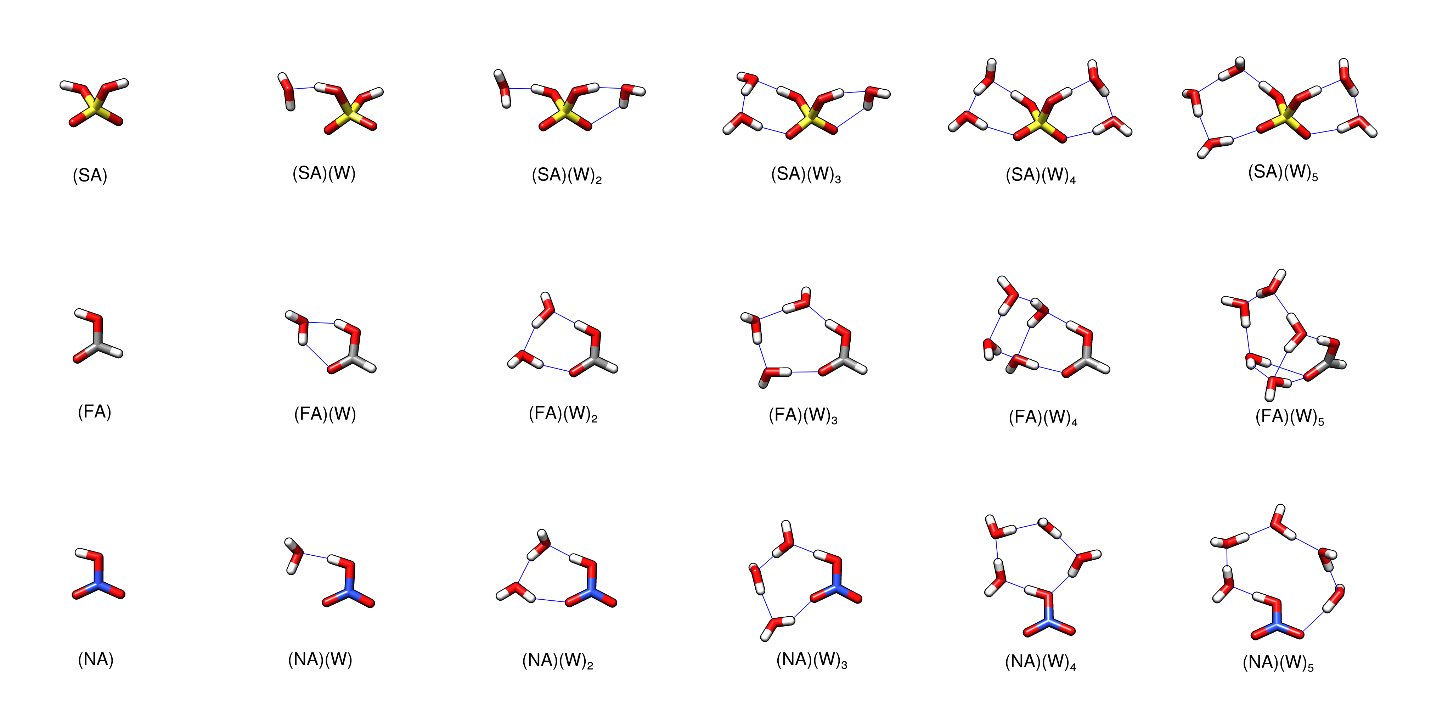
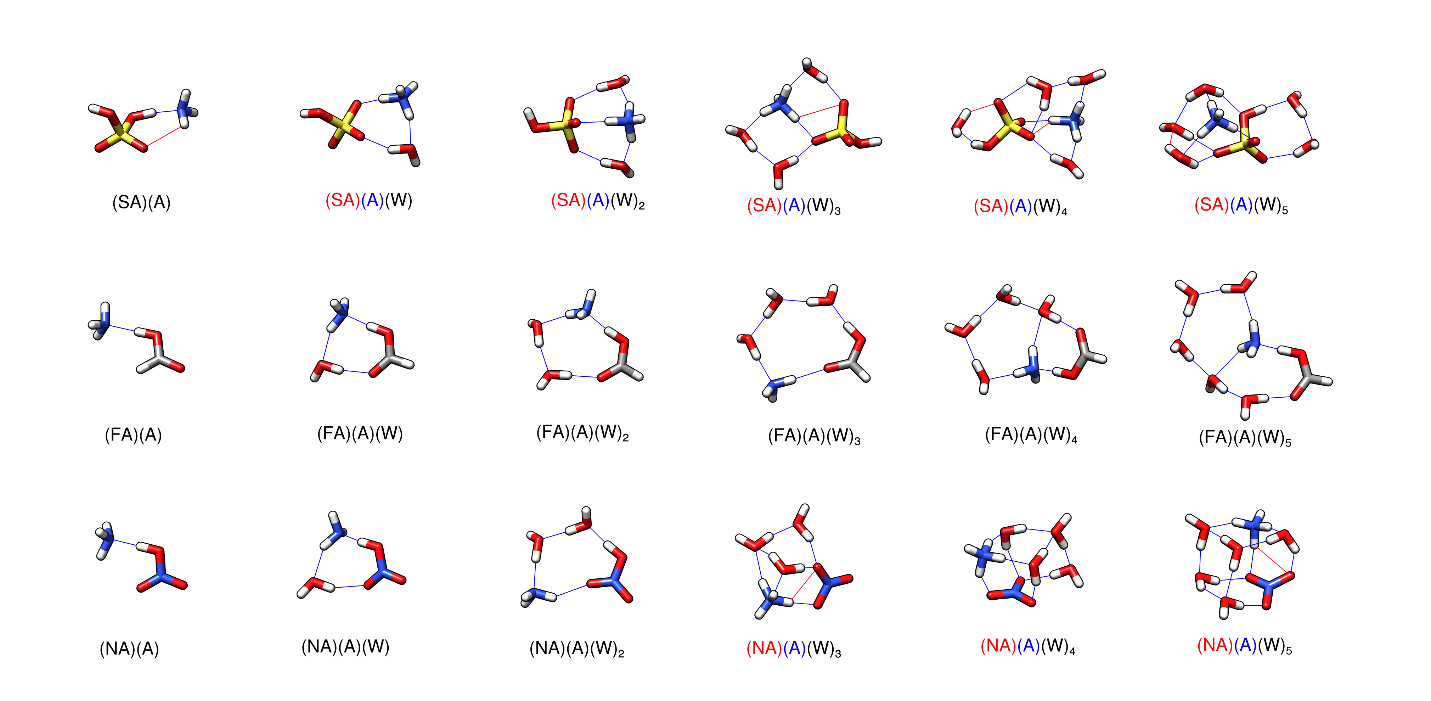


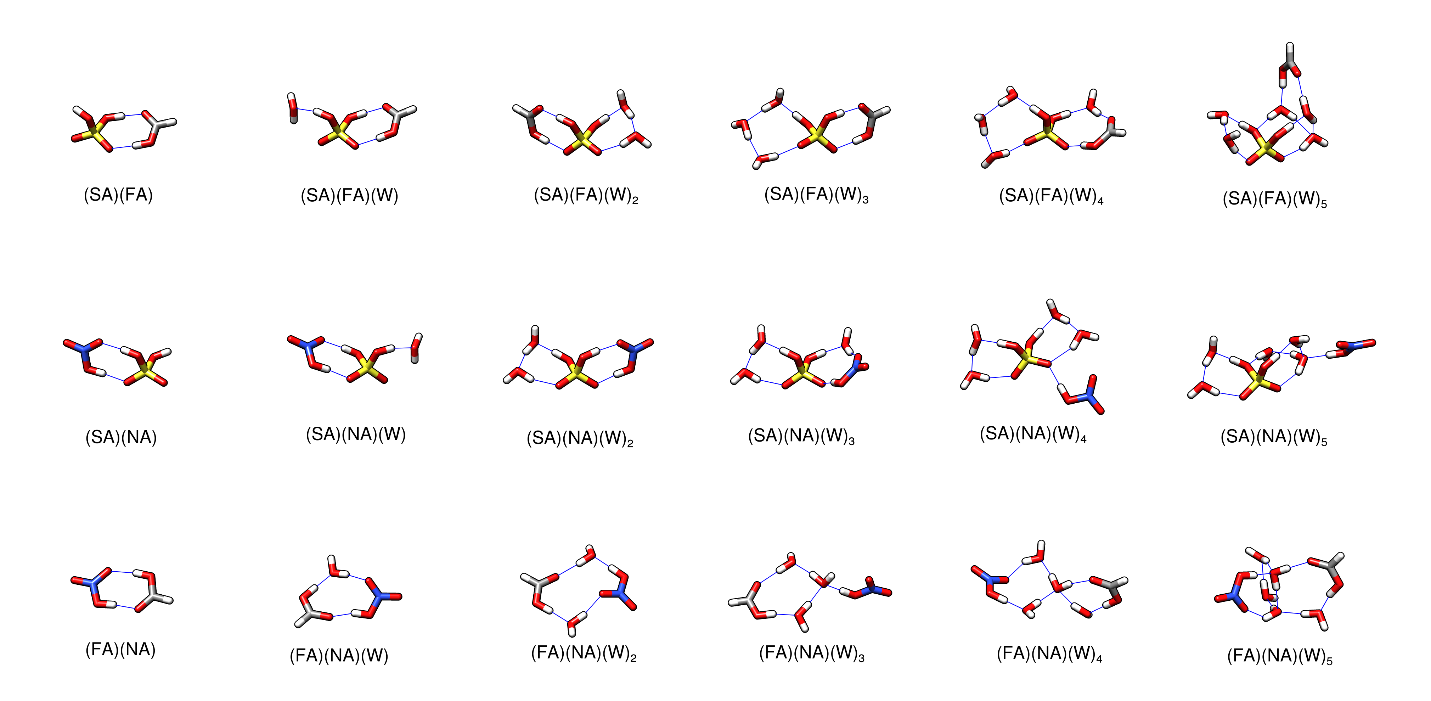
**Figure S2.** DLPNO-CCSD(T)/CBS//ωb97xD/6-31++G\*\* minimum energy clusters for the sequential hydration of base monomers. Strong hydrogen bonds are drawn in blue while weaker Van der Waals interactions are in red. The molecule labels are colored according to charge as follows: blue = +1, black = 0, red = -1, orange = -2. Atoms are drawn in the following colors: hydrogen –white, carbon –gray, nitrogen –blue, oxygen –red, sulfur –yellow.



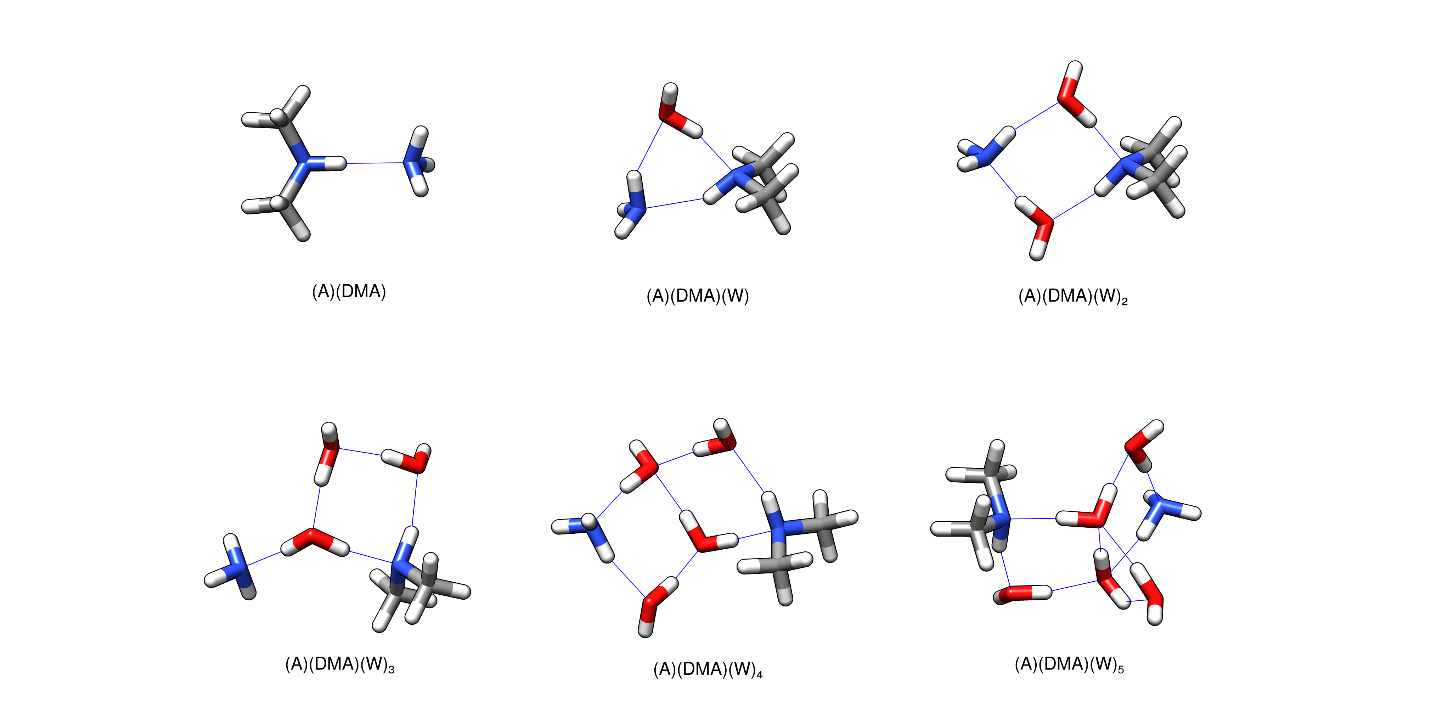
**Figure S1.** DLPNO-CCSD(T)/CBS//ωb97xD/6-31++G\*\* minimum energy clusters for the sequential hydration of acid monomers. Strong hydrogen bonds are drawn in blue while weaker Van der Waals interactions are in red. The molecule labels are colored according to charge as follows: blue = +1, black = 0, red = -1, orange = -2. Atoms are drawn in the following colors: hydrogen –white, carbon –gray, nitrogen –blue, oxygen –red, sulfur –yellow.



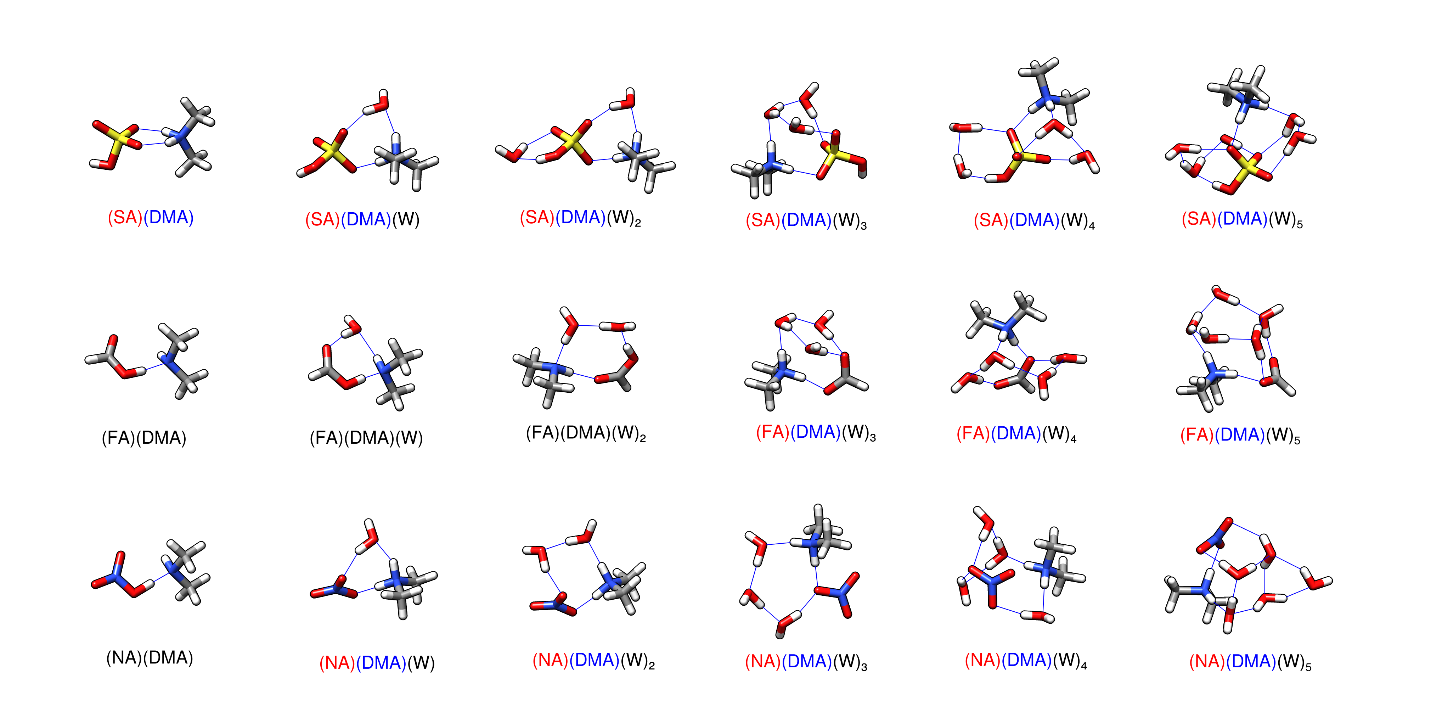
**Figure S4.** DLPNO-CCSD(T)/CBS//ωb97xD/6-31++G\*\* minimum energy clusters for the sequential hydration of one acid and ammonia. Strong hydrogen bonds are drawn in blue while weaker Van der Waals interactions are in red. The molecule labels are colored according to charge as follows: blue = +1, black = 0, red = -1, orange = -2. Atoms are drawn in the following colors: hydrogen –white, carbon –gray, nitrogen –blue, oxygen –red, sulfur –yellow.



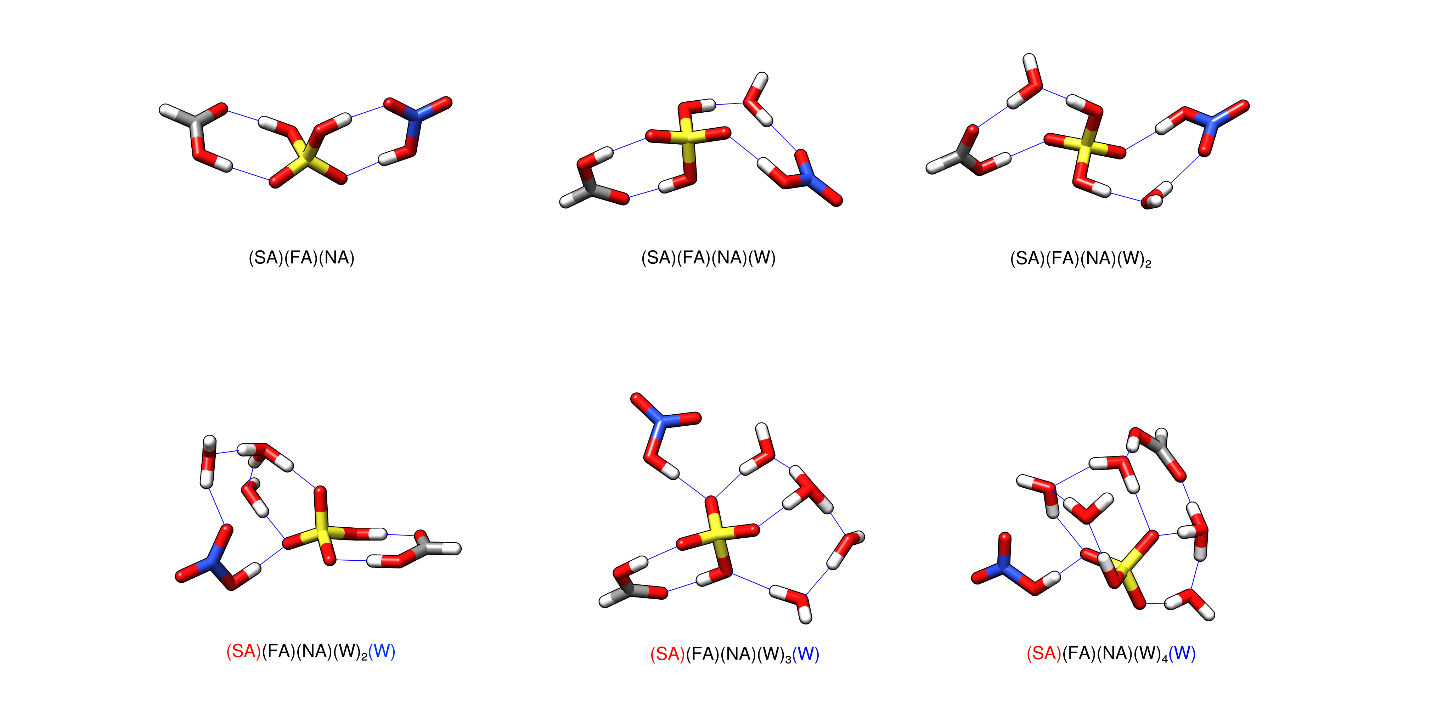
**Figure S3.** DLPNO-CCSD(T)/CBS//ωb97xD/6-31++G\*\* minimum energy clusters for the sequential hydration of two acids. Strong hydrogen bonds are drawn in blue while weaker Van der Waals interactions are in red. The molecule labels are colored according to charge as follows: blue = +1, black = 0, red = -1, orange = -2. Atoms are drawn in the following colors: hydrogen –white, carbon –gray, nitrogen –blue, oxygen –red, sulfur –yellow.



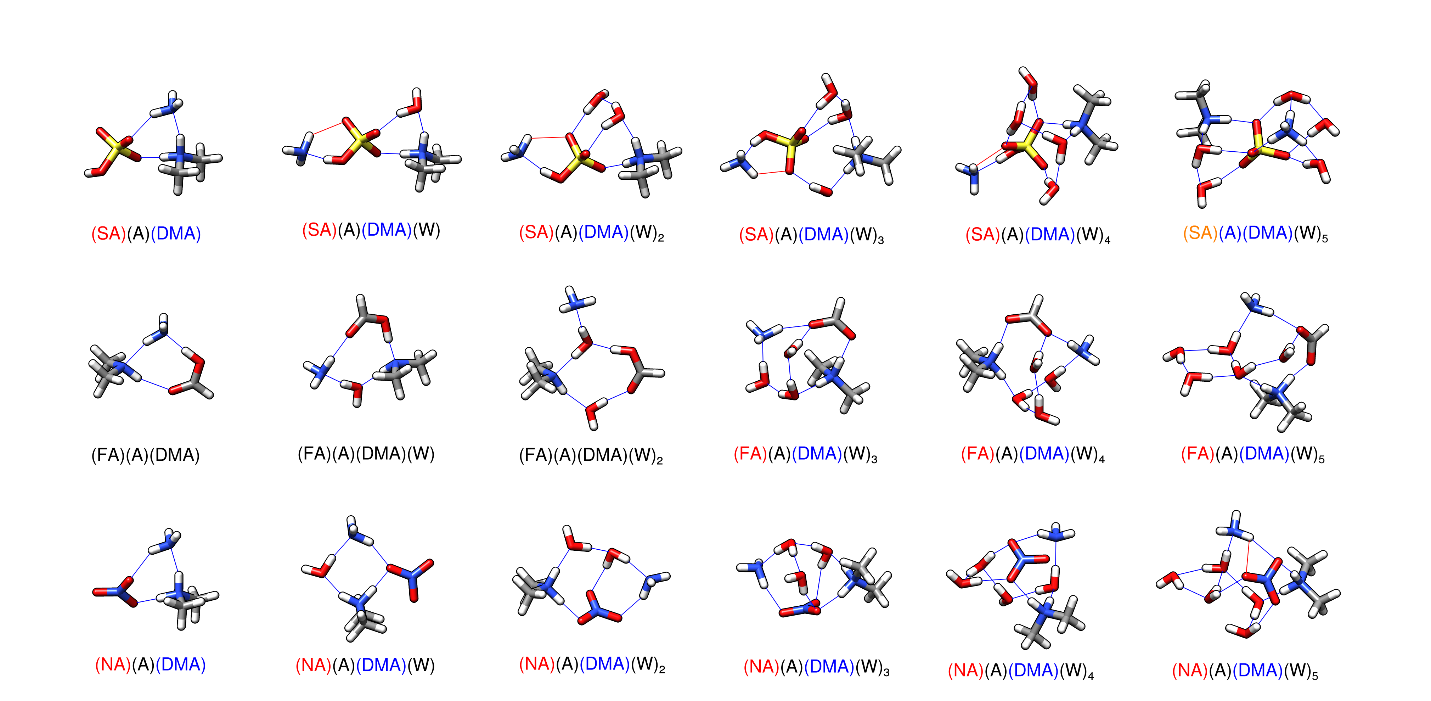
**Figure S6.** DLPNO-CCSD(T)/CBS//ωb97xD/6-31++G\*\* minimum energy clusters for the sequential hydration of two bases. Strong hydrogen bonds are drawn in blue while weaker Van der Waals interactions are in red. The molecule labels are colored according to charge as follows: blue = +1, black = 0, red = -1, orange = -2. Atoms are drawn in the following colors: hydrogen –white, carbon –gray, nitrogen –blue, oxygen –red, sulfur –yellow.



**Figure S5.** DLPNO-CCSD(T)/CBS//ωb97xD/6-31++G\*\* minimum energy clusters for the sequential hydration of one acid and dimethylamine. Strong hydrogen bonds are drawn in blue while weaker Van der Waals interactions are in red. The molecule labels are colored according to charge as follows: blue = +1, black = 0, red = -1, orange = -2. Atoms are drawn in the following colors: hydrogen –white, carbon –gray, nitrogen –blue, oxygen –red, sulfur –yellow.



**Figure S8.** DLPNO-CCSD(T)/CBS//ωb97xD/6-31++G\*\* minimum energy clusters for the sequential hydration of three acids. Strong hydrogen bonds are drawn in blue while weaker Van der Waals interactions are in red. The molecule labels are colored according to charge as follows: blue = +1, black = 0, red = -1, orange = -2. Atoms are drawn in the following colors: hydrogen –white, carbon –gray, nitrogen –blue, oxygen –red, sulfur –yellow.



**Figure S7.** DLPNO-CCSD(T)/CBS//ωb97xD/6-31++G\*\* minimum energy clusters for the sequential hydration of one acid and two bases. Strong hydrogen bonds are drawn in blue while weaker Van der Waals interactions are in red. The molecule labels are colored according to charge as follows: blue = +1, black = 0, red = -1, orange = -2. Atoms are drawn in the following colors: hydrogen –white, carbon –gray, nitrogen –blue, oxygen –red, sulfur –yellow.