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Supporting Information for Theoretical Understanding of Two-photon-induced Fluorescence of Isomorphic Nucleoside Analogs†

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The 2PA cross sections (σ_{2P}) for five lowest transitions are given in Table S1 in the unit of a.u. (atomic unit). $a.u. = 1.896788$ GM and 1 GM $= 10^{-50}$ cm^4 s/photon.

Table S1: Five Low Energy Transition Peaks of the Nucleoside Analogs in both Gas phase and in implicit Solvent. Oscillator Strength (f) for 1PA and σ_{2p} (in a.u.) for 2PA are given in bracket.

Molecules	Transition Energy (eV)				
	Calculated				
	Excitation	in gas		in water	
		1PA	2PA	1PA	2PA
1	$S_0 \rightarrow S_1$	3.48 (0.25)	3.49 (3.73)	3.42 (0.29)	3.30 (16.50)
	$S_0 \rightarrow S_2$	4.06 (0.03)	4.06 (0.41)	4.01 (0.06)	3.99 (1.70)
	$S_0 \rightarrow S_3$	4.07 (0.01)	4.07 (0.80)	4.14 (0.00)	4.16 (4.25)
	$S_0 \rightarrow S_4$	4.15 (0.00)	4.14 (1.80)	4.22 (0.00)	4.23 (21.1)
	$S_0 \rightarrow S_5$	4.62 (0.00)	4.61 (6.05)	4.68 (0.19)	4.62 (69.0)
2	$S_0 \rightarrow S_1$	3.70 (0.28)	3.69 (2.40)	3.75 (0.23)	3.64 (9.61)
	$S_0 \rightarrow S_2$	4.50 (0.03)	4.50 (1.41)	4.53 (0.10)	4.46 (19.3)
	$S_0 \rightarrow S_3$	4.58 (0.00)	4.58 (0.11)	4.59 (0.21)	4.54 (8.81)
	$S_0 \rightarrow S_4$	4.65 (0.22)	4.65 (13.1)	4.76 (0.01)	4.77 (12.7)
	$S_0 \rightarrow S_5$	4.91 (0.00)	4.89 (2.65)	4.99 (0.01)	4.98 (115.0)
3	$S_0 \rightarrow S_1$	3.75 (0.28)	3.75 (5.99)	3.71 (0.31)	3.75 (6.17)
	$S_0 \rightarrow S_2$	4.66 (0.00)	4.65 (0.54)	4.65 (0.41)	4.59 (0.08)
	$S_0 \rightarrow S_3$	4.76 (0.32)	4.76 (1.31)	4.78 (0.00)	4.77 (1.58)
	$S_0 \rightarrow S_4$	4.80 (0.02)	4.78 (2.64)	5.04 (0.00)	4.78 (2.11)
	$S_0 \rightarrow S_5$	5.00 (0.00)	4.98 (1.73)	5.09 (0.00)	5.03 (2.37)
4	$S_0 \rightarrow S_1$	4.40 (0.11)	4.40 (1.96)	4.26 (0.28)	4.10 (38.30)
	$S_0 \rightarrow S_2$	4.65 (0.12)	4.65 (5.72)	4.51 (0.07)	4.46 (14.70)
	$S_0 \rightarrow S_3$	4.77 (0.00)	4.76 (0.05)	4.92 (0.20)	4.80 (1.49)
	$S_0 \rightarrow S_4$	4.89 (0.00)	4.86 (1.55)	4.93 (0.00)	4.96 (0.14)
	$S_0 \rightarrow S_5$	5.07 (0.16)	5.07 (1.01)	5.23 (0.00)	5.20 (2.23)
5	$S_0 \rightarrow S_1$	3.64 (0.16)	3.64 (0.39)	3.59 (0.20)	3.49 (2.10)
	$S_0 \rightarrow S_2$	3.94 (0.00)	3.94 (0.02)	4.21 (0.00)	4.17 (1.30)
	$S_0 \rightarrow S_3$	4.67 (0.01)	4.64 (3.91)	4.56 (0.06)	4.51 (25.4)
	$S_0 \rightarrow S_4$	4.68 (0.01)	4.68 (3.80)	4.83 (0.00)	4.88 (59.7)
	$S_0 \rightarrow S_5$	4.70 (0.04)	4.70 (5.42)	4.88 (0.00)	4.93 (27.9)
6	$S_0 \rightarrow S_1$	4.17 (0.07)	4.17 (1.97)	4.07 (0.08)	4.01 (6.76)
	$S_0 \rightarrow S_2$	4.49 (0.00)	4.49 (0.02)	4.69 (0.00)	4.68 (0.19)
	$S_0 \rightarrow S_3$	5.00 (0.01)	4.99 (0.37)	4.83 (0.03)	4.82 (3.00)
	$S_0 \rightarrow S_4$	5.11 (0.02)	5.10 (1.03)	5.00 (0.12)	4.98 (1.46)
	$S_0 \rightarrow S_5$	5.19 (0.07)	5.18 (0.40)	5.20 (0.00)	5.32 (1.22)
7	$S_0 \rightarrow S_1$	3.86 (0.10)	3.86 (2.92)	3.66 (0.13)	3.57 (8.91)
	$S_0 \rightarrow S_2$	4.54 (0.01)	4.52 (3.35)	4.69 (0.02)	4.63 (5.15)
	$S_0 \rightarrow S_3$	4.72 (0.00)	4.72 (1.11)	4.76 (0.00)	4.79 (0.14)
	$S_0 \rightarrow S_4$	4.75 (0.00)	4.75 (2.18)	4.99 (0.01)	4.98 (9.78)
	$S_0 \rightarrow S_5$	4.88 (0.00)	4.88 (7.02)	5.01 (0.00)	5.00 (2.84)
8	$S_0 \rightarrow S_1$	3.66 (0.08)	3.67 (2.52)	3.85 (0.10)	3.78 (5.97)
	$S_0 \rightarrow S_2$	4.52 (0.03)	4.52 (0.63)	4.61 (0.01)	4.57 (6.26)
	$S_0 \rightarrow S_3$	4.66 (0.00)	4.65 (0.03)	4.71 (0.25)	4.63 (0.30)
	$S_0 \rightarrow S_4$	4.70 (0.12)	4.70 (0.92)	4.88 (0.02)	4.85 (7.26)
	$S_0 \rightarrow S_5$	4.76 (0.03)	4.76 (1.91)	4.93 (0.03)	4.87 (2.27)