Supporting Information for

Highly Sensitive MoS$_2$-Indocyanine Green Hybrid for Photoacoustic Imaging of Orthotopic Brain Glioma at Deep Site

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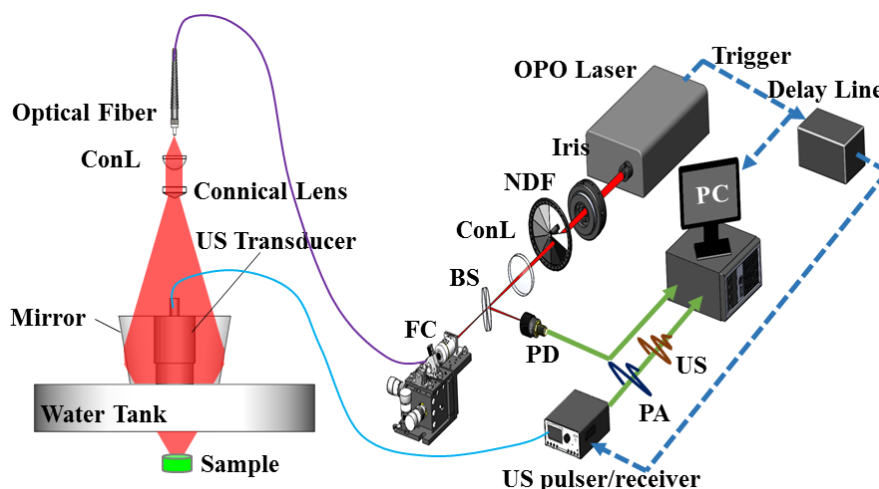# Supplementary Figures and Table

Fig. S1 Schematic illustration of the custom-built acoustic-resolution photoacoustic microscopy (AR-PAM) system. OPO: optical parametric oscillator; BS: beam splitter; PD: photodiode; FC: optical fiber coupler; PA: photoacoustic; US: ultrasound; ConL: convex lens; PC: personal computer. The OPO laser was reshaped by Iris, and then focused by a convex lens before coupling into an optical fiber via a coupler. A beam sampler and a photodiode were used to monitor the fluctuation of laser energy per pulse. The laser beam coming out of the fiber was collimated by another convex lens and focused by a conical lens to create a cone-shaped beam, which was able to pass through the ultrasound transducer and reflected by a custom-made mirror to illuminate the imaging objects. For system control, the trigger-out signal from the OPO laser was used to trigger the data acquisition board to acquire photoacoustic signals first, and a delay line was added to the trigger-out signal to trigger an ultrasonic pulser-receiver to emit an ultrasound pulse and subsequently receive the echo signals by the transducer. Both the photoacoustic and the ultrasound signals were amplified using the ultrasonic pulser-receiver, and then digitized with the DAQ in a personal computer. The motion controller manages a precision scanning stage to motorize the imaging head (dashed box) for 2D raster scanning.
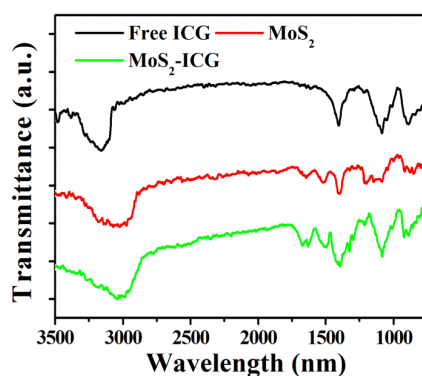

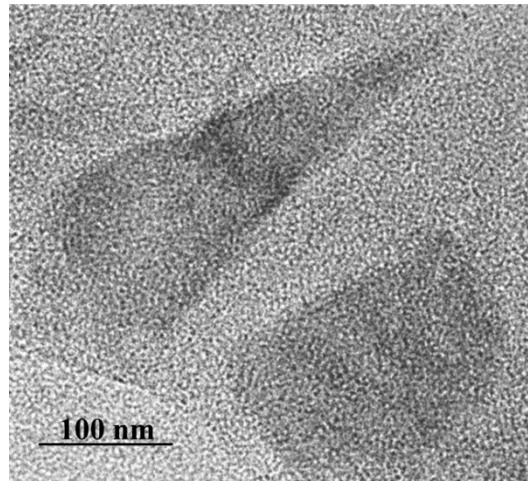
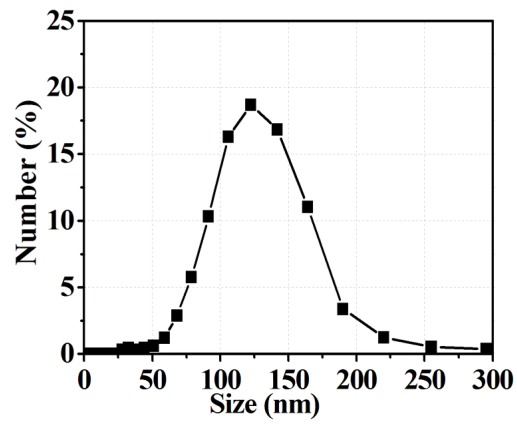**Fig. S2** FT-IR spectra of free ICG and MoS_2 and MoS_2-ICG

Fig. S3 TEM image of MoS$_2$-ICG

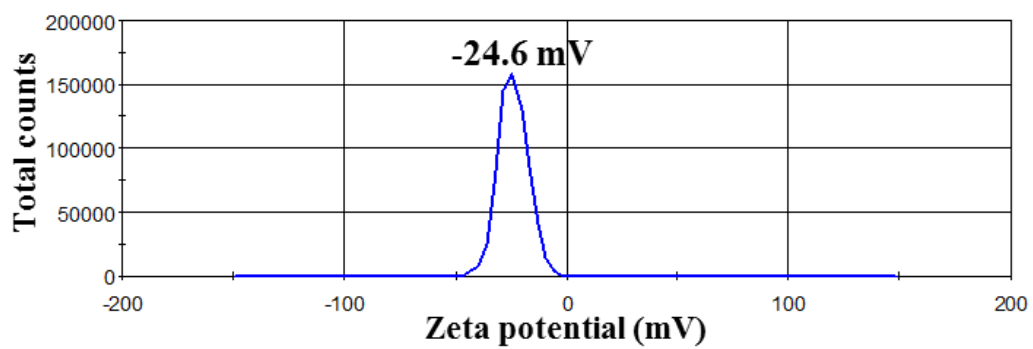**Fig. S4** Size distribution of MoS$_2$-ICG

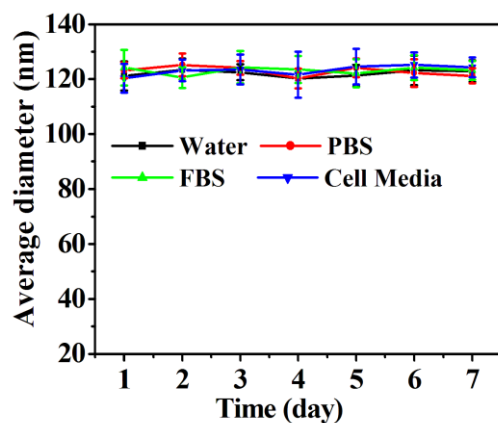**Fig. S5** Zeta potential distribution of MoS$_2$-ICG

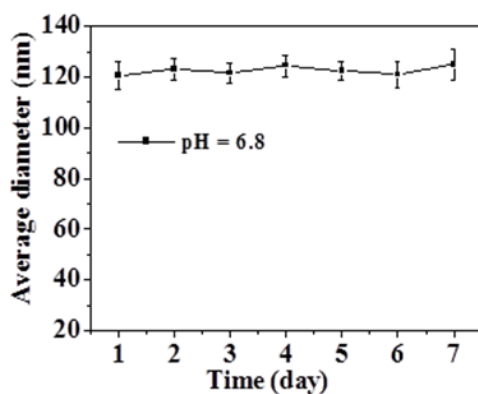**Fig. S6** Average size change of MoS$_2$-ICG in several media including water, PBS, FBS and cell media

Fig. S7 Average diameter change of MoS$_2$-ICG in pH 6.8 condition
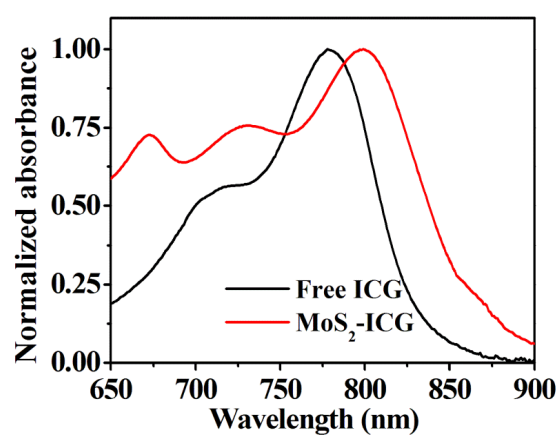

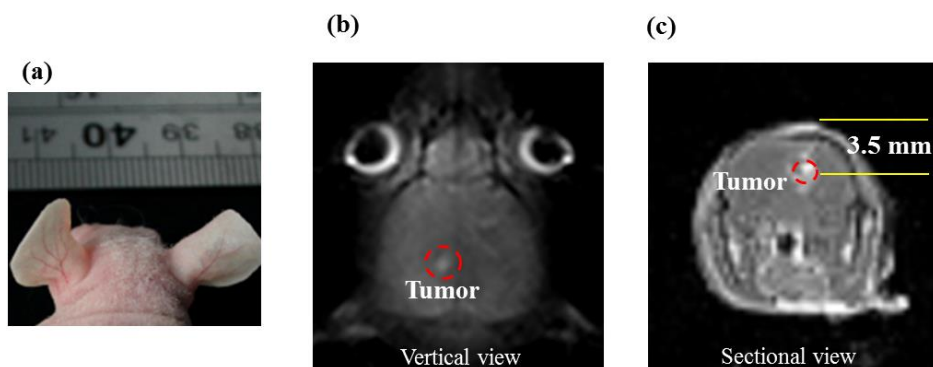**Fig. S8** Normalized absorbance spectrum of MoS$_2$-ICG and ICG

Fig. S9 a Photo of orthotopic brain glioma bearing mouse. (**b, c**) MRI images of orthotopic brain glioma, **b** is MAP image, **c** is cross sectional image. Red dashed line delineates the tumor region

Table S1 The comparison of the imaging depth and applied laser wavelength for the reported photoacoustic brain tumor imaging studies using various types of nanoparticles in the NIR I spectral region

Types of Nanoparticles	Wavelength (nm)	Depth (mm)	Craniotomy	References
Gold-silica based NPs	532	~3	/	[1]
Perylene-Diimide-Based NPs	700	3-4	/	[2]
Coomassie Blue-loaded NPs	590	/	Yes	[3]
HAuNS	800	/	/	[4]
IRDye800-c(KRGDf)	804	3	/	[5]
Prussian blue NPs	800	/	/	[6]
MoS_2 nanosheets	675	1.8	/	[7]
MoS_2-ICG	800	3.5	/	This work

"/": no data or ambiguity in literature