Structural resolutions of 3-Arylamino and 3-alkoxy-nor-Beta-Lapachone derivatives with cytotoxicity against cancer cells lines

C. A. De Simone,[a,e] E. N. da Silva Júnior,[b] C. F. de Deus,[b] J. B. L. Martins,[b] A. B. Lima,[b] B. C. Cavalcanti,[c] C. Pessoa,[c] L. V. Costa-Lotufo,[c] R. C. Montenegro,[c] M. O. de Moraes,[c] M. do Carmo F. R. Pinto,[d] C.K. Z. Andrade,[b] M. O. F. Goulart,[e] and A. V. Pinto.[d]

[a] Instituto de Física da USP, São Carlos SP, CEP 13560-160, Brasil. e-mail: casimone@ifsc.usp.br
[b] Instituto de Química,Universidade de Brasília, Brasília DF, CEP 70910-970, Brasil.
[c] Universidade Federal do Ceará, Fortaleza CE, CEP 60430-270, Brasil.
[d] Núcleo de Pesquisas em Produtos Naturais, UFRJ,Rio de Janeiro RJ, CEP 21944-971, Brasil.
[e] Instituto de Química e Biotecnologia, UFAL, Maceió AL, 57072-970, Brasil.

Keywords: *Lapachol, naphthodihydrofuranquinones ,arylamino, X-ray Diffraction.*

Quinonoid compounds in the last times have been having great interest due to their multiple biological activities that are endowed[1]. The number of reports concerning the biological evaluation of new naturally occurring quinones and semi-synthetic analogues containing naphthalenic type structures (NQs) are constantly increasing in the pertinent literature[2]. With the aim of discovering cytotoxic naphthoquinones, in the last years, were synthesized and evaluated the pharmacological activity of naphthodihydrofuranquinones obtained from nor-lapachol and arylamino derivatives of nor-β-lapachone [3] .In this work the structures of four compounds of this series were performed using X-ray diffraction.

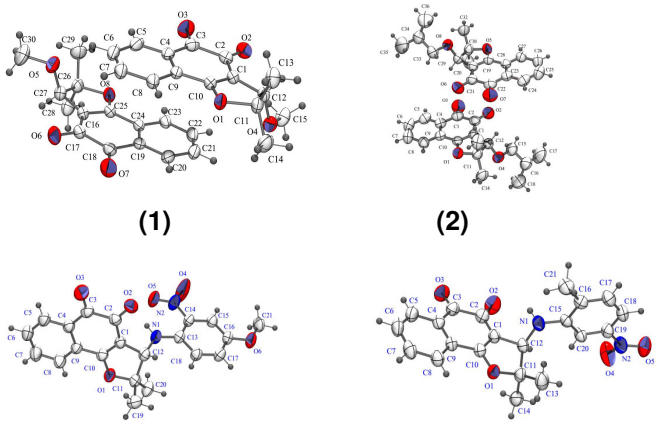
X-ray diffraction data collections for all the compounds were performed on an Enraf-Nonius Kappa-CCD diffractometer (95 mm CCD camera on κ-goniostat) using graphite monochromated MoKα radiation (0.71073 Å), at room temperature. The structure of compounds were solved by direct methods with SHELXS-97 and the models were refined by full-matrix least squares on F^2 using SHELXL-97[4].

Crystal Data (1): $C_{15}H_{14}O_4$, M=258.3, D_x= 1.32 g. cm^{-3}, a=7.3350(2), b=10.1350(5), c= 18.2510(6) Å, α=97.052(2),β=93.12(3),γ=104.100(2)°, V=1300.8 (8)$Å^3$,triclinic P-1, Z= 4, F(000) =544, μ= 0.09 mm^{-1}, S= 1.037, R_1=0.06 for 4043 reflections with I.>4σ(I) and 343 refined parameters.

Crystal Data (2): $C_{18}H_{19}O_4$,M= 299.3, D_x= 1.23 $g.cm^{-3}$, a=9.2360(3),b=18.0740(6),c=19.4330(3)Å, V=3243.9(2)$Å^3$,orthorhombic Pbn2_1, Z=8 ,F(000) =1272, μ= 0.09 mm^{-1}, S= 1.054, R_1=0.05 for 4247 reflections with I.>4σ(I) and 397 refined parameters.

Crystal Data (3): $C_{21}H_{18}N_2O_6$, M= 394.4, D_x= 1.41 $g.cm^{-3}$, a=8.0284(4),b=11.4548(5),c=12.1526(6)Å, α=62.49(4),β= 76.73(3),γ=69.54(3)° ,V=1224.0(8) $Å^3$,triclinic P-1, Z=2 ,F(000)=412, μ= 0.11 mm^{-1}, S= 1.029, R_1=0.06 for 2315 reflections with I.>4σ(I) and 262 refined parameters.

Crystal Data (4):$C_{15}H_9N_1O_5$, M= 378.4, D_x= 1.38$g.cm^{-3}$,a=9.2660(3),b=25.6250(8),c=7.6640(2) Å, β=90.61(3)° ,V=1819.6(1)$Å^3$,monoclinic P21/c, Z=4,F(000)=792,μ= 0.10 mm^{-1}, S= 1.102, R_1=0.06 for 2988 reflections with I.>4σ(I) and 253 refined parameters .



(1) **(2)** **(3)** **(4)**

Figure 1. A projection ORTEP3 of four structures with displacement ellipsoids at the 50% probability level.

References

[1] Hillard, E. A et al., *Chem. Comm.* **2008**, 2612-2628.
[2] Plyta, Z. F. et al., *J. Braz. Chem. Soc.* **2001**, *12*, 339-345
[3] da Silva Júnior, E. N. et al., *Bioorg. Med. Chem.* **2007**, *15*, 7035-7041.
[4] Sheldrick, G. M. SHELXL-97. Program for Crystal Structure Refinement. University of Göttingen, Göttingen, Germany, **1997**.

Acknowledgements

CNPq, FAPEAL,CAPES,FAPERJ, USP, UFRJ, UFAL,UFC and Proj. FINEP-CTINFRA n° 0970/01.