Synthesis, Characterization and X-ray Attenuation Properties of Ultrasmall BiOI Nanoparticles: Towards Renal Clearable Particulate CT Contrast Agents

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Summary of structure determination for BiOI by X-ray powder diffraction

Table S1 *Crystal data*

BiOI	F_{000} = 288
M_r = 351.88	D_x = 8.002 Mg m^{-3}
Tetragonal, *P*4/*nmm*	Melting point: ? K
Hall symbol: -P 4a 2a	$K\alpha_1$, $K\alpha_2$ radiation, λ = 1.540600, 1.544400 Å
a = 3.99399(4) Å	*T* = 295 K
b = 3.99399(4) Å	Specimen shape: disk
c = 9.15486(8) Å	12 × 12 × 0.2 mm
V = 146.038 (3) Å^3	Particle morphology: plate-like, red-orange
Z = 2	

Data collection

D8 Advance powder diffractometer	*T* = 295 K
Radiation source: sealed tube	$2\theta_{min}$ = 7.00°

Monochromator: Ni beta-filter	$2\theta_{max}$ = 109.07°
Specimen mounted in reflection mode	Increment in 2θ = 0.02°
Background-less sample holder	Scan method: step

Refinement

Least-squares matrix: full	54 parameters
R_p = 0.027	2 constraints
R_{wp} = 0.036	S = 1.39
R_{exp} = 0.026	$(\Delta/\sigma)_{max}$ = 0.04
R_{F2} = 0.016	
Profile function: CW Profile function number 3 with 19 terms, Pseudovoigt profile coefficients as parameterized in P. Thompson, D.E. Cox & J.B. Hastings (1987). J. Appl. Cryst.,20,79-83. Asymmetry correction of L.W. Finger, D.E. Cox & A. P. Jephcoat (1994). J. Appl. Cryst.,27,892-900. #1(GU) = 119.081 #2(GV) = -5.084 #3(GW) = 11.207 #4(GP) = 25.131 #5(LX) = 1.863 #6(LY) = 26.859 #7(S/L) = 0.0103 #8(H/L) = 0.0103 #9(trns) = 2.18 #10(shft)= -8.9199 #11(stec)= -9.60 #12(ptec)= 14.58 #13(sfec)= 0.00 #14(L11) = -0.469 #15(L22) = -1.237 #16(L33) = 0.031 #17(L12) = 0.358 #18(L13) = 0.126 #19(L23) = 0.292 Peak tails are ignored where the intensity is below 0.005 times the peak Aniso. broadening axis 0 0 1.	Preferred orientation correction: March-Dollase, Ratio= 0.64143, h= 0, k= 0, l= 1; Preferred orientation correction range: Min= 0.4097, Max= 5.3361

Table S2 *Fractional atomic coordinates and isotropic displacement parameters (Å^2)*

	x	*y*	*z*	U_{iso}
Bi1	0.25	0.25	0.13358 (3)	0.01169 (7)
O1	0.25	0.75	0.0	0.01169 (7)
I1	0.25	0.25	0.66586 (5)	0.01169 (7)

Table S3 *Geometric parameters* (Å, °)

Bi1—O1^{i}	2.3417(2)	O1—Bi1	2.3417(2)
Bi1—O1	2.3417(2)	O1—Bi1^{viii}	2.3417(2)
Bi1—O1^{ii}	2.3417(2)	O1—Bi1^{ix}	2.3417(2)
Bi1—O1^{iii}	2.3417(2)	O1—Bi1^{x}	2.3417(2)
Bi1—I1^{iv}	3.3686(3)	I1—Bi1^{iv}	3.3686(3)
Bi1—I1^{v}	3.3686(3)	I1—Bi1^{v}	3.3686(3)
Bi1—I1^{vi}	3.3686(3)	I1—Bi1^{vi}	3.3686(3)
Bi1—I1^{vii}	3.3686(3)	I1—Bi1^{vii}	3.3686(3)
O1^{i}—Bi1—O1	117.036(13)	O1^{iii}—Bi1—I1^{vi}	77.237(5)
O1^{i}—Bi1—O1^{ii}	74.174(6)	O1^{iii}—Bi1—I1^{vii}	77.237(5)
O1^{i}—Bi1—O1^{iii}	74.174(6)	I1^{iv}—Bi1—I1^{v}	72.716 (7)
O1^{i}—Bi1—I1^{iv}	77.237 (5)	I1^{iv}—Bi1—I1^{vi}	72.716 (7)
O1^{i}—Bi1—I1^{v}	142.2063 (14)	I1^{iv}—Bi1—I1^{vii}	113.940 (15)
O1^{i}—Bi1—I1^{vi}	77.237 (5)	I1^{v}—Bi1—I1^{vi}	113.940 (15)
O1^{i}—Bi1—I1^{vii}	142.2063 (14)	I1^{v}—Bi1—I1^{vii}	72.716 (7)
O1—Bi1—O1^{ii}	74.174(6)	I1^{vi}—Bi1—I1^{vii}	72.716 (7)
O1—Bi1—O1^{iii}	74.174(6)	Bi1—O1—Bi1^{viii}	117.036 (13)
O1—Bi1—I1^{iv}	142.2063 (14)	Bi1—O1—Bi1^{ix}	105.826 (6)
O1—Bi1—I1^{v}	77.237 (5)	Bi1—O1—Bi1^{x}	105.826 (6)
O1—Bi1—I1^{vi}	142.2063 (14)	Bi1^{viii}—O1—Bi1^{ix}	105.826 (6)
O1—Bi1—I1^{vii}	77.237 (5)	Bi1^{viii}—O1—Bi1^{x}	105.826 (6)
O1^{ii}—Bi1—O1^{iii}	117.036 (13)	Bi1^{ix}—O1—Bi1^{x}	117.036 (13)
O1^{ii}—Bi1—I1^{iv}	77.237 (5)	Bi1^{iv}—I1—Bi1^{v}	72.716 (7)

O1^{ii}—Bi1—I1^{v}	77.237 (5)	Bi1^{iv}—I1—Bi1^{vi}	72.716 (7)
O1^{ii}—Bi1—I1^{vi}	142.2063 (14)	Bi1^{iv}—I1—Bi1^{vii}	113.940 (15)
O1^{ii}—Bi1—I1^{vii}	142.2063 (14)	Bi1^{v}—I1—Bi1^{vi}	113.940 (15)
O1^{iii}—Bi1—I1^{iv}	142.2063 (14)	Bi1^{v}—I1—Bi1^{vii}	72.716 (7)
O1^{iii}—Bi1—I1^{v}	142.2063 (14)	Bi1^{vi}—I1—Bi1^{vii}	72.716 (7)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) 1/2−*y*, *x*, *z*; (iii) 3/2−*y*, *x*, *z*; (iv) −*x*, −*y*, 1−*z*; (v) −*x*, 1−*y*, 1−*z*; (vi) 1−*x*, −*y*, 1−*z*; (vii) 1−*x*, 1−*y*, 1−*z*; (viii) *x*, *y*+1, *z*; (ix) −*x*, 1−*y*, −*z*; (x) 1−*x*, 1−*y*, −*z*.

Data collection: *XRD commander*; cell refinement: *GSAS*; program(s) used to refine structure: *GSAS*; software used to prepare material for publication: *Platon*, *publCIF*.

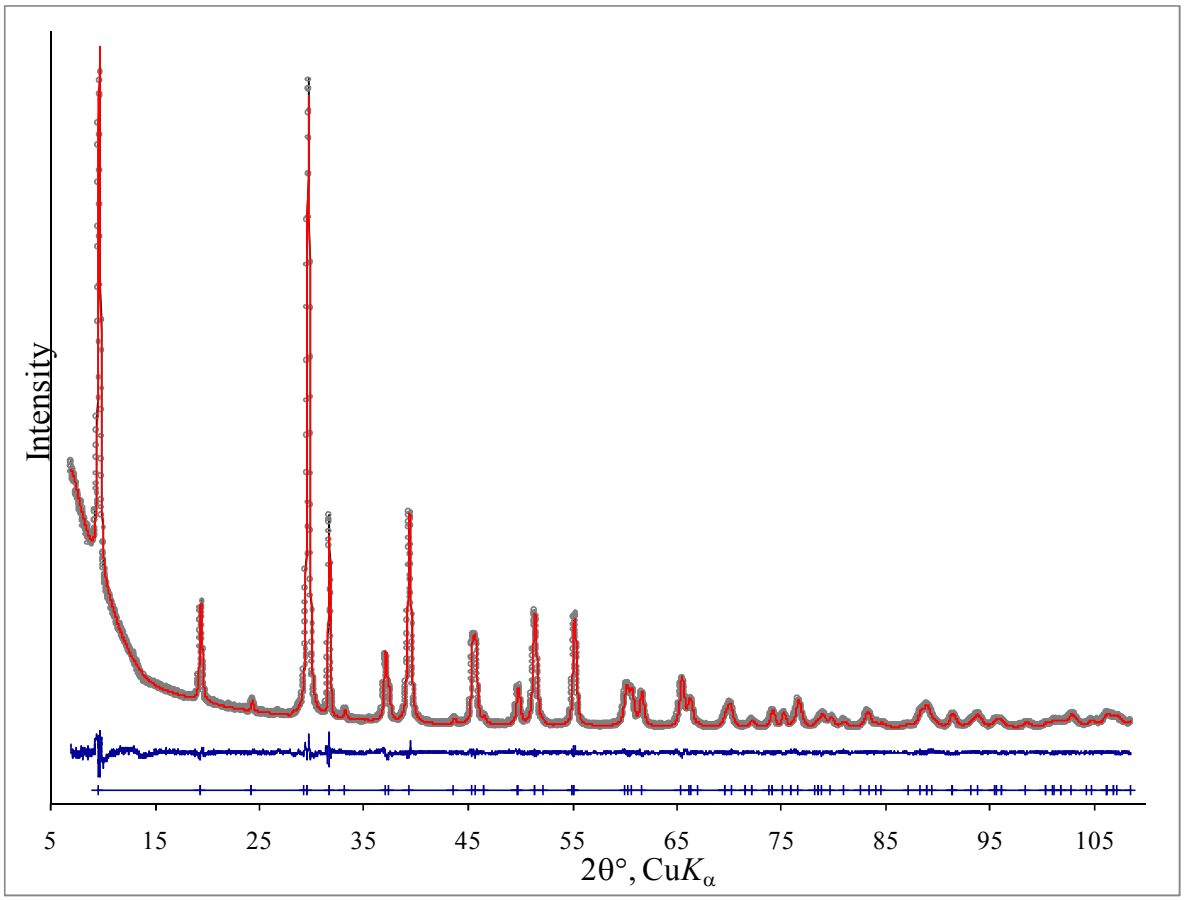

Figure S1 Rietveld refinement plot of BiOI with the difference between observed and calculated patterns shown at the bottom and the reflection positions shown as the vertical lines

Other spectroscopic characterization data

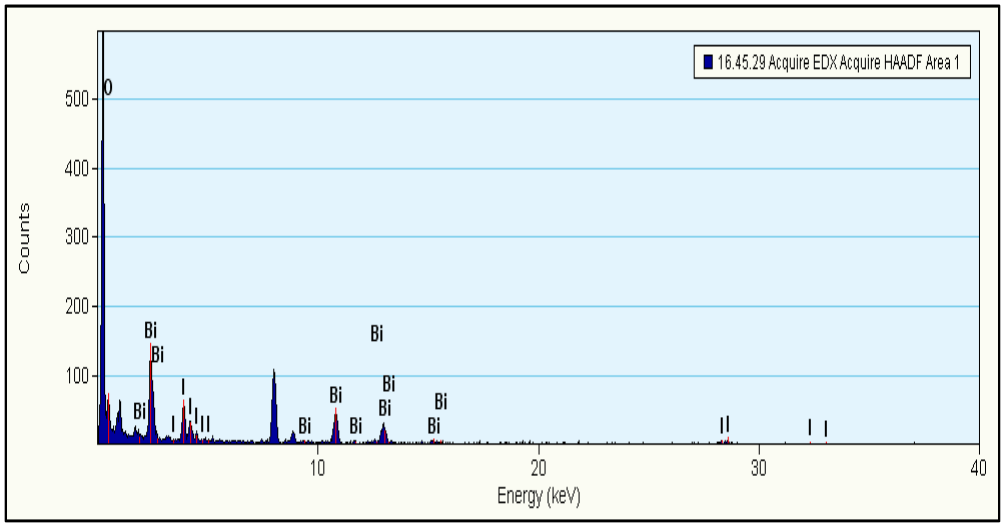

Figure S2 EDX spectrum of a typical PVP-coated BiOI nanoparticle

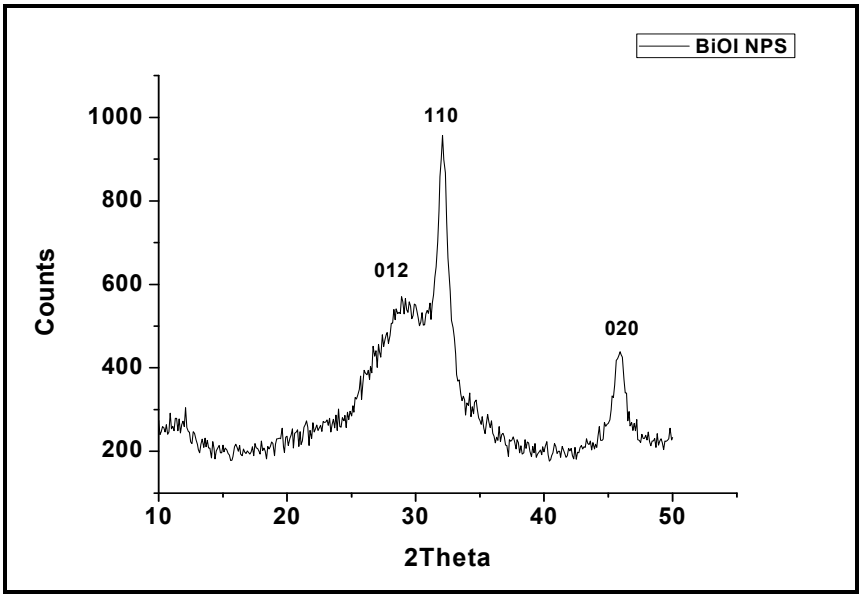

Figure S3 X-ray powder diffraction patterns of the BiOI NPs

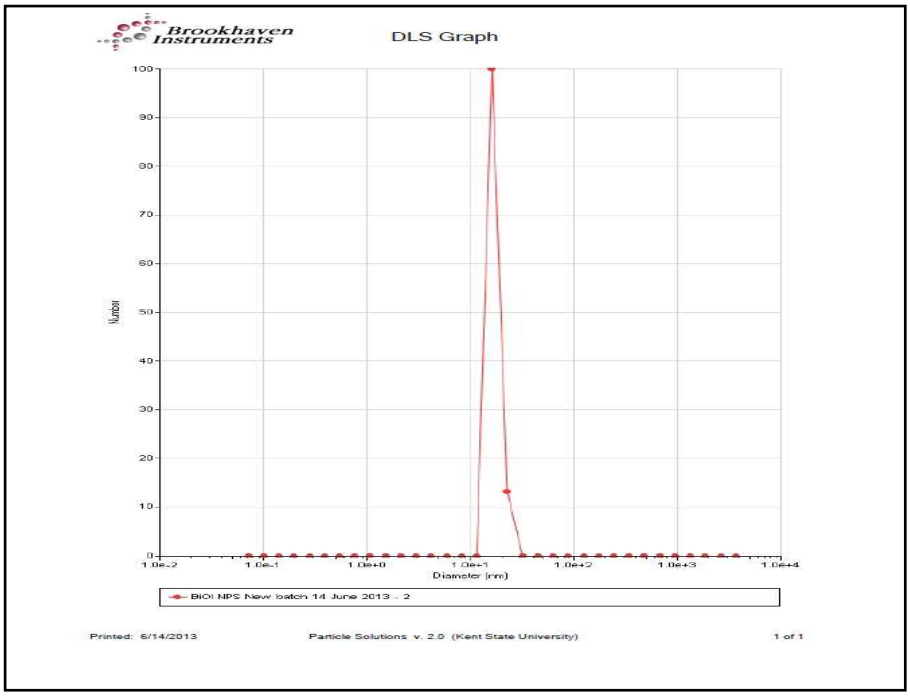

Figure S4 Particle size distribution of PVP-coated BiOI NPs in water dispersion

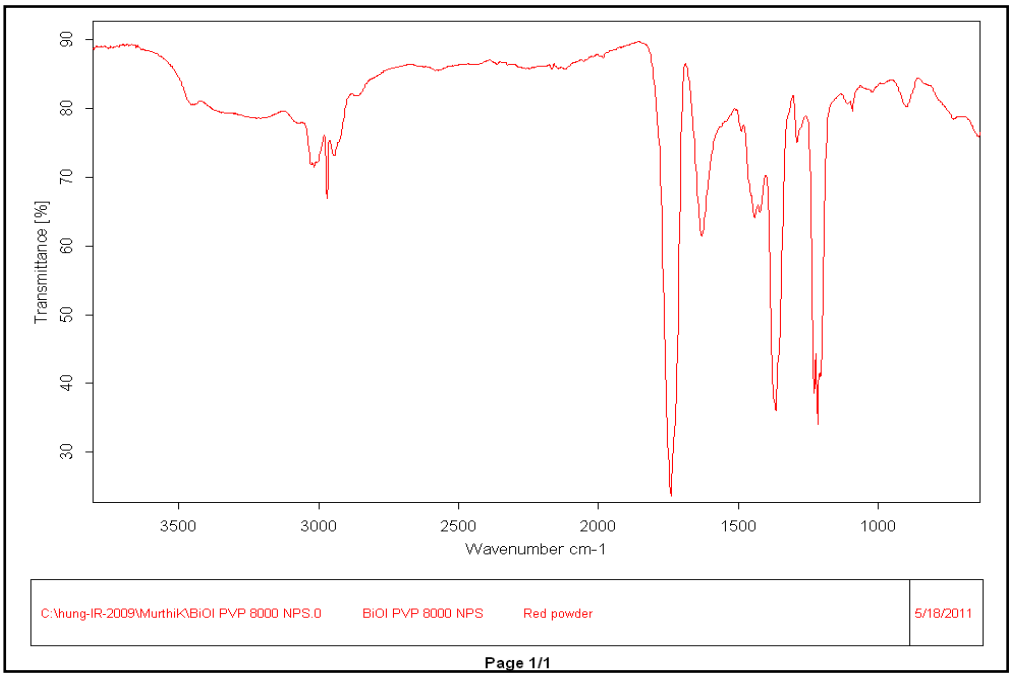

Figure S5 The FT-IR spectrum of PVP-coated BiOI NPs

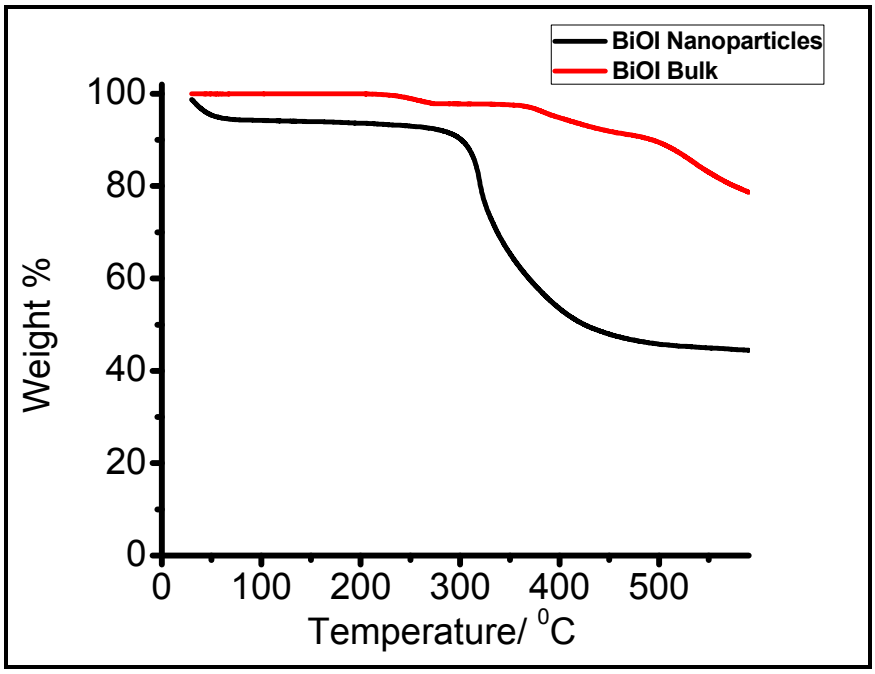

Figure S6 The TGA curve of PVP-coated BiOI NP

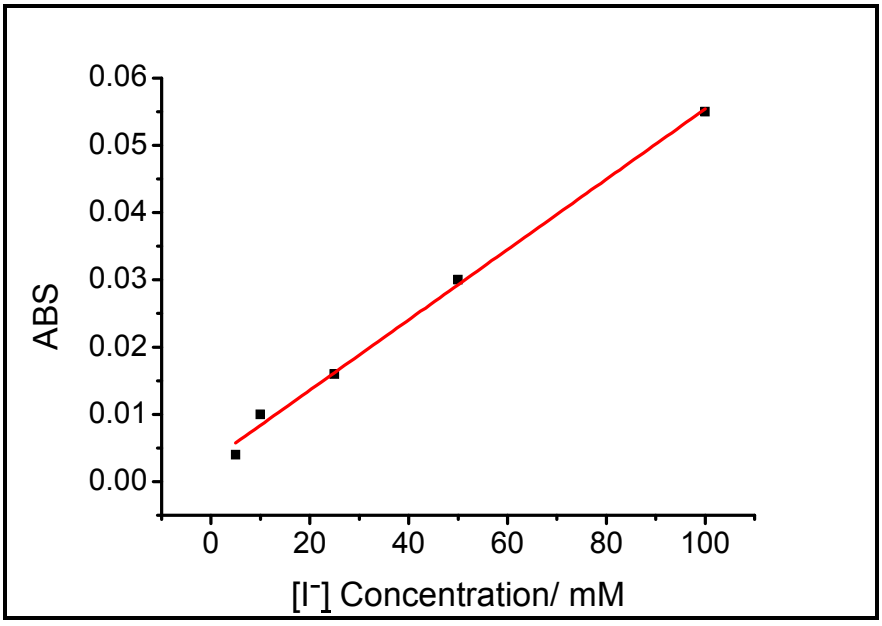

Figure S7 Calibration curve of absorbance *vs*. I^- concentration

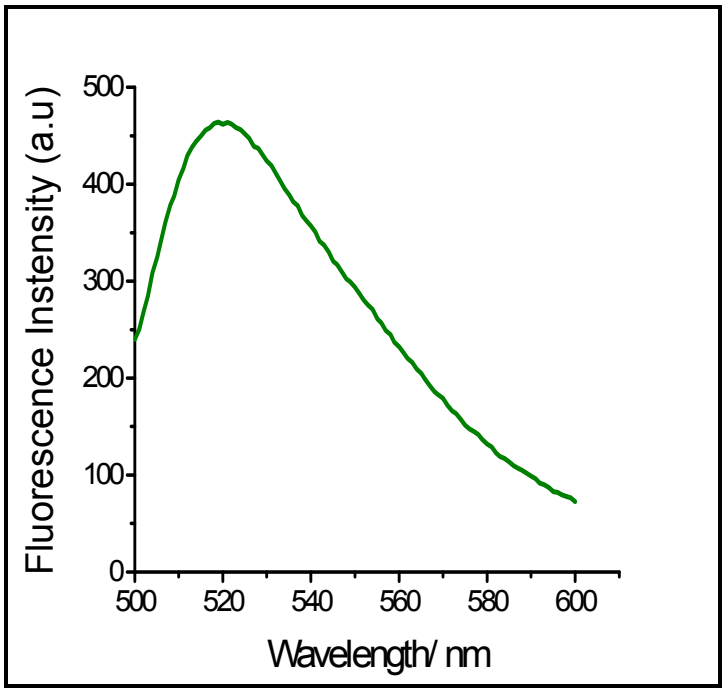

Figure S8 Fluorescence emission spectrum of dye-conjugated BiOI NPs