Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting information

Stability of doubly and triply H-bonded complexes governed by acidity-basicity relationships

Wilmer E. Vallejo Narváez,[a] Eddy I. Jiménez,[a] Margarita Cantú-Reyes,[a] Anatoly K. Yatsimirsky,[b] Marcos Hernández-Rodríguez,*[a] and Tomás Rocha-Rinza*[a]

[a]Instituto de Química and [b]Facultad de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Delegación Coyoacán 04510 Ciudad de México, México.

E-mail: marcoshr@unam.mx, tomasrocharinza@gmail.com

Contents

1. Experimental section

Compounds **A1**-**A3** and **I1-I3** are commercially available. The association constants for the considered triply H-bonded complexes were obtained from the literature as indicated in the manuscript.

1.1 ^{1}H-NMR titrations of amide-imide heterodimers

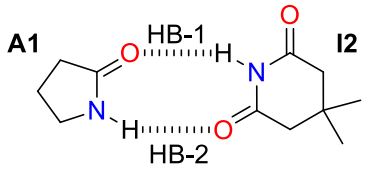
0 to 20 equivalents of imide (from a 2.0 M stock solution) were added to 0.5 mL of a 0.1 M solution of the amide in $CDCl_3$. We proceed in this way because the imide usually self-associates to a smaller degree than the amide. Nonetheless, for the systems **A1**-**I3** and **A2**-**I3**, we performed the inverse process since amides **A1** and **A2** dimerise to a lesser degree than imide **I3**. These experiments were carried out on a 300 MHz spectrometer and N-H chemical shifts of the amide and imide are reported in ppm downfield from TMS. NMR spectra were recorded at 25 ^{o}C and analysed using the MestReNova NMR software.[1]

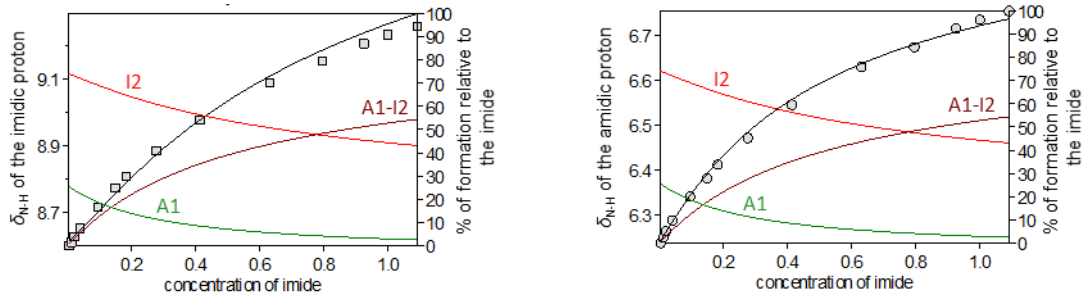
Heterodimerisation constants were calculated with the HypNMR 2008 program[2] considering the self-associations constants for each amide and imide[3] as well as the chemical shift and concentration data obtained from the heterodimerisation process. The association constant of the **A1a**-**I1** adduct was determined from the downfield shifting of the N-H proton using the online tool supramolecular.org.[4]

We also calculated the heterodimerisation constant when the amide is in excess for the **A1**-**I1** and **A2**-**I1** adducts. We obtained similar values to the direct and inverse processes. We averaged the values of association constants for these systems and their corresponding results are presented in Table 1 in the manuscript. The similarity of the outcome for the direct and the inverse processes confirms the fact that only one titration (for example that wherein there is an excess of imide) suffices for the calculation of the heterodimerisation constant. A statistical factor of two was applied to systems that involve imides **I1** and **I2**, which contain equivalent (or nearly equivalent) carbonyl groups.

1.2 Determination of heterodimerisation constants by ^{1}H-NMR

(a)



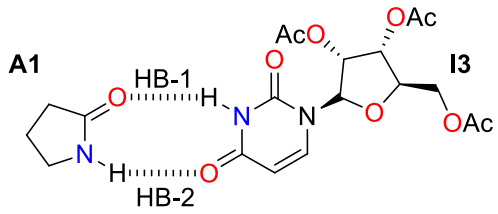


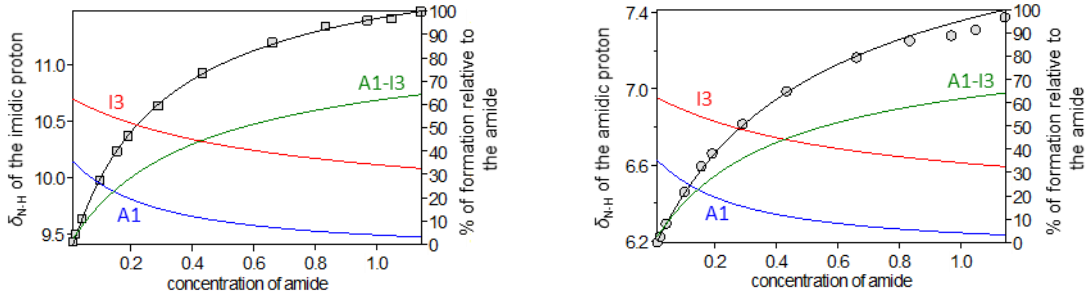
K_{exp} = 2.0 ± 0.4 M^{-1}

HB-1
$\Delta\delta_{N\text{-}H}$ (imide) = 3.43 ppm

HB-2
$\Delta\delta_{N\text{-}H}$ (amide) = 1.85 ppm

(b)



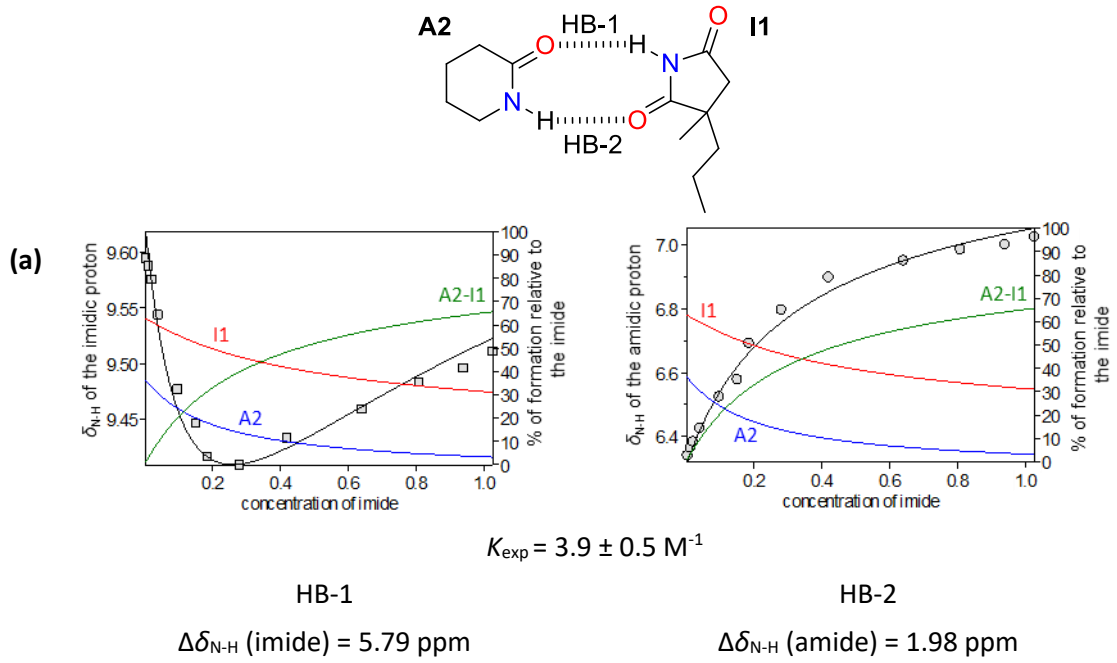


K_{exp} = 11.0 ± 1.0 M^{-1}

HB-1
$\Delta\delta_{N\text{-}H}$ (imide) = 4.50 ppm

HB-2
$\Delta\delta_{N\text{-}H}$ (amide) = 2.21 ppm

Fig. S1 Profiles of chemical shift as a function of concentration for the heterodimerisations **A1**-**I2** and **A1**-**I3**, in $CDCl_3$ at 25 °C, for the N-H signal of the imide (left) and the amide (right). **(a)** Amide **A1** (0.1 M) upon titration with 0 to 20 equivalents of imide **I2** and **(b)** the inverse titration of the system **A1**-**I3**.



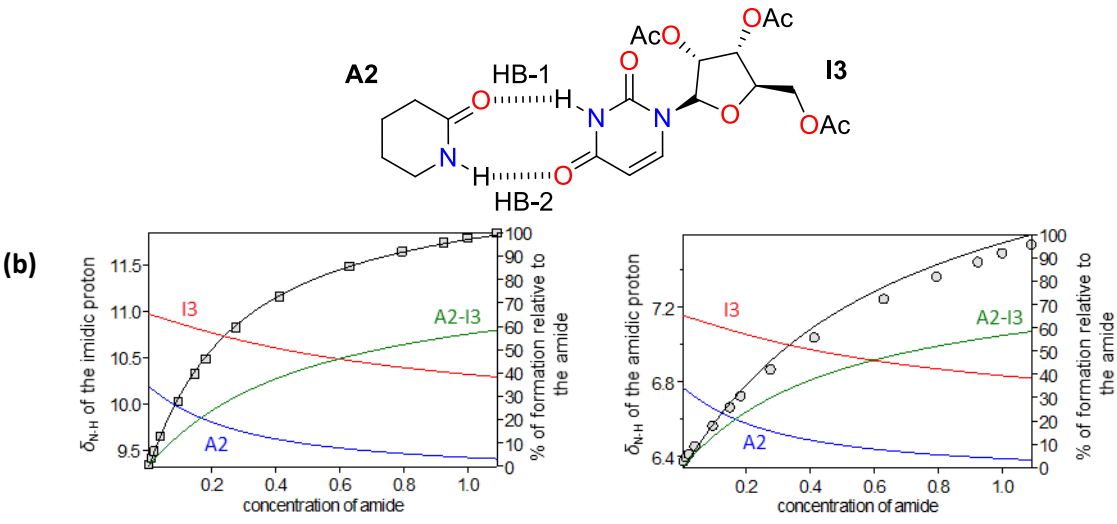
K_{exp} = 3.9 ± 0.5 M^{-1}

HB-1

$\Delta\delta_{N\text{-}H}$ (imide) = 5.79 ppm

HB-2

$\Delta\delta_{N\text{-}H}$ (amide) = 1.98 ppm



K_{exp} = 10.2 ± 1.0 M^{-1}

HB-1

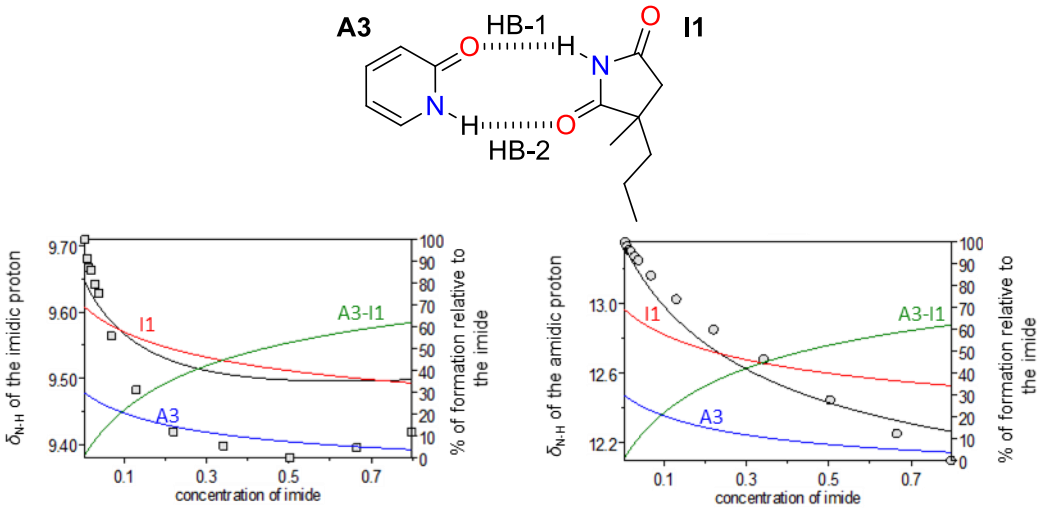
$\Delta\delta_{N\text{-}H}$ (imide) = 4.91 ppm

HB-2

$\Delta\delta_{N\text{-}H}$ (amide) = 2.08 ppm

Fig. S2 Profiles of chemical shift as a function of concentration for the heterodimerisations **A2**-**I1** and **A2**-**I3** in $CDCl_3$ at 25 °C, for the N-H signal of the imide (left) and the amide (right). **(a)** Amide **A2** (0.1 M) upon titration with 0 to 20 equivalents of imide **I1** and **(b)** the inverse titration of the system **A2**-**I3**.

(a)



K_{exp} = 30.3 ± 0.1 M^{-1}

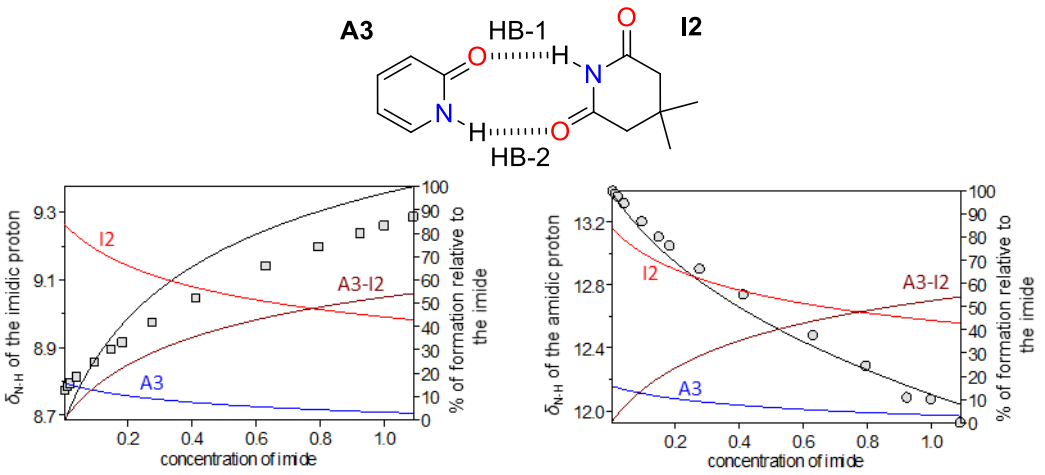
HB-1

$\Delta\delta_{N\text{-}H}$ (imide) = 7.15 ppm

HB-2

$\Delta\delta_{N\text{-}H}$ (amide) = 4.11 ppm

(b)



K_{exp} = 11.9 ± 0.6 M^{-1}

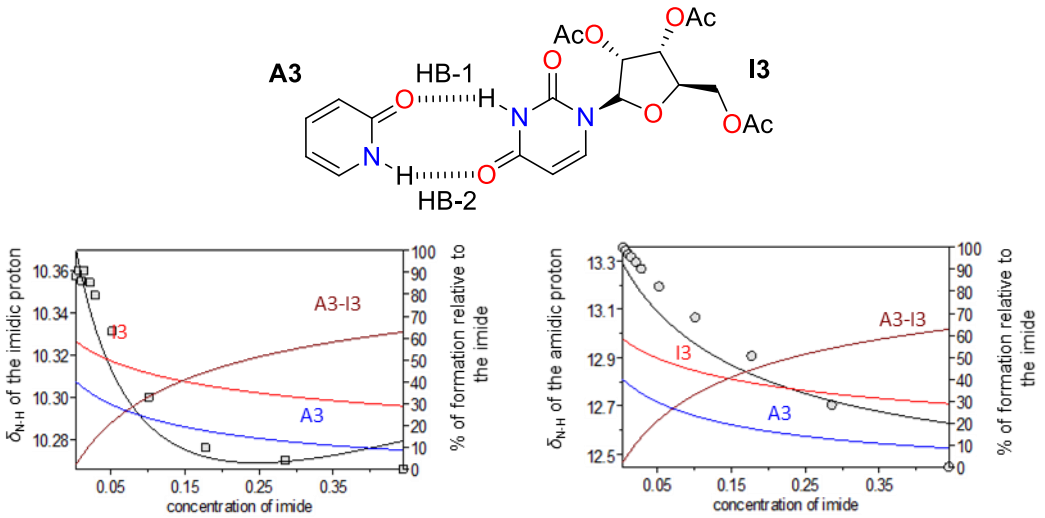
HB-1

$\Delta\delta_{N\text{-}H}$ (imide) = 5.96 ppm

HB-2

$\Delta\delta_{N\text{-}H}$ (amide) = 3.57 ppm

Fig. S3 Profiles of chemical shift as a function of concentration for the heterodimerisations **A3**-**I1** and **A3-I2** in $CDCl_3$ at 25 °C, for the N-H signal of the imide (left) and the amide (right). **(a)** and **(b)** amide **A3** (0.1 M) was titrated with 0 to 20 equivalents of imides **I1** and **I2** respectively.



K_{exp} = 105.2 ± 1.0 M^{-1}

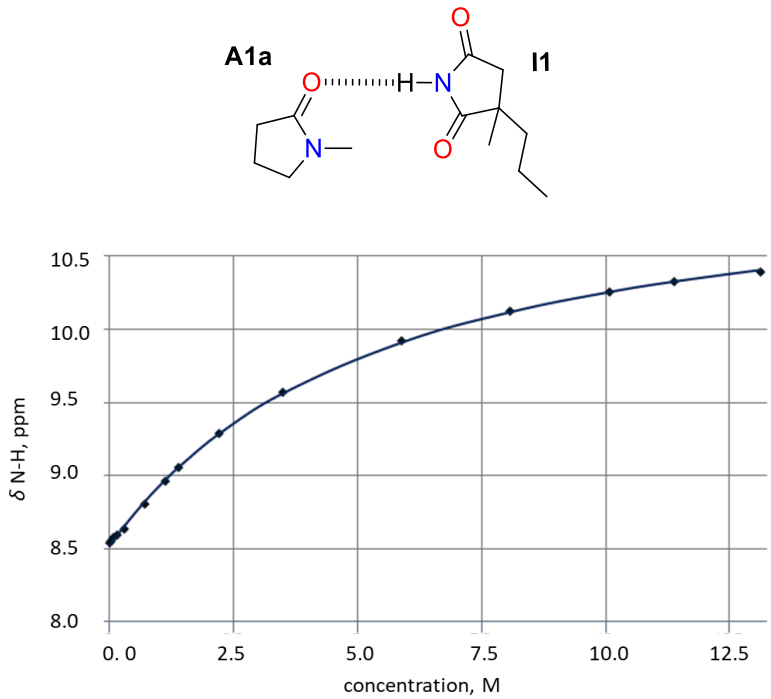
HB-1

$\Delta\delta_{N\text{-}H}$ (imide) = 6.13 ppm

HB-2

$\Delta\delta_{N\text{-}H}$ (imide) = 4.44 ppm

Fig. S4 Profiles of chemical shift as a function of concentration for the heterodimerisation **A3**-**I3** in $CDCl_3$ at 25 °C, for the N-H signal of the imide (left) and the amide (right). Amide **A3** (0.1 M) was titrated with 0 to 20 equivalents of imide **I3**.



K_{exp} = 1.12 ± 0.01 M^{-1}

$\Delta\delta_{N\text{-}H}$ = 3.49 ppm

Fig. S5 Profile of chemical shift as a function of concentration for the heterodimerisation **A1a**-**I1** in $CDCl_3$ at 25 °C, for the N-H signal of the imide. Imide **I1** (0.1 M) was titrated with 0 to 20 equivalents of amide **A1a**.

2. Computational details

All geometrical parameters of monomers, adducts and the species involved in the calculation of proton acceptor and donor capacities were computed using the M06-2x[5] functional with the 6-311++G(2d,2p) basis set as implemented in the Gaussian 09 package.[6] We selected this level of theory because it yields a good description of (i) intermolecular interactions such as hydrogen bonds and (ii) energetics of protonation and deprotonation processes.[7] The calculation of the corresponding harmonic frequencies was performed to characterise each stationary structure as a minimum. We used an implicit solvent model in the calculations by using the SMD method[8] and considering chloroform as solvent. We also consider vacuum, water and acetonitrile to compute proton affinities in different environments discussed in section 2.7.1 of the ESI. We performed the IQA energy partition with M06-2x/6-311++G(2d,2p) electron densities to get further insights about the chemical bonding of the studied complexes. The IQA calculations were carried out with the AIMAll program.[9]

2.1 Interacting quantum atoms energy partition

The Interacting Quantum Atoms (IQA) approach is an electronic energy partition, E, in one (E_{net}^{A}) and two-atoms (E_{int}^{AB}) terms[10]

$$E = \sum_{A} E_{net}^{A} + \sum_{A} \sum_{B>A} E_{int}^{AB}, \qquad \text{(S1)}$$

where the sums run over atomic regions which cover completely the three-dimensional space. E_{net}^{A} and E_{int}^{AB} are denoted as (i) the IQA net energy of atom A and (ii) the IQA interaction energy between two atoms, A and B.[11] The IQA method is based on the first order reduced density matrix and the pair density. None of these scalar fields is defined in conventional density functional theory. However, it is possible to scale one and two terms of the Kohn-Sham exchange correlation energy in a similar way to QTAIM.[12] This process allows to obtain the total DFT electronic energy according to equation (S1). The IQA method has been successfully used to study molecular adducts.[13] Considering that the IQA approach is invariant with respect to the gathering of QTAIM atoms in molecules or functional groups, the energy of a bimolecular complex $M \cdots N$ can be written as

$$E^{M\cdots N} = E_{net}^{M} + E_{net}^{N} + E_{int}^{M,N}, \qquad \text{(S2)}$$

where E_{net}^{M} equals the sum of the net energies of the atoms within M and their corresponding interactions

$$E_{net}^{M} = \sum_{A\in M} E_{net}^{A} + \sum_{A\in M} \sum_{\substack{B\in M \\ B>A}} E_{int}^{AB}. \qquad \text{(S3)}$$

A similar definition holds for E_{net}^{N}. The term $E_{int}^{M,N}$ is written as

$$E_{int}^{M,N} = \sum_{A\in M} \sum_{B\in N} E_{int}^{AB}. \qquad \text{(S4)}$$

The difference in energy related to the formation of the molecular group $M \cdots N$ from the isolated monomers can be defined as the sum of the IQA deformation energies of the monomers and its corresponding interaction,

$$\Delta E = E^{M\cdots N} - \left(E_{iso}^{M} + E_{iso}^{N}\right)$$
$$= E_{def}^{M} + E_{def}^{N} + E_{int}^{M,N}. \qquad \text{(S5)}$$

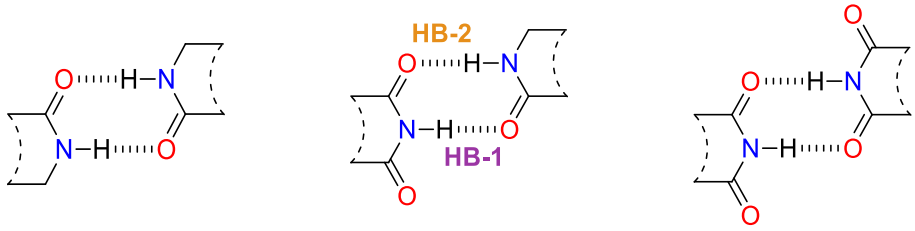
The deformation energy of monomer G is expressed as

$$E_{def}^{G} = E_{net}^{G} - E_{iso}^{G}, \qquad \text{(S6)}$$

E_{def}^{G} is related with the changes of the electron density and the nuclear geometry associated to the interaction of monomer G with other molecules.

2.2 Hydrogen bond distances of homo- and heterodimers of the examined amides and imides

Table S1. Hydrogen bond lengths (Å) of the homo- and heterodimers involved in amide-imide heterodimerisation.



dimer	amide-amide	HB-1	HB-2	imide-imide
A1-I1		1.79	1.97	1.90
A1-I2	1.89	1.83	1.97	1.92
A1-I3		1.77	1.94	1.83
A2-I1		1.77	1.99	1.90
A2-I2	1.89	1.81	1.97	1.92
A2-I3		1.75	1.95	1.83
A3-I1		1.77	1.88	1.90
A3-I2	1.74	1.81	1.86	1.92
A3-I3		1.74	1.84	1.83

2.3 Correlation of the experimental (ln K_{exp}) and computed heterodimerisation constants

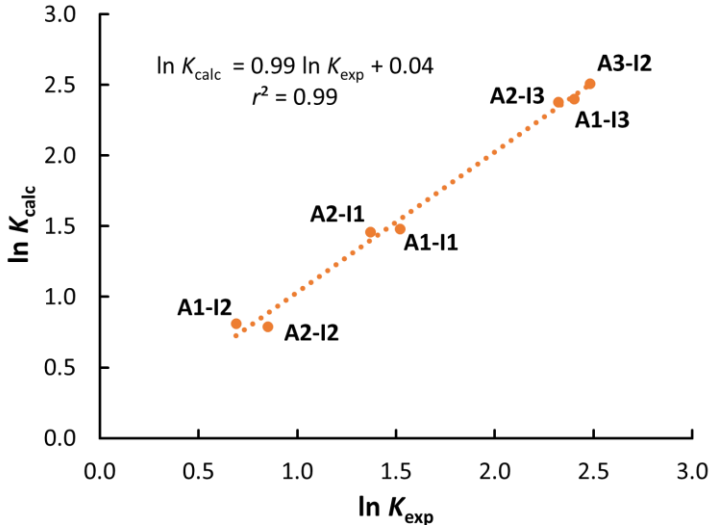
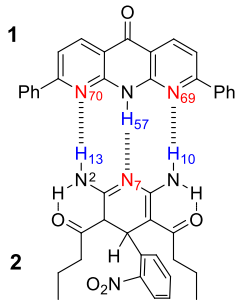
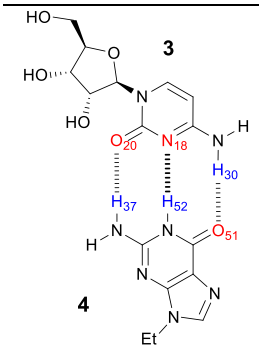
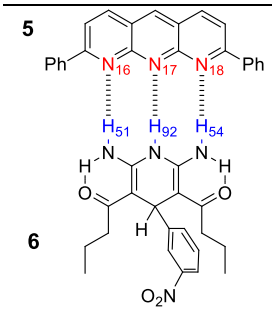


Fig. S6 Correlation of experimental (ln K_{exp}) and calculated (ln K_{calc}) heterodimerisation constants for the compounds indicated in Table 1. The values of ln K_{calc} were calculated according to Eq. (2) in the body of the manuscript.

2.4 IQA analyses of triply hydrogen-bonded complexes

Table S2. Representative IQA energies (kcal/mol) of the **1-2**, **3-4** and **5-6** adducts.

	Interaction	IQA energy atom-atom	atom – molecule intermolecular interaction	IQA energy
 **1-2**	$N_{70}\cdots H_{13}$	−34.1	$N_{70}\cdots$**2**	−25.0
	$N_{70}\cdots N_{7}$	109.1	$H_{57}\cdots$**2**	−18.0
	$H_{57}\cdots H_{13}$	28.8	$N_{69}\cdots$**2**	−40.4
	$H_{57}\cdots N_{7}$	−97.1	$H_{13}\cdots$**1**	−21.0
	$H_{57}\cdots H_{10}$	27.4	$N_{7}\cdots$**1**	−33.7
	$N_{69}\cdots H_{10}$	−33.1	$H_{10}\cdots$**1**	−15.4
	$N_{69}\cdots N_{7}$	114.7		
 **3-4**	$O_{20}\cdots H_{37}$	−107.5	$O_{20}\cdots$**4**	−64.7
	$O_{20}\cdots H_{52}$	−66.2	$N_{18}\cdots$**4**	−52.9
	$N_{18}\cdots H_{37}$	−59.3	$H_{30}\cdots$**4**	−31.0
	$N_{18}\cdots H_{52}$	−104.7	$H_{37}\cdots$**3**	−40.1
	$N_{18}\cdots O_{51}$	125.5	$H_{52}\cdots$**3**	−33.4
	$H_{30}\cdots H_{52}$	31.4	$O_{51}\cdots$**3**	−39.7
	$H_{30}\cdots O_{51}$	−112.5		
 **5-6**	$N_{16}\cdots H_{51}$	−88.6	$N_{16}\cdots$**6**	−54.9
	$N_{16}\cdots H_{92}$	−47.8	$N_{17}\cdots$**6**	−57.7
	$N_{17}\cdots H_{51}$	−52.1	$N_{18}\cdots$**6**	−54.8
	$N_{17}\cdots H_{92}$	−75.2	$H_{51}\cdots$**5**	−29.9
	$N_{17}\cdots H_{54}$	−52.1	$H_{92}\cdots$**5**	−27.0
	$N_{18}\cdots H_{92}$	−47.8	$H_{54}\cdots$**5**	−29.8
	$N_{18}\cdots H_{54}$	−88.5		

2.5 Experimental and theoretical correlations for the triply H-bonded systems

The following model contains all parameters of the acidity $|E(A)|$ and basicity $|E(B)|$ for each hydrogen bond in the system:

The expression is:

$$\ln K_{calc} = -0.12|E(A)|_{HB\text{-}1} + 1.08|E(B)|_{HB\text{-}1} - 0.51|E(A)|_{HB\text{-}2} - 0.05|E(B)|_{HB\text{-}2} + 0.24|E(A)|_{HB\text{-}3} - 0.09|E(B)|_{HB\text{-}3} \quad \text{(S7)}$$

with $r^2 = 0.99$

Table S3. $|E(A)|$ and $|E(B)|$ values (kcal/mol) for the three hydrogen bonds of the AAA-DDD, AAD-DDA and ADA-DAD complexes studied in this work. The quantities ln K_{exp} and ln K_{calc} (determined by the model) are also indicated.

adduct	ln K_{exp}	HB-1		HB-2		HB-3		ln K_{calc}
		$\|E(A)\|$	$\|E(B)\|$	$\|E(A)\|$	$\|E(B)\|$	$\|E(A)\|$	$\|E(B)\|$	
5-6	11.51	67.3	43.2	78.0	40.3	78.0	40.3	11.88
3-4	10.71	73.7	39.7	78.2	35.4	87.4	25.0	11.11
1-2	4.36	74.6	34.5	79.9	30.2	89.5	30.2	4.81
7-8	4.61	82.5	36.9	88.2	21.5	94.8	16.1	5.20
9-8	5.14	78.5	36.9	88.2	21.5	94.8	16.1	5.68
10-8	5.35	79.0	36.9	88.2	21.3	94.8	18.2	5.44
11-8	6.31	74.0	36.9	88.2	15.5	94.8	12.8	6.82

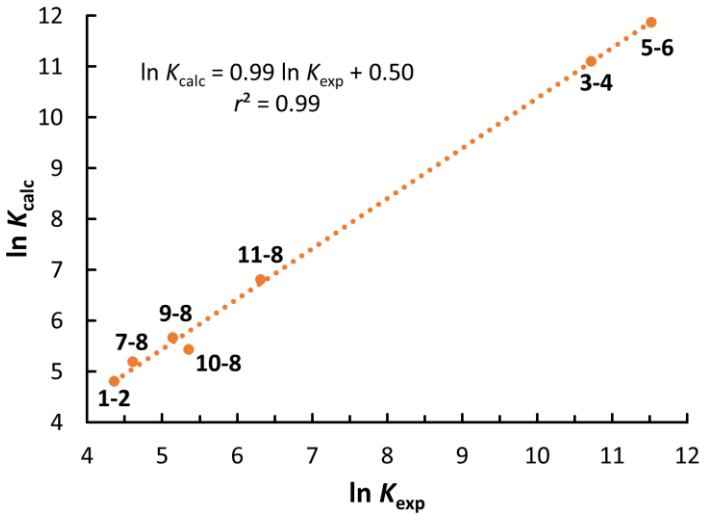


Fig. S7 Correlation of experimental (ln K_{exp}) and calculated (ln K_{calc}) association constants for the complexes indicated in Table S3. The values of ln K_{cal} were computed with Eq. (S7).

2.6 Experimental and theoretical correlations of triply H-bonded adducts considering only the strongest hydrogen bond

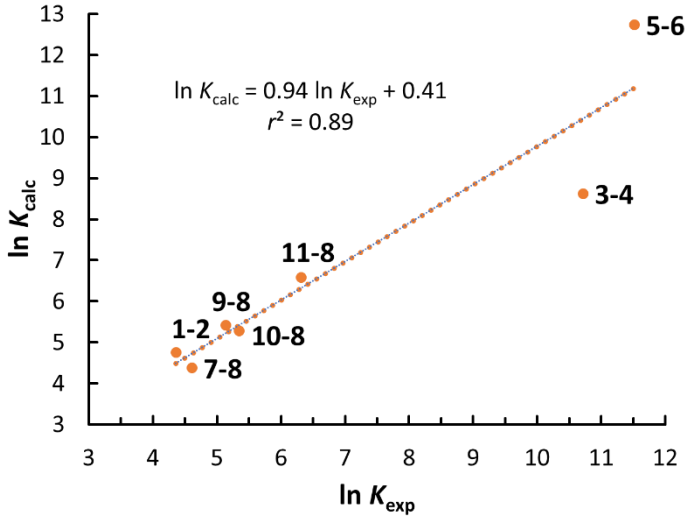


Fig. S8 Correlation of the experimental ln K_{exp} and its theoretical counterpart computed with Eq. 3 in the manuscript.

We note that when the most acidic HB donor is not paired with the most basic HB acceptor, it is not straightforward to determine which hydrogen bond has the largest formation energy. This situation might occur, for example, in a DDD–AAA complex in which the most acidic donor is the central one in DDD and the most basic acceptor is located in the periphery of AAA. Under such circumstances, it is not clear whether the system will present (a) three hydrogen bonds or (b) only two of these interactions to ensure the pairing of the most acidic and basic sites. For these systems, there are other strategies like the use of (i) the Interacting Quantum Atoms[10] or (ii) the potential energy density as described in Ref. 14 to identify the strongest H-bond in the system.

2.7 Rationalisation of the relative basicities of compounds 1, 1' and 5

The relative basicities of **1**, **1'** and **5** might at first sight be surprising as correctly pointed out by one of the reviewers. **1** and **1'** are analogues of 2-aminopyridine (pK_a = 6.71) on one hand, while on the other **5** can be related to 1,8 naphtyridine (pK_a = 3.39). Thus, one could expect **1** and **1'** to be more basic than **5** as opposed to the relative basicities indicated by the computed |E(B)| values reported in Fig. 5 in the body of the manuscript.

First, we consider the structure of **1** in more detail. We note that this compound has an additional carbonyl group in position 3 of the ring of pyridine. This group might considerably diminish the basicity of pyridine due to (i) the inductive effect as previously observed for halogen substituents[15] and (ii) the conjugation between the carbonyl and the amino groups as shown in Fig. S9.

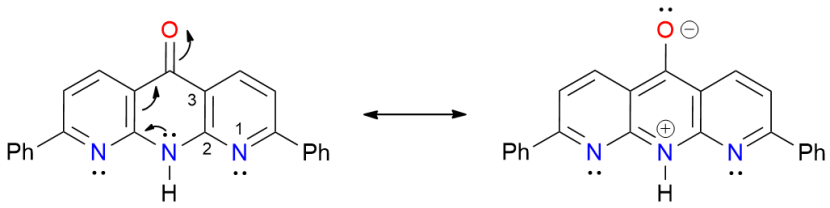
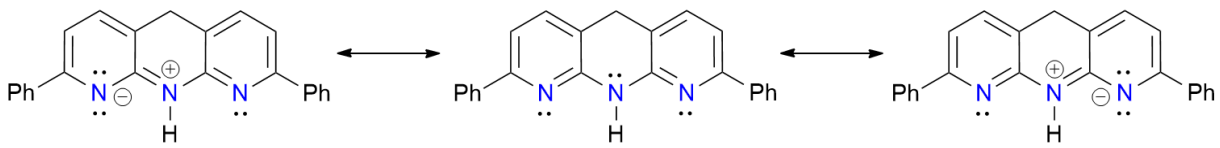
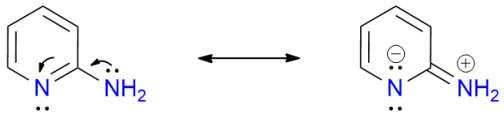


Fig. S9 Conjugation between the amino and carbonyl groups within molecule **1**.

To further investigate this effect, we computed values of |E(B)| for a series of heterocycles related with compounds **1**, **1'** and **5**, namely, pyridine, 1,8-naphthyridine, quinoline, 2-aminopyridine and 3-acetylpyridine. We observed that the magnitudes of the calculated energies |E(B)| are in agreement with the experimental tendency of pK_a in H_2O as shown in Fig. S10. This figure also indicates that an acetyl in position 3 induces a considerable diminution of the basicity of pyridine: pK_a (3-acetylpyridine) − pK_a (pyridine) = 3.18 − 5.14 = −1.96. This effect is larger in magnitude than the corresponding increase on basicity because of an amino group in position 2: pK_a (2-aminopyridine) − pK_a (pyridine) = 6.71 − 5.14 = 1.57. Hence, we can explain the differences of basicities between compounds **1** and **5** by considering the carbonyl group in the middle ring in the former molecule. Concerning the comparison between **1'** and **5**, one can conjecture that the electron donating effect of the central nitrogen in the former compound is shared by the two pyridine nitrogens,



as opposed to 2-aminopyridine in which this action occurs only on one pyridine nitrogen



Thus, the electron donating effect of the amino group in **1'** is reduced to the extent than its basicity is lower than that of **5**.

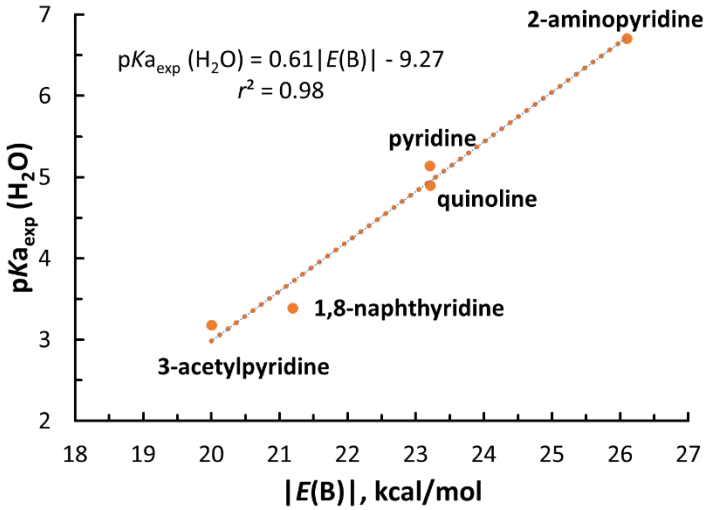


Fig. S10 Correlation of the experimental pK_a (in water) and energies $|E(B)|$ computed with the model indicated in Figure 3 in the body of the manuscript and considering water as a solvent via the SMD method.

Second, one can suggest another explanation based on the application of the JSIH model to examine the structure of **1**, **1'** and **5** along with their corresponding conjugated acids. We note that the basic pyridine rings in **5** have a repulsion between the lone pairs of the molecule as opposed to **1** and **1'** (Fig. S11).

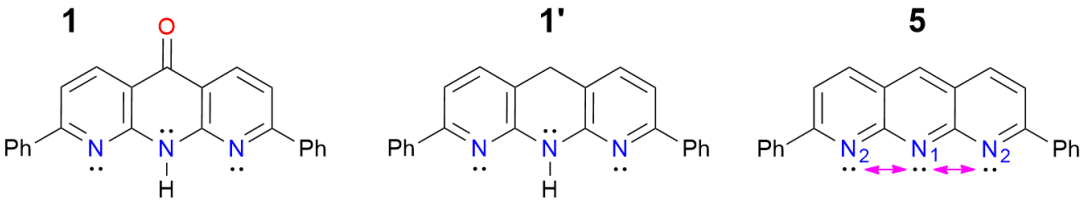
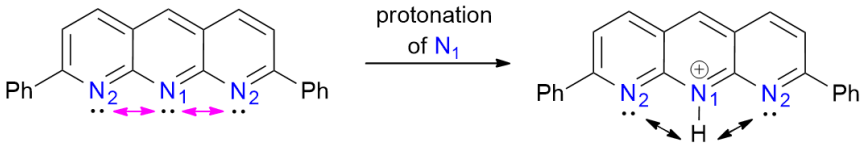
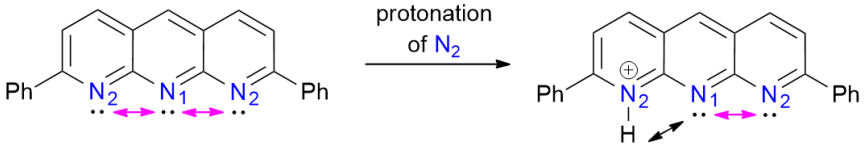


Fig. S11 Jorgensen secondary interactions repulsions among lone pairs in molecule **5** indicated by magenta arrows. Such repulsions are not present in compounds **1** and **1'**.

The conjugated acids can also be analysed under this approach; the protonation of **5** would release repulsions among lone pairs. For example, the protonation of the central nitrogen (N_1) would alleviate the two repulsions among the lone pairs and it would result in two new attractive hydrogen-lone pair interactions,

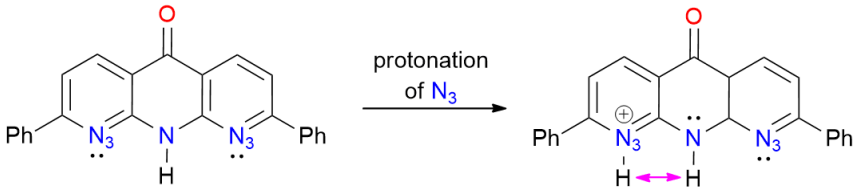


while the addition of an H^+ to N_2 would mitigate only one of those repulsions and it would form only one attractive interaction between a proton and a lone pair,

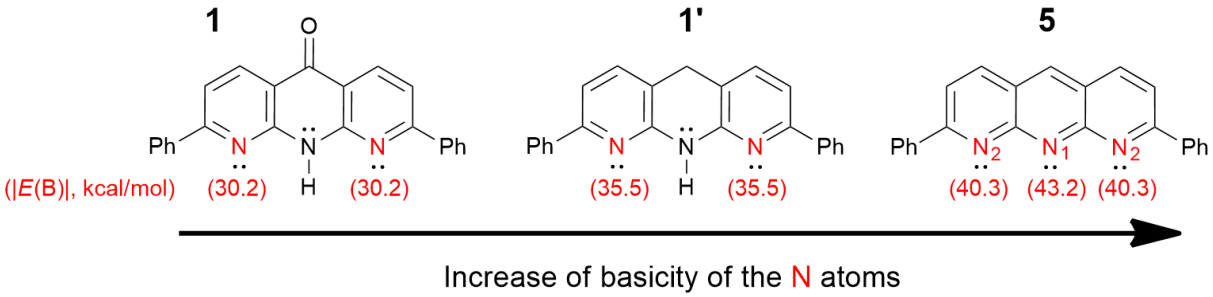


These observations are consistent with the fact that N_1 is more basic than N_5 in **5**.

On the contrary, the protonation of molecule **1** would be accompanied by an H···H repulsion within the conjugated acid, a condition which furthers reduces the basicity of this molecule,



A similar situation arises for **1'**. We observe, thus, the following order of basicity,



This discussion suggests the importance of JSIH in the relative basicites of **1**, **1'** and **5**.

In conclusion, the JSIH could be exploited in the explanation of the apparently surprising relative basicities of **1**, **1'** and **5**. Although the paper is mainly concerned with intermolecular Jorgensen secondary interactions, this model might provide valuable insights to rationalise the proton affinity of these molecules.

2.7.1 Relative basicity of pyridine and 1,8-naphthyridine in different solvents

An important issue to reckon with in the analysis of the apparently surprising relative basicities of **1**, **1'** and **5** is the solvent in which they are measured. For this purpose, we considered (i) the pyridine ring in compounds **1** and **1'** and (ii) the naphthyridine moiety in system **5**. First, we point out that in water, a solvent with a dielectric constant value of ε = 80.1, pyridine (pK_a = 5.2) is considerably more basic than 1,8-naphthyridine (pK_a = 3.4). This result is consistent with the M06-2X/6-311++G(2d,2p) calculations (considering water as solvent via the SMD method) presented in Figure S10 for which the respective values of |E(B)| for C_6H_5N and $C_8H_6N_2$ are 23.2 and 21.2 kcal/mol respectively. Furthermore, Table 1 in Ref. 16 suggest that pyridine is more basic than 1,8-naphthyridine in acetonitrile (ε = 37.5). This chart reports the pK_a values in MeCN of pyridine and **5** which comprises the 1,8-naphthyridine fragment. The difference in basicities is, however, considerably smaller than it is in H_2O as reflected by the pK_a values under consideration (12.5 and 12.2 for pyridine and **5** respectively). These results indicate that the relative basicities of C_6H_5N and $C_8H_6N_2$ are strongly dependent upon the surrounding medium. Indeed, the relative acid/base properties of two compounds can change very noticeably as a function of the solvent.[17] A well-known example is the relative basicity of secondary and tertiary amines. The former are more basic in water and polar solvents whereas the relative basicities are inverted in CCl_4.[18] Hereof, the gas proton affinities and basicities *"calculated as protonation enthalpies and free-energies, respectively, employing the M06-2X/6-311++G(2df,2pd)//M06-2X/6-31+G(d,p) level of theory*" (Ref. 19) indicate that 1,8-naphthyridine is more basic than pyridine in vacuum (ε = 1). In other words, the relative basicity of pyridine and 1,8-naphthyridine is reversed when we move from gas phase to acetonitrile as solvent and even more conspicuously when we consider water as the surrounding environment. Indeed, our

calculations show the following trend in the values of |*E*(B)| for vacuum, $CHCl_3$, MeCN and H_2O as presented in Figure S12.

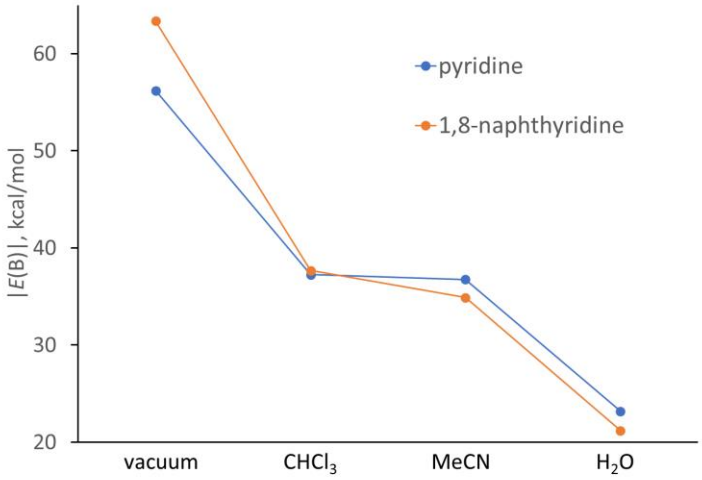


Fig. S12 Values of |*E*(B)| for pyridine and 1,8-naphthyridine in different environments, vacuum, $CHCl_3$, MeCN and H_2O.

In virtue of (i) the agreement of our calculations with the experimental trends of basicity for pyridine and 1,8-naphthyridine in water and acetonitrile, and (ii) the low dielectric constant of $CHCl_3$ (ε = 4.81), we expect that the relative order of the basicities of pyridine and 1,8-naphthyridine to be the same than that observed in vacuum as reflected in the above graph and in consistence with the relative stabilities of the triply hydrogen-bonded adducts presented in Figure 5.

2.8 XYZ coordinates

2.8.1 Amide-imide heterodimers

XYZ coordinates of the monomers of the addressed amides and imides as well as the corresponding protonated and deprotonated species are reported in Ref. 3.

A1-I2 heterodimer

O	2.01931700	1.37153000	-0.07353700
N	2.86008100	-0.75611500	-0.06604200
C	2.95797600	0.57989000	-0.00564400
C	4.14294600	-1.44494100	-0.07559200
C	5.09244300	-0.38301000	0.50240800
C	4.42234900	0.94403000	0.13469300
H	1.96744200	-1.19573200	-0.26776800
H	4.10407200	-2.34766000	0.52966100
H	4.42061300	-1.72187200	-1.09479400
H	5.13252900	-0.48747600	1.58585500
H	6.10094800	-0.48152900	0.11063300
H	4.55159200	1.73560500	0.86807900
H	4.75708300	1.32161800	-0.83394200
C	-1.69850300	1.49028700	-0.23337200
C	-0.89942900	-0.82488100	-0.45717300
C	-2.32034100	-1.31671200	-0.53236600
C	-3.32063800	-0.41691500	0.19765900
C	-3.12283600	1.00662000	-0.32998500
H	-2.57415500	-1.36676700	-1.59641800
H	-2.33264900	-2.33452700	-0.14474800
H	-3.39436400	1.04920400	-1.38992700
H	-3.74682700	1.72606100	0.19844400
H	0.27094600	0.85749900	-0.27407200
N	-0.70423200	0.52922400	-0.34237900
O	0.05463400	-1.58210900	-0.51402500
O	-1.39966100	2.65417800	-0.09064000
C	-3.07513400	-0.46311300	1.70832000
H	-3.78403900	0.18327100	2.22764300
H	-3.20441800	-1.47919300	2.08377800
H	-2.06795700	-0.13391700	1.97236000
C	-4.74179900	-0.88395800	-0.10286500
H	-4.89356900	-1.90420000	0.25384900
H	-5.46995700	-0.24096100	0.39430900
H	-4.94476400	-0.86376300	-1.17487800

A1-I3 heterodimer

C	-1.25379100	-1.68092900	-0.98380900

H	-1.64911900	-2.67320300	-1.20098900
C	-1.97678100	-1.14299800	0.26695200
H	-1.35718400	-1.11251000	1.15678700
C	-2.47456500	0.23109300	-0.18949500
H	-1.70495200	0.96176600	0.02521100
C	-2.64394600	0.03344600	-1.69075300
H	-3.58893500	-0.48628800	-1.88655200
C	-2.62182500	1.28967200	-2.52838500
H	-2.53127200	1.02499700	-3.57955900
H	-3.54160800	1.84838500	-2.36932500
O	-1.48797700	2.10055100	-2.22395200
C	-1.65524800	3.06059100	-1.29456500
C	-0.35956600	3.72973800	-0.96724400
H	-0.54715400	4.61802000	-0.37304700
H	0.18247400	3.97762900	-1.87750600
H	0.24835400	3.02498300	-0.39657000
O	-2.71998200	3.30683600	-0.78748600
O	-1.54234000	-0.79776700	-2.04616200
O	-3.09023800	-2.02065000	0.46261800
C	-3.68112400	-2.00482400	1.67664300
O	-3.26190600	-1.36573200	2.60295300
C	-4.89661800	-2.87729800	1.69146000
H	-4.64605200	-3.87170700	1.32558600
H	-5.64273200	-2.45231700	1.01934700
H	-5.29360200	-2.93303100	2.69950200
O	-3.70627900	0.61252200	0.38744700
C	-3.62932500	1.37990100	1.50432300
O	-2.59127400	1.69381800	2.01323700
C	-4.99636600	1.75017100	1.98351800
H	-4.91774200	2.36668000	2.87255700
H	-5.55760300	0.84263200	2.20650200
H	-5.52181200	2.28833800	1.19513700
N	0.18570900	-1.84671400	-0.87274400
C	0.96239900	-0.76872500	-0.45586800
N	2.31565300	-0.99031500	-0.45546600
H	2.90149300	-0.19261100	-0.14772400
C	2.96405800	-2.15415800	-0.82326100
C	2.09464300	-3.22153600	-1.26536000
H	2.52940200	-4.15494700	-1.58093300
C	0.76872700	-3.02209700	-1.27784000
H	0.07662000	-3.78448800	-1.60604700
O	0.46948500	0.28263000	-0.10869900
O	4.18551000	-2.22979100	-0.76448600
C	7.20276200	-0.03585400	0.89812400
C	5.10874300	0.99393500	0.66057400
C	6.04795300	2.06559600	1.17354600
C	7.24314700	1.27097600	1.70626900
H	6.31644400	2.69331000	0.32079900

H	5.55224600	2.69132600	1.91090700
H	8.19158000	1.78919000	1.59618800
H	7.09323300	1.04667200	2.76153000
H	5.37058300	-0.96565400	0.11775400
N	5.78899900	-0.15634300	0.56868100
O	3.92527900	1.15381900	0.35921200
H	7.80260800	0.03176500	-0.01186100
H	7.54030800	-0.89540100	1.47258100

A2-I1 heterodimer

O	0.28574100	-0.91618700	0.77944500
N	0.52487800	1.23739300	0.04877200
C	0.99237600	0.02841200	0.48720900
C	1.52996900	2.14853700	-0.21185000
C	2.85693300	1.47762900	0.07148400
C	2.51585900	0.05666700	0.55314600
H	-0.48497400	1.42452900	-0.07245100
H	3.44443700	1.48775600	-0.84631900
H	3.39436100	2.06590100	0.81447500
O	1.34976600	3.27552100	-0.60142100
C	3.04662400	-1.03731900	-0.38813400
H	2.58865300	-1.98773900	-0.10402800
H	2.70670800	-0.81274300	-1.40455300
C	4.56522600	-1.18584900	-0.38891100
H	5.03520700	-0.21215300	-0.55174200
H	4.90073600	-1.53600800	0.58859200
C	5.03013600	-2.16463800	-1.46162100
H	6.11273100	-2.28983700	-1.44437600
H	4.57755300	-3.14667700	-1.31305300
H	4.74776200	-1.81664500	-2.45645800
C	2.93185000	-0.18182800	2.00684400
H	2.65040000	-1.18520800	2.32640200
H	4.00969000	-0.06852100	2.11562800
H	2.44979000	0.53916400	2.66898200
C	-3.04119600	0.57041200	-0.17928600
C	-3.49881700	-1.82084300	0.40032700
C	-4.80525000	-1.68438700	-0.36013900
C	-5.42616900	-0.32507400	-0.06584800
C	-4.49047100	0.77630800	-0.55284300
H	-4.61808800	-1.77813100	-1.43269800
H	-5.46897300	-2.49676000	-0.06662900
H	-1.66563400	-0.73824100	0.45655000
N	-2.64796200	-0.64811400	0.20831000
O	-2.24130200	1.51241800	-0.26653100
H	-4.77728100	1.75937400	-0.18292100
H	-4.50923000	0.83464800	-1.64455200

H	-6.39741200	-0.22397700	-0.54881000
H	-5.58765300	-0.22583300	1.01049200
H	-3.70222800	-1.94529500	1.46691000
H	-2.94102200	-2.69472000	0.06676400

A2-I3 heterodimer

C	-1.57685100	-1.70788300	-0.92264600
H	-2.01696500	-2.68244000	-1.13206900
C	-2.30167700	-1.11202500	0.30021600
H	-1.69999200	-1.08797900	1.20197700
C	-2.72974200	0.27264800	-0.19657400
H	-1.93569700	0.97575700	0.02146300
C	-2.87269400	0.04932600	-1.69698600
H	-3.83242600	-0.43769200	-1.90378000
C	-2.77951000	1.28470200	-2.56056400
H	-2.67959400	0.99299500	-3.60356200
H	-3.67577100	1.88745800	-2.43366000
O	-1.61654300	2.04954200	-2.24793700
C	-1.76087700	3.04860000	-1.35620800
C	-0.44063000	3.66053700	-1.01464400
H	-0.59328800	4.55042300	-0.41337600
H	0.11249900	3.89585200	-1.92197600
H	0.13773700	2.92594000	-0.45158800
O	-2.82565900	3.36892900	-0.89283900
O	-1.79627800	-0.83073200	-2.00699200
O	-3.45750900	-1.93474900	0.49031000
C	-4.08451300	-1.84354400	1.68235900
O	-3.66248100	-1.19007900	2.59766400
C	-5.34460000	-2.65022200	1.68924100
H	-5.14149200	-3.66562700	1.35337800
H	-6.05087200	-2.20148200	0.98998700
H	-5.76679700	-2.65747400	2.68849700
O	-3.95817500	0.71420500	0.34323500
C	-3.87696800	1.50281800	1.44510500
O	-2.83811000	1.80126000	1.96175300
C	-5.23965500	1.92400800	1.89345200
H	-5.15778600	2.52455600	2.79295900
H	-5.84824400	1.04068100	2.08517700
H	-5.71672900	2.49835000	1.09967000
N	-0.14986300	-1.94036800	-0.77880200
C	0.66675000	-0.89554900	-0.35186100
N	2.00942800	-1.17017100	-0.34471000
H	2.63140700	-0.39994800	-0.03291400
C	2.61394200	-2.35301100	-0.72458500
C	1.70622000	-3.38607300	-1.17106600
H	2.10587000	-4.33391300	-1.48981100

C	0.38911700	-3.13556600	-1.18789000
H	-0.32978300	-3.86848200	-1.52478400
O	0.21214600	0.17260300	-0.00333200
O	3.83256800	-2.47034300	-0.67264500
H	5.04608900	-1.08818500	-0.03699900
C	7.05999900	-0.52104200	0.38821900
C	4.94865300	0.80524100	0.59015700
C	7.71843600	0.52098300	1.27450300
C	5.72177900	1.99609900	1.10616400
C	7.22742000	1.90808400	0.88018500
H	8.79972300	0.43796700	1.17170500
H	7.46702100	0.32630600	2.31996700
H	5.28322700	2.88144800	0.64884800
H	5.50086100	2.05296100	2.17539400
H	7.73334600	2.68219300	1.45566700
H	7.45514500	2.08601000	-0.17372400
N	5.61417300	-0.32226700	0.31963700
O	3.71888700	0.87909600	0.45505900
H	7.24019100	-1.52588700	0.76719000
H	7.47779100	-0.46679000	-0.62017400

A3-I1 heterodimer

O	0.10903200	-0.97697000	0.42164100
N	0.35089300	1.24904100	-0.04049900
C	0.81418900	0.00585400	0.28280900
C	1.35804300	2.18870300	-0.17117200
C	2.68139500	1.48311300	0.03410300
C	2.32541500	0.05257500	0.47438600
H	-0.65694300	1.44094300	-0.15923300
H	3.21568800	1.50437500	-0.91685000
H	3.27521000	2.03263600	0.76218600
O	1.17823800	3.35383700	-0.42071500
C	2.97512800	-1.03624600	-0.38921900
H	2.51778200	-1.99569300	-0.13679600
H	2.73431500	-0.83686900	-1.43818600
C	4.48970800	-1.13515100	-0.23304000
H	4.94325200	-0.15151100	-0.38426300
H	4.73538600	-1.43916000	0.78585400
C	5.09168500	-2.13307800	-1.21605600
H	6.17128600	-2.21347200	-1.08945800
H	4.66254900	-3.12630700	-1.07222900
H	4.89540600	-1.83344500	-2.24680600
C	2.59270800	-0.16040200	1.96969400
H	2.29436500	-1.16373000	2.27364300
H	3.65196100	-0.02872300	2.18483700
H	2.03626200	0.56259300	2.56874300

C	-3.22422900	0.51997900	-0.19734100
C	-3.55138900	-1.84694000	0.18793200
C	-4.89727300	-1.75247100	0.03947100
C	-5.44337600	-0.47421100	-0.23750200
C	-4.64755400	0.62383200	-0.35333000
H	-1.75072100	-0.84883500	0.19172600
N	-2.76303400	-0.74982700	0.07272900
O	-2.42613500	1.46753600	-0.28843900
H	-5.04759600	1.60438700	-0.56433500
H	-6.51390600	-0.37085100	-0.36002400
H	-5.51973100	-2.62768900	0.13034600
H	-3.03536700	-2.77169800	0.40093600

A3-I2 heterodimer

C	-1.91477100	1.49768600	-0.23735100
C	-1.03388400	-0.78995700	-0.40003600
C	-2.43318100	-1.33371800	-0.50114500
C	-3.48485700	-0.45513500	0.18144300
C	-3.31883400	0.96502300	-0.36541300
H	-2.65436300	-1.41425000	-1.57057200
H	-2.42074400	-2.34333600	-0.09261200
H	-3.55983800	0.98042900	-1.43340300
H	-3.98188200	1.67191700	0.13150400
H	0.07942200	0.92660700	-0.23105100
N	-0.88562600	0.56801900	-0.30602300
O	-0.05269100	-1.51830300	-0.41999400
O	-1.65610600	2.67161600	-0.10473100
C	-3.28597400	-0.46678100	1.69949200
H	-4.03519500	0.16099400	2.18379400
H	-3.38940500	-1.48042500	2.08917500
H	-2.30129100	-0.09460200	1.98950300
C	-4.87998600	-0.97488600	-0.15282900
H	-5.00833400	-1.99382200	0.21647100
H	-5.64279900	-0.34897400	0.31323600
C	3.71279500	-1.54857400	-0.04439400
C	4.98530900	-1.11464200	0.14363700
C	5.19564800	0.28202600	0.26736000
C	4.15916400	1.16153200	0.20102300
C	2.81356800	0.69875100	0.00341300
N	2.68412200	-0.66874000	-0.11049700
H	6.20074900	0.65474300	0.41700600
H	3.44532800	-2.58986100	-0.14963700
H	5.80010600	-1.81832100	0.19569500
H	4.30336000	2.22768700	0.29354400
H	1.72995800	-1.01338600	-0.24735800
O	1.80986300	1.42533600	-0.06660800

H	-5.05307100	-0.97749600	-1.23017500

A3-I3 heterodimer

C	1.38203800	-1.65941700	0.97386300
H	1.79647300	-2.62892500	1.25109200
C	2.17097200	-1.13236600	-0.24151800
H	1.60529600	-1.12425000	-1.16643000
C	2.61804400	0.25816800	0.22022400
H	1.85111600	0.97219900	-0.05597600
C	2.68944100	0.09034300	1.73295500
H	3.61683500	-0.42941400	2.00064200
C	2.61279100	1.35935600	2.54802900
H	2.43172500	1.11030800	3.59137300
H	3.54883300	1.90622500	2.45950500
O	1.51835400	2.17981800	2.14102300
C	1.77724500	3.12830500	1.21990800
C	0.52652400	3.82887900	0.79672000
H	0.77938300	4.69749400	0.19767900
H	-0.06118700	4.11470000	1.66688100
H	-0.06983100	3.13334400	0.20348000
O	2.88220000	3.34543900	0.79270600
O	1.56288900	-0.73275500	2.02344600
O	3.30629000	-1.99551300	-0.35655500
C	3.96527200	-1.99474200	-1.53470300
O	3.59611900	-1.37399100	-2.49441900
C	5.18474300	-2.85903500	-1.46565900
H	4.92074100	-3.84618300	-1.08977800
H	5.89320700	-2.41382700	-0.76637000
H	5.63390600	-2.93565700	-2.45023600
O	3.87793600	0.64467000	-0.28687200
C	3.86323200	1.40079500	-1.41378500
O	2.85516200	1.71084800	-1.98221600
C	5.25482600	1.76449000	-1.82183400
H	5.22443400	2.38153300	-2.71354000
H	5.82074800	0.85346400	-2.01761300
H	5.74375600	2.29867000	-1.00783000
N	-0.04002000	-1.87868600	0.77496100
C	-0.81567200	-0.84509000	0.25450700
N	-2.16314700	-1.09714400	0.20422800
H	-2.75740900	-0.33541200	-0.17551800
C	-2.80322000	-2.24515700	0.62187600
C	-1.93856200	-3.26900200	1.16005000
H	-2.37039500	-4.19097200	1.51111000
C	-0.61827200	-3.04015200	1.22205500
H	0.07206700	-3.76604400	1.62756800
O	-0.32578200	0.19278000	-0.13315000

O	-4.02382800	-2.34510100	0.52752300
H	-5.16721800	-1.02879600	-0.05328900
C	-7.10174000	-0.36746200	-0.33699300
C	-5.07806200	0.88409600	-0.76776700
C	-7.89883500	0.65849800	-0.73133100
C	-5.91585200	1.97224300	-1.18458800
C	-7.27183700	1.85378500	-1.16350600
N	-5.75244900	-0.24463500	-0.36069200
O	-3.83513800	0.90561600	-0.75433800
H	-5.42160700	2.87540600	-1.51011700
H	-7.88394600	2.68819500	-1.48087200
H	-8.97152600	0.55544200	-0.71111200
H	-7.47816100	-1.31795900	0.01167500

2.8.2 AAA-DDD, AAD-DDA and ADA-DAD adducts

XYZ coordinates of the monomers of **7** and **11** and their corresponding protonated and deprotonated species are reported in Ref. 3.

1

C	-3.48830900	0.24730700	-0.00005500
C	-1.20143500	0.42971000	-0.00030400
C	-1.23670200	1.83222900	0.00002200
C	-2.49663300	2.42882700	0.00031300
C	-3.62751800	1.64784600	0.00030200
C	0.00000100	2.62285100	0.00015000
C	1.23670000	1.83222200	-0.00000600
C	1.20142500	0.42970400	-0.00039800
C	3.48829800	0.24729000	-0.00012100
C	3.62751500	1.64782800	0.00024600
C	2.49663400	2.42881400	0.00025400
H	-0.00000900	-1.23705100	-0.00086000
H	-2.55991000	3.50871600	0.00056100
H	-4.59980300	2.11150100	0.00057500
H	4.59980500	2.11147500	0.00056800
H	2.55991600	3.50870300	0.00055500
O	0.00000400	3.84627600	-0.00013400
N	2.29237200	-0.33560000	-0.00041800
N	-0.00000700	-0.22594300	-0.00067800
N	-2.29238500	-0.33558800	-0.00033800
C	-4.66783700	-0.66160300	-0.00001500
C	-4.47751100	-2.04628000	0.00004600
C	-5.97505600	-0.16864100	0.00000100
C	-5.56095000	-2.91100800	0.00011900

H	-3.47152400	-2.43782100	0.00001000
C	-7.05875800	-1.03515900	0.00010300
H	-6.16581300	0.89388900	-0.00003400
C	-6.85692500	-2.40907800	0.00016300
H	-5.39273200	-3.97932400	0.00016900
H	-8.06294800	-0.63398600	0.00013700
H	-7.70282400	-3.08298600	0.00024900
C	4.66783100	-0.66161300	-0.00002900
C	4.47752400	-2.04629300	0.00013100
C	5.97504200	-0.16863200	-0.00005900
C	5.56097600	-2.91100500	0.00027300
H	3.47154400	-2.43784900	0.00015900
C	7.05875600	-1.03513400	0.00005000
H	6.16577900	0.89390200	-0.00021200
C	6.85694300	-2.40905600	0.00022700
H	5.39277300	-3.97932300	0.00042400
H	8.06294000	-0.63394600	0.00000700
H	7.70285200	-3.08295100	0.00033100

1 (protonated)

C	-3.48762400	0.24985700	0.00195600
C	-1.20096500	0.43619100	-0.00218000
C	-1.23636600	1.83770600	-0.00060000
C	-2.49889700	2.43397500	0.00339300
C	-3.62752300	1.65337600	0.00495400
C	-0.00000400	2.62334400	-0.00117700
C	1.23635700	1.83770300	-0.00078400
C	1.20095700	0.43618600	-0.00046100
C	3.48762600	0.24986600	0.00242200
C	3.62752000	1.65339000	0.00142500
C	2.49888800	2.43397900	0.00026600
H	-0.00001500	-1.23188100	-0.00420200
H	-2.55950900	3.51377800	0.00416000
H	-4.60103200	2.11300500	0.00700200
H	4.60102300	2.11303100	0.00241400
H	2.55949300	3.51378300	-0.00037400
O	0.00000100	3.84787800	0.00070600
N	2.29331100	-0.33119000	-0.00037400
N	-0.00000300	-0.21899800	-0.00279400
N	-2.29331700	-0.33118600	-0.00428700
C	-4.66661400	-0.66099300	0.00124800
C	-4.46932700	-2.04484200	0.00890900
C	-5.97658100	-0.17467900	-0.00746000
C	-5.54784200	-2.91522000	0.00741000
H	-3.46174400	-2.43142200	0.01501900
C	-7.05526200	-1.04719900	-0.00811000

H	-6.17291300	0.88631800	-0.01357000
C	-6.84600000	-2.41986500	-0.00077300
H	-5.37458600	-3.98247400	0.01290500
H	-8.06147200	-0.65194600	-0.01483400
H	-7.68829200	-3.09789500	-0.00191600
C	4.66662200	-0.66099200	0.00117600
C	4.50414336	-1.99926910	-0.36846813
C	5.94277858	-0.21895572	0.35981879
C	5.58345531	-2.86860178	-0.37832815
H	3.52276510	-2.35153759	-0.64687019
C	7.02247943	-1.09014011	0.34853830
H	6.11172728	0.80618623	0.65108501
C	6.84785609	-2.41744986	-0.01998915
H	5.43728729	-3.90038935	-0.66665257
H	8.00227997	-0.72947355	0.62896621
H	7.69073778	-3.09470764	-0.02730052
H	2.21359966	-1.32800596	-0.00238274

1 (deprotonated)

C	-3.46790400	0.23953300	-0.00000500
C	-1.14586800	0.38380700	0.00000700
C	-1.21638800	1.80630400	0.00005900
C	-2.47482500	2.41283300	0.00008500
C	-3.61194300	1.64754900	0.00005700
C	0.00000000	2.60193600	0.00009500
C	1.21638800	1.80630400	0.00006200
C	1.14586800	0.38380700	0.00000300
C	3.46790400	0.23953200	0.00000900
C	3.61194200	1.64754800	0.00007500
C	2.47482500	2.41283200	0.00009800
H	-2.52492600	3.49425400	0.00013300
H	-4.58276800	2.11493200	0.00009300
H	4.58276800	2.11493100	0.00011900
H	2.52492600	3.49425400	0.00015100
O	0.00000000	3.84250200	0.00012200
N	2.29278800	-0.35511600	-0.00002200
N	0.00000000	-0.31506300	-0.00002400
N	-2.29278800	-0.35511600	-0.00002700
C	-4.66480400	-0.65899400	-0.00003500
C	-4.49052200	-2.04584700	0.00005800
C	-5.96809700	-0.15676100	-0.00015200
C	-5.58245600	-2.90059700	0.00004700
H	-3.48546200	-2.44077700	0.00013600
C	-7.06190500	-1.01258100	-0.00016700
H	-6.14850000	0.90771400	-0.00023900
C	-6.87495600	-2.38823000	-0.00006400

H	-5.42327800	-3.97064100	0.00012400
H	-8.06211800	-0.60055600	-0.00026300
H	-7.72728700	-3.05431000	-0.00007200
C	4.66480400	-0.65899400	-0.00002600
C	4.49052200	-2.04584700	0.00007500
C	5.96809700	-0.15676000	-0.00015700
C	5.58245700	-2.90059700	0.00006000
H	3.48546200	-2.44077800	0.00016200
C	7.06190500	-1.01258000	-0.00017700
H	6.14849800	0.90771400	-0.00025300
C	6.87495700	-2.38822900	-0.00006400
H	5.42327900	-3.97064100	0.00014400
H	8.06211800	-0.60055500	-0.00028500
H	7.72728800	-3.05430800	-0.00007600

1’

C	3.44978600	0.37936900	-0.03616300
C	1.20769300	0.66048300	0.34816000
C	1.24401800	2.02814900	0.03646400
C	2.46281800	2.53351300	-0.36793800
C	3.58415500	1.71257500	-0.40915500
C	0.00000200	2.86069700	0.20313400
C	-1.24401700	2.02815300	0.03647400
C	-1.20769100	0.66048300	0.34815500
C	-3.44979500	0.37938100	-0.03612700
C	-3.58415900	1.71258600	-0.40912800
C	-2.46281900	2.53352100	-0.36791700
H	-0.00000100	-0.92584800	0.80502000
H	2.54206300	3.57667900	-0.64885100
H	4.53465000	2.10046200	-0.74199500
H	-4.53465000	2.10047700	-0.74197200
H	-2.54206300	3.57668700	-0.64883100
N	-2.26548200	-0.13642900	0.31988600
N	0.00000000	0.08061300	0.71081000
N	2.26547900	-0.13643500	0.31987800
C	4.60822200	-0.55174300	-0.04073700
C	4.40739100	-1.92092000	-0.22290400
C	5.91062700	-0.08124700	0.13537200
C	5.48396100	-2.79587900	-0.24031400
H	3.40126600	-2.29231100	-0.35628200
C	6.98665200	-0.95776900	0.12323800
H	6.08695600	0.97221900	0.30510600
C	6.77784800	-2.31787700	-0.06793900
H	5.31225200	-3.85332500	-0.39023500
H	7.98848300	-0.57723600	0.26976700
H	7.61663900	-3.00051900	-0.07824100

C	-4.60822600	-0.55173800	-0.04072200
C	-4.40738500	-1.92091100	-0.22290900
C	-5.91063700	-0.08125600	0.13538700
C	-5.48394800	-2.79587700	-0.24034100
H	-3.40125600	-2.29229300	-0.35628000
C	-6.98665500	-0.95778500	0.12323200
H	-6.08697600	0.97220300	0.30515700
C	-6.77784000	-2.31788800	-0.06797000
H	-5.31223100	-3.85331800	-0.39029100
H	-7.98849000	-0.57726000	0.26975500
H	-7.61662600	-3.00053800	-0.07828200
H	0.00000800	3.29926600	1.20767300
H	0.00000100	3.69229900	-0.50134400

1’ (protonated)

C	-3.49312800	0.36230700	-0.04003600
C	-1.25236000	0.63105900	0.30406000
C	-1.28366700	2.01120600	0.11838700
C	-2.51847600	2.54667300	-0.20420100
C	-3.63343000	1.72674900	-0.28818000
C	-0.03902300	2.83705600	0.31172900
C	1.21284300	2.01759900	0.13963700
C	1.14692000	0.62813700	0.33081000
C	3.50862600	0.41798400	0.00004200
C	3.60106300	1.76882700	-0.21454900
C	2.44473800	2.55534800	-0.15004600
H	-2.60914100	3.60963700	-0.38944700
H	-4.59247200	2.14038700	-0.55914900
H	4.56586200	2.21442900	-0.39963400
H	2.52295900	3.62306800	-0.31205100
N	2.27477000	-0.10271800	0.25556200
N	-0.02264400	-0.00144400	0.56974600
N	-2.29560700	-0.17141900	0.23658300
C	-4.64744300	-0.56928100	-0.09317700
C	-4.44343700	-1.92468900	-0.35761800
C	-5.94917100	-0.11240300	0.11931100
C	-5.51750100	-2.80002000	-0.41896200
H	-3.43838700	-2.28636700	-0.52137700
C	-7.02236300	-0.99019400	0.06233600
H	-6.12983700	0.92831600	0.35135100
C	-6.81085500	-2.33587600	-0.21003700
H	-5.34487300	-3.84630200	-0.63192400
H	-8.02423500	-0.62221100	0.23649400
H	-7.64781600	-3.01921900	-0.25532400
C	4.64781100	-0.51449100	-0.03559400
C	4.73553600	-1.57478200	0.86796900

C	5.65610700	-0.32700100	-0.98218500
C	5.82053400	-2.43747200	0.82194800
H	3.97880000	-1.70872300	1.63140500
C	6.73547000	-1.19527100	-1.02591300
H	5.58169000	0.48186800	-1.69680400
C	6.81950000	-2.25056700	-0.12536800
H	5.89057400	-3.24899100	1.53271400
H	7.50804100	-1.05209800	-1.76845200
H	7.66376700	-2.92513200	-0.16010100
H	-0.02850200	3.67820100	-0.38032600
H	-0.04214000	3.25956100	1.32159600
H	-0.05248200	-1.01126200	0.63627700
H	2.19278700	-1.11149000	0.34934600

1’ (deprotonated)

C	-3.49474500	0.39907400	-0.00000200
C	-1.16317900	0.56148700	-0.00036100
C	-1.25181900	1.98656400	-0.00007100
C	-2.49893300	2.56246900	0.00024300
C	-3.65474200	1.78080500	0.00028200
C	0.00000000	2.82831500	-0.00017300
C	1.25181900	1.98656400	-0.00005600
C	1.16318100	0.56148800	-0.00034300
C	3.49474600	0.39907600	0.00000400
C	3.65474300	1.78080700	0.00031200
C	2.49893300	2.56247000	0.00027300
H	-2.58349800	3.64455700	0.00046600
H	-4.62593700	2.24807800	0.00055700
H	4.62593700	2.24808100	0.00060300
H	2.58349800	3.64455800	0.00050500
N	2.29387700	-0.18169500	-0.00029200
N	0.00000100	-0.12675800	-0.00065800
N	-2.29387600	-0.18169600	-0.00029800
C	-4.67034200	-0.52784300	0.00003200
C	-4.46721100	-1.91048300	-0.00003400
C	-5.98671400	-0.05817500	0.00013300
C	-5.54002900	-2.79090200	0.00002100
H	-3.45341600	-2.28189600	-0.00013200
C	-7.06058200	-0.93793200	0.00018500
H	-6.18920600	1.00285000	0.00016300
C	-6.84385100	-2.31035900	0.00013400
H	-5.35538700	-3.85706200	-0.00002500
H	-8.06990500	-0.54811100	0.00026200
H	-7.68092000	-2.99550400	0.00017800
C	4.67034300	-0.52784200	0.00003400
C	4.46721000	-1.91048200	-0.00002300

C	5.98671500	-0.05817600	0.00012100
C	5.54002600	-2.79090200	0.00003000
H	3.45341300	-2.28189300	-0.00011500
C	7.06058200	-0.93793500	0.00017000
H	6.18920900	1.00284800	0.00014000
C	6.84384900	-2.31036200	0.00013100
H	5.35538200	-3.85706200	-0.00000800
H	8.06990500	-0.54811500	0.00023600
H	7.68091600	-2.99550800	0.00017400
H	0.00000400	3.48933800	-0.87298700
H	-0.00000400	3.48954500	0.87247900

2

C	-0.43280000	-0.88616700	-1.11929200
C	0.14860700	0.04639600	-0.08355800
C	-0.24399400	1.48203700	-0.47769000
C	0.16043900	1.71518600	-1.91151500
C	-0.47037500	-0.42617200	-2.43664800
H	-0.30389800	-0.15943200	0.87916800
N	0.02055800	0.80851500	-2.82620700
N	0.66587000	2.91079000	-2.21984700
N	-0.93315500	-1.16006700	-3.45330800
H	-0.94194300	-0.75692200	-4.37455900
H	0.69112700	3.65000900	-1.53875500
H	-1.28866400	-2.08502700	-3.25795500
H	0.85350900	3.13437500	-3.18515800
C	-1.75443900	1.74657800	-0.32985200
C	-0.83910300	-2.21965900	-0.77765600
O	-2.35266300	2.34353300	-1.19074000
O	-1.30757600	-3.02363900	-1.59810900
C	-0.67210800	-2.66290900	0.66938700
H	0.35589100	-2.45603300	0.98547400
H	-1.30636700	-2.02991600	1.29972600
C	-1.00741900	-4.12743600	0.90568500
H	-0.37945700	-4.74854000	0.26511900
H	-2.03642100	-4.31562300	0.59794600
C	-0.81545600	-4.51872200	2.36621000
H	-1.05503200	-5.56935700	2.53066900
H	0.21699800	-4.35786900	2.68244800
H	-1.45723300	-3.92318900	3.01839600
C	-2.41579500	1.28463900	0.94352600
H	-2.46597600	0.19052900	0.90361000
H	-1.75618800	1.52285100	1.78366200
C	-3.80702800	1.86661700	1.14442100
H	-4.43157700	1.60030100	0.29147500
H	-3.74243400	2.95606000	1.15248100

C	-4.44213600	1.36878400	2.43699400
H	-3.83736100	1.64248800	3.30331700
H	-5.43609000	1.79399400	2.57516300
H	-4.54140600	0.28194000	2.42996600
C	1.66883100	-0.06978300	0.09950700
C	2.42799500	-0.85216800	-0.76791700
C	2.39681600	0.61524700	1.08036800
C	3.80869600	-0.95476900	-0.65643000
H	1.91736500	-1.39597400	-1.54948600
C	3.77661100	0.54842800	1.19939600
C	4.49057500	-0.25516900	0.32781000
H	4.35142700	-1.58327300	-1.34909300
H	4.27002300	1.10820100	1.98009400
H	5.56436900	-0.33174600	0.42048400
N	1.72747000	1.46448100	2.07915500
O	2.29571400	2.47921200	2.42912600
O	0.65002900	1.10575300	2.51687500
H	0.24260800	2.22149800	0.16356500

2 (protonated)

C	-0.46203500	0.79362100	1.13566600
C	0.19159900	-0.05943200	0.07203900
C	-0.16494300	-1.53256800	0.35768700
C	0.20714700	-1.88783300	1.75916200
C	-0.53479400	0.30710500	2.41252600
H	-0.26091300	0.18073200	-0.88308500
N	-0.00999900	-0.97497600	2.69494300
N	0.68147000	-3.06417000	2.05147300
N	-1.00499800	0.93954500	3.49417000
H	0.81882900	-3.74773600	1.31985900
H	-1.43189500	1.84293400	3.33025600
C	-1.68744000	-1.80204000	0.20711800
C	-0.95707700	2.13309900	0.83637600
O	-2.27256900	-2.39516200	1.07682400
O	-1.45512100	2.84980200	1.70082900
C	-0.82822200	2.63315600	-0.58641700
H	0.21079800	2.50323600	-0.90731800
H	-1.42060100	1.97613300	-1.23359200
C	-1.26369200	4.07931200	-0.76181000
H	-0.66257200	4.71522800	-0.11021500
H	-2.29590000	4.18729400	-0.42780800
C	-1.12918800	4.53468200	-2.20969100
H	-1.44353300	5.57148200	-2.32583900
H	-0.09593500	4.45828500	-2.55254400
H	-1.74541000	3.92284600	-2.87098200
C	-2.33846300	-1.32386000	-1.05944000

H	-2.39432000	-0.23009500	-0.99907000
H	-1.67132200	-1.54428400	-1.89836600
C	-3.72710700	-1.90955900	-1.27341400
H	-4.35533800	-1.65806400	-0.41886200
H	-3.65630700	-2.99802400	-1.29899500
C	-4.35731400	-1.39245300	-2.56037100
H	-3.74993300	-1.65284300	-3.42859800
H	-5.34945500	-1.81830800	-2.70612200
H	-4.45973600	-0.30630400	-2.53682700
C	1.70363100	0.15553600	-0.07448400
C	2.39046200	0.95305000	0.83736800
C	2.48885200	-0.42748300	-1.07875300
C	3.76091600	1.16710700	0.74779400
H	1.83813200	1.43196100	1.63262500
C	3.85896400	-0.24351800	-1.17660000
C	4.50167600	0.57073500	-0.25974600
H	4.24497500	1.80721200	1.47235000
H	4.40022600	-0.72430500	-1.97773000
H	5.56613900	0.73710300	-0.33869000
N	1.89837000	-1.28142200	-2.12256600
O	2.57743400	-2.18350400	-2.56409500
O	0.76577000	-1.03618200	-2.49841600
H	0.33465500	-2.21930700	-0.32702300
H	-1.25670800	0.41419100	4.31709400
H	0.87700600	-3.34583300	3.00425700
H	0.16326900	-1.20793900	3.66789900

2 (deprotonated H1)

C	-0.48261600	0.75852300	1.23837100
C	0.14302800	-0.03159100	0.11605600
C	-0.09817700	-1.52652300	0.38366300
C	0.37838800	-1.84090800	1.78265700
C	-0.40530900	0.21218400	2.58051300
H	-0.34367200	0.21345500	-0.81940000
N	0.24774900	-1.04271800	2.76917700
N	1.02832400	-3.03713100	1.93893800
N	-0.83951800	0.75968100	3.66876700
H	0.78520500	-3.76814400	1.28885500
H	-1.27112600	1.64364400	3.40716200
H	1.12615800	-3.34412900	2.89602600
C	-1.55948000	-1.95984000	0.21500500
C	-1.01802600	2.03594600	0.98548500
O	-2.01719800	-2.83139700	0.91623200
O	-1.54869500	2.78192300	1.84680500
C	-0.94522900	2.57683300	-0.45303500
H	0.08116400	2.49050900	-0.82554100

H	-1.55142300	1.94062500	-1.10830100
C	-1.41382900	4.01814000	-0.58441700
H	-0.81844500	4.65161400	0.07501100
H	-2.44156700	4.09651800	-0.22856900
C	-1.31652700	4.52021600	-2.02123600
H	-1.65597800	5.55332600	-2.10767300
H	-0.28768200	4.47606100	-2.38464100
H	-1.92828500	3.91180300	-2.69092100
C	-2.35864000	-1.32356400	-0.89458200
H	-2.49580000	-0.27011100	-0.62778100
H	-1.74415900	-1.32538800	-1.80081000
C	-3.70231200	-1.99262800	-1.13635700
H	-4.28600400	-1.96428000	-0.21577700
H	-3.54339700	-3.04717500	-1.36884100
C	-4.47064800	-1.31645400	-2.26568100
H	-3.90808600	-1.35392100	-3.20042500
H	-5.43304300	-1.80011100	-2.43402500
H	-4.65975700	-0.26685600	-2.03376900
C	1.64647100	0.21855100	-0.09668400
C	2.37301100	0.95540100	0.83773400
C	2.39655300	-0.29339800	-1.16245900
C	3.73717000	1.17767300	0.70898400
H	1.84150200	1.36361400	1.68545400
C	3.76359000	-0.10202500	-1.30684000
C	4.44044600	0.65346900	-0.36670100
H	4.25174500	1.76105600	1.46036900
H	4.27237900	-0.53294500	-2.15632800
H	5.50179000	0.82614000	-0.47391500
N	1.76866300	-1.08704900	-2.23165500
O	2.40992500	-2.00562200	-2.70492100
O	0.65218900	-0.78159200	-2.60683500
H	0.45501300	-2.15132100	-0.32587000

2 (deprotonated H2)

C	-0.51864500	0.83406300	1.11213000
C	0.14680600	-0.05100800	0.08888100
C	-0.08955800	-1.51439500	0.51552900
C	0.43787100	-1.71024400	1.93106300
C	-0.47211100	0.36457900	2.46011100
H	-0.31589900	0.09490900	-0.87896600
N	0.09706500	-0.77640800	2.85830600
N	1.15835700	-2.72923600	2.25749200
N	-0.96533500	1.14458000	3.45105000
H	1.28633200	-3.32633900	1.44560200
H	-1.46856700	1.97830200	3.18186500
C	-1.56809100	-1.90105600	0.41134700

C	-1.06663900	2.08691900	0.75156300
O	-2.10999700	-2.55150300	1.27261800
O	-1.63273600	2.88186200	1.54015900
C	-0.95539100	2.51244800	-0.71600100
H	0.07667300	2.37599300	-1.05436700
H	-1.55837700	1.83167700	-1.32752200
C	-1.39424500	3.94637500	-0.97206600
H	-0.79790200	4.62001600	-0.35437400
H	-2.42684400	4.07083800	-0.64521400
C	-1.25822500	4.32699000	-2.44222100
H	-1.56985500	5.35737200	-2.61775800
H	-0.22441600	4.22899700	-2.77935400
H	-1.87282100	3.68099500	-3.07262700
C	-2.29827300	-1.49524500	-0.85064900
H	-2.42818200	-0.40828700	-0.81514700
H	-1.64333500	-1.69113100	-1.70572600
C	-3.64764000	-2.17656400	-1.01953900
H	-4.27281000	-1.94648600	-0.15628800
H	-3.50830900	-3.25917300	-1.01971000
C	-4.34263500	-1.73806300	-2.30322300
H	-3.74010100	-1.98522000	-3.17930500
H	-5.31162800	-2.22503600	-2.41552600
H	-4.50840500	-0.65918200	-2.30802900
C	1.65009900	0.19449500	-0.09320000
C	2.34664500	1.01573600	0.79184900
C	2.43360200	-0.42290700	-1.07503300
C	3.71643200	1.21820800	0.69247000
H	1.79046500	1.50365800	1.57928400
C	3.80631600	-0.25528900	-1.18463100
C	4.45456800	0.58530900	-0.29783900
H	4.20822900	1.86946400	1.40216900
H	4.34273700	-0.77162900	-1.96700400
H	5.52110100	0.73869400	-0.37908800
N	1.83677900	-1.31117100	-2.08610500
O	2.47535200	-2.28859200	-2.42477100
O	0.75099300	-1.01995600	-2.55158000
H	0.42815900	-2.20426300	-0.15818300
H	-1.04849600	0.73488200	4.36541300

1-2 adduct (ADA-DAD)

C	-2.24562900	1.19531300	-0.13746100
C	-2.89909500	-0.15384600	-0.30613200
C	-2.23172800	-1.12317200	0.68534500
C	-0.73788800	-1.06254200	0.49020600
C	-0.87835400	1.21249700	0.15914600
H	-3.94500300	-0.08302500	-0.03583200

N	-0.11282000	0.06116800	0.28142300
N	-0.06137400	-2.20279000	0.56222500
N	-0.17959300	2.33963200	0.29732700
H	0.82615200	2.29278600	0.41340100
H	-0.53671800	-3.06409400	0.77221300
H	-0.66541300	3.21433000	0.15180300
H	0.95700000	-2.20017700	0.50618200
C	-2.56660100	-0.79363100	2.15171200
C	-2.97509100	2.40624800	-0.37969000
O	-1.70106300	-0.80122900	2.99179200
O	-2.48320400	3.54039500	-0.26648000
C	-4.43231800	2.28293100	-0.80864800
H	-4.49507000	1.59201400	-1.65615600
H	-4.99333700	1.80540900	0.00213900
C	-5.08122100	3.61066600	-1.16763900
H	-4.50874400	4.08952500	-1.96349700
H	-5.02843500	4.28120400	-0.30926000
C	-6.53079200	3.42853300	-1.60281600
H	-6.99393200	4.38408700	-1.84961900
H	-6.59801600	2.78723000	-2.48378400
H	-7.12255300	2.96542600	-0.81074600
C	-4.01322000	-0.52878800	2.48231000
H	-4.26221900	0.45629500	2.07153000
H	-4.63105500	-1.24596000	1.93346500
C	-4.30750900	-0.56559600	3.97475100
H	-3.69922700	0.18608800	4.47811300
H	-4.00023700	-1.53246100	4.37737100
C	-5.78462000	-0.32431600	4.26048800
H	-6.40547300	-1.08351600	3.78177600
H	-5.98745200	-0.35189900	5.33088900
H	-6.10208900	0.65006200	3.88516400
C	-2.83799900	-0.72346300	-1.73120800
C	-2.03350700	-0.12405300	-2.69781800
C	-3.50898400	-1.88140100	-2.14401500
C	-1.91949900	-0.63212300	-3.98552700
H	-1.48434000	0.76678300	-2.42916600
C	-3.39846900	-2.41928500	-3.41754200
C	-2.60342500	-1.78126200	-4.35310600
H	-1.28742500	-0.12502700	-4.70151200
H	-3.94592200	-3.31693600	-3.66355400
H	-2.52032000	-2.18033800	-5.35367600
N	-4.39939700	-2.62024000	-1.23393000
O	-4.43046600	-3.83022800	-1.33527700
O	-5.07122400	-1.99098100	-0.43761700
H	-2.57969100	-2.14840000	0.53161300
C	3.61941600	1.29481800	0.01009200
C	3.44856100	3.58228400	0.08131700
C	4.93629000	1.34654100	-0.47252000

C	4.75815300	3.73584300	-0.40476000
C	3.64557400	-1.09592700	0.03118700
H	2.00480000	0.08889600	0.45968600
C	5.68764200	0.11693200	-0.74661800
C	5.49584400	2.60843300	-0.67521000
H	5.17778300	4.72232600	-0.53063200
C	4.96272600	-1.12586000	-0.45422600
H	6.51314600	2.67142700	-1.03772000
C	3.53680600	-3.38679000	0.14828600
C	5.55102600	-2.37614900	-0.64142900
C	4.84336000	-3.51798300	-0.34760000
H	6.56764200	-2.41959200	-1.00862600
H	5.28480400	-4.49660800	-0.45993300
N	3.00349000	0.09345300	0.23024900
N	2.89903500	2.38709700	0.28241000
N	2.95533400	-2.20311700	0.32704600
O	6.83143700	0.12490700	-1.17970500
C	2.74356300	-4.58048800	0.52842900
C	1.90221300	-4.53092800	1.64126600
C	2.83245600	-5.76133400	-0.20851100
C	1.15874800	-5.64390900	2.00692500
H	1.85036900	-3.62275500	2.22761800
C	2.07919900	-6.86982900	0.15258400
H	3.47224900	-5.80469500	-1.07995800
C	1.24227300	-6.81392000	1.26044800
H	0.52054500	-5.60144600	2.87929100
H	2.14208000	-7.77643900	-0.43351400
H	0.65990800	-7.68033000	1.54339900
C	2.61543300	4.76190700	0.41648700
C	2.72403700	5.94549900	-0.31435900
C	1.70677600	4.69416600	1.47376300
C	1.92792800	7.03775600	0.00029400
H	3.41177100	6.00512100	-1.14722800
C	0.91754000	5.78950200	1.79119400
H	1.63153900	3.78303600	2.05176800
C	1.02455100	6.96257500	1.05348400
H	2.00724200	7.94579200	-0.58163000
H	0.21907000	5.72674700	2.61438300
H	0.40502200	7.81467900	1.29801200

3

O	-1.71022800	2.65015000	0.17628700
C	-2.74869300	1.92984200	-0.47041600
H	-2.89382800	2.29120400	-1.49141800
H	-3.69334900	2.02883100	0.07216200
C	-2.39212300	0.46773000	-0.51494500

H	-3.23629600	-0.07437700	-0.95142100
O	-1.22729100	0.26637200	-1.32266400
C	-0.44121100	-0.78286200	-0.81220800
H	-0.27082800	-1.53840600	-1.57415100
N	0.87897600	-0.26012900	-0.41205400
C	1.11102100	1.06256000	-0.24243700
H	0.26767200	1.71815300	-0.40444900
C	2.33666400	1.51009800	0.11000300
H	2.53397700	2.56074600	0.24840500
C	3.35634300	0.52360300	0.27602900
N	4.59766600	0.90710100	0.62708900
H	4.84719100	1.88025900	0.64951400
N	3.13664000	-0.76792300	0.11457300
C	1.89862000	-1.21482800	-0.22008700
O	1.61640400	-2.39812500	-0.36169500
C	-2.04029300	-0.17023200	0.82312700
H	-1.43256500	0.51261300	1.41979300
C	-1.20375100	-1.37173700	0.37312500
H	-0.52860800	-1.75013200	1.14077900
O	-3.22235000	-0.53851900	1.50056600
H	-1.92349800	3.58699900	0.14617400
H	-3.03708300	-0.60686700	2.44238000
O	-2.04295900	-2.38976200	-0.12222300
H	-2.82320500	-2.42468800	0.44509700
H	5.32937500	0.21635000	0.65455400

3 (N-protonated)

O	1.62282000	2.64246200	-0.17945500
C	2.71332700	1.98498800	0.45097200
H	2.86152900	2.36544600	1.46413400
H	3.63910700	2.12307500	-0.11384700
C	2.42389500	0.50980400	0.51368800
H	3.27674200	0.00528900	0.97401200
O	1.25198500	0.27999700	1.31467700
C	0.50551800	-0.78234900	0.80886100
H	0.32542100	-1.53403700	1.57357200
N	-0.83698600	-0.27224200	0.39572300
C	-1.09726500	1.04780300	0.24133700
H	-0.25530500	1.70841000	0.40129800
C	-2.32581700	1.51449300	-0.09391500
H	-2.51364300	2.56827800	-0.21334300
C	-3.36753100	0.57718300	-0.27159500
N	-4.60171300	0.91497700	-0.58385600
H	-4.84161100	1.88770400	-0.69975600
N	-3.06615200	-0.72894200	-0.10907900
C	-1.81279200	-1.23436100	0.21667600

O	-1.61119400	-2.41709300	0.32745900
C	2.11292000	-0.15989900	-0.81990500
H	1.51465900	0.50404700	-1.44677400
C	1.27882600	-1.36736600	-0.37246000
H	0.61667100	-1.75309800	-1.14943900
O	3.31498600	-0.53081600	-1.45203500
H	1.82717800	3.57983900	-0.24617100
H	3.17528300	-0.58323800	-2.40289900
O	2.11154500	-2.37513500	0.14236800
H	2.91508900	-2.39551500	-0.39355200
H	-5.33083300	0.22665200	-0.70220000
H	-3.78394600	-1.43649600	-0.23062500

3 (O-protonated)

O	1.66081400	2.64376500	-0.15862600
C	2.73339600	1.95901200	0.47206400
H	2.88260800	2.32528600	1.49026900
H	3.66578400	2.08395900	-0.08499300
C	2.41553200	0.48922000	0.51771700
H	3.25708000	-0.03645400	0.97506800
O	1.23707400	0.27220400	1.31461600
C	0.47985800	-0.77610600	0.80422400
H	0.29419900	-1.52703000	1.56765700
N	-0.86245100	-0.24127700	0.39676800
C	-1.09166500	1.09400200	0.22730300
H	-0.23978000	1.74085500	0.38287700
C	-2.31875300	1.54228100	-0.11608300
H	-2.50796100	2.59543800	-0.25050600
C	-3.35203700	0.57883400	-0.28318900
N	-4.58732900	0.92753300	-0.60123800
H	-4.83787800	1.89496800	-0.72647400
N	-3.10045100	-0.73411300	-0.12224000
C	-1.89203800	-1.09253300	0.20355100
O	-1.58603300	-2.36418600	0.36506100
C	2.09339100	-0.16095300	-0.82279900
H	1.50652700	0.51891500	-1.44288800
C	1.23867900	-1.35944300	-0.38876500
H	0.56820000	-1.71960200	-1.17115500
O	3.28757900	-0.54974000	-1.45750900
H	1.87630300	3.58026800	-0.19976600
H	3.15563500	-0.56573600	-2.41077000
O	2.05203000	-2.39013900	0.10911200
H	2.85844900	-2.41162400	-0.42309600
H	-5.29751300	0.21907200	-0.70766400
H	-2.37992300	-2.90444300	0.22305200

3 (deprotonated)

O	1.73335100	2.75834900	-0.03462900
C	2.73185000	1.89681400	0.48315700
H	2.91283200	2.21853800	1.50853000
H	3.66872100	1.99792500	-0.07219900
C	2.34552900	0.43432900	0.49528900
H	3.20767500	-0.13114200	0.86640400
O	1.22430100	0.21573000	1.35099800
C	0.39401200	-0.81286900	0.83968700
H	0.24554500	-1.57964300	1.59442400
N	-0.91217700	-0.26649700	0.47410300
C	-1.13176700	1.07290500	0.32123500
H	-0.29364100	1.71854600	0.53801500
C	-2.33170300	1.53016500	-0.06906000
H	-2.50228600	2.59143300	-0.17588800
C	-3.41090200	0.57926700	-0.33465200
N	-4.59537900	0.95504000	-0.73227800
H	-4.60500700	1.96856400	-0.80747100
N	-3.15444200	-0.75302300	-0.15700900
C	-1.95808300	-1.19747000	0.22981000
O	-1.66605200	-2.39429100	0.38926500
C	1.92257300	-0.16670100	-0.83816300
H	1.25866700	0.51458700	-1.37768700
C	1.12709600	-1.38613000	-0.37134600
H	0.42947300	-1.77131200	-1.11400600
O	3.06519300	-0.48806100	-1.60505200
H	1.71727900	2.68258100	-0.99293600
H	2.79934600	-0.61639800	-2.52116000
O	2.00709300	-2.39413700	0.08123400
H	2.75266400	-2.42491100	-0.53001000

3-4 adduct (AAD-DDA)

O	-6.24459700	1.61295100	0.03170800
C	-6.81092600	0.39733800	-0.43359700
H	-7.14860700	0.49607600	-1.46794400
H	-7.66288600	0.09892400	0.18412700
C	-5.77801600	-0.69564800	-0.35836100
H	-6.25580500	-1.63693100	-0.64548800
O	-4.69577400	-0.41721800	-1.25404900
C	-3.47776700	-0.86890900	-0.71982600
H	-2.98328200	-1.54560400	-1.41120000
N	-2.57388300	0.28216900	-0.51691000
C	-3.02292600	1.56248000	-0.48357100
H	-4.08861500	1.69296900	-0.60641100
C	-2.16848600	2.59197400	-0.30409300

H	-2.51683800	3.61175600	-0.27676600
C	-0.78209800	2.27420400	-0.16103300
N	0.11876500	3.24006600	0.01139200
H	-0.17449800	4.20123300	0.04284000
N	-0.34805300	1.01559900	-0.19384200
C	-1.21626600	-0.00672000	-0.35657500
O	-0.86552800	-1.19045200	-0.36498000
C	-5.10818100	-0.88153200	0.99724800
H	-4.89792700	0.08858400	1.45140700
C	-3.80173300	-1.57392000	0.59672300
H	-3.00201100	-1.45541300	1.32813100
O	-5.92546500	-1.67817700	1.82629700
H	-6.86860400	2.32578800	-0.13108600
H	-5.70586800	-1.50641600	2.74747500
O	-4.03885200	-2.93222500	0.30773100
H	-4.68164200	-3.25621900	0.95129600
H	1.10457400	3.00679500	0.13592100
C	3.35006000	1.38132300	0.27342200
C	2.90447900	-0.99415000	-0.18759800
C	4.70795700	0.96785500	0.39504000
C	4.99871700	-0.37606400	0.21159900
N	2.51120700	0.30681800	-0.02252500
N	1.93618100	-1.87199700	-0.50444400
H	0.95161100	-1.61948700	-0.42928500
H	2.18876600	-2.84579200	-0.50038600
N	6.34532800	-0.48589000	0.39048000
N	5.85517400	1.67761100	0.68077600
C	6.80063600	0.78055200	0.66571800
N	4.15472600	-1.38924500	-0.07665700
C	7.13621100	-1.70234500	0.25346300
H	8.08084000	-1.52545400	0.76451900
H	6.61165700	-2.49872300	0.77909500
C	7.36128300	-2.07370300	-1.20293600
H	7.95541300	-2.98509800	-1.26358800
H	6.40985100	-2.24789300	-1.70379100
H	7.89120500	-1.27785300	-1.72593900
H	7.84737600	0.96156200	0.85078700
O	2.88061300	2.51275900	0.39580800
H	1.50833300	0.53377600	-0.10544400

4

C	-1.80051600	-1.06191400	0.14657200
C	-1.41777600	1.37711400	-0.08520600
C	-0.38164800	-1.14703300	-0.01034600
C	0.33746800	0.02459800	-0.17934700
N	-2.22063300	0.28425600	0.08990900

N	-2.03189300	2.59148000	-0.05074300
H	-3.00780300	2.63543100	-0.30017000
H	-1.47030400	3.35898800	-0.38560300
N	1.63846600	-0.35795600	-0.30268600
N	0.45846900	-2.23705800	-0.02670100
C	1.64599600	-1.72620800	-0.19991300
N	-0.12204800	1.29916100	-0.23032800
C	2.79028200	0.52321700	-0.45655600
H	3.60562600	-0.08836500	-0.83799800
H	2.54175100	1.26419500	-1.21478300
C	3.17231600	1.19368000	0.85239200
H	4.04051900	1.83374600	0.69873600
H	2.35211800	1.80784400	1.22183300
H	3.41931800	0.44892700	1.60862800
H	2.56922300	-2.27897600	-0.26674400
O	-2.62115700	-1.94583900	0.31187400
H	-3.21445700	0.42502000	0.21937700

4 (protonated)

C	-1.73713200	-0.94212500	0.12557200
C	-1.39274700	1.43755300	-0.07668000
C	-0.38094200	-1.09845700	-0.02618900
C	0.36619300	0.08142400	-0.19274900
N	-2.20707400	0.33231100	0.08979500
N	-1.99408600	2.62920100	-0.11410200
H	-1.41066900	3.44974200	-0.16112400
N	1.64605800	-0.32583400	-0.32328600
N	0.43995600	-2.20568600	-0.05205500
C	1.62466800	-1.70422300	-0.22741600
N	-0.09105300	1.33468000	-0.21396400
C	2.82519100	0.53053400	-0.46485200
H	3.57551800	-0.05239900	-0.99440200
H	2.53772700	1.36906300	-1.09579200
C	3.33725900	1.00422100	0.88404600
H	4.21134600	1.63728300	0.73917700
H	2.57442000	1.58271700	1.40399500
H	3.62331300	0.15804800	1.50792000
H	2.54081900	-2.26867000	-0.30330200
O	-2.55101700	-1.95198000	0.29960100
H	-2.96515200	2.74395600	0.12674800
H	-3.20780100	0.48563500	0.16929800
H	-3.48292800	-1.69580100	0.37556700

4 (deprotonation H1)

C	-1.86184800	-0.95079200	0.15179900
C	-1.41508000	1.51642400	-0.09667100
C	-0.45210800	-1.09911500	-0.02196400
C	0.30647000	0.05649000	-0.19303100
N	-2.23090500	0.38770500	0.09561000
N	-2.03468800	2.66090100	-0.11658200
H	-1.33800300	3.38578800	-0.25804800
N	1.59879600	-0.38818300	-0.31605500
N	0.35330500	-2.22437900	-0.04000000
C	1.55722900	-1.76026700	-0.21172900
N	-0.07593700	1.33667900	-0.24026100
C	2.77531600	0.45321300	-0.44647200
H	3.57664900	-0.16888800	-0.84326900
H	2.55252800	1.22508200	-1.18254000
C	3.17720900	1.08275000	0.87836500
H	4.05772400	1.71124300	0.74390900
H	2.36661000	1.70061500	1.26270900
H	3.40790200	0.31354600	1.61571500
H	2.46005300	-2.34649500	-0.27859300
O	-2.70808600	-1.82503600	0.33605500
H	-3.21590400	0.57811000	0.21090200

4 (deprotonation H2)

C	-1.85318900	-0.98755100	0.15546000
C	-1.47450000	1.32879900	-0.06826500
C	-0.42434900	-1.11545200	-0.01218500
C	0.31260700	0.04204000	-0.18465600
N	-2.31532300	0.31075700	0.10838200
N	-2.04953200	2.59621200	-0.04533300
H	-1.51420300	3.29487700	-0.53710500
N	1.61781000	-0.35967500	-0.31581400
N	0.41001800	-2.22027400	-0.03601400
C	1.60559800	-1.72783500	-0.21267700
N	-0.14596000	1.30596900	-0.22646700
C	2.77532800	0.50746200	-0.45103000
H	3.59583500	-0.10558900	-0.82190400
H	2.54740200	1.25679600	-1.20881400
C	3.14643600	1.17664100	0.86341000
H	4.02174000	1.81198800	0.72697600
H	2.32269700	1.79417400	1.21915100
H	3.37347800	0.42925400	1.62386000
H	2.52119600	-2.29382700	-0.28334100
O	-2.62314200	-1.94482900	0.32860200
H	-3.02967800	2.59540100	-0.28126100

5

C	-3.45465100	0.37568300	-0.00003200
C	-1.14687400	0.52825800	0.00000800
C	-1.19638800	1.95802900	0.00001500
C	-2.47623800	2.57622200	0.00002500
C	-3.58906700	1.80568500	0.00001100
C	0.00000000	2.66078100	0.00002800
C	1.19638800	1.95802900	0.00003500
C	1.14687400	0.52825800	0.00005000
C	3.45465100	0.37568400	-0.00003400
C	3.58906700	1.80568600	0.00001900
C	2.47623800	2.57622200	0.00004600
H	-2.54118800	3.65687500	0.00004500
H	-4.56281400	2.26684200	0.00004000
H	4.56281300	2.26684400	0.00001900
H	2.54118700	3.65687500	0.00004900
N	2.28917100	-0.21808000	0.00001000
N	0.00000000	-0.15118100	0.00001700
N	-2.28917100	-0.21808000	-0.00003100
C	-4.65885100	-0.50321000	-0.00001100
C	-4.49581000	-1.89220100	-0.00006000
C	-5.95552300	0.01603200	0.00002700
C	-5.59594000	-2.73408500	-0.00007300
H	-3.49601800	-2.30008700	-0.00010500
C	-7.05725200	-0.82914100	0.00002300
H	-6.12822800	1.08144300	0.00005800
C	-6.88249900	-2.20584000	-0.00002600
H	-5.44911500	-3.80554000	-0.00012300
H	-8.05331900	-0.40812000	0.00005000
H	-7.74159300	-2.86300100	-0.00003800
C	4.65885000	-0.50321000	-0.00004000
C	4.49581000	-1.89220000	0.00014400
C	5.95552300	0.01603100	-0.00019300
C	5.59594000	-2.73408400	0.00017500
H	3.49601900	-2.30008900	0.00027900
C	7.05725200	-0.82914200	-0.00016500
H	6.12822900	1.08144200	-0.00032800
C	6.88250000	-2.20584100	0.00001800
H	5.44911400	-3.80554000	0.00033300
H	8.05331900	-0.40811900	-0.00027500
H	7.74159300	-2.86300200	0.00005100
H	0.00000000	3.74468400	0.00002800

5 (N1-protonated)

C	3.47099600	-0.38140900	0.00000700

C	1.19481900	-0.55499900	-0.00000400
C	1.20755900	-1.97394500	0.00000300
C	2.48840200	-2.58517500	0.00001900
C	3.59897300	-1.80624400	0.00002200
C	0.00000000	-2.66446500	-0.00000500
C	-1.20755900	-1.97394500	-0.00001500
C	-1.19481900	-0.55499900	-0.00001400
C	-3.47099600	-0.38140900	-0.00001400
C	-3.59897300	-1.80624400	-0.00002600
C	-2.48840200	-2.58517500	-0.00002500
H	2.55784000	-3.66453900	0.00002700
H	4.57281700	-2.26603300	0.00003500
H	-4.57281700	-2.26603300	-0.00003400
H	-2.55784000	-3.66453900	-0.00003000
N	-2.28615100	0.20928400	-0.00001200
N	0.00000000	0.08191900	-0.00001200
N	2.28615100	0.20928400	-0.00000400
C	4.65715600	0.50074700	0.00000200
C	4.48289700	1.88995900	-0.00002700
C	5.95761100	-0.01454400	0.00002700
C	5.57732900	2.73711000	-0.00003000
H	3.48320000	2.29682900	-0.00004800
C	7.05150400	0.83714400	0.00002400
H	6.13656700	-1.07863900	0.00004800
C	6.86567200	2.21326100	-0.00000400
H	5.42645500	3.80758500	-0.00005300
H	8.05048700	0.42425100	0.00004500
H	7.72088800	2.87526600	-0.00000500
C	-4.65715600	0.50074700	0.00000000
C	-4.48289700	1.88995900	0.00005600
C	-5.95761100	-0.01454400	-0.00004000
C	-5.57732900	2.73711000	0.00006900
H	-3.48320000	2.29682900	0.00009100
C	-7.05150400	0.83714400	-0.00002900
H	-6.13656700	-1.07863900	-0.00008100
C	-6.86567200	2.21326100	0.00002500
H	-5.42645500	3.80758500	0.00011200
H	-8.05048700	0.42425100	-0.00006300
H	-7.72088800	2.87526600	0.00003300
H	0.00000000	-3.74831200	-0.00000200
H	0.00000000	1.09937600	-0.00001500

5 (N2-protonated)

C	-3.46535900	0.35556300	-0.03666900

C	-1.17164100	0.51152500	-0.03231500
C	-1.21828800	1.94439200	-0.00059600
C	-2.50151200	2.56234100	-0.01319100
C	-3.60760400	1.78470700	-0.03375000
C	-0.02983000	2.65685800	0.03052400
C	1.17697600	1.96120300	0.03107000
C	1.09393000	0.54532000	-0.00515100
C	3.48740000	0.38804300	0.02223600
C	3.58923400	1.79656200	0.05948500
C	2.45993300	2.56119700	0.06390200
H	-2.56752900	3.64233400	-0.01593700
H	-4.59105200	2.22627900	-0.07284400
H	4.56842600	2.24399900	0.11733100
H	2.53017900	3.64054500	0.10462700
N	2.27723300	-0.16136200	-0.01286900
N	-0.01123900	-0.16179600	-0.03852600
N	-2.29636900	-0.24117300	-0.04729700
C	-4.66582000	-0.51016900	-0.04035900
C	-4.57607100	-1.81436500	-0.53389900
C	-5.88819000	-0.05259200	0.45674200
C	-5.69012000	-2.63749400	-0.54269400
H	-3.62948200	-2.17004700	-0.91465900
C	-6.99850900	-0.88463200	0.45996900
H	-5.97490200	0.94314000	0.86886500
C	-6.90394100	-2.17510000	-0.04468700
H	-5.61270700	-3.64126200	-0.93721900
H	-7.93689700	-0.52443800	0.85846800
H	-7.77236500	-2.81981400	-0.04775900
C	4.65600100	-0.49667100	0.03578000
C	4.58760300	-1.75193700	0.64774600
C	5.84628300	-0.08061300	-0.56626000
C	5.69777700	-2.57946500	0.65373800
H	3.68552200	-2.06796400	1.15633900
C	6.94800400	-0.92007100	-0.56786800
H	5.90293100	0.88150100	-1.05654200
C	6.87621500	-2.16657400	0.04276700
H	5.64561200	-3.54202100	1.14231900
H	7.86248000	-0.60223200	-1.04839300
H	7.74120900	-2.81545400	0.04605400
H	-0.03558800	3.73969300	0.05434700
H	2.18195600	-1.17211600	-0.08328500

6

C	1.62082400	-1.26121800	-0.03076200
C	0.77553800	-0.00021800	-0.13458400
C	1.62206800	1.25998100	-0.03107100

C	2.79586200	1.20838000	0.68793200
C	2.79466600	-1.21067700	0.68824500
H	0.29699300	-0.00014200	-1.11116100
N	3.25267900	-0.00130600	1.16960400
N	3.56404500	2.26973000	1.00770100
N	3.56159000	-2.27288000	1.00849200
H	4.53281800	-2.12527500	1.23188000
H	3.28820100	3.14139000	0.57089800
H	3.28483000	-3.14423400	0.57148900
H	4.53494000	2.12106800	1.23178500
C	1.20640600	2.50627600	-0.63930100
C	1.20419000	-2.50706700	-0.63915500
O	1.81464800	3.57139700	-0.47791800
O	1.81126600	-3.57283100	-0.47750700
C	-0.02887600	-2.49825800	-1.52444400
H	-0.87978400	-2.16281400	-0.92369300
H	0.10381800	-1.73985900	-2.30216900
C	-0.33680900	-3.84596600	-2.15877700
H	-0.46838600	-4.59274800	-1.37509600
H	0.52135900	-4.16998900	-2.74919100
C	-1.58158300	-3.78091500	-3.03625200
H	-1.79151700	-4.74674900	-3.49598700
H	-2.45806400	-3.49040700	-2.45389700
H	-1.45888900	-3.04966200	-3.83749200
C	-0.02681400	2.49862100	-1.52421400
H	0.10549000	1.74063000	-2.30243400
H	-0.87779700	2.16313500	-0.92361700
C	-0.33417600	3.84685500	-2.15767400
H	0.52408900	4.17084800	-2.74795800
H	-0.46534100	4.59323300	-1.37352900
C	-1.57906200	3.78295600	-3.03507800
H	-2.45563000	3.49240400	-2.45286700
H	-1.78865200	4.74919100	-3.49414100
H	-1.45674300	3.05221500	-3.83684100
C	-0.35572100	0.00025300	0.89432700
C	-0.07809000	0.00039300	2.26348400
C	-1.68345200	0.00050100	0.48903300
C	-1.09454500	0.00069600	3.20677100
H	0.95260400	0.00023600	2.59607300
C	-2.68538300	0.00077200	1.44860500
C	-2.42392100	0.00087300	2.80595500
H	-0.85567400	0.00079900	4.26086400
H	-3.23374700	0.00113700	3.51880000
H	-1.94530900	0.00055800	-0.55984300
N	-4.08429700	0.00103200	0.99807100
O	-4.29823400	0.00108700	-0.19883300
O	-4.95694400	0.00124000	1.84343500
H	4.09966000	-0.00157700	1.71940600

6 (deprotonated H1)

C	1.65111100	1.25462200	0.04821200
C	0.80201500	-0.00062900	0.17387500
C	1.64875300	-1.25747400	0.04830300
C	2.83330200	-1.15680800	-0.71378000
C	2.83549200	1.15166700	-0.71381500
H	0.31973300	-0.00014900	1.14921600
N	3.36277700	-0.00307900	-1.16657500
N	3.53478300	-2.26511600	-1.05625900
N	3.53910700	2.25862700	-1.05628700
H	4.47506600	2.11264300	-1.39466500
H	3.26403300	-3.12804700	-0.60270000
H	3.27002200	3.12206100	-0.60269800
H	4.47100500	-2.12093100	-1.39468000
C	1.23734200	-2.49169600	0.62446400
C	1.24201500	2.48968000	0.62424400
O	1.83798900	-3.58186100	0.48148700
O	1.84471600	3.57869300	0.48114200
C	-0.01553400	2.49858300	1.49199000
H	-0.86467100	2.18025100	0.87999900
H	0.08621700	1.74214700	2.27597800
C	-0.31910800	3.84884400	2.12382600
H	-0.43134400	4.59903300	1.34026600
H	0.53363100	4.16433200	2.72668300
C	-1.57686800	3.79792700	2.98470800
H	-1.78729900	4.76622000	3.44049200
H	-2.44775300	3.51188000	2.39130100
H	-1.47153000	3.06688900	3.78893900
C	-0.02029300	-2.49813300	1.49210700
H	0.08266200	-1.74159000	2.27583200
H	-0.86881700	-2.17856300	0.87990000
C	-0.32625800	-3.84764400	2.12439500
H	0.52588000	-4.16438200	2.72744800
H	-0.43971800	-4.59792300	1.34109900
C	-1.58401000	-3.79425100	2.98513700
H	-2.45434500	-3.50692400	2.39154100
H	-1.79614900	-4.76201800	3.44124700
H	-1.47749700	-3.06310700	3.78911700
C	-0.33070600	0.00034600	-0.85500200
C	-0.04571600	0.00037200	-2.22435000
C	-1.66293400	0.00121500	-0.46251900
C	-1.05514300	0.00122600	-3.17518500
H	0.98929700	-0.00027900	-2.54407300
C	-2.65957400	0.00205700	-1.42978700
C	-2.38830000	0.00207800	-2.78579400

H	-0.80724000	0.00122600	-4.22745500
H	-3.19246800	0.00274900	-3.50474500
H	-1.93208100	0.00124100	0.58442400
N	-4.06001200	0.00296600	-0.99195900
O	-4.28796400	0.00300600	0.20322900
O	-4.92933400	0.00360800	-1.84349300

6 (deprotonated H2)

C	1.46771200	1.49635100	0.06492500
C	0.80775900	0.12565600	0.15824000
C	1.80816800	-1.01749000	0.04906900
C	2.96123300	-0.79770700	-0.69489600
C	2.65520800	1.64065500	-0.71979500
H	0.32523900	0.04720300	1.13024400
N	3.22079400	0.43335700	-1.20764500
N	3.85865100	-1.76305400	-1.00196100
N	3.31895100	2.69753100	-1.06104700
H	3.71903500	-2.63997200	-0.51343300
H	2.83019500	3.49787900	-0.66969600
H	4.79321700	-1.48171900	-1.25174900
C	1.57602500	-2.29346700	0.65962400
C	0.88439000	2.63660500	0.66404100
O	2.33169000	-3.27552800	0.53049100
O	1.33841900	3.80207400	0.56331000
C	-0.38897700	2.45300400	1.49722200
H	-1.17219000	2.03729400	0.85645100
H	-0.21100900	1.70392000	2.27535600
C	-0.89320700	3.73723000	2.13778700
H	-1.08169300	4.47849700	1.36041200
H	-0.10997700	4.15682900	2.77071400
C	-2.15972500	3.50293700	2.95415900
H	-2.52187200	4.42788200	3.40493200
H	-2.96005100	3.10190800	2.32840100
H	-1.98228400	2.78692400	3.75947900
C	0.33700500	-2.45877100	1.52930700
H	0.38186100	-1.72618400	2.34143400
H	-0.54291800	-2.19240700	0.93737200
C	0.17050000	-3.85812200	2.10149300
H	1.05371700	-4.11784200	2.68623100
H	0.12393200	-4.57858600	1.28367400
C	-1.08095200	-3.96535500	2.96597000
H	-1.97751300	-3.72815000	2.38971800
H	-1.20055300	-4.97076300	3.37081500
H	-1.03625100	-3.27050100	3.80690900
C	-0.30830800	-0.03292100	-0.87636300
C	-0.02602100	-0.00877200	-2.24589300
C	-1.63085700	-0.19638900	-0.48385000

C	-1.02752400	-0.14245400	-3.19580000
H	0.99864700	0.12165000	-2.57009100
C	-2.62009500	-0.32500200	-1.45028900
C	-2.35090800	-0.30258800	-2.80606300
H	-0.78097800	-0.11974200	-4.24813200
H	-3.14793600	-0.40651000	-3.52541900
H	-1.89845100	-0.22385400	0.56292300
N	-4.01016100	-0.49379400	-1.01134500
O	-4.23730300	-0.50615200	0.18378300
O	-4.87129900	-0.61464600	-1.86245800
H	4.09958400	0.57156100	-1.68689500

8

C	-1.82171900	-0.81496200	0.11779500
C	-1.37026200	1.44253200	-0.07141600
C	-0.44230200	-1.05703900	-0.01669500
C	0.35615700	0.06493900	-0.18234900
N	-2.71319600	-1.81851500	0.24220600
N	-2.26100100	0.44278600	0.09138900
H	-2.37667500	-2.74806600	0.42994600
H	-3.65891300	-1.59045100	0.50148500
N	-1.89372000	2.70855300	-0.03466200
H	-2.87957000	2.78118300	-0.22619800
H	-1.31553700	3.43355900	-0.42738800
N	1.63167900	-0.41206100	-0.30207200
N	0.31991400	-2.20934000	-0.02801000
C	1.53994600	-1.77756000	-0.19655900
N	-0.05008700	1.33840800	-0.22145700
C	2.84133200	0.38596100	-0.45529600
H	3.61568200	-0.28048800	-0.83105000
H	2.64641900	1.13852900	-1.21816800
C	3.26292500	1.03903800	0.85041400
H	4.17352400	1.61723300	0.69636700
H	2.48469700	1.71038700	1.21115100
H	3.45538500	0.28515500	1.61356300
H	2.42339700	-2.39330800	-0.25683200

8 (protonated)

C	1.72090800	1.06226600	0.00597200
C	1.63533700	-1.36133400	0.00292000
C	0.32817600	1.02404100	-0.00034300
C	-0.27430400	-0.23090000	-0.01022100
N	2.46020600	2.15733100	0.00875900
N	2.31970200	-0.16219300	0.00687500

H	2.00598400	3.05829600	0.00446000
H	3.46749200	2.12499000	0.01186900
N	2.39404800	-2.47003600	-0.03334900
H	3.36918700	-2.42965400	0.21712300
H	1.91959800	-3.34954500	0.09881800
N	-1.60747300	0.00886200	-0.01967800
N	-0.61686800	2.02301900	-0.00309600
C	-1.75062200	1.37949700	-0.01513700
N	0.32890300	-1.43147800	-0.00332400
C	-2.64492600	-1.02968000	-0.05193200
H	-2.52731300	-1.58018100	-0.98437400
H	-2.43919700	-1.71364900	0.76969000
C	-4.04039900	-0.45292600	0.06195000
H	-4.75429100	-1.27415500	0.04674300
H	-4.17127300	0.09236900	0.99610000
H	-4.27137900	0.20882000	-0.77199900
H	-2.72487100	1.83804300	-0.01916700
H	3.33141500	-0.19966000	-0.02183100

8 (deprotonated H1)

C	1.83699400	0.90606000	0.02440300
C	1.72086600	-1.44654300	0.00591100
C	0.42838900	0.97024600	-0.00019600
C	-0.21302000	-0.26252300	-0.00600200
N	2.58403000	2.06142100	0.08918200
N	2.45073700	-0.25385600	0.02763400
H	2.12549000	2.89185800	-0.25295600
H	3.54328600	1.95777200	-0.20510200
N	2.41152100	-2.56028800	-0.01408600
H	1.74275700	-3.32510800	-0.02902400
N	-1.55713100	0.03821600	-0.02624300
N	-0.48872800	2.00938300	-0.02396000
C	-1.64987400	1.41365000	-0.04006200
N	0.33585000	-1.46542700	-0.00068300
C	-2.61469000	-0.96113400	-0.05269200
H	-2.53336400	-1.52322900	-0.98437500
H	-2.42537100	-1.66195800	0.76074700
C	-3.99844300	-0.35508400	0.07973600
H	-4.73585800	-1.15641600	0.08215000
H	-4.10008700	0.20229300	1.01095400
H	-4.22746400	0.30935800	-0.75323200
H	-2.60467800	1.91125600	-0.05865100

8 (deprotonated H2)

C	-1.86895700	-0.95112600	0.14619200
C	-1.46515000	1.35795200	-0.06022700
C	-0.43842900	-1.08772600	-0.00603400
C	0.31172200	0.05626600	-0.17879600
N	-2.71030500	-1.93239800	0.30765300
N	-2.31894700	0.35388100	0.10360300
H	-2.17876500	-2.80013100	0.30901700
N	-2.02485000	2.63367300	-0.02528600
H	-3.00478000	2.64467000	-0.26242000
H	-1.48242000	3.32602000	-0.51825200
N	1.61107000	-0.36692600	-0.31226900
N	0.37465000	-2.20554500	-0.02830300
C	1.58085000	-1.73377800	-0.20778400
N	-0.13280100	1.32837700	-0.21844500
C	2.77862000	0.48381900	-0.46288700
H	3.57923900	-0.13303200	-0.86930100
H	2.53900400	1.25015600	-1.19969200
C	3.19596900	1.12365300	0.85203700
H	4.06996600	1.75729100	0.69982900
H	2.38753300	1.73777100	1.24677500
H	3.44392600	0.35995500	1.58937500
H	2.48681300	-2.31448900	-0.27902300

9

O	-0.36818800	1.95130700	-0.00016000
C	-3.29045200	-0.10887300	-0.00009600
C	-1.02738000	0.93087400	-0.00013900
N	-0.47687500	-0.33880100	0.00000700
N	-2.40517700	0.96409300	-0.00016200
H	-2.81050500	1.89189400	-0.00019200
C	-1.28809700	-1.44408900	0.00015100
H	-0.76160500	-2.38761200	0.00030100
C	-2.63132200	-1.39456400	0.00014900
H	-3.22803700	-2.29130300	0.00032100
C	0.99566300	-0.51114100	0.00005800
C	1.64818900	0.03714400	-1.26748100
C	1.64814100	0.03757900	1.26743300
H	1.13797700	-1.59365500	0.00024400
C	3.14375500	-0.28529100	-1.25905000
H	1.50469700	1.11655700	-1.31024000
H	1.16517000	-0.40103600	-2.14275900
C	3.14370800	-0.28485700	1.25917100
H	1.50464500	1.11700800	1.30981300
H	1.16508800	-0.40029900	2.14284200

C	3.81875600	0.25725100	-0.00002000
H	3.61089400	0.13010800	-2.15249900
H	3.28203300	-1.37021100	-1.30193000
H	3.61081200	0.13084900	2.15249500
H	3.28198600	-1.36976300	1.30242900
H	4.87877600	-0.00097500	0.00004400
H	3.75406900	1.34938200	-0.00020800
O	-4.49273700	0.08592000	0.00008300

9 (protonated)

O	-0.34946100	1.94742200	0.00015100
C	-3.16871000	-0.13406700	-0.00000700
C	-0.97915700	0.92599300	0.00006100
N	-0.43290300	-0.35276000	-0.00003200
N	-2.37945800	0.94633500	0.00007900
H	-2.78413700	1.87974200	0.00017100
C	-1.22178100	-1.44271700	-0.00012800
H	-0.70194900	-2.38993400	-0.00021400
C	-2.58586600	-1.39621300	-0.00012300
H	-3.19282800	-2.28524900	-0.00020200
C	1.05477700	-0.51297000	-0.00005100
C	1.69066800	0.04614600	-1.26935400
C	1.69068700	0.04580500	1.26939500
H	1.19815100	-1.59445600	-0.00019100
C	3.18694900	-0.27670500	-1.25994800
H	1.55013000	1.12607400	-1.30729100
H	1.20781700	-0.39125500	-2.14469800
C	3.18696700	-0.27704700	1.25987900
H	1.55015500	1.12572200	1.30762400
H	1.20784900	-0.39182900	2.14463000
C	3.86149600	0.26354400	0.00003400
H	3.65045000	0.14267300	-2.15266600
H	3.32435400	-1.36099900	-1.30759800
H	3.65048200	0.14208900	2.15270400
H	3.32436900	-1.36135400	1.30723500
H	4.91974400	0.00057200	-0.00000900
H	3.80190000	1.35567000	0.00018100
O	-4.46778300	-0.01141000	0.00002000
H	-4.77818200	0.90879900	0.00008400

9 (deprotonated)

O	-0.35060300	1.94284600	-0.00137800
C	-3.26609800	-0.02092100	0.00002600
C	-1.10852300	0.96375800	-0.00096700

N	-0.51268700	-0.32415100	0.00025800
N	-2.44972200	1.06567400	-0.00089500
C	-1.31065200	-1.43094400	0.00119000
H	-0.79147000	-2.38040500	0.00202800
C	-2.65049300	-1.34514900	0.00107600
H	-3.27039900	-2.22798800	0.00180200
C	0.94813300	-0.49854600	0.00050800
C	1.61615200	0.03911500	-1.26548100
C	1.61605700	0.04224600	1.26521200
H	1.09613600	-1.58228100	0.00184100
C	3.10923700	-0.29369300	-1.25851000
H	1.47330300	1.11808800	-1.30915200
H	1.13034600	-0.39678300	-2.14092100
C	3.10914700	-0.29055800	1.25917400
H	1.47320000	1.12132500	1.30619700
H	1.13018800	-0.39148200	2.14169500
C	3.78963000	0.24493400	-0.00031300
H	3.58234400	0.11601700	-2.15235300
H	3.24124500	-1.38018900	-1.29858600
H	3.58219000	0.12137300	2.15202900
H	3.24114900	-1.37695000	1.30196400
H	4.84897400	-0.01928400	0.00005300
H	3.73070700	1.33750400	-0.00167500
O	-4.50522200	0.09327100	-0.00011700

10

O	0.42501300	2.59511400	0.00014000
N	2.29407700	1.31455100	-0.00012500
N	0.20535500	0.31233200	-0.00020500
C	0.92714200	1.48599200	-0.00012300
C	0.84166600	-0.90748800	0.00001700
C	2.17631500	-1.07222600	0.00010900
C	3.00466600	0.12230200	-0.00011300
C	2.85271000	-2.40582200	0.00044500
H	2.83694800	2.16902500	-0.00007700
H	3.49162300	-2.51538000	0.87744700
H	2.11926100	-3.21015000	0.00049600
H	3.49188000	-2.51570800	-0.87631300
O	4.22320000	0.13078500	-0.00024500
H	0.18080700	-1.76334800	0.00007000
C	-1.27011800	0.37789900	-0.00023100
C	-1.85633100	-0.24572100	-1.26499200
C	-1.85621600	-0.24506400	1.26492100
H	-1.50258800	1.44070800	-0.00050000
C	-3.37925300	-0.10931900	-1.25930900
H	-1.59094200	-1.30623900	-1.31130900

H	-1.42514800	0.23905200	-2.14223300
C	-3.37913700	-0.10871400	1.25932600
H	-1.59070900	-1.30553600	1.31179700
H	-1.42496000	0.24022600	2.14184400
C	-3.98416900	-0.72813900	0.00019200
H	-3.79456000	-0.57581900	-2.15313100
H	-3.64246900	0.95177200	-1.30089800
H	-3.79432500	-0.57478700	2.15342400
H	-3.64234600	0.95240200	1.30043700
H	-5.06717800	-0.59826200	0.00020600
H	-3.79069200	-1.80553500	0.00044000

10 (protonated)

O	0.40284300	2.58121700	0.00015200
N	2.26827300	1.29488200	0.00005300
N	0.16864100	0.29192800	0.00002700
C	0.88268900	1.47804800	0.00010700
C	0.79151100	-0.90455800	-0.00003400
C	2.14828100	-1.07308000	-0.00005100
C	2.89122100	0.11235300	-0.00001900
C	2.83063000	-2.40631200	-0.00009500
H	2.80154500	2.16109100	0.00008400
H	3.46266000	-2.51889400	0.88018700
H	2.09058300	-3.20318400	-0.00011900
H	3.46265600	-2.51883600	-0.88038700
O	4.19572500	0.05079700	-0.00004600
H	0.13966400	-1.76829700	-0.00004400
C	-1.32091200	0.37066300	0.00004800
C	-1.89938200	-0.24936200	-1.26788100
C	-1.89933500	-0.24975100	1.26780400
H	-1.53858400	1.43607500	0.00020700
C	-3.42125000	-0.09745600	-1.25979500
H	-1.64400300	-1.31235600	-1.31099400
H	-1.46421200	0.23371000	-2.14380500
C	-3.42120300	-0.09784200	1.25982400
H	-1.64394600	-1.31275900	1.31057000
H	-1.46412900	0.23305000	2.14386000
C	-4.03122300	-0.71016100	-0.00006800
H	-3.83744100	-0.56168500	-2.15363800
H	-3.67336500	0.96586500	-1.30401100
H	-3.83735900	-0.56234200	2.15354200
H	-3.67331600	0.96546600	1.30437400
H	-5.11185600	-0.56621000	-0.00002500
H	-3.85149800	-1.78962600	-0.00023600
H	4.62949900	0.91990200	-0.00001400

10 (deprotonated)

O	-0.38616000	2.58437400	0.00045500
N	-2.33729700	1.41357700	0.00033000
N	-0.23357100	0.31392100	-0.00010000
C	-0.99496900	1.50319900	0.00014900
C	-0.86507900	-0.89951600	-0.00032600
C	-2.20258400	-1.01950200	-0.00026800
C	-2.98777000	0.22264500	-0.00002600
C	-2.90921900	-2.33841400	-0.00042100
H	-3.55526000	-2.43632100	-0.87465900
H	-2.19740300	-3.16459000	-0.00052700
H	-3.55525400	-2.43652900	0.87379600
O	-4.23098200	0.15730500	0.00073100
H	-0.21757300	-1.76742700	-0.00048700
C	1.23079100	0.37169500	-0.00003500
C	1.82756900	-0.25290900	1.26190300
C	1.82770000	-0.25237200	-1.26217800
H	1.46715000	1.43336200	0.00019200
C	3.35039800	-0.11663800	1.25920900
H	1.56230600	-1.31392100	1.30942600
H	1.39520300	0.22948900	2.14015800
C	3.35052800	-0.11609100	-1.25926400
H	1.56246100	-1.31336700	-1.31018800
H	1.39542500	0.23039600	-2.14027500
C	3.95721000	-0.73472400	-0.00013100
H	3.76914900	-0.58196800	2.15295700
H	3.61315900	0.94490400	1.29941300
H	3.76937300	-0.58103200	-2.15316900
H	3.61329000	0.94546900	-1.29897900
H	5.04106900	-0.60632700	-0.00004800
H	3.76266500	-1.81228900	-0.00037500

7-8 adduct (ADA-DAD)

O	0.43706500	3.25123600	0.16229900
N	3.31948900	0.42282600	-0.01292500
N	1.08097100	1.09162500	0.07361100
C	2.02138800	0.07445200	-0.12802300
C	1.33679300	2.43284500	0.08153400
C	3.66713200	1.72521200	0.55048200
C	2.78552700	2.80554800	-0.04501100
H	4.70959300	1.93032700	0.32438000
H	2.99541200	2.92221000	-1.11146900
H	0.09524700	0.78880600	0.05709200
O	1.62050100	-1.05403800	-0.39207100
H	2.94118100	3.76468600	0.44212300

H	3.55685500	1.70403000	1.63819800
C	4.35522300	-0.61418100	-0.11427000
C	5.37160600	-0.29394300	-1.21014200
C	5.04351500	-0.85475000	1.22981500
H	3.82871700	-1.52420800	-0.39609100
C	6.39884300	-1.42116100	-1.32528800
H	5.89268800	0.63899100	-0.97539000
H	4.84928300	-0.14957000	-2.15709800
C	6.07068700	-1.98052600	1.10765600
H	5.55228400	0.05981300	1.55016900
H	4.29327300	-1.09539600	1.98556600
C	7.09171100	-1.67740000	0.01213200
H	7.13197300	-1.17671500	-2.09498500
H	5.89095800	-2.33531200	-1.64706900
H	6.57006000	-2.13112200	2.06550700
H	5.55143600	-2.91295800	0.86728700
H	7.80010200	-2.50166000	-0.08211900
H	7.66909400	-0.79099400	0.29365000
C	-2.75424800	1.19127100	-0.03194100
C	-2.16446100	-1.05426500	0.08586200
C	-4.10188100	0.78357800	-0.05266500
C	-4.32717300	-0.58150200	-0.00297000
N	-2.40329200	2.48259500	-0.09361600
N	-1.80325700	0.25133000	0.03858900
H	-3.12451200	3.18335300	-0.07977000
H	-1.43357600	2.76043900	0.01057400
N	-1.14236100	-1.94585500	0.20533800
H	-0.21091500	-1.63852400	-0.04943300
H	-1.37384500	-2.90757300	0.01943300
N	-5.68615300	-0.73010100	-0.03516600
N	-5.29472600	1.47641100	-0.11419500
C	-6.20573500	0.54082800	-0.10175200
N	-3.40426800	-1.54673200	0.06309400
C	-6.38347500	-2.01399100	-0.00391900
H	-6.06781800	-2.58727600	-0.87550200
H	-6.04580400	-2.55069400	0.88229000
C	-7.89053900	-1.85531900	0.01225900
H	-8.34541600	-2.84365400	0.04765600
H	-8.22256900	-1.29878000	0.88841300
H	-8.25006300	-1.35022400	-0.88384700
H	-7.26847000	0.70954900	-0.13707000

9-8 adduct (ADA-DAD)

O	0.43931000	3.22525500	0.31041600
N	3.33755300	0.45234500	-0.03396800
N	1.09420000	1.06970100	0.08309800

C	2.01371500	0.05966600	-0.03921100
C	1.35928600	2.42106100	0.21230900
C	3.66844700	1.77315900	0.10361600
C	2.76123500	2.75805400	0.22054900
H	0.10205200	0.77457300	0.08935200
O	1.66897000	-1.10815500	-0.14327400
C	4.39708100	-0.57686300	-0.11509500
C	5.31594600	-0.34531200	-1.31277900
C	5.17613000	-0.65847700	1.19540400
H	3.86665800	-1.51446300	-0.26416900
C	6.37211900	-1.44920100	-1.38252200
H	5.81951200	0.62087600	-1.21615600
H	4.72136600	-0.31679600	-2.22708600
C	6.23707800	-1.75574600	1.11324200
H	5.66354600	0.30186000	1.38982300
H	4.48393100	-0.84781000	2.01725900
C	7.16595700	-1.53689200	-0.07998500
H	7.03865300	-1.26429900	-2.22540100
H	5.87833500	-2.40732300	-1.56889700
H	6.80706600	-1.78612700	2.04225100
H	5.74134100	-2.72544000	1.01005400
H	7.89858600	-2.34267500	-0.14015100
H	7.72403000	-0.60642100	0.06432800
C	-2.70628000	1.19046500	-0.06505900
C	-2.14309800	-1.04920900	0.20882700
C	-4.05491100	0.79042300	-0.12360400
C	-4.29516900	-0.56767700	-0.00512400
N	-2.34060300	2.47324300	-0.18725100
N	-1.76736300	0.24852800	0.10063300
H	-3.05954600	3.17623500	-0.22040200
H	-1.38085700	2.75311800	-0.00746100
N	-1.13757800	-1.94142500	0.42970000
H	-0.19288800	-1.66132300	0.19685600
H	-1.37256900	-2.91001400	0.28985200
N	-5.65274400	-0.70869900	-0.08622000
N	-5.23773200	1.48682600	-0.27468600
C	-6.15715800	0.55986200	-0.24764900
N	-3.38467700	-1.53347600	0.15825100
C	-6.36235600	-1.98423800	-0.01379600
H	-6.05109700	-2.59125900	-0.86398200
H	-6.03043200	-2.49140600	0.89155800
C	-7.86774500	-1.81029700	-0.00550600
H	-8.33240200	-2.79117100	0.07824300
H	-8.19269900	-1.20793300	0.84258400
H	-8.22380900	-1.34643400	-0.92493300
H	-7.21605700	0.73386400	-0.33682300
H	3.05373000	3.78934000	0.32368800
H	4.72825700	1.98226400	0.11388000

10-8 adduct (ADA-DAD)

O	0.41404100	3.03383700	0.23296300
N	3.21532600	0.17001900	-0.04721100
N	0.99879900	0.85408800	0.05752300
C	1.88723600	-0.18682400	-0.03988700
C	1.30611200	2.19566100	0.15197300
C	3.58667000	1.48947200	0.05521500
C	2.72086200	2.51425600	0.15037600
H	-0.00255000	0.59260700	0.07144300
O	1.50360300	-1.34701200	-0.11300500
C	4.24761200	-0.88618500	-0.11676400
C	5.15971700	-0.70021200	-1.32724400
C	5.03800100	-0.96467500	1.18748700
H	3.69249200	-1.81302100	-0.24300500
C	6.18729600	-1.83132900	-1.38809300
H	5.68769500	0.25480100	-1.25293400
H	4.55638600	-0.67281700	-2.23588900
C	6.07093900	-2.08935700	1.11425700
H	5.55037600	-0.01354500	1.36171700
H	4.34912300	-1.12316500	2.01862000
C	6.99207100	-1.91554500	-0.09203100
H	6.84999300	-1.67871300	-2.24046200
H	5.66833200	-2.78016200	-1.55238100
H	6.65002000	-2.11729700	2.03777000
H	5.55031900	-3.04815600	1.03410700
H	7.70361000	-2.74057600	-0.14417500
H	7.57502900	-0.99702900	0.02928500
C	-2.79568100	1.10774400	-0.09926100
C	-2.30475800	-1.14145100	0.22865700
C	-4.15649200	0.75026700	-0.14905200
C	-4.44061700	-0.59610100	0.00202300
N	-2.38850600	2.37473100	-0.25183200
N	-1.88764000	0.14047000	0.08955700
H	-3.08426000	3.09971000	-0.30215800
H	-1.42001300	2.62640000	-0.07692900
N	-1.32866300	-2.05996500	0.47096600
H	-0.37411400	-1.81731900	0.23430700
H	-1.59540100	-3.02367200	0.35754200
N	-5.80227500	-0.69462800	-0.07568800
N	-5.31600100	1.48111000	-0.31714800
C	-6.26503800	0.58540000	-0.26813300
N	-3.56165000	-1.58650600	0.18854000
C	-6.55206700	-1.94517100	0.02330600
H	-6.26478400	-2.57672600	-0.81736700
H	-6.23089100	-2.44629700	0.93583700
C	-8.05122200	-1.72370100	0.03640400
H	-8.54564400	-2.68815100	0.13823200

H	-8.35276000	-1.09788200	0.87612000
H	-8.39781700	-1.26405200	-0.88874900
H	-7.31768200	0.79186800	-0.36168300
H	4.65351000	1.66344700	0.05510400
C	3.13046000	3.94789400	0.25614300
H	2.71273500	4.52973700	-0.56618200
H	2.75828600	4.38812600	1.18190100
H	4.21453500	4.04120300	0.23504500

11-8 adduct (ADA-DAD)

O	0.28505300	2.54864800	0.13707500
N	2.78288500	-0.60945400	-0.00790200
N	0.64604000	0.31497400	0.04903900
C	1.41713200	-0.81771500	-0.01109200
C	1.07940500	1.62428300	0.10460700
C	3.29462700	0.65518400	0.05513500
C	2.52438500	1.75456800	0.11587400
H	-0.38266400	0.15926900	0.05502900
O	0.91562200	-1.92906600	-0.06415600
C	3.69606700	-1.77194600	-0.09756300
C	4.47775900	-1.75314200	-1.40851300
C	4.61879300	-1.85194900	1.11637500
H	3.04087900	-2.63984500	-0.09357400
C	5.37660600	-2.98645800	-1.50129200
H	5.09597400	-0.85111600	-1.45284200
H	3.78108600	-1.71597200	-2.24728400
C	5.51263200	-3.08805600	1.01096600
H	5.25042000	-0.95992200	1.16170400
H	4.02029100	-1.87877600	2.02809600
C	6.30788000	-3.08430100	-0.29379600
H	5.95106000	-2.95319800	-2.42734000
H	4.74983700	-3.88193000	-1.54543100
H	6.18376400	-3.12728100	1.86929000
H	4.88878800	-3.98569600	1.05034700
H	6.92054200	-3.98403800	-0.36215300
H	6.99174200	-2.22977700	-0.29613400
C	-3.05727400	0.90567400	-0.30815900
C	-2.80583100	-1.28987600	0.41719200
C	-4.44612600	0.68423800	-0.33136000
C	-4.87113900	-0.57613300	0.05402000
N	-2.51707600	2.08042000	-0.67070900
N	-2.25685400	-0.10067100	0.06809400
H	-3.14030100	2.85697800	-0.82039200
H	-1.55340500	2.28162100	-0.42503000
N	-1.92854300	-2.24979400	0.83057700
H	-0.96877200	-2.16712300	0.51879300

H	-2.30240500	-3.18404700	0.87053000
N	-6.23463100	-0.54673300	-0.03391500
N	-5.52205600	1.48804500	-0.65160500
C	-6.55986400	0.71865100	-0.46177600
N	-4.10134100	-1.60126500	0.43387700
C	-7.11259500	-1.66705000	0.29863300
H	-6.81482400	-2.51503200	-0.31739700
H	-6.92707900	-1.93523600	1.33856100
C	-8.57668100	-1.34000600	0.08502800
H	-9.17161300	-2.21225000	0.35006500
H	-8.89635200	-0.50944200	0.71376800
H	-8.78258100	-1.09344200	-0.95632800
H	-7.58485800	1.01042600	-0.61601700
H	4.37287600	0.72309200	0.05300000
Br	3.26681700	3.47747500	0.22227200

3. References

[1] M. R. Willcott, *J. Am. Chem. Soc.*, 2009, **131**, 13180–13180.

[2] C. Frassineti, S. Ghelli, P. Gans, A. Sabatini, M. S. Moruzzi and A. Vacca, *Anal. Biochem.*, 1995, **231**, 374–382.

[3] W. E. Vallejo Narváez, E. I. Jiménez, E. Romero-Montalvo, A. Sauza-De La Vega, B. Quiroz-García, M. Hernández-Rodríguez and T. Rocha-Rinza, *Chem. Sci.*, 2018, **9**, 4402–4413.

[4] www.supramolecular.org (accessed from January to April 2018)

[5] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.

[6] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, et al. Gaussian 09; Gaussian, Inc., Wallingford, CT, 2013.

[7] Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157–167.

[8] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378–6396.

[9] Keith, T. A. AIMAll (Version 16.10.31); TK Gristmill Software, Overland Parks KS, USA, 2016 (aim.tkgristmill.com).

[10] M. A. Blanco, A. Martín Pendás and E. Francisco, *J. Chem. Theory Comput.*, 2005, **1**, 1096–1109.

[11] J. M. Guevara-Vela, R. Chávez-Calvillo, M. García-Revilla, J. Hernández-Trujillo, O. Christiansen, E. Francisco, Á. Martín Pendás and T. Rocha-Rinza, *Chem. A Eur. J.*, 2013, **19**, 14304–14315.

[12] E. Francisco, J. L. Casals-Sainz, T. Rocha-Rinza and A. Martín Pendás, *Theor. Chem. Acc.*, 2016, **135**, 170.

[13] (a) J. M. Guevara-Vela, E. Romero-Montalvo, V. A. Mora Gómez, R. Chávez-Calvillo, M. García-Revilla, E. Francisco, Á. M. Pendás and T. Rocha-Rinza, *Phys. Chem. Chem. Phys*., 2016, **18**, 19557–19566. (b) E. Romero-Montalvo, J. M. Guevara-Vela, W. E. Vallejo Narváez, A. Costales, Á. M. Pendás, M. Hernández-Rodríguez and T. Rocha-Rinza, *Chem. Commun*., 2017, **53**, 3516–35129.

[14] E. Espinosa, E. Molins and C. Lecomte, *Chem. Phys. Lett*., 1998, **285**, 170–173.

[15] A. Buschauer, *J. Med. Chem*., 1989, **32**, 1970–1977.

[16] Hannon, C. L.; Bell, D. A.; Kelly-Rowley, A. M.; Cabell, L. A.; Anslyn, E. V. *J. Phys. Org. Chem.* 1997, **10**, 396–404.

[17] E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2006.

[18] C.-H. Li and T. D. Stewart, *J. Am. Chem. Soc.*, 1937, **59**, 2596–2599.

[19] I. Despotović and R. Vianello, *Chem. Commun.* , 2014, **50**, 10941–10944.