Supporting Information

Detection of Dopamine in Human Fluids Using N-Doped Carbon Dots

by

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CONTENTS

Synthesis of CDs

Following the previous publications for our group, the synthesis of CDs was as follow [Milenković, I.; Algarra, M.; Alcoholado, C.; Cifuentes, M.; Lázaro-Martínez, J. M.; Rodríguez-Castellón, E.; Mutavdžić, D.; Radotić, K.; Bandosz, T. J. Fingerprint imaging using N-doped carbon dots. *Carbon* **2019**, *144*, 791-797.]: Polyvinylpyrrolidone (PVP, average mol. Wt. 40000) from Sigma-Aldrich, (500 mg) were dissolved in H_2O (15 mL) and transferred into a 50 mL teflon-steel reactor and kept at 180 ºC for 2 h to obtain an aqueous solution, which showed a green shinny fluorescent under UV light.

***Materials and Methods*.** Polyvinylpyrrolidone (PVP, average mol. Wt. 40000), L-dopamine hydrochloride (DA), L-Histidine (His), L-(+)-Arginine (Arg) (98%), L-Cysteine (Cys), Magnesium sulfate (≥99.5%), Potassium bromide (99%), L-Tyrosine (Tyr), Serotonin hydrochloride, Leucine Enkephalin acetate hydrate (Leu), Epinephrine (EPI) (95%), DL-Norepinephrine hydrochloride (NE), DL-3,4-Dihydroxymandelic Acid (DOMA) and DL-Tryptophan (Trp) were purchased from Sigma-Aldrich. D-(+)-Glucose anhydrous PA-ACS (Glc), Acido L-(+)-Ascorbico (AA) and hydrochloric acid (37%) were purchased from Panreac SAU (Barcelona, Spain). Uric acid (UA) (99%) was purchased from Alfa Aesar. Sodium borohydride was purchased from Fluka Analytical. Ultrapure water, used throughout all experiments, was purified through a Millipore system. Reagents were not further purified

Characterization Methods. The morphology of N-CDs was analysed using a high-resolution transmission electron microscopy (HRTEM) and examined under a FEI Talos F200X. XPS studies were acquired on a Physical Electronics PHI VersaProbe II spectrometer using monochromatic Al-K□ radiation (49.1 W, 15 kV and 1486.6 eV) for analyzing the core-level signals of the elements of interest with a hemispherical multichannel detector. The sample spectra were recorded with a constant pass energy value at 29.35 eV, using a 200 μm diameter circular analysis area. The X-ray photoelectron spectra obtained were analyzed using PHI SmartSoft software and processed using MultiPak 9.3 package. The binding energy values were referenced to adventitious carbon C 1*s* signal (284.8 eV). Shirleytype background and Gauss-Lorentz curves were used to determine the binding energies. Equinox 55 FT-IR spectrometer fitted with a Golden Gate single reflection ATR accessory kit from Specac. All spectra were recorded using a resolution of 2 cm^{-1}; 50 scans were collected. The fluorescence measurements were performed with a Jovin Yvon Fluoromax 4 TCSPC

(Horiba), and measured between 400 and 700 nm using an integration time of 0.1 s and 5 nm slits for excitation and emission.

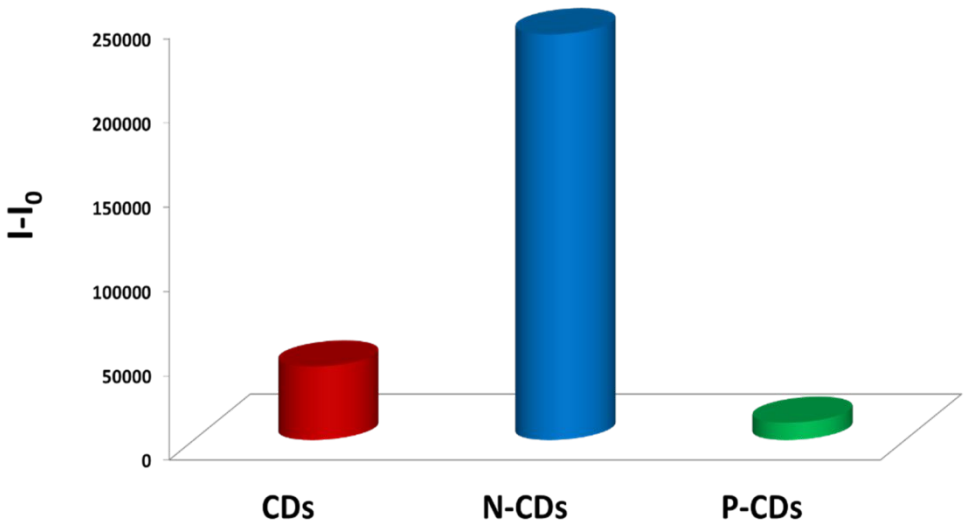

Figure S1. Selection of carbon nanoparticles based on the interaction with DA (1ppm) (λ_{ex} =350 nm λ_{em} =430 nm).

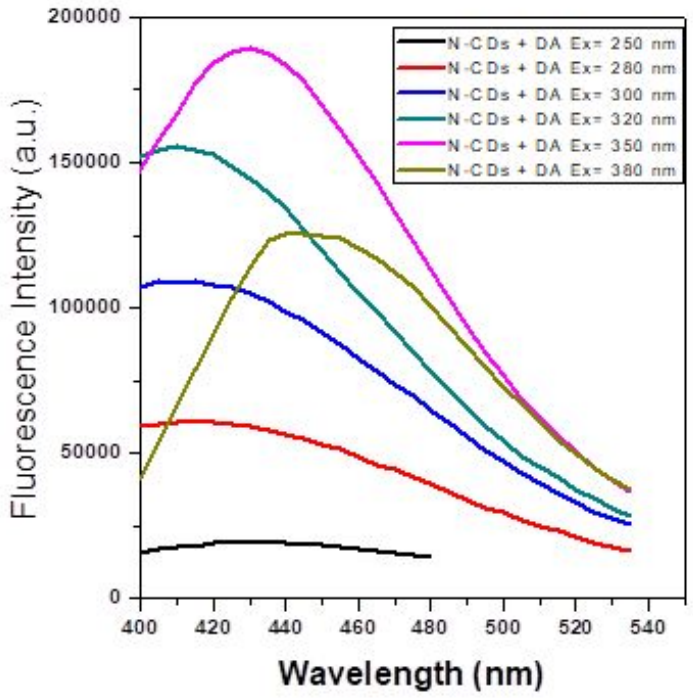

Figure S2. Fluorescence spectra (under different excitation wavelengths) of aqueous dissolutions of N-CDs+DA. All data were the average values obtained by three parallel experiments.

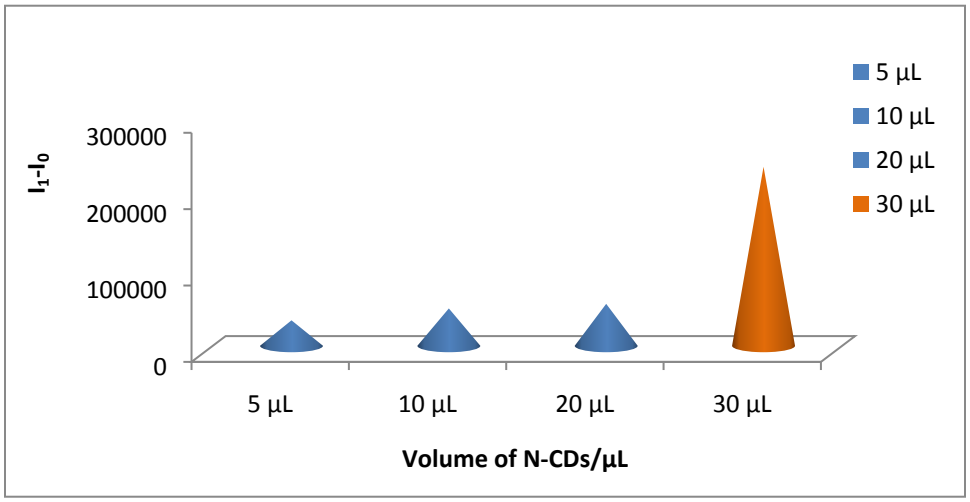

Figure S3. Optimization of the difference of the intensities for different volume of N-CDs with 1 ppm DA. λ_{max} = 430 nm. Excitation at 350 nm.

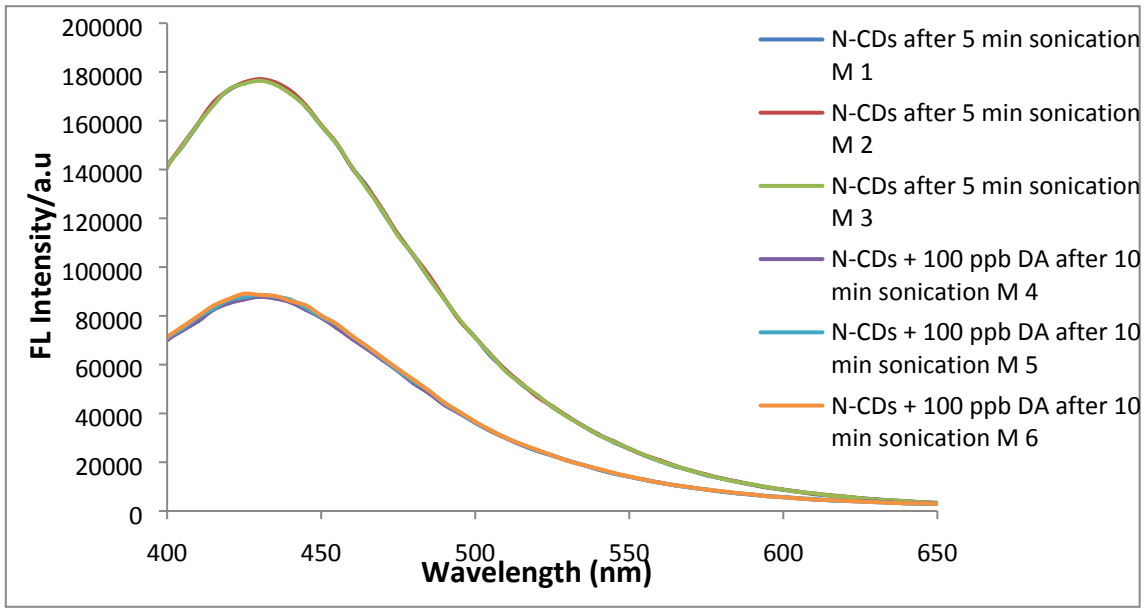

Figure S4. Fluorescence spectra of N-CDs and N-CDs + 100 ppb DA for each of the three repetitions. The mixtures of N-CDs were sonicated for 5 min and N-CDs + 100 ppb DA were sonicated for 10 min before the fluorescence intensity of the solution was measured. Excitation at 350 nm.

Abbreviations: N-CDs, N-doped carbon dots; DA, dopamine; M 1, M 2 and M 3, each mixture contains: 30 µL of N-CDs diluted to 2 mL with 0.1 M HCl; M 4, M 5 and M 6, each mixture contains: 30 µL of N-CDs + 100 ppb DA diluted to 2 mL with 0.1 M HCl.

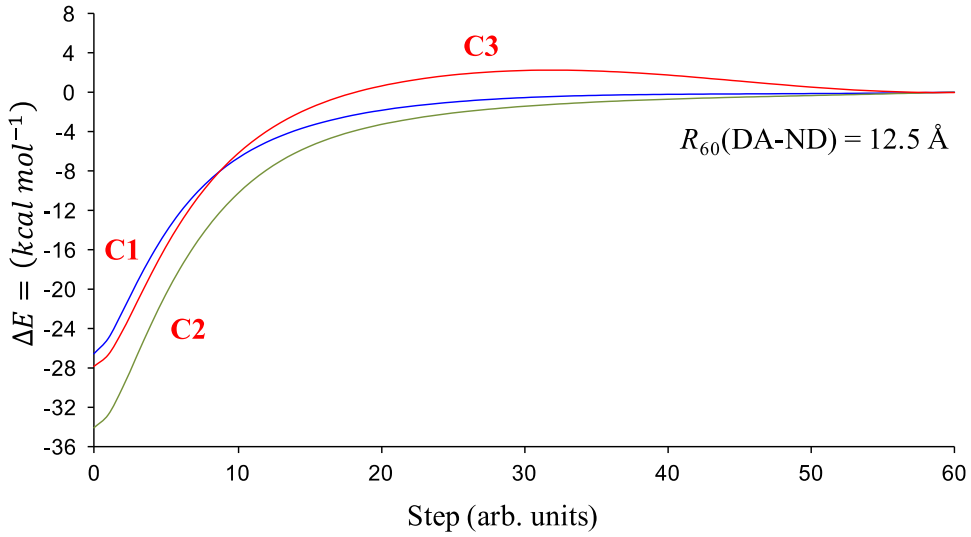

Figure S5. M05-2X/def2-TZVPP potential energy surfaces (electronic energy) of the complexes formed between dopamine (DA) and N-CDs. (a) **C1** (-COOH); (b) **C2** (-$CONH_2$); (c) **C3** (-CH_2NH_2). Origin corresponds to equilibrium geometry. Final point corresponds to a separation of 12.5 Å between DA and N-CDs.

Table S1. Calculated vertical excitation and emission energies in nm [eV] of the DA/N-CDS complexes and N-CDS.[a]

Complex[b]	Absorption	Emission
C1	354 [3.50]	426 [2.91]
C1(0)[b]	351 [3.53]	423 [2.93]
C2	353 [3.51]	445 [2.79]
C2(0)[b]	353 [3.51]	423 [2.93]
C3	355 [3.50]	428 [2.89]
C3(0)[b]	353 [3.51]	422 [2.94]

[a]M05-2X(D3)/def2-TZVPP. Vertical excitations at the S_0 minimum and emission from S_1 minimum. [b]N-CDs without dopamine.

OPTIMIZED CARTESIAN COORDINATES OF THE GEOMETRICAL MODELS FOR N-CDs NANOPARTICLES AND DA/N-CDs COMPLEXES IN ANGTROMS

C1(0)

C	6	2.545927000000	0.278675000000	-2.136647000000
C	6	1.260706000000	0.135241000000	-1.591355000000
C	6	3.502398000000	-0.731184000000	-1.947753000000
C	6	3.180842000000	-1.874520000000	-1.150534000000
C	6	0.950752000000	-1.012216000000	-0.795078000000
C	6	1.918850000000	-1.983421000000	-0.584344000000
C	6	4.160426000000	-2.890750000000	-0.952740000000
C	6	4.804729000000	-0.683821000000	-2.535792000000
C	6	-0.352206000000	-1.145848000000	-0.232958000000
C	6	0.217023000000	1.088107000000	-1.807103000000
C	6	5.706958000000	-1.678228000000	-2.333559000000
C	6	5.386390000000	-2.799656000000	-1.523305000000
C	6	-1.015992000000	0.919357000000	-1.264313000000
C	6	-1.308257000000	-0.211709000000	-0.456652000000
H	1	1.681770000000	-2.846569000000	0.021932000000
H	1	3.897186000000	-3.739598000000	-0.338803000000
H	1	5.079551000000	0.146138000000	-3.165921000000
H	1	-0.558877000000	-2.015809000000	0.372991000000
H	1	0.398122000000	1.952154000000	-2.424767000000
H	1	6.680603000000	-1.618947000000	-2.794942000000
H	1	6.120119000000	-3.575713000000	-1.370860000000
H	1	-1.786447000000	1.651728000000	-1.449549000000
H	1	-2.292806000000	-0.323228000000	-0.029956000000
C	6	2.886491000000	1.490390000000	-2.960557000000
C	6	2.567822000000	1.254438000000	-4.448779000000
H	1	2.334088000000	2.356582000000	-2.609860000000
H	1	3.937489000000	1.738232000000	-2.853686000000
C	6	2.936402000000	2.471966000000	-5.239779000000
H	1	3.132889000000	0.397788000000	-4.807647000000
H	1	1.506443000000	1.070562000000	-4.579299000000
O	8	2.181647000000	3.329727000000	-5.602588000000
O	8	4.265372000000	2.539462000000	-5.467348000000
H	1	4.430223000000	3.366315000000	-5.936341000000

C2(0)

C	6	2.513669000000	0.158011000000	-2.116277000000
C	6	1.227725000000	0.190883000000	-1.554865000000
C	6	3.378894000000	-0.905792000000	-1.816967000000
C	6	2.967669000000	-1.919419000000	-0.895060000000
C	6	0.827226000000	-0.828128000000	-0.634216000000
C	6	1.708234000000	-1.851819000000	-0.317266000000
C	6	3.856103000000	-2.990150000000	-0.585626000000
C	6	4.672812000000	-1.042638000000	-2.409107000000
C	6	-0.475498000000	-0.781737000000	-0.057729000000
C	6	0.268914000000	1.202439000000	-1.872655000000
C	6	5.486615000000	-2.083812000000	-2.097836000000
C	6	5.078452000000	-3.073562000000	-1.164816000000
C	6	-0.967399000000	1.206332000000	-1.311714000000
C	6	-1.348427000000	0.202868000000	-0.381875000000
H	1	1.403380000000	-2.617053000000	0.382847000000
H	1	3.525825000000	-3.737998000000	0.120291000000
H	1	5.010807000000	-0.319599000000	-3.132812000000
H	1	-0.750715000000	-1.557458000000	0.641688000000
H	1	0.516810000000	1.971674000000	-2.585132000000
H	1	6.454900000000	-2.164949000000	-2.567026000000
H	1	5.742330000000	-3.890085000000	-0.927557000000
H	1	-1.672964000000	1.978422000000	-1.576935000000
H	1	-2.333836000000	0.227108000000	0.056454000000
C	6	2.949422000000	1.240443000000	-3.069505000000
C	6	2.593183000000	0.884567000000	-4.513777000000
H	1	2.479668000000	2.179590000000	-2.788047000000
H	1	4.021563000000	1.393566000000	-2.974070000000
C	6	2.965894000000	1.883141000000	-5.591679000000
H	1	3.062551000000	-0.056976000000	-4.794826000000
H	1	1.520641000000	0.721959000000	-4.606932000000
O	8	2.700559000000	1.672086000000	-6.755513000000
N	7	3.604796000000	3.011406000000	-5.194395000000
H	1	3.856006000000	3.677053000000	-5.900274000000
H	1	3.828823000000	3.197434000000	-4.239048000000

C3(0)

C	6	2.408472000000	0.134796000000	-2.216495000000
C	6	1.103947000000	0.013361000000	-1.710212000000
C	6	3.387018000000	-0.799273000000	-1.840424000000
C	6	3.066252000000	-1.833172000000	-0.904801000000
C	6	0.793424000000	-1.024299000000	-0.775888000000
C	6	1.782181000000	-1.916505000000	-0.386813000000
C	6	4.070056000000	-2.769803000000	-0.520778000000
C	6	4.716267000000	-0.780322000000	-2.366176000000
C	6	-0.530877000000	-1.131886000000	-0.259538000000
C	6	0.041109000000	0.886416000000	-2.100314000000
C	6	5.642815000000	-1.695920000000	-1.983948000000
C	6	5.320180000000	-2.707065000000	-1.040003000000
C	6	-1.210829000000	0.745825000000	-1.594024000000
C	6	-1.505349000000	-0.275972000000	-0.652538000000
H	1	1.544833000000	-2.696735000000	0.322952000000
H	1	3.805046000000	-3.535560000000	0.193538000000
H	1	4.990966000000	-0.033633000000	-3.092231000000
H	1	-0.738094000000	-1.918584000000	0.451125000000
H	1	0.227804000000	1.665614000000	-2.820419000000
H	1	6.637048000000	-1.659167000000	-2.401902000000
H	1	6.072017000000	-3.422455000000	-0.745142000000
H	1	-1.994449000000	1.416855000000	-1.910410000000
H	1	-2.505552000000	-0.367226000000	-0.258444000000
C	6	2.735390000000	1.233419000000	-3.191221000000
C	6	2.479550000000	0.805724000000	-4.633933000000
H	1	2.147677000000	2.122458000000	-2.985820000000
H	1	3.774585000000	1.536627000000	-3.085294000000
N	7	2.730377000000	1.925723000000	-5.534190000000
H	1	3.081957000000	-0.081970000000	-4.850928000000
H	1	1.435196000000	0.514514000000	-4.733315000000
H	1	2.514697000000	1.678711000000	-6.487643000000
H	1	3.704195000000	2.190203000000	-5.507986000000

DOPAMINE

N	7	-1.991324000000	-1.536274000000	-2.306018000000
H	1	-2.334127000000	-0.749382000000	-1.738128000000
H	1	-1.109344000000	-1.244979000000	-2.722288000000
H	1	-2.649986000000	-1.735222000000	-3.054233000000
C	6	-1.792636000000	-2.709779000000	-1.380374000000
C	6	-1.073296000000	-2.219218000000	-0.127898000000
C	6	-1.810266000000	-1.052929000000	0.476100000000
C	6	-3.007698000000	-1.262878000000	1.165740000000
C	6	-1.365429000000	0.244824000000	0.282813000000
C	6	-3.737247000000	-0.201974000000	1.666543000000
C	6	-2.100478000000	1.321545000000	0.776087000000
C	6	-3.279650000000	1.113930000000	1.462615000000
H	1	-3.361706000000	-2.270280000000	1.345357000000
H	1	-0.420332000000	0.430019000000	-0.208765000000
O	8	-4.883556000000	-0.337002000000	2.356173000000
H	1	-1.739459000000	2.330583000000	0.639781000000
O	8	-4.040155000000	2.097545000000	1.974133000000
H	1	-0.051560000000	-1.933715000000	-0.375126000000
H	1	-1.015275000000	-3.057182000000	0.563051000000
H	1	-1.241242000000	-3.468245000000	-1.924880000000
H	1	-2.785748000000	-3.076122000000	-1.143092000000
H	1	-5.083933000000	-1.261187000000	2.518616000000
H	1	-3.630537000000	2.954914000000	1.838686000000

C1

C	6	2.596835000000	0.394421000000	-2.024265000000
C	6	1.302289000000	0.275766000000	-1.494607000000
C	6	3.514407000000	-0.658517000000	-1.878857000000
C	6	3.114263000000	-1.853967000000	-1.199484000000
C	6	0.921494000000	-0.918852000000	-0.805784000000
C	6	1.832381000000	-1.956774000000	-0.678703000000
C	6	4.032862000000	-2.940430000000	-1.084267000000
C	6	4.848160000000	-0.616703000000	-2.395016000000
C	6	-0.395298000000	-1.038086000000	-0.273812000000
C	6	0.314732000000	1.302063000000	-1.620897000000
C	6	5.695473000000	-1.671787000000	-2.266208000000
C	6	5.282766000000	-2.861386000000	-1.609401000000
C	6	-0.931646000000	1.150085000000	-1.103099000000
C	6	-1.298225000000	-0.038100000000	-0.417327000000
H	1	1.535992000000	-2.864589000000	-0.172710000000
H	1	3.712068000000	-3.825690000000	-0.553338000000
H	1	5.207026000000	0.267403000000	-2.894499000000
H	1	-0.654153000000	-1.947263000000	0.247842000000
H	1	0.558421000000	2.227688000000	-2.116017000000
H	1	6.697491000000	-1.605673000000	-2.660416000000
H	1	5.970999000000	-3.686115000000	-1.512657000000
H	1	-1.652451000000	1.947083000000	-1.200685000000
H	1	-2.291753000000	-0.133993000000	-0.009178000000
C	6	2.942297000000	1.590188000000	-2.876012000000
C	6	2.429730000000	1.305913000000	-4.288009000000
H	1	2.495632000000	2.498574000000	-2.486469000000
H	1	4.009454000000	1.769683000000	-2.898287000000
C	6	2.781251000000	2.273272000000	-5.373331000000
H	1	2.796054000000	0.333046000000	-4.621303000000
H	1	1.341174000000	1.227105000000	-4.275450000000
O	8	2.412049000000	2.137384000000	-6.528568000000
O	8	3.535618000000	3.286748000000	-5.002453000000
H	1	3.714343000000	3.849395000000	-5.769080000000
H	1	1.382649000000	0.899442000000	-7.008038000000
N	7	0.672417000000	0.165856000000	-7.254440000000
H	1	0.709312000000	-0.549778000000	-6.525164000000
H	1	-0.246084000000	0.597666000000	-7.249035000000
C	6	0.962981000000	-0.496106000000	-8.566644000000
C	6	2.278668000000	-1.263137000000	-8.468658000000
C	6	2.339001000000	-2.089135000000	-7.209732000000
C	6	1.410522000000	-3.109804000000	-6.978332000000
C	6	3.260295000000	-1.794204000000	-6.221270000000
C	6	1.403413000000	-3.815679000000	-5.788250000000
C	6	3.259204000000	-2.497219000000	-5.019903000000
C	6	2.334768000000	-3.495591000000	-4.785298000000
H	1	0.698341000000	-3.384575000000	-7.746975000000
H	1	4.002856000000	-1.026829000000	-6.388966000000
O	8	0.541143000000	-4.817105000000	-5.517240000000
H	1	3.988928000000	-2.271425000000	-4.255451000000
O	8	2.278558000000	-4.203002000000	-3.642946000000
H	1	3.109772000000	-0.561148000000	-8.479601000000
H	1	2.362681000000	-1.881087000000	-9.360659000000
H	1	0.994301000000	0.277802000000	-9.325627000000
H	1	0.131619000000	-1.163172000000	-8.769705000000
H	1	0.011321000000	-5.028064000000	-6.288395000000
H	1	2.939644000000	-3.875933000000	-3.021305000000

C2

C	6	2.664869000000	0.383009000000	-2.105310000000
C	6	1.373134000000	0.308627000000	-1.561372000000
C	6	3.569344000000	-0.675020000000	-1.922258000000
C	6	3.158028000000	-1.832024000000	-1.185487000000
C	6	0.981763000000	-0.848358000000	-0.816834000000
C	6	1.879396000000	-1.892235000000	-0.650566000000
C	6	4.062468000000	-2.924199000000	-1.024175000000
C	6	4.898619000000	-0.678424000000	-2.451248000000
C	6	-0.331191000000	-0.924442000000	-0.267958000000
C	6	0.398714000000	1.341875000000	-1.725506000000
C	6	5.732959000000	-1.736916000000	-2.275963000000
C	6	5.310167000000	-2.887072000000	-1.558352000000
C	6	-0.844446000000	1.231618000000	-1.189655000000
C	6	-1.221062000000	0.081443000000	-0.447232000000
H	1	1.574925000000	-2.771652000000	-0.101157000000
H	1	3.732418000000	-3.778782000000	-0.450453000000
H	1	5.265548000000	0.170366000000	-3.003507000000
H	1	-0.597858000000	-1.806044000000	0.295361000000
H	1	0.646671000000	2.238615000000	-2.269477000000
H	1	6.731450000000	-1.705117000000	-2.683148000000
H	1	5.988306000000	-3.715173000000	-1.426045000000
H	1	-1.555650000000	2.032699000000	-1.318980000000
H	1	-2.211937000000	0.018538000000	-0.026532000000
C	6	3.021078000000	1.540675000000	-3.005113000000
C	6	2.489278000000	1.224528000000	-4.404063000000
H	1	2.591399000000	2.465081000000	-2.627839000000
H	1	4.096432000000	1.683002000000	-3.031201000000
C	6	2.813729000000	2.156677000000	-5.538042000000
H	1	2.848026000000	0.240822000000	-4.709196000000
H	1	1.401576000000	1.149669000000	-4.363053000000
O	8	2.408056000000	1.907790000000	-6.683326000000
N	7	3.544314000000	3.237054000000	-5.292571000000
N	7	0.677861000000	0.010373000000	-7.218585000000
H	1	0.696485000000	-0.685461000000	-6.471945000000
H	1	-0.232228000000	0.458149000000	-7.226493000000
H	1	1.419994000000	0.757897000000	-6.987904000000
C	6	0.953932000000	-0.685717000000	-8.511941000000
C	6	2.260173000000	-1.467454000000	-8.404358000000
C	6	2.317672000000	-2.272972000000	-7.132005000000
C	6	1.367998000000	-3.265166000000	-6.867651000000
C	6	3.262166000000	-1.985965000000	-6.163558000000
C	6	1.360108000000	-3.948645000000	-5.664449000000
C	6	3.261131000000	-2.666877000000	-4.949983000000
C	6	2.314137000000	-3.634959000000	-4.682476000000
H	1	0.635552000000	-3.533490000000	-7.619333000000
H	1	4.019375000000	-1.239210000000	-6.355988000000
O	8	0.474071000000	-4.921352000000	-5.362272000000
H	1	4.007662000000	-2.446043000000	-4.200781000000
O	8	2.257212000000	-4.317574000000	-3.522721000000
H	1	3.098486000000	-0.774743000000	-8.428606000000
H	1	2.335329000000	-2.102479000000	-9.285176000000
H	1	0.997806000000	0.069545000000	-9.289089000000
H	1	0.115187000000	-1.346907000000	-8.705388000000
H	1	-0.073712000000	-5.128034000000	-6.121858000000
H	1	2.939020000000	-3.995245000000	-2.922515000000
H	1	3.762410000000	3.859698000000	-6.050390000000
H	1	3.868629000000	3.453652000000	-4.370034000000

C3

C	6	2.505523000000	0.316551000000	-2.163386000000
C	6	1.249008000000	0.172095000000	-1.553888000000
C	6	3.488962000000	-0.671978000000	-1.988347000000
C	6	3.183581000000	-1.841034000000	-1.218842000000
C	6	0.965780000000	-0.991552000000	-0.771429000000
C	6	1.932977000000	-1.974892000000	-0.631803000000
C	6	4.165042000000	-2.866727000000	-1.073604000000
C	6	4.803591000000	-0.585944000000	-2.545043000000
C	6	-0.312873000000	-1.137270000000	-0.158735000000
C	6	0.207866000000	1.143934000000	-1.680963000000
C	6	5.718540000000	-1.576423000000	-2.371905000000
C	6	5.394709000000	-2.746732000000	-1.636578000000
C	6	-0.997691000000	0.970595000000	-1.080748000000
C	6	-1.268897000000	-0.189176000000	-0.307276000000
H	1	1.708499000000	-2.861767000000	-0.056194000000
H	1	3.911753000000	-3.734831000000	-0.481524000000
H	1	5.098618000000	0.286188000000	-3.103259000000
H	1	-0.498546000000	-2.023651000000	0.429076000000
H	1	0.379534000000	2.047113000000	-2.243204000000
H	1	6.706634000000	-1.472353000000	-2.792467000000
H	1	6.133112000000	-3.522754000000	-1.511521000000
H	1	-1.759423000000	1.728253000000	-1.180751000000
H	1	-2.232697000000	-0.304317000000	0.162459000000
C	6	2.727573000000	1.449277000000	-3.133546000000
C	6	2.107885000000	1.033383000000	-4.468665000000
H	1	2.282684000000	2.374820000000	-2.777560000000
H	1	3.783569000000	1.653155000000	-3.273377000000
N	7	2.389344000000	1.898536000000	-5.627584000000
H	1	2.462130000000	0.034030000000	-4.714049000000
H	1	1.026340000000	0.969986000000	-4.347731000000
H	1	3.386331000000	1.953223000000	-5.788546000000
H	1	2.073657000000	2.844407000000	-5.457635000000
H	1	1.514172000000	1.000719000000	-6.767367000000
N	7	0.818070000000	0.309724000000	-7.226500000000
H	1	0.695831000000	-0.456668000000	-6.561310000000
H	1	-0.070791000000	0.787041000000	-7.335561000000
C	6	1.278511000000	-0.275770000000	-8.523158000000
C	6	2.536181000000	-1.116018000000	-8.312808000000
C	6	2.448806000000	-1.989262000000	-7.086175000000
C	6	1.357844000000	-2.842964000000	-6.882121000000
C	6	3.419892000000	-1.914240000000	-6.105466000000
C	6	1.232171000000	-3.582524000000	-5.718267000000
C	6	3.303828000000	-2.655845000000	-4.934372000000
C	6	2.211213000000	-3.470034000000	-4.716819000000
H	1	0.602781000000	-2.961965000000	-7.650246000000
H	1	4.282007000000	-1.277803000000	-6.245235000000
O	8	0.204744000000	-4.421993000000	-5.472459000000
H	1	4.066978000000	-2.590731000000	-4.172845000000
O	8	2.030633000000	-4.184438000000	-3.590321000000
H	1	-0.345975000000	-4.523828000000	-6.250971000000
H	1	2.716654000000	-3.961156000000	-2.951983000000
H	1	3.400357000000	-0.462042000000	-8.217954000000
H	1	2.681594000000	-1.706831000000	-9.215975000000
H	1	1.453278000000	0.541888000000	-9.214023000000
H	1	0.460532000000	-0.880759000000	-8.901003000000

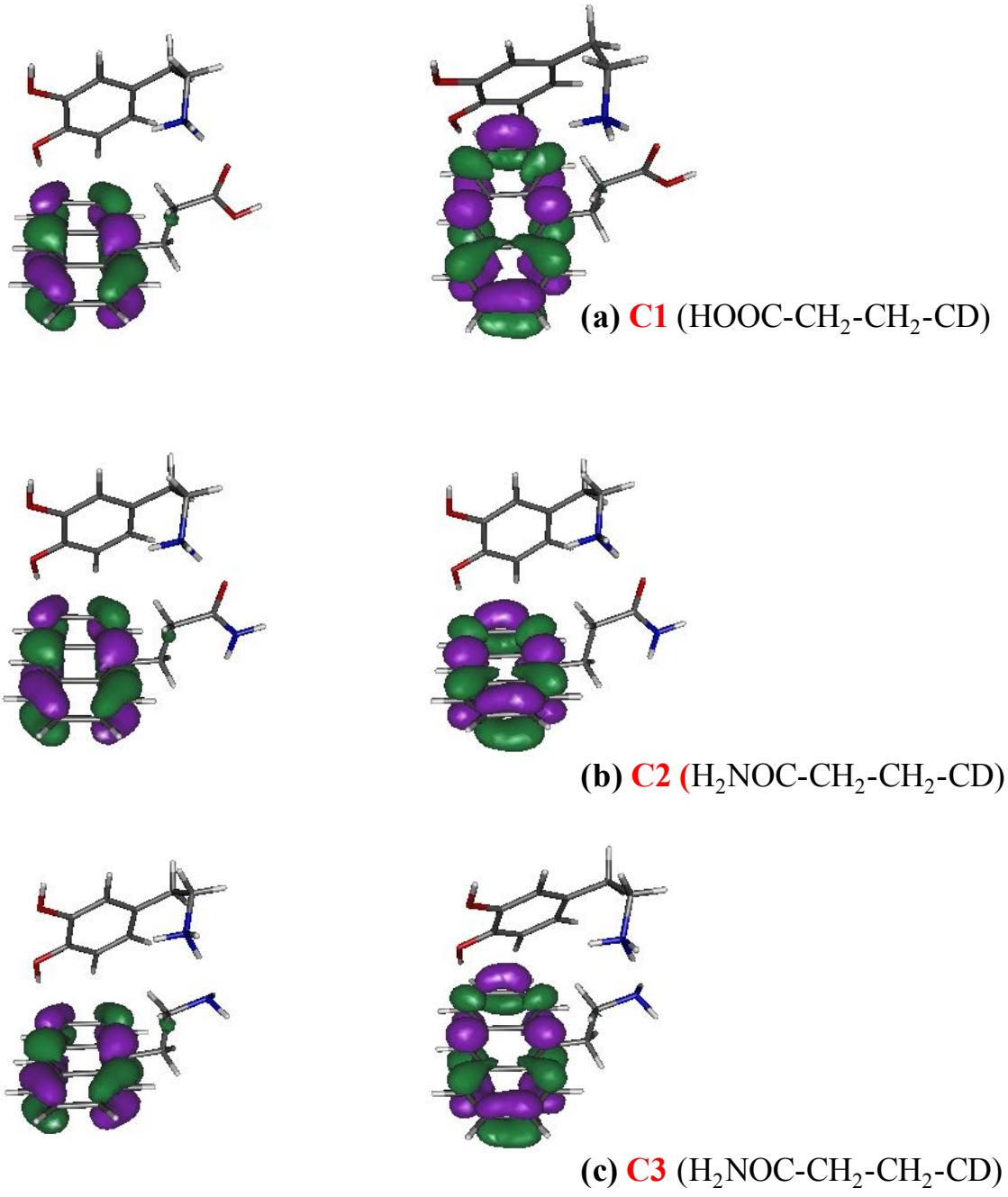

Figure S6. Main molecular orbitals involved on the $S_0 \rightarrow S_1$ transition of the N-CDs complexes. (a) **C1** (-COOH); (b) **C2** (-$CONH_2$); (c) **C3** (-CH_2NH_2).