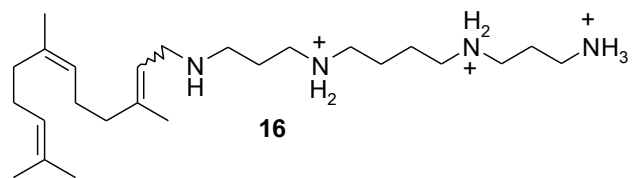
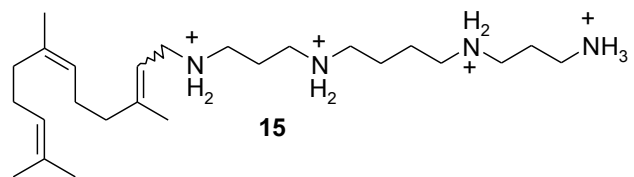


Chemical parameters

a) Estimation of protonated species encountered at various pH for compound **3**.



At pH 7.0 species **16** in 90.7% and species **15** in 4.99%

At pH 7.2 species **16** at 85.89% and species **15** in 7.49%

b) Identification of the major species according to pH theoretical values.

