal Blocking Mechanism. 2017 , 139, 11460-11470 | 10 |

| | | |
|-----|--|----|
| 654 | Site of Tagging Influences the Ochratoxin Recognition by Peptide NFO4: A Molecular Dynamics Study. 2017 , 57, 2035-2044 | 3 |
| 653 | Modulation of polypeptide conformation through donor-acceptor transformation of side-chain hydrogen bonding ligands. 2017 , 8, 92 | 33 |
| 652 | An optimal distance cutoff for contact-based Protein Structure Networks using side-chain centers of mass. 2017 , 7, 2838 | 44 |
| 651 | A novel HPV prophylactic peptide vaccine, designed by immunoinformatics and structural vaccinology approaches. 2017 , 54, 402-416 | 41 |
| 650 | Activation processes in ligand-activated G protein-coupled receptors: A case study of the adenosine A receptor. 2017 , 39, 1700072 | 13 |
| 649 | Amino Acid Insertion Frequencies Arising from Photoproducts Generated Using Aliphatic Diazirines. 2017 , 28, 2011-2021 | 32 |
| 648 | Blocking protein quality control to counter hereditary cancers. 2017 , 56, 823-831 | 18 |
| 647 | Network of Conformational Transitions Revealed by Molecular Dynamics Simulations of the Carbonic Anhydrase II Apo-Enzyme. 2017 , 2, 8414-8420 | 6 |
| 646 | Insight into the molecular recognition mechanism of the coactivator NCoA1 by STAT6. 2017 , 7, 16845 | 5 |
| 645 | Initial Structural Models of the A β 2 Dimer from Replica Exchange Molecular Dynamics Simulations. 2017 , 2, 7621-7636 | 7 |
| 644 | Changes in Enzyme Structural Dynamics Studied by Hydrogen Exchange-Mass Spectrometry: Ligand Binding Effects or Catalytically Relevant Motions?. 2017 , 89, 13326-13333 | 9 |
| 643 | Ligand Recognition Mechanism of Thiamine Pyrophosphate Riboswitch Aptamer. 2017 , 38, 1465-1473 | 2 |
| 642 | Real-Time Conformational Changes and Controlled Orientation of Native Proteins Inside a Protein Nanoreactor. 2017 , 139, 18640-18646 | 60 |
| 641 | HyRes: a coarse-grained model for multi-scale enhanced sampling of disordered protein conformations. 2017 , 19, 32421-32432 | 13 |
| 640 | Deciphering Conformational Changes Associated with the Maturation of Thrombin Anion Binding Exosite I. 2017 , 56, 6343-6354 | 1 |
| 639 | Role of Conformational Dynamics in the Evolution of Retro-Aldolase Activity. 2017 , 7, 8524-8532 | 62 |
| 638 | Induced-Fit Recognition of CCG Trinucleotide Repeats by a Nickel-Chromomycin Complex Resulting in Large-Scale DNA Deformation. 2017 , 129, 8887-8891 | |
| 637 | Reaction-diffusion with stochastic decay rates. 2017 , 19, 18863-18879 | 20 |

| | | |
|-----|--|----|
| 636 | Direct examination of the relevance for folding, binding and electron transfer of a conserved protein folding intermediate. 2017 , 19, 19021-19031 | 1 |
| 635 | Enhanced Binding Affinity via Destabilization of the Unbound State: A Millisecond Hydrogen-Deuterium Exchange Study of the Interaction between p53 and a Pleckstrin Homology Domain. 2017 , 56, 4127-4133 | 6 |
| 634 | Electrostatic Control of Chemistry in Terpene Cyclases. 2017 , 7, 5461-5465 | 28 |
| 633 | Conformational Selection as the Mechanism of Guest Binding in a Flexible Supramolecular Host. 2017 , 139, 8013-8021 | 74 |
| 632 | Conformational Heterogeneity of the HIV Envelope Glycan Shield. 2017 , 7, 4435 | 22 |
| 631 | Understanding the core of RNA interference: The dynamic aspects of Argonaute-mediated processes. 2017 , 128, 39-46 | 7 |
| 630 | Osmolyte-Like Stabilizing Effects of Low GdnHCl Concentrations on d-Glucose/d-Galactose-Binding Protein. 2017 , 18, | 1 |
| 629 | Evaluation of Ochratoxin Recognition by Peptides Using Explicit Solvent Molecular Dynamics. 2017 , 9, | 6 |
| 628 | Molecular Modeling and Simulation Tools in the Development of Peptide-Based Biosensors for Mycotoxin Detection: Example of Ochratoxin. 2017 , 9, 395 | 8 |
| 627 | Peptide and Peptide-Dependent Motions in MHC Proteins: Immunological Implications and Biophysical Underpinnings. 2017 , 8, 935 | 27 |
| 626 | Binding kinetics in drug discovery - A current perspective. 2017 , 22, 21-47 | 6 |
| 625 | Determinants of Macromolecular Specificity from Proteomics-Derived Peptide Substrate Data. 2017 , 18, 905-913 | 0 |
| 624 | The Design of Repeat Proteins: Stability Conflicts with Functionality. 2017 , 03, | 3 |
| 623 | Allosteric Modulators. 2017 , 276-296 | 4 |
| 622 | Specific Interaction Sites Determine Differential Adsorption of Protein Structural Isomers on Nanoparticle Surfaces. 2018 , 24, 5911-5919 | 9 |
| 621 | Introduction of Intrinsic Kinetics of Protein-Ligand Interactions and Their Implications for Drug Design. 2018 , 61, 2292-2302 | 13 |
| 620 | Allosterically Activated Protein Self-Assembly for the Construction of Helical Microfilaments with Tunable Helicity. 2018 , 130, 5123-5126 | 3 |
| 619 | AFD: an application for bi-molecular interaction using axial frequency distribution. 2018 , 24, 84 | 14 |

| | | |
|-----|---|-----|
| 618 | Molecular recognition by synthetic receptors: Application in field-effect transistor based chemosensing. 2018 , 109, 50-62 | 14 |
| 617 | Identifying Conformational-Selection and Induced-Fit Aspects in the Binding-Induced Folding of PMI from Markov State Modeling of Atomistic Simulations. 2018 , 122, 5649-5656 | 15 |
| 616 | Allosterically Activated Protein Self-Assembly for the Construction of Helical Microfilaments with Tunable Helicity. 2018 , 57, 5029-5032 | 13 |
| 615 | Epoxide Hydrolase Conformational Heterogeneity for the Resolution of Bulky Pharmacologically Relevant Epoxide Substrates. 2018 , 24, 12254-12258 | 7 |
| 614 | Efficiently Photocontrollable or Not? Biological Activity of Photoisomerizable Diarylethenes. 2018 , 24, 11245-11254 | 23 |
| 613 | Targeting Intrinsically Disordered Transcription Factors: Changing the Paradigm. 2018 , 430, 2321-2341 | 61 |
| 612 | Peptidic Macrocycles - Conformational Sampling and Thermodynamic Characterization. 2018 , 58, 982-992 | 38 |
| 611 | A Long Cytoplasmic Loop Governs the Sensitivity of the Anti-viral Host Protein SERINC5 to HIV-1 Nef. 2018 , 22, 869-875 | 35 |
| 610 | Partner-Specific Prediction of Protein-Dimer Stability from Unbound Structure of Monomer. 2018 , 58, 733-745 | 3 |
| 609 | Programmable DNA switches and their applications. 2018 , 10, 4607-4641 | 69 |
| 608 | On the folding of a structurally complex protein to its metastable active state. 2018 , 115, 1998-2003 | 13 |
| 607 | Importance of protein flexibility in molecular recognition: a case study on Type-11/2 inhibitors of ALK. 2018 , 20, 4851-4863 | 21 |
| 606 | Chain Assembly and Disassembly Processes Differently Affect the Conformational Space of Ubiquitin Chains. 2018 , 26, 249-258.e4 | 11 |
| 605 | Binding of Zn(II) to Tropomyosin Receptor Kinase A in Complex with Its Cognate Nerve Growth Factor: Insights from Molecular Simulation and in Vitro Essays. 2018 , 9, 1095-1103 | 1 |
| 604 | Unified understanding of folding and binding mechanisms of globular and intrinsically disordered proteins. 2018 , 10, 163-181 | 22 |
| 603 | Enhanced spontaneous DNA twisting/bending fluctuations unveiled by fluorescence lifetime distributions promote mismatch recognition by the Rad4 nucleotide excision repair complex. 2018 , 46, 1240-1255 | 16 |
| 602 | A Map of Protein-Metabolite Interactions Reveals Principles of Chemical Communication. 2018 , 172, 358-372.e23 | 192 |
| 601 | Applications of the NRGsuite and the Molecular Docking Software FlexAID in Computational Drug Discovery and Design. 2018 , 1762, 367-388 | 4 |

| | | |
|-----|---|----|
| 600 | Endo- and Exocyclic Coordination of a 20-Membered NOS-Macrocyclic and Cascade Complexation of a 40-Membered NOS-Macrocyclic. 2018 , 57, 6289-6299 | 8 |
| 599 | Effect of Methylation on Local Mechanics and Hydration Structure of DNA. 2018 , 114, 1791-1803 | 18 |
| 598 | Conformational Ensemble and Biological Role of the TCTP Intrinsically Disordered Region: Influence of Calcium and Phosphorylation. 2018 , 430, 1621-1639 | 2 |
| 597 | The Role of the Active Site Flap in Streptavidin/Biotin Complex Formation. 2018 , 140, 5434-5446 | 12 |
| 596 | Structural Ensemble Modulation upon Small-Molecule Binding to Disordered Proteins. 2018 , 430, 2288-2292 | 30 |
| 595 | Conformational Sampling of the Intrinsically Disordered C-Terminal Tail of DERA Is Important for Enzyme Catalysis. 2018 , 8, 3971-3984 | 10 |
| 594 | Measuring the signs of the methyl H chemical shift differences between major and 'invisible' minor protein conformational states using methyl H multi-quantum spectroscopy. 2018 , 70, 187-202 | 6 |
| 593 | From Optimization to Mapping: An Evolutionary Algorithm for Protein Energy Landscapes. 2018 , 15, 719-731 | 6 |
| 592 | Structure-Guided Protein Transition Modeling with a Probabilistic Roadmap Algorithm. 2018 , 15, 1783-1796 | 6 |
| 591 | Incorporation of Solvent Effect into Multi-Objective Evolutionary Algorithm for Improved Protein Structure Prediction. 2018 , 15, 1365-1378 | 33 |
| 590 | Conformational Selection of Dimethylarginine Recognition by the Survival Motor Neuron Tudor Domain. 2018 , 130, 495-499 | |
| 589 | Conformational Selection of Dimethylarginine Recognition by the Survival Motor Neuron Tudor Domain. 2018 , 57, 486-490 | 1 |
| 588 | Discovery of hidden allosteric sites as novel targets for allosteric drug design. 2018 , 23, 359-365 | 73 |
| 587 | Solution NMR views of dynamical ordering of biomacromolecules. 2018 , 1862, 287-306 | 19 |
| 586 | Technical Basis for Nuclear Magnetic Resonance Approach for Glycoproteins. 2018 , 415-438 | 7 |
| 585 | Inter-Enzyme Allosteric Regulation of Chorismate Mutase in <i>Corynebacterium glutamicum</i> : Structural Basis of Feedback Activation by Trp. 2018 , 57, 557-573 | 14 |
| 584 | Structural vaccinology considerations for in silico designing of a multi-epitope vaccine. 2018 , 58, 96-109 | 56 |
| 583 | Laboratory evolution of protein conformational dynamics. 2018 , 50, 49-57 | 56 |

| | | |
|-----|---|-----|
| 582 | The price of flexibility - a case study on septanoses as pyranose mimetics. 2018 , 9, 646-654 | 20 |
| 581 | Molecular dynamics simulations and novel drug discovery. 2018 , 13, 23-37 | 151 |
| 580 | Peptide mediated facile fabrication of silver nanoparticles over living diatom surface and its application. 2018 , 249, 600-608 | 29 |
| 579 | Sample-Based Models of Protein Energy Landscapes and Slow Structural Rearrangements. 2018 , 25, 33-50 | 6 |
| 578 | Structure-based prediction of protein allostery. 2018 , 50, 1-8 | 57 |
| 577 | The application of ion-mobility mass spectrometry for structure/function investigation of protein complexes. 2018 , 42, 25-33 | 71 |
| 576 | Single-molecule imaging and manipulation of biomolecular machines and systems. 2018 , 1862, 241-252 | 9 |
| 575 | Refinement of Highly Flexible Protein Structures using Simulation-Guided Spectroscopy. 2018 , 130, 17356-17360 | |
| 574 | Reconstructing and Decomposing Protein Energy Landscapes to Organize Structure Spaces and Reveal Biologically-active States. 2018 , | |
| 573 | How Human Alpha-lactalbumin Recognize DNA and RNA. 2018 , 07, | |
| 572 | An Energy Landscape Treatment of Decoy Selection in Template-Free Protein Structure Prediction. 2018 , 6, 39 | 7 |
| 571 | . 2018 , | 1 |
| 570 | Generating Two-Dimensional Repertoire of siRNA Linc-ROR and siRNA mRNA ARF6 from the lincRNA-RoR/miR-145/ARF6 expression Pathway that involved in the progression of Triple Negative Breast Cancer. 2018 , 299, 012059 | |
| 569 | Understanding Allostery to Design New Drugs. 2018 , 281-300 | |
| 568 | The entropic force generated by intrinsically disordered segments tunes protein function. 2018 , 563, 584-588 | 66 |
| 567 | Imaginative Order from Reasonable Chaos: Conformation-Driven Activity and Reactivity in Exploring ProteinLigand Interactions. 2018 , 71, 917 | |
| 566 | Millisecond Timescale Motions Connect Amino Acid Interaction Networks in Alpha Tryptophan Synthase. 2018 , 5, 92 | 5 |
| 565 | Transition path times of coupled folding and binding reveal the formation of an encounter complex. 2018 , 9, 4708 | 51 |

| | | |
|-----|--|----|
| 564 | 2018 ISCB accomplishments by a senior scientist award. 2018 , 14, e1006138 | 0 |
| 563 | Molecular DynamicsBased Approaches Describing Protein Binding. 2018 , 29-42 | 1 |
| 562 | Refinement of Highly Flexible Protein Structures using Simulation-Guided Spectroscopy. 2018 , 57, 17110-17114 | |
| 561 | Oxidative damage to epigenetically methylated sites affects DNA stability, dynamics and enzymatic demethylation. 2018 , 46, 10827-10839 | 12 |
| 560 | Diversification of Device Platforms by Molecular Layers: Hybrid Sensing Platforms, Monolayer Doping, and Modeling. 2018 , 34, 14103-14123 | 9 |
| 559 | Autoinhibition in Ras effectors Raf, PI3K and RASSF5: a comprehensive review underscoring the challenges in pharmacological intervention. 2018 , 10, 1263-1282 | 29 |
| 558 | Redox Kinetics of the Amyloid-ECu Complex and Its Biological Implications. 2018 , 57, 6228-6233 | 4 |
| 557 | 'Negative' and 'positive catalysis': complementary principles that shape the catalytic landscape of enzymes. 2018 , 47, 94-100 | 21 |
| 556 | From mutations to mechanisms and dysfunction via computation and mining of protein energy landscapes. 2018 , 19, 671 | 3 |
| 555 | Computational Studies for Structure-Based Drug Designing Against Transmembrane Receptors: pLGICs and Class A GPCRs. 2018 , 6, | 4 |
| 554 | Induced-fit expansion and contraction of a self-assembled nanocube finely responding to neutral and anionic guests. 2018 , 9, 4530 | 23 |
| 553 | DNA-Based Nanodevices Controlled by Purely Entropic Linker Domains. 2018 , 140, 14725-14734 | 19 |
| 552 | Regional conformational flexibility couples substrate specificity and scissile phosphate diester selectivity in human flap endonuclease 1. 2018 , 46, 5618-5633 | 7 |
| 551 | Proteins That Chaperone RNA Regulation. 2018 , 383-397 | 6 |
| 550 | Mechanical variations in proteins with large-scale motions highlight the formation of structural locks. 2018 , 203, 195-204 | 2 |
| 549 | Role of conformational dynamics in the evolution of novel enzyme function. 2018 , 54, 6622-6634 | 83 |
| 548 | Intrinsic structural versatility of the highly conserved 412-423 epitope of the Hepatitis C Virus E2 protein. 2018 , 116, 620-632 | 5 |
| 547 | Message from the ISCB: 2018 ISCB Accomplishments by a Senior Scientist Award. 2018 , 34, 2332-2333 | |

| | | |
|-----|---|----|
| 546 | Conserved conformational selection mechanism of Hsp70 chaperone-substrate interactions. 2018 , 7, | 50 |
| 545 | Dissecting conformational changes in APP's transmembrane domain linked to inefficiency in familial Alzheimer's disease. 2018 , 13, e0200077 | 9 |
| 544 | DNA-binding induced conformational change of c-Myb R2R3 analyzed using diffracted X-ray tracking. 2018 , 503, 338-343 | 4 |
| 543 | Magnesium Activates Microsecond Dynamics to Regulate Integrin-Collagen Recognition. 2018 , 26, 1080-1090.e5 | 5 |
| 542 | Improving Prediction Accuracy of Binding Free Energies and Poses of HIV Integrase Complexes Using the Binding Energy Distribution Analysis Method with Flattening Potentials. 2018 , 58, 1356-1371 | 6 |
| 541 | The use of residual dipolar couplings for conformational analysis of non-steroidal anti-inflammatory drugs dissolved in weakly ordering media. 2018 , 45, 2033-2047 | 3 |
| 540 | The Role of Molecular Modeling in Predicting Carbohydrate Antigen Conformation and Understanding Vaccine Immunogenicity. 2018 , 139-173 | 5 |
| 539 | Electrostatic control of calcineurin's intrinsically-disordered regulatory domain binding to calmodulin. 2018 , 1862, 2651-2659 | 4 |
| 538 | Proteins That Chaperone RNA Regulation. 2018 , 6, | 38 |
| 537 | Lead Identification Through the Synergistic Action of Biomolecular NMR and In Silico Methodologies. 2018 , 1824, 299-316 | 2 |
| 536 | Evolutionary repurposing of a sulfatase: A new Michaelis complex leads to efficient transition state charge offset. 2018 , 115, E7293-E7302 | 28 |
| 535 | Inhibition of the precursor and mature forms of HIV-1 protease as a tool for drug evaluation. 2018 , 8, 10438 | 9 |
| 534 | Effects of Disease-Causing Mutations on the Conformation of Human Apolipoprotein A-I in Model Lipoproteins. 2018 , 57, 4583-4596 | 5 |
| 533 | Determination of the conformational states of strychnine in solution using NMR residual dipolar couplings in a tensor-free approach. 2018 , 148, 4-8 | 7 |
| 532 | Reverse Binding Mode of Phosphotyrosine Peptides with SH2 Protein. 2018 , 57, 5257-5269 | 3 |
| 531 | Tunable order-disorder continuum in protein-DNA interactions. 2018 , 46, 8700-8709 | 13 |
| 530 | A Dynamic Overview of Antimicrobial Peptides and Their Complexes. 2018 , 23, | 11 |
| 529 | The different modes of binding of the dust mite allergens, Der f 7 and Der p 7, on a monoclonal antibody WH9 contribute to the differential reactivity. 2018 , 51, 478-484 | 1 |

| | | |
|-----|--|----|
| 528 | Entropic Control of an Excited Folded-Like Conformation in a Disordered Protein Ensemble. 2018 , 430, 2688-2694 | 7 |
| 527 | Allosteric Modulators of HSP90 and HSP70: Dynamics Meets Function through Structure-Based Drug Design. 2019 , 62, 60-87 | 59 |
| 526 | Prediction of Protein-Protein Interactions: Looking Through the Kaleidoscope. 2019 , 834-848 | |
| 525 | Study of the Variability of the Native Protein Structure. 2019 , 606-619 | 2 |
| 524 | Conformational Control of Macrocycles by Remote Structural Modification. 2019 , 119, 9724-9752 | 51 |
| 523 | O sensitivity and H production activity of hydrogenases-A review. 2019 , 116, 3124-3135 | 23 |
| 522 | Tuning a timing device that regulates lateral root development in rice. 2019 , 73, 493-507 | 4 |
| 521 | How B-DNA Dynamics Decipher Sequence-Selective Protein Recognition. 2019 , 431, 3845-3859 | 15 |
| 520 | : Consistent Identification of Plausible Binding Sites Despite the Elusive Nature of Cavities and Grooves in Protein Dynamics. 2019 , 59, 3506-3518 | 9 |
| 519 | Network analysis of dynamically important residues in protein structures mediating ligand-binding conformational changes. 2019 , 48, 559-568 | 4 |
| 518 | Decreasing the immunogenicity of Erwinia chrysanthemi asparaginase via protein engineering: computational approach. 2019 , 46, 4751-4761 | 0 |
| 517 | Uncovering the Molecular Interactions in the Catalytic Loop That Modulate the Conformational Dynamics in Protein Tyrosine Phosphatase 1B. 2019 , 141, 12634-12647 | 14 |
| 516 | Structure and Function of GPCRs. 2019 , | |
| 515 | In-silico Methods of Drug Design: Molecular Simulations and Free Energy Calculations. 2019 , 521-533 | 4 |
| 514 | NMR Characterization of Conformational Dynamics and Molecular Assemblies of Proteins. 2019 , 42, 867-872 | 1 |
| 513 | Experimental studies of binding of intrinsically disordered proteins to their partners. 2019 , 139-187 | 2 |
| 512 | Beclin1-mediated ferroptosis activation is associated with isoflurane-induced toxicity in SH-SY5Y neuroblastoma cells. 2019 , 51, 1134-1141 | 10 |
| 511 | Exploring and Engineering the Conformational Landscape of Calmodulin through Specific Interactions. 2019 , 123, 9321-9327 | 1 |

| | | |
|-----|---|----|
| 510 | Single-Molecule Observation of Ligand Binding and Conformational Changes in FeuA. 2019 , 117, 1642-1654 | 14 |
| 509 | Can Conformational Changes of Proteins Be Represented in Torsion Angle Space? A Study with Rescaled Ridge Regression. 2019 , 59, 4929-4941 | 6 |
| 508 | Target Discovery Using Thermal Proteome Profiling. 2019 , 267-291 | 3 |
| 507 | The static and dynamic structural heterogeneities of B-DNA: extending Calladine-Dickerson rules. 2019 , 47, 11090-11102 | 18 |
| 506 | Protein Allostery in Drug Discovery. 2019 , | 5 |
| 505 | Structures of SF3b1 reveal a dynamic Achilles heel of spliceosome assembly: Implications for cancer-associated abnormalities and drug discovery. 2019 , 1862, 194440 | 8 |
| 504 | Binding-induced folding under unfolding conditions: Switching between induced fit and conformational selection mechanisms. 2019 , 294, 16942-16952 | 13 |
| 503 | Does Ras Activate Raf and PI3K Allosterically?. 2019 , 9, 1231 | 29 |
| 502 | Branch site bulge conformations in domain 6 determine functional sugar puckers in group II intron splicing. 2019 , 47, 11430-11440 | 7 |
| 501 | Direct observation of Thermomyces lanuginosus lipase diffusional states by Single Particle Tracking and their remodeling by mutations and inhibition. 2019 , 9, 16169 | 14 |
| 500 | Selektive Synthese von Iridium(III)-Metalla[2]catenänen durch Präorganisation der Komponenten über Wechselwirkungen. 2019 , 131, 5941-5946 | 10 |
| 499 | An ensemble of flexible conformations underlies mechanotransduction by the cadherin-catenin adhesion complex. 2019 , 116, 21545-21555 | 15 |
| 498 | Cell size effects in the molecular dynamics of the intrinsically disordered A β peptide. 2019 , 151, 085101 | 14 |
| 497 | Using subpopulation EAs to map molecular structure landscapes. 2019 , | 1 |
| 496 | Switching of and Mechanisms in Host-Guest Binding Associated with Chemical Reactions. 2019 , 141, 15597-15604 | 10 |
| 495 | Involvement of Local, Rapid Conformational Dynamics in Binding of Flexible Recognition Motifs. 2019 , 123, 8387-8396 | 3 |
| 494 | A reinforcement-learning-based approach to enhance exhaustive protein loop sampling. 2020 , 36, 1099-1106 | 5 |
| 493 | The pressure and temperature perturbation approach reveals a whole variety of conformational substates of amyloidogenic hIAPP monitored by 2D NMR spectroscopy. 2019 , 254, 106239 | 7 |

| | | |
|-----|--|----|
| 492 | Discovery and Characterization of a Cellular Potent Positive Allosteric Modulator of the Polycomb Repressive Complex 1 Chromodomain, CBX7. 2019 , 26, 1365-1379.e22 | 21 |
| 491 | Engineering of lysine cyclodeaminase conformational dynamics for relieving substrate and product inhibitions in the biosynthesis of L-pipecolic acid. 2019 , 9, 398-405 | 7 |
| 490 | Fluorometric Recognition of Nucleotides within a Water-Soluble Tetrahedral Capsule. 2019 , 58, 4200-4204 | 32 |
| 489 | Computational approach to suggest a new multi-target-directed ligand as a potential medication for Alzheimer's disease. 2019 , 37, 4825-4839 | 10 |
| 488 | Experimental free ligand conformations: a missing link in structure-based drug discovery. 2019 , 11, 79-82 | 17 |
| 487 | Extending the Lifetime of Native GTP-Bound Ras for Site-Resolved NMR Measurements: Quantifying the Allosteric Dynamics. 2019 , 131, 2756-2759 | |
| 486 | Duplexed aptamers: history, design, theory, and application to biosensing. 2019 , 48, 1390-1419 | 89 |
| 485 | Internal Coordinate Normal Mode Analysis: A Strategy To Predict Protein Conformational Transitions. 2019 , 123, 1294-1301 | 10 |
| 484 | Thrombin Exosite Maturation and Ligand Binding at ABE II Help Stabilize PAR-Binding Competent Conformation at ABE I. 2019 , 58, 1048-1060 | 2 |
| 483 | Dynamic Control of Intramolecular Rotation by Tuning the Surrounding Two-Dimensional Matrix Field. 2019 , 13, 2410-2419 | 29 |
| 482 | Fluorometric Recognition of Nucleotides within a Water-Soluble Tetrahedral Capsule. 2019 , 131, 4244-4248 | 9 |
| 481 | Extending the Lifetime of Native GTP-Bound Ras for Site-Resolved NMR Measurements: Quantifying the Allosteric Dynamics. 2019 , 58, 2730-2733 | 8 |
| 480 | Gynoecium development: networks in Arabidopsis and beyond. 2019 , 70, 1447-1460 | 20 |
| 479 | Intermolecular distance measurement with TNT suppressor on the M13 bacteriophage-based Förster resonance energy transfer system. 2019 , 9, 496 | 1 |
| 478 | Selective Inhibitors of FKBP51 Employ Conformational Selection of Dynamic Invisible States. 2019 , 131, 9529-9533 | 3 |
| 477 | On the relationship between docking scores and protein conformational changes in HIV-1 protease. 2019 , 91, 186-193 | 4 |
| 476 | Topochemical Synthesis of Single-Crystalline Hydrogen-Bonded Cross-Linked Organic Frameworks and Their Guest-Induced Elastic Expansion. 2019 , 141, 10915-10923 | 34 |
| 475 | Attenuating dependence on structural data in computing protein energy landscapes. 2019 , 20, 280 | |

| | | |
|-----|--|-----|
| 474 | The roles of structural dynamics in the cellular functions of RNAs. 2019 , 20, 474-489 | 144 |
| 473 | Hybrid Refinement of Heterogeneous Conformational Ensembles Using Spectroscopic Data. 2019 , 10, 3410-3414 | 5 |
| 472 | Modulating Hinge Flexibility in the APP Transmembrane Domain Alters β Secretase Cleavage. 2019 , 116, 2103-2120 | 16 |
| 471 | Conformational Selection in Anion Recognition: cGMP-Selective Binding by a Naphthalimide-Functionalized Amido-Amine Macrocycle. 2019 , 84, 9034-9043 | 9 |
| 470 | Self-assembly in elastin-like recombinamers: a mechanism to mimic natural complexity. 2019 , 2, 100007 | 14 |
| 469 | Mechanisms of Specific versus Nonspecific Interactions of Aggregation-Prone Inhibitors and Attenuators. 2019 , 62, 5063-5079 | 18 |
| 468 | Prescient Indices of Activity: The Application of Functional System Sensitivity to Measurement of Drug Effect. 2019 , 40, 529-539 | 3 |
| 467 | Selective Inhibitors of FKBP51 Employ Conformational Selection of Dynamic Invisible States. 2019 , 58, 9429-9433 | 7 |
| 466 | Symmetry, Rigidity, and Allosteric Signaling: From Monomeric Proteins to Molecular Machines. 2019 , 119, 6788-6821 | 41 |
| 465 | Detection of molecular behavior that characterizes systems using a deep learning approach. 2019 , 11, 10064-10071 | 2 |
| 464 | Conformational Stability Adaptation of a Double-Stranded RNA-Binding Domain to Transfer RNA Ligand. 2019 , 58, 2463-2473 | 2 |
| 463 | Predicted dynamical couplings of protein residues characterize catalysis, transport and allostery. 2019 , 35, 4971-4978 | 10 |
| 462 | Intrinsically disordered proteins and phenotypic switching: Implications in cancer. 2019 , 166, 63-84 | 9 |
| 461 | Holo-like and Druggable Protein Conformations from Enhanced Sampling of Binding Pocket Volume and Shape. 2019 , 59, 1515-1528 | 22 |
| 460 | Highly Selective Synthesis of Iridium(III) Metalla[2]catenanes through Component Pre-Orientation by π - π Stacking. 2019 , 58, 5882-5886 | 36 |
| 459 | LARP4A recognizes polyA RNA via a novel binding mechanism mediated by disordered regions and involving the PAM2w motif, revealing interplay between PABP, LARP4A and mRNA. 2019 , 47, 4272-4291 | 12 |
| 458 | A Semi-Empirical Framework for Interpreting Traveling Wave Ion Mobility Arrival Time Distributions. 2019 , 30, 956-966 | 3 |
| 457 | Biased Receptor Signaling in Drug Discovery. 2019 , 71, 267-315 | 115 |

| | | |
|-----|--|----|
| 456 | Graph-Based Community Detection for Decoy Selection in Template-Free Protein Structure Prediction. 2019 , 24, | 5 |
| 455 | Conformational studies of RGDechi peptide by natural-abundance NMR spectroscopy. 2019 , 25, e3166 | 6 |
| 454 | Review: Precision medicine and driver mutations: Computational methods, functional assays and conformational principles for interpreting cancer drivers. 2019 , 15, e1006658 | 45 |
| 453 | General mathematical formula for near equilibrium relaxation kinetics of basic enzyme reactions and its applications to find conformational selection steps. 2019 , 313, 61-70 | 1 |
| 452 | Learning Organizations of Protein Energy Landscapes: An Application on Decoy Selection in Template-Free Protein Structure Prediction. 2019 , 1958, 147-171 | 2 |
| 451 | Single-Molecule FRET Kinetics of the Mn Riboswitch: Evidence for Allosteric Mg Control of "Induced-Fit" vs "Conformational Selection" Folding Pathways. 2019 , 123, 2005-2015 | 17 |
| 450 | Dissecting a novel allosteric mechanism of cruzain: A computer-aided approach. 2019 , 14, e0211227 | 9 |
| 449 | Interaction Force Fluctuations in Antigen-Antibody Biorecognition Studied by Atomic Force Spectroscopy. 2019 , 4, 3627-3634 | 2 |
| 448 | Massive-Scale Binding Free Energy Simulations of HIV Integrase Complexes Using Asynchronous Replica Exchange Framework Implemented on the IBM WCG Distributed Network. 2019 , 59, 1382-1397 | 3 |
| 447 | Effects of a remote mutation from the contact paratope on the structure of CDR-H3 in the anti-HIV neutralizing antibody PG16. 2019 , 9, 19840 | 3 |
| 446 | Leveraging protein dynamics to identify cancer mutational hotspots using 3D structures. 2019 , 116, 18962-18970 | 14 |
| 445 | Coordination-driven self-assembly of ML metal-organic bi-capped square antiprisms with adaptable cavities. 2019 , 48, 17713-17717 | 7 |
| 444 | Kinetics analysis of ubiquitin local fluctuations with Markov state modeling of the LE4PD normal modes. 2019 , 151, 164119 | 3 |
| 443 | Quantitative structural assessment of graded receptor agonism. 2019 , 116, 22179-22188 | 10 |
| 442 | From molecular energy landscapes to equilibrium dynamics via landscape analysis and markov state models. 2019 , 17, 1940014 | 3 |
| 441 | Emergent Concepts of Receptor Pharmacology. 2019 , 260, 17-41 | 5 |
| 440 | Unsupervised and Supervised Learning over the Energy Landscape for Protein Decoy Selection. 2019 , 9, | 2 |
| 439 | . 2019 , | 3 |

| | | |
|-----|---|----|
| 438 | p38 β Mitogen-Activated Protein Kinase Is a Druggable Target in Pancreatic Adenocarcinoma. 2019 , 9, 1294 | 14 |
| 437 | Hidden Conformations in <i>Aspergillus niger</i> Monoamine Oxidase are Key for Catalytic Efficiency. 2019 , 58, 3097-3101 | 12 |
| 436 | Evaluating the effect of BDNF Val66Met polymorphism on complex formation with HAP1 and Sortilin1 via structural modeling. 2019 , 78, 282-289 | 2 |
| 435 | Pillar[5]-bis-thiacrown: An Adaptive Tricyclic Host Selectively Recognizing an Organic Guest by Dimetalation. 2019 , 25, 949-953 | 8 |
| 434 | Toward mechanistic models for genotype-phenotype correlations in phenylketonuria using protein stability calculations. 2019 , 40, 444-457 | 36 |
| 433 | Hidden Conformations in <i>Aspergillus niger</i> Monoamine Oxidase are Key for Catalytic Efficiency. 2019 , 131, 3129-3133 | |
| 432 | Precision medicine review: rare driver mutations and their biophysical classification. 2019 , 11, 5-19 | 26 |
| 431 | Improving Coarse-Grained Protein Force Fields with Small-Angle X-ray Scattering Data. 2019 , 123, 1026-1034 | 16 |
| 430 | Solid-State NMR and MD Study of the Structure of the Statherin Mutant SNa15 on Mineral Surfaces. 2019 , 141, 1998-2011 | 10 |
| 429 | Atomic Force Microscopy. 2019 , | 3 |
| 428 | Single-Molecule Force Spectroscopy: Experiments, Analysis, and Simulations. 2019 , 1886, 163-189 | 12 |
| 427 | SNAREs. 2019 , | |
| 426 | Quantifying Intramolecular Protein Conformational Dynamics Under Lipid Interaction Using smFRET and FCCS. 2019 , 1860, 345-359 | 0 |
| 425 | Protein dynamics revealed by hydrogen/deuterium exchange mass spectrometry: Correlation between experiments and simulation. 2019 , 33 Suppl 3, 83-89 | 14 |
| 424 | Observation of preQ-II riboswitch dynamics using single-molecule FRET. 2019 , 16, 1086-1092 | 8 |
| 423 | Elucidation of conformational diversity of druggable enzymes and classification of chemical modulators based on inhibitor-bound structures. 2019 , 37, 4563-4568 | 0 |
| 422 | Engineering an Osmosensor by Pivotal Histidine Positioning within Disordered Helices. 2019 , 27, 302-314.e4 | 1 |
| 421 | Computational Design of Synthetic Enzymes. 2019 , 119, 6613-6630 | 79 |

| | | |
|-----|--|----|
| 420 | Deep analysis of N-cadherin/ADH-1 interaction: a computational survey. 2019 , 37, 210-228 | 5 |
| 419 | Allosteric transitions in hemoglobin revisited. 2020 , 1864, 129335 | 13 |
| 418 | Accelerating structural life science by paramagnetic lanthanide probe methods. 2020 , 1864, 129332 | 12 |
| 417 | Protein-Protein Interaction Networks. 2020 , | 0 |
| 416 | Pre- and post-docking sampling of conformational changes using ClustENM and HADDOCK for protein-protein and protein-DNA systems. 2020 , 88, 292-306 | 21 |
| 415 | Allosteric Cooperativity in Proton Energy Conversion in A1-Type Cytochrome c Oxidase. 2020 , 432, 534-551 | 2 |
| 414 | Combined strategies in structure-based virtual screening. 2020 , 22, 3149-3159 | 39 |
| 413 | Emission Control by Molecular Manipulation of Double-Paddled Binuclear Pt Complexes at the Air-Water Interface. 2020 , 15, 406-414 | 19 |
| 412 | Discovery of novel nonpeptide small-molecule NRP1 antagonists: Virtual screening, molecular simulation and structural modification. 2020 , 28, 115183 | 3 |
| 411 | Unveiling invisible protein states with NMR spectroscopy. 2020 , 60, 39-49 | 47 |
| 410 | Off-Pocket Activity Cliffs: A Puzzling Facet of Molecular Recognition. 2020 , 60, 152-161 | 5 |
| 409 | Patterns of Dynamics Comprise a Conserved Evolutionary Trait. 2020 , 432, 497-507 | 7 |
| 408 | Conformational flexibility and oligomerization of BRCA2 regions induced by RAD51 interaction. 2020 , 48, 9649-9659 | 6 |
| 407 | BMPQ-1 binds selectively to (3+1) hybrid topologies in human telomeric G-quadruplex multimers. 2020 , 48, 11259-11269 | 7 |
| 406 | KRAS(G12C)-AMG 510 interaction dynamics revealed by all-atom molecular dynamics simulations. 2020 , 10, 11992 | 12 |
| 405 | Synergistic Allostery in Multiligand-Protein Interactions. 2020 , 119, 1833-1848 | 12 |
| 404 | Differentiating and Quantifying Gas-Phase Conformational Isomers Using Coulomb Explosion Imaging. 2020 , 11, 10205-10211 | 4 |
| 403 | Polarizable and non-polarizable force fields: Protein folding, unfolding, and misfolding. 2020 , 153, 185102 | 11 |

| | | |
|-----|--|---------|
| 402 | Exploring the Molecular Conformation Space by Soft Molecule-Surface Collision. 2020 , 142, 21420-21427 | 18 |
| 401 | Hydrogen-Deuterium Exchange within Adenosine Deaminase, a TIM Barrel Hydrolase, Identifies Networks for Thermal Activation of Catalysis. 2020 , 142, 19936-19949 | 4 |
| 400 | T-Cell Receptor CDR3 Loop Conformations in Solution Shift the Relative V _H /D Domain Distributions. 2020 , 11, 1440 | 8 |
| 399 | Driving Protein Conformational Cycles in Physiology and Disease: "Frustrated" Amino Acid Interaction Networks Define Dynamic Energy Landscapes: Amino Acid Interaction Networks Change Progressively Along Alpha Tryptophan Synthase's Catalytic Cycle. 2020 , 42, e2000092 | 1 |
| 398 | Exploring the Conformational Landscape of Bioactive Small Molecules. 2020 , 16, 6575-6585 | 10 |
| 397 | Structural dissimilarity from self drives neoepitope escape from immune tolerance. <i>Nature Chemical Biology</i> , 2020 , 16, 1269-1276 | 11.7 17 |
| 396 | Conformational gating, dynamics and allostery in human monoacylglycerol lipase. 2020 , 10, 18531 | 3 |
| 395 | Intrinsically Disordered Proteins: Insights from Poincaré-Waddington, and Lamarck. 2020 , 10, | 5 |
| 394 | Simulating Multiple Substrate-Binding Events by β -Glutamyltransferase Using Accelerated Molecular Dynamics. 2020 , 124, 10104-10116 | 1 |
| 393 | Molecular insights into the differential structure-dynamics-stability features of interleukin-8 orthologs: Implications to functional specificity. 2020 , 164, 3221-3234 | 3 |
| 392 | Regulation and Function of RNA Pseudouridylation in Human Cells. 2020 , 54, 309-336 | 23 |
| 391 | Evolving Role of Conformational Dynamics in Understanding Fundamental Biomolecular Behavior. 2020 , 57-81 | 0 |
| 390 | Relevance of Electrostatic Charges in Compactness, Aggregation, and Phase Separation of Intrinsically Disordered Proteins. 2020 , 21, | 20 |
| 389 | Ligand-bound glutamine binding protein assumes multiple metastable binding sites with different binding affinities. 2020 , 3, 419 | 2 |
| 388 | Dynamically encoded reactivity of Ras enzymes: opening new frontiers for drug discovery. 2020 , 39, 1075-1089 | 4 |
| 387 | Complete Dynamic Reconstruction of C, C, and (CN) Encapsulation into an Adaptable Supramolecular Nanocapsule. 2020 , 142, 16051-16063 | 20 |
| 386 | Hierarchical Graph Representation of Pharmacophore Models. 2020 , 7, 599059 | 0 |
| 385 | Dynamic Instability from Non-equilibrium Structural Transitions on the Energy Landscape of Microtubule. 2020 , 11, 608-624.e9 | 2 |

| | | |
|-----|---|----|
| 384 | Seeking the Source of Catalytic Efficiency of Lindane Dehydrochlorinase, LinA. 2020 , 124, 10353-10364 | 0 |
| 383 | Mechanisms of ligand binding. 2020 , 1, 011303 | 10 |
| 382 | Statistical Mechanical Model of Gas Adsorption in a Metal-Organic Framework Harboring a Rotaxane Molecular Shuttle. 2020 , 36, 13112-13123 | 1 |
| 381 | Backbone assignments and conformational dynamics in the <i>S. typhimurium</i> tryptophan synthase β subunit from solution-state NMR. 2020 , 74, 341-354 | 3 |
| 380 | A supramolecular system that strictly follows the binding mechanism of conformational selection. 2020 , 11, 2740 | 21 |
| 379 | NMR Spectroscopic Studies Reveal the Critical Role of the Isopeptide Bond in Forming the Otherwise Unstable SpyTag-SpyCatcher Mutant Complexes. 2020 , 59, 2226-2236 | 1 |
| 378 | PI3K inhibitors: review and new strategies. 2020 , 11, 5855-5865 | 46 |
| 377 | Sequence specificity, energetics and mechanism of mismatch recognition by DNA damage sensing protein Rad4/XPC. 2020 , 48, 2246-2257 | 5 |
| 376 | Pseudouridine Synthase RsuA Captures an Assembly Intermediate that Is Stabilized by Ribosomal Protein S17. 2020 , 10, | 2 |
| 375 | Allosteric Communications between Domains Modulate the Activity of Matrix Metalloprotease-1. 2020 , 119, 360-374 | 6 |
| 374 | Analysis of Temperature-Dependent H/D Exchange Mass Spectrometry Experiments. 2020 , 92, 10058-10067 | 11 |
| 373 | Microsecond dynamics in proteins by two-dimensional ESR: Predictions. 2020 , 152, 214112 | 3 |
| 372 | The Regulatory Role of Key Metabolites in the Control of Cell Signaling. 2020 , 10, | 9 |
| 371 | Dynamics Rationalize Proteolytic Susceptibility of the Major Birch Pollen Allergen Bet v 1. 2020 , 7, 18 | 4 |
| 370 | T-Cell Receptor Variable β Domains Rigidify During Affinity Maturation. 2020 , 10, 4472 | 11 |
| 369 | Exploring Conformational Space with Thermal Fluctuations Obtained by Normal-Mode Analysis. 2020 , 60, 3068-3080 | 2 |
| 368 | The physical basis and practical consequences of biological promiscuity. 2020 , | 5 |
| 367 | Pinpoint analysis of a protein in slow exchange using FF-selective ZZ-exchange spectroscopy: assignment and kinetic analysis. 2020 , 74, 205-211 | 2 |

| | | |
|-----|---|----|
| 366 | Difference contact maps: From what to why in the analysis of the conformational flexibility of proteins. 2020 , 15, e0226702 | 3 |
| 365 | Investigation of anomalous charge variant profile reveals discrete pH-dependent conformations and conformation-dependent charge states within the CDR3 loop of a therapeutic mAb. 2020 , 12, 1763138 | 6 |
| 364 | Protein-Protein Binding as a Two-Step Mechanism: Preselection of Encounter Poses during the Binding of BPTI and Trypsin. 2020 , 119, 652-666 | 8 |
| 363 | Engineering Stability, Viscosity, and Immunogenicity of Antibodies by Computational Design. 2020 , 109, 1631-1651 | 19 |
| 362 | Strategies to Support Fragment-to-Lead Optimization in Drug Discovery. 2020 , 8, 93 | 48 |
| 361 | Structure-Activity Relationships of Hydroxyapatite-Binding Peptides. 2020 , 36, 2729-2739 | 7 |
| 360 | Mapping Structural Dynamics of Proteins with Femtosecond Stimulated Raman Spectroscopy. 2020 , 71, 239-265 | 17 |
| 359 | RNA-Dependent Structures of the RNA-Binding Loop in the Flavivirus NS3 Helicase. 2020 , 124, 2371-2381 | 1 |
| 358 | Long-range correlation in protein dynamics: Confirmation by structural data and normal mode analysis. 2020 , 16, e1007670 | 14 |
| 357 | Emerging functional materials based on chemically designed molecular recognition. 2020 , 2, | 40 |
| 356 | Allostery as Structure-Encoded Collective Dynamics. 2020 , 125-141 | 1 |
| 355 | Dynamic design: manipulation of millisecond timescale motions on the energy landscape of cyclophilin A. 2020 , 11, 2670-2680 | 10 |
| 354 | Structure-Activity Relationship of HER2 Receptor Targeting Peptide and Its Derivatives in Targeted Tumor Therapy. 2020 , 10, | 2 |
| 353 | Domain sliding of two <i>Staphylococcus aureus</i> N-acetylglucosaminidases enables their substrate-binding prior to its catalysis. 2020 , 3, 178 | 4 |
| 352 | Conformational selection in the flaviviral NS2B-NS3 protease. 2020 , 174, 117-125 | 10 |
| 351 | Investigating the Conformational Ensembles of Intrinsically Disordered Proteins with a Simple Physics-Based Model. 2020 , 124, 4097-4113 | 7 |
| 350 | Backbone-Directed Self-Assembly of Interlocked Molecular Cyclic Metalla[3]Catenanes. 2020 , 59, 13516-13520 | 18 |
| 349 | Conformational Studies of Oligosaccharides. 2020 , 26, 9814-9825 | 16 |

| | | |
|-----|--|----|
| 348 | Backbone-Directed Self-Assembly of Interlocked Molecular Cyclic Metalla[3]Catenanes. 2020 , 132, 13618-13622 | |
| 347 | Strategies for identifying dynamic regions in protein complexes: Flexibility changes accompany methylation in chemotaxis receptor signaling states. 2020 , 1862, 183312 | 2 |
| 346 | Mechanism of Action of an EPAC1-Selective Competitive Partial Agonist. 2020 , 63, 4762-4775 | 9 |
| 345 | NMR-Derived Conformational Ensemble of State 1 of Activated Ras Reveals Insights into a Druggable Pocket. 2020 , 11, 3642-3646 | 7 |
| 344 | Rational drug repurposing for cancer by inclusion of the unbiased molecular dynamics simulation in the structure-based virtual screening approach: Challenges and breakthroughs. 2021 , 68, 249-257 | 11 |
| 343 | Structural dynamics in the La-module of La-related proteins. 2021 , 18, 194-206 | 5 |
| 342 | Current advances in design and engineering strategies of industrial enzymes. 2021 , 1, 15-23 | 11 |
| 341 | Comparison of Different Reweighting Approaches for the Calculation of Conformational Variability of Macromolecules from Molecular Simulations. 2021 , 22, 127-138 | 3 |
| 340 | Structural Transition Dynamics in Carbon Electrode-Based Single-Molecule Junctions. 2021 , 39, 223-231 | 5 |
| 339 | Conformational Ensembles of Antibodies Determine Their Hydrophobicity. 2021 , 120, 143-157 | 10 |
| 338 | Structurally silent peptide anchor modifications allosterically modulate T cell recognition in a receptor-dependent manner. 2021 , 118, | 6 |
| 337 | Exploring conformational preferences of proteins: ionic liquid effects on the energy landscape of avidin. 2020 , 12, 196-209 | 6 |
| 336 | The dynamic nature of the Mre11-Rad50 DNA break repair complex. 2021 , 163, 14-22 | 0 |
| 335 | The challenge of predicting distal active site mutations in computational enzyme design. 2021 , 11, e1502 | 20 |
| 334 | Exploring the different states of wild-type T-cell receptor and mutant conformational changes towards understanding the antigen recognition. 2021 , 39, 188-201 | 2 |
| 333 | Pharmacological Receptor Theory. 2021 , | |
| 332 | Conformational Dynamics of Deubiquitinase A and Functional Implications. 2021 , 60, 201-209 | 2 |
| 331 | A perspective on the molecular simulation of DNA from structural and functional aspects. 2021 , 12, 5390-5409 | 3 |

| | | |
|-----|--|----|
| 330 | Protein Structure, Dynamics and Assembly: Implications for Drug Discovery. 2021 , 91-122 | |
| 329 | Disrupting enzyme fluidity. 2021 , 10, | |
| 328 | Agonism and Biased Signaling. 2021 , | |
| 327 | A Highly Specific DNA Aptamer for RNase H2 from. 2021 , 13, 9464-9471 | 5 |
| 326 | Controlled Self-Assembly and Multistimuli-Responsive Interconversions of Three Conjoined Twin-Cages. 2021 , 143, 2016-2024 | 17 |
| 325 | Dimerization of PHGDH via the catalytic unit is essential for its enzymatic function. 2021 , 296, 100572 | 3 |
| 324 | Comparison between slow, anisotropic LE4PD fluctuations and the Principal Component Analysis modes of Ubiquitin. | |
| 323 | Folding-controlled assembly of -phenylene-based macrocycles. 2021 , 12, 6992-7002 | 3 |
| 322 | Inhibition of Nonfunctional Ras. 2021 , 28, 121-133 | 11 |
| 321 | Structural basis for peptide substrate specificities of glycosyltransferase GalNAc-T2. 2021 , 11, 2977-2991 | 3 |
| 320 | Recent developments in deuterium solid-state NMR for the detection of slow motions in proteins. 2021 , 111, 101710 | 2 |
| 319 | REPROGRAMMING CBX8-PRC1 FUNCTION WITH A POSITIVE ALLOSTERIC MODULATOR. | 2 |
| 318 | Simultaneous measurement of H-R's for rapid acquisition of backbone and sidechain paramagnetic relaxation enhancements (PREs) in proteins. 2021 , 75, 109-118 | |
| 317 | The Perturbed Free-Energy Landscape: Linking Ligand Binding to Biomolecular Folding. 2021 , 22, 1499-1516 | 2 |
| 316 | Computational compound screening of biomolecules and soft materials by molecular simulations. 2021 , 29, 023001 | 8 |
| 315 | Inference of Joint Conformational Distributions from Separately Acquired Experimental Measurements. 2021 , 12, 1606-1611 | 2 |
| 314 | Stability of ligand-induced protein conformation influences affinity in maltose-binding protein. | 0 |
| 313 | Extraction of protein dynamics information from cryo-EM maps using deep learning. 2021 , 3, 153-160 | 23 |

| | | |
|-----|--|----|
| 312 | NMR spectroscopy captures the essential role of dynamics in regulating biomolecular function. 2021 , 184, 577-595 | 27 |
| 311 | Generative Adversarial Learning of Protein Tertiary Structures. 2021 , 26, | 2 |
| 310 | Unraveling the Coupling between Conformational Changes and Ligand Binding in Ribose Binding Protein Using Multiscale Molecular Dynamics and Free-Energy Calculations. 2021 , 125, 2898-2909 | 2 |
| 309 | Protein structural heterogeneity: A hypothesis for the basis of proteolytic recognition by the main protease of SARS-CoV and SARS-CoV-2. 2021 , 182, 177-184 | 10 |
| 308 | Pervasive cooperative mutational effects on multiple catalytic enzyme traits emerge via long-range conformational dynamics. 2021 , 12, 1621 | 17 |
| 307 | Allostery-Mimicking Self-assembly of Helical Poly(phenylacetylene) Block Copolymers and the Chirality Transfer. 2021 , 60, 9686-9692 | 15 |
| 306 | Comparison between slow anisotropic LE4PD fluctuations and the principal component analysis modes of ubiquitin. 2021 , 154, 124111 | 1 |
| 305 | Conformational Strain Indicated by Ramachandran Angles for the Protein Backbone Is Only Weakly Related to the Flexibility. 2021 , 125, 2597-2606 | 1 |
| 304 | Structural Proteomics Methods to Interrogate the Conformations and Dynamics of Intrinsically Disordered Proteins. 2021 , 9, 603639 | 8 |
| 303 | Coupling Monte Carlo, Variational Implicit Solvation, and Binary Level-Set for Simulations of Biomolecular Binding. 2021 , 17, 2465-2478 | 1 |
| 302 | Composition-dependent multivalency of peptide-peptide interactions revealed by tryptophan-scanning mutagenesis. 2021 , 27, e3310 | 3 |
| 301 | Allostery-Mimicking Self-assembly of Helical Poly(phenylacetylene) Block Copolymers and the Chirality Transfer. 2021 , 133, 9772-9778 | 2 |
| 300 | X-Entropy: A Parallelized Kernel Density Estimator with Automated Bandwidth Selection to Calculate Entropy. 2021 , 61, 1533-1538 | 5 |
| 299 | Tying the knot in the tetrahydrofolate (THF) riboswitch: A molecular basis for gene regulation. 2021 , 213, 107703 | 1 |
| 298 | Unveiling the "invisible" druggable conformations of GDP-bound inactive Ras. 2021 , 118, | 1 |
| 297 | Host assisted molecular recognition by human serum albumin: Study of molecular recognition controlled protein/drug mimic binding in a microfluidic channel. 2021 , 176, 137-144 | 1 |
| 296 | Remdesivir and Ledipasvir among the FDA-Approved Antiviral Drugs Have Potential to Inhibit SARS-CoV-2 Replication. 2021 , 10, | 10 |
| 295 | Effect of Stapling on the Thermodynamics of mdm2-p53 Binding. 2021 , 61, 1989-2000 | 4 |

| | | |
|-----|---|----|
| 294 | Native or non-native protein-protein docking models? Molecular dynamics to the rescue. | 0 |
| 293 | Extending the New Generation of Structure Predictors to Account for Dynamics and Allostery. 2021 , 433, 167007 | 6 |
| 292 | How does a small molecule bind at a cryptic binding site?. | |
| 291 | The 'Shape-Shifter' Peptide from the Disulphide Isomerase PmScsC Shows Context-Dependent Conformational Preferences. 2021 , 11, | 1 |
| 290 | Bcl-xL Dynamics under the Lens of Protein Structure Networks. 2021 , 125, 4308-4320 | 3 |
| 289 | Biased cytochrome P450-mediated metabolism via small-molecule ligands binding P450 oxidoreductase. 2021 , 12, 2260 | 9 |
| 288 | Stimuli-Responsive Topological Transformation of a Molecular Borromean Ring via Controlled Oxidation of Thioether Moieties. 2021 , 133, 15594-15599 | 0 |
| 287 | Metal ion coordination in peptide fragments of neurotrophins: A crucial step for understanding the role and signaling of these proteins in the brain. 2021 , 435, 213790 | 3 |
| 286 | Unusual RNA binding of FUS RRM studied by molecular dynamics simulation and enhanced sampling method. 2021 , 120, 1765-1776 | 1 |
| 285 | Sequence of Events during Peptide Unbinding from RNase S: A Complete Experimental Description. 2021 , 12, 5201-5207 | 4 |
| 284 | Development of Kinetically Controlled New Functional Supramolecular Complexes. 2021 , 77, 26-36 | |
| 283 | Stimuli-Responsive Topological Transformation of a Molecular Borromean Ring via Controlled Oxidation of Thioether Moieties. 2021 , 60, 15466-15471 | 4 |
| 282 | Switching on H-Tunneling through Conformational Control. 2021 , 143, 8266-8271 | 3 |
| 281 | Biocatalysis. 2021 , 1, | 57 |
| 280 | The oxidoreductase PYROXD1 uses NAD(P) as an antioxidant to sustain tRNA ligase activity in pre-tRNA splicing and unfolded protein response. 2021 , 81, 2520-2532.e16 | 2 |
| 279 | A Minireview on Temperature Dependent Protein Conformational Sampling. 2021 , 40, 545-553 | 0 |
| 278 | A multiscale approach for computing gated ligand binding from molecular dynamics and Brownian dynamics simulations. | 1 |
| 277 | Structural Flexibility in Metal-Organic Cages. 2021 , 9, 706462 | 12 |

| | | |
|-----|--|---|
| 276 | Unified Approach to Gated Reactions on Networks. 2021 , 127, 018301 | 4 |
| 275 | Damaged goods? Evaluating the impact of X-ray damage on conformational heterogeneity in room temperature and cryo-cooled protein crystals. | 1 |
| 274 | Fibril fragments from the amyloid core of lysozyme: An accelerated molecular dynamics study. 2021 , 106, 107917 | 2 |
| 273 | Understanding the Binding Transition State After the Conformational Selection Step: The Second Half of the Molecular Recognition Process Between NS1 of the 1918 Influenza Virus and Host p85□ 2021 , 8, 716477 | 2 |
| 272 | What's in a name? From "fluctuation fit" to "conformational selection": rediscovery of a concept. 2021 , 43, 88 | 1 |
| 271 | Predicting 3D protein structures in light of evolution. 2021 , 5, 1195-1198 | 2 |
| 270 | Reduced efficacy of a Src kinase inhibitor in crowded protein solution. 2021 , 12, 4099 | 5 |
| 269 | Looking for the Elusive Imine Tautomer of Creatinine: Different States of Aggregation Studied by Quantum Chemistry and Molecular Spectroscopy. 2021 , 86, 1374-1386 | 4 |
| 268 | Stability of Ligand-induced Protein Conformation Influences Affinity in Maltose-binding Protein. 2021 , 433, 167036 | 2 |
| 267 | A Framework for Investigating Rules of Life by Establishing Zones of Influence. 2021 , | 1 |
| 266 | Competing stress-dependent oligomerization pathways regulate self-assembly of the periplasmic protease-chaperone DegP. 2021 , 118, | 5 |
| 265 | Correlated Response of Protein Side-Chain Fluctuations and Conformational Entropy to Ligand Binding. 2021 , 125, 9641-9651 | 3 |
| 264 | Across scales: novel insights into kidney health and disease by structural biology. 2021 , 100, 281-288 | |
| 263 | Intrinsically disordered electronegative clusters improve stability and binding specificity of RNA-binding proteins. 2021 , 297, 100945 | 3 |
| 262 | Allosteric regulation of 3CL protease of SARS-CoV-2 and SARS-CoV observed in the crystal structure ensemble. | |
| 261 | Native or Non-Native Protein-Protein Docking Models? Molecular Dynamics to the Rescue. 2021 , 17, 5944-5954 | 2 |
| 260 | 1,3,4-oxadiazole conjugates of capsaicin as potent NorA efflux pump inhibitors of <i>Staphylococcus aureus</i> . 2021 , 113, 105031 | 2 |
| 259 | Guest-Induced Transformations in Metal-Organic Cages. | 4 |

| | | |
|-----|--|----|
| 258 | Cyclosporin Structure and Permeability: From A to Z and Beyond. 2021 , 64, 13131-13151 | 7 |
| 257 | A new mathematical formula to link near equilibrium relaxation kinetics and conformational selection steps in enzymatic reactions. 2021 , 59, 2270 | |
| 256 | Ligand binding remodels protein side chain conformational heterogeneity. | 0 |
| 255 | Ensemblefunction relationships to evaluate catalysis in the ketosteroid isomerase oxyanion hole. | |
| 254 | Repositioning of Fungal-based Peptides as Modulators of Angiotensin-converting Enzyme-related Carboxypeptidase, SARS-coronavirus HR2 Domain, and Coronavirus Disease 2019 Main Protease.. 2021 , 9, 190-199 | 1 |
| 253 | Designing an effective therapeutic siRNA to silence RdRp gene of SARS-CoV-2. 2021 , 93, 104951 | 8 |
| 252 | Probing allosteric regulations with coevolution-driven molecular simulations. 2021 , 7, eabj0786 | 0 |
| 251 | Self-assembling systems comprising intrinsically disordered protein polymers like elastin-like recombinamers. 2021 , e3362 | 0 |
| 250 | Mutual Protein-Ligand Conformational Selection Drives cGMP vs. cAMP Selectivity in Protein Kinase G. 2021 , 433, 167202 | 4 |
| 249 | Developments in solution-state NMR yield broader and deeper views of the dynamic ensembles of nucleic acids. 2021 , 70, 16-25 | 9 |
| 248 | Allosteric Switching of Calmodulin in a Mycobacterium smegmatis porin A (MspA) Nanopore-Trap. 2021 , 133, 24056 | 0 |
| 247 | Allosteric Switching of Calmodulin in a Mycobacterium smegmatis porin A (MspA) Nanopore-Trap. 2021 , 60, 23863-23870 | 3 |
| 246 | Designing a therapeutic and prophylactic candidate vaccine against human papillomavirus through vaccinomics approaches. 2021 , 95, 105084 | 3 |
| 245 | Solution Structure, Dynamics, and New Antifungal Aspects of the Cysteine-Rich Mini-protein PAFC. 2021 , 22, | 1 |
| 244 | Effects of electrostatic interactions on global folding and local conformational dynamics of a multidomain Y-family DNA polymerase. 2021 , 23, 20841-20847 | 2 |
| 243 | Loquacious-PD regulates the terminus-dependent molecular recognition of Dicer-2 toward double-stranded RNA. 2021 , 57, 10879-10882 | 0 |
| 242 | Biomineralization: Apatite Protein Interaction. 2012 , 135-159 | 1 |
| 241 | Molecular docking to flexible targets. 2015 , 1215, 445-69 | 15 |

| | | |
|-----|---|----|
| 240 | Embedding Alternative Conformations of Proteins in Protein-Protein Interaction Networks. 2020 , 2074, 113-124 | 4 |
| 239 | Expanding the conformational selection paradigm in protein-ligand docking. 2012 , 819, 59-74 | 10 |
| 238 | Revisiting the Concept of Human Disease. 2020 , 1-34 | 1 |
| 237 | Exploiting protein intrinsic flexibility in drug design. 2014 , 805, 245-69 | 7 |
| 236 | Resurrected Ancestral Proteins as Scaffolds for Protein Engineering. 2017 , 229-255 | 7 |
| 235 | Structure, Dynamics, and Fidelity of RNA-Dependent RNA Polymerases. 2014 , 309-333 | 6 |
| 234 | Computational Methods for Predicting DNA-Binding Sites at a Genomic Scale. 2011 , 165-182 | 1 |
| 233 | (How to) Profit from Molecular Dynamics-based Ensemble Docking. 2014 , 501-538 | 2 |
| 232 | Enzyme Catalysis. 2017 , 101-110 | 1 |
| 231 | Dynamic Protein Allosteric Regulation and Disease. 2019 , 1163, 25-43 | 8 |
| 230 | Integration of Evolutionary Theory into Cancer Biology and Caspase Signaling. 2019 , 131-155 | 1 |
| 229 | Recent advances in measuring the kinetics of biomolecules by NMR relaxation dispersion spectroscopy. 2017 , 628, 81-91 | 19 |
| 228 | Isoform-Selective Enzyme Inhibitors by Exploring Pocket Size According to the Lock-and-Key Principle. 2020 , 119, 1513-1524 | 1 |
| 227 | The dynamics of β -secretase and its substrates. 2020 , 105, 86-101 | 7 |
| 226 | Breaking the law: unconventional strategies for antibody diversification. 2019 , 19, 355-368 | 39 |
| 225 | Sodium-induced population shift drives activation of thrombin. 2020 , 10, 1086 | 5 |
| 224 | Fuzzy protein theory for disordered proteins. 2020 , 48, 2557-2564 | 5 |
| 223 | Assessment of enzyme active site positioning and tests of catalytic mechanisms through X-ray-derived conformational ensembles. 2020 , 117, 33204-33215 | 13 |

| | | |
|-----|---|-----|
| 222 | Identifying the natural polyphenol catechin as a multi-targeted agent against SARS-CoV-2 for the plausible therapy of COVID-19: an integrated computational approach. 2021 , 22, 1346-1360 | 26 |
| 221 | Extraction of Protein Dynamics Information Hidden in Cryogenic Electron Microscopy Maps Using Deep Learning. | 1 |
| 220 | The relation between intrinsic protein conformational changes and ligand binding. | 2 |
| 219 | Pervasive cooperative mutational effects on multiple catalytic enzyme traits emerge via long-range conformational dynamics. | 1 |
| 218 | A kinetic ensemble of the Alzheimer's A β peptide. | 2 |
| 217 | Modulating hinge flexibility in the APP transmembrane domain alters β secretase cleavage. | 2 |
| 216 | An enhanced-sampling MD-based protocol for molecular docking. | 1 |
| 215 | 7-Transmembrane Helical (7TMH) Proteins: Pseudo-Symmetry and Conformational Plasticity. | 1 |
| 214 | Calcium-ligand variants of the myocilin olfactomedin propeller selected from invertebrate phyla reveal cross-talk with N-terminal blade and surface helices. 2019 , 75, 817-824 | 3 |
| 213 | Markov State Models Reveal a Two-Step Mechanism of miRNA Loading into the Human Argonaute Protein: Selective Binding followed by Structural Re-arrangement. 2015 , 11, e1004404 | 39 |
| 212 | Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. 2016 , 12, e1004619 | 124 |
| 211 | Predicting Allosteric Effects from Orthosteric Binding in Hsp90-Ligand Interactions: Implications for Fragment-Based Drug Design. 2016 , 12, e1004840 | 17 |
| 210 | How to Distinguish Conformational Selection and Induced Fit Based on Chemical Relaxation Rates. 2016 , 12, e1005067 | 43 |
| 209 | Bayesian refinement of protein structures and ensembles against SAXS data using molecular dynamics. 2017 , 13, e1005800 | 34 |
| 208 | Atomic-level characterization of the activation mechanism of SERCA by calcium. 2011 , 6, e26936 | 42 |
| 207 | Unique structure and dynamics of the EphA5 ligand binding domain mediate its binding specificity as revealed by X-ray crystallography, NMR and MD simulations. 2013 , 8, e74040 | 13 |
| 206 | New conformational state of NHERF1-CXCR2 signaling complex captured by crystal lattice trapping. 2013 , 8, e81904 | 7 |
| 205 | Flexibility of PCNA-protein interface accommodates differential binding partners. 2014 , 9, e102481 | 12 |

| | | |
|-----|--|----|
| 204 | Dynamics Govern Specificity of a Protein-Protein Interface: Substrate Recognition by Thrombin. 2015 , 10, e0140713 | 19 |
| 203 | Pharmacokinetic modeling optimizes inhibition of the 'undruggable' EWS-FLI1 transcription factor in Ewing Sarcoma. 2014 , 5, 338-50 | 34 |
| 202 | Building a macro-mixing dual-basin G^- model using the Multistate Bennett Acceptance Ratio. 2019 , 16, 310-321 | 3 |
| 201 | Use of Molecular Dynamics Simulations in Structure-Based Drug Discovery. 2019 , 25, 3339-3349 | 20 |
| 200 | Protein flexibility, not disorder, is intrinsic to molecular recognition. 2013 , 5, 2 | 54 |
| 199 | Protein-Ligand Docking Methodologies and Its Application in Drug Discovery. 2017 , 891-914 | 1 |
| 198 | Intrinsically disordered proteins and prostate cancer: pouring new wine in an old bottle. 2016 , 18, 659-61 | 5 |
| 197 | Single-molecule FRET unveils induced-fit mechanism for substrate selectivity in flap endonuclease 1. 2017 , 6, | 26 |
| 196 | Probing protein flexibility reveals a mechanism for selective promiscuity. 2017 , 6, | 14 |
| 195 | Promiscuous binding by Hsp70 results in conformational heterogeneity and fuzzy chaperone-substrate ensembles. 2017 , 6, | 57 |
| 194 | Local frustration determines loop opening during the catalytic cycle of an oxidoreductase. 2020 , 9, | 4 |
| 193 | Residue-resolved monitoring of protein hyperpolarization at sub-second time resolution. 2021 , 4, | 1 |
| 192 | Why are large conformational changes well described by harmonic normal modes?. 2021 , 120, 5343-5354 | 1 |
| 191 | Mechanism of activation and the rewired network: New drug design concepts. 2021 , | 2 |
| 190 | Analytical and functional aspects of protein-ligand interactions: Beyond induced fit and conformational selection. 2021 , 714, 109064 | 2 |
| 189 | AlphaDesign: A de novo protein design framework based on AlphaFold. | 9 |
| 188 | Coarse-Grained Modeling of Large Protein Complexes for Understanding Their Conformational Dynamics. 2011 , 61-93 | |
| 187 | Preparation and optimization of protein-DNA complexes suitable for detailed NMR studies. 2012 , 831, 219-32 | |

- 186 General Overview of Basic Concepts in Molecular Biophysics. 1-25
- 185 References. 575-608
- 184 Self Organizing Maps to efficiently cluster and functionally interpret protein conformational ensembles. 130, 83-86 2
- 183 Dynamics of Small, Folded Proteins. **2014**, 223-248
- 182 Protein-Ligand Docking Methodologies and Its Application in Drug Discovery. **2016**, 196-219
- 181 Pressure Perturbation: A Prime Tool to Study Conformational Substates and Volume Fluctuations of Biomolecular Assemblies. **2016**, 29-64
- 180 NMR Explorations of Biomolecular Systems with Rapid Conformational Exchanges. **2016**, 87-103 1
- 179 Understanding properties of the master effector of phage shock operon in Mycobacterium tuberculosis via bioinformatics approach. 2
- 178 Macromolecular Interactions. **2017**, 115-137
- 177 Peptide Suboptimal Conformation Sampling for the Prediction of Protein-Peptide Interactions. **2017**, 1561, 21-34
- 176 High Performance Virtual Screening by Targeting a High-resolution RNA Dynamic Ensemble.
- 175 Mechanical variations in proteins with large-scale motions highlight the formation of structural locks.
- 174 Dissecting Conformational Changes in APP's Transmembrane Domain Linked to Efficiency in Familial Alzheimer's Disease.
- 173 Dual roles of electrostatic-steering and conformational dynamics in the binding of calcineurin's intrinsically-disordered recognition domain to calmodulin.
- 172 Speciflex: A Protocol for Mining Binding Site Conformational Selectivity in Structure-Based Inhibitor Discovery.
- 171 Analysis of Molecular Structure Data [Systematic Study of Different Design Decisions in Markov Model-based Analysis of Molecular Structure Data. **2018**,
- 170 Ligand modulation of allosteric networks in an ancestral steroid receptor.
- 169 Leveraging protein dynamics to identify cancer mutational hotspots in 3D-structures.

| | | |
|-----|---|---|
| 168 | Dynamic design: manipulation of millisecond timescale motions on the energy landscape of Cyclophilin A. | |
| 167 | Difference contact maps: from what to why in the analysis of the conformational flexibility of proteins. | |
| 166 | Bcl-xL dynamics and cancer-associated mutations under the lens of protein structure network and biomolecular simulations. | 3 |
| 165 | Quantitative Structural Assessment of Graded Receptor Agonism. | |
| 164 | Hybrid Refinement of Heterogeneous Conformational Ensembles using Spectroscopic Data. | |
| 163 | Single-molecule observation of ligand binding and conformational changes in FeuA. | |
| 162 | Dancing Molecules: Rewiring Cooperative Communications within 14-3-3 Docking Proteins. | |
| 161 | Local frustration determines loop opening during the catalytic cycle of an oxidoreductase. | |
| 160 | Assessment of enzyme active site positioning and tests of catalytic mechanisms through X-ray-derived conformational ensembles. | 1 |
| 159 | Allosteric communications between domains modulate the activity of matrix metalloprotease-1. | 0 |
| 158 | Strategies for identifying dynamic regions in protein complexes: flexibility changes accompany methylation in chemotaxis receptor signaling states. | |
| 157 | Structural basis for peptide substrate specificities of glycosyltransferase GalNAc-T2. | |
| 156 | Allosteric Regulation of 3CL Protease of SARS-CoV-2 and SARS-CoV Observed in the Crystal Structure Ensemble. 2021 , 433, 167324 | 1 |
| 155 | Identification and Experimental Validation of Distal Activity-Enhancing Mutations in Tryptophan Synthase. 2021 , 11, 13733-13743 | 5 |
| 154 | Impact of protein conformational diversity on AlphaFold predictions. | 3 |
| 153 | Comparative Study on Acyl Transferases in Fatty Acid and Polyketide Synthases. | |
| 152 | Effect of Stapling on the Thermodynamics of mdm2-p53 Binding. | |
| 151 | Structure prediction of cyclic peptides by molecular dynamics + machine learning. 2021 , 12, 14927-14936 | 6 |

- 150 RNA-dependent structures of the RNA-binding loop in the flavivirus NS3 helicase.
- 149 Structure-Dynamic and Regulatory Specificities of Epithelial Na⁺/Ca²⁺ Exchangers. **2020**, 325-380
- 148 Investigating the Conformational Ensembles of Intrinsically-Disordered Proteins with a Simple Physics-Based Model.
- 147 Simulating Multiple Substrate Binding Events by β Glutamyltransferase using Accelerated Molecular Dynamics.
- 146 A patch of positively charged residues regulates the efficacy of clinical DR5 antibodies in solid tumors. **2021**, 37, 109953 1
- 145 CIFDock: A novel CHARMM-based flexible receptor-flexible ligand docking protocol. **2022**, 43, 84-95 0
- 144 Multiscale Approach for Computing Gated Ligand Binding from Molecular Dynamics and Brownian Dynamics Simulations. **2021**, 0
- 143 Neutral and charged forms of inubosin B in aqueous solutions at different pH and on the surface of Ag nanoparticles. **2021**, 1250, 131828 0
- 142 Reconstruction and Decomposition of High-Dimensional Landscapes via Unsupervised Learning. **2020**, 1
- 141 Across kingdom biased CYP-mediated metabolism via small-molecule ligands docking on P450 oxidoreductase.
- 140 A Fast Lysine Cross-linker DOPA Enables Mass Spectrometry Analyses of Protein Unfolding and Weak Protein-protein Interactions.
- 139 Binding of dsRNA by *D. melanogaster* Dicer-2 is substrate-dependent and regulated by Loquacious-PD.
- 138 From Interatomic Distances to Protein Tertiary Structures with a Deep Convolutional Neural Network. **2020**,
- 137 Protein conformational dynamics and phenotypic switching.. **2021**, 13, 1127-1138 0
- 136 Generating Tertiary Protein Structures via Interpretable Graph Variational Autoencoders. 1
- 135 Sampling the conformational landscapes of transporters and receptors with AlphaFold2. 1
- 134 Gated reactions in discrete time and space.. **2021**, 155, 234112 0
- 133 Docking and molecular dynamics simulation for therapeutic repurposing in small cell lung cancer (SCLC) patients infected with COVID-19. **2021**, 1-10 0

| | | |
|-----|---|---|
| 132 | Genetic perturbation enhances functional heterogeneity in alkaline phosphatase. | |
| 131 | Plant-Derived Natural Non-Nucleoside Analog Inhibitors (NNAs) against Complex (nsp7/nsp8/nsp12) of SARS-CoV-2. 2021 , 1-30 | 0 |
| 130 | Biophysical and characterization of NrtA: a protein-based host for aqueous nitrate and nitrite recognition.. 2021 , | 0 |
| 129 | Possibilities and challenges of small molecule organic compounds for the treatment of repeat diseases.. 2022 , 98, 30-48 | 0 |
| 128 | Structural Determinants for Ligand Accommodation in Voltage Sensors. | |
| 127 | Antimicrobial Peptides from Human Microbiome Against Multidrug Efflux Pump of Pseudomonas aeruginosa: a Computational Study.. 2022 , 14, 180 | 0 |
| 126 | Intrinsically disordered proteins/regions and insight into their biomolecular interactions.. 2022 , 283, 106769 | 5 |
| 125 | Superphanes: Facile and efficient preparation, functionalization and unique properties. 2022 , 1, 100006 | 2 |
| 124 | The native state conformational heterogeneity in the energy landscape of protein folding.. 2022 , 283, 106761 | 1 |
| 123 | Elucidating the mechanisms underlying protein conformational switching using NMR spectroscopy.. 2022 , 10-11, 100034 | 0 |
| 122 | Early-stage structure-based drug discovery for small GTPases by NMR spectroscopy.. 2022 , 236, 108110 | 0 |
| 121 | Using azobenzene photocontrol to set proteins in motion. 2022 , 6, 112-124 | 5 |
| 120 | Structure and chemistry of enzymatic active sites that play a role in the switch and conformation mechanism.. 2022 , 130, 59-83 | |
| 119 | Dissecting the Protein Dynamics Coupled Ligand Binding with Kinetic Models and Single-Molecule FRET.. 2022 , | 1 |
| 118 | Intrinsically Disordered Proteins: Critical Components of the Wetware.. 2022 , | 4 |
| 117 | Signal propagation within the MCL-1/BIM protein complex.. 2022 , 167499 | 1 |
| 116 | When Dynamic Diselenide Bonds meet Dynamic Imine Bonds in Polymeric Materials.. 2022 , e2200083 | 3 |
| 115 | Helical remodeling augments 5-lipoxygenase activity. | |

| | | |
|-----|---|---|
| 114 | Hierarchical assembly of uranyl metallacycles involving macrocyclic hosts. 2022 , | |
| 113 | Sampling alternative conformational states of transporters and receptors with AlphaFold2.. 2022 , 11, | 8 |
| 112 | How does a small molecule bind at a cryptic binding site?. 2022 , 18, e1009817 | 2 |
| 111 | In silico screening and testing of FDA approved small molecules to block SARS-CoV-2 entry to the host cell by inhibiting Spike protein cleavage. | 1 |
| 110 | Ligand binding remodels protein side chain conformational heterogeneity.. 2022 , 11, | 2 |
| 109 | Characterization of protein unfolding by fast cross-linking mass spectrometry using di-ortho-phthalaldehyde cross-linkers.. 2022 , 13, 1468 | 0 |
| 108 | Intrinsically disordered proteins: Ensembles at the limits of Anfinsen's dogma. 2022 , 3, 011306 | 1 |
| 107 | Impact of protein conformational diversity on AlphaFold predictions.. 2022 , | 5 |
| 106 | AB-DB: Force-Field parameters, MD trajectories, QM-based data, and Descriptors of Antimicrobials.. 2022 , 9, 148 | 3 |
| 105 | Deuteron rotating frame relaxation for the detection of slow motions in rotating solids.. 2022 , 337, 107171 | |
| 104 | Insights of conformational dynamics on catalytic activity in the computational stability design of Bacillus subtilis LipA.. 2022 , 109196 | |
| 103 | Dynophore-Based Approach in Virtual Screening: A Case of Human DNA Topoisomerase IIβ 2021 , 22, | 2 |
| 102 | Rational Protein Engineering of Bacterial N-demethylases to Create Biocatalysts for the Production of Methylxanthines. | 0 |
| 101 | Generating Physically-Realistic Tertiary Protein Structures with Deep Latent Variable Models Learning Over Experimentally-available Structures. 2021 , | 0 |
| 100 | Entropy in the Molecular Recognition of Membrane Protein-Lipid Interactions.. 2021 , 12, 12218-12224 | 3 |
| 99 | Molecular enantiodiscrimination by NMR spectroscopy in chiral oriented systems: Concept, tools, and applications.. 2021 , | 3 |
| 98 | Recent Developments in Data-Assisted Modeling of Flexible Proteins.. 2021 , 8, 765562 | 1 |
| 97 | Identifying the leading dynamics of ubiquitin: A comparison between the tICA and the LE4PD slow fluctuations in amino acids' position.. 2021 , 155, 244108 | 0 |

- 96 Origin of Protein Quake: Energy Waves Conducted by a Precise Mechanical Machine.
- 95 Chapter 3. Designing Chemical Tools with Computational Chemistry. 69-86
- 94 Data_Sheet_1.docx. **2020**,
- 93 Data_Sheet_1.docx. **2020**,
- 92 Data_Sheet_1.PDF. **2020**,
- 91 Table_1.DOCX. **2019**,
- 90 Video_1.mp4. **2019**,
- 89 Video_2.mp4. **2019**,
- 88 Video_3.mp4. **2019**,
- 87 Video_4.mp4. **2019**,
- 86 Structural basis of protein substrate processing by human mitochondrial high-temperature requirement A2 protease.. **2022**, 119, e2203172119 0
- 85 Cosolvent Simulations with Fragment-Bound Proteins Identify Hot Spots to Direct Lead Growth.. **2022**, 0
- 84 Construction of L-Asparaginase Stable Mutation for the Application in Food Acrylamide Mitigation. **2022**, 8, 218
- 83 Quinolinate Synthase: An Example of the Roles of the Second and Outer Coordination Spheres in Enzyme Catalysis.. **2022**, 1
- 82 An electrostatically-steered conformational selection mechanism promotes SARS-CoV-2 Spike protein variation. **2022**, 167637 0
- 81 Electrostatic Complementarity in Structure-Based Drug Design.. **2022**, 2
- 80 In Silico Screening and Testing of FDA-Approved Small Molecules to Block SARS-CoV-2 Entry to the Host Cell by Inhibiting Spike Protein Cleavage. **2022**, 14, 1129 1
- 79 Structural and ITC Characterization of Peptide-Protein Binding: Thermodynamic Consequences of Cyclization Constraints, a Case Study on Vascular Endothelial Growth Factor Ligands.

| | | |
|----|--|---|
| 78 | Learning Strategies in Protein Directed Evolution. 2022 , 225-275 | 1 |
| 77 | Allosteric Modulators of Metabotropic Glutamate Receptors as Novel Therapeutics for Neuropsychiatric Disease. 2022 , 74, 630-661 | 2 |
| 76 | Molecular Docking and Dynamics of Phytochemicals From Chinese Herbs With SARS-CoV-2 RdRp. 2022 , 17, 1934578X2211056 | 1 |
| 75 | Spontaneously Restoring Specific Bioaffinity of RGD in Linear RGD-containing Peptides by Conjugation with Zwitterionic Dendrimers. 2022 , | 0 |
| 74 | What the protein data bank tells us about the evolutionary conservation of protein conformational diversity. 2022 , 31, | 1 |
| 73 | Data Size and Quality Matter: Generating Physically-Realistic Distance Maps of Protein Tertiary Structures. 2022 , 12, 908 | 0 |
| 72 | Essential Dynamics Ensemble Docking for Structure-Based GPCR Drug Discovery. 9, | 0 |
| 71 | In silico identification and in vitro antiviral validation of potential inhibitors against Chikungunya virus. | |
| 70 | Evaluating the impact of X-ray damage on conformational heterogeneity in room-temperature (277 K) and cryo-cooled protein crystals. 2022 , 78, | 0 |
| 69 | Helical remodeling augments 5-lipoxygenase activity in the synthesis of pro-inflammatory mediators. 2022 , 102282 | 0 |
| 68 | A litmus test for classifying recognition mechanisms of transiently binding proteins. 2022 , 13, | 0 |
| 67 | Kinetic solvent viscosity effects uncover an internal isomerization of the enzyme-substrate complex in <i>Pseudomonas aeruginosa</i> PAO1 NADH:Quinone oxidoreductase. 2022 , 727, 109342 | 0 |
| 66 | New fluorinated diarylureas linked to pyrrolo[2,3-d]pyrimidine scaffold as VEGFR-2 inhibitors: Molecular docking and biological evaluation. 2022 , 127, 106006 | |
| 65 | NKCC1 and KCC2: Structural insights into phospho-regulation. 15, | 1 |
| 64 | Functional roles of enzyme dynamics in accelerating active site chemistry: Emerging techniques and changing concepts. 2022 , 75, 102434 | 2 |
| 63 | Chapter 8. Structural Insight into the Slowly Exchanging Dark States at the Functional Interaction Interface. 2022 , 203-235 | |
| 62 | Origin of Protein Quake: Energy Waves Conducted by a Precise Mechanical Machine. | |
| 61 | A photochemically covalent lock stabilizes aptamer conformation and strengthens its performance for biomedicine. | 0 |

| | | |
|----|---|---|
| 60 | AlphaFold, Artificial Intelligence (AI), and Allostery. | 4 |
| 59 | Chemical Composition, Antiaging Activities and Molecular Docking Studies of Essential Oils from <i>Acca sellowiana</i> (Feijoa). | 1 |
| 58 | Impact of aromatic residues on the intrinsic disorder and transitional behaviour of model IDPs. 2022 , 100400 | |
| 57 | Large-Scale Ligand Perturbations of the Protein Conformational Landscape Reveal State-Specific Interaction Hotspots. | 1 |
| 56 | Temperature-dependent hydrogen deuterium exchange shows impact of analog binding on adenosine deaminase flexibility but not embedded thermal networks. 2022 , 102350 | 0 |
| 55 | Conformational Selection Governs Carrier Domain Positioning in <i>Staphylococcus aureus</i> Pyruvate Carboxylase. | |
| 54 | Threading single proteins through pores to compare their energy landscapes. 2022 , 119, | 0 |
| 53 | Estimating conformational heterogeneity of tryptophan synthase with a template-based AlphaFold2 approach. 2022 , 31, | 1 |
| 52 | Protection and Transformation of Natural Products within Aqueous Metal-Organic Cages. | 0 |
| 51 | Design, Synthesis, and Characterization of Stapled Oligosaccharides. | 0 |
| 50 | The Evolution of Our Understanding of GPCRs 2022 , 60-80 | 0 |
| 49 | Pre-Training of Equivariant Graph Matching Networks with Conformation Flexibility for Drug Binding. 2203796 | 0 |
| 48 | Detecting and Characterizing Interactions of Metabolites with Proteins by Saturation Transfer Difference Nuclear Magnetic Resonance (STD NMR) Spectroscopy. 2023 , 123-139 | 0 |
| 47 | Entropic control of the free energy landscape of an archetypal biomolecular machine. | 0 |
| 46 | Molecular and thermodynamic mechanisms for protein adaptation. | 0 |
| 45 | Reweighting methods for elucidation of conformation ensembles of proteins. 2022 , 77, 102470 | 0 |
| 44 | Graph Representation Learning for Protein Conformation Sampling. 2022 , 16-28 | 0 |
| 43 | No dance, no partner! A tale of receptor flexibility in docking and virtual screening. 2022 , | 0 |

- 42 Ensemble-function relationships to dissect mechanisms of enzyme catalysis. **2022**, 8, 1
- 41 MicroED structure of a protoglobin reactive carbene intermediate. 0
- 40 Anti-CRISPR proteins function through thermodynamic tuning and allosteric regulation of CRISPR RNA-guided surveillance complex. 1
- 39 Recent Advances and Potential Applications of Flexible Adsorption and Separation Materials: A review. 0
- 38 Dynamical activation of function in metalloenzymes. 1
- 37 Clustering conformational ensembles of intrinsically disordered proteins with t-distributed stochastic neighbor embedding. 1
- 36 Fullerene Complexation in a Hydrogen-Bonded Porphyrin Receptor via Induced-Fit: Cooperative Action of Tautomerization and CH π Interactions. 0
- 35 Small-angle x-ray and neutron scattering of MexR and its complex with DNA supports a conformational selection binding model. **2022**, 0
- 34 Screening of the Active Compounds against Neural Oxidative Damage from Ginseng Phloem Using UPLC-Q-Exactive-MS/MS Coupled with the Content-Effect Weighted Method. **2022**, 27, 9061 0
- 33 High Pressure CPMG and CEST Reveal That Cavity Position Dictates Distinct Dynamic Disorder in the PP32 Repeat Protein. **2022**, 126, 10597-10607 0
- 32 Phosphorylation of the Hsp90 co-chaperone Hop changes its conformational dynamics and biological function. **2022**, 167931 0
- 31 Functional dynamics of SARS-CoV-2 3C-like protease as a member of clan PA. 0
- 30 Harnessing Pressure-Axis Experiments to Explore Volume Fluctuations, Conformational Substates, and Solvation of Biomolecular Systems. 12099-12115 0
- 29 Conformational Control of ortho-Phenylenes by Terminal Amides. 0
- 28 DMSO-Induced Unfolding of the Antifungal Disulfide Protein PAF and Its Inactive Variant: A Combined NMR and DSC Study. **2023**, 24, 1208 0
- 27 Preferential molecular recognition of heterochiral guests within a cyclophane receptor. **2023**, 14, 0
- 26 Equivariant Encoding based GVAE (EqEn-GVAE) for Protein Tertiary Structure Generation. **2022**, 0
- 25 Expanding the Cation Cage: Squalene-Hopene Cyclase-Mediated Enantioselective Semipinacol Rearrangement. **2023**, 13, 1946-1951 0

- 24 Genetic Perturbation Alters Functional Substates in Alkaline Phosphatase. **2023**, 145, 2806-2814 ○
- 23 Principles Governing Molecular Recognition. **2023**, 1-36 ○
- 22 Description of conformational ensembles of disordered proteins by residue-local probabilities. **2023**, 25, 10512-10524 ○
- 21 Easy Not Easy: Comparative Modeling with High-Sequence Identity Templates. **2023**, 83-100 ○
- 20 Single-Particle Tracking of *Thermomyces lanuginosus* Lipase Reveals How Mutations in the Lid Region Remodel Its Diffusion. **2023**, 13, 631 ○
- 19 Atomic insights into the mechanism of trace water influence on lipase catalysis in organic media. **2023**, 464, 142610 ○
- 18 (Re-)Directing Oligomerization of a Single Building Block into Two Specific Dynamic Covalent Foldamers through pH. **2023**, 145, 2822-2829 ○
- 17 Peptidase Activation by a Leader Peptide-Bound RiPP Recognition Element. **2023**, 62, 956-967 ○
- 16 MCL-1 promiscuity and the structural resilience of its binding partners. **2023**, 158, 095101 1
- 15 Solvato-Controlled Assembly and Structural Transformation of Emissive Poly-NHC-Based Organometallic Cages and Their Applications in Amino Acid Sensing and Fluorescence Imaging. ○
- 14 mRNA interactions with disordered regions control protein activity. ○
- 13 Pathogen-driven cancers from a structural perspective: Targeting host-pathogen protein-protein interactions. 13, ○
- 12 Photoallosteric Polymersomes toward On-Demand Drug Delivery and Multimodal Cancer Immunotherapy. ○
- 11 An NMR portrait of functional and dysfunctional allosteric cooperativity in cAMP -dependent protein kinase A. ○
- 10 Photo- and Temperature-Induced Reversible Structural Transformation between Dodecanuclear and Pentadecanuclear Gold(I) Sulfido Complexes. **2023**, 145, 7454-7461 ○
- 9 MicroED Structure of a Protoglobin Reactive Carbene Intermediate. **2023**, 145, 7159-7165 ○
- 8 Insights into receptor structure and dynamics at the surface of living cells. **2023**, 14, ○
- 7 Effect of Cross-Seeding of Wild-Type Amyloid- β 40 Peptides with Post-translationally Modified Fibrils on Internal Dynamics of the Fibrils Using Deuterium Solid-State NMR. **2023**, 127, 2887-2899 ○

- 6 Dynamics-Based Regulatory Switches of Type II Antitoxins: Insights into New Antimicrobial Discovery. **2023**, 12, 637 ○
- 5 Mutational and Environmental Effects on the Dynamic Conformational Distributions of Lys48-Linked Ubiquitin Chains. **2023**, 24, 6075 ○
- 4 Binding to the Conserved and Stably Folded Guide RNA Pseudoknot Induces Cas12a Conformational Changes During Ribonucleoprotein Assembly. **2023**, 104700 ○
- 3 Conformational dynamics of lipid transfer domains provide a general framework to decode their functional mechanism. ○
- 2 Dynamic Self-assembled Supramolecular Catalysts. **2023**, 469-493 ○
- 1 Structural insights into SARS-CoV-2 main protease conformational plasticity. ○