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> Evaluation of substituent-bioactivity and anion impact of linear and T-shaped Silver(I) pyridinyl complexes as potential antiproliferative, antioxidant, antimicrobial agents and DNA- and BSA- binders

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Supplementary information

Table of Contents

Table S1: ¹H-NMR chemical shifts of some protons in E_{a-d} complexes 1–12 and the IR band of (C=N) and pyridinyl N for E_{a-d} complexes 1–12 7 8 **Table S2:** ¹⁵N NMR chemical shifts of E_{a-d} and selected complexes (2, 7, 8 and 9) Table S3: Physical and chemical data of Silver(I) complexes 1–12 8 Figure S1: Electronic Absorption Spectra of Ligand E_a at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 285 nm λ_{max} . (inset) A stern-volmer plot of E_a interaction with CT-DNA 9 Figure S2: Electronic Absorption Spectra of Ligand E_{h} at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 302 nm λ_{max} . (inset) A stern-volmer plot of E_b interaction with CT-DNA 9 Figure S3: Electronic Absorption Spectra of Ligand E_c at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 327 nm λ_{max} . (inset) A stern-volmer plot of E_c interaction with CT-DNA 10 Figure S4: Electronic Absorption Spectra of Ligand E_d at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA ($0 - 3.0 \times 10^5 \text{ M}$) at 333 nm λ_{max} . (inset) A stern-volmer plot of E_d interaction with CT-DNA 10 Figure S5: Electronic Absorption Spectra of complex 2 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 306 nm λ_{max} . (inset) A stern-volmer plot of 2 interaction with CT-DNA 11

Page

Figure S6: Electronic Absorption Spectra of complex 3 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 330 nm λ_{max} . (inset) A stern-volmer plot of **3** interaction with CT-DNA 11 Figure S7: Electronic Absorption Spectra of complex 4 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 332 nm λ_{max} . (inset) A stern-volmer plot of 4 interaction with CT-DNA 12 Figure S8: Electronic Absorption Spectra of complex 5 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 285 nm λ_{max} . (inset) A stern-volmer plot of 5 interaction with CT-DNA 13 Figure S9: Electronic Absorption Spectra of complex 6 at 2.0×10^{-5} M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 306 nm λ_{max} . (inset) A stern-volmer plot of **6** interaction with CT-DNA 13 Figure S10: Electronic Absorption Spectra of complex 7 at 2.0×10^{-5} M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 328 nm λ_{max} . (inset) A stern-volmer plot of 7 interaction with CT-DNA 14 Figure S11: Electronic Absorption Spectra of complex 8 at 2.0 x 10^{-5} M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 332 nm λ_{max} . (inset) A stern-volmer plot of **8** interaction with CT-DNA 14 Figure S12: Electronic Absorption Spectra of complex 9 at 2.0×10^{-5} M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 282 nm λ_{max} . (inset) A stern-volmer plot of 9 interaction with CT-DNA 15 Figure S13: Electronic Absorption Spectra of complex 10 at 2.0×10^{-5} M in the absence (dashed line) and the presence of different concentrations of CT-DNA ($0 - 3.0 \times 10^5 \text{ M}$) at 300 nm λ_{max} . (inset) A stern-volmer plot of **10** interaction with CT-DNA 15 Figure S14: Electronic Absorption Spectra of complex 11 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 331 nm λ_{max} . (inset) A stern-volmer plot of **11** interaction with CT-DNA 16 Figure S15: Electronic Absorption Spectra of complex 12 at 2.0 x 10-5 M in the absence (dashed line) and the presence of different concentrations of CT-DNA $(0 - 3.0 \times 10^5 \text{ M})$ at 340 nm λ_{max} . (inset) A stern-volmer plot of 12 interaction with CT-DNA 16 Figure S16: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentration of complex 3. (inset) Stern-Volmer plot of 3 interactions with EB-CT- DNA 17 Figure S17: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentration of complex 4. (inset) Stern-Volmer plot of 4 interaction with EB-CT- DNA 17

Figure S18: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations s of complex **5**. (inset) Stern-Volmer plot of **5** interaction with EB-CT- DNA 18

Figure S19: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex 7. (inset) Stern-Volmer plot of 7 interaction with EB-CT-DNA 18

Figure S20: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentration of complex **8**. (inset) Stern-Volmer plot of **8** interaction with EB-CT-DNA 19

Figure S21: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex **9**. (inset) Stern-Volmer plot of **9** interaction with EB-CT-DNA 19

Figure S22: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex **11**. (inset) Stern-Volmer plot of **11** interaction with EB-CT- DNA 20

Figure S23: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex 12. (inset) Stern-Volmer plot of 12 interaction with EB-CT-DNA 20

Figure S24: The Fluorescence spectra of Hoechst 33342-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex **6**. (inset) Stern-Volmer plot of **6** interaction with Hoechst 33342-CT-DNA 21

Figure S25: The Fluorescence spectra of Hoechst 33342-CT-DNA in the absence (dashed line) and the presence of different concentration of complex **10**. (inset) Stern-Volmer plot of **10** interaction with Hoechst 33342-CT-DNA 21

The double-logarithmic plot of EB-CT-DNA–Complexes interactions at room temperature.

22

Figure S26: The double-logarithmic plot of EB-CT-DNA–Complex 1 interaction at roomtemperature.22

Figure S27: The double-logarithmic plot of EB-CT-DNA–Complex 4 interaction at roomtemperature.22

Figure S28: The double-logarithmic plot of EB-CT-DNA–Complex **5** interaction at room temperature. 23

Figure S29: The double-logarithmic plot of EB-CT-DNA–Complex 7 interaction at room temperature. 23

Figure S30: The double-logarithmic plot of EB-CT-DNA–Complex **8** interaction at room temperature. 24

Figure S31: The double-logarithmic plot of EB-CT-DNA–Complex **9** interaction at room temperature. 24

Figure S32: The double-logarithmic plot of EB-CT-DNA–Complex 11 interaction at room temperature. 25

Figure S33: The double-logarithmic plot of EB-CT-DNA–Complex 12 interaction at room temperature. 25

Figure S34: The double-logarithmic plot of Hoechst 33342-CT-DNA –Complex **2** interaction at room temperature. 26

Figure S35: The double-logarithmic plot of Hoechst 33342-CT-DNA –Complex **6** interaction at room temperature. 27

Figure S36: The double-logarithmic plot of Hoechst 33342-CT-DNA–Complex **10** interaction at room temperature. 27

BSA Binding studies using Electronic Absorption method

27

Figure S37: Electronic Absorption Spectra of BSA in the absence (dashed line) and thepresence of different concentrations of complexes 1. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \times 10^{-4} M^{-1}$ 28

Figure S38: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes **2**. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 28

Figure S39: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complex **3**. (inset) plot of 3 $1/(A-A_0)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 29

Figure S40: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes **4**. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 29

Figure S41: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes **5**. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 30

Figure S42: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes **6**. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 30

Figure S43: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 7. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 31

Figure S44: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes **8**. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 31

Figure S45: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes **9**. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 32

Figure S46: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes **11**. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 32

Figure S47: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes **12**. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$ 33

BSA Binding studies using the Fluorescence method

Figure S48: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentration of complex 2. (inset) Stern-Volmer plot of complex 2 interaction with BSA 33

33

Figure S49: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex **3**. (inset) Stern-Volmer plot of complex **3** interaction with BSA. 34

Figure S50: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex **6**. (inset) Stern-Volmer plot of complex **6** interaction with BSA 34

Figure S51: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 10. (inset) Stern-Volmer plot of complex 10 interaction with BSA 35

Figure S52: Fluorescence emission spectra of BSA in the absence(dashed line) and thepresence of different concentrations of complex 11. (inset) Stern-Volmer plot of complex11 interaction with BSA35

Figure S53: Fluorescence emission presence of different concentration	on spectra of BSA in the absence(dashed line) and the n of complex 1	36
Figure S54: Fluorescence emission presence of different concentration	on spectra of BSA in the absence(dashed line) and the ns of complex 4.	36
Figure S55: Fluorescence emission presence of different concentration	on spectra of BSA in the absence(dashed line) and the n of complex 5	37
Figure S56: Fluorescence emission presence of different concentration	on spectra of BSA in the absence(dashed line) and the ns of complex 8.	37
Figure S57: Fluorescence emission presence of different concentration interaction with BSA	on spectra of BSA in the absence(dashed line) and the ns of complex 9. (inset) Stern-Volmer plot of complex 38	x 9
Figure S58: Fluorescence emission presence of different concentration 12 interaction with BSA	on spectra of BSA in the absence(dashed line) and the ns of complex 12. (inset) Stern-Volmer plot of complex 38	ex
The double-logarithmic plot of BS	A–Complexes interactions at room temperature.	38
Figure S59: The double-logarithr	nic plot of BSA–Complex 2 interactions.	39
Figure S60: The double-logarithr	nic plot of BSA–Complex 3 interactions.	39
Figure S61: The double-logarithm	nic plot of BSA–Complex 6 interactions	40
Figure S62: The double-logarithr	nic plot of BSA–Complex 7 interactions	40
Figure S63: The double-logarithr	nic plot of BSA–Complex 11 interactions	41
H-NMR Spectra of Ligands E _{a-d}		42
Figure S64: E)-2-((pyridin-4-ylmo	ethylene)amino)phenol E _a	42
Figure S65: 2-(pyridin-4-yl)benzo	$[d]$ thiazole E_b	43
Figure S66: (E)-N-(2-fluoropheny	l)-1-(pyridin-4-yl)methanimine E _c	43
Figure S67: (E)-1-(pyridin-4-yl)-1	N-(p-tolyl)methanimine E _d	43
H-NMR SPECTRA OF COMPL	EXES 1-12	44
Figure S68: $[Ag(E_a)_2]NO_3$ 1	44	
Figure S69: $[Ag(E_b)_2]NO_3$ 2	44	
Figure S70: $[Ag(E_c)_2]NO_3$ 3	45	
Figure S71: $[Ag(E_d)_2]NO_3$ 4	45	
Figure S72: [Ag(E _a) ₂]ClO ₄	5	46
Figure S73: [Ag(E _b) ₂]ClO ₄	6	46
Figure S74: [Ag(E _c) ₂]ClO ₄	7	47
Figure S75: [Ag(E _d) ₂]ClO ₄	8	47
Figure S76: $[Ag(E_a)_2]CF_3SO_3$	9	48
Figure S77: $[Ag(E_b)_2]CF_3SO_3$	10	48
Figure S78: $[Ag(E_c)_2]CF_3SO_3$	11	49
Figure S79: [Ag(E _d) ₂]CF ₃ SO ₃	12	49
Figure S80: Time dependent ¹ H	NMR spectra of [Ag(E _a) ₂]NO ₃ 1	50
~ 1	NMD shoot $of \left[A_{\alpha}(F) \right] Clock$	50
Figure S81: Time dependent ¹ H	NMR spectra of $[Ag(E_b)_2]C(O_4 = 0$	50

Figure S83: Time dependent ¹ H NMR spectra of [Ag(E _d) ₂]CF ₃ SO ₃	12	51
¹⁵ N-NMR SPECTRA OF E _{a-d}		52
Figure S84: ¹⁵ N NMR spectrum of E)-2-((pyridin-4-ylmethylene)amino)phenol	E _a	52
Figure S85: ¹⁵ N NMR spectrum of 2-(pyridin-4-yl)benzo[d]thiazole E_b		53
Figure S86: ¹⁵ N NMR spectrum of (E)-N-(2-fluorophenyl)-1-(pyridin-4-yl)meth E _c 53	animine	e
Figure S87: ¹⁵ N NMR spectrum of (E)-1-(pyridin-4-yl)-N-(p-tolyl)methanimine	E_{d}	54
Figure S88: ¹⁵ N NMR spectrum of $[Ag(E_b)_2]NO_3 = 2$		54
Figure S89: ¹⁵ N NMR spectrum of $[Ag(E_c)_2]ClO_4$ 7		55
Figure S90: ¹⁵ N NMR spectrum of $[Ag(E_d)_2]ClO_4$ 8		55
Figure S91: ¹⁵ N NMR spectrum of $[Ag(E_a)_2]CF_3SO_3$ 9		55
¹³ C-NMR SPECTRA OF E _{a-d}		56
Figure S92: E)-2-((pyridin-4-ylmethylene)amino)phenol E_a		56
Figure S94: 2-(pyridin-4-yl)benzo[d]thiazole E _b		57
Figure S95: (E)-N-(2-fluorophenyl)-1-(pyridin-4-yl)methanimine E_c		58
Figure S96: (E)-1-(pyridin-4-yl)-N-(p-tolyl)methanimine E _d		58
¹³ C-NMR SPECTRA OF COMPLEXES 1-12		59
Figure S97: $[Ag(E_a)_2]NO_3 = 1 = 59$		
Figure S98: $[Ag(E_b)_2]NO_3 = 2 = 59$		
Figure S99: $[Ag(E_c)_2]NO_3 = 3 = 60$		
Figure S100: $[Ag(E_d)_2]NO_3 = 4 = 60$		
Figure S101: $[Ag(E_a)_2]ClO_4$ 5		61
Figure S102: $[Ag(E_b)_2]ClO_4$ 6		61
Figure S103: $[Ag(E_c)_2]ClO_4$ 7		62
Figure S104: $[Ag(E_d)_2]ClO_4$ 8		62
Figure S105: $[Ag(E_a)_2]CF_3SO_3$ 9		63
Figure S106: $[Ag(E_b)_2]CF_3SO_3$ 10		63
Figure S107: $[Ag(E_c)_2]CF_3SO_3$ 11		64
Figure S108: $[Ag(E_d)_2]CF_3SO_3$ 12		64
IR SPECTRA OF LIGANDS E _{a-d}		65
Figure S109: (E)-2-((pyridin-4-ylmethylene)amino)phenol E_a		65
Figure S110: 2-(pyridin-4-yl)benzo[d]thiazole E_b		65
Figure S111: (E)-N-(2-fluorophenyl)-1-(pyridin-4-yl)methanimine E _c		66
Figure S112: (E)-1-(pyridin-4-yl)-N-(p-tolyl)methanimine E _d		66
IR SPECTRA OF COMPLEXES 1-12		67
Figure S113: $[Ag(E_a)_2]NO_3 = 1 - 67$		
Figure S114: $[Ag(E_b)_2]NO_3 = 2$ 67		
Figure S115: $[Ag(E_c)_2]NO_3 = 3 = 68$		
Figure S116: $[Ag(E_d)_2]NO_3 = 4 = 68$		

Figure S117: $[Ag(E_a)_2]ClO_4$	5	69
Figure S118: [Ag(E _b) ₂]ClO ₄	6	69
Figure S119: [Ag(E _c) ₂]ClO ₄	7	70
Figure S121: [Ag(E _a) ₂]CF ₃ SO ₃	9	71
Figure S122: [Ag(E _b) ₂]CF ₃ SO ₃	10	71
Figure S123: [Ag(E _c) ₂]CF ₃ SO ₃	11	72
Figure S124: [Ag(E _d) ₂]CF ₃ SO ₃	12	72
Mass Spectra of Ligands E _{a-d}		73
Figure S125: (E)-2-((pyridin-4-y	lmethylene)amino)phenol E _a	73
Figure S126: 2-(pyridin-4-yl)ber	$zo[d]$ thiazole E_b	73
Figure S127: (E)-N-(2-fluorophe	nyl)-1-(pyridin-4-yl)methanimine E _c	74
Figure S128: (E)-1-(pyridin-4-yl)-N-(p-tolyl)methanimine E _d	74
MASS SPECTRA OF COMPLE	XES 1-12	75
Figure S129: $[Ag(E_a)_2]NO_3$ 1	75	
Figure S130: $[Ag(E_b)_2]NO_3$ 2	76	
Figure S132: $[Ag(E_d)_2]NO_3$ 4	77	
Figure S133: [Ag(E _a) ₂]ClO ₄	5	77
Figure S134: [Ag(E _b) ₂]ClO ₄	6	78
Figure S135: [Ag(E _c) ₂]ClO ₄	7	79
Figure S136: [Ag(E _d) ₂]ClO ₄	8	79
Figure S137: [Ag(E _a) ₂]CF ₃ SO ₃	9	80
Figure S138: [Ag(E _b) ₂]CF ₃ SO ₃	10	80
Figure S139: [Ag(E _c) ₂]CF ₃ SO ₃	11	81
Figure S140: [Ag(E _d) ₂]CF ₃ SO ₃	12	81

Table S1: ¹H-NMR chemical shifts of some protons in E_{a-d} complexes 1–12 and the IR band of (C=N) and pyridinyl N for E_{a-d} complexes 1–12

Ligands (Complex)	δC(H=N)ppm	Δδ	Hb-py	Δδ	$v(C=N) \text{ cm}^{-1}$	Δv	$v(py-N) cm^{-1}$	Δv
1 (Ea)	8.78 (9.20)	0.42	8.74 (8.78)	0.04	1627 (1627)	0	1584 (1580)	4
2 (Eb)	-	-	8.81 (8.78)	0.03	-	-	1606 (1586)	20
3 (Ec)	8.76 (8.74)	0.02	8.78 (8.78)	0.00	1610 (1612)	2	1552 (1585)	33
4 (Ed)	8.74 (8.68)	0.06	8.75 (8.74)	0.01	1608 (-)	-	1586 (1589)	3
5 (Ea)	8.78 (9.20)	0.42	8.74 (8.78)	0.04	1624 (1627)	3	1585 (1580)	5
6 (Eb)	-	-	8.79 (8.78)	0.01		-	1611 (1586)	25
7 (Ec)	8.76 (8.74)	0.02	8.79 (8.78)	0.01	1613 (1612)	1	1557 (1585)	28
8 (Ed)	8.74 (8.68)	0.06	8.76 (8.74)	0.02	1610 (-)	-	- (1589)	-

9 (Ea)	8.79 (9.20)	0.41	8.74 (8.78)	0.04	1625 (1627)	2	1585 (1580)	5
10 (Eb)	-	-	8.79 (8.78)	0.01		-	1609 (1586)	23
11 (Ec)	8.76 (8.74)	0.02	8.78 (8.78)	0.00	1609 (1612)	3	1552 (1585)	33
12 (Ed)	8.74 (8.68)	0.06	8.76 (8.74)	0.02	1609 (-)	-	- (1589)	-

Table S2: ¹⁵ N NM	R chemical shifts of E_a	- d and selected com	plexes (2, 7, 8 and 9)
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Ligand (Complex)	$\delta^{15}N_{py}$ (ppm)	$\Delta\delta^{15}N_{py}$ (ppm)	δ ¹⁵ N=C(ppm)	$\Delta\delta^{15}N_{im}$ (ppm)
2 (Eb)	323 (314)	9	-	-
7 (Ec)	7 (Ec) 303 (327)		326 (327)	1
8 (Ed)	324 (317)	7	339 (339)	0
9 (Ea)	329 (333)	4	-	-

 Table S3:
 Physical and chemical data of Silver(I) complexes 1–12

Comp.	Anal. (Calcd. (Anal. f	ound)	M.pt.	MS	5	MC
	С	Η	Ν	(°C)	Calcd.	Found	$(\Lambda_{\rm m}/{\rm ~S~m^2~mol^{-1}})$
							X 10 ⁻⁴
1	50.90 (50.62)	3.56 (3.23)	12.37 (12.39)	157-158	504.32	504	22.5
2	48.50 (48.49)	2.71 (2.54)	11.78 (11.58)	186-187	532.41	532	19.8
3	50.55 (50.49)	3.18 (3.13)	12.28 (12.06)	146-147	508.30	508	13.4
4	55.53 (55.80)	4.30 (4.00)	12.45 (12.24)	164-165	500.37	501	20.4
5	47.74 (47.52)	3.34 (3.11)	9.28 (9.09)	169-170	504.32	504	26.3
6	45.62 (45.38)	2.55 (2.55)	8.87 (8.61)	168-169	532.41	532	15.7
7	47.43 (47.40)	2.99 (2.74)	9.22 (9.00)	209-210	508.30	508	24.4
8	52.06 (52.05)	4.03 (3.89)	9.34 (9.27)	227-228	500.37	501	19.2
9	45.96 (45.82)	3.09 (2.85)	8.58 (8.52)	165-166	504.32	504	29.0
10	44.06 (43.93)	2.37 (2.27)	8.22 (8.04)	183-184	532.41	532	23.3
11	45.68 (45.68)	2.76 (2.74)	8.52 (8.38)	171-172	508.30	508	27.8
12	49.94 (49.73)	3.73 (3.41)	8.63 (8.60)	220-221	500.37	501	20.8

DNA Binding Studies



Figure S1: Electronic Absorption Spectra of Ligand E_a at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 285 nm λ_{max} . (inset) A stern-volmer plot of E_a interaction with CT-DNA



Figure S2: Electronic Absorption Spectra of Ligand E_b at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 302 nm λ_{max} . (inset) A stern-volmer plot of E_b interaction with CT-DNA



Figure S3: Electronic Absorption Spectra of Ligand E_c at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 327 nm λ_{max} . (inset) A stern-volmer plot of E_c interaction with CT-DNA



Figure S4: Electronic Absorption Spectra of Ligand E_d at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 333 nm λ_{max} . (inset) A stern-volmer plot of E_d interaction with CT-DNA



Figure S5: Electronic Absorption Spectra of complex 2 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 306 nm λ_{max} . (inset) A stern-volmer plot of 2 interaction with CT-DNA



Figure S6: Electronic Absorption Spectra of complex 3 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 330 nm λ_{max} . (inset) A stern-volmer plot of 3 interaction with CT-DNA



Figure S7: Electronic Absorption Spectra of complex 4 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 332 nm λ_{max} . (inset) A stern-volmer plot of 4 interaction with CT-DNA



Figure S8: Electronic Absorption Spectra of complex 5 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 285 nm λ_{max} . (inset) A stern-volmer plot of 5 interaction with CT-DNA



Figure S9: Electronic Absorption Spectra of complex 6 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 306 nm λ_{max} . (inset) A stern-volmer plot of 6 interaction with CT-DNA



Figure S10: Electronic Absorption Spectra of complex 7 at 2.0 x 10^{-5} M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10^{5} M) at 328 nm λ_{max} . (inset) A stern-volmer plot of 7 interaction with CT-DNA



Figure S11: Electronic Absorption Spectra of complex 8 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 332 nm λ_{max} . (inset) A stern-volmer plot of 8 interaction with CT-DNA



Figure S12: Electronic Absorption Spectra of complex 9 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 282 nm λ_{max} . (inset) A stern-volmer plot of 9 interaction with CT-DNA



Figure S13: Electronic Absorption Spectra of complex 10 at 2.0 x 10^{-5} M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10^{5} M) at 300 nm λ_{max} . (inset) A stern-volmer plot of 10 interaction with CT-DNA



Figure S14: Electronic Absorption Spectra of complex 11 at 2.0 x 10⁻⁵ M in the absence (dashed line) and the presence of different concentrations of CT-DNA (0 – 3.0 x 10⁵ M) at 331 nm λ_{max} . (inset) A stern-volmer plot of 11 interaction with CT-DNA



Figure S15: Electronic Absorption Spectra of complex **12** at 2.0 x 10-5 M in the absence (dashed line) and the presence of different concentrations of CT-DNA ($0 - 3.0 \times 10^5$ M) at 340 nm λ_{max} . (inset) A stern-volmer plot of **12** interaction with CT-DNA



Figure S16: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentration of complex 3. (inset) Stern-Volmer plot of 3 interactions with EB-CT-DNA



Figure S17: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentration of complex 4. (inset) Stern-Volmer plot of 4 interaction with EB-CT- DNA



Figure S18: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations s of complex 5. (inset) Stern-Volmer plot of 5 interaction with EB-CT-DNA



Figure S19: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex 7. (inset) Stern-Volmer plot of 7 interaction with EB-CT- DNA



Figure S20: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentration of complex 8. (inset) Stern-Volmer plot of 8 interaction with EB-CT- DNA



Figure S21: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex 9. (inset) Stern-Volmer plot of 9 interaction with EB-CT- DNA



Figure S22: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex 11. (inset) Stern-Volmer plot of 11 interaction with EB-CT-DNA



Figure S23: The Fluorescence spectra of EB-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex 12. (inset) Stern-Volmer plot of 12 interaction with EB-CT-DNA



Figure S24: The Fluorescence spectra of Hoechst 33342-CT-DNA in the absence (dashed line) and the presence of different concentrations of complex 6. (inset) Stern-Volmer plot of 6 interaction with Hoechst 33342-CT-DNA



Figure S25: The Fluorescence spectra of Hoechst 33342-CT-DNA in the absence (dashed line) and the presence of different concentration of complex 10. (inset) Stern-Volmer plot of 10 interaction with Hoechst 33342-CT-DNA

The double-logarithmic plot of EB-CT-DNA-Complexes interactions at room temperature.



Figure S26: The double-logarithmic plot of EB-CT-DNA–Complex 1 interaction at room temperature.



Figure S27: The double-logarithmic plot of EB-CT-DNA-Complex 4 interaction at room temperature.



Figure S28: The double-logarithmic plot of EB-CT-DNA–Complex 5 interaction at room temperature.



Figure S29: The double-logarithmic plot of EB-CT-DNA–Complex 7 interaction at room temperature.



Figure S30: The double-logarithmic plot of EB-CT-DNA–Complex 8 interaction at room temperature.



Figure S31: The double-logarithmic plot of EB-CT-DNA–Complex 9 interaction at room temperature.



Figure S32: The double-logarithmic plot of EB-CT-DNA–Complex 11 interaction at room temperature.



Figure S33: The double-logarithmic plot of EB-CT-DNA–Complex 12 interaction at room temperature.



Figure S34: The double-logarithmic plot of Hoechst 33342-CT-DNA –Complex 2 interaction at room temperature.



Figure S35: The double-logarithmic plot of Hoechst 33342-CT-DNA –Complex 6 interaction at room temperature.



Figure S36: The double-logarithmic plot of Hoechst 33342-CT-DNA–Complex 10 interaction at room temperature.

BSA Binding studies using Electronic Absorption method



Figure S37: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 1. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$



Figure S38: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 2. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \times 10^{-4} M^{-1}$



Figure S39: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complex **3**. (inset) plot of 3 1/(A-A₀) vs. 1/[Complex] x 10⁻⁴ M⁻¹



Figure S40: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 4. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$



Figure S41: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 5. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$



Figure S42: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 6. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$



Figure S43: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 7. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$



Figure S44: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 8. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$



Figure S45: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 9. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$



Figure S46: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 11. (inset) Plot of $1/(A_o - A)$ vs. $1/[Complex] \ge 10^{-4} M^{-1}$



Figure S47: Electronic Absorption Spectra of BSA in the absence (dashed line) and the presence of different concentrations of complexes 12. (inset) Plot of 1/(A_o – A) vs. 1/[Complex] x 10⁻⁴ M⁻¹



BSA Binding studies using the Fluorescence method

Figure S48: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentration of complex 2. (inset) Stern-Volmer plot of complex 2 interaction with BSA



Figure S49: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 3. (inset) Stern-Volmer plot of complex 3 interaction with BSA.



Figure S50: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 6. (inset) Stern-Volmer plot of complex 6 interaction with BSA



Figure S51: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 10. (inset) Stern-Volmer plot of complex 10 interaction with BSA



Figure S52: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 11. (inset) Stern-Volmer plot of complex 11 interaction with BSA



Figure S53: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentration of complex 1



Figure S54: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 4.


Figure S55: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentration of complex 5



Figure S56: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 8.



Figure S57: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 9. (inset) Stern-Volmer plot of complex 9 interaction with BSA



Figure S58: Fluorescence emission spectra of BSA in the absence(dashed line) and the presence of different concentrations of complex 12. (inset) Stern-Volmer plot of complex 12 interaction with BSA

The double-logarithmic plot of BSA-Complexes interactions at room temperature.



Figure S59: The double-logarithmic plot of BSA–Complex 2 interactions.



Figure S60: The double-logarithmic plot of BSA–Complex 3 interactions.



Figure S61: The double-logarithmic plot of BSA-Complex 6 interactions



Figure S62: The double-logarithmic plot of BSA-Complex 7 interactions



Figure S63: The double-logarithmic plot of BSA–Complex 11 interactions







Figure S66: (E)-N-(2-fluorophenyl)-1-(pyridin-4-yl)methanimine E_c

8.0

8.2

8.4

1

7.8

7.6

7.4

[ppm]

2.290

8.6

8.8





44













Figure S75: [Ag(E_d)₂]ClO₄



Figure S76: $[Ag(E_a)_2]CF_3SO_3 \qquad 9$



Figure S77: $[Ag(E_b)_2]CF_3SO_3$ 10











 $^1\mathrm{H}$ NMR spectra of the complexes 1, 6, 7 and 12 between 0-48 h





Figure S81: Time dependent ¹H NMR spectra of $[Ag(E_b)_2]ClO_4$





Figure S83: Time dependent ¹H NMR spectra of [Ag(E_d)₂]CF₃SO₃





Figure S84: ¹⁵N NMR spectrum of E)-2-((pyridin-4-ylmethylene)amino)phenol E_a





Figure S86: ¹⁵N NMR spectrum of (E)-N-(2-fluorophenyl)-1-(pyridin-4-yl)methanimine E_c



53



400 300 200

Figure S88: ¹⁵N NMR spectrum of [Ag(E_b)₂]NO₃ 2



Figure S87: ¹⁵N NMR spectrum of (E)-1-(pyridin-4-yl)-N-(p-tolyl)methanimine E_d



Figure S90: ¹⁵N NMR spectrum of $[Ag(E_d)_2]ClO_4$



Figure S91: ¹⁵N NMR spectrum of [Ag(E_a)₂]CF₃SO₃ 9



Figure S92: E)-2-((pyridin-4-ylmethylene)amino)phenol E_a



Figure S93: 2-(pyridin-4-yl)benzo[d]thiazole E_b



Figure S94: (E)-N-(2-fluorophenyl)-1-(pyridin-4-yl)methanimine E_c



Figure S95: (E)-1-(pyridin-4-yl)-N-(p-tolyl)methanimine E_d



Figure S96: $[Ag(E_a)_2]NO_3 = 1$



Figure S97: $[Ag(E_b)_2]NO_3 = 2$











Figure S100: $[Ag(E_a)_2]ClO_4$ 5



Figure S101: $[Ag(E_b)_2]ClO_4$ 6



Figure S102: $[Ag(E_c)_2]ClO_4$ 7



61



Figure S104: [Ag(E_a)₂]CF₃SO₃ 9







Figure S106: [Ag(E_c)₂]CF₃SO₃ 11





IR SPECTRA OF LIGANDS Ea-d

Ea 100 1920.546 1991.660 90 2089.118 2739.373 80 2845.269 2122.138 %Transmittance 70 2926.521 943 489 1092.94 3035.837 385.966 60 3389.920 1324.92 878.391 50 1239.642 1473,553,770 1626.963 803.048 1022.778 1580.317 1209.323 1700.995 30 2400 2200 2000 1800 1600 1400 3800 3400 3200 3000 2800 2600 1200 1000 800 3600 Wavenumber

Figure S108: (E)-2-((pyridin-4-ylmethylene)amino)phenol E_a





Figure S109: 2-(pyridin-4-yl)benzo[d]thiazole E_b

Agilent Resolutions Pro



Figure S110: (E)-N-(2-fluorophenyl)-1-(pyridin-4-yl)methanimine E_c



Figure S111: (E)-1-(pyridin-4-yl)-N-(p-tolyl)methanimine E_d

IR SPECTRA OF COMPLEXES 1-12



Agilent Resolutions Pro





Figure S113: $[Ag(E_b)_2]NO_3 = 2$



Figure S114: $[Ag(E_c)_2]NO_3 = 3$



Figure S115: $[Ag(E_d)_2]NO_3 = 4$











Figure S117: [Ag(E_b)₂]ClO₄















Figure S121: $[Ag(E_b)_2]CF_3SO_3$ 10



Figure S122: [Ag(E_c)₂]CF₃SO₃ 11



Agilent Resolutions Pro

Figure S123: $[Ag(E_d)_2]CF_3SO_3$ 12





MS Spectrum Ea

ESI Negative Spectrum Mode:Averaged 1.081-1.088(650-654) Base Peak:197(178763) BG Mode:Averaged 0.751-1.101(452-662) Segment 1 - Event 2



Figure S124: (E)-2-((pyridin-4-ylmethylene)amino)phenol E_a

==== Shimadzu LabSolutions Data Report ====





Figure S125: 2-(pyridin-4-yl)benzo[d]thiazole E_b
<Spectrum>

MS Spectrum Ec

ESI Positive Spectrum Mode:Averaged 0.687-0.693(413-417) Base Peak:233(5450048) BG Mode:Averaged 0.750-1.100(451-661) Segment 1 - Event 1



Figure S126: (E)-N-(2-fluorophenyl)-1-(pyridin-4-yl)methanimine E_c

==== Shimadzu LabSolutions Data Report ====

<Spectrum>

MS Spectrum Ed

ESI Positive Spectrum Mode:Averaged 0.687-0.693(413-417) Base Peak:197(2367075) BG Mode:Averaged 0.750-1.100(451-661) Segment 1 - Event 1



Figure S127: (E)-1-(pyridin-4-yl)-N-(p-tolyl)methanimine E_d

MASS SPECTRA OF COMPLEXES 1-12

==== Shimadzu LabSolutions Data Report ====

<Spectrum>

MS Spectrum E1

ESI Positive Spectrum Mode:Averaged 1.093-1.100(657-661) Base Peak:270(6715298) BG Mode:Averaged 0.750-1.100(451-661) Segment 1 - Event 1





<Spectrum>



Figure S129: [Ag(E_b)₂]NO₃ 2

==== Shimadzu LabSolutions Data Report ====

<Spectrum>





Figure S131: $[Ag(E_d)_2]NO_3 = 4$



<Spectrum>

MS Spectrum E5

ESI Positive Spectrum Mode:Averaged 1.097-1.103(659-663) Base Peak:288(6383200) BG Mode:Averaged 0.750-1.100(451-661) Segment 1 - Event 1







Figure S133: $[Ag(E_b)_2]ClO_4$ 6

<Spectrum>

MS Spectrum

E7

ESI Positive Spectrum Mode Averaged 0,680-0,687(409-413) Base Peak:631(2911334) BG Mode:Averaged 0,200-0,600(121-361) Segment 1 - Event 1



Figure S134: [Ag(E_c)₂]ClO₄ 7



<Spectrum>

MS Spectrum E8

ESI Positive Spectrum Mode:Single 1.107(665) Base Peak:197(1017698) BG Mode:Averaged 0.750-1.090(451-655) Segment 1 - Event 1



Figure S135: $[Ag(E_d)_2]ClO_4$ 8

<Spectrum>

MS Spectrum E9

ESI Positive Spectrum Mode:Averaged 1.093-1.100(657-661) Base Peak:270(6715298) BG Mode:Averaged 0.750-1.100(451-661) Segment 1 - Event 1





<Spectrum>

MS Spectrum E10

ESI Positive Spectrum Mode:Averaged 1.093.1.100(657.661) Base Peak:533(3123840) BG Mode:Averaged 0.750.1.100(451.661) Segment 1 - Event 1





<Spectrum>

MS Spectrum E11



Figure S138: $[Ag(E_c)_2]CF_3SO_3$ 11



<Spectrum>



Spectrum Mode:Averaged 1.100-1.107(661-665) Base Peak:359(1976196) BG Mode:Averaged 0.750-1.100(451-661) Segment 1 - Event 1

ESI Positive



