Electronic Supplementary Material (ESI) for RSC Advances.

Interaction of a Synthesized Pyrene Based Fluorescent Probe with CT-DNA: Spectroscopic, Thermodynamic and Molecular modeling studies

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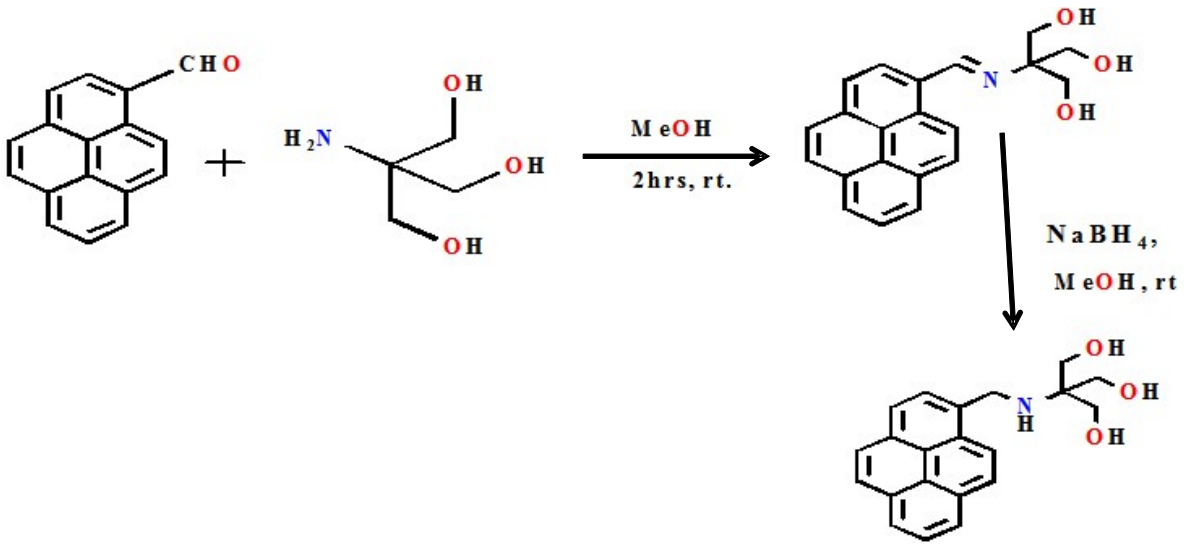


Scheme S1. Synthetic route of compound **1.**

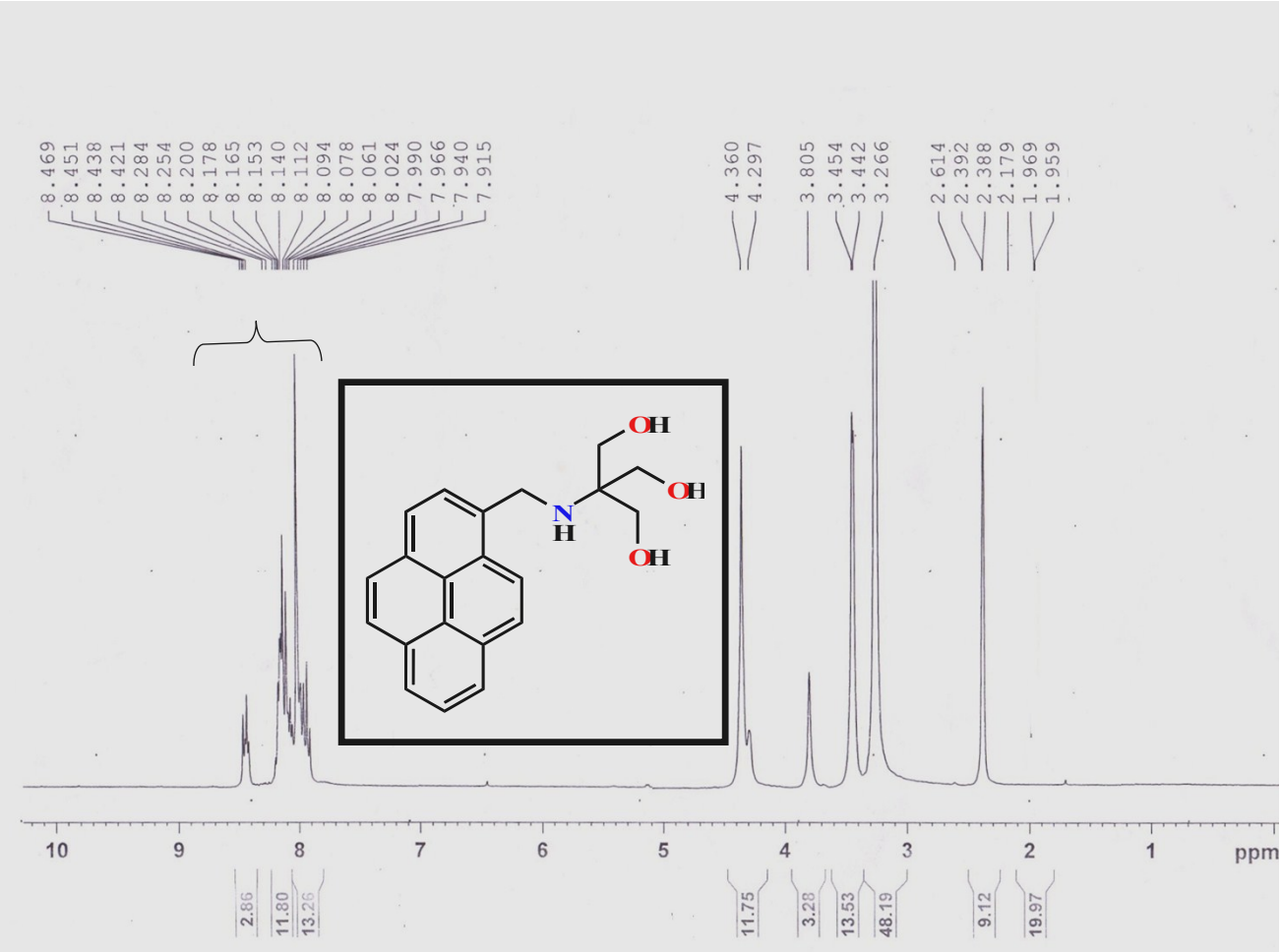


Figure S1. ^{1}H NMR (300 MHz) spectrum of **1** in DMSO–d_6 at 20 ºC

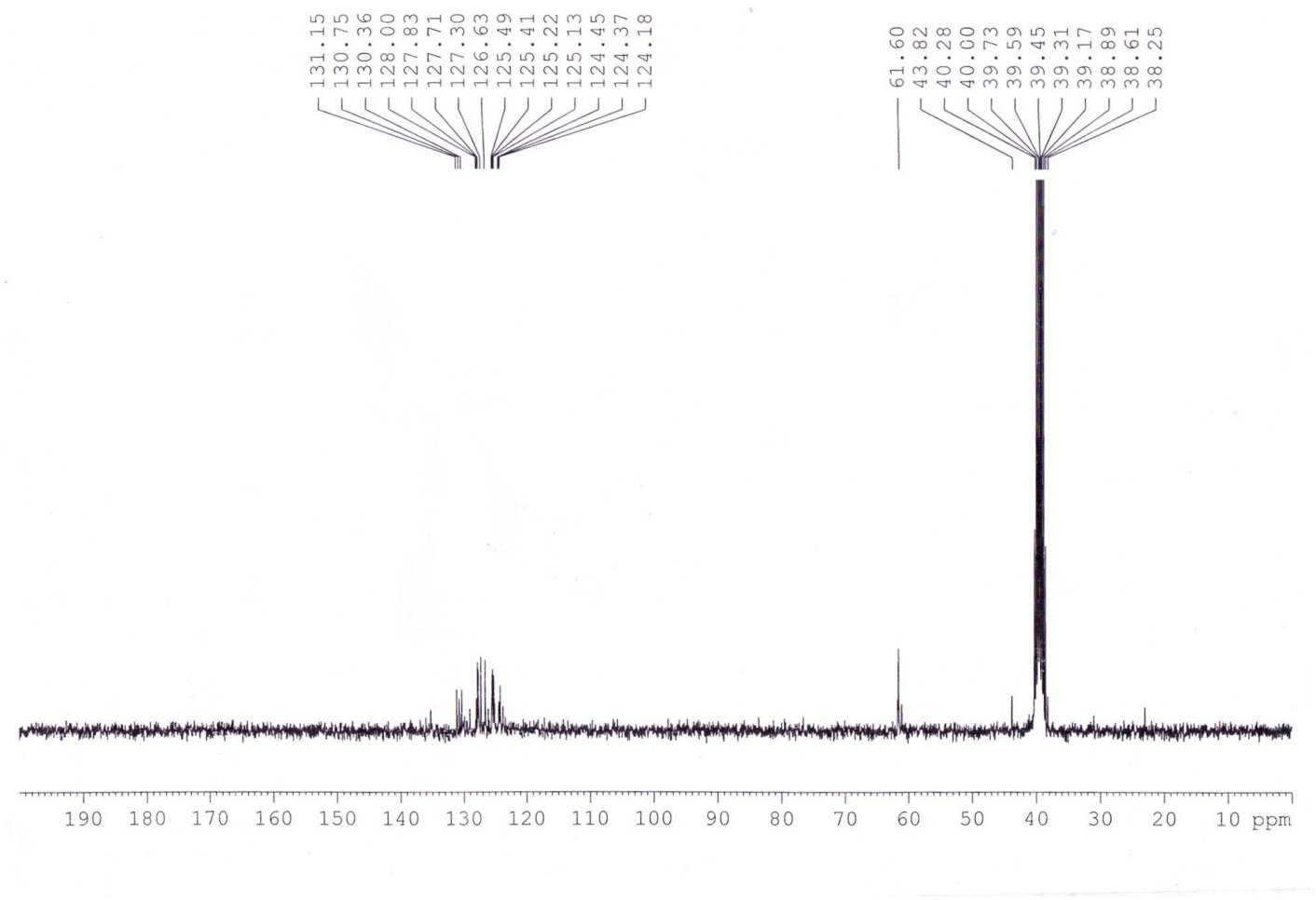


Figure S2. ^{13}C NMR (75.5 MHz) spectrum of **1** in d_6-DMSO at 20 ºC

Table S1. Four DNA decamer sequences

S.No.	DNA	Sequence
1	S1	5'-d(GATGGCCATC)$_2$
2	S2	5'-d(GATCCGGATC)$_2$
3	S3	5'-d(GGCAATTGCC)$_2$
4	S4	5'-d(GGCTTAAGCC)$_2$

S1-pytris docking table				
S	rmsd	E_conf	E_place	E_score1
-6.4546618	7.179431	0	-668.33075	-6.4546618
-6.9276376	7.1241064	1.8063836	-674.39392	-6.9276376
-7.7952886	7.105413	0	-669.61407	-7.7952886
-8.4600554	7.0959425	2.0509024	-679.12665	-8.4600554
-6.4867949	7.0909152	0	-670.79437	-6.4867949
-6.3626819	7.0853705	0	-672.44769	-6.3626819
-6.3328075	7.0820994	0	-669.20404	-6.3328075
-7.3279901	7.0621223	0	-665.3371	-7.3279901
-6.3158188	7.0573668	0	-671.45886	-6.3158188
-7.9114366	7.0262923	0	-672.1687	-7.9114366
-8.5631628	7.0082469	2.0513055	-679.55054	-8.5631628
-7.6667867	6.9982057	0	-671.11646	-7.6667867
-6.3457031	6.9916921	0	-671.67682	-6.3457031
-8.8124399	6.9690537	2.2563903	-687.34387	-8.8124399
-8.4452066	6.9598751	2.2561491	-686.63971	-8.4452066
-8.7948046	6.9373326	1.998136	-678.63818	-8.7948046
-8.9760923	2.7277198	1.5962512	-785.32898	-8.9760923
-9.3244419	2.6845901	1.59613	-779.87915	-9.3244419
-10.555079	2.6388922	1.5963793	-778.24445	-10.555079
-10.474515	2.6342528	1.5963116	-778.34509	-10.474515
-9.4319153	2.5617173	1.6351231	-779.85431	-9.4319153

-9.9312782	2.5442975	1.7154114	-775.35364	-9.9312782
-8.7853031	2.5160537	1.9945502	-767.75281	-8.7853031
-9.915637	2.5110061	1.6817863	-779.30719	-9.915637
-10.51836	2.5022755	1.6352916	-778.41888	-10.51836
-10.186988	2.4944973	1.7154398	-769.52301	-10.186988
-10.191694	2.4622648	1.6818099	-773.41003	-10.191694
-9.4528351	2.432831	1.7154876	-778.23621	-9.4528351
-9.4138355	2.3993895	1.6818545	-782.16907	-9.4138355
-9.7803926	2.3774307	2.2563462	-762.89679	-9.7803926

S2-pytris docking table				
S	**rmsd**	**E_conf**	**E_place**	**E_score1**
-10.034606	6.8968883	1.6975729	-622.12256	-10.034606
-9.7919636	6.8823619	1.5182332	-612.32928	-9.7919636
-10.204964	6.8735442	1.3769805	-645.50311	-10.204964
-9.5849695	6.8422637	1.7013464	-610.50824	-9.5849695
-9.8206396	6.7628417	1.3769788	-643.96552	-9.8206396
-10.059402	6.7492332	1.7419789	-658.20728	-10.059402
-10.583174	6.7233791	1.6980435	-658.53894	-10.583174
-9.9027309	6.5937419	1.7420311	-659.10406	-9.9027309
-10.530219	6.5864015	1.6980658	-658.25964	-10.530219
-1.4828229	6.4732137	1.5182403	-587.99823	-1.4828229
-1.4340451	6.3915849	1.5181806	-588.30975	-1.4340451
-1.6817904	6.3449621	1.7888666	-603.5791	-1.6817904
-2.0954382	6.3367147	1.7013464	-586.98895	-2.0954382
-1.6723944	6.2518449	1.7888476	-604.22632	-1.6723944
-0.85963154	6.1890893	1.7013148	-590.99493	-0.85963154
-13.053338	2.2384264	0	-667.19012	-13.053338
-12.721235	2.1680107	0	-665.71368	-12.721235
-11.335208	1.9214787	0	-663.76135	-11.335208
-10.992325	1.8861812	0	-670.3316	-10.992325
-11.538211	1.864049	0	-664.17596	-11.538211
-10.89166	1.8328191	0	-669.31128	-10.89166

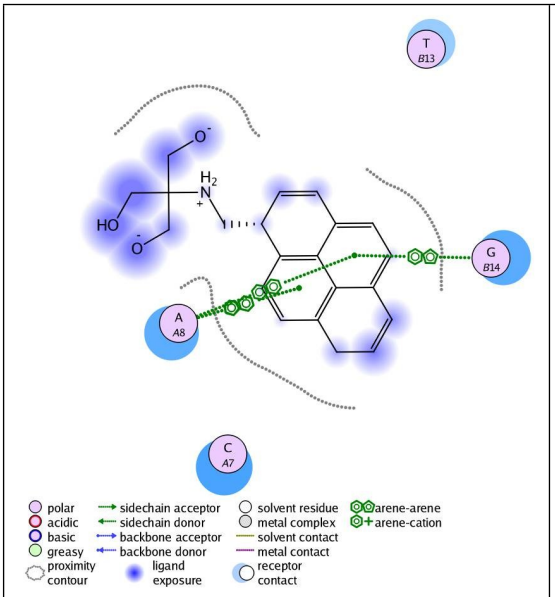
-11.922042	1.794799	0	-668.28589	-11.922042
-11.601603	1.7777536	0	-673.83838	-11.601603
-11.743905	1.5099301	0	-671.711	-11.743905
-11.77538	1.5027348	0	-671.58643	-11.77538
-11.587506	1.4267851	0	-661.77747	-11.587506
-11.458681	1.4265821	0	-660.94049	-11.458681
-11.599536	1.4146892	0	-673.94769	-11.599536
-11.59997	1.4130015	0	-670.08167	-11.59997
-10.963889	1.2992067	0	-659.75641	-10.963889

S3-pytris dockin table				
S	**rmsd**	**E_conf**	**E_place**	**E_score1**
-10.141603	6.9137802	1.4802929	-689.4436	-10.141603
-10.009198	6.8776774	1.4803308	-688.50928	-10.009198
-10.30027	6.8583522	1.4592804	-690.04401	-10.30027
-9.5048351	6.8468351	1.4802989	-689.27686	-9.5048351
-10.197693	6.8467264	1.4593091	-688.90265	-10.197693
-9.6938133	6.8164277	1.459278	-689.66986	-9.6938133
-9.4734163	6.6056628	0.043115843	-599.25256	-9.4734163
-9.3524256	6.5624537	0	-594.47003	-9.3524256
-9.4462204	6.5423951	0	-592.16217	-9.4462204
-9.5140982	6.521142	0.043113727	-599.92206	-9.5140982
-9.8149042	6.4616256	0	-594.17664	-9.8149042
-9.7813759	6.4401097	0.043112118	-598.76245	-9.7813759
-10.877054	6.2290454	0.15002993	-687.83417	-10.877054
-11.144661	6.1475258	0.15003026	-687.5954	-11.144661
-10.676573	6.1318712	0.17941804	-691.75067	-10.676573
-10.932964	6.0480628	0.17941876	-691.47571	-10.932964
-9.775733	6.036365	0.15003374	-685.01965	-9.775733
-11.619782	4.1934342	0.60000002	-672.43811	-11.619782
-9.4616261	4.1088805	0.60000002	-672.32452	-9.4616261
-9.8311424	3.448595	0.15045162	-713.87164	-9.8311424
-9.4071321	3.4408824	0.15045534	-713.95142	-9.4071321

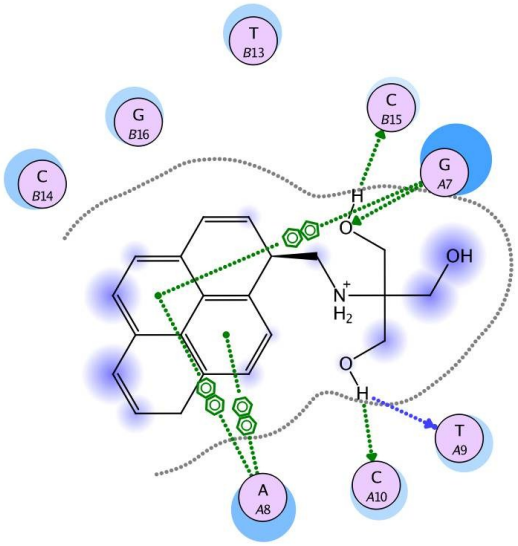
-9.5048923	3.4151387	0.17983626	-713.97797	-9.5048923
-10.924271	3.1644521	1.4802989	-724.12	-10.924271
-9.3308001	3.156287	1.4802929	-724.15997	-9.3308001
-9.9733047	2.0062029	0.17983767	-707.28589	-9.9733047
-11.489121	1.9539614	0.15045534	-707.49316	-11.489121
-9.8017664	1.9114515	0	-670.58667	-9.8017664
-9.7758608	1.8978614	0.043115843	-671.67792	-9.7758608
-9.6469202	1.7481135	0	-671.013	-9.6469202
-11.684961	1.5173985	0	-657.56439	-11.684961

S4-pytris docking table				
S	**rmsd**	**E_conf**	**E_place**	**E_score1**
-7.3543439	6.8449535	2.3977594	-657.85327	-7.3543439
-12.003634	3.3526378	1.1591526	-660.59705	-12.003634
-10.874158	3.3524058	1.0730581	-662.64423	-10.874158
-10.375343	3.3506923	0.60000002	-630.40167	-10.375343
-10.834942	3.3495309	1.1591526	-660.01318	-10.834942
-11.720356	3.3073516	1.0730581	-661.09021	-11.720356
-10.579964	3.305783	1.0730581	-660.51135	-10.579964
-8.6411629	3.2964044	1.0052307	-654.98016	-8.6411629
-9.2367783	3.27966	1.2830637	-662.41882	-9.2367783
-10.802885	3.2787411	1.3731635	-661.63263	-10.802885
-10.890466	3.2746527	1.389603	-703.6015	-10.890466
-11.897175	3.269079	1.3731608	-662.84094	-11.897175
-10.923158	3.2482934	1.4475715	-702.07471	-10.923158
-11.496552	3.239063	1.3731623	-661.72498	-11.496552
-11.37088	3.237813	1.3731633	-659.97534	-11.37088
-11.86519	3.2318439	1.389603	-704.34729	-11.86519
-11.99263	3.2079558	1.4475714	-702.9317	-11.99263
-10.59781	3.207428	1.3731633	-658.87494	-10.59781
-11.323713	3.1977823	1.389603	-702.5542	-11.323713
-9.0633535	3.1944628	1.4544754	-658.95349	-9.0633535
-10.585618	3.1799052	1.0052327	-656.53918	-10.585618

-11.866062	3.1755123	1.4475713	-701.39337	-11.866062
-11.360275	3.1715798	1.4475706	-701.09546	-11.360275
-10.136869	3.1696568	1.2830637	-668.43518	-10.136869
-10.083429	3.1487181	1.45446	-659.94318	-10.083429
-12.155	3.1273401	1.3731612	-667.68359	-12.155
-11.586825	3.0943685	1.3731633	-664.87238	-11.586825
-10.735434	3.0727437	1.45444	-661.01099	-10.735434
-12.086841	2.7308867	2.3977592	-703.77454	-12.086841
-11.935977	2.7161479	2.3977597	-703.52759	-11.935977



S1-pyrine 2D interaction



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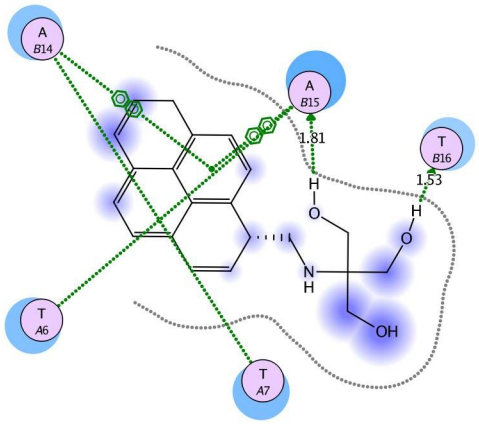
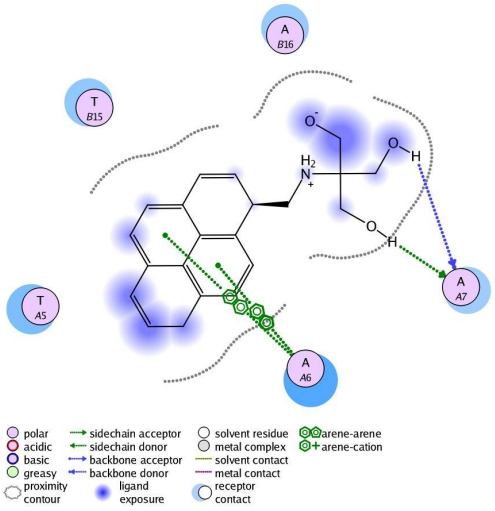


S3- pyrine 2D interaction



S4- pyrine 2D interaction