and its outcomes may be also used to constraint the generation of more reliable structural models. The method has been applied to a large number of protein test structures, showing a good discriminant power with respect to the complexity of the structure, the space group symmetry and the presence of additional beta domains. The accuracy in the determination of the direction of the alpha helix depends on its length, and only helices greater than ten residues may be found with a reliable precision. The automatic procedure has been tested in Matlab and will be included in the software package ILMILIONE, devoted to protein crystal structure solution [3].

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Keywords: alpha-helix, patterson map, pattern recognition

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Structural and computational analysis of 3,6-dioctyloxiphenyl-2,5-dimethyl-1,4-diketopyrrolo[3,4-c]pyrrole-1,4-dione

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Diketodiphenylpyrrolopyrroles are industrially important red pigments[1]. The success of these compounds as pigments relies, in part, on their high light fastness and very low solubility in most common solvents.

The title compound was synthesized, structural and spectroscopic properties were investigated. Molecular and crystal structure of 3,6-dioctyloxiphenyl-2,5-dimethyl-1,4-diketopyrrolo[3,4-c]pyrrole-1,4-dione, $C_{36}H_{48}N_2O_4$, have been determined by single crystal X-ray diffraction study. The title compound is triclinic, with *a*=6.2419(6) Å, *b*= 9.5847 (9) Å, *c*=13.4568 (8) Å, α=106.573(7) °, β=94.244(6)°, γ=93.154(8)°; Z=1, D_x=1.24 g/cm^3, μ(CuK_α)=0.08 mm^{-1}, and space group is P-1. The structure was solved by direct methods and refined to a final R=0.055 for 3214 reflections with I>2σ(I). The structure is devoid of classical hydrogen bonds. However, there are two intra-molecular weak interactions between C9-H9···O2 and its inversion counterpart C9^i-H9^i···O2^i (Symmetry code i: 4-x, 1-y, 1-z), with the geometrical parameters: D-A=3.06 Å, H···A= 2.18 Å, D-H···A=158 °.

Optimized geometry and NMR spectra of the title compound were investigated and analyzed using DFT at B3LYP functional by 6-31g(d) basis set. Experimental and computational NMR spectra were determined and compared.

Computational and crystallographic results, NMR spectra and molecular geometry, are in good agreement. RMSD (Root Mean Square Distance) value between crystallographic result and optimized geometry is 9,507·10^{-3}Å. The geometry of diketopyrrolopyyrole ring is in agreement with previous study [2, 3].

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Keywords: diketopyrrolopyrroles, crystal structure, dye-pigment.

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Automatic structure determination for small molecule crystallography

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When the automatic structure determination algorithm was proposed over two decades ago [1], it had some technical problems. For example, it took more than a half day to solve a structure because of the limited capability of computers at that time. Recently, the situation has dramatically been changed. We can solve the structure of a small molecule several tens of seconds or sometimes in a few seconds. We have developed a software, AutoSolve, for small molecule crystallography to determine structures automatically.

AutoSolve was designed for organic and metal-organic compounds. This software uses SIR [2] as a direct method and SHELXL[3] as a refinement tool. In addition, we have incorporated a feature to switch among direct methods, SIR, SHELXS and Superflip[4] when a method does not give an initial structure.

In the initial step, AutoSolve assumes all atoms as carbons except heavy atoms and executes refinement by using SHELXL. After that, AutoSolve assigns atoms by taking temperature factors (Biso/Beq), bond distances, and chemical valencies into account. AutoSolve decides when to convert temperature factors to anisotropic and when to add hydrogen atoms by checking the R1 value in every refinement cycle. Finally, the hydrogen atoms are generated by using the SHELXL's HFIX command. Our algorithm follows the conventional structure determination procedure but it gives good results.

In order to evaluate the performance, we picked up 50 samples from Acta Cryst. C and ran AutoSolve. We did not get good results for inorganic compounds. However, AutoSolve gave structures close to final structures for organic compounds with success rate of about 100% and 60% for organic and metal-organic compounds, respectively.

AutoSolve can reach nearly a complete structure in a few seconds or several tens of seconds, except for inorganic compounds.

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Partial observations, partial models and partial residuals in least squares refinement

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Certain features of the standard use of least squares methods should cause concern as they are the result of a number of misconceptions. In particular one has to seriously question the use of a global scale, *K*, to assess errors in variables by creating a variance-covariance matrix **M** as *K* times the inverse of the matrix used to describe the least squares equations. There is also the oversight of not calculating variances for components of the model of the observations, the failure to take sufficient notice of how information is distributed in the observations and how easy it is to make mistakes in the description of twins, powders and pseudo symmetric structures that will not self correct during refinement. Ideas have been developed using partial observations, partial models and partial residuals that suggest how to better identify