Supplementary Material

Effect of Novel Schiff Base-Platinum Complexes on Amyloid Beta Aggregation and Their Interactions with Histidine

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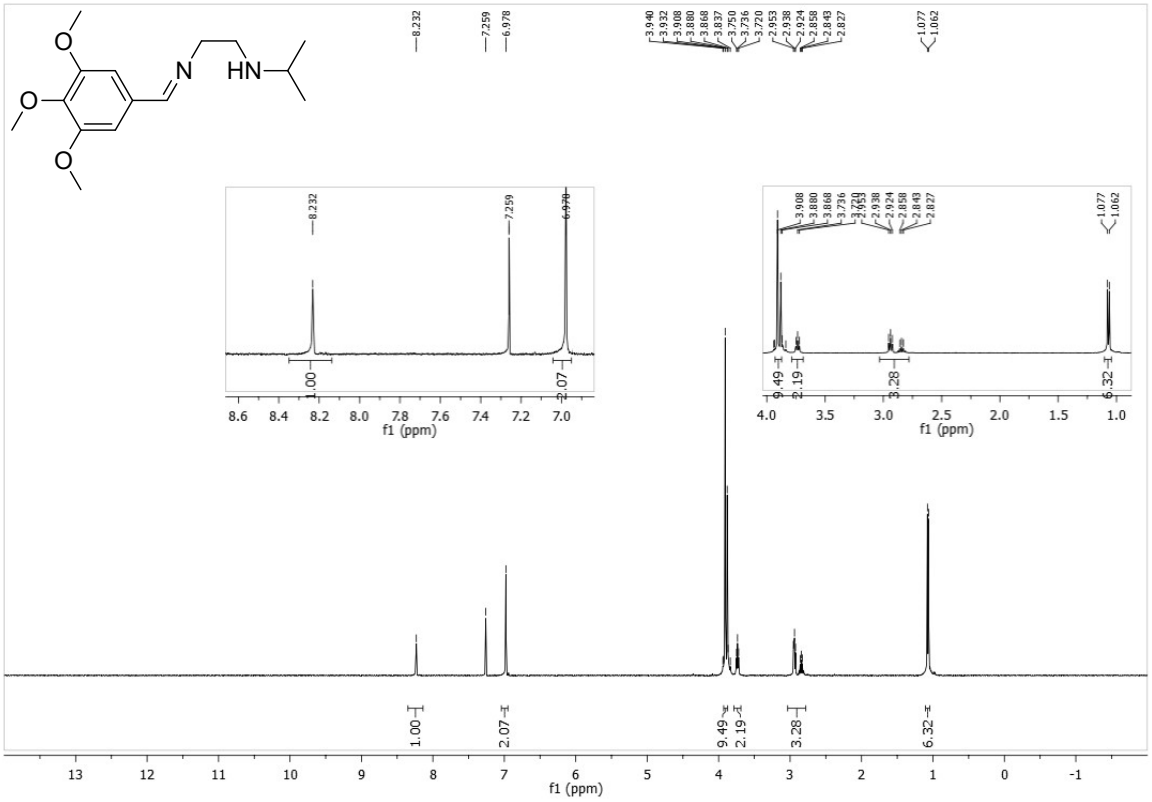
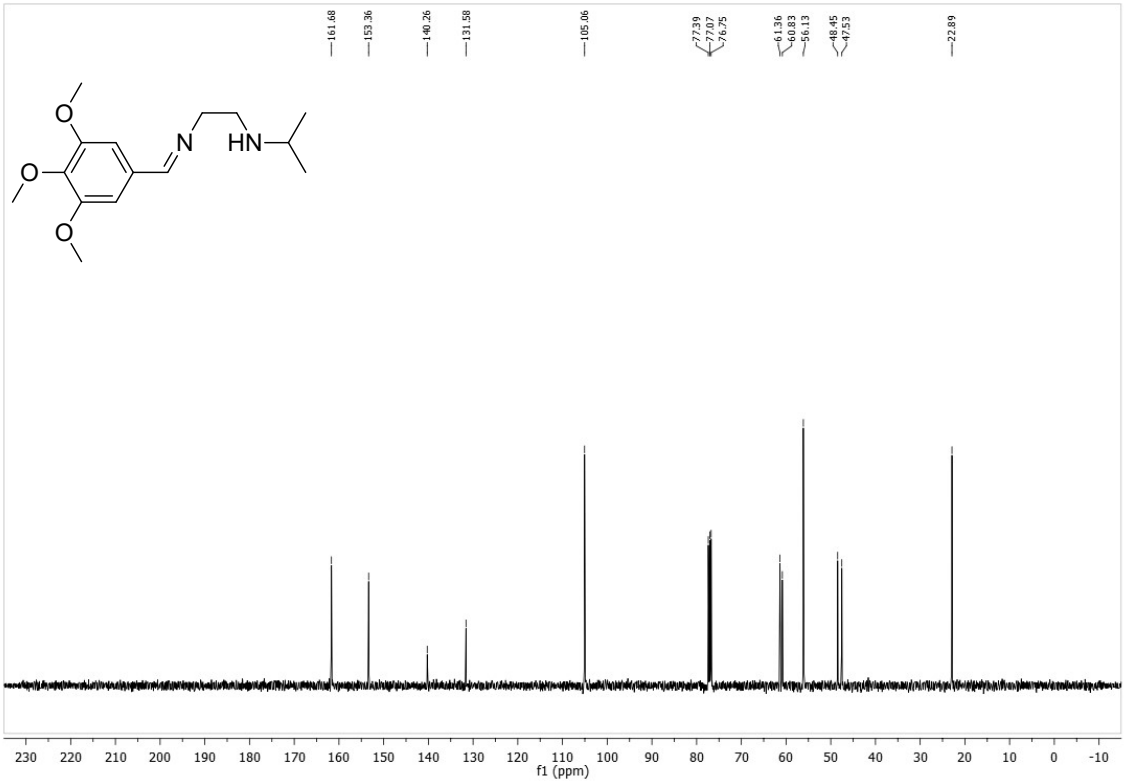
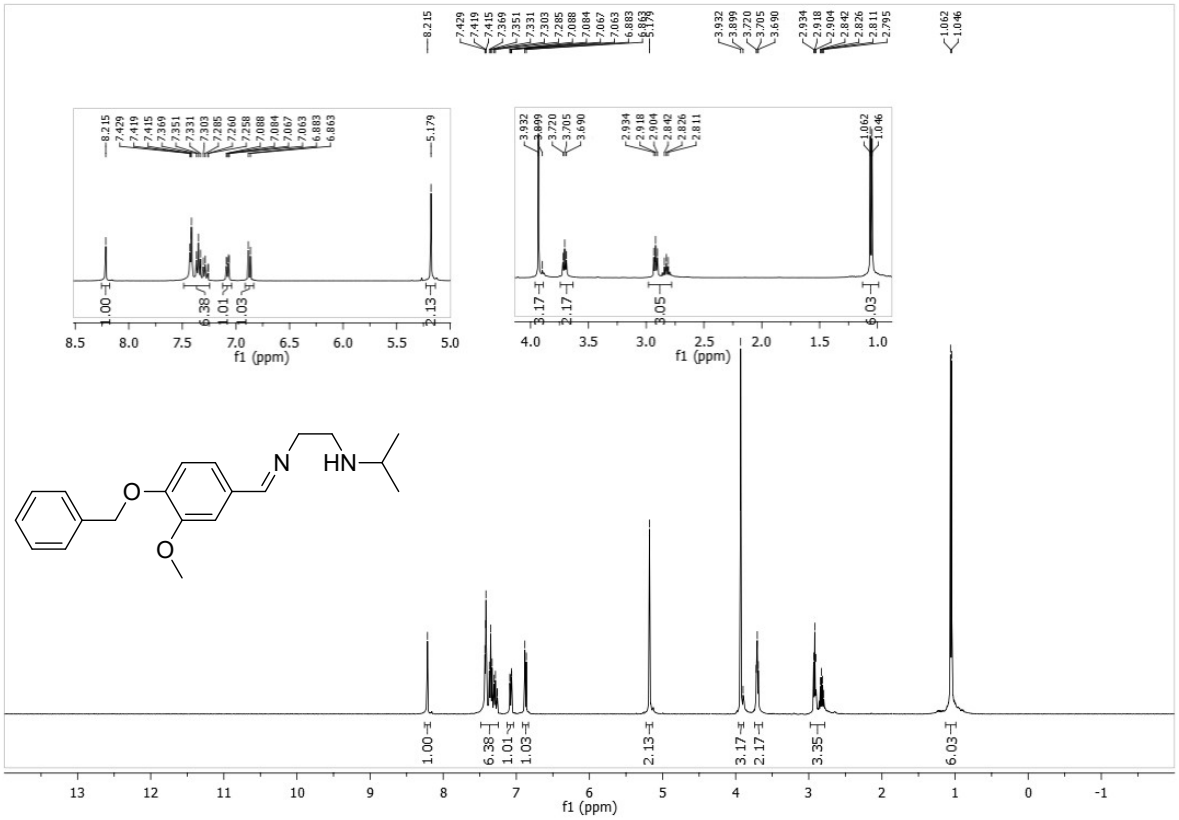


(a)

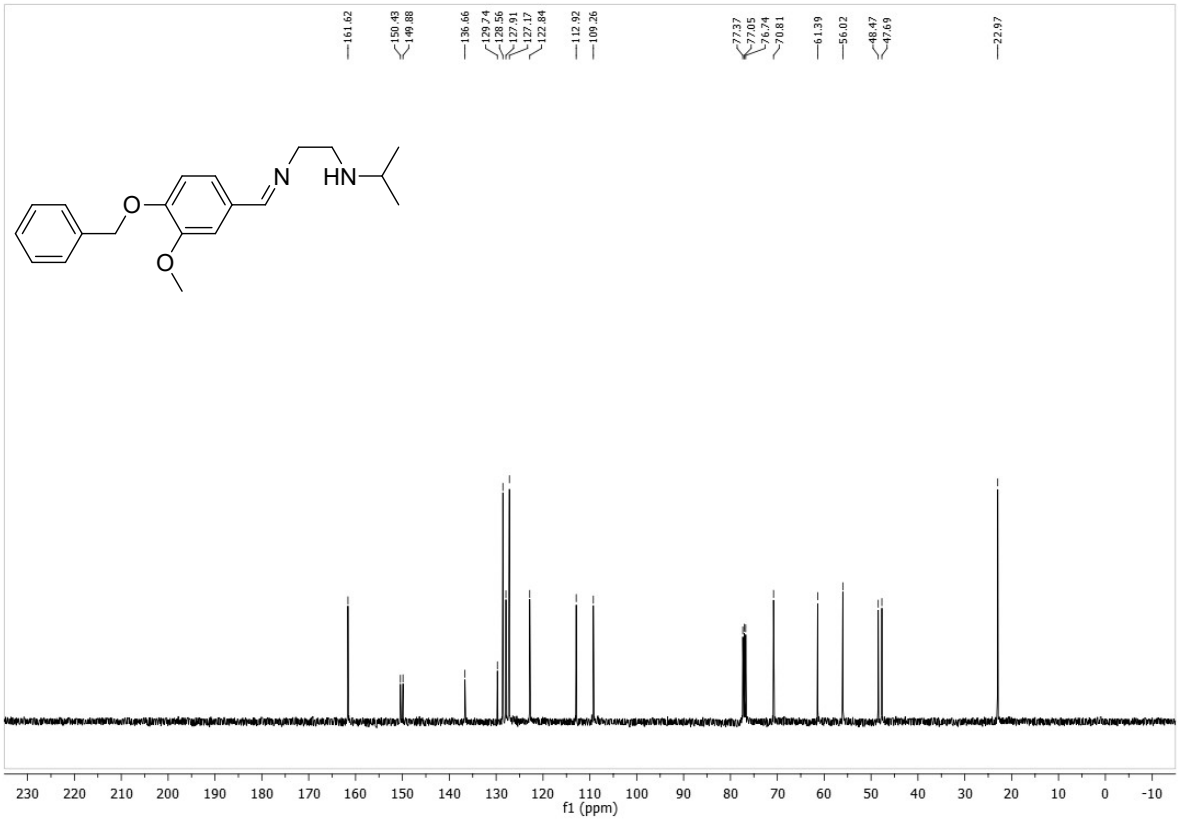


(b)

Figure S1. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of Ligand I, 400 MHz, $CDCl_3$, 25 °C.

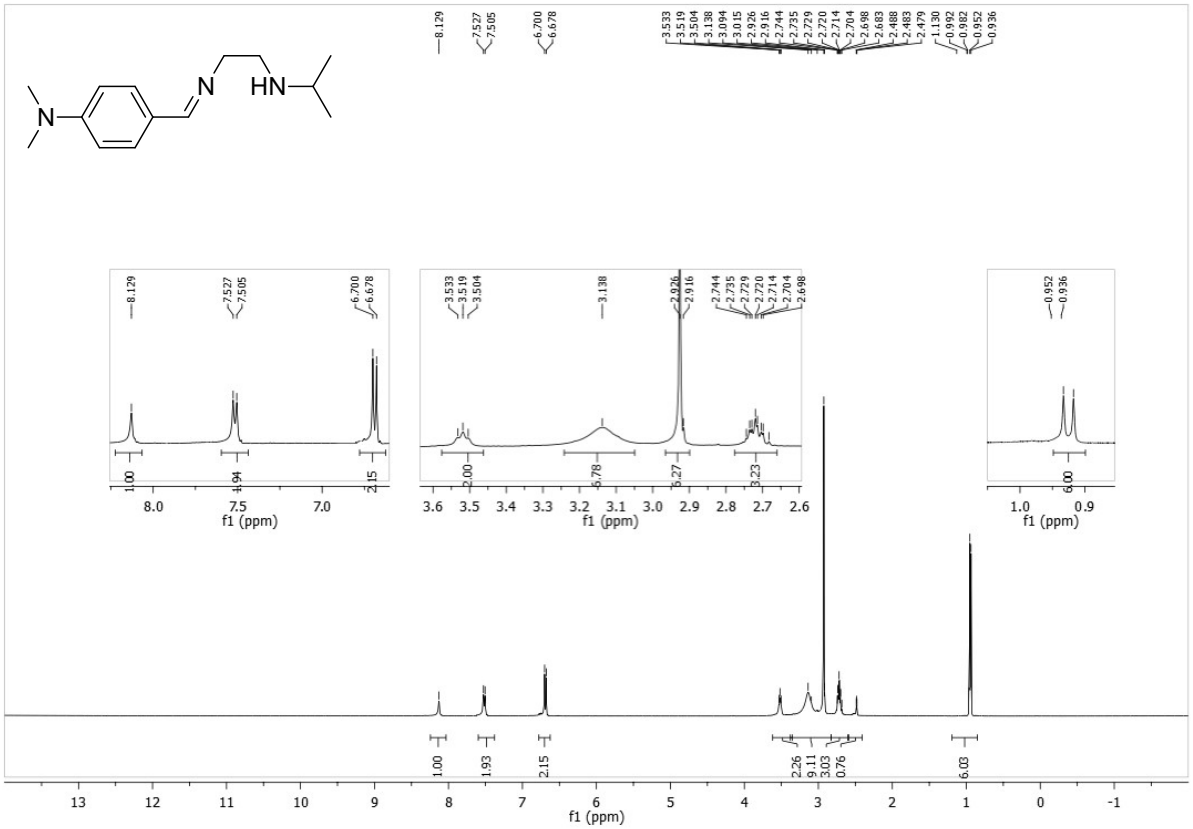


(a)

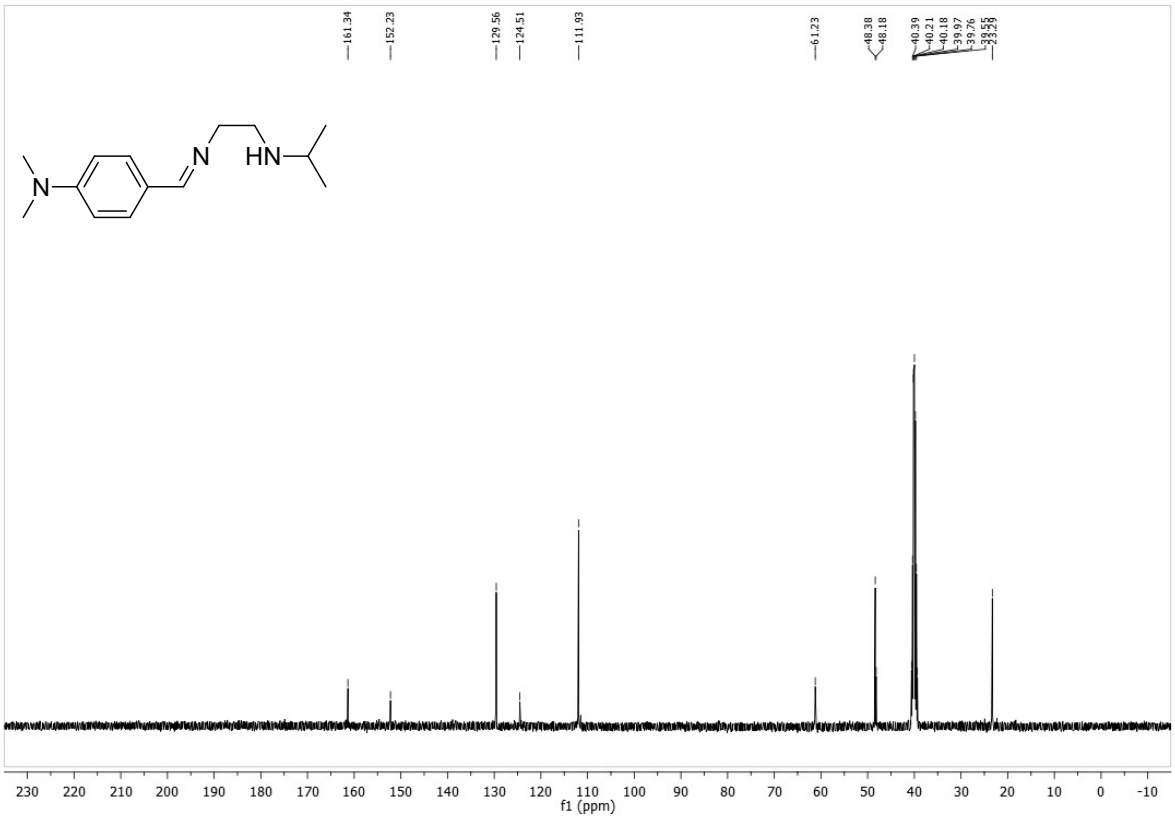


(b)

Figure S2. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of Ligand II, 400 MHz, $CDCl_3$, 25 °C.

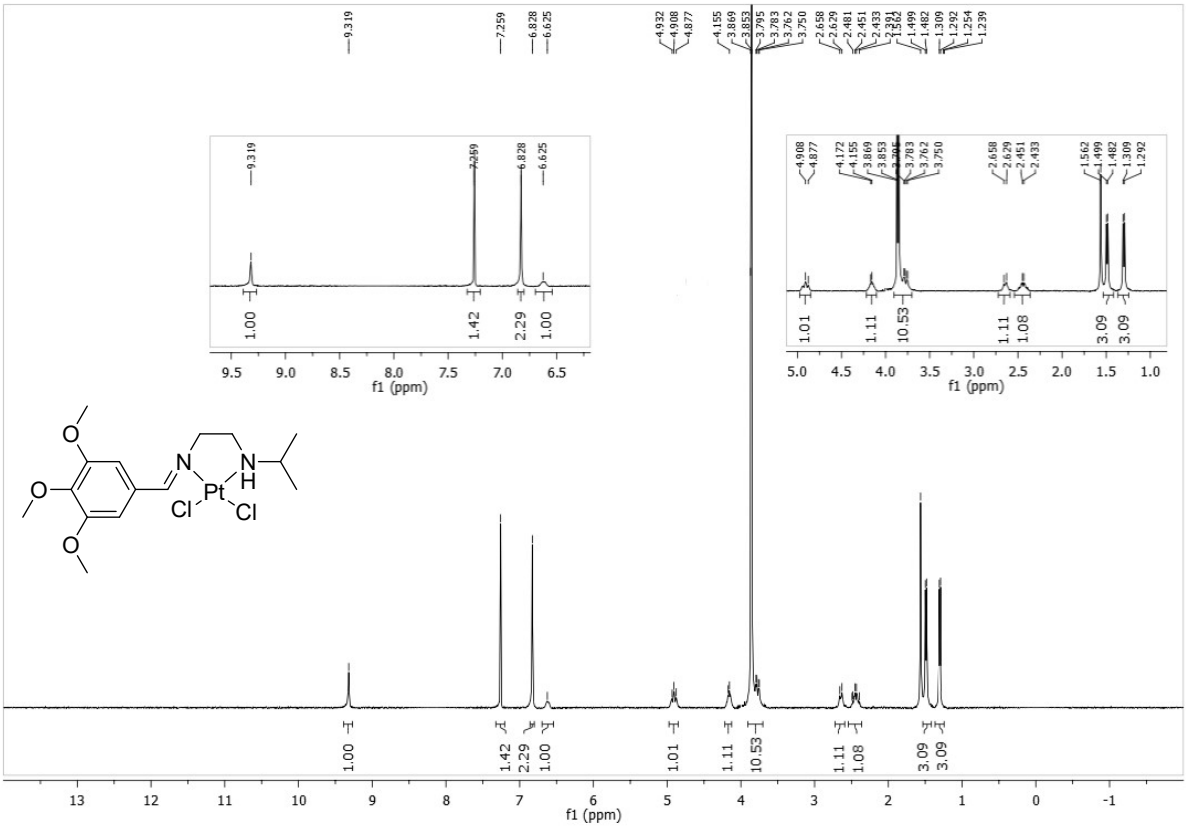


(a)

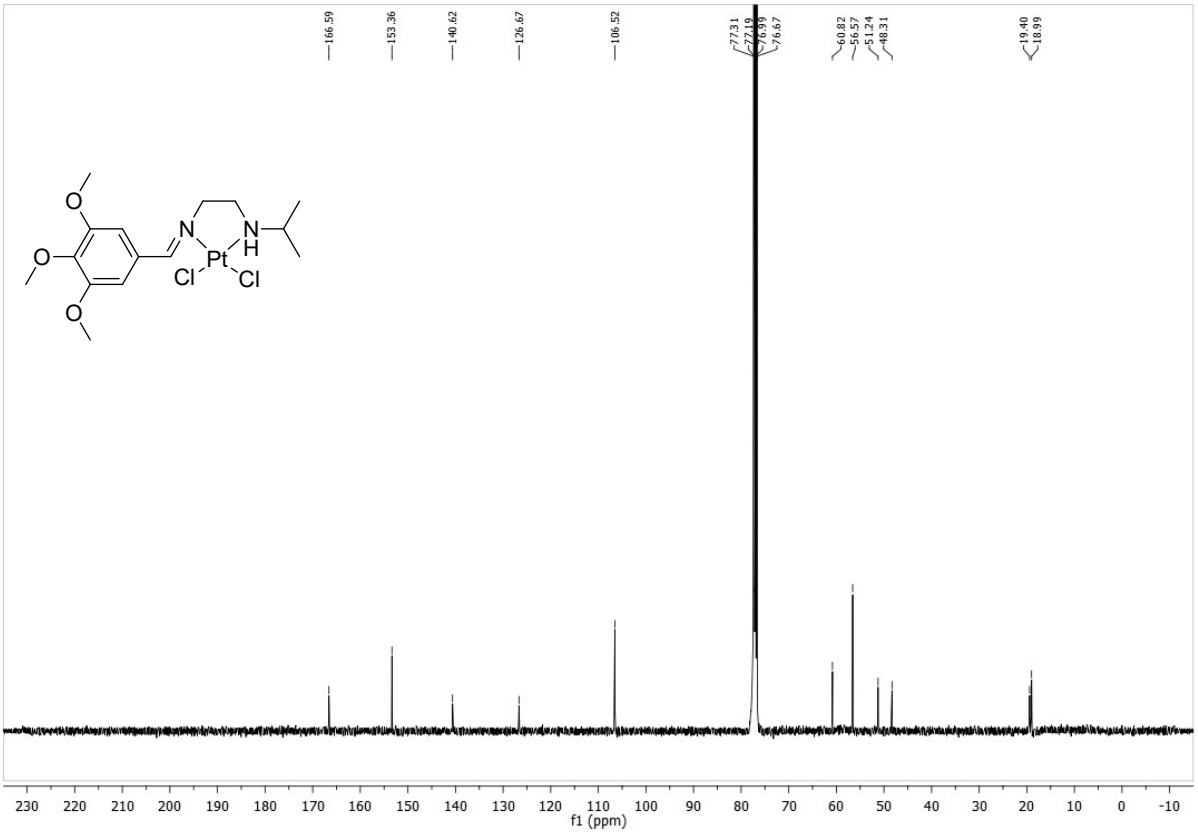


(b)

Figure S3. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of Ligand III, 400 MHz, $CDCl_3$, 25 °C.

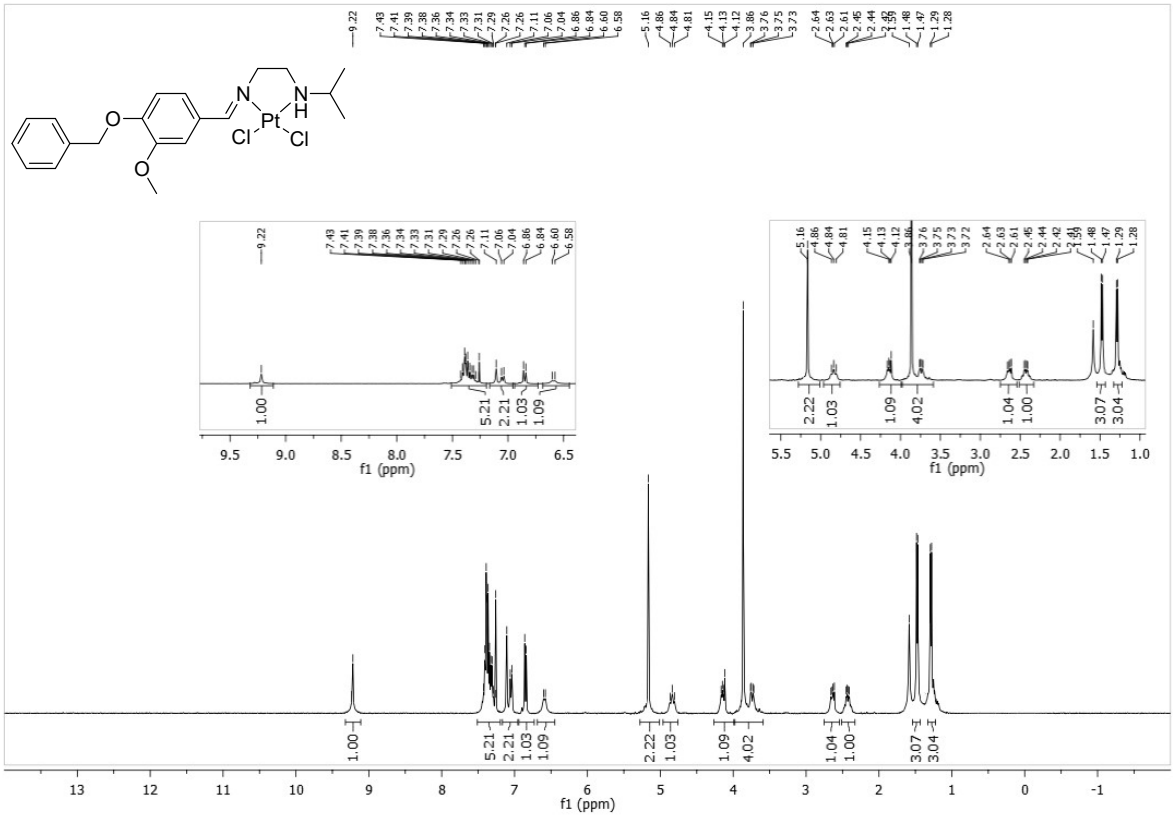


(a)



(b)

Figure S4. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of complex I, 400 MHz, $CDCl_3$, 25 °C.



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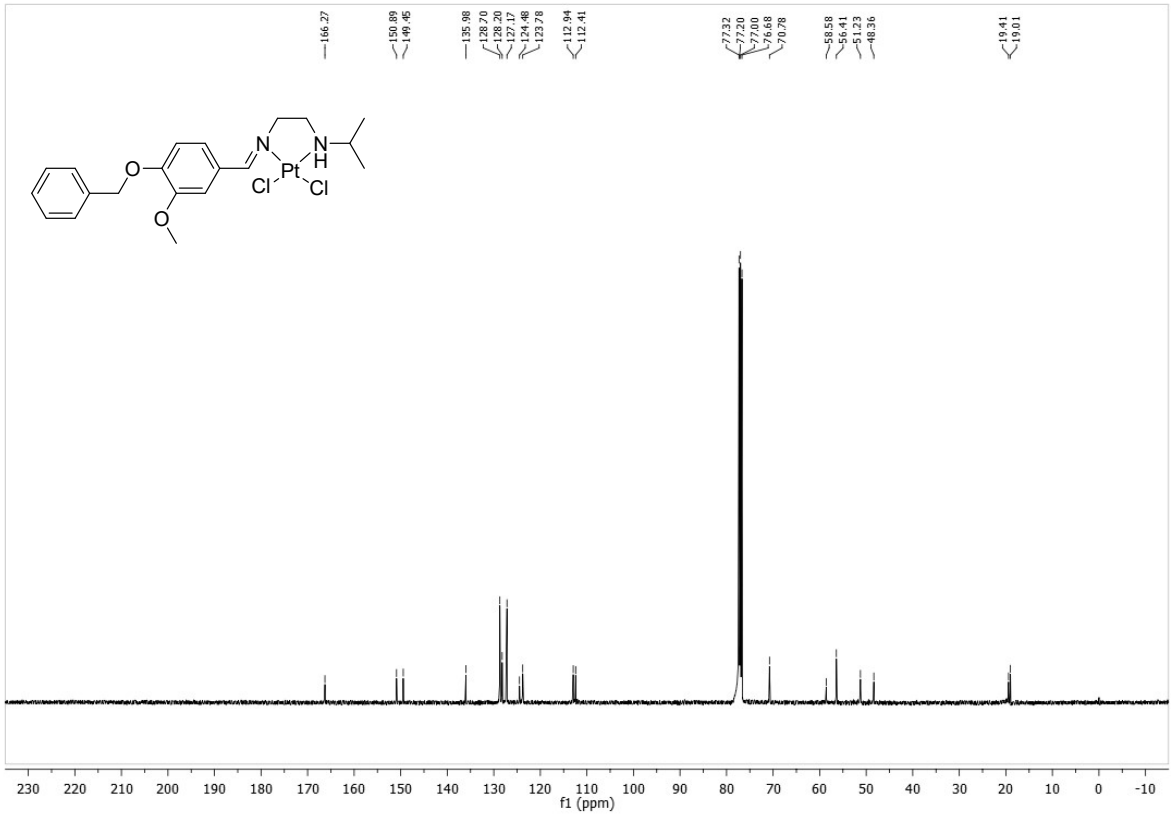
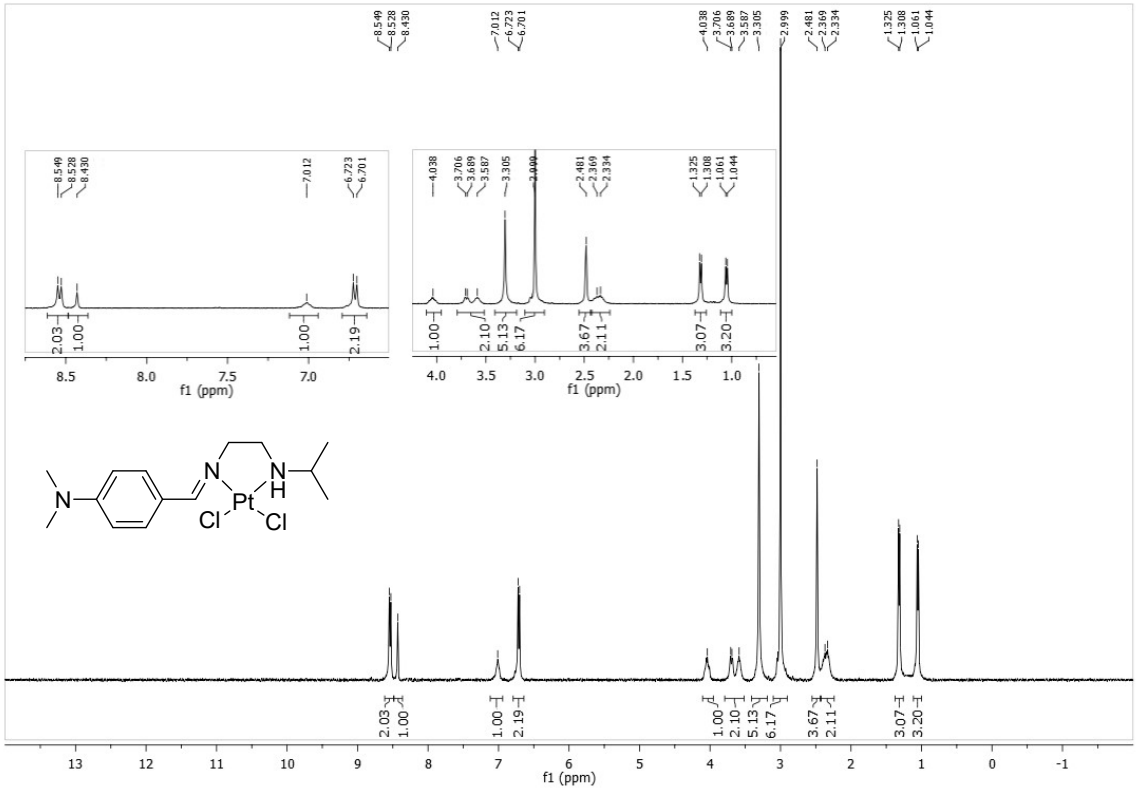
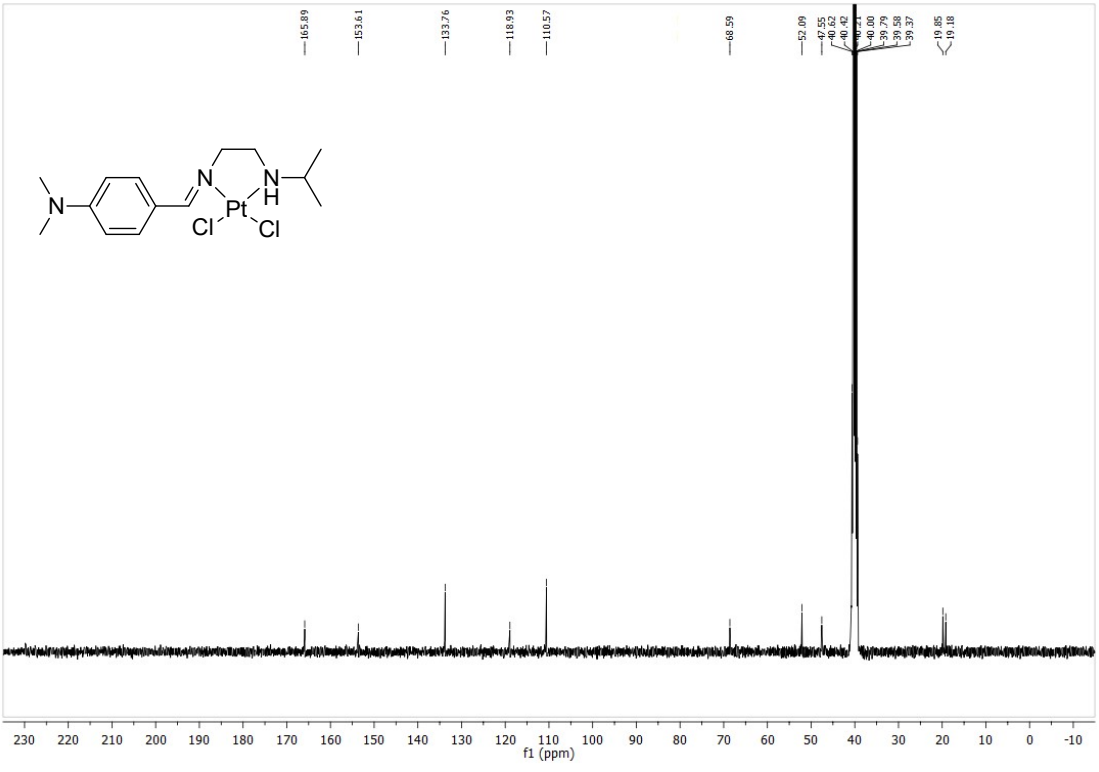


(b)

Figure S5. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of complex II, 400 MHz, $CDCl_3$, 25 °C.



(a)



(b)

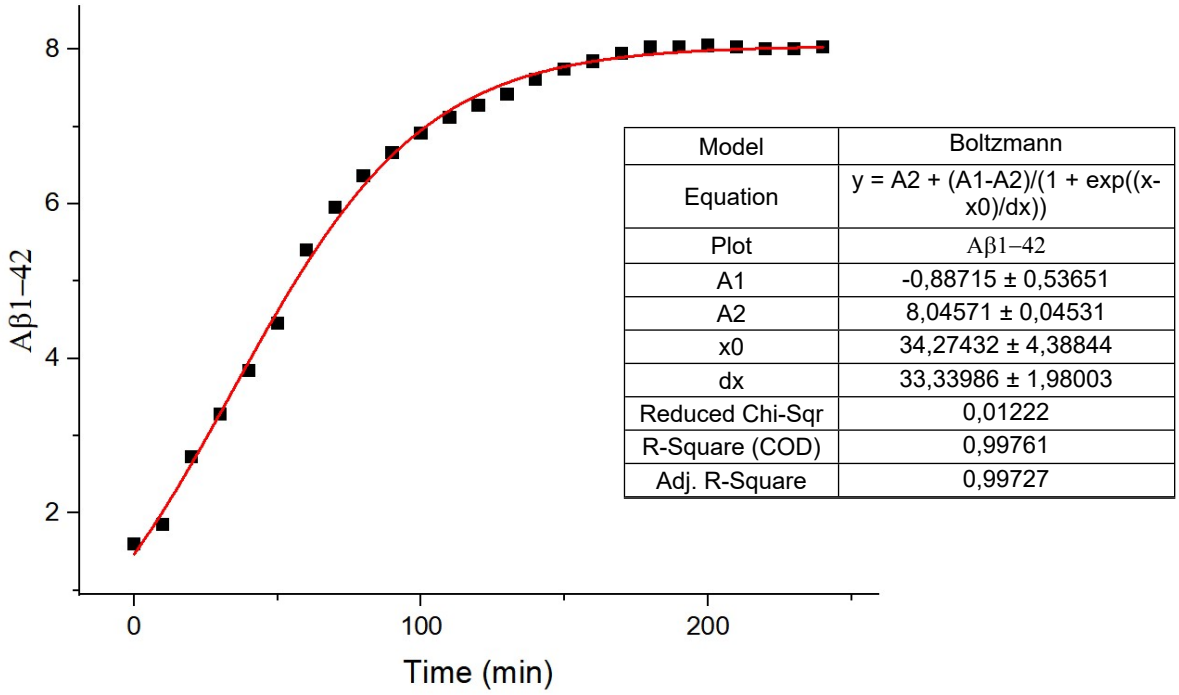
Figure S6. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of complex III, 400 MHz, DMSO-d6, 25 °C.

Figure S7. Kinetic data derived from fluorescence measurements.

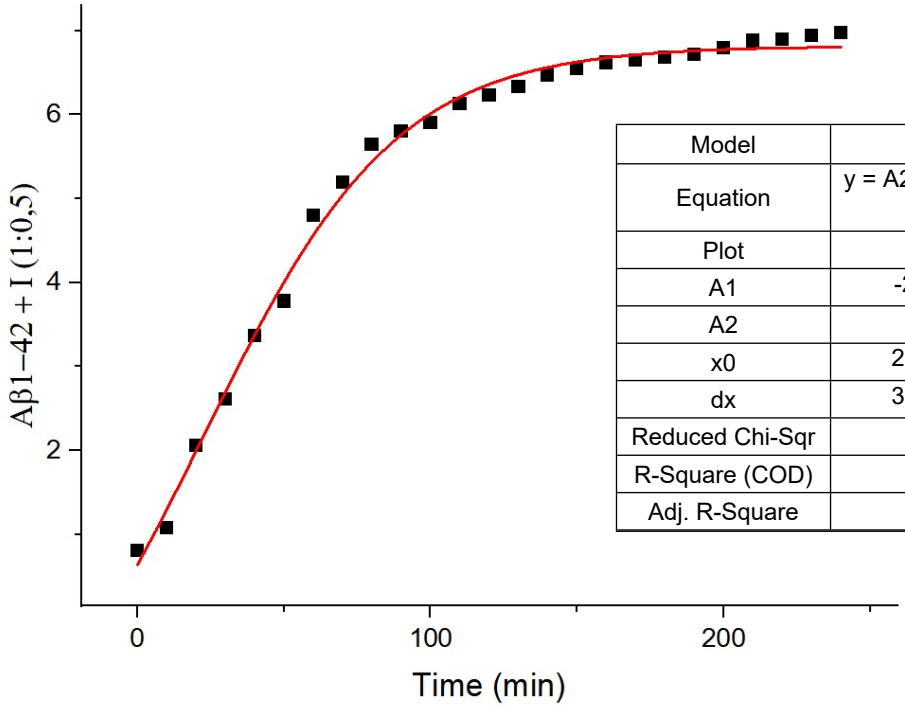
The detailed fitting results for the Thioflavin-T aggregation kinetics are presented below. The data were fitted using the Boltzmann sigmoidal model as implemented in OriginPro software.

Notes on Fitting Results

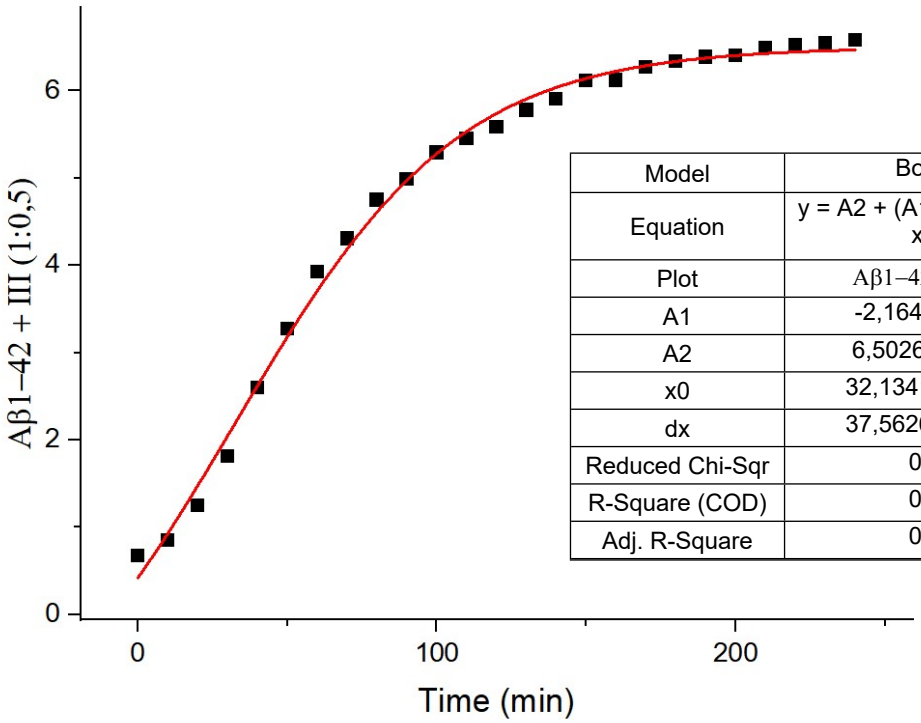
Negative A_1 values were observed in the fitting results for several samples. This phenomenon is attributed to very low initial ThT fluorescence signals and minor fluctuations in background readings during measurement. The negative A_1 values did not significantly impact the quality of the model fits, as evidenced by high R^2 values (>0.99) across all conditions. Therefore, these negative values are considered within acceptable experimental variance and do not affect the interpretation of the aggregation kinetics.



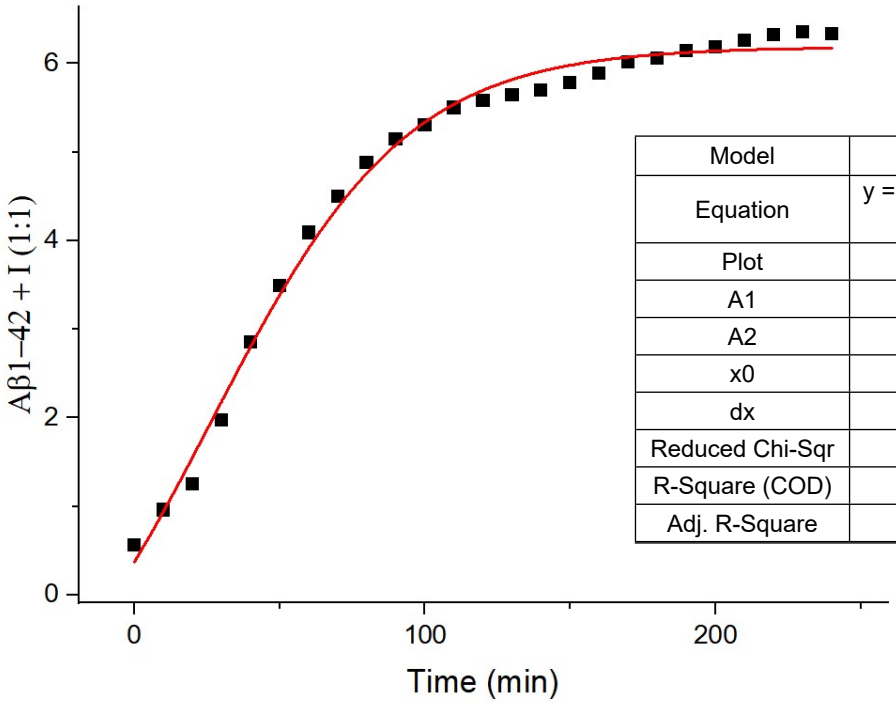
Model	Boltzmann
Equation	y = A2 + (A1-A2)/(1 + exp((x-x0)/dx))
Plot	Aβ1–42
A1	-0,88715 ± 0,53651
A2	8,04571 ± 0,04531
x0	34,27432 ± 4,38844
dx	33,33986 ± 1,98003
Reduced Chi-Sqr	0,01222
R-Square (COD)	0,99761
Adj. R-Square	0,99727



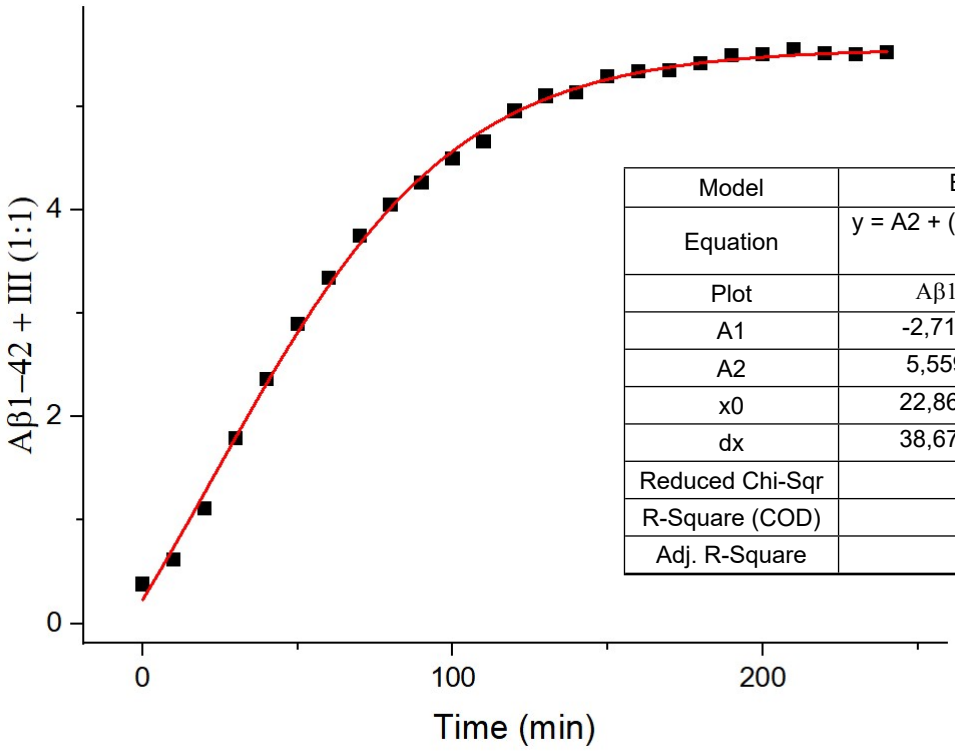
Model	Boltzmann
Equation	y = A2 + (A1-A2)/(1 + exp((x-x0)/dx))
Plot	Aβ1–42 + I (1:0,5)
A1	-2,46502 ± 1,01489
A2	6,81667 ± 0,0545
x0	22,60411 ± 7,53007
dx	32,87462 ± 2,80754
Reduced Chi-Sqr	0,01971
R-Square (COD)	0,99532
Adj. R-Square	0,99465



Model	Boltzmann
Equation	y = A2 + (A1-A2)/(1 + exp((x-x0)/dx))
Plot	Aβ1–42 + III (1:0,5)
A1	-2,1643 ± 0,79916
A2	6,50261 ± 0,06352
x0	32,13414 ± 7,32212
dx	37,56263 ± 3,14327
Reduced Chi-Sqr	0,01813
R-Square (COD)	0,99581
Adj. R-Square	0,99522



Model	Boltzmann
Equation	y = A2 + (A1-A2)/(1 + exp((x-x0)/dx))
Plot	Aβ1–42 + I (1:1)
A1	-2,27603 ± 0,99239
A2	6,18759 ± 0,06217
x0	26,38437 ± 8,34834
dx	33,56601 ± 3,30758
Reduced Chi-Sqr	0,02395
R-Square (COD)	0,99375
Adj. R-Square	0,99286



Model	Boltzmann
Equation	y = A2 + (A1-A2)/(1 + exp((x-x0)/dx))
Plot	Aβ1–42 + III (1:1)
A1	-2,71825 ± 0,59705
A2	5,55986 ± 0,03451
x0	22,86806 ± 5,68592
dx	38,67502 ± 2,11282
Reduced Chi-Sqr	0,00529
R-Square (COD)	0,99834
Adj. R-Square	0,9981

A_1 (Initial fluorescence intensity), A_2 (Maximum fluorescence intensity), x_0 (Lag time), dx (Aggregation rate parameter), R-Square (COD) (R^2 =Coefficient of determination)

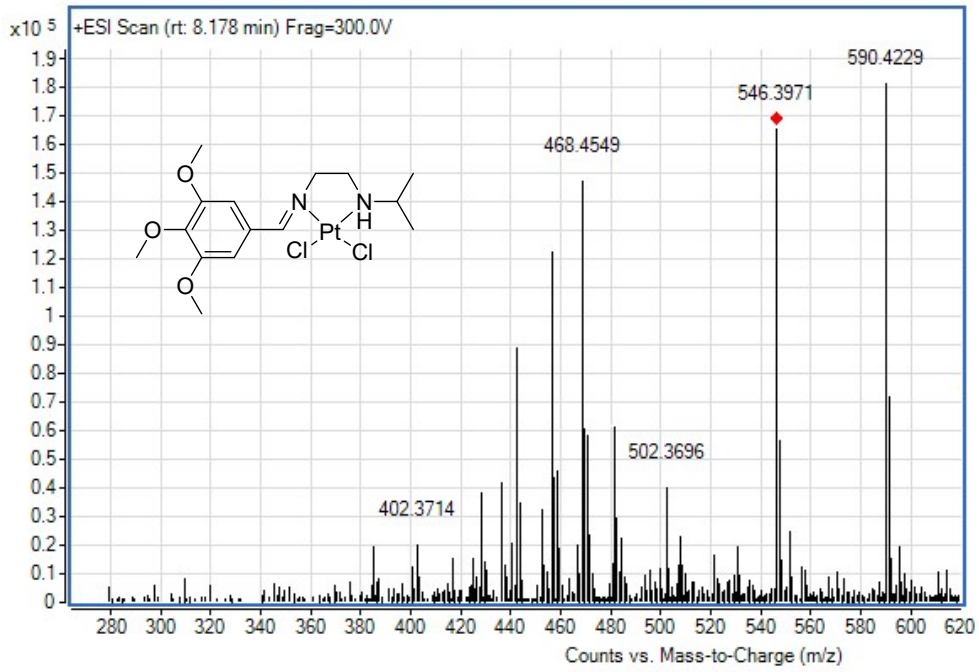


Figure S8. Mass spectrum of the complex I.

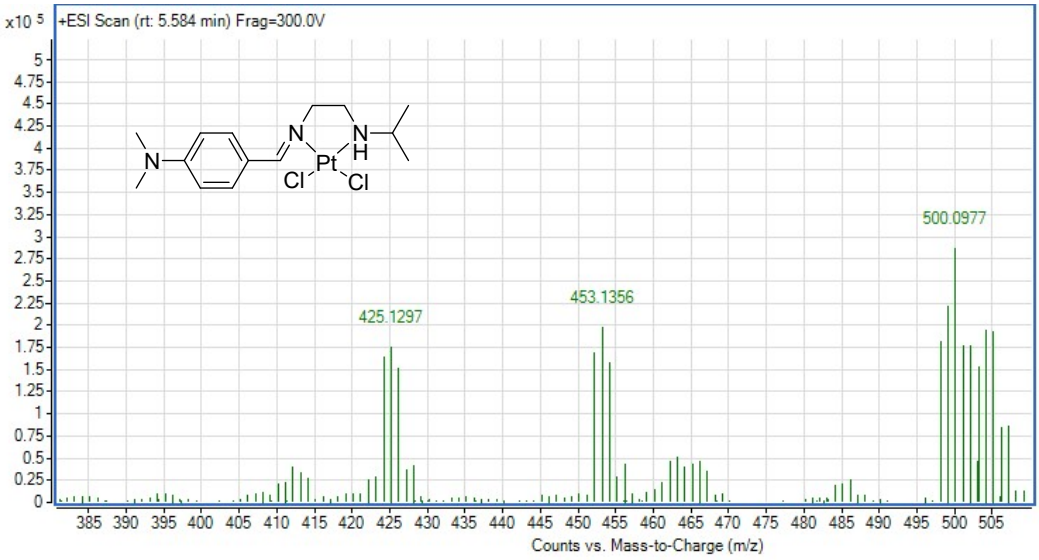


Figure S9. Mass spectrum of the complex III.

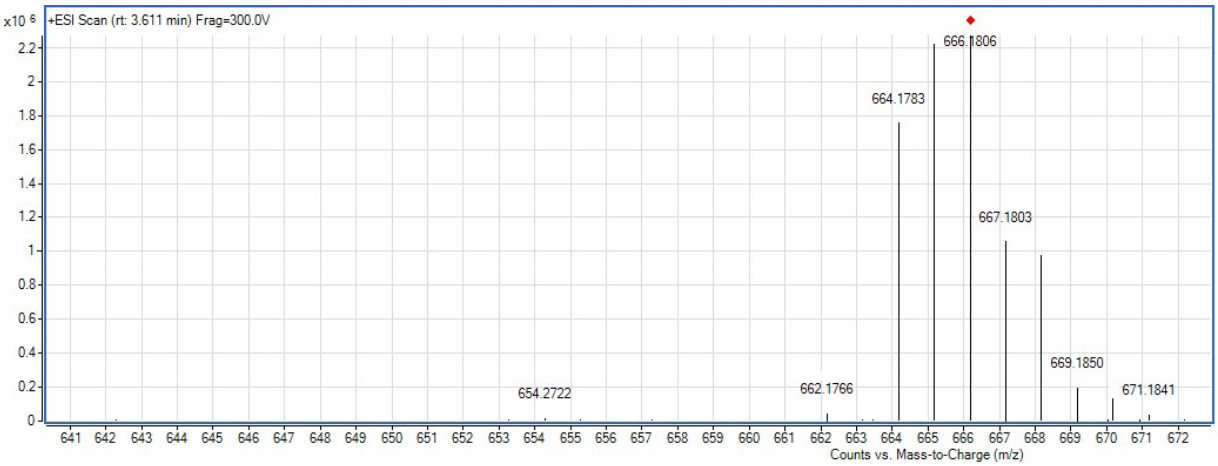
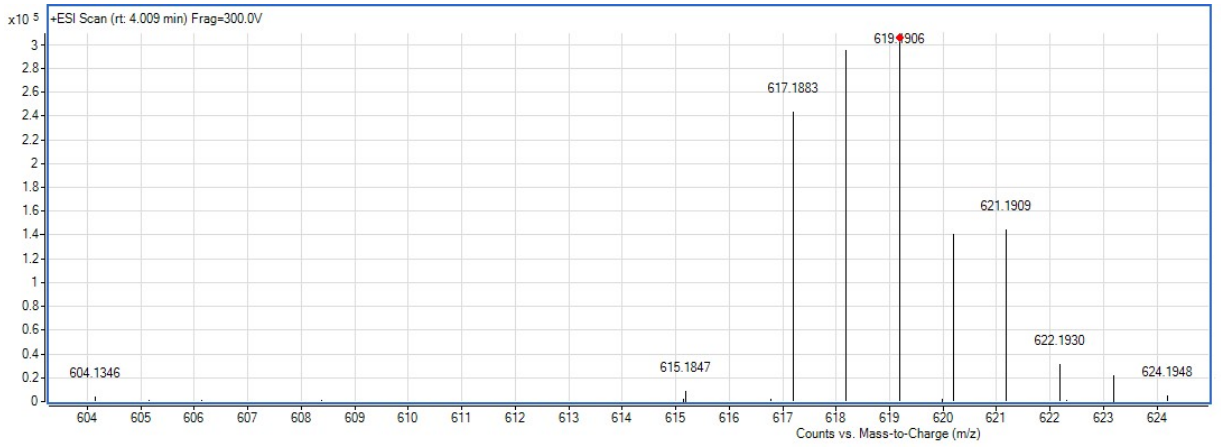


Figure S10. Mass spectrum of the complex I–Histidine interaction.



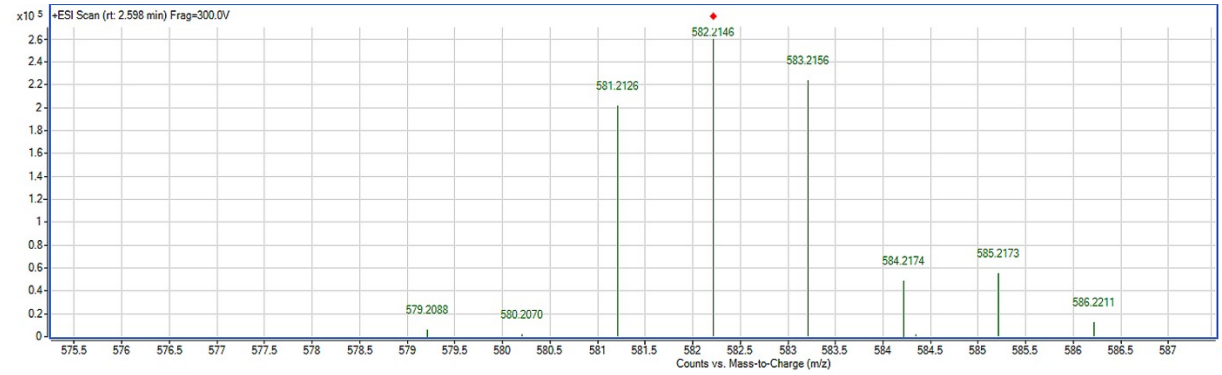


Figure S11. Mass spectra of the complex III–Histidine interaction.

Table S1. Raw fluorescence intensity values obtained from ThT assay for $A\beta_{1-42}$ aggregation.

Time (min)	$A\beta_{1-42}$	$A\beta_{1-42}$+ I (1:0,5)	$A\beta_{1-42}$+ III (1:0,5)	$A\beta_{1-42}$+ I (1:1)	$A\beta_{1-42}$+ III (1:1)
0	1,599	0,805	0,676	0,563	0,381
10	1,847	1,082	0,852	0,962	0,619
20	2,720	2,059	1,246	1,254	1,116
30	3,273	2,613	1,810	1,970	1,792
40	3,840	3,371	2,598	2,856	2,362
50	4,452	3,779	3,277	3,492	2,893
60	5,398	4,800	3,929	4,090	3,339
70	5,951	5,193	4,309	4,495	3,747
80	6,358	5,645	4,750	4,876	4,048
90	6,664	5,805	4,988	5,149	4,260
100	6,911	5,907	5,293	5,307	4,496
110	7,115	6,125	5,450	5,502	4,660
120	7,275	6,227	5,585	5,582	4,953
130	7,421	6,328	5,778	5,647	5,100
140	7,610	6,474	5,904	5,696	5,133
150	7,741	6,546	6,115	5,785	5,288
160	7,843	6,619	6,122	5,890	5,337
170	7,945	6,648	6,271	6,012	5,346
180	8,032	6,676	6,339	6,060	5,411
190	8,032	6,720	6,387	6,141	5,493
200	8,046	6,792	6,400	6,190	5,502
210	8,032	6,879	6,488	6,262	5,551
220	8,003	6,893	6,522	6,319	5,511
230	8,003	6,937	6,550	6,351	5,503
240	8,032	6,980	6,577	6,334	5,519

Notes

Raw fluorescence intensity data from ThT assay over 240 min.
Each column represents a single measurement condition.
Measurements were taken using excitation λ = 440 nm and emission λ = 485 nm.
These data correspond to the ThT aggregation assay results shown in the manuscript.
No normalization or background subtraction applied to the values.

Table S2. Raw data from cytotoxicity assay for cell viability.

	Control	I	I	I	II	II	II	III	III	III
100,00	0,851	0,083	0,083	0,085	0,072	0,066	0,071	0,091	0,060	0,073
50,00	0,781	0,090	0,144	0,078	0,077	0,069	0,078	0,088	0,069	0,098
25,00	0,851	0,562	0,562	0,634	0,062	0,076	0,083	0,175	0,176	0,199
12,75	0,751	0,615	0,612	0,612	0,340	0,161	0,161	0,725	0,588	0,588
6,75	0,648	0,658	0,657	0,657	0,662	0,662	0,763	0,655	0,648	0,648
3,375	0,948	0,674	0,675	0,674	0,664	0,664	0,765	0,677	0,619	0,619
1,68	0,675	0,684	0,684	0,752	0,737	0,737	0,782	0,657	0,657	0,696

	PBS	DMSO	Cisplatine	Cisplatine	Cisplatine
100,00	0,189	0,072	0,113	0,090	0,095
50,00	0,481	0,081	0,096	0,106	0,100
25,00	0,797	0,074	0,325	0,315	0,314
12,75	0,639	0,116	0,631	0,546	0,363
6,75	0,746	0,296	0,723	0,565	0,539
3,38	0,855	0,672	0,796	0,510	0,537
1,68	0,692	0,522	0,646	0,646	0,661

Cytotoxicity I				
	Average	**std**	**Avg. (%)**	**std (%)**
Control	0,79	0,11	100,00	13,47
100	0,08	0,00	10,64	1,38
50	0,10	0,04	13,22	11,00
25	0,59	0,04	74,51	7,09
12,75	0,61	0,00	77,95	0,28
6,75	0,66	0,00	83,58	0,09
3,38	0,67	0,00	85,75	0,09
1,68	0,71	0,04	89,86	5,56
Cytotoxicity II				
	Average	**std**	**Avg. (%)**	**std (%)**
Control	0,79	0,11	100,00	13,47
100	0,07	0,00	8,86	4,61
50	0,07	0,00	9,49	6,61
25	0,07	0,01	9,37	14,51
12,75	0,22	0,10	28,06	46,83
6,75	0,70	0,06	88,46	8,38
3,375	0,70	0,06	88,71	8,36
1,68	0,75	0,03	95,62	3,45
Cytotoxicity III				
	Average	**std**	**Avg. (%)**	**std (%)**
Control	0,79	0,11	100,00	13,47
100	0,07	0,02	9,49	20,85
50	0,09	0,01	10,81	17,33
25	0,18	0,01	23,31	7,41
12,75	0,63	0,08	80,58	12,48
6,75	0,65	0,00	82,69	0,62
3,375	0,64	0,04	81,17	6,42
1,68	0,67	0,02	85,20	3,36

Cell Viability (%) Based on MTT Assay at 570 nm

		Average	std	Avg. (%)	std (%)
	Control	0,382	0,029	100,0	7,5
	Amyloid	0,236	0,031	64,8	13,3
10μM	**I**	0,293	0,036	80,5	12,2
	II	0,012	0,015	40,4	8,4
	II	0,282	0,029	77,5	10,5
5μM	**I**	0,269	0,052	73,9	19,3
	II	0,156	0,025	42,9	16,1
	III	0,255	0,082	70,1	32,2