Supplementary Information:

Structural Behaviour of Isolated Asphaltene Molecules at the Oil-Water Interface

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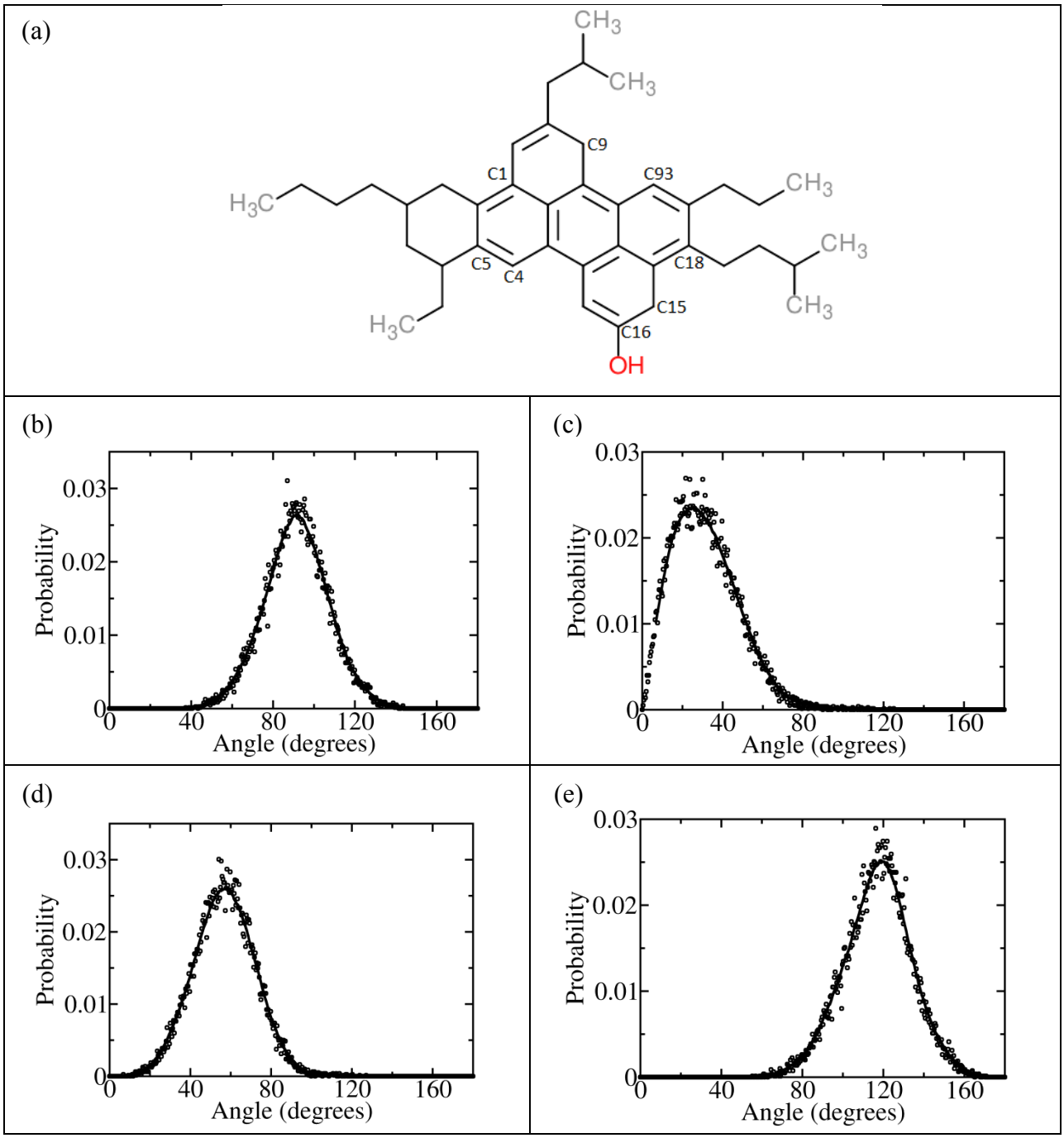

Figure S1: *(a) Structure of asphaltene-phenol (APH) molecule. Orientational distribution of the APH molecule defined by the angle formed between oil-water interface normal (i.e. z-axis) and vector formed by (b) C5 and C18 atoms, (c) C9 and C16 atoms, (d) C1-C15 atoms and (e) C4-C93 atoms of APH molecule*

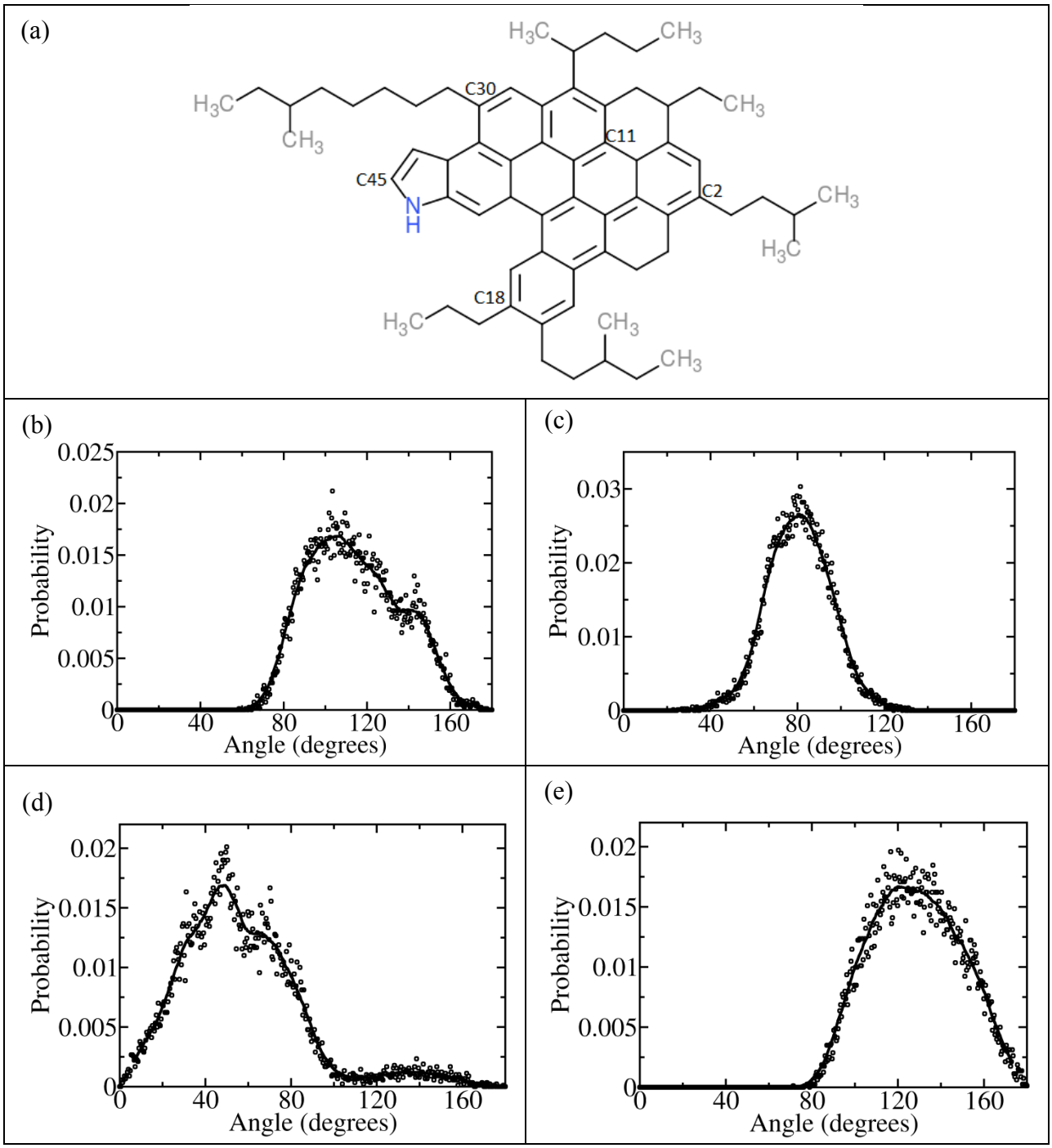

Figure S2: *(a) Structure of asphaltene-pyrol (APY) molecule. Orientational distribution of the APY molecule defined by the angle formed between oil-water interface normal (i.e. z-axis) and vector formed by (b) C30 and C18 atoms, (c) C30 and C2 atoms, (d) C45 and C2 atoms and (e) C18 and C11 atoms of APY molecule*

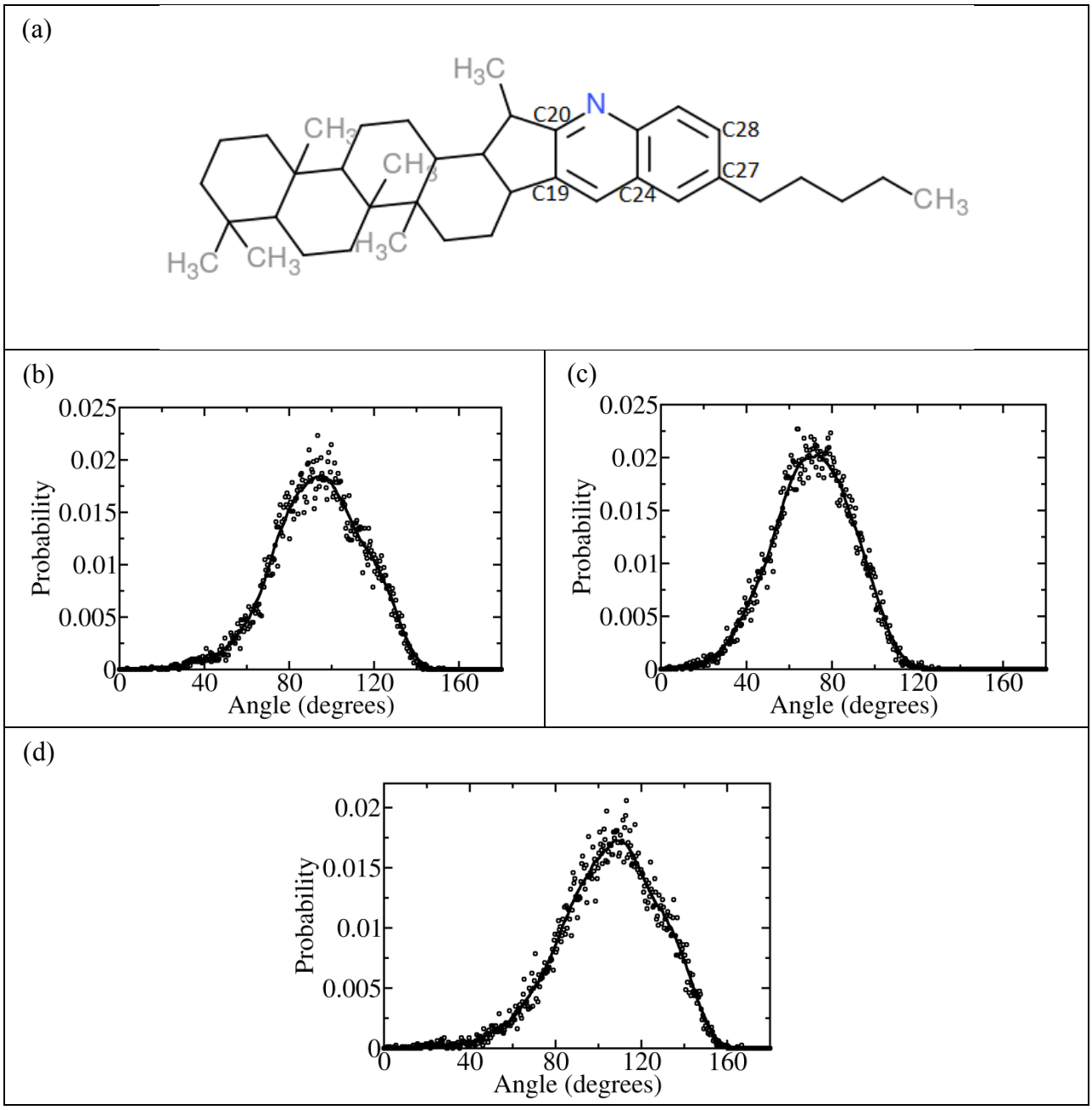

Figure S3: *(a) Structure of quinilinohopane (QHP) molecule. Orientational distribution of the QHP molecule defined by the angle formed between oil-water interface normal (i.e. z-axis) and vector formed by (b) C20 and C27 atoms, (c) C19 and C28 atoms, and (d) C20 and C24 atoms of QHP molecule.*

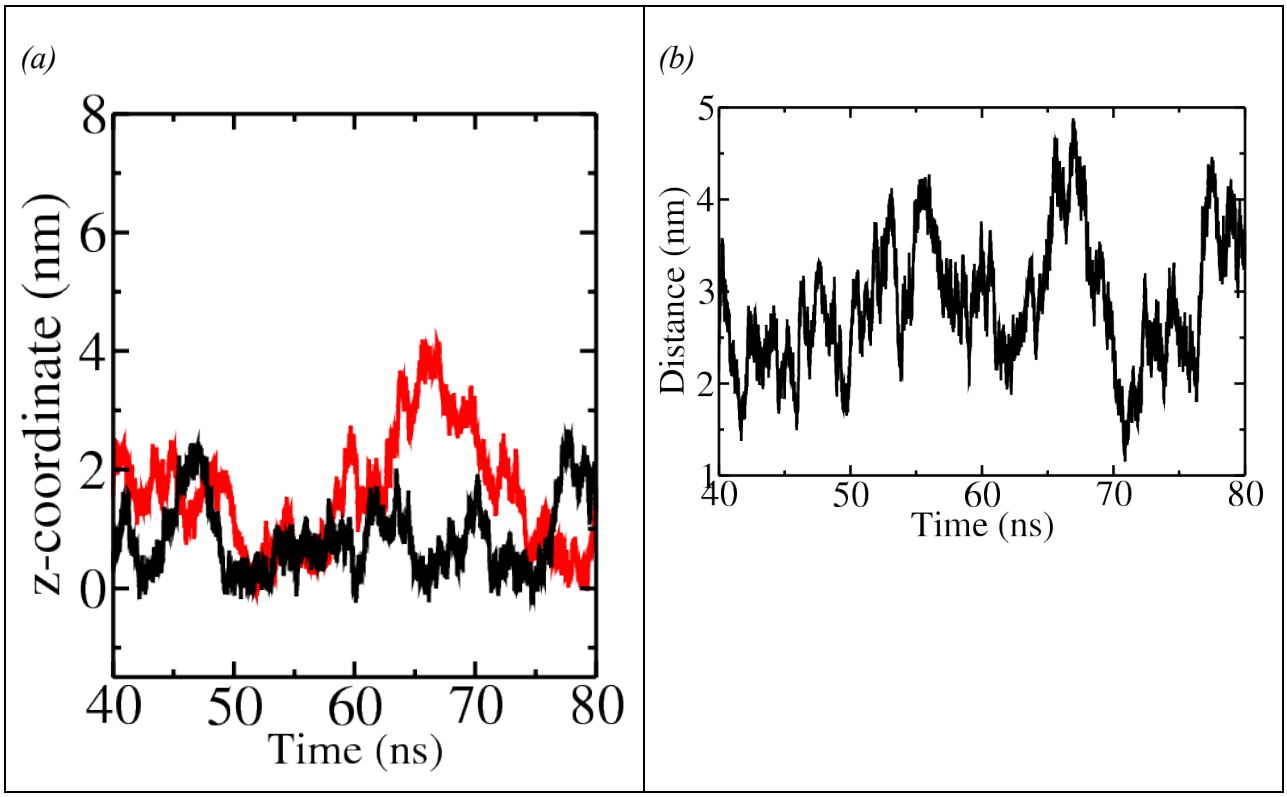

Figure S4: *Variation in (a) z- coordinate and (b) distance between two ATH molecules center of mass with respect to time obtained from additional 40ns simulations. Both ATH molecule neither aggregate nor adsorb at the oil-water interface.*