Supporting Information for

B-O-B Bridged BOPPY Derivatives: Synthesis, Structures, and Acid-Catalyzed Cis-Trans Interconversion

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1 Cis-trans interconversion characterization

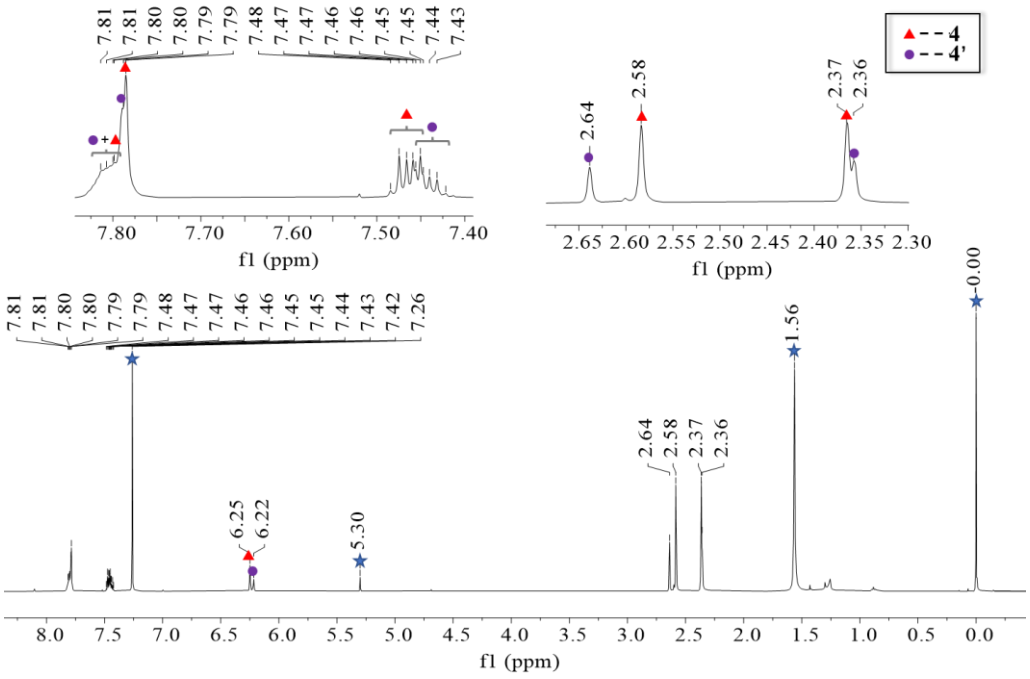


Figure S1. ^{1}H NMR spectrum of compound **4'** (400 MHz, acidic CD_3Cl).

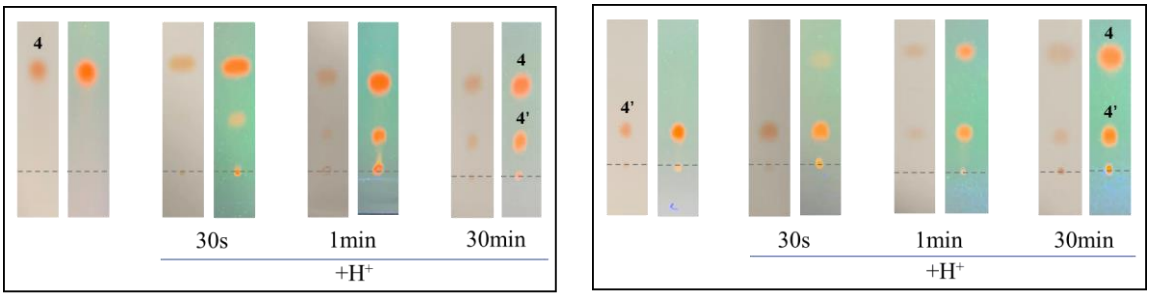


Figure S2. TLC analysis of dichloromethane solutions (ca. 10^{-3}M) of **4** (left) and **4'** (right) at different times after the addition of hydrochloric acid (1 equiv.) (eluent: n-hexane:CH_2Cl_2 = 1:4).

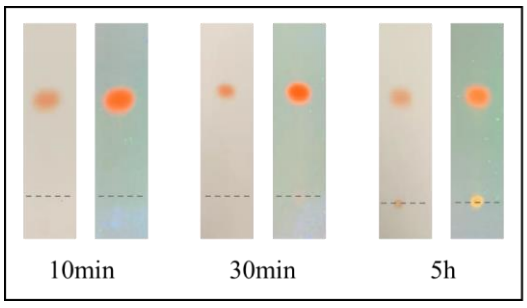


Figure S3. TLC analysis of toluene solution (ca. 10^{-3} M) of **4** at different times after reflux (eluent: n-hexane:CH_2Cl_2 = 1:4).

As shown in Figures S2-3, the addition of hydrochloric acid induced the interconversion of trans-cis isomers **4** and **4'**, whereas heating did not, further indicating that the above cis-trans isomerization processes were triggered by the acid. In addition, similar isomerization occurred between their brominated products **4Br** and **4Br'**, as evidenced by the appearance of mixed signal peaks of the isomers in ^{1}H NMR.

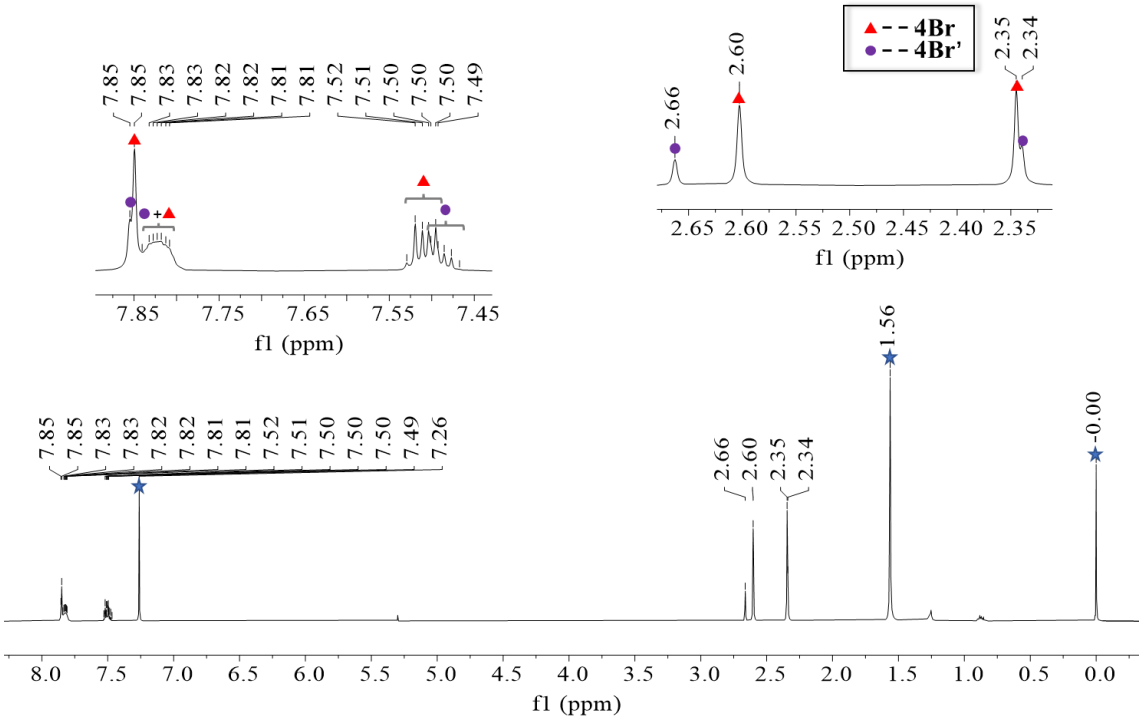


Figure S4. ^{1}H NMR spectrum of compound **4Br** (400 MHz, acidic CD_3Cl).

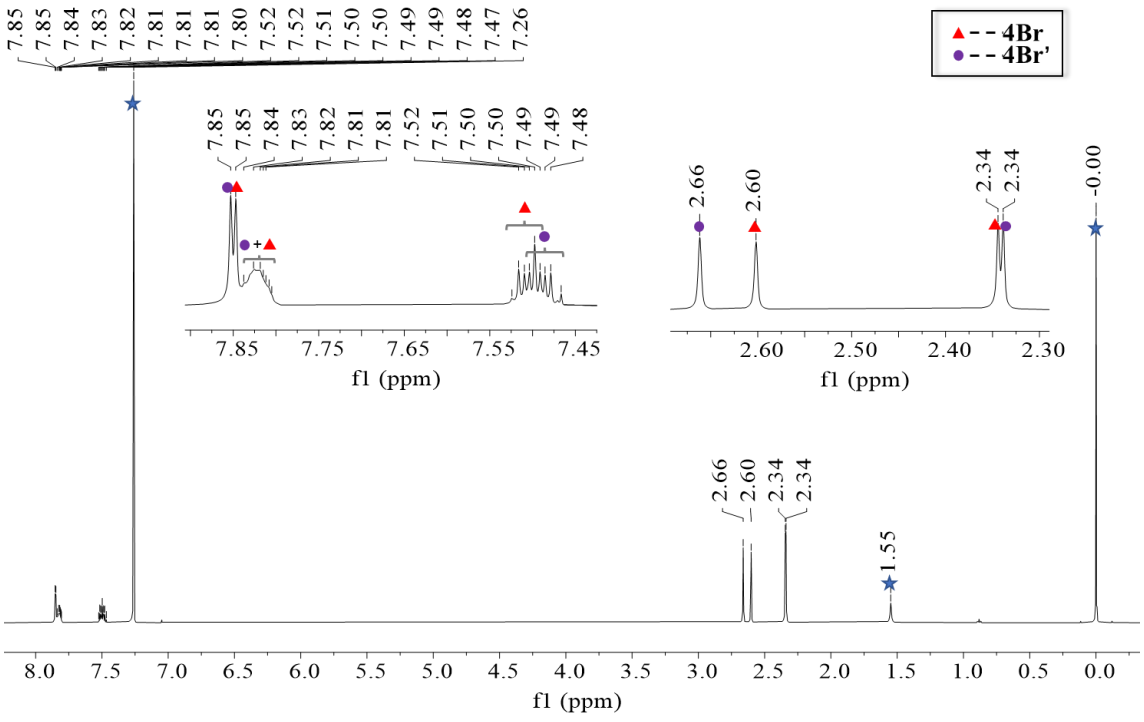


Figure S5. ^{1}H NMR spectrum of compound **4Br'** (400 MHz, acidic CD_3Cl).

2 Crystal packings and selected parameters

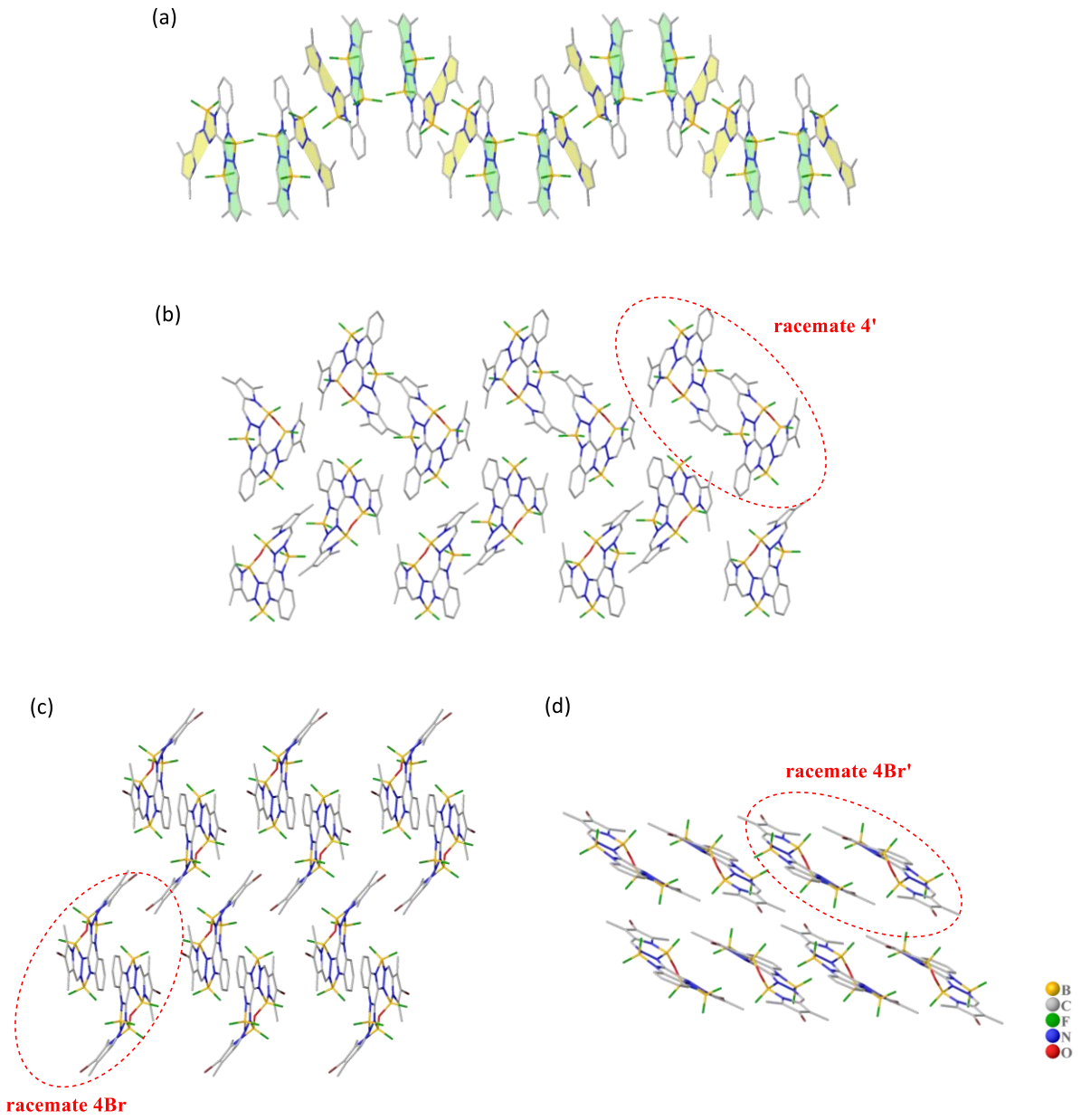
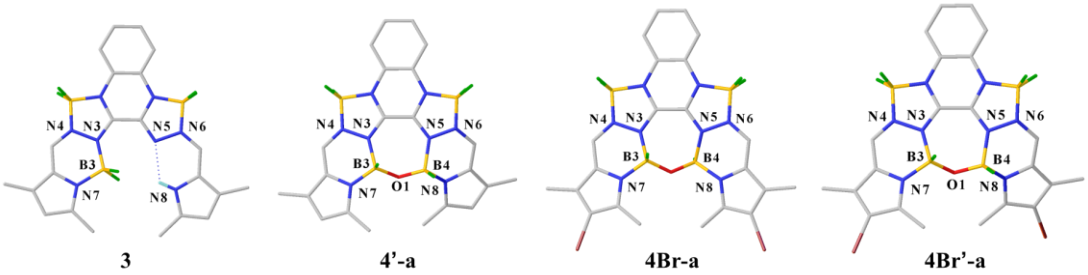


Figure S6. Crystal-packing pattern of **3** (a), **4'** (b), **4Br** (c) **and 4Br'** (d). Two halves of the ligand of **3** are marked in yellow and green, respectively. Each B-O-B bridge compound has an equal number of enantiomers in the crystal unit cell.

Table S1. Crystal data and collection parameters for **3**, **4'**, **4Br** and **4Br'** obtained from crystallography.

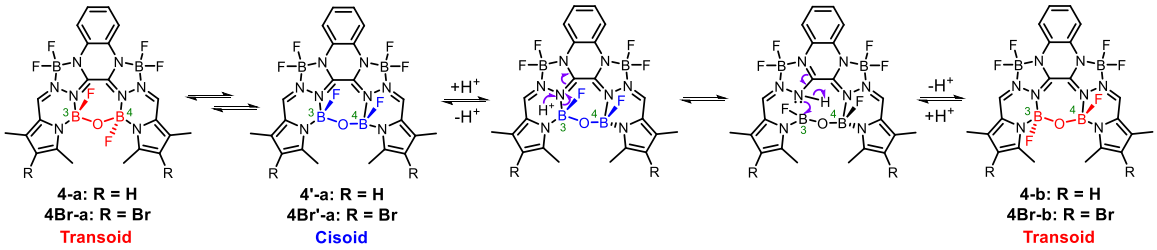
	3	**4'**	**4Br**	**4Br'**
CCDC. No.	2091170	2091171	2091172	2091174
formula	$C_{22}H_{21}B_3F_6N_8$	$C_{22}H_{20}B_4F_6N_8O$	$C_{22}H_{18}B_4Br_2F_6N_8O$	$C_{22}H_{18}B_4Br_2F_6N_8O$
fw	543.90	569.70	727.50	727.50
T (K)	199(2)	189.99	193.0	296.15
λ (Å)	1.34139	1.34139	1.34139	0.71073
crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
space group	C 2/c	P 21/n	C 1 2/c 1	P -1
a (Å)	21.593(13)	8.3897(2)	12.6730(10)	9.2437(8)
b (Å)	17.946(12)	21.0157(6)	24.2903(19)	12.7062(10)
c (Å)	15.446(10)	13.7432(4)	8.7967(8)	13.7867(10)
α (deg)	90	90	90	107.288(2)
β (deg)	112.98(3)	100.3310(10)	107.285(5)	98.865(3)
γ (deg)	90	90	90	96.501(3)
v (Å^3)	5510(6)	2383.85(11)	2585.6(4)	1505.8(2)
Z	8	4	4	2
D_{calcd} (mg/m^3)	1.311	1.587	1.869	1.605
μ mm^{-1}	0.600	0.730	3.099	0.0517
F(000)	2224	1160	1432	716
θ range (deg)	2.89-43.11	3.382-53.879	2.79-54.37	1.915-27.498
reflections collected / unique	20895/4889	18845/4316	9672/2873	13774/6792
R (int)	0.0923	0.0415	0.0462	0.0517
goodness-of-fit on F^2	0.983	1.056	1.059	1.040
R_1, wR_2 [$I>2\sigma(I)$]	0.0617, 0.1495	0.0363, 0.0966	0.0352, 0.0849	0.0425, 0.1117
R_1, wR_2 (all data)	0.1521, 0.1908	0.0433, 0.1035	0.0471, 0.0902	0.0517, 0.1173
Largest diff. peak and hole, e. Å^{-3}	0.233/-0.159	0.275/-0.208	0.350/-0.519	0.715/-0.785

Table S2. Selected bond lengths [Å] and dihedral angles [deg] of crystals **3**, **4'**, **4Br** and **4Br'** obtained from crystallography.

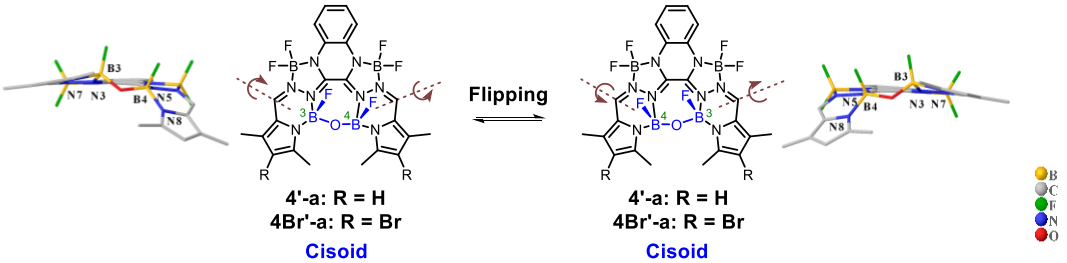


dyes	B-N bonds distances (Å)				N-N bonds distances (Å)		B-O-B bond angles (deg)
	B3-N3	B3-N7	B4-N5	B4-N8	N3-N4	B5-N6	B3-O1-B4
3	1.538 (8)	1.609 (8)	––	––	1.413 (4)	1.401 (4)	––
4'	1.619 (2)	1.548 (8)	1.620 (2)	1.555 (2)	1.399 (2)	1.407 (2)	127.0 (1)
4Br	1.610 (4)	1.552 (4)	1.610 (4)	1.552 (4)	1.402 (2)	1.402 (2)	134.9 (3)
4Br'	1.606 (3)	1.548 (4)	1.614 (3)	1.558 (4)	1.395 (3)	1.410 (3)	124.0 (2)

3 Proposed mechanism of enantiomeric isomerization



Scheme S1. Proposed mechanism for the conversion process of trans- enantiomers.



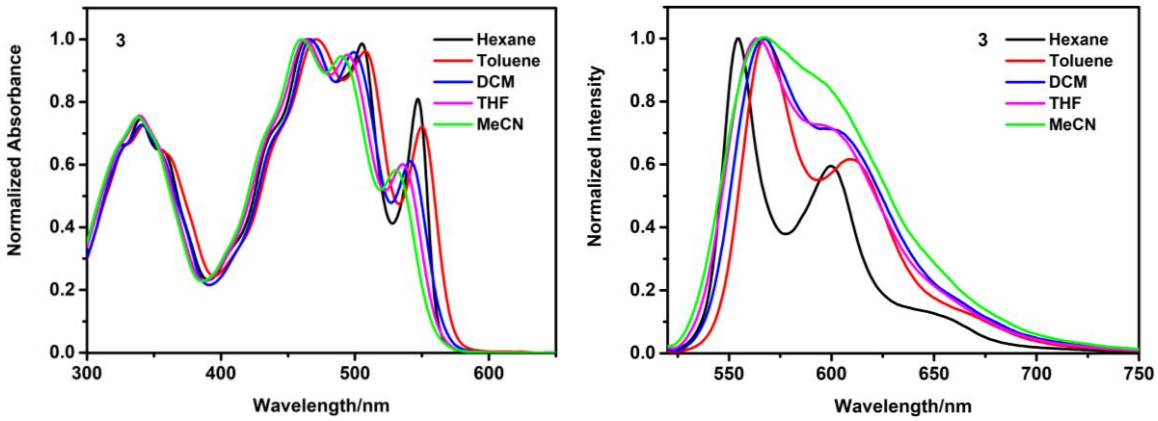
Scheme S2. Proposed mechanism for the conversion process of cis-enantiomers.

4 Photophysical properties

Table S3 Photophysical properties of complex **3** and racemates **4, 4', 4Br** and **4Br'** in different solvents.

	Solvent	λ_{abs}^{max} /nm (log ε_{max})[a]	λ_{em}^{max} /nm	$\Delta\nu_{em\text{-}abs}$ /cm^{-1}	Φ_F	τ_f /ns
3	Hexane	465 (4.50), 505 (4.50), 547 (4.41)	554, 600	4839	0.50	3.13
	Toluene	471 (4.51), 508 (4.50), 550 (4.37)	568, 609	4811	0.52	3.47
	CH_2Cl_2	467 (4.56), 499 (4.54), 541 (4.35)	567, 596 (sh)	4635	0.59	3.60
	THF	463 (4.54), 495 (4.52), 536 (4.32)	563, 593 (sh)	4735	0.39	3.35
	CH_3CN	460 (4.54), 508 (4.51), 550 (4.31)	565	4040	0.47	3.28
4	Hexane	470 (4.52), 498 (4.56)	560, 605	4748	0.16	2.13
	Toluene	496 (4.56)	576, 610 (sh)	3768	0.07	1.10
	CH_2Cl_2	473 (4.54), 498 (4.57)	579, 613 (sh)	4828	0.08	0.93
	THF	470 (4.57)	581, 608 (sh)	4829	0.02	0.54
	CH_3CN	470 (4.57)	598	4554	<0.01	0.42
4'	Hexane	491 (4.57)	556, 599	3672	0.21	2.63
	Toluene	490 (4.58)	567, 604 (sh)	3852	0.14	1.61
	CH_2Cl_2	492 (4.56)	576, 608 (sh)	3878	0.08	1.16
	THF	473 (4.57)	579	3870	0.06	0.78
	CH_3CN	488 (4.57)	588	3485	0.02	0.47
4Br	Hexane	476 (4.48), 505 (4.54)	566, 611	4642	0.11	1.52
	Toluene	504 (4.55)	583, 622 (sh)	3764	0.06	0.94
	CH_2Cl_2	480 (4.51), 506 (4.55)	586	3768	0.04	0.77
	THF	484 (4.55)	591	3741	0.02	0.46
	CH_3CN	488 (4.55)	605	3963	<0.01	0.28
4Br'	Hexane	480 (4.51), 500 (4.55)	564, 605	4304	0.19	1.71
	Toluene	496 (4.51)	576, 604 (sh)	3605	0.07	1.10
	CH_2Cl_2	499 (4.55)	585, 612 (sh)	3700	0.04	0.82
	THF	478 (4.50)	590	3971	0.03	0.50
	CH_3CN	478 (4.56)	600	4254	<0.01	0.27

[a]Molar absorption coefficients were obtained at the maximum of the highest peak.



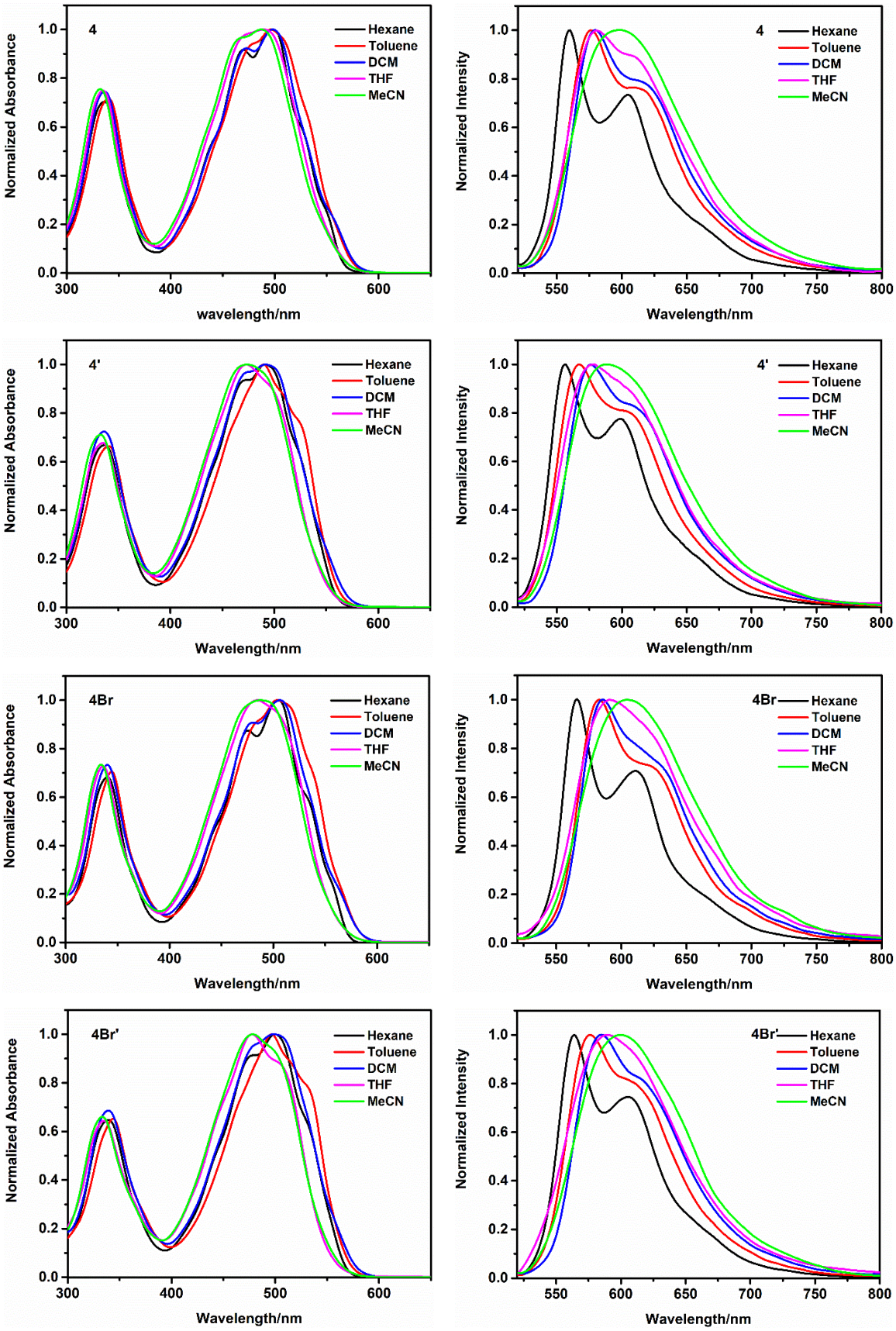


Figure S7. The absorption and emission spectra of complex **3** and racemates **4, 4', 4Br** and **4Br'** in different solvents.

5 Electrochemical properties

Table S4. Electrochemical data acquired and HOMO-LUMO gaps of selected components **3, 4** and **4'**.

dyes	E_{ox} (V)	E_{red} (V)	E_{red}^{onset} (V)	E_{ox}^{onset} (V)	LUMO (eV)	HOMO (eV)[c]	E_g (eV)[d]
3	1.29	-1.01	-0.89	1.17	-3.39	-5.57	2.18
4	1.59	-0.76	-0.64	1.47	-3.64	-5.87	2.23
4'	1.60	-0.77	-0.65	1.48	-3.63	-5.88	2.25

E_{ox} = irreversible oxidation potentials; E_{red} = half-wave potential of the first reduction; E_{red}^{onset} = the onset reduction potentials; E_{ox}^{onset} = the onset oxidative potentials; $E_{LUMO} = -e(E_{red}^{onset} + 4.4)$; $E_{HOMO} = -e(E_{ox}^{onset} + 4.4)$; $E_g = E_{LUMO} - E_{HOMO}$.

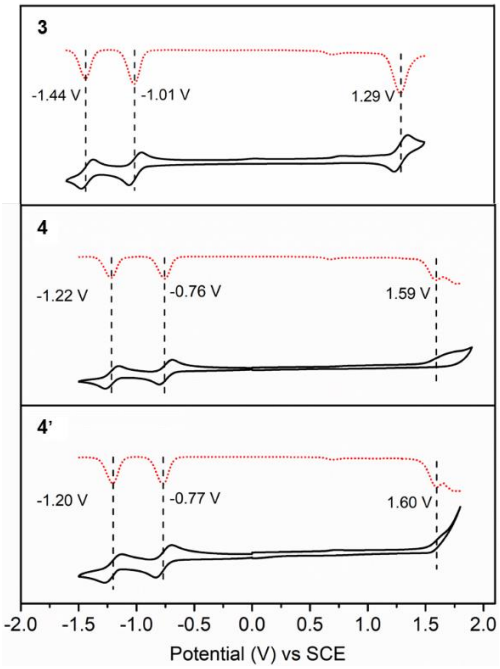


Figure S8. Cyclic voltammograms of selected components **3, 4** and **4'** (1 mM) measured in MeCN at a scan rate of 100 mVs^{-1}, containing 0.1m $TBAPF_6$ as the supporting electrolyte at room temperature. Glassy carbon electrode as a working electrode.

6 Computational Details

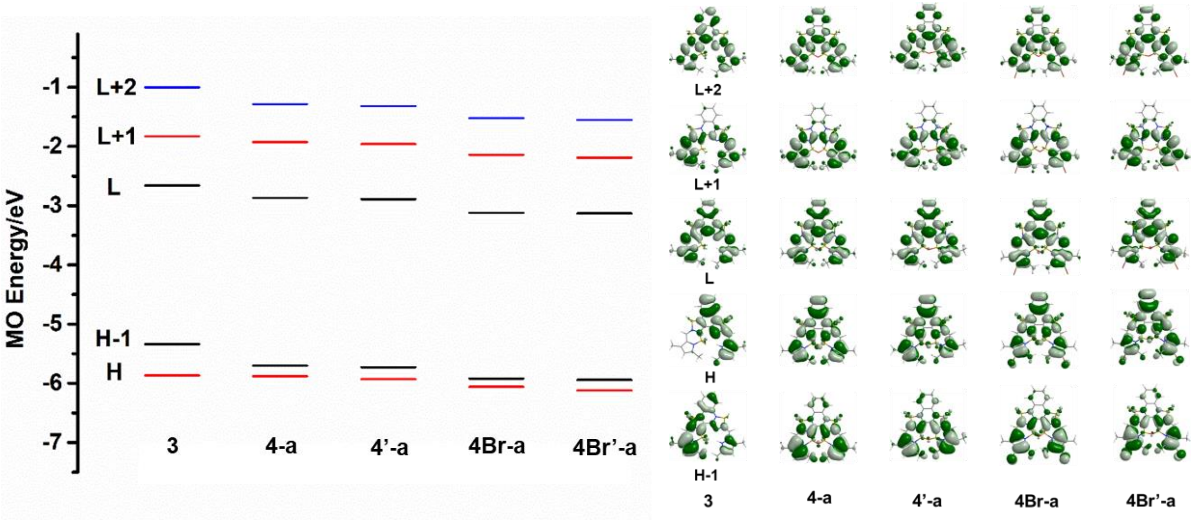


Figure S9. Selected frontier MOs and energies (in a.u.).

Table S5. Calculated electronic excitation energies, oscillator strengths, and eigenvectors for the TD-DFT spectra of compound **3** as well as the enantiomers **a** in all racemates.

	State[a]	Energy [eV]	λ [nm]	*f* [b]	Orbitals (coefficient)[c]
3	S_1	2.38	522	0.2683	H→L (96%)
	S_2	2.83	439	0.3209	H − 1→L (97%)
	S_3	3.07	405	0.2035	H→L + 1 (91%)
	S_9	3.76	312	0.3219	H − 1→L + 1 (29%), H→L + 2 (26%), H − 2→L + 1 (10%), H − 2→L (8%)
4-a	S_1	2.58	481	0.1804	H − 1→L (100%)
	S_2	2.59	480	0.4344	H→L (98%)
	S_8	3.73	333	0.4603	H − 1→L + 1 (70%), H→L + 1 (21%)
4'-a	S_1	2.60	478	0.4046	H→L (86%), H − 1→L (13%),
	S_2	2.61	476	0.2041	H − 1→L (87%), H→L (13%)
	S_8	3.74	332	0.4424	H − 1→L + 1 (69%), H→L + 2 (22%)
4Br-a	S_1	2.50	496	0.1648	H − 1→L (100%)
	S_2	3.56	386	0.4752	H→L (98%)
	S_8	3.69	337	0.4969	H − 1→L + 1 (73%), H→L + 2 (16%), H − 4→L (7%)
4Br'-a	S_1	2.55	488	0.1673	H − 1→L (97%), H→L (3%)
	S_2	2.57	483	0.4581	H→L (96%), H − 1→L (3%)
	S_8	3.71	335	0.4197	H − 1→L + 1 (63%), H→L + 2 (20%), H − 4→L (10%)

[a] Excited state. [b] Oscillator strength. [c] MOs involved in the transitions.

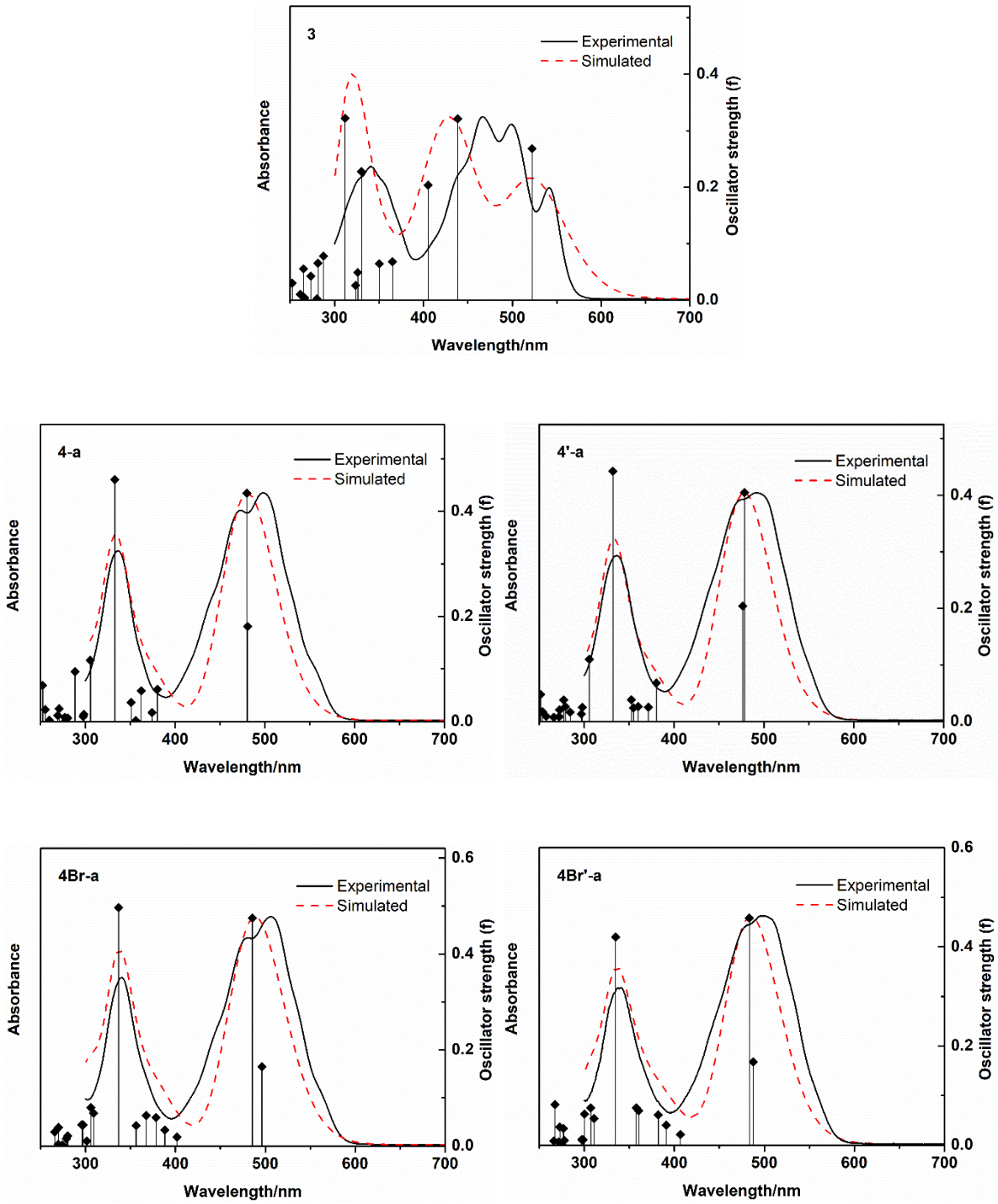
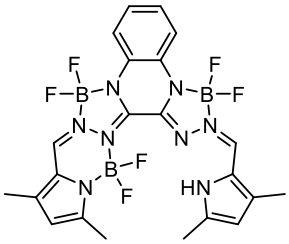


Figure S10. The experimental absorption spectra in dichloromethane (red dotted line) and the calculated absorption spectra (black solid line) of complex **3** and enantiomers **4-a, 4'-a, 4Br-a** and **4Br'-a**. The calculated oscillator strengths are plotted against a secondary axis.

DFT optimized coordinates of all newly-designed BF_2 complexes in the S0 geometry

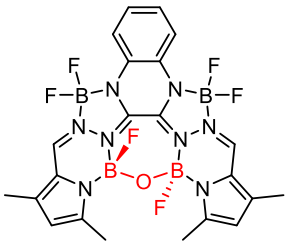


3

3 in the S_0 geometry

F	-3.03337012	2.33919391	-1.93421255
B	-2.80971490	2.04291813	-0.61288311
N	-1.30880115	2.28129179	-0.20798020
C	-0.65899878	3.51672308	-0.10691799
F	-3.71394541	2.65013854	0.22325083
B	2.92312069	2.04842639	0.49776401
N	1.39221670	2.31855576	0.26491926
C	0.72999799	3.52781736	0.15101113
F	3.72979950	2.64751640	-0.44226206
N	-1.47780190	0.02440842	-0.10685714
C	1.40243299	4.75485164	0.26053438
H	2.47217099	4.75815473	0.43507521
C	0.69196900	5.94034768	0.12770668
H	1.21681601	6.88742520	0.21205054
F	3.32337212	2.33099258	1.78230736
N	-2.77048710	0.48097288	-0.36185091
N	1.51126394	0.03706272	0.09938534
C	-0.68976743	5.92563142	-0.11292007
H	-1.23686725	6.85861949	-0.20641270
N	2.81261963	0.47594105	0.25227361
C	-1.36766889	4.71908475	-0.22905459
H	-2.43810472	4.69343806	-0.39575591
C	-0.67860651	1.11468486	-0.04699540
N	-2.50276912	-2.23254482	0.35912169
C	0.76414386	1.11885901	0.12348115
N	2.58831194	-2.44784500	-0.45579511
H	1.65618401	-2.03256751	-0.42874920
C	-3.80933310	-0.32385281	-0.30324879
H	-4.76014970	0.15276918	-0.51528907
C	-3.73320733	-1.67121085	0.02792454
C	-4.75002875	-2.64492003	0.18486807
C	-4.09650350	-3.79589890	0.62435522
H	-4.55534179	-4.74750514	0.86112157
C	-2.71956322	-3.51720420	0.72646722

C	-6.21433275	-2.46570795	-0.08314607
H	-6.79842463	-3.23784425	0.42641410
H	-6.43993641	-2.53733687	-1.15516652
H	-6.57949061	-1.49162794	0.26178152
C	-1.62129495	-4.43216815	1.16122496
H	-2.03775667	-5.33507575	1.61543379
H	-0.96612547	-3.93555749	1.88314352
H	-0.99816327	-4.73295723	0.31022489
C	3.81093343	-0.37215130	0.13529162
H	4.79034522	0.07310427	0.28009485
C	3.75075060	-1.74114050	-0.17137609
C	4.83551418	-2.64476421	-0.31492484
C	6.28845440	-2.33876759	-0.09832744
H	6.91086791	-3.17297928	-0.43502980
H	6.51400731	-2.16607134	0.96167837
H	6.60749509	-1.44551175	-0.64851013
C	4.28261619	-3.87379159	-0.68847647
H	4.82658844	-4.78805837	-0.88785883
C	2.88806720	-3.72441415	-0.77203257
C	1.82869008	-4.71636234	-1.13066365
H	2.10950361	-5.28088763	-2.02631650
H	0.87756962	-4.21177013	-1.31869657
H	1.67642545	-5.44347020	-0.32238139
B	-1.14379919	-1.49142766	0.30627018
F	-0.33321030	-2.08296164	-0.67310378
F	-0.52965744	-1.50295147	1.53804145



4-a

4-a in the S_0 geometry

F	3.18427461	2.32599164	1.90779802
F	3.72073459	2.68213429	-0.28149993
F	0.87861005	-1.03746745	-1.97446008
O	-0.00150061	-1.94893837	0.00060502
N	2.79529681	0.49522057	0.32333575
N	1.34770807	2.32503863	0.28264602
N	1.49506893	0.07278128	0.08524124
N	2.39808709	-2.20491751	-0.50841237
C	0.71682717	1.15779719	0.09452782
C	0.69088859	3.54753770	0.16398425

C	3.63340372	-1.70969236	-0.08701595
C	4.61066817	-2.73606694	-0.19970916
C	1.37494688	4.76108473	0.32037726
H	2.43427582	4.74916482	0.54863873
C	3.78524172	-0.37712806	0.26996015
H	4.76175352	0.03069410	0.50729749
C	3.93459498	-3.83782925	-0.71128566
C	1.48852798	-4.31320536	-1.49037991
H	0.75655467	-4.59917037	-0.72786108
H	1.90285331	-5.22308676	-1.93279987
H	0.94620141	-3.75539541	-2.26058942
C	0.68820018	5.95670974	0.15928194
H	1.21834015	6.89667093	0.27806138
C	6.05874411	-2.63900985	0.17625961
H	6.51522987	-1.70902009	-0.18285995
H	6.62515945	-3.47201053	-0.25038303
H	6.19659907	-2.66982749	1.26477986
C	2.58101859	-3.48045730	-0.90499329
B	1.09571655	-1.35215023	-0.63234499
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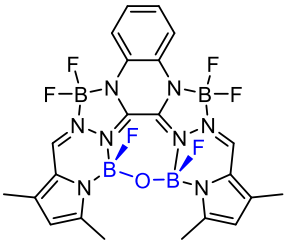

4'-a

4’-a in the S_0 geometry

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B	-3.53155288	-0.26711353	0.73068407
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C	-3.69839447	-3.28150289	0.12485799
H	-4.59728599	-2.71945978	0.34764661
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C	-2.58267948	-5.35674979	-0.44981112
H	-2.63511944	-6.42264983	-0.64930036
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H	3.19050968	3.52076009	0.62062193
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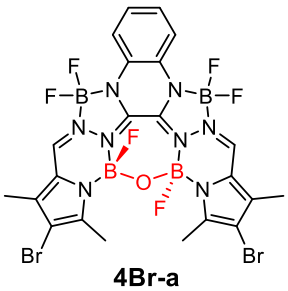

4Br-a

4Br-a in the S_0 geometry

Br	4.50663856	4.68736283	-0.53097845
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F	-3.75807847	3.72391826	-0.11207837

F	-0.01214883	1.04991164	-1.90914966
O	0.86198467	0.00008781	0.00023630
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N	1.15009376	2.42668784	-0.29886320
C	-2.23019220	0.71028348	0.13284590
C	-4.62151631	0.67914017	0.19495439
C	0.64032581	3.63759768	0.17400165
C	1.66955528	4.61502219	0.19080471
C	-5.83549666	1.35495641	0.38315797
H	-5.82520877	2.40227377	0.66117501
C	-0.70464061	3.76878747	0.49816987
H	-1.11990913	4.72983814	0.78038957
C	2.78783962	3.94765984	-0.29248016
C	3.32457142	1.57871641	-1.23149677
H	4.32628199	1.61425002	-0.79147106
H	3.43623370	1.78238262	-2.30450176
H	2.90305659	0.58102410	-1.11247014
C	-7.02977902	0.67493737	0.19021963
H	-7.97040227	1.19765956	0.33344874
C	1.57826377	6.03377372	0.65405098
H	2.25250072	6.66881520	0.07124351
H	1.87377060	6.12788313	1.70705109
H	0.56377288	6.43308288	0.55759477
C	2.44978438	2.61005028	-0.60355847
B	0.27996967	1.14724958	-0.55264665
B	-3.14006302	2.84209195	0.73538498
Br	4.50734727	-4.68669522	0.53089642
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C	-5.83527869	-1.35575815	-0.38332932
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H	-1.11920227	-4.72995106	-0.78045615

C	2.78842930	-3.94725728	0.29243484
C	3.32482823	-1.57830271	1.23159792
H	4.32645000	-1.61345261	0.79133341
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H	2.90302409	-0.58069266	1.11291699
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H	-7.97020970	-1.19876649	-0.33375497
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H	2.25380523	-6.66839345	-0.07182079
H	1.87424619	-6.12738766	-1.70741615
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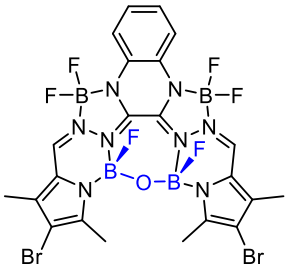

4Br'-a

4Br'-a in the S_0 geometry

Br	0.69667742	6.24595120	-1.27747176
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F	-1.02486037	-0.97107235	2.07484676
F	5.27045186	-0.16691040	0.22702422
F	4.52496263	-0.74232347	2.30956459
F	-0.18055677	-5.23186974	-0.31792754
F	0.07500096	-4.26721266	-2.37040725
O	-0.62073220	0.58941768	0.34020840
N	0.99751945	2.46722962	0.17518614
N	3.09779956	0.68685905	0.90323293
N	1.82495132	0.16846934	0.66542838
N	3.23916336	-1.57460173	0.40983364
N	1.29982834	-3.27481087	-0.49050622
N	-0.38208189	-1.82178599	-0.09344427
N	-1.00264297	-2.94366692	-0.62044146
N	-2.65065465	-0.81423018	0.30252715
C	-1.17621444	3.47375414	-0.58962409
H	-1.49837060	2.48438524	-0.91573604
H	-1.43318471	4.22298447	-1.34285626
H	-1.72761247	3.72344045	0.32651660

C	0.29232831	3.49557043	-0.33586148
C	1.18334257	4.57514395	-0.54811518
C	2.46318829	4.21636279	-0.14430559
C	3.70764116	5.04089467	-0.22241742
H	4.06355769	5.12535628	-1.25708058
H	4.51854844	4.61970372	0.37878009
H	3.51364471	6.05869897	0.13240603
C	2.32776301	2.87660975	0.30272900
C	3.30913424	1.97561624	0.69782634
H	4.34146278	2.28594125	0.81469904
C	1.97074043	-1.12859535	0.36462243
C	0.93496644	-2.05894457	-0.05465030
C	3.61446691	-2.84853164	0.00068451
C	2.61633461	-3.72136310	-0.48132001
C	2.95789490	-5.00924192	-0.91941319
H	2.18229041	-5.67731569	-1.27448037
C	4.28532671	-5.41055775	-0.87659962
H	4.55219641	-6.40811555	-1.21151774
C	5.28029533	-4.53936957	-0.40549824
H	6.31664674	-4.86197107	-0.38295314
C	4.95472115	-3.26272610	0.02917852
H	5.71759724	-2.57580177	0.37479080
C	-2.31176272	-2.95168774	-0.78256109
H	-2.70545399	-3.84886258	-1.24688500
C	-3.15439832	-1.92028184	-0.38294409
C	-4.56501602	-1.81308119	-0.48620229
C	-4.87247117	-0.62660482	0.17092395
C	-3.68885568	-0.03457207	0.66746092
C	-3.55168078	1.20108805	1.49004691
H	-2.76807164	1.08430003	2.24295941
H	-4.50242200	1.42134499	1.98208889
H	-3.28813329	2.06291093	0.86694667
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H	-5.05847562	-3.72782118	-1.35520215
H	-5.86015214	-2.34569680	-2.11635609
H	-6.40212458	-2.90994568	-0.53716486
B	-1.15881470	-0.65017865	0.73113350
B	0.52989766	1.14692792	0.90293642
B	4.18275544	-0.45146537	1.01695731
B	0.03658109	-4.07146616	-1.01326406

7 Copies of ^{1}H, ^{11}B, ^{19}F and ^{13}C NMR spectra

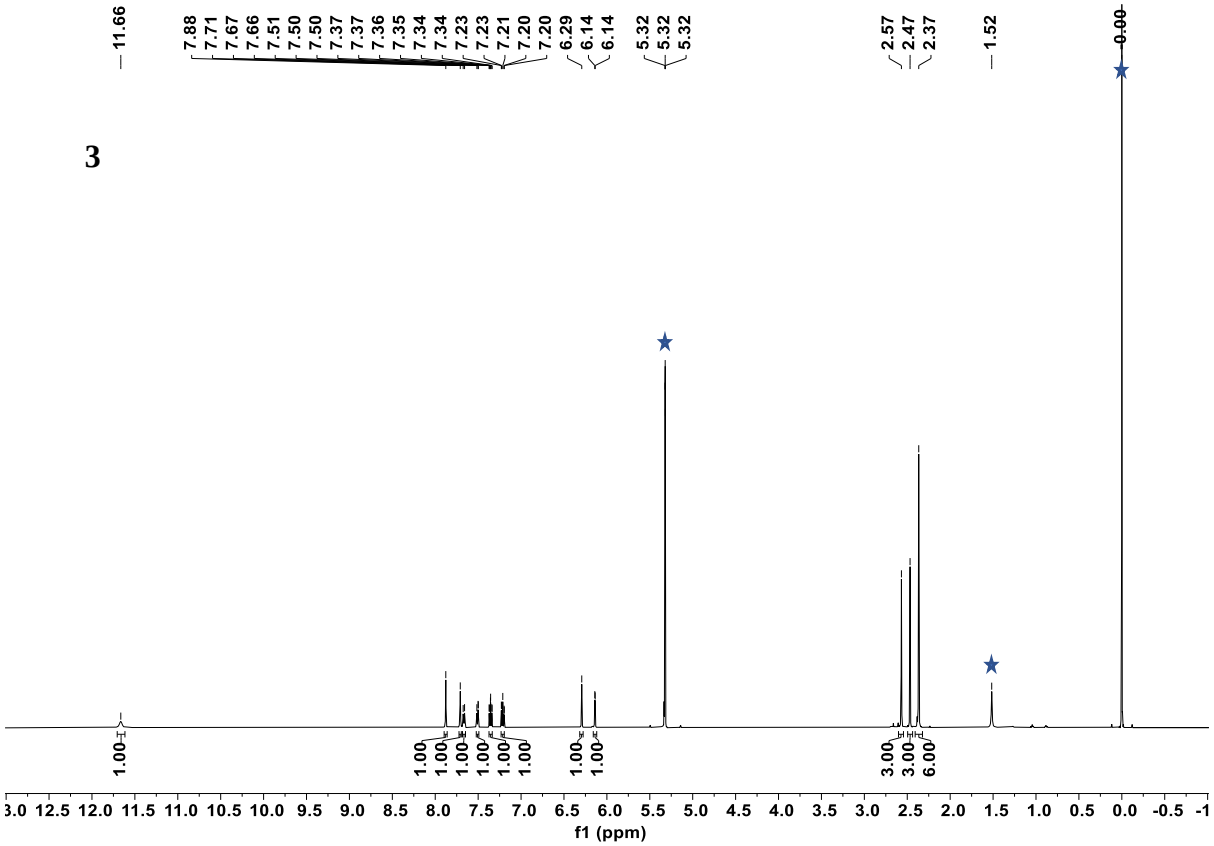

Figure S11. ^{1}H NMR spectra of compound **3** (500 MHz, CD_2Cl_2).

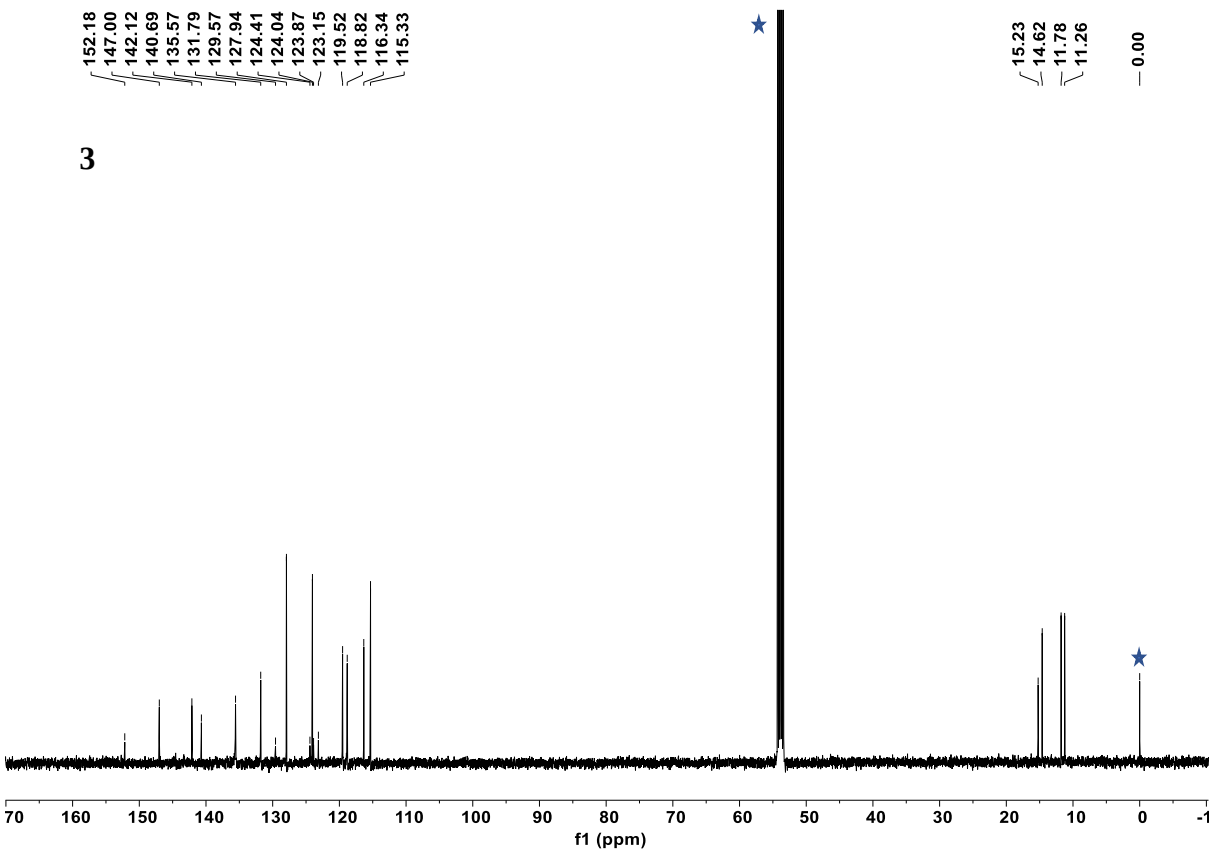

Figure S12. ^{13}C NMR spectrum of compound **3** (125 MHz, CD_2Cl_2).

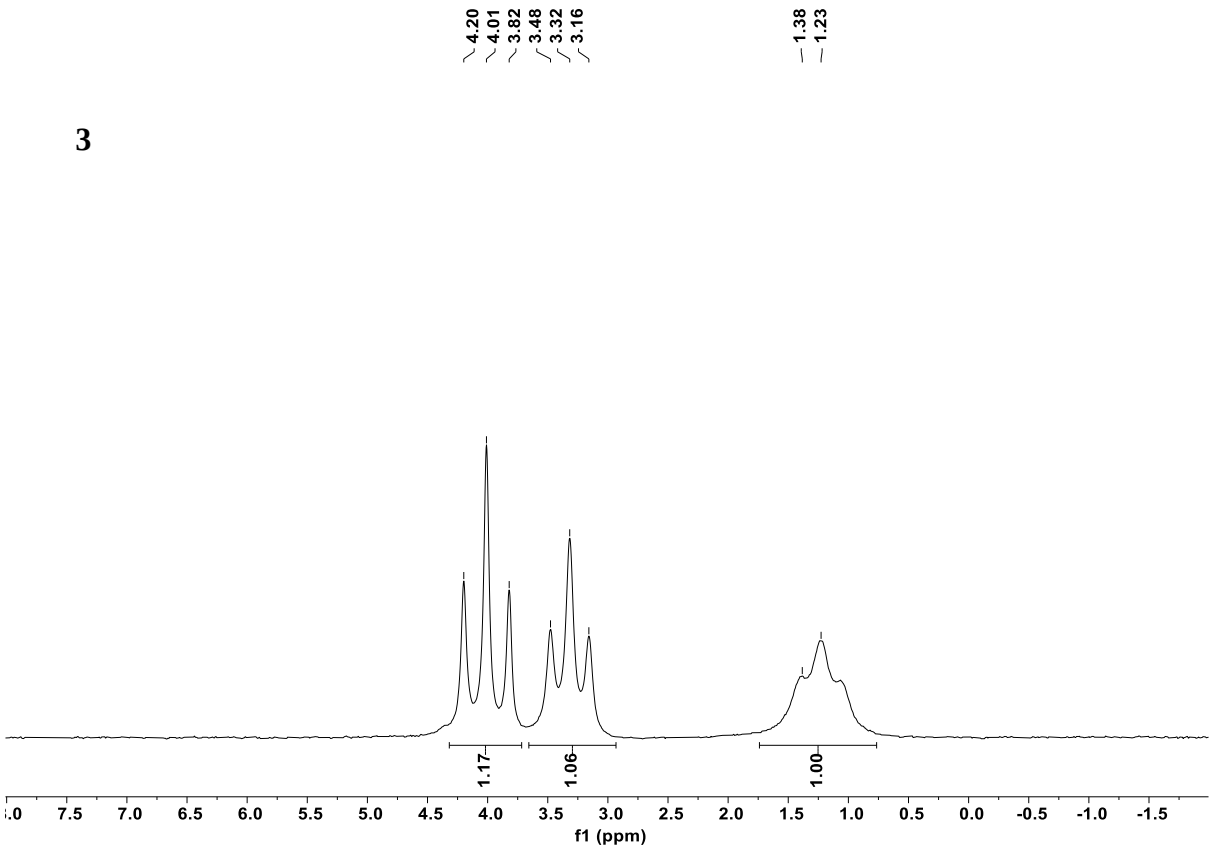

Figure S13. ^{11}B NMR spectrum of compound **3** (160 MHz, CD_2Cl_2).

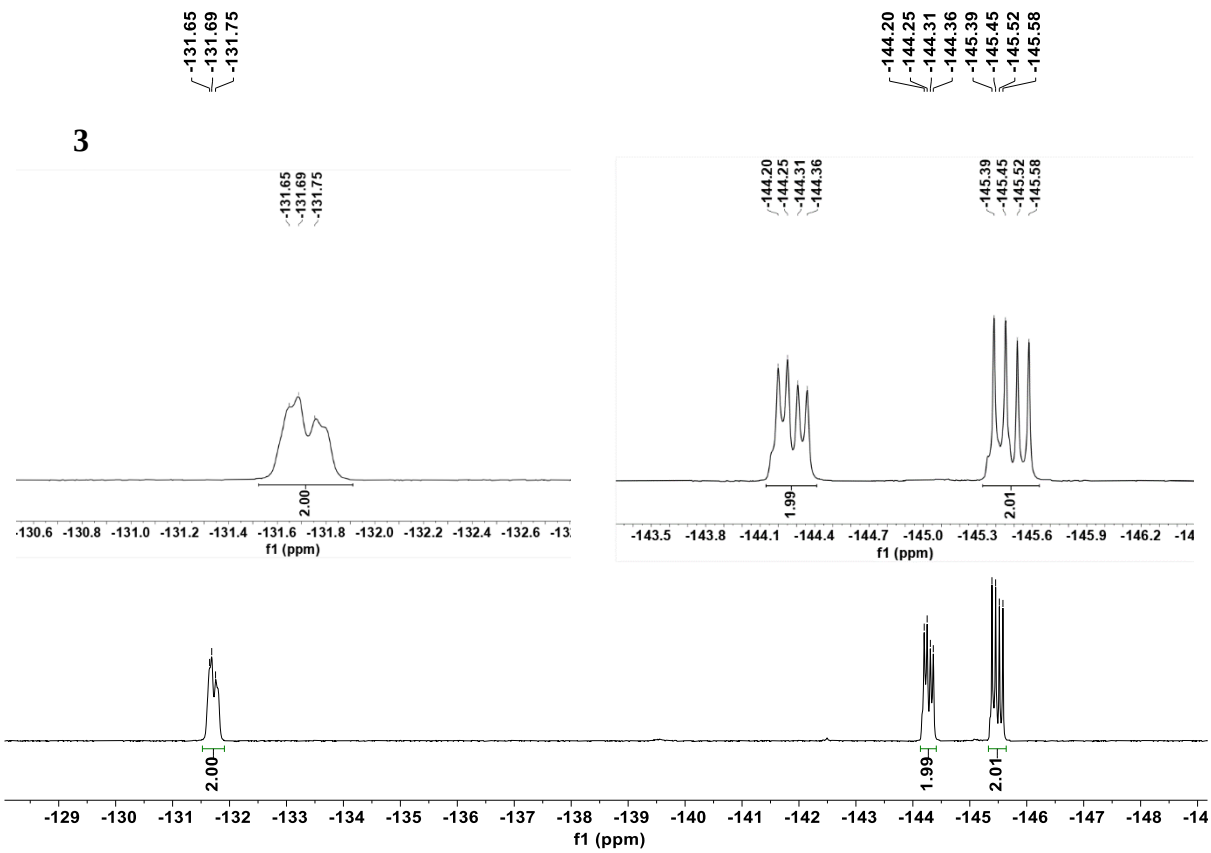

Figure S14. ^{19}F NMR spectrum of compound **3** (471 MHz, CD_2Cl_2).

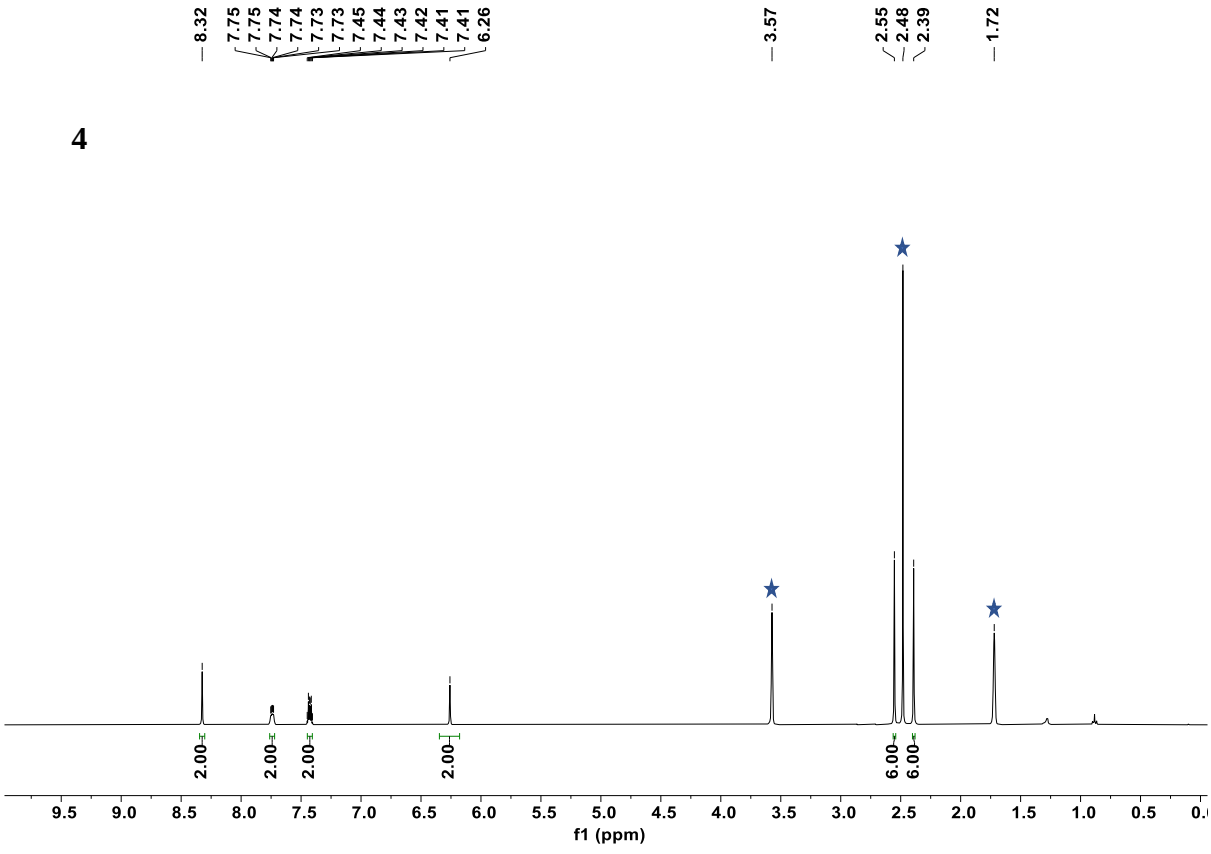

Figure S15. ^{1}H NMR spectrum of compound **4** (400 MHz, THF-d_8).

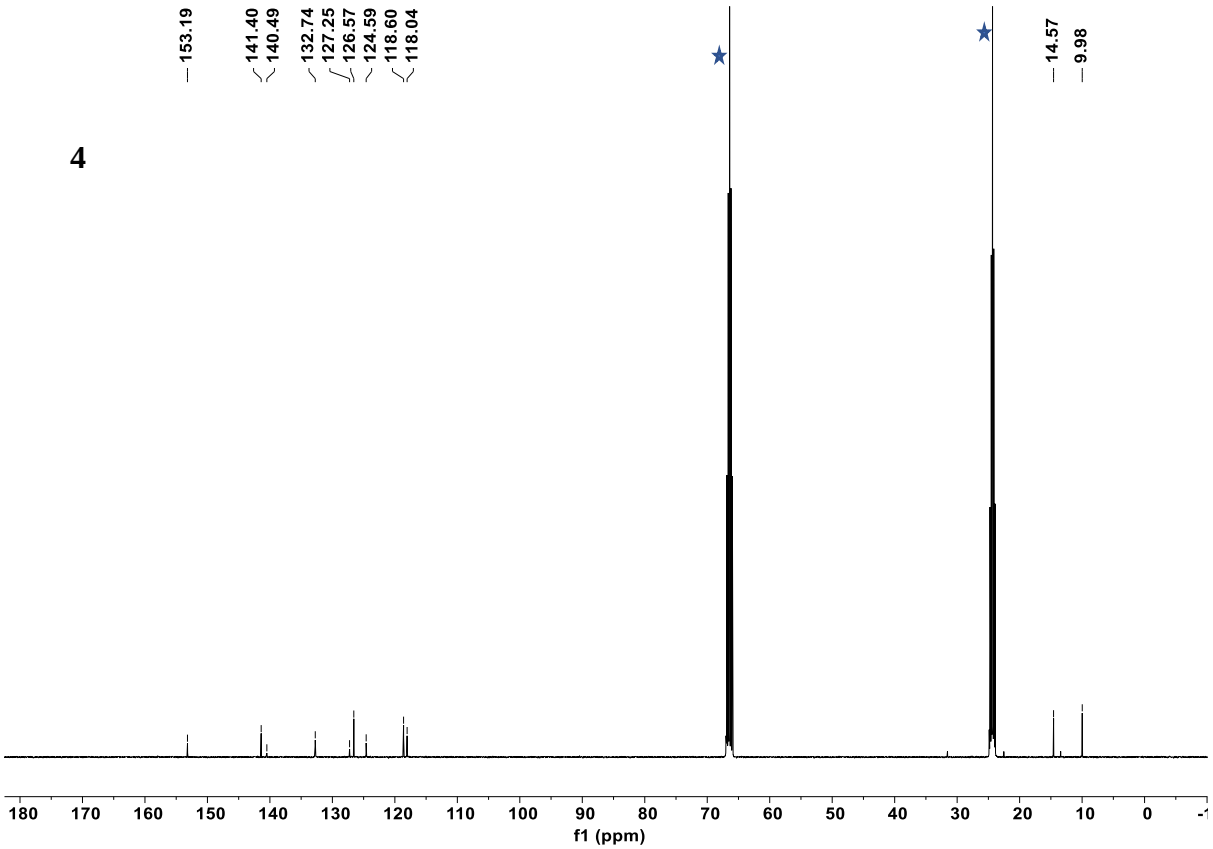

Figure S16. ^{13}C NMR spectrum of compound **4** (100 MHz, THF-d_8).

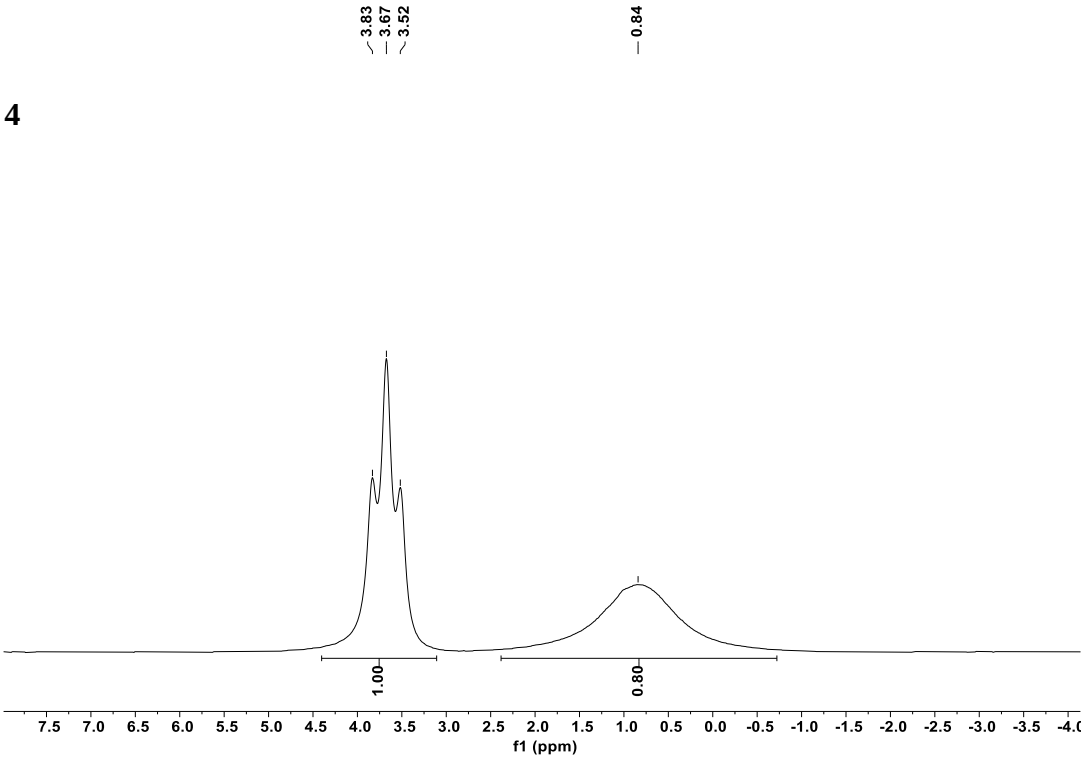

Figure S17. ^{11}B NMR spectrum of compound **4** (160 MHz, THF-d_8).

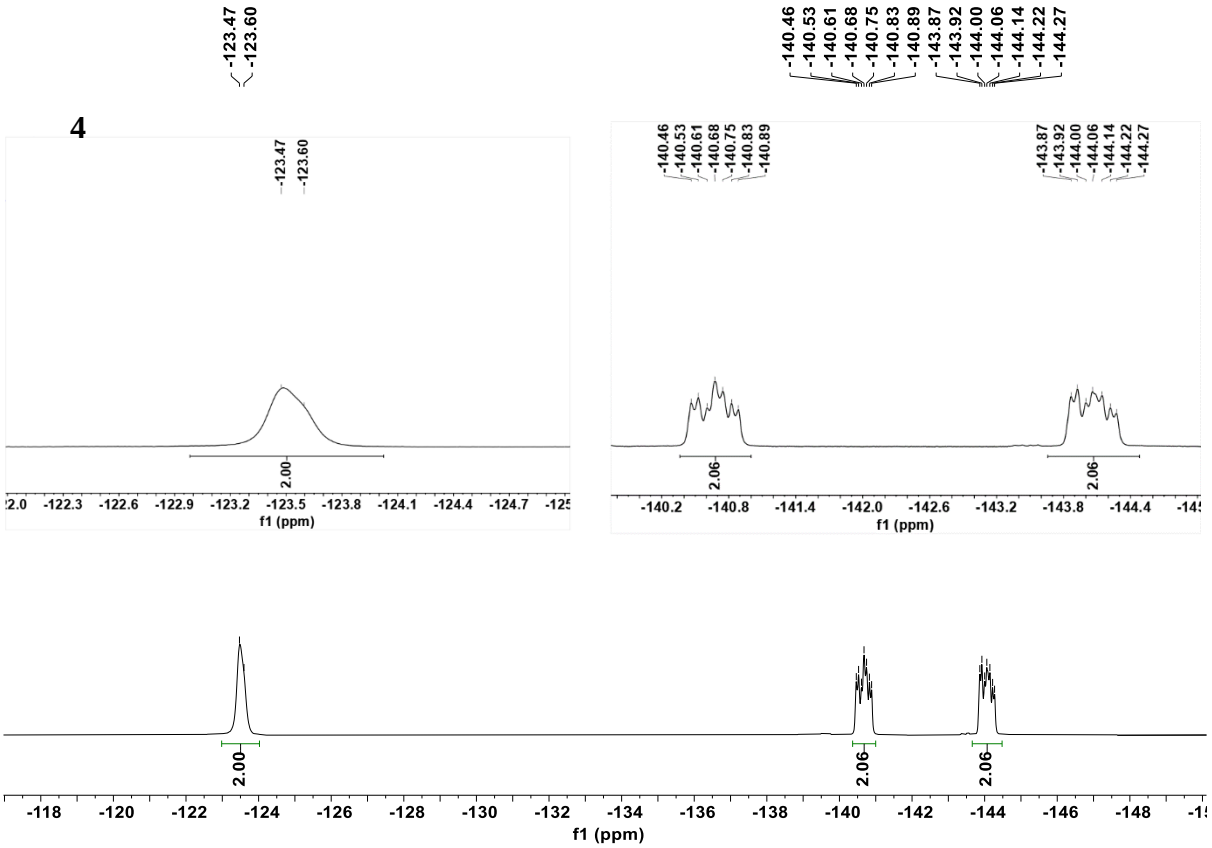

Figure S18. ^{19}F NMR spectrum of compound **4** (377 MHz, THF-d_8).

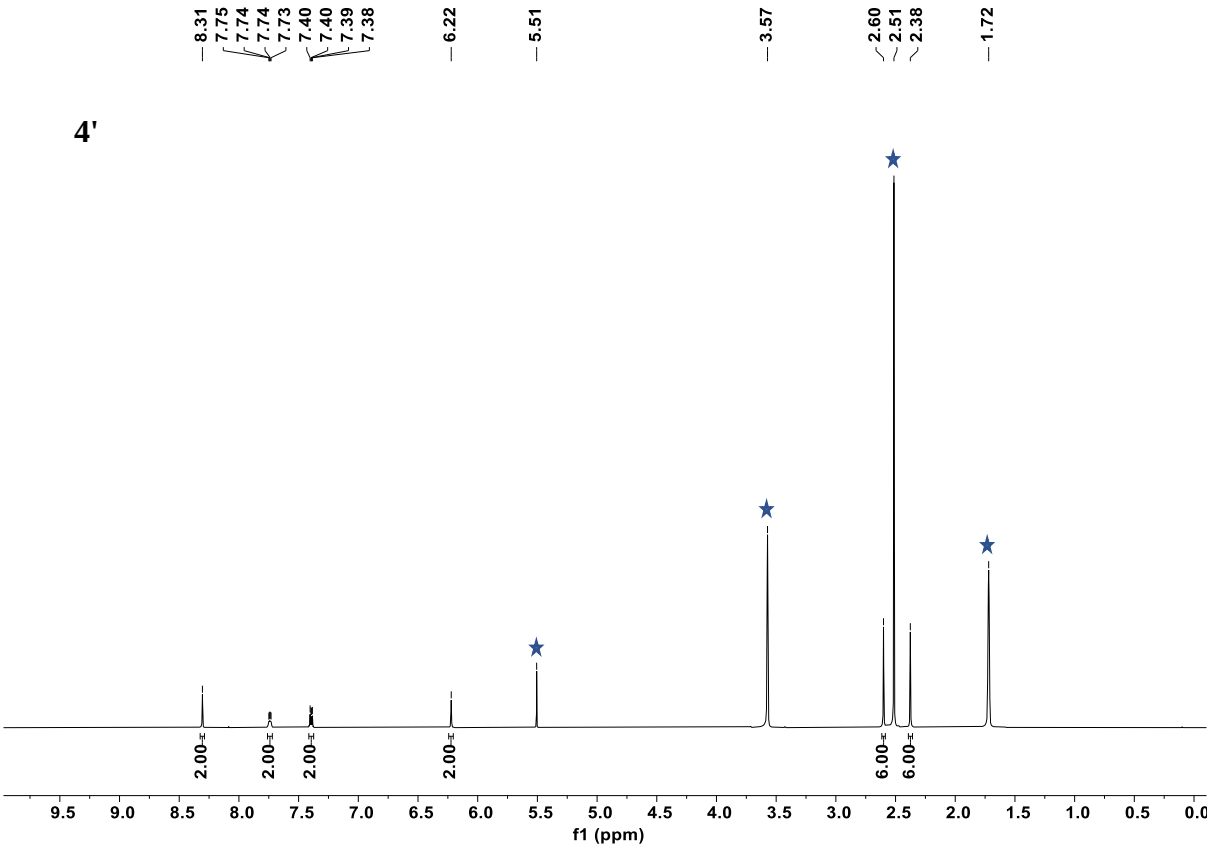

Figure S19 ^{1}H NMR spectra of compound **4'** (500 MHz, THF-d_8).

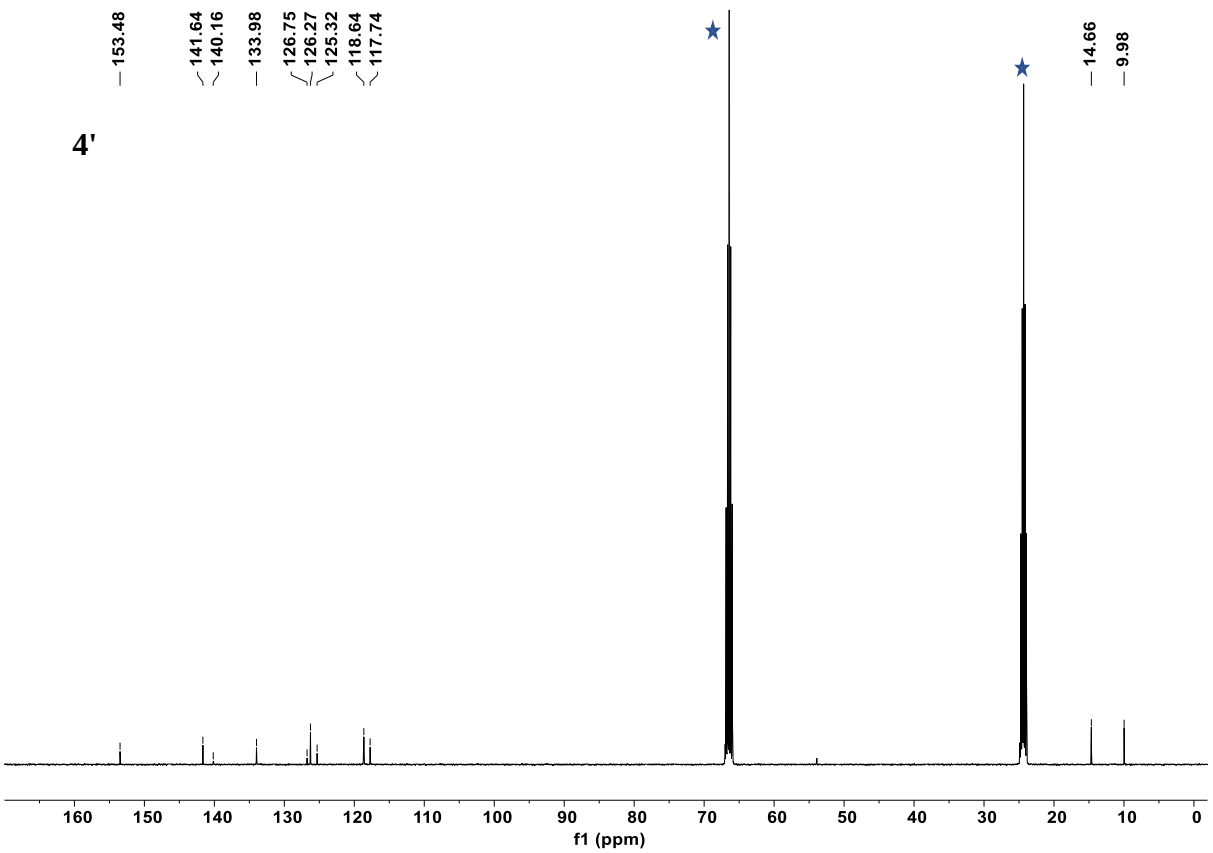

Figure S20. ^{13}C NMR spectrum of compound **4'** (100 MHz, THF-d_8).

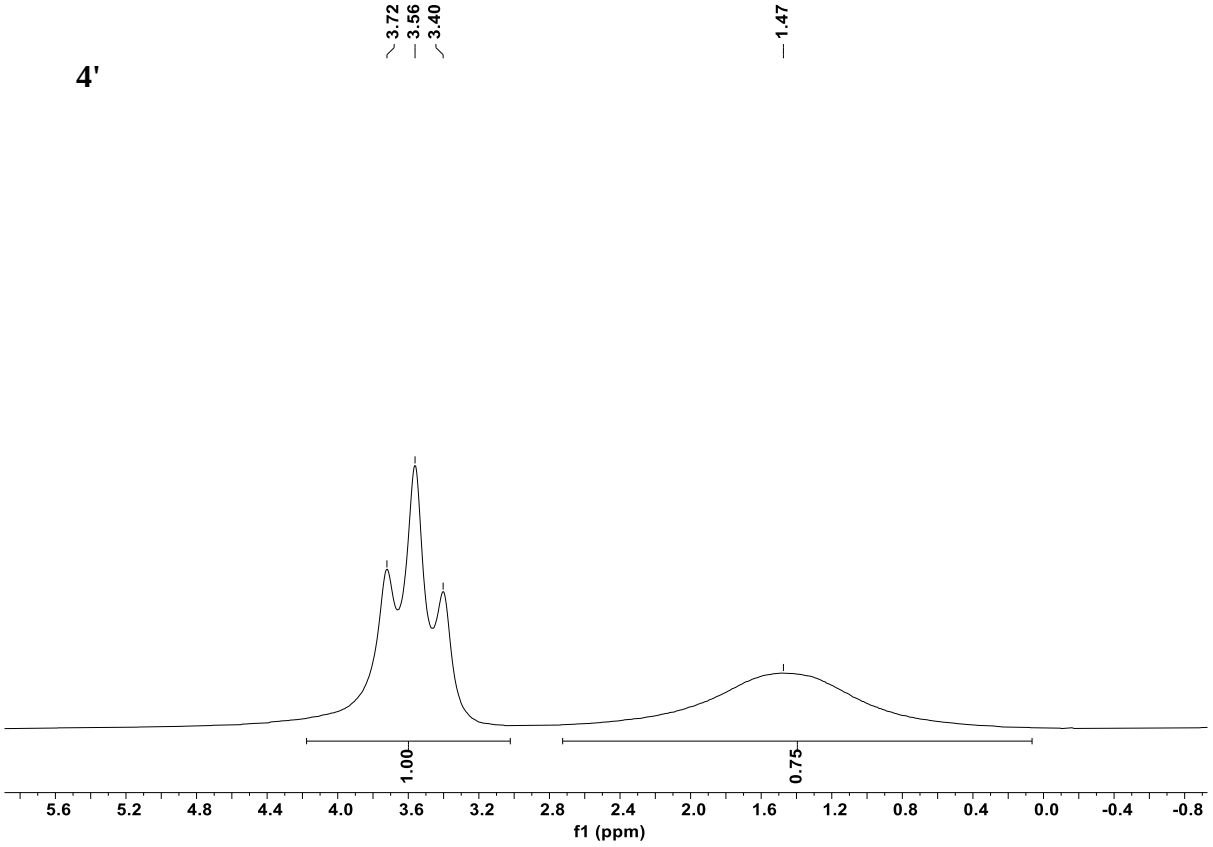

Figure S21. ^{11}B NMR spectrum of compound **4'** (160 MHz, THF-d_8).

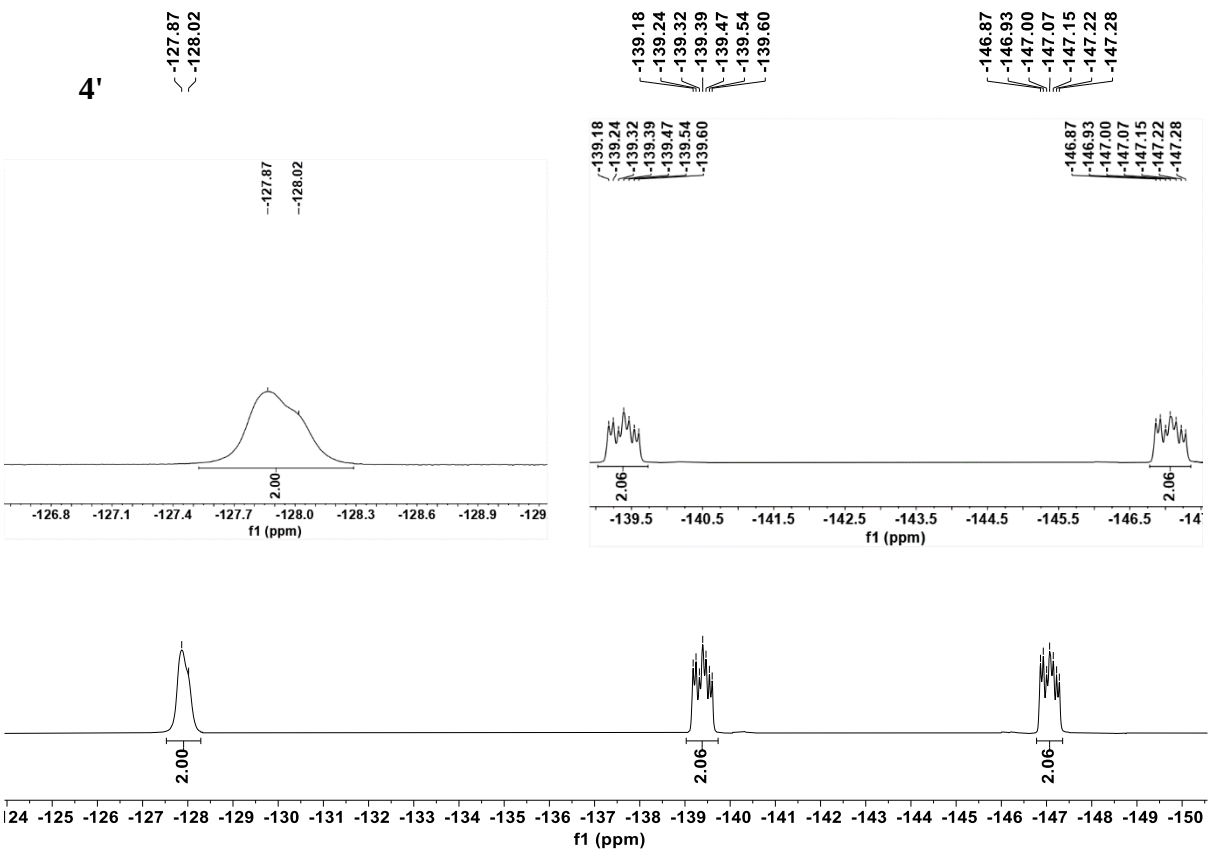

Figure S22. ^{19}F NMR spectrum of compound **4'** (377 MHz, THF-d_8).

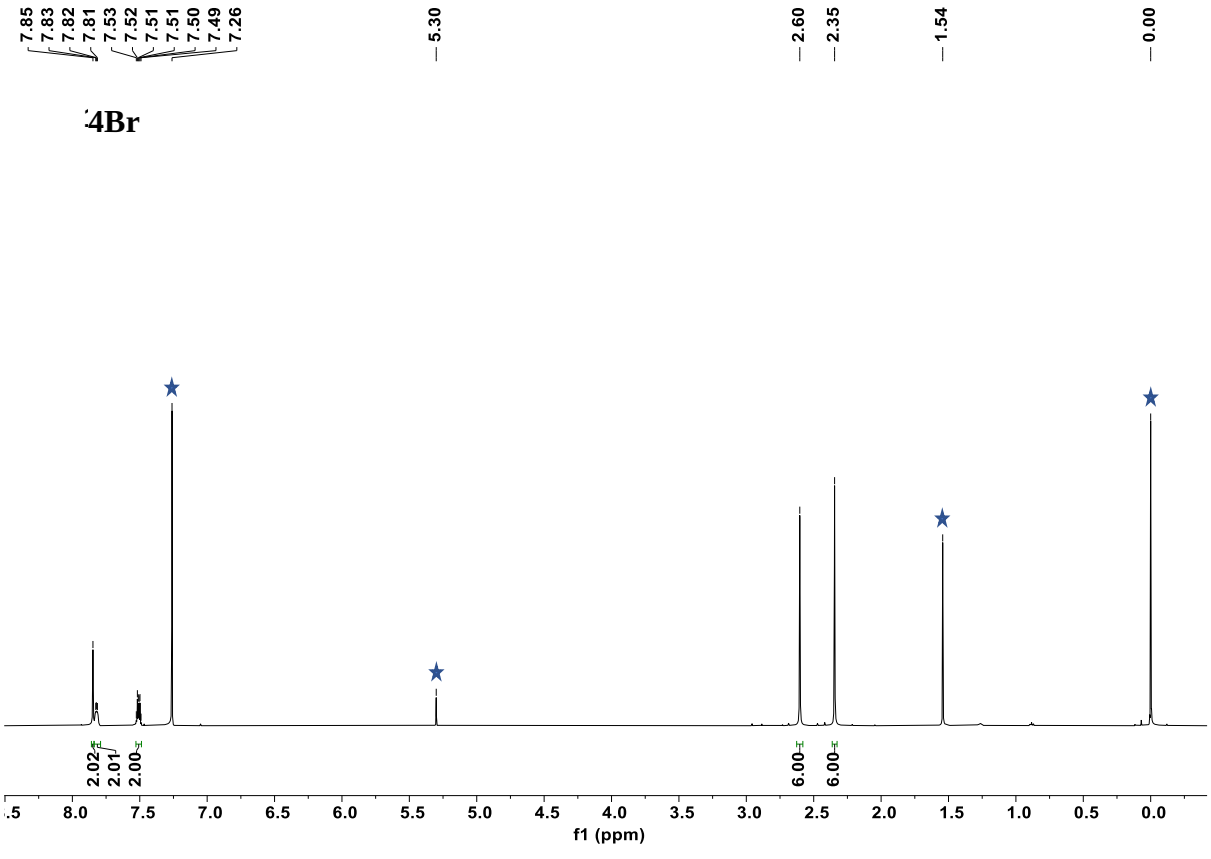

Figure S23. ^{1}H NMR spectrum of compound **4Br** (500 MHz, CD_3Cl stab. with Ag).

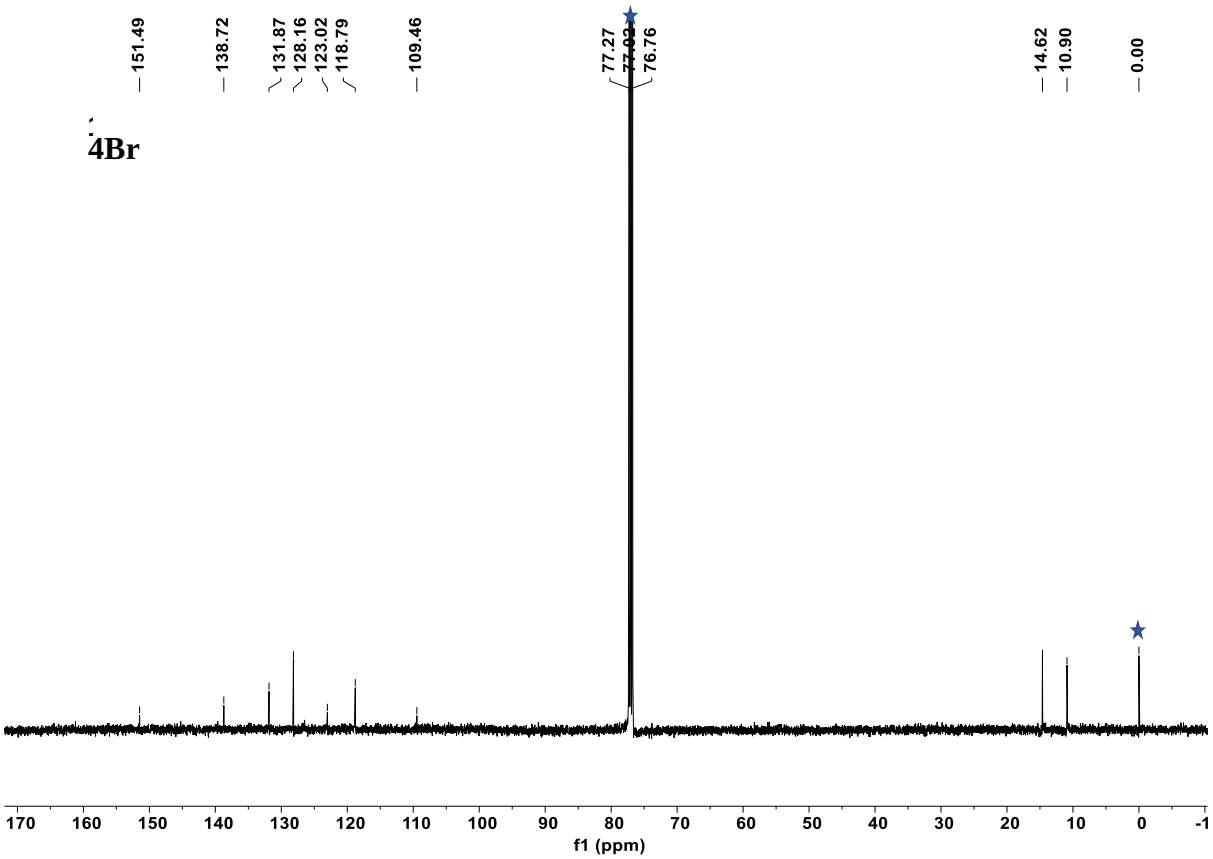

Figure S24. ^{13}C NMR spectrum of compound **4Br** (125 MHz, CD_3Cl stab. with Ag).

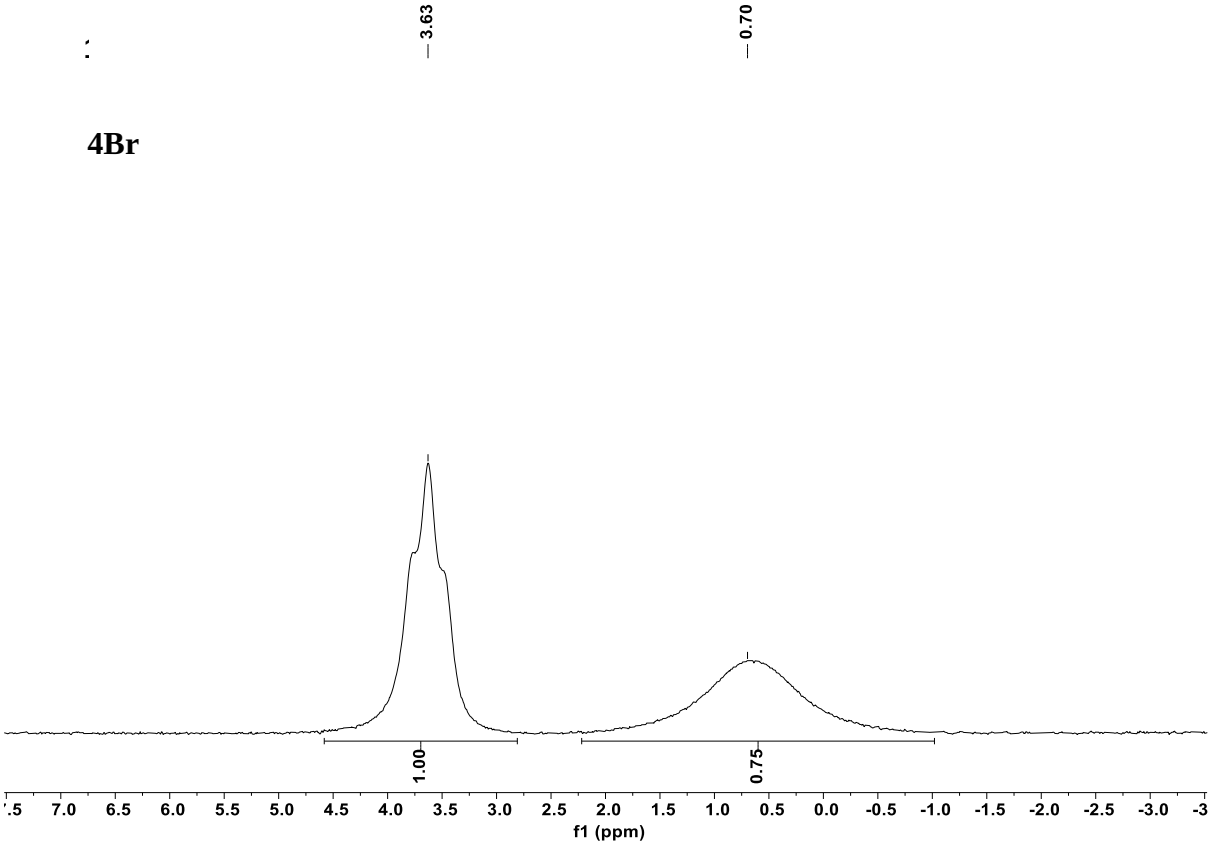

Figure S25. ^{11}B NMR spectrum of compound **4Br** (160 MHz, CD_3Cl stab. with Ag).

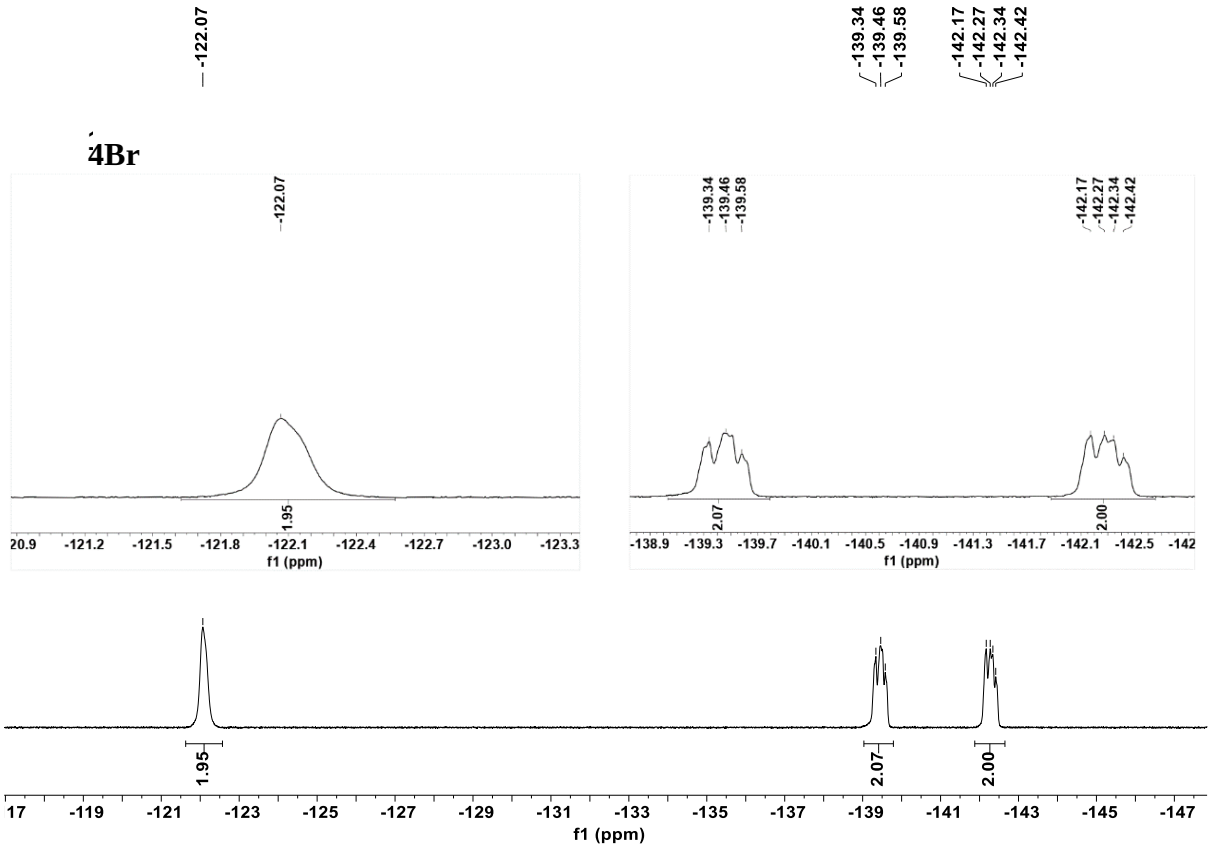

Figure S26. ^{19}F NMR spectrum of compound **4Br** (471 MHz, CD_3Cl stab. with Ag).

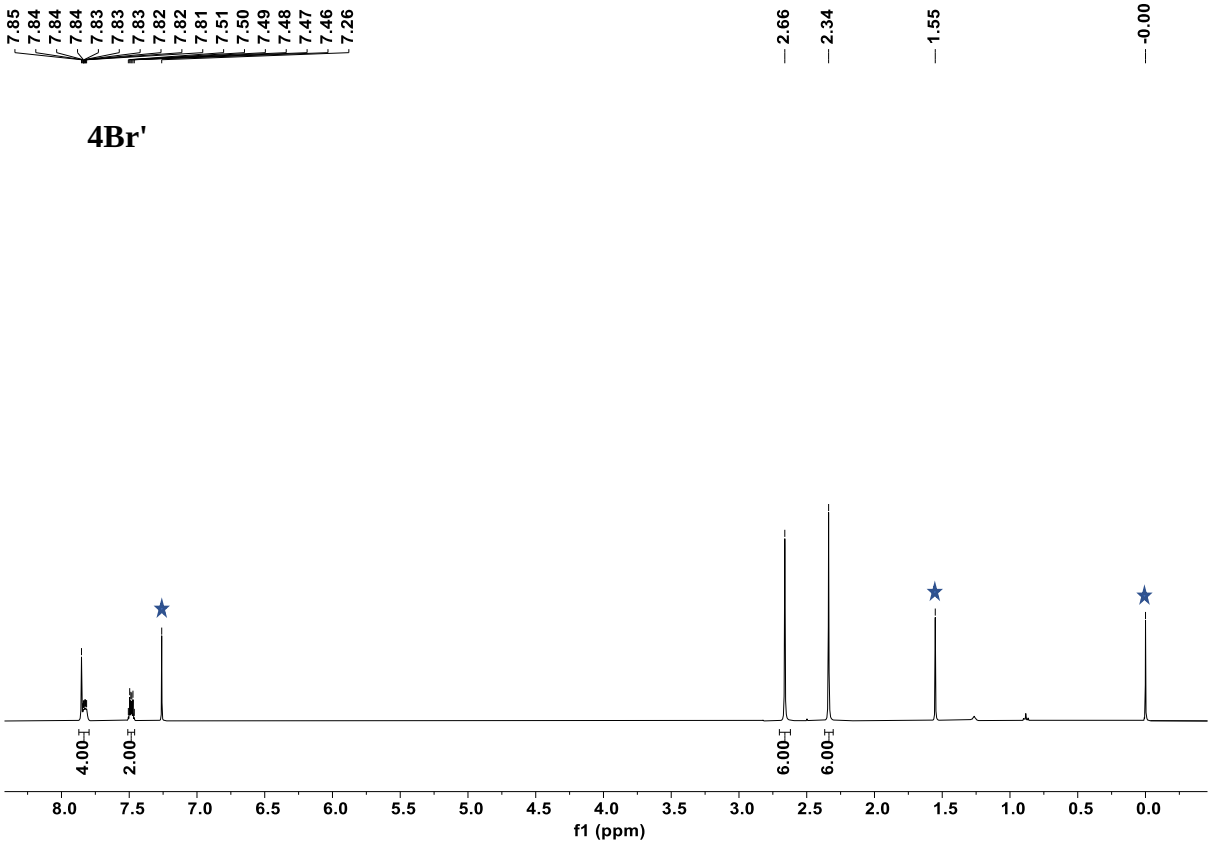

Figure S27. ^{1}H NMR spectrum of compound **4Br'** (400 MHz, CD_3Cl stab. with Ag).

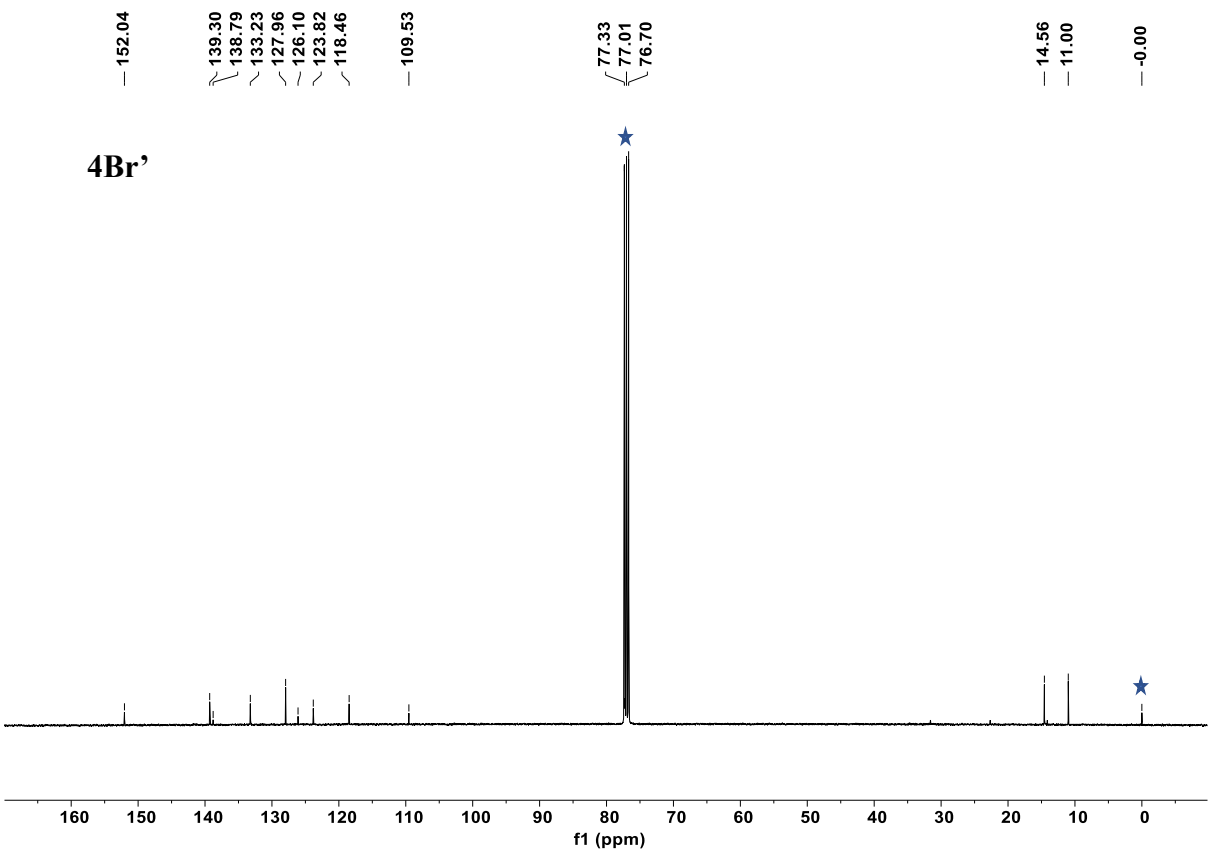

Figure S28. ^{13}C NMR spectrum of compound **4Br'** (100 MHz, CD_3Cl stab. with Ag).

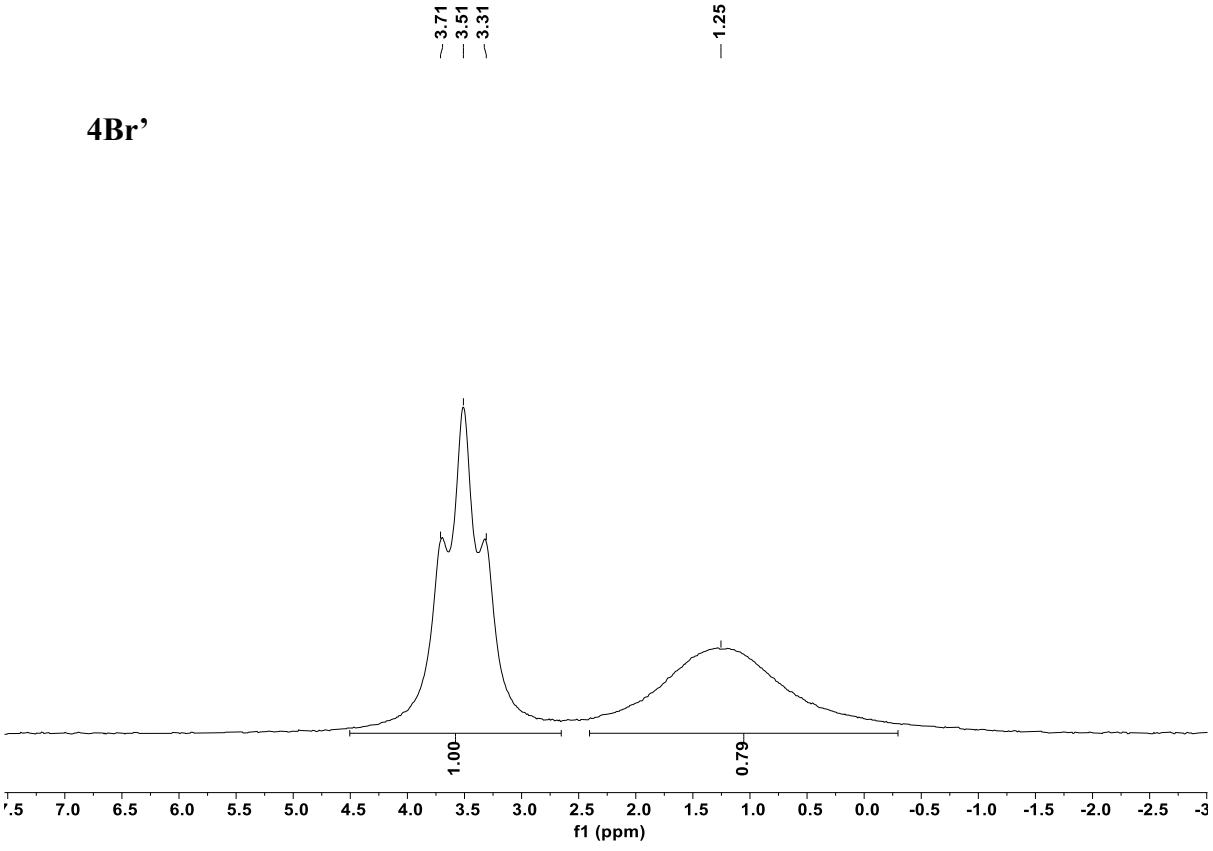

Figure S29. ^{11}B NMR spectrum of compound **4Br'** (128 MHz, CD_3Cl stab. with Ag).

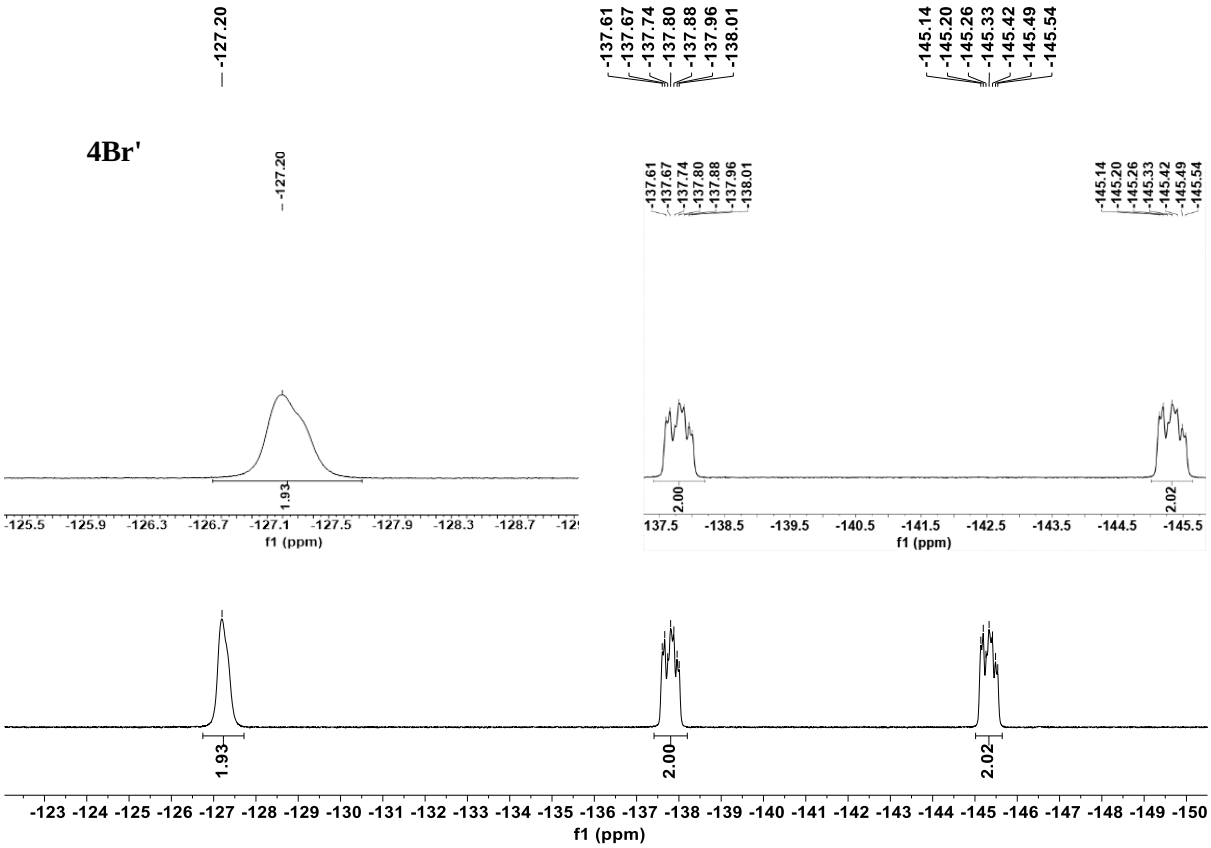

Figure S30. ^{19}F NMR spectrum of compound **4Br'** (377 MHz, CD_3Cl stab. with Ag).

8 Copies of HRMS spectra

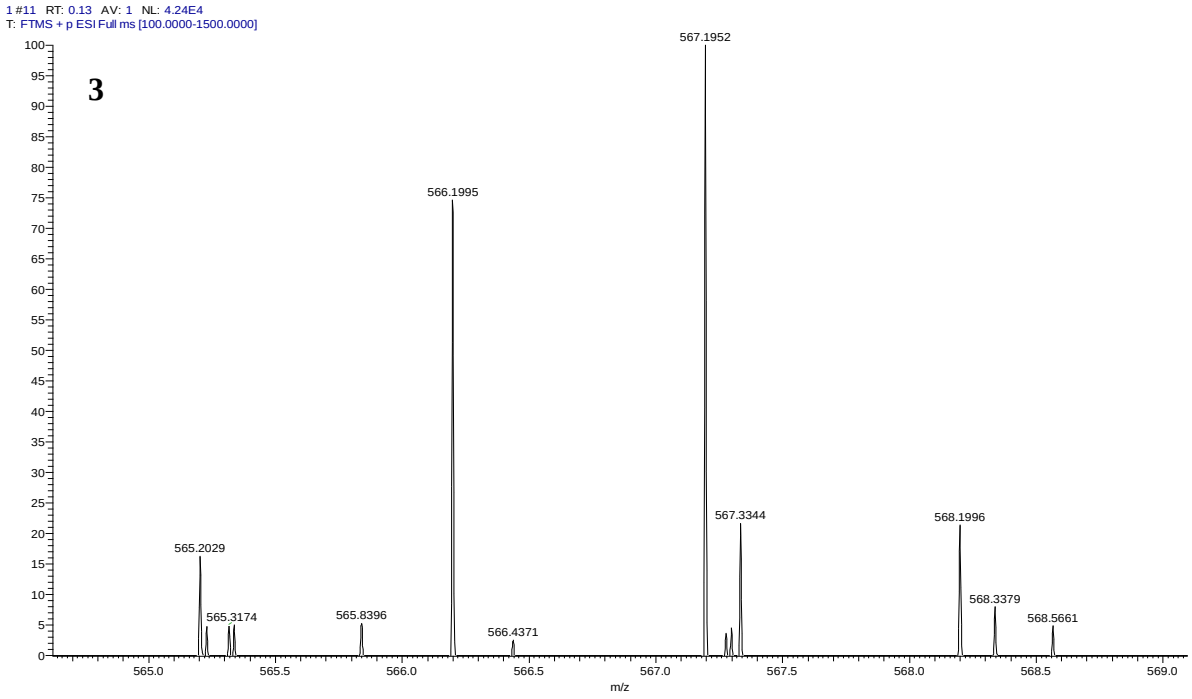

Figure S31. HR-MS spectrum of compound **3**.

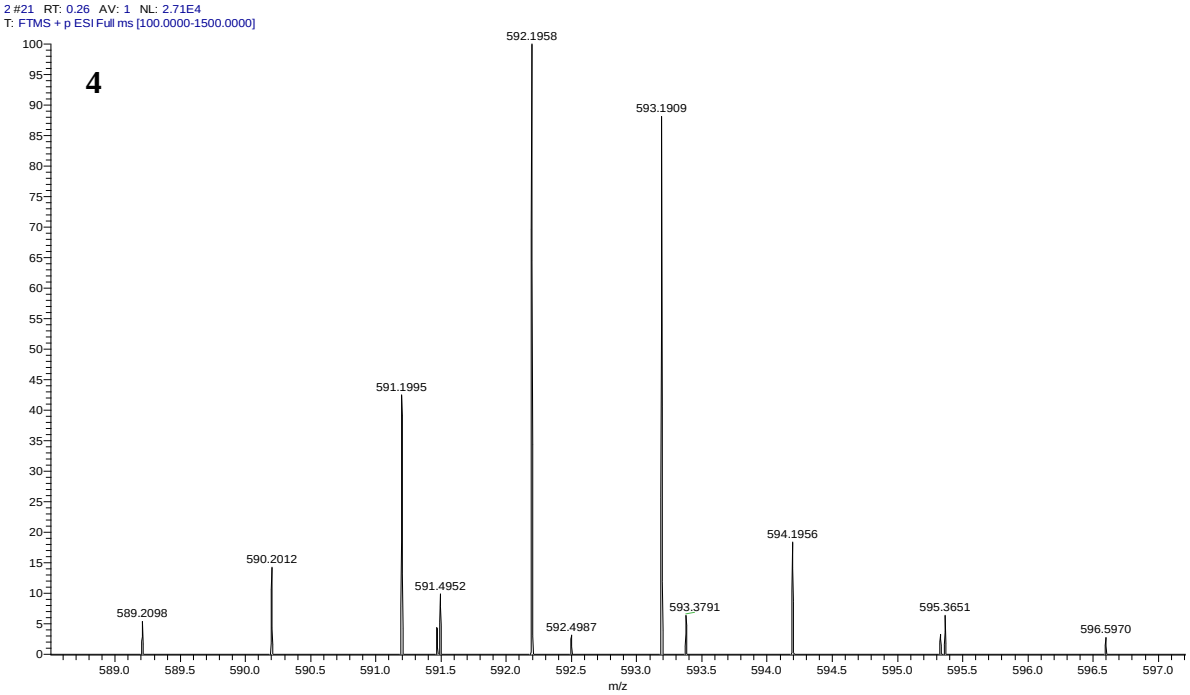

Figure S32. HR-MS spectrum of compound **4**.

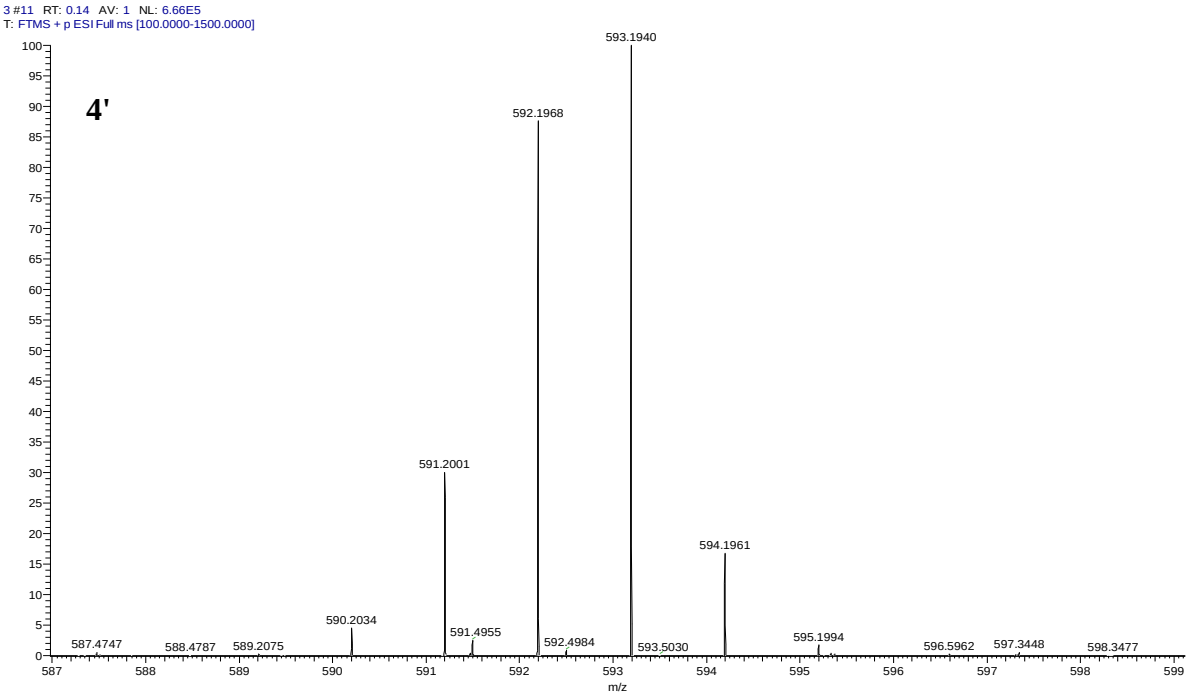

Figure S33. HR-MS spectrum of compound **4'**.

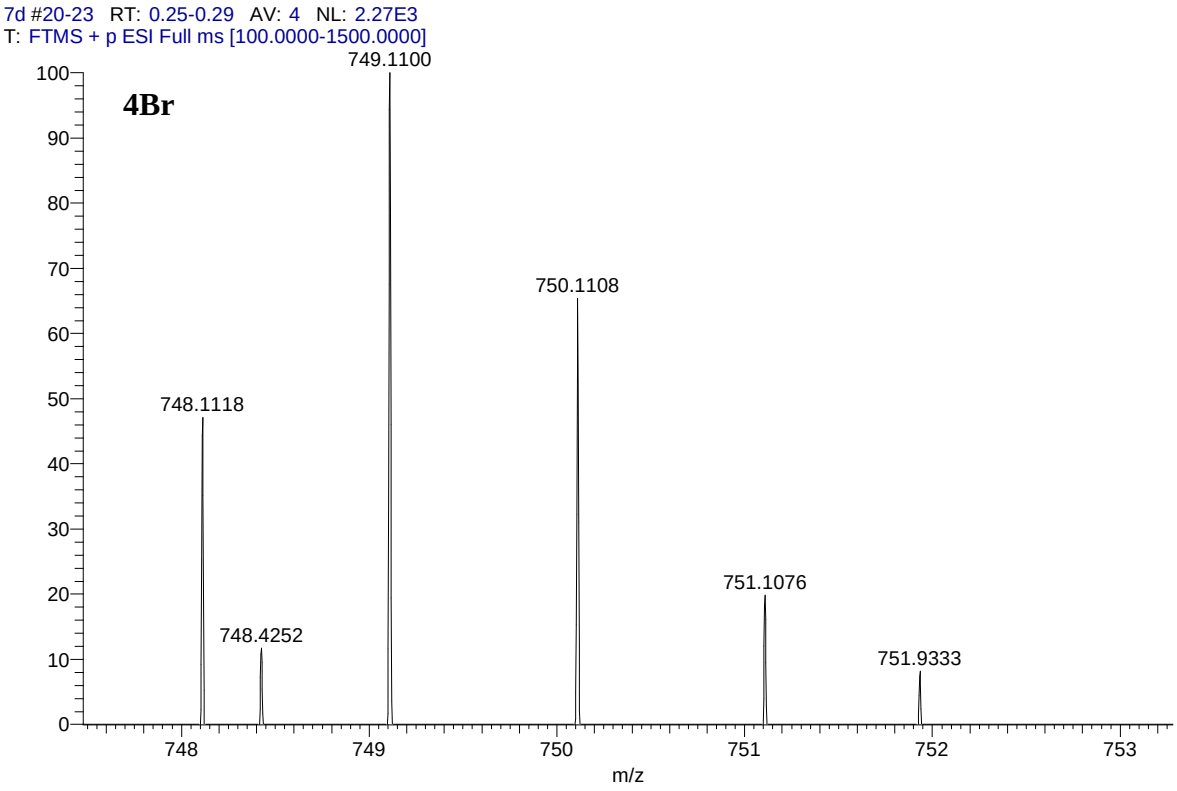

Figure S34. HR-MS spectrum of compound **4Br**.

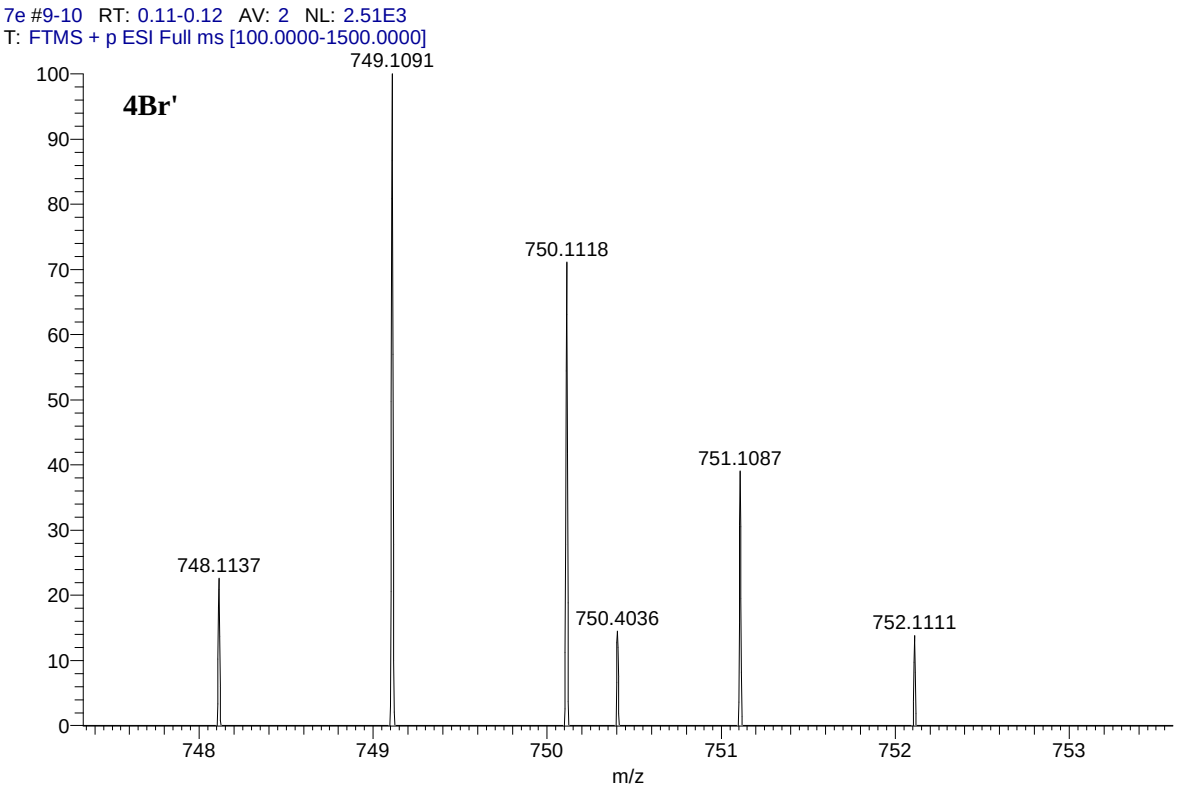

Figure S35. HR-MS spectrum of compound **4Br'**.