

Supporting information

Solvent- and functional-group-assisted tautomerism of 3-alkyl substituted 5-(2-pyridyl)-1,2,4-triazoles in DMSO-Water

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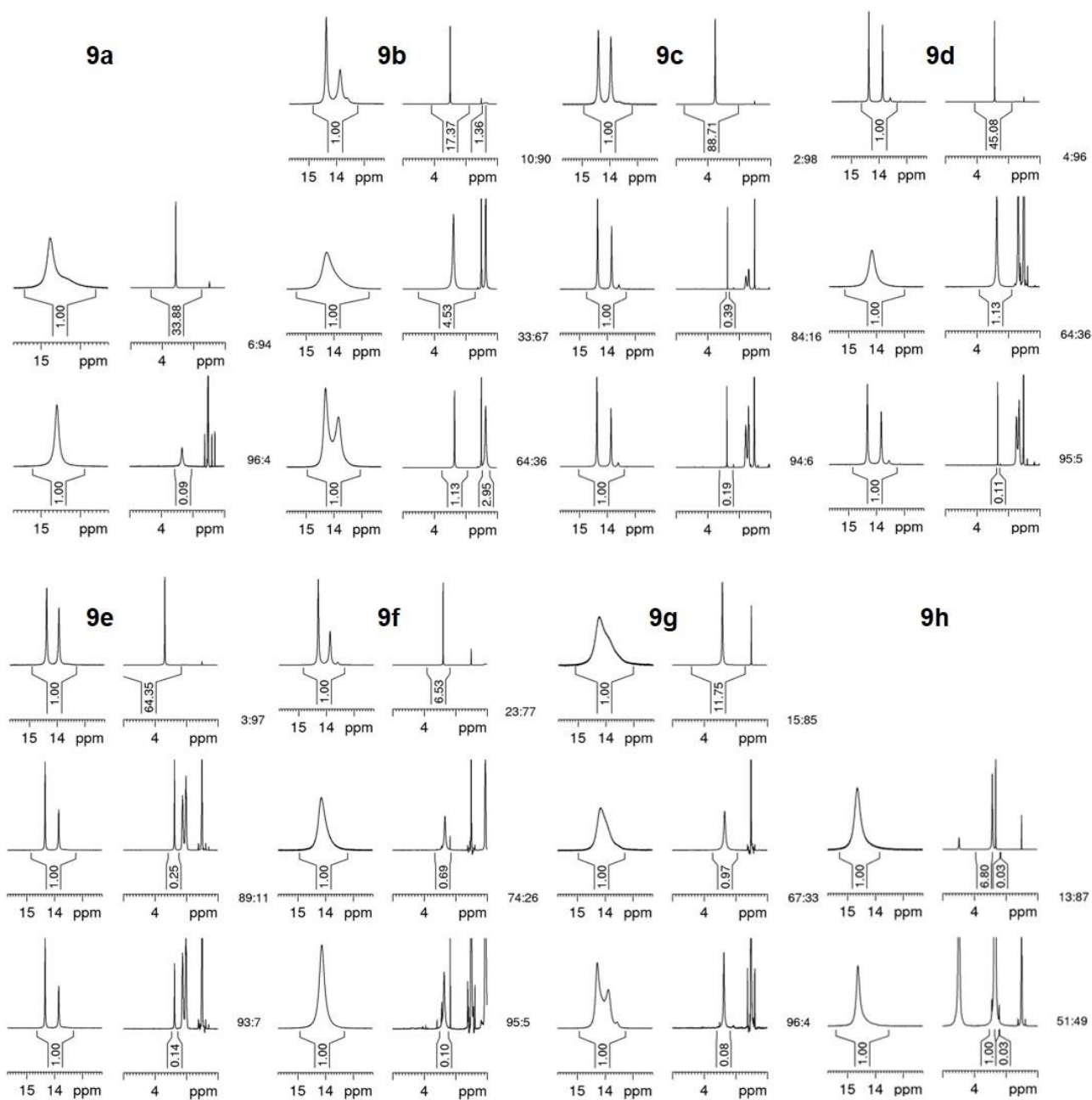


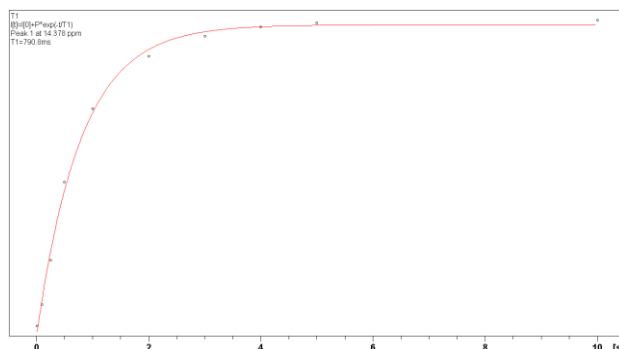
Figure S1. Expansions of the NH and H₂O signals of the ^1H NMR spectra of compounds **9a-9h** with increasing amounts of H₂O (from bottom to top). The ratio **9**:H₂O is indicated on the right of the NMR spectra. For **9h**, the integral of the H₂O signal has been obtained by integrating half the signal and subtracting the integral of one of the OMe ^{13}C satellites due to the overlap of the H₂O and OMe signals.

INTENSITY fit : $I[t]=I[0]+P*\exp(-t/T1)$

10 points for Peak 1, Peak Point at 14.378 ppm

$I[0] = 9.713e-001$; $P = -1.915e+000$; $T1 = 790.788$ ms; SD = 3.452e-002

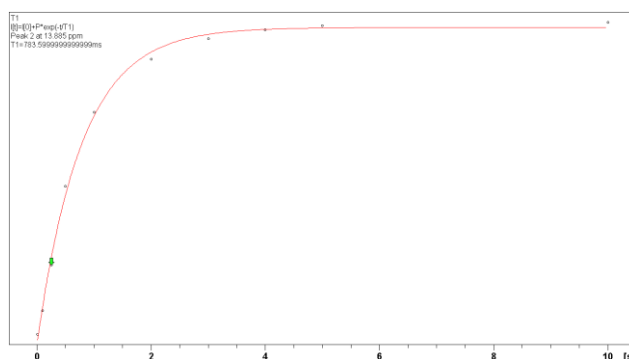
tau	ppm	integral	intensity
10.000m	14.378	-1.1314e+007	-1.4254e+006
100.000m	14.378	-9.5841e+006	-1.2153e+006
250.000m	14.378	-5.9609e+006	-7.7034e+005
500.000m	14.376	3.9622e+005	6752.8
1.000s	14.378	6.5521e+006	7.3668e+005
2.000s	14.378	1.106e+007	1.2579e+006
3.000s	14.378	1.2946e+007	1.4597e+006
4.000s	14.378	1.3816e+007	1.5483e+006
5.000s	14.378	1.4274e+007	1.5885e+006
10.000s	14.378	1.4981e+007	1.6182e+006



10 points for Peak 2, Peak Point at 13.885 ppm

$I[0] = 9.701e-001$; $P = -1.904e+000$; $T1 = 783.595$ ms; SD = 3.269e-002

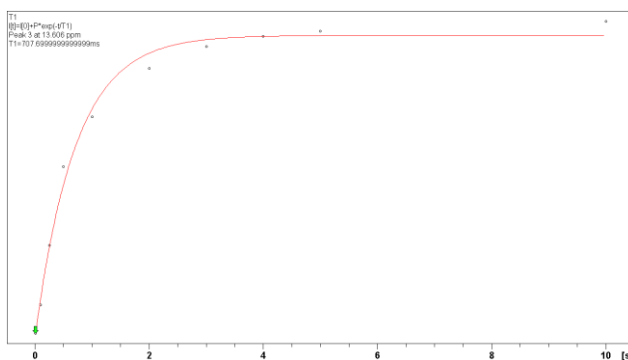
tau	ppm	integral	intensity
10.000m	13.883	-8.9749e+006	-1.0352e+006
100.000m	13.882	-7.4661e+006	-8.6828e+005
250.000m	13.882	-4.601e+006	-5.431e+005
500.000m	13.881	4.1777e+005	16118
1.000s	13.882	5.2829e+006	5.4368e+005
2.000s	13.882	8.8438e+006	9.1933e+005
3.000s	13.882	1.0324e+007	1.065e+006
4.000s	13.882	1.1004e+007	1.1288e+006
5.000s	13.882	1.1359e+007	1.1585e+006
10.000s	13.882	1.1884e+007	1.1804e+006



10 points for Peak 3, Peak Point at 13.606 ppm

$I[0] = 9.236e-001$; $P = -1.677e+000$; $T1 = 707.724$ ms; SD = 5.306e-002

tau	ppm	integral	intensity
10.000m	13.605	-4.9625e+005	-54153
100.000m	13.604	-3.1041e+005	-42445
250.000m	13.605	-1228	-18052
500.000m	13.603	4.9998e+005	14327
1.000s	13.604	8.3465e+005	34807
2.000s	13.605	1.1495e+006	54738
3.000s	13.604	1.3502e+006	63735
4.000s	13.604	1.4568e+006	67946
5.000s	13.604	1.5534e+006	69933
10.000s	13.604	1.8239e+006	73908



10 points for Peak 6, Peak Point at 3.450 ppm

$I[0] = 9.462e-001$; $P = -1.951e+000$; $T1 = 561.890$ ms; SD = 5.495e-002

tau	ppm	integral	intensity
10.000m	3.450	-1.122e+009	-4.1017e+008
100.000m	3.450	-8.438e+008	-3.1389e+008
250.000m	3.450	-3.2756e+008	-1.1888e+008
500.000m	3.449	2.2689e+008	1.0132e+008
1.000s	3.449	6.001e+008	2.2683e+008
2.000s	3.449	9.8795e+008	3.4514e+008
3.000s	3.449	1.148e+009	3.9053e+008
4.000s	3.449	1.2178e+009	4.1007e+008
5.000s	3.449	1.2491e+009	4.1769e+008
10.000s	3.450	1.2688e+009	4.2528e+008

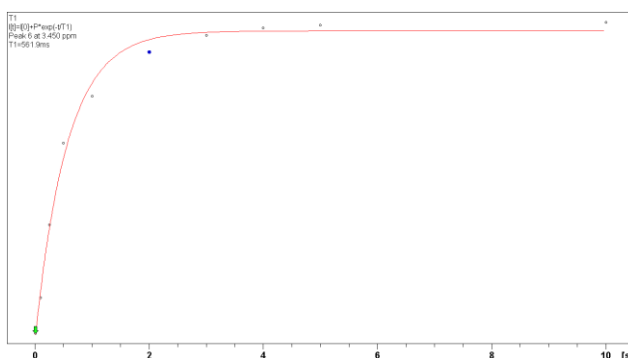


Figure S2. Inversion-recovery measurement of T_1 for the NH and H₂O signals of **9d** in DMSO-*d*₆ at 17 °C, ratio triazoles:H₂O of 4:96.

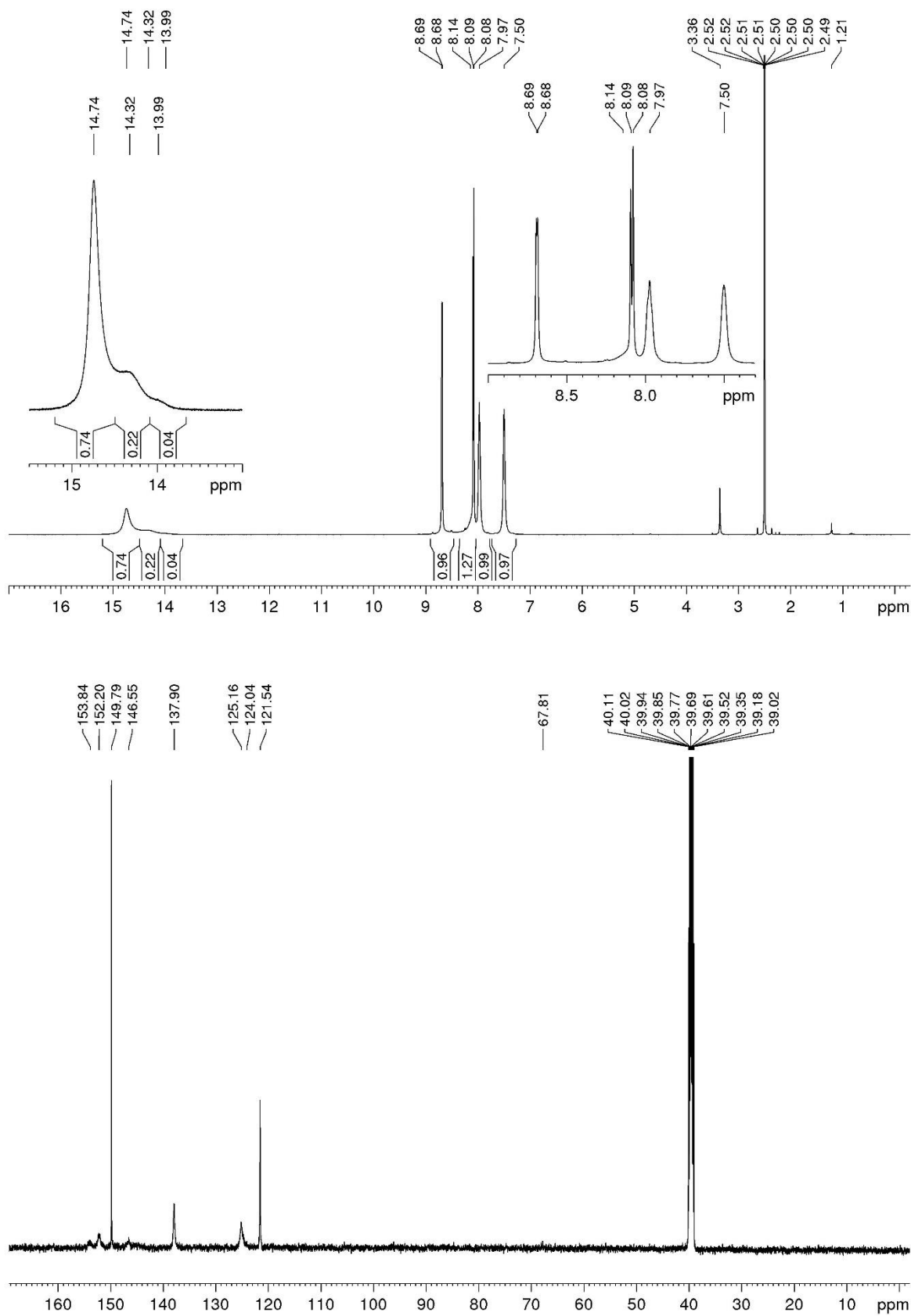


Figure S3. (Top) ^1H - (500.13 MHz) and (bottom) ^{13}C -NMR (125.76 MHz) spectra of pyridinetriazol **9a** in $\text{DMSO-}d_6$ at 17 °C.

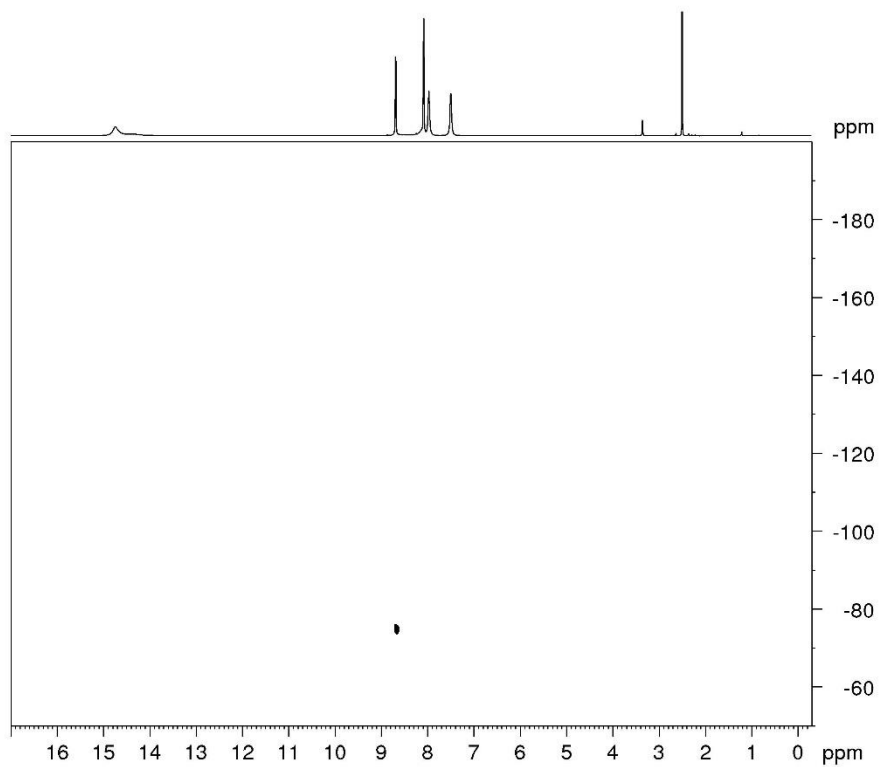


Figure S4. ^1H , ^{15}N HMQC (500.13 MHz) spectrum of pyridinetriazol **9a** in $\text{DMSO-}d_6$ at 17 °C. The broad singlet of H3 narrowed to a signal of half line-width of 8.5 Hz upon heating at 110 °C. However, no ^1H , ^{15}N correlations were observed.

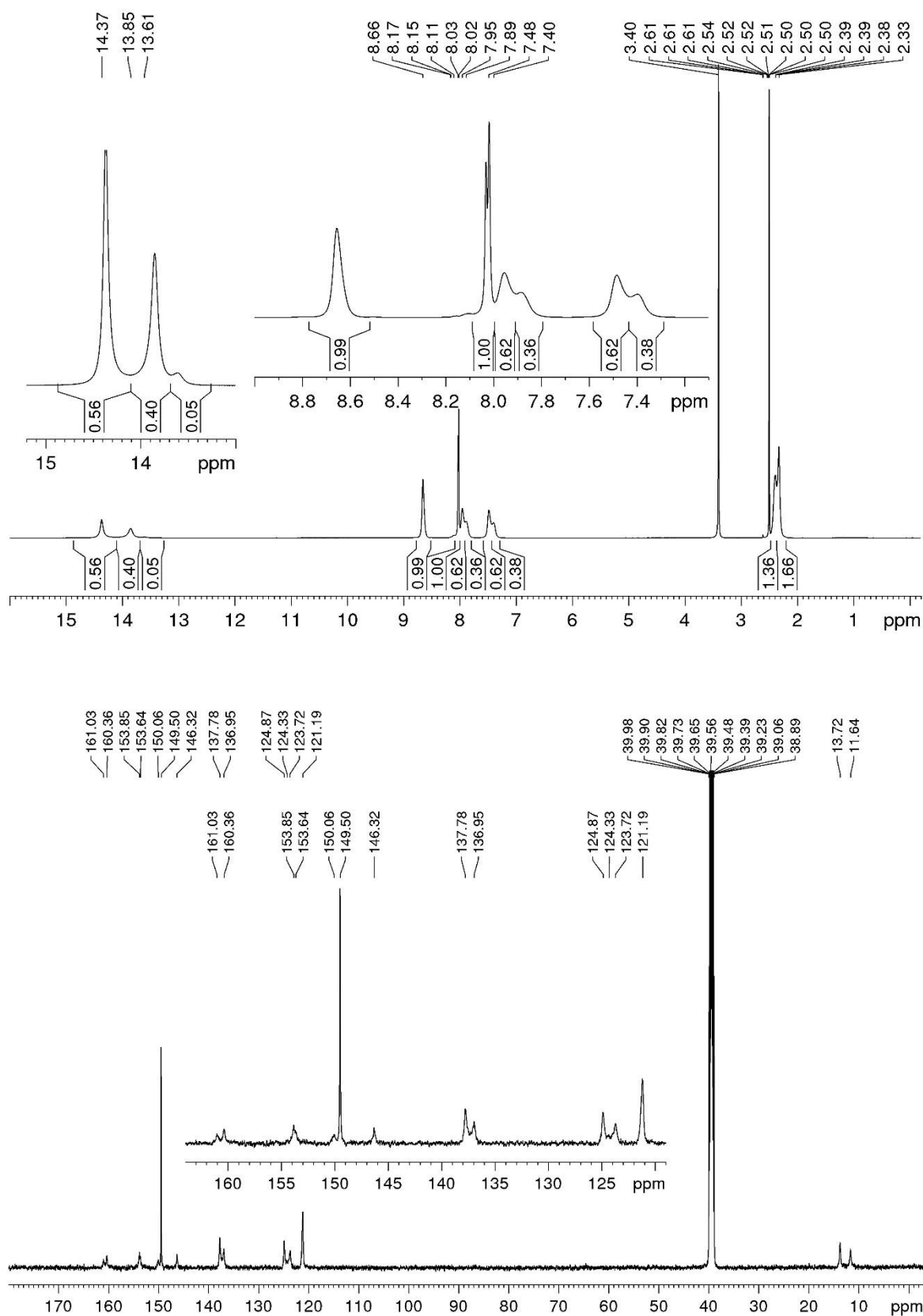


Figure S5. (Top) ¹H- (600.13 MHz) and (bottom) ¹³C-NMR (125.76 MHz) spectra of pyridinetriazol **9b** in DMSO-*d*₆ at 17 °C.

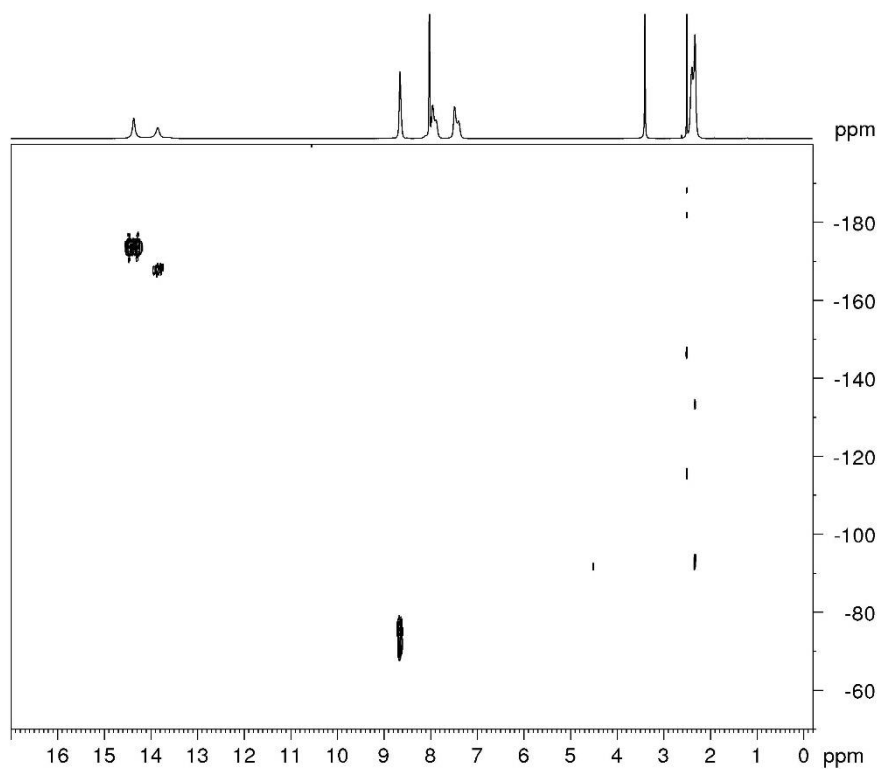


Figure S6. $^1\text{H},^{15}\text{N}$ HMQC (600.13 MHz) spectrum of pyridinetriazol **9b** in $\text{DMSO-}d_6$ at 17 °C.

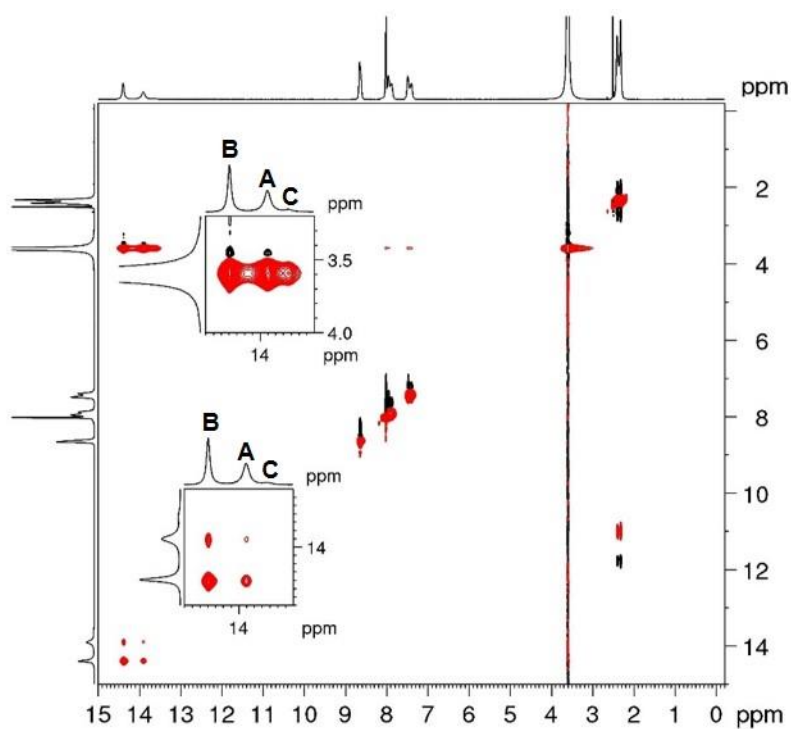


Figure S7. ^1H EXSY spectrum (500.13 MHz, negative peaks in red) of pyridinetriazol **9b** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 6:94, mixing time of 25 ms.

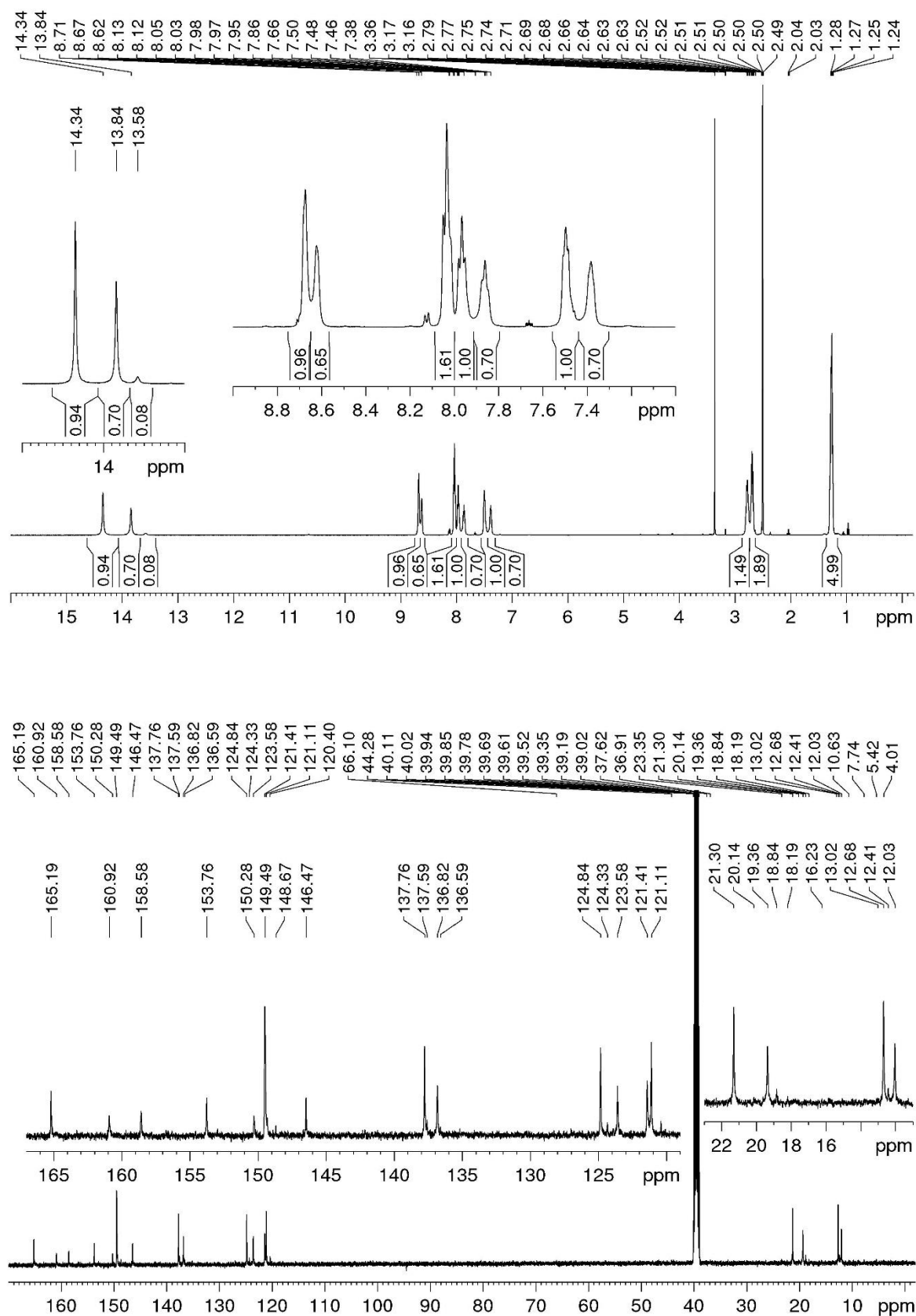


Figure S8. (Top) ¹H- (500.13 MHz) and (bottom) ¹³C-NMR (125.76 MHz) spectra of pyridinetriazol **9c** in DMSO-*d*₆ at 17 °C.

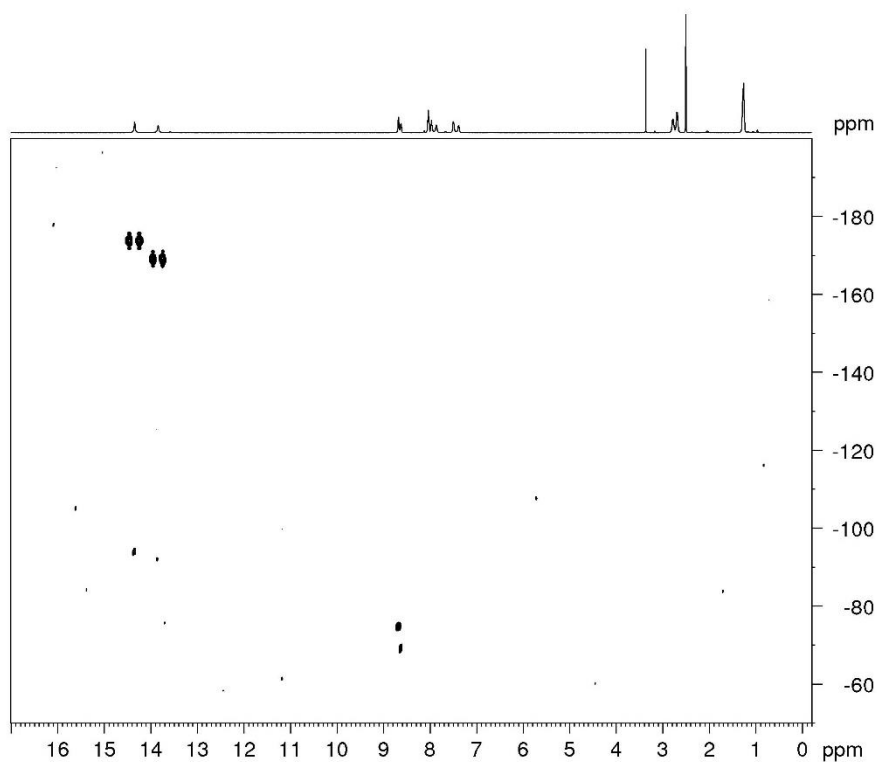


Figure S9. ^1H , ^{15}N HMQC spectrum (500.13 MHz) of pyridinetriazol **9c** in $\text{DMSO-}d_6$ at 17 °C.

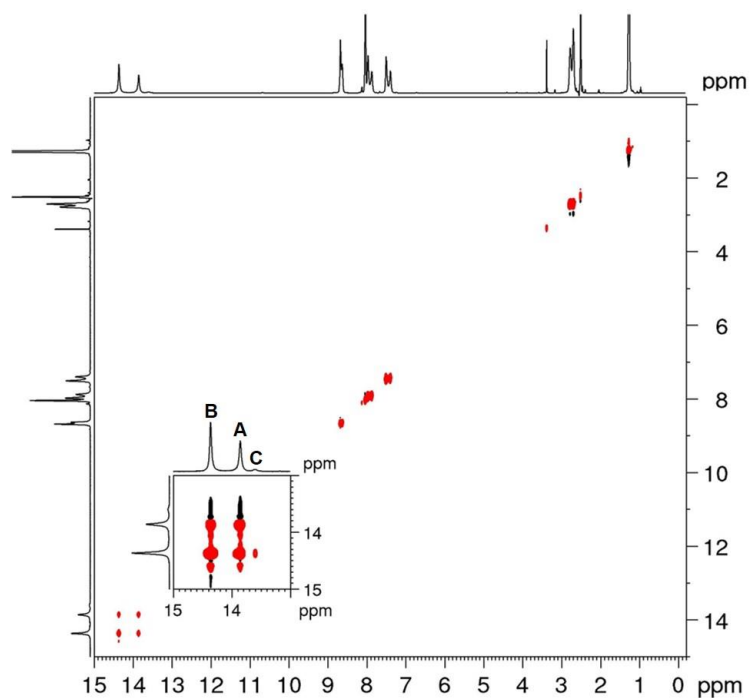


Figure S10. ^1H EXSY spectrum (600.13 MHz, negative peaks in red) of pyridinetriazol **9c** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 94:6, mixing time of 25 ms. The inset shows the expansion of the NH region at a lower threshold. The peaks detected do not allow to obtain the exchange parameters of tautomer **C**.

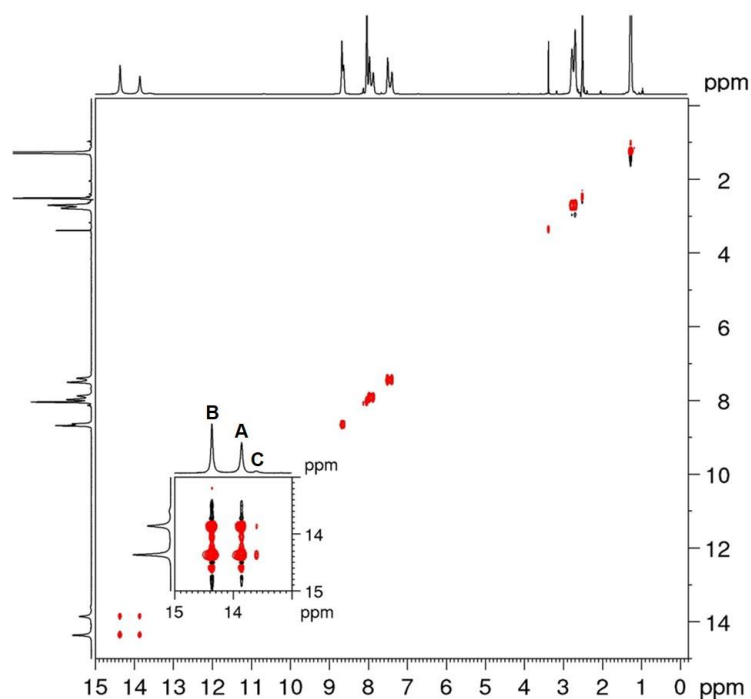


Figure S11. ^1H EXSY spectrum (600.13 MHz, negative peaks in red) of pyridinetriazol **9c** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 94:6, mixing time of 50 ms. The inset shows the expansion of the NH region at a lower threshold. The peaks detected do not allow to obtain the exchange parameters of tautomer **C**.

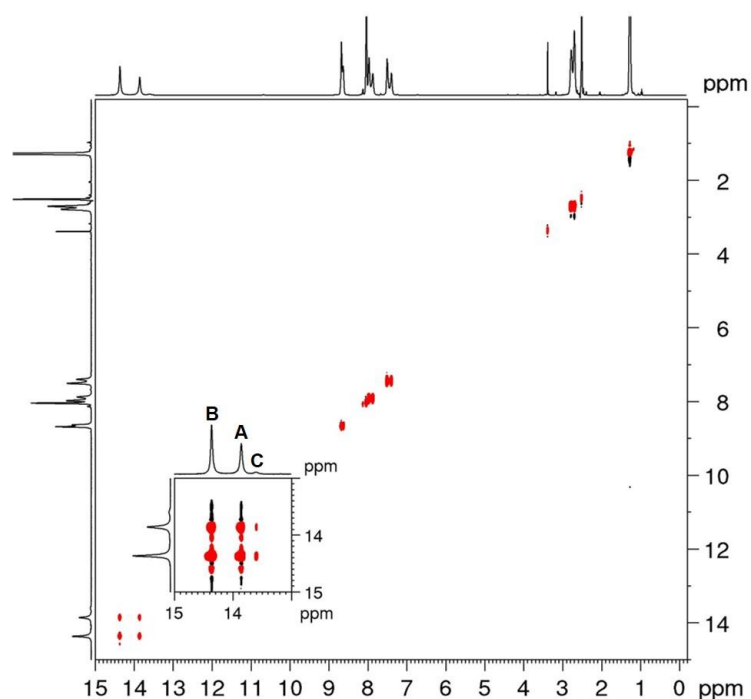


Figure S12. ^1H EXSY spectrum (600.13 MHz, negative peaks in red) of pyridinetriazol **9c** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 94:6, mixing time of 100 ms. The inset shows the expansion of the NH region at a lower threshold. The peaks detected do not allow to obtain the exchange parameters of tautomer **C**.

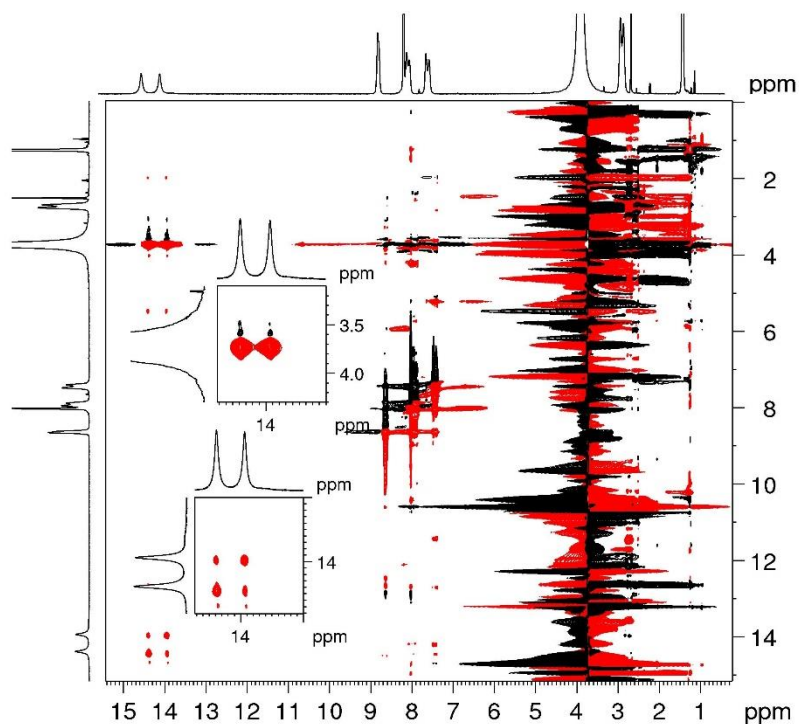


Figure S13. ^1H EXSY spectrum (500.13 MHz, negative peaks in red) of pyridinetriazol **9c** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 2:98, mixing time of 25 ms.

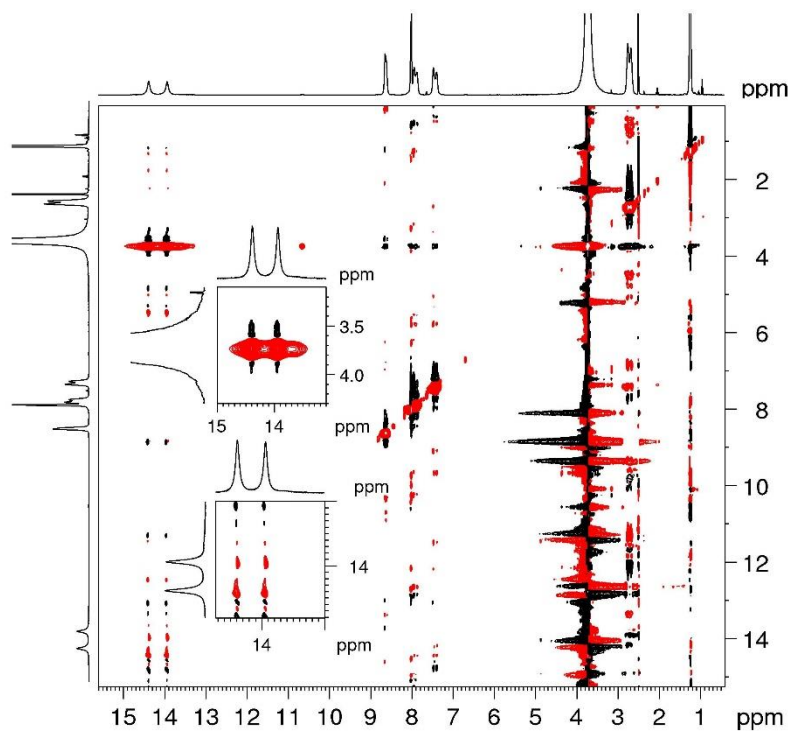


Figure S14. ^1H EXSY spectrum (500.13 MHz, negative peaks in red) of pyridinetriazol **9c** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 2:98, mixing time of 50 ms.

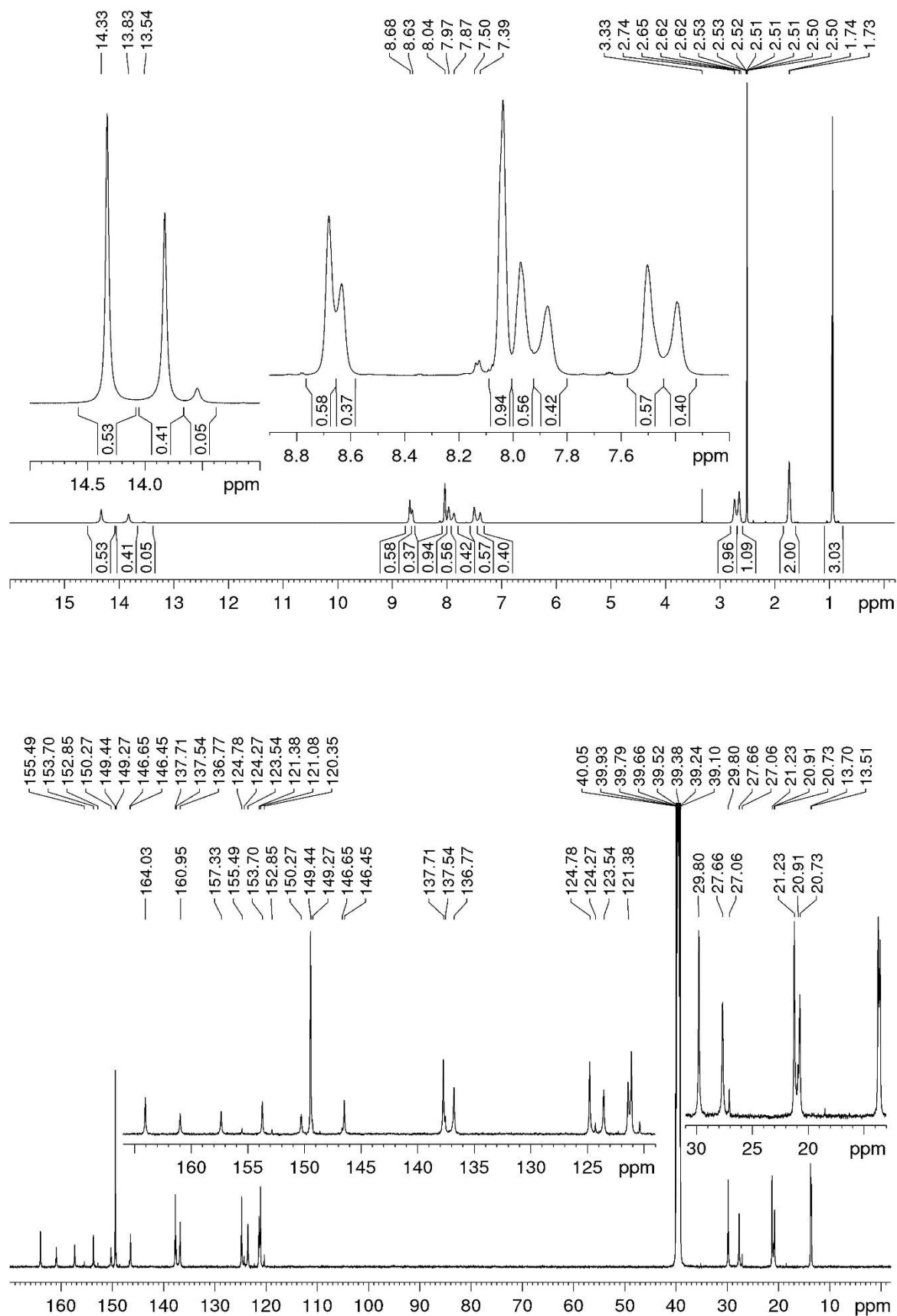


Figure S15. (Top) ^1H - (600.13 MHz) and (bottom) ^{13}C -NMR (150.9 MHz) spectra of pyridinetriazol **9d** in $\text{DMSO-}d_6$ at 17 °C.

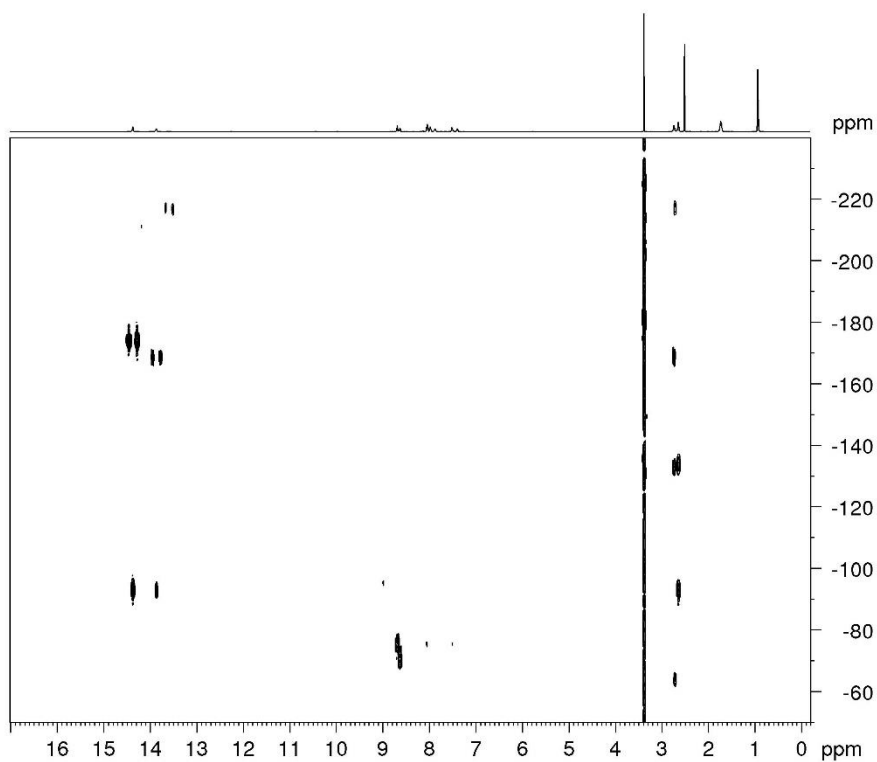


Figure S16. $^1\text{H},^{15}\text{N}$ HMQC spectrum (600.13 MHz) of pyridinetriazol **9d** optimized for $J_{\text{NH}} = 10$ Hz in $\text{DMSO}-d_6$ at 17°C .

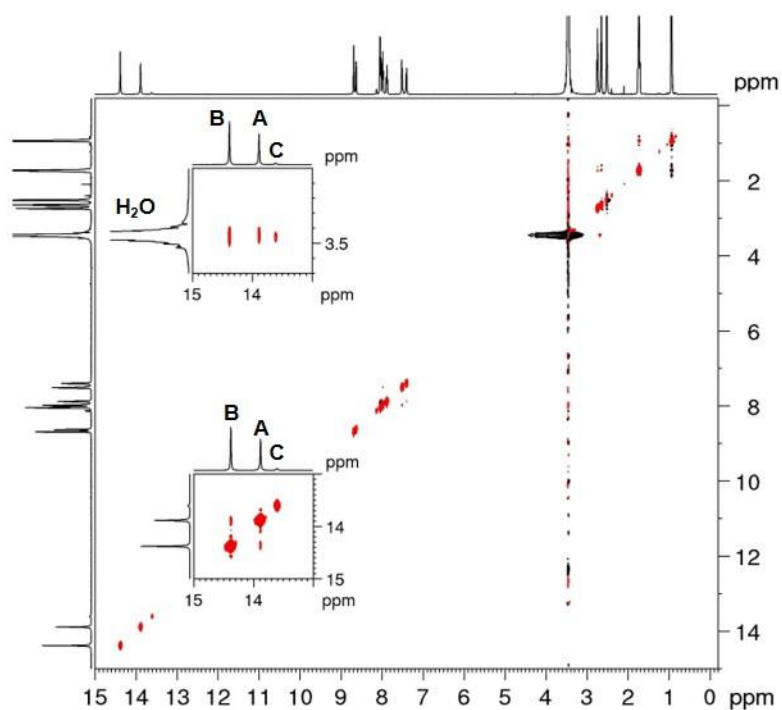


Figure S17. ^1H EXSY spectra (600.13 MHz, negative peaks in red) of pyridinetriazol **9d** in $\text{DMSO}-d_6$ at 17°C , ratio triazoles: H_2O of 4:96, mixing time of 2.6 ms.

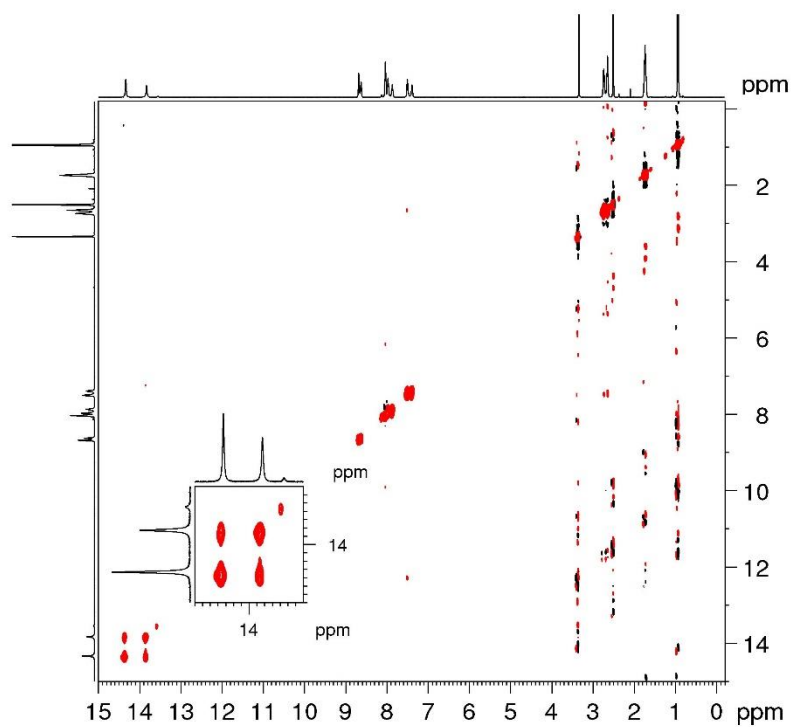


Figure S18. ^1H EXSY spectra (600.13 MHz, negative peaks in red) of pyridinetriazol **9d** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 58:42, mixing time of 50 ms.

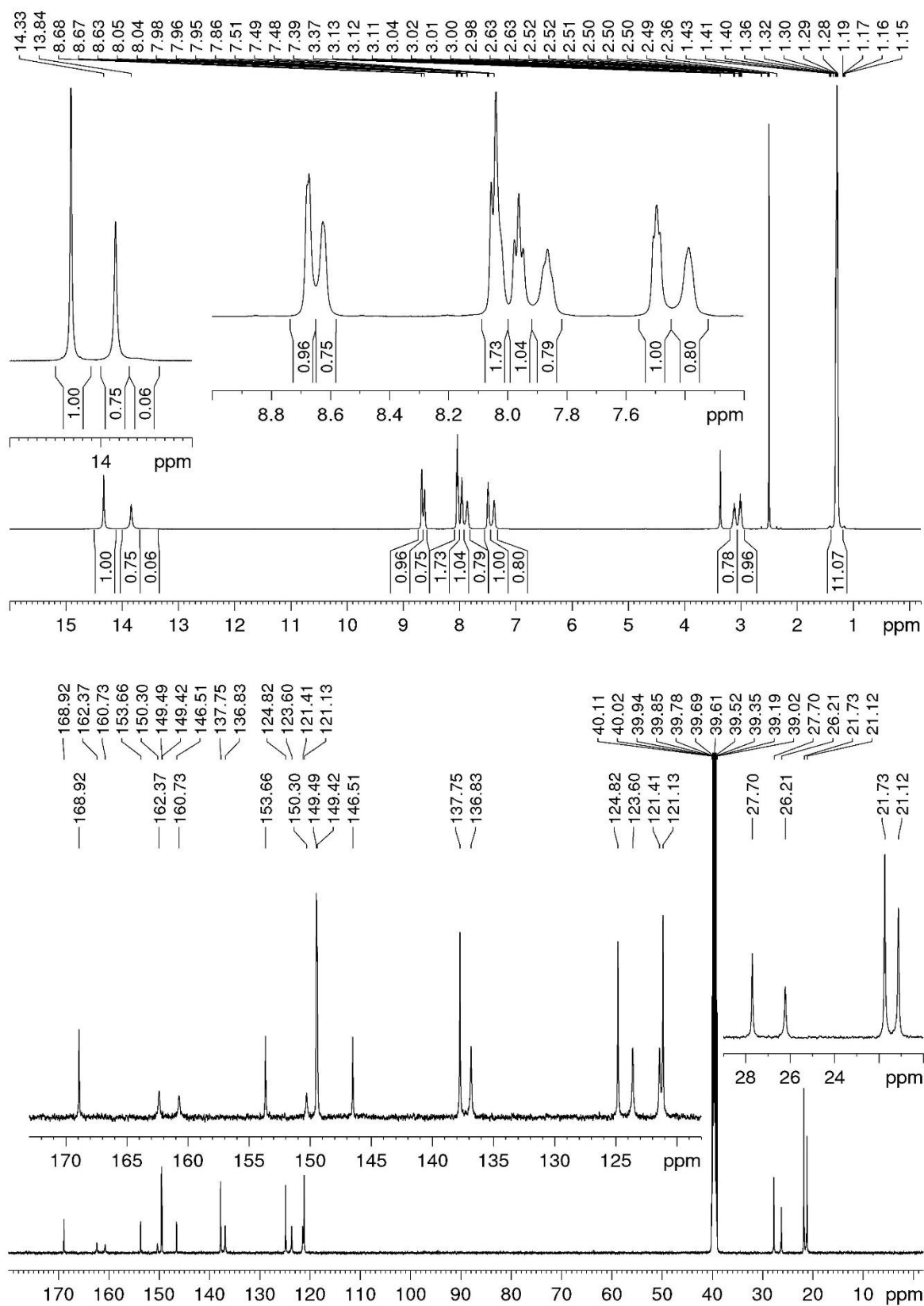


Figure S19. (Top) ¹H- (500.13 MHz) and (bottom) ¹³C-NMR (125.76 MHz) spectra of pyridinetriazol **9e** in DMSO-*d*₆ at 17 °C.

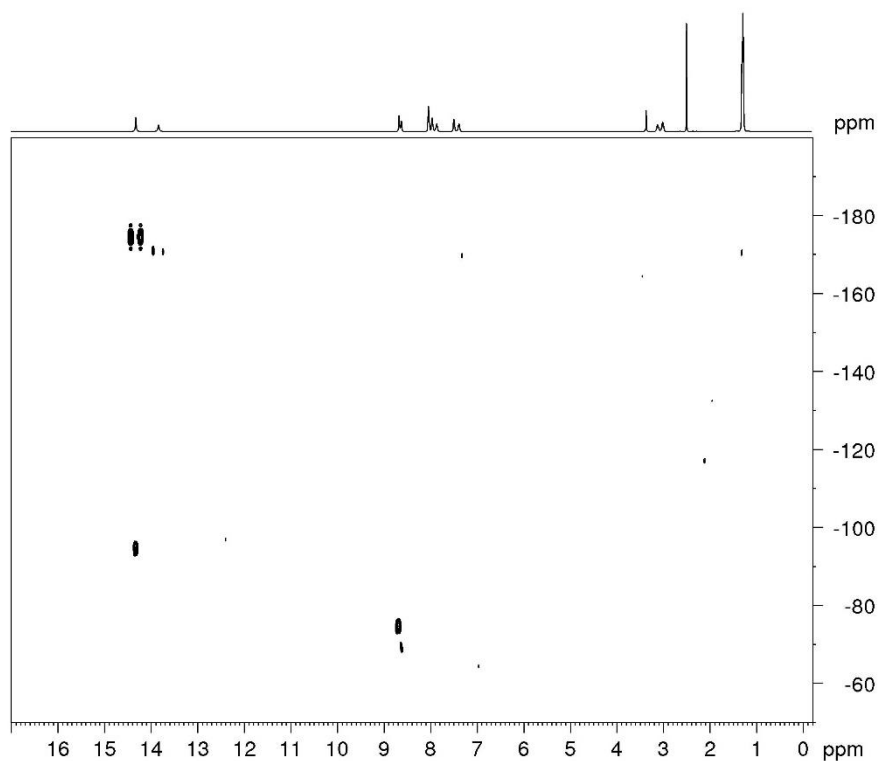


Figure S20. ^1H , ^{15}N HMQC spectrum (500.13 MHz) of pyridinetriazol **9e** in $\text{DMSO-}d_6$ at 17 °C.

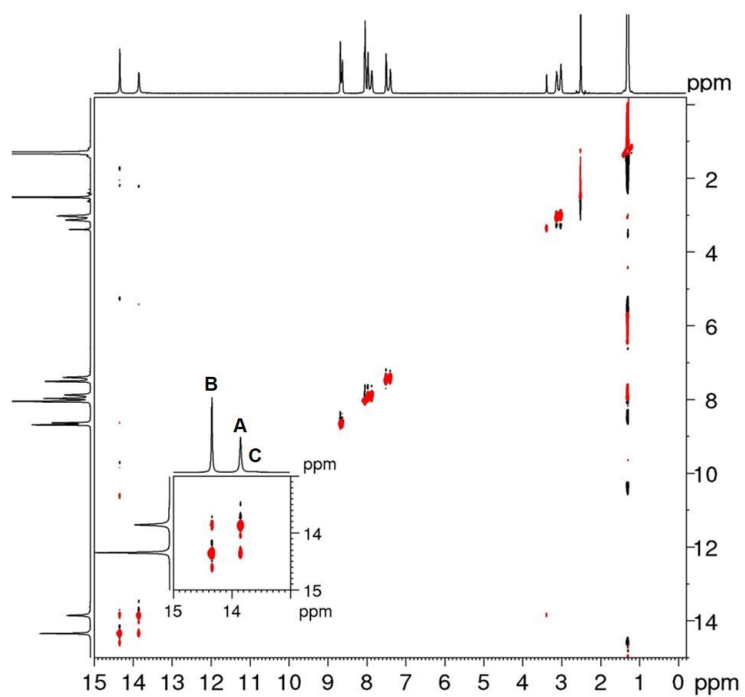


Figure S21. ^1H EXSY spectrum (600.13 MHz, negative peaks in red) of pyridinetriazol **9e** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 93:7, mixing time of 25 ms.

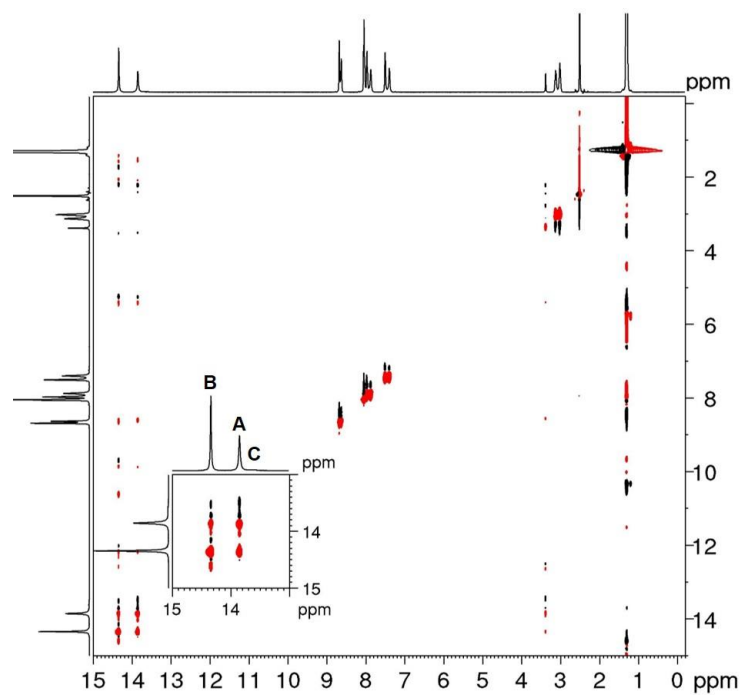


Figure S22. ^1H EXSY spectrum (600.13 MHz, negative peaks in red) of pyridinetriazol **9e** in $\text{DMSO-}d_6$ at 17 $^\circ\text{C}$, ratio triazoles: H_2O of 93:7, mixing time of 50 ms.

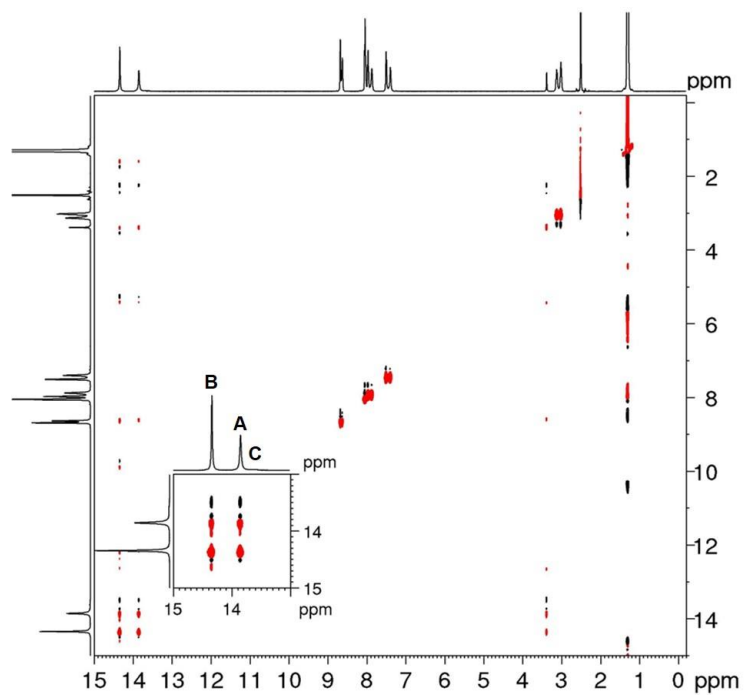


Figure S23. ^1H EXSY spectrum (600.13 MHz, negative peaks in red) of pyridinetriazol **9e** in $\text{DMSO-}d_6$ at 17 $^\circ\text{C}$, ratio triazoles: H_2O of 93:7, mixing time of 100 ms.

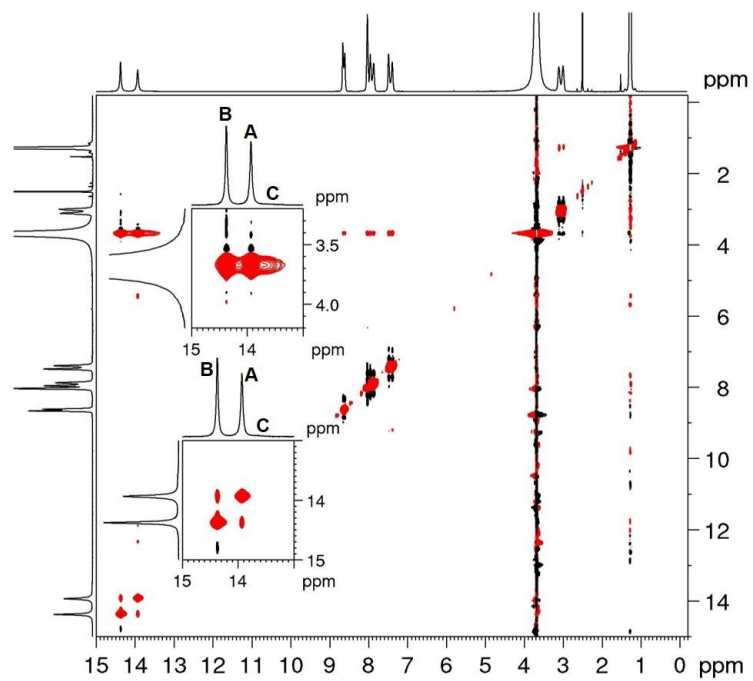


Figure S24. ^1H EXSY spectrum (500.13 MHz, negative peaks in red) of pyridinetriazol **9e** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 13:87, mixing time of 25 ms.

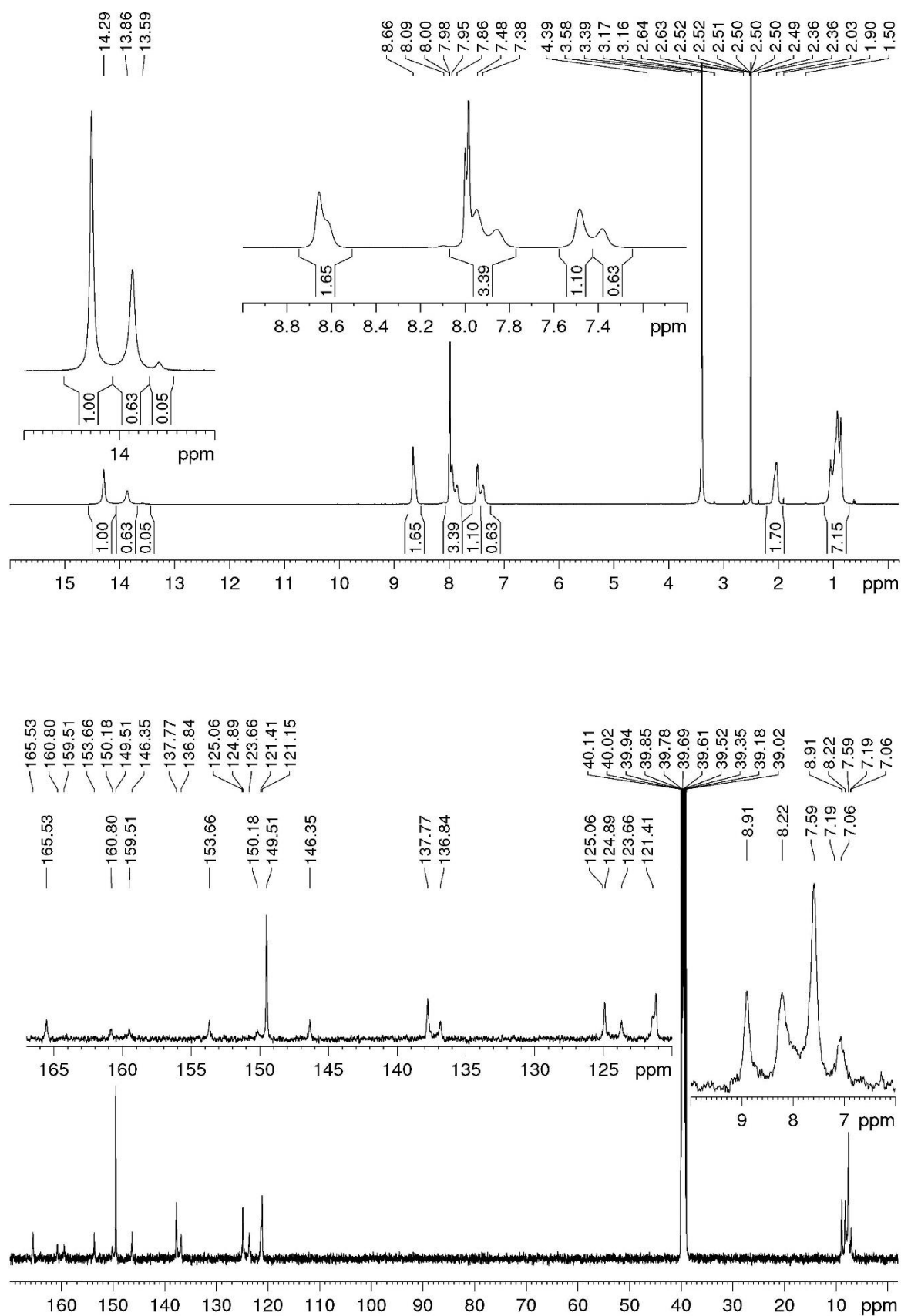


Figure S25. (Top) ¹H- (500.13 MHz) and (bottom) ¹³C-NMR (125.76 MHz) spectra of pyridinetriazol **9f** in DMSO-*d*₆ at 17 °C.

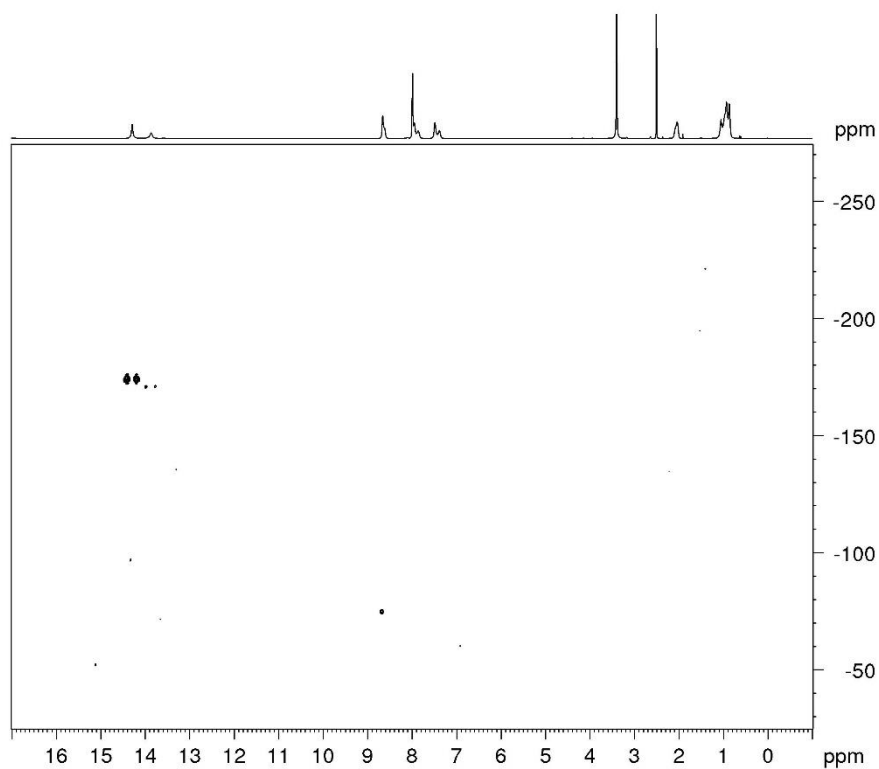


Figure S26. ^1H , ^{15}N HMQC spectrum (500.13 MHz) of pyridinetriazol **9f** in $\text{DMSO-}d_6$ at 17 °C.

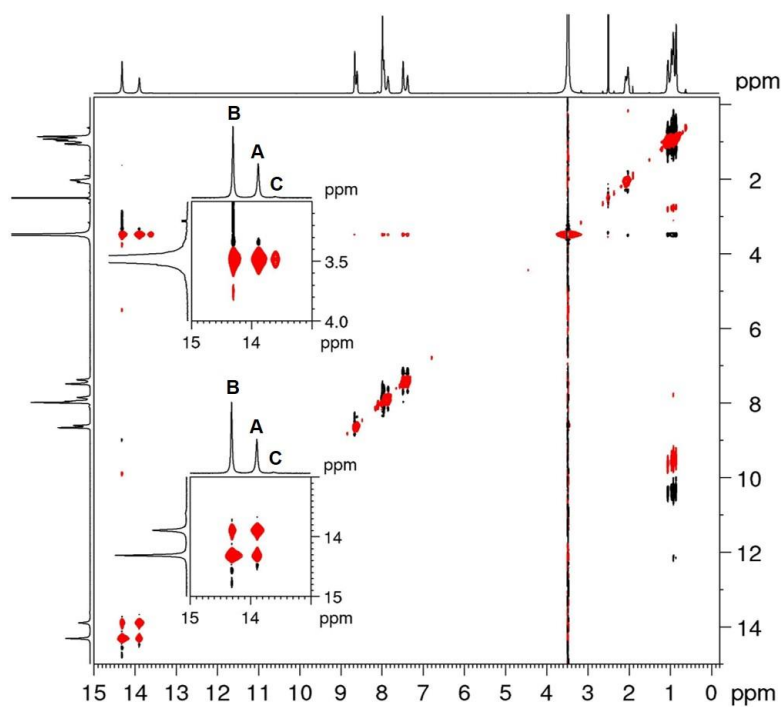


Figure S27. ^1H EXSY spectrum (500.13 MHz, negative peaks in red) of pyridinetriazol **9f** in $\text{DMSO-}d_6$ at 17 °C, ratio triazoles: H_2O of 13:87, mixing time of 25 ms.

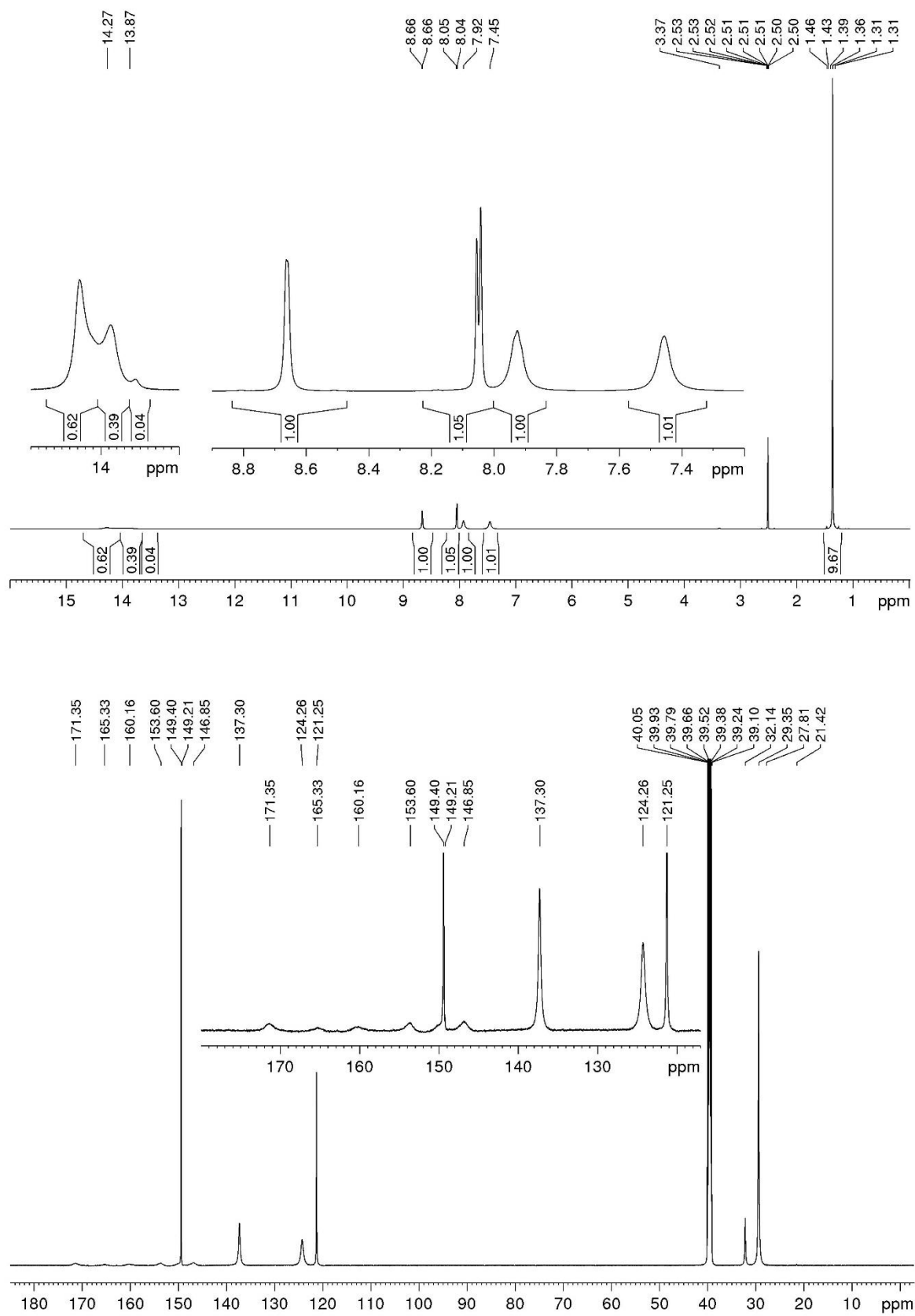


Figure S28. (Top) ¹H- (500.13 MHz) and (bottom) ¹³C-NMR (150.9 MHz) spectra of pyridinetriazol **9g** in DMSO-*d*₆ at 17 °C.

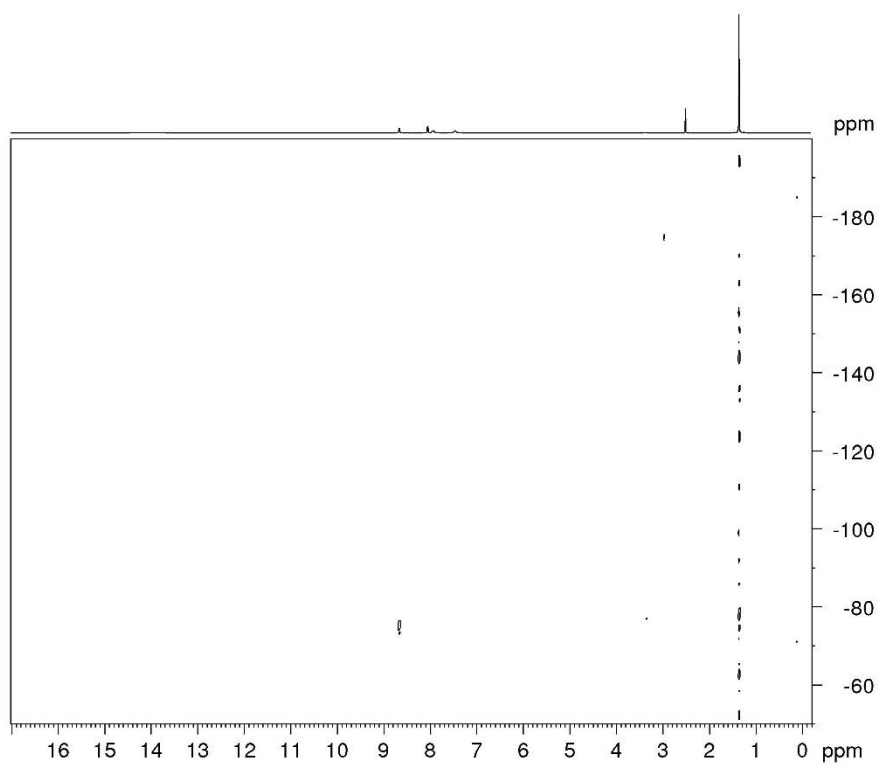


Figure S29. ^1H , ^{15}N HMQC spectrum (500.13 MHz) of pyridinetriazol **9g** in $\text{DMSO-}d_6$ at 17 °C.

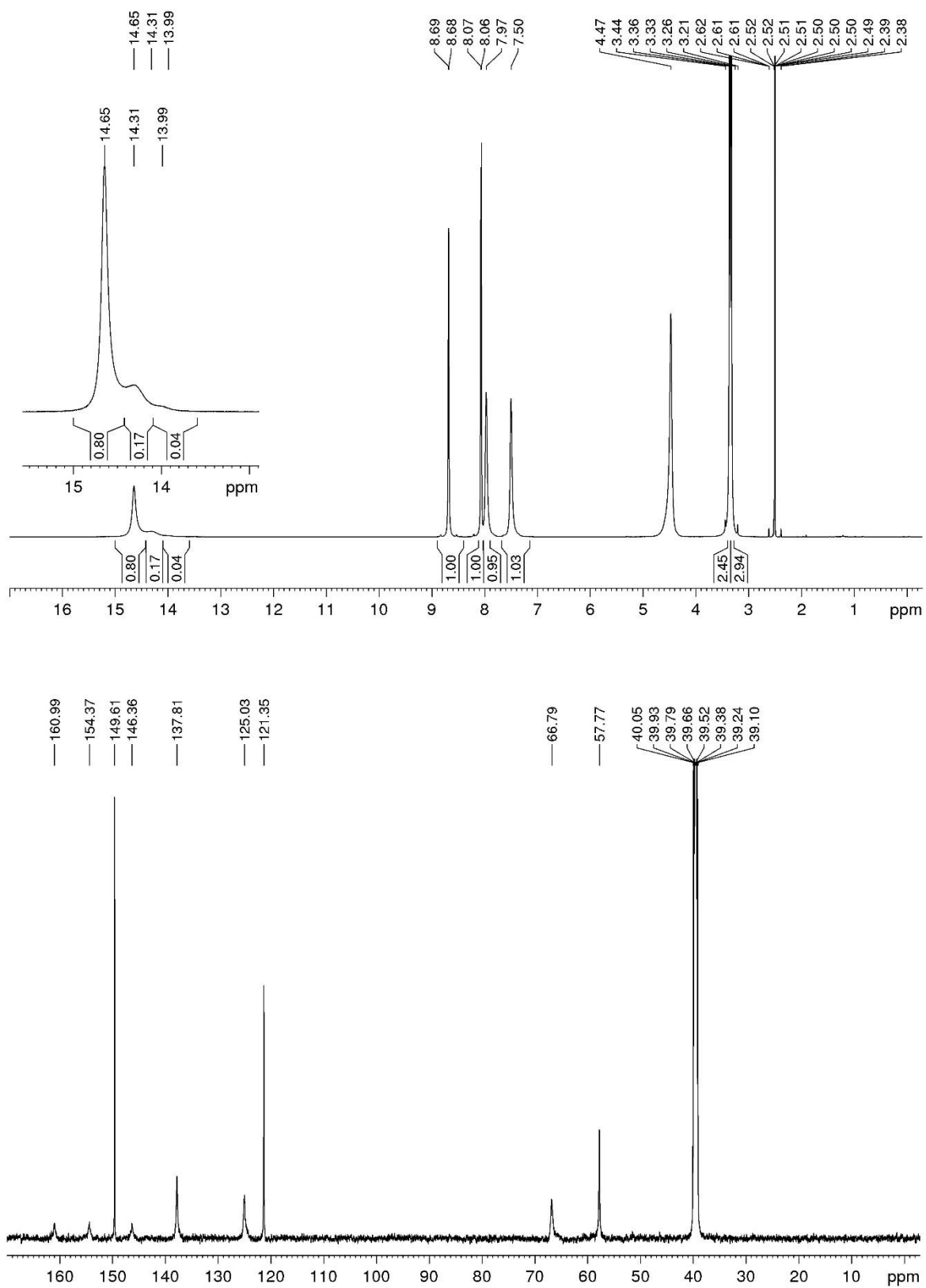


Figure S30. (Top) ¹H- (500.13 MHz) and (bottom) ¹³C-NMR (125.76 MHz) spectra of pyridinetriazol **9h** in DMSO-*d*₆ at 17 °C.

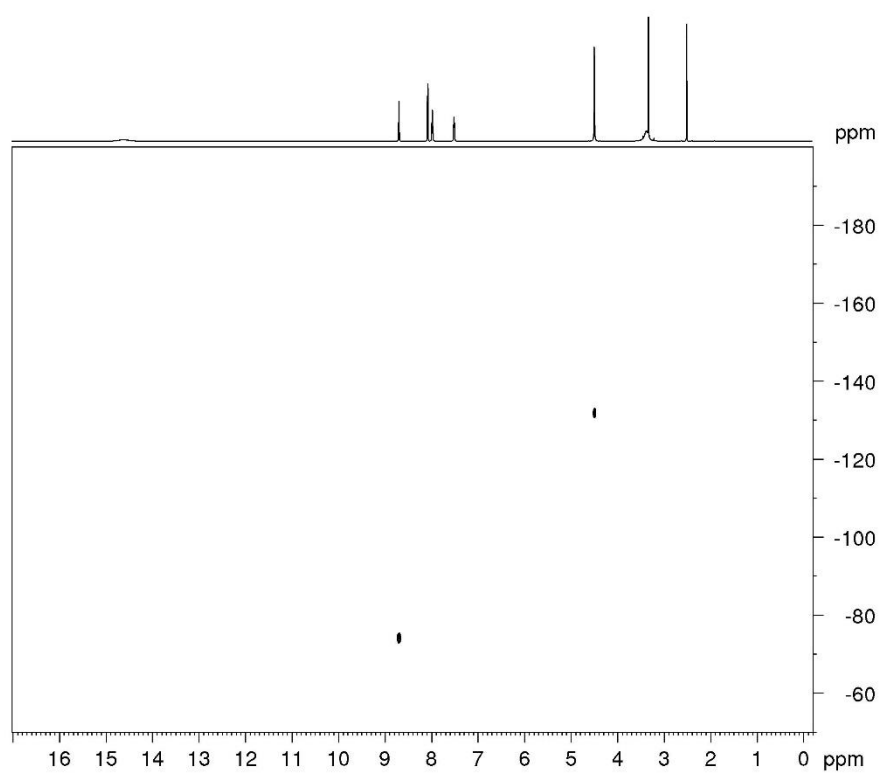


Figure S31. ^1H , ^{15}N HMQC spectrum (500.13 MHz) of pyridinetriazol **9h** in $\text{DMSO-}d_6$ at 17 °C.

Table S1. Rates of exchange (k in s^{-1}) and activation energies (ΔG^\ddagger , in $\text{kcal}\cdot\text{mol}^{-1}$) obtained from EXSY spectra for compounds **9b**, **9c**, **9d**, **9e** and **9f** in $\text{DMSO-}d_6$ at 17°C .^a

	9b		9c^b		9c^{c,d}		9d		9d^b		9e		9e^{b,d}		9f	
	k	ΔG^\ddagger	k	ΔG^\ddagger	k	ΔG^\ddagger	k	ΔG^\ddagger	k	ΔG^\ddagger	k	ΔG^\ddagger	k	ΔG^\ddagger	k	ΔG^\ddagger
A → B	47.17	14.74	13.81	15.47	31.77	14.87	3.43	16.25	11.29	15.56	4.93	16.04	10.28	15.54	15.76	15.38
B → A	27.92	15.04	26.93	15.63	31.38	15.00	2.69	16.39	8.79	15.71	3.16	16.30	9.02	15.67	9.15	15.70
A → C							0.08	18.39	0.50	17.36						
C → A							1.37	16.78								
B → C							0.04	18.88	0.22	17.84						
C → B																
A → H₂O							4.13	16.14					3.57	16.26	18.79	15.28
B → H₂O							4.17	16.14							7.68	15.55
C → H₂O							27.6	15.05								
H₂O → A	1.26	16.83	1.22	17.74			0.04	18.88			0.29	17.67	5.03	16.03	0.34	17.60
H₂O → B	0.43	17.45	0.98	17.73			0.05	18.73			0.26	17.75			0.28	17.70
H₂O → C							0.02	19.24								

a) Proportion of water with respect to triazoles $\geq 87\%$. b) Average value of 2 mixing times. c) Proportion of water with respect to triazoles $\leq 7\%$. d) Average value of 3 mixing times.

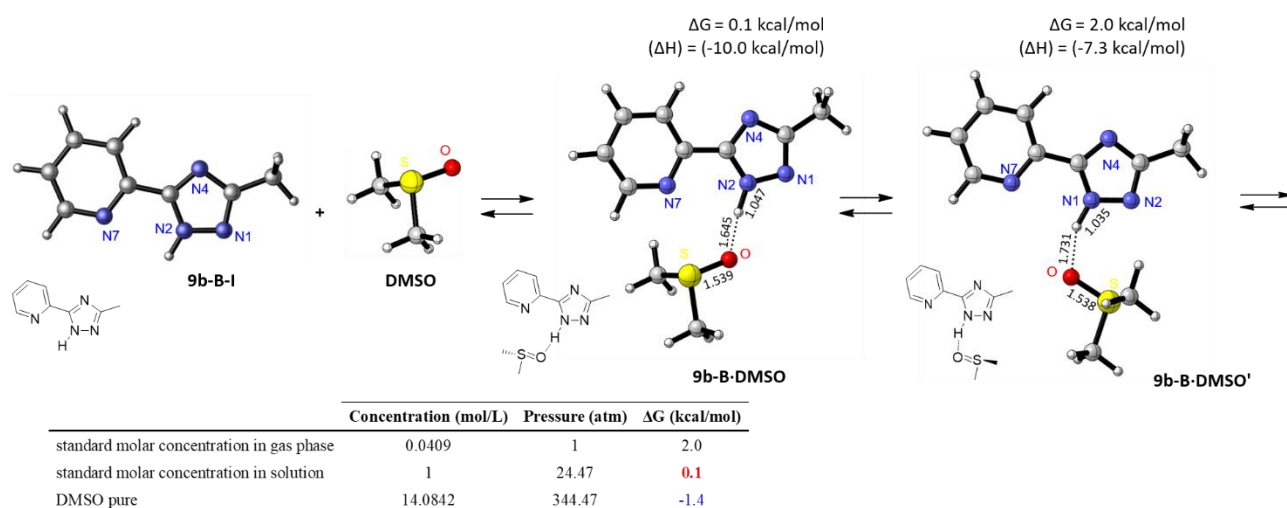


Figure S32. Computed explicit solvation of **9b-B** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

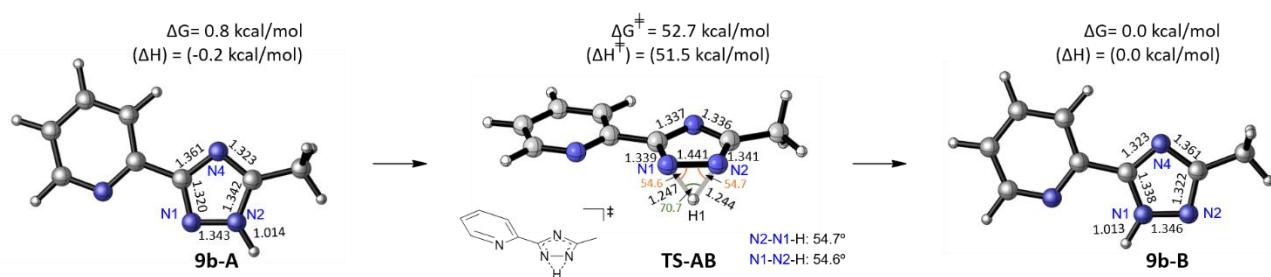


Figure S33. Computed 1,2-proton transfer pathway of **9b-A** to **9b-B** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

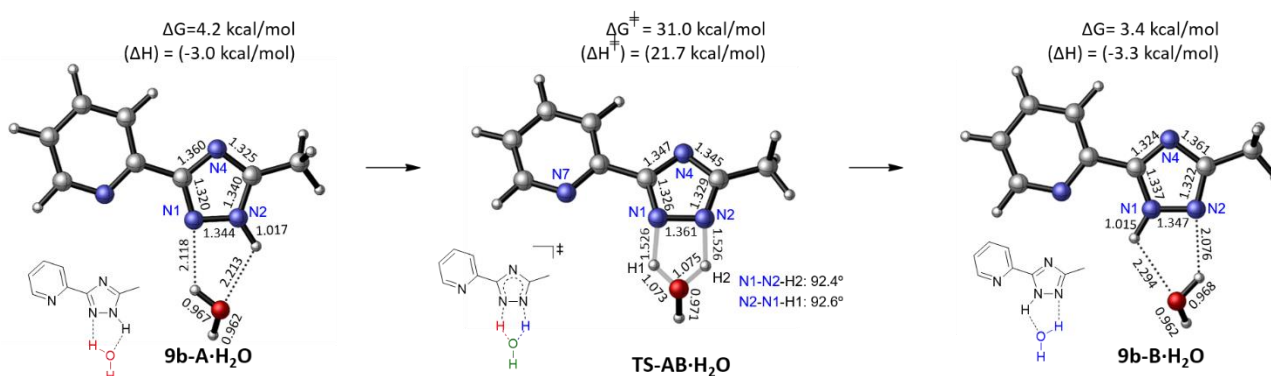


Figure S34. Computed 1,2-proton transfer pathway of **9b-A·H₂O** to **9b-B·H₂O** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

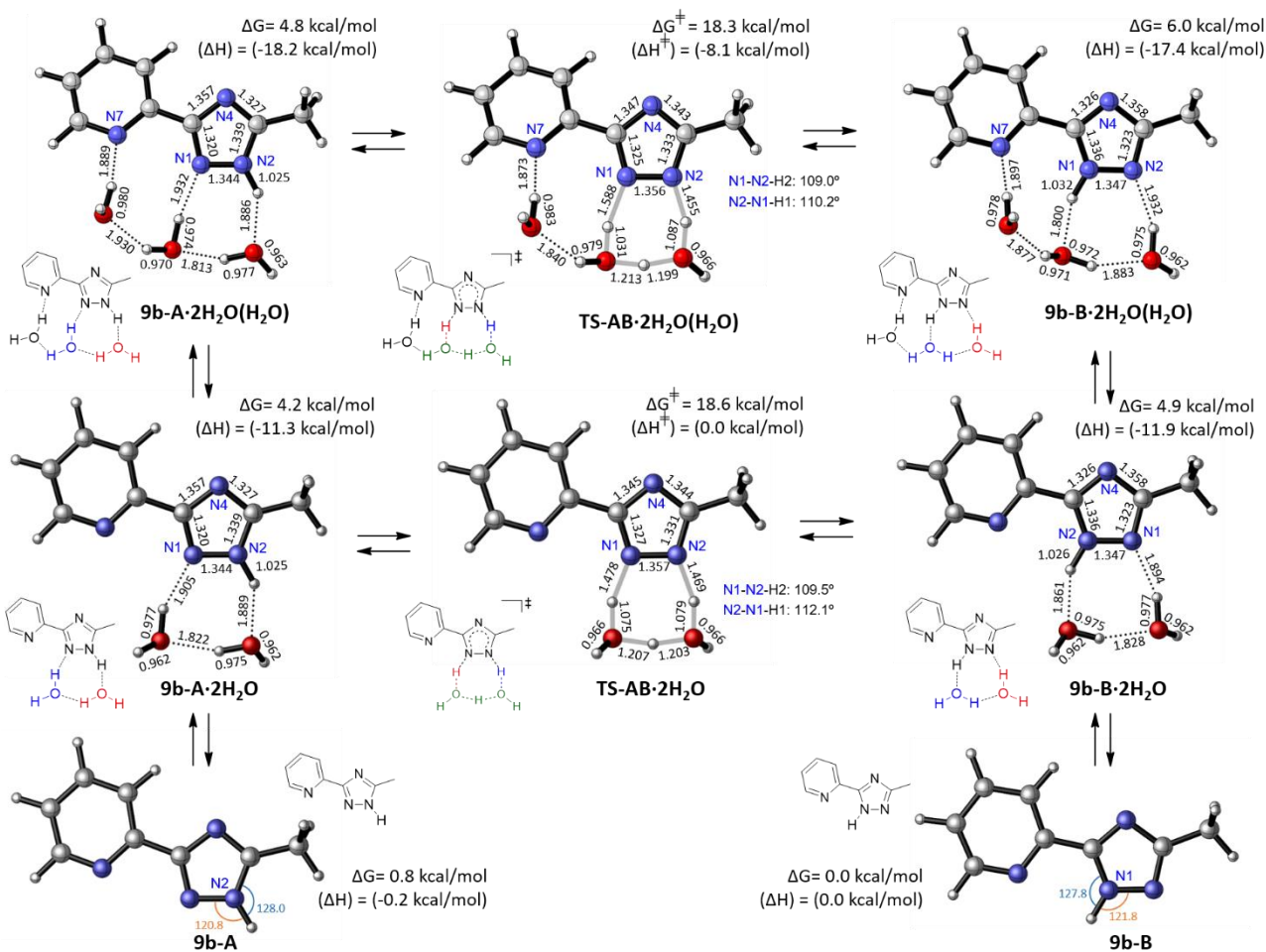


Figure S35. Computed 1,2-proton transfer pathway of **9b-A·2H₂O** to **9b-B·2H₂O** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

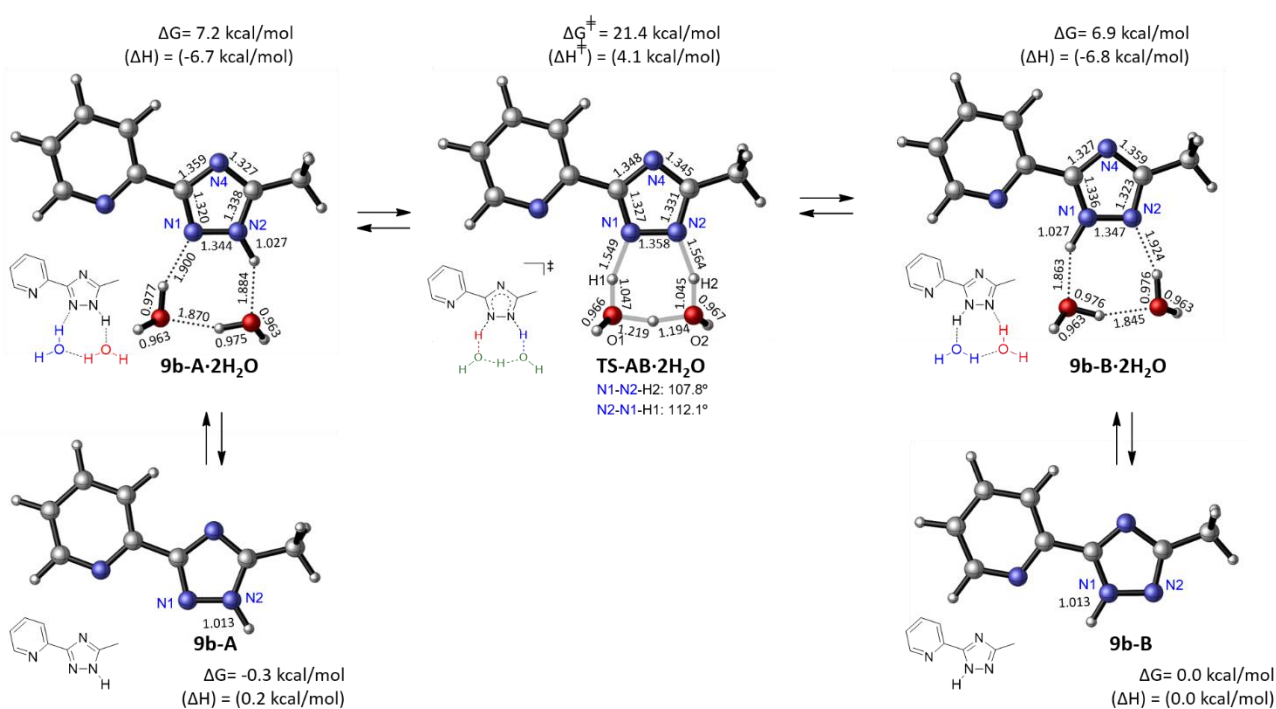


Figure S36. Computed 1,2-proton transfer pathway of **9b-A·2H₂O** to **9b-B·2H₂O** in H₂O [M06-2X/6-311+G(d,p)/SMD(H₂O)].

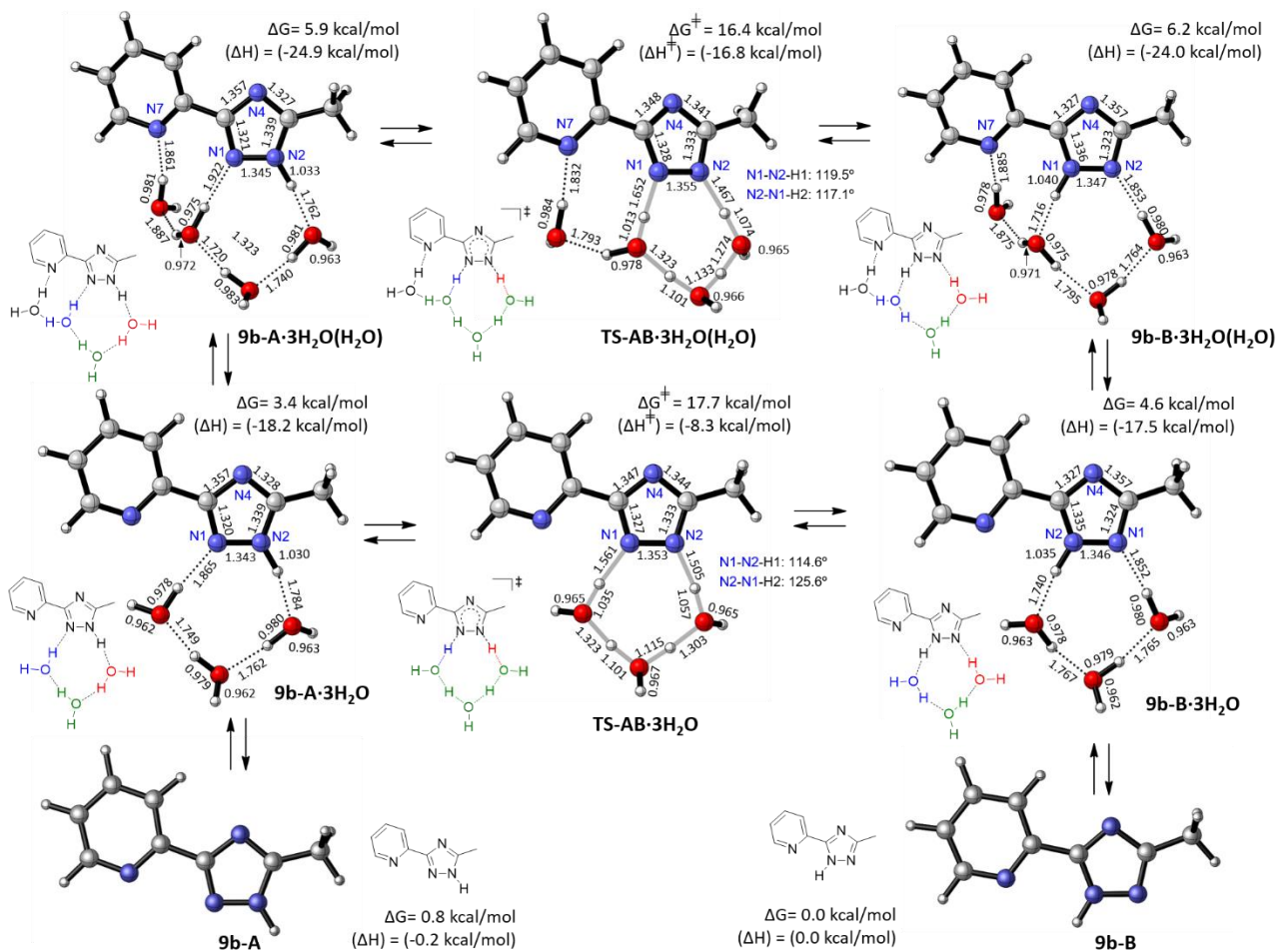


Figure S37. Computed 1,2-proton transfer pathway of **9b-A·3H₂O/9b-A·3H₂O(H₂O)** to **9b-B·3H₂O/9b-B·3H₂O(H₂O)** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

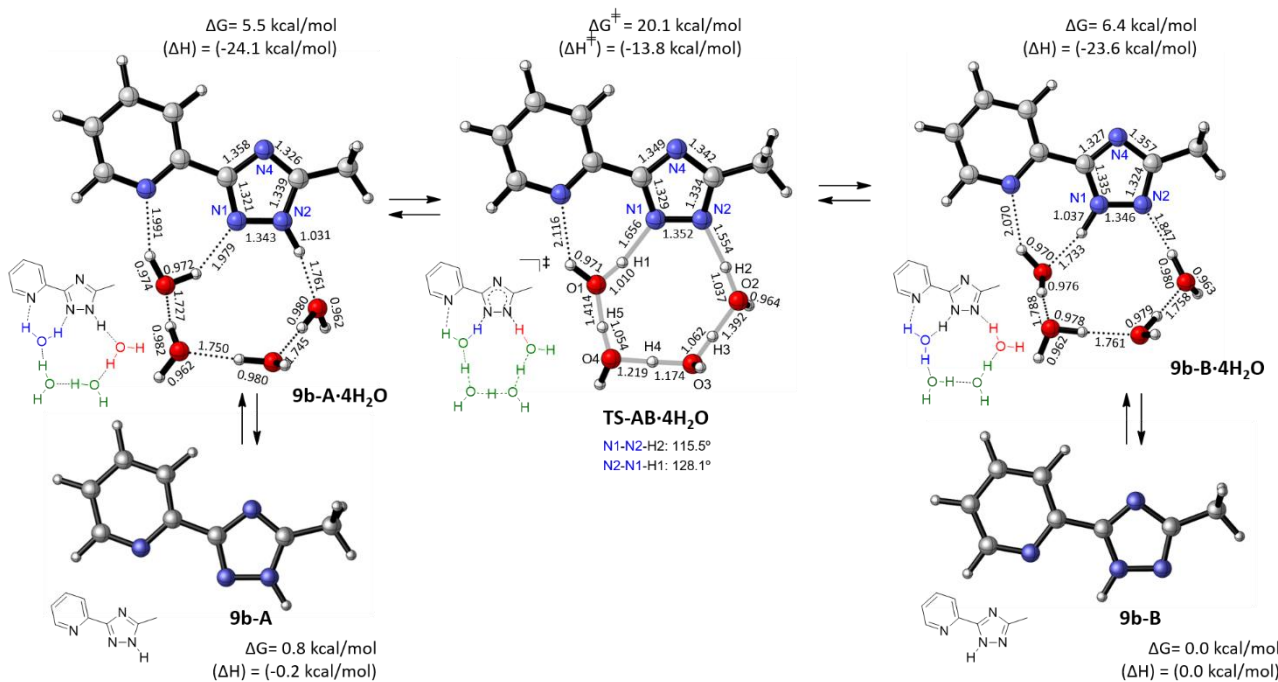


Figure S38. Computed 1,2-proton transfer pathway of **9b-A·4H₂O** to **9b-B·4H₂O** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

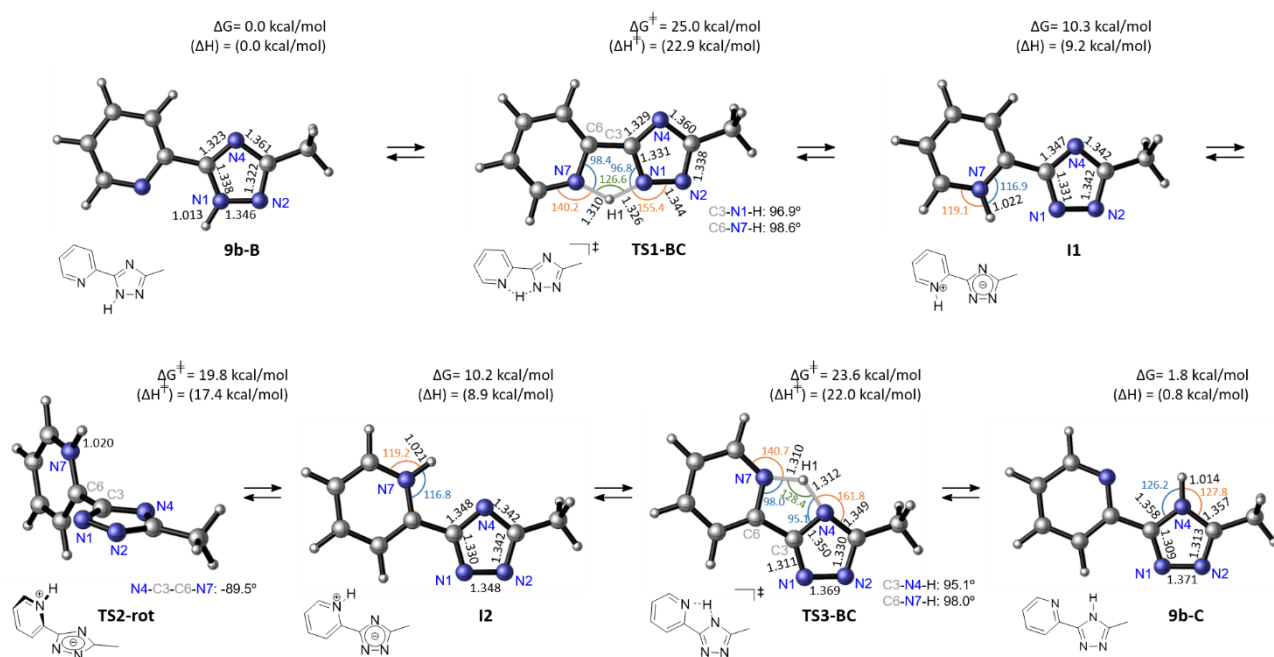


Figure S39. Computed proton transfer pathway of **9b-B** \rightleftharpoons **9b-C** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

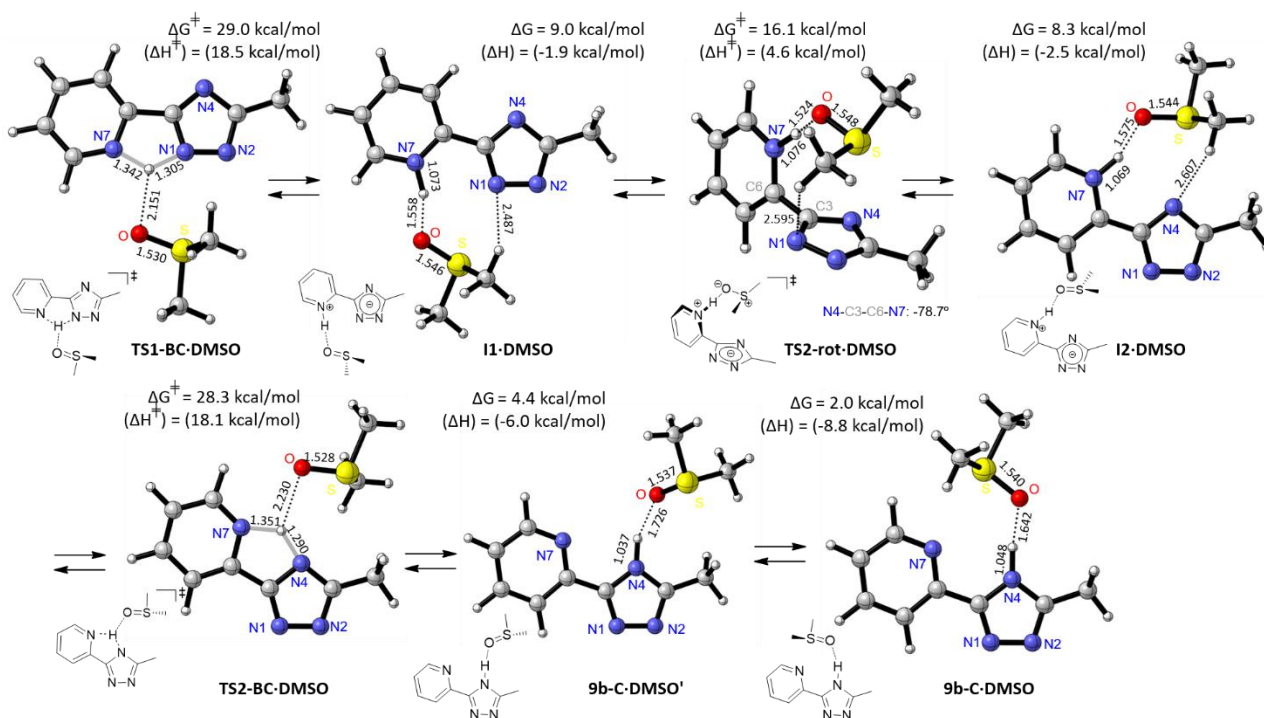


Figure S40. Computed proton transfer pathway of **9b-B·DMSO** \rightleftharpoons **9b-C·DMSO** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

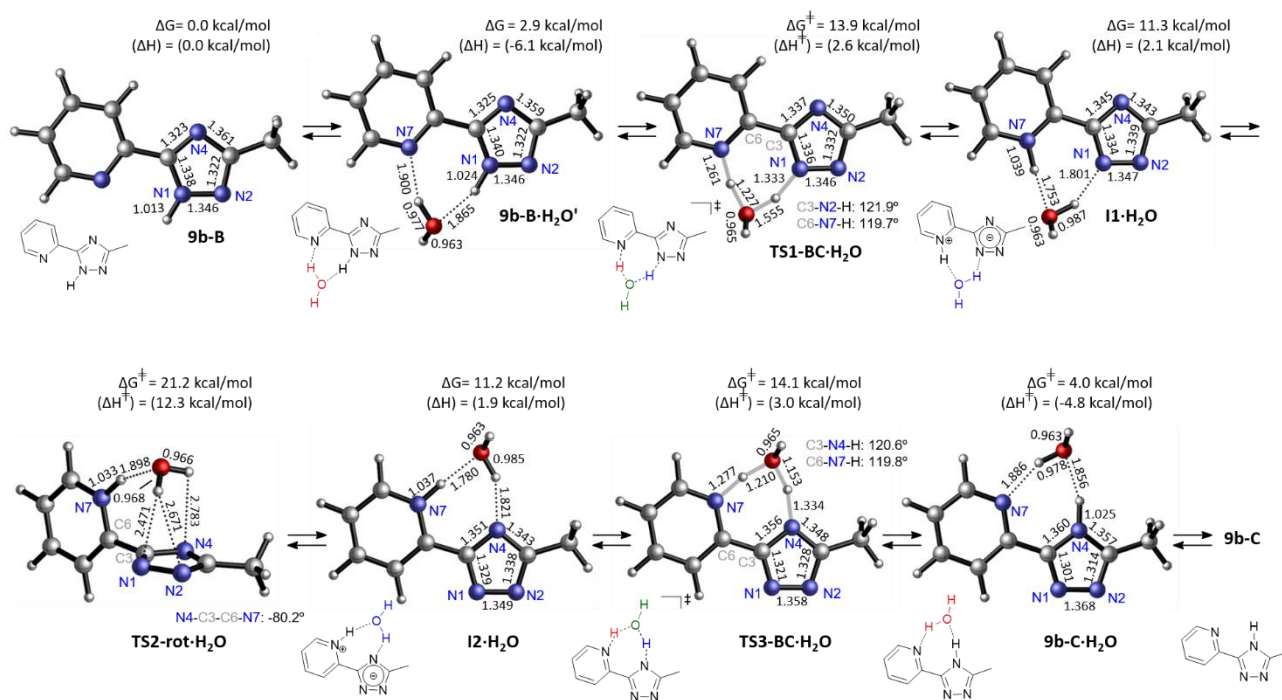


Figure S41. Computed proton transfer pathway of **9b-B·H₂O** \rightleftharpoons **9b-C·H₂O** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

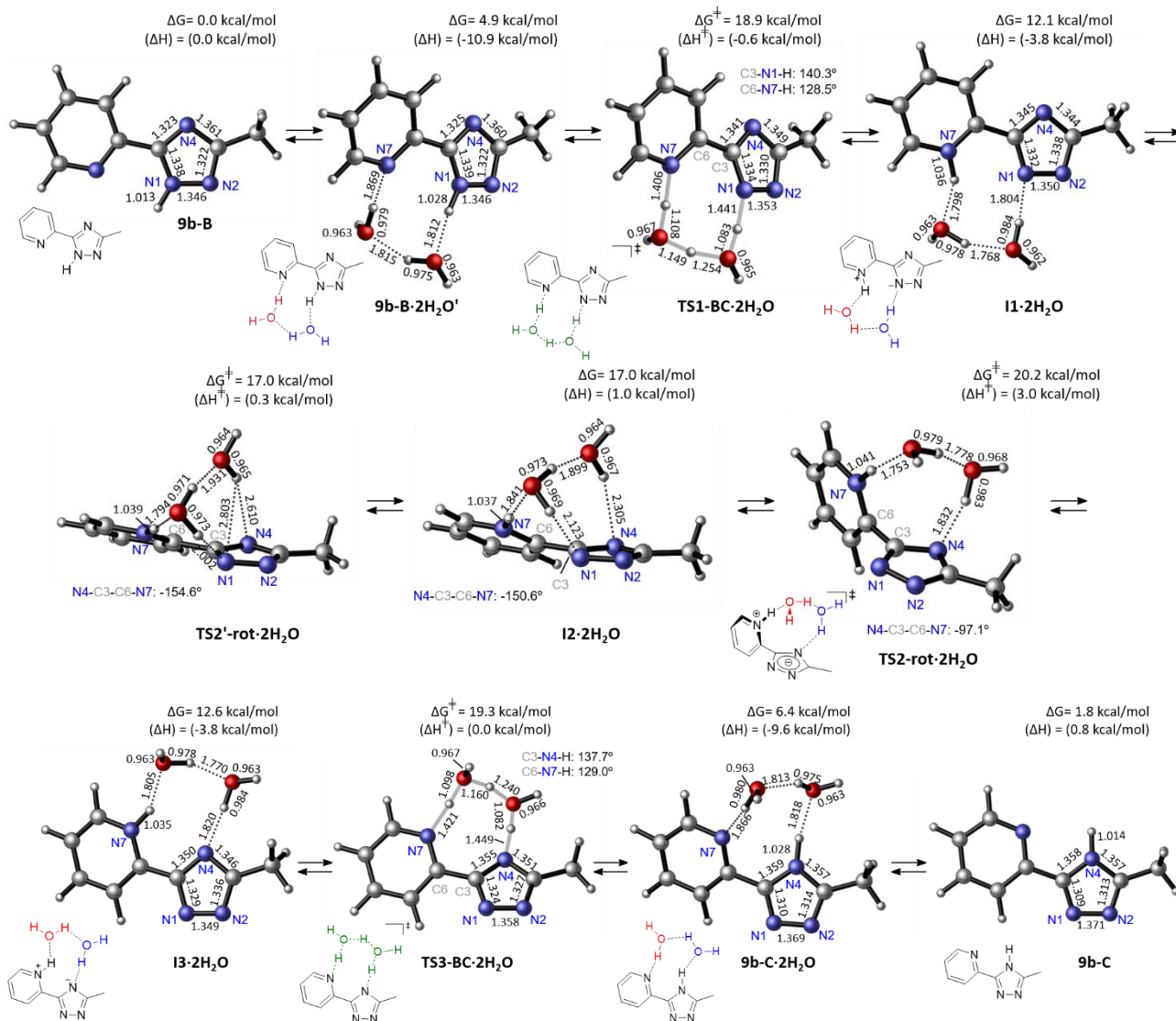


Figure S42. Computed proton transfer pathway of $9b\text{-B}\cdot 2\text{H}_2\text{O} \rightleftharpoons 9b\text{-C}\cdot 2\text{H}_2\text{O}$ in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

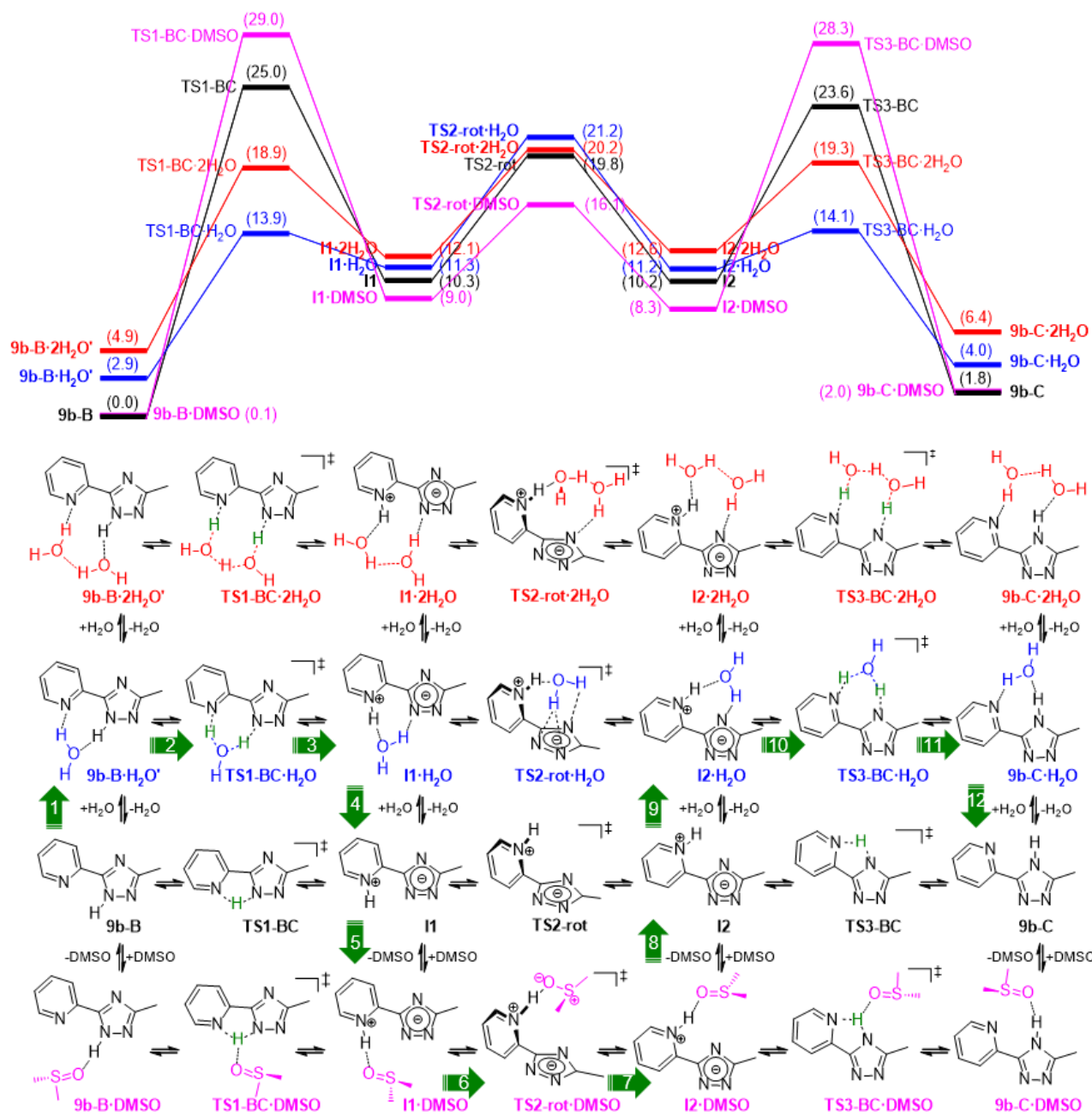


Figure S43. Graphical overview of the computed proton transfer pathway of $9b\text{-B}\cdot nS \rightleftharpoons 9b\text{-C}\cdot nS$ in DMSO, S = DMSO, H₂O, n = 0, 1, 2. The favored transfer pathway is highlighted using green arrows.

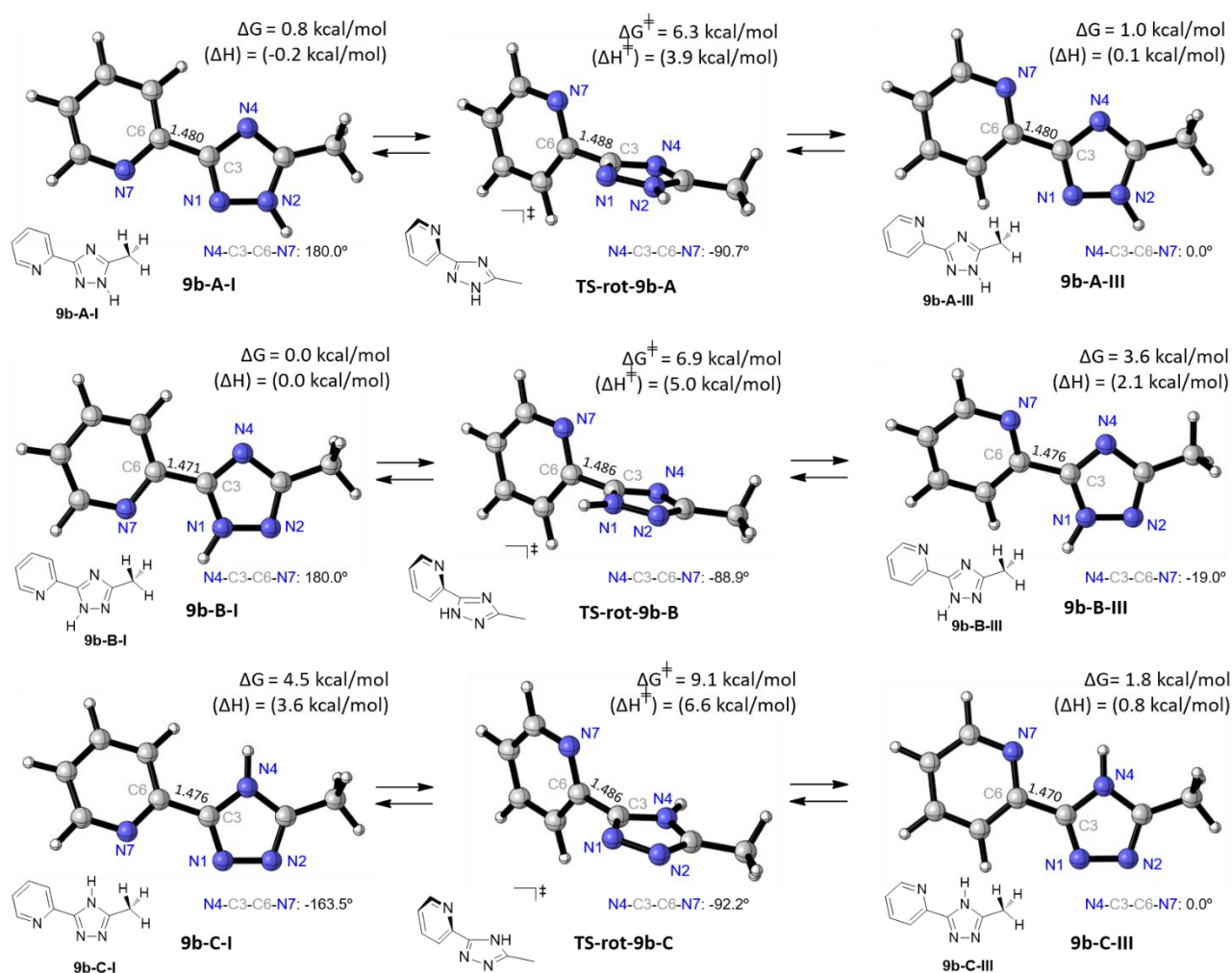
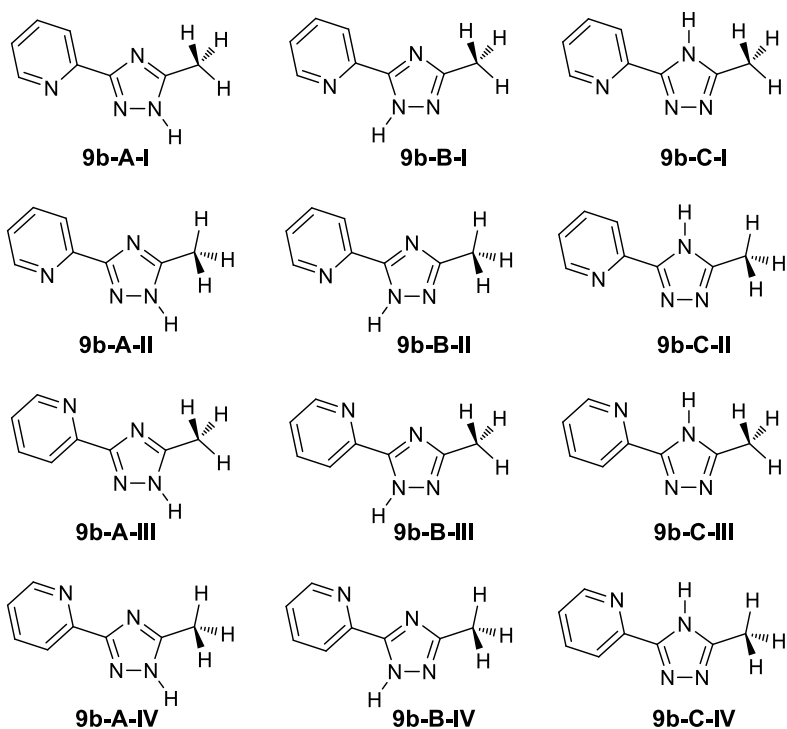


Figure S44. Computed rotamerization of the pyridine substituent in **9b-A,B,C** in DMSO [M06-2X/6-311+G(d,p)/SMD(DMSO)].

Table S2. Distribution of tautomers **9b-A**, **9b-B** and **9b-C** computed at the M06-2X/6-311+G(d,p)/SMD(DMSO) level.



	DMSO	
	ΔG (kcal·mol ⁻¹)	%
9b-B-I	0.5	18.5
9b-B-II	0.0	42.7
9b-B-IV	4.7	0.0
9b-B-III	3.6	0.1
9b-C-II	5.3	0.0
9b-C-I	4.5	0.0
9b-C-IV	2.3	0.8
9b-C-III	1.8	1.9
9b-A-III	1.0	8.5
9b-A-IV	1.0	8.3
9b-A-II	1.0	7.6
9b-A-I	0.8	11.5

61.4

2.7

35.9

Table S3. Computed energy and thermodynamic parameters for the conformers of tautomer **9b-A**, **9b-B** and **9b-C** and the species involved in the tautomerization $9b-A \rightleftharpoons 9b-B \rightleftharpoons 9b-C$ at the level M06-2X/6-311+G(d,p)/SMD(DMSO) (E = electronic energy, H = enthalpy, G = Gibbs free energy; G_{correct} = correction due to entropy, in Hartrees).

	E	H	G	G_{correction}
9b-B-I	-528.62061627	-528.45229600	-528.49889100	-528.49587909
9b-B-II	-528.61958844	-528.45137200	-528.49967900	-528.49666709
9b-B-IV	-528.61544729	-528.44787500	-528.49219600	-528.48918409
9b-B-III	-528.61643522	-528.44796000	-528.49387100	-528.49085909
9b-C-II	-528.61292552	-528.44462800	-528.49123500	-528.48822309
9b-C-I	-528.61378591	-528.44565900	-528.49248100	-528.48946909
9b-C-IV	-528.61709132	-528.44902800	-528.49593900	-528.49292709
9b-C-III	-528.61806170	-528.45007800	-528.49674200	-528.49373009
9B-A-III	-528.61967049	-528.45126400	-528.49815700	-528.49514509
9B-A-IV	-528.61937921	-528.45111400	-528.49813000	-528.49511809
9B-A-II	-528.61988621	-528.45155900	-528.49804600	-528.49503409
9B-A-I	-528.62015107	-528.45172700	-528.49843800	-528.49542609
TS-AB	-528.53128803	-528.36936600	-528.41570500	-528.41269309
9b-A·H₂O	-605.05607108	-604.86032500	-604.91562600	-604.91261409
TS-AB·H₂O	-605.01124704	-604.82095100	-604.87290800	-604.86989609
9b-B·H₂O	-605.05643821	-604.86081100	-604.91677300	-604.91376109
H₂O	-76.42921659	-76.40415400	-76.42558000	-76.42256809
9b-A·2H₂O	-681.50150770	-681.27767200	-681.33819300	-681.33518109
9b-B·2H₂O	-681.50149059	-681.27859200	-681.33701600	-681.33400409
TS-AB·2H₂O	-681.47493762	-681.25963600	-681.31512800	-681.31211609
9b-A·3H₂O	-757.94433500	-757.69287600	-757.76204300	-757.75903109
9b-B·3H₂O	-757.94311400	-757.69172300	-757.75998500	-757.75697309
TS-AB·3H₂O	-757.92008100	-757.67713000	-757.73910600	-757.73609409
9b-A·4H₂O	-834.38609600	-834.10643700	-834.18120500	-834.17819309
9b-B·4H₂O	-834.38512300	-834.10552000	-834.17978700	-834.17677509
TS-AB·4H₂O	-834.36024400	-834.08997500	-834.15796500	-834.15495309
I2	-528.60570378	-528.43713400	-528.48336900	-528.48035709
I1	-528.60517128	-528.43673000	-528.48332000	-528.48030809
TS1-BC	-528.57817661	-528.41486900	-528.45984400	-528.45683209
TS3-BC	-528.57925495	-528.41625600	-528.46211600	-528.45910409
TS2-rot	-528.59146933	-528.42370300	-528.46816200	-528.46515009
9b-B·H₂O'	-605.06126323	-604.86520700	-604.91760700	-604.91459509
TS1-BC·H₂O	-605.03957896	-604.85137900	-604.90011900	-604.89710709
I1·H₂O	-605.04803864	-604.85225100	-604.90421100	-604.90119909
TS2-rot·H₂O	-605.03102539	-604.83589300	-604.88851000	-604.88549809
I2·H₂O	-605.04838773	-604.85244800	-604.90435200	-604.90134009
TS3-BC·H₂O	-605.03897012	-604.85082000	-604.89976000	-604.89674809
9b-C·H₂O	-605.05891904	-604.86321800	-604.91592000	-604.91290809
9b-B·2H₂O'	-681.50078967	-681.27704800	-681.33693500	-681.33392309
TS1-BC·2H₂O	-681.47566930	-681.26056700	-681.31474400	-681.31173209
I1·2H₂O	-681.48929451	-681.26571000	-681.32547700	-681.32246509

Table S3, continuation. Computed energy and thermodynamic parameters for the conformers of tautomer **9b-A**, **9b-B** and **9b-C** and the species involved in the tautomerization **9b-A** \rightleftharpoons **9b-B** \rightleftharpoons **9b-C** at the level M06-2X/6-311+G(d,p)/SMD(DMSO) (E = electronic energy, H = enthalpy, G = Gibbs free energy; G_{correct} = correction due to entropy, in Hartrees).

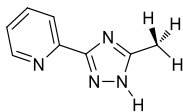
	E	H	G	G_{correct}
TS2'-rot·2H₂O	-681.48187983	-681.25916700	-681.31768600	-681.31467409
I2·2H₂O	-681.48198531	-681.25801200	-681.31760700	-681.31459509
TS2-rot·2H₂O	-681.47749013	-681.25482700	-681.31259400	-681.30958209
I3·2H₂O	-681.48953204	-681.26577500	-681.32476800	-681.32175609
TS3-BC·H₂O	-681.47472831	-681.25962800	-681.31405400	-681.31104209
9b-C·H₂O	-681.49853141	-681.27496200	-681.33456800	-681.33155609
9b-B-I·DMSO	-1081.80153300	-1081.54512100	-1081.60868500	-1081.60567309
DMSO	-553.16423300	-553.07781500	-553.11223700	-553.10922509
9b-B-I·DMSO'	-1081.79738000	-1081.54081600	-1081.60577800	-1081.60276609
TS1-BC·DMSO	-1081.75116200	-1081.49970200	-1081.56263300	-1081.55962109
I1·DMSO	-1081.78821900	-1081.53229200	-1081.59454400	-1081.59153209
TS2-rot·DMSO	-1081.77676300	-1081.52194300	-1081.58326100	-1081.58024909
I2·DMSO	-1081.78900900	-1081.5332500	-1081.59564500	-1081.59263309
TS2-BC·DMSO	-1081.75190600	-1081.50028500	-1081.56377500	-1081.56076309
9b-C·DMSO'	-1081.79522700	-1081.5387100	-1081.60186900	-1081.59885709
9b-C·DMSO	-1081.79946600	-1081.54320500	-1081.60572800	-1081.60271609
9b-B·2H₂O(H₂O)	-757.94364400	-757.69161600	-757.75775500	-757.75474309
TS-AB·2H₂O(H₂O)	-757.92098100	-757.67679200	-757.73821600	-757.73520409
9b-A·2H₂O(H₂O)	-757.94487500	-757.69276200	-757.75976900	-757.75675709
9b-B·3H₂O(H₂O)	-834.38586100	-834.10622700	-834.18013200	-834.17712009
TS-AB·3H₂O(H₂O)	-834.36560400	-834.09474800	-834.16381500	-834.16080309
9b-A·3H₂O(H₂O)	-834.38751900	-834.10771700	-834.18055200	-834.17754009
TS-rot-9b-A	-528.612582	-528.445081	-528.489687	-528.48667509
TS-rot-9b-B	-528.610689	-528.44345	-528.488635	-528.48562309
TS-rot-9b-C	-528.607985	-528.440921	-528.48513	-528.48211809
9b-B-I·DMSO'	-1081.79738000	-1081.54081600	-1081.60577800	-1081.60276609

Table S4. Computed energy and thermodynamic parameters for the conformers of tautomer **9b-A**, and **9b-B** and the species involved in the tautomerization **9b-A** \rightleftharpoons **9b-B** at the level M06-2X/6-311+G(d,p)/SMD(H₂O) (E = electronic energy, H = enthalpy, G = Gibbs free energy; G_{correct} = correction due to entropy, in Hartrees).

	E	H	G	G_{correct}
9b-B-I	-528.62101000	-528.45267700	-528.49867600	-528.49566409
9b-A-I	-528.62073600	-528.45238000	-528.49915200	-528.49614009
H₂O	-76.43468700	-76.40962300	-76.43105200	-76.42804009
9b-A·2H₂O	-681.50615800	-681.28264800	-681.34328900	-681.34027709
9b-B·2H₂O	-681.50613600	-681.28269400	-681.34381600	-681.34080409
TS-AB·2H₂O	-681.48157217	-681.26537600	-681.32057700	-681.31756509

Cartesian coordinates and total energies (hartrees) the optimized stationary points. Imaginary frequencies of transition structures are in cm^{-1} .

9b-A-I



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.62657000	0.23923000	0.00008500
C	-0.57022700	-0.23815800	0.00006000
N	-1.15796800	-1.41953600	-0.00047200
N	-2.46054300	-1.09233100	-0.00042300
N	-1.43481100	0.81332200	0.00042900
C	-3.95158200	0.91346600	0.00024100
H	-4.05110900	1.54455100	0.88448700
H	-4.05040000	1.54625400	-0.88286500
H	-4.75491100	0.17678500	-0.00076300
C	0.89771400	-0.06131800	0.00009600
C	1.43898400	1.22424700	-0.00027100
C	2.82060900	1.36197300	-0.00034200
H	0.78459700	2.08621100	-0.00051300
C	2.97384300	-1.01974400	0.00033900
C	3.60912200	0.21857300	-0.00004300
H	3.27239200	2.34712500	-0.00063900
H	3.55830800	-1.93456900	0.00059500
H	4.69039100	0.27557100	-0.00010000
N	1.64979200	-1.16733300	0.00041300
H	-3.17591000	-1.81039800	-0.00082100

M06-2X/6-311+G(d,p)/SMD(H₂O)

Cartesian coordinates

ATOM	X	Y	Z
C	0.57183300	-0.23221100	-0.00007900
C	2.62706700	0.24018100	0.00008800
N	2.45753700	-1.08957200	-0.00031900
H	3.17481700	-1.80542200	-0.00040800
N	1.15498200	-1.41521200	-0.00039700
N	1.43725200	0.81993400	0.00022100
C	-0.89447300	-0.05925000	-0.00006400
C	-1.44261900	1.22320500	-0.00032800
C	-2.82431000	1.35863000	-0.00022500
H	-0.79675700	2.09047600	-0.00059600
C	-2.97081000	-1.02043000	0.00034200
C	-3.61016100	0.21413300	0.00012100
H	-3.27677100	2.34312700	-0.00041500
H	-3.55275800	-1.93600800	0.00058000
H	-4.69127800	0.26728500	0.00023100
N	-1.64569300	-1.16793600	0.00025400
C	3.95324900	0.90481900	0.00032200
H	4.05153100	1.53510300	0.88520800
H	4.75262000	0.16444900	-0.00009200
H	4.05138800	1.53603600	-0.88390200

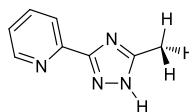
B3LYP /6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	2.63536800	0.23882100	0.00001500
C	0.56745600	-0.23930400	0.00000000
N	1.16030200	-1.42595700	0.00001900
N	2.47149500	-1.09504900	0.00003100
N	1.43951500	0.81129700	0.00000100
C	3.95728800	0.91877400	0.00001800

H	4.76741600	0.18910400	0.00002200
H	4.06010400	1.55401400	-0.88203500
H	4.06010000	1.55401800	0.88206800
C	-0.89648600	-0.06096100	-0.00001100
C	-1.44502200	1.22373700	0.00002200
C	-2.82583600	1.36219600	0.00001700
H	-0.79561400	2.08833100	0.00005400
C	-2.98230900	-1.01816000	-0.00005500
C	-3.61630000	0.22016200	-0.00002200
H	-3.27609900	2.34769600	0.00004300
H	-3.56779500	-1.93241000	-0.00008600
H	-4.69738900	0.27976100	-0.00002800
N	-1.65705100	-1.16721000	-0.00005000
H	3.18450500	-1.81367300	0.00004800

9b-A-II



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.62641400	0.24142600	0.00005400
C	-0.56971100	-0.23893700	-0.00001200
N	-1.15824600	-1.41906600	-0.00029700
N	-2.46106100	-1.09142800	-0.00024300
N	-1.43439700	0.81392300	0.00021900
C	-3.95263400	0.91319800	0.00019600
H	-4.52671000	0.63116000	-0.88436200
H	-4.52665700	0.63086100	0.88469400
H	-3.80689700	1.99192900	0.00036900
C	0.89794200	-0.06200700	0.00002000
C	1.43886200	1.22379000	-0.00017600
C	2.82040700	1.36198300	-0.00017700
H	0.78419900	2.08555700	-0.00032500
C	2.97440800	-1.01965100	0.00020800
C	3.60932500	0.21884400	0.00001300
H	3.27182000	2.34731200	-0.00032900
H	3.55919600	-1.93427100	0.00037000
H	4.69057100	0.27620900	0.00001400
N	1.65039700	-1.16777100	0.00021600
H	-3.17549200	-1.81024400	-0.00045500

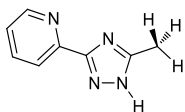
B3LYP /6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	2.63544900	0.24022900	0.00001600
C	0.56689600	-0.24117700	0.00000000
N	1.16086800	-1.42606000	0.00001700
N	2.47248900	-1.09515800	0.00002900
N	1.43952600	0.81095600	0.00000200
C	3.95686300	0.92096200	0.00001700
H	3.81045100	1.99989000	0.00002900
H	4.53859900	0.64533900	0.88277100
H	4.53859100	0.64535700	-0.88274700
C	-0.89666300	-0.06215800	-0.00001000
C	-1.44428300	1.22305500	0.00001900
C	-2.82493800	1.36266500	0.00001300
H	-0.79423300	2.08715400	0.00004600
C	-2.98338600	-1.01751200	-0.00005000
C	-3.61640100	0.22130400	-0.00002100
H	-3.27430200	2.34858400	0.00003700

H	-3.56966200	-1.93125900	-0.00007800
H	-4.69743500	0.28182900	-0.00002600
N	-1.65823700	-1.16776900	-0.00004500
H	3.18424900	-1.81488100	0.00004500

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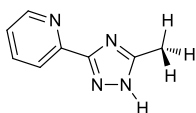


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	2.63578700	-0.24135600	0.00000300
C	0.57326900	0.19962100	0.00000200
N	1.14287400	1.39115600	-0.00001700
N	2.45001200	1.08789200	-0.00000800
N	1.45407600	-0.83655200	0.00001000
C	3.97255900	-0.89190300	0.00000800
H	4.08316900	-1.52196600	0.88369600
H	4.08316700	-1.52198200	-0.88367000
H	4.76233600	-0.14072300	0.00000000
C	-0.89780100	0.04024200	0.00000300
C	-1.72730500	1.16417500	0.00000900
C	-3.10096700	0.97430700	0.00000600
H	-1.29763100	2.15775800	0.00001600
C	-2.69397900	-1.37655800	-0.00000700
C	-3.60089000	-0.32322100	-0.00000200
H	-3.77110800	1.82615000	0.00001100
H	-3.04630600	-2.40331100	-0.00001300
H	-4.66557400	-0.52021000	-0.00000500
N	-1.37065400	-1.20891700	-0.00000500
H	3.15375300	1.81738800	-0.00001700

9b-A-IV

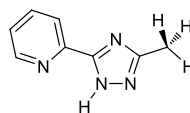


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.63570600	-0.24340900	-0.00000600
C	-0.57269700	0.20161200	0.00000500
N	-1.14383700	1.39135500	0.00003000
N	-2.45125600	1.08731700	0.00002100
N	-1.45353900	-0.83636500	-0.00001900
C	-3.97289100	-0.89315400	-0.00002100
H	-4.54187100	-0.60137800	0.88463900
H	-4.54191400	-0.60124200	-0.88460700
H	-3.84515800	-1.97415900	-0.00010300
C	0.89808500	0.04166500	0.00000000
C	1.72875900	1.16480400	-0.00002200
C	3.10219600	0.97352900	-0.00002200
H	1.30017900	2.15887300	-0.00004100
C	2.69310800	-1.37688100	0.00001800
C	3.60101400	-0.32449000	-0.00000100
H	3.77319200	1.82470000	-0.00003800
H	3.04432100	-2.40402600	0.00003400
H	4.66551100	-0.52247700	0.00000000
N	1.36992900	-1.20793800	0.00002000
H	-3.15454900	1.81707500	0.00005200

9b-B-I



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

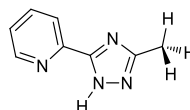
ATOM	X	Y	Z
C	2.66866600	0.16668200	0.00003900
C	0.57996700	-0.12816000	-0.00004600
N	1.19736200	-1.31545500	0.00006400
H	0.77475500	-2.23633800	0.00015600
N	2.53254700	-1.14836800	-0.00026800
N	1.48428300	0.83780600	-0.00014300
C	3.99404800	0.84713300	0.00013700
H	4.79487700	0.10835900	-0.00009900
H	4.09790000	1.48161100	-0.88209200
H	4.09801700	1.48117100	0.88267100
C	-0.88415800	0.01422100	-0.00002000
C	-1.47512000	1.27435100	-0.00000400
C	-2.86245900	1.34347100	0.00004000
H	-0.85962400	2.16506700	-0.00002500
C	-2.90614000	-1.04719400	0.00004800
C	-3.59464500	0.16307100	0.00006800
H	-3.36261400	2.30472300	0.00005300
H	-3.44720600	-1.98776600	0.00007100
H	-4.67737400	0.17064100	0.00010400
N	-1.57700300	-1.12954300	0.00000300

B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	2.67612100	0.17056900	0.00001300
C	0.57733300	-0.13508100	0.00000000
N	1.20161500	-1.32282200	0.00002500
H	0.78683200	-2.24530500	0.00003800
N	2.54526700	-1.15044800	0.00002600
N	1.48679800	0.83440400	-0.00000300
C	3.99945200	0.85407500	0.00001300
H	4.80578900	0.12096300	0.00001500
H	4.10704400	1.49142100	-0.88086400
H	4.10704400	1.49142500	0.88088700
C	-0.88220500	0.01154800	-0.00001100
C	-1.47863800	1.27190900	0.00002400
C	-2.86479200	1.34539900	0.00001900
H	-0.86729000	2.16428500	0.00005700
C	-2.91760000	-1.04350700	-0.00005100
C	-3.60223800	0.16813000	-0.00001900
H	-3.36083900	2.30841800	0.00004700
H	-3.46208100	-1.98216400	-0.00008100
H	-4.68480000	0.18077600	-0.00002300
N	-1.58743600	-1.13085800	-0.00004800

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M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.66764300	0.17006800	0.00007700
C	-0.57888200	-0.12869400	-0.00005300
N	-1.19827800	-1.31405900	-0.00006700
H	-0.77655600	-2.23558200	-0.00004900

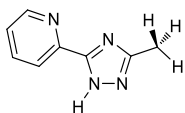
N	-2.53211000	-1.14602100	-0.00078100
N	-1.48328800	0.83909700	-0.00004800
C	-3.99859500	0.84379200	0.00025200
H	-3.86176500	1.92442400	0.00048100
H	-4.57494800	0.56371400	-0.88324000
H	-4.57490900	0.56334300	0.88365400
C	0.88487400	0.01347500	0.00003500
C	1.47570900	1.27378200	-0.00016400
C	2.86297200	1.34329900	-0.00010000
H	0.85985700	2.16424200	-0.00038900
C	2.90725400	-1.04726000	0.00034800
C	3.59552500	0.16313400	0.00016000
H	3.36273500	2.30475800	-0.00026800
H	3.44867200	-1.98763500	0.00055500
H	4.67822600	0.17095800	0.00021400
N	1.57816200	-1.13013100	0.00028300

B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.67537300	0.17277400	-0.00002100
C	-0.57631600	-0.13680500	0.00000600
N	-1.20282900	-1.32248200	-0.00006600
H	-0.78900200	-2.24561500	-0.00010900
N	-2.54514100	-1.14937600	-0.00007500
N	-1.48614300	0.83445500	0.00001800
C	-4.00193500	0.85400400	0.00000900
H	-3.86479100	1.93474000	-0.00012600
H	-4.58526100	0.57882500	-0.88167200
H	-4.58511200	0.57903600	0.88185600
C	0.88275300	0.01010200	0.00002300
C	1.47824500	1.27110700	-0.00004400
C	2.86424300	1.34592300	-0.00004100
H	0.86609300	2.16292500	-0.00010400
C	2.91932500	-1.04285100	0.00009100
C	3.60289400	0.16935600	0.00002900
H	3.35928800	2.30947100	-0.00009500
H	3.46472700	-1.98098000	0.00014500
H	4.68543800	0.18306400	0.00003200
N	1.58919900	-1.13161600	0.00008900

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M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.66714200	-0.18035300	0.03555000
C	-0.58326100	0.15427900	-0.03034000
N	-1.23176400	1.31099300	-0.23467900
H	-0.85209400	2.22947600	-0.43207200
N	-2.56291300	1.11549700	-0.19919200
N	-1.46772500	-0.81396400	0.14511500
C	-3.97460000	-0.87852700	0.17662600
H	-4.79352700	-0.17800900	0.01561900
H	-4.05279700	-1.69000600	-0.54924500
H	-4.06918200	-1.31048500	1.17499200
C	0.88732000	0.02384500	-0.00395600
C	1.70173000	1.13900200	0.18849000
C	3.07858700	0.95699900	0.19648800
H	1.27517100	2.12313300	0.34162800
C	2.68934900	-1.37223000	-0.15405500
C	3.58690900	-0.32270800	0.02160600
H	3.74014300	1.80224500	0.34439600
H	3.05112300	-2.38637800	-0.29037800

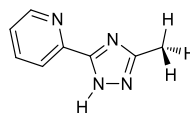
H	4.65270800	-0.51316600	0.02294500
N	1.36741800	-1.21233500	-0.16986400

B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.67497900	-0.18546200	0.00712400
C	-0.58096700	0.16802500	0.00227000
N	-1.23818900	1.34069000	-0.05882200
H	-0.86866800	2.28043500	-0.11237500
N	-2.57731100	1.13608100	-0.05647800
N	-1.47098400	-0.81869300	0.04599700
C	-3.98024400	-0.90215100	0.03665800
H	-4.80547700	-0.19309500	-0.02598300
H	-4.05527100	-1.60243300	-0.79855700
H	-4.08557300	-1.47944600	0.95837900
C	0.88604100	0.03135500	0.00903700
C	1.72266800	1.14956100	0.05416500
C	3.09678000	0.95660800	0.04435500
H	1.31858600	2.15257400	0.10119000
C	2.68553900	-1.39111900	-0.04194900
C	3.59440400	-0.33852900	-0.00572300
H	3.76633100	1.80752400	0.07659600
H	3.03667000	-2.41749400	-0.07824700
H	4.65892500	-0.53533500	-0.01503000
N	1.36348700	-1.22128600	-0.03663900

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M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.66611900	-0.18287300	0.03791400
C	-0.58192200	0.15337500	-0.03117900
N	-1.23150500	1.30796800	-0.23798400
H	-0.85162300	2.22669000	-0.43490900
N	-2.56135400	1.11340700	-0.20055300
N	-1.46764300	-0.81534400	0.14787300
C	-3.98192000	-0.87374500	0.17711100
H	-3.81993000	-1.93279400	0.37380100
H	-4.55657600	-0.44758000	1.00122000
H	-4.57177400	-0.77207000	-0.73535600
C	0.88829700	0.02330800	-0.00436900
C	1.70214500	1.13880300	0.18964100
C	3.07901200	0.95768900	0.19791000
H	1.27479500	2.12244000	0.34381600
C	2.69144200	-1.37142100	-0.15483300
C	3.58828900	-0.32160000	0.02205500
H	3.73994300	1.80322800	0.34699600
H	3.05387900	-2.38525300	-0.29177600
H	4.65420200	-0.51137500	0.02373100
N	1.36932300	-1.21238800	-0.17119600

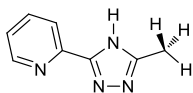
B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.67398700	-0.18588100	0.03481000
C	-0.57949700	0.15914600	-0.02805000
N	-1.23391900	1.31741600	-0.22015300
H	-0.85876200	2.23948400	-0.40162600
N	-2.57216300	1.11900100	-0.18773100
N	-1.47170500	-0.81450900	0.13756300
C	-3.98726600	-0.88225200	0.16391600
H	-3.82830300	-1.94376000	0.35040500

H	-4.56982300	-0.46812800	0.98989900
H	-4.58034500	-0.77456700	-0.74689000
C	0.88646700	0.02585300	-0.00186300
C	1.71097100	1.13897600	0.17729900
C	3.08655300	0.95595900	0.18372400
H	1.29168300	2.12655700	0.32234900
C	2.69673100	-1.37479500	-0.14522600
C	3.59519200	-0.32525000	0.01859700
H	3.74836900	1.80222200	0.32218500
H	3.05767500	-2.39029500	-0.27380800
H	4.66112100	-0.51461600	0.01895300
N	1.37313000	-1.21439900	-0.15835200

9b-C-I



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

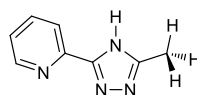
ATOM	X	Y	Z
C	-2.70125900	0.10506000	0.02432500
C	-0.56362700	-0.28237700	-0.03459800
N	-1.17958200	-1.42085400	-0.23171400
N	-2.52741900	-1.17598500	-0.19691200
N	-1.48725900	0.70555600	0.12848100
C	-3.99728000	0.81918200	0.14909200
H	-4.81072900	0.10602900	0.02310700
H	-4.08444100	1.29013900	1.13013800
H	-4.08234900	1.59623600	-0.61301300
C	0.89658600	-0.07098800	-0.00678300
C	1.43736200	1.20552900	-0.16098300
C	2.81895000	1.34679000	-0.13463500
H	0.80227100	2.06941900	-0.31477000
C	2.97101700	-1.01379300	0.17755600
C	3.60628900	0.21707000	0.03818500
H	3.26936100	2.32507500	-0.25430000
H	3.55403100	-1.91914200	0.31401400
H	4.68691800	0.27832800	0.06365800
N	1.64841300	-1.16449500	0.15876300
H	-1.32236500	1.68552400	0.32787700

B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	2.70967900	0.10714500	-0.00002400
C	0.56098400	-0.28179800	-0.00000900
N	1.17832000	-1.44372600	-0.00008200
N	2.53650200	-1.19733500	-0.00008400
N	1.49499300	0.71534400	0.00003300
C	4.00930200	0.82703300	-0.00001000
H	4.82306300	0.10292500	-0.00005600
H	4.10629700	1.46381500	-0.88253300
H	4.10632400	1.46373100	0.88257000
C	-0.89511400	-0.06720800	0.00001300
C	-1.44240700	1.21851600	0.00008200
C	-2.82372200	1.35761900	0.00009500
H	-0.81315300	2.09904100	0.00012200
C	-2.98272600	-1.02134700	-0.00003000
C	-3.61562600	0.21807000	0.00003800
H	-3.27059900	2.34437100	0.00014800
H	-3.56857500	-1.93519100	-0.00007800
H	-4.69645700	0.27968500	0.00004400
N	-1.65905500	-1.17156200	-0.00004300
H	1.33554500	1.71439100	0.00008800

9b-C-II



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

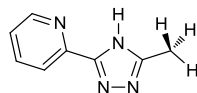
ATOM	X	Y	Z
C	-2.70238700	0.10492900	0.00008700
C	-0.56257500	-0.28032900	0.00012800
N	-1.17787700	-1.43708700	-0.00042200
N	-2.52495100	-1.19517400	-0.00007500
N	-1.49175800	0.71675300	0.00036300
C	-4.00510700	0.82320100	0.00027300
H	-3.84532200	1.90117100	0.00019600
H	-4.58470900	0.55382400	-0.88393000
H	-4.58438300	0.55390500	0.88471600
C	0.89748500	-0.06661700	0.00009100
C	1.43806100	1.21942900	-0.00018800
C	2.82040000	1.35692800	-0.00038000
H	0.80622800	2.09901600	-0.00024900
C	2.97481200	-1.02322100	0.00005300
C	3.60976900	0.21579400	-0.00028200
H	3.26898300	2.34328700	-0.00061400
H	3.55895600	-1.93805800	0.00018300
H	4.69082900	0.27438500	-0.00044900
N	1.65218800	-1.17110400	0.00024000
H	-1.33655700	1.71807200	0.00071600

B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.70885400	0.10703400	0.00002600
C	-0.56046900	-0.28354900	0.00001200
N	-1.17972800	-1.44501200	0.00008700
N	-2.53664500	-1.19807700	0.00008700
N	-1.49466300	0.71347100	-0.00003000
C	-4.00897300	0.82990700	0.00000700
H	-3.85074700	1.90850800	-0.00002600
H	-4.59503400	0.56582000	-0.88259200
H	-4.59503100	0.56587400	0.88262300
C	0.89519000	-0.06843300	-0.00001200
C	1.44149200	1.21794200	-0.00008400
C	2.82253800	1.35847200	-0.00010000
H	0.81150900	2.09795800	-0.00012500
C	2.98402400	-1.02021000	0.00003000
C	3.61573700	0.21972300	-0.00004200
H	3.26828900	2.34575200	-0.00015600
H	3.57082400	-1.93345000	0.00007800
H	4.69649600	0.28251700	-0.00005100
N	1.66039600	-1.17193800	0.00004500
H	-1.33594500	1.71259600	-0.00008600

9b-C-III



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.68231500	-0.12138800	0.00003300
C	-0.55940300	0.31866800	-0.00008800
N	-1.19625500	1.46176200	0.00009200
N	-2.53921300	1.18426800	-0.00061300
N	-1.45553600	-0.70205200	0.00002900
C	-3.96532400	-0.87127600	0.00017100
H	-4.79179600	-0.16218000	-0.00013600

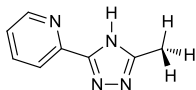
H	-4.04182600	-1.50737600	-0.88366100
H	-4.04200000	-1.50682400	0.88438700
C	0.89542400	0.11075500	-0.00002600
C	1.77337600	1.19286800	0.00005900
C	3.13542800	0.92768500	0.00012300
H	1.39035700	2.20553700	0.00007700
C	2.60713400	-1.40311800	0.00003200
C	3.56502500	-0.39463600	0.00010700
H	3.85078500	1.74175100	0.00018800
H	2.90572400	-2.44629300	0.00009000
H	4.61814300	-0.64578100	0.00015200
N	1.29545500	-1.16461900	-0.00003400
H	-1.23660300	-1.69169700	0.00021500

B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.68931900	-0.12399800	-0.00001900
C	-0.55775200	0.32097000	-0.00001500
N	-1.19866600	1.46854300	-0.00009300
N	-2.55154100	1.18618700	-0.00009000
N	-1.45904900	-0.69974600	0.00002400
C	-3.97056800	-0.87611900	0.00001100
H	-4.80293300	-0.17348800	-0.00006800
H	-4.05067800	-1.51560300	-0.88228600
H	-4.05072400	-1.51545500	0.88241100
C	0.89338000	0.11406900	0.00000800
C	1.78078000	1.19160500	-0.00006000
C	3.14181900	0.92546700	-0.00003900
H	1.40630300	2.20651200	-0.00012800
C	2.61361300	-1.40391100	0.00011200
C	3.57196900	-0.39677300	0.00004900
H	3.85696600	1.73932500	-0.00009000
H	2.91210700	-2.44718800	0.00018100
H	4.62524700	-0.64691500	0.00006700
N	1.30063300	-1.16461400	0.00009300
H	-1.23945700	-1.68763800	0.00008200

9b-C-IV



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

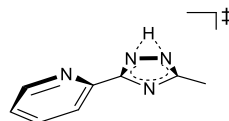
ATOM	X	Y	Z
C	2.68128300	-0.12169000	0.00001900
C	0.55903900	0.31993900	-0.00000800
N	1.19794000	1.46241300	0.00010600
N	2.53970900	1.18429700	-0.00017500
N	1.45498400	-0.70099600	0.00001400
C	3.96542900	-0.87252000	0.00006000
H	3.77775300	-1.94586400	-0.00003800
H	4.55201800	-0.61845800	-0.88409800
H	4.55188000	-0.61860800	0.88435500
C	-0.89557500	0.11184200	-0.00000300
C	-1.77475000	1.19320000	0.00016000
C	-3.13649500	0.92682500	0.00014800
H	-1.39240400	2.20615100	0.00029500
C	-2.60634700	-1.40349200	-0.00017300
C	-3.56509300	-0.39585800	-0.00002600
H	-3.85259700	1.74027600	0.00027200
H	-2.90414800	-2.44693100	-0.00031200
H	-4.61798700	-0.64789700	-0.00004500
N	-1.29486400	-1.16389600	-0.00016200
H	1.23614600	-1.69086500	0.00001500

B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.68841100	-0.12361600	-0.00002000
C	-0.55727900	0.32325100	-0.00001600
N	-1.20025900	1.47021000	-0.00009000
N	-2.55186100	1.18723600	-0.00007000
N	-1.45866600	-0.69750500	0.00001400
C	-3.96944200	-0.87988700	0.00000700
H	-3.78242600	-1.95379300	0.00003200
H	-4.56260200	-0.63183500	0.88251200
H	-4.56261300	-0.63187900	-0.88250300
C	0.89342400	0.11562200	0.00000600
C	1.78250700	1.19190300	-0.00007200
C	3.14313500	0.92381200	-0.00004800
H	1.40958700	2.20740000	-0.00015000
C	2.61195500	-1.40473100	0.00012300
C	3.57169000	-0.39902300	0.00005200
H	3.85940100	1.73669300	-0.00010800
H	2.90890900	-2.44846800	0.00020100
H	4.62462500	-0.65059400	0.00007300
N	1.29928300	-1.16364500	0.00010200
H	-1.23983400	-1.68558100	0.00005900

TS-AB



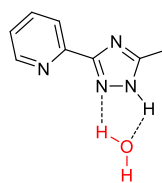
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -1703.5935 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
N	1.15826700	-1.42831500	-0.02635800
H	1.93837100	-1.70017700	0.90708200
C	0.57504900	-0.22337200	-0.04428100
N	1.44732100	0.78783300	-0.09915500
C	2.64473900	0.20234700	-0.01344900
N	2.56891700	-1.13688900	-0.00519800
C	-0.89205400	-0.04426400	-0.02517000
C	-1.43403500	1.23841800	0.02349600
C	-2.81683200	1.36813500	0.04991900
H	-0.78378900	2.10338200	0.04374500
C	-2.95881200	-1.01567400	-0.02155000
C	-3.59796400	0.22078400	0.02671700
H	-3.27389700	2.34981000	0.08986500
H	-3.53949600	-1.93238200	-0.04139700
H	-4.67935600	0.27227700	0.04539400
C	3.94096300	0.93225600	0.02299000
H	4.10385900	1.45490000	-0.92173700
H	3.93076100	1.67584800	0.82117800
H	4.76171000	0.23555100	0.18754600
N	-1.63514600	-1.15562600	-0.04696200

9b-A·H₂O



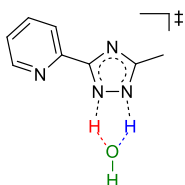
M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-0.26831100	-0.25892200	-0.02455100

C	-2.17444800	-1.16894700	-0.01916900
N	-2.30318200	0.16504000	-0.04694200
H	-3.14748500	0.73096600	-0.05980500
N	-1.10034300	0.76519700	-0.05036300
N	-0.88490500	-1.47123300	-0.00687200
H	-1.98388100	2.68918700	0.01503800
O	-2.91588600	2.92452000	0.12212600
H	-3.05245100	3.71027300	-0.41603500
C	1.20177700	-0.10391500	-0.01183000
C	2.02068600	-1.23256500	0.01159400
C	3.39746300	-1.05199200	0.02639500
H	1.58126200	-2.22152300	0.01789700
C	3.00534400	1.30192400	-0.00582800
C	3.90550500	0.24058500	0.01792200
H	4.06153500	-1.90835500	0.04446400
H	3.36609600	2.32577000	-0.01288500
H	4.97131500	0.43096100	0.02948600
N	1.68284000	1.14398300	-0.02070000
C	-3.32188700	-2.11179900	0.02899400
H	-3.44753100	-2.49312300	1.04455800
H	-4.24158900	-1.61046900	-0.27266400
H	-3.13783100	-2.95696400	-0.63408200

TS-AB



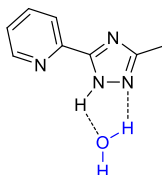
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -671. 6740 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	0.29464600	-0.23364700	-0.00010200
C	2.25329000	-1.01688800	0.00067300
N	2.37171800	0.30718600	-0.00034800
H	2.99857400	1.69835500	-0.01617200
N	1.10809000	0.81389400	-0.00142000
N	0.96490800	-1.40151500	0.00219400
H	1.61007100	2.25504100	-0.01852400
O	2.58958600	2.69055600	-0.07528200
H	2.79477800	3.20744900	0.72121900
C	-1.17772100	-0.12453500	0.00052200
C	-1.96520600	-1.27656000	0.01939700
C	-3.34618000	-1.13687200	0.01848300
H	-1.49560500	-2.25154900	0.03464000
C	-3.02391400	1.22740700	-0.01920000
C	-3.89245500	0.14057500	-0.00163000
H	-3.98496900	-2.01240900	0.03291300
H	-3.41479900	2.24011200	-0.03493400
H	-4.96346000	0.29933500	-0.00352700
C	3.41768300	-1.94628100	-0.00952300
H	3.43530900	-2.52838700	-0.93336800
H	4.34813900	-1.38376700	0.06706000
H	3.35799000	-2.64643300	0.82565100
N	-1.69665600	1.10880800	-0.01820000

9b-B·H₂O



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.22038400	-1.11724900	-0.00603200
C	-0.25136500	-0.35632600	-0.00674100
N	-1.11740100	0.66223300	-0.02096200
H	-0.93198100	1.66074000	-0.03066500
N	-2.38054500	0.19509100	-0.02068300
N	-0.91533900	-1.50221300	0.00253100
H	-3.18049500	2.11046000	0.00124100
O	-2.79533400	2.99262500	0.10020600
H	-3.26079200	3.55313000	-0.52805700
C	1.20775600	-0.16715500	-0.00295500
C	2.06605300	-1.26267500	0.00422800
C	3.43366200	-1.01943100	0.00737200
H	1.66541100	-2.26843500	0.00692800
C	2.94013500	1.32025300	-0.00361900
C	3.88258400	0.29499200	0.00355400
H	4.13617600	-1.84453700	0.01267600
H	3.25634800	2.35820300	-0.00655100
H	4.93939300	0.53027800	0.00602000
C	-3.36026000	-2.07353400	0.00787200
H	-3.34728200	-2.66633500	0.92474000
H	-3.29141600	-2.76058700	-0.83743200
H	-4.30400400	-1.53204800	-0.04986500
N	1.62646000	1.10272900	-0.00699500

H₂O

M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

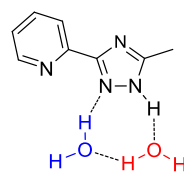
ATOM	X	Y	Z
O	0.00000000	0.00000000	0.11793700
H	0.00000000	0.76072700	-0.47174800
H	0.00000000	-0.76072700	-0.47174800

M06-2X/6-311+G(d,p)/H₂O

Cartesian coordinates

ATOM	X	Y	Z
O	0.00000000	0.00000000	0.11831800
H	0.00000000	0.75973900	-0.47327400
H	0.00000000	-0.75973900	-0.47327400

9b-A·2H₂O



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-0.03077200	-0.57290300	0.00019500
C	1.74172000	-1.71982700	-0.00967300
N	2.04815400	-0.41615200	0.00142500
H	2.95856700	0.05432900	0.00685200
N	0.93101100	0.33109200	0.00908900
N	0.42171100	-1.85264800	-0.01118700
H	3.21379900	2.35762400	-0.02316400
O	3.91557100	1.68155800	-0.06623300
H	4.60315800	1.96616300	0.54380900
O	1.54769400	3.08869400	0.08188000
H	1.08542700	2.22935900	0.03202600
H	1.13100900	3.66108400	-0.56978900
C	-1.46371100	-0.21512200	0.00052400

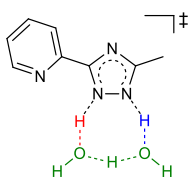
C	-2.43248700	-1.21716400	0.01970000
C	-3.76996100	-0.84404200	0.02008200
H	-2.13482900	-2.25765000	0.03376700
C	-3.04842200	1.43182800	-0.01679900
C	-4.08928200	0.50739500	0.00180100
H	-4.54875400	-1.59775200	0.03478700
H	-3.26201100	2.49607800	-0.03179100
H	-5.11763700	0.84610100	0.00157700
N	-1.76104800	1.08910000	-0.01804200
C	2.74442300	-2.81698800	-0.01314500
H	3.75467700	-2.41469100	-0.08556700
H	2.66006500	-3.39968900	0.90574900
H	2.56256800	-3.48177300	-0.85853900

M06-2X/6-311+G(d,p)/SMD(H₂O)

Cartesian coordinates

ATOM	X	Y	Z
C	-0.08120100	-0.54220900	-0.00195900
C	1.67510100	-1.71228000	-0.01535500
N	1.99960000	-0.41430700	-0.00495700
H	2.92226400	0.03568500	-0.00222300
N	0.89322300	0.34925100	0.00423700
N	0.35333400	-1.83028900	-0.01393900
H	3.43708700	2.18423000	-0.00100900
O	4.12067100	1.48927000	-0.03454500
H	4.63656300	1.60352300	0.77091200
O	1.78241800	3.05375900	0.03828800
H	1.29897600	2.20557400	-0.00559900
H	1.53912500	3.52687400	-0.76477200
C	-1.50950600	-0.17152800	0.00304800
C	-2.48307000	-1.16901200	0.00484300
C	-3.81984000	-0.79439800	0.00996600
H	-2.19249000	-2.21059000	0.00263900
C	-3.09368400	1.47769100	0.01089300
C	-4.13631900	0.55727300	0.01314700
H	-4.59944200	-1.54687100	0.01162300
H	-3.30502800	2.54171600	0.01319400
H	-5.16310800	0.89965000	0.01733200
N	-1.80512000	1.13494100	0.00584700
C	2.67355400	-2.80991700	-0.01782100
H	3.68270300	-2.40841900	-0.10311600
H	2.59700100	-3.38380300	0.90713200

TS-AB·2H₂O



M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -979.4594 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-1.79206600	-1.58505300	0.01274300
C	0.03247700	-0.53527200	-0.00064700
N	-0.92086700	0.38738600	-0.00756200
H	-1.12263800	1.85163600	-0.01288900
N	-2.09714400	-0.28981900	0.00195700
N	-0.46348800	-1.78556500	0.01144300
H	-2.77360600	2.34645100	-0.00366000
O	-1.65090000	2.78670600	-0.04874200
H	-1.41527800	3.33643100	0.71017400
O	-3.72676800	1.61326700	0.03293000
H	-3.21318400	0.66509000	-0.00202000
H	-4.31335700	1.70970700	-0.72901000
C	1.47098100	-0.20794000	-0.00397900

C	2.42296100	-1.22749900	-0.02183800
C	3.76668100	-0.87980200	-0.02264200
H	2.10534700	-2.26216300	-0.03417500
C	3.08912500	1.40908700	0.01038200
C	4.11223300	0.46590200	-0.00624800
H	4.53124100	-1.64809200	-0.03601600
H	3.32258000	2.46924900	0.02360300
H	5.14687300	0.78485800	-0.00604500
N	1.79498300	1.09071900	0.01202700
C	-2.80954300	-2.67414800	0.02994200
H	-2.72507200	-3.25970900	0.94771500
H	-3.81438200	-2.25538700	-0.02760200
H	-2.65865500	-3.34855700	-0.81491100

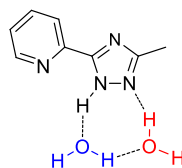
M06-2X/6-311+G(d,p)/SMD(H₂O)

Imaginary frequency: -917.2093 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-1.77823000	-1.61348300	0.01533100
C	0.03404700	-0.55035300	0.00542400
N	-0.92658700	0.36461700	-0.00111200
H	-1.14713800	1.89778700	0.02447100
N	-2.09888100	-0.32137400	0.00530100
N	-0.44780000	-1.80889100	0.01551300
H	-2.78460700	2.36296000	-0.00394200
O	-1.65194400	2.81475400	-0.00011700
H	-1.47356900	3.27982500	0.82811700
O	-3.74319800	1.65047700	-0.01165300
H	-3.26444000	0.72150600	-0.02763400
H	-4.23005500	1.75157600	-0.84087500
C	1.46722200	-0.20779400	-0.00176700
C	2.43043600	-1.21741600	-0.01196700
C	3.77157100	-0.86159400	-0.02089000
H	2.12506100	-2.25496000	-0.01402500
C	3.07822000	1.41976000	-0.00869200
C	4.10814400	0.48625000	-0.01923600
H	4.54075700	-1.62485600	-0.02966000
H	3.30390000	2.48104100	-0.00722200
H	5.13961300	0.81420100	-0.02647600
N	1.78432700	1.09506700	0.00029100
C	-2.79142300	-2.70477800	0.03179200
H	-2.71870400	-3.28077000	0.95675900
H	-3.79632800	-2.28985000	-0.04264000
H	-2.63068700	-3.38979400	-0.80263900

9b-B·2H₂O



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	1.72173100	-1.65963600	-0.00764200
C	-0.11343300	-0.61765900	-0.00065800
N	0.88663500	0.26762500	-0.00157700
H	0.86314700	1.29334100	-0.00091700
N	2.06655000	-0.38223700	-0.00689100
N	0.37675400	-1.84969500	-0.00410200
H	2.65564400	2.69537600	0.02315600
O	1.71459600	2.94650300	0.07024500
H	1.58909800	3.65653500	-0.56712400
O	4.10207700	1.58161900	-0.06369400
H	3.58003300	0.75684300	-0.01688500
H	4.77720900	1.51579600	0.61911300

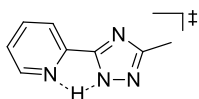
C	-1.53096300	-0.22351300	0.00160300
C	-2.53434000	-1.18779700	0.00793000
C	-3.85443800	-0.75579800	0.00903600
H	-2.27772100	-2.23960800	0.01171300
C	-3.03790800	1.49178500	-0.00196000
C	-4.11471300	0.60850200	0.00407600
H	-4.66561300	-1.47438800	0.01372600
H	-3.20629300	2.56378100	-0.00593200
H	-5.12813300	0.98945500	0.00474300
C	2.70950500	-2.77347200	-0.01055500
H	2.58161800	-3.39358300	0.87867300
H	2.56275000	-3.40598300	-0.88794000
H	3.72434400	-2.37675200	-0.02395400
N	-1.76738600	1.09284000	-0.00339500

M06-2X/6-311+G(d,p)/SMD(H₂O)

Cartesian coordinates

ATOM	X	Y	Z
C	1.75353100	-1.68192300	-0.02878900
C	-0.08144700	-0.64154700	-0.01798200
N	0.91802700	0.24346400	-0.05699900
H	0.88969200	1.26992400	-0.07123100
N	2.09898900	-0.40523700	-0.06397400
N	0.40870500	-1.87506200	-0.00016200
H	2.47875100	2.74421900	0.01613100
O	1.54032700	3.01312800	0.01343700
H	1.42541400	3.52984400	-0.79142400
O	4.01494500	1.72240300	0.04617000
H	3.53220700	0.87373700	0.04193500
H	4.49676000	1.73765900	0.88012300
C	-1.49617200	-0.24611700	0.00032500
C	-2.49976600	-1.20964100	0.02702800
C	-3.82059900	-0.78079800	0.04256500
H	-2.24727300	-2.26148700	0.03518600
C	-3.00804400	1.46519500	0.00451400
C	-4.08309400	0.58254500	0.03105300
H	-4.62991400	-1.50066900	0.06302200
H	-3.17908200	2.53609500	-0.00475700
H	-5.09621300	0.96327100	0.04229100
C	2.74651700	-2.78795600	-0.01447200
H	2.65731000	-3.36285200	0.90926600
H	2.57035400	-3.46565500	-0.85148500
H	3.75731800	-2.38898800	-0.08687000
N	-1.73472900	1.07142300	-0.01093600

TS1-BC



M06-2X/6-311+G(d,p)/SMD(DMSO)

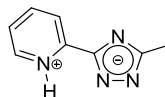
Imaginary frequency: -1627.3150 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-0.62121800	0.14284900	0.00000000
N	-1.65184700	0.98117200	0.00000000
N	-0.98683300	-1.13668700	0.00000100
C	0.84450200	0.27178500	0.00000000
C	1.65766800	1.39082800	-0.00000200
C	3.03738400	1.18208700	-0.00000200
H	1.22539900	2.38480200	-0.00000200
C	2.66999100	-1.18822400	0.00000000
C	3.55277200	-0.11154200	-0.00000100
H	3.71041200	2.03348100	-0.00000300
H	3.00373500	-2.21985600	0.00000100
H	4.62104700	-0.29169800	-0.00000200
N	1.35825800	-0.97679300	0.00000000
C	-2.69267900	0.10605800	0.00000100

C	-4.12276400	0.53812000	0.00000100
H	-4.34918400	1.14332600	0.88316400
H	-4.34918400	1.14332800	-0.88316200
H	-4.77764500	-0.33589900	0.00000000
N	-2.33015900	-1.18171300	0.00000200
H	0.23555200	-1.65110200	0.00000100

II

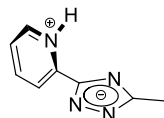


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-0.63156300	-0.15048300	-0.00005500
N	-1.53912200	0.84427900	-0.00050400
N	-1.16452300	-1.37035800	0.00010100
C	0.80654500	0.05033200	-0.00019000
C	1.43528300	1.29244800	-0.00025800
C	2.81813000	1.35141700	-0.00034100
H	0.82580800	2.18575700	-0.00021900
C	2.92390700	-1.02874100	-0.00032800
C	3.57962100	0.17931100	-0.00036600
H	3.31354800	2.31492200	-0.00037300
H	3.41938600	-1.98956000	-0.00035200
H	4.66022400	0.20313400	-0.00042200
N	1.58051100	-1.05401700	-0.00025400
C	-2.68788500	0.14968100	0.00039400
C	-4.04299300	0.77815700	0.00078300
H	-4.81315000	0.00638100	0.00094000
H	-4.18176300	1.40743900	0.88275700
H	-4.18221700	1.40757800	-0.88101300
N	-2.49800600	-1.17886200	0.00081000
H	1.09987700	-1.95567000	-0.00023000

TS2-rot



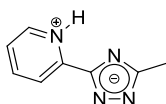
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -82.7341 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-0.64761000	0.03200900	0.21947800
N	-1.49409300	-0.05312600	-0.82137900
N	-1.23599600	0.11227700	1.40434200
C	0.82322500	0.06987300	-0.06297500
C	1.55420300	1.23780700	-0.07414400
C	2.93543900	1.17177300	-0.22075600
H	1.03324600	2.18558500	-0.06546800
C	2.82405900	-1.20388100	-0.08848200
C	3.58065600	-0.06076100	-0.23005600
H	3.50891900	2.08456300	-0.32880900
H	3.23099100	-2.20540600	-0.08051500
H	4.65269100	-0.14130400	-0.34398500
N	1.49364700	-1.10042700	0.05112600
C	-2.68659300	-0.01626900	-0.18697100
C	-4.00142200	-0.06368800	-0.89676900
H	-4.81649000	-0.05024800	-0.17235200
H	-4.11699500	0.79458500	-1.56296600
H	-4.09066200	-0.96777500	-1.50306100
N	-2.57067400	0.07840800	1.13572400
H	0.95637100	-1.96110400	0.15681200

I2

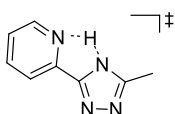


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	0.62540800	0.29683800	-0.00003400
N	1.45254500	-0.76798300	-0.00001700
N	1.25143900	1.47036600	-0.00026500
C	-0.81973700	0.16076900	-0.00008700
C	-1.72644600	1.21896600	-0.00030400
C	-3.08222600	0.94662700	-0.00032500
H	-1.34771200	2.23185700	-0.00044200
C	-2.62082900	-1.39136900	0.00004600
C	-3.54373700	-0.37418400	-0.00014700
H	-3.79288800	1.76460200	-0.00048300
H	-2.87339100	-2.44257500	0.00018600
H	-4.59921100	-0.60697500	-0.00016600
N	-1.30877400	-1.09486800	0.00006900
C	2.65291300	-0.16843700	0.00026900
C	3.95460900	-0.90100500	0.00054000
H	4.78158600	-0.19046000	-0.00009900
H	4.04543000	-1.53870600	0.88269300
H	4.04508000	-1.53995300	-0.88074200
N	2.56583000	1.17070800	0.00008200
H	-0.62589900	-1.85457800	0.00022000

TS3-BC

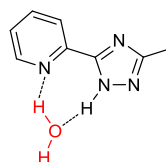


M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -1500.9010 cm⁻¹

Cartesian coordinates

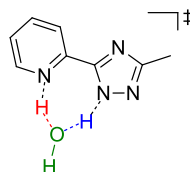
ATOM	X	Y	Z
C	0.58678100	0.57826300	0.00063100
N	1.37163700	1.62787200	-0.00200400
N	1.25805700	-0.59301300	0.00065100
C	-0.86766700	0.36404600	0.00080200
C	-1.91688100	1.26380500	0.00264700
C	-3.20737300	0.74000700	0.00184100
H	-1.72771500	2.32930300	0.00468600
C	-2.29969200	-1.47744500	-0.00209400
C	-3.40641000	-0.63718700	-0.00076300
H	-4.05920900	1.40970200	0.00323700
H	-2.38664400	-2.55679200	-0.00404300
H	-4.40191600	-1.06018900	-0.00170100
N	-1.07257400	-0.96717400	-0.00114900
H	0.18207600	-1.34414900	-0.00089500
C	2.55037700	-0.20491000	-0.00185400
C	3.71736900	-1.12859300	0.00310400
H	4.64043100	-0.55138200	-0.04402400
H	3.72788900	-1.73478500	0.91149000
H	3.68019300	-1.80628500	-0.85206800
N	2.64372000	1.12183900	-0.00357900

9b-B·H₂O'

M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	0.64288800	-0.18375700	0.00180900
N	1.56954900	-1.13048600	0.00345600
N	1.23309800	1.01956300	-0.00115200
C	-0.81337600	-0.40702200	0.00163900
C	-1.31069400	-1.70750700	0.00520600
C	-2.68731900	-1.88735700	0.00397200
H	-0.62684200	-2.54629400	0.00862700
C	-2.92375900	0.48866900	-0.00470500
C	-3.51312200	-0.77057500	-0.00103300
H	-3.10731200	-2.88618100	0.00657500
H	-3.53418700	1.38578000	-0.00920700
H	-4.59149300	-0.86395200	-0.00254200
N	-1.60309900	0.67431700	-0.00325500
H	0.80146600	1.94830300	-0.00111600
C	2.73787000	-0.43588200	0.00115400
C	4.07794700	-1.08721500	0.00126500
H	4.19501700	-1.72006600	0.88302200
H	4.19602500	-1.71822900	-0.88170100
H	4.86275600	-0.33145600	0.00236500
N	2.57141400	0.87575700	-0.00159300
O	-0.50305100	3.27822000	-0.08383900
H	-0.73339700	3.87073700	0.63893700
H	-1.09697100	2.50543000	-0.01227400

TS1-BC·H₂O

M06-2X/6-311+G(d,p)/SMD(DMSO)

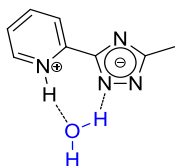
Imaginary frequency: -1271.9375 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	0.65675700	-0.12716200	0.00126000
N	1.56331400	-1.10966700	0.01461700
N	1.23104500	1.07883800	-0.02138900
C	-0.79755300	-0.35022200	0.00240700
C	-1.32428500	-1.63835600	0.01643500
C	-2.70131600	-1.80357300	0.01225000
H	-0.65022300	-2.48419300	0.02947700
C	-2.94452100	0.56584300	-0.01946500
C	-3.53112000	-0.68644600	-0.00654800
H	-3.12614700	-2.80024800	0.02277700
H	-3.52794200	1.47866700	-0.03403300
H	-4.60872500	-0.77858000	-0.01160000
N	-1.61636900	0.71863400	-0.01455800
H	0.51254500	2.20201100	-0.01945800
C	2.72878900	-0.42784900	-0.00086900
C	4.06988000	-1.08281200	0.00467200
H	4.19111500	-1.71047100	0.88998400
H	4.19399300	-1.71930400	-0.87399900
H	4.85563300	-0.32738000	0.00195400
N	2.56449700	0.89366300	-0.02173300
O	-0.41962200	2.88210300	-0.05990500
H	-0.49381800	3.43538100	0.72688500

H -1.12664700 1.88048300 -0.01215300

I1·H₂O

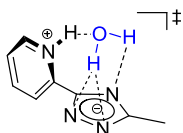


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	0.67091800	-0.14938400	0.00223400
N	1.58114100	-1.13961900	0.01529800
N	1.21655800	1.06768700	-0.01868000
C	-0.76647500	-0.39895800	0.00379400
C	-1.30111900	-1.68522600	0.00484400
C	-2.67474500	-1.85482300	0.00131900
H	-0.62336200	-2.52759700	0.00690600
C	-2.95680100	0.50777100	-0.00248700
C	-3.52248800	-0.74546000	-0.00286700
H	-3.09190100	-2.85469800	0.00097300
H	-3.52698300	1.42703800	-0.00511500
H	-4.59823400	-0.85028800	-0.00658500
N	-1.61987200	0.64621000	0.00098900
H	0.34601000	2.64422000	-0.02433300
C	2.73369500	-0.44983800	0.00116900
C	4.08517000	-1.08536000	0.00677400
H	4.21568200	-1.71617000	0.88873600
H	4.22372600	-1.71477700	-0.87509200
H	4.85954000	-0.31794600	0.01050800
N	2.54981100	0.87609800	-0.01868400
O	-0.47522600	3.18886800	-0.07615800
H	-0.45968400	3.79869000	0.66866300
H	-1.24539300	1.61561700	0.00346000

TS2-rot·H₂O



M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -68.8816 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-0.51492800	-0.49675300	0.19059600
N	-1.35806400	-0.46043100	-0.85543600
N	-1.10776900	-0.46999600	1.37655700
C	0.95378700	-0.39520500	0.04486000
C	1.84201500	-1.45526000	0.06778700
C	3.20289900	-1.20663400	-0.08309600
H	1.46298200	-2.45982600	0.19834500
C	2.74727300	1.12585800	-0.26635400
C	3.66363800	0.09469600	-0.25361600
H	3.90508300	-2.03169800	-0.06870200
H	3.01005100	2.16817100	-0.38529000
H	4.71560200	0.31396500	-0.37281600
N	1.44421700	0.85133600	-0.11920200
H	-1.26261700	1.96034600	0.95983400
C	-2.55404300	-0.43302700	-0.22558500
C	-3.86493800	-0.40982100	-0.94343000
H	-3.89910400	0.40771800	-1.66683300
H	-4.02995000	-1.34168200	-1.48965200
H	-4.67983200	-0.27998100	-0.23053400

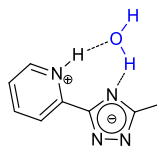
N -2.44293200 -0.43095400 1.10169400

O -0.89061000 2.49586100 0.24471100

H -1.45898700 2.29939400 -0.51117500

H 0.75926800 1.62389400 -0.10311900

I2·H₂O

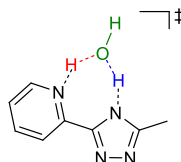


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-0.54693000	-0.61953000	-0.00002300
N	-1.45973600	0.37696500	-0.01378400
N	-1.09238000	-1.83177300	0.01516400
C	0.89608100	-0.41996400	-0.00052600
C	1.81009500	-1.47320500	0.00758900
C	3.16549600	-1.19996800	0.00619400
H	1.43523600	-2.48727200	0.01470100
C	2.69045200	1.13154400	-0.01086600
C	3.62121000	0.12132200	-0.00381600
H	3.87712300	-2.01707400	0.01267100
H	2.94095000	2.18391100	-0.01781100
H	4.67533000	0.36043400	-0.00551700
N	1.37693200	0.83994200	-0.00881400
H	-0.69677400	3.50588600	0.68123000
C	-2.61529500	-0.30730700	-0.00492100
C	-3.96247100	0.33509100	-0.01174200
H	-4.09895400	0.96455700	0.87053900
H	-4.08920200	0.96679400	-0.89374900
H	-4.73970800	-0.42925000	-0.01657000
N	-2.42619400	-1.63183800	0.01193100
O	-0.50530200	2.93328900	-0.06857700
H	-1.11938000	2.16582200	-0.01189600
H	0.71560400	1.63890600	-0.00778700

TS3-BC·H₂O



M06-2X/6-311+G(d,p)/SMD(DMSO)

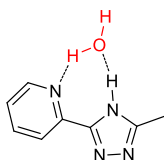
Imaginary frequency: -1271.4869 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-0.55034900	-0.57784300	0.00082000
N	-1.11589300	-1.77152800	0.01447400
N	-1.47167700	0.41746900	-0.01378000
C	0.90541100	-0.37329100	-0.00001100
C	1.78757400	-1.45245700	0.01316700
C	3.15114300	-1.20773600	0.00975100
H	1.39300100	-2.45949900	0.02525800
C	2.69236200	1.12883900	-0.01908600
C	3.61929100	0.10424900	-0.00711200
H	3.84884500	-2.03683200	0.01968600
H	2.98364900	2.17238800	-0.03211200
H	4.67691500	0.33074500	-0.01089300
N	1.37606400	0.88740000	-0.01521000
H	-1.09023400	1.69599500	-0.01444500
O	-0.39323500	2.61373400	-0.06115000
H	-0.47341400	3.16588100	0.72626400

H	0.56052400	1.86999000	-0.01440500
N	-2.45736900	-1.56010300	0.01001800
C	-2.64505000	-0.24586100	-0.00640500
C	-3.97857800	0.41942900	-0.01343000
H	-4.09387700	1.05188700	-0.89610500
H	-4.10353100	1.05014400	0.86929600
H	-4.76470100	-0.33521200	-0.01801900

9b-C·H₂O

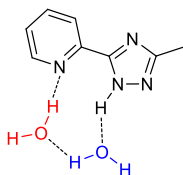


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	0.50793500	-0.64681500	0.00223700
N	1.07962900	-1.82592500	0.00116900
N	1.46183100	0.32310200	0.00205100
C	-0.94368000	-0.40403400	0.00178200
C	-1.83009200	-1.48038100	0.00695000
C	-3.19114100	-1.21428000	0.00532900
H	-1.44989300	-2.49366200	0.01193200
C	-2.66487000	1.11332400	-0.00649600
C	-3.62228200	0.10755900	-0.00143300
H	-3.90600800	-2.02874800	0.00909300
H	-2.95783900	2.15811100	-0.01242700
H	-4.67487000	0.35979000	-0.00308000
N	-1.35193700	0.87046800	-0.00497500
H	1.32057800	1.33857300	0.00462800
O	0.49368400	2.99756100	-0.08375600
H	0.44933300	3.63633600	0.63491500
H	-0.30792200	2.44107800	-0.01452900
C	2.64975000	-0.33261400	0.00062500
C	3.97455200	0.34140500	0.00009600
H	4.08545000	0.97491000	-0.88191900
H	4.08948600	0.96849800	0.88618500
H	4.75933100	-0.41365200	-0.00426900
N	2.43359900	-1.62860300	-0.00039000

9b-B·2H₂O'



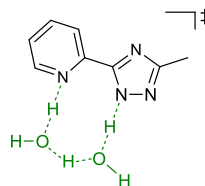
M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.75280900	-0.76362200	0.11166300
C	-0.66046300	-0.54209100	-0.03318900
N	-1.24511700	0.63153300	-0.30269200
H	-0.83985000	1.52817700	-0.60000700
N	-2.58292900	0.50554400	-0.21720700
N	-1.58586800	-1.45175100	0.23410700
H	0.10396000	3.44205200	-0.24246900
O	-0.42190700	3.23638300	-1.03682100
O	1.17698900	2.92129300	1.12600700
H	0.91462000	2.89457400	2.05177300
C	0.79462100	-0.76487600	-0.04721900
C	1.29848600	-2.05512800	-0.18608400
C	2.67597900	-2.22550800	-0.21811400

H	0.61857200	-2.89265900	-0.27524200
C	2.89986600	0.13853300	0.03151200
C	3.49550600	-1.10885200	-0.11345900
H	3.10156300	-3.21588700	-0.32828800
H	3.50614900	1.03303600	0.13143900
H	4.57426600	-1.19438000	-0.13682500
C	-4.09259200	-1.37471200	0.33839800
H	-4.24971600	-2.21681400	-0.33823000
H	-4.17296700	-1.74801100	1.36126000
H	-4.87511500	-0.63538300	0.16972900
N	1.57755800	0.31498000	0.06829100
H	-1.08384300	3.92989300	-1.12299600
H	1.26463000	1.98938000	0.83781800

TS1-BC·2H₂O



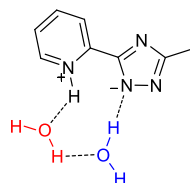
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -779.1254 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-2.71620900	-0.80932400	0.10451300
C	-0.65420400	-0.45589500	-0.02441100
N	-1.25915800	0.70822400	-0.26679800
H	-0.94421300	2.06520600	-0.63574600
N	-2.59063400	0.48344600	-0.18276600
N	-1.53027900	-1.44365000	0.20967500
H	0.28272400	3.07700400	0.05160400
O	-0.63744400	3.09054400	-0.79966900
O	1.14792600	2.76792900	0.74082600
H	0.92465200	2.89053400	1.67357200
C	0.80268100	-0.67097500	-0.03147400
C	1.31342400	-1.95325600	-0.23427900
C	2.68633700	-2.14201100	-0.25449400
H	0.62699900	-2.77611800	-0.38210600
C	2.95091400	0.19086700	0.13251400
C	3.52826100	-1.04937400	-0.07410300
H	3.09662200	-3.13206000	-0.41517100
H	3.55587800	1.07638300	0.29485300
H	4.60519400	-1.15127700	-0.08642900
C	-4.03574000	-1.47745900	0.30668300
H	-4.16202300	-2.31256500	-0.38558700
H	-4.11817800	-1.87257700	1.32176600
H	-4.84434200	-0.76445300	0.14383300
N	1.62514700	0.37436300	0.15815000
H	-1.37046700	3.68741800	-0.60641200
H	1.29498800	1.69260900	0.51904500

II·2H₂O



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	2.70510500	-0.89301200	0.09226500

C	0.64821500	-0.56357700	0.03105700
N	1.20723400	0.64535100	0.00781800
H	-1.48034200	3.38928900	1.35271300
N	2.53957100	0.43418100	0.04835200
N	1.54232600	-1.56660700	0.08185000
H	-0.53127900	3.38100900	0.12212900
O	-1.36890500	3.01661000	0.47176300
H	-1.21365700	1.24036100	0.24257600
O	1.04578300	3.34122300	-0.67600600
H	1.15138000	2.38804800	-0.45503100
H	1.85244400	3.77808900	-0.38592100
C	-0.79238600	-0.77751100	-0.00655700
C	-1.37291600	-2.03458900	-0.15288200
C	-2.75218200	-2.14765100	-0.19664100
H	-0.72861800	-2.89897200	-0.23533600
C	-2.94467200	0.21059900	0.05587400
C	-3.55728300	-1.01147500	-0.09615300
H	-3.20727200	-3.12397200	-0.31332600
H	-3.47694700	1.14767900	0.15073400
H	-4.63589100	-1.07245600	-0.13087500
C	4.04725000	-1.54631300	0.13733800
H	4.83114100	-0.78875900	0.15274200
H	4.14968800	-2.17165900	1.02675500
H	4.19757400	-2.18440100	-0.73641100
N	-1.60484900	0.29196800	0.09874900

TS2'-rot·2H₂O

M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -38.9111 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-2.60216800	-0.74707300	-0.16641100
C	-0.54796700	-0.43405400	-0.35324000
N	-1.12475000	0.51811900	-1.08731900
H	-0.47680400	2.41044000	-0.99542900
N	-2.45304300	0.31279200	-0.97014700
N	-1.42786400	-1.25622600	0.25118600
H	-0.12835600	2.81626900	0.41679000
O	0.17100500	2.93968000	-0.49873000
H	1.17788800	1.45564200	-0.55916900
O	-0.68610200	1.73817200	1.91798300
H	-1.09888700	0.89566200	1.69041400
H	-1.08055300	1.99901700	2.75786100
C	0.89792100	-0.54989000	-0.18483700
C	1.53316800	-1.73499700	0.17196100
C	2.91262900	-1.75600300	0.29877400
H	0.93367600	-2.62069100	0.33231600
C	2.99220600	0.55637100	-0.26343100
C	3.65959700	-0.59923900	0.07164100
H	3.41347800	-2.67762400	0.57037600
H	3.47951700	1.50625200	-0.43829000
H	4.73676600	-0.59054800	0.16143600
C	-3.93521300	-1.27775000	0.24622200
H	-4.72653500	-0.75929500	-0.29588500
H	-4.01248400	-2.34736900	0.04147100
H	-4.09674500	-1.13118300	1.31688400
N	1.65405300	0.55051800	-0.37612900

I2·2H₂O

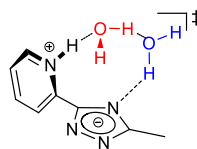
M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.56562200	-0.72451000	-0.20244900
C	-0.51091500	-0.42791300	-0.40827900
N	-1.08202900	0.45506300	-1.22489400
H	-0.57807400	2.49350200	-0.90891100
N	-2.41236000	0.25907000	-1.09560300

N	-1.39236100	-1.19429100	0.26542800
H	-0.28634700	2.59536300	0.57171500
O	0.04007400	2.90886800	-0.28938200
H	1.16574000	1.48495200	-0.59863300
O	-0.84896800	1.45514900	1.98250300
H	-1.13666500	0.56680600	1.73098800
H	-1.40652600	1.70888800	2.72646600
C	0.93353600	-0.51519300	-0.21212300
C	1.58863000	-1.67614900	0.18443900
C	2.96639000	-1.66271700	0.33175700
H	1.00666500	-2.57097200	0.35852800
C	3.00361300	0.63733600	-0.28608100
C	3.69081700	-0.49598200	0.08392700
H	3.48332800	-2.56550400	0.63462400
H	3.47195100	1.59433000	-0.47285500
H	4.76618400	-0.46165600	0.18804200
C	-3.89902700	-1.22316900	0.24747800
H	-4.69196100	-0.70890300	-0.29615400
H	-3.99481700	-2.29689400	0.07290400
H	-4.03827000	-1.04467300	1.31635000
N	1.66752400	0.59764400	-0.41636500

TS2-rot·2H₂O



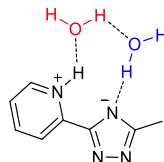
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -78.2570 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-2.52754000	-0.69652400	0.04774800
C	-0.45665900	-0.76788300	-0.21373300
N	-0.96611700	-1.24898500	-1.33567500
H	-1.04306400	2.32096200	-1.71797100
N	-2.31766700	-1.20862900	-1.15975900
N	-1.37784800	-0.39840800	0.69703700
H	-0.61853000	2.52837700	-0.23722900
O	-0.27575000	2.45917700	-1.15189300
H	0.92121800	1.18592700	-1.01871300
O	-0.91648100	2.21538300	1.48726300
H	-1.14768200	1.26100700	1.43852600
H	-1.56416300	2.63277200	2.06382700
C	1.00023500	-0.59635700	-0.01783100
C	1.81182400	-1.47819100	0.67498300
C	3.17543000	-1.21915700	0.76875600
H	1.37282700	-2.35789200	1.12593400
C	2.86980200	0.77490100	-0.49990300
C	3.71480300	-0.08533500	0.17028100
H	3.81829500	-1.90647900	1.30550800
H	3.19458900	1.68688000	-0.98266900
H	4.77131500	0.13777700	0.22468700
C	-3.88267300	-0.46106000	0.63017500
H	-4.65158300	-0.78744500	-0.07060800
H	-4.00689300	-1.01042000	1.56597200
H	-4.03521300	0.59995500	0.84392400
N	1.56097500	0.49741300	-0.57117500

I3·2H₂O

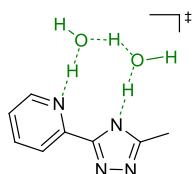


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-2.43075500	-0.88677700	-0.10319700
C	-0.34459800	-0.99282500	-0.03514700
N	-0.76308000	-2.24880400	-0.14615300
H	0.06222400	3.41093400	-1.44411200
N	-2.10996000	-2.18122900	-0.19047900
N	-1.34948300	-0.09116500	-0.00530800
H	-0.67911000	3.11766000	-0.11047900
O	0.19297800	3.07644000	-0.55061500
H	0.70455400	1.36732800	-0.27886100
O	-2.03979500	2.49257800	0.83280800
H	-1.82951200	1.56692400	0.57217900
H	-2.97329200	2.62253800	0.63737200
C	1.06965300	-0.65257700	0.01770600
C	2.07940500	-1.59782400	0.18987500
C	3.39915000	-1.18531600	0.22568800
H	1.80525000	-2.63821800	0.29740300
C	2.69647600	1.06823300	-0.07847800
C	3.72061100	0.16847100	0.09480300
H	4.18682200	-1.91706200	0.35983100
H	2.83905400	2.13400400	-0.19763600
H	4.74372200	0.51592500	0.12255600
C	-3.83695000	-0.38520700	-0.09920000
H	-4.52156400	-1.20820300	-0.30603400
H	-4.10135000	0.04240600	0.87160200
H	-3.97967700	0.38583500	-0.85969800
N	1.42244600	0.63987200	-0.11434100

TS3-BC·2H₂O



M06-2X/6-311+G(d,p)/SMD(DMSO)

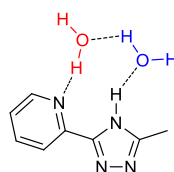
Imaginary frequency: -805.8607 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	2.51142800	-0.77590600	0.02591800
C	0.40196200	-0.87868800	0.09458300
N	0.84521500	-2.08663100	0.40640100
H	0.02975200	2.88132200	1.63616700
N	2.20109400	-2.01999200	0.36681900
N	1.41252500	-0.01213500	-0.15646600
H	0.72815500	2.76409000	0.01680800
O	-0.20663600	2.80486500	0.70179200
H	-0.70011200	1.84215700	0.51215600
O	1.59737500	2.42355800	-0.79867700
H	1.56194300	1.36381900	-0.58477900
H	2.48270400	2.76673900	-0.62441700
C	-1.03619000	-0.57802700	0.00842300
C	-1.95072000	-1.60755800	-0.22266100
C	-3.30053700	-1.30900200	-0.31070800
H	-1.58785800	-2.61948500	-0.34216000
C	-2.75707800	0.97731900	0.05973500
C	-3.71876200	0.01138200	-0.17402100
H	-4.02036300	-2.09798100	-0.49421000
H	-3.02309400	2.02152000	0.18487400
H	-4.76201700	0.28921600	-0.24390000
C	3.90434000	-0.27283400	-0.15845200
H	4.61332000	-1.07891900	0.03061700
H	4.05611900	0.09075800	-1.17759300
H	4.12271700	0.54830700	0.52861400

N -1.45223800 0.69032300 0.15410400

9b-C·2H₂O

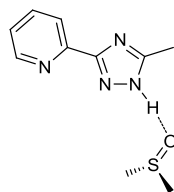


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	2.49124600	-0.87387000	0.02193500
C	0.33359500	-0.98621400	0.09713400
N	0.79945000	-2.16119900	0.44180600
H	0.14173600	2.88586500	2.00555700
N	2.16591700	-2.09018200	0.39698200
N	1.36421000	-0.14272700	-0.17132700
H	1.19784700	2.97065000	-0.24986600
O	-0.04926900	2.96735300	1.06563400
H	-0.48119200	2.12956100	0.79853800
O	1.64077300	2.54893500	-1.00919700
H	1.33832600	0.82613600	-0.51413700
H	2.53110200	2.91292500	-1.05149400
C	-1.08772800	-0.62376000	-0.00517900
C	-2.05312500	-1.61594500	-0.16295800
C	-3.38166700	-1.23223900	-0.27445900
H	-1.75578200	-2.65579500	-0.20738200
C	-2.66876000	1.03636200	-0.06644200
C	-3.69951400	0.12024100	-0.23221400
H	-4.15692800	-1.97867900	-0.40125000
H	-2.87645600	2.10048600	-0.01687000
H	-4.72166300	0.46474000	-0.32228000
C	3.86649600	-0.34727000	-0.18024100
H	4.58647800	-1.13334700	0.04348200
H	4.00643800	-0.02196500	-1.21315500
H	4.05560800	0.50516300	0.47530100
N	-1.38683700	0.67983900	0.04919700

9b-A-I·DMSO



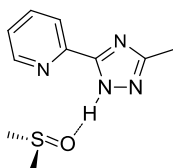
B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	0.10007300	2.13138700	0.09404000
N	1.40511900	1.90016900	0.00235300
N	-0.54886500	0.95855600	0.17719000
C	-0.56308300	3.46300800	0.10244500
H	-1.56569900	0.77022900	0.24726900
O	-3.24998600	0.36261000	0.41060200
S	-3.84683400	-0.81007600	-0.37647500
C	-4.13055400	-2.13408800	0.82746100
H	-4.65821100	-2.94786500	0.32768500
H	-3.15157800	-2.47797700	1.16036100
H	-4.70959900	-1.74408800	1.66482900
N	0.32677200	-0.07261100	0.13706500
C	1.49903700	0.53943300	0.02908200
C	-5.57480300	-0.36575900	-0.68587100
H	-6.04428500	-0.07042300	0.25265500

H	-5.57212900	0.46171300	-1.39483700
H	-6.08023400	-1.22701900	-1.12503100
C	2.78545300	-0.17844200	-0.02781900
C	3.98783300	0.53302900	-0.06079300
N	2.74663500	-1.52051000	-0.04145600
C	5.18272100	-0.17078500	-0.10713100
H	3.97698600	1.61418600	-0.04804900
C	3.90345700	-2.18312200	-0.08504900
C	5.14623800	-1.55939900	-0.11920500
H	6.12772300	0.35880600	-0.13221700
H	3.83503300	-3.26669700	-0.09430200
H	6.05330300	-2.14956900	-0.15400800
H	-1.58102100	3.39115400	0.48623200
H	0.00075900	4.15762900	0.72646400
H	-0.60767700	3.87946800	-0.90728400

9b-B-I-DMSO



M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.66861100	-0.02995100	-0.00119700
N	-2.97788100	-0.24888200	0.02185000
N	-1.00944800	-1.19259000	0.00512400
C	-0.99435600	1.27741700	-0.03552400
C	-1.73658600	2.45563800	-0.07640400
C	-1.05029900	3.66169200	-0.12224800
H	-2.81849100	2.41575800	-0.07458500
C	0.98671500	2.41435300	-0.08035000
C	0.33916000	3.64532500	-0.12710300
H	-1.59279100	4.59920700	-0.15563900
H	2.07237400	2.36552500	-0.07992000
H	0.91499700	4.56133200	-0.16481500
N	0.34279600	1.24932600	-0.03314300
H	0.02281500	-1.36669300	-0.00686200
O	1.60258300	-1.82638300	0.00708300
S	2.71557200	-0.81524800	-0.32081700
C	3.17339000	-0.08077800	1.25615200
H	4.01808400	0.59206000	1.10004500
H	2.30695600	0.47462100	1.61294300
H	3.43289100	-0.87967700	1.95222900
N	-1.88996800	-2.21008900	0.03225100
C	-3.06704700	-1.60492500	0.04235900
C	-4.36091000	-2.34332400	0.06873400
H	-4.17776900	-3.41760600	0.07819800
H	-4.93742600	-2.07586600	0.95666900
H	-4.96237600	-2.09543400	-0.80819500
C	4.18103700	-1.83242700	-0.54528300
H	4.28809600	-2.49097600	0.31723400
H	4.04148500	-2.41154900	-1.45762000
H	5.04787200	-1.17815600	-0.65065900

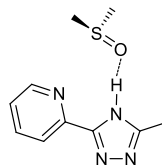
B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.67215400	-0.24167200	0.00438700
N	-2.90989200	-0.73497500	0.02771000
N	-0.78681200	-1.24906800	0.01267900
C	-1.30368300	1.17872400	-0.03415600
C	-2.28657800	2.16743400	-0.10062300
C	-1.88834700	3.49579200	-0.14187800
H	-3.33256300	1.89292000	-0.12028500

C	0.37530900	2.73945100	-0.04848100
C	-0.53114400	3.79287200	-0.11632400
H	-2.62716800	4.28654600	-0.19432900
H	1.44279900	2.93552600	-0.02609800
H	-0.17662500	4.81531900	-0.14821600
N	0.00895200	1.45800000	-0.00704300
H	0.24946700	-1.22703700	-0.00052000
O	1.95591000	-1.57736500	0.03106700
S	2.96755700	-0.47783000	-0.30732900
C	3.44717300	0.27378200	1.27026900
H	4.25525200	0.98301600	1.08459600
H	2.57215800	0.79720700	1.65308000
H	3.76294000	-0.50856000	1.96100600
N	-1.44260700	-2.43532900	0.04130900
C	-2.72259300	-2.08165300	0.04945600
C	-3.84095500	-3.06555300	0.08067800
H	-3.45359500	-4.08401500	0.05496600
H	-4.43969500	-2.94345000	0.98679000
H	-4.50542700	-2.92175900	-0.77457800
C	4.52187900	-1.34403800	-0.65281400
H	4.76132800	-2.00728100	0.17868800
H	4.37438600	-1.91367100	-1.56998400
H	5.30763100	-0.60180600	-0.80205600

9b-C-I-DMSO

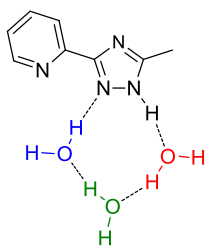


B3LYP/6-311+G(2d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	1.67774400	0.86829900	-0.01094200
N	2.65337000	1.75322100	-0.01868300
N	0.47648200	1.50879900	0.03656400
C	1.83922600	-0.58961200	-0.04033300
C	3.10891100	-1.16800900	-0.12228500
C	3.20692100	-2.55051600	-0.14009800
H	3.98984200	-0.54212100	-0.17095000
C	0.82564700	-2.64727300	-0.00130900
C	2.04414400	-3.31121300	-0.07828700
H	4.17725500	-3.02847400	-0.20195000
H	-0.10273300	-3.20775300	0.04725100
H	2.07617000	-4.39338700	-0.08921700
N	0.71395900	-1.31739200	0.01912000
H	-0.47231500	1.09121900	0.04321000
O	-2.19999300	0.77002400	0.08508200
S	-2.72315200	-0.60966100	-0.32621600
C	-2.92566500	-1.55461100	1.20787100
H	-3.38529200	-2.51405900	0.96604000
H	-1.92995300	-1.71125200	1.62001000
H	-3.54610600	-0.98676900	1.90173600
C	-4.47964800	-0.36571700	-0.69944200
H	-4.95878300	0.14866200	0.13377200
H	-4.53707700	0.23353900	-1.60776000
H	-4.93625600	-1.34169800	-0.87212400
N	2.07423600	3.00359100	0.02589300
C	0.76628500	2.83494400	0.05767000
C	-0.24814600	3.91858900	0.13599300
H	-0.94710000	3.87197500	-0.70220300
H	-0.82954500	3.84212300	1.05813100
H	0.25343600	4.88555300	0.11957000

9b-A·3H₂O

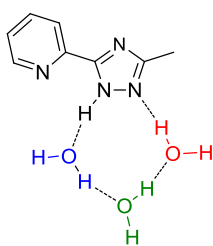


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.04320900	2.18524400	-0.05024700
C	0.56328300	0.81908600	-0.04253000
N	-0.57885400	0.13722900	-0.15955900
H	-0.72965800	-0.88367400	-0.23805400
N	-1.61491900	0.99668500	-0.16486200
N	0.31030000	2.12009700	0.02562900
O	-1.25015000	-2.53636200	-0.39467900
O	-4.23983400	-0.02227700	0.10706500
H	-3.35761600	0.39066300	-0.00311700
H	-4.68806600	0.48741300	0.78982200
C	1.87981600	0.16392600	0.00526000
C	3.04697200	0.91967300	0.06796700
C	4.25990400	0.24444500	0.11597300
H	2.99529500	2.00111700	0.07823100
C	3.03304500	-1.80604500	0.03241700
C	4.25677400	-1.14441800	0.09779400
H	5.19161200	0.79550400	0.16614000
H	2.99512200	-2.89061500	0.01708700
H	5.17854300	-1.71122500	0.13340200
N	1.86221500	-1.17319900	-0.01157000
C	-1.81544600	3.45779200	-0.01689800
H	-1.56456900	4.07918900	-0.87894200
H	-2.88512800	3.24871600	-0.03339100
H	-1.57769700	4.02353700	0.88574400
H	-4.12508100	-1.77810300	0.24753000
O	-3.88400200	-2.72550800	0.29384800
H	-4.53476800	-3.19620700	-0.23633900
H	-2.16980900	-2.74650500	-0.13570400
H	-0.67431500	-3.15054800	0.07184100

9b-B·3H₂O



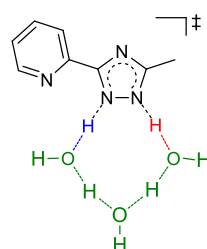
M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	1.10993000	2.26309500	0.02939300
C	-0.42970100	0.82109700	0.00507400
N	0.67826900	0.10343400	0.02871000
H	0.75217900	-1.74797200	0.23959700
N	1.64458000	1.03537000	0.04466300
N	-0.21353900	2.16069100	0.00707800
O	0.92566900	-2.70720200	0.32360300
O	4.15195000	-0.18829700	-0.06156200
H	2.63219100	0.74172100	0.03053000
H	4.82824500	0.02398900	-0.71270900
C	-1.76883300	0.19919900	-0.02015100
C	-2.91390600	0.99282300	0.01420900

C	-4.15320000	0.36597400	-0.00853400
H	-2.82472100	2.07079100	0.05835900
C	-3.00246300	-1.72430300	-0.09487800
C	-4.20338000	-1.02084700	-0.06324700
H	-5.06414400	0.95258600	0.01721100
H	-3.00435700	-2.80919700	-0.13913300
H	-5.14591800	-1.55329100	-0.08231900
N	-1.80682300	-1.13768700	-0.07542000
C	1.91195100	3.51492400	0.03690600
H	1.67211400	4.10888800	0.92027800
H	2.97747200	3.28435800	0.04483600
H	1.68480200	4.11210800	-0.84744000
H	4.02526200	-1.15862800	-0.10564900
O	3.58624900	-2.86445400	-0.17261700
H	4.00311700	-3.47844800	0.44021700
H	2.62159500	-2.95027500	-0.02837200
H	0.11142400	-3.12145000	0.02135200

TS-AB·3H₂O

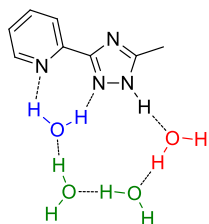


M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -329.9241 cm⁻¹

Cartesian coordinates

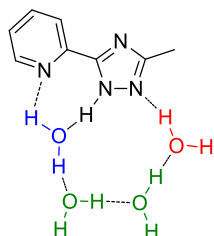
ATOM	X	Y	Z
C	-1.24474400	2.12103400	-0.04280400
C	0.38669100	0.79979000	-0.03169300
N	-0.69721200	0.03812900	-0.10302500
H	-0.77898100	-1.51102600	-0.28101400
N	-1.74883200	0.88879500	-0.10992300
N	0.09802900	2.11471400	0.00415000
O	-0.96182000	-2.52486400	-0.38096300
O	-3.95208100	-0.37686500	0.15799500
H	-3.09249700	0.22630300	0.03751300
H	-4.42580100	-0.07990900	0.94449700
C	1.74722100	0.23211700	0.01172200
C	2.86556400	1.06615300	-0.01198000
C	4.12667000	0.48767600	0.02830300
H	2.73572500	2.13976000	-0.06201900
C	3.05580300	-1.64391400	0.10896000
C	4.22962400	-0.89693600	0.08859500
H	5.01504800	1.10851200	0.01118300
H	3.09821100	-2.72783000	0.15809700
H	5.19137200	-1.39316200	0.12085800
N	1.83807200	-1.10359900	0.07403200
C	-2.09160400	3.34958200	-0.02643200
H	-1.87750000	3.97877000	-0.89286500
H	-3.14765700	3.07813300	-0.04659400
H	-1.89941900	3.94065200	0.87117200
H	-3.65186000	-1.64479600	0.17802100
O	-3.30615200	-2.70506800	0.17161300
H	-3.80016000	-3.22509300	-0.47719800
H	-2.22960500	-2.71953900	-0.05628500
H	-0.25820100	-2.97567500	0.10080900

9b-A·4H₂O

M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-0.40288500	2.63783300	-0.10189900
C	0.83429900	0.93422100	0.04226000
N	-0.36478800	0.48498300	0.36810800
H	-0.93860300	-1.35305900	0.82570400
N	-1.13547400	1.57987900	0.26959200
N	0.85926800	2.25990900	-0.25237400
O	-0.72804900	-2.30163000	0.80107500
H	0.20257000	-2.23868700	0.52071200
O	-3.82575400	0.99755400	0.62391800
H	-2.14870700	1.50435100	0.44406600
H	-4.32511600	1.04310600	1.44515900
C	2.04306200	0.08295200	-0.00279800
C	3.29183300	0.67007100	-0.20278700
C	4.41309200	-0.14720200	-0.24940500
H	3.37026700	1.74327400	-0.31703500
C	2.96856500	-2.01255500	0.10027100
C	4.25343700	-1.51806700	-0.09497700
H	5.39625200	0.28220000	-0.40304800
H	2.80173400	-3.07810400	0.22387800
H	5.09775800	-2.19496400	-0.12429100
N	1.88348200	-1.23893900	0.14515700
C	-0.96055900	4.00126400	-0.30503600
H	-0.77844300	4.33277600	-1.32827900
H	-2.03438400	4.00454800	-0.11782800
H	-0.48094600	4.70826500	0.37359200
H	-4.10890800	0.17454700	0.17397000
O	-4.58020700	-1.30423900	-0.62424700
H	-4.95957900	-1.26609600	-1.50779400
H	-3.97233000	-2.07299800	-0.62024800
O	-2.79540300	-3.36664200	-0.56861900
H	-1.98524700	-3.07223600	-0.09723700
H	-3.04350600	-4.20919000	-0.17548700

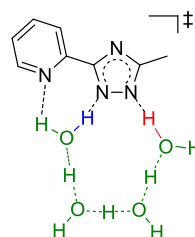
9b-B·4H₂O

M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-0.50595600	2.57606500	-0.03466700
C	0.86868900	0.97735800	0.04312600
N	-0.33744700	0.52570900	0.40052000
H	-0.61448800	-0.43335200	0.67967400
N	-1.22580400	1.53574600	0.35578700
N	0.80047800	2.27252600	-0.23772200

O	-0.71056600	-2.12401200	1.04669800
H	0.19197100	-2.20856000	0.70303900
O	-3.97933000	0.91523600	0.42793100
H	-3.03649000	1.18144400	0.44699600
H	-4.33603500	1.12862900	1.29618500
C	2.07615300	0.13535400	-0.02362000
C	3.30741300	0.71058900	-0.32494400
C	4.42223100	-0.11528100	-0.38511600
H	3.37680300	1.77557300	-0.50561000
C	2.99436300	-1.95377900	0.15168400
C	4.26678300	-1.47378400	-0.14243000
H	5.39667600	0.29789300	-0.61740300
H	2.83443100	-3.00931400	0.34661900
H	5.10759200	-2.15471600	-0.17797000
N	1.91555000	-1.17320300	0.21044700
C	-1.08106600	3.93495700	-0.23260800
H	-0.92557500	4.26675300	-1.26079900
H	-2.15019200	3.92452000	-0.02116700
H	-0.59556300	4.65371200	0.43023700
H	-4.35857700	-0.63398400	-0.31103600
O	-4.54291800	-1.49601500	-0.73603700
H	-4.98346000	-1.29346800	-1.56720600
H	-3.30591900	-2.74576100	-0.64720400
O	-2.57593700	-3.38794700	-0.53770900
H	-1.30251200	-2.65903200	0.48455100
H	-2.98975300	-4.22275100	-0.29774300

TS-AB·4H₂O

M06-2X/6-311+G(d,p)/SMD(DMSO)

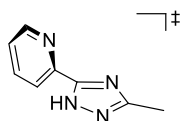
Imaginary frequency: -525.2808 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	0.59358500	2.51831000	0.03848100
C	-0.77025700	0.92530600	-0.05590200
N	0.41147800	0.41203500	-0.38066100
H	0.72272500	-1.18225600	-0.70165700
N	1.28977300	1.43821300	-0.31894400
N	-0.70926800	2.24551600	0.21226900
O	0.71411600	-2.18942700	-0.77756100
H	-0.20149800	-2.35624800	-0.50061100
O	3.76009600	0.69113200	-0.49620500
H	2.78686300	1.04540200	-0.45976200
H	4.07312700	0.74871500	-1.40569600
C	-2.01875000	0.13742800	0.00546100
C	-3.23843600	0.78595000	0.21273000
C	-4.39905300	0.02881300	0.27250000
H	-3.26084800	1.86239400	0.32143200
C	-3.05599100	-1.90912700	-0.07885100
C	-4.31237000	-1.35039000	0.12332200
H	-5.35759300	0.50943700	0.43145100
H	-2.94595900	-2.98273300	-0.19823600
H	-5.19041700	-1.98248600	0.16201500
N	-1.93124700	-1.19367600	-0.13605100
C	1.20697200	3.86550600	0.22578100
H	1.05640000	4.21920800	1.24789600
H	2.27810700	3.82313200	0.02515900
H	0.75372700	4.59361900	-0.45030500
H	4.04938600	-0.48951100	0.18178400
O	4.27068600	-1.38725000	0.70500400

H 4.47627600 -1.18834300 1.62797100
H 3.47663200 -2.24380100 0.58992200
O 2.63741300 -3.11771300 0.45377100
H 1.78224100 -2.77353900 -0.05794800
H 2.98299400 -3.90233200 0.00910100

TS-rot-9b-A



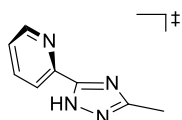
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -63.3261 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	2.63107200	0.01422200	0.26933100
C	0.57824000	-0.00118800	-0.21567700
N	1.16708700	-0.06641300	-1.39114000
N	2.47292400	-0.05546200	-1.05904700
N	1.43390500	0.05554200	0.83902400
C	3.95089400	0.02972800	0.95384800
H	3.96639000	0.81507400	1.70983900
H	4.75319900	0.20513300	0.23731500
H	4.12817700	-0.92595600	1.45084400
C	-0.90206300	0.00605400	-0.06540700
C	-1.60189100	1.20908000	-0.03221800
C	-2.98280000	1.16912600	0.11890100
H	-1.07210800	2.14928800	-0.12576500
C	-2.81993500	-1.21268900	0.18873000
C	-3.60631500	-0.06615900	0.23253300
H	-3.55880200	2.08672500	0.14664800
H	-3.27525700	-2.19418400	0.27411200
H	-4.67934600	-0.14806900	0.35270400
N	-1.49342000	-1.18808000	0.04360300
H	3.19105400	-0.09616700	-1.77301600

TS-rot-9b-B



M06-2X/6-311+G(d,p)/SMD(DMSO)

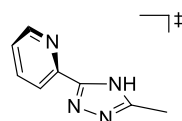
Imaginary frequency: -69.8957 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-2.66982700	-0.02434900	-0.20057200
C	-0.58843200	0.00558800	0.14954900
N	-1.23930300	0.12326600	1.31251300
H	-0.85138800	0.21243600	2.24449000
N	-2.57149400	0.10550400	1.10854300
N	-1.46349100	-0.09126400	-0.83549800
C	-3.97187100	-0.08691900	-0.92089600
H	-4.79665900	-0.00303800	-0.21389000
H	-4.06379100	-1.02989100	-1.46315700
H	-4.04183600	0.72567500	-1.64665000
C	0.89287800	0.00250300	0.02635200
C	1.58148300	1.20091700	-0.13091800
C	2.96519100	1.15231300	-0.25579000
H	1.04344400	2.14048800	-0.15662700
C	2.81606100	-1.22438900	-0.05390700
C	3.59598800	-0.08330700	-0.21655600
H	3.53640500	2.06453400	-0.38156700
H	3.27793600	-2.20564000	-0.01852600
H	4.67120700	-0.17083300	-0.30973600

N 1.48798200 -1.19291600 0.06617000

TS-rot-9b-C



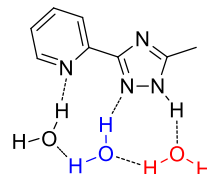
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -63.1629 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	2.69950200	0.02160600	0.14502700
C	0.57161700	-0.04077900	-0.28184300
N	1.20223900	-0.25908500	-1.40416400
N	2.55048200	-0.22116300	-1.13330300
N	1.47195800	0.14415400	0.71920500
C	3.98187700	0.14939400	0.88374300
H	4.80806600	-0.02768800	0.19657500
H	4.03064500	-0.57814900	1.69601000
H	4.08156300	1.14881900	1.31165600
C	-0.90176200	-0.00488200	-0.09405500
C	-1.59384300	1.19933000	-0.17782900
C	-2.97285300	1.18079600	-0.00221400
H	-1.06298600	2.12190000	-0.37821000
C	-2.81536900	-1.18130800	0.32146600
C	-3.59722800	-0.03215000	0.25177200
H	-3.54550900	2.09863700	-0.06444300
H	-3.27206600	-2.14539500	0.52061900
H	-4.66853600	-0.09569200	0.39576400
N	-1.49219800	-1.17842000	0.15396800
H	1.26980500	0.32711200	1.69568900

9b-A·2H₂O(H₂O)



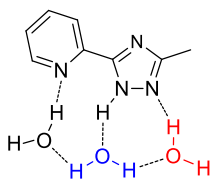
M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.85595500	-1.91021200	0.18496200
C	-0.03842900	-0.85310100	0.00940800
N	-0.95996600	0.08012200	-0.13762600
H	-1.19420700	1.89299500	-0.76328600
N	-2.10666800	-0.61064600	-0.02073900
N	-0.54243300	-2.09794100	0.20550300
H	-3.19415600	2.18793100	-0.43446200
O	-1.53545400	2.80299500	-0.83011700
H	-0.99194800	3.25437800	-0.16533500
O	-3.89833000	1.54500800	-0.22031300
H	-2.99675100	-0.10628000	-0.08840800
H	-4.64798200	1.76292500	-0.78262700
C	1.40773900	-0.56232900	-0.05091500
C	2.31948600	-1.59574500	-0.25466500
C	3.67127200	-1.28575400	-0.32437600
H	1.96575500	-2.61299300	-0.36210800
C	3.08451800	1.00041100	0.02247400
C	4.06607200	0.03870700	-0.18826600
H	4.40367600	-2.06801400	-0.48578700
H	3.35280400	2.04506800	0.14595900
H	5.10804600	0.32786200	-0.23744000
N	1.78357800	0.71494900	0.09340300

C	-2.91435800	-2.94018500	0.35787000
H	-2.79776500	-3.44241300	1.31914900
H	-3.90160500	-2.48034600	0.31538400
H	-2.84086200	-3.69170000	-0.42973100
H	0.86349100	2.23823100	0.72737000
O	0.52609300	3.11120000	1.01808800
H	0.46938700	3.06258900	1.97730800

9b-B·2H₂O(H₂O)

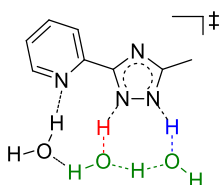


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.84850600	-1.86550800	0.15867300
C	0.01433100	-0.89127700	-0.01938100
N	-0.95900300	-0.00942400	-0.26459000
H	-0.92197800	0.98240400	-0.54802800
N	-2.15610900	-0.61704700	-0.15380600
N	-0.51020000	-2.07917500	0.24877000
H	-2.43321000	2.54901600	-0.62603700
O	-1.49658700	2.66009000	-0.85999500
H	-1.05174200	3.05333200	-0.09175800
O	-3.98147900	1.58065900	-0.16631600
H	-3.57475500	0.69457300	-0.17550000
H	-4.78046700	1.51778200	-0.69912000
C	1.44649100	-0.55487400	-0.06211900
C	2.39858400	-1.56105800	-0.19104200
C	3.73737900	-1.19645500	-0.24796100
H	2.08653400	-2.59579500	-0.25234900
C	3.04950800	1.08187900	-0.04244800
C	4.07229400	0.14957000	-0.17844500
H	4.50605600	-1.95334900	-0.35014300
H	3.27251800	2.14164400	0.02825200
H	5.10237500	0.47904800	-0.22268200
N	1.76032900	0.74443600	0.01899100
C	-2.87329400	-2.91969600	0.39455500
H	-2.78349100	-3.31708000	1.40735200
H	-3.87273500	-2.50542700	0.26430700
H	-2.73866500	-3.74739100	-0.30418400
H	0.81533500	2.19252400	0.79916600
O	0.36864900	2.99495100	1.13427100
H	0.32371700	2.89609600	2.09049600

TS-AB·2H₂O(H₂O)



M06-2X/6-311+G(d,p)/SMD(DMSO)

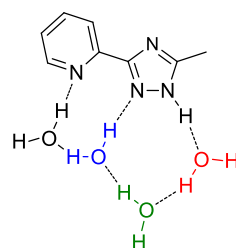
Imaginary frequency: -894.0984 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-1.88922100	-1.79483000	0.17356600
C	-0.03193000	-0.83006600	-0.02187500
N	-0.94581500	0.10477000	-0.23689400
H	-1.15912400	1.62293100	-0.65199900
N	-2.14396700	-0.51684700	-0.10480600

N	-0.57001900	-2.03904200	0.23025900
H	-2.74092900	2.14690100	-0.44497900
O	-1.63085800	2.53563700	-0.74012900
H	-1.15871400	3.06359700	-0.06481100
O	-3.68115000	1.45579200	-0.16868600
H	-3.20199300	0.48069000	-0.14463900
H	-4.37918200	1.47845800	-0.83633700
C	1.41605200	-0.55238400	-0.05797500
C	2.33124100	-1.59326000	-0.21015400
C	3.68513900	-1.29105300	-0.25334600
H	1.97528500	-2.61162500	-0.29938500
C	3.10181000	1.00609300	0.01350600
C	4.08366700	0.03573500	-0.14488400
H	4.41795600	-2.08038400	-0.37436900
H	3.37170100	2.05290900	0.11395800
H	5.12793700	0.31892600	-0.17612400
N	1.79747100	0.72777000	0.06123600
C	-2.95725200	-2.81271000	0.39183900
H	-2.87690800	-3.24889800	1.38935900
H	-3.93991700	-2.35176100	0.28864500
H	-2.87180100	-3.62205100	-0.33593300
H	0.83439300	2.22263000	0.65156500
O	0.40006000	3.06509500	0.91199000
H	0.49616200	3.13376400	1.86701700

9b-A·3H₂O(H₂O)



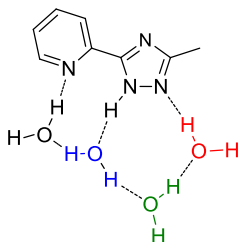
M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.06394100	2.40525800	0.15495700
C	0.48579600	0.97948300	0.03938800
N	-0.61295400	0.24755200	0.09161900
N	-1.58674600	1.17262800	0.16331400
N	0.25747800	2.31623600	0.07445200
O	0.40970700	-2.98485700	1.30825900
H	0.86962800	-2.17674700	0.99476700
O	-4.20111800	0.19994300	0.21762600
H	-2.57680700	0.88364300	0.21407300
C	1.84003600	0.39992800	-0.06115700
C	2.91176300	1.20564200	-0.44064500
C	4.17199700	0.63236900	-0.54388600
H	2.74762500	2.25375500	-0.65414500
C	3.19535900	-1.44256400	0.11203800
C	4.32112300	-0.72033400	-0.26636100
H	5.02361700	1.23380900	-0.83960200
H	3.27045800	-2.49964000	0.34758100
H	5.28332000	-1.21137300	-0.33519400
N	1.98022200	-0.90230700	0.21647200
C	-1.87012500	3.65209400	0.23003100
H	-1.65374600	4.28956700	-0.62826100
H	-2.93525000	3.42106600	0.24054800
H	-1.61915200	4.20539600	1.13666300
H	-4.26745100	-0.70553200	-0.15321500
O	-4.08956200	-2.31945400	-0.77910600
H	-3.11674700	-2.46154200	-0.79042200
O	-1.39920500	-2.41451800	-0.71350100
H	-0.92337200	-2.90818600	-0.02521500
H	-1.11441400	-1.49974600	-0.53209800

H	-4.74877100	0.20935000	1.00910700
H	-4.41246200	-2.56654700	-1.65115500
H	0.19689300	-2.82621200	2.23314800

9b-B·3H₂O(H₂O)

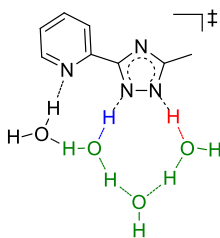


M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.09343600	2.32651300	0.19918900
C	0.53200800	0.99744400	-0.00053400
N	-0.60436800	0.30200300	-0.10593000
N	-1.65133500	1.14012300	0.01791100
N	0.26253500	2.28243600	0.19131900
O	0.33948000	-2.79124700	1.53363000
H	0.87629100	-2.08062000	1.12882300
O	-4.32710600	0.22207500	-0.09668100
H	-3.41842200	0.58476500	-0.03860900
C	1.87450300	0.40167000	-0.09908500
C	2.96457400	1.19873900	-0.43569000
C	4.21208600	0.59817300	-0.54060900
H	2.82468700	2.25670900	-0.61685900
C	3.17779900	-1.47788500	0.02910800
C	4.32351600	-0.76690400	-0.30966500
H	5.08240200	1.18781900	-0.80334100
H	3.22757800	-2.54308000	0.23043700
H	5.27505800	-1.27753600	-0.38348500
N	1.97427800	-0.91202200	0.13741400
C	-1.87774900	3.57266100	0.41932400
H	-1.57616800	4.34235100	-0.29291700
H	-2.94288500	3.37463300	0.30003000
H	-1.70069800	3.95659100	1.42613000
H	-4.27438100	-1.50266600	-0.46275000
O	-4.05873800	-2.43785600	-0.65189500
H	-2.26375000	-2.45828200	-0.64611200
O	-1.30048200	-2.30715400	-0.61718400
H	-0.95449000	-2.74373200	0.17795500
H	-0.77219500	-0.70171100	-0.32035100
H	-4.79136300	0.54038300	0.68425300
H	-4.56509900	-2.67932400	-1.43364400
H	0.20063100	-2.53310100	2.45025700

TS-AB·3H₂O(H₂O)



M06-2X/6-311+G(d,p)/SMD(DMSO)

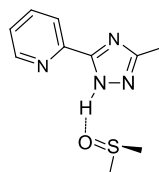
Imaginary frequency: -443.4829 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-1.23684200	2.26974700	0.18607600
C	0.39967000	0.96449000	0.02626900

N	-0.67918200	0.19458800	-0.05250400
N	-1.73298500	1.03977000	0.05108200
N	0.10418300	2.27148600	0.17198900
O	0.50662800	-2.98505300	1.22630000
H	0.97187900	-2.16759500	0.93606300
O	-4.05607600	0.01726500	0.01123500
H	-3.09628700	0.49866600	0.04729500
C	1.78132700	0.45404600	-0.06307800
C	2.82291300	1.32395700	-0.38975900
C	4.11257100	0.82140200	-0.48197100
H	2.60979000	2.36914100	-0.57202100
C	3.23326200	-1.32243800	0.07581900
C	4.32764000	-0.53186900	-0.24881400
H	4.93779900	1.47643600	-0.73617900
H	3.35808500	-2.38207800	0.27683000
H	5.31584400	-0.96917000	-0.31069900
N	1.98820900	-0.84923500	0.17191700
C	-2.08318900	3.48639900	0.35248100
H	-1.78849200	4.25602200	-0.36299600
H	-3.13479200	3.24464900	0.19484800
H	-1.96854700	3.90037000	1.35682200
H	-3.94033900	-1.20934300	-0.31313200
O	-3.71382700	-2.28206900	-0.59786100
H	-2.61771800	-2.37514500	-0.63770600
O	-1.29646400	-2.32142500	-0.65881100
H	-0.81839800	-2.82783100	0.02840200
H	-1.00536900	-1.36823700	-0.47715000
H	-4.50575100	0.14901600	0.85467400
H	-4.11217000	-2.51911000	-1.44587000
H	0.36668000	-2.89619500	2.17440200

9b-B·DMSO'



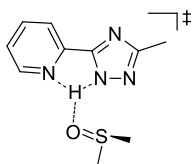
M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.23868100	0.84253500	-0.06052500
N	-1.43667300	2.15450800	-0.04753200
N	0.07002200	0.58230700	-0.12961500
C	-2.26933500	-0.20555200	0.00348400
C	-3.61653100	0.13238200	0.10701900
C	-4.54746800	-0.89682500	0.15677400
H	-3.91393300	1.17263200	0.14570500
C	-2.73083200	-2.44276300	0.00300000
C	-4.09995700	-2.21114200	0.10380800
H	-5.60529700	-0.67487300	0.23548600
H	-2.34663300	-3.45681500	-0.04021100
H	-4.79036200	-3.04446600	0.13877900
N	-1.82680300	-1.46605200	-0.04804300
C	-0.17811500	2.66420600	-0.11588500
C	0.11453700	4.12481900	-0.12526300
H	-0.23829300	4.59136800	0.79683900
H	1.18758600	4.29199700	-0.21541200
H	-0.39127600	4.61161000	-0.96128100
N	0.76353100	1.73538000	-0.16681900
H	0.58912900	-0.31261600	-0.17128000
S	3.34625500	-0.67037500	-0.34227200
O	1.97081000	-1.35287200	-0.25091100
C	4.53206800	-2.02146600	-0.30920200
H	4.42443400	-2.57222700	-1.24316500
H	5.53798400	-1.60544100	-0.23563500
H	4.30760500	-2.66221900	0.54448700

C	3.66491700	-0.01647300	1.30263800
H	4.67869600	0.38568300	1.33411800
H	2.94198300	0.78165100	1.47323400
H	3.53766300	-0.81864000	2.03094500

TS1-BC·DMSO



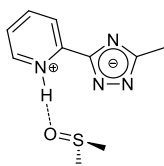
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -1522.7992 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-1.35106100	1.08372600	-0.02688100
N	-1.64166500	2.37912000	-0.06473500
N	-0.04458200	0.84671600	-0.02543200
C	-2.11503900	-0.17640400	0.00453700
C	-3.47508200	-0.41641300	0.00947300
C	-3.88659400	-1.74951600	0.03943400
H	-4.18190600	0.40300600	-0.00982400
C	-1.59382000	-2.44524100	0.05572700
C	-2.94730300	-2.77380800	0.06277400
H	-4.94426900	-1.98528700	0.04405500
H	-0.80576500	-3.18881000	0.07158600
H	-3.24975200	-3.81223400	0.08553700
N	-1.21488100	-1.17689200	0.02834300
C	-0.39771600	2.93123500	-0.08908900
C	-0.15521700	4.40189100	-0.14488300
H	-0.63573000	4.90628200	0.69597300
H	0.91513700	4.60544300	-0.11188100
H	-0.56282400	4.82628300	-1.06518500
N	0.58975300	2.03425200	-0.06591300
H	-0.08159600	-0.45779900	0.00666300
S	2.76125900	-0.70814300	-0.34586600
O	1.65974600	-1.72051900	-0.02727000
C	4.28483900	-1.66327600	-0.46625000
H	4.20801400	-2.28919400	-1.35491200
H	5.12637200	-0.97637800	-0.56916400
H	4.38689000	-2.27872900	0.42848000
C	3.13150300	0.12366800	1.20830000
H	3.95842000	0.81835100	1.05146400
H	2.23541600	0.67263000	1.49612400
H	3.38604400	-0.62667700	1.95842300

I1·DMSO



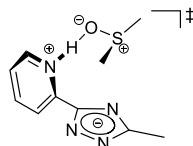
M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.23570700	0.78186800	-0.03293900
N	-2.08465800	1.82911000	-0.06007200
N	0.04830600	1.12822000	-0.03694800
C	-1.66435700	-0.60982000	0.00087000
C	-3.00298100	-0.99735200	-0.02779600
C	-3.32305400	-2.34353500	0.00364300
H	-3.76584900	-0.23226700	-0.07616800
C	-1.00480500	-2.87360400	0.09233100

C	-2.31225800	-3.30466600	0.06329200
H	-4.36196400	-2.65041300	-0.01945200
H	-0.15571000	-3.54320000	0.13954500
H	-2.53283900	-4.36269700	0.08747800
N	-0.71560200	-1.56397400	0.06249700
C	-1.22642700	2.86188600	-0.07974400
C	-1.64855700	4.29491100	-0.10365900
H	-2.21611400	4.55049700	0.79435600
H	-0.77255600	4.94242400	-0.15358100
H	-2.28391200	4.50171700	-0.96778600
N	0.05792900	2.47662400	-0.06722400
H	0.32605100	-1.30706700	0.09507500
S	2.74308200	-0.23438200	-0.36434100
O	1.87913300	-1.38760900	0.19502300
C	4.37805200	-0.97193200	-0.49074600
H	4.33983500	-1.72549700	-1.27687900
H	5.09214000	-0.19197700	-0.75937900
H	4.63652600	-1.42689100	0.46582300
C	3.07729000	0.84011100	1.03581600
H	3.80912400	1.58891800	0.72807800
H	2.13597400	1.31710500	1.30133600
H	3.46191400	0.23328300	1.85665700

TS2-rot·DMSO

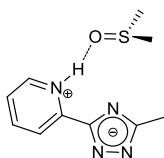


M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -59.2259 cm⁻¹

Cartesian coordinates

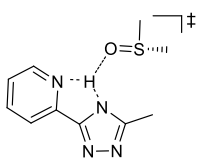
ATOM	X	Y	Z
C	-0.52580500	1.17127900	-0.15588900
N	0.14729600	1.61323800	0.92207400
N	0.06091200	1.43448100	-1.31556300
C	-1.80054500	0.42514200	-0.05555100
C	-3.05245300	0.98412800	-0.25752400
C	-4.18354500	0.18790000	-0.11357600
H	-3.12933700	2.03198800	-0.51541200
C	-2.78372800	-1.66886200	0.40820000
C	-4.05223300	-1.15358100	0.22996000
H	-5.16735000	0.61546800	-0.26636700
H	-2.58854100	-2.70291000	0.66061700
H	-4.91399500	-1.79519900	0.35176900
N	-1.71305200	-0.87926200	0.26294900
C	1.21725700	2.19618500	0.33883000
C	2.32228500	2.85041000	1.10267100
H	1.93667000	3.62645400	1.76753900
H	3.03447900	3.30563800	0.41340300
H	2.85593200	2.12174700	1.71865400
N	1.20315900	2.10267900	-0.98895900
H	-0.72571400	-1.30098700	0.33394000
S	1.97609000	-1.15457400	0.13009200
O	0.65083700	-1.94797600	0.23196000
C	3.22023300	-2.34581100	0.63795300
H	3.07338900	-2.53789400	1.70031400
H	4.20624100	-1.90935400	0.47078600
H	3.08860600	-3.25901500	0.05688400
C	2.36021700	-1.10870700	-1.62367100
H	3.32662400	-0.61761300	-1.75043600
H	1.57851400	-0.51894200	-2.10142900
H	2.38206700	-2.12883300	-2.00933800

I2-DMSO

M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.03558500	1.31080800	-0.03541400
N	0.30653700	1.19516100	0.01446800
N	-1.46557100	2.56629100	-0.14181400
C	-1.93386500	0.16584100	0.00155900
C	-3.32443500	0.27129700	-0.04850500
C	-4.09467900	-0.87632500	-0.00819300
H	-3.77155100	1.25343900	-0.11887700
C	-2.11170900	-2.18536300	0.12576500
C	-3.48552900	-2.13080400	0.08302600
H	-5.17487200	-0.80070400	-0.04756900
H	-1.55007600	-3.10807800	0.19095500
H	-4.06390400	-3.04347000	0.11654400
N	-1.38219400	-1.05864200	0.08516800
C	0.68719500	2.47959200	-0.07056200
C	2.11225600	2.92794800	-0.04192200
H	2.72204300	2.33148000	-0.72421200
H	2.18172500	3.97580900	-0.33646000
H	2.53825800	2.82611100	0.95988000
N	-0.34938400	3.32509000	-0.16426800
H	-0.32073800	-1.18397600	0.11005400
S	2.33278800	-1.07192400	-0.34530600
O	1.10223600	-1.85732800	0.15831600
C	3.57894100	-2.34720500	-0.58273100
H	3.26091500	-2.96637600	-1.42110300
H	4.52856000	-1.86413800	-0.81927000
H	3.65781500	-2.94202600	0.32762300
C	3.03865700	-0.31164400	1.12224300
H	3.95806000	0.20547800	0.84238900
H	2.30006000	0.39640500	1.49243600
H	3.23800800	-1.09072600	1.85950100

TS2-BC-DMSO

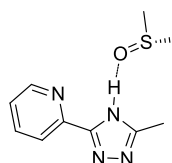
M06-2X/6-311+G(d,p)/SMD(DMSO)

Imaginary frequency: -1497.3696 cm⁻¹

Cartesian coordinates

ATOM	X	Y	Z
C	-1.51432600	1.33754500	-0.01563900
N	-1.85813300	2.60137800	-0.01632800
N	-0.17671300	1.14693800	-0.07665300
C	-2.24096400	0.05768800	0.01561500
C	-3.59345300	-0.22241300	0.08773100
C	-3.96369500	-1.56598100	0.09378400
H	-4.32359300	0.57503400	0.13629600
C	-1.65523800	-2.19504700	-0.03927600
C	-2.99513500	-2.56318400	0.03034200
H	-5.01231500	-1.83375300	0.14861600
H	-0.84268300	-2.90974100	-0.09247300
H	-3.26804100	-3.61008800	0.03354900
N	-1.31517300	-0.91376600	-0.04373200
H	-0.20789200	-0.14232100	-0.09574200

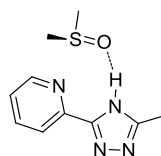
S	2.67846300	-0.72576300	-0.27569000
O	1.44581100	-1.62825200	-0.26498500
C	4.10090100	-1.81605500	-0.46900100
H	4.05218500	-2.23907900	-1.47209000
H	5.01366200	-1.22821700	-0.35795200
H	4.04710100	-2.60374300	0.28372600
C	2.96090200	-0.27304000	1.44548400
H	3.86292700	0.33679100	1.51704400
H	2.09224600	0.29910800	1.77311400
H	3.05908400	-1.18514700	2.03640100
C	0.30967800	2.40693500	-0.12254800
N	-0.67881000	3.29445500	-0.08506000
C	1.75036300	2.77524500	-0.21288200
H	2.31384300	2.37730100	0.63357600
H	2.19622700	2.38757300	-1.13071100
H	1.84295300	3.86131700	-0.21167600

9b-C-DMSO'

M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.43188100	1.13229600	-0.03253100
N	-1.75195500	2.38649200	-0.24494700
N	-0.09018400	1.01931300	0.13897200
C	-2.36057200	-0.00712100	0.01187500
C	-3.73096200	0.18521300	-0.16359500
C	-4.55997000	-0.92583100	-0.11696800
H	-4.12359900	1.18010600	-0.33057000
C	-2.61858800	-2.26383300	0.26516700
C	-3.99665400	-2.17848200	0.10038800
H	-5.62993700	-0.81568800	-0.24945400
H	-2.14387700	-3.22459100	0.43739000
H	-4.60586100	-3.07251900	0.14254200
N	-1.80857600	-1.20519900	0.22429800
H	0.49085600	0.17808900	0.31276500
S	3.07241500	-0.82053200	-0.41320200
O	1.90126200	-0.78028400	0.58059500
C	3.56313300	-2.54804100	-0.49352000
H	2.75793700	-3.09380500	-0.98437400
H	4.47839300	-2.62542300	-1.08237400
H	3.71544100	-2.91397600	0.52270400
C	4.48892000	-0.19885600	0.50288800
H	5.38565900	-0.32564200	-0.10533800
H	4.31419400	0.85980300	0.69357800
H	4.56691700	-0.75279000	1.43924300
C	0.39564500	2.27912000	0.01912600
N	-0.59307100	3.11500400	-0.21139600
C	1.83775300	2.62686200	0.13183400
H	2.26035900	2.22943600	1.05625000
H	2.40318400	2.21964800	-0.71013400
H	1.94714500	3.71090400	0.12778200

9b-C-DMSO

M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
C	1.77864300	0.51662300	0.00004700
N	2.94716700	1.11071500	0.05486400
N	0.78492300	1.44023600	-0.01378100
C	1.53783100	-0.93310900	-0.04225300
C	2.60183400	-1.83517100	-0.05376300
C	2.31148800	-3.19082700	-0.09635800
H	3.62168800	-1.47264600	-0.02928100
C	-0.00658400	-2.61750600	-0.11416900
C	0.98119500	-3.59555300	-0.12928800
H	3.11195700	-3.92146000	-0.10483900
H	-1.05666700	-2.89687200	-0.13677900
H	0.71006700	-4.64307100	-0.16454200
N	0.25589900	-1.31110600	-0.06862900
H	-0.24908300	1.27008600	-0.04614300
O	-1.89001700	1.21845200	-0.04973400
S	-2.62985900	-0.10497000	-0.31812000
C	-2.79902800	-0.89118900	1.29086300
H	-3.39775100	-1.79663000	1.18025700
H	-1.79537900	-1.14109900	1.63225000
H	-3.27543000	-0.18813500	1.97565200
C	-4.34753600	0.38364300	-0.52830900
H	-4.64459300	1.00554300	0.31687400
H	-4.41780200	0.94282000	-1.46086100
H	-4.96095900	-0.51673100	-0.58885200
N	2.71530100	2.45955300	0.07819300
C	1.41186600	2.63958100	0.03836200
C	0.70491500	3.94813900	0.04087000
H	0.09149300	4.05856400	-0.85548800
H	0.05103400	4.03500100	0.91087700
H	1.43852300	4.75295400	0.06813400

DMSO

M06-2X/6-311+G(d,p)/SMD(DMSO)

Cartesian coordinates

ATOM	X	Y	Z
S	0.26356300	0.42155400	0.00000000
O	-1.12055000	1.05977900	0.00000000
C	0.26356300	-0.77211500	1.35090500
H	1.19791000	-1.33509800	1.33185400
H	0.19027900	-0.20993600	2.28155500
H	-0.59587300	-1.43382400	1.23436900
C	0.26356300	-0.77211500	-1.35090500
H	0.19027900	-0.20993600	-2.28155500
H	1.19791000	-1.33509800	-1.33185400
H	-0.59587300	-1.43382400	-1.23436900

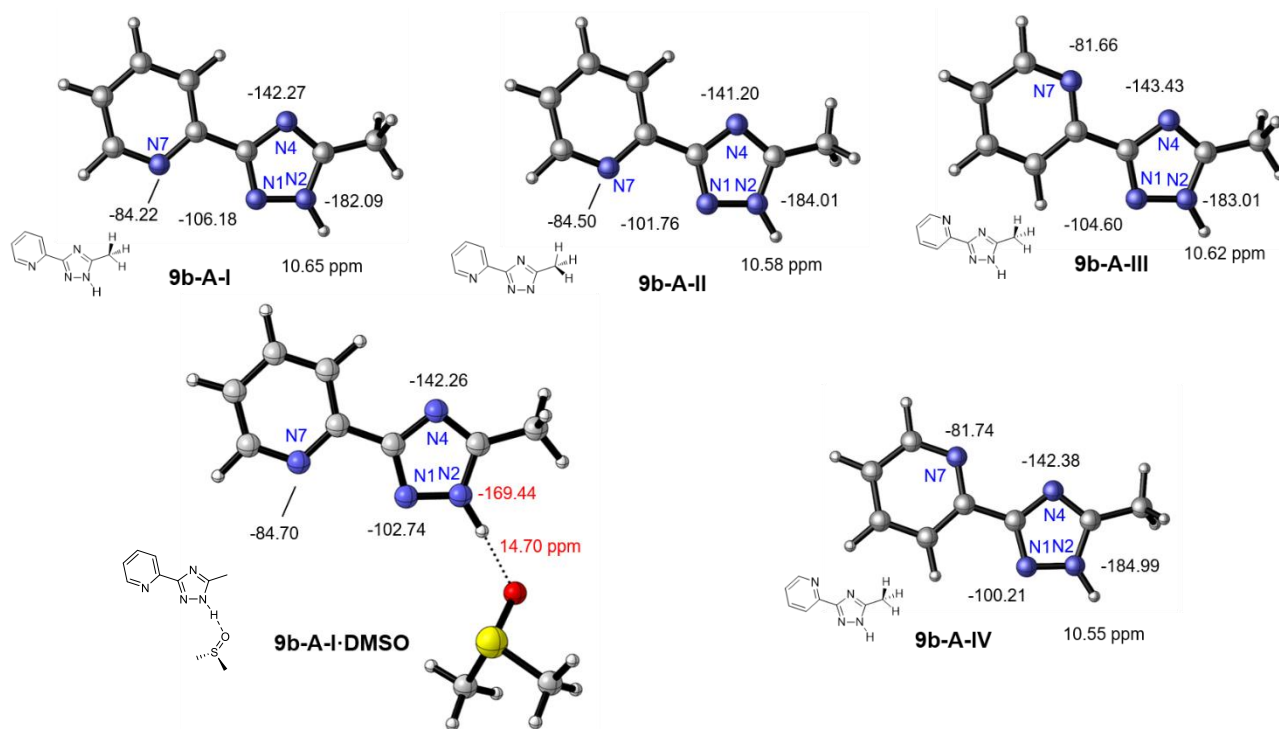


Figure S44. Computed ^{15}N chemical shifts of **9b-A** at the level GIAO/B3LYP/6-311+G(2d,p)/SMD(DMSO).

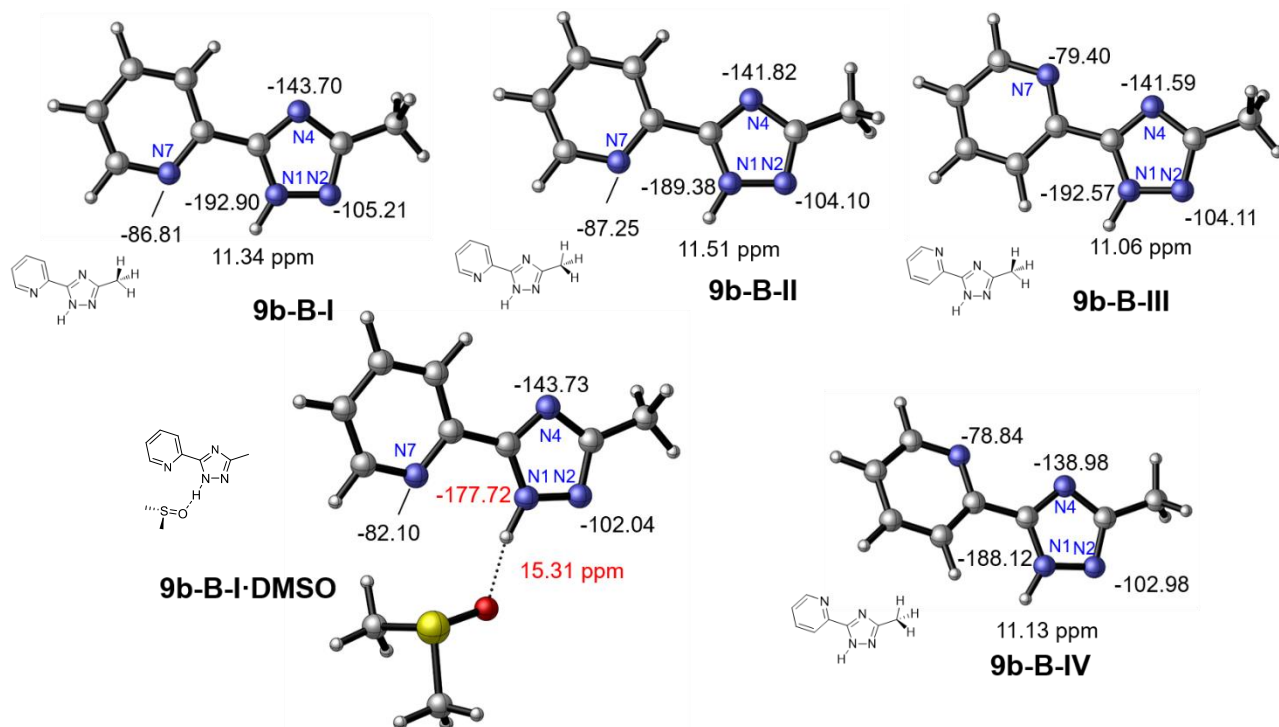


Figure S45. Computed ^{15}N chemical shifts of **9b-B** at the level B3LYP/6-311+G(2d,p)/SMD(DMSO)/GIAO.

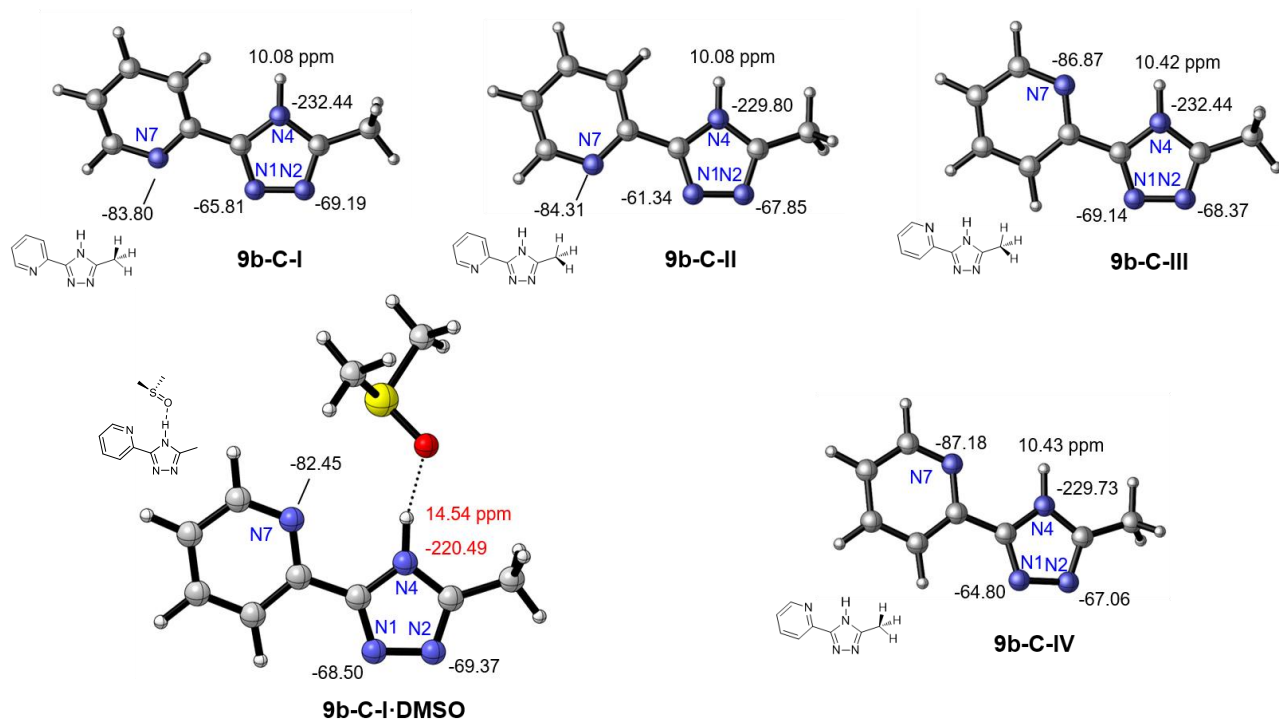


Figure S46. Computed ^{15}N chemical shifts of **9b-C** at the level B3LYP/6-311+G(2d,p)/SMD(DMSO)/GIAO.