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DFT calculations on the hydrogen bonding interactions between adrenaline and trimethoxysilylpropylamine

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Abstract. The hydrogen bonding interactions between adrenaline (**Drug**) and 3-(trimethoxysilyl)-1-propanamine (**TMSA**) have been calculated using Gaussian 98 software. Ten possible forms (**1**–**10**) for the hydrogen bonding interactions were computed at HF and B3LYP levels of theory with 6-31 G(d) and 6-31 + G(d,p) standard basis sets. The binding energies, $\Delta E_{(binding)}$, were obtained from the equation $\Delta E_{(binding)} = E_{(complex)} - [E_{(\mathbf{Drug})} + E_{(\mathbf{TMSA})}] + BSSE$. The most stable forms (complexes **4** and **5**) interact through O–H . . . N hydrogen bond, with calculated binding energies at B3LYP/6-31G* level equal to –10.93 and –12.84 kcal mol^{-1}, respectively. Other compounds containing N–H . . . N (**1**), N–H . . . O (**2**, **3**, **6**, **9**) and O–H . . . O (**7**, **8** and **10**) hydrogen bonds show lower $\Delta E_{(binding)}$ values. The nuclear quadrupole coupling constants (NQCCs or χs) were calculated for ^{17}O, ^{14}N and ^{2}H nuclei about 10.0, 4.0–5.0 MHz and 180.0–360.0 kHz, respectively, that are in agreement with the experimental data.

Keywords: DFT computations, adrenaline, hydrogen bonding, BSSE, NQR

1. Introduction

Hydrogen bonds play a vital role in biological systems [1–3] and the biological properties are certainly affected by these linkages [4, 5]. Several computational and experimental studies have been performed to estimate the hydrogen bonding energies [6–8]. *Ab initio* calculations predicted the nuclear quadrupole coupling constants (χ) of some amide groups and the NQCCs for the ^{14}N and ^{2}H atoms were computed about 5.0 MHz and 200 kHz, respectively [9]. Adrenaline (or Epinephrine, Fig. 1) is a hormone and neurotransmitter [10] that increases heart rate, contracts blood vessels, dilates air passages and participates

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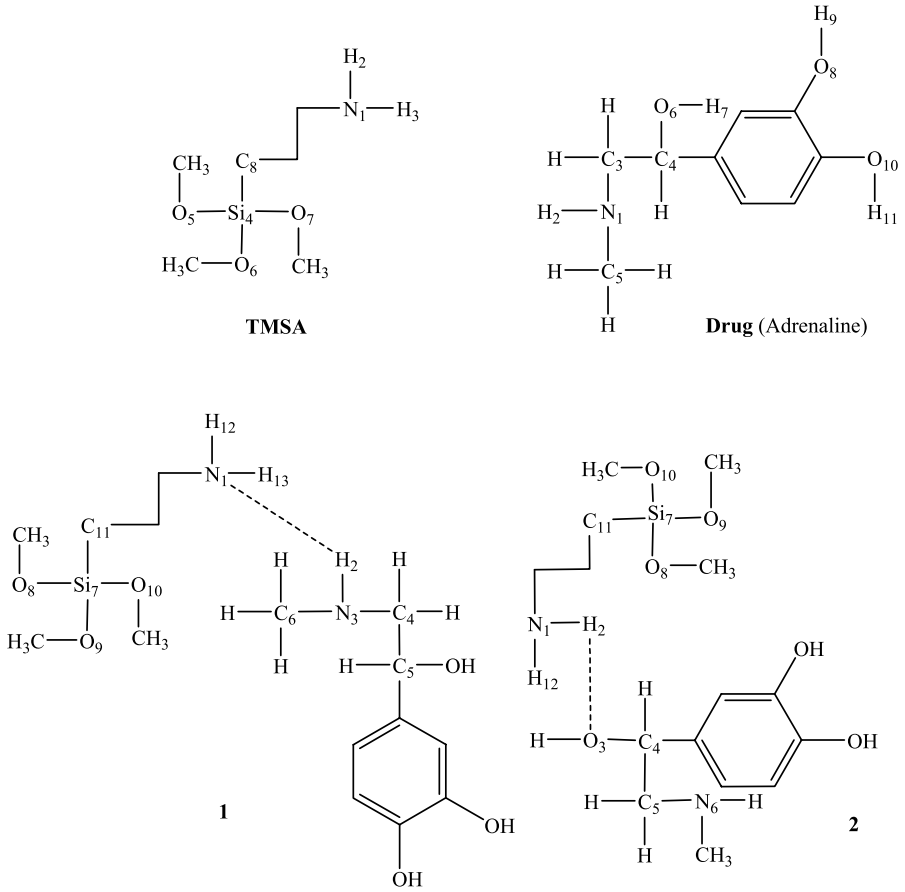
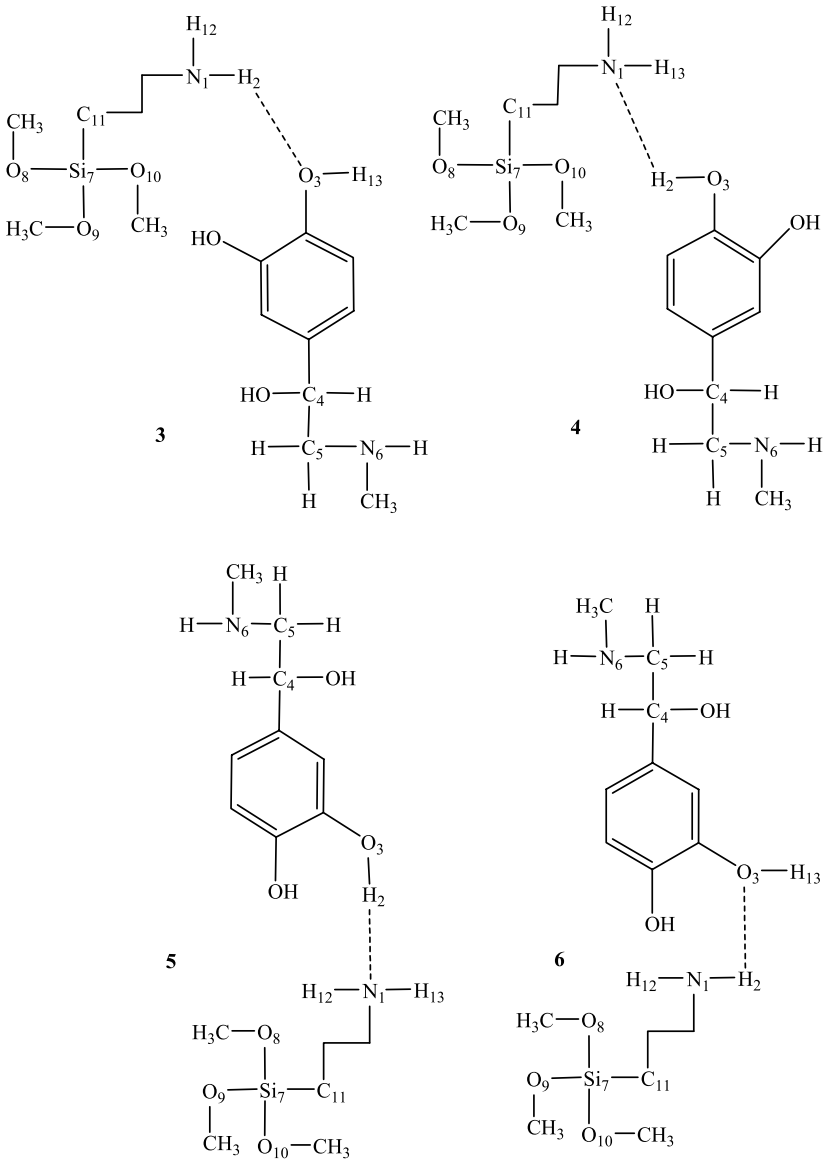


Scheme 1. The chemical structures of **Drug**, **TMSA** and compounds **1**, **2** with atom labeling scheme.

in the "fight or flight" response of the sympathetic nervous system [11]. The hydrogen bonding interactions of this hormone in biological systems are important. One of these systems is molecularly imprinted polymers (MIPs) that are of great interest due to their significant applications in separations, sensing and analysis [12–16]. The sol-gel synthesis of a molecular imprinted ormosil (MIS) for solid-phase extraction of methylxanthines was reported [17]. Computational design of molecularly imprinted silica xerogels was performed by Azenha et al. [18]. In these compounds, the H-bonds play significant role. The molecularly imprinted polymers bearing epinephrine as a template have been prepared in order to substitute with antibodies and receptors [12, 19]. Recently, a chemiluminescence sensor has been introduced for determination of epinephrine using graphene oxide–magnetite-molecularly imprinted polymers [20]. Interestingly, Matsui et al. have designed a composite of Au nanoparticles and molecularly imprinted polymer for sensing adrenaline [21].

Herein, the hydrogen bonding interactions between adrenaline (**Drug**) and trimethoxysilylpropylamine (**TMSA**) have been studied using DFT quantum chemical calculations with Gaussian 98 program suite [22]. Moreover, the nuclear quadrupole coupling constants (χ) for ^{17}O, ^{14}N and ^{2}H nuclei were calculated by NQR computations.

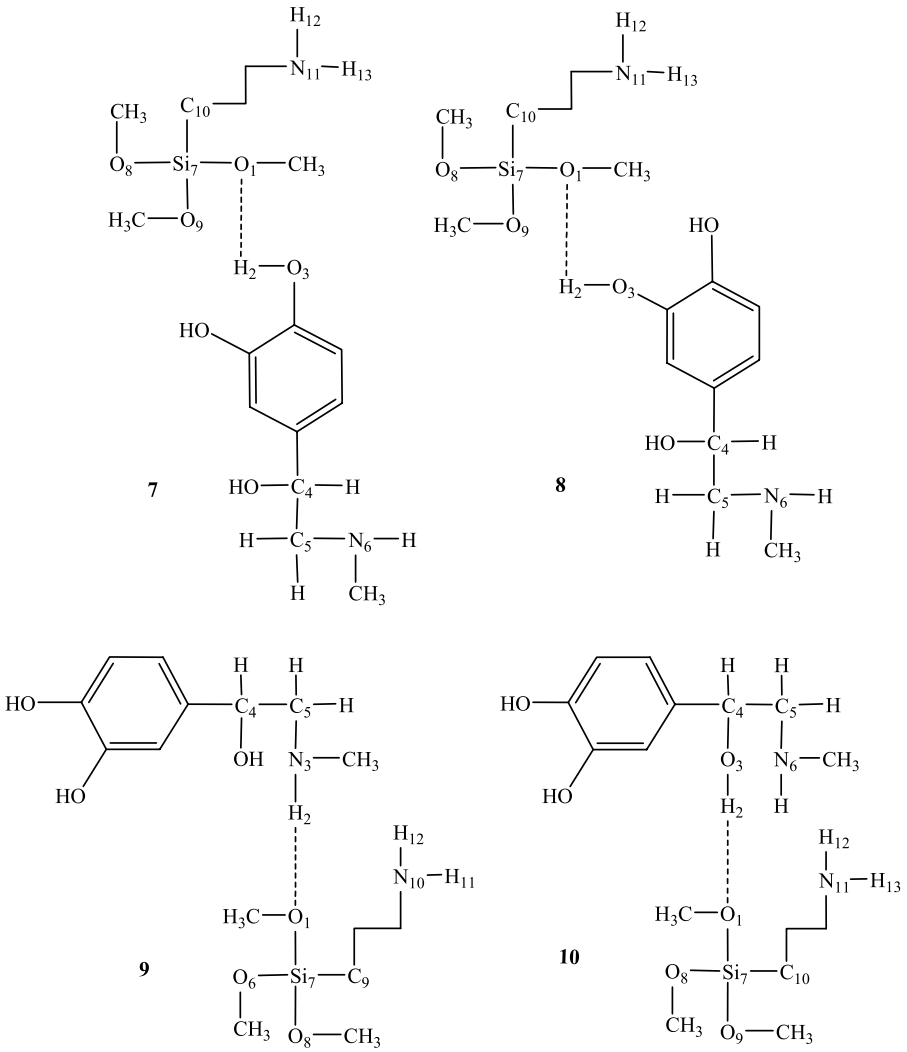


Scheme 2. The chemical structures of compounds **3–6** with atom labeling scheme.

2. Results and discussion

In order to study the hydrogen bonding interactions, the geometries of trimethoxysilyl propylamine (**TMSA**) and adrenaline (**Drug**) as well as ten possible H-bonded forms among them (compounds **1–10**) were fully optimized at HF and B3LYP methods with 6-31G* and 6-31 + G** standard basis sets. The optimized structures of **TMSA**, **Drug** and compounds **1–10** are represented in Schemes 1–3.

The binding energies for H-bond interactions, $\Delta E_{(binding)}$, are obtained from the equation $\Delta E_{(binding)} = E_{(complex)} - [E_{(\mathbf{Drug})} + E_{(\mathbf{TMSA})}] + BSSE$, Table 1. The basis sets superposition errors (BSSE) using counterpoise correction was developed by Boys and Bernardi [23]. Among complexes **1–10**,



Scheme 3. The chemical structures of compounds **7–10** with atom labeling scheme.

compounds **4** and **5** (containing O–H . . . N hydrogen bond) yield the highest binding energies at B3LYP/6-31G* level equal to –10.93 and –12.84 kcal mol^{-1}, respectively. Other compounds containing N–H . . . N (**1**), N–H . . . O (**2**, **3**, **6**, **9**) and O–H . . . O (**7**, **8** and **10**) hydrogen bonds indicate smaller $\Delta E_{(binding)}$ values. Figure 2 indicates the optimized structure of the most stable form at B3LYP/6-31 + G** level (compound **5**).

Huang et al. studied the hydrogen bonding interactions between adrenaline, protonated adrenaline and 12-crown-4 (12C4) [24]. They indicated that the most stable complex between adrenaline and 12C4 contains one O–H . . . O hydrogen bond. Also, the most stable complex between protonated adrenaline and 12C4 contains one O–H . . . O and one N–H . . . O hydrogen bonds. They obtained the hydrogen bonding interaction energies, $\Delta E_{(binding)}$, in the range of –4.99 to –18.99 kcal/mol at B3LYP/6-31 G(d) level for eight possible H-bonded forms. It has been shown that $\Delta E_{(binding)}$ for the hydrogen bonded forms of protonated adrenaline and formate anion can be as great as 119.99 kcal/mol in the gas phase [25].

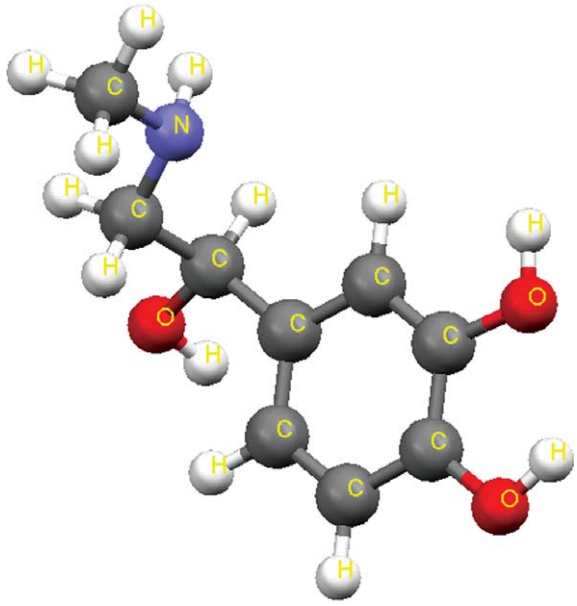


Fig. 1. The structure of adrenaline (Epinephrine) with atom labeling scheme.

Table 1
The corrected binding energies with BSSE, ΔE^{CP}, (kcal mole^{-1}) for compounds **1**–**10**

Method	Compound									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
HF/6-31G*	–2.19	–0.42	–0.04	–7.71	–5.68	0.42	–4.66	–4.66	–0.22	–0.80
HF/6-31 + G**	–1.68	–0.16	0.24	–7.78	–4.53	0.65	–4.66	–4.66	–0.12	–2.87
B3LYP/6-31G*	–5.11	–2.20	–0.50	–10.93	–12.84	–1.38	–5.55	–3.24	–1.92	–2.72
B3LYP/6-31 + G**	–2.63	–1.12	–0.32	–10.34	–10.11	0.23	–5.20	–3.10	–0.34	–3.67

Another investigation revealed the molecular recognition of protonated adrenaline by supramolecular complexation with crown ethers [26] in which the $\Delta E_{(binding)}$ were measured in the range of –28.98 (in **I**) to –48.62 (in **II**) kcal/mol in the gas phase. The $\Delta E_{(binding)}$ values reported for the hydrogen bonding interactions between adrenaline and 15-crown-5 at B3LYP/6-31 + G(d) level were in the range of –4.27 to –32.18 kcal/mol [27] while they vary from –2.41 to –9.19 kcal/mol for the interaction between adrenaline and formamide at B3LYP/6-311 + G(d,p) level [28].

The hydrogen bonding data and dipole moments of these complexes are represented in Table 2 where the D, H, and A introduce the donor, bridging hydrogen and acceptor atoms, respectively. Acceptable values result for the D–H, H ... A, D–H ... A distances and ∠DHA about 1.0, 2.0–2.5 and 3.0–3.5 $\AA$ and 150–170°, respectively. The dipole moments of compounds **1**–**10** are affected by H-bonds and vary in the range of ∼1.0 D in **6** to ∼7.5 D in **5**. It is interesting that the most stable compound (**5**) has the greatest dipole moment. The dipole moments of **TMSA** and **Drug** were measured as 0.668 and 3.222 D at B3LYP/6-31 + G** level, respectively. In fact, when a hydrogen bond is formed, the polarity of the resulting compound is changed due to varying the electron cloud distribution. The effects of hydrogen

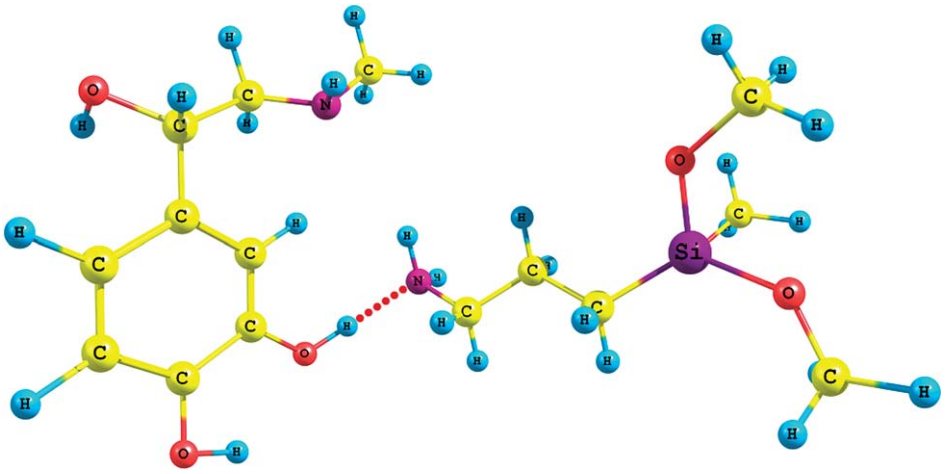


Fig. 2. The optimized structure of the most stable compound **5** at B3LYP/6-31 + G** level with atom labeling scheme.

Table 2
Hydrogen bonding data (*Å*, °) and dipole moments (Debye) for compounds **1–10** at B3LYP/6-31 + G** level

Compound	D–H ... A	*d*(D–H)	*d*(H ... A)	*d*(D ... A)	∠DHA	Dipole moment
1	N(3)–H(2) ... N(1)	1.023	2.228	3.240	169.64	4.259
2	N(1)–H(2) ... O(3)	1.017	2.252	3.190	152.52	3.056
3	N(1)–H(2) ... O(3)	1.018	2.270	3.262	164.35	2.928
4	O(3)–H(2) ... N(1)	1.005	1.742	2.733	167.92	2.860
5	O(3)–H(2) ... N(1)	1.003	1.766	2.762	171.54	7.628
6	N(1)–H(2) ... O(3)	1.018	2.246	3.257	171.89	0.905
7	O(3)–H(2) ... O(1)	0.976	1.960	2.841	148.97	4.026
8	O(3)–H(2) ... O(1)	0.974	1.864	2.836	174.69	4.032
9	N(3)–H(2) ... O(1)	1.020	2.193	3.209	174.19	4.079
10	O(3)–H(2) ... O(1)	0.977	1.879	2.850	172.66	4.028

bonding on the dipole moments have been indicated [29–31]. It has been even shown that different conformations of a H-bonded structure affects the dipole moment values [32]. Similarly, various dipole moments were obtained for three conformers (rotamers) of thiodiglycol [33].

Calculation of nuclear quadrupole coupling constants (χs) of nuclei with spin ≥ 1 is a powerful tool to estimate the electronic and structural properties [34, 35]. For instance, it has been shown that the nuclear quadrupole coupling constants of van der Waals complexes contain valuable information on intermolecular forces [36]. Moreover, the numbers and energies of electronic transitions from ground to excited states can be evaluated from NQCCs [37]. Oxygen-17, nitrogen-14 and deuterium are quadrupolar nuclei with nuclear spin angular moments of $I = 5/2$, 1 and 1, respectively, and electric quadrupole moments, eQ, which interact with electric field gradient, EFG, tensors. The computed nuclear quadrupole coupling constants (χ) for ^{17}O, ^{14}N (MHz) and ^{2}H (kHz) atoms of **Drug**, **TMSA** and compounds **1–10** at different levels of theory are given in Table 3. The χ values for ^{17}O, and ^{14}N atoms are about 10.0, 4.0–5.0 MHz, and for ^{2}H nuclei differ from about 180.0–260.0 kHz to approximately 360.0 kHz. Previous investigations have reported the χ value for ^{2}H nucleus about to 200 kHz [9]. The B3LYP method yields

Table 3
The selected calculated NQCCs (χs) for ^{17}O, ^{14}N (MHz) and ^{2}H (kHz) atoms of **TMSA**, **Drug** and compounds **1–6** at B3LYP/6-31 + G** level

Compound/Atom	NQCC	Compound/Atom	NQCC
TMSA		**4**	
N1	4.737	N1	4.100
H2	258.6	H2	179.1
H3	256.1	O3	9.000
O5	9.362		
O6	9.417	**5**	
O7	9.501	N1	4.021
		H2	180.5
Drug		O3	8.773
N1	5.268		
H2	253.8	**6**	
H7	138.7	N1	4.601
H9	155.3	H2	242.7
H11	195.3	O3	9.168
O6	10.509		
O8	9.601	**7**	
O10	9.257	O1	9.089
		H2	258.6
1		O3	9.061
N1	4.468		
H2	217.9	**8**	
N3	5.070	O1	8.622
		H2	257.0
		O3	9.314
2			
N1	4.570	**9**	
H2	257.6	O1	9.222
O3	10.559	H2	230.9
		N3	5.012
3		**10**	
N1	4.568	O1	9.003
H2	242.8	H2	251.7
O3	9.166	O3	9.766

smaller values for χs, but there are not considerable differences between the outcomes of 6-31G* and 6-31 + G** levels. Moreover, comparing the NQCCs of donor, hydrogen and acceptor atoms in the H-bonded forms **3–6** and **9** with those of their corresponding atoms in **Drug** and **TMSA** exhibits smaller NQCC values upon hydrogen bonding. For the H-bonded form in **2**, the NQCCs are reduced for donor and H atoms but it is increased for the acceptor atom. The NQCCs of donor and acceptor atoms have been reduced in **7**, **8**, **10** while that of H atom are increased. In fact, the reduction in the NQCCs of the atoms contributing in the hydrogen bonding formation reveals the effect of this interaction on the EFG tensors. This subject has been also studied for the H-bond interaction in sulfamerazine by DFT calculations [38].

3. Conclusions

DFT computations at HF and B3LYP levels of theory with 6-31G* and 6-31 + G** basis sets were conducted by Gaussian 98 software to fully optimize the structures of adrenaline (**Drug**) and trimethoxysilylpropylamine (**TMSA**) as well as the ten possible complexes formed due to the hydrogen bonding interactions. Among compounds **1–10**, compounds **4** and **5** each containing one O–H ... N hydrogen bond indicate the most negative $\Delta E_{(binding)}$. This reveals that the O–H ... N is more preferred than other hydrogen bonds (i.e. N–H ... N, N–H ... O and O–H ... O). Nuclear quadrupole coupling constants (χ) were calculated about 10.0, 4.0–5.0 MHz and 180.0–260.0 kHz for ^{17}O, ^{14}N and ^{2}H atoms, respectively.

4. Computational details

The structures of **TMSA**, **Drug**, and hydrogen bonded compounds **1–10** were drawn and optimized in Hyperchem 7.0 program suite. DFT calculations were performed to fully optimize the geometry of the structures using Gaussian 98 program [22] at HF and B3LYP levels of theory and standard 6-31G*, 6-31 + G** basis sets. The optimizations were followed by computations of the harmonic and the vibrational frequencies. Nuclear quadruple coupling constants (χ) were calculated from the equation $\chi = e^2 q_{zz} Q/h$ [39], supposing that the electric quadrupole moments (Q) of ^{2}H, ^{17}O and ^{14}N nuclei are 2.860, –25.58, and 20.44 mb, respectively [40]. The principal components of the EFG tensor, q_{ii}, are computed in atomic unit (1 au = 9.717365×10^{21} V m^{-2}), with $|q_{zz}| \geq |q_{yy}| \geq |q_{xx}|$ and $q_{xx} + q_{yy} + q_{zz} = 0$. These diagonal elements relate to each other by the asymmetry parameter: $\eta_Q = |q_{yy} - q_{xx}|/|q_{zz}|$, $0 \leq \eta_Q \leq 1$, which measures the EFG tensor deviation from axial symmetry. The computed q_{zz} component of EFG tensor is used to obtain the nuclear quadrupole coupling constants NQCCs (χs).

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References

[1] G.A. Kumar and M.A. McAllister, Theoretical investigation of the relationship between proton NMR chemical shift and hydrogen bond strength, *J Org Chem* **63** (1998), 6968–6972.
[2] P. Cieplak and P.A. Kollman, On the use of electrostatic potential derived charges in molecular mechanics force fields. The relative solvation free energy of cis- and trans-N-methyl-acetamide, *J Comput Chem* **12** (1991), 1232–1236.
[3] Z. Gu, C.F. Ridenour, C.E. Bronniamann, T. Iwashita and A. McDermott, Hydrogen bonding and distance studies of amino acids and peptides using solid state 2D ^{1}H–^{13}C heteronuclear correlation spectra, *J Am Chem Soc* **118** (1996), 822–829.
[4] C. Alemán, On the ability of modified peptide links to form hydrogen bonds, *J Phys Chem A* **105** (2001), 6717–6723.
[5] S. Khodaei, N.L. Hadipour and M.R. Kasaai, Theoretical investigation of hydrogen bonding effects on oxygen, nitrogen, and hydrogen chemical shielding and electric field gradient tensors of chitosan/HI salt, *Carbohydrate Res* **342** (2007), 2396–2403.

[6] B.T. Mmereki and D.J. Donaldson, Ab Initio and density functional study of complexes between the methylamines and water, *J Phys Chem A* **106** (2002), 3185–3190.
[7] N. Huang and A.D. MacKerell Jr, An ab initio quantum mechanical study of hydrogen-bonded complexes of biological interest, *J Phys Chem A* **106** (2002), 7820–7827.
[8] P.R. Rablen, J.W. Lockman and W.L. Jorgenson, Ab initio study of hydrogen-bonded complexes of small organic molecules with water, *J Phys Chem A* **102** (1998), 3782–3797.
[9] F. Elmi, N.L. Hadipour and F. Safinezhad, Investigation hydrogen-bonding capabilities of modified amide groups using calculated nuclear quadruple coupling constants, *Chem Phys Lett* **375** (2003), 273–278.
[10] K.H. Berecek and M.J. Brody, Evidence for a neurotransmitter role for epinephrine derived from the adrenal medulla, *Am J Physiol* **242** (1982), H593–H601.
[11] W.B. Cannon, H.T. Newton, E.M. Bright, V. Menkin and R.M. Moore, Some aspects of the physiology of animals surviving complete exclusion of the sympathetic nerve impulses, *Am J Physiol* **89** (1929), 84–107.
[12] S.A. Piletsky, E.V. Piletska, B. Chen, K. Karim, D. Weston, G. Barrett, P. Lowe and A.P.F. Turner, Chemical grafting of molecularly imprinted homopolymers to the surface of microplates. Application of artificial adrenergic receptor in enzyme-linked assay for β-agonists determination, *Anal Chem* **72** (2000), 4381–4385.
[13] J.M. Lin and M. Yamada, Chemiluminescent flow-through sensor for 1,10-phenanthroline based on the combination of molecular imprinting and chemiluminescence, *Analyst* **126** (2001), 810–815.
[14] F.L. Dickert, K. Halikias, O. Hayden, L. Piu and R. Sikorski, Sensors based on fingerprints of neutral and ionic analytes in polymeric materials, *Sensor Actuator B* **76** (2001), 295–298.
[15] H.Y. Liu, K.H. Row and G.L. Yan, Monolithic molecularly imprinted columns for chromatographic separation, *Chromatographia* **61** (2005), 429–432.
[16] S.H. Cheong, S. McNiven, A. Rachkov, R. Levi, K. Yano and I. Karube, Testosterone receptor binding mimic constructed using molecular imprinting, *Macromolecules* **30** (1997), 1317–1322.
[17] R. Gomes da Costa Silva and F. Augusto, Sol-gel molecular imprinted ormosil for solid-phase extraction of methylxanthines, *J Chromatogr A* **1114** (2006), 216–223.
[18] M. Azenha, P. Kathirvel, P. Nogueira and A. Fernando-Silva, The requisite level of theory for the computational design of molecularly imprinted silica xerogels, *Biosensor Bioelectron* **23** (2008), 1843–1849.
[19] S.A. Piletsky, E.V. Piletska, A. Bossi, K. Karim, P. Lowe and A.P.F. Turner, Substitution of antibodies and receptors with molecularly imprinted polymers in enzyme-linked and fluorescent assays, *Biosensor Bioelectron* **16** (2001), 701–707.
[20] H. Qiu, C. Luo, M. Sun, F. Lu, L. Fan and X. Li, A chemiluminescence sensor for determination of epinephrine using graphene oxide-magnetite-molecularly imprinted polymers, *Carbon* **50** (2012), 4052–4060.
[21] J. Matsui, K. Akamatsu, S. Nishiguchi, D. Miyoshi, H. Nawafune, K. Tamaki and N. Sugimoto, Composite of Au nanoparticles and molecularly imprinted polymer as a sensing material, *Anal Chem* **76** (2004), 1310–1315.
[22] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, J.A. Montgomery, R.E.J. Stratmann Jr, C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Ortiz, A.G. Baboul, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M.P. Challacombe, M.W. Gill, B. Johnson, W. Chen, M.W. Wong, J.L. Andres, C. Gonzalez, M. Head-Gordon, E.S. Replogle and J.A. Pople, Gaussian 98, Revision A9, Gaussian, Inc; Pittsburgh, PA 1998.
[23] S.B. Boys and F. Bernardi, The calculation of small molecular interactions by the differences of separate total energies. Some procedures with reduced errors, *Mol Phys* **19** (1970), 553–566.
[24] T. Liu, M.-B. Huang, Z.-Y. Yu and D.-Y. Yan, Theoretical study on the supramolecular complexes of 12-crown-4 with adrenaline, *J Mol Struct: Theochem* **776** (2006), 97–104.
[25] Z. Yu, T. Liu, D. Zhang and C. Liu, Theoretical study on the hydrogen bond interaction of 1:1 supermolecular complexes of protonated adrenaline with formate anion and its derivatives, *J Mol Struc: Theochem* **960** (2010), 10–14.
[26] T. Liu, L. Han, Z. Yu, D. Zhang and C. Liu, Theoretical and experimental study on the molecular recognition of adrenaline by supramolecular complexation with crownethers, *Comput Biol Med* **42** (2012), 480–484.
[27] T. Liu and Z.-Y. Yu, Experimental and theoretical study on the supramolecular complexes of 15-crown-5 with adrenaline, *Bioorg Med Chem Lett* **20** (2010), 4845–4849.
[28] T. Liu, Z. Yu, L. Han, X. Wang and C. Liu, Experimental and theoretical study on the 1:1 supramolecular complexes of formamide with adrenaline, *Gene* **496** (2012), 136–140.

[29] B.J.C. Cabral, R.C. Guedes, R.S. Pai-Panandiker and C.A. Nieto de Castro, Hydrogen bonding and the dipole moment of hydrofluorocarbons by density functional theory, *Phys Chem Chem Phys* **3** (2001), 4200–4207.
[30] A.E. Lutskii and N.I. Gorokhova, Intramolecular hydrogen bonds and molecular dipole moments, *Theor Exp Chem* **4** (1971), 532–534.
[31] P.J. Dyer and P.T. Cummings, Hydrogen bonding and induced dipole moments in water: Predictions from the Gaussian charge polarizable model and Car-Parrinello molecular dynamics, *J Chem Phys* **125** (2006), 144519.
[32] K.-M. Marstokk and H. Møllendal, Microwave spectrum, conformational equilibrium, intramolecular hydrogen bonding, inversion tunneling, dipole moments and centrifugal distortion of ethylenediamine, *J Mol Struct* **49** (1978), 221–237.
[33] L.-H. Xu, Q. Liu, R.D. Suenram, F.J. Lovas, A.R. Hight Walker, J.O. Jensen and A.C. Samuels, Rotational spectra, conformational structures, and dipole moments of thiodiglycol by jet-cooled FTMW and ab initio calculations, *J Mol Spect* **228** (2004), 243–250.
[34] M.H. Palmer and A.D. Nelson, The nuclear quadrupole coupling of the halogen pseudohalides: A comparison of ab initio and DFT studies with spectroscopic data, *J Mol Struct* **828** (2007), 91–101.
[35] A.H. Brunetti, NQR in tert-butyl chloride, *J Mol Struct* **690** (2004), 83–88.
[36] J.M. Hutson, Calculating nuclear quadrupole coupling constants for van der Waals complexes, *Mol Phys* **84** (2006), 185–199.
[37] Y. Kawashima, R.D. Suenram and E. Hirota, Determination of nuclear quadrupole coupling constants of NaOH, KOH, RbOH, and CsOH and electric dipole moment of NaOH, *J Mol Spect* **175** (1996), 99–103.
[38] M. Aghazadeh and M. Mirzaei, Hydrogen bond interactions in sulfamerazine: DFT study of the O-17, N-14, and H-2 electric field gradient tensors, *Chem Phys* **351** (2008), 159–162.
[39] R. Bersohn, Nuclear electric quadrupole spectra in solids, *J Chem Phys* **20** (1952), 1505–1509.
[40] P. Pyykö, Spectroscopic nuclear quadrupole moments, *Mol Phys* **99** (2001), 1617–1629.