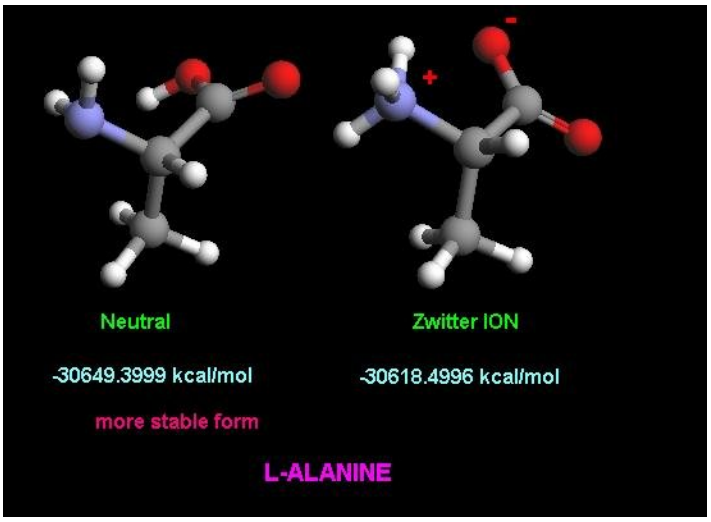
http://www.ugc-inno-nehu.com/ToxicHE.html

	NO Solvent	6H2O	12H2O	24H2O
L-Alanine_neut	-30649.3999 kcal/mol	-78913.5039 kcal/mol	-127191.4901 kcal/mol	-223743.5204 kcal/mol
L_Alanine_ZI	-30618.4996 kcal/mol	-78901.9898 kcal/mol	-127195.3701 kcal/mol	-223746.0048 kcal/mol
Remarks On Stability of neutral form vs ZI form	NEUT is more Stable than ZI Neut-ZI= **-30.9003**	NEUT is more Stable than ZI Neut-ZI= **-11.5141**	ZI is more stable than NEUT Neut-ZI= **+3.88**	ZI ismore stable than NEUT= Neut-ZI= **+2.4844**
			NOTE the reversal in Stability trend as compared to the previous two columns for No Solvent & 6H2O	
singlept	In the solvated ZI structure the Aminoacid is deleted and the Water system was subjected to single point energy calculation	-48234.4488 kcal/mol	-96500.8360 kcal/mol	-193048.9025 kcal/mol
G.O.	After Calculating the single point energy, the same was subjected to Optimization	-48262.7168 kcal/mol	-96543.5626 kcal/mol	-193107.6346 kcal/mol
One H2O G.O.	Single h2o optimized -8036.9395 kcal/mol	6 x -8036.9395= -48221.637 kcal/mol	12 x -8036.9395= -96443.274 kcal/mol	24 x -8036.0395= 192886.548 kcal/mol

http://www.ugc-inno-nehu.com/ToxicHE.html

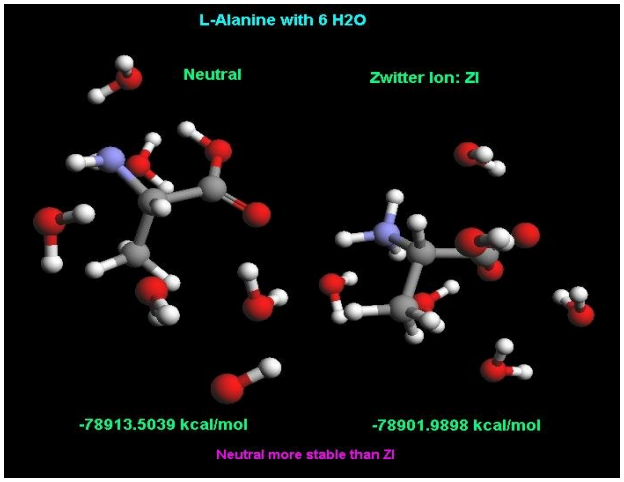


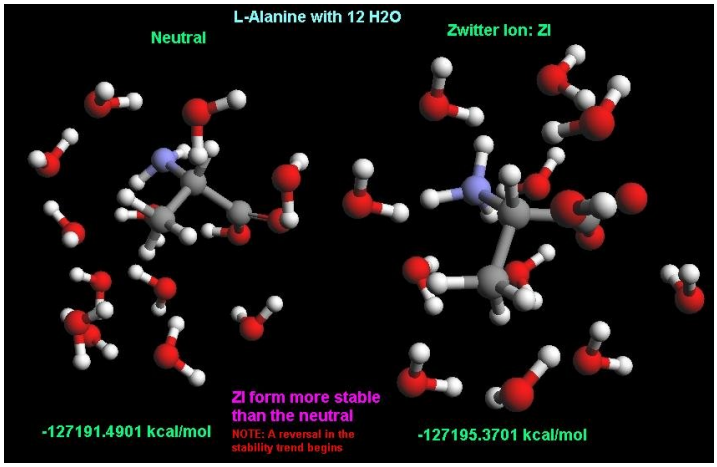
Results on Alanine using a relatively speedy method: the AM1 semiempirical method. **Conclusion:** *Nonionic form is more stable than the Zwitterionic form for the isolated molecule in the absence of surrounding water molecules*

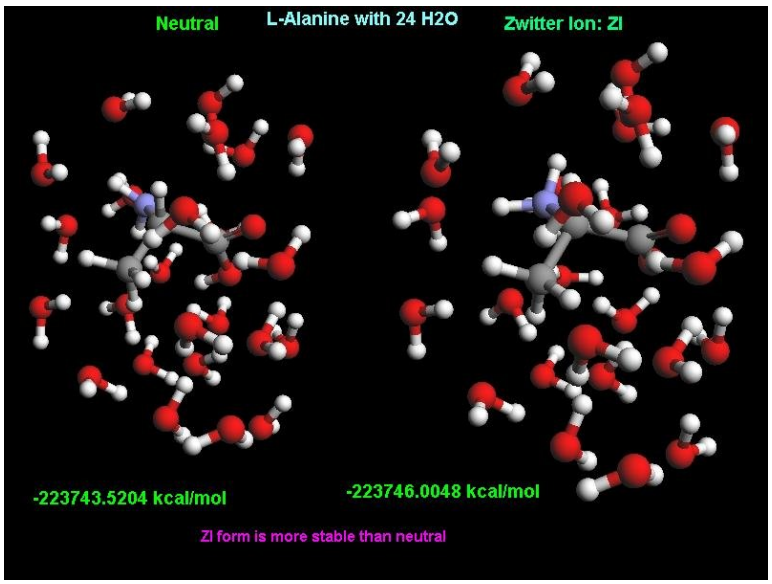
http://www.ugc-inno-nehu.com/ToxicHE.html
http://www.ugc-inno-nehu.com/the_gamess.html

How to ascertain the role of neighboring water molecules for the detailing after conclusions as above? **"This question is nothing new!"**

http://www.ugc-inno-nehu.com/crsi_13nsc_nmrs2007.html







http://www.ugc-inno-nehu.com/crsi_13nsc_nmrs2007.html