Excited-State Absorption of DNA bases in the gas phase and in chloroform solution: a comparative quantum mechanical study. Supplementary Information

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S1 Results

IPs

Table S1: First ionization energy of the four nucleobases (FC geometries) in gas phase.

	CCSD [eV]	CC3 [eV]	CAM-B3LYP
Adenine	8.257	8.236	8.38
Cytosine	8.683	8.616	8.82
Guanine	7.858	7.799	7.97
Thymine	9.045	8.930	9.44

SS1.1 ESA summary

Table S2: Summary of energy region and number of excited states (in parenthesis) computed with various methods for a particular target state of all four nucleobases.

	State	EOM-CC3	EOM-CCSD	CAM-B3LYP
Thymine	1π	4.08(50)	4.15(50)	4.13(43)
	1n	4.30(51)	4.40(51)	4.25(45)
Cytosine	1π	3.95(44)	4.3(51)	4.05(43)
	1n	3.51(43)	3.8(50)	3.74(43)
Adenine	L_a	1.69(17)	2.71(39)	3.02(43)
	L_b	1.79(19)	2.84(39)	2.96(42)
	1n	1.75(18)	2.73(39)	3.10(43)
Guanine	L_a	1.7(14)	2.56(28)	3.17(43)
	L_b	1.2(12)	2.02(25)	2.73(41)
	1n	1.1(11)	2.03(26)	2.71(42)

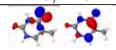
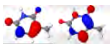
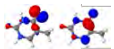
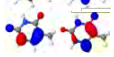
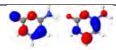
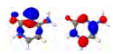
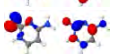
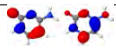
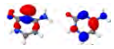
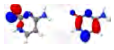
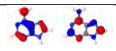
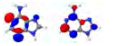
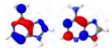
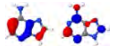
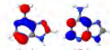
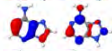
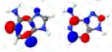
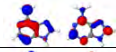
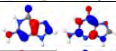
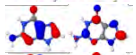
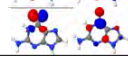
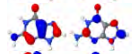
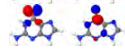
		State					
Molecule	Method	Sym	Energy	f×100	Character	MO/NTO	Weight
Thymine	CAM-B3LYP	1A″	5.13	0.00	1n/nπ^*		1.00
		1A′	5.25	17.5	1$\pi/\pi\pi^*$		0.97
	CCSD	1A″	5.26 (5.01)	0.00	1n/nπ^*		0.80
		1A′	5.51 (5.28)	20.7 (15.9)	1$\pi/\pi\pi^*$		0.76
Cytosine	CAM-B3LYP	1A′	4.98	6.56	1$\pi/\pi\pi^*$		0.96
		1A″	5.29	0.19	1n/nπ^*		1.0
		3A″	5.92	0.01	2n/nπ^*		0.94
	CCSD	1A′	4.99 (4.76)	6.57 (5.09)	1$\pi/\pi\pi^*$		0.74
		1A″	5.46 (5.20)	0.26 (0.21)	1n/nπ^*		0.8
		6A″	6.34	0.00	n/nπ^*		0.7
Adenine	CAM-B3LYP	1A′	5.34	27.7	$L_a/\pi\pi^*$		0.95
		1A″	5.35	0.06	1n/nπ^*		0.98
		2A′	5.49	1.32	$L_b/\pi\pi^*$		0.72
							0.27
	CCSD	1A′	5.41 (5.24)	0.56 (0.55)	$L_b/\pi\pi^*$		0.49
							0.28
		1A″	5.51 (5.28)	0.18 (0.11)	1n/nπ^*		0.78
		2A′	5.53 (5.31)	29.7 (26.31)	$L_a/\pi\pi^*$		0.73
Guanine	CAM-B3LYP	1A′	5.13	14.8	$L_a/\pi\pi^*$		0.95
		2A′	5.57	33.7	$L_b/\pi\pi^*$		0.96
		3A″	5.59	0.00	nπ^*		1.0
	CCSD	1A′	5.21 (5.03)	16.6 (13.43)	$L_a/\pi\pi^*$		0.73
		2A′	5.751 (5.51)	34.8 (30.42)	$L_b/\pi\pi^*$		0.76
		3A″ (1A″)	5.750 (5.61)	0.00	nπ^*		0.82

Figure S1: Excited states considered for each molecule in gas phase and their characterization via Natural Transition Orbitals. Energies in eV. The EOM-CC3 data is shown in parenthesis beside the corresponding EOM-CCSD values.

SS1.2 Comparison with RASPT2/ANO-L results

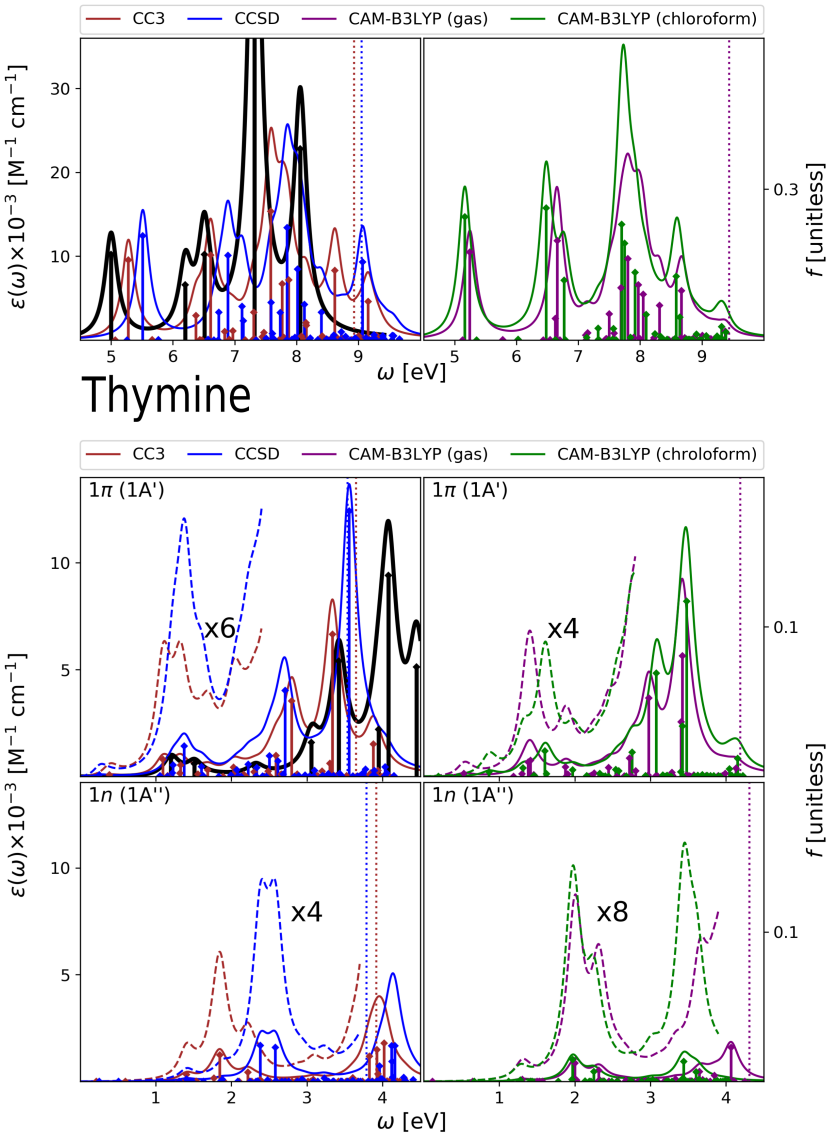


Figure S2: Thymine. Comparison of our results with RASPT2 (in thick black) from Ref. [1]. The top panels refer to OPA and the middle and bottom panels to ESA (notice the excited state labels).

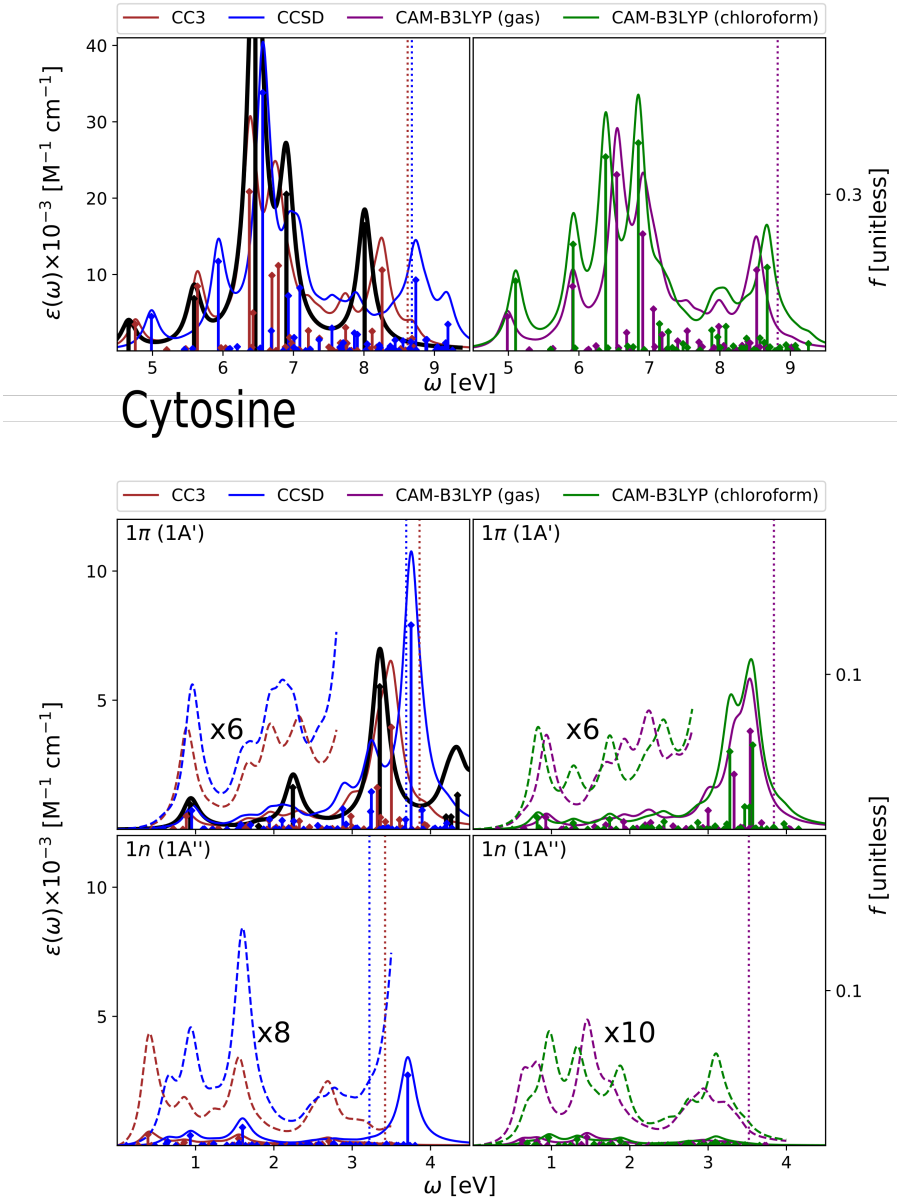


Figure S3: Cytosine. Comparison of our results with RASPT2 (in thick black) from Ref. [1]. The top panels refer to OPA and the middle and bottom panels to ESA (notice the excited state labels).

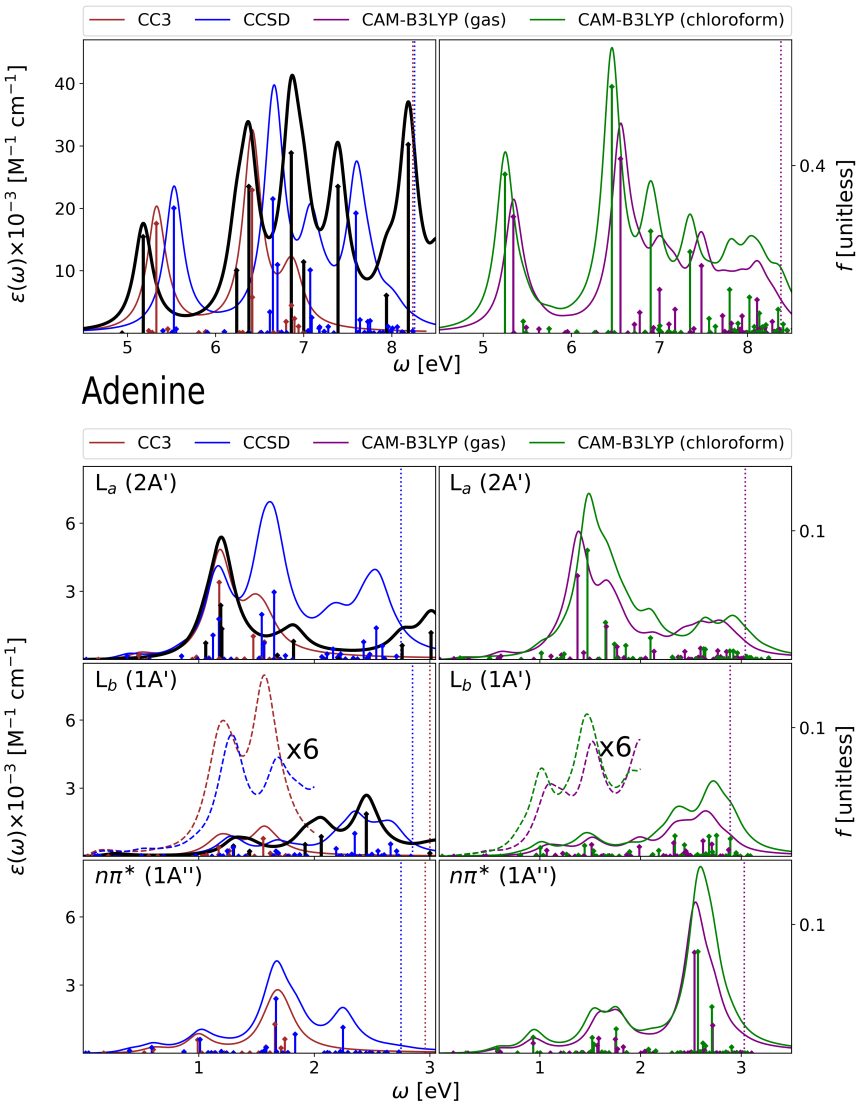


Figure S4: Adenine. Comparison of our results with RASPT2 (in thick black) from Ref. [1]. The top panels refer to OPA and the middle and bottom panels to ESA (notice the excited state labels).

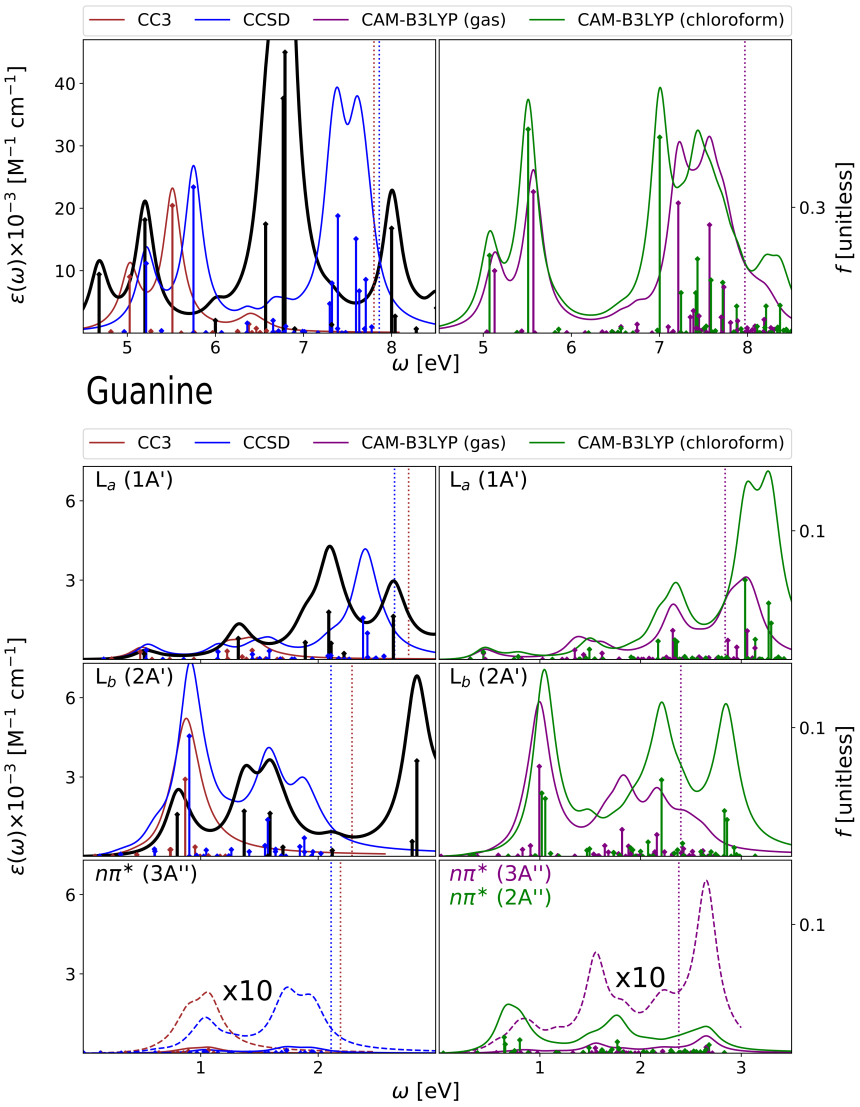


Figure S5: Guanine. Comparison of our results with RASPT2 (in thick black) from Ref. [1]. The top panels refer to OPA and the middle and bottom panels to ESA (notice the excited state labels).

SS1.3 One-photon Absorption: Comparison with Experiment

Computed OPA spectra for the four nucleobases are compared with available experimental results in Figures S6–S9. Computed spectra have been red-shifted by an amount specified by the inset in the Figures so to approximately overlap the lowest-energy computed and experimental bands; their shape nicely compare with the low-energy part of the experimental spectra. Data in the figures clearly suggest that the employed levels of electronic structure theory overestimate the excitation energies of the bright states, EOM-CC3 generally being the most accurate. However, it is not possible to precisely define the error of the electronic calculations. In fact, the experimental spectrum of adenine was measured at ∼500 K, and the one adopted to compare with thymine was actually measured for 1-methyl-thymine at 370 K. Spectra for cytosine and guanine were obtained at lower temperatures, but in any case it is known that they arise from a contribution of a mixture of different tautomers [2, 3]. On the contrary, the computed spectra were obtained considering a single tautomer for each nucleobase at 0 K, neglecting both vibronic and non-adiabatic effects, and simply broadening the stick electronic intensities with a phenomenological Lorentzian. For instance, it is well known that vibronic effects usually induce a red-shift by 0.1–0.2 eV of the spectral maximum at room temperature, and analytical expressions of the first spectral moment suggest that larger red-shifts should occur at larger temperatures [4].

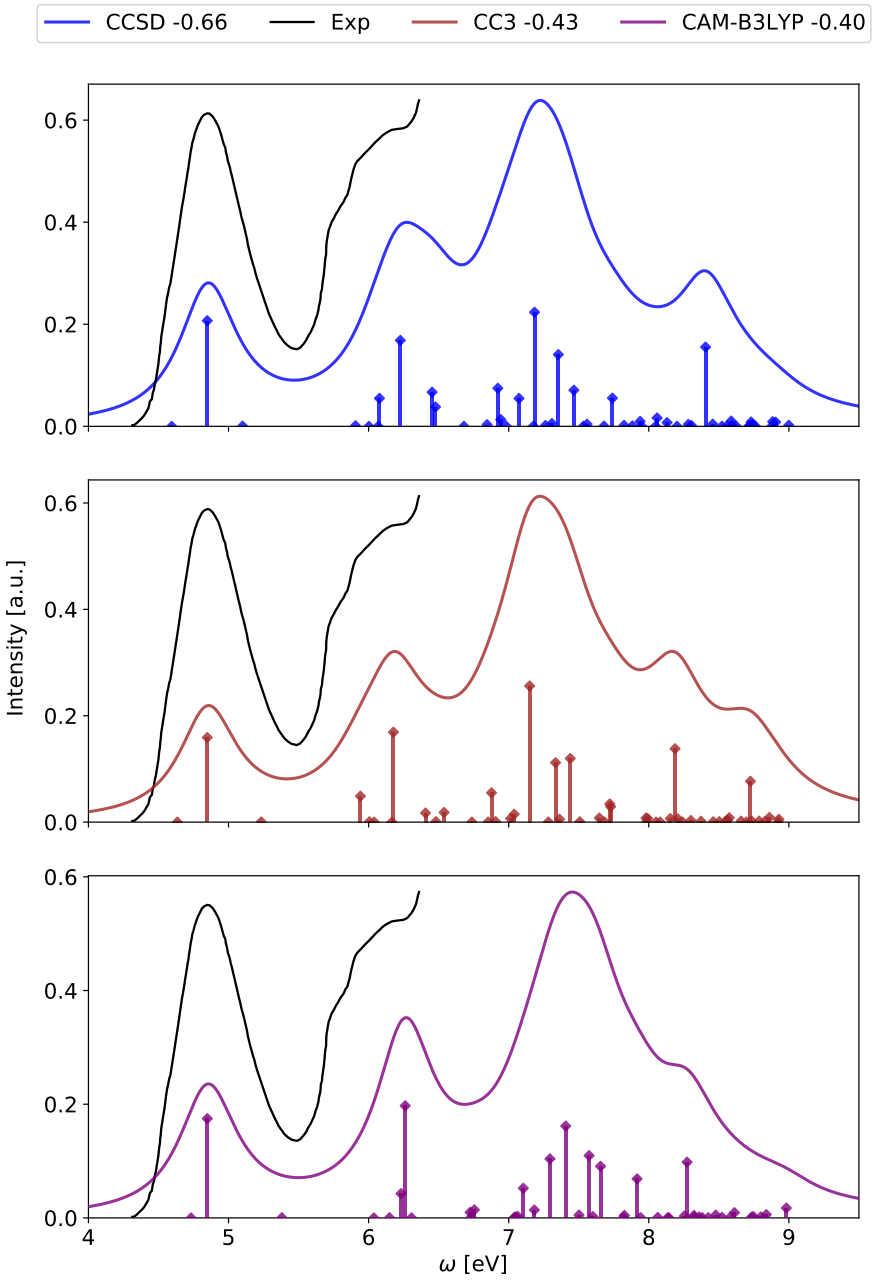


Figure S6: Thymine. Comparison of our results for OPA with experimental spectrum for 1-methyl-thymine in vapor phase at 370K taken from Ref. [5].

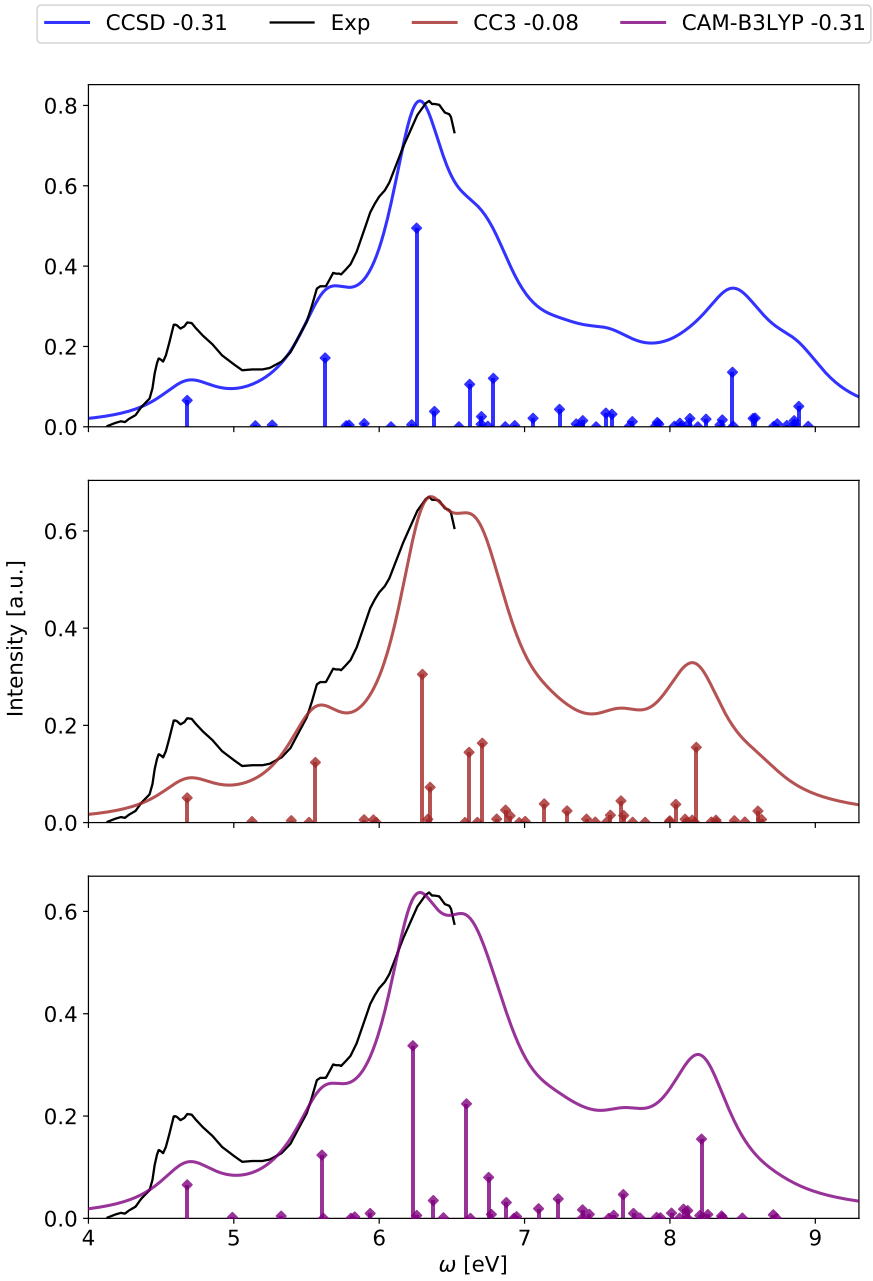


Figure S7: Cytosine. Comparison of our results for OPA with the experimental spectrum measured in an Argon matrix at low-temperature taken from Ref. [2].

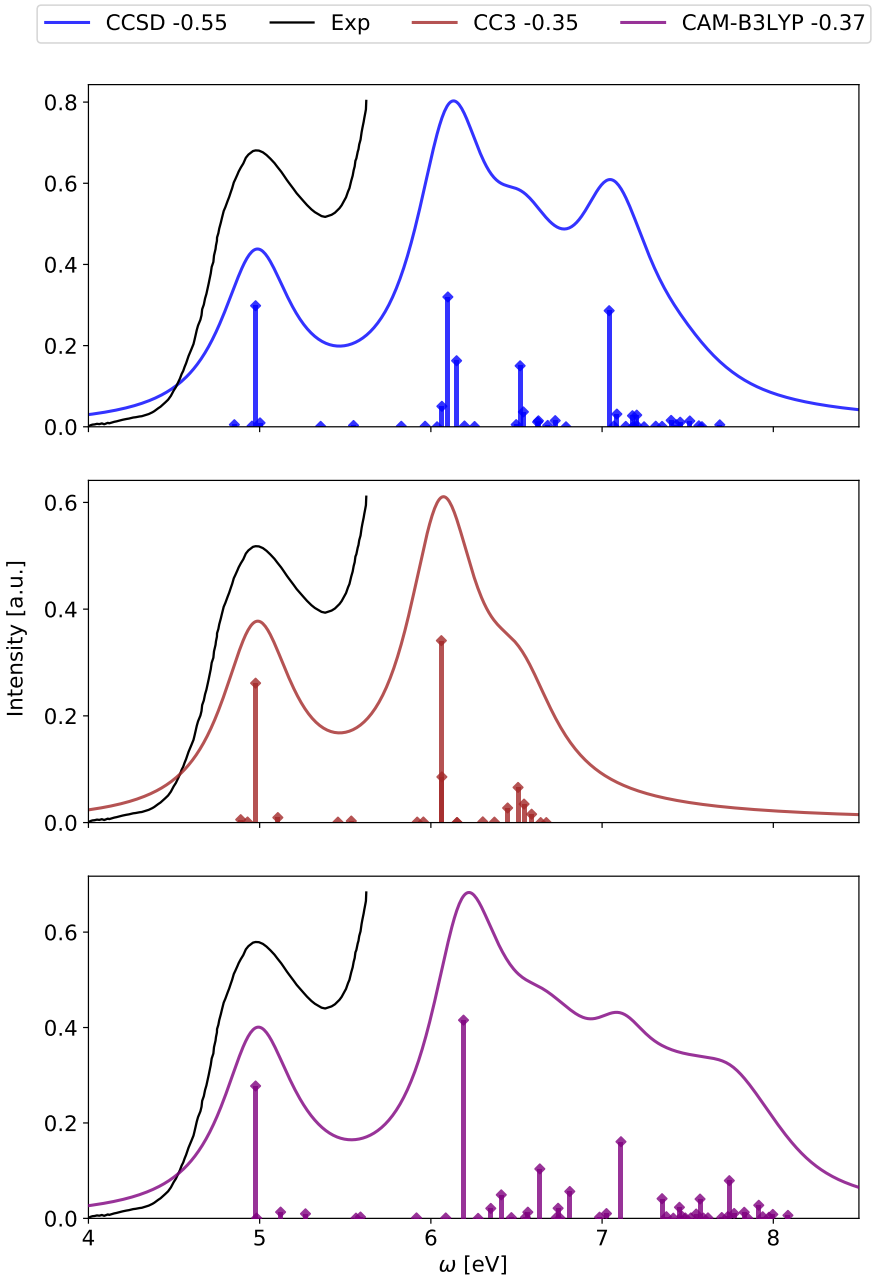


Figure S8: Adenine. Comparison of our results for OPA with the experimental spectrum in vapor phase at 500K taken from Ref. [5].

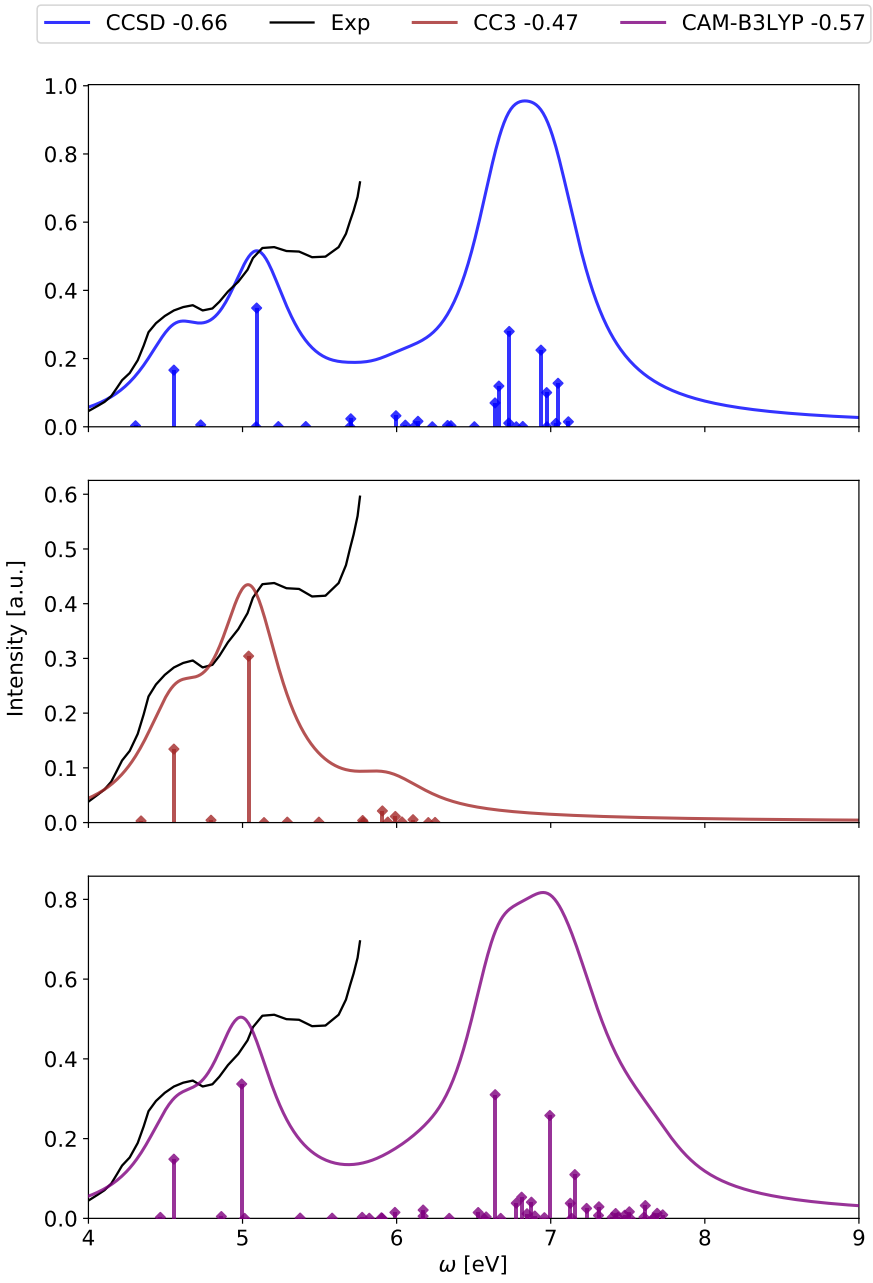


Figure S9: Guanine. Comparison of our results for OPA with the experimental spectrum in nitrogen matrix at 15 K taken from Ref. [3].

SS1.4 PCM/OPA at gas-phase versus PCM optimized ground-state geometry

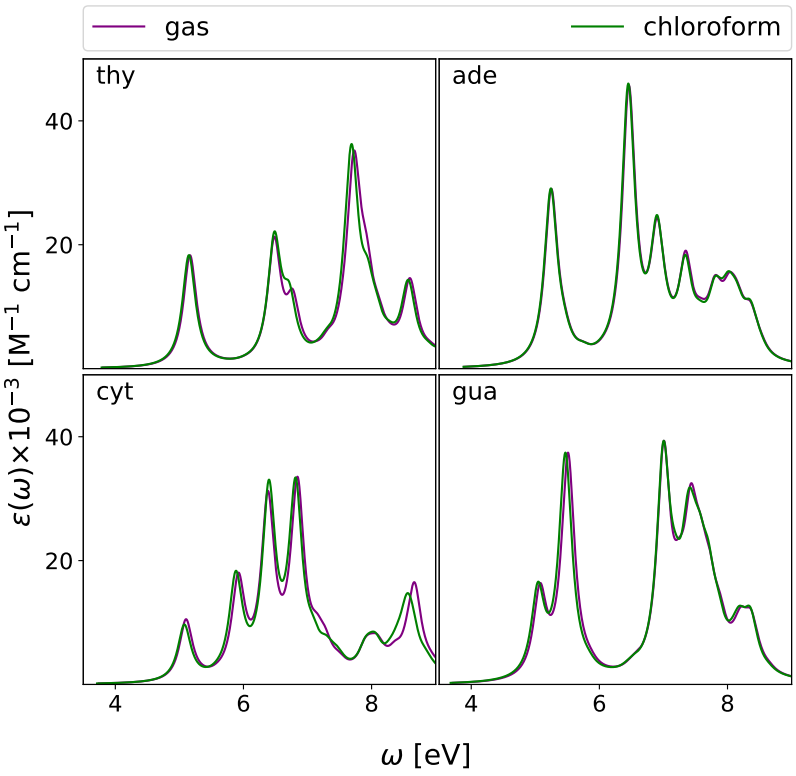


Figure S10: PCM/TD-CAMB3LYP OPA using gas-phase and PCM optimized geometries for the ground state.

SS1.5 Experimental transition absorption spectra

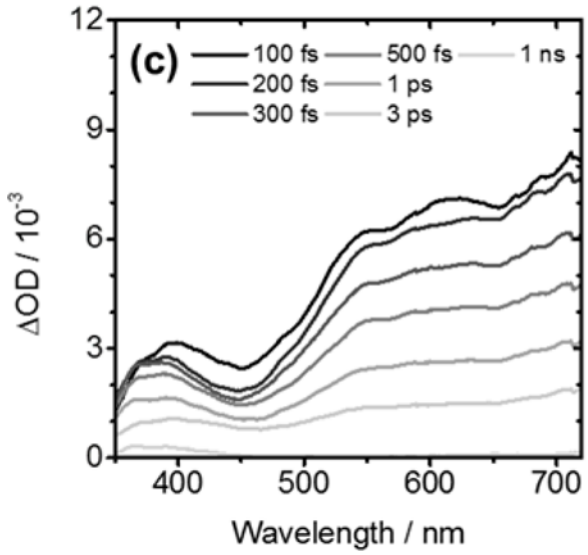


Figure S11: Thymine. TEA spectra recorded in chloroform after 260 nm excitation for 3',5'-Di-O-(tert-butyldimethylsilyl)-2'-deoxythymidine, reproduced with permission from *Is UV-Induced Electron-Driven Proton Transfer Active in a Chemically Modified A·T DNA Base Pair?*, J. Phys. Chem. B 2017, 121, 4448-4455 [6], main text.

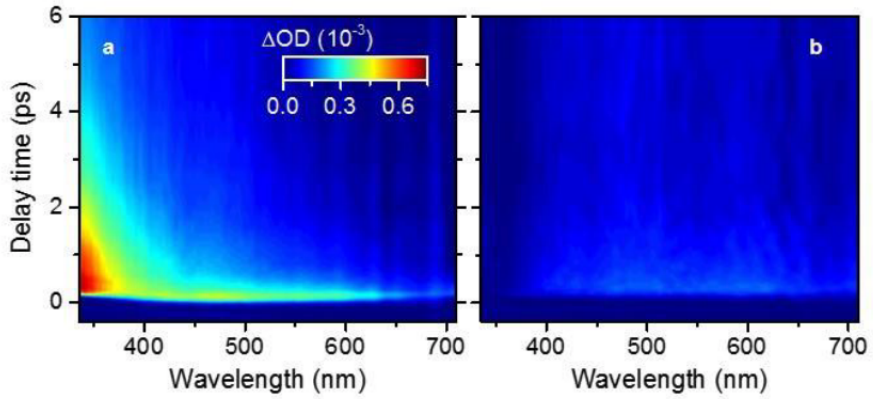


Figure S12: Cytosine and Guanine. Transient absorption maps after 260 nm excitation of (a) 2',3',5'-Tri-O-(tert-butyldimethylsilyl)-guanosine and (b) 3',5'-Di-O-(tert-butyldimethylsilyl)-2'-deoxycytidine, measured separately and scaled according to their actinometric factors to a concentration $c = 5.6$ mM. Both absorption maps are shown on the same intensity scale. Reproduced with permission from *Ultraviolet Absorption Induces Hydrogen-Atom Transfer in G·C Watson–Crick DNA Base Pairs in Solution*, Angew. Chem. Int. Ed., 54(49), 14719-14722, 2015 (see ESI file) [7].

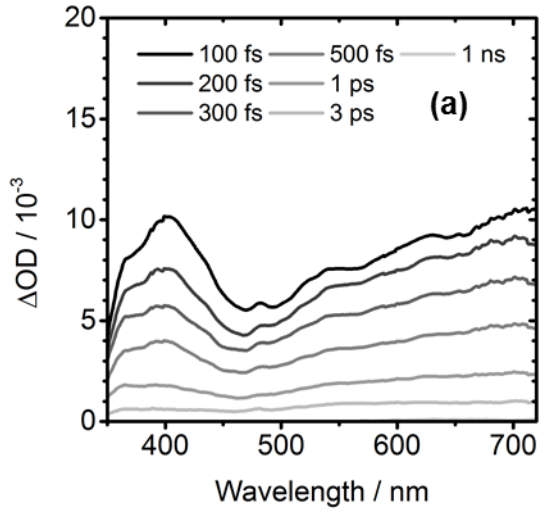


Figure S13: Adenine. TEAS measurements after 260 nm excitation of the 8-tert-butyl-9-ethyladenine in $CHCl_3$ ($c_0 = 50$ mM). Reproduced with permission from: *Is UV-Induced Electron-Driven Proton Transfer Active in a Chemically Modified A·T DNA Base Pair?*, J. Phys. Chem. B 2017, 121, 4448-4455 (SI) [6]. Please notice that $CHCl_3$ also absorbs in that region (see SI in the same paper).

SS1.6 Cartesian coordinates

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#Thymine, ground state opt  Cs sym  cam-b3lyp/6-311+G(d,p)
0 1
   7         0.155116   -1.658819    0.000000
   6         1.355869   -0.978682    0.000000
   7         1.196269    0.390701    0.000000
   6        -0.000000    1.114923    0.000000
   6        -1.214111    0.296415    0.000000
   6        -1.073416   -1.036928    0.000000
   8         2.430202   -1.531746    0.000000
   8         0.018245    2.326017    0.000000
   1         0.230151   -2.663902    0.000000
   1         2.049617    0.934284    0.000000
   6        -2.532996    1.000762    0.000000
   1        -1.925568   -1.704714    0.000000
   1        -3.357798    0.287281    0.000000
   1        -2.627877    1.645382    0.875945
   1        -2.627877    1.645382   -0.875945

#Cytosine, ground state opt  Cs sym  cam-b3lyp/6-311+G(d,p)
0 1
  6      -0.066548   -1.714527   -0.000000
  6      -1.219007    0.431513    0.000000
  6       1.101517    0.340693   -0.000000
  6       1.131900   -1.097127   -0.000000
  7      -1.203699   -0.985159    0.000000
  7      -0.000000    1.047554    0.000000
  7       2.271670    1.018994   -0.000000
  8      -2.290717    0.994921    0.000000
  1      -2.112424   -1.423553    0.000000
  1       2.056960   -1.653675   -0.000000
  1      -0.176634   -2.791533   -0.000000
  1       3.159550    0.551294   -0.000000
  1       2.235310    2.025069   -0.000000

#Adenine, ground state opt  Cs sym  cam-b3lyp/6-311+G(d,p)
0 1
   6             0.664555   -2.021821    0.000000
   7             1.659008   -1.127792    0.000000
   6             1.353886    0.171290    0.000000
   6             0.000000    0.543282    0.000000
   6            -0.918721   -0.495494    0.000000
   7            -0.641588   -1.798863    0.000000
   1             0.973540   -3.061995    0.000000
   7             2.348282    1.080832    0.000000
   1             3.301658    0.761362    0.000000
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```
   1             2.137417    2.063682    0.000000
   7            -0.633203    1.770424    0.000000
   7            -2.142670    0.123487    0.000000
   6            -1.899333    1.476588    0.000000
   1            -3.038351   -0.337796    0.000000
   1            -2.705393    2.195054    0.000000

#Guanine CAM-B3LYP in gas ground state opt  Cs sym
0 1
 N                -2.16454700    0.72937400    0.00000000
 C                -1.82366900    2.06621000    0.00000000
 N                -0.54093100    2.25385700    0.00000000
 C                 0.00000000    0.98762100    0.00000000
 C                 1.36857000    0.55796600    0.00000000
 O                 2.40041600    1.18612500    0.00000000
 N                 1.42415700   -0.86968100    0.00000000
 C                 0.35668200   -1.72300200    0.00000000
 N                 0.62752800   -3.05317200    0.00000000
 N                -0.88207600   -1.32079900    0.00000000
 C                -0.99616000    0.02807900    0.00000000
 H                -2.57319600    2.84264900    0.00000000
 H                 2.36755200   -1.23274000    0.00000000
 H                 1.56178000   -3.41861300    0.00000000
 H                -0.15200300   -3.68733400    0.00000000
 H                -3.08891000    0.32874100    0.00000000

#thymine  ground-state opt cam-b3lyp/6-311+G(d,p) (pcm,solvent=chloroform)
0 1
              7                 0.155861   -1.656905    0.000000
              6                 1.348122   -0.978122    0.000000
              7                 1.193813    0.389891    0.000000
              6                -0.000000    1.111096    0.000000
              6                -1.211715    0.299008    0.000000
              6                -1.070916   -1.036322    0.000000
              8                 2.431872   -1.527412    0.000000
              8                 0.024973    2.328337    0.000000
              1                 0.219125   -2.664176    0.000000
              1                 2.049189    0.931542    0.000000
              6                -2.535469    0.996251    0.000000
              1                -1.920442   -1.706492    0.000000
              1                -3.353100    0.275165    0.000000
              1                -2.638688    1.637095    0.878043
              1                -2.638688    1.637095   -0.878043
```

```
#Cytosine ground-state opt  cam-b3lyp/6-311+G(d,p) (pcm,solvent=chloroform)
0 1
             6                -0.078238   -1.711082    0.000000
             6                -1.210691    0.429367    0.000000
             6                 1.109917    0.332531   -0.000000
             6                 1.124246   -1.101646   -0.000000
             7                -1.212279   -0.972910    0.000000
             7                 0.000000    1.046281    0.000000
             7                 2.277309    1.000355   -0.000000
             8                -2.284814    1.015877    0.000000
             1                -2.119118   -1.416904    0.000000
             1                 2.045734   -1.663820   -0.000000
             1                -0.199219   -2.786045    0.000000
             1                 3.160971    0.521282   -0.000000
             1                 2.263537    2.007372   -0.000000

#Adenine ground-state opt  cam-b3lyp/6-311+G(d,p) (pcm,solvent=chloroform)
0 1
           6                 0.667236   -2.022050    0.000000
           7                 1.660884   -1.127134    0.000000
           6                 1.356343    0.176061    0.000000
           6                -0.000000    0.544006    0.000000
           6                -0.920311   -0.494227    0.000000
           7                -0.638823   -1.800140    0.000000
           1                 0.977071   -3.062083    0.000000
           7                 2.349455    1.082195    0.000000
           1                 3.306220    0.769954    0.000000
           1                 2.144312    2.066945    0.000000
           7                -0.636766    1.769518    0.000000
           7                -2.142902    0.121699    0.000000
           6                -1.905190    1.471307    0.000000
           1                -3.043690   -0.333133    0.000000
           1                -2.715312    2.184771    0.000000

#Guanine ground-state opt cam-b3lyp/6-311+G(d,p) (pcm,solvent=chloroform)
0 1
             7                2.165508    0.731179    0.000000
             6                1.825250    2.064017    0.000000
             7                0.539098    2.251115    0.000000
             6               -0.000000    0.980487    0.000000
             6               -1.360687    0.546722    0.000000
             8               -2.391516    1.196786    0.000000
             7               -1.427933   -0.865854   -0.000000
             6               -0.362075   -1.726001   -0.000000
             7               -0.637636   -3.046651   -0.000000
             7                0.882261   -1.320604   -0.000000
             6                1.001166    0.024156    0.000000
```

1	2.576099	2.839064	0.000000
1	-2.369422	-1.236510	-0.000000
1	-1.575599	-3.407522	-0.000000
1	0.133343	-3.692663	-0.000000
1	3.096696	0.342769	0.000000

Planar pi-pi* (pseudo) minima

Adenine

N	-0.697490	-1.769678	0.000000
N	1.669399	-1.168025	0.000000
N	2.351188	1.063074	0.000000
N	-0.567259	1.762213	0.000000
N	-2.169000	0.162960	0.000000
C	0.684943	-2.051103	0.000000
C	-1.902479	1.516037	0.000000
C	1.380496	0.129048	0.000000
C	-0.000000	0.562268	0.000000
C	-0.950417	-0.500774	0.000000
H	0.944736	-3.099893	0.000000
H	-3.074357	-0.277988	0.000000
H	-2.672239	2.268913	0.000000
H	3.319578	0.782075	0.000000
H	2.099160	2.040225	0.000000

Cytosine

N	-1.261581	-0.946724	-0.000000
N	0.000000	1.057446	0.000000
N	2.302981	1.013240	0.000000
C	-0.146083	-1.757929	-0.000000
C	-1.144191	0.431935	-0.000000
C	1.159818	0.269821	0.000000
C	1.105110	-1.102763	0.000000
O	-2.261029	1.039129	-0.000000
H	-2.201067	-1.312637	-0.000000
H	2.008875	-1.697630	0.000000
H	-0.285426	-2.824776	-0.000000
H	3.214111	0.593980	0.000000
H	2.214005	2.013915	0.000000

Thymine

N	0.123521	-1.656065	0.000000
N	1.230515	0.393695	0.000000
C	-2.495838	1.014589	0.000000
C	1.336531	-0.961713	0.000000
C	0.000000	1.125746	0.000000
C	-1.187662	0.335086	0.000000
C	-1.122795	-1.103864	0.000000

```
O                2.382223   -1.582508    0.000000
O                0.052431    2.358156    0.000000
H                0.248475   -2.660995    0.000000
H                2.086585    0.929853    0.000000
H               -1.978781   -1.758536    0.000000
H               -3.324893    0.306774    0.000000
H               -2.584144    1.677620    0.869282
H               -2.584144    1.677620   -0.869282

Guanine
N               -1.504040   -0.849086    0.000000
N                0.556158    2.225279    0.000000
N                2.230442    0.711210    0.000000
N               -0.670828   -3.053095    0.000000
N                0.883191   -1.316980    0.000000
C                1.851700    2.030473    0.000000
C               -0.418679   -1.716037    0.000000
C                1.052850   -0.033805    0.000000
C               -0.000000    0.986680    0.000000
C               -1.360861    0.580539    0.000000
O               -2.377676    1.251963    0.000000
H                2.583330    2.825465    0.000000
H               -2.454747   -1.183812    0.000000
H               -1.602011   -3.428506    0.000000
H                0.112342   -3.683515    0.000000
H                3.167967    0.346265    0.000000

Non-planar pi-pi* minima (true absolute minima)
Cyt
N            -1.310699    0.834832   -0.231937
N             0.090817   -1.043719    0.211651
N             2.383591   -0.807160   -0.152892
C            -1.124346   -0.547209    0.052548
C            -0.318735    1.718012    0.056533
C             1.157692   -0.199170    0.016515
C             0.992431    1.181690    0.061997
O            -2.172580   -1.194973    0.148854
H            -2.271685    1.128587   -0.319936
H             1.840089    1.849008    0.119361
H            -0.555979    2.760468    0.172795
H             3.195405   -0.253072    0.066999
H             2.429075   -1.746901    0.209461

Ade
N               0.009749   -0.025352    0.024966
N              -0.706910    0.135680    3.632378
N               2.135018    0.021967    0.743346
```

```
N              1.665997    0.155249    3.116799
N             -2.315182   -0.071336    1.963855
C              0.561341    0.089513    3.990673
C             -1.033513    0.071449    2.345281
C              0.018916   -0.060082    1.351304
C              1.342976   -0.006738    1.871682
C              1.307119   -0.006795   -0.346393
H              3.140435    0.049261    0.730127
H              1.668081   -0.068104   -1.356762
H              0.795494    0.091290    5.043260
H             -3.047044   -0.116762    2.653226
H             -2.544237   -0.166080    0.989005

Gua
N            1.519395    0.646576    0.560140
N            0.536361   -1.483818    0.054940
N           -2.090886    0.843536   -0.192269
N           -1.894114   -1.374044    0.104300
N            2.789727   -1.098671   -0.389088
C           -0.604792   -0.866258    0.194007
C           -0.780109    0.558797    0.001775
C            0.364004    1.398553    0.060758
C            1.592693   -0.628274    0.010983
C           -2.711480   -0.320792   -0.118879
O            0.492054    2.590759   -0.194554
H            2.354564    1.200833    0.424976
H            3.640341   -0.667801   -0.064182
H            2.841251   -2.069372   -0.646684
H           -3.777362   -0.444265   -0.216567
H           -2.180506   -2.332675    0.200869

Thy
N             -0.334220    1.300743   -0.635740
N              0.914074   -0.613781   -0.209139
C              2.047554    0.109194   -0.068124
C             -0.327999   -0.064115   -0.514437
C              0.620234    2.124717    0.028830
C              1.858153    1.490160    0.321425
C              2.902194    2.173131    1.100966
O             -1.294809   -0.777279   -0.694571
O              0.296182    3.282989    0.315494
H              0.929933   -1.626264   -0.203617
H             -1.248432    1.713393   -0.748326
H              2.994316   -0.402702   -0.074978
H              3.096916    1.649929    2.045133
H              3.854146    2.157522    0.557567
```

H	2.617205	3.198230	1.315253

S2 Basis set comparison

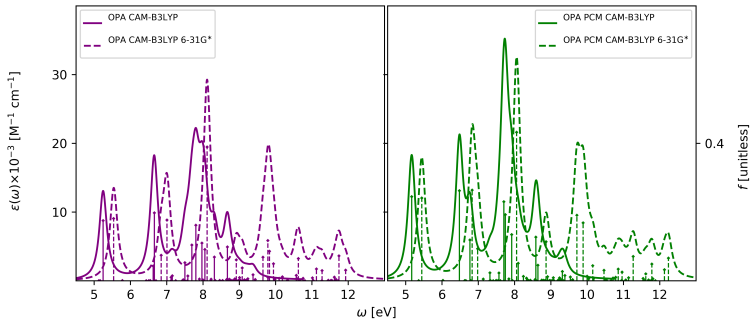

Figure S14: Thymine. Comparison of CAMB3LYP OPA using two different basis sets: aug-cc-pVDZ and 6-31G*.

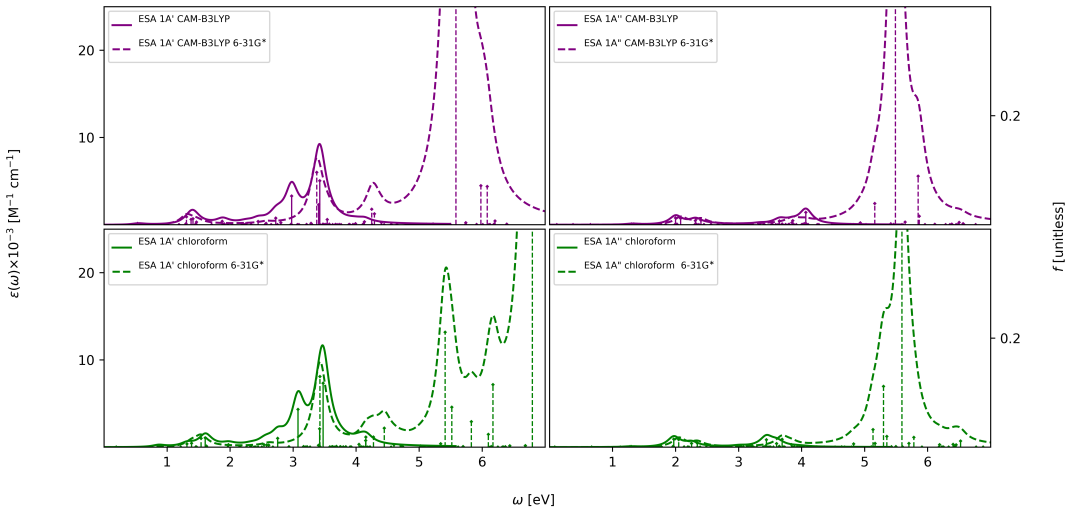

Figure S15: Thymine. CAMB3LYP ESA of S_2 (left) and S_1 (right) computed using the aug-cc-pVDZ and 6-31G* basis sets.

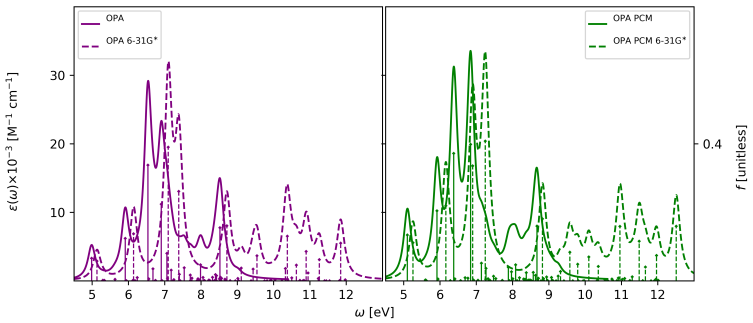

Figure S16: Cytosine. Comparison of OPA computed at CAMB3LYP/aug-cc-pVDZ and CAMB3LYP/6-31G* levels of theory.

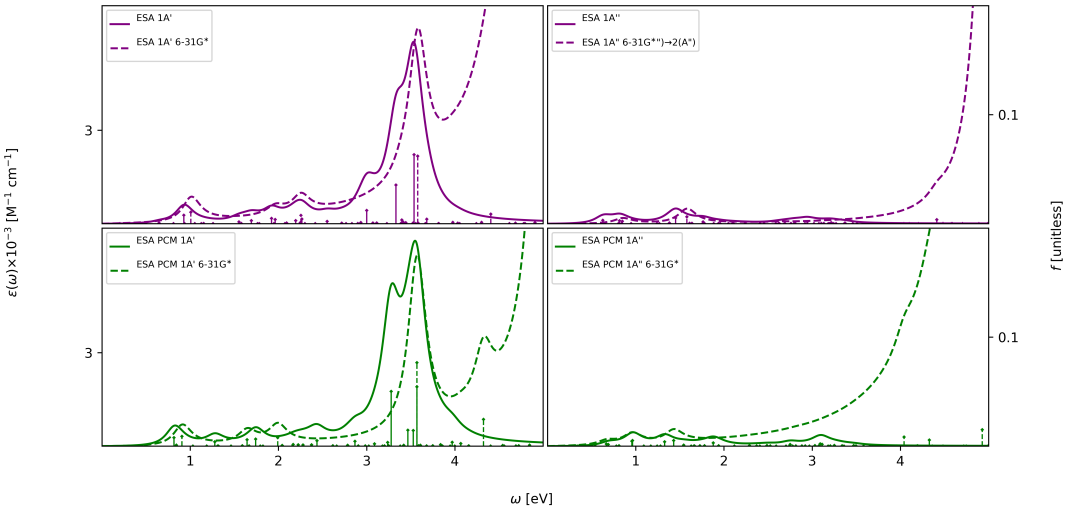

Figure S17: Cytosine. Comparison of ESA computed at CAMB3LYP/aug-cc-pVDZ and CAMB3LYP/6-31G* levels of theory.

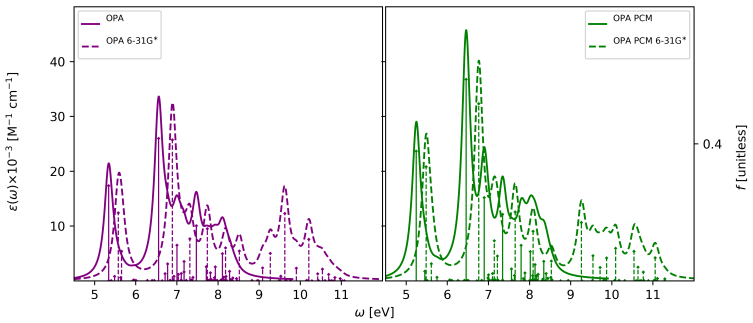

Figure S18: Adenine. Comparison of CAMB3LYP OPA using the aug-cc-pVDZ and 6-31G* basis sets.

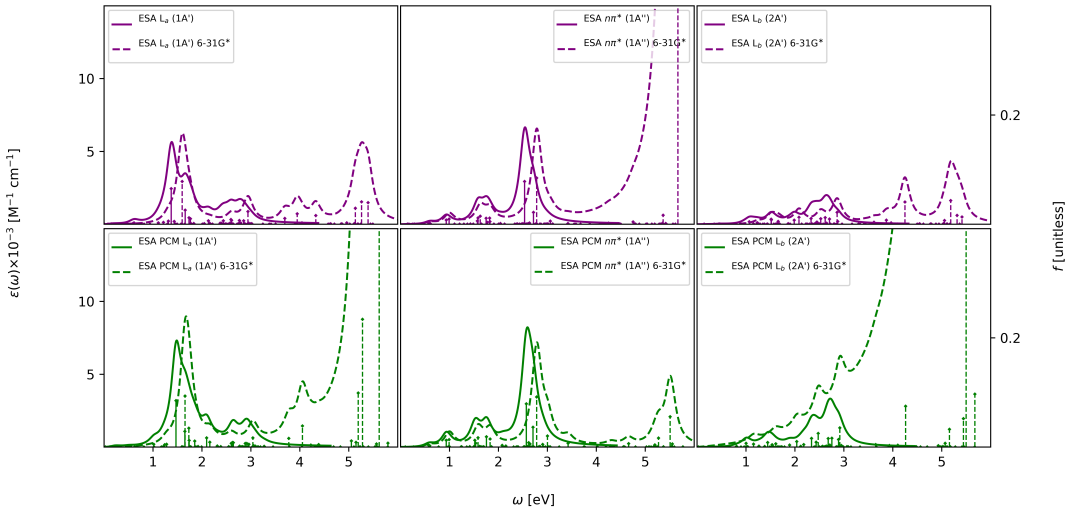

Figure S19: Adenine. Comparison of CAMB3LYP ESA using the aug-cc-pVDZ and 6-31G* basis sets.

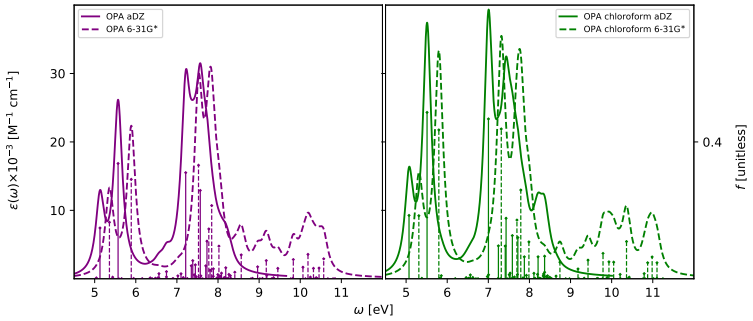

Figure S20: Guanine. Comparison of OPA computed at CAM-B3LYP/aug-cc-pVDZ and CAM-B3LYP/6-31G* levels of theory.

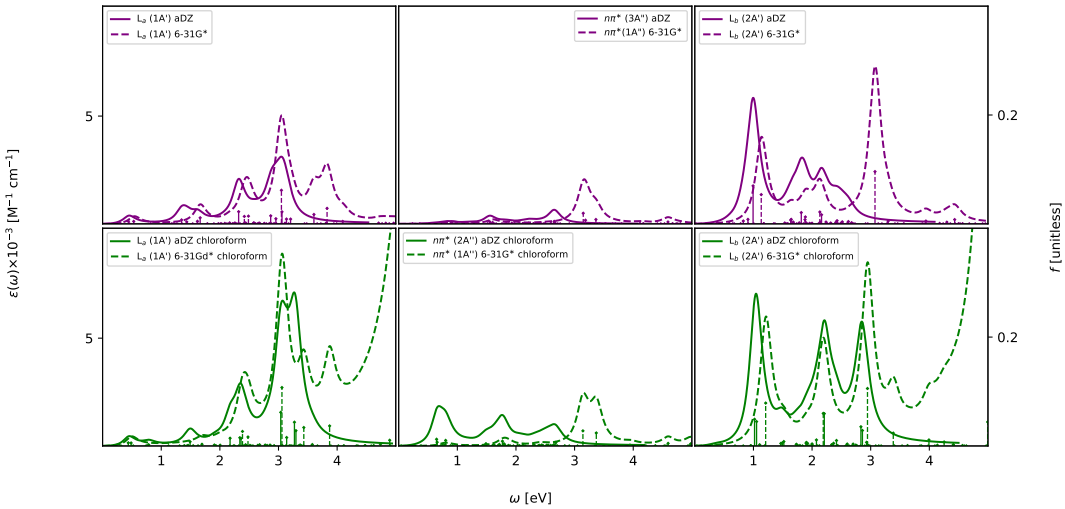

Figure S21: Guanine. Comparison of CAM-B3LYP ESA computed using the aug-cc-pVDZ and CAM-B3LYP/6-31G* basis sets.

S3 Tamm-Dancoff (TDA) results: ESA from quadratic response versus ESA from maximum-overlap-method

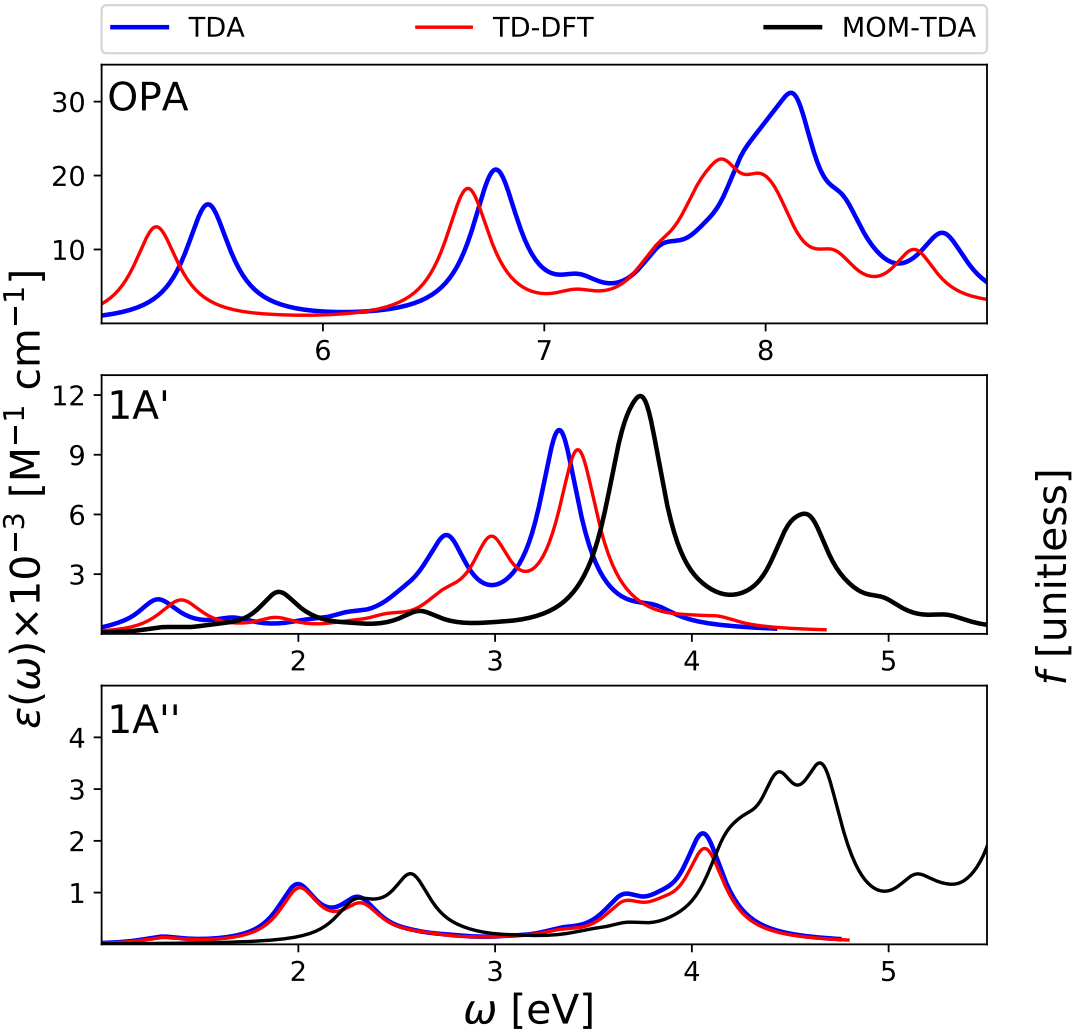

Figure S22: Thymine. Comparison of TDA and TDDFT results using the CAMB3LYP functional for OPA, as well as TDA ESA from quadratic response theory and OPA of MOM-optimized excited states. [8]

Table S3: Thymine. MOM-TDA/CAM-B3LYP ESA results.

$1n$		1π	
ω_j	$f \times 100$	ω_j	$f \times 100$
0.31	0.00	0.78	0.00
1.42	0.00	1.31	0.31
2.28	0.84	1.57	0.28
2.40	0.20	1.90	2.66
2.57	1.59	2.06	0.11
2.83	0.03	2.25	0.16
3.10	0.02	2.28	0.00
3.48	0.12	2.61	1.21
3.66	0.24	2.99	0.09
3.93	0.06	3.09	0.01
4.06	0.00	3.43	0.02
4.16	0.01	3.46	0.14
4.20	0.01	3.64	7.81
4.27	1.17	3.76	11.4
4.37	0.00	4.01	0.11
4.44	2.81	4.07	0.16
4.58	0.42	4.21	0.00
4.67	3.31	4.28	0.14
4.77	0.14	4.46	0.01

S4 TABLES OF RAW DATA

SS4.1 Thymine

Table S4: Thymine. CAM-B3LYP/aug-cc-pVDZ OPA excitation energies (ΔE, eV) and oscillator strengths (f) computed with the Tamm-Dancoff approximation (CIS), at TDDFT level in gas phase and at TDDFT in non-equilibrium PCM (chloroform). First IP is 9.44 eV.

One-Photon Absorption ($S_0 \rightarrow S_n$)											
TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
0→1	5.15	0.00	0→1	5.13	0.00	0→1A”	5.13	0.00	0→1A’	5.16	24.47
0→2	5.48	21.48	0→2	5.25	17.48	0→1A’	5.25	17.47	0→1A”	5.36	0.00
0→3	5.79	0.06	0→3	5.78	0.04	0→2A”	5.78	0.04	0→2A”	6.03	0.10
0→4	6.45	0.00	0→4	6.44	0.00	0→3A”	6.43	0.00	0→2A’	6.48	26.21
0→5	6.56	0.06	0→5	6.55	0.04	0→4A”	6.55	0.04	0→3A”	6.62	0.01
0→6	6.72	0.01	0→6	6.63	4.28	0→2A’	6.63	4.27	0→4A”	6.64	0.01
0→7	6.76	13.44	0→7	6.66	19.72	0→3A’	6.66	19.73	0→3A’	6.77	11.86
0→8	6.80	14.11	0→8	6.72	0.01	0→5A”	6.70	0.01	0→5A”	6.79	0.03
0→9	7.14	0.08	0→9	7.13	0.98	0→4(A’)	7.12	0.98	0→4(A’)	7.14	0.49
0→10	7.14	1.85	0→10	7.13	0.09	0→6A”	7.13	0.09	0→5A’	7.32	2.31
0→11	7.17	2.00	0→11	7.16	1.43	0→5A’	7.15	1.42	0→6A”	7.33	0.13
0→12	7.44	0.01	0→12	7.44	0.01	0→7A”	7.43	0.01	0→7A”	7.49	0.08
0→13	7.45	0.10	0→13	7.45	0.09	0→8A”	7.45	0.19	0→8A”	7.55	0.06
0→14	7.48	0.31	0→14	7.48	0.31	0→9A”	7.46	0.26	0→9(A”)	7.57	2.27
0→15	7.52	6.57	0→15	7.51	5.27	0→6A’	7.50	5.22	0→10A”	7.61	0.00
0→16	7.60	1.61	0→16	7.59	1.48	0→10A”	7.58	1.39	0→6A’	7.70	22.97
0→17	7.72	5.08	0→17	7.70	12.04	0→7A’	7.69	10.39	0→7A’	7.75	19.23
0→18	7.89	13.50	0→18	7.81	15.66	0→8A’	7.80	16.16	0→11A”	7.85	0.50
0→19	7.92	0.52	0→19	7.92	0.48	0→11A”	7.90	0.49	0→8A’	7.92	13.44
0→20	8.00	12.44	0→20	7.99	10.34	0→9A’	7.97	10.96	0→9A’	8.10	5.08
0→21	8.01	0.27	0→21	8.01	0.25	0→12A”	8.00	0.23	0→10A’	8.24	1.25
0→22	8.13	27.90	0→22	8.06	8.71	0→10A’	8.05	9.08	0→11A’	8.33	0.72
0→23	8.22	0.04	0→23	8.22	0.03	0→13A”	8.22	0.03	0→12A”	8.36	0.21
0→24	8.24	0.18	0→24	8.23	0.47	0→11A’	8.22	0.44	0→13A”	8.39	0.03
0→25	8.35	11.37	0→25	8.32	6.83	0→12A’	8.31	6.87	0→14A”	8.44	0.13
0→26	8.35	0.05	0→26	8.35	0.05	0→14A”	8.34	0.05	0→15A”	8.57	0.33
0→27	8.48	1.37	0→27	8.47	0.10	0→13A’	8.46	0.09	0→12A’	8.59	12.69
0→28	8.55	0.01	0→28	8.55	0.01	0→15A”	8.53	0.00	0→16A”	8.60	0.04
0→29	8.60	0.04	0→29	8.60	0.04	0→16A”	8.54	0.03	0→13A’	8.64	4.52
0→30	8.68	0.99	0→30	8.66	2.76	0→14A’	8.65	0.34	0→17A”	8.75	0.17
0→31	8.74	0.35	0→31	8.68	7.41	0→15A’	8.67	9.81	0→14A’	8.79	0.10
0→32	8.75	0.68	0→32	8.73	0.13	0→17A”	8.72	0.44	0→18A”	8.80	0.07
0→33	8.77	0.24	0→33	8.74	0.34	0→16A’	8.72	0.13	0→19A”	8.83	0.00
0→34	8.79	0.04	0→34	8.77	0.23	0→18A”	8.76	0.16	0→15A’	8.85	0.09
0→35	8.80	10.76	0→35	8.78	0.04	0→19A”	8.78	0.05	0→16A’	8.91	1.18
0→36	8.83	0.04	0→36	8.83	0.03	0→20A”	8.82	0.04	0→20A”	8.96	0.06
0→37	8.89	1.18	0→37	8.89	0.50	0→17A’	8.88	0.50	0→21A”	9.00	0.03
0→38	8.93	0.09	0→38	8.93	0.08	0→21A”	8.92	0.09	0→17A’	9.07	0.86
0→39	8.99	0.09	0→39	8.98	0.07	0→22A”	8.98	0.07	0→22A”	9.09	0.00
0→40	9.03	0.99	0→40	9.02	0.99	0→18A’	9.01	0.93	0→23A”	9.21	0.15
0→41	9.15	0.17	0→41	9.14	0.17	0→23A”	9.13	0.14	0→18A’	9.24	0.81
0→42	9.16	0.25	0→42	9.15	0.24	0→191A’	9.14	0.26	0→24A”	9.29	0.24
0→43	9.21	0.19	0→43	9.21	0.18	0→24A”	9.20	0.18	0→19A’	9.32	2.69
0→44	9.26	0.59	0→44	9.25	0.55	0→25A”	9.24	0.58	0→25A”	9.35	0.01
0→45	9.30	0.25	0→45	9.30	0.23	0→20A’	9.38	1.74	0→20A’	9.39	1.53

Table S5: Thymine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from 1A' = $\pi\pi^*$, computed with the Tamm-Dancoff approximation (CIS), TDDFT and TDDFT in non-equilibrium PCM (chloroform).

ESA: S_2 (1A') $\rightarrow$ S_n											
TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
2→3	0.31	0.13	2→3	0.54	0.20	1A'→2A"	0.53	0.20	1A'→1A"	0.19	0.00
2→4	0.97	0.00	2→4	1.19	0.00	1A'→3A"	1.19	0.00	1A'→2A"	0.86	0.30
2→5	1.08	0.15	2→5	1.31	0.16	1A'→4A"	1.30	0.17	1A'→2A'	1.32	0.57
2→6	1.24	0.11	2→6	1.38	0.99	1A'→2A'	1.38	0.97	1A'→3A"	1.46	0.04
2→7	1.28	1.83	2→7	1.41	1.09	1A'→3A'	1.41	1.07	1A'→4A"	1.47	0.01
2→8	1.32	0.28	2→8	1.47	0.12	1A'→5A"	1.46	0.11	1A'→3A'	1.61	1.70
2→9	1.66	0.00	2→9	1.88	0.60	1A'→4A'	1.88	0.63	1A'→5A"	1.63	0.17
2→10	1.66	0.56	2→10	1.88	0.00	1A'→6A"	1.88	0.00	1A'→4A'	1.97	0.43
2→11	1.69	0.11	2→11	1.91	0.16	1A'→5A'	1.91	0.15	1A'→5A'	2.16	0.05
2→12	1.96	0.00	2→12	2.19	0.00	1A'→7A"	2.19	0.00	1A'→6A"	2.16	0.00
2→13	1.97	0.00	2→13	2.20	0.00	1A'→8A"	2.20	0.00	1A'→7A"	2.33	0.19
2→14	2.00	0.07	2→14	2.23	0.08	1A'→9A"	2.22	0.07	1A'→8A"	2.38	0.00
2→15	2.05	0.28	2→15	2.26	0.20	1A'→6A'	2.26	0.21	1A'→9A"	2.41	0.01
2→16	2.12	0.00	2→16	2.35	0.00	1A'→10A"	2.33	0.00	1A'→10A"	2.45	0.00
2→17	2.24	0.62	2→17	2.45	0.55	1A'→7A'	2.45	0.59	1A'→6A'	2.54	0.45
2→18	2.41	0.21	2→18	2.57	0.03	1A'→8A'	2.56	0.03	1A'→7A'	2.58	0.37
2→19	2.44	0.01	2→19	2.67	0.01	1A'→11A"	2.65	0.02	1A'→11A"	2.68	0.01
2→20	2.53	0.98	2→20	2.74	1.19	1A'→9A'	2.73	1.21	1A'→8A'	2.76	1.61
2→21	2.53	0.00	2→21	2.76	0.00	1A'→12A"	2.75	0.00	1A'→9A'	2.94	0.05
2→22	2.65	1.00	2→22	2.82	0.37	1A'→10A'	2.81	0.37	1A'→10A'	3.08	6.92
2→23	2.75	0.16	2→23	2.98	0.09	1A'→13A"	2.97	0.09	1A'→11A'	3.17	0.08
2→24	2.76	4.98	2→24	2.98	5.45	1A'→11A'	2.98	5.24	1A'→12A"	3.19	0.01
2→25	2.87	0.07	2→25	3.08	0.02	1A'→12A'	3.07	0.02	1A'→13A"	3.22	0.07
2→26	2.87	0.01	2→26	3.10	0.01	1A'→14A"	3.09	0.01	1A'→14A"	3.27	0.01
2→27	3.00	0.06	2→27	3.23	0.04	1A'→13A'	3.22	0.04	1A'→15A"	3.40	0.31
2→28	3.07	0.15	2→28	3.30	0.16	1A'→15A"	3.29	0.25	1A'→12A'	3.42	3.36
2→29	3.12	0.23	2→29	3.35	0.20	1A'→16A"	3.30	0.06	1A'→16A"	3.43	0.00
2→30	3.20	0.17	2→30	3.41	9.04	1A'→14A'	3.41	3.65	1A'→13A'	3.48	11.71
2→31	3.27	0.04	2→31	3.43	4.55	1A'→15A'	3.43	8.05	1A'→17A"	3.58	0.02
2→32	3.27	0.03	2→32	3.48	0.01	1A'→17A"	3.47	0.09	1A'→14A'	3.63	0.07
2→33	3.29	0.06	2→33	3.50	0.04	1A'→16A'	3.48	0.01	1A'→18A"	3.63	0.02
2→34	3.31	0.00	2→34	3.52	0.06	1A'→18A"	3.51	0.05	1A'→19A"	3.66	0.00
2→35	3.32	12.93	2→35	3.53	0.01	1A'→19A"	3.53	0.01	1A'→15A'	3.69	0.11
2→36	3.35	0.12	2→36	3.58	0.08	1A'→20A"	3.58	0.09	1A'→16A'	3.75	0.07
2→37	3.42	0.05	2→37	3.64	0.01	1A'→17A'	3.63	0.01	1A'→20A"	3.80	0.04
2→38	3.46	0.04	2→38	3.69	0.04	1A'→21A"	3.67	0.04	1A'→21A"	3.84	0.05
2→39	3.51	0.03	2→39	3.73	0.03	1A'→22A"	3.73	0.03	1A'→17A'	3.91	0.02
2→40	3.55	0.03	2→40	3.78	0.02	1A'→18A'	3.76	0.01	1A'→22A"	3.93	0.00
2→41	3.67	0.00	2→41	3.90	0.00	1A'→23A"	3.89	0.00	1A'→23A"	4.05	0.50
2→42	3.68	0.03	2→42	3.91	0.03	1A'→19A'	3.90	0.05	1A'→18A'	4.08	0.06
2→43	3.73	0.06	2→43	3.96	0.04	1A'→24A"	3.95	0.05	1A'→24A"	4.12	0.01
2→44	3.78	0.23	2→44	4.01	0.20	1A'→25A"	3.99	0.18	1A'→19A'	4.15	1.19
2→45	3.82	0.57	2→45	4.06	0.58	1A'→20A'	4.13	0.54	1A'→25A"	4.18	0.01
2→46	3.88	0.01	2→46	4.11	0.01				1A'→20A'	4.22	0.03

Table S6: Thymine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from 1A" = nπ^* computed in the Tamm-Dancoff approximation (CIS), TDDFT and TDDFT with non-equilibrium PCM (chloroform).

ESA: S_1/1A'/n$\pi^* \rightarrow S_n$											
TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
1→2	0.33	0.00	1→2	0.12	0.00	1A"→1A'	0.12	0.00	1A"→2A"	0.67	0.00
1→3	0.64	0.00	1→3	0.66	0.00	1A"→2A"	0.65	0.00	1A"→2A'	1.12	0.00
1→4	1.30	0.16	1→4	1.31	0.15	1A"→3A"	1.31	0.14	1A"→3A"	1.27	0.01
1→5	1.41	0.00	1→5	1.43	0.00	1A"→4A"	1.42	0.00	1A"→4A"	1.28	0.08
1→6	1.57	0.00	1→6	1.50	0.00	1A"→2A'	1.50	0.00	1A"→3A'	1.41	0.00
1→7	1.61	0.00	1→7	1.53	0.00	1A"→3A'	1.53	0.00	1A"→5A"	1.43	0.00
1→8	1.65	0.00	1→8	1.59	0.00	1A"→5A"	1.57	0.00	1A"→4A'	1.78	0.01
1→9	1.99	1.31	1→9	2.00	0.05	1A"→4A'	1.99	0.05	1A"→5A'	1.96	0.13
1→10	1.99	0.05	1→10	2.00	1.28	1A"→6A"	2.00	1.22	1A"→6A"	1.97	1.46
1→11	2.02	0.09	1→11	2.03	0.08	1A"→5A'	2.02	0.09	1A"→7A"	2.14	0.02
1→12	2.29	0.00	1→12	2.31	0.00	1A"→7A"	2.31	0.00	1A"→8A"	2.19	0.00
1→13	2.30	0.94	1→13	2.32	0.95	1A"→8A"	2.32	0.73	1A"→9A"	2.21	0.00
1→14	2.33	0.03	1→14	2.35	0.02	1A"→9A"	2.33	0.09	1A"→10A"	2.25	0.66
1→15	2.37	0.02	1→15	2.38	0.02	1A"→6A'	2.37	0.02	1A"→6A'	2.35	0.00
1→16	2.45	0.01	1→16	2.46	0.01	1A"→10A"	2.45	0.01	1A"→7A'	2.39	0.01
1→17	2.57	0.06	1→17	2.57	0.04	1A"→10A"	2.45	0.00	1A"→11A"	2.49	0.00
1→18	2.74	0.05	1→18	2.68	0.06	1A"→7A'	2.56	0.05	1A"→8A'	2.56	0.00
1→19	2.77	0.00	1→19	2.79	0.00	1A"→8A'	2.67	0.06	1A"→9A'	2.74	0.04
1→20	2.85	0.01	1→20	2.86	0.00	1A"→11A"	2.77	0.00	1A"→10A'	2.89	0.00
1→21	2.86	0.01	1→21	2.88	0.01	1A"→9A'	2.84	0.00	1A"→11A'	2.97	0.06
1→22	2.98	0.00	1→22	2.93	0.01	1A"→12A"	2.87	0.01	1A"→12A"	3.00	0.00
1→23	3.07	0.04	1→23	3.10	0.04	1A"→10A'	2.92	0.01	1A"→13A"	3.03	0.11
1→24	3.08	0.00	1→24	3.10	0.00	1A"→13A"	3.09	0.04	1A"→14A"	3.08	0.00
1→25	3.20	0.00	1→25	3.19	0.01	1A"→11A'	3.09	0.00	1A"→15A"	3.21	0.01
1→26	3.20	0.00	1→26	3.22	0.00	1A"→12A'	3.18	0.01	1A"→12A'	3.23	0.01
1→27	3.33	0.18	1→27	3.35	0.17	1A"→14A"	3.21	0.00	1A"→16A"	3.24	0.00
1→28	3.40	0.00	1→28	3.42	0.00	1A"→13A'	3.33	0.16	1A"→13A'	3.29	0.00
1→29	3.45	0.00	1→29	3.47	0.00	1A"→15A"	3.40	0.00	1A"→17A"	3.39	0.00
1→30	3.52	0.02	1→30	3.53	0.00	1A"→16A"	3.41	0.00	1A"→14A'	3.43	0.22
1→31	3.59	0.01	1→31	3.55	0.01	1A"→14A'	3.52	0.01	1A"→18A"	3.44	1.33
1→32	3.60	0.00	1→32	3.60	0.00	1A"→15A'	3.54	0.01	1A"→19A"	3.47	0.00
1→33	3.62	0.01	1→33	3.61	0.01	1A"→17A"	3.59	0.01	1A"→15A'	3.50	0.00
1→34	3.64	0.75	1→34	3.64	0.01	1A"→16A'	3.59	0.00	1A"→16A'	3.55	0.01
1→35	3.65	0.00	1→35	3.65	0.81	1A"→18A"	3.63	0.00	1A"→20A"	3.60	0.64
1→36	3.68	0.15	1→36	3.70	0.11	1A"→19A"	3.65	0.66	1A"→21A"	3.65	0.14
1→37	3.74	0.00	1→37	3.76	0.01	1A"→20A"	3.69	0.11	1A"→17A'	3.71	0.00
1→38	3.78	0.01	1→38	3.80	0.01	1A"→17A'	3.75	0.01	1A"→22A"	3.73	0.00
1→39	3.84	0.43	1→39	3.85	0.46	1A"→21A"	3.79	0.01	1A"→23A"	3.85	0.01
1→40	3.88	0.01	1→40	3.90	0.01	1A"→22A"	3.85	0.39	1A"→18A'	3.88	0.04
1→41	3.99	0.00	1→41	4.02	0.00	1A"→18A'	3.88	0.02	1A"→24A"	3.93	0.00
1→42	4.01	0.02	1→42	4.02	0.02	1A"→23A"	4.00	0.00	1A"→19A'	3.96	0.00
1→43	4.06	2.63	1→43	4.08	2.62	1A"→19A'	4.01	0.02	1A"→25A"	3.99	0.04
1→44	4.10	0.01	1→44	4.12	0.01	1A"→24A"	4.07	2.27	1A"→20A'	4.03	0.03
1→45	4.15	0.01	1→45	4.17	0.01	1A"→25A"	4.11	0.02			
1→46	4.21	0.01	1→46	4.23	0.01	1A"→20A'	4.25	0.00			

Table S7: Thymine. CCSD/aug-cc-pVDZ OPA and ESA transition energies (ω, eV) and oscillator strengths (f).

OPA			ESA($n\pi^*/S_1$)			ESA($\pi\pi^*/S_2$)		
$S_0 \rightarrow S_n$	ω [eV]	$f \times 100$	$S_1 \rightarrow S_n$	ω [eV]	$f \times 100$	$S_2 \rightarrow S_n$	ω [eV]	$f \times 100$
$0 \rightarrow 1$	5.258	0.00	$1 \rightarrow 2$	0.253	0.00	$2 \rightarrow 3$	0.253	0.11
$0 \rightarrow 2$	5.512	20.70	$1 \rightarrow 3$	0.506	0.00	$2 \rightarrow 4$	1.058	0.05
$0 \rightarrow 3$	5.764	0.04	$1 \rightarrow 4$	1.312	0.00	$2 \rightarrow 5$	1.155	0.00
$0 \rightarrow 4$	6.570	0.11	$1 \rightarrow 5$	1.408	0.16	$2 \rightarrow 6$	1.220	0.23
$0 \rightarrow 5$	6.666	0.00	$1 \rightarrow 6$	1.473	0.00	$2 \rightarrow 7$	1.229	0.76
$0 \rightarrow 6$	6.732	0.00	$1 \rightarrow 7$	1.483	0.00	$2 \rightarrow 8$	1.378	2.04
$0 \rightarrow 7$	6.741	5.49	$1 \rightarrow 8$	1.632	0.00	$2 \rightarrow 9$	1.606	0.65
$0 \rightarrow 8$	6.890	16.84	$1 \rightarrow 9$	1.859	0.03	$2 \rightarrow 10$	1.629	0.04
$0 \rightarrow 9$	7.117	6.69	$1 \rightarrow 10$	1.883	0.13	$2 \rightarrow 11$	1.833	0.00
$0 \rightarrow 10$	7.141	3.80	$1 \rightarrow 11$	2.086	0.00	$2 \rightarrow 12$	1.997	0.08
$0 \rightarrow 11$	7.344	0.00	$1 \rightarrow 12$	2.251	0.01	$2 \rightarrow 13$	2.074	0.43
$0 \rightarrow 12$	7.509	0.32	$1 \rightarrow 13$	2.328	0.01	$2 \rightarrow 14$	2.095	0.03
$0 \rightarrow 13$	7.586	7.46	$1 \rightarrow 14$	2.349	0.02	$2 \rightarrow 15$	2.131	0.00
$0 \rightarrow 14$	7.607	1.33	$1 \rightarrow 15$	2.385	2.40	$2 \rightarrow 16$	2.226	0.81
$0 \rightarrow 15$	7.643	0.10	$1 \rightarrow 16$	2.479	0.08	$2 \rightarrow 17$	2.328	0.01
$0 \rightarrow 16$	7.737	5.47	$1 \rightarrow 17$	2.581	2.28	$2 \rightarrow 18$	2.336	0.58
$0 \rightarrow 17$	7.840	0.04	$1 \rightarrow 18$	2.590	0.04	$2 \rightarrow 19$	2.415	0.01
$0 \rightarrow 18$	7.848	22.36	$1 \rightarrow 19$	2.668	0.00	$2 \rightarrow 20$	2.460	0.00
$0 \rightarrow 19$	7.926	0.16	$1 \rightarrow 20$	2.713	0.01	$2 \rightarrow 21$	2.506	1.38
$0 \rightarrow 20$	7.972	0.55	$1 \rightarrow 21$	2.760	0.00	$2 \rightarrow 22$	2.618	1.02
$0 \rightarrow 21$	8.018	14.06	$1 \rightarrow 22$	2.871	0.00	$2 \rightarrow 23$	2.685	0.14
$0 \rightarrow 22$	8.129	7.08	$1 \rightarrow 23$	2.939	0.15	$2 \rightarrow 24$	2.711	5.74
$0 \rightarrow 23$	8.197	0.03	$1 \rightarrow 24$	2.965	0.00	$2 \rightarrow 25$	2.832	0.00
$0 \rightarrow 24$	8.223	0.42	$1 \rightarrow 25$	3.086	0.00	$2 \rightarrow 26$	2.892	0.03
$0 \rightarrow 25$	8.344	0.06	$1 \rightarrow 26$	3.146	0.01	$2 \rightarrow 27$	2.975	0.09
$0 \rightarrow 26$	8.404	5.53	$1 \rightarrow 27$	3.229	0.22	$2 \rightarrow 28$	3.036	0.01
$0 \rightarrow 27$	8.487	0.20	$1 \rightarrow 28$	3.289	0.01	$2 \rightarrow 29$	3.090	0.02
$0 \rightarrow 28$	8.547	0.09	$1 \rightarrow 29$	3.344	0.00	$2 \rightarrow 30$	3.101	0.40
$0 \rightarrow 29$	8.602	0.96	$1 \rightarrow 30$	3.355	0.00	$2 \rightarrow 31$	3.200	0.01
$0 \rightarrow 30$	8.613	0.01	$1 \rightarrow 31$	3.453	0.00	$2 \rightarrow 32$	3.211	0.04
$0 \rightarrow 31$	8.712	0.01	$1 \rightarrow 32$	3.465	0.01	$2 \rightarrow 33$	3.283	0.17
$0 \rightarrow 32$	8.723	1.65	$1 \rightarrow 33$	3.536	0.01	$2 \rightarrow 34$	3.353	0.05
$0 \rightarrow 33$	8.794	0.73	$1 \rightarrow 34$	3.607	0.06	$2 \rightarrow 35$	3.434	0.19
$0 \rightarrow 34$	8.865	0.01	$1 \rightarrow 35$	3.687	0.00	$2 \rightarrow 36$	3.457	0.07
$0 \rightarrow 35$	8.946	0.38	$1 \rightarrow 36$	3.710	0.00	$2 \rightarrow 37$	3.558	17.74
$0 \rightarrow 36$	8.968	0.17	$1 \rightarrow 37$	3.811	0.00	$2 \rightarrow 38$	3.609	0.01
$0 \rightarrow 37$	9.069	15.53	$1 \rightarrow 38$	3.862	0.01	$2 \rightarrow 39$	3.674	0.02
$0 \rightarrow 38$	9.120	0.43	$1 \rightarrow 39$	3.928	0.03	$2 \rightarrow 40$	3.708	0.02
$0 \rightarrow 39$	9.186	0.03	$1 \rightarrow 40$	3.962	1.03	$2 \rightarrow 41$	3.740	0.22
$0 \rightarrow 40$	9.220	0.02	$1 \rightarrow 41$	3.994	0.18	$2 \rightarrow 42$	3.747	0.03
$0 \rightarrow 41$	9.252	1.03	$1 \rightarrow 42$	4.001	0.02	$2 \rightarrow 43$	3.776	0.47
$0 \rightarrow 42$	9.259	0.21	$1 \rightarrow 43$	4.029	0.01	$2 \rightarrow 44$	3.869	0.05
$0 \rightarrow 43$	9.288	0.02	$1 \rightarrow 44$	4.122	2.38	$2 \rightarrow 45$	3.873	0.06
$0 \rightarrow 44$	9.380	0.08	$1 \rightarrow 45$	4.126	1.34	$2 \rightarrow 46$	3.883	0.01
$0 \rightarrow 45$	9.384	0.10	$1 \rightarrow 46$	4.136	0.28	$2 \rightarrow 47$	3.893	0.38
$0 \rightarrow 46$	9.394	0.85	$1 \rightarrow 47$	4.146	0.00	$2 \rightarrow 48$	3.911	0.00
$0 \rightarrow 47$	9.404	0.35	$1 \rightarrow 48$	4.165	2.38	$2 \rightarrow 49$	4.029	0.03
$0 \rightarrow 48$	9.423	0.06	$1 \rightarrow 49$	4.282	0.27	$2 \rightarrow 50$	4.036	0.64
$0 \rightarrow 49$	9.541	0.00	$1 \rightarrow 50$	4.290	0.00	$2 \rightarrow 51$	4.058	0.22
$0 \rightarrow 50$	9.548	0.91	$1 \rightarrow 51$	4.311	0.00	$2 \rightarrow 52$	4.151	0.04
$0 \rightarrow 51$	9.569	0.83	$1 \rightarrow 52$	4.405	0.12			
$0 \rightarrow 52$	9.663	0.21						

Table S8: Thymine: CC3/aug-cc-pVDZ OPA and ESA transition energies (ω, eV) and oscillator strengths (f).

OPA			ESA ($n\pi^*/S_1$)			ESA ($\pi\pi^*/S_2$)		
$S_0 \rightarrow S_n$	ω [eV]	$f \times 100$	$S_1 \rightarrow S_n$	ω [eV]	$f \times 100$	$S_2 \rightarrow S_n$	ω [eV]	$f \times 100$
$0 \rightarrow 1$	5.066	0.00	$1 \rightarrow 2$	0.213	0.00	$2 \rightarrow 3$	0.385	0.11
$0 \rightarrow 2$	5.280	15.91	$1 \rightarrow 3$	0.599	0.00	$2 \rightarrow 4$	1.094	1.13
$0 \rightarrow 3$	5.665	0.04	$1 \rightarrow 4$	1.307	0.00	$2 \rightarrow 5$	1.158	0.04
$0 \rightarrow 4$	6.373	4.89	$1 \rightarrow 5$	1.371	0.00	$2 \rightarrow 6$	1.192	0.00
$0 \rightarrow 5$	6.438	0.08	$1 \rightarrow 6$	1.406	0.47	$2 \rightarrow 7$	1.319	0.21
$0 \rightarrow 6$	6.472	0.00	$1 \rightarrow 7$	1.532	0.00	$2 \rightarrow 8$	1.329	0.77
$0 \rightarrow 7$	6.598	0.00	$1 \rightarrow 8$	1.543	0.01	$2 \rightarrow 9$	1.558	0.14
$0 \rightarrow 8$	6.609	16.91	$1 \rightarrow 9$	1.772	0.21	$2 \rightarrow 10$	1.632	0.00
$0 \rightarrow 9$	6.838	1.72	$1 \rightarrow 10$	1.846	1.78	$2 \rightarrow 11$	1.690	0.44
$0 \rightarrow 10$	6.912	0.10	$1 \rightarrow 11$	1.904	0.00	$2 \rightarrow 12$	1.890	0.00
$0 \rightarrow 11$	6.970	1.82	$1 \rightarrow 12$	2.103	0.00	$2 \rightarrow 13$	2.005	0.00
$0 \rightarrow 12$	7.169	0.00	$1 \rightarrow 13$	2.219	0.62	$2 \rightarrow 14$	2.029	0.61
$0 \rightarrow 13$	7.285	0.02	$1 \rightarrow 14$	2.242	0.00	$2 \rightarrow 15$	2.058	0.13
$0 \rightarrow 14$	7.309	5.51	$1 \rightarrow 15$	2.272	0.00	$2 \rightarrow 16$	2.165	0.13
$0 \rightarrow 15$	7.338	0.10	$1 \rightarrow 16$	2.379	0.11	$2 \rightarrow 17$	2.191	0.02
$0 \rightarrow 16$	7.445	0.67	$1 \rightarrow 17$	2.404	0.00	$2 \rightarrow 18$	2.301	0.31
$0 \rightarrow 17$	7.471	1.48	$1 \rightarrow 18$	2.515	0.00	$2 \rightarrow 19$	2.435	0.00
$0 \rightarrow 18$	7.581	25.60	$1 \rightarrow 19$	2.648	0.00	$2 \rightarrow 20$	2.487	0.35
$0 \rightarrow 19$	7.715	0.03	$1 \rightarrow 20$	2.700	0.02	$2 \rightarrow 21$	2.514	0.00
$0 \rightarrow 20$	7.766	11.18	$1 \rightarrow 21$	2.728	0.00	$2 \rightarrow 22$	2.592	1.40
$0 \rightarrow 21$	7.794	0.55	$1 \rightarrow 22$	2.805	0.00	$2 \rightarrow 23$	2.659	0.15
$0 \rightarrow 22$	7.871	11.97	$1 \rightarrow 23$	2.873	0.08	$2 \rightarrow 24$	2.799	5.05
$0 \rightarrow 23$	7.939	0.07	$1 \rightarrow 24$	3.013	0.00	$2 \rightarrow 25$	2.836	0.00
$0 \rightarrow 24$	8.079	0.78	$1 \rightarrow 25$	3.050	0.00	$2 \rightarrow 26$	2.873	0.15
$0 \rightarrow 25$	8.116	0.02	$1 \rightarrow 26$	3.086	0.14	$2 \rightarrow 27$	2.879	0.03
$0 \rightarrow 26$	8.153	3.42	$1 \rightarrow 27$	3.092	0.07	$2 \rightarrow 28$	3.132	0.01
$0 \rightarrow 27$	8.159	2.91	$1 \rightarrow 28$	3.346	0.01	$2 \rightarrow 29$	3.138	0.00
$0 \rightarrow 28$	8.412	0.78	$1 \rightarrow 29$	3.352	0.00	$2 \rightarrow 30$	3.144	0.03
$0 \rightarrow 29$	8.418	0.08	$1 \rightarrow 30$	3.357	0.01	$2 \rightarrow 31$	3.203	0.34
$0 \rightarrow 30$	8.423	0.69	$1 \rightarrow 31$	3.417	0.00	$2 \rightarrow 32$	3.233	0.02
$0 \rightarrow 31$	8.483	0.00	$1 \rightarrow 32$	3.447	0.00	$2 \rightarrow 33$	3.305	0.88
$0 \rightarrow 32$	8.513	0.02	$1 \rightarrow 33$	3.519	0.01	$2 \rightarrow 34$	3.339	9.50
$0 \rightarrow 33$	8.585	0.67	$1 \rightarrow 34$	3.552	0.00	$2 \rightarrow 35$	3.358	0.06
$0 \rightarrow 34$	8.619	13.81	$1 \rightarrow 35$	3.572	0.01	$2 \rightarrow 36$	3.392	0.05
$0 \rightarrow 35$	8.638	0.63	$1 \rightarrow 36$	3.606	0.23	$2 \rightarrow 37$	3.452	0.09
$0 \rightarrow 36$	8.672	0.02	$1 \rightarrow 37$	3.666	0.01	$2 \rightarrow 38$	3.524	0.03
$0 \rightarrow 37$	8.732	0.31	$1 \rightarrow 38$	3.738	0.00	$2 \rightarrow 39$	3.612	0.02
$0 \rightarrow 38$	8.804	0.17	$1 \rightarrow 39$	3.826	1.68	$2 \rightarrow 40$	3.656	0.00
$0 \rightarrow 39$	8.892	0.07	$1 \rightarrow 40$	3.869	0.00	$2 \rightarrow 41$	3.701	0.04
$0 \rightarrow 40$	8.935	0.09	$1 \rightarrow 41$	3.914	0.00	$2 \rightarrow 42$	3.716	0.01
$0 \rightarrow 41$	8.980	0.15	$1 \rightarrow 42$	3.929	2.12	$2 \rightarrow 43$	3.726	0.06
$0 \rightarrow 42$	8.995	0.38	$1 \rightarrow 43$	3.940	0.50	$2 \rightarrow 44$	3.810	0.02
$0 \rightarrow 43$	9.006	0.83	$1 \rightarrow 44$	4.024	2.55	$2 \rightarrow 45$	3.849	0.23
$0 \rightarrow 44$	9.090	0.18	$1 \rightarrow 45$	4.063	0.02	$2 \rightarrow 46$	3.878	2.17
$0 \rightarrow 45$	9.129	0.02	$1 \rightarrow 46$	4.091	0.00	$2 \rightarrow 47$	3.884	0.25
$0 \rightarrow 46$	9.157	7.68	$1 \rightarrow 47$	4.098	0.05	$2 \rightarrow 48$	3.940	0.40
$0 \rightarrow 47$	9.164	0.24	$1 \rightarrow 48$	4.153	0.00	$2 \rightarrow 49$	3.981	0.00
$0 \rightarrow 48$	9.219	0.19	$1 \rightarrow 49$	4.194	0.00	$2 \rightarrow 50$	4.014	0.02
$0 \rightarrow 49$	9.261	0.10	$1 \rightarrow 50$	4.227	0.01	$2 \rightarrow 51$	4.075	0.02
$0 \rightarrow 50$	9.293	0.88	$1 \rightarrow 51$	4.288	0.18	$2 \rightarrow 52$	4.080	0.09
$0 \rightarrow 51$	9.355	0.00	$1 \rightarrow 52$	4.294	0.09			
$0 \rightarrow 52$	9.360	0.53						

SS4.2 Cytosine

Table S9: Cytosine. CAM-B3LYP/aug-cc-pVDZ OPA excitation energies (ΔE, eV) and oscillator strengths (f): computed in the Tamm-Dancoff approximation (CIS), with TDFT in gas phase, and with non-equilibrium PCM (chloroform). First IP is 8.82 eV.

OPA ($\mathbf{S}_0 \rightarrow \mathbf{S}_n$)											
TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
0→1	5.17	8.34	0→1	4.99	6.57	0→1A'	4.98	6.56	0→1A'	5.10	13.37
0→2	5.32	0.22	0→2	5.30	0.19	0→1A"	5.30	0.19	0→1A"	5.60	0.27
0→3	5.64	0.47	0→3	5.64	0.44	0→2A"	5.63	0.44	0→2A'	5.92	20.42
0→4	5.94	0.03	0→4	5.91	12.38	0→2A'	5.91	12.37	0→2A"	5.94	0.52
0→5	6.07	11.68	0→5	5.92	0.01	0→3A"	5.92	0.01	0→3A"	6.29	0.02
0→6	6.12	0.01	0→6	6.11	0.01	0→4A"	6.11	0.02	0→3A'	6.38	37.17
0→7	6.15	0.30	0→7	6.15	0.31	0→5A"	6.14	0.28	0→4A"	6.41	0.55
0→8	6.26	0.99	0→8	6.26	0.94	0→6A"	6.24	0.96	0→5A"	6.56	0.01
0→9	6.58	0.58	0→9	6.54	33.95	0→3A'	6.54	33.75	0→6A"	6.69	0.90
0→10	6.66	15.51	0→10	6.58	0.57	0→7A"	6.56	0.57	0→7A"	6.77	0.76
0→11	6.75	18.89	0→11	6.69	3.40	0→4A'	6.68	3.49	0→4A'	6.84	39.84
0→12	6.76	0.16	0→12	6.75	0.12	0→8A"	6.75	0.12	0→8A"	6.93	0.22
0→13	6.95	0	0→13	6.91	22.84	0→5A'	6.91	22.39	0→5A'	7.14	5.17
0→14	6.99	19.99	0→14	6.95	0.00	0→9A"	6.93	0	0→9A"	7.26	0.46
0→15	7.09	0.86	0→15	7.07	7.46	0→6A'	7.06	8.01	0→6A'	7.27	3.65
0→16	7.13	25.72	0→16	7.08	0.81	0→10A"	7.08	0.78	0→10A"	7.33	0.61
0→17	7.20	12.83	0→17	7.18	3.20	0→7A'	7.18	3.10	0→11A"	7.38	0.15
0→18	7.25	0.00	0→18	7.25	0.00	0→11A"	7.23	0.02	0→7A'	7.48	1.36
0→19	7.28	0.41	0→19	7.27	0.38	0→12A"	7.25	0.34	0→12A"	7.54	0.63
0→20	7.42	4.00	0→20	7.42	1.92	0→8A'	7.40	1.89	0→13A"	7.72	0.14
0→21	7.56	4.10	0→21	7.56	3.80	0→9A'	7.54	3.81	0→8A'	7.89	3.95
0→22	7.72	2.04	0→22	7.72	1.73	0→13A"	7.70	0.05	0→9A'	7.97	2.65
0→23	7.72	0.05	0→23	7.72	0.04	0→10A'	7.70	1.67	0→14A"	8.01	0.62
0→24	7.77	0.87	0→24	7.77	0.80	0→14A"	7.75	0.78	0→10A'	8.09	4.67
0→25	7.90	0.01	0→25	7.90	0.00	0→15A"	7.88	0.01	0→15A"	8.13	0.04
0→26	7.94	0.35	0→26	7.93	0.36	0→11A'	7.92	0.60	0→11A'	8.19	0.91
0→27	8.02	9.59	0→27	7.99	4.91	0→12A'	7.98	4.66	0→16A"	8.30	0.52
0→28	8.08	0.62	0→28	8.07	0.93	0→13A'	8.05	0.98	0→12A'	8.34	0.45
0→29	8.10	0.08	0→29	8.10	0.07	0→16A"	8.10	0.07	0→17A"	8.35	0.35
0→30	8.24	0.23	0→30	8.24	0.22	0→17A"	8.21	0.20	0→13A'	8.38	2.40
0→31	8.27	0.04	0→31	8.26	0.11	0→14A'	8.24	0.12	0→18A"	8.48	0.25
0→32	8.33	1.62	0→32	8.32	1.09	0→15A'	8.32	1.03	0→19A"	8.52	0.03
0→33	8.39	0.06	0→33	8.38	0.05	0→18A"	8.37	0.04	0→14A'	8.57	2.45
0→34	8.42	2.09	0→34	8.41	1.76	0→16A'	8.40	1.80	0→15A'	8.63	1.59
0→35	8.45	2.30	0→35	8.44	1.59	0→19A"	8.43	0.02	0→16A'	8.67	15.99
0→36	8.45	0.03	0→36	8.45	0.02	0→17A'	8.43	1.52	0→17A'	8.69	0.47
0→37	8.51	0.57	0→37	8.51	0.53	0→20A"	8.51	0.55	0→20A"	8.71	0.74
0→38	8.60	0.01	0→38	8.52	15.45	0→18A'	8.52	15.50	0→21A"	8.78	0
0→39	8.62	3.31	0→39	8.57	0.79	0→21A"	8.54	0.01	0→22A"	8.85	0.21
0→40	8.68	9.39	0→40	8.60	0.01	0→19A'	8.57	0.75	0→18A'	8.85	0.64
0→41	8.71	6.08	0→41	8.68	0.16	0→22A"	8.66	0.47	0→19A'	8.94	1.14
0→42	8.73	0.50	0→42	8.73	0.47	0→20A'	8.67	0.14	0→23A"	8.96	0.11
0→43	8.85	0.06	0→43	8.85	0.06	0→23A"	8.80	0.06	0→20A'	9.07	1.01
0→44	8.94	3.66	0→44	8.93	3.19	0→24A"	9.02	0.70	0→24A"	9.10	0.12
0→45	8.98	0.41	0→45	8.96	0.32	0→25A"	9.04	0	0→25A"	9.26	1.37

Table S10: Cytosine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from $1A''S_2/n\pi^*/S_2$, computed in the Tamm-Dancoff approximation (CIS), with TDDFT in gas phase, and (TDDFT in non-equilibrium PCM (chloroform).

ESA: S_2 (1A") $\rightarrow S_n$											
TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
2→3	0.32	0.00	2→3	0.35	0.00	1A"→2A"	0.34	0.00	1A"→2A'	0.32	0.00
2→4	0.62	0.34	2→4	0.62	0.00	1A"→2A'	0.62	0.00	1A"→2A"	0.35	0.00
2→5	0.74	0.00	2→5	0.63	0.31	1A"→3A"	0.63	0.32	1A"→3A"	0.69	0.15
2→6	0.80	0.28	2→6	0.82	0.27	1A"→4A"	0.82	0.27	1A"→3A'	0.78	0.00
2→7	0.83	0.04	2→7	0.85	0.03	1A"→5A"	0.84	0.03	1A"→4A"	0.81	0.02
2→8	0.94	0.01	2→8	0.96	0.01	1A"→6A"	0.95	0.01	1A"→5A"	0.96	0.51
2→9	1.26	0.00	2→9	1.24	0.00	1A"→3A'	1.24	0.00	1A"→6A"	1.09	0.00
2→10	1.34	0.03	2→10	1.28	0.00	1A"→7A"	1.27	0.00	1A"→7A"	1.17	0.00
2→11	1.42	0.04	2→11	1.39	0.06	1A"→4A'	1.38	0.06	1A"→4A'	1.24	0.00
2→12	1.44	0.52	2→12	1.45	0.53	1A"→8A"	1.45	0.53	1A"→8A"	1.33	0.40
2→13	1.63	0.03	2→13	1.61	0.02	1A"→5A'	1.61	0.03	1A"→5A'	1.54	0.08
2→14	1.67	0.09	2→14	1.65	0.03	1A"→9A"	1.64	0.03	1A"→9A"	1.66	0.01
2→15	1.77	0.01	2→15	1.77	0.15	1A"→6A'	1.76	0.16	1A"→6A'	1.67	0.00
2→16	1.81	0.06	2→16	1.79	0.01	1A"→10A"	1.78	0.01	1A"→10A"	1.73	0.03
2→17	1.88	0.01	2→17	1.88	0.01	1A"→7A'	1.88	0.01	1A"→11A"	1.78	0.03
2→18	1.93	0.02	2→18	1.95	0.02	1A"→11A"	1.94	0.01	1A"→7A'	1.88	0.29
2→19	1.95	0.02	2→19	1.98	0.01	1A"→12A"	1.96	0.02	1A"→12A"	1.94	0.04
2→20	2.10	0.02	2→20	2.12	0.02	1A"→8A'	2.11	0.02	1A"→13A"	2.12	0.00
2→21	2.24	0.01	2→21	2.26	0.01	1A"→9A'	2.24	0.01	1A"→8A'	2.29	0.01
2→22	2.40	0.00	2→22	2.42	0.00	1A"→13A"	2.41	0.00	1A"→9A'	2.37	0.02
2→23	2.40	0.00	2→23	2.42	0.00	1A"→10A'	2.41	0.00	1A"→14A"	2.41	0.00
2→24	2.45	0.00	2→24	2.47	0.00	1A"→14A"	2.46	0.00	1A"→10A'	2.49	0.04
2→25	2.58	0.01	2→25	2.60	0.01	1A"→15A"	2.59	0.01	1A"→15A"	2.53	0.01
2→26	2.62	0.02	2→26	2.64	0.02	1A"→11A'	2.62	0.03	1A"→11A'	2.59	0.00
2→27	2.70	0.04	2→27	2.69	0.04	1A"→12A'	2.69	0.03	1A"→16A"	2.70	0.00
2→28	2.75	0.03	2→28	2.77	0.03	1A"→13A'	2.76	0.02	1A"→12A'	2.74	0.00
2→29	2.78	0.07	2→29	2.80	0.07	1A"→16A"	2.80	0.08	1A"→17A"	2.75	0.14
2→30	2.92	0.00	2→30	2.94	0.00	1A"→17A"	2.92	0.00	1A"→13A'	2.78	0.00
2→31	2.94	0.18	2→31	2.97	0.17	1A"→14A'	2.94	0.18	1A"→18A"	2.88	0.01
2→32	3.01	0.00	2→32	3.02	0.01	1A"→15A'	3.02	0.00	1A"→19A"	2.92	0.01
2→33	3.06	0.01	2→33	3.09	0.01	1A"→18A"	3.08	0.01	1A"→14A'	2.97	0.00
2→34	3.09	0.02	2→34	3.12	0.02	1A"→16A'	3.10	0.02	1A"→15A'	3.03	0.04
2→35	3.13	0.01	2→35	3.15	0.01	1A"→19A"	3.13	0.01	1A"→16A'	3.07	0.00
2→36	3.13	0.00	2→36	3.15	0.00	1A"→17A'	3.13	0.02	1A"→17A'	3.09	0.21
2→37	3.19	0.08	2→37	3.21	0.08	1A"→20A"	3.21	0.09	1A"→20A"	3.11	0.16
2→38	3.28	0.00	2→38	3.23	0.02	1A"→18A'	3.23	0.02	1A"→21A"	3.18	0.00
2→39	3.30	0.03	2→39	3.28	0.00	1A"→21A"	3.24	0.00	1A"→22A"	3.25	0.00
2→40	3.35	0.03	2→40	3.31	0.00	1A"→19A'	3.27	0.01	1A"→18A'	3.25	0.05
2→41	3.39	0.01	2→41	3.38	0.05	1A"→22A"	3.37	0.00	1A"→19A'	3.34	0.03
2→42	3.41	0.00	2→42	3.43	0.00	1A"→20A'	3.37	0.06	1A"→23A"	3.36	0.00
2→43	3.53	0.00	2→43	3.55	0.00	1A"→23A"	3.51	0.00	1A"→20A'	3.47	0.04
2→44	3.61	0.11	2→44	3.63	0.10	1A"→24A"	3.72	0.00	1A"→24A"	3.50	0.00
2→45	3.65	0.03	2→45	3.66	0.04	1A"→25A"	3.74	0.00	1A"→25A"	3.66	0.00

Table S11: Cytosine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from S_1/ 1A'/$\pi\pi^*$, computed with the Tamm-Dancoff approximation (CIS), TDDFT in gas phase and TDDFT in non-equilibrium PCM (chloroform)

ESA: S_1 (1A') $\rightarrow S_n$											
TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
1→2	0.15	0.00	1→2	0.31	0.00	1A'→1A"	0.31	0.00	1A'→1A"	0.50	0.00
1→3	0.47	0.05	1→3	0.66	0.07	1A'→2A"	0.65	0.07	1A'→2A'	0.82	0.77
1→4	0.77	0.00	1→4	0.93	0.79	1A'→2A'	0.93	0.78	1A'→2A"	0.84	0.09
1→5	0.90	0.76	1→5	0.94	0.00	1A'→3A"	0.94	0.00	1A'→3A"	1.19	0.00
1→6	0.95	0.00	1→6	1.13	0.01	1A'→4A"	1.13	0.00	1A'→3A'	1.28	0.40
1→7	0.98	0.02	1→7	1.16	0.02	1A'→5A"	1.15	0.02	1A'→4A"	1.31	0.00
1→8	1.09	0.01	1→8	1.27	0.01	1A'→6A"	1.26	0.01	1A'→5A"	1.46	0.00
1→9	1.41	0.02	1→9	1.55	0.18	1A'→3A'	1.55	0.17	1A'→6A"	1.59	0.02
1→10	1.49	0.05	1→10	1.59	0.02	1A'→7A"	1.58	0.02	1A'→7A"	1.67	0.02
1→11	1.58	0.37	1→11	1.70	0.27	1A'→4A'	1.69	0.28	1A'→4A'	1.74	0.64
1→12	1.59	0.00	1→12	1.76	0.00	1A'→8A"	1.76	0.00	1A'→8A"	1.82	0.00
1→13	1.78	0.00	1→13	1.92	0.46	1A'→5A'	1.92	0.49	1A'→5A'	2.04	0.06
1→14	1.82	0.49	1→14	1.96	0.00	1A'→9A"	1.95	0.00	1A'→9A"	2.16	0.00
1→15	1.92	0.07	1→15	2.08	0.00	1A'→6A'	2.07	0.00	1A'→6A'	2.17	0.14
1→16	1.96	0.09	1→16	2.10	0.07	1A'→10A"	2.09	0.07	1A'→10A"	2.22	0.11
1→17	2.03	0.22	1→17	2.19	0.26	1A'→7A'	2.20	0.28	1A'→11A"	2.28	0.10
1→18	2.08	0.02	1→18	2.26	0.04	1A'→11A"	2.25	0.09	1A'→7A'	2.38	0.11
1→19	2.11	0.49	1→19	2.29	0.49	1A'→12A"	2.27	0.43	1A'→12A"	2.44	0.49
1→20	2.25	0.02	1→20	2.43	0.01	1A'→8A'	2.42	0.01	1A'→13A"	2.62	0.03
1→21	2.39	0.32	1→21	2.57	0.21	1A'→9A'	2.55	0.21	1A'→8A'	2.78	0.08
1→22	2.55	0.02	1→22	2.73	0.01	1A'→13A"	2.72	0.05	1A'→9A'	2.87	0.44
1→23	2.55	0.06	1→23	2.73	0.05	1A'→10A'	2.72	0.01	1A'→14A"	2.90	0.02
1→24	2.60	0.00	1→24	2.78	0.00	1A'→14A"	2.77	0.00	1A'→10A'	2.98	0.02
1→25	2.73	0.03	1→25	2.91	0.02	1A'→15A"	2.90	0.02	1A'→15A"	3.02	0.00
1→26	2.77	0.17	1→26	2.95	0.16	1A'→11A'	2.93	0.11	1A'→11A'	3.09	0.21
1→27	2.85	1.37	1→27	3.00	1.16	1A'→12A'	3.00	1.22	1A'→16A"	3.20	0.01
1→28	2.91	0.06	1→28	3.08	0.07	1A'→13A'	3.07	0.07	1A'→12A'	3.24	0.34
1→29	2.93	0.10	1→29	3.11	0.06	1A'→16A"	3.11	0.06	1A'→17A"	3.25	0.02
1→30	3.07	0.00	1→30	3.25	0.00	1A'→17A"	3.23	0.00	1A'→13A'	3.28	5.02
1→31	3.10	0.06	1→31	3.28	0.16	1A'→15A'	3.33	3.55	1A'→18A"	3.38	0.00
1→32	3.16	3.28	1→32	3.33	3.61	1A'→18A"	3.39	0.00	1A'→19A"	3.42	0.07
1→33	3.21	0.00	1→33	3.40	0.00	1A'→16A'	3.41	0.13	1A'→14A'	3.47	1.45
1→34	3.25	0.09	1→34	3.43	0.10	1A'→19A"	3.44	0.03	1A'→15A'	3.53	1.43
1→35	3.28	0.12	1→35	3.46	0.11	1A'→17A'	3.44	0.09	1A'→16A'	3.57	5.44
1→36	3.28	0.04	1→36	3.46	0.03	1A'→20A"	3.53	0.06	1A'→17A'	3.59	0.04
1→37	3.34	0.09	1→37	3.52	0.05	1A'→18A'	3.54	6.33	1A'→20A"	3.61	0.08
1→38	3.43	0.02	1→38	3.54	7.67	1A'→21A"	3.56	0.01	1A'→21A"	3.68	0.01
1→39	3.45	0.39	1→39	3.59	0.02	1A'→19A'	3.58	0.06	1A'→22A"	3.75	0.00
1→40	3.51	4.11	1→40	3.62	0.01	1A'→22A"	3.68	0.01	1A'→18A'	3.75	0.03
1→41	3.54	3.90	1→41	3.69	0.45	1A'→20A'	3.68	0.42	1A'→19A'	3.84	0.13
1→42	3.56	0.01	1→42	3.74	0.02	1A'→23A"	3.82	0.00	1A'→23A"	3.86	0.00
1→43	3.68	0.00	1→43	3.86	0.00	1A'→24A"	4.03	0.05	1A'→20A'	3.97	0.36
1→44	3.76	0.24	1→44	3.94	0.23	1A'→25A"	4.05	0.00	1A'→24A"	4.00	0.00
1→45	3.81	0.39	1→45	3.97	0.27				1A'→25A"	4.16	0.02

Table S12: Cytosine. CCSD/aug-cc-pVDZ OPA and ESA transition energies (ω) and oscillator strengths (f).

OPA			ESA(S_1)			ESA(S_2)		
Transition	ω [eV]	$f \times 100$	Transition	ω [eV]	$f \times 100$	Transition	ω [eV]	$f \times 100$
$0 \rightarrow 1$	4.985	6.58	$1 \rightarrow 2$	0.469	0.00	$2 \rightarrow 3$	0.116	0.00
$0 \rightarrow 2$	5.454	0.26	$1 \rightarrow 3$	0.585	0.04	$2 \rightarrow 4$	0.480	0.00
$0 \rightarrow 3$	5.570	0.42	$1 \rightarrow 4$	0.950	1.21	$2 \rightarrow 5$	0.626	0.11
$0 \rightarrow 4$	5.934	17.14	$1 \rightarrow 5$	1.095	0.01	$2 \rightarrow 6$	0.645	0.26
$0 \rightarrow 5$	6.079	0.27	$1 \rightarrow 6$	1.114	0.02	$2 \rightarrow 7$	0.749	0.00
$0 \rightarrow 6$	6.099	0.42	$1 \rightarrow 7$	1.218	0.00	$2 \rightarrow 8$	0.933	0.65
$0 \rightarrow 7$	6.203	0.79	$1 \rightarrow 8$	1.402	0.00	$2 \rightarrow 9$	1.075	0.00
$0 \rightarrow 8$	6.387	0.00	$1 \rightarrow 9$	1.544	0.03	$2 \rightarrow 10$	1.110	0.00
$0 \rightarrow 9$	6.529	0.51	$1 \rightarrow 10$	1.579	0.31	$2 \rightarrow 11$	1.232	0.10
$0 \rightarrow 10$	6.563	49.47	$1 \rightarrow 11$	1.701	0.29	$2 \rightarrow 12$	1.400	0.02
$0 \rightarrow 11$	6.686	3.83	$1 \rightarrow 12$	1.870	0.01	$2 \rightarrow 13$	1.474	0.01
$0 \rightarrow 12$	6.854	0.01	$1 \rightarrow 13$	1.943	0.65	$2 \rightarrow 14$	1.553	0.01
$0 \rightarrow 13$	6.928	10.57	$1 \rightarrow 14$	2.022	0.03	$2 \rightarrow 15$	1.555	0.15
$0 \rightarrow 14$	7.007	0.64	$1 \rightarrow 15$	2.024	0.01	$2 \rightarrow 16$	1.600	1.17
$0 \rightarrow 15$	7.009	2.54	$1 \rightarrow 16$	2.069	0.00	$2 \rightarrow 17$	1.637	0.00
$0 \rightarrow 16$	7.053	0.14	$1 \rightarrow 17$	2.106	0.57	$2 \rightarrow 18$	1.719	0.04
$0 \rightarrow 17$	7.091	12.07	$1 \rightarrow 18$	2.189	0.05	$2 \rightarrow 19$	1.784	0.01
$0 \rightarrow 18$	7.173	0.02	$1 \rightarrow 19$	2.253	0.53	$2 \rightarrow 20$	1.910	0.03
$0 \rightarrow 19$	7.238	0.30	$1 \rightarrow 20$	2.380	0.00	$2 \rightarrow 21$	2.092	0.00
$0 \rightarrow 20$	7.364	2.13	$1 \rightarrow 21$	2.561	0.24	$2 \rightarrow 22$	2.207	0.00
$0 \rightarrow 21$	7.546	4.35	$1 \rightarrow 22$	2.676	0.06	$2 \rightarrow 23$	2.230	0.00
$0 \rightarrow 22$	7.661	0.70	$1 \rightarrow 23$	2.700	0.00	$2 \rightarrow 24$	2.252	0.00
$0 \rightarrow 23$	7.684	0.19	$1 \rightarrow 24$	2.721	0.01	$2 \rightarrow 25$	2.345	0.00
$0 \rightarrow 24$	7.706	1.53	$1 \rightarrow 25$	2.814	0.03	$2 \rightarrow 26$	2.411	0.00
$0 \rightarrow 25$	7.798	0.00	$1 \rightarrow 26$	2.880	1.32	$2 \rightarrow 27$	2.453	0.08
$0 \rightarrow 26$	7.865	3.41	$1 \rightarrow 27$	2.922	0.33	$2 \rightarrow 28$	2.572	0.08
$0 \rightarrow 27$	7.907	3.13	$1 \rightarrow 28$	3.041	0.06	$2 \rightarrow 29$	2.593	0.04
$0 \rightarrow 28$	8.026	0.11	$1 \rightarrow 29$	3.063	0.08	$2 \rightarrow 30$	2.752	0.00
$0 \rightarrow 29$	8.047	1.29	$1 \rightarrow 30$	3.221	0.00	$2 \rightarrow 31$	2.765	0.13
$0 \rightarrow 30$	8.206	0.14	$1 \rightarrow 31$	3.235	1.15	$2 \rightarrow 32$	2.776	0.06
$0 \rightarrow 31$	8.219	1.07	$1 \rightarrow 32$	3.245	2.42	$2 \rightarrow 33$	2.882	0.01
$0 \rightarrow 32$	8.229	0.63	$1 \rightarrow 33$	3.351	0.00	$2 \rightarrow 34$	2.921	0.02
$0 \rightarrow 33$	8.336	0.13	$1 \rightarrow 34$	3.390	0.05	$2 \rightarrow 35$	2.928	0.00
$0 \rightarrow 34$	8.374	0.89	$1 \rightarrow 35$	3.397	0.05	$2 \rightarrow 36$	2.971	0.06
$0 \rightarrow 35$	8.382	0.09	$1 \rightarrow 36$	3.440	0.05	$2 \rightarrow 37$	2.989	0.00
$0 \rightarrow 36$	8.425	0.40	$1 \rightarrow 37$	3.458	0.10	$2 \rightarrow 38$	3.044	0.00
$0 \rightarrow 37$	8.443	2.06	$1 \rightarrow 38$	3.513	0.00	$2 \rightarrow 39$	3.100	0.01
$0 \rightarrow 38$	8.498	0.00	$1 \rightarrow 39$	3.570	0.00	$2 \rightarrow 40$	3.196	0.00
$0 \rightarrow 39$	8.554	1.90	$1 \rightarrow 40$	3.665	0.02	$2 \rightarrow 41$	3.212	0.09
$0 \rightarrow 40$	8.650	0.45	$1 \rightarrow 41$	3.682	0.63	$2 \rightarrow 42$	3.282	0.00
$0 \rightarrow 41$	8.666	1.71	$1 \rightarrow 42$	3.752	13.18	$2 \rightarrow 43$	3.288	0.00
$0 \rightarrow 42$	8.736	13.58	$1 \rightarrow 43$	3.757	0.00	$2 \rightarrow 44$	3.424	0.01
$0 \rightarrow 43$	8.741	0.15	$1 \rightarrow 44$	3.893	1.24	$2 \rightarrow 45$	3.438	0.09
$0 \rightarrow 44$	8.878	2.08	$1 \rightarrow 45$	3.907	0.00	$2 \rightarrow 46$	3.566	0.01
$0 \rightarrow 45$	8.892	2.17	$1 \rightarrow 46$	4.036	0.01	$2 \rightarrow 47$	3.590	0.00
$0 \rightarrow 46$	9.020	0.11	$1 \rightarrow 47$	4.059	0.07	$2 \rightarrow 48$	3.656	0.05
$0 \rightarrow 47$	9.044	0.74	$1 \rightarrow 48$	4.125	0.00	$2 \rightarrow 49$	3.706	0.00
$0 \rightarrow 48$	9.110	0.33	$1 \rightarrow 49$	4.175	0.04	$2 \rightarrow 50$	3.709	4.54
$0 \rightarrow 49$	9.160	1.52	$1 \rightarrow 50$	4.178	0.01	$2 \rightarrow 51$	3.738	0.00
$0 \rightarrow 50$	9.163	0.67	$1 \rightarrow 51$	4.208	0.39	$2 \rightarrow 52$	3.803	0.00
$0 \rightarrow 51$	9.192	5.08	$1 \rightarrow 52$	4.272	0.08			
$0 \rightarrow 52$	9.257	0.12						

Table S13: Cytosine. CC3/aug-cc-pVDZ ESA transition energies (ω) and oscillator strengths (f).

OPA			ESA(S_1)			ESA(S_2)		
Transition	ω [eV]	$f \times 100$	Transition	ω [eV]	$f \times 100$	Transition	ω [eV]	$f \times 100$
$0 \rightarrow 1$	4.756	5.09	$1 \rightarrow 2$	0.446	0.00	$2 \rightarrow 3$	0.269	0.00
$0 \rightarrow 2$	5.202	0.21	$1 \rightarrow 3$	0.715	0.04	$2 \rightarrow 4$	0.392	0.71
$0 \rightarrow 3$	5.472	0.40	$1 \rightarrow 4$	0.838	0.00	$2 \rightarrow 5$	0.436	0.00
$0 \rightarrow 4$	5.594	0.05	$1 \rightarrow 5$	0.882	0.85	$2 \rightarrow 6$	0.771	0.01
$0 \rightarrow 5$	5.638	12.38	$1 \rightarrow 6$	1.217	0.03	$2 \rightarrow 7$	0.834	0.00
$0 \rightarrow 6$	5.973	0.58	$1 \rightarrow 7$	1.280	0.00	$2 \rightarrow 8$	0.855	0.19
$0 \rightarrow 7$	6.037	0.55	$1 \rightarrow 8$	1.301	0.00	$2 \rightarrow 9$	1.172	0.01
$0 \rightarrow 8$	6.057	0.00	$1 \rightarrow 9$	1.618	0.11	$2 \rightarrow 10$	1.209	0.00
$0 \rightarrow 9$	6.374	30.50	$1 \rightarrow 10$	1.655	0.02	$2 \rightarrow 11$	1.224	0.10
$0 \rightarrow 10$	6.411	0.68	$1 \rightarrow 11$	1.670	0.27	$2 \rightarrow 12$	1.465	0.01
$0 \rightarrow 11$	6.427	7.27	$1 \rightarrow 12$	1.911	0.00	$2 \rightarrow 13$	1.493	0.02
$0 \rightarrow 12$	6.667	0.03	$1 \rightarrow 13$	1.939	0.59	$2 \rightarrow 14$	1.550	0.45
$0 \rightarrow 13$	6.695	14.46	$1 \rightarrow 14$	1.996	0.00	$2 \rightarrow 15$	1.584	0.04
$0 \rightarrow 14$	6.752	0.05	$1 \rightarrow 15$	2.030	0.13	$2 \rightarrow 16$	1.682	0.00
$0 \rightarrow 15$	6.786	16.34	$1 \rightarrow 16$	2.128	0.02	$2 \rightarrow 17$	1.743	0.00
$0 \rightarrow 16$	6.885	0.73	$1 \rightarrow 17$	2.189	0.10	$2 \rightarrow 18$	1.775	0.01
$0 \rightarrow 17$	6.946	2.57	$1 \rightarrow 18$	2.221	0.09	$2 \rightarrow 19$	1.838	0.02
$0 \rightarrow 18$	6.977	1.39	$1 \rightarrow 19$	2.284	0.03	$2 \rightarrow 20$	1.879	0.00
$0 \rightarrow 19$	7.040	0.00	$1 \rightarrow 20$	2.325	0.53	$2 \rightarrow 21$	2.009	0.01
$0 \rightarrow 20$	7.081	0.24	$1 \rightarrow 21$	2.455	0.14	$2 \rightarrow 22$	2.167	0.00
$0 \rightarrow 21$	7.212	3.85	$1 \rightarrow 22$	2.613	0.03	$2 \rightarrow 23$	2.301	0.00
$0 \rightarrow 22$	7.369	2.41	$1 \rightarrow 23$	2.747	0.05	$2 \rightarrow 24$	2.360	0.00
$0 \rightarrow 23$	7.503	0.72	$1 \rightarrow 24$	2.806	0.01	$2 \rightarrow 25$	2.437	0.00
$0 \rightarrow 24$	7.563	0.11	$1 \rightarrow 25$	2.883	0.03	$2 \rightarrow 26$	2.465	0.07
$0 \rightarrow 25$	7.639	0.02	$1 \rightarrow 26$	2.911	0.07	$2 \rightarrow 27$	2.538	0.02
$0 \rightarrow 26$	7.667	1.52	$1 \rightarrow 27$	2.984	0.84	$2 \rightarrow 28$	2.556	0.03
$0 \rightarrow 27$	7.740	4.46	$1 \rightarrow 28$	3.002	0.14	$2 \rightarrow 29$	2.618	0.08
$0 \rightarrow 28$	7.759	1.45	$1 \rightarrow 29$	3.064	0.05	$2 \rightarrow 30$	2.703	0.28
$0 \rightarrow 29$	7.820	0.07	$1 \rightarrow 30$	3.149	0.02	$2 \rightarrow 31$	2.871	0.00
$0 \rightarrow 30$	7.906	0.06	$1 \rightarrow 31$	3.317	0.00	$2 \rightarrow 32$	2.874	0.01
$0 \rightarrow 31$	8.073	0.15	$1 \rightarrow 32$	3.320	2.69	$2 \rightarrow 33$	2.915	0.00
$0 \rightarrow 32$	8.076	0.36	$1 \rightarrow 33$	3.360	0.77	$2 \rightarrow 34$	2.979	0.01
$0 \rightarrow 33$	8.117	3.75	$1 \rightarrow 34$	3.425	0.49	$2 \rightarrow 35$	2.990	0.01
$0 \rightarrow 34$	8.181	0.69	$1 \rightarrow 35$	3.436	0.00	$2 \rightarrow 36$	3.028	0.02
$0 \rightarrow 35$	8.193	0.04	$1 \rightarrow 36$	3.474	0.07	$2 \rightarrow 37$	3.045	0.00
$0 \rightarrow 36$	8.230	0.50	$1 \rightarrow 37$	3.491	0.02	$2 \rightarrow 38$	3.055	0.02
$0 \rightarrow 37$	8.248	0.00	$1 \rightarrow 38$	3.501	6.58	$2 \rightarrow 39$	3.159	0.05
$0 \rightarrow 38$	8.258	15.48	$1 \rightarrow 39$	3.605	0.62	$2 \rightarrow 40$	3.191	0.02
$0 \rightarrow 39$	8.361	0.11	$1 \rightarrow 40$	3.637	0.07	$2 \rightarrow 41$	3.196	0.00
$0 \rightarrow 40$	8.393	0.49	$1 \rightarrow 41$	3.642	0.01	$2 \rightarrow 42$	3.317	0.00
$0 \rightarrow 41$	8.398	0.00	$1 \rightarrow 42$	3.763	0.01	$2 \rightarrow 43$	3.390	0.00
$0 \rightarrow 42$	8.520	0.39	$1 \rightarrow 43$	3.836	0.00	$2 \rightarrow 44$	3.480	0.05
$0 \rightarrow 43$	8.592	0.12	$1 \rightarrow 44$	3.926	0.30	$2 \rightarrow 45$	3.505	0.03
$0 \rightarrow 44$	8.682	2.37	$1 \rightarrow 45$	3.951	0.23			
$0 \rightarrow 45$	8.707	0.64						

SS4.3 Adenine

Table S14: Adenine. CAM-B3LYP/aug-cc-pVDZ OPA excitation energies (ΔE, eV) and oscillator strengths (f), computed with the Tamm-Dancoff approximation (CIS), TDDFT in gas phase and TDDFT with non-equilibrium PCM (chloroform). First IP is 8.38 eV. Note the inversion of the state ordering in TDA, and the relatively large intensity of L_b.

OPA											
TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
0→1	5.37	0.07	0→1 L_a	5.34	27.76	1A'L_a	5.34	27.75	1A'L_a	5.25	37.85
0→2	5.54	25.82	0→2 $n\pi^*$	5.35	0.06	1A"$n\pi^*$	5.35	0.06	2A'L_b	5.45	2.79
0→3	5.57	9.56	0→3 L_b	5.49	1.31	2A'L_b	5.49	1.32	1A"$n\pi^*$	5.48	0.07
0→4	5.64	0.96	0→4	5.64	0.96	2A"	5.63	0.96	2A"	5.75	1.06
0→5	5.95	0.01	0→5	5.93	0.09	3A"	5.93	0.05	3A"	6.06	0.25
0→6	5.98	0.37	0→6	5.96	0.23	4A"	5.95	0.28	4A"	6.26	0.08
0→7	6.31	0.12	0→7	6.28	0.10	5A"	6.28	0.10	5A"	6.42	0.13
0→8	6.47	0.11	0→8	6.47	0.10	6A"	6.45	0.09	3A'	6.46	58.79
0→9	6.65	0	0→9	6.56	41.68	3A'	6.56	41.55	6A"	6.49	0.08
0→10	6.72	20.57	0→10	6.65	0.00	7A"	6.64	0	4A'	6.72	0
0→11	6.79	8.21	0→11	6.72	1.99	4A'	6.72	2.09	7A"	6.84	0.14
0→12	6.82	25.87	0→12	6.78	5.07	5A'	6.78	4.93	5A'	6.90	24.30
0→13	6.86	0.18	0→13	6.86	0.17	8A"	6.84	0.16	6A'	6.99	0.85
0→14	6.93	0.01	0→14	6.92	0.53	9A"	6.92	0.21	8A"	7.00	1.74
0→15	6.98	2.07	0→15	6.94	0.98	10A"	6.93	1.30	9A"	7.02	0.27
0→16	7.09	8.48	0→16	7.00	10.28	6A'	7.00	10.37	7A'	7.10	0.34
0→17	7.13	0.25	0→17	7.10	0.11	11A"	7.10	0.14	10A"	7.13	0
0→18	7.15	0.01	0→18	7.11	2.09	7A'	7.11	2.12	11A"	7.17	0.25
0→19	7.23	3.39	0→19	7.14	0.13	12A"	7.12	0.08	12A"	7.24	0.12
0→20	7.25	16.41	0→20	7.19	5.85	8A'	7.18	5.64	8A'	7.35	19.38
0→21	7.36	0.27	0→21	7.36	0.25	13A"	7.35	0.25	9A'	7.56	3.45
0→22	7.42	1.63	0→22	7.41	0.94	9A'	7.39	1.01	13A"	7.58	0.17
0→23	7.70	26.74	0→23	7.48	16.06	10A'	7.48	16.07	10A'	7.64	1.55
0→24	7.76	0.40	0→24	7.73	4.09	11A'	7.72	4.13	11A'	7.80	10.36
0→25	7.77	3.97	0→25	7.75	0.37	14A"	7.74	0.35	14A"	7.85	0.65
0→26	7.80	0.03	0→26	7.79	0.03	15A"	7.78	0.04	15A"	7.87	0.28
0→27	7.83	2.40	0→27	7.82	2.63	12A'	7.82	2.32	12A'	7.89	2.31
0→28	7.87	0.06	0→28	7.84	0.20	13A'	7.83	0.42	16A"	8.00	0.04
0→29	7.89	0.12	0→29	7.86	0.06	16A"	7.85	0.08	13A'	8.02	8.53
0→30	7.89	3.88	0→30	7.88	0.11	17A"	7.88	0.09	17A"	8.05	0.13
0→31	7.94	0.05	0→31	7.92	2.04	14A'	7.92	0.91	14A'	8.08	1.51
0→32	7.97	0.08	0→32	7.94	2.94	15A'	7.94	4.05	18A"	8.10	0.10
0→33	8.00	0.18	0→33	7.97	0.08	18A"	7.96	0.06	19A"	8.13	0.29
0→34	8.02	4.23	0→34	8.00	0.16	19A"	7.98	0.10	15A'	8.13	4.73
0→35	8.07	0.17	0→35	8.07	0.15	20A"	8.06	0.18	16A'	8.17	1.44
0→36	8.12	0.35	0→36	8.11	8.69	21A"	8.10	0.37	20A"	8.19	0.06
0→37	8.15	7.49	0→37	8.12	0.35	16A'	8.11	7.91	17A'	8.21	1.92
0→38	8.17	4.10	0→38	8.15	0.40	17A'	8.14	1.03	21A"	8.30	0.04
0→39	8.23	0.01	0→39	8.20	1.14	18A'	8.20	1.28	22A"	8.33	0.57
0→40	8.24	0.52	0→40	8.23	0.01	22A"	8.22	0	18A'	8.35	5.66
0→41	8.30	3.21	0→41	8.30	2.93	19A'	8.28	2.75	23A"	8.39	0.03
0→42	8.32	0.23	0→42	8.32	0.17	23A"	8.30	0.34	19A'	8.40	2.11
0→43	8.36	0.28	0→43	8.35	0.31	24A"	8.34	0.23	24A"	8.45	0.73
0→44	8.39	0.84	0→44	8.37	5.79	20A'	8.36	0.83	20A'	8.52	1.05
0→45	8.45	18.04	0→45	8.39	3.58	25A"	8.45	0.63	25A"	8.55	0.31

Table S15: Adenine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from L_a/1A', computed in the Tamm-Dancoff approximation (CIS), with TDDFT in gas phase, and and TDDFT with non-equilibrium PCM (chloroform).

TDA (Turbomole) - S_2			TDDFT (Turbomole) - S_1			TDDFT (Dalton) - 1A'			TDDFT PCM (Dalton) 1A'		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
$2 \rightarrow 3$	0.03	0.01	$1 \rightarrow 2$	0.01	0.00	1A'→1A"	0.01	0.00	1A'→2A'	0.21	0.11
$2 \rightarrow 4$	0.10	0.00	$1 \rightarrow 3$	0.15	0.05	1A'→2A'	0.15	0.05	1A'→1A"	0.24	0.00
$2 \rightarrow 5$	0.41	0.11	$1 \rightarrow 4$	0.30	0.01	1A'→2A"	0.29	0.01	1A'→2A"	0.50	0.07
$2 \rightarrow 6$	0.44	0.07	$1 \rightarrow 5$	0.59	0.05	1A'→3A"	0.59	0.09	1A'→3A"	0.81	0.00
$2 \rightarrow 7$	0.77	0.00	$1 \rightarrow 6$	0.62	0.30	1A'→4A"	0.61	0.25	1A'→4A"	1.02	0.49
$2 \rightarrow 8$	0.93	0.30	$1 \rightarrow 7$	0.94	0.00	1A'→5A"	0.94	0.00	1A'→5A"	1.17	0.01
$2 \rightarrow 9$	1.11	0.01	$1 \rightarrow 8$	1.13	0.24	1A'→6A"	1.11	0.25	1A'→3A'	1.21	0.07
$2 \rightarrow 10$	1.18	3.02	$1 \rightarrow 9$	1.21	0.34	1A'→3A'	1.21	0.34	1A'→6A"	1.24	0.42
$2 \rightarrow 11$	1.25	0.26	$1 \rightarrow 10$	1.31	0.04	1A'→7A"	1.30	0.03	1A'→4A'	1.47	8.47
$2 \rightarrow 12$	1.28	2.32	$1 \rightarrow 11$	1.37	6.70	1A'→4A'	1.37	6.50	1A'→7A"	1.59	0.02
$2 \rightarrow 13$	1.32	0.01	$1 \rightarrow 12$	1.44	0.42	1A'→5A'	1.43	0.52	1A'→5A'	1.65	2.87
$2 \rightarrow 14$	1.39	0.01	$1 \rightarrow 13$	1.52	0.02	1A'→8A"	1.49	0.02	1A'→6A'	1.74	1.18
$2 \rightarrow 15$	1.44	0.01	$1 \rightarrow 14$	1.58	0.00	1A'→9A"	1.58	0.00	1A'→8A"	1.76	0.00
$2 \rightarrow 16$	1.54	4.60	$1 \rightarrow 15$	1.59	0.01	1A'→10A"	1.59	0.01	1A'→9A"	1.77	0.02
$2 \rightarrow 17$	1.59	0.10	$1 \rightarrow 16$	1.66	2.79	1A'→6A'	1.66	2.56	1A'→7A'	1.85	1.08
$2 \rightarrow 18$	1.61	0.07	$1 \rightarrow 17$	1.76	0.00	1A'→11A"	1.76	0.01	1A'→10A"	1.88	0.00
$2 \rightarrow 19$	1.69	0.99	$1 \rightarrow 18$	1.77	1.04	1A'→7A'	1.77	0.98	1A'→11A"	1.92	0.07
$2 \rightarrow 20$	1.71	0.00	$1 \rightarrow 19$	1.79	0.14	1A'→12A"	1.78	0.12	1A'→12A"	1.99	0.00
$2 \rightarrow 21$	1.82	0.04	$1 \rightarrow 20$	1.85	0.15	1A'→8A'	1.83	0.13	1A'→8A'	2.10	1.67
$2 \rightarrow 22$	1.88	0.19	$1 \rightarrow 21$	2.02	0.00	1A'→13A"	2.01	0.00	1A'→9A'	2.32	0.17
$2 \rightarrow 23$	2.16	0.17	$1 \rightarrow 22$	2.07	0.13	1A'→9A'	2.05	0.10	1A'→13A"	2.33	0.00
$2 \rightarrow 24$	2.21	0.16	$1 \rightarrow 23$	2.14	0.69	1A'→10A'	2.13	0.62	1A'→10A'	2.39	0.05
$2 \rightarrow 25$	2.23	0.07	$1 \rightarrow 24$	2.39	0.19	1A'→11A'	2.37	0.17	1A'→11A'	2.55	0.06
$2 \rightarrow 26$	2.25	0.46	$1 \rightarrow 25$	2.41	0.21	1A'→14A"	2.40	0.15	1A'→14A"	2.60	0.01
$2 \rightarrow 27$	2.29	0.17	$1 \rightarrow 26$	2.45	0.53	1A'→15A"	2.44	0.61	1A'→15A"	2.63	0.81
$2 \rightarrow 28$	2.32	0.00	$1 \rightarrow 27$	2.48	0.01	1A'→12A'	2.48	0.02	1A'→12A'	2.64	0.78
$2 \rightarrow 29$	2.34	0.00	$1 \rightarrow 28$	2.50	0.00	1A'→13A'	2.49	0.00	1A'→16A"	2.75	0.00
$2 \rightarrow 30$	2.35	0.02	$1 \rightarrow 29$	2.52	0.00	1A'→16A"	2.51	0.00	1A'→13A'	2.77	0.15
$2 \rightarrow 31$	2.40	0.05	$1 \rightarrow 30$	2.54	0.03	1A'→17A"	2.54	0.00	1A'→17A"	2.81	0.00
$2 \rightarrow 32$	2.43	0.03	$1 \rightarrow 31$	2.58	0.38	1A'→14A'	2.57	0.16	1A'→14A'	2.83	0.06
$2 \rightarrow 33$	2.46	0.04	$1 \rightarrow 32$	2.60	0.61	1A'→15A'	2.60	0.86	1A'→18A"	2.86	0.01
$2 \rightarrow 34$	2.48	1.23	$1 \rightarrow 33$	2.62	0.11	1A'→18A"	2.62	0.11	1A'→19A"	2.88	0.03
$2 \rightarrow 35$	2.53	0.00	$1 \rightarrow 34$	2.66	0.00	1A'→19A"	2.64	0.01	1A'→15A'	2.89	0.65
$2 \rightarrow 36$	2.58	0.16	$1 \rightarrow 35$	2.72	0.01	1A'→20A"	2.72	0.01	1A'→16A'	2.92	0.64
$2 \rightarrow 37$	2.61	0.60	$1 \rightarrow 36$	2.77	0.75	1A'→21A"	2.76	0.15	1A'→20A"	2.95	0.00
$2 \rightarrow 38$	2.63	0.80	$1 \rightarrow 37$	2.78	0.17	1A'→16A'	2.77	0.67	1A'→17A'	2.96	0.50
$2 \rightarrow 39$	2.69	0.04	$1 \rightarrow 38$	2.80	0.19	1A'→17A'	2.79	0.20	1A'→21A"	3.05	0.22
$2 \rightarrow 40$	2.70	0.91	$1 \rightarrow 39$	2.86	0.57	1A'→18A'	2.85	0.61	1A'→22A"	3.08	0.14
$2 \rightarrow 41$	2.76	0.07	$1 \rightarrow 40$	2.89	0.06	1A'→22A"	2.88	0.05	1A'→18A'	3.10	0.13
$2 \rightarrow 42$	2.78	0.17	$1 \rightarrow 41$	2.95	0.07	1A'→19A'	2.94	0.09	1A'→23A"	3.14	0.01
$2 \rightarrow 43$	2.82	0.11	$1 \rightarrow 42$	2.97	0.12	1A'→23A"	2.96	0.17	1A'→19A'	3.16	0.01
$2 \rightarrow 44$	2.85	0.14	$1 \rightarrow 43$	3.01	0.13	1A'→24A"	3.00	0.07	1A'→24A"	3.20	0.00
$2 \rightarrow 45$	2.90	0.82	$1 \rightarrow 44$	3.03	0.12	1A'→20A'	3.02	0.11	1A'→20A'	3.27	0.11

Table S16: Adenine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from nπ^*/1A$''$, computed in the Tamm-Dancoff approximation (CIS), at TDDFT level in gas phase, and TDDFT with non-equilibrium PCM (chloroform)

TDA (Turbomole) - S_1			TDDFT (Turbomole) - S_2			TDDFT (Dalton) - 1A"			TDDFT PCM (Dalton) - 1A"		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
$1 \rightarrow 2$	0.17	0.00	$2 \rightarrow 3$	0.14	0.00	1A"→2A'	0.14	0.00	1A"→2A"	0.26	0.00
$1 \rightarrow 3$	0.20	0.00	$2 \rightarrow 4$	0.29	0.00	1A"→2A"	0.29	0.00	1A"→3A"	0.58	0.30
$1 \rightarrow 4$	0.27	0.00	$2 \rightarrow 5$	0.58	0.18	1A"→3A"	0.58	0.15	1A"→4A"	0.78	0.00
$1 \rightarrow 5$	0.58	0.08	$2 \rightarrow 6$	0.62	0.05	1A"→4A"	0.61	0.08	1A"→5A"	0.93	1.23
$1 \rightarrow 6$	0.61	0.15	$2 \rightarrow 7$	0.93	0.78	1A"→5A"	0.93	0.77	1A"→3A'	0.97	0.00
$1 \rightarrow 7$	0.94	0.81	$2 \rightarrow 8$	1.12	0.00	1A"→6A"	1.10	0.00	1A"→6A"	1.00	0.02
$1 \rightarrow 8$	1.10	0.00	$2 \rightarrow 9$	1.21	0.00	1A"→3A'	1.21	0.00	1A"→4A'	1.24	0.00
$1 \rightarrow 9$	1.28	0.00	$2 \rightarrow 10$	1.30	0.00	1A"→7A"	1.29	0.00	1A"→7A"	1.35	0.00
$1 \rightarrow 10$	1.35	0.00	$2 \rightarrow 11$	1.37	0.00	1A"→4A'	1.37	0.00	1A"→5A'	1.41	0.05
$1 \rightarrow 11$	1.42	0.04	$2 \rightarrow 12$	1.44	0.04	1A"→5A'	1.43	0.04	1A"→6A'	1.50	0.09
$1 \rightarrow 12$	1.45	0.00	$2 \rightarrow 13$	1.51	0.01	1A"→8A"	1.49	0.01	1A"→8A"	1.52	1.21
$1 \rightarrow 13$	1.49	0.01	$2 \rightarrow 14$	1.57	1.09	1A"→9A"	1.57	0.59	1A"→9A"	1.54	0.69
$1 \rightarrow 14$	1.56	0.03	$2 \rightarrow 15$	1.59	0.78	1A"→10A"	1.58	1.14	1A"→7A'	1.62	0.08
$1 \rightarrow 15$	1.61	1.64	$2 \rightarrow 16$	1.65	0.01	1A"→6A'	1.65	0.01	1A"→10A"	1.64	0.02
$1 \rightarrow 16$	1.71	0.00	$2 \rightarrow 17$	1.75	1.30	1A"→11A"	1.75	1.08	1A"→11A"	1.69	0.03
$1 \rightarrow 17$	1.76	0.32	$2 \rightarrow 18$	1.76	0.00	1A"→7A'	1.76	0.00	1A"→12A"	1.76	1.88
$1 \rightarrow 18$	1.78	1.31	$2 \rightarrow 19$	1.79	0.17	1A"→12A"	1.77	0.32	1A"→8A'	1.86	0.04
$1 \rightarrow 19$	1.86	0.07	$2 \rightarrow 20$	1.84	0.46	1A"→8A'	1.83	0.48	1A"→9A'	2.08	0.29
$1 \rightarrow 20$	1.88	0.45	$2 \rightarrow 21$	2.01	0.00	1A"→13A"	2.00	0.00	1A"→13A"	2.09	0.01
$1 \rightarrow 21$	1.99	0.00	$2 \rightarrow 22$	2.06	0.15	1A"→9A'	2.04	0.14	1A"→10A'	2.15	0.16
$1 \rightarrow 22$	2.05	0.09	$2 \rightarrow 23$	2.13	0.01	1A"→10A'	2.13	0.01	1A"→11A'	2.31	0.00
$1 \rightarrow 23$	2.33	0.02	$2 \rightarrow 24$	2.38	0.00	1A"→11A'	2.37	0.00	1A"→14A"	2.37	0.01
$1 \rightarrow 24$	2.38	0.03	$2 \rightarrow 25$	2.40	0.03	1A"→14A"	2.39	0.03	1A"→15A"	2.39	0.01
$1 \rightarrow 25$	2.40	0.00	$2 \rightarrow 26$	2.45	0.01	1A"→15A"	2.43	0.01	1A"→12A'	2.41	0.01
$1 \rightarrow 26$	2.42	0.01	$2 \rightarrow 27$	2.47	0.00	1A"→12A'	2.47	0.01	1A"→16A"	2.52	0.01
$1 \rightarrow 27$	2.46	0.00	$2 \rightarrow 28$	2.50	0.01	1A"→13A'	2.48	0.01	1A"→13A'	2.54	0.04
$1 \rightarrow 28$	2.50	0.25	$2 \rightarrow 29$	2.52	0.28	1A"→16A"	2.50	0.08	1A"→17A"	2.57	7.89
$1 \rightarrow 29$	2.52	7.59	$2 \rightarrow 30$	2.54	7.65	1A"→17A"	2.54	7.83	1A"→14A'	2.59	0.12
$1 \rightarrow 30$	2.52	0.00	$2 \rightarrow 31$	2.57	0.02	1A"→14A'	2.57	0.04	1A"→18A"	2.62	0.78
$1 \rightarrow 31$	2.57	0.05	$2 \rightarrow 32$	2.60	0.02	1A"→15A'	2.59	0.01	1A"→19A"	2.65	0.56
$1 \rightarrow 32$	2.60	0.07	$2 \rightarrow 33$	2.62	0.08	1A"→18A"	2.61	0.10	1A"→15A'	2.65	0.00
$1 \rightarrow 33$	2.63	0.19	$2 \rightarrow 34$	2.65	0.18	1A"→19A"	2.64	0.20	1A"→16A'	2.68	0.00
$1 \rightarrow 34$	2.65	0.00	$2 \rightarrow 35$	2.72	2.30	1A"→20A"	2.72	2.16	1A"→20A"	2.71	3.60
$1 \rightarrow 35$	2.70	2.33	$2 \rightarrow 36$	2.76	0.00	1A"→21A"	2.75	0.01	1A"→17A'	2.72	0.00
$1 \rightarrow 36$	2.75	0.01	$2 \rightarrow 37$	2.77	0.00	1A"→16A'	2.76	0.00	1A"→21A"	2.82	0.00
$1 \rightarrow 37$	2.78	0.00	$2 \rightarrow 38$	2.80	0.01	1A"→17A'	2.79	0.00	1A"→22A"	2.85	0.08
$1 \rightarrow 38$	2.80	0.00	$2 \rightarrow 39$	2.85	0.00	1A"→18A'	2.85	0.00	1A"→18A'	2.86	0.00
$1 \rightarrow 39$	2.86	0.01	$2 \rightarrow 40$	2.88	0.01	1A"→22A"	2.87	0.01	1A"→23A"	2.90	0.47
$1 \rightarrow 40$	2.87	0.00	$2 \rightarrow 41$	2.95	0.00	1A"→19A'	2.93	0.00	1A"→19A'	2.92	0.00
$1 \rightarrow 41$	2.93	0.00	$2 \rightarrow 42$	2.97	0.03	1A"→23A"	2.96	0.04	1A"→24A"	2.96	0.00
$1 \rightarrow 42$	2.95	0.02	$2 \rightarrow 43$	3.00	0.02	1A"→24A"	2.99	0.07	1A"→20A'	3.04	0.01
$1 \rightarrow 43$	2.99	0.02	$2 \rightarrow 44$	3.02	0.00	1A"→20A'	3.01	0.02	1A"→25A"	3.06	0.01
$1 \rightarrow 44$	3.02	0.05	$2 \rightarrow 45$	3.04	0.05	1A"→25A"	3.10	0.00			

Table S17: Adenine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from $L_b/2A'$, computed in the Tamm-Dancoff approximation at TDDFT level in gAs phase, and with TDDFT in non-equilibrium PCM (chloroform).

TDA (Turbomole) - S_3			TDDFT (Turbomole) - S_3			TDDFT (Dalton) - 2A'			TDDFT PCM (Dalton) - 2A'		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
$3 \rightarrow 4$	0.07	0.00	$3 \rightarrow 4$	0.15	0.00	2A'→2A"	0.15	0.00	2A'→1A"	0.03	0.00
$3 \rightarrow 5$	0.38	0.07	$3 \rightarrow 5$	0.44	0.00	2A'→3A"	0.44	0.00	2A'→2A"	0.29	0.01
$3 \rightarrow 6$	0.41	0.07	$3 \rightarrow 6$	0.48	0.03	2A'→4A"	0.47	0.03	2A'→3A"	0.61	0.00
$3 \rightarrow 7$	0.74	0.00	$3 \rightarrow 7$	0.79	0.00	2A'→5A"	0.79	0.00	2A'→4A"	0.81	0.11
$3 \rightarrow 8$	0.90	0.00	$3 \rightarrow 8$	0.98	0.08	2A'→6A"	0.96	0.07	2A'→5A"	0.96	0.00
$3 \rightarrow 9$	1.08	0.10	$3 \rightarrow 9$	1.07	0.45	2A'→3A'	1.07	0.46	2A'→3A'	1.00	0.66
$3 \rightarrow 10$	1.15	0.89	$3 \rightarrow 10$	1.16	0.07	2A'→7A"	1.15	0.07	2A'→6A"	1.03	0.06
$3 \rightarrow 11$	1.22	0.11	$3 \rightarrow 11$	1.23	0.22	2A'→4A'	1.23	0.22	2A'→4A'	1.27	0.15
$3 \rightarrow 12$	1.25	0.59	$3 \rightarrow 12$	1.30	0.01	2A'→5A'	1.29	0.01	2A'→7A"	1.38	0.08
$3 \rightarrow 13$	1.29	0.02	$3 \rightarrow 13$	1.37	0.00	2A'→8A"	1.35	0.00	2A'→5A'	1.44	0.83
$3 \rightarrow 14$	1.36	0.00	$3 \rightarrow 14$	1.43	0.00	2A'→9A"	1.43	0.00	2A'→6A'	1.53	0.41
$3 \rightarrow 15$	1.41	0.00	$3 \rightarrow 15$	1.45	0.00	2A'→10A"	1.44	0.00	2A'→8A"	1.55	0.01
$3 \rightarrow 16$	1.51	0.00	$3 \rightarrow 16$	1.51	0.88	2A'→6A'	1.51	0.90	2A'→9A"	1.57	0.00
$3 \rightarrow 17$	1.56	0.00	$3 \rightarrow 17$	1.61	0.00	2A'→11A"	1.61	0.00	2A'→7A'	1.65	0.01
$3 \rightarrow 18$	1.58	0.00	$3 \rightarrow 18$	1.62	0.01	2A'→7A'	1.62	0.01	2A'→10A"	1.67	0.02
$3 \rightarrow 19$	1.66	0.10	$3 \rightarrow 19$	1.65	0.05	2A'→12A"	1.63	0.04	2A'→11A"	1.72	0.03
$3 \rightarrow 20$	1.68	0.15	$3 \rightarrow 20$	1.70	0.03	2A'→8A'	1.69	0.04	2A'→12A"	1.79	0.01
$3 \rightarrow 21$	1.79	0.07	$3 \rightarrow 21$	1.87	0.11	2A'→13A"	1.86	0.11	2A'→8A'	1.89	0.35
$3 \rightarrow 22$	1.85	0.02	$3 \rightarrow 22$	1.92	0.02	2A'→9A'	1.90	0.02	2A'→9A'	2.11	0.01
$3 \rightarrow 23$	2.13	0.33	$3 \rightarrow 23$	1.99	0.76	2A'→10A'	1.99	0.74	2A'→13A"	2.12	0.13
$3 \rightarrow 24$	2.18	0.06	$3 \rightarrow 24$	2.24	0.05	2A'→11A'	2.23	0.04	2A'→10A'	2.18	0.45
$3 \rightarrow 25$	2.20	0.33	$3 \rightarrow 25$	2.26	0.00	2A'→14A"	2.25	0.00	2A'→11A'	2.34	1.58
$3 \rightarrow 26$	2.22	0.16	$3 \rightarrow 26$	2.31	0.00	2A'→15A"	2.29	0.01	2A'→14A"	2.40	0.00
$3 \rightarrow 27$	2.26	1.13	$3 \rightarrow 27$	2.33	1.07	2A'→12A'	2.33	1.04	2A'→15A"	2.42	0.01
$3 \rightarrow 28$	2.29	0.01	$3 \rightarrow 28$	2.36	0.01	2A'→13A'	2.34	0.05	2A'→12A'	2.44	0.88
$3 \rightarrow 29$	2.31	0.01	$3 \rightarrow 29$	2.38	0.01	2A'→16A"	2.36	0.02	2A'→16A"	2.55	0.00
$3 \rightarrow 30$	2.32	0.45	$3 \rightarrow 30$	2.40	0.00	2A'→17A"	2.40	0.00	2A'→13A'	2.57	0.13
$3 \rightarrow 31$	2.37	0.09	$3 \rightarrow 31$	2.43	0.35	2A'→14A'	2.43	0.21	2A'→17A"	2.60	0.00
$3 \rightarrow 32$	2.40	0.26	$3 \rightarrow 32$	2.46	0.25	2A'→15A'	2.45	0.40	2A'→14A'	2.62	0.08
$3 \rightarrow 33$	2.43	0.04	$3 \rightarrow 33$	2.48	0.15	2A'→18A"	2.47	0.16	2A'→18A"	2.65	0.15
$3 \rightarrow 34$	2.45	0.19	$3 \rightarrow 34$	2.51	0.07	2A'→19A"	2.50	0.06	2A'→19A"	2.68	0.11
$3 \rightarrow 35$	2.50	0.01	$3 \rightarrow 35$	2.58	0.00	2A'→20A"	2.58	0.00	2A'→15A'	2.68	1.55
$3 \rightarrow 36$	2.55	0.06	$3 \rightarrow 36$	2.62	1.31	2A'→21A"	2.61	0.00	2A'→16A'	2.71	0.34
$3 \rightarrow 37$	2.58	0.12	$3 \rightarrow 37$	2.63	0.00	2A'→16A'	2.62	1.20	2A'→20A"	2.74	0.00
$3 \rightarrow 38$	2.60	0.21	$3 \rightarrow 38$	2.66	0.11	2A'→17A'	2.65	0.18	2A'→17A'	2.75	1.62
$3 \rightarrow 39$	2.66	0.06	$3 \rightarrow 39$	2.71	0.89	2A'→18A'	2.71	0.94	2A'→21A"	2.85	0.02
$3 \rightarrow 40$	2.67	0.41	$3 \rightarrow 40$	2.74	0.01	2A'→22A"	2.73	0.01	2A'→22A"	2.88	0.00
$3 \rightarrow 41$	2.73	0.06	$3 \rightarrow 41$	2.81	0.02	2A'→19A'	2.79	0.02	2A'→18A'	2.89	1.36
$3 \rightarrow 42$	2.75	0.01	$3 \rightarrow 42$	2.83	0.01	2A'→23A"	2.82	0.01	2A'→23A"	2.93	0.00
$3 \rightarrow 43$	2.79	0.01	$3 \rightarrow 43$	2.86	0.01	2A'→24A"	2.85	0.00	2A'→19A'	2.95	0.26
$3 \rightarrow 44$	2.82	0.02	$3 \rightarrow 44$	2.88	1.51	2A'→20A'	2.87	0.50	2A'→24A"	2.99	0.01
$3 \rightarrow 45$	2.87	1.56	$3 \rightarrow 45$	2.90	0.18	2A'→25A"	2.96	0.00	2A'→20A'	3.07	0.06
$3 \rightarrow 46$	2.91	0.00	$3 \rightarrow 46$	2.99	0.00				2A'→25A"	3.09	0.03

Table S18: Adenine. CCSD/aug-cc-pVDZ OPA and ESA transition energies (ω) and oscillator strengths (f).

OPA			ESA(S_1)			ESA(S_2)			ESA(S_3)		
Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$
$0 \to 1$	5.406	0.52	$1 \to 2$	0.103	0.00	$2 \to 3$	0.021	0.00	$3 \to 4$	0.026	0.00
$0 \to 2$	5.509	0.17	$1 \to 3$	0.124	0.04	$2 \to 4$	0.047	0.00	$3 \to 5$	0.380	0.27
$0 \to 3$	5.530	29.83	$1 \to 4$	0.149	0.00	$2 \to 5$	0.401	0.19	$3 \to 6$	0.572	0.00
$0 \to 4$	5.556	0.96	$1 \to 5$	0.503	0.04	$2 \to 6$	0.593	0.44	$3 \to 7$	0.851	0.26
$0 \to 5$	5.910	0.11	$1 \to 6$	0.695	0.01	$2 \to 7$	0.872	0.10	$3 \to 8$	0.990	0.00
$0 \to 6$	6.102	0.32	$1 \to 7$	0.975	0.04	$2 \to 8$	1.011	1.06	$3 \to 9$	1.060	0.01
$0 \to 7$	6.381	0.13	$1 \to 8$	1.114	0.00	$2 \to 9$	1.081	0.03	$3 \to 10$	1.088	0.05
$0 \to 8$	6.520	0.14	$1 \to 9$	1.184	0.07	$2 \to 10$	1.109	0.03	$3 \to 11$	1.123	1.88
$0 \to 9$	6.590	0.00	$1 \to 10$	1.211	0.02	$2 \to 11$	1.144	0.02	$3 \to 12$	1.174	3.14
$0 \to 10$	6.618	5.05	$1 \to 11$	1.247	0.41	$2 \to 12$	1.195	0.13	$3 \to 13$	1.220	0.01
$0 \to 11$	6.653	31.99	$1 \to 12$	1.298	0.68	$2 \to 13$	1.241	0.01	$3 \to 14$	1.279	0.02
$0 \to 12$	6.704	16.28	$1 \to 13$	1.344	0.00	$2 \to 14$	1.300	0.02	$3 \to 15$	1.522	0.09
$0 \to 13$	6.750	0.20	$1 \to 14$	1.403	0.00	$2 \to 15$	1.543	0.06	$3 \to 16$	1.545	3.49
$0 \to 14$	6.809	0.07	$1 \to 15$	1.645	0.03	$2 \to 16$	1.566	0.18	$3 \to 17$	1.564	1.26
$0 \to 15$	7.052	0.53	$1 \to 16$	1.668	0.40	$2 \to 17$	1.585	0.44	$3 \to 18$	1.647	0.00
$0 \to 16$	7.075	15.03	$1 \to 17$	1.688	0.25	$2 \to 18$	1.668	4.23	$3 \to 19$	1.652	5.23
$0 \to 17$	7.094	3.67	$1 \to 18$	1.770	0.00	$2 \to 19$	1.673	0.11	$3 \to 20$	1.706	0.01
$0 \to 18$	7.177	1.18	$1 \to 19$	1.775	0.00	$2 \to 20$	1.727	0.01	$3 \to 21$	1.750	0.29
$0 \to 19$	7.182	1.47	$1 \to 20$	1.829	0.11	$2 \to 21$	1.771	0.04	$3 \to 22$	1.813	0.00
$0 \to 20$	7.236	0.34	$1 \to 21$	1.873	0.11	$2 \to 22$	1.834	1.47	$3 \to 23$	2.065	0.20
$0 \to 21$	7.280	1.52	$1 \to 22$	1.936	0.01	$2 \to 23$	2.086	0.01	$3 \to 24$	2.092	0.00
$0 \to 22$	7.343	0.00	$1 \to 23$	2.189	0.59	$2 \to 24$	2.113	0.04	$3 \to 25$	2.110	0.42
$0 \to 23$	7.595	28.61	$1 \to 24$	2.215	0.00	$2 \to 25$	2.131	0.00	$3 \to 26$	2.162	0.80
$0 \to 24$	7.622	0.17	$1 \to 25$	2.233	0.04	$2 \to 26$	2.183	0.01	$3 \to 27$	2.201	0.15
$0 \to 25$	7.640	3.13	$1 \to 26$	2.286	0.04	$2 \to 27$	2.222	0.00	$3 \to 28$	2.205	0.19
$0 \to 26$	7.692	0.10	$1 \to 27$	2.324	0.16	$2 \to 28$	2.226	0.13	$3 \to 29$	2.227	0.41
$0 \to 27$	7.731	2.73	$1 \to 28$	2.329	0.00	$2 \to 29$	2.248	0.00	$3 \to 30$	2.227	0.00
$0 \to 28$	7.735	0.07	$1 \to 29$	2.350	1.77	$2 \to 30$	2.248	2.00	$3 \to 31$	2.269	0.03
$0 \to 29$	7.756	2.88	$1 \to 30$	2.350	0.04	$2 \to 31$	2.290	0.04	$3 \to 32$	2.337	0.09
$0 \to 30$	7.757	0.27	$1 \to 31$	2.393	0.00	$2 \to 32$	2.358	0.04	$3 \to 33$	2.374	0.03
$0 \to 31$	7.799	0.00	$1 \to 32$	2.460	0.04	$2 \to 33$	2.395	0.04	$3 \to 34$	2.427	1.36
$0 \to 32$	7.867	0.14	$1 \to 33$	2.498	0.15	$2 \to 34$	2.448	0.00	$3 \to 35$	2.458	0.12
$0 \to 33$	7.904	0.10	$1 \to 34$	2.551	0.41	$2 \to 35$	2.479	0.03	$3 \to 36$	2.480	0.40
$0 \to 34$	7.957	1.58	$1 \to 35$	2.582	0.03	$2 \to 36$	2.501	0.00	$3 \to 37$	2.536	2.44
$0 \to 35$	7.988	0.48	$1 \to 36$	2.604	0.11	$2 \to 37$	2.557	0.00	$3 \to 38$	2.589	1.05
$0 \to 36$	8.010	1.13	$1 \to 37$	2.660	0.95	$2 \to 38$	2.610	0.00	$3 \to 39$	2.607	0.07
$0 \to 37$	8.066	1.43	$1 \to 38$	2.712	0.40	$2 \to 39$	2.628	0.06	$3 \to 40$	2.711	0.24
$0 \to 38$	8.119	0.24	$1 \to 39$	2.731	0.01	$2 \to 40$	2.732	0.08			
$0 \to 39$	8.137	0.02	$1 \to 40$	2.835	0.00						
$0 \to 40$	8.241	0.48									

Table S19: Adenine. CC3/aug-cc-pVDZ OPA and ESA transition energies (ω) and oscillator strengths (f).

OPA			ESA(S_1)			ESA(S_2)			ESA(S_3)		
Transit.	ω [eV]	$f \times 100$	Transit.	ω [eV]	$f \times 100$	Transit.	ω [eV]	$f \times 100$	Transit.	ω [eV]	$f \times 100$
$0 \rightarrow 1$	5.244	0.55	$1 \rightarrow 2$	0.040	0.00	$2 \rightarrow 3$	0.047	0.00	$3 \rightarrow 4$	0.130	0.00
$0 \rightarrow 2$	5.284	0.11	$1 \rightarrow 3$	0.086	0.04	$2 \rightarrow 4$	0.177	0.00	$3 \rightarrow 5$	0.481	0.32
$0 \rightarrow 3$	5.331	26.13	$1 \rightarrow 4$	0.216	0.01	$2 \rightarrow 5$	0.528	0.01	$3 \rightarrow 6$	0.559	0.01
$0 \rightarrow 4$	5.461	0.94	$1 \rightarrow 5$	0.567	0.00	$2 \rightarrow 6$	0.606	0.28	$3 \rightarrow 7$	0.944	0.00
$0 \rightarrow 5$	5.812	0.09	$1 \rightarrow 6$	0.645	0.01	$2 \rightarrow 7$	0.991	1.03	$3 \rightarrow 8$	0.980	0.17
$0 \rightarrow 6$	5.890	0.29	$1 \rightarrow 7$	1.030	0.00	$2 \rightarrow 8$	1.027	0.00	$3 \rightarrow 9$	1.086	0.03
$0 \rightarrow 7$	6.275	0.09	$1 \rightarrow 8$	1.066	0.10	$2 \rightarrow 9$	1.132	0.00	$3 \rightarrow 10$	1.088	0.11
$0 \rightarrow 8$	6.311	0.11	$1 \rightarrow 9$	1.172	0.70	$2 \rightarrow 10$	1.135	0.01	$3 \rightarrow 11$	1.177	0.05
$0 \rightarrow 9$	6.416	34.10	$1 \rightarrow 10$	1.174	0.13	$2 \rightarrow 11$	1.223	0.01	$3 \rightarrow 12$	1.177	5.99
$0 \rightarrow 10$	6.419	8.56	$1 \rightarrow 11$	1.263	0.04	$2 \rightarrow 12$	1.223	0.00	$3 \rightarrow 13$	1.328	0.01
$0 \rightarrow 11$	6.508	0.00	$1 \rightarrow 12$	1.263	0.42	$2 \rightarrow 13$	1.374	0.00	$3 \rightarrow 14$	1.396	0.03
$0 \rightarrow 12$	6.507	0.00	$1 \rightarrow 13$	1.414	0.00	$2 \rightarrow 14$	1.442	0.01	$3 \rightarrow 15$	1.472	1.80
$0 \rightarrow 13$	6.658	0.14	$1 \rightarrow 14$	1.482	0.00	$2 \rightarrow 15$	1.519	0.01	$3 \rightarrow 16$	1.533	0.10
$0 \rightarrow 14$	6.726	0.09	$1 \rightarrow 15$	1.558	1.38	$2 \rightarrow 16$	1.580	0.47	$3 \rightarrow 17$	1.568	1.35
$0 \rightarrow 15$	6.803	2.74	$1 \rightarrow 16$	1.619	0.23	$2 \rightarrow 17$	1.615	0.01	$3 \rightarrow 18$	1.612	0.01
$0 \rightarrow 16$	6.864	6.59	$1 \rightarrow 17$	1.655	0.03	$2 \rightarrow 18$	1.659	2.25	$3 \rightarrow 19$	1.665	0.06
$0 \rightarrow 17$	6.899	3.47	$1 \rightarrow 18$	1.698	0.01	$2 \rightarrow 19$	1.712	0.40	$3 \rightarrow 20$	1.699	0.00
$0 \rightarrow 18$	6.943	1.57	$1 \rightarrow 19$	1.751	0.05	$2 \rightarrow 20$	1.745	1.09			
$0 \rightarrow 19$	6.996	0.00	$1 \rightarrow 20$	1.785	0.01						
$0 \rightarrow 20$	7.029	0.00									

SS4.4 Guanine

Table S20: Guanine. CAM-B3LYP/aug-cc-pVDZ OPA excitation energies (ΔE, eV) and oscillator strengths (f), computed in the Tamm-Dancoff approximation (CIS), with TDDFT in gas phase, and TDDFT in non-equilibrium PCM (chloroform). First IP is 7.97 eV.

TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
0→1	5.05	0.27	0→1	5.05	0.26	0→1A"	5.04	0.25	0→1A' L_a	5.07	18.52
0→2	5.29	18.77	0→2 L_a	5.13	14.86	0→1A' L_a	5.13	14.85	0→1A"	5.38	0.12
0→3	5.45	0.47	0→3	5.45	0.46	0→2A"	5.44	0.46	0→2A' L_b	5.51	48.63
0→4	5.61	0.00	0→4 L_b	5.57	33.72	0→2A' L_b	5.57	33.70	0→2A" $n\pi^*$	5.82	0.08
0→5	5.74	39.85	0→5 $n\pi^*$	5.59	0.00	0→3A" $n\pi^*$	5.59	0.00	0→3A"	5.86	0.90
0→6	5.96	0.08	0→6	5.96	0.08	0→4A"	5.95	0.08	0→4A"	6.20	0.03
0→7	6.16	0.07	0→7	6.16	0.05	0→5A"	6.16	0.05	0→5A"	6.46	0.34
0→8	6.40	0.40	0→8	6.35	0.25	0→6A"	6.35	0.26	0→6A"	6.47	0.07
0→9	6.42	0.00	0→9	6.42	0.04	0→7A"	6.40	0.03	0→3A'	6.53	0.16
0→10	6.49	0.01	0→10	6.47	0.14	0→3A'	6.48	0.14	0→4A'	6.56	1.12
0→11	6.50	0.78	0→11	6.48	0.01	0→8A"	6.48	0.01	0→7A"	6.62	0.00
0→12	6.67	1.72	0→12	6.56	1.49	0→4A'	6.56	1.50	0→8A"	6.70	0.00
0→13	6.76	0.59	0→13	6.75	2.11	0→9A"	6.75	0.54	0→9A"	6.98	0.66
0→14	6.77	2.08	0→14	6.75	0.55	0→5A'	6.75	2.09	0→5A'	7.00	46.72
0→15	6.93	0.02	0→15	6.93	0.02	0→10A"	6.92	0.01	0→10A"	7.24	0.14
0→16	7.12	0.96	0→16	7.11	1.63	0→6A'	7.10	1.47	0→6A'	7.25	9.62
0→17	7.15	0.00	0→17	7.14	0.00	0→11A"	7.14	0.00	0→11A"	7.30	0.00
0→18	7.17	0.33	0→18	7.16	0.34	0→12A"	7.16	0.36	0→7A'	7.41	9.58
0→19	7.26	0.00	0→19	7.21	31.17	0→7A'	7.21	31.02	0→8A'	7.43	17.68
0→20	7.31	28.20	0→20	7.26	0.00	0→13A"	7.25	0.00	0→12A"	7.46	0.00
0→21	7.38	19.17	0→21	7.36	3.05	0→8A'	7.35	3.81	0→9A'	7.51	1.19
0→22	7.42	5.79	0→22	7.39	5.83	0→9A'	7.39	5.31	0→13A"	7.53	1.64
0→23	7.45	1.79	0→23	7.42	1.14	0→14A"	7.42	1.16	0→10A'	7.58	12.63
0→24	7.48	0.22	0→24	7.45	4.14	0→10A'	7.45	4.06	0→14A"	7.60	0.22
0→25	7.55	0.26	0→25	7.48	0.62	0→15A"	7.47	0.59	0→15A"	7.63	0.52
0→26	7.56	4.12	0→26	7.54	0.19	0→16A"	7.53	0.17	0→11A'	7.72	12.07
0→27	7.68	12.33	0→27	7.57	25.83	0→11A'	7.57	25.81	0→16A"	7.84	0.26
0→28	7.72	0.03	0→28	7.71	4.11	0→12A'	7.70	3.78	0→12A'	7.88	6.41
0→29	7.75	22.47	0→29	7.72	0.02	0→17A"	7.71	0.02	0→13A'	7.93	1.00
0→30	7.82	7.38	0→30	7.73	11.00	0→13A'	7.73	10.98	0→17A"	7.94	0.02
0→31	7.89	13.15	0→31	7.82	2.00	0→14A'	7.81	2.50	0→14A'	8.11	1.59
0→32	7.91	0.94	0→32	7.90	2.96	0→18A"	7.88	0.72	0→18A"	8.12	0.09
0→33	7.93	4.78	0→33	7.90	0.89	0→15A'	7.89	2.90	0→15A'	8.14	0.10
0→34	8.01	0.19	0→34	7.99	1.35	0→19A"	7.97	0.23	0→19A"	8.20	1.30
0→35	8.03	1.85	0→35	8.00	0.24	0→16A'	8.00	1.22	0→16A'	8.21	6.43
0→36	8.03	0.34	0→36	8.01	0.16	0→20A"	8.01	0.28	0→20A"	8.26	0.08
0→37	8.07	2.11	0→37	8.06	0.68	0→17A'	8.05	0.78	0→21A"	8.28	0.03
0→38	8.11	0.01	0→38	8.09	1.82	0→18A'	8.08	1.65	0→22A"	8.34	0.83
0→39	8.12	2.86	0→39	8.11	0.01	0→21A"	8.09	0.00	0→17A'	8.34	1.39
0→40	8.23	0.38	0→40	8.20	3.35	0→22A"	8.18	0.30	0→18A'	8.37	6.60
0→41	8.24	1.52	0→41	8.23	0.37	0→19A'	8.19	3.22	0→23A"	8.41	0.64
0→42	8.24	0.11	0→42	8.24	0.10	0→23A"	8.24	0.00	0→19A'	8.44	0.87
0→43	8.26	0.05	0→43	8.26	0.05	0→24A"	8.24	0.08	0→24A"	8.46	0.15
0→44	8.31	0.82	0→44	8.27	1.25	0→20A'	8.27	1.27	0→25A"	8.50	0.42
0→45	8.32	3.78	0→45	8.31	0.73	0→25A"	8.30	0.88	0→20A'	8.65	0.78
0→46	8.41	0.82	0→46	8.41	0.73						
0→47	8.44	0.11	0→47	8.44	0.08						
0→48	8.46	0.50	0→48	8.46	0.47						
0→49	8.51	0.75	0→49	8.49	0.24						
0→50	8.51	0.03	0→50	8.51	0.03						
0→51	8.52	0.00	0→51	8.52	0.00						
0→52	8.55	0.06	0→52	8.55	0.05						
0→53	8.60	0.01	0→53	8.59	3.81						
0→54	8.61	0.03	0→54	8.60	0.02						
0→55	8.61	1.08	0→55	8.60	3.11						
0→56	8.64	4.24	0→56	8.61	0.02						
0→57	8.68	4.57	0→57	8.66	3.69						

Table S21: Guanine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from $S_{3A''}$ ($n\pi^*$), computed in the Tamm-Dancoff approximation, TDDFT in gas phase and TDDFT in non-equilibrium PCM (chloroform). Estimated first IP is 2.38 eV. Note the different state number for the initial state at TDA and TDDFT level.

TDA (Turbomole)			TDDFT(Turbomole)			TDDFT(Dalton)			TDDFT/PCM(Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
4→5	0.13	0.00	5→6	0.37	0.00	3A"→4A"	0.36	0.00	3A"→4A"	0.34	0.59
4→6	0.35	0.00	5→7	0.57	0.04	3A"→5A"	0.57	0.04	3A"→5A"	0.60	26.96
4→7	0.55	0.03	5→8	0.76	0.08	3A"→6A"	0.76	0.07	3A"→6A"	0.61	3.67
4→8	0.79	0.08	5→9	0.83	0.04	3A"→7A"	0.81	0.03	3A"→3A'	0.67	0.00
4→9	0.81	0.03	5→10	0.89	0.00	3A"→3A'	0.89	0.00	3A"→4A'	0.71	2.75
4→10	0.88	0.06	5→11	0.89	0.07	3A"→8A"	0.89	0.08	3A"→7A"	0.76	18.04
4→11	0.89	0.00	5→12	0.97	0.00	3A"→4A'	0.98	0.00	3A"→8A"	0.84	0.07
4→12	1.06	0.01	5→13	1.16	0.03	3A"→9A"	1.16	0.02	3A"→9A"	1.12	1.30
4→13	1.15	0.02	5→14	1.17	0.02	3A"→5A'	1.16	0.04	3A"→5A'	1.15	0.00
4→14	1.16	0.03	5→15	1.34	0.01	3A"→10A"	1.33	0.01	3A"→10A"	1.39	0.24
4→15	1.32	0.01	5→16	1.52	0.02	3A"→6A'	1.52	0.02	3A"→6A'	1.39	0.10
4→16	1.51	0.03	5→17	1.55	0.27	3A"→11A"	1.55	0.40	3A"→11A"	1.45	7.15
4→17	1.54	0.26	5→18	1.57	0.01	3A"→12A"	1.57	0.04	3A"→7A'	1.56	0.77
4→18	1.56	0.02	5→19	1.63	0.00	3A"→7A'	1.63	0.00	3A"→8A'	1.58	5.03
4→19	1.65	0.00	5→20	1.67	0.00	3A"→13A"	1.66	0.00	3A"→12A"	1.60	0.16
4→20	1.70	0.00	5→21	1.77	0.03	3A"→8A'	1.76	0.02	3A"→9A'	1.65	0.08
4→21	1.77	0.02	5→22	1.80	0.01	3A"→9A'	1.80	0.01	3A"→13A"	1.67	0.02
4→22	1.81	0.01	5→23	1.83	0.11	3A"→14A"	1.83	0.10	3A"→10A'	1.73	15.56
4→23	1.84	0.11	5→24	1.86	0.00	3A"→10A'	1.86	0.00	3A"→14A"	1.75	0.05
4→24	1.87	0.01	5→25	1.89	0.00	3A"→15A"	1.88	0.00	3A"→15A"	1.78	0.20
4→25	1.94	0.00	5→26	1.95	0.00	3A"→16A"	1.95	0.00	3A"→11A'	1.86	0.00
4→26	1.94	0.00	5→27	1.98	0.01	3A"→11A'	1.98	0.01	3A"→16A"	1.99	1.31
4→27	2.07	0.05	5→28	2.12	0.03	3A"→12A'	2.11	0.03	3A"→12A'	2.02	0.10
4→28	2.11	0.03	5→29	2.13	0.03	3A"→17A"	2.12	0.03	3A"→13A'	2.07	0.35
4→29	2.14	0.00	5→30	2.14	0.00	3A"→13A'	2.14	0.00	3A"→17A"	2.08	2.77
4→30	2.21	0.09	5→31	2.23	0.14	3A"→14A'	2.22	0.14	3A"→14A'	2.25	0.04
4→31	2.28	0.06	5→32	2.31	0.03	3A"→18A"	2.30	0.02	3A"→18A"	2.26	0.00
4→32	2.30	0.01	5→33	2.31	0.01	3A"→15A'	2.30	0.02	3A"→15A'	2.28	0.00
4→33	2.32	0.00	5→34	2.40	0.00	3A"→19A"	2.39	0.01	3A"→19A"	2.34	2.02
4→34	2.39	0.01	5→35	2.41	0.00	3A"→16A'	2.41	0.00	3A"→16A'	2.35	0.04
4→35	2.41	0.00	5→36	2.43	0.06	3A"→20A"	2.42	0.04	3A"→20A"	2.40	2.90
4→36	2.41	0.05	5→37	2.47	0.00	3A"→17A'	2.47	0.01	3A"→21A"	2.42	0.86
4→37	2.46	0.01	5→38	2.50	0.00	3A"→18A'	2.50	0.00	3A"→22A"	2.48	1.01
4→38	2.50	0.00	5→39	2.52	0.00	3A"→21A"	2.50	0.00	3A"→17A'	2.49	0.00
4→39	2.51	0.00	5→40	2.61	0.01	3A"→22A"	2.59	0.05	3A"→18A'	2.51	0.04
4→40	2.62	0.18	5→41	2.64	0.17	3A"→19A'	2.60	0.02	3A"→23A"	2.55	1.42
4→41	2.63	0.03	5→42	2.65	0.63	3A"→23A"	2.65	0.46	3A"→19A'	2.58	0.00
4→42	2.63	0.61	5→43	2.67	0.00	3A"→24A"	2.66	0.28	3A"→24A"	2.61	5.90
4→43	2.65	0.00	5→44	2.68	0.02	3A"→20A'	2.68	0.03	3A"→25A"	2.64	0.02
4→44	2.70	0.00	5→45	2.72	0.00	3A"→25A"	2.71	0.00	3A"→20A'	2.79	0.03
4→45	2.71	0.00	5→46	2.82	0.00						
4→46	2.80	0.00	5→47	2.85	0.04						
4→47	2.83	0.05	5→48	2.87	0.13						
4→48	2.85	0.14	5→49	2.90	0.00						
4→49	2.90	0.00	5→50	2.92	0.09						
4→50	2.90	0.10	5→51	2.93	3.21						
4→51	2.91	3.15	5→52	2.96	0.01						
4→52	2.94	0.01	5→53	3.00	0.00						
4→53	2.99	0.04	5→54	3.01	0.02						
4→54	3.00	0.00	5→55	3.01	0.03						
4→55	3.00	0.00	5→56	3.02	0.01						
4→56	3.03	0.04	5→57	3.08	0.03						
4→57	3.07	0.01	5→58	3.11	0.00						
4→58	3.14	0.26	5→59	3.15	0.26						
4→59	3.14	0.00	5→60	3.17	0.02						
4→60	3.15	0.02									

Table S22: Guanine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from $S_{1A'}$ (L_a), computed using the Tamm-Dancoff approximation (CIS), TDDFT in gas phase, TDDFT with non-equilibrium PCM (chloroform). Estimated first IP is 2.84 eV.

TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT/PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
$2 \rightarrow 3$	0.16	0.02	$2 \rightarrow 3$	0.32	0.03	1A'→2A"	0.31	0.03	1A'→1A"	0.31	0.00
$2 \rightarrow 4$	0.32	0.00	$2 \rightarrow 4$	0.44	0.48	1A'→2A'	0.44	0.48	1A'→2A'	0.44	0.57
$2 \rightarrow 5$	0.45	0.47	$2 \rightarrow 5$	0.46	0.00	1A'→3A"	0.46	0.00	1A'→2A"	0.74	0.02
$2 \rightarrow 6$	0.67	0.00	$2 \rightarrow 6$	0.83	0.00	1A'→4A"	0.82	0.00	1A'→3A"	0.79	0.22
$2 \rightarrow 7$	0.87	0.00	$2 \rightarrow 7$	1.03	0.00	1A'→5A"	1.03	0.00	1A'→4A"	1.12	0.01
$2 \rightarrow 8$	1.10	0.00	$2 \rightarrow 8$	1.22	0.00	1A'→6A"	1.22	0.00	1A'→5A"	1.39	0.02
$2 \rightarrow 9$	1.13	0.01	$2 \rightarrow 9$	1.29	0.01	1A'→7A"	1.27	0.01	1A'→6A"	1.40	0.01
$2 \rightarrow 10$	1.20	0.01	$2 \rightarrow 10$	1.34	0.72	1A'→3A'	1.35	0.73	1A'→3A'	1.46	0.10
$2 \rightarrow 11$	1.21	0.61	$2 \rightarrow 11$	1.35	0.01	1A'→8A"	1.35	0.01	1A'→4A'	1.49	0.78
$2 \rightarrow 12$	1.38	0.44	$2 \rightarrow 12$	1.43	0.38	1A'→4A'	1.43	0.36	1A'→7A"	1.54	0.03
$2 \rightarrow 13$	1.47	0.03	$2 \rightarrow 13$	1.62	0.45	1A'→9A"	1.62	0.03	1A'→8A"	1.63	0.02
$2 \rightarrow 14$	1.48	0.97	$2 \rightarrow 14$	1.62	0.03	1A'→5A'	1.62	0.48	1A'→9A"	1.91	0.17
$2 \rightarrow 15$	1.64	0.03	$2 \rightarrow 15$	1.80	0.03	1A'→10A"	1.79	0.03	1A'→5A'	1.93	0.06
$2 \rightarrow 16$	1.83	0.05	$2 \rightarrow 16$	1.98	0.03	1A'→6A'	1.97	0.03	1A'→10A"	2.17	0.00
$2 \rightarrow 17$	1.86	0.01	$2 \rightarrow 17$	2.01	0.00	1A'→11A"	2.01	0.00	1A'→6A'	2.17	1.42
$2 \rightarrow 18$	1.87	0.00	$2 \rightarrow 18$	2.03	0.00	1A'→12A"	2.03	0.00	1A'→11A"	2.23	0.00
$2 \rightarrow 19$	1.97	0.00	$2 \rightarrow 19$	2.08	0.09	1A'→7A'	2.08	0.08	1A'→7A'	2.34	1.51
$2 \rightarrow 20$	2.01	0.08	$2 \rightarrow 20$	2.13	0.00	1A'→13A"	2.12	0.00	1A'→8A'	2.36	1.37
$2 \rightarrow 21$	2.09	0.01	$2 \rightarrow 21$	2.23	0.02	1A'→8A'	2.22	0.02	1A'→12A"	2.39	0.02
$2 \rightarrow 22$	2.13	0.10	$2 \rightarrow 22$	2.26	0.14	1A'→9A'	2.26	0.17	1A'→9A'	2.44	0.22
$2 \rightarrow 23$	2.16	0.01	$2 \rightarrow 23$	2.29	0.00	1A'→14A"	2.29	0.00	1A'→13A"	2.46	0.00
$2 \rightarrow 24$	2.19	0.03	$2 \rightarrow 24$	2.32	2.46	1A'→10A'	2.32	2.24	1A'→10A'	2.51	0.10
$2 \rightarrow 25$	2.25	0.00	$2 \rightarrow 25$	2.35	0.02	1A'→15A"	2.34	0.02	1A'→14A"	2.53	0.00
$2 \rightarrow 26$	2.26	2.35	$2 \rightarrow 26$	2.41	0.00	1A'→16A"	2.40	0.00	1A'→15A"	2.56	0.01
$2 \rightarrow 27$	2.39	0.21	$2 \rightarrow 27$	2.44	0.20	1A'→11A'	2.44	0.17	1A'→11A'	2.65	0.10
$2 \rightarrow 28$	2.43	0.20	$2 \rightarrow 28$	2.58	0.11	1A'→12A'	2.57	0.13	1A'→16A"	2.77	0.16
$2 \rightarrow 29$	2.45	0.53	$2 \rightarrow 29$	2.59	0.18	1A'→17A"	2.58	0.19	1A'→12A'	2.81	0.09
$2 \rightarrow 30$	2.53	0.07	$2 \rightarrow 30$	2.60	0.06	1A'→13A'	2.60	0.05	1A'→13A'	2.86	0.16
$2 \rightarrow 31$	2.60	0.10	$2 \rightarrow 31$	2.69	0.14	1A'→14A'	2.68	0.13	1A'→17A"	2.87	0.01
$2 \rightarrow 32$	2.61	0.00	$2 \rightarrow 32$	2.77	0.12	1A'→18A"	2.76	0.00	1A'→14A'	3.04	6.17
$2 \rightarrow 33$	2.64	0.10	$2 \rightarrow 33$	2.77	0.00	1A'→15A'	2.76	0.08	1A'→18A"	3.05	0.01
$2 \rightarrow 34$	2.71	0.08	$2 \rightarrow 34$	2.86	1.60	1A'→19A"	2.84	0.06	1A'→15A'	3.07	0.05
$2 \rightarrow 35$	2.73	1.03	$2 \rightarrow 35$	2.87	0.04	1A'→16A'	2.87	1.48	1A'→19A"	3.13	0.00
$2 \rightarrow 36$	2.73	0.02	$2 \rightarrow 36$	2.88	0.03	1A'→20A"	2.88	0.01	1A'→16A'	3.14	1.55
$2 \rightarrow 37$	2.78	0.00	$2 \rightarrow 37$	2.93	0.06	1A'→17A'	2.93	0.05	1A'→20A"	3.18	0.03
$2 \rightarrow 38$	2.82	0.00	$2 \rightarrow 38$	2.96	1.32	1A'→18A'	2.96	0.95	1A'→21A"	3.21	0.00
$2 \rightarrow 39$	2.83	0.51	$2 \rightarrow 39$	2.98	0.00	1A'→21A"	2.96	0.00	1A'→22A"	3.27	0.01
$2 \rightarrow 40$	2.94	0.04	$2 \rightarrow 40$	3.07	2.36	1A'→22A"	3.05	0.01	1A'→17A'	3.27	4.37
$2 \rightarrow 41$	2.95	1.25	$2 \rightarrow 41$	3.10	0.03	1A'→19A'	3.06	2.21	1A'→18A'	3.30	2.82
$2 \rightarrow 42$	2.95	0.14	$2 \rightarrow 42$	3.11	0.09	1A'→23A"	3.11	0.10	1A'→23A"	3.34	0.01
$2 \rightarrow 43$	2.97	0.01	$2 \rightarrow 43$	3.13	0.01	1A'→24A"	3.12	0.02	1A'→19A'	3.37	0.18
$2 \rightarrow 44$	3.02	0.00	$2 \rightarrow 44$	3.14	0.94	1A'→20A'	3.14	0.89	1A'→24A"	3.39	0.02
$2 \rightarrow 45$	3.03	2.56	$2 \rightarrow 45$	3.18	0.00	1A'→25A"	3.17	0.00	1A'→25A"	3.42	0.05
$2 \rightarrow 46$	3.12	0.04	$2 \rightarrow 46$	3.28	0.02				1A'→20A'	3.58	0.26
$2 \rightarrow 47$	3.15	0.02	$2 \rightarrow 47$	3.31	0.01						
$2 \rightarrow 48$	3.17	0.02	$2 \rightarrow 48$	3.33	0.01						
$2 \rightarrow 49$	3.21	1.03	$2 \rightarrow 49$	3.36	1.58						
$2 \rightarrow 50$	3.22	0.00	$2 \rightarrow 50$	3.38	0.00						
$2 \rightarrow 51$	3.23	0.00	$2 \rightarrow 51$	3.39	0.00						
$2 \rightarrow 52$	3.26	0.01	$2 \rightarrow 52$	3.42	0.01						
$2 \rightarrow 53$	3.31	0.06	$2 \rightarrow 53$	3.46	2.83						
$2 \rightarrow 54$	3.31	0.00	$2 \rightarrow 54$	3.47	0.18						
$2 \rightarrow 55$	3.32	2.39	$2 \rightarrow 55$	3.47	0.19						
$2 \rightarrow 56$	3.35	0.13	$2 \rightarrow 56$	3.48	0.00						
$2 \rightarrow 57$	3.39	0.01	$2 \rightarrow 57$	3.53	0.05						
$2 \rightarrow 58$	3.45	0.00	$2 \rightarrow 58$	3.57	2.71						
$2 \rightarrow 59$	3.45	2.51	$2 \rightarrow 59$	3.61	0.00						
$2 \rightarrow 60$	3.47	0.21	$2 \rightarrow 60$	3.63	0.18						

Table S23: Guanine. CAM-B3LYP/aug-cc-pVDZ ESA transition energies (ΔE, eV) and oscillator strengths (f) from $S_{2A'}$ (L_b), computed with Tamm-Dancoff approximation (CIS), TDDFT and TDDFT in non-equilibrium PCM (chloroform). Estimated first IP is 2.4 eV.

TDA (Turbomole)			TDDFT (Turbomole)			TDDFT (Dalton)			TDDFT/PCM (Dalton)		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
$4 \rightarrow 5$	0.13	0.00	$4 \rightarrow 5$	0.02	0.00	2A'→3A"	0.02	0.00	2A'→2A"	0.31	0.00
$4 \rightarrow 6$	0.35	0.00	$4 \rightarrow 6$	0.39	0.00	2A'→4A"	0.38	0.00	2A'→3A"	0.35	0.07
$4 \rightarrow 7$	0.55	0.03	$4 \rightarrow 7$	0.59	0.08	2A'→5A"	0.59	0.08	2A'→4A"	0.69	0.01
$4 \rightarrow 8$	0.79	0.08	$4 \rightarrow 8$	0.78	0.01	2A'→6A"	0.78	0.02	2A'→5A"	0.95	0.03
$4 \rightarrow 9$	0.81	0.03	$4 \rightarrow 9$	0.85	0.54	2A'→7A"	0.83	0.53	2A'→6A"	0.96	0.00
$4 \rightarrow 10$	0.88	0.06	$4 \rightarrow 10$	0.91	0.83	2A'→3A'	0.91	0.82	2A'→3A'	1.02	4.90
$4 \rightarrow 11$	0.89	0.00	$4 \rightarrow 11$	0.91	0.00	2A'→8A"	0.91	0.00	2A'→4A'	1.05	4.48
$4 \rightarrow 12$	1.06	0.01	$4 \rightarrow 12$	0.99	7.09	2A'→4A'	0.99	6.98	2A'→7A"	1.11	0.22
$4 \rightarrow 13$	1.15	0.02	$4 \rightarrow 13$	1.18	0.02	2A'→9A"	1.18	0.04	2A'→8A"	1.19	0.00
$4 \rightarrow 14$	1.16	0.03	$4 \rightarrow 14$	1.19	0.04	2A'→5A'	1.18	0.02	2A'→9A"	1.47	0.46
$4 \rightarrow 15$	1.32	0.01	$4 \rightarrow 15$	1.36	0.01	2A'→10A"	1.35	0.01	2A'→5A'	1.49	0.58
$4 \rightarrow 16$	1.51	0.03	$4 \rightarrow 16$	1.54	0.16	2A'→6A'	1.53	0.16	2A'→10A"	1.73	0.29
$4 \rightarrow 17$	1.54	0.26	$4 \rightarrow 17$	1.57	0.00	2A'→11A"	1.57	0.00	2A'→6A'	1.74	0.27
$4 \rightarrow 18$	1.56	0.02	$4 \rightarrow 18$	1.60	0.04	2A'→12A"	1.59	0.04	2A'→11A"	1.79	0.08
$4 \rightarrow 19$	1.65	0.00	$4 \rightarrow 19$	1.65	0.83	2A'→7A'	1.64	0.83	2A'→7A'	1.90	0.64
$4 \rightarrow 20$	1.70	0.00	$4 \rightarrow 20$	1.69	0.35	2A'→13A"	1.68	0.32	2A'→8A'	1.92	0.49
$4 \rightarrow 21$	1.77	0.02	$4 \rightarrow 21$	1.79	0.29	2A'→8A'	1.78	0.19	2A'→12A"	1.95	0.01
$4 \rightarrow 22$	1.81	0.01	$4 \rightarrow 22$	1.82	1.82	2A'→9A'	1.82	2.07	2A'→9A'	2.00	0.38
$4 \rightarrow 23$	1.84	0.11	$4 \rightarrow 23$	1.85	0.00	2A'→14A"	1.85	0.00	2A'→13A"	2.02	0.00
$4 \rightarrow 24$	1.87	0.01	$4 \rightarrow 24$	1.88	0.77	2A'→10A'	1.88	0.78	2A'→10A'	2.07	1.10
$4 \rightarrow 25$	1.94	0.00	$4 \rightarrow 25$	1.91	0.15	2A'→15A"	1.90	0.17	2A'→14A"	2.09	0.00
$4 \rightarrow 26$	1.94	0.00	$4 \rightarrow 26$	1.97	0.01	2A'→16A"	1.96	0.01	2A'→15A"	2.13	0.02
$4 \rightarrow 27$	2.07	0.05	$4 \rightarrow 27$	2.00	0.12	2A'→11A'	2.00	0.12	2A'→11A'	2.21	5.93
$4 \rightarrow 28$	2.11	0.03	$4 \rightarrow 28$	2.14	0.28	2A'→12A'	2.13	0.16	2A'→16A"	2.33	0.24
$4 \rightarrow 29$	2.14	0.00	$4 \rightarrow 29$	2.15	0.32	2A'→17A"	2.14	0.34	2A'→12A'	2.37	0.49
$4 \rightarrow 30$	2.21	0.09	$4 \rightarrow 30$	2.16	1.82	2A'→13A'	2.16	1.68	2A'→13A'	2.42	1.01
$4 \rightarrow 31$	2.28	0.06	$4 \rightarrow 31$	2.25	0.30	2A'→14A'	2.24	0.34	2A'→17A"	2.43	0.05
$4 \rightarrow 32$	2.30	0.01	$4 \rightarrow 32$	2.33	0.19	2A'→18A"	2.32	0.04	2A'→14A'	2.60	0.35
$4 \rightarrow 33$	2.32	0.00	$4 \rightarrow 33$	2.33	0.02	2A'→15A'	2.32	0.16	2A'→18A"	2.61	0.00
$4 \rightarrow 34$	2.39	0.01	$4 \rightarrow 34$	2.43	0.71	2A'→19A"	2.40	0.26	2A'→15A'	2.63	0.00
$4 \rightarrow 35$	2.41	0.00	$4 \rightarrow 35$	2.43	0.22	2A'→16A'	2.43	0.58	2A'→19A"	2.69	0.04
$4 \rightarrow 36$	2.41	0.05	$4 \rightarrow 36$	2.45	0.05	2A'→20A"	2.44	0.00	2A'→16A'	2.70	0.34
$4 \rightarrow 37$	2.46	0.01	$4 \rightarrow 37$	2.49	0.05	2A'→17A'	2.49	0.06	2A'→20A"	2.75	0.16
$4 \rightarrow 38$	2.50	0.00	$4 \rightarrow 38$	2.52	0.50	2A'→18A'	2.52	0.37	2A'→21A"	2.77	0.00
$4 \rightarrow 39$	2.51	0.00	$4 \rightarrow 39$	2.54	0.04	2A'→21A"	2.52	0.05	2A'→22A"	2.83	0.00
$4 \rightarrow 40$	2.62	0.18	$4 \rightarrow 40$	2.63	0.41	2A'→22A"	2.61	0.16	2A'→17A'	2.83	3.53
$4 \rightarrow 41$	2.63	0.03	$4 \rightarrow 41$	2.66	0.22	2A'→19A'	2.62	0.42	2A'→18A'	2.86	2.84
$4 \rightarrow 42$	2.63	0.61	$4 \rightarrow 42$	2.67	0.00	2A'→23A"	2.67	0.01	2A'→23A"	2.90	0.00
$4 \rightarrow 43$	2.65	0.00	$4 \rightarrow 43$	2.69	0.01	2A'→24A"	2.68	0.00	2A'→19A'	2.93	0.67
$4 \rightarrow 44$	2.70	0.00	$4 \rightarrow 44$	2.71	0.05	2A'→20A'	2.70	0.05	2A'→24A"	2.95	0.12
$4 \rightarrow 45$	2.71	0.00	$4 \rightarrow 45$	2.74	0.01	2A'→25A"	2.73	0.01	2A'→25A"	2.99	0.00
$4 \rightarrow 46$	2.80	0.00	$4 \rightarrow 46$	2.84	0.03				2A'→20A'	3.14	0.01
$4 \rightarrow 47$	2.83	0.05	$4 \rightarrow 47$	2.87	0.03						
$4 \rightarrow 48$	2.85	0.14	$4 \rightarrow 48$	2.89	0.05						
$4 \rightarrow 49$	2.90	0.00	$4 \rightarrow 49$	2.92	1.94						
$4 \rightarrow 50$	2.90	0.10	$4 \rightarrow 50$	2.94	0.00						
$4 \rightarrow 51$	2.91	3.15	$4 \rightarrow 51$	2.95	0.00						
$4 \rightarrow 52$	2.94	0.01	$4 \rightarrow 52$	2.98	0.00						
$4 \rightarrow 53$	2.99	0.04	$4 \rightarrow 53$	3.02	1.42						
$4 \rightarrow 54$	3.00	0.00	$4 \rightarrow 54$	3.03	0.04						
$4 \rightarrow 55$	3.00	0.00	$4 \rightarrow 55$	3.03	1.75						
$4 \rightarrow 56$	3.03	0.04	$4 \rightarrow 56$	3.04	0.14						
$4 \rightarrow 57$	3.07	0.01	$4 \rightarrow 57$	3.10	0.33						
$4 \rightarrow 58$	3.14	0.26	$4 \rightarrow 58$	3.13	2.70						
$4 \rightarrow 59$	3.14	0.00	$4 \rightarrow 59$	3.17	0.01						
$4 \rightarrow 60$	3.15	0.02	$4 \rightarrow 60$	3.19	0.33						

Table S24: Guanine. CC3/aug-cc-pVDZ ESA transition energies (ω) and oscillator strengths (f)

Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$
$0 \rightarrow 1$	4.814	0.30	$2 \rightarrow 3$	0.241	0.03	$4 \rightarrow 5$	0.100	0.00	$5 \rightarrow 6$	0.151	0.00
$0 \rightarrow 2$	5.027 L_a	13.43	$2 \rightarrow 4$	0.485	0.59	$4 \rightarrow 6$	0.251	0.00	$5 \rightarrow 7$	0.357	0.00
$0 \rightarrow 3$	5.268	0.43	$2 \rightarrow 5$	0.585	0.00	$4 \rightarrow 7$	0.456	0.12	$5 \rightarrow 8$	0.640	0.00
$0 \rightarrow 4$	5.512 L_b	30.42	$2 \rightarrow 6$	0.736	0.00	$4 \rightarrow 8$	0.739	0.51	$5 \rightarrow 9$	0.645	0.01
$0 \rightarrow 5$	5.612 $n\pi^*$	0.00	$2 \rightarrow 7$	0.942	0.00	$4 \rightarrow 9$	0.745	0.52	$5 \rightarrow 10$	0.768	0.00
$0 \rightarrow 6$	5.763	0.08	$2 \rightarrow 8$	1.225	0.64	$4 \rightarrow 10$	0.868	5.98	$5 \rightarrow 11$	0.804	0.03
$0 \rightarrow 7$	5.968	0.08	$2 \rightarrow 9$	1.230	0.03	$4 \rightarrow 11$	0.903	0.00	$5 \rightarrow 12$	0.853	0.02
$0 \rightarrow 8$	6.252	0.38	$2 \rightarrow 10$	1.353	0.20	$4 \rightarrow 12$	0.952	0.72	$5 \rightarrow 13$	0.895	0.14
$0 \rightarrow 9$	6.257	0.04	$2 \rightarrow 11$	1.389	0.01	$4 \rightarrow 13$	0.995	0.00	$5 \rightarrow 14$	0.967	0.00
$0 \rightarrow 10$	6.380	2.13	$2 \rightarrow 12$	1.438	0.70	$4 \rightarrow 14$	1.066	0.03	$5 \rightarrow 15$	1.066	0.24
$0 \rightarrow 11$	6.415	0.09	$2 \rightarrow 13$	1.480	0.01	$4 \rightarrow 15$	1.165	0.00	$5 \rightarrow 16$	1.110	0.00
$0 \rightarrow 12$	6.464	1.12	$2 \rightarrow 14$	1.552	0.04	$4 \rightarrow 16$	1.210	0.01			
$0 \rightarrow 13$	6.507	0.12	$2 \rightarrow 15$	1.651	0.00						
$0 \rightarrow 14$	6.579	0.53	$2 \rightarrow 16$	1.695	0.03						
$0 \rightarrow 15$	6.678	0.00									
$0 \rightarrow 16$	6.722	0.03									

Table S25: Guanine: CCSD/aug-cc-pVDZ ESA transition energies (ω) and oscillator strengths (f)

Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$	Trans.	ω [eV]	$f \times 100$
$0 \rightarrow 1$	4.965	0.30	$2 \rightarrow 3$	0.174	0.02	$4 \rightarrow 5$	0.005	0.00	$5 \rightarrow 6$	0.140	0.01
$0 \rightarrow 2$	5.214 L_a	16.62	$2 \rightarrow 4$	0.533	0.00	$4 \rightarrow 6$	0.145	0.00	$5 \rightarrow 7$	0.318	0.16
$0 \rightarrow 3$	5.388	0.54	$2 \rightarrow 5$	0.537	0.74	$4 \rightarrow 7$	0.323	0.00	$5 \rightarrow 8$	0.606	0.56
$0 \rightarrow 4$	5.747 $n\pi^*$	0.00	$2 \rightarrow 6$	0.677	0.00	$4 \rightarrow 8$	0.610	0.01	$5 \rightarrow 9$	0.610	0.39
$0 \rightarrow 5$	5.751 L_b	34.83	$2 \rightarrow 7$	0.855	0.00	$4 \rightarrow 9$	0.615	0.00	$5 \rightarrow 10$	0.903	9.34
$0 \rightarrow 6$	5.892	0.07	$2 \rightarrow 8$	1.143	0.02	$4 \rightarrow 10$	0.908	0.00	$5 \rightarrow 11$	0.903	0.00
$0 \rightarrow 7$	6.070	0.08	$2 \rightarrow 9$	1.147	0.60	$4 \rightarrow 11$	0.908	0.02	$5 \rightarrow 12$	0.965	0.07
$0 \rightarrow 8$	6.357	0.03	$2 \rightarrow 10$	1.440	0.40	$4 \rightarrow 12$	0.969	0.01	$5 \rightarrow 13$	1.025	0.00
$0 \rightarrow 9$	6.362	2.35	$2 \rightarrow 11$	1.441	0.01	$4 \rightarrow 13$	1.030	0.11	$5 \rightarrow 14$	1.047	0.48
$0 \rightarrow 10$	6.655	3.00	$2 \rightarrow 12$	1.502	0.06	$4 \rightarrow 14$	1.051	0.04	$5 \rightarrow 15$	1.140	0.01
$0 \rightarrow 11$	6.655	0.24	$2 \rightarrow 13$	1.562	0.02	$4 \rightarrow 15$	1.145	0.00	$5 \rightarrow 16$	1.239	0.03
$0 \rightarrow 12$	6.716	0.48	$2 \rightarrow 14$	1.584	0.66	$4 \rightarrow 16$	1.243	0.00	$5 \rightarrow 17$	1.261	0.52
$0 \rightarrow 13$	6.777	0.17	$2 \rightarrow 15$	1.677	0.03	$4 \rightarrow 17$	1.265	0.03	$5 \rightarrow 18$	1.413	0.36
$0 \rightarrow 14$	6.798	1.61	$2 \rightarrow 16$	1.776	0.02	$4 \rightarrow 18$	1.418	0.01	$5 \rightarrow 19$	1.547	0.83
$0 \rightarrow 15$	6.891	0.01	$2 \rightarrow 17$	1.798	0.02	$4 \rightarrow 19$	1.551	0.00	$5 \rightarrow 20$	1.571	2.84
$0 \rightarrow 16$	6.990	0.39	$2 \rightarrow 18$	1.950	0.02	$4 \rightarrow 20$	1.576	0.00	$5 \rightarrow 21$	1.636	0.36
$0 \rightarrow 17$	7.012	0.31	$2 \rightarrow 19$	2.084	0.27	$4 \rightarrow 21$	1.640	0.03	$5 \rightarrow 22$	1.638	0.54
$0 \rightarrow 18$	7.164	0.02	$2 \rightarrow 20$	2.108	0.30	$4 \rightarrow 22$	1.643	0.00	$5 \rightarrow 23$	1.685	0.02
$0 \rightarrow 19$	7.298	7.00	$2 \rightarrow 21$	2.173	0.04	$4 \rightarrow 23$	1.689	0.04	$5 \rightarrow 24$	1.726	0.00
$0 \rightarrow 20$	7.323	11.94	$2 \rightarrow 22$	2.175	0.07	$4 \rightarrow 24$	1.731	0.21	$5 \rightarrow 25$	1.844	0.75
$0 \rightarrow 21$	7.387	1.07	$2 \rightarrow 23$	2.222	0.00	$4 \rightarrow 25$	1.849	0.01	$5 \rightarrow 26$	1.882	1.42
$0 \rightarrow 22$	7.390	27.96	$2 \rightarrow 24$	2.264	0.01	$4 \rightarrow 26$	1.887	0.03	$5 \rightarrow 27$	1.884	0.34
$0 \rightarrow 23$	7.436	0.00	$2 \rightarrow 25$	2.382	3.22	$4 \rightarrow 27$	1.889	0.01	$5 \rightarrow 28$	1.942	0.00
$0 \rightarrow 24$	7.478	0.10	$2 \rightarrow 26$	2.419	2.04	$4 \rightarrow 28$	1.946	0.10	$5 \rightarrow 29$	1.955	0.35
$0 \rightarrow 25$	7.596	22.48	$2 \rightarrow 27$	2.421	0.17	$4 \rightarrow 29$	1.960	0.07	$5 \rightarrow 30$	2.023	0.22
$0 \rightarrow 26$	7.633	10.03	$2 \rightarrow 28$	2.479	0.01	$4 \rightarrow 30$	2.027	0.01			
$0 \rightarrow 27$	7.635	0.00	$2 \rightarrow 29$	2.492	0.10						
$0 \rightarrow 28$	7.693	1.00	$2 \rightarrow 30$	2.560	0.25						
$0 \rightarrow 29$	7.707	12.76									
$0 \rightarrow 30$	7.774	1.47									

Table S26: Guanine. CAM-B3LYP/aug-cc-pVDZ and CAM-B3LYP/6-31G* ESA transition energies (ΔE, eV) and oscillator strengths (f) from $S_{1A'}$ (L_a) and $S_{1A''}$ ($n\pi^*$) : (section 1) $S_{1A'}$ (L_a) at CAM-B3LYP/aug-cc-pVDZ; (section 2) $S_{1A'}$ (L_a) at CAM-B3LYP/6-31G*; (section 3) $S_{1A"}$ ($n\pi^*$) at CAM-B3LYP/aug-cc-pVDZ, (section 4) $S_{1A"}$ ($n\pi^*$) at CAM-B3LYP/6-31G*

$S_{1A'}$ (L_a) aDZ			$S_{1A'}$ (L_a) 6-31G*			$S_{1A"}$ ($n\pi^*$) aDZ			$S_{1A"}$ ($n\pi^*$) 6-31G*		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
1A'→2A"	0.31	0.03	1A'→1A"	0.30	0.00	1A"→1A'	0.09	0.02	1A"→2A'	0.23	0.00
1A'→2A'	0.44	0.48	1A'→2A'	0.53	0.46	1A"→2A"	0.40	10.44	1A"→2A"	0.88	0.05
1A'→3A"	0.46	0.00	1A'→2A"	1.18	0.00	1A"→2A'	0.53	0.57	1A"→3A"	0.91	0.17
1A'→4A"	0.82	0.00	1A'→3A"	1.20	0.01	1A"→3A"	0.55	0.04	1A"→4A"	1.24	0.01
1A'→5A"	1.03	0.00	1A'→4A"	1.54	0.00	1A"→4A"	0.91	18.61	1A"→3A'	1.37	0.00
1A'→6A"	1.22	0.00	1A'→3A'	1.66	1.12	1A"→5A"	1.11	3.08	1A"→5A"	1.60	0.27
1A'→7A"	1.27	0.01	1A'→5A"	1.90	0.00	1A"→6A"	1.31	0.00	1A"→4A'	1.87	0.00
1A'→3A'	1.35	0.73	1A'→4A'	2.17	0.18	1A"→7A"	1.36	0.04	1A"→6A"	1.93	0.13
1A'→8A"	1.35	0.01	1A'→6A"	2.22	0.00	1A"→3A'	1.43	18.90	1A"→7A"	1.97	0.00
1A'→4A'	1.43	0.36	1A'→7A"	2.27	0.00	1A"→8A"	1.44	0.01	1A"→5A'	2.12	0.00
1A'→9A"	1.62	0.03	1A'→5A'	2.42	1.37	1A"→4A'	1.52	1.33	1A"→6A'	2.19	0.00
1A'→5A'	1.62	0.48	1A'→6A'	2.49	1.42	1A"→9A"	1.70	1.18	1A"→8A"	2.34	0.01
1A'→10A"	1.79	0.03	1A'→8A"	2.64	0.00	1A"→5A'	1.71	0.00	1A"→7A'	2.37	0.00
1A'→6A'	1.97	0.03	1A'→7A'	2.66	0.10	1A"→10A"	1.87	9.07	1A"→9A"	2.50	0.05
1A'→11A"	2.01	0.00	1A'→9A"	2.79	0.01	1A"→6A'	2.06	0.07	1A"→10A"	2.67	0.00
1A'→12A"	2.03	0.00	1A'→10A"	2.96	0.00	1A"→11A"	2.10	0.21	1A"→8A'	2.75	0.00
1A'→7A'	2.08	0.08	1A'→8A'	3.05	6.18	1A"→12A"	2.11	1.33	1A"→9A'	2.91	0.00
1A'→13A"	2.12	0.00	1A'→9A'	3.21	0.88	1A"→7A'	2.17	0.14	1A"→11A"	3.15	1.96
1A'→8A'	2.22	0.02	1A'→11A"	3.44	0.00	1A"→13A"	2.21	3.46	1A"→12A"	3.19	0.68
1A'→9A'	2.26	0.17	1A'→12A"	3.48	0.00	1A"→8A'	2.31	0.17	1A"→10A'	3.31	0.00
1A'→14A"	2.29	0.00	1A'→10A'	3.60	1.73	1A"→9A'	2.34	2.71	1A"→13A"	3.36	0.81
1A'→10A'	2.32	2.24	1A'→13A"	3.66	0.00	1A"→14A"	2.38	0.02	1A"→14A"	3.43	0.01
1A'→15A"	2.34	0.02	1A'→14A"	3.72	0.00	1A"→10A'	2.41	0.00	1A"→11A'	3.52	0.00
1A'→16A"	2.40	0.00	1A'→11A'	3.82	0.16	1A"→15A"	2.43	2.51	1A"→12A'	3.53	0.00
1A'→11A'	2.44	0.17	1A'→12A'	3.83	2.85	1A"→16A"	2.49	6.33	1A"→15A"	3.65	0.00
1A'→12A'	2.57	0.13	1A'→15A"	3.94	0.00	1A"→11A'	2.53	0.47	1A"→16A"	3.70	0.00
1A'→17A"	2.58	0.19	1A'→16A"	3.99	0.00	1A"→12A'	2.66	0.00	1A"→13A'	3.80	0.00
1A'→13A'	2.60	0.05	1A'→13A'	4.10	0.45	1A"→17A"	2.67	0.30	1A"→17A"	4.12	0.11
1A'→14A'	2.68	0.13	1A'→17A"	4.41	0.00	1A"→13A'	2.69	0.00	1A"→18A"	4.17	0.00
1A'→18A"	2.76	0.00	1A'→18A"	4.46	0.00	1A"→14A'	2.77	0.00	1A"→14A'	4.18	0.00
1A'→15A'	2.76	0.08	1A'→14A'	4.47	0.01	1A"→18A"	2.84	3.66	1A"→15A'	4.41	0.00
1A'→19A"	2.84	0.06	1A'→15A'	4.71	0.14	1A"→15A'	2.85	0.00	1A"→19A"	4.47	0.00
1A'→16A'	2.87	1.48	1A'→19A"	4.77	0.02	1A"→19A"	2.93	3.51	1A"→16A'	4.53	0.00
1A'→20A"	2.88	0.01	1A'→16A'	4.83	0.11	1A"→16A'	2.95	0.13	1A"→20A"	4.59	0.47
1A'→17A'	2.93	0.05	1A'→20A"	4.89	0.02	1A"→20A"	2.97	0.03	1A"→17A'	4.67	0.00
1A'→18A'	2.96	0.95	1A'→17A'	4.96	0.11	1A"→17A'	3.01	0.02	1A"→21A"	4.68	0.01
1A'→21A"	2.96	0.00	1A'→21A"	4.97	0.00	1A"→18A'	3.04	0.14	1A"→18A'	4.73	0.01
1A'→22A"	3.05	0.01	1A'→18A'	5.03	0.06	1A"→21A"	3.05	3.55	1A"→22A"	4.76	0.00
1A'→19A'	3.06	2.21	1A'→22A"	5.06	0.01	1A"→22A"	3.14	1.05	1A"→19A'	4.80	0.03
1A'→23A"	3.11	0.10	1A'→19A'	5.10	0.09	1A"→19A'	3.15	0.08	1A"→20A'	4.92	0.00
1A'→24A"	3.12	0.02	1A'→20A'	5.21	0.07	1A"→23A"	3.20	0.44	1A"→23A"	5.02	0.00
1A'→20A'	3.14	0.89	1A'→23A"	5.31	0.00	1A"→24A"	3.20	0.47	1A"→24A"	5.14	0.00
1A'→25A"	3.17	0.00	1A'→24A"	5.44	0.00	1A"→20A'	3.22	0.00	1A"→25A"	5.19	0.01
			1A'→25A"	5.49	0.11	1A"→25A"	3.26	0.38			

SS4.5 ESA from $\pi\pi^*$

Table S27: ESA from the 1A' state at $\pi\pi^*$ minima. CAM-B3LYP/aug-cc-pVDZ excitation energies (ΔE, eV) and oscillator strengths (f) for Cytosine, Thymine, Adenine, Guanine.

Cytosine			Thymine			Adenine			Guanine		
Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$	Trans.	ΔE	$f \times 100$
→1A"	0.84	0.00	→1A"	0.63	0.00	→1A"	0.45	0.00	→2A'	0.55	0.77
→2A'	0.90	1.44	→2A"	1.32	0.43	→2A'	0.64	0.50	→1A"	0.55	0.03
→2A"	0.98	0.00	→2A'	1.75	0.47	→2A"	0.81	0.03	→2A"	1.02	0.19
→3A"	1.60	0.17	→3A'	1.87	2.22	→3A"	1.32	0.40	→3A"	1.26	0.00
→4A"	1.74	0.00	→3A"	1.89	0.04	→4A"	1.48	0.05	→4A"	1.35	0.00
→3A'	2.01	0.27	→4A"	1.92	0.00	→5A"	1.51	0.61	→5A"	1.61	0.11
→5A"	2.08	0.00	→5A"	2.05	0.19	→3A'	1.66	9.78	→6A"	1.62	0.00
→6A"	2.27	0.06	→4A'	2.39	0.15	→6A"	1.70	0.00	→3A'	1.66	0.18
→4A'	2.29	0.11	→6A"	2.56	0.00	→4A'	1.88	0.60	→4A'	1.74	1.20
→7A"	2.41	0.08	→7A"	2.75	0.20	→7A"	1.89	0.00	→7A"	1.76	0.00
→5A'	2.49	0.93	→8A"	2.83	0.00	→8A"	2.01	0.02	→8A"	1.85	0.00
→8A"	2.74	0.01	→5A'	2.85	0.01	→5A'	2.07	0.83	→9A"	2.14	0.08
→6A'	2.87	0.51	→9A"	2.96	0.01	→9A"	2.21	0.14	→10A"	2.44	0.00
→9A"	2.87	0.01	→10A"	3.07	0.00	→6A'	2.24	3.97	→5A'	2.55	0.51
→10A"	2.93	0.03	→6A'	3.13	0.85	→10A"	2.34	0.01	→11A"	2.56	0.00
→11A"	3.02	0.21	→7A'	3.24	0.23	→7A'	2.38	0.27	→6A'	2.60	2.66
→12A"	3.12	0.49	→11A"	3.24	0.02	→11A"	2.84	0.00	→7A'	2.65	0.36
→7A'	3.16	0.53	→8A'	3.27	0.73	→8A'	2.85	0.05	→8A'	2.73	0.59
→8A'	3.26	2.97	→9A'	3.47	0.64	→12A"	2.87	0.01	→12A"	2.75	0.01
→9A'	3.28	4.05	→12A"	3.57	0.02	→9A'	2.89	0.11	→13A"	2.80	0.01
→13A"	3.31	0.00	→10A'	3.65	0.38	→10A'	2.92	0.22	→9A'	2.87	0.40
→10A'	3.36	0.94	→13A"	3.67	0.05	→13A"	2.92	0.55	→10A'	2.88	0.23
→14A"	3.59	0.07	→11A'	3.72	6.46	→11A'	3.08	0.16	→14A"	2.94	0.00
→15A"	3.60	0.00	→14A"	3.78	0.15	→14A"	3.13	0.04	→15A"	3.01	0.05
→11A'	3.63	1.79	→12A'	3.91	0.08	→15A"	3.18	0.11	→11A'	3.04	0.18
→16A"	3.73	0.00	→15A"	3.94	0.09	→16A"	3.21	0.01	→12A'	3.09	0.18
→12A'	3.80	0.06	→16A"	3.95	0.04	→12A'	3.24	0.64	→16A"	3.11	0.00
→17A"	3.88	0.03	→17A"	4.04	0.00	→17A"	3.27	0.35	→13A'	3.24	0.05
→13A'	3.90	0.08	→18A"	4.07	0.01	→13A'	3.38	0.74	→17A"	3.41	0.00
→14A'	3.94	0.00	→19A"	4.12	0.00	→14A'	3.45	0.03	→18A"	3.43	0.00
→15A'	4.05	0.24	→13A'	4.14	0.41	→18A"	3.48	0.05	→14A'	3.47	5.27
→16A'	4.08	5.84	→20A"	4.15	0.01	→15A'	3.51	0.29	→19A"	3.48	0.04
→18A"	4.09	0.00	→14A'	4.34	0.92	→19A"	3.51	0.01	→15A'	3.53	0.72
→19A"	4.18	0.03	→15A'	4.37	1.11	→20A"	3.58	0.00	→16A'	3.59	1.78
→17A'	4.19	0.93	→21A"	4.43	0.58	→16A'	3.62	0.05	→20A"	3.60	0.00
→20A"	4.25	0.02	→16A'	4.46	12.62	→21A"	3.66	0.02	→21A"	3.64	0.02
→18A'	4.30	33.29	→22A"	4.53	0.00	→17A'	3.75	0.97	→22A"	3.75	0.00
→19A'	4.37	256.39	→17A'	4.53	125.71	→22A"	3.75	0.01	→17A'	3.76	0.06
→21A"	4.43	0.02	→23A"	4.54	0.07	→18A'	3.87	0.14	→18A'	3.80	0.16
→22A"	4.52	0.01	→18A'	4.54	62.43	→23A"	3.89	0.06	→23A"	3.82	0.00
→23A"	4.52	0.01	→24A"	4.62	0.00	→24A"	3.92	0.23	→24A"	3.84	0.03
→24A"	4.59	0.00	→19A'	4.65	0.24	→19A'	3.95	0.47	→25A"	3.92	0.01
→20A'	4.63	0.11	→20A'	4.72	8.01	→25A"	3.96	0.00	→19A'	3.93	0.53
→20A'	4.63	0.10	→25A"	4.83	0.03	→20A'	4.05	0.03	→20A'	4.01	2.45
→25A"	4.70	0.04									

S5 Additional figures

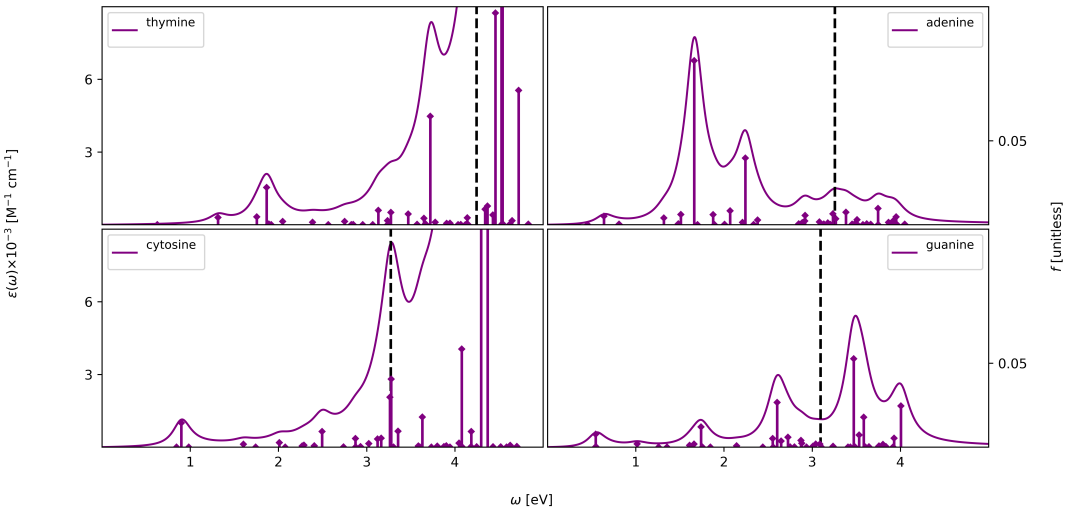

Figure S23: CAMB3LYP/aug-cc-pVDZ ESA in solution computed, at the non-equilibrium level, applying PCM in chloroform from $\pi\pi^*$ state at the $\pi\pi^*$-minima for four nucleobases. A vertical dashed line indicates the estimated value of the first ionization energy in the excited state for ESA. This was obtained as difference of the IE of the ground state and the energy of $\pi\pi^*$ state. Structures were optimised in gas-phase.

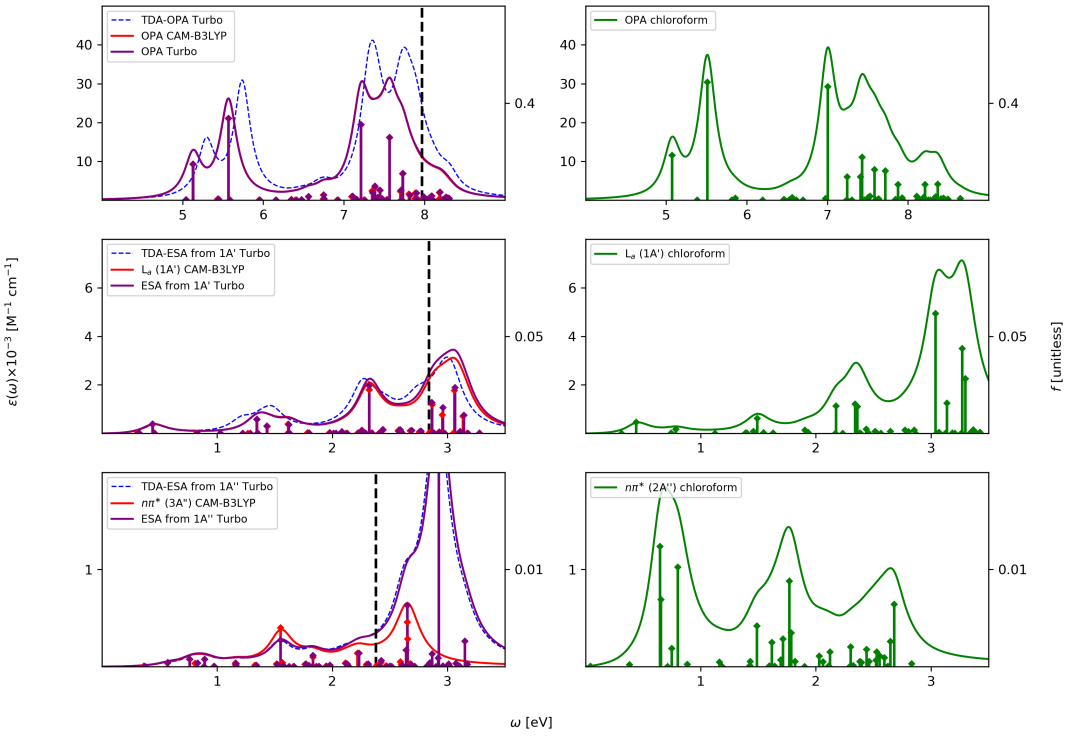

Figure S24: Guanine. OPA and ESA computed at CAMB3LYP/aug-cc-pVDZ level of theory. A vertical dashed line indicates the first ionisation energy for OPA and the estimated value of the first ionisation energy in the excited state for ESA, obtained as IE of the ground state minus the energy of $\mathbf{1}\pi$ and $\mathbf{1n}$.

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