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

Supporting Information

peri-Interactions in 1,8-bis(dimethylamino)naphthalene *ortho*-ketimine cations facilitate [1,5]-hydride shift: selective synthesis of 1,2,3,4-tetrahydrobenzo[h]quinazolines

Vladimir Y. Mikshiev*, Peter M. Tolstoy, Aleksandra M. Puzyk, Sergey O. Kirichenko and Alexander S. Antonov*.

Institute of Chemistry, St. Petersburg State University, Universitetskij pr. 26, 198504 St. Petersburg, Russian Federation

E-mail: vladimirmikshiev@mail.ru

Table of Contents

NMR spectra of reaction mixtures

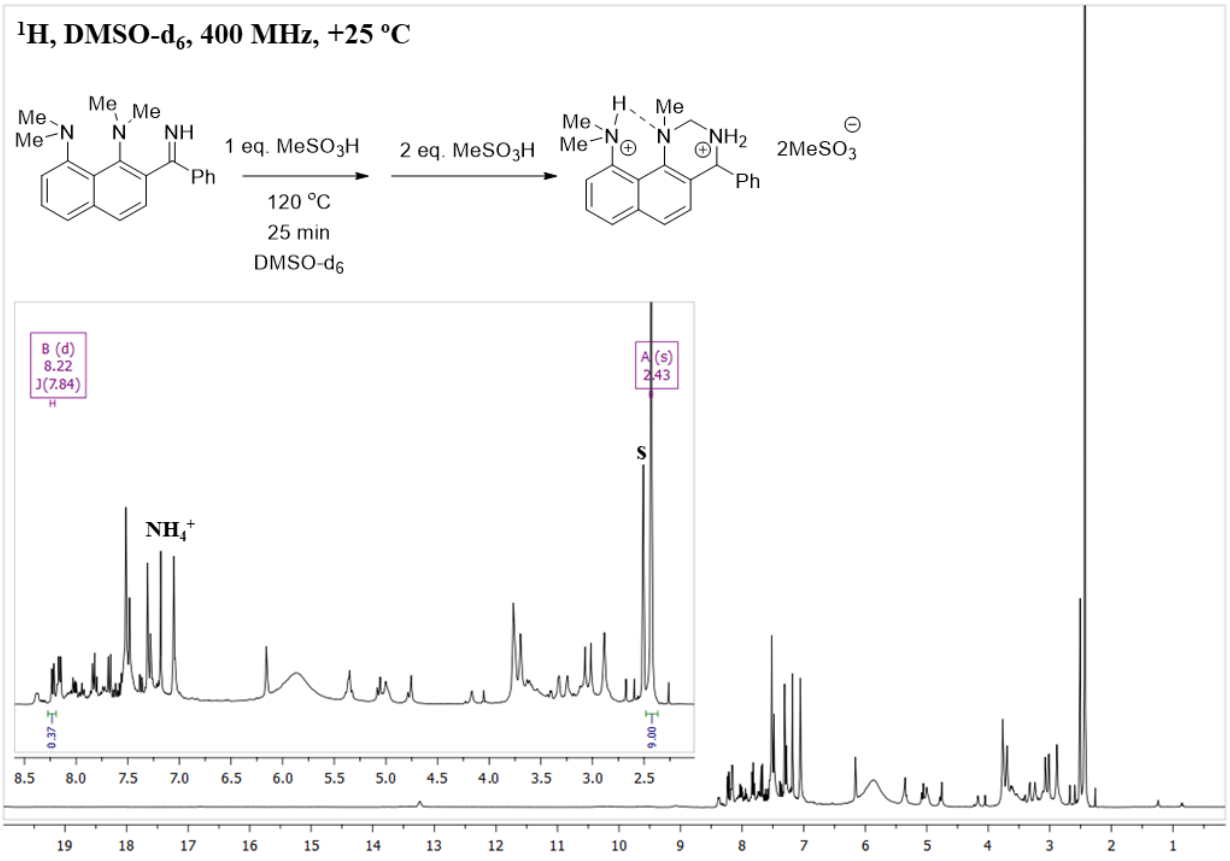

Figure S1. ^{1}H NMR spectrum of the reaction mixture for entry 1 (table 1).

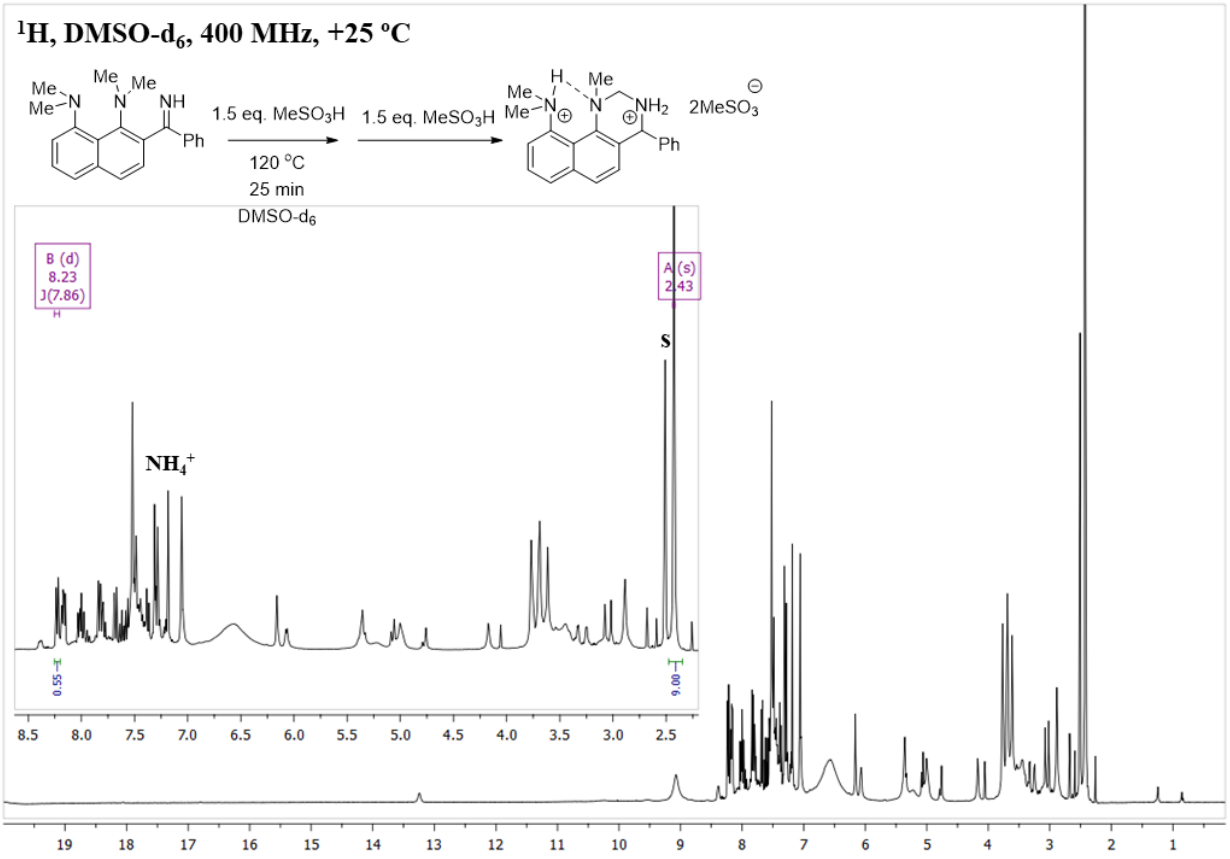

Figure S2. ^{1}H NMR spectrum of the reaction mixture for entry 2 (table 1).

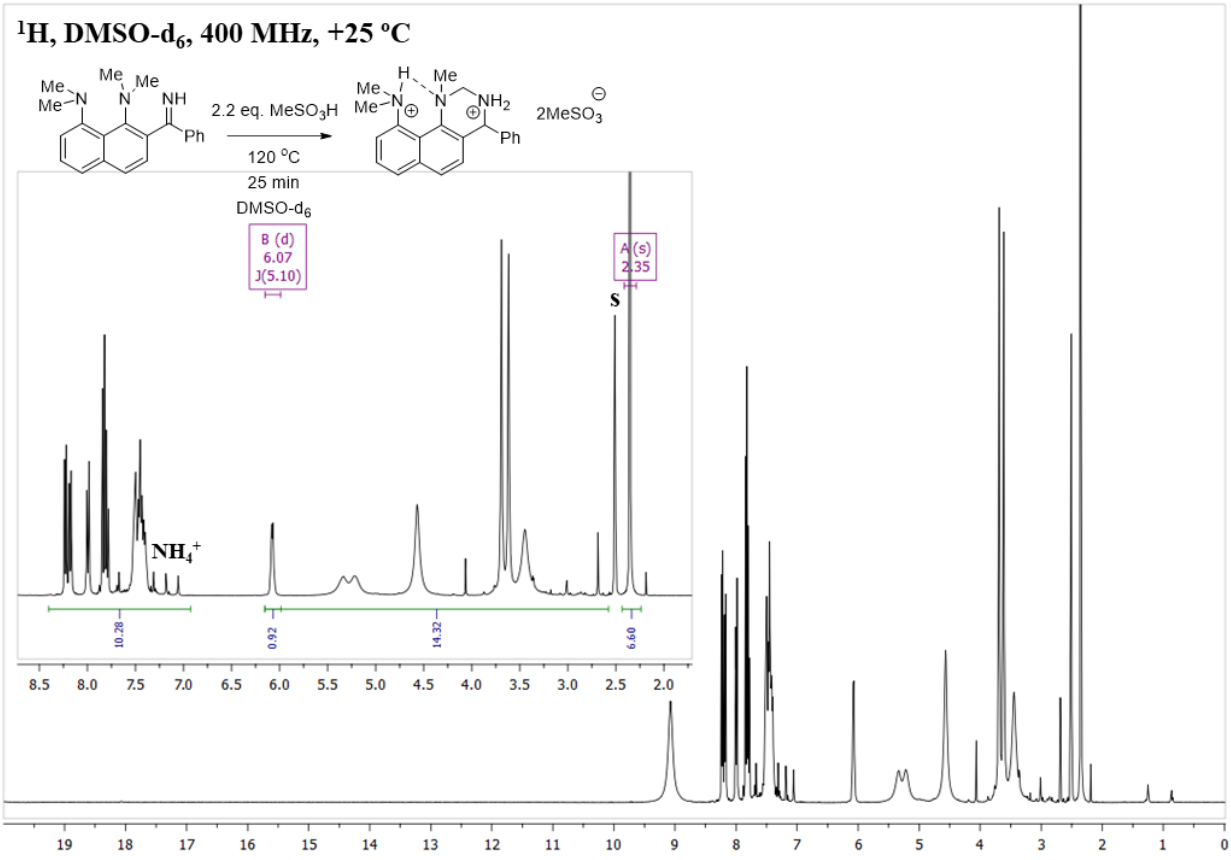

Figure S3. ^{1}H NMR spectrum of the reaction mixture for entry 3 (table 1).

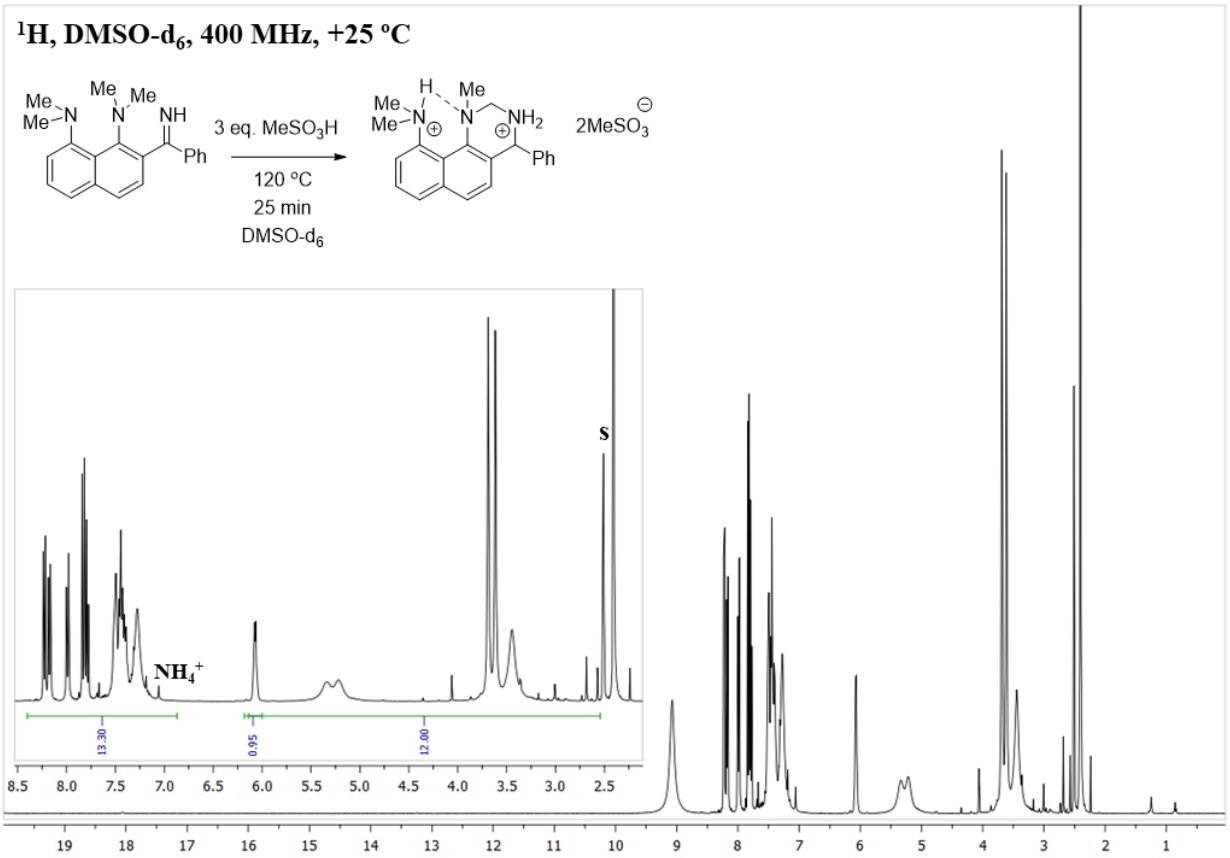

Figure S4. ^{1}H NMR spectrum of the reaction mixture for entry 4 (table 1).

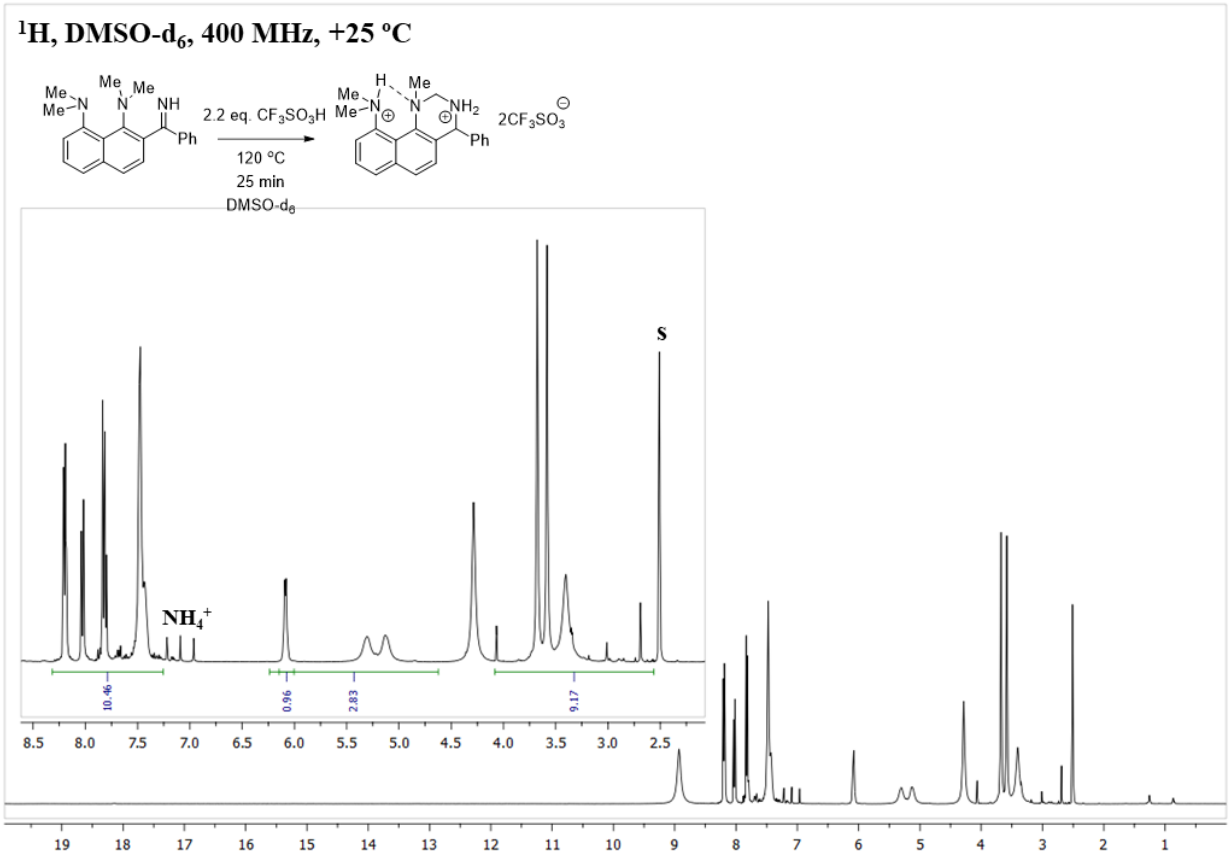

Figure S5. ^{1}H NMR spectrum of the reaction mixture for entry 5 (table 1).

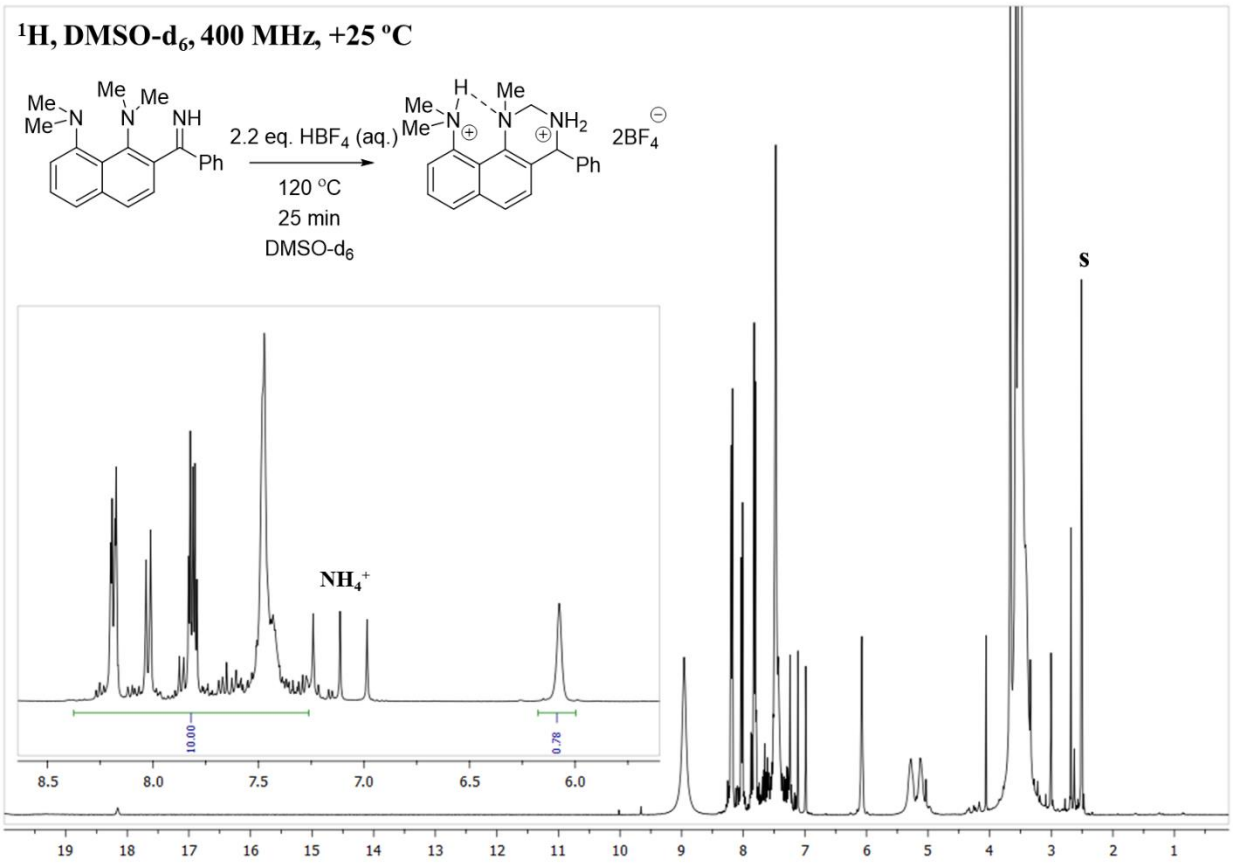

Figure S6. ^{1}H NMR spectrum of the reaction mixture for entry 6 (table 1).

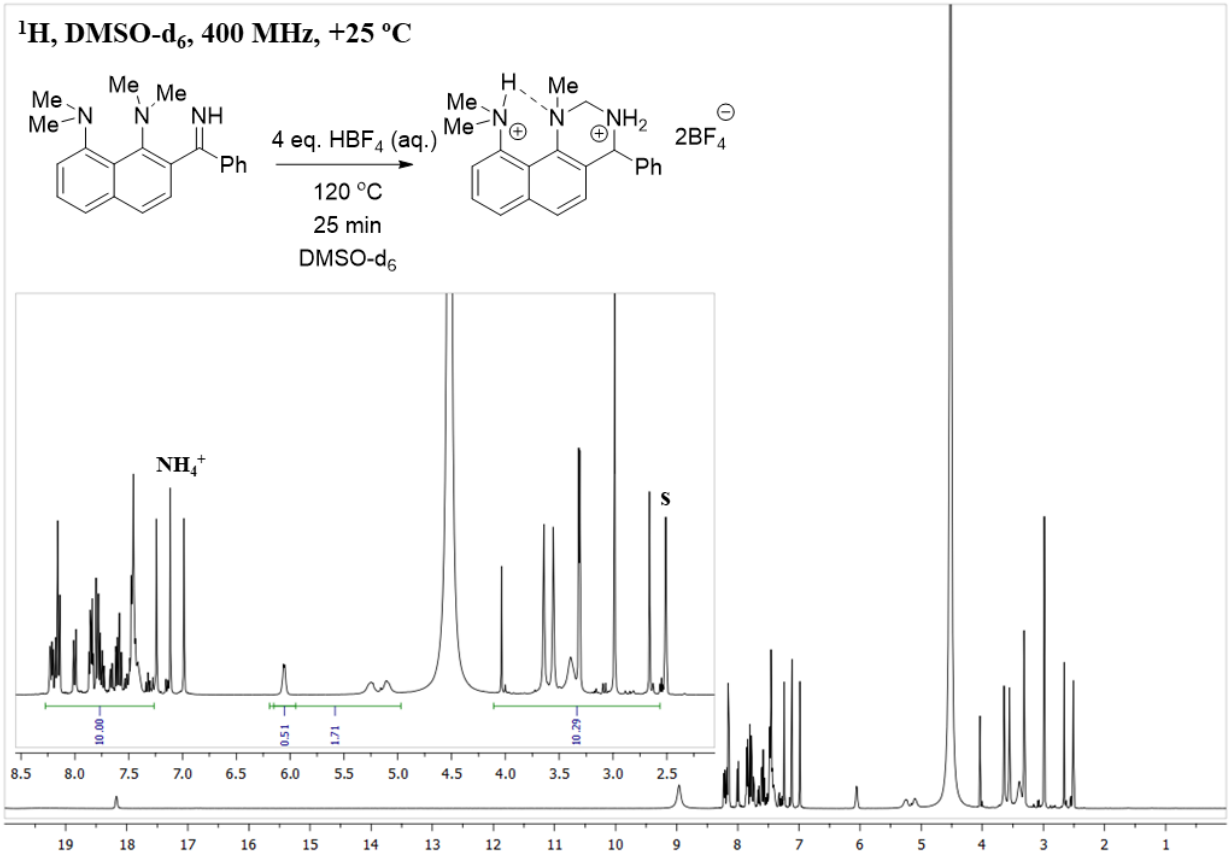

Figure S7. ^{1}H NMR spectrum of the reaction mixture for entry 7 (table 1).

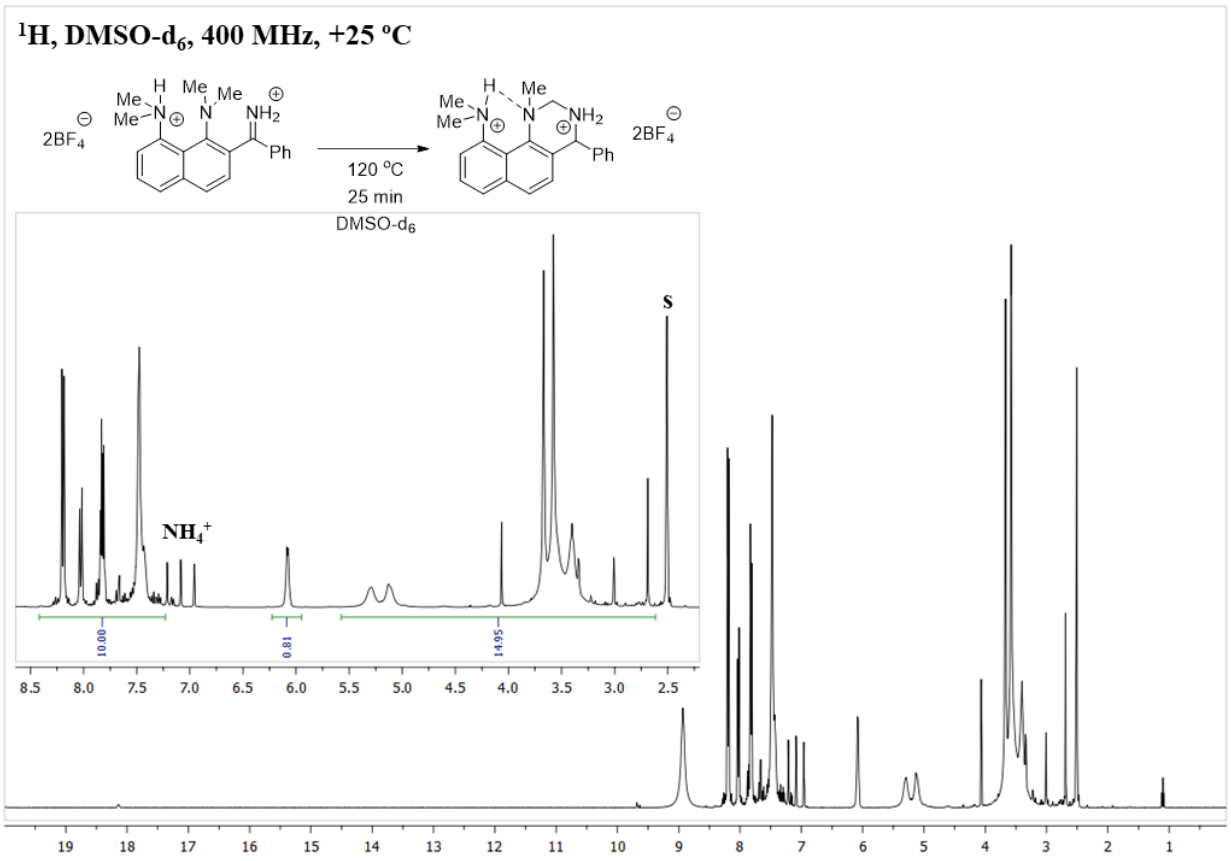

Figure S8. ^{1}H NMR spectrum of the reaction mixture for entry 8 (table 1).

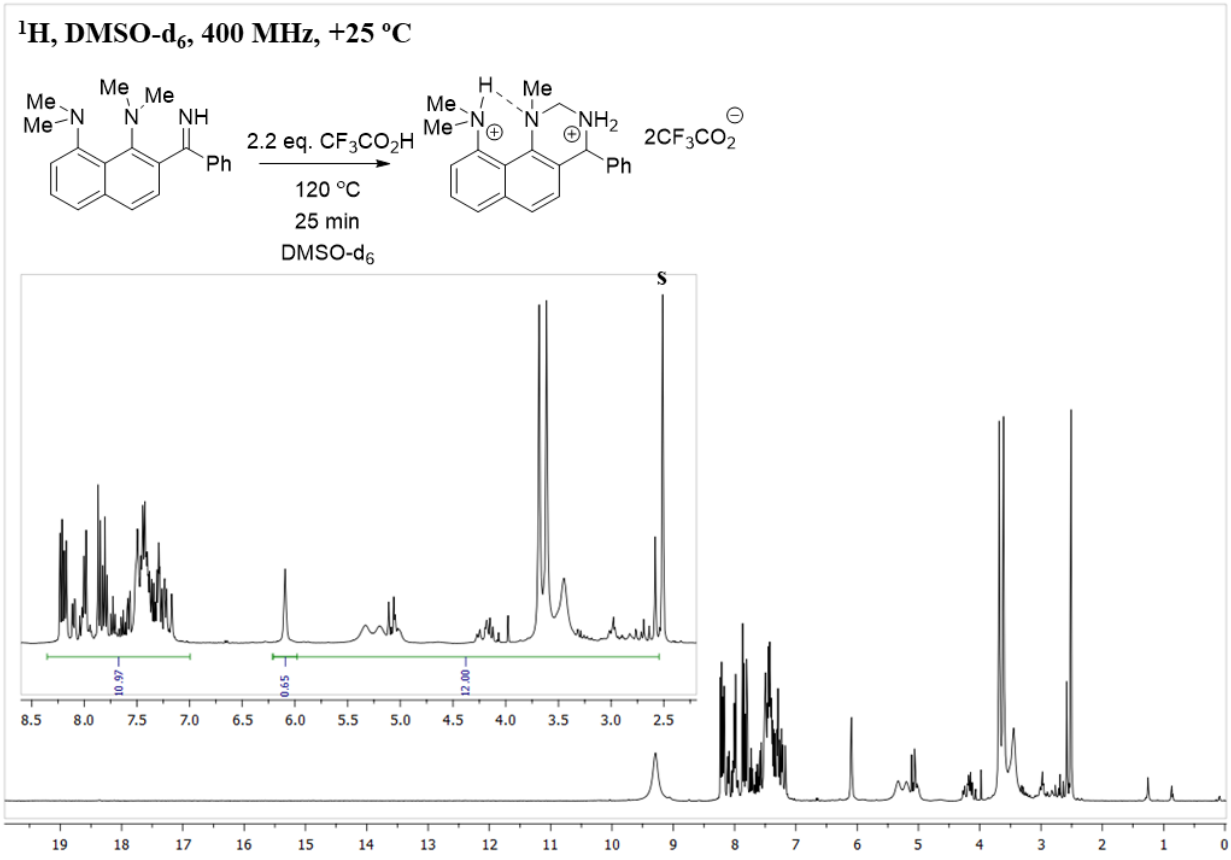

Figure S. ^{1}H NMR spectrum of the reaction mixture for entry 9 (table 1).

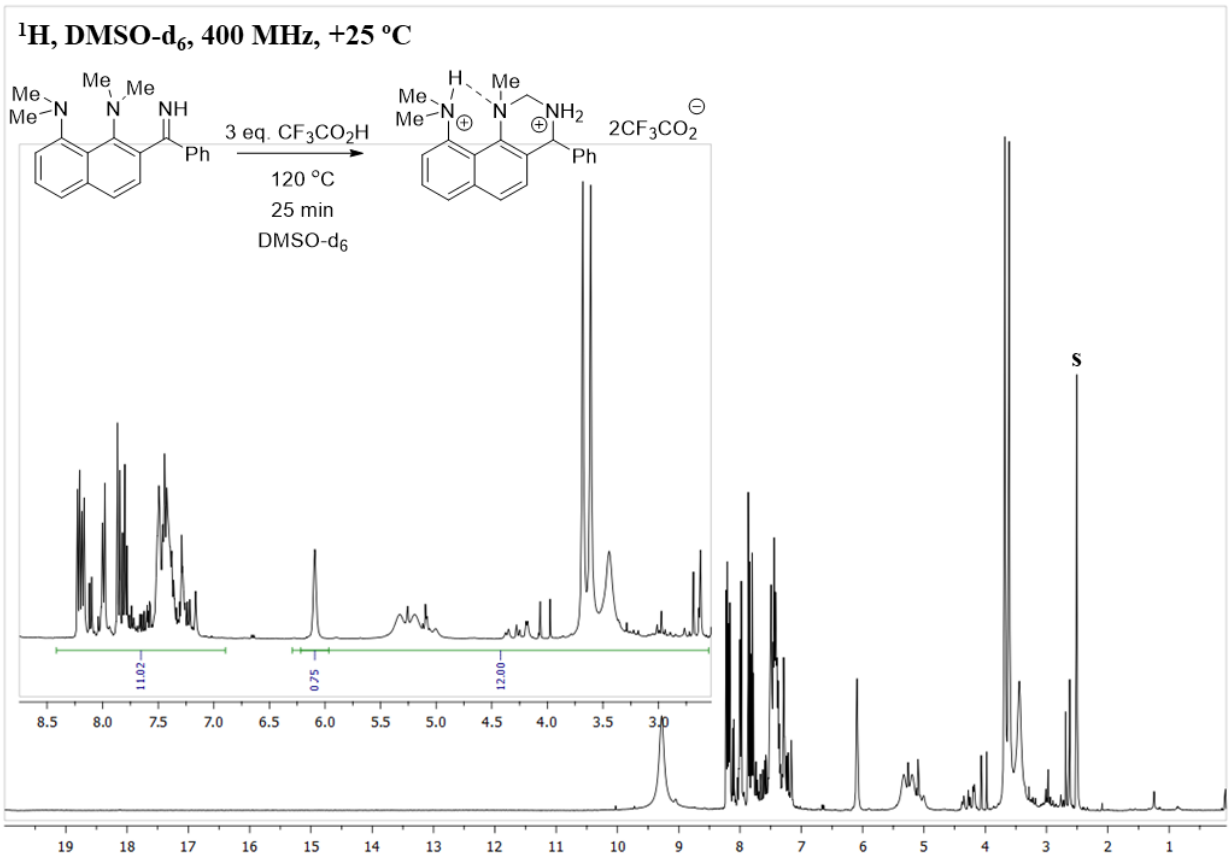

Figure S10. ^{1}H NMR spectrum of the reaction mixture for entry 10 (table 1).

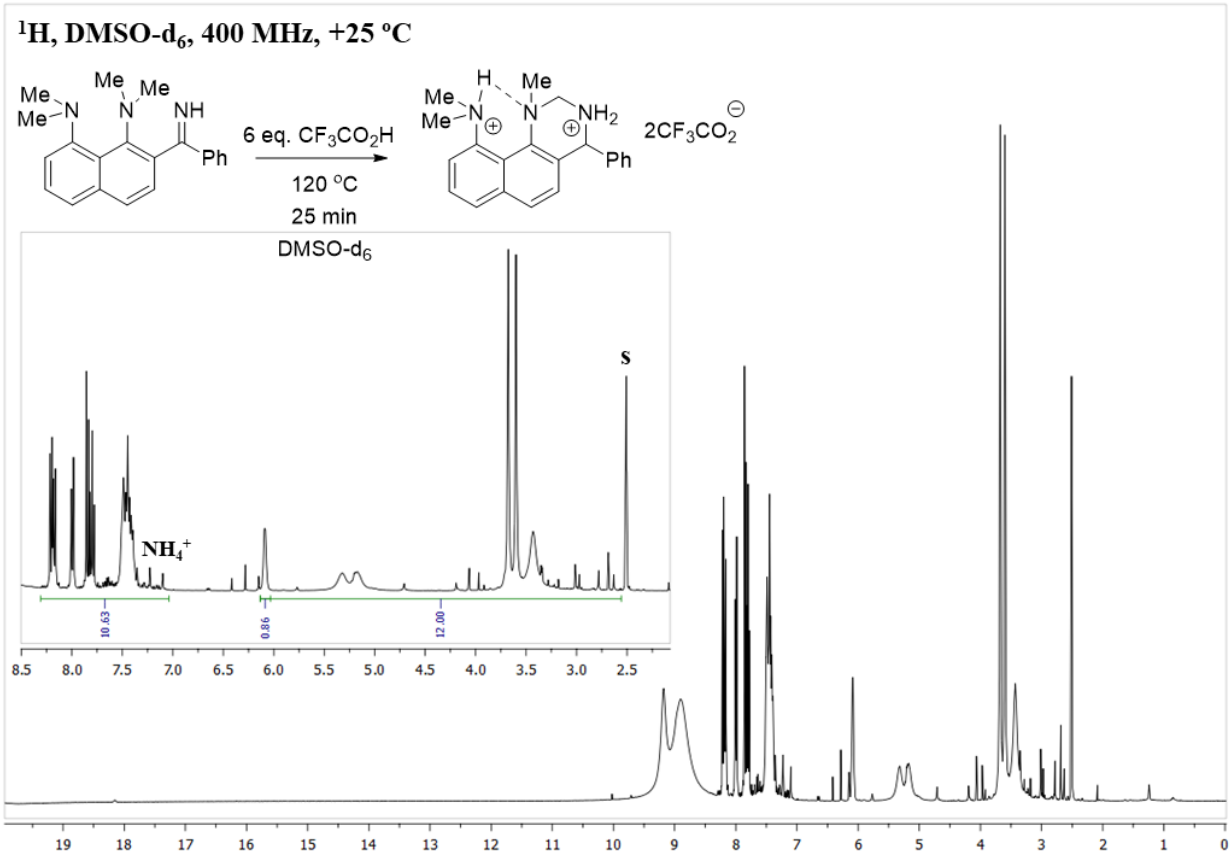

Figure S11. ^{1}H NMR spectrum of the reaction mixture for entry 11 (table 1).

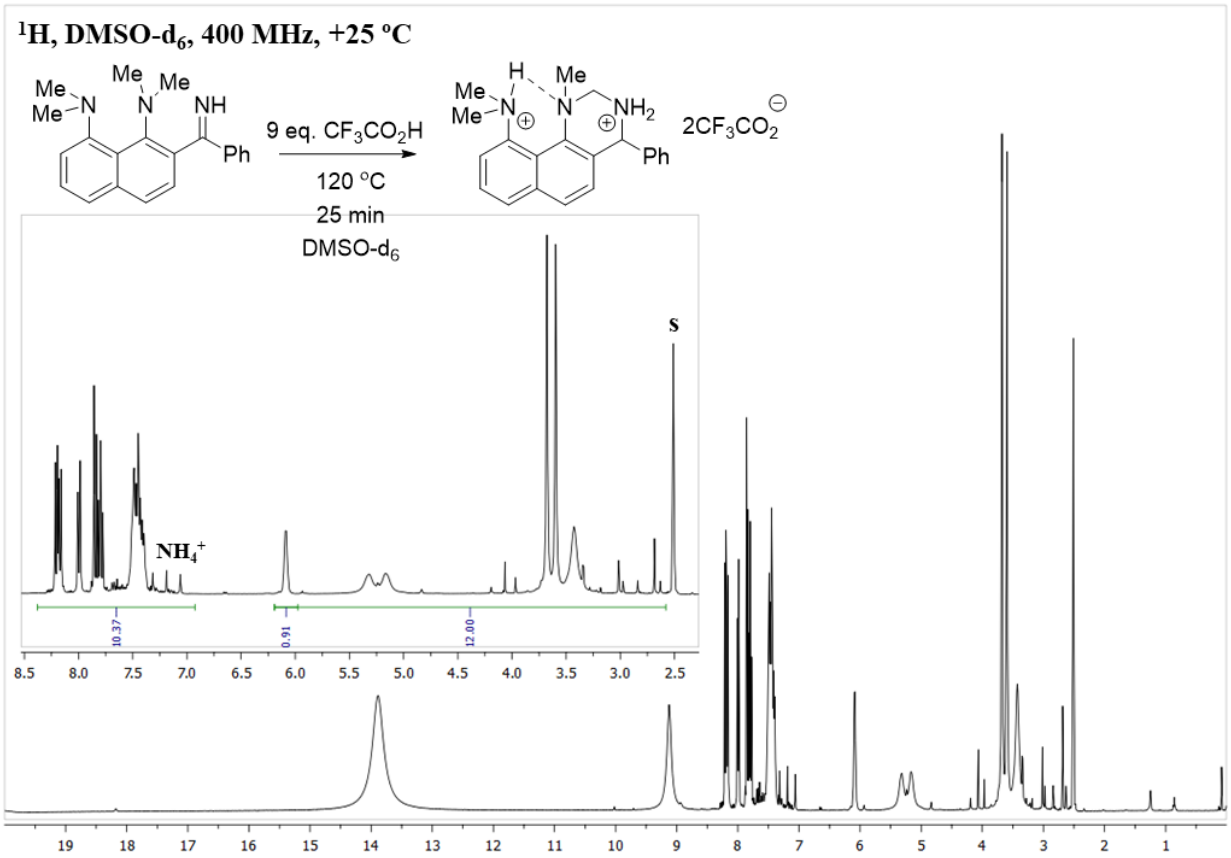

Figure S12. ^{1}H NMR spectrum of the reaction mixture for entry 12 (table 1).

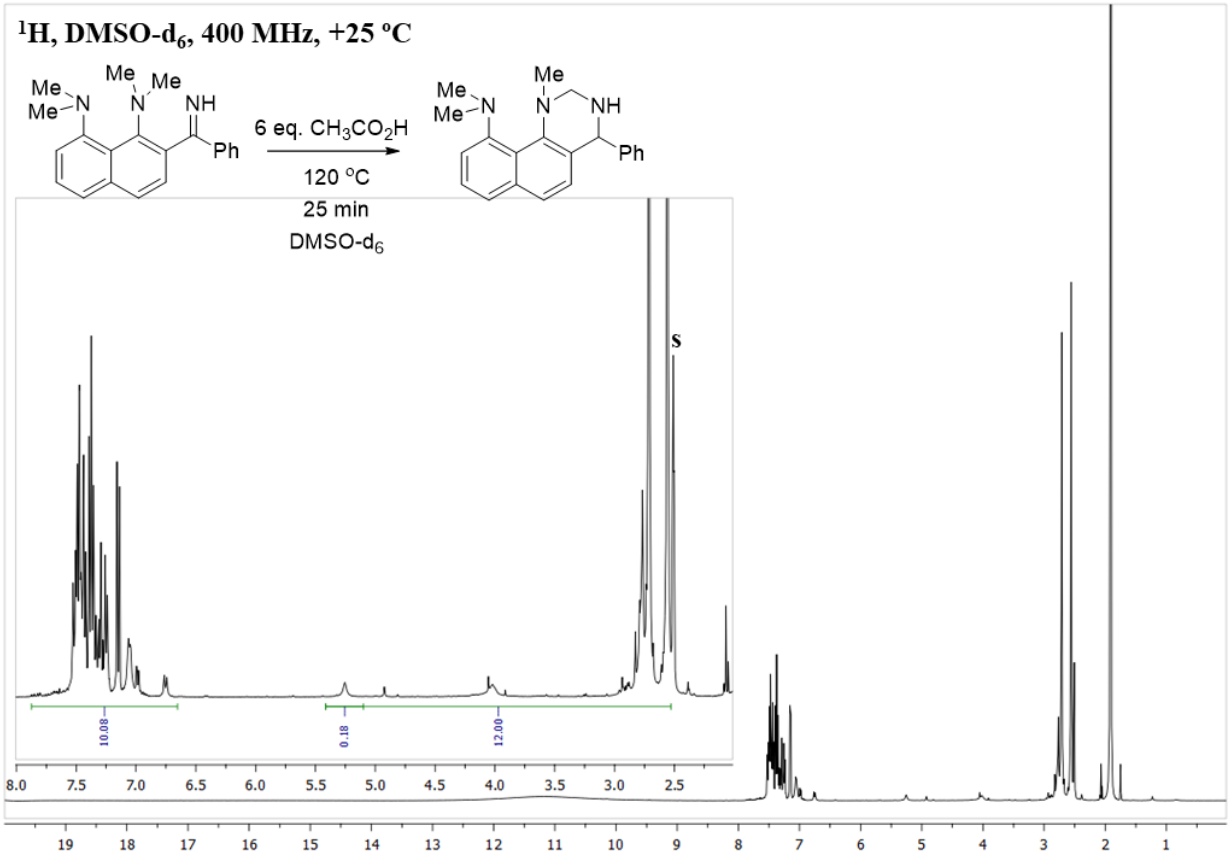

Figure S13. ^{1}H NMR spectrum of the reaction mixture for entry 13 (table 1).

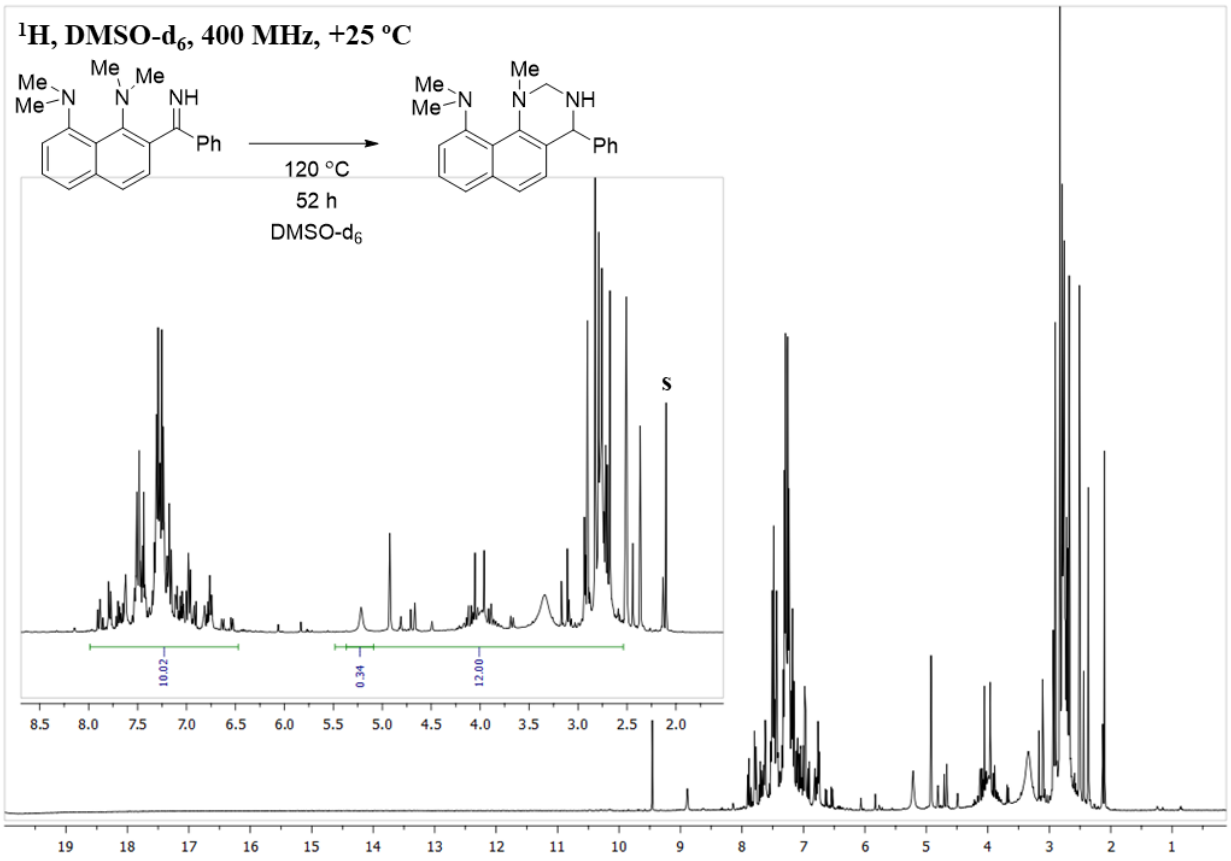

Figure S14. ^{1}H NMR spectrum of the reaction mixture for entry 14 (table 1).

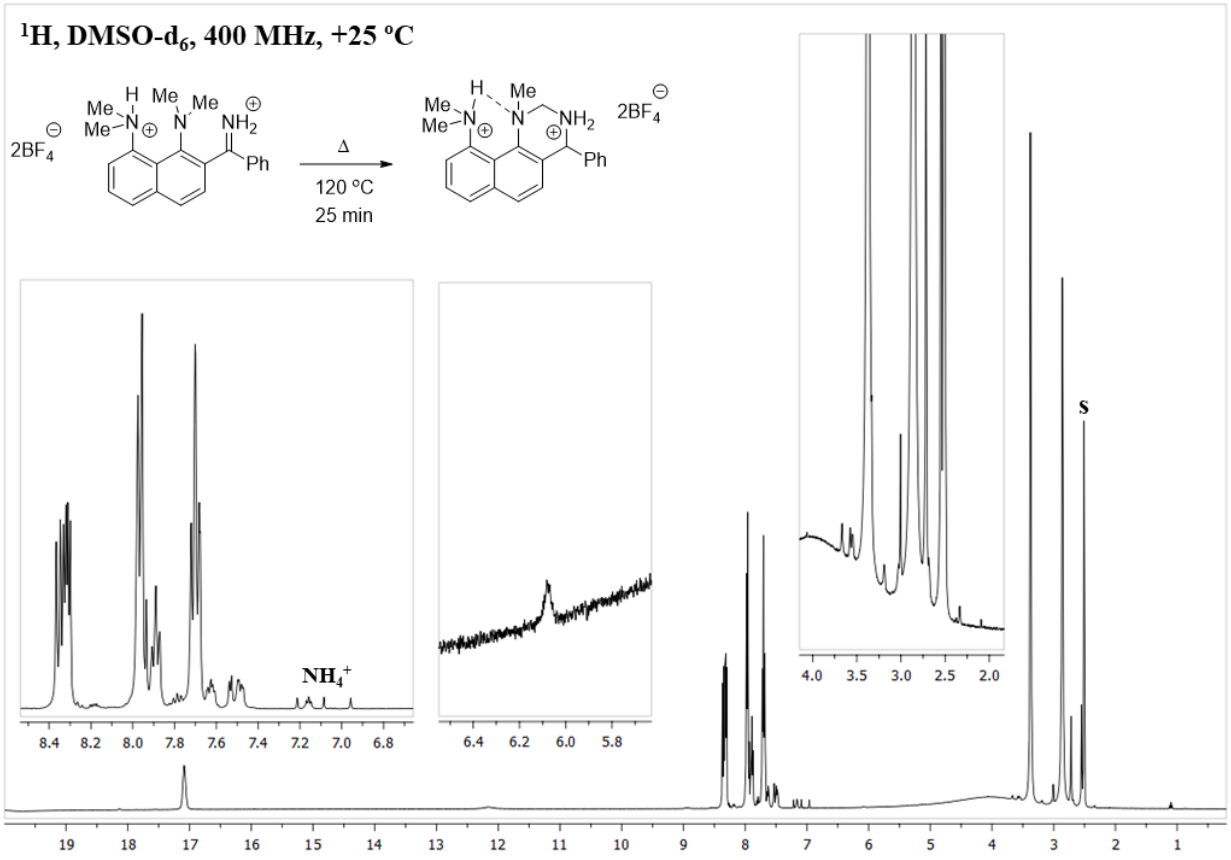

Figure S15. ^{1}H NMR spectrum of the reaction mixture for entry 15 (table 1).

NMR spectra of protonated 1,8-bis(dimethylamino)naphtalene *ortho*-ketimines

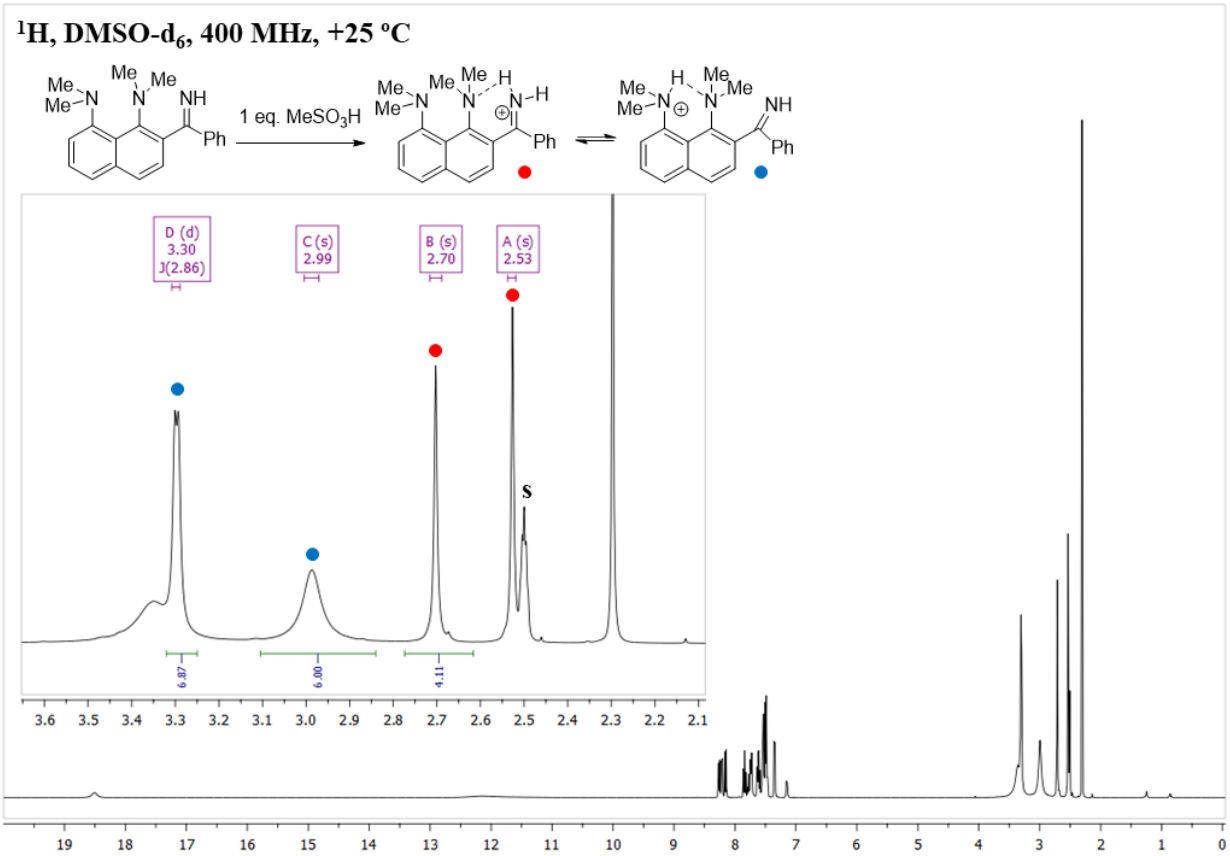

Figure S16. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

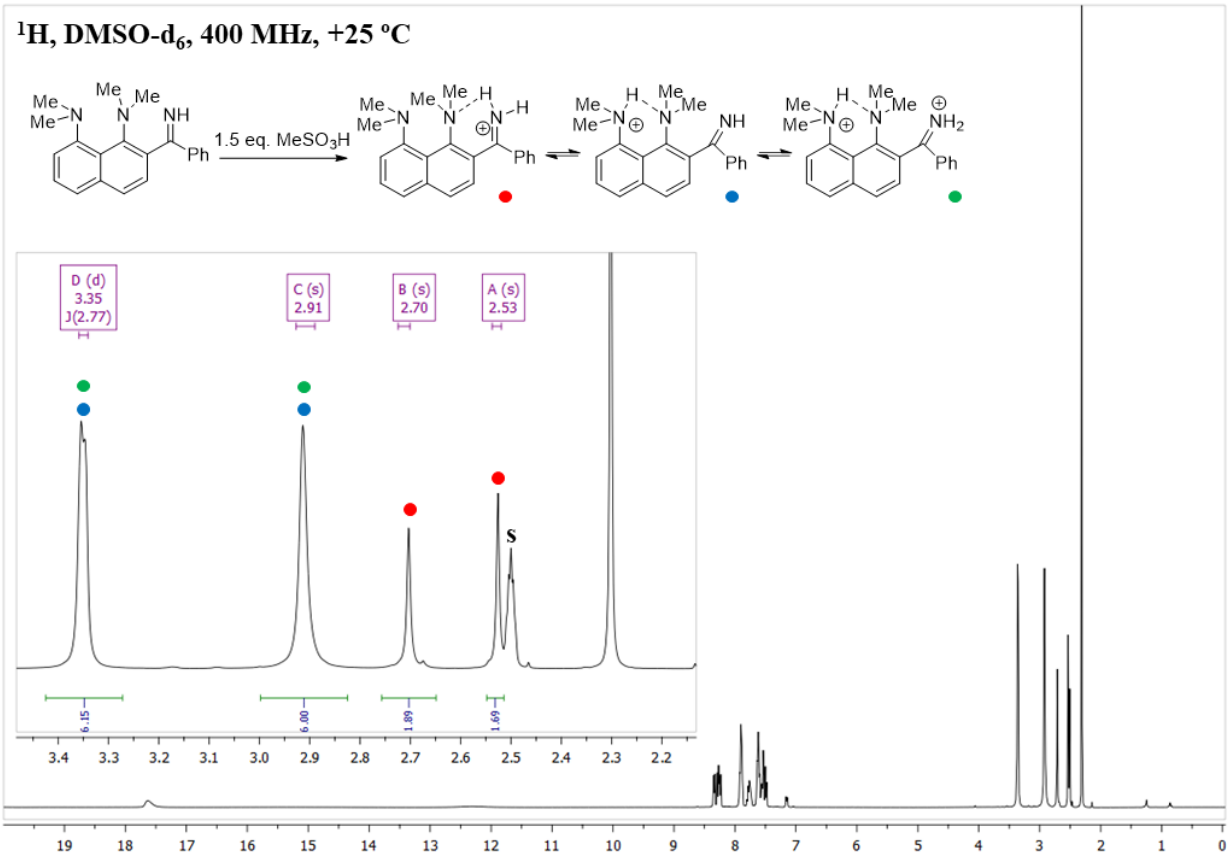

Figure S17. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

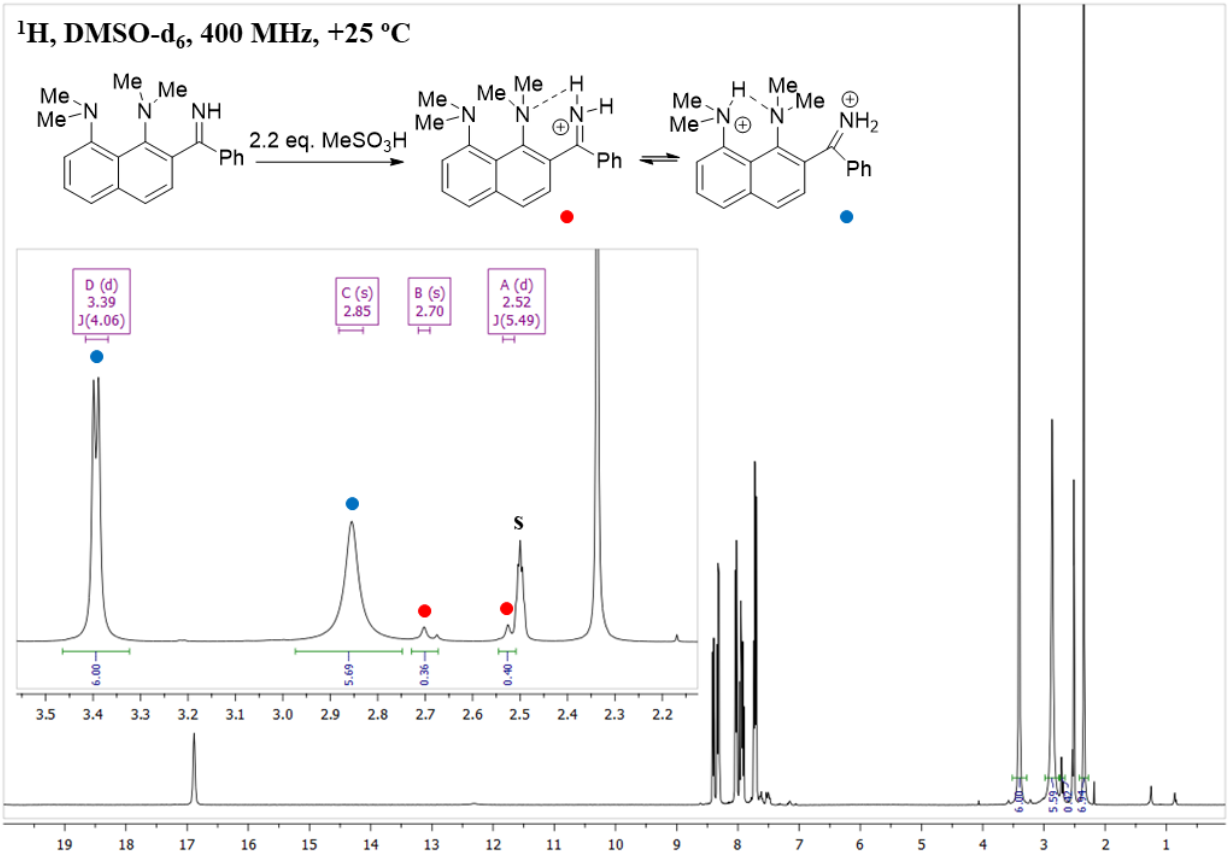

Figure S18. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

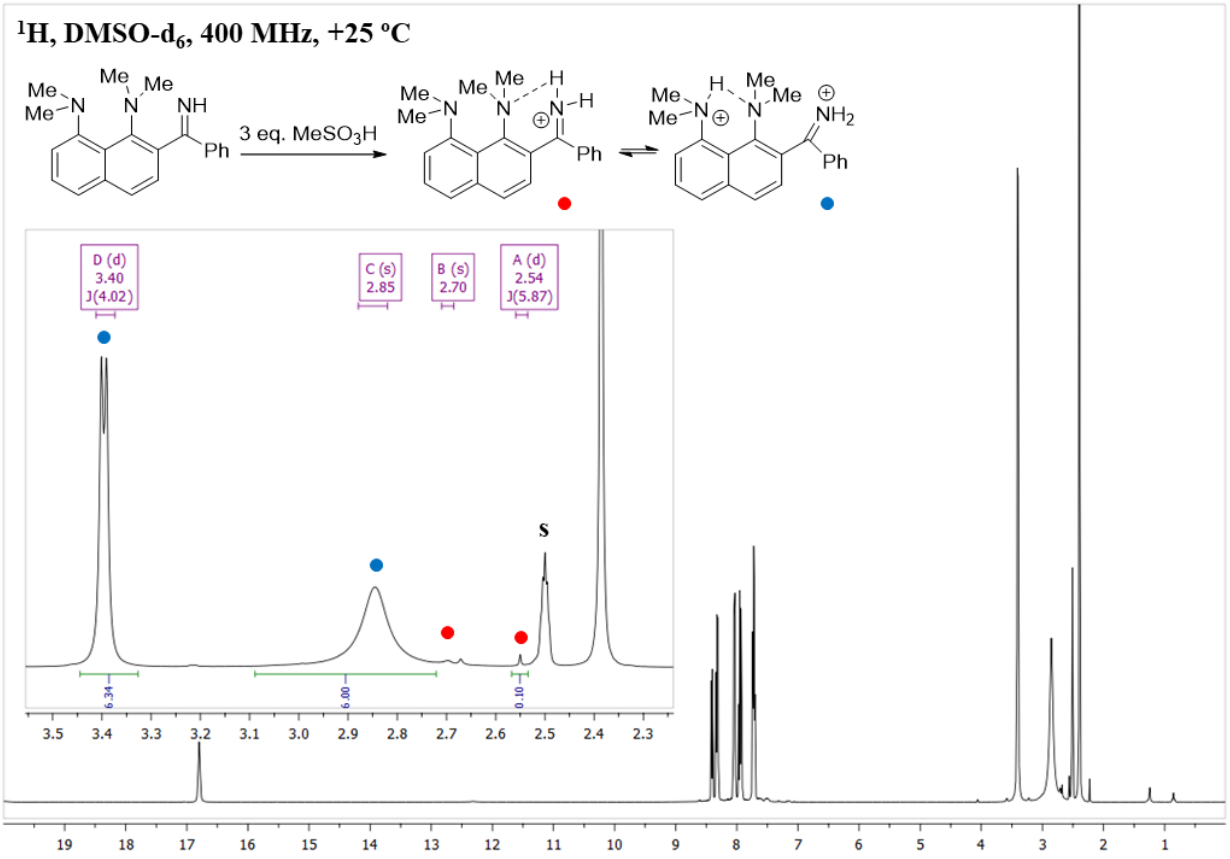

Figure S19. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

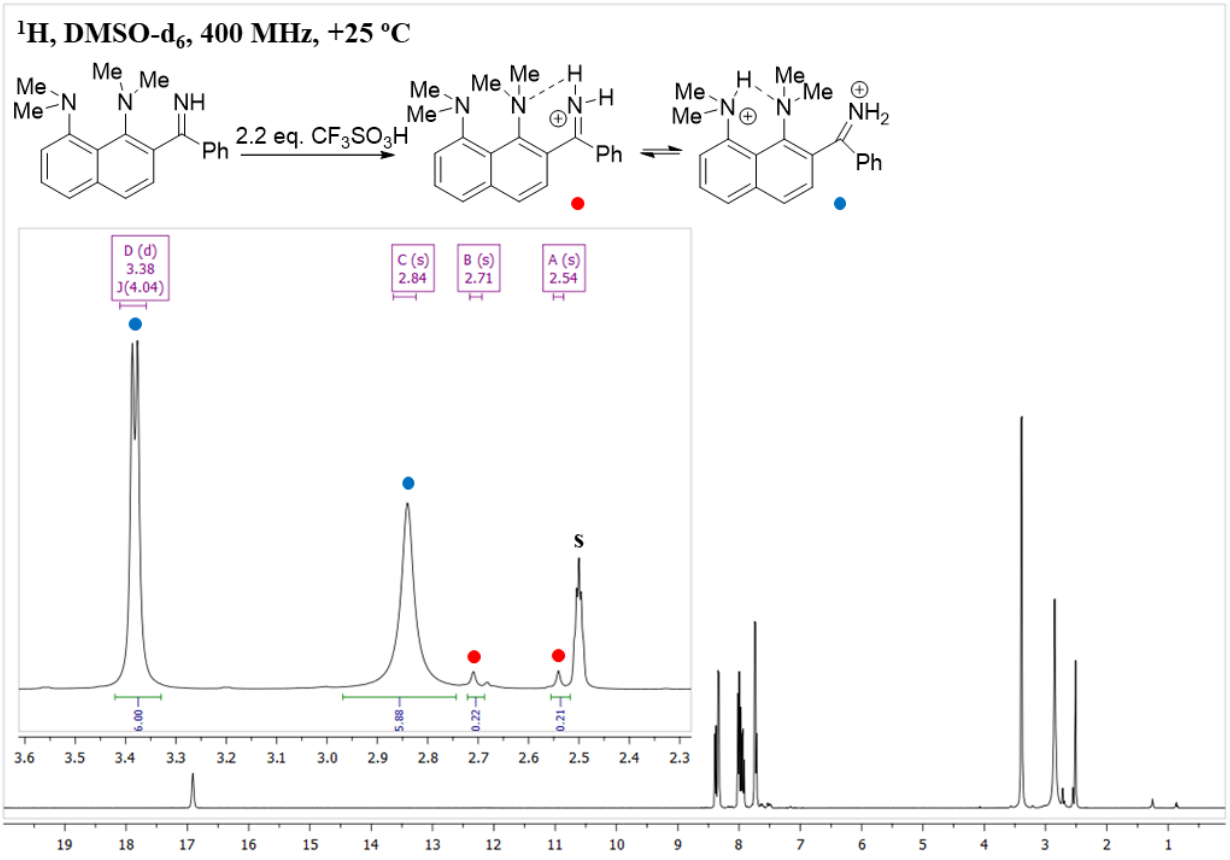

Figure S20. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

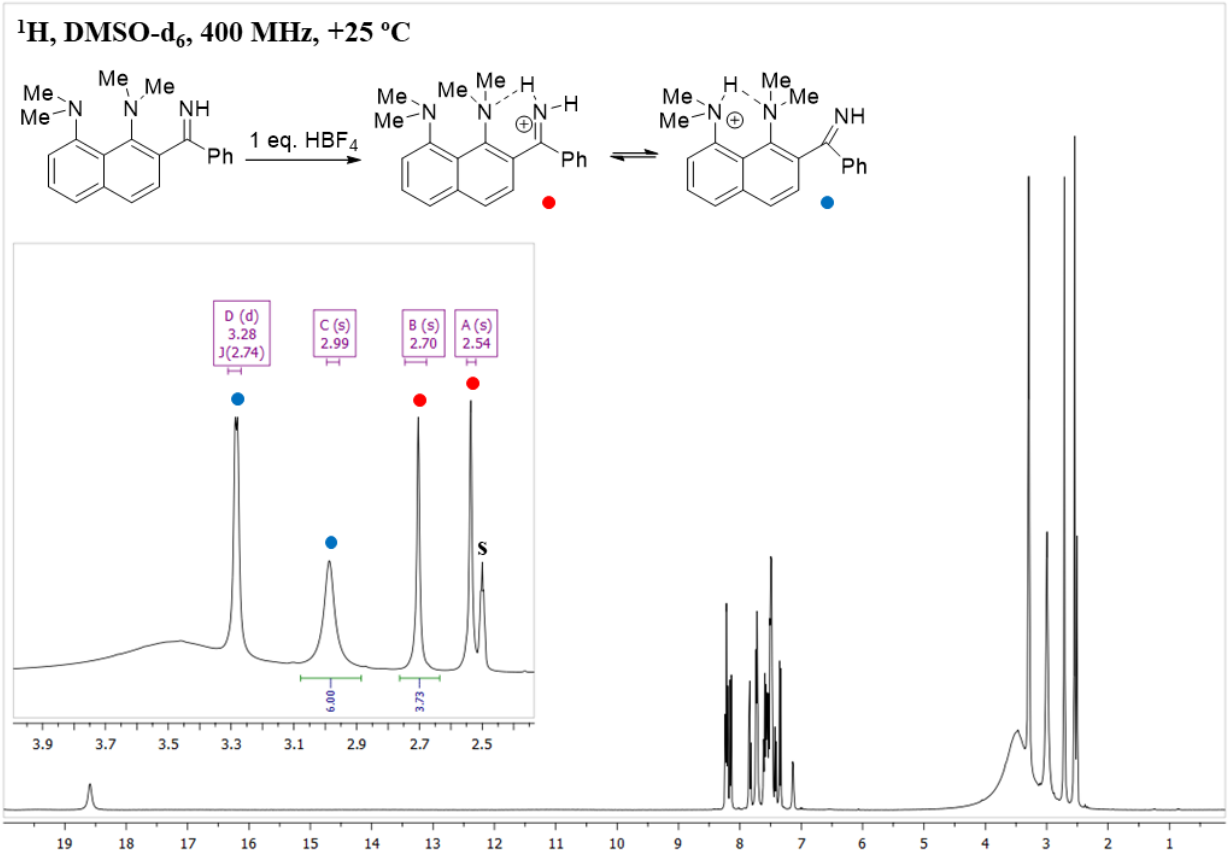

Figure S21. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

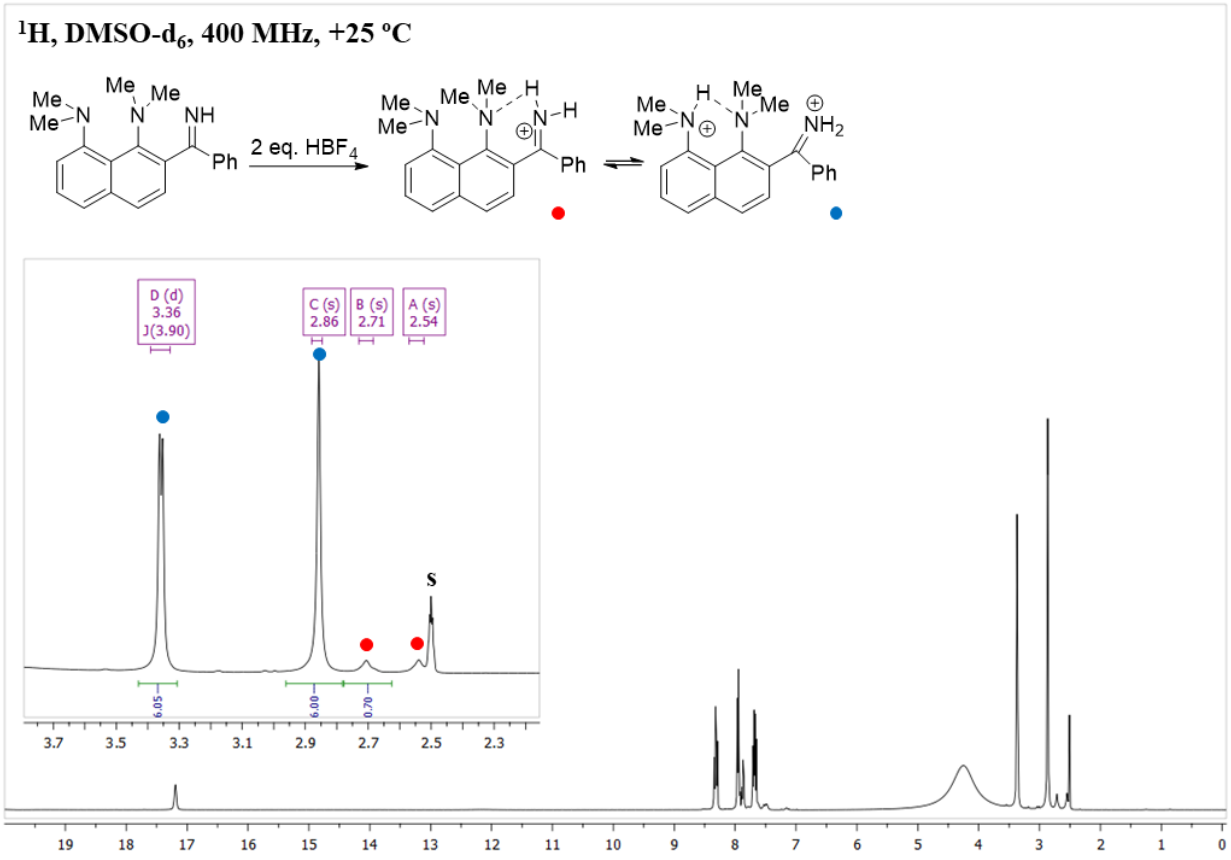

Figure S22. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

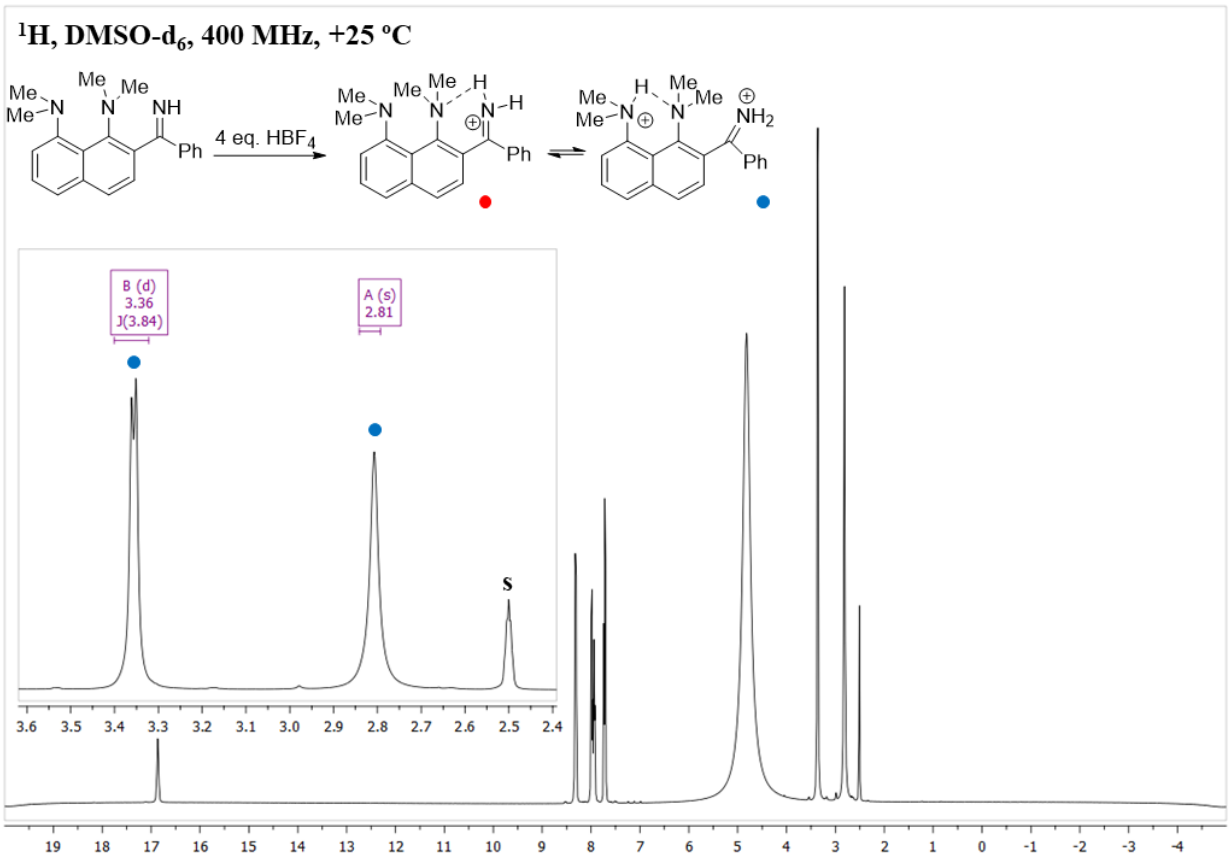

Figure S23. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

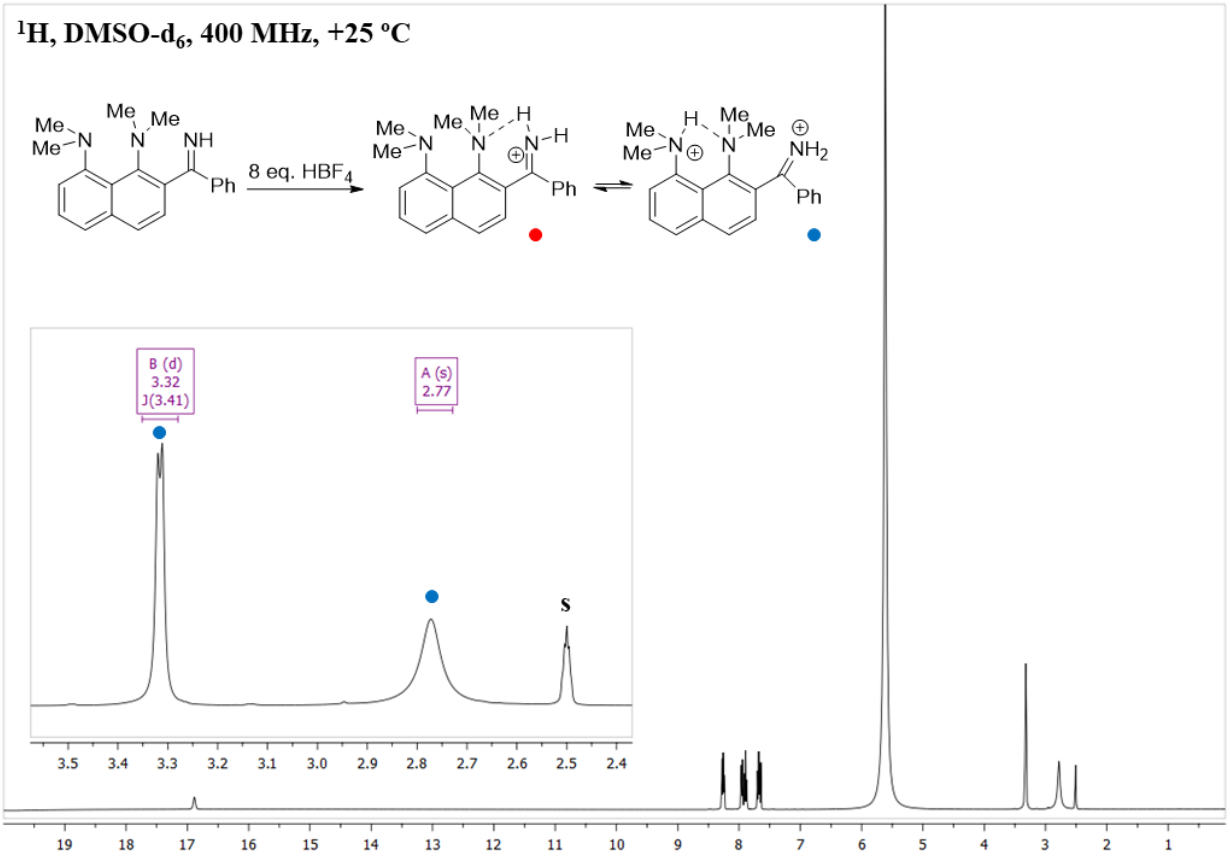

Figure S24. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

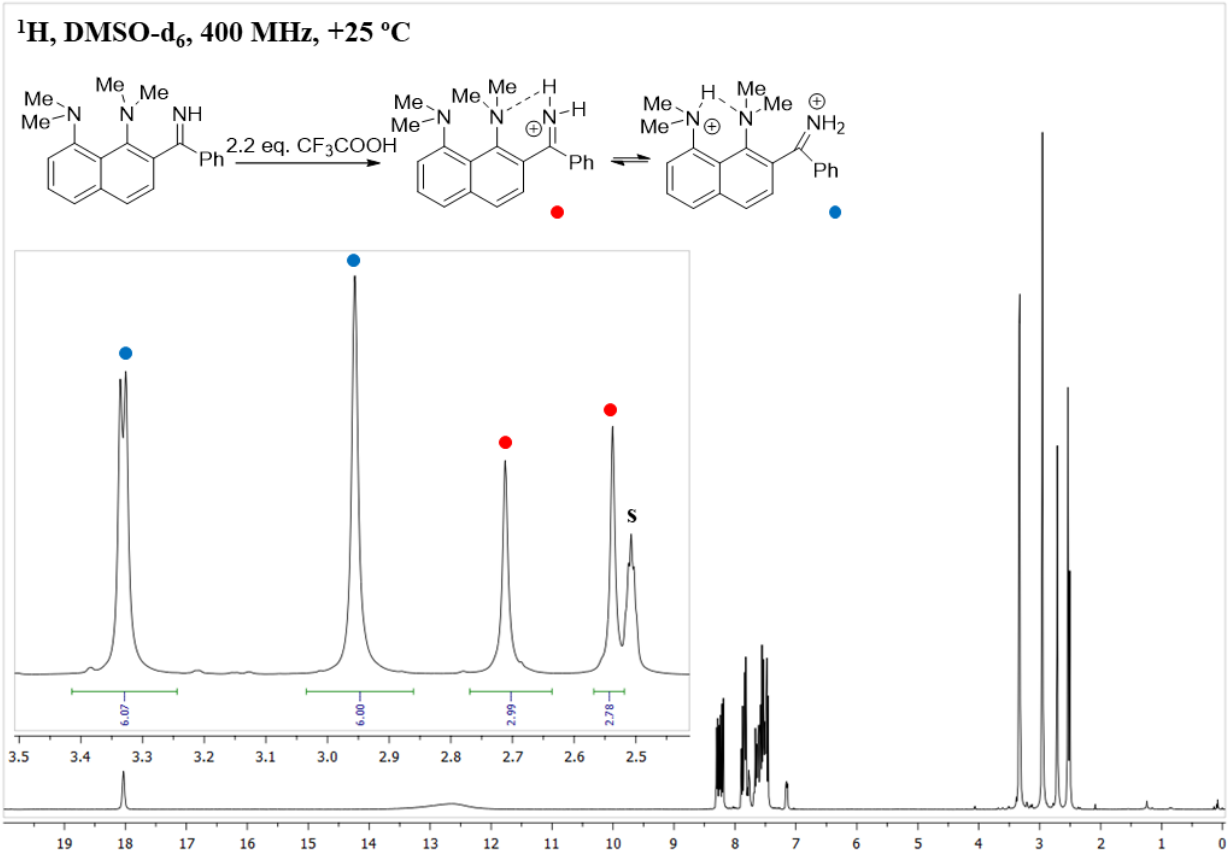

Figure S25. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

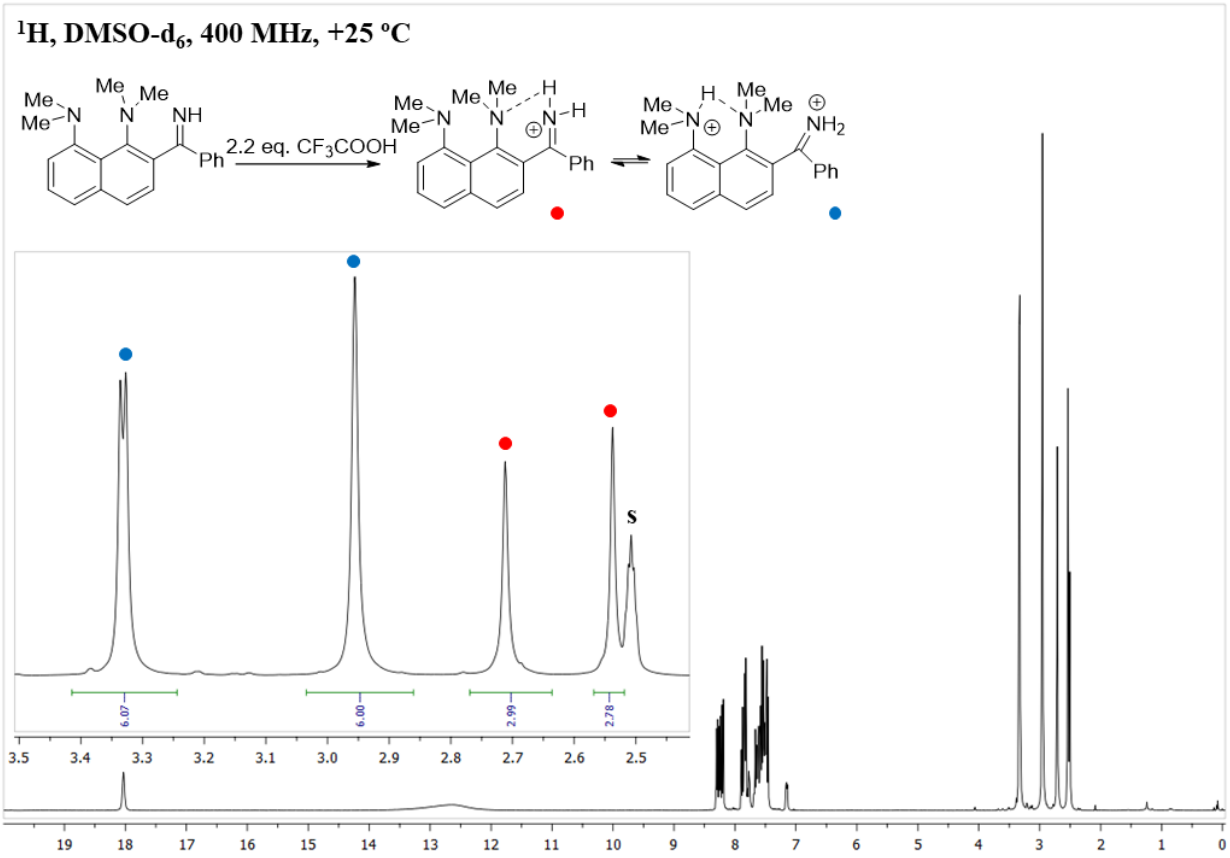

Figure S26. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

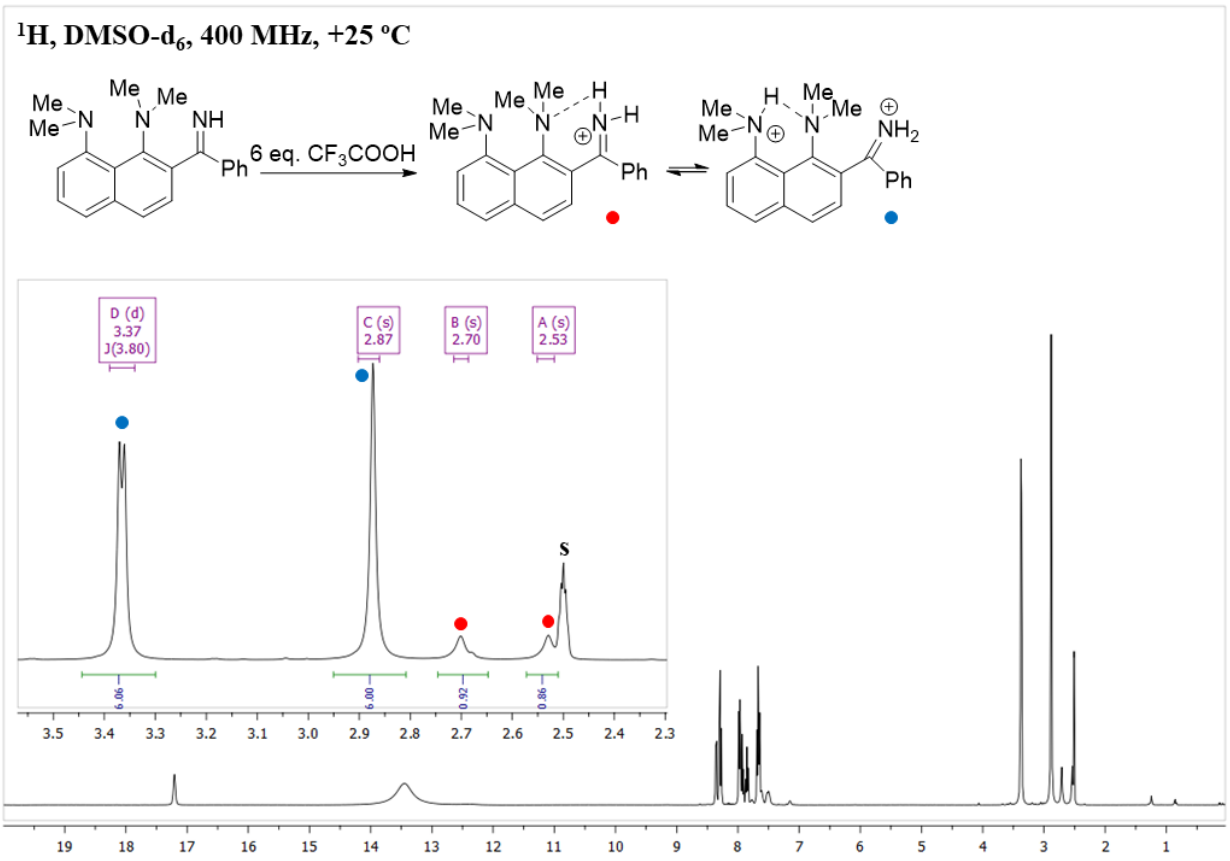

Figure S27. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

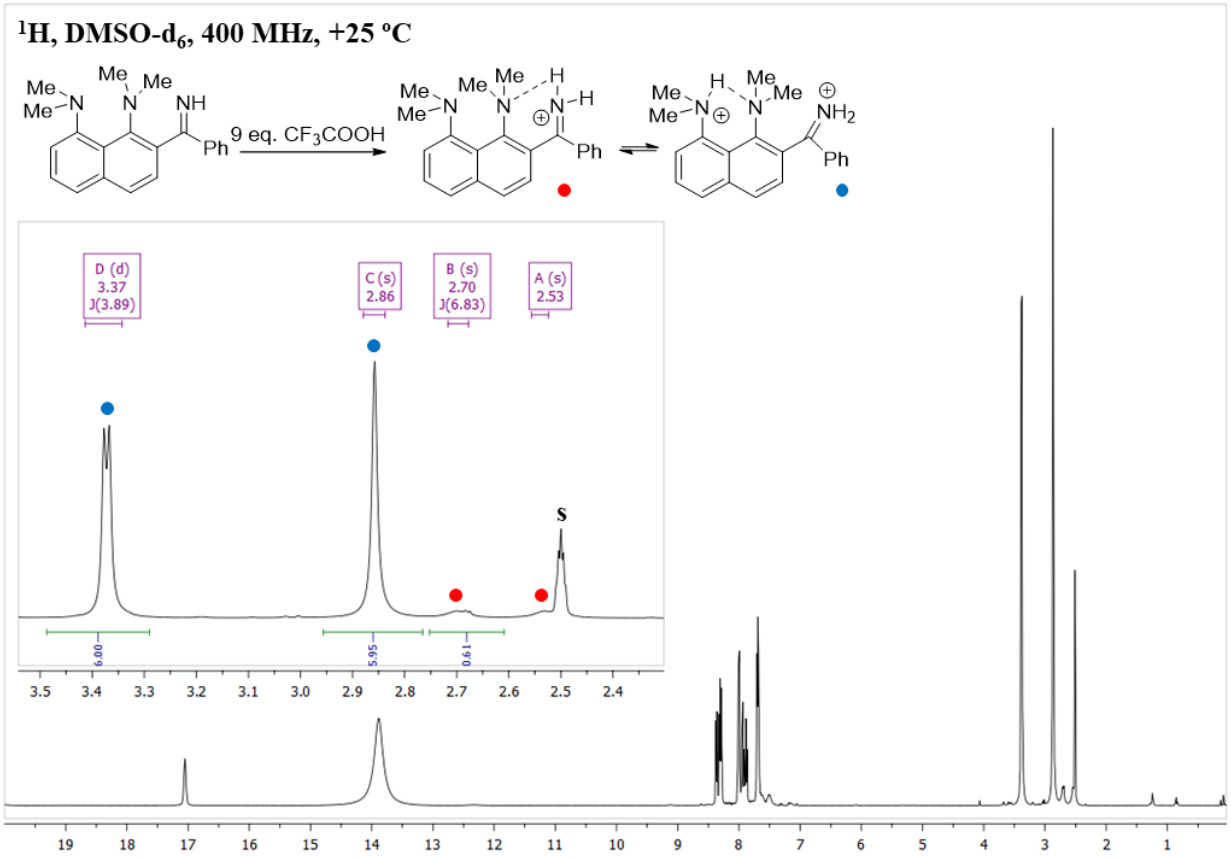

Figure S28. ^{1}H NMR spectrum of the protonated *ortho*-ketimine **7a**.

Compounds NMR spectra

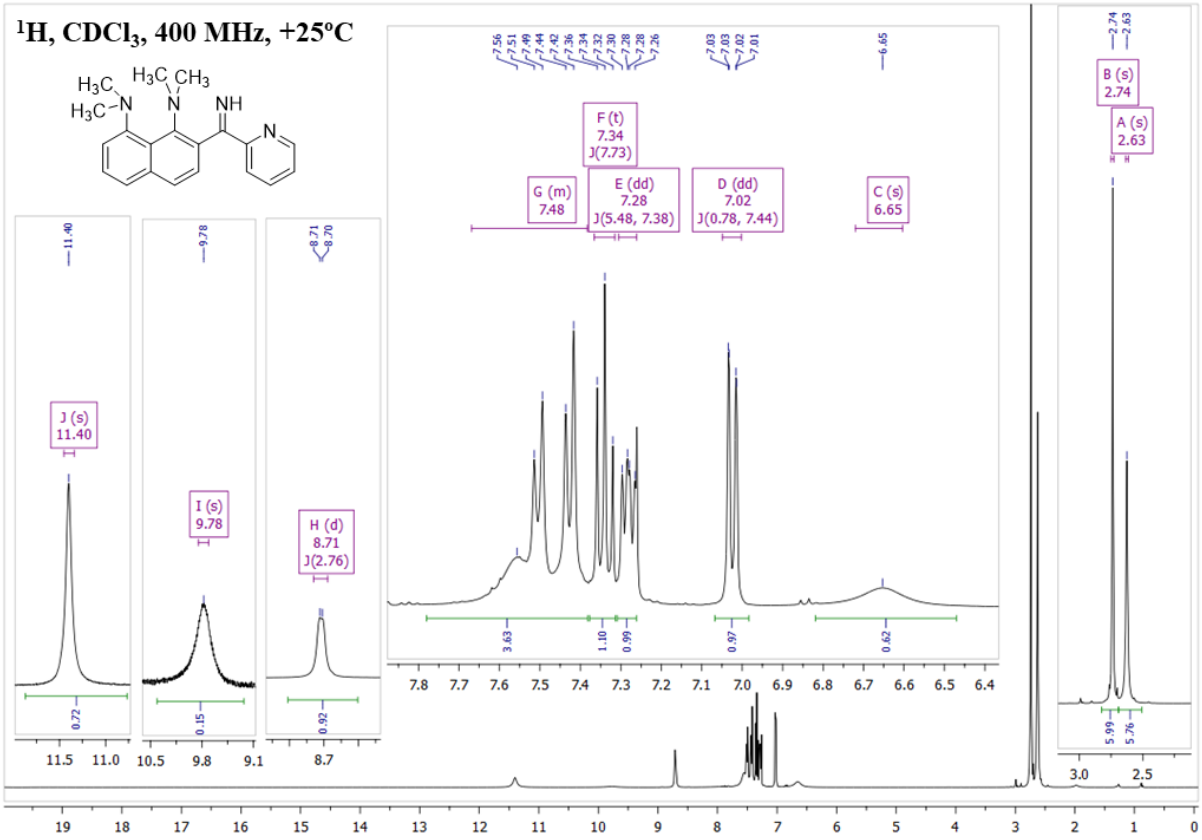

Figure S29. ^{1}H NMR spectrum of **7h**.

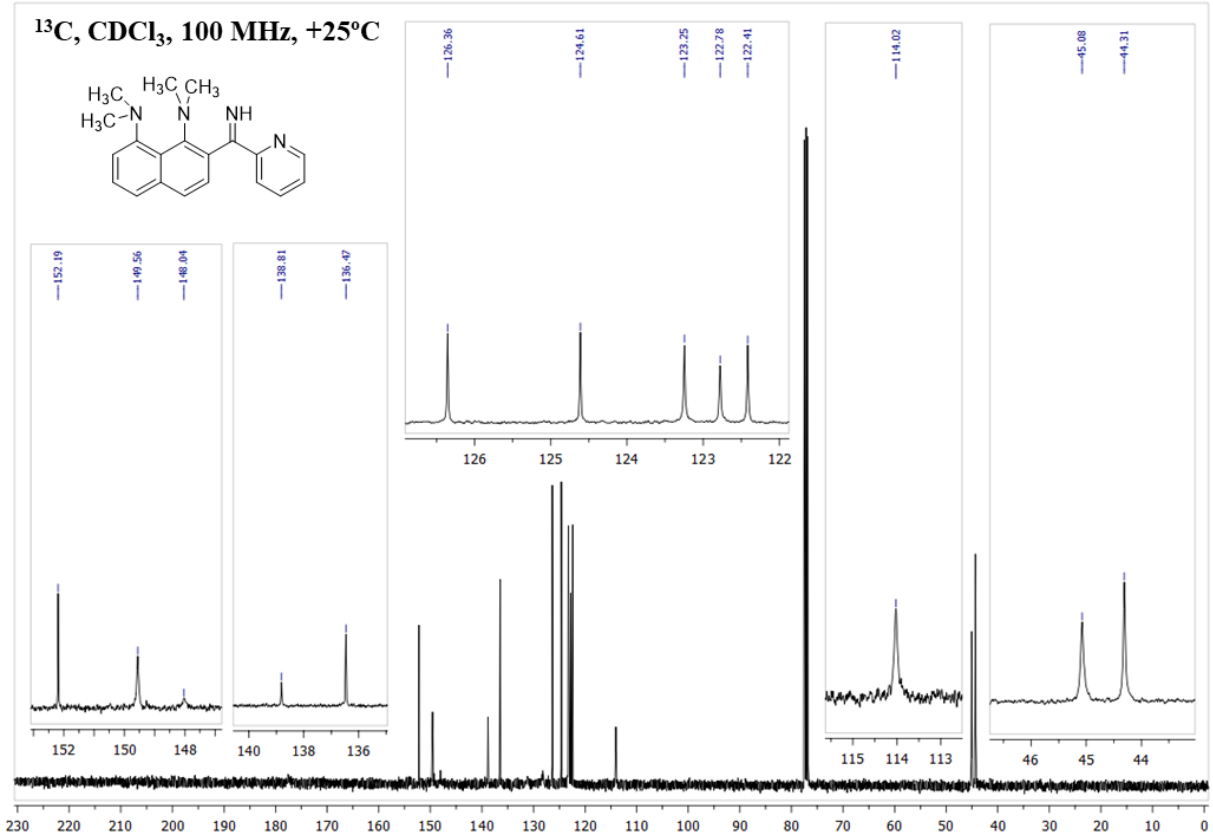

Figure S30. ^{13}C NMR spectrum of **7h**.

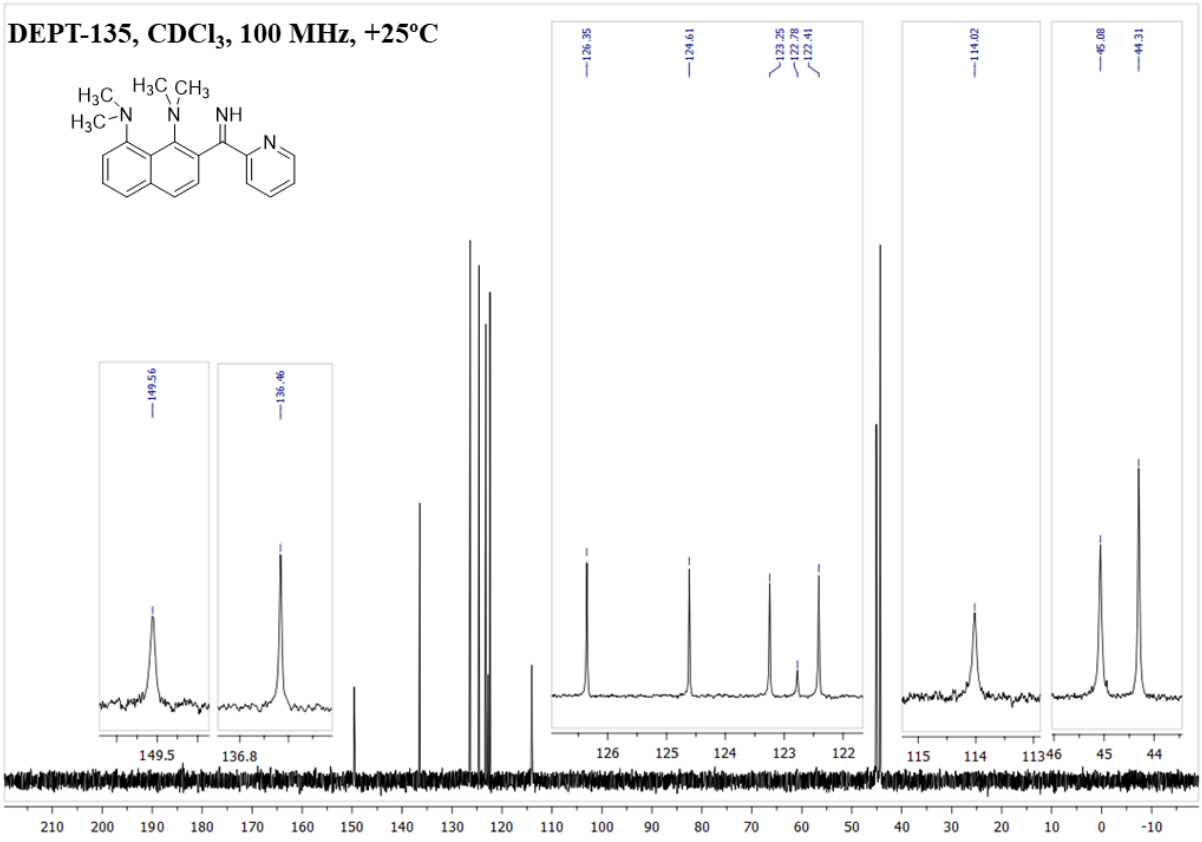

Figure S31. ^{13}C DEPT NMR spectrum of **7h**.

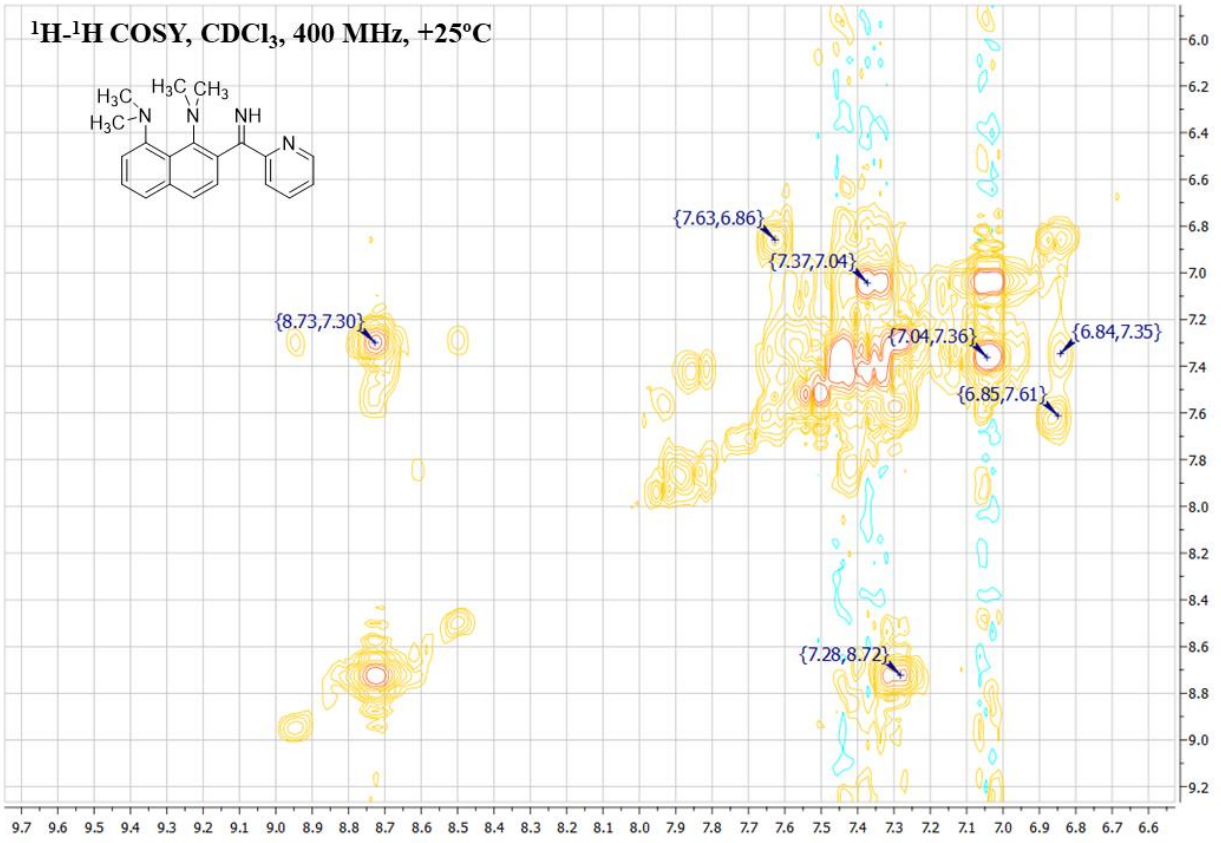

Figure S32. ^{1}H-^{1}H COSY NMR spectrum of **7h**.

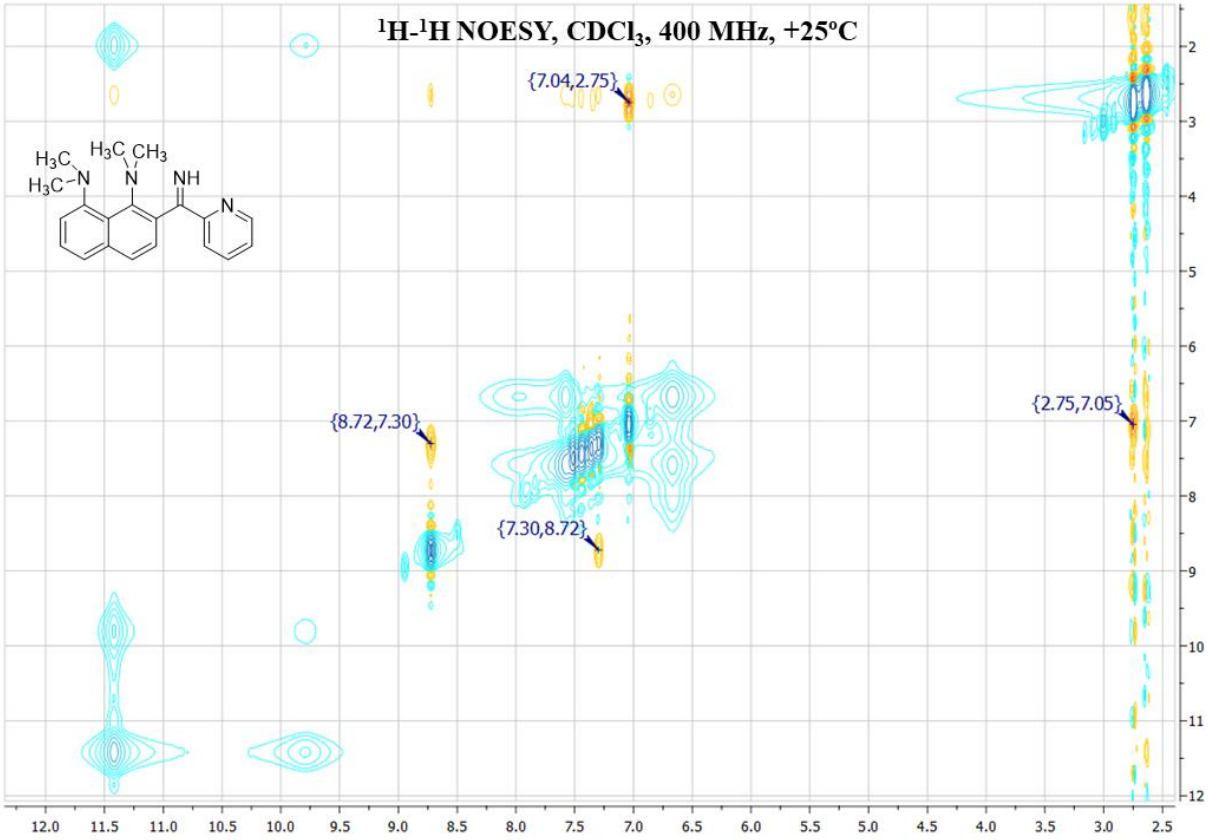

Figure S33. ^{1}H-^{1}H NOESY NMR spectrum of **7h**.

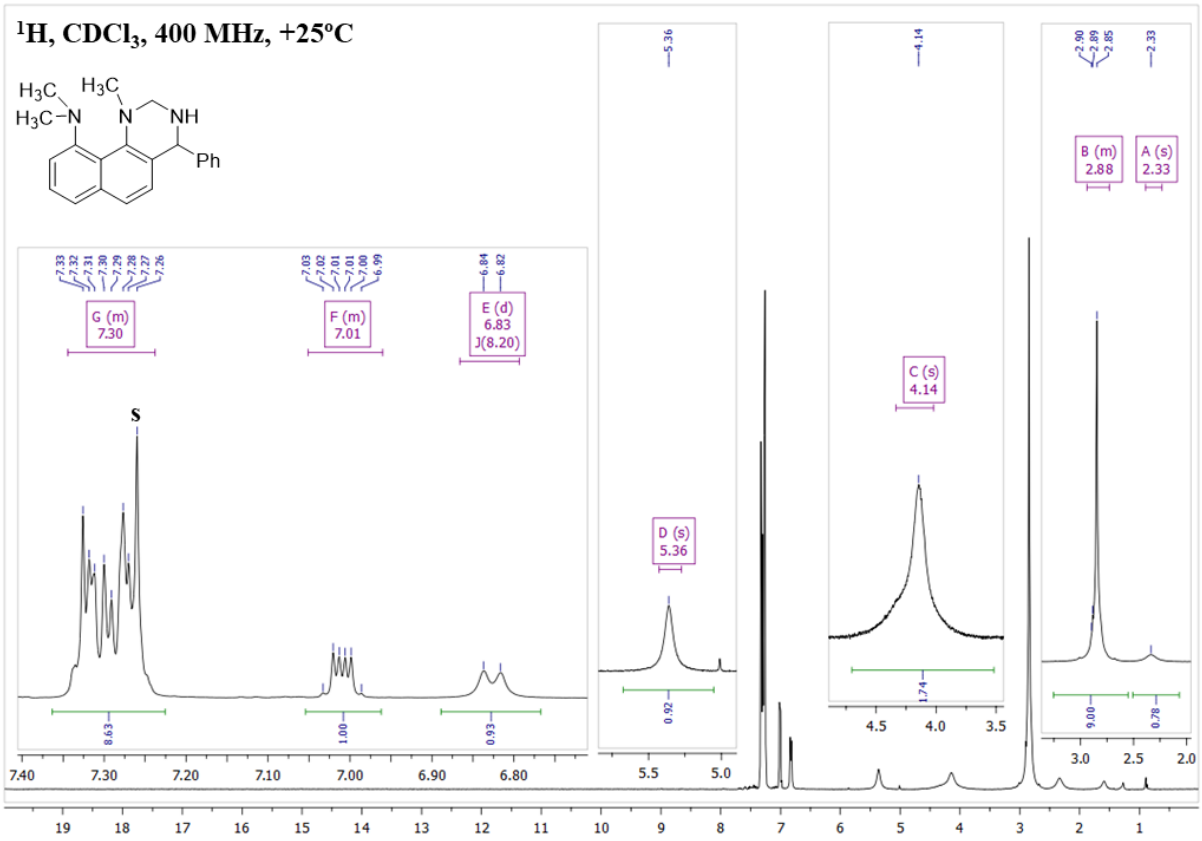

Figure S34. ^{1}H NMR spectrum of **8a**.

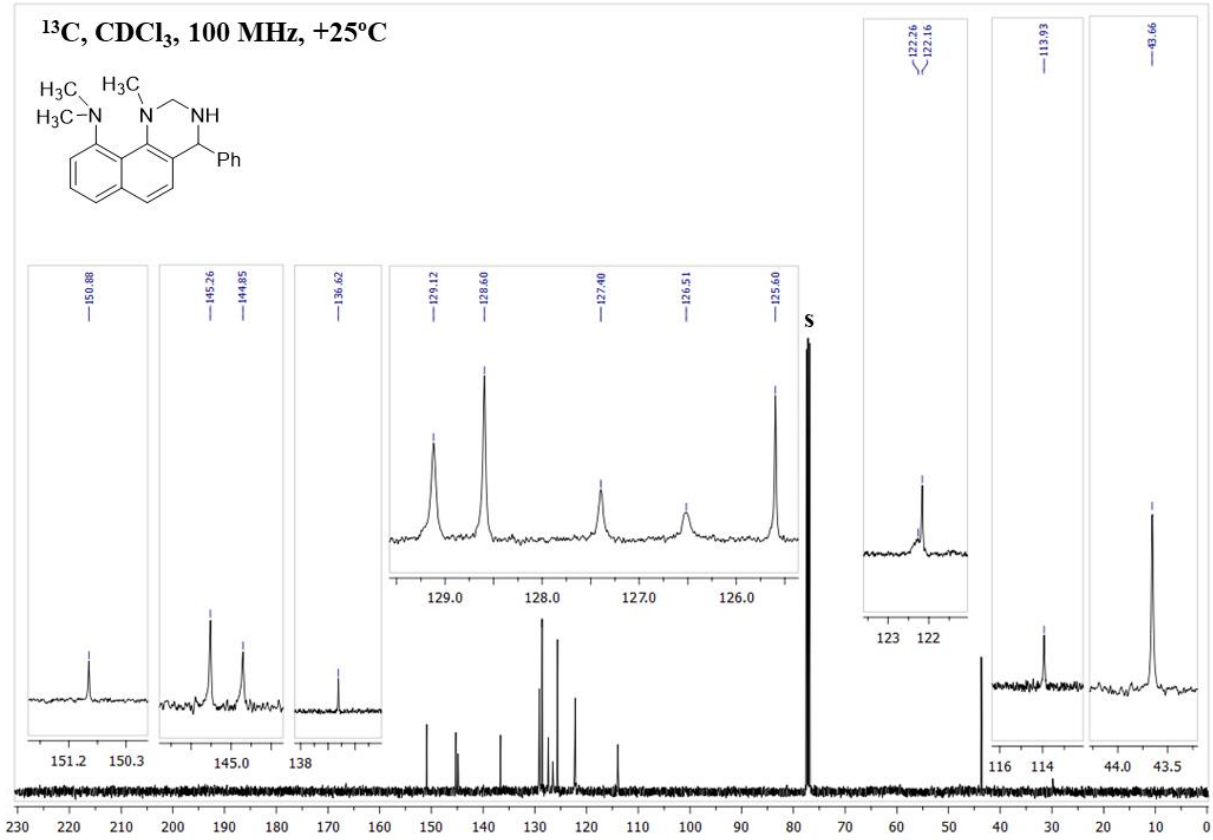

Figure S35. ^{13}C NMR spectrum of **8a**.

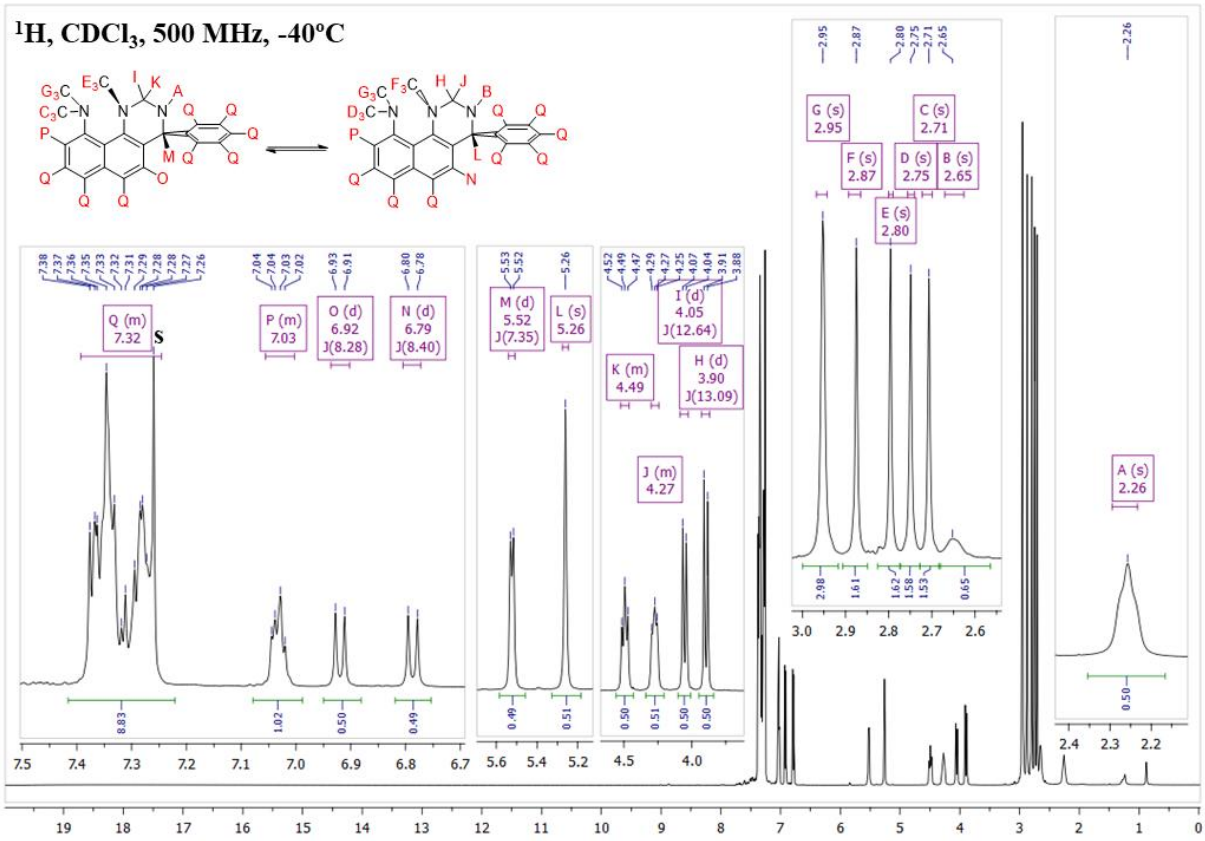

Figure S36. ^{1}H NMR spectrum of **8a**.

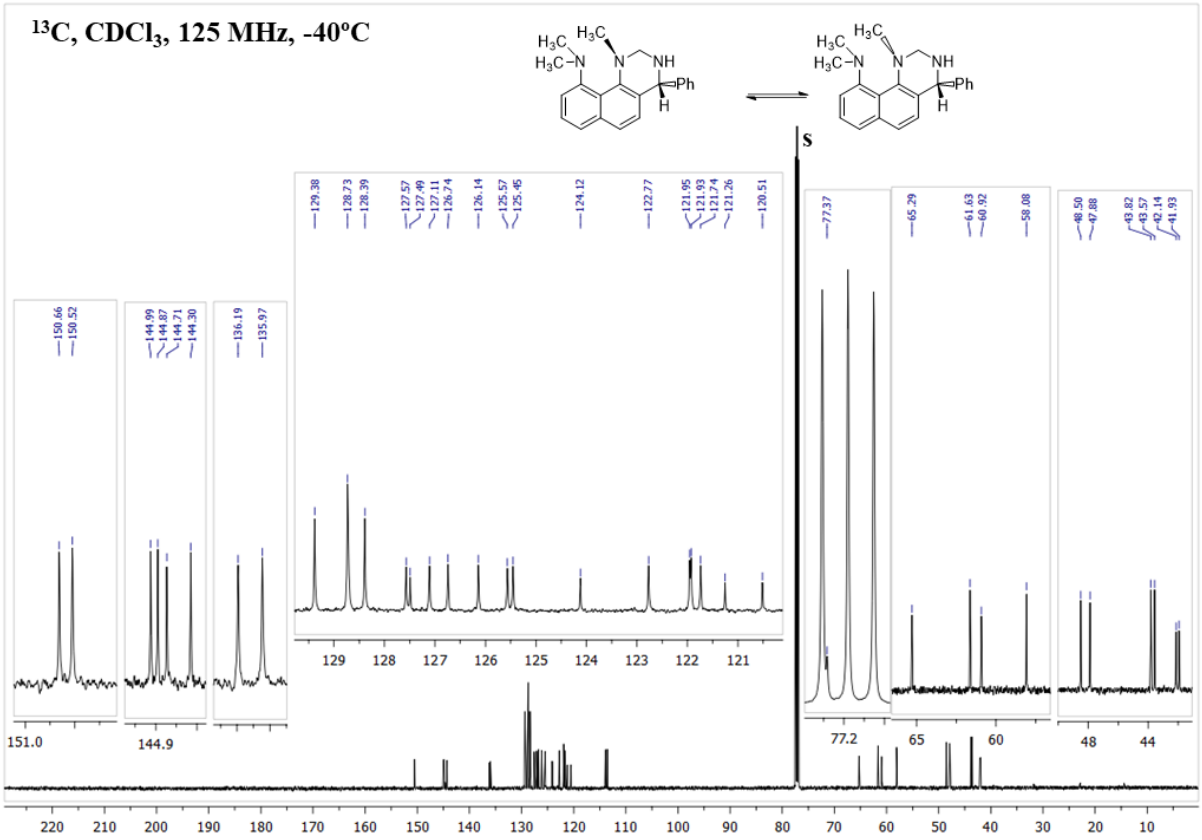

Figure S37. 13C NMR spectrum of **8a**.

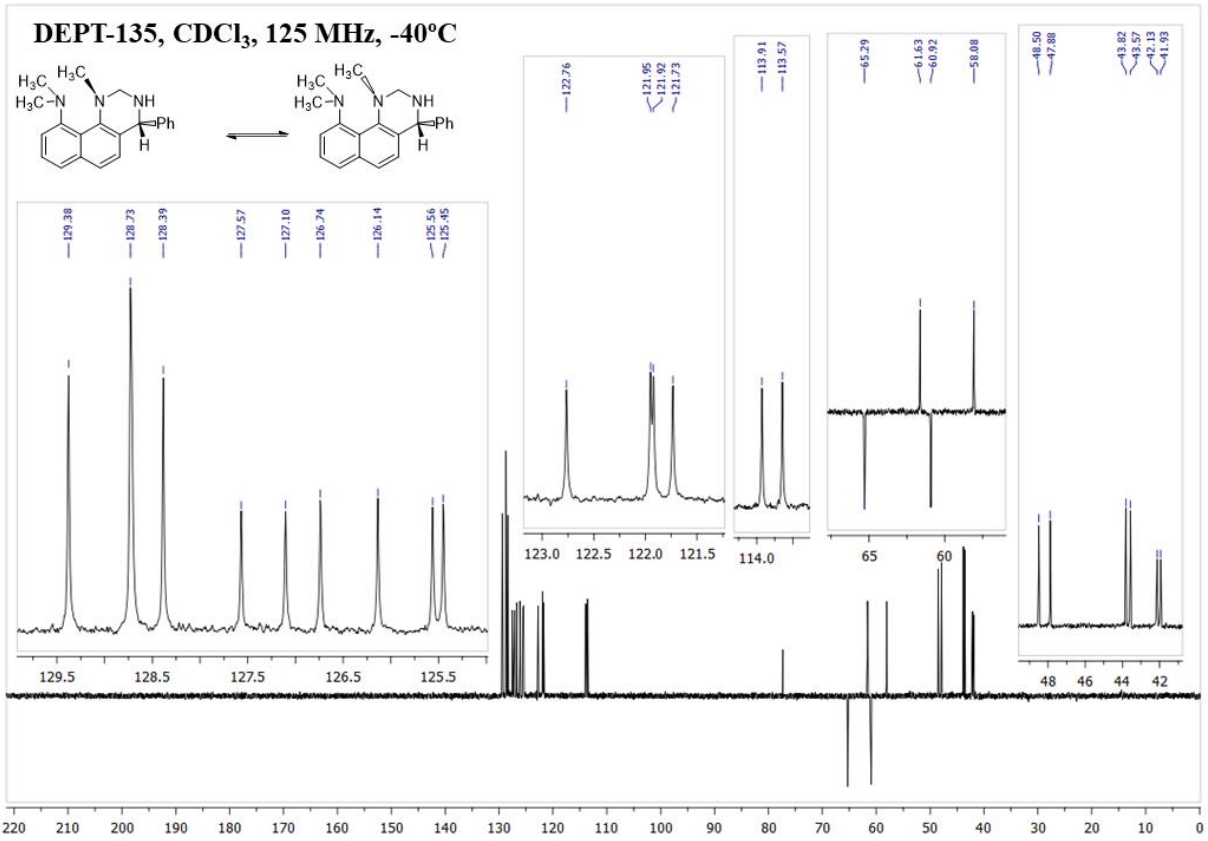

Figure S38. ^{13}C DEPT NMR spectrum of **8a**.

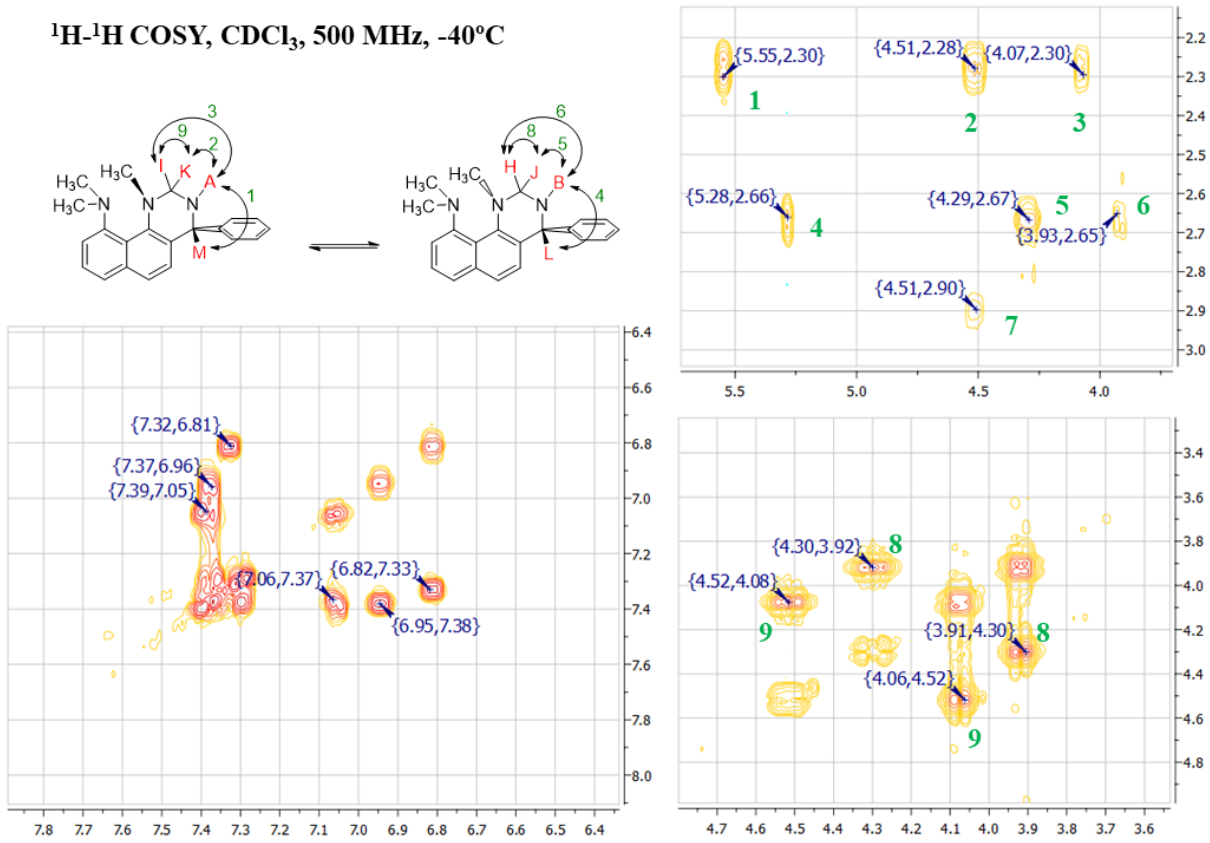

Figure S39. ^{1}H-^{1}H COSY NMR spectrum of **8a**.

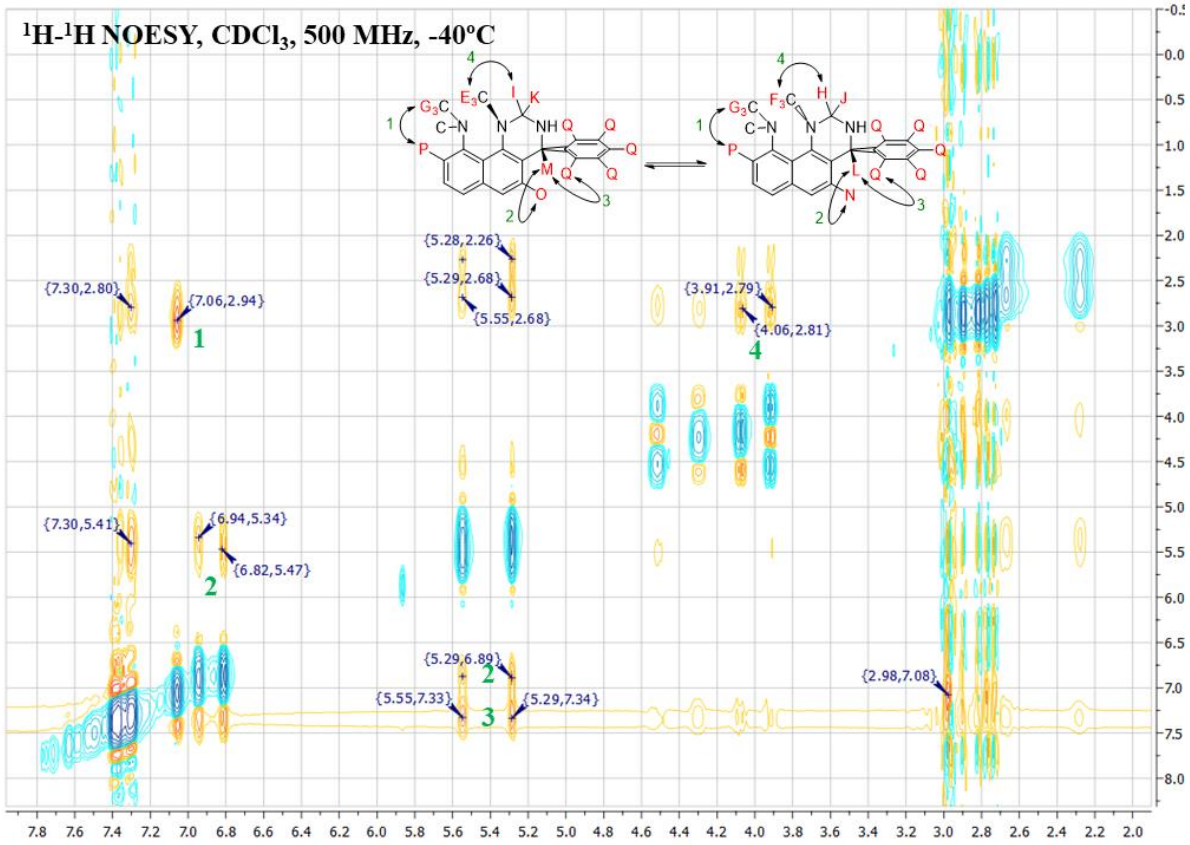

Figure S40. ^{1}H-^{1}H NOESY NMR spectrum of **8a**.

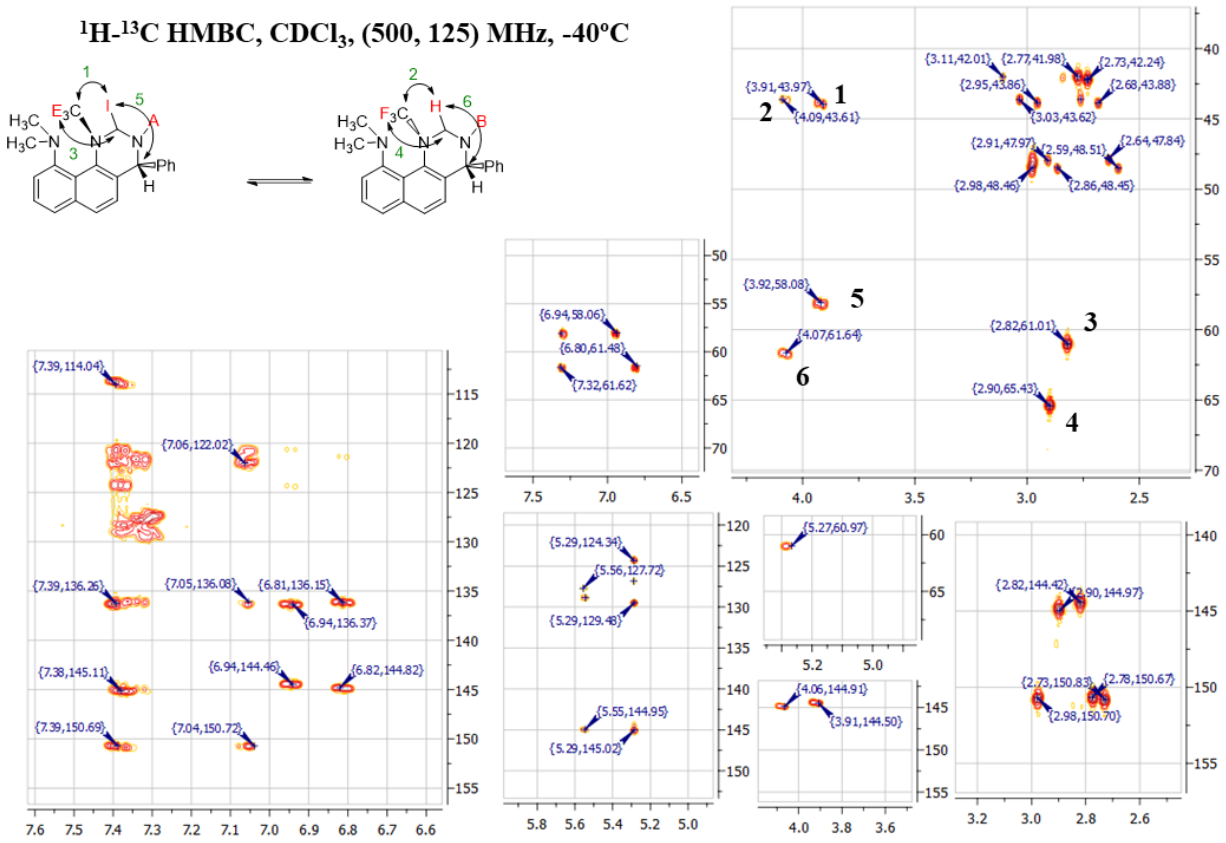

Figure S41. ^{1}H-^{13}C HMBC NMR spectrum of **8a**.

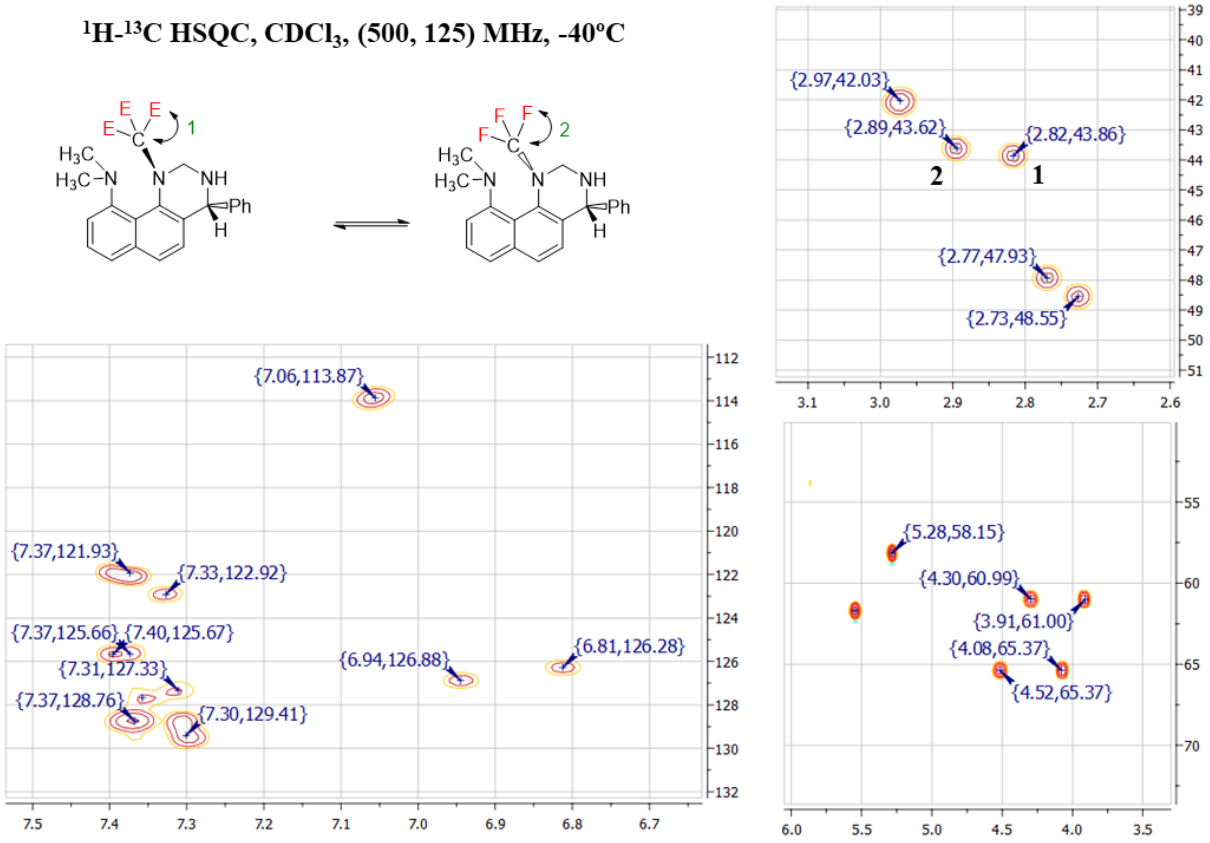

Figure S42. ^{1}H-^{13}C HSQC NMR spectrum of **8a**.

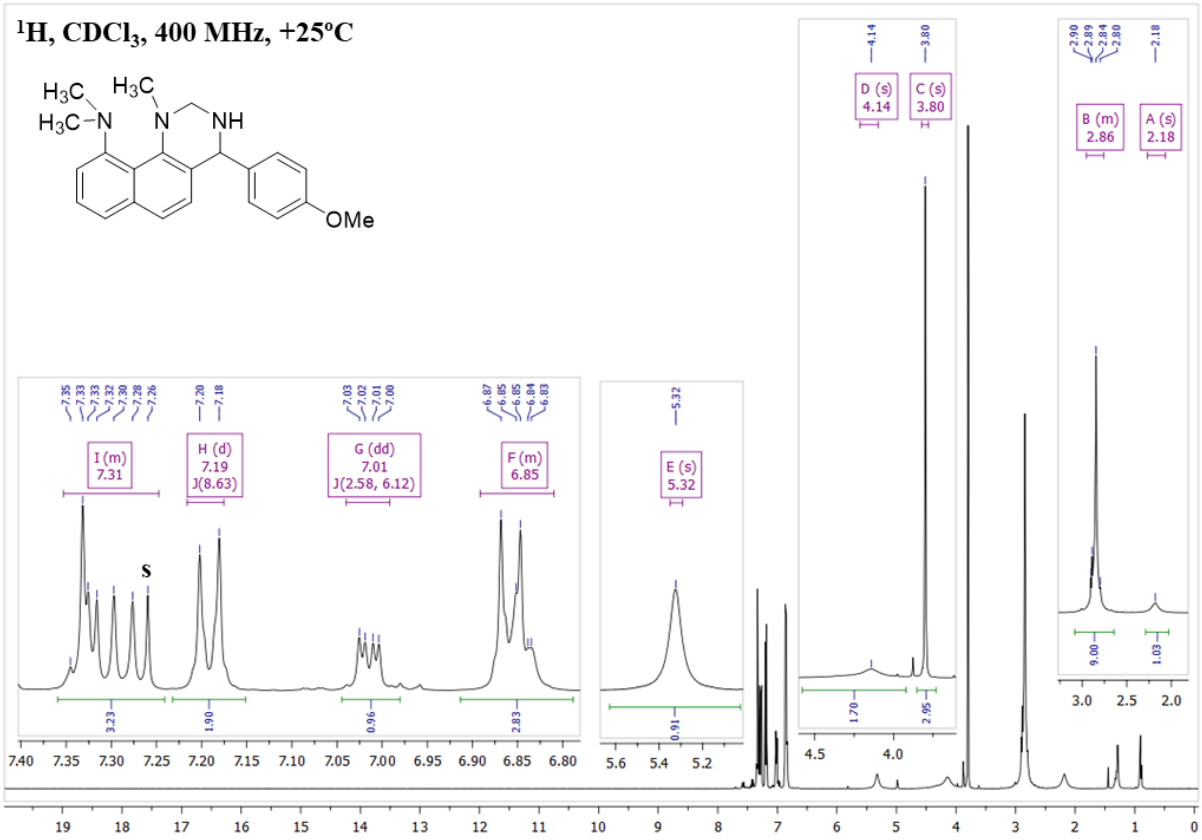

Figure S43. ^{1}H NMR spectrum of **8b**.

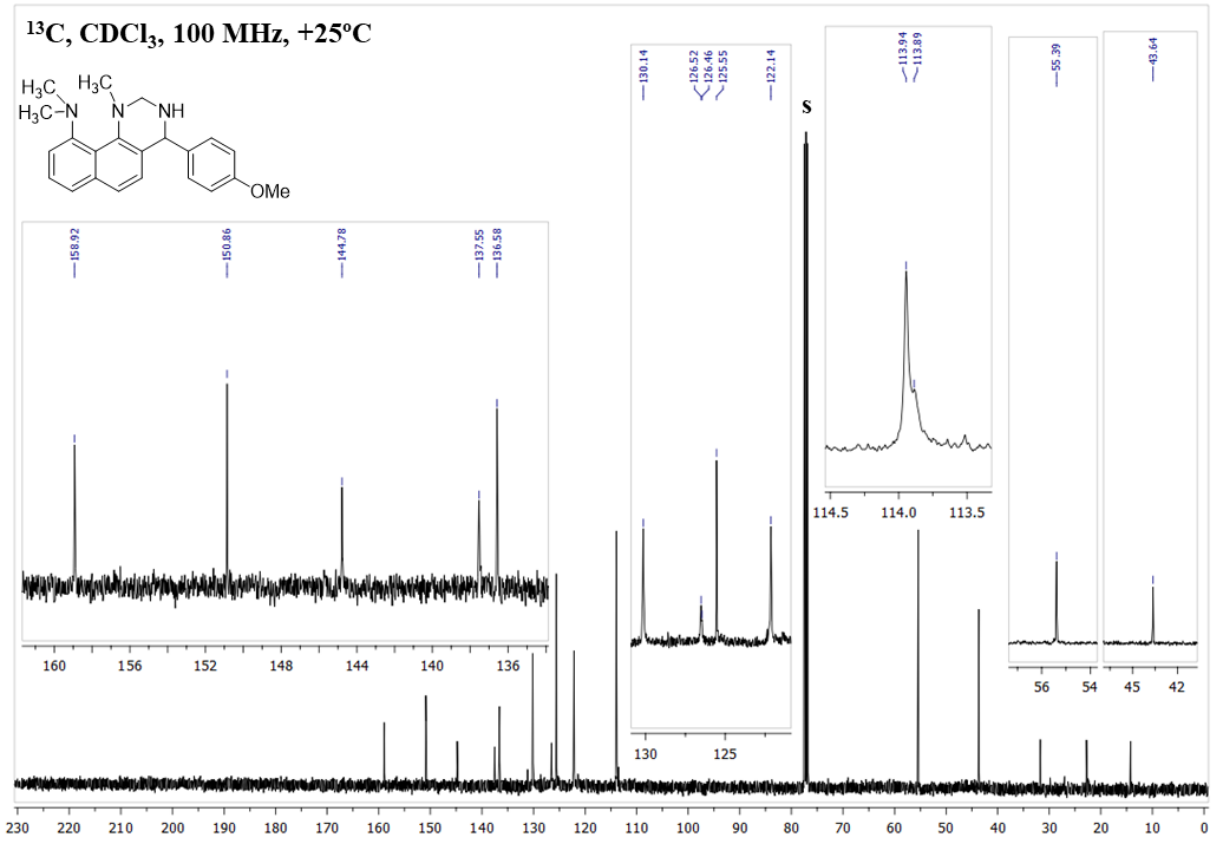

Figure S44. ^{13}C NMR spectrum of **8b**.

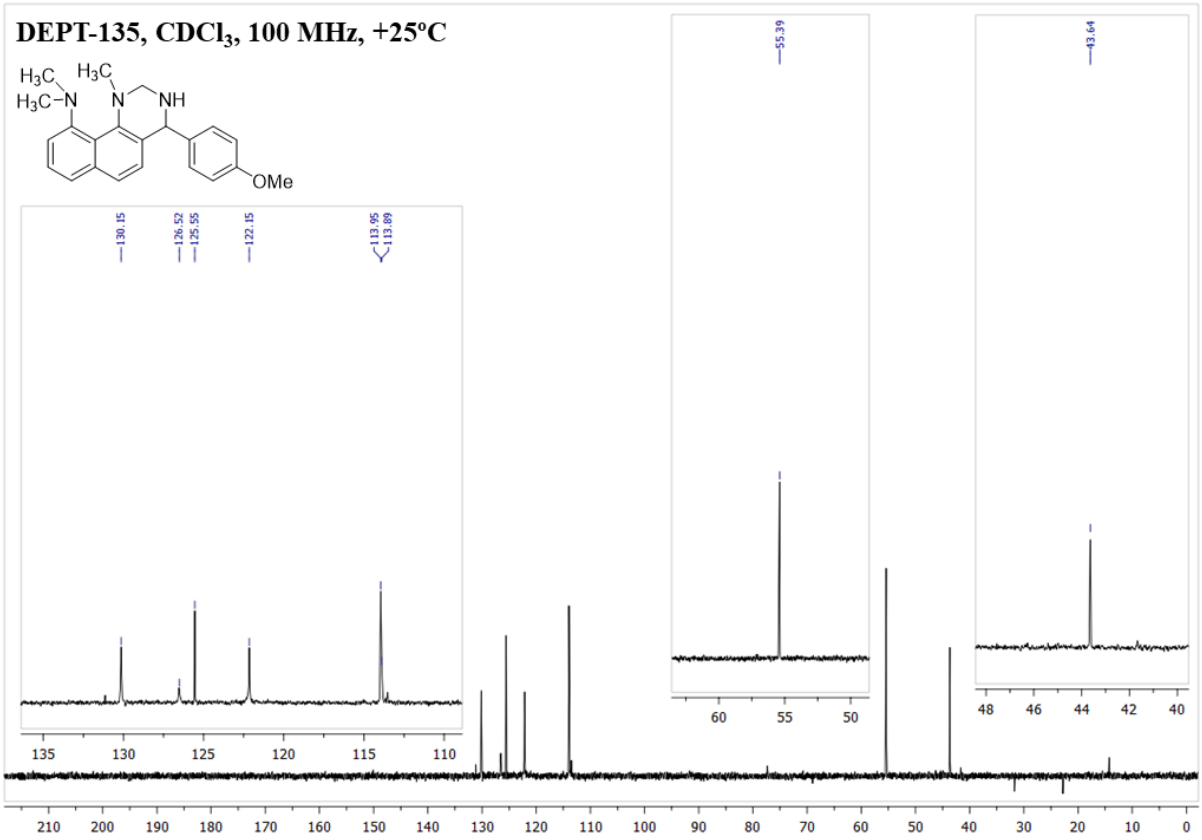

Figure S45. ^{13}C DEPT NMR spectrum of **8b**.

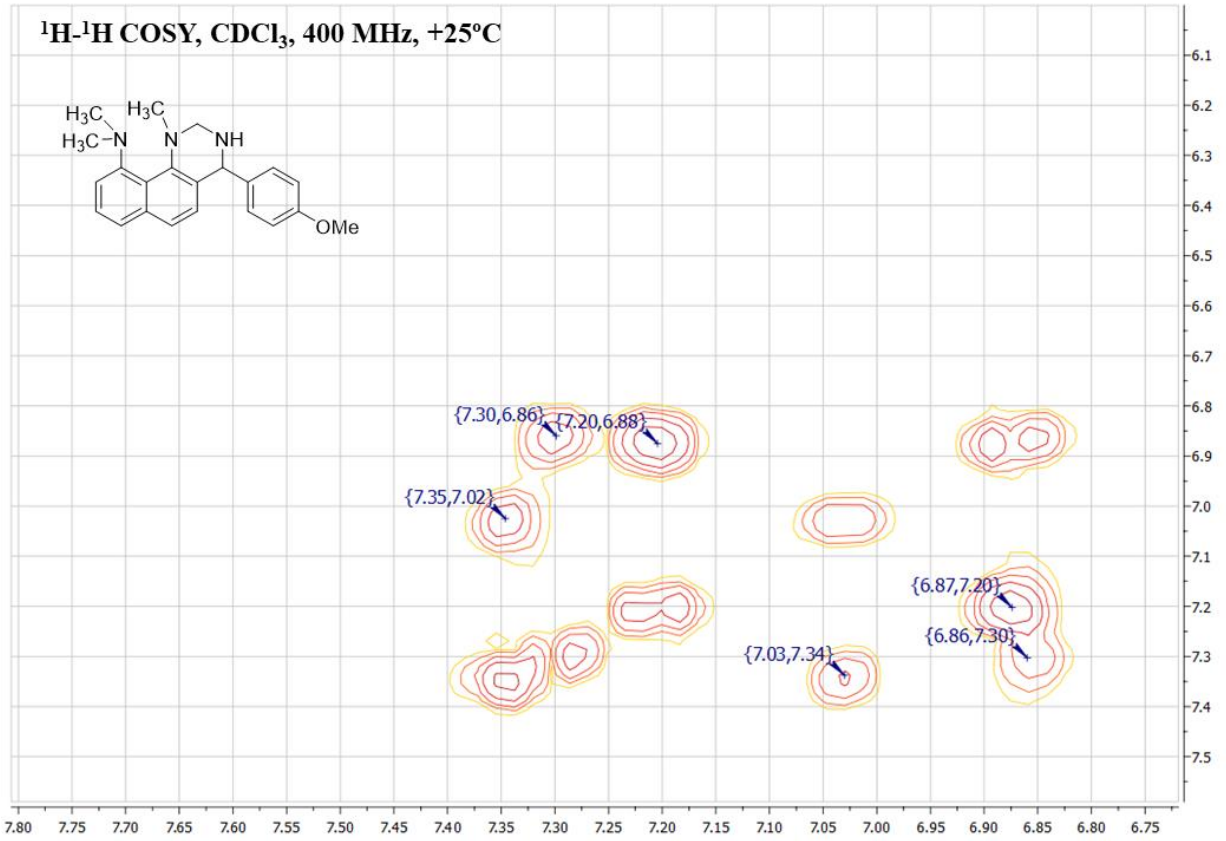

Figure S46. ^{1}H-^{1}H COSY NMR spectrum of **8b**.

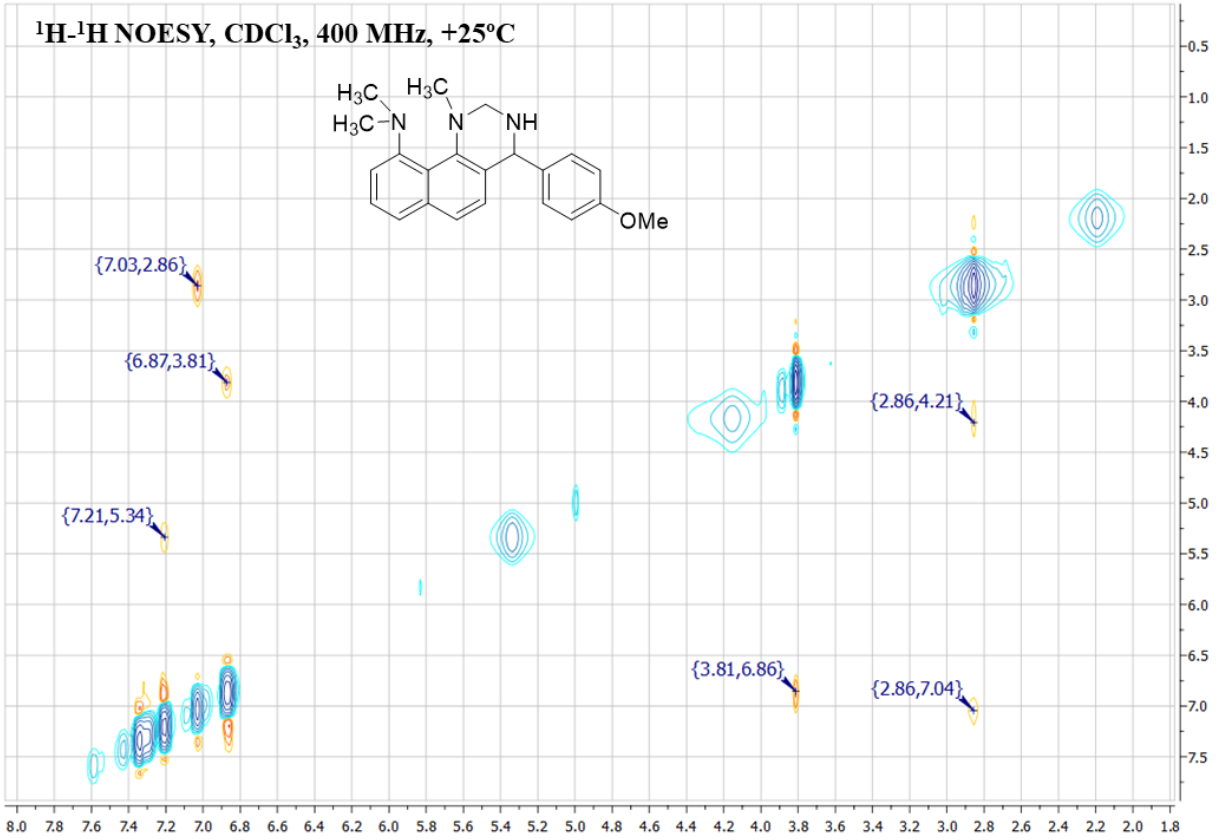

Figure S47. ^{1}H-^{1}H NOESY NMR spectrum of **8b**.

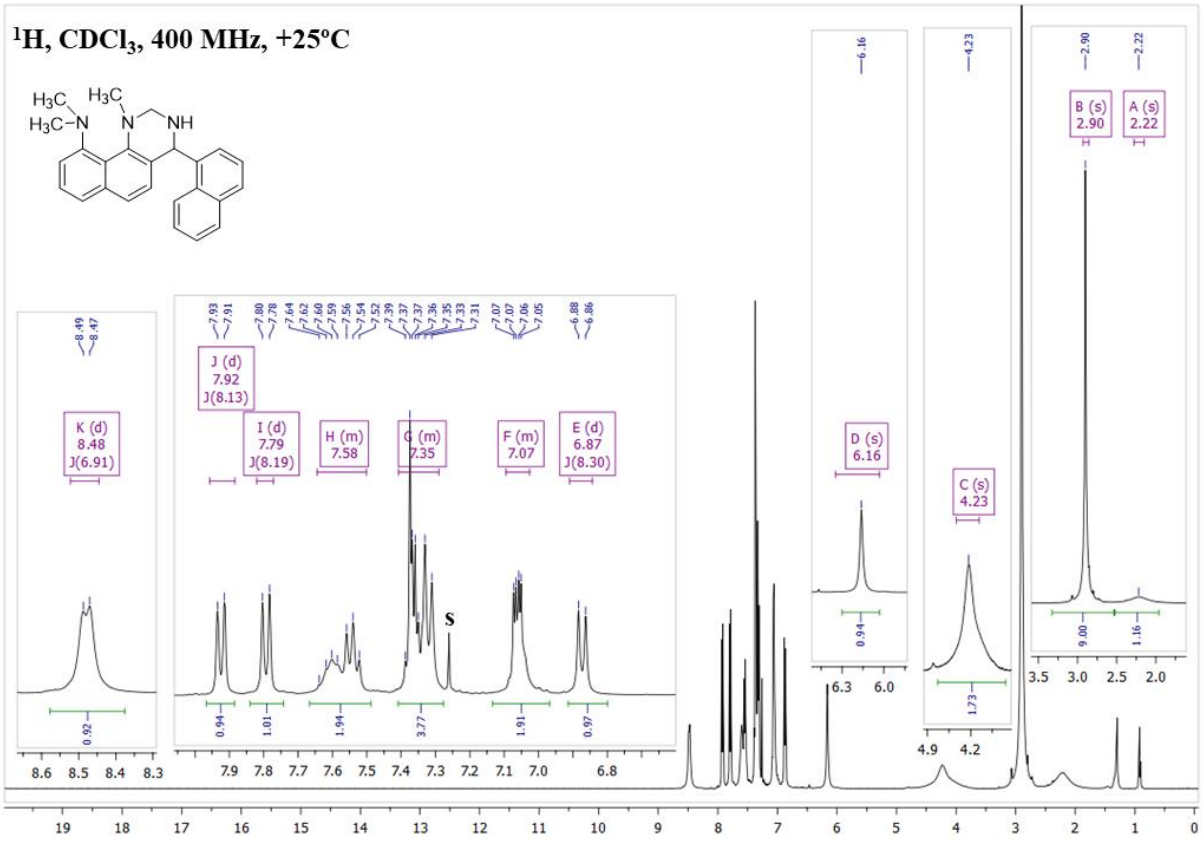

Figure S48. ^{1}H NMR spectrum of **8c**.

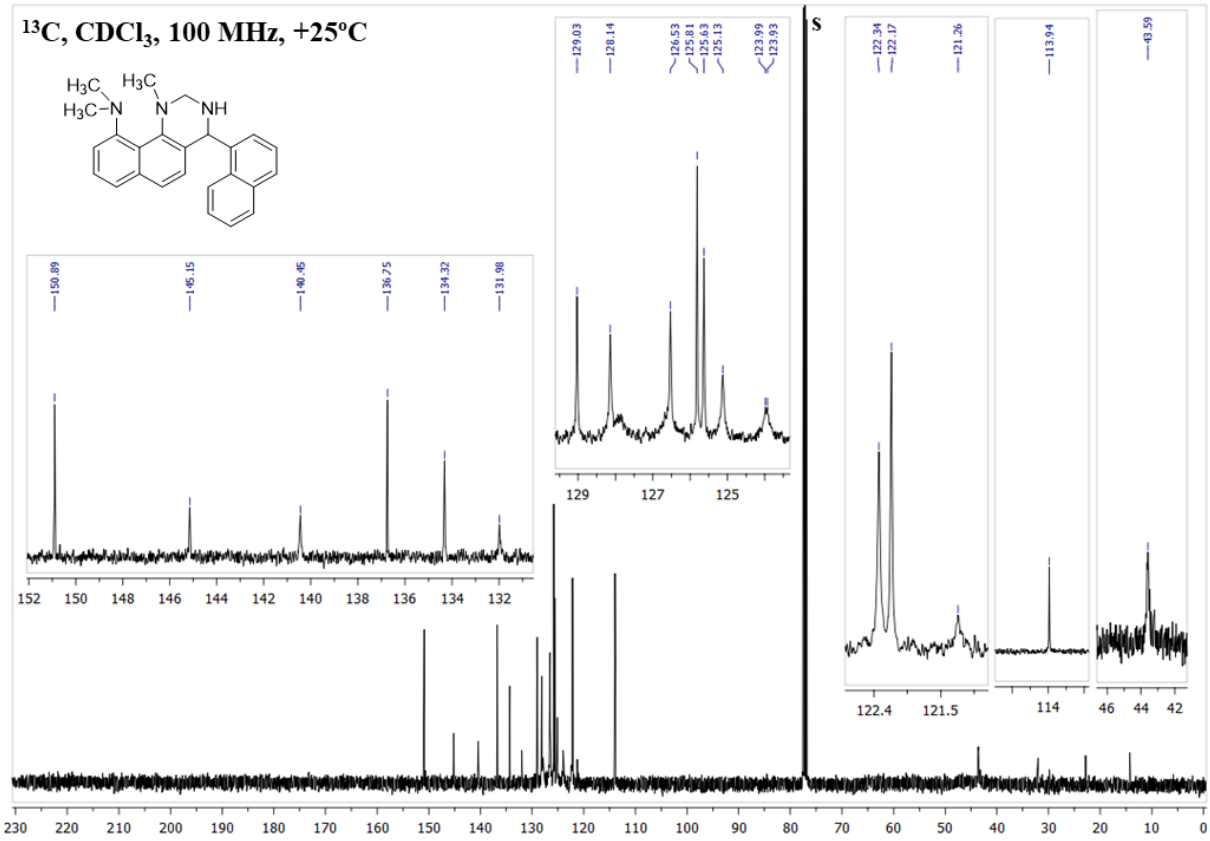

Figure S49. ^{13}C NMR spectrum of **8c**.

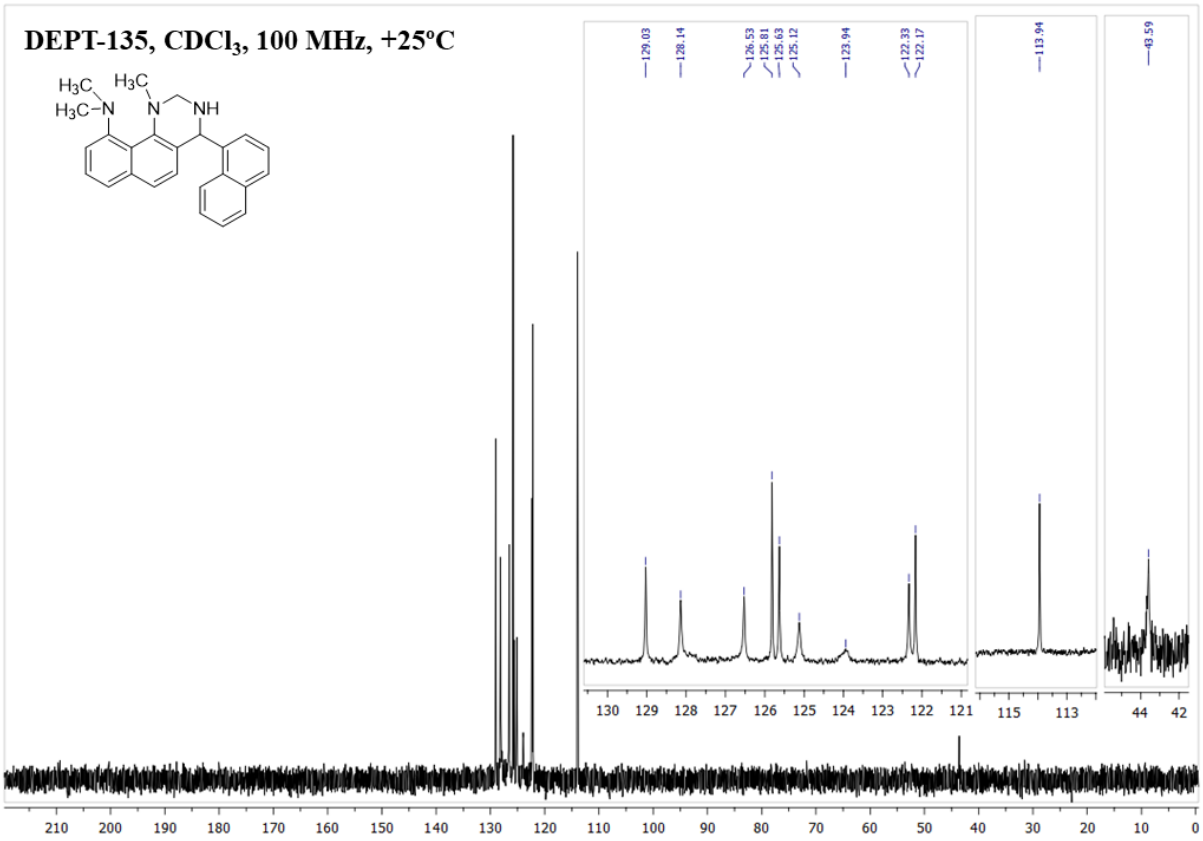

Figure S50. ^{13}C DEPT NMR spectrum of **8c**.

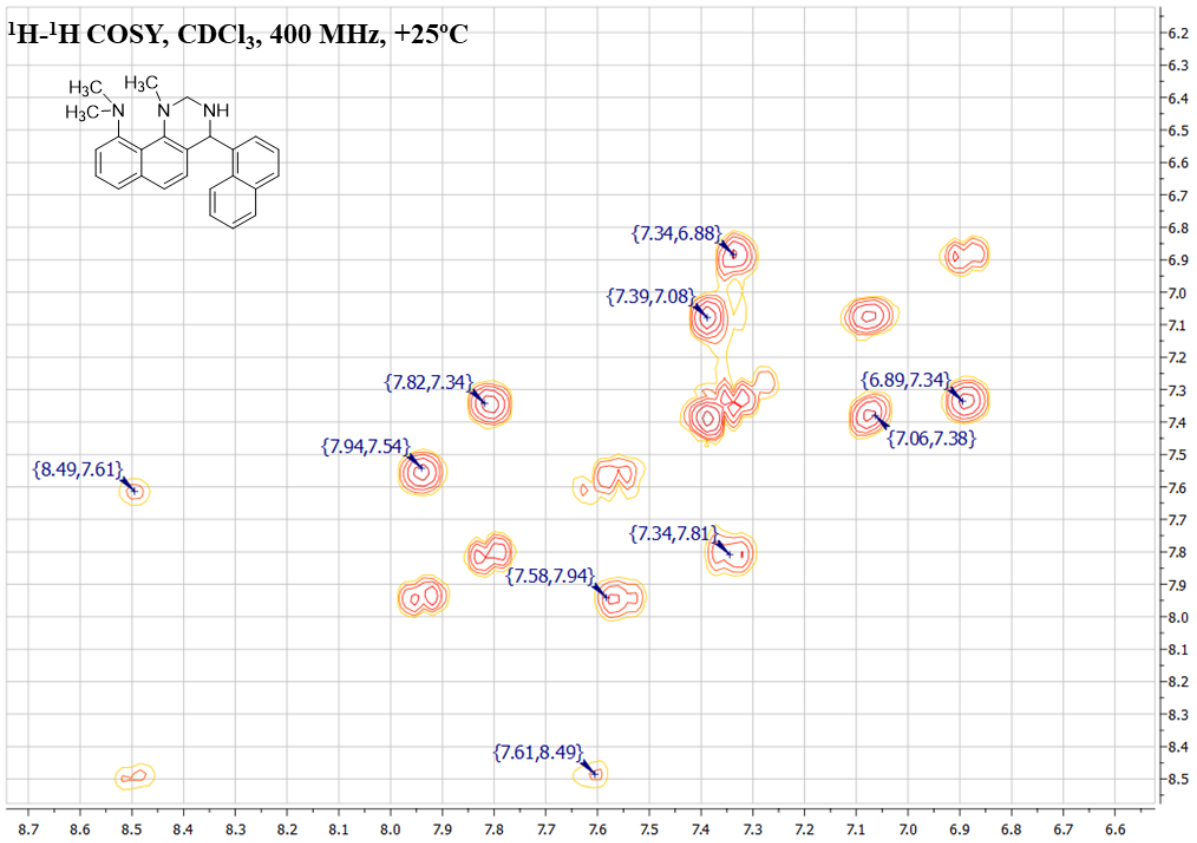

Figure S51. ^{1}H-^{1}H COSY NMR spectrum of **8c**.

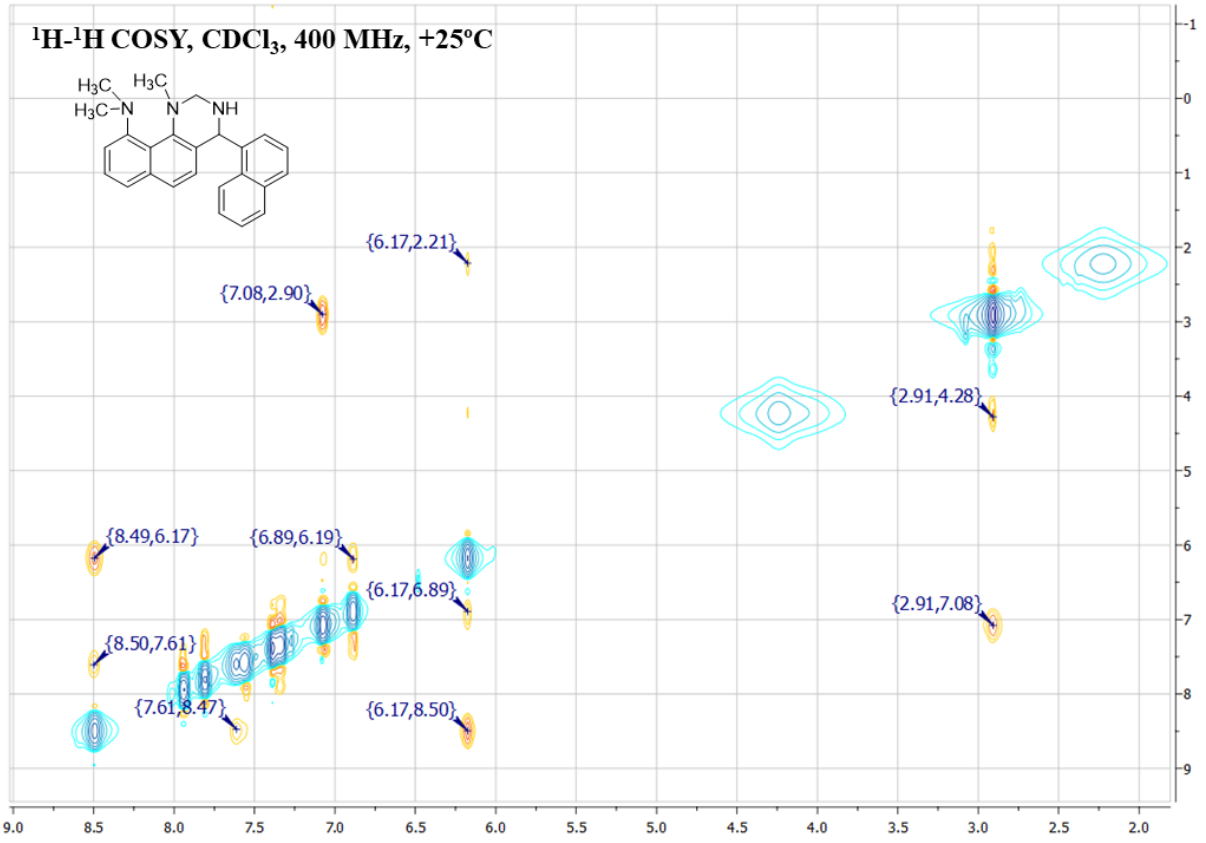

Figure S52. ^{1}H-^{1}H NOESYNMR spectrum of **8c**.

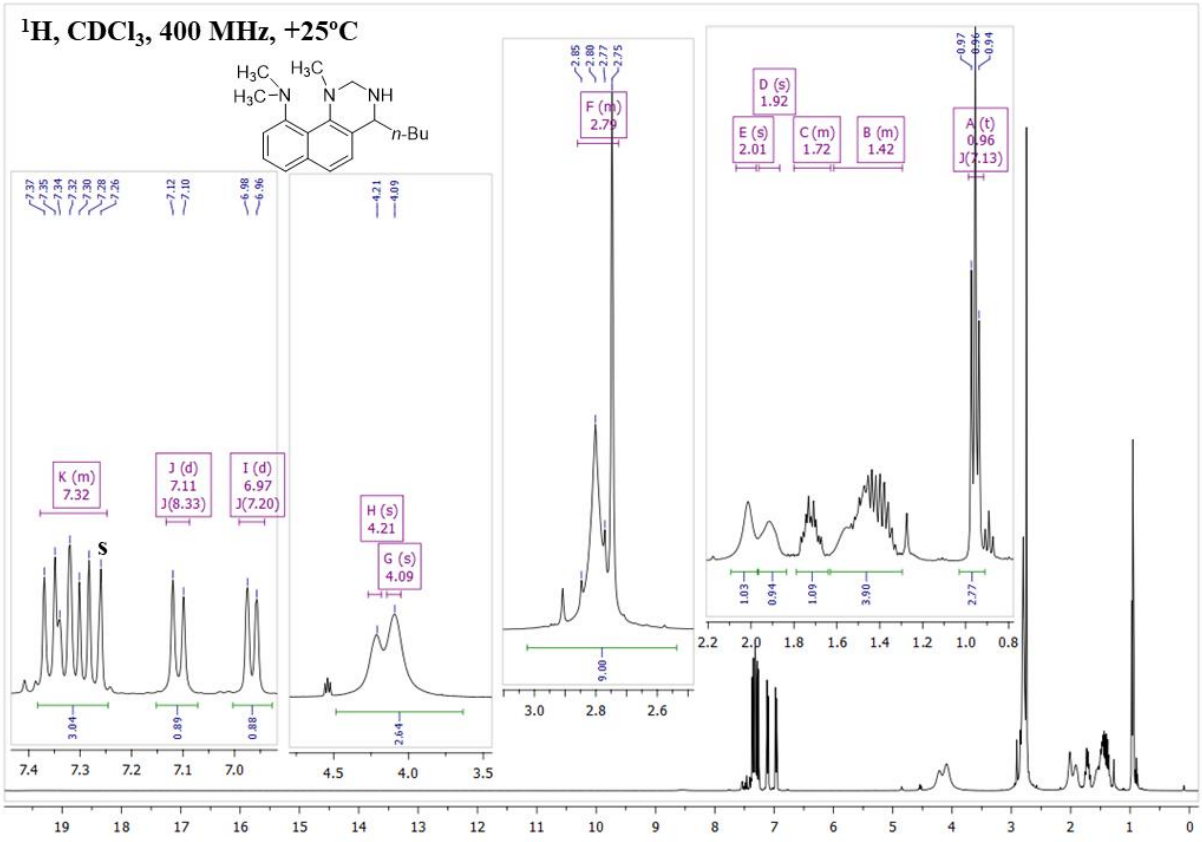

Figure S53. ^{1}H NMR spectrum of **8d**.

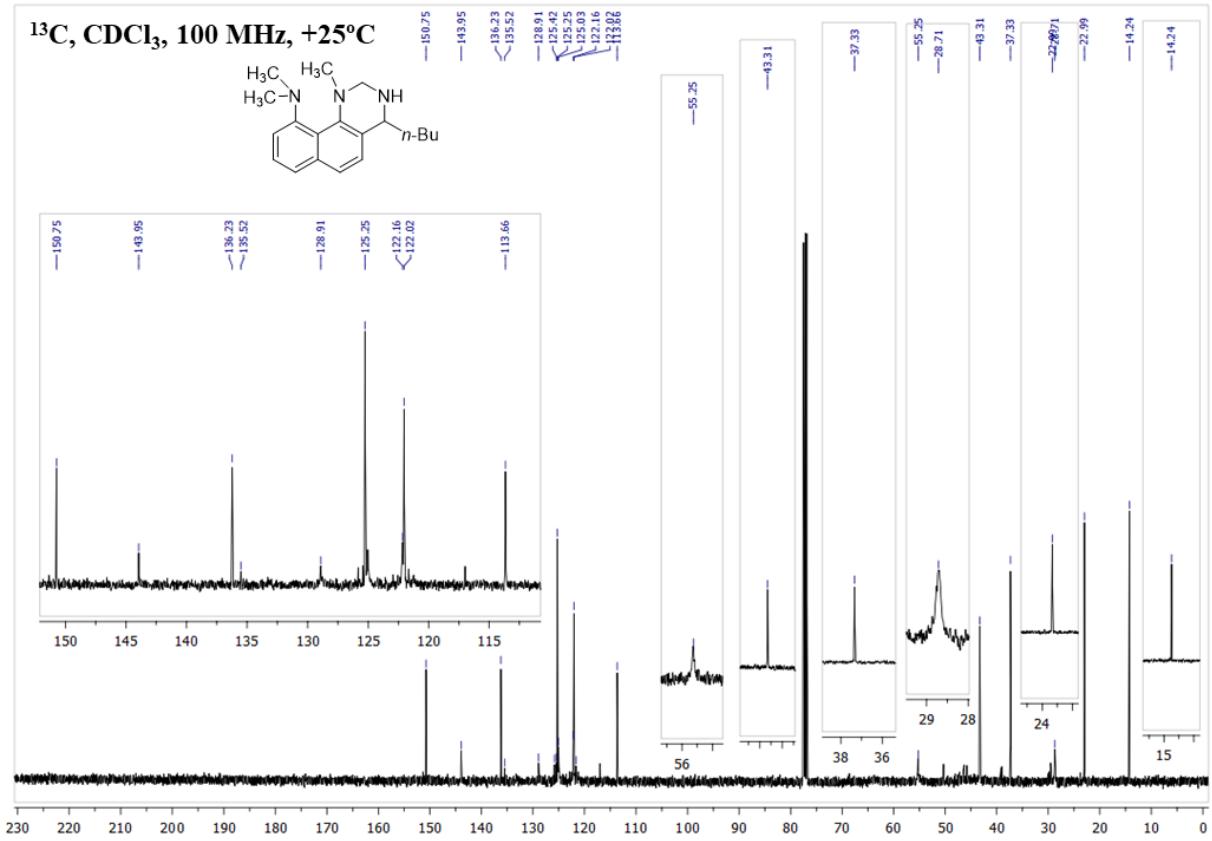

Figure S54. ^{13}C NMR spectrum of **8d**.

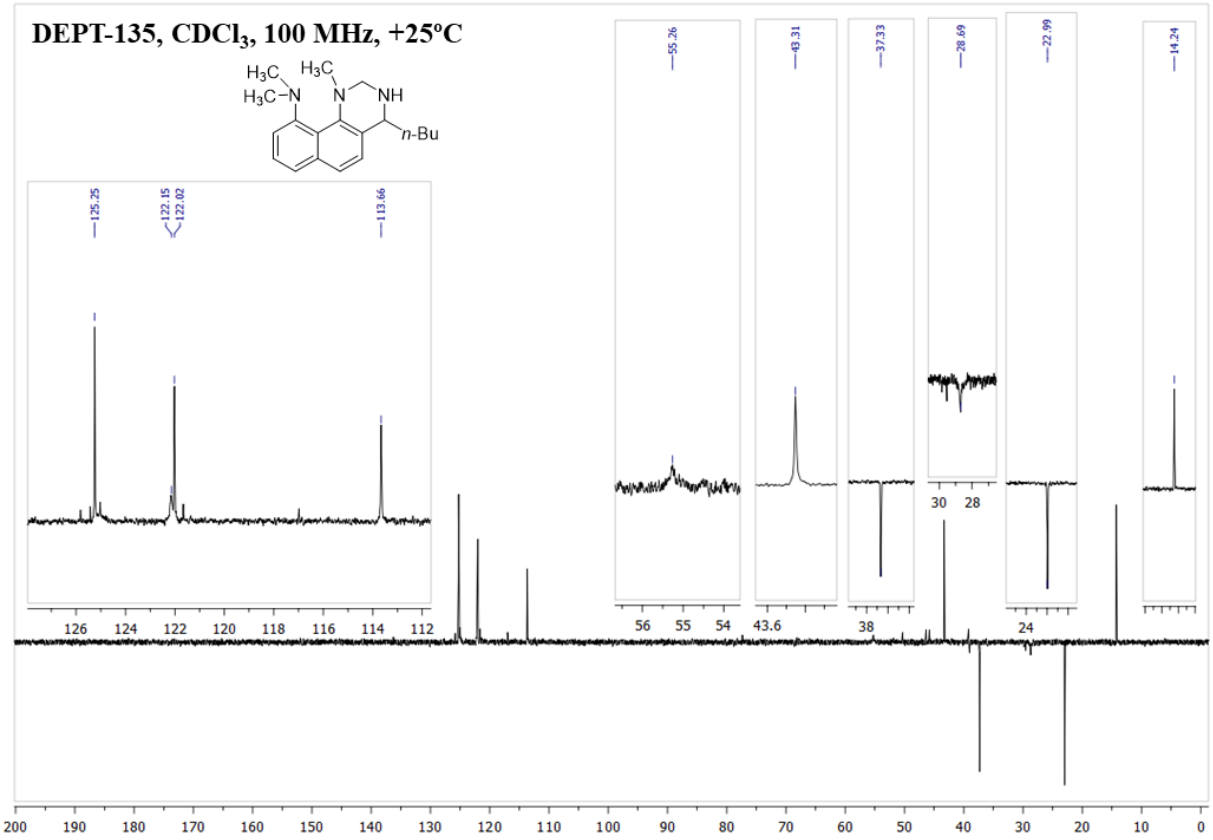

Figure S55.[13]C DEPT NMR spectrum of **8d**.

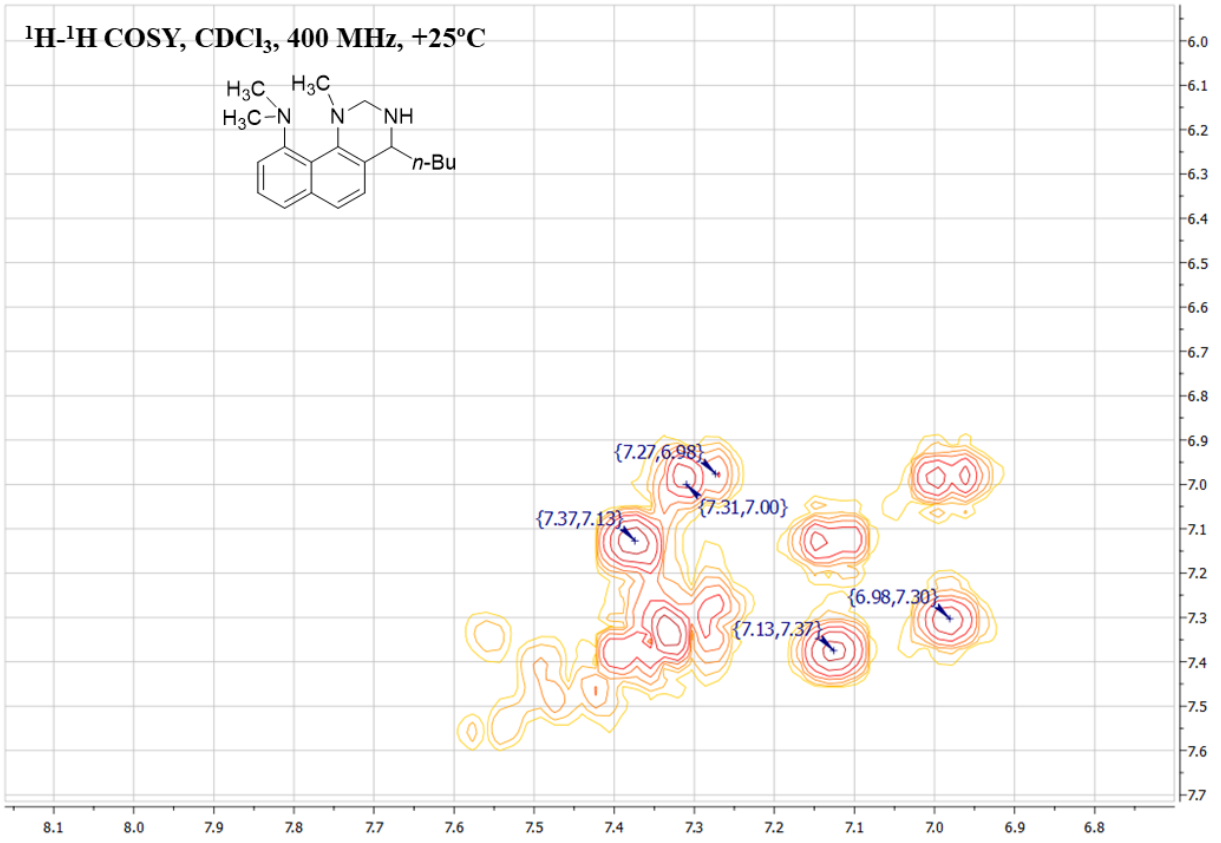

Figure S56. [1]H-[1]H COSY NMR spectrum of **8d**.

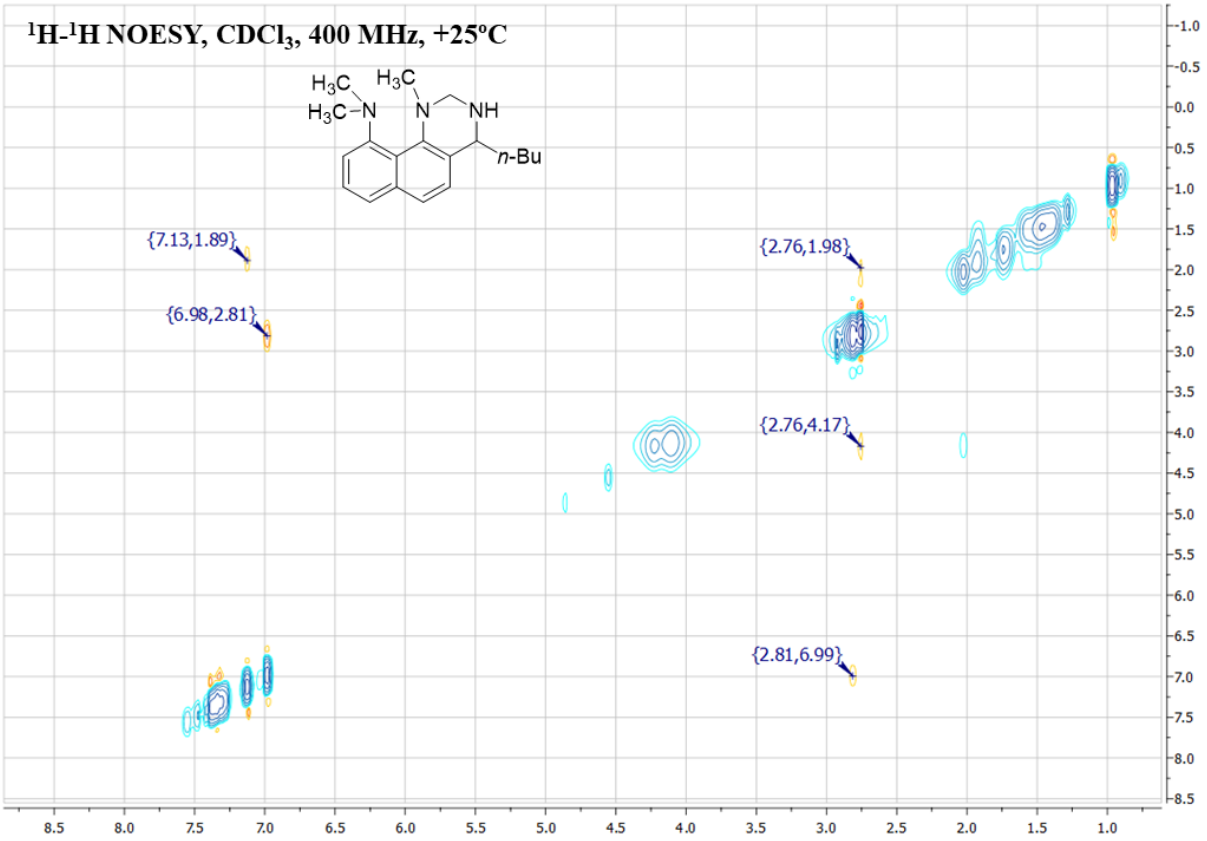

Figure S57. ^{1}H-^{1}H NOESY NMR spectrum of **8d**.

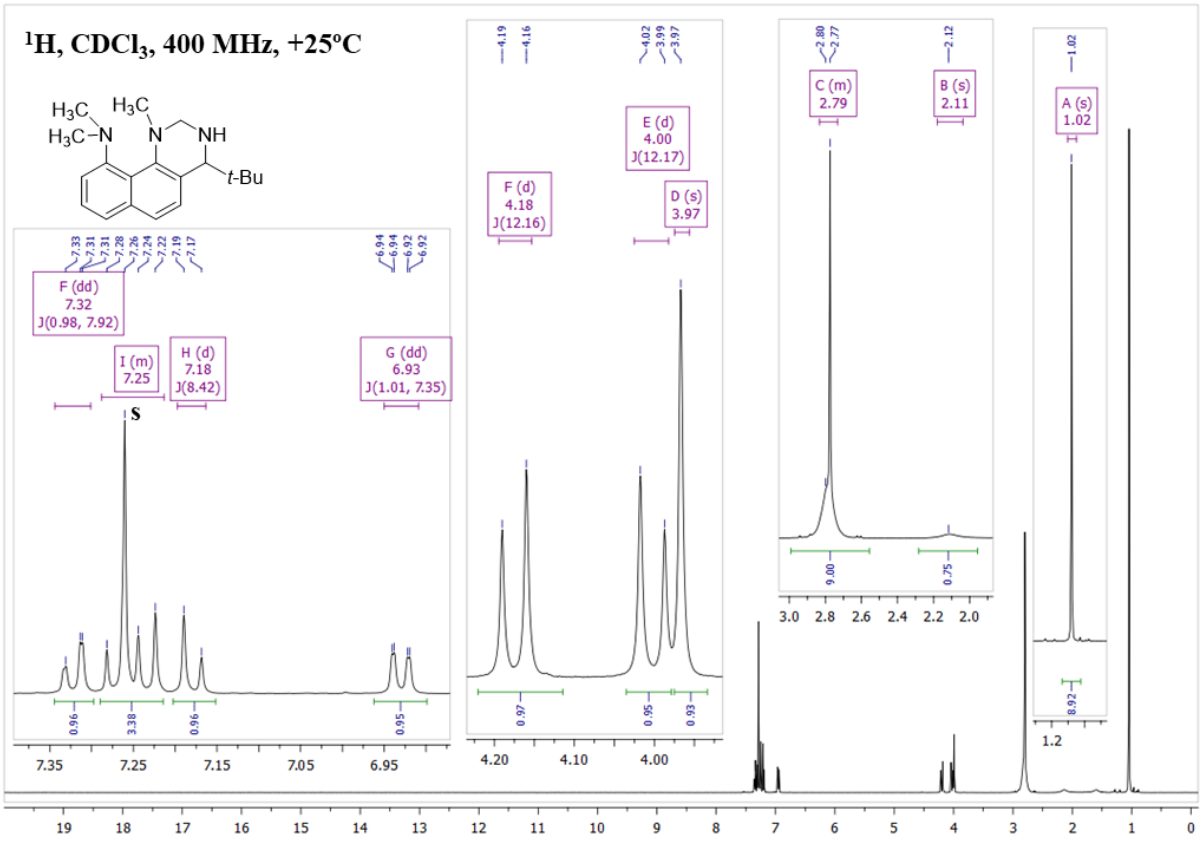

Figure S58. ^{1}H NMR spectrum of **8e**.

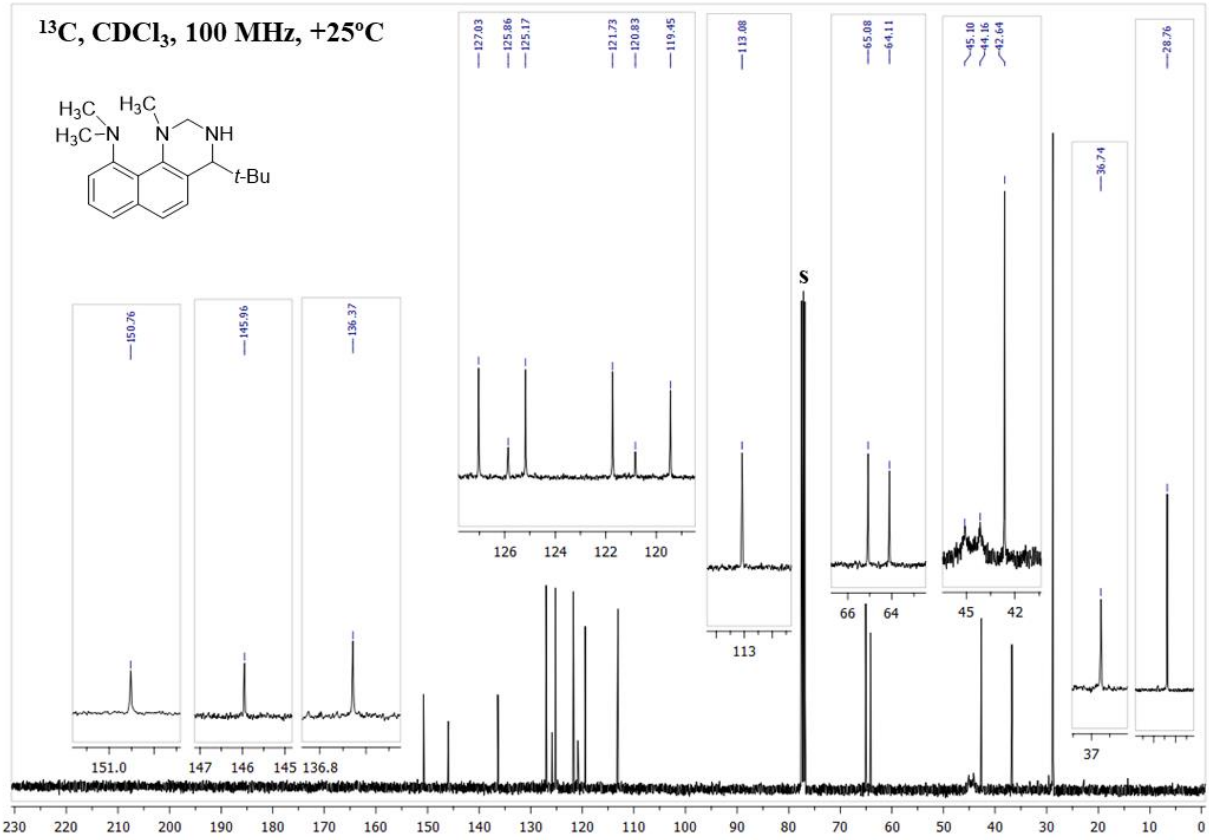

Figure S59.1^{3}C NMR spectrum of **8e**.

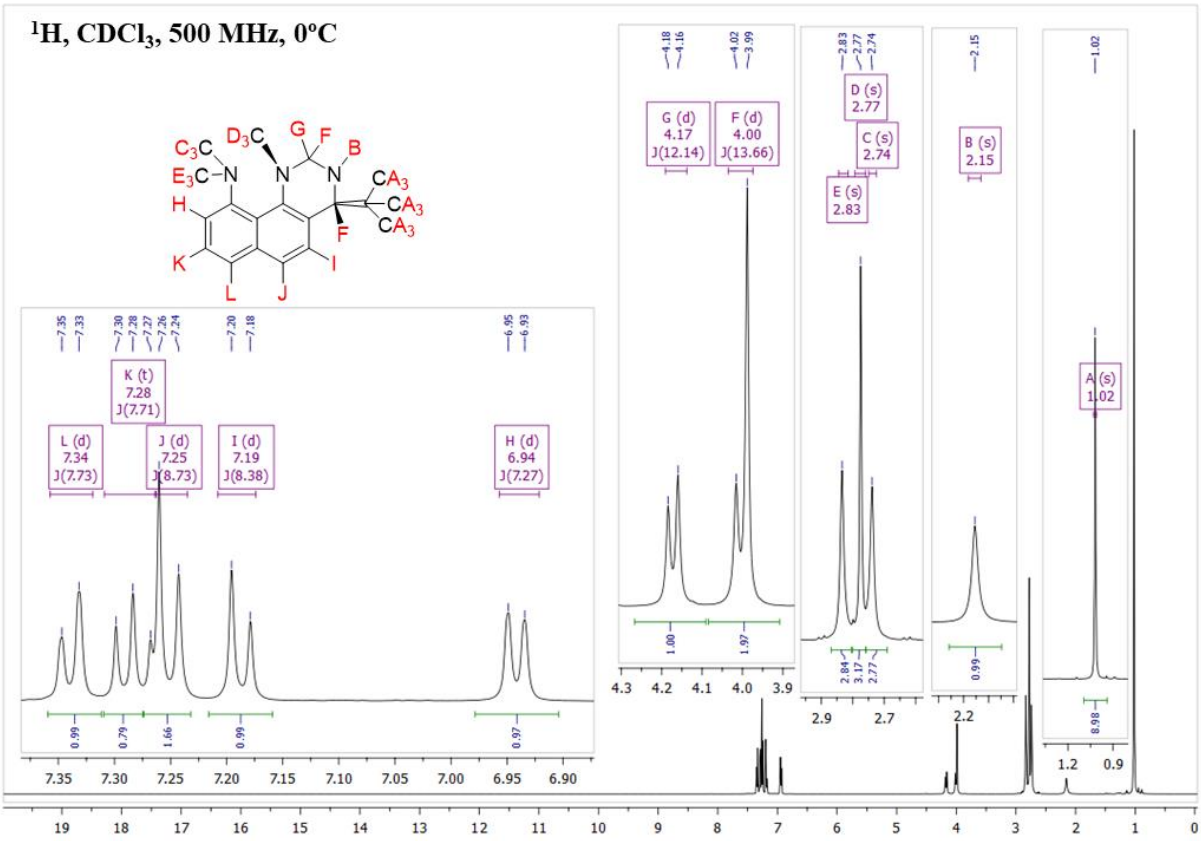

Figure S60. ^{1}H NMR spectrum of **8e**.

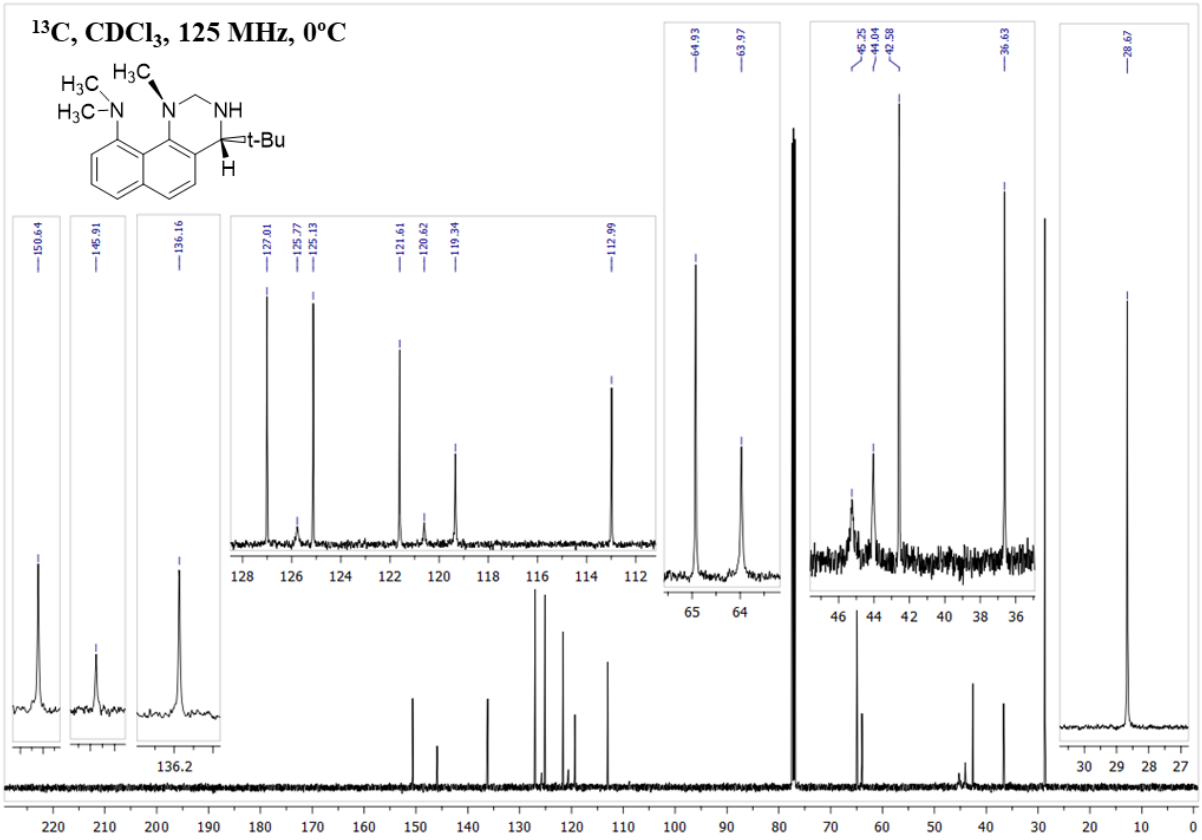

Figure S61.[13]C NMR spectrum of **8e**.

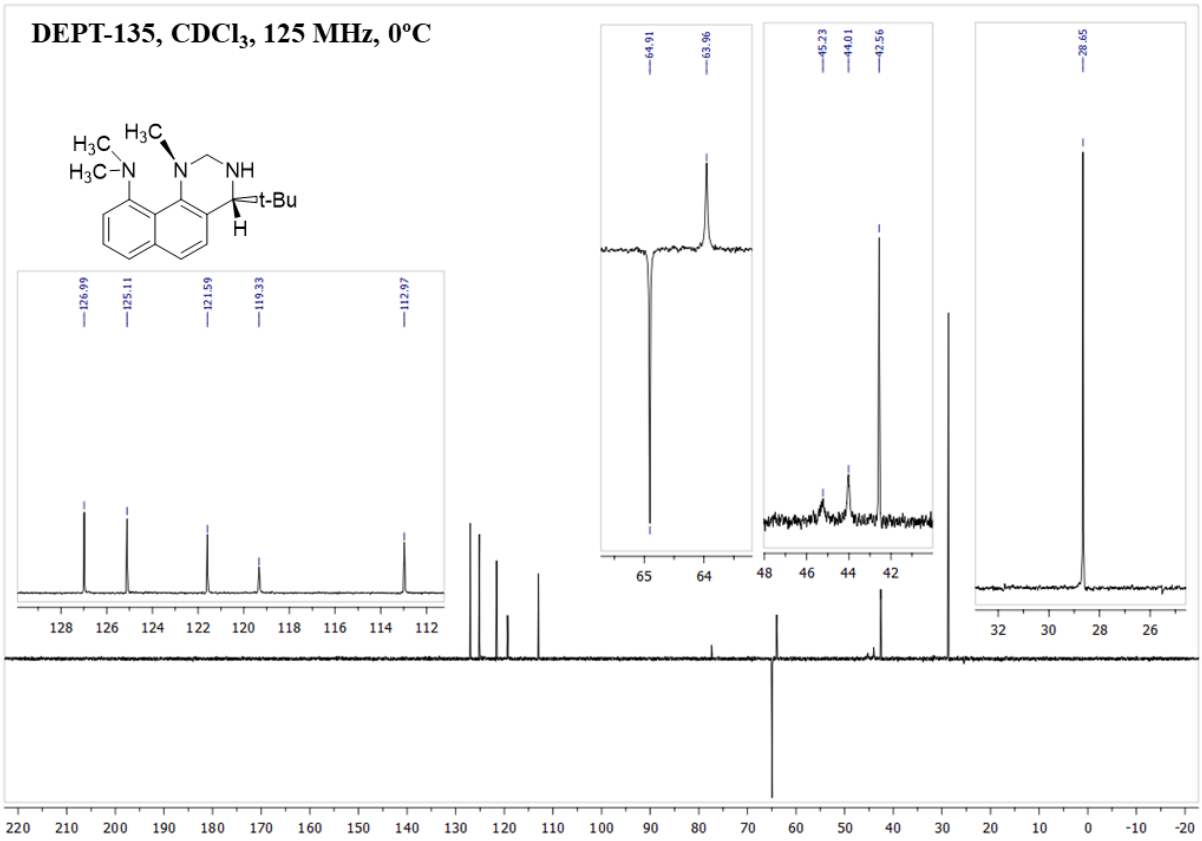

Figure S62.[13]C DEPT NMR spectrum of **8e**.

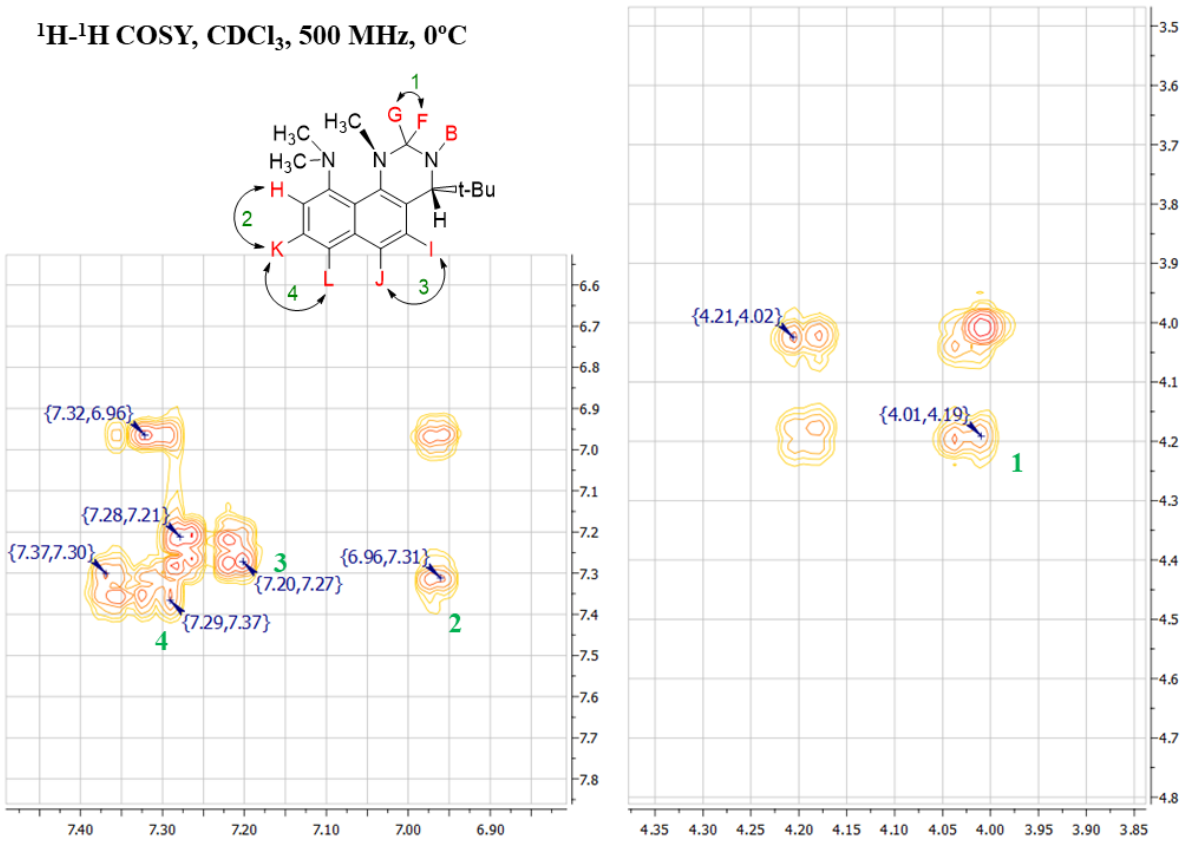

Figure S63. ^{1}H-^{1}H COSY NMR spectrum of **8e**.

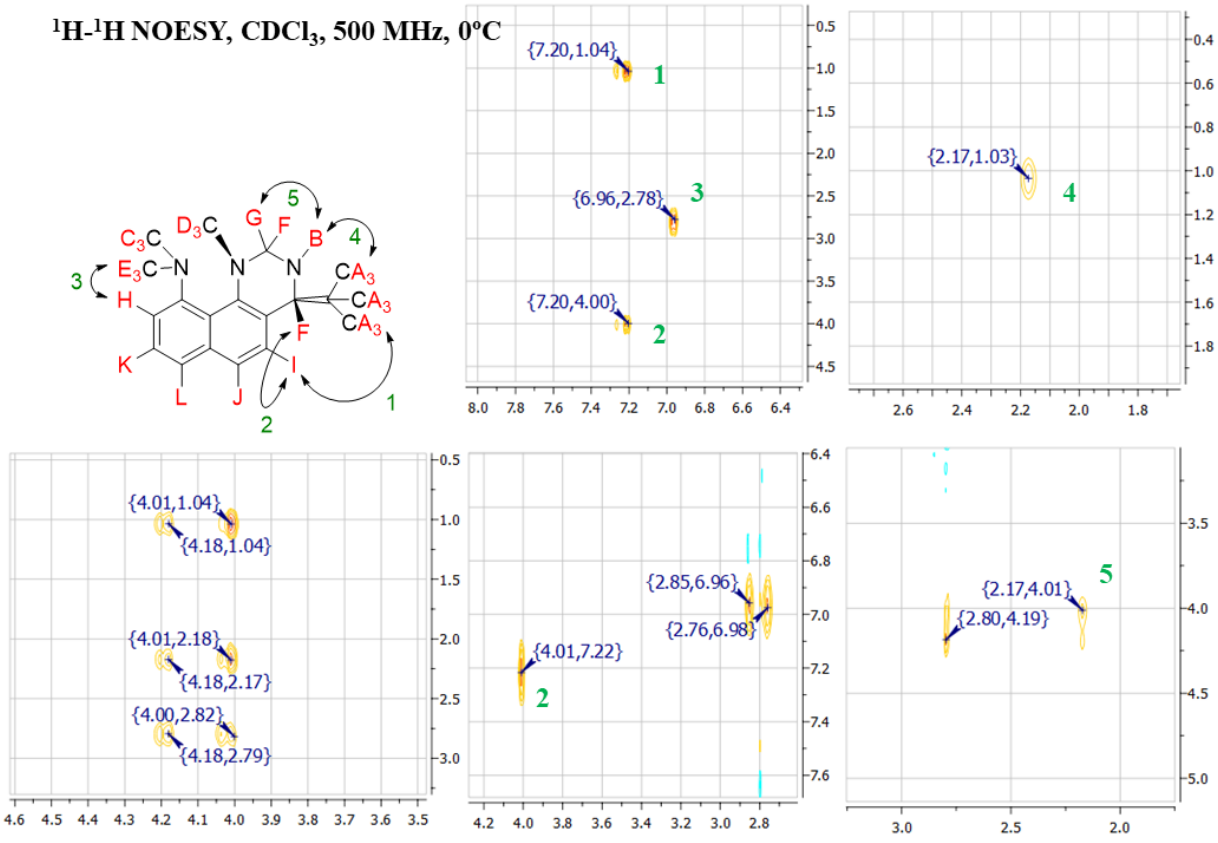

Figure S64. ^{1}H-^{1}H NOESY NMR spectrum of **8e**.

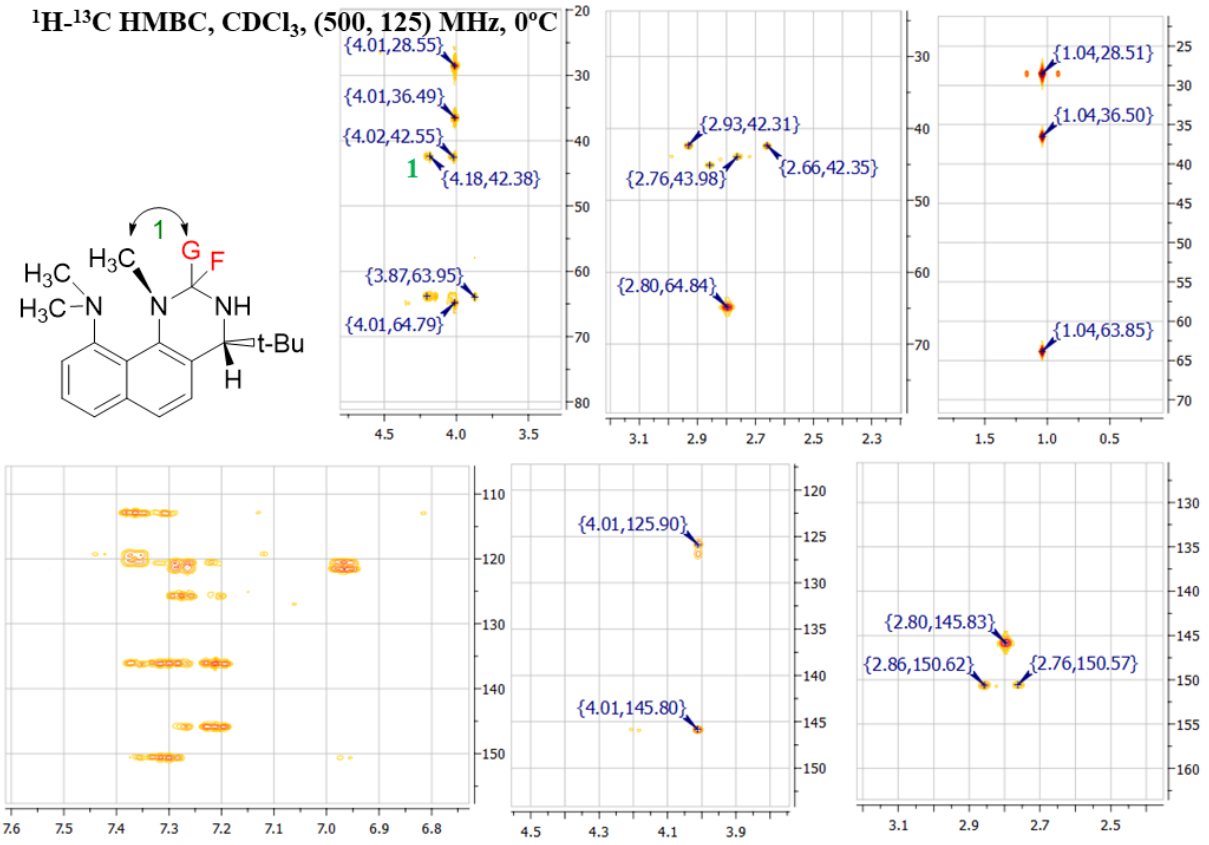

Figure S65. ^{1}H-^{13}C HMBC NMR spectrum of **8e**.

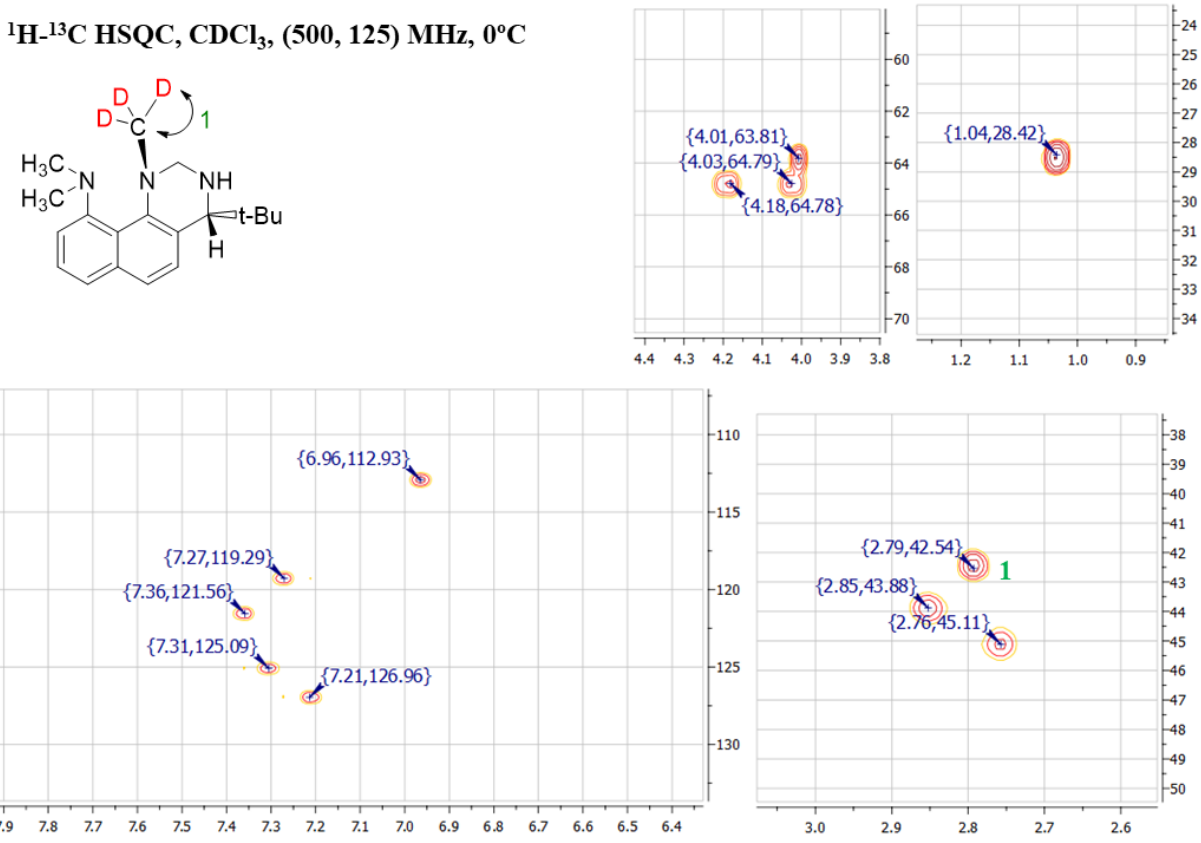

Figure S66. ^{1}H-^{13}C HSQC NMR spectrum of **8e**.

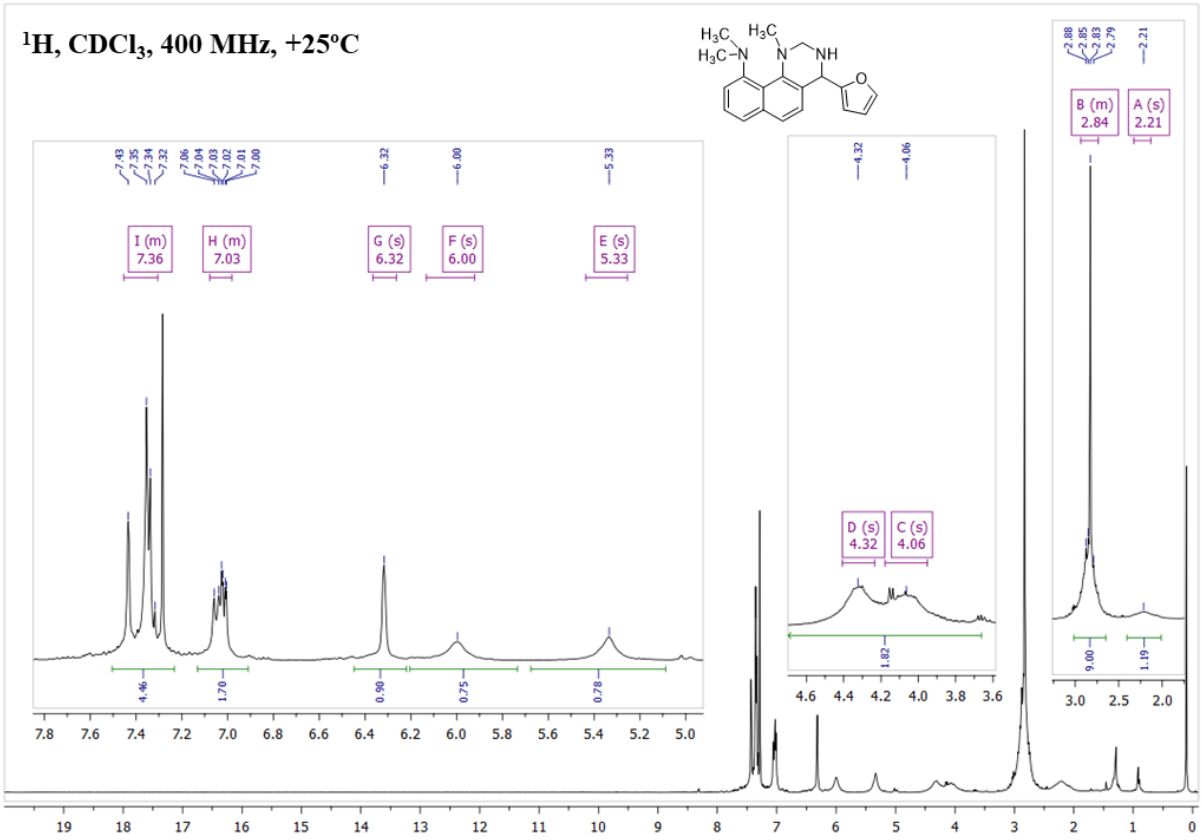

Figure S67. ^{1}H NMR spectrum of **8f**.

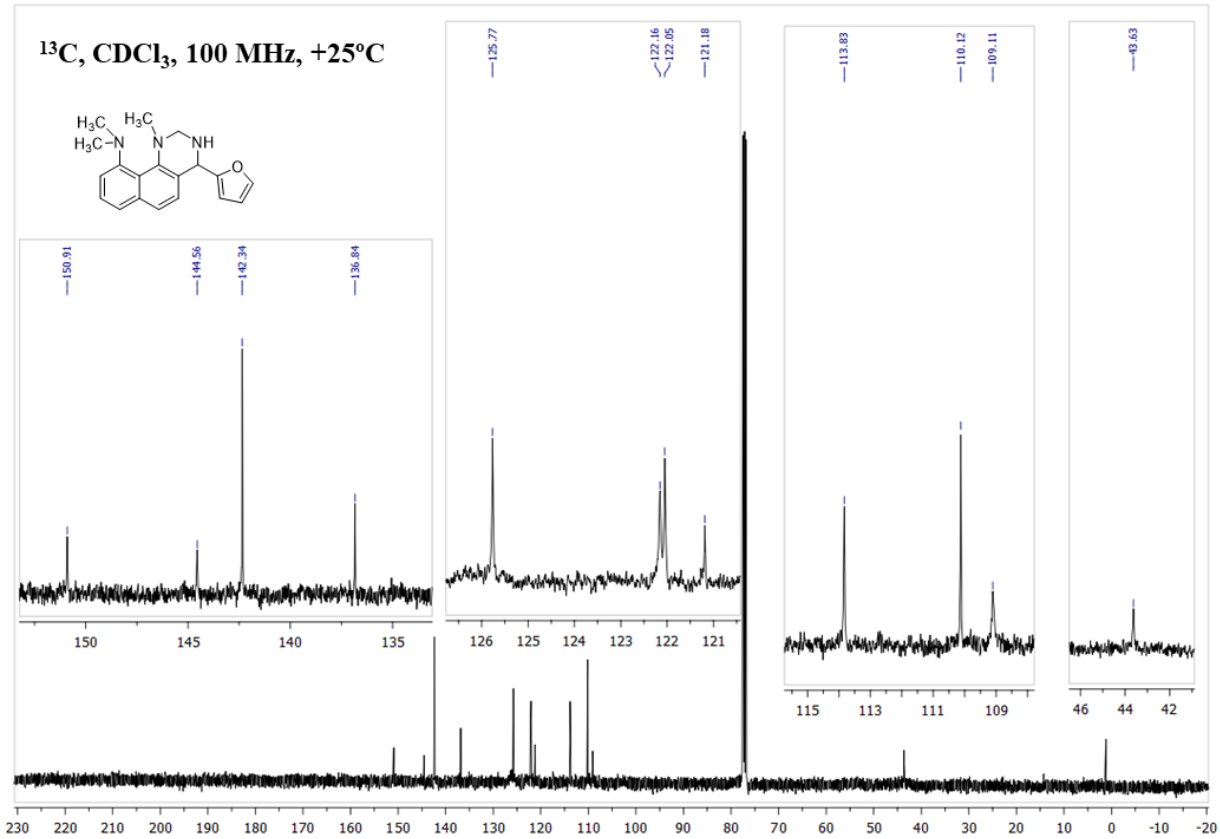

Figure S68. ^{13}C NMR spectrum of **8f**.

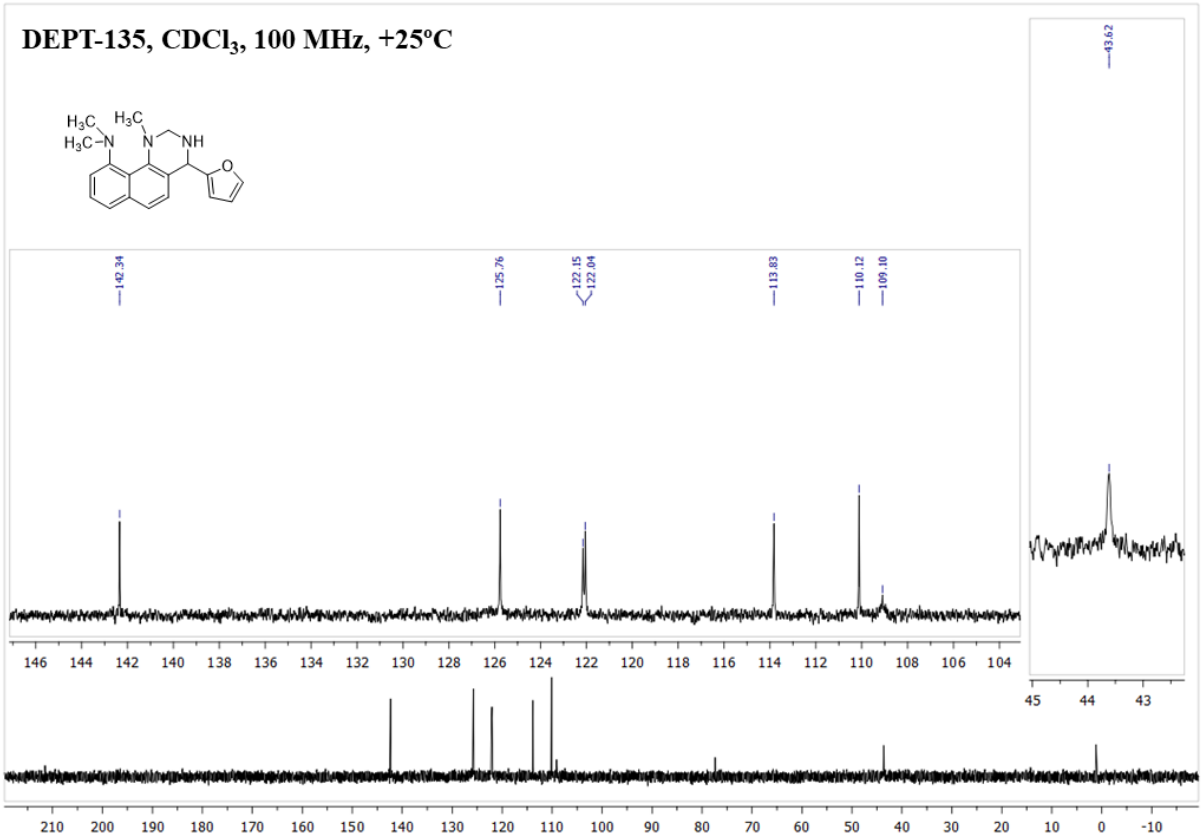

Figure S69. ^{13}C DEPT NMR spectrum of **8f**.

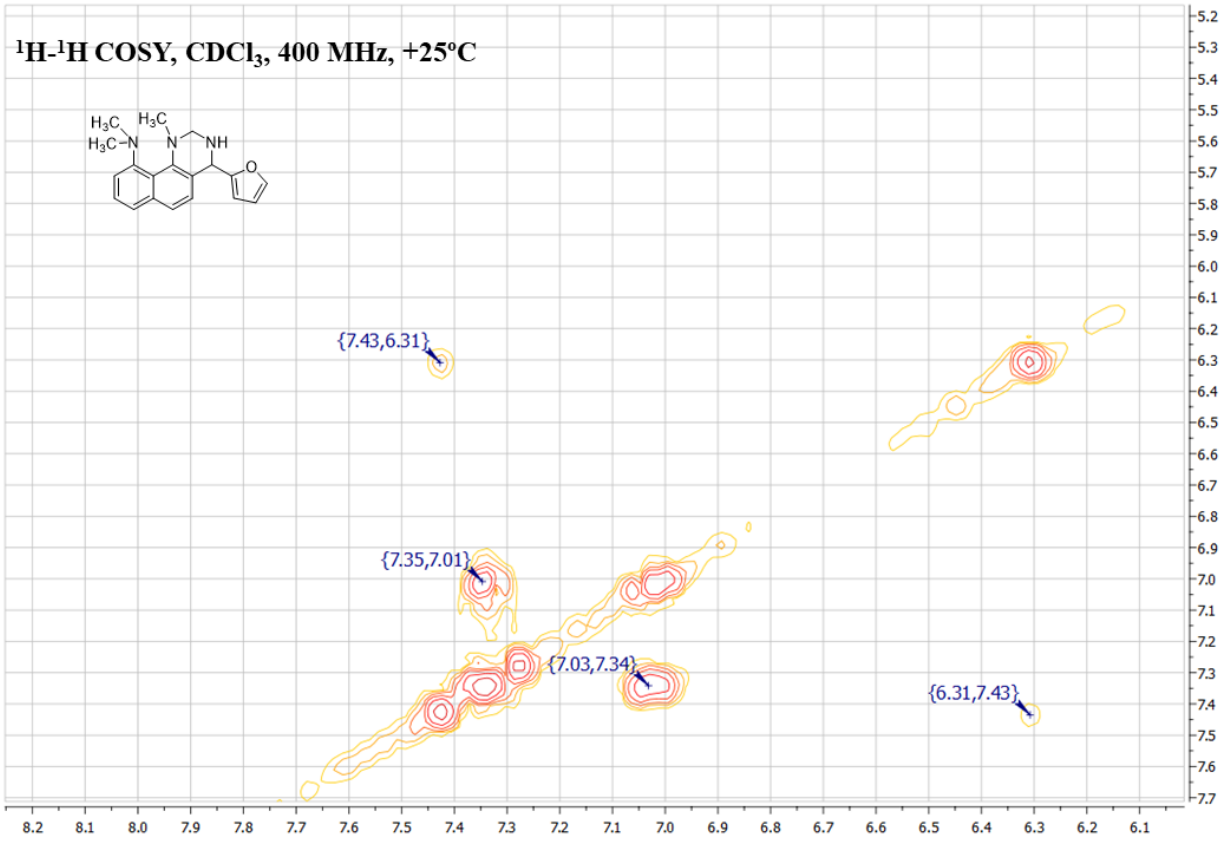

Figure S70. ^{1}H-^{1}H COSY NMR spectrum of **8f**.

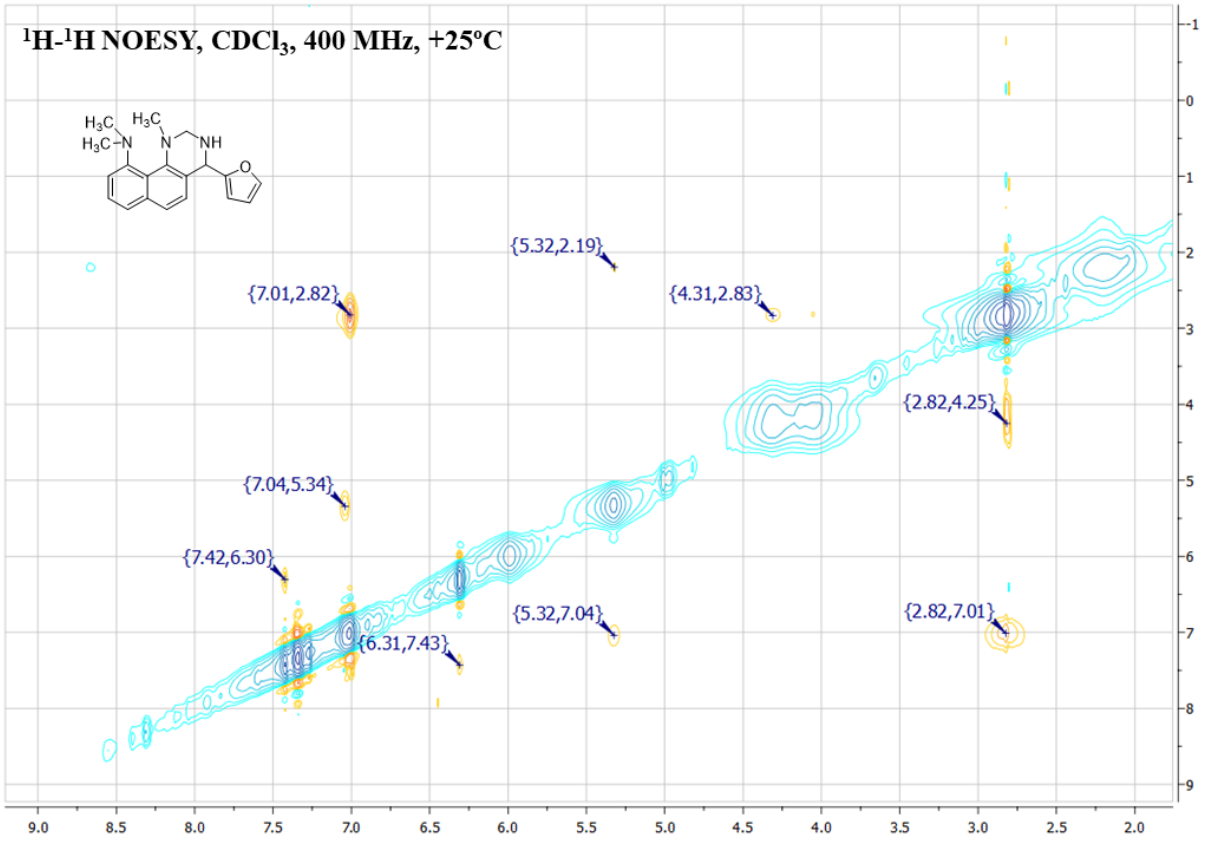

Figure S71. ^{1}H-^{1}H NOESY NMR spectrum of **8f**.

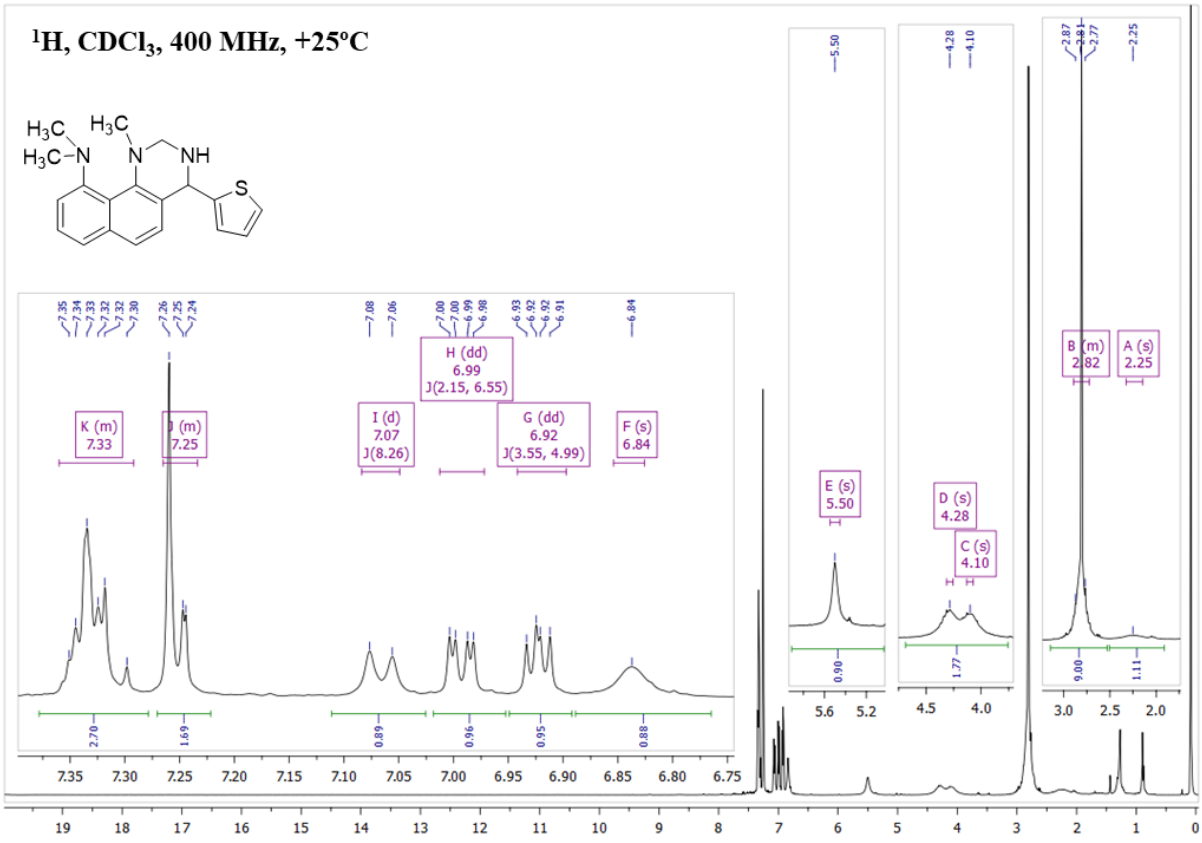

Figure S72. ^{1}H NMR spectrum of **8g**.

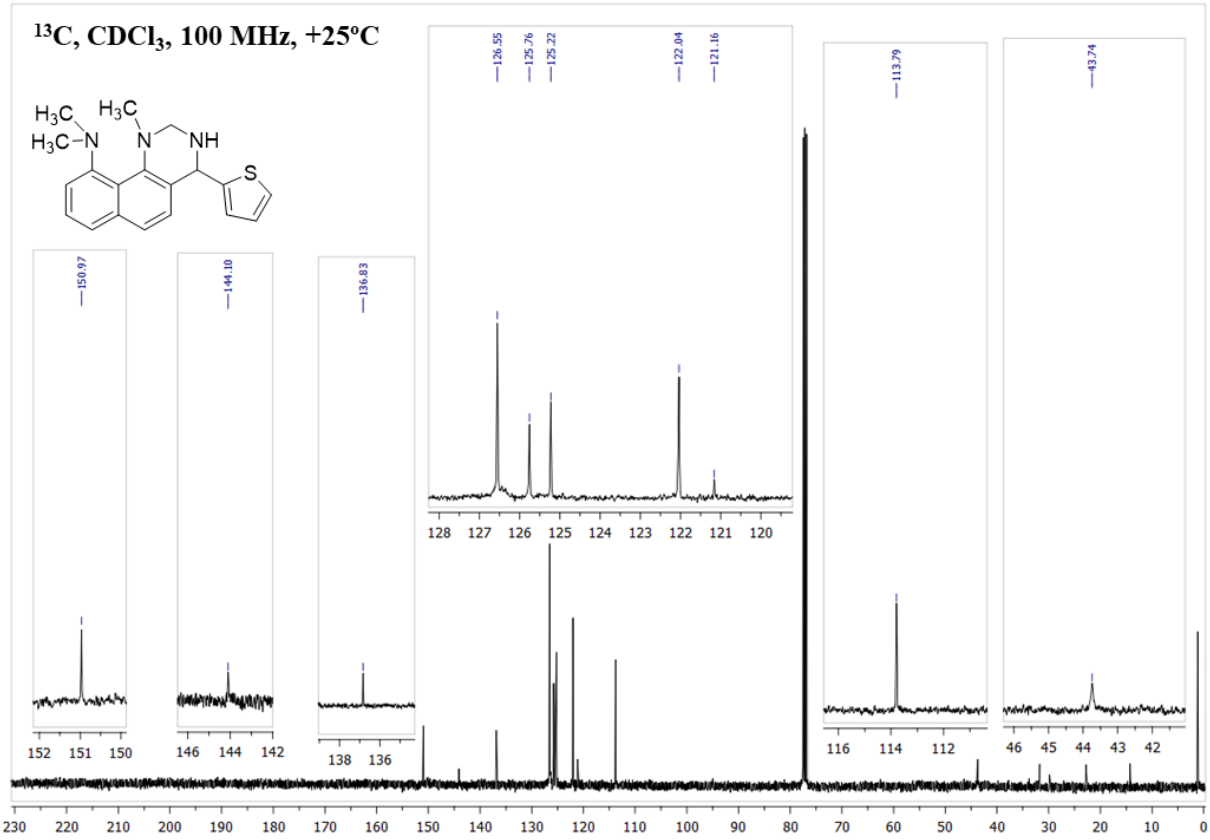

Figure S73. ^{13}C NMR spectrum of **8g**.

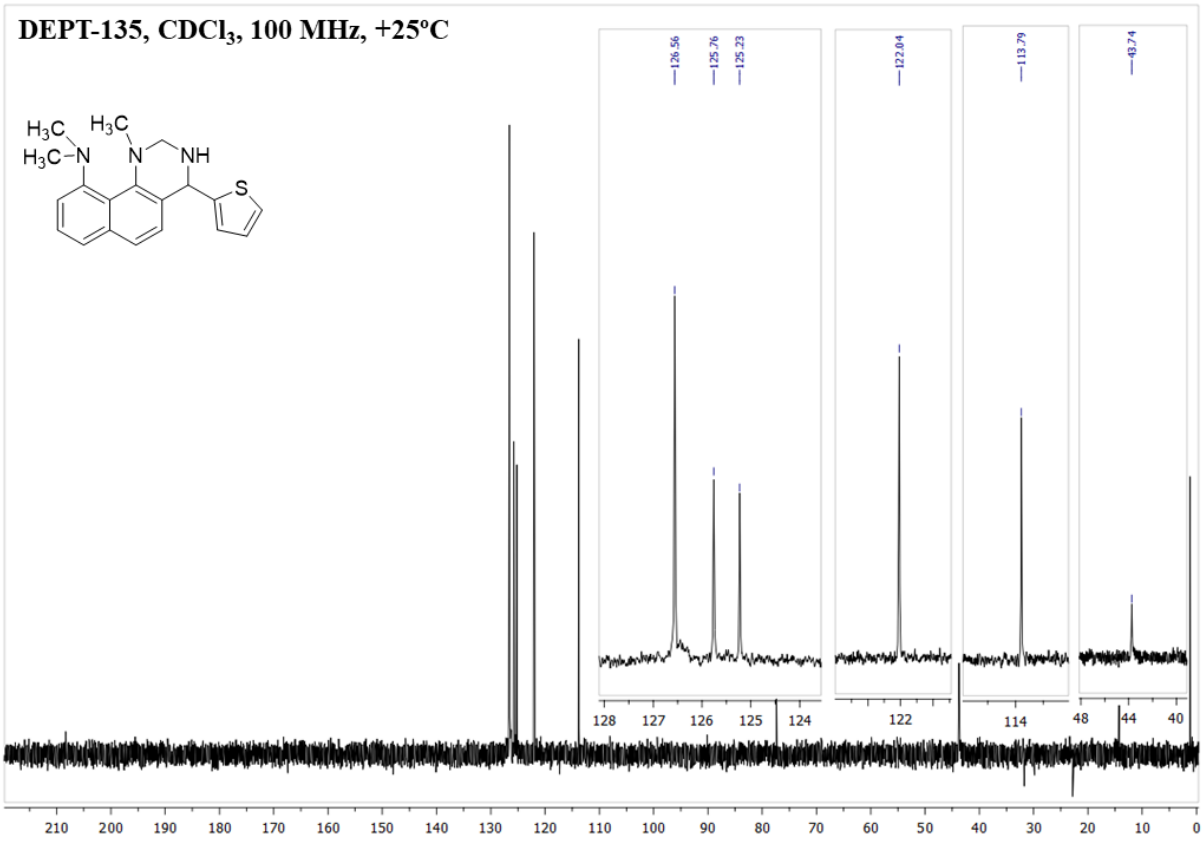

Figure S74. ^{13}C DEPT NMR spectrum of **8g**.

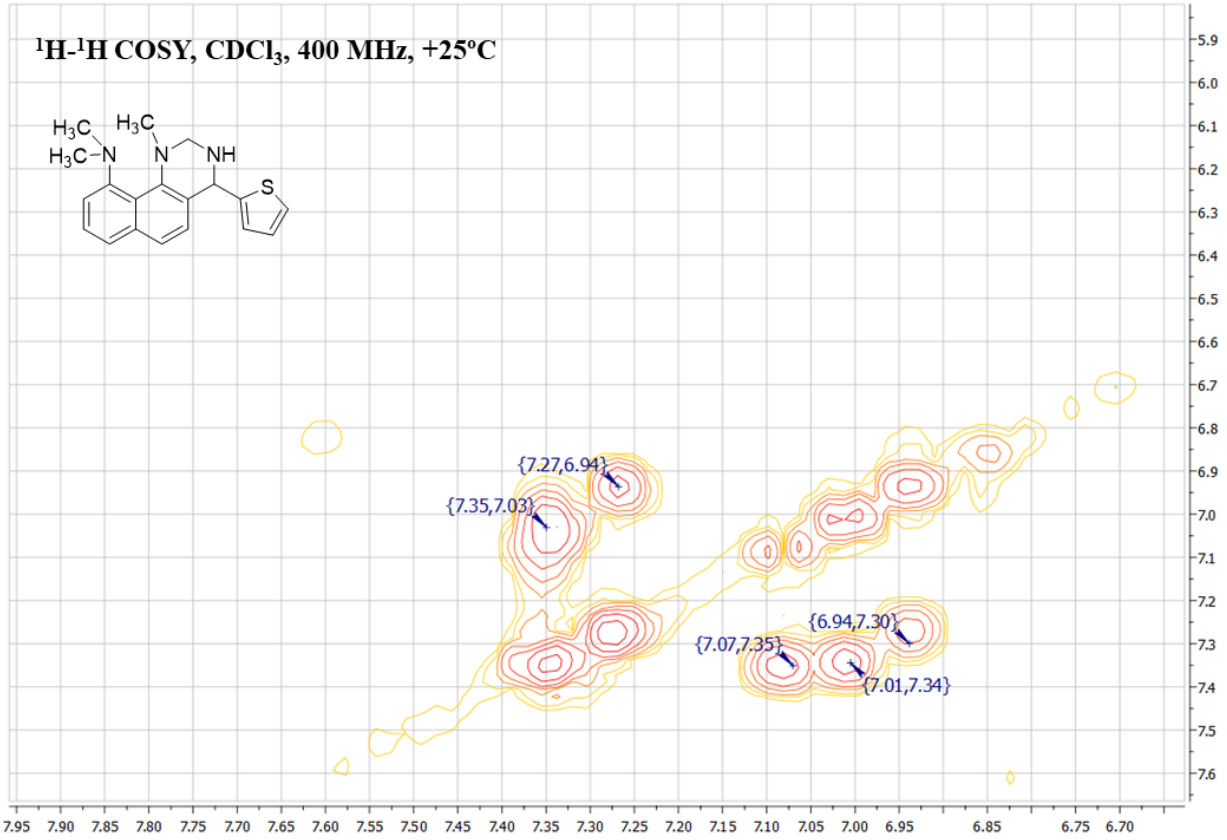

Figure S75. ^{1}H-^{1}H COSY NMR spectrum of **8g**.

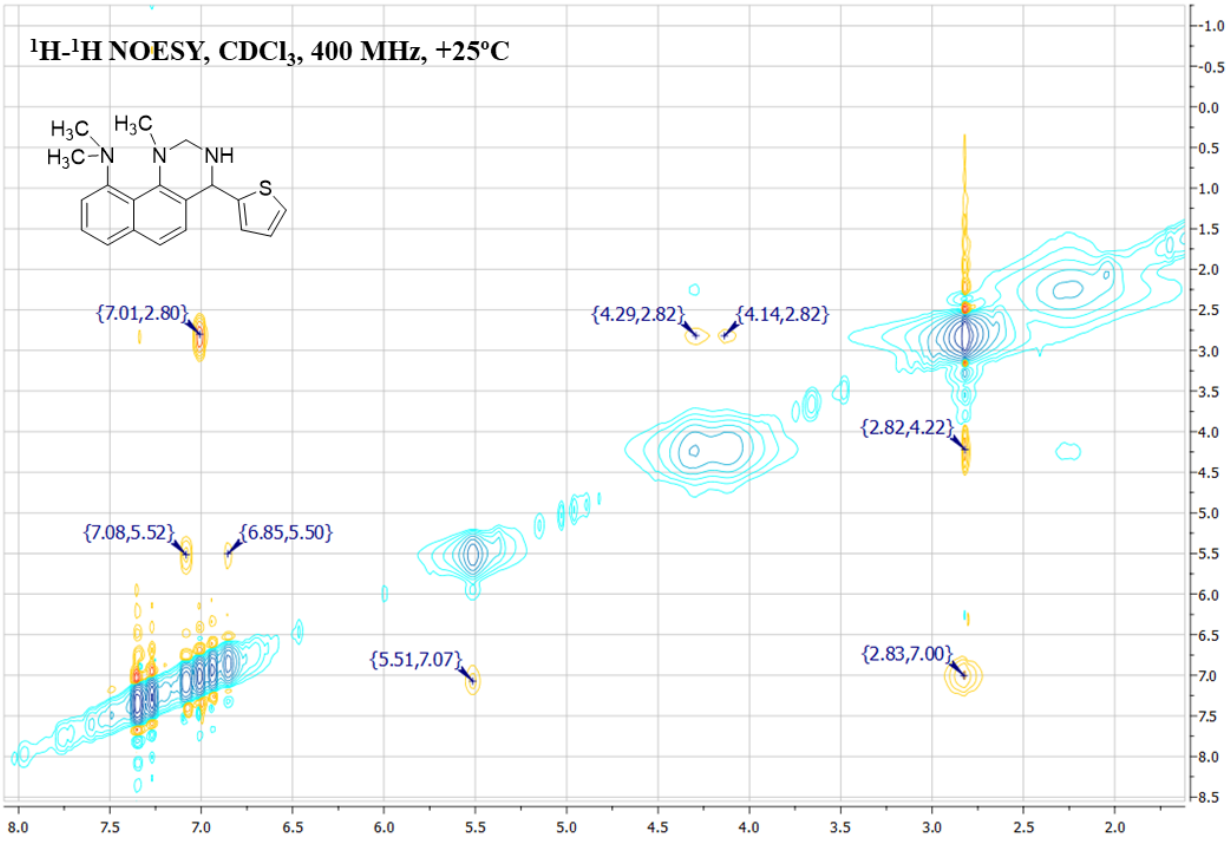

Figure S76. ^{1}H-^{1}H NOESY NMR spectrum of **8g**.

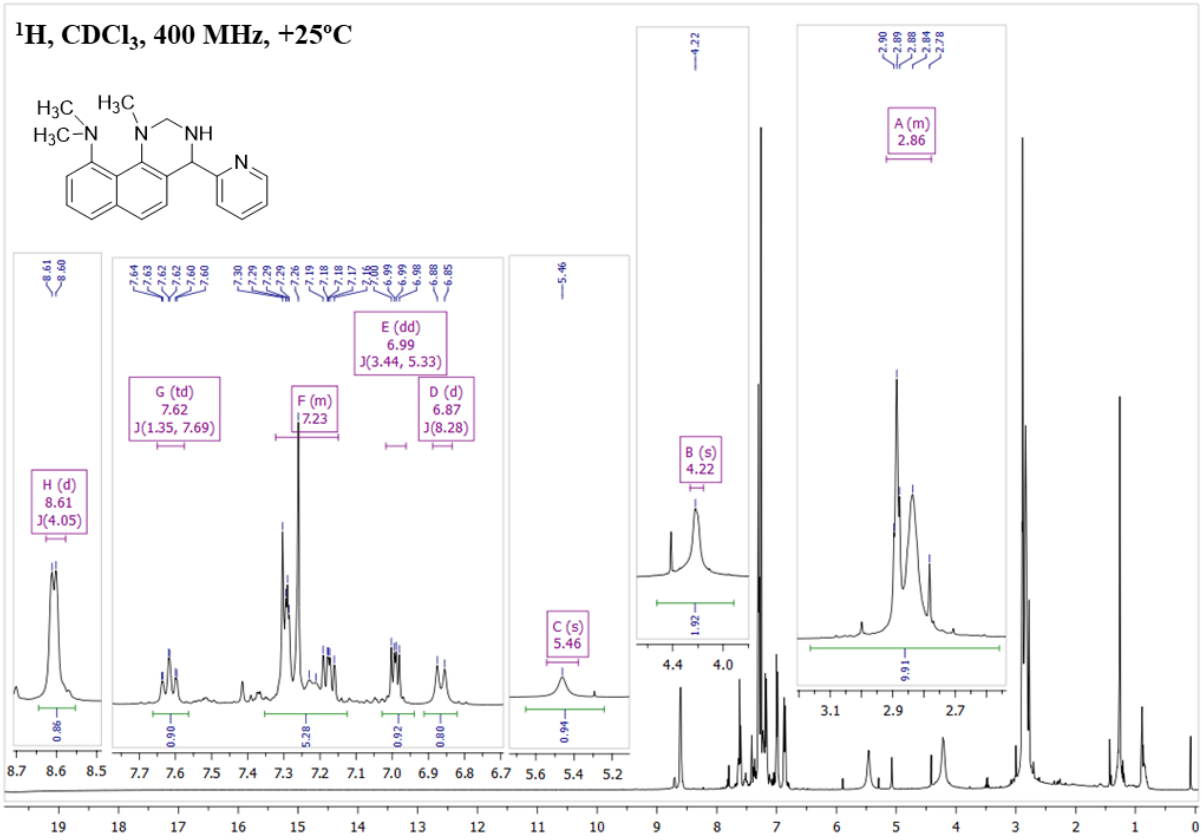

Figure S77. ^{1}H NMR spectrum of **8h**.

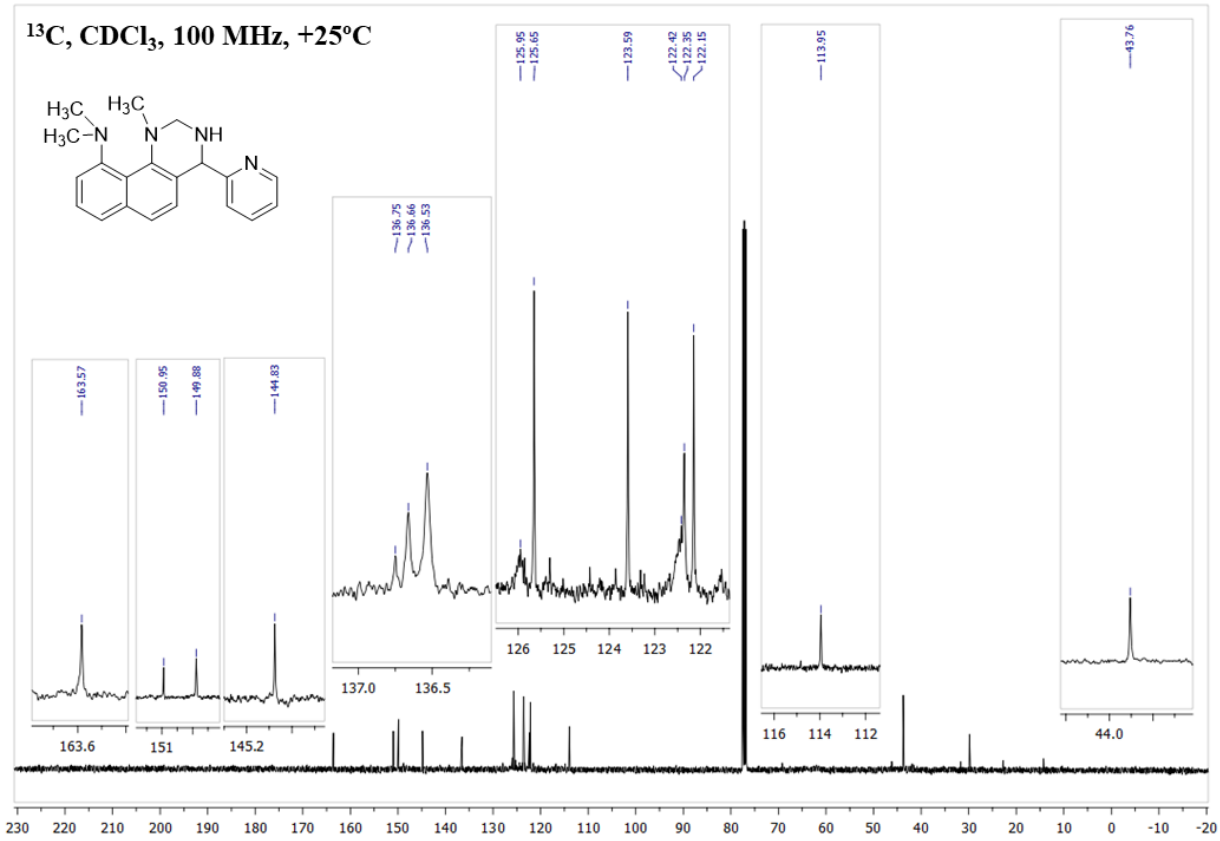

Figure S78. ^{13}C NMR spectrum of **8h**.

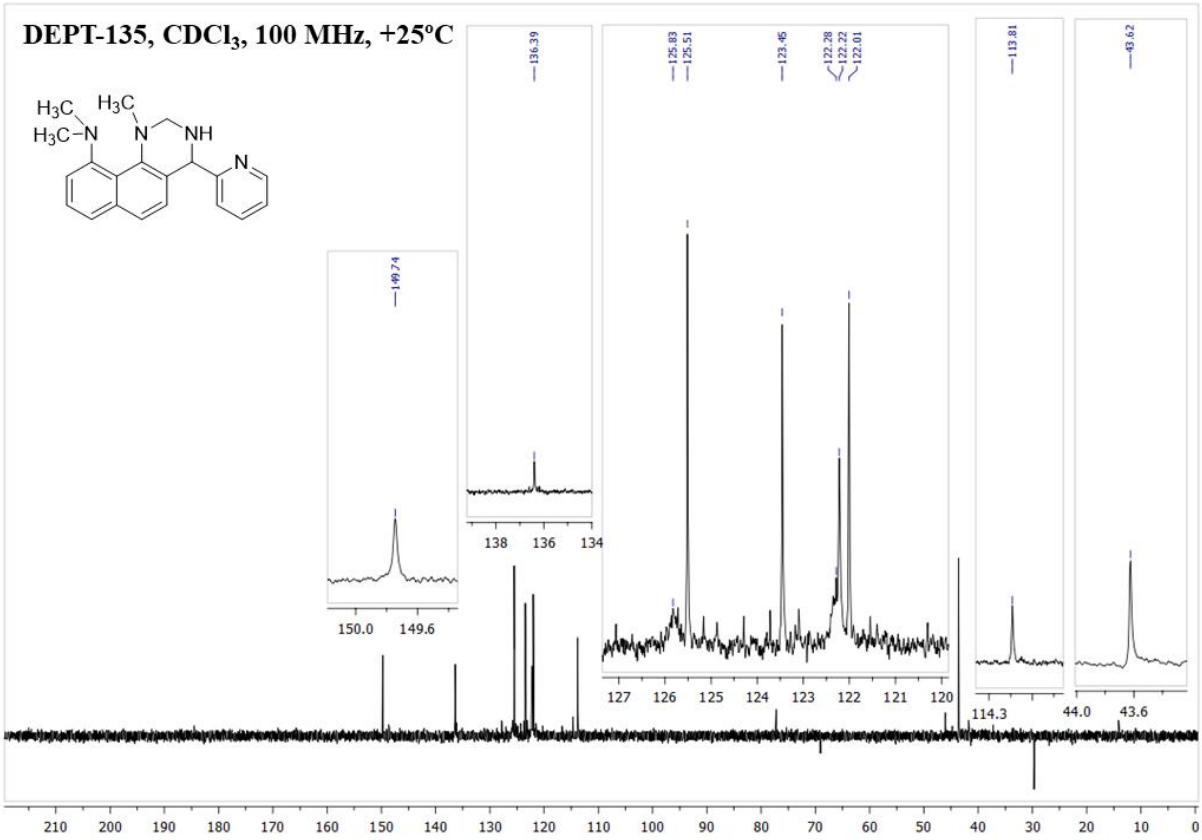

Figure S79. ^{13}C DEPT NMR spectrum of **8h**.

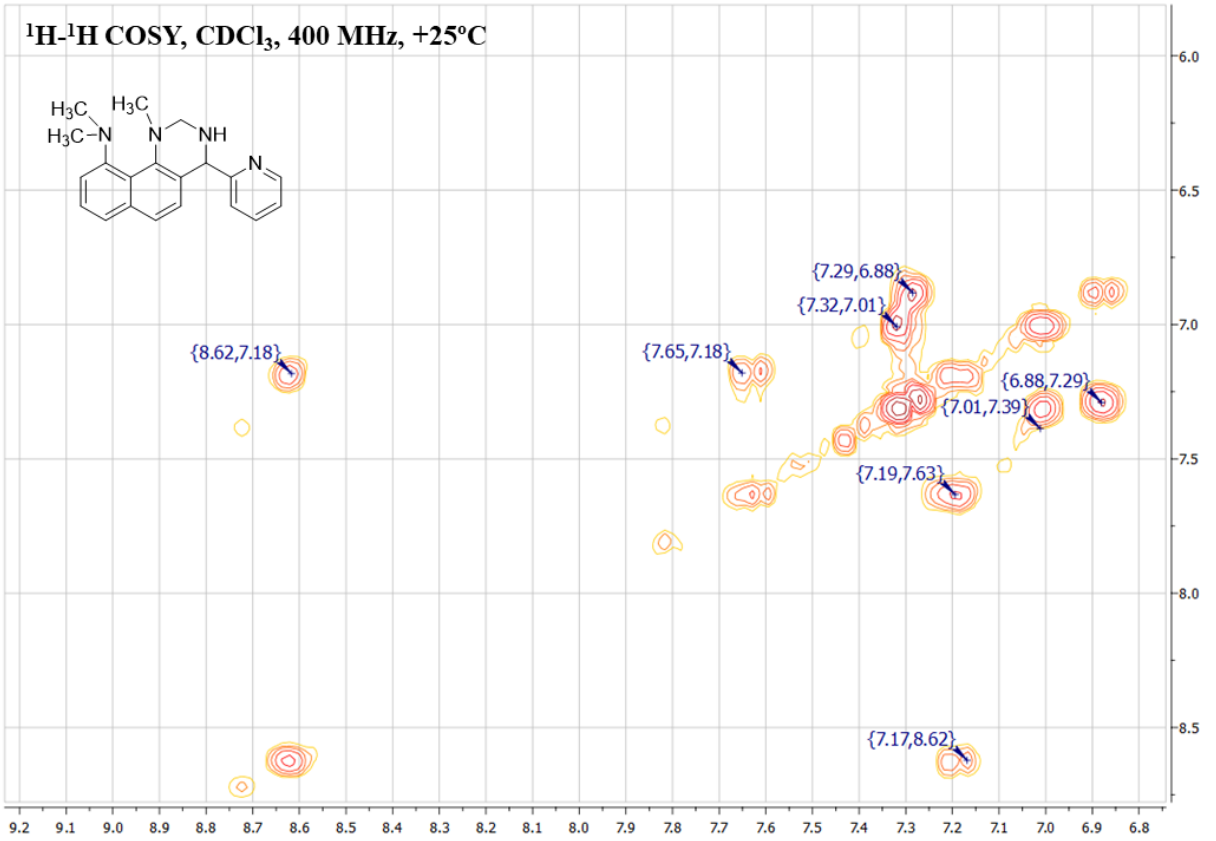

Figure S80. ^{1}H-^{1}H COSY NMR spectrum of **8h**.

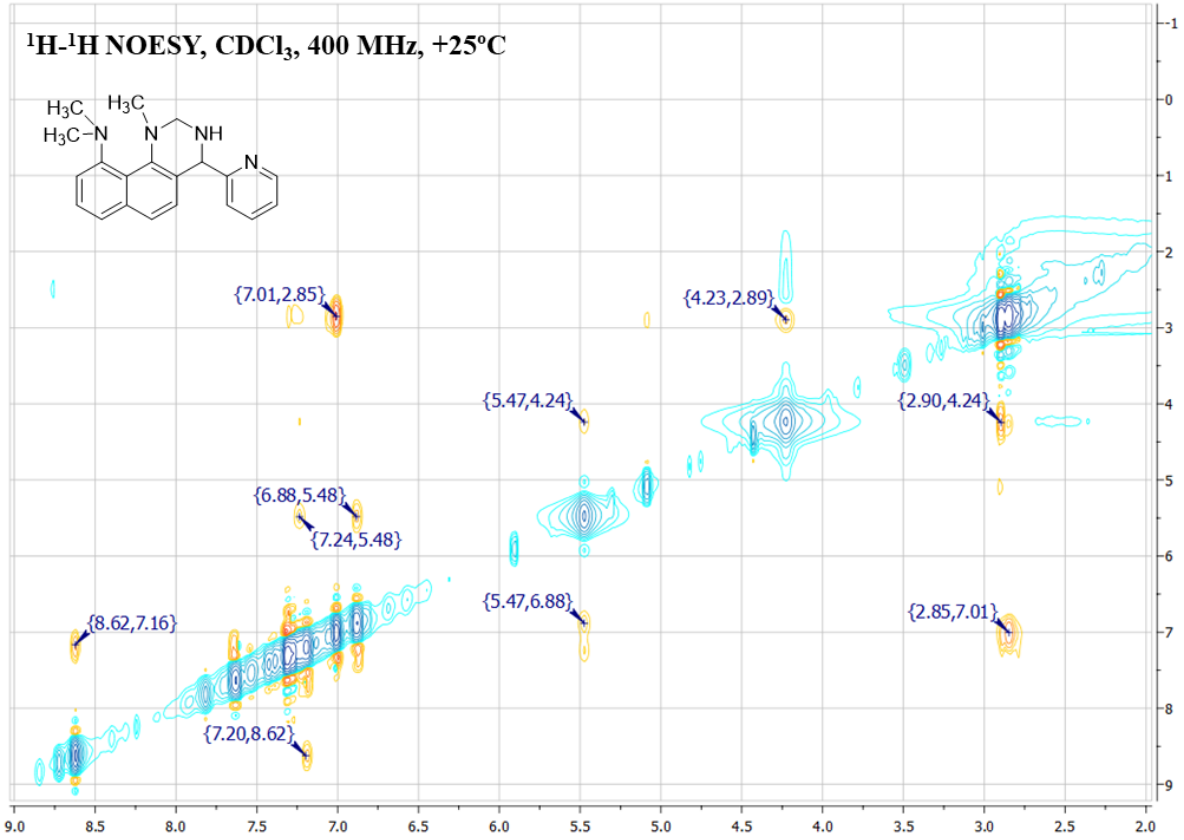

Figure S81. ^{1}H-^{1}H NOESY NMR spectrum of **8h**.

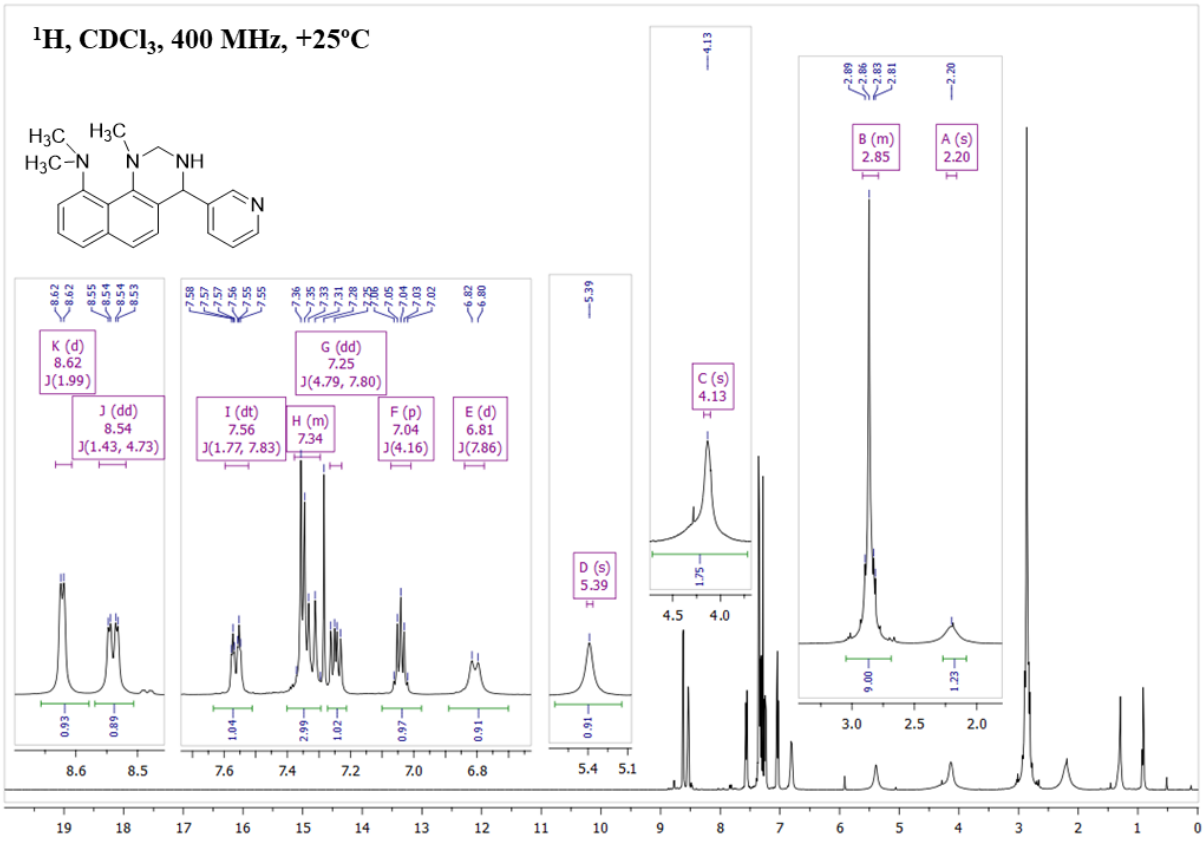

Figure S82. ^{1}H NMR spectrum of **8i**.

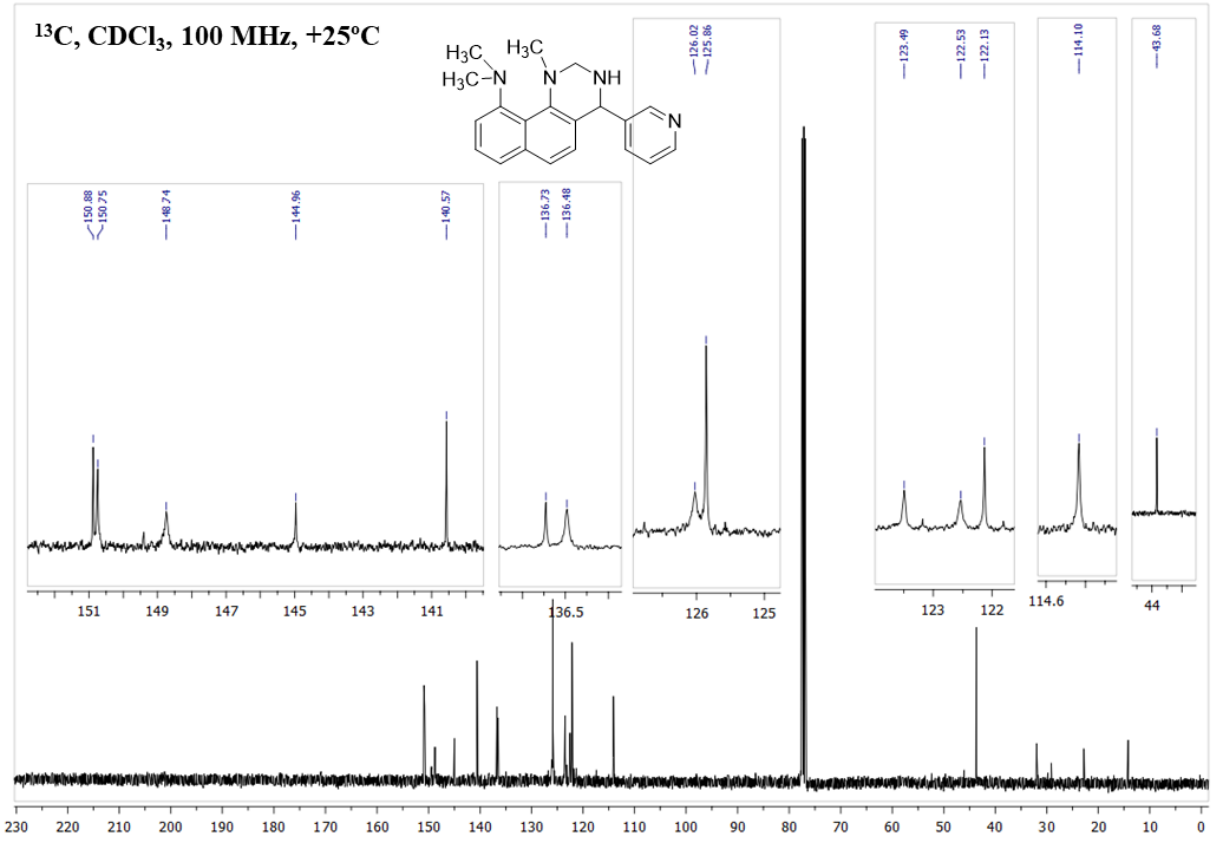

Figure S83. ^{13}C NMR spectrum of **8i**.

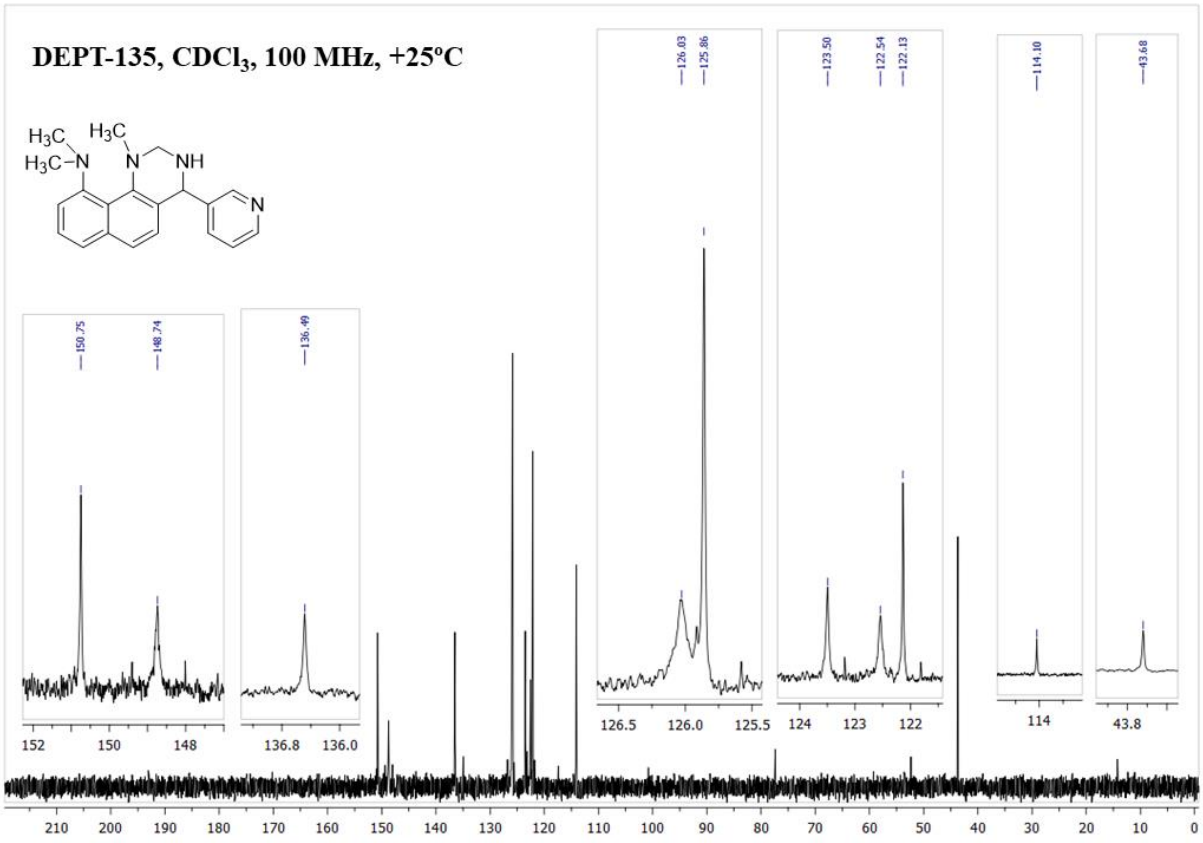

Figure S84. ^{13}C DEPT NMR spectrum of **8i**.

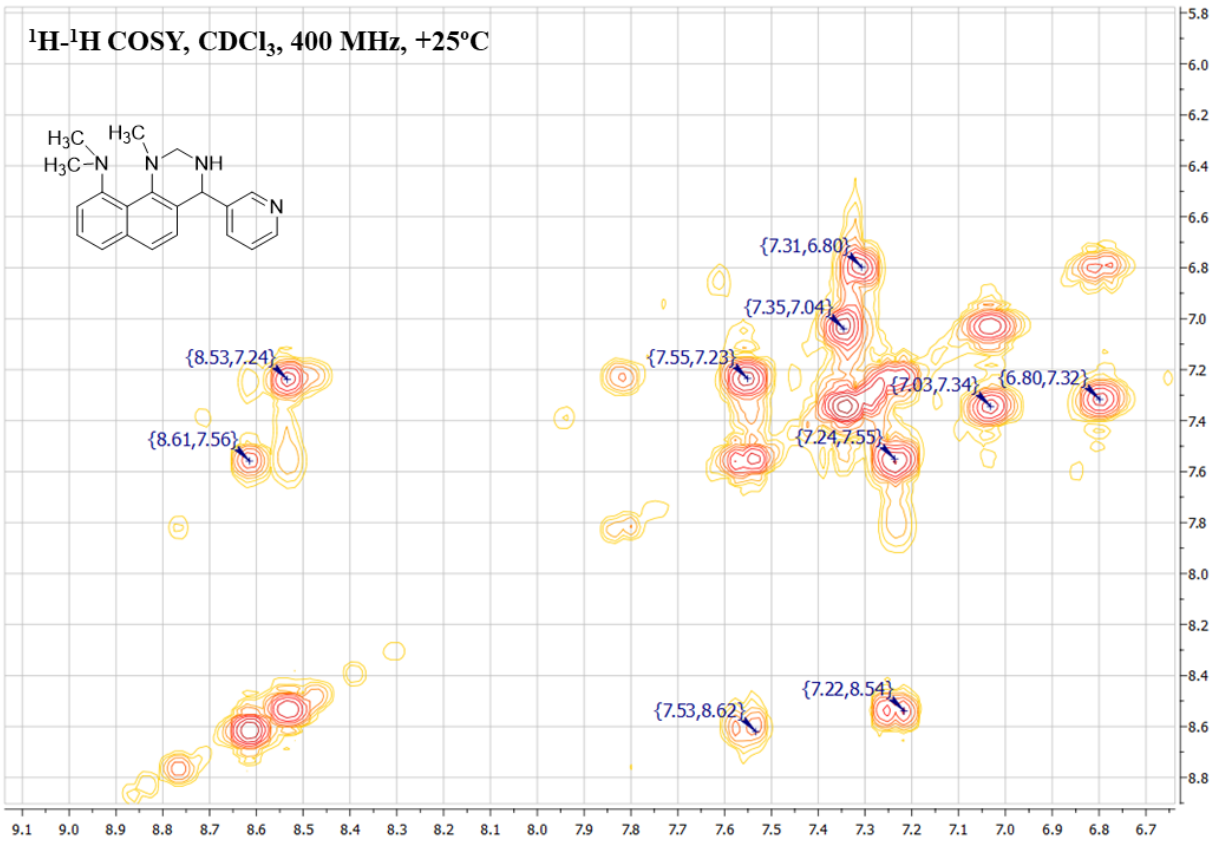

Figure S85. ^{1}H-^{1}H COSY NMR spectrum of **8i**.

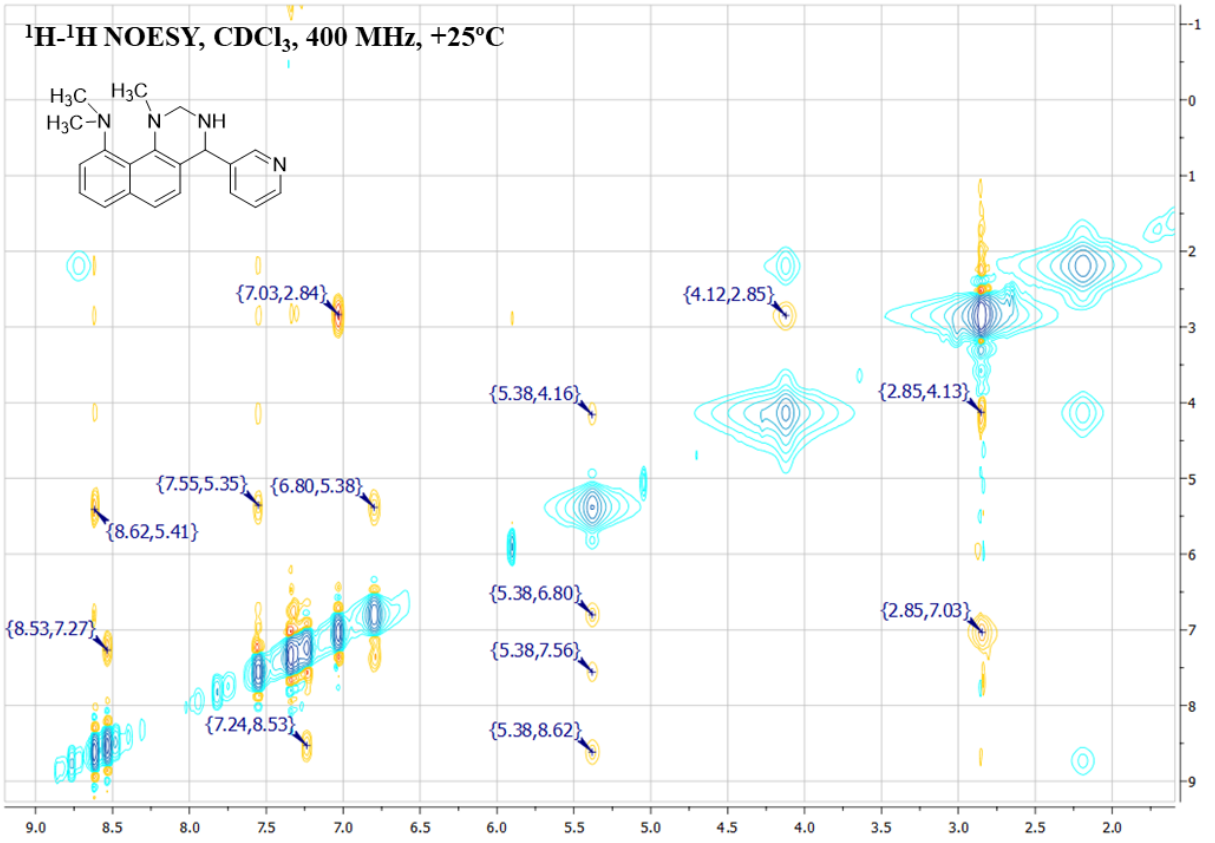

Figure S86. ^{1}H-^{1}H NOESY NMR spectrum of **8i**.

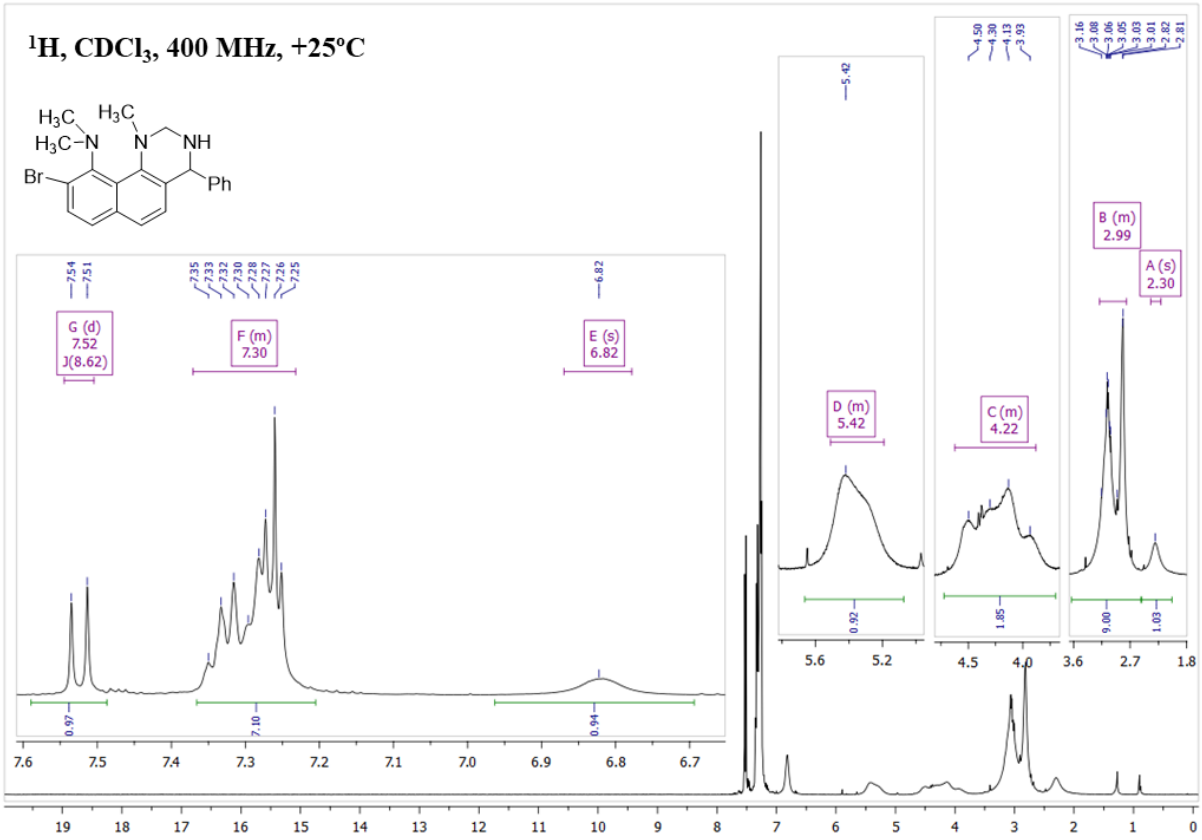

Figure S87. ^{1}H NMR spectrum of **8j**.

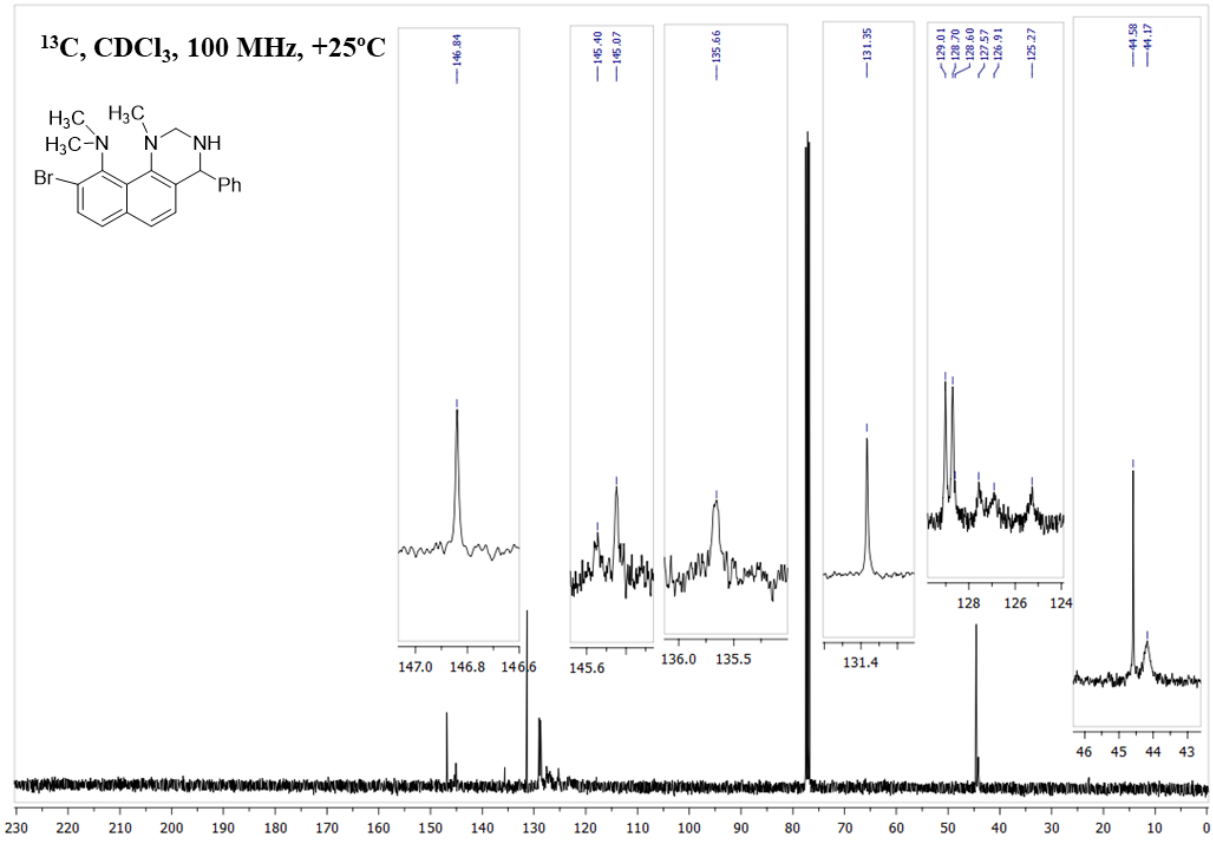

Figure S88. ^{13}C NMR spectrum of **8j**.

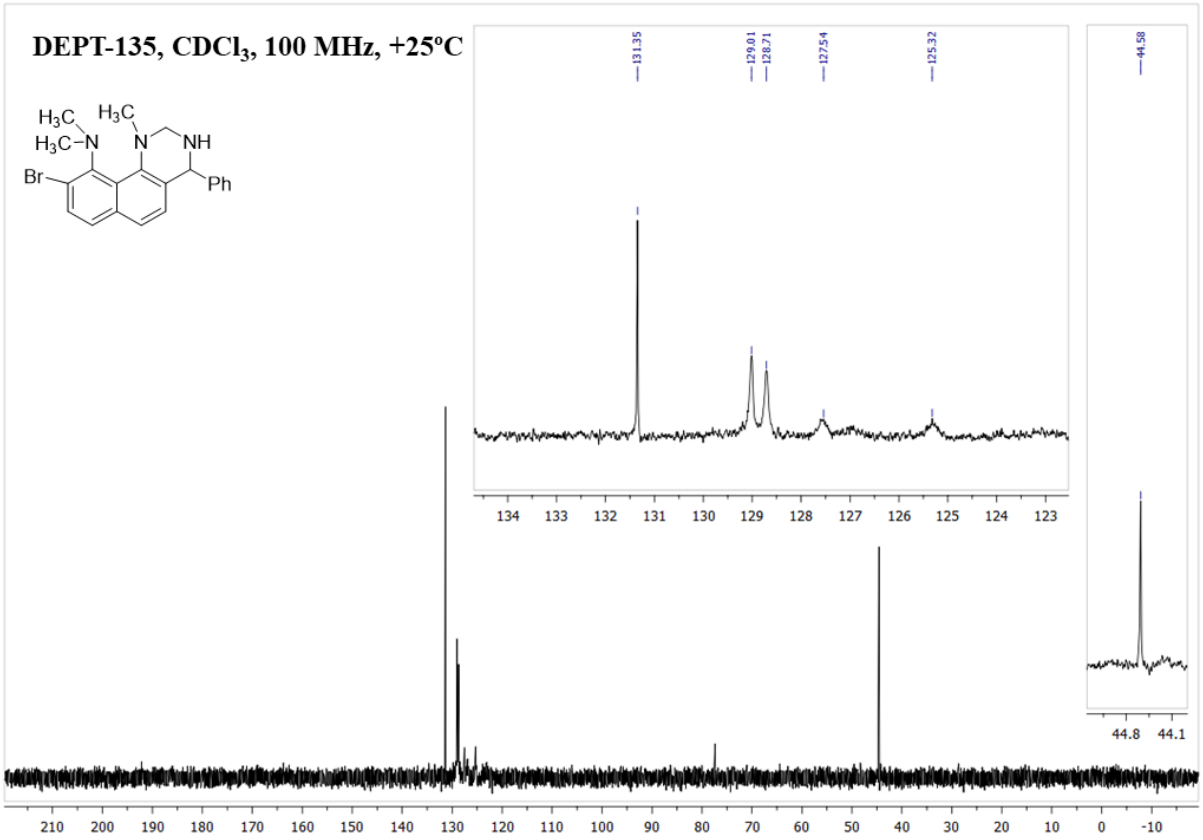

Figure S89. ^{13}C DEPT NMR spectrum of **8j**.

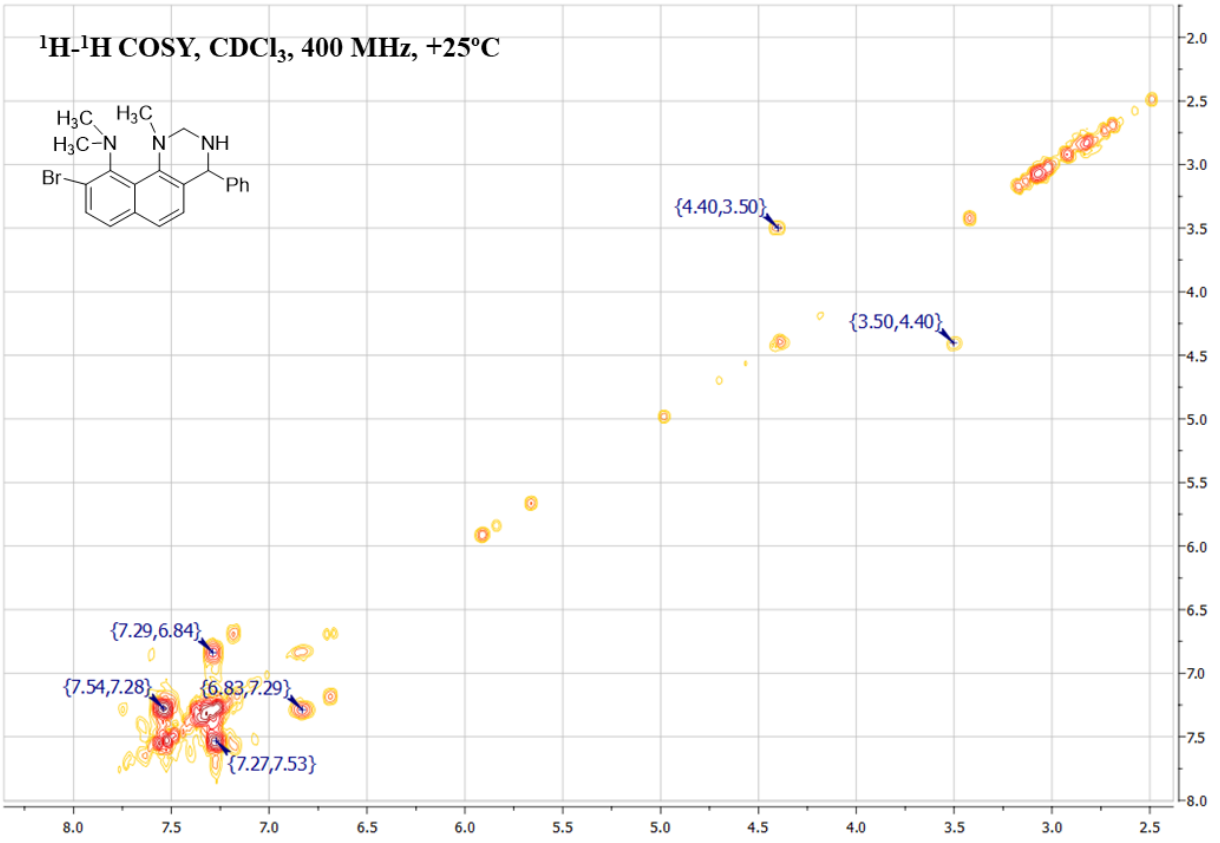

Figure S90. ^{1}H-^{1}H COSY NMR spectrum of **8j**.

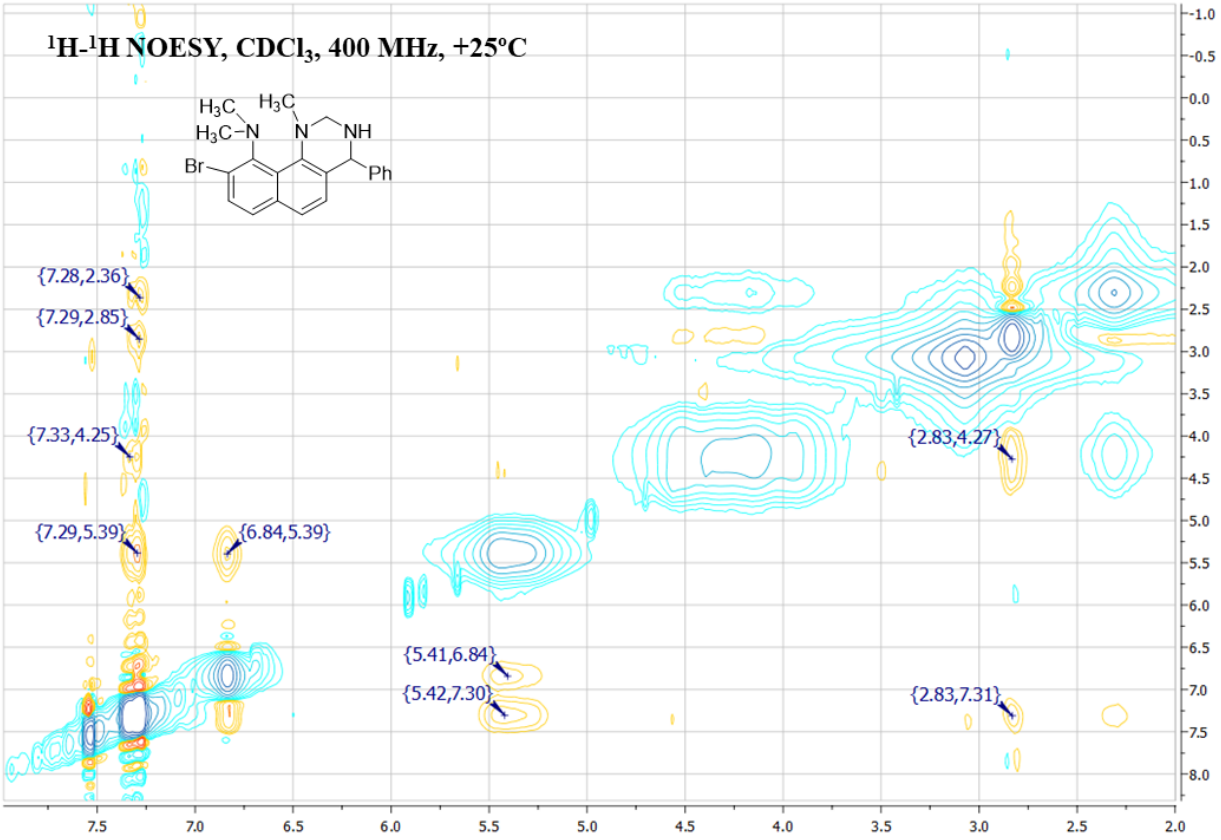

Figure S91. ^{1}H-^{1}H NOESY NMR spectrum of **8j**.

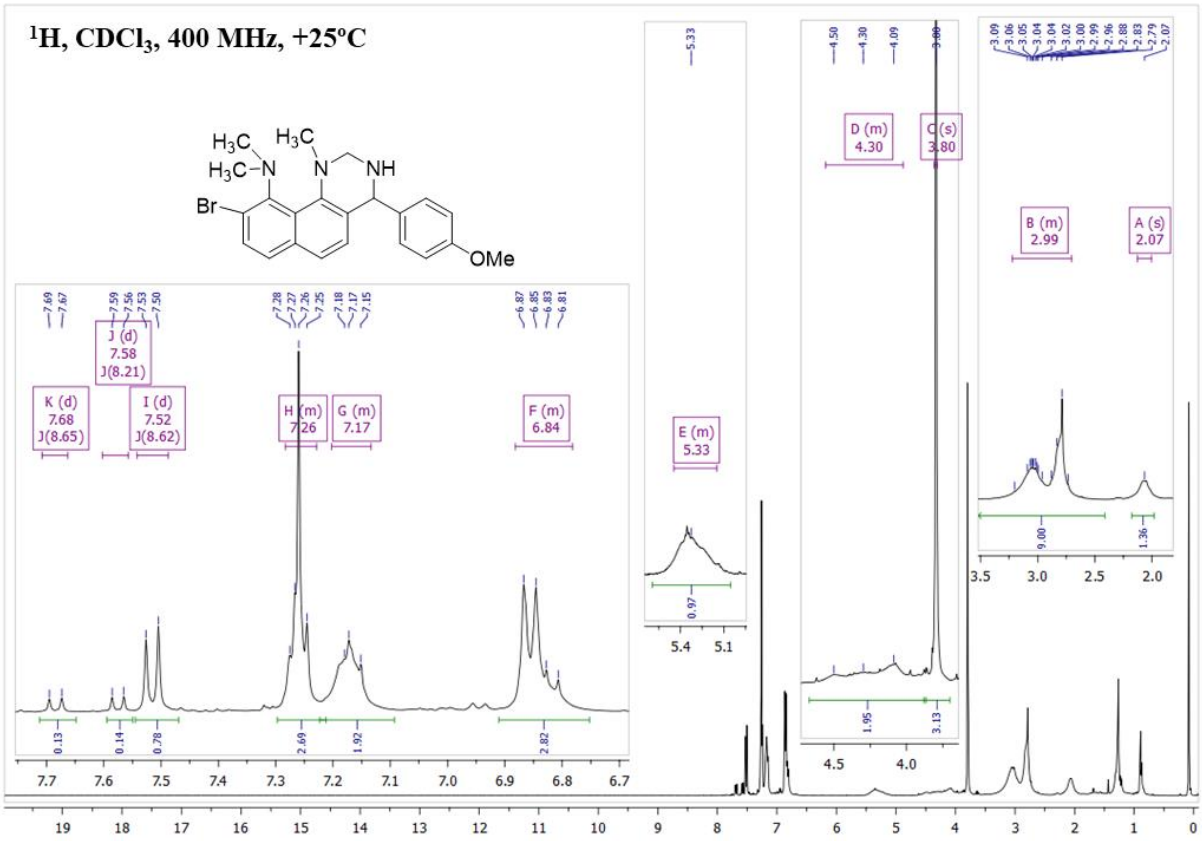

Figure S92. ^{1}H NMR spectrum of **8k**.

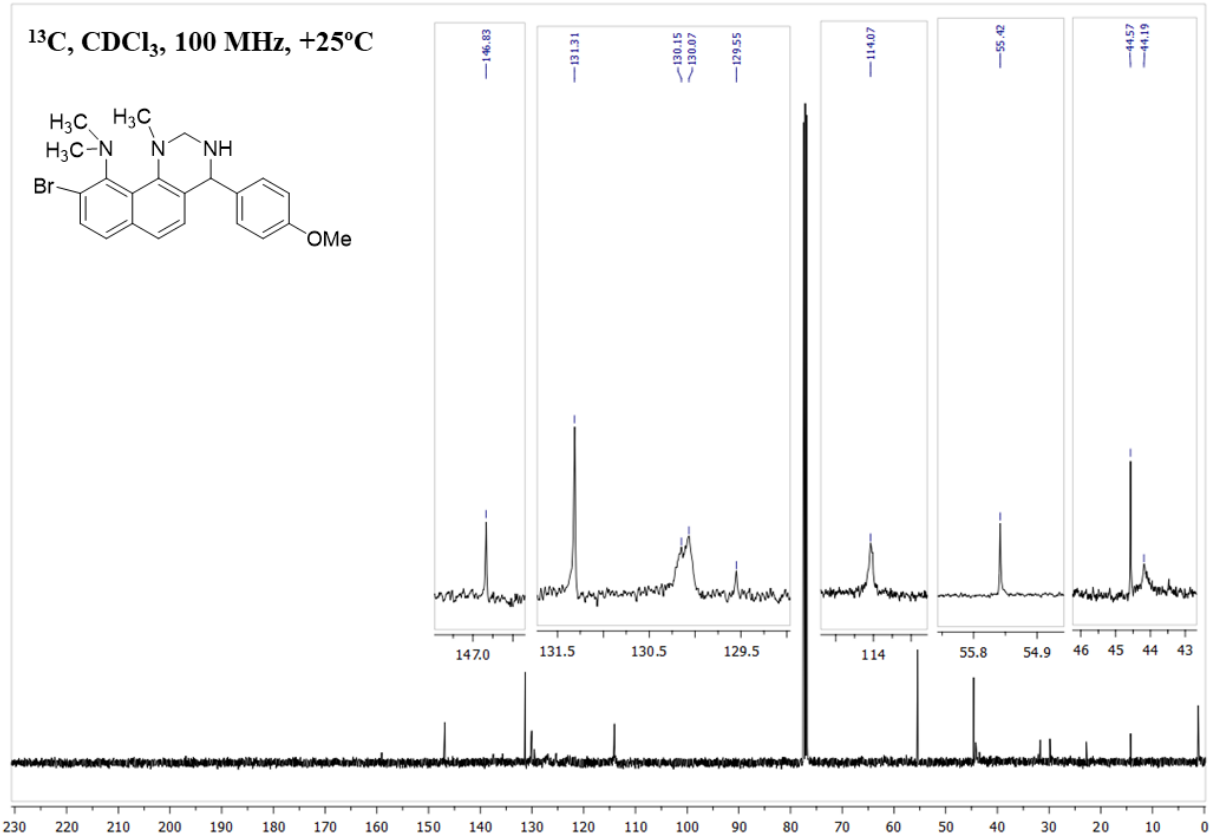

Figure S93. ^{13}C NMR spectrum of **8k**.

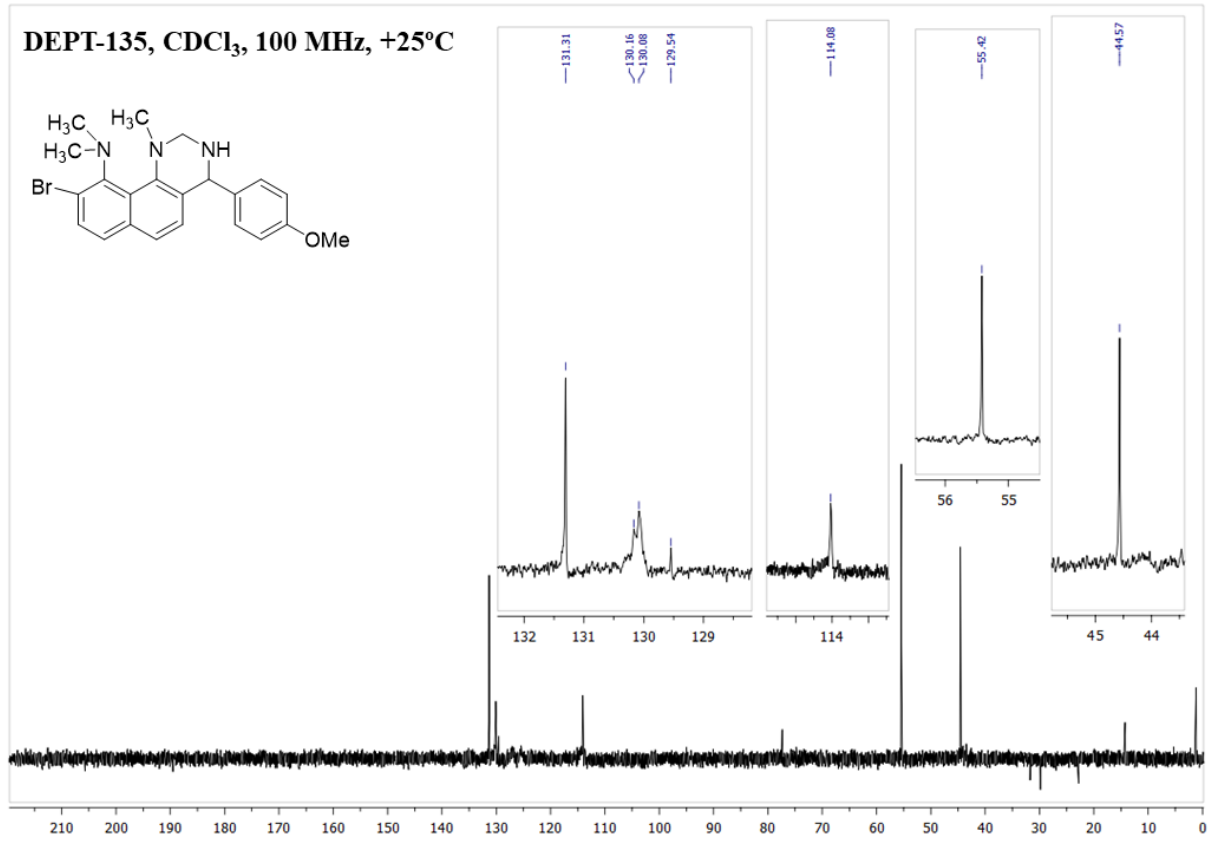

Figure S94. ^{13}C DEPT NMR spectrum of **8k**.

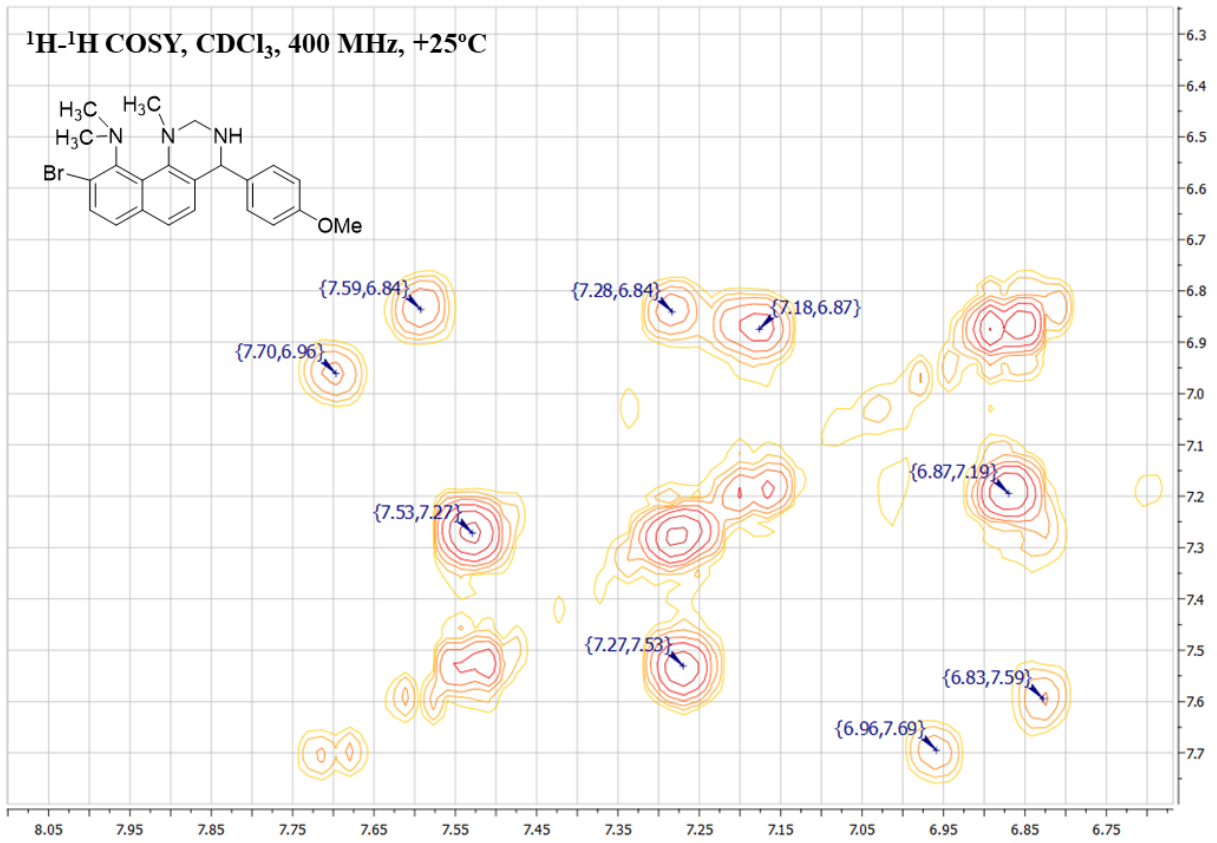

Figure S95. ^{1}H-^{1}H COSY NMR spectrum of **8k**.

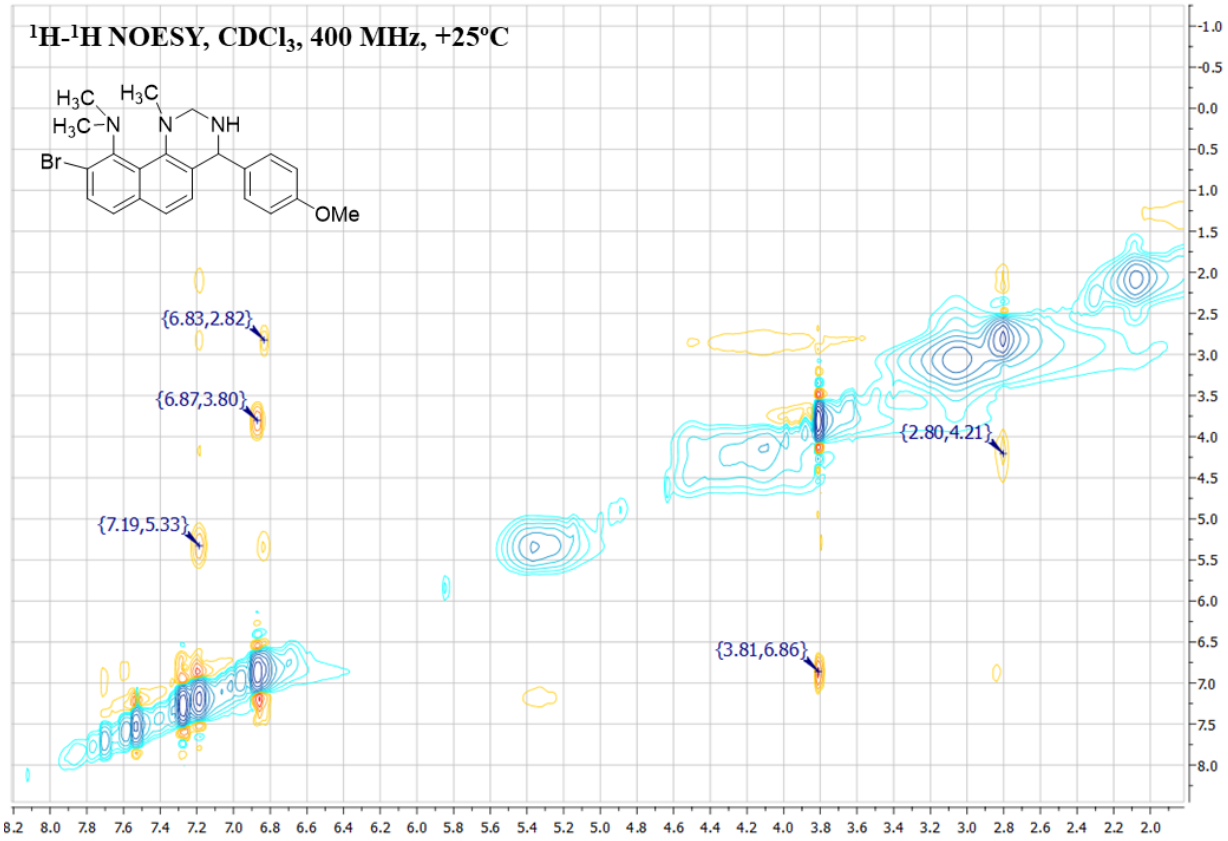

Figure S96. ^{1}H-^{1}H NOESY NMR spectrum of **8k**.

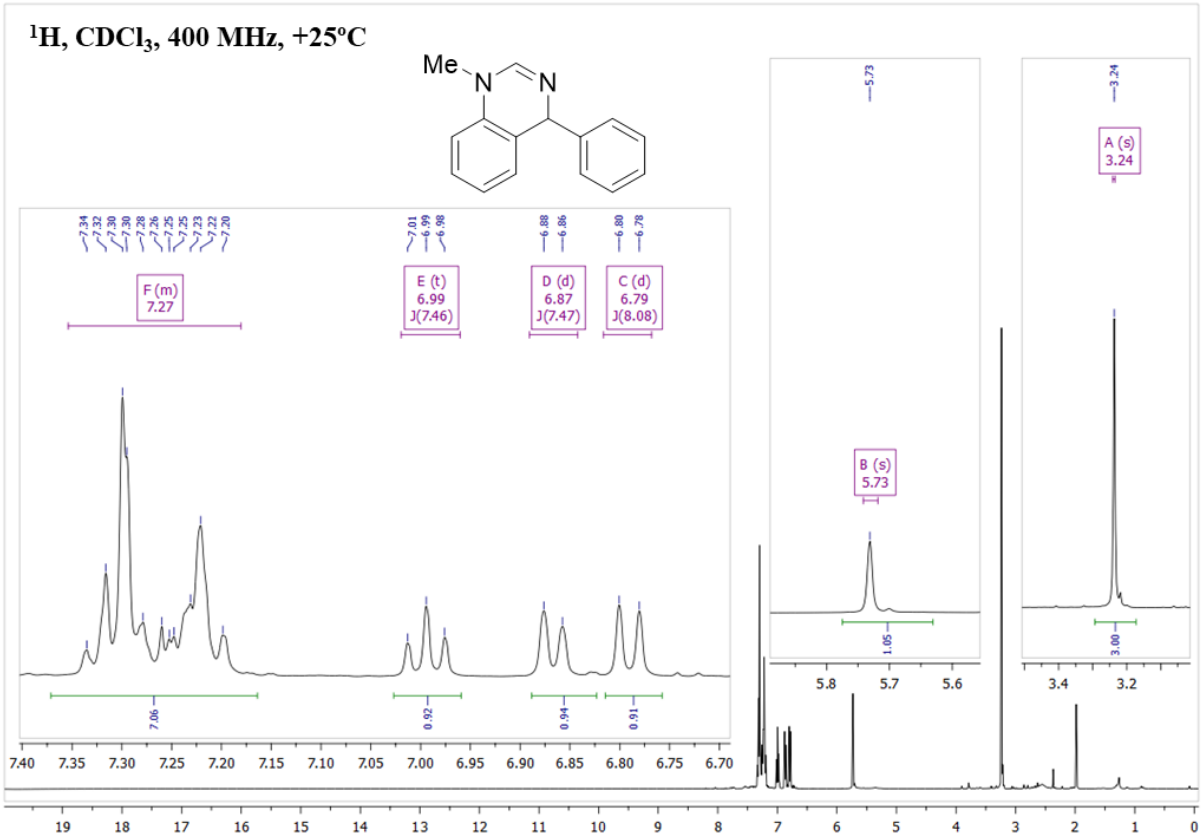

Figure S97. ^{1}H NMR spectrum of **15**.

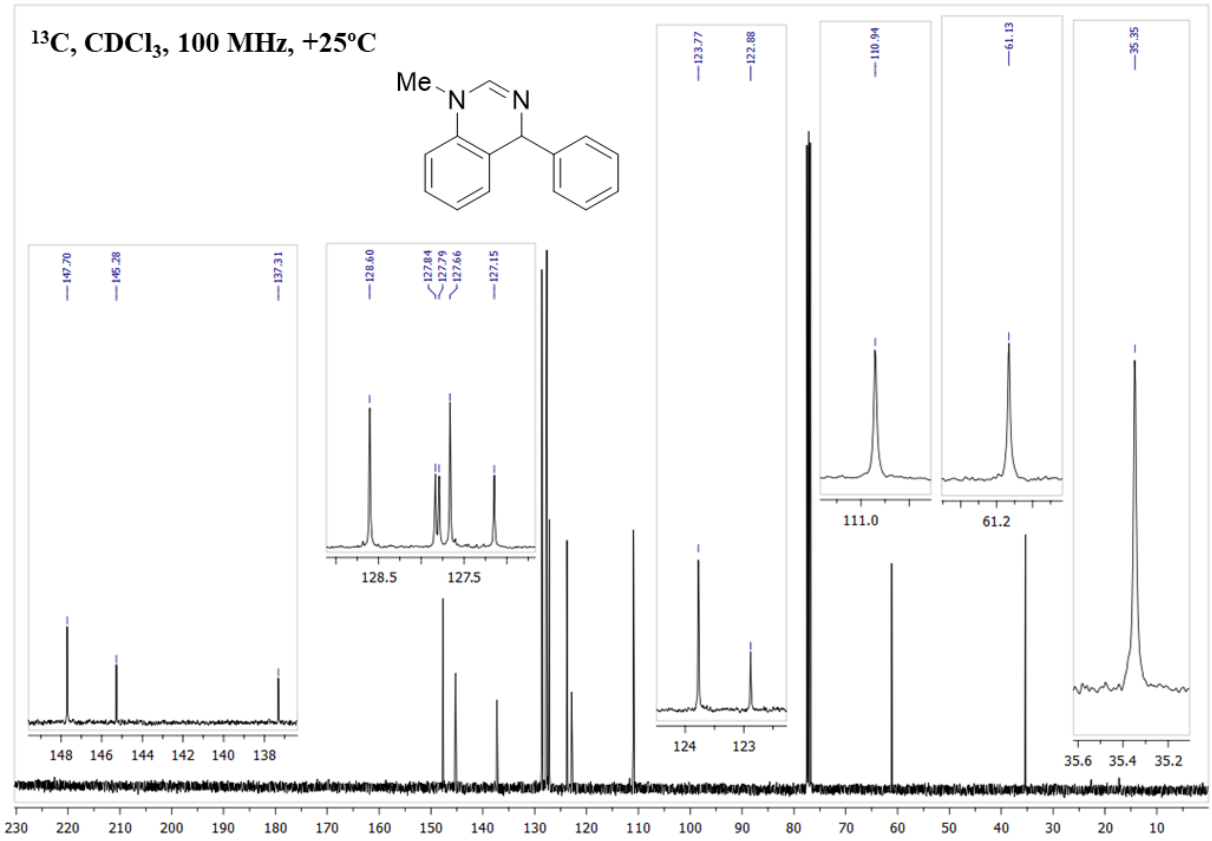

Figure S98. ^{13}C NMR spectrum of **12**.

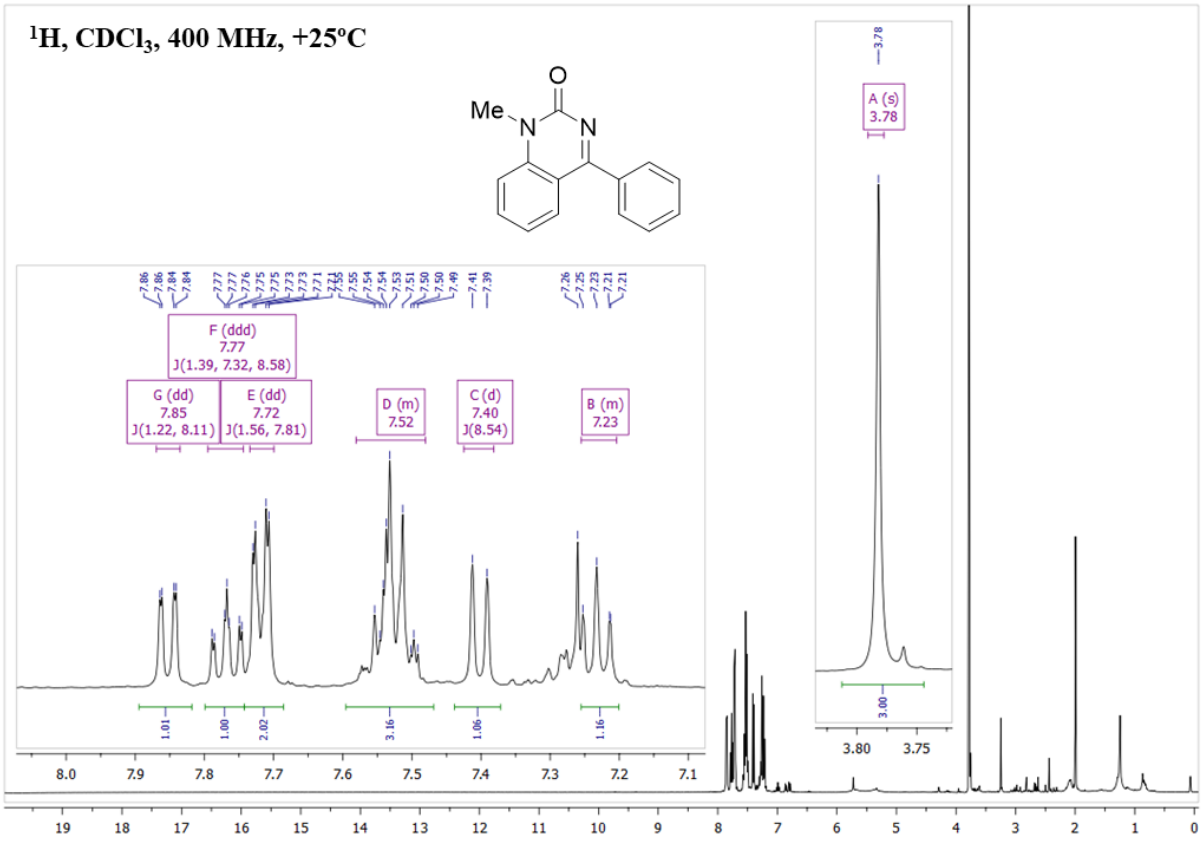

Figure S99. ^{1}H NMR spectrum of **13**.

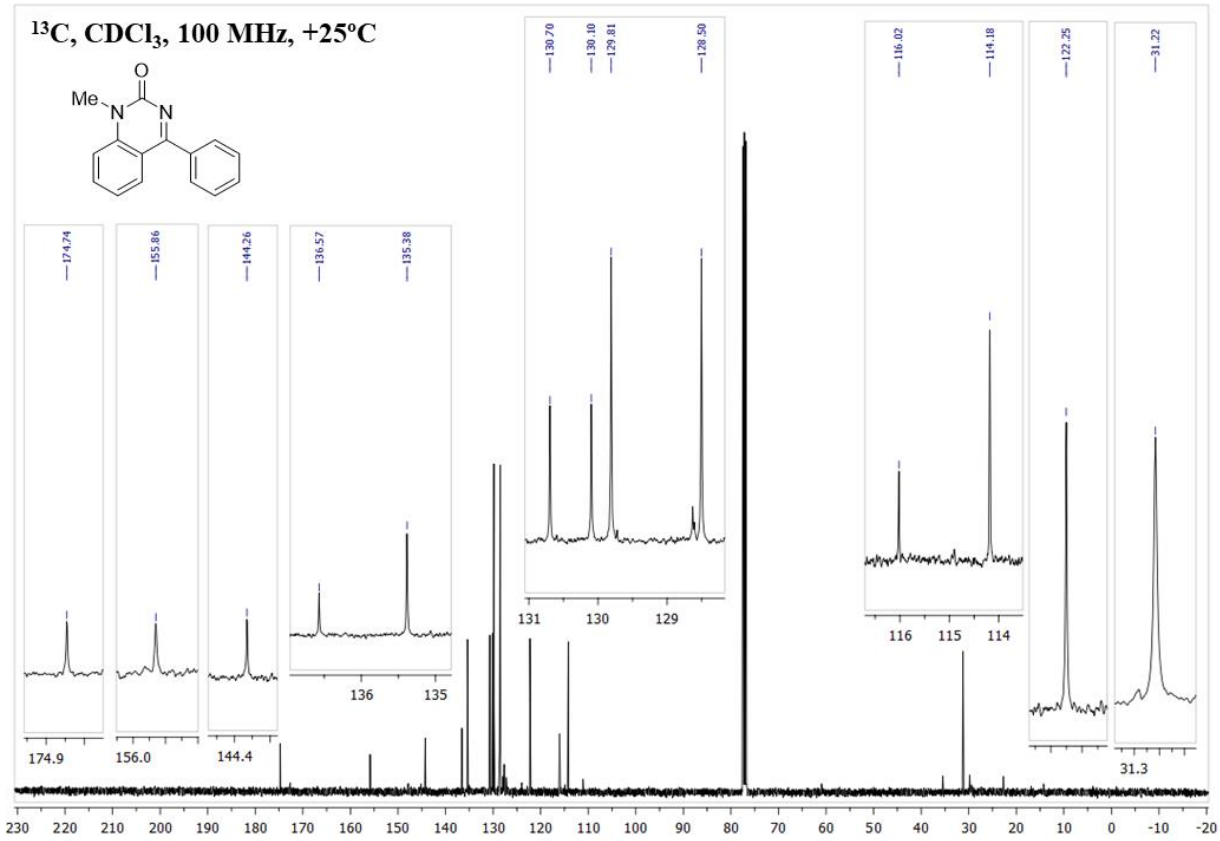

Figure S100. ^{13}C NMR spectrum of **13**.

X-Ray data

Appropriate for X-ray analysis crystals were grown by slow evaporation of solutions of **8c**, **8e** in n-hexane. For single crystal X-ray diffraction experiment crystals were fixed on a micro mount and placed on a Rigaku XtaLAB Synergy single crystal diffractometer using CuKα monochromated radiation (λ = 1.5418 Å). Crystals were kept at 100 K throughout the experiment. The unit cell parameters were refined by least square techniques. The structures have been solved by ShelXT[9] program, using Intrinsic Phasing and refined with the ShelXL package[10] incorporated in the OLEX2 program package[11]. Empirical absorption correction was applied in CrysAlisPro (Agilent Technologies, 2014) program complex using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The hydrogen atoms were introduced to the geometrically calculated positions and refined by attaching themselves to the corresponding parent atoms.

Supplementary crystallographic data for this paper have been deposited at Cambridge Crystallographic Data Centre (CCDC 2130455, 2130475) and can be obtained free of charge via www.ccdc.cam.ac.uk/structures/.

Table S1. Crystal data and structure refinement for compounds **8c**, **8e**.

Parameter	8e	8c
Empirical formula	$C_{19}H_{27}N_3$	$C_{25}H_{25}N_3$
Formula weight	297.43	367.48
Temperature/K	100(2)	100(2)
Crystal system	orthorhombic	triclinic
Space group	$P2_12_12_1$	P–1
a/Å	9.6026(2)	8.9740(3)
b/Å	12.0411(3)	10.1567(3)
c/Å	14.2206(4)	11.2275(3)
α/°	90	72.713(2)
β/°	90	89.359(2)
γ/°	90	80.928(2)
Volume/Å^3	1644.27(7)	964.20(5)
Z	4	2
ρ_{calc}g/cm^3	1.202	1.266
μ/mm^{-1}	0.546	0.577
F(000)	648.0	392.0
Crystal size/mm^3	0.20×0.16×0.10	0.12×0.12×0.08
Radiation	CuKα (λ=1.54184)	CuKα (λ=1.54184)
2Θ range for data collection/°	11.118 to 139.92	8.254 to 139.992
Index ranges	-11 ≤ h ≤ 10, -14 ≤ k ≤ 14, -17 ≤ l ≤ 15	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14
Reflections collected	10544	11725
Independent reflections	3091 R_{int} = 0.0331, R_{sigma} = 0.0354	3647 R_{int} =0.0314, R_{sigma} = 0.0345
Data/restraints/parameters	3091/0/209	3647/0/259
Goodness-of-fit on F^2	1.052	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0335, wR_2 = 0.0900	R_1 = 0.0423, wR_2 = 0.1157
Final R indexes [all data]	R_1 = 0.0366, wR_2 = 0.0918	R_1 = 0.0473, wR_2 = 0.1212
Largest diff. peak/hole / e Å^{-3}	0.17/-0.17	0.58/-0.19
Flack parameter	0.2(2)	0
CCDC	2130455	2130475

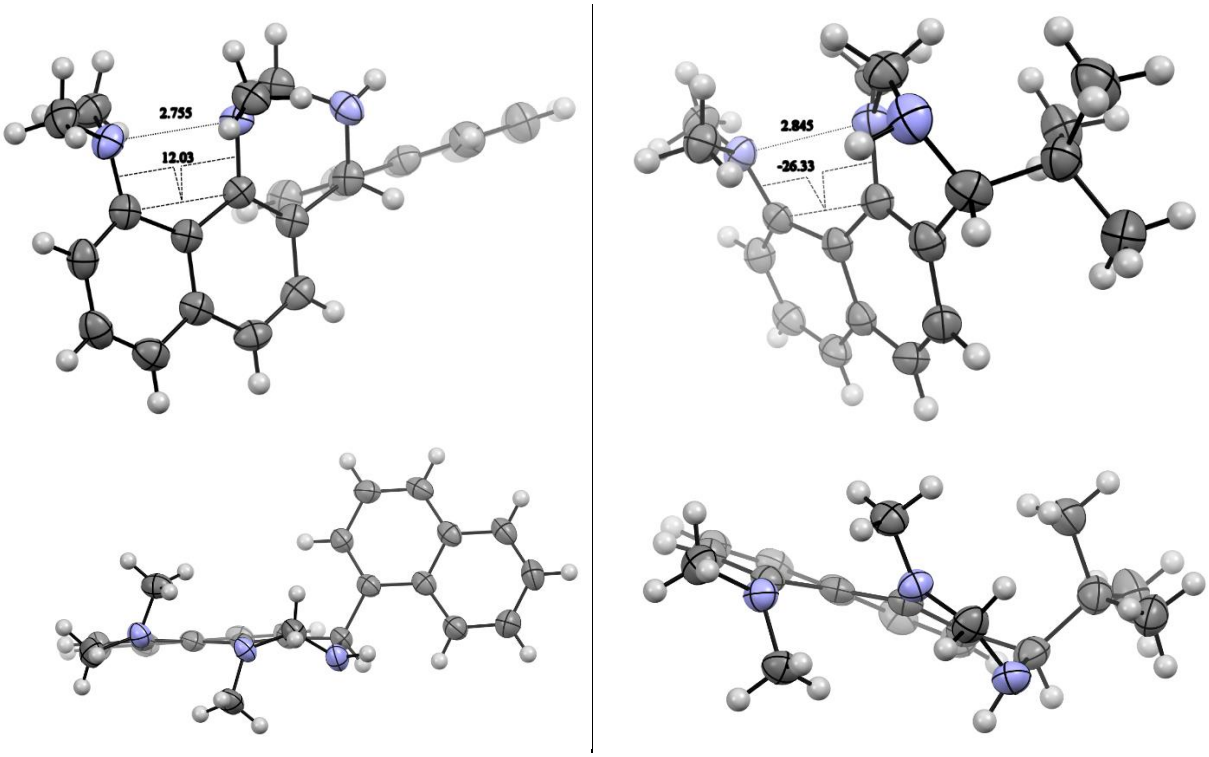

Figure S101. Molecular structure of 1,2,3,4-tetrahydrobenzo[*h*]quinazolines **8c** (left side) and **8e** (right side)

Computational data

General Remarks. The geometry optimization of all model structures was carried out at the B3LYP/6-311++G** (empiricaldispersion=gd3bj) level of theory with the use of Gaussian-16 program package.[12] The geometry optimization was performed using analytical calculations of gradients according to the scheme of Berny[13]. The Hessian matrices were calculated analytically for all optimized model structures to prove the correct location of the extremum points on the potential energy surface - no imaginary frequencies for minima and one imaginary frequency for transition state. The standard grid size for Gaussian-16 was used (UltraFine grid). Solvation effects were taken into account by Tomasi polarizable continuum model (PCM).[14] The lack of the minima corresponding to intermediate in case of dication **9**2H$^+$ was confirmed by means of scan procedure - the distance *r* (NCH_2-H…C=NH) is stepwise shortened (Fig. S102). In case of intermediates **9**2H$^+$Cl$^-$ and **9**2H$^+$$MeSO_3^-$ with counterion the IRC approach was utilized – the geometry with frozen *r* distance (*r* = 1.09Å) was optimized and applied as starting point in IRC procedure.

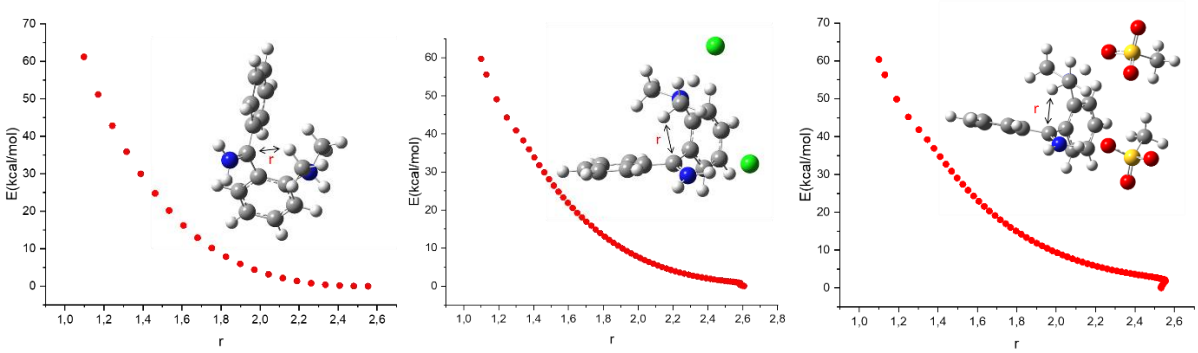

Figure S102. Calculated energy curves for the hydride transfer in dications **9**2H$^+$ (left), **9**2H$^+$Cl$^-$ (middle), **9**2H$^+$$MeSO_3^-$ (right).

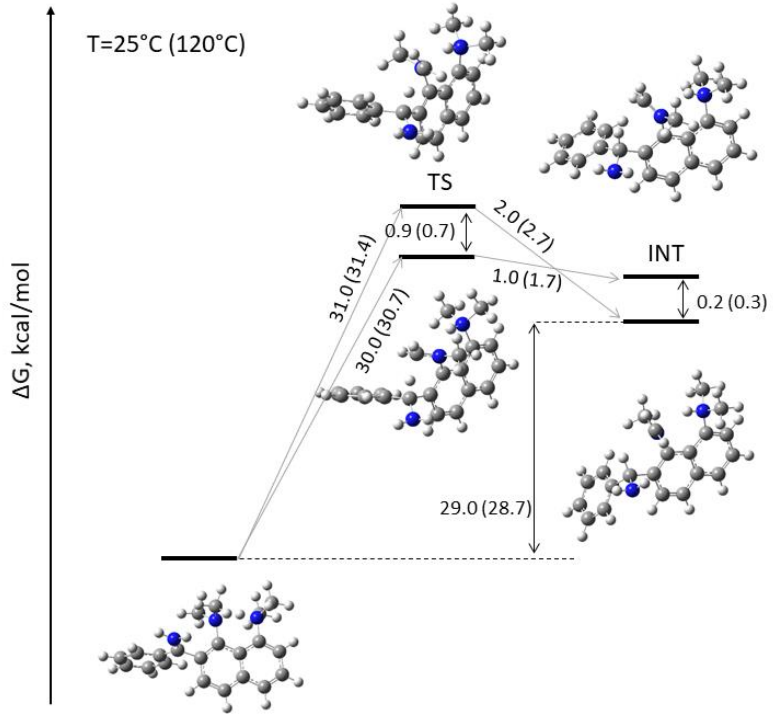

Figure S103. Reaction profile for the hydride transfer in **10a**

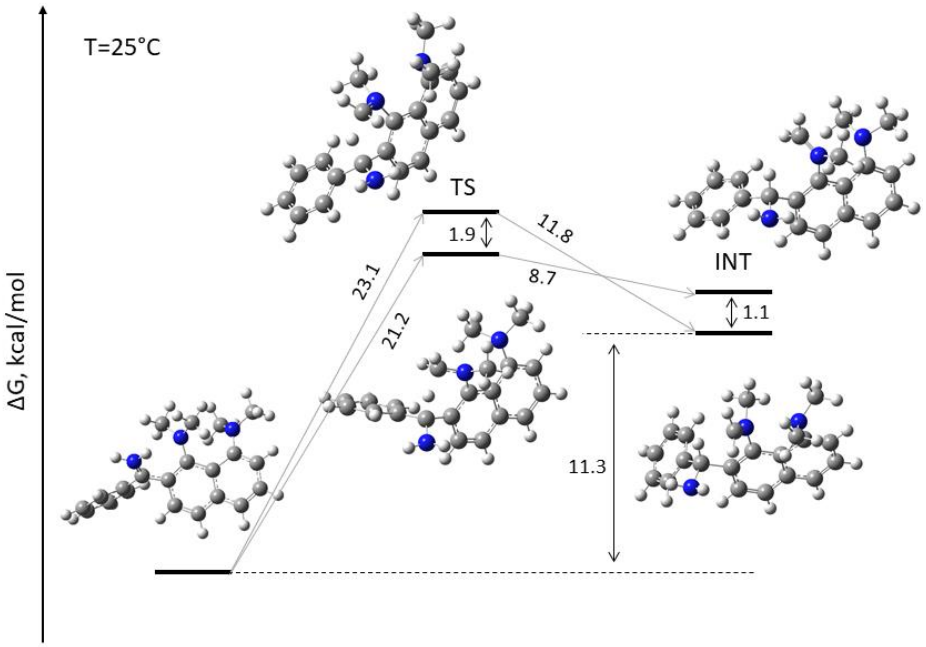

Figure S104. Reaction profile for the hydride transfer in **9a'''**

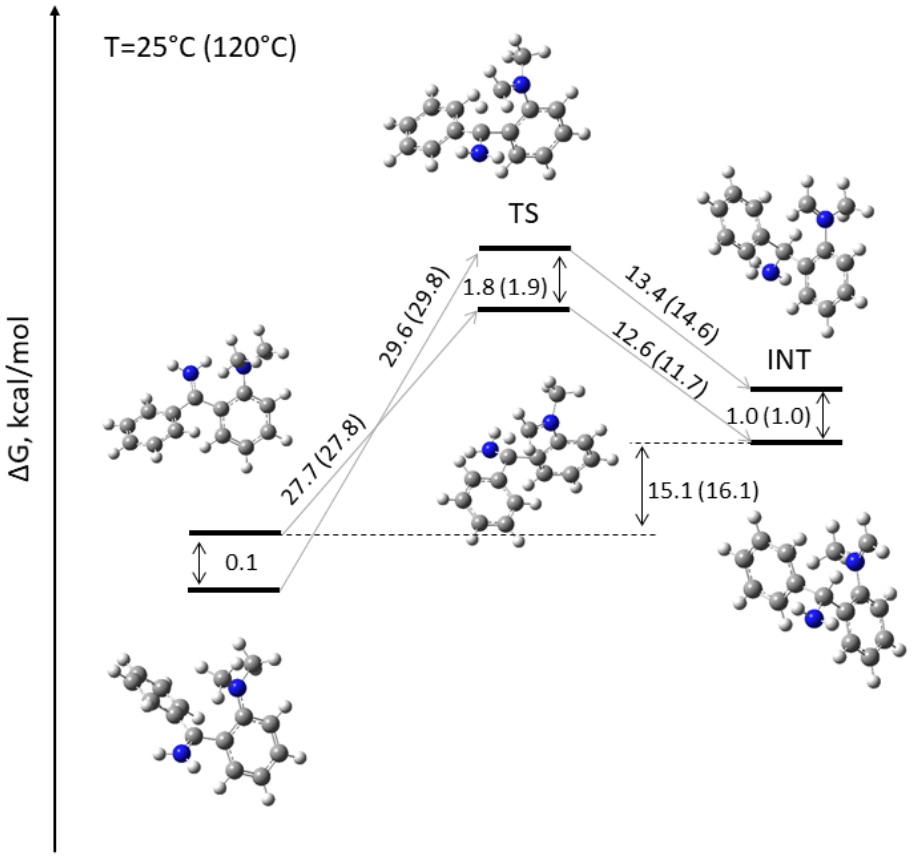

Figure S105. Reaction profile for the hydride transfer in **17**

Cartesian coordinates and total energies

Imine monocation **9**H^+ (conformer-1)

E = -691.431305389

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.548818	0.550330	1.195232
2	6	0	2.702987	-0.538415	1.112658
3	1	0	3.983353	2.562595	0.521374
4	6	0	3.313565	1.715945	0.449522
5	6	0	1.569068	-0.522360	0.266063
6	6	0	1.266628	0.707556	-0.400592
7	6	0	2.183768	1.784292	-0.335837
8	1	0	1.941085	2.711622	-0.839437
9	7	0	0.820736	-1.653073	0.082932
10	6	0	0.928268	-2.763083	1.021997
11	1	0	0.988678	-2.393230	2.044817
12	1	0	0.028337	-3.372165	0.934570
13	1	0	1.797796	-3.398865	0.814266
14	6	0	0.221108	-2.015832	-1.197647
15	1	0	0.622838	-2.982596	-1.516609
16	1	0	-0.865955	-2.096683	-1.123664
17	1	0	0.468458	-1.281750	-1.961335
18	6	0	-0.022116	0.969436	-1.005981
19	7	0	-0.089600	1.708750	-2.092961
20	1	0	-0.970266	2.077114	-2.427039
21	6	0	-1.280927	0.536000	-0.391175
22	6	0	-1.372133	0.427855	1.005112
23	6	0	-2.406253	0.261396	-1.183909
24	6	0	-2.572190	0.058620	1.594906
25	1	0	-0.509163	0.652238	1.617883
26	6	0	-3.602955	-0.116281	-0.587198
27	1	0	-2.335613	0.296816	-2.264378
28	6	0	-3.687649	-0.216266	0.800908
29	1	0	-2.641422	-0.013163	2.673097
30	1	0	-4.463505	-0.342335	-1.204123
31	1	0	-4.621078	-0.511223	1.264956
32	1	0	0.741602	1.955651	-2.613330
33	1	0	2.948440	-1.437575	1.658317
34	1	0	4.422123	0.488338	1.834082

Imine monocation **9**H^+ (Transition state-1)

E = -691.379855608

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.036186	-1.789439	-0.880355
2	6	0	3.069379	-0.427260	-0.617358
3	1	0	1.891589	-3.608121	-0.724737
4	6	0	1.916666	-2.544104	-0.525636
5	6	0	1.988751	0.183910	0.020922
6	6	0	0.858832	-0.569176	0.399181
7	6	0	0.834083	-1.932391	0.093993

8	1	0	-0.039299	-2.512900	0.365283
9	7	0	1.944443	1.595759	0.189877
10	6	0	2.136368	2.433679	-1.005495
11	1	0	1.373593	2.215181	-1.756795
12	1	0	2.083228	3.479247	-0.712618
13	1	0	3.119446	2.235904	-1.428043
14	6	0	1.178587	2.028204	1.206483
15	1	0	0.860228	3.064625	1.181323
16	1	0	1.362614	1.596833	2.188145
17	6	0	-0.340649	0.033764	1.089737
18	7	0	-0.449791	-0.347399	2.423676
19	1	0	-1.135912	0.139576	2.985002
20	6	0	-1.614384	0.029267	0.295860
21	6	0	-1.583034	0.449345	-1.040018
22	6	0	-2.827047	-0.386651	0.854933
23	6	0	-2.743979	0.458324	-1.802859
24	1	0	-0.647693	0.764639	-1.486409
25	6	0	-3.990083	-0.375814	0.088511
26	1	0	-2.863330	-0.746647	1.874526
27	6	0	-3.952956	0.047968	-1.238497
28	1	0	-2.706981	0.782988	-2.835558
29	1	0	-4.923103	-0.708027	0.527507
30	1	0	-4.858814	0.053329	-1.832731
31	1	0	0.414690	-0.524753	2.915957
32	1	0	3.932631	0.163860	-0.893265
33	1	0	3.883045	-2.262669	-1.361143
34	1	0	-0.015201	1.282218	1.061282

Imine monocation **9**H^+ (Intermediate-1)

E = -691.405906516

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.995461	2.511221	1.239462
2	6	0	1.956242	1.139720	1.008578
3	1	0	1.052884	4.398581	0.830991
4	6	0	1.035653	3.330294	0.652672
5	6	0	0.965141	0.621091	0.185000
6	6	0	-0.015198	1.416097	-0.422717
7	6	0	0.046037	2.786678	-0.163667
8	1	0	-0.708278	3.424628	-0.602581
9	7	0	0.952406	-0.827880	-0.002894
10	6	0	0.496765	-1.637718	1.146494
11	1	0	-0.504265	-1.308596	1.417060
12	1	0	0.499636	-2.688213	0.870501
13	1	0	1.178741	-1.456749	1.975939
14	6	0	1.335440	-1.349987	-1.102575
15	1	0	1.304854	-2.425141	-1.227005
16	1	0	1.688702	-0.708951	-1.899927
17	6	0	-1.119221	0.815282	-1.291208
18	7	0	-1.927757	1.871344	-1.915389
19	1	0	-2.717606	1.441940	-2.386692
20	6	0	-2.023153	-0.092503	-0.470109
21	6	0	-2.571182	0.353851	0.736475
22	6	0	-2.313483	-1.382748	-0.914698
23	6	0	-3.387950	-0.483855	1.490784
24	1	0	-2.346327	1.353220	1.089884
25	6	0	-3.127489	-2.226192	-0.158355

26	1	0	-1.895053	-1.734615	-1.851732
27	6	0	-3.663210	-1.778900	1.047379
28	1	0	-3.803523	-0.131019	2.427292
29	1	0	-3.337710	-3.229545	-0.509272
30	1	0	-4.290662	-2.434010	1.640030
31	1	0	-1.387514	2.351553	-2.630733
32	1	0	2.693126	0.481399	1.451509
33	1	0	2.768843	2.928477	1.871449
34	1	0	-0.641645	0.186978	-2.053891

Imine monocation **9**H^+ (Conformer-2)

E = -691.431405661

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.542686	0.048595	-0.692148
2	6	0	2.579717	1.013085	-0.411168
3	1	0	4.070573	-2.041357	-0.598804
4	6	0	3.322206	-1.291305	-0.379539
5	6	0	1.365716	0.671899	0.190694
6	6	0	1.114744	-0.706864	0.474998
7	6	0	2.117392	-1.658350	0.194588
8	1	0	1.918252	-2.703137	0.384018
9	7	0	0.394517	1.647920	0.494368
10	6	0	0.491991	2.926783	-0.211755
11	1	0	0.605776	2.754040	-1.281402
12	1	0	-0.435913	3.474958	-0.045566
13	1	0	1.324076	3.547090	0.146553
14	6	0	0.131800	1.848581	1.933733
15	1	0	0.914100	2.472897	2.382284
16	1	0	-0.831635	2.344845	2.058133
17	1	0	0.105401	0.898913	2.462516
18	6	0	-0.194400	-1.219207	0.857854
19	7	0	-1.277594	-0.523409	0.627142
20	1	0	-2.188674	-0.865782	0.901172
21	6	0	-0.357180	-2.547066	1.470000
22	6	0	0.479085	-2.934009	2.527303
23	6	0	-1.381660	-3.402375	1.039627
24	6	0	0.280828	-4.159312	3.152206
25	1	0	1.260067	-2.267861	2.870159
26	6	0	-1.557905	-4.635822	1.654955
27	1	0	-2.010303	-3.121359	0.203276
28	6	0	-0.731722	-5.012559	2.714025
29	1	0	0.916981	-4.448449	3.979329
30	1	0	-2.335164	-5.303947	1.305845
31	1	0	-0.875221	-5.972258	3.195528
32	1	0	-1.186185	0.410494	0.223194
33	1	0	2.789652	2.047177	-0.641985
34	1	0	4.477492	0.353235	-1.147648

Imine monocation **9**H^+ (Transition state-2)

E = -691.382561528

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.160602	-1.824792	-0.458745
2	6	0	-2.980076	-0.507341	-0.848320
3	1	0	-2.375715	-3.468220	0.695538
4	6	0	-2.236866	-2.437861	0.393022
5	6	0	-1.855731	0.198901	-0.410835
6	6	0	-0.902094	-0.412000	0.429183
7	6	0	-1.133925	-1.729433	0.845036
8	1	0	-0.418506	-2.194334	1.511835
9	7	0	-1.717409	1.584717	-0.678944
10	6	0	-2.832017	2.470203	-0.299839
11	1	0	-3.033795	2.389765	0.770614
12	1	0	-2.569679	3.493477	-0.557706
13	1	0	-3.722649	2.185415	-0.856626
14	6	0	-0.455718	2.047065	-0.695206
15	1	0	-0.315995	3.116038	-0.581458
16	1	0	0.257155	1.521325	-1.323188
17	6	0	0.310675	0.303002	0.955737
18	1	0	-3.700020	-0.021657	-1.493749
19	1	0	-4.022189	-2.375628	-0.814742
20	1	0	0.101004	1.489640	0.499856
21	6	0	1.633221	0.019246	0.283686
22	6	0	1.756407	-0.967122	-0.697399
23	6	0	2.754640	0.781386	0.635575
24	6	0	2.991242	-1.204856	-1.300448
25	1	0	0.896784	-1.556854	-0.986023
26	6	0	3.984876	0.540249	0.035158
27	1	0	2.666176	1.581418	1.362506
28	6	0	4.106679	-0.457481	-0.933489
29	1	0	3.076808	-1.976749	-2.055679
30	1	0	4.845049	1.136321	0.314660
31	1	0	5.065090	-0.643654	-1.403043
32	7	0	0.370521	0.303623	2.343395
33	1	0	1.231520	0.605648	2.776765
34	1	0	-0.462489	0.592903	2.837318

Imine monocation **9**H^+ (Intermediate-2)

E = -691.407187884

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.321340	0.040546	-1.591528
2	6	0	2.793541	0.762320	-0.524461
3	1	0	3.078550	-1.680746	-2.854326
4	6	0	2.674465	-1.113453	-2.024648
5	6	0	1.633110	0.306171	0.085662
6	6	0	0.956939	-0.847945	-0.324910
7	6	0	1.508745	-1.550032	-1.397962
8	1	0	1.012621	-2.450829	-1.731648
9	7	0	1.099294	1.087451	1.197734
10	6	0	0.259319	2.248642	0.845142
11	1	0	-0.558653	1.903886	0.214324
12	1	0	-0.121534	2.709140	1.752691
13	1	0	0.873609	2.952465	0.285025
14	6	0	1.351304	0.755444	2.406492
15	1	0	0.935392	1.336289	3.219663
16	1	0	1.997587	-0.089279	2.602021
17	6	0	-0.300514	-1.328167	0.393996

18	1	0	3.277048	1.662039	-0.164593
19	1	0	4.228427	0.380482	-2.074705
20	1	0	-0.950503	-0.455680	0.543291
21	6	0	0.033808	-1.868087	1.778672
22	6	0	1.054552	-2.806537	1.954730
23	6	0	-0.676596	-1.414997	2.893780
24	6	0	1.366869	-3.273873	3.228149
25	1	0	1.613413	-3.158718	1.095993
26	6	0	-0.362502	-1.880570	4.171879
27	1	0	-1.474547	-0.692002	2.761986
28	6	0	0.662587	-2.807728	4.340643
29	1	0	2.164628	-3.996062	3.355794
30	1	0	-0.915632	-1.515945	5.029174
31	1	0	0.914104	-3.166385	5.331616
32	7	0	-0.979647	-2.372413	-0.383564
33	1	0	-1.753508	-2.739597	0.161187
34	1	0	-1.378711	-1.974277	-1.229809

Imine dication **7a**$2H^+$

E = -979.580720817

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.639803	-1.099361	0.090351
2	6	0	-3.344235	-1.252252	-0.327362
3	6	0	-2.504231	-0.128706	-0.525214
4	6	0	-3.003046	1.202601	-0.319200
5	6	0	-4.348653	1.295932	0.155472
6	6	0	-5.137485	0.191786	0.348147
7	1	0	-0.788903	-1.335136	-1.032146
8	1	0	-5.280101	-1.958287	0.242468
9	1	0	-2.934125	-2.238730	-0.505335
10	6	0	-1.152858	-0.324541	-0.896385
11	6	0	-2.127050	2.314724	-0.576615
12	1	0	-6.150072	0.303523	0.713524
13	6	0	-0.808982	2.059890	-0.928269
14	6	0	-0.312925	0.738520	-1.060320
15	1	0	0.726311	0.587318	-1.321846
16	7	0	-2.654828	3.650050	-0.406556
17	7	0	-4.905903	2.618366	0.500733
18	6	0	-5.142755	2.776198	1.972451
19	1	0	-5.427020	3.809604	2.159404
20	1	0	-5.938756	2.104746	2.285137
21	1	0	-4.222787	2.536895	2.500346
22	6	0	-6.114501	2.982828	-0.305142
23	1	0	-6.945806	2.339384	-0.026411
24	1	0	-6.362647	4.020834	-0.094530
25	1	0	-5.883855	2.853771	-1.359405
26	6	0	-1.942975	4.525648	0.541277
27	1	0	-1.035490	4.966473	0.117848
28	1	0	-2.612060	5.341065	0.820627
29	1	0	-1.686823	3.962948	1.437570
30	6	0	-3.052636	4.352906	-1.646538
31	1	0	-3.827183	5.083627	-1.407460
32	1	0	-2.216018	4.892109	-2.098587
33	1	0	-3.449216	3.638127	-2.366202
34	6	0	0.184443	3.127228	-1.217576
35	7	0	0.057273	3.777135	-2.339984

36	1	0	0.683745	4.527319	-2.607891
37	6	0	1.286097	3.367958	-0.308546
38	6	0	1.220665	2.840255	0.995481
39	6	0	2.413769	4.120946	-0.695380
40	6	0	2.246876	3.080152	1.896440
41	1	0	0.363356	2.256404	1.300670
42	6	0	3.436310	4.350088	0.208376
43	1	0	2.515342	4.501934	-1.703632
44	6	0	3.352034	3.835367	1.505694
45	1	0	2.187157	2.679504	2.899977
46	1	0	4.304806	4.920134	-0.094999
47	1	0	4.155486	4.018556	2.208655
48	1	0	-0.652156	3.516180	-3.013683
49	1	0	-4.100498	3.270389	0.225943

Imine dication **7a**$2H^+$ (Transition state-1)

E = 979.530439375

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.060088	1.929878	0.649293
2	6	0	2.954346	2.654799	0.283596
3	6	0	1.750199	2.007679	-0.080196
4	6	0	1.682378	0.577347	-0.104102
5	6	0	2.828405	-0.124804	0.365917
6	6	0	3.982378	0.527337	0.721773
7	1	0	0.662955	3.846921	-0.371255
8	1	0	4.982437	2.424458	0.922994
9	1	0	2.981994	3.737357	0.276807
10	6	0	0.595112	2.766637	-0.403828
11	6	0	0.461075	-0.007294	-0.560361
12	1	0	4.834716	-0.025328	1.092332
13	6	0	-0.679283	0.749252	-0.789076
14	6	0	-0.588361	2.160574	-0.716930
15	1	0	-1.474354	2.742468	-0.933113
16	7	0	0.415165	-1.382662	-0.980688
17	7	0	2.752224	-1.582685	0.643303
18	6	0	2.611361	-1.847758	2.123922
19	1	0	2.438078	-2.912567	2.259683
20	1	0	3.530681	-1.542275	2.615416
21	1	0	1.769966	-1.269376	2.495710
22	6	0	3.874900	-2.390283	0.043432
23	1	0	4.792874	-2.175279	0.581749
24	1	0	3.619664	-3.441890	0.148944
25	1	0	3.978601	-2.123151	-1.004121
26	6	0	-0.721509	-2.028529	-0.722354
27	1	0	-0.953153	-2.916457	-1.298795
28	1	0	-1.167816	-1.904258	0.256591
29	6	0	1.133168	-1.687813	-2.250090
30	1	0	1.273542	-2.763579	-2.327361
31	1	0	0.551795	-1.317395	-3.095589
32	1	0	2.095131	-1.182584	-2.242117
33	6	0	-2.006602	0.144103	-1.168646
34	7	0	-2.541856	0.728907	-2.331875
35	1	0	-3.506433	0.501444	-2.532574
36	6	0	-3.017232	0.035772	-0.039791
37	6	0	-2.795841	0.608015	1.213991
38	6	0	-4.195268	-0.686154	-0.267407

39	6	0	-3.753206	0.480074	2.220277
40	1	0	-1.886547	1.159035	1.413151
41	6	0	-5.149210	-0.809771	0.736435
42	1	0	-4.362313	-1.171391	-1.223051
43	6	0	-4.930838	-0.223191	1.983791
44	1	0	-3.573915	0.933107	3.187801
45	1	0	-6.056438	-1.371082	0.548893
46	1	0	-5.672673	-0.321494	2.767143
47	1	0	-1.955296	0.675623	-3.154866
48	1	0	1.886706	-1.922529	0.216466
49	1	0	-1.745298	-1.019927	-1.353889

Imine dication **7a**$2H^+$ (Intermediate-1)

E = -979.534295697

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.818119	2.237813	0.161502
2	6	0	2.619310	2.790104	-0.208293
3	6	0	1.473687	1.983787	-0.395949
4	6	0	1.544289	0.559421	-0.235570
5	6	0	2.790219	0.051526	0.239986
6	6	0	3.887369	0.859996	0.417559
7	1	0	0.207785	3.672743	-0.826732
8	1	0	4.698323	2.851151	0.298635
9	1	0	2.525164	3.858672	-0.355823
10	6	0	0.236218	2.595011	-0.724329
11	6	0	0.347923	-0.175495	-0.542677
12	1	0	4.813933	0.447063	0.791451
13	6	0	-0.859999	0.442552	-0.819434
14	6	0	-0.897680	1.856484	-0.883735
15	1	0	-1.845315	2.327872	-1.105042
16	7	0	0.424674	-1.612401	-0.768218
17	7	0	2.933991	-1.349876	0.721476
18	6	0	2.909201	-1.412325	2.233944
19	1	0	2.898566	-2.460277	2.524938
20	1	0	3.800672	-0.916590	2.606831
21	1	0	2.015742	-0.902516	2.583357
22	6	0	4.133167	-2.079385	0.164666
23	1	0	5.035851	-1.651888	0.588087
24	1	0	4.045702	-3.123274	0.453383
25	1	0	4.133440	-1.975941	-0.916446
26	6	0	-0.294352	-2.446592	-0.103417
27	1	0	-0.329356	-3.484311	-0.412399
28	1	0	-0.828516	-2.113800	0.776336
29	6	0	1.151975	-2.034246	-1.998928
30	1	0	1.390766	-3.092201	-1.932747
31	1	0	0.507005	-1.837926	-2.853348
32	1	0	2.052704	-1.434361	-2.096560
33	6	0	-2.175383	-0.270799	-1.096990
34	7	0	-2.664085	0.143958	-2.413148
35	1	0	-3.490352	-0.389901	-2.664194
36	6	0	-3.171849	0.061306	0.018516
37	6	0	-2.765502	-0.003645	1.356410
38	6	0	-4.494392	0.406206	-0.263996
39	6	0	-3.663340	0.250491	2.388800
40	1	0	-1.733470	-0.221090	1.605758
41	6	0	-5.395771	0.662645	0.770031

42	1	0	-4.832447	0.492093	-1.287518
43	6	0	-4.986206	0.582698	2.098260
44	1	0	-3.326294	0.199902	3.417331
45	1	0	-6.418602	0.929602	0.531395
46	1	0	-5.686698	0.785462	2.899573
47	1	0	-1.966822	-0.058138	-3.122541
48	1	0	2.122372	-1.877765	0.415451
49	1	0	-2.032219	-1.360552	-1.063574

Imine dication **7a**$2H^+$ (Transition state-2)

E = -979.527205714

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.094340	1.685621	-1.139669
2	6	0	-2.993286	2.483223	-0.970070
3	6	0	-1.790329	1.959315	-0.436842
4	6	0	-1.699807	0.567692	-0.091042
5	6	0	-2.893464	-0.199606	-0.227726
6	6	0	-4.046388	0.336165	-0.740427
7	1	0	-0.772650	3.856547	-0.469562
8	1	0	-5.012462	2.084923	-1.549282
9	1	0	-3.026520	3.533196	-1.233357
10	6	0	-0.678659	2.807483	-0.218004
11	6	0	-0.438854	0.104987	0.376619
12	1	0	-4.941263	-0.265593	-0.824939
13	6	0	0.621167	0.959246	0.620262
14	6	0	0.486758	2.330970	0.322207
15	1	0	1.324391	2.988336	0.514392
16	7	0	-0.150802	-1.310157	0.548789
17	7	0	-2.952997	-1.590779	0.285631
18	6	0	-3.419996	-2.595165	-0.734911
19	1	0	-3.276172	-3.587819	-0.316023
20	1	0	-4.472175	-2.426979	-0.943312
21	1	0	-2.832068	-2.469271	-1.639623
22	6	0	-3.749861	-1.680135	1.564899
23	1	0	-4.786991	-1.443957	1.344127
24	1	0	-3.660580	-2.695053	1.945348
25	1	0	-3.338670	-0.965567	2.273191
26	6	0	0.480009	-1.595849	1.693388
27	1	0	1.010476	-2.538652	1.767960
28	1	0	0.117598	-1.122587	2.599623
29	6	0	0.251393	-2.043116	-0.684965
30	1	0	0.209219	-3.111604	-0.485227
31	1	0	-0.440834	-1.787355	-1.483233
32	1	0	1.257413	-1.751517	-0.984716
33	6	0	1.947998	0.460560	1.164363
34	7	0	2.447621	1.284575	2.182695
35	1	0	3.369767	1.044199	2.522043
36	6	0	2.995945	0.100563	0.128650
37	6	0	2.907778	0.550902	-1.190094
38	6	0	4.073086	-0.703744	0.513898
39	6	0	3.898893	0.212036	-2.109087
40	1	0	2.072328	1.160413	-1.508179
41	6	0	5.060397	-1.041662	-0.405936
42	1	0	4.131495	-1.084469	1.527992
43	6	0	4.975273	-0.582583	-1.720421
44	1	0	3.825563	0.568617	-3.129314

45	1	0	5.888365	-1.669333	-0.099811
46	1	0	5.740845	-0.849364	-2.438971
47	1	0	1.802646	1.508871	2.931002
48	1	0	-1.993309	-1.848173	0.538954
49	1	0	1.666028	-0.628696	1.628859

Imine dication **7a**$2H^+$ (Intermediate-2)

E = -979.534546105

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.516279	2.467451	0.973336
2	6	0	2.264421	2.886199	0.609411
3	6	0	1.281617	1.964087	0.183713
4	6	0	1.555689	0.551325	0.132769
5	6	0	2.896878	0.182261	0.465729
6	6	0	3.828899	1.104655	0.878668
7	1	0	-0.149894	3.529076	-0.178425
8	1	0	4.269937	3.168520	1.305155
9	1	0	2.002630	3.936475	0.636607
10	6	0	0.013425	2.459040	-0.211564
11	6	0	0.450894	-0.280262	-0.264671
12	1	0	4.834280	0.787816	1.119126
13	6	0	-0.787595	0.221878	-0.624692
14	6	0	-0.979429	1.622762	-0.621888
15	1	0	-1.942578	2.011905	-0.920362
16	7	0	0.561053	-1.740369	-0.212054
17	7	0	3.421316	-1.205030	0.320678
18	6	0	3.970206	-1.779111	1.606920
19	1	0	4.134471	-2.842380	1.451792
20	1	0	4.907479	-1.284317	1.839782
21	1	0	3.250334	-1.608015	2.401521
22	6	0	4.433595	-1.307577	-0.801002
23	1	0	5.304568	-0.717986	-0.533269
24	1	0	4.701096	-2.355347	-0.914650
25	1	0	3.974482	-0.921904	-1.707302
26	6	0	0.602735	-2.440395	-1.286599
27	1	0	0.567373	-3.521746	-1.224776
28	1	0	0.692003	-1.940300	-2.242299
29	6	0	0.382486	-2.369268	1.124168
30	1	0	0.773703	-3.383173	1.112731
31	1	0	0.883685	-1.756939	1.867895
32	1	0	-0.683934	-2.378921	1.343380
33	6	0	-1.989931	-0.637661	-1.017093
34	7	0	-2.221987	-0.456528	-2.454079
35	1	0	-2.974445	-1.065350	-2.763104
36	6	0	-3.216966	-0.225814	-0.205428
37	6	0	-3.295872	-0.583015	1.143874
38	6	0	-4.254282	0.519405	-0.768070
39	6	0	-4.385973	-0.200790	1.919356
40	1	0	-2.501567	-1.160626	1.601737
41	6	0	-5.350670	0.900418	0.006550
42	1	0	-4.201019	0.806196	-1.809878
43	6	0	-5.419841	0.544406	1.351024
44	1	0	-4.429983	-0.486508	2.963675
45	1	0	-6.149553	1.477464	-0.444479
46	1	0	-6.271215	0.841376	1.951963
47	1	0	-1.398402	-0.701443	-2.992865

48	1	0	2.658595	-1.813215	0.043698
49	1	0	-1.794678	-1.683429	-0.758314

Imine monocation **7a**H^+

E = -979.131973939

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.939701	2.185579	-0.672095
2	6	0	2.698805	2.774253	-0.544198
3	6	0	1.567539	1.972558	-0.302657
4	6	0	1.692182	0.541042	-0.233869
5	6	0	3.031636	0.002315	-0.078668
6	6	0	4.113178	0.821699	-0.410189
7	1	0	0.233035	3.655882	-0.031937
8	1	0	4.810718	2.792626	-0.890966
9	1	0	2.577831	3.847527	-0.624893
10	6	0	0.295153	2.575791	-0.084379
11	6	0	0.490003	-0.247253	-0.342371
12	1	0	5.117878	0.427888	-0.366416
13	6	0	-0.764875	0.402971	-0.201843
14	6	0	-0.820201	1.812394	0.049092
15	1	0	-1.782921	2.279350	0.203721
16	7	0	0.541723	-1.608566	-0.584606
17	7	0	3.240963	-1.275140	0.409676
18	6	0	2.551599	-1.681775	1.634863
19	1	0	2.285647	-2.739501	1.587889
20	1	0	3.207976	-1.530102	2.502477
21	1	0	1.650507	-1.096082	1.785996
22	6	0	4.559345	-1.875931	0.280649
23	1	0	5.295583	-1.438539	0.970403
24	1	0	4.474197	-2.939816	0.507132
25	1	0	4.925344	-1.772626	-0.741097
26	6	0	-0.310790	-2.574712	0.091848
27	1	0	-1.058053	-3.018461	-0.575336
28	1	0	0.313767	-3.385883	0.475528
29	1	0	-0.824253	-2.108593	0.930812
30	6	0	1.442936	-2.193911	-1.569105
31	1	0	2.151898	-2.883232	-1.106479
32	1	0	0.847218	-2.748751	-2.304549
33	1	0	1.996256	-1.415735	-2.088354
34	6	0	-2.028470	-0.192771	-0.568303
35	7	0	-2.129850	-1.031265	-1.579809
36	1	0	-3.002519	-1.492867	-1.794619
37	6	0	-3.268975	0.173954	0.128766
38	6	0	-3.246822	0.370133	1.517921
39	6	0	-4.479958	0.295977	-0.570195
40	6	0	-4.421442	0.668460	2.196932
41	1	0	-2.314548	0.269401	2.058313
42	6	0	-5.648570	0.608234	0.113202
43	1	0	-4.501938	0.189181	-1.648024
44	6	0	-5.621772	0.789671	1.496412
45	1	0	-4.401651	0.805484	3.270876
46	1	0	-6.577199	0.719143	-0.432558
47	1	0	-6.535147	1.030215	2.026952
48	1	0	-1.328894	-1.252596	-2.154328

Imine monocation **7a**H^+(Transition state-1)

E = -979.094106047

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.214192	1.722965	-0.726235
2	6	0	-3.121670	2.534121	-0.543530
3	6	0	-1.871741	1.967095	-0.196436
4	6	0	-1.749706	0.553003	-0.025415
5	6	0	-2.871574	-0.283366	-0.367505
6	6	0	-4.084328	0.323131	-0.661614
7	1	0	-0.835477	3.861738	-0.168453
8	1	0	-5.178525	2.151665	-0.972515
9	1	0	-3.197851	3.609280	-0.651330
10	6	0	-0.734433	2.796112	0.000262
11	6	0	-0.507329	0.058051	0.489752
12	1	0	-4.942685	-0.289570	-0.899158
13	6	0	0.609226	0.884070	0.627915
14	6	0	0.469301	2.272466	0.376569
15	1	0	1.335527	2.908010	0.508298
16	7	0	-0.414331	-1.238721	1.057901
17	7	0	-2.718675	-1.679860	-0.393916
18	6	0	-1.790790	-2.206409	-1.398565
19	1	0	-1.412963	-3.179535	-1.077391
20	1	0	-2.291098	-2.326030	-2.370734
21	1	0	-0.947563	-1.533817	-1.536343
22	6	0	-3.920385	-2.492993	-0.283009
23	1	0	-4.530948	-2.490536	-1.199148
24	1	0	-3.620358	-3.523747	-0.084314
25	1	0	-4.533191	-2.145159	0.549344
26	6	0	0.793783	-1.821305	0.986158
27	1	0	0.984224	-2.644381	1.666656
28	1	0	1.263100	-1.875102	0.008535
29	6	0	-1.278963	-1.545605	2.213379
30	1	0	-1.493034	-2.612001	2.223874
31	1	0	-0.774324	-1.249368	3.137243
32	1	0	-2.208425	-0.995833	2.118131
33	6	0	1.944820	0.407635	1.116446
34	7	0	2.413718	1.123615	2.210382
35	1	0	3.376723	0.988307	2.482742
36	6	0	2.993025	0.121219	0.068337
37	6	0	2.755805	0.381828	-1.283515
38	6	0	4.214370	-0.446994	0.452952
39	6	0	3.735622	0.099933	-2.234754
40	1	0	1.814644	0.814431	-1.595575
41	6	0	5.190702	-0.724038	-0.497170
42	1	0	4.399804	-0.699302	1.491238
43	6	0	4.954382	-0.448046	-1.844882
44	1	0	3.542935	0.312937	-3.279303
45	1	0	6.130757	-1.164643	-0.188035
46	1	0	5.714958	-0.666052	-2.584959
47	1	0	1.778886	1.237095	2.988452
48	1	0	1.653967	-0.811123	1.445069

Imine monocation **7a**H^+(Intermediate-1)

E = -979.112420949

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.746760	2.531782	0.210818
2	6	0	2.478523	3.017234	0.010170
3	6	0	1.390250	2.126166	-0.153285
4	6	0	1.613786	0.714891	-0.116058
5	6	0	2.924199	0.241208	0.219914
6	6	0	3.963146	1.145798	0.335961
7	1	0	-0.084778	3.686985	-0.371975
8	1	0	4.583732	3.211405	0.316548
9	1	0	2.290127	4.083051	-0.036679
10	6	0	0.076077	2.615263	-0.371373
11	6	0	0.501563	-0.133988	-0.428615
12	1	0	4.957122	0.786274	0.566809
13	6	0	-0.774019	0.358171	-0.641348
14	6	0	-0.969313	1.761591	-0.575406
15	1	0	-1.970008	2.141861	-0.732543
16	7	0	0.753390	-1.546910	-0.682174
17	7	0	3.106811	-1.147228	0.431799
18	6	0	2.606861	-1.631967	1.716710
19	1	0	2.419396	-2.709233	1.656317
20	1	0	3.328695	-1.454082	2.526048
21	1	0	1.680882	-1.123054	1.982661
22	6	0	4.409692	-1.709529	0.095290
23	1	0	5.191783	-1.450869	0.823456
24	1	0	4.321385	-2.797807	0.071835
25	1	0	4.719123	-1.363945	-0.891351
26	6	0	0.214905	-2.468713	0.022191
27	1	0	0.345089	-3.504341	-0.263980
28	1	0	-0.350733	-2.211395	0.905123
29	6	0	1.500202	-1.873883	-1.921633
30	1	0	1.976045	-2.842786	-1.803232
31	1	0	0.790595	-1.892048	-2.748964
32	1	0	2.244638	-1.104384	-2.090562
33	6	0	-1.993112	-0.476660	-1.011849
34	7	0	-2.412245	-0.105423	-2.370601
35	1	0	-3.136042	-0.740584	-2.695012
36	6	0	-3.111021	-0.246509	0.005691
37	6	0	-2.862997	-0.482146	1.362861
38	6	0	-4.381224	0.184128	-0.377991
39	6	0	-3.862850	-0.304861	2.313492
40	1	0	-1.875238	-0.785044	1.690486
41	6	0	-5.387186	0.362693	0.573959
42	1	0	-4.587699	0.395311	-1.418415
43	6	0	-5.133794	0.117683	1.920504
44	1	0	-3.648991	-0.489613	3.359723
45	1	0	-6.368359	0.697597	0.257661
46	1	0	-5.914403	0.258534	2.658774
47	1	0	-1.631721	-0.206863	-3.010987
48	1	0	-1.744515	-1.542038	-0.957392

Imine monocation **7a**H^+(Transition state-2)

E = -979.090934539

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.795942	2.450403	0.277816
2	6	0	2.586995	2.923714	-0.168234
3	6	0	1.521529	2.022992	-0.409645

4	6	0	1.700737	0.622787	-0.175044
5	6	0	3.020014	0.140179	0.144091
6	6	0	4.017709	1.066782	0.409988
7	1	0	0.158651	3.556561	-1.081819
8	1	0	4.609675	3.136086	0.482651
9	1	0	2.426429	3.982002	-0.334462
10	6	0	0.266486	2.498985	-0.872032
11	6	0	0.542513	-0.213727	-0.265745
12	1	0	5.007543	0.722414	0.675178
13	6	0	-0.667257	0.272678	-0.762697
14	6	0	-0.786256	1.649103	-1.068411
15	1	0	-1.733165	2.019038	-1.441089
16	7	0	0.526114	-1.513121	0.313133
17	7	0	3.264054	-1.242011	0.185164
18	6	0	4.416228	-1.703188	0.944786
19	1	0	4.330530	-2.783523	1.077131
20	1	0	5.374769	-1.500261	0.442880
21	1	0	4.427984	-1.234473	1.929412
22	6	0	3.114350	-1.962747	-1.081515
23	1	0	4.037573	-1.906625	-1.676551
24	1	0	2.889073	-3.013012	-0.883532
25	1	0	2.306947	-1.538940	-1.674153
26	6	0	-0.322275	-2.390238	-0.251216
27	1	0	-0.596249	-3.255406	0.343586
28	1	0	-0.241802	-2.544945	-1.324948
29	6	0	0.798121	-1.632285	1.759487
30	1	0	1.325175	-2.565422	1.945806
31	1	0	1.419830	-0.801950	2.074924
32	1	0	-0.141819	-1.613118	2.317553
33	6	0	-1.895320	-0.577498	-0.948533
34	7	0	-2.142257	-0.884673	-2.284851
35	1	0	-2.849274	-1.584168	-2.469702
36	6	0	-3.088762	-0.196217	-0.124451
37	6	0	-2.900322	0.150487	1.219838
38	6	0	-4.381193	-0.181694	-0.659602
39	6	0	-3.983544	0.500759	2.016088
40	1	0	-1.902446	0.153511	1.641595
41	6	0	-5.466076	0.166918	0.141132
42	1	0	-4.544957	-0.413182	-1.703638
43	6	0	-5.271724	0.506224	1.478845
44	1	0	-3.824316	0.770491	3.053006
45	1	0	-6.462121	0.182161	-0.284560
46	1	0	-6.117449	0.779484	2.098381
47	1	0	-1.329332	-0.980092	-2.877981
48	1	0	-1.502556	-1.671430	-0.364105

Imine monocation **7a**H^+(Intermediate-2)

E = -979.113231410

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.394041	2.784513	-0.683836
2	6	0	-2.155910	3.132995	-0.204955
3	6	0	-1.224646	2.132608	0.165175
4	6	0	-1.571719	0.751649	0.033568
5	6	0	-2.911035	0.421958	-0.354619
6	6	0	-3.775097	1.429689	-0.738033
7	1	0	0.298881	3.532373	0.778576
8	1	0	-4.101078	3.548152	-0.984622

9	1	0	-1.866691	4.172810	-0.110835
10	6	0	0.060456	2.482562	0.653729
11	6	0	-0.540895	-0.208562	0.296580
12	1	0	-4.778926	1.176319	-1.052498
13	6	0	0.720473	0.149829	0.737674
14	6	0	0.987286	1.525738	0.952491
15	1	0	1.965827	1.805504	1.318270
16	7	0	-0.785587	-1.609908	-0.024503
17	7	0	-3.310684	-0.938539	-0.318637
18	6	0	-4.276837	-1.375407	-1.320826
19	1	0	-4.294536	-2.467404	-1.331991
20	1	0	-5.298713	-1.024600	-1.117253
21	1	0	-3.973442	-1.021557	-2.306345
22	6	0	-3.636477	-1.427968	1.019005
23	1	0	-4.653843	-1.141528	1.320859
24	1	0	-3.569056	-2.520770	1.037272
25	1	0	-2.946426	-1.014917	1.754477
26	6	0	-0.789325	-2.513879	0.880179
27	1	0	-0.873881	-3.554303	0.594590
28	1	0	-0.717107	-2.233026	1.921222
29	6	0	-0.821799	-1.966198	-1.462420
30	1	0	-1.403755	-2.874026	-1.592335
31	1	0	-1.267461	-1.145685	-2.012605
32	1	0	0.205962	-2.119209	-1.793876
33	6	0	1.867659	-0.827611	0.981499
34	7	0	2.146342	-0.856076	2.423545
35	1	0	2.840592	-1.569303	2.628486
36	6	0	3.102247	-0.404541	0.189676
37	6	0	3.126696	-0.610891	-1.193101
38	6	0	4.200408	0.202322	0.800580
39	6	0	4.222248	-0.213536	-1.953419
40	1	0	2.282967	-1.082603	-1.683883
41	6	0	5.302230	0.598539	0.040984
42	1	0	4.189650	0.367404	1.869896
43	6	0	5.316763	0.394691	-1.336633
44	1	0	4.224093	-0.381009	-3.024167
45	1	0	6.148695	1.067370	0.529554
46	1	0	6.172454	0.702920	-1.925831
47	1	0	1.309291	-1.095957	2.944090
48	1	0	1.589422	-1.814463	0.598548

References

[1] A. S. Antonov, V. Y. Mikshiev, A. F. Pozharskii, V. A. Ozeryanskii, *Synth.* **2014**, *46*, 3273–3282.
[2] H. Ott, M. Denzer, *J. Org. Chem.* **2002**, *33*, 4263–4266.
[3] H. Quast, S. Ivanova, E.-M. Peters, K. Peters, *European J. Org. Chem.* **2000**, *2000*, 1577–1587.
[4] K. Mori, Y. Ohshima, K. Ehara, T. Akiyama, *Chem. Lett.* **2009**, *38*, 524–525.
[5] C. Zhang, S. Murarka, D. Seidel, *J. Org. Chem.* **2008**, *74*, 419–422.
[6] Y.-B. Shen, L.-X. Wang, Y.-M. Sun, F.-Y. Dong, L. Yu, Q. Liu, J. Xiao, *J. Org. Chem.* **2019**, *85*, 1915–1926.
[7] Y.-P. He, Y.-L. Du, S.-W. Luo, L.-Z. Gong, N. B. Ar, -h N N Co, N. N. Co, -h -b, **2011**, DOI 10.1016/j.tetlet.2011.10.062.
[8] H. Shi, L. Xu, D. Ren, L. Wang, W. Guo, S.-S. Li, *Org. Biomol. Chem.* **2020**, *18*, 895–904.
[9] G. M. Sheldrick, *Acta Crystallogr. Sect. A Found. Crystallogr.* **2015**, *71*, 3–8.
[10] G. M. Sheldrick, *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71*, 3–8.
[11] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339–341.
[12] M. J. Frisch, G. W. Trucks, G. E. Schlegel, **2010**.
[13] X. Li, M. J. Frisch, *J. Chem. Theory Comput.* **2006**, *2*, 835–839.
[14] J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev.* **2005**, *105*, 2999–3093.