

# CURRICULUM VITAE



## INFORMAZIONI PERSONALI

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Nazionalità	Italiana
Data di nascita	13/12/1954

## ESPERIENZA LAVORATIVA

Esperienze professionali (incarichi ricoperti e funzioni svolte)	2006-presente Preside della Facoltà di Scienze Matematiche, Fisiche e Naturali Università di Pavia
	2006-presente Componente del Senato Accademico Università di Pavia
	2004-presente Professore Ordinario di Chimica Organica Dipartimento di Chimica Organica (ora Dipartimento di Chimica) Università di Pavia
	2005-2006 Componente del Nucleo di Valutazione Università di Pavia
	2001-2004 Professore Straordinario di Chimica Organica Dipartimento di Chimica Organica Università di Pavia
	1987-2001 Professore Associato di Chimica Organica Dipartimento di Chimica Organica Università di Pavia
	1981-1987 Ricercatore confermato di Chimica Organica Dipartimento di Chimica Organica e Industriale Università di Milano
	1979-1981 Assegnista Dipartimento di Chimica Organica e Industriale

**ISTRUZIONE E FORMAZIONE**

Titolo di studio      Laurea in Chimica  
conseguita il 20/7/1978  
presso l'Università di Pavia

**CAPACITÀ LINGUISTICHE.**

PRIMA LINGUA	Italiano
ALTRE LINGUE	
• Capacità di lettura	Inglese
• Capacità di scrittura	Ottimo
• Capacità di espressione orale	Ottimo
• Capacità di espressione orale	Buono

**CAPACITÀ E COMPETENZE  
NELL'USO DI TECNOLOGIE**  
*Con computer, attrezzature specifiche,  
macchinari, ecc.*

Uso corrente dei principali pacchetti di applicativi Office.

**ALTRO / CAPACITÀ E  
COMPETENZE**  
*Competenze non precedentemente  
indicate.*

Le competenze scientifiche rientrano principalmente nel campo della chimica organica. I temi di fondo sono l'interesse per problematiche di tipo biorganico e l'utilizzo di metodi computazionali applicati alla modellistica molecolare. Nel corso della sua attività professionale Lucio Toma si è occupato, in particolare, di studi sintetici e biosintetici su sostanze organiche naturali e su molecole bio-attive sia con procedure chimiche sia enzimatiche e di studi conformazionali applicati alla correlazione struttura, proprietà molecolari e attività di molecole di interesse biologico, alla indagine strutturale di molecole organiche ed alla razionalizzazione del decorso di trasformazioni organiche. L'attività scientifica è documentata da oltre 150 pubblicazioni su riviste internazionali.

**PUBBLICAZIONI**

1. Gandolfi, R.; Toma, L.; De Micheli, C. "1,3-Dipolar cycloreversions of isoxazolidines and pyrazolidines" *Heterocycles*, 1979, 12, 5-10.
2. Gandolfi, R.; Ratti, M.; Toma, L.; De Micheli, C. "Syn selectivity in the reactions of azomethine imines and azomethine oxides with cis-3,4- disubstituted cyclobutenes" *Heterocycles*, 1979, 12, 897-902.
3. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L. "Role of 24- and 28-hydroxylated intermediates in the metabolism of  $\beta$ -sitosterol in the insect *Tenebrio molitor*" *Biochem J.*, 1979, 183, 495-499.
4. Gandolfi, R.; Toma, L. "Site specificity in cycloadditions of diphenylnitrile imine with 8-substituted-8-azahepta- fulvenes and tricarbonyl(8-azaheptafulvene)iron complexes" *Tetrahedron*, 1980, 36, 935-941.
5. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis of (24R,28S)- and (24S,28R)- 24,28-epoxy-5-stigmasten-3 $\beta$ -ol" *Gazz. Chim. Ital.*, 1980, 110, 151-153.
6. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L. "Conversion of isofucosterol-(24R,28S)- epoxide into cholesterol in the insect *Tenebrio molitor*" *J. Chem. Soc., Chem. Commun.*, 1980, 479-480.

7. Nicotra, F.; Ranzi, B. M.; Ronchetti, F.; Russo, G.; Toma, L. "Origin of the 28-pro-R and 28-pro-S hydrogens in the biosynthesis of poriferasterol in *Ochromonas malhamensis*" *J. Chem. Soc., Chem. Commun.*, 1980, 752-753.
8. Nicotra, F.; Toma, L. "A convenient procedure for the conversion of fucosterol into isofucosterol" *Gazz. Chim. Ital.*, 1980, 110, 579-580.
9. Nicotra, F.; Pizzi, P.; Ronchetti, F.; Russo, G.; Toma, L. "Substrate stereospecificity in the metabolism of fucosterol and isofucosterol 24,28- epoxides in *Tenebrio molitor*" *J. Chem. Soc., Perkin Trans. I*, 1981, 480-483.
10. Ranzi, B. M.; Ronchetti, F.; Russo, G.; Toma, L. "Stereochemistry of the introduction of the hydrogen atom at C-2 of cis-aconitic acid during its transformation into itaconic acid in *Aspergillus terreus*: a <sup>2</sup>H N.M.R. approach" *J. Chem. Soc., Chem. Commun.*, 1981, 1050-1051.
11. Ranzi, B. M.; Ronchetti, F.; Russo, G.; Toma, L. "2H NMR in stereochemical problems: stereochemistry of hydrogen introduction at C-3 during the transformation of cis-aconitic acid into itaconic acid" *Ital. J. Biochem.*, 1981, 30, 5.
12. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L. "Metabolism of C28 phytosterols in the insect *Tenebrio molitor*: migration of the C-25 hydrogen atm to C-24" *J. Chem. Soc., Chem. Commun.*, 1982, 922-923.
13. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L. "Migration of tritium to C-24 during the metabolism of 24-methylene[23,23,25-<sup>3</sup>H3]-cholesterol by the insect *Tenebrio molitor*" *J. Chem. Soc., Perkin Trans. I*, 1983, 787.
14. Nicotra, F.; Russo, G.; Ronchetti, F.; Toma, L. "Stereospecific synthesis of ethyl(2-acetamido-2-deoxy- $\alpha$ -D-glucopyranosyl)acetate" *Carbohydr. Res.*, 1983, 124, C5-C7.
15. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L.; Gariboldi, P.; Ranzi, B. M. "Stereochemistry of hydride migration from C-24 to C-25 in the biosynthesis of poriferasterol in *Ochromonas malhamensis*" *J. Chem. Soc., Chem. Commun.*, 1984, 383-384.
16. Nicotra, F.; Perego, R.; Ronchetti, F.; Russo, G.; Toma, L. "Stereochemistry of C-glycosidation through a Wittig-mercuriocyclization procedure" *Gazz. Chim. Ital.*, 1984, 114, 193-195.
17. Nicotra, F.; Perego, R.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis of the phosphono analogues of  $\alpha$ - and  $\beta$ -D-mannopyranosyl phosphate" *Carbohydr. Res.*, 1984, 131, 180-184.
18. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis of (24R)- and (24S)-24,28-epoxyergost-5-en-3 $\beta$ -ols. Substrate stereospecificity in their metabolism in the insect *Tenebrio molitor*" *J. Chem. Soc., Perkin Trans. I*, 1984, 2039-2042.
19. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L. "C-glycosides through the Wittig-cyclization procedure: observations on the influence of the nature of the substrate" *Tetrahedron Lett.*, 1984, 25, 5697-5700.
20. Nicotra, F.; Panza, L.; Ronchetti, F.; Russo, G.; Toma, L. "High stereoselective synthesis of diethyl (2,3-isopropylidene-5-trityl- $\alpha$ -D-ribofuranosyl)-methanephosphonate, a precursor to the phosphono analog of  $\alpha$ -D-ribose 1-phosphate" *Tetrahedron Lett.*, 1984, 25, 5937-5938.
21. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L. "Conversion of clionasterol into both fucosterol and isofucosterol by the insect *Tenebrio molitor*" *Experientia*, 1985, 41, 65-66.
22. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L.; Ranzi, B. M. "Application of biosynthetic <sup>13</sup>C enrichment using [1,2-<sup>13</sup>C2]acetate as precursor for <sup>13</sup>C NMR spectral assignment of the isopropyl methyls of (24 $\beta$ )-ethylsterols" *Magn. Res. Chem.*, 1985, 23, 134-136.
23. Nicotra, F.; Ronchetti, F.; Russo, G.; Toma, L.; Gariboldi, P.; Ranzi, B. M. "Mechanism of the transmethylation reaction by S-adenosylmethionine: stereochemistry of hydride migration from C-24 to C-25 in the biosynthesis of poriferasterol in the chrysophyte *Ochromonas malhamensis*" *J. Chem. Soc., Perkin Trans. I*, 1985, 521-524.
24. Nicotra, F.; Panza, L.; Ronchetti, F.; Russo, G.; Toma, L. "A novel approach to the synthesis of 1,2-cis-glycopyranosides" *Tetrahedron Lett.*, 1985, 26, 807-808.
25. Michelini, E.; Nicotra, F.; Panza, L.; Ronchetti, F.; Toma, L. "A new approach to the synthesis of  $\beta$ -glycosidically linked oligosaccharides containing 2-acetamido-2-deoxy-D-mannose residues" *Carbohydr. Res.*, 1985, 139, C1-C3.
26. Nicotra, F.; Panza, L.; Ronchetti, F.; Toma, L. "Stereoselective hydroboration of the 22(23)-double bond of stigmasterol-like side chain: an easy approach to 22 and 23-hydroxylated 24-ethylsterols" *Gazz. Chim. Ital.*, 1985, 115, 649-651.
27. Nicotra, F.; Panza, L.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis of enantiomerically pure 24-alkylsterol side chains, in both enantiomeric forms, starting from (R)-(+)-limonene" *J. Org. Chem.*, 1986, 51, 1272-1276.

28. Ronchetti, F.; Toma, L. "Cis and trans  $\beta,\gamma$ -disubstituted  $\delta$ -valerolactones: conformational studies and configurational assignments by molecular mechanics" *Tetrahedron*, 1986, 42, 6535-6540.
29. Nicotra, F.; Panza, L.; Ronchetti, F.; Russo, G.; Toma, L. "Formation of glycosides by epoxidation-ring closure of open-chain hydroxyenol ethers obtained from sugars" *J. Chem. Soc., Perkin Trans. I*, 1987, 1319-1324.
30. Nicotra, F.; Panza, L.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis of C-glycosyl compounds by the Wittig iodocyclization procedure. Differences from mercuriocyclization" *Carbohydr. Res.*, 1987, 171, 49-57.
31. Panza, L.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis of the trisaccharide component of the repeating unit of the capsular polysaccharide of *Streptococcus pneumoniae* type 19F" *J. Chem. Soc., Perkin Trans. I*, 1987, 2745-2747.
32. De Amici, M.; De Micheli, C.; Pratesi, P.; Toma, L.; Grana, E.; Santagostino-Barbone, M. G. "Synthesis, biological activity and conformational analysis of some acyclic cholinergic ligands" *Farmaco, Ed. Sc.*, 1987, 42, 921-930.
33. Mella, M.; Panza, L.; Ronchetti, F.; Toma, L. "1,2-Dideoxy-3,4:5,7-bis-O-(1-methyl-ethylidene)-D-glucos- and D-galacto-hept-1-ytol: synthesis and conformational studies" *Tetrahedron*, 1988, 44, 1673-1678.
34. Panza, L.; Ronchetti, F.; Toma, L. "Streptococcus pneumoniae type 19A polysaccharide. Synthesis of the trisaccharide component of the repeating unit" *Carbohydr. Res.*, 1988, 180, 242-245.
35. Ronchetti, F.; Russo, G.; Toma, L. "Biosynthesis of the C<sub>29</sub>-phytosterol side-chain: evidence that the same stereochemistry at C-25 can originate from different mechanisms" *J. Chem. Soc., Chem. Commun.*, 1988, 1375-1376.
36. Boschetti, A.; Panza, L.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis of ketofuranosides by epoxidation-ring closure of enol ethers" *J. Chem. Soc., Perkin Trans. I*, 1988, 3353-3357.
37. De Amici, M.; De Micheli, C.; Ortisi, A.; Gatti, G.; Gandolfi, R.; Toma, L. "Face selectivity of the nitrile oxides cycloaddition to unsaturated sugars" *J. Org. Chem.*, 1989, 54, 793-798.
38. Banfi, A.; Benedini, F.; Casanova, G.; Perego, R.; Toma, L. "Synthesis of rigid analogues of (D,L-arginine methyl ester with antiarrhythmic activity" *Synthetic Commun.*, 1989, 19, 1787-1799.
39. Ciuffreda, P.; Ronchetti, F.; Toma, L. "An efficient synthesis of the  $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 2)- $\alpha$ -L-rhamnopyranosidic unit" *J. Carbohydr. Chem.*, 1989, 8, 805-811.
40. Colombo, D.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis of 24-methyl sterols stereospecifically labelled with 2H in the isopropyl methyl groups. <sup>13</sup>C NMR spectral assignment of C-26 and C-27 resonances" *J. Chem. Soc., Chem. Commun.*, 1990, 263-264.
41. Palmisano, G.; Gabetta, B.; Lesma, G.; Pilati, T.; Toma, L. "Hexacyclic indole alkaloids. The structure of cuanzine as an experimental test of molecular mechanics calculations" *J. Org. Chem.*, 1990, 55, 2182-2185.
42. Desimoni, G.; Faita, G.; Gamba, A.; Righetti, P. P.; Tacconi, G.; Toma, L. "Substituents effect on the Claisen rearrangement" *Tetrahedron*, 1990, 46, 2165-2178.
43. Ciuffreda, P.; Ronchetti, F.; Toma, L. "Acylation of 6-deoxy-L-hexoses: regioselectivity in the enzymatic transesterification as compared to chemical esterification" *J. Carbohydr. Chem.*, 1990, 9, 125-129.
44. Toma, L.; Cignarella, G.; Barlocco, D.; Ronchetti, F. "Conformationally constrained congeners of 6-aryl-5-methyl-4,5-dihydro-3(2H)-pyridazinones active on the cardiovascular system: conformational studies by molecular mechanics calculations and <sup>1</sup>H NMR spectroscopy" *J. Med. Chem.*, 1990, 33, 1591-1594.
45. Burdisso, M.; Gamba, A.; Gandolfi, R.; Toma, L.; Rastelli, A.; Schiatti, E. "Syn-anti isomerism in the 1,3-dipolar cycloaddition to cis 3,4-disubstituted cyclobutenes. 5. Diastereoselectivity in the reaction with diazoalkanes" *J. Org. Chem.*, 1990, 55, 3311-3321.
46. Ciuffreda, P.; Colombo, D.; Ronchetti, F.; Toma, L. "Regioselective acylation of 6-deoxy-L- and -D-hexosides through lipase-catalyzed transesterification. Enhanced reactivity of the 4-OH function in the L series" *J. Org. Chem.*, 1990, 55, 4187-4190.
47. Desimoni, G.; Faita, G.; Righetti, P. P.; Toma, L. "Solvent effect as the result of frontier molecular orbital interaction. V. Diels-Alder with heterodienophiles: a unified approach to the solvent effect of the Diels-Alder reactions" *Tetrahedron*, 1990, 46, 7951-7970.
48. Colombo, D.; Ronchetti, F.; Toma, L. "Enzymic acylation of sugars. Rationale of the regioselective butyrylation of secondary hydroxy groups of D- and L-galacto and mannopyranosides" *Tetrahedron*, 1991, 47, 103-110.
49. Colombo, D.; Ronchetti, F.; Russo, G.; Toma, L. "Biosynthesis of poriferasterol in *Ochromonas malhamensis*: <sup>13</sup>C NMR assignment of the isopropyl methyl groups of 2-

- methylpentan-3-ol" *J. Chem. Soc., Perkin Trans. I*, 1991, 962-964.
50. Palmisano, G.; Danieli, B.; Lesma, G.; Passarella, D.; Toma, L. "Hexacyclic indole alkaloids. A highly convergent total synthesis of cuanzine" *J. Org. Chem.*, 1991, 56, 2380-2386.
  51. D'Alessandro, N.; Mella, M.; Fasani, E.; Toma, L.; Albini, A. "The photochemical reaction between 1,4-dicyanonaphthalene and benzyl ethers" *Tetrahedron*, 1991, 47, 5043-5050.
  52. Burdisso, M.; Gandolfi, R.; Toma, L.; Oberti, R. "Hexafluoroisopropanol as a suitable solvent for rearrangements via zwitterionic intermediates" *Tetrahedron*, 1991, 47, 6725-6736.
  53. De Bernardi, M.; Garlaschelli, L.; Toma, L.; Vidari, G.; Vita-Finzi, P. "Fungal metabolites XXVI: the structure of saponeaceolides B, C and D, new C-30 terpenoids from *Tricholoma saponaceum*" *Tetrahedron*, 1991, 47, 7109-7116.
  54. Carroll, P. J.; De Amici, M.; De Micheli, C.; Toma, L. "Conformational studies of muscarone analogs: X-ray analysis and molecular mechanics calculations" *J. Med. Chem.*, 1992, 35, 305-309.
  55. Colombo, D.; Ronchetti, F.; Scala, A.; Toma, L. "Enzymic acylation of methyl D- and L-glucopyranosides and 6-deoxy-glucopyranosides" *J. Carbohydr. Chem.*, 1992, 11, 89-94.
  56. Toma, L.; Cignarella, G.; Barlocco, D.; Ronchetti, F. "Molecular mechanics and <sup>1</sup>H NMR conformational study of 3,8-diazabicyclo[3.2.1]octanes and related cis-2,6-dimethylpiperazines active on opioid receptors" *Tetrahedron*, 1992, 48, 159-166.
  57. Palmisano, G.; Danieli, B.; Lesma, G.; Santagostino, M.; Fiori, G.; Toma, L. "Aspidosperma alkaloids. A new didehydrodimerization mode of  $\beta$ -anilinoacrylic alkaloids by anodic oxidation" *Helv. Chim. Acta*, 1992, 75, 813-824.
  58. Ciuffreda, P.; Colombo, D.; Ronchetti, F.; Toma, L. "Conformational analysis of the trisaccharide components of the repeating units of the capsular polysaccharides of *Streptococcus pneumoniae* types 19F and 19A" *Carbohydr. Res.*, 1992, 232, 327-339.
  59. De Bernardi, M.; Garlaschelli, L.; Toma, L.; Vidari, G.; Vita-Finzi, P. "The chemical basis of hot-tasting and yellowing of the mushrooms *Lactarius chrysorrheus* and *L. scrobiculatus*" *Tetrahedron*, 1993, 49, 1489-1504.
  60. Colombo, D.; Ronchetti, F.; Scala, A.; Taino, I. M.; Toma, L. "Enzymic acylation of methyl D- and L-glucopyranosides: influence of the 3-hydroxyl group" *Bioorg. Med. Chem.*, 1993, 1, 375-380.
  61. Garlaschelli, L.; Toma, L.; Vidari, G.; Colombo, D. "Conformational studies and stereochemical assignments of the lactarane sesquiterpenes Furoscrobiculin D and Blennin D" *Tetrahedron*, 1994, 50, 1211-1216.
  62. Toma, L.; Ciuffreda, P.; Colombo, D.; Ronchetti, F.; Lay, L.; Panza, L. "Oligosaccharides related to tumor-associate antigens. Conformational analysis of the trisaccharide  $\alpha$ -L-Fucp-(1 $\rightarrow$ 2)- $\beta$ -D-Galp-(1 $\rightarrow$ 3)- $\beta$ -D-GalpNAc, epitope structure recognized by the MBr1 antibody" *Helv. Chim. Acta*, 1994, 77, 668-678.
  63. Colombo, D.; Ronchetti, F.; Scala, A.; Taino, I. M.; Marinone Albini, F.; Toma, L. "Regio- and diastereoselective lipase-catalyzed preparation of acetylated 2-O-glucosylglycerols" *Tetrahedron: Asymmetry*, 1994, 5, 1377-1384.
  64. Mei, G.; Pugliese, L.; Rosato, N.; Toma, L.; Bolognesi, M.; Finazzi-Agrò, A. "Biotin and biotin analogues specifically modify the fluorescence decay of avidin" *J. Mol. Biol.*, 1994, 242, 559-565.
  65. Appendino, G.; Cravotto, G.; Toma, L.; Annunziata, R.; Palmisano, G. "Diels-Alder trapping of 3-methylene-2,4-chromandione. A new entry to substituted pyrano[3,2-c]coumarins" *J. Org. Chem.*, 1994, 59, 5556-5564.
  66. Colombo, D.; Marinone Albini, F.; Scala, A.; Taino, I. M.; Toma, L. "<sup>1</sup>H NMR acetyl methyl resonances of peracetylated Lilioside B: a tool for the stereochemical identification of its partially acetylated derivatives" *Tetrahedron: Asymmetry*, 1994, 5, 1993-1998.
  67. Toma, L.; Colombo, D.; Ronchetti, F.; Panza, L.; Russo, G. "Oligosaccharides related to tumor-associate antigens. Modeling of the terminal tetrasaccharide of an antigen recognized by the MBr1 antibody and overlapping di- and trisaccharide sequences" *Helv. Chim. Acta*, 1995, 78, 636-646.
  68. Colombo, D.; Ronchetti, F.; Scala, A.; Taino, I. M.; Marinone Albini, F.; Toma, L. "Optically pure 1-O- and 3-O- $\beta$ -D-glucosyl- and galactosyl-sn-glycerols through lipase-catalyzed transformations" *Tetrahedron Lett.*, 1995, 36, 4865-4868.
  69. Barlocco, D.; Villa, S.; Fratta, W.; Fadda, P.; Colombo, D.; Toma, L. "Monocyclic analogues of the  $\mu$ -opioid agonist 3,8-diazabicyclo[3.2.1]octanes: synthesis, modeling, and activity" *Tetrahedron*, 1995, 51, 11547-11556.
  70. Toma, L.; Toma, S. "Contact interaction method: a new algorithm for protein folding simulations" *Protein Sci.*, 1996, 5, 147-153.

71. Colombo, D.; Ronchetti, F.; Scala, A.; Taino, I. M.; Toma, L. "A facile lipase catalyzed access to fatty acid monoesters of 2-O- $\beta$ -D-glucosylglycerol" *Tetrahedron: Asymmetry*, 1996, 7, 771-777.
72. Colombo, D.; Scala, A.; Taino, I. M.; Toma, L.; Ronchetti, F.; Tokuda, H.; Nishino, H.; Nagatsu, A.; Sakakibara, J. "1-O, 2-O, and 3-O- $\beta$ -D-glycosyl-sn-glycerols: structure - anti-tumor-promoting activity relationship" *Bioorg. Med. Chem. Lett.*, 1996, 6, 1187-1190.
73. Ballabio, M.; Barlocco, D.; Cignarella, G.; Colombo, D.; Toma, L. "2,2,6- and 2,3,5-trimethylpiperazines as monocyclic analogues of the  $\mu$ -opioid agonist 3,8-diazabicyclo[3.2.1]octanes: synthesis, modeling, and activity" *Tetrahedron*, 1997, 53, 1481-1490.
74. Colombo, D.; Scala, A.; Taino, I. M.; Toma, L.; Ronchetti, F.; Tokuda, H.; Nishino, H.; Nagatsu, A.; Sakakibara, J. "Inhibitory effects of fatty acid monoesters of 2-O- $\beta$ -D-glucosylglycerol on Epstein-Barr virus activation" *Cancer Lett.*, 1998, 123, 83-86.
75. Barlocco, D.; Cignarella, G.; Tondi, D.; Vianello, P.; Villa, S.; Bartolini, A.; Ghelardini, C.; Galeotti, N.; Anderson, D. J.; Kuntzweiler, T. A.; Colombo, D.; Toma, L. "Mono- and disubstituted-3,8-diazabicyclo[3.2.1]octane derivatives as analgesics structurally related to epibatidine: synthesis, activity, and modeling" *J. Med. Chem.*, 1998, 41, 674-681.
76. Toma, L.; Toma, S.; Subirana, J. A. "Simulation of polymer crystallization through a dynamic Monte Carlo lattice model" *Macromolecules*, 1998, 31, 2328-2334.
77. Toma, L.; Subirana, J. A. "3D Simulations of polymer crystallization" *Polym. Mat. Sci. Eng.*, 1998, 79, 367-368.
78. Colombo, D.; Ronchetti, F.; Scala, A.; Toma, L. "Bioactive glycoglycerolipid analogues: An expeditious enzymatic approach to mono- and diesters of 2-O- $\beta$ -D-galactosylglycerol" *Tetrahedron: Asymmetry*, 1998, 9, 2113-2119.
79. Cignarella, G.; Barlocco, D.; Vianello, P.; Villa, S.; Pinna, G. A.; Fadda, P.; Fratta, W.; Toma, L.; Gessi, S. "Benzocondensed derivatives as rigid analogues of the  $\mu$ -opioid agonist 3(8)-cinnam-yl-8(3)-propionyl-3,8-diazabicyclo[3.2.1]octanes: synthesis, modeling, and affinity" *Farmaco*, 1998, 53, 667-674.
80. Toma, L.; Toma, S. "Folding simulation of protein models on the structure-based cubooctahedral lattice with the Contact Interactions algorithm" *Protein Sci.*, 1999, 8, 196-202.
81. Barlocco, D.; Cignarella, G.; Montesano, F.; Leonardi, A.; Mella, M.; Toma, L. "Novel adrenoceptor antagonists with a tricyclic pyrrolodipyridazine skeleton" *J. Med. Chem.*, 1999, 42, 173-177.
82. Canevari, S.; Colombo, D.; Compostella, F.; Panza L.; Ronchetti, F.; Russo, G.; Toma, L. "Synthesis, modeling and binding affinity of an ester analogue of the terminal trisaccharide of the tumor-associate antigen globo-H" *Tetrahedron*, 1999, 55, 1469-1478.
83. Colombo, D.; Compostella, F.; Ronchetti, Scala, A.; Toma, L.; Mukainaka, T.; Nagatsu, A.; Konoshima, T.; Tokuda, H.; Nishino, H. "Inhibitory effects of monoacylated 2-O- $\beta$ -galactosylglycerols on Epstein-Barr virus activation: the significant role of the hexanoyl chain" *Cancer Lett.*, 1999, 143, 1-4.
84. Clericuzio, M.; Toma, L.; Vidari, G. "Isolation of a new caryophyllane ester from *Lactarius subumbonatus*: Conformational analysis and absolute configuration" *Eur. J. Org. Chem.*, 1999, 2059-2065.
85. Colombo, D.; Compostella, F.; Ronchetti, F.; Scala, A.; Toma, L.; Tokuda, H.; Nishino, H. "Chemoenzymatic synthesis and antitumour promoting activity of 6'- and 3-esters of 2-O- $\beta$ -D-glucosylglycerol" *Bioorg. Med. Chem.*, 1999, 7, 1867-1871.
86. Conti, P.; De Amici, M.; De Sarro, G.; Rizzo, M.; Stensbøl, T. B.; Bräuner-Osborne, H.; Madsen, U.; Toma, L.; De Micheli, C. "Synthesis and enantioselectivity of new AMPA-kainate receptor agonists" *J. Med. Chem.*, 1999, 42, 4099-4107.
87. Villa, S.; Cignarella, G.; Curzu, M. M.; Pinna, G. A.; Pini, E.; Toma, L. "Behaviour of 5,6-dihydrothieno[2,3-h]cinnolin-3(2H)-one and 5,6-dihydrothieno[3,2-h]cinnolin-3(2H)-one towards hydrazine. Synthesis of thienocinnolinones and of 4-amino-thienocinnolinones" *J. Heterocyclic Chem.*, 1999, 36, 1253-1257.
88. Toma, L.; Subirana, J. A. "Simulation of melting transitions in crystalline polymers" Chapter 6 in "Scattering from polymers: characterization by X-rays, neutrons and light", Cebe, P.; Hsiao, B. S.; Loshe, D. J. Editors. 2000. ACS Book Symposium Series No. 739.
89. Consonni, R.; Zetta, L.; Longhi, R.; Toma, L.; Zanaboni, G.; Tenni, R. "Conformational analysis and stability of collagen peptides by CD and by  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR spectroscopies" *Biopolymers*, 2000, 53, 99-111.
90. Barlocco, D.; Cignarella, G.; Giardina, G. A. M.; Toma, L. "The opioid-receptor-like 1 (ORL-1) as a potential target for new analgesics" *Eur. J. Med. Chem.*, 2000, 35, 275-282.
91. Toma, L.; Toma, S. "A lattice study of multimolecular ensembles of protein models. Effect of

- sequence on the final state: globules, aggregates, dimers, fibrillae" *Biomacromolecules*, 2000, 1, 232-238.
92. Toma, L.; Quadrelli, P.; Perrini, G.; Gandolfi, R.; Di Valentin, C.; Corsaro, A.; Caramella, P. "Cycloaddition of nitrile oxides to  $\alpha,\beta$ -unsaturated aldehydes. Frontier orbital interactions and secondary orbital interactions at work in determining regiochemistry" *Tetrahedron*, 2000, 56, 4299-4309.
  93. Clericuzio, M.; Alagona, G.; Ghio, C.; Toma, L. "Ab initio and density functional evaluations of the molecular conformations of  $\beta$ -caryophyllene and 6-hydroxycaryophyllene" *J. Org. Chem.*, 2000, 65, 6910-6916.
  94. Pinna, G. A.; Murineddu, G.; Curzu, M. M.; Villa, S.; Vianello, P.; Borea, P. A.; Gessi, S.; Toma, L.; Colombo, D.; Cignarella, G. "Synthesis, modelling, and  $\mu$ -opioid receptor affinity of N-3(9)-arylpropenyl-N-9(3)-propionyl-3,9-diazabicyclo[3.3.1]nonanes" *Farmaco*, 2000, 55, 553-562.
  95. Toma, L.; Nava, D.; Celentano, G.; Giovannoni, M. P.; Dal Piaz, V.; Kwon, B. M.; Kim, M. K.; Kim, Y. K.; Barlocco, D. "5,6-Dinitrophenyl and 5-aminophenyl-6-nitrophenyl Analogues of the ACAT Inhibitor 5,6-diphenyl-3-alkylaminopyridazines" *Heterocycles*, 2000, 53, 2709-2718.
  96. Colombo, D.; Compostella, F.; Ronchetti, F.; Scala, A.; Toma, L.; Kuchide, M.; Tokuda, H.; Nishino, H. "Anti-tumor-promoting effects of glycoglycerolipid analogues on two-stage mouse skin carcinogenesis" *Cancer Lett.*, 2000, 161, 201-205.
  97. Colombo, D.; Compostella, F.; Ronchetti, F.; Scala, A.; Toma, L.; Tokuda, H.; Nishino H. "Glycoglycerolipid analogues active as anti-tumor-promoters: the influence of the anomeric configuration" *Eur. J. Med. Chem.*, 2000, 35, 1109-1113.
  98. Toma, L.; Quadrelli, P.; Caramella, P. "Classical and non-classical secondary orbital interactions and Coulombic attraction in the regiospecific dimerization of acrolein" *Tetrahedron Lett.*, 2001, 42, 731-733.
  99. Castronovo, F.; Clericuzio, M.; Toma, L.; Vidari, G. "Fungal Metabolites. Part 45: The Sesquiterpenes of *Collybia maculata* and *Collybia peronata*" *Tetrahedron*, 2001, 57, 2791-2798.
  100. Barlocco, D.; Toma, L.; Cignarella, G. "Non Peptidic Ligands at the Opioid Receptor Like-1 (ORL-1)" *Mini-Reviews Med. Chem.*, 2001, 1, 363-375.
  101. Toma, L.; Romano, S.; Quadrelli, P.; Caramella, P. "Merging of 4+2 and 2+4 cycloaddition paths in the regiospecific dimerization of methacrolein. A case of concerted cryptodiradical cycloaddition" *Tetrahedron Lett.*, 2001, 42, 5077-5080.
  102. Giovannoni, M. P.; Dal Piaz, V.; Kwon, B. M.; Kim, M. K.; Kim, Y. K.; Toma, L.; Barlocco, D.; Bernini, F.; Canavesi, M. "5,6-Diphenylpyridazine derivatives as acyl-CoA:cholesterol acyltransferase inhibitors" *J. Med. Chem.*, 2001, 44, 4292-4295.
  103. Compostella, F.; Colombo, D.; Modica, E.; Scala, A.; Toma, L.; Bovio, B.; Ronchetti, F. "Base promoted air oxidation of 13 $\beta$ -ethyl-11-methylenegon-4-en-17-one" *Steroids*, 2002, 67, 111-117.
  104. Clericuzio, M.; Mella, M.; Toma, L.; Vita Finzi, P.; Vidari, G. "Fungal metabolites. Part 46: Atlanticones, new protoilludane sesquiterpenes from the mushroom *Lactarius atlanticus* (Basidiomycetes)" *Eur. J. Org. Chem.*, 2002, 988-994.
  105. Caramella, P.; Toma, L.; Quadrelli, P. "An unexpected bispericyclic transition structure leading to 4+2 and 2+4 cycloadducts in the endo dimerization of cyclopentadiene" *J. Am. Chem. Soc.*, 2002, 124, 1130-1131.
  106. Toma, L.; Giovannoni, M. P.; Dal Piaz, V.; Kwon, B. M.; Kim, Y. K.; Gelain, A.; Barlocco, D. "Mono- and di-substituted 5,6-diphenyl-3-alkylaminopyridazines active as ACAT inhibitors" *Heterocycles*, 2002, 57, 39-46.
  107. Colombo, D.; Ronchetti, F.; Toma, L.; Pisano, B.; Ianaro, A. "Inhibition of activated murine T-lymphocytes by synthetic glycoglycerolipid analogues" *Farmaco*, 2002, 57, 337-339.
  108. Compostella, F.; Colombo, D.; Ferraboschi, P.; Scala, A.; Toma, L.; Ronchetti, F. "Synthesis of Isosteric Analogues of Acylglycosylglycerols Active as Chemoprevention Agents" *Eur. J. Org. Chem.*, 2002, 1429-1435.
  109. Colombo, D.; Compostella, F.; Ronchetti, F.; Reza-Elahi, S.; Scala, A.; Toma, L.; Aoi, W.; Kuchide, M.; Takayasu, J.; Tokuda, H.; Nishino, H. "Inhibitory effect of stabilized analogues of glycoglycerolipids on Epstein-Barr virus activation and mouse skin tumor promotion" *Cancer Lett.*, 2002, 186, 37-41.
  110. Colombo, D.; Ferraboschi, P.; Ronchetti, F.; Toma, L. "Stereoechemical analysis of the 3 $\alpha$ - and 3 $\beta$ -hydroxy metabolites of tibolone through NMR and quantum-chemical investigations. An experimental test of GIAO calculations" *Magn. Res. Chem.*, 2002, 40,

111. Toma, L.; Quadrelli, P.; Bunnelle, W. H.; Anderson, D. J.; Meyer, M. D.; Cignarella, G.; Gelain, A.; Barlocco, D. "6-Chloropyridazin-3-yl Derivatives Active as Nicotinic Agents: Synthesis, Binding, and Modeling Studies" *J. Med. Chem.*, 2002, 45, 4011-4017.
112. Micale, N.; Zappalà, M.; Grasso, S.; Puja, G.; De Sarro, G.; Ferreri, G.; De Sarro, A.; Toma, L.; De Micheli, C. "Novel Potent AMPA/Kainate Receptor Antagonists: Synthesis and Anticonvulsant Activity of a Series of 2-[(4-Alkylsemicarbazono)-(4-aminophenyl)-methyl]-4,5-methylenedioxyphenylacetic Acid Alkyl Esters" *J. Med. Chem.*, 2002, 45, 4433-4442.
113. Quadrelli, P.; Romano, S.; Toma, L.; Caramella, P. "Merging and bifurcation of 4+2 and 2+4 cycloaddition modes in the archetypal dimerization of butadiene. A case of competing bispericyclic, pericyclic and diradical paths" *Tetrahedron Lett.*, 2002, 43, 8785-8789.
114. Conti, P.; De Amici, M.; Bräuner-Osborne, H.; Madsen, U.; Toma, L.; De Micheli, C. "Synthesis and pharmacology of 3-hydroxy- $\Delta$ 2-isoxazoline-cyclopentane analogues of glutamic acid" *Farmaco*, 2002, 57, 889-895.
115. Toma, L.; Giovannoni, M. P.; Dal Piaz, V.; Kwon, B. M.; Kim, Y. K.; Gelain, A.; Barlocco, D. "Novel 3-arylamino- and 3-cycloalkylamino-5,6-diphenyl-pyridazines active as ACAT inhibitors" *Arch. Pharm. Pharm. Med. Chem.*, 2002, 335, 563-566.
116. Colombo, D.; Ronchetti, F.; Scala, A.; Toma, L.; Tokuda, H.; Nishino, H. "Synthesis and anti-tumor-promoting activity of glycoglycerolipid analogues lacking the glycerol backbone" *Bioorg. Med. Chem.*, 2003, 11, 909-912.
117. Conti, P.; De Amici, M.; Roda, G.; Vistoli, G.; Stensbol, T. B.; Bräuner-Osborne, H.; Madsen, U.; Toma, L.; De Micheli, C. "Design of novel conformationally restricted analogues of glutamic acid" *Tetrahedron*, 2003, 59, 1443-1452.
118. Quadrelli, P.; Romano, S.; Toma, L.; Caramella, P. "A bispericyclic transition structure allows for efficient relief of antiaromaticity enhancing reactivity and endo stereoselectivity in the dimerization of the fleeting cyclopentadiene" *J. Org. Chem.*, 2003, 68, 6035-6038.
119. Modica, E.; Bombieri, G.; Colombo, D.; Marchini, N.; Ronchetti, F.; Scala, A.; Toma, L. "Novel Estrones by Oxidation of the Benzylic Positions of the Estrane Skeleton with tert-Butyl Hydroperoxide and Cobalt Acetate" *Eur. J. Org. Chem.*, 2003, 2964-2971.
120. Conti, P.; De Amici, M.; Grazioso, G.; Roda, G.; Stensbøl, T. B.; Bräuner-Osborne, H.; Madsen, U.; Toma, L.; De Micheli, C. "Design of Cyclopentaisoxazoline Amino Acids as Conformationally Constrained Agonists at Glutamate Receptors" *Eur. J. Org. Chem.*, 2003, 4455-4461.
121. Compostella, F.; Marinone Albini, F.; Ronchetti, F.; Toma, L. "A theoretical study of the conformational behavior of analogues of  $\alpha$ -L-rhamnose-1-phosphate" *Carbohydr. Res.*, 2004, 339, 1323-1330.
122. Toma, L.; Barlocco, D.; Gelain A. "Neuronal nicotinic acetylcholine receptor agonists" *Expert Opin. Ther. Patents*, 2004, 14, 1029-1040.
123. Conti, P.; De Amici, M.; Grazioso, G.; Roda, G.; Barberis Negra, F. F.; Nielsen, B.; Stensbøl, T. B.; Madsen, U.; Bräuner-Osborne, H.; Frydenvang, K.; De Sarro, G.; Toma, L.; De Micheli, C. "Design, synthesis, and pharmacological characterization of novel, potent NMDA receptor antagonists" *J. Med. Chem.*, 2004, 47, 6740-6748.
124. Colombo, D.; Franchini, L.; Toma, L.; Ronchetti, F.; Nakabe, N.; Konoshima, T.; Nishino, H.; Tokuda, H. "Anti-tumor-promoting activity of simple models of galactoglycerolipids with branched and unsaturated acyl chains" *Eur. J. Med. Chem.*, 2005, 40, 69-74.
125. Caramella, P.; Quadrelli, P.; Toma, L.; Romano, S.; Khuong, K. S.; Northrop, B.; Houk, K. N. "Three corrugated surfaces of 1,4-divinyltetramethylene diradical intermediates and their connections to 1,2-divinylcyclobutane, 4-vinylcyclohexene, 1,5-cyclooctadiene, and two butadienes" *J. Org. Chem.*, 2005, 70, 2994-3008.
126. Modica, E.; Colombo, D.; Ronchetti, F.; Scala, A.; Bombieri, G.; Marchini, N.; Toma, L. "Crystal structures of 10 $\alpha$ -gon-5-enes from the synthetic pathway to desogestrel" *Steroids*, 2005, 70, 660-666.
127. Ronchi, S.; Compostella, F.; Lay, L.; Ronchetti, F.; Toma, L. " $(\alpha$ -L-Rhamnopyranosyl)-methylphosphonic acids: experimental evidence of the analogy with  $\alpha$ -L-rhamnopyranosyl phosphate" *Eur. J. Org. Chem.*, 2005, 4459-4463.
128. Murineddu, G.; Ruiu, S.; Loriga, G.; Manca, I.; Lazzari, P.; Reali, R.; Pani, L.; Toma, L.; Pinna, G. A. "Tricyclic Pyrazoles. 3. Synthesis, biological evaluation, and molecular modeling of analogues of the cannabinoid antagonist 8-chloro-1-(2',4'-dichlorophenyl)-N-piperidin-1-yl-1,4,5,6-tetrahydrobenzo[6,7]cyclohepta[1,2-c]pyrazole-3-carboxamide" *J. Med. Chem.*, 2005, 48, 7351-7362.

129. Gelain, A.; Bettinelli, I.; Barlocco, D.; Kwon, B.-M.; Jeong, T.-S.; Cho, K.-H.; Toma, L. "Mono- or diphenylpyridazines connected to N-(2,4-difluorophenyl)-N'-heptylurea as acyl-CoA:cholesterol acyltransferase inhibitors" *J. Med. Chem.*, 2005, 48, 7708-7713.
130. Colombo, D.; Ferraboschi, P.; Prestileo, P.; Toma, L. "A comparative molecular modeling study of dydrogesterone with other progestational agents through theoretical calculations and nuclear magnetic resonance spectroscopy" *J. Steroid. Biochem. Mol. Biol.*, 2006, 98, 56-62.
131. Loriga, G.; Manca, I.; Murineddu, G.; Chelucci, G.; Villa, S.; Gessi, S.; Toma, L.; Cignarella, G.; Pinna, G. A. "Synthesis of 3,6-diazabicyclo[3.1.1]heptanes as novel ligands for the opioid receptors" *Bioorg. Med. Chem.*, 2006, 14, 676-691.
132. Gelain, A.; Bettinelli, I.; Barlocco, D.; Kwon, B.-M.; Jeong, T.-S.; Im, K.-R.; Legnani, L.; Toma, L. "Ureidopyridazine derivatives as Acyl-CoA:cholesterol acyltransferase inhibitors" *Sci. Pharm.*, 2006, 74, 85-97.
133. Gelain, A.; Barlocco, D.; Kwon, B.-M.; Jeong, T.-S.; Im, K.-R.; Legnani, L.; Toma, L. "3-Heptylamino-5-phenylpyridazine derivatives as analogues of acyl-CoA: cholesterol acyltransferase inhibitors containing the N-heptyl-N'-arylureidic moiety" *Arch. Pharm.* 2006, 339, 645-651.
134. Colombo, D.; Franchini, L.; Toma, L.; Ronchetti, F.; Tanaka, R.; Takayasu, J.; Nishino, H.; Tokuda, H. "Cyclic and branched acyl chain galactoglycerolipids and their effect on anti-tumor-promoting activity" *Eur. J. Med. Chem.*, 2006, 41, 1456-1463.
135. Colombo, D.; Ferraboschi, P.; Legnani, L.; Prestileo, P.; Toma, L. "A full conformational characterization of 13-ethylprogestogens through theoretical calculations and nuclear magnetic resonance spectroscopy" *J. Steroid. Biochem. Mol. Biol.*, 2007, 103, 163-169.
136. Palmisano, G.; Toma, L.; Annunziata, R.; Tagliapietra, S.; Barge, A.; Cravotto, G. "Cyclization reactions of coumarin derivatives: chemo- and regioselectivity effects of oxygen/sulfur isosteric replacement" *J. Heterocyclic Chem.*, 2007, 44, 411-418.
137. Legnani, L.; Lunghi, C.; Marinone Albini, F.; Nativi, C.; Richichi, B.; Toma, L. "Alternative mechanistic paths in the hetero-Diels-Alder reaction of  $\alpha$ -oxothiones: a theoretical study" *Eur. J. Org. Chem.*, 2007, 3547-3554.
138. Bunnelle, W. H.; Daanen, J. F.; Ryther, K. B.; Schrimpf, M. R.; Dart, M. J.; Gelain, A.; Meyer, M. D.; Frost, J. M.; Anderson, D. J.; Buckley, M.; Curzon, P.; Cao, Y. J.; Puttfarcken, P.; Searle, X.; Ji, J.; Putman, C. B.; Surowy, C.; Toma, L.; Barlocco, D. "Structure-activity studies and analgesic efficacy of N-(3-pyridinyl)-bridged bicyclic diamines, exceptionally potent agonists at nicotinic acetylcholine receptors" *J. Med. Chem.*, 2007, 50, 3627-3644.
139. Toma, L.; Di Cola, E.; Ienco, A.; Legnani, L.; Lunghi, C.; Moneti, G.; Richichi, B.; Ristori, S.; Dell'Atti, D.; Nativi, C. "Synthesis, conformational studies, binding assessment and liposome insertion of a thioether-bridged mimetic of the antigen GM3-ganglioside lactone" *ChemBioChem*, 2007, 8, 1646-1649.
140. Estruch, I.; Tagliani, A. R.; Guisán, J. M.; Fernández-Lafuente, R.; Alcántara, A. R.; Toma, L.; Terreni, M. "Immobilization of the acylase from Escherichia coli on glyoxylagarose gives efficient catalyst for the synthesis of cephalosporins" *Enzyme Microb. Technol.*, 2008, 42, 121-129.
141. Gelain, A.; Barlocco, D.; Kwon, B.-M.; Jeong, T.-S.; Im, K.-R.; Legnani, L.; Toma, L. "Biphenyl versus phenylpyridazine derivatives: the role of the heterocycle in a series of acyl-CoA:cholesterol acyl transferase inhibitors" *J. Med. Chem.*, 2008, 51, 1474-1477.
142. Catelani, G.; D'Andrea, F.; Griselli, A.; Guazzelli, L.; Legnani, L.; Toma, L. "A new stereoselective approach to a selectively protected derivative of D-pinitol and its evaluation as  $\alpha$ -L-rhamnopyranose mimetic" *Tetrahedron Lett.* 2008, 49, 4534-4536.
143. Legnani, L.; Luparia, M.; Zanoni, G.; Toma, L.; Vidari, G. "A full conformational characterization of natural ionones and irones, as well as 13-alkyl-substituted  $\alpha$ -ionones" *Eur. J. Org. Chem.*, 2008, 4755-4762.
144. Murineddu, G.; Murruzzu, C.; Curzu, M. M.; Chelucci, G.; Gotti, C.; Gaimarri, A.; Legnani, L.; Toma, L.; Pinna, G. A. "Synthesis of 3,6-diazabicyclo[3.1.1]heptanes as novel ligands for neuronal nicotinic acetylcholine receptors" *Bioorg. Med. Chem. Lett.* 2008, 18, 6147-6150.
145. Altamura, M.; Dragoni, E.; Infantino, A. S.; Legnani, L.; Ludbrook, S. B.; Menchi, G.; Toma, L.; Nativi, C. "Cyclic glycopeptidomimetics through a versatile sugar-based scaffold" *Bioorg. Med. Chem. Lett.* 2009, 19, 3841-3844.
146. Colombo, D.; Villa, S.; Solano, L.; Legnani, L.; Marinone Albini, F.; Toma, L. "An exhaustive conformational evaluation of the HIV-1 inhibitor BMS-378806 through theoretical calculations and nuclear magnetic resonance spectroscopy" *Eur. J. Org. Chem.*

- Chem. 2009, 3178-3183.
- 147. Toma, L.; Legnani, L.; Rencurosi, A.; Poletti, L.; Lay, L.; Russo, G. "Modeling of synthetic phosphono and carba analogues of N-acetyl- $\alpha$ -D-mannosamine 1-phosphate, the repeating unit of the capsular polysaccharide from *Neisseria meningitidis* serovar A" Org. Biomol. Chem. 2009, 7, 3734-3740.
  - 148. Legnani, L.; Ronchi, S.; Fallarini, S.; Lombardi, G.; Campo, F.; Panza L.; Lay, L.; Poletti, L.; Toma, L.; Ronchetti, F.; Compostella, F. "Synthesis, molecular dynamics simulations, and biology of a carba-analogue of the trisaccharide repeating unit of *Streptococcus pneumoniae* 19F capsular polysaccharide" Org. Biomol. Chem. 2009, 7, 4428-4436.
  - 149. Luparia, M.; Legnani, L.; Porta, A.; Zanoni, G.; Toma, L.; Vidari, G. "Enantioselective synthesis and olfactory evaluation of bicyclic  $\alpha$ - and  $\gamma$ -ionone derivatives: The 3D Arrangement of key molecular features relevant to the violet odor of ionones" J. Org. Chem., 2009, 74, 7100-7110.
  - 150. Shin, D.-S.; Masciocchi, D.; Gelain, A.; Villa, S.; Barlocco, D.; Meneghetti, F.; Pedretti, A.; Han, Y.-M.; Han, D. C.; Kwon, B.-M.; Legnani, L.; Toma, L. "Synthesis, modeling, and crystallographic study of 3,4-disubstituted-1,2,5-oxadiazoles and evaluation of their ability to decrease STAT3 activity" Med. Chem. Commun., 2010, 1, 156-164.
  - 151. Arcangeli, A.; Toma, L.; Contiero, L.; Crociani, O.; Legnani, L.; Lunghi, C.; Nesti, E.; Moneti, G.; Richichi, B.; Nativi, C. "Stable GM3 lactone mimetic raises antibodies specific for the antigens expressed on melanoma cells" Bioconjugate Chem., 2010, 21, 1432-1438.
  - 152. Legnani, L.; Colombo, D.; Cocchi, E.; Solano, L.; Villa, S.; Lopalco, L.; Asti, V.; Diomedè, L.; Marinone Albini, F.; Toma, L. "Modeling and spectroscopic studies of synthetic diazabicyclo analogs of the HIV-1 inhibitor BMS-378806 and evaluation of their antiviral activity" Eur. J. Org. Chem., 2011, 287-294.
  - 153. Legnani, L.; Compostella, F.; Grazioso, G.; Marinone Albini, F.; Toma, L. "Molecular dynamics simulations of the *Salmonella typhi* Vi antigenic polysaccharide and effects of the introduction of a zwitterionic motif" Org. Biomol. Chem., 2011, 9, 5554-5559.
  - 154. Masciocchi, D.; Villa, S.; Meneghetti, F.; Pedretti, A; Barlocco, D.; Legnani, L.; Toma, L.; Kwon, B.-M.; Nakano, S.; Asai, A.; Gelain, A. "Biological and computational evaluation of an oxadiazole derivative (MD77) as a new lead for direct STAT3 inhibitors" Med. Chem. Commun., 2012, 3, in stampa.

<b>DIRETTORE DI DIPARTIMENTO</b>	<b>Indennità di Carica</b>	<b>Gettone di presenza per seduta</b>
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