Article

Sensing Performance Investigations on Two-Photon Fluorescent Probes for Detecting β-Amyloid in Alzheimer's Disease

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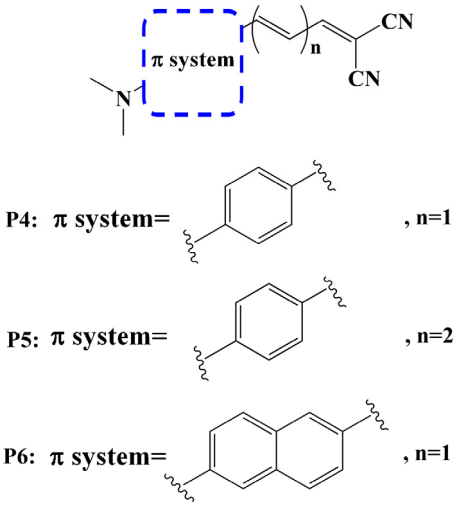

Figure 1. Molecular structures of P4, P5 and P6.

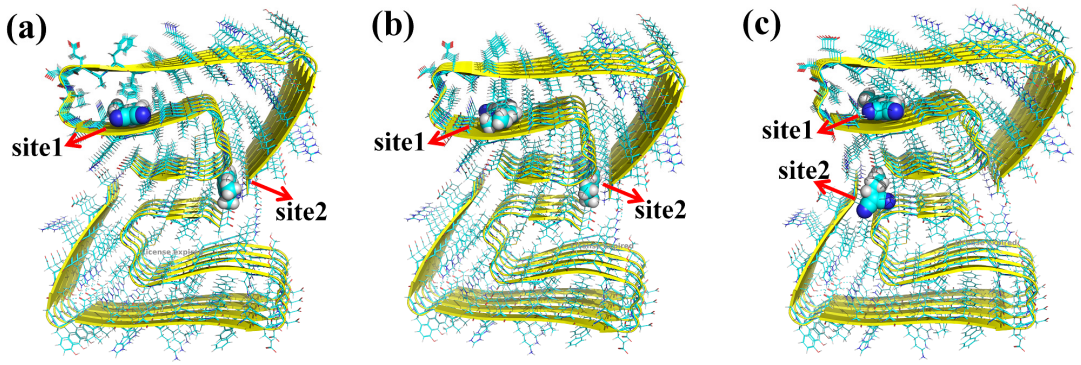

Figure 2. Binding sites of (a) P4, (b) P5, (c) P6 in β-amyloid.

Table S1. Energy parameters (in kcal/mol) and inhibition constant (in nM) for P4, P5 and P6 in various binding sites in β-amyloid.

Site	P4		P5		P6	
	site1	site2	site1	site2	site1	site2
Binding energy	-9.27	-6.44	-10.07	-6.77	-11.1	-8.12
Inhibition constant	160.77	18930	41.45	10890	7.33	1120
Intermolecular Energy	-10.16	-7.34	-11.26	-7.96	-11.99	-9.01
Internal Energy	-0.4	-0.41	-0.49	-0.43	-0.32	-0.59
Torsional Energy	0.89	0.89	1.19	1.19	0.89	0.89
Unbound Energy	-0.4	-0.41	-0.49	-0.43	-0.32	-0.59

Table S2. OPA wavelength λ_{OPA}(nm), oscillator strength δ_{OPA}(a.u.) and the corresponding transition nature for P1, P2, P3, P4, P5 and P6 in different microenvironments at long wavelength region. H(L) donates HOMO(LUMO).

	P1			P2(Exp. 557)			P3(Exp. 559)		
Site	**gas**	**site1**	**site2**	**gas**	**site1**	**site2**	**gas**	**site1**	**site2**
λ_{OPA}	560	549	541	524	538	533	573	568	606
δ_{OPA}	0.55	0.90	0.96	0.73	0.79	0.82	0.81	0.85	0.66
Transition Nature	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%
	P4(Exp. 489)			**P5(Exp. 519)**			**P6**		
Site	**gas**	**site1**	**site2**	**gas**	**site1**	**site2**	**gas**	**site1**	**site2**
λ_{OPA}	441	455	439	498	498	509	508	503	501
δ_{OPA}	0.71	0.89	1.05	0.81	0.90	1.06	0.48	0.97	0.80
Transition Nature	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%	H-L 98%

Table S3. OPE wavelength λ_{OPE}(nm), oscillator strength δ_{OPE}(a.u.) and the corresponding transition nature for P1, P2, P3, P4, P5 and P6 in different microenvironments at long wavelength region. H(L) donates HOMO(LUMO).

	P1(Exp. 678)			P2(Exp. 660)			P3(Exp. 710)		
Site	**gas**	**site1**	**site2**	**gas**	**site1**	**site2**	**gas**	**site1**	**site2**
λ_{OPA}	859	600	591	892	593	589	924	614	656
δ_{OPA}	0	0.69	0.73	0	0.58	0.60	0	0.71	0.53
Transition Nature	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%
	P4(Exp. 577)			**P5(Exp. 665)**			**P6(Exp. 615)**		
Site	**gas**	**site1**	**site2**	**gas**	**site1**	**site2**	**gas**	**site1**	**site2**
λ_{OPA}	725	493	471	769	574	552	801	598	589
δ_{OPA}	0	0.67	0.83	0	0.54	0.77	0	0.41	0.39
Transition Nature	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%	L-H 98%

Table S4. The maximum TPA wavelength λ_{TPA}(nm), TPA cross section σ_{TPA}(GM, 1GM=10^{-50} cm^4×s/photon), and the corresponding two-photon transition matrix element $S_{\alpha\beta}$ for P1, P2, P3, P4, P5 and P6 in different microenvironments.

Site	λ_{TPA}	σ_{TPA}	S_{xx}	S_{yy}	S_{zz}	S_{xy}	S_{xz}	S_{yz}
P1-gas	1119	411	757.9	2.8	0.8	15.8	10.6	2.3
P1-site1	1206	1099	1335.2	1.1	1.1	43.6	7.5	0.2
P1-site2	1183	1088	1303.1	0.3	1.1	33.9	15.0	0.6
P2-gas	1048	166	449.1	3.9	1.1	30.0	0.0	0.0
P2-site1	1129	338	690.9	5.6	1.6	40.4	1.5	0.8
P2-site2	1140	366	726.0	4.0	1.4	36.0	4.2	0.3
P3-gas	1080	344	664.4	10.2	0.9	34.7	0.0	0.0
P3-site1	1224	894	1222.0	3.3	1.5	23.4	9.6	0.6
P3-site2	1281	934	1308.8	2.8	1.4	33.6	0.2	0.1
Site	λ_{TPA}	σ_{TPA}	S_{xx}	S_{yy}	S_{zz}	S_{xy}	S_{xz}	S_{yz}
P4-gas	1039	238	2.2	8.6	533.2	4.1	12.3	20.3
P4-site1	962	136	1.7	4.4	372.5	0.8	5.1	15.0
P4-site2	933	155	1.9	1.7	387.6	0.9	0.5	7.2
P5-gas	1200	668	1.7	7.4	1035.2	2.7	17.9	13.6
P5-site1	1048	441	2.3	2.7	735.1	0.5	4.3	3.3
P5-site2	1085	356	2.0	2.7	684.1	0.5	2.1	0.4
P6-gas	1195	647	1.9	1.6	1015.9	7.7	10.7	3.6
P6-site1	1052	538	1.2	0.2	813.9	0.9	3.6	37.2
P6-site2	1061	409	0.8	4.8	715.3	2.8	17.1	45.9