Supporting Information
of

Supramolecular Catalysis with Chiral Mono- and Bis-(Thio)Urea-Derivatives

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NMR Spectra

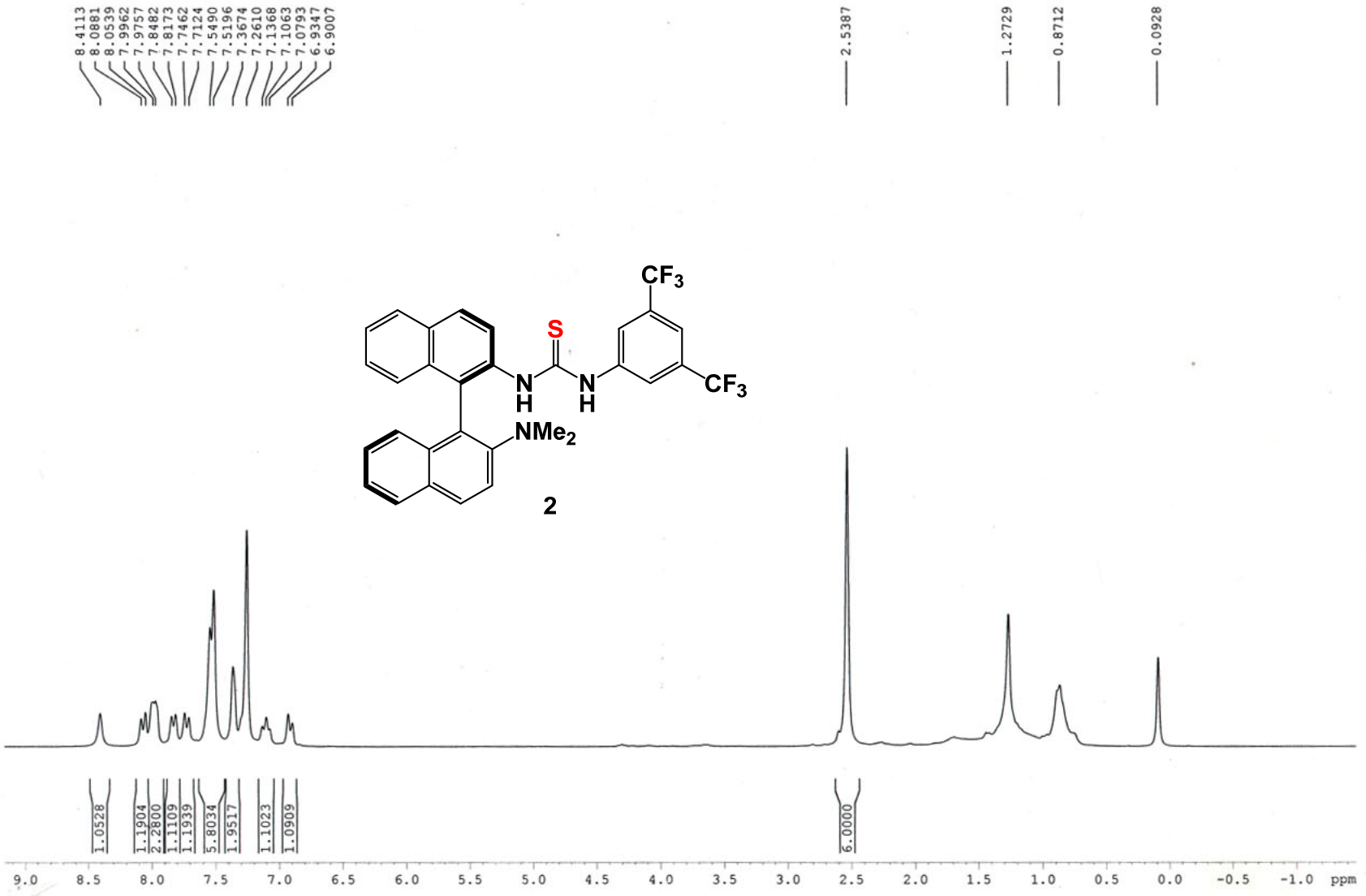


Figure S1. ^{1}H NMR spectrum of organocatalyst **2** (250 MHz, $CDCl_3$, 298 K).

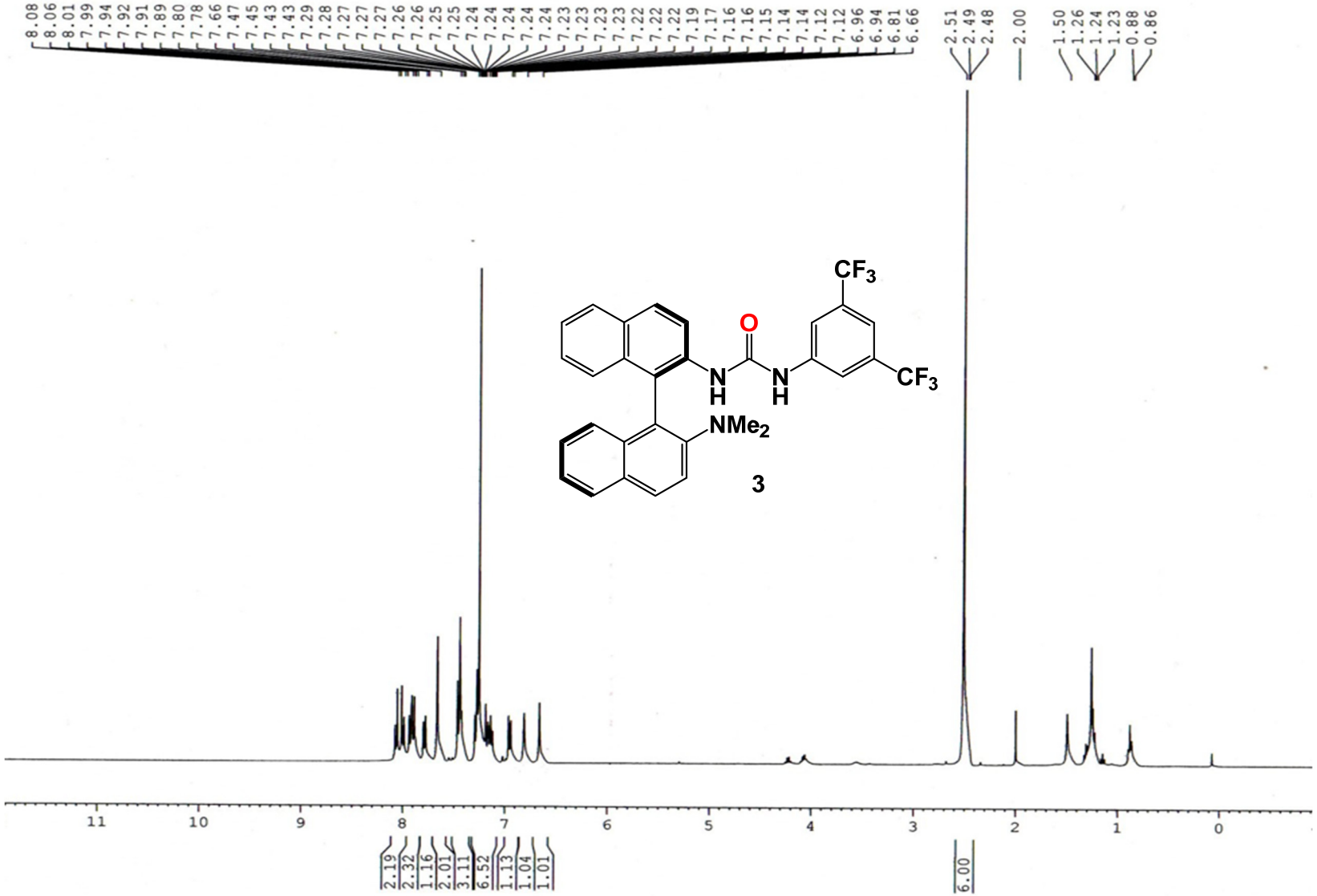


Figure S2. ^{1}H NMR spectrum of organocatalyst **3** (400 MHz, $CDCl_3$, 298 K).

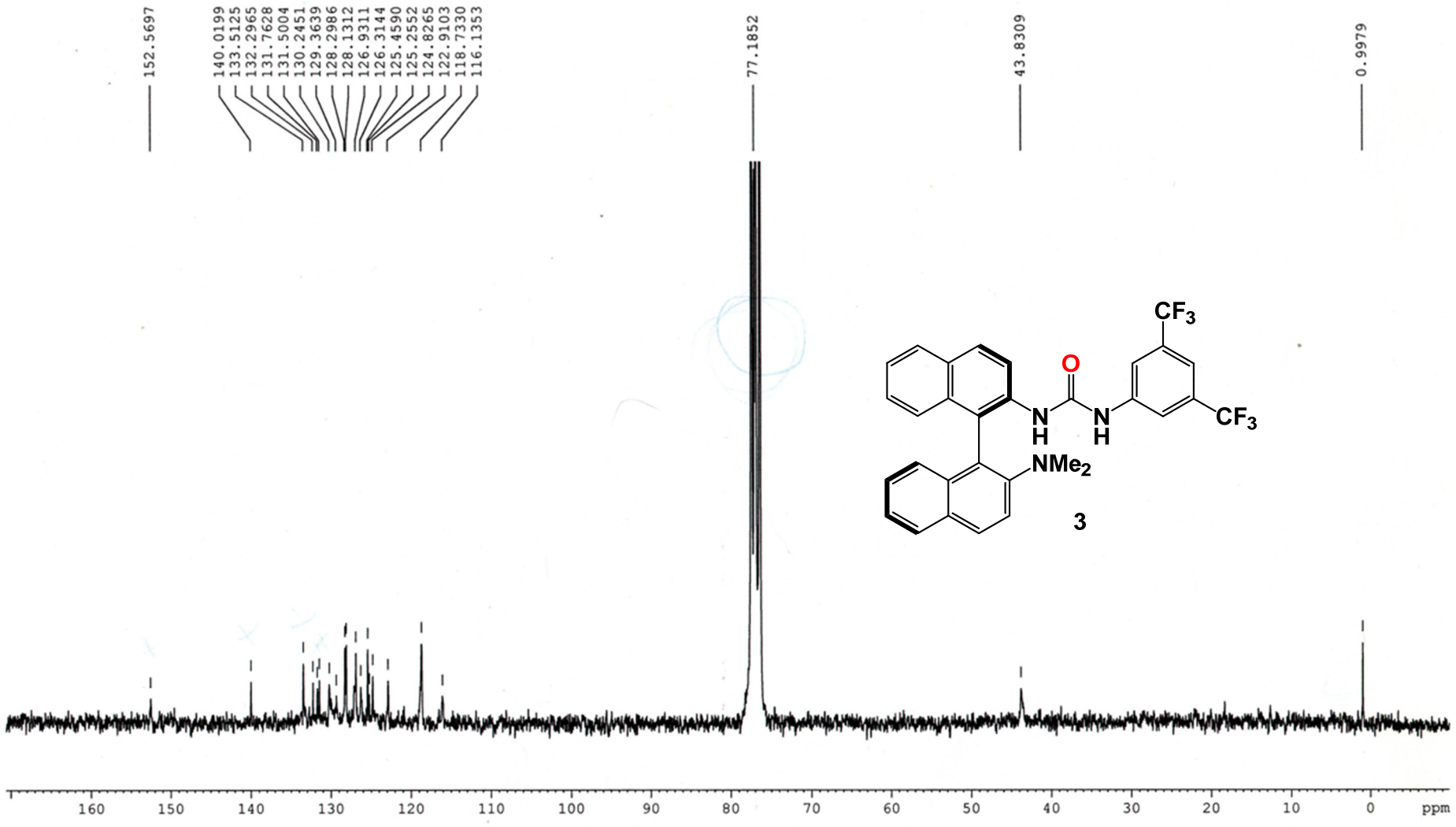


Figure S3. ^{13}C NMR spectrum of organocatalyst **3** (100 MHz, $CDCl_3$, 298 K).

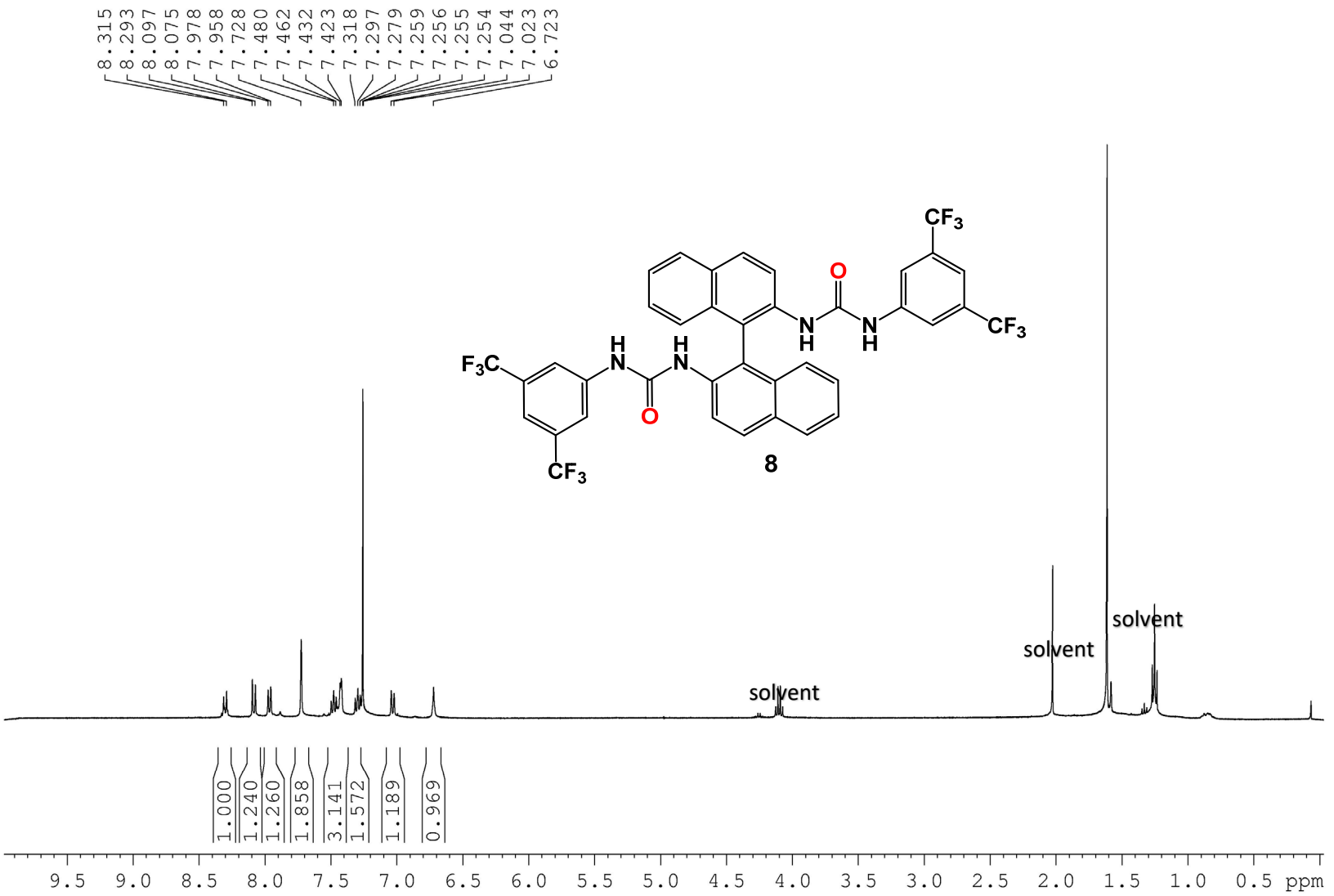


Figure S4. ^{1}H NMR spectrum of organocatalyst **8** (400 MHz, $CDCl_3$, 298 K).

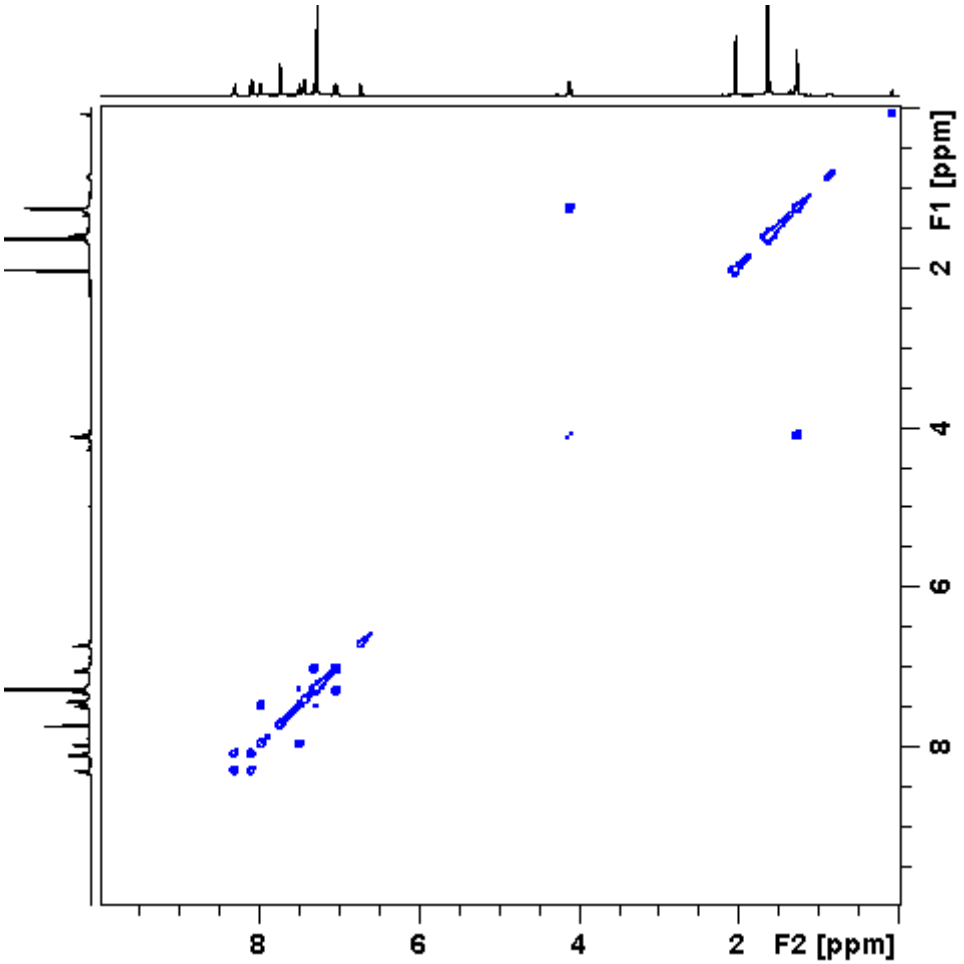
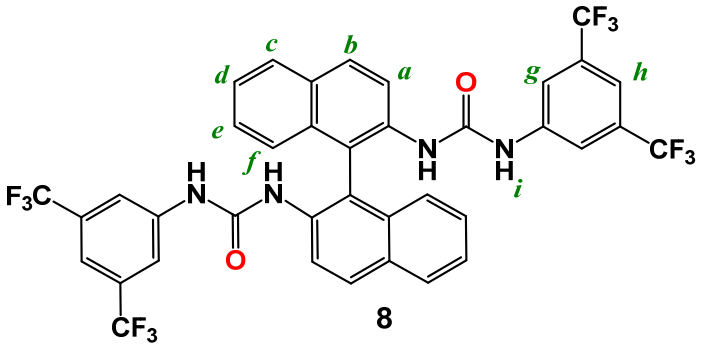


Figure S5. 2D COSY spectrum of organocatalyst **8** (400 MHz, $CDCl_3$, 298 K).



8

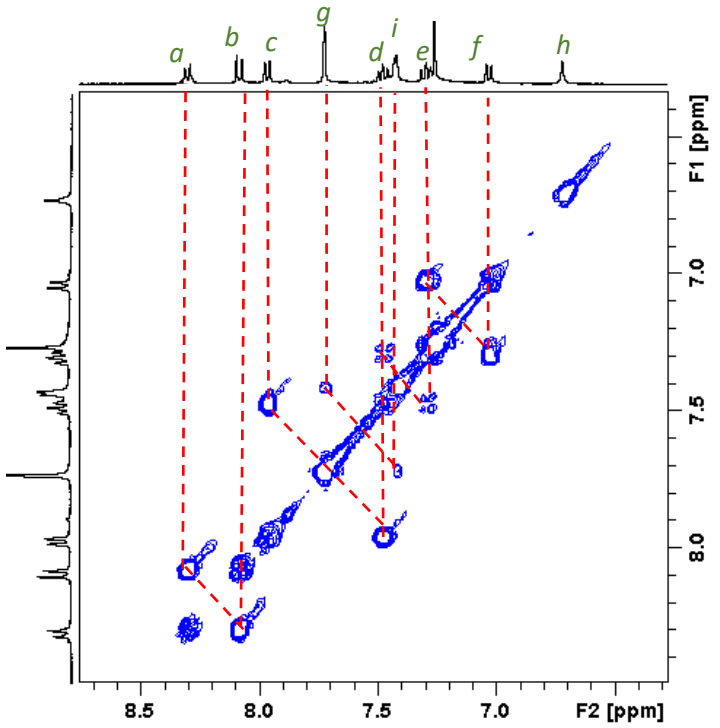


Figure S6. Portion of 2D COSY spectrum of organocatalyst **8** (400 MHz, $CDCl_3$, 298 K).

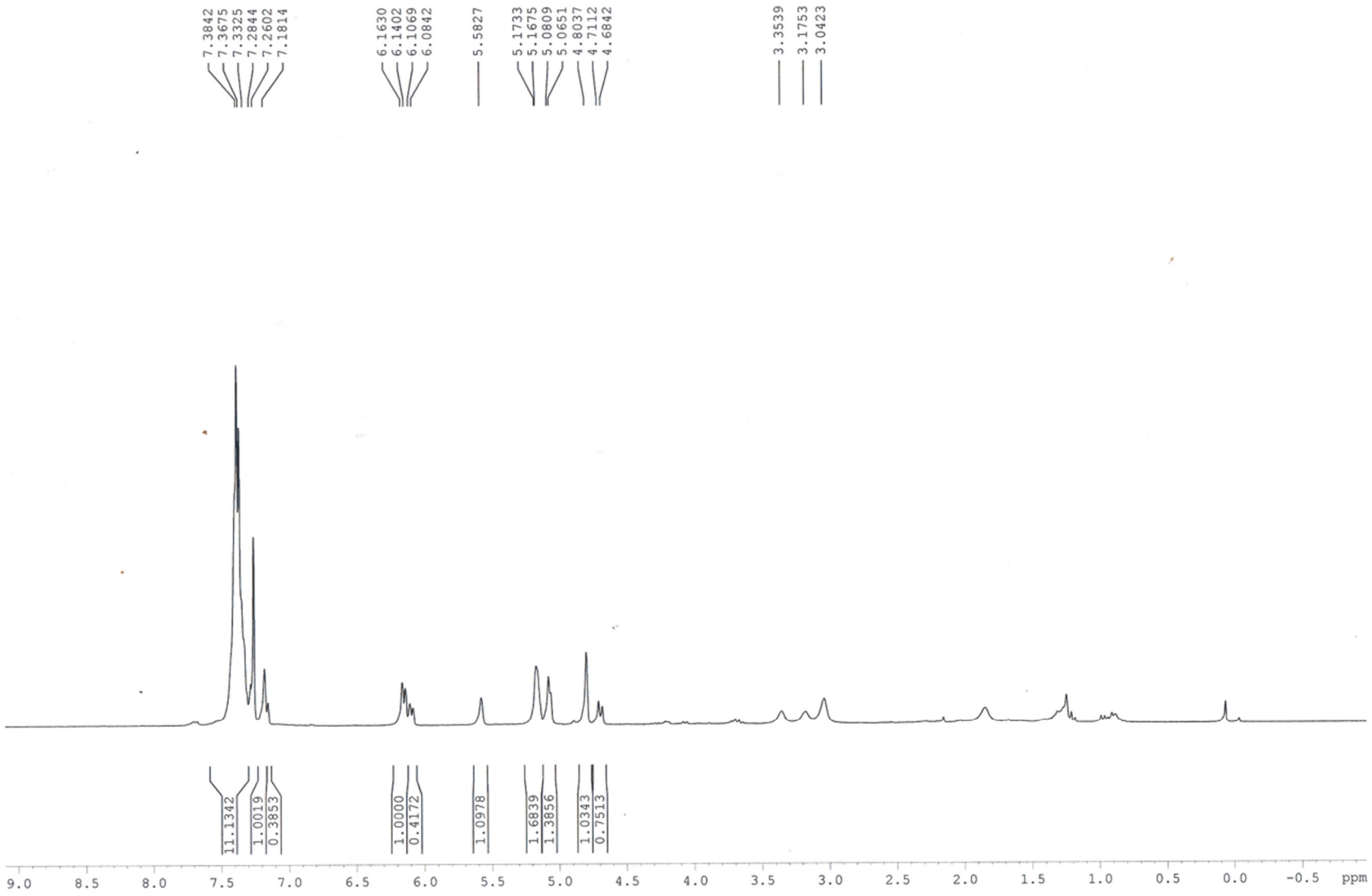


Figure S7. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 1 of Table 1 (250 MHz, $CDCl_3$, 298 K).

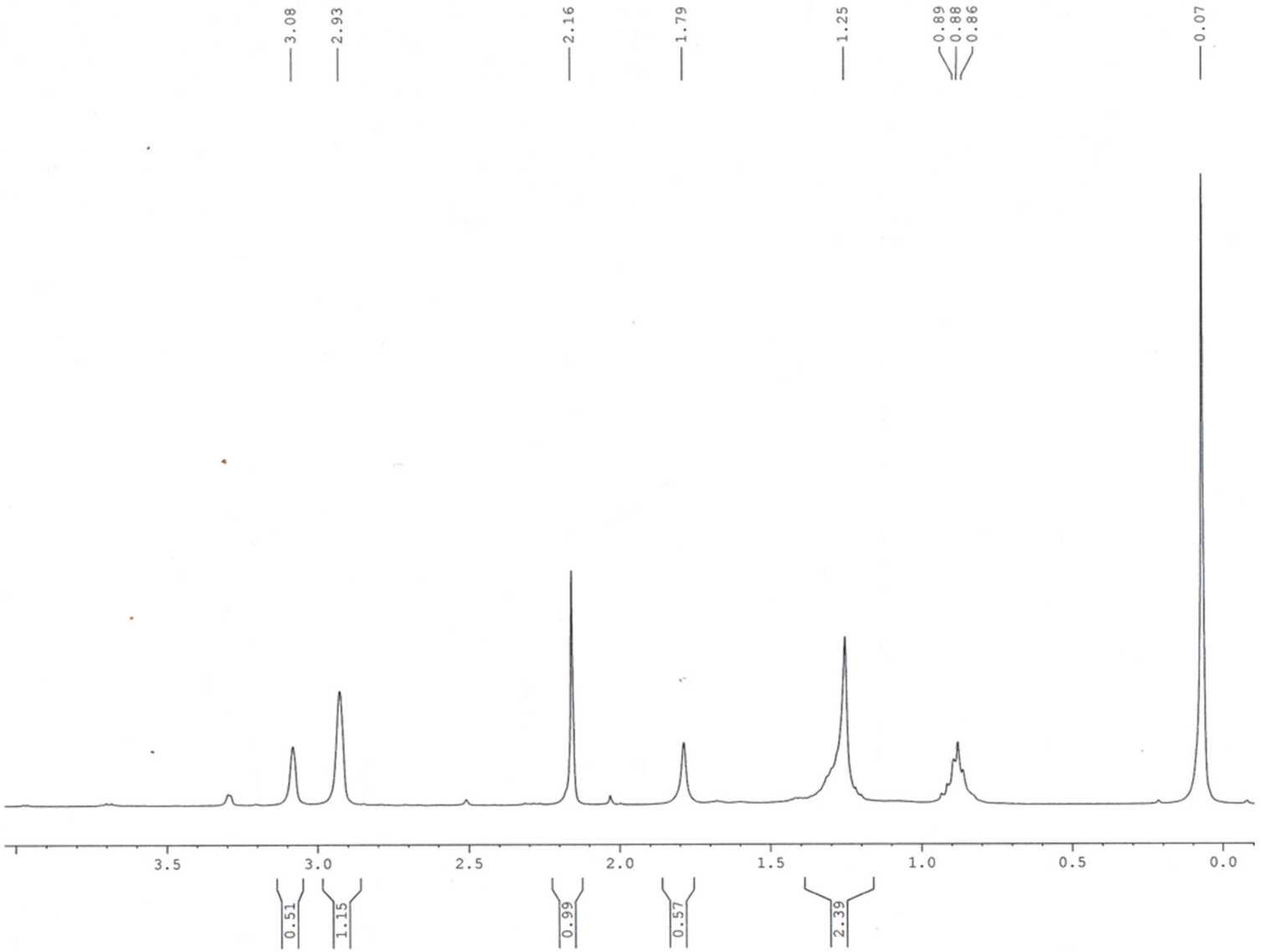


Figure S8. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 2 of Table 1 (250 MHz, $CDCl_3$, 298 K).

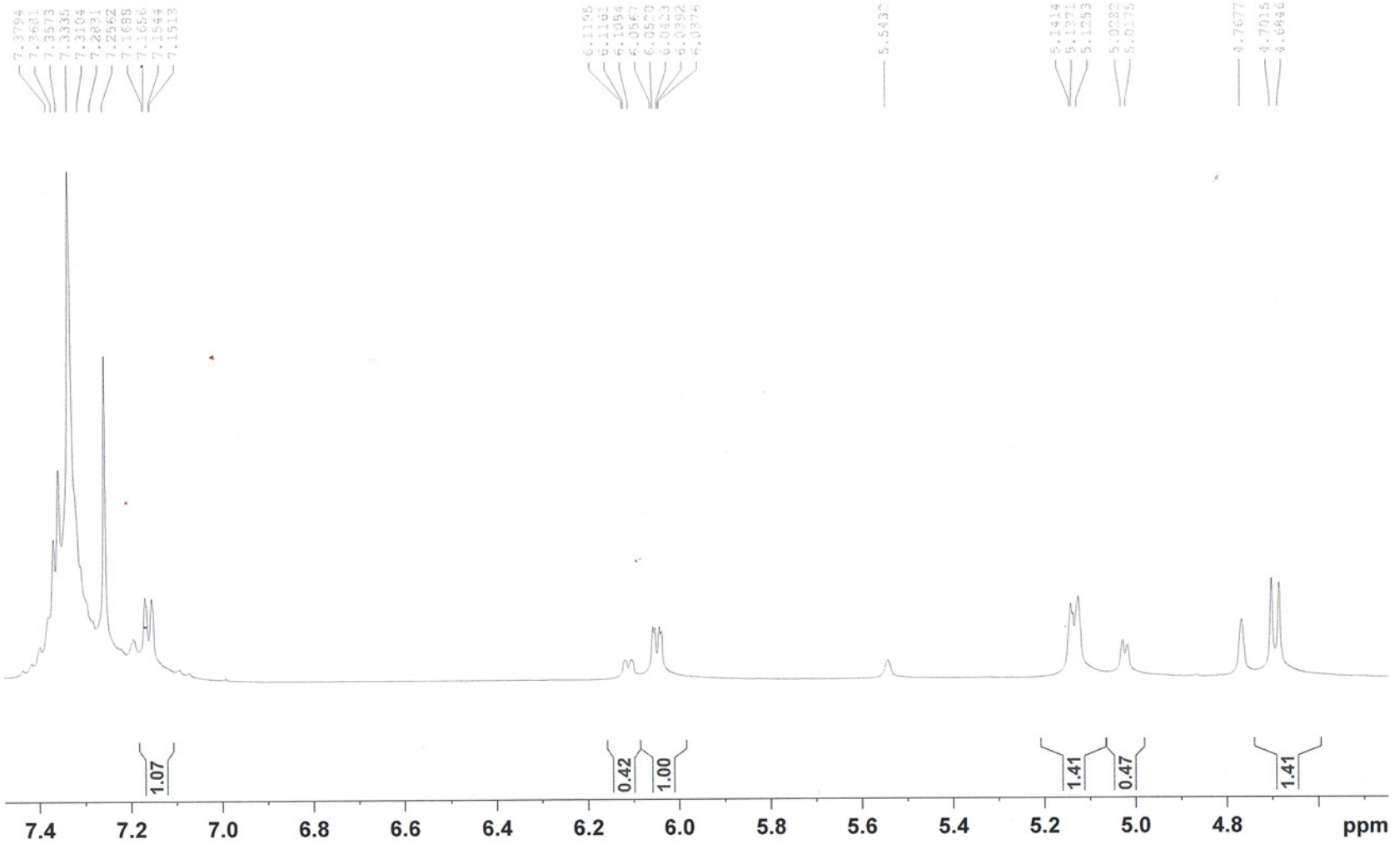


Figure S9. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 1 of Table 3 (400 MHz, $CDCl_3$, 298 K).

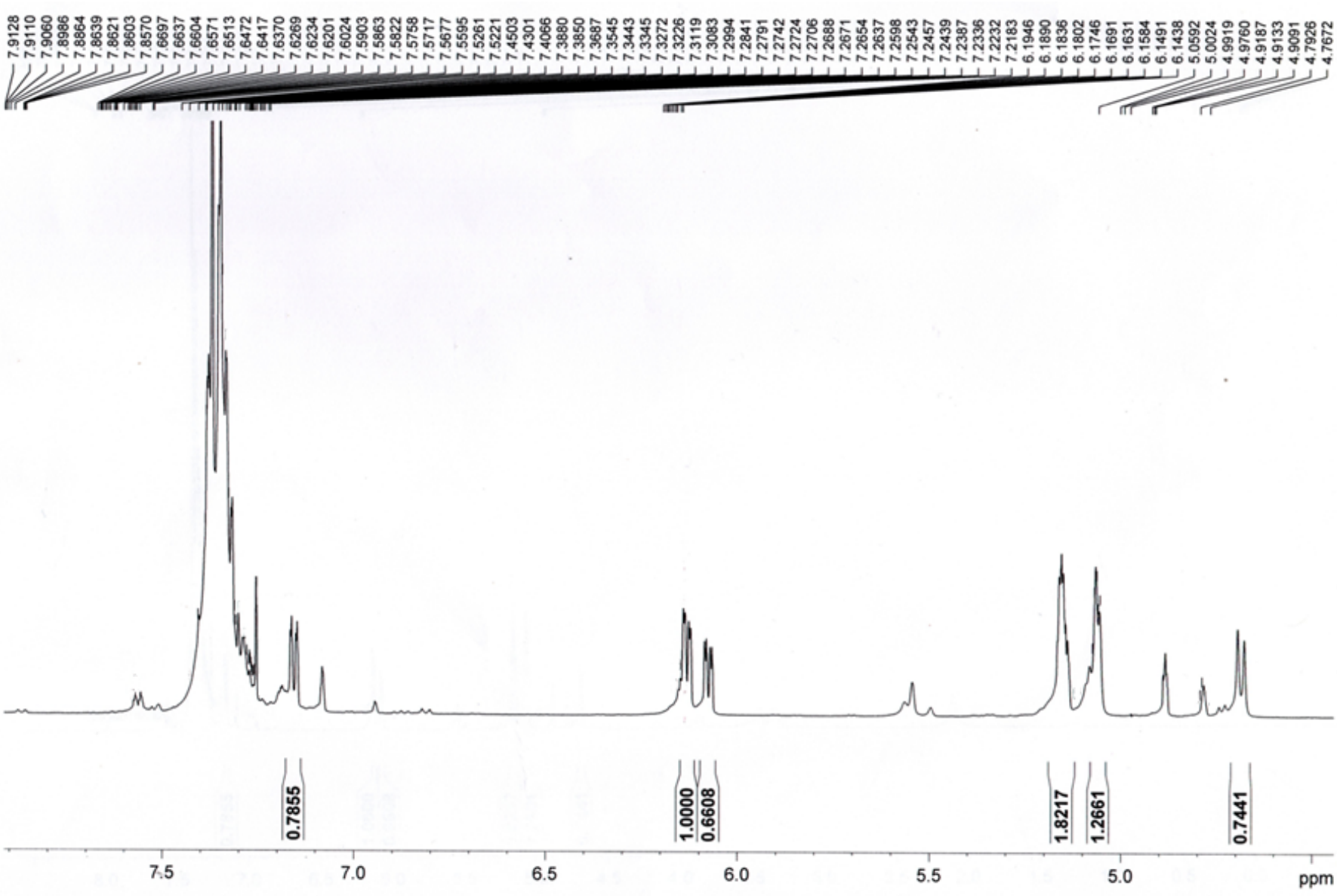


Figure S10. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 2 of Table 3 (400 MHz, $CDCl_3$, 298 K).

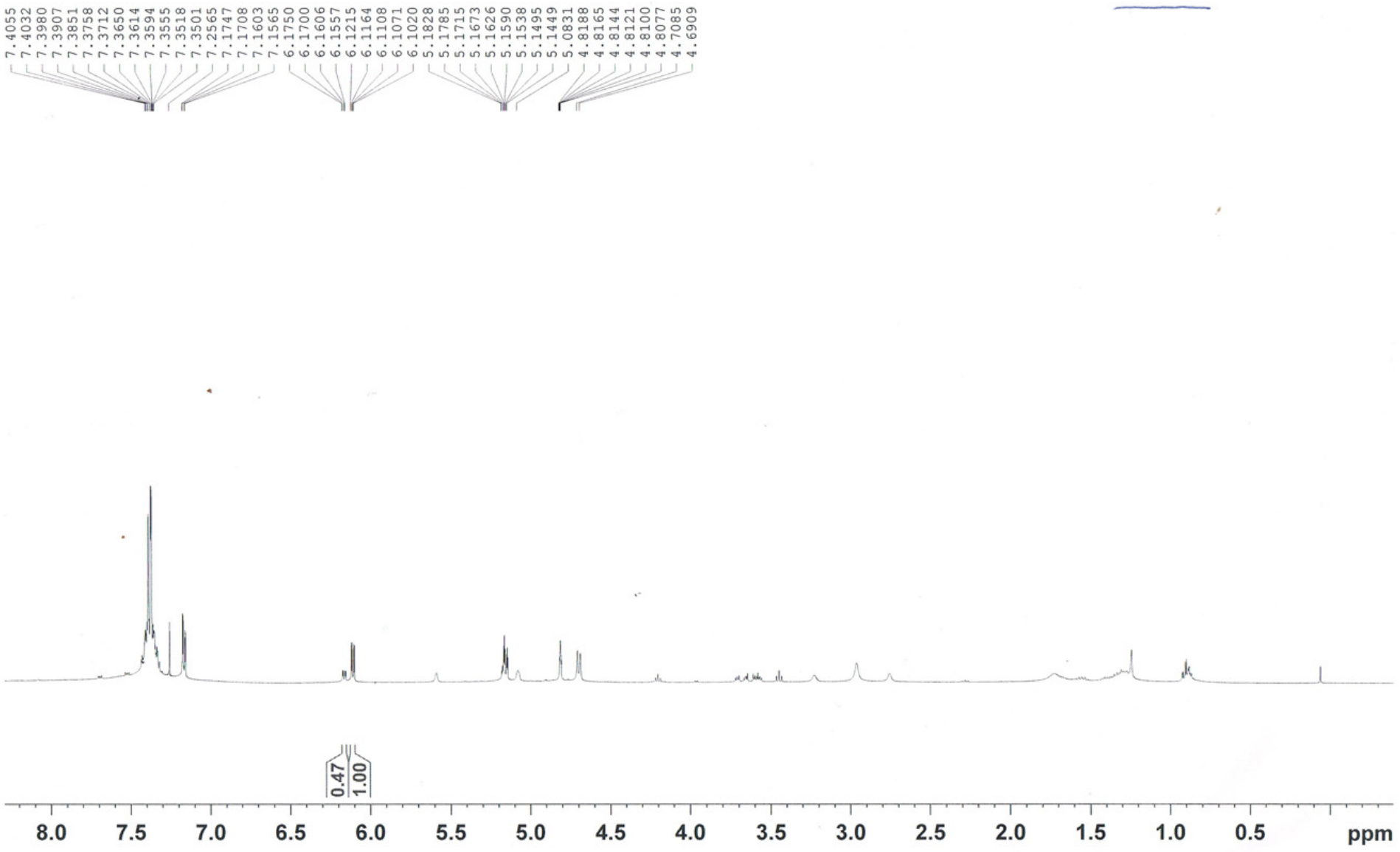


Figure S11. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 3 of Table 3 (400 MHz, $CDCl_3$, 298 K)

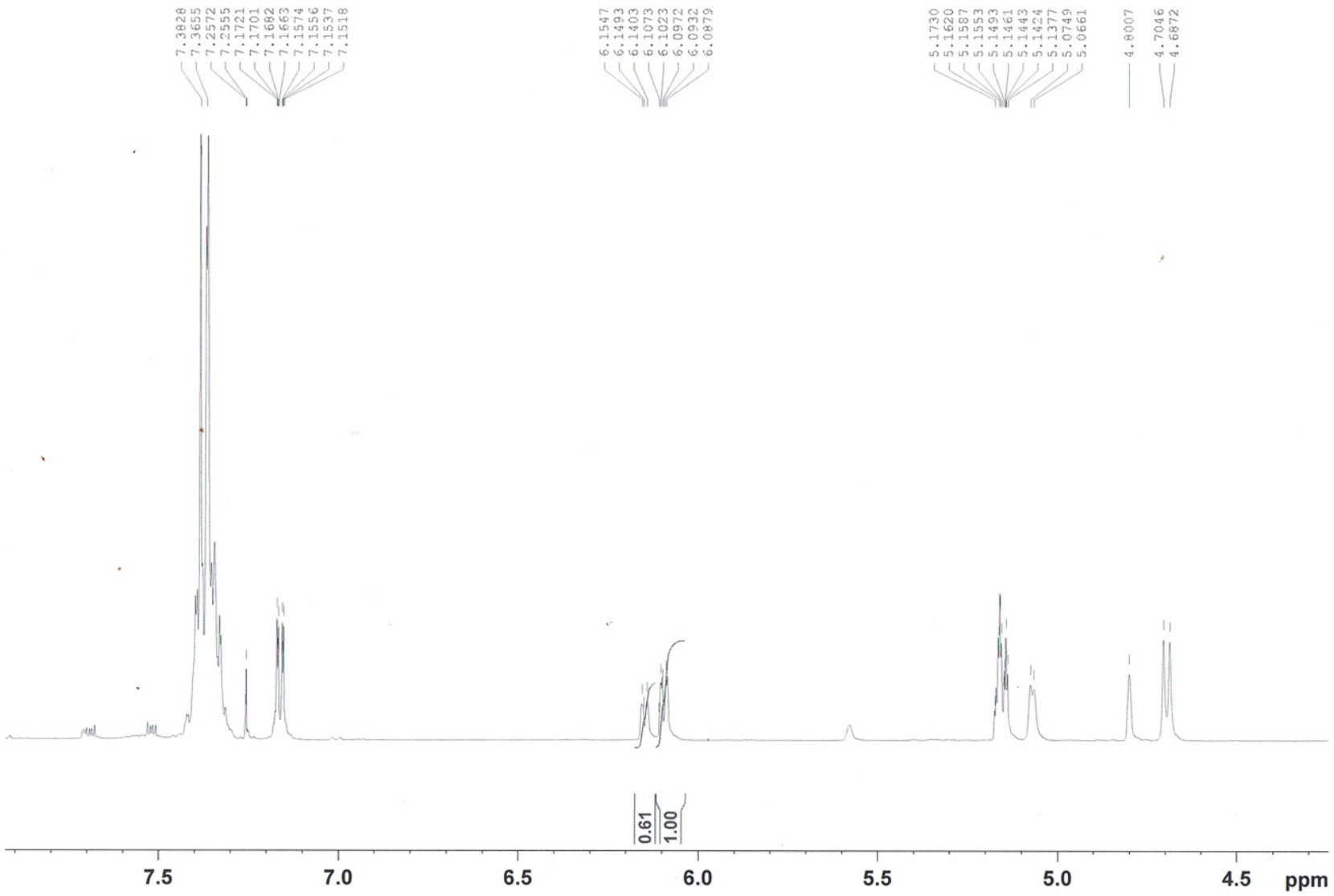


Figure S12. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 4 of Table 3 (400 MHz, $CDCl_3$, 298 K)

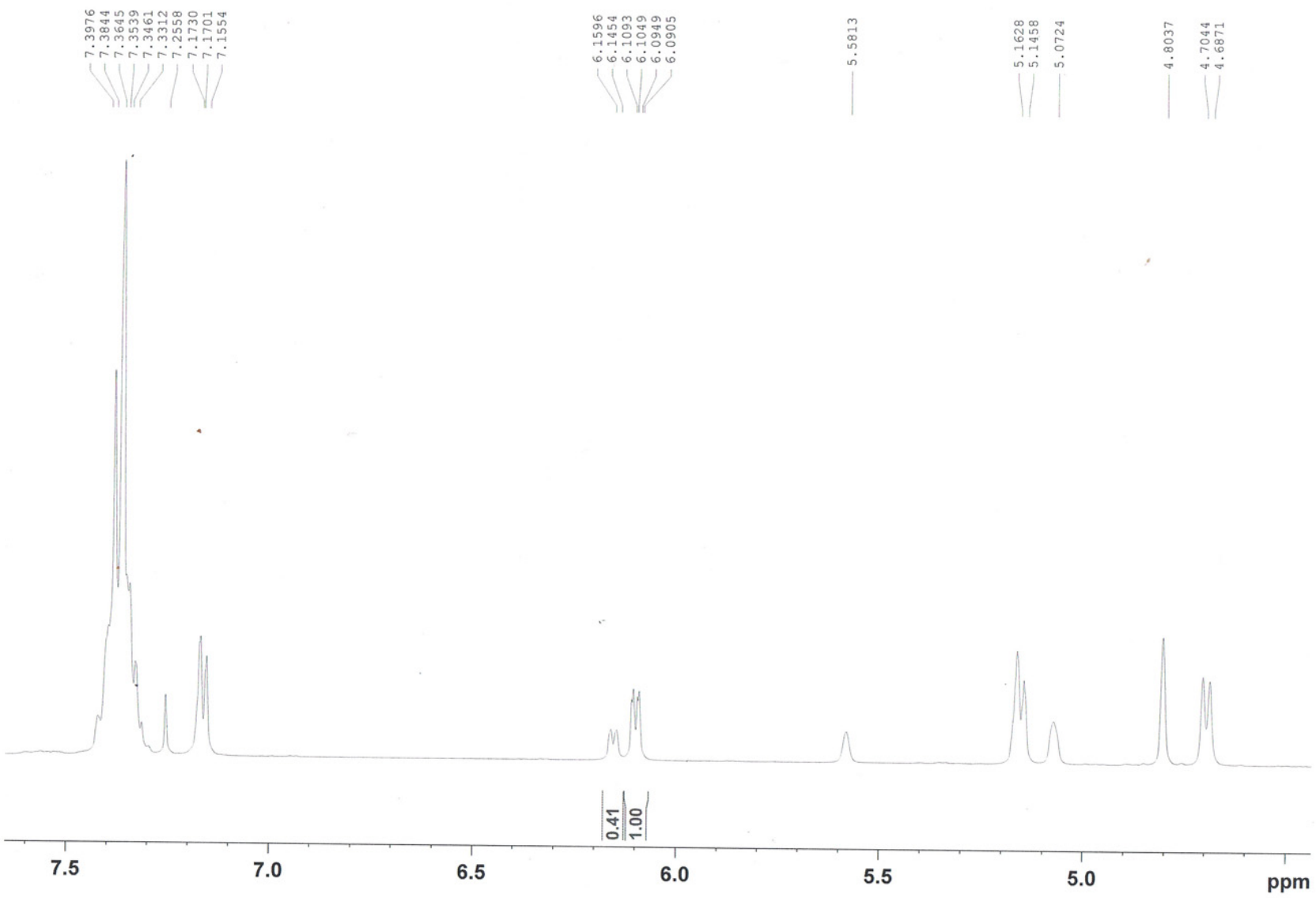


Figure S13. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 5 of Table 3 (400 MHz, $CDCl_3$, 298 K)

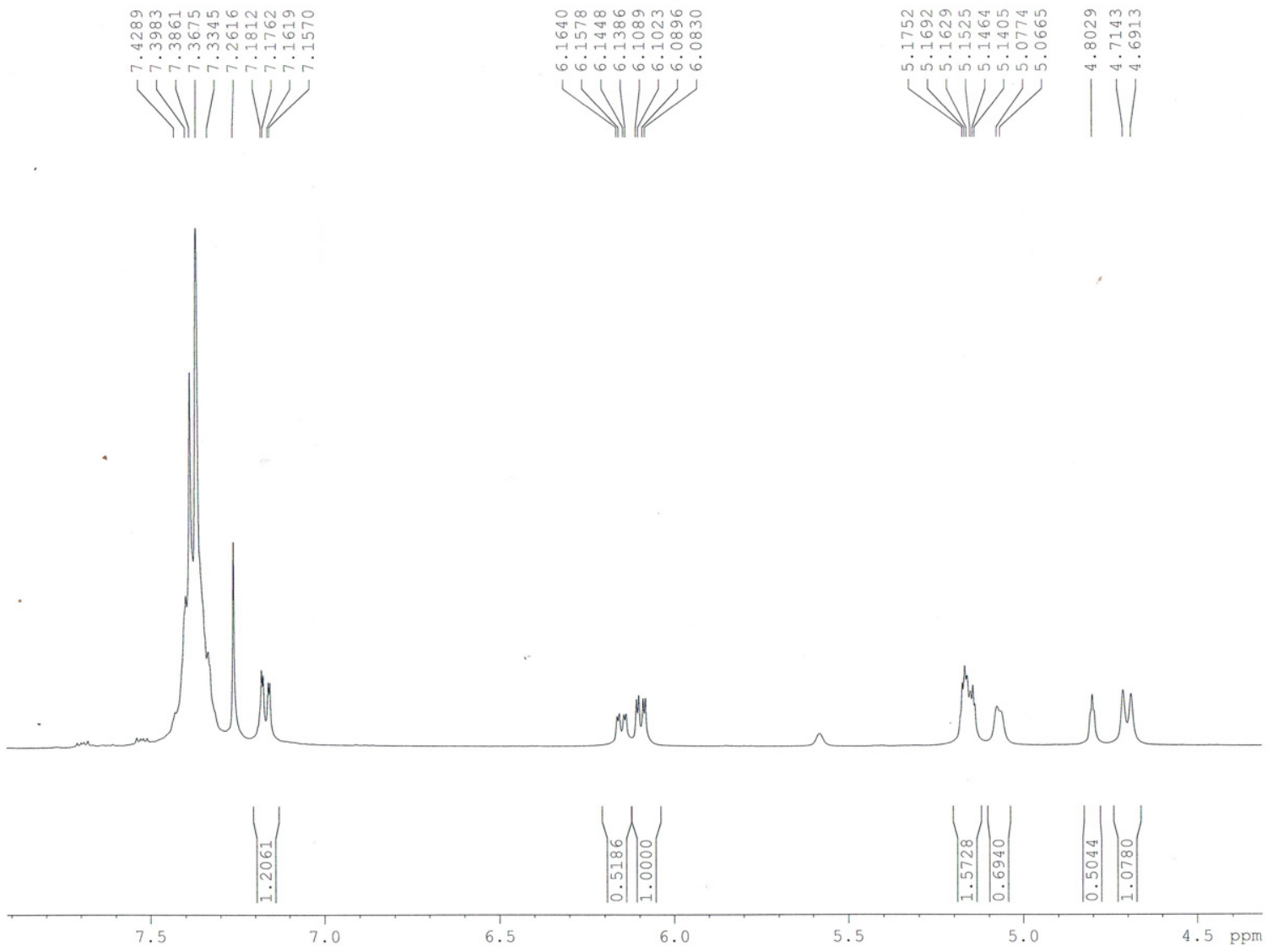


Figure S14. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 6 of Table 3 (400 MHz, $CDCl_3$, 298 K)

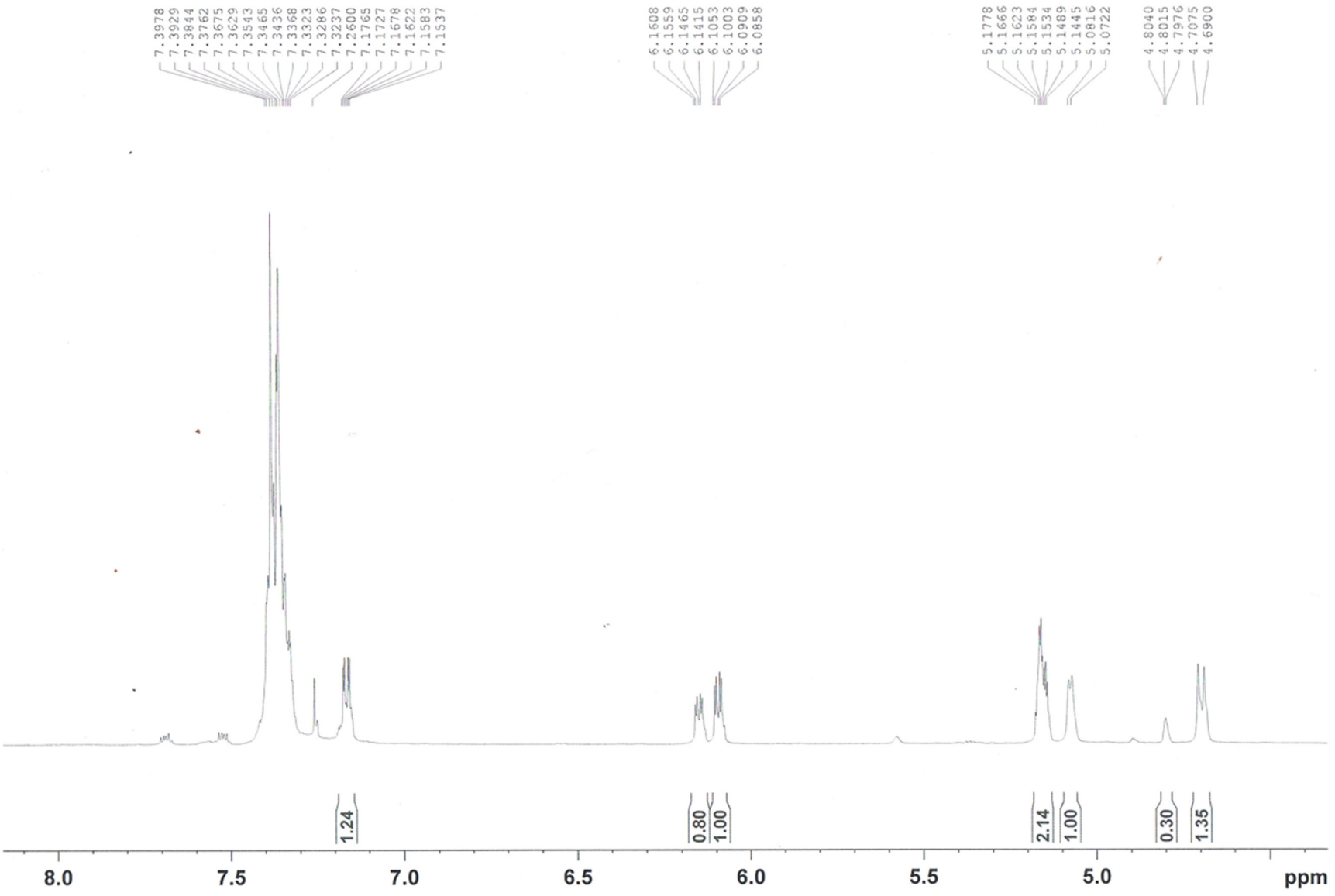


Figure S15. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 2 of Table 4 (400 MHz, $CDCl_3$, 298 K)

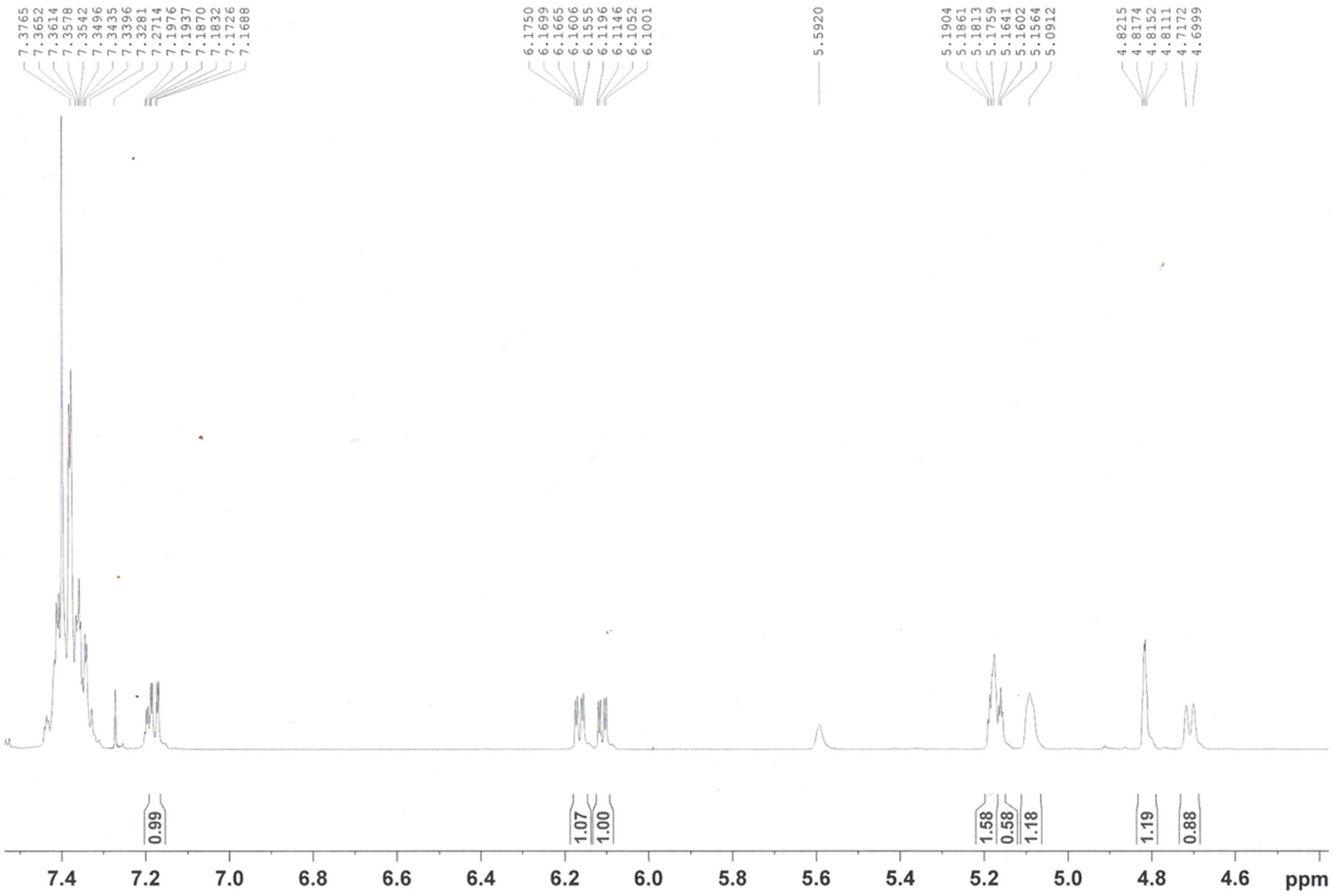


Figure S16. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 3 of Table 4 (400 MHz, $CDCl_3$, 298 K)

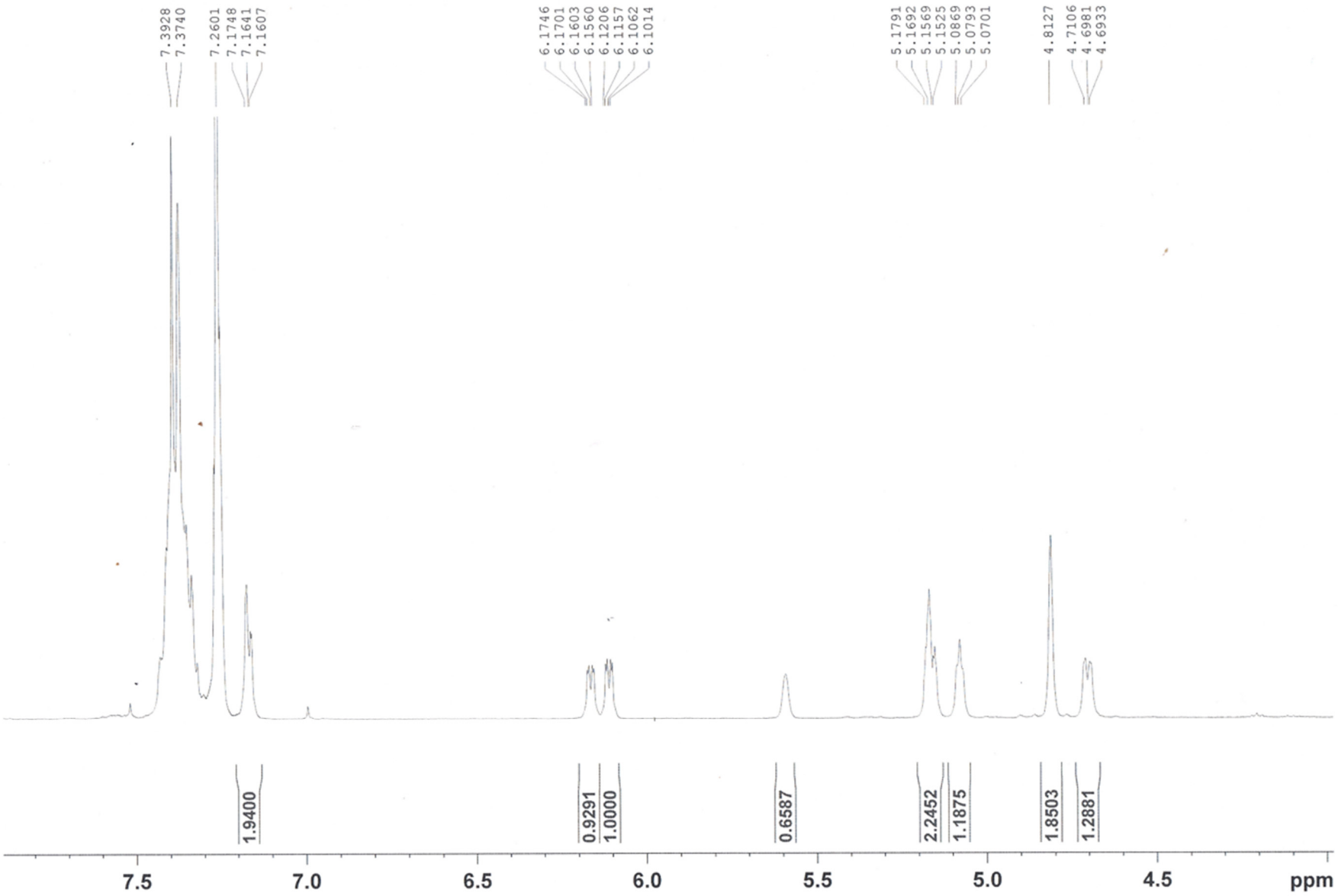


Figure S17. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 4 of Table 4 (400 MHz, $CDCl_3$, 298 K)

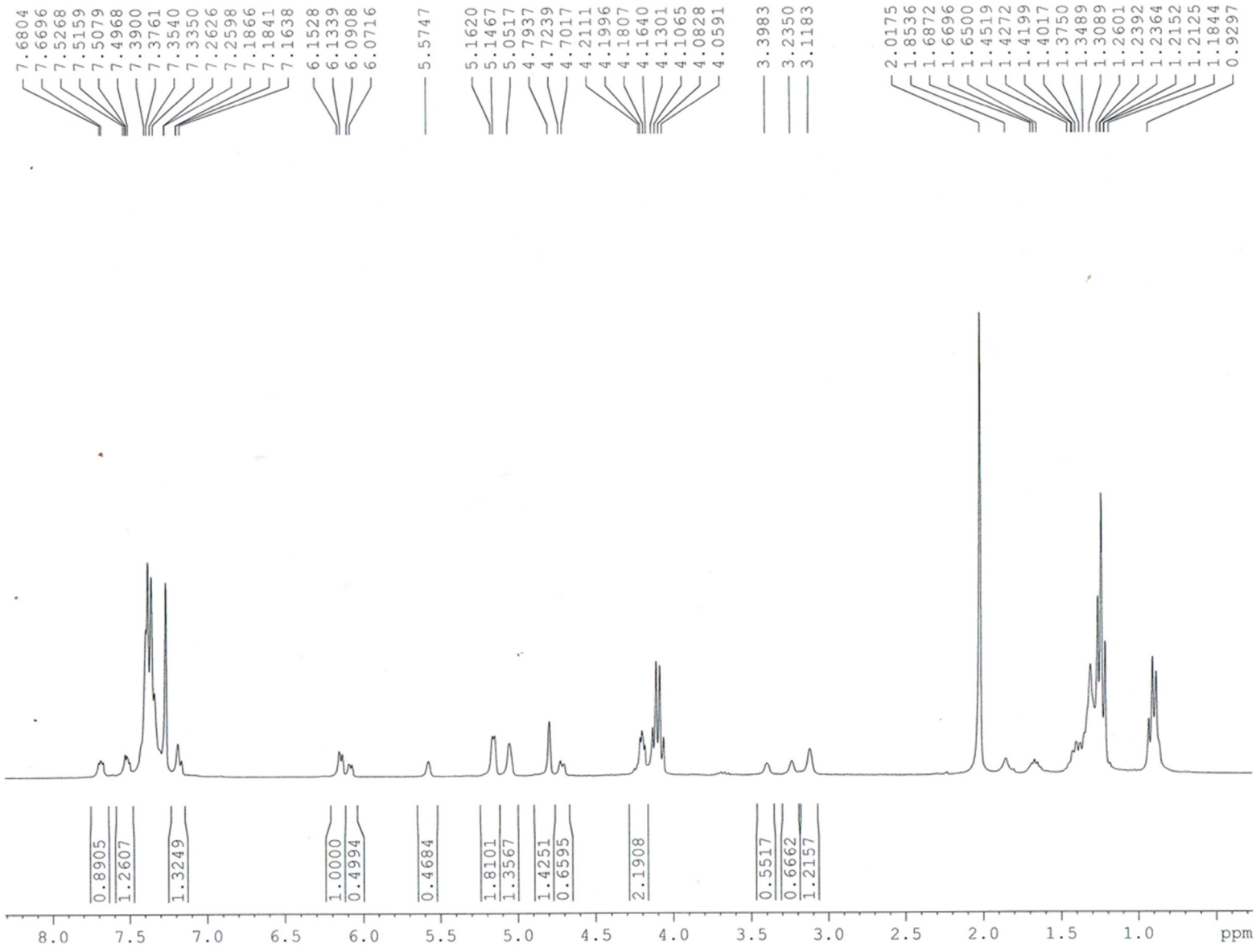


Figure S18. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 5 of Table 4 (400 MHz, $CDCl_3$, 298 K)

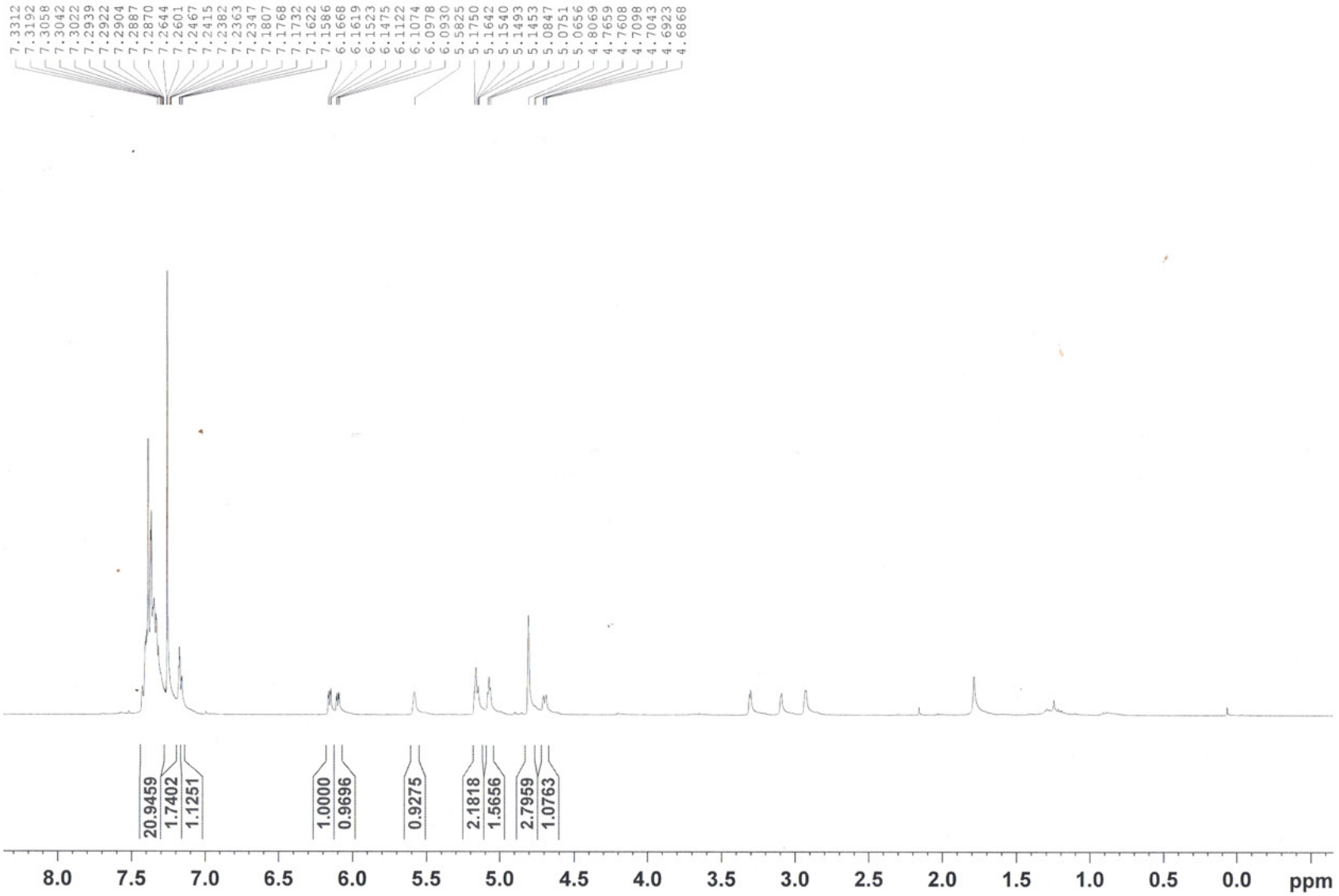


Figure S19. ^{1}H NMR spectrum of *Erythro*/*Threo* mixture, entry 6 of Table 4 (400 MHz, $CDCl_3$, 298 K)

HPLC Chromatograms

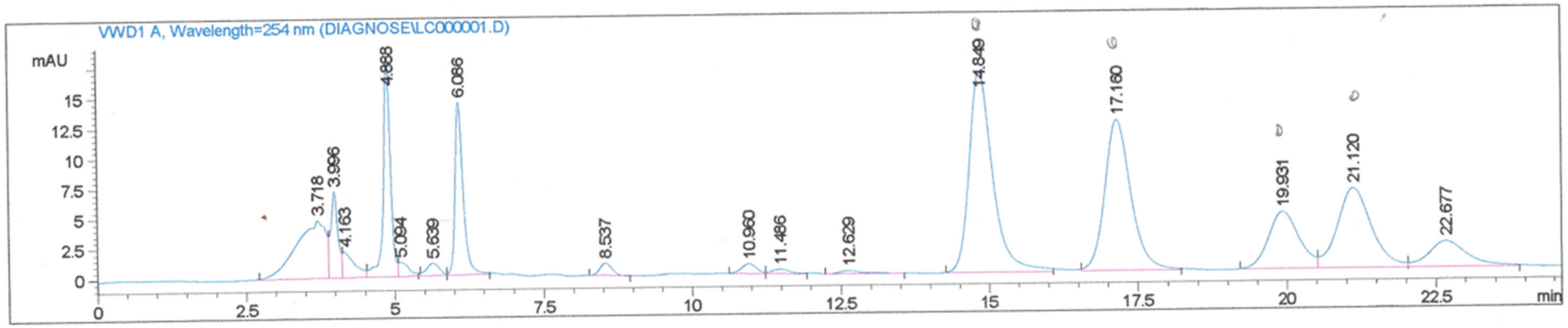


Figure S20. HPLC Chromatogram of *Erythro*/*Threo* mixture entry 1, table 1.

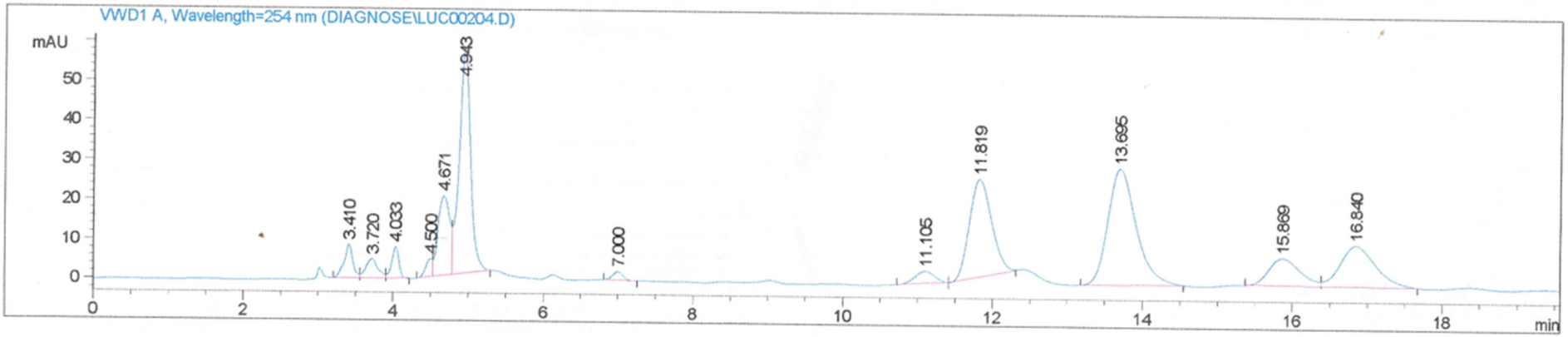


Figure S21. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 2 table 1.

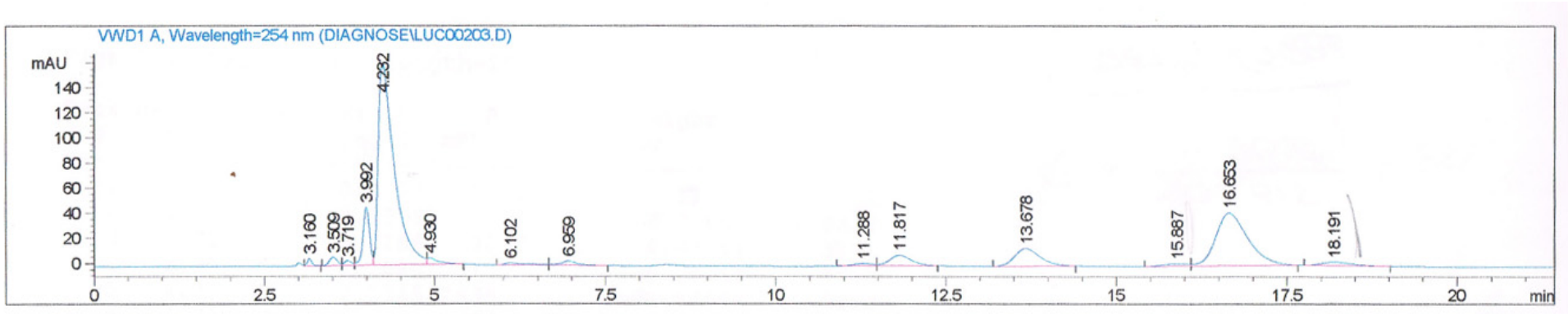


Figure S22. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 1 of Table 3.

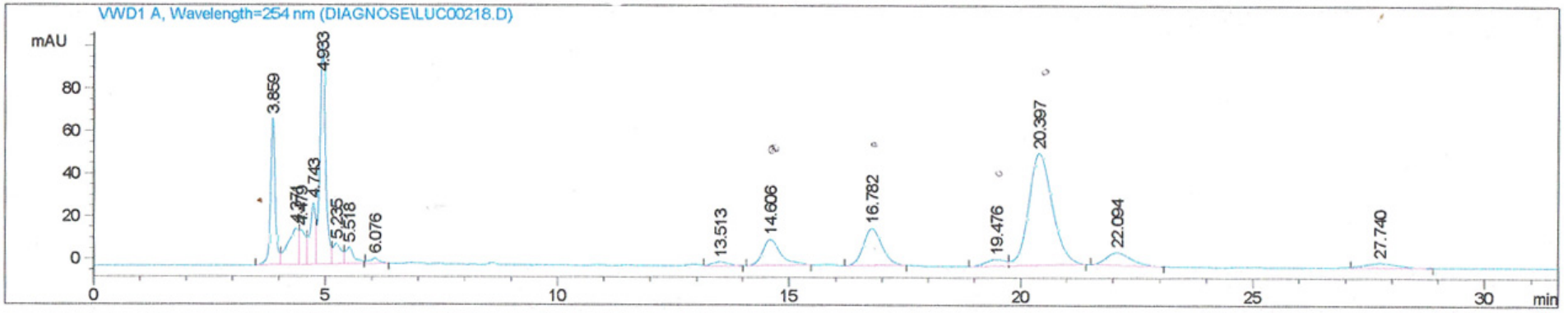


Figure S23. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 3 of Table 3.

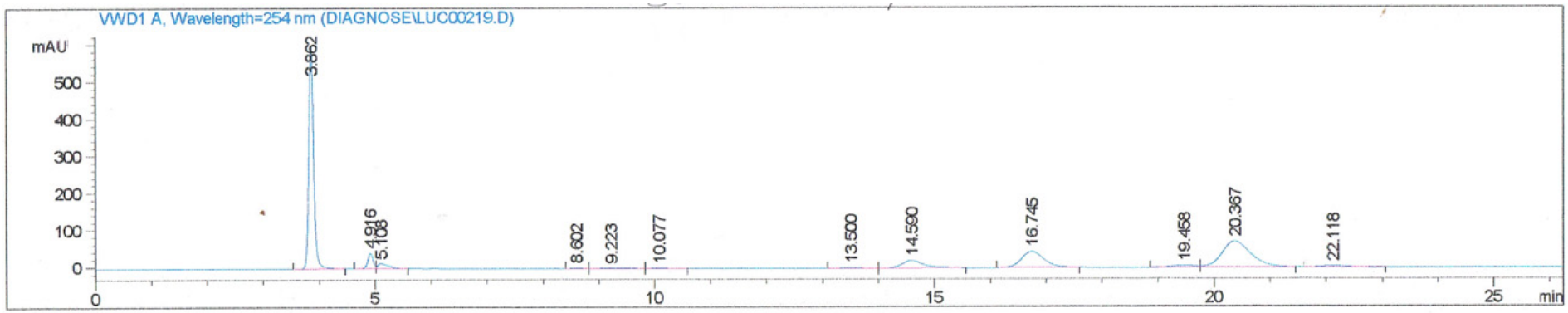


Figure S24. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 4 of Table 3.

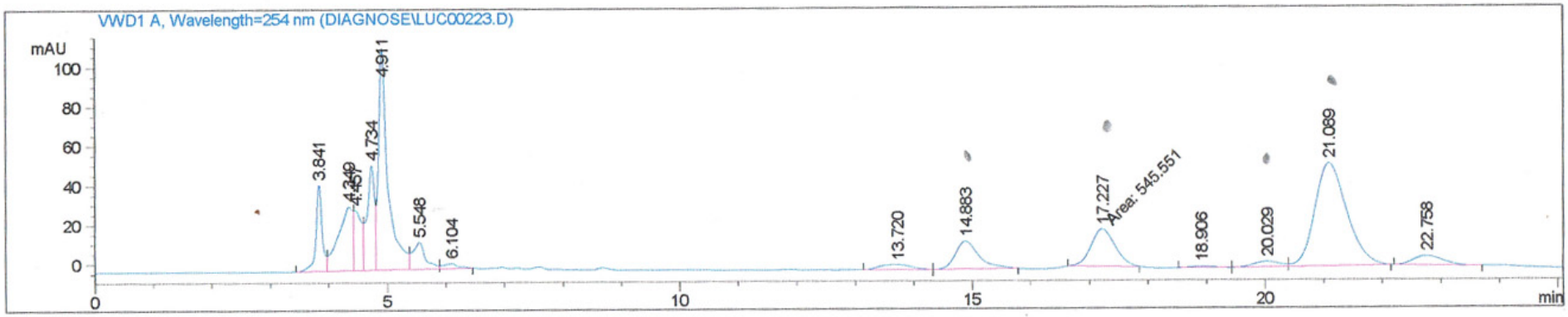


Figure S25. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 5 of Table 3.

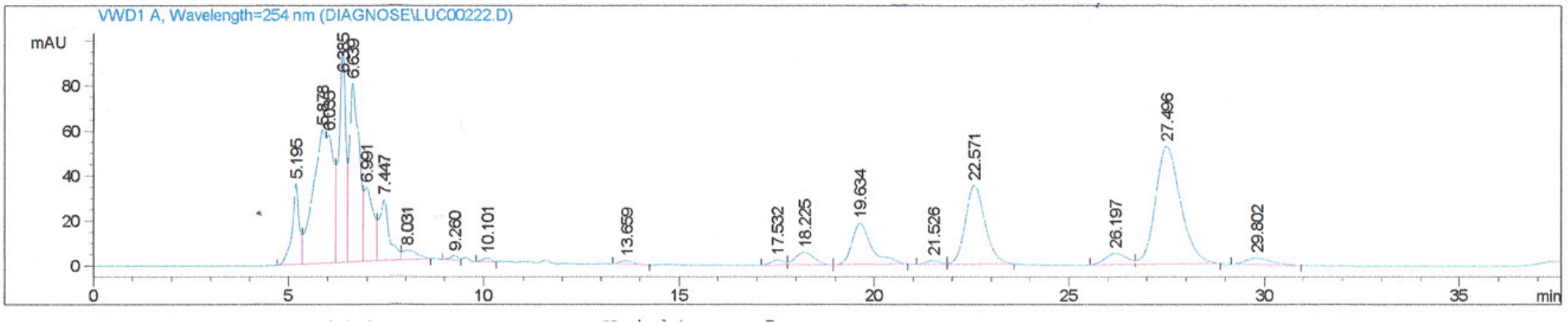


Figure S26. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 6 of Table 3.

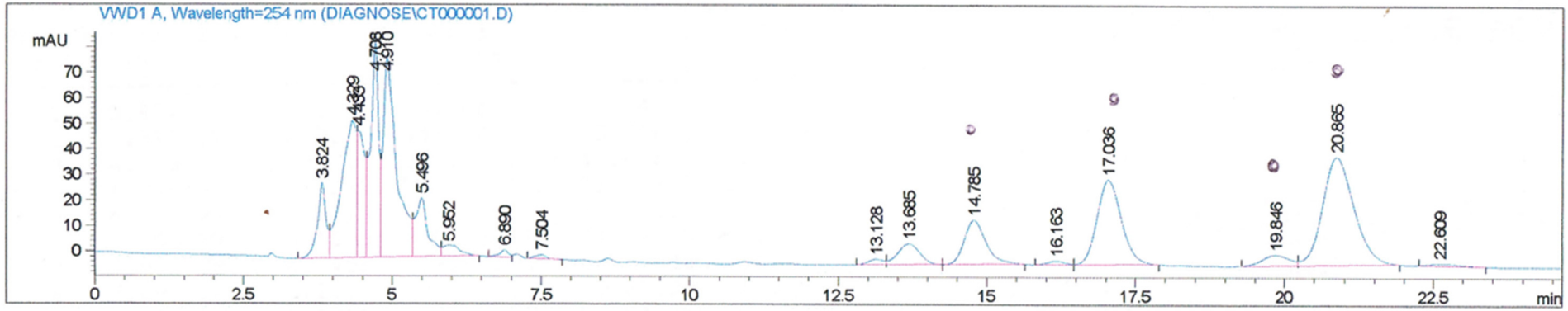


Figure S27. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 2 of Table 4.

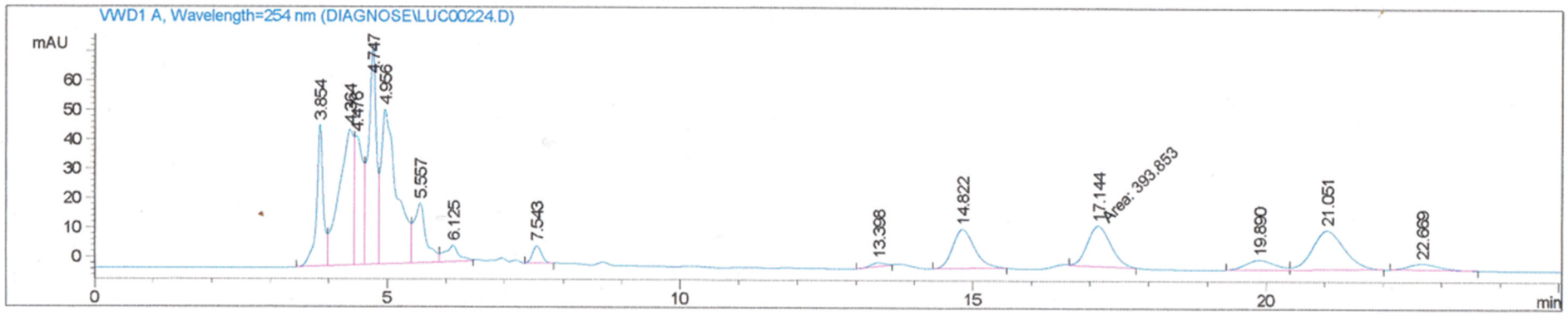


Figure S28. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 3 of Table 4.

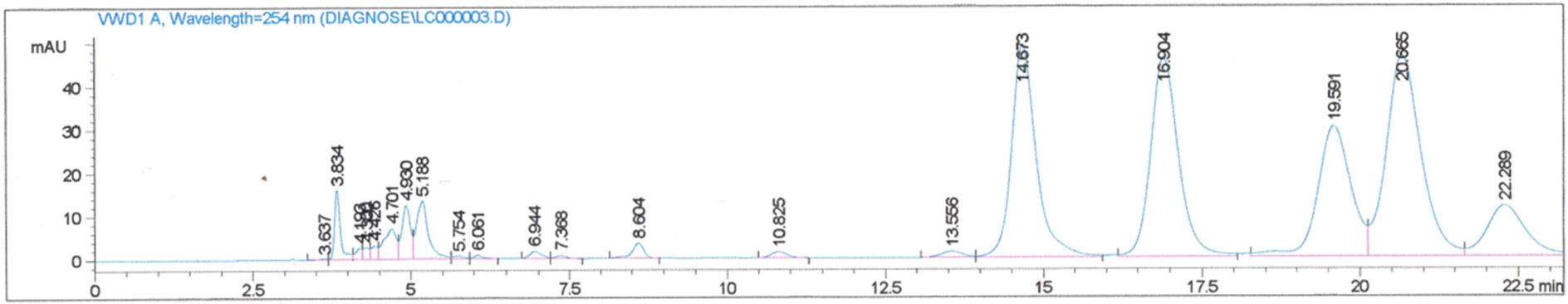


Figure S29. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 4 of Table 4.

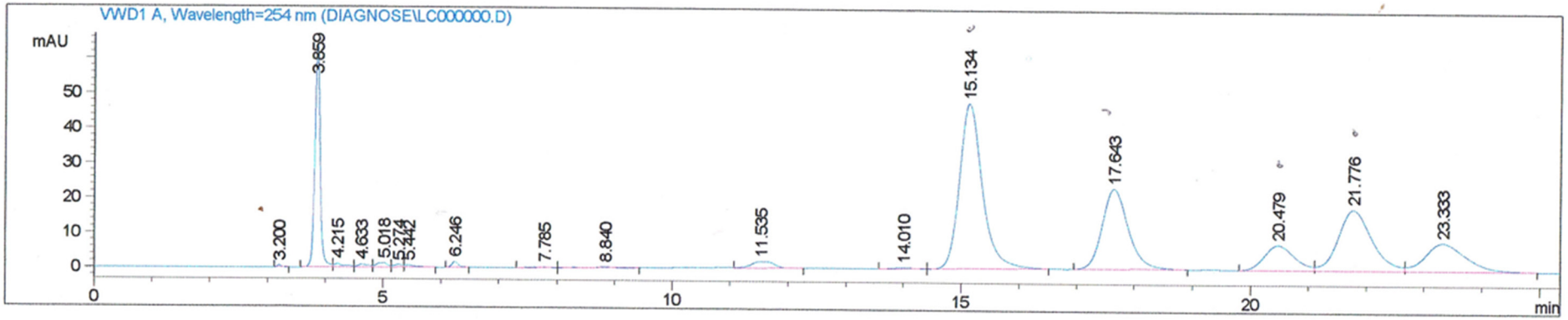


Figure S30. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 5 of Table 4.

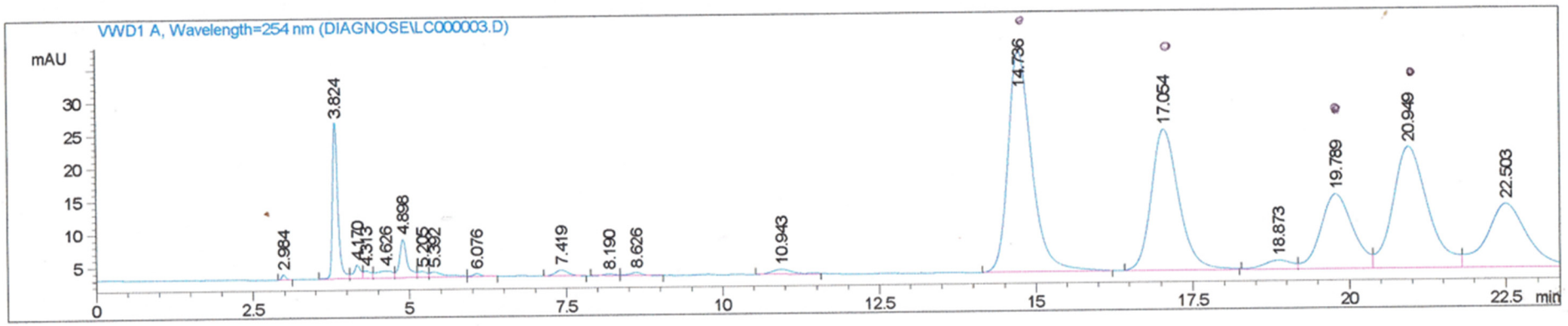


Figure S31. HPLC Chromatogram of *Erythro*/*Threo* mixture, entry 6 of Table 4.

Computational Details

Computational studies have been performed using the DFT method incorporated in the Gaussian 16 package[4], and using b3lyp/6-31G(d,p) level of theory in benzaldehyde as solvent. The starting structure for DFT calculations were obtained by molecular mechanics calculation performed by YASARA software. All optimized structures were characterized by 0 imaginary frequency.

The non-covalent interaction (NCI) investigations were carried out with the Multiwfn program[13] and its plot was graphed with VMD program[14] Plots describe the RDG values versus the electron density multiplied by the sign of the second Hessian eigenvalue (s = 0.5 a.u.; left) and gradient isosurfaces (s = 0.4 a.u.; right) for the complexes.

The coloring scheme was chosen to assist in distinguishing the amplitude of the electron density corresponding to different types of interactions. Marked in green color represent medium-strong (cation···π, Van der Waals and C-H···π) interactions whereas the red color represents the repulsive ones. The coordination energy of benzaldehyde to organocatalyst is calculated according to eqn 1:

$$E_{Coord} = E_{C/A} - E^0_C - E^0_A$$

where $E_{C/A}$ is the energy of the system composed by an aldehyde molecule bonded to the organocatalyst, while E^0_A and E^0_C are the total energies of the free reactants, aldehyde and organocatalysts, respectively.

Table S1. Relative stabilities between isomers of Figure 5

Systems	ΔE_{isomer} [a] (kcal/mol)	E_{coord} (kcal/mol)
7-cis-cis	1.77	-
7-trans-cis	2.41	-
7-trans-trans	0.00	-
8-cis-cis	0.00	-
8-trans-cis	5.33	-
8-trans-trans	8.07	-
5@8-cis-cis	-	-8.9
$(5)_2$@8-cis-cis	-	-12.9

[a] ΔE_{isomer} is calculated assuming as zero the energy of most stable conformer.

Atomic Coordinates

2-cis-A

C	-4.1341	-3.1117	0.6411
C	-3.3039	-2.0989	0.076
C	-3.5717	-1.6907	-1.2693
C	-4.6408	-2.2874	-1.9847
C	-5.4274	-3.2694	-1.3909
C	-5.1752	-3.6792	-0.0882
C	-2.2187	-1.4927	0.799
C	-1.4453	-0.5091	0.1532
C	-1.7114	-0.1327	-1.1633
C	-2.7626	-0.7012	-1.8688
C	-3.3822	-1.4358	5.6745
C	-2.5163	-1.8458	4.6294
C	-2.7993	-1.4646	3.2806
C	-3.9518	-0.6554	3.0492
C	-4.7806	-0.2644	4.097
C	-4.4999	-0.6546	5.3997
C	-1.372	-2.6207	4.9029
C	-0.5198	-2.996	3.8748
C	-0.7691	-2.6436	2.545
C	-1.9224	-1.8894	2.2221
N	-0.337	0.0454	0.8203
C	-0.0232	1.342	1.1158
N	1.1828	1.4243	1.7552
S	-0.9979	2.6592	0.7473
C	1.842	2.5211	2.3361
N	0.1504	-3.0369	1.5374
C	-0.3092	-4.1389	0.6956
C	1.5731	-3.0908	1.8719
C	1.2101	3.3554	3.266
C	1.9029	4.4229	3.8513
C	3.2442	4.6333	3.5076
C	3.8954	3.794	2.5943
C	3.1838	2.7357	2.0136
C	1.222	5.3381	4.87
C	5.3569	4.0495	2.2216
F	2.0561	5.6222	5.8721
F	0.8752	6.4768	4.2709
F	0.1269	4.7797	5.3899
F	6.1428	3.4516	3.1166
F	5.6461	3.5657	1.0119
F	5.6291	5.3561	2.2213
H	-3.9563	-3.4471	1.6525
H	-4.8414	-1.9767	-3.0001
H	-6.2391	-3.7187	-1.9459
H	-5.7926	-4.4439	0.3616
H	-1.0962	0.6157	-1.6426
H	-2.9617	-0.3933	-2.8855
H	-3.1656	-1.7284	6.6921
H	-4.1896	-0.3327	2.0458
H	-5.6479	0.3483	3.8958
H	-5.1518	-0.3435	6.2037
H	-1.1561	-2.9112	5.9218
H	0.3481	-3.5873	4.1235
H	0.213	-0.6602	1.288
H	1.7473	0.5898	1.7139
H	-1.3552	-4.0321	0.4089
H	0.2676	-4.1811	-0.2292
H	-0.2128	-5.0933	1.2151
H	1.8648	-2.239	2.4885
H	1.8248	-4.004	2.4129
H	2.1772	-3.0478	0.9646
H	0.1757	3.1717	3.5245
H	3.7854	5.4559	3.9581
H	3.6744	2.085	1.3024

Energy = -2356.738413 a.u.
0 imaginary frequency

2-trans-A

C	-4.5452	0.7849	-3.3783
C	-4.0267	1.8609	-2.5978
C	-3.6447	3.0584	-3.2834
C	-3.8081	3.1448	-4.6890
C	-4.3284	2.0730	-5.4074
C	-4.6913	0.9012	-4.7574
C	-3.8701	1.7806	-1.1705
C	-3.3126	2.8854	-0.4933
C	-2.9297	4.035	-1.1772
C	-3.1022	4.1359	-2.5502
C	-7.4371	-1.2246	0.6684
C	-6.0643	-0.9152	0.5015
C	-5.6812	0.2379	-0.2529
C	-6.7232	1.0432	-0.8049
C	-8.063	0.7109	-0.6268
C	-8.4175	-0.4153	0.1037
C	-5.0676	-1.7305	1.0731
C	-3.7266	-1.4203	0.9027
C	-3.3169	-0.3025	0.17
C	-4.2843	0.5451	-0.4181
N	-3.0578	2.8679	0.8874
C	-3.9332	3.0264	1.9155
N	-5.2609	3.0901	1.5943
S	-3.2969	3.1031	3.4515
C	-6.3622	3.2827	2.4361
N	-1.9312	-0.0387	0.0201
C	-1.0462	-0.3216	1.1487
C	-1.3881	-0.3992	-1.2866
C	-6.5629	4.5035	3.0859
C	-7.6871	4.6926	3.9005
C	-8.6061	3.6452	4.0491
C	-8.4152	2.4193	3.396
C	-7.2846	2.2481	2.5893
C	-7.9273	6.0149	4.6292
C	-9.4082	1.269	3.5675
F	-6.9559	6.9029	4.4059
F	-9.0811	6.5436	4.2199
F	-8.0026	5.7944	5.9422

F	-8.7621	0.1158	3.7471
F	-10.2167	1.4586	4.6124
F	-10.1564	1.1728	2.4685
H	-4.8296	-0.1397	-2.8972
H	-3.5184	4.0494	-5.2044
H	-4.4465	2.1486	-6.4791
H	-5.0882	0.0733	-5.3275
H	-2.4947	4.8654	-0.6377
H	-2.8084	5.038	-3.0681
H	-7.721	-2.0975	1.2395
H	-6.4787	1.9217	-1.3839
H	-8.8352	1.3309	-1.0611
H	-9.462	-0.6618	0.2369
H	-5.3543	-2.603	1.6435
H	-2.9905	-2.0764	1.3414
H	-2.0864	2.7863	1.1498
H	-5.4878	2.8191	0.6485
H	-1.506	-0.015	2.0902
H	-0.8007	-1.3825	1.2147
H	-0.1187	0.2448	1.0529
H	-1.2778	-1.4807	-1.3756
H	-2.0352	-0.0707	-2.1002
H	-0.4155	0.0692	-1.4431
H	-5.8345	5.2929	2.9575
H	-9.4745	3.7921	4.678
H	-7.1167	1.3039	2.0895

Energy = -2356.741769 a.u.
0 imaginary frequency

2-cis-B

C	0.026	-0.9561	0.7967
C	0.2118	-2.0108	1.7388
C	-0.2536	-3.3158	1.3758
C	-0.848	-3.5223	0.1053
C	-0.9973	-2.4644	-0.7856
C	-0.5671	-1.1906	-0.4406
C	0.8219	-1.8049	3.0248
C	0.9338	-2.9091	3.8945
C	0.43	-4.1596	3.5461
C	-0.133	-4.3777	2.2976
C	4.0492	2.0333	2.6572
C	2.9179	1.4382	3.2704
C	2.4543	0.16	2.8251
C	3.1731	-0.4671	1.7648
C	4.2799	0.143	1.1809
C	4.7159	1.3837	1.6246
C	2.2424	2.0938	4.3172
C	1.1347	1.5073	4.9089
C	0.6522	0.2621	4.4964
C	1.3035	-0.4388	3.4516
N	1.4401	-2.7392	5.1893
C	2.6185	-3.1222	5.7625
N	3.5581	-3.894	5.1453
S	2.9342	-2.6101	7.2992
C	3.5279	-4.5479	3.9164
N	-0.4957	-0.2778	5.1325
C	-0.6716	-0.048	6.5666
C	-1.7224	-0.1755	4.3466
C	3.1578	-5.8927	3.8665
C	3.1369	-6.5738	2.6438
C	3.5312	-5.898	1.4809
C	3.9346	-4.5565	1.5269
C	3.9357	-3.8856	2.7579
C	2.7002	-8.0383	2.5958
C	4.3965	-3.8498	0.2525
F	1.3737	-8.0965	2.7096
F	3.055	-8.6314	1.4544
F	3.2449	-8.7186	3.6058
F	3.3496	-3.2703	-0.3309
F	5.3079	-2.914	0.5235
F	4.9385	-4.7123	-0.6099
H	0.3493	0.0452	1.0417
H	-1.1957	-4.5084	-0.1674
H	-1.4568	-2.6306	-1.7498
H	-0.6947	-0.3746	-1.138
H	0.4828	-4.9759	4.252
H	-0.5012	-5.3588	2.0324
H	4.3929	3.0001	2.997
H	2.8491	-1.427	1.3933
H	4.8037	-0.348	0.3733
H	5.5759	1.8478	1.1617
H	2.5917	3.059	4.6561
H	0.6334	2.0459	5.6975
H	0.9095	-2.0723	5.7332
H	4.3804	-4.0756	5.7033
H	-1.3684	-0.7745	6.9855
H	0.2723	-0.1679	7.1025
H	-1.0529	0.9537	6.7704
H	-2.4602	-0.8995	4.6946
H	-2.1509	0.8254	4.4188
H	-1.5511	-0.3844	3.2899
H	2.8669	-6.4022	4.7752
H	3.5241	-6.4173	0.5311
H	4.2467	-2.8513	2.8213

Energy = -2356.737794 a.u.
0 imaginary frequency

2-trans-B

C	3.7978	1.9161	0.2557
C	3.5492	0.6639	0.892
C	4.1073	0.4535	2.1938
C	4.8826	1.4754	2.799
C	5.1004	2.6812	2.1396
C	4.5617	2.9	0.8782
C	2.7643	-0.3739	0.2831
C	2.5321	-1.5582	1.0081

C	3.1072	-1.7598	2.2628
C	3.8814	-0.7729	2.8565
C	-1.1408	0.3688	-2.785
C	0.2501	0.1621	-2.6028
C	0.7801	0.0123	-1.2823
C	-0.1351	0.0872	-0.1895
C	-1.4978	0.2756	-0.4021
C	-1.9973	0.4152	-1.6902
C	1.1202	0.0977	-3.7095
C	2.4756	-0.1306	-3.5213
C	3.0241	-0.2942	-2.2453
C	2.1916	-0.2092	-1.1038
N	1.7471	-2.5421	0.3921
C	0.7418	-3.3483	0.8476
N	0.0767	-4.0502	-0.1072
S	0.1838	-3.4823	2.4075
C	0.299	-4.0255	-1.4852
N	4.4098	-0.5664	-2.1155
C	5.333	0.117	-3.0213
C	4.7318	-1.9717	-1.8781
C	-0.6905	-3.4971	-2.3126
C	-0.473	-3.3969	-3.6919
C	0.7419	-3.8425	-4.2263
C	1.7355	-4.3853	-3.4024
C	1.5034	-4.4837	-2.0257
C	-1.519	-2.7766	-4.6123
C	3.06	-4.8284	-4.0141
F	-1.9949	-3.7114	-5.432
F	-2.5385	-2.2479	-3.9368
F	-0.9607	-1.8129	-5.342
F	3.9626	-5.1491	-3.0871
F	2.8528	-5.8906	-4.789
F	3.5598	-3.8445	-4.7601
H	3.3885	2.1093	-0.7255
H	5.305	1.3132	3.7811
H	5.6924	3.4539	2.6106
H	4.7382	3.8416	0.3767
H	2.9618	-2.6919	2.7892
H	4.3134	-0.9387	3.8338
H	-1.537	0.4802	-3.7851
H	0.2247	-0.0139	0.8247
H	-2.1726	0.3178	0.4419
H	-3.0576	0.5644	-1.8412
H	0.7221	0.2105	-4.7089
H	3.1071	-0.2032	-4.3939
H	1.8084	-2.5	-0.6147
H	-0.7646	-4.5178	0.1995
H	5.0501	1.1633	-3.1491
H	6.3424	0.1123	-2.6077
H	5.3582	-0.3525	-4.006
H	4.0399	-2.4422	-1.1805
H	4.7024	-2.5411	-2.8074
H	5.7278	-2.0649	-1.443
H	-1.6103	-3.1312	-1.8759
H	0.92	-3.7551	-5.2906
H	2.2594	-4.8926	-1.3685

Energy = -2356.737066 a.u.
0 imaginary frequency

3-cis-A

C	-7.5139	0.7179	1.7318
C	-8.7258	1.1143	2.3791
C	-8.7186	2.2163	3.2711
C	-7.5422	2.9167	3.52
C	-6.359	2.5456	2.8944
C	-7.5266	-0.3997	0.8298
C	-8.7379	-1.0883	0.6037
C	-9.9127	-0.6741	1.2411
C	-9.9149	0.4028	2.117
C	-4.6579	-0.579	-3.2747
C	-4.8637	-0.9098	-1.9119
C	-6.0573	-0.4834	-1.25
C	-6.9971	0.2832	-2.0021
C	-6.7659	0.5922	-3.3398
C	-5.6061	0.1626	-3.9719
C	-3.9036	-1.6526	-1.1958
C	-4.1149	-1.9667	0.139
C	-5.2741	-1.5706	0.8116
C	-6.2654	-0.8297	0.1296
N	-8.7167	-2.1675	-0.3088
C	-9.5741	-3.1914	-0.4524
N	-9.1971	-3.9801	-1.474
O	-10.5651	-3.3864	0.2462
C	-9.7847	-5.1845	-1.9056
N	-5.4433	-1.9293	2.1704
C	-6.2666	-3.1156	2.3847
C	-4.2825	-1.8188	3.0513
C	-9.5608	-5.5633	-3.2322
C	-10.093	-6.7555	-3.7405
C	-10.8543	-7.5755	-2.8984
C	-11.0805	-7.2213	-1.5626
C	-10.5381	-6.0268	-1.073
C	-9.8663	-7.143	-5.203
C	-11.8854	-8.1359	-0.6372
F	-10.8583	-7.9068	-5.6655
F	-9.7819	-6.0607	-5.9789
F	-8.7253	-7.8245	-5.2986
F	-13.1468	-7.709	-0.5925
F	-11.8806	-9.399	-1.069
F	-11.3852	-8.1223	0.5997
H	-9.6363	2.512	3.7595
H	-7.5473	3.7538	4.2039
H	-5.4509	3.0961	3.097
H	-10.8509	-1.1773	1.0629
H	-10.8325	0.7037	2.6022
H	-3.7533	-0.9017	-3.7706
H	-7.902	0.6387	-1.5305
H	-7.49	1.1759	-3.8911
H	-5.4363	0.4134	-5.0098
H	-2.9992	-1.9746	-1.6923

H	-3.3644	-2.5438	0.6579
H	-7.8887	-2.1913	-0.8797
H	-8.4223	-3.6526	-2.0249
H	-7.1521	-3.1154	1.75
H	-5.7092	-4.0282	2.1689
H	-6.6193	-3.1533	3.4162
H	-4.6058	-1.7568	4.0908
H	-3.6089	-2.6703	2.9445
H	-3.7201	-0.9072	2.842
H	-8.9757	-4.9265	-3.8814
H	-11.2709	-8.4971	-3.2852
H	-10.7033	-5.7633	-0.0377
C	-6.3341	1.4681	2.0134
H	-5.4009	1.1964	1.5421

Energy = -2033.788689 a.u.
0 imaginary frequency

3-trans-A

C	-4.5228	0.5042	-1.0097
C	-3.778	-0.7006	-0.83
C	-4.2267	-1.8677	-1.529
C	-5.3572	-1.7877	-2.3816
C	-6.0431	-0.5873	-2.5351
C	-5.6313	0.5489	-1.8512
C	-2.6194	-0.7824	0.0222
C	-1.9974	-2.0397	0.1786
C	-2.4549	-3.166	-0.4962
C	-3.5414	-3.089	-1.3544
C	-0.3078	3.6727	-0.0935
C	-0.9057	2.6216	0.6484
C	-1.4714	1.4983	-0.0338
C	-1.3837	1.4825	-1.461
C	-0.7954	2.533	-2.1613
C	-0.2633	3.6212	-1.4827
C	-0.9449	2.6673	2.0556
C	-1.5378	1.6392	2.7735
C	-2.1125	0.5337	2.1403
C	-2.083	0.4368	0.728
N	-0.9542	-2.2639	1.0839
C	0.3193	-1.8588	1.0284
N	0.6523	-1.0306	0.0256
O	1.1133	-2.2609	1.8731
C	1.9455	-0.6011	-0.2976
N	-2.7251	-0.474	2.9282
C	-4.1837	-0.4141	2.9532
C	-2.1019	-0.8305	4.2022
C	3.0709	-1.4309	-0.2035
C	4.3392	-0.9541	-0.556
C	4.472	0.3634	-1.0153
C	3.3525	1.1985	-1.1203
C	2.0966	0.7022	-0.7631
C	5.5478	-1.8789	-0.4434
C	3.4677	2.6386	-1.6091
F	6.6383	-1.3578	-1.0061
F	5.8045	-2.1052	0.8429
F	5.2888	-3.0427	-1.0382
F	2.7314	2.7927	-2.7077
F	3.0071	3.4636	-0.6709
F	4.7243	2.9817	-1.8919
H	-4.2269	1.4024	-0.4863
H	-5.6897	-2.6703	-2.9104
H	-6.9056	-0.5382	-3.1855
H	-6.1768	1.4745	-1.9738
H	-1.9671	-4.1208	-0.3538
H	-3.8835	-3.9723	-1.8762
H	0.1181	4.5189	0.4282
H	-1.7852	0.6503	-2.0212
H	-0.7481	2.5016	-3.2414
H	0.196	4.4275	-2.0382
H	-0.5153	3.5135	2.5744
H	-1.5637	1.719	3.85
H	-1.1584	-2.8968	1.8404
H	-0.1109	-0.6396	-0.5038
H	-4.5985	-0.2259	1.9619
H	-4.6022	-1.3603	3.2989
H	-4.5307	0.3856	3.6096
H	-1.0157	-0.8785	4.1036
H	-2.3416	-0.1104	4.986
H	-2.4334	-1.8186	4.5242
H	2.963	-2.4494	0.1441
H	5.4488	0.7403	-1.289
H	1.2381	1.3495	-0.8317

Energy = -2033.789796 a.u.
0 imaginary frequency

3-cis-B

C	-3.2823	-0.486	2.5869
C	-2.1841	-1.253	2.0959
C	-1.4886	-2.088	3.0257
C	-1.8941	-2.1197	4.3841
C	-2.9679	-1.3496	4.819
C	-3.6577	-0.54	3.9264
C	-1.7673	-1.2224	0.7202
C	-0.6889	-2.0381	0.3121
C	-0.0268	-2.8475	1.2432
C	-0.409	-2.8746	2.5764
C	-4.8964	-0.6682	-3.1601

C	-4.0349	-0.0937	-2.1917
C	-3.3656	-0.9337	-1.2475
C	-3.6153	-2.3373	-1.3163
C	-4.466	-2.8715	-2.2798
C	-5.1007	-2.0436	-3.1961
C	-3.8303	1.2994	-2.1449
C	-2.9912	1.8515	-1.1885
C	-2.317	1.0586	-0.2558
C	-2.484	-0.3461	-0.2742
N	-0.318	-2.0177	-1.0527
C	0.3615	-2.9709	-1.7092
N	1.6911	-3.0806	-1.5382
O	-0.2184	-3.7414	-2.4589
C	2.589	-2.1966	-0.9186
N	-1.4694	1.6784	0.6958
C	-1.883	2.9622	1.2593
C	-0.0461	1.5775	0.395
C	3.6202	-2.7445	-0.1532
C	4.5725	-1.9188	0.4576
C	4.4948	-0.5334	0.2672
C	3.4799	0.0308	-0.515
C	2.5265	-0.8094	-1.1055
C	5.7033	-2.5197	1.2942
C	3.4496	1.5439	-0.7322
F	6.8217	-1.8018	1.1745
F	5.3372	-2.5275	2.5753
F	5.9735	-3.7723	0.9214
F	2.5507	1.9051	-1.6501
F	3.1512	2.1486	0.4171
F	4.6483	1.9666	-1.1359
H	-3.8332	0.1542	1.9139
H	-1.364	-2.75	5.0839
H	-3.2691	-1.381	5.8566
H	-4.4905	0.0539	4.2756
H	0.7964	-3.4773	0.944
H	0.1158	-3.5072	3.2785
H	-5.3977	-0.0295	-3.8736
H	-3.1364	-3.0069	-0.6163
H	-4.6323	-3.939	-2.3176
H	-5.7582	-2.4721	-3.9395
H	-4.3348	1.9367	-2.8578
H	-2.8533	2.922	-1.1851
H	-1.0189	-1.5776	-1.6286
H	2.0806	-3.9146	-1.9477
H	-2.9522	2.965	1.4775
H	-1.3682	3.1423	2.204
H	-1.6688	3.7899	0.5819
H	0.2261	0.5843	0.0412
H	0.2396	2.2931	-0.3772
H	0.5474	1.7684	1.29
H	3.6788	-3.817	-0.0244
H	5.2332	0.1132	0.7248
H	1.7475	-0.3889	-1.7261

Energy =-2033.775586 a.u.
0 imaginary frequency

3-trans-B

C	-3.5991	0.2423	0.0897
C	-3.0562	-0.2668	1.307
C	-3.7609	0.0164	2.5197
C	-4.9516	0.7861	2.4792
C	-5.4421	1.2641	1.2684
C	-4.7717	0.9934	0.0826
C	-1.8513	-1.0492	1.3545
C	-1.4072	-1.5456	2.5975
C	-2.103	-1.2421	3.7725
C	-3.2588	-0.4749	3.7425
C	-0.4699	-4.2465	-2.2562
C	-0.4158	-2.9503	-1.6844
C	-1.1452	-2.6707	-0.486
C	-1.9135	-3.7305	0.0847
C	-1.9386	-4.9958	-0.4961
C	-1.2224	-5.2518	-1.658
C	0.3523	-1.9307	-2.2808
C	0.4069	-0.6687	-1.7065
C	-0.285	-0.3631	-0.5302
C	-1.0805	-1.3541	0.0936
N	-0.2444	-2.3366	2.5837
C	0.2673	-3.1667	3.5094
N	1.2957	-3.9285	3.1038
O	-0.1486	-3.2853	4.6556
C	1.8752	-3.9743	1.832
N	-0.172	0.9391	0.0218
C	-0.0875	2.0774	-0.8935
C	0.6889	1.0481	1.1974
C	1.7944	-5.1582	1.1001
C	2.3453	-5.232	-0.1854
C	2.9875	-4.1075	-0.7182
C	3.0881	-2.9198	0.017
C	2.5306	-2.8602	1.2988
C	2.2082	-6.5014	-1.0209
C	3.7601	-1.6928	-0.5904
F	2.0281	-6.2042	-2.307
F	3.3212	-7.2214	-0.903
F	1.1761	-7.2438	-0.6215
F	3.636	-1.6807	-1.917
F	3.2265	-0.5682	-0.1176
F	5.0543	-1.7121	-0.2825
H	-3.0959	0.0467	-0.8459
H	-5.4799	1.0007	3.3977
H	-6.351	1.8493	1.2483

H	-5.1643	1.3703	-0.8518
H	-1.7633	-1.5877	4.7362
H	-3.7846	-0.2534	4.6609
H	0.0859	-4.454	-3.1604
H	-2.4852	-3.5586	0.9858
H	-2.5228	-5.7851	-0.0426
H	-1.2495	-6.2389	-2.0992
H	0.9087	-2.1406	-3.1845
H	1.0241	0.0796	-2.1808
H	0.2237	-2.3665	1.692
H	1.6749	-4.546	3.8044
H	-0.7615	1.9494	-1.7423
H	-0.3917	2.994	-0.3862
H	0.9244	2.2125	-1.2793
H	0.3737	1.892	1.8128
H	0.6392	0.1654	1.8335
H	1.731	1.198	0.9118
H	1.2822	-6.0122	1.5225
H	3.4051	-4.1549	-1.7156
H	2.5984	-1.9494	1.8786

Energy = -2033.784316 a.u.
0 imaginary frequency

7-cis-cis

C	-0.4914	5.944	0.1064
C	-0.6468	4.7963	0.9347
C	-0.4566	4.95	2.3473
C	-0.1251	6.2272	2.8711
C	0.0172	7.3171	2.0416
C	-0.1686	7.17	0.6467
C	-0.988	3.5079	0.4057
C	-1.115	2.4231	1.27
C	-0.9024	2.5797	2.6662
C	-0.5924	3.8108	3.1841
N	-1.3505	1.1458	0.7123
C	-2.0764	0.094	1.1995
N	-1.8078	-1.0463	0.4781
S	-3.1476	0.1823	2.4961
C	-2.4189	-2.3135	0.5168
C	-3.7874	-2.5014	0.7516
C	-4.3166	-3.7908	0.7337
C	-3.5163	-4.9023	0.4678
C	-2.1605	-4.7038	0.2135
C	-1.6097	-3.4237	0.2417
C	-5.7975	-3.9812	0.9346
C	-1.2848	-5.8772	-0.1376
F	-6.0762	-5.1706	1.5134
F	-6.3341	-3.0158	1.7101
F	-6.4661	-3.9552	-0.244
F	-0.0114	-5.6994	0.2788
F	-1.7359	-7.0253	0.4125
F	-1.2334	-6.0768	-1.4763
H	-0.637	5.8475	-0.9641
H	0.0151	6.3277	3.9439
H	0.2702	8.2892	2.4535
H	-0.0578	8.0324	-0.0038
H	-0.984	1.7151	3.3103
H	-0.4301	3.9217	4.2525
H	-0.947	1.0054	-0.2118
H	-0.9712	-1.0043	-0.099
H	-4.4241	-1.6532	0.9559
H	-3.9375	-5.8997	0.4687
H	-0.5479	-3.2878	0.0652
C	-3.5769	4.095	-0.8915
C	-2.4732	3.6366	-1.6613
C	-2.6495	3.4639	-3.0735
C	-3.9094	3.7616	-3.6568
C	-4.9576	4.2062	-2.8827
C	-4.7879	4.371	-1.4879
C	-1.2011	3.3328	-1.0676
C	-0.1771	2.8704	-1.8814
C	-0.3497	2.7116	-3.2804
C	-1.5588	2.9994	-3.858
N	1.1124	2.6132	-1.3127
C	1.7367	1.4067	-1.2644
N	3.0096	1.4774	-0.774
S	0.9772	-0.0342	-1.7459
C	3.9244	0.4312	-0.4959
C	4.1566	-0.6203	-1.3883
C	5.1012	-1.5945	-1.0668
C	5.8356	-1.5266	0.1172
C	5.6137	-0.4606	0.9873
C	4.6596	0.5121	0.6908
C	5.384	-2.6976	-2.0542
C	6.4387	-0.3316	2.241
F	5.8175	-3.82	-1.4415
F	4.2902	-3.0211	-2.7754
F	6.3448	-2.3354	-2.9377
F	5.7566	0.2857	3.2306
F	6.8368	-1.5337	2.7068
F	7.5585	0.3982	2.0233
H	-3.4579	4.2194	0.1788
H	-4.0311	3.6285	-4.7281
H	-5.9173	4.4285	-3.3391
H	-5.6203	4.7161	-0.8825
H	0.4865	2.3629	-3.8751
H	-1.6943	2.8797	-4.9289
H	1.5502	3.3991	-0.8442
H	3.3165	2.3864	-0.447
H	3.6028	-0.68	-2.3142

H	6.5603	-2.2936	0.3602
H	4.4751	1.3215	1.3889

Energy = -3674.921618 a.u.
0 imaginary frequency

7-trans-cis

C	-1.2881	4.7559	-1.5176
C	-1.1257	4.1319	-0.2486
C	-0.8251	4.9615	0.8813
C	-0.7044	6.365	0.7035
C	-0.868	6.9365	-0.5383
C	-1.1607	6.1208	-1.6568
C	-1.2361	2.711	-0.0712
C	-1.0374	2.1669	1.1958
C	-0.7722	2.997	2.3165
C	-0.6654	4.3545	2.1552
N	-1.2069	0.7711	1.3564
C	-0.4858	-0.0966	2.1194
N	-0.9637	-1.3829	2.143
S	0.9312	0.266	2.9634
C	-2.1763	-1.9155	1.6501
C	-3.3959	-1.2358	1.7699
C	-4.5661	-1.8246	1.2892
C	-4.5506	-3.0959	0.7201
C	-3.3359	-3.778	0.6302
C	-2.1539	-3.1964	1.0801
C	-5.8744	-1.0962	1.4649
C	-3.296	-5.1306	-0.0346
F	-6.7945	-1.4895	0.5599
F	-6.404	-1.3172	2.6907
F	-5.7223	0.2407	1.3396
F	-3.1806	-5.0187	-1.3776
F	-2.2522	-5.8715	0.3929
F	-4.4233	-5.8353	0.205
C	-4.0151	2.3653	-1.0087
C	-2.9404	1.7124	-1.6757
C	-3.2455	0.8901	-2.8096
C	-4.5944	0.7601	-3.2336
C	-5.6105	1.4036	-2.5638
C	-5.3145	2.2093	-1.4389
C	-1.5789	1.8271	-1.2339
C	-0.5828	1.1164	-1.9024
C	-0.8875	0.3384	-3.0502
C	-2.1844	0.2304	-3.4833
N	0.756	1.2706	-1.4642
C	1.7352	0.3256	-1.314
N	2.8765	0.8668	-0.7707
S	1.5694	-1.3037	-1.7058
C	4.1055	0.2283	-0.4891
C	4.7401	-0.6068	-1.4161
C	5.9838	-1.155	-1.1076
C	6.6206	-0.8687	0.1007
C	5.9894	-0.0205	1.0084
C	4.7359	0.5218	0.7241
C	6.6368	-2.0964	-2.0856
C	6.6351	0.2652	2.3386
F	7.9852	-2.0512	-2.0018
F	6.2732	-3.3803	-1.8608
F	6.3002	-1.8113	-3.3627
F	6.3016	1.4888	2.8064
F	6.2589	-0.6306	3.2802
F	7.9832	0.2125	2.2636
H	-0.2965	-2.0441	2.5186
H	-1.5132	4.1427	-2.3832
H	-0.4788	6.9808	1.5699
H	-0.7731	8.0106	-0.6632
H	-1.2871	6.5757	-2.6347
H	-0.662	2.5457	3.293
H	-0.4656	4.9857	3.0163
H	-1.8055	0.3471	0.6547
H	-3.4385	-0.2625	2.2426
H	-5.4649	-3.548	0.357
H	-1.2142	-3.7291	0.9874
H	-3.8028	2.9867	-0.1458
H	-4.8095	0.1362	-4.0969
H	-6.6389	1.2935	-2.8935
H	-6.1199	2.7095	-0.9099
H	-0.0853	-0.1609	-3.5746
H	-2.4109	-0.3656	-4.3627
H	0.9293	2.1684	-1.0258
H	2.788	1.7852	-0.3517
H	4.2729	-0.8139	-2.3682
H	7.5958	-1.284	0.3215
H	4.2486	1.1693	1.4449

Energy = -3674.920594 a.u.
0 imaginary frequency

7-trans-trans

C	-1.9639	2.8306	0.1243
C	-1.4487	1.9811	-0.8954
C	-2.0964	1.9857	-2.1747
C	-3.2239	2.8234	-2.3806
C	-3.7049	3.623	-1.3683
C	-3.0654	3.6256	-0.1063
C	-0.3278	1.1125	-0.6753
C	0.113	0.2936	-1.7122

C	-0.5059	0.3339	-2.9891
C	-1.5846	1.1529	-3.2044
N	1.257	-0.5105	-1.4896
C	1.5051	-1.7844	-1.9028
N	2.7606	-2.2538	-1.604
S	0.4107	-2.8107	-2.6756
C	3.8967	-1.571	-1.1129
C	4.2631	-0.301	-1.5831
C	5.4142	0.3107	-1.0911
C	6.2289	-0.3315	-0.158
C	5.8725	-1.6051	0.2831
C	4.7117	-2.223	-0.1792
C	5.8365	1.6589	-1.6171
C	6.7108	-2.2908	1.332
F	6.2459	2.473	-0.6186
F	6.8726	1.5502	-2.4803
F	4.8378	2.2885	-2.2718
F	6.3129	-1.9557	2.5807
F	6.6302	-3.6351	1.2389
F	8.0139	-1.9512	1.2298
C	2.0031	2.8249	-0.0658
C	1.4855	1.9323	0.915
C	2.1365	1.8739	2.1913
C	3.2705	2.6934	2.4321
C	3.754	3.5357	1.4561
C	3.1104	3.6013	0.1979
C	0.3586	1.0814	0.6584
C	-0.0861	0.2207	1.6588
C	0.5361	0.1984	2.9346
C	1.6217	0.9985	3.1836
N	-1.2376	-0.5636	1.4052
C	-1.4904	-1.8544	1.7584
N	-2.7544	-2.2993	1.4573
S	-0.3915	-2.9255	2.4604
C	-3.8973	-1.5863	1.0308
C	-4.235	-0.3306	1.5584
C	-5.3892	0.3139	1.1192
C	-6.237	-0.282	0.1845
C	-5.9107	-1.543	-0.3113
C	-4.7459	-2.192	0.0958
C	-5.7728	1.6536	1.6946
C	-6.8439	-2.2326	-1.2737
F	-6.1633	2.5132	0.7268
F	-6.8091	1.5423	2.5572
F	-4.7556	2.2331	2.3667
F	-6.1789	-3.0379	-2.129
F	-7.7412	-3.0068	-0.6203
F	-7.5488	-1.3472	-2.0096
H	2.8437	-3.256	-1.7125
H	-1.4792	2.8458	1.0946
H	-3.705	2.8165	-3.3548
H	-4.5733	4.2528	-1.5339
H	-3.4508	4.2546	0.6896
H	-0.1169	-0.2882	-3.7834
H	-2.0567	1.1767	-4.1824
H	1.872	-0.1579	-0.7638
H	3.6664	0.2003	-2.334
H	7.1261	0.1483	0.214
H	4.4353	-3.2065	0.1841
H	1.5157	2.888	-1.0328
H	3.7544	2.6383	3.4034
H	4.6272	4.1513	1.6478
H	3.4971	4.2648	-0.5689
H	0.1442	-0.4559	3.7012
H	2.0969	0.974	4.16
H	-1.8578	-0.1704	0.7053
H	-2.8423	-3.3053	1.5161
H	-3.6108	0.1366	2.3087
H	-7.129	0.229	-0.1569
H	-4.4857	-3.1584	-0.3214

Energy = -3674.924437 a.u.
0 imaginary frequency

8-cis-cis

C	-6.3009	1.1525	0.4644
C	-5.1884	0.6518	1.2003
C	-5.1919	0.8233	2.6238
C	-6.2923	1.4668	3.2493
C	-7.3533	1.9355	2.5078
C	-7.3512	1.7763	1.1013
C	-4.0776	0.0042	0.5684
C	-2.9942	-0.4233	1.3453
C	-3.0124	-0.2586	2.7589
C	-4.0844	0.3424	3.3685
N	-1.8847	-0.975	0.6856
C	-0.7112	-1.4793	1.2225
N	0.277	-1.5718	0.2504
O	-0.5635	-1.8068	2.3956
C	1.5354	-2.1723	0.3735
C	1.9472	-2.8935	1.5043
C	3.2145	-3.4784	1.5234
C	4.0902	-3.3658	0.4467
C	3.6743	-2.6421	-0.6728
C	2.4163	-2.052	-0.7162
C	3.61	-4.3039	2.7196
C	4.6295	-2.4796	-1.8258
F	4.9518	-4.3674	2.8706
F	3.097	-3.8105	3.8682
F	3.1677	-5.5804	2.6123
F	4.0163	-2.0425	-2.9458

F	5.6168	-1.5985	-1.5404
F	5.238	-3.6507	-2.1299
H	-6.3155	1.0387	-0.6141
H	-6.2783	1.5846	4.3296
H	-8.1892	2.4273	2.9956
H	-8.1874	2.1503	0.5178
H	-2.1748	-0.6235	3.3355
H	-4.0878	0.4614	4.4485
H	-1.9322	-0.9414	-0.3247
H	0.1267	-1.0225	-0.5927
H	1.2877	-2.9773	2.355
H	5.0701	-3.8256	0.4777
H	2.1136	-1.5013	-1.5998
C	-5.6908	-2.1376	-0.6876
C	-4.8677	-1.2924	-1.4819
C	-4.8135	-1.5315	-2.8946
C	-5.5913	-2.5798	-3.4543
C	-6.3847	-3.3733	-2.6571
C	-6.4284	-3.1505	-1.2608
C	-4.0761	-0.2349	-0.9117
C	-3.2761	0.5287	-1.7537
C	-3.2236	0.2852	-3.1508
C	-3.9727	-0.7205	-3.7037
N	-2.4998	1.6043	-1.2304
C	-1.1207	1.5822	-1.2781
N	-0.5392	2.7357	-0.7939
O	-0.4864	0.6221	-1.7292
C	0.8265	3.0071	-0.6098
C	1.8483	2.1554	-1.051
C	3.179	2.4962	-0.8127
C	3.526	3.6795	-0.164
C	2.5024	4.5301	0.2545
C	1.1661	4.2015	0.0433
C	4.2569	1.5192	-1.2072
C	2.8465	5.8502	0.8931
F	5.4135	2.1405	-1.5214
F	4.5311	0.6599	-0.1981
F	3.8936	0.7707	-2.2734
F	1.8777	6.2716	1.7363
F	3.9972	5.7835	1.5959
F	3.0083	6.8232	-0.0346
H	-5.7299	-1.9792	0.3838
H	-5.5437	-2.7463	-4.5269
H	-6.9736	-4.1733	-3.0951
H	-7.0484	-3.7851	-0.6348
H	-2.589	0.9127	-3.7663
H	-3.9352	-0.9047	-4.7735
H	-2.946	2.1836	-0.531
H	-1.1659	3.4846	-0.5315
H	1.5972	1.2499	-1.5795
H	4.5637	3.9338	0.0113
H	0.3881	4.8716	0.3935

Energy = -3029.033710 a.u.
0 imaginary frequency

8-trans-cis

C	0.1911	4.4367	1.5262
C	0.3957	3.9511	0.2042
C	0.0885	4.8218	-0.892
C	-0.4046	6.1273	-0.6302
C	-0.5919	6.5658	0.6614
C	-0.29	5.709	1.7466
C	0.885	2.6275	-0.0582
C	1.066	2.2143	-1.3795
C	0.7683	3.0879	-2.4624
C	0.2894	4.349	-2.2159
N	1.6133	0.9375	-1.617
C	1.3663	0.1402	-2.7173
N	2.0528	-1.0692	-2.7342
O	0.5889	0.4214	-3.6226
C	3.1412	-1.5261	-1.9665
C	4.1966	-0.6789	-1.592
C	5.2706	-1.1902	-0.8675
C	5.3324	-2.5416	-0.5237
C	4.2933	-3.3817	-0.9187
C	3.2002	-2.8837	-1.627
C	6.4312	-0.3013	-0.4996
C	4.3077	-4.8329	-0.5124
F	6.7581	-0.4296	0.8058
F	7.5389	-0.6224	-1.209
F	6.1749	1.0027	-0.7302
F	3.658	-5.0263	0.6589
F	3.7013	-5.6162	-1.4311
F	5.5648	-5.2964	-0.3471
C	3.5428	2.5546	1.228
C	2.5002	1.6918	1.6721
C	2.7833	0.7892	2.7492
C	4.0792	0.7776	3.3297
C	5.0668	1.6188	2.8702
C	4.7904	2.5156	1.8105
C	1.1979	1.6938	1.0744
C	0.2177	0.8165	1.5518
C	0.5036	-0.0684	2.6289
C	1.7515	-0.0728	3.2002
N	-1.0468	0.8586	0.9355
C	-2.1414	0.0415	1.1457
N	-3.2168	0.3973	0.3391
O	-2.1763	-0.8886	1.9448
C	-4.4705	-0.2233	0.2566
C	-4.8576	-1.3134	1.0509

C	-6.1345	-1.855	0.8975
C	-7.0442	-1.3425	-0.0247
C	-6.6504	-0.258	-0.8095
C	-5.3823	0.2982	-0.6764
C	-6.5098	-3.0612	1.719
C	-7.5904	0.281	-1.855
F	-7.8464	-3.1574	1.8944
F	-6.1087	-4.2108	1.1249
F	-5.9414	-3.037	2.9442
F	-7.3551	1.5842	-2.1262
F	-7.471	-0.3899	-3.0255
F	-8.8816	0.1725	-1.473
H	1.6744	-1.7055	-3.4231
H	0.4211	3.7901	2.366
H	-0.6313	6.7757	-1.4723
H	-0.9688	7.5661	0.8512
H	-0.4378	6.0592	2.7639
H	0.9155	2.7375	-3.4743
H	0.0639	5.0101	-3.0481
H	2.0088	0.4859	-0.8017
H	4.1884	0.3646	-1.8785
H	6.1761	-2.9334	0.0313
H	2.3928	-3.5465	-1.9185
H	3.3442	3.2489	0.4187
H	4.2768	0.0856	4.144
H	6.0563	1.598	3.3159
H	5.572	3.1779	1.4512
H	-0.2725	-0.7328	2.9777
H	1.9603	-0.755	4.0198
H	-1.1161	1.5616	0.2106
H	-3.0978	1.1874	-0.2794
H	-4.1693	-1.7155	1.7784
H	-8.0359	-1.7654	-0.1213
H	-5.1028	1.1457	-1.2937

Energy = -3029.025215 a.u.
0 imaginary frequency

8-trans-trans

C	-1.8856	3.1158	0.2145
C	-1.4807	2.2115	-0.8077
C	-2.222	2.2011	-2.0346
C	-3.3265	3.0794	-2.1903
C	-3.6957	3.9371	-1.1788
C	-2.9647	3.9528	0.0328
C	-0.3752	1.3128	-0.6413
C	-0.0315	0.4492	-1.6828
C	-0.7621	0.4554	-2.9031
C	-1.8269	1.3051	-3.0622
N	1.0956	-0.3823	-1.5231
C	1.2948	-1.6098	-2.1223
N	2.5088	-2.2213	-1.8228
O	0.4849	-2.1749	-2.8487
C	3.6855	-1.7125	-1.2428
C	4.1428	-0.4101	-1.501
C	5.3373	0.0291	-0.9351
C	6.1077	-0.8109	-0.1295
C	5.6598	-2.1097	0.1043
C	4.4569	-2.5605	-0.4372
C	5.862	1.4086	-1.2416
C	6.4458	-3.017	1.0155
F	6.2212	2.0628	-0.1143
F	6.9664	1.3506	-2.0232
F	4.9574	2.1731	-1.8867
F	6.0483	-2.8931	2.3031
F	6.2954	-4.3173	0.6815
F	7.7668	-2.7383	0.9832
C	1.9256	3.1082	-0.1553
C	1.5149	2.1734	0.8366
C	2.2578	2.1159	2.0612
C	3.3696	2.9797	2.2445
C	3.7444	3.8677	1.2616
C	3.0117	3.9299	0.0525
C	0.4025	1.289	0.6417
C	0.0537	0.3935	1.6541
C	0.7858	0.3532	2.8728
C	1.8572	1.189	3.0588
N	-1.0795	-0.4244	1.4688
C	-1.2845	-1.6706	2.026
N	-2.5046	-2.2629	1.713
O	-0.4744	-2.2665	2.727
C	-3.6852	-1.7258	1.1679
C	-4.126	-0.4272	1.4701
C	-5.3211	0.0412	0.9294
C	-6.1089	-0.7664	0.1077
C	-5.6784	-2.0628	-0.1679
C	-4.4742	-2.5417	0.3458
C	-5.8222	1.4213	1.2708
C	-6.5444	-2.9749	-0.9978
F	-6.1568	2.1148	0.1595
F	-6.9361	1.3621	2.0388
F	-4.9103	2.1492	1.9471
F	-5.8133	-3.8836	-1.6789
F	-7.4132	-3.669	-0.2254
F	-7.2809	-2.2874	-1.8968
H	2.5086	-3.198	-2.0846
H	-1.332	3.1389	1.1469
H	-3.8788	3.0583	-3.126
H	-4.5452	4.6008	-1.3057
H	-3.2594	4.6304	0.8282
H	-0.4734	-0.2261	-3.6906

H	-2.3822	1.3015	-3.9961
H	1.6702	-0.1679	-0.7174
H	3.5818	0.2478	-2.1518
H	7.0406	-0.4646	0.2985
H	4.1155	-3.5703	-0.2374
H	1.3709	3.1671	-1.0856
H	3.9229	2.9228	3.1781
H	4.5994	4.5198	1.4093
H	3.3108	4.6315	-0.7202
H	0.493	-0.3523	3.6373
H	2.4139	1.1495	3.9911
H	-1.6548	-0.1787	0.6727
H	-2.5098	-3.2479	1.9417
H	-3.5493	0.2068	2.1307
H	-7.0352	-0.3928	-0.3116
H	-4.1386	-3.5432	0.1007

Energy= -3029.020844 a.u.
0 imaginary frequency

5@2-cis-A

C	-5.9373	-0.6802	-0.4669
C	-4.5891	-1.1325	-0.5779
C	-4.3659	-2.4216	-1.1584
C	-5.47	-3.2014	-1.5869
C	-6.7687	-2.7207	-1.4533
C	-7.0002	-1.4687	-0.8988
C	-3.4674	-0.3457	-0.1412
C	-2.1675	-0.8552	-0.3336
C	-1.9731	-2.1236	-0.8837
C	-3.046	-2.8998	-1.2968
C	-3.4759	4.6543	-0.479
C	-3.709	3.4793	0.2793
C	-3.4363	2.198	-0.2934
C	-2.9386	2.1628	-1.6296
C	-2.7133	3.334	-2.3466
C	-2.9804	4.5712	-1.7761
C	-4.208	3.5573	1.5942
C	-4.4372	2.4009	2.3248
C	-4.1861	1.1329	1.7929
C	-3.6837	1.0093	0.4765
N	-1.0507	-0.1193	0.1162
C	0.1126	0.2279	-0.5146
N	0.9836	0.8119	0.3631
S	0.4298	-0.0533	-2.1403
C	2.3107	1.2611	0.2206
N	-4.443	-0.0138	2.5866
C	-3.2544	-0.6244	3.1743
C	-5.6154	-0.0019	3.4599
C	3.2946	0.5229	-0.45
C	4.6105	0.9952	-0.536
C	4.9394	2.2098	0.079
C	3.9725	2.9496	0.7721
C	2.6636	2.4592	0.8449
C	5.6838	0.184	-1.2642
C	4.3292	4.2657	1.4643
F	6.8715	0.3244	-0.6718
F	5.3869	-1.1171	-1.287
F	5.7818	0.6205	-2.5192
F	5.649	4.4343	1.5717
F	3.8296	5.2801	0.7592
F	3.8062	4.2978	2.6911
H	-6.1425	0.2903	-0.0399
H	-5.2972	-4.1755	-2.0217
H	-7.6032	-3.3229	-1.7839
H	-8.0133	-1.1052	-0.8014
H	-0.9713	-2.5134	-0.9953
H	-2.8743	-3.875	-1.7296
H	-3.6777	5.6204	-0.0388
H	-2.7235	1.2138	-2.1
H	-2.3279	3.2785	-3.3549
H	-2.8022	5.4729	-2.3445
H	-4.4072	4.526	2.0308
H	-4.8111	2.4974	3.3323
H	-1.2158	0.3519	0.997
H	0.566	1.0655	1.2509
H	-2.9014	-0.048	4.0303
H	-3.4674	-1.6441	3.4978
H	-2.4327	-0.684	2.4621
H	-6.4716	0.4484	2.9548
H	-5.9034	-1.0216	3.7184
H	-5.4297	0.5525	4.3809
H	3.0365	-0.4246	-0.9023
H	5.9559	2.5768	0.0174
H	1.9203	3.025	1.388
C	-0.5531	3.9517	2.6089
C	-0.3421	5.0485	3.4532
C	-0.0785	6.303	2.9088
C	-0.0229	6.4603	1.5257
C	-0.2328	5.3743	0.6795
C	-0.4994	4.1193	1.2188
H	-0.3722	4.9462	4.5303
H	0.0874	7.1524	3.5566
H	0.1833	7.4341	1.1048
H	-0.198	5.5029	-0.3933
H	-0.6763	3.2888	0.5455
C	-0.7948	2.612	3.2033
O	-0.7675	1.5586	2.5634
H	-1.0068	2.6142	4.2731

Energy= -2702.335348 a.u.
0 imaginary frequency

5@2-trans-A

C	-4.8558	1.6925	-0.1513
C	-3.6399	1.3753	-0.8212
C	-3.0622	2.3738	-1.6749
C	-3.6962	3.6396	-1.7995
C	-4.8641	3.9150	-1.1254
C	-5.4504	2.9264	-0.2999
C	-2.9975	0.0948	-0.6847
C	-1.8568	-0.1576	-1.4418
C	-1.3001	0.8280	-2.2994
C	-1.8774	2.0685	-2.3960
C	-3.8137	-1.4135	4.0116
C	-3.9261	-1.6545	2.6153
C	-3.4254	-0.6881	1.6808
C	-2.7909	0.4725	2.2136
C	-2.6872	0.6730	3.5723
C	-3.2113	-0.2719	4.4868
C	-4.5090	-2.8449	2.1169
C	-4.5790	-3.0827	0.7676
C	-4.0877	-2.1407	-0.1793
C	-3.5329	-0.9347	0.2676
N	-1.3294	-1.4785	-1.4586
C	-0.0612	-1.9228	-1.2900
N	0.8527	-1.0097	-0.8615
S	0.2824	-3.5609	-1.6276
C	2.2296	-1.2170	-0.5964
N	-4.1056	-2.4551	-1.5759
C	-4.2229	-3.8744	-1.9247
C	-5.0162	-1.6473	-2.4046
C	3.1308	-0.2386	-1.0264
C	4.4877	-0.3549	-0.7229
C	4.9686	-1.4534	-0.0137
C	4.0628	-2.4277	0.4082
C	2.6997	-2.3125	0.1368
C	5.4198	0.7524	-1.1298
C	4.5517	-3.5838	1.2393
F	5.1106	1.2541	-2.3458
F	5.3624	1.7951	-0.2577
F	6.7072	0.3513	-1.1697
F	3.8058	-4.6943	1.0516
F	5.8340	-3.9031	0.9545
F	4.5055	-3.3025	2.5646
H	-5.3186	0.9439	0.4810
H	-3.2427	4.3852	-2.4467
H	-5.3416	4.8843	-1.2309
H	-6.3795	3.1420	0.2189
H	-0.4270	0.5782	-2.8928
H	-1.4504	2.8207	-3.0529
H	-4.2090	-2.1576	4.6980
H	-2.3724	1.2059	1.5352
H	-2.1943	1.5656	3.9464
H	-3.1276	-0.0974	5.5551
H	-4.9001	-3.5760	2.8192
H	-5.0291	-4.0031	0.4169
H	-2.0324	-2.1873	-1.6727
H	0.5511	-0.0452	-0.7097
H	-3.5063	-4.4665	-1.3518
H	-5.2332	-4.2822	-1.7632
H	-3.9864	-3.9845	-2.9864
H	-6.0648	-1.9538	-2.2655
H	-4.9288	-0.5904	-2.1614
H	-4.7553	-1.7815	-3.4581
H	2.7676	0.6145	-1.5851
H	6.0249	-1.5514	0.2021
H	2.0073	-3.0662	0.4837
C	1.3569	6.3783	1.3726
C	2.7513	6.3276	1.4472
C	3.4387	5.1528	1.1152
C	2.7339	4.0252	0.7102
C	1.3304	4.0707	0.6341
C	0.6465	5.2509	0.9649
H	0.8299	7.2913	1.6301
H	3.3067	7.2054	1.7636
H	4.5222	5.1242	1.1738
H	3.2516	3.1095	0.4456
H	-0.4381	5.2782	0.9019
C	0.5588	2.8948	0.2081
H	-0.5362	3.0419	0.1511
O	1.0524	1.8099	-0.0786

Energy = -2702.337656 a.u.
0 imaginary frequency

5@3-cis-A

C	4.7471	-1.5864	-0.2778
C	4.8948	-2.9055	-0.8181
C	6.1811	-3.5070	-0.8633
C	7.2893	-2.8449	-0.3854
C	7.1477	-1.5471	0.1621
C	3.4473	-0.9793	-0.2231
C	2.3413	-1.6993	-0.6787
C	2.5001	-3.0027	-1.2294
C	3.7408	-3.5821	-1.2918
C	2.1890	1.9415	3.6349
C	2.7000	1.8161	2.3147
C	2.7681	0.5236	1.6960
C	2.3342	-0.5978	2.4622
C	1.8480	-0.4447	3.7418
C	1.7662	0.8370	4.3379
C	3.1677	2.9403	1.5903
C	3.6646	2.8033	0.3179

C	3.7312	1.5319	-0.3255
C	3.2936	0.3917	0.3650
N	1.0691	-1.0867	-0.6534
C	-0.1453	-1.7402	-0.5442
N	-1.2134	-0.8553	-0.5438
O	-0.2729	-2.9611	-0.4682
C	-2.5682	-1.1612	-0.3982
N	4.2817	1.4244	-1.6294
C	3.3654	1.0560	-2.7104
C	5.2036	2.4734	-2.0493
C	-3.4843	-0.1185	-0.6108
C	-4.8489	-0.3198	-0.4211
C	-5.3438	-1.5679	-0.0479
C	-4.4326	-2.6099	0.1314
C	-3.0600	-2.4261	-0.0316
C	-5.7719	0.8581	-0.5787
C	-4.9460	-3.9867	0.4608
F	-5.6546	1.7232	0.4631
F	-5.4941	1.5689	-1.6957
F	-7.0683	0.4928	-0.6422
F	-4.0616	-4.6998	1.1926
F	-6.1033	-3.9418	1.1587
F	-5.1952	-4.7079	-0.6597
H	6.2715	-4.5064	-1.2809
H	8.2679	-3.3138	-0.4226
H	8.0214	-1.0288	0.5467
H	1.6266	-3.5271	-1.5888
H	3.8511	-4.5767	-1.7153
H	2.1428	2.9319	4.0804
H	2.3955	-1.5886	2.0269
H	1.5243	-1.3179	4.3009
H	1.3771	0.9423	5.3461
H	3.1229	3.9224	2.0539
H	4.0048	3.6839	-0.2139
H	1.0620	-0.0760	-0.5437
H	-0.9943	0.1349	-0.6185
H	2.7248	0.2276	-2.4152
H	2.7252	1.9010	-3.0166
H	3.9459	0.7389	-3.5824
H	5.7570	2.1180	-2.9241
H	4.7067	3.4166	-2.3347
H	5.9234	2.6860	-1.2557
H	-3.1247	0.8530	-0.9306
H	-6.4045	-1.7239	0.0976
H	-2.3693	-3.2407	0.1244
C	5.9143	-0.9354	0.2132
H	5.8213	0.0568	0.6389
C	-0.8314	5.3099	-0.7444
C	-1.0180	3.9536	-0.4325
C	-2.2479	3.5196	0.0920
C	-3.2846	4.4256	0.2783
C	-3.0958	5.7751	-0.0467
C	-1.8707	6.2183	-0.5525
H	0.1226	5.6436	-1.1431
H	-2.3705	2.4770	0.3607
H	-4.2376	4.0823	0.6672
H	-3.9065	6.4826	0.0984
H	-1.7297	7.2659	-0.7975
C	0.0776	3.0099	-0.6799
O	-0.0052	1.7895	-0.5630
H	1.0340	3.4617	-0.9968

Energy = -2379.389386 a.u.
0 imaginary frequency

5@3-trans-A

C	-5.0016	0.5544	-1.0595
C	-3.6526	0.2706	-1.4181
C	-3.0941	0.9785	-2.5341
C	-3.8800	1.9460	-3.2161
C	-5.1767	2.2032	-2.8321
C	-5.7412	1.4925	-1.7466
C	-2.8562	-0.7003	-0.7153
C	-1.5753	-0.9838	-1.1892
C	-1.0365	-0.2881	-2.3066
C	-1.7674	0.6806	-2.9449
C	-4.2275	-0.4087	4.0848
C	-4.0658	-1.1887	2.9076
C	-3.5600	-0.5807	1.7107
C	-3.2009	0.7977	1.7778
C	-3.3587	1.5254	2.9365
C	-3.8869	0.9237	4.1040
C	-4.3770	-2.5701	2.8902
C	-4.1820	-3.3198	1.7581
C	-3.6789	-2.7396	0.5595
C	-3.3886	-1.3697	0.5194
N	-0.8651	-2.0615	-0.6134
C	0.4786	-2.2524	-0.3877
N	1.2559	-1.1052	-0.3558
O	0.9216	-3.3859	-0.1903
C	2.6446	-1.0558	-0.1686
N	-3.4117	-3.5684	-0.5756
C	-4.2661	-3.3459	-1.7531
C	-3.2568	-5.0026	-0.3194
C	3.4897	-2.1700	-0.3019
C	4.8644	-2.0210	-0.1143
C	5.4345	-0.7882	0.2000
C	4.5874	0.3129	0.3267
C	3.2128	0.1897	0.1471
C	5.7532	-3.2188	-0.3167
C	5.1617	1.6731	0.6148

F	5.1581	-4.3675	0.0763
F	6.0840	-3.3820	-1.6220
F	6.9147	-3.1126	0.3673
F	4.3298	2.4247	1.3787
F	6.3432	1.6008	1.2650
F	5.3815	2.3787	-0.5209
H	-5.4503	0.0156	-0.2330
H	-3.4372	2.4749	-4.0559
H	-5.7695	2.9419	-3.3628
H	-6.7690	1.6860	-1.4543
H	-0.0446	-0.5477	-2.6595
H	-1.3487	1.2065	-3.7982
H	-4.6208	-0.8924	4.9751
H	-2.7850	1.2777	0.9009
H	-3.0711	2.5725	2.9553
H	-4.0115	1.5110	5.0086
H	-4.7715	-3.0345	3.7899
H	-4.4284	-4.3743	1.7748
H	-1.4234	-2.9106	-0.5260
H	0.7788	-0.2063	-0.3116
H	-4.3789	-2.2829	-1.9556
H	-3.8037	-3.8161	-2.6258
H	-5.2664	-3.7851	-1.6130
H	-2.5777	-5.1678	0.5197
H	-4.2090	-5.5161	-0.1119
H	-2.8195	-5.4628	-1.2097
H	3.0660	-3.1372	-0.5249
H	6.5011	-0.6912	0.3552
H	2.5679	1.0525	0.2620
C	1.4384	4.5496	0.5057
C	0.2322	4.2082	-0.1317
C	-0.6482	5.2168	-0.5542
C	-0.3314	6.5563	-0.3385
C	0.8676	6.8896	0.2964
C	1.7519	5.8875	0.7162
H	2.1176	3.7644	0.8202
H	-1.5772	4.9448	-1.0484
H	-1.0121	7.3367	-0.6630
H	1.1172	7.9330	0.4642
H	2.6826	6.1570	1.2055
C	-0.1334	2.8056	-0.3717
O	0.5325	1.8385	-0.0169
H	-1.0834	2.6506	-0.9158

Energy = -2379.387225 a.u.
0 imaginary frequency

5@8-cis-cis

C	-5.3193	-2.3246	-0.0787
C	-4.1876	-2.1463	0.7693
C	-4.4235	-1.7955	2.1396
C	-5.7569	-1.6476	2.6060
C	-6.8282	-1.8287	1.7592
C	-6.6011	-2.1684	0.4031
C	-2.8442	-2.2875	0.2945
C	-1.7774	-2.0407	1.1649
C	-2.0208	-1.7084	2.5273
C	-3.3067	-1.5980	2.9922
N	-0.4739	-2.0791	0.6434
C	0.7318	-1.9280	1.3051
N	1.7481	-1.6064	0.4151
O	0.8868	-2.0691	2.5157
C	3.1204	-1.5502	0.6767
C	3.6944	-1.8972	1.9095
C	5.0799	-1.8340	2.0669
C	5.9184	-1.4315	1.0305
C	5.3389	-1.0817	-0.1910
C	3.9616	-1.1380	-0.3728
C	5.6771	-2.2768	3.3763
C	6.2311	-0.6038	-1.3061
F	5.8609	-3.6196	3.4128
F	6.8844	-1.7124	3.6016
F	4.8845	-1.9664	4.4267
F	6.6492	0.6690	-1.1068
F	7.3491	-1.3620	-1.4035
F	5.6177	-0.6363	-2.5078
H	-5.1631	-2.5831	-1.1203
H	-5.9154	-1.3853	3.6487
H	-7.8436	-1.7144	2.1259
H	-7.4467	-2.3072	-0.2641
H	-1.1770	-1.5509	3.1836
H	-3.4805	-1.3418	4.0337
H	-0.4196	-2.1258	-0.3663
H	1.4495	-1.2653	-0.4974
H	3.0585	-2.1977	2.7285
H	6.9915	-1.3901	1.1685
H	3.5368	-0.8698	-1.3333
C	-3.1325	-5.0945	-0.5899
C	-2.7188	-4.0873	-1.5054
C	-2.4128	-4.4786	-2.8506
C	-2.5503	-5.8411	-3.2285
C	-2.9619	-6.7887	-2.3186
C	-3.2501	-6.4091	-0.9864
C	-2.5771	-2.7085	-1.1195
C	-2.1434	-1.7884	-2.0667
C	-1.8354	-2.1852	-3.3946
C	-1.9672	-3.4956	-3.7749
N	-2.0175	-0.4112	-1.7246
C	-0.8010	0.2154	-1.6976
N	-0.8900	1.5642	-1.4099
O	0.2662	-0.3830	-1.9106

C	0.1577	2.4682	-1.2035
C	1.5020	2.1750	-1.4781
C	2.4814	3.1378	-1.2390
C	2.1608	4.4039	-0.7521
C	0.8195	4.6934	-0.4983
C	-0.1736	3.7421	-0.7137
C	3.9267	2.7703	-1.4493
C	0.4468	6.0332	0.0784
F	4.0769	1.8047	-2.3849
F	4.6702	3.8292	-1.8382
F	4.4838	2.2986	-0.3078
F	1.2776	7.0117	-0.3434
F	-0.8113	6.3983	-0.2550
F	0.5056	6.0280	1.4321
H	-3.3530	-4.8170	0.4343
H	-2.3193	-6.1218	-4.2525
H	-3.0618	-7.8275	-2.6180
H	-3.5659	-7.1614	-0.2700
H	-1.5050	-1.4295	-4.0986
H	-1.7361	-3.7966	-4.7927
H	-2.8261	0.0840	-1.3470
H	-1.8233	1.9205	-1.2272
H	1.7628	1.2096	-1.8814
H	2.9297	5.1478	-0.5863
H	-1.2093	3.9889	-0.5070
C	-5.0154	4.0886	0.2561
C	-6.6187	2.6148	1.3459
C	-7.2695	3.7221	1.8851
C	-6.7946	5.0068	1.6079
C	-5.6693	5.1905	0.7934
H	-8.1415	3.5878	2.5168
H	-7.3022	5.8706	2.0263
H	-5.3104	6.1929	0.5830
C	-5.4883	2.7931	0.5314
H	-6.9751	1.6096	1.5549
H	-4.1456	4.2096	-0.3808
C	-4.8225	1.6096	-0.0170
O	-3.8025	1.6352	-0.7056
H	-5.2973	0.6415	0.2196

Energy = -3374.636198 a.u.
0 imaginary frequency

$(5)_2$@8-cis-cis

C	-1.6940	5.4372	-0.0316
C	-1.2383	4.4668	-0.9693
C	-1.8049	4.4872	-2.2861
C	-2.7769	5.4696	-2.6163
C	-3.1908	6.3967	-1.6853
C	-2.6438	6.3730	-0.3800
C	-0.2567	3.4751	-0.6326
C	0.1231	2.5345	-1.5925
C	-0.4434	2.5661	-2.8985
C	-1.3772	3.5144	-3.2272
N	1.1223	1.5962	-1.2713
C	1.2362	0.3205	-1.7940
N	2.3227	-0.3590	-1.2659
O	0.4673	-0.1578	-2.6261
C	2.7559	-1.6481	-1.5829
C	3.7838	-2.1871	-0.7928
C	4.3201	-3.4395	-1.0802
C	3.8270	-4.2046	-2.1353
C	2.7815	-3.6794	-2.8966
C	2.2450	-2.4179	-2.6422
C	5.4725	-3.9281	-0.2449
C	2.2626	-4.4634	-4.0731
F	6.6059	-3.2256	-0.5075
F	5.2326	-3.7820	1.0782
F	5.7549	-5.2281	-0.4647
F	2.3922	-5.7967	-3.8901
F	0.9568	-4.2145	-4.3157
F	2.9346	-4.1600	-5.2111
H	-1.2857	5.4315	0.9727
H	-3.1889	5.4743	-3.6220
H	-3.9338	7.1436	-1.9475
H	-2.9762	7.1007	0.3543
H	-0.1239	1.8304	-3.6225
H	-1.7967	3.5333	-4.2293
H	1.7403	1.8444	-0.5035
H	2.9106	0.1504	-0.6105
H	4.1547	-1.6266	0.0584
H	4.2355	-5.1834	-2.3494
H	1.4382	-2.0259	-3.2428
C	1.8850	5.3535	0.1435
C	1.3860	4.3997	1.0761
C	1.9567	4.3838	2.3912
C	2.9757	5.3160	2.7248
C	3.4309	6.2289	1.7989
C	2.8796	6.2405	0.4952
C	0.3583	3.4571	0.7350
C	-0.0622	2.5287	1.6894
C	0.5067	2.5261	2.9946
C	1.4852	3.4265	3.3273
N	-1.1025	1.6364	1.3659
C	-1.2529	0.3558	1.8675
N	-2.3692	-0.2769	1.3439
O	-0.4892	-0.1627	2.6800
C	-2.8395	-1.5575	1.6412
C	-2.3325	-2.3702	2.6702
C	-2.9060	-3.6191	2.9055
C	-3.9843	-4.0905	2.1544

C	-4.4737	-3.2829	1.1301
C	-3.9024	-2.0416	0.8626
C	-2.3906	-4.4494	4.0514
C	-5.6508	-3.7136	0.2975
F	-1.0756	-4.2412	4.2816
F	-3.0387	-4.1623	5.2074
F	-2.5575	-5.7732	3.8322
F	-5.3855	-3.6347	-1.0267
F	-6.0346	-4.9791	0.5589
F	-6.7291	-2.9161	0.5183
H	1.4740	5.3744	-0.8595
H	3.3910	5.2934	3.7289
H	4.2094	6.9376	2.0640
H	3.2442	6.9566	-0.2352
H	0.1538	1.8021	3.7149
H	1.9070	3.4192	4.3286
H	-1.7183	1.9180	0.6079
H	-2.9468	0.2619	0.7030
H	-1.5006	-2.0205	3.2625
H	-4.4212	-5.0600	2.3536
H	-4.2741	-1.4460	0.0362
C	-6.3957	0.7224	-0.5851
C	-6.7366	2.6934	-1.9670
C	-8.0289	2.2622	-2.2597
C	-8.4991	1.0619	-1.7198
C	-7.6831	0.2922	-0.8806
H	-8.6673	2.8555	-2.9062
H	-9.5049	0.7244	-1.9508
H	-8.0484	-0.6412	-0.4651
C	-5.9103	1.9223	-1.1335
H	-6.3589	3.6223	-2.3855
H	-5.7609	0.1455	0.0764
C	-4.5440	2.3872	-0.8694
O	-3.6969	1.7648	-0.2325
H	-4.2860	3.3719	-1.2966
C	6.4074	0.5527	0.4585
C	6.9346	2.6078	1.6453
C	8.2474	2.1716	1.8129
C	8.6352	0.9272	1.3084
C	7.7154	0.1175	0.6295
H	8.9656	2.7953	2.3349
H	9.6573	0.5862	1.4421
H	8.0164	-0.8501	0.2413
C	6.0057	1.7981	0.9719
H	6.6212	3.5714	2.0376
H	5.6902	-0.0565	-0.0776
C	4.6245	2.2726	0.8318
O	3.7062	1.6314	0.3255
H	4.4257	3.2836	1.2285

Energy = -3720.230942 a.u.
0 imaginary frequency

Derivative 5

C	1.4385	4.5497	0.5057
C	0.2323	4.2082	-0.1318
C	-0.6482	5.2168	-0.5543
C	-0.3314	6.5564	-0.3386
C	0.8677	6.8897	0.2964
C	1.752	5.8876	0.7163
H	2.1176	3.7644	0.8203
H	-1.5772	4.9449	-1.0485
H	-1.0121	7.3368	-0.663
H	1.1173	7.933	0.4643
H	2.6826	6.1571	1.2055
C	-0.1335	2.8057	-0.3718
O	0.5326	1.8386	-0.017
H	-1.0834	2.6507	-0.9159

Energy = -345.588295 a.u.
0 imaginary frequency

NCI studies

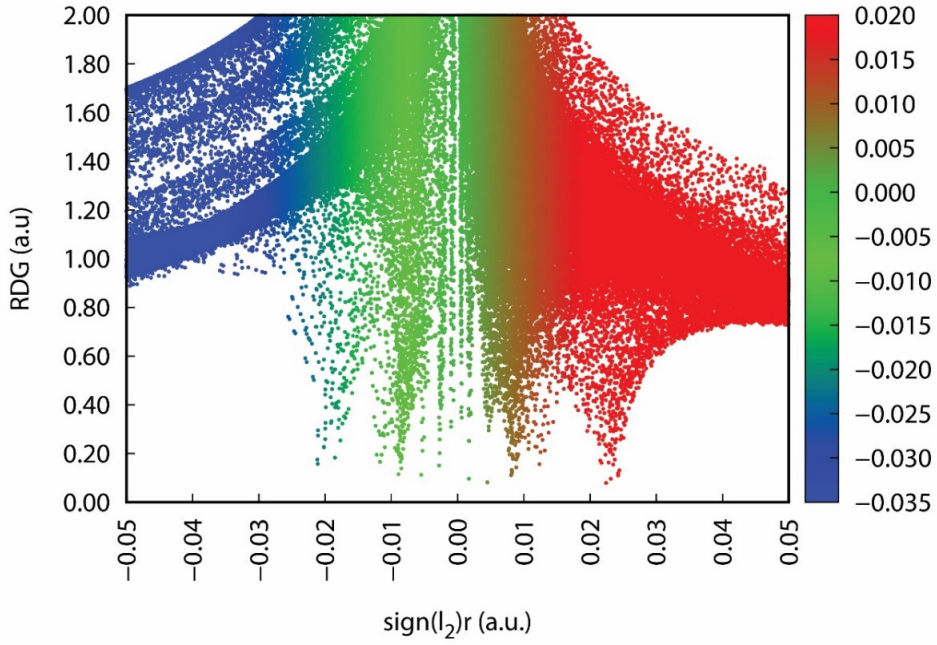


Figure S32. Plot of RDG versus sign(I_2)r for **5@2-trans-A** complex (NCI-RDG isosurfaces with S = 0.5).

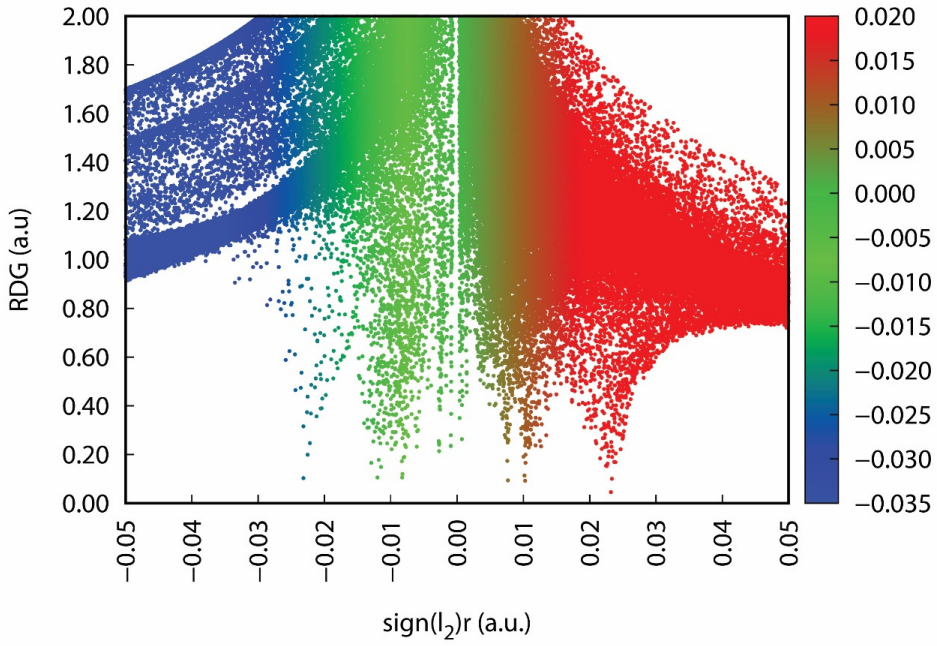


Figure S33. Plot of RDG versus sign(I_2)r for **5@3-cis-A** complex (NCI-RDG isosurfaces with S = 0.5).

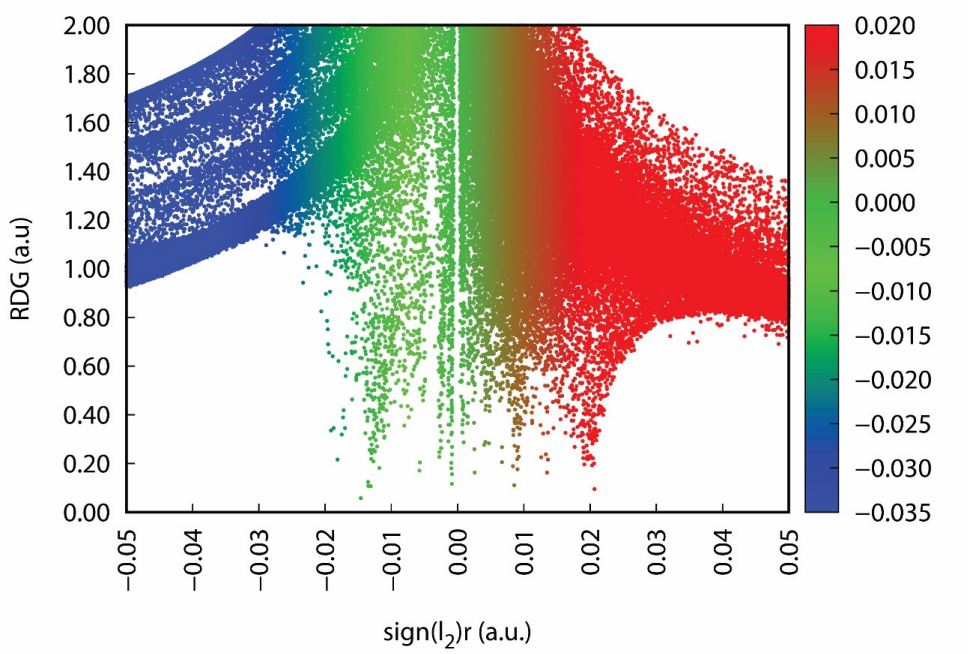


Figure S34. Plot of RDG versus sign(I_2)r for **5@8-cis-cis** 1:1 complex (NCI-RDG isosurfaces with S = 0.5).

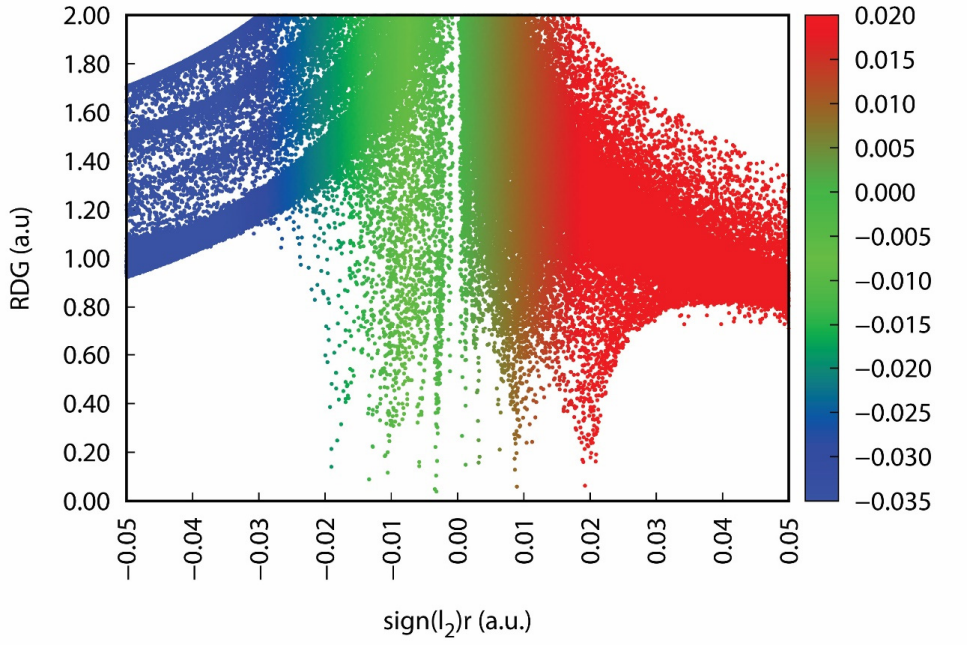


Figure S35. Plot of RDG versus sign(I_2)r for (**5**)$_2$**@8-cis-cis** 1:2 complex (NCI-RDG isosurfaces with S = 0.5).

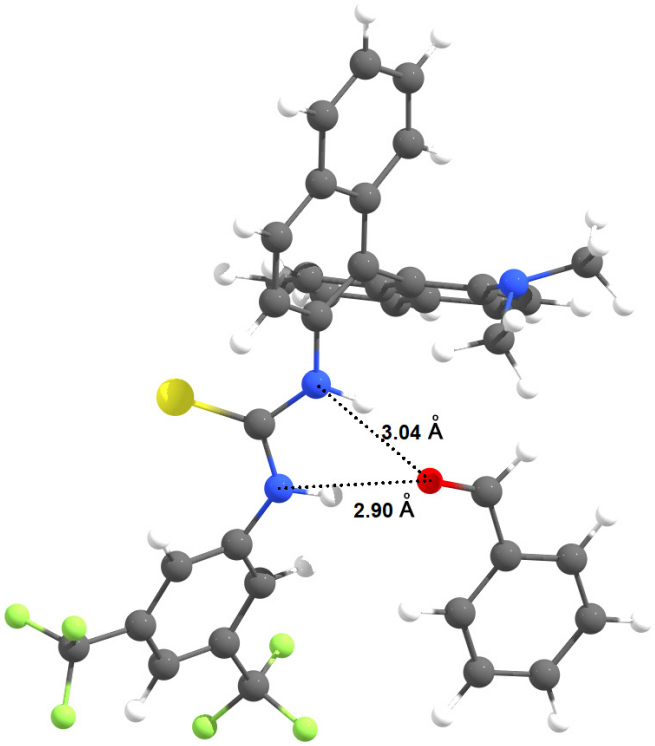


Figure S36. DFT optimized structure of **5@2-cis-A** complex.

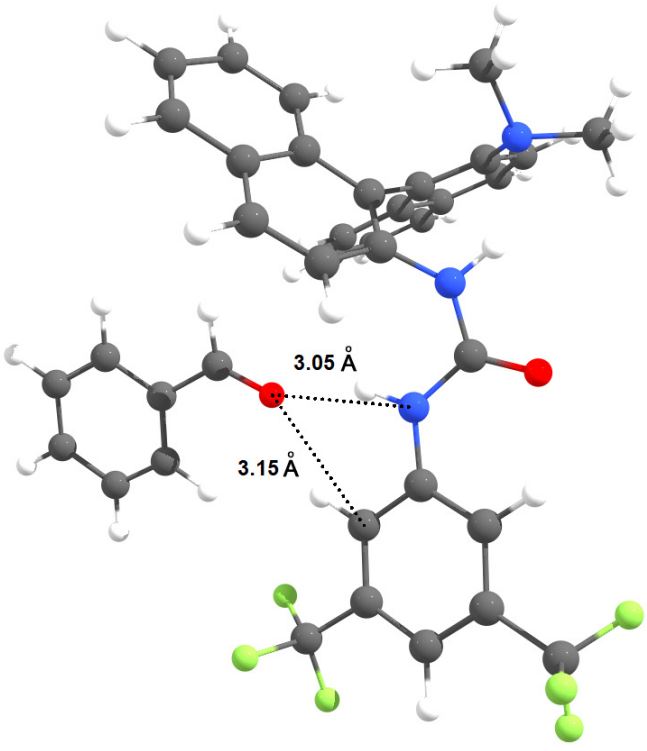


Figure S37. DFT optimized structure of **5@3-trans-A** complex.

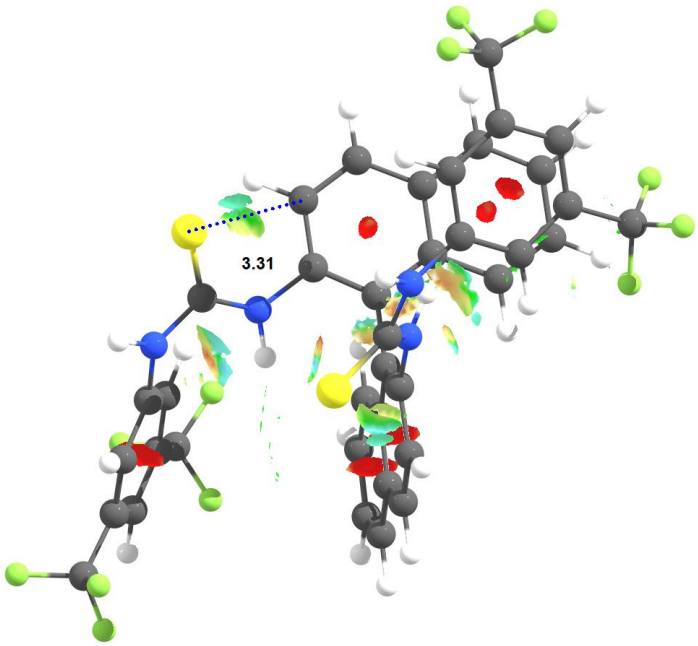


Figure S38. Non-covalent interaction plots by the sign of the second Hessian eigenvalue (gradient isosurfaces s = 0.5 a.u.) of **7-trans-trans**.

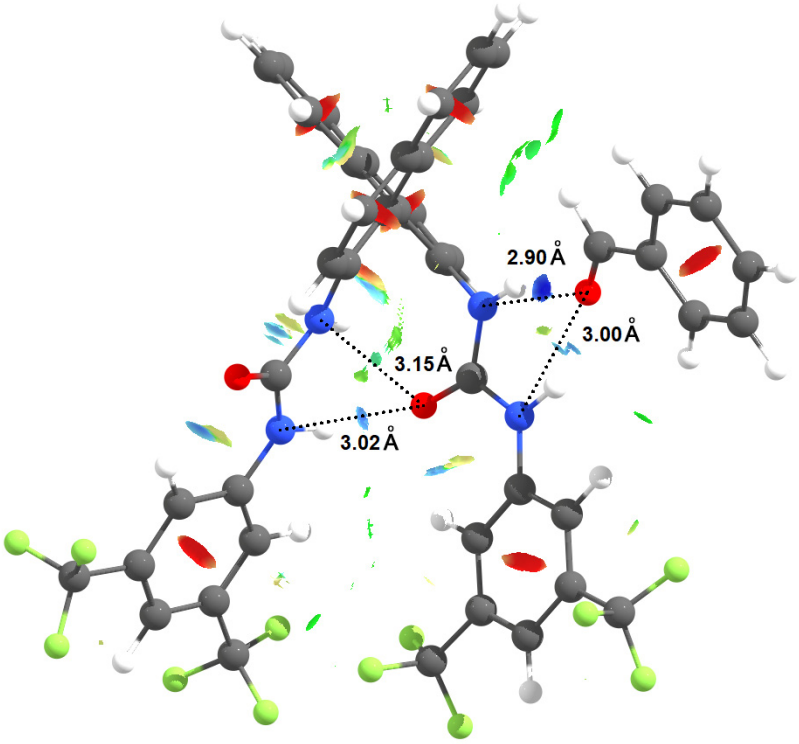


Figure S39. Gradient RDG isosurfaces (0.5) for the noncovalent interaction (NCI) regions in **5@8-cis-cis** 1:1 complex.

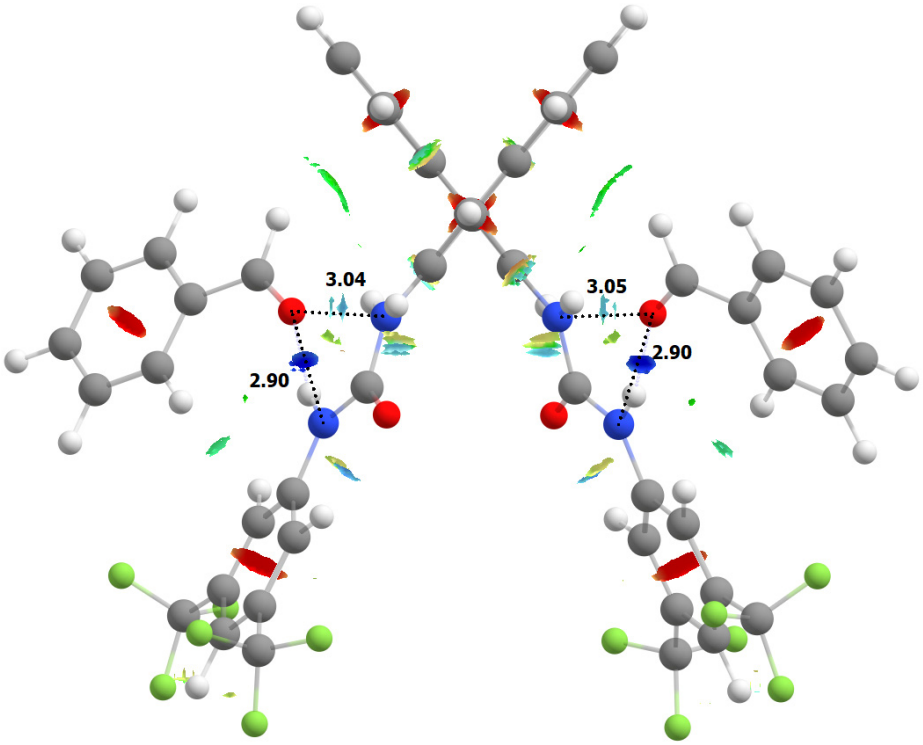


Figure S40. Gradient RDG isosurfaces (0.5) for the noncovalent interaction (NCI) regions in **(5)$_2$@8-cis-cis** 1:2 complex.