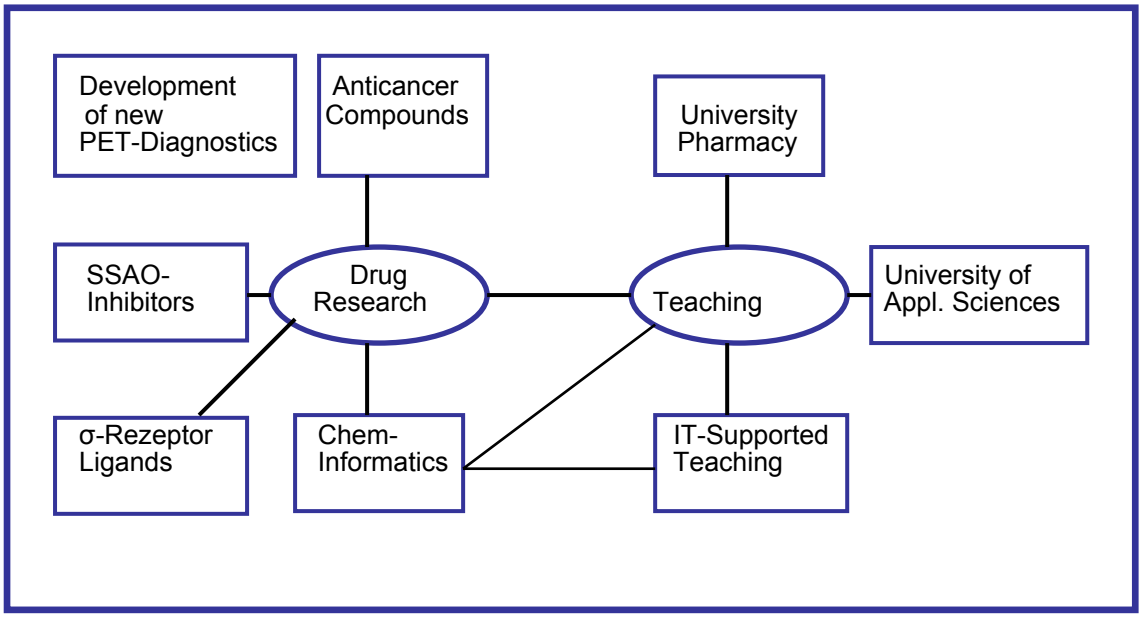
Annual Report 2010
Department of Drug and Natural Product Synthesis

1. The Year 2010 - Milestones and Highlights

One of the most challenging goals of science is the search for new medicines. The mission of the Department of Drug and Natural Product Synthesis is to develop in strong co-operation with the pharmaceutical industry and other outside partners new lead structures in the following fields:

- Anticancer Drugs
- Development of new PET-Diagnostics
- Semicarbazide-sensitive Amine Oxidase (SSAO) Inhibitors
- Sigma-receptor Ligands

The main strength of the Department of Drug and Natural Product Synthesis is a very tight connection of drug research and students' education. Therefore, the department is also engaged as a competent partner in educational programs outside the university. Innovative teaching methods include "blended learning" with a high integration of personal teaching and e-learning.



2. Structure of the Department

2.1.Personnel paid by the University

Scientific Staff:
- Ao. Univ. Prof. Dr. Helmut Spreitzer
- Ao. Univ. Prof. Dr. Norbert Haider
- Ao. Univ. Prof. Dr. Wolfgang Holzer

Teaching Assistants:
- Mag. pharm. Barbara Datterl (since 1. 2. 2009)
- Mag. pharm. Eva Schirmer (since 1. 2. 2009)

Technical Staff:
- Mag. pharm. Birgit Bornatowicz
- Angelika Ebner

2.2. Personnel Paid by third-party funds

Nipawan Pongprom (ASEA-UNET, 18. 10. – 17. 11. 2010)
Suriyan Thengay (OeAD, 19. 07. – 30. 11. 2010)
Chiaranan Kerdsamut (OeAD, 01. 07. – 30. 09. 2010)
M.Sc. Egle Arbaciauskiene (until 01. 10. 2009)
Dr. Pavel Dallakian (IMI PharmaTrain, 1.4.2010 – 30.6.2011)
M.Sc. Gyte Vilkauskaite (Erasmus, 1.3.2010 – 31.8.2010; Lithuanian Science Council, 1.10-2010 – 31.1.2011)
Dr. Vittorio Pace (Ernst Mach Stipendium, 1.10.2010 – 28.2.2011)

2.3. Visiting Scientist

2.4. Laboratory and Office Space

a) Research: 358m^2 Laboratory Space; 138 m^2 Office Space
b) Student's Education: 448 m^2 Laboratory Space; 13 m^2 Office Space

3. Publications

3.1. Publications in peer-reviewed journals in 2006, 2007, 2008, 2009 and 2010

3.1.1 Publications in journals listed in Journal Citation Report (ISI)

E. Arbačiauskienė, K. Kazlauskas, A. Miasojedovas, S. Juršėnas, V. Jankauskas, W. Holzer, V. Getautis, A. Sackus (2010) Pyrazolyl-substituted polyconjugated molecules for optoelectronic applications; *Dyes and Pigments*, *85*, 79–85
[Dyes and Pigments: IF 2.855; Category Chemistry, Applied: Rank 7/64 (Top 25%) or Category Engeneering, Chemical: Rank 11/127 (Top 10%)]

E. Arbačiauskienė, K. Kazlauskas, A. Miasojedovas, S. Juršėnas, V. Jankauskas, W. Holzer, V. Getautis, A.Šačkus (2010) Multifunctional polyconjugated molecules with carbazolyl and pyrazolyl segments for optoelectronic applications; *Synthetic Metals*, *160*, 490–498
[Synthetic Metals: IF 1.901; Category Material Sciences, Multidisciplinary: Rank 53/214 (Top 25%)]

V. Huemer, G. A. Eller, W. Holzer (2010) Heterocyclic analogues of xanthiones: 5,6-fused 3-methyl-1-phenylpyrano[2,3-*c*]pyrazol-4(1*H*)thiones – synthesis and NMR (^{1}H, ^{13}C, ^{15}N) data; *Magn. Reson. Chem*., *48*, 476–482
[Magnetic Resonance in Chemistry: IF 1.612; Category Chemistry, Multidisciplinary: Rank 51/136]

W. Holzer, A. Ebner, K. Schalle, G. Batezila, G. Eller (2010) Novel fluoro-substituted benzo- and benzothieno fused pyrano[2,3-*c*]pyrazol-4(1*H*)-ones; *J. Fluorine Chem*., *131*, 1013−1024
[Journal of Fluorine Chemistry, IF 1.730; Category Chemistry; Inorganic&Nuclear: Rank 16/40]

B. Datterl, N. Tröstner, D. Kucharski, W. Holzer (2010) Heterocyclic Analogues of Xanthone and Xanthione. 1*H*-Pyrano[2,3-*c*:6,5-*c*]dipyrazol-4(7*H*)-ones and thiones: Synthesis and NMR Data; *Molecules*, *15*, 6106−6126
[Molecules, IF 1.738; Category Chemistry, Organic: Rank 26/53]

P. Singh, J. Kaur, W. Holzer (2010) Acridone based Cu^{2+}−F^-/F^-−Cu^{2+} responsive ON/OFF key pad; *Sensor. Actuat. B-Chem.*, *150*, 50−56
[Sensors and Actuators B-Chemical, IF 3.083; Category Chemistry, Analytical: Rank 12/70 (Top 25%) or Category Instruments&Instrumentation: Rank 5/58 (Top 10%)]

P. Singh, M. Kaur and W. Holzer (2010) Synthesis and evaluation of indole, pyrazole, chromone and pyrimidine based conjugates for tumor growth inhibitory activities – Development of highly efficacious cytotoxic agents; *Eur. J. Med. Chem*., 45, 4968−4982

[European Journal of Medicinal Chemistry, IF 3.269; Category Chemistry, Medicinal: Rank 6/42 (Top 25%)]

N. Haider, I. Hochholdinger, P. Mátyus, A. Wobus (2010) Synthesis of ortho-Functionalized 4-Aminomethylpyridazines as Substrate-Like Semicarbazide-Sensitive Amine Oxidase Inhibitors; *Chem. Pharm. Bull.*, 58, 964-970
[Chemical and Pharmaceutical Bulletin: IF 1.698; Category Chemistry, Multidisciplinary: Rank 49/137]

N. Haider (2010) Functionality Pattern Matching as an Efficient Complementary Structure/Reaction Search Tool: an Open-Source Approach; *Molecules*, 15, 5079-5092
[Molecules: IF 1.738; Category Chemistry, Organic: Rank 26/53]

D. Häusler, L. Nics, L.-K. Mien, J. Ungersböck, R.R. Lanzenberger, K. Shanab, H. Spreitzer, K. M. Sindelar, H. Viernstein, K.-H. Wagner, R. Dudczak, K. Kletter, W. Wadsak, M. Mitterhauser (2010) [^{18}F]FE@SUPPY and [^{18}F]FE@SUPPY:2 – metabolic considerations; *Nucl. Med. Biol.* 37, 421-426.
[Nuclear Medicine and Biology: IF 2.456; Category Radiology, Nuclear Medinine & Medical Imaging: Rank 35/104]

K. Shanab, E. Schirmer, H. Knafl, E. Wulz, W. Holzer, H. Spreitzer, P. Schmidt, B. Aicher, G. Müller, E. Günther (2010) *Bioorg. Med. Chem. Lett.* 20, 3950-3952.
[Bioorganic and Medicinal Chemistry Letters: IF 2.650, Category Chemistry, Medicinal: Rank 15/42]

N. Pongprom, H. Bachitsch, A. Bauchinger, H. Ettefagh, T. Haider, M. Hofer, H. Knafl, R. Slanz, M. Waismayer, F. Wieser, H. Spreitzer (2010) Synthesis of new Benzo[f]isoindole-4,9-diones as anticancer compounds; *Monatsh. Chem.* 141, 53-62.
[Monatshefte f. Chemie: IF 1.312; Category Chemistry, Multidisciplinary: Rank 67/140]

W. Holzer, G.A. Eller, B. Datterl, D. Habicht (2009) Derivatives of Pyrazinecarboxylic Acid: ^{1}H, ^{13}C and ^{15}N NMR Spectroscopic Investigations; *Magn. Reson. Chem*. 47, 617-624.
[Magnetic Resonance in Chemistry: IF 1.443; Category Chemistry, Multidisciplinary: Rank 49/124]

E. Arbaciauskiene, G. Vilkauskaite, G.A. Eller, W. Holzer, A. Sackus (2009) Pd-Catalyzed Cross-Coupling Reactions of Halogenated 1-Phenylpyrazol-3-ols and Related Triflates; *Tetrahedron* 65, 7817-7824.
[Tetrahedron: IF 2.897, Category Chemistry, Organic: Rank 12/50 (Top 25%)]

F.C. Fuchs, G.A. Eller, W. Holzer (2009) Heterocyclic analogs of thioflavones: synthesis and NMR spectroscopic investigations; *Molecules* 14, 3814-3832.
[Molecules: IF 1.252; Category Chemistry, Organic: Rank 30/50]

J. Solovjova, V. Martynaitis, W. Holzer, S. Mangelinckx, N. DeKimpe, A. Sackus (2009) Synthesis and reactions of 1-amino-1,5,6,10b-tetrahydroimidazo[2,1-*a*]isoquinolin-2(3*H*)-ones; ARKIVOC vi, 48-62.
[ARKIVOC: IF 1.377; Category Chemistry, Organic: Rank 28/50]

J. Solovjova, V. Martynaitis, S. Mangelinckx, W. Holzer, N. DeKimpe, A. Sackus (2009) Synthesis and ring opening of alkaloid-type compounds with a novel indolo[2,3-*c*][2]-benzazepine skeleton; *Synlett,* 3119-3122.
[Synlett: IF 2.659; Category Chemistry, Organic: Rank 14/50]

G.A. Eller, Q. Zhang, D. Habicht, B. Datterl, W. Holzer (2009) Synthesis and NMR Data of Pyrazolo[4',3':5,6]pyrano[2,3-*b*]pyrazin-4(1*H*)-ones: Derivatives of a Novel Tricyclic Ring System; *Acta Chim. Slov*. 56, 521-526.
[Acta Chimica Slovenica: IF: 0.909; Category Chemistry, Multidisciplinary: Rank 72/124]

N. Haider, R. Jbara, J. Käferböck and U. Traar (2009) Synthesis of Tetra- and Pentacyclic Carbazole-Fused Imides as Potential Antitumor Agents; *ARKIVOC*, 38-47.
[ARKIVOC: IF 1.377; Category Chemistry, Organic: Rank 28/50]

D. Hauesler, M. Mitterhauser, L.-K. Mien, K. Shanab, R.R. Lanzenberger, E. Schirmer, J. Ungersboeck, L. Nics, H. Spreitzer, H. Viernstein, R. Dudczak, K. Kletter, W. Wadsak (2008) Radiosynthesis of a novel potential adenosine A_3 receptor ligand, 5-ethyl 2,4-diethyl-3-((2-[^{18}F]fluoroethyl)sulfanylcarbonyl)-6-phenylpyridine-5-carboxylate ([^{18}F]FE@SUPPY:2). *Radiochim. Acta* 97, 753-758.
[Radiochimica Acta: IF 1.084; Category Chemistry, Inorganic & Nuclear: Rank 27/43]

N. Pongprom, G. Mueller, P. Schmidt, W. Holzer, H. Spreitzer (2009) Synthesis of anticancer compounds, III, carbinol derivatives of azanaphthoquinone annelated pyrroles. *Monatsh. Chem.* 140, 309-313.
[Monatshefte f. Chemie: IF 1.426; Category Chemistry, Multidisciplinary: Rank 57/127]

Mihovilovic MD, Groetzl B, Kandioller W, Muskotal A, Snajdrova R, Rudroff F, Spreitzer H (2008) Recombinant whole-cell mediated baer-villiger oxidation of perhydropyran-type ketones. *Chem. Biodivers*. 5: 490-498.
[Chemistry & Biodiversity: IF 1.420; Category Chemistry, Multidisciplinary: Rank 46/124]

Wadsak W, Mien L-K, Shanab K, Weber K, Schmidt B, Sindelar KM, Ettlinger DE, Haesler D, Spreitzer H, Keppler BK, Viernstein H, Dudzak R, Kletter K, Mitterhauser M (2008): Radiosynthesis of the adenosine A3 receptor ligand 5-(2-[18F}fluoroethyl)2,4-diethyl-3-(ethylsulfanylcarbonyl)-6-phenylpyridine-5-carboxylate ([18F]FE@SUPPY). *Radiochim. Acta* 96: 119-124.
[Radiochimica Acta: IF 1.210; Category Chemistry, Inorganic & Nuclear: Rank 21/40]

Shanab K, Wadsak W, Mien L-K, Mitterhauser M, Holzer W, Polster V, Viernstein H, Spreitzer H (2008) Synthesis of in Vivo Metabolites of the New Adenosine A3 Receptor PET-Radiotracer [18F]FE@SUPPY. *Heterocycles* 75: 339-356.
[Heterocycles: IF 1.066; Category Chemistry, Organic: Rank 33/53]

Wadsak W, Mien L-K, Shanab K, Ettlinger DE, Haeusler D, Sindelar K, Lanzenberger RR, Spreitzer H, Viernstein H, Keppler BK, Dudzak R, Kletter K, Mitterhauser M (2008) Preparation and first evaluation of [18F]FE@SUPPY: a new PET tracer fort he adenosine A3 receptor. *Nucl. Med. Biol.* 35: 61-66.
[Nuclear Medicine and Biology: IF 2.478; Category Radiology, Nuclear Medinine & Medical Imaging: Rank 25/86]

Dunkel P, Gelain A, Barlocco D, Haider N, Gyires K, Sperlágh B, Magyar K, Maccioni E, Fadda A, Mátyus P (2008) Semicarbazide-Sensitive Amine Oxidase/Vascular Adhesion Protein 1: Recent Developments Concerning Substrates and Inhibitors of a Promising Therapeutic Target. *Curr. Med. Chem.* 15: 1827-1839.
[Current Medicinal Chemistry: IF 4.944; Category Chemistry, Medicinal: Rank 3/41 (Top 20%); Category Biochemistry & Molecular Biology: Rank 49/263 (Top 20%); Category Pharmacology & Pharmacy: Rank 16/205 (Top 20%)]

Haider N, Wobus A (2008) Concise syntheses of 5-substituted pyridazino[4,5-b]indolones and –diones. *ARKIVOC* 16-25.
[ARKIVOC: IF 1.253; Category Chemistry, Organic: Rank 30/53]

Holzer W, Eller GA, Schönberger S (2008) On the Tautomerism of Cinnolin-4-ol, Cinnoline-4-thiol, and Cinnolin-4-amine. *Heterocycles* 75: 77-86.
[Heterocycles: IF 1.066; Category Chemistry, Organic: Rank 33/53]

Singh P, Mittal A, Kaur S, Holzer W, Kumar S (2008) 2,3-Diaryl-5-ethylsulfanylmethyltetrahydrofurans as a new class of COX-2 inhibitors and cytotoxic agents. *Org. Biomol. Chem*. 6: 2706-2712.
[Organic & Biomolecular Chemistry: IF 3.167; Category Chemistry, Organic: Rank 8/53 (Top 20%)]

Eller GA, Habicht D, Holzer W (2008) Synthesis of a Novel Pentacycle: 8-Methyl-10-phenylpyrazolo[4',3':5,6]pyrano[3,2-*c*][1,10]phenanthrolin-7(10*H*)-one. *Khim. Geterotsikl.*

Soedin. 844-890 (*Chem. Heterocycl. Comp*. 44: 709-714).
[Khimiya Geterotsiklicheskh Soedinenii (Engl. Transl. Chemistry of Heterocyclic Compounds, NY): IF 0.463; Category Chemistr, Organic: Rank 47/53]

Wolf BMT, Eller GA, Holzer W (2008) 2-Pyrazolin-5-ones Bearing a Basic Dialkylaminoalkyl Substituent at the N-1 Position: Preparation and NMR Spectroscopic Studies. *Heterocycles* 75: 2035-2042.
[Heterocycles: IF 1.066; Category Chemistry, Organic: Rank 33/53]

Holzer W, Claramunt RM, Lopez C, Alkorta I, Elguero J (2008) A study in desmotropy. *Solid State Nuclear Magn. Reson.* 34: 68-76.
[Solid State Nuclear Magnetic Resonance: IF 1.508; Category Spectroscopy: Rank 15/36]

Yerin A, Wilks ES, Moss GP, Harada A, Hartshorn RM, Damhus T, Brecher J, Degtyarenko K, Heller SR, Hellwich K-H, Hodge P, Hutton AT, Leigh GJ, Wilson J, Kahovec J, Jones RG, Lawson A, Norlander E, Nyitrai J, Powell WH, Ansari FL, Do Y, Dukov IL, Hashem MdA, Lajunen LHJ, Ogino H, Reedijk J, Schomburg D, Powell WH, Metanomski WV, Hellwich K-H, Favre HA, Eller G (2008) Nomenclature for rotaxanes and pseudorotaxanes (IUPAC Recommendations 2008), *Pure Appl. Chem.* 80: 2041–2068.
[Pure and Applied Chemistry: IF 2.232; Category Chemistry, Multidisciplinary: Rank 31/124]

Shanab K, Pongprom N, Wulz E, Holzer W, Spreitzer H, Schmidt P, Aicher B, Mueller G, Guenther E (2007) Synthesis and biological evaluation of novel cytotoxic azanaphthoquinone annelated pyrrolo oximes. *Bioorg. Med. Chem. Lett.* 17: 6091-6095.
[Bioorganic and Medicinal Chemistry Letters: IF 2.604, Category Chemistry, Medicinal: Rank 9/36]

Spreitzer H, Puschmann C (2007) Synthesis of anticancer compounds, I. *Monatshefte für Chemie* 138: 517-522.
[Monatshefte für Chemie: IF 0.972; Category Chemistry, Multidisciplinary: Rank 65/124]

Haider N, Kabicher T, Kaeferboeck J, Plenk A (2007) Synthesis and in vitro antitumor activity of 1-[3-(indolyl-1-yl)prop-1-yn-1-yl]phthalazines and related compounds. *Molecules* 12:1900-1909.
[Molecules: IF 0.940; Category Chemistry, Organic: Rank 36/53]

Eller GA, Haring AW, Datterl B, Zwettler M, Holzer W (2007) Tri- and Tetracyclic Heteroaromatic Systems: Synthesis of Novel Benzo-, Benzothieno- and Thieno-Fused Pyrano[2,3-*c]*pyrazol-4(1*H*)-ones. *Heterocycles* 71: 87-104.
[Heterocycles: IF 1.066; Category Chemistry, Organic: Rank 33/53]

Eller GA, Holzer W (2007) A Convenient Approach to Heterocyclic Building Blocks: Synthesis of Novel Ring Systems Containing a [5,6]Pyrano[2,3-*c*]pyrazol-4(1*H*)-one Moiety. *Molecules* 12: 60-73.
[Molecules: IF 0.940; Category Chemistry, Organic: Rank 36/53]

Eller GA, Datterl B, Holzer W (2007) Pyrazolo[4',3':5,6]pyrano[2,3-*b*]quinoxalin-4(1*H*)-one: Synthesis and Characterization of a Novel Tetracyclic System. *J. Heterocycl. Chem*. 44: 1139-1144.
[Journal of Heterocyclic Chemistry: IF 0.813; Category Chemistry, Organic: Rank 38/53]

Eller GA, Wimmer V, Holzer W (2007) Synthesis of Novel Polycyclic Ring Systems Containing two Pyrano[2,3-*c*]pyrazol-4(1*H*)-one Moieties. *Khim. Geterotsikl. Soedin*. 1251-1255 (*Chem. Heterocycl. Comp.* 43: 1060-1064).
[Khimiya Geterotsiklicheskh Soedinenii (Engl. Transl. Chemistry of Heterocyclic Compounds, NY): IF 0.463; Category Chemistr, Organic: Rank 47/53]

Jirovetz L, Buchbauer G, Eller GA, Ngassoum MB, Maponmetsam PM (2007) Composition and Antimicrobial Activity of *Cymbopogon giganteus* (Hoechst.) Chiov. Essential Flower, Leaf and Stem Oils from Cameroon. *J. Essent. Oil Res*. 19: 485–489:
[Journal of Essential Oil Research: IF 0.368; Category Chemistry, Applied: Rank 50/61]

Haider N, Wobus A (2006) Thermolysis of 5-azido-4-arylpyridazin-3(2*H*)-ones: An efficient and versatile synthesis of pyridazino[4,5-b]indoles. *Heterocycles* 68: 2549-2561.
[Heterocycles: IF 1.066; Category Chemistry, Organic: Rank 33/53]

Haider N (2006) Diazine analogues of the pyridocarbazole alkaloids. *Curr. Org. Chem.*10: 363-375.
[Current Organic Chemistry: IF 3.961; Category Chemistry, Organic: Rank 8/56 (Top 20%)]

Dumciute J, Martynaitis V, Holzer W, Mangelinckx S, DeKimpe N, Sackus A (2006) Synthesis and Ring Transformations of 1-Amino-1,2,3,9a-tetrahydroimidazo[1,2-*a*]indol-2(9*H*)-ones. *Tetrahedron* 62: 3309-3319.
[Tetrahedron: IF 2.869; Category Chemistry, Organic: Rank 11/53 (Top 20%)]

Eller GA, Holzer W (2006) First Synthesis of 3-Acetyl-2-aminothiophenes Using the Gewald Reaction. *Molecules* 11: 371-376.
[Molecules: IF 0.940; Category Chemistry, Organic: Rank 36/53]

Singh P, Paul K, Holzer W (2006) Synthesis of pyrazole-based hybrid molecules: Search for potent multidrug resistance modulators. *Bioorg. Med. Chem*. 14: 5061-5071.
[Bioorganic & Medicinal Chemistry: IF 2.662; Category Chemistry, Medicinal: Rank 8/36]

Höfinghoff J, Buchbauer G, Holzer W, Wolschann P (2006) Synthesis and odor of ‚bulky-group'-modified sandalwood odorants: Isophorono-β-santalol analogues. *Eur. J. Med. Chem*. 41: 905-913.
[European Journal of Medicinal Chemistry: IF 2.301; Category Chemistry, Medicinal: Rank 12/36]

Bieringer S, Holzer W (2006) 4-Acyl-5-hydroxy-1-phenyl-3-trifluoromethylpyrazoles: Synthesis and NMR-Investigations. *Heterocycles* 68: 1825-1836.
[Heterocycles: IF 1.066; Category Chemistry, Organic: Rank 33/53]

Eller GA, Wimmer V, Haring AW, Holzer W (2006) An Efficient Approach to Heterocyclic Analogues of Xanthone: A Short Synthesis of all Possible Pyrido[5,6]pyrano[2,3-c]pyrazol-4(1***H***)-ones. *Synthesis* 4219-4229.
[Synthesis: IF 2.257; Category Chemistry, Organic: Rank 20/53]

Eller GA (2006) Improving the Quality of Published Chemical Names with Nomenclature Software. *Molecules* 11: 915–928.
[Molecules: IF 0.940; Category Chemistry, Organic: Rank 36/53]

3.1.2. Other peer-reviewed journals

V. Huemer, W. Holzer (2010) 1-Phenylpyrazolo[4',3':5,6]pyrano[3,2-*c*]pyridine-4(1*H*)-thione; *Molbank* M678.

G. Batezila, W. Holzer (2010) (2-Chlorophenyl)-3-methylchromeno[2,3-*c*]pyrazol-4(1*H*)-one; *Molbank* M661.

A. Ebner, W. Holzer (2010) 5-Dimethylamino-1-phenylchromeno[2,3-*c*]pyrazol-4(1*H*)-one; *Molbank* M706.

M. Emich, N. Haider (2010) 5-Methyl-4-oxo-4,6-dihydro-3H-pyridazino[4,5-b]carbazole-1-carbonitrile; *Molbank* M657.

H. Spreitzer and Ch. Puschmann (2010) 2-[4-[2-chloroethyl)amino]benzyl]-5,5-dimethyl-2,5-dihydro-4H-benzo[e]isoindol-4-one (Cytotoxic Oxonaphthalene-Pyrroles, Part I); *Molbank* M651.

H. Spreitzer and Ch. Puschmann (2010) 1-[4-[2-chloroethyl)amino]benzyl]-5,5-dimethyl-2,5-dihydro-4H-benzo[e]isoindol-4-one (Cytotoxic Oxonaphthalene-Pyrroles, Part II); *Molbank* M654

M. Emich and N. Haider (2009) 5-Methyl-4-oxo-4,6-dihydro-3H-pyridazino[4,5-b]-carbazole-1-carbaldehyde; *Molbank* M623.

M. Mitterhauser, D. Haeusler, L.-K. Mien, J. Ungersboeck, L. Nics, R. R. Lanzenberger, K. Sindelar, H. Viernstein, R. Dudczak, K. Kletter, H. Spreitzer, W. Wadsak (2009) Automatisation and First Evaluation of [^{18}F]FE@SUPPY:2, an Alternative PET-Tracer for the Adenosine A_3 Receptor: A Comparison with [^{18}F]FE@SUPPY. *The Open Nucl. Med. J.* 1, 15-23.

H. Spreitzer, C. Puschmann (2009) Regioselective Alkylation of an Oxonaphthalene-Annelated Pyrrol System, *Molbank* M619.

W. Holzer, C. Guo, K. Schalle (2009) 3-Methyl-1-phenyl-1*H*-pyrazol-5-yl 2-Bromo-3-furancarboxylate; *Molbank* M603.

W. Holzer, C. Guo (2009) 4,4'-[(2-chlorophenyl)methylene]bis[1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5-ol]; *Molbank* M605.

G.A. Eller, G. Vilkauskaite, A. Sackus, W. Holzer (2009) 5-Chloro-4-iodo-1,3-dimethyl-1*H*-pyrazole; *Molbank* M620.

N. Kleiziene, E. Arbaciauskiene, W. Holzer, A. Sackus (2009) 4-Bromo-3-methoxy-1-phenyl-1*H*-pyrazole; *Molbank* M639.

N. Kleiziene, E. Arbaciauskiene, W. Holzer, A. Sackus (2009) (2*E*)-3-(3-Methoxy-1-phenyl-1*H*-pyrazol-4-yl)-2-propenal; *Molbank* M644.

Haider N, Kabicher T (2008) Methyl 1-prop-2-yn-1-yl-1H-indole-5-carboxylate. *Molbank* M560.

Holzer W, Eller GA, Schönberger S (2008) On the Synthesis and Reactivity of 4-(Oxiran-2-ylmethoxy)cinnoline: Towards a Cinnoline Analogue of Propranolol. *Sci. Pharm*. 76: 19-32.

Eller GA, Holzer W (2008) Synthesis of 4,4'-(Cyclohexane-1,1-diyl)bis(1-methyl-1*H*-pyrazol-5-ol). *Molbank* M569.

Nedzelskyte E, Martynaitis V, Sackus A, Eller GA, Holzer W (2007) Synthesis of Mono- and Dibromo-Derivatives of 1-Phenylpyrazol-3-ol. *Molbank* M551.

Eller GA, Holzer W (2006) A one-step synthesis of pyrazolone. *Molbank* M464.

Eller GA, Holzer W (2006) Synthesis and Detailed Spectroscopic Characterization of Two Novel *N*-(3-Acetyl-2-thienyl)acetamides. *Molbank* M520.

Schmidt E, Jirovetz L, Buchbauer G, Eller GA, Stoilova I, Krastanov A, Stoyanaova A, Geissler M (2006) Composition and antioxidant activities of the essential oil of cinnamon (Cinnamomum zeylanicum Blume) leaves from Sri Lanka. *Journal of Essential Oil-Bearing Plants* 9: 170-182.

Jirovetz L, Eller G, Buchbauer G, Schmidt E, Denkova Z, Stoyanova AS, Nikolova R, Geissler M (2006) Chemical composition, antimicrobial activities and odor descriptions of some essential oils with characteristic floral-rosy scent and of their principal aroma compounds. *Recent Research Developments in Agronomy & Horticulture* 2: 1–12

Patents

Compounds for inhibiting semicarbazide-sensitive amine oxidase (SSAO)/vascular adhesion protein-1 (VAP-1) and uses thereof for treatment and prevention of diseases. P. Mátyus, K. Magyar, M. Pihlavista, K. Gyires, N. Haider, Y. Wang, P. Woda, P. Dunkel, E. Tóth-Sarudy, G. Túrós. *PCT Int. Appl.* (2010), WO 2010029379 A1; *Chem. Abstr.* 152, 358062 (2010).

4. Grants

a. Current Projects

Cooperation agreement („Development of new anticancer compounds“) [2006-open end] with Zentaris GmbH; PI Spreitzer H, Haider N, Holzer W, € 2560.- in 2008.

Granted application of N. Haider as a project partner in EU FP7 / IMI project „PharmaTrain“; 5 months FTE

b. Grant Applications in 2010

5. Teaching

Completed PhD and Diploma/Master theses in 2010

Nicole Tröstner: 5-Chlor-1-phenyl-1*H*-Pyrazol-4-carbonsäure als Synthesebaustein für neue kondensierte Pyrazol-Derivate (Diploma Thesis), Supervisor: Holzer, December 2010.

Veronika Schreiber: Synthese neuer Adenosin-A3-Rezeptor-Antagonisten als PET-Tracer-Precursoren (Diploma thesis) Supervisor: Spreitzer. August 2010.

Thomas Nagel: Synthese neuartiger Adenosin-A3-Rezeptor-Antagonisten für PET-diagnostische Studien (Diploma thesis) Supervisor: Spreitzer. July 2010.

Johanna Beichl: Studien zur Herstellung einer neuen Vorstufe eine MCH1-Rezeptor-Antagonisten für PET-diagnostische Studien (Diploma thesis) Supervisor: Spreitzer. September 2010.

Catharina Neudorfer: Synteses of new adenosine-A3-receptor antagonists (Diploma thesis) Supervisor: Spreitzer. December 2010.

Patrick Woda: Synthese neuer 5-Cycloaminopyridazin-3(2H)-one mit 4-Carbaldehydoxim-Funktion als potentielle Inhibitoren der humanen SSAO (Diploma thesis) Supervisor: Haider. March 2009

Theerachart Leepasert: Synthesis of new anticancer compounds with a tetracyclic nucleus (PhD thesis) Supervisor: Spreitzer. October 2009.

Karin Schalle: Synthese neuer Tri- und Tetracyclen aus 2-Pyrazolin-5-onen (Diploma Thesis) Supervisor: Holzer. February 2009.

Birgit Bornatowicz: Synthese von 4,6-Diethyl-5-[[2-fluorethyl)sulfanyl]carbonyl]-2-phenylpyridin-3-carbonsäure als Metabolit eines A3-Rezeptor-Antagonisten als PET Diagonstikum (Diploma thesis) Supervisor: Spreitzer. May 2008

Alexander Thiem: Synthese von Tracern zu Positronen-Emissions-Tomographie (Diploma thesis) Supervisor: Spreitzer. November 2008.

Davidova Ema: Versuche zur Herstellung eine MCH1-Rezeptor-Antagonisten in enantiomerenreiner Form (Diploma thesis) Supervisor: Spreitzer, November 2008.

Daniela Habicht: Synthese kondensierter heterocyclischer Systeme mit Pyrano[2,3-*c*]pyrazol-4(1*H*)-on Teilstruktur (Master thesis). Supervisor: W. Holzer. Februar 2008.

Barbara Wolf: Synthese neuer 2-Pyrazolin-5-one mit basischem N1-Substituenten (Master thesis).

Supervisor: W. Holzer. Februar 2008.

Current PhD and Diploma/Master theses

Thomas Nagel: Synthesis of new azanaphthoquinone annelated indoles as cytotoxic agents (PhD thesis, start: October 2010)

Stefan Deibl: Untersuchungen zur Reaktivität von 1-(2-Pyridinyl)-2-pyrazolin-5-onen (Master thesis), Supervisor: Holzer, start: October 2010

Helmut Julian Heiter: Pd-Katalysierte cross-coupling Reaktionen mit 4-substituierten Cinnolinen (Master thesis), Supervisor: Holzer, start: October 2010.

Alice Wittig: Pd-Katalysierte cross-coupling Reaktionen mit Pyrazolo[3,4-*b*]pyrazolen (Master thesis), Supervisor: Holzer, start: October 2010

Manochehr Shahabi: Synthese von 9-Azaanthrapyrazolen als Zytostatika (PhD thesis, start: April 2007).

Eva Schirmer: Synthese von Diagnostika für die Positronen-Emissions-Tomographie (PhD thesis, start: March 2007)

Brigitte Bornatowicz: Synthese neuer Precursoren für PET-Diagnostika (PhD thesis, start October 2008)

Verena Wieder: Herstellung eines chiralen MCH-Rezeptor-Antagonisten für PET-diagnostische Zwecke (Master thesis, start: October 2010).

Valerie Huemer: 2-Pyrazolin-5-thione als Precursoren zur Synthese von Pyrazol-Derivaten mit potentiell biologischer Aktivität (Master Thesis, start: October 2009).

Dorota Kucharski: 5-Chlor-3-methyl-1-phenyl-1*H*-pyrazol-4-carbaldehyd bzw. 4-carbonsäure als Synthesebausteine für neue Pyrazol-Derivate (Master Thesis, start: October 2009).

Gyselle Esambo Obonga Wella: Synthese halogenierter 1-Phenylchromeno[2,3-*c*]pyrazol-4-4(1*H*)-one (Master Thesis, start: March 2009).

Angelika Ebner: Synthese neuer Tri- bzw. Tetracyclen mit Pyrazol-Partialstruktur (Master Thesis, start: September 2007).

Barbara Datterl: Synthese neuer kondensierter Pyrazol-Derivate mit potentieller biologischer Aktivität (PhD thesis, start: April 2007).

Miriam Emich: Synthesis and Biological Evaluation of new Functionalized 3-Aza Analogs of the Ellipticine/Olivacine Type of Antitumor Alkaloids (PhD Thesis, Start: Oct 2007). Supervisor: N. Haider

Simon Nuß: Synthesis of New Ring-A-Modified Derivatives of the Alkaloid Luotonin A (Master Thesis, start: March 2010)

Stefan Eckerstorfer: Symthesis of New Luotonin A derivatives with Basic Substituents at Ring A (Master Thesis, start: November 2010)

Katharina Tropper: Synthesis of New Key Synthons for Ring-A-Substituted 3-Aza-Ellipticines (Master Thesis, start: November 2010)

a. Teaching Activities (summer term 09, winter term 09/10)

Summer term 10:

H. Spreitzer:
“Arzneistoffsynthese“, PR, 12 SWS, 9.0 ECTS (aliquoter Anteil: 6 SWS)
“Grundlagen der Arzneistoffsynthese (einschl. Nomenklatur)“, VO, 5 SWS, 7.5 ECTS (aliquoter Anteil: 4 SWS)
“Pharmazeutisch chemisches Praktikum f. Fortgeschrittene“, PR, 10 SWS, 5 ECTS (aliquoter Anteil: 0.91 SWS)
“Aktuelle Forschungsergebnisse i. d. pharm. Chemie“, SE, 3 SWS, 1.5 ECTS (aliquoter Anteil: 0.25 SWS)

N. Haider:
“Arzneistoffsynthese“, PR, 12 SWS, 9.0 ECTS (aliquoter Anteil: 9 SWS)
“Trenn- und Analysenmethoden organischer Arzneistoffe“, VO, 2 SWS, 3.0 ECTS (aliquoter Anteil: 1 SWS)
“Arzneimittelanalytik und Wirkstoffentwicklung“, PR, 9 SWS, 6 ECTS (aliquoter Anteil: 1 SWS)
“Pharm. chemisches Praktikum f. Fortgeschrittene“, PR, 10 SWS, 5 ECTS (aliquoter Anteil: 1.66 SWS)
“Aktuelle Forschungsergebnisse i. d. pharm. Chemie“, SE, 3 SWS, 1.5 ECTS (aliquoter Anteil: 0.25 SWS)

W. Holzer:
“Arzneistoffsynthese“, PR, 12 SWS, 9.0 ECTS (aliquoter Anteil: 7 SWS)
“Instrumentelle pharm. Analytik“, VO, 2 SWS, 3 ECTS
“Anwendung neuerer spektroskopischer Techniken“, VO, 1 SWS, 0.5 ECTS
“Pharm. chemisches Praktikum f. Fortgeschrittene“, PR, 10 SWS, 5 ECTS (aliquoter Anteil: 1.66 SWS)
“Aktuelle Forschungsergebnisse i. d. pharm. Chemie“, SE, 3 SWS, 1.5 ECTS (aliquoter Anteil: 0.25 SWS)

Winter term 09/10:

H. Spreitzer:
“Arzneistoffsynthese“, PR, 12 SWS, 9.0 ECTS (aliquoter Anteil: 10 SWS)
“Pharmazeutisch chemisches Praktikum f. Fortgeschrittene“, PR, 10 SWS, 5 ECTS (aliquoter Anteil: 0.91 SWS)
“Aktuelle Forschungsergebnisse i. d. pharm. Chemie“, SE, 3 SWS, 1.5 ECTS (aliquoter Anteil: 0.25 SWS)

N. Haider
“Arzneistoffsynthese“, PR, 12 SWS, 9.0 ECTS (aliquoter Anteil: 6 SWS)
“Computeranwendungen in der pharm. Chemie“, Seminar, 2 SWS, ECTS
“Arzneimittelanalytik und Wirkstoffentwicklung“, PR, 9 SWS, 6 ECTS (aliquoter Anteil: 1 SWS)
“Pharm. chemisches Praktikum f. Fortgeschrittene“, PR, 10 SWS, 5 ECTS (aliquoter Anteil: 2 SWS)
“Aktuelle Forschungsergebnisse i. d. pharm. Chemie“, SE, 3 SWS, 1.5 ECTS (aliquoter Anteil: 0.27 SWS)

W. Holzer:
“Arzneistoffsynthese“, PR, 12 SWS, 9.0 ECTS (aliquoter Anteil: 8 SWS)
“Pharm. chemisches Praktikum f. Fortgeschrittene“, PR, 10 SWS, 5 ECTS (aliquoter Anteil: 2 SWS)
“Aktuelle Forschungsergebnisse i. d. pharm. Chemie“, SE, 3 SWS, 1.5 ECTS (aliquoter Anteil: 0.27 SWS)

6. Invited Talks

N. Haider: The Department of Drug and Natural Product Synthesis at the University of Vienna – Research Areas and Teaching Activities; University of Catania, Italy, Nov. 2010

H. Spreitzer: Neu am Markt, Seggau, 10. Oktober 2010 (Seggauer Fortbildungstage).

W. Holzer: Techniques for Heteronuclear Correlations, Niederöblarn, 14. September 2010 (NMR Summerschool: 1D- and 2D-NMR Spectroscopy in Liquids).

H. Spreitzer: Neues am Markt, Innsbruck, 6. November 2010 und Wien 13. November 2010 (Zentrale Fortbildungstagsveranstaltungen der Österr. Apothekerkammer).

H. Spreitzer: Neues am Markt, Innsbruck, 7. November 2009 und Wien 14. November 2009 (Zentrale Fortbildungstagsveranstaltung der Österr. Apothekerkammer).

W. Holzer: Pyrazolones as synthetic building blocks and objects for tautomerism studies, 13th Blue Danube Symposium on Heterocyclic Chemistry, Bled, Slovenia, 2009-09-22.

H. Spreitzer: Neu am Markt, Seggau, 4. Oktober 2008 (Seggauer Fortbildungstage).

H. Spreitzer: Neu am Markt, Salzburg, 8. November 2008 und Wien 15. November 2008 (Zentrale Fortbildungstagsveranstaltungen der Österr. Apothekerkammer).

N. Haider: Computer-Aided Learning in the Pharmaceutical Sciences at the University of Vienna; 2nd European Workshop on Computer-Aided Learning in the Pharmaceutical Sciences, Vienna, 7 Nov 2008.

W. Holzer: Techniques for Heteronuclear Correlations, Niederöblarn, 16. September 2008 (NMR Summerschool: 1D- and 2D-NMR Spectroscopy in Liquids).

7. Outreach Activities

---

8. Further Activities of Staff

a. Awards, Prizes, Promotion, Position Offers

---

b. Professional and Public Services

H. Spreitzer:

(i) Head of Department
(ii) Study Programme Director
(iii) referee for various international journals

N. Haider:

Acts as IT manager of the faculty and as the e-learning coordinator of the faculty
N. Haider acts as international reviewer for the Slovenian Research Agency (ARRS) in the 2008/2009 and 2009/2010 research project and mentor programmes.

c. W. Holzer:

(i) main instruments coordinator of the faculty of life sciences;

Sicherheitsvertrauensperson of the Department of Drug- and Natural Product Synthesis; in charge for the NMR spectrometers at the pharmacy center

(ii) referee for various international journals

(iii) Editorenschaft von wissenschaftlichen Zeitschriften

N. Haider is Editor-in-Chief of the online journal, MolBank (http://www.mdpi.net/molbank/) and he is member of the editorial board of the journals, Molecules and ARKIVOC.

(iv) Organisation von Kongressen, Tagungen, etc.

N. Haider and his team at the EUFEPS Branch Office for in-silico Systems and Learning organized the "2nd European Workshop on Computer-Aided Learning in the Pharmaceutical Sciences" in Nov. 2008 at the Pharma Center, University of Vienna (30 participants from 10 countries)

d. Other Activities

Since July 2007, N. Haider acts as chief executive of the Branch Office for in-silico Systems and Learning of EUFEPS (European Federation for Pharmaceutical Sciences). The office is located within the Department of Drug and Natural Product Synthesis, it is operated by NH and one part-time coworker, S. Parth (until June 2009). Main activities are the coordination, evaluation, categorization, and information exchange of all matters related to pharmaceutical e-learning on a European level. This includes running a dedicated website and organising international workshops. The office was established in July 2007 by a 5-year frame contract between the University of Vienna and EUFEPS, human resources were funded by the faculty until June 2009. Since 2008, N. Haider acts as secretary of the EUFEPS Committee for Education and Training and the corresponding Steering Committee.

9. Research Focus and Future Perspectives for the Year 2011

Kurze (nicht mehr als einseitige) Zusammenfassung der
(i) derzeitigen Forschungsziele und Forschungsschwerpunkte des Departments und
(ii) Ausblick auf die erwarteten Entwicklungen im Jahr 2010

H. Spreitzer:

(i) anticancer drugs based on intercalation
synthesis of PET precursors

(ii) Continuing development of anticancer drugs based on intercalation
extension and diversification of the synthesis of PET precursors

N. Haider:

(i) In the research group of N. Haider, a new line of antitumor research was opened, targeting the enzyme topoisomerase-I with new derivatives/analogs of the natural product, luotonin A. These activities complement the previous (and ongoing) work on topoisomerase-II inhibitors. Another field, the development of inhibitors of the diabetes-related enzyme SSAO (semicarbazide-sensitive amine oxidase), was successfully completed by a joint patent application with our Hungarian cooperation partners at the Semmelweis University, Budapest (Prof. P. Mátyus).
(ii) The first series of potential topoisoisomerase-I inhibitors has become available and will be extended.

W. Holzer:

(i) Medicinal Heterocyclic Chemistry (the pyrazole system as a structural element of biologically active compounds – antitumor agents, sigma-receptor ligands, novel heterocyclic scaffolds); Heterocyclic Tautomerism (investigation of tautomeric equilibria, investigation of desmotropy); NMR Spectroscopy (systematic ^{13}C and ^{15}N NMR studies of azoles and azines, configurational studies)
(ii) extension of antitumor research, fluorine-labeled bioactive compounds – synthesis and interaction with their biological targets by ^{19}F NMR