TABLE S1: VIBRATIONAL ASSIGNMENTS

WAVE NUMBER (cm-1)

INH INH OH I INH OH 2 INH OH 4 INH OH 5 INH OH N

C-C 1300.20 1334.22 1357.39 1325.34 1329.41 1323.43

C=C 1604.88 1618.98 1601.69 1607.23 1621.00 1652.89

NH2-BEND 1686.55 1686.55 1683.04 1688.49 1685.26 1676.35

C=O 1778.91 1777.07 1732.58 1769.27 1781.81 1732.57

C-H 3171.21 3174.84 3178.63 3126.87 3180.12 3207.26

NH2 SYMM 3505.31 3505.20 3508.25 3500.83 3505.00 3490.89

N-H 3564.99 3570.42 3600.75 3583.45 3555.42 3537.94

NH2 ASSYM 3614.16 3612.39 3613.64 3601.12 3616.01 3616.87

O-H - 3827.37 3291.51 3812.46 3831.26 3775.37

Table S2: Theoretical Excitation Energies, Absorption Wavelength and Oscillator Strength of studied molecules in water.

Compound Energy (eV) Wavelength (λmax nm) Oscillator Strength

INH 4.4376 279 0.0045

INH OH 1 4.0967 275 0.0554

INH OH 2 4.1908 295 0.1443

INH OH 4 4.5331 273 0.1047

INH OH 5 4.5218 274 0.0636

INH OH N 2.2657 547 0.0015

Table S3: Second Order Perturbation Theory Analysis of Fock Matrix on Isoniazid

Donor Occupancy Acceptor Occupancy E2 [Kcal/mol] E (j) – (i) [a. u.] F (i, j) [a. u.]

NBO (j) NBO (i)

Π C1-C2 1.61579 \*ΠC3-C4 0.35004 22.88 0.28 0.071

\*ΠC5-N6 0.36725 18.34 0.26 0.062

ΠC3-C4 1.64706 \*ΠC1-C2 0.27861 16.75 0.29 0.063

\*ΠC5-N6 0.36725 26.45 0.27 0.076

ΠC5-N6 1.70956 \*ΠC1-C2 0.27861 24.75 0.32 0.000

\*ΠC3-C4 0.35004 13.51 0.32 0.059

LP(1)N6 1.92428 \*ΠC1-C2 0.27861 9.83 0.91 0.085

\*ΠC4-C5 0.02725 10.22 0.90 0.087

LP(2)O12 1.85778 \*ΠC3-C11 0.07289 20.71 0.65 0.105

\*ΠC11-N13 0.08757 28.09 0.68 0.125

LP(1)N13 1.73954 \*ΠC11-O12 0.26449 3.97 0.33 0.107

\*ΠC3-C4 0.35004 \*ΠC11-O12 0.26449 61.28 0.03 0.069

\*ΠC5-N6 0.36725 \*ΠC1-C2 0.27861 121.45 0.02 0.079

\*ΠC3-C4 0.35004 236.93 0.01 0.084

Table S4: Second Order Perturbation Theory Analysis of Fock Matrix on NBO of Isoniazid OH 1

Donor Occupancy Acceptor Occupancy E2 [Kcal/mol] E (j) – (i) [a. u.] F (i, j) [a. u.]

NBO (j) NBO (i)

Π C1-C6 1.69236 \*ΠC2-C3 0.03700 11.60 0.32 0.055

\*ΠC4-C5 0.31238 28.85 0.32 0.086

ΠC2-C3 1.67704 \*ΠC1-N6 0.42286 27.96 0.27 0.079

\*ΠC4-C5 0.31238 15.57 0.28 0.059

ΠC4-C5 1.66207 \*ΠC1-N6 0.42286 14.44 0.26 0.056

\*ΠC2-C3 0.33828 24.79 0.28 0.011

LP(1)N6 1.90600 \*ΠC1-C2 0.03700 10.98 0.88 0.089

\*ΠC4-C5 0.31238 9.83 0.90 0.086

LP(1)N12 1.73518 \*ΠC10-O11 0.27000 46.56 0.32 0.109

LP(2)O11 1.85828 \*ΠC3-C10 0.07288 20.70 0.65 0.105

\*ΠC10-N12 0.08646 27.93 0.69 0.125

LP(2)O17 1.85677 \*ΠC1-N6 0.42286 34.00 0.32 0.101

\*ΠC1-N6 0.42286 \*ΠC2-C3 0.03700 180.40 0.02 0.085

\*ΠC4-C5 0.31238 167.74 0.02 0.079

\*ΠC2-C3 0.33828 \*ΠC10-O11 0.27000 82.66 0.02 0.070

Table S5: Second Order Perturbation Theory Analysis of Fock Matrix on NBO of Isoniazid OH 2

Donor Occupancy Acceptor Occupancy E2 [Kcal/mol] E (j) – (i) [a. u.] F (i, j) [a. u.]

NBO (j) NBO (i)

Π C1-C6 1.75413 \*ΠC2-C3 0.40723 14.91 0.31 0.063

\*ΠC4-C5 0.31222 21.62 0.32 0.075

ΠC2-C3 1.60921 \*ΠC1-N6 0.33985 19.45 0.28 0.066

\*ΠC4-C5 0.30222 20.90 0.29 0.071

\*ΠC10-O11 0.34028 24.04 0.26 0.071

ΠC4-C5 1.68930 \*ΠC1-N6 0.33985 18.23 0.28 0.064

\*ΠC2-C3 0.40723 17.05 0.28 0.063

LP(1)N6 1.92225 \*ΠC1-C2 0.03580 10.33 0.87 0.085

\*ΠC4-C5 0.30222 9.83 0.91 0.086

LP(1)N12 1.72320 \*ΠC10-O11 0.34028 61.97 0.28 0.119

LP(2)O11 1.84724 \*ΠC3-C10 0.05729 12.72 0.71 0.087

LP(1)O11 1.96550 \*ΠC3-C10 0.05729 5.05 1.10 0.067 LP(2)O17 1.81447 \*ΠC2-C3 0.40723 38.78 0.32 0.105 \*ΠC10-O11 0.34028 \*ΠC2-C3 0.03580 141.83 0.02 0.072

Table S6: Second Order Perturbation Theory Analysis of Fock Matrix on NBO of Isoniazid OH 4

Donor Occupancy Acceptor Occupancy E2 [Kcal/mol] E (j) – (i) [a. u.] F (i, j) [a. u.]

NBO (j) NBO (i)

Π C1-C2 1.62380 \*ΠC3-C4 0.39461 20.46 0.27 0.066

\*ΠC5-N6 0.40020 21.67 0.25 0.067

ΠC3-C4 1.62284 \*ΠC1-C2 0.28517 18.60 0.30 0.068

\*ΠC5-N6 0.40020 23.80 0.27 0.072

\*ΠC10-O11 0.31173 15.78 0.30 0.062

ΠC5-N6 1.74526 \*ΠC1-C2 0.28517 20.64 0.33 0.075

\*ΠC3-C4 0.39461 15.07 0.32 0.064

LP(1)N6 1.92154 \*ΠC1-C2 0.28517 9.34 0.92 0.084

\*ΠC4-C5 0.03625 10.43 0.87 0.086

LP(1)N12 1.71208 \*ΠC10-O11 0.31173 63.31 0.28 0.120

LP(2)O11 1.85405 \*ΠC3-C10 0.07689 21.84 0.63 0.107

\*ΠC10-N12 0.08161 26.60 0.70 0.124

LP(1)O17 1.96475 \*ΠC4-C5 0.03625 5.26 1.15 0.070 \*ΠC3-C4 0.39461 24.68 0.36 0.091

\*ΠC3-C4 0.39461 \*ΠC1-C2 0,28517 145.63 0.02 0.072

\*ΠC10-O11 0.07689 174.77 0.01 0.072

\*ΠC5-N6 0.40020 \*ΠC1-C2 0.28517 89.00 0.03 0.080

\*ΠC3-C4 0.39461 282.82 0.01 0.085

Table S7: Second Order Perturbation Theory Analysis of Fock Matrix on NBO of Isoniazid OH 5

Donor Occupancy Acceptor Occupancy E2 [Kcal/mol] E (j) – (i) [a. u.] F (i, j) [a. u.]

NBO (j) NBO (i)

Π C1-C2 1.64102 \*ΠC3-C4 0.35906 26.18 0.27 0.075

\*ΠC5-N6 0.41630 15.66 0.26 0.057

ΠC3-C4 1,98189 \*ΠC1-C2 0.28697 14.20 0.30 0.058

\*ΠC5-N6 0.41630 27.26 0.27 0.079

\*ΠC10-O11 0.25530 11.78 0.32 0.056

ΠC5-N6 1.70147 \*ΠC1-C2 0.28697 26.67 0.33 0.084

\*ΠC3-C4 0.36906 11.09 0.32 0.054

LP(1)N6 1.90522 \*ΠC1-C2 0.02438 9.46 0.91 0.084

\*ΠC4-C5 1,98403 11.40 0.86 0.090

LP(1)N12 1.74332 \*ΠC10-O11 0.25530 40.02 0.34 0.104

LP(2)O11 1.8566 \*ΠC3-C10 0.07238 20.81 0.65 0.105

\*ΠC10-N12 0.08856 28.22 0.68 0.125

LP(1)O17 1.86099 \*ΠC5-N6 0.41630 33.27 0.33 0.100

\*ΠC3-C4 0.35906 \*ΠC1-C2 0.28697 215.08 0.01 0.080

\*ΠC10-O11 0.25530 45.60 0.04 0.069

\*ΠC5-N6 0.41630 \*ΠC1-C2 0.28697 102.79 0.03 0.077

\*ΠC3-C4 0.35906 245.78 0.01 0.083

Table S8: Second Order Perturbation Theory Analysis of Fock Matrix on NBO of Isoniazid OH N

Donor Occupancy Acceptor Occupancy E2 [Kcal/mol] E (j) – (i) [a. u.] F (i, j) [a. u.]

NBO (j) NBO (i)

LP(1)C3 0.70875 \*ΠC1-C2 0.09887 21.66 0.23 0.079

\*ΠC4-C5 0.01717 25.70 0,21 0.102

\*ΠC11-O12 0.18680 31.23 0.21 0.108

LP(1)N6 0.94643 \*ΠC1-C2 0.09887 3.72 0.45 0.053

\*ΠC4-C5 0.01717 4.33 0.42 0.056

LP(1)N13 0.90076 \*ΠC11-O12 0.18680 14.10 0.35 0.098

LP(2)O12 0.93196 \*ΠC3-C10 0.03156 9.46 0.69 0.104

\*ΠC11-N13 0.04405 14.01 0.66 0.123

\*ΠC1-C2 0.09887 \*ΠC1-C2 0.00643 4.95 0.46 0.177

\*ΠC4-C5 0.01717 \*ΠC4-C5 0.01717 4.33 0.48 0.160

\*ΠC11-O12 0.18680 \*ΠC11-O12 0.00923 5.89 0.50 0.150

Table S9: Binding Energies for studied molecules

System Electronic Energy (a. u.) Electronic Energy ( Kcal/mol)

OH -75.739015 -47,526

INH -472.331243 -296,389

INH OH 1 -547.563596 -343,597

Binding Energy 0.506752 317.988

OH -75.739015 -47,526

INH -472.331243 -296,389

INH OH 2 -547.567260 -343,600

Binding Energy 0.502998 315.633

OH -75.739015 -47,526

INH -472.331243 -296,389

INH OH 4 -547.558703 -343,694

Binding Energy 0.511555 321.0023

OH -75.739015 -47,526

INH -472.331243 -296,389

INH OH 5 -547.561845 -343,596

Binding Energy 0.508413 319.0360

OH -75.739015 -47,526

INH -472.331243 -296,389

INH OH N -548.066931 -343,913

Binding Energy 0.003327 2.0877

Table S10: Dipole Moment of Studied Molecules

System Dipole moment (Debye)

INH 4.74865

INH OH1 4.62283

INH OH 2 6.12820

INH OH 4 5.51269

INH OH 5 5.97766

INH OH N 5.97766

OH 1.85767