Designing Dual-State and Aggregation-Induced Emissive Luminogens from Lignocellulosic Biosourced Molecules

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Figure S1: ^{1}H NMR spectra of compound CS-BeFu in DMSO d$_6$.
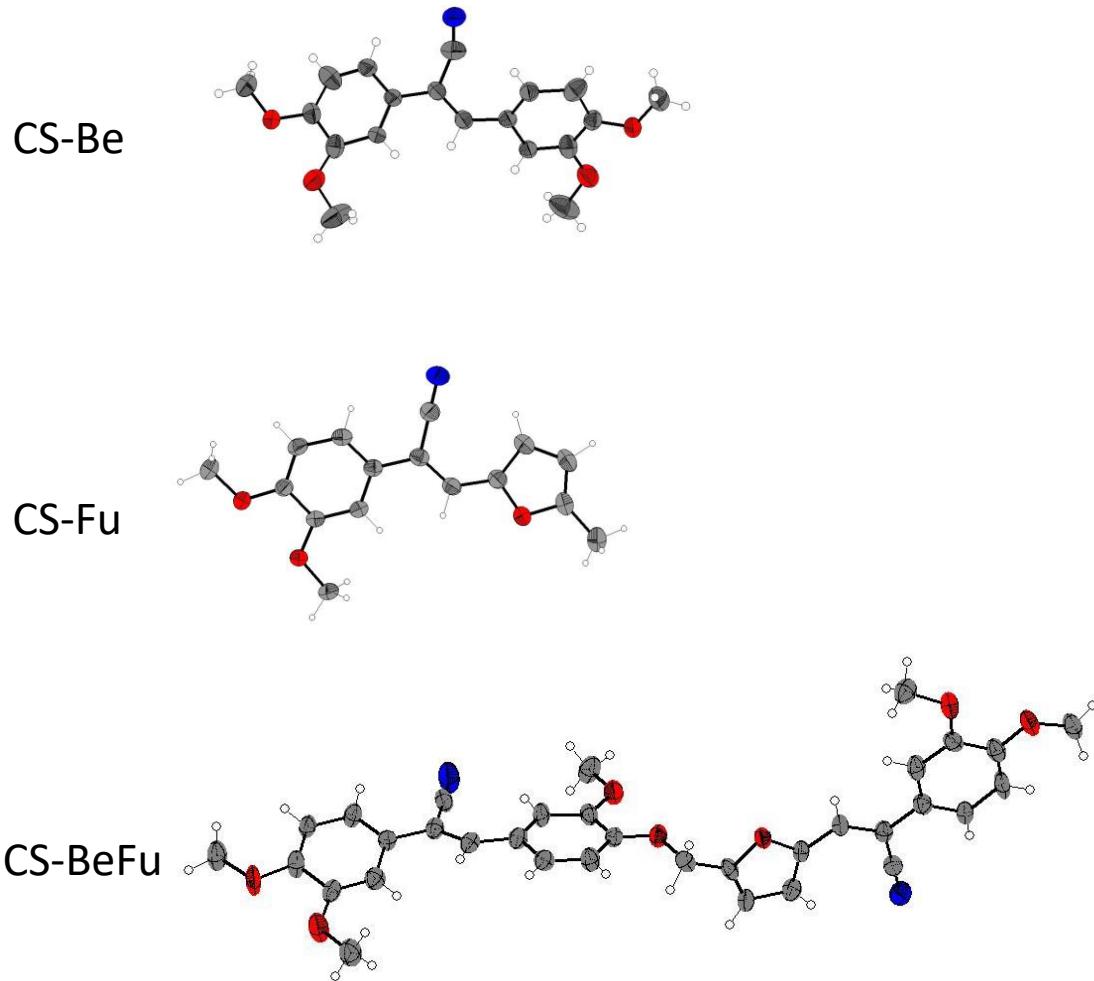
CS-Be

CS-Fu

CS-BeFu

Figure S2: Ortep views of **CS-Be**, **CS-Fu** and **CS-BeFu** showing the Z-configurations of all the cyanovinyl bonds
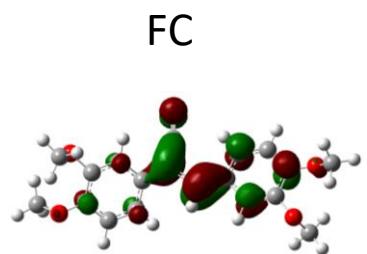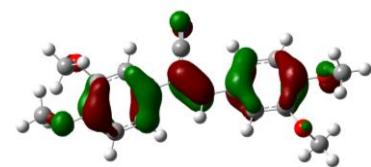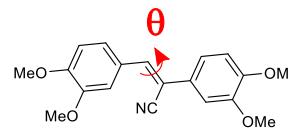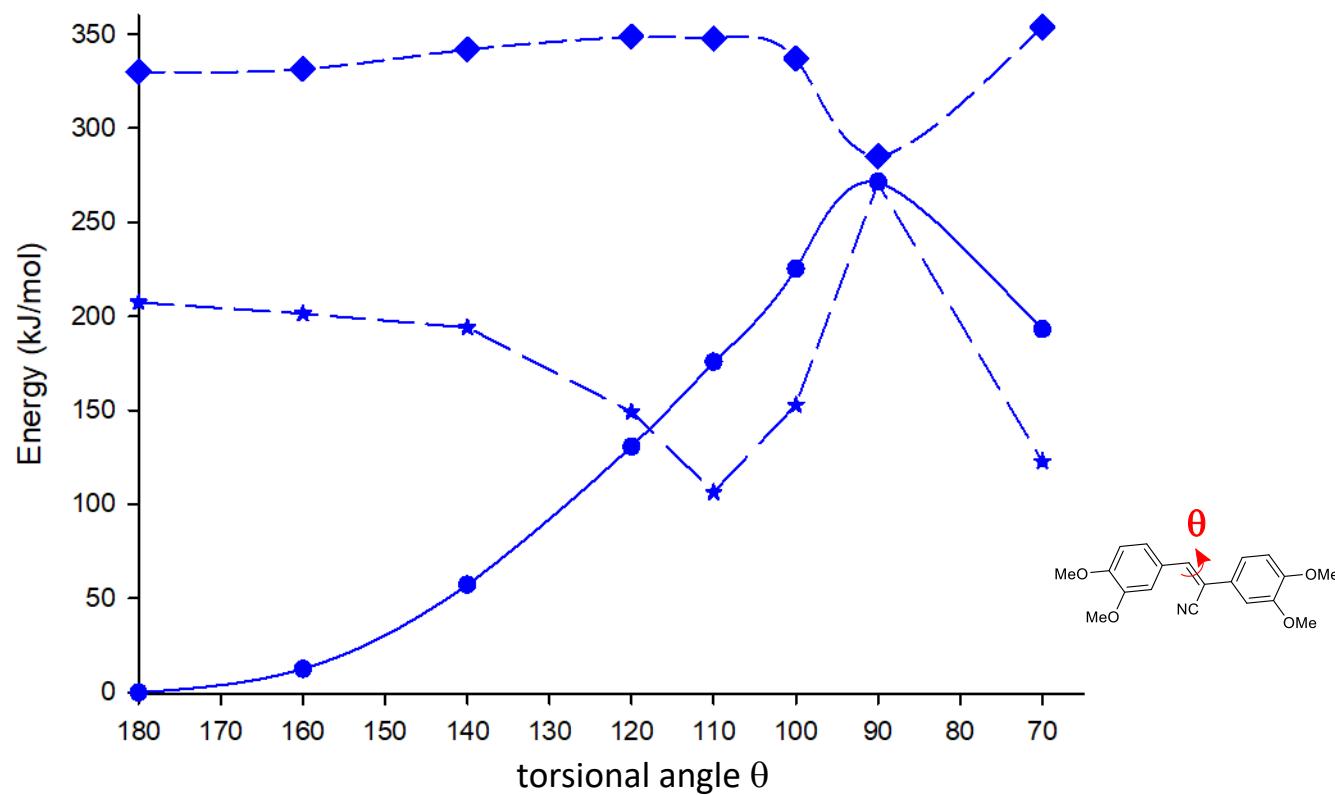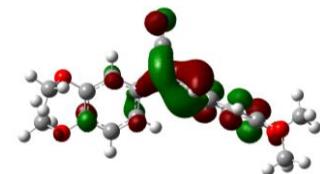
Figure S3 : TD-DFT torsional scans of double bonds θ for **CS-Be**, using the optimized S0 state at the TD-B3LYP/6.31G(d,p) level. S0, S1 and T1 energies were computed for each data point.
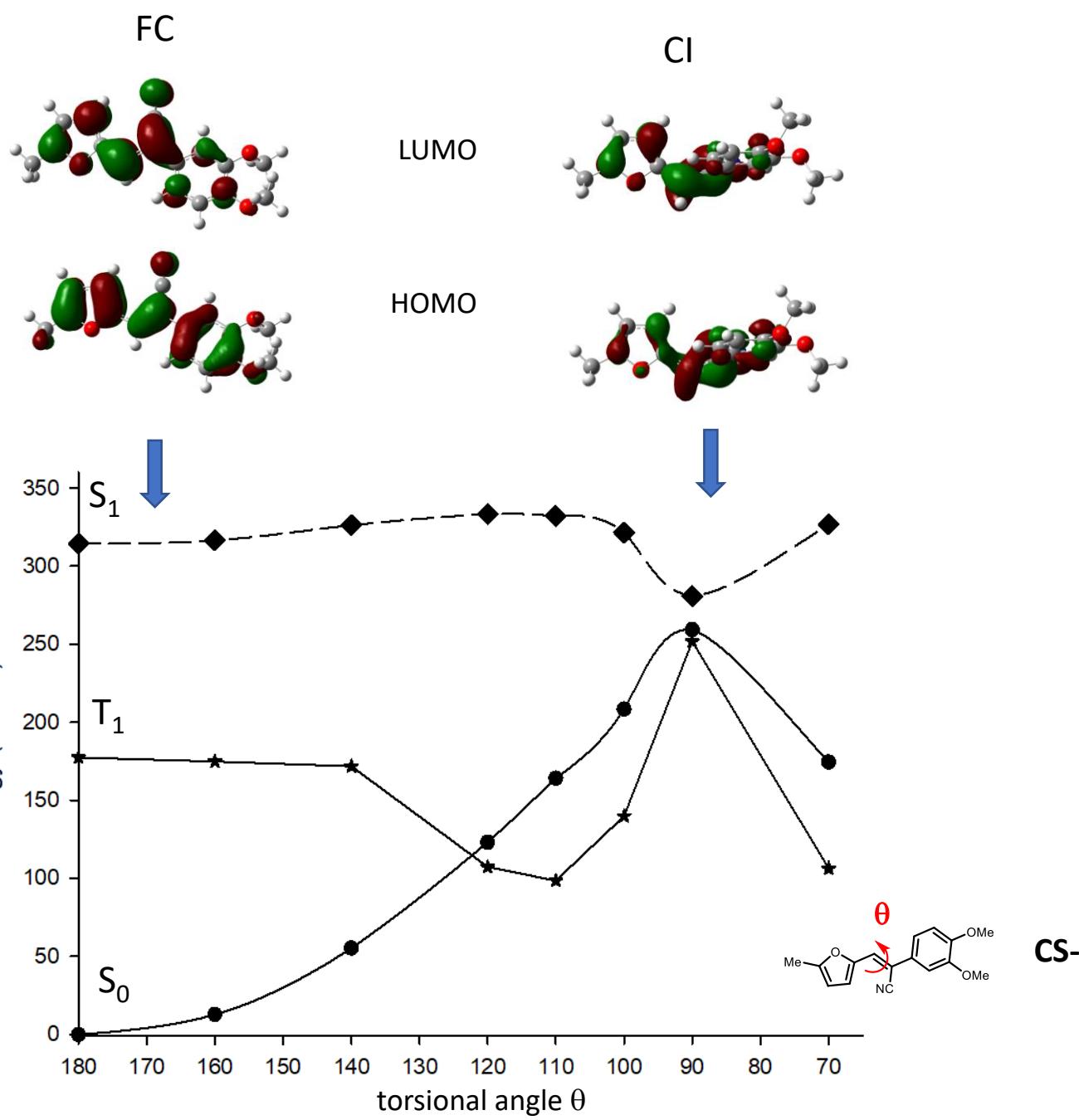
**Figure S4** : TD-DFT torsional scans of double bonds q for **CS-Fu**, using the optimized S0 state at the TD-B3LYP/6.31G(d,p) level. S0, S1 and T1 energies were computed for each data point.
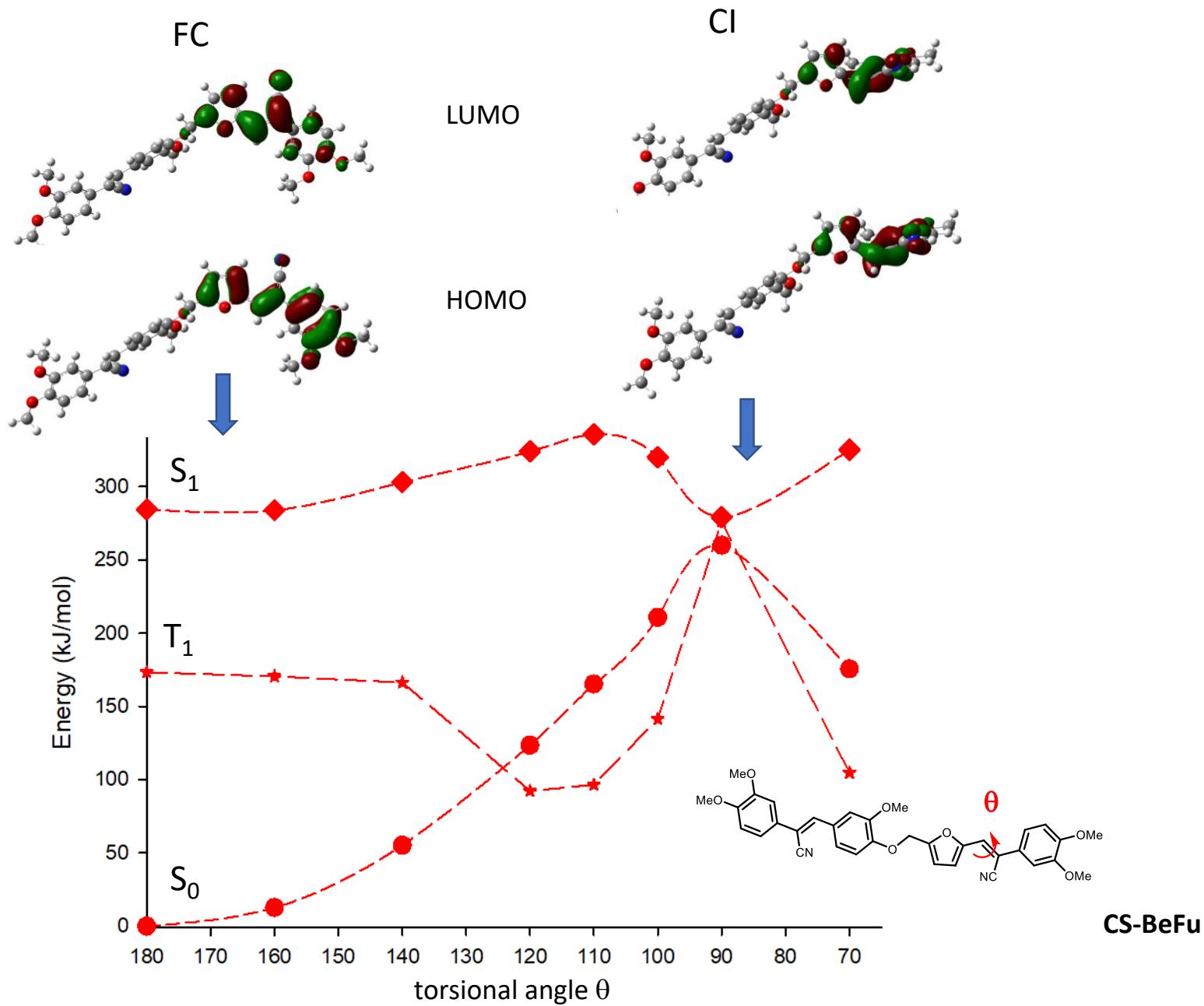
Figure S5 : TD-DFT torsional scans of double bonds θ for **CS-BeFu**, using the optimized S_0 state at the TD-B3LYP/6.31G(d,p) level. S0, S1 and T1 energies were computed for each data point.
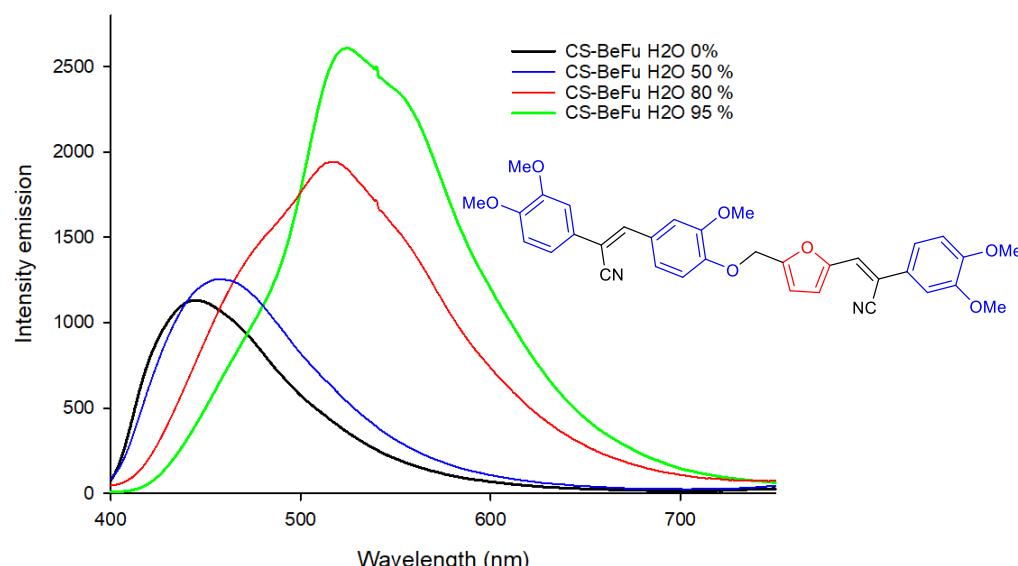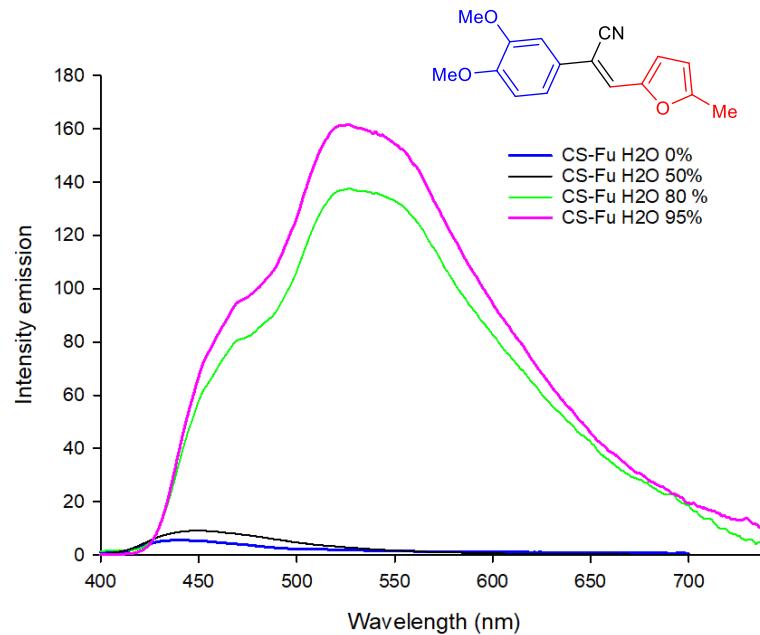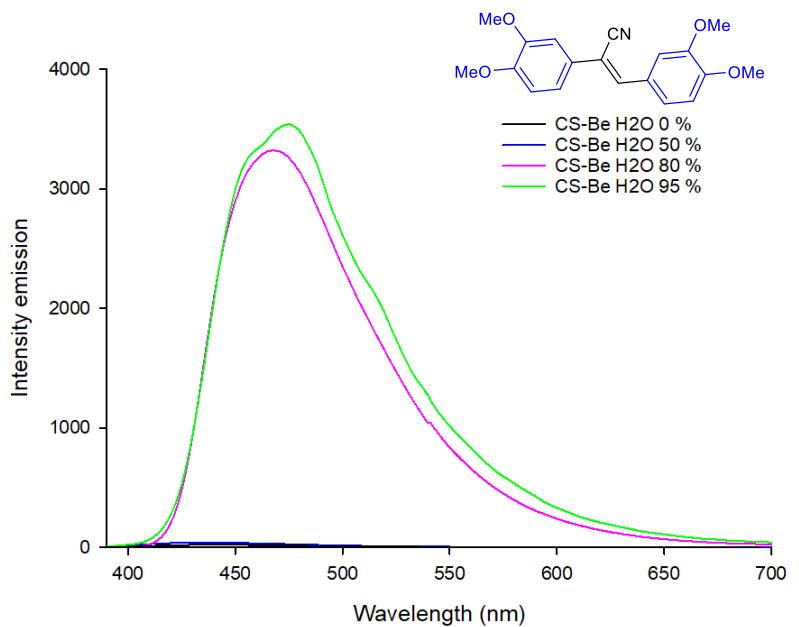
Figure S6, Emission spectra of CS-Be, CS-Fu and CS-BeFu in mixture of THF-Water : THF 100% (black), 50 % vol H2O (blue), 80 % vol H2O (pink) and 95 % vol H2O (green)

Table S1: X-ray crystallographic data of single crystals of **CS-Fu**, **CS-BeFu** and **CS-Be**

	CS-Fu	CS-BeFu	CS-Be
Formula	C16 H15 N O3	C34 H30 N2 O7	C19 H19 N O4
M	269.29	578.60	325.35
T (K)	200.00	200	200
Crystal system Space group	Triclinic, P -1	Triclinic, P 1	Monoclinic, I 2/a
Unit cell.: a (Å) b (Å) c (Å) a (°) b (°) g (°) Volume (Å³)	6.9278(3) 8.9012(4) 11.6478(5) 71.891(4) 85.089(4) 82.065(4) 675.46(5)	7.1041(3) 13.1195(6) 17.0173(10) 112.145(5) 100.909(5) 91.569(4) 1433.98(13)	9.2182(5) 7.4082(4) 24.5864(14) 90 93.688(5) 90 1675.54(16)
Z	2	2	4
Calculated density	1.324	1.340	1.290
F(000)	284	608	688
θ range (°)	3.997 to 71.889	2.871 to 72.014	3.603 to 75.926
Limiting indices	-8≤h≤7, -9≤k≤10, -26≤l≤24	-8≤h≤8 -16≤k≤14 -20≤l≤17	-10≤h≤8 -7≤k≤9 -30≤l≤30
Reflection coll. Unique R (int)	4776 2577 0.0096	11718 6800 0.0436	3742 1686 0.0198
Final R indices, [I>2sigma(I)], R1 wR2	0.0357 0.1032	0.0461 0.1206	0.0433 0.114
R indices (all data), R1 wR2	0.0368 0.1046	0.0587 0.1348	0.0495 0.1190
Largest diff. Peak and hole (e A⁻³)	0.287 -0.283	0.194 -0.217	0.144 -0.151
CCDC number	2335531	2335530	2335527

CS-Be

^{1}H NMR of **CS-Be** in CDCl$_3$

^{13}C NMR of **CS-Be** in CDCl$_3$

CS-Fu

^{1}H NMR of **CS-Fu** in CDCl$_3$

155.3 149.6 149.2 148.9 126.8 126.4 118.5 118.2 116.2 111.3 109.5 109.4 108.0 105.3 56.0 14.0

MeO CN
MeO Me

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

^{13}C NMR of **CS-Fu** in CDCl$_3$
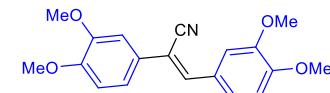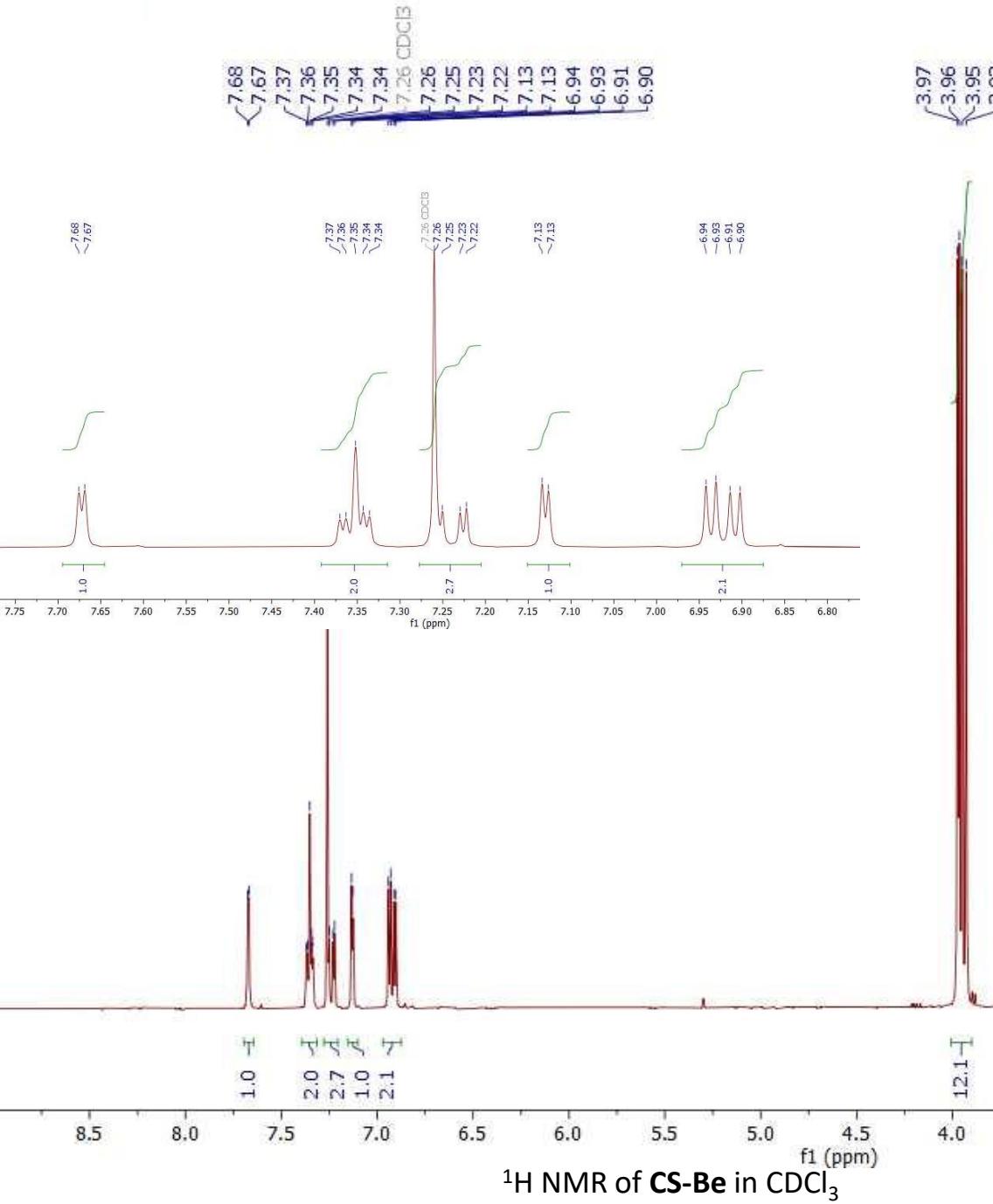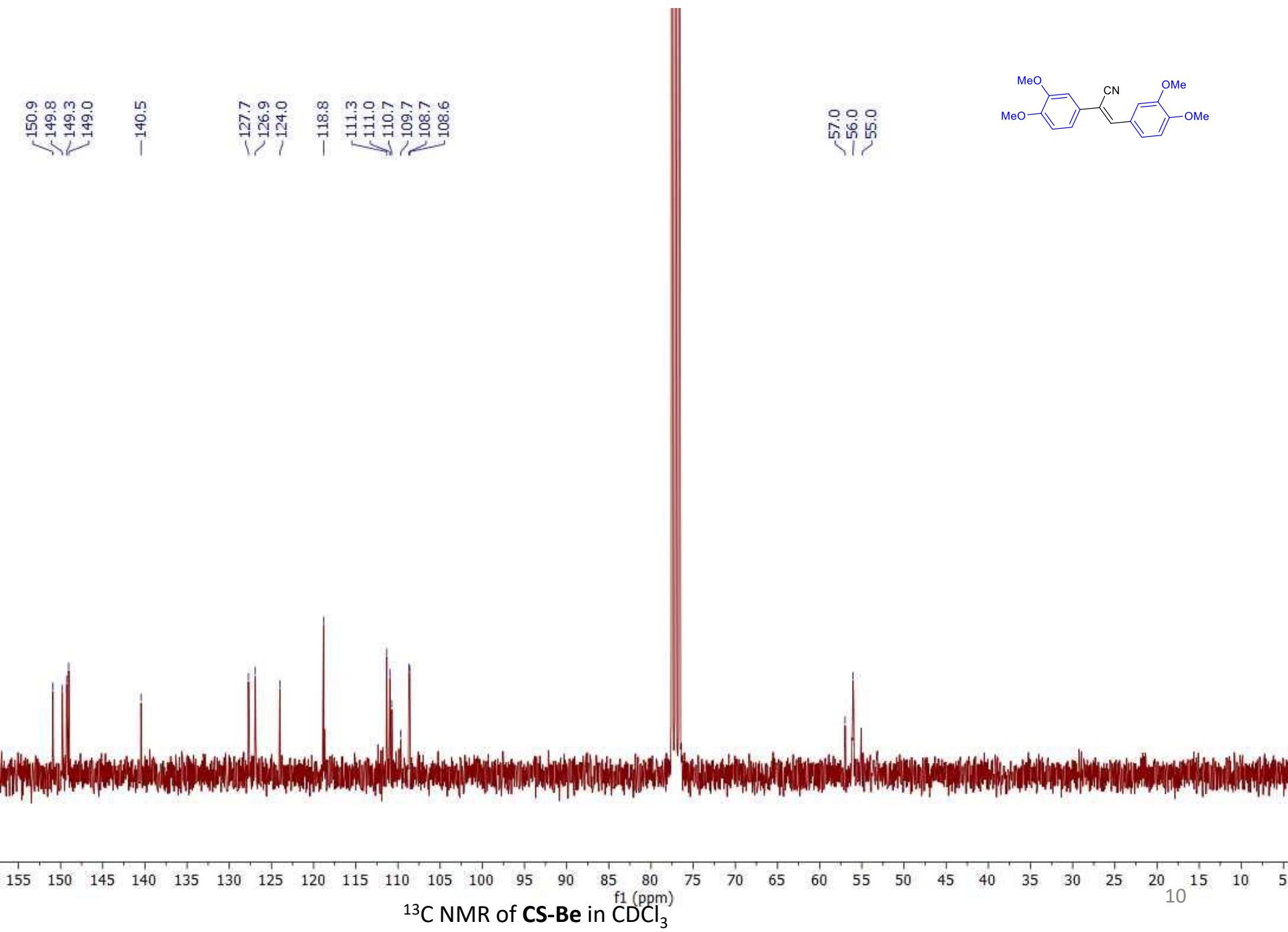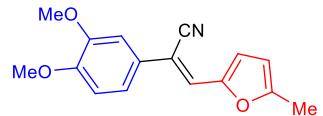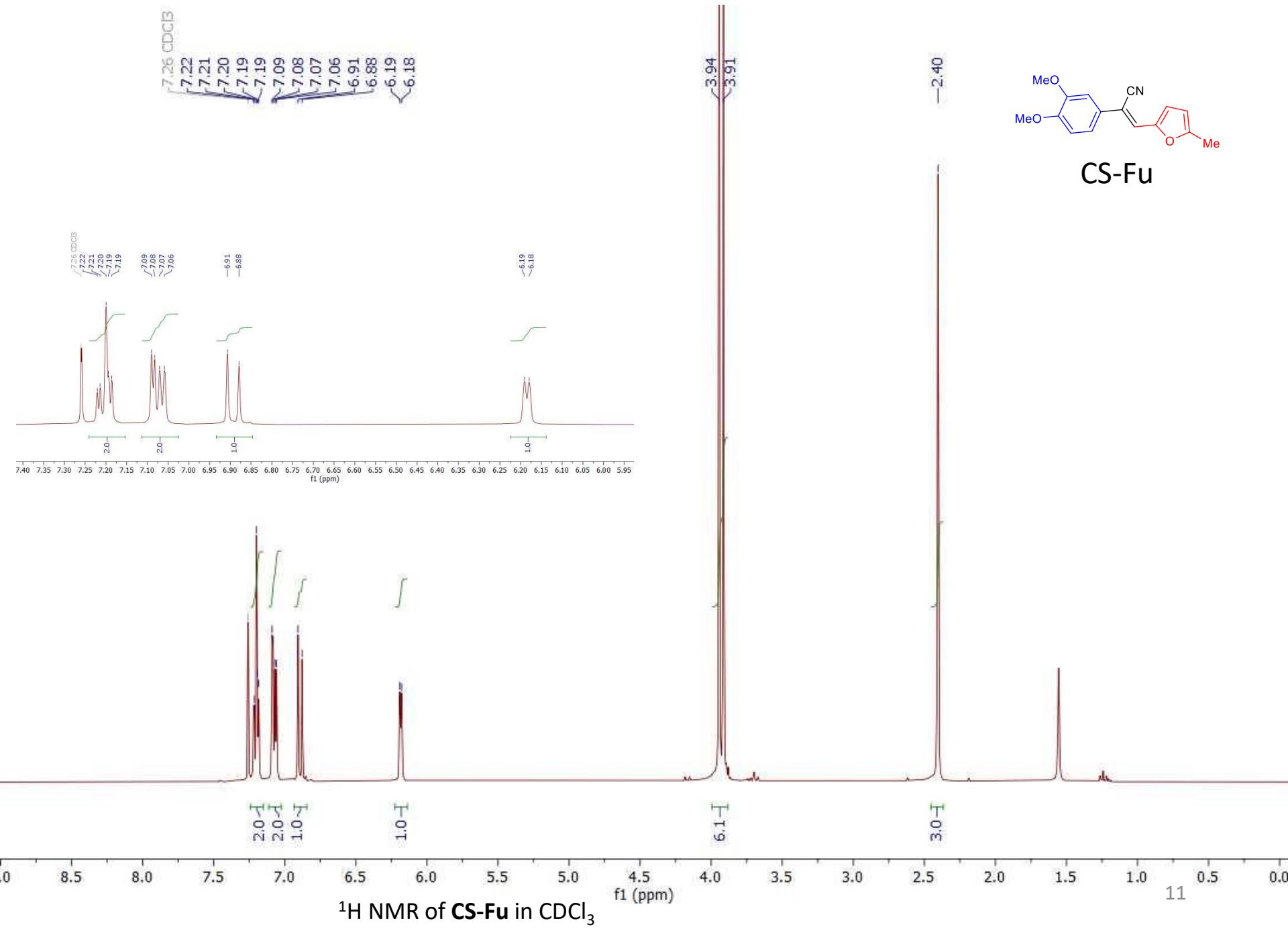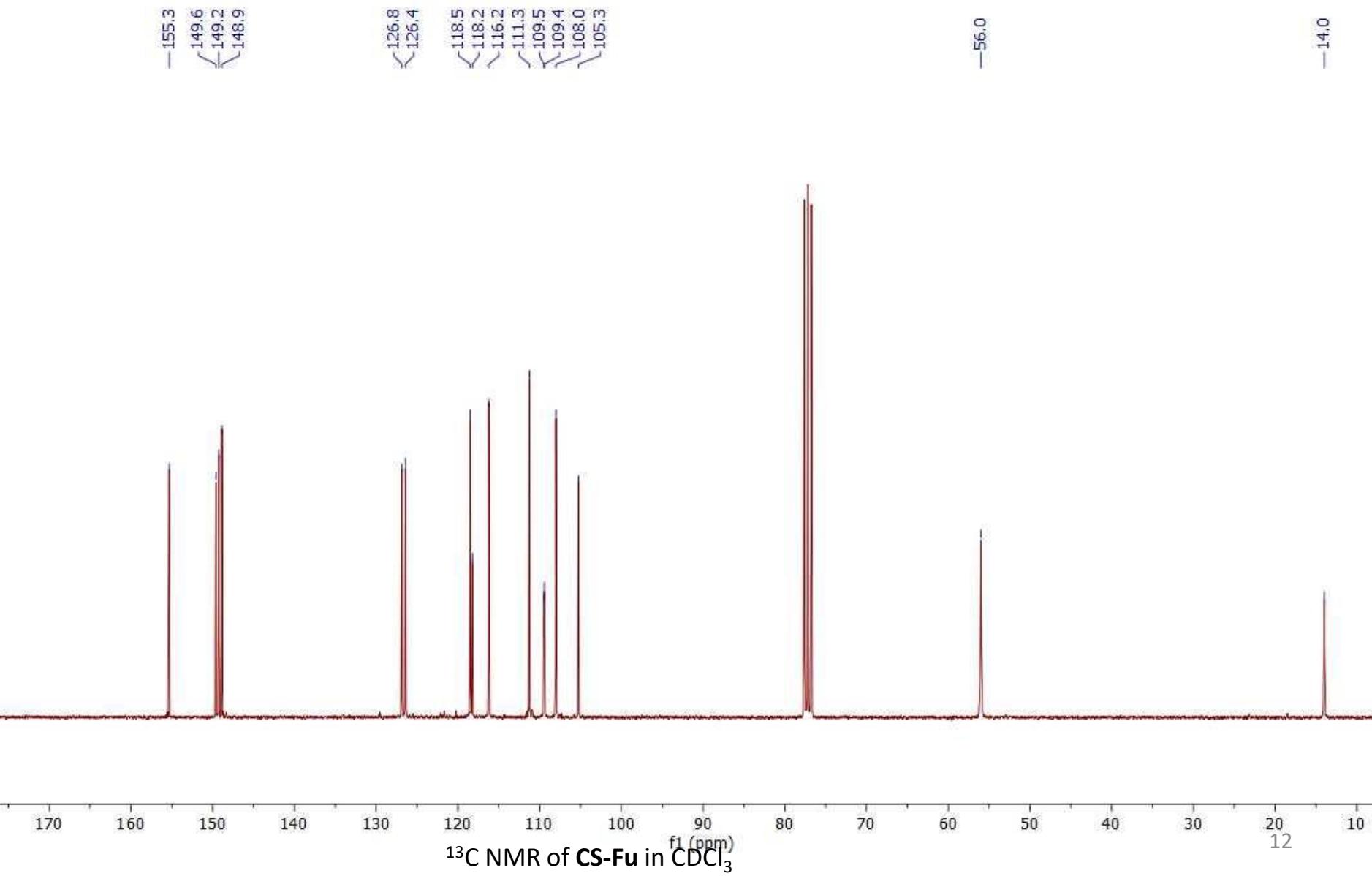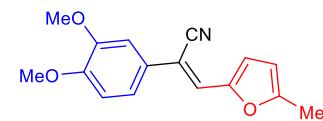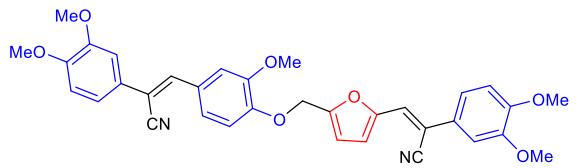
CS-BeFu

^{1}H NMR spectra of compound **CS-BeFu** in DMSO d$_6$.
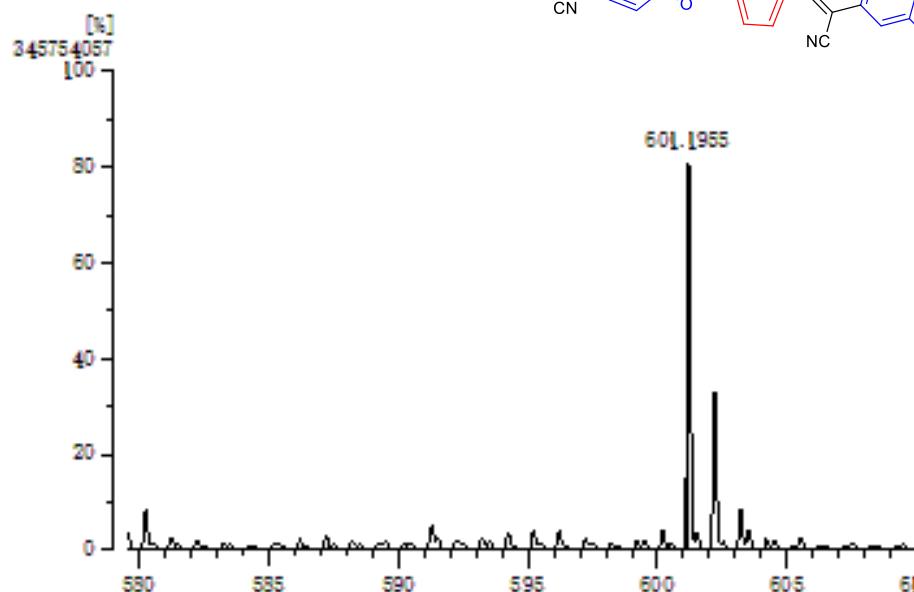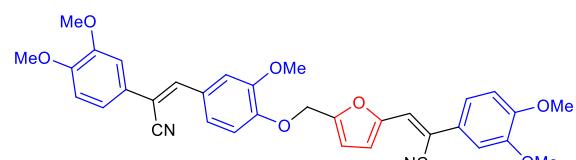
CS-BeFu

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1 601.1955	81.15	+0.7 / +0.4	20.5	C34 H30 N2 O7 Na

Mass Spectra (FAB) of **CS-BeFu**

14