Supporting Information

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The Synthesis and Spectral Properties of Merocyanine Dyes Based on 9H-Fluorene-2,7-Dicarbonitrile

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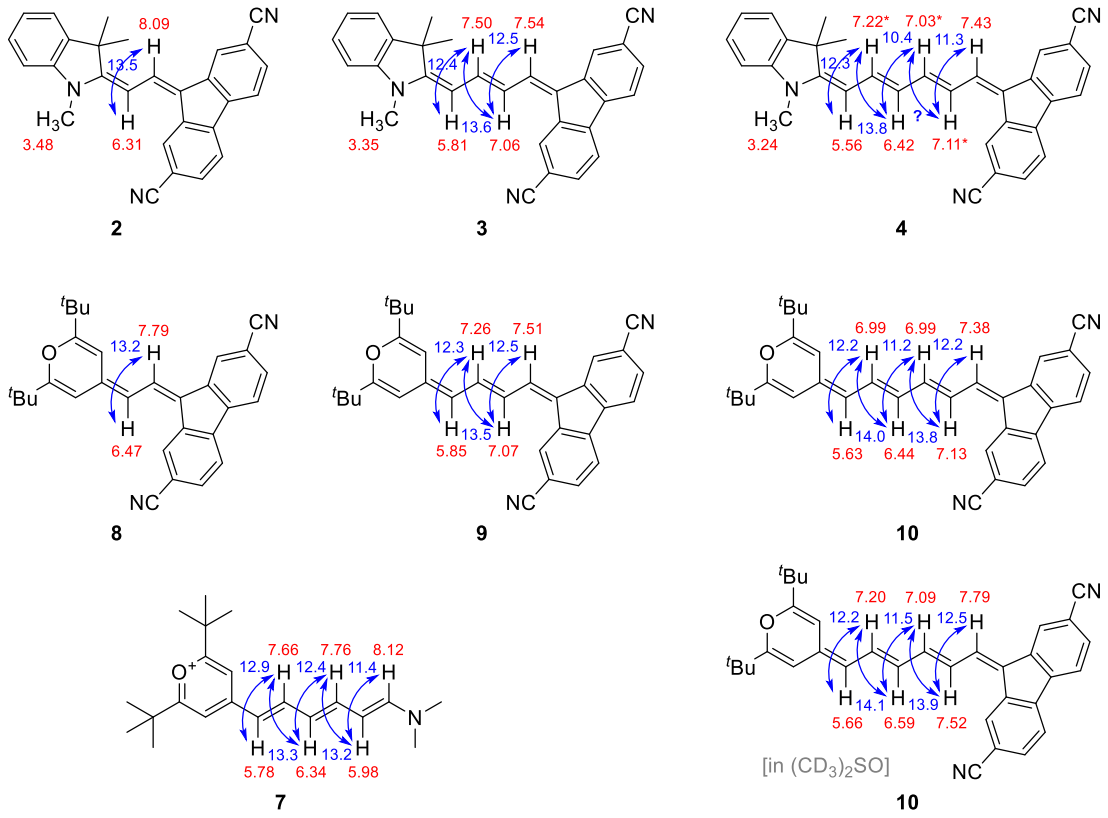
Figure S1. Some ^{1}H NMR parameters of the studied dyes



• *measured in $CDCl_3$ if not stated otherwise*

• *spin-spin coupling constants in the polymethine chain are shown in blue*

• *chemical shifts of selected H-atoms are shown in red (* those, estimated via deconvolution of complex multiplets)*

UV–Vis spectra of merocyanines 2–4 and 8–10

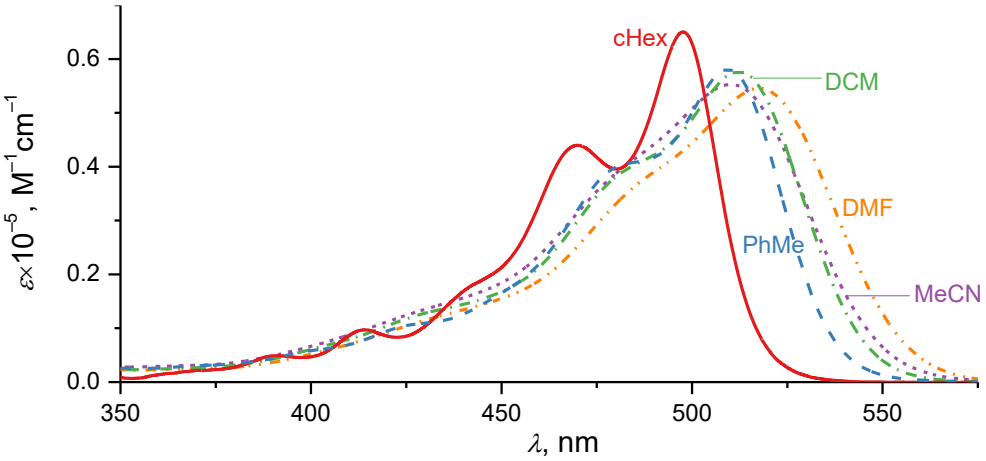


Figure S2. Electronic absorption spectra of dye **2** in solvents of varying polarity.

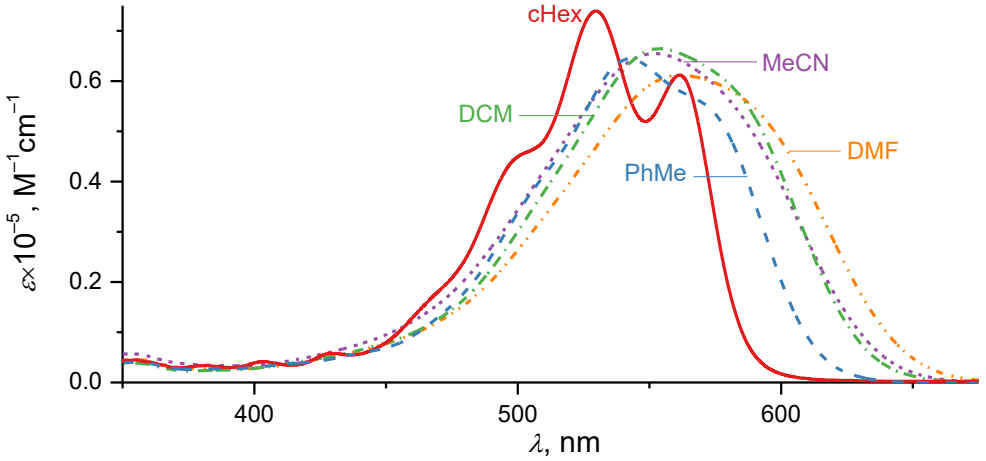


Figure S3. Electronic absorption spectra of dye **3** in solvents of varying polarity (Figure 2A).

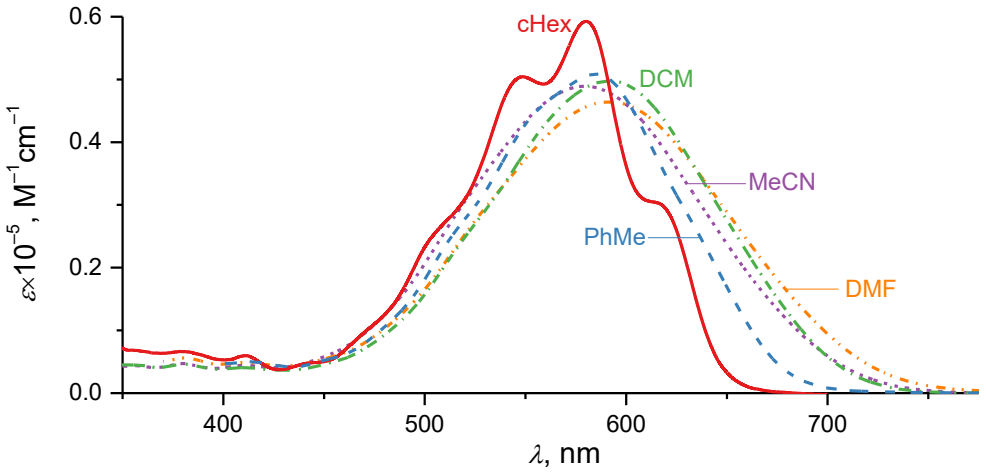


Figure S4. Electronic absorption spectra of dye **4** in solvents of varying polarity.

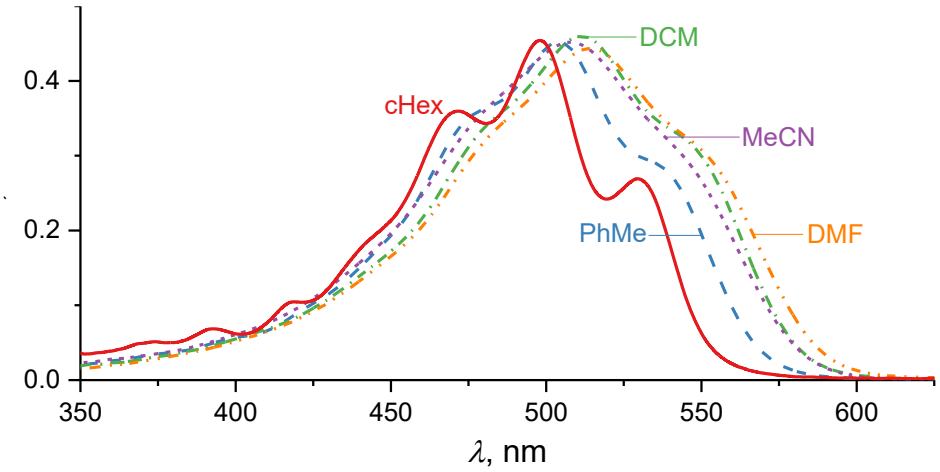


Figure S5. Electronic absorption spectra of dye **8** in solvents of varying polarity.

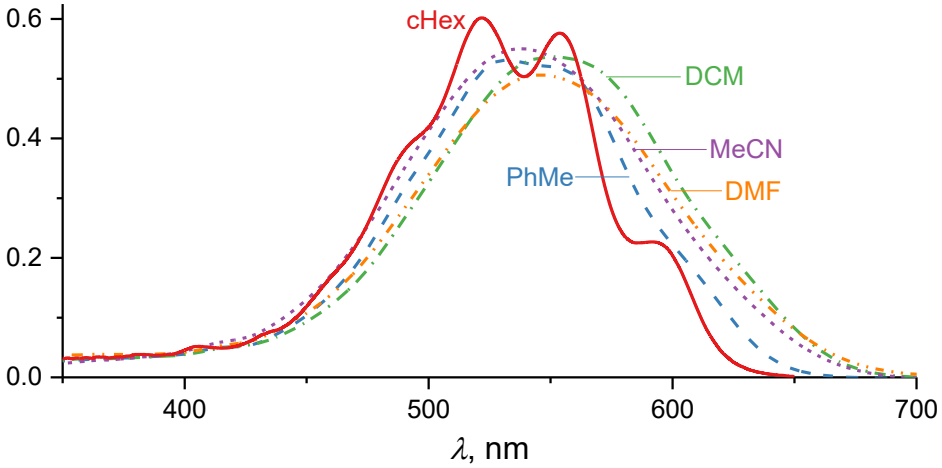


Figure S6. Electronic absorption spectra of dye **9** in solvents of varying polarity (Figure 2B).

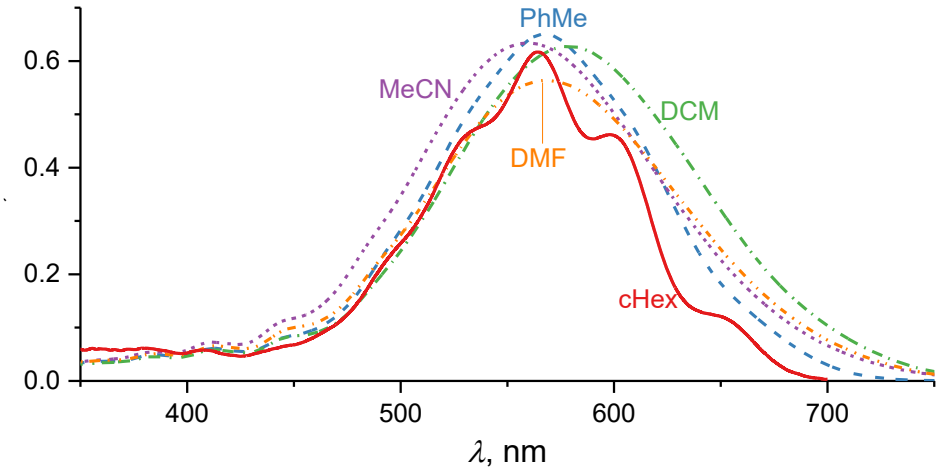
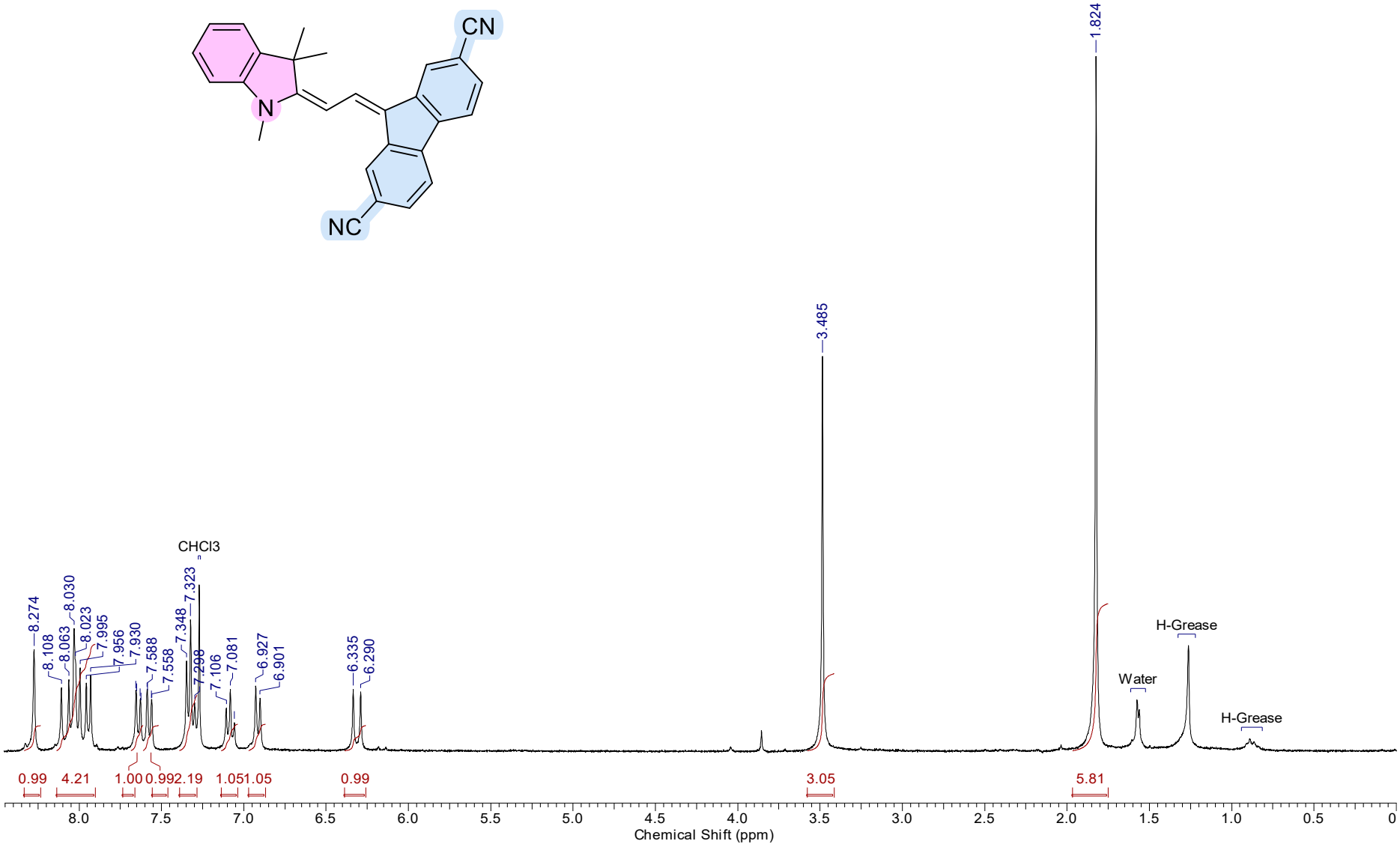


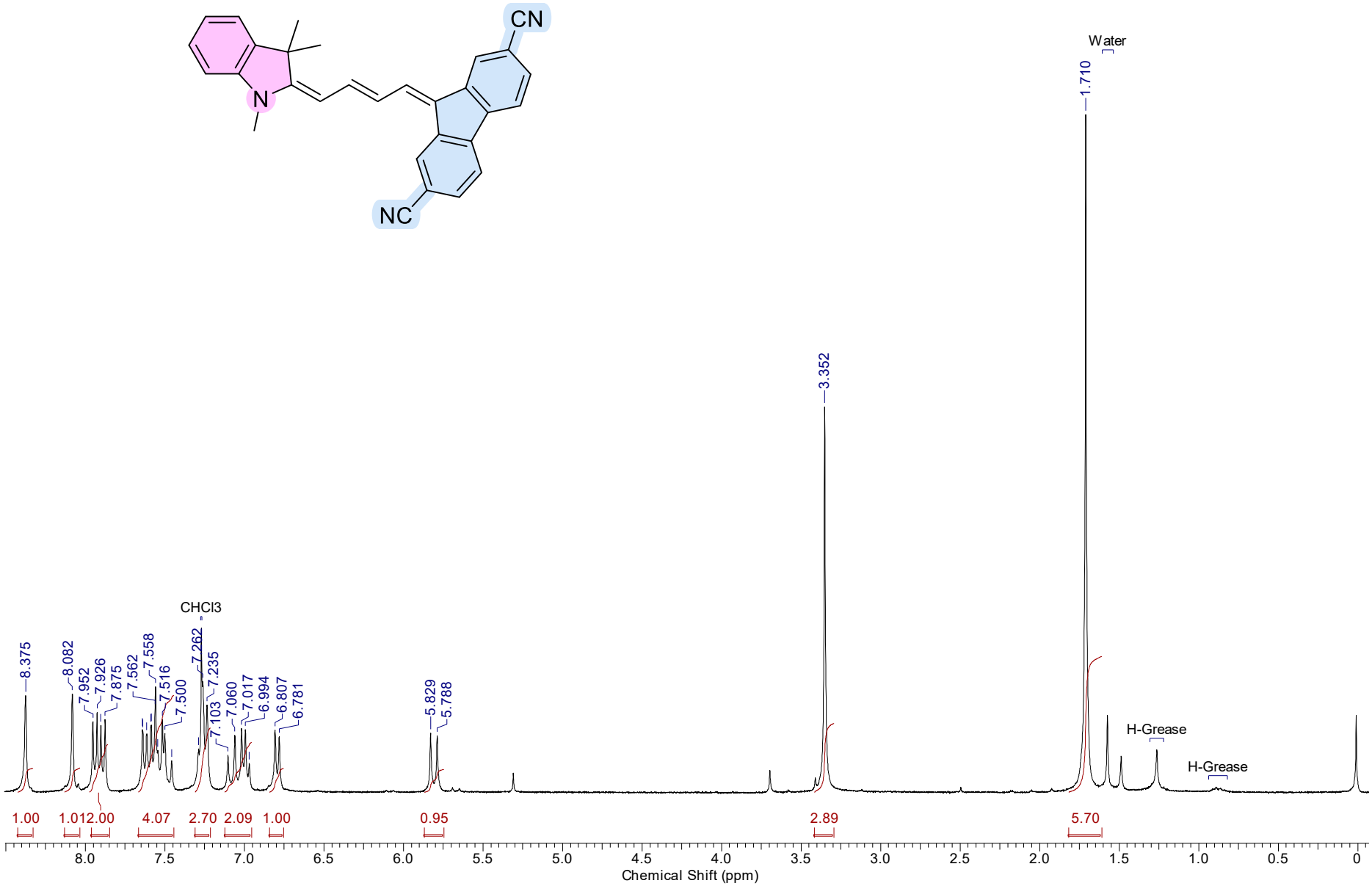
Figure S7. Electronic absorption spectra of dye **10** in solvents of varying polarity.

^{1}H NMR spectra of the synthesized dyes

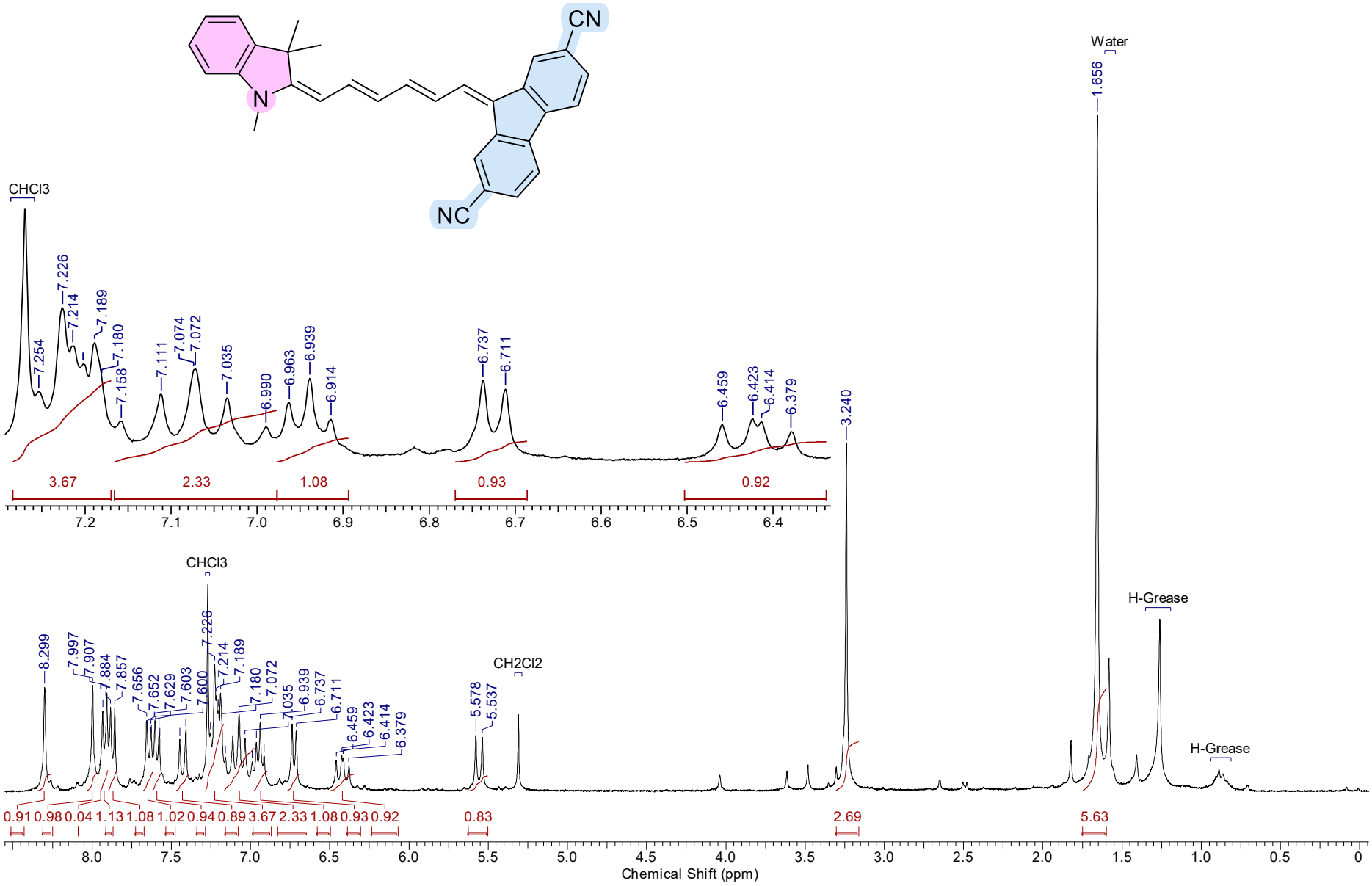
Dye 2 — ^{1}H NMR spectrum in $CDCl_3$



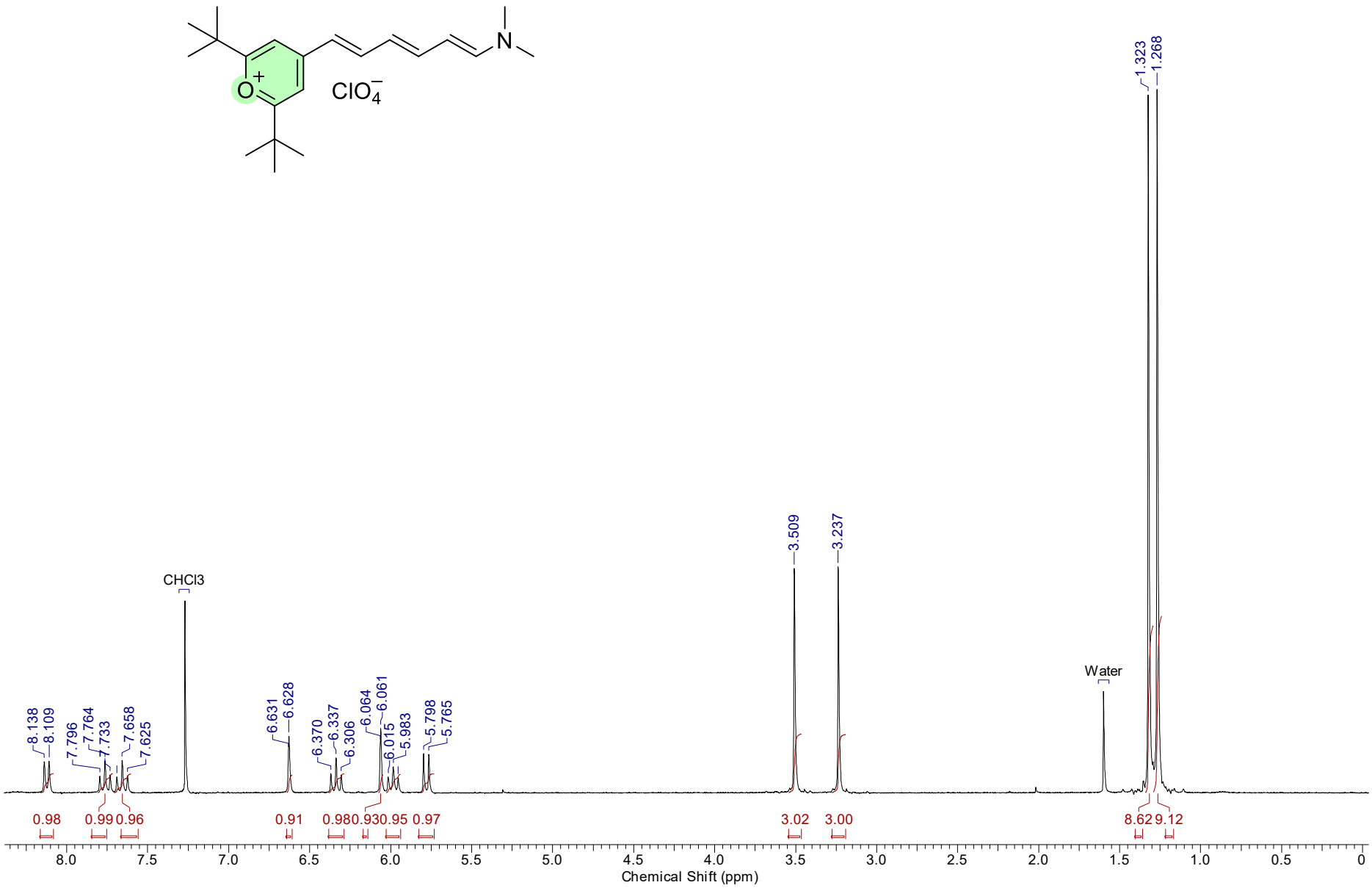
Dye 3 — ^{1}H NMR spectrum in $CDCl_3$



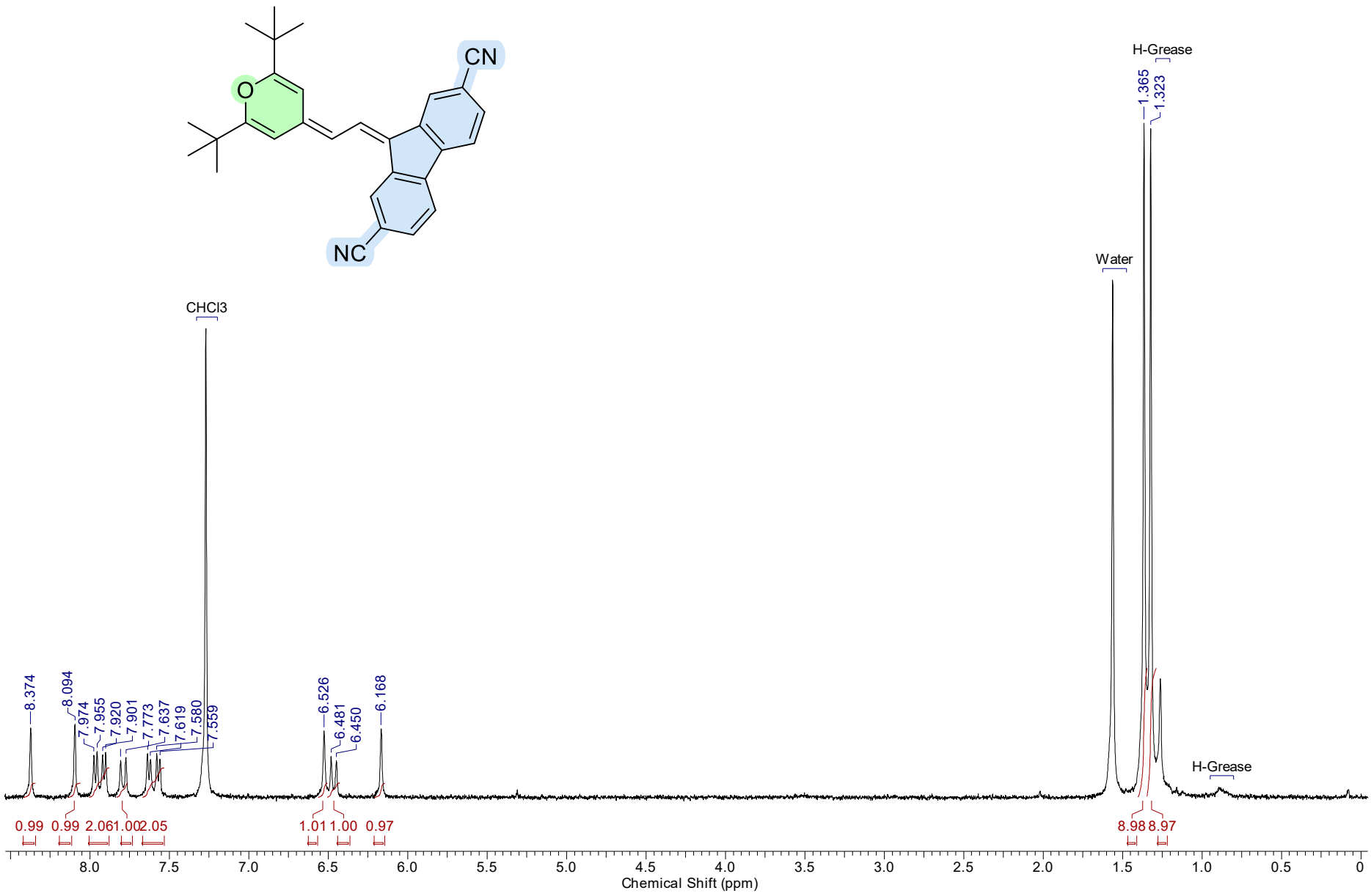
Dye 4 — ^{1}H NMR spectrum in $CDCl_3$



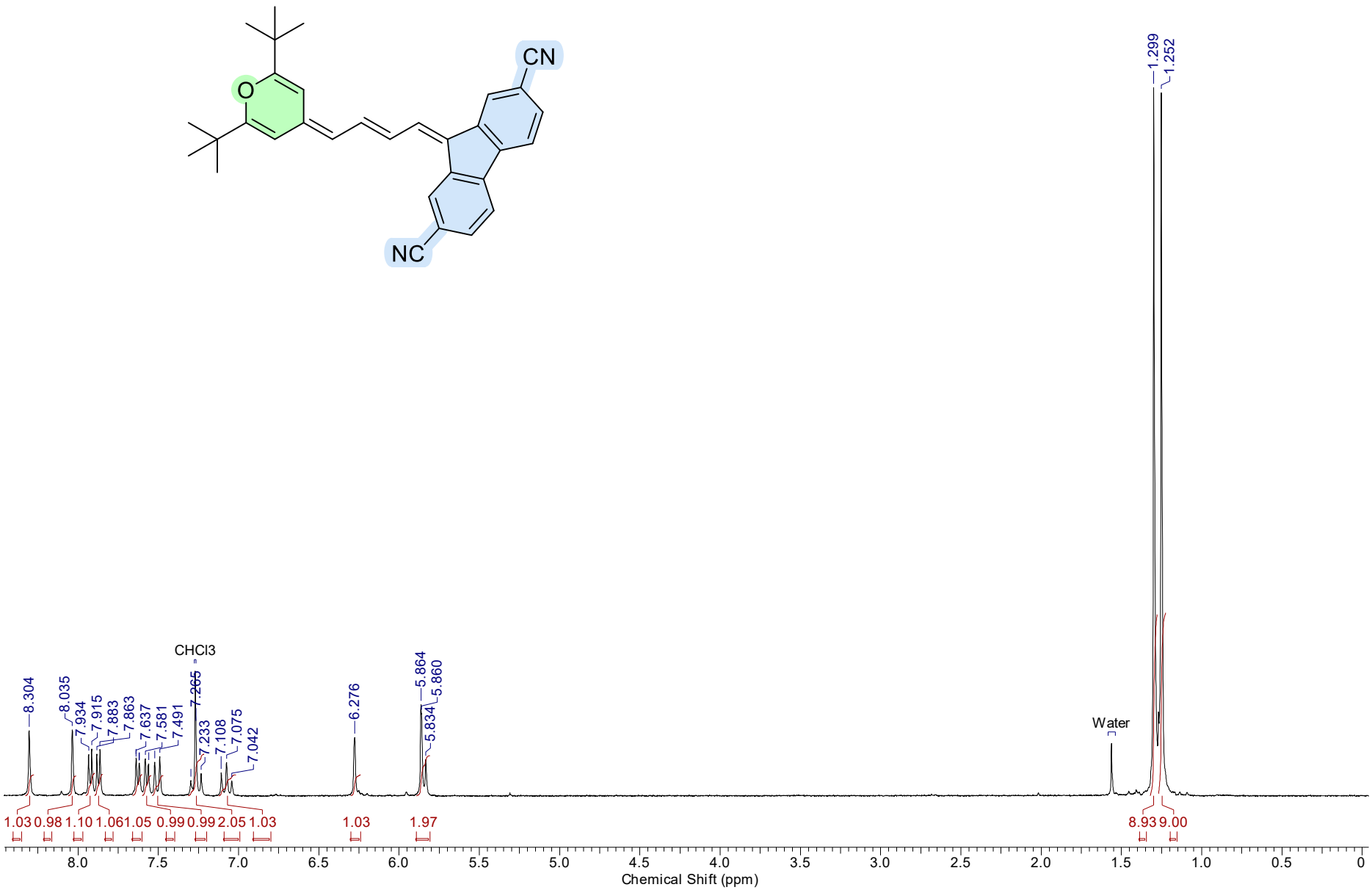
Hemicyanine 7 — ^{1}H NMR spectrum in $CDCl_3$



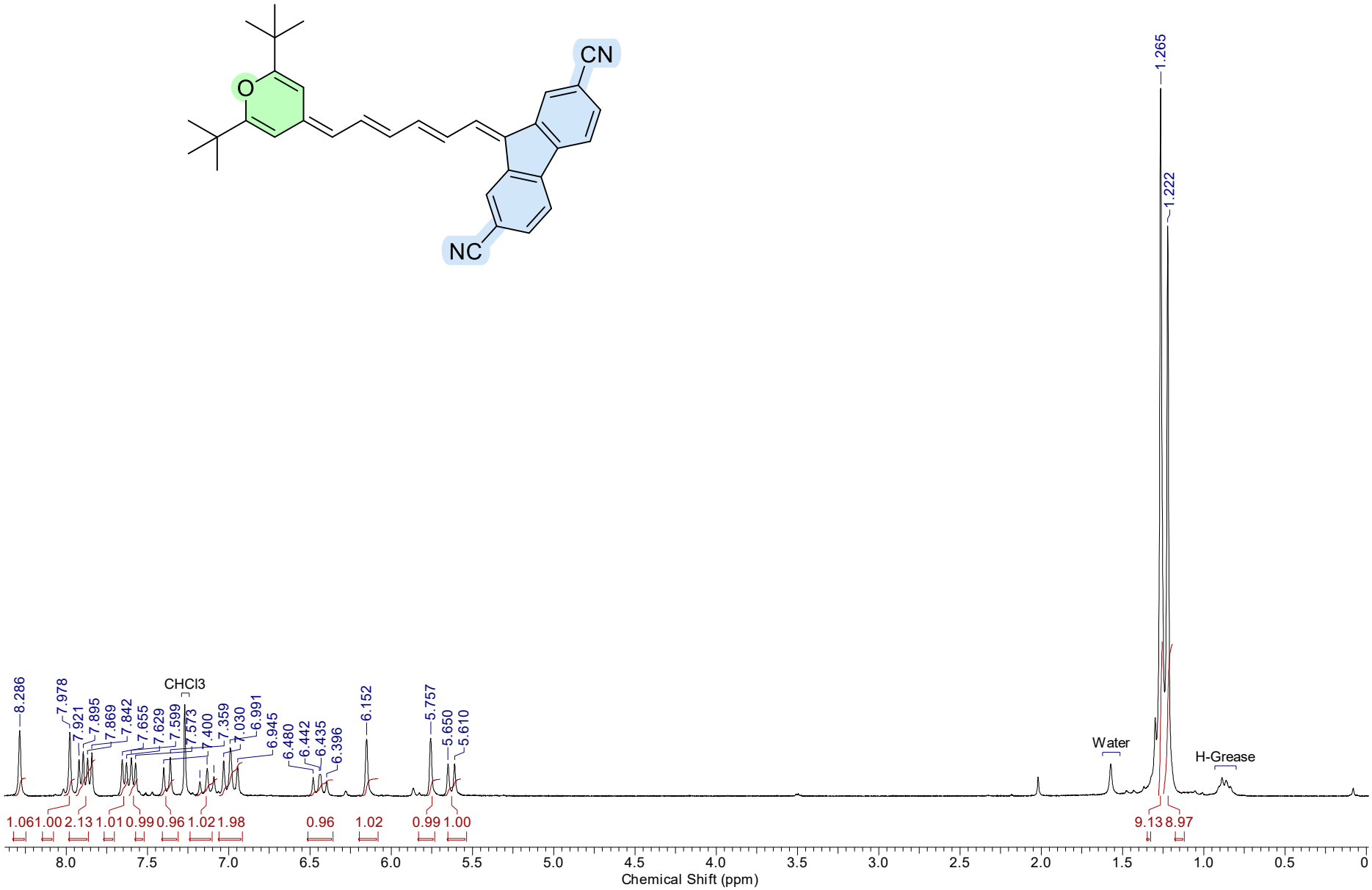
Dye 8 — ^{1}H NMR spectrum in $CDCl_3$



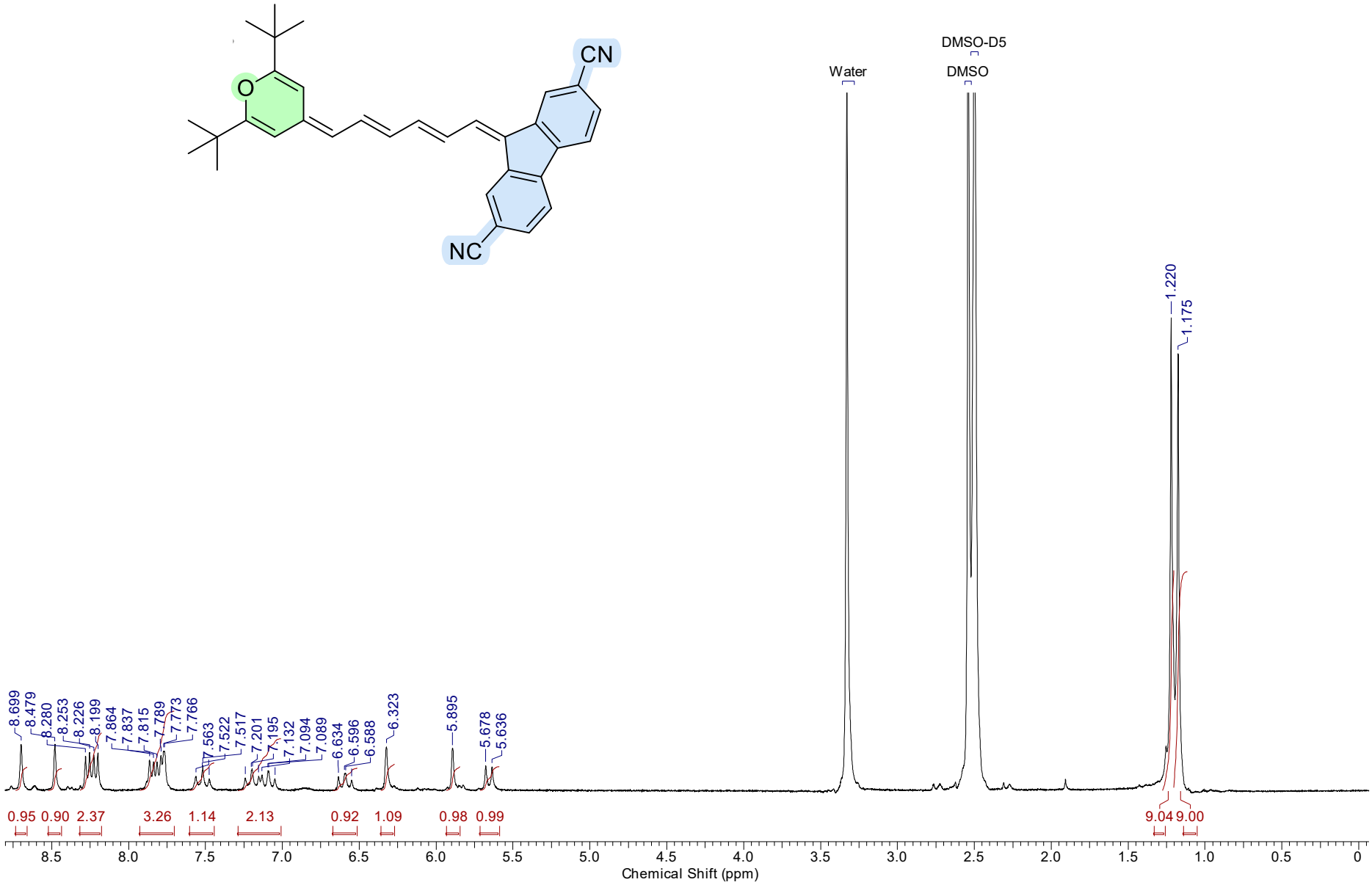
Dye 9 — ^{1}H NMR spectrum in $CDCl_3$



Dye 10 — ^{1}H NMR spectrum in $CDCl_3$ (~20 mg in 0.67 mL)



Dye 10 — ^{1}H NMR spectrum in $(CD_3)_2SO$ (low solubility)



Cartesian atomic coordinates (in Å) and final energies for the optimized ground-state geometries of molecules 2–4 and 8–10

***Dye 2**, DFT-B3LYP/6-31G(d,p) optimization; final energy -1243.90592889 Hartree*

C	-2.269147	1.239647	0.007062
C	-1.833477	2.565390	0.042302
H	-0.785094	2.827999	0.081061
C	-2.777637	3.606207	0.044545
C	-4.160424	3.334112	0.016189
H	-4.865961	4.157504	0.017255
C	-4.604536	2.017397	-0.007455
H	-5.669387	1.805323	-0.021578
C	-3.672332	0.978047	-0.009284
C	-3.870842	-0.464268	-0.017448
C	-5.038395	-1.231756	-0.031161
H	-6.015658	-0.758423	-0.040811
C	-4.939996	-2.618012	-0.032069
H	-5.830918	-3.235931	-0.041991
C	-3.670549	-3.236147	-0.020218
C	-2.494245	-2.469724	-0.008470
H	-1.535111	-2.977146	-0.001354
C	-2.590744	-1.079128	-0.005634
C	2.229792	0.201199	-0.042094
C	2.870879	-1.198065	0.050851
N	3.240146	1.137343	-0.104892
C	4.353672	-0.851787	0.040841
C	4.509753	0.535778	-0.052936
C	5.468817	-1.673223	0.105385
C	6.745685	-1.095227	0.076338
C	6.886034	0.290172	-0.016725
C	5.768970	1.130802	-0.082973
H	7.626557	-1.726916	0.126714
H	7.878214	0.730560	-0.038237
H	5.898484	2.205179	-0.153951
C	-1.548605	-0.042026	-0.000302
C	-0.205329	-0.329503	-0.012374
C	0.901669	0.560718	-0.060406
H	0.031810	-1.388295	0.007156
H	0.689983	1.618411	-0.130939
C	2.522798	-2.072480	-1.177845
C	2.498299	-1.915825	1.369617
C	3.006631	2.565766	-0.199988
H	5.359691	-2.751836	0.178071
H	2.786212	-1.562030	-2.107983
H	3.085946	-3.009703	-1.134437
H	1.459505	-2.319927	-1.215553
H	1.433057	-2.153101	1.417122
H	3.057623	-2.852888	1.450850
H	2.747440	-1.296610	2.235428
H	2.458325	2.930828	0.675863
H	3.959684	3.088747	-0.253271
H	2.429198	2.805376	-1.099607
C	-2.317580	4.963255	0.078430
N	-1.932143	6.061326	0.105183
C	-3.578942	-4.666686	-0.020967
N	-3.499565	-5.827944	-0.021588

***Dye 3**, DFT-B3LYP/6-31G(d,p) optimization; final energy -1321.31631799 Hartree*

C	2.656874	-0.112892	0.000000
C	3.718617	-1.129903	-0.000001
C	3.646706	-2.521710	-0.000003
H	2.696262	-3.044973	-0.000005
C	4.837375	-3.266063	-0.000003
C	6.094847	-2.624015	-0.000001
H	6.997238	-3.225212	-0.000002
C	6.168062	-1.235881	0.000000
H	7.136574	-0.744824	0.000001
C	4.986538	-0.490567	0.000001
C	4.760362	0.948435	0.000002
C	5.671566	2.006055	0.000003
H	6.740639	1.815904	0.000004
C	5.199813	3.313433	0.000003
H	5.888396	4.151093	0.000004
C	3.811446	3.558262	0.000003
C	2.888280	2.498792	0.000001
H	1.833377	2.737342	0.000000
C	3.353093	1.182956	0.000001
C	-3.574886	0.321263	-0.000002
C	-4.133173	-1.115305	0.000005
N	-4.639668	1.200971	-0.000003
C	-5.633695	-0.855977	0.000004
C	-5.870346	0.524084	-0.000002
C	-3.723408	-1.889777	1.274984
C	-3.723409	-1.889793	-1.274963
C	-4.487372	2.642552	-0.000013
C	-6.698870	-1.743320	0.000005
C	-8.007811	-1.240829	0.000002
C	-8.228859	0.137074	-0.000004
C	-7.162978	1.044217	-0.000005
H	-4.014277	-1.342216	2.175379
H	-4.223551	-2.863051	1.293727
H	-2.645511	-2.063057	1.315635
H	-2.645512	-2.063079	-1.315612
H	-4.223555	-2.863066	-1.293694
H	-4.014276	-1.342243	-2.175365
H	-3.941464	2.976262	-0.889599
H	-5.468795	3.113511	-0.000014
H	-3.941461	2.976274	0.889566
H	-6.526436	-2.816164	0.000010
H	-8.850088	-1.925003	0.000003
H	-9.245178	0.519221	-0.000006
H	-7.355465	2.111535	-0.000009
C	-2.270169	0.749534	-0.000004
C	-1.100661	-0.061125	-0.000002
H	-2.096169	1.822249	-0.000006
H	-1.214960	-1.141923	-0.000003
C	1.319247	-0.421248	0.000000
H	1.083273	-1.485835	0.000000
C	0.181079	0.430161	0.000000
H	0.312081	1.506881	0.000001
C	3.327226	4.907424	0.000004
N	2.926917	6.000441	-0.000002
C	4.773863	-4.698148	-0.000004
N	4.718853	-5.860807	-0.000006

***Dye 4**, DFT-B3LYP/6-31G(d,p) optimization; final energy -1398.72649325 Hartree*

C	-3.784364	-0.164057	0.000001
C	-4.854674	-1.172348	0.000001
C	-4.793702	-2.564611	0.000003
H	-3.847443	-3.095330	0.000005
C	-5.990511	-3.299214	0.000003
C	-7.242534	-2.646773	0.000001
H	-8.149833	-3.240552	0.000002
C	-7.304597	-1.257964	0.000000
H	-8.269093	-0.759093	-0.000002
C	-6.117076	-0.522582	-0.000001
C	-5.878914	0.914728	-0.000003
C	-6.781565	1.979410	-0.000005
H	-7.852140	1.797976	-0.000006
C	-6.298969	3.282890	-0.000008
H	-6.980687	4.126153	-0.000010
C	-4.908751	3.516627	-0.000008
C	-3.994043	2.449743	-0.000005
H	-2.937205	2.679614	-0.000005
C	-4.469936	1.137870	-0.000002
C	-2.449545	-0.484770	0.000003
H	-2.222210	-1.551015	0.000005
C	-1.304127	0.356835	0.000006
H	-1.425129	1.434623	0.000007
C	-0.026665	-0.144587	0.000007
H	0.095308	-1.229025	0.000005
C	1.161368	0.635680	0.000009
H	1.053919	1.720098	0.000012
C	2.421857	0.096102	0.000009
H	2.494767	-0.988178	0.000006
C	3.622886	0.862216	0.000013
H	3.488276	1.940687	0.000018
C	4.909895	0.386493	0.000009
C	5.414725	-1.069750	-0.000005
C	4.976472	-1.828791	-1.274732
H	5.288275	-1.292850	-2.175124
H	5.439206	-2.820490	-1.293227
H	3.892698	-1.960526	-1.315682
C	4.976480	-1.828812	1.274712
H	3.892707	-1.960549	1.315668
H	5.439215	-2.820512	1.293187
H	5.288290	-1.292887	2.175112
C	6.924024	-0.866448	-0.000008
C	7.955113	-1.793031	-0.000021
H	7.742225	-2.858623	-0.000031
C	9.282271	-1.340516	-0.000023
H	10.098165	-2.055960	-0.000033
C	9.554798	0.028091	-0.000011
H	10.584780	0.371843	-0.000012
C	8.523801	0.974707	0.000003
H	8.756487	2.034024	0.000011
C	7.212065	0.504152	0.000005
N	6.008656	1.226592	0.000017
C	5.909930	2.672093	0.000034
H	5.376499	3.026162	0.889545
H	6.908068	3.106717	0.000061
H	5.376535	3.026189	-0.889487
C	-5.939412	-4.731807	0.000005
N	-5.895416	-5.894920	0.000006
C	-4.415306	4.862483	-0.000011
N	-4.010047	5.953635	-0.000013

***Dye 8**, DFT-B3LYP/6-31G(d,p) optimization; final energy -1344.81015661 Hartree*

C	-2.987174	1.281351	0.014040
C	-2.583011	2.617157	0.051914
H	-1.540538	2.903410	0.081380
C	-3.552924	3.633738	0.062410
C	-4.928985	3.327479	0.038426
H	-5.654395	4.133404	0.046561
C	-5.341070	2.000627	0.008198
H	-6.400450	1.762564	-0.005314
C	-4.383354	0.984888	-0.002148
C	-4.545502	-0.461843	-0.023025
C	-5.692695	-1.259004	-0.042305
H	-6.681902	-0.811028	-0.045558
C	-5.558623	-2.642392	-0.057250
H	-6.433449	-3.282841	-0.071956
C	-4.273643	-3.227824	-0.053629
C	-3.117493	-2.431455	-0.035726
H	-2.145413	-2.913457	-0.034958
C	-3.249636	-1.043789	-0.019249
C	-2.234869	0.018650	-0.002590
C	-0.882490	-0.234028	-0.009308
C	0.206490	0.670360	-0.031388
H	-0.620996	-1.290355	-0.005676
H	0.000400	1.732974	-0.074232
C	-3.130212	5.002914	0.099840
N	-2.780405	6.112734	0.129848
C	-4.144705	-4.655357	-0.068938
N	-4.034126	-5.814051	-0.081251
C	2.572401	1.334660	-0.061423
C	3.889440	1.030801	-0.051549
O	4.302236	-0.277881	0.001315
C	3.384024	-1.295588	0.046420
C	2.056858	-1.035894	0.038449
C	1.546871	0.316769	-0.018485
C	5.070195	1.985805	-0.093541
C	4.596089	3.448288	-0.152473
C	5.928762	1.780864	1.177964
C	5.922692	1.677286	-1.348126
C	4.065585	-2.653269	0.103621
C	3.032272	-3.792109	0.151712
C	4.950760	-2.824533	-1.154577
C	4.951006	-2.717904	1.371578
H	2.273416	2.374021	-0.103626
H	1.374545	-1.872272	0.078844
H	5.466254	4.110458	-0.181585
H	3.999063	3.646228	-1.048055
H	4.002938	3.719148	0.726436
H	5.352181	2.001698	2.081838
H	6.793061	2.452110	1.153983
H	6.297203	0.754624	1.249201
H	6.291002	0.648590	-1.337008
H	5.341708	1.823572	-2.264243
H	6.786929	2.348114	-1.383236
H	3.553467	-4.752908	0.191364
H	2.394390	-3.725498	1.038563
H	2.393121	-3.799315	-0.736688
H	5.460557	-3.792504	-1.119860
H	5.710658	-2.041922	-1.217274
H	4.347806	-2.790980	-2.067575
H	4.348108	-2.607980	2.278590
H	5.461338	-3.685095	1.418250
H	5.710468	-1.932367	1.368089

***Dye 9**, DFT-B3LYP/6-31G(d,p) optimization; final energy -1422.22059722 Hartree*

C	3.403580	-0.047699	-0.000001
C	4.443382	-1.086228	0.000001
C	4.342433	-2.476386	0.000001
H	3.381192	-2.979510	0.000000
C	5.517186	-3.245534	0.000003
C	6.787942	-2.629982	0.000005
H	7.677538	-3.249966	0.000006
C	6.890223	-1.243631	0.000004
H	7.868852	-0.773024	0.000005
C	5.724722	-0.473592	0.000002
C	5.528388	0.969598	0.000001
C	6.461165	2.008144	0.000001
H	7.526118	1.796035	0.000003
C	6.016292	3.324858	-0.000001
H	6.721857	4.148269	-0.000001
C	4.633123	3.598340	-0.000004
C	3.688127	2.558391	-0.000004
H	2.638244	2.818354	-0.000006
C	4.126013	1.233078	-0.000001
C	-1.510146	0.892127	0.000000
C	-0.354557	0.073287	-0.000001
H	-1.346633	1.968362	0.000001
H	-0.486624	-1.008253	-0.000003
C	2.058782	-0.329656	-0.000001
H	1.802474	-1.389504	-0.000001
C	0.938438	0.541747	-0.000001
H	1.087627	1.616039	0.000000
C	4.178795	4.957897	-0.000006
N	3.805541	6.060430	-0.000008
C	5.423473	-4.675937	0.000004
N	5.343704	-5.837194	0.000004
H	-3.682470	2.470053	0.000005
C	-3.914385	1.412853	0.000002
C	-2.825302	0.461643	-0.000001
C	-3.246744	-0.923097	-0.000003
H	-2.509107	-1.712466	-0.000005
C	-4.553737	-1.268323	-0.000003
O	-5.537055	-0.310460	-0.000001
C	-5.208553	1.024112	0.000002
C	-5.147036	-2.667932	-0.000006
C	-4.043085	-3.739418	-0.000008
H	-4.501686	-4.732488	-0.000011
H	-3.407704	-3.668351	-0.888332
H	-3.407704	-3.668356	0.888317
C	-6.023072	-2.842879	1.264030
H	-6.830871	-2.107766	1.293941
H	-5.425862	-2.732926	2.174823
H	-5.425864	-2.732921	-2.174834
H	-6.830871	-2.107760	-1.293951
C	-6.023074	-2.842875	-1.264041
H	-6.470846	-3.841714	-1.269981
C	-6.449078	1.901106	0.000006
C	-7.286457	1.589696	1.263975
H	-7.586640	0.539501	1.294367
H	-7.586649	0.539504	-1.294351
C	-7.286465	1.589699	-1.263958
H	-8.192891	2.203402	-1.269390
H	-6.720865	1.810880	-2.174690
H	-8.192883	2.203399	1.269414
H	-6.720851	1.810875	2.174704
C	-6.071417	3.392555	0.000006
H	-6.982830	3.997502	0.000008
H	-5.492615	3.664914	-0.888006
H	-5.492612	3.664913	0.888017
H	-6.470843	-3.841719	1.269968

***Dye 10**, DFT-B3LYP/6-31G(d,p) optimization; final energy -1499.63088861 Hartree*

C	4.587896	0.107954	0.000007
C	5.639826	1.134721	-0.000010
C	5.554359	2.525837	-0.000019
H	4.598848	3.039712	-0.000011
C	6.737921	3.281503	-0.000040
C	8.001422	2.651369	-0.000053
H	8.898049	3.261148	-0.000070
C	8.088039	1.263877	-0.000044
H	9.061236	0.782168	-0.000055
C	6.913817	0.507443	-0.000022
C	6.700998	-0.933628	-0.000007
C	7.622108	-1.982362	-0.000006
H	8.689362	-1.782224	-0.000023
C	7.162368	-3.294027	0.000020
H	7.858658	-4.125299	0.000021
C	5.776336	-3.552091	0.000047
C	4.843015	-2.501545	0.000045
H	3.790310	-2.749779	0.000075
C	5.295922	-1.181367	0.000014
C	3.246870	0.405795	0.000008
H	3.001876	1.468130	0.000014
C	2.116571	-0.453861	-0.000006
H	2.254510	-1.529636	-0.000036
C	0.829784	0.027636	0.000006
H	0.691169	1.110058	0.000034
C	-0.343913	-0.769738	-0.000016
H	-0.221474	-1.852414	-0.000045
C	-1.615539	-0.249358	-0.000003
H	-1.704321	0.836485	0.000029
C	-2.803469	-1.022467	-0.000028
H	-2.680654	-2.104206	-0.000059
C	6.661371	4.712945	-0.000050
N	6.596672	5.875116	-0.000056
C	5.307479	-4.906719	0.000080
N	4.923521	-6.005544	0.000109
H	-5.035185	-2.517002	-0.000076
C	-5.226326	-1.451618	-0.000046
C	-4.100778	-0.543017	-0.000014
C	-4.469657	0.857255	0.000028
H	-3.702104	1.617642	0.000057
C	-5.762139	1.252220	0.000034
O	-6.782536	0.332912	0.000000
C	-6.504411	-1.013851	-0.000038
C	-6.301455	2.673561	0.000079
C	-5.157336	3.702013	0.000115
H	-5.577476	4.712006	0.000143
H	-4.525134	3.606237	0.888401
H	-4.525125	3.606289	-0.888171
C	-7.170137	2.882344	-1.263856
H	-8.004995	2.178143	-1.294174
H	-6.577326	2.750140	-2.174585
H	-6.577340	2.749989	2.174746
H	-8.005007	2.178064	1.294285
C	-7.170144	2.882261	1.264022
H	-7.580022	3.897292	1.269817
C	-7.777618	-1.842770	-0.000069
C	-8.602749	-1.499773	-1.263896
H	-8.862111	-0.438767	-1.294342
H	-8.862129	-0.438845	1.294273
C	-8.602762	-1.499848	1.263769
H	-9.532243	-2.078118	1.269179
H	-8.046056	-1.742617	2.174500
H	-9.532233	-2.078038	-1.269345
H	-8.046038	-1.742494	-2.174635
C	-7.457400	-3.347559	-0.000112
H	-8.391201	-3.917403	-0.000135
H	-6.889259	-3.641607	0.887887
H	-6.889247	-3.641554	-0.888122
H	-7.580022	3.897372	-1.269581