

CURRICULUM VITAE INVESTIGATOR**PERSONAL DATA**

Surname Cassels		Name Bruce K.	
Birth date August 20, 1939	Age (on 20/08/2011) 72	Gender (M or F) M	Nationality(ies) Chilean
Title Chemist		Academic Degree Ph.D. Chemistry	
Current position Full Professor	Institution(Department, Faculty, Institution) University of Chile, Faculty of Sciences		
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EDUCATION, ACADEMIC AND PROFESSIONAL EXPERIENCE

Universidad de Buenos Aires, Argentina	Licenciado (B.Sc.)	1963	Chemistry
Universidad de Buenos Aires, Argentina	Ph.D.	1966	Chemistry
Universität Bonn, Germany, Alexander von Humboldt Fellow		1972-3	Natural Products

RESEARCH AND/OR PROFESSIONAL EXPERIENCE**ACADEMIC EMPLOYMENT**

1967-1981	Chemistry Lecturer-Reader, State Technical University, Santiago, Chile.
1982-1983	Visiting Lecturer, SUNY – Stony Brook, USA.
1984 and 1985-1987	Professeur Associé, Université de Paris-Sud, France.
1984-1985	Visiting Scientist, Universität München, Germany.
1985-1987	Professeur Associé, Université de Paris-Sud, France
1988-present	Full Professor, Universidad de Chile
1988-present	Director of the Chemobiodynamics Laboratory, Department of Chemistry, Faculty of Sciences, University of Chile.
2000-2005 (Feb.)	Senior Scientist, Millennium Institute for Advanced Studies in Cell Biology and Biotechnology (CBB).
2007-present	Associate Researcher, Institute for Cell Dynamics and Biotechnology: a Centre for Systems Biology(ICDB)

HONORS AND AWARDS

1973 and 1984	“Dozentenstipendium”, Alexander von Humboldt Foundation, Germany
1997-1999	Presidential Chair in Sciences, Chile

EDITORIAL POSITIONS

1991-2001	Editorial Board: Journal of the Chilean Chemical Society
2001-present	Editorial Board: ARKIVOC
2003-present	Editorial Board: Letters in Drug Design and Discovery
2003-present	Editorial Board: Drug Discovery Research - Online
2004-present	Associate Editor: Journal of the Chilean Chemical Society

ADMINISTRATIVE AND PROFESSIONAL SERVICE

1971 National Director for Research, Universidad Técnica del Estado (Chile)
1972-1973 Member, National Research Committee, Universidad Técnica del Estado (Chile)
1974-1981 Chairman, Organic Chemistry Teaching, Universidad Técnica del Estado (Chile)
1977-1978 Chairman, Academic Assessment Board, Universidad Técnica del Estado (Chile)
1979-1981 Member, CONICYT (Chile)/UNESCO Committee for the Chemical Sciences
1992-present Director Chemobiodynamics Laboratory, University of Chile
1994-2003 Member, Academic Assessment Board, Faculty of Sciences, University of Chile
1997-2000 Academic Director, Faculty of Sciences, University of Chile
2004-2006 Member, Chemistry Study Group, FONDECYT (Chile)
2006-2009 Secretary, Higher Assessment Council, University of Chile
2010-present Member, Higher Academic Assessment Board, University of Chile

GRADUATE STUDENTS SUPERVISED

15 PhD students graduated, 5 current PhD students.

MAIN PUBLICATIONS IN MEDIA WITH EDITORIAL COMMITTEE

Iturriaga-Vaásquez, P., Zapata-Torres, G., Rezende, M.C., and Cassels, B.K. (2004) 1-Benzyl-1,2,3,4-tetrahydroisoquinolines. ¹H NMR conformational studies and rotational barriers. J. Chil. Chem. Soc. 49, 17-23.

Zapata-Torres, G., Opazo, F., Salgado, C., Mascayano, C., Sepúlveda-Boza, S., Krautwurst, H., Muñoz, J.P., Maccioni, R.B. and Cassels, B.K. (2004) Effects of natural flavones and flavonols on the kinase activity of cdk5, J. Nat. Prod. 67, 416-420.

Villalobos, C., Bull, P., Sáez, P., Cassels, B.K. and Huidobro-Toro, J.P. (2004) 4-Bromo-2,5-dimethoxyphenethylamine (2C-B) and structurally related phenylethylamines are potent 5-HT_{2A} receptor antagonists in *Xenopus laevis* oocytes. Br. J. Pharmacol. 141, 1167-1174.

Osorio, M., Rezende, M.C., Sepúlveda-Boza, S., Cassels, B.K. and Fierro, A., MAO inhibition by arylisopropylamines: The effect of oxygen substituents at the beta position. Bioorg. Med. Chem. 12, 4055-4066.

Valiente, M., D'Ocon, P., Noguera, M.A., Cassels, B.K., Lugnier, C. and Ivorra, M.D. (2004) Vascular activity of (-)-anonaine, (-)-roemerine and (-)-pukateine, three natural 6a(R)-1,2-methylenedioxyaporphines with different affinities for α_1 -adrenoceptor subtypes. Planta Med. 70, 603-609.

Hurtado-Guzmán, C., Iturriaga-Vásquez, P., Zapata-Torres, G., and Cassels, B.K. (2004) Geometrical isomerism in β -nitrostyrenes: preferred conformations of (*E*) and (*Z*)-1-(4-methylthiophenyl)-2-nitrobutenes. J. Chil. Chem. Soc. 49, 257-260

Bustamante, D., Díaz-Véliz, G., Paeile, C., Zapata-Torres, G. and Cassels, B.K. (2004) Analgesic and behavioral effects of amphetamine enantiomers, *p*-methoxyamphetamine and *N*-alkyl-*p*-methoxyamphetamine derivatives. Pharmacol. Biochem. Behav. 79, 199-212.

Galdámez, A., Iturriaga-Vásquez, P., and Cassels, B.K. (2005) Crystal structure of isotetrandrine, C₃₈H₄₂N₂O₆,. Z. Kristallogr. NCS, 220, 1-2.

Reyes-Parada, M., Fierro, A., Iturriaga-Vásquez, P. and Cassels, B.K. (2005) Monoamine oxidase inhibition in the light of new structural data. Curr. Enz. Inhib. 1, 85-95.

Gallardo-Godoy, A., Fierro, A., McLean, T.H., Castillo, M., Cassels, B.K., Reyes-Parada, M., and Nichols, D.E. (2005) Sulfur-substituted α -alkyl phenethylamines as selective and reversible MAO-A inhibitors: Biological activities, ComFA analysis, and active site modeling. J. Med. Chem. 48, 2407-2419.

Asencio, M., Hurtado-Guzmán, C., López, J.J., Cassels, B.K., Protais, P. and Chagraoui, A. (2005) **Structure-affinity relationships of halogenated predicentrine and glaucine derivatives at D1 and D2 dopaminergic receptors: halogenation and D1 receptor selectivity.** Bioorg. Med. Chem.13, 3699-3704.

Exley, R., Iturriaga-Vásquez, P., Lukas, R.J., Sher, E., Cassels, B.K. and Bermúdez, I. (2005) evaluation of benzyltetrahydroisoquinolines as ligands for brain nicotinic acetylcholine receptors. Br. J. Pharmacol., advance online publication, June 27.

Pérez, E.G., Saez, J. and Cassels, B.K. (2005) A convenient, renewable source of the anxiolytic proaporphine alkaloid glaziovine: *Duguetia vallicola* leaves. J. Chil. Chem. Soc. 50, 553-557.

Ivorra, M.D., Valiente, M., Martinez, S., Madrero, Y., Noguera, M.A., Cassels, B.K., Sobarzo, E.M. and D'Ocon, P. (2005) 8-NH₂-Boldine, an antagonist of α_{1A} and α_{1B} adrenoceptors without affinity for the α_{1D} subtype: Structural requirements for aporphines at α_1 -adrenoceptor subtypes. Planta Med. 71, 897-903.

Cassels, B.K., Bermúdez, I., Dajas, F., Abin-Carriquiry, J.A. and Wonnacott, S. (2005) From ligand design to therapeutic efficacy: The challenge for nicotinic receptor research. Drug Discov. Today, 10, 1657-1665.

Varas, R., Valdés, V., Iturriaga-Vásquez, P., Cassels, B.K., Alcayaga, J. and Iturriaga, R. (2006) Electrophysiological characterization of nicotinic receptors in cat petrosal ganglion neurons in culture by cytisine and its bromo derivatives, Brain Res., 1072, 72-78.

Abin-Carriquiry, J.A., Voutilainen, M.H., Barik, J., Cassels, B.K., Iturriaga-Vásquez, P., Bermúdez, I., Durand, C., Dajas, F. and Wonnacott, S. (2006) **C3-Halogenation of cytisine generates potent and efficacious nicotinic receptor agonists,** Eur. J. Pharmacol., 536, 1-11.

Iturriaga-Vásquez, P., Lühr-Sierra, S., Rezende, M.C. and Cassels, B.K. (2006) Synthesis of 2-aryl-1,3-propanediamines using a one-pot Knoevenagel-Michael sequence, J. Chil. Chem. Soc., 51, 781-783.

Mazariegos, D.I., Cabantchik, I.Z., Cassels, B.K. and Núñez, M.T. (2006) Characterization of mitochondrial iron uptake in HepG2 cells. Biol. Res., 39, 199-201.

Araya-Maturana, R., Cardona, W., Cassels, B.K., Delgado-Castro, T., Ferreira, J., Miranda, D., Pavani, M., Pessoa-Mahana, H., Soto-Delgado, J. and Weiss-López, B. (2006) Effects of 9,10-dihydroxy-4,4-dimethyl-5,8-dihydro-1(4*H*)-anthracenone derivatives on tumor cell respiration. *Bioorg. Med. Chem.*, 14, 4664-4669.

Iturriaga-Vásquez, P., Cassels, B.K., Prez, E.G., Slater, E.Y. and Bermúdez, I. (2007) Aporphine metho salts as neuronal nicotinic acetylcholine receptor blockers. *Bioorg. Med.Chem.*,15, 3368-3372.

Moya, P.R., Berg, K.A., Gutiérrez-Hernández, M.A., Sáez-Briones, P., Reyes-Parada, M., Cassels, B.K. and Clarke, W.P. (2007) **Functional selectivity of hallucinogenic phenethylamine and phenylisopropylamine derivatives at human 5-hydroxytryptamine (5-HT)_{2A} and 5-HT_{2C} receptors.** *J. Pharmacol. Exp.Ther.*, 321, 1054-1061.

Cassels, B.K., Reyes-Parada, M., Fierro, A., Osorio-Olivares, M., Edmondson, D.E. and Sepúlveda-Boza, S. (2007) Human and rat monoamine oxidase-A are differentially inhibited by (S)-4-alkylthioamphetamine derivatives. Insights from molecular modeling studies. *Bioorg. Med.Chem.* 15, 5198-5206.

Cassels, B.K., Iturriaga-Vásquez, P., Maya, J.D., Ferreira, J., Faúndez, M., Galanti, N., Ferreira, A. and Morello, A. (2007) Mode of action of natural and synthetic drugs against *Trypanosoma cruzi* and their interaction with the mammalian host. *Comp. Biochem. Physiol.*, 146, 601-620.

Cassels, B.K. and Asencio, M. (2008) Monoaminergic, ion channel and enzyme inhibitory activities of natural aporphines, their analogues and derivatives, *Nat. Prod. Commun.* 3, 643-653.

Zapata-Torres, G., Cassels, B.K., Parra-Mouchet, J., Mascarenhas, Y.P., Ellena, J. and de Araujo, A.S. (2008) Quantum-chemical, NMR and X-ray diffraction studies on (±)-1-[3,4-(methylenedioxy)phenyl]-2-methylaminopropane, *J. Mol. Graph. Model.* 26, 1296-1305.

Abin-Carriquiry, J.A., Costa, G., Urbanavicius, J., Cassels, B.K., Rebolledo-Fuentes, M., Wonnacott, S. and Dajas, F. (2008) *In vivo* modulation of dopaminergic nigrostriatal pathways by cytisine derivatives: Implications for Parkinson's disease, *Eur. J. Pharmacol.* 589, 80-84.

Cassels, B.K., Cytisine and smoking, http://topics.scirus.com/Cytisine_and_Smoking.html
Pérez, E.G., Cassels, B.K. and Zapata-Torres, G. (2009) Molecular modeling of the $\alpha 9\alpha 10$ nicotinic acetylcholine receptor subtype, *Bioorg. Med. Chem. Lett.* 19, 251-254

Zambrano, C.A., Marks, M.J., Cassels, B.K. and Maccioni, R.B. (2009) *In vivo* effects of 3-iodocytisine: Pharmacological and genetic analysis of hypothermia and evaluation of chronic treatment on nicotinic binding sites, *Neuropharmacology* 57, 332-342.

Vilches-Herrera, M., Miranda-Sepúlveda, J., Rebolledo-Fuentes, M., Fierro, A., Lühr, S., Iturriaga-Vásquez, P., Cassels, B.K. and Reyes-Parada, M. (2009) Naphthylisopropylamine and *N*-benzylamphetamine derivatives as monoamine oxidase inhibitors, *Bioorg. Med. Chem.* 17, 2452-2460.

Galdámez, A., Castro-Castillo, V. and Cassels, B.K. (2009) Crystal structure of 5,6,8,12b-tetrahydrodioxolo[4,5-*g*]isoindolo[1,2-*a*]isoquinolin-8-one (C₁₇H₁₃NO₃). *J. Chil. Chem. Soc.* 54, 327-329.

Castro-Castillo, V., Rebolledo-Fuentes, M. and Cassels, B.K. (2009) Synthesis of A-ring-substituted 5,6,8,12b-tetrahydroisoindolo[1,2-*a*]isoquinolin-8-ones. *J. Chil. Chem. Soc.* 54, 417-423.

Lühr, S., Vilches-Herrera, M., Fierro, A., Ramsay, R.R., Edmondson, D.E., Reyes-Parada, M., Cassels, B.K. and Iturriaga-Vásquez, P. (2010) **2-Arylthiomorpholine derivatives as selective and reversible monoamine oxidase B inhibitors**. *Bioorg. Med. Chem.* 18, 1388-1395.

Abin-Carriquiry, J.A., Urbanavicius, J., Scorza, C., Costa, G., Wonnacott, S., Rebolledo-Fuentes, M., Cassels, B.K. and Dajas, F. (2010) Increase in locomotor activity after acute administration of the nicotinic receptor agonist 3-bromocytisine in rats. *Eur. J. Pharmacol.* 634, 89-94.

Abin-Carriquiry, J.A., Paulino-Zunini, M., Cassels, B.K., Wonnacott, S. and Dajas, F. (2010) In silico characterization of cytisinoids docked into an acetylcholine binding protein. *Bioorg. Med. Chem. Lett.* 20, 3683-3687.

Di Liberto, M., Svetaz, L., Furlán, R.L.E., Zacchino, S.A., Delporte, C., Novoa, M.A., Asencio, M. and Cassels, B.K. (2010) Antifungal activity of saponin-rich extracts of *Phytolacca dioica* L. and of the saponin obtained through hydrolysis. *Nat. Prod. Commun.* 5, 1013-1018.

Iturriaga-Vásquez, P., Carbone, A., García-Beltrán, O., Livingstone, P.D., Biggin, P., Cassels, B.K., Wonnacott, S., Zapata-Torres, G. and Bermúdez, I. (2010) **Molecular determinants for competitive inhibition of $\alpha 4\beta 2$ nicotinic acetylcholine receptors**. *Mol. Pharmacol.* 78, 366-375.

Quinteros-Muñoz, D., Sáez-Briones, P., Díaz-Véliz, G., Mora-Gutiérrez, S., Rebolledo-Fuentes, M. and Cassels, B.K. (2010) Behavioral profiles in rats distinguish among 'ecstasy', methamphetamine and 2,5-dimethoxy-4-iodoamphetamine: Mixed effects for 'ecstasy' analogues. *Behav. Neurosci.* 124, 662-674.

Castro-Castillo, V., Rebolledo-Fuentes, M., Theoduloz, C. and Cassels, B.K. (2010) Synthesis of lakshminine and antiproliferative testing of related oxoisoaporphines. *J. Nat. Prod.* 73, 1951-1953.

Cassels, B.K. and Asencio, M. (2010) Anti-HIV activity of natural triterpenoids and hemisynthetic derivatives 2004 – 2009. *Phytochem. Rev.* Published online: 25 March 2010.

Arrau, S., Delporte, C., Cartagena, C., Rodríguez, M., González, P., Silva, X., Cassels, B.K. and Miranda, H.F. (2011) Antinociceptive activity of *Quillaja saponaria* Mol. saponin extract, quillaic acid and derivatives in mice. *J. Ethnopharmacol.* 133, 164-167.

Rodríguez-Díaz, M., Delporte, C., Cartagena, C., Cassels, B.K., González, P., Silva, X., León, F. and Wessjohann, L.A. (2011) Topical anti-inflammatory activity of quillaic acid from *Quillaja saponaria* Mol. and some derivatives. *J. Pharm. Pharmacol.* 63, 718-724.

Galdámez, A., García-Beltrán, O. and Cassels, B.K. (2011) Hydrogen-bonded supramolecular array in the crystal structure of ethyl 7-hydroxy-2-oxo-2*H*-chromene-3-carboxylate monohydrate. *J. Chil. Chem. Soc.* 56, 546-548.

Galdámez, A., Gutiérrez-Hernández, M., Cassels, B.K. and Sáez-Briones, P. (2011) Crystal structure of (1*R*,5*S*)-9-nitro-1,2,3,4,5,6-hexahydro-1,5-methanopyrido[1,2-*a*][1,5]diazocin-8-one (9-nitrocytisine), C₁₁H₁₃O₃N₃. *J. Chil. Chem. Soc.* 56, 595-597.

PATENTS

B.K. Cassels, F.J. Dajas, J.H. Medina y A.C. Paladini,
Flavonoid and biflavonoid derivatives, their pharmaceutical compositions,
their anxiolytic activity
WO 95/05169, February 23, 1995.

B.K. Cassels, F.J. Dajas, J.H. Medina, A.C. Paladini y R.H. Silveira,
Flavonoid and biflavonoid derivatives, their pharmaceutical compositions,
their anxiolytic activity
United States Patent 5,756,538, May 26, 1998.

B.K. Cassels, F.J. Dajas, J.H. Medina, A.C. Paladini y R.H. Silveira,
Flavonoid and biflavonoid derivatives, their pharmaceutical compositions,
their anxiolytic activity
United States Patent 6,004,998, December 21, 1999.

B.K. Cassels, F.J. Dajas, J.H. Medina, A.C. Paladini y R.H. Silveira,
Flavonoid and biflavonoid derivatives, their pharmaceutical compositions,
Their anxiolytic activity
European Patent 0 714 296 B1, November 07, 2001.