

Supplementary Materials

Synthesis and Structure of 5-Methyl-9-(trifluoromethyl)-12*H*-quino[3,4-*b*][1,4]benzothiazinium Chloride as Anticancer Agent

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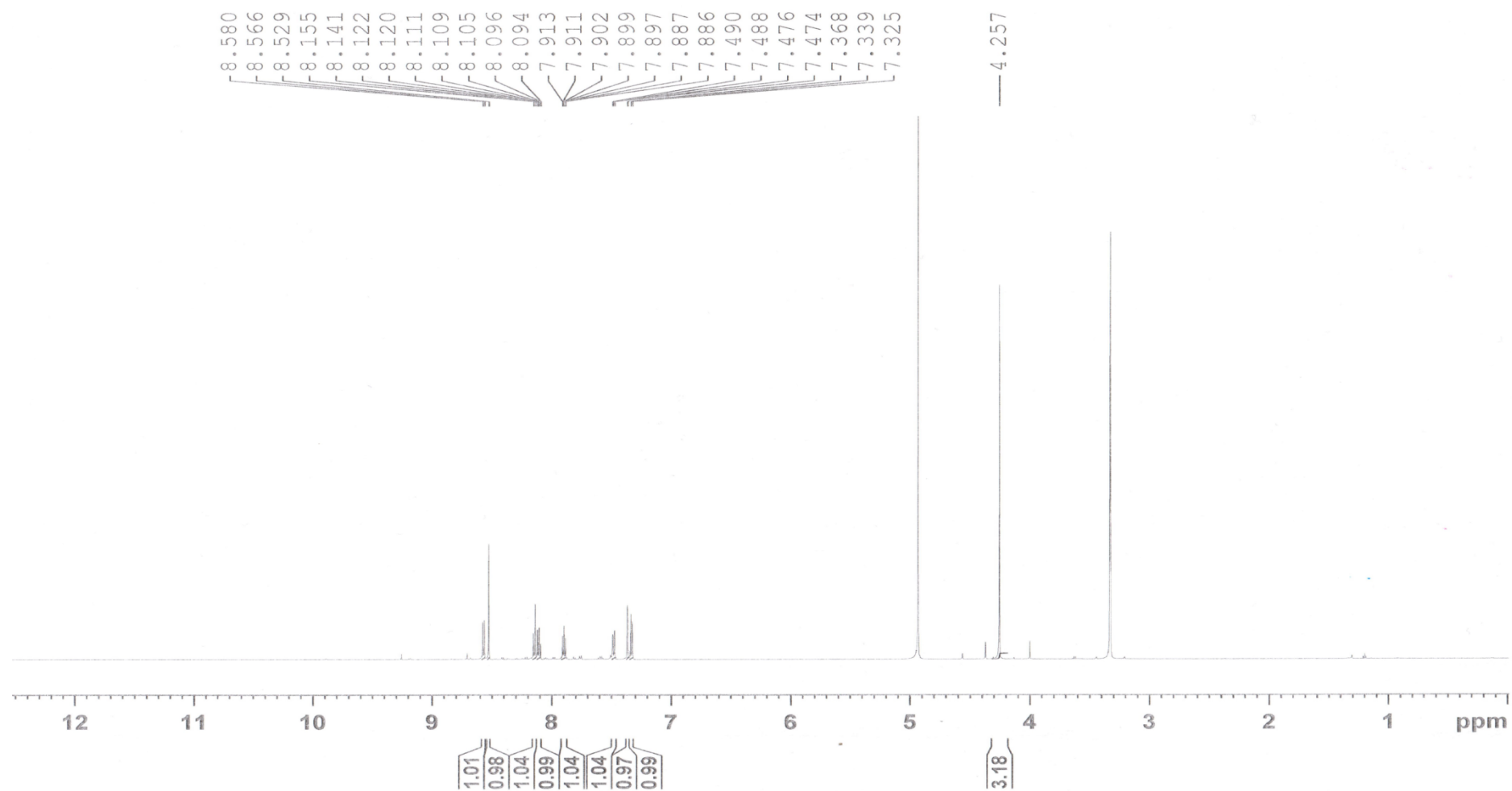


Figure S1. ¹H NMR spectrum of 5-methyl-9-(trifluoromethyl)-12H-quino[3,4-b][1,4]benzothiazinium chloride (3) in CD₃OD.

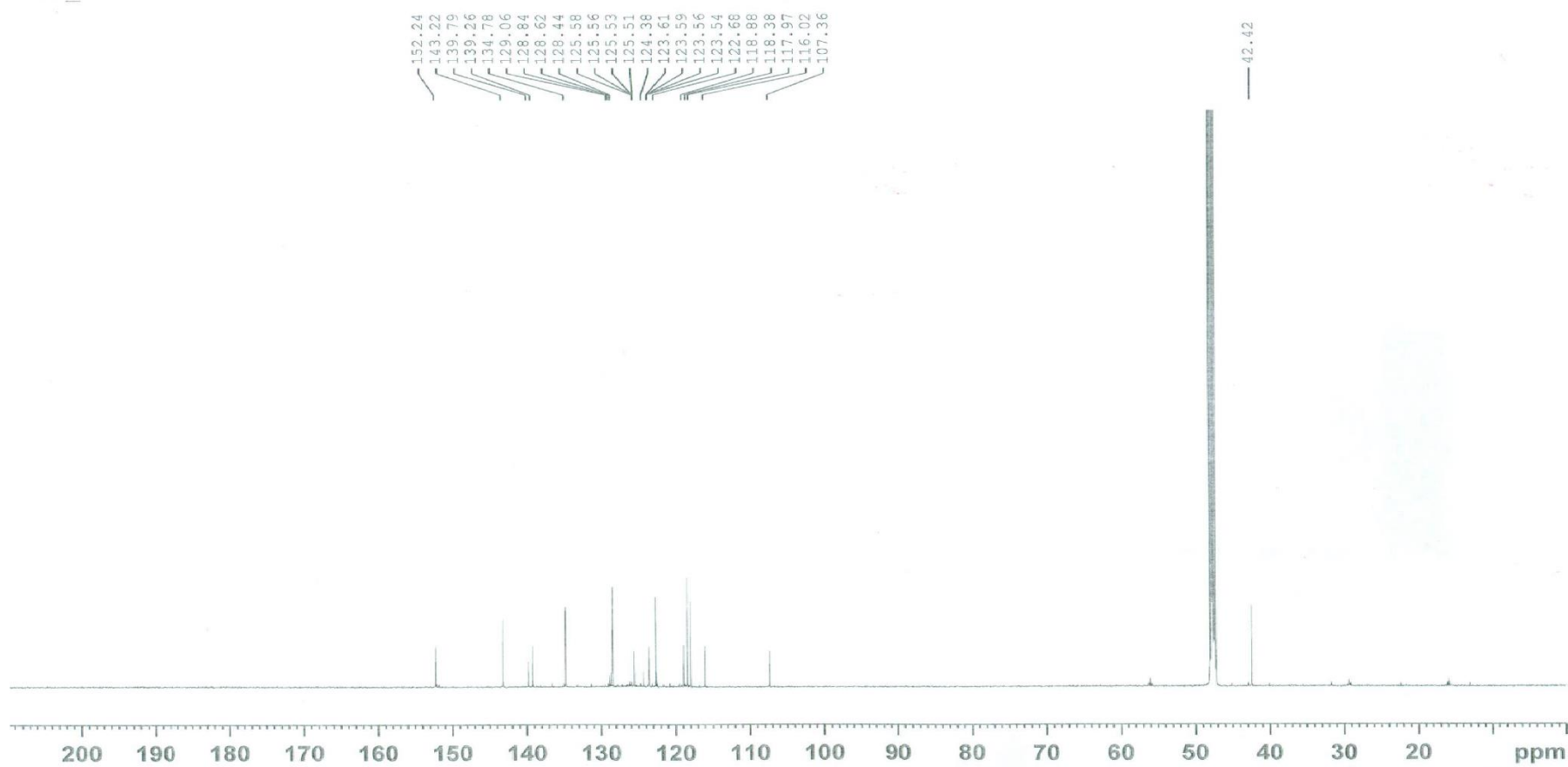


Figure S2. ^{13}C NMR spectrum of 5-methyl-9-(trifluoromethyl)-12H-quino[3,4-b][1,4]benzothiazinium chloride (3) in CD_3OD .

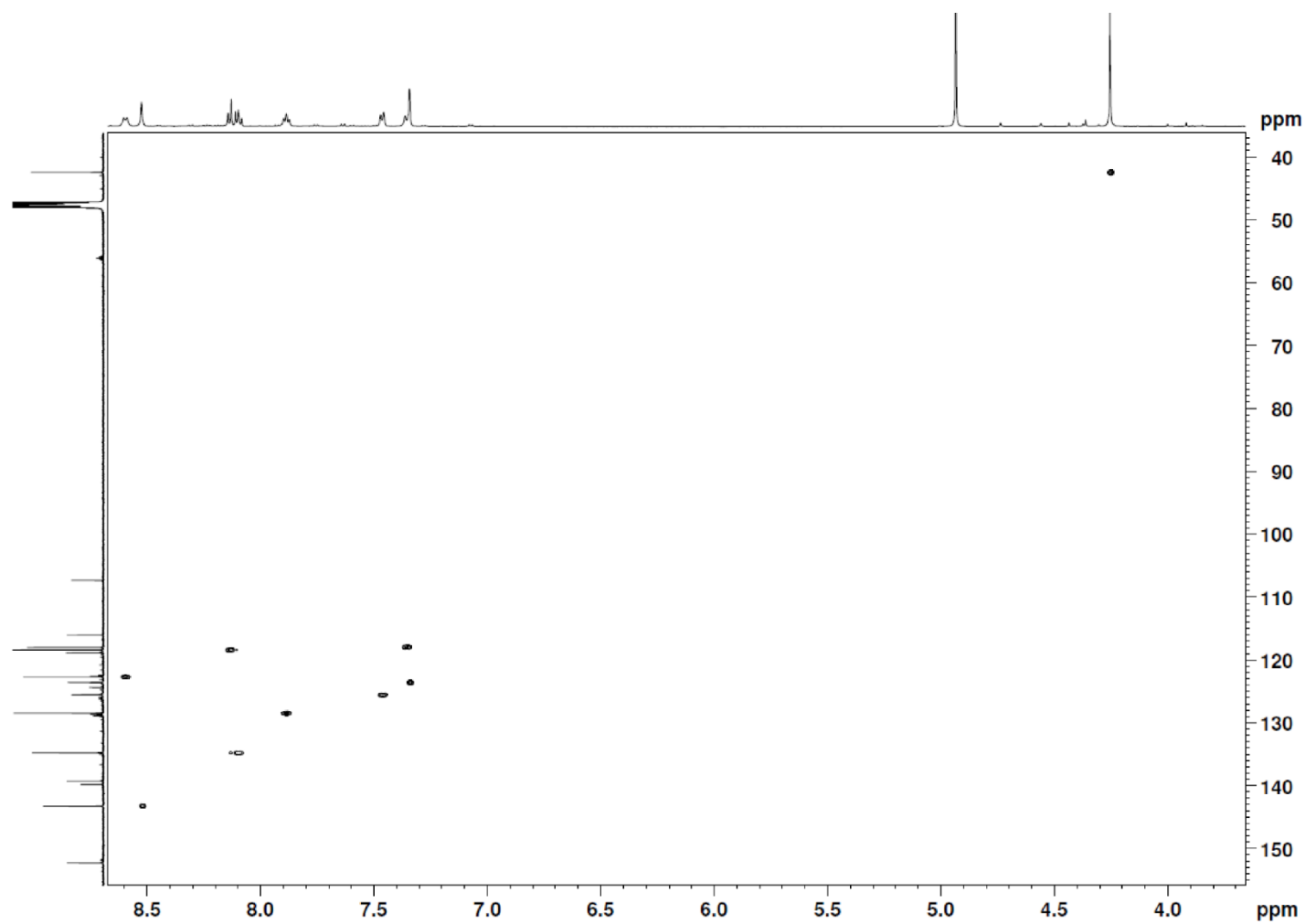


Figure S3. HSQC spectrum of 5-methyl-9-(trifluoromethyl)-12*H*-quino[3,4-*b*][1,4]benzothiazinium chloride (3) in CD_3OD .

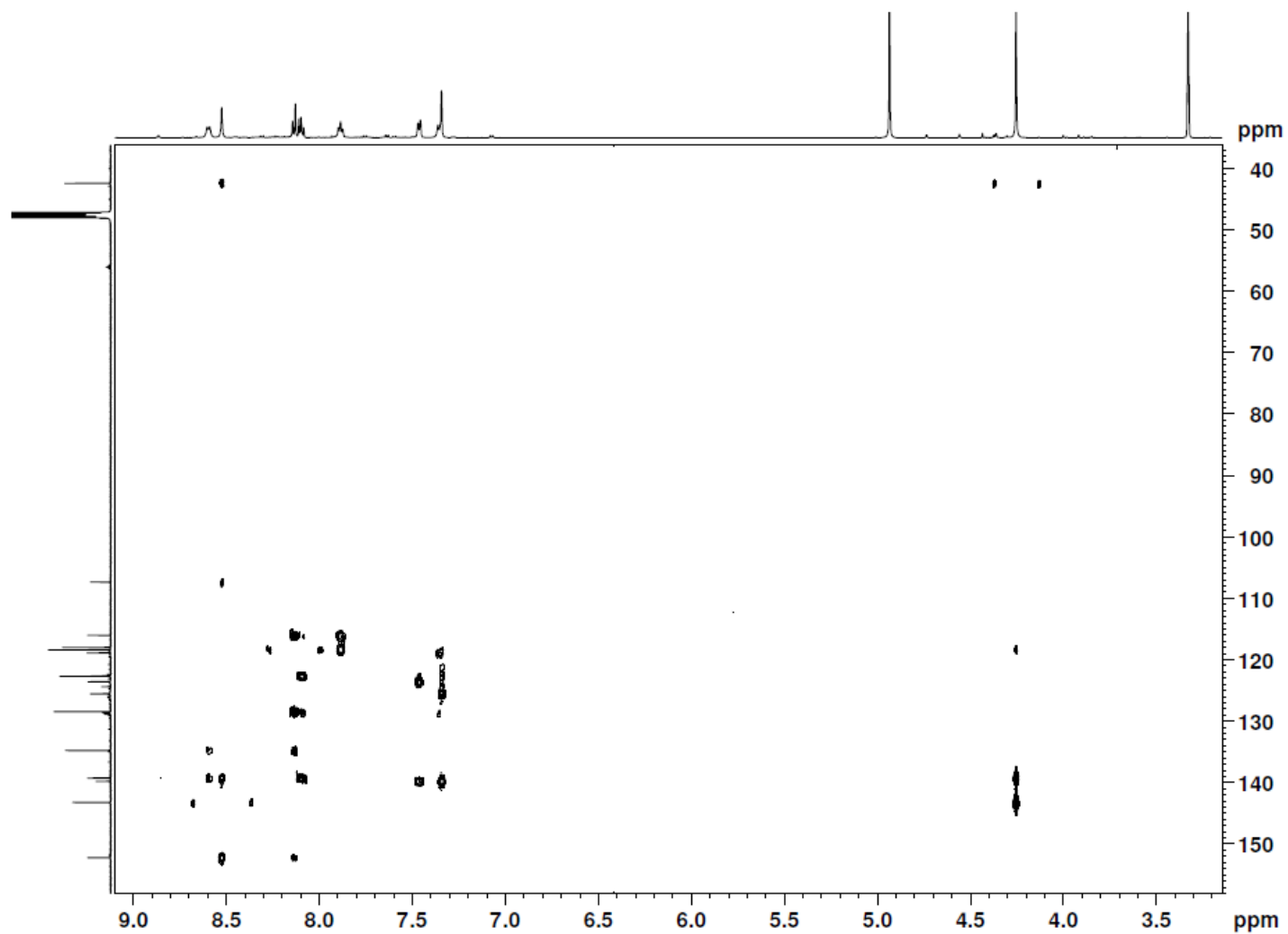


Figure S4. HMBC spectrum of 5-methyl-9-(trifluoromethyl)-12*H*-quino[3,4-*b*][1,4]benzothiazinium chloride (3) in CD₃OD.

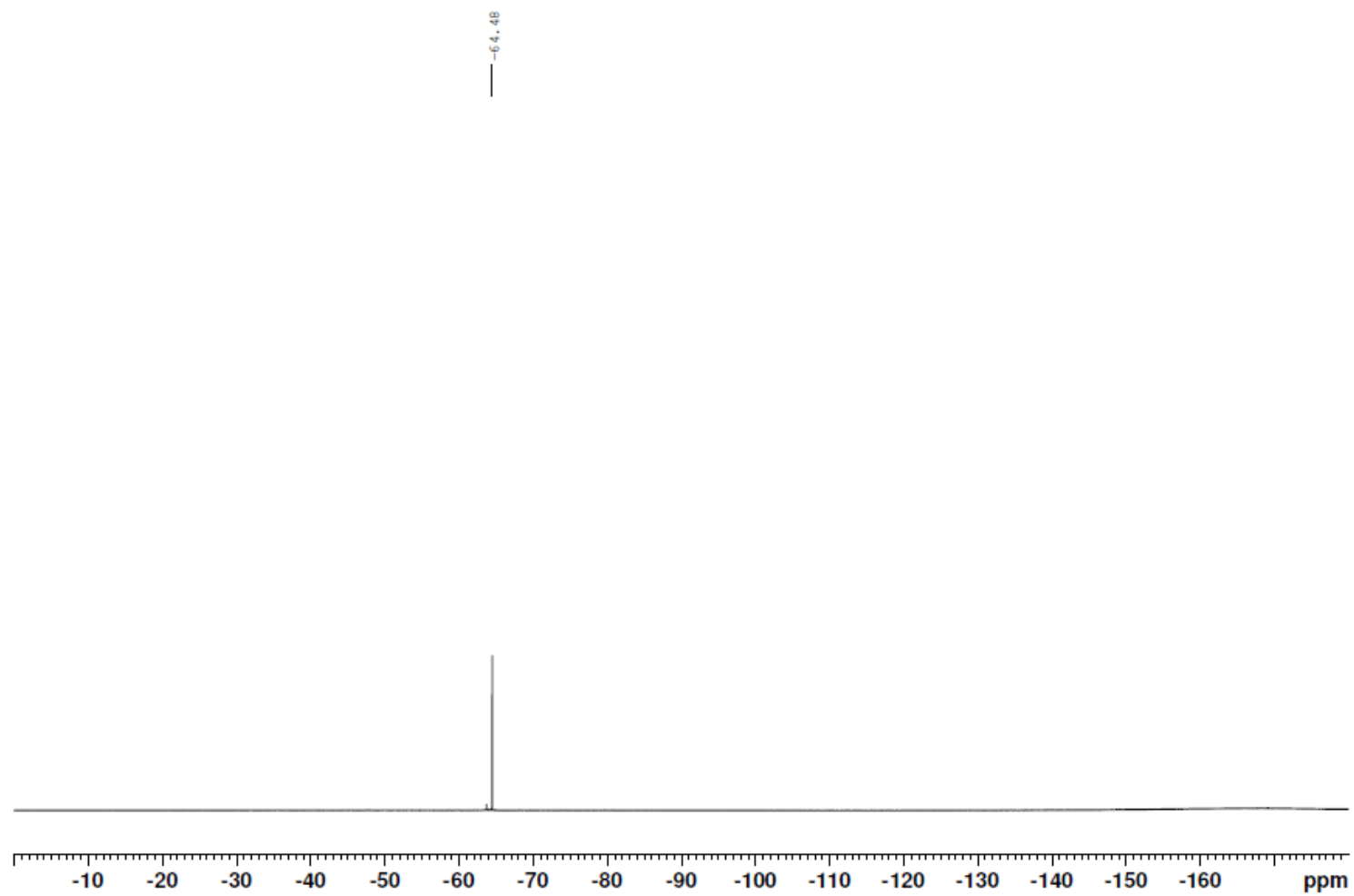


Figure S5. ^{19}F -NMR spectrum of 5-methyl-9-(trifluoromethyl)-12*H*-quino[3,4-*b*][1,4]benzothiazinium chloride (3) in CD_3OD .

Charge distribution of the studied molecule (**3**) as given by the Hirshfeld population analysis.

a) Crystal structure as given (cif format)

Total integrated alpha density = 93.999921339

Total integrated beta density = 93.999921339

ATOM	CHARGE	SPIN
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0 Cl	-0.721181	0.000000
1 S	-0.000790	0.000000
2 F	-0.178764	0.000000
3 N	0.015460	0.000000
4 N	-0.061465	0.000000
5 H	0.085324	0.000000
6 C	-0.040860	0.000000
7 H	0.034464	0.000000
8 C	0.073411	0.000000
9 C	0.063967	0.000000
10 H	0.059796	0.000000
11 C	-0.011102	0.000000
12 C	-0.014286	0.000000
13 H	0.044113	0.000000
14 C	0.009981	0.000000
15 H	0.031806	0.000000
16 C	0.071052	0.000000
17 C	-0.003094	0.000000
18 H	0.057687	0.000000
19 H	0.050632	0.000000
20 H	0.051218	0.000000
21 C	0.133741	0.000000
22 C	-0.000017	0.000000
23 C	0.302284	0.000000
24 C	-0.029918	0.000000
25 C	-0.048109	0.000000
26 H	0.026453	0.000000
27 C	-0.007715	0.000000

28 C	0.018856	0.000000
29 H	0.026259	0.000000
30 C	0.003019	0.000000
31 H	0.051441	0.000000
32 C	0.005245	0.000000
33 H	0.044276	0.000000
34 F	-0.077720	0.000000
35 F	-0.065308	0.000000
TOTAL	0.000157	0.000000

b) Structure optimized in the gas phase

Total integrated alpha density = 94.000008501

Total integrated beta density = 94.000008501

ATOM	CHARGE	SPIN
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0 Cl	-0.555604	0.000000
1 S	-0.010525	0.000000
2 F	-0.110031	0.000000
3 N	-0.020858	0.000000
4 N	-0.059394	0.000000
5 H	0.086556	0.000000
6 C	-0.051977	0.000000
7 H	0.039067	0.000000
8 C	0.065958	0.000000
9 C	0.055530	0.000000
10 H	0.061847	0.000000
11 C	-0.028269	0.000000
12 C	-0.018663	0.000000
13 H	0.051079	0.000000
14 C	-0.017120	0.000000
15 H	0.041364	0.000000
16 C	0.063800	0.000000
17 C	0.009934	0.000000
18 H	0.053451	0.000000
19 H	0.048536	0.000000

20 H	0.050244	0.000000
21 C	0.123695	0.000000
22 C	-0.009236	0.000000
23 C	0.289377	0.000000
24 C	-0.038590	0.000000
25 C	-0.034500	0.000000
26 H	0.042175	0.000000
27 C	-0.011469	0.000000
28 C	-0.003510	0.000000
29 H	0.032422	0.000000
30 C	-0.020978	0.000000
31 H	0.054722	0.000000
32 C	-0.006188	0.000000
33 H	0.050456	0.000000
34 F	-0.105794	0.000000
35 F	-0.117525	0.000000
TOTAL	-0.000017	0.000000

c) Structure optimized in the presence of the water molecule. Continuum C-PCM scheme applied.

Total integrated alpha density = 93.999869974

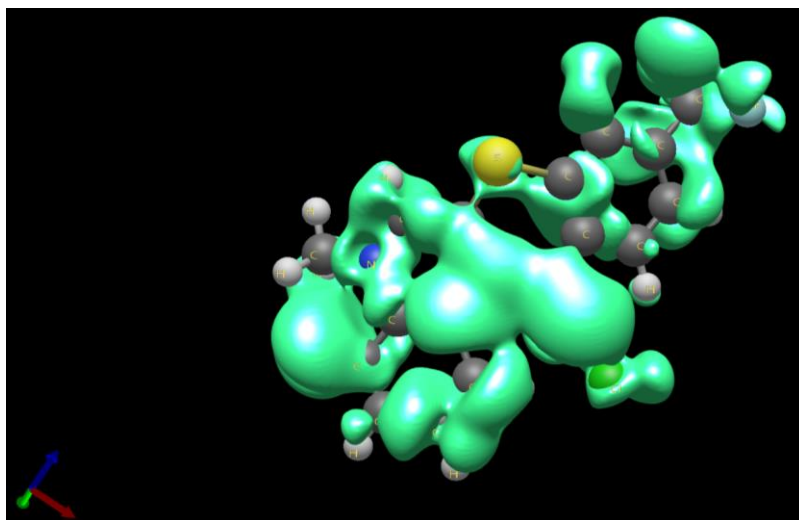
Total integrated beta density = 93.999869974

ATOM	CHARGE	SPIN
0 Cl	-0.736462	0.000000
1 S	-0.012725	0.000000
2 F	-0.120723	0.000000
3 N	0.015309	0.000000
4 N	-0.078043	0.000000
5 H	0.096428	0.000000
6 C	-0.030811	0.000000
7 H	0.063273	0.000000
8 C	0.080234	0.000000
9 C	0.097557	0.000000
10 H	0.092716	0.000000
11 C	-0.036544	0.000000

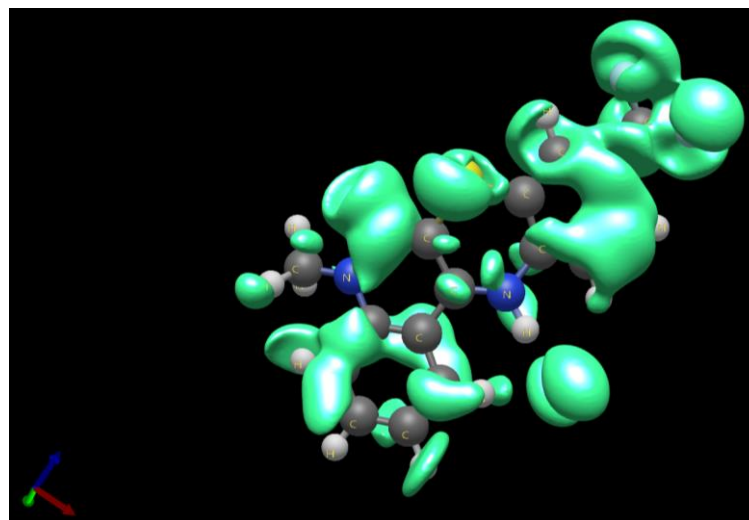
12 C	-0.022811	0.000000
13 H	0.059310	0.000000
14 C	-0.035055	0.000000
15 H	0.035377	0.000000
16 C	0.065442	0.000000
17 C	0.025042	0.000000
18 H	0.071318	0.000000
19 H	0.064856	0.000000
20 H	0.064446	0.000000
21 C	0.118126	0.000000
22 C	-0.005047	0.000000
23 C	0.290651	0.000000
24 C	-0.030382	0.000000
25 C	-0.027132	0.000000
26 H	0.055296	0.000000
27 C	-0.013198	0.000000
28 C	-0.024257	0.000000
29 H	0.022451	0.000000
30 C	-0.026015	0.000000
31 H	0.058463	0.000000
32 C	-0.004514	0.000000
33 H	0.064210	0.000000
34 F	-0.108235	0.000000
35 F	-0.128292	0.000000
TOTAL	0.000260	0.000000

Table S1. HOMO-LUMO gap, electric dipole momentum. HOMO-LUMO gap in eV, dipole moment in Debyes.

Structure	HOMO-LUMO [eV]	Dipole moment [Debyes]
a)	1.291	18.41
b)	1.315	14.29
c)	1.304	24.09



(a)



(b)

Figure S6. HOMO (a) and LUMO (b) orbitals for molecule **3** optimized in the gas phase.