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References (85)

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1

Micellization of dodecyldimethyl-N-2-phenoxyethylammonium bromide (domiphen) in aqueous solution. Comparison with other alkyl ammonium surfactants

2 Substances • 0 Reactions • 0 Citations

By: Vazquez-Gomez, Silvia; Vazquez-Tato, M. Pilar; Seijas, Julio A.; Meijide, Francisco; Tato, Jose Vazquez; Fraga, Francisco

Journal of Molecular Liquids (2023), 390(Part_B), 123109 | Language: English, Database: CAplus

Dodecyldimethyl-N-2-phenoxyethylammonium bromide (domiphen) is a quaternary ammonium salt which has been used in oral hygiene long time ago. The published studies on its characterization as surfactant evidence several contradictory results. In this paper, measurements of surface tension, conductimetry, fluorescence and mainly isotermal titration calorimetry (ITC) have been performed at different temperatures The enthalpy of demicell ization, ΔHodem, varies linearly with temper ature in the interval 15-45°C, from which a value of 704 ± 39 J mol- 1K-1 in water has been determined for the change of heat capacity, Δ CoP,dem. The obtained results are compared with published values for alkyltrimethylammonium bromides with different alkyl chain lengths (Cn TAB). For instance, its critical micelle concent ration, cmc, is almost ten times lower than that of C12 TAB. The substitution of one Me group by the phenoxyethyl has a strong influence on the behavior of domiphen making it equivalent to a Cn TAB surfactant with n = 15-19 methylene groups, the number depending on the studied property. From I TC an average aggregation number of 45 ± 3 is obtained in good agreement with the one from fluorescence quenching of pyrene equal to 44.5-47.6. From the anal. of specific conductivity, the fraction of bound counterions to micelles was obtained, the values linearly decreasing with temper ature Below cmc domiphen behaves as a strong 1:1 electrolyte without associ ation of monomers. Other themodynamic parameters have also been obtained. The fjord and reef hydration models are used to propose a structure for domiphen micelles.

Keywords: dodecyldimethyl phenoxyethylammonium bromide surfactant aqueous solution

Substances (2) Reactions (0) Citing (0)

2

Effect of Gold Nanoparticles on the Physical Properties of an Epoxy Resin

6 Substances • 1 Reaction • 1 Citation

By: Fraga-Lopez, F.; Carrillo, Lisbeth Jimenez; Vazquez-Tato, Maria Pilar; **Seijas, Julio A.** ; Meijide, Francisco; Vazquez Tato, Jose; Jover, Aida

International Journal of Molecular Sciences (2023), 24(6), 5638 | Language: English, Database: CAplus and MEDLINE

The effect of doping the bisphenol A diglycidyl ether (DGEBA)/m-xylylenediamine (mXDA) system with gold nanoparticles (AuNP) has been studied with differential scanning calorimetry (DSC), thermogravimetric anal., dynamic mech. anal. (DMA), and dielec. anal. (DEA). The evolved heat (ΔHt), the glass transition temperature (T_g), and the associated activation energies of this relaxation process have been determined Below a certain concentration of AuNPs (= 8.5%, in mg Au NP/g epoxy matrix), T_g decreases linearly with the concentration of AuNPs, but above it, T_g is not affected. The degree of conversion α of this epoxy system was analyzed by the semiempirical Kamal's model, evidencing that diffusion correction is required at high values of α. Activation energy values suggest that AuNPs can cause some impediments at the beginning of the crosslinking process (n-order mechanism). The slight difference between the initial decomposition temperature, as well as the temperature for which the degradation rate is at a maximum, for both systems can be accepted to be within exptl. error. Mech. properties (tension, compression, and bending tests) are not affected by the presence of AuNPs. Dielec. measurements show the existence of a second T_g at high temperatures, which was analyzed using the Tsagarapoulos and Eisenberg model of the mobility restrictions of network chains bound to the filler.

Keywords: epoxy resin gold nanoparticle phys property; bisphenol A diglycidyl ether (D GEBA); degree of conversion; epoxy resin; glass transition temperature; gold nanoparticles; m-xylylenediamine

Substances (6) | Reaction (1) | Citing (1)

3

Analysis of the Electron Density of a Water Molecule Encapsulated by Two Cholic Acid Residues

4 Substances • 0 Reactions • 0 Citations

By: Vazquez-Tato, Maria Pilar; **Seijas, Julio A.** ; Meijide, Francisco; de Frutos, Santiago; Vazquez Tato, Jose

International Journal of Molecular Sciences (2023), 24(6), 5359 | Language: English, Database: CAplus and MEDLINE

Cholic acid is a trihydroxy bile acid with a nice peculiarity: the average distance between the oxygen atoms (O7 and O12) of the hydroxy groups located at C7 and C12 carbon atoms is 4.5 Å, a value which perfectly matches with the O/O tetrahedral edge distance in Ih ice. In the solid phase, they are involved in the formation of hydrogen bonds with other cholic acid units and solvents. This fact was satisfactorily used for designing a cholic dimer which encaps ulates one single water mol. between two cholic residues, its oxygen atom (Ow) being exactly located at the centroid of a distorted tetrahedron formed by the four steroid hydroxy groups. The water mol. participates in four hydrogen bonds, with the water simultaneously being an acceptor from the 2 O12 (hydrogen lengths are 2.177 Å and 2.114 Å) and a donor towards the 2 O7 (hydrogen bond lengths are 1.866 Å and 1.920 Å). These facts suggest that this system can be a nice model for the theor. study of the formation of ice-like structures. These are frequently proposed to describe the water structure found in a plethora of systems (water interfaces, metal complexes, solubilized hydrop hobic species, proteins, and confined carbon nanotubes) . The above tetrah edral structure is proposed as a reference model for those systems, and the results obtained from the application of the atoms in mols. theory are presented here. Furthe rmore, the structure of the whole system allows a division into two interesting subsystems in which water is the acceptor of one hydrogen bond and the donor of another. The anal. of the calculated electron d. is performed through its gradient vector and the Laplacian. The calculation of the complexation energy used correction of the basis set superpo sition error (BSSE) with the counterpoise method. As expected, four critical points located in the H...O bond paths were identified. All calculated parameters obey the proposed criteria for hydrogen bonds. The total energy for the interaction in the tetrahedral structure is 54.29 kJ/mol, while the summation obtained of the two independent subsystems and the one between the alkyl rings without water is only 2.5 k J/mol higher. This concordance, together with the calculated values for the electron d., the Laplacian of the electron d., and the lengths of the oxygen atom and the hydrogen atom (involved in the formation of each hydrogen bond) to the hydrogen bond critical point, suggests that each pair of hydrogen bonds can be considered independent of each other.

Keywords: cholic acid residue water mol encapsulation electron density; atoms in molecules theory; bile acid; cholic acid; critical points; electronic density; hydrogen bond

Substances (4) | Reactions (0) | Citing (0)

4

Efficient Synthesis of 2-Aminopyridine Derivatives: Antibacterial Activity Assessment and Molecular Docking Studies

25 Substances • 27 Reactions • 8 Citations

By: Kibou, Zahira; Aissaoui, Nadia; Daoud, Ismail; Seijas, Julio A. ; Vazquez-Tato, Maria Pilar; Klouche Khelil, Nihel; Choukchou-Braham, Noureddine

Molecules (2022), 27(11), 3439 | Language: English, Database: CAplus and MEDLINE

A new and suitable multicomponent one-pot reaction was developed for the synthesis of 2- amino-3-cyanopyridine derivatives This synthesis was demonstrated by the efficient and easy access to a variety of substi tuted 2-aminopyridines using enaminones as key precursors under solvent-free conditions. The antimicrobial potency of synthe sized compounds was tested using disk diffusion assays, and the Min. Inhibitory Concentration (MIC) for the active compounds was determined against a panel of microorg anisms, including Gram-pos. and Gram-neg. bacteria and yeasts. Moreover, a docking anal. was conducted by Mol. Operating Enviro nment (MOE) software to provide supplem entary information about the potential, as well as an ADME-T prediction to describe the pharmacokinetic properties of the best compound and its toxicity. The results of the antimic robial activity indicated that compound 2-(cyclohexylamino)-4-phenylnicotinonitrile showed the highest activity against Gram- pos. bacteria, particularly S. aureus and B. subtilis whose MIC values were 0.039 ± 0.000μg·m L^{-1}. The results of the theor. study of compound 2- (cyclohexylamino)-4-phenyln icotinonitrile were in line with the exptl. data and exhibited excellent antibac terial potential. On the basis of the obtained results, compound 2-(cyclohexylamino)-4-phenylnicotinonitrile can be used as an antibac terial agent model with high antibac terial potency.

Keywords: aminopyridine preparation antibacterial mol docking; 2- aminopyridine derivatives; ADME-T prediction; antimicrobial study; enaminones; molecular docking; multico mponent reactions

Substances (25) | Reactions (27) | Citing (8)

5

Asian Hornet, Vespa velutina Lepeletier 1836 (Hym.: Vespidae), Venom Obtention Based on an Electric Stimulation Protocol

0 Substances • 0 Reactions • 3 Citations

By: Feas, Xesus; Vidal, Carmen ; Vazquez-Tato, M. Pilar; Seijas, Julio A.

Molecules (2022), 27(1), 138 | Language: English, Database: CAplus and MEDLINE

The yellow-legged Asian hornet (Vespa velutina Lepeletier 1836 (Hymeno ptera: Vespidae)) is naturally distributed in China, Southeast Asia, and India; however, recently it has been detected outside of its native area, confirmed as being established in South Korea, Europe, and Japan. Health risks and deaths caused by the invasive Vespa velutina stings have become a public health concern, being the most common cause of anaphylaxis due to hymenop terans in some European regions. This in turn has led to increased demand from medical practitioners and resear chers for Vespa velutina venom for diagnostic and therap eutic purposes. In this study, a straightforward, quick, and inexpensive method for obtaining Vespa velutina venom by elec. stimul ation is described. The venom extracts were analyzed by NMR spectroscopy (^{1}H-NMR). The availability of Vespa velutina venom will lead to improved diagnostic and therapeutic methods, mainly by venom immunot herapy (VIT), in patients allergic to this invasive species.

Keywords: Vespa velutina venom elec stimulation protocol; Asian hornet; Vespa velutina; allergy; electr ical; invasive species; stimul ation; stings; venom

Substances (0) | Reactions (0) | Citing (3)

6

Strange behaviour of transport properties in novel metal thiocyanate based ionic liquids

1 Substance • 0 Reactions • 3 Citations

By: Cabeza, Oscar; Segade, Luisa; Dominguez-Perez, Montserrat; Rilo, Esther; Ausin, David; **Seijas, Julio A.**; Vazquez-Tato, M. Pilar; Matleev, Vladimir; Ievlev, Alexandr; Salgado, Josefa; et al

Journal of Molecular Liquids (2021), 340, 117164 | Language: English, Database: CAplus

In a previous paper some of us presented the structure and some properties of a new family of ionic liquids, ILs, with a common cation, 1-butyl-3-Me imidazolium (the popular $[C4C1Im]^{+}$ or $[BMIM]^{+}$) and a variety of anions based in thiocy anate $(SCN)^{-}$: one reference sample and ten with anionic metal complexes of different valences: Al^{III}, Mn^{II}, Fe^{III}, Cr^{III}, Ni^{II}, Hg^{II}, Zn^{II}, Co^{II} and Cu^{I}, resulting, resp., [BMIM](SCN), $[BMIM]_3$ $Al(SCN)_6$, $[BMIM]_4$ $Mn(SCN)_6$, $[BMIM]_3$ $Fe(SCN)_6$, $[BMIM]_3$ $Cr(SCN)_6$, $[BMIM]_4$ $Ni(SCN)_6$, $[BMIM]_2$ $Hg(SCN)_4$, $[BMIM]_2$ $Zn(SCN)_4$, $[BMIM]_2$ $Co(SCN)_4$ and $[BMIM]_3$ $Cu(SCN)_4$. In this paper we show exptl. measur ements of elec. conduc tivity of these I Ls in a broad temper ature range (about 90 K). Viscosity has been measured for six compounds in a wide temper ature range. In addition, the diffusion coefficient for both ions forming the I L has been measured for some of the samples using N MR-Dosy technique. In spite of being very similar compounds from a chem. point of view, they present very different transport property values. Thus, viscosity varies more than two orders of magnitude among those metal thiocyanate ILs, being the highest for the compound with Al and the lowest for that with Hg. Moreover, differences between ionic conduc tivity and diffusion coefficient values extend more than one order of magnitude among the thiocyanate ILs. These three properties will be related in pairs, thus through Walden's rule we compare molar conductivity and fluidity, while using Kohlra usch's law and Nerst-Einstein equation molar conductivity and diffusion coefficient are related. Also, diffusion coeffi cient and fluidity (the inverse of viscosity) are compared by means of Stokes-Einstein relationship. In addition, we calculate the Laity interionic friction coeffi cients for both anions of the I L with Hg. Finally, a theor. model is suggested to explain all the exptl. evidences reported.

Keywords: metal thiocyanate ionic liquid transport property

Substance (1) | Reactions (0) | Citing (3)

7

Highly Hydrophilic and Lipophilic Derivatives of Bile Salts

3 Substances • 0 Reactions • 4 Citations

By: Vazquez-Tato, M. Pilar; **Seijas, Julio A.**; Meijide, Francisco; Fraga, Francisco; de Frutos, Santiago; Miragaya, Javier; Trillo, Juan Ventura; Jover, Aida; Soto, Victor H.; Vazquez Tato, Jose

International Journal of Molecular Sciences (2021), 22(13), 6684 | Language: English, Database: CAplus and MEDLINE

Lipophilicity of 15 derivatives of sodium cholate, defined by the octan- 1-ol/water partition coefficient (log P), has been theor. determined by the Virtual log P method. These derivatives bear highly hydrop hobic or highly hydrop hilic substituents at the C3 position of the steroid nucleus, being linked to it through an amide bond. The difference between the maximum value of log P and the min. one is enlarged to 3.5. The partition coefficient and the critical micelle concent ration (cmc) are tightly related by a double-logarithm relationship (VirtuallogP=-(1.00 ±0.09)log(cmcmM)+(2.79±0.09)), meaning that the Gibbs free energies for the transfer of a bile anion from water to either a micelle or to octan-1-ol differ by a constant The equation also means that cmc can be used as a measurement of lipophilicity. The demicellization of the aggregates formed by three deriva tives of sodium cholate bearing bulky hydrophobic substituents has been studied by surface tension and isothermal titration calori metry. Aggregation numbers, enthal pies, free energies, entropies, and heat capaci ties, δCP,demic, were obtained. δCP,demic, being pos., means that the interior of the aggregates is hydrophobic.

Keywords: bile salt hydrophilicity lipophilicity heat capacity partition coeffi cient; bile acids and salts; demicellization thermody namics; hydrophilic-lipophilic balance; isothermal titration calori metry; lipophilicity; partition coeffi cient

Substances (3) | Reactions (0) | Citing (4)

8

Structure-based site of metabolism (SOM) prediction of ligand for CYP3A4 enzyme: comparison of glide XP and induced fit docking (IFD)

0 Substances • 0 Reactions • 10 Citations

By: Lokwani, Deepak K. ; Sarkate, Aniket P.; Karnik, Kshipra S.; Nikalje, Anna Pratima G.; **Seijas, Julio A.**
Molecules (2020), 25(7), 1622 | Language: English, Database: CAplus and MEDLINE

Metabolism is one of the prime reasons where most of drugs fail to accomplish their clin. trials. The enzyme CYP3A4, which belongs to the superfamily of cytochrome P 450 enzymes (CYP), helps in the metabolism of a large number of drugs in the body. The enzyme CYP3A4 catalyzes oxidative chem. processes and shows a very broad range of ligand specif icity. The understanding of the compound's structure where oxidation would take place is crucial for the successful modification of mols. to avoid unwanted metabolism and to increase its bioavailability. For this reason, it is required to know the site of metabolism (S OM) of the compounds, where compounds undergo enzymic oxidation It can be identified by predicting the accessibility of the substrate's atom toward oxygenated Fe atom of heme in a CYP protein. The CYP3A4 enzyme is highly flexible and can take signifi cantly different conformations depending on the ligand with which it is being bound. To predict the accessi bility of substrate atoms to the heme iron, conventional protein-rigid docking methods failed due to the high flexib ility of the CYP3A4 protein. Herein, we demons trated and compared the ability of the Glide extra precision (X P) and Induced Fit docking (I FD) tool of Schrodinger software suite to reproduce the binding mode of co-crystallized ligands into six X- ray crystallog. structures. We extend our studies toward the prediction of SOM for compounds whose exptl. S OM is reported but the ligand- enzyme complex crystal structure is not available in the Protein Data Bank (PDB). The quality and accuracy of Glide X P and IFD was determined by calculating RMSD of docked ligands over the corresponding co-crystallized bound ligand and by measuring the distance between the S OM of the ligand and Fe atom of heme. It was observed that IFD reproduces the exact binding mode of available co- crystallized structures and correctly predicted the SOM of exptl. reported compounds Our approach using I FD with multiple conformer structures of CYP3A4 will be one of the effective methods for SOM prediction.

Keywords: CYP3A4; Glide XP; Induced Fit Docking (IFD); Site of Metabolism (SOM)

Substances (0) Reactions (0) Citing (10)

9

Extraction and physicochemical characterization of chitin derived from the Asian hornet, Vespa velutina Lepeletier 1836 (Hym.: Vespidae)

3 Substances • 0 Reactions • 18 Citations

By: Feas, Xesus; Pilar Vazquez-Tato, M.; **Seijas, Julio A.** ; Nikalje, Anna Pratima G.; Fraga-Lopez, Francisco
Molecules (2020), 25(2), 384 | Language: English, Database: CAplus and MEDLINE

Fifteen years ago, at least one multimated female yellow-legged Asian hornet (Vespa velutina Lepeletier 1836) arrived in France, which gave rise to a pan-European invasion. In this study, the isolation and characte rization of chitin (CHI) that was obtained from Vespa velutina (CHIVV) is described. In addition, an easy procedure is carried out to capture the raw insect, select ively and with high rates of success. The chitin contents of dry VV was observed to be 11.7%. Fourier transform I R spectroscopy (FTIR), solid-state NMR (ssNMR), elemental anal. (EA), SEM, and thermogravimetric anal. (TG) characterized the physicochem. properties of CHIVV. The obtained CHIVV is close to pure (43.47% C, 6.94% H, and 6.85% N) , and full acetylated with a value of 95.44%. Addnl., lifetime and kinetic parameters such as activation E and the frequency factor A using model-free and model-fitting methods, were determined For CHIVV the solid state mechanism that follows the thermod egrdn. is of type F2 (random nucleation around two nuclei) . The invasive Asian hornet is a promising alternative source of CHI, based on certain factors, such as the current and probable continued abundance of the quantity and quality of the product obtained.

Keywords: vespa velutina chitin extraction physicochem property; Asian hornet; Vespa velutina; chitin; insects; invasive species; polymer

Substances (3) Reactions (0) Citing (18)

10

Thermodynamics of the aggregation of the bile anions of obeticholic and chenodeoxycholic acids in aqueous solution

2 Substances • 0 Reactions • 3 Citations

By: Vazquez-Gomez, Silvia; Vazquez-Tato, M. Pilar; **Seijas, Julio A.**; Meijide, Francisco; de Frutos, Santiago; Tato, Jose Vazquez
Journal of Molecular Liquids (2019), 296, 112092 | Language: English, Database: CAplus

A complete characterization of the aggregation process of the sodium salts of chenodeo xycholic (NaCDC) and obeticholic (NaObC) acids has been carried out by using different exptl. techniques. Since it is well known that the presence of hydrop hobic groups strongly reduce the critical aggregation concentrations and modifies the type of aggregation structures which can be formed, it could be expected that the introduction of an Et group into the structure of the chenodeo xycholic acid, to form the obeticholic derivative, could give rise to important modific ations in its aggregation behavior. However, it has been observed that the aggreg ation numbers (determined in the range of temper atures 10-40°C from ITC measurements) are identical to each other, a fact which was supported by the determination of the hydrodynamic radius from dynamic light scatte ring. This similarity was also observed for the fraction of bound counterions determined from the well-known Corrin-Harkins plot, being equal to 0.33 for both compounds Finally, the polarity of the interior of the aggregate as measured by the ratio of the fluorescence intensities of the first and third vibronic peaks, I_1/I_3, of monomeric pyrene solubilized within the aggregates is also identical within the exptl. error. The main differences correspond to: (1) the temper atures at which the enthalpy of demicell ization is zero (31.4 (NaObC) and 26.8°C (Na CDC)); and (2) the cmc value for Na ObC is roughly half the one for Na CDC as observed from surface tension, fluore scence and ITC measurements. This implies that the free energy for the demicell ization process is around 2 kJ mol^{-1} larger for NaObC than for NaC DC. (3) Finally, the difference in the change in the heat capacity of the aggreg ation (being 60 J mol^{-1} K^{-1} higher for ObCA) is due to the different number of water mols. which are lost during the monomer transfer from the bulk solution to the micellar aggregate.

Keywords: bile anion obeticholic chenodeoxycholic acid aqueous solution thermodn aggreg ation

Substances (2) | Reactions (0) | Citing (3)

11

Synthesis and Evaluation of Aromatic Surfactants as Potential Antibacterial and Cytotoxic Agents

15 Substances • 22 Reactions • 1 Citation

By: Barrantes, Kenia; Fuentes, Mary; Chacon, Luz; Achi, Rosario; Granados-Zuniga, Jorge; Alvarado, Maria Jose; Somarribas, Luis; Vazquez-Tato, Jose; Vazquez-Tato, M. Pilar; **Seijas, Julio A.**; et al
Letters in Organic Chemistry (2019), 16(6), 478-484 | Language: English, Database: CAplus

Two ether and one ester derivatives of the 4-nitro-3-hydroxybenzoic acid were synthesized and characterized. The in vitro antimic robial and cytotoxic activities of the three novel compounds were also evaluated. The aromatic deriva tives showed antibacterial activity against one of the four microorganisms tested and two compounds (C8 and N OBA) had a lower IC50 in HeLa cells.

Keywords: aromatic surfactant preparation antimicrobial cytotoxicity

Substances (15) | Reactions (22) | Citing (1)

12

Synthesis, microstructure and volumetry of novel metal thiocyanate ionic liquids with [BMIM] cation

0 Substances • 0 Reactions • 11 Citations

By: Cabeza, Oscar; Varela, Luis M.; Rilo, Esther; Segade, Luisa; Dominguez-Perez, Montserrat; Ausin, David; de Pedro, Imanol; Fernandez, Jesus Rodriguez; Gonzalez, Jesus; Vazquez-Tato, M. Pilar; et al
Journal of Molecular Liquids (2019), 283, 638-651 | Language: English, Database: CAplus

We present a new family of ionic liquids (ILs) with a common cation, 1-butyl-3-Me imidazolium, the popular $[BMIM]^+$ (also written $C_4C_1Im^+$) and a variety of anionic complexes (also called adducts) based in thiocyanate $(SCN)^-$: one blank compound, BMIM(SCN), and ten doped with metals having different oxidation states: Al^{+3}, Mn^{+2}, Fe^{+3}, Cr^{+3}, Ni^{+2}, Hg^{+2}, Zn^{+2}, Co^{+2}, Cd^{+2} and Cu^+, forming, resp., $[BMIM]_3[Al(SCN)_6]$, $[BMIM]_4$ $Mn(SCN)_6$, $[BMIM]_3$ $Fe(SCN)_6$, $[BMIM]_3$ $Cr(SCN)_6$, $[BMIM]_4$ $Ni(SCN)_6$, $[BMIM]_2$ $Hg(SCN)_4$, $[BMIM]_2$ $Zn(SCN)_4$, $[BMIM]_2$ $Co(SCN)_4$, $[BMIM]_2$ $Cd(SCN)_4$ and $[BMIM]_3$ $Cu(SCN)_4$. All of them were synthesized by us, except the blank IL and the Co thiocyanate, which are com. Obtained products have been characterized by NMR, and also by electrospray ionization, MS-ES, which allows the determination of the new ILs purities. Then, compounds have been analyzed using FT-IR and Raman spectroscopy. In addition, magnetic susceptibility and refractive index measurements were performed in some of the compounds studied, as well as thermal characterization using DSC and TGA. Finally, exptl. measurements of d. on all those ILs have been performed, and for some of the samples in a broad temperature range (about 100 K). In spite of being very similar compounds from the chem. point of view, they present quite different phys. properties, including optical, thermal and magnetic ones... Also, they show different oxidation states (one with +1, six with +2 and other three with +3). We guess that this family of ILs will have interesting applications, mainly for photonic devices.

Substances (0) | Reactions (0) | Citing (11)

13

Crystal structure of a cationic bile salt derivative ([3β,5β,7α,12α]-3-(2-naphthyloylamino)-7,12-dihydroxycholan-24-triethylammonium iodide)

1 Substance • 0 Reactions • 0 Citations

By: Meijide, Francisco; Vazquez-Tato, Maria Pilar; Seijas, Julio A.; de Frutos, Santiago; Novo, Juan V. Trillo; Soto, Victor H.; Tato, Jose Vazquez
Crystals (2019), 9(3), 135/1-135/13 | Language: English, Database: CAplus

The crystal structure of the iodide salt of a quaternary ammonium derivative of cholic acid having a naphthalene group attached to the 3rd position of the steroid nucleus through an amide bond ([3β,5β,7α,12α]-3-(2-naphthyloylamino)-7,12-dihydroxycholan-24-triethylammonium iodide) has been resolved. The compound crystallizes in the P212121 orthorhombic space group (a/Å = 10.9458 (3); b/Å = 12.1625 (3); c/Å = 28.4706 (7)). The lateral chain adopts a fully extended tttt conformation because the quaternary ammonium group cannot participate in the formation of hydrogen bonds. The iodide ion is involved in the formation of hydrogen bonds as well as the amide group and the two steroid hydroxy groups. Hirshfeld surface anal. confirms that these contacts, as well as the electrostatic interactions, stabilize the structure. The helixes around the 21 screw axis are right- handed ones.

Keywords: dihydroxycholan naphthyloylamino quaternary ammonium crystal structure

Substance (1) | Reactions (0) | Citing (0)

14

Physicochemical Characterization of BADGE n = 0/Zinc Meso-tetra(4-pyridyl) Porphyrin Resin

3 Substances • 1 Reaction • 0 Citations

By: Lopez, Francisco Fraga; Vazquez Barreiro, Eva C.; Jover, Aida; **Seijas, Julio A.**; Meijide, Francisco; Vazquez Tato, Jose
Polymer Science, Series B: Polymer Chemistry (2018), 60(4), 481-496 | Language: English, Database: CAplus

In this work we introduce the zinc 5,10,15,20-tetra(4-pyridyl)-21H,23H-porphine (ZnTPyP) macrocycle as a crosslinking agent of the epoxy resin BADGE n = 0. NMR, TEM and FTIR confirm that both homopolymerization and heteropolymn. (resulting in the formation of a pyridone) are taken place. DSC evidences two exothermic signals at 170 and 290 °, with enthalpy values of 262.3 and - 20.7 J/g, resp. Crystal powder diffraction supports that the second one corresponds to a phys. process. The introduction of the ZnTPyP into the epoxy network improves the thermal stability of the material, which, although very weakly, shows ferromagnetic properties.

Keywords: epoxy resin zinc pyridylporphyrin copolymer preparation thermal physiochem property

Substances (3) | Reaction (1) | Citing (0)

15

Analysis of an old controversy: The compensation temperature for micellization of surfactants

0 Substances • 0 Reactions • 11 Citations

By: Vazquez-Tato, M. Pilar; Meijide, Francisco; **Seijas, Julio A.**; Fraga, Francisco; Vazquez Tato, Jose
Advances in Colloid and Interface Science (2018), 254, 94-98 | Language: English, Database: CAplus and MEDLINE

The actual significance of the so-called compensation temperature T_c for micellization of surfactants is reviewed. It is demonstrated that it is possible to obtain as many T_c values as the number of temperature intervals in which the dependencies of enthalpy and entropy changes with temperature are analyzed. The value of each T_c will be the central value T_o of each temperature interval. These two facts suggest that T_c is simply such exptl. T_o. Thus any phys. interpretation derived from T_c is unfounded.

Keywords: micellization compensation analysis temperature enthalpy entropy; Compensation temperature; Demicellization; Enthalpy-entropy compensation; Isothermal titration calorimetry; Surfactants

Substances (0) | Reactions (0) | Citing (11)

16

Aggregation behavior of sodium 3-(octyloxy)-4-nitrobenzoate in aqueous solution

8 Substances • 9 Reactions • 0 Citations

By: Soto, Victor H.; Vazquez-Tato, M. Pilar; Meijide, Francisco; Alvarado, Maria Jose; Seijas, Julio A.; de Frutos, Santiago; Lomonte, Bruno; Vazquez Tato, Jose

New Journal of Chemistry (2018), 42(24), 19407-19414 | Language: English, Database: CAplus

Ester 3-(octanoyloxy)-4-nitrobenzoic acid is a standard for the assay of the activity of phospho lipase enzymes (the main toxins involved in tissue-damaging after snake bites). Because of its amphiphilic nature, it probably behaves as a surfactant but the instab ility of the ester bond prevents its character ization. Its ether analog, 3-(octyloxy)-4-nitrobenzoic acid, is also an interesting compound as it is an inhibitor of the phospholipase activity and can be accepted as a model of the ester derivative Its sodium salt, stable at basic pH, was studied by surface tension measure ments, isothermal titration calorimetry, dynamic light scattering (DLS), and transmission electron microscopy (TEM). The aggregation number, fraction of bound counterions, critical micelle concentration and thermodn. parameters involved in demicellization were obtained. The pos. value for the change in the heat capacity for demicellization indicates that a larger hydrophobic surface area of each monomer is exposed to a hydrop hilic environment after dissociation Semiempirical calculations are in agreement with DLS and TEM measurements. For several carboxylate surfactants, the plot of enthalpy vs. entropy is linear. Although the slope has been named the compensation temperature, T_c, it merely is an exptl. temperature without any extra-thermodn. meaning.

Keywords: aggregation behavior sodium octyloxynitrobenzoate aqueous solution

Substances (8) | Reactions (9) | Citing (0)

17

Ultrasound assisted synthesis of 4-(benzyloxy)-N-(3-chloro-2-(substituted phenyl)-4-oxoazetidin-1-yl)benzamide as challenging anti-tubercular scaffold

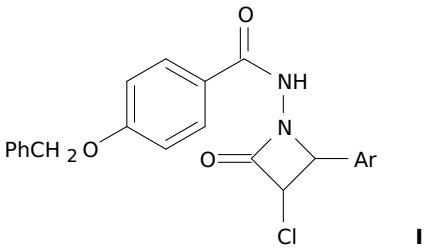
38 Substances • 73 Reactions • 10 Citations

By: Nimbalkar, Urja D.; Seijas, Julio A.; Borkute, Rachna; Damale, Manoj G.; Sangshetti, Jaiprakash N.; Sarkar, Dhiman; Nikalje, Anna Pratima G.

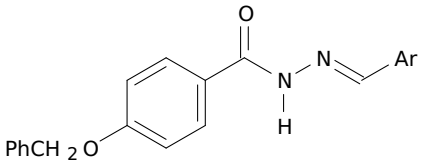
Molecules (2018), 23(8), 1945/1-1945/19 | Language: English, Database: CAplus and MEDLINE

A series of ten novel azetidinyl-benzamide derivatives **I** (Ar = 4-HOC_6H_4, 4-$MeOC_6H_4$, 4-FC_6H_4, etc.) were synthesized in good yield from Schiff bases **II** by Staudinger reaction ([2+2] ketene-imine cycloaddition) with chloroacetyl chloride in the presence of catalyst TEA and solvent DMF, by using ultra-sonication as one of the green chem. tools. **I** were evaluated for in vitro anti-tubercular activity against Mycobacterium tuberculosis (MTB) and most of them showed promising activity with an I C_{50} value of less than 1 μg/mL. To establish the safety, **I** were further tested for cytotoxicity against the human cancer cell line HeLa and all were found to be non-cytotoxic in nature. The mol. docking study was carried out with essential enzyme InhA (FabI/ENR) of Mycobacterium responsible for cell wall synthesis which suggests that **I** (Ar = 4-HOC_6H_4, 3-$O_2NC_6H_4$) are the most active derivatives of the series. The theor. evaluation of cell permeability based on Lipinski's rule of five has helped to rationalize the biol. results; and hence, the synthesized azetidinone derivatives were also analyzed for physicochem. evaluation, i.e., absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties and the results showed that all the derivatives could comply with essential features required for a potential lead in the anti-tubercular drug discovery process.

Keywords: azetidinone green preparation antitubercular cytotoxicity docking ADMET; ADMET study; anti-tubercular screening; azetidinone; cytotoxicity study; green chemistry; molecular docking; ultra- sonication



I



II

Substances (38) Reactions (73) Citing (10)

18

A standard structure for bile acids and derivatives

4 Substances • 0 Reactions • 5 Citations

By: Meijide, Francisco; de Frutos, Santiago; Soto, Victor H.; Jover, Aida; **Seijas, Julio A.**; Vazquez-Tato, Maria Pilar; Fraga, Francisco; Tato, Jose Vazquez

Crystals (2018), 8(2), 86/1-86/17 | Language: English, Database: CAplus

The crystal structures of two ester compounds (a monomer in its Me ester form, with an amino isophthalic group, and a dimer in which the two steroid units are linked by a urea bridge recrystallized from Et acetate/methanol) derived from cholic acid are described. Average bond lengths and bond angles from the crystal structures of 26 monomers and four dimers (some of them in several solvents) of bile acids and esters (and derivatives) are used for proposing a standard steroid nucleus. The hydrogen bond network and conformation of the lateral chain are also discussed. This standard structure was used to compare with the structures of both progesterone and cholesterol.

Keywords: bile acid derivative crystal structure recrystallization

Substances (4) Reactions (0) Citing (5)

19

Ionic liquid-promoted synthesis of novel chromone-pyrimidine coupled derivatives, antimicrobial analysis, enzyme assay, docking study and toxicity study

4 Substances • 0 Reactions • 13 Citations

By: Tiwari, Shailee V.; **Seijas, Julio A.**; Vazquez-Tato, Maria Pilar; Sarkate, Aniket P.; Karnik, Kshipra S.; Nikalje, Anna Pratima G.

Molecules (2018), 23(2), 23020440/1-23020440/22 | Language: English, Database: CAplus and MEDLINE

Herein, we report an environmentally friendly, rapid, and convenient ionic liquid ([Et3NH][HSO4])-promoted facile synthesis of Et 4-(6-substituted-4-oxo-4H-chromen-3-yl)-6-methyl-2-thioxo/oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate derivatives 4(a-f) and 4-(6-substituted-4-oxo-4H-chromen-3-yl)-6-methyl-2-thioxo/oxo-1,2,3,4-tetrahydropyrimidine-5- carbohydrazide derivatives 6(a-f). All the synthesized derivatives 4(a-f) and 6(a-f) were evaluated for their in vitro antifungal and antibac terial activity, by method recomm ended by National Committee for Clin. Laboratory Standards (N CCLS). The compound 6c bearing a fluoro group on the chromone ring and oxygen and a hydrazino group (-NHNH2) on the pyrimidine ring, was found to be the most potent antibac terial compound amongst the synthesized derivatives The compound 6f bearing a methoxy group (- OCH3) on the chromone ring and sulfur group on the pyrimidine ring, was found to exhibit equipotent antifungal activity when compared with the standard drug miconazole. A d-alanine-d-alanine ligase (DdlB) enzyme assay study and an ergosterol extraction and quanti tation assay study were performed to predict the mode of action of the synthesized compounds A mol. docking study was performed to predict the binding intera ctions with receptors and mode of action of the synthesized derivatives Further, anal. of the ADMET parameters for the synthe sized compounds has shown that these compounds have good oral drug-like properties and can be developed as oral drug candid ates. To establish the antimicrobial selectivity and safety, the most active compounds 6c and 6f were further tested for cytoto xicity against the human cancer cell line HeLa and were found to be non-cytotoxic in nature. An in vivo acute oral toxicity study was also performed for the most active compounds 6c and 6f and the results indicated that the compounds are non-toxic in nature.

Keywords: chromone pyrimidine coupled derivative antimicrobial docking toxicity; antibac terial activity; antifungal activity; cytotox icity; in vivo acute oral toxicity; ionic liquid; molecular docking

Substances (4) Reactions (0) Citing (13)

20

Structural and physical properties of a new reversible and continuous thermochromic ionic liquid in a wide temperature interval: $[BMIM]_4[Ni(NCS)_6]$

3 Substances • 1 Reaction • 10 Citations

By: Lopez Lago, Elena; **Seijas, Julio A.**; de Pedro, Imanol; Rodriguez Fernandez, Jesus; Vazquez-Tato, M. Pilar; Gonzalez, Jesus Antonio; Rilo, Esther; Segade, Luisa; Cabeza, Oscar; Rodriguez Fernandez, Carlos Damian; et al
New Journal of Chemistry (2018), 42(19), 15561-15571 | Language: English, Database: CAplus

We report spectroscopic, structural, optical and magnetic characterization of tetra(1-butyl-3-methylimidazolium)hexaisothiocyanatonickelate. This paramagnetic ionic liquid exhibits reversible and continuous thermochromism from 298 K up to 400 K and it is solar responsive resisting numerous heating-cooling cycles. Its appearance changes from pale blue to grass green from 298 K to 343 K. Well above these temperatures it becomes brown and gray. Thermochromism is observed both in the solid and liquid phase.

Keywords: ionic liquid crystal structure phase transition magnetic susceptibility IR

Substances (3) Reaction (1) Citing (10)

21

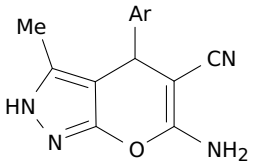
Ionic liquid-catalyzed green protocol for multi-component synthesis of dihydropyrano[2,3-c]pyrazoles as potential anticancer scaffolds

24 Substances • 11 Reactions • 32 Citations

By: Nimbalkar, Urja D.; **Seijas, Julio A.**; Vazquez-Tato, Maria Pilar; Damale, Manoj G.; Sangshetti, Jaiprakash N.; Nikalje, Anna Pratima G.
Molecules (2017), 22(10), 1628/1-1628/17 | Language: English, Database: CAplus and MEDLINE

A series of 6-amino-4-substituted-3-methyl-2,4-dihydropyrano[2,3-c]pyrazole-5-carbonitriles **I** (Ar = 4-hydroxypehnyl, thiophen-2-yl, 3,4-dimethoxyphenyl, etc.) was synthesized via one-pot, four-component condensation reactions of aryl aldehydes ArCHO, propanedinitrile, hydrazine hydrate and Et acetoacetate under solvent-free conditions. The use of the Bronsted acid ionic liquid (BAIL) triethylammonium hydrogen sulfate $[Et_3NH][HSO_4]$ as catalyst for this multi-component synthesis has been reported. Compared with the available reaction methodol., this new method has consistent advantages, including excellent yields, a short reaction time, mild reaction conditions and catalyst reusability. Selected synthesized derivatives were evaluated for in vitro anticancer activity against four human cancer cell lines viz. melanoma cancer cell line (SK-MEL-2), breast cancer cell line (MDA-MB-231), leukemia cancer cell line (K-562) and cervical cancer cell line (HeLa). Compounds **I** (Ar = 4-chlorophenyl, 4-methoxyphenyl, 3,4-dimethoxyphenyl, 3-nitrophenyl, 4-benzyloxyphenyl) exhibited promising anticancer activity against all selected human cancer cell lines, except HeLa. Mol. docking studies also confirmed **I** (Ar = 4-chloropehnyl and 4-methoxyphenyl) as good lead mols. An in silico ADMET study of the synthesized anticancer agents indicated good oral drug-like behavior and non-toxic nature.

Keywords: dihydropyranopyrazole carbonitrile preparation antitumor mol docking green chem solvent less; aldehyde propanedinitrile hydrazine ethyl acetoacetate condensation reaction ionic liquid; ADMET prediction; anticancer activity; dihydropyrano[2,3-c]pyrazoles; ionic liquid; molecular docking study; multi-component synthesis



I

Substances (24) Reactions (11) Citing (32)

22

Facile synthesis of novel coumarin derivatives, antimicrobial analysis, enzyme assay, docking study, ADMET prediction and toxicity study

34 Substances • 15 Reactions • 28 Citations

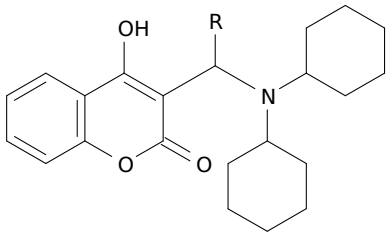
By: Tiwari, Shailee V.; Seijas, Julio A.; Vazquez-Tato, Maria Pilar; Sarkate, Aniket P.; Karnik, Kshipra S.; Nikalje, Anna Pratima G.

Molecules (2017), 22(7), 1172/1-1172/18 | Language: English, Database: CAplus and MEDLINE

Analytical Methods available

The synthesis of fifteen novel 3-((dicyclohexylamino)(substituted phenyl/heteryl)methyl)-4-hydroxy-2H-chromen-2-one derivatives **I** (R = Ph, 4-$MeOC_6H_4$, 2-thienyl, etc.) as potential antimicrobial agents was reported under solvent-free condition using the ionic liquid [Et_3NH][HSO_4] as a catalyst. All the synthesized compounds were evaluated for their in vitro antifungal and antibacterial activity. The compound **I** [R = 4-OH-3-$MeOC_6H_3$ (**II**)] was found to be the most active antifungal agent and compound **I** (R = 2,4-$F_2C_6H_3$) was found to be the most active antibacterial agent. The mode of action of the most promising antifungal compound **II** was established by an ergosterol extraction and quantitation assay and it was found that it acts by inhibition of ergosterol biosynthesis in C. albicans. Mol. docking studies revealed a highly spontaneous binding ability of the tested compounds to the active site of lanosterol 14α-demethylase, which suggests that the tested compounds inhibit the synthesis of this enzyme. The synthesized compounds were analyzed for in silico ADMET properties to establish oral drug like behavior and showed satisfactory results. To establish the antimicrobial selectivity and safety, the most active compounds were further tested for cytotoxicity against human cancer cell line HeLa and were found to be non-cytotoxic in nature. An in vivo acute oral toxicity study was also performed for the most active compounds and results indicated that the compounds are non-toxic.

Keywords: coumarin preparation green chem antibacterial antifungal antitumor human; antibacterial activity; antifungal activity; cytotoxicity; in vivo acute oral toxicity; ionic liquid; molecular docking



I

Substances (34) | Reactions (15) | Citing (28)

23

Microwave-assisted facile synthesis, anticancer evaluation and docking study of N-((5-(substituted methylene amino)-1,3,4-thiadiazol-2-yl)methyl) benzamide derivatives

32 Substances • 0 Reactions • 24 Citations

By: Tiwari, Shailee V.; Siddiqui, Sumaiya; **Seijas, Julio A.**; Vazquez-Tato, M. Pilar; Sarkate, Aniket P.; Lokwani, Deepak K.; Nikalje, Anna Pratima G.

Molecules (2017), 22(6), 995/1-995/14 | Language: English, Database: CAplus and MEDLINE

In the present work, 12 novel Schiff's bases containing a thiadiazole scaffold and benzamide groups coupled through appropriate pharmacophore were synthesized. These moieties are associated with important biol. properties. A facile, solvent-free synthesis of a series of novel 7(a-l) N-((5-(substituted methylene amino)-1,3,4-thiadiazol-2-yl)methyl) benzamide was carried out under microwave irradiation Structures of the synthesized compounds were confirmed by IR, NMR, mass spectral study and elemental anal. All the synthesized hybrids were evaluated for their in vitro anticancer activity against a panel of four human cancer cell lines, viz. SK-MEL-2 (melanoma), HL-60 (leukemia), HeLa (cervical cancer), MCF-7 (breast cancer) and normal breast epithelial cell (MCF-10A) using 3-(4,5-dimethythiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT) assay method. Most of the synthesized compounds exhibited promising anticancer activity, showed comparable GI50 values comparable to that of the standard drug Adriamycin. The compounds 7k, 7l, 7b, and 7a were found to be the most promising anticancer agents in this study. A mol. docking study was performed to predict the probable mechanism of action and computational study of the synthesized compounds 7(a-l) was performed to predict absorption, distribution, metabolism, excretion and toxicity (ADMET) properties, by using QikProp v3.5 (Schrödinger LLC). The results showed the good oral drug-like behavior of the synthesized compounds 7(a-l).

Keywords: methylene amino thiadiazol methyl benzamide anticancer agent cancer; ADMET; in vitro anticancer activity; microwave-assisted synthesis; molecular docking; thiadiazoles

Substances (32) | Reactions (0) | Citing (24)

24

Nonlinear absorption in ionic liquids with transition metallic atoms in the anion

7 Substances • 0 Reactions • 10 Citations

By: Novoa-Lopez, Jose A.; Lopez Lago, Elena; **Seijas, Julio A.**; Pilar Vazquez-Tato, M.; Troncoso, Jacobo; de la Fuente, Raul; Salgueiro, Jose R.; Michinel, Humberto

Optical Materials (Amsterdam, Netherlands) (2016), 52, 144-149 | Language: English, Database: CAplus

Nonlinear absorption has been investigated by open aperture Z-scan in ionic liquids obtained by combination of 1-butyl-3-methyl-imidazolium cations with anions containing a transition metal (Co, Zn, Cu or Ni) and thiocyanate groups. The laser source was a Ti:Sapphire oscillator (80-fs pulses, λ = 810 nm, repetition rate of 80.75 MHz). All liquids present quite low heat capacities that favor the development of strong thermal effects. Thermal effects and nonlinear absorption make them potential materials for optical limiting purposes.

Keywords: transition metallic atom anion ionic liquid nonlinear absorption

Substances (7) | Reactions (0) | Citing (10)

25

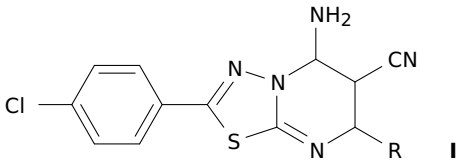
Ultrasound mediated one-pot, three component synthesis, docking and ADME prediction of novel 5-amino-2-(4-chlorophenyl)-7-substituted phenyl-8,8a-dihydro-7H-(1,3,4)thiadiazolo(3,2-α)pyrimidine-6-carbonitrile derivatives as anticancer agents

25 Substances • 10 Reactions • 43 Citations

By: Tiwari, Shailee V.; Seijas, Julio A.; Vazquez-Tato, M. Pilar; Sarkate, Aniket P.; Lokwani, Deepak K.; Nikalje, Anna Pratima G.
Molecules (2016), 21(8), 894/1-894/13 | Language: English, Database: CAplus and MEDLINE

Herein, an environmentally friendly, rapid, and convenient one-pot ultrasound-promoted synthesis of 5-amino-2-(4-chlorophenyl)-7-substituted phenyl-8,8a-dihydro-7H-(1,3,4)thiadiazolo(3,2-α)pyrimidine-6-carbonitrile derivatives **I** (R = 4-ClC_6H_4, 4-$MeOC_6H_4$, Ph, etc.) is reported. The in-vitro anticancer activities of these compounds were evaluated against four human tumor cell lines. Among all the synthesized derivatives, compound which has substituent 3-hydroxy-4-methoxyphenyl **I** (R = 3-HO-4-$MeOC_6H_3$) is found to have the highest GI_{50} value of 32.7 μM, 55.3 μM, 34.3 μM, 28.9 μM for MCF-7, K562, HeLa and PC-3 cancer cell lines resp. A docking study of the newly synthesized compounds were performed, and the results showed good binding mode in the active site of thymidylate synthase enzyme. ADME properties of synthesized compounds were also studied and showed good drug like properties.

Keywords: thiadiazolopyrimidine carbonitrile green preparation antitumor ultrasound irradiation; mol docking ADME property human; 1,3,4-thiadiazolo(3,2-α)pyrimidine; ADME; docking; ultrasound-promoted synthesis



I

Substances (25) Reactions (10) Citing (43)

26

A rapid and sensitive determination of hypoxic radiosensitizer agent nimorazole in rat plasma by LC-MS/MS and its application to a pharmacokinetic study

2 Substances • 0 Reactions • 6 Citations

By: Das, Soumyajit; Dubey, Ramkumar; Roychowdhury, Subhradip; Ghosh, Manik ; Sinha, Barij Nayan; Kumar Pradhan, Kishanta; Bal, Trishna; Muthukrishnan, Venkateswari; **Seijas, Julio A.**; Pujarid, Abhijit
Biomedical Chromatography (2015), 29(10), 1575-1580 | Language: English, Database: CAplus and MEDLINE
Analytical Methods available

A highly sensitive, accurate and robust LC-MS/MS method was developed and validated for determi nation of nimorazole (NMZ) in rat plasma using metronidazole (MNZ) as internal standard (IS). The analyte and I S were extracted from plasma by precipi tating protein with acetonitrile and were chromato graphed using an Agilent Poroshell 120, E C-C_{18} column. The mobile phase was composed of a mixture of acetonitrile and 0.1 % formic acid (85: 15 volume/volume). The total run time was 1.5 min and injection volume was 5 µL. Multiple reaction monitoring mode using the transitions of m/z 227.1 → m/z 114.0 for M NZ and m/z 172.10 → m/z 128.1 for IS were monitored on a triple quadrupole mass spectro meter, operating in pos. ion mode. The calibr ation curve was linear in the range of 0.25-200 ng/mL (r^2 > 0.9996) and the lower limit of quantif ication was 0.25 ng/mL in the rat plasma samples. Recoveries of NMZ ranged between 88.05 and 95.25%. The precision (intra- day and inter-day) and accuracy of the quality control samples were 1.25-8.20% and -2.50-3.10, resp. The analyte and I S were found to be stable during all sample storage and anal. procedures. The LC-MS/MS method described here was validated and succes sfully applied to pharmacokinetic study in rats.

Keywords: nimorazole antiinfective agent pharmaco kinetics LC MS hypoxia; LC-MS/MS; hypoxic sensitizer; metronidazole; nimora zole; pharmacokinetic

Substances (2) Reactions (0) Citing (6)

27

Novel microwave-assisted synthesis of the immunomodulator organotellurium compound ammonium trichloro(dioxoethylene-O,O')tellurate (AS101)

2 Substances • 1 Reaction • 8 Citations

By: Vazquez-Tato, M. Pilar; Mena-Menendez, Alberto; Feas, Xesus; **Seijas, Julio A.**
International Journal of Molecular Sciences (2014), 15(2), 3287-3298, 12 pp. | Language: English, Database: CAplus and MEDLINE

Ammonium trichloro(1,2-ethanediolato-O,O')-tellurate (AS101) is the most important synthetic Te compound from the standpoint of its biol. activity. It is a potent immunomodulator with a variety of potential therap eutic applic ations and antitumoral action in several preclin. and clin. studies. An exptl. design has been used to develop and optimize a novel microwave-assisted synthesis (M A OS) of the AS101. In comparison to the results observed in the literature, refluxing Te(IV) chloride and ethylene glycol in aceton itrile (Method A), or by refluxing Te(IV) chloride and ammonium chloride in ethylene glycol (Method B) , it was found that the developed methods in the present work are an effective alternative, because although perfor mance slightly decreases compared to conven tional procedures (75% vs. 79% by Method A, and 45% vs. 51% by Method B) , reaction times decreased from 4 h to 30 min and from 4 h to 10 min, by Methods A and B resp. MAOS is proving to be of value in the rapid synthesis of compounds with new and improved biol. activities, specially based on the benefit of its shorter reaction times.

Keywords: microwave assisted preparation immunomodulator organotellurium ammonium trichlorodioxoethylene tellurate AS101

Substances (2) Reaction (1) Citing (8)

28

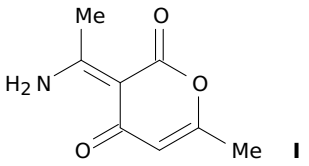
Microwave assisted synthesis, crystal structure and modeling of cytotoxic dehydroacetic acid enamine: a natural alkaloid from Fusarium incarnatum (HKI0504)

3 Substances • 1 Reaction • 2 Citations

By: **Seijas, Julio A.** ; Crecente-Campo, Jose; Feas, Xesus; Vazquez-Tato, M. Pilar
RSC Advances (2014), 4(33), 17054-17059 | Language: English, Database: CAplus

A novel, fast and efficient method for the synthesis of (3E)-3-(1-aminoethylidene)-6-methyl-3,4-dihydro-2H-pyran-2,4-dione (**I**), a natural antiproliferative and cytotoxic product isolated from Fusarium incarnatum (HKI0504), was developed from dehydroacetic acid and urea under solvent-free microwave irradiation The anal. of the co-crystal structure revealed an asym. unit formed by a pair of mols. Each mol. is joined by two different hydrogen bonds to another two mols., ordered as four-unit clusters linked by π-stacking, assembled in a brick like layered structure in a set of parallel walls. Besides, the preferred tautomer for crystal structure is the enamine form. This is corroborated by computational NBO anal., outlining the contribution of enamine resonance and modeling the non-covalent interactions involved by means of Hirshfeld surfaces and G09 counte rpoise calculations

Keywords: urea dehydroacetic acid condensation microwave irradiation; dehydroacetic acid enamine preparation crystal mol structure modeling



I

Substances (3) Reaction (1) Citing (2)

29

Structure elucidation and HPLC-MS/MS determination of a potential biomarker for estradiol administration in cattle

6 Substances • 1 Reaction • 7 Citations

By: Regal, Patricia; **Seijas, Julio A.** ; Cepeda, Alberto; Fente, Cristina
Analytical and Bioanalytical Chemistry (2013), 405(29), 9537-9546 | Language: English, Database: CAplus and MEDLINE
Analytical Methods available

Administration of hormonal compounds as growth promoters in livestock farming was banned by Council Directive 96/22/E C. However, this kind of substances is sometimes reported within the framework of European monitoring residue plans. Various anal. methods have been previously developed to screen for their misuse, and they are now especially efficient for monitoring the illegal administration of synthetic and semisynthetic hormones. Nevertheless, proving an exogenous administration of hormones from natural origin (i.e., estradiol-17β or progesterone) still remains a challenge for European author ities. These target compounds are indeed always present in the animal matrix, and the establishment of reference thresholds appears very difficult because of the extreme variability existing among animals. In 2011, a metabo lomics study was performed on serum samples obtained from cows treated with estradiol-17β (or its ester estradiol benzoate) and from control animals using a high- performance liquid chromatog. (H PLC)-LTQ-Orbitrap system. After appropriate data processing and multivariate statistical anal. (orthogonal partial least squares discriminant anal.), it was possible to highlight one potential biomarker candidate of estradiol treatments in bovine animals. Now, this biomarker has been structurally elucidated as a dipeptide, and its usefulness has been tested through a targeted H PLC-MS/MS method. Its presence in the previous samples has been confirmed and also in addnl. samples from estradiol-treated animals.

Keywords: forensic illegal hormone HPLC MS biomarker estradiol cattle

Substances (6) Reaction (1) Citing (7)

30

Palynological, physicochemical, and microbiological attributes of organic lavender (Lavandula stoechas) honey from Portugal

3 Substances • 0 Reactions • 2 Citations

By: Estevinho, M. L.; Vazquez-Tato, M. P.; **Seijas, J. A.**; Feas, X.
Acta Alimentaria (2013), 42(1), 36-44 | Language: English, Database: CAplus

At the present time, the quality, integrity, sanitation, and nutritional value of honeys receive attention on an interna tional level due to the increasing content of chems. in the aforementioned matrix. The present study aims to charac terize organic honey (n=73) from Northeast Portugal, with respect to floral nectar origin, physicochem. parameters, microbial safety, and com. quality. All organic honey samples can be classified as monofloral lavender (Lavandula stoechas L.), exceed in quality the international physic ochem. standards, and show low microbiol. counts (yeast, molds, and aerobic mesophiles) , with neg. results in respect to faecal coliforms, Salmonella, and sulphite-reducing clostridia. Correlating the palynol., physico chem., and microbiol. results is necessary in order to check the authenticity, quality, and sanitation of honey.

Keywords: organic honey lavender microbial safety physicochem property

Substances (3) | Reactions (0) | Citing (2)

31

Triacylglyceride, antioxidant and antimicrobial features of virgin Camellia oleifera, C. reticulata and C. sasanqua oils

8 Substances • 0 Reactions • 47 Citations

By: Feas, Xesus; Estevinho, Leticia M.; Salinero, Carmen; Vela, Pilar; Sainz, Maria J.; Vazquez-Tato, Mara Pilar; **Seijas, Julio A.**
Molecules (2013), 18, 4573-4587 | Language: English, Database: CAplus and MEDLINE

Virgin oils obtained from seeds of Camellia oleifera (CO), Camellia reticulata (CR) and Camellia sasanqua (CS) were studied for their triacylglyceride composition, antioxidant and antimicrobial activities. Levels of fatty acids determined by ^{1}H-NMR anal. were similar to those reported for olive oils (82.30%-84.47%; 5.69%-7.78%; 0.26%-0.41% and 8.04%-11.2%, for oleic, linoleic, linolenic and saturated acids, resp.). The CR oil showed the best antiox idant potential in the three in vitro models tested. With regard to E C_{50} values (μg/mL), the order in DPPH radical-scavenging was CR (33.48) < C O (35.20) < CS (54.87). Effectiveness in reducing power was CR (2.81) < C O (3.09) < CS (5.32). IC_{50} for LPO inhibition were 0.37, 0.52 and 0.75 μg/m L for CR, CO and CS, resp. All the oils showed antimicrobial activity and exhibited different selectivity and MICs for each microor ganism tested (E. coli, B. cereus and C. albicans) . B. cereus was the less sensitive species (MIC: 52.083 ± 18.042 for C O; 41.667 ± 18.042 for C R; 104.167 ± 36.084 for C S mg/mL) and the E. coli was the most sensitive to camellia oil's effect. The standard gentamicin presented higher MIC for E. coli (4.2) than the C R (MIC = 2.6) and C O (MIC = 3.9) oils.

Keywords: seed oil Camellia triacylglyceride antioxidant antimicrobial

Substances (8) | Reactions (0) | Citing (47)

32

Organic honey from Tras-Os-Montes region (Portugal): Chemical, palynological, microbiological and bioactive compounds characterization

3 Substances • 0 Reactions • 59 Citations

By: Estevinho, Leticia M.; Feas, Xesus; Seijas, Julio A.; Pilar Vazquez-Tato, M.
Food and Chemical Toxicology (2012), 50(2), 258-264 | Language: English, Database: CAplus and MEDLINE

At the present time, the quality, integrity, sanitation and nutritional value of honeys receive attention on an interna tional level due to the increasing content of chems. in the aforementioned matrix. This work was conducted to evaluate the quality of 75 organic honey samples from the Tras-Os-Montes region (Portugal). Mean values obtained for physico-chem. parameters were: p H 3.7; 15.6% moisture; 0.26 mS/cm elec. conductivity; 0.25% ash; 1.1 mg/kg H MF; 15.3 Gothe diastase activity; 40.3 meq/kg free acidity; 67.8% invert sugars and 2.7% apparent sucrose. All honey samples can be classified as monofloral Erica sp., as showed by pollen features. The amounts of phenols and flavonoids in the samples were also determined In respect to sanitary quality (fecal coliforms) and safety (sulfite-reducing clostridia and Salmonella), all organic honey samples were neg. Furthe rmore, yeast and molds were detected in low counts, with mean values obtained of 5.5 cfu/g and the value of total aerobic mesophiles obtained from honeys was established in 1.3×10^{2} cfu/g ± 7.5×10^{1} cfu/g. The levels of flavonoids had a stronger impact on both mesophiles (p = 0.0004) and molds (p = 0.0138) than the sucrose concentration (p = 0.001 and 0.0278; resp.) . The results reported in this study should be introduced in the organic honey label, and may help beekeepers, the industry, researchers and consumers better understand honey properties.

Keywords: organic honey sucrose diastase hydroxymethylfurfural phenol flavonoid microor ganism

Substances (3) | Reactions (0) | Citing (59)

33

Comprehensive study of honey with Protected Denomination of Origin and contribution to the enhancement of legal specifications

2 Substances • 0 Reactions • 24 Citations

By: Iglesias, Antonio; Feas, Xesus; Rodrigues, Sandra; Seijas, Julio A.; Vazquez-Tato, M. Pilar; Dias, Luis G.; Estevinho, Leticia M.
Molecules (2012), 17, 8561-8577 | Language: English, Database: CAplus and MEDLINE

In this study the characterization of a total of 60 honey samples with Protected Denomi nation of Origin (P DO) collected over three harvests (2009-2011, inclusive), from the Northeast of Portugal was carried out based on the presence of pollen, physic ochem. and microbiol. characteristics. All samples were found to meet the European Legisl ation, but some didn't meet the requir ements of the PDO specifications. Concerning the floral origin of honey, our results showed the prevalence of rosemary (Lavandula pedunc ulata) pollen. The microbiol. quality of all the analyzed samples was satisfactory, since fecal coliforms, sulfite-reducing clostridia and Salmonella were absent, and molds and yeasts were detected in low counts. Significant differences between the results were studied using one-way anal. of variance (A NOVA), followed by Tukey's HSD test. The samples were submitted to discri minant function anal., in order to determine which variables differentiate between two or more naturally occurring groups (Forward Stepwise Anal.). The variables selected were in this order: diastase activity, p H, reducing sugars, free acidity and H MF. The pollen spectrum has perfect discriminatory power. This is the first study in which a honey with P DO was tested, in order to assess its compliance with the PDO book of specifications.

Keywords: honey Lavandula pollen

Substances (2) | Reactions (0) | Citing (24)

34

Organic bee pollen: botanical origin, nutritional value, bioactive compounds, antioxidant activity and microbiological quality

8 Substances • 0 Reactions • 145 Citations

By: Feas, Xesus; Vazquez-Tato, M. Pilar; Estevinho, Leticia; **Seijas, Julio A.**; Iglesias, Antonio
Molecules (2012), 17, 8359-8377 | Language: English, Database: CAplus and MEDLINE

Organic bee pollen (BP, n = 22) harvested from the Douro Interna tional Natural Park (DINP, Portugal) was studied. Nine botanical families were found in the mixture of the samples. The water activity and pH ranged 0.21-0.37 and 4.3-5.2, resp. The BP analyses averaged 67.7% carbohydrates, 21.8% crude protein, 5.2% crude fat and 2.9% ash. The energy ranged from 396.4 to 411.1 kcal/100 g. The principal fatty acid found was linolenic, followed by linoleic acid, palmitic acid and oleic acid. The phenolic and flavonoid contents varied from 12.9 to 19.8 mg of gallic acid equivalent/g of extract and from 4.5 to 7.1 mg of catechin equiva lent/g of extract, resp. The scavenger activity and β-carotene bleaching assays values (EC_{50}) were 3.0 ± 0.7 mg/m L and 4.6 mg/m L ± 0.9 mg/m L, resp. E. coli, sulphite-reducing Clostridia, Salmonella and S. aureus were not found. Since there are studies indicating apprec iable differ ences among BPs from different regions, the full characterization of BP from diverse origins still appears to be a sound research priority in order to obtain reliable data about this beehive product.

Keywords: bee pollen bioactive compound antioxidant

Substances (8) | Reactions (0) | Citing (145)

35

The 1st Electronic Conference on Pharmaceutical Sciences, ECPS2011 on 1-31 March

0 Substances • 0 Reactions • 0 Citations

By: **Seijas, Julio A.**; Vazquez Tato, Pilar; Rantanen, Jukka; Naelapaa, Kaisa; He, Jely; Editors
2012, No pp. given | Language: English, Database: CAplus

There is no abstract available for this document.

Keywords: pharmaceutical science book

Substances (0) | Reactions (0) | Citing (0)

36

^{1}H-nuclear magnetic resonance analysis of the triacylglyceride composition of cold-pressed oil from Camellia japonica

3 Substances • 0 Reactions • 26 Citations

By: Salinero, Carmen; Feas, Xesus; Mansilla, J. Pedro; **Seijas, Julio A.**; Vazquez-Tato, M. Pilar; Vela, Pilar; Sainz, Maria J.
Molecules (2012), 17, 6716-6727 | Language: English, Database: CAplus and MEDLINE

Camellia japonica (CJ) has oil-rich seeds, but the study of these oils has received little attention and has mainly focused only on their health properties. In the present work the relative composition of the fatty acid (FA) components of the triglycerides in cold-pressed oil from CJ is studied by ^{1}H-NMR. The results obtained were: 75.75%, 6.0%, 0.17% and 18.67%, for oleic, linoleic, linolenic and saturated FA resp. Levels of C_{18} unsaturated FA found in CJ oil were similar to those reported for olive oils. We also checked the possibility of using ^{13}C-NMR spectroscopy; however, the results confirmed the drawback of ^{13}C over ^{1}H-NMR for the study of FA components of CJ triglycerides due to its low gyromagnetic ratio and its very low natural abundance.

Keywords: triacylglyceride cold pressed oil Camellia 1 H NMR spectroscopy

Substances (3) | Reactions (0) | Citing (26)

37

15th International Electronic Conference on Synthetic Organic Chemistry (ECSOC-15) held 1-30 November 2011

0 Substances • 0 Reactions • 0 Citations

By: **Seijas, Julio A.**; Vazquez-Tato, M. Pilar; Editors
2011, No pp. given | Language: English, Database: CAplus

There is no abstract available for this document.

Keywords: book synthetic organic chem

Substances (0) | Reactions (0) | Citing (0)

38

Efficient synthesis of heterophosphole-2-sulfides by solvent-free microwave reaction

26 Substances • 13 Reactions • 6 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Crecente-Campo, Jose
Tetrahedron (2010), 66(41), 8210-8213 | Language: English, Database: CAplus

Microwave irradiation of a stoichiometric amount of Lawesson's reagent in the presence of o-aminophenols, o-aminothiophenols, o-phenylenediamines, or catechols leads to benzoxazaphosphole-, benzothiazaphosphole-, benzodiazaphosphole-, and benzodioxa phosphole-2-sulfides, resp., in good yields in a fast and direct way under solven tless conditions. The procedure requires short reaction times and is similar for all reagents; thus it may be used in parallel synthesis.

Keywords: phosphole sulfide hetero preparation; Lawessons reagent microwave irradi ation aminophenol aminothiophenol phenylenediamine catechol

Substances (26) Reactions (13) Citing (6)

39

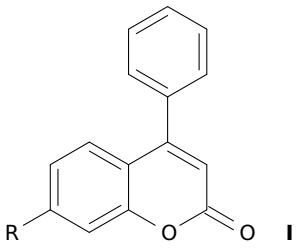
Microwave-Promoted, One-Pot, Solvent-Free Synthesis of 4-Arylcoumarins from 2-Hydroxybenzophenones

28 Substances • 40 Reactions • 20 Citations

By: Crecente-Campo, Jose; Pilar Vazquez-Tato, M.; Seijas, Julio A.
European Journal of Organic Chemistry (2010), (21), 4130-4135, S4130/1-S4130/14 | Language: English, Database: CAplus

4-Arylcoumarins are synthesized in very good yields through solvent- free microwave irradiation of 2-hydroxybenzophenones and alkyl malonate in the presence of DBU. The one-pot synthesis is carried out with Knoeve nagel condensation, intramol. lactonization, and decarboxylation reactions. The method can be applied to a broad scope of neoflav onoids, e.g., **I** (R = H, Me O, EtO, OH).

Keywords: hydroxybenzophenone dialkyl malonate Knoevenagel condensation intramol lactonization decarboxylation microwave; aryl coumarin preparation solventless; neoflavonoid preparation solventless; microwave irradiation Knoevenagel condensation intramol lactonization decarboxylation mediator



I

Substances (28) Reactions (40) Citing (20)

40

Direct syntheses of 4-aryl-1,2,3,4-tetrahydroisoquinolines and 1-aryl-2,3,4,5-tetrahydro-3-benzazepines via hydroamination of enol carbamates

29 Substances • 38 Reactions • 20 Citations

By: Crecente-Campo, Jose; Vazquez-Tato, M. Pilar; **Seijas, Julio A.**
Tetrahedron (2009), 65(13), 2655-2659 | Language: English, Database: CAplus

An efficient and simple procedure for the syntheses of 4-aryl-1,2,3,4-tetrahydroisoquinolines and 1-aryl-2,3,4,5-tetrahydro-3-benzazepines has been developed. The approach uses easily available starting materials and requires just three steps. The hydroamination of an enol carbamate is the key step. This general and direct method has been applied to the total synthesis of the natural alkaloid cherylline and to biol. active 3-benzazepines as well.

Keywords: hydroamination enol carbamate tetrahydroisoquinoline tetrahydrobenzazepine preparation

Substances (29) | Reactions (38) | Citing (20)

41

Use of acrylic acid in the synthesis of molecularly imprinted polymers for the analysis of cyproheptadine

4 Substances • 0 Reactions • 21 Citations

By: Feas, Xesus; Fente, Cristina A.; Hosseini, S. Vali; **Seijas, Julio A.**; Vazquez, Beatriz I.; Franco, Carlos M.; Cepeda, Alberto
Materials Science & Engineering, C: Materials for Biological Applications (2009), 29(2), 398-404 | Language: English, Database: CAplus

The synthesis and comparative characterization of molecularly imprinted polymers (MIP$_s$) with cyproheptadine (CYP), using two different monomers, acrylic acid (AA) and methacrylic acid (MAA), are described. Polyacids (PA) [poly(methacrylic acid) (PMAA) and poly(acrylic acid) (PAA)] were obtained by the radical polymerization of MAA and AA, resp., in dichloromethane as the porogen solvent-imprinted medium. The non-covalent imprinting process was performed via thermal decomposition of an azo-initiator at 60°, using ethylene glycol dimethacrylate as the cross-linker and 2,2'-azobis(2-methylpropionitrile) as the initiator. The selectivities of MIP$_s$ and NIP$_s$ particles were evaluated in binding experiments of the four synthesized polymeric materials (MIP$_{aa}$, MIP$_{maa}$, NIP$_{maa}$, and NIP$_{aa}$) with CYP. The effects of monomers on: (a) the surface morphol., (b) the binding capacity and (c) the swelling properties of imprinted and non-imprinted polymers were studied and are presented here. Polymer material morphol. was assessed with SEM. This revealed differences in monomer function, depending on which one was employed, as well as differences in function when polymerization occurred in the presence of template or without it. Non-specific retention of the template to NIP$_s$ was higher for NIP$_s$-PAA polymers than for NIP$_s$-PMAA materials. In terms of specific binding ($\Delta Q = Q_{MIP}-Q_{NIP}$), MIP$_{maa}$ showed the greatest value (53.47%) in comparison with MIP$_{aa}$ (50.07%).

Keywords: cyproheptadine determination gas chromatog MS MIP; GC separation cyproheptadine mass spectroscopy

Substances (4) | Reactions (0) | Citing (21)

42

NMR analysis of a series of substituted pyrazolo[3,4-d]pyrimidines-4-amines

21 Substances • 0 Reactions • 1 Citation

By: Rodrigues, Ligia M.; Sivasubramanian, Aravind; Pinto, Elisa M.; Oliveira-Campos, Ana M. F.; **Seijas, Julio A.**; Vazquez-Tato, M. Pilar
Magnetic Resonance in Chemistry (2009), 47(1), 84-86 | Language: English, Database: CAplus and MEDLINE

A series of 21 substituted pyrazolo[3,4-d]pyrimidines-4-amines were studied by ^{1}H and ^{13}C NMR. The application of two-dimens ional techniques, HMQC and HMBC, allowed the complete assignment of the spectra for all the compounds

Keywords: NMR analysis substituted pyrazolo d pyrimidines amine

Substances (21) | Reactions (0) | Citing (1)

43

Syntheses of molecularly imprinted polymers: Molecular recognition of cyproheptadine using original print molecules and azatadine as dummy templates

11 Substances • 0 Reactions • 80 Citations

By: Feas, X.; **Seijas, J. A.**; Vazquez-Tato, M. P.; Regal, P.; Cepeda, A.; Fente, C.
Analytica Chimica Acta (2009), 631(2), 237-244 | Language: English, Database: CAplus and MEDLINE

The use of custom-made polymeric materials with high selectivities as target mols. in solid-phase extraction (SPE), known as molecu larly imprinted solid-phase extraction (MISPE), is becoming an increasingly important sample preparation technique. However, the potential risk of leakage of the imprinting mols. during the desorption phase has limited application. The use of a mimicking template, called a dummy mol. imprinting polymer (DMIP), that bears the structure of a related mol. and acts as a putative imprinting mol. may provide a useful solution to this problem. In the current study, cyproheptadine (CPH) and azatadine (AZA) were used as templates in the development of an MIP and DMIP for acrylic acid and methac rylic acid monomers. Our results indicate that DMIPs have equal recognition of CPH, avoiding the problem of leakage of original template during the desorption phase relative to MIPs synthesized in presence of the print mol. C PH. Examination of the surface structure of the two polymer products by SEM shows appreciable differences in structural morphol. and function of the monomers employed. These results are well supple mented by data obtained for swelling ratios and solvent uptake. Mol. modeling of C PH and AZA suggests that both substrates are similar in shape and volume

Keywords: molecularly imprinted polymer cyproheptadine azatadine extraction

Substances (11) | Reactions (0) | Citing (80)

44

13th International Electronic Conference on Synthetic Organic Chemistry held 1-30 November 2009

0 Substances • 0 Reactions • 0 Citations

By: Seijas, Julio A. ; Vazquez Tato, M. Pilar
2009, No pp. given | Language: English, Database: CAplus

There is no abstract available for this document.

Keywords: book review synthetic organic chem

Substances (0) Reactions (0) Citing (0)

45

Straightforward microwave-assisted synthesis of 2-thiazolines using Lawesson's reagent under solvent-free conditions

68 Substances • 43 Reactions • 35 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Crecente-Campo, Jose
Tetrahedron (2008), 64(39), 9280-9285 | Language: English, Database: CAplus

2-Thiazolines are synthesized from carboxylic acids and 1,2-amino alcs. in the presence of Lawesson's reagent under solventless conditions. The method is valid for either substituted or unsubstituted amino alcs. and a wide variety of aromatic, heteroaromatic and aliphatic carboxylic acids; thus it constitutes a general synthetic method for these kinds of compounds The role of Lawesson's reagent is dual: to transform the 1,2-amino alc. into 1,2-amino thiol and to activate its reaction with the carboxylic acid leading to the formation of a thiazoline ring, all in one pot.

Keywords: carboxylic acid heterocyclization amino alc Lawesson reagent; thiazoline derivative microwave assisted solventless preparation

Substances (68) Reactions (43) Citing (35)

46

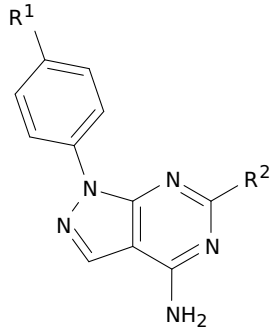
Substituted pyrazolo[3,4-d]pyrimidines: microwave-assisted, solvent-free synthesis and biological evaluation

32 Substances • 21 Reactions • 17 Citations

By: Oliveira-Campos, Ana M. F.; Sivasubramanian, Aravind; Rodrigues, Ligia M.; **Seijas, Julio A.**; Vazquez-Tato, M. Pilar; Peixoto, Francisco; Abreu, Carlos G.; Cidade, Honorina; Oliveira, Ana Elizabete; Pinto, Madalena
Helvetica Chimica Acta (2008), 91(7), 1336-1345 | Language: English, Database: CAplus
Analytical Methods available

A simple and efficient method has been developed for the synthesis of various pyrazolo[3,4-d]pyrimidines **I** (R^1 = H, Cl, Br; R^2 = Ph, Bn, 3-CNC_6H_4, 3-pyridyl, 4-pyridyl, 2-thiophenyl, 2-furanyl) by using microwave irradiation under solvent-free conditions. The advantages of applying microwave irradiation compared with the classical method were demonstrated. The structures of all the compounds were confirmed by the usual techniques and, in two cases, by X-ray anal. The compounds did not display appreciable ability to inhibit xanthine oxidase activity. Screening for antifungal activity showed that some derivatives were active against four fungi, with more significant results for Botrytis.

Keywords: arylaminopyrazolecarbonitrile nitrile microwave irradiation heterocyclization; pyrimidine pyrazolo derivative preparation crystal structure; pyrazolopyrimidine derivative preparation agrochem antifungal activity xanthine oxidase inhibition



I

Substances (32) | Reactions (21) | Citing (17)

47

Microwave-assisted solvent-free synthesis of enol carbamates

42 Substances • 20 Reactions • 11 Citations

By: **Seijas, Julio A.**; Vazquez-Tato, M. Pilar; Crecente-Campo, Jose
Synlett (2007), (15), 2420-2424 | Language: English, Database: CAplus

An efficient and simple method for the synthesis of enol carbamates by irradiation with microwaves under solvent-free conditions has been developed. The method has been applied to substituted acetophenones, cyclic aryl ketones and α-aryl ketones. Its main advantages are short reaction times, good conversions except for nitro acetophenones, and the environmentally friendly nature of the process. For α-aryl ketones the reaction shows regio-selectivity to afford conjugated products.

Keywords: enol carbamate preparation; arylketone diisopropylcarbamoyl chloride enolation acylation microwave irradiation; microwave irradiation enolation acylation mediator

Substances (42) | Reactions (20) | Citing (11)

48

Lawesson's reagent and microwaves: a new efficient access to benzoxazoles and benzothiazoles from carboxylic acids under solvent-free conditions

56 Substances • 37 Reactions • 129 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Carballido-Reboredo, M. Raquel; Crecente-Campo, Jose; Romar-Lopez, Lucia
Synlett (2007), (2), 313-317 | Language: English, Database: CAplus

Lawesson's reagent acts as an efficient promoter in the solvent-free microwave-assisted synthesis of 2-substituted benzoxazoles from carboxylic acids and 2-aminophenol, and thus, constitutes a general synthetic method for these compounds This new applic ation of Lawesson's reagent is valid also for benzoth iazoles with very high efficiency level. A variety of aromatic, heteroar omatic, and aliphatic carboxylic acids react under the conditions developed with good yields in all cases. Thiobenzoic acid is a good altern ative for microwave-assisted synthesis of 2-phenylbenzoxazole and 2-phenylbenzothiazole in the absence of solvents.

Keywords: carboxylate aminophenol solventfree cyclocondensation Lawesson reagent microwave; aminothiophenol carboxylate solventfree cyclocondensation Lawesson reagent microwave; benzoxazole preparation; benzothiazole preparation

Substances (56) Reactions (37) Citing (129)

49

Proceedings of ECSOC-10, 10th International Electron Conference on Synthetic Organic Chemistry held 1-30 November 2006

0 Substances • 0 Reactions • 0 Citations

By: Seijas, Julio A. ; Vazquez Tato, Pilar; Editors
2006, No pp. given | Language: English, Database: CAplus

There is no abstract available for this document.

Keywords: synthetic organic chem book

Substances (0) Reactions (0) Citing (0)

50

Oxazoline as a useful tool in organic synthesis: preparation of 4-aryl-1,2,3,4-tetrahydroisoquinoline alkaloid skeleton

11 Substances • 21 Reactions • 14 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Martinez, M. Montserrat; Pizzolatti, Moacir G.
Tetrahedron Letters (2005), 46(35), 5827-5830 | Language: English, Database: CAplus

New direct strategy for the synthesis of 4-aryl-1,2,3,4-tetrahydroisoquinolines. The key steps are based on oxazoline chem.: nucleophilic substitution in an (2-methoxyphenyl)oxazoline with a Grignard reagent and a 1, 6-conjugate addition of a lithium amide to [2-(1-phenylethenyl)phenyl]oxazoline.

Keywords: isoquinoline alkaloid skeleton preparation nucleophilic substitution conjugate addition; methoxyphenyloxazoline styrylmagnesium bromide nucleophilic substitution

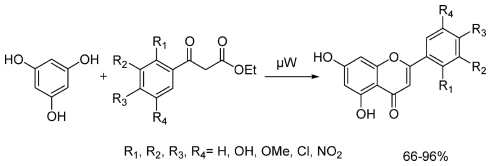
Substances (11) | Reactions (21) | Citing (14)

51

Solvent-free synthesis of functionalized flavones under microwave irradiation

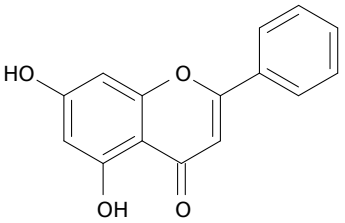
21 Substances • 10 Reactions • 110 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Carballido-Reboredo, Raquel
Journal of Organic Chemistry (2005), 70(7), 2855-2858 | Language: English, Database: CAplus and MEDLINE



Eco-friendly direct solvent-free synthesis of flavones, e.g., **I**, was achieved by microwave irradiation of phloroglucinol and β-keto esters. Heating with microwaves vs. under classical conditions was shown to be higher yielding, cleaner, and faster. The reaction went through a cycloaddition of an α-oxo ketene intermediate followed by an uncatalyzed thermal Fries rearrangement.

Keywords: phloroglucinol keto ester cyclization microwave irradiation; flavone preparation; microwave irradiation cyclization mediator



I

Substances (21) | Reactions (10) | Citing (110)

52

Effect of counterion on thermodynamic micellar properties of tetradecylpyridinium in aqueous solutions

2 Substances • 0 Reactions • 19 Citations

By: Galan, J. J.; Gonzalez-Perez, A.; **Seijas, J. A.**; Uriarte, E.; Rodriguez, J. R.
Colloid and Polymer Science (2005), 283(4), 456-460 | Language: English, Database: CAplus

Elec. conductivity of aqueous solutions of tetradecylpyridinium bromide and chloride has been measured as a function of surfactant molal concentration and temperature From the molal dependence of conductivity, the critical micelle concentration and the micellar ionization degree were estimated The temperature dependence of these parameters has been used for calcul ating the thermodn. parameters related with the micellization process by using the classical charged pseudo phase separation model. The effect of the counterion on the conventional thermodn. potentials of micelli zation such as standard Gibbs free energy, enthalpy and entropy has also been a matter of study. Finally, the occurrence of the enthalpy-entropy compensation phenomenon was verified and the relevant parameters discussed.

Keywords: counterion thermodn micelle tetradecylpyridinium aqueous solution cmc

Substances (2) | Reactions (0) | Citing (19)

53

Proceedings of the ECSOC-9, the Ninth International Electronic Conference on Synthetic Organic Chemistry held 1-30 November 2005

0 Substances • 0 Reactions • 0 Citations

By: **Seijas, Julio A.**; Vazquez-Tato, M. Pilar; Editors
2005, No pp. given | Language: English, Database: CAplus

There is no abstract available for this document.

Keywords: synthetic organic chem book

Substances (0) | Reactions (0) | Citing (0)

54

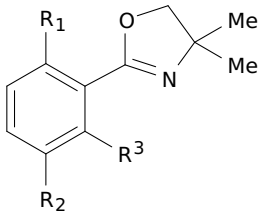
Synthesis of anacardic acids by nucleophilic substitution on 2-aryloxazolines

20 Substances • 13 Reactions • 7 Citations

By: Seijas, Julio A. ; Pilar Vazquez-Tato, M.; Montserrat Martinez, M.; Santiso, Veronica
Tetrahedron Letters (2004), 45(9), 1937-1939 | Language: English, Database: CAplus

A new direct synthesis for anacardic acids based on a nucleophilic substitution of a methoxy group in 2- aryloxazolines by long-chained Grignard reagents is reported. Thus, reacting (methoxy phenyl)oxazoline **I** (R^1 = H, R^2 = R^3 = MeO; R^1 = R^3 = MeO, R^2 = H) with $C_{11}H_{23}MgCl$ gave **I** (R^3 = $C_{11}H_{23}$).

Keywords: nucleophilic substitution aryloxazoline anacardic acid preparation; oxazoline aryl nucleophilic substitution anacardic acid preparation



I

Substances (20) Reactions (13) Citing (7)

55

Synthetic Organic Chemistry, ECSOC. (8th International Electronic Conference held 1-30 November 2004.)

0 Substances • 0 Reactions • 0 Citations

By: Seijas, Julio A. ; Vazquez Tato, M. Pilar; Editors
2004, No pp. given | Language: English, Database: CAplus

There is no abstract available for this document.

Keywords: synthetic organic chem book

Substances (0) Reactions (0) Citing (0)

56

Microwave enhanced synthesis of acridines. A new aspect in the Bernthsen reaction

16 Substances • 7 Reactions • 40 Citations

By: **Seijas, Julio A.** ; Vazquez-Tato, M. Pilar; Martinez, M. Montserrat; Rodriguez-Parga, Jacobo
Green Chemistry (2002), 4(4), 390-391 | Language: English, Database: CAplus

The Bernthsen reaction is studied using microwaves as the heat source. This leads to acridines with aromatic and aliphatic substi tuents in position 9, shortening reaction times and increasing yields, with a reduction in Lewis acid catalyst (Zn Cl_2), allowing a more environmentally friendly reaction.

Keywords: Lewis acid catalyst Bernthsen reaction acridine derivative microwave synthesis

Substances (16) Reactions (7) Citing (40)

57

Microwave promoted synthesis of a rehabilitated drug: Thalidomide

5 Substances • 2 Reactions • 38 Citations

By: **Seijas, Julio A.** ; Vazquez-Tato, M. Pilar; Gonzalez-Bande, Cristobal; Martinez, M. Montserrat; Pacios-Lopez, Beatriz
Synthesis (2001), (7), 999-1000 | Language: English, Database: CAplus

A new direct synthesis of thalidomide in high yield by microwave irradi ation of N-phthaloyl-L-glutamic in the presence of thiourea is described. Thalidomide was also obtained in good yield from L-glutamic acid, phthalic anhydride and thiourea in a one- pot procedure.

Keywords: thalidomide preparation

Substances (5) Reactions (2) Citing (38)

58

β-Phenylethylamines, indolines and isoquinolones via hydroamination of styrenes by microwave irradiation

17 Substances • 9 Reactions • 23 Citations

By: **Seijas, Julio A.** ; Vazquez-Tato, M. Pilar; Martinez, M. Montserrat
Synlett (2001), (6), 875-877 | Language: English, Database: CAplus

Microwave irradiation promotes hydroamination of styrenes. This method can be used as a direct way of producing different kinds of bioactive compounds: open chain compounds like β-phenylethylamines or cyclized products like indolines or isoquinolones.

Keywords: hydroamination styrene microwave irradi ation

Substances (17) Reactions (9) Citing (23)

59

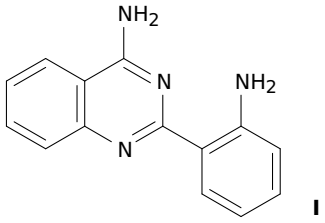
Microwave-enhanced synthesis of 4-aminoquinazolines

20 Substances • 10 Reactions • 104 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Martinez, M. Montserrat
Tetrahedron Letters (2000), 41(13), 2215-2217 | Language: English, Database: CAplus

Aromatic nitriles react with anthranilonitrile in a domestic microwave oven to afford good yields of the corresp onding 4-aminoquin azolines, e.g. **I**, in a very short irradi ation time.

Keywords: quinazolinamine preparation; anthranilonitrile aromatic nitrile microwave assisted cyclocond ensation



I

Substances (20) Reactions (10) Citing (104)

60

Complexation of Sodium Cholate and Sodium Deoxycholate by β-Cyclodextrin and Derivatives

8 Substances • 0 Reactions • 33 Citations

By: Ramos Cabrer, P.; Alvarez-Parrilla, E.; Meijide, F.; Seijas, J. A. ; Rodriguez Nunez, E.; Vazquez Tato, J.
Langmuir (1999), 15(17), 5489-5495 | Language: English, Database: CAplus

The complexation behavior of two bile salts-sodium cholate (NaC) and sodium deoxycholate (NaDC)-with β-cyclodextrin (β-CD), 6-deoxy-6-amino-β-cyclodextrin (β-CDNH$_2$), and dimer I (N,N'-bis(6-deoxy-β-cyclodextrin)pyromellic acid diamide) was studied by N M R techniques. Complexes formed between β-CD and β-CDNH$_2$ with NaC and NaDC have 1:1 and 2:1 (host:guest) stoichiometries, resp. Complexes with β-CDNH$_2$ show higher equili brium constants than those with β-CD because of the electrostatic effect of the protonated amine group. Dimer I showed 1:2 and n:n stoichiometries with NaC and NaDC, resp. ROESY spectra indicated that bile salts enter first with their 5-C ring toward the inner cavity by the side of the secondary hydroxyl groups of cyclode xtrins. In the complexes formed with β-CDNH$_2$, the steroid body of the bile salt enters deeper into the cavity, while the carbox ylated side chain is extended toward the protonated amine group at C-6, allowing an electrostatic interaction between both groups. In complexes with 2:1 stoichiometry, the second cyclodextrin complexes with ring A of the steroid body.

Keywords: bile salt complex beta cyclodextrin dimer; beta cyclodextrin complex sodium cholate deoxycholate

Substances (8) Reactions (0) Citing (33)

61

Direct synthesis of imides from dicarboxylic acids using microwaves

23 Substances • 13 Reactions • 54 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Martinez, M. Montserrat; Nunez-Corredoira, Gonzalo
Journal of Chemical Research, Synopses (1999), (7), 420-421 | Language: English, Database: CAplus

1,4- And 1,5-dicarboxylic acids, when treated with amines in a domestic microwave oven, afford good yields of the corresp onding imides. For example, the reaction of butanedioic acid with aniline gave 1- phenyl-2,5-pyrrolidinedione. The reaction of 2-carboxyben zeneacetic acid with aniline gave 2- phenyl-1,3(2*H*,4*H*)-isoquinolinedione.

Keywords: imide preparation; phenylsuccinimide phenylpyrrolidinedione preparation; pyrrolidinedione hydroxypyrrolidinedione phenyl preparation; isoquinolinedione phenyl preparation

Substances (23) Reactions (13) Citing (54)

62

Synthesis of β-phenylethylamines from styrene derivatives

0 Substances • 0 Reactions • 0 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Entenza, Cesar; Martinez, M. Montserrat; Onega, M. Gabriela; Veiga, Susana
Tetrahedron Letters (1998), 39(35), 6261 | Language: English, Database: CAplus

There is no abstract available for this document.

Substances (0) Reactions (0) Citing (0)

63

Synthesis of β-phenylethylamines from styrene derivatives

50 Substances • 34 Reactions • 40 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Entenza, Cesar; Martinez, M. Montserrat; Onega, M. Gabriela; Veiga, Susana
Tetrahedron Letters (1998), 39(28), 5073-5076 | Language: English, Database: CAplus

β-Phenylethylamines are prepared from the styrene deriva tives, such as 4,4-dimethyl-2-(2-vinylphenyl)-2-oxazoline, 2-(3-methoxy-2-vinylphenyl)-4,4-dimethyl-2-oxazoline, 2-vinylbenzoic acid, styrene, β-methylstyrene, and α-methylstyrene. For example, the addition of diethylamine to 2-(2-vinylphenyl)-4,5-dihydro-4,4-dimethyloxazole gave 2-(4,5-dihydro-4,4-dimethyl-2-oxazolyl) benzeneethanamine.

Keywords: phenylethylamine benzeneethanamine preparation; styrene vinylbenzene ethenylbenzoate amination addition

Substances (50) Reactions (34) Citing (40)

64

1,6-Conjugate addition to o-vinylphenyloxazolines. Syntheses of chuangxinol and 3-n-butylphthalide

7 Substances • 5 Reactions • 10 Citations

By: Martinez, M. Montserrat; Onega, M. Gabriela; Fe Tellado, M.; **Seijas, Julio A.**; Vazquez-Tato, M. Pilar
Tetrahedron (1997), 53(41), 14127-14130 | Language: English, Database: CAplus

Phtalhides are prepared from o-vinylphenyloxazolines in one pot reaction by 1,6-conjugate addition of alkyllithium and trapping of the benzylic anion with MoOPH, followed by hydrolysis with aqueous oxalic acid. This method was applied to the syntheses of two natural products: chuangxinol and 3-n-butylphthalide.

Keywords: chuangxinol butylphthalide synthesis; conjugate addition alkyllithium vinylphenyloxazoline

Substances (7) | Reactions (5) | Citing (10)

65

Synthesis, affinity at 5-HT_{2A}, 5-HT_{2B} and 5-HT_{2C} serotonin receptors and structure-activity relationships of a series of cyproheptadine analogs

22 Substances • 18 Reactions • 15 Citations

By: Honrubia, Maria Angeles; Rodriguez, Jesus; Dominguez, Rosa; Lozoya, Estrella; Manaut, Francesc; **Seijas, Julio A.**; Villaverde, Maria Carmen; Calleja, Jose M.; Cadavid, Maria Isabel
Chemical & Pharmaceutical Bulletin (1997), 45(5), 842-848 | Language: English, Database: CAplus and MEDLINE

Cyproheptadine (Cyp) is a drug that shows high affinity for type 2 (5-HT_2)receptors. The authors studied a series of compounds obtained by modification of the tricyclic system of Cyp (dibenzocycloheptadiene ring) to make the thioxanthene, xanthene, dihydrodibenzocycloheptadiene, di-Ph, fluorene, and phenylmethyl analogs. Their activities at the rat cerebral cortex 5- HT_{2A} receptor were (pK_i):8.80 (Cyp), 8.60 (thioxanthene analog), 8.40 (xanthene analog), 8.05 (dihydrodibenzocycloheptadiene analog), 7.87 (di-Ph analog), 6.70 (fluorene analog) and 6.45 (phenyl methyl analog); those at the rat stomach fundus 5- HT_{2B} receptor (pA_2) were: 9.14 (Cyp), 8.49 (thioxanthene analog), 7.58 (xanthene analog), 7.02 (dihydrodibenzocycloheptadiene analog), 6.07 (di-Ph analog), and undetectable (fluorene analog, phenylmethyl analog); and those at the pig choroidal plexus 5- HT_{2C} receptor (pK_i) were: 8.71 (Cyp), 8.68 (thioxanthene analog), 8.58 (xanthene analog), 7.95 (dihydrodibenzocycloheptadiene analog), 7.57 (di-Ph analog), 6.98 (fluorene analog) and 6.63 (phenylmethyl analog). The slopes did not differ signifi cantly from unity. The compounds exhibited the same order of activities at every type of receptor, and the most active mols. presented certain steric (butterfly conformation of the tricyclic system) and electrostatic (proton affinity on the top of the central rings) patterns. It is concluded that the activity of cyproheptadine derivatives at 5-HT_2 receptors is related to these mol. features, which make feasible a common dispos ition to interact with all three 5-HT_2 subtypes.

Keywords: cyproheptadine analog preparation serotonin receptor affinity; serotonin receptor affinity cyprohe ptadine analog structure

Substances (22) | Reactions (18) | Citing (15)

66

Synthesis of (3S,5S)-quinuclidine-3,5-diol and of [3S-(3α,3aα,7aα)]-octahydro-2-furo[2,3-c]pyridinol from D-arabinose

34 Substances • 238 Reactions • 22 Citations

By: Vazquez-Tato, M. Pilar; Seijas, Julio A.; Fleet, George W. J.; Mathews, Christopher J.; Hemmings, Philippa R.; Brown, David
Tetrahedron (1995), 51(3), 959-74 | Language: English, Database: CAplus

The synthesis of (3S,5S)-quinuclidine-3,5-diol is achieved by an introd uction of a 2 carbon chain at C- 3 of D-arabinose, followed by joining the terminus of the chain extension to C-1 and C-5 of the sugar; the synthesis of [3 S-(3α,3aα,7aα)]-octahydro-2-furo[2,3-c] pyridinol, a potential muscarine mimic, is described.

Keywords: furopyridinol octahydro; quinuclidinediol; arabinose synthon bicyclic nitrogen hetero cycle

Substances (34) Reactions (238) Citing (22)

67

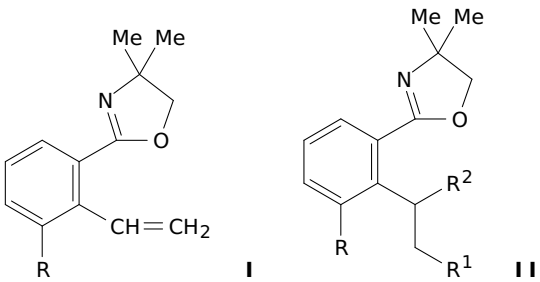
Reactivity of o-styryloxazolines with nucleophiles

16 Substances • 12 Reactions • 14 Citations

By: Seijas, Julio A.; Vazquez-Tato, M. Pilar; Castedo, Luis; Estevez, Ramon J.; Ruiz, Maria
Journal of Organic Chemistry (1992), 57(20), 5283-4 | Language: English, Database: CAplus

The *o*-styryloxazolines **I** (R = MeO, H) react with organolithium reagents affording, as a result of conjugate addition to the exocyclic double bond, substituted benzenes **II** (R = MeO, R^1 = Bu, Me_3C, Me, H, Ph, R^2 = Me, H; R = H, R^1 = Bu, Me_3C, Me, R^2 = Me) in good yields. The presence of a methoxy substituent in position 3 of the benzene ring enhances reacti vity. **I** (R = MeO) reacts with aryl- and alkyllithium reagents, while **I** (R = H) (no MeO in the ring) reacts only with alkyll ithium reagents.

Keywords: styryloxazoline addition nucleophile; oxazoline styryl addition nucleo phile



Substances (16) Reactions (12) Citing (14)

68

Synthesis of pyrrolizidines via copper(I) catalyzed radical atom transfer cyclization. [Erratum to document cited in CA116(25):255857r]

12 Substances • 8 Reactions • 0 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Castedo, Luis; Estevez, Ramon J.; Onega, M. Gabriela; Ruiz, Maria
Tetrahedron (1992), 48(35), 7057 | Language: English, Database: CAplus

Errors in the ^{1}H NMR spectrum of (1R,8S)-1-chloromethyl-2-dichloro-3-oxo-hexahydropyrrolizidine have been corrected The errors were not reflected in the abstract or the index entries.

Keywords: erratum trachelanthamidine synthesis; pseudoheliotridane synthesis erratum; pyrrolizidine alkaloid erratum; cyclization trichloroacetylvinylpyrrolidine copper catalyst erratum; radical transfer cyclization erratum

Substances (12) Reactions (8) Citing (0)

69

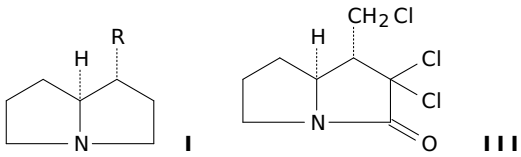
Synthesis of pyrrolizidines via copper(I) catalyzed radical atom transfer cyclization

12 Substances • 19 Reactions • 42 Citations

By: Seijas, Julio A. ; Vazquez-Tato, M. Pilar; Castedo, Luis; Estevez, Ramon J.; Onega, M. Gabriela; Ruiz, Maria
Tetrahedron (1992), 48(9), 1637-42 | Language: English, Database: CAplus

Trachelanthamidine (**I**, R = CH_2OH) and pseudoheliotridane (**I**, R = Me) were synthesized from (2*S*)-*N*-trichloroacetyl-2-vinylpyrrolidine (**II**) by a 5-exo-trig radical cyclization. The intermediate radical is generated heating **II** in a sealed tube (CH_3CN/160°C) using CuCl as catalyst and the cyclization occurs in very good yield (93%). Cyclized product **III** is transformed either into (-)-trachelanthamidine (55% yield from **II**) or into (-)-pseudoheliotridane (42% yield from **II**).

Keywords: trachelanthamidine synthesis; pseudoheliotridane synthesis; pyrrolizidine alkaloid; cyclization trichloroacetylvinylpyrrolidine copper catalyst; radical transfer cyclization



I III

Substances (12) Reactions (19) Citing (42)

70

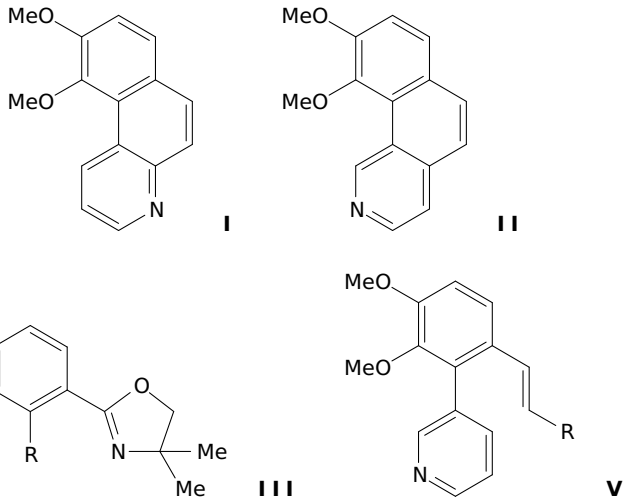
A new synthesis of azaphenanthrenes

14 Substances • 41 Reactions • 7 Citations

By: Castedo, Luis; Cid, M. Magdalena; Seijas, Julio A.; Villaverde, M. Carmen
Tetrahedron Letters (1991), 32(31), 3871-2 | Language: English, Database: CAplus

A new synthesis of azaphenanthrenes **I** and **II** starting from aryloxazoline **III** (R = OMe) is reported. Lithiation of 3-bromopyridine, followed by coupling with **III** (R = OMe) gave **III** (R = 3-pyridinyl) (**IV**). Hydrolysis of **IV**, followed by esterification, $LiAlH_4$ redn, and Swern oxidation, and Wittig reaction gave styrenes **V** (R = H, Br). **V** were then irradiated to give **I** and **II**.

Keywords: azaphenanthrene dimethoxy; benzisoquinoline dimethoxy; benzoquinoline dimethoxy; pyridylstyrene preparation photochem cyclization



Substances (14) | Reactions (41) | Citing (7)

71

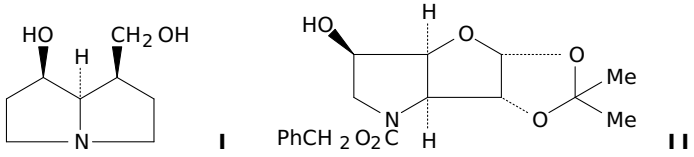
Synthesis of the necine base platynecine from glucose

14 Substances • 22 Reactions • 13 Citations

By: Fleet, George W. J.; Seijas, Julio A.; Vazquez-Tato, M. Pilar
Tetrahedron (1991), 47(3), 525-30 | Language: English, Database: CAplus

A synthesis of platynecine (**I**) from an intermediate **II** is described which has previously been used for the synthesis of the enantiomers of retronecine; the stereochem. of the necine base is determined by the formation of a tricyclic amide interme diate.

Keywords: platynecine synthesis



Substances (14) | Reactions (22) | Citing (13)

72

Reactivity of heteroaromatic aldehydes with low valent titanium

26 Substances • 11 Reactions • 3 Citations

By: Castedo, Luis; Cid, M. Magdalena; Dominguez, Rosa; **Seijas, Julio A.**; Villaverde, M. Carmen
Heterocycles (1990), 31(7), 1271-4 | Language: English, Database: CAplus

Ti-catalyzed coupling reaction of aromatic hetero cycles was studied. Coupling of 4-pyridinecarboxaldehyde gave exclusively the reduced product, i.e., 1,2-bis(4-pyridyl)ethane, while 3-pyridinecarboxaldehyde gave both 1,2-bis(3-pyridyl)ethene and 1,2-dihydroxy-1,2-bis(3-pyridyl)ethane. Coupling of 3-bromo-4-pyridine-, 2- and 3-thiophene-, 3-furan-, and *N*-acyl-2-pyrrolecarboxaldehydes gave the corresponding bis(heteroaryl)ethenes, and 1-methyl-2-imidazolecarboxaldehyde gave the -ethane. Thus, compounds with low electron d. at the benzylic position gave reduced products.

Keywords: coupling heteroaromatic aldehyde titanium catalysis; pyridinecarboxaldehyde coupling reduction titanium catalysis; ethene bisheteroaryl; electronic effect coupling reduction heteroa romatic aldehyde

Substances (26) | Reactions (11) | Citing (3)

73

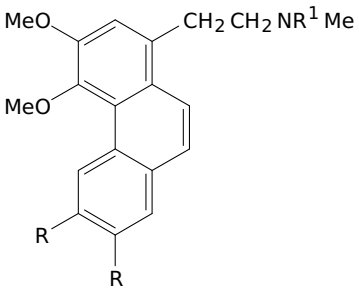
New total synthesis of phenanthrene alkaloids

23 Substances • 23 Reactions • 13 Citations

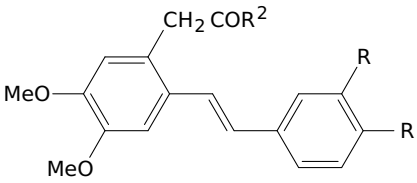
By: Estevez, Juan C.; Villaverde, M. Carmen; Estevez, Ramon J.; **Seijas, Julio A.**; Castedo, Luis
Canadian Journal of Chemistry (1990), 68(6), 964-8 | Language: English, Database: CAplus

A new synthesis of phenanthrene alkaloids **I** (R = H, O Me; R^1 = H, Me) is based on the photocyc lization of stilbene **II** (R^2 = OMe, NH_2) prepared by Friedel-Crafts reaction of 3,4-$(MeO)_2C_6H_3CH_2CO_2Me$ with 3,4-$R_2C_6H_3COCl$, reduction, and dehydration.

Keywords: phenanthrene alkaloid; aminoethylphenanthrene; stilbene intramol photochem cycload dition



I



II

Substances (23) | Reactions (23) | Citing (13)

74

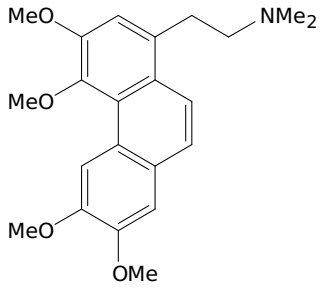
N-Methylsecoglaucine, a new phenanthrene alkaloid from fumariaceae

8 Substances • 8 Reactions • 7 Citations

By: Blanco, Olga; Castedo, Luis; Cid, Magdalena; **Seijas, Julio A.**; Villaverde, Carmen
Heterocycles (1990), 31(6), 1077-80 | Language: English, Database: CAplus

The isolation and its total synthesis of the new phenanthrene alkaloid *N*-methylsecoglaucine (**I**) from *Platycapnos spicata* are reported.

Keywords: secoglaucine methyl Platycapnos; methylsecoglaucine Platycapnos isolation total synthesis; fumariaceae methylsec oglaucine



I

Substances (8) Reactions (8) Citing (7)

75

A new simple route to styryl amides

16 Substances • 15 Reactions • 9 Citations

By: Estevez, J. C.; Villaverde, M. C.; Estevez, R. J.; **Seijas, J. A.**; Castedo, L.
Synthetic Communications (1990), 20(4), 503-7 | Language: English, Database: CAplus

Treatment of $BzNHCH_2CH_2C_6H_3RR^1$-3,4 (R = R^1 = H, OMe; R = H, R^1 = OMe) with DDQ and AcOH gave $BzNHCH_2CH(OAc)C_6H_3RR^1$-3,4 quant. Thermolysis of the latter at 250° gave 3:1 *E*-*Z* mixtures of $BzNHCH{:}CHC_6H_3RR^1$-3,4.

Keywords: styrylbenzamide; phenethylbenzamide acetoxylation; amide styryl; benzamide acetoxyp henethyl preparation thermal elimination

Substances (16) Reactions (15) Citing (9)

76

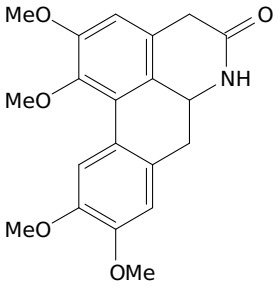
Total synthesis of oxoaporphines

10 Substances • 24 Reactions • 2 Citations

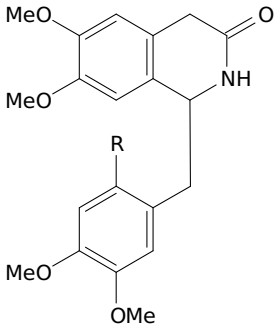
By: Castedo, L.; Estevez, J. C.; Estevez, R. J.; Seijas, J. A.; Vazquez Tato, M. P.; Villaverde, M. C.
Anales de Quimica (1990), 86(7), 805-7 | Language: Spanish, Database: CAplus

The total synthesis of oxoaporphine derivative **I** from benzyltetrahydroisoquinolone **II** (R = H) was investigated by two routes. Pschorr cyclization of **II** (R = NH_2) did not lead to **I** and photolysis of **II** (R = iodo) gave norpontevedrine. The synthesis of **II** (R = H) is described.

Keywords: oxoaporphine methoxy; aporphine oxo; isoquinolone benzyltetrahydro preparation reaction



I



II

Substances (10) | Reactions (24) | Citing (2)

77

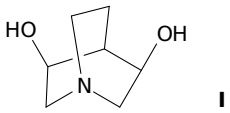
Complex quinuclidines (1-azabicyclo[2.2.2]octanes) from sugars: synthesis of (1α,3α,4α,5α)-quinuclidine-3,5-diol from D-glucose

19 Substances • 47 Reactions • 3 Citations

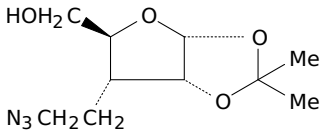
By: Fleet, George W. J.; Mathews, Christopher J.; Seijas, Julio A.; Vazquez Tato, M. P.; Brown, David
Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1989), (5), 1067-8 | Language: English, Database: CAplus

The synthesis of (1α,3α,4α,5α)-quinuclidine-3,5-diol (**I**) from D-glucose by 2 alternative ring closures is described. Azido alc. **II** is a key intermediate.

Keywords: quinuclidinediol; glucose conversion quinuclidinediol



I



II

Substances (19) | Reactions (47) | Citing (3)

78

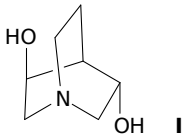
Chiral quinuclidines (1-azabicyclo[2.2.2]octanes) from sugars: synthesis of (3S,5S)-quinuclidine-3,5-diol from D-arabinose

16 Substances • 16 Reactions • 5 Citations

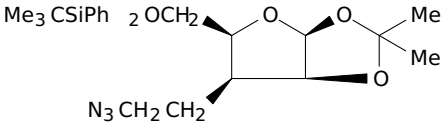
By: Fleet, George W. J.; Mathews, Christopher J.; Seijas, Julio A.; Vazquez Tato, M. P.; Brown, David J.
Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1989), (5), 1065-6 | Language: English, Database: CAplus

The synthesis of (3*S*,5*S*)-quinuclidine-3,5-diol (**I**) from D-arabinose by 2 alternative ring closures is described. Protected *lyxo*-furanose **II** is the key intermediate.

Keywords: chiral quinuclidinediol; arabinose conversion chiral quinuclidinediol



I



II

Substances (16) Reactions (16) Citing (5)

79

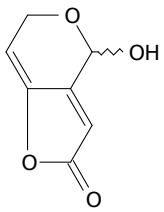
New total synthesis of patulin

11 Substances • 21 Reactions • 8 Citations

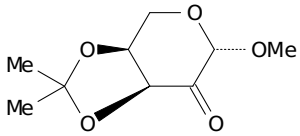
By: Seijas, Julio A.; Vazquez Tato, M. Pilar; Estevez, Ramon; Castedo, Luis; Riguera, Ricardo
Heterocycles (1989), 29(1), 181-4 | Language: English, Database: CAplus

Patulin (**I**) was prepared in 23% overall yield from L-arabinose via Wittig reaction of pentopyranosidulose **II**.

Keywords: patulin total synthesis; arabinose synthon patulin



I



II

Substances (11) Reactions (21) Citing (8)

80

Oxidation with Fremy's salt of aryl oximes and benzylamine to carbonyl compounds

32 Substances • 16 Reactions • 0 Citations

By: Vazqueztato, M. P.; **Seijas, J. A.**; Castedo, L.; Riguera, R.
Anales de Quimica, Serie C: Quimica Organica y Bioquimica (1988), 84(3), 374-5 | Language: Spanish, Database: CAplus

The oxidation of aryl oximes ArCR:NOH (Ar = aryl, R = H, Me) and benzyl amines with Fremy's salt, $(KO_3S)_2NO$, afforded carbonyl compounds in good yields. The reaction proceeds via a benzylic radical. Aliphatic oximes and amines do not react under these conditions.

Keywords: oxidation aryl oxime benzylamine Fremys salt; carbonyl compound aromatic; acetop henone methoxy; benzoic acid methoxy

Substances (32) | Reactions (16) | Citing (0)

81

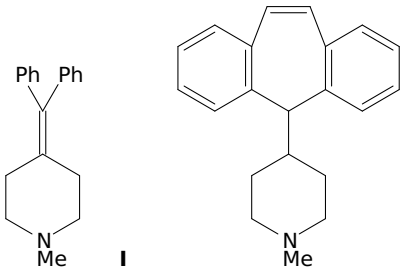
New synthesis of cyproheptadine and related compounds using low valent titanium

22 Substances • 23 Reactions • 14 Citations

By: Cid, M. M.; **Seijas, J. A.**; Villaverde, M. C.; Castedo, L.
Tetrahedron (1988), 44(19), 6197-200 | Language: English, Database: CAplus

A simple method is described for the preparation of biphenylmethylenepiperidine (**I**), cyproheptadine (**II**) and related compounds based on asym. dicarbonyl coupling of two suitable ketones with low valent titanium. Thus, Ph_2CO and *N*-ethoxycarbonyl-4-piperidone gave **I** after reduction of the cross-coupling product.

Keywords: biphenylmethylenepiperidine; piperidine diphenylmethylene; cyproheptadine; reductive dicarbonyl coupling benzop henone piperidone; suberenone reductive dicarbonyl coupling piperidone



I **II**

Substances (22) | Reactions (23) | Citing (14)

82

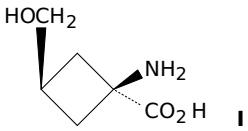
Synthesis of cis- and trans-1-amino-3-(hydroxymethyl)cyclobutane-1-carboxylic acids

5 Substances • 6 Reactions • 0 Citations

By: Fleet, George W. J.; **Seijas, Julio A.**; Vazquez Tato, M. P.
Tetrahedron (1988), 44(7), 2077-80 | Language: English, Database: CAplus

The stereospecific synthesis of the title compounds **I** and **II** from bicyclo compd **III** is described.

Keywords: aminohydroxymethylcyclobutanecarboxylic acid; cyclobutanecarboxylic acid amino hydroxymethyl



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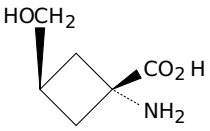
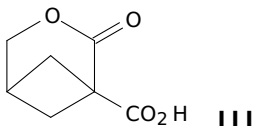


II



III

Substances (5) | Reactions (6) | Citing (0)

83

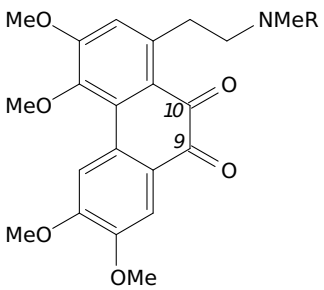
A direct conversion of phenanthrenes to aporphinoids

17 Substances • 31 Reactions • 5 Citations

By: **Seijas, Julio A.**; Rodriguez de Lera, Angel; Villaverde, Carmen; Castedo, Luis
Heterocycles (1985), 23(12), 3079-84 | Language: English, Database: CAplus

The (aminoethyl)phenanthrenediones **I** (R = H, C OCF$_3$), prepared by oxidation of the corresp onding 9,10-unsaturated derivatives, were cyclized by treatment with Na_2CO_3 to give aporphinoids **II** and **III**.

Keywords: phenanthrenedione aminoethyl cyclization; aporphinoid; cyclization aminoethylphenanthrenedione



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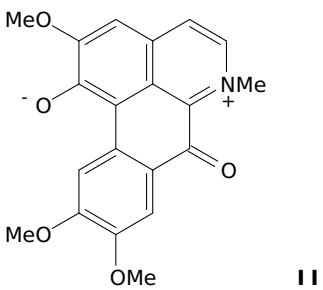
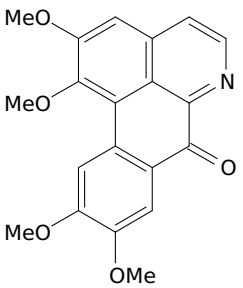


II



III

Substances (17) | Reactions (31) | Citing (5)

84

4,5-O-Substituted phenanthrenes from cyclophanes. The total synthesis of cannithrene II

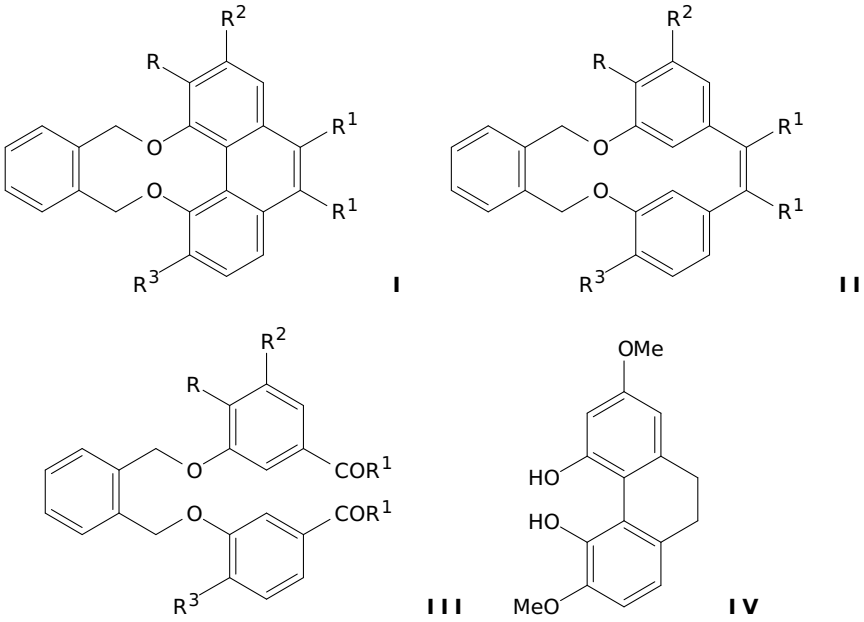
28 Substances • 63 Reactions • 28 Citations

By: Ben, Ines; Castedo, Luis; Saa, Jose M.; Seijas, Julio A.; Suau, Rafael; Tojo, Gabriel

Journal of Organic Chemistry (1985), 50(13), 2236-40 | Language: English, Database: CAplus

A new procedure for the synthesis of phenathrenes **I** (R = OMe, R^1 = R^2 = H, R^3 = H, OMe; R = R^1 = H, R^2 = R^3 = H, OMe; R = R^2 = R^3 = H, R^1 = Me) is based on the regiose lective cyclization of the conformationally rigid *cis*-stilbene moiety of a cyclophane **II**. **II** were obtained by the intramol. reductive carbonyl coupling of dicarbonyl compounds **III** by active Ti. This new approach was succes sfully applied to obtain cannithrene II (**IV**).

Keywords: phenathrenediol ether; cannithrene 2; cyclophane photochem ring closure



Substances (28) | Reactions (63) | Citing (28)

85

Reductive dicarbonyl coupling with low-valent titanium reagents: a new entry to phenanthrene alkaloids

13 Substances • 25 Reactions • 6 Citations

By: Seijas, Julio A.; De Lera, Angel R.; Villaverde, M. Carmen; Castedo, Luis

Journal of the Chemical Society, Chemical Communications (1985), (12), 839-40 | Language: English, Database: CAplus

Phenanthrene alkaloids were prepared using a low-valent Ti reagent which is compatible with ethoxyc arbonyl as the N-protecting group. E.g., atherosperminine was prepared in 5 steps from 6, 7-dimethoxy-3,4-dihydroisoquinoline. The key step was the mixed reductive coupling of 6,4,3-HCO$(MeO)_2C_6H_2(CH_2)_2NMeCO_2Et$ with PhCHO in the presence of $TiCl_3$ and Li in refluxing $(MeOCH_2)_2$ to give 55% (*E*)-6,4,3-PhCH:CH$(MeO)_2C_6H_2(CH_2)_2NMeCO_2Et$.

Keywords: phenanthrene alkaloid preparation; atherosperminine

Substances (13) | Reactions (25) | Citing (6)