CURRICULUM VITAE

Ibon Alkorta

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DATOS PERSONALES

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FORMACION ACADEMICA

Comienza la carrera de Química en el curso 1981-82 en la Universidad del Pais Vasco, campus de Leioa (Vizcaya). En el curso 1984-85 se traslada a la Universidad Autonoma de Madrid para llevar a cabo la especializacion de Química Orgánica. Finaliza la carrera el año 1986.

En Febrero de 1987 presenta su memoria de Licenciatura en la Facultad de Ciencias (U.A.M.) obteniendo la calificación de Sobresaliente.

Durante los cursos 1986-87 y 1987-88 lleva a cabo los correspondientes cursos de doctorado (Facultad de Ciencias-U.A.M.).

En 26 de Noviembre de 1990 presenta su memoria de Doctorado en la Facultad de Ciencias (U.A.M.) obteniendo la calificación de Apto "Cum Laude".

CURSOS

En Octubre de 1986 asiste al curso de "Diseño de fármacos" organizado por la Asociación Nacional de Químicos de España y la Sociedad Española de Química Terapéutica.

En Enero de 1987 participa en el curso "Introducción al análisis estadístico de datos con los paquetes BMDP, SPSS y CLUSTAN", en Septiembre de ese mismo año asiste al curso sobre "Base de datos cristalográfica de Cambridge, sistema CSD y Banco de Datos de Proteinas Brookhaven", en Diciembre al curso "Métodos de mecanica molecular en analisis conformacional: Introducción a los programas MM2, MOLTWS y ECEPP", y en Marzo de

1988 al curso "Sistema operativo NOS2. Curso avanzado" impartidos por el Centro de Calculo del C.S.I.C.

En Mayo de 1990 asiste al curso " Química Orgánica Teórica", impartido por el Prof. Santiago Olivella en la Universidad de las Islas Baleares, Palma de Mallorca.

En Junio de 1998 asiste al curso “Mantenimiento y reparación de ordenadores” organizado por el CSIC.

En Marzo de 2004 asiste al curso “Programación en shell scripts” organizado por el CSIC.

En Noviembre de 2005 asiste al curso “Excel Avanzado. 1ª Edición” organizado por el CSIC.

En Junio de 2006 asiste al curso “Linux Avanzado” organizado por el CSIC.

En Mayo de 2018 asiste al curso “Excel 2010 Avanzado, 1ª edición” organizado por el CSIC.

ACTIVIDAD INVESTIGADORA

Desde Octubre de 1985 hasta Enero de 1987 realiza su trabajo de Licenciatura en el Instituto de Química Médica, del C.S.I.C., sobre el tema "Reactividad de sulfamidas N-sustituidas frente a 1,2- y 1,3-dinitrilos".

Desde Febrero de 1987 hasta Diciembre de 1990 realiza su trabajo de Tesis Doctoral en el mismo Instituto sobre "Aplicaciones de la modelización en química orgánica y química médica", disfrutando de una beca de Formación de Personal Investigador del Ministerio de Educación y Ciencia.

Desde Marzo de 1991 hasta Febrero de 1993 realizó una estancia post-doctoral en el Molecular Research Institute (Palo Alto, EEUU) gracias a una beca del Programa de Perfeccionamiento de Doctores y Tecnologos del Ministerio de Educación y Ciencia.

Durante el mes de Mayo de 1992 permaneció en la Universidad de Saskatchewan (Saskatoon, Canada) gracias a la beca post-doctoral anteriomente comentada.

Desde Marzo hasta Septiembre de 1993 permaneció en el Molecular Research Institute contratado como Químico Computacional.

A partir de Octubre de 1993 y hasta Febrero de 1996 trabaja en el Instituto de Química Médica con un contrato del Programa de Incorporación de Doctores y Tecnólogos a Grupos de Investigación en España.

Desde Junio hasta Agosto de 1994 permaneció en el Molecular Research Institute gracias a una beca de la Comunidad de Madrid.

Durante el mes de Junio de 1995 permaneció en la Universidad Politécnica de Barcelona gracias a una beca del Centro de Supercomputación de Cataluña (CESCA).

Desde 29 de Abril de 1996 es Colaborador Científico del Instituto de Química Médica (CSIC).

Desde el 25 de Noviembre de 2004 es Investigador Científico del Instituto de Química Médica (CSIC).

Desde el 19 de Julio de 2008 es Profesor de Investigación del Instituto de Química Médica (CSIC).

PARTICIPACION EN PROYECTOS

De Enero de 1987 a Febrero de 1991 en el proyecto PA 86-0431 titulado: "Aplicaciones de la informática en Investigación terapéutica", que se ejecutó en el Instituto de Química Médica del CSIC y fué financiado por la CICYT y el CSIC.

De Marzo de 1991 a Febrero de 1993, en el proyecto titulado "Modelización del receptor D1 de la dopamina" que se ejecuto en el Molecular Research Institute (EEUU) bajo la dirección de la Dra. Gilda Loew y que fué financiado por el Ministerio de Educación y Ciencia.

De Marzo de 1993 a Septiembre de 1993, en el proyecto titulado "CADD of D1/D2 receptor ligands for cocaine abuse therapy", " que se ejecuto en el Molecular Research Institute (EEUU) bajo la dirección del Dr. Hugo Villar y que fué financiado por el National Institute of Drugs (EEUU).

De Octubre de 1993 a Diciembre de 1994 en el proyecto FAR90-0746 titulado: "Modelización molecular de compuestos con actividad biológica" del que era investigador principal Dª. Pilar Goya Laza, que se ejecutó en el Instituto de Química Médica del CSIC y fué financiado por la CICYT y el CSIC.

De Enero de 1995 a Marzo de 1996 en el proyecto SAF 94-0705 titulado: "Miméticos de neuropéptidos. Busqueda de nuevos fármacos con acción sobre el sistema nervioso

central" del que era investigador principal Dª. Maria Teresa Garcia Lopez, que se ejecutó en el Instituto de Química Médica del CSIC y fué financiado por la CICYT.

De Marzo de 1997 a Marzo 2000 en el proyecto SAF97-0044-CO2-01 titulado "Analgésicos No Convencionales" del que es investigador principal Dª. Pilar Goya Laza, que se está realizando en el Instituto de Química Médica del CSIC y está financiado por la CICYT.

De Enero de 1996 a Septiembre de 1997 participó en el proyecto europeo CHRX CT 940582 titulado "Localization and transfer of hydrogen".

Desde Diciembre de 2000 hasta Noviembre 2003 participa en el proyecto (SAF 00-0-114-C02-01) titulado "Diseño y síntesis de nuevos opioides, antagonistas de bradiquinina y canabinoides", del que es investigador princial Dª. Pilar Goya Laza y que fue financiado por la CICYT.

Desde Diciembre del 2000 hasta Noviembre del 2003 participa en el proyecto (BQU2000-0906) titulado "Estudio teórico de interacciones entre acidos nucleicos y proteinas" del que soy investigador principal y que fue financiado por el Ministerio de Ciencia y Tecnología.

Desde Diciembre 2003 hasta Noviembre de 2006 participa en el proyecto (BQU2003-01251) titulado "Reconocimiento quiral en complejos con puentes de hidrógeno" del que soy investigador principal y que está financiado por el Ministerio de Ciencia y Tecnología.

Desde Enero 2006 hasta Diciembre 2009, es coordinador en el CSIC del proyecto (S-0505/PPQ/0225) titulado "Materiales foto- y electroactivos para células solares orgánicas e híbridas" del que es investigador principal el Dr. Nazario Martín y que está financiado por la Comunidad de Madrid.

Desde Diciembre 2006 hasta Noviembre 2007 participa en el proyecto (CTQ2006-14487-C02-01) titulado "Estudio de organocatalisis quiral por interacciones débiles" del que soy investigador principal y que está financiado por el Ministerio de Educación y Ciencia.

Desde Diciembre de 2007 hasta Noviembre 2008 participa en el proyecto (CTQ2007-61901/BQU) titulado "Racionalizacion y optimización de la discriminacion quiral a través de enlaces de hidrógeno" del que soy investigador principal y que esta financiado por el Ministerio de Educación y Ciencia.

Desde Enero de 2010 y hasta Diciembre de 2012 participa en el proyecto "Reactividad en fase gas: nuevos materiales moleculares y discriminación quiral" (CTQ2009-

13129-C02-02) del que el Prof. Alkorta es el investigador principal del subproyecto y que está financiado por el Ministerio de Ciencia e Innovación.

Desde Enero de 2010 y hasta Diciembre de 2013 participa en el proyecto "Materiales foto- y electroactivos para células solares orgánicas e híbridas" (MADRISOLAR2, S2009/PPQ-1533) del que es investigador principal el Dr. Nazario Martín y que está financiado por la Comunidad de Madrid.

Desde Enero de 2013 y hasta Diciembre de 2015 participa en el proyecto "Interacciones no-covalentes y quiralidad en nuevos materiales" (CTQ2012-35513-C02-02) del que el Prof. Alkorta es el investigador principal del subproyecto y que está financiado por el Ministerio de Economía y Competitividad.

Desde Octubre de 2014 y hasta Diciembre de 2018 participa en el proyecto "Materiales avanzados de carbono para fotovoltaica molecular" (FOTOCARBON, S2013/MIT-2841) del que es investigador principal el Dr. Nazario Martín y que está financiado por la Comunidad de Madrid.

Desde Enero de 2016 y hasta Diciembre de 2018 participa en el proyecto "Modificación de la reactividad y diseño de nuevos materiales mediante enlaces berilio y otras interacciones no-covalentes" (CTQ2015-63997-C2-2-P) del que el Prof. Alkorta es el investigador principal del subproyecto y que está financiado por el Ministerio de Economía y Competitividad.

Desde Enero de 2019 y hasta la actualidad participa en el proyecto "Evaluación Integral de la Calidad del Aire Urbano y Cambio Climático" (AIRTEC-CM, P2018/EMT-4329) del que es investigador principal el Dr. Rafael Borge García y que está financiado por la Comunidad de Madrid.

Desde Enero de 2019 y hasta la actualidad participa en el proyecto "Diseño y Caracterización de nuevos Materiales Moleculares y optimización de fármacos: Sinergia experimento y teoría" (PGC2018-094644-B-C22) del que el Prof. Alkorta es el investigador principal del subproyecto y que está financiado por el Ministerio de Ciencia, Innovación y Universidades.

FORMACION DE PERSONAL INVESTIGADOR

De Enero de 1996 a Septiembre de 1996, Dra. María del Mar Ramos Gallego realizó una estancia post-doctoral bajo mi dirección trabajando sobre el estudio teórico de puentes de hidrógeno.

De Mayo de 1997 a Septiembre de 1997, Dra. Pilar Sánchez Andrada realizó una estancia post-doctoral bajo mi dirección trabajando sobre el estudio teórico de adiciones nucleófilas sobre cumulenos.

De Septiembre de 1997 a Noviembre de 1997, Dr. Rostislav Trifonov realizó una estancia post-doctoral bajo mi dirección trabajando sobre el estudio de reactividad y tautomería en azoles.

Durante el mes de Julio de 2000, Dr. Pilar Prieto realizó una estancia post-doctoral bajo mi dirección trabajando sobre puentes de hidrógeno.

Desde Junio de 2002 dirige la tesis doctoral de Oscar Picazo con el tíuto "Discriminación quiral en complejos con puentes de hidrógeno". En Julio de 2004, Oscar Picazo, obtiene el Diploma de Estudios Avanzados con la calificación de Sobresaliente.

De Octubre a Noviembre de 2004, la Dra. Marina Sanchez realizó una estancia bajo mi dirección trabajando en el estudio teórico de rotaciones ópticas.

De Enero de 2005 a Diciembre de 2005, el Dr. Markku Sundberg ha realizado un año sabatico bajo mi dirección trabajando sobre la discriminación quiral en complejos metálicos.

De Mayo de 2005 a Abril de 2006, el Dr. Krzysztof Zborowski ha trabajado en nuestro grupo con una beca post-doctoral del MEC, en el estudio de discriminación quiral en procesos reactivos.

De Octubre a Noviembre de 2006, la Dra. Marina Sanchez realizó una estancia bajo mi dirección trabajando en el estudio teórico de constantes de acoplamiento en RMN.

De Septiembre a Diciembre de 2007, Daniel H O' Donovan realizó una estancia bajo mi dirección trabajando en el reconocimiento quiral de guanidinas biciclicas

Desde Enero 2007 hasta Diciembre de 2009, el Dr. Fernando Blanco realiza una estancia bajo mi dirección trabajando en el estudio de discriminación quiral.

De Septiembre a Diciembre de 2009, Amanda Sotoodeh realizó una estancia bajo mi dirección trabajando en el estudio de la complejación de guanidinas quirales con aniones

Desde Junio de 2010 a Diciembre de 2010, la Dra. Cristina Trujillo estuvo contratada bajo mi dirección trabajando en el estudio de nuevos materiales fotovoltaicos.

Desde Enero de 2011 a Julio de 2012, el Dr. Goar Sánchez-Sanz estuvo contratado (proyecto (MADRISOLAR2, S2009/PPQ-1533) bajo mi dirección trabajando en el estudio de nuevas interacciones intermoleculares.

Desde Octubre de 2010 a Septiembre de 2014, Luis Miguel Azofra realiza su tesis doctoral bajo mi dirección en el estudio de reactividad de carbohidratos.

Desde Octubre de 2014 a Septiembre de 2015, Marta Marín-Luna estuvo contratada (proyecto (CTQ2015-63997-C2-2-P) bajo mi dirección trabajando en el estudio de enlaces de berilio.

Desde Febrero de 2016 a Julio de 2016, Carlos Martín Fernández estuvo contratado (proyecto FOTOCARBON, S2013/MIT-2841) bajo mi dirección trabajando en el estudio mecanocuántico de propiedades químico-físicas de compuestos con interés fotoquímico.

Desde Octubre de 2016 hasta Marzo de 2017 Saber Mohammadi Chalanchi ha trabajando bajo mi dirección con una beca del Gobierno de Irán.

Desde Enero de 2017 hasta Febrero de 2018, M. Merced Montero-Campillo estuvo contratada (proyecto FOTOCARBON, S2013/MIT-2841) bajo mi dirección trabajando en el estudio mecanocuántico de propiedades químico-físicas de compuestos con interés fotoquímico.

De Enero de 2017 a Julio de 2018 Iñigo Irribarren e I-Ting realizaron una estancia para desarrollar el trabajo fin de master en el Máster Universitario en Química Teórica y Modelización [European Master in Theoretical Chemistry and Computational Modelling (TCCM)].

Desde Octubre de 2020 y hasta la actualidad Maxime Ferrer realiza su tesis doctoral bajo mi dirección.

PUBLICACIONES EN REVISTAS EXTRANJERAS

1 I. Alkorta, V.J. Arán, A.G. Bielsa, y M. Stud, "Reactivity of malononitrile towards sulphamide and N-sustituted sulfamides: Synthesis and hydrolysis reactions of 3,5-diamino-1,2,6-thiadiazine 1,1-dioxides", J. Chem. Soc., Perkin I, **1988**, 1271-1275.

2 V.J. Arán, J.R. Ruiz, E. Davila, I. Alkorta, y M. Stud, "Synthesis and reactivity of some aminosubstituted 1,2,5-thiadiazole 1,1-dioxides", Liebigs Ann. Chem., **1988**, 337-341.

3 I. Alkorta, J. Elguero, P. Goya, y C. Roussel, "Energy calculations and computer modeling of chromatographic separations on microcristalline cellulose triacetate", Chromatographia, **27**, 77-81 (1989). DOI: 10.1007/BF02290410

4 O. Mó, J.L.G. de Paz, M. Yáñez, I. Alkorta, J. Elguero, P. Goya, e I. Rozas, "A molecular study of the conformation (inversion and rotation barriers) and electronic properties of sulphamide", Can. J. Chem., **67**, 2227-2236 (1989). DOI: 10.1139/v89-347

5 I. Alkorta, V.J. Arán, E. Davila, J.R. Ruiz, y M. Stud, "Reactivity of cyanogen towards N-substituted sulfamides: Synthesis of 1,2,5-thiadiazole 1,1-dioxides derivatives", Liebigs Ann. Chem., **1989**, 1135-1137.

6 I. Alkorta, J. Elguero, I. Rozas, y A.T. Balaban, "Theoretical studies of azaanalogs of platonic hydrocarbons. I. Cubane and its azaderivatives", J. Mol. Struct. (Theochem), **206**, 67-75 (1990).

7 I. Alkorta, P. Goya, J.A. Páez, y W. Pfleiderer, "Synthesis and physico-chemical properties of 6- and 7- monosubtituted pyrazino[2,3-*c*]-1,2,6-thiadiazine 2,2-dioxides", Pteridines, **2**, 3-7 (1990).

8 I. Alkorta, J. Elguero, I. Rozas, y A.T. Balaban, "Theoretical studies of azaanalogs of platonic hydrocarbons. II. Tetrahedrane and its azaderivatives", J. Mol. Struct. (Theochem), **208**, 63-77 (1990).

9 I. Alkorta, J. Elguero, I. Rozas, y A.T. Balaban, "Theoretical studies of azaanalogs of platonic hydrocarbons. III. Dodecahedrane and its azaderivatives", J. Mol. Struct. (Theochem), **228**, 47-60 (1991).

10 I. Alkorta, P. Goya, C. Nombela, R. Medina, y C. Pérez-Martín, "Synthesis and biological screening of aminothiadiazine dioxides related to trimetoprim", Arzneim. Forsch./Drug Res., **41**, 264-266 (1991).

11 I. Alkorta, P. Goya, J.A. Páez, y C. Pérez, "Pyrazino[2,3-*c*]-1,2,6-thiadiazine 2,2-dioxides. Synthesis of SO_2 analoques of folic acid antagonist", Liebigs Ann. Chem., **1991**, 301-303.

12 I. Alkorta, P. Goya, y J.A. Páez, "Selective bromination of pyrido[2,3-*c*]-1,2,6-thiadiazine 2,2-dioxides", Synthetic Communication, **21**, 827-831 (1991).

13 I. Alkorta, P. Goya, y J.A. Páez, "Synthesis and E/Z stereoisomerism of 6-carbaldoxime derivatives of pyrazino[2,3-*c*]-1,2,6-thiadiazine 2,2-dioxides", Heterocycles, **32**, 279-284 (1991).

14 I. Alkorta y H.O. Villar, "Quantum mechanical parametrization of a hydrophobic index", Int. J. of Quantum Chemistry, **44**, 203-218 (1992).

15 I. Alkorta y J. Elguero, "The use of additive models for discussing the heats of formation of polyazaderivatives of aromatic hydrocarbons", Acta Chim. Hung. Models in Chemistry, **129**, 709-718 (1992).

16 P. Goya, J.A. Páez, I. Alkorta, E. Carrasco, M. Grau F. Anton, S. Julia, y M. Martínez-Ripoll, "N-Substituted pyrazino[2,3-*c*]-1,2,6-thiadiazine 2,2-dioxides. a new class of diuretics", J. Med. Chem., **35**, 3977-3983 (1992).

17 I. Alkorta, H.O. Villar, y G.A. Arteca, "Comparative study between ab initio and semiempirical electrostatic potentials on molecular surfaces", J. Comput. Chem., **14**, 530-540 (1993).

18 I. Alkorta, H.O. Villar, y R.E. Cachau, "Conformational analysis of 2,3,6,7-tetrahydroazepines with implications for D1 selective benzazepines", J. Comput. Chem., **14**, 571-578 (1993).

19 H.O. Villar, G. H. Loew, e I. Alkorta, "Strategies for indirect computer-aided drug design", Pharmaceut. Res., **10**, 475-487 (1993).

20 I. Alkorta, H.O. Villar, y J.J. Pérez, "Comparation of methods to estimate the free energy of solvation: Importance in the modulation of the affinity of 3-benzazepines for the D1 receptor", J. Comput. Chem., **14**, 620-626 (1993).

21 I. Alkorta y H.O. Villar, "Considerations on the recognition of the D1 receptor by agonists", J. Comp-Aided Mol. Design, **7**, 659-670 (1993).

22 I. Alkorta, H.O. Villar, y J.J. Perez, "Effect of the basis set on the computation of molecular polarization", J. Phys. Chem., **97**, 9113-9119 (1993).

23 I. Alkorta y H.O. Villar, "Molecular electrostatic potential of D1 and D2 dopamine agonists", J. Med. Chem., **37**, 210-213 (1994).

24 I. Alkorta, J.J. Pérez, y H.O. Villar, "Molecular polarization maps as a tool for drugs design and in chemical reactivity studies", J. Mol. Graph., **12**, 3-13 (1994).

25 I. Alkorta, "Comparison of methods to estimate geometric and electronic properties on sulfur containing compounds", Theor. Chim. Acta, **89**, 1-12 (1994).

26 I. Alkorta, M.Bachs, y J.J. Perez, " The induced polarization of the water molecule", Chem. Phys. Lett., **224**, 160-165 (1994).

27 P. Du e I. Alkorta, "Sequence divergence analysis for the prediction of membrane proteins I. Comparison with bacteriorhodopsin", Prot. Eng., **7**, 1221-1229 (1994).

28 I. Alkorta y P. Du, "Sequence divergence analysis for the prediction of membrane proteins II. A 3-D model of human rhodopsin", Prot. Eng., **7**, 1231-1238 (1994).

29 C. Escolástico, M.D. Santa María, R.M. Claramunt, M.L. Jimeno, I. Alkorta, C. Foces-Foces, F.H. Cano, y J. Elguero, "Imidazole and Benzimidazole addition to quinones. Formation of meso and d,l isomers and crystal structure of d,l isomer of 2,3-bis(benzimidazol-1´-yl)-1,4-dihydroxybenzene", Tetrahedron, **50**, 12489-12510 (1994).

30 I. Alkorta y S. Maluendes, "Theoretical study of CH···O hydrogen bonds in H_2O-CH_3F, H_2O-CH_2F_2, and H_2O-CHF_3", J. Phys. Chem., **99**, 6457-60 (1995).

31 I. Alkorta y J.J. Perez, "Molecular polarization potential maps of nucleic acid bases", Int. J. Quant. Chem., **57**, 123-135 (1996).

32 N. Figuera, I. Alkorta, M.T. García-López, y R. González-Muñiz, "2-Amino-3-oxohexahydroindolizino[8,7-*b*]indole-5-carboxylate derivatives as new scaffolds for mimicking β-turn secondary structures. Molecular dynamics and stereoselective synthesis", Tetrahedron, **51**, 7841-7856 (1995).

33 M.T. García-López, I. Alkorta, M.J. Domínguez, R. González-Muñiz, R. Herranz, N.L. Johansen, K. Madsen, H. ThØgersen, y P. Suzdak, "Constrained C-terminal hexapeptide neurotensin analogues containing a 3-oxoindolizidine skeleton", Lett. Pep. Sci., **1**, 269-276 (1995).

34 I. Alkorta, C. García-Gómez, J.A. Páez, y P. Goya, "Theoretical and experimental analysis of properties in heterocycles containing the aminosulfonylamino moeity", J. Phys. Org. Chem., **9**, 203-211 (1996).

35 N. Jagerovic, C. Fernández-Castaño, C. Foces-Foces, A.L. Llamas-Saiz, I. Alkorta y J. Elguero, "Hexadeca(pyrazol-1-yl)phtalocyanine: a soluble phtalocyanine absorbing at 772 nm.", New Journal of Chemistry, **20**, 1081-1086 (1996).

36 I. Alkorta y J.J. Perez, "Approximations in the computation of molecular polarization maps", Elect. J. Theor. Chem., **1**, 26-37 (1995).

37 I. Alkorta, M.L. Suarez, R. Herranz, R. González-Muniz y M.T. García-López, "Similarity study on peptide γ-turn conformation mimetics", J. Mol. Modeling, **2**, 16-25 (1996).

38 I. Alkorta, C. García-Gómez, J.L. G. de Paz, M.L. Jimeno y V.J. Arán, "Synthesis, hydrolysis reactions and conformational study of 2-substituted 3,5-diamino-4-nitroso-2*H*-1,2,6-thiadiazine 1,1-dioxides", J. Chem. Soc., Perkin Trans II, **1996**, 293-297.

39 I. Alkorta, I. Rozas, J. Elguero, C. Foces-Foces y F. H. Cano, "A statistical survey of the Cambridge Structural Database concerning density and paking", J. Mol. Struct., **382**, 205-213 (1996).

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41 I. Alkorta y G. Loew, "A 3D model of the δ opioid receptor and ligand-receptor complexes", Prot. Eng., **9**, 573-583 (1996).

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43 I. Alkorta y J. Elguero, "Tautomerism and Mills-Nixon-like effect in pyrazols", Structural Chemistry, **8**, 189-195 (1997).

44 I. Alkorta y J. Elguero, " Carbenes and Silylenes as hydrogen bond acceptors", J. Phys. Chem. **100**, 19367-19370 (1996).

45 M. Ramos, I. Alkorta y J. Elguero, " The Mills-Nixon effect on enol-enol tautomerism in β-dicarbonyl compounds and on annular tautomerism in N*H*-pyrazoles: a semi-empirical study", Tetrahedron, **53**, 1403-1410 (1997).

46 I. Rozas, I. Alkorta y J. Elguero, “Inverse hydrogen-bonded complexes”, J. Phys. Chem. A, **101**, 4236-4244 (1997).

47 I. Rozas, I. Alkorta y J. Elguero, “Field effects on Dihydrogen Bonded Systems”, Chem. Phys. Lett. **275**, 423-428 (1997).

48 I. Alkorta y J. Elguero, “Carbon acidity and ring strain: a hybrid HF-DFT approach (Becke3LYP/6-311++G**)”, Tetrahedron **53**, 9741-9748 (1997).

49 P. Goya, N. Campillo, C. García-Gómez, J.A. Páez e I. Alkorta, "Heterocyclic structures useful in medicinal chemistry: the case of pyrazino [2,3-c][1,2,6]thiadiazine 2,2-dioxide", Il Farmaco, **52**, 283-387 (1997).

50 I. Rozas, I. Alkorta y J. Elguero, “Unusual hydrogen bonds: H···π interactions", J. Phys. Chem., **101,** 9457-9463 (1997).

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OTROS

Organización del Curso sobre "Modelización Molecular y diseño de moléculas bioactivas" en los Cursos de Verano de El Escorial, 1997.

Desde 2004 es miembro de la International Union of Pure and Applied Chemitry (IUPAC).

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