CROATICA CT CHEMICA

Croat. Chem. Acta 2016, *89*(4)
Published online: December 12, 2016

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INTRODUCTION

FOREWORD

Bono Lučić, Hrvoj Vančik, Jerzy Ciosłowski

Croat. Chem. Acta **2016**, *89*(*4*), 373

AUTOBIOGRAPHICAL NOTES

Nenad Trinajstić

Croat. Chem. Acta **2016**, *89*(*4*), 375–389
DOI: 10.5562/cca3171

REMINISCENCES

How Information Theory Met Chemical Graph Theory in Ruđer Bošković Institute

Reminiscence for the years of collaboration with the jubilee

Danail Bonchev

Croat. Chem. Acta **2016**, *89*(*4*), 391–392
DOI: 10.5562/cca3035

Celebrating my Ph.D. Thesis Mentor Birthday

Predrag-Peter Ilich

Croat. Chem. Acta **2016**, *89*(*4*), 393–394
DOI: 10.5562/cca3089

Professor Nenad Trinajstić - a Strong Supporter of Young Researchers

Bono Lučić

Croat. Chem. Acta **2016**, *89*(*4*), 395–396
DOI: 10.5562/cca3167

SCIENTIFIC ARTICLES

ESSAY

Chemistry 4.0 Challenges and Solutions for the Digital Transformation

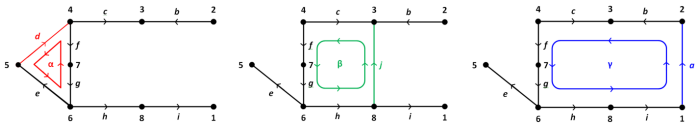
Jan von Knop

Croat. Chem. Acta **2016**, *89*(*4*), 397–402
DOI: 10.5562/cca3132

ORIGINAL SCIENTIFIC ARTICLE - REVIEW

What Kirchhoff Actually did Concerning Spanning Trees in Electrical Networks and its Relationship to Modern Graph-Theoretical Work

Edward C. Kirby, Roger B. Mallion,
Paul Pollak, Paweł J. Skrzyński

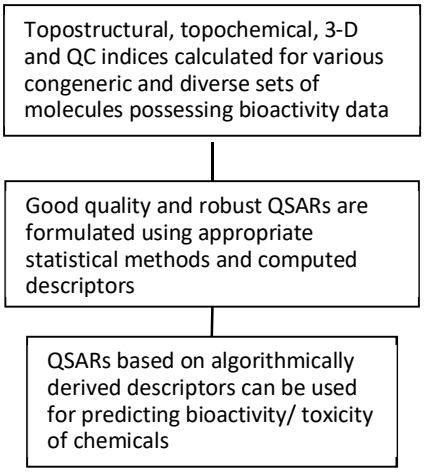


Croat. Chem. Acta **2016**, *89*(*4*), 403–417
DOI: 10.5562/cca2995

ORIGINAL SCIENTIFIC ARTICLE - AUTHOR'S REVIEW

Use of Graph Invariants in Quantitative Structure-Activity Relationship Studies

Subhash C. Basak

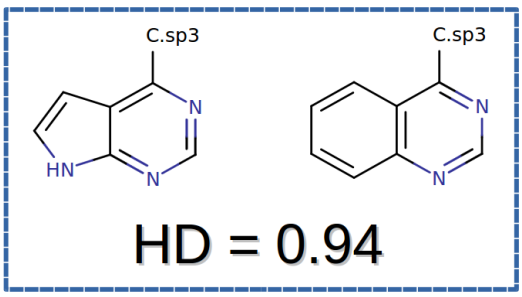


Croat. Chem. Acta **2016**, *89*(*4*), 419–429
DOI: 10.5562/cca3029

ORIGINAL SCIENTIFIC ARTICLE

Scaffold Hopping and Bioisosteric Replacements Based on Binding Site Alignments

Samo Lešnik, Janez Konc, Dušanka Janežič

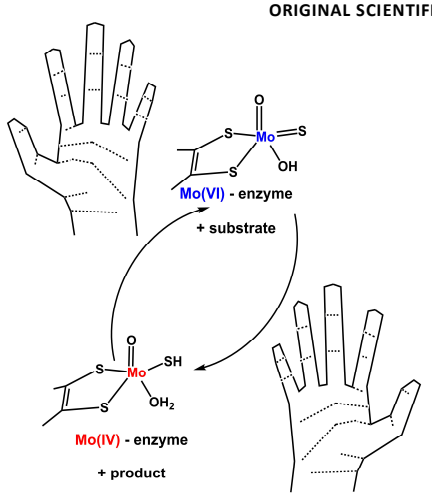


Croat. Chem. Acta **2016**, *89*(*4*), 431–437
DOI: 10.5562/cca2993

ORIGINAL SCIENTIFIC ARTICLE

Xanthine Dehydrogenase Active Site: Chiral Switching and Substrate Coordination

Predrag-Peter Ilich

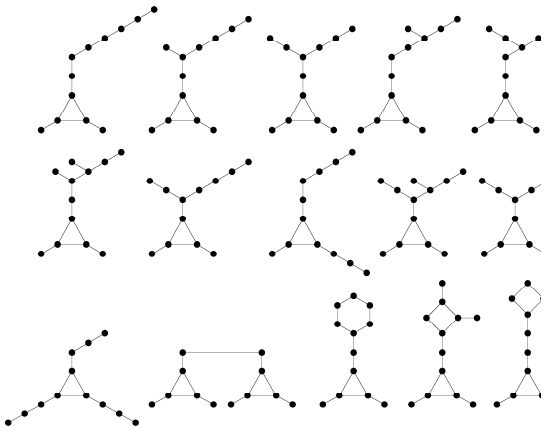


Croat. Chem. Acta **2016**, *89*(*4*), 439–447
DOI: 10.5562/cca3047

ORIGINAL SCIENTIFIC ARTICLE

Constructing NSSD Molecular Graphs

Ivan Gutman, Boris Furtula, Alexander Farrugia, Irene Sciriha

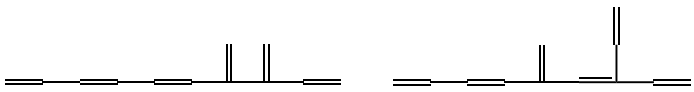


Croat. Chem. Acta **2016**, *89*(*4*), 449–454
DOI: 10.5562/cca2997

ORIGINAL SCIENTIFIC ARTICLE

Chemistry-Relevant Isospectral Graphs. Acyclic Conjugated Polyenes

Haruo Hosoya

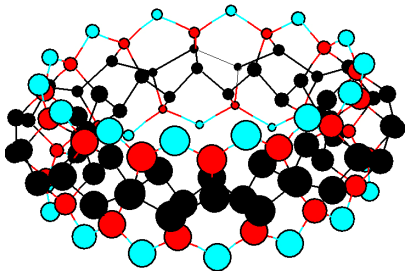


Croat. Chem. Acta **2016**, *89*(*4*), 455–461
DOI: 10.5562/cca3036

ORIGINAL SCIENTIFIC ARTICLE

Energies for Cyclic and Acyclic Aggregations of Adamantane Sharing Six-membered Rings

Alexandru T. Balaban, Yenni P. Ortiz, Douglas J. Klein, Debojit Bhattacharya



Croat. Chem. Acta **2016**, *89*(*4*), 463–470
DOI: 10.5562/cca3055

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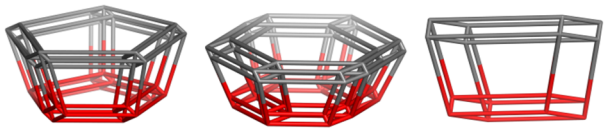
ORIGINAL SCIENTIFIC ARTICLE

Euler Characteristic of Polyhedral Graphs

Atena Pîrvan-Moldovan, Mircea V. Diudea

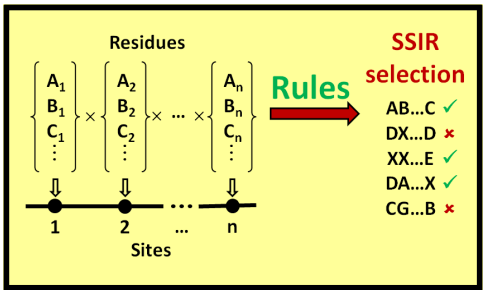


Croat. Chem. Acta **2016**, *89*(*4*), 471–479
DOI: 10.5562/cca3008

ORIGINAL SCIENTIFIC ARTICLE

Superposing Significant Interaction Rules (SSIR) Method: A simple Procedure for Rapid Ranking of Congeneric Compounds

Emili Besalú, Lionello Pogliani, Jesús Vicente de Julián-Ortiz

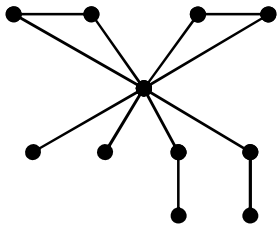


Croat. Chem. Acta **2016**, *89*(*4*), 481–492
DOI: 10.5562/cca3027

NOTE

On the Signless Laplacian Spectral Radius of Cacti

Mingzhu Chen, Bo Zhou



Croat. Chem. Acta **2016**, *89*(*4*), 493–498
DOI: 10.5562/cca3018

NOTE

Comparison Between Two Eccentricity-based Topological Indices of Graphs

Kexiang Xu, Xia Li,

$$E_1(T) > \xi^c(T)$$

$$E_1(G\square K_2) \geq \xi^c(G\square K_2) \quad (E_1(G\square K_2) < \xi^c(G\square K_2)$$

Croat. Chem. Acta **2016**, *89*(*4*), 499–504
DOI: 10.5562/cca3028

NOTE

Comparison Between Zagreb Eccentricity Indices and the Eccentric Connectivity Index, the Second Geometric-arithmetic Index and the Graovac-Ghorbani Index

Kinkar Ch. Das

$$E_1(G) = \sum_{v_i \in V(G)} \varepsilon_G^2(v_i)$$

$$E_2(G) = \sum_{v_i v_j \in E(G)} \varepsilon_G(v_i) \cdot \varepsilon_G(v_j)$$

$$\xi^C(G) = \sum_{v_i \in V(G)} d_G(v_i) \cdot \varepsilon_G(v_i) = \sum_{v_i v_j \in E(G)} (\varepsilon_G(v_i) + \varepsilon_G(v_j))$$

$$GA_2(G) = \sum_{v_i v_j \in E(G)} \frac{\sqrt{n_i \cdot n_j}}{\frac{1}{2}[n_i + n_j]}$$

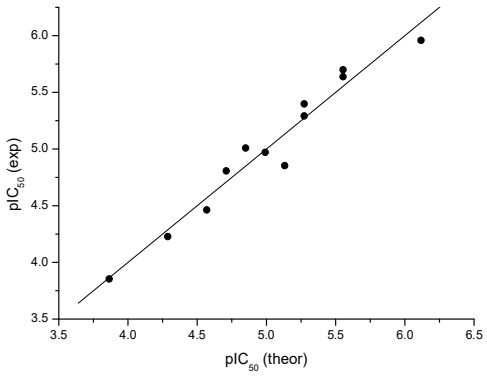
$$ABC_{GG}(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{n_i + n_j - 2}{n_i \cdot n_j}}$$

Croat. Chem. Acta **2016**, *89*(*4*), 505–510
DOI: 10.5562/cca3007

PRELIMINARY COMMUNICATION

Modelling of Protective Mechanism of Iron(II)-polyphenol Binding with OH-related Molecular Descriptors

Ante Miličević, Nenad Raos

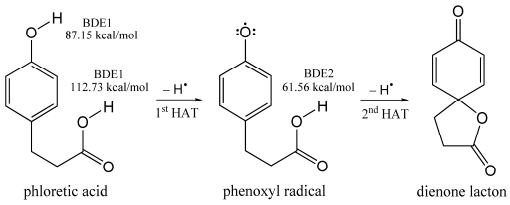


Croat. Chem. Acta **2016**, *89*(*4*), 511–515
DOI: 10.5562/cca2996

ORIGINAL SCIENTIFIC ARTICLE

Carboxyl Group as a Radical Scavenging Moiety: Thermodynamics of $2H^+/2e^-$ Processes of Phloretic Acid

Ana Amić, Bono Lučić, Zoran Marković, Dragan Amić



Croat. Chem. Acta **2016**, *89*(*4*), 517–525
DOI: 10.5562/cca3024

ORIGINAL SCIENTIFIC ARTICLE

The Difference Between the Accuracy of Real and the Corresponding Random Model is a Useful Parameter for Validation of Two-State Classification Model Quality

Jadranko Batista, Dražen Vikić-Topić, Bono Lučić

$$Q_2 = 100\frac{p+n}{p+n+u+o}\ (\%)$$

$$Q_{2,rnd} = 100\frac{(p+u)(p+o)+(n+o)(n+u)}{N^2}(\%)$$

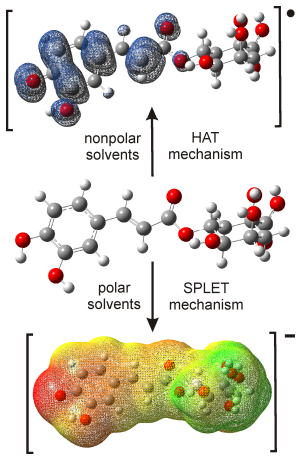
$$\Delta \boldsymbol{Q_2} = \boldsymbol{Q_2} - \boldsymbol{Q_{2,rnd}}\ (\%)$$

Croat. Chem. Acta **2016**, *89*(*4*), 527–534
DOI: 10.5562/cca3117

ORIGINAL SCIENTIFIC ARTICLE

Structural and Antioxidative Features of Chlorogenic Acid

Jelena Tošović, Svetlana Marković

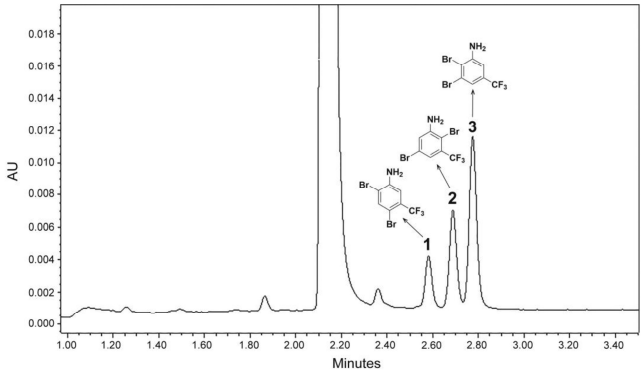


Croat. Chem. Acta **2016**, *89*(*4*), 535–541
DOI: 10.5562/cca3026

PRELIMINARY COMMUNICATION

Rapid Identification of Unknown Impurities in 3-Bromo-5-(trifluoromethyl)aniline by LC-SPE/NMR

Miroslava Harča, Iva Habinovec, Ernest Meštrović, Ivana Biljan, Predrag Novak

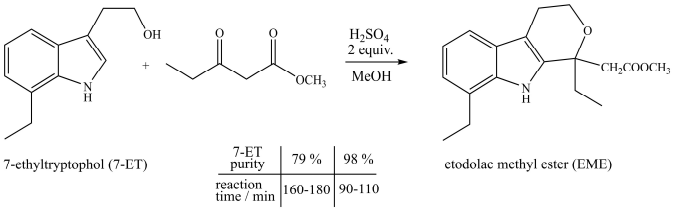


Croat. Chem. Acta **2016**, *89*(*4*), 543–547
DOI: 10.5562/cca3042

ORIGINAL SCIENTIFIC ARTICLE

HPLC Monitoring of Acid Catalyzed Conversion of 7-Ethyltryptophol to Methyl Ester of Etodolac

Iva Habinovec, Željka Car, Rosana Ribić, Nives Galić, Predrag Novak, Ernest Meštrović, Srđanka Tomić



Croat. Chem. Acta **2016**, *89*(*4*), 549–553
DOI: 10.5562/cca3016

BOOK REVIEWS

Ivan Gutman:
Selected Theorems in Chemical Graph Theory
Mathematical Chemistry Monographs, Vol. 18

Nenad Trinajstić

Croat. Chem. Acta **2016**, *89*(*4*), 555–557
DOI: 10.5562/cca3148