Supporting Information

Acridine-based near-infrared dyes as high-performanced Raman

reporter molecules for cancer cell imaging

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Figure S1 UV–Vis absorption spectra of (a) C3AD, (b) C5AD, and (c) C7AD in EtOH (blue), CH_2Cl_2 (green) and $CHCl_3$ (red).



Figure S2 UV–Vis absorption spectra, hydrodynamic diameter distributions and average zeta potential of (a-c) C3AD (d-f) C5AD and (g-i) C7AD nanotags.



Figure S3 TEM images of (a,b) AuNS-C3AD-BSA, (c,d) AuNS-C5AD-BSA and (e,f) AuNS-C7AD-BSA.



Figure S4 The relationship between the concentration of AD dyes and SERS intensity of 1277 cm⁻¹ SERS band. (n=3) (785 nm wavelenth, 0.85 mW laser power, 10 s exposure time and 50L× objective lens.)



Figure S5 SERS images of (a) AuNS-C3AD-BSA and (c) AuNS-C7AD-BSA and (b and d) the corresponding SERS spectra of 16.2 pM inside the vessel (positions 1 and 2) and outside the vessel (position 3).



Figure S6 SERS images of AuNS-DTTC-BSA. The SERS images were acquired under a $5 \times$ objective lens with 1.7 mW laser power on the samples, 2 s exposure time and 50 µm step size. The SERS images were created with the intensity of 1239 cm⁻¹ SERS band after removing the baseline via Wire 5.1.



Figure S7 (a) and (c) are bright field image of A549. (b) and (d) are corresponding SERS spectra of position 1, 2, and 3. The SERS imaging was carried out using a $100 \times$ objective lens at 8.5 mW laser power with 5 s exposure time and 5 µm step size. Scale bar : 5 µm.



Figure S8 (c) SERS spectra of position 1, 2, and 3 in (a) overlay of bright field image and (b) bright field image of A549 cell. The SERS imaging was carried out using a $100 \times$ objective lens at 8.5 mW laser power with 5 s exposure time and 3 µm step size. Scale bar : 5 µm.



Figure S9¹H NMR spectra of C3AD







Figure S11¹H NMR spectra of C7AD

Nanostructures	Molecular probe	Detection Limit	Reference
gold nanostar	$\langle \rangle \langle \rangle$	0.4 pM (n=3)	This Work
		0.5 pM (n=5)	
		0.51 pM (n=7)	
	AD dyes (n=3, 5, 7)		
gold particles	CH ₃	2.3 μM	1
(60 nm)	H ₃ C		
	Malachite Green		
gold nanoparticle	\square	0.26 nM	2
(40 nm)			
	P4		
gold nanostar	"O ₃ S, N, SO ₃ "	0.8 pM	3
	s s		
	↓ s s√ IR7n		
Au NSs	0 ₂ N	0.13 pM	4
	SH		
	4-NTP		
Hollow AgAu		1 pM	5
	strands ²		
	DTTC		
hollow CuS NPs	DTTC	1 pM	6
gold particles		1 fM	7
(60 nm)			
	IR729		
	s⊋	100 aM,	
	s⁺		
	3		
Gap-enhanced	SH SH	0.1 pM	8
Raman tags	HS		
(GERT)	1,4-Benzenedithiol		

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