**Job Plot**



Figure S1: Job plot for **3a** with acetate.
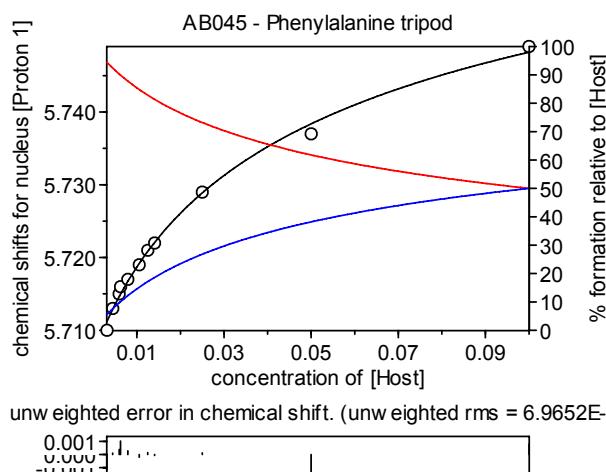


Fig. S2: Self Association in **3a**

AB041 - Leucine Tripod (2)

unweighted error in chemical shift. (unweighted rms = 1.2522E-3
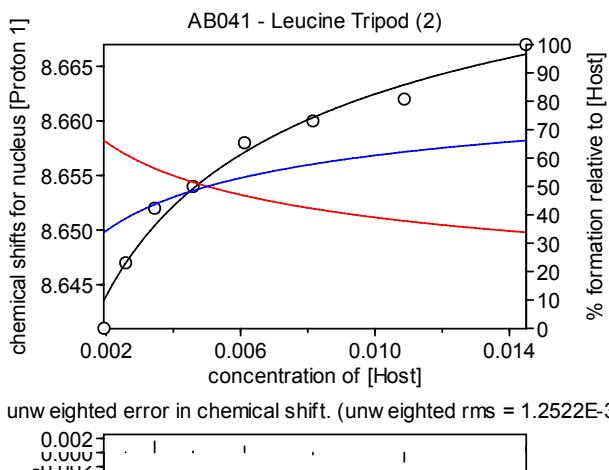
Fig. S3: Self Association in **3b**
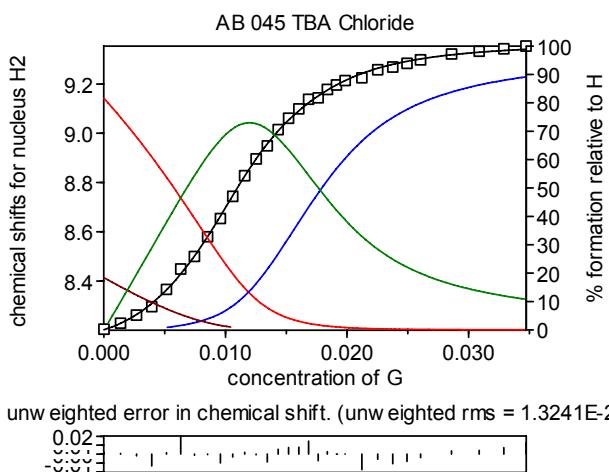
AB 045 TBA Chloride

unweighted error in chemical shift. (unweighted rms = 1.3241E-2

Fig. S4: Cl⁻ binding by **3a**

AB 045 TBA Bromide

unweighted error in chemical shift. (unweighted rms = 8.0824E-3

Fig. S5: Br⁻ binding by **3a**

AB 045 TBA Iodide

unweighted error in chemical shift. (unweighted rms = 3.7913E-3

Fig. S6: $I^-$ binding by **3a**

AB 045 TBA Nitrate

unweighted error in chemical shift. (unweighted rms = 2.1932E-3

Fig. S7: $NO_3^-$ binding by **3a**

Project title

unweighted error in chemical shift. (unweighted rms = 6.4360E-3
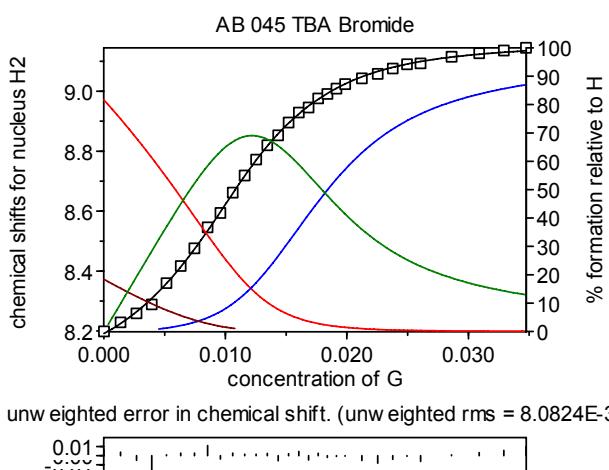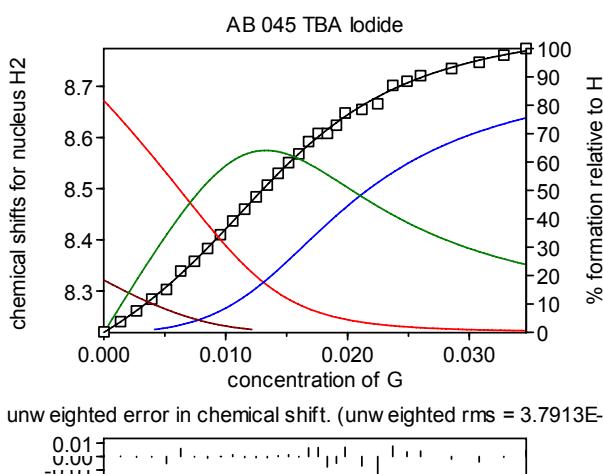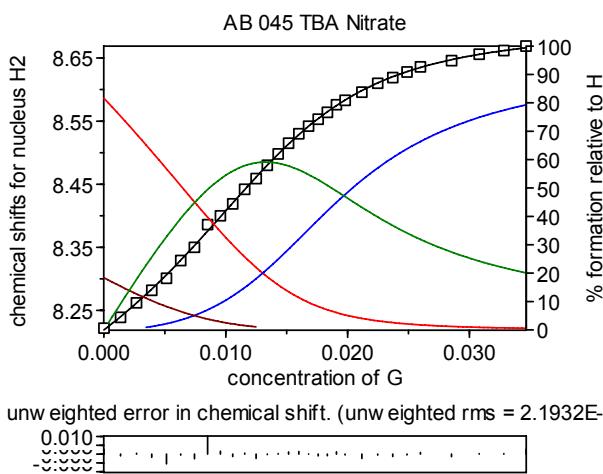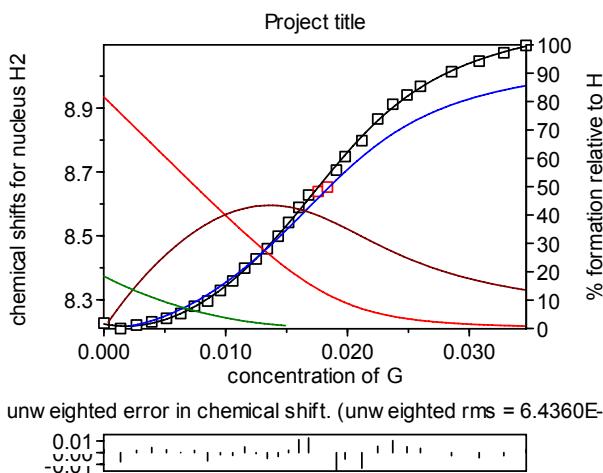
Fig. S8: $MeCO_2^-$ binding by **3a**

AB 045 TBA L-Lactic Acid

unweighted error in chemical shift. (unweighted rms = 3.1947E-3)

Fig. S9: L-lactate binding by **3a**

AB 045 TBA DL-Lactic Acid

unweighted error in chemical shift. (unweighted rms = 4.2976E-3)
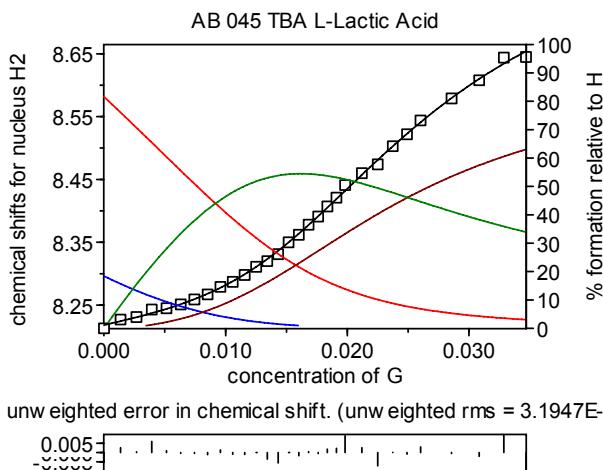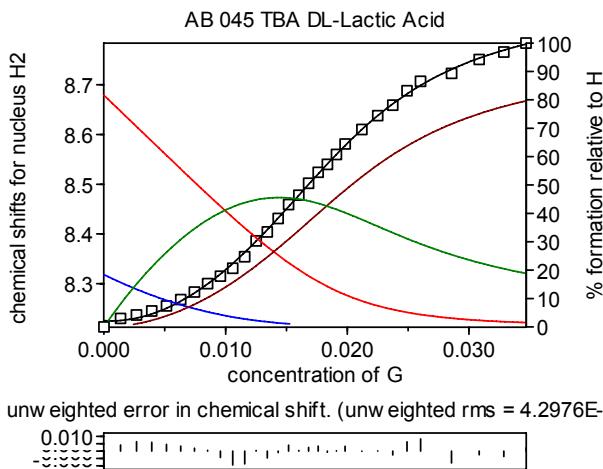
Fig. S10: racemic lactate binding by **3a**

Project title

weighted error in chemical shift. (weighted rms = 2.5976E0)

Fig. S11: Cl⁻ binding by **3b**

**Project title**

unweighted error in chemical shift. (unweighted rms = 4.9475E-3

Fig. S12: Br⁻ binding by **3b**

**AB 041 TBA Iodide**

unweighted error in chemical shift. (unweighted rms = 3.3494E-3

Fig. S13: I⁻ binding by **3b**

**AB 041 TBA Acetate**

unweighted error in chemical shift. (unweighted rms = 4.1525E-3
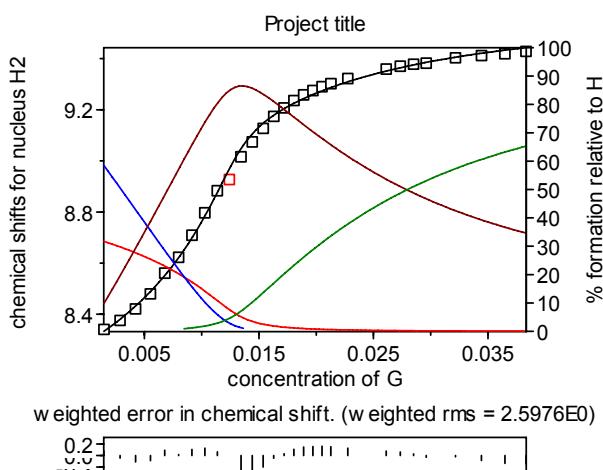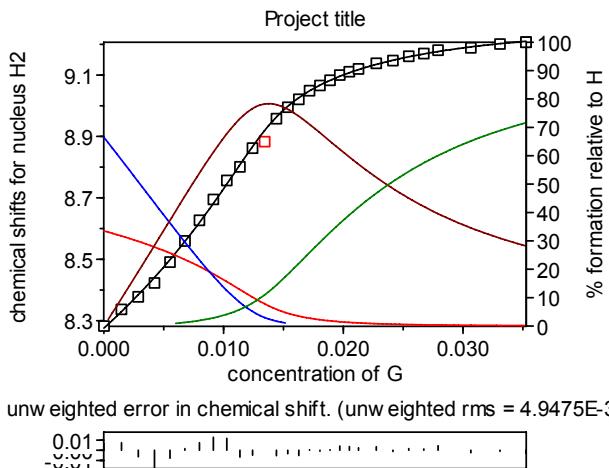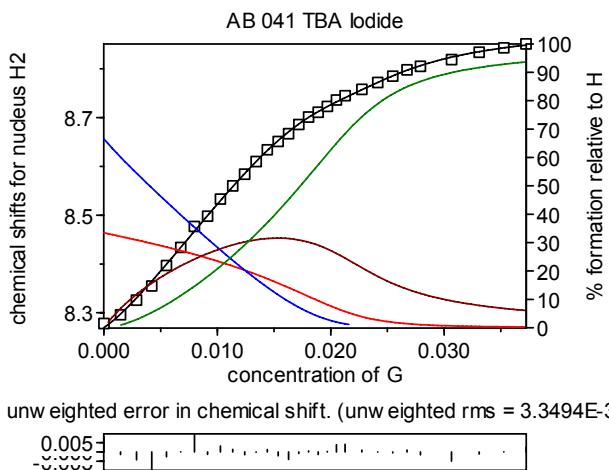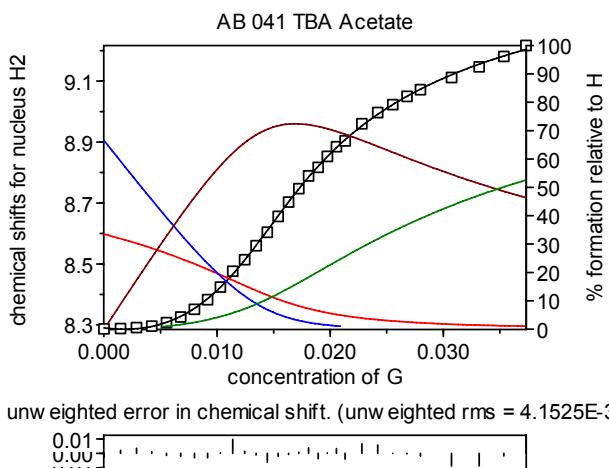
## Fig. S14: MeCO$_2^-$ binding by **3b**

**AB 041 TBA L-Lactic Acid**

unweighted error in chemical shift. (unweighted rms = 2.9934E-3
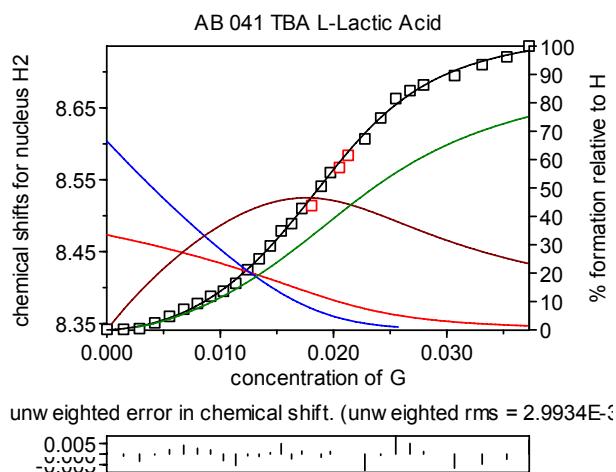
## Fig. S15: L-lactate binding by **3b**

**AB 041 TBA DL-Lactic Acid**

unweighted error in chemical shift. (unweighted rms = 2.8167E-3
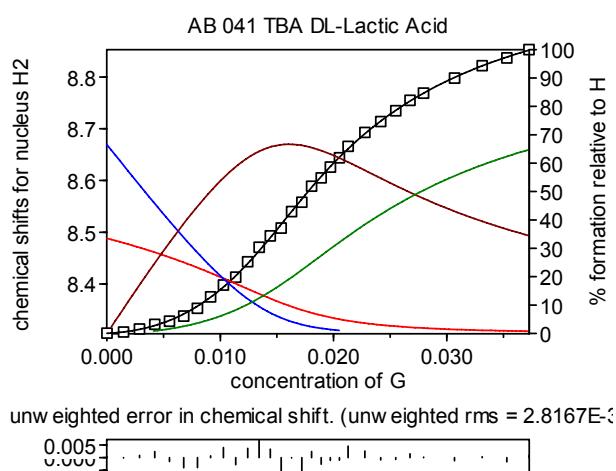
## Fig. S16: racemic lactate binding by **3b**

**Project title**

unweighted error in chemical shift. (unweighted rms = 8.3970E-3
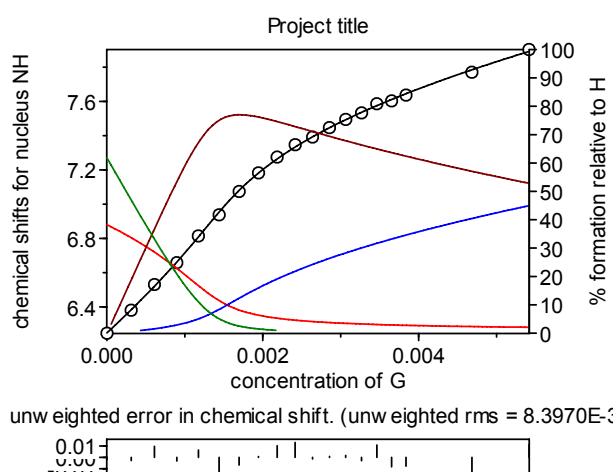
## Fig. S17: Chloride binding by **4b**

**Nitro Host + Acetate**



unweighted error in chemical shift. (unweighted rms = 2.8215E-2
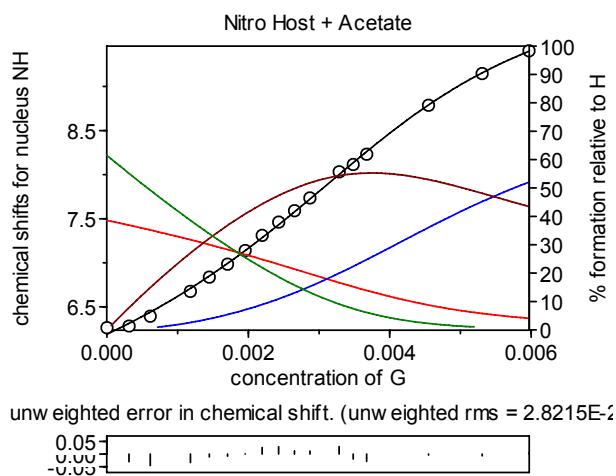
## Fig. S18: Acetate binding by **4b**
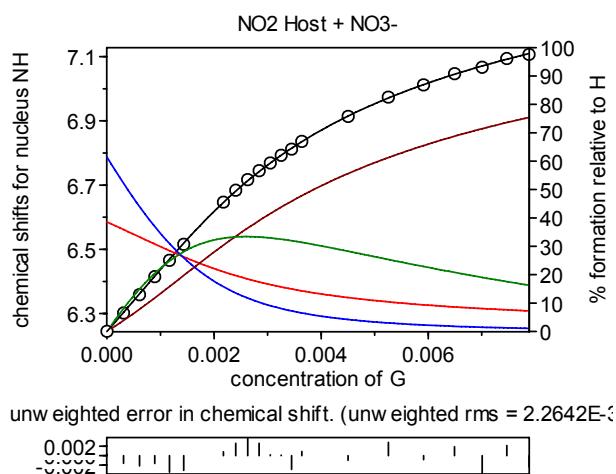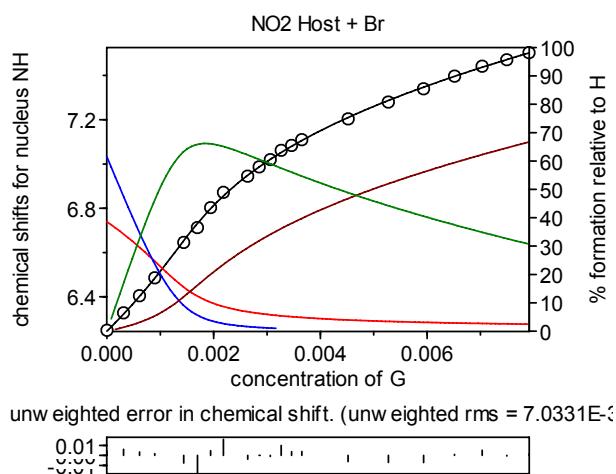
**NO2 Host + NO3-**



unweighted error in chemical shift. (unweighted rms = 2.2642E-3

## Fig. S19: NO$_3^-$ binding by **4b**

**NO2 Host + Br**



unweighted error in chemical shift. (unweighted rms = 7.0331E-3

Fig. S20: Br⁻ binding by **4b**

**Phenyl host + Cl**



unweighted error in chemical shift. (unweighted rms = 1.4030E-2

Fig. S21: Cl⁻ binding by **4a**

**Phenyl Host + Br**



unweighted error in chemical shift. (unweighted rms = 3.3659E-3

Fig. S22: Br⁻ binding by **4a**

**Pehnyl Host + NO3-**



unweighted error in chemical shift. (unweighted rms = 2.7814E-3

Fig. S23: NO₃⁻ binding by **4a**

$E_{orb} = -0.234$ au

$E_{orb} = -0.241$ au

$E_{orb} = -0.247$ au
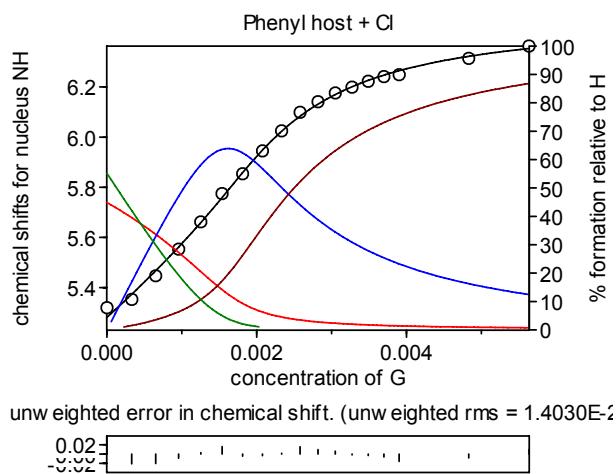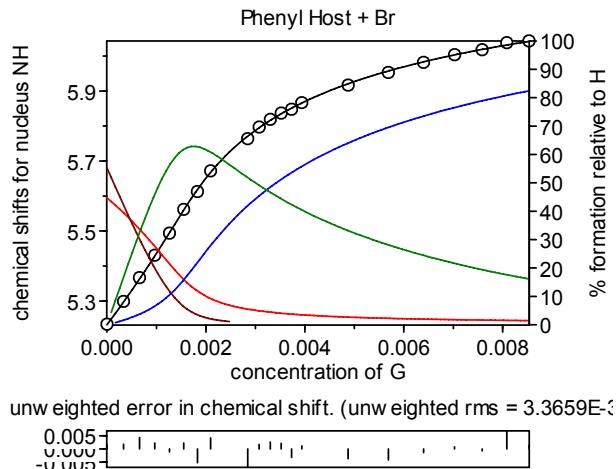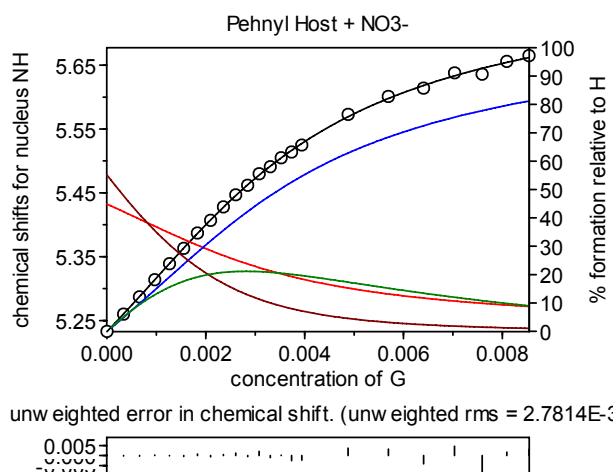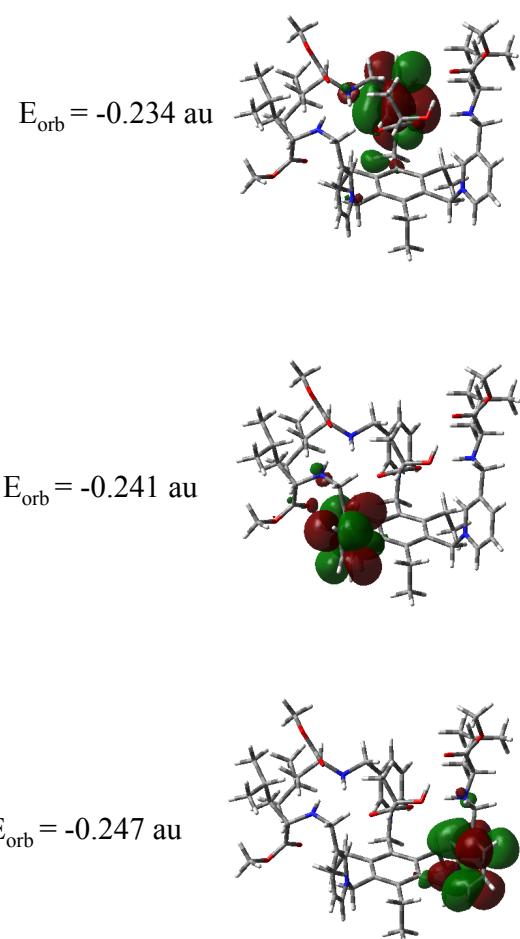
Fig S24: LUMOs from TD DFT calculations.
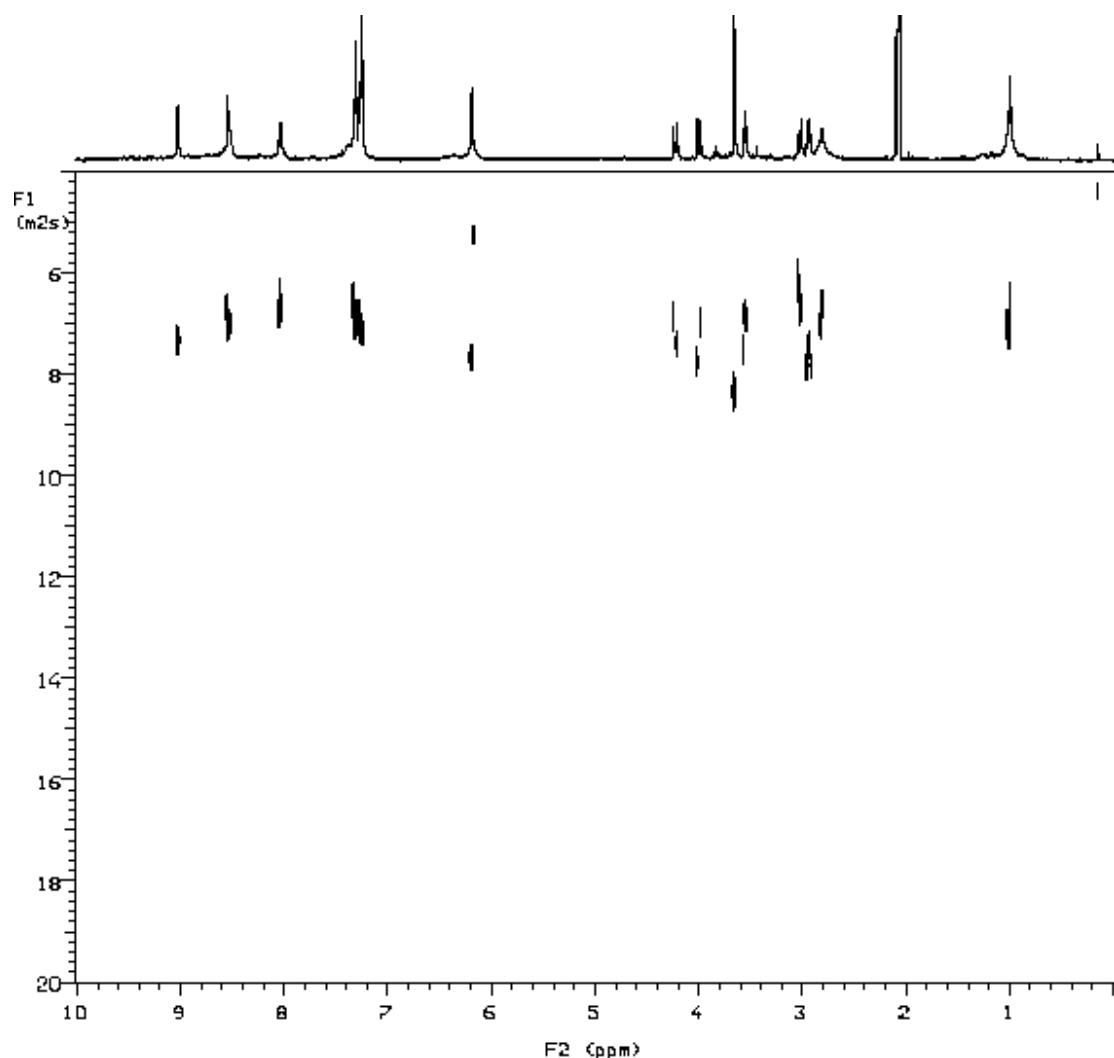
Fig S25 DOSY spectrum for **3a**
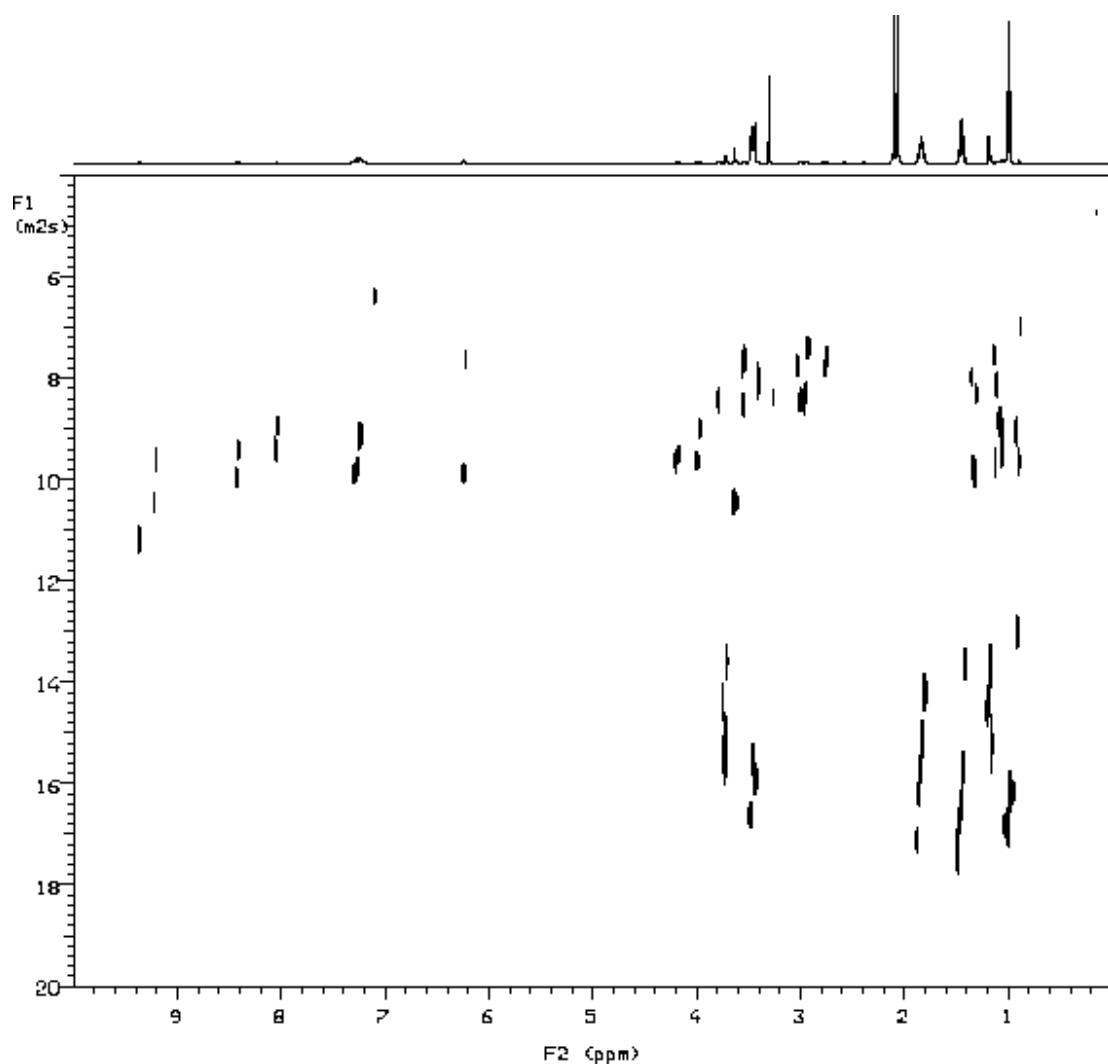
Fig S25 DOSY spectrum for **3a** in the presence of 3 equivalents of $NBu_4^+$ lactate.