Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Disulphide Bond Exchange Inhibited by Air - Kinetic and Thermodynamic Products in a Library of Macrocyclic Cysteine Derivatives

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Supporting Information

1. Contents

2. NMR Spectra

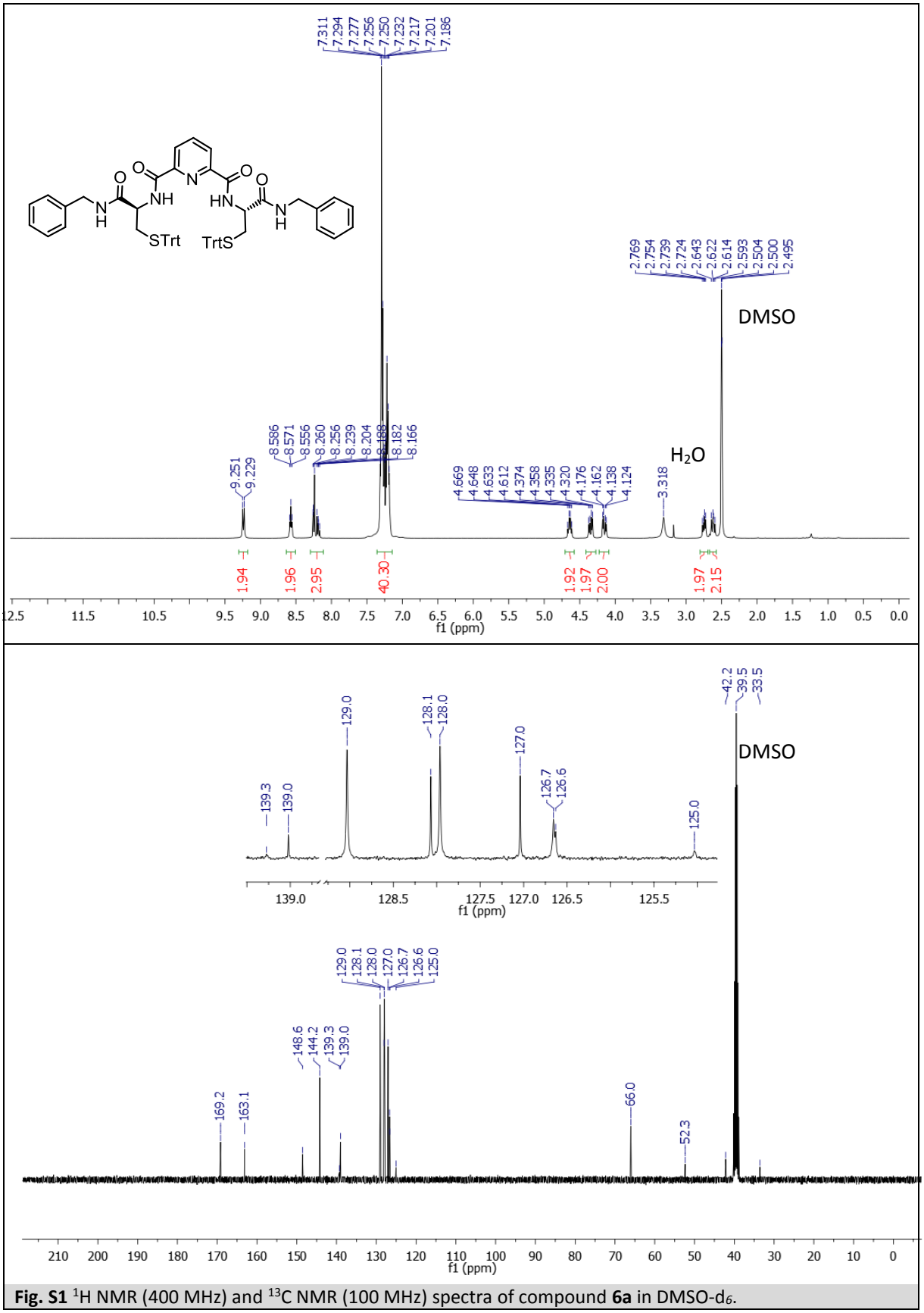

Fig. S1 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **6a** in DMSO-d_6.

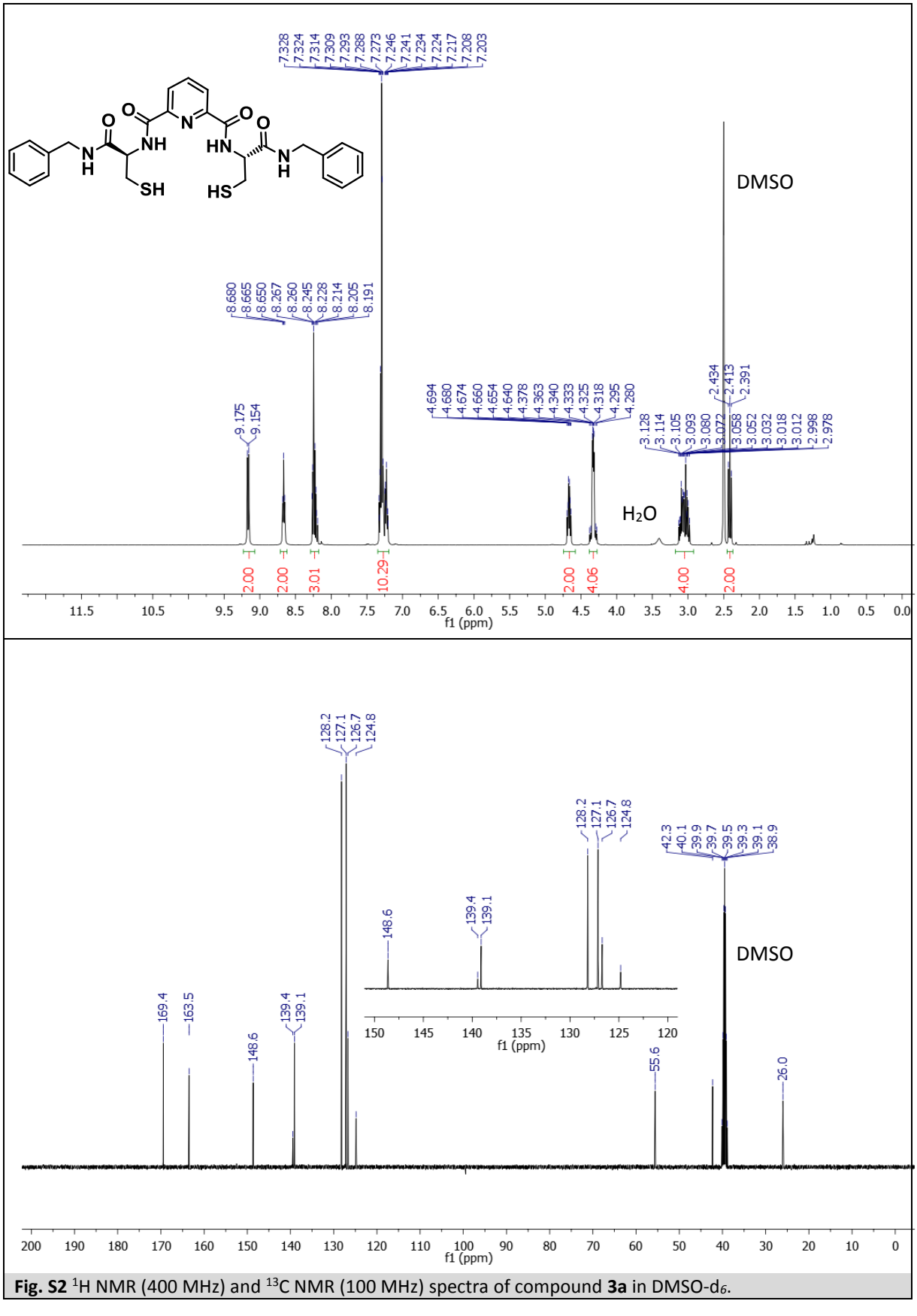

Fig. S2 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **3a** in DMSO-d_6.

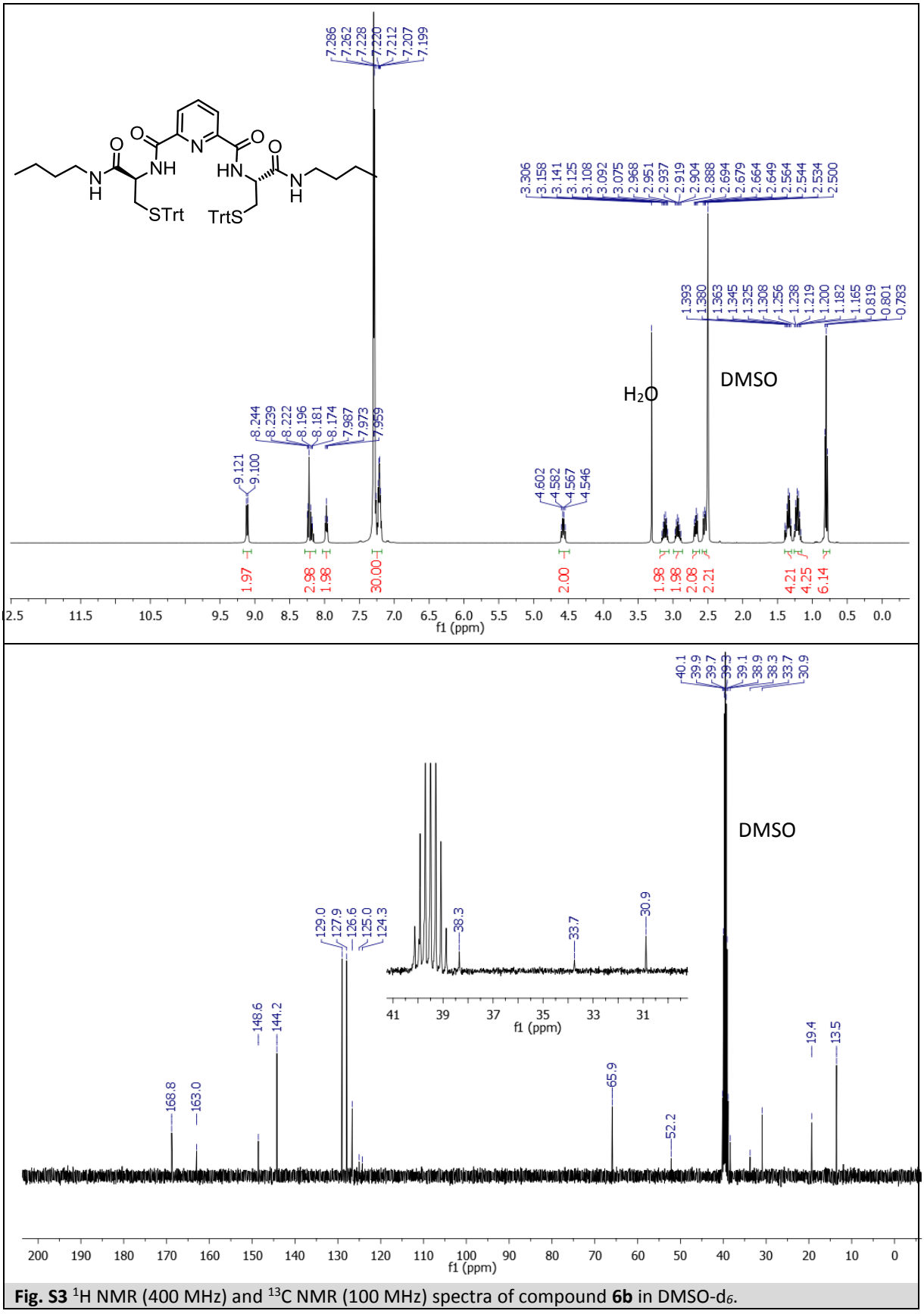

Fig. S3 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **6b** in DMSO-d_6.

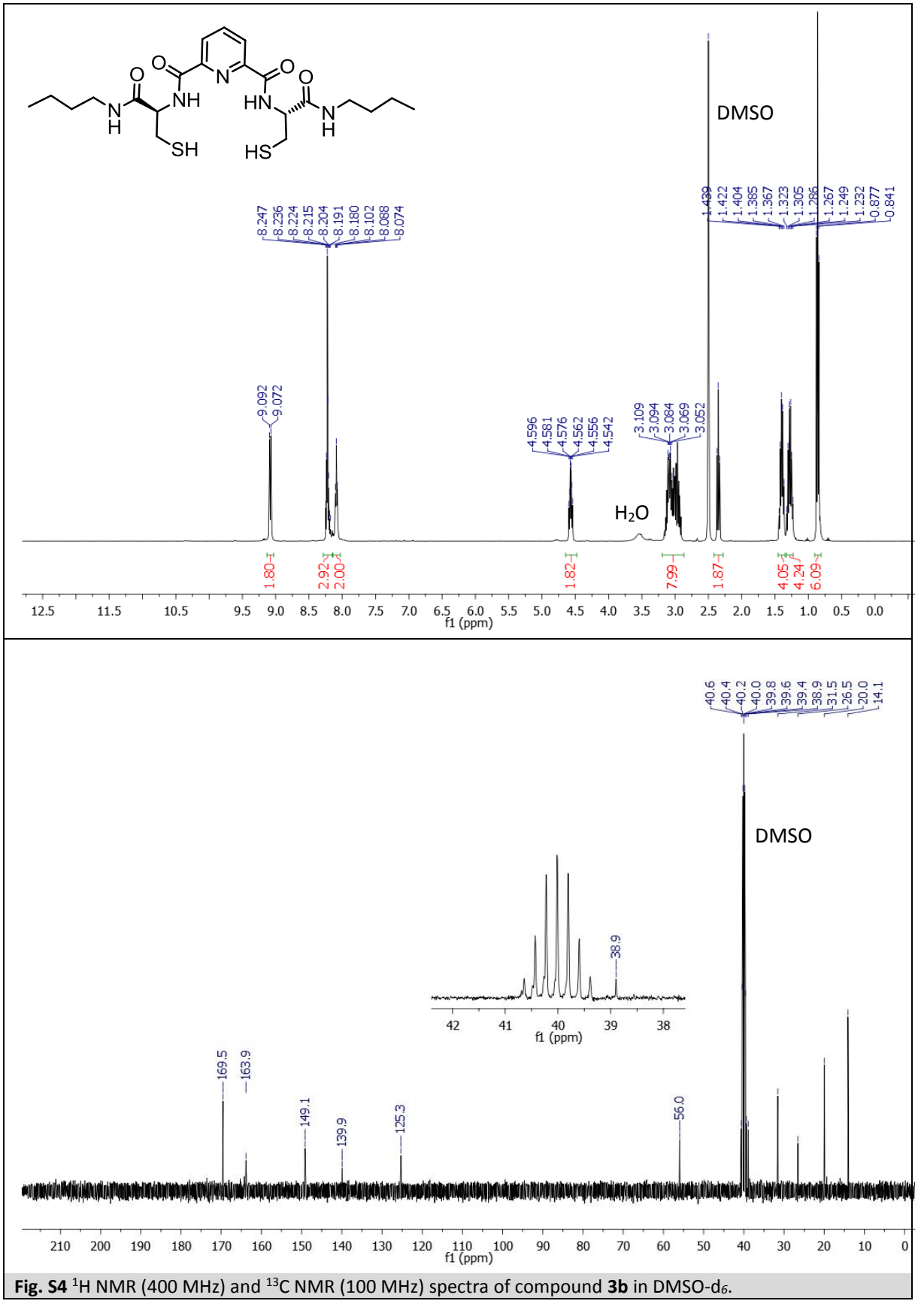

Fig. S4 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **3b** in DMSO-d_6.

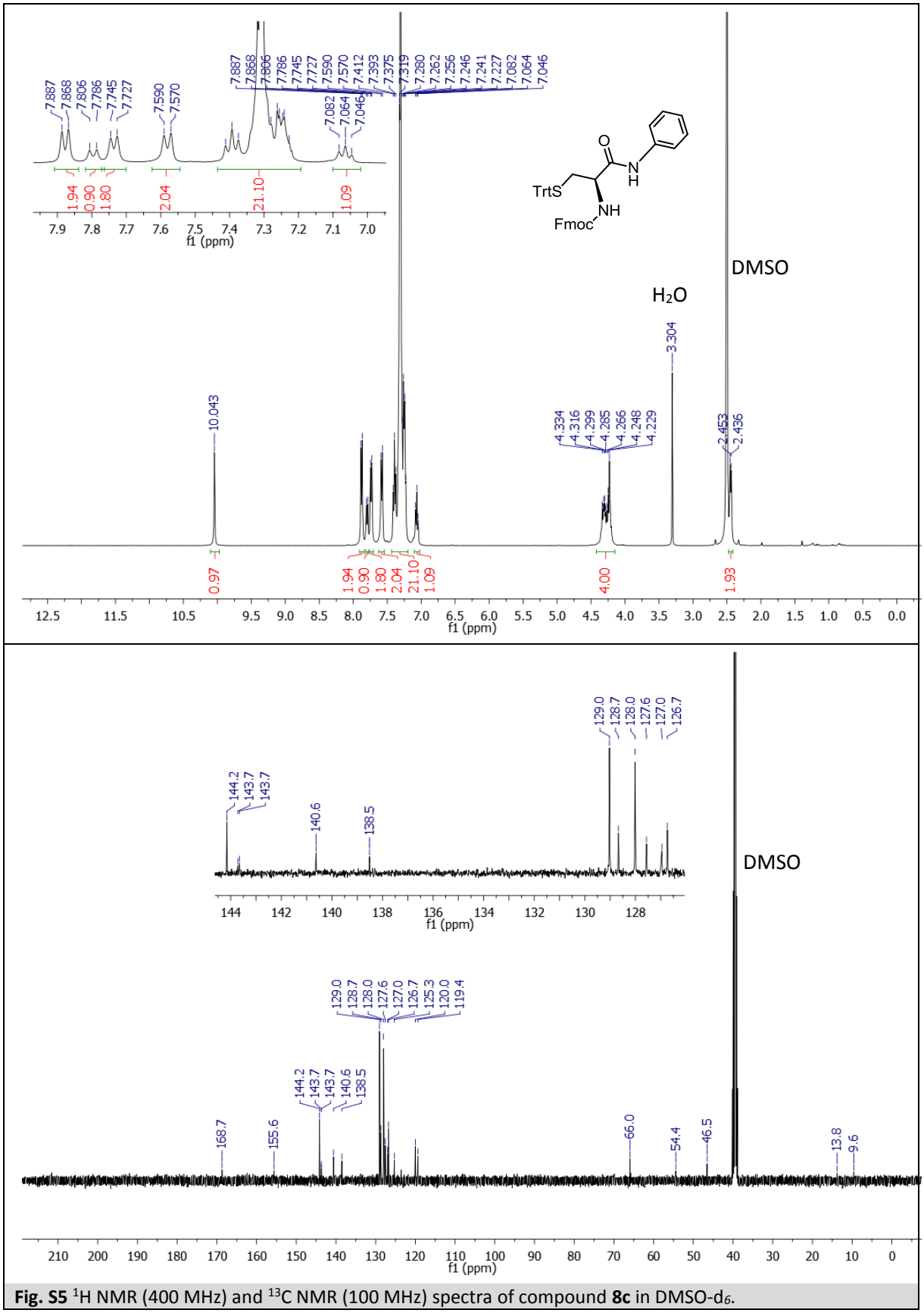

Fig. S5 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **8c** in DMSO-d$_6$.

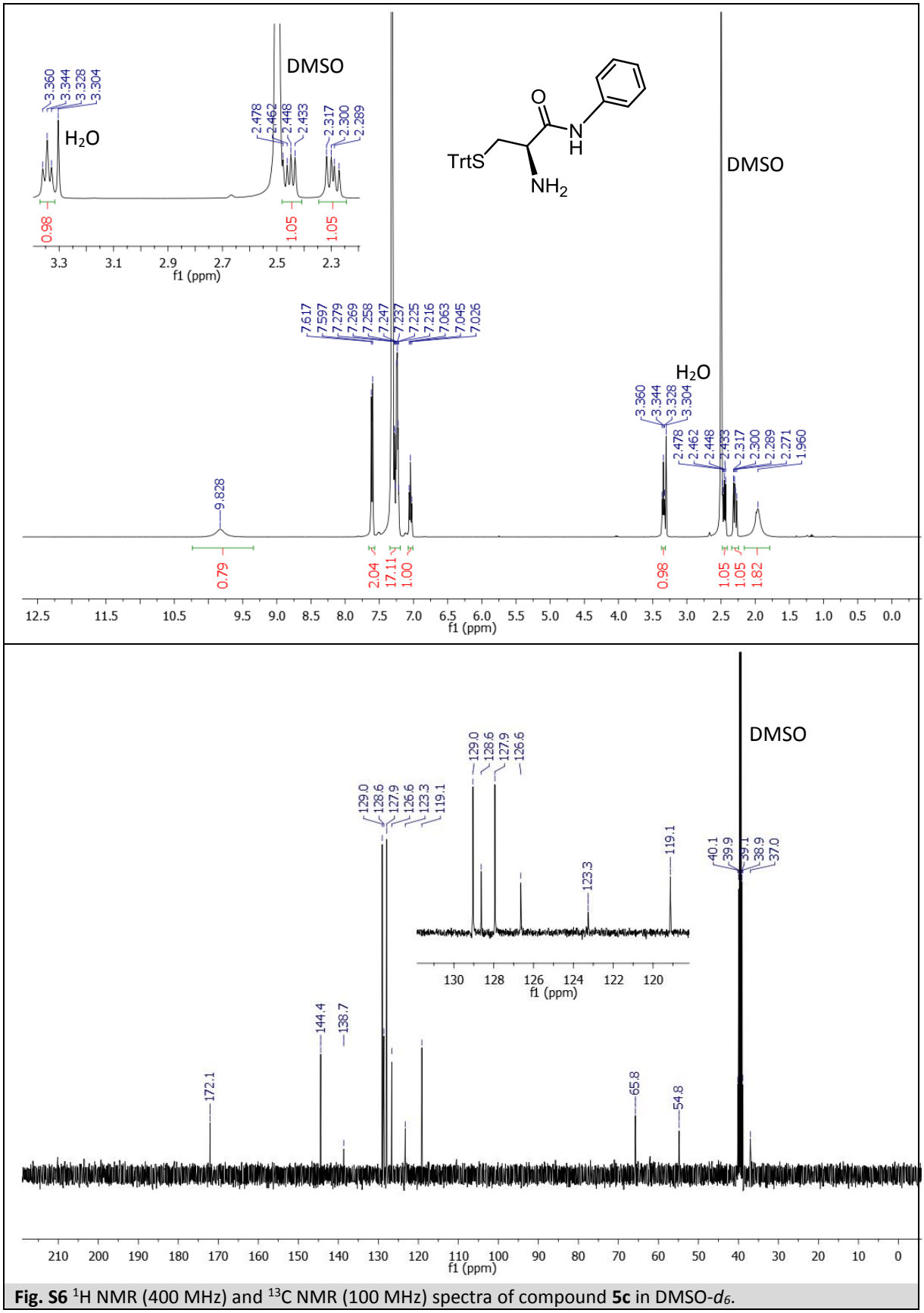

Fig. S6 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **5c** in DMSO-*d*$_6$.

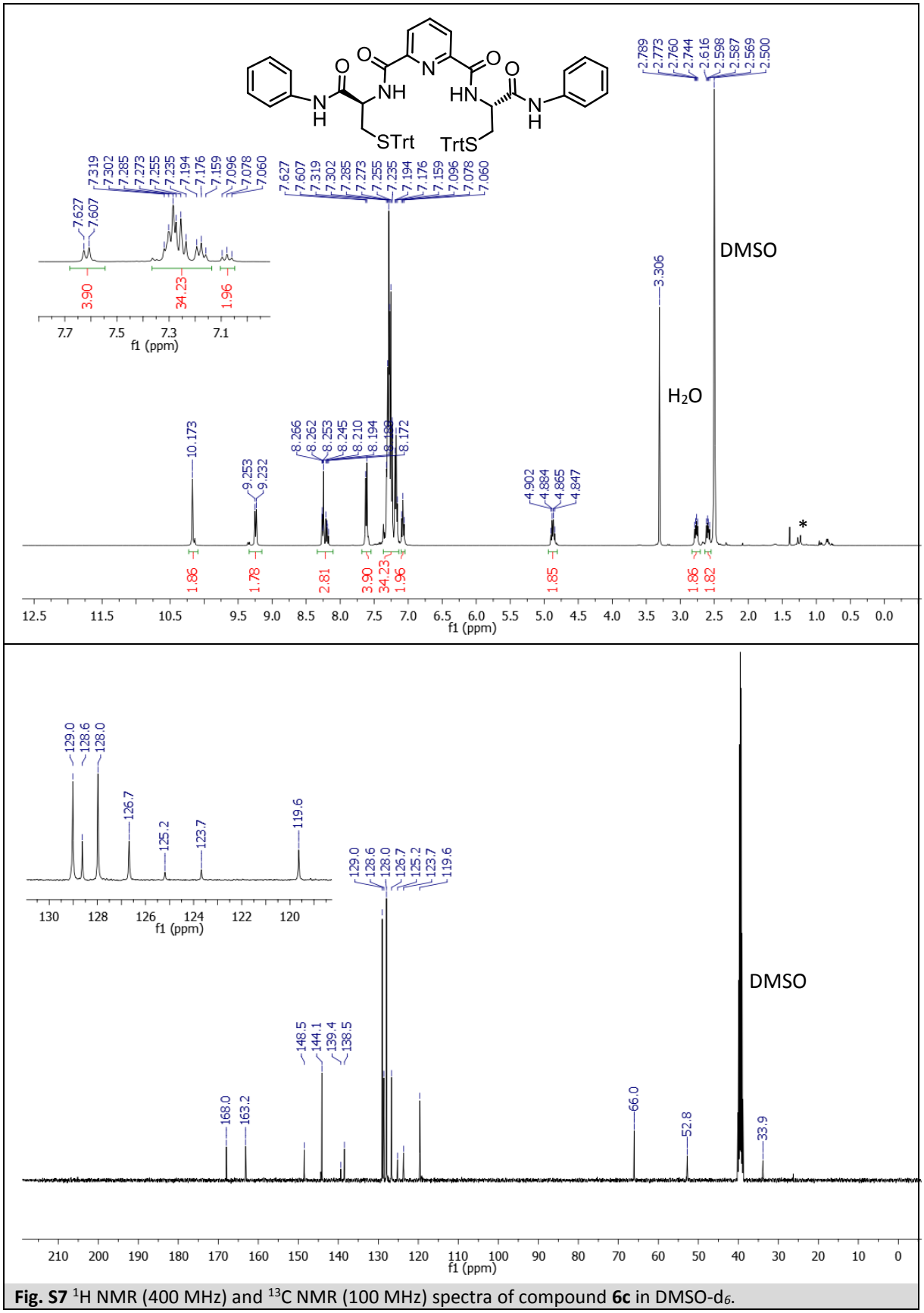

Fig. S7 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **6c** in DMSO-d_6.

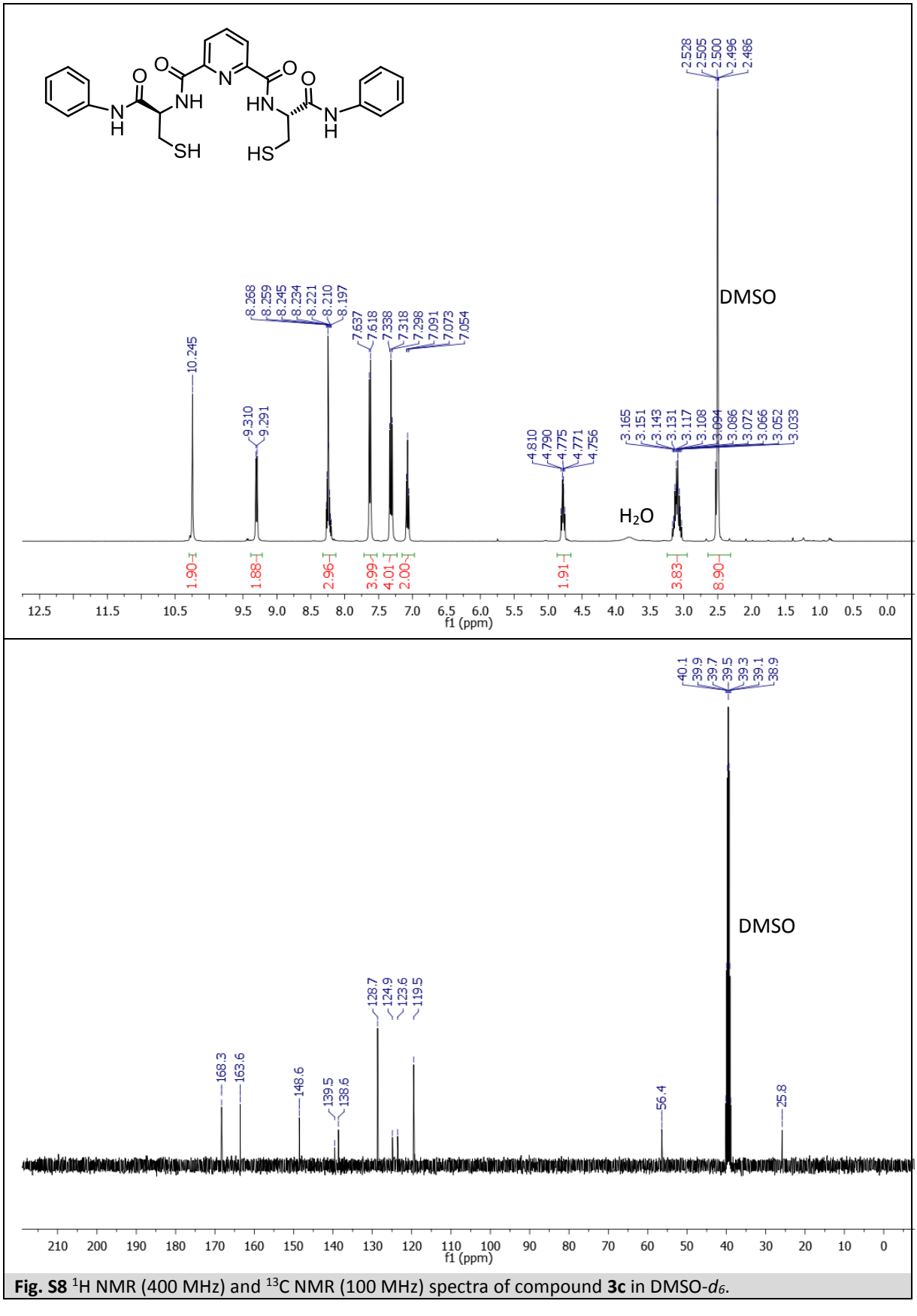

Fig. S8 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **3c** in DMSO-*d*$_6$.

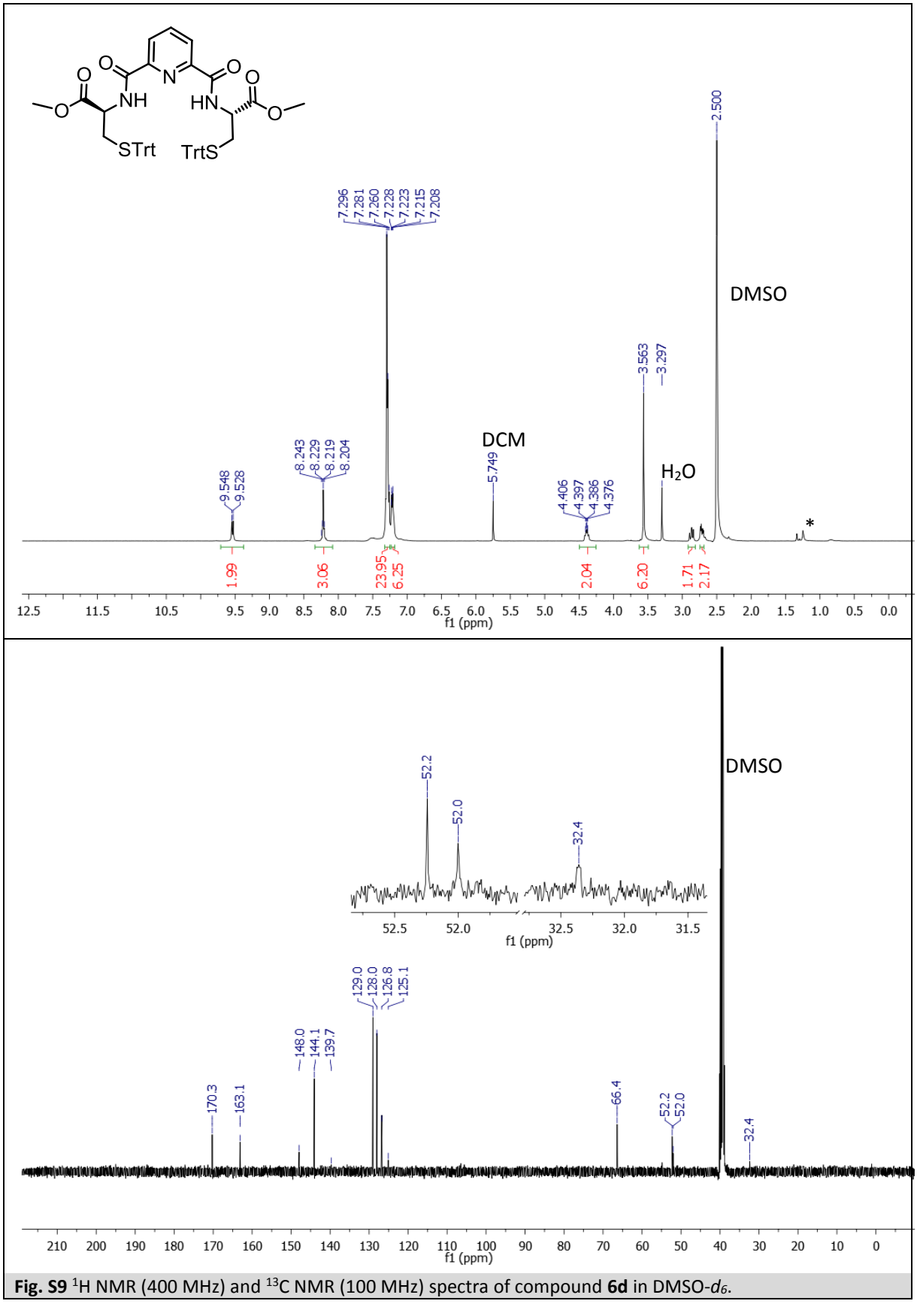

Fig. S9 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **6d** in DMSO-*d*$_6$.

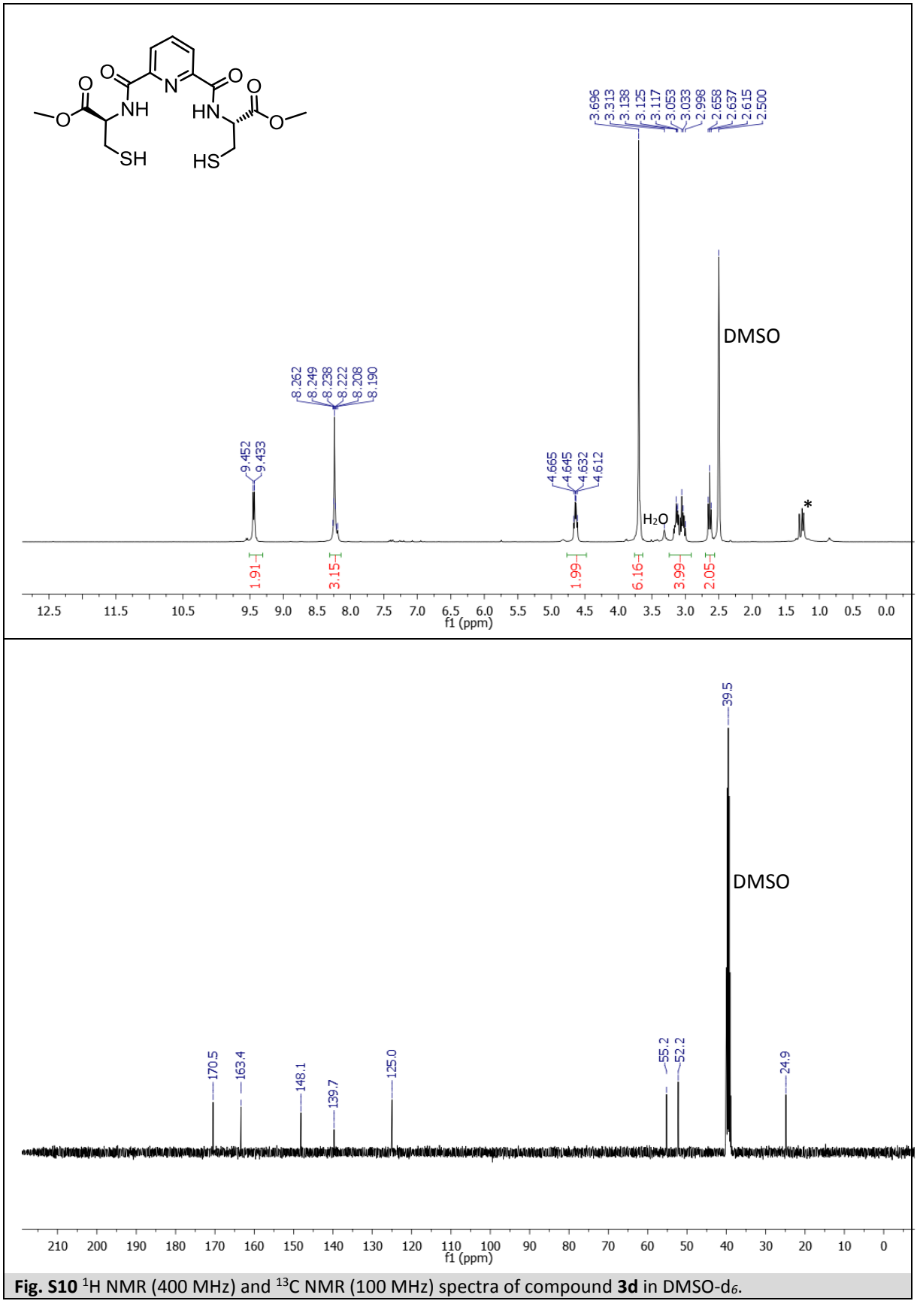

Fig. S10 ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **3d** in DMSO-d_6.

3. HPLC traces

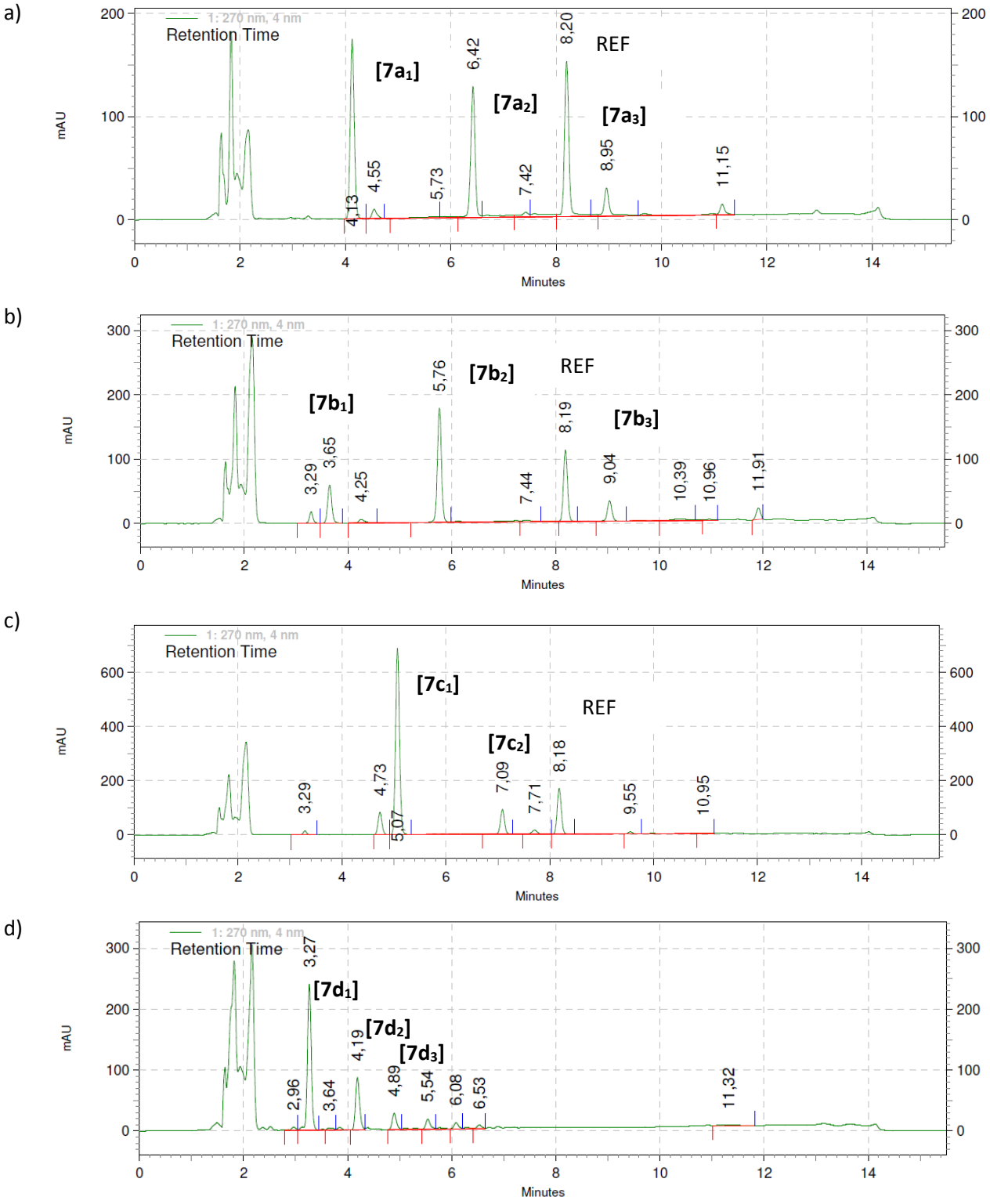

Fig. S11 Chromatograms of mixtures obtained upon oxidation of dithios a) **3a**, b) **3b**, c) **3c**, and d) **3d**.

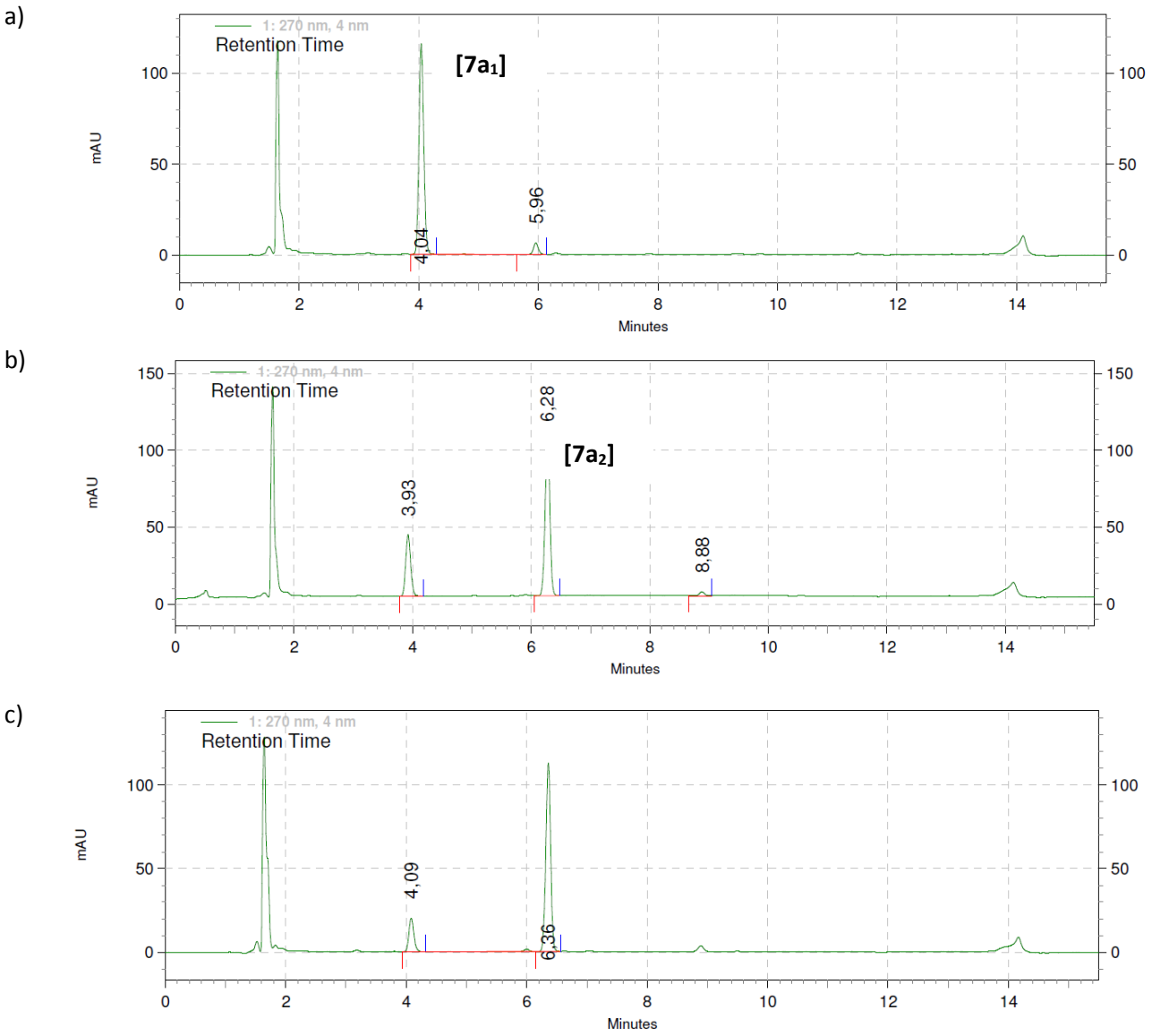

Fig. S12 Chromatograms of (a) **[7a$_1$]**, after heating for (b) 2h, (c) 4h at 80^{o}C.

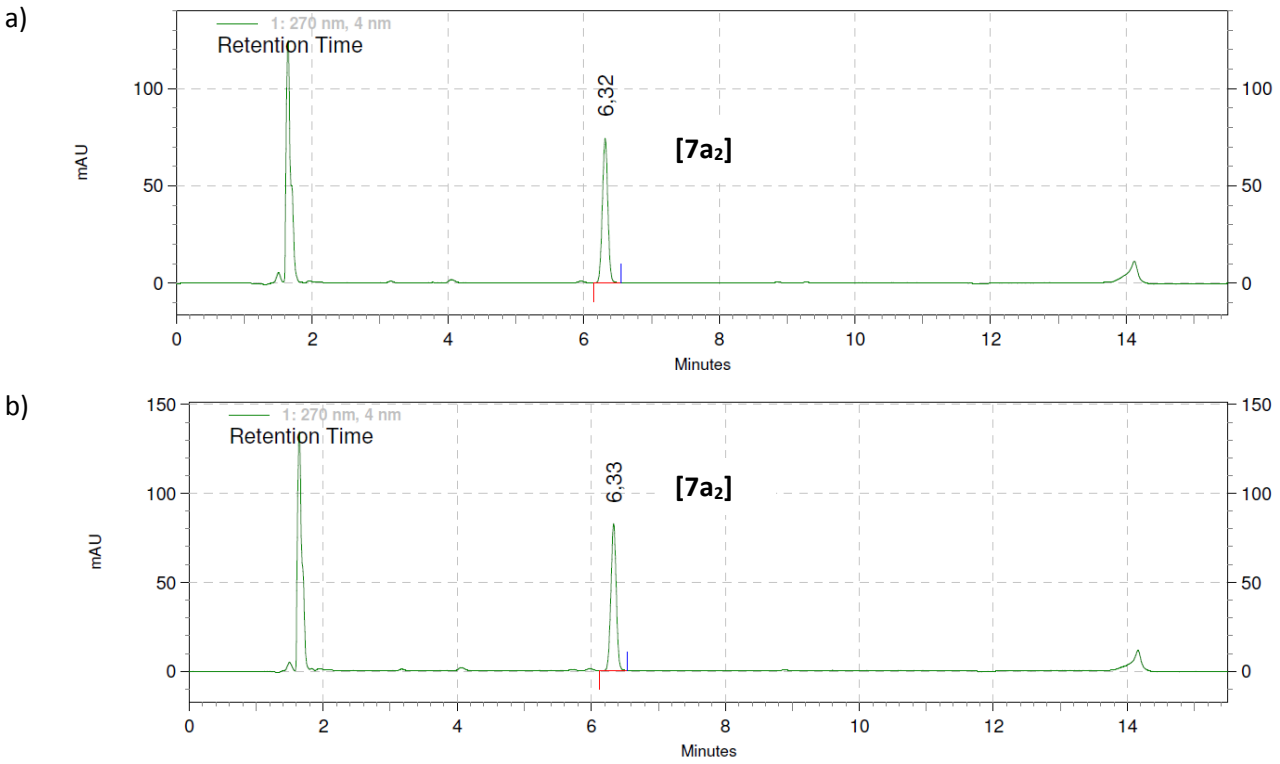

Fig. S13 Chromatograms of (a) **[7a$_2$]**, after heating for 6h at 80^{o}C

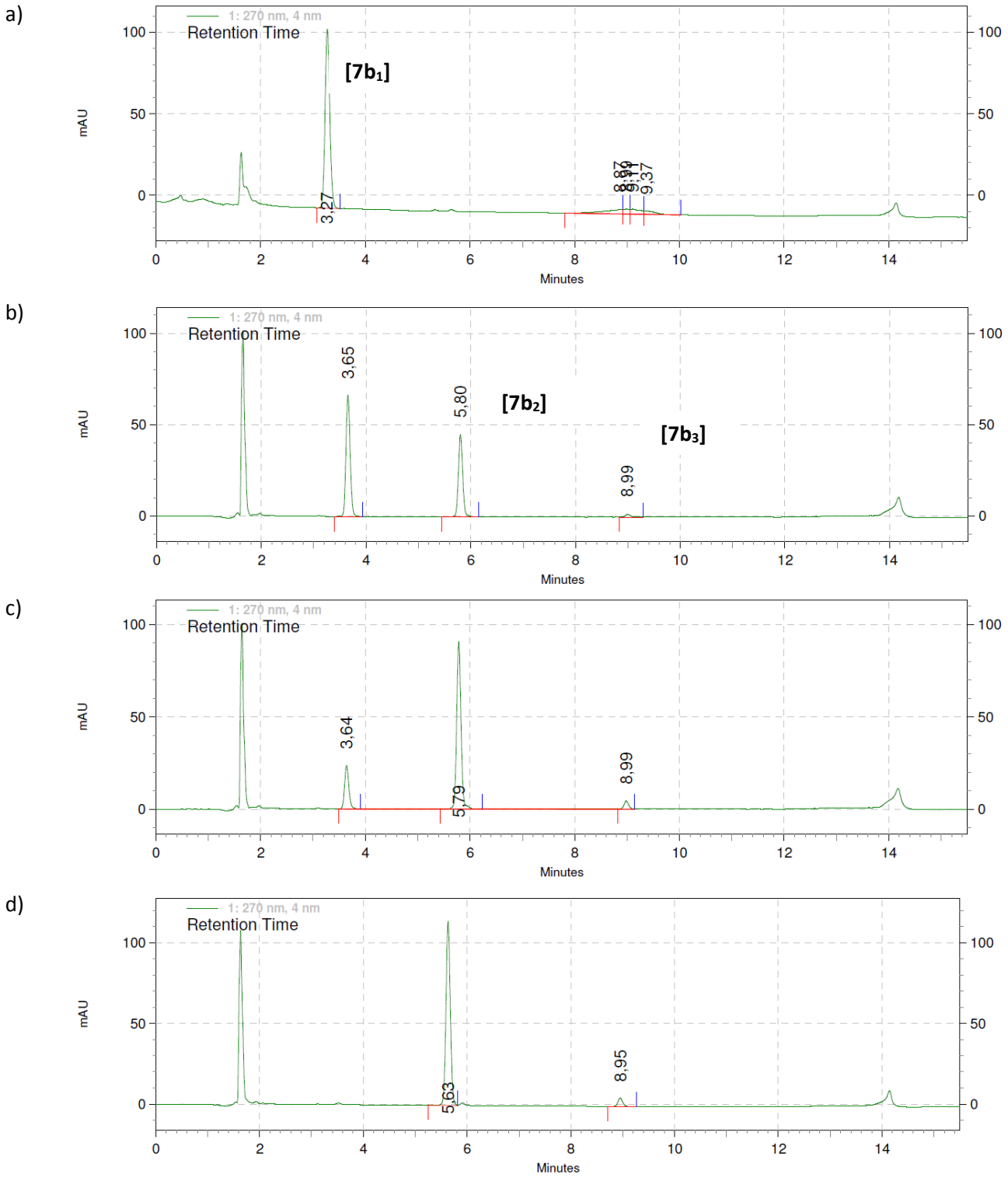

Fig. S14 Chromatograms of (a) **[7b$_1$]**, after addition of TBAOH: (b) 5 min, (c) 15 min, (d) 60min.

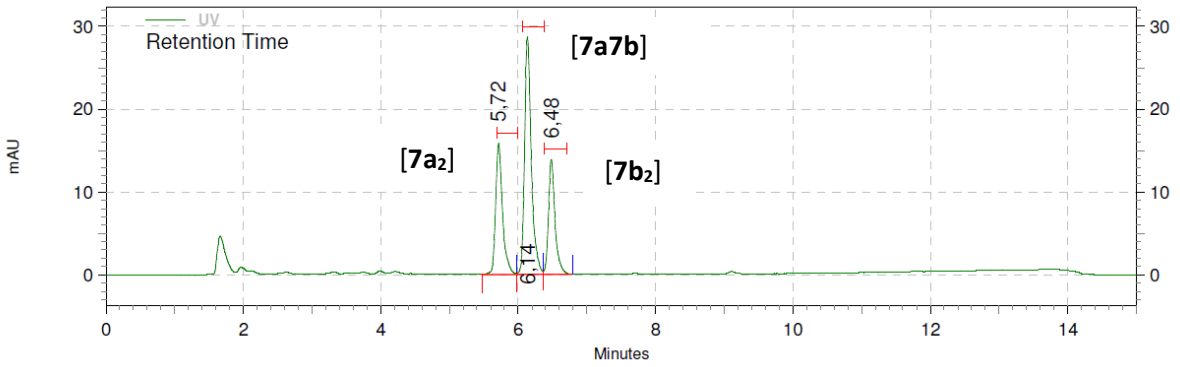

Fig. S15 Chromatogram of mixture of [**7a$_2$**] and [**7b$_2$**] 120 min after addition of 20 mol% of thiols **3a** and **3b** and TBAOH.

4. X-ray measurments

The X-ray measurement of **[2$_2$]** was performed at 100(2) K on a Bruker D8 Venture Photon100 diffractometer equipped with a TRIUMPH monochromator and a MoKα fine focus sealed tube (λ = 0.71073 Å). A total of 1450 frames were collected with Bruker APEX2 program [1]. The frames were integrated with the Bruker SAINT software package [2] using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 22761 reflections to a maximum θ angle of 25.49° (0.83 Å resolution), of which 3094 were independent (average redundancy 7.356, completeness = 100.0%, R_{int} = 2.26%, R_{sig} = 1.39%) and 2777 (89.75%) were greater than 2σ(F^2). The final cell constants of a = 15.4619(9) Å, b = 9.5378(5) Å, c = 22.6171(12) Å, β = 92.5215(13)°, volume = 3332.2(3) Å^3, are based upon the refinement of the XYZ-centroids of 9931 reflections above 20 σ(I) with 5.019° < 2θ < 52.21°. Data were corrected for absorption effects using the multi-scan method (SADABS) [7]. The ratio of minimum to maximum apparent transmission was 0.933. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8320 and 0.9250.

The structure was solved and refined using SHELXTL Software Package [4] using the space group C 1 2/c 1, with Z = 4 for the formula unit, $C_{26}H_{38}N_6O_6S_6$. The final anisotropic full-matrix least-squares refinement on F^2 with 209 variables converged at R1 = 2.75%, for the observed data and wR2 = 7.02% for all data. The goodness-of-fit was 1.099. The largest peak in the final difference electron density synthesis was 0.391 e$^-$/Å^3 and the largest hole was -0.159 e$^-$/Å^3 with an RMS deviation of 0.055 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.441 g/cm^3 and F(000), 1520 e$^-$.

The non-hydrogen atoms were refined anisotropically. Most of hydrogen atoms were placed in calculated positions and refined within the riding model. The temperature factors of these hydrogen atoms were not refined and were set to be equal to either 1.2 or 1.5 times larger than U_{eq} of the corresponding heavy atom. Positions of two hydrogen atoms engaged in hydrogen bonds were refined together with their isotropic temperature factors. The atomic scattering factors were taken from the International Tables [5].

These data are deposited at CCDC base under number CCDC 1551580

The X-ray measurement of **[7a$_2$]** was performed at 100(2) K on a Bruker D8 Venture Photon100 diffractometer equipped with a TRIUMPH monochromator and a MoKα fine focus sealed tube (λ = 0.71073 Å). A total of 870 frames were collected with Bruker APEX2 program [1]. The frames were integrated with the Bruker SAINT software package [2] using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 210438 reflections to a maximum ϑ angle of 25.05° (0.84 Å resolution), of which 30740 were independent, but not fully merged due to twinning and HKLF5 format of the data (average redundancy 6.84 , completeness = 99.9%, R_{int} = 10.44%, R_{sig} = 11.59%). 20093 reflections (65.36%) were greater than 2σ(F^2). The final cell constants of a = 19.763(2) Å, b = 21.594(2) Å, c = 33.712(4) Å, V = 14387.(3) Å^3, are based upon the refinement of the XYZ-centroids of 9331 reflections above 20 σ(I) with 4.465° < 2ϑ < 40.06°. Data were

corrected for absorption effects using the multi-scan method (TWINABS) [6]. The ratio of minimum to maximum apparent transmission was 0.759. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.893 and 0.968.

The structure was solved and refined using SHELXTL Software Package [4] using the space group $P2_12_12_1$, with Z = 4 for the formula unit, $C_{124.40}H_{156.62}N_{20}O_{25.40}S_{16.20}$. and the Flack parameter equal to 0.00(4) [7]. The final anisotropic full-matrix least-squares refinement on F^2 with 2035 variables converged at $R1$ = 9.64%, for the observed data and $wR2$ = 25.99% for all data. The goodness-of-fit was 1.091. The largest peak in the final difference electron density synthesis was 0.560 $e^-/Å^3$ and the largest hole was -0.427 $e^-/Å^3$ with an RMS deviation of 0.080 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.319 g/cm^3 and F(000), 6022 e^-.

The investigated crystal is twinned by reticular pseudomerohedry, with partial overlap of some reflection. Due to twinning effect data integration and scaling was based on two domains resulting the HKLF5 format of the reflection data. The refined twin fractions are equal to 0.732(2) and 0.268(2). In addition the structure is heavily disordered thus resulting in weak scattering power, especially at higher 2ϑ diffraction angles. In spite of the disorder, twinning effects and use of MoKα X-ray radiation the diffraction experiment confirmed optical purity of investigated compound. It was possible due to relatively high sulfur atoms contents coming from both the macrocycle compound and large amount of dimethyl sulfoxide (DMSO) solvent molecules in the crystal lattice. The compound crystallizes the chiral $P2_12_12_1$ space group with Flack parameter equal to 0.00(4) with both twin components belonging to the same enantiomorphic phase.

The structure in the asymmetric part of the unit cell contains two macrocycle molecules, 8.2 DMSO molecules and 1.2 species of H_2O. In the latter case H atoms were not assigned. As mentioned above structure is severely disordered with many atoms both in macrocycle molecules and the solvent moieties disordered over two sites. In most cases the occupancy ratios of both disordered fragments were refined. DMSO molecules is located in 9 sites, with only one moiety fully ordered. Among the other DMSO molecules 6 sites are fully occupied whereas in two cases the sum occupation of the atoms is equal to 0.5 and 0.7. The occupancy of the water molecules located at three sites, in the asymmetric part of the unit cell, is equal to 0.6, 0.3 and 0.3. To preserve reasonable geometry of disordered fragments number of restraints was applied.

All ordered non-hydrogen atoms and major component (occupancy ≥50%) disordered non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in calculated positions and refined within the riding model. The temperature factors of the hydrogen atoms were not refined and were set to be equal to either 1.2 or 1.5 times larger than U_{eq} of the corresponding heavy atom. The atomic scattering factors were taken from the International Tables [5].

These data are deposited at CCDC base under number CCDC 1551754

5. Coordinates of optimised geometries

Compound **1**, conformation A:

H	-4.049355	2.611814	-0.206692
C	-3.209553	1.925624	-0.153145
N	-1.050411	0.163603	-0.017308
C	-2.685212	1.542878	1.079981
C	-2.641493	1.410800	-1.316648
C	-1.563341	0.528655	-1.198916
C	-1.601583	0.660018	1.097989
H	-3.090084	1.909145	2.015774
H	-3.011179	1.670478	-2.301651

C	-1.010891	0.243638	2.424452
C	-0.947787	-0.052430	-2.453430
N	0.054761	-0.581820	2.330874
H	0.384300	-0.800445	1.397260
N	0.040273	-0.946993	-2.234738
H	0.304390	-1.115404	-1.270819
O	-1.500007	0.641875	3.487663
O	-1.359174	0.278225	-3.571601
C	0.851186	-0.985862	3.472420
H	1.052193	-2.061904	3.404625
H	0.255035	-0.808776	4.370452
C	2.195822	-0.254704	3.568973
H	2.765331	-0.655367	4.412569
H	2.784518	-0.412374	2.659495
C	0.796108	-1.583044	-3.295870
H	0.852454	-2.660089	-3.095129
H	0.243030	-1.441599	-4.227204
C	2.226244	-1.050019	-3.433929
H	2.760022	-1.631594	-4.191221
H	2.767144	-1.152736	-2.487607
S	2.065838	1.577918	3.731057
H	1.325099	1.594466	4.857972
S	2.340900	0.743878	-3.847584
H	1.655423	0.692146	-5.008063

Compound **1**, conformation B:

H	-2.600278	2.516796	3.324132
C	-2.023709	1.952777	2.597175
N	-0.544678	0.504935	0.729613
C	-2.424204	1.902576	1.262837
C	-0.873068	1.267784	2.984297
C	-0.168402	0.549968	2.013856
C	-1.646823	1.169442	0.361788
H	-3.311044	2.414610	0.908082
H	-0.517123	1.273082	4.007719
C	-2.047025	1.118411	-1.097158
C	1.073962	-0.215701	2.405847
N	-1.145086	0.518213	-1.903963
H	-0.320493	0.129209	-1.460509
N	1.558991	-1.022423	1.436412
H	1.091029	-0.985183	0.537266
O	-3.110669	1.617885	-1.481666
O	1.561488	-0.100905	3.536042
C	-1.326248	0.337913	-3.331277
H	-0.450400	0.740640	-3.856321
H	-2.198165	0.923407	-3.631269
C	-1.491494	-1.128846	-3.741409
H	-1.492128	-1.205238	-4.832413
H	-0.657047	-1.727525	-3.362521
C	2.813647	-1.739075	1.542263
H	3.138780	-1.684224	2.583520
H	2.651068	-2.795385	1.293008
C	3.895825	-1.190452	0.606157
H	3.550266	-1.214579	-0.432458
H	4.791787	-1.813642	0.677860
S	-3.003710	-1.946906	-3.072342
H	-3.905061	-1.156460	-3.690669
S	4.346987	0.572363	0.909527
H	4.783025	0.416532	2.176575

Compound **1**, conformation C:

H	-4.021805	2.798287	0.838230
C	-3.184654	2.111026	0.761059
N	-1.042747	0.341565	0.569193
C	-2.451596	1.761960	1.893600
C	-2.828265	1.566374	-0.472231
C	-1.750500	0.679799	-0.515308
C	-1.373157	0.879456	1.747395
H	-2.695526	2.155153	2.873281
H	-3.359422	1.809632	-1.385410
C	-0.597256	0.481209	2.979540
C	-1.313055	0.086408	-1.836670
N	0.699696	0.084584	2.873892
H	1.097859	-0.139542	3.781489

N	-0.370372	-0.873737	-1.725873
H	-0.022539	-1.081446	-0.792393
O	-1.167163	0.505091	4.077639
O	-1.804028	0.476947	-2.902920
C	1.672623	0.221472	1.788913
H	2.406258	0.989589	2.068311
H	1.162955	0.541867	0.884317
C	2.432198	-1.084543	1.545366
H	3.191395	-0.921585	0.774735
H	2.940524	-1.408031	2.458871
C	0.349217	-1.432071	-2.852243
H	0.304939	-2.527834	-2.808606
H	-0.152739	-1.109919	-3.767544
C	1.825813	-1.017229	-2.864139
H	2.345754	-1.523767	-3.682279
H	2.307043	-1.308314	-1.924653
S	1.388081	-2.472983	0.920064
H	0.425213	-2.372274	1.859324
S	2.103756	0.801445	-2.990955
H	1.481498	0.981412	-4.173994

Compound **3d**, conformation D:

H	0.258023	-5.716988	-0.967341
C	0.170844	-4.662300	-0.725104
N	-0.054001	-1.957908	-0.107206
C	1.268674	-3.957569	-0.231519
C	-1.041120	-3.995503	-0.902718
C	-1.104792	-2.638851	-0.574978
C	1.106472	-2.601451	0.062469
H	2.231445	-4.429402	-0.073938
H	-1.924059	-4.497311	-1.281550
C	2.266357	-1.788665	0.581756
C	-2.400924	-1.880439	-0.736364
O	3.383415	-2.283078	0.754432
O	-3.420956	-2.419542	-1.177509
N	1.949875	-0.498272	0.836819
H	1.023573	-0.191200	0.557541
N	-2.334714	-0.587543	-0.347365
H	-1.437095	-0.236350	-0.037242
C	2.924416	0.506496	1.176600
H	3.733090	0.013835	1.731084
C	-3.453703	0.318896	-0.452829
H	-4.370013	-0.270793	-0.315754
C	3.597042	1.154141	-0.046499
C	-3.445322	1.375609	0.653657
C	2.317327	1.588269	2.081756
H	3.085597	2.310866	2.358228
H	1.924040	1.121847	2.987679
C	-3.556751	0.989238	-1.836216
H	-3.630033	0.207269	-2.595370
H	-4.452786	1.610264	-1.883212
S	-2.085363	1.997751	-2.298686
S	0.885335	2.482944	1.326662
O	4.258761	2.172249	0.032036
O	-4.128858	2.380065	0.602478
O	3.388561	0.471752	-1.173804
O	-2.620964	1.071855	1.659390
C	4.016644	1.003678	-2.363652
H	3.727437	0.328850	-3.168459
H	5.102356	1.017150	-2.240908
H	3.654620	2.016189	-2.557336
C	-2.550391	2.038122	2.735177
H	-3.528276	2.138397	3.211776
H	-2.223751	3.004464	2.345435
H	-1.815953	1.637157	3.432356
H	-2.309117	3.010838	-1.437362
H	1.595473	3.161892	0.402503

Compound **3d**, conformation E:

H	-2.181322	-4.988653	-1.053754
C	-1.817975	-4.027191	-0.704095
N	-0.895553	-1.550815	0.191693
C	-0.451268	-3.782124	-0.594188
C	-2.712179	-3.017165	-0.362365

C	-2.208521	-1.785045	0.078001
C	-0.038939	-2.529069	-0.137132
H	0.291035	-4.527704	-0.853209
H	-3.783431	-3.158340	-0.433588
C	1.438373	-2.241636	-0.025514
C	-3.222529	-0.709802	0.407087
O	2.282200	-3.054930	-0.412674
O	-4.426560	-0.974154	0.316819
N	1.728201	-1.047731	0.537927
H	0.954317	-0.423464	0.726512
N	-2.833778	0.532815	0.810196
H	-3.624875	1.166093	0.880387
C	3.057553	-0.483670	0.575448
H	3.753442	-1.297719	0.339367
C	-1.526398	1.160029	0.852000
H	-0.870664	0.611728	1.532973
C	3.232074	0.574791	-0.525712
C	-0.785971	1.198020	-0.487879
C	3.418564	0.067287	1.959349
H	4.412775	0.516246	1.926433
H	3.427862	-0.756120	2.677267
C	-1.623214	2.585376	1.427511
H	-2.042239	2.536751	2.435663
H	-0.615918	3.000742	1.488433
S	-2.719933	3.746612	0.505176
S	2.220737	1.291875	2.649282
O	3.719089	1.675707	-0.351291
O	0.386078	1.523930	-0.558207
O	2.806982	0.113760	-1.705056
O	-1.544881	0.872577	-1.532100
C	2.839869	1.053647	-2.801785
H	2.503390	0.493017	-3.673354
H	3.854617	1.429654	-2.952133
H	2.157597	1.879282	-2.589237
C	-0.863882	0.796610	-2.806783
H	-0.047277	0.073396	-2.743150
H	-0.468571	1.776865	-3.082481
H	-1.619953	0.468738	-3.518876
H	-1.992123	3.807263	-0.628696
H	2.412765	2.239853	1.711700

Compound **3d**, conformation F:

H	0.258023	-5.716988	-0.967341
C	0.170844	-4.662300	-0.725104
N	-0.054001	-1.957908	-0.107206
C	1.268674	-3.957569	-0.231519
C	-1.041120	-3.995503	-0.902718
C	-1.104792	-2.638851	-0.574978
C	1.106472	-2.601451	0.062469
H	2.231445	-4.429402	-0.073938
H	-1.924059	-4.497311	-1.281550
C	2.266357	-1.788665	0.581756
C	-2.400924	-1.880439	-0.736364
O	3.383415	-2.283078	0.754432
O	-3.420956	-2.419542	-1.177509
N	1.949875	-0.498272	0.836819
H	1.023573	-0.191200	0.557541
N	-2.334714	-0.587543	-0.347365
H	-1.437095	-0.236350	-0.037242
C	2.924416	0.506496	1.176600
H	3.733090	0.013835	1.731084
C	-3.453703	0.318896	-0.452829
H	-4.370013	-0.270793	-0.315754
C	3.597042	1.154141	-0.046499
C	-3.445322	1.375609	0.653657
C	2.317327	1.588269	2.081756
H	3.085597	2.310866	2.358228
H	1.924040	1.121847	2.987679
C	-3.556751	0.989238	-1.836216
H	-3.630033	0.207269	-2.595370
H	-4.452786	1.610264	-1.883212
S	-2.085363	1.997751	-2.298686
S	0.885335	2.482944	1.326662
O	4.258761	2.172249	0.032036

O	-4.128858	2.380065	0.602478
O	3.388561	0.471752	-1.173804
O	-2.620964	1.071855	1.659390
C	4.016644	1.003678	-2.363652
H	3.727437	0.328850	-3.168459
H	5.102356	1.017150	-2.240908
H	3.654620	2.016189	-2.557336
C	-2.550391	2.038122	2.735177
H	-3.528276	2.138397	3.211776
H	-2.223751	3.004464	2.345435
H	-1.815953	1.637157	3.432356
H	-2.309117	3.010838	-1.437362
H	1.595473	3.161892	0.402503

Compound **[7d$_1$]**, conformation A:

H	-5.211256	0.922791	-1.165586
C	-4.167231	0.850434	-0.876662
N	-1.516423	0.678980	-0.141643
C	-3.824614	0.629339	0.461960
C	-3.165799	0.941076	-1.846650
C	-1.837367	0.853600	-1.422393
C	-2.469691	0.535681	0.780799
H	-4.578232	0.506416	1.231865
H	-3.398091	1.063821	-2.898994
C	-1.961209	0.138582	2.150290
C	-0.660087	0.784608	-2.369807
O	-2.692426	0.005242	3.133245
O	-0.784460	0.464840	-3.551884
N	-0.626202	-0.089578	2.132676
H	-0.201697	-0.056719	1.211751
N	0.527819	1.022892	-1.750565
H	0.451131	1.243694	-0.764207
C	0.128617	-0.684246	3.205556
H	-0.060810	-0.133200	4.134005
C	1.788335	0.447802	-2.173435
H	1.572373	-0.331726	-2.916384
C	-0.234965	-2.143970	3.509496
C	2.724128	1.439080	-2.883161
C	1.636627	-0.569258	2.898258
H	2.206477	-0.787692	3.806827
H	1.865292	0.450442	2.578286
C	2.528377	-0.155847	-0.960898
H	3.478131	-0.583932	-1.280532
H	2.717835	0.623261	-0.216275
S	1.484369	-1.473524	-0.166864
S	2.374872	-1.779193	1.697690
O	0.120802	-2.699755	4.530328
O	3.925399	1.271189	-2.972778
O	-0.928051	-2.723049	2.526123
O	2.060527	2.463176	-3.422587
C	-1.254598	-4.119237	2.719563
H	-0.338859	-4.707679	2.817925
H	-1.807838	-4.412474	1.828206
H	-1.869711	-4.240971	3.614248
C	2.863650	3.413086	-4.162355
H	3.611022	3.863029	-3.504810
H	2.162438	4.164806	-4.522870
H	3.361393	2.914181	-4.997758

Compound **[7d$_1$]**, conformation B:

H	-4.966196	-0.763770	-2.342047
C	-4.032819	-0.765192	-1.787657
N	-1.638198	-0.760181	-0.356088
C	-4.033309	-0.612320	-0.404228
C	-2.815942	-0.920217	-2.449284
C	-1.646334	-0.906250	-1.688790
C	-2.807297	-0.614988	0.276928
H	-4.954269	-0.495476	0.153734
H	-2.755680	-1.043720	-3.524506
C	-2.847719	-0.499248	1.781493
C	-0.313067	-1.038738	-2.376978
O	-3.919149	-0.681649	2.368794
O	-0.211408	-1.256599	-3.588664
N	-1.725485	-0.200660	2.495865

H	-1.886390	-0.238547	3.498009
N	0.750037	-0.878282	-1.562017
H	0.563652	-0.662646	-0.593675
C	-0.346583	0.087881	2.101664
H	-0.330142	0.467392	1.084938
C	2.107879	-0.941660	-2.045139
H	2.311337	-1.928135	-2.474613
C	0.170501	1.220627	2.993479
C	2.386387	0.061289	-3.174782
C	0.499633	-1.196081	2.234575
H	0.209482	-1.907755	1.458117
H	0.312710	-1.648660	3.211605
C	3.095434	-0.652425	-0.905433
H	4.114961	-0.673807	-1.297974
H	2.906114	0.331897	-0.468664
S	3.025517	-1.913690	0.456098
S	2.332984	-0.906846	2.143118
O	0.517243	2.310271	2.589094
O	3.158964	-0.167363	-4.083816
O	0.182171	0.843324	4.279637
O	1.744708	1.218892	-2.990766
C	0.618563	1.838291	5.236713
H	1.658131	2.111037	5.040210
H	0.520829	1.363638	6.212112
H	-0.017034	2.724285	5.169674

Compound **[2$_1$]**:

H	3.509916	-1.814597	-0.554814
C	3.062798	-0.849613	-0.345554
C	1.757978	1.505191	0.172422
C	1.694156	-0.783394	-0.079519
C	3.796506	0.334997	-0.325419
C	3.140107	1.532569	-0.055152
N	1.051771	0.367239	0.173490
H	4.865875	0.325197	-0.516581
H	3.660285	2.482082	-0.010816
C	0.881113	-2.059454	-0.088936
C	1.077965	2.820702	0.477067
N	-0.257896	2.979878	0.217799
H	-0.569110	3.908497	0.480095
N	-0.404954	-1.892293	0.313580
H	-0.665238	-0.961013	0.607485
C	-1.377913	-2.961715	0.359074
H	-1.591524	-3.244237	1.399320
H	-0.913938	-3.825891	-0.127345
C	-2.682365	-2.607620	-0.355891
H	-3.333100	-3.488826	-0.383223
H	-2.502473	-2.283576	-1.384353
C	-1.201074	2.153719	-0.528154
H	-1.745094	2.805053	-1.223710
H	-0.655853	1.422749	-1.122894
C	-2.189834	1.439093	0.403493
H	-1.652051	0.774264	1.081792
H	-2.743732	2.162522	1.009790
S	-3.713392	-1.308100	0.486062
S	-3.409324	0.453347	-0.592307
O	1.736684	3.741857	0.953080
O	1.373712	-3.128625	-0.439879

Compound **[2$_2$]**:

H	7.630436	-2.024135	-0.769314
C	7.137406	-1.100120	-0.490723
C	5.725550	1.132548	0.211182
C	5.743089	-1.086542	-0.391591
C	7.833473	0.077337	-0.229360
C	7.118014	1.218344	0.125249
N	5.046430	0.005140	-0.044678
H	8.917150	0.105606	-0.300917
H	7.595532	2.167298	0.339200
C	4.990018	-2.363283	-0.689063
C	4.952492	2.369729	0.606205
N	3.624229	2.171193	0.814070
H	3.257716	1.244527	0.635352
N	3.637661	-2.234930	-0.701423

H	3.254321	-1.321650	-0.491537
C	2.750869	-3.356571	-0.933666
H	3.384163	-4.202199	-1.216185
H	2.079314	-3.137731	-1.773137
C	1.926570	-3.728257	0.300004
H	2.581300	-3.891132	1.163860
H	1.359728	-4.647681	0.123501
C	2.724828	3.260164	1.137383
H	2.072398	2.968695	1.968845
H	3.349091	4.095255	1.467753
C	1.875372	3.709830	-0.053508
H	1.316458	4.618754	0.189614
H	2.514307	3.924270	-0.917539
S	0.689682	2.425285	-0.657031
S	0.757275	-2.405325	0.851356
O	5.517491	3.454180	0.734467
O	5.589909	-3.413761	-0.907841
H	-7.595532	-2.167298	0.339200
C	-7.118014	-1.218344	0.125249
C	-5.743089	1.086542	-0.391591
C	-5.725550	-1.132548	0.211182
C	-7.833473	-0.077337	-0.229360
C	-7.137406	1.100120	-0.490723
N	-5.046430	-0.005140	-0.044678
H	-8.917150	-0.105606	-0.300917
H	-7.630436	2.024135	-0.769314
C	-4.952492	-2.369729	0.606205
C	-4.990018	2.363283	-0.689063
N	-3.637661	2.234930	-0.701423
H	-3.254321	1.321650	-0.491537
N	-3.624229	-2.171193	0.814070
H	-3.257716	-1.244527	0.635352
C	-2.724828	-3.260164	1.137383
H	-3.349091	-4.095255	1.467753
H	-2.072398	-2.968695	1.968845
C	-1.875372	-3.709830	-0.053508
H	-2.514307	-3.924270	-0.917539
H	-1.316458	-4.618754	0.189614
C	-2.750869	3.356571	-0.933666
H	-2.079314	3.137731	-1.773137
H	-3.384163	4.202199	-1.216185
C	-1.926570	3.728257	0.300004
H	-1.359728	4.647681	0.123501
H	-2.581300	3.891132	1.163860
S	-0.757275	2.405325	0.851356
S	-0.689682	-2.425285	-0.657031
O	-5.589909	3.413761	-0.907841
O	-5.517491	-3.454180	0.734467

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