

SUPPLEMENTARY INFORMATION

The reactivity properties of platinum-containing anticancer drugs

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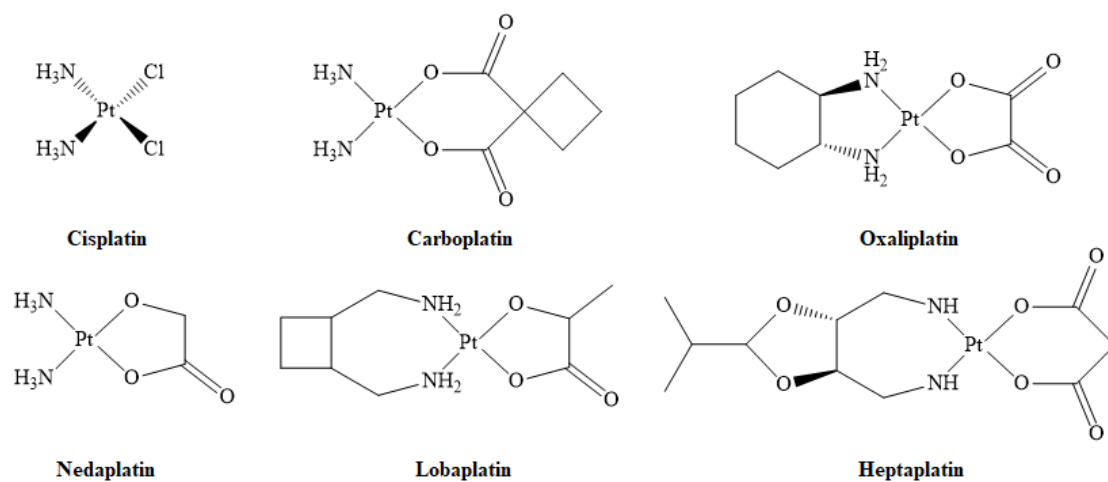


Fig. S1. Molecular structures of cisplatin and derivatives

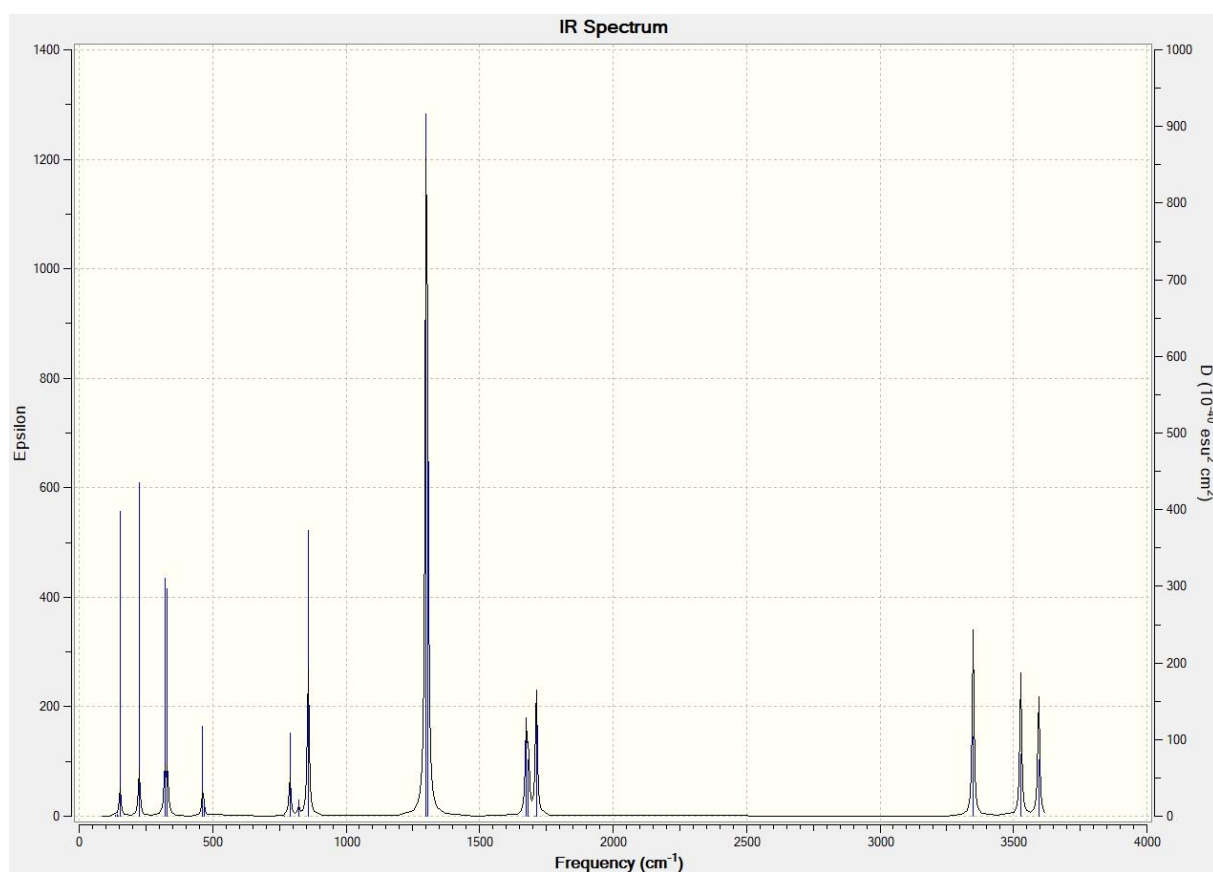


Fig. S2. Calculated IR spectrum of cisplatin

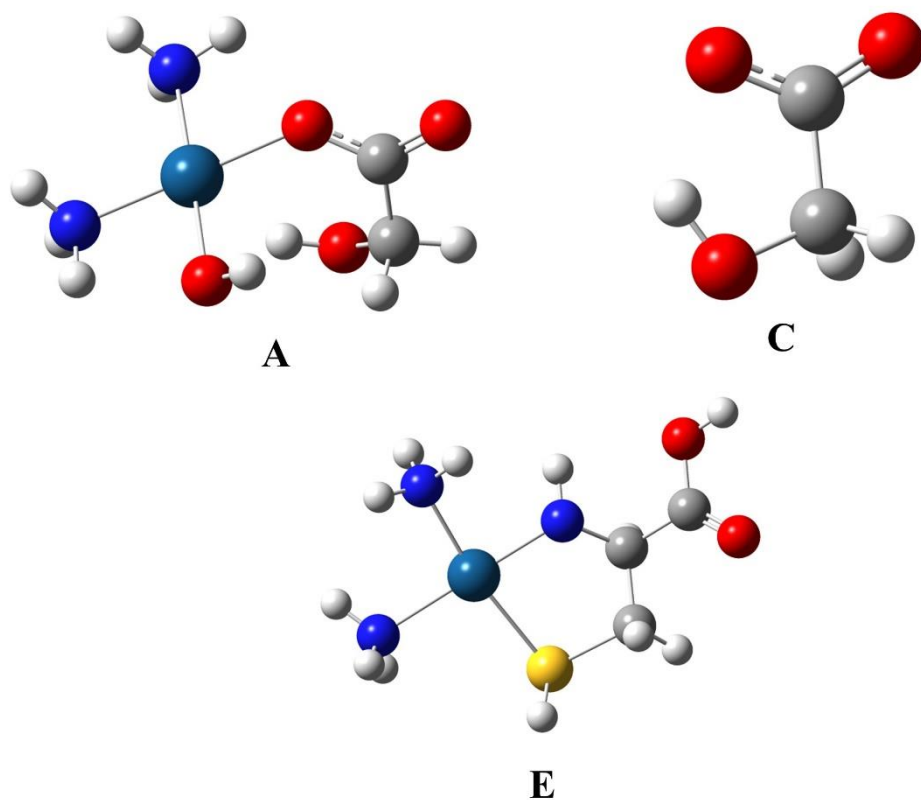


Fig. S3. Optimized geometries of reaction intermediates

Table S1. Comparison of the calculated geometric and IR data of cisplatin with the experimental ones

	Calculated	Experimental ^{1,2}
<i>Bond length (Å)</i>		
Pt-Cl	2.41	2.33
Pt-N	2.11	2.00
<i>Bond angle (°)</i>		
Cl-Pt-Cl	96.71	91.9
N-Pt-N	99.30	87.0
N-Pt-Cl	81.99	90.3
<i>IR vibrations (cm⁻¹)</i>		
ν_{NH_3}	3349	3285
δ_{NH_3}	1676	1625
$\nu_{\text{Pt-N}}$	467	519
$\nu_{\text{Pt-Cl}}$	321	324

Table S2. Fukui indices of cisplatin

		f ⁺	f ⁻	f ⁰
1	Pt	0.360	0.642	0.501
2	Cl	0.159	0.095	0.127
3	Cl	0.159	0.095	0.127
4	N	0.052	0.017	0.034
5	N	0.052	0.017	0.034

Table S3. Fukui indices of carboplatin

		f ⁺	f ⁻	f ⁰
1	Pt	0.418	0.482	0.450
2	N	0.046	0.016	0.031
6	N	0.046	0.015	0.031
10	O	0.008	0.036	0.022
11	O	0.008	0.040	0.024
12	C	0.067	0.050	0.059
13	C	0.073	0.054	0.064
14	O	0.047	0.059	0.053
15	O	0.046	0.056	0.051
16	C	0.006	0.006	0.006
19	C	0.015	0.015	0.015
22	C	0.015	0.013	0.014
25	C	-0.049	-0.051	-0.050

Table S4. Fukui indices of oxaliplatin

		f ⁺	f ⁻	f ⁰
1	Pt	0.170	0.489	0.330
2	O	0.059	0.043	0.051
3	O	0.059	0.043	0.051
4	C	0.179	0.050	0.115
5	C	0.179	0.050	0.115
6	O	0.140	0.067	0.104
7	O	0.140	0.067	0.104
8	N	-0.001	-0.021	-0.011
9	N	-0.001	-0.021	-0.011
14	C	0.000	0.011	0.005
15	C	0.001	0.002	0.001
16	C	0.000	-0.001	-0.001
17	C	0.000	-0.001	-0.001
18	C	0.001	0.002	0.001
19	C	0.000	0.011	0.005

Table S5. Fukui indices of lobaplatin

		f ⁺	f ⁻	f ⁰
1	Pt	0.440	0.418	0.429
2	O	0.034	0.175	0.105
3	O	0.015	0.018	0.016
4	C	0.062	0.049	0.055
5	O	0.045	0.041	0.043
6	C	0.014	-0.026	-0.006
7	C	0.016	0.021	0.019
12	N	-0.004	-0.011	-0.008
13	N	-0.013	-0.018	-0.016
18	C	0.016	0.008	0.012
19	C	0.016	0.007	0.012
20	C	-0.015	-0.012	-0.014
21	C	-0.015	-0.009	-0.012
22	C	0.010	0.005	0.008
23	C	0.011	0.007	0.009

Table S6. Fukui indices of heptaplatin

		f ⁺	f ⁻	f ⁰
1	Pt	0.394	0.446	0.420
2	O	0.008	0.048	0.028
3	O	0.006	0.038	0.022
4	C	0.062	0.047	0.054
5	C	0.061	0.045	0.053
6	O	0.048	0.064	0.056
7	O	0.049	0.071	0.060
8	N	-0.001	-0.019	-0.010
11	N	0.004	-0.017	-0.006
14	O	0.007	0.005	0.006
15	O	0.009	0.007	0.008
16	C	0.001	0.000	0.001
20	C	0.002	0.002	0.002
24	C	-0.002	-0.002	-0.002
27	C	-0.002	-0.001	-0.002
29	C	-0.001	-0.001	-0.001
31	C	-0.004	-0.003	-0.003
33	C	0.006	0.005	0.005
36	C	-0.016	-0.011	-0.014
38	C	0.022	0.012	0.017

Table S7. Energies of molecules

Molecules	Energies (Hartree)
Nedaplatin	-535.43
A	-611.87
B	-384.57
C	-303.81
D	-641.74
E	-565.30
Cysteine	-333.80
Water	-76.41

REFERENCES

1. G. H. W. Milburn, M. R. Truter, *J. Chem. Soc. A: Inorg. Phys. Theor.*, 1609 (1966), <https://doi.org/10.1039/J19660001609>
2. M. Malik, D. Michalska, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **125**, 431 (2014), <http://dx.doi.org/10.1016/j.saa.2014.01.107>