Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Photoacidity as tool to rationalize excited state intramolecular proton transfer reactivity in flavonols

Luís Gustavo Teixeira Alves Duarte,[a,b] José Carlos Germino,[b] Cláudia de Ávila Braga,[a] Cristina Aparecida Barboza,[c] Teresa Dib Zambon Atvars,[b] Fabiano da Silveira Santos,*[a] and Fabiano Severo Rodembusch*[a]

[a]Grupo de Pesquisa em Fotoquímica Orgânica Aplicada, Universidade Federal do Rio Grande do Sul - Instituto de Química, Avenida Bento Gonçalves 9500. CEP 91501-970 Porto Alegre-RS, Brazil. E-mail: fabiano@ufrgs.br (F. S. Santos) and fabiano.rodembusch@ufrgs.br (F. S. Rodembusch)

[b]Chemistry Institute, University of Campinas, Rua Sérgio Buarque de Holanda s/n, Poste Code 6154, Campinas SP - CEP 13083-970.

[c]Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668, Warsaw, Poland.

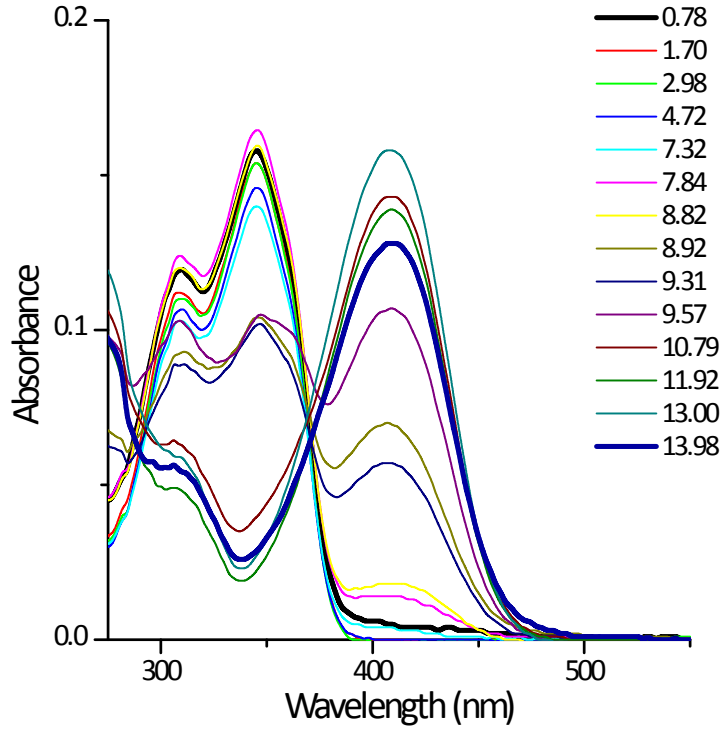


Fig S1. UV-Vis absorption spectra of **3HF** in ethanol/water (1:1 vol) at different acid solutions. [Flavonol]=8.5x10^{-6} Molar.

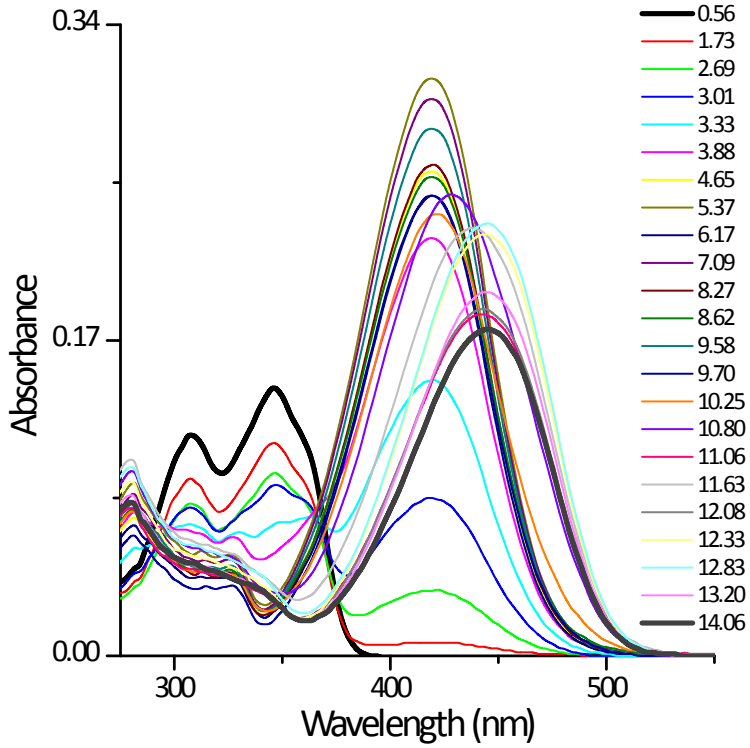


Fig S2. UV-Vis absorption spectra of **DEA3HF** in ethanol/water (1:1 vol) at different acid solutions. [Flavonol]=8.5x10^{-6} Molar.

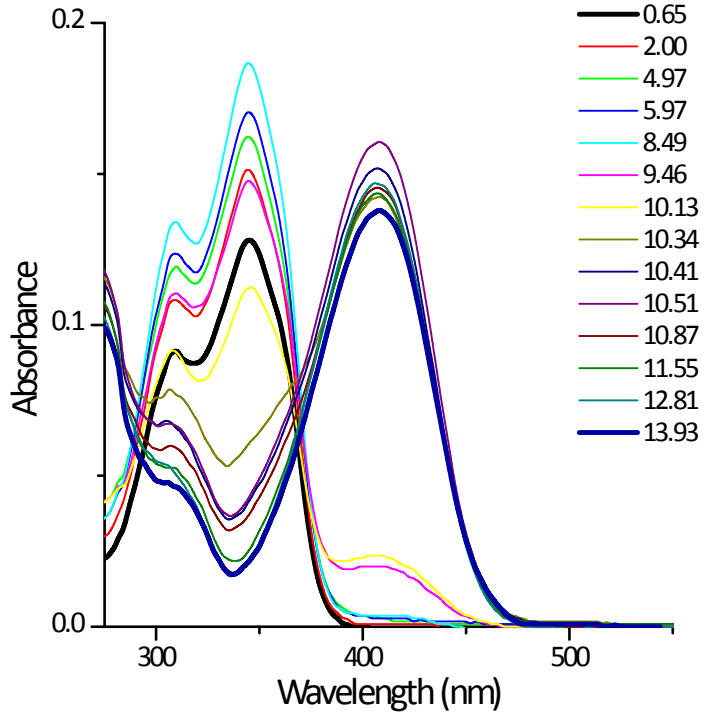


Fig S3. UV-Vis absorption spectra of **F3HF** in ethanol/water (1:1 vol) at different acid solutions. [Flavonol]=8.5x10^{-6} Molar.

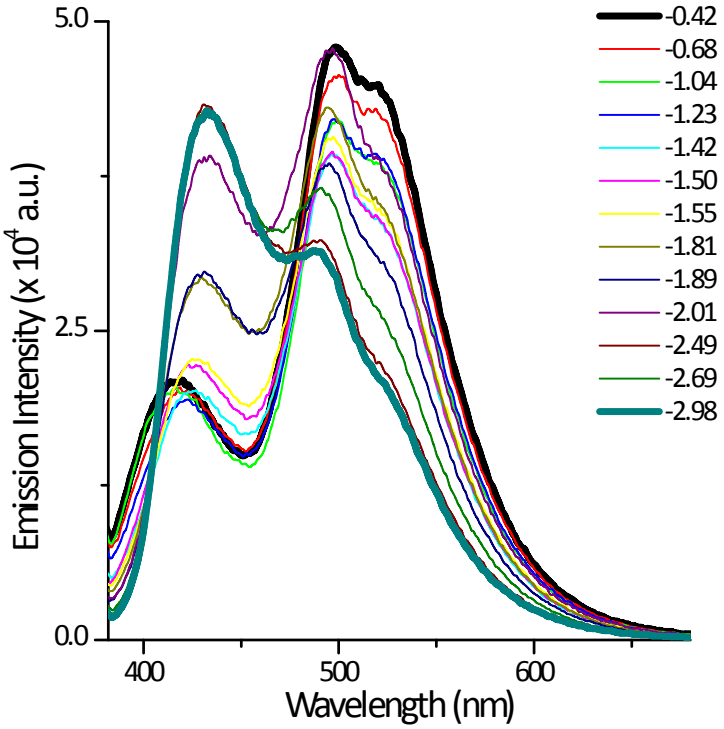


Fig S4. Fluorescence emission spectra of **3HF** at different acid solutions from HCl 7.11 mol·L^{-1} (H_0 -2.98) to 1.34 mol·L^{-1} (H_0 -0.42). [Flavonol]=8.5x10^{-6} Molar.

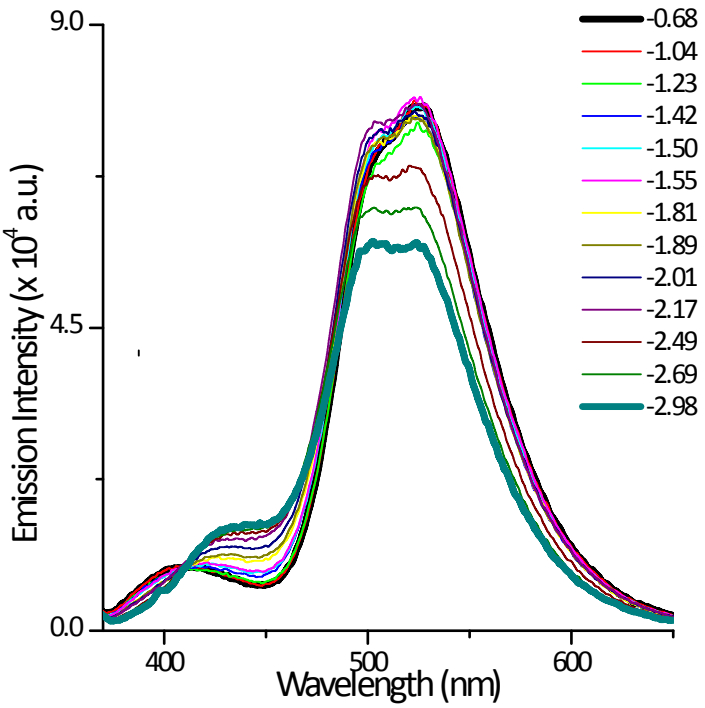


Fig S5. Fluorescence emission spectra of **DEA3HF** at different acid solutions from HCl 7.11 Molar (H_0 -2.98) to 2.01 Molar (H_0 -0.68). [Flavonol]=8.5x10^{-6} Molar.

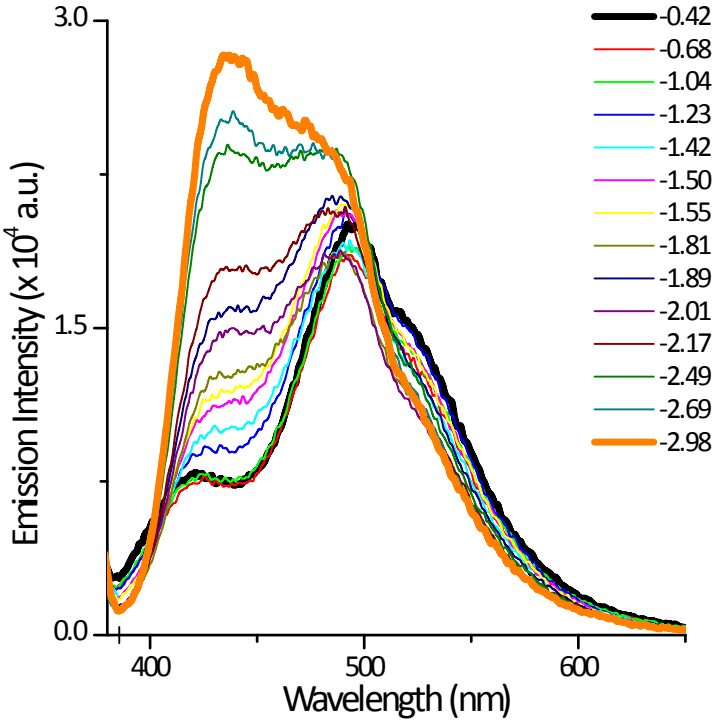


Fig S6. Fluorescence emission spectra of **F3HF** at different acid solutions from HCl 7.11 Molar (H_0 -2.98) to 1.34 Molar (H_0 -0.42). [Flavonol]=8.5x10^{-6} Molar.

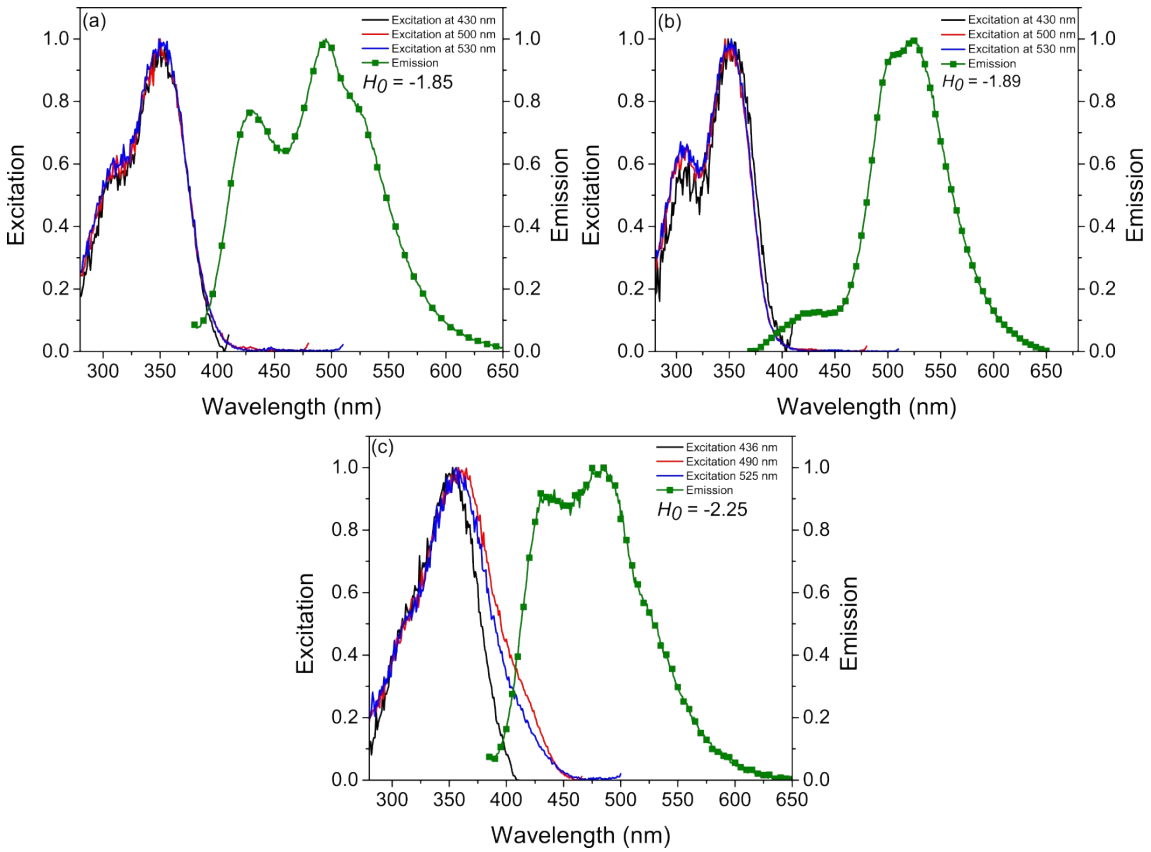
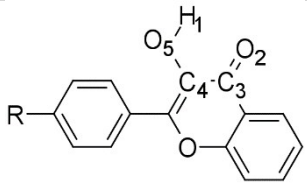


Fig S7. Excitation spectra at all curves inflection point of the compounds **3HF, DEA3HF** and **F3HF**.

Table S1. Molecular structure showing the labels used in selected geometry parameters in Å for the ground state structures obtained at CAM-B3LYP/6-311++G(d,p) using water as solvent.



Species	Comp.	Geometry parameters			
		H_1-O_2	O_2-C_3	C_3-C_4	C_4-O_5
Protonated	**3HF**	0.968	1.346	1.396	1.318
	DEA3HF	0.967	1.351	1.380	1.329
	F3HF	0.968	1.346	1.396	1.318
Neutral	**3HF**	0.976	1.349	1.457	1.228
	DEA3HF	0.975	1.354	1.449	1.236
	F3HF	0.975	1.352	1.452	1.235
Deprotonated	**3HF**	-	1.236	1.518	1.215
	DEA3HF	-	1.244	1.507	1.220
	F3HF	-	1.236	1.517	1.215

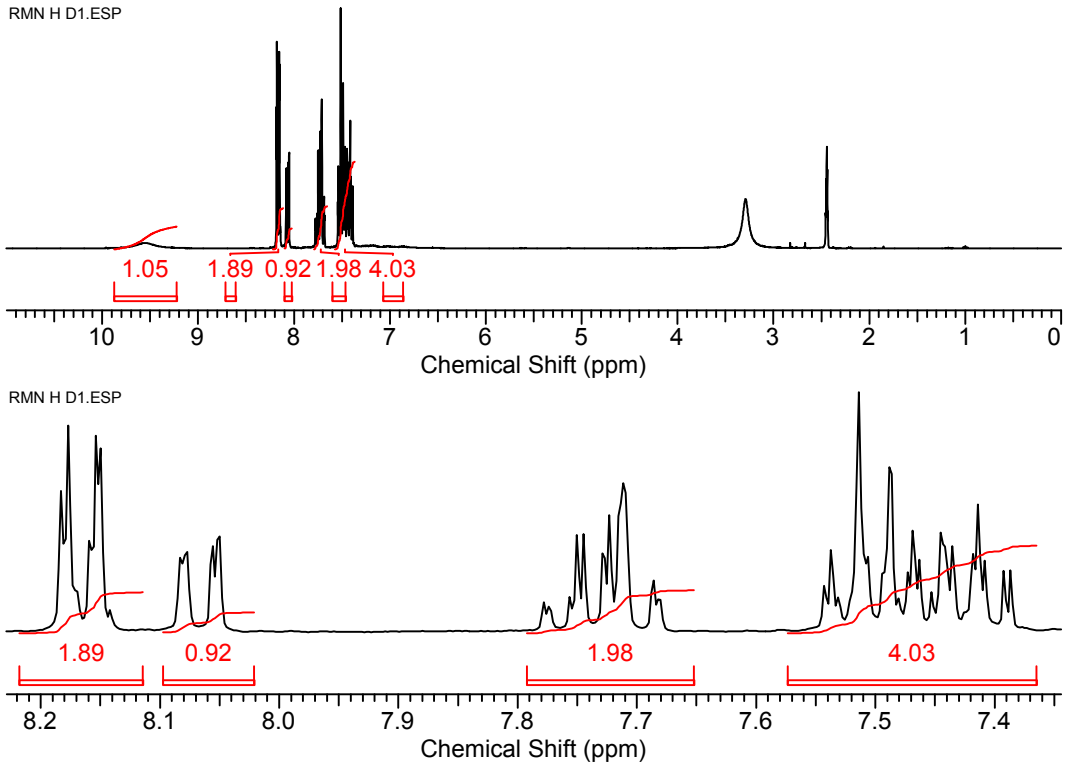


Fig S8. ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of compound **3HF**.

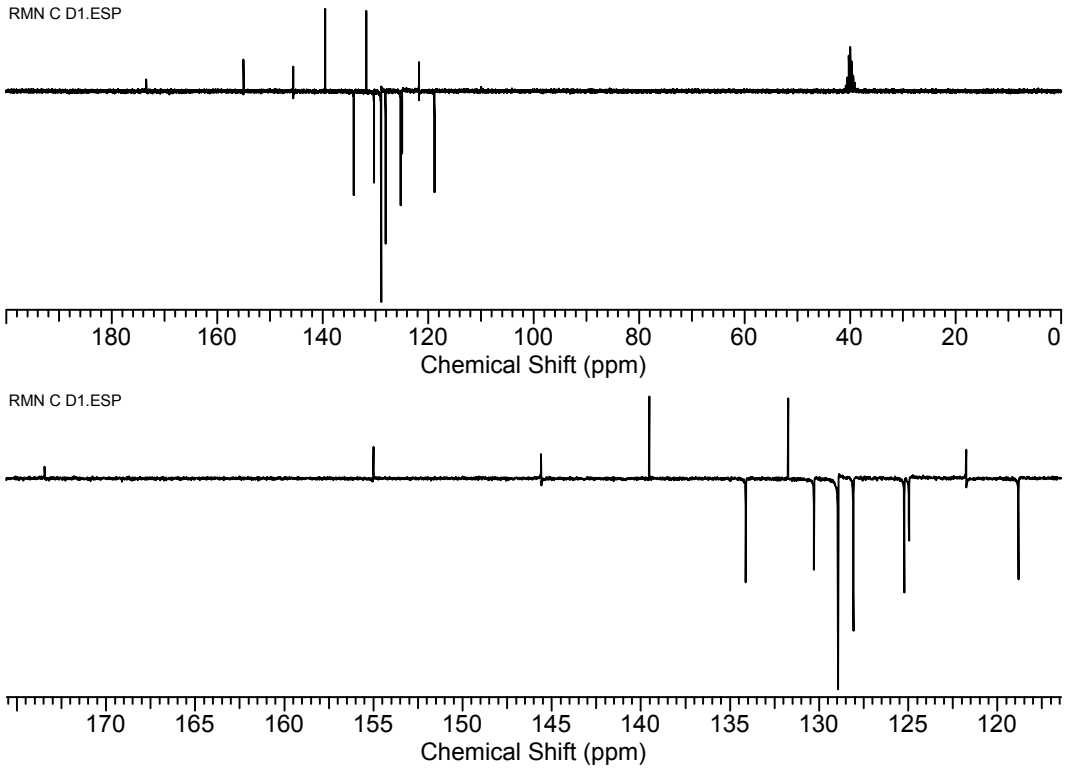


Fig S9. ^{13}C NMR spectrum (75.4 MHz, DMSO-d_6) of compound **3HF**.

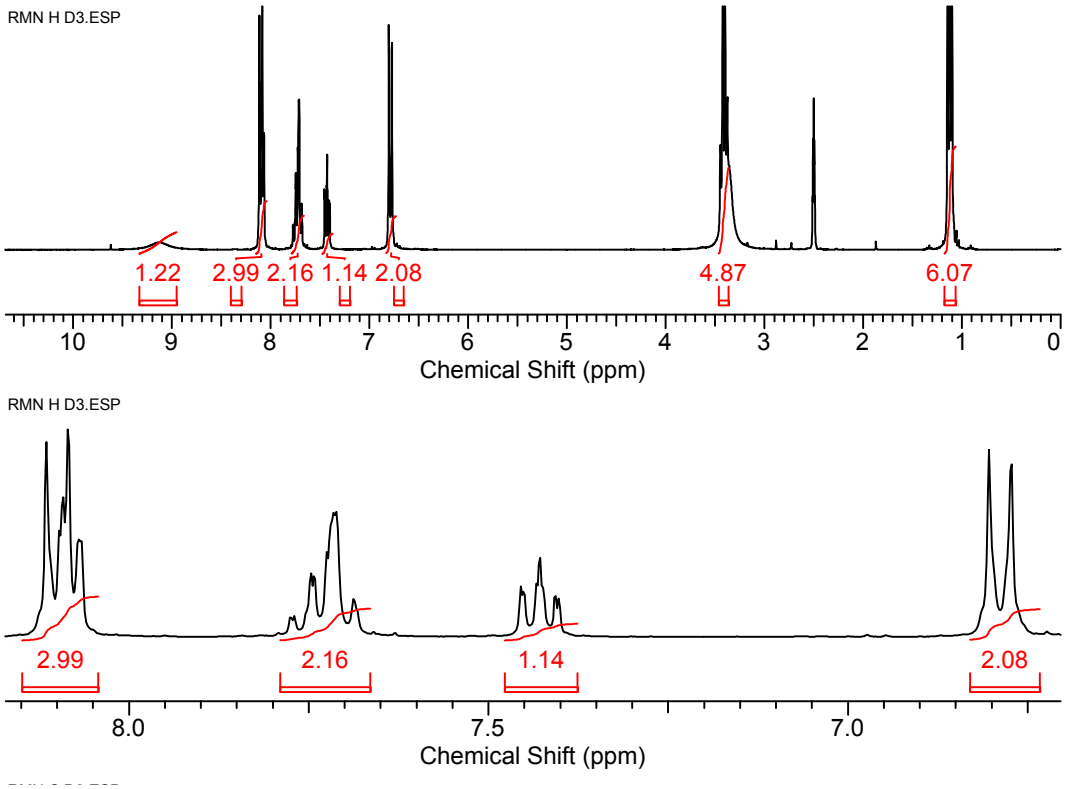


Fig S10. ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of compound **DEA3HF**.

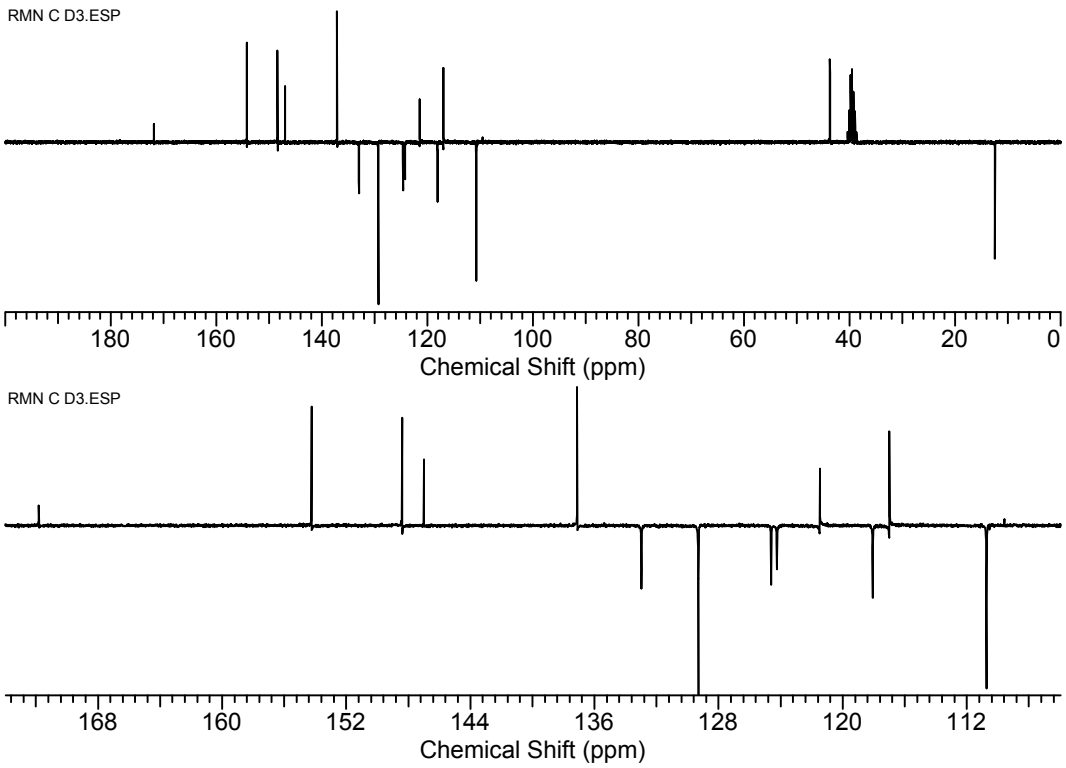


Fig S11. ^{13}C NMR spectrum (75.4 MHz, DMSO-d_6) of compound **DEA3HF**.

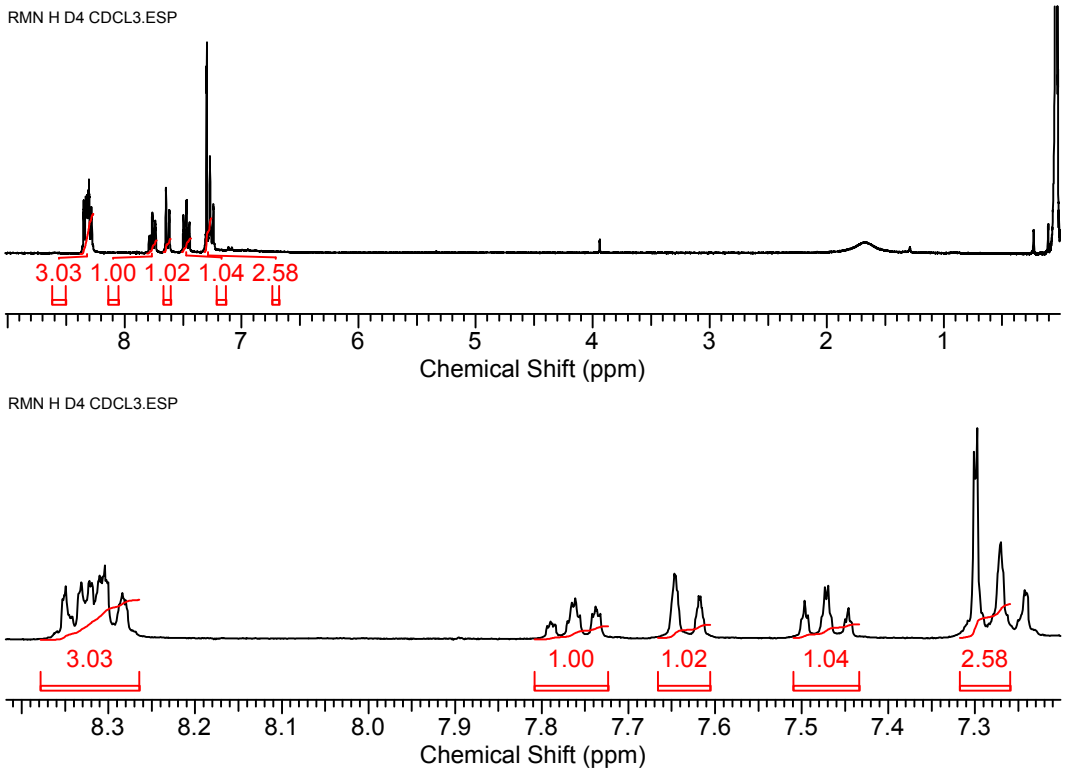


Fig S12. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **F3HF**.

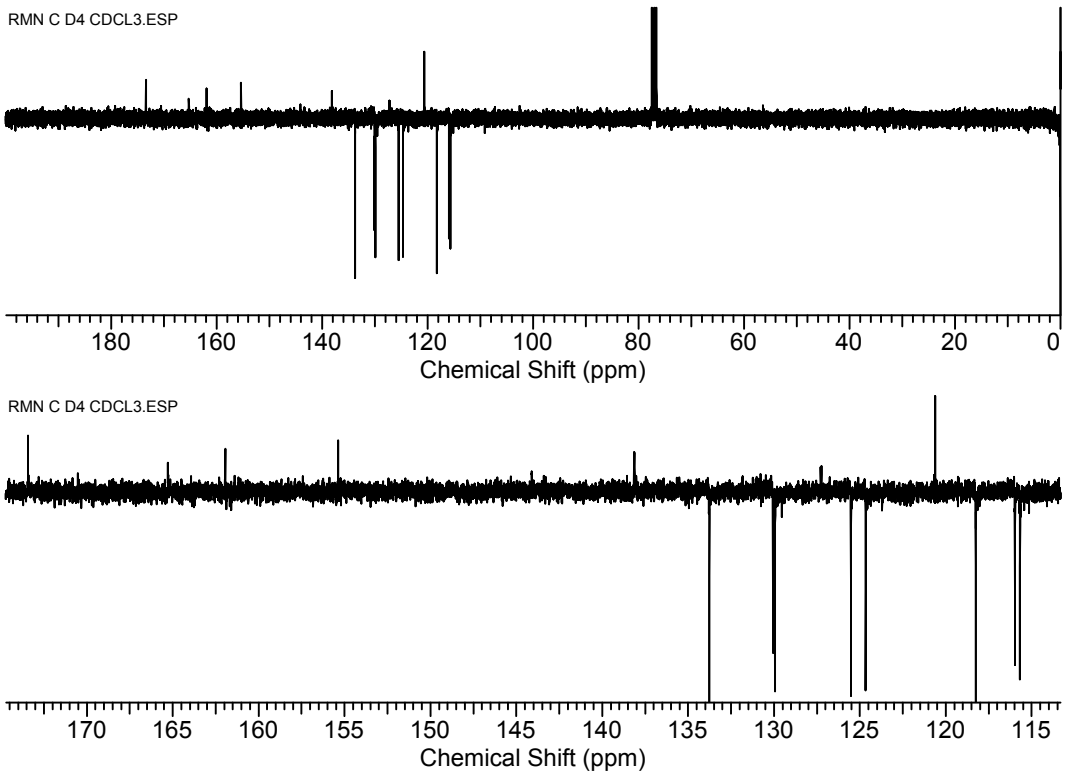


Fig S13. ^{13}C NMR spectrum (75.4 MHz, $CDCl_3$) of compound **F3HF**.

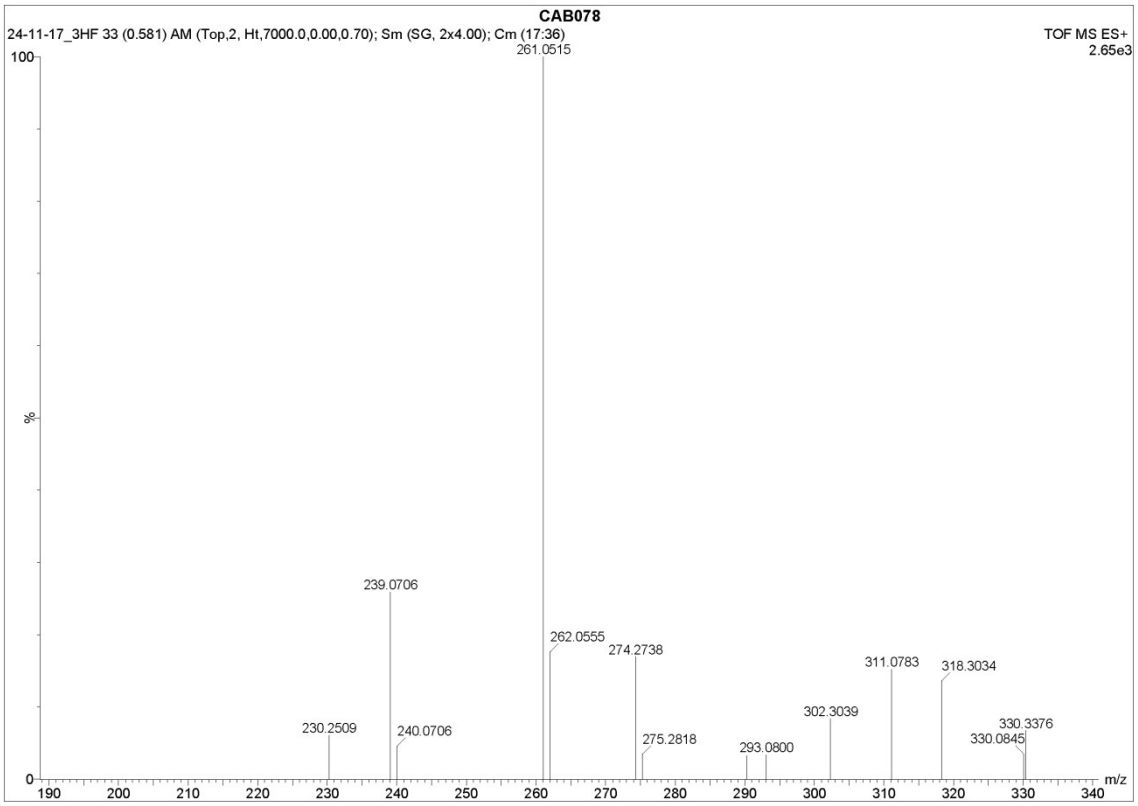


Fig S14. HRMS spectra of compound **3HF**.

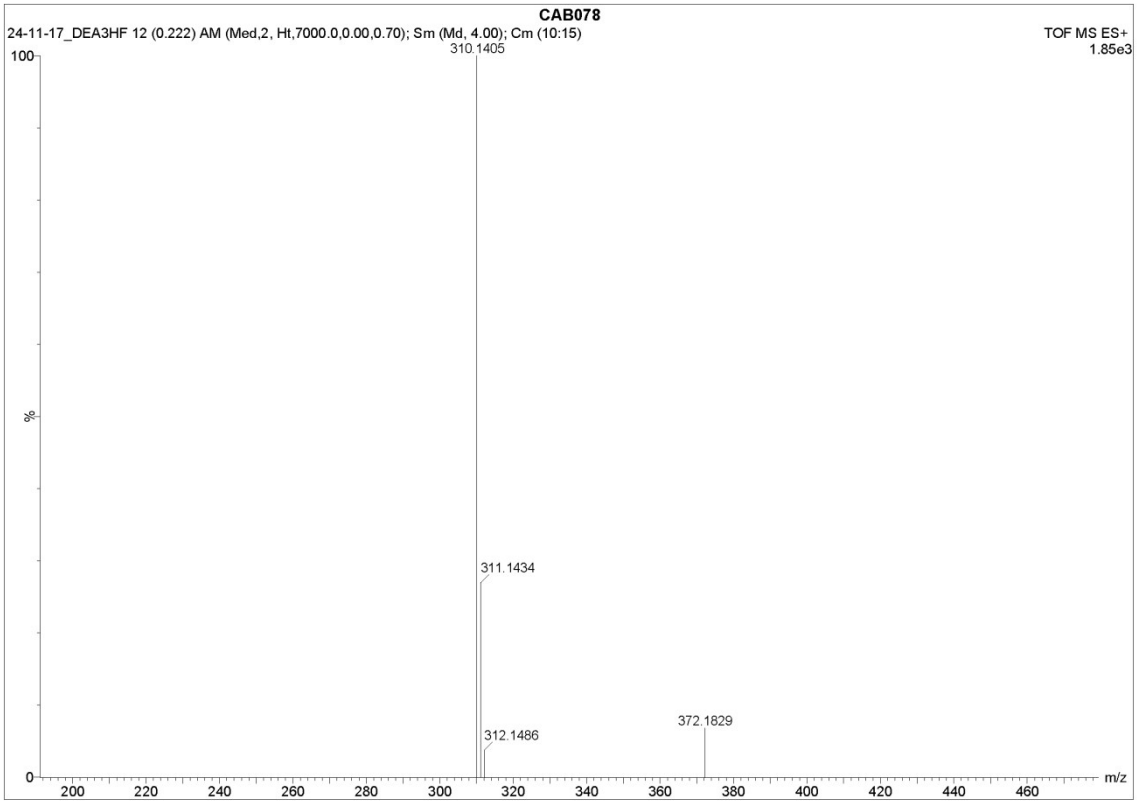


Fig S15. HRMS spectra of compound **DE3HF**.

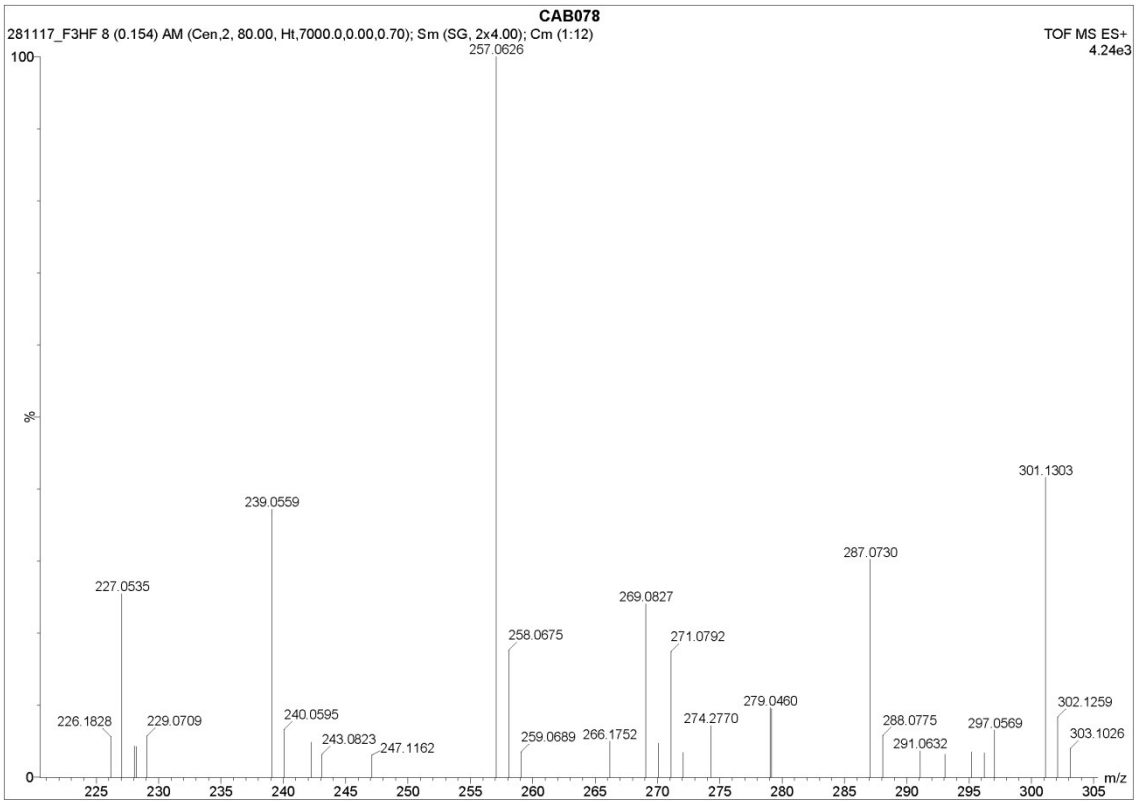


Fig S16. HRMS spectra of compound **F3HF**.