Supplementary Material

Contents

Table S1. Comparison of the sensing properties of different Spm/Spd selective optical probes.

Probe	Detection technique	Selectivity	Limit of detection	Application	Reference
Tetraphenylethylene derivative	Fluorescence "turn on"	For Spm and Spd	0.70 µM (Spm) 1.17 µM (Spd)	Aqueous media and urine	This study
Sulfonated derivative	Fluorescence "turn on"	For Spm and Spd	0.6 µM (Spm)	Aqueous media and artificial urine	Kim *et al.*, 2016
Polymer-Surfactant complexation	Fluorescence "turn off"	For Spm	66 ppb	Aqueous media and urine	Malik *et al.*, 2016
Tetraphenylethylene conjugated pentiptycene	Fluorescence "turn on"	For Spm	0.3 µM	Artificial urine	Huang *et al.*, 2021
Chemosensor based on pyrocatechol violet and anionic phenylboronic acid	Abs	For Spm	6.24 µM	Aqueous media	Fukushima *et al.*, 2021
Ionic self-assembly of benzimidazolium based dipod and dodecylsulfate	Fluorescence "turn off"	For Spm	ENS1 - 6 nM ENS2- 500 nM	Urine and blood serum	Tripathi *et al.*,2018
Terphenyl derivative	Fluorescence "turn on"	For Spd	46 nM	Aqueous media and artificial urine	Tejpal *et al.*, 2018

Kim, T. I.; & Kim, Y. Analyte-directed formation of emissive excimers for the selective detection of polyamines. *ChemComm* **2016**, *52*, 10648-10651.

Malik, A. H.; Hussain, S.; Iyer, P. K. Aggregation-induced FRET via polymer–surfactant complexation: A new strategy for the detection of spermine. *Anal. Chem.* **2016**, *88*, 7358-7364.

Huang, J.; Ye, W.; Zha, S.; Tao, Y.; Yang, M.; Huang, K.; Lee, C. S. Sensitive and responsive pentiptycene-based molecular fluorescence chemosensor for detection of polyamines. *J. Lumin.* **2021**, *232*, 117856.

Fukushima, Y.; Aikawa, S. Colorimetric chemosensor for spermine based on pyrocatechol violet and anionic phenylboronic acid in aqueous solution. *Microchem. J.* **2021**, *162*, 105867.

Tripathi, N.; Singh, P.; Luxami, V.; Mahajan, D.; Kumar, S. Spermine detection from urine and blood serum using ionic self-assembly of benzimidazolium based dipod and dodecylsulfate. *Sens.* **2018**, *270*, 552-561.

Tejpal, R., Kumar, M., & Bhalla, V. Spermidine induced aggregation of terphenyl derivative: An efficient probe for detection of spermidine in living cells. *Sens. Actuators B: Chem.* **2018**, *258*, 841-849.

Compound 1 ^{1}H NMR (300 MHz, DMSO-d_6) δ 13.36 (s, 2H), 8.17 (s, 2H), 7.19 – 7.04 (m, 6H), 7.00 – 6.94 (m, 4H), 6.89 (d, J = 8.8 Hz, 4H), 6.81 (d, J = 8.9 Hz, 4H), 5.28 (s, 4H), 5.06 (s, 4H).
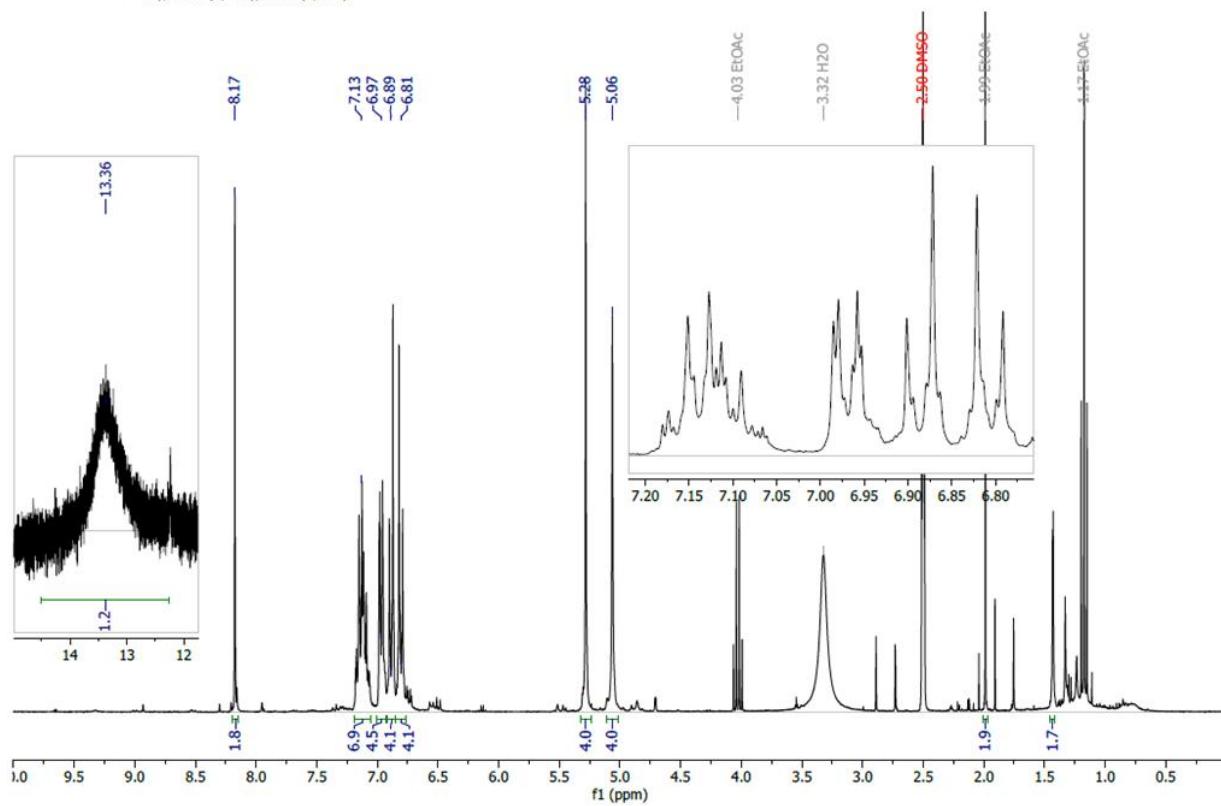
Figure S1. ^{1}H NMR compound 1 in DMSO-d_6.

Compound 1 ^{13}C NMR (75 MHz, DMSO) δ 168.60, 156.63, 143.75, 142.48, 139.70, 138.99, 135.95, 132.03, 130.72, 127.88, 125.99, 113.87, 60.86, 50.55, 39.52.
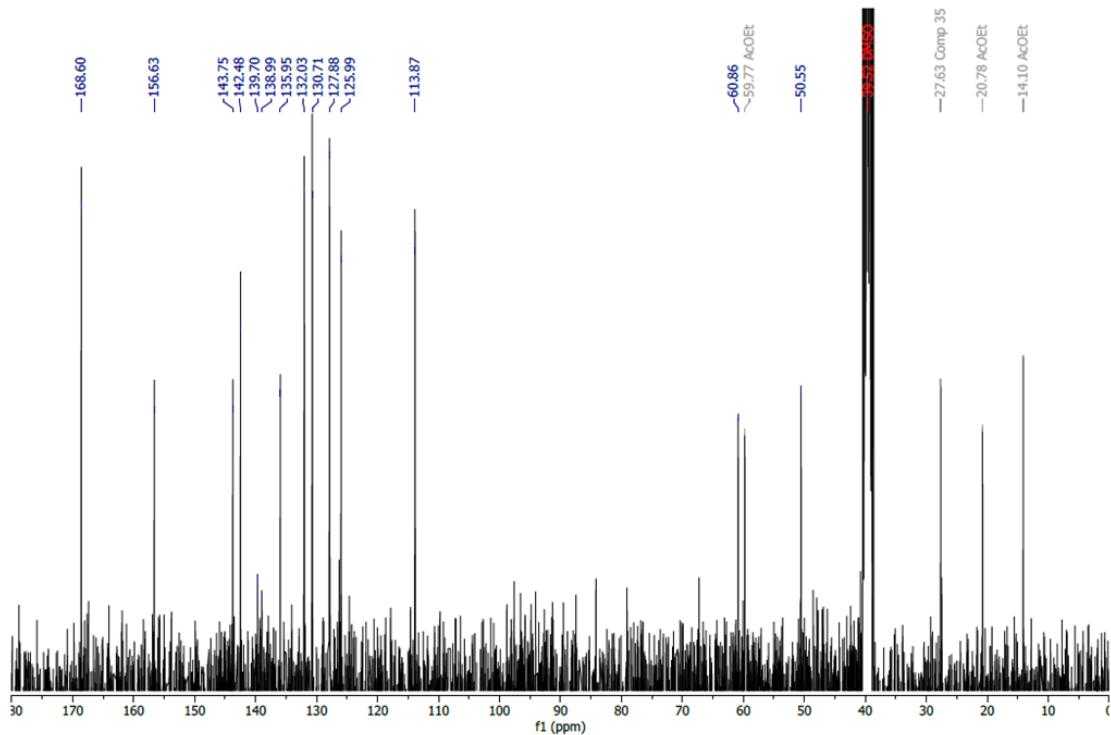
Figure S2. ^{13}C NMR compound 1 in DMSO-d_6.
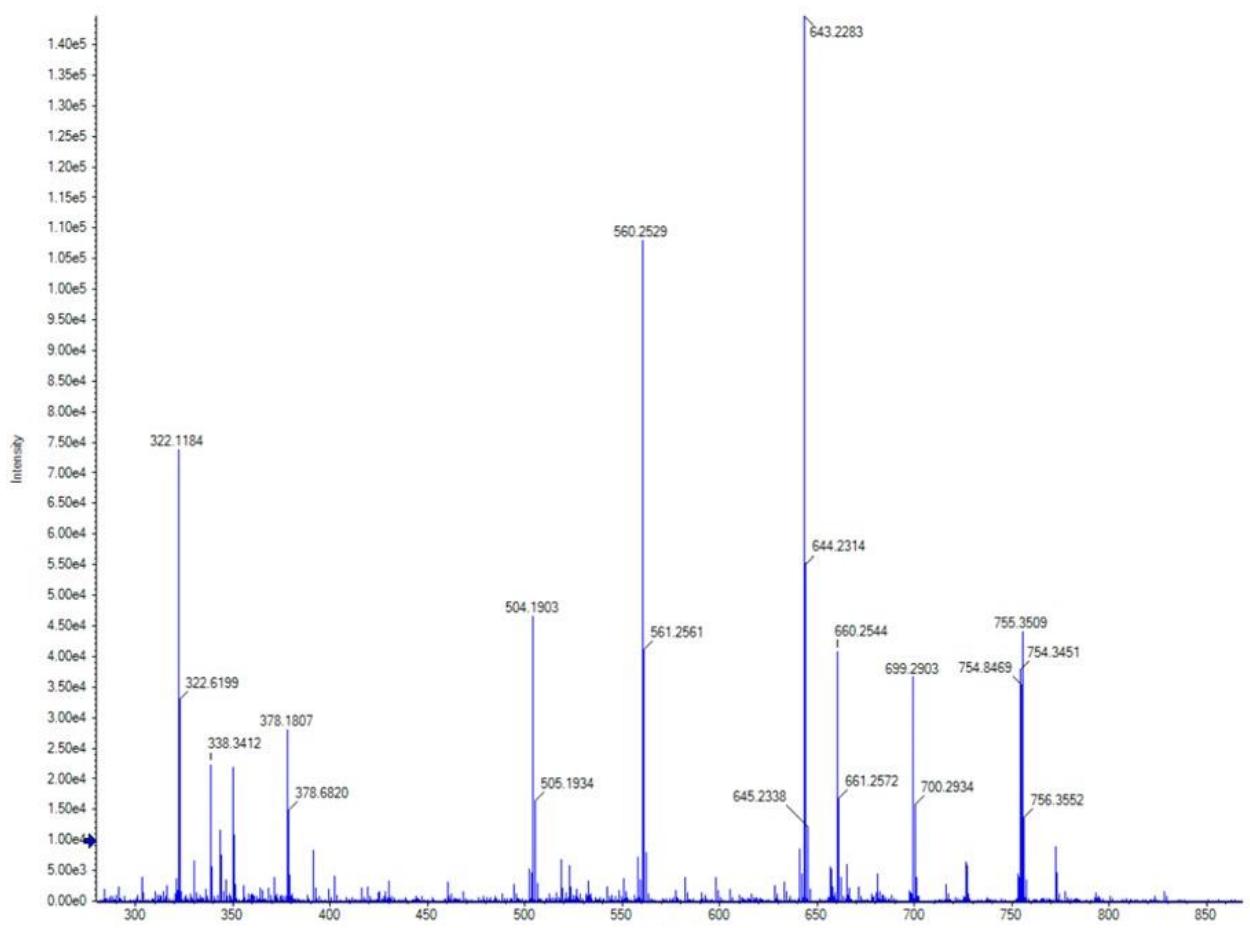
Figure S3. Mass Spectroscopy data of compound 1.

Compound 2 ^{1}H NMR (300 MHz, Chloroform-d) δ 7.15 – 7.06 (m, 6H), 7.06 – 7.00 (m, 4H), 6.95 (d, J = 8.9 Hz, 4H), 6.64 (d, J = 8.8 Hz, 4H), 3.74 (s, 6H).
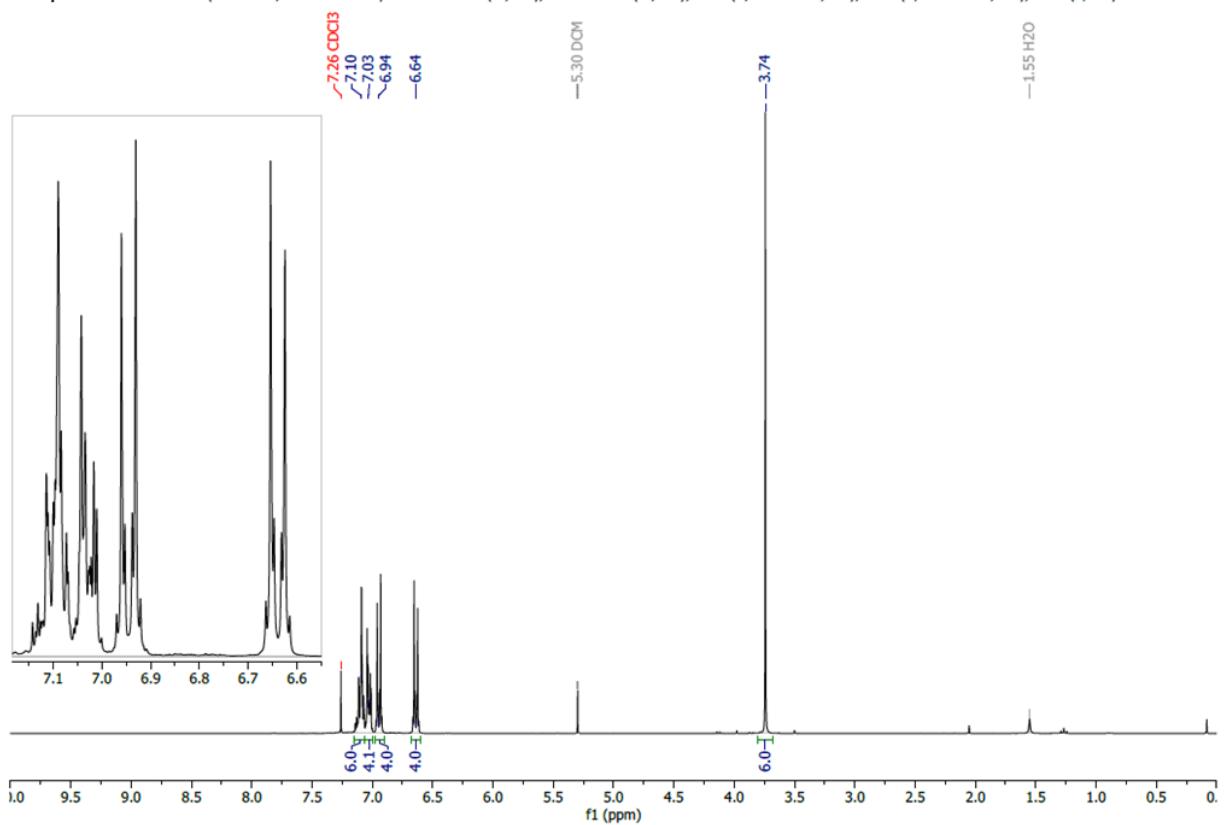
Figure S4. ^{1}H NMR compound 2 in CDCl$_3$-d.

Compound 3 ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.30 (s, 2H), 7.17 – 7.02 (m, 6H), 6.95 – 6.91 (m, 4H), 6.74 (d, J = 8.6 Hz, 4H), 6.48 (d, J = 8.6 Hz, 4H).
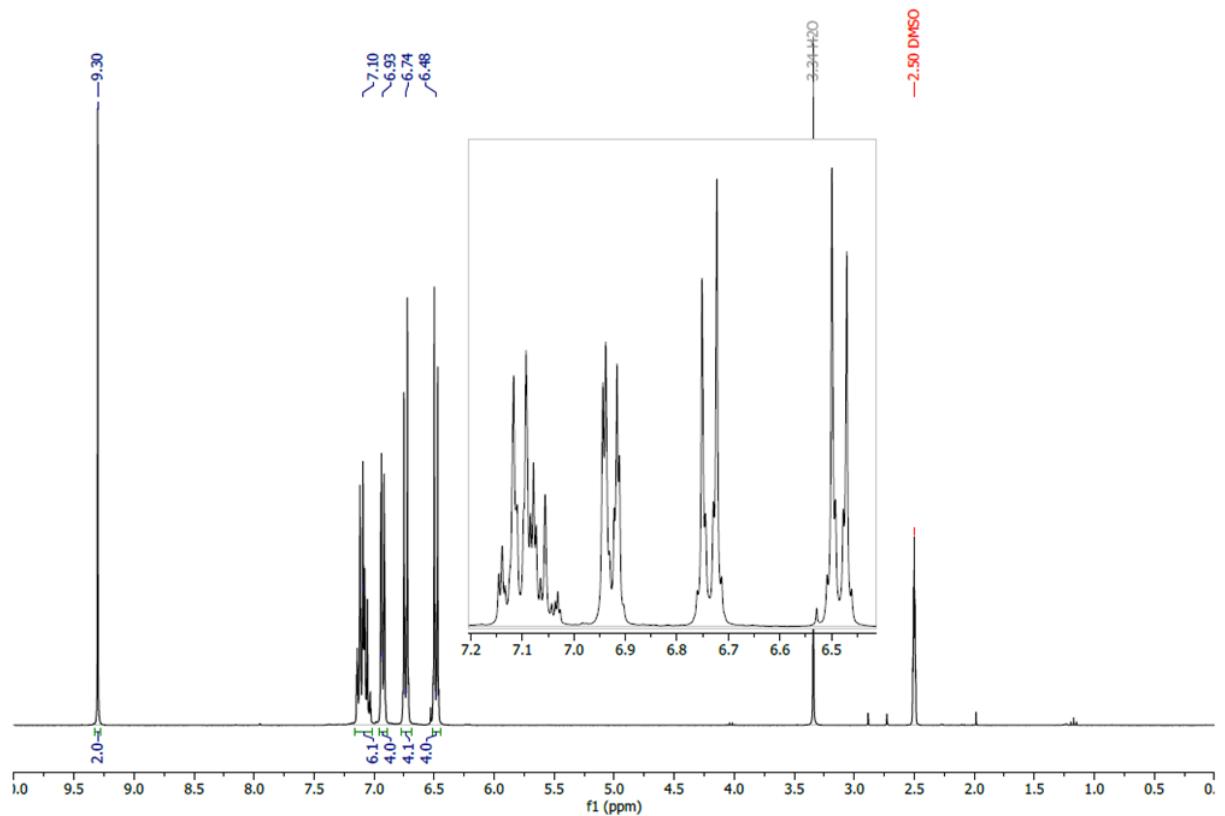
Figure S5. ^{1}H NMR compound 3 in DMSO-d$_6$.

Compound 3 ^{13}C NMR (75 MHz, DMSO) δ 155.86, 144.17, 140.61, 137.69, 134.12, 132.03, 130.76, 127.74, 125.94, 114.56.
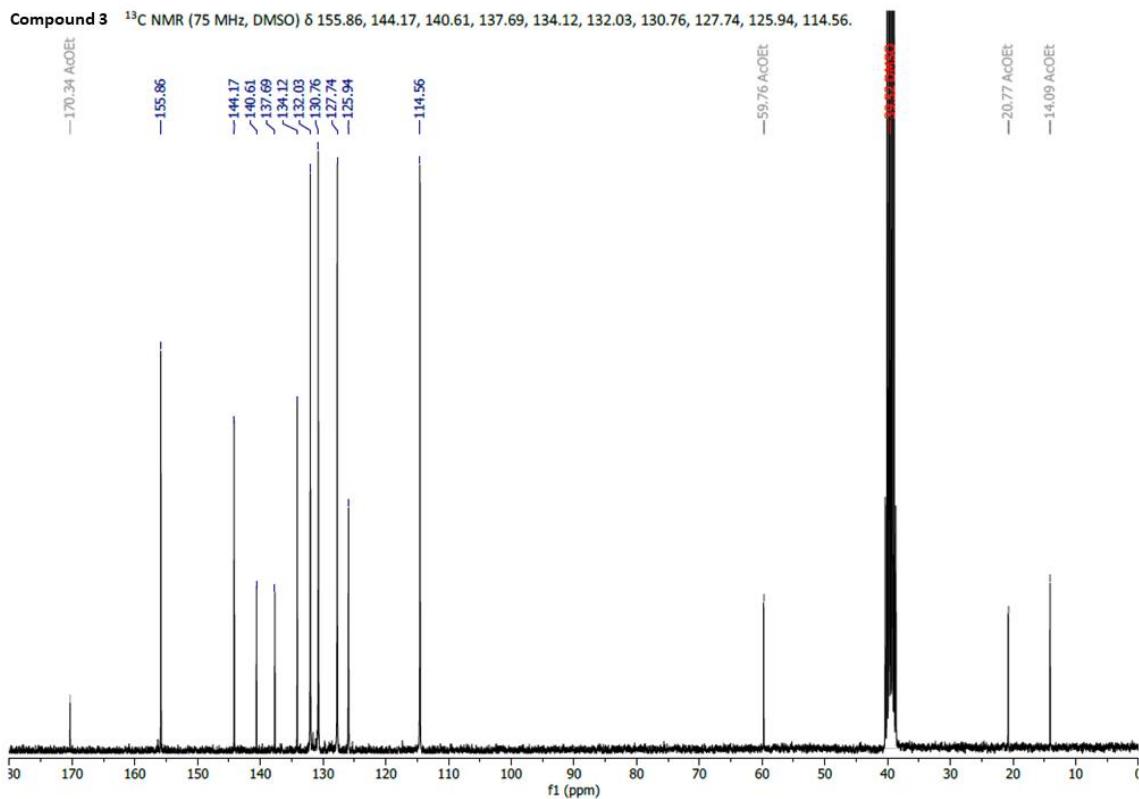
Figure S6. ^{13}C NMR compound 3 in DMSO-d$_6$.

Compound 4 ^{1}H NMR (300 MHz, DMSO-d$_6$) δ 7.19 – 7.07 (m, 6H), 7.00 – 6.92 (m, 4H), 6.88 (d, J = 8.7 Hz, 4H), 6.73 (d, J = 8.8 Hz, 4H), 4.71 (d, J = 2.4 Hz, 4H), 3.54 (t, J = 2.3 Hz, 2H).
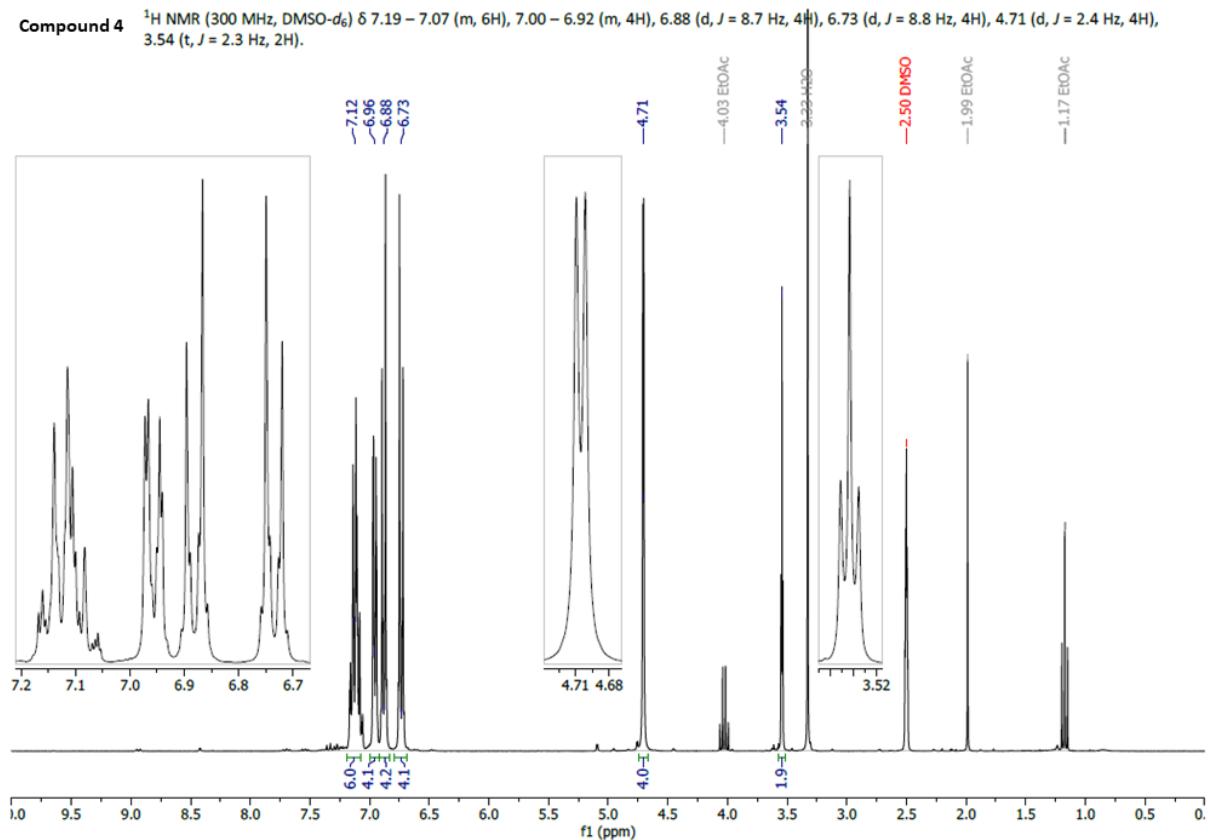
Figure S7. ^{1}H NMR compound 4 in DMSO-d$_6$.

Compound 4 ^{13}C NMR (75 MHz, DMSO) δ 155.74, 143.63, 139.53, 139.23, 136.27, 131.90, 130.67, 127.85, 126.30, 114.01, 79.21, 78.19, 55.28.
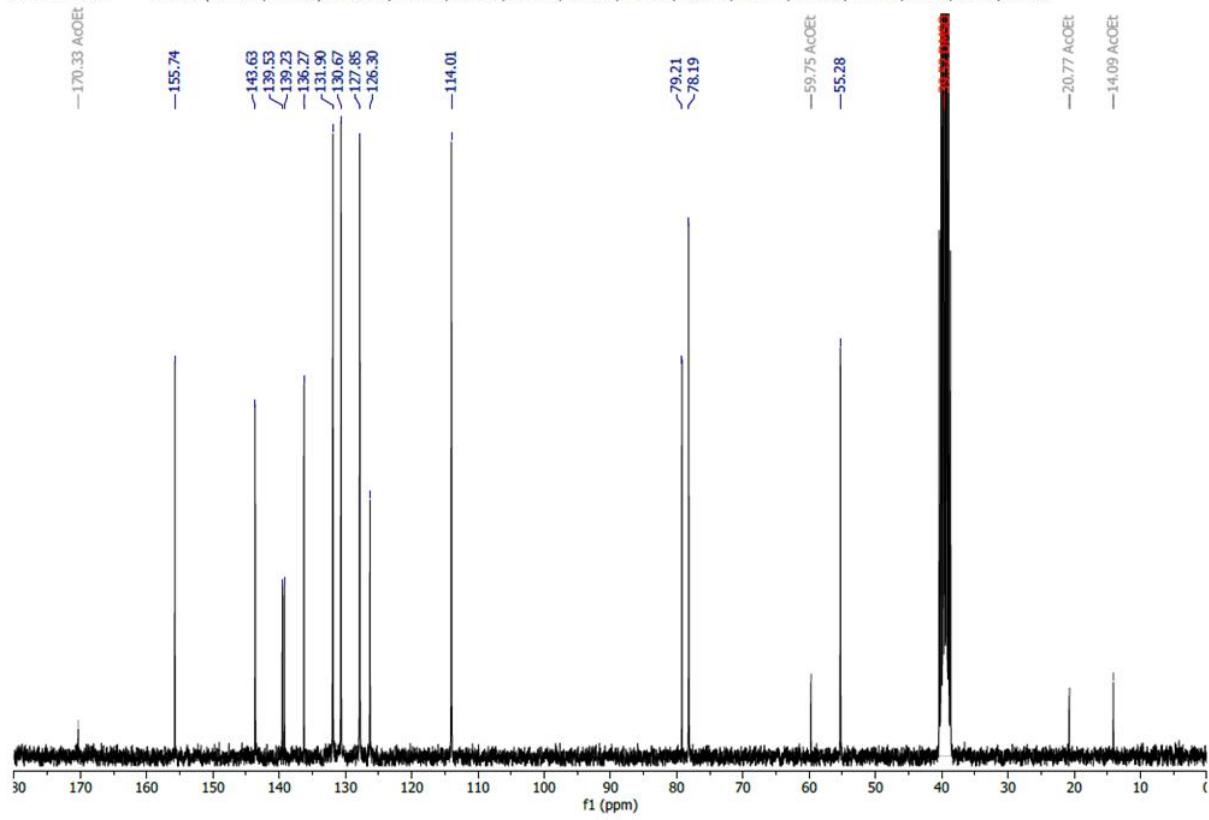
Figure S8. ^{13}C NMR compound 4 in DMSO-d_6.

Compound 5 ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.95 (s, 2H), 1.45 (s, 9H).
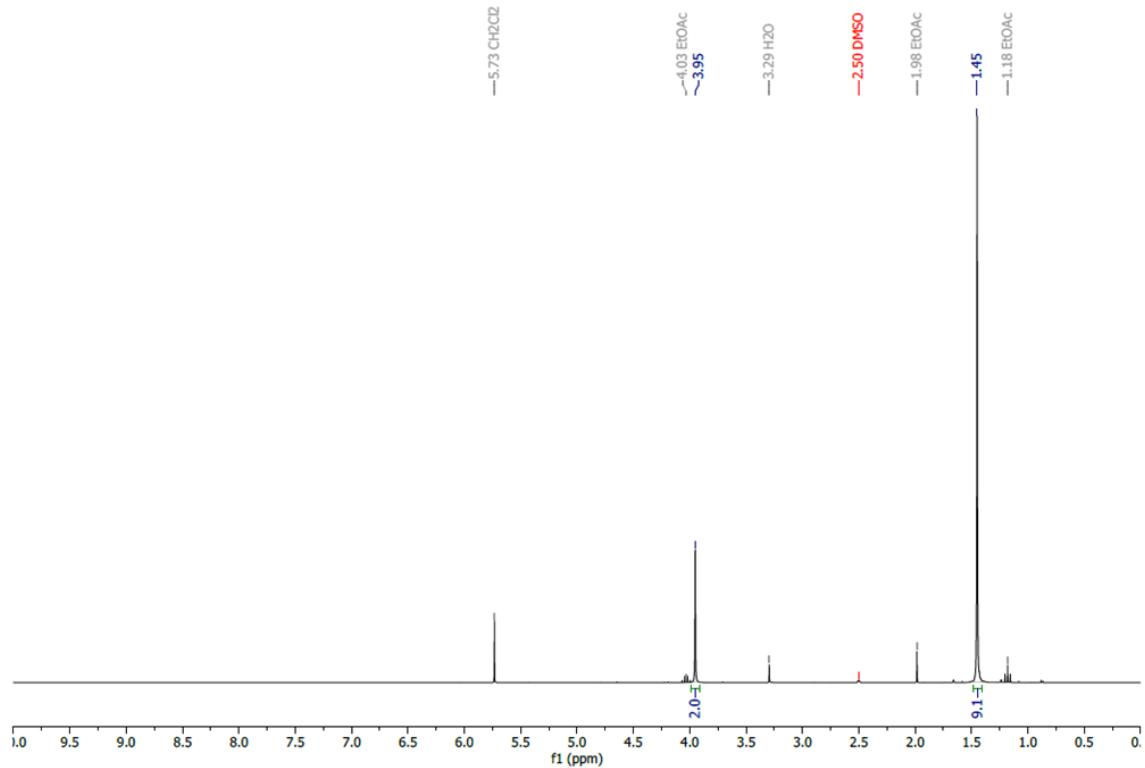
Figure S9. ^{1}H NMR compound 5 in DMSO-d_6.

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Compound 6 ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.17 (s, 2H), 7.17 – 7.05 (m, 6H), 6.99 – 6.94 (m, 4H), 6.88 (d, J = 8.8 Hz, 4H), 6.80 (d, J = 8.9 Hz, 4H), 5.28 (s, 4H), 5.06 (s, 4H), 1.43 (s, 18H).
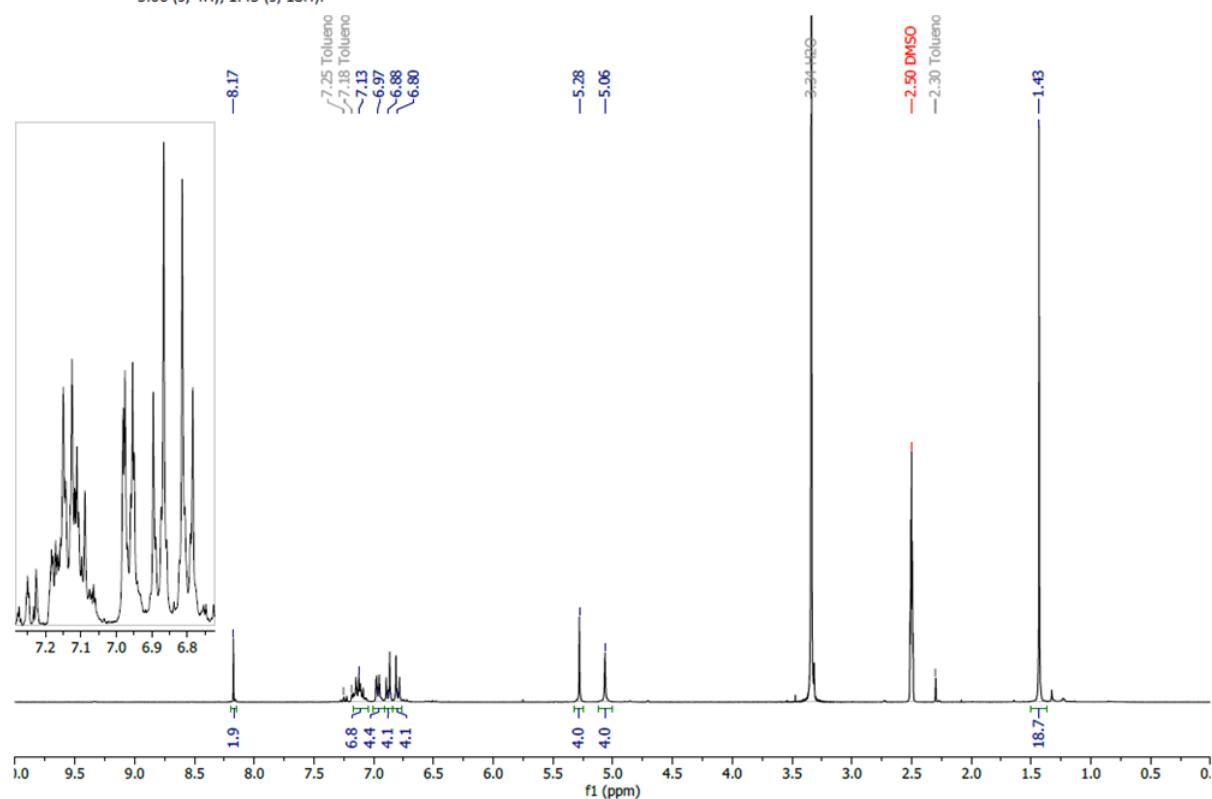
Figure S10. ^{1}H NMR compound 6 in DMSO-d$_6$.

Compound 6 ^{13}C NMR (75 MHz, DMSO) δ 166.22, 156.60, 143.74, 142.55, 139.68, 138.98, 135.94, 132.01, 130.70, 127.86, 126.26, 126.00, 113.85, 82.38, 60.82, 50.94, 27.63.
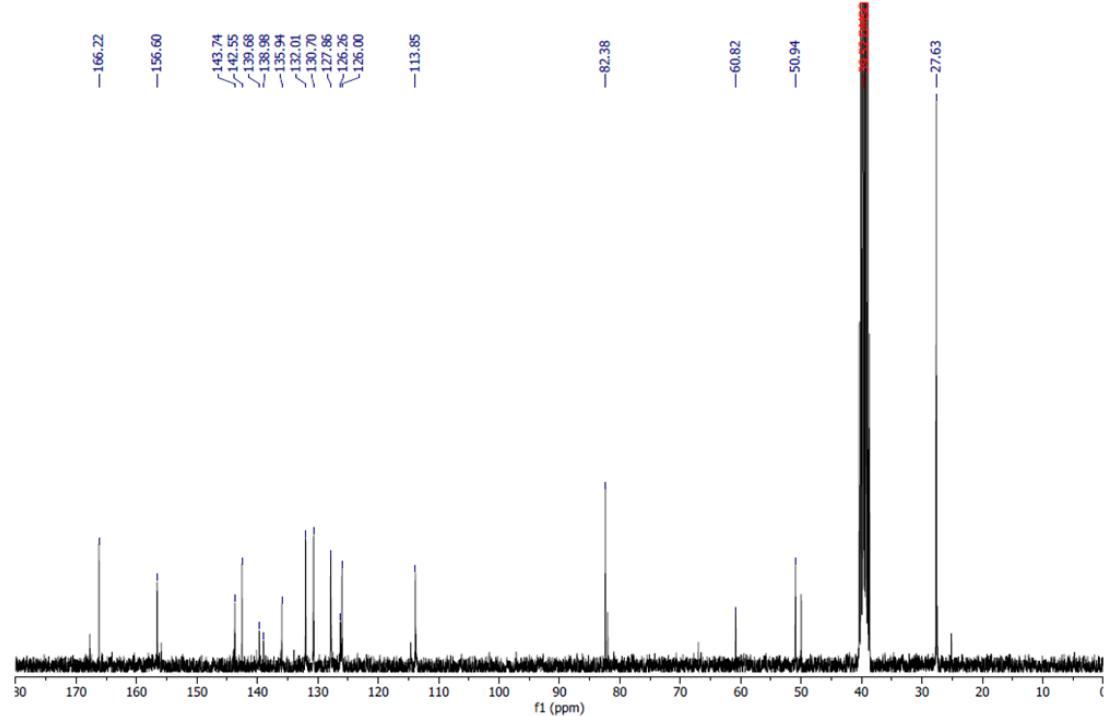
Figure S11. ^{13}C NMR compound 6 in DMSO-d$_6$.

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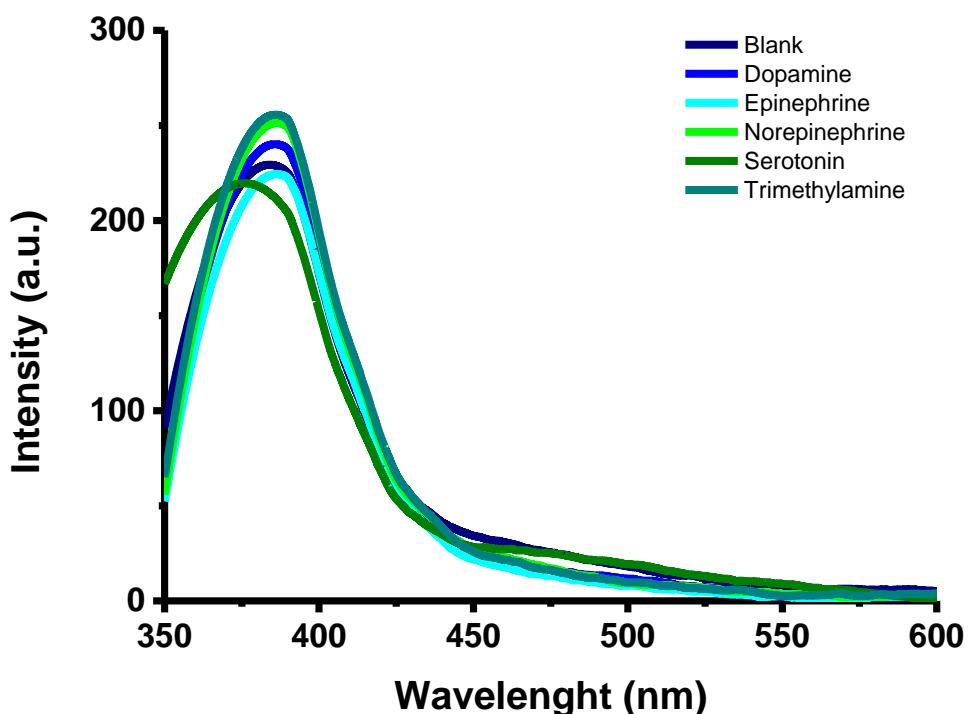
Figure S12. 50 μM of the sensor in acetonitrile in the presence of 2 equiv of different amines (in phosphate buffer =7.4) (final solvent acetonitrile:water 98:2) (λem at 473 nm, λexc = 340 nm).
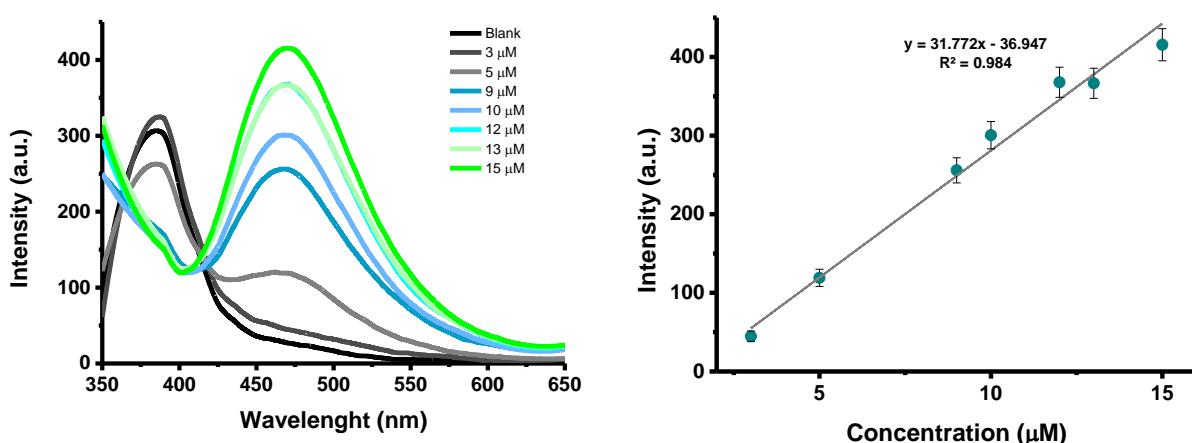
Figure S13. (left) Fluorescence titration of sensor (50 μM in acetonitrile) with Spd (in urine). (final solvent acetonitrile:water 98:2) (right) Calibration curve: emission at λem = 470 nm.

Determination of recovery and accuracy of the method

Table S2. Recovery and accuracy of the method were calculated according to reference K. A. Rawat, R. K. Singhal, S. K. Kailasa, RSC Adv. 6 (2016) 32025-32036.

Analite	Known concentration (μM)	Found concentration (μM)	Recovery %[a]	Accuracy %[b]
Spm	10	9	90	-10
Spd	18	24	133	33

[a] recovery % (found concentration/Known concentration) x 100

[b] accuracy % (found concentration – known concentration/Known concentration) x 100

Complete citation for reference [44] in the main text.

Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

Computational methods for theoretical calculations.

a) Computational methods for molecular dynamics simulation.

The protonation state of the amines was obtained with the Chemicalize tool[41] of ChemAxon. The main species obtained for each amine at the pH of 7.4 used at the experimental tests is shown in the legend of Figure 4. All the molecules under study were parameterized following the protocol stablished by AMBER. First, geometric optimization at the HF/6-31G (d) [1] *ab initio* method to obtain the equilibrium atom coordinates and the RESP charges on the atoms of each molecule was performed. Subsequently, the antechamber module was used together with the *general AMBER force field* (GAFF) [2] for organic molecules included in the AmberTools18 [3] to generate the parameters file for each molecule. For building the system, an amine molecule was placed at approximately 6 Å from the sensor. All molecular dynamics simulations were performed using the Amber18 program [3]. The implicit Generalized Born solvation model [4] implemented in sander was used to simulate the role of the solvent stabilizing ionic charges. Long range interactions were not considered by setting a cutoff of 999. The simulation protocol included a short geometric optimization process of the system (500 steps) to relax the possible deviations from the equilibrium positions when constructing the system, followed by a molecular dynamics simulation of 50 ns with a time step of 0.001 ps at constant temperature of 300 K, resulting on a molecular dynamics trajectory formed by 50,000 snapshots of every amine together with the

chemosensor. The *hbond* utility considers a hydrogen bond, A···H-D, if the distance between an acceptor heavy atom of the sensor, A, and a polar heavy atom of the amine, D, bound to a polar hydrogen, H, is less of 3.0 Å, and the angle formed by A-H-D is less of 135.0 degrees.

To obtain the binding energy of each sensor:amine complex, the *cluster* command of the *ptraj* program of Amber12 [5] was used to process the 50,000 snapshots of the molecular dynamic trajectories to end up with 250 representative structures which were submitted for a binding energy calculation.

1. Cornell, W. D.; P. Cieplak, C. I. Bayly, I. R. Gould, K. M. Merz Jr., D. M. Ferguson, D. C. Spellmeyer, T. Fox, J. W. Caldwell, P. A. Kollman. A second generation force field for the simulation of proteins, nucleic acids, and organic molecules. *J. Am. Chem. Soc.*, **1995**, *117*, 5179–5197. https://doi.org/10.1021/ja00124a002
2. Wang, J.; Wolf, R. M.; Caldwell, J. W.; Kollman, P. A.; Case, D. A. Development and Testing of a General Amber Force Field, *J. Comp. Chem.*, **2004**, *25*, 1157–1174. https://doi.org/10.1002/jcc.20035
3. Case, D. A.; Ben-Shalom, I. Y.; Brozell, S. R.; Cerutti, D. S.; Cheatham III, T. E.; Cruzeiro, V. W. D.; Darden, T. A.; Duke, R. E.; Ghoreishi, D.; Gilson, M. K.; Gohlke, H.; Goetz, A. W.; Greene, D.; Harris, R.; Homeyer, N.; Huang, Y.; Izadi, S.; Kovalenko, A.; Kurtzman, T.; Lee, T. S.; LeGrand, S.; Li, P.; Lin, C.; Liu, J.; Luchko, T.; Luo, R.; Mermelstein, D. J.; Merz, K. M.; Miao, Y.; Monard, G.; Nguyen, C.; Nguyen, H.; Omelyan, I.; Onufriev, A.; Pan, F.; Qi, R.; Roe, D. R.; Roitberg, A.; Sagui, C.; Schott-Verdugo, S.; Shen, J.; Simmerling, C. L.; Smith, J.; SalomonFerrer, R.; Swails, J.; Walker, R. C.; Wang, J.; Wei, H.; Wolf, R. M.; Wu, X.; Xiao, L.; York, D. M.; Kollman, P. A. AMBER 18, **2018**, University of California, San Francisco.
4. Tsui, V.; Case, D. A. Theory and applications of the generalized Born solvation model in macromolecular simulations, *Biopolymers*, **2000–2001**, *56*, 275–291. https://doi.org/10.1002/1097-0282(2000)56:4%3C275::aid-bip10024%3E3.0.co;2-e
5. Case, D. A.; Darden, T. A.; Cheatham III, T. E.; Simmerling, C. L.; Wang, J.; Duke, R. E.; Luo, R.; Walker, R. C.; Zhang, W.; Merz, K. M.; Roberts, B.; Hayik, S.; Roitberg, A.; Seabra, G.; Swails, J.; Götz, A. W.; Kolossváry, I.; Wong, K. F.; Paesani, F.; Vanicek, J.; Wolf, R. M.; Liu, J.; Wu, X.; Brozell, S. R.; Steinbrecher, T.; Gohlke, H.; Cai, Q.; Ye, X.; Wang, J.; Hsieh, M.-J.; Cui, G.; Roe, D. R.; Mathews, D. H.; Seetin, M. G.; Salomon-Ferrer, R.; Sagui, C.; Babin, V.; Luchko, T.; Gusarov, S.; Kovalenko, A.; Kollman, P. A. AMBER 12, **2012**, University of California, San Francisco.

b) Computational methods for DFT calculations.

Selected structures of the complexes between the chemosensor **1** and the biogenic amines/neurotransmitters that remained hydrogen-bonded along the molecular dynamics simulation (that is, Det, Cad, Put, Spm, Spd and Dop) were further optimized at M062X/6-31+G(2d-p)/PCM(acetonitrile) level was carried out taking into account the empirical dispersion through the D3 version of Grimme's dispersion parametrisation as well as the original D3 damping function using Gaussian16 Rev. A.03 package. Also, the isolated chemosensor **1** (in its dicarboxylate form) and the isolated amines/neurotransmitters (in the same protonation state they were simulated through molecular dynamics) were submitted for its optimization at the same theory level.

Furthermore, over the optimized geometries, a frequency calculation was performed to ensure that no imaginary frequencies were present, and the common thermochemical calculations were

performed using a scale factor of 0.952 at the same theory level in order to compute the stabilization of the complex respect to the isolated components.

Energy results for DFT calculations.

The electronic energy, enthalpy, and free energy of the studied species (isolated and forming hydrogen-bonded complexes) are collected in the following table (see Table S3):

Table S3. Computed energies (E, H and G in atomic units, a.u.) for the chemosensor and the biogenic amines/neurotransmitters studied at the same protonation state predicted by Chemicalize and simulated throught molecular dynamics.

Species	E (in a.u.)	H (in a.u.)	G^a (in a.u.)
TPE **1** (dicarboxylate)	-2168.14322459	-2167.541581	-2167.665915
Cad2+	-309.24211844	-309.013680	-309.060097
Dop1+	-516.96428098	-516.761644	-516.810915
Det2+	-325.26680434	-325.048447	-325.093812
Put2+	-269.94342236	-269.743317	-269.785164
Spd3+	-443.60511201	-443.285450	-443.340342
Spm3+	-616.82409867	-616.401341	-616.470399
Spm4+	-617.26603604	-616.826892	-616.895389
1:Cad2+ complex	-2477.45579131	-2476.626897	-2476.773346
1:Dop1+ complex	-2685.16257526	-2684.359040	-2684.506257
1:Det2+ complex	-2493.48397007	-2492.665029	-2492.809916
1:Put2+ complex	-2438.16037466	-2437.359067	-2437.500291
1:Spd3+ complex	-2611.85008179	-2610.930254	-2611.081082
1:Spm3+ complex	-2785.08616218	-2784.062565	-2784.222149
1:Spm4+ complex	-2785.53992547	-2784.500597	-2784.659287

[a]Calculated at 298.15 K. 1 atm and with a scale factor of 0.952.

The energy stabilization of the complexes present in Table S3 was calculated in terms of ΔG ($\Delta G_{stabilization} = G_{complex} - G_{chemosensor} - G_{amine/neurotransmitter}$) at 298.15 K and 1 atm and are depicted in the following Table S4:

Table S4. Stabilization (ΔE. ΔH and ΔG in kcal/mol) of the chemosensor: biogenic amines/neurotransmitters complexes computed at the same protonation state predicted by Chemicalize and simulated through molecular dynamics.

Energy stabilized species	ΔE (in kcal/mol)	ΔG[a] (in kcal/mol)	ΔG[a] per positively charged amine nitrogen (in kcal/mol)
1:Cad2+ complex	-44.2	-29.7	-14.9
1:Dop1+ complex	-34.6	-18.5	-18.5
1:Det2+ complex	-46.4	-31.5	-15.7
1:Put2+ complex	-46.3	-30.9	-15.4
1:Spd3+ complex	-63.8	-47.0	-15.7
1:Spm3+ complex	-74.6	-53.9	-18.0
1:Spm4+ complex	-82.0	-61.5	-15.4

[a]Calculated at 298.15 K. 1 atm and with a scale factor of 0.952.

Cartesian coordinates of optimized DFT structures (complexes between chemosensor **1** and biogenic amines/neurotransmitters and isolated species).

Cad(2+):**1** complex

E = -2477.45579131 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2476.773346 hartree

charge=0; multiplicity=1

O	-5.45852600	-1.58587800	-1.04130000
C	-4.32685500	-2.11430800	-1.13377400
O	-3.30704400	-1.85931900	-0.46524800
C	-4.23525400	-3.20314800	-2.21576500
H	-4.48224400	-2.76045100	-3.18142900
H	-4.96525700	-3.98419200	-1.99903800
N	-2.92304300	-3.80092100	-2.32133400
N	-2.01442600	-3.28851900	-3.14771600
N	-0.91045700	-3.95464800	-2.98531900
C	-2.40546600	-4.81264500	-1.60257300
H	-2.97876800	-5.35687900	-0.87015400
C	-1.10262000	-4.91187200	-2.03967700
C	-0.00543400	-5.81497900	-1.58545300
H	-0.35540200	-6.84200000	-1.47811700
H	0.80856700	-5.78758000	-2.31800600
O	0.48989400	-5.45442300	-0.28785400

C	1.07310700	-4.20909100	-0.23947400
C	0.35385700	-3.13880400	0.28343700
C	0.94957100	-1.88596800	0.34515900
H	0.40072200	-1.04446200	0.75333800
H	-0.66256700	-3.29961900	0.62644500
C	2.37605900	-4.02634000	-0.69363200
H	2.92153500	-4.86981400	-1.10356300
C	2.96450800	-2.76910400	-0.61268200
H	3.98354500	-2.62673100	-0.95815600
C	2.26094900	-1.68202900	-0.08731400
C	2.86934500	-0.32355600	-0.01509200
C	4.05833000	-0.10157700	0.59159100
C	4.78796700	1.19406800	0.48207400
C	5.27464900	1.82707600	1.62979000
C	5.95655500	3.03674300	1.53952700
C	6.18358000	3.61958600	0.29474700
C	5.72596800	2.98330100	-0.85740600
C	5.03296600	1.78101300	-0.76344200
H	4.67324200	1.28867400	-1.66156300
H	5.91090300	3.42231700	-1.83180400
H	6.72009900	4.55910900	0.22219600
H	6.31363900	3.52207900	2.44125900
H	5.10659300	1.37063100	2.60085000
C	4.74166100	-1.14499000	1.40796300
C	6.09335000	-1.43144200	1.19065300
C	6.74222500	-2.40908700	1.93792300
C	6.05369900	-3.10002500	2.93290100
C	4.71419500	-2.80383300	3.17576900
C	4.06412200	-1.83473200	2.41846800
H	3.02028000	-1.60624300	2.60896700
H	4.17437500	-3.32577200	3.95842200
H	6.55982700	-3.85805500	3.52030500
H	7.78658900	-2.62912000	1.74530500

H	6.63473700	-0.88915500	0.42103400
C	2.09391300	0.75626300	-0.68419200
C	1.85551100	1.98462500	-0.06843800
C	1.19390400	3.01969700	-0.72723600
H	1.02331100	3.95448200	-0.20845200
H	2.20538500	2.14783300	0.94603600
C	1.59020500	0.56353200	-1.97823200
H	1.73175400	-0.39412200	-2.47042700
C	0.94683000	1.58550200	-2.65500200
H	0.58759200	1.44644300	-3.66846200
C	0.76820900	2.82988200	-2.04237300
O	0.18364600	3.78481800	-2.81577500
C	0.02124000	5.09075800	-2.27794500
H	0.94387100	5.44016200	-1.80280400
H	-0.17510400	5.72009200	-3.14736700
C	-1.10863800	5.16383300	-1.30194600
N	-0.99610500	5.76568100	-0.09033100
N	-2.13328000	5.67391200	0.53590000
C	-2.39122700	4.67899400	-1.41526300
H	-2.90512800	4.12943000	-2.18648400
N	-2.98071600	5.02646900	-0.25651500
C	-4.28372400	4.61616600	0.21899800
H	-4.55467700	5.26486300	1.05379700
H	-5.01669600	4.74447500	-0.57764300
C	-4.28577600	3.15160200	0.69707500
O	-5.41505400	2.63679600	0.82952000
O	-3.17074100	2.63292700	0.91955400
N	-6.39348200	0.04275100	0.85618800
H	-7.35013400	0.23291200	0.55755000
H	-5.91984400	0.97051500	0.94842200
H	-5.92713900	-0.52444000	0.08618700
C	-6.39226200	-0.75658200	2.11485900
H	-6.94548300	-0.19693100	2.87251700

H	-6.92928300	-1.68214100	1.90195300
C	-4.96518000	-1.03860200	2.56189800
H	-4.99706800	-1.78797900	3.35943600
H	-4.42706500	-1.49430700	1.72043100
C	-4.26297100	0.22558000	3.05641300
H	-4.36800800	1.02834700	2.31914800
H	-4.77187700	0.58365900	3.95824500
C	-2.77861000	0.05271700	3.37906200
H	-2.36770700	1.02611000	3.66601700
H	-2.64893600	-0.61345200	4.23845700
C	-1.93655700	-0.52266300	2.24471000
H	-0.87912400	-0.40832800	2.48366500
H	-2.13685700	-1.58576100	2.09207500
N	-2.20364800	0.15477400	0.93648800
H	-2.65957300	1.10706000	1.02513100
H	-1.34189000	0.29723300	0.40927000
H	-2.80252700	-0.47089300	0.34545900

Det(2+):**1** complex

E = -2493.48397007 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2492.809916 hartree

charge=0; multiplicity=1

O	5.69193400	0.72642400	1.38987100
C	5.14098100	-0.34173500	1.12824400
O	4.85057300	-0.78941700	-0.02424100
C	4.76004500	-1.21422600	2.34109400
H	4.11099800	-0.63903000	3.00170800
H	5.66631500	-1.47854200	2.88704100
N	4.08040800	-2.43865900	1.97328000
N	4.77807200	-3.50404500	1.60703500
N	3.93578000	-4.41569600	1.20619500
C	2.75965500	-2.64144600	1.80079600
H	2.02407400	-1.89188500	2.04214100

C	2.67527800	-3.92516800	1.30560000
C	1.49435700	-4.74796000	0.89303500
H	1.30693500	-4.66428200	-0.18461000
H	1.70570200	-5.79559900	1.11300300
O	0.32363600	-4.42223400	1.61840700
C	-0.45871600	-3.39497100	1.18234600
C	-0.09915500	-2.48377800	0.18987300
C	-0.98993300	-1.47189000	-0.16646300
H	-0.69848600	-0.76240000	-0.93543900
H	0.86407800	-2.53729400	-0.30341300
C	-1.69769000	-3.27650100	1.81668400
H	-1.95339100	-3.98253700	2.59860500
C	-2.57629200	-2.27737800	1.43728200
H	-3.54243400	-2.20110100	1.92590300
C	-2.24646200	-1.36571000	0.42627800
C	-3.21592400	-0.31253100	0.01529600
C	-4.49136500	-0.62317200	-0.32215700
C	-5.55982000	0.40570800	-0.47289000
C	-6.38397000	0.41229600	-1.60258800
C	-7.38594100	1.36721800	-1.74646300
C	-7.59505300	2.31681700	-0.74867000
C	-6.79696200	2.30241900	0.39351100
C	-5.78758100	1.35512200	0.52854200
H	-5.16343700	1.34801000	1.41673600
H	-6.96199200	3.02840900	1.18222800
H	-8.37957600	3.05757400	-0.85664400
H	-8.00603000	1.36699700	-2.63628800
H	-6.22919700	-0.33198700	-2.37826200
C	-4.93565000	-2.02815400	-0.54881600
C	-6.09842800	-2.50775800	0.06317900
C	-6.52003600	-3.81837500	-0.13760000
C	-5.79686200	-4.66498800	-0.97502400
C	-4.65164500	-4.18987300	-1.61070600

C	-4.22526000	-2.88300200	-1.39807600
H	-3.33186800	-2.51557000	-1.89288800
H	-4.09038900	-4.83669000	-2.27634500
H	-6.12774900	-5.68479200	-1.13730300
H	-7.41564900	-4.17741900	0.35762500
H	-6.66916100	-1.84854900	0.71062900
C	-2.71929500	1.08876400	0.04270100
C	-3.00772100	1.98669700	-0.99493300
C	-2.61637500	3.31117700	-0.92497900
H	-2.85122100	4.00735400	-1.72238500
H	-3.56167800	1.63999800	-1.86112600
C	-1.96596200	1.55876100	1.11815900
H	-1.69804300	0.87713000	1.91985300
C	-1.56930900	2.89253600	1.21079900
H	-0.99383200	3.21659700	2.06841600
C	-1.92292700	3.78067600	0.19542700
O	-1.65378000	5.11435900	0.19927400
C	-0.99430700	5.67057500	1.32903600
H	-1.16005400	6.74514600	1.23791000
H	-1.45528400	5.33047300	2.26220500
C	0.46754300	5.35997400	1.34636200
N	1.10001500	4.86861300	2.44164300
N	2.36406800	4.71741600	2.16916900
C	1.40532600	5.51199800	0.34992200
H	1.34767800	5.85668800	-0.66915800
N	2.55697600	5.10650000	0.91370400
C	3.84767600	4.95786100	0.27824400
H	4.02548300	5.81562900	-0.37151500
H	4.60664100	4.95332600	1.06213900
C	3.96411900	3.65600800	-0.53656600
O	3.06528900	2.81156500	-0.45432100
O	5.02481200	3.58117300	-1.22123500
N	4.98244000	1.07841200	-2.07986100

H	5.07152300	2.10449600	-1.76591800
H	4.95696300	0.46838700	-1.23060200
H	5.80387200	0.79838900	-2.61298600
C	3.74359900	0.89749300	-2.88032200
H	3.94928300	1.22679600	-3.90145100
H	2.98732000	1.54823100	-2.44093500
C	3.27905700	-0.54661700	-2.84729800
H	2.35779600	-0.63376100	-3.44275600
H	3.03156200	-0.80937300	-1.81276000
N	4.33538700	-1.43835700	-3.31582000
H	4.57935000	-1.19234500	-4.27087800
C	3.96490000	-2.84711300	-3.28128600
H	4.65017800	-3.39720700	-3.93289500
H	2.94347300	-3.03387200	-3.64549200
C	4.06294300	-3.41396700	-1.87342100
H	3.32794800	-2.97087700	-1.19811700
H	3.92209500	-4.49473100	-1.88325000
N	5.40031300	-3.10883400	-1.28427200
H	5.63707400	-3.78111300	-0.55132100
H	6.13614600	-3.11576600	-1.99234700
H	5.35928800	-2.16364300	-0.82559400

Put(2+):**1** complex

E = -2438.16037466 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2437.500291 hartree

charge=0; multiplicity=1

O	-2.92582400	2.15021600	0.24407600
C	-3.89687900	2.93190300	0.21713100
O	-5.05498100	2.69780700	-0.20019100
C	-3.72687600	4.34289300	0.80105600
H	-4.23030500	4.36681000	1.76982100
H	-4.20839500	5.06863900	0.14618900
N	-2.35225700	4.74100300	1.00428400

N	-1.71315100	4.45126600	2.13350100
N	-0.49380500	4.89154500	2.02181400
C	-1.54380100	5.38085700	0.14044600
H	-1.87401500	5.70225500	-0.83362600
C	-0.34281300	5.48007700	0.80712200
C	0.94685100	6.08001100	0.35449500
H	0.81644700	7.11970300	0.05157400
H	1.66928600	6.03848000	1.17660800
O	1.46251200	5.41819700	-0.80484800
C	1.86456300	4.12120100	-0.58398300
C	1.09920700	3.07602200	-1.09059600
C	1.52789900	1.76459100	-0.91676800
H	0.93174400	0.94796600	-1.31357800
H	0.17936000	3.30122900	-1.61879500
C	3.04187000	3.85955500	0.11213400
H	3.62409600	4.68294700	0.51211700
C	3.46717800	2.54732500	0.26965400
H	4.39301300	2.34146700	0.79684000
C	2.72789600	1.48344200	-0.25778200
C	3.19912600	0.07861200	-0.12024400
C	4.46132200	-0.29598800	-0.43586200
C	5.00137200	-1.64607900	-0.10602900
C	5.65667900	-2.39999800	-1.08466600
C	6.15975600	-3.66352200	-0.79059400
C	6.03629400	-4.18270900	0.49626300
C	5.40933100	-3.42831600	1.48589000
C	4.89551400	-2.17103600	1.18596600
H	4.40435600	-1.58630100	1.95738100
H	5.32208400	-3.81795100	2.49431000
H	6.43311500	-5.16477300	0.72843200
H	6.65118900	-4.24102100	-1.56594800
H	5.76114500	-1.99485800	-2.08684100
C	5.41317100	0.60845000	-1.14167000

C	6.71199300	0.78230400	-0.65322000
C	7.60791600	1.62697200	-1.30083300
C	7.22501500	2.29285800	-2.46329100
C	5.94204500	2.10552900	-2.97340700
C	5.04385900	1.27069000	-2.31672700
H	4.04368500	1.12825800	-2.71374500
H	5.64025300	2.60806100	-3.88593900
H	7.92425300	2.94677200	-2.97247800
H	8.60639200	1.76236000	-0.89970100
H	7.01572900	0.25813400	0.24816000
C	2.19169800	-0.89330800	0.38275500
C	1.95353800	-2.09310200	-0.28554700
C	1.04954300	-3.03522700	0.19570400
H	0.88331500	-3.94295800	-0.36715900
H	2.49173200	-2.30419900	-1.20408700
C	1.45671500	-0.63152200	1.54542000
H	1.60455700	0.30501100	2.07490500
C	0.56807300	-1.56750200	2.05404900
H	0.03424100	-1.38388700	2.98046700
C	0.37088900	-2.78292800	1.38785000
O	-0.49253500	-3.64926600	1.98568700
C	-0.78721900	-4.88276400	1.33105200
H	0.13421600	-5.38866700	1.02792500
H	-1.27401000	-5.48392300	2.09912100
C	-1.69212800	-4.71521100	0.15341400
N	-1.26788300	-4.84155700	-1.13211900
N	-2.27176700	-4.65055300	-1.93277000
C	-3.04113000	-4.43570300	0.12173800
H	-3.77719400	-4.28867200	0.89565300
N	-3.34738400	-4.40951300	-1.18778700
C	-4.61846200	-4.09240600	-1.80194500
H	-4.56384600	-4.40540500	-2.84558400
H	-5.40778300	-4.66215800	-1.31008300

C	-4.97570000	-2.59686000	-1.74628600
O	-4.08162100	-1.79039700	-1.36027100
O	-6.13069300	-2.30751500	-2.08077000
N	-2.36099500	-0.53989100	0.45232700
H	-2.67296000	0.45307000	0.31015100
H	-1.33958100	-0.54624400	0.38228100
H	-2.75165400	-1.12380600	-0.30843900
C	-2.78533100	-1.08191000	1.78125000
H	-2.25116500	-2.02310800	1.92451100
H	-2.45399300	-0.37022000	2.54099700
C	-4.28875200	-1.30744300	1.83476700
H	-4.57169800	-1.93195400	0.98120200
H	-4.49222900	-1.90252800	2.72826600
C	-5.13617700	-0.02001500	1.86438800
H	-5.52061100	0.14186400	2.87353100
H	-4.52489400	0.85840200	1.62980000
C	-6.32179700	-0.05159100	0.90801700
H	-6.83993800	-1.01273200	0.94284100
H	-7.03505400	0.73873400	1.14524200
N	-5.86617100	0.18613200	-0.48941700
H	-5.47595400	1.17435600	-0.53345100
H	-5.14749500	-0.50336700	-0.80485300
H	-6.63710300	0.08385700	-1.14996200

Spm(4+):**1** complex

E = -2785.53992547 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2784.659287 hartree

charge=+2; multiplicity=1

O	0.22640200	-0.00476000	0.02052500
C	0.13330300	-0.06815000	1.27007200
O	1.10691900	-0.07368700	2.05582700
C	-1.23778200	-0.13327400	1.94167400
H	-1.28793600	0.65378200	2.69617800

H	-1.33347400	-1.09531000	2.44614700
N	-2.34585100	0.01874700	1.02479600
N	-2.52999900	1.17952900	0.39873700
N	-3.60305100	1.07276300	-0.32566800
C	-3.30974500	-0.86156800	0.70050200
H	-3.35291800	-1.85632700	1.11250700
C	-4.12293600	-0.17401900	-0.17615900
C	-5.36752400	-0.63937800	-0.86163700
H	-5.84043900	-1.41495400	-0.25889200
H	-6.07500500	0.18595500	-0.97792000
O	-5.11300600	-1.26065600	-2.11964600
C	-5.02058400	-0.48429900	-3.23548100
C	-4.95248700	-1.17864800	-4.44686700
C	-4.87202900	-0.48416100	-5.64439900
H	-4.83917800	-1.03113400	-6.58164600
H	-4.97604300	-2.26260300	-4.42924500
C	-4.97479900	0.90992800	-3.23316100
H	-4.99908100	1.47282800	-2.30959700
C	-4.86821100	1.58968600	-4.44446000
H	-4.81821400	2.67516300	-4.43459800
C	-4.83724000	0.91410500	-5.66292300
C	-4.72922700	1.67858300	-6.93747200
C	-5.66373500	1.61910500	-7.90773900
C	-5.48597000	2.29257200	-9.22589100
C	-4.32951400	2.10904900	-9.98993700
C	-4.18468600	2.74172800	-11.22074200
C	-5.19395700	3.57065900	-11.70527500
C	-6.35533600	3.75129700	-10.95714600
C	-6.50344400	3.10750500	-9.73283600
H	-7.41390400	3.24194900	-9.15624200
H	-7.14860800	4.39060800	-11.32885700
H	-5.07963100	4.06640900	-12.66286700
H	-3.28361800	2.58366600	-11.80332500

H	-3.54245700	1.46242900	-9.61601300
C	-6.94652700	0.87928200	-7.73165400
C	-7.76869500	1.09986700	-6.62249700
C	-8.96549400	0.40502500	-6.47707900
C	-9.35703200	-0.52399800	-7.43838600
C	-8.55091100	-0.74265200	-8.55355400
C	-7.36105400	-0.03730200	-8.70324800
H	-6.73936200	-0.20216800	-9.57840500
H	-8.85053100	-1.45988800	-9.30985800
H	-10.28802500	-1.06796800	-7.32356800
H	-9.59413800	0.59283700	-5.61342000
H	-7.46702200	1.82404800	-5.87277200
C	-3.50365000	2.51886800	-7.03399400
C	-2.24612200	1.92173300	-6.97270200
C	-1.07668200	2.67430800	-7.01193300
H	-0.12022700	2.16974100	-6.96214900
H	-2.17309300	0.83956700	-6.90424000
C	-3.57182000	3.91187800	-7.12851700
H	-4.54195600	4.39665500	-7.17929900
C	-2.41722600	4.67953800	-7.14955500
H	-2.46443300	5.76092900	-7.21117600
C	-1.16521000	4.06418700	-7.08867700
O	-0.09423500	4.90456100	-7.10766200
C	1.19922300	4.34161900	-7.15359100
H	1.27649600	3.61646200	-7.97229400
H	1.86372900	5.17664000	-7.38263000
C	1.60428300	3.70373300	-5.85492400
N	0.91038400	3.85953100	-4.70270900
N	1.51892000	3.20619700	-3.75475200
C	2.69496100	2.90319600	-5.58988700
H	3.50011700	2.53050900	-6.20073200
N	2.59604500	2.63045600	-4.27570000
C	3.49319400	1.87349500	-3.42588200

H	4.25318500	1.41038900	-4.05778800
H	3.99502400	2.54843400	-2.73022200
C	2.77106200	0.76559500	-2.64557500
O	3.37813700	0.37146300	-1.61391900
O	1.68152900	0.35842300	-3.07648000
N	-0.43185200	-1.22691700	-2.34885500
H	-0.41748300	-2.24694900	-2.35048200
H	0.45764800	-0.87194500	-2.75540200
H	-0.40185500	-0.91882800	-1.35964600
C	-1.63375900	-0.71788900	-3.08942600
H	-2.47357500	-0.71852800	-2.38980200
H	-1.84611700	-1.44670600	-3.87098200
C	-1.43315800	0.64930800	-3.73970700
H	-0.48322900	0.67812800	-4.28565400
H	-2.22682000	0.73497700	-4.48944000
C	-1.58184300	1.88915500	-2.86684200
H	-2.52655300	1.88359800	-2.31958200
H	-1.53929900	2.77847500	-3.50273200
N	-0.49432000	2.05011300	-1.85524100
H	-0.49969300	1.28473700	-1.16013100
H	0.40438700	2.00816300	-2.35842700
C	-0.58285600	3.33955900	-1.10131900
H	-0.38091400	4.13862500	-1.81964300
H	-1.61062800	3.41913500	-0.74507500
C	0.39910500	3.35717900	0.06371000
H	0.15063100	4.21173300	0.69835600
H	0.23278700	2.46215500	0.67317300
C	1.85593000	3.46835700	-0.39132800
H	2.04244000	2.82298800	-1.25574100
H	2.04279300	4.48528300	-0.74722100
C	2.89615500	3.14140500	0.67018100
H	3.87804900	3.50085600	0.35662400
H	2.65821400	3.57494900	1.64359500

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N	3.03473900	1.66159600	0.85398100
H	2.23943900	1.25634900	1.38084700
H	3.02610500	1.22663000	-0.08851200
C	4.31490500	1.27793200	1.52577000
H	4.44084800	1.95252000	2.37424700
H	5.11406700	1.47023100	0.80558600
C	4.33875300	-0.16345400	2.01838600
H	5.27932500	-0.27459100	2.56435400
H	3.53676700	-0.32737200	2.74433100
C	4.32183900	-1.26905000	0.96755400
H	4.58551200	-2.21133900	1.44506100
H	5.02875500	-1.07703000	0.15851500
N	2.97225100	-1.45706200	0.34057500
H	2.89080200	-0.86510900	-0.52099200
H	2.83066400	-2.42963900	0.06703000
H	2.22134800	-1.18446600	0.99729100

Spd(3+):**1** complex

E = -2611.85008179 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2611.081082 hartree

charge=+1; multiplicity=1

O	4.51645000	1.66976000	-0.04460200
C	3.41362200	2.27539800	-0.00425000
O	2.28044800	1.76463400	0.01357900
C	3.53504300	3.80479500	0.03536700
H	4.03386600	4.14127100	-0.87551900
H	4.15241300	4.08745900	0.88874100
N	2.26512000	4.48163800	0.16247400
N	1.81989200	4.86453400	1.35616600
N	0.62871000	5.35921400	1.19740900
C	1.34243700	4.70955000	-0.79054800
H	1.49973600	4.45134100	-1.82507400
C	0.28886500	5.28038900	-0.11519900

C	-1.02090500	5.77978400	-0.64125700
H	-1.05338400	6.87001300	-0.60452300
H	-1.14802800	5.47060500	-1.68491100
O	-2.12976900	5.36860700	0.14315100
C	-2.50049100	4.05960500	0.12107100
C	-3.62174500	3.73706100	0.89202900
C	-4.09595500	2.43620400	0.92289200
H	-4.97478600	2.20011900	1.51479700
H	-4.10934200	4.52376700	1.45680700
C	-1.85003400	3.05967300	-0.60149700
H	-0.97777700	3.27323700	-1.20313300
C	-2.32449200	1.75204600	-0.53665400
H	-1.80235300	0.97732200	-1.09091600
C	-3.45796500	1.41896200	0.20270800
C	-3.94613300	0.01327200	0.22483600
C	-5.22471000	-0.32606600	-0.05051400
C	-5.73402500	-1.71623200	0.12576900
C	-5.54756400	-2.41265800	1.32404000
C	-6.03321700	-3.70749600	1.47599600
C	-6.71236200	-4.32797500	0.42969600
C	-6.91520300	-3.63858300	-0.76388100
C	-6.43954800	-2.33914100	-0.90881500
H	-6.60672000	-1.80114600	-1.83733500
H	-7.44744000	-4.11137400	-1.58206100
H	-7.08801700	-5.33844900	0.54655200
H	-5.88402800	-4.23062500	2.41434000
H	-5.01917000	-1.93151500	2.14077700
C	-6.22234100	0.65756400	-0.56031900
C	-5.94165900	1.46998300	-1.66328000
C	-6.88509300	2.37703000	-2.13508600
C	-8.12447600	2.48795800	-1.50830000
C	-8.41910200	1.67447000	-0.41626100
C	-7.47875400	0.75885600	0.04536900

H	-7.71420200	0.11969700	0.89131900
H	-9.38319800	1.75010600	0.07467400
H	-8.85850100	3.19781500	-1.87317200
H	-6.65264800	2.99596000	-2.99490500
H	-4.97565400	1.38700100	-2.15114300
C	-2.90616000	-1.00094900	0.55371100
C	-2.19425000	-0.92224800	1.75594500
C	-1.22389400	-1.85833900	2.07216300
H	-0.69918700	-1.82054100	3.02049200
H	-2.41914300	-0.12692400	2.46041800
C	-2.58587700	-2.02488700	-0.33375200
H	-3.11911100	-2.09700300	-1.27673600
C	-1.58581100	-2.95304400	-0.04942700
H	-1.33873000	-3.70303300	-0.78710800
C	-0.90574700	-2.87454800	1.16455800
O	0.07880800	-3.72904100	1.56986000
C	0.52069500	-4.75488300	0.68527900
H	1.00627700	-5.48917400	1.32831800
H	-0.33279500	-5.23821300	0.20263400
C	1.50768200	-4.26587300	-0.32675300
N	1.16196900	-3.55638100	-1.43695400
N	2.23024300	-3.30130900	-2.12947900
C	2.87396600	-4.44919300	-0.35888400
H	3.56087700	-4.95529300	0.29971600
N	3.26644600	-3.84700400	-1.49765600
C	4.60573300	-3.64485300	-2.00600400
H	5.24381400	-4.46212200	-1.66775700
H	4.56793500	-3.66244900	-3.09571000
C	5.20468700	-2.31468300	-1.54547000
O	6.35218200	-2.04484400	-1.95262100
O	4.51663200	-1.57803900	-0.79505300
N	2.00825100	-0.90876600	0.31980700
H	2.11807600	0.11086000	0.04912000

H	2.81303000	-1.41631300	-0.08898100
H	1.14838700	-1.28404700	-0.09021700
C	1.97430900	-0.97865800	1.81230400
H	1.70258900	-1.99736200	2.09877700
H	1.18538800	-0.29703100	2.13150000
C	3.32066900	-0.56664500	2.38967800
H	3.17568200	-0.27087900	3.43140700
H	3.64368700	0.33407300	1.85605700
C	4.36493200	-1.68978600	2.31108600
H	4.20235800	-2.30877300	1.42330100
H	4.25326300	-2.35168700	3.17383100
C	5.80476900	-1.19768500	2.29258900
H	6.49971700	-2.03675600	2.22387400
H	6.05158300	-0.60947200	3.17943400
N	6.05849400	-0.32562800	1.10394400
H	5.54811700	0.56304100	1.19273700
H	5.60082400	-0.77649200	0.27453700
C	7.50718100	-0.03942600	0.87510600
H	7.95611100	0.06909200	1.86351800
H	7.94286700	-0.91843300	0.39359500
C	7.74091500	1.24352600	0.07914500
H	8.75412000	1.58048500	0.31151800
H	7.06273700	2.02572800	0.43600400
C	7.67038500	1.14957200	-1.43867400
H	7.86284300	2.13287600	-1.86650700
H	8.41380500	0.45113100	-1.82751100
N	6.33960800	0.68894600	-1.93660600
H	6.20422800	0.97450900	-2.90702300
H	6.29890600	-0.36575000	-1.92094200
H	5.55949200	1.08470400	-1.37504500

Dop(1+):**1** complex

E = -2685.16257526 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2684.506257 hartree

charge=-1; multiplicity=1

O	4.90967400	-0.25293900	1.34899400
C	4.44581200	-1.15380500	0.58661400
O	4.82039100	-2.33103400	0.51514000
C	3.33462300	-0.64970700	-0.34209500
H	3.80133300	-0.01377500	-1.09827200
H	2.61431400	-0.05393900	0.22331500
N	2.64536400	-1.70144900	-1.05783500
N	2.84139400	-1.87191700	-2.35957500
N	2.10638300	-2.87492600	-2.74468100
C	1.78013100	-2.61603200	-0.57395700
H	1.48131300	-2.64319400	0.46066900
C	1.43653000	-3.36753900	-1.67355500
C	0.48300000	-4.51420300	-1.81794200
H	-0.02215000	-4.44727600	-2.78881000
H	1.01409000	-5.46719400	-1.77895500
O	-0.46136900	-4.58189800	-0.76416100
C	-1.42954300	-3.62397200	-0.69785000
C	-1.50659700	-2.51740900	-1.54451900
C	-2.49956400	-1.56623200	-1.33110700
H	-2.52795400	-0.68543000	-1.96600200
H	-0.79097100	-2.36470600	-2.34162300
C	-2.37806300	-3.79129600	0.31347000
H	-2.30661800	-4.66035500	0.95790600
C	-3.37979100	-2.84866600	0.49068500
H	-4.10982800	-2.98272400	1.28321000
C	-3.44774900	-1.71181100	-0.32025400
C	-4.43844600	-0.62981000	-0.05673700
C	-5.77243800	-0.84253100	-0.06420900
C	-6.75163100	0.18450100	0.39270400
C	-7.85585100	0.50317700	-0.40421400
C	-8.77707000	1.46153700	0.00660500

C	-8.61973200	2.10061100	1.23448500
C	-7.53699000	1.77224900	2.04762600
C	-6.61038700	0.82278800	1.62885600
H	-5.76582600	0.57049800	2.26226900
H	-7.41432200	2.25429100	3.01149100
H	-9.33987500	2.84359000	1.55894800
H	-9.61966900	1.70659000	-0.63080800
H	-7.98575700	0.00026400	-1.35804500
C	-6.36528800	-2.13335900	-0.51645200
C	-7.32178000	-2.77864400	0.27446200
C	-7.87975300	-3.98796300	-0.12756900
C	-7.50550700	-4.56116600	-1.34098000
C	-6.57190000	-3.91487900	-2.14816400
C	-6.00610900	-2.71188000	-1.73801600
H	-5.27974300	-2.21024400	-2.36909900
H	-6.28519500	-4.34597300	-3.10124900
H	-7.94404900	-5.50059100	-1.65886600
H	-8.60930800	-4.48111400	0.50559800
H	-7.62207500	-2.33011100	1.21691200
C	-3.81488400	0.68572300	0.25449000
C	-4.20421900	1.87221700	-0.37853700
C	-3.56987100	3.07199300	-0.09715100
H	-3.85968100	3.98812200	-0.59967200
H	-5.00797400	1.85011500	-1.10787200
C	-2.76966600	0.74925400	1.17542000
H	-2.43714500	-0.16039900	1.66644400
C	-2.13706900	1.94810600	1.48874300
H	-1.33271200	1.94690100	2.21145800
C	-2.53380700	3.11748500	0.84071900
O	-1.97604100	4.34173000	1.05168600
C	-0.89306300	4.44017100	1.96964500
H	-0.74988900	5.51321100	2.10235500
H	-1.16178500	4.00587300	2.93872600

C	0.36093000	3.79348900	1.47125400
N	1.00942400	2.83262800	2.17910200
N	2.05980500	2.45031200	1.51612300
C	1.06370000	4.00250000	0.30574900
H	0.91278600	4.65435900	-0.53858200
N	2.10227100	3.15137800	0.38610400
C	3.14389600	2.92056900	-0.58942200
H	3.57925200	3.87672300	-0.88573700
H	3.92423900	2.32949900	-0.09853900
C	2.65237100	2.16440300	-1.84114200
O	3.54517400	2.04402500	-2.74380700
O	1.50358100	1.73746800	-1.87980400
C	8.07300800	1.45166700	0.26501000
H	8.73699900	1.76030400	1.06719100
C	7.34579600	2.41303800	-0.42699500
H	7.43280200	3.46526100	-0.17705300
C	6.50201500	2.05994100	-1.47869200
O	5.86690100	3.04005900	-2.17120100
H	4.96124000	2.72553100	-2.45983700
C	6.38300700	0.70192700	-1.82127300
O	5.62171900	0.27915200	-2.87057800
H	4.82771600	0.84013100	-2.97049600
C	7.10516700	-0.25399800	-1.11125700
H	6.98352300	-1.29480300	-1.39785700
C	7.95796200	0.10144600	-0.06946000
C	8.73791400	-0.94780700	0.68775200
H	8.62796500	-1.92223900	0.19944700
H	9.80563900	-0.70592700	0.67197600
C	8.33850800	-1.07307500	2.15391100
H	8.41144600	-0.11223400	2.66657400
H	8.98491300	-1.78863200	2.66465200
N	6.93447600	-1.53852800	2.29440900
H	6.14769400	-0.85642600	1.91389700

H	6.71801600	-1.73517800	3.27155200
H	6.75945600	-2.39901000	1.76734600

Spm(3+):**1** complex

E = -2785.08616218 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2784.222149 hartree

charge=+1; multiplicity=1

O	-0.00121200	-0.02017400	-0.23499300
C	0.02549400	-0.07032000	1.00844200
O	1.03978800	-0.24321400	1.72872000
C	-1.32765400	0.13383600	1.70532700
H	-2.08547600	-0.48384800	1.22304500
H	-1.61291500	1.18206500	1.58439200
N	-1.33726200	-0.21090100	3.11302400
N	-2.18197600	-1.14018000	3.56381000
N	-2.00986600	-1.24815600	4.84489800
C	-0.60314900	0.29707400	4.11890600
H	0.13771100	1.06342800	3.96577100
C	-1.04262500	-0.37637300	5.23896800
C	-0.60428800	-0.22490600	6.65890900
H	-0.37198300	0.81930100	6.86866100
H	-1.40173400	-0.53863700	7.33780500
O	0.61111600	-0.91853300	6.93724000
C	0.59377900	-2.28161600	6.95400300
C	1.83671600	-2.90157400	6.80294300
C	1.93082200	-4.28418800	6.80398800
H	2.90093200	-4.75605200	6.66971400
H	2.71548000	-2.27769800	6.67536200
C	-0.54859100	-3.06092700	7.12624300
H	-1.52819700	-2.61187900	7.21695000
C	-0.43250500	-4.45046600	7.15932500
H	-1.32403900	-5.05246100	7.30765700
C	0.79878700	-5.08208600	7.00090900

C	0.92414200	-6.56911800	7.01540600
C	0.73395600	-7.30621300	8.12653100
C	0.76929300	-8.79745800	8.10428300
C	1.59411600	-9.48474400	9.00031800
C	1.64982400	-10.87479900	8.99157700
C	0.86189200	-11.59977400	8.09997700
C	0.01865900	-10.92523900	7.22034700
C	-0.02550400	-9.53415400	7.22165700
H	-0.68496400	-9.01160300	6.53670100
H	-0.60890100	-11.48192800	6.53292500
H	0.89927400	-12.68347000	8.09629300
H	2.30540700	-11.39178900	9.68373800
H	2.20132100	-8.92163100	9.70305900
C	0.46869700	-6.69083600	9.45903600
C	-0.62682700	-7.12324500	10.21345400
C	-0.90301500	-6.55858500	11.45448900
C	-0.07194300	-5.56680500	11.97099400
C	1.03591000	-5.14677500	11.23881600
C	1.30309600	-5.70396700	9.99176900
H	2.16900800	-5.37646200	9.42627600
H	1.69686700	-4.38597600	11.63960900
H	-0.28193500	-5.12992900	12.94096600
H	-1.76477700	-6.89597600	12.01986900
H	-1.27055200	-7.90312100	9.81721400
C	1.27642800	-7.17217900	5.69752100
C	2.51322800	-7.78362600	5.47238800
C	2.83149900	-8.30087000	4.22539000
H	3.79015600	-8.77385600	4.04419900
H	3.23188800	-7.85288000	6.28329800
C	0.37658900	-7.09696200	4.63841900
H	-0.58829900	-6.62639500	4.80285900
C	0.67539200	-7.61634700	3.38081900
H	-0.05491300	-7.52821800	2.58528800

C	1.91293000	-8.22488100	3.17525800
O	2.31163800	-8.80265500	2.00612200
C	1.56362600	-8.55302700	0.82892800
H	1.88107300	-9.33076600	0.13180600
H	0.48836500	-8.67119200	0.98733300
C	1.85892800	-7.20280500	0.25141300
N	0.92329000	-6.45986400	-0.38909600
N	1.49381100	-5.40209900	-0.89530400
C	3.06670500	-6.54804400	0.13906000
H	4.06123500	-6.77650700	0.48419200
N	2.78267900	-5.44546900	-0.58175400
C	3.69659300	-4.40234300	-1.01112900
H	4.71388900	-4.77250400	-0.89562200
H	3.51756600	-4.20211700	-2.07022200
C	3.52869700	-3.08909400	-0.23720400
O	4.53132000	-2.34323800	-0.18906000
O	2.40704800	-2.83788100	0.26045800
N	-0.12205400	-2.78553200	-0.82141500
H	-0.09363600	-3.03470700	0.19526700
H	0.56509100	-3.40767100	-1.25828700
H	0.15674600	-1.80010200	-0.92468500
C	-1.50924800	-3.04517900	-1.29667500
H	-1.51103600	-2.99769400	-2.38580900
H	-2.13221400	-2.23345200	-0.91288600
C	-2.00223100	-4.39661900	-0.79068300
H	-2.97319700	-4.59418500	-1.25212000
H	-1.31902300	-5.18704800	-1.12492300
C	-2.15167100	-4.45364000	0.72975000
H	-2.61763600	-5.40674700	1.02135000
H	-2.81777300	-3.64889600	1.06408500
N	-0.85250100	-4.25478900	1.38087200
H	-0.24878800	-5.02744500	1.09976500
C	-0.91547100	-4.20080000	2.84266900

H	-1.79743400	-3.61818800	3.12162300
H	-1.03772500	-5.20423900	3.27114600
C	0.32008000	-3.50911200	3.41226400
H	0.28723700	-2.47240200	3.04496900
H	0.24289500	-3.47119400	4.50528100
C	1.63142600	-4.18503700	3.00200700
H	1.71786800	-5.15694200	3.49834900
H	1.64407600	-4.36527700	1.92133500
C	2.88090000	-3.39683000	3.36757900
H	2.99092900	-3.29544000	4.44814300
H	3.77692000	-3.87858000	2.96711300
N	2.85172900	-2.01500500	2.80236700
H	2.64632000	-2.11422000	1.77529600
H	2.05627200	-1.48949500	3.18006300
C	4.11262900	-1.25719800	3.05677900
H	4.88906500	-1.70943900	2.43400300
H	4.36375200	-1.43182900	4.10441300
C	3.97085100	0.24516500	2.80890100
H	2.97912100	0.58079100	3.12907500
H	4.69359300	0.74845600	3.45533900
C	4.25669600	0.73351900	1.39376600
H	5.29120600	0.52712700	1.11213600
H	4.09340200	1.80979500	1.34413200
N	3.38221100	0.08565500	0.37598000
H	3.78224100	-0.85338200	0.11693700
H	2.40296100	-0.03942800	0.74996900
H	3.33611600	0.64517900	-0.47530400

Spm(4+):**1** complex

E = -2785.53372629 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2784.653954 hartree

charge=+2; multiplicity=1

O	-3.17852300	1.91163600	0.40106800

C	-3.99372500	2.59211800	-0.25807800
O	-4.84973400	2.15765800	-1.06666000
C	-3.97476100	4.11255800	-0.05887200
H	-4.54230500	4.35579400	0.84197400
H	-4.42532400	4.61092200	-0.91484000
N	-2.62204000	4.60081900	0.08899400
N	-1.92880800	4.92211900	-1.00107200
N	-0.71530400	5.19188600	-0.63011600
C	-1.84787200	4.65143300	1.18986500
H	-2.22217300	4.42291500	2.17436600
C	-0.61341400	5.03660500	0.71570200
C	0.67905500	5.27369300	1.42853300
H	1.44262100	5.54026300	0.68970300
H	0.58201200	6.09307500	2.14217400
O	1.11495800	4.16703100	2.21150000
C	1.74598400	3.13871100	1.57683300
C	1.59896600	2.83648700	0.22195700
C	2.28762100	1.74883000	-0.31389100
H	2.16115400	1.51577200	-1.36783800
H	0.96403800	3.43148000	-0.42111700
C	2.58219400	2.35429400	2.37380000
H	2.69186300	2.60660400	3.42264900
C	3.28048500	1.29204900	1.81701300
H	3.94937300	0.70762100	2.44153200
C	3.14418300	0.97116400	0.46226200
C	3.83675000	-0.22385900	-0.10960300
C	5.10916600	-0.19047100	-0.54796700
C	5.84063400	-1.41526100	-0.98448400
C	6.51243200	-1.42392000	-2.21063700
C	7.20089400	-2.55611200	-2.63496700
C	7.24702700	-3.68941200	-1.82596100
C	6.60209800	-3.68163400	-0.59127500
C	5.90262500	-2.55325500	-0.17488400

H	5.40166000	-2.54925800	0.78779600
H	6.64553800	-4.55423400	0.05133300
H	7.78918700	-4.57007500	-2.15199200
H	7.70541700	-2.55139500	-3.59492100
H	6.48738700	-0.53728500	-2.83745100
C	5.90203000	1.07254600	-0.58832000
C	7.11731800	1.14255700	0.10109100
C	7.87531100	2.30841700	0.08747100
C	7.43913100	3.41670200	-0.63631600
C	6.24299800	3.34895000	-1.34531000
C	5.47928900	2.18477100	-1.32009400
H	4.55335900	2.13246900	-1.88210400
H	5.90312500	4.20146500	-1.92321200
H	8.03238500	4.32417100	-0.65340900
H	8.80855800	2.35067400	0.63823900
H	7.46362400	0.27598400	0.65680300
C	3.00838200	-1.46337900	-0.10219600
C	2.72194500	-2.17687500	-1.27077400
C	1.91993200	-3.30923900	-1.23584800
H	1.67736100	-3.84978700	-2.14402700
H	3.12621600	-1.83455100	-2.21839300
C	2.47525800	-1.93016100	1.09821800
H	2.67697600	-1.39437300	2.02078200
C	1.69288100	-3.07754900	1.15550700
H	1.29388000	-3.38905700	2.10970100
C	1.39575300	-3.76221000	-0.02176900
O	0.59609700	-4.86345500	-0.08967000
C	-0.14054900	-5.23539500	1.07090300
H	-0.50518000	-6.23993600	0.85760500
H	0.51439600	-5.29313000	1.94408200
C	-1.31407300	-4.34372300	1.33766700
N	-1.24291600	-3.14720300	1.97636400
N	-2.43935000	-2.64541300	2.07141900

C	-2.64033400	-4.57205300	1.03151900
H	-3.14817200	-5.39081400	0.54883300
N	-3.29031700	-3.49902000	1.50697600
C	-4.71204600	-3.22952000	1.51371400
H	-5.21793800	-4.06704100	1.03390000
H	-5.06098900	-3.16936100	2.54645500
C	-5.10040300	-1.93671700	0.78772900
O	-4.21156500	-1.21992500	0.27442300
O	-6.33142300	-1.71449000	0.79647900
N	-7.03697300	0.56948300	-0.30741100
H	-6.72397600	-0.32054300	0.20965800
H	-6.21423800	1.17248400	-0.47625700
H	-7.67337200	1.09365300	0.29314100
C	-7.71864800	0.19411400	-1.57890200
H	-7.86604100	1.09991000	-2.17041100
H	-8.69719800	-0.19700300	-1.30086200
C	-6.96689100	-0.87555900	-2.36512400
H	-6.69219600	-1.70517700	-1.70410800
H	-7.68516100	-1.28405500	-3.08083300
C	-5.76904900	-0.43327100	-3.19708600
H	-5.97511900	0.49326700	-3.73900000
H	-5.53647900	-1.21065300	-3.92628800
N	-4.52009400	-0.20546300	-2.41217200
H	-4.60287800	0.67205600	-1.83903700
H	-4.38094400	-0.95216100	-1.71674500
C	-3.31970800	-0.06178800	-3.29058300
H	-3.24556600	-0.96590600	-3.89954500
H	-3.51830000	0.78801700	-3.94581000
C	-2.06532600	0.16403800	-2.46328600
H	-1.28797400	0.55738600	-3.12342900
H	-2.27843600	0.95723400	-1.73609600
C	-1.55107400	-1.11042900	-1.78260200
H	-2.37334300	-1.71294100	-1.37600400

H	-1.04014000	-1.73691500	-2.51873600
C	-0.57769000	-0.81791200	-0.65465100
H	-0.11117200	-1.72632800	-0.27058800
H	0.20629700	-0.11610600	-0.95105200
N	-1.30705300	-0.20001300	0.49557300
H	-1.77119700	0.67646500	0.20565400
H	-2.08099900	-0.84024900	0.73060500
C	-0.42605600	0.06343200	1.68158400
H	0.53401500	0.39432300	1.27699900
H	-0.27978700	-0.89309000	2.19012600
C	-0.98423600	1.15146000	2.58901300
H	-0.17106500	1.45654200	3.25408700
H	-1.24213400	2.03135500	1.98910500
C	-2.14751800	0.76511100	3.49066500
H	-2.46810300	1.63122200	4.06831900
H	-1.87297700	-0.03527200	4.17922600
N	-3.34460000	0.28044000	2.72642000
H	-3.51635600	0.84868800	1.87346700
H	-3.22562400	-0.70692000	2.45195200
H	-4.18373900	0.32560300	3.30868900

TPE (dicarboxylate)

E = -2168.14322459 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -2167.665915 hartree

charge=-2; multiplicity=1

C	2.71800600	-0.31663800	-0.22068300
C	4.00467900	-0.68594700	-0.02008400
C	4.38839400	-2.05981600	0.41205200
C	5.40726200	-2.74862700	-0.25394500
C	3.77077400	-2.67173900	1.50759200
C	5.77542600	-4.03090800	0.14119800
H	5.90682500	-2.27638500	-1.09472200
C	4.14574400	-3.94849900	1.91268900

H	2.99052100	-2.13885900	2.04190100
C	5.14459700	-4.63591400	1.22604000
H	6.55751100	-4.55619100	-0.39611600
H	3.65927600	-4.40575600	2.76748400
H	5.43471900	-5.63270600	1.53923200
C	5.14222700	0.25818300	-0.21114900
C	6.12704800	0.38371700	0.77418000
C	5.26634400	1.01194800	-1.38258200
C	7.18816400	1.26856000	0.61044100
H	6.05122400	-0.20986400	1.68049900
C	6.33297600	1.88812000	-1.55423600
H	4.51775100	0.90772600	-2.16160400
C	7.29394500	2.02520100	-0.55468700
H	7.93428700	1.36485300	1.39168500
H	6.41513100	2.46193800	-2.47093600
H	8.12348300	2.71106700	-0.68616500
C	2.31900300	1.10330300	-0.42907800
C	2.71889600	2.10464300	0.46058800
C	1.48433200	1.45102800	-1.49556800
C	2.29328600	3.41815400	0.29704800
H	3.36333300	1.84803700	1.29535600
C	1.06284900	2.76252400	-1.67396700
H	1.15247300	0.68163500	-2.18610100
C	1.45900900	3.74204800	-0.76878400
H	2.59220700	4.18823600	1.00037500
H	0.40157500	3.03495700	-2.48931500
C	1.59259800	-1.29086300	-0.23770400
C	0.42495900	-1.04130100	0.48295500
C	1.65554500	-2.46820000	-0.99458600
C	-0.63697400	-1.94406700	0.49738400
H	0.34151000	-0.12521300	1.06114100
C	0.60496800	-3.36844400	-1.00489800
H	2.54363400	-2.67691600	-1.58256100

C	-0.54365000	-3.12087100	-0.24564900
H	-1.51745600	-1.71735200	1.08436600
H	0.65273500	-4.27779800	-1.59345200
O	-1.49403100	-4.08967700	-0.29383800
O	0.98301700	5.02338000	-0.92441100
C	-2.69893100	-3.91333800	0.44037600
H	-3.14526500	-4.90929600	0.46087400
H	-2.48623300	-3.61799900	1.47304100
C	-0.01777100	5.37903600	0.04887100
H	-0.33385500	6.38732600	-0.21973100
H	0.43201000	5.39679900	1.04674000
C	-3.64474000	-2.94561900	-0.19663800
C	-4.33195900	-1.88610600	0.35451300
H	-4.33906500	-1.40619400	1.32271500
C	-1.17359100	4.43938700	0.01372100
C	-1.37043900	3.26684700	0.71031900
H	-0.81431700	2.77671500	1.49316100
C	-6.12961400	-0.41331700	-0.59762500
H	-5.88346300	0.25799700	0.22894200
H	-6.12019800	0.14452600	-1.53496300
C	-3.19922200	1.55046700	0.59156400
H	-3.87896600	1.29300300	-0.22243500
H	-2.47432100	0.73999400	0.69695300
N	-2.49851800	2.75342000	0.19366200
N	-2.99133600	3.54870100	-0.75372700
N	-2.19298400	4.56802100	-0.87475000
N	-5.09459600	-1.42619900	-0.65547600
N	-4.02778100	-3.06286900	-1.49498300
N	-4.90467700	-2.13845200	-1.76003300
C	-7.54753000	-0.99205800	-0.34945600
C	-4.00159500	1.69107300	1.91224700
O	-3.96665400	2.78333700	2.50255800
O	-7.64148600	-2.20269900	-0.07512600

O	-4.60872100	0.64502900	2.23432400
O	-8.45780600	-0.13990400	-0.43814800

Cad(2+)

E = -309.24211844 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -309.060097 hartree

charge=+2; multiplicity=1

C	-2.50304900	0.51630300	-0.04397500
H	-2.55876900	1.08110000	-0.97487400
H	-2.55520200	1.20749300	0.79762200
C	-1.26304700	-0.35685400	0.01308200
H	-1.28266700	-0.96922100	0.92161500
H	-1.25451500	-1.03869600	-0.84490100
C	-0.00000300	0.50241300	0.00082800
H	-0.00551300	1.15215900	-0.88169600
H	0.00553600	1.15500700	0.88124900
C	1.26300900	-0.35688600	-0.00895000
H	1.25534300	-1.03525000	0.85177500
H	1.28161500	-0.97297400	-0.91497600
N	-3.74326600	-0.32596100	0.01847300
H	-3.80069800	-0.83925500	0.90139500
H	-4.58927200	0.24316000	-0.06261400
H	-3.76200000	-1.01384000	-0.73865800
C	2.50320100	0.51636700	0.04301700
H	2.55283000	1.20612000	-0.79992000
H	2.56178500	1.08276700	0.97276400
N	3.74318700	-0.32609300	-0.02173400
H	3.79879000	-0.83948000	-0.90471800
H	4.58944500	0.24289500	0.05760900
H	3.76336000	-1.01388300	0.73545900

Det(2+)

E = -325.26680434 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -325.093812 hartree

charge=+2; multiplicity=1

C	-1.20898000	-0.38393800	0.09135600
H	-1.16038900	-1.08212800	-0.75105400
H	-1.32055200	-0.97872700	1.01135900
C	-2.40555600	0.53722800	-0.08359000
H	-2.48672100	1.25513400	0.73323000
H	-2.35435400	1.07135100	-1.03126100
N	-0.00000100	0.42639900	0.08178900
H	-0.00000800	1.02881700	0.90212600
N	-3.67560800	-0.25525200	-0.08704100
H	-3.80380900	-0.76838800	0.78932700
H	-4.49021400	0.35152900	-0.20776000
H	-3.68927800	-0.93846400	-0.84896800
C	1.20898000	-0.38393500	0.09137300
H	1.16038700	-1.08214900	-0.75101600
H	1.32055600	-0.97869800	1.01139300
C	2.40555200	0.53722900	-0.08360400
H	2.35434300	1.07132700	-1.03128900
H	2.48672000	1.25515700	0.73319600
N	3.67560700	-0.25524700	-0.08704300
H	3.68927900	-0.93846900	-0.84896100
H	4.49021100	0.35153600	-0.20777000
H	3.80381000	-0.76836900	0.78933200

Put(2+)

E = -269.94342236 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -269.785164 hartree

charge=+2; multiplicity=1

C	0.00056000	0.00006200	0.00658700
H	-0.01599900	-0.00095700	1.09678500
H	1.03596400	-0.00104700	-0.33501600
C	-0.78569100	1.16444400	-0.56938300

H	-0.77411400	1.11255400	-1.66332000
H	-1.82945700	1.10137300	-0.24387500
C	-0.18150100	2.49075700	-0.10867300
H	-0.19327000	2.54273400	0.98526200
H	0.86237300	2.55363000	-0.43392300
C	-0.96740800	3.65523600	-0.68489300
H	-0.95076000	3.65614700	-1.77508700
H	-2.00284700	3.65679300	-0.34339800
N	-0.59647300	-1.30320300	-0.43124000
H	-0.59124500	-1.39569300	-1.45042300
H	-0.07617000	-2.09609600	-0.04795900
N	-0.36993600	4.95840600	-0.24750100
H	0.60034700	5.04897500	-0.55958400
H	-0.89065800	5.75136200	-0.63000100
H	-0.37413500	5.05074700	0.77167900
H	-1.56712300	-1.39358000	-0.12018100

Spm(3+)

E = -616.82409867 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -616.470399 hartree

charge=+3; multiplicity=1

C	1.97203100	1.61015200	0.16488200
H	1.96219400	1.60465700	1.26879800
H	1.71778200	2.62522500	-0.15628200
C	0.90307600	0.65036500	-0.34962200
H	0.91771800	0.65876300	-1.44518300
H	1.12568800	-0.37351200	-0.02898600
C	-0.48352800	1.04281000	0.15849700
H	-0.48890300	1.04178700	1.25486300
H	-0.72380500	2.06043900	-0.17117700
C	-1.53665400	0.07722900	-0.35484600
H	-1.58836000	0.07299600	-1.44502800
H	-1.35826300	-0.94048700	-0.00330500

N	3.29665800	1.29626200	-0.36563700
H	3.89409500	2.10638000	-0.22740700
N	-2.90265100	0.46381600	0.13345900
H	-2.88547200	0.52653900	1.15631700
H	-3.11925400	1.40715500	-0.20402000
C	3.92133100	0.15133600	0.28505600
H	3.93803200	0.25970300	1.38351200
H	3.33644600	-0.74680500	0.05963000
C	5.34314000	-0.03737800	-0.23225900
H	5.93046700	0.86485900	-0.02413600
H	5.31655400	-0.17540900	-1.31803400
C	5.99750500	-1.23567400	0.42988400
H	6.07025700	-1.11643500	1.51108200
H	5.46824400	-2.16304100	0.20838800
N	7.39876200	-1.41539700	-0.07346700
H	7.97426400	-0.59262300	0.12365700
H	7.85294900	-2.21982100	0.36528000
H	7.41481400	-1.56690300	-1.08536600
C	-3.97831100	-0.48230900	-0.29043400
H	-3.70359700	-1.46284800	0.10173300
H	-3.95452100	-0.51616200	-1.38074800
C	-5.33556700	-0.02988000	0.23077300
H	-5.31543500	0.01680200	1.32426300
H	-5.56694200	0.96958800	-0.15082100
C	-6.39908600	-1.01747200	-0.22604200
H	-6.21378400	-2.01842200	0.16263900
H	-6.47001200	-1.06282100	-1.31267700
N	-7.74887000	-0.60788500	0.27428900
H	-8.46560400	-1.27266200	-0.02888700
H	-7.77946000	-0.57184300	1.29689900
H	-8.02044900	0.31470800	-0.07760200

Spm(4+)

E = -617.26603604 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -616.895389 hartree

charge=+4; multiplicity=1

C	-1.85837700	0.48304400	0.14358000
H	-1.86207200	1.06941400	-0.77649200
H	-1.92126500	1.15953200	0.99754600
C	-0.63894900	-0.42046200	0.22345100
H	-0.68191900	-1.02930800	1.13260500
H	-0.63123800	-1.10201600	-0.63437300
C	0.63894700	0.42048700	0.22347200
H	0.63119800	1.10214300	-0.63427000
H	0.68196100	1.02922100	1.13269800
C	1.85836700	-0.48301600	0.14343600
H	1.92128400	-1.15961300	0.99731300
H	1.86202500	-1.06926700	-0.77671200
N	-3.12282700	-0.32282400	0.13992200
H	-3.18186900	-0.86106400	1.01013700
N	3.12282400	0.32284200	0.13983800
H	3.07986100	1.01142200	-0.61787600
H	3.18188000	0.86100100	1.01010200
C	-4.35540300	0.50908900	-0.01706300
H	-4.35928300	1.22372000	0.80761300
H	-4.24807700	1.05091100	-0.95806900
C	-5.60207500	-0.36510900	-0.01239400
H	-5.68351100	-0.89402700	0.94232600
H	-5.53864400	-1.11126200	-0.81122000
C	-6.82601700	0.51331900	-0.22410900
H	-6.93963900	1.24888500	0.57200400
H	-6.79485200	1.02648400	-1.18520700
N	-8.07053200	-0.31786500	-0.22049500
H	-8.18849600	-0.81723000	0.66530500
H	-8.90178500	0.26394700	-0.35572600
H	-8.06167200	-1.01475500	-0.97025800

C	4.35539000	-0.50907300	-0.01722600
H	4.24806900	-1.05080100	-0.95828800
H	4.35924600	-1.22378600	0.80737900
C	5.60207700	0.36510300	-0.01244500
H	5.53870700	1.11129800	-0.81123600
H	5.68346500	0.89397200	0.94230600
C	6.82601600	-0.51333700	-0.22412100
H	6.79491400	-1.02644900	-1.18525000
H	6.93956300	-1.24894900	0.57195900
N	8.07054900	0.31782000	-0.22036400
H	8.90180300	-0.26400700	-0.35552800
H	8.06177900	1.01472900	-0.97011200
H	8.18843800	0.81716100	0.66546000
H	-3.07986500	-1.01133700	-0.61785200

Spd(3+)

E = -443.60511201 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -443.340342 hartree

charge=+3; multiplicity=1

C	0.64190200	0.44263800	0.11733700
H	0.59728200	1.11091100	-0.74410800
H	0.63026400	1.03902500	1.03090100
C	1.85318200	-0.47246700	0.04899000
H	1.84957100	-1.16284500	0.89895400
H	1.80815500	-1.07133000	-0.86712800
C	3.14030200	0.35292500	0.06002600
H	3.11710800	1.08600700	-0.75369000
H	3.21862800	0.90436300	1.00290000
C	4.34578000	-0.55571100	-0.10683100
H	4.42510900	-1.28046700	0.70380000
H	4.32409200	-1.08528600	-1.05955200
N	-0.63045000	-0.35131900	0.10630500
H	-0.66928100	-0.93918800	0.94504400

N	5.61272100	0.24506600	-0.09123600
H	6.43407200	-0.35301200	-0.21100200
H	5.62567900	0.93714100	-0.84503300
H	5.72601900	0.74952200	0.79191400
H	-0.61785500	-0.99693900	-0.68974300
C	-1.85790700	0.49908100	0.03018500
H	-1.81231100	1.19546900	0.86868600
H	-1.78835400	1.06015500	-0.90305800
C	-3.11465200	-0.35893300	0.07818800
H	-3.17891100	-0.87154300	1.04332400
H	-3.07993100	-1.11752800	-0.71096600
C	-4.33228500	0.53171900	-0.11908500
H	-4.42370900	1.27713400	0.67085600
H	-4.31244900	1.03406900	-1.08634800
N	-5.58543500	-0.28558800	-0.08675900
H	-5.69383500	-0.77799300	0.80403700
H	-6.41271600	0.30379500	-0.21298800
H	-5.59553400	-0.98738700	-0.83194100

Dop(1+)

E = -516.96428098 hartree

G (298.15 K. 1 atm. scale factor 0.952) = -516.810915 hartree

charge=+1; multiplicity=1

C	0.00847900	0.07561600	-0.00806400
C	-0.01384400	-0.04812900	1.38382400
C	1.18847600	-0.16719900	2.07414400
C	2.40294500	-0.16572600	1.38802800
C	2.41615400	-0.04443800	0.00832600
C	1.21157200	0.07721400	-0.69498800
H	-0.91273500	0.16470600	-0.57598600
H	1.18608700	-0.26783200	3.15446000
H	3.33968200	-0.26361600	1.92708400
C	-1.32851000	-0.00889100	2.12523800

H	-2.11026800	-0.49723200	1.53468300
H	-1.23795300	-0.54830200	3.07314600
C	-1.72889500	1.43491100	2.40055800
H	-0.99075000	1.94492000	3.01977200
H	-1.87419800	1.99705000	1.47774500
N	-3.02955200	1.48814600	3.14797200
H	-3.30759600	2.45271500	3.34348700
H	-3.78588400	1.05148100	2.61437600
H	-2.96355400	0.99912200	4.04445200
O	1.21608900	0.19147200	-2.04867800
H	2.13083900	0.16182700	-2.36001700
O	3.54242400	-0.03646100	-0.76181300
H	4.32985100	-0.14434200	-0.21657100