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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; 1H NMR (CDCl3) δ 4.75 (dd, CHOAc), 3.37 (s, 3H, C-3´´OCH3), 3.01 (s, 3H, C-6 OCH3), 2.26 (s, 6H, N(CH3)2), 2.05 (s, 3H, OCOCH3), 1.14 (s, 3H, C-12 CH3); 13C NMR (CDCl3) δ 175.7 (C-1), 170 (OCOCH3), 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 (1H and 13C) of the compound are available in the Supplementary Material (Figure S-1).

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a)

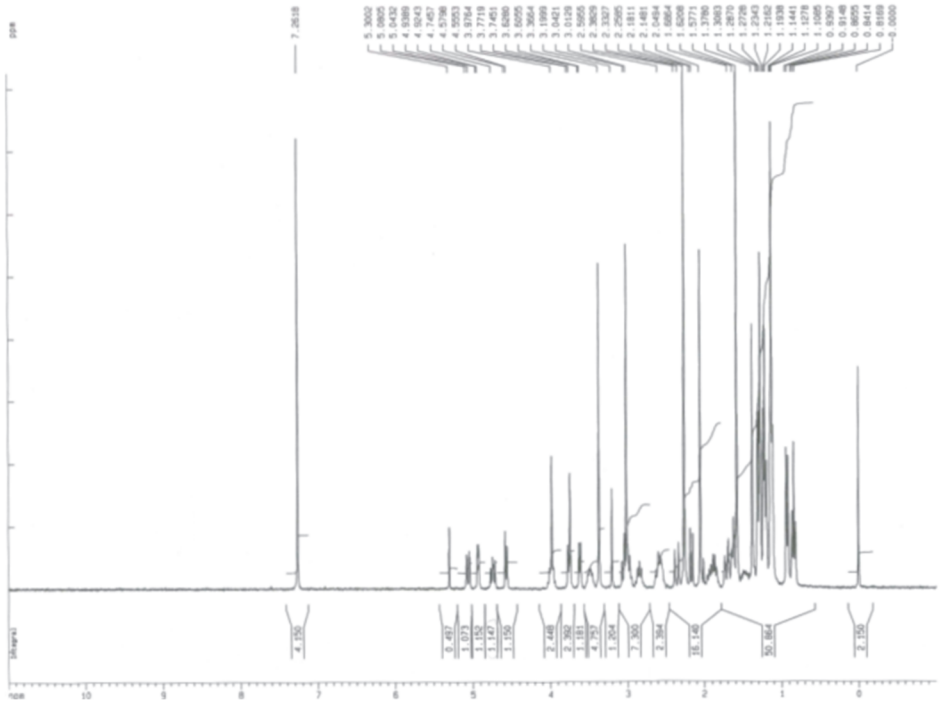

Fig. S-1. a) The ^{1}H NMR spectrum of 2′-*O*-acetyl-clarithromycin A (**1**).

b)

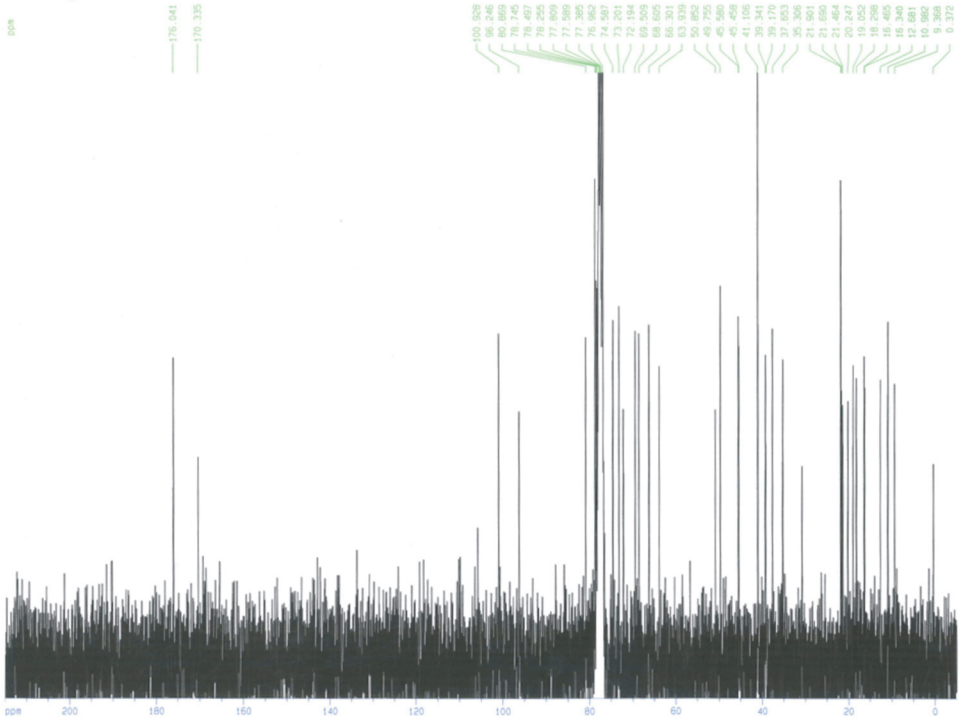

Fig. S-1. b) ^{13}C NMR spectrum of 2′-*O*-acetyl-clarithromycin A (**1**).

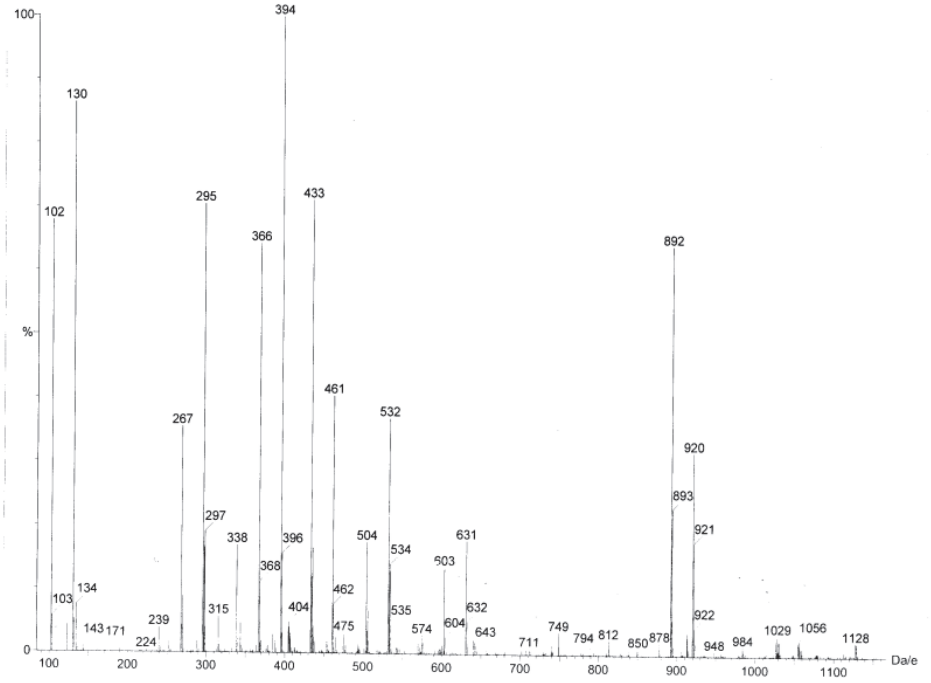

Fig. S-2. Mass spectrum (ES+) of 2′-*O*-acetyl-4"-*O*-(2-cyanoethyldiisopropylphosphoramidite)-clarithromycin A (**2**).

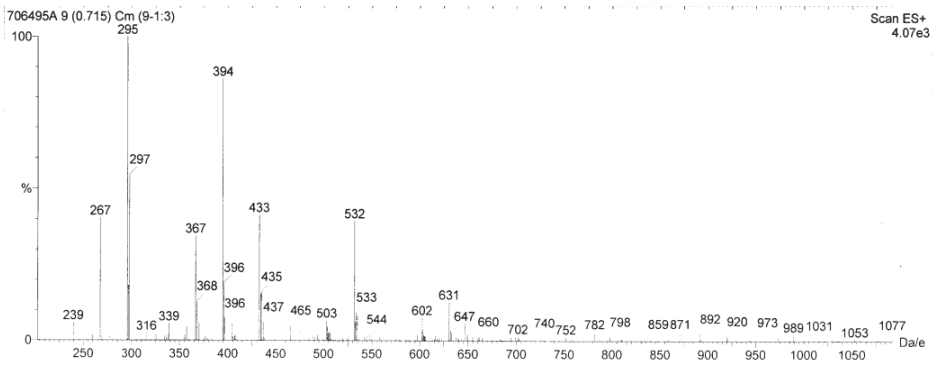

Fig. S-3. Mass spectrum (ES+) of 2′-*O*-acetyl-4′′-*O*-(2-cyanoethyldiisopropylphosphoramidite)-clarithromycin A (**2**).

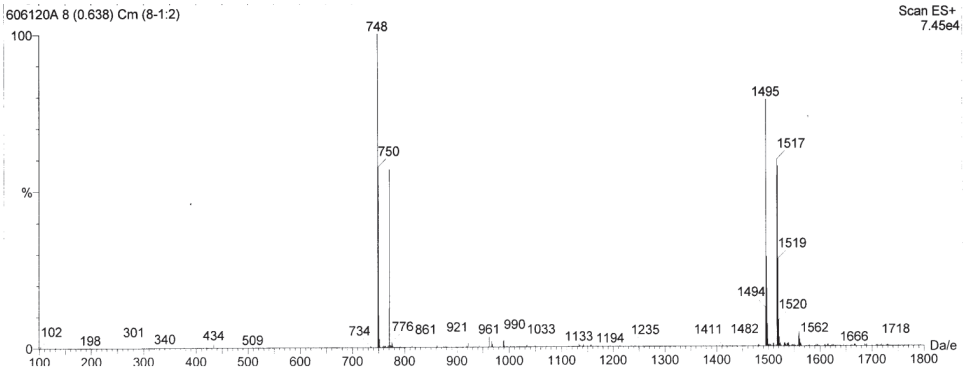

Fig. S-4. Mass spectrum (ES+) of 4´´-*O*-phosphonyl-clarithromycin A (**3**).

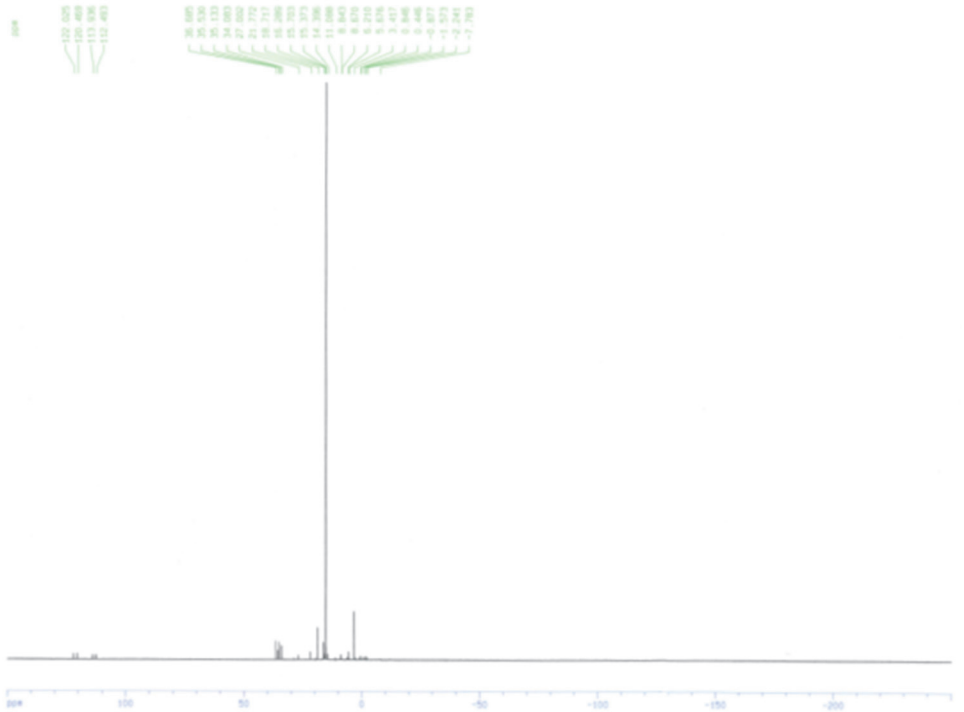

Fig. S-5. ^{31}P NMR spectrum of the mixture 2-cyanoethyl *N,N*-diisopropylchlorophosphoramidite, *N*-ethyldiisopropylamine and water.

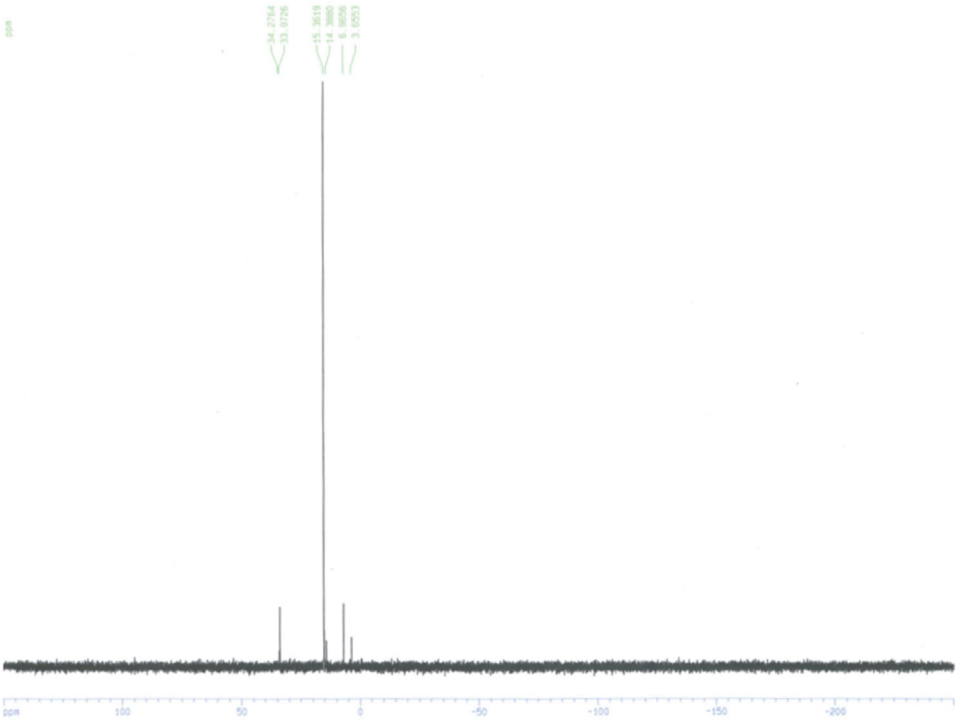

Fig. S-6. ^{31}P NMR spectrum of the reaction mixture after 1 day when 2-cyanoethyl *N,N*-diisopropylchlorophosphoramidite was in 5 fold excess.

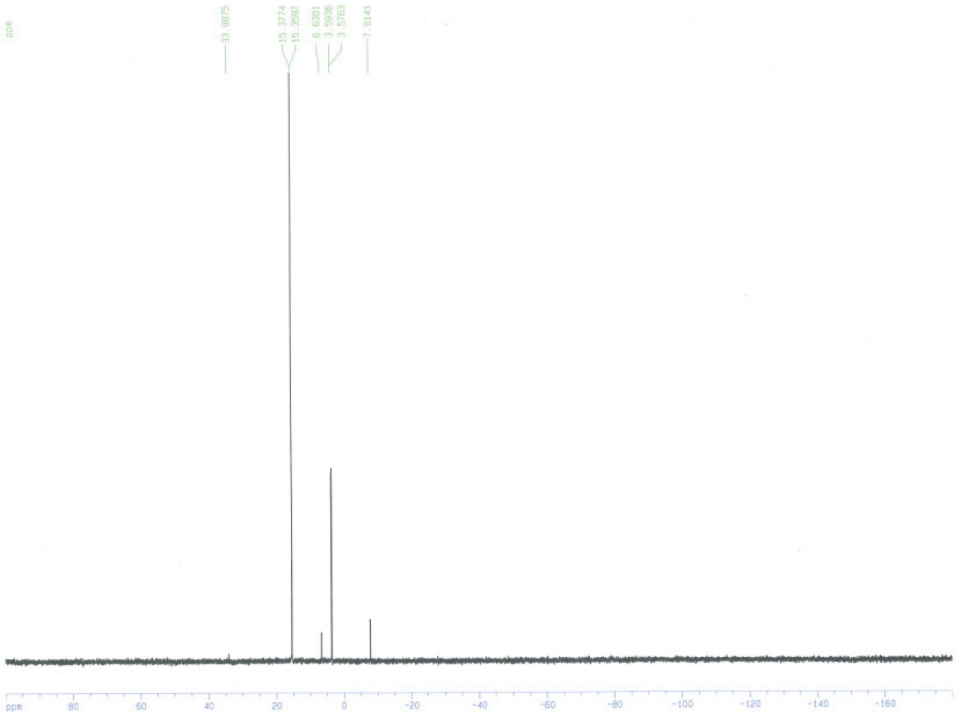

Fig. S-7. ^{31}P NMR spectrum of a reaction mixture with DMAP (4-dimethylaminopyridine) as a catalyst.

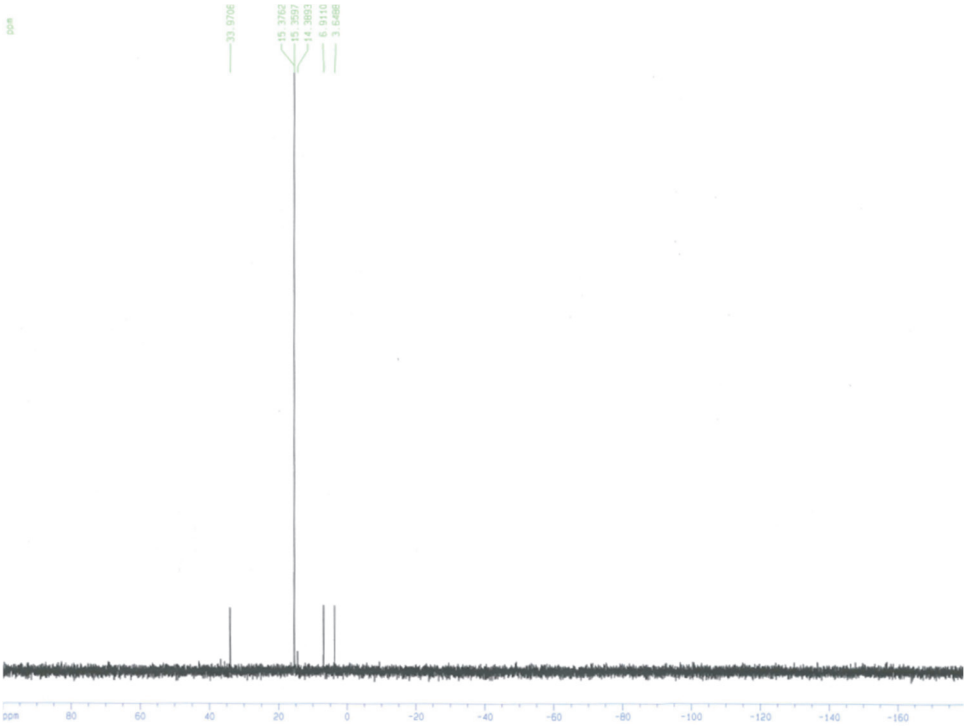

Fig. S-8. ^{31}P NMR spectrum of the reaction mixture on heating at 40 ºC under reflux.

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).