Supplementary Materials for :

1-Benzyl-1-[2,8-bis(trifluoromethyl)quinolin-4-yl]-hexahydro-oxazolo[3,4-*a*]pyridin-3-one

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S1. Plots of NMR spectra

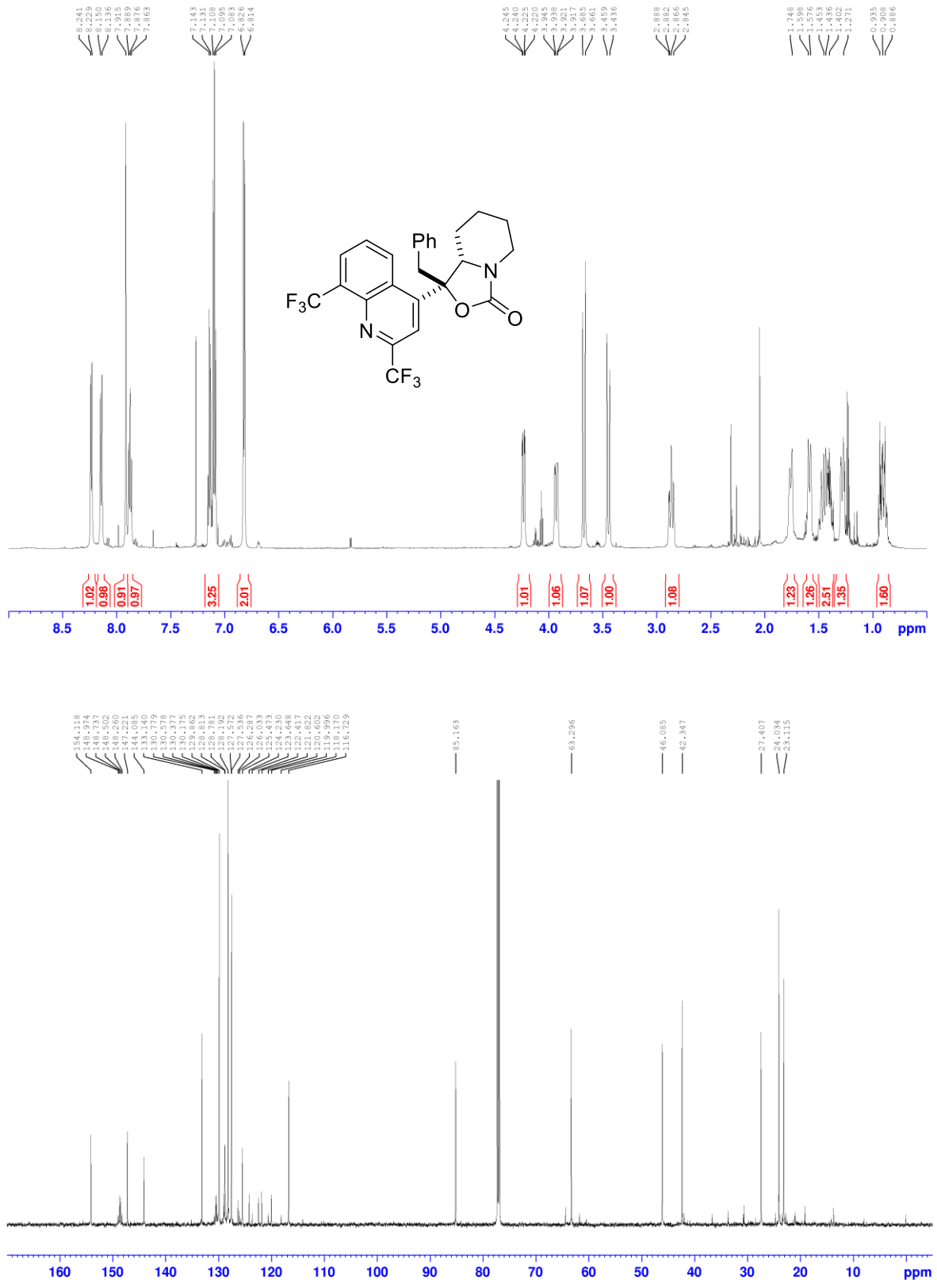

Figure S1. ^{1}H (600 MHz) and $^{13}C\{^{1}H\}$ NMR (151 MHz) spectra for **1** in $CDCl_3$+TMS.

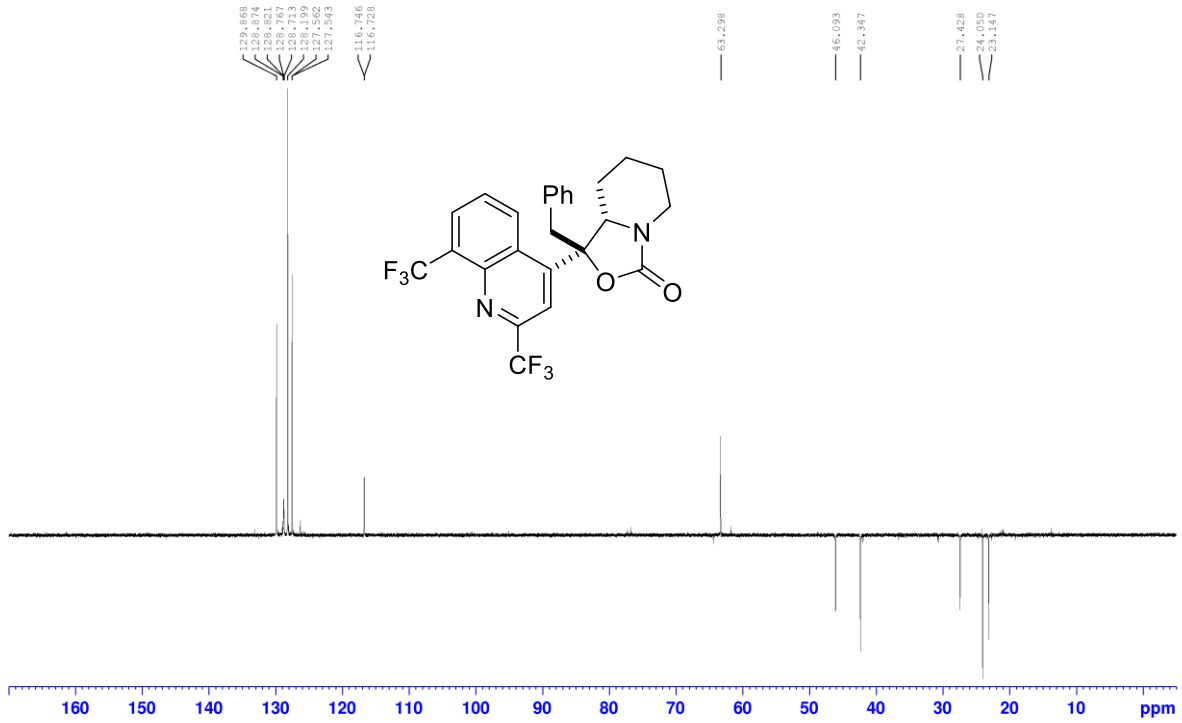

Figure S2. ^{13}C DEPT-135 (100 MHz) spectrum for **1** in $CDCl_3$+TMS. Positive phase (CH/CH_3), negative phase (CH_2).

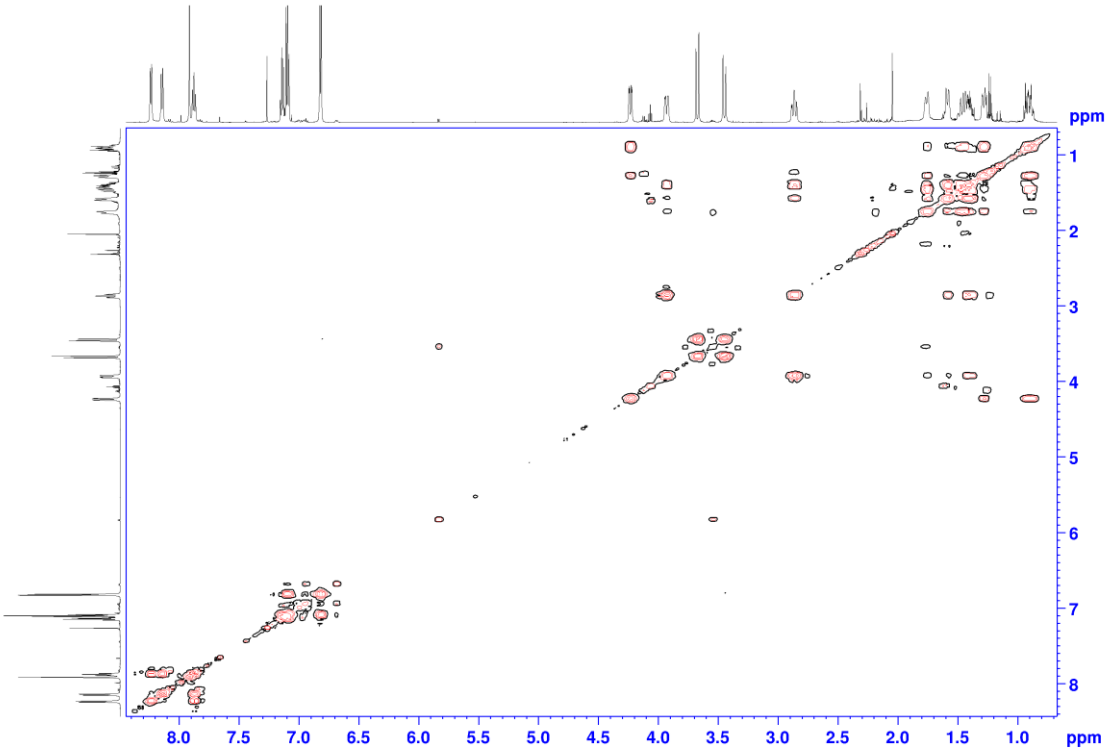

Figure S3. ^{1}H COSY experiment (600 MHz) for **1** in $CDCl_3$. For spectral assignment, see Figure 2.

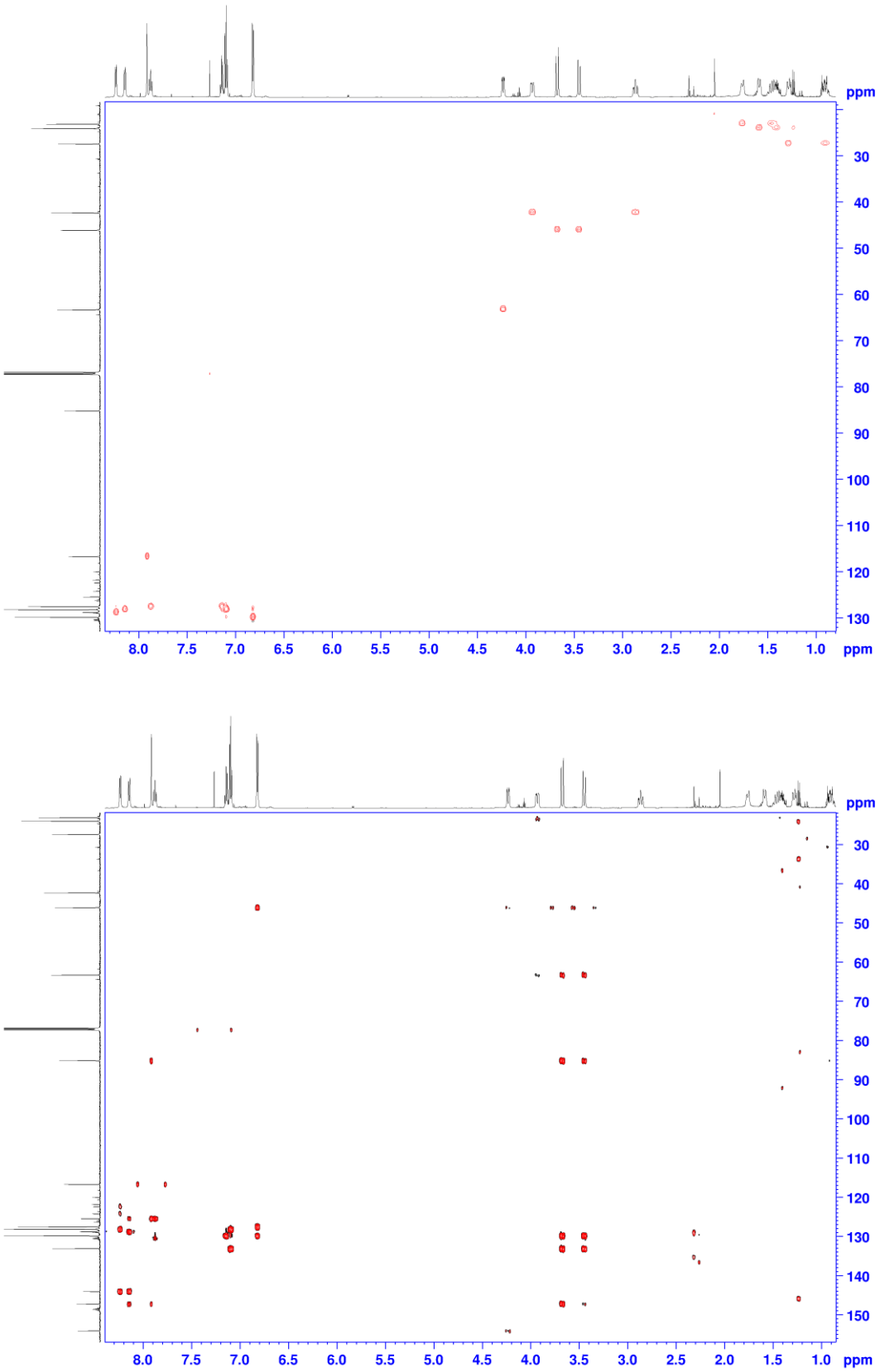

Figure S4. $^{1}H,^{13}C$ HSQC and HMBC experiments (600 / 151 MHz) for **1** in $CDCl_3$. For spectral assignment, see Figure 2.

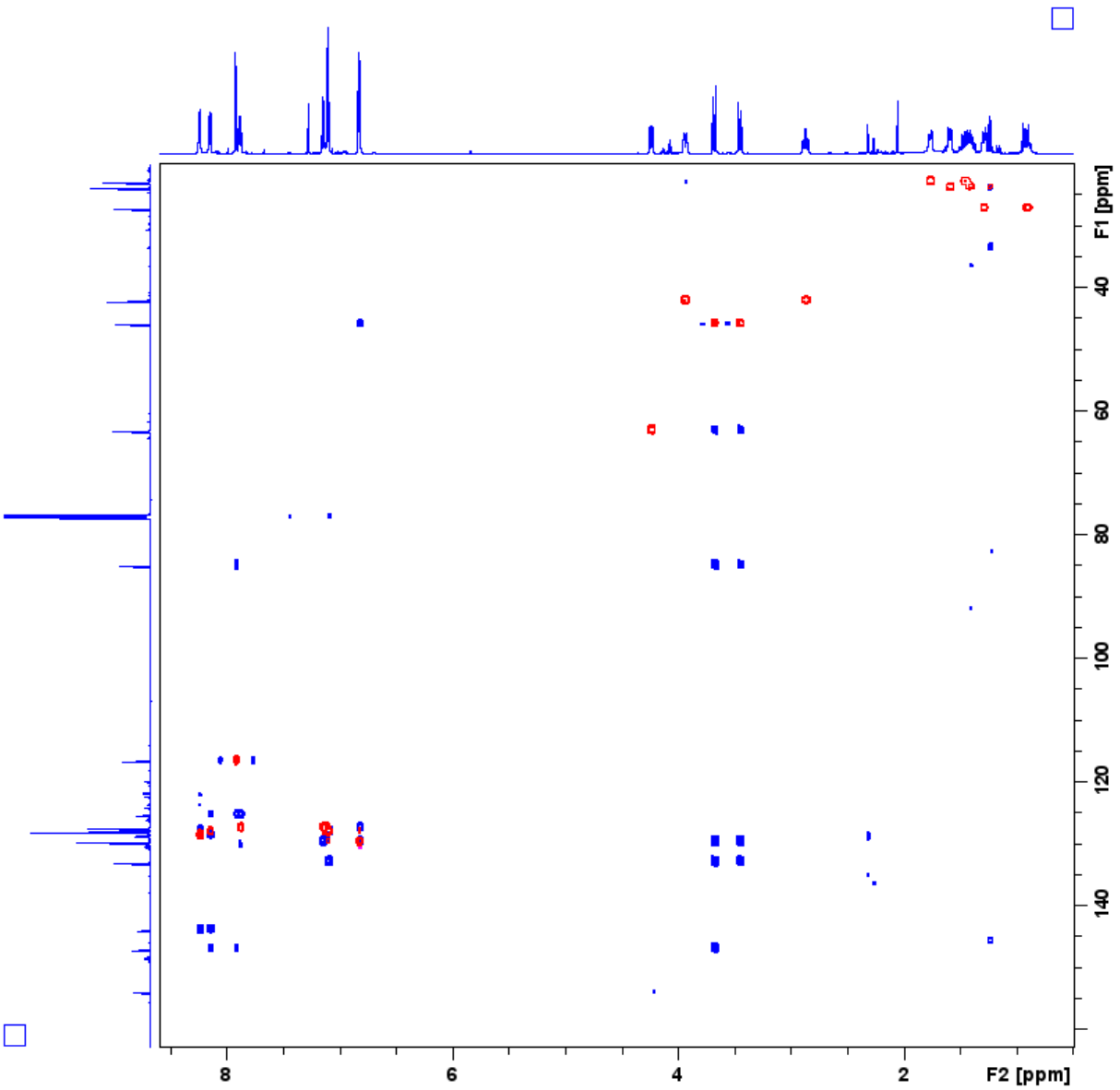

Figure S5. Superimposed $^{1}H,^{13}C$ HSQC and $^{1}H,^{13}C$ HMBC experiments (600 / 151 MHz) for **1** in $CDCl_3$. For spectral assignment, see Figure 2.

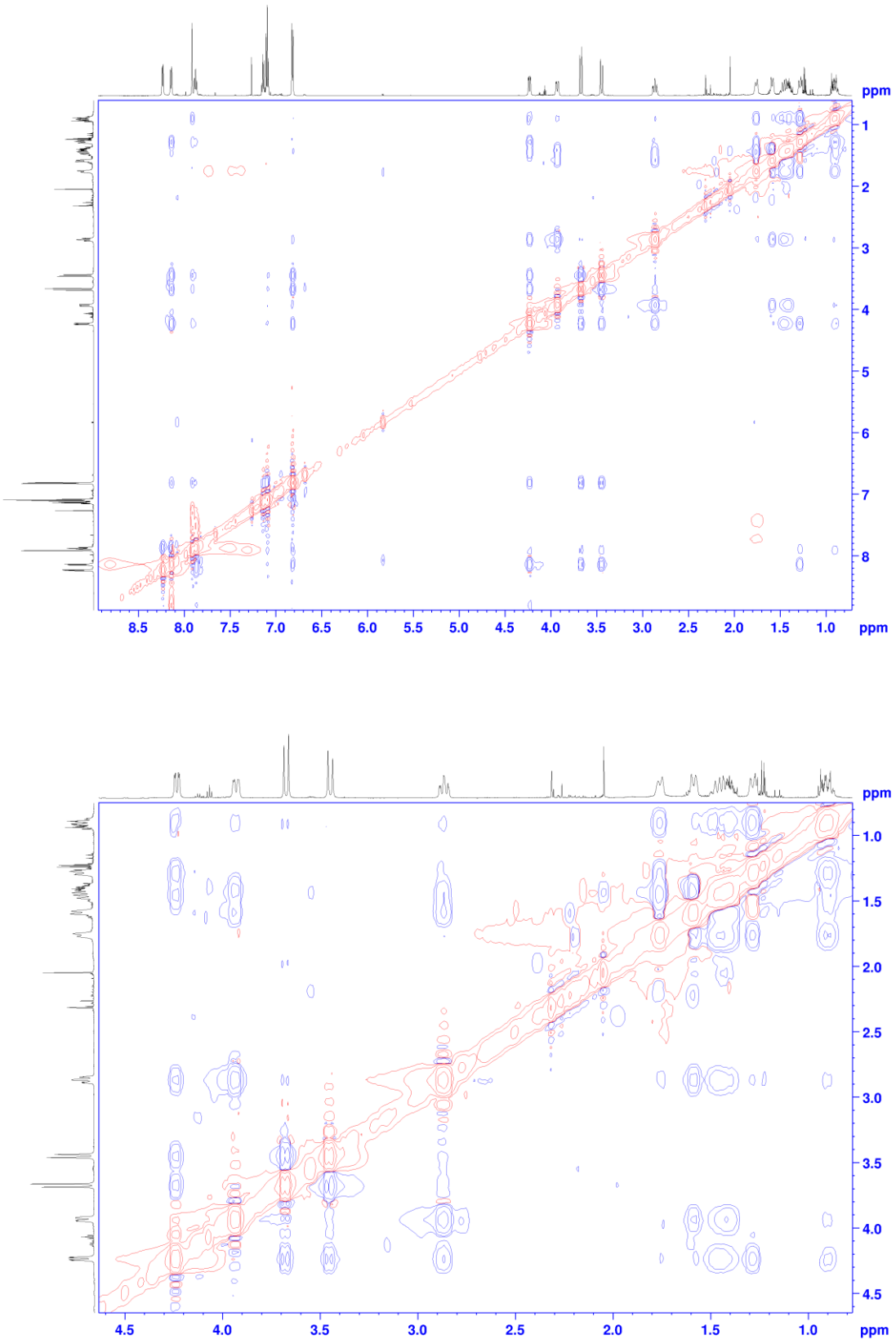

Figure S6. ^{1}H NOESY experiment (600 MHz) for **1** in $CDCl_3$ and expansion of aliphatic region. For spectral assignment, see Figure 2.

S2. Spectral data for compound **2**

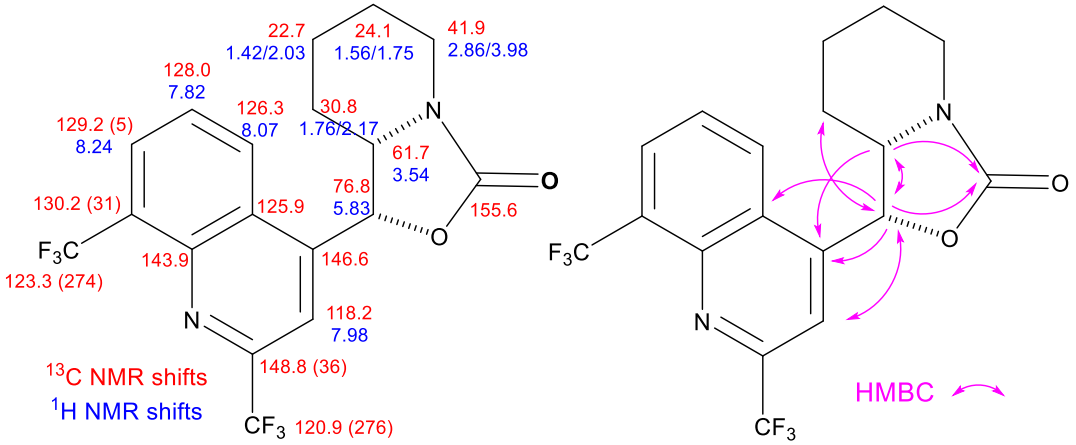

Figure S7. Spectral assignment, and ^{1}H,^{13}C-HMBC correlations for compound **2**.

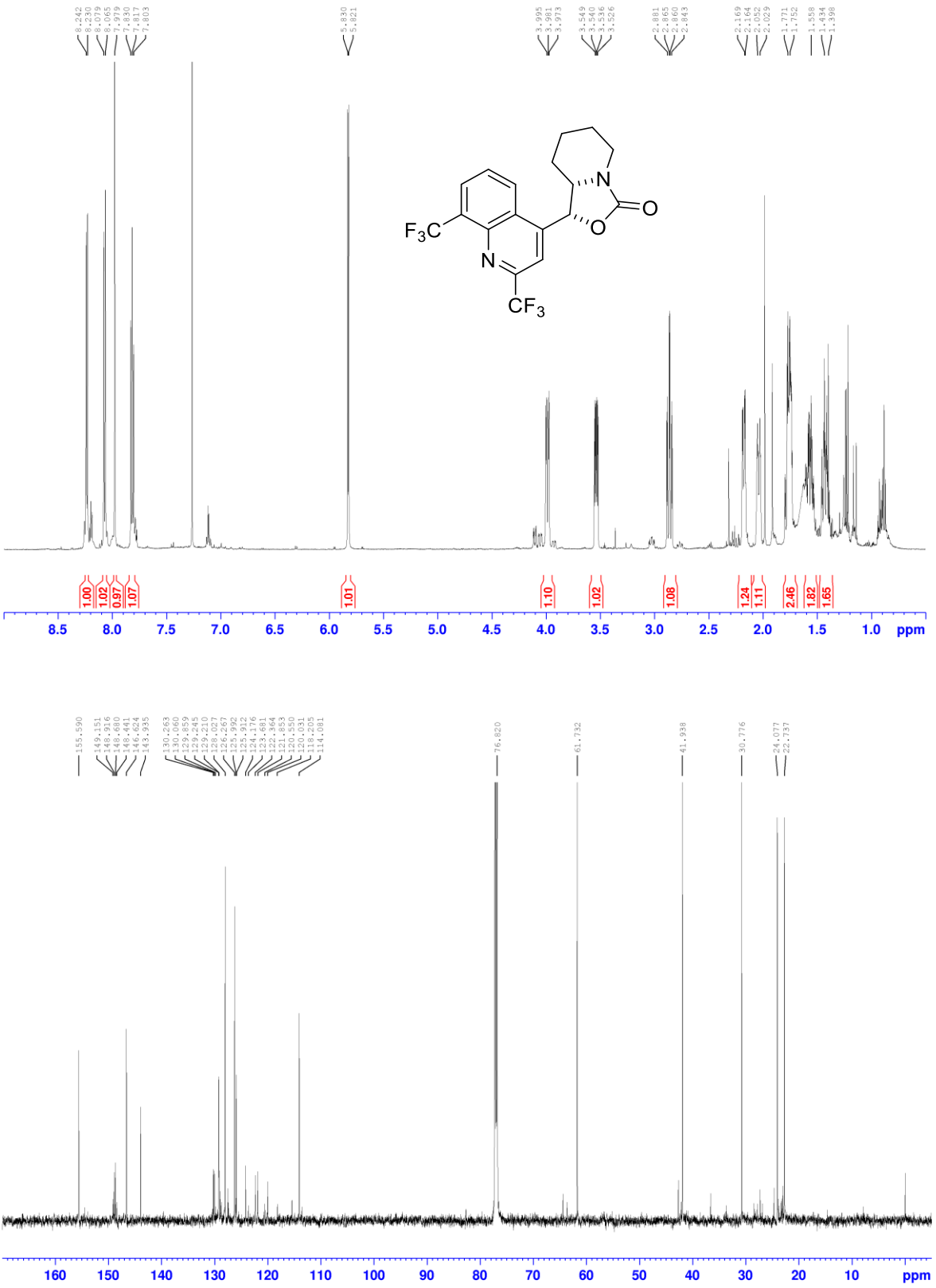

Figure S8. ^{1}H (600 MHz) and $^{13}C\{^{1}H\}$ NMR (151 MHz) spectra for **2** in $CDCl_3$+TMS.

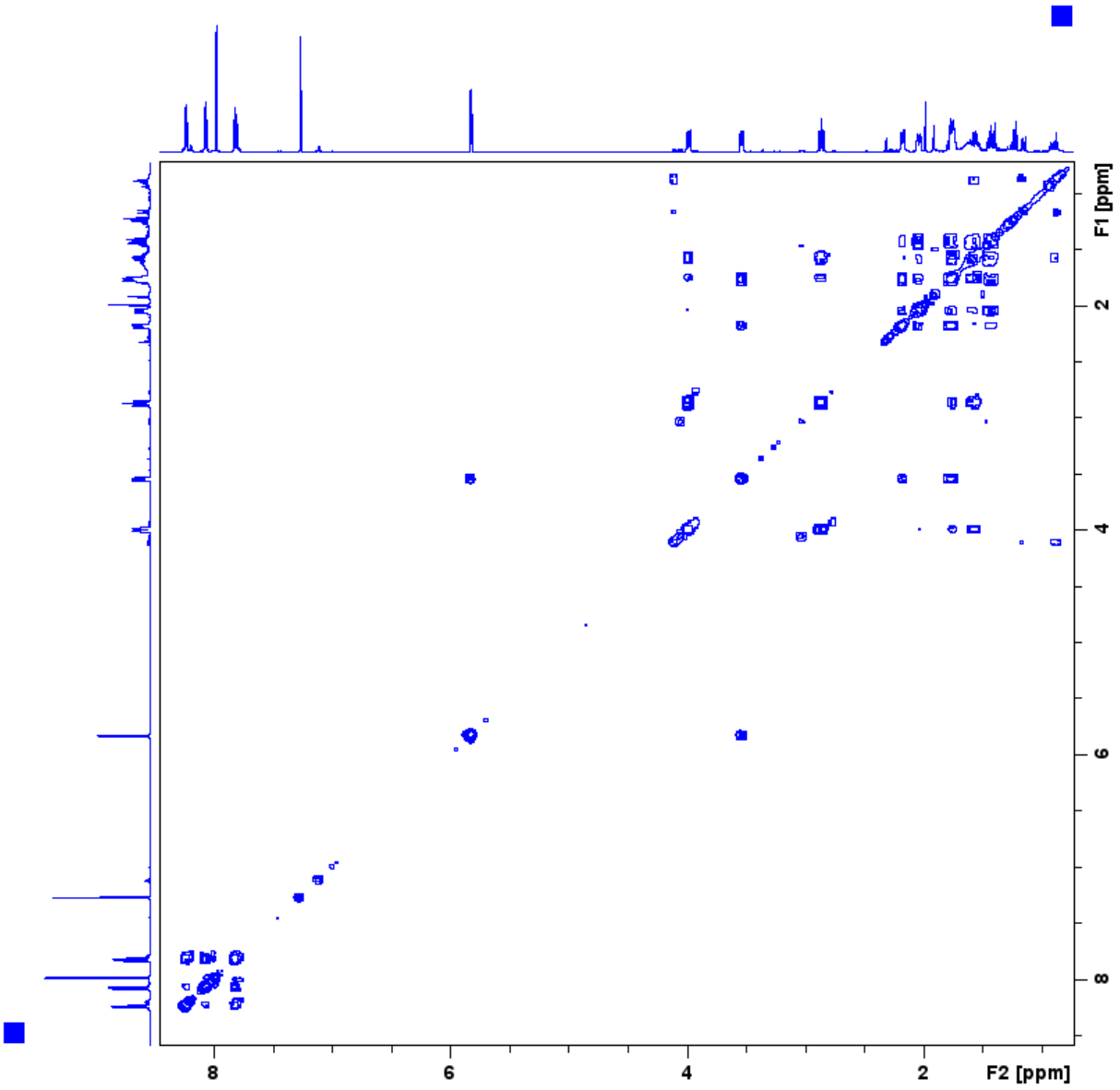

Figure S9. ^{1}H COSY experiment (600 MHz) for **2** in $CDCl_3$. For spectral assignment, see Figure S7.

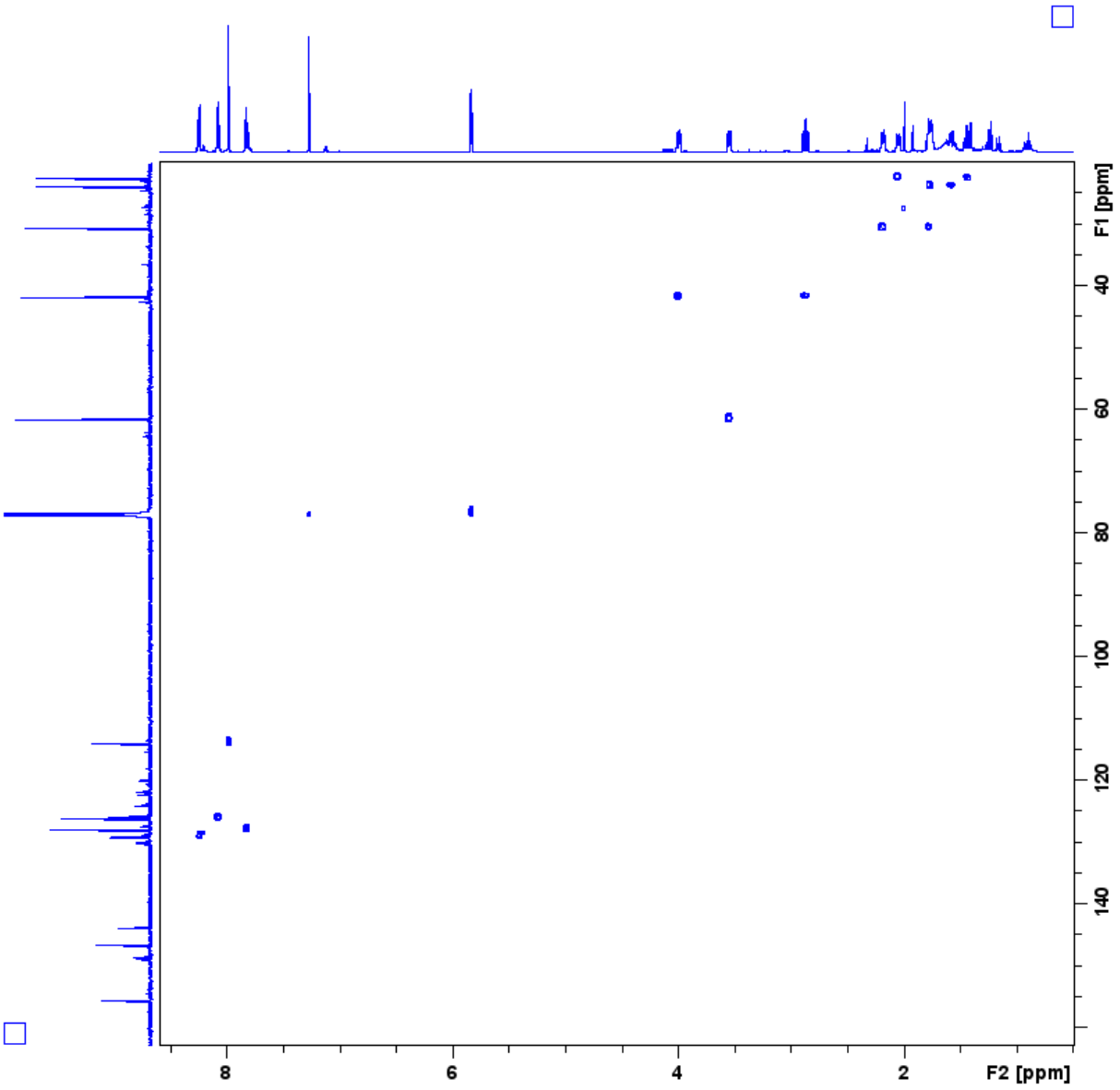

Figure S10. $^{1}H,^{13}C$ HSQC experiment (600 / 151 MHz) for **2** in $CDCl_3$. For spectral assignment, see Figure S7.

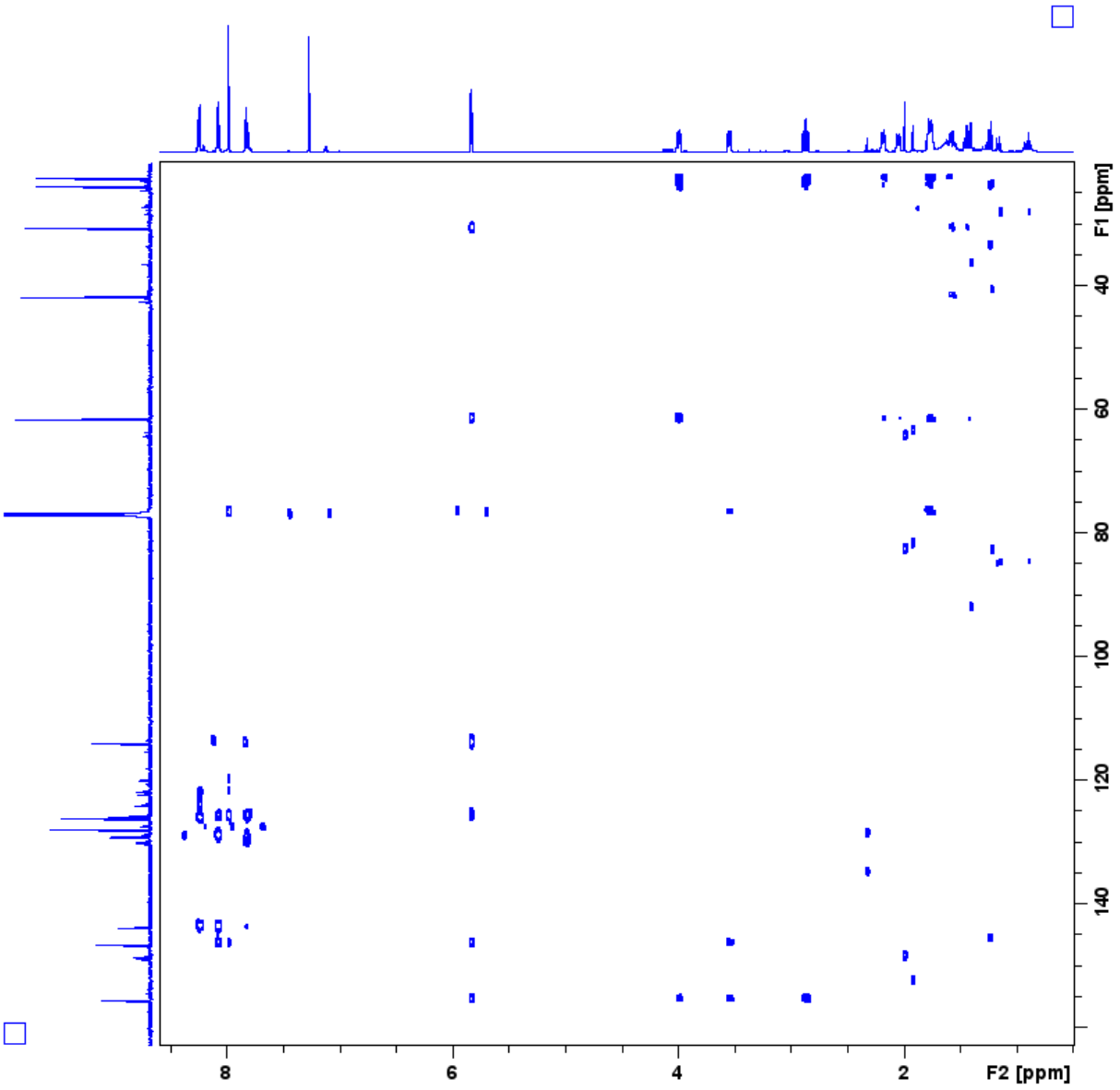

Figure S11. $^{1}H,^{13}C$ HMBC experiment (600 / 151 MHz) for **2** in $CDCl_3$. For spectral assignment, see Figure S7.

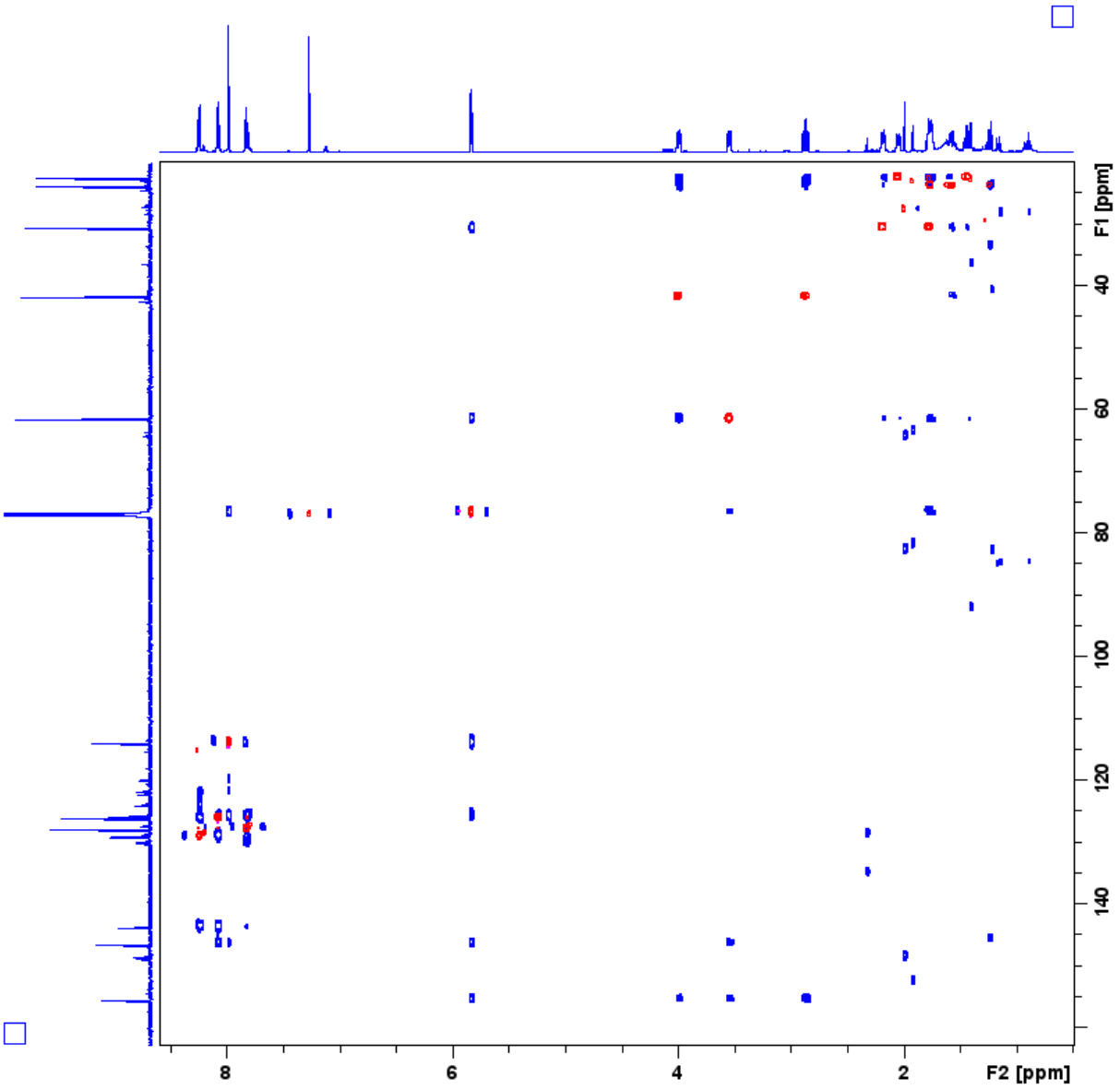

Figure S12. Superimposed $^{1}H,^{13}C$ HSQC and $^{1}H,^{13}C$ HMBC experiments (600 / 151 MHz) for **2** in $CDCl_3$. For spectral assignment, see Figure S7.

S3. Computational details

erythro-**1**; (cf. Figure 2)

E = -1823.78398906 Hartree

C	-1.830078	0.111063	-0.418478
O	-4.676601	-0.435328	1.493033
C	-3.820133	0.019553	0.773570
N	-3.875334	1.133761	-0.027197
C	-2.541828	1.507350	-0.493213
H	-2.606435	1.842300	-1.536922
C	-1.971994	2.641975	0.375915
H	-1.026207	3.000798	-0.040120
H	-1.756277	2.248766	1.377241
C	-2.983800	3.797252	0.479892
H	-2.574680	4.588164	1.117228
H	-3.130159	4.243689	-0.514432
C	-4.335354	3.315119	1.029069
H	-5.059998	4.136752	1.051185
H	-4.210306	2.966752	2.061897
C	-4.889821	2.163214	0.180038
H	-5.743371	1.677600	0.657114
H	-5.211578	2.533302	-0.801950
C	-0.362520	0.132979	0.003984
C	0.659351	0.790244	-0.757758
C	0.016746	-0.547448	1.143199
C	0.426050	1.546674	-1.941401
C	2.011411	0.685356	-0.281751
C	1.377094	-0.575625	1.514114
H	-0.718504	-1.064191	1.741973
C	1.459757	2.148917	-2.618432
H	-0.581306	1.661953	-2.319846
C	3.065552	1.322089	-1.010569
C	2.788466	2.034292	-2.154022
H	1.256864	2.720765	-3.518225
H	3.595276	2.511718	-2.696290
N	2.344448	0.005342	0.843826
C	1.817496	-1.305904	2.774087
C	4.493593	1.214475	-0.518965
F	4.647502	1.749338	0.706165
F	5.338006	1.880290	-1.347430
F	4.917623	-0.061418	-0.473334
F	2.761888	-2.222233	2.503141
F	2.326803	-0.444988	3.676097
F	0.780290	-1.943798	3.360535
O	-2.582509	-0.562876	0.620437
C	-2.059680	-0.697180	-1.733988
H	-1.571878	-0.173821	-2.560176
H	-3.137595	-0.659265	-1.927195
C	-1.582357	-2.133719	-1.698771
C	-0.379387	-2.496343	-2.319080
C	-2.332486	-3.129432	-1.056682
C	0.069939	-3.817056	-2.294617
H	0.210056	-1.738917	-2.829721

C	-1.884187	-4.449699	-1.029692
H	-3.266404	-2.867837	-0.569731
C	-0.681696	-4.797910	-1.647437
H	1.004582	-4.078061	-2.782388
H	-2.477564	-5.207737	-0.526873
H	-0.335221	-5.826961	-1.627552

threo-**1**

E = -1823.77730420 Hartree

C	-1.668910	0.598845	-0.669518
O	-2.309286	3.973415	-0.146661
C	-2.252737	2.769553	-0.078475
N	-2.603045	1.944586	0.961686
C	-2.727278	0.565408	0.483031
H	-2.437044	-0.120586	1.280587
C	-4.189708	0.270302	0.108753
H	-4.304546	-0.787554	-0.139846
H	-4.470117	0.854887	-0.776543
C	-5.118989	0.640571	1.280593
H	-6.158966	0.440298	1.001677
H	-4.896646	-0.010246	2.138394
C	-4.952093	2.110624	1.695025
H	-5.581071	2.341895	2.561987
H	-5.277969	2.764287	0.876212
C	-3.485391	2.422160	2.022949
H	-3.310840	3.494748	2.127326
H	-3.188749	1.934643	2.959884
C	-0.230147	0.357519	-0.158604
C	0.931088	0.945027	-0.775810
C	-0.014336	-0.533333	0.874986
C	0.904364	1.834372	-1.891526
C	2.219380	0.585109	-0.239409
C	1.295348	-0.805601	1.316791
H	-0.826684	-1.053885	1.359502
C	2.067372	2.331871	-2.429042
H	-0.043445	2.142163	-2.305272
C	3.407943	1.134506	-0.815977
C	3.325715	1.988301	-1.890211
H	2.018354	3.007665	-3.276784
H	4.231739	2.396465	-2.321197
N	2.375926	-0.275215	0.798663
C	1.536836	-1.788142	2.451564
C	4.761435	0.765680	-0.248778
F	4.884836	1.118171	1.044277
F	5.754450	1.397837	-0.924346
F	5.008171	-0.555428	-0.343244
F	2.186949	-2.883651	2.015729
F	2.270922	-1.237817	3.431797
F	0.367947	-2.202672	2.998822
O	-1.795610	1.978966	-1.112649
C	-1.967271	-0.260809	-1.932358
H	-1.256305	0.075395	-2.693993
H	-2.957939	0.030319	-2.290470
C	-1.886378	-1.772133	-1.808739
C	-0.649603	-2.435502	-1.778284
C	-3.051432	-2.552225	-1.795499
C	-0.581811	-3.825949	-1.696111
H	0.270204	-1.862184	-1.833595
C	-2.988487	-3.944272	-1.715291
H	-4.020729	-2.068364	-1.874505

C	-1.751893	-4.585865	-1.655852
H	0.387375	-4.315120	-1.671485
H	-3.906287	-4.524944	-1.708842
H	-1.698916	-5.668600	-1.593571

Anion conformation *E*

E = -1552.84842321 Hartree

C	1.929337	0.370598	-0.318660
O	4.751117	2.367999	-0.363597
C	3.938532	1.461180	-0.381374
N	4.193335	0.118490	-0.522848
C	2.998090	-0.695232	-0.306668
H	2.908387	-1.412647	-1.140977
C	3.145468	-1.504801	1.008501
H	2.305048	-2.197001	1.113685
H	3.090202	-0.800274	1.847316
C	4.488602	-2.251928	1.040203
H	4.589422	-2.815900	1.975426
H	4.516093	-2.992658	0.226527
C	5.665150	-1.275229	0.878021
H	6.621795	-1.813065	0.863879
H	5.689528	-0.590940	1.735963
C	5.519251	-0.450907	-0.411352
H	6.227217	0.380833	-0.446590
H	5.710224	-1.097676	-1.281917
C	0.560411	0.379092	-0.281567
C	-0.325169	-0.804063	-0.356732
C	-0.141411	1.637407	-0.153377
C	0.129038	-2.098399	-0.656936
C	-1.743168	-0.609270	-0.135595
C	-1.500288	1.652530	0.018168
H	0.421916	2.558713	-0.158266
C	-0.714338	-3.204116	-0.692171
H	1.174593	-2.255890	-0.888341
C	-2.584399	-1.774318	-0.151624
C	-2.075650	-3.034732	-0.422873
H	-0.317934	-4.187855	-0.926525
H	-2.745771	-3.887013	-0.431534
N	-2.328839	0.588934	0.064256
C	-2.218521	2.970892	0.185908
C	-4.055987	-1.622348	0.110122
F	-4.334823	-1.090072	1.321879
F	-4.694089	-2.836440	0.088528
F	-4.693597	-0.864058	-0.810862
F	-3.144611	3.176902	-0.783005
F	-2.879449	3.047306	1.367246
F	-1.380614	4.040947	0.146497
O	2.600482	1.633249	-0.271779

Anion-conformation *Z* (Cf. Figure 3)

E = -1552.85231553 Hartree

C	-1.870528	-0.551448	-0.116177
O	-4.357257	-2.917996	-0.442569
C	-3.685745	-1.904260	-0.387590
N	-4.101945	-0.611358	-0.590252
C	-3.067244	0.357900	-0.229582
H	-2.950322	1.097519	-1.041286
C	-3.486515	1.121483	1.052835
H	-2.768537	1.923227	1.251993
H	-3.435122	0.425394	1.899568
C	-4.914199	1.674455	0.917206
H	-5.206978	2.208365	1.829488
H	-4.945406	2.412502	0.101515
C	-5.913255	0.544214	0.618603
H	-6.927531	0.942276	0.486603
H	-5.944157	-0.147399	1.470566
C	-5.499993	-0.235986	-0.640123
H	-6.075762	-1.157671	-0.755266
H	-5.673493	0.387514	-1.530446
C	-0.545820	-0.213978	-0.091049
C	0.610319	-1.132217	0.002874
C	-0.187918	1.186641	-0.158849
C	0.474306	-2.529680	0.082358
C	1.937101	-0.559451	0.018213
C	1.129748	1.567756	-0.140299
H	-0.957390	1.942413	-0.239010
C	1.574868	-3.374592	0.172516
H	-0.518002	-2.959555	0.073671
C	3.049264	-1.460967	0.112761
C	2.863476	-2.833258	0.186969
H	1.432059	-4.449732	0.232942
H	3.729426	-3.482149	0.257299
N	2.205225	0.766300	-0.050384
C	1.482410	3.034397	-0.223871
C	4.446187	-0.909954	0.132730
F	4.771794	-0.220199	-0.985331
F	5.377559	-1.912148	0.226953
F	4.690021	-0.092420	1.183576
F	2.173920	3.460489	0.860656
F	2.249753	3.319554	-1.303367
F	0.385323	3.839127	-0.314527
O	-2.354724	-1.889911	-0.110177