

2022

Dauer K, Werner C, Lindenblatt D, Wagner KG. *Impact of process stress on protein stability in highly-loaded solid protein/PEG formulations from small-scale melt extrusion.* International Journal of Pharmaceutics: X, 2022, 100154, <https://doi.org/10.1016/j.ijpx.2022.100154>

Keuler T, Lemke C, Elsinghorst PW, Iriepa I, Chioua M, Martínez-Grau MA, Beadle CD, Vetman T, López-Muñoz F, Wille T, U. Bartz U, Deuther-Conrad W, J. Marco-Contelles J, Gütschow M. *The Chemotype of Chromanones as a Privileged Scaffold for Multineurotarget Anti-Alzheimer Agents;* ACS Pharmacol. Transl. Sci. 2022, 5, 1097-1108.

Pepanian A, Sommerfeld P, Kasprzyk R, Kühl T, Binbay F, Hauser C, Löser R, Wodkite R, Bednarczyk M, Chrominski M, Kowalska J, Jemielity I, Imhof D, Pietsch M. *A fluorescence anisotropy assay with guanine nucleotides provides access to functional analysis of Gai1 proteins.* Anal.Chem., 94 (41), 14418

Müller CE, Claff T; *Activated microglia nibbling glycosaminoglycans from spinal cord perineural nets: a new mechanism for neuropathic pain.* Signal Transduction and targeted Therapy 2022, 7: 333; <https://doi.org/10.1038/s41392-022-01162-0>

Keuler T, König B, Bückreiß N, Kraft FB, König P, Steinebach C, Bendes G, Hansen FK: *Development of the first non-hydroxamate selective HDAC6 degraders* ChemRxiv:DOI: 10.26434/chemrxiv--2022-3rhqf.

Hopp MT, Rathod D, Imhof D: *Host and viral proteins involved in SARS-CoV-2 infection differentially bind heme.* Protein Sci., e4451

Abram M, Jakubiec M, Reeb K, Cheng MH, Gedschold R, Rapacz A, Mogilski S, Socała K, Nieoczym D, Szafarz M, Latacz G, Szulczyk B, Kalinowska-Tłuścik J, Gawel K, Esguerra CV, Wyska E, Müller CE, Bahar I, Fontana ACK, Wlaź P, Kamiński RM, Kamiński K. *Discovery of (R)-N-benzyl-2-(2,5-dioxopyrrolidin-1-yl)propanamide [(R)-AS-1], a novel orally bioavailable EAAT2 modulator with drug-like properties and potent antiseizure activity in vivo.* J. Med. Chem. 2022; <https://doi.org/10.1021/acs.jmedchem.2c00534>

Kohgo H, Mori T, Tanako Y, Yoshihaie K, Taniguchi K, Fujimoto K, Fritz L, Schneider T, Tsukazaki T: *Crystal structure of the lipid flippase Mur J in a "squeezed" form distinct from its inward-and outward-facing forms* Structure 2022, 4;30(8): 1085-1097

Haerdlein A, Boehmer A, Dafonde KK, Rottenkolber M, Jaehde U, Dreischulte T: *Prioritisation of Adverse Drug Events Leading to Hospital Admission and Occuring during Hospitalisation: A RAND Survey* J.Clin.Med. 2022 11 (15) 4254

Niemann B, Hauf-Brunberg S, Puetz Laura, Freikert M, Yaeckstein MJ, Hoffmann A, Zurkovic J, Heine M, Trautmann EM, Mueller CE, Toenjes A, Schlein C, Jafari A, Eltzschig HK, Gnad T, Blüher M, Krahmer N, Kovacs P, Heeren J, Pfeifer A: *Apoptotic brown adipocytes enhance energy expenditure via extracellular inosine.* Nature (2022)

Mähler B, Janssen K, Tahoun M, Tomaschek F, Schellhorn R, Müller CE, Bierbaum G, Rust J; Adipocere formation in biofilms as a first step in soft tissue preservation. *Sci. Rep.* 2022, 12:10122. doi: 10.1038/s41598-022-14119-8.

Pillaiyar T, Flury P, Krüger N, Su H, Schäkel L, Barbosa da Silva E, Eppler O, Kronenberger T, Nie T, Luedtke S, Rocha C, Sylvester K, Petry MRI, McKerrow J, Poso A, . Pohlmann S, Gütschow M, O'Donoghue A, Xu Y, Müller CE, Laufer S. *Small Molecule Thioesters as SARS-CoV-2 Main Protease Inhibitors: Enzyme Inhibition, Structure-activity Relationships, Antiviral Activity, and X-ray Structure Determination*; *J. Med. Chem.* 2022, 65, 9376-9395.

Miller DSJ, Voell SA, Sosič I, Proj M, Rossanese OW, Schnakenburg G, M. Gütschow M, Collins I, Steinebach C. *Encoding BRAF Inhibitor Functions in Protein Degraders*; RSC Med. Chem. 2022, 13, 731-736.

Modemann DJ, Mahardhika AB, Yamoune S, Kreyenschmidt AK, Maaß F, Kremers S, Breunig C, Sahlmann CO, Bucerius J, Stalke D, Wiltfang J, Bouter Y, Müller CE, Bouter C, Beller B. *Development of high-affinity fluorinated ligands for cannabinoid subtype 2 receptor, and in vitro evaluation of a radioactive tracer for imaging*. *Eur. J. Med. Chem.* 2022, 232, 114138; <https://doi.org/10.1016/j.ejmech.2022.114138>.

Büscher B, Manga P, Penner E, Schiedel AC: *The Many Faces of G Protein-Coupled Receptor 143, an Atypical Intracellular Receptor*. *Front. Mol. Biosci.*, 2022 doi.org/10.3389/fmolsb.2022.873777

Murgai A, Sosič I, Gobec M, Lemnitzer P, Proj M, Wittenburg S, Voget R, Gütschow M, Krönke J, Steinebach C: *Expanding the PROTAC Toolbox: Targeted Degradation of the Deubiquitinase USP7 in Cancer*; *Chem. Commun.* 2022, 58, 8858-8861.

Sosič I, Bricelj A, Steinebach C. *E3 Ligase Ligand Chemistries: From Building Blocks to Protein Degraders*; *Chem. Soc. Rev.* 2022, 51, 3487-3534.

Voss JH, Müller CE: Heteromeric G protein β-subunits - structure, peptide-derived inhibitors, and mechanisms. *Curr. Med. Chem.*

Vu LP, Zyulina M, Hingst A, Schnakenburg G, Gütschow M. Combinatorial Assembly, Traceless Generation and *In Situ* Evaluation of Inhibitors for Therapeutically Relevant Serine Proteases. *Bioorg. Chem.* 2022 121, 1105676.

Caniceiro AB, Büschbell B, Schiedel AC, Moreira IS: *Class A and C GPCR dimers in neurodegenerative diseases*. *Current Neuropharmacology*, 2022 doi:10.2174/1570159X20666220327221830

Neumann A, Attah IY, Al-Hroub H, Namasivayam V, Müller CE: Discovery of P2Y2 receptor antagonists scaffolds through virtual high-throughput screening. *J. Chem. Inf. Model.* 2022, 62, 1538-49

Voss JH, Mahardhika AB, Inoue A, Müller CE. *Agonist-Dependent Coupling of the Promiscuous Adenosine A_{2B} Receptor to G_P Protein Subunits*. ACS Pharmacol. Transl. Sci.

Gockel LM, Nekipelov K, Ferro V, Bendas G, Schlesinger M. *Tumour cell-activated platelets modulate the immunological activity of CD4+, CD8+, and NK cells, which is efficiently antagonized by heparin*. Cancer Immunol Immunother. doi: 10.1007/s00262-022-03186-5.

Losenkova K, Tkeda A, Ragauskas S, Cerrad-Gimenez M, Vähätupa M, Kaja S, Paul ML, Schmies CC, Rolshoven G, Müller CE, Sandholm J, Jalkanen S, Kalesnykas G, Yegutkin GG: *CD73 controls ocular adenosine levels and protects retina from light-induced phototoxicity*. Cell.Mol.Life Sci. 2022, 79,152

Claff T, Klapschinski TA, Udaya K, Subhramanyam T, Vaaßen VJ, Schlegel JG, Vielmuth C, Voß JH, Labahn J, Müller CE: *Single stabilizing point mutation enables high-resolution co-crystal structures of the adenosine A_{2A} receptor with preladdenant conjugates*. Angew. Chem. Int. Ed. 2022, e2022115545; doi.org/10.1002/anie.202115545

Gockel LM, Pfeifer V, Baltes F, Bachmaier RD, Wagner KG, Bendas G, Gütschow M, Sosić I, Steinebach C. Design, synthesis, and characterization of PROTACs targeting the androgen receptor in prostate and lung cancer models. *Arch Pharm (Weinheim)* 2022:e202100467. doi: 10.1002/ardp.202100467.

Keuler T, D. Ferber, Marleaux M, Geyer M, Gütschow M. Structure-Stability Relationship of NLRP3 Inflammasome-Inhibiting Sulfonylureas. *ACS Omega* 2022, 7, 8158-8162.

Ng YLD, Ramberger E, Bohl S, Dolnik A, Steinebach C, Conrad T, Müller S, Popp O, Kull M, Haji M, Gütschow M, Döhner H, Walther W, Keller U, Bullinger L, Mertins P, Krönke J. Proteomic Profiling Reveals CDK6 Upregulation as a Targetable Resistance Mechanism for Lenalidomide in Multiple Myeloma. *Nat. Commun.* 2022, 13, 1009

von Bredow L, Schäfer TM, Hogenkamp J, Tretbar M, Stopper D, Kraft FB, Schliehe-Diecks J, Schöler A, Borkhardt A, Bhatia S, Held J, Hansen FK. *Synthesis, Antiplasmodial, and Antileukemia Activity of Dihydroartemisinin.HDAC Inhibitor Hybrids as Multitarget Drugs*. Pharmaceuticals, 15(3):333.

Tahoun M, Engeser M, Namasivayam V, Saner PM, Müller CE. *Chemistry and Analysis of Organic Compounds in Dinosaurs* Biology 2022, 11(5), 670

Scorticchini M, Idris RM, Moschütz S, Keim A, Slamaso V, Dobermann C, Oliva P, Losenkova K, Irjala H, Vaittinen S, Sandholm J, Yegutkin GG, Sträter N, Junker A, Müller CE, Jacobson KA; *Structure-activity relationship of 3-methylcytidine-5'-α,β-methylenediphosphates as CD73 inhibitors*. *J. Med. Chem.* 2022, 65, 2409-2433;
<https://doi.org/10.1021/acsjmedchem.1c01852>.

Schäker-Hübner L, Haschemi R, Büch T, Kraft FB, Brumme B, Schöler A, Jenke R, Meiler J, Aigner A, Bendas G, Hansen FK. *Balancing Histone Deacetylase (HDAC) Inhibitors and Drug-likeness: Biological and Physicochemical Evaluation of Class I Selective HDAC Inhibitors*. ChemMedChem.

Schulte B, König M, Escher BI, Wittenburg S, Proj M, Wolf V, Lemke C, Schnakenburg G, Sosič I, Streeck H, Müller CE, Gütschow M, Steinebach C. *Andrographolide Derivatives Target the KEAP1/NRF2 Axis and Possess Potent anti-SARS-CoV-2 Activity* *ChemMedChem* 2022, 17, e202100732

Nubbemeyer B, Ajay Abisheck PG, Kühl T, Pepanian A, Beck MS, Maghraby R, Boushehri MS, Mühlhaupt M, Pfeil EM, Annala SK, Ammer H, Imhof D, Pei D. *Targeting Gai/s Proteins with peptidyl Nucleotide Exchange Modulators* *ACS Chem. Bio.* 2022