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SUPPLEMENTARY MATERIAL TO

Syntheses and computational analyses of selected macrolide derivatives derived from clarithromycin A

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*2′-O-acetyl-clarithromycin A (**1**)*. m.p. 249-251 ºC; ^{1}H NMR ($CDCl_3$) δ 4.75 (dd, CHOAc), 3.37 (s, 3H, C-3′′OCH_3), 3.01 (s, 3H, C-6 OCH_3), 2.26 (s, 6H, $N(CH_3)_2$), 2.05 (s, 3H, $OCOCH_3$), 1.14 (s, 3H, C-12 CH_3); ^{13}C NMR ($CDCl_3$) δ 175.7 (C-1), 170 ($OCOCH_3$), 71.8 (C-2′); MS (ES^+) (*m/z*): $[M+H]^+$ 790. The melting point was in accordance with the previously published value.[1] NMR spectra (^{1}H and ^{13}C) of the compound are available in the Supplementary Material (Figure S-1).

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a)

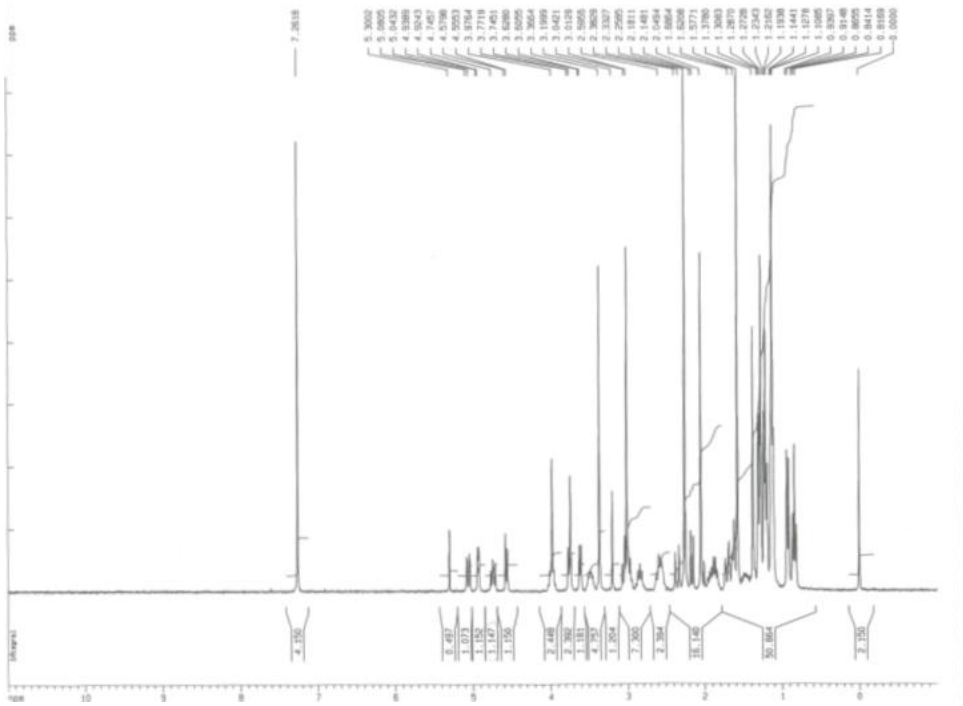

Figure S-1. a) The ^{1}H NMR spectrum of 2′-*O*-acetyl-clarithromycin A (**1**).

b)

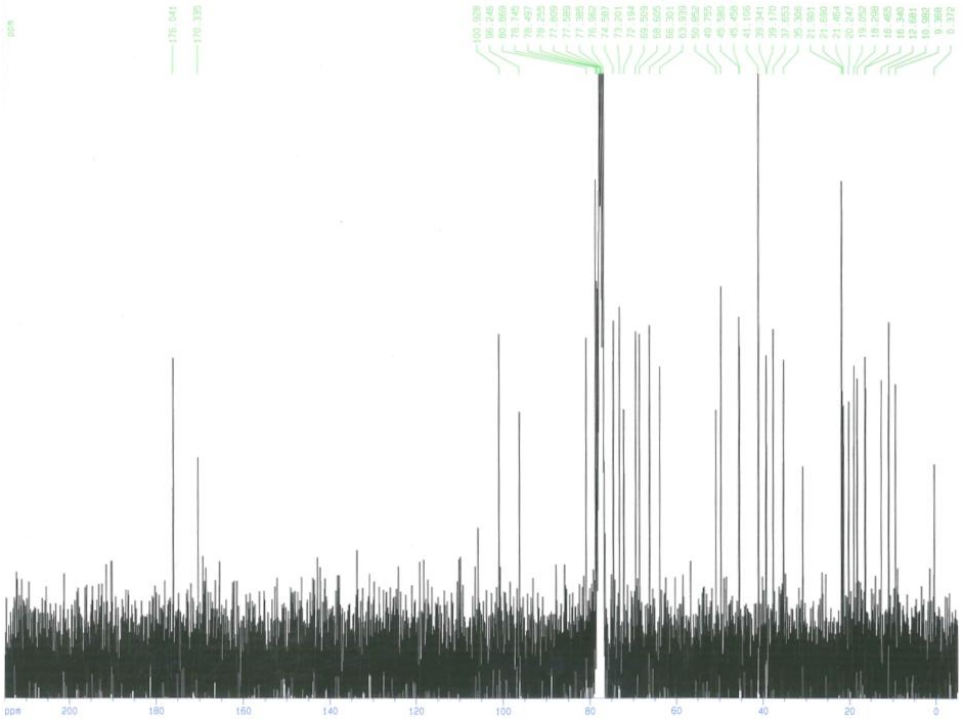

Figure S-1. b) ^{13}C NMR spectrum of 2′-*O*-acetyl-clarithromycin A (**1**).

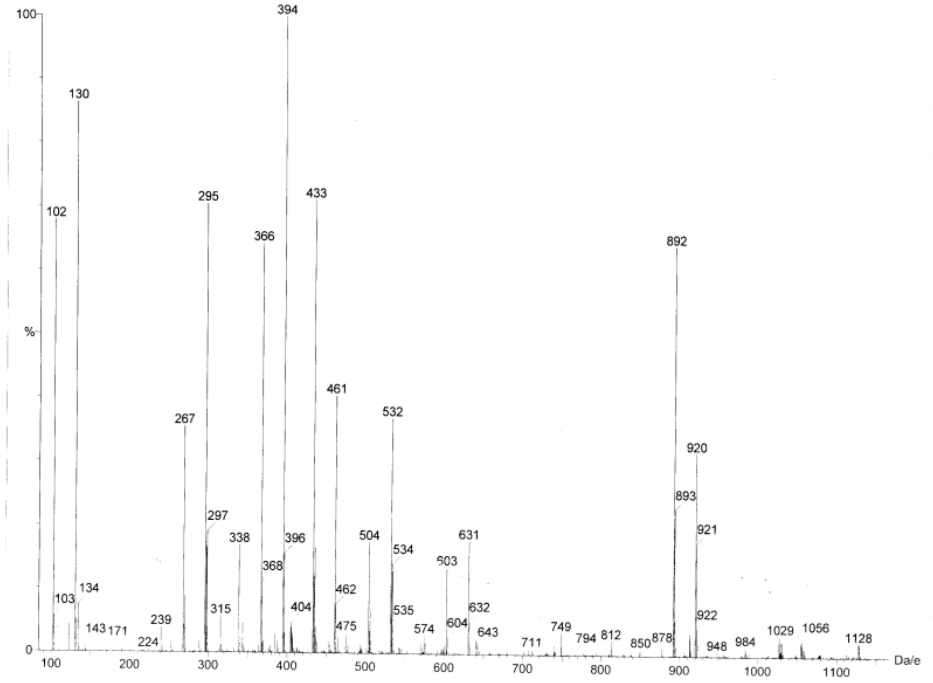

Figure S-2. Mass spectrum (ES+) of 2′-*O*-acetyl-4"-*O*-(2-cyanoethyldiisopropylphosphoramidite)-clarithromycin A (**2**).

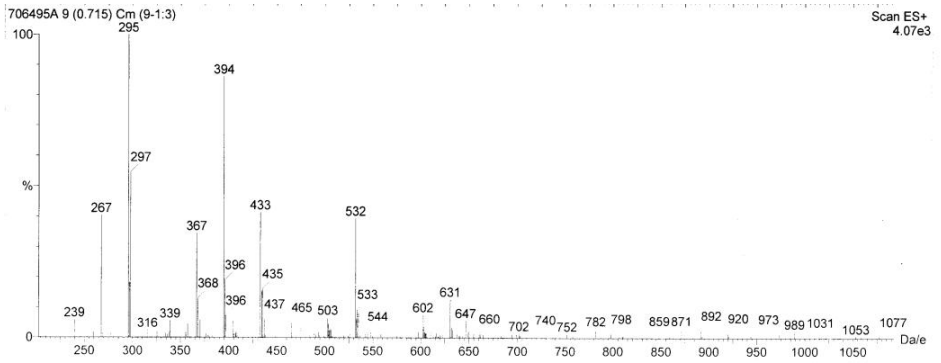

Figure S-3. Mass spectrum (ES+) of 2′-*O*-acetyl-4′′-*O*-(2-cyanoethyldiisopropylphosphoramidite)-clarithromycin A (**2**).

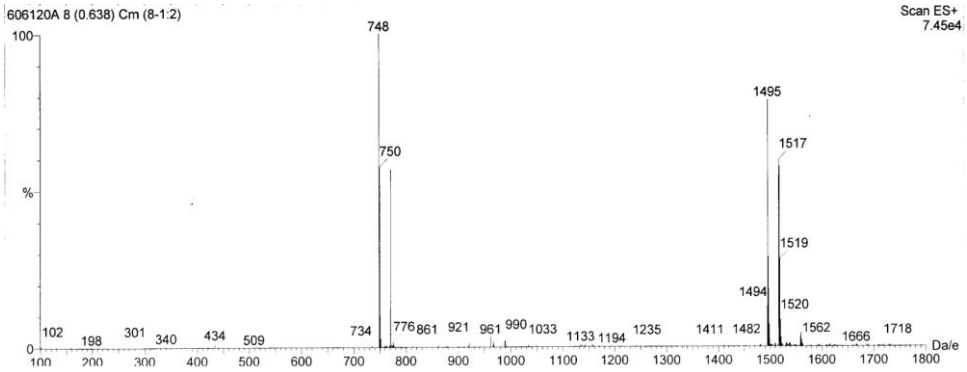

Figure S-4. Mass spectrum (ES+) of 4´´-*O*-phosphonyl-clarithromycin A (**3**).

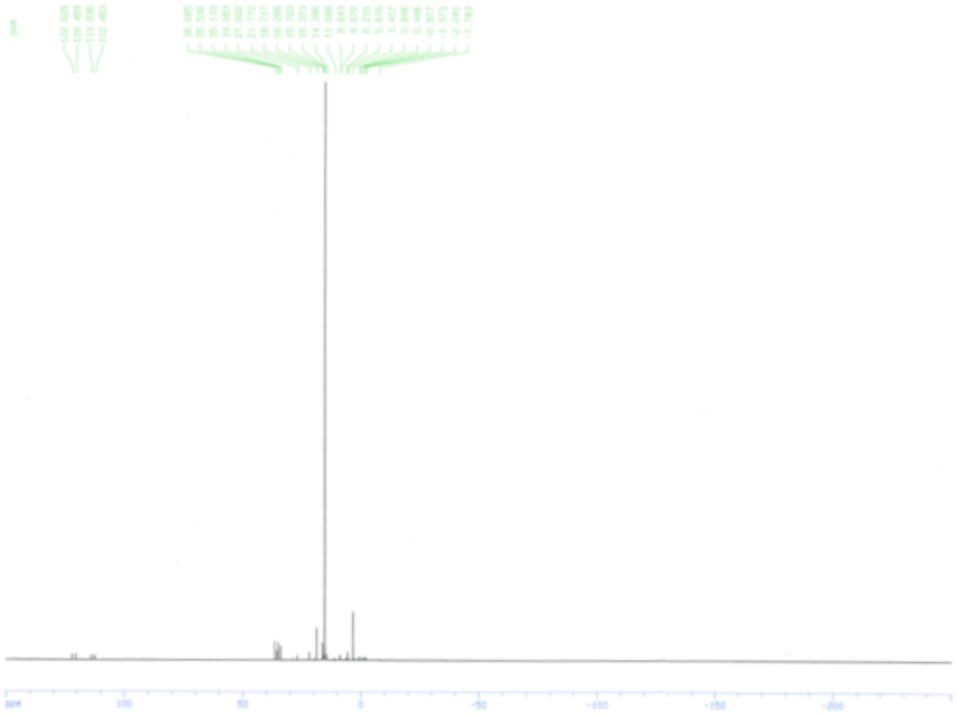

Figure S-5. ^{31}P NMR spectrum of the mixture 2-cyanoethyl *N,N*-diisopropylchlorophosphoramidite, *N*-ethyldiisopropylamine and water.

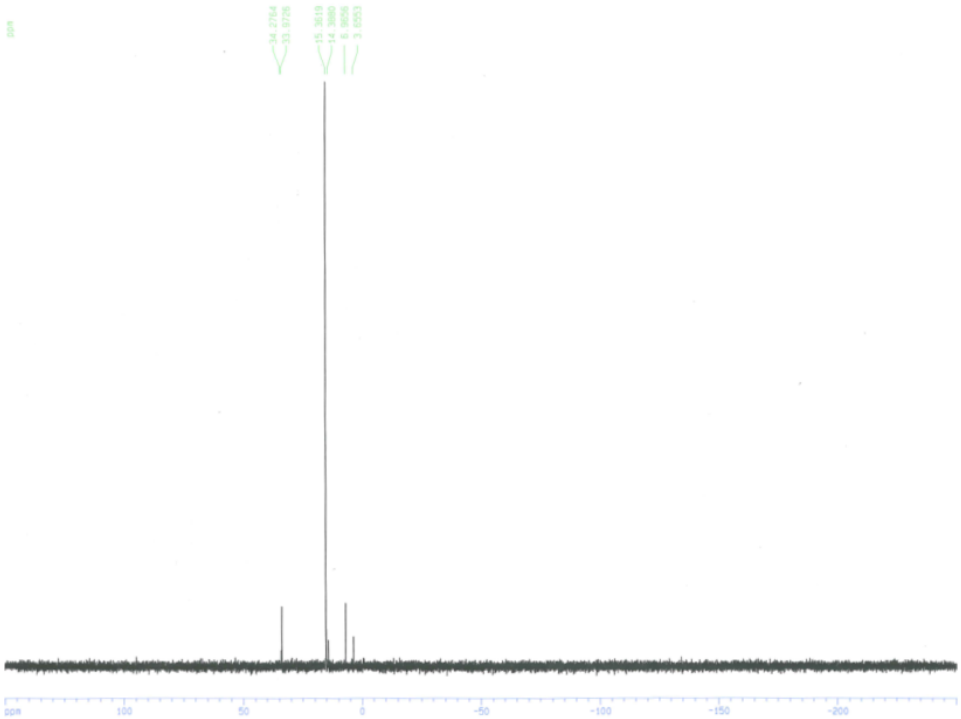

Figure S-6. ^{31}P NMR spectrum of the reaction mixture after 1 day when 2-cyanoethyl *N,N*-diisopropylchlorophosphoramidite was in 5 fold excess.

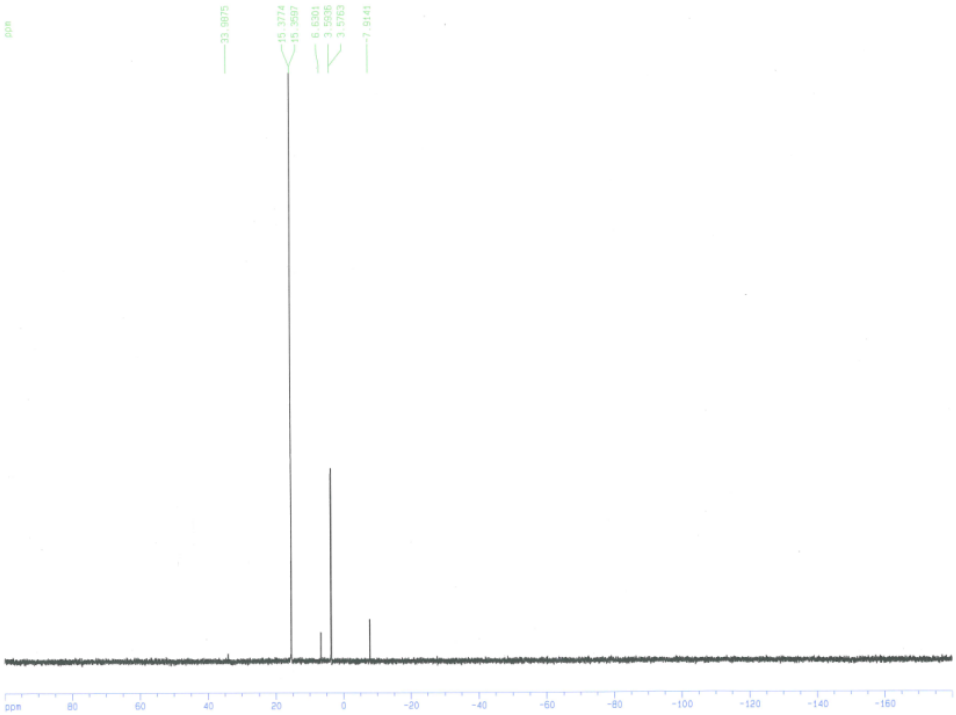

Figure S-7. ^{31}P NMR spectrum of a reaction mixture with DMAP (4-dimethylaminopyridine) as a catalyst.

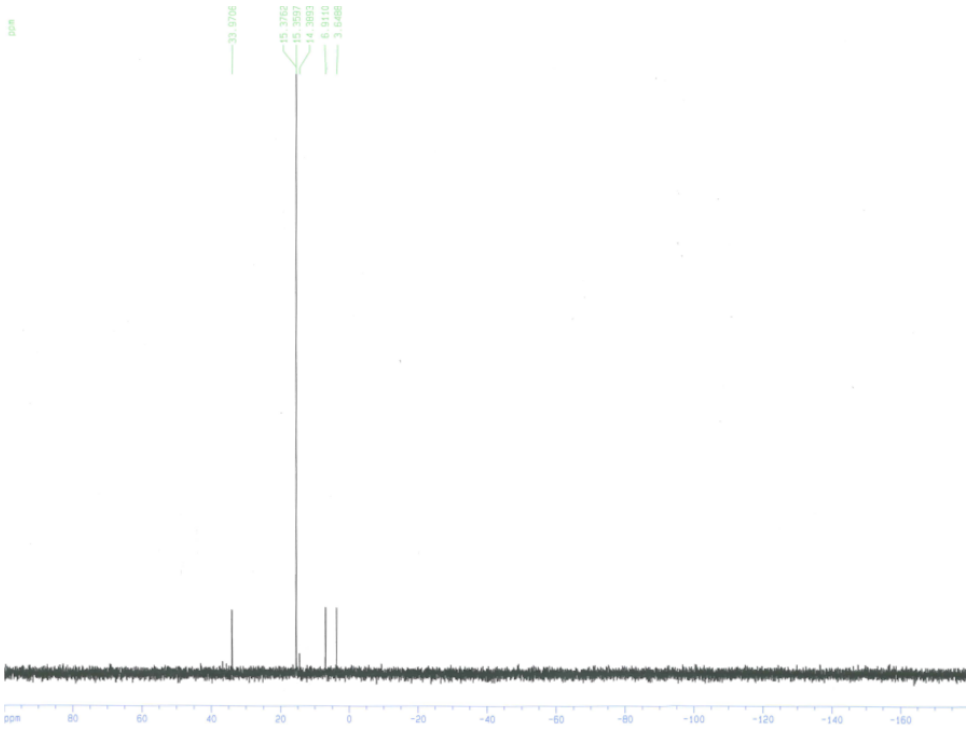

Figure S-8. ^{31}P NMR spectrum of the reaction mixture on heating at 40 ºC under reflux.

REFERENCES

1. W. R. Baker, J. D. Clark, R. L. Stephens, K. H. Kim, *J. Org. Chem.* **53** (1988) 2340 (https://doi.org/10.1021/jo00245a038).