Supplementary Data

Synthesis, radiolabelling and biodistribution studies of triazole derivatives

for targeting melanoma.

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Figure S1: ^1H NMR of compound **4e** (CDCl_3 , 600 MHz)

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Figure S3: High Resolution Mass Spectrum (ESI^+) of compound **4e**

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Figure S9: ^1H NMR of compound **4h** (CDCl_3 , 600 MHz)

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Figure S12: ^{13}C NMR of compound **4i** (CDCl_3 , 150 MHz)

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Figure S13: ¹H NMR of compound **5e** (CDCl₃, 600 MHz)

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Figure S14: ^{13}C NMR of compound **5e** (CDCl_3 , 150 MHz)

Figure S15: ^1H NMR of compound **5f** (CDCl_3 , 600 MHz)

Figure S16: ^{13}C NMR of compound **5f** (CDCl_3 , 150 MHz)

Figure S17: High Resolution Mass Spectrum (ESI^+) of compound **5f**

Figure S18: ^1H NMR of compound **5g** (CDCl_3 , 600 MHz)

Figure S19: ^{13}C NMR of compound **5g** (CDCl_3 , 150 MHz)

Figure S20: ^1H NMR of compound **5h** (CDCl_3 , 600 MHz)

Figure S21: ¹³C NMR of compound **5h** (CDCl₃, 150 MHz)

Figure S23: ^{13}C NMR of compound **5i** (CDCl_3 , 150 MHz)

Figure S24: ¹H NMR of compound **6a** (600 MHz, MeOD)

Figure S25: ¹³C NMR of compound **6a** (MeOD, 150 MHz)

Figure S26: IR spectrum of compound **6a**

Figure S27: High Resolution Mass Spectrum (ESI⁺) of compound **6a**

Figure S28: ^1H NMR of compound **6b** (CDCl_3 , 600 MHz)

Figure S29: ¹³C NMR of compound **6b** (CDCl₃, 150 MHz)

Figure S30: IR Spectrum of compound **6b**

Figure S31: High Resolution Mass Spectrum (ESI⁺) of compound **6b**

Figure S32: ¹H NMR of compound **6c** (CDCl₃, 600 MHz)

Figure S33: ^{13}C NMR of compound **6c** (CDCl_3 , 150 MHz)

Figure S34: IR spectrum of compound **6c**

Figure S35: High Resolution Mass Spectrum (ESI⁺) of compound **6c**

Figure S36: ^1H NMR of compound **6d** (CDCl_3 , 600 MHz)

Figure S37: ¹³C NMR of compound **6d** (CDCl₃, 150 MHz)

Figure S38: IR spectrum of compound **6d**

Figure S39: High Resolution Mass Spectrum (ESI⁺) of compound **6d**

Figure S40: ^1H NMR of compound **6e** (CDCl_3 , 600 MHz)

Figure S41: ^{13}C NMR of compound **6e** (CDCl_3 , 150 MHz)

Figure S42: IR spectrum of compound **6e**

Figure S43: High Resolution Mass Spectrum (ESI⁺) of compound **6e**

Figure S44: ^1H NMR of compound **6f** (CDCl_3 , 600 MHz)

Figure S45: ^{13}C NMR of compound **6f** (CDCl_3 , 150 MHz)

Figure S46: IR spectrum of compound **6f**

Figure S47: High Resolution Mass Spectrum (ESI⁺) of compound **6f**

Figure S49: ^{13}C NMR of compound **6g** (CDCl_3 , 150 MHz)

Figure S50: IR spectrum of compound **6g**

Figure S51: High Resolution Mass Spectrum (ESI⁺) of compound **6g**

Figure S52: ^1H NMR of compound **6h** (CDCl_3 , 600 MHz)

Figure S53: ^{13}C NMR of compound **6h** (CDCl_3 , 150 MHz)

Figure S54: IR spectrum of compound **6h**

Figure S55: High Resolution Mass Spectrum (ESI⁺) of compound **6h**

Figure S56: ^1H NMR of compound **6i** (CDCl_3 , 600 MHz)

Figure S57: ^{13}C NMR of compound **6i** (CDCl_3 , 150 MHz)

Figure S58: IR spectrum of compound **6i**

Figure S59: High Resolution Mass Spectrum (ESI⁺) of compound **6i**

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Figure S60: ^1H NMR of compound **7a** (D_2O , 600 MHz)

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PL13W 0.07535660 W
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SF 150.9028090 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 1.00

Figure S61: ^{13}C NMR of compound **7a** (D_2O , 150 MHz)

Figure S62: IR spectrum of compound **7a**

Figure S63 : High Resolution Mass Spectrum (ESI⁺) of compound **7a**

Figure S64: γ -HPLC chromatogram (bottom) of [^{125}I]-**7a** with co-injection of **7a**

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Figure S65: ^1H NMR of compound **7b** (chloroform-d, 600 MHz)

Figure S66: Low resolution mass spectrum ESI⁺ of compound **7b**

Figure S67: γ -HPLC chromatogram (bottom) of [^{125}I]-**7b** with co-injection of **7b**

Figure S68: ¹H NMR of compound **7c** (MeOD, 600 MHz)

Figure S69: ^{13}C NMR of compound **7c** (MeOD , 150 MHz)

Figure S70: IR spectrum of compound **7c**

Figure S71 : High Resolution Mass Spectrum (ESI⁺) of compound **7c**

Figure S72: γ -HPLC chromatogram (bottom) of [^{125}I]-**7c** with co-injection of **7c**

Figure S73: ^1H NMR of compound **7d** (MeOD, 600 MHz)

Figure S74: ¹³C NMR of compound **7d** (MeOD, 150 MHz)

Figure S75: IR of compound **7d**

Figure S76: High Resolution Mass Spectrum (ESI⁺) of compound **7d**

Figure S77: γ -HPLC chromatogram (bottom) of [^{125}I]-**7d** with co-injection of **7d**

ITAAGDMeABP

JFV4B23755 (0.027) Is (0.10,0.01) C₁₈H₂₄IN₅O₃H

15-Oct-2013

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7.96e12

Figure S78: High Resolution Mass Spectrum (ESI⁺) of compound **7e**

Figure S79: γ -HPLC chromatogram (bottom) of [¹²⁵I]-**7e** with co-injection of **7e**

ITAAGDNABP

JFV4B23756 (0.027) Is (0.10,0.01) C₁₆H₁₈IN₇O₅H

15-Oct-2013

1: TOF MS ES+
8.05e12

Figure S80: High Resolution Mass Spectrum (ESI⁺) of compound **7f**

Figure S81: γ -HPLC chromatogram (bottom) of [¹²⁵I]-**7f** with co-injection of **7f**

1TAAGoFABP

JFV423905 (0.028) Is (1.00,1.00) C₁₆H₁₉FIN₅OH

1: TOF MS ES+
8.18e12

JFV423905 126 (2.403) AM (Cen,4, 80.00, Ht,5000.0,922.01,1.00); Sb (99,10.00); Sm (Mn, 2x3.00); Cm (124:138)

1.86e3

Figure S82: High Resolution Mass Spectrum (ESI⁺) of compound **7g**

Figure S83: γ -HPLC chromatogram (bottom) of [¹²⁵I]-**7g** with co-injection of **7g**

1TAAGmFABP

JFV4B23903 (0.027) Is (1.00,1.00) C₁₆H₁₉FIN₅OH

1: TOF MS ES+
8.18e12

JFV4B23903 31 (0.596) AM (Cen,4, 80.00, Ht,5000.0,922.01,1.00); Sb (99,10.00); Sm (Mn, 2x3.00); Cm (6:31) 1: TOF MS ES+
1.75e3

Figure S84: High Resolution Mass Spectrum (ESI⁺) of compound **7h**

Figure S85: γ -HPLC chromatogram (bottom) of [¹²⁵I]-**7h** with co-injection of **7h**

1TAAGpFABP

JFV4B23904 (0.027) Is (1.00,1.00) C₁₆H₁₉FIN₅OH

1: TOF MS ES+
8.18e12

Figure S86: High Resolution Mass Spectrum (ESI⁺) of compound **7i**

Figure S87: γ -HPLC chromatogram (bottom) of [¹²⁵I]-**7i** with co-injection of **7i**

General procedure 4: Preparation of non-radioactive standards (7a-i).

To a solution of tin precursor (1 equiv.) in THF (1 mL) was added molecular iodine (1.2 equiv.) and the reaction was stirred for 10 min. The reaction mixture was subsequently quenched with an excess of saturated Na₂S₂O₃(aq) and the product used as an HPLC reference standard.

7a *N*-(2-Diethylamino-ethyl)-2-(4-iodo-[1,2,3]triazol-1-yl)-acetamide. Following general procedure 4, product was isolated as a clear oil (41%, 0.020 g). ¹H NMR (D₂O, 600 MHz) δ: 8.46 (s, 1H), 8.18 (s, 1H), 5.31 (s, 2H), 3.49 (t, 2H), 2.91 (t, 2H), 2.84 (m, 4H), 1.12 (t, 6H). ¹³C NMR (D₂O, 150 MHz) δ: 171.0, 167.7, 132.6, 87.1, 50.0, 47.0, 35.8, 9.3. IR: (KBr disc) $\bar{\nu}$ = 3267, 2967, 1599 cm⁻¹. HRMS-ESI (*m/z*): [M+H]⁺ calcd for C₁₀H₁₈N₅OIH: 352.0634; found 352.0626.

7b *N*-(2-Diethylamino-ethyl)-2-(4-iodo-[1,2,3]triazol-1-yl)-acetamide. Following general procedure 4, the product was isolated as a clear oil (0.0010g, 79%). ¹H NMR (CDCl₃, 600 MHz) δ: 7.50 (m, 3H), 7.43 (m, 2H), 7.08 (s, 1H), 5.02 (s, 2H), 3.60 (s, 2H), 3.15 (m, 6H), 1.30 (m, 6H). LRMS-ESI (*m/z*): 421.

7c 2-(4-Iodo-1*H*-1,2,3-triazol-1-yl)-*N*-(2-(piperidin-1-yl)ethyl)acetamide. Following general procedure 4, the product was isolated as a clear oil (81%, 0.010 g). ¹H NMR (MeOD, 600 MHz) δ: 8.20 (s, 1H), 5.29 (s, 2H), 3.64 (m, 4H), 3.26 (t, 2H, J=6.0 Hz), 2.95 (s, 2H), 1.88 (s, 5H), 1.54 (s, 1H). ¹³C NMR (MeOD, 150 MHz) δ: 169.0, 133.4, 87.8, 57.6, 54.8, 53.2, 35.5, 24.2, 22.7. IR: (KBr disc) $\bar{\nu}$ = 3315, 2936, 1684, 1623, 1559, 1447, 1253, 1203, 1130 cm⁻¹. HRMS-ESI (*m/z*): [M+H]⁺ calcd for C₁₁H₁₉N₅OI: 365.0660; found 365.0717.

7d *N*-(1-Benzylpiperidin-4-yl)-2-(4-iodo-1*H*-1,2,3-triazol-1-yl)acetamide. Following general procedure 4, the product was isolated as a white solid (22%, 0.018 g yield). ¹H NMR (MeOD, 600 MHz) δ: 8.13 (s, 1H), 7.34 (m, 4H), 7.28 (m, 1H), 5.15 (s, 2H), 3.70 (m, 1H), 3.57 (s, 2H), 2.91 (m, 2H), 2.20 (m, 2H), 1.90 (m, 2H), 1.57 (m, 2H). ¹³C NMR (MeOD, 150 MHz) δ: 166.7, 133.2,

130.8, 129.4, 128.7, 87.6, 63.8, 53.1, 48.2, 32.1. IR: (KBr disc) $\bar{\nu}$ = 3293, 2924, 2802, 2761, 1668, 1551, 1450. HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{20}N_5OI$: 427.0827; found 427.0819.

7e *N-(1-(3,5-Dimethoxybenzyl)piperidin-4-yl)-2-(4-iodo-1H-1,2,3-triazol-1-yl)acetamide.*

See general procedure 4. HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{18}H_{24}N_5O_3IH$: 486.1002; found 486.0998.

7f *N-(1-(3,5-Dinitrobenzyl)piperidin-4-yl)-2-(4-iodo-1H-1,2,3-triazol-1-yl)acetamide.*

See general procedure 4. HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{18}N_7O_5IH$: 516.0493; found 516.0486.

7g *N-(1-(2-Fluorobenzyl)piperidin-4-yl)-2-(4-iodo-1H-1,2,3-triazol-1-yl)acetamide.*

See general procedure 4. HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{19}N_5OIFH$: 444.0697; found 444.0716.

7h *N-(1-(3-Fluorobenzyl)piperidin-4-yl)-2-(4-iodo-1H-1,2,3-triazol-1-yl)acetamide.*

See general procedure 4. HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{19}N_5OIF$: 444.0697; found 444.0695.

7i *N-(1-(4-Fluorobenzyl)piperidin-4-yl)-2-(4-iodo-1H-1,2,3-triazol-1-yl)acetamide.*

See general procedure 4. HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{19}N_5OIFH$: 444.0697; found 444.0706.

Table S1.

Biodistribution Data at 24h post-injection of [$^{123/125}$ I]-labelled BZA and **7a-7d**

	Compound									
Tissue	BZA		7a		7b		7c		7d	
	%ID/g	SEM	%ID/g	SEM	%ID/g	SEM	%ID/g	SEM	%ID/g	SEM
Blood	0.04	0.00	0.01	0.00	0.01	0.00	0.05	0.01	0.01	0.00
Adipose	0.03	0.01	0.00	0.00	0.00	0.00	0.02	0.01	0.00	0.00
Adrenals	0.06	0.03	0.00	0.00	0.04	0.02	0.03	0.02	0.01	0.00
Bone	0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Brain	0.02	0.01	0.00	0.00	0.00	0.00	0.04	0.01	0.00	0.00
Eyes	13.55	1.59	1.50	0.16	6.84	1.05	3.17	0.73	6.59	0.41
Gall Bladder	0.42	0.15	0.00	0.00	1.01	0.42	0.19	0.11	0.02	0.01
Heart	0.06	0.01	0.00	0.00	0.01	0.00	0.06	0.03	0.01	0.00
Kidney	0.17	0.04	0.00	0.00	0.41	0.04	0.08	0.02	0.02	0.00
Lg Intest.	0.11	0.02	0.03	0.00	1.36	0.34	0.33	0.19	0.18	0.05
Liver	0.99	0.03	0.00	0.00	2.42	0.51	0.12	0.04	0.08	0.00
Lungs	0.13	0.04	0.00	0.00	0.01	0.00	0.16	0.04	0.02	0.01
Skeletal Muscle	0.02	0.01	0.00	0.00	0.00	0.00	0.02	0.01	0.00	0.00
Sm Intest.	0.08	0.03	0.01	0.00	0.49	0.09	0.10	0.05	0.05	0.01
Spleen	1.04	0.98	0.04	0.02	0.01	0.00	0.04	0.01	0.38	0.38
Stomach	0.21	0.07	0.03	0.00	0.08	0.02	0.22	0.07	0.10	0.02
Thyroid-Trachea	5.43	1.86	5.03	1.13	11.78	0.17	24.52	4.92	7.71	2.21
Tumour	6.50	0.31	0.09	0.04	0.89	0.21	0.77	0.11	2.21	0.46
Urine-Bladder	3.04	1.24	0.25	0.08	0.39	0.09	0.63	0.08	0.30	0.01

Table S2.

Biodistribution Data at 24h post-injection of [$^{123/125}\text{I}$]-labelled BZA, and **7e-7i**

	Compound											
Tissue	BZA		7e		7f		7g		7h		7i	
	%ID/g	SEM	%ID/g	SEM	%ID/g	SEM	%ID/g	SEM	%ID/g	SEM	%ID/g	SEM
Blood	0.04	0.00	0.02	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00
Adipose	0.03	0.01	0.04	0.03	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.00
Adrenals	0.06	0.03	0.00	0.00	0.01	0.00	0.03	0.01	0.01	0.01	0.08	0.02
Bone	0.03	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00
Brain	0.02	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Eyes	13.55	1.59	7.36	0.20	8.06	1.30	4.61	0.41	4.68	1.02	8.39	0.71
Gall Bladder	0.42	0.15	0.01	0.01	0.02	0.02	0.28	0.09	0.20	0.10	0.03	0.02
Heart	0.06	0.01	0.03	0.00	0.04	0.00	0.01	0.00	0.01	0.00	0.03	0.00
Kidney	0.17	0.04	0.07	0.00	0.07	0.01	0.05	0.01	0.07	0.01	0.06	0.00
Lg Intest.	0.11	0.02	0.24	0.04	0.40	0.09	0.36	0.14	0.27	0.05	0.24	0.08
Liver	0.99	0.03	0.13	0.01	0.14	0.01	0.09	0.01	0.03	0.01	0.11	0.03
Lungs	0.13	0.04	0.02	0.01	0.04	0.00	0.02	0.00	0.02	0.00	0.04	0.01
Skeletal Muscle	0.02	0.01	0.00	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00
Sm Intest.	0.08	0.03	0.13	0.07	0.09	0.01	0.12	0.05	0.08	0.02	0.07	0.02
Spleen	1.04	0.98	0.02	0.01	0.01	0.00	0.01	0.00	0.02	0.00	0.66	0.63
Stomach	0.21	0.07	0.13	0.03	0.26	0.06	0.15	0.04	0.11	0.04	0.16	0.05
Thyroid-Trachea	5.43	1.86	12.8	1.39	9.48	3.06	1.46	0.30	5.93	4.02	2.21	0.77
Tumour	6.50	0.31	1.32	0.27	1.15	0.47	1.03	0.19	1.89	0.72	1.91	0.26
Urine-Bladder	3.04	1.24	0.48	0.06	0.22	0.10	0.55	0.50	0.55	0.50	1.85	0.76

Table S3.

Crystal data and structure refinement for **7d**.

Identification code	ITAAG
Empirical formula	C ₁₆ H ₂₀ I N ₅ O
Formula weight	425.27
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P b c a
Unit cell dimensions	a = 11.1319(19) Å α = 90°. b = 9.6191(17) Å β = 90°. c = 33.175(6) Å γ = 90°.
Volume	3552.3(11) Å ³
Z	8
Density (calculated)	1.590 Mg/m ³
Absorption coefficient	1.814 mm ⁻¹
F(000)	1696
Crystal size	0.222 x 0.044 x 0.020 mm ³
Theta range for data collection	2.203 to 26.473°.
Index ranges	-13 ≤ h ≤ 12, -12 ≤ k ≤ 12, -41 ≤ l ≤ 41
Reflections collected	35669
Independent reflections	3648 [R(int) = 0.0689]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9955 and 0.7294
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3648 / 0 / 211
Goodness-of-fit on F ²	1.028
Final R indices [I > 2σ(I)]	R1 = 0.0339, wR2 = 0.0579
R indices (all data)	R1 = 0.0674, wR2 = 0.0665
Extinction coefficient	n/a
Largest diff. peak and hole	0.932 and -0.778 e.Å ⁻³

Table S4.

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	9314(1)	5772(1)	4472(1)	46(1)
O(1)	7582(2)	8091(2)	5954(1)	42(1)
N(1)	8782(3)	8986(3)	5290(1)	29(1)
N(2)	7009(3)	10245(3)	6134(1)	26(1)
N(3)	5604(2)	10554(3)	7312(1)	29(1)
N(4)	10277(2)	7793(3)	5080(1)	35(1)
N(5)	9975(3)	8803(3)	5329(1)	37(1)
C(1)	9278(3)	7364(3)	4888(1)	28(1)
C(2)	8321(3)	8109(3)	5018(1)	28(1)
C(3)	8174(3)	10009(3)	5535(1)	38(1)
C(4)	7564(3)	9353(3)	5898(1)	28(1)
C(5)	6351(3)	9863(3)	6496(1)	25(1)
C(6)	5394(3)	10950(4)	6586(1)	36(1)
C(7)	4760(3)	10633(4)	6978(1)	37(1)
C(8)	7179(3)	9717(4)	6856(1)	31(1)
C(9)	6482(3)	9460(3)	7242(1)	34(1)
C(10)	4976(3)	10352(4)	7694(1)	34(1)
C(11)	5701(3)	10708(3)	8060(1)	31(1)
C(12)	5543(3)	10020(4)	8422(1)	41(1)
C(13)	6171(4)	10393(5)	8765(1)	54(1)
C(14)	6958(4)	11495(5)	8752(1)	51(1)
C(15)	7116(3)	12214(4)	8397(1)	48(1)
C(16)	6499(3)	11818(4)	8052(1)	39(1)

Table S5.

Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **7d**.

I(1)-C(1)	2.061(3)
O(1)-C(4)	1.228(4)
N(1)-C(2)	1.337(4)
N(1)-N(5)	1.346(4)
N(1)-C(3)	1.445(4)
N(2)-C(4)	1.316(4)
N(2)-C(5)	1.454(4)
N(2)-H(2)	0.70(3)
N(3)-C(7)	1.455(4)
N(3)-C(9)	1.455(4)
N(3)-C(10)	1.459(4)
N(4)-N(5)	1.319(4)
N(4)-C(1)	1.346(4)
C(1)-C(2)	1.354(4)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.521(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(5)-C(8)	1.516(4)
C(5)-C(6)	1.523(4)
C(5)-H(5A)	1.0000
C(6)-C(7)	1.511(5)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.518(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900

C(10)-C(11)	1.500(5)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.380(5)
C(11)-C(16)	1.389(5)
C(12)-C(13)	1.383(6)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.376(6)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.377(5)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.388(5)
C(15)-H(15A)	0.9500
C(16)-H(16A)	0.9500

C(2)-N(1)-N(5)	111.2(3)
C(2)-N(1)-C(3)	129.0(3)
N(5)-N(1)-C(3)	119.8(3)
C(4)-N(2)-C(5)	124.2(3)
C(4)-N(2)-H(2)	117(3)
C(5)-N(2)-H(2)	119(3)
C(7)-N(3)-C(9)	110.5(3)
C(7)-N(3)-C(10)	111.0(3)
C(9)-N(3)-C(10)	111.3(3)
N(5)-N(4)-C(1)	108.1(3)
N(4)-N(5)-N(1)	106.7(3)
N(4)-C(1)-C(2)	109.8(3)
N(4)-C(1)-I(1)	121.8(2)
C(2)-C(1)-I(1)	128.4(3)
N(1)-C(2)-C(1)	104.3(3)
N(1)-C(2)-H(2A)	127.9
C(1)-C(2)-H(2A)	127.9
N(1)-C(3)-C(4)	111.8(3)
N(1)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3A)	109.2
N(1)-C(3)-H(3B)	109.2

C(4)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	107.9
O(1)-C(4)-N(2)	124.3(3)
O(1)-C(4)-C(3)	121.5(3)
N(2)-C(4)-C(3)	114.2(3)
N(2)-C(5)-C(8)	111.6(3)
N(2)-C(5)-C(6)	109.9(3)
C(8)-C(5)-C(6)	109.6(3)
N(2)-C(5)-H(5A)	108.6
C(8)-C(5)-H(5A)	108.6
C(6)-C(5)-H(5A)	108.6
C(7)-C(6)-C(5)	110.9(3)
C(7)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6A)	109.5
C(7)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	108.1
N(3)-C(7)-C(6)	111.4(3)
N(3)-C(7)-H(7A)	109.3
C(6)-C(7)-H(7A)	109.3
N(3)-C(7)-H(7B)	109.3
C(6)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	108.0
C(9)-C(8)-C(5)	111.7(3)
C(9)-C(8)-H(8A)	109.3
C(5)-C(8)-H(8A)	109.3
C(9)-C(8)-H(8B)	109.3
C(5)-C(8)-H(8B)	109.3
H(8A)-C(8)-H(8B)	107.9
N(3)-C(9)-C(8)	111.1(3)
N(3)-C(9)-H(9A)	109.4
C(8)-C(9)-H(9A)	109.4
N(3)-C(9)-H(9B)	109.4
C(8)-C(9)-H(9B)	109.4
H(9A)-C(9)-H(9B)	108.0
N(3)-C(10)-C(11)	114.5(3)

N(3)-C(10)-H(10A)	108.6
C(11)-C(10)-H(10A)	108.6
N(3)-C(10)-H(10B)	108.6
C(11)-C(10)-H(10B)	108.6
H(10A)-C(10)-H(10B)	107.6
C(12)-C(11)-C(16)	117.8(3)
C(12)-C(11)-C(10)	121.8(3)
C(16)-C(11)-C(10)	120.3(3)
C(11)-C(12)-C(13)	121.7(4)
C(11)-C(12)-H(12A)	119.2
C(13)-C(12)-H(12A)	119.2
C(14)-C(13)-C(12)	119.8(4)
C(14)-C(13)-H(13A)	120.1
C(12)-C(13)-H(13A)	120.1
C(15)-C(14)-C(13)	119.6(4)
C(15)-C(14)-H(14A)	120.2
C(13)-C(14)-H(14A)	120.2
C(14)-C(15)-C(16)	120.3(4)
C(14)-C(15)-H(15A)	119.9
C(16)-C(15)-H(15A)	119.9
C(15)-C(16)-C(11)	120.8(4)
C(15)-C(16)-H(16A)	119.6
C(11)-C(16)-H(16A)	119.6

Symmetry transformations used to generate equivalent atoms:

Table S6.

Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
I(1)	66(1)	41(1)	30(1)	-5(1)	1(1)	12(1)
O(1)	59(2)	20(1)	45(1)	4(1)	15(1)	9(1)
N(1)	31(2)	24(2)	32(2)	3(1)	6(1)	3(1)
N(2)	32(2)	15(1)	32(2)	2(1)	4(1)	-1(1)
N(3)	23(2)	33(2)	32(1)	-2(1)	3(1)	4(1)
N(4)	26(2)	36(2)	42(2)	2(2)	4(1)	5(1)
N(5)	36(2)	33(2)	42(2)	-1(1)	-1(2)	-2(1)
C(1)	30(2)	27(2)	26(2)	4(1)	4(2)	3(2)
C(2)	26(2)	28(2)	28(2)	6(2)	2(2)	1(2)
C(3)	50(2)	26(2)	38(2)	1(2)	14(2)	6(2)
C(4)	30(2)	22(2)	31(2)	1(2)	0(1)	2(2)
C(5)	27(2)	20(2)	30(2)	-3(1)	3(2)	0(1)
C(6)	31(2)	39(2)	37(2)	-1(2)	-5(2)	6(2)
C(7)	24(2)	44(2)	44(2)	-5(2)	0(2)	7(2)
C(8)	27(2)	36(2)	30(2)	-1(2)	1(2)	8(2)
C(9)	32(2)	36(2)	32(2)	1(2)	2(2)	9(2)
C(10)	26(2)	38(2)	39(2)	-1(2)	9(2)	-3(2)
C(11)	28(2)	31(2)	35(2)	-4(2)	8(2)	7(2)
C(12)	37(2)	43(2)	44(2)	7(2)	5(2)	2(2)
C(13)	51(3)	67(3)	44(2)	11(2)	9(2)	19(2)
C(14)	45(3)	73(3)	35(2)	-20(2)	-2(2)	21(2)
C(15)	38(2)	48(2)	57(3)	-18(2)	4(2)	0(2)
C(16)	37(2)	39(2)	41(2)	-4(2)	4(2)	1(2)

Table S7.

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7d**.

	x	y	z	U(eq)
H(2)	7090(30)	10950(30)	6092(11)	31
H(2A)	7507	8028	4935	33
H(3A)	7564	10494	5369	46
H(3B)	8763	10710	5628	46
H(5A)	5945	8950	6448	31
H(6A)	5773	11880	6603	43
H(6B)	4800	10969	6364	43
H(7A)	4160	11368	7033	45
H(7B)	4329	9737	6953	45
H(8A)	7739	8934	6810	37
H(8B)	7661	10575	6886	37
H(9A)	6065	8553	7224	40
H(9B)	7047	9419	7473	40
H(10A)	4723	9368	7713	41
H(10B)	4240	10930	7693	41
H(12A)	4988	9270	8435	50
H(13A)	6060	9889	9008	65
H(14A)	7389	11759	8987	62
H(15A)	7649	12985	8388	57
H(16A)	6625	12311	7808	47

Table S8.

Torsion angles [°] for **7d**.

C(1)-N(4)-N(5)-N(1)	0.3(3)
C(2)-N(1)-N(5)-N(4)	-0.3(4)
C(3)-N(1)-N(5)-N(4)	178.4(3)
N(5)-N(4)-C(1)-C(2)	-0.2(4)
N(5)-N(4)-C(1)-I(1)	-179.2(2)
N(5)-N(1)-C(2)-C(1)	0.1(3)
C(3)-N(1)-C(2)-C(1)	-178.3(3)
N(4)-C(1)-C(2)-N(1)	0.1(3)
I(1)-C(1)-C(2)-N(1)	178.9(2)
C(2)-N(1)-C(3)-C(4)	79.4(4)
N(5)-N(1)-C(3)-C(4)	-99.0(4)
C(5)-N(2)-C(4)-O(1)	0.6(5)
C(5)-N(2)-C(4)-C(3)	179.2(3)
N(1)-C(3)-C(4)-O(1)	-2.2(5)
N(1)-C(3)-C(4)-N(2)	179.2(3)
C(4)-N(2)-C(5)-C(8)	83.7(4)
C(4)-N(2)-C(5)-C(6)	-154.5(3)
N(2)-C(5)-C(6)-C(7)	-175.7(3)
C(8)-C(5)-C(6)-C(7)	-52.7(4)
C(9)-N(3)-C(7)-C(6)	-60.3(4)
C(10)-N(3)-C(7)-C(6)	175.7(3)
C(5)-C(6)-C(7)-N(3)	57.4(4)
N(2)-C(5)-C(8)-C(9)	174.3(3)
C(6)-C(5)-C(8)-C(9)	52.4(4)
C(7)-N(3)-C(9)-C(8)	59.2(4)
C(10)-N(3)-C(9)-C(8)	-177.0(3)
C(5)-C(8)-C(9)-N(3)	-56.2(4)
C(7)-N(3)-C(10)-C(11)	-161.4(3)
C(9)-N(3)-C(10)-C(11)	75.1(4)
N(3)-C(10)-C(11)-C(12)	-148.5(3)
N(3)-C(10)-C(11)-C(16)	36.0(4)
C(16)-C(11)-C(12)-C(13)	-1.3(5)

C(10)-C(11)-C(12)-C(13)	-176.9(3)
C(11)-C(12)-C(13)-C(14)	1.4(6)
C(12)-C(13)-C(14)-C(15)	-0.3(6)
C(13)-C(14)-C(15)-C(16)	-1.0(6)
C(14)-C(15)-C(16)-C(11)	1.1(5)
C(12)-C(11)-C(16)-C(15)	0.1(5)
C(10)-C(11)-C(16)-C(15)	175.7(3)

Symmetry transformations used to generate equivalent atoms: