

**Discovery of Cisplatin Binding to Thymine and Cytosine on a
Single-stranded Oligodeoxynucleotide by High Resolution FT-ICR
Mass Spectrometry**

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Table S1. Full MS peak assignments of ODN15 for Figure 1a. Red-highlighted species were used for the internal calibration.

5' HO-CCTTCTTGCTTCTCC-OH 3' (ODN15, C₁₄₃H₁₈₈N₄₀O₉₅P₁₄)	Observed m/z	Exact m/z	Mass error/ ppm
[ODN15 – 3H] ³⁻	1472.24136	1472.241555	-0.13
[ODN15 – 4H] ⁴⁻	1103.92967	1103.929347	0.29
[ODN15 – 5H] ⁵⁻	882.94202	882.942022	0.00
[ODN15 – 6H] ⁶⁻	735.61733	735.617139	0.26

Table S2. Full MS peak assignments of the reaction mixture of ODN15 with cisplatin for Figure 1b. Red-highlighted species were used for the internal calibration.

	Observed m/z	Exact m/z	Mass error/ ppm
[ODN15 + 2Pt(NH ₃) ₂ – 7H] ³⁻	1623.90939	1623.910057	-0.41
[ODN15 + 1Pt(NH ₃) ₂ – 5H] ³⁻	1548.24333	1548.242972	0.23
[ODN15 – 3H] ³⁻	1472.24262	1472.241555	0.72
[ODN15 + 2Pt(NH ₃) ₂ – 8H] ⁴⁻	1217.68075	1217.680724	0.02
[ODN15 + 1Pt(NH ₃) ₂ – 6H] ⁴⁻	1160.92891	1160.930410	-1.29
[ODN15 – 4H] ⁴⁻	1103.93047	1103.929347	1.02
[ODN15 + 2Pt(NH ₃) ₂ – 9H] ⁵⁻	973.94292	973.943124	-0.21
[ODN15 + 1Pt(NH ₃) ₂ – 7H] ⁵⁻	928.54282	928.542873	-0.06
[ODN15 – 5H] ⁵⁻	882.94279	882.942022	0.87
[ODN15 + 1Pt(NH ₃) ₂ – 8H] ⁶⁻	773.61994	773.617848	2.70
[ODN15 – 6H] ⁶⁻	735.61969	735.617139	3.46

Table S3. CID MS/MS fragments assignment of [ODN15 – 5H]⁵⁻ for Figure S1a. Red-highlighted species were used for the internal calibration.

Fragment	Observed m/z	Exact m/z	Mass error/ ppm	Chemical formula of neutral fragment
[w1] ⁻	306.04966	306.049660	0.00	C ₉ H ₁₄ N ₃ O ₇ P
[w2] ⁻	595.09650	595.096032	0.79	C ₁₈ H ₂₆ N ₆ O ₁₃ P ₂
[w3] ⁻	899.14180	899.142069	-0.30	C ₂₈ H ₃₉ N ₈ O ₂₀ P ₃
[w3] ²⁻	449.06751	449.067397	0.25	C ₂₈ H ₃₉ N ₈ O ₂₀ P ₃
[w4] ⁻	1188.18895	1188.18844	0.43	C ₃₇ H ₅₁ N ₁₁ O ₂₆ P ₄
[w4] ²⁻	593.59108	593.590583	0.84	C ₃₇ H ₅₁ N ₁₁ O ₂₆ P ₄
[w5] ²⁻	745.61421	745.613601	0.82	C ₄₇ H ₆₄ N ₁₃ O ₃₃ P ₅
[w6] ²⁻	897.63694	897.636620	0.36	C ₅₇ H ₇₇ N ₁₅ O ₄₀ P ₆
[w6] ³⁻	598.08880	598.088654	0.24	C ₅₇ H ₇₇ N ₁₅ O ₄₀ P ₆
[w7] ²⁻	1042.15903	1042.15981	-0.74	C ₆₆ H ₈₉ N ₁₈ O ₄₆ P ₇
[w7] ³⁻	694.43766	694.437445	0.31	C ₆₆ H ₈₉ N ₁₈ O ₄₆ P ₇
[w8] ³⁻	804.12195	804.121618	0.41	C ₇₆ H ₁₀₁ N ₂₃ O ₅₂ P ₈
[w9] ⁴⁻	678.85154	678.850904	0.94	C ₈₆ H ₁₁₄ N ₂₅ O ₅₉ P ₉

[w9] ³⁻	905.46996	905.470297	-0.37	C86H114N25O59P9
[w10] ⁴⁻	754.86246	754.862413	0.06	C96H127N27O66P10
[w11] ⁴⁻	827.12432	827.124006	0.38	C105H139N30O72P11
[w12] ⁴⁻	903.13541	903.135516	-0.12	C115H152N32O79P12
[w13] ⁴⁻	979.14746	979.147025	0.44	C125H165N34O86P13
[w13] ⁵⁻	783.11687	783.116165	0.90	C125H165N34O86P13
[a2 – C5] ⁻	386.07598	386.075875	0.27	C14H18N3O8P
[a3 – T3] ⁻	675.12276	675.122247	0.76	C23H30N6O14P2
[a4] ⁻	1105.21176	1105.211210	0.50	C38H49N10O23P3
[a5 – C5] ⁻	1283.21464	1283.214320	0.25	C43H56N10O28P4
[a5 – C5] ²⁻	641.10360	641.103523	0.12	C43H56N10O28P4
[a5] ⁻	1394.25907	1394.257580	1.07	C47H61N13O29P4
[a6] ²⁻	848.64911	848.648172	1.10	C57H74N15O36P5
[a7 – T7] ²⁻	937.64974	937.649727	0.01	C62H81N15O41P6
[a8 – G8] ³⁻	726.11292	726.112739	0.25	C72H94N17O48P7
[a8 – G8] ²⁻	1089.67270	1089.672750	-0.04	C72H94N17O48P7
[a8] ²⁻	1165.19639	1165.197450	-0.91	C77H99N22O49P7
[a9 – C9] ³⁻	835.79744	835.796912	0.63	C82H106N22O54P8
[a9 – C9] ²⁻	1254.19810	1254.199010	-0.72	C82H106N22O54P8
[a12 – C12] ³⁻	1134.84408	1134.843060	0.90	C111H144N29O74P11
[a12 – C12] ⁴⁻	850.88101	850.880476	0.63	C111H144N29O74P11
[a14 – C12] ⁴⁻	999.15333	999.153579	-0.25	C130H169N34O87P13
[T3: T4 or T6: T7 or T10: T11] ⁻	785.08769	785.087908	-0.28	C25H33N4O19P3
[T6: G8] ²⁻	556.56698	556.566576	0.72	C35H45N9O25P4
[T6: G8] ⁻	1114.14052	1114.140430	0.08	C35H45N9O25P4
[C2: T7] ³⁻	656.41951	656.419391	0.18	C63H83N14O45P7
[C2: T7] ²⁻	985.13319	985.132725	0.47	C63H83N14O45P7
[T3: T7] ²⁻	840.60936	840.609540	-0.21	C54H71N11O39P6
[T3: T7] ⁻	1682.22732	1682.226360	0.57	C54H71N11O39P6
[C2: T6 or C9: T13 or T10: C14] ²⁻	833.10982	833.109707	0.14	C53H70N12O38P6
[C2: T6 or C9: T13 or T10: C14] ⁻	1667.22835	1667.226690	1.00	C53H70N12O38P6

Table S4. CID MS/MS fragments assignment of [ODN15 + Pt(NH₃)₂ – 7H]⁵⁻ for Figure 3. Red-highlighted species were used for the internal calibration.

Fragment	Observed m/z	Exact m/z	Mass error/ ppm	Chemical formula of neutral fragment
[w7 + Pt] ³⁻	759.08848	759.087344	1.49	C66H87N18O46P7Pt
[w7 + Pt(NH ₃)] ³⁻	764.76398	764.762859	1.46	C66H90N19O46P7Pt
[w7 + Pt(NH ₃) ₂] ³⁻	770.43957	770.4383743	1.55	C66H93N20O46P7Pt

[w7 + Pt] ²⁻	1139.1367	1139.134654	1.79	C66H87N18O46P7Pt
[w7 + Pt(NH ₃) ₂] ²⁻	1147.64902	1147.647927	0.95	C66H90N19O46P7Pt
[w7 + Pt(NH ₃) ₂] ²⁻	1156.16248	1156.1612	1.11	C66H93N20O46P7Pt
[a8 – G8 + Pt] ³⁻	790.76357	790.7634657	0.13	C72H92N17O48P7Pt
[a8 – G8 + Pt(NH ₃) ₂] ³⁻	796.43932	796.438981	0.43	C72H95N18O48P7Pt
[a8 – G8 + Pt(NH ₃) ₂] ³⁻	802.11504	802.1144963	0.68	C72H98N19O48P7Pt
[a8 – G8 + Pt] ²⁻	1186.64877	1186.648837	-0.06	C72H92N17O48P7Pt
[a8 – G8 + Pt(NH ₃) ₂] ²⁻	1195.16194	1195.16211	-0.14	C72H95N18O48P7Pt
[a8 – G8 + Pt(NH ₃) ₂] ²⁻	1203.67438	1203.675383	-0.83	C72H98N19O48P7Pt
[w10 + Pt] ⁴⁻	803.35116	803.350266	1.11	C96H125N27O66P10Pt
[w10 + Pt(NH ₃) ₂] ⁴⁻	807.60749	807.6069	0.73	C96H128N28O66P10Pt
[w10 + Pt(NH ₃) ₂] ⁴⁻	811.8643	811.863534	0.94	C96H131N29O66P10Pt
[w10 + Pt] ³⁻	1071.46945	1071.469447	0.00	C96H125N27O66P10Pt
[w10 + Pt(NH ₃) ₂] ³⁻	1077.14567	1077.144959	0.66	C96H128N28O66P10Pt
[w10 + Pt(NH ₃) ₂] ³⁻	1082.82142	1082.820471	0.88	C96H131N29O66P10Pt
[w13 + Pt(NH ₃) ₂] ⁵⁻	825.31257	825.311805	0.93	C125H166N35O86P13Pt
[w13 + Pt(NH ₃) ₂] ⁵⁻	828.71791	828.7171124	0.96	C125H169N36O86P13Pt
[w13 + Pt] ⁴⁻	1027.63449	1027.634941	-0.44	C125H163N34O86P13Pt
[w13 + Pt(NH ₃) ₂] ⁴⁻	1031.89221	1031.891575	0.61	C125H166N35O86P13Pt
[w13 + Pt(NH ₃) ₂] ⁴⁻	1036.1491	1036.14821	0.86	C125H169N36O86P13Pt
[a8 + Pt] ³⁻	840.77967	840.77904	0.75	C77H97N22O49P7Pt
[a8 + Pt(NH ₃) ₂] ³⁻	846.78947	846.7887857	0.81	C77H100N23O49P7Pt
[a8 + Pt(NH ₃) ₂] ³⁻	852.46488	852.464301	0.68	C77H103N24O49P7Pt
[a8 + Pt(NH ₃) ₂] ²⁻	1270.68536	1270.686817	-1.15	C77H100N23O49P7Pt
[a8 + Pt(NH ₃) ₂] ²⁻	1279.19885	1279.20009	-0.97	C77H103N24O49P7Pt
[w14 + Pt] ⁵⁻	879.71657	879.7157826	0.89	C134H175N37O92P14Pt
[w14 + Pt(NH ₃) ₂] ⁵⁻	883.12161	883.1210902	0.59	C134H178N38O92P14Pt
[w14 + Pt(NH ₃) ₂] ⁵⁻	886.52753	886.5263976	1.28	C134H181N39O92P14Pt
[ODN15 + Pt(NH ₃) – G8] ⁵⁻	894.72829	894.7272292	1.18	C138H184N36O94P14Pt
[ODN15 + Pt – C] ⁵⁻	899.32379	899.323148	0.71	C139H181N37O94P14Pt
[ODN15 + Pt(NH ₃) – C] ⁵⁻	902.72903	902.7284556	0.64	C139H184N38O94P14Pt
[ODN15 + Pt(NH ₃) ₂ – C] ⁵⁻	906.13434	906.1337632	0.64	C139H187N39O94P14Pt
[ODN15 + Pt] ⁵⁻	921.73289	921.7322602	0.68	C143H186N40O95P14Pt
[ODN15 + Pt(NH ₃) ₂] ⁵⁻	925.13772	925.1375664	0.17	C143H189N41O95P14Pt
[ODN15 + Pt(NH ₃) ₂] ⁵⁻	928.54361	928.5428726	0.79	C143H192N42O95P14Pt
[a9 – C9 + Pt(NH ₃) ₂] ³⁻	906.12358	906.1231627	0.46	C82H107N23O54P8Pt
[a9 – C9 + Pt(NH ₃) ₂] ³⁻	911.79942	911.7986783	0.81	C82H110N24O54P8Pt
[a9 – C9 + Pt] ²⁻	1351.17528	1351.175109	0.13	C82H104N22O54P8Pt
[a9 – C9 + Pt(NH ₃) ₂] ²⁻	1359.68805	1359.688382	-0.24	C82H107N23O54P8Pt
[a9 – C9 + Pt(NH ₃) ₂] ²⁻	1368.20063	1368.201656	-0.75	C82H110N24O54P8Pt
[a9 + Pt] ³⁻	937.46244	937.46207	0.39	C86H109N25O55P8Pt
[a9 + Pt(NH ₃) ₂] ³⁻	943.13757	943.1375857	-0.02	C86H112N26O55P8Pt
[a9 + Pt(NH ₃) ₂] ³⁻	948.81376	948.813101	0.69	C86H115N27O55P8Pt

[w6 + Pt] ²⁻	994.61317	994.611457	1.72	C57H75N15O40P6Pt
[w6 + Pt(NH ₃)] ²⁻	1003.12584	1003.12473	1.11	C57H78N16O40P6Pt
[a14 - C14 + Pt] ⁴⁻	1047.64331	1047.641507	1.72	C130H167N34O87P13Pt
[a14 - C14 + Pt(NH ₃)] ⁴⁻	1051.89936	1051.898142	1.16	C130H170N35O87P13Pt
[a14 - C14 + Pt(NH ₃) ₂] ⁴⁻	1056.15637	1056.154776	1.51	C130H173N36O87P13Pt
[a12 - C12 + Pt] ³⁻	1199.49403	1199.493584	0.37	C111H142N29O74P11Pt
[a12 - C12 + Pt(NH ₃)] ³⁻	1205.16828	1205.169097	-0.68	C111H145N30O74P11Pt
[a12 - C12 + Pt(NH ₃) ₂] ³⁻	1210.84412	1210.844609	-0.40	C111H148N31O74P11Pt
[a12 - C12 + Pt(NH ₃) ₂] ⁴⁻	903.62564	903.6250035	0.70	C111H145N30O74P11Pt
[a12 - C12 + Pt(NH ₃) ₂] ⁴⁻	907.88211	907.8816375	0.52	C111H148N31O74P11Pt
[T6: G8 + Pt(NH ₃)] ⁻	1324.1156	1324.116325	-0.55	C35H46N10O25P4Pt
[T6: G8 + Pt(NH ₃) ₂] ⁻	1341.14373	1341.142861	0.65	C35H49N11O25P4Pt
[a5 - C5 + Pt] ⁻	1476.16467	1476.16373	0.64	C43H54N10O28P4Pt
[a5 - C5 + Pt(NH ₃)] ⁻	1493.19076	1493.190267	0.33	C43H57N11O28P4Pt
[a5 - C5 + Pt(NH ₃) ₂] ⁻	1510.21711	1510.216804	0.20	C43H60N12O28P4Pt
[a5 + Pt] ⁻	1587.20856	1587.206982	0.99	C47H59N13O29P4Pt
[a5 + Pt(NH ₃)] ⁻	1604.23226	1604.23352	-0.78	C47H62N14O29P4Pt
[w14 - C + Pt(NH ₃)] ⁵⁻	860.91327	860.9124374	0.97	C130H173N35O91P14Pt
[w14 - C + Pt(NH ₃) ₂] ⁵⁻	864.31809	864.3177448	0.40	C130H176N36O91P14Pt
[a9 - C9 - C + Pt] ²⁻	1295.6523	1295.653475	-0.91	C78H99N19O53P8Pt
[a9 - C9 - C + Pt(NH ₃)] ²⁻	1304.16614	1304.166748	-0.47	C78H102N20O53P8Pt
[a9 - C9 - C + Pt(NH ₃) ₂] ²⁻	1312.67988	1312.680022	-0.11	C78H105N21O53P8Pt
[C2: G8 + Pt(NH ₃)] ³⁻	836.43043	836.4298067	0.74	C73H96N20O51P8Pt
[C2: G8 + Pt] ²⁻	1246.63411	1246.635075	-0.77	C73H93N19O51P8Pt
[C2: G8 + Pt(NH ₃) ₂] ²⁻	1255.14711	1255.148348	-0.99	C73H96N20O51P8Pt
[C2: G8 + Pt(NH ₃) ₂] ²⁻	1263.66057	1263.661622	-0.83	C73H99N21O51P8Pt
[C2: T7 + Pt] ²⁻	1082.10928	1082.107576	1.57	C63H81N14O45P7Pt
[C2: T7 + Pt(NH ₃)] ²⁻	1090.62237	1090.620849	1.39	C63H84N15O45P7Pt
[C2: T7 + Pt(NH ₃) ₂] ²⁻	1099.13529	1099.134122	1.06	C63H87N16O45P7Pt
[T3: G8 + Pt] ²⁻	1102.11104	1102.110648	0.36	C64H81N16O45P7Pt
[T3: G8 + Pt(NH ₃)] ²⁻	1110.62522	1110.623921	1.17	C64H84N17O45P7Pt
[T3: G8 + Pt(NH ₃) ₂] ²⁻	1119.13879	1119.137193	1.43	C64H87N18O45P7Pt
[C2: T11 + Pt] ³⁻	1129.80041	1129.800215	0.17	C102H131N26O71P11Pt
[C2: T11 + Pt(NH ₃)] ³⁻	1135.47679	1135.475727	0.94	C102H134N27O71P11Pt
[w2] ⁻	595.09644	595.096032	0.68	C18H26N6O13P2
[w3] ⁻	899.14198	899.142069	-0.10	C28H39N8O20P3
[w3] ²⁻	449.0674	449.0673965	0.01	C28H39N8O20P3
[w4] ⁻	1188.19246	1188.188441	3.38	C37H51N11O26P4
[w4] ²⁻	593.59109	593.5905825	0.85	C37H51N11O26P4
[w5] ²⁻	745.61429	745.613601	0.92	C47H64N13O33P5
[w6] ²⁻	897.63717	897.6366195	0.61	C57H77N15O40P6
[w6] ³⁻	598.0888	598.0886543	0.24	C57H77N15O40P6
[w7] ²⁻	1042.15992	1042.159806	0.11	C66H89N18O46P7

[w7] ³⁻	694.43799	694.437445	0.78	C66H89N18O46P7
[w8] ³⁻	804.12222	804.1216183	0.75	C76H101N23O52P8
[w10] ⁴⁻	754.86278	754.8624133	0.49	C96H127N27O66P10
[a3 – T3] ⁻	675.12285	675.122247	0.89	C23H30N6O14P2
[a5 – C5] ⁻	1283.21455	1283.214321	0.18	C43H56N10O28P4
[a5 – C5] ²⁻	641.10372	641.1035225	0.31	C43H56N10O28P4
[a7 – T7] ²⁻	937.65014	937.649727	0.44	C62H81N15O41P6
[a8 – G8] ³⁻	726.11321	726.1127387	0.65	C72H94N17O48P7
[a8 – G8] ²⁻	1089.67292	1089.672746	0.16	C72H94N17O48P7
[a9 – C9] ³⁻	835.79775	835.7969117	1.00	C82H106N22O54P8
[a9 – C9] ²⁻	1254.19796	1254.199006	-0.83	C82H106N22O54P8
[a12 – C12] ⁴⁻	850.88123	850.8804763	0.88	C111H144N29O74P11
[T3: T4 or T6: T7 or T10: T11] ⁻	785.08774	785.087908	-0.21	C25H33N4O19P3
[C2: T6] ²⁻	833.11013	833.1097065	0.51	C53H70N12O38P6
[T3: T7] ²⁻	840.60979	840.6095395	0.30	C54H71N11O39P6
[a6] ²⁻	848.64886	848.648172	0.81	C57H74N15O36P5
[y6] ²⁻	857.65402	857.6534545	0.66	C57H76N15O37P5
[C2: T7] ³⁻	656.41981	656.4193913	0.64	C63H83N14O45P7
[C2: T7] ²⁻	985.13372	985.132725	1.01	C63H83N14O45P7
[y7] ²⁻	1002.17713	1002.176641	0.49	C66H88N18O43P6
[a4] ⁻	1105.21191	1105.211211	0.63	C38H49N10O23P3
[C2: T4 or C9: T11 or T11: T13] ⁻	1074.13391	1074.13428	-0.34	C34H45N7O25P4
[C2: T4 or C9: T11 or T11: T13] ²⁻	536.56389	536.563502	0.72	C34H45N7O25P4
[T3: T6 or T4: T7 or T10: T13] ²⁻	688.58713	688.5865205	0.88	C44H58N9O32P5
[T3: T6 or T4: T7 or T10: T13] ⁻	1378.17878	1378.180317	-1.11	C44H58N9O32P5
[a5] ⁻	1394.25756	1394.257583	-0.02	C47H61N13O29P4
[y3] ⁻	819.1764	819.175739	0.81	C28H38N8O17P2

Table S5. CID MS/MS fragments assignment of [ODN15 + 2Pt(NH₃)₂ – 9H]⁵⁻ for Figure 5. Red-highlighted species were used for the internal calibration.

Fragment	Observed m/z	Exact m/z	Mass error/ppm	Chemical formula of neutral fragment
[w6 + Pt] ³⁻	662.73951	662.738546	1.45	C57H75N15O40P6Pt
[w6 + Pt(NH ₃)] ³⁻	668.41467	668.4140613	0.91	C57H78N16O40P6Pt
[w6 + Pt] ²⁻	994.61232	994.611457	0.87	C57H75N15O40P6Pt
[w6 + Pt(NH ₃)] ²⁻	1003.1251	1003.12473	0.37	C57H78N16O40P6Pt

$[\text{w7} + \text{Pt}]^{3-}$	759.08836	759.087344	1.34	C66H87N18O46P7Pt
$[\text{w7} + \text{Pt}(\text{NH}_3)]^{3-}$	764.76361	764.762859	0.98	C66H90N19O46P7Pt
$[\text{w7} + \text{Pt}(\text{NH}_3)_2]^{3-}$	770.43911	770.4383743	0.95	C66H93N20O46P7Pt
$[\text{w7} + \text{Pt}]^{2-}$	1139.13496	1139.134654	0.27	C66H87N18O46P7Pt
$[\text{w7} + \text{Pt}(\text{NH}_3)]^{2-}$	1147.64834	1147.647927	0.36	C66H90N19O46P7Pt
$[\text{w7} + \text{Pt}(\text{NH}_3)_2]^{2-}$	1156.16167	1156.161200	0.41	C66H93N20O46P7Pt
$[\text{a8} - \text{G8} + \text{Pt}]^{3-}$	790.76328	790.7634657	-0.23	C72H92N17O48P7Pt
$[\text{a8} - \text{G8} + \text{Pt}(\text{NH}_3)]^{3-}$	796.43894	796.438981	-0.05	C72H95N18O48P7Pt
$[\text{a8} - \text{G8} + \text{Pt}(\text{NH}_3)_2]^{3-}$	802.11458	802.1144963	0.10	C72H98N19O48P7Pt
$[\text{a8} - \text{G8} + \text{Pt}]^{2-}$	1186.64828	1186.648837	-0.47	C72H92N17O48P7Pt
$[\text{a8} - \text{G8} + \text{Pt}(\text{NH}_3)]^{2-}$	1195.16139	1195.16211	-0.60	C72H95N18O48P7Pt
$[\text{a8} - \text{G8} + \text{Pt}(\text{NH}_3)_2]^{2-}$	1203.67385	1203.675383	-1.27	C72H98N19O48P7Pt
$[\text{w10} + \text{Pt}]^{4-}$	803.35077	803.350266	0.63	C96H125N27O66P10Pt
$[\text{w10} + \text{Pt}(\text{NH}_3)]^{4-}$	807.60724	807.6069	0.42	C96H128N28O66P10Pt
$[\text{w10} + \text{Pt}(\text{NH}_3)_2]^{4-}$	811.86409	811.863534	0.68	C96H131N29O66P10Pt
$[\text{a8} + \text{Pt}(\text{NH}_3)]^{3-}$	846.78905	846.7887857	0.31	C77H100N23O49P7Pt
$[\text{a8} + \text{Pt}(\text{NH}_3)_2]^{3-}$	852.46456	852.464301	0.30	C77H103N24O49P7Pt
$[\text{a8} + \text{Pt}(\text{NH}_3)]^{2-}$	1270.68533	1270.686817	-1.17	C77H100N23O49P7Pt
$[\text{a8} + \text{Pt}(\text{NH}_3)_2]^{2-}$	1279.19838	1279.20009	-1.34	C77H103N24O49P7Pt
$[\text{a5} - \text{C5} + \text{Pt}]^{2-}$	737.57866	737.578227	0.59	C43H54N10O28P4Pt
$[\text{a5} - \text{C5} + \text{Pt}]^{-}$	1476.16366	1476.16373	-0.05	C43H54N10O28P4Pt
$[\text{a5} - \text{C5} + \text{Pt}(\text{NH}_3)]^{-}$	1493.1902	1493.190267	-0.04	C43H57N11O28P4Pt
$[\text{a5} + \text{Pt}]^{-}$	1587.20792	1587.206982	0.59	C47H59N13O29P4Pt
$[\text{a5} + \text{Pt}(\text{NH}_3)]^{-}$	1604.23204	1604.23352	-0.92	C47H62N14O29P4Pt
$[\text{C2: G8} + \text{Pt}(\text{NH}_3)]^{3-}$	836.42961	836.4298067	-0.23	C73H96N20O51P8Pt
$[\text{C2: T7} + \text{Pt}]^{2-}$	1082.10797	1082.107576	0.36	C63H81N14O45P7Pt
$[\text{C2: T7} + \text{Pt}(\text{NH}_3)]^{2-}$	1090.6218	1090.620849	0.87	C63H84N15O45P7Pt
$[\text{C2: T7} + \text{Pt}(\text{NH}_3)_2]^{2-}$	1099.13378	1099.134122	-0.31	C63H87N16O45P7Pt
$[\text{T3: G8} + \text{Pt}]^{2-}$	1102.11075	1102.110648	0.09	C64H81N16O45P7Pt
$[\text{T3: G8} + \text{Pt}(\text{NH}_3)]^{2-}$	1110.62419	1110.623921	0.24	C64H84N17O45P7Pt
$[\text{T3: G8} + \text{Pt}(\text{NH}_3)_2]^{2-}$	1119.1376	1119.137193	0.36	C64H87N18O45P7Pt
$[\text{w14} + 2\text{Pt}(\text{NH}_3)_2 - 4\text{NH}_3]^{5-}$	918.50657	918.5058694	0.76	C134H173N37O92P14Pt2
$[\text{w14} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{5-}$	921.91135	921.9111762	0.19	C134H176N38O92P14Pt2
$[\text{w14} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{5-}$	925.31668	925.3164828	0.21	C134H179N39O92P14Pt2
$[\text{w14} + 2\text{Pt}(\text{NH}_3)_2 - 1\text{NH}_3]^{5-}$	928.72235	928.7217894	0.60	C134H182N40O92P14Pt2
$[\text{a12} - \text{C12} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{4-}$	951.86229	951.8621293	0.17	C111H143N30O74P11Pt2
$[\text{a12} - \text{C12} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{4-}$	956.1192	956.118763	0.46	C111H146N31O74P11Pt2
$[\text{ODN15} + 2\text{Pt}(\text{NH}_3)_2 - \text{G8} - 3\text{NH}_3]^{5-}$	933.51768	933.5173226	0.38	C138H182N36O94P14Pt2
$[\text{ODN15} + 2\text{Pt}(\text{NH}_3)_2 - \text{G8} - 2\text{NH}_3]^{5-}$	936.92253	936.9226292	-0.11	C138H185N37O94P14Pt2

$[\text{ODN15} + 2\text{Pt}(\text{NH}_3)_2 - 4\text{NH}_3]^{5-}$	960.32223	960.3218964	0.35	C143H184N40O95P14Pt2
$[\text{ODN15} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{5-}$	963.72756	963.7272032	0.37	C143H187N41O95P14Pt2
$[\text{ODN15} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{5-}$	967.13273	967.13251	0.23	C143H190N42O95P14Pt2
$[\text{ODN15} + 2\text{Pt}(\text{NH}_3)_2 - 1\text{NH}_3]^{5-}$	970.53788	970.5378168	0.07	C143H193N43O95P14Pt2
$[\text{ODN15} + 2\text{Pt}(\text{NH}_3)_2]^{5-}$	973.94306	973.9431236	-0.07	C143H196N44O95P14Pt2
$[\text{w13} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{4-}$	1080.12812	1080.128708	-0.54	C125H164N35O86P13Pt2
$[\text{w13} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{4-}$	1084.38475	1084.385342	-0.55	C125H167N36O86P13Pt2
$[\text{w13} + 2\text{Pt}(\text{NH}_3)_2 - 1\text{NH}_3]^{4-}$	1088.64156	1088.641977	-0.38	C125H170N37O86P13Pt2
$[\text{a14} - \text{C14} + 2\text{Pt}(\text{NH}_3)_2 - 4\text{NH}_3]^{4-}$	1096.12968	1096.129111	0.52	C130H165N34O87P13Pt2
$[\text{a14} - \text{C14} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{4-}$	1100.38611	1100.385745	0.33	C130H168N35O87P13Pt2
$[\text{a14} - \text{C14} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{4-}$	1104.6428	1104.642378	0.38	C130H171N36O87P13Pt2
$[\text{w10} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{3-}$	1141.46129	1141.461118	0.15	C96H126N28O66P10Pt2
$[\text{w10} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{3-}$	1147.13523	1147.13663	-1.22	C96H129N29O66P10Pt2
$[\text{w10} + 2\text{Pt}(\text{NH}_3)_2 - 1\text{NH}_3]^{3-}$	1152.81224	1152.812141	0.09	C96H132N30O66P10Pt2
$[\text{w7} + 2\text{Pt}(\text{NH}_3)_2 - 4\text{NH}_3]^{2-}$	1235.10838	1235.108645	-0.21	C66H85N18O46P7Pt2
$[\text{w7} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{2-}$	1244.12297	1244.122978	-0.01	C66H88N19O46P7Pt2
$[\text{w7} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{2-}$	1252.63603	1252.636251	-0.18	C66H91N20O46P7Pt2
$[\text{a8} - \text{G8} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{2-}$	1291.63534	1291.635929	-0.46	C72H93N18O48P7Pt2
$[\text{a8} - \text{G8} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{2-}$	1300.14868	1300.149202	-0.40	C72H96N19O48P7Pt2
$[\text{a8} - \text{G8} + 2\text{Pt}(\text{NH}_3)_2 - 1\text{NH}_3]^{2-}$	1308.66248	1308.662379	0.08	C72H99N20O48P7Pt2
$[\text{a8} + 2\text{Pt}(\text{NH}_3)_2 - 4\text{NH}_3]^{2-}$	1358.6462	1358.647279	-0.79	C77H95N22O49P7Pt2
$[\text{a8} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{2-}$	1367.15929	1367.160546	-0.92	C77H98N23O49P7Pt2
$[\text{a8} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{2-}$	1375.67363	1375.673813	-0.13	C77H101N24O49P7Pt2
$[\text{a8} + 2\text{Pt}(\text{NH}_3)_2 - 1\text{NH}_3]^{2-}$	1384.18703	1384.18708	-0.04	C77H104N25O49P7Pt2
$[\text{a9} - \text{C9} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{2-}$	1456.15984	1456.162144	-1.58	C82H105N23O54P8Pt2
$[\text{a9} - \text{C9} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{2-}$	1464.67562	1464.675411	0.14	C82H108N24O54P8Pt2
$[\text{a9} - \text{C9} + 2\text{Pt}(\text{NH}_3)_2 - 1\text{NH}_3]^{2-}$	1473.18718	1473.188678	-1.02	C82H111N25O54P8Pt2
$[\text{a9} - \text{C9} + 2\text{Pt}(\text{NH}_3)_2]^{2-}$	1481.70272	1481.701945	0.52	C82H114N26O54P8Pt2
$[\text{a9} + 2\text{Pt}(\text{NH}_3)_2 - 3\text{NH}_3]^{2-}$	1511.68401	1511.683781	0.15	C86H110N26O55P8Pt2
$[\text{a9} + 2\text{Pt}(\text{NH}_3)_2 - 2\text{NH}_3]^{2-}$	1520.1961	1520.197049	-0.62	C86H113N27O55P8Pt2
$[\text{a9} + 2\text{Pt}(\text{NH}_3)_2 - 1\text{NH}_3]^{2-}$	1528.71202	1528.710316	1.11	C86H116N28O55P8Pt2
$[\text{w2}]^-$	595.09621	595.096032	0.30	C18H26N6O13P2
$[\text{w3}]^-$	899.14205	899.142069	-0.02	C28H39N8O20P3
$[\text{w3}]^{2-}$	449.0674	449.0673965	0.01	C28H39N8O20P3
$[\text{w4}]^-$	1188.18859	1188.188441	0.13	C37H51N11O26P4
$[\text{w4}]^{2-}$	593.59076	593.5905825	0.30	C37H51N11O26P4
$[\text{w5}]^{2-}$	745.61388	745.613601	0.37	C47H64N13O33P5
$[\text{w6}]^{2-}$	897.63696	897.6366195	0.38	C57H77N15O40P6
$[\text{w6}]^{3-}$	598.0888	598.0886543	0.24	C57H77N15O40P6
$[\text{w7}]^{2-}$	1042.15936	1042.159806	-0.43	C66H89N18O46P7

[w7] ³⁻	694.43773	694.437445	0.41	C66H89N18O46P7
[a3 – T3] ⁻	675.12248	675.122247	0.34	C23H30N6O14P2
[a5 – C5] ⁻	1283.21407	1283.214321	-0.20	C43H56N10O28P4
[a5 – C5] ²⁻	641.10364	641.1035225	0.18	C43H56N10O28P4
[a7 – T7] ²⁻	937.6497	937.649727	-0.03	C62H81N15O41P6
[a8 – G8] ³⁻	726.11289	726.1127387	0.21	C72H94N17O48P7
[a8 – G8] ²⁻	1089.67257	1089.672746	-0.16	C72H94N17O48P7
[a9 – C9] ³⁻	835.79738	835.7969117	0.56	C82H106N22O54P8
[a9 – C9] ²⁻	1254.19822	1254.199006	-0.63	C82H106N22O54P8
[C2: T7] ³⁻	656.41958	656.4193913	0.29	C63H83N14O45P7
[C2: T7] ²⁻	985.13306	985.132725	0.34	C63H83N14O45P7
[T3: T4 or T6: T7 or T10: T11] ¹⁻	785.08781	785.087908	-0.12	C25H33N4O19P3
[C2: T6] ²⁻	833.10995	833.1097065	0.29	C53H70N12O38P6
[T3: T7] ²⁻	840.60968	840.6095395	0.17	C54H71N11O39P6
[a6] ²⁻	848.64849	848.648172	0.37	C57H74N15O36P5
[y6] ²⁻	857.65376	857.6534545	0.36	C57H76N15O37P5
[y7] ²⁻	1002.17666	1002.176641	0.02	C66H88N18O43P6
[a4] ⁻	1105.21124	1105.211211	0.03	C38H49N10O23P3
[C2: T4 or C9: T11 or T11: T13] ⁻	1074.13396	1074.13428	-0.30	C34H45N7O25P4
[C2: T4 or C9: T11 or T11: T13] ²⁻	536.56367	536.563502	0.31	C34H45N7O25P4
[T3: T6 or T4: T7 or T10: T13] ²⁻	688.5868	688.5865205	0.41	C44H58N9O32P5
[T3: T6 or T4: T7 or T10: T13] ⁻	1378.17846	1378.180317	-1.35	C44H58N9O32P5
[y3] ⁻	819.17601	819.175739	0.33	C28H38N8O17P2

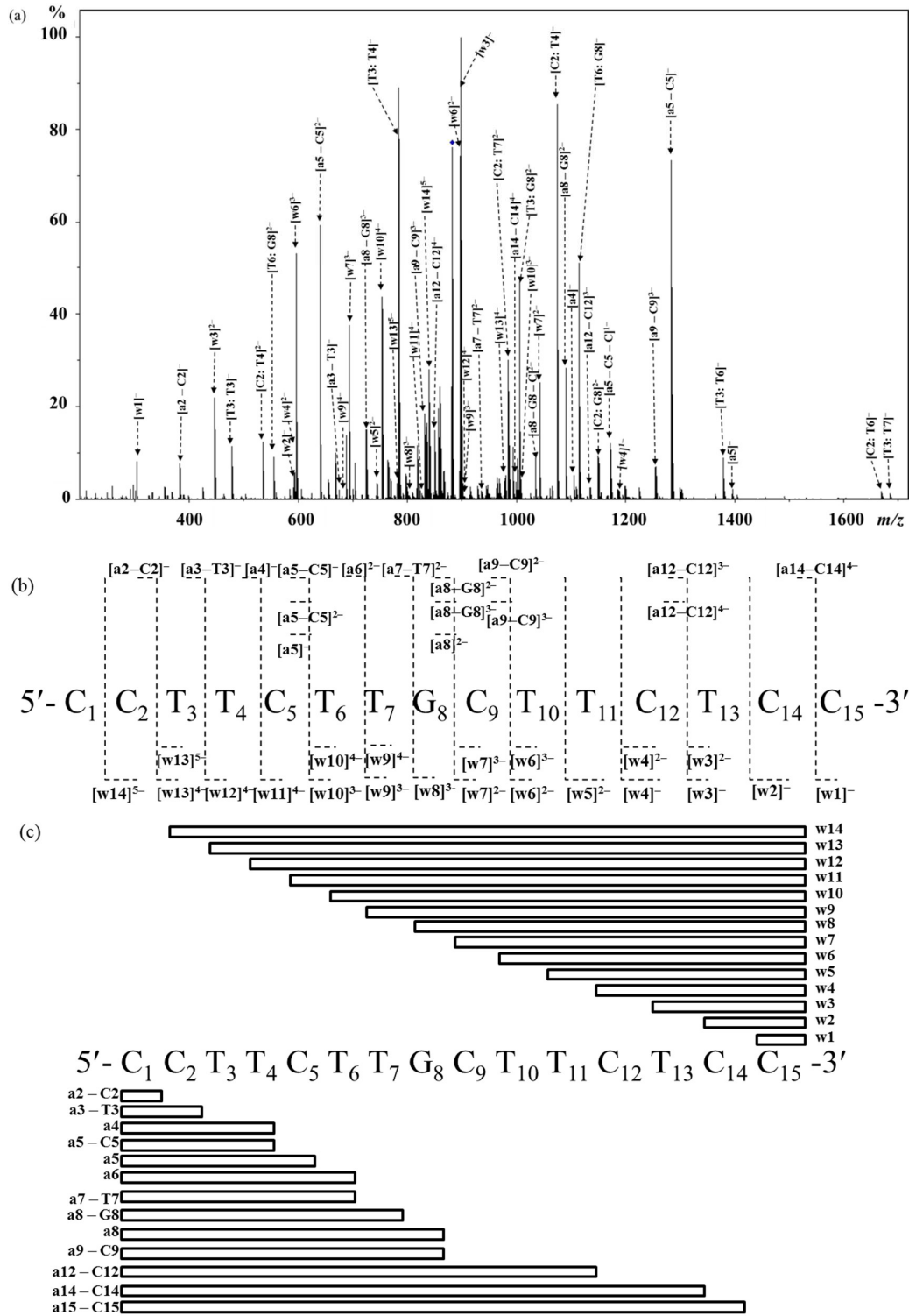


Figure S1. FT-ICR CID MS/MS spectrum of $[\text{ODN15} - 5\text{H}]^{5-}$ (a), along with corresponding fragmentation maps (b) and fragments sequence of ODN15 (c). Main fragments were assigned and labeled in the spectrum shown in (a).