Giulia CARON: Curriculum Vitae et Studiorum

- 1992: Laurea in Chimica e Tecnologia Farmaceutiche conseguita presso la Facoltà di Farmacia dell'Università di Torino.

  1993: Borsa di studio annuale post-lauream per attività di perfezionamento all'estero conferita dall'Università degli Studi di Torino (D.R. n. 461 del 26-1-1993).
- 1994: Laurea in Farmacia conseguita presso la Facoltà di Farmacia dell'Università di Torino.

  1997: Dottorato di ricerca in Scienze Farmaceutiche conseguito presso Institut de Chimie Thèrapeutique, Ecole de Pharmacie, BEP, UNIL, CH-1015 Lausanne-Dorigny, Suisse (aprile).

  Tesi dal titolo: Physicochemical determinants of drug binding and distribution. Direttore prof. B.Testa
- Aprile 1997-dicembre 1997: Primo Assistente con incarichi di ricerca e didattica presso Institut de Chimie Thèrapeutique, Ecole de Pharmacie, BEP, UNIL, CH-1015 Lausanne-Dorigny, Suisse.
- 1998: Borsa di studio per il supporto didattico conferita dall'Università degli Studi di Torino (D.R. n. 1352 del 23-2-1998)
- 16 aprile 1999: Ricercatore presso la Facoltà di Farmacia di Torino (settore disciplinare CHIM08).
- 16 aprile 2002: Conferma in ruolo come ricercatore
- 2005/2006 – oggi: Professore aggregato

Attività didattica

La dott. Caron, in qualità di ricercatore/ricercatore confermato afferente al Consiglio di corso di Laurea in Farmacia, ha svolto la seguente attività didattica:

- Assistenza agli studenti nella preparazione di Tesi di Laurea sperimentali e compilative.
- Svolgimento dell'attività didattica integrativa in particolare rivolta ad esercitazioni pratiche di laboratorio (Analisi dei Farmaci II ed Analisi dei Medicinali I e II)
- Seminari nell'ambito di corsi del settore CHIM08: Analisi dei Farmaci II (CTF), Analisi dei Medicinali II (F), Chimica Farmaceutica II (CTF), Chimica Farmaceutica II (Farmacia Ospedaliera) e cicli di lezioni nell'ambito del corso in Chimica Farmaceutica (Corso di laurea in Chimica).

- Affidamento del corso di Analisi dei Medicinali I (primo semestre) del corso di Laurea in Farmacia (da a.a.2001/2002 ad oggi).
- Attività libera "Comprensione e classificazione di dati mediante analisi grafica e chemiometrica di base" (da a.a.2003/2004 ad oggi).
- Coaffidamento del corso "Molecular modeling and chemometrics to investigate chemical topics in bio and enviromental sciences" della Scuola di Dottorato in Scienza ed Alta Tecnologia, Indirizzo Scienze Chimiche (a.a. 2007-2008).

Attività scientifica

- La dott. Caron si è dapprima misurata con un' esperienza internazionale (5 anni tra dottorato e post-dottorato trascorsi in Svizzera) sotto la guida del prof. Testa, premio Nauta della medicinal chemistry nel 2002. In questa fase la dott.Caron si è occupata di filoni di ricerca relativi alle proprietà fisico-chimiche dei farmaci e della loro applicazione nel settore QSAR. Al termine di questa esperienza, la candidata ha lavorato per nell'ambito del gruppo di ricerca coordinato dal prof. Gasco e rivolta alla progettazione, sintesi, caratterizzazione fisico-chimica e biologica di molecole biologicamente attive, con particolare interesse nei confronti della funzione N-ossidica. Infine, nel 2002 la dott. Caron ha fondato con il prof.Ermondi il gruppo di ricerca CASMedChem (www.casmedchem.unito.it) per mettere a frutto le specifiche competenze scientifiche acquisite negli anni e per poter sviluppare una propria autonomia di ricerca nel campo del QSAR, delle predizioni ADMET nell'ambito del processo del drug design e di tematiche correlate.
- Coautore di più di 40 pubblicazioni tra articoli su riviste internazionali e capitoli di libro e di circa 35 presentazioni a congresso.
- Referee per le riviste: J.Med.Chem. Eur.J.Med.Chem., Int.J.Pharm. QSAR & Combinatorial Science, Pharm. Res., Bioorganic and Med.Chem., J.Inclusion Phenom.Mol.Recognit.Chem and Journal of Chemical Information and Modeling.
- Coautore del software BIOCUBE4mf. Il software è stato ideato e realizzato nell'ambito del gruppo di ricerca CASMedChem per estrarre le informazioni più rilevanti dai Molecular Interaction Fields generati da software come GRID Molecular Discovery Ltd., Pinner, Middlesex, UNITED KINGDOM). Il software è distribuito gratuitamente per le Università attraverso il sito www.casmedchem.unito.it.

- Responsabile della gestione del sito web (www.cdtec.unito.it) e del settore informatico della Associazione Italiana Chimica e Tecnologia delle Ciclodestrine di cui la dott. Caron è anche membro.
- Membro American Chemical Society (ACS)

Pubblicazioni

Articoli su riviste

1. **Caron,G.**; Carrupt,P.A.; Testa,B.; Ermondi,G.; Gasco,A.;
   Insight into the lipophilicity of the aromatic N-oxide moiety.
   Pharm. Res. **1996**, *13,* 1186-1190. (New York, NY, USA)
   IF 2.847
2. **Caron,G**.; Pagliara,A.; Gaillard,P.; Carrupt,P.A.; Testa,B.;
   143. Ionization and Partitioning Profiles of Zwitterions: The Case of the Anti-Inflammatory Drug Azapropazone.
   Helv. Chim. Acta **1996**, *79,* 1683-1685. (Berlin, Germany)
   IF 2.483
3. Zahouily,M.; **Caron,G.**; Carrupt,P.A.; Knouzi,N.; Renaud,P.
   Diastereoselective radical alkylations of alkyl aryl sulfoxides.
   Tetrahedron Lett. **1996**, *37,* 8387-8390. (Kidlington, Oxford, England)
   IF 2.400
4. **Caron,G.**; Gaillard,P.; Carrupt,P.A.; Testa,B.
   Lipophilicity behavior of model and medicinal compounds containing a sulfide, sulfoxide, or sulfone moiety.
   Helv. Chim. Acta **1997**, *80,* 449-462. (Berlin, Germany)
   IF 2.483
5. Pagliara,A.; Carrupt,P.A.; **Caron,G.**; Gaillard,P.; Testa,B.
   Lipophilicity profiles of ampholytes.
   Chem. Rev. **1997**, *97,* 3385-3400. (Washington, DC 20036, USA).
   IF 22.757
6. Pagliara,A.; **Caron,G.**; Lisa,G.; Fan,W.; Gaillard,P.; Carrupt,P.A.; Testa,B.; Abraham,M.H.
   Solvatochromic analysis of di-n-butyl ether/water partition coefficients as compared to other solvent systems.
   J. Chem. Soc. , Perkin Trans. 2 **1997**, 2639-2643. (Cambridge, UK).
   IF 1.845
7. Hervé,F.; **Caron,G**.; Duché,J-C; Gaillard,P.; Rahman,.A.; Tsantili-Kakoulidou, A.; Carrupt,P-A.; d'Athib,P.; Tillement,J-P. And Testa,B.

Ligand specificity of the genetic variants of human α1-acid glycoprotein: generation of a three dimensional quantitative structure-activity relationship model for drug binding to the A variant.
Mol. Pharmacol. **1998**, *54,* 129-138. (Bethesda, MD 20814-3998, USA).
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8. Fruttero,R.; **Caron,G.**; Fornatto,E.; Boschi,D.; Ermondi,G.; Gasco,A.; Carrupt,P.A.; Testa,B.
Mechanisms of Liposomes/Water Partitioning of (p-Methylbenzyl)alkylamines.
Pharm. Res. **1998**, *15,* 1407-1413. (New York, NY, USA)
IF 2.847
9. Megson,I.L.; Morton,S.; Greig,I.R.; Mazzei,F.A.; Field,R.A.; Butler,A.R.; **Caron,G.**; Gasco,A.; Fruttero,R. And Webb,D.J.
N-substituted analogues of S-nitroso-N-acetyl-D,L-penicillamine: chemical stability and prolonged nitric oxide mediated vasodilation in isolated rat femoral arteries.
Br. J. Pharmacol. **1999**, *126,* 639-648. (Houndmills, Hampshire, England).
IF 3.722
10. Got,P.; Raimbaud,E.; Bussey,C.; **Caron,G.**; Carrupt,P-A; Walther,B.; Bensussan,A. ; Scherrmann,J-M.
Production and characterization of 22 monoclonal antibodies directed against S 20499, a new potent 5-HT1A chiral agonist: influence of the hapten structure on specificity and stereorecognition.
Pharm. Res. **1999**, *16,* 725-735. (New York, NY, USA)
IF 2.847
11. **Caron,G.**; Steyaert,G.; Pagliara,A.; Reymond,F.; Crivori,P.; Gaillard,P.; Carrupt,P.A.; Avdeef,A.; Comer,J.E.; Box,K.J.; Girault,H.H.; Testa,B.
Structure-lipophilicity relationships of neutral and protonated β–blockers. Part I. Intra- and Intermolecular Effects in Isotropic Solvent Systems.
Helv. Chim. Acta **1999**, *82,* 1211-1222. (Berlin, Germany)
IF 2.483
12. **Caron,G.**; Ermondi,G.; Boschi,D.; Carrupt,P.A.; Fruttero,R.; Testa,B.; Gasco,A.
Structure-Property Relationships in the Basicity and Lipophilicity of Arylalkylamine Oxides.
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13. **Caron,G.**; Reymond,F.; Carrupt,P.A.; Girault,H.H.; Testa,B.
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PSTT **1999**, *2,* 327-335.(Oxford, Oxon, England).
14. Testa,B.; **Caron,G.**; Crivori,P.; Rey,S.; Reist,M.; Carrupt,P.A.
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15. Ermondi,G.; **Caron,G.**; Bouchard,G.; Plemper van Balen,G.; Pagliara,A.; Grandi,T.; Carrupt,P.A.; Fruttero,R.; Testa,B.
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16. Bouchard,G.; Pagliara,A.; Plemper van Balen,G.; Carrupt,P.A.; Testa,B.; Gobry,V.; Girault,H.H.; **Caron,G.**; Ermondi,G.; Fruttero,R.
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Helv. Chim. Acta **2001**, *84,* 375-387. (Berlin, Germany)
IF 2.027
17. Plemper van Balen,G.; **Caron,G.**; Ermondi,G.; Pagliara,A.; Grandi,T.; Bouchard,G.; Fruttero,R.; Carrupt,P.A.; Testa,B.
Lipophilicity behaviour of the zwitterionic antihistamine cetirizine in phosphatidylcholine liposomes/water systems.
Pharm. Res. **2001**, *18,* 694-701. (New York, NY, USA)
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18. Rey,S.; **Caron,G.**; Ermondi,G.; Gaillard,P.; Pagliara,A.; Carrupt,P.A.; Testa,B.
Development of Molecular Hydrogen-Bonding Potentials (MHBPs) and their Application to Structure-Permeation Relations.
J.Mol.Graphics and Model, **2001**, *19,* 521-535. (New York, NY, USA).
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19. Boschi,D.; **Caron,G**.; Visentin,S.; Di Stilo,A.; Rolando,B.; Fruttero,R.; Gasco,A.
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Pharm. Res. **2001**, *18,* 987-991. (New York, NY, USA)
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20. Taillardat-Bertschinger,A.; a Marca Martinet,C.; Carrupt,P.A.; Reist,M.; **Caron,G**.; Fruttero,R.; Testa,B.
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Pharm. Res. **2002**, *19,* 729-737. (New York, NY, USA)
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21. Rolando,B.; Cena, C., **Caron,G**.; Marini,E.; Grosa,G.; Fruttero,R.; Gasco,A.
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22. **Caron,G.**; Ermondi,G.
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23. Plempler van Balen,G.; a Marca Martinet,C.; **Caron,G**.; Bouchard,G.; Reist,M.; Carrupt,P.A.; Fruttero,R.; Gasco,A.; Testa,B.
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24. Ermondi,G.; Lorenti,M.; **Caron,G**.
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J. Med. Chem **2004**, *47,* 3949-3961 (Washington, DC, USA)
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25. Ermondi,G.; **Caron,G**.; Lawrence, R. Longo,D.

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J. Comput. -Aided Mol. Design **2004**, *18,* 683-696. (Dordrecht, Netherlands)
IF 2.729
26. **Caron,G**.; Ermondi,G.; Damiano,A.; Novaroli,L.; Tsinman,O.; Ruell,J.A.; Avdeef,A.
Ionization, Lipophilicity, and Molecular Modeling to investigate Permeability and other Biological Properties of Amlodipine.
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27. **Caron,G.**; Ermondi,G.
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IF 4.926
28. Ermondi, G.; **Caron, G.**
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Biochem. Pharmacol. **2006**, *72*, 1633-1645. (Kidlington, Oxford, England)
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29. Ermondi,G.; Anghilante,C.; **Caron,G.**
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30. Ermondi, G.; Cillis, G.I.; **Caron, G.**
In silico strategies to describe the formation of inclusion complex between β-cyclodextrin and β-naphtyloxyacetic acid: a preliminary step towards prediction of log K.
J.Incl. Phenom. Macrocycl. Chem. **2007**, 57, 355-361. (Dordrecht, Netherlands)
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31. **Caron,G.**; Ermondi,G.
Classification of ·α–cyclodextrins inclusion complexes into Type 1 and Type 2: A prelude to log K prediction .

J.Mol.Graphics and Model, **2007**, 25, 731-739. (New York, NY, USA)
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32. **Caron, G**.; Ermondi, G.
Influence of Conformation on GRIND-Based Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR).
J. Med. Chem. **2007**, 50, 5039-5042. (Washington, DC, USA)
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33. **Caron,G**.; Ermondi,G.; Testa,B.
Predicting the oxidative metabolism of statins: An application of the MetaSite® algorithm.
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34. Ermondi, G.; **Caron, G.**
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35. Sapino,S.; Trotta,M.; Ermondi,G.; **Caron,G.**; Cavalli,R.; Carlotti,M.E.
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36. Sapino, S., Carlotti, M.E., **Caron, G.**, Ugazio, E., Cavalli, R.
In silico design, photostability and biological properties of the complex resveratrol/hydroxypropyl-β-cyclodextrin
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37. **Caron, G**., Nurisso, A., Ermondi, G.
How to Extend the Use of Grid-Based Interaction Energy Maps from Chemistry to Biotopics
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38. Ermondi, G.; Visentin, S., **Caron, G.**
GRIND-based 3D-QSAR and CoMFA to investigate topics dominated by hydrophobic interactions: The case of hERG K+ channel blockers.
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Capitoli di libri

1. **Caron,G.**; Rey,S.; Ermondi,G.; Crivori,P.; Gaillard,P.; Carrupt,P.A.; Testa,B.
Molecular Hydrogen-Bonding Potentials (MHBPs) in Structure-Permeation Relations.
In B. Testa, H.van de Waterbeemd, G. Folkers, and R. H. Guy (eds.), Pharmacokinetic Optimization in Drug Research: Biological, Physicochemical and Computational Chemistry, Wiley-VHCA, Zürich ***2001****; 525-538.*
2. **Caron,G.**; Ermondi,G.
New insights into the lipophilicity of ionized species.
In Testa,B., Kraemer,S., Wunderli-Allenspach,H., Folkers,G. (eds.), Pharmacokinetic Profiling in Drug Research: Biological, Physicochemical and Computational Strategies, Wiley-VHCA: Zürich, ***2005****, 165-185.*
3. **Caron,G**.; Ermondi,G. and Scherrer,R.A.
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In B. Testa and H. van de Waterbeemd (eds.), Comprehensive Medicinal Chemistry, 2nd Edition, Volume 5, Elsevier, Oxford, UK, ***2006****, 425-452*
4. **Caron, G.**; Ermondi, G.
Lipophilicity:chemical nature and biological relevance.
In Mannhold, R., Kubinyi,H., Folkers, G., (eds.); Molecular Drug Properties, Wiley VCH, Weinheim, ***2007****; 315-329.*

Comunicazioni a congressi

Comunicazioni orali

1. Drug-Membrane interactions as described by partitioning in liposome/water system
Chimia, 51 (1997), 597 (Bern (CH), Assemblée d'automne de la NSSC 1997)
2. pH-Metric method as a powerful tool to investigate physicochemical determinants of drugs

European Journal of Pharmaceutical Sciences, 6 (1998), S17 (Milano, IV European Congress of Pharmaceutical Sciences, 1998).

3. Lipophilicity of neutral and ionised species: the *diff*(log P^{N-I}) parameter
   Third European Symposium on Ionisation, Partitioning and Lipophilicity, Paris (F) 1998.
4. Hydrogen Bonding Potentials in Structure-Permeation Relations (invited)
   Lipophilicity in Drug Disposition, Lausanne (CH), March 5-9, 2000.
5. Methods for calculating hydrogen bonding descriptors (invited)
   Sirius 2002 User Meeting: Measurement and beyond, Brighton (UK) 2002.
6. Lipophilicity of ions and zwitterions (invited)
   LogP2004 Symposium, Zurigo (CH), February 29-March 4 2004.
7. Computational chemistry for experimental scientists (invited)
   Molecules, Membranes and Measurements, Barcelona (Spain) April 14-15 2005
8. The use of Web resources to share information about cyclodextrins
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Posters

1. Physicochemical and structural properties of the anti-inflammatory drug azapropazone.
   Caron Giulia; Zhu Fenggang; Carrupt Pierre-Alain; Tsai Ruey-Shiuan; Testa Bernard.
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2. Study of the interaction between amphiphilic alkylbenzylamines and phospholipids.
   R. Fruttero, **G.Caron**, G. Ermondi, E. Fornatto
   Symposium on Lipophilicity in Drug Research and Toxicology, Lausanne, 1995. Abstract book pag. P26.
3. CoMFA models for drug binding to the main variants of α_1-acid glycoprotein.
   Giulia Caron, Noorsaadah Abd. Rahman, Pierre-Alain Carrupt, Patrick Gaillard, Bernard Testa, Anna Tsantili-Kakoulidou, Françoise Hervé and Jean-Paul Tillement.
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4. Significance of lipophilicity profiles for ionisable compounds.

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11th European Symposium on Quantitative Structure-Activity Relationships: Computer-Assisted Lead Finding and Optimization, Lausanne, 1996. Abstract book pag. P3C.

5. Physicochemical properties of drugs containing the sulfoxide moiety and their sulfone and sulfide metabolites.
   G. Caron, P. Gaillard, P.-A. Carrupt and B. Testa.
   11th European Symposium on Quantitative Structure-Activity Relationships: Computer-Assisted Lead Finding and Optimization, Lausanne, 1996. Abstract book pag. P4C.
6. Intramolecular interactions affecting lipophilicity of zwitterionic molecules.
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   14th international Symposium on Medicinal Chemistry, Maastricht, 1996. Abstract book pag. OC8.
8. Lipophilicity profiles of ampholites.
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9. Mechanism governing the partitioning of neutral and cationic forms of (p-methylbenzyl)alkylamines in biomimetic media as revealed by lipophilicity and NMR studies.
   R. Fruttero, E Fornatto, D Boschi, G. Ermondi, A. Gasco, **G. Caron**, P.-A. Carrupt and B. Testa
   1th Italian Swiss-meeting on Medicinal Chemistry, Torino, 1997. Abstract book pag. B87.

10. Evaluations virologiques et physico-chimiques de derives a motif ferulique
    L. Vergnes, S. Barthelemy, **G. Caron**, D. Guyot, P.-A. Carrupt, E. Bahraoui, B. Testa and S. Labidalle.
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11. 3D Computational indices for the prediction of passive drug absorption in humans
    G. Caron, G. Ermondi, P. Gaillard, A. Pagliara, P.-A. Carrupt and B. Testa
    The Second Electronic Molecular Graphics and Modelling Conference (MGM EC-2) 1997.
12. Lipophilicity studies on SNAP and related compounds
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    Biological Chemistry and Cellular Targets of Nitric Oxide, Graz 1998. Abstract book pag. 54.
13. pH-Metric method as a powerful tool to investigate drug molecular physicochemical descriptors
    G.Caron, R.Fruttero, A.Pagliara, P.-A.Carrupt, A.Gasco and B.Testa
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14. Lipophilicity of the antihistamine cetirizine in phosphatidylcholine liposomes/water systems
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    Lipophilicity in Drug Disposition, Lausanne 2000. Abstract book pag. P-A16.
15. Development and applications of Molecular Hydrogen Bonding Potentials (MHBP)
    S. Rey, M. Rabii, **G. Caron**, G. Ermondi, P. Gaillard, A. Pagliara, P.-A. Carrupt and B. Testa.
    Lipophilicity in Drug Disposition, Lausanne 2000. Abstract book pag. P-B25.
16. Lipophilicity behavior of the zwitterionic antihistamine cetirizine in 1,2-dichloroethane/water system
    Bouchard B., Gobry V., **Caron G.**, Ermondi G., Fruttero R., Girault H.H., Carrupt P.-A., Testa, B.
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17. New NO-Donor analogues of Nicardipine and Amlodipine
    Boschi, D.; **Caron, G.**; Cena, C.; Visentin, S.; Di Stilo, A.; Fruttero, R.; Gasco, A.

XVIth International Symposium on Medicinal Chemistry, Bologna (I) 2000. Abstract book pag. 220.

18. Descrittori molecolari di lipofilia quale utile criterio per l'inserimento dei farmaci nel Prontuario Terapeutico Ospedaliero
    Bretto, C.; Rizza, V.; **Caron, G.**, Rolando, B., Fruttero, R.; Gasco, A.
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19. Synthesis of new gemcitabine prodrugs for liposomes and nanoparticle encapsulation
    Stella, B.; Rocco, F.; Immordino, M.L.; **Caron, G.**; Ceruti, M.; Tumiatti, K.; Cattel, L.
    4th World Meeting on Pharmaceutics Biopharmaceutics Pharmaceutical Technology, Florence 2002. Abstract book pag. 697
20. Galland,A.; Bouchard,G.; **Caron,G**.; Plemper van Balen,G.; a Marca Martinet,C.; Geinoz,S.; Rey,S.; Ermondi,G.; Vacondio,F.; Mor,M.; Plazzi,P.V.; Carrupt,P.A.; Testa,B.;
    The 1,2-dichloroethane/water vs the n-octanol/water system: more about intra- or intermolecular H-bond interactions
    *Chimia **2002**, 56, 373*
21. Novaroli,L.; Bouchard,G.; **Caron,G**.; Fruttero,R.; Carrupt,P.A.; Gasco,A.; Testa,B.;
    The lipophilicity behaviour of COMT inhibitors.
    *Chimia **2002**, 56, 344*
22. Cyanoacrylate nanospheres and nanocapsules containing lipophilic prodrugs of gemcitabine
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