Synthesis, characterization and *in-vitro* studies of metallacyclic derivatives of titanium(IV) incorporated with Schiff's bases: DNA/BSA binding, computational aspects and cytotoxic potential

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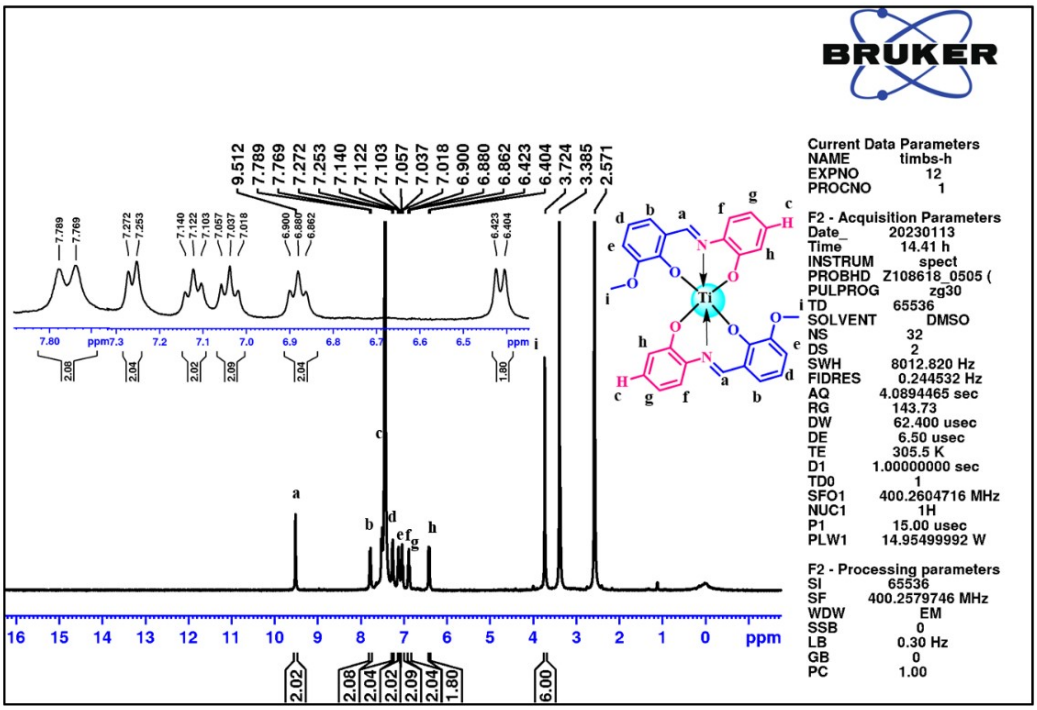
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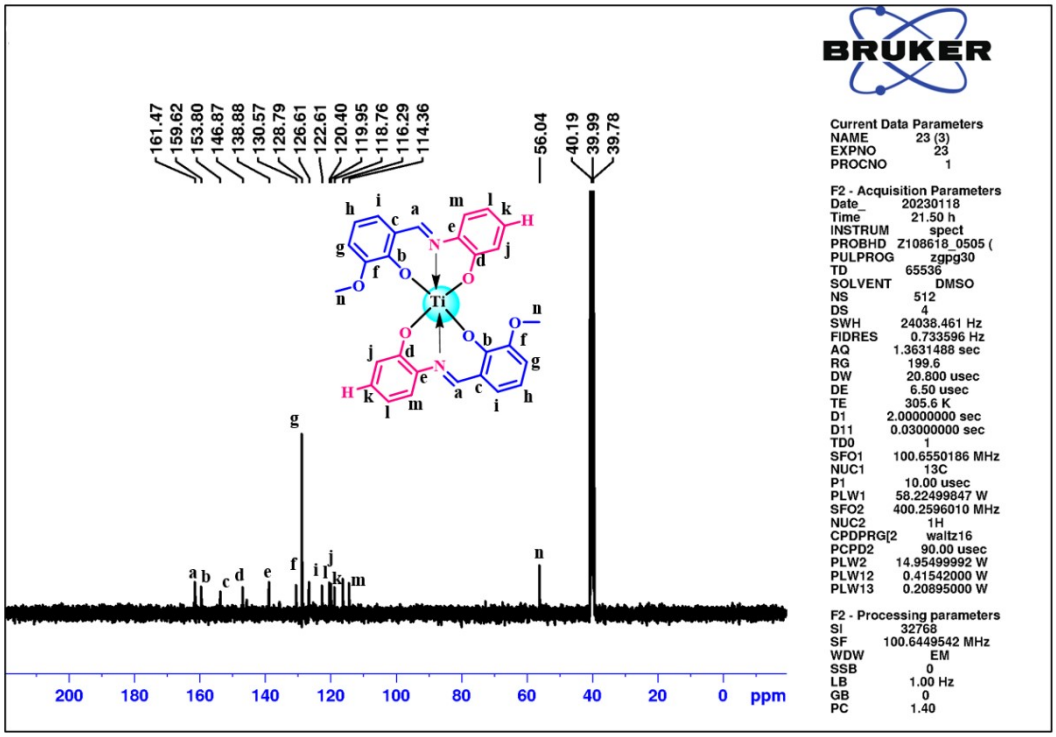
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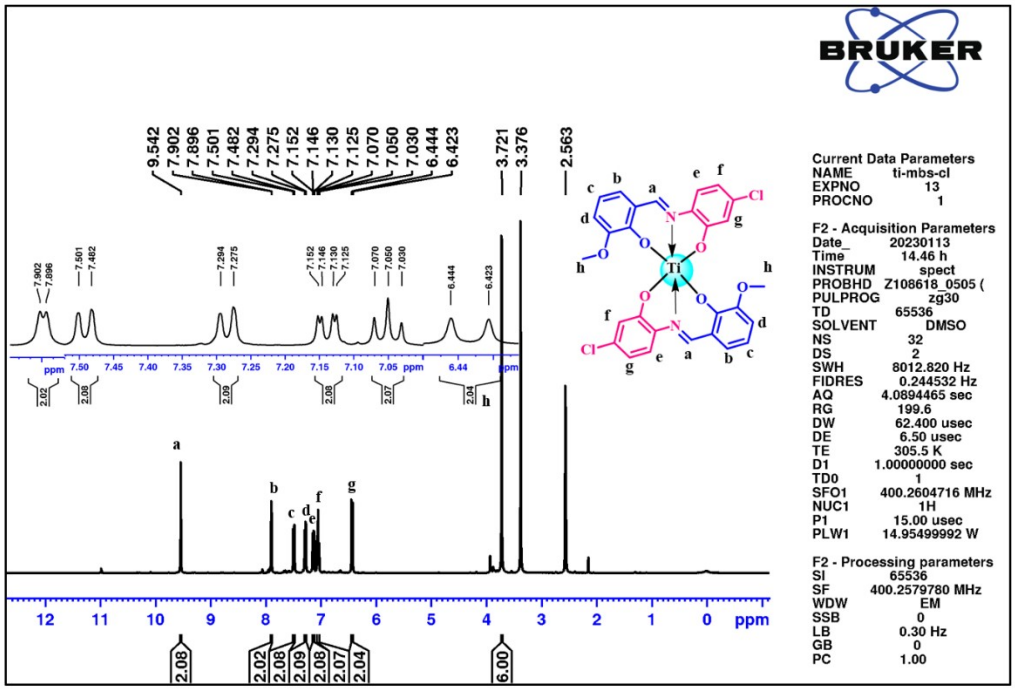
Figure 1. ^{1}H (400 MHz) and $^{13}C\{^{1}H\}$ (100 MHz) NMR spectra of $[Ti^{IV}(L^{1})_2]$ recorded in DMSO-d_6.



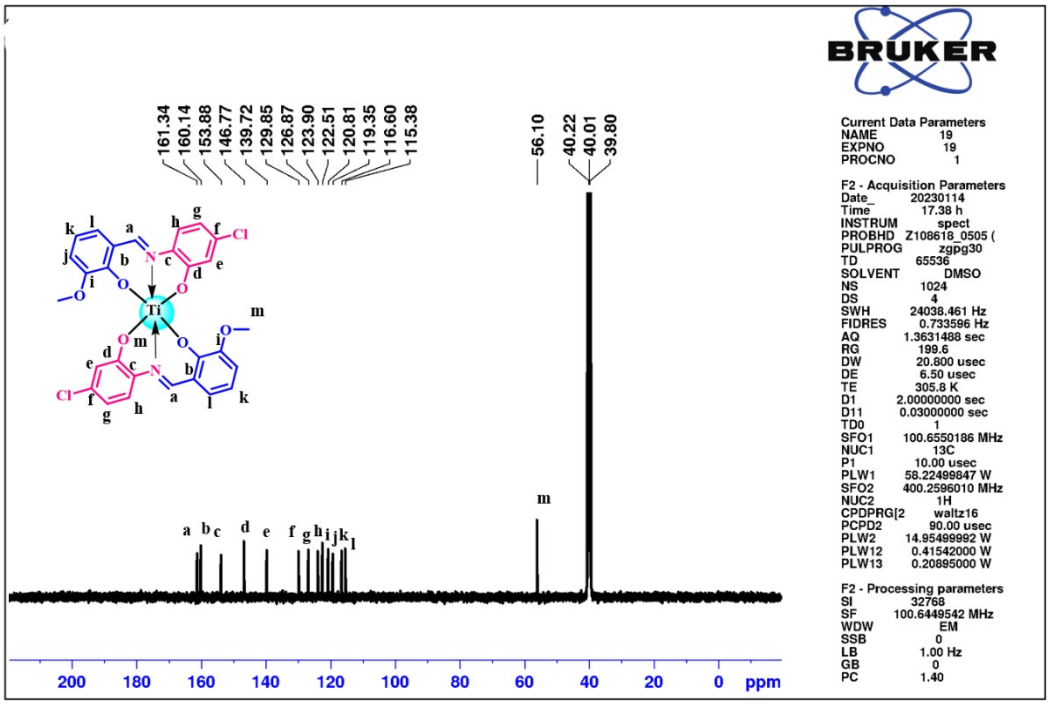
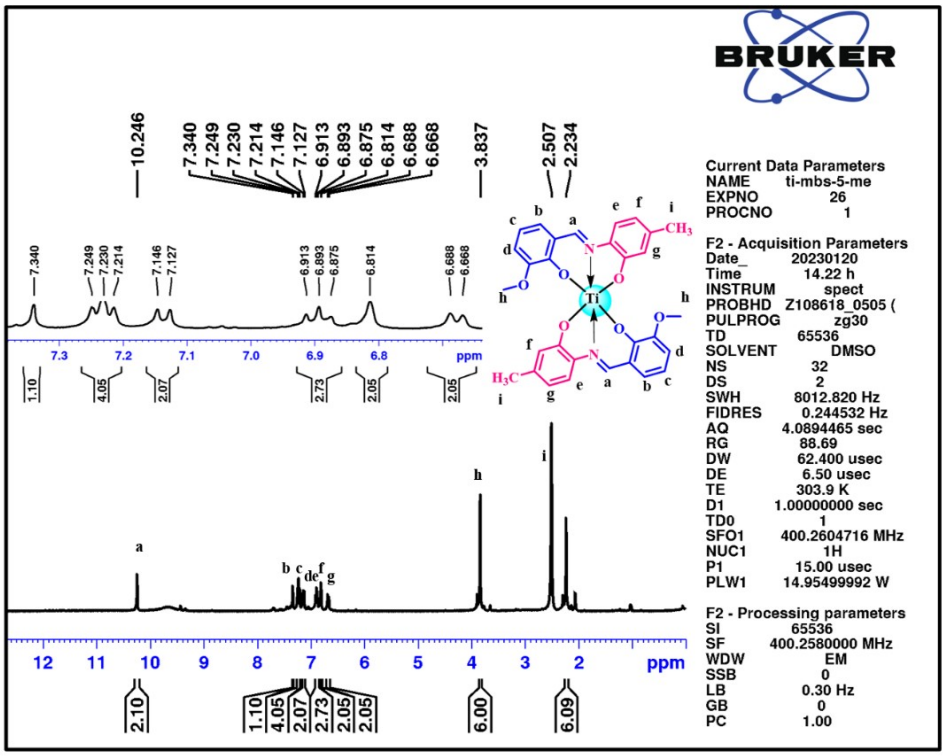


Figure 2. ^{1}H (400 MHz) and $^{13}C\{^{1}H\}$ (100 MHz) NMR spectra of $[Ti^{IV}(L^{2})_2]$ recorded in DMSO-d6.



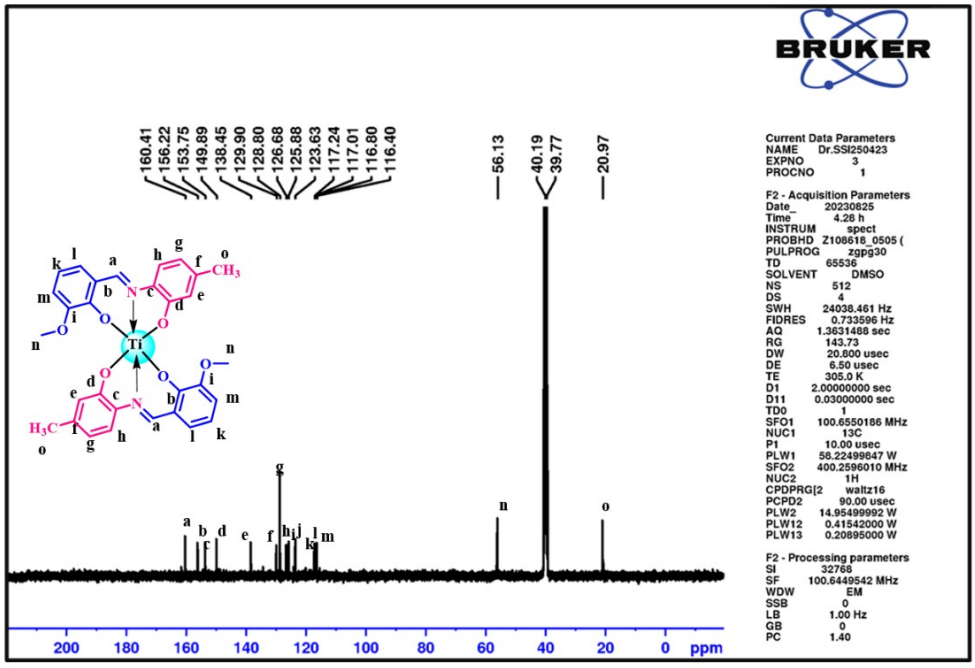
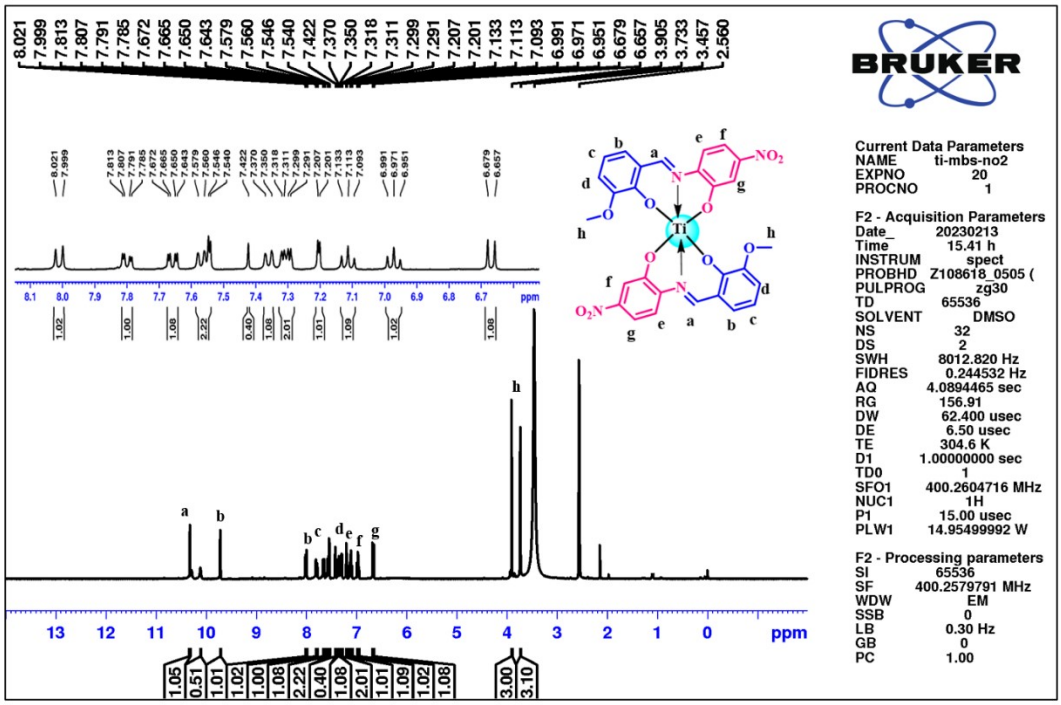


Figure 3. ^{1}H (400 MHz) and $^{13}C\{^{1}H\}$ (100 MHz) NMR spectra of $[Ti^{IV}(L^{3})_2]$ recorded in DMSO-d_6.



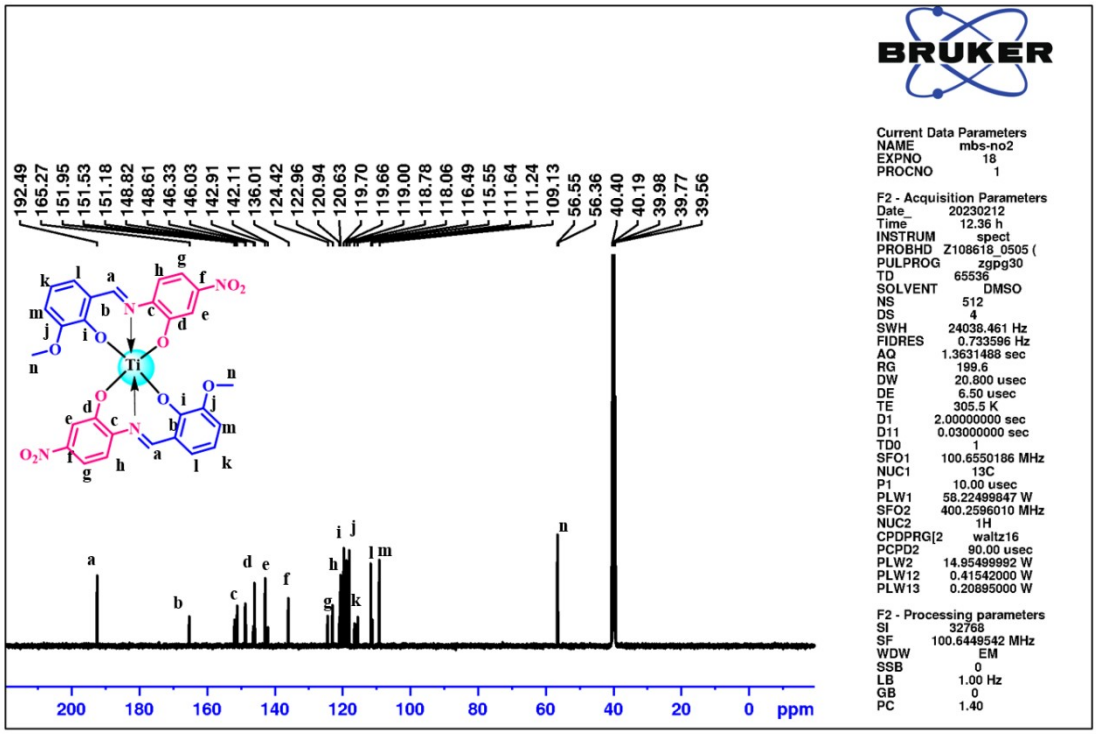
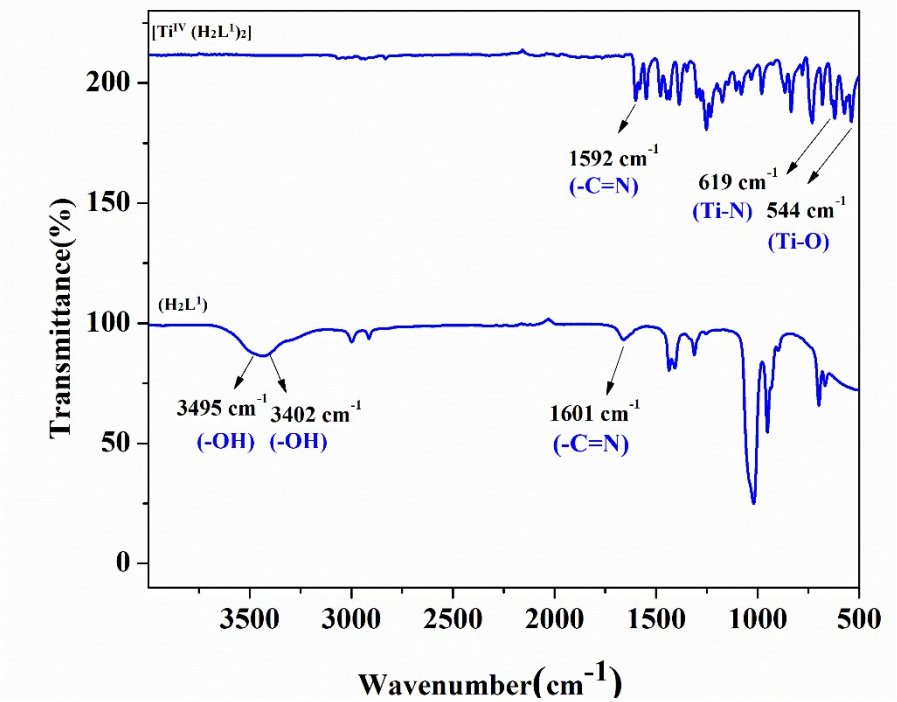


Figure 4. ^{1}H (400 MHz) and $^{13}C\{^{1}H\}$ (100 MHz) NMR spectra of $[Ti^{IV}(L^{4})_2]$ recorded in DMSO-d_6.



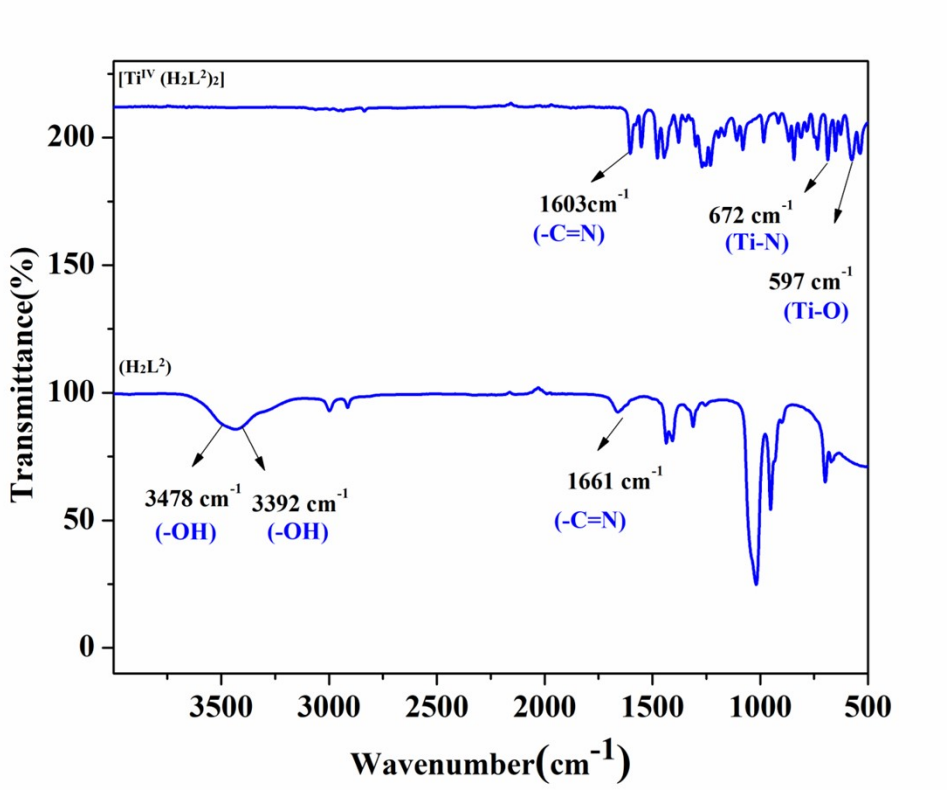
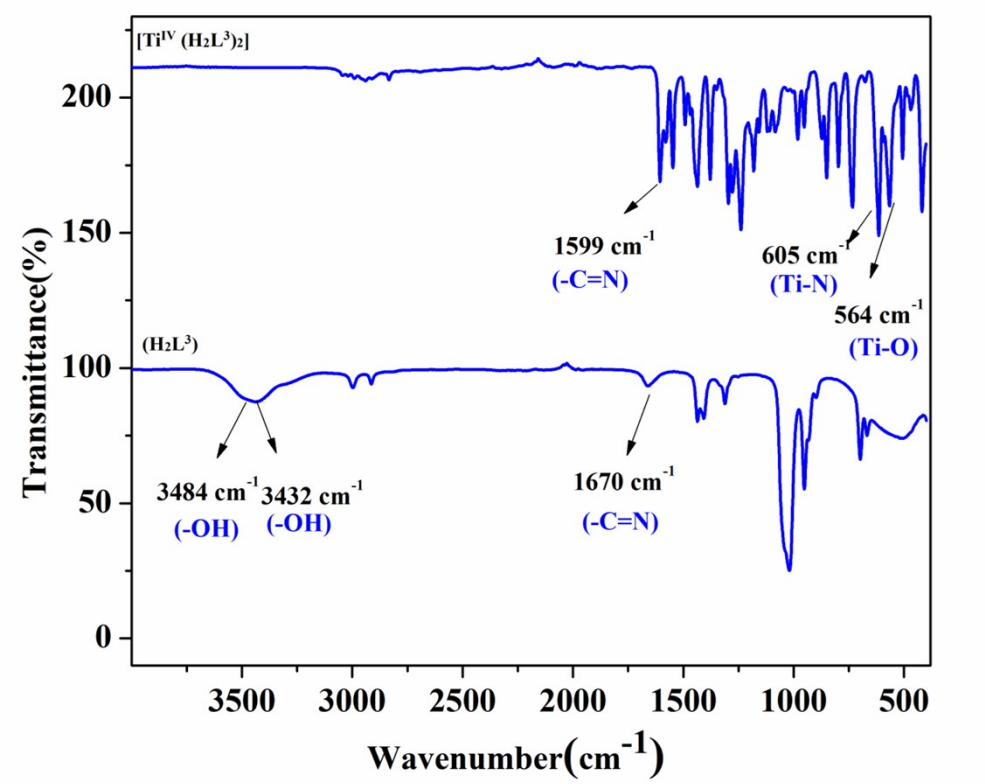


Figure 5. FTIR spectra of (H_2L^1) and [$Ti^{IV}(L^1)_2$]

Figure 6. FTIR spectra of (H_2L^2) and [$Ti^{IV}(L^2)_2$]



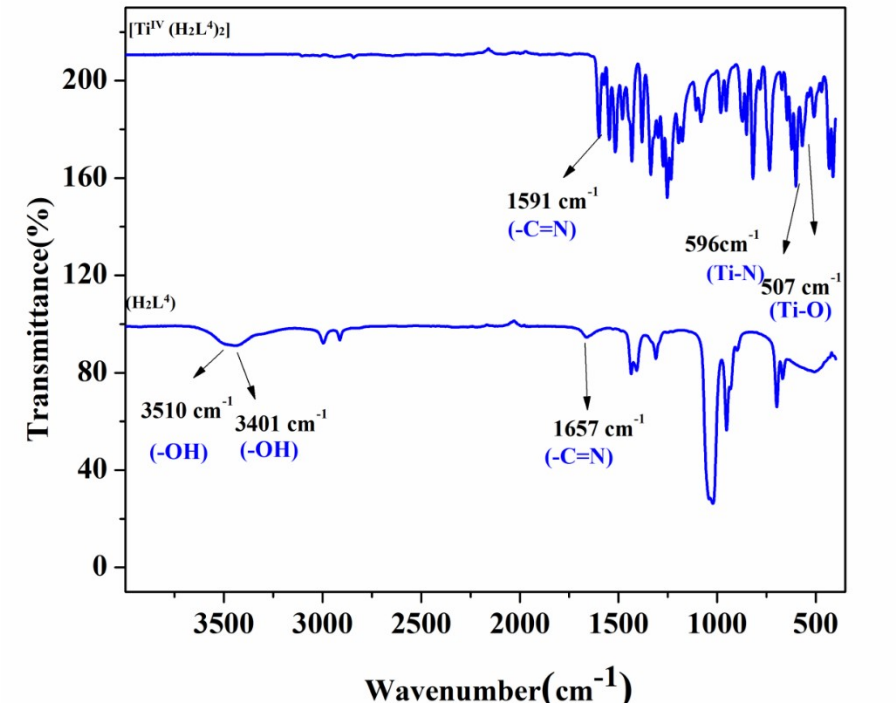


Figure 7. FTIR spectra of (H_2L^3) and [$Ti^{IV}(L^3)_2$]

Figure 8. FTIR spectra of (H_2L^4) and [$Ti^{IV}(L^4)_2$]

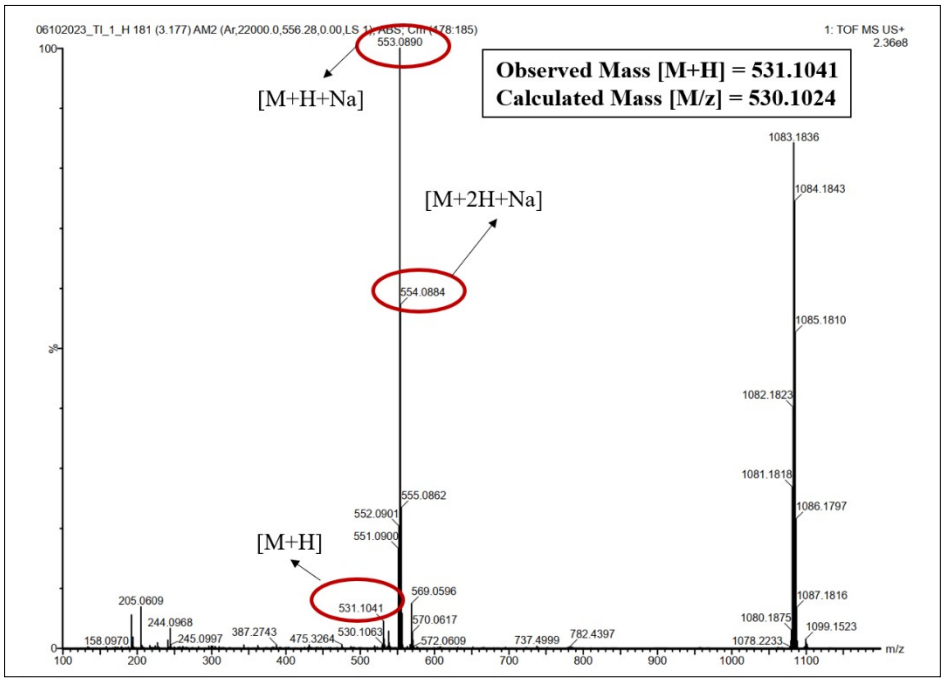


Figure 9. HRMS (ESI+) spectrum of [$Ti^{IV}(L^1)_2$]

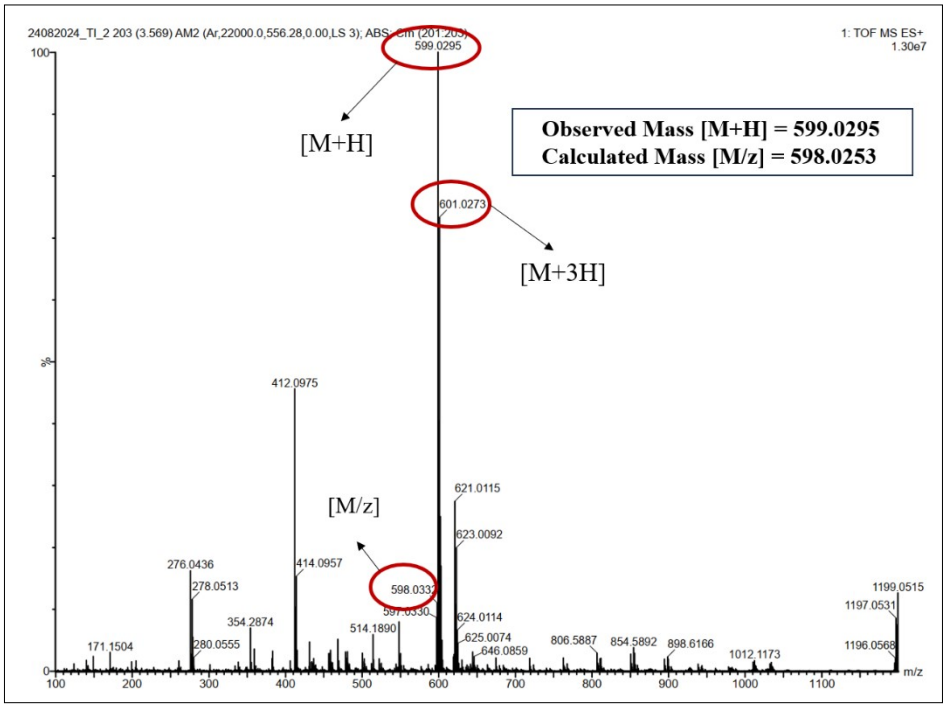


Figure 10. HRMS (ESI$^+$) spectrum of $[Ti^{IV}(L^2)_2]$

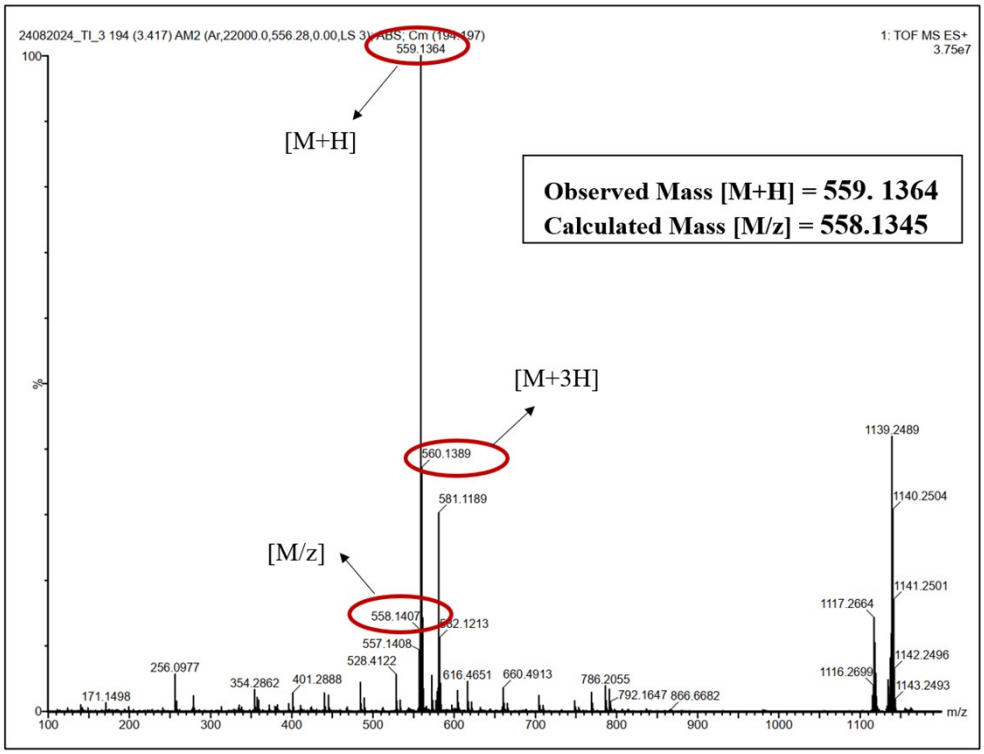


Figure 11. HRMS (ESI$^+$) spectrum of $[Ti^{IV}(L^3)_2]$

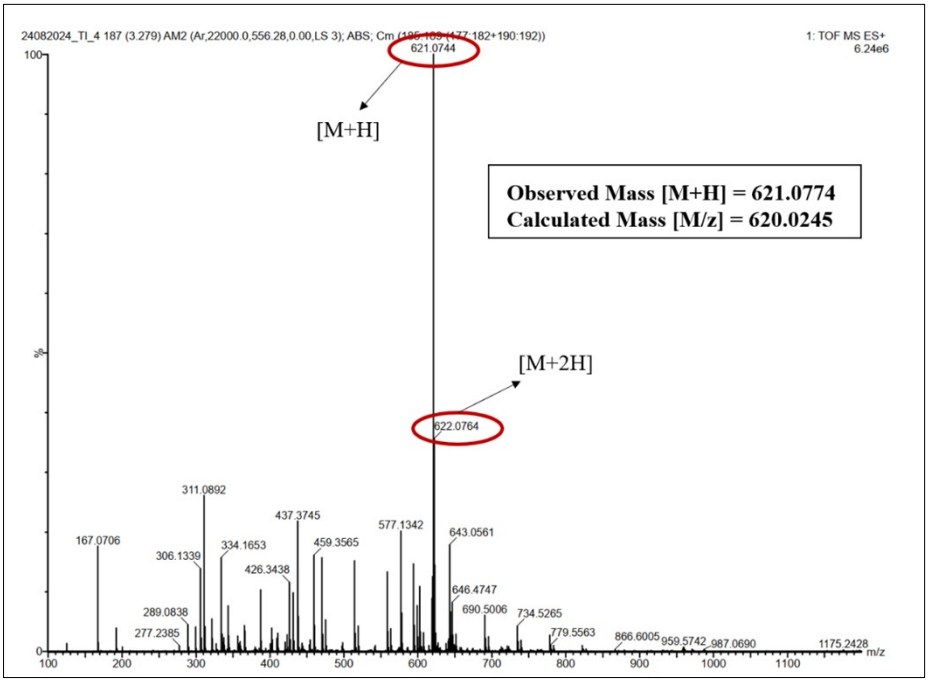


Figure 12. HRMS (ESI^+) spectrum of $[Ti^{IV}(L^4)_2]$

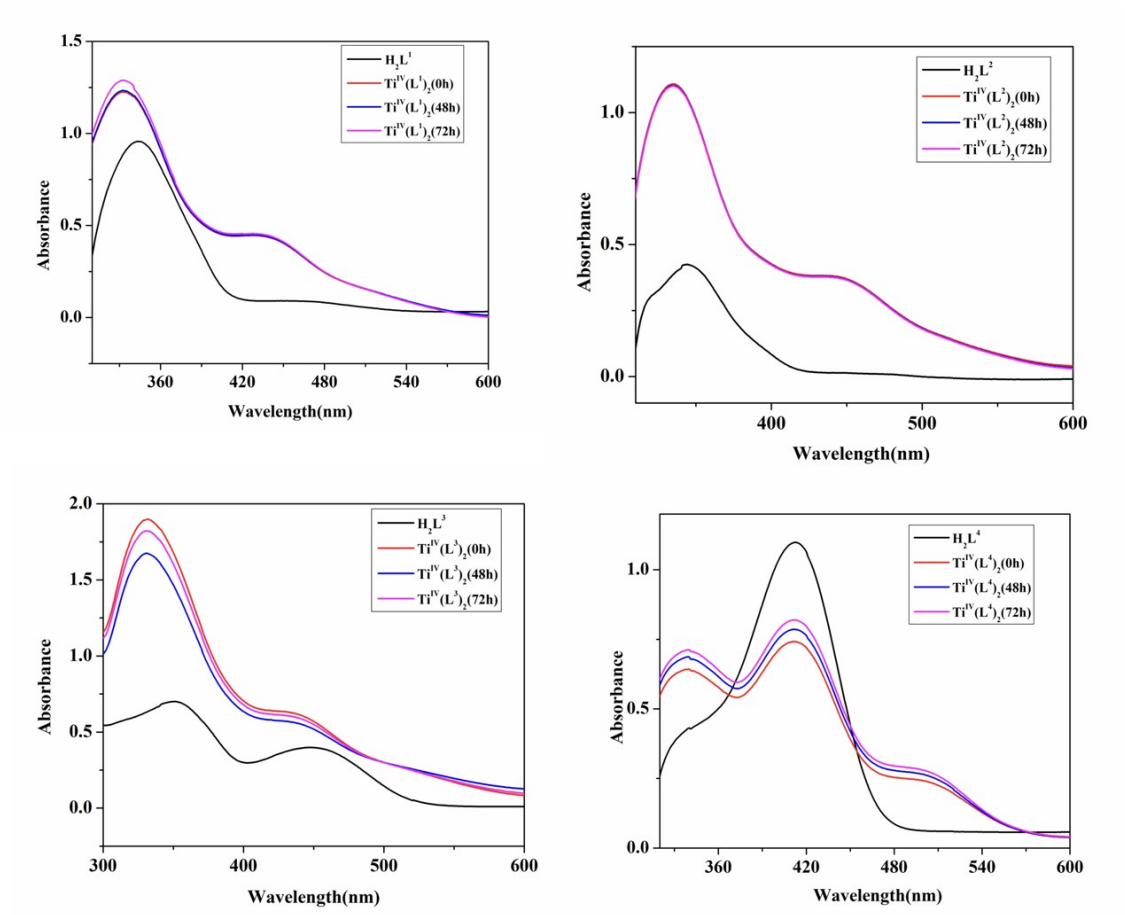
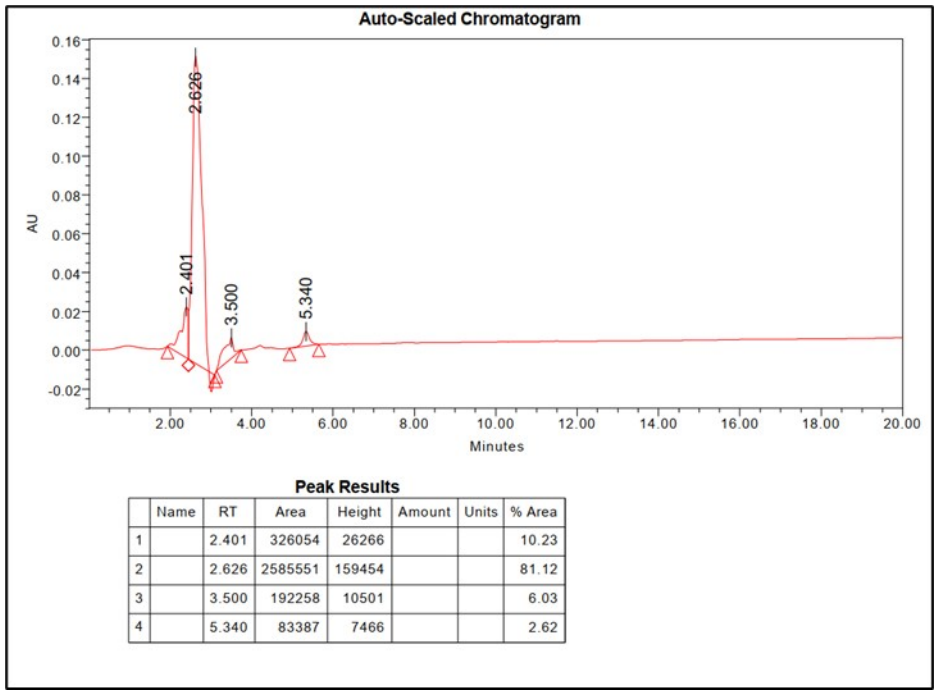


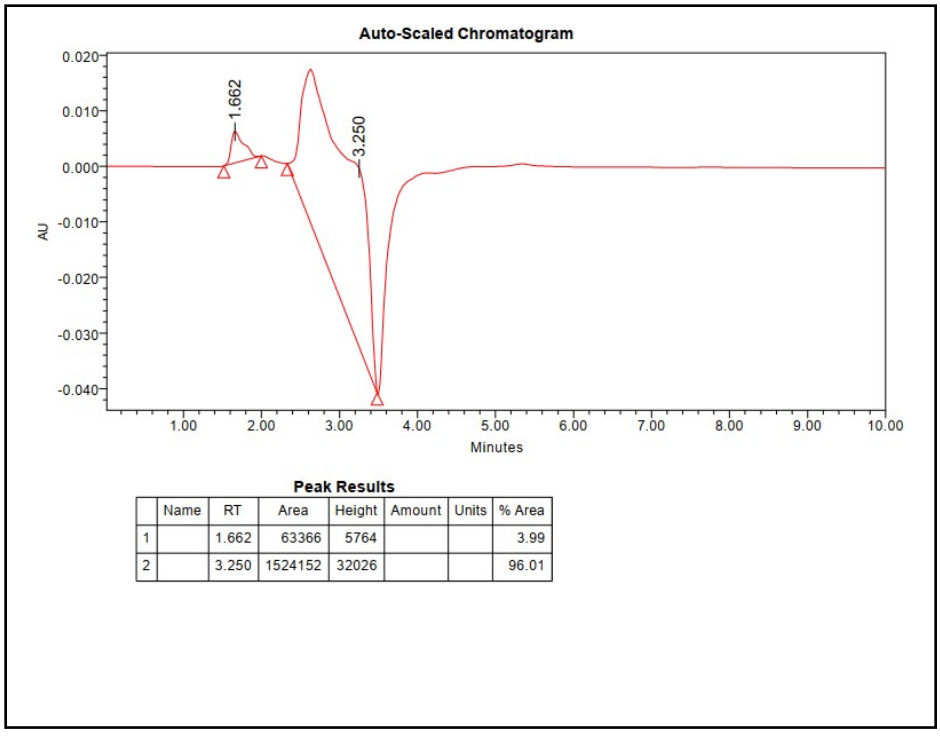
Figure 13. UV-Vis spectra of ($L^{1\text{-}4}$) and $[Ti^{IV}(L^{1\text{-}4})_2]$ recorded in DMSO medium



Peak Results

	Name	RT	Area	Height	Amount	Units	% Area
1		2.401	326054	26266			10.23
2		2.626	2585551	159454			81.12
3		3.500	192258	10501			6.03
4		5.340	83387	7466			2.62

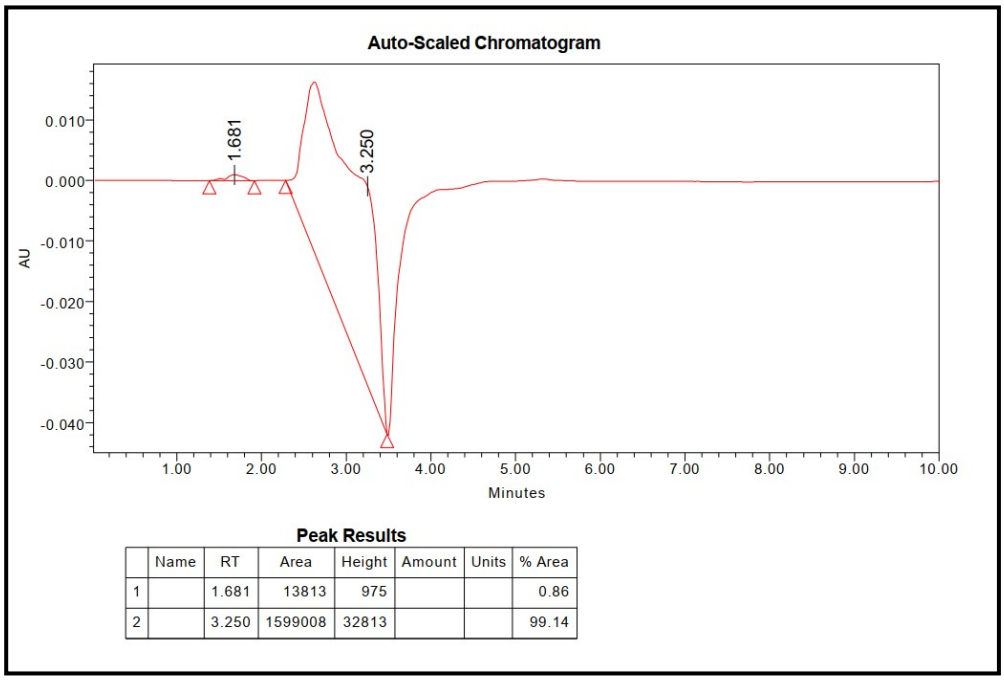
Figure 14. HPLC chromatograms of complex $[Ti^{IV}(L^1)_2]$



Peak Results

	Name	RT	Area	Height	Amount	Units	% Area
1		1.662	63366	5764			3.99
2		3.250	1524152	32026			96.01

Figure 15. HPLC chromatograms of complex $[Ti^{IV}(L^2)_2]$



Peak Results

	Name	RT	Area	Height	Amount	Units	% Area
1		1.681	13813	975			0.86
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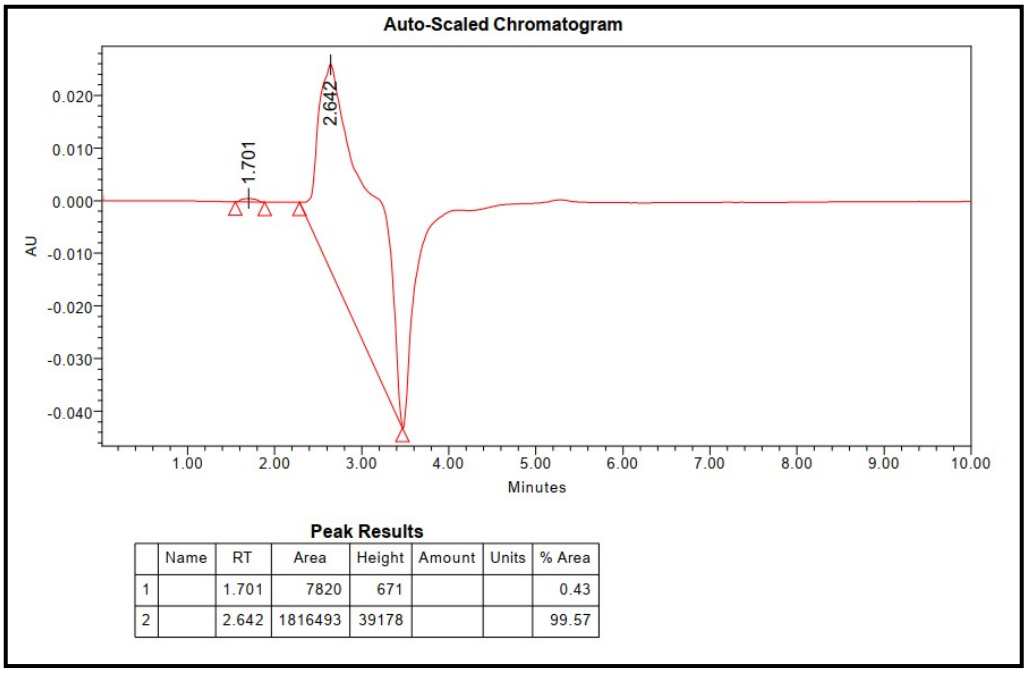
Figure 16. HPLC chromatograms of complex $[Ti^{IV}(L^3)_2]$



Peak Results

	Name	RT	Area	Height	Amount	Units	% Area
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Figure 17. HPLC chromatograms of complex $[Ti^{IV}(L^4)_2]$

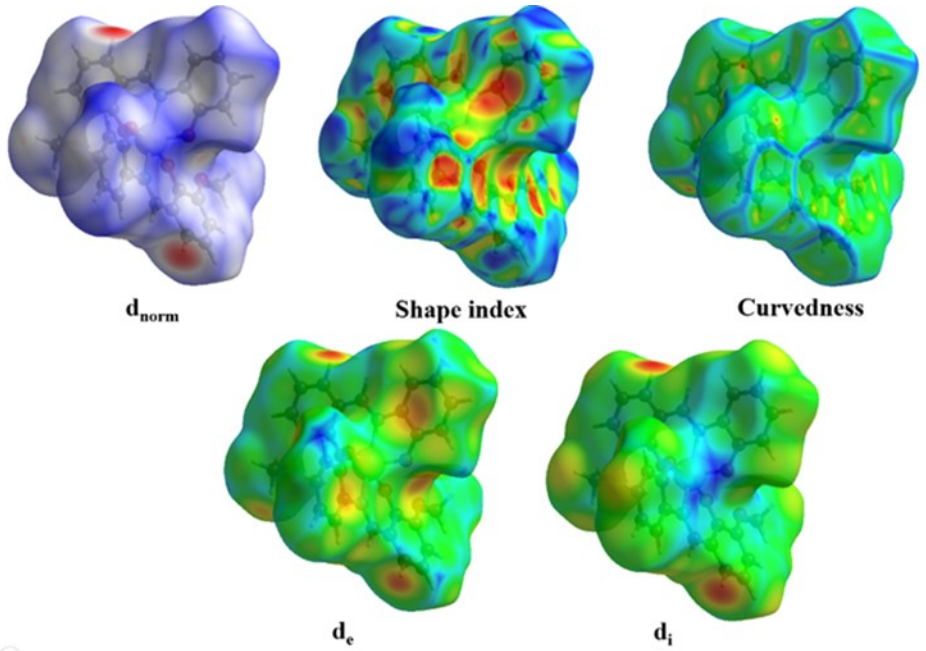

Figure 18. Molecular surface images of the d_{norm}, Shape index, Curvedness, d_e and d_i for the complex of $[Ti^{IV}(L^3)_2]$

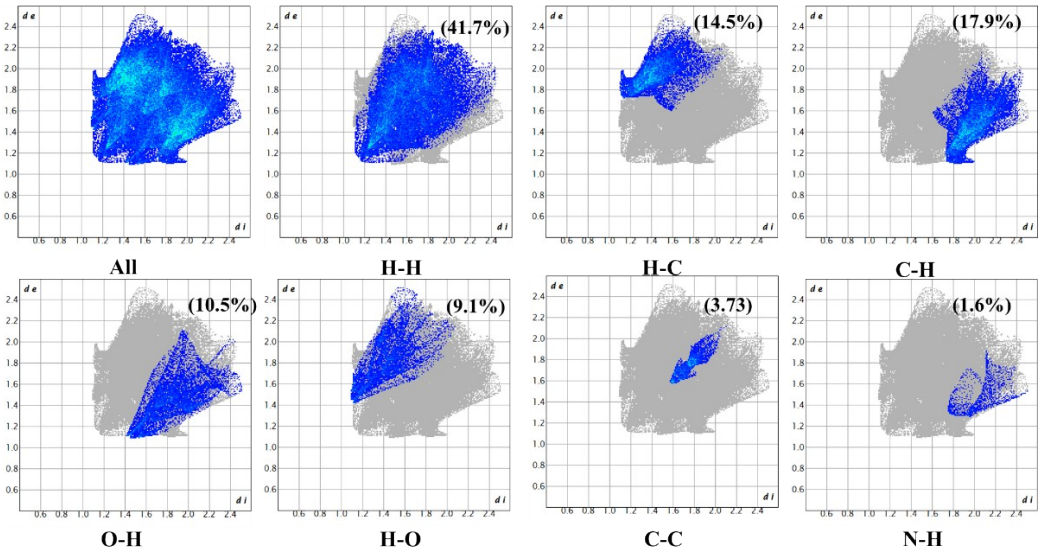

Figure 19. Fingerprint 2D-plot of $[Ti^{IV}(L^3)_2]$ with the intermolecular interactions for the specific contact

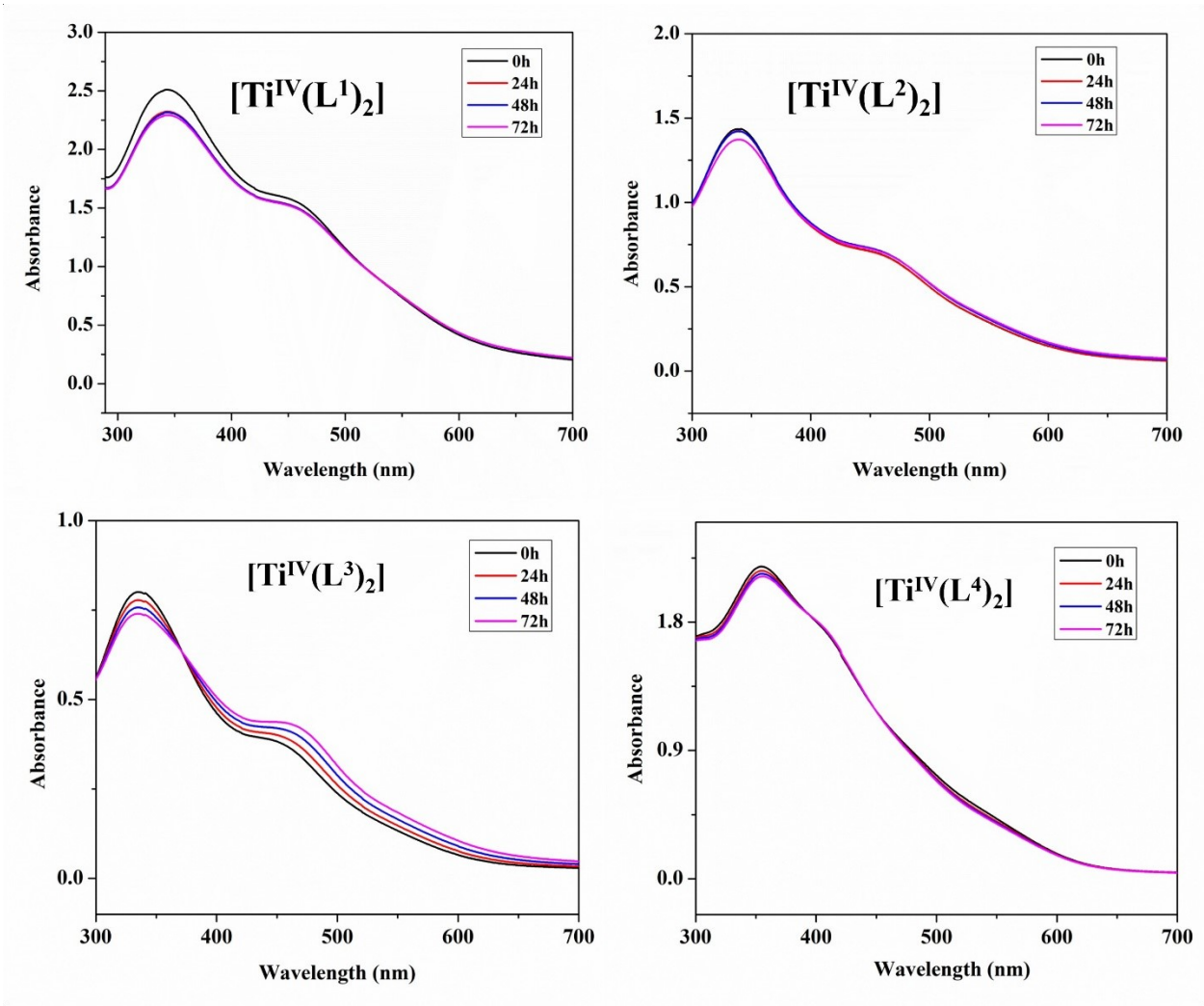

Figure 20. UV-Vis stability study of $[Ti^{IV}(L^{1\text{-}4})_2]$ complexes in GSH medium

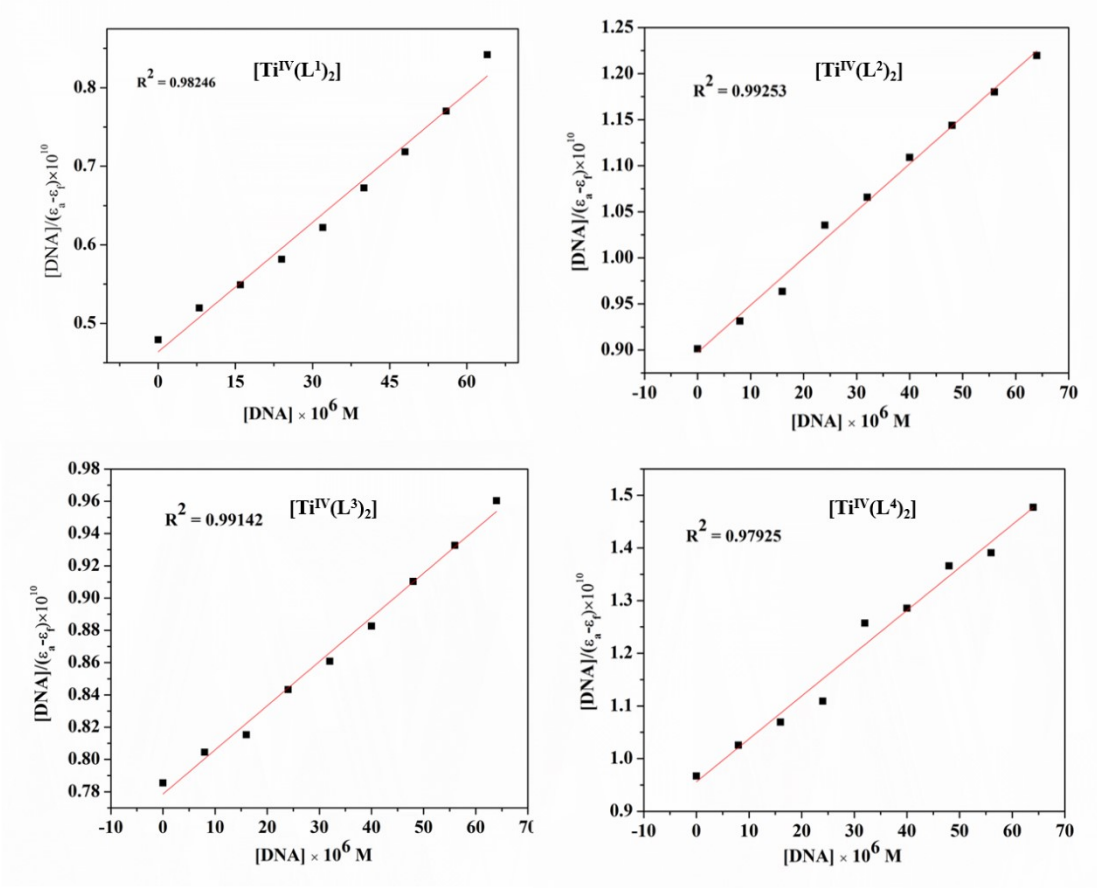

Figure 21. Linear plots of (DNA)/($\varepsilon_a - \varepsilon_f$) *vs* (DNA) [$Ti^{IV}(L^{1\text{-}4})_2$]

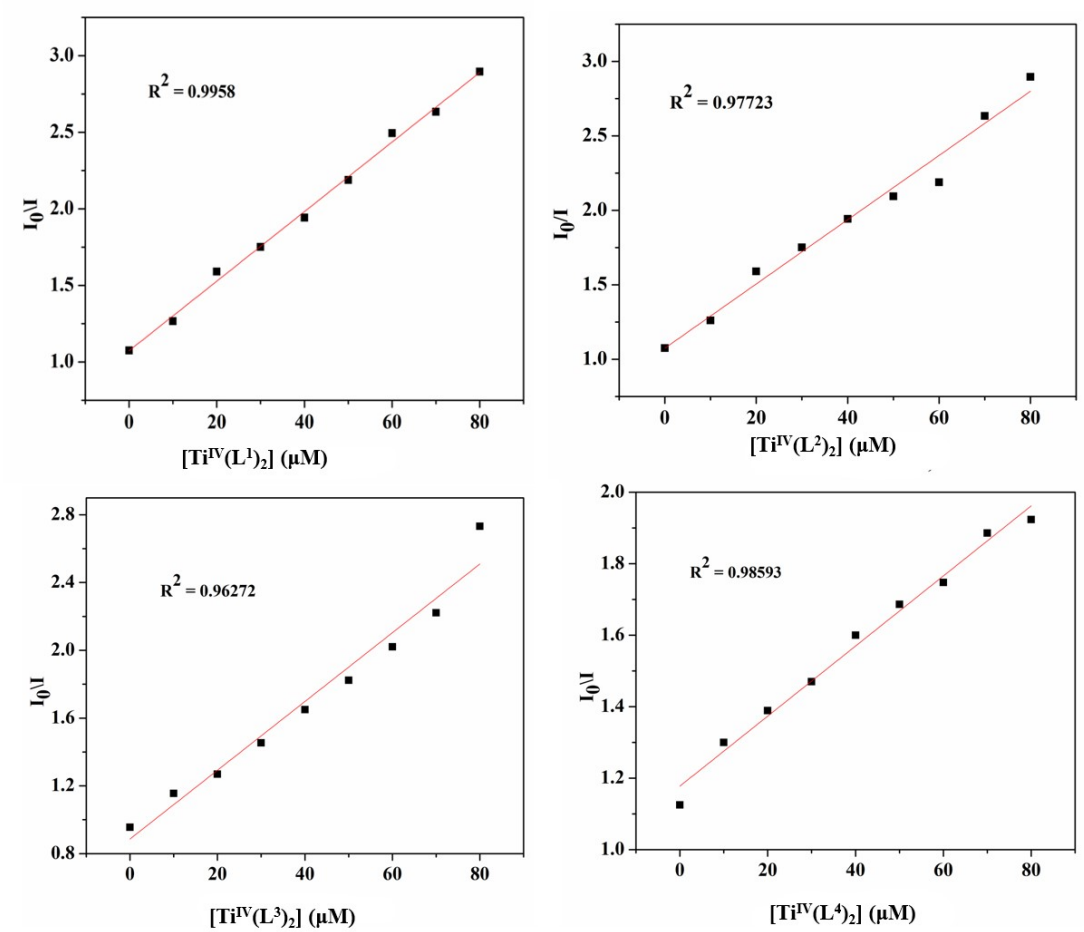

Figure 22. Stern–Volmer plots I_0/I *vs* complexes $[Ti^{IV}(L^{1\text{-}4})_2]$

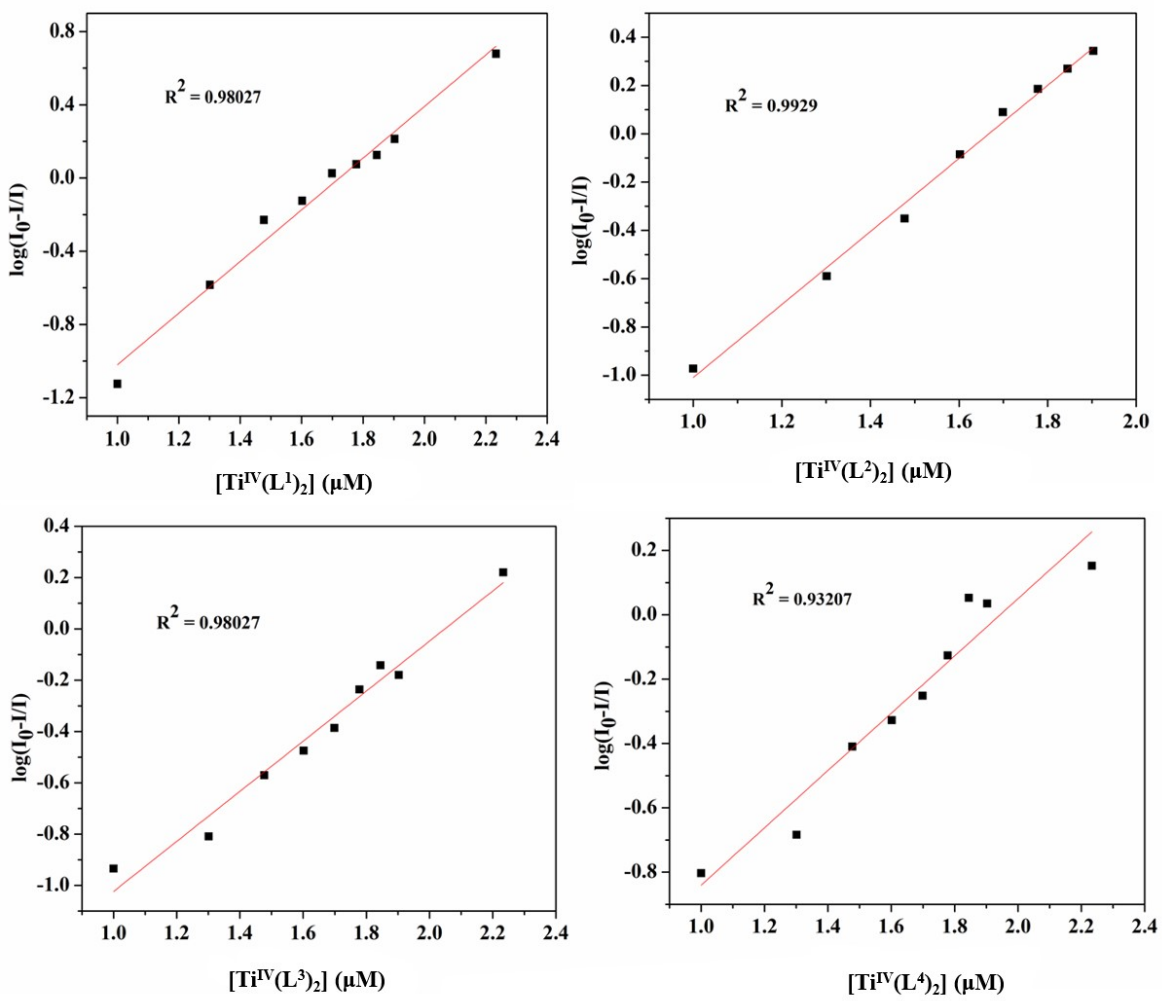

Figure 23. Scatchard plots of log $(I_0–I)/I$ *vs* log (Q)

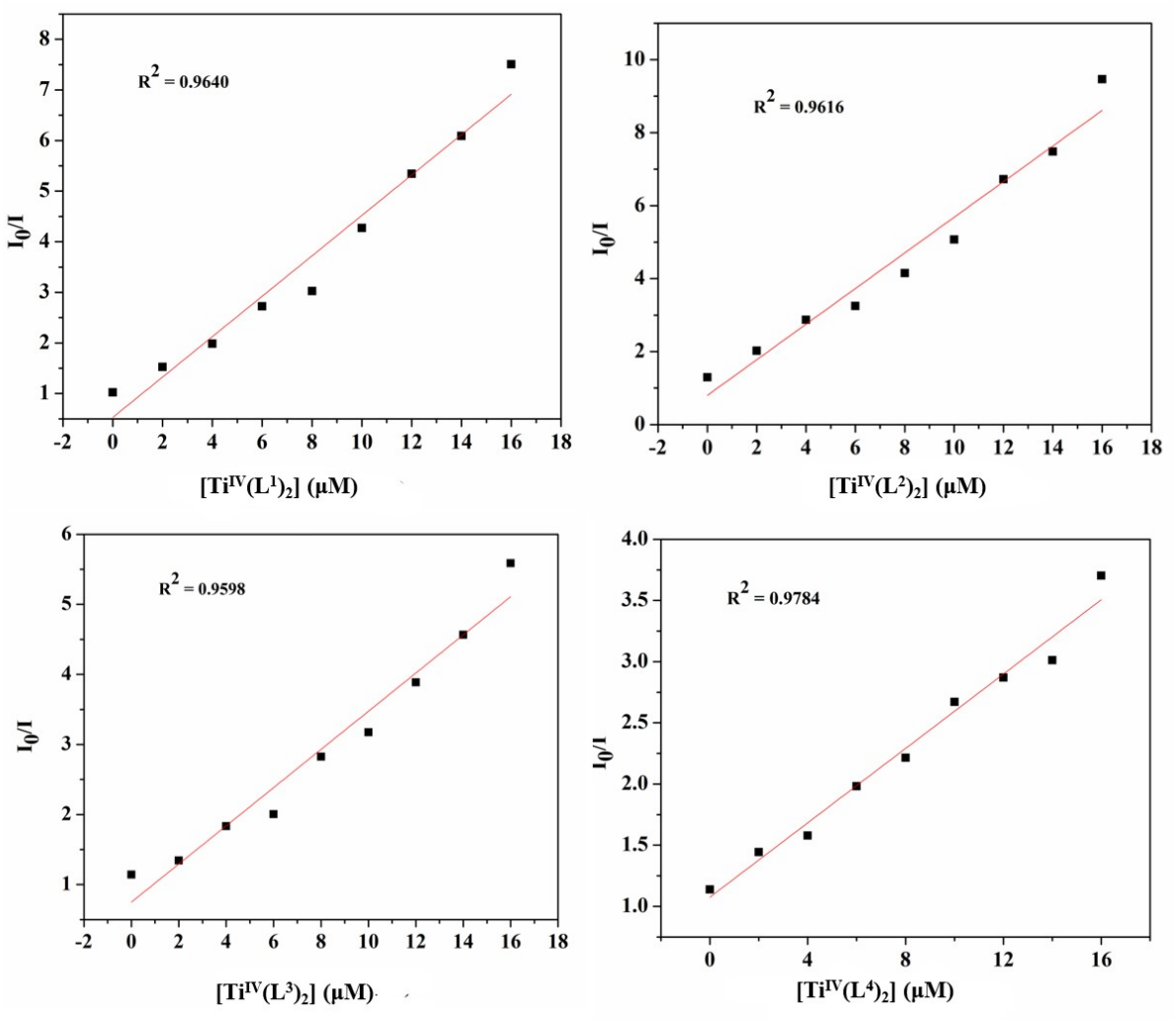

Figure 24. Stern–Volmer plots I_0/I *vs* complexes $[Ti^{IV}(L^{1\text{-}4})_2]$

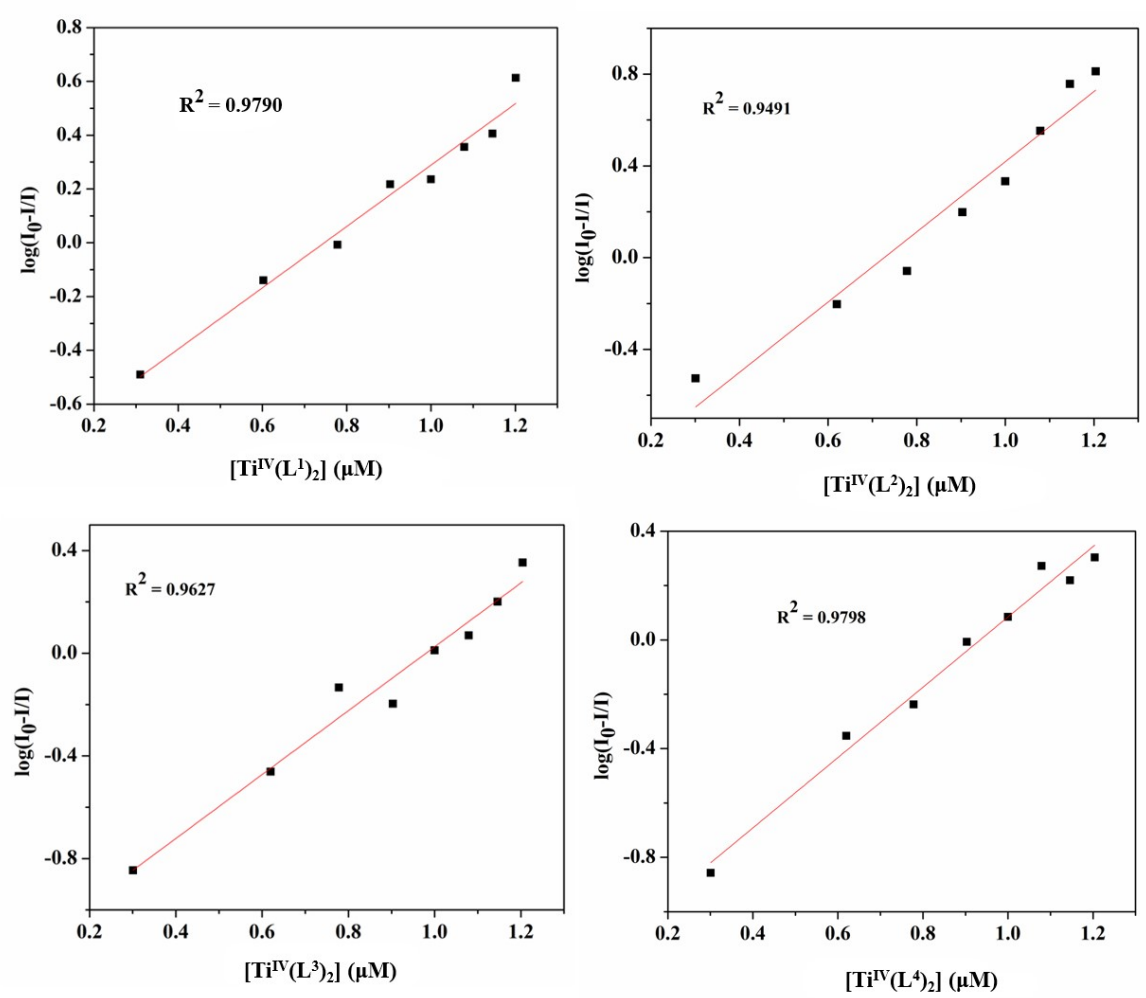

Figure 25. Scatchard plots of log $(I_0–I)/I$ *vs* log (Q)

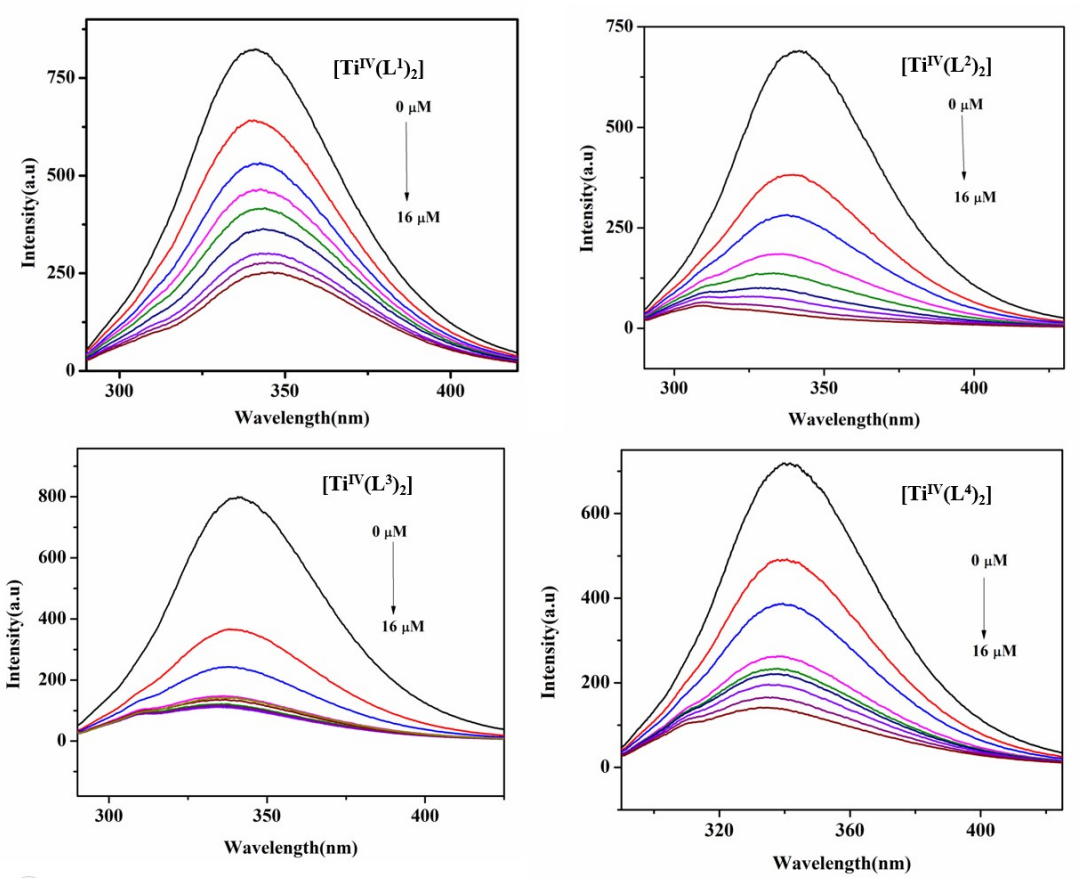

Figure 26. Synchronous fluorescence spectra of BSA of complexes $[Ti^{IV}(L^{1-4})_2]$ (0-16 μM) at $\Delta\lambda$ = 60 nm (Recorded in DMSO medium)

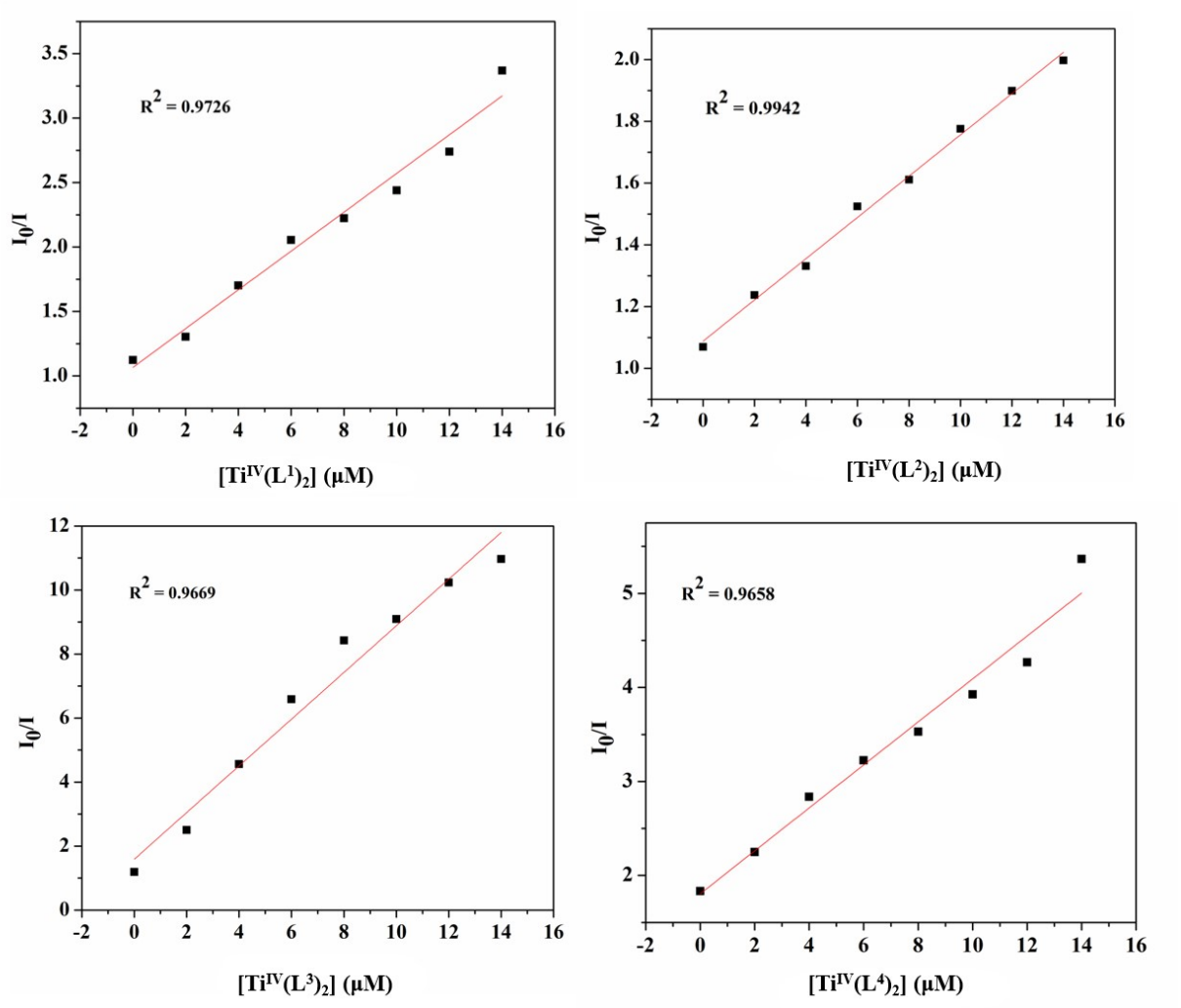

Figure 27. Linear Stern -Volmer plots of complexes $[Ti^{IV}(L^{1\text{-}4})_2]$

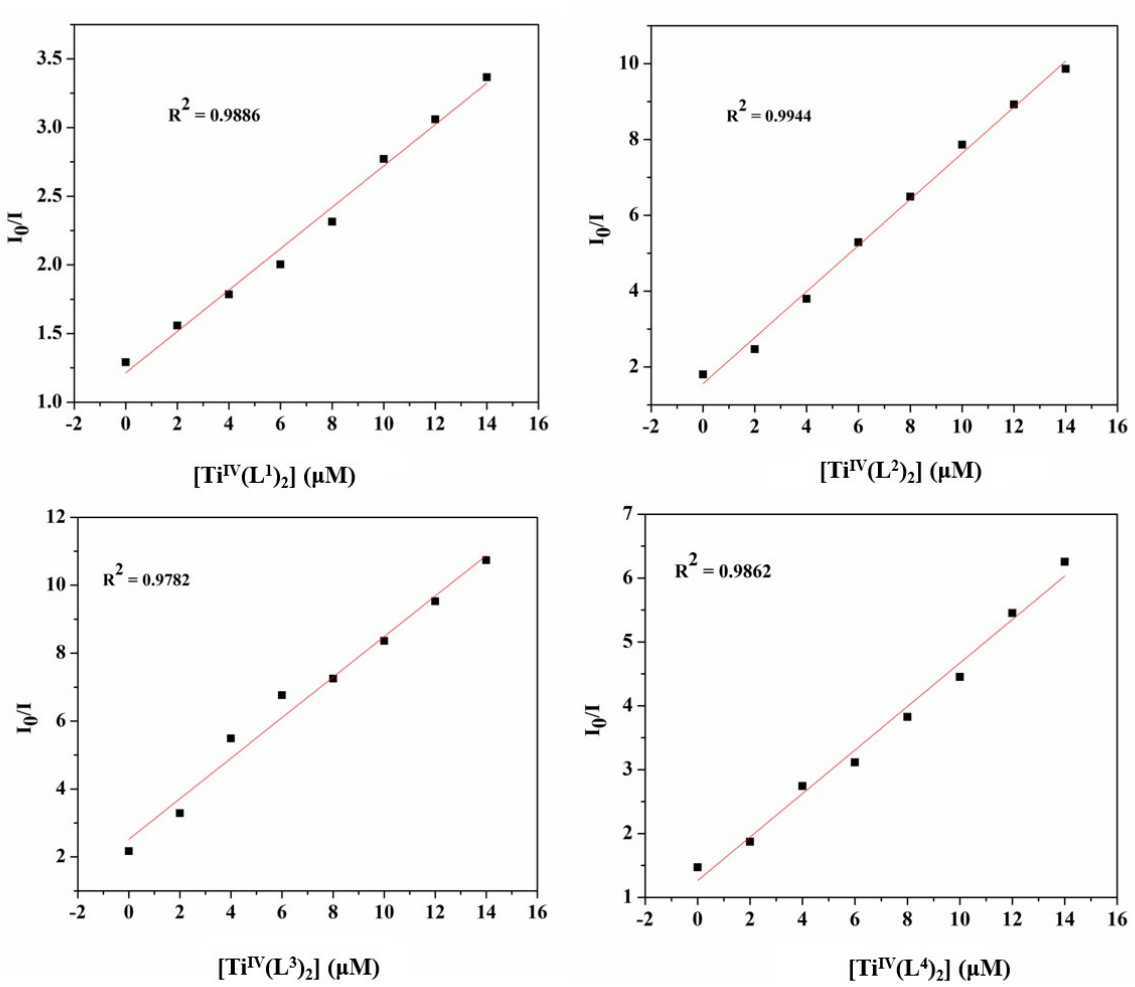

Figure 28. Stern–Volmer plots complexes $[Ti^{IV}(L^{1\text{-}4})_2]$

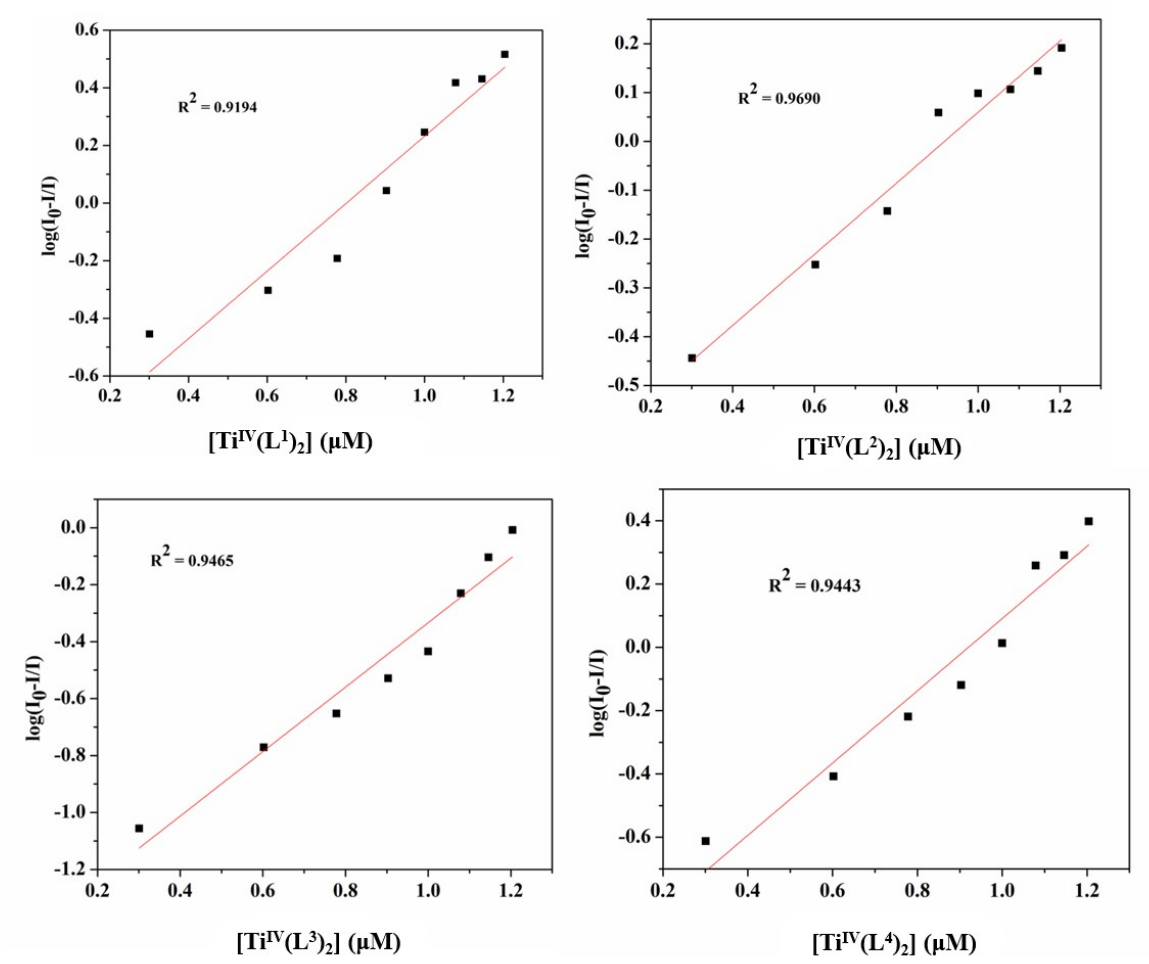

Figure 29. Site marker study of Warfarin bound BSA double log plots of complexes $[Ti^{IV}(L^{1\text{-}4})_2]$

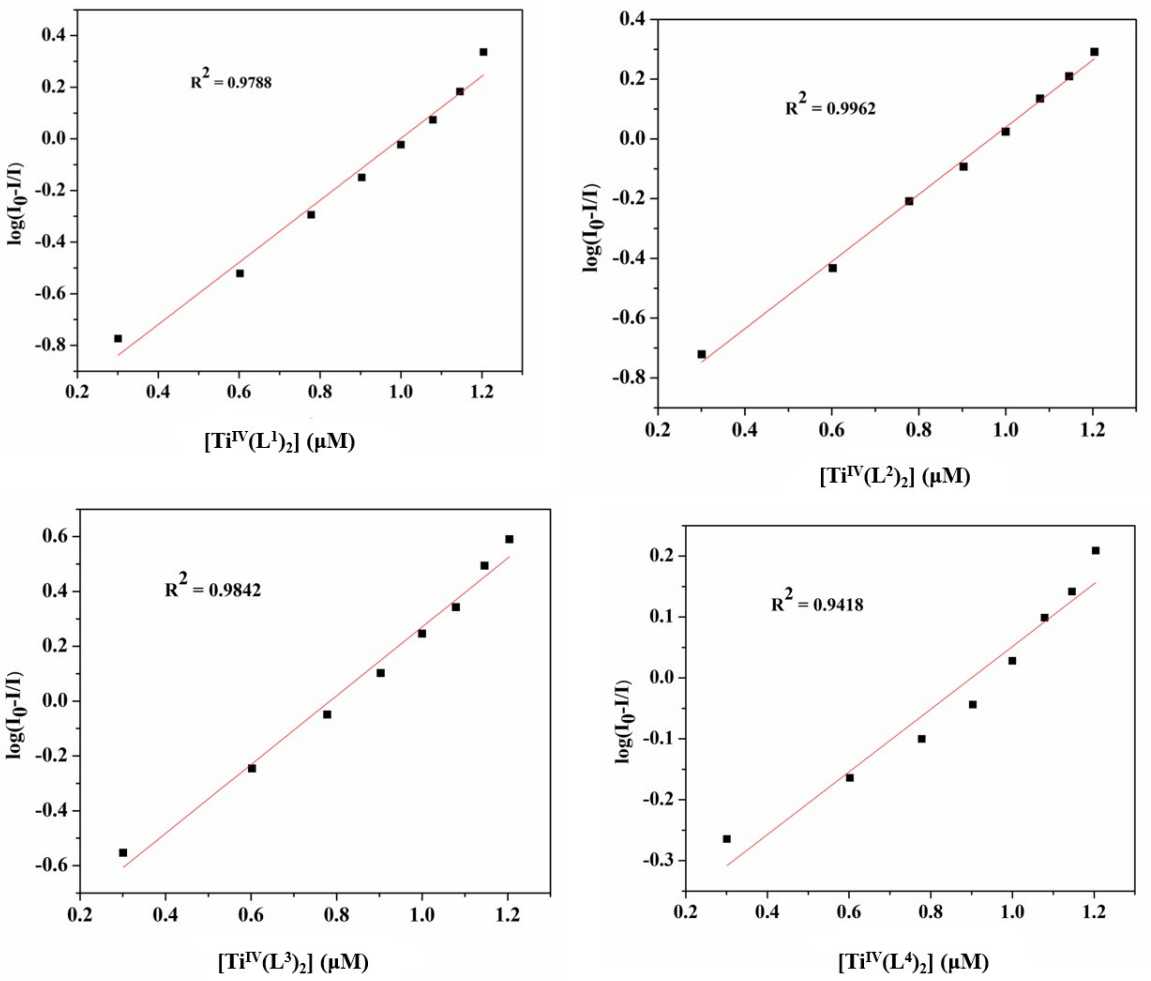

Figure 30. Site marker study of Ibuprofen bound BSA double log plots of complexes $[Ti^{IV}(L^{1-4})_2]$

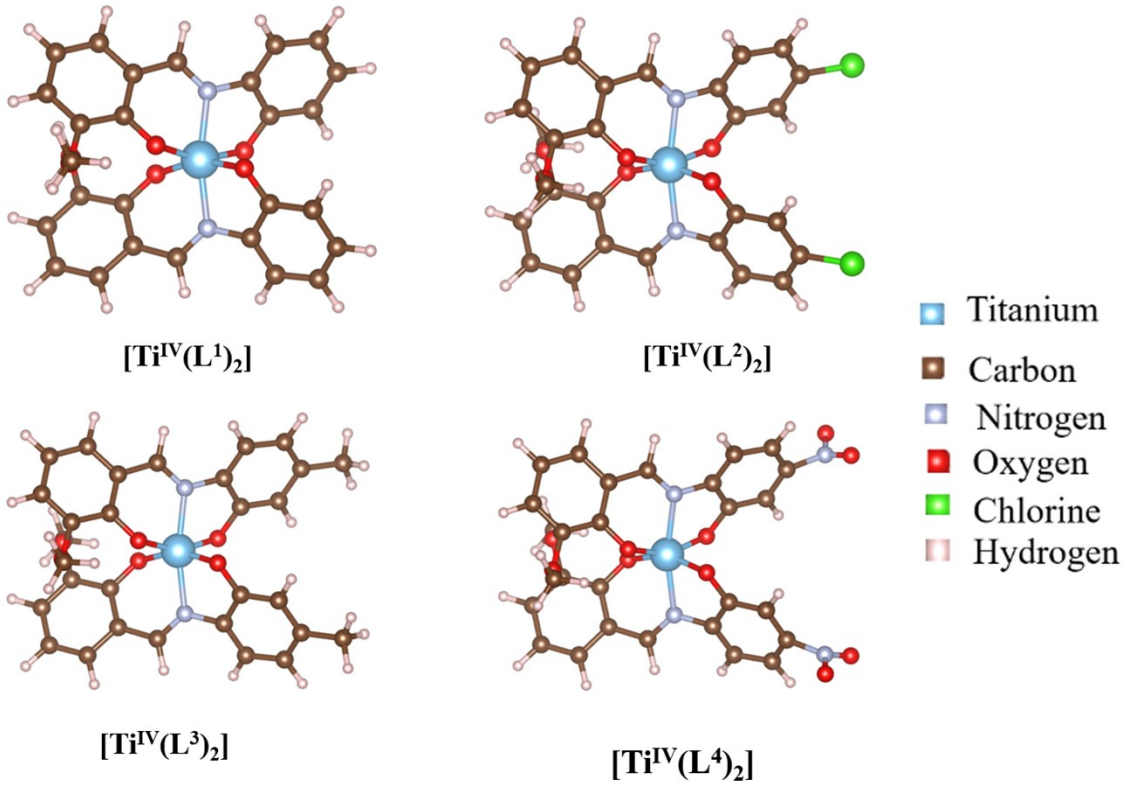

Figure 31. Optimized geometry of $[Ti^{IV}(L^{1\text{-}4})_2]$ derivatives

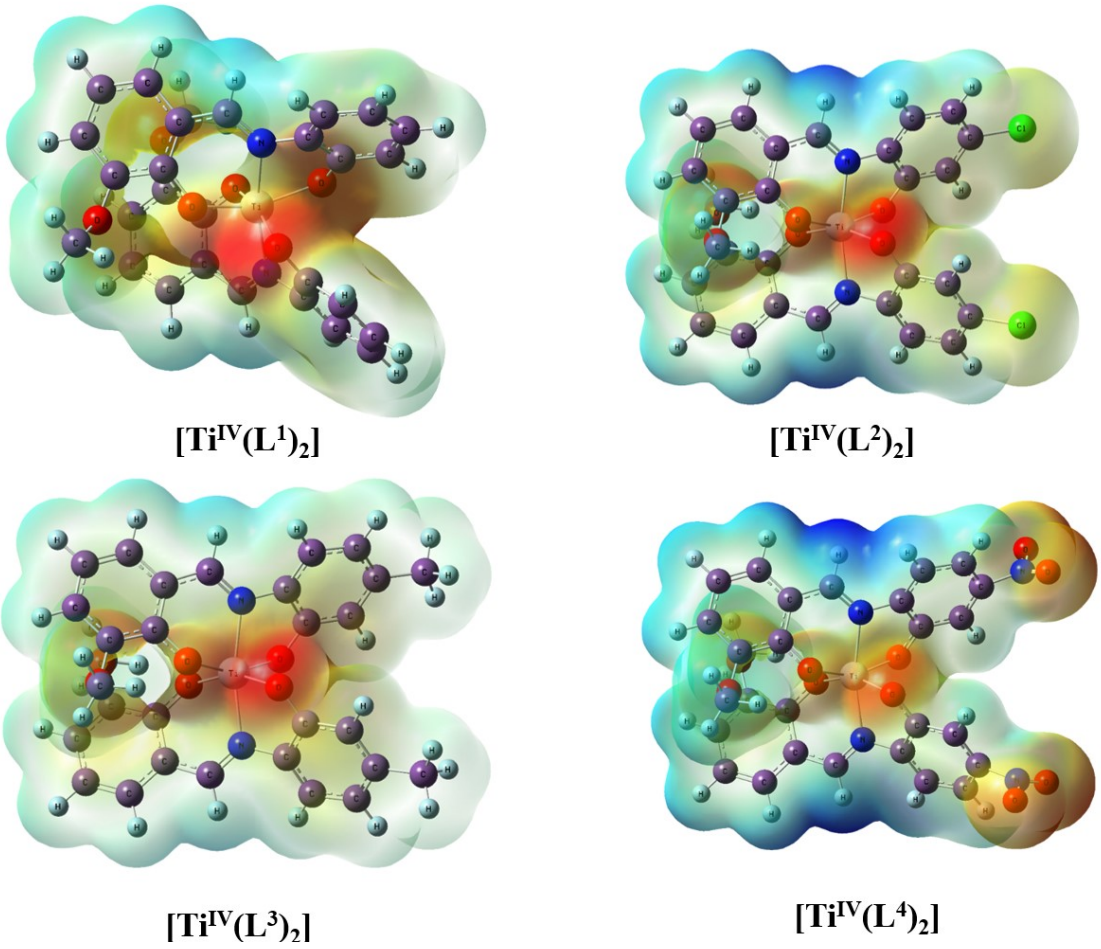

Figure 32. ESP mapping images of titanium(IV) $[Ti^{IV}(L^{1\text{-}4})_2]$

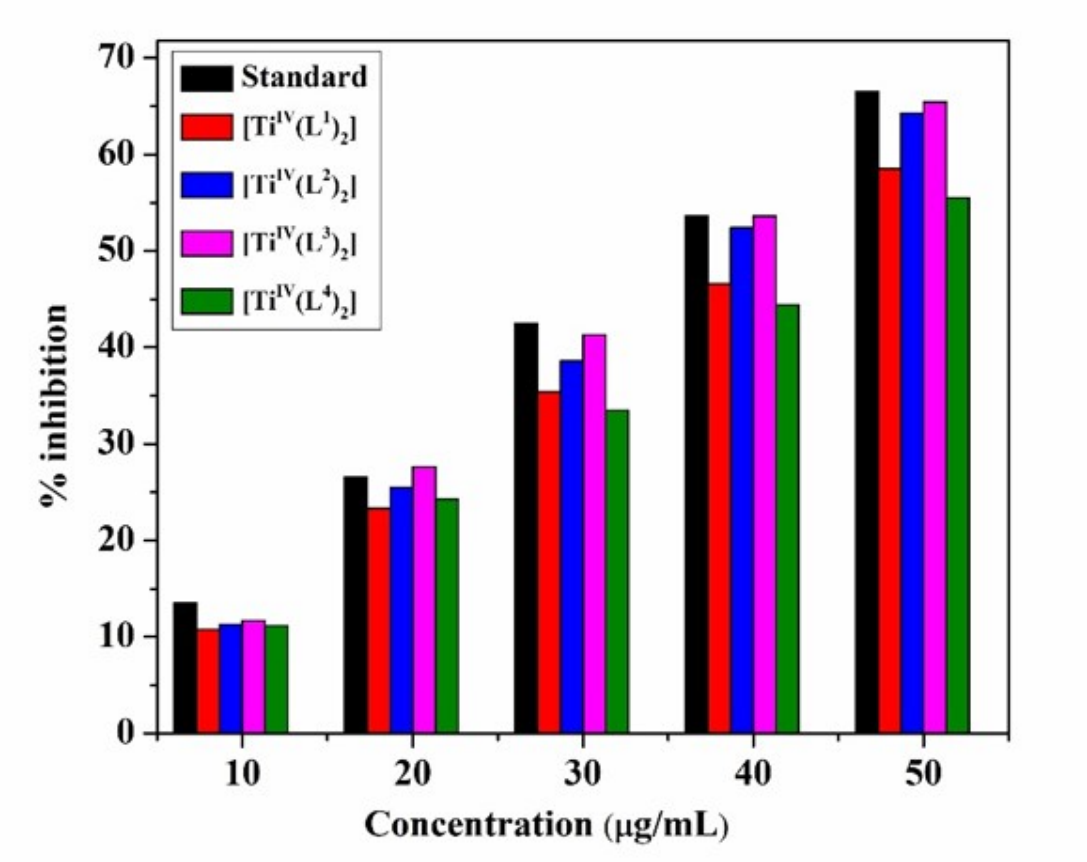

Figure 33. DPPH assay of $[Ti^{IV}(L^{1\text{-}4})_2]$ derivatives

Table 1. Bond lengths (Å) for $[Ti^{IV}(L^1)_2]$

Ti1-O2	1.871(6)	Ti1-O1	1.886(7)
Ti1-O4	1.910(5)	Ti1-O3	1.919(7)
Ti1-N2	2.182(6)	Ti1-N1	2.183(6)
O1-C1	1.303(12)	O2-C14	1.295(9)
O3-C20	1.364(12)	O4-C13	1.286(9)
O5-C12	1.312(12)	O5-C27	1.435(12)
O6-C19	1.326(11)	O6-C28	1.451(13)
N1-C7	1.321(11)	N1-C2	1.486(11)
N2-C26	1.341(10)	N2-C21	1.440(11)
C1-C2	1.378(13)	C1-C6	1.441(15)
C2-C3	1.362(13)	C3-C4	1.443(15)
C3-H3	0.930000	C4-C5	1.377(16)
C4-H4	0.930000	C5-C6	1.402(15)
C5-H5	0.930000	C6-H6	0.930000
C7-C8	1.357(13)	C7-H7	0.930000
C8-C9	1.418(12)	C8-C13	1.439(11)
C9-C10	1.363(17)	C9-H9	0.930000
C10-C11	1.359(17)	C10-H10	0.930000
C11-C12	1.361(13)	C11-H11	0.930000
C12-C13	1.458(13)	C14-C15	1.393(10)
C14-C19	1.459(12)	C15-C26	1.362(12)
C15-C16	1.378(11)	C16-C17	1.354(14)
C16-H16	0.930000	C17-C18	1.299(15)
C17-H17	0.930000	C18-C19	1.403(12)
C18-H18	0.930000	C20-C25	1.382(15)
C20-C21	1.398(13)	C21-C22	1.398(11)
C22-C23	1.358(15)	C22-H22	0.930000
C23-C24	1.367(16)	C23-H23	0.930000
C24-C25	1.370(15)	C24-H24	0.930000
C25-H25	0.930000	C26-H26	0.930000
C27-H27	0.960000	C27-H27	0.960000
C27-H27	0.960000	C28-H28	0.960000
C28-H28	0.960000	C28-H28	0.960000

Table 2. Bond angles (°) for $[Ti^{IV}(L^1)_2]$

O2-Ti1-O1	96.6(3)	O2-Ti1-O4	89.2(3)
O1-Ti1-O4	156.9(3)	O2-Ti1-O3	151.3(3)
O1-Ti1-O3	97.8(4)	O4-Ti1-O3	87.2(3)
O2-Ti1-N2	80.9(3)	O1-Ti1-N2	84.4(3)
O4-Ti1-N2	118.7(2)	O3-Ti1-N2	76.0(3)
O2-Ti1-N1	115.1(3)	O1-Ti1-N1	76.7(3)
O4-Ti1-N1	80.5(2)	O3-Ti1-N1	92.4(3)
N2-Ti1-N1	156.3(3)	C1-O1-Ti1	121.2(7)
C14-O2-Ti1	141.0(5)	C20-O3-Ti1	122.2(6)
C13-O4-Ti1	138.5(5)	C12-O5-C27	119.6(10)
C19-O6-C28	117.2(8)	C7-N1-C2	119.0(7)
C7-N1-Ti1	128.6(6)	C2-N1-Ti1	112.0(5)
C26-N2-C21	120.5(7)	C26-N2-Ti1	126.9(6)
C21-N2-Ti1	111.9(5)	O1-C1-C2	122.8(10)
O1-C1-C6	122.0(10)	C2-C1-C6	115.1(10)
C3-C2-C1	128.9(10)	C3-C2-N1	124.3(9)
C1-C2-N1	106.5(7)	C2-C3-C4	113.0(10)
C2-C3-H3	123.500000	C4-C3-H3	123.50000
C5-C4-C3	123.4(10)	C5-C4-H4	118.30000
C3-C4-H4	118.300000	C4-C5-C6	119.3(11)
C4-C5-H5	120.400000	C6-C5-H5	120.40000
C5-C6-C1	120.3(11)	C5-C6-H6	119.80000
C1-C6-H6	119.800000	N1-C7-C8	123.5(8)
N1-C7-H7	118.300000	C8-C7-H7	118.30000
C7-C8-C9	119.5(9)	C7-C8-C13	124.2(7)
C9-C8-C13	115.9(9)	C10-C9-C8	123.7(12)
C10-C9-H9	118.200000	C8-C9-H9	118.20000
C11-C10-C9	119.1(10)	C11-C10-H10	120.40000
C9-C10-H10	120.400000	C10-C11-C12	123.3(12)
C10-C11-H11	118.400000	C12-C11-H11	118.40000
O5-C12-C11	128.0(11)	O5-C12-C13	113.3(7)

C11-C12-C13	118.6(11)	O4-C13-C8	120.1(7)

Table 3. Bond lengths (Å) for $[Ti^{IV}(L^3)_2]$

Ti5-O3	1.889(2)	Ti5-O3	1.889(2)
Ti5-O1	1.904(2)	Ti5-O1	1.904(2)
Ti5-N1	2.193(3)	Ti5-N1	2.193(3)
O1-C2	1.341(4)	O2-C12	1.362(4)
O2-C15	1.414(4)	O3-C13	1.323(4)
N1-C7	1.299(4)	N1-C1	1.426(4)
C1-C6	1.386(4)	C1-C2	1.392(4)
C2-C3	1.389(4)	C3-C4	1.382(5)
C4-C5	1.390(5)	C5-C6	1.384(5)
C5-C14	1.510(5)	C7-C8	1.423(4)
C8-C13	1.395(4)	C8-C9	1.412(5)
C9-C10	1.359(5)	C10-C11	1.389(5)
C11-C12	1.376(5)	C12-C13	1.413(4)

Table 4. Bond angles (°) for $[Ti^{IV}(L^3)_2]$

O3-Ti5-O3	100.47(16)	O3-Ti5-O1	154.18(9)
O3-Ti5-O1	91.81(10)	O3-Ti5-O1	91.81(10)
O3-Ti5-O1	154.18(9)	O1-Ti5-O1	86.52(14)
O3-Ti5-N1	91.84(9)	O3-Ti5-N1	81.13(9)
O1-Ti5-N1	112.59(9)	O1-Ti5-N1	75.82(9)
O3-Ti5-N1	81.13(9)	O3-Ti5-N1	91.83(9)
O1-Ti5-N1	75.82(9)	O1-Ti5-N1	112.60(9)
N1-Ti5-N1	169.03(14)	C2-O1-Ti5	122.37(19)
C12-O2-C15	117.3(3)	C13-O3-Ti5	141.4(2)
C7-N1-C1	120.2(3)	C7-N1-Ti5	128.2(2)
C1-N1-Ti5	111.62(19)	C6-C1-C2	120.4(3)
C6-C1-N1	128.1(3)	C2-C1-N1	111.5(3)
O1-C2-C3	123.1(3)	O1-C2-C1	117.0(3)
C3-C2-C1	119.8(3)	C4-C3-C2	118.7(3)
C3-C4-C5	122.3(3)	C6-C5-C4	118.2(3)
C6-C5-C14	120.5(3)	C4-C5-C14	121.3(3)
C5-C6-C1	120.5(3)	N1-C7-C8	125.7(3)
C13-C8-C9	119.8(3)	C13-C8-C7	121.6(3)
C9-C8-C7	118.6(3)	C10-C9-C8	120.4(3)
C9-C10-C11	120.0(3)	C12-C11-C10	121.2(3)
O2-C12-C11	124.6(3)	O2-C12-C13	115.7(3)
C11-C12-C13	119.6(3)	O3-C13-C8	121.5(3)
O3-C13-C12	119.6(3)	C8-C13-C12	118.9(3)

Table 5. Optimized Cartesian coordinates of all structures obtained from DFT calculations

Complex	Coordinates			
$[Ti^{IV}(L^1)_2]$	C	-3.74587100	-3.24223900	-0.65756000
	C	-4.01715000	-2.01569900	-1.28154800
	C	-3.00480200	-1.08620900	-1.52627200
	C	-1.67708300	-1.34186900	-1.11198600
	C	-1.40229900	-2.60793200	-0.51423600
	C	-2.44061500	-3.54140300	-0.29723700
	C	-0.07091400	-2.96575900	-0.13990700
	N	0.85457600	-2.07771300	0.07231500
	O	-0.71257500	-0.43785100	-1.33625400
	O	-3.30756500	0.10280000	-2.15176700
	C	-3.27530000	0.03328200	-3.59070500
	C	2.17243900	-2.36897300	0.41670000
	C	2.73994100	-1.34570300	1.20582400
	C	4.04757900	-1.51907200	1.68673500
	C	4.77954800	-2.64608900	1.29823000
	C	4.22818600	-3.61593600	0.44452800
	C	2.91292300	-3.48302500	0.00582100
	O	1.96792100	-0.26246500	1.44337000
	C	-3.74669300	3.24141500	0.65497900
	C	-4.01828700	2.01502100	1.27872600
	C	-3.00645900	1.08494900	1.52449000
	C	-1.67845700	1.34013100	1.11053400
	C	-1.40323800	2.60652100	0.51339000
	C	-2.44116700	3.54040200	0.29591900
	C	-0.07172700	2.96514500	0.14032000
	N	0.85409400	2.07747400	-0.07187500
	O	-0.71393700	0.43639700	1.33600900
	O	-3.31412400	-0.10014700	2.15429100
	C	-3.27290800	-0.03363800	3.59416500
	C	2.17181000	2.36923100	-0.41600900
	C	2.73944900	1.34651300	-1.20573500
	C	4.04658700	1.52070200	-1.68747900
	C	4.77824400	2.64782800	-1.29893600
	C	4.22723400	3.61675500	-0.44406400
	C	2.91210600	3.48334900	-0.00490300
	O	1.96787700	0.26300900	-1.44304500
	Ti	0.62605300	-0.00025400	0.00028700
	H	-4.54513400	-3.94964000	-0.46797000

	H	-5.02787700	-1.76405100	-1.58746600
	H	-2.20111700	-4.48714500	0.17904300
	H	0.16266600	-4.02190900	0.00209800
	H	-3.66485700	0.98615600	-3.95319900
	H	-2.25247300	-0.10862900	-3.95145000
	H	-3.90761000	-0.78262000	-3.95467400
	H	4.48283900	-0.76611400	2.33549900
	H	5.79881400	-2.76489200	1.65243400
	H	4.81988900	-4.46654900	0.12373000
	H	2.46883700	-4.21299300	-0.66365100
	H	-4.54585800	3.94887200	0.46511800
	H	-5.02890700	1.76338600	1.58490700
	H	-2.20124300	4.48651500	-0.17940600
	H	0.16137800	4.02145500	-0.00109900
	H	-3.84585000	-0.88692100	3.96211900
	H	-2.24250700	-0.09631300	3.95606500
	H	-3.73018600	0.89296500	3.95324900
	H	4.48160200	0.76833600	-2.33708000
	H	5.79718400	2.76735700	-1.65382900
	H	4.81919400	4.46690000	-0.12239500
	H	2.46812600	4.21298600	0.66503200
$[Ti^{IV}(L^2)_2]$	C	-4.42096800	-3.09597700	-1.20500700
	C	-4.68922800	-1.78273900	-1.60534400
	C	-3.67910100	-0.82884900	-1.68009100
	C	-2.35865100	-1.15421100	-1.30910400
	C	-2.08512000	-2.50425400	-0.95022200
	C	-3.12149700	-3.45616700	-0.90405800
	C	-0.74704600	-2.91985500	-0.65302300
	N	0.17942300	-2.08153900	-0.30325900
	O	-1.39157600	-0.22917500	-1.34610000
	O	-3.97776800	0.45236100	-2.08586900
	C	-3.94361700	0.63367700	-3.51281300
	C	1.50376100	-2.43529500	-0.01456500
	C	2.06936600	-1.55648300	0.93028700
	C	3.36864500	-1.80276500	1.38772200
	C	4.09040800	-2.84795900	0.81388500
	C	3.55830600	-3.66422900	-0.19002300
	C	2.24440100	-3.45928800	-0.59886200
	O	1.29944500	-0.52842200	1.32949900
	C	-4.42067000	3.09809900	1.20107000
	C	-4.69074500	1.78529100	1.60089100
	C	-3.68226600	0.82943600	1.67694200
	C	-2.36103000	1.15271900	1.30698900
	C	-2.08558500	2.50279900	0.94890300
	C	-3.12039700	3.45639600	0.90179300
	C	-0.74694500	2.91781200	0.65380600

	N	0.17984700	2.07927800	0.30572500
	O	-1.39472500	0.22693400	1.34615500
	O	-3.98877400	-0.44830900	2.08670700
	C	-3.94394600	-0.63575400	3.51357200
	C	1.50379200	2.43385600	0.01657500
	C	2.07091900	1.55326000	-0.92567900
	C	3.37011700	1.79982700	-1.38314200
	C	4.08949000	2.84901100	-0.81364900
	C	3.55542200	3.66846000	0.18657700
	C	2.24222000	3.46171700	0.59686700
	O	1.30158300	0.52472800	-1.32438700
	Ti	-0.04731600	-0.00133700	0.00161800
	H	-5.21947500	-3.81897000	-1.14105700
	H	-5.69442900	-1.47970600	-1.86416500
	H	-2.88383600	-4.46762700	-0.60611100
	H	-0.51735600	-3.98119700	-0.68879800
	H	-4.32718200	1.63264400	-3.70704100
	H	-2.92356400	0.55315800	-3.89395200
	H	-4.57659500	-0.10172000	-4.01346400
	H	3.80605100	-1.17156000	2.14763500
	H	4.15869300	-4.43903700	-0.64345400
	H	1.81140700	-4.06808800	-1.37969800
	H	-5.21820400	3.82217400	1.13681400
	H	-5.69624900	1.48329800	1.85962800
	H	-2.88081300	4.46776100	0.60506000
	H	-0.51718700	3.97913100	0.68946700
	H	-4.50877400	-1.54021900	3.72866400
	H	-2.91537000	-0.75610500	3.85970300
	H	-4.40373400	0.20837800	4.03012000
	H	3.80862200	1.16711900	-2.14119000
	H	4.15394500	4.44675200	0.63653700
	H	1.80775500	4.07311700	1.37485700
	Cl	5.73597500	3.13385700	-1.34733300
	Cl	5.73794600	-3.13034000	1.34543500
$[Ti^{IV}(L^3)_2]$	C	-4.10770800	-3.20198500	-1.02745100
	C	-4.36761300	-1.92352800	-1.53414500
	C	-3.35589300	-0.97677000	-1.66470600
	C	-2.04340700	-1.27386100	-1.23907000
	C	-1.77413400	-2.59202500	-0.77423600
	C	-2.81268200	-3.53941300	-0.68136400
	C	-0.43660900	-2.98624100	-0.41856900
	N	0.49735300	-2.13051600	-0.14466100
	O	-1.07744300	-0.34660300	-1.30049700
	O	-3.65880200	0.28289100	-2.13466200
	C	-3.61550400	0.37371200	-3.57137900
	C	1.82497800	-2.46365700	0.19694300

	C	2.39320200	-1.49068400	1.04203600
	C	3.68660100	-1.68556200	1.52546000
	C	4.44798900	-2.78129400	1.08818900
	C	3.88482400	-3.68528400	0.17293800
	C	2.57057400	-3.54360400	-0.26333600
	O	1.61547800	-0.41589500	1.31897600
	C	-4.10692900	3.20335300	1.02445400
	C	-4.36798400	1.92536300	1.53115800
	C	-3.35785300	0.97700400	1.66354000
	C	-2.04445000	1.27221800	1.23862600
	C	-1.77418600	2.59050600	0.77441100
	C	-2.81138100	3.53940700	0.68048600
	C	-0.43655100	2.98461200	0.41979500
	N	0.49727600	2.12907600	0.14568700
	O	-1.07817500	0.34481000	1.30069100
	O	-3.67161200	-0.27851300	2.13633500
	C	-3.61334100	-0.37639600	3.57308600
	C	1.82442700	2.46304200	-0.19630500
	C	2.39239700	1.49083400	-1.04239200
	C	3.68554600	1.68659500	-1.52619400
	C	4.44693300	2.78196400	-1.08781500
	C	3.88362100	3.68546000	-0.17212100
	C	2.56951200	3.54327700	0.26415800
	O	1.61476100	0.41577700	-1.31891600
	Ti	0.26993000	-0.00064300	0.00025700
	H	-4.91153300	-3.91698100	-0.91811300
	H	-5.37062500	-1.63772800	-1.82567300
	H	-2.58085100	-4.52978400	-0.31044100
	H	-0.21924900	-4.05050600	-0.35423800
	H	-3.97013700	1.36746400	-3.83570100
	H	-2.59512900	0.24129000	-3.93968200
	H	-4.26589600	-0.37689600	-4.02626900
	H	4.11310200	-0.96359700	2.21094900
	H	4.48811800	-4.50171500	-0.20411800
	H	2.14477800	-4.23419800	-0.98023100
	H	-4.91012000	3.91897200	0.91448900
	H	-5.37116600	1.64022800	1.82269100
	H	-2.57772100	4.52950600	0.31006200
	H	-0.21913900	4.04885800	0.35579400
	H	-4.12950300	-1.29298600	3.85113900
	H	-2.57769000	-0.42305400	3.91862400
	H	-4.11361100	0.47593600	4.03756900
	H	4.11247400	0.96492500	-2.21170900
	H	4.48702600	4.50130100	0.20606200
	H	2.14374700	4.23288700	0.98200000
	C	5.86941900	2.97285100	-1.55455000

	H	6.02208900	3.97492200	-1.98084100
	H	6.57932100	2.87828100	-0.71884500
	H	6.15480800	2.23650400	-2.31592800
	C	5.87114800	-2.97015400	1.55386100
	H	6.03744100	-3.98728900	1.93660700
	H	6.58370300	-2.82758100	0.72701800
	H	6.14157600	-2.26271600	2.34748800
$[Ti^{IV}(L^4)_2]$	C	-4.02709100	-3.26877300	-0.63654600
	C	-4.29690200	-2.04887300	-1.26447800
	C	-3.28961900	-1.12279200	-1.50939700
	C	-1.96911700	-1.37429300	-1.08573000
	C	-1.69333500	-2.63747900	-0.49080200
	C	-2.72791600	-3.56751200	-0.27694400
	C	-0.35544200	-2.99076200	-0.12163400
	N	0.57040700	-2.10333900	0.07246300
	O	-1.00400200	-0.47017500	-1.28586400
	O	-3.59156800	0.06434800	-2.13728600
	C	-3.55540200	-0.01177100	-3.57295900
	C	1.89694400	-2.39883900	0.41940900
	C	2.46099300	-1.36202500	1.18728400
	C	3.75804200	-1.52839300	1.67374100
	C	3.95233000	-3.64630600	0.46463600
	C	2.63570900	-3.51177700	0.02846400
	O	1.68267400	-0.27609200	1.39171900
	C	-4.03158000	3.26477700	0.63364900
	C	-4.30054300	2.04499000	1.26162200
	C	-3.29298500	1.11906300	1.50772100
	C	-1.97251500	1.37082000	1.08443000
	C	-1.69747000	2.63470700	0.49014300
	C	-2.73228900	3.56430300	0.27542900
	C	-0.35976500	2.98986900	0.12239300
	N	0.56713600	2.10361400	-0.07148000
	O	-1.00636400	0.46785800	1.28515200
	O	-3.59985300	-0.06423100	2.13981600
	C	-3.55379600	0.00756900	3.57649500
	C	1.89299300	2.40069200	-0.41873200
	C	2.45720600	1.36488400	-1.18774000
	C	3.75374500	1.53298600	-1.67509500
	C	3.94695200	3.65031300	-0.46457700
	N	2.63066400	3.51433700	-0.02778000
	O	1.67996100	0.27822300	-1.39214200
	Ti	0.34077200	0.00003400	0.00077800
	H	-4.82437500	-3.96970600	-0.44536400
	H	-5.30173000	-1.79867400	-1.57243600
	H	-2.48938300	-4.50894600	0.19552400
	H	-0.12480800	-4.04018500	0.03174600

	H	-3.93864900	0.93510300	-3.94389500
	H	-2.53512800	-0.15817800	-3.93070200
	H	-4.18629900	-0.82508800	-3.93455300
	H	4.19258300	-0.76949000	2.30799100
	H	2.19699200	-4.24755200	-0.63081600
	H	-4.82923400	3.96506700	0.44196500
	H	-5.30498500	1.79403200	1.57015400
	H	-2.49380200	4.50613500	-0.19640200
	H	-0.13040600	4.03963300	-0.03061100
	H	-4.11470600	-0.84447000	3.95193400
	H	-2.52507600	-0.04497400	3.93597800
	H	-4.01551300	0.92887000	3.93290500
	H	4.18883700	0.77494700	-2.31005900
	H	2.19144200	4.24930300	0.63207700
	C	4.48205900	2.66635300	-1.30518000
	H	5.49063300	2.78310700	-1.66888800
	C	4.48720900	-2.66127300	1.30413800
	H	5.49611300	-2.77687400	1.66723400
	C	4.77859400	4.84933300	-0.02877700
	H	5.81856400	4.71561200	-0.30557400
	H	4.41749500	5.76189900	-0.49528600
	H	4.72312600	4.98162800	1.04744800
	C	4.78462500	-4.84520600	0.02973100
	H	5.82315200	-4.71413100	0.31311400
	H	4.41927600	-5.75867900	0.49110300
	H	4.73552700	-4.97402700	-1.04725200

Table 6. Electronic properties of **$[Ti^{IV}(L^{1\text{-}4})_2]$** in DMSO phase

Code	Energy	DM	HOMO	LUMO	Gap	χ	μ	η	S	ω
$[Ti^{IV}(L^1)_2]$	-1070541.48	4.22	-5.76	-2.73	-3.02	4.24	-4.24	-1.51	-0.76	-13.61
$[Ti^{IV}(L^2)_2]$	-1649585.10	9.08	-5.87	-2.73	-3.14	4.30	-4.30	-1.57	-0.79	-14.54
$[Ti^{IV}(L^3)_2]$	-1120091.42	2.15	-5.69	-2.53	-3.16	4.11	-4.11	-1.58	-0.79	-13.34
$[Ti^{IV}(L^4)_2]$	-1328200.35	15.30	-6.07	-2.95	3.13	4.1	-4.51	-1.56	-0.78	-15.86

Complex	Abs	OS	LHE	LHE (%)	State
$[Ti^{IV}(L^{1})_2]$	338.6	0.3206	0.522	52	20
	452.02	0.0611	0.131	13	5
$[Ti^{IV}(L^{2})_2]$	320.51	0.2701	0.463	46	19
	440.73	0.0689	0.147	15	3
$[Ti^{IV}(L^{3})_2]$	322.11	0.4257	0.625	62	19
	431.94	0.0569	0.123	12	4
$[Ti^{IV}(L^{4})_2]$	335.28	0.1944	0.36	36	21
	445.11	0.1025	0.211	21	4

Table 7. TD-DFT absorbance spectral characteristic of **$[Ti^{IV}(L^{1-4})_2]$** in DMSO phase

Table 8. Molecular docking scores of $[Ti^{IV}(L^{1-4})_2]$ with DNA and BSA

Ligand	Binding free energy ($\Delta G_{binding}$)[a]	Vdw_hb_desolv energy ($\Delta G_{vdW+hb+desolv}$)	Electrostatic energy (ΔG_{elec})	Total internal energy (ΔG_{total})	Torsional free energy (ΔG_{tor})	Unbound system energy (ΔG_{unb})	H bonding
			DNA				
$[Ti^{IV}(L^1)_2]$	-5.91	-6.48	-0.02	-0.54	0.6	-0.54	ADE06 (2.421)
$[Ti^{IV}(L^2)_2]$	-5.52	-5.99	-0.13	-0.54	0.6	-0.54	ADE18 (2.828)
$[Ti^{IV}(L^3)_2]$	-5.39	-5.85	-0.13	-0.58	0.6	-0.58	ADE18 (2.881)
$[Ti^{IV}(L^4)_2]$	-4.09	-6.65	1.37	-0.55	1.19	-0.55	ADE18 (1.923)
			BSA				
$[Ti^{IV}(L^1)_2]$	-5.71	-6.47	-0.17	-0.54	0.6	-0.54	GLU424 (2.452)
$[Ti^{IV}(L^2)_2]$	-5.83	-6.51	-0.08	-0.53	0.6	-0.53	ASN44 (2.185)
$[Ti^{IV}(L^3)_2]$	-5.76	-6.33	-0.02	-0.52	0.6	-0.52	ASN44 (2.246)
$[Ti^{IV}(L^4)_2]$	-6.25	-5.99	-1.45	-0.55	1.19	-0.55	ARG (1.816)