Supporting information of

Dual anticancer and antibacterial activity of fluorescent NaphthoImidazolium salts

Dung Ngoc Tran,[a,‡.] Thi Thuy Hang Hoang,[b,‡] Sondavid Nandanwar,[c] Vuong Thi Thanh Xuan Ho,[d] Van Thong Pham,[e] Huy Duc Vu,[f] Xuan Ha Nguyen,[g] Huy trung Nguyen,[h] Trang Van Nguyen,[h] Thuy Kieu Van Nguyen,[i] Lam Dai Tran,[h] Myeongkee Park,[j] Songyi Lee,*[i,j] Thanh Chung Pham,*[h]

[a.]   *Faculty of Chemistry, Hanoi National University of Education, Hanoi, Vietnam*

[b.]   *Department of Chemistry, Soongsil University, Seoul 06978, South Korea.*

[c.]   *Eco-friendly New Materials Research Center, Korea Research Institute of Chemical Technology, 141 Gajeong-ro, Yuseong-gu, Daejeon City, Republic of Korea*

[d.]   *Faculty of Pharmacy, Dong A University, Danang, Vietnam*

[e.]   *R&D Center, Vietnam Education and Technology transfer JSC, Cau Giay, Hanoi, Vietnam*

[f.]   *Department of Radiology, School of Medicine, Daegu Catholic University, Daegu 42472, Korea*

[g.]   *Institute of Natural Products Chemistry, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam*

[h.]   *Institute for Tropical Technology, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam. Email: ptchung@itt.vast.vn*
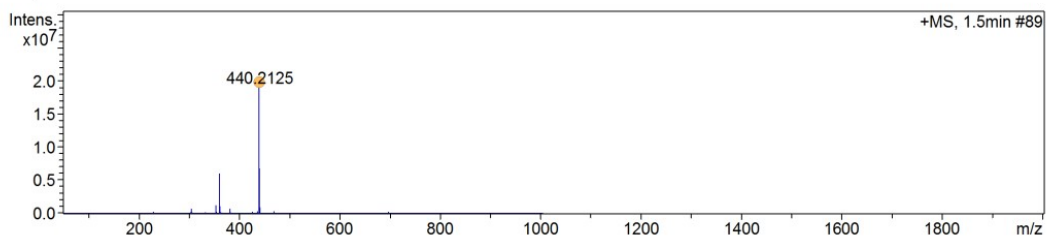
[i.]   *Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Busan 48513, Korea. Email: slee@pknu.ac.kr*

[j.]   *Department of Chemistry, Pukyong National University, Busan 48513, Korea*

[k.]   *‡ These authors equally contributed to this work.*

Figure S1. ^{1}H-NMR, ^{13}C-NMR and HR-MS spectra of **NI-TPA**
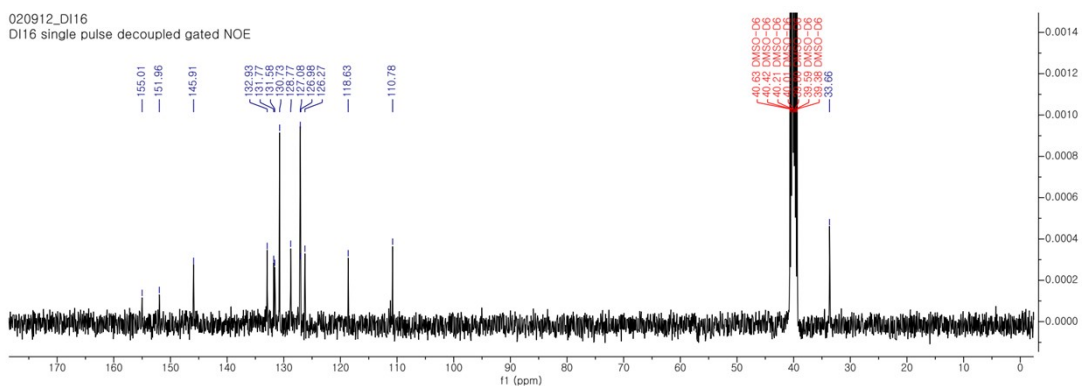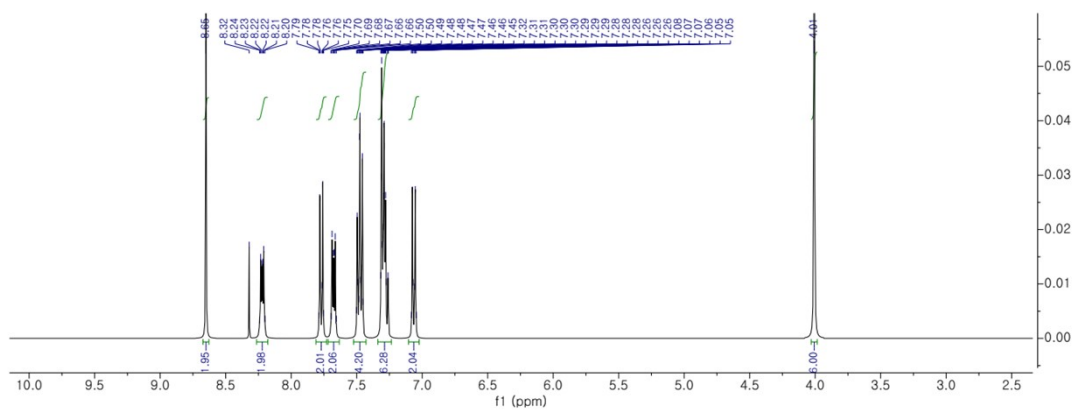
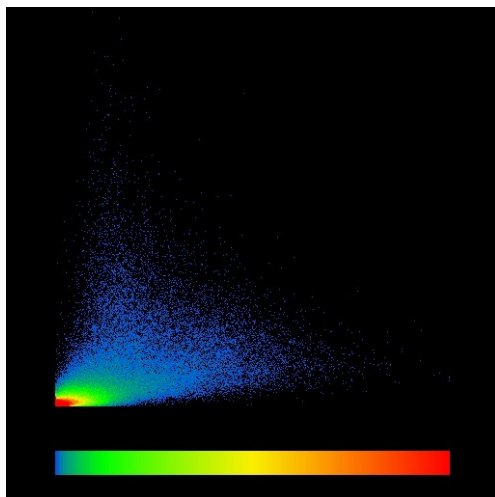| Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
440.2125	1	C31H26N3	440.2127	0.4	9.1	1	100.00	20.5	even	ok

Figure S2. Colocalization analysis plot of the Lysotracker and **NI-TPA**.
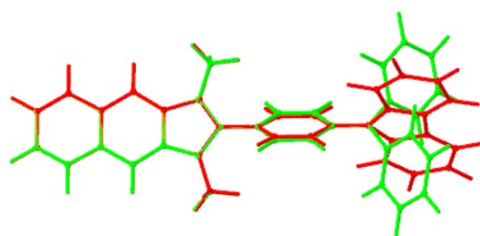

Figure S3. Merge S_0 geometry of **NI-Cbz** (red) and **NI-TPA** (green)

Table S1. RMSD of the backbone protein, RMSD of the ligand, and Rg analysis for the MD simulations at different times.

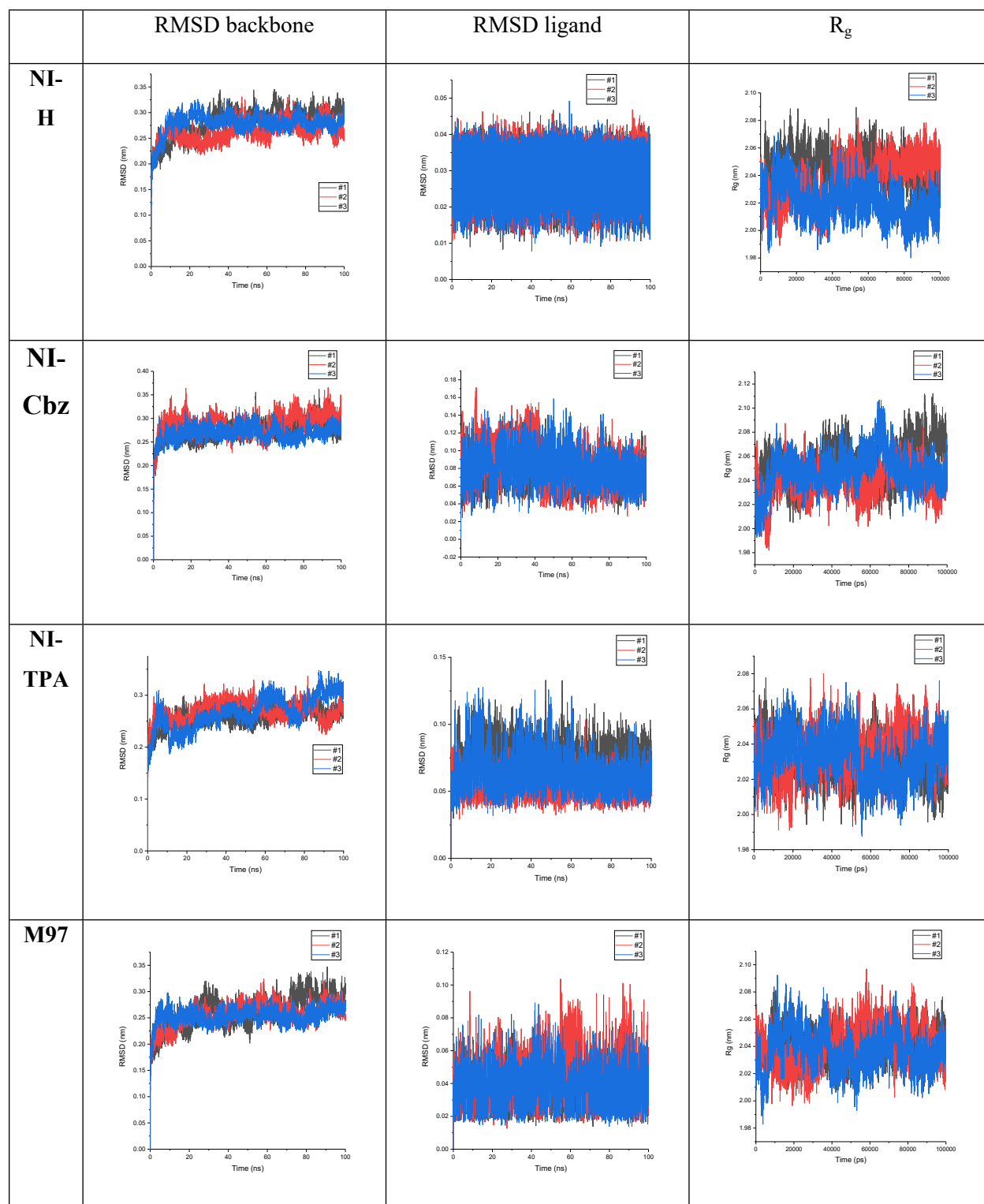|	RMSD backbone	RMSD ligand	R$_g$
NI-H			
NI-Cbz			
NI-TPA			
M97			

Table S2. Value of RMSD of the backbone protein, RMSD of the ligand, and Rg analysis for the MD simulations at different times and its average

	Time	**NI-H**	**NI-Cbz**	**NI-TPA**	**M97**
Average RMSD backbone (nm)	1	0.280	0.271	0.258	0.261
	2	0.262	0.288	0.269	0.255
	3	0.278	0.268	0.266	0.253
	Average	0.273±0.010	0.276±0.011	0.264±0.006	0.256±0.004
Average RMSD Ligand (nm)	1	0.029	0.076	0.074	0.037
	2	0.030	0.083	0.053	0.042
	3	0.029	0.081	0.064	0.036
	Average	0.029±0.0002	0.080±0.003	0.064±0.010	0.038±0.003
Average Rg (nm)	1	2.044	2.053	2.030	2.041
	2	2.037	2.039	2.035	2.040
	3	2.021	2.049	2.032	2.037
	Average	2.034±0.012	2.047±0.007	2.032±0.002	2.039±0.002