

Electronic Supplementary Information (ESI)

Novel C,N-Chelate Rhodium(III) and Iridium(III) Antitumor Complexes Incorporating a Lipophilic Steroidal Conjugate and their interaction with DNA

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Calculated structures: cartesian coordinates (in Å) and energies for all computed species.-

Complex 1':

E = -1439.394618427 au

Rh	0.00000000	0.00000000	0.00000000	C	0.12748441	2.83765659	1.10603869
Cl	2.39405049	0.00000000	0.00000000	C	0.14487642	4.22060436	1.07435209
N	0.02670713	2.09486443	0.00000000	C	0.07017150	4.85303775	-0.16570613

C	-0.00171996	4.08483335	-1.31343136	C	0.45069059	-3.22483773	-0.12213511
C	-0.01760052	2.68965259	-1.21812640	H	0.21848338	-4.17138007	0.37907675
C	-0.03342790	1.75541327	-2.33334049	H	1.51382239	-3.01613904	0.00875333
C	0.03331353	0.39175086	-1.97693798	H	0.25892028	-3.35055230	-1.18839648
C	0.14417716	-0.54705930	-3.00053385	C	0.99510553	-1.84222395	2.64191153
C	0.13800270	-0.15557597	-4.33543312	H	0.89761524	-2.87451637	2.99516598
C	0.03349862	1.19396156	-4.67865304	H	1.03018414	-1.18397697	3.51072515
C	-0.04238383	2.14859671	-3.67733490	H	1.94087392	-1.74922355	2.10239406
H	0.20244025	2.29064145	2.03455799	C	-1.29256517	0.36567658	3.13053205
H	0.22317662	4.78102606	1.99558889	H	-2.01322161	-0.06176599	3.83659742
H	0.08243009	5.93388159	-0.23388682	H	-1.67333433	1.34649339	2.83778901
H	-0.03417086	4.54995905	-2.28781143	H	-0.34839935	0.50543433	3.65897407
H	0.25650710	-1.59570803	-2.75615215	C	-3.20033863	0.35012795	0.60300911
H	0.22660264	-0.90349573	-5.11514998	H	-4.06440930	-0.10425302	1.10111652
H	0.03160975	1.49534490	-5.71854283	H	-3.44520588	0.47473326	-0.45281606
H	-0.09455342	3.19821384	-3.94000975	H	-3.04970171	1.34007535	1.03687285
C	-0.36163133	-2.10457055	0.43664328	C	-2.26761208	-1.98595755	-1.34144666
C	-0.13907207	-1.49240459	1.74182440	H	-3.08639864	-2.66417095	-1.07734271
C	-1.12275039	-0.51920685	1.94148894	H	-1.59734927	-2.51303102	-2.01821889
C	-1.98007679	-0.49576853	0.76558272	H	-2.68699647	-1.13531623	-1.87943678
C	-1.55729335	-1.54646731	-0.10638207				

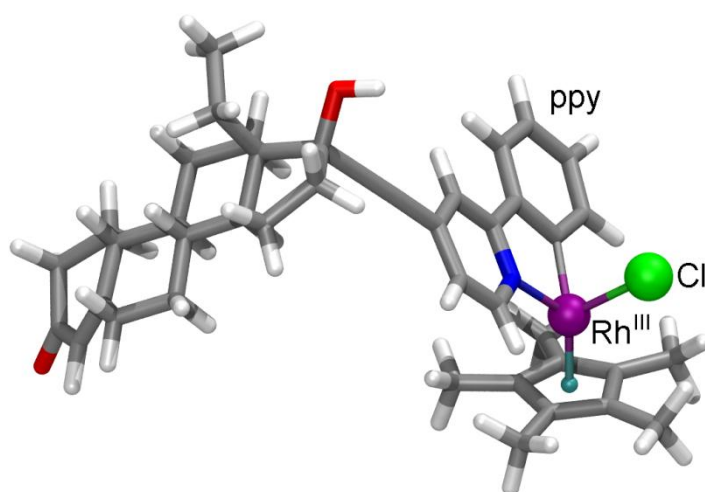
Complex 1:

E = -2405.599578147 au (RIJCOSX-B3LYPD/def2-TZVPecp)

E = -2405.422352956 au

Rh	0.00000000	0.00000000	0.00000000	H	1.03679062	-1.30471263	-3.50123061
Cl	2.39243161	0.00000000	0.00000000	C	0.38966074	-3.23037612	0.18355424
N	0.03157087	2.09433330	0.00000000	H	0.13086705	-4.18282386	-0.29284041
C	0.15455444	2.84244287	-1.10076415	H	0.18895990	-3.32259619	1.25178478
C	0.18291023	4.22102338	-1.06879203	H	1.45894623	-3.05632595	0.05276374
C	0.10016079	4.86809433	0.17522625	C	-2.32033035	-1.92106497	1.33443053
C	0.00133967	4.07981846	1.32026386	H	-3.11117868	-2.63414315	1.07621258
C	-0.02671289	2.68959010	1.21767195	H	-2.77909096	-1.06168293	1.82314810
C	-0.06585068	1.75558294	2.33254263	H	-1.65697456	-2.40044906	2.05193148
C	0.01813786	0.39216414	1.97758274	C	0.13302051	6.28721318	0.26347578
C	0.11548615	-0.54512709	3.00454452	C	0.15328235	7.49055117	0.32690598
C	0.06898987	-0.15331857	4.33865857	C	0.22825323	8.95280164	0.42012599
C	-0.06311564	1.19450096	4.67866423	C	-1.17355918	9.62310801	0.24020767
C	-0.11678403	2.14861440	3.67571397	C	-2.08723570	9.02529344	-0.82744216
H	0.23843080	2.29978814	-2.03153543	C	-3.50328646	9.60078667	-0.69504196
H	0.28006572	4.78929530	-1.98257339	C	-4.10739986	9.35861414	0.69610656
H	-0.03743923	4.54701669	2.29293196	C	-5.53326604	9.94670623	0.81734274
H	0.24706565	-1.59202108	2.76292517	C	-6.46487669	9.36459388	-0.25479169
H	0.14395755	-0.90035196	5.12075094	C	-7.93837486	9.66435920	0.01361401
H	-0.10221996	1.49399737	5.71823198	C	-8.35598170	9.18768124	1.39111742
H	-0.18832485	3.19731502	3.93859731	C	-7.34481265	9.34651480	2.44642726
C	-1.97327829	-0.47420086	-0.79436716	C	-6.08637963	9.75297976	2.21454410
C	-1.09582239	-0.53349805	-1.95574166	C	-5.16255141	10.08117844	3.35345187
C	-0.13535698	-1.52090857	-1.72079612	C	-3.76647624	9.47916966	3.17922359
C	-0.38787192	-2.10217036	-0.40774942	C	-3.18565365	9.86552806	1.82245730
C	-1.58520899	-1.51504876	0.10349127	C	-1.78599751	9.30598102	1.62312890
C	-3.17746624	0.39972128	-0.66634340	C	-0.68872796	9.69417627	2.62135765
H	-4.03043488	-0.02358986	-1.20916740	C	0.63179999	9.37478086	1.87451970
H	-2.98217455	1.39280737	-1.07519028	O	1.14632753	9.43650109	-0.56425487
H	-3.46399614	0.51283853	0.37984364	H	1.97226969	8.94763984	-0.47343191
C	-1.22670793	0.33302872	-3.16419186	C	-0.98660804	11.15238482	0.03300925
H	-1.94478453	-0.09144229	-3.87456212	H	-1.86185657	11.66513599	0.43247381
H	-0.27081036	0.44206499	-3.67918438	C	-0.13918384	11.49371513	0.62917638
H	-1.58851975	1.32679125	-2.89411934	H	-0.78775835	11.61575612	-1.41280021
C	1.00484366	-1.91118495	-2.59549195	H	-0.59414150	12.69135413	-1.42957973
H	0.91682674	-2.96269380	-2.88708677	H	0.05237686	11.10621514	-1.88121405
H	1.94844114	-1.78088763	-2.05966936	H	-1.68135433	11.43264771	-2.01389457

H	-2.13190149	7.94191450	-0.68692512	H	-7.69019936	9.17695625	3.46106596
H	-1.69500891	9.20634629	-1.82897112	H	-5.05419939	11.17438877	3.38552949
H	-3.49136525	10.67789342	-0.89370041	H	-5.61400781	9.77639876	4.29976542
H	-4.13830922	9.14672593	-1.45656069	H	-3.81922063	8.38626764	3.24641475
H	-4.19647946	8.27115798	0.83143751	H	-3.11446321	9.82340139	3.98536272
H	-5.44352032	11.03257548	0.65720741	H	-3.15503109	10.96085583	1.77852326
H	-6.31961884	8.27858453	-0.27899687	H	-1.89068225	8.21375221	1.66364832
H	-6.18377194	9.74611769	-1.23645406	H	-0.75002916	10.76036006	2.85118714
H	-8.10680951	10.74842444	-0.01562288	H	-0.77599383	9.14957387	3.56178940
H	-8.59270034	9.20849667	-0.73050674	H	1.20859689	8.58893015	2.36173474
O	-9.47073522	8.75834912	1.62225598	H	1.26802214	10.25620202	1.79175479



Complex **1** *diaster.*:

$E = -2405.599680774$ au (RIJCOSX-B3LYPD/def2-TZVPecp)

$E = -2405.422285677$ au

Rh	0.00000000	0.00000000	0.00000000	H	-3.33272281	-1.19378059	0.28299380
Cl	0.00000000	0.00000000	2.39301918	C	-1.84327918	2.64153863	0.99968814
N	2.09228404	0.00000000	0.02243447	H	-2.88198215	2.97696709	0.91396655
C	2.83883322	1.10409800	0.12288216	H	-1.19795328	3.51989669	1.02277509
C	4.21757065	1.07583371	0.13298622	H	-1.73045386	2.10696059	1.94641981
C	4.86681466	-0.16699139	0.05063316	C	0.35928848	3.13475111	-1.29579862
C	4.08051492	-1.31568665	-0.01838121	H	-0.06930750	3.83663265	-2.01947208
C	2.68949612	-1.21724247	-0.02658241	H	1.34059622	2.84062358	-1.67376052
C	1.75709526	-2.33360968	-0.04849275	H	0.49657595	3.66822918	-0.35393070
C	0.39269509	-1.97891625	0.02361514	C	0.33547143	0.60423617	-3.20382257
C	-0.54458077	-3.00563670	0.12222026	H	-0.12046512	1.10850635	-4.06365668
C	-0.15079072	-4.33981614	0.09553695	H	0.45239031	-0.45100634	-3.45395978
C	1.19899252	-4.68014294	-0.01666047	H	1.32873181	1.03181155	-3.05577090
C	2.15238758	-3.67694834	-0.07717432	C	-1.98998301	-1.33897749	-2.26609019
H	2.29488684	2.03430402	0.20215090	H	-2.66497893	-1.07152459	-3.08643916
H	4.78389253	1.99269609	0.21054259	H	-2.52261858	-2.01482716	-1.59928770
H	4.55111252	-2.28657111	-0.05903392	H	-1.13951721	-1.87815076	-2.68394145
H	-1.59333771	-2.76414970	0.23822094	C	6.28659853	-0.25144629	0.03669830
H	-0.89775763	-5.12169922	0.17268712	C	7.48823442	-0.33056168	-0.00826958
H	1.50023709	-5.71967453	-0.03725719	C	8.95118611	-0.42389532	-0.06104861
H	3.20200533	-3.93895717	-0.13545300	C	9.45595875	-0.71262826	-1.51450561
C	-2.10349876	0.43605802	-0.35411541	C	8.63790956	-1.70565165	-2.33882717
C	-1.49429957	1.74319030	-0.13538484	C	9.07344871	-1.66161063	-3.80935995
C	-0.52447488	1.94427339	-1.12187579	C	8.93698722	-0.25690615	-4.41380728
C	-0.50254966	0.76760393	-1.97904131	C	9.33752244	-0.22576758	-5.90831438
C	-1.55044565	-0.10548395	-1.55295962	C	8.48422116	-1.20949121	-6.72319451
C	-3.21634317	-0.12469122	0.46623009	C	8.56897385	-0.97011649	-8.22956794
H	-4.16829090	0.36541366	0.23251157	C	8.20907101	0.46086751	-8.57942751
H	-3.00368354	0.01628609	1.52722481	C	8.69118597	1.47796233	-7.63434064

C	9.26414192	1.18391641	-6.45653225	H	8.46645747	-2.36903740	-4.37561056
C	9.89542931	2.25739804	-5.61713304	H	7.87456660	0.02067292	-4.36570263
C	9.45628934	2.18908098	-4.15210004	H	10.39224706	-0.53628754	-5.96421020
C	9.70137144	0.79418142	-3.58539770	H	7.44143603	-1.09987633	-6.40480380
C	9.26805579	0.69205180	-2.13098770	H	8.78129888	-2.23326809	-6.49470439
C	9.89226549	1.64274528	-1.10300146	H	9.59716352	-1.13707697	-8.57414746
C	9.59441274	0.96825133	0.26122126	H	7.91875470	-1.64418694	-8.78869010
O	9.38877554	-1.44808589	0.83628198	O	7.61420588	0.75449054	-9.59928900
H	8.99124520	-1.28491105	1.69925865	H	8.61490331	2.50791122	-7.96750303
C	10.95494867	-1.11975416	-1.46440045	H	10.98347641	2.10827765	-5.64942517
H	11.43054364	-0.80350573	-2.39334186	H	9.69097001	3.23889601	-6.04959023
H	11.45021494	-0.56371373	-0.66731386	H	8.38873969	2.42408217	-4.07250918
C	11.23910715	-2.61196110	-1.27197128	H	9.99874960	2.93701851	-3.56891564
H	12.31522137	-2.76973907	-1.16420179	H	10.77479075	0.58815765	-3.67005252
H	10.74318442	-2.99884787	-0.38334812	H	8.18660841	0.88048022	-2.13055675
H	10.90499558	-3.19258639	-2.13476923	H	10.97013035	1.71836844	-1.26549772
H	7.58205849	-1.43022273	-2.27846990	H	9.47861336	2.64927356	-1.16826805
H	8.73158586	-2.71743081	-1.94259259	H	8.93269705	1.56676716	0.88720206
H	10.11456002	-1.98846051	-3.90445819	H	10.50971779	0.78093711	0.82305160

Complex 2':

E = -1433.190723725 au

Ir	0.00000000	0.00000000	0.00000000	C	-1.03899802	-0.52509467	2.00659164
Cl	2.40916425	0.00000000	0.00000000	C	-1.95665400	-0.42181701	0.87639671
N	0.13297734	2.09223903	0.00000000	C	-1.61799592	-1.45748103	-0.05893998
C	0.26993222	2.81984552	1.11581848	C	0.26783026	-3.27778179	-0.19616057
C	0.37968299	4.19693148	1.09545981	H	-0.07721067	-4.21440257	0.25714710
C	0.36678734	4.84495264	-0.13932012	H	1.34751064	-3.20415095	-0.05328819
C	0.25472445	4.09311050	-1.29301916	H	0.07193264	-3.33232699	-1.26838259
C	0.14057922	2.70083080	-1.21353404	C	1.03791728	-1.97779580	2.56301988
C	0.05697264	1.78467947	-2.33593705	H	0.90020934	-3.01868855	2.87341097
C	0.03405170	0.41529168	-1.98600828	H	1.13420929	-1.36137047	3.45643065
C	0.05373147	-0.51455311	-3.02948869	H	1.97023941	-1.90875369	1.99671616
C	0.04212745	-0.10617302	-4.35887117	C	-1.12107214	0.30529690	3.24678702
C	0.02517706	1.25206029	-4.68781611	H	-1.81984386	-0.13751137	3.96531513
C	0.04380750	2.19584360	-3.67520350	H	-1.48268383	1.31116092	3.02259569
H	0.29726245	2.26471716	2.04250186	H	-0.14811592	0.38974155	3.73447127
H	0.48555311	4.74202034	2.02320994	C	-3.16949238	0.45142074	0.82711384
H	0.45740674	5.92269958	-0.19659134	H	-3.99451090	0.00319342	1.39294960
H	0.26604697	4.56738442	-2.26351555	H	-3.50232859	0.59604738	-0.20127734
H	0.09741523	-1.57318667	-2.80543701	H	-2.96578348	1.43289336	1.25897470
H	0.05666402	-0.84908981	-5.14840996	C	-2.42043210	-1.84580896	-1.25530815
H	0.01529752	1.56398472	-5.72444495	H	-3.18460853	-2.57554825	-0.96527320
H	0.05571868	3.24976594	-3.92618901	H	-1.79556522	-2.30048489	-2.02300512
C	-0.42047116	-2.09876641	0.41090792	H	-2.91980613	-0.98256394	-1.69610064
C	-0.11217565	-1.53843655	1.72194314				

Complex 2:

E = -2399.395364365 au

Ir	0.00000000	0.00000000	0.00000000	C	1.78369552	2.33714952	0.03824102
Cl	0.00000000	0.00000000	2.40789323	C	0.41489203	1.98559669	0.03705270
N	2.09026686	0.00000000	0.10959665	C	-0.51566013	3.02825649	0.07653984
C	2.82719337	-1.11260485	0.23020441	C	-0.10915155	4.35762001	0.06432217
C	4.20281946	-1.09326188	0.30476412	C	1.24830220	4.68852812	0.02606625
C	4.86599118	0.14601640	0.27620663	C	2.19341479	3.67702701	0.02435132
C	4.09091565	1.29924114	0.18219906	H	2.27832516	-2.04239649	0.27045804
C	2.70068056	1.21408432	0.10239809	H	4.75804965	-2.01577231	0.39459091

H	4.56705147	2.26827545	0.18078171	C	9.25630254	2.08805003	-7.95368130
H	-1.57308918	2.80298989	0.13594874	C	9.44004324	3.03892276	-6.84807889
H	-0.85271133	5.14612552	0.09302301	C	9.83355995	2.67885371	-5.61581579
H	1.55822833	5.72566061	0.01539182	C	10.18743305	3.71815628	-4.58990431
H	3.24697315	3.92982909	0.02021989	C	9.56535198	3.43366893	-3.22123254
C	-0.42976639	-0.87958564	-1.95319863	C	9.91724780	2.02181946	-2.76274131
C	-0.54248024	-2.00583494	-1.03211037	C	9.33995702	1.70816220	-1.39127893
C	-1.55403002	-1.70899629	-0.10677076	C	9.72708520	2.60108803	-0.20663726
C	-2.10308739	-0.39391993	-0.41946957	C	9.38203630	1.74610918	1.03894534
C	-1.45781722	0.06595210	-1.61797577	O	9.41317928	-0.72755719	1.34047571
C	0.44673017	-0.84450549	-3.16450516	H	8.92961518	-0.68929203	2.17350035
H	0.00515215	-1.42845181	-3.98063051	C	11.15844686	0.03072155	-0.71424238
H	1.43114310	-1.26563847	-2.94969882	H	11.68715976	0.50062196	-1.54396595
H	0.58468302	0.17849660	-3.51651018	H	11.49485211	0.54382744	0.18753929
C	0.27583137	-3.25356997	-1.11037143	C	11.60297432	-1.43227851	-0.64143527
H	-0.17380031	-3.96986862	-1.80717795	H	12.67434525	-1.47994581	-0.43001879
H	0.35548858	-3.74007600	-0.13665585	H	11.07220176	-1.96999294	0.14225841
H	1.28300009	-3.03988755	-1.47350254	H	11.43080864	-1.94619478	-1.58985382
C	-2.00269882	-2.54478391	1.04407426	H	7.95300635	-0.55024842	-1.94941293
H	-3.04767338	-2.84118480	0.90673335	H	9.20502968	-1.73807246	-1.60886166
H	-1.92470381	-1.98008946	1.97609183	H	10.69596324	-0.65835566	-3.30453039
H	-1.39902929	-3.44814013	1.13959802	H	9.16419618	-1.14793870	-4.00888800
C	-3.27785463	0.22780686	0.26381187	H	8.31111451	1.14993699	-3.86065441
H	-4.21655858	-0.23314139	-0.06433534	H	11.06793150	1.03325906	-5.12304673
H	-3.33392076	1.29539737	0.04462482	H	8.28829172	0.26446548	-6.07866726
H	-3.19705817	0.10885174	1.34576014	H	9.72537612	-0.74684513	-6.03364812
C	-1.83438448	1.26605606	-2.41987434	H	10.77027024	0.61578543	-7.83435842
H	-2.58295056	0.98704854	-3.17004620	H	9.21050887	-0.00265144	-8.38466697
H	-0.97079530	1.68475776	-2.93644673	O	8.84450913	2.43675402	-9.04432752
H	-2.26162276	2.04659392	-1.79216521	H	9.30275667	4.08577554	-7.09768576
C	6.28423452	0.21780962	0.35186629	H	11.27950713	3.70605030	-4.46965010
C	7.48741534	0.26681193	0.40471651	H	9.91498118	4.71049176	-4.95459035
C	8.94916602	0.33728677	0.50559636	H	8.47514598	3.52988748	-3.27900090
C	9.63409860	0.27252454	-0.89935018	H	9.91955411	4.16900841	-2.49485098
C	9.03461551	-0.70365737	-1.91015979	H	11.01072167	1.95179282	-2.72792302
C	9.62052552	-0.45030708	-3.30553204	H	8.24986031	1.77157025	-1.50444530
C	9.39605843	0.99201063	-3.78433123	H	10.79693057	2.82089402	-0.23508038
C	9.98712424	1.23113095	-5.19455558	H	9.19569762	3.55284527	-0.21768591
C	9.37493090	0.26810460	-6.22162878	H	8.59407802	2.19130396	1.64609634
C	9.68691622	0.66317537	-7.66415060	H	10.25421012	1.59794792	1.67607743

Complex 3':

E = -1423.224134519 au

Ru	0.00000000	0.00000000	0.00000000	H	-0.02159808	1.60066398	-5.72521831
Cl	2.40740270	0.00000000	0.00000000	H	0.04822297	3.27203552	-3.91404245
N	0.13640320	2.08687241	0.00000000	C	-2.04417316	-0.76913000	-0.09788672
C	0.25919982	2.81043607	1.12030619	C	-1.87667822	-0.01091932	1.08653893
C	0.35851219	4.18859978	1.11089448	C	-0.93310658	-0.38302142	2.10130103
C	0.34731092	4.84425731	-0.11917876	C	-0.02855874	-1.41367570	1.87640789
C	0.24788567	4.09906166	-1.27867759	C	-0.11127689	-2.12087632	0.62402572
C	0.14621498	2.70627660	-1.20783345	C	-1.13105509	-1.85092297	-0.30036726
C	0.06701457	1.79545423	-2.33599432	H	-2.48464022	0.86927702	1.23844539
C	0.04958601	0.42395447	-1.99298291	H	-0.85419253	0.21160009	3.00151641
C	0.04265174	-0.49586544	-3.04601674	H	0.64689725	-2.85338051	0.38761918
C	0.01294908	-0.07889453	-4.37303759	H	-1.16456826	-2.39499111	-1.23361383
C	0.00117423	1.28054960	-4.69135284	C	-3.08385459	-0.45824955	-1.14497416
C	0.03810824	2.21627918	-3.67084499	H	-2.64227265	-0.73708963	-2.10579146
H	0.28409178	2.24376660	2.04010844	C	-3.43952658	1.02617311	-1.21404969
H	0.45178901	4.72887175	2.04264855	H	-4.10559700	1.20647760	-2.06035942
H	0.42748424	5.92297140	-0.16867179	H	-3.95893025	1.35105923	-0.30824076
H	0.25833064	4.57986448	-2.24598446	H	-2.54076924	1.63094725	-1.34165386
H	0.08121075	-1.55645902	-2.83174168	C	-4.33378454	-1.31832357	-0.91666721
H	0.00651647	-0.81689320	-5.16731218	H	-5.06410255	-1.14772920	-1.71203480

H	-4.08422918	-2.38213880	-0.89947594	H	1.06568878	-2.75911594	3.13319135
H	-4.80105843	-1.06247011	0.03885981	H	2.04442085	-1.53190333	2.30345764
C	1.09468458	-1.71244265	2.81628749	H	1.04721861	-1.07461377	3.70001729

Complex 3':

E = -2389.359347968 au

Ru	0.00000000	0.00000000	0.00000000	C	-1.01287286	9.56615474	-0.15554476
Cl	2.40720024	0.00000000	0.00000000	C	-2.07737291	8.88563211	-1.01375615
N	0.12814591	2.08251642	0.00000000	C	-3.47291970	9.40300576	-0.63909619
C	0.25123318	2.81096326	1.11807921	C	-3.79434100	9.18701793	0.84809092
C	0.33188924	4.18618852	1.11151055	C	-5.21674916	9.67553500	1.21458532
C	0.29995223	4.86053942	-0.12111873	C	-6.27722625	8.96754725	0.35857974
C	0.20451359	4.09631802	-1.28156364	C	-7.69394551	9.13520345	0.90352487
C	0.12428959	2.70593491	-1.20682636	C	-7.78555498	8.67458779	2.34483235
C	0.04679049	1.79641601	-2.33554446	C	-6.61954393	8.99257435	3.18071682
C	0.04313062	0.42476316	-1.99196484	C	-5.47865468	9.50912089	2.69755553
C	0.03770172	-0.49475603	-3.04541279	C	-4.39471119	9.98196462	3.62342924
C	-0.00602236	-0.07772315	-4.37179578	C	-3.01041670	9.46781648	3.21954369
C	-0.03320951	1.28171008	-4.69005344	C	-2.71736641	9.80599803	1.76019649
C	0.00403978	2.21762648	-3.67004786	C	-1.34893310	9.29991712	1.32995484
H	0.29095075	2.24789632	2.03953616	C	-0.10711253	9.78277380	2.08898858
H	0.42537303	4.73223595	2.03908046	C	1.06803347	9.46559203	1.12901685
H	0.19767256	4.58225749	-2.24567860	O	1.12799208	9.40854181	-1.36317919
H	0.08639875	-1.55506218	-2.83154834	H	1.97603336	8.95153816	-1.40265485
H	-0.01340659	-0.81567095	-5.16605030	C	-0.93154486	11.08981339	-0.45724460
H	-0.06822152	1.60137839	-5.72367760	H	-1.74197480	11.59080774	0.07420302
H	0.00259614	3.27343682	-3.91333954	H	-0.00664390	11.48746043	-0.03945047
C	-2.04097088	-0.77867382	-0.09793576	C	-1.01722115	11.49023079	-1.93237761
C	-1.87778244	-0.01818497	1.08578610	H	-0.87430602	12.56995099	-2.02779758
C	-0.93423983	-0.38563186	2.10208805	H	-0.25463788	10.98713998	-2.52440631
C	-0.02596469	-1.41297647	1.87941026	H	-1.99583592	11.24781376	-2.35176739
C	-0.10476905	-2.12169661	0.62769041	H	-2.04231626	7.80779563	-0.83313525
C	-1.12428096	-1.85749054	-0.29785253	H	-1.88585770	9.04171630	-2.07630861
H	-2.48924765	0.85957268	1.23701467	H	-3.55196106	10.47142267	-0.86767687
H	-0.85862814	0.20883153	3.00275648	H	-4.21293141	8.89223740	-1.925587173
H	0.65617271	-2.85160704	0.39223414	H	-3.77445831	8.10369063	1.03442989
H	-1.15646103	-2.40346463	-1.22995827	H	-5.24937604	10.75538692	1.00171330
C	-3.08416313	-0.47635867	-1.14328768	H	-6.03199317	7.89989300	0.32783237
H	-2.64559188	-0.75843048	-2.10434596	H	-6.23020405	9.33438254	-0.66716745
C	-3.44750709	1.00559940	-1.21765391	H	-7.97508579	10.19578455	0.88672137
H	-4.12072459	1.17837093	-2.05971744	H	-8.42846174	8.58838465	0.31107094
H	-3.96259543	1.33241592	-0.31002132	O	-8.77680203	8.13215113	2.79601217
H	-2.55275089	1.61429509	-1.35545793	H	-6.74728823	8.84218289	4.24791707
C	-4.32976051	-1.34064606	-0.90378818	H	-4.37203300	11.07944077	3.57542165
H	-5.06474291	-1.17700008	-1.69619475	H	-4.63734642	9.70970349	4.65281503
H	-4.07544965	-2.40325470	-0.88268900	H	-2.96649299	8.38001534	3.34958453
H	-4.79274942	-1.08138825	0.05261193	H	-2.24942612	9.90413126	3.87063859
C	1.09651743	-1.70879326	2.82077013	H	-2.76041221	10.89709867	1.65779342
H	1.07918805	-2.75942750	3.12439861	H	-1.39148078	8.20873683	1.43887716
H	2.04619017	-1.51131979	2.31389227	H	-0.17264593	10.85792157	2.27203739
H	1.03799878	-1.08310309	3.71279482	H	0.00238477	9.29056062	3.05559843
C	0.36295078	6.28020000	-0.17401922	H	1.75517637	8.72591443	1.54026964
C	0.38655788	7.48488821	-0.20397583	H	1.64225178	10.36068822	0.88933677
C	0.42558225	8.95157807	-0.20522074				

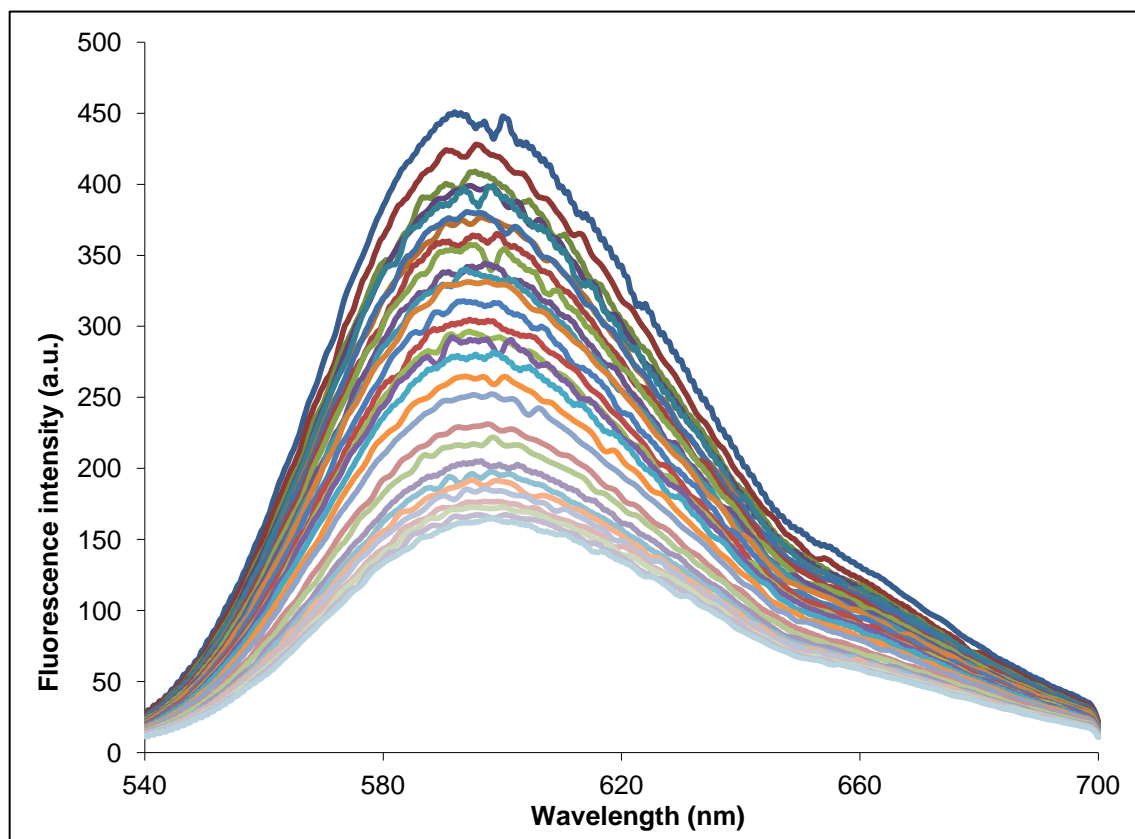


Figure S1. Fluorescence quenching of EB bound ct-DNA with **1** (0 – 70 μ M in 2.5 μ M increments)

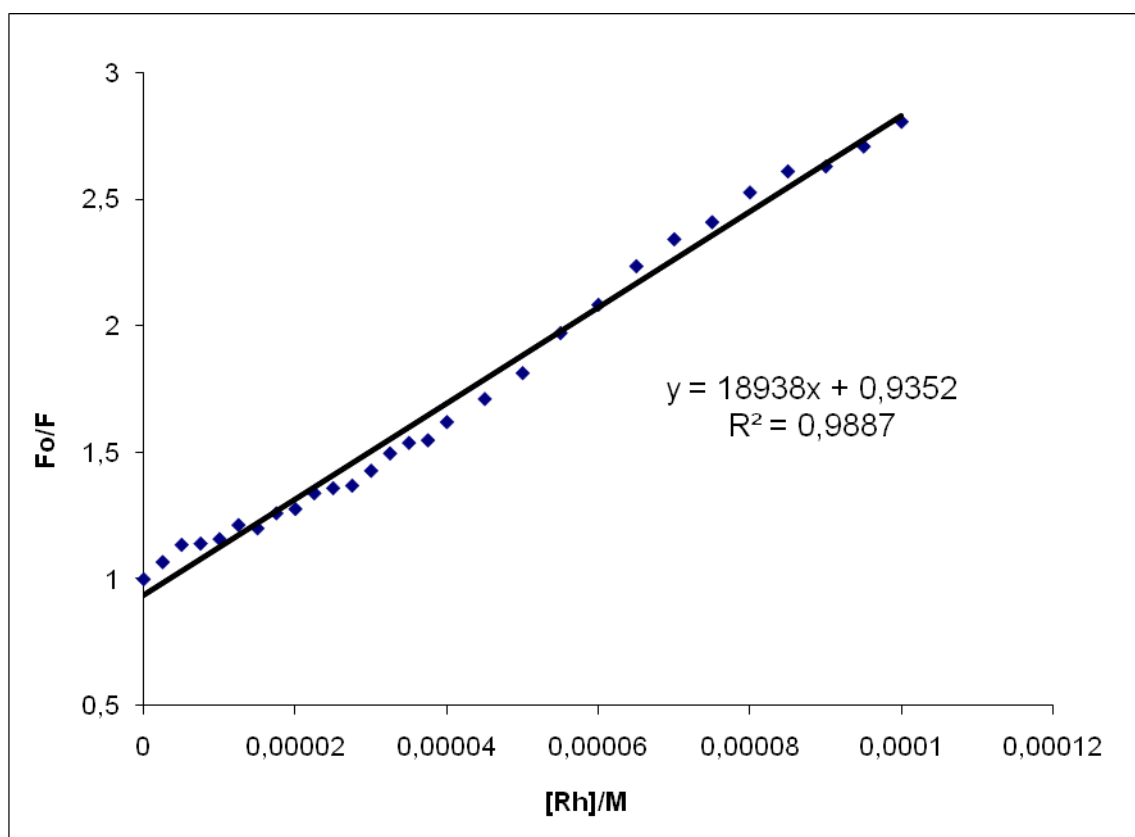


Figure S2. Stern-Volmer plot of the titration of BE bound ct-DNA with **1**

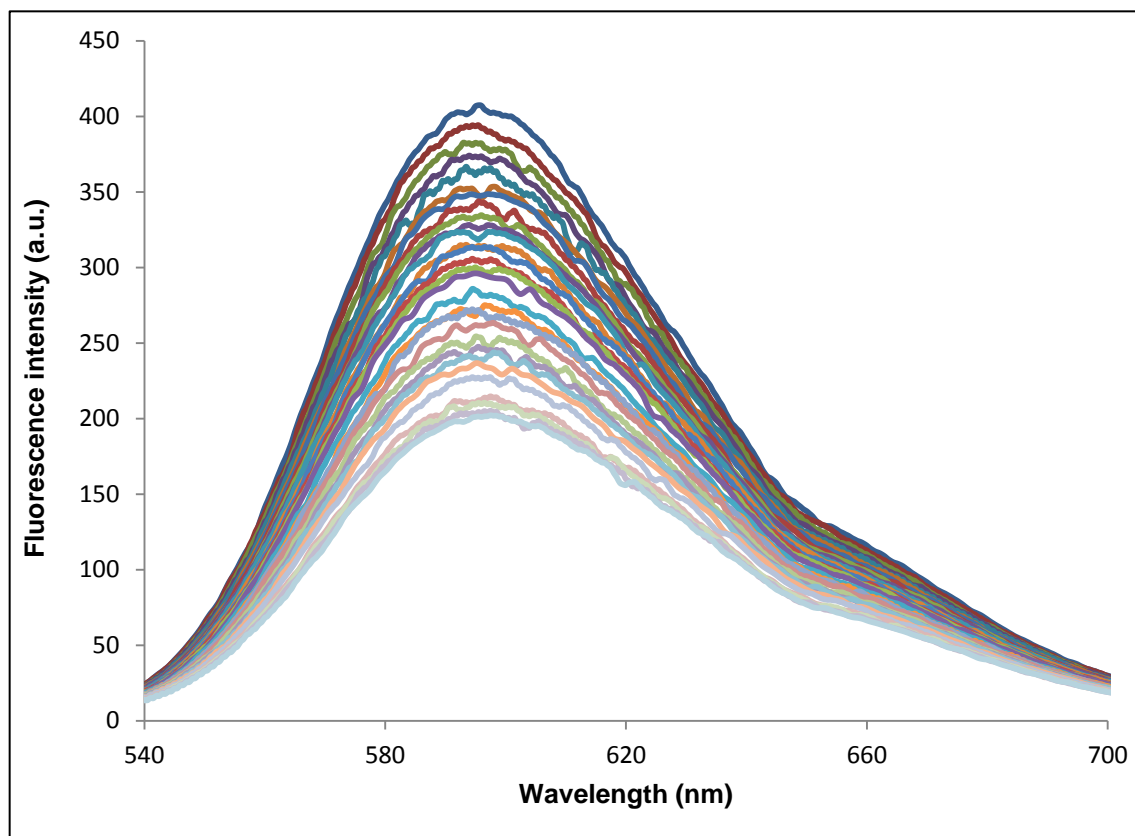


Figure S3. Fluorescence quenching of EB bound ct-DNA with **2** (0 – 70 μM in 2.5 μM increments)

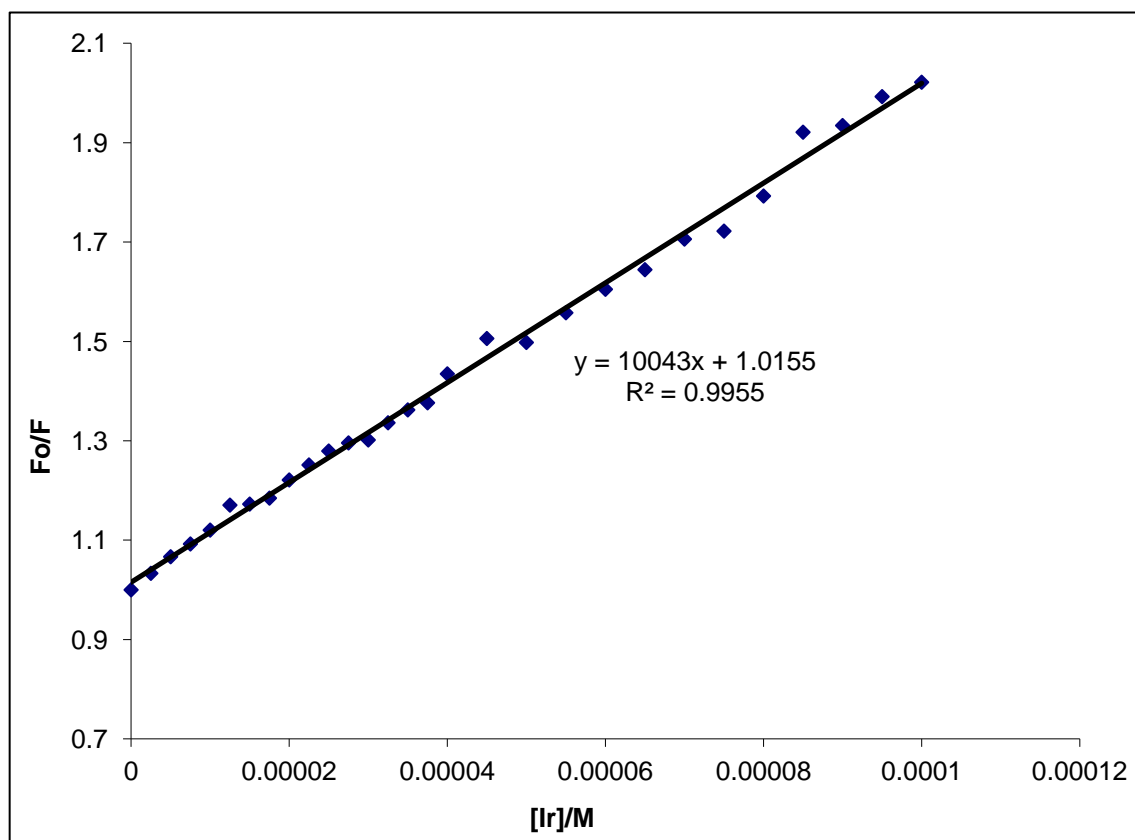


Figure S4. Stern-Volmer plot of the titration of BE bound ct-DNA with **2**

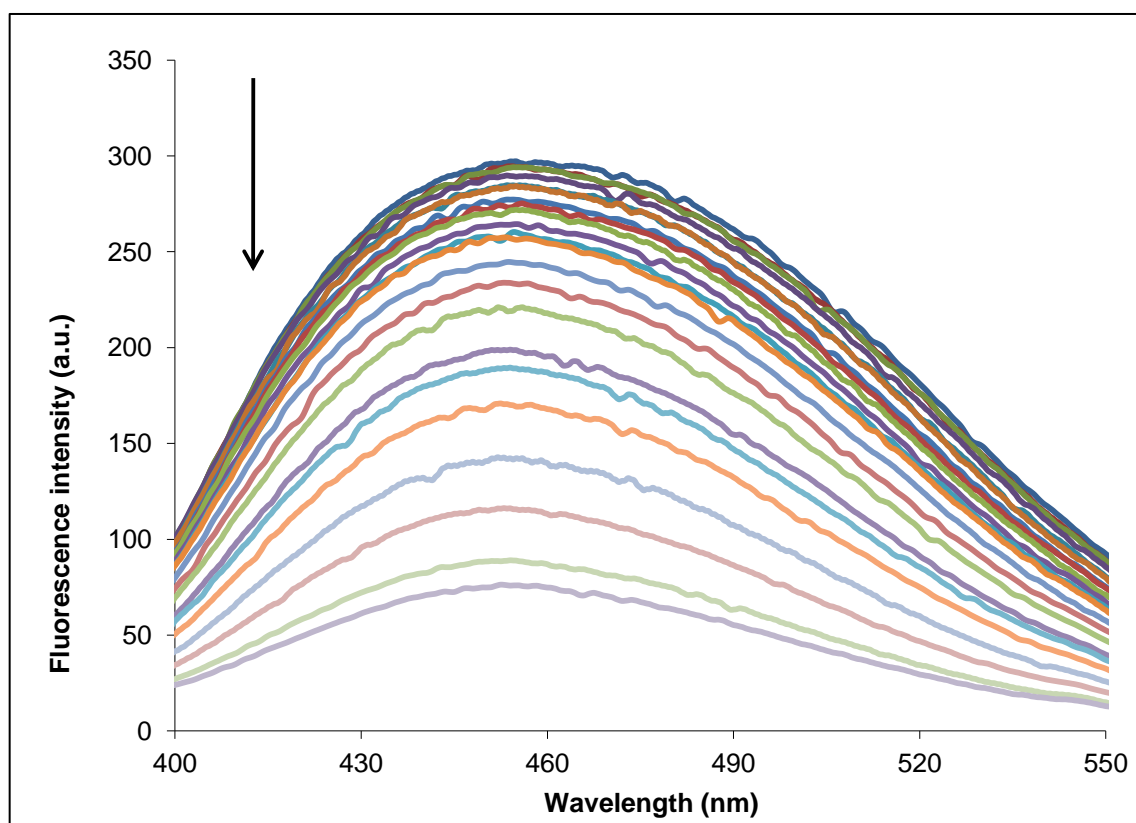


Figure S5. Fluorescence quenching of Hoechst 33258-DNA with **1** (0 – 55 μM in 2.5 μM increments)

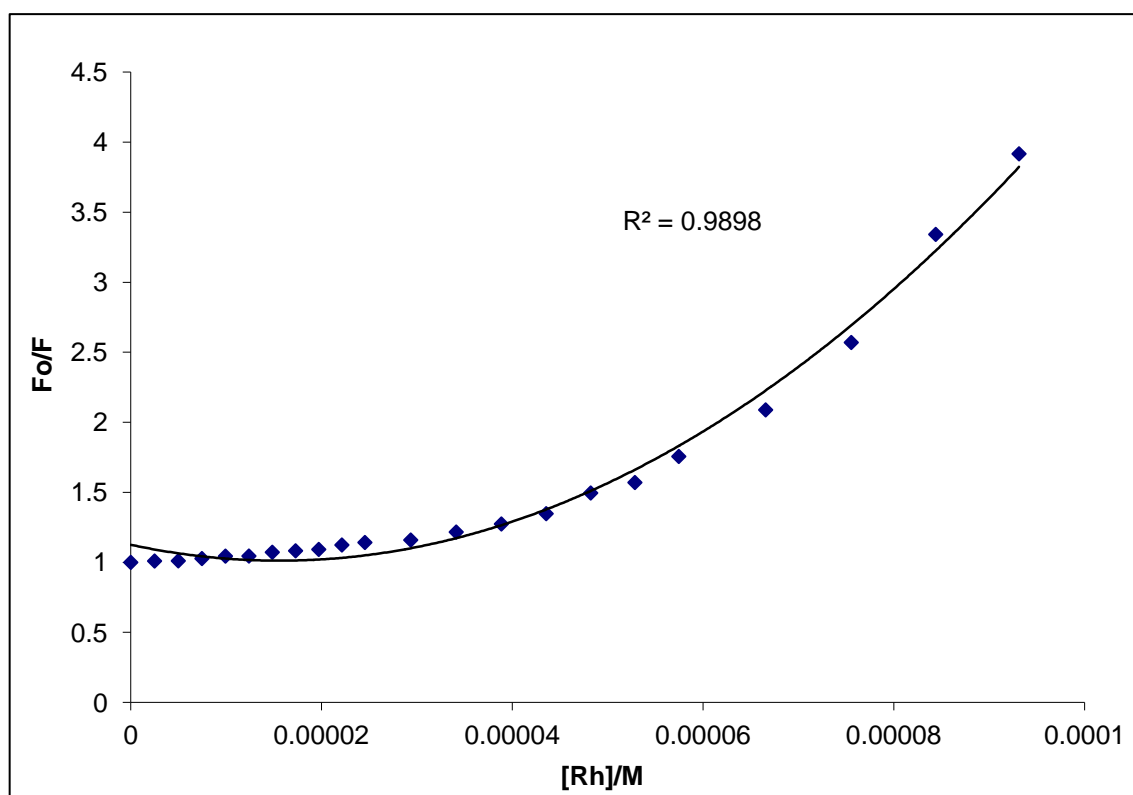


Figure S6. Stern-Volmer plot of the titration of Hoechst 33258-DNA with **1**

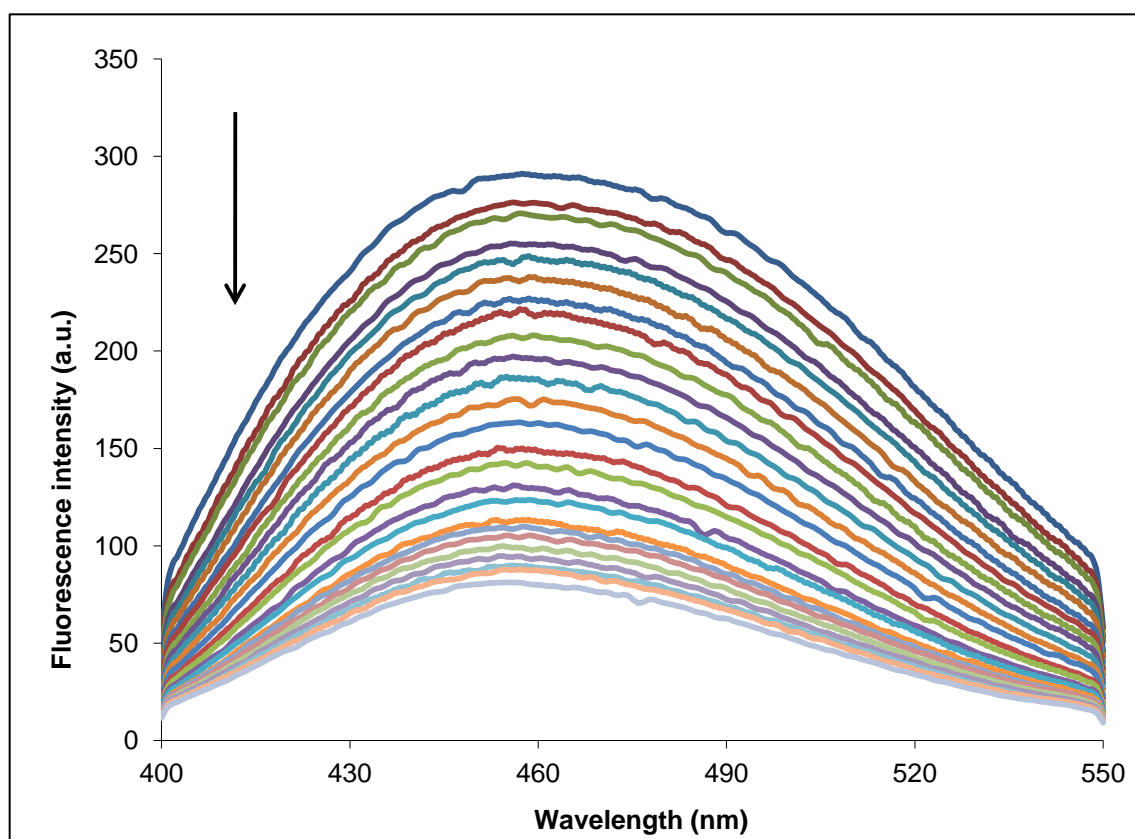


Figure S7. Fluorescence quenching of Hoechst 33258-DNA with **2** (0 – 62.5 μM in 2.5 μM increments)

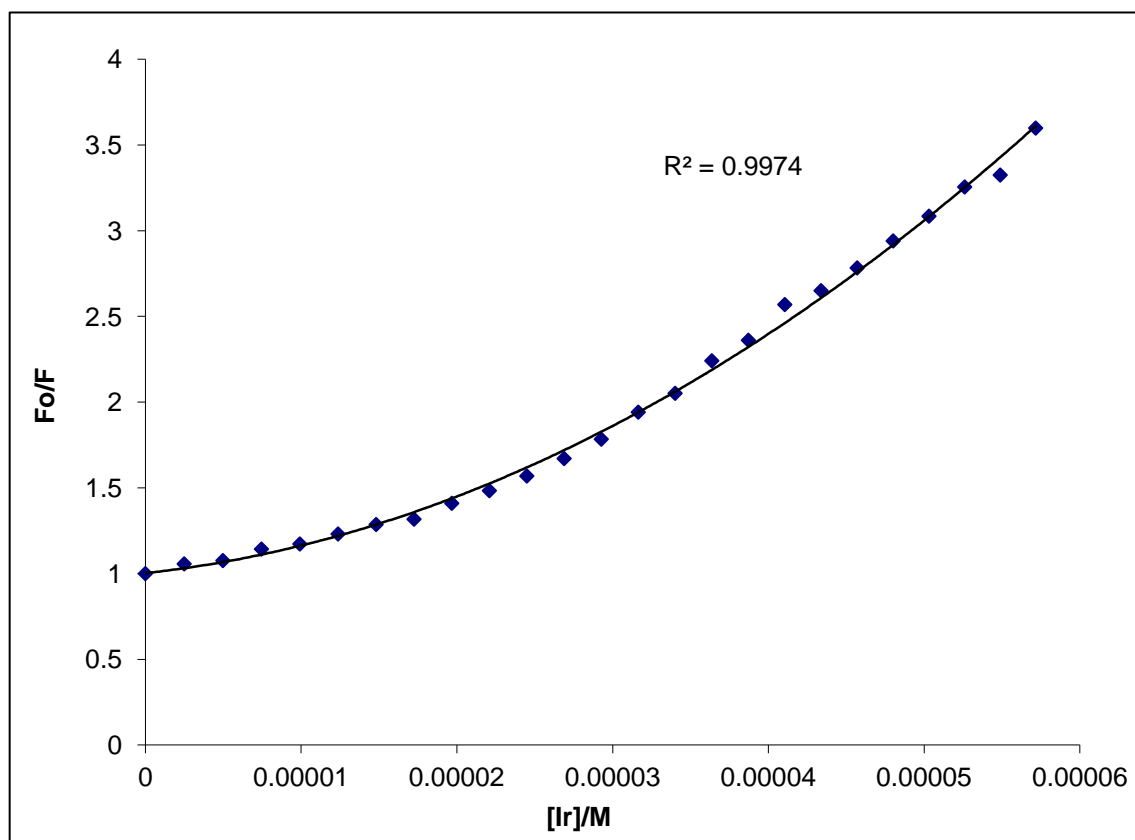


Figure S8. Stern-Volmer plot of the titration of Hoechst 33258-DNA with **2**

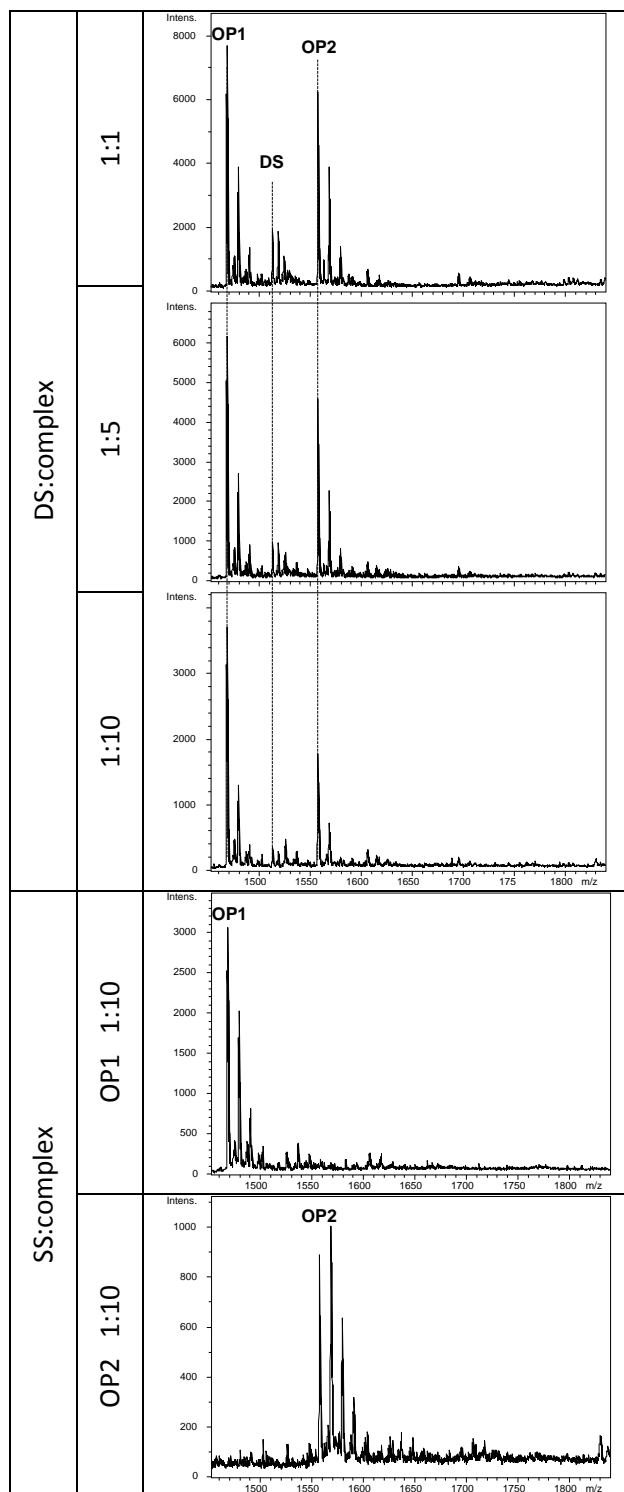


Figure S9. Negative ESI-TOF MS spectra obtained after the mixture of the Ir complex **2** with the corresponding solution containing the oligonucleotides assayed after incubation during 24 h. At the m/z range shown, the peaks related with the single oligonucleotides (OP1 and OP2) exhibit the -2 charge, while those related with the DS are -4 charged.