Electronic Supplementary Information

Synthesis, structural characterization, biological evaluation and molecular docking studies of new platinum(II) complexes bearing isocyanides

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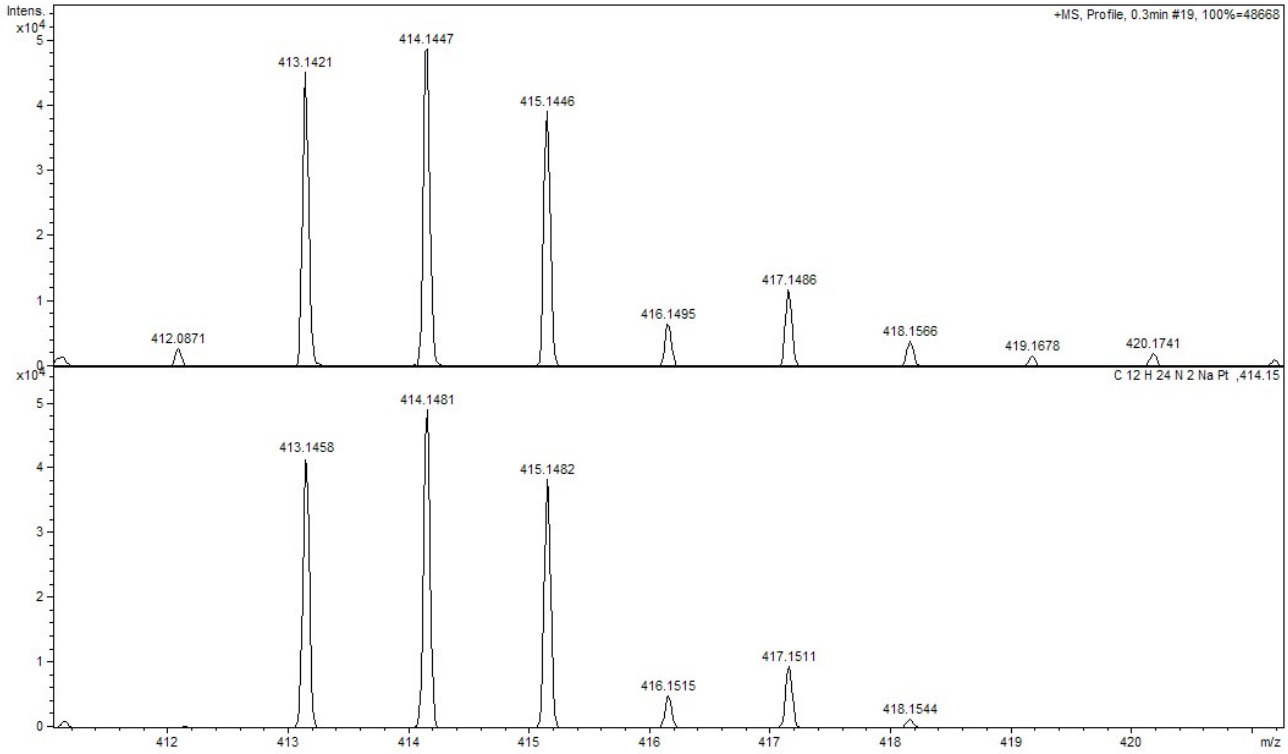

Figure S1. Experimental (top) and calculated (bottom) HR ESI-MS spectra of **1a** showing the ion [**1a** + Na]$^+$.

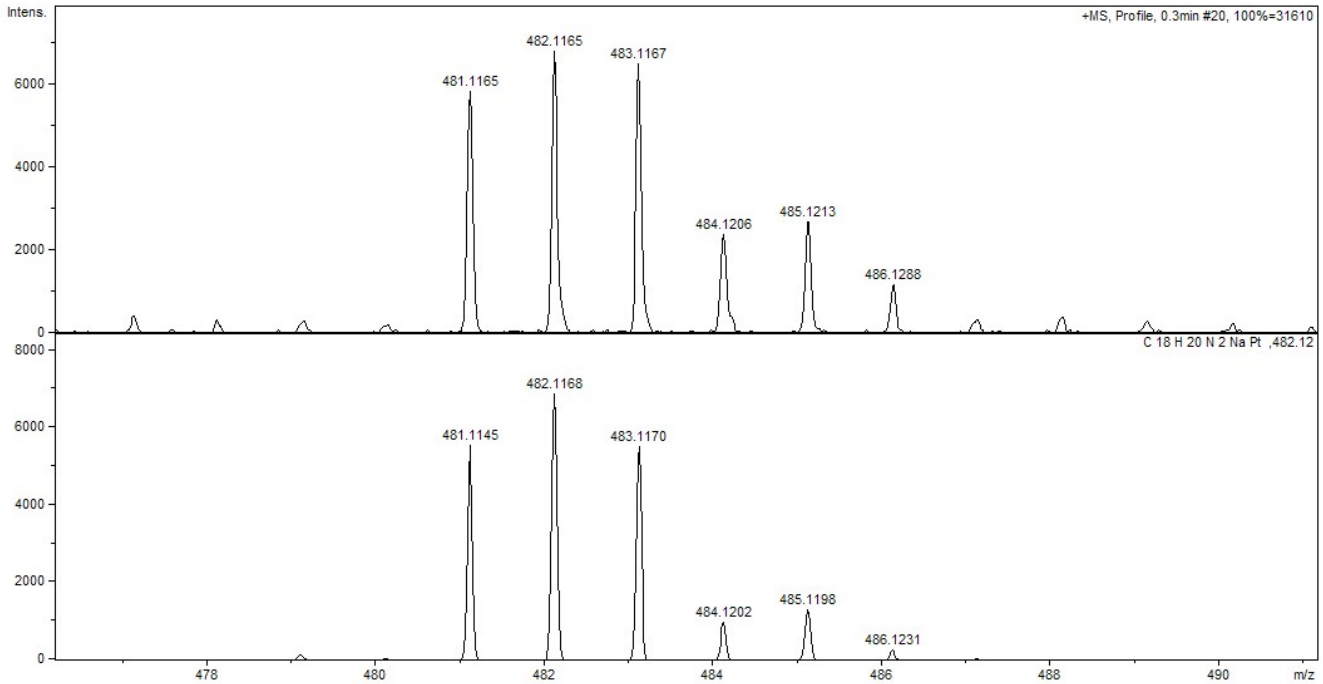

Figure S2. Experimental (top) and calculated (bottom) HR ESI-MS spectra of **1b** showing the ion [**1b** + Na]$^+$.

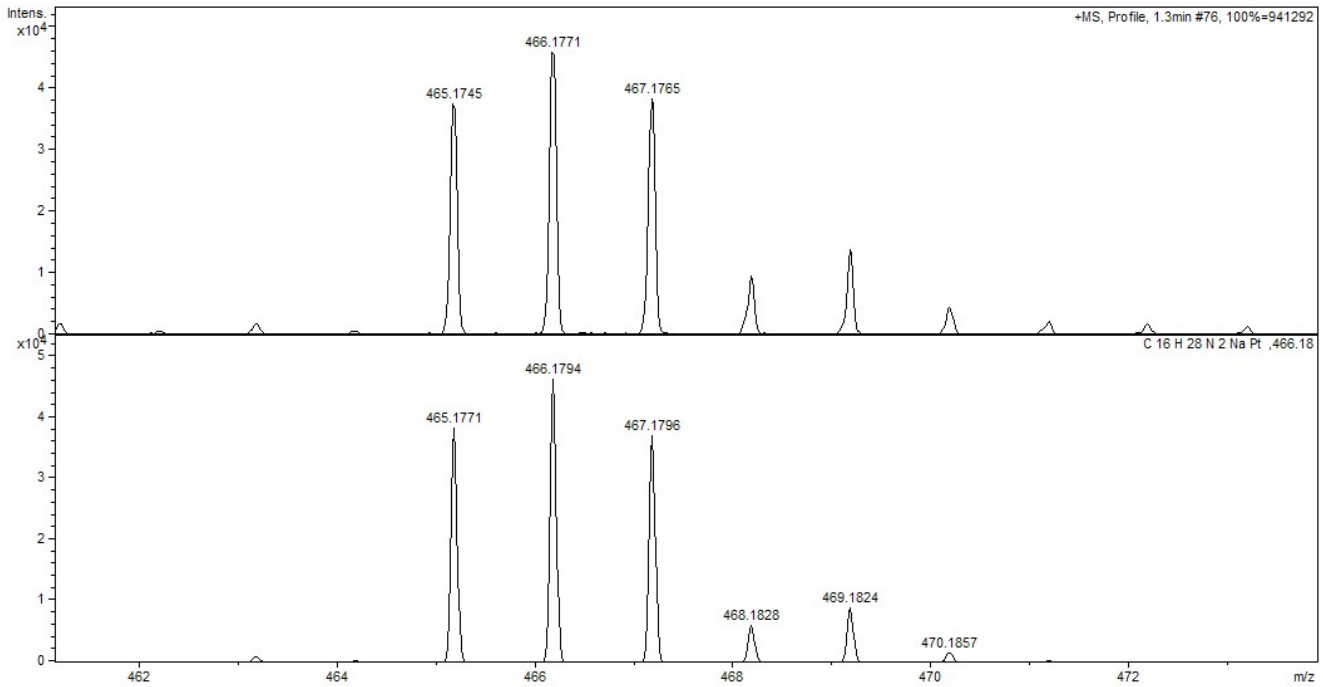

Figure S3. Experimental (top) and calculated (bottom) HR ESI-MS spectra of **1c** showing the ion [**1c** + Na]$^+$.

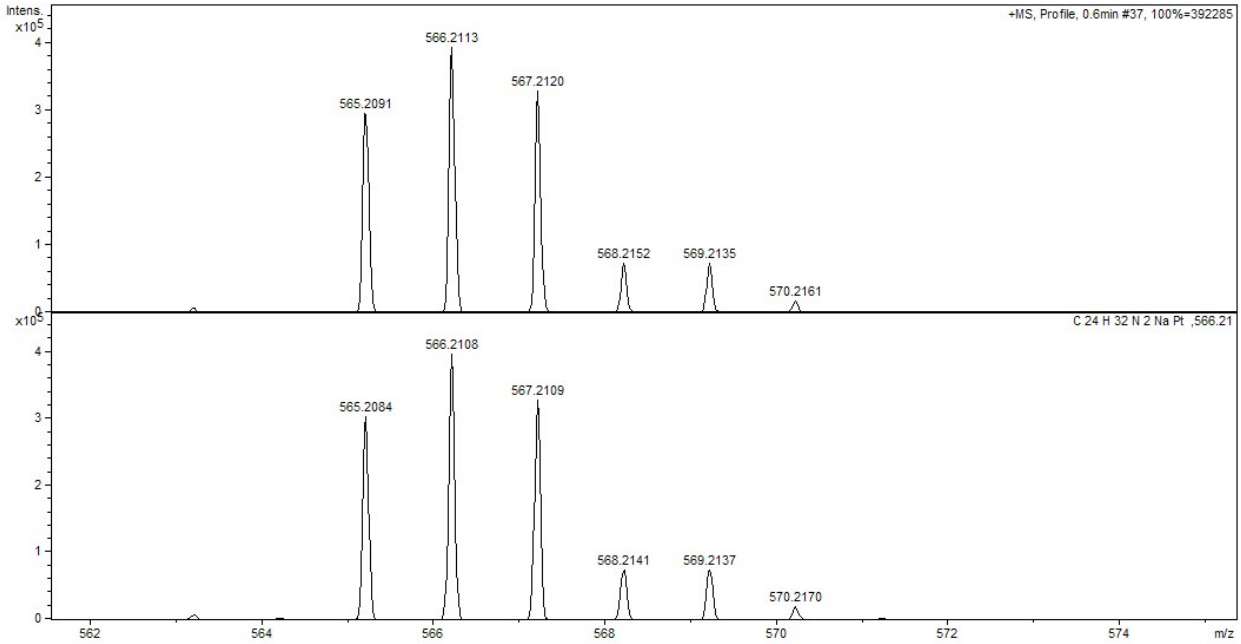

Figure S4. Experimental (top) and calculated (bottom) HR ESI-MS spectra of **2a** showing the ion [**2a** + Na]$^+$.

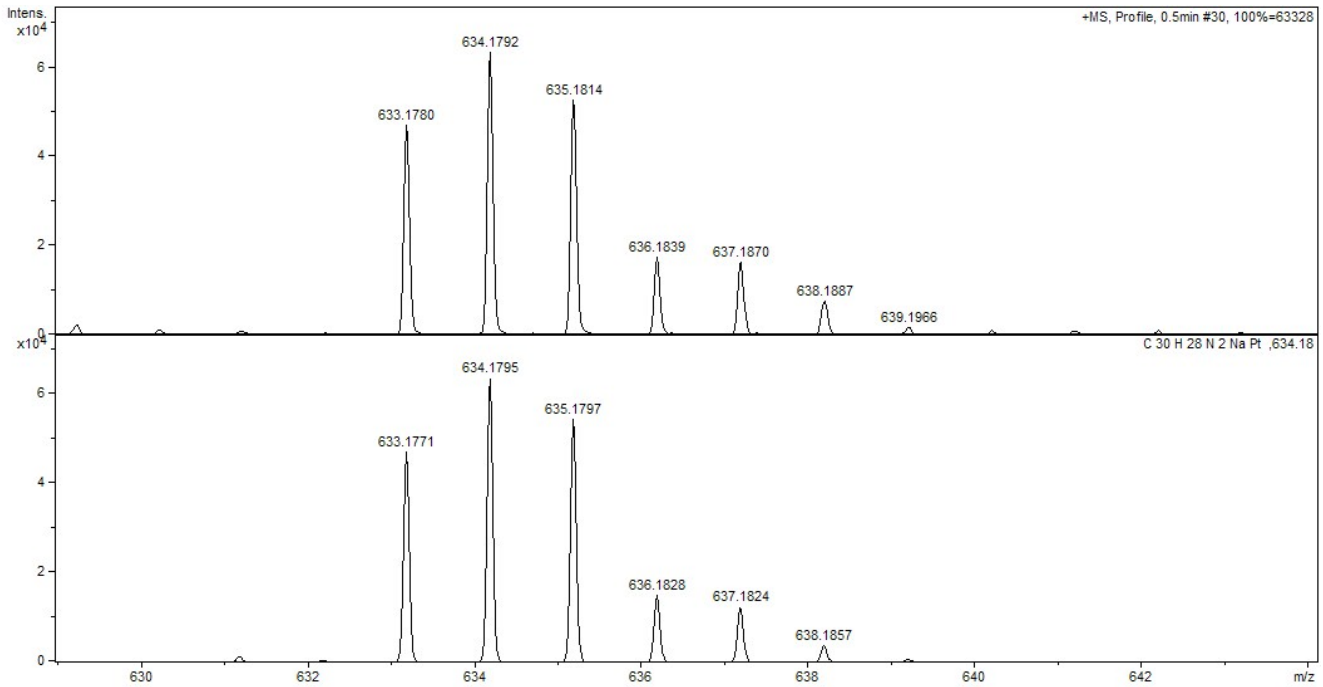

Figure S5. Experimental (top) and calculated (bottom) HR ESI-MS spectra of **2b** showing the ion [**2b** + Na]$^+$.

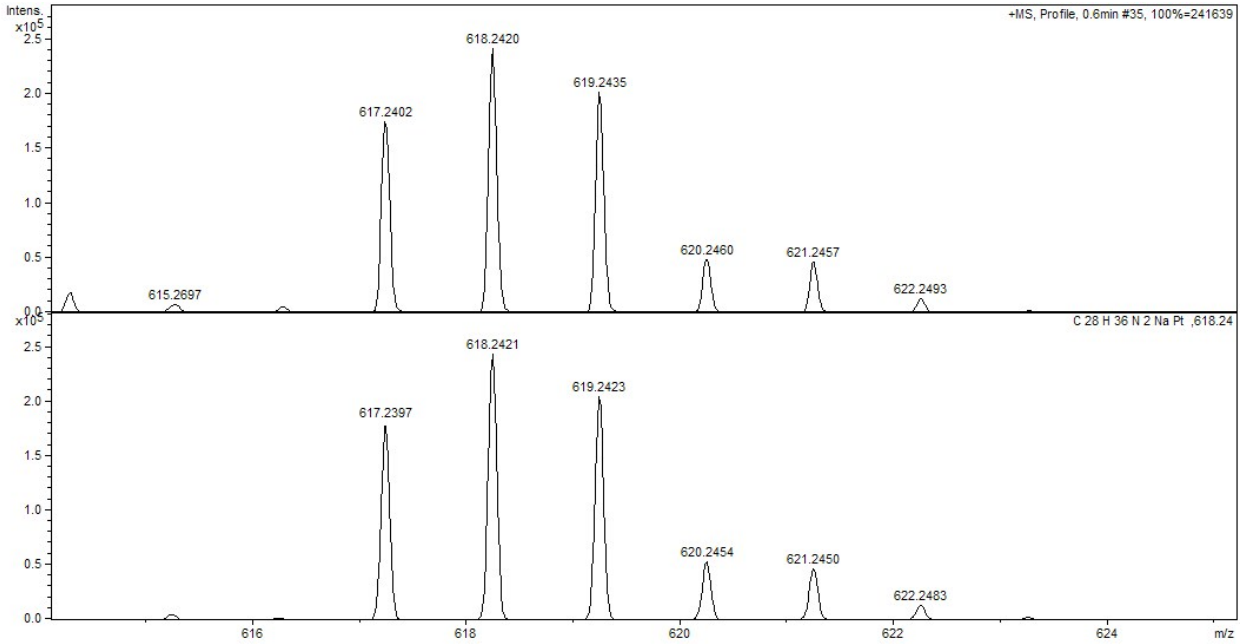

Figure S6. Experimental (top) and calculated (bottom) HR ESI-MS spectra of **2c** showing the ion [**2c** + Na]$^+$.

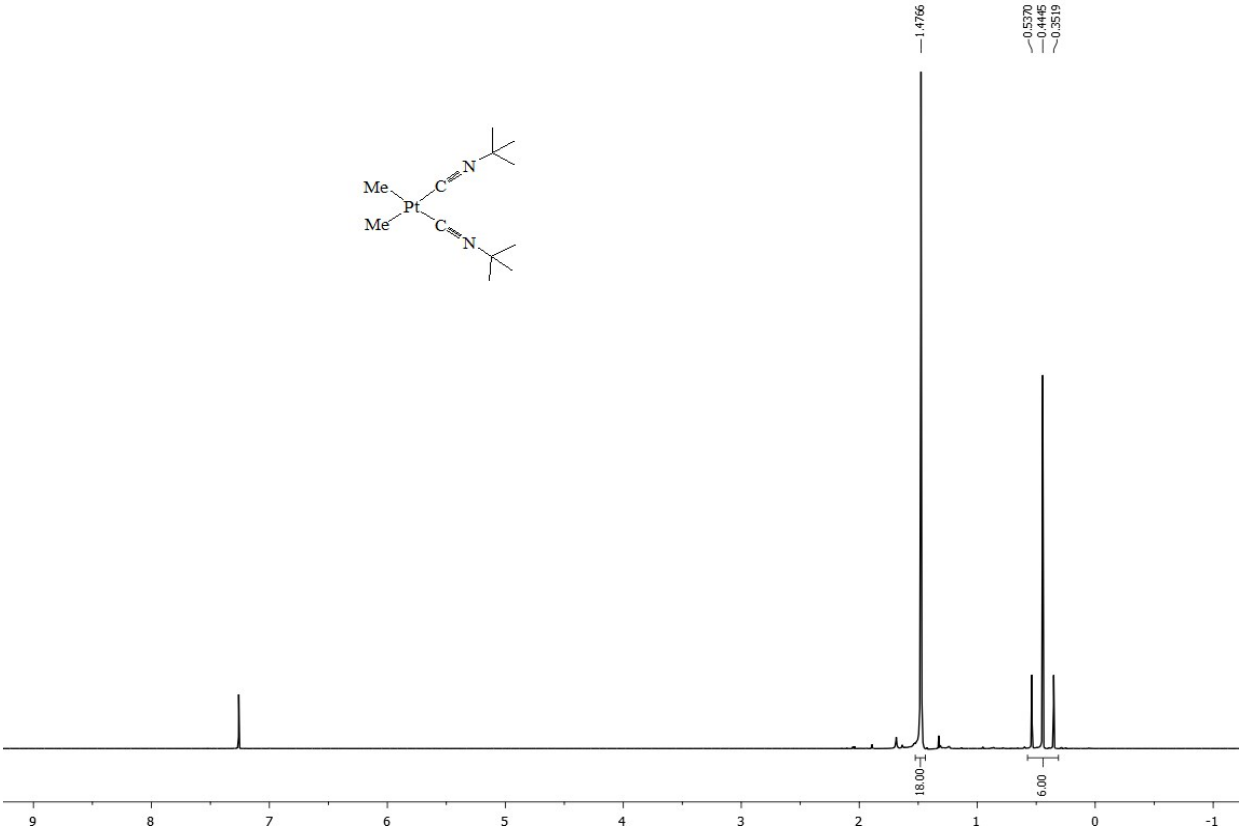

Figure S7. ^{1}H NMR spectrum of **1a** in $CDCl_3$ at room temperature.

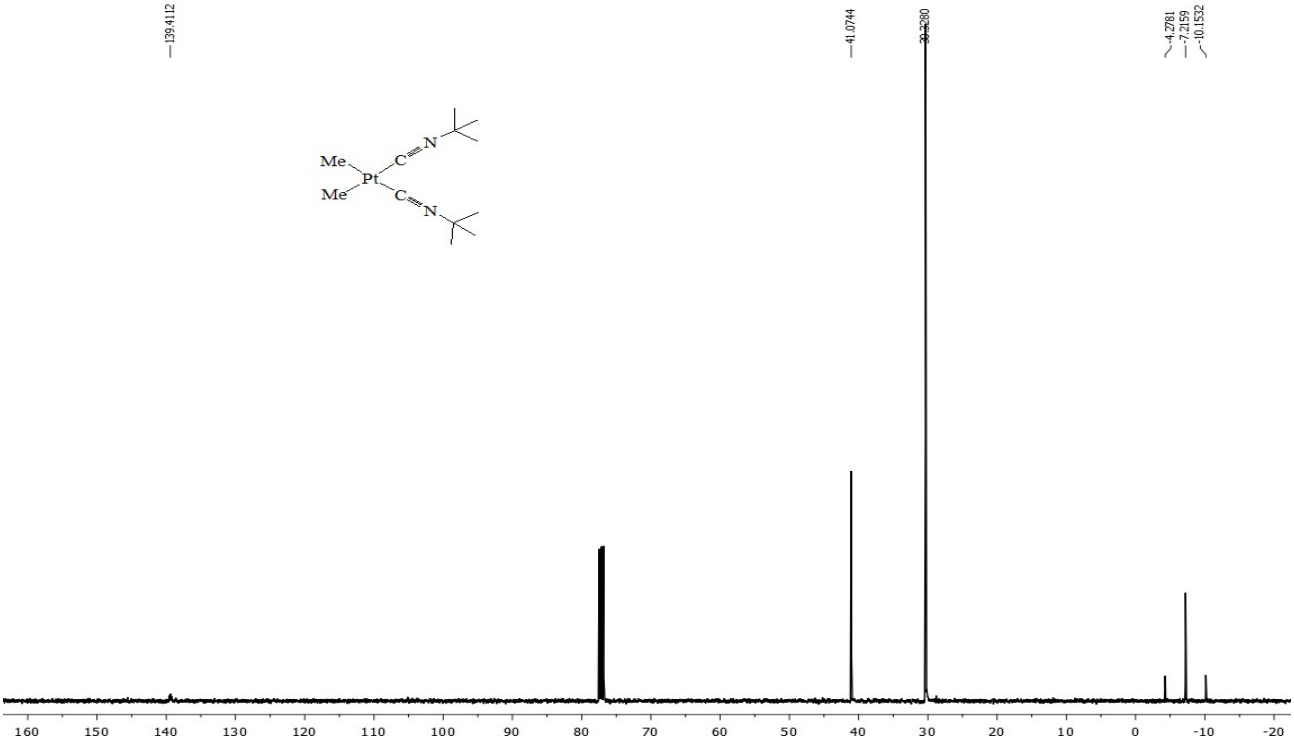

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **1a** in $CDCl_3$ at room temperature.

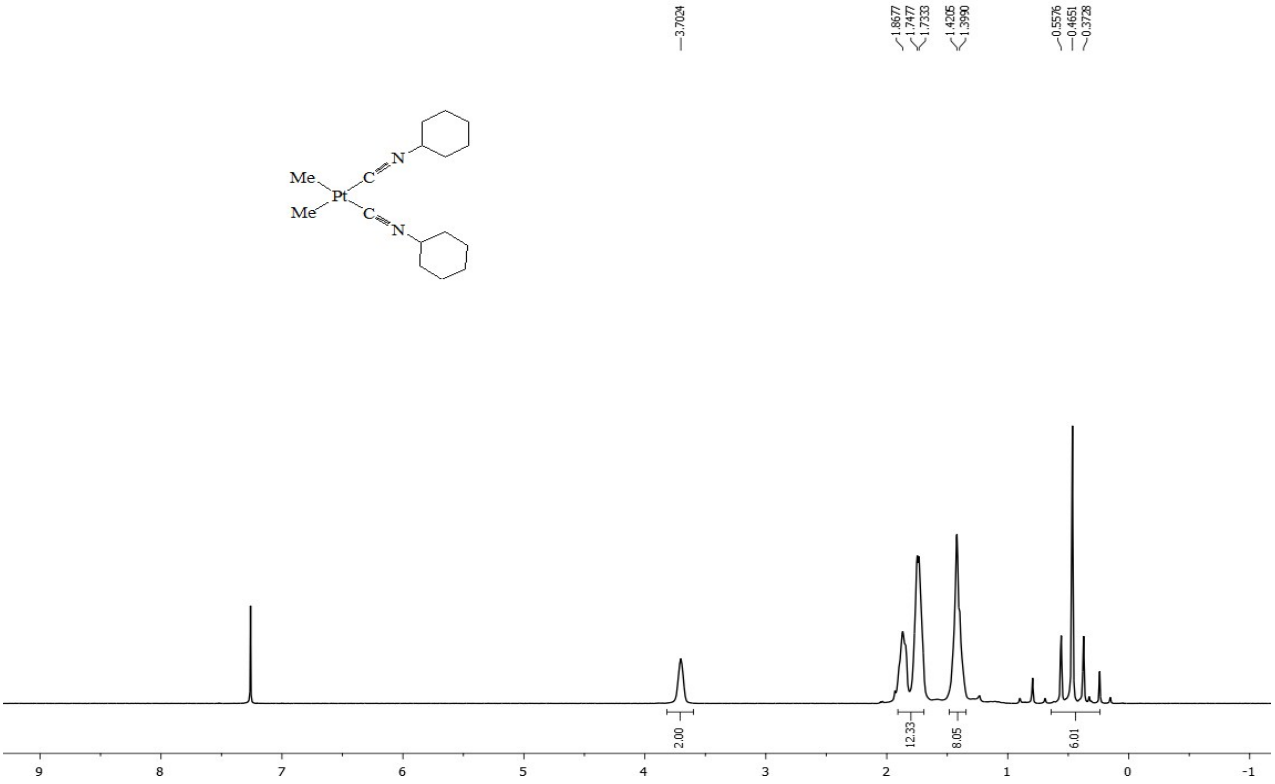

Figure S9. ^{1}H NMR spectrum of **1c** in $CDCl_3$ at room temperature.

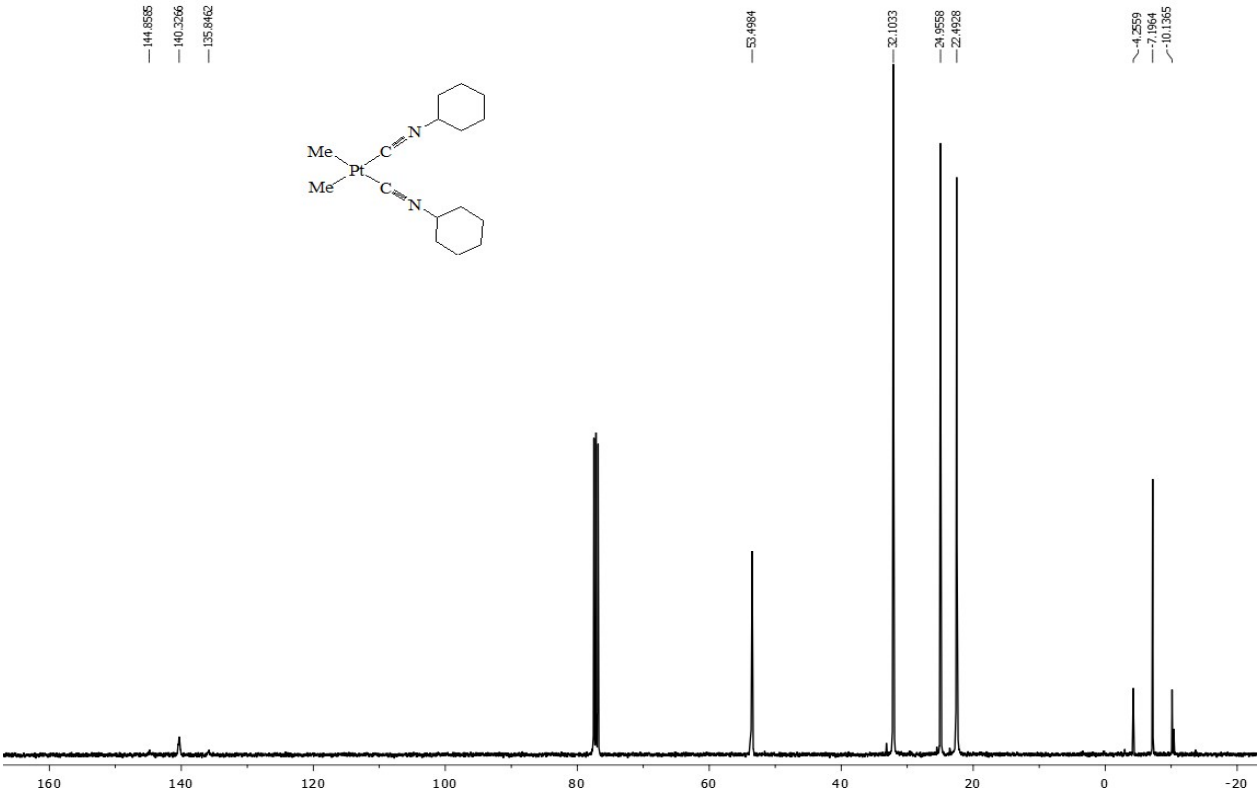

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **1c** in $CDCl_3$ at room temperature.

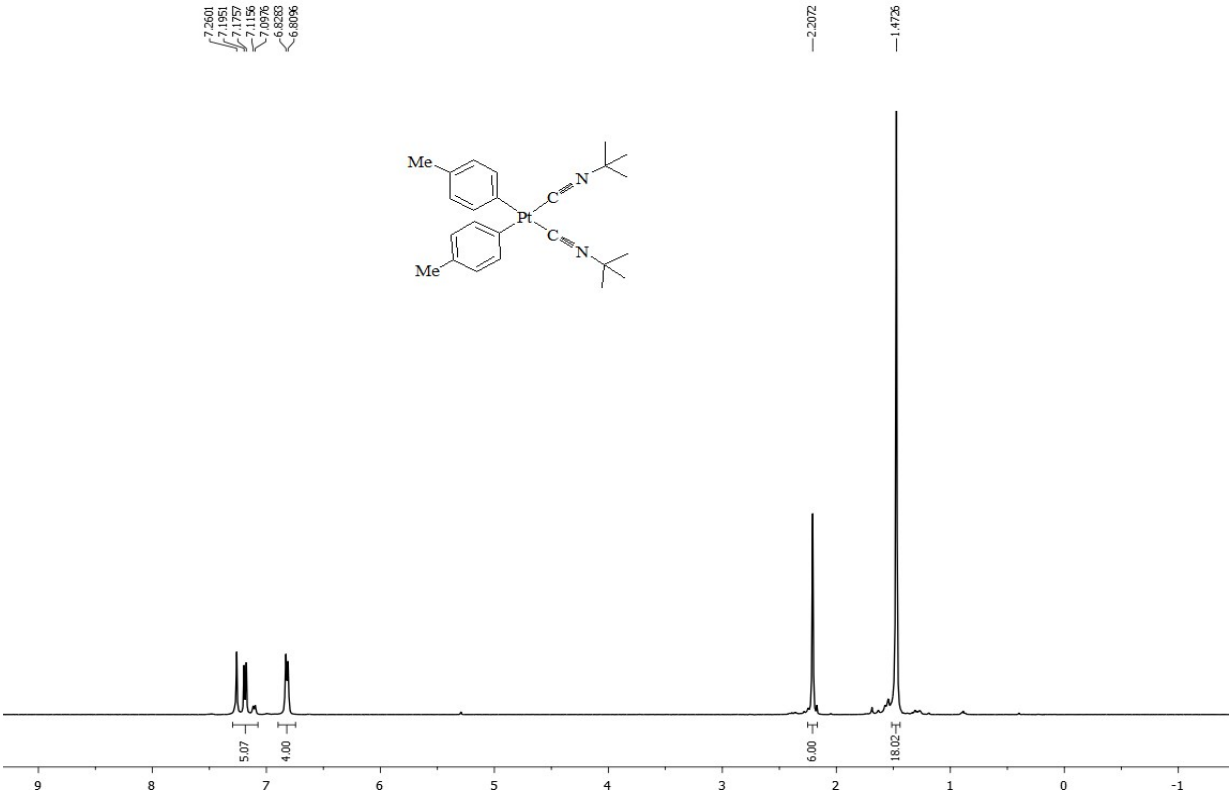

Figure S11. ^{1}H NMR spectrum of **2a** in $CDCl_3$ at room temperature.

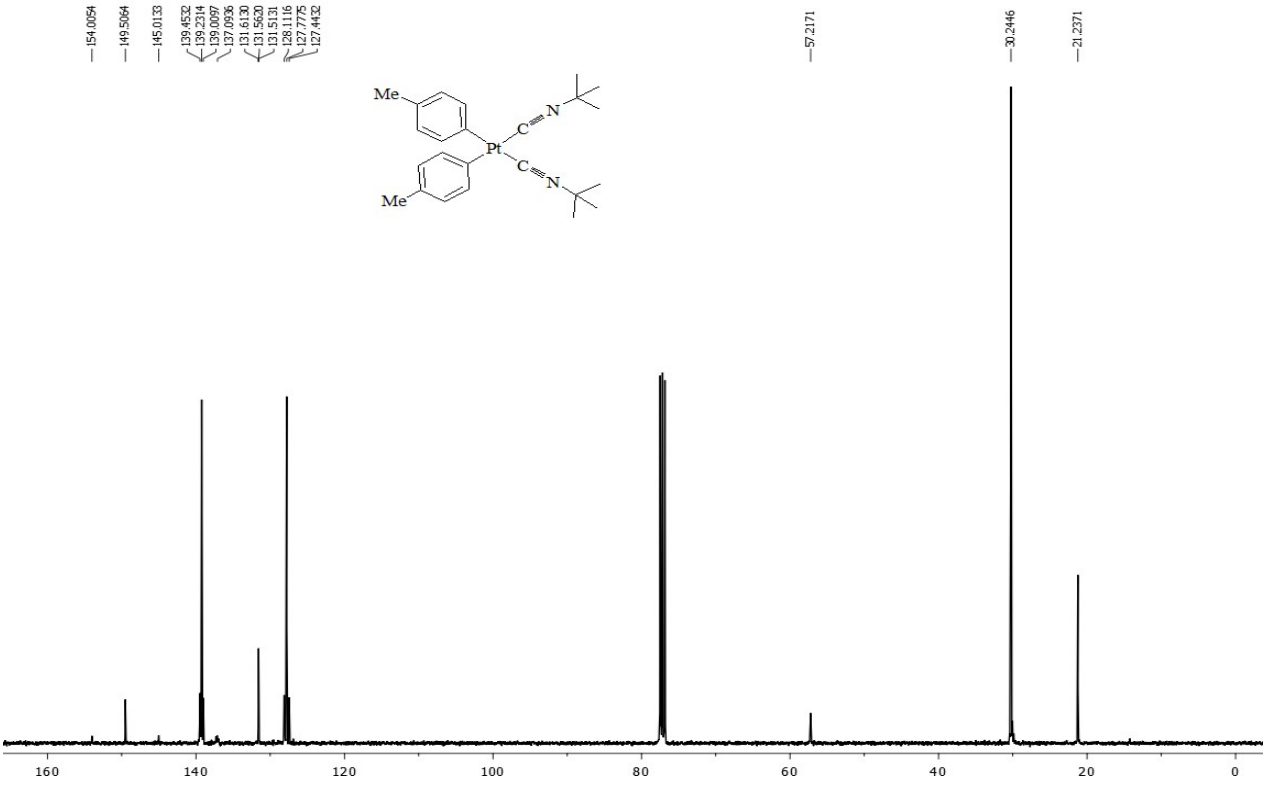

Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of **2a** in $CDCl_3$ at room temperature.

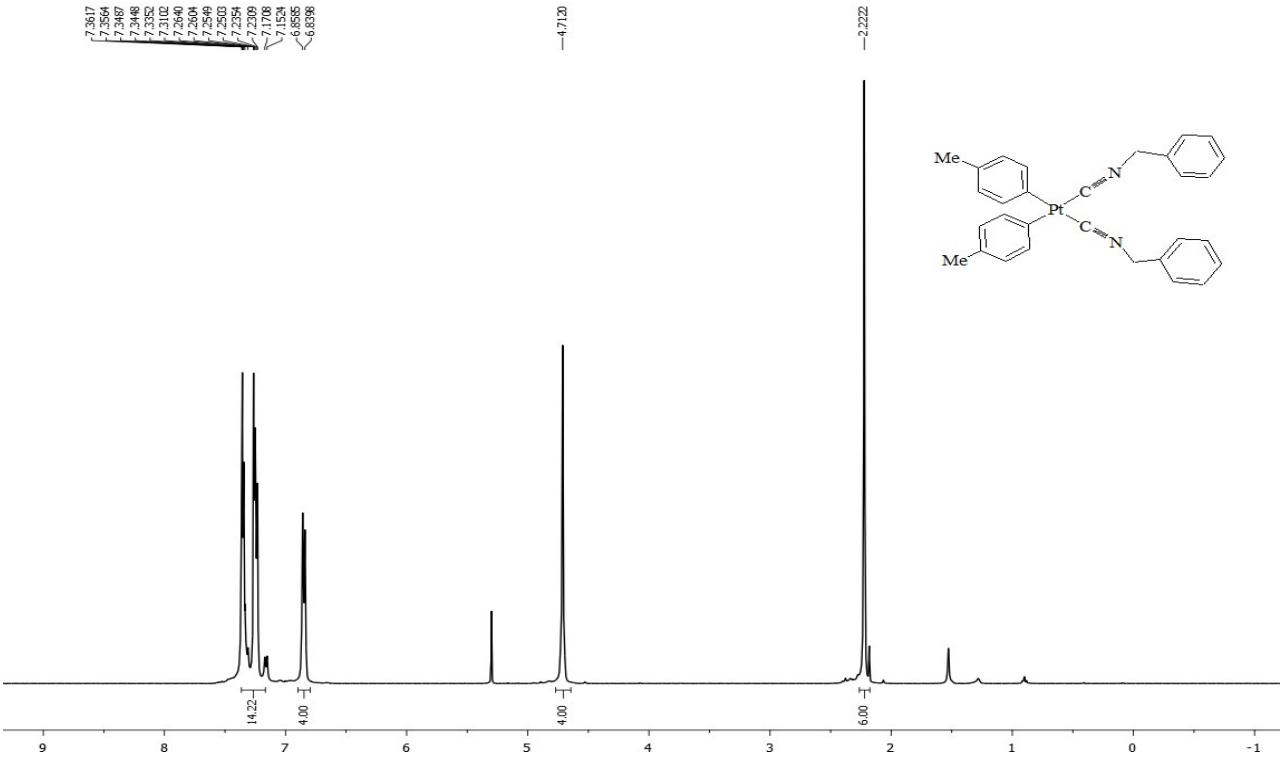

Figure S13. ^{1}H NMR spectrum of **2b** in $CDCl_3$ at room temperature.

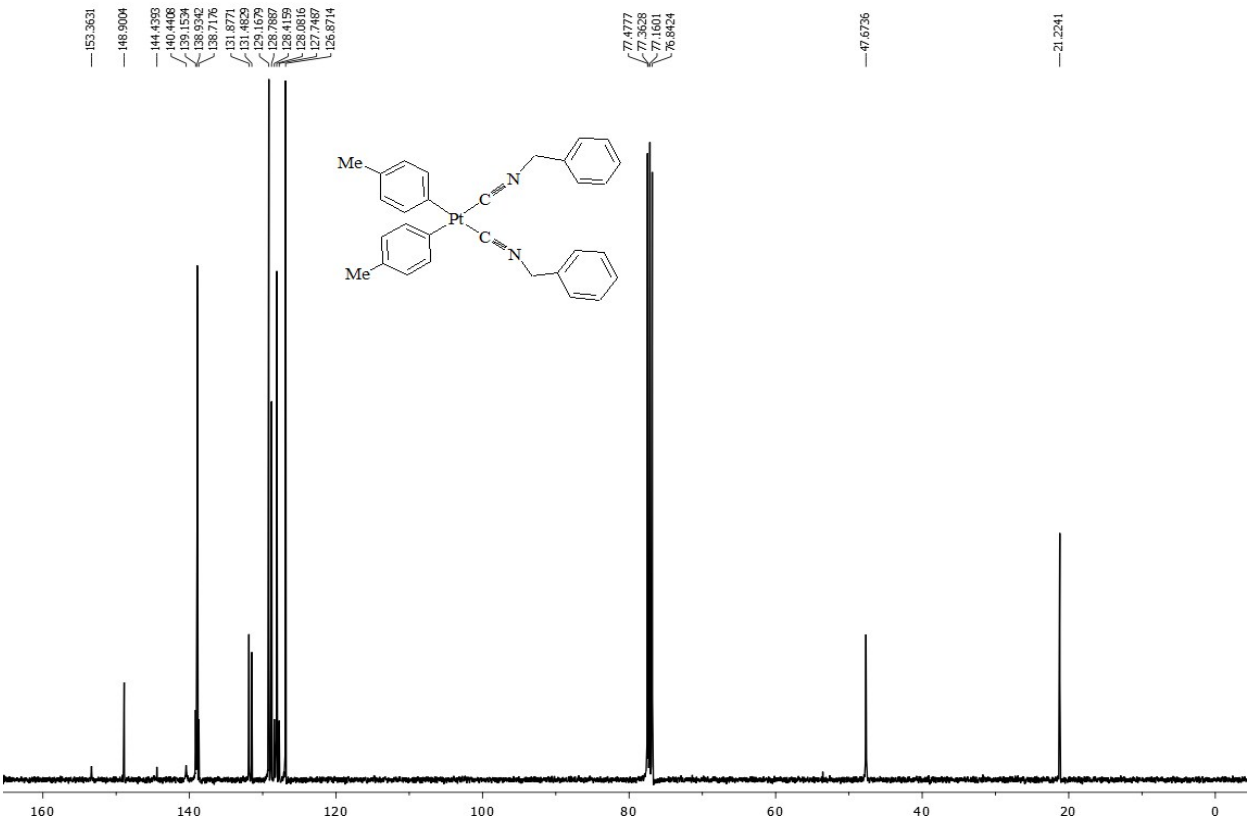

Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **2b** in $CDCl_3$ at room temperature.

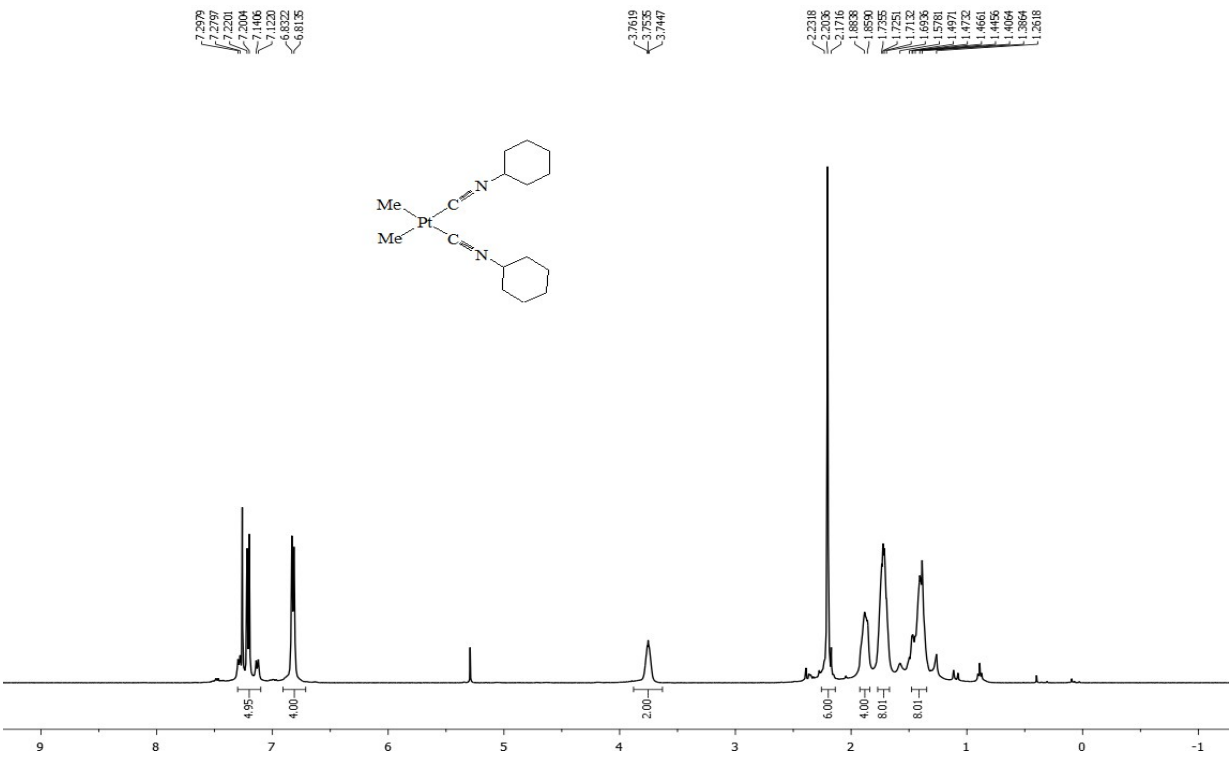

Figure S15. ^{1}H NMR spectrum of **2c** in $CDCl_3$ at room temperature.

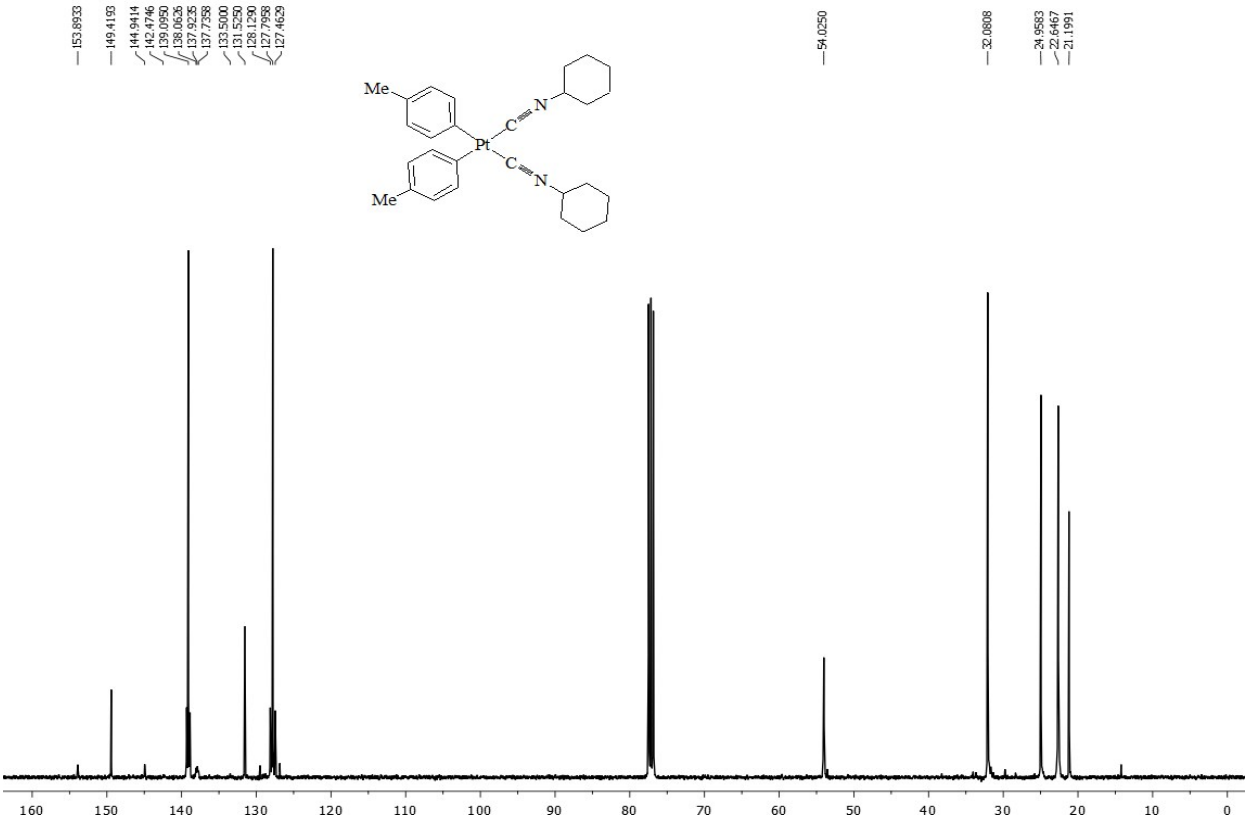

Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of **2c** in $CDCl_3$ at room temperature.

Table S1. Crystal data and structure refinements of **2b**.

Empirical formula	$C_{30}H_{28}N_2Pt$
Formula weight	611.63
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.994(2) Å, α= 94.44(3)°
	b = 10.991(2) Å, β= 111.73(3)°
	c = 13.402(3) Å, γ = 106.35(3)°
Volume	1284.7(6) $Å^3$
Z	2
Density (calculated)	1.581 Mg/m^3
Absorption coefficient	5.480 mm^{-1}
F(000)	600
Crystal size	0.500 x 0.450 x 0.400 mm^3
Theta range for data collection	1.671 to 24.993°.
Index ranges	-11<=h<=10
	-13<=k<=13
	-15<=l<=15
Reflections collected	9678
Independent reflections	4390 [R(int) = 0.1178]
Completeness to theta = 24.993°	97.1 %
Absorption correction	Integration
Max. and min. transmission	0.9882 and 0.977
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4390 / 294 / 298
Goodness-of-fit on F^2	1.012
Final R indices [I>2sigma(I)]	R1 = 0.0567, wR2 = 0.1255
R indices (all data)	R1 = 0.0684, wR2 = 0.1298
CCDC No.	1574855

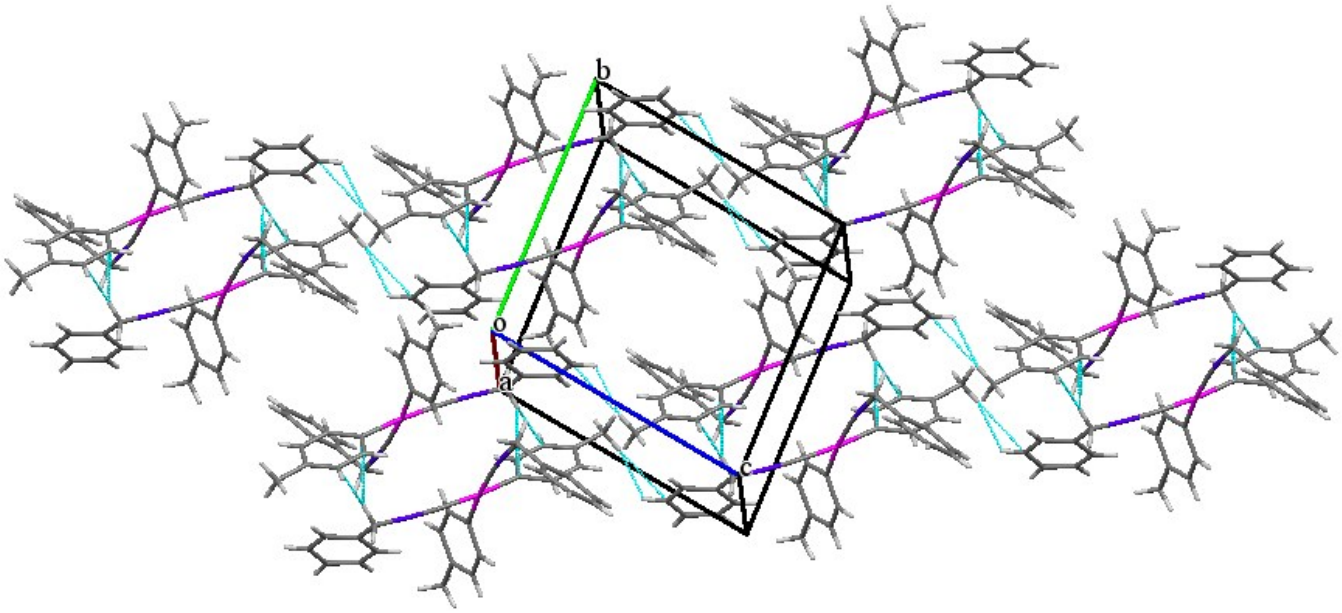

Figure S17. Packing diagram of **2b** showing CH···π interactions.

Table S2. Calculated chemical descriptors for the compounds.

Name	SA (ap) [1]	SA(Grid)[2]	Vol.[3]	HE[4]	LogP[5]	Ref[6]	Pol[7]	Mass	PIC_{50}-A549	PIC_{50}-SKOV3	PIC_{50}-MCF7
1a	716.34	578.48	906.76	4.8	1.49	57.39	25.17	391.43	4.583	4.539	4.597
1b	598.59	562.05	944.79	-1.04	1.85	87.29	33.48	459.46	4.669	4.799	4.903
1c	599.12	596.33	1007.63	4.49	2.99	71.81	30.96	443.5	4.294	4.350	4.165
2a	877.05	753.91	1296.6	3.16	2.78	115.13	44.49	543.62	4.717	4.732	4.955
2b	797.74	818.87	1399.36	-2.88	3.14	145.02	52.8	611.66	4.506	4.257	4.205
2c	759.84	796.64	1392.67	2.85	4.28	129.55	50.28	595.7	4.353	4.173	4.140

[1] Surface area (Approx)
[2] Surface area (Grid)
[3] Volume
[4] Hydration Energy
[5] Log partition coefficient
[6] Refractivity
[7] Polarizability
[8] PIC_{50}**:** -log IC_{50}

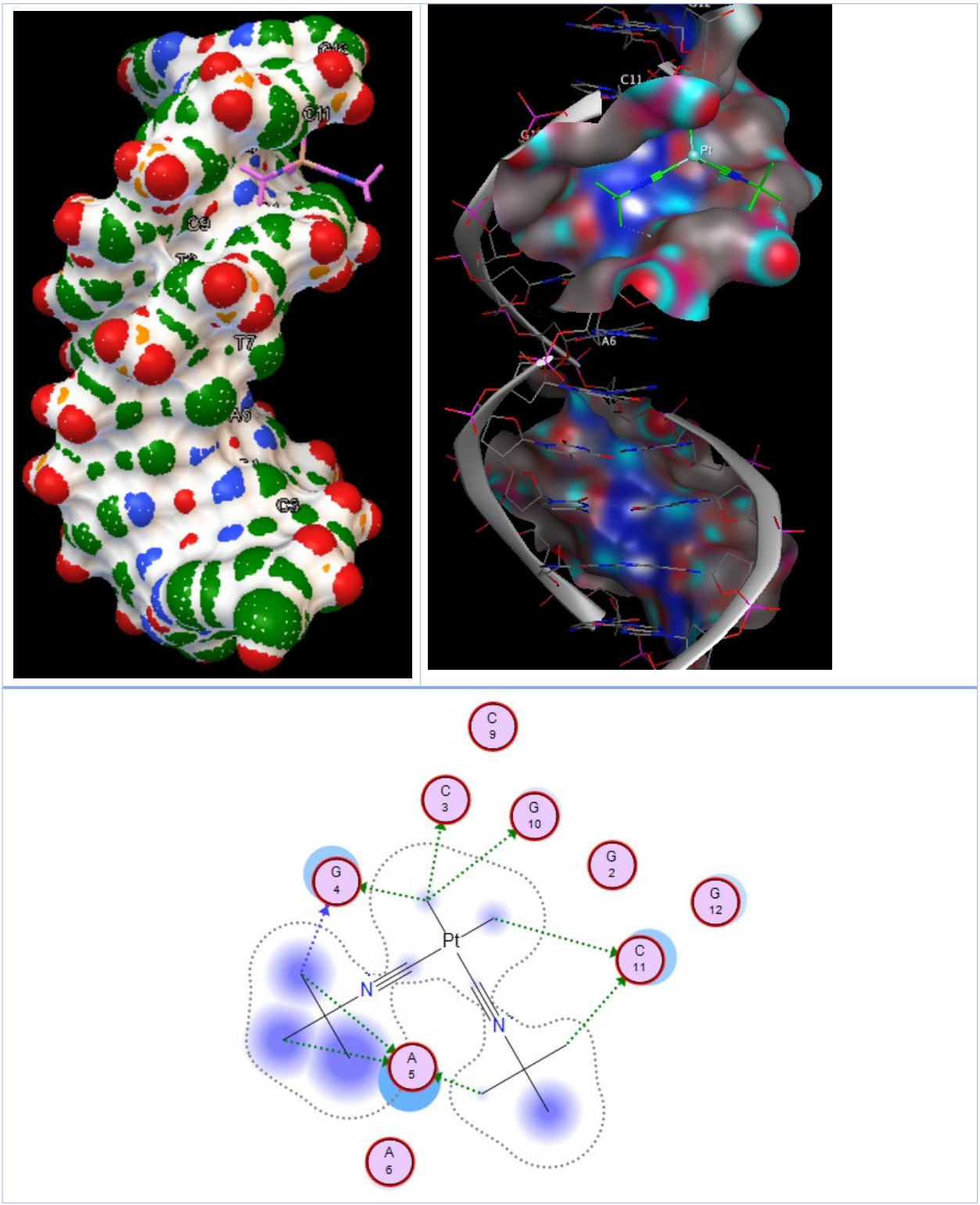

Figure S18. Molecular docking simulation studies of the interaction between **1a** and DNA (PDB ID: 1BNA).

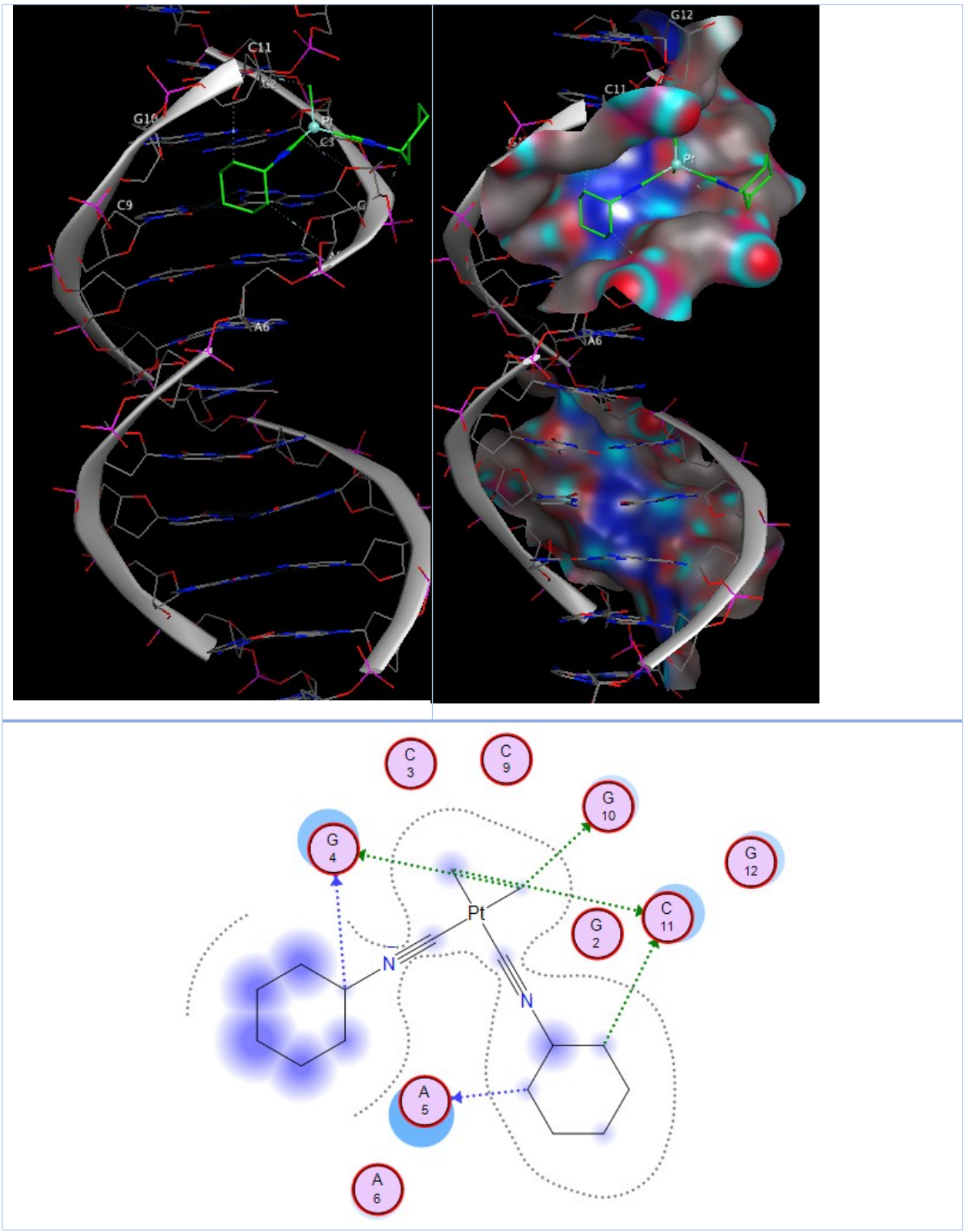

Figure S19. Molecular docking simulation studies of the interaction between **1c** and DNA (PDB ID: 1BNA).

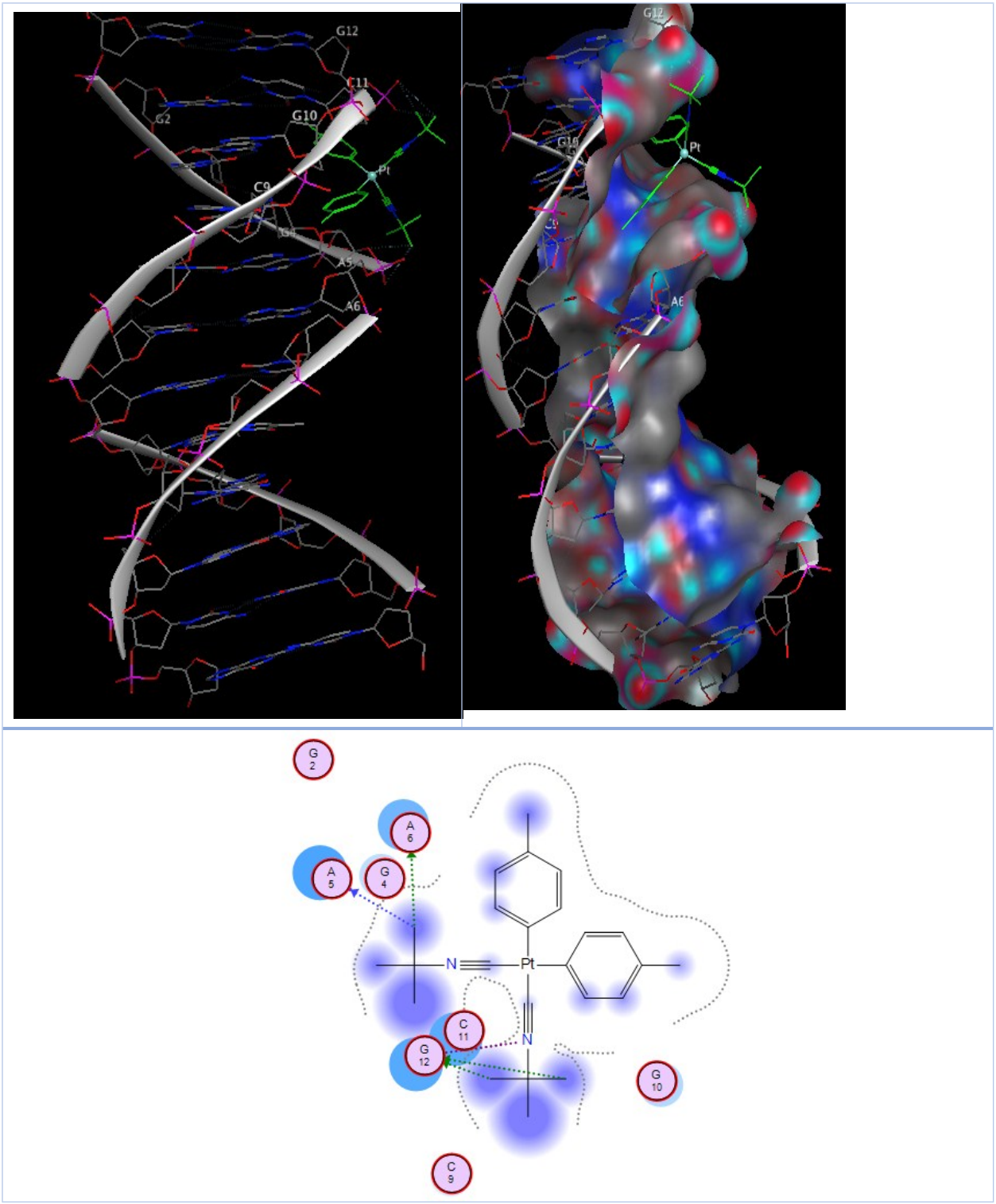

Figure S20. Molecular docking simulation studies of the interaction between **2a** and DNA (PDB ID: 1BNA).

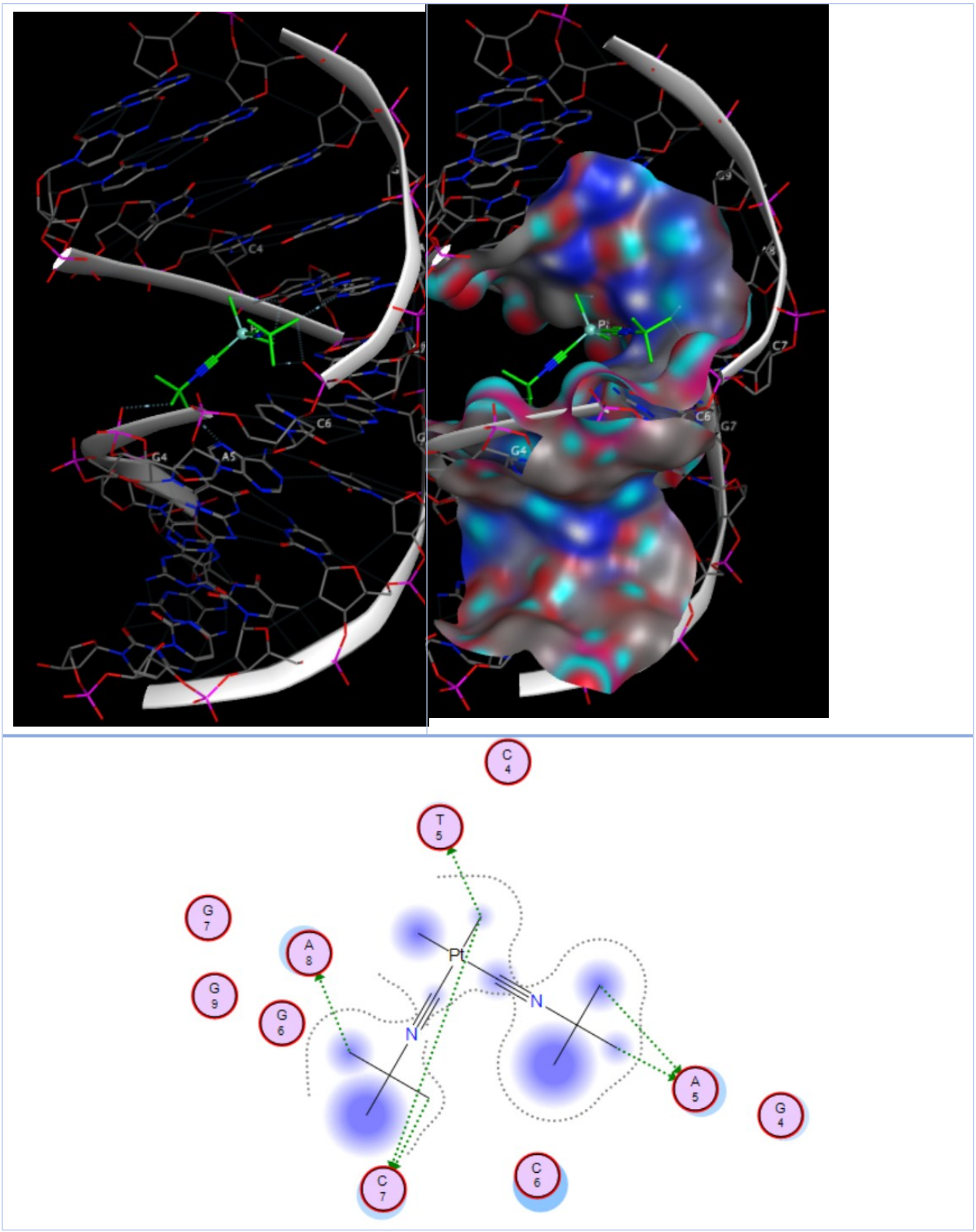

Figure S21. Molecular docking simulation studies of the interaction between **1a** and DNA (PDB ID: 1LU5).

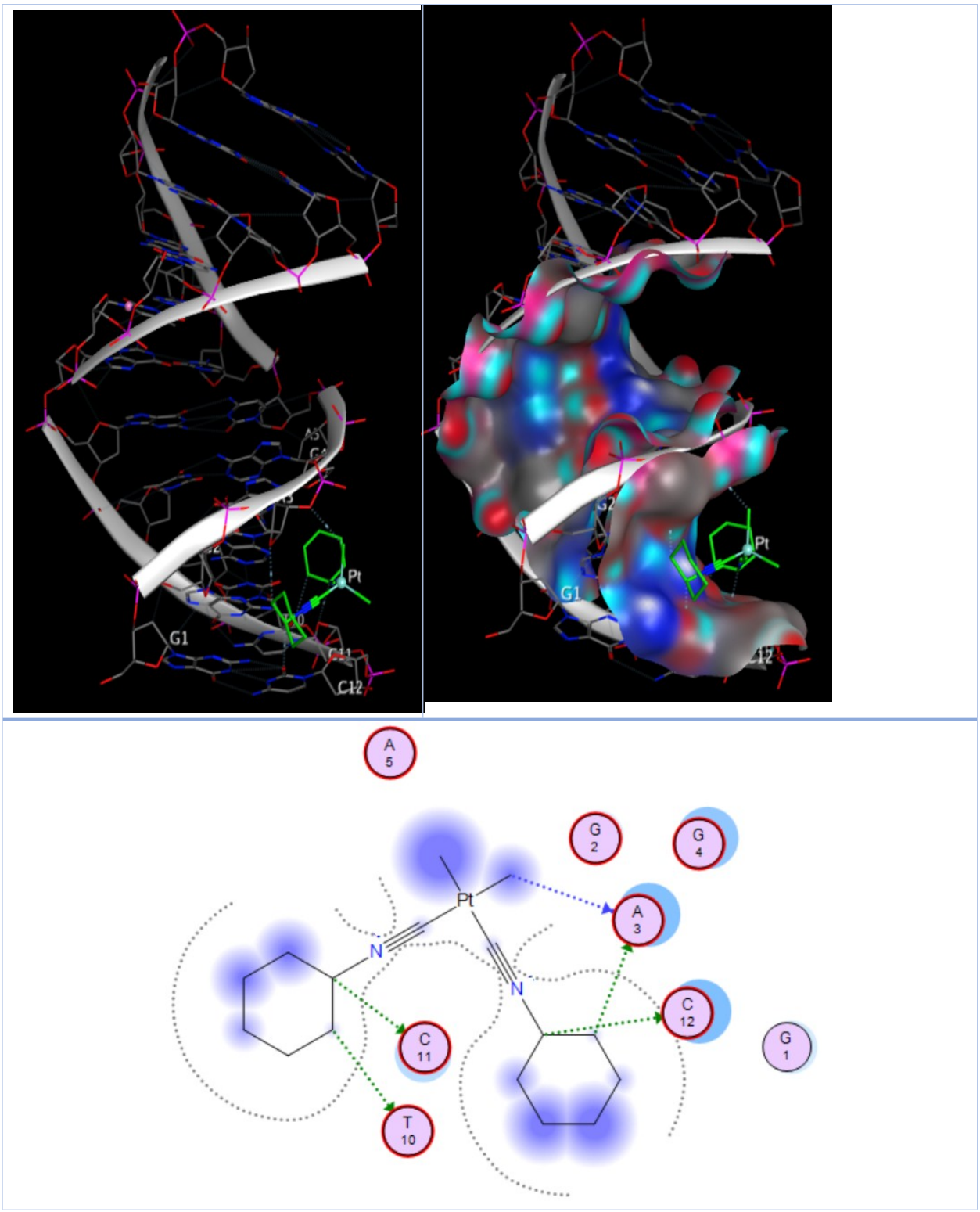

Figure S22. Molecular docking simulation studies of the interaction between **1c** and DNA (PDB ID: 1LU5).

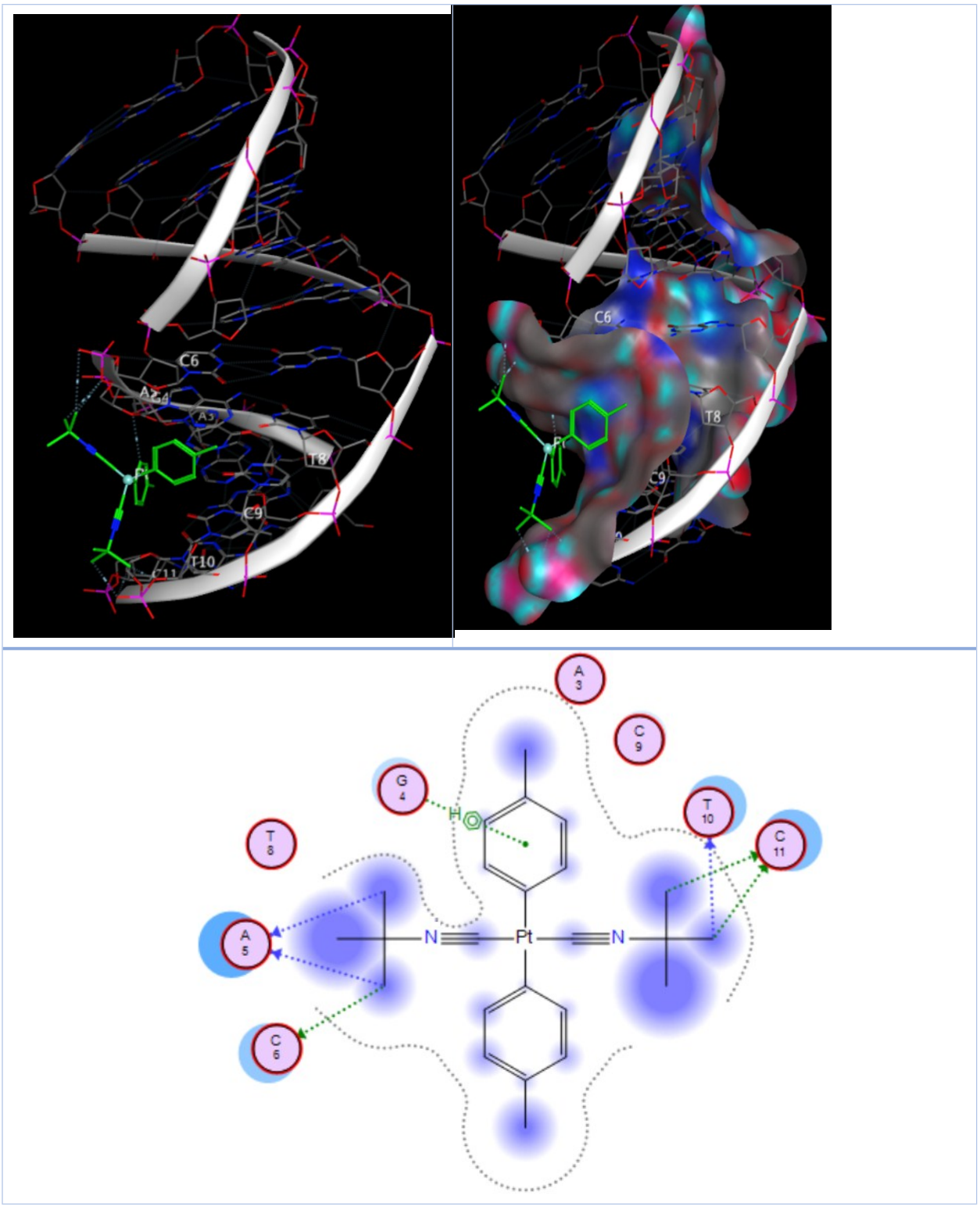

Figure S23. Molecular docking simulation studies of the interaction between **2a** and DNA (PDB ID: 1LU5).

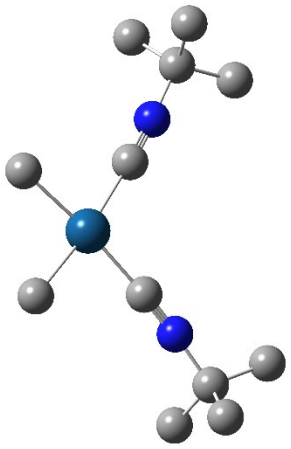

Figure S24. The optimized structures of **1a**. Hydrogen atoms were omitted for clarity.

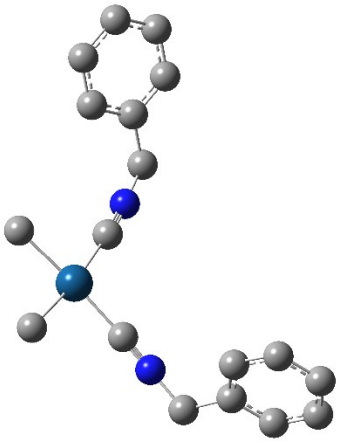

Figure S25. The optimized structures of **1b**. Hydrogen atoms were omitted for clarity.

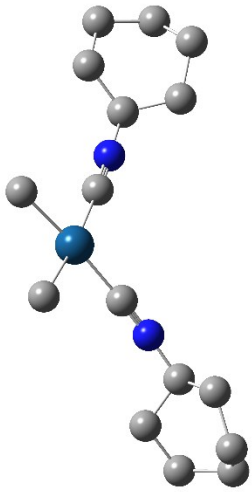

Figure S26. The optimized structures of **1c**. Hydrogen atoms were omitted for clarity.

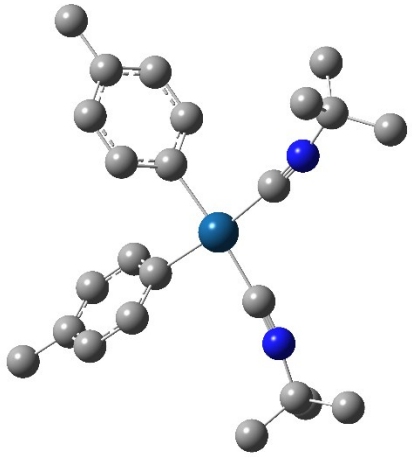

Figure S27. The optimized structures of **2a**. Hydrogen atoms were omitted for clarity.

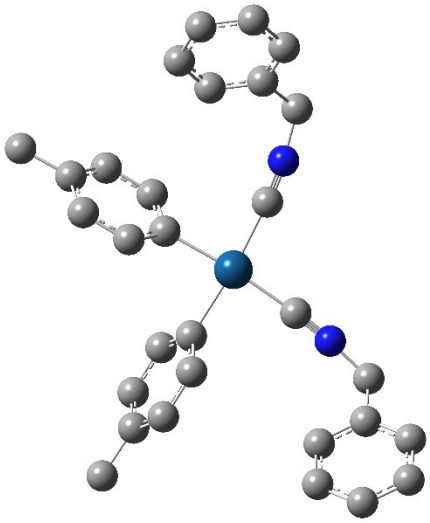

Figure S28. The optimized structures of **2b**. Hydrogen atoms were omitted for clarity.

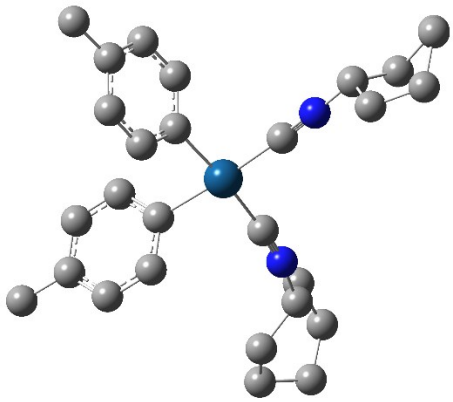

Figure S29. The optimized structures of **2c**. Hydrogen atoms were omitted for clarity.

Table S3. XYZ coordinates for **1a**.

Symbol	X	Y	Z
Pt	0.002723	1.144013	0.000089
C	1.513003	-0.160068	0.000367
C	-1.512977	-0.158562	0.00014
N	2.45213	-0.864551	0.000127
N	-2.45212	-0.862718	0.00012
C	-1.442045	2.678453	-0.00046
H	-2.088012	2.599438	-0.885299
H	-2.083765	2.603273	0.887818
H	-0.978571	3.668876	-0.003692
C	1.412656	2.705394	-0.000047
H	2.457759	2.374543	0.001769
H	1.253476	3.329729	-0.88752
H	1.251144	3.33216	0.885274
C	-3.649029	-1.666784	-0.000031
C	3.652488	-1.663347	-0.000103
C	-4.455659	-1.322363	1.266593
H	-5.37415	-1.918332	1.291466
H	-3.874311	-1.539741	2.168033
H	-4.726609	-0.262255	1.276276
C	-4.452592	-1.326448	-1.269703
H	-3.869056	-1.546709	-2.169028
H	-5.371012	-1.922513	-1.294891
H	-4.723538	-0.266383	-1.28345
C	-3.232808	-3.149625	0.002859
H	-2.640058	-3.384666	0.89253
H	-4.126056	-3.783031	0.002786
H	-2.637879	-3.387527	-0.884594
C	4.514237	-1.229411	-1.201243
H	4.778526	-0.170314	-1.125116
H	5.436647	-1.819377	-1.224928
H	3.976094	-1.385289	-2.141396
C	3.24604	-3.143634	-0.125
H	4.142204	-3.772917	-0.127746
H	2.612648	-3.444528	0.715497
H	2.696017	-3.317901	-1.05516
C	4.39505	-1.40999	1.325832
H	4.658713	-0.352697	1.425622

H	3.77228	-1.693827	2.179905
H	5.314897	-2.003819	1.351981

Table S4. XYZ coordinates for **1b**.

Symbol	**X**	**Y**	**Z**
Pt	0.048217	-1.636364	0.003884
C	-1.738013	-0.927226	0.527848
C	1.175285	-0.151663	0.722501
N	-2.819629	-0.56108	0.798576
N	1.908411	0.67458	1.117984
C	-4.152028	-0.131947	1.056089
H	-4.251569	0.0539	2.131617
H	-4.82001	-0.969896	0.814549
C	2.874098	1.618236	1.56914
H	3.233196	1.277737	2.550208
H	2.367743	2.576436	1.731713
C	-4.55409	1.109792	0.272122
C	-4.043038	1.370172	-1.003228
C	-5.498194	1.98186	0.825161
C	-4.473911	2.490512	-1.715666
H	-3.302127	0.703828	-1.43573
C	-5.93325	3.098174	0.109525
H	-5.894488	1.789984	1.820091
C	-5.420779	3.355424	-1.163392
H	-4.067075	2.68629	-2.703909
H	-6.664878	3.7697	0.55049
H	-5.753841	4.227287	-1.719629
C	4.043388	1.801156	0.610853
C	4.701055	3.035937	0.581755
C	4.504471	0.757141	-0.197127
C	5.812871	3.224889	-0.239997
H	4.342177	3.855139	1.201474
C	5.612789	0.949929	-1.02378
H	3.994157	-0.2017	-0.191911
C	6.270958	2.180995	-1.046043
H	6.313462	4.189178	-0.256617
H	5.959164	0.134391	-1.652494
H	7.132275	2.328025	-1.691815
C	1.836275	-2.541264	-0.650747

H	2.294313	-1.932181	-1.442292
H	2.560669	-2.626604	0.170446
H	1.658776	-3.542304	-1.053278
C	-0.903847	-3.316184	-0.830692
H	-1.998232	-3.2897	-0.779839
H	-0.611295	-3.408545	-1.883199
H	-0.559023	-4.214627	-0.304707

Table S5. XYZ coordinates for **1c**.

Symbol	**X**	**Y**	**Z**
Pt	0.00163	-1.455071	-0.033267
C	1.542122	-0.200191	0.181369
C	-1.476517	-0.117315	0.050092
N	2.491868	0.478564	0.302293
N	-2.396512	0.61071	0.08975
C	3.687326	1.252954	0.405847
C	4.936561	0.35427	0.386578
C	3.746698	2.313845	-0.726744
C	6.197984	1.188906	0.713961
H	4.815929	-0.46764	1.099235
C	5.199154	2.761024	-1.017783
H	3.296458	1.884909	-1.628344
C	6.082302	2.656592	0.233403
H	6.384898	1.171605	1.794429
H	5.627871	2.132246	-1.808981
H	5.650796	3.279595	1.029108
C	-3.578378	1.412079	0.119306
C	-4.280165	1.391851	-1.266076
C	-4.537265	0.949142	1.230815
C	-5.786746	1.725153	-1.150606
H	-3.772818	2.104319	-1.926488
C	-5.704641	1.954086	1.380896
H	-4.910251	-0.047724	0.966229
C	-6.070709	2.645625	0.044493
H	-6.134528	2.182273	-2.08382
H	-6.57647	1.419135	1.7752
H	-5.490162	3.571509	-0.070733
H	-6.36221	0.79809	-1.030037
H	-4.146202	0.399096	-1.708425

H	-7.12405	2.947913	0.054956
H	-5.446728	2.714786	2.12767
H	-3.991608	0.840963	2.173665
H	5.015327	-0.100285	-0.608468
H	7.064689	0.709616	0.244075
H	7.079221	3.066186	0.035
H	5.197537	3.785216	-1.407544
H	3.12597	3.170039	-0.438576
H	-3.25504	2.435885	0.347524
H	3.644051	1.762249	1.377376
C	-1.441892	-2.965999	-0.276835
H	-1.326325	-3.703556	0.526461
H	-2.478675	-2.610046	-0.267104
H	-1.265205	-3.477635	-1.230738
C	1.409362	-3.019534	-0.143671
H	2.128033	-2.840787	-0.954646
H	1.976723	-3.087575	0.794483
H	0.92696	-3.984703	-0.321272

Table S6. XYZ coordinates for **2a**.

Symbol	**X**	**Y**	**Z**
Pt	-0.000085	0.230922	-0.000047
C	-1.529486	1.527359	0.026117
C	1.529172	1.527558	-0.026291
N	-2.494331	2.190318	0.06268
N	2.493998	2.190544	-0.062789
C	-1.432968	-1.268767	-0.01688
C	-1.528697	-2.225348	1.010016
C	-2.378437	-1.369723	-1.05338
C	-2.513872	-3.214748	1.004986
H	-0.812911	-2.206833	1.827583
C	-3.356281	-2.370312	-1.069025
H	-2.357162	-0.656623	-1.87575
C	-3.444509	-3.311816	-0.038153
H	-2.554935	-3.932095	1.823948
H	-4.062297	-2.418129	-1.897637
C	1.433128	-1.26846	0.016972
C	1.529492	-2.224586	-1.010337
C	2.378083	-1.369701	1.053849

C	2.514804	-3.213804	-1.005294
H	0.814053	-2.205828	-1.828204
C	3.356116	-2.370157	1.069488
H	2.35627	-0.657007	1.876558
C	3.445011	-3.311146	0.038252
H	2.556336	-3.930812	-1.824535
H	4.061723	-2.418259	1.898427
C	-4.483643	-4.41015	-0.060298
H	-4.062096	-5.358512	-0.421637
H	-4.889785	-4.602211	0.940154
H	-5.321458	-4.156603	-0.719699
C	4.484506	-4.409147	0.060115
H	5.318305	-4.158976	0.725839
H	4.061288	-5.359778	0.413411
H	4.896657	-4.595278	-0.939031
C	3.794393	2.817152	-0.135568
C	-3.794692	2.816973	0.13563
C	-3.6288	4.316507	-0.167635
H	-4.605506	4.80925	-0.123567
H	-2.967351	4.791643	0.563842
H	-3.208822	4.467618	-1.167077
C	-4.698028	2.135649	-0.9101
H	-4.754597	1.058539	-0.726622
H	-5.706442	2.559095	-0.85443
H	-4.30919	2.294956	-1.920849
C	-4.34177	2.599166	1.559221
H	-3.679909	3.052387	2.303882
H	-5.330905	3.061172	1.645219
H	-4.433287	1.531246	1.778554
C	4.342114	2.598392	-1.558759
H	5.331293	3.060328	-1.644621
H	4.433714	1.530324	-1.777336
H	3.680596	3.051126	-2.304023
C	4.697254	2.136525	0.911032
H	4.753954	1.059301	0.728272
H	5.705679	2.559975	0.855568
H	4.307923	2.296467	1.92149
C	3.628365	4.316881	0.166648
H	2.967257	4.791557	-0.565438
H	3.207928	4.468634	1.165798
H	4.605094	4.809592	0.122711

Table S7. XYZ coordinates for **2b**.

Symbol	X	Y	Z
Pt	-0.0205	-0.060558	-0.555811
C	-1.630007	-1.209161	-0.889256
C	1.400751	-1.447879	-0.835838
N	-2.616869	-1.80208	-1.10107
N	2.299007	-2.188175	-0.960649
C	-3.884623	-2.404819	-1.362214
H	-3.718211	-3.461819	-1.595361
H	-4.28439	-1.932132	-2.269294
C	3.497946	-2.958514	-1.057474
H	3.900057	-2.802799	-2.067491
H	3.230456	-4.017503	-0.978183
C	-4.864623	-2.267337	-0.207236
C	-5.022823	-1.049743	0.465464
C	-5.655373	-3.362899	0.152848
C	-5.964945	-0.936585	1.487909
H	-4.403254	-0.194822	0.207243
C	-6.603337	-3.24468	1.171378
H	-5.531038	-4.313144	-0.361977
C	-6.758999	-2.030608	1.841273
H	-6.076698	0.010448	2.008413
H	-7.211382	-4.102728	1.44457
H	-7.491832	-1.937846	2.638121
C	4.5293	-2.591683	-0.000908
C	5.247986	-3.609324	0.634189
C	4.800433	-1.254062	0.311024
C	6.236717	-3.296134	1.569147
H	5.034794	-4.650403	0.401075
C	5.782096	-0.944527	1.252514
H	4.241357	-0.453121	-0.165645
C	6.503975	-1.962401	1.880892
H	6.78812	-4.094177	2.058825
H	5.976737	0.096305	1.494498
H	7.267184	-1.716879	2.614342
C	-1.329939	1.502147	-0.18168
C	-1.435614	2.611829	-1.038821
C	-2.168717	1.499136	0.946458
C	-2.330971	3.652955	-0.786309

H	-0.798826	2.673901	-1.917672
C	-3.056979	2.549243	1.208506
H	-2.133181	0.665163	1.645127
C	-3.156565	3.646113	0.346164
H	-2.383181	4.492507	-1.478579
H	-3.680392	2.514069	2.101569
C	1.515842	1.293325	-0.224222
C	1.66823	1.966681	1.000924
C	2.478978	1.568485	-1.212051
C	2.723348	2.852598	1.227788
H	0.943698	1.806028	1.794723
C	3.528665	2.467864	-0.992503
H	2.416579	1.075638	-2.180897
C	3.672274	3.126765	0.233824
H	2.806312	3.348079	2.19439
H	4.246795	2.659108	-1.789231
C	-4.096456	4.79477	0.635432
H	-3.562002	5.658548	1.05444
H	-4.601565	5.142488	-0.273876
H	-4.868094	4.508864	1.35902
C	4.786152	4.122717	0.466661
H	5.642353	3.92965	-0.189782
H	4.454503	5.151885	0.270554
H	5.142835	4.094315	1.503084

Table S8. XYZ coordinates for **2c**.

Symbol	**X**	**Y**	**Z**
Pt	0.087537	-0.265614	-0.011113
C	1.808522	0.76334	0.034708
C	-1.182831	1.286238	-0.090268
N	2.850627	1.296863	0.04221
N	-2.013237	2.111697	-0.118024
C	1.215943	-1.999716	0.113807
C	1.187973	-2.98635	-0.88883
C	2.060677	-2.247454	1.210052
C	1.962159	-4.144673	-0.802977
H	0.539625	-2.8557	-1.751224
C	2.823968	-3.415744	1.306583
H	2.129491	-1.518239	2.015529

C	2.791205	-4.386867	0.300694
H	1.91431	-4.880247	-1.605292
H	3.458687	-3.571499	2.178427
C	-1.591408	-1.480928	-0.09348
C	-1.910811	-2.387999	0.933256
C	-2.487643	-1.424767	-1.17628
C	-3.058932	-3.181	0.88469
H	-1.24421	-2.487961	1.785679
C	-3.630298	-2.230576	-1.23517
H	-2.295421	-0.741835	-2.002063
C	-3.939733	-3.12338	-0.203703
H	-3.270238	-3.86591	1.705225
H	-4.291081	-2.16272	-2.09894
C	3.597189	-5.661805	0.408553
H	2.974892	-6.508142	0.73129
H	4.041402	-5.941773	-0.554422
H	4.410318	-5.561589	1.136372
C	-5.160099	-4.013792	-0.270822
H	-5.898133	-3.629731	-0.984134
H	-4.900284	-5.032791	-0.589803
H	-5.650938	-4.100944	0.706101
C	4.156194	1.878203	0.016771
C	4.60161	2.138984	-1.447506
C	4.213186	3.169069	0.851714
C	5.691632	3.234586	-1.525875
H	4.961382	1.196915	-1.875462
C	5.678356	3.650896	0.983199
H	3.596345	3.927603	0.353867
C	6.540436	3.277156	-0.247658
H	6.322511	3.061778	-2.404828
H	5.676758	4.738332	1.121878
H	7.006936	2.294342	-0.094857
C	-3.170016	2.954201	-0.111137
C	-4.302931	2.306571	-0.955284
C	-3.638659	3.234047	1.32801
C	-5.699249	2.797764	-0.507181
H	-4.129353	2.543366	-2.011315
C	-4.764408	4.295447	1.323633
H	-3.991968	2.290223	1.760062
C	-5.641757	4.227274	0.048928

H	-6.395946	2.737122	-1.350727
H	-5.386083	4.145097	2.213858
H	-5.234543	4.895104	-0.72302
H	-6.095648	2.128169	0.266971
H	-4.232993	1.218202	-0.857255
H	-6.650052	4.596388	0.267966
H	-4.330244	5.298343	1.416894
H	-2.793324	3.565177	1.940121
H	3.724169	2.436897	-2.0316
H	5.221254	4.215653	-1.67353
H	7.365058	3.990369	-0.357685
H	6.128674	3.225511	1.887959
H	3.769652	2.997312	1.837835
H	-2.866546	3.904561	-0.567854
H	4.824264	1.138263	0.474955

Table S9. The participating atom in bonding on 1BNA.

Name	DNA bases	The participating atom in bonding	Type of Interactions
		Ligand	
1a	G4, A5, C11	CH_3 of *t*-Bu-NC	Vanderwaals
	G4, C3, G10, C11	CH_3 attached to Pt	Vanderwaals
1b	T7, T8	CH_3 attached to Pt	Vanderwaals
	G10, T7, T8	CH_2 of benzyl	Vanderwaals
1c	G10, C11	CH_3 attached to Pt	Vanderwaals
	G4, A5, C11	cyclohexyl-NC	Vanderwaals
2a	A6, A5, G12	CH_3 of *t*-Bu-NC	Vanderwaals
	G12	Nitrogen of *t*-Bu-NC	H.B
2b	G10, G12, C11	CH_2 of benzyl	Vanderwaals
	G12	phenyl of benzyl-NC	Vanderwaals
2c	G10, C11	Nitrogen of cyclohexyl-NC	H.B
	G10, C11	carbon of isocyanide	Vanderwaals
	G4	phenyl attached to Pt	Arene-hydrogen

Table S10. The participating atom in bonding on 1LU5.

Name	DNA bases	The participating atom in bonding	Type of Interactions
		Ligand	
1a	T5, C7	CH_3 attached to Pt	Vanderwaals
	A8, C7, A5	CH_3 of *t*-Bu-NC	Vanderwaals
1b	C11	CH_3 attached to Pt	Vanderwaals
	G4, G10, C9	CH_2 of benzyl	Vanderwaals
	G10	Nitrogen of benzyl-NC	H.B
1c	A3	CH_3 attached to Pt	Vanderwaals
	C11, T10, A3, C12	cyclohexyl-NC	Vanderwaals
2a	A5, C6, T10, C11	CH_3 of *t*-Bu-NC	Vanderwaals
	G4	phenyl attached to Pt	Arene-hydrogen
2b	G6	phenyl attached to Pt	Vanderwaals
	G2, G4, G6	CH_2 of benzyl	Vanderwaals
	G6	Nitrogen of benzyl-NC	H.B
2c	A5, G4, C11	Nitrogen of cyclohexyl-NC	H.B
	C11	carbon of isocyanide	Vanderwaals