Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Zn(II) and Cd(II) Pincer Complexes Bearing Meta Alkylated Pyridinium Amidates; Synthesis & Preliminary Anticancer Evaluation

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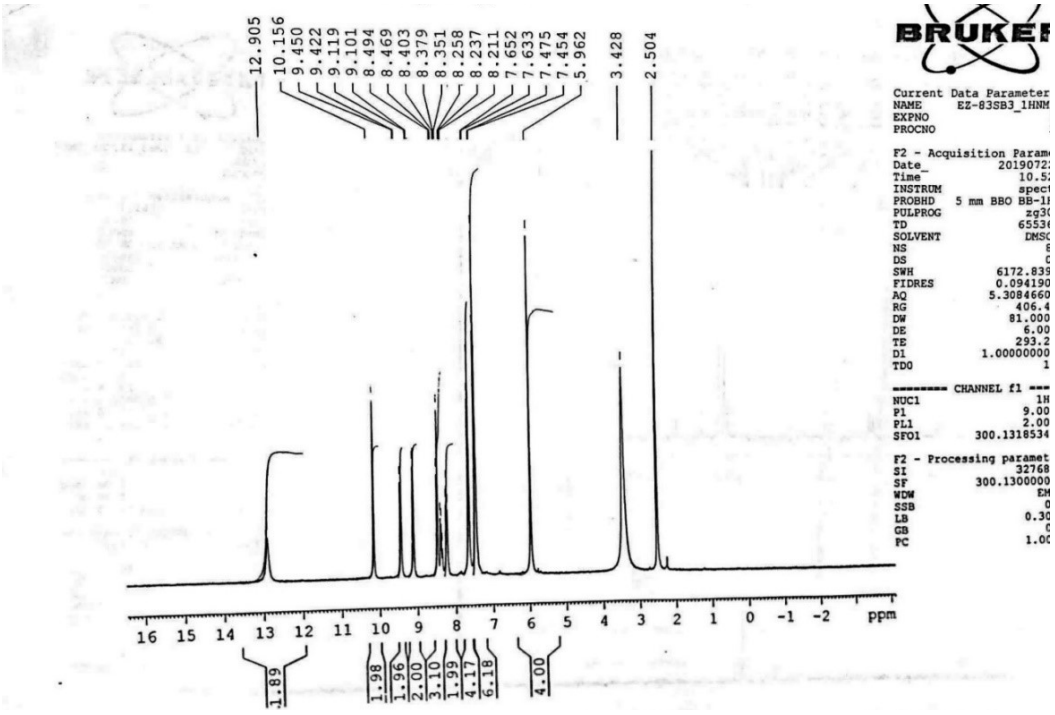


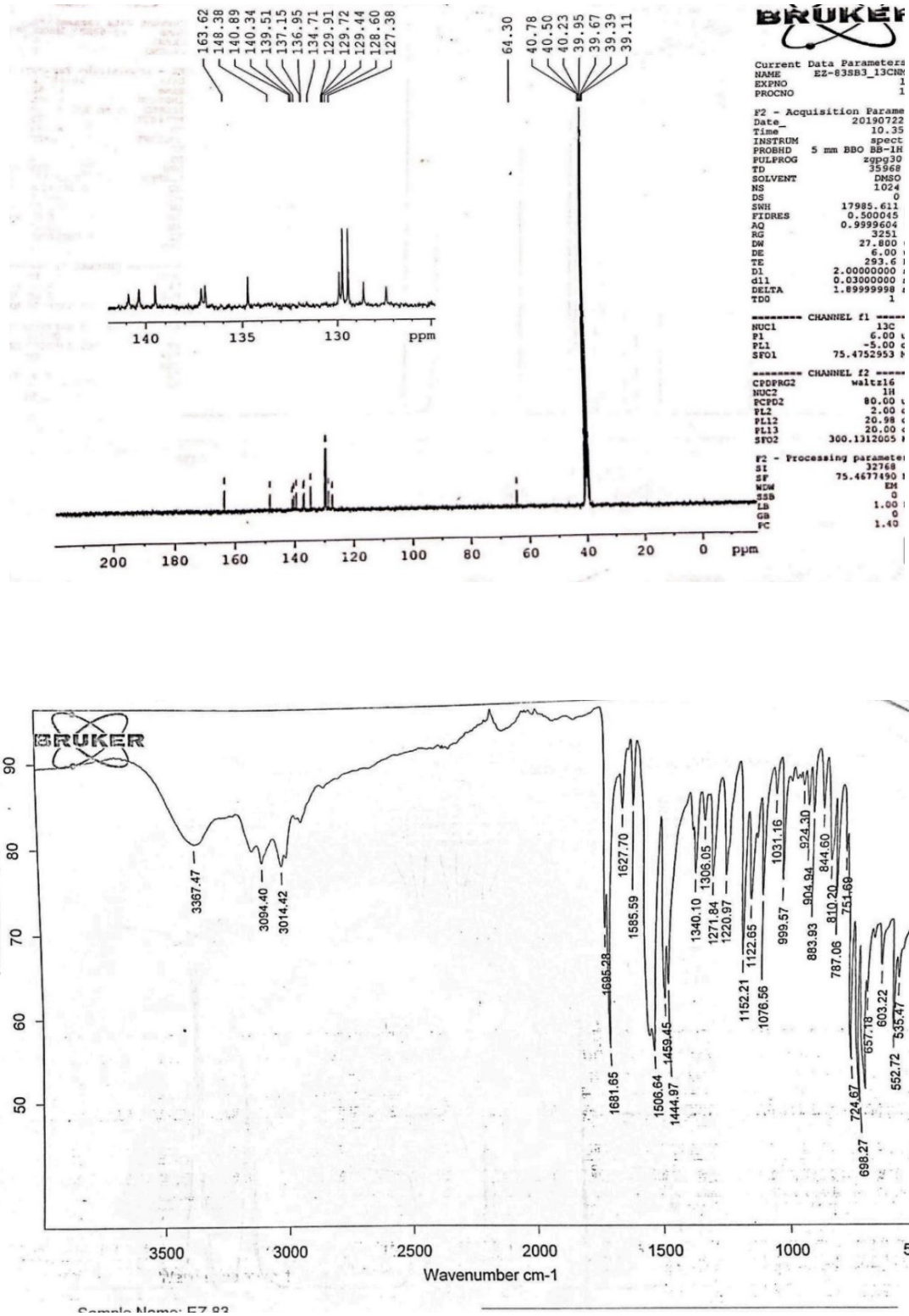
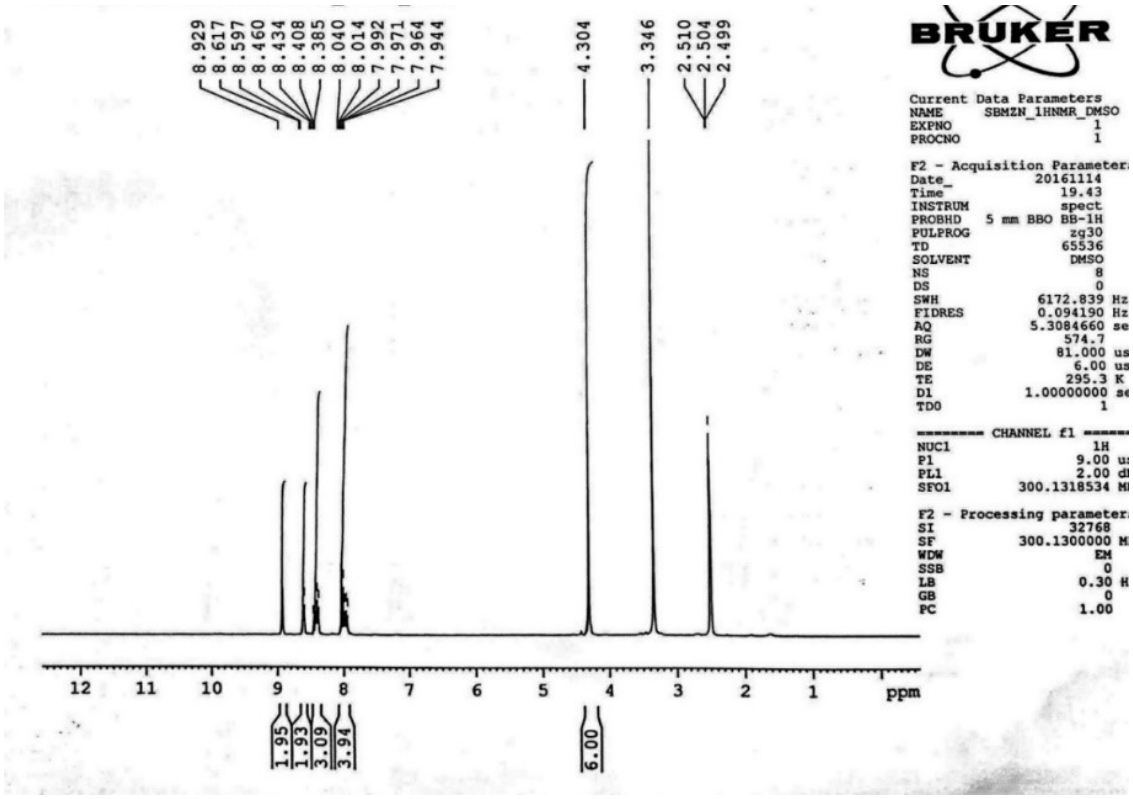


Fig. S1. ^{1}H, ^{13}CNMR and FT-IR spectra of $H_2L_{Bn}^{m}(Cl)_2$



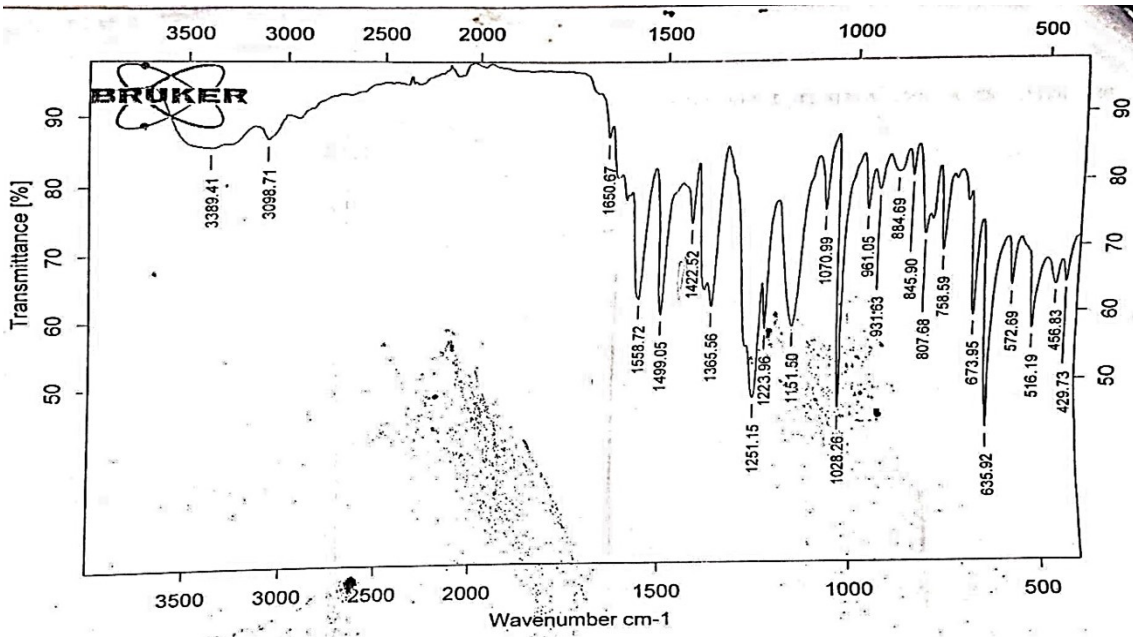
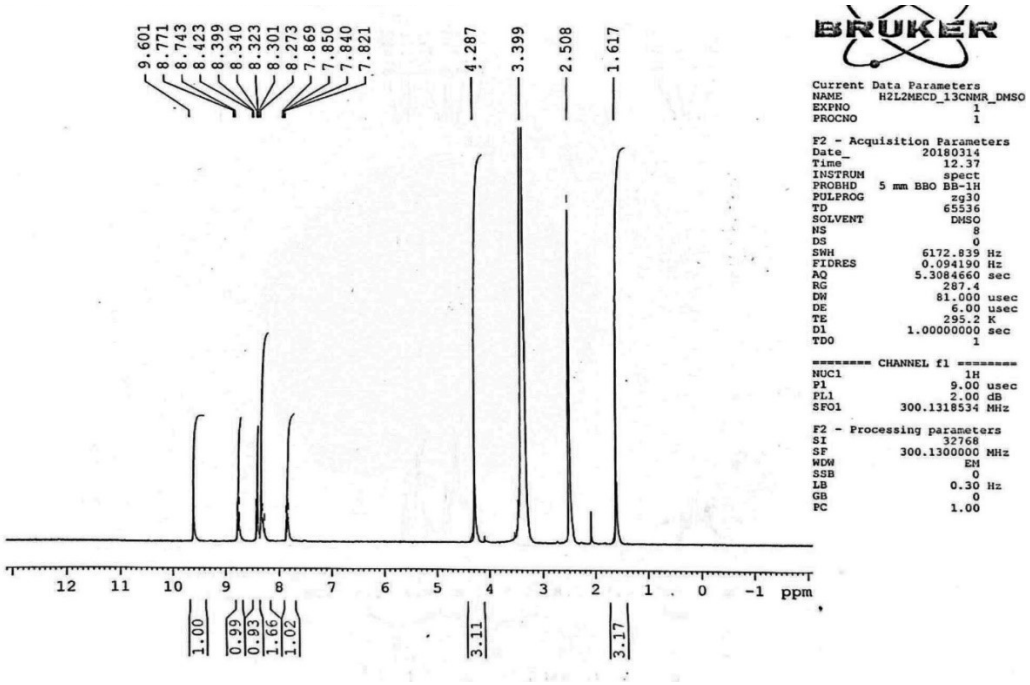


Fig. S2. ^{1}H and FT-IR spectra of $[Zn(L^m_{Me})(OTf)_2]$ (C1)



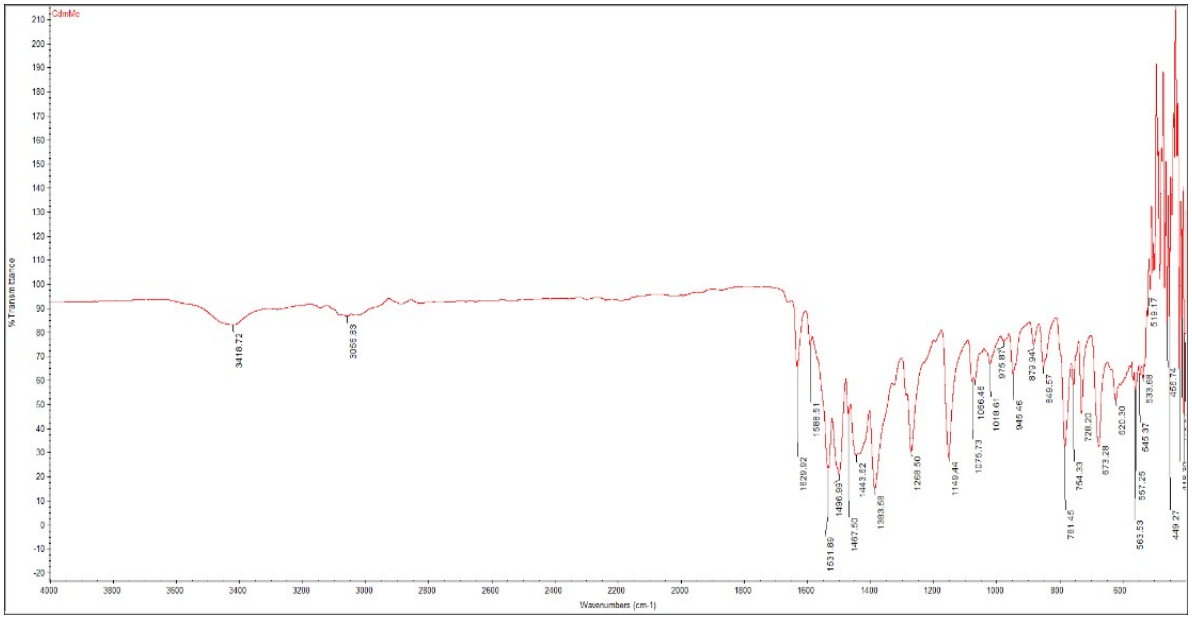
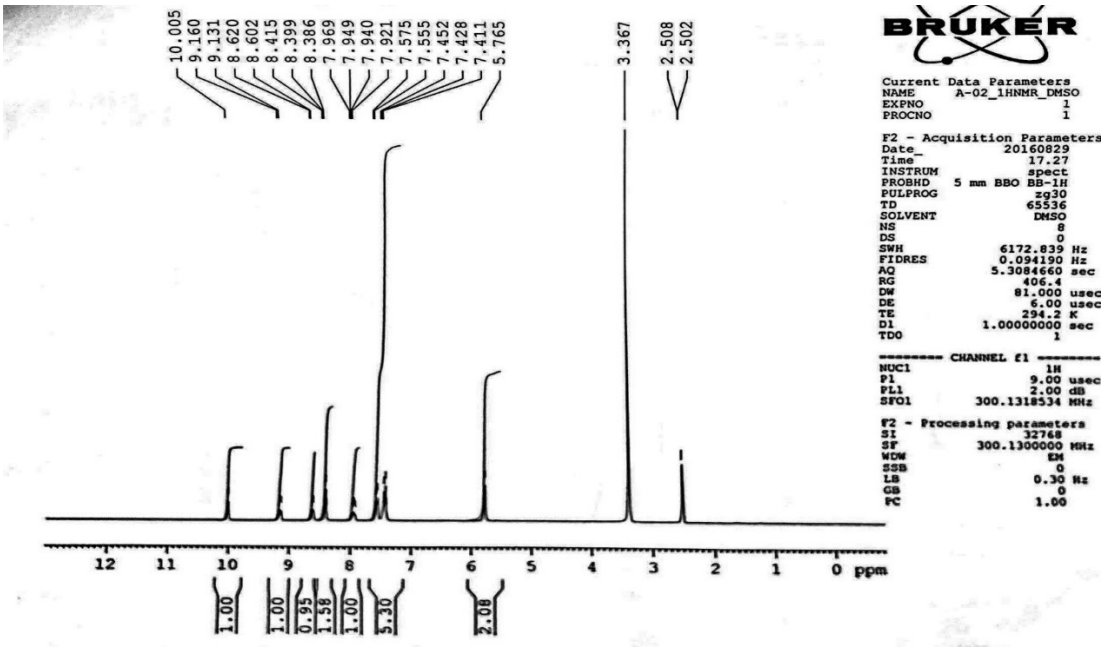


Fig. S3. ^{1}H and FT-IR spectra of $[Cd(L^m_{Me})(Cl)(OAc)]$ (C2)



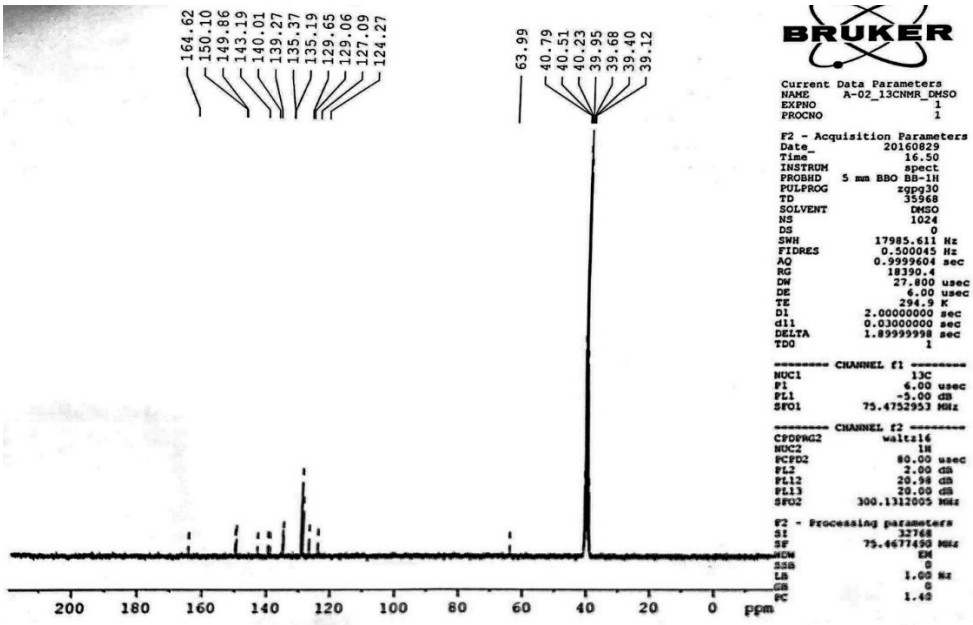
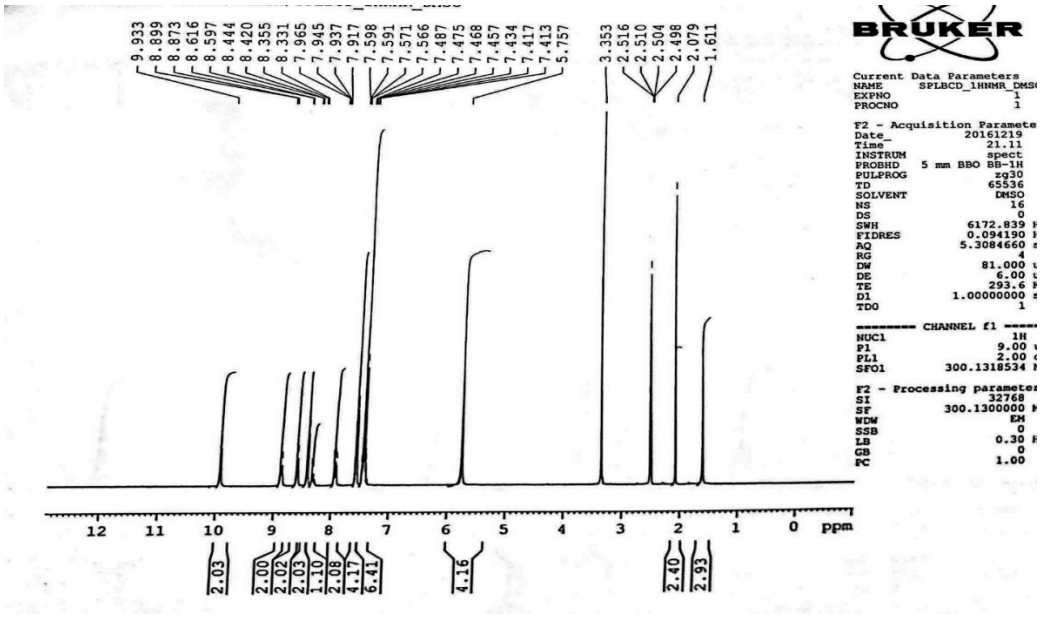


Fig. S4. ^{1}H, and ^{13}CNMR spectra of $[Zn(L_{Bn}^{m})(Cl)_2]$ (C3)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7.917
7.598
7.591
7.571
7.566
7.487
7.475
7.468
7.457
7.434
7.417
7.413
5.757
3.353
2.516
2.510
2.504
2.498
2.079
1.611
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2.00
2.02
2.03
1.10
2.08
4.17
6.41
4.16
2.40
2.93
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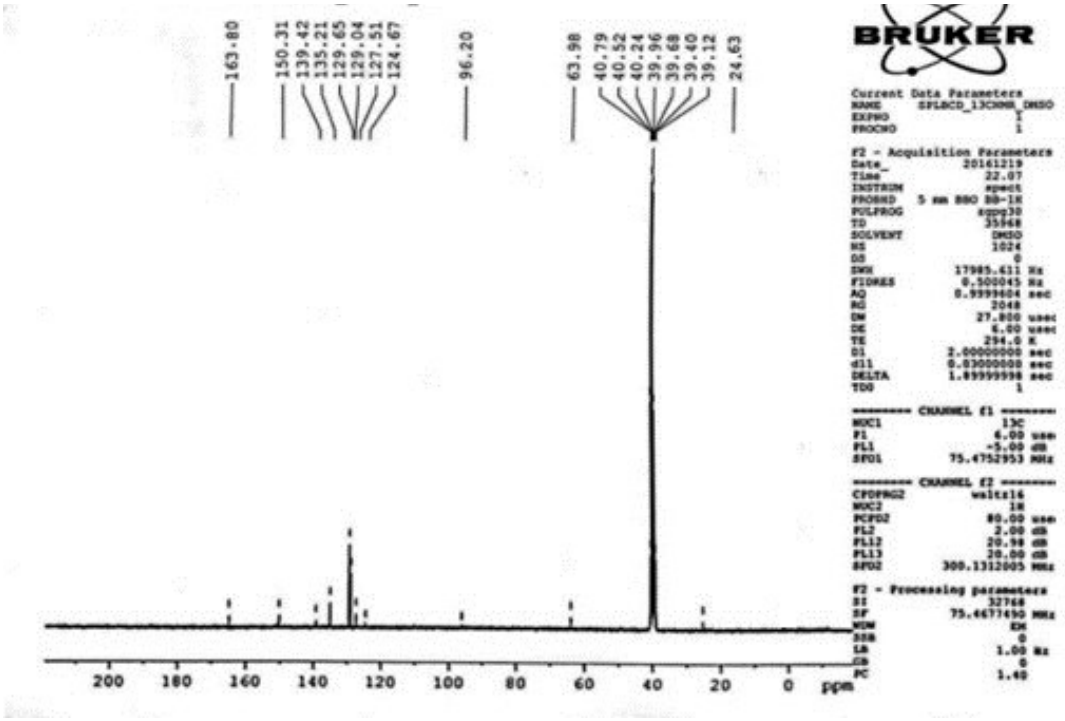
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129.65
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124.67
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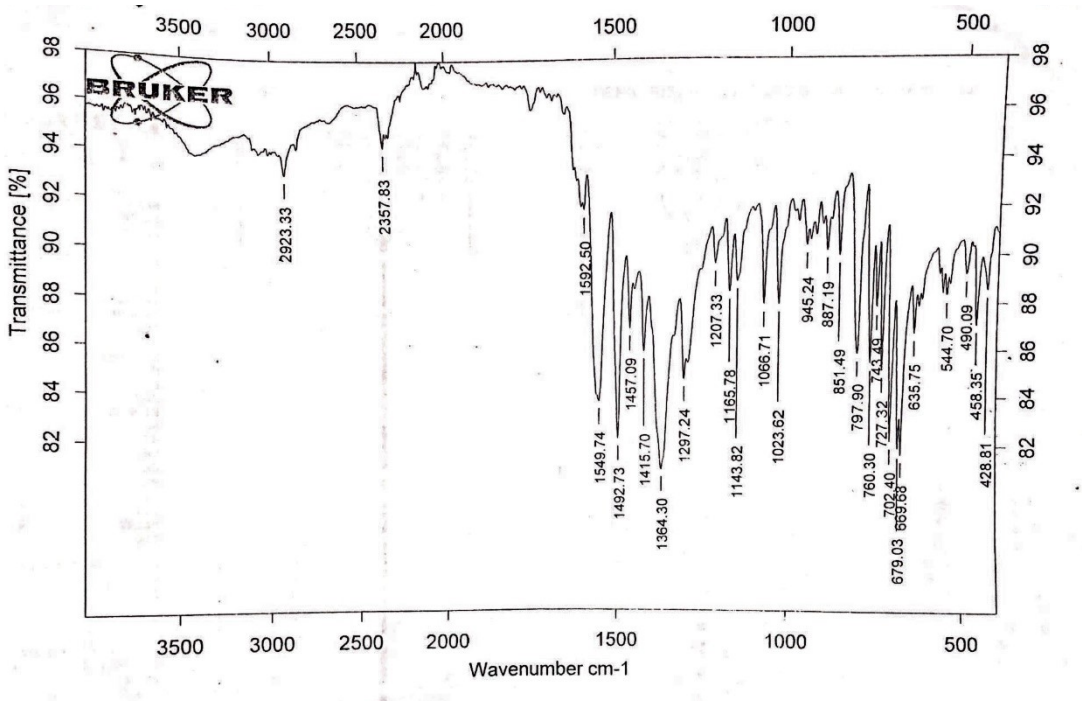

Fig. S5. ^{1}H, ^{13}CNMR and FT-IR spectra of $[Cd(L_{Bn}^{m})(Cl)(OAc)$] (C4)

Table S1. Experimental details of C3 and C4		
Crystal data	**C3**	**C4**
CCDC	**2265862**	**2265863**
Chemical formula	$C_{62}H_{52}Cl_4N_{10}O_5Zn_2$	$C_{35}H_{31}CdClN_6O_4$
M_r	1289.67	747.51
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/n$
Temperature (K)	296	296
***a*, *b*, *c* (Å)**	9.1405 (14), 13.016 (2), 13.591 (3)	13.5644 (14), 9.4204 (9), 26.700 (2)
β (°)	107.064 (5), 101.287 (5), 99.980 (6)	95.262 (4)
***V* (Å³)**	1469.2 (4)	3397.4 (6)
Z	1	4
Radiation type	Mo *K*α	Mo *K*α
μ (mm⁻¹)	1.06	0.77
Crystal size (mm)	0.38 × 0.24 × 0.20	0.42 × 0.20 × 0.18
Diffractometer	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)	Multi-scan (*SADABS*; Bruker, 2007)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15334, 6557, 3603	18149, 7880, 5313
R_{int}	0.057	0.051
$(\sin\theta/\lambda)_{max}$ (Å⁻¹)	0.652	0.653
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.061, 0.169, 0.96	0.055, 0.128, 1.04
No. of reflections	6557	7880
No. of parameters	320	455
No. of restraints	3	186
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å⁻³)	0.82, −0.63	1.15, −0.71

Table S2. Important bond lengths (Å) and bond angles (°) in C3 and C4				
	Bond lengths (Å)		Bond Angles (°)	
C3	Zn1—N2	2.033 (3)	N2—Zn1—N1	76.43 (13)
	Zn1—N1	2.211 (3)	N2—Zn1—N3	75.80 (13)
	Zn1—N3	2.226 (3)	N1—Zn1—N3	152.16 (13)
	Zn1—Cl1	2.2907 (12)	N2—Zn1—Cl1	125.54 (10)
	Zn1—Cl2	2.3009 (12)	N1—Zn1—Cl1	98.42 (10)
			N3—Zn1—Cl1	96.01 (10)
			N2—Zn1—Cl2	117.44 (11)
			N1—Zn1—Cl2	98.17 (10)
			N3—Zn1—Cl2	96.28 (10)
			Cl1—Zn1—Cl2	116.96 (5)
C4	Cd1—N2	2.278 (3)	N2—Cd1—O3	142.64 (12)
	Cd1—O3	2.292 (3)	N2—Cd1—N1	71.01 (12)
	Cd1—N1	2.369 (3)	O3—Cd1—N1	112.47 (12)
	Cd1—N3	2.387 (3)	N2—Cd1—N3	70.34 (11)
	Cd1—Cl1	2.5023 (11)	O3—Cd1—N3	98.80 (13)
	Cd1—O4	2.538 (3)	N1—Cd1—N3	141.34 (11)
			N2—Cd1—Cl1	124.41 (8)
			O3—Cd1—Cl1	92.36 (9)
			N1—Cd1—Cl1	99.99 (9)
			N3—Cd1—Cl1	100.87 (8)
			N2—Cd1—O4	91.03 (12)
			O3—Cd1—O4	52.65 (12)
			N1—Cd1—O4	90.37 (11)
			N3—Cd1—O4	91.13 (12)
			Cl1—Cd1—O4	144.56 (9)

Table S3. Hydrogen bond geometry (Å, °) in C3 and C4.					
	D—H···A	**D—H**	**H···A**	**D···A**	**<(D—H···A)°**
C3	C5—H5···O2^{i}	0.93	2.53	3.188 (6)	128
	C9—H9···O2	0.93	2.27	2.800 (6)	115
	C10—H10···Cl2^{ii}	0.93	2.82	3.590 (5)	141
	C11—H11···Cl2^{iii}	0.93	2.86	3.459 (5)	124
	C12—H12···Cl1	0.93	2.87	3.411 (4)	119
	C12—H12···Cl2	0.93	2.85	3.550 (5)	133
	C21—H21···Cl1	0.93	2.98	3.551 (5)	122
	C21—H21···Cl2	0.93	2.89	3.555 (4)	130
	C23—H23···Cl1^{iv}	0.93	2.87	3.679 (5)	147
	C24—H24···O1	0.93	2.11	2.735 (6)	124
	C24—H24···O3^{iv}	0.93	2.53	3.221 (11)	132
	C25—H25B···Cl1^{v}	0.97	2.97	3.785 (6)	142
	O3—H3A···O1^{ii}	0.82 (1)	2.12 (6)	2.890 (9)	156 (15)
	O3—H3B···O2^{i}	0.82 (1)	2.26 (4)	3.054 (9)	166 (12)
C4	C5—H5···O2^{i}	0.93	2.48	3.206 (6)	135
	C11—H11···O4^{vi}	0.93	2.30	3.135 (6)	149
	C12—H12···O1	0.93	2.14	2.717 (6)	119
	C21—H21···O2	0.93	2.28	2.810 (6)	115
	C22—H22···Cl1^{vii}	0.93	2.97	3.704 (5)	137
	C24—H24···Cl1	0.93	2.72	3.598 (5)	158
	C25—H25A···Cl1^{viii}	0.97	2.72	3.617 (5)	154

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

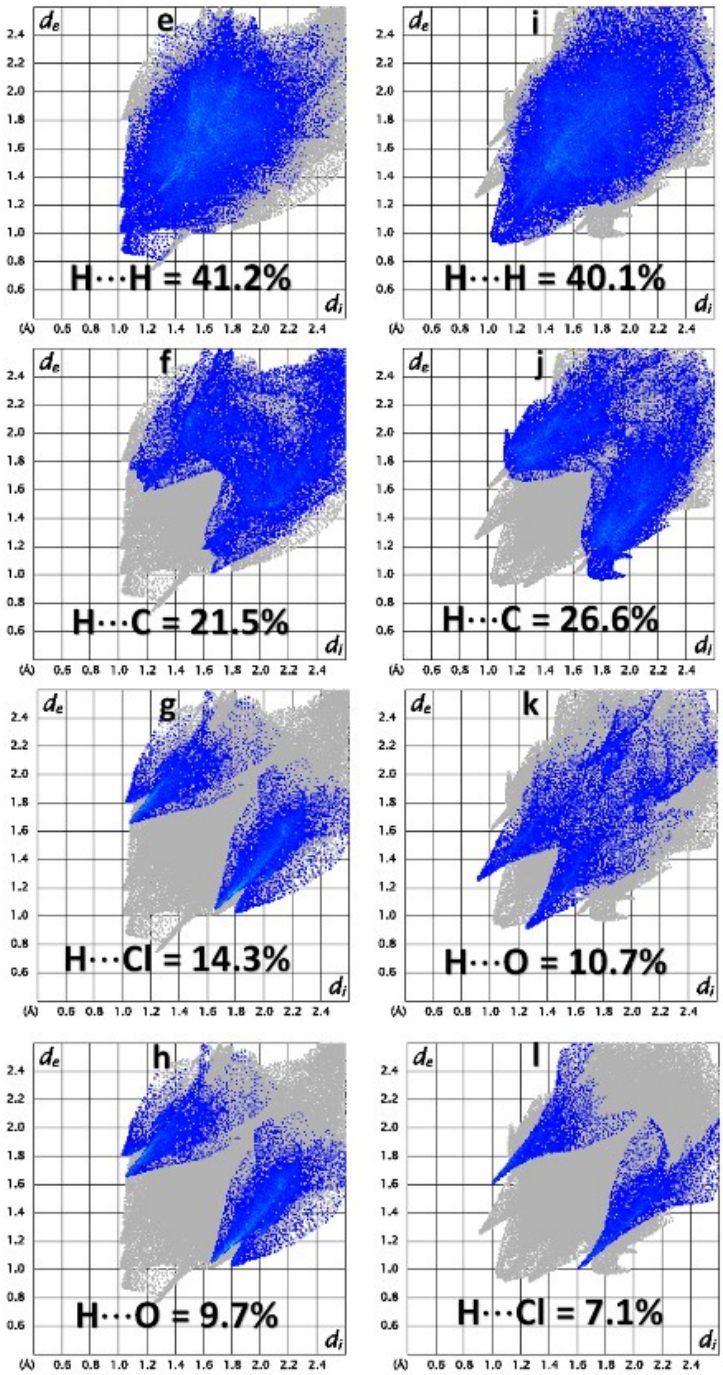

Fig. S6. 2D fingerprint plots for main molecule of **(e-h) C3**, **(i-l) C4**

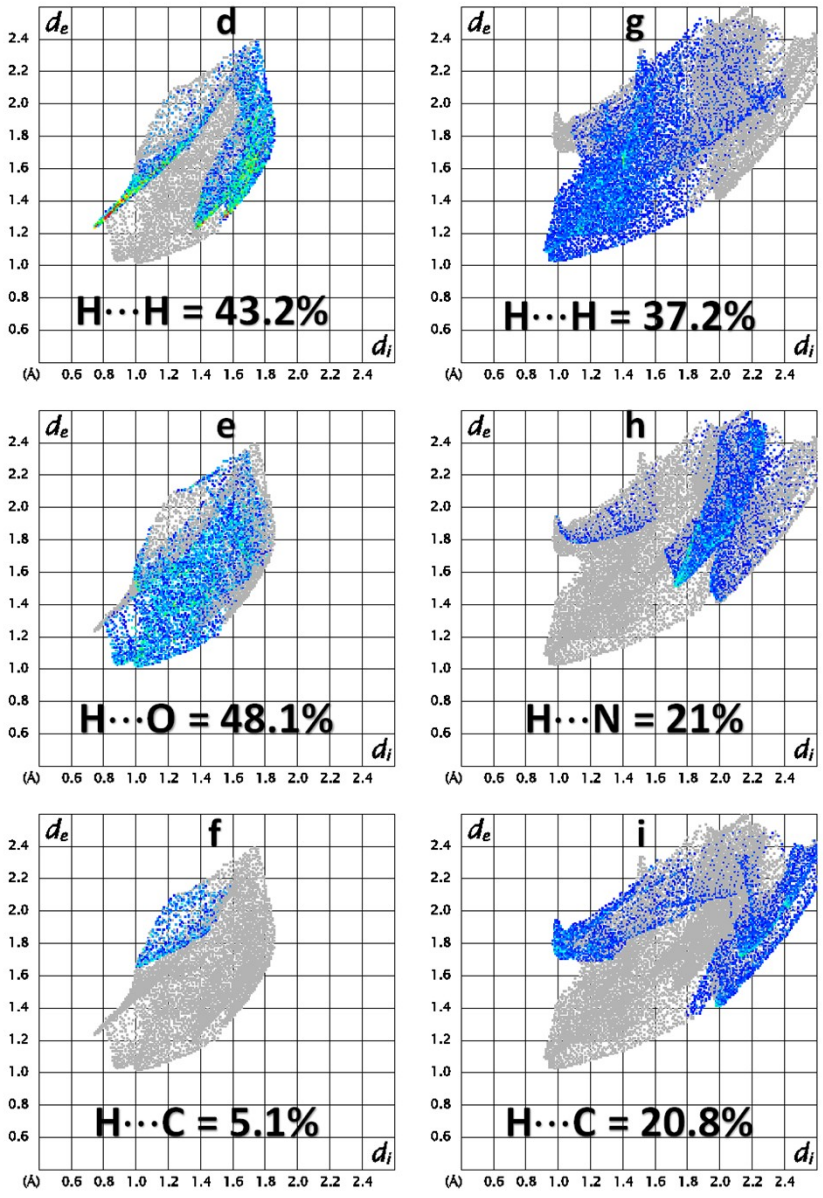

Fig. S7. 2D fingerprint plots for solvent molecules of **(d-f) C3**, **(g-i) C4**.

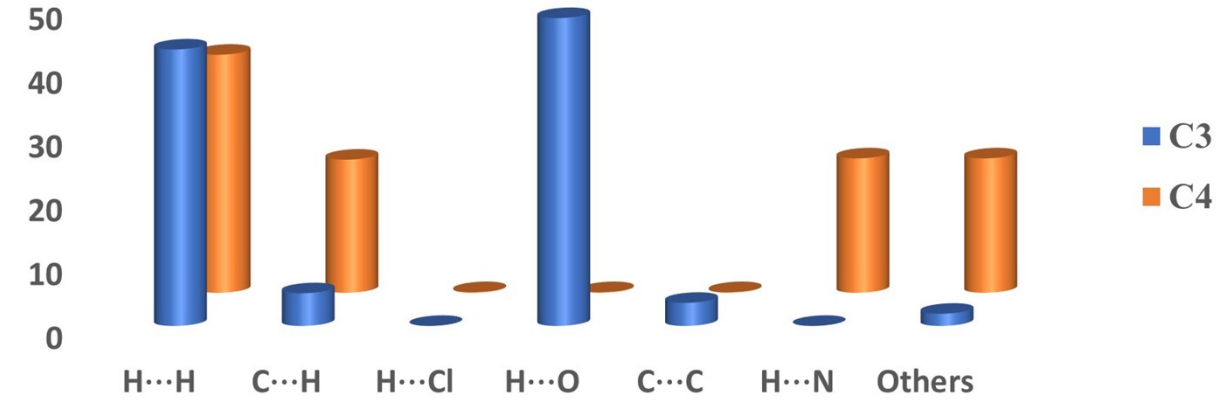

Fig. S8. Contribution of some important intermolecular contacts in the solvent molecules for the Hirshfeld surface of the complexes (**C3** and **C4**)

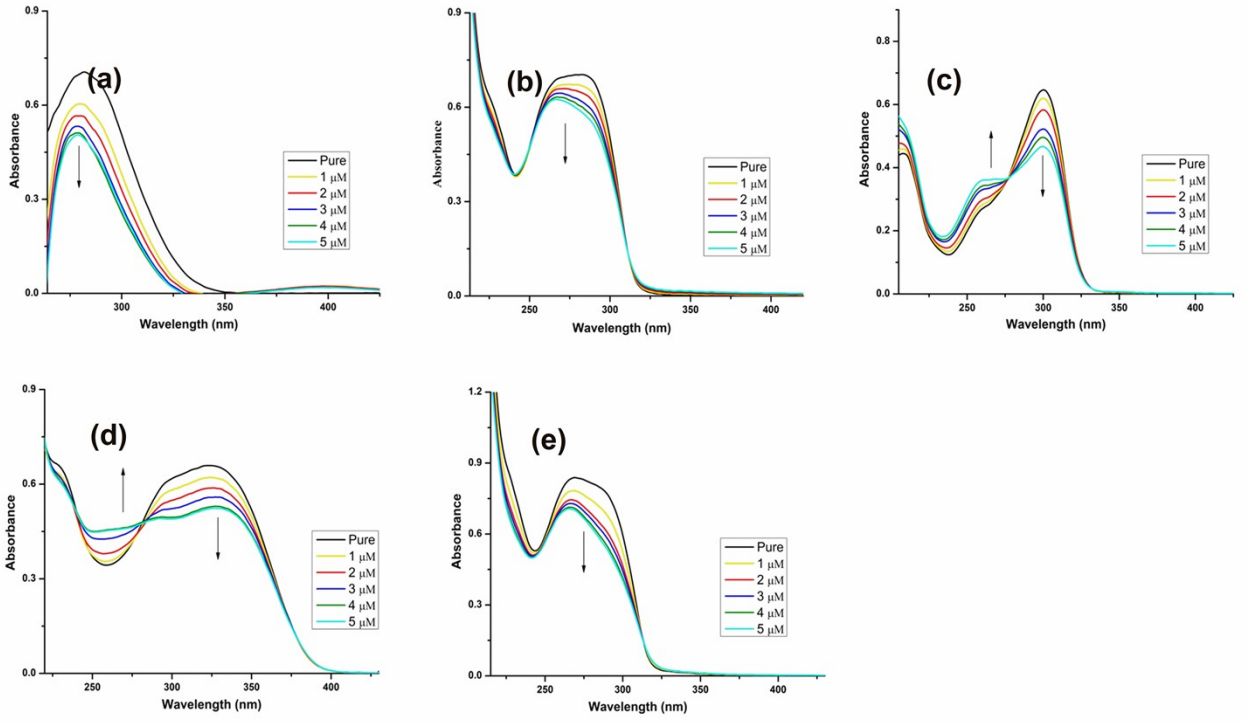

Fig. S9. Absorption titration curves of compounds (a) $^{H_2L^m}$ (b) $^{H_2L^m_{Me}(OTf)_2}$ (c) **C1** (d) **C2** (e) **C3** in Tris-HCl buffer solution containing varied CT-DNA concentrations.

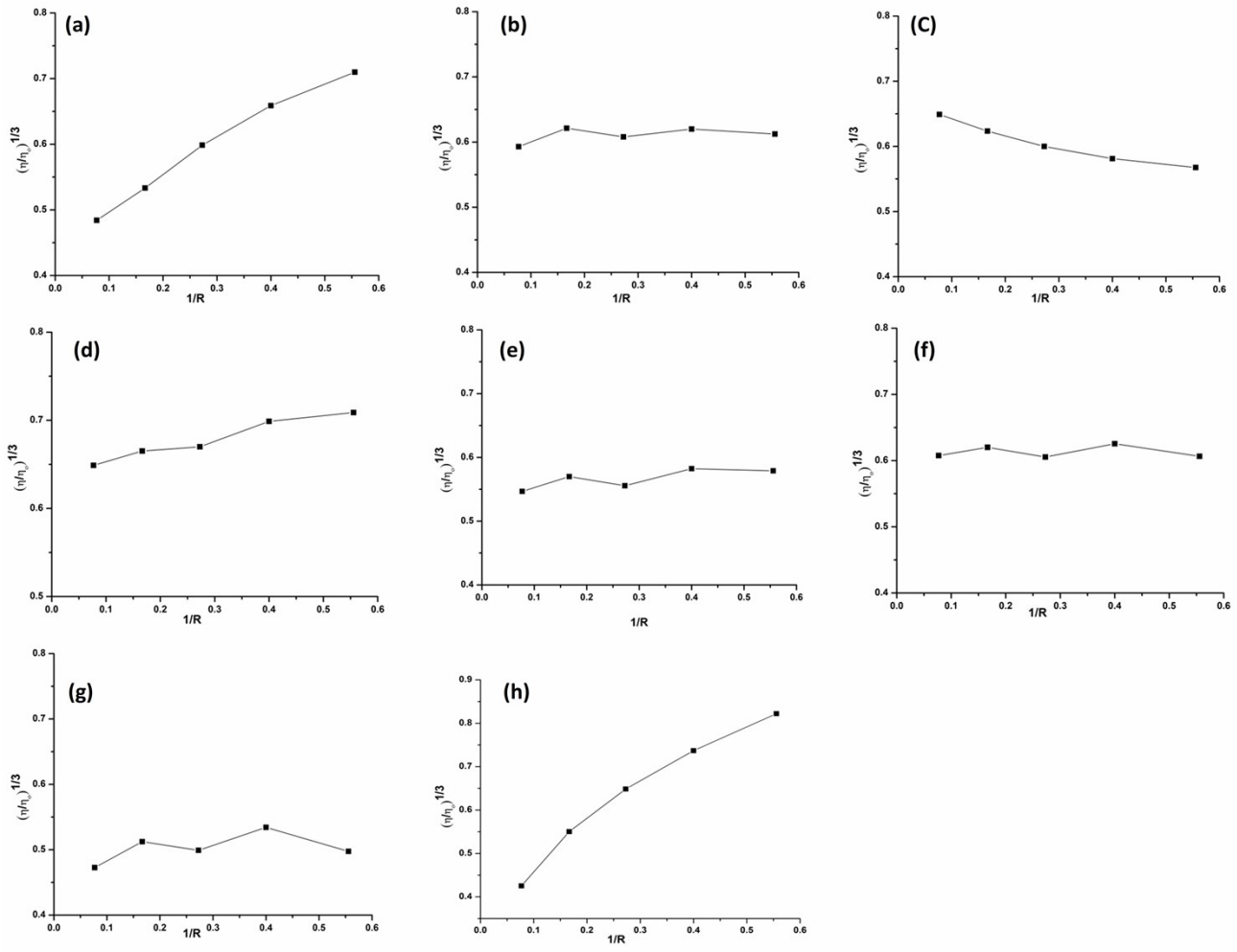

Fig. S10. Variation of the relative specific viscosity parameter $[(\eta/\eta_0)^{1/3}]$ *vs* 1/R (a) $^{H_2L^m}$ (b) $H_2L^m_{Me}(OTf)_2$ (c) $H_2L^m_{Bn}(Cl)_2$ (d) **C1** (e) **C2** (f) **C3** (g) **C4** (h) EtBr by keeping constant CT-DNA concentration