Electronic Supplementary Material (ESI) for RSC Advances

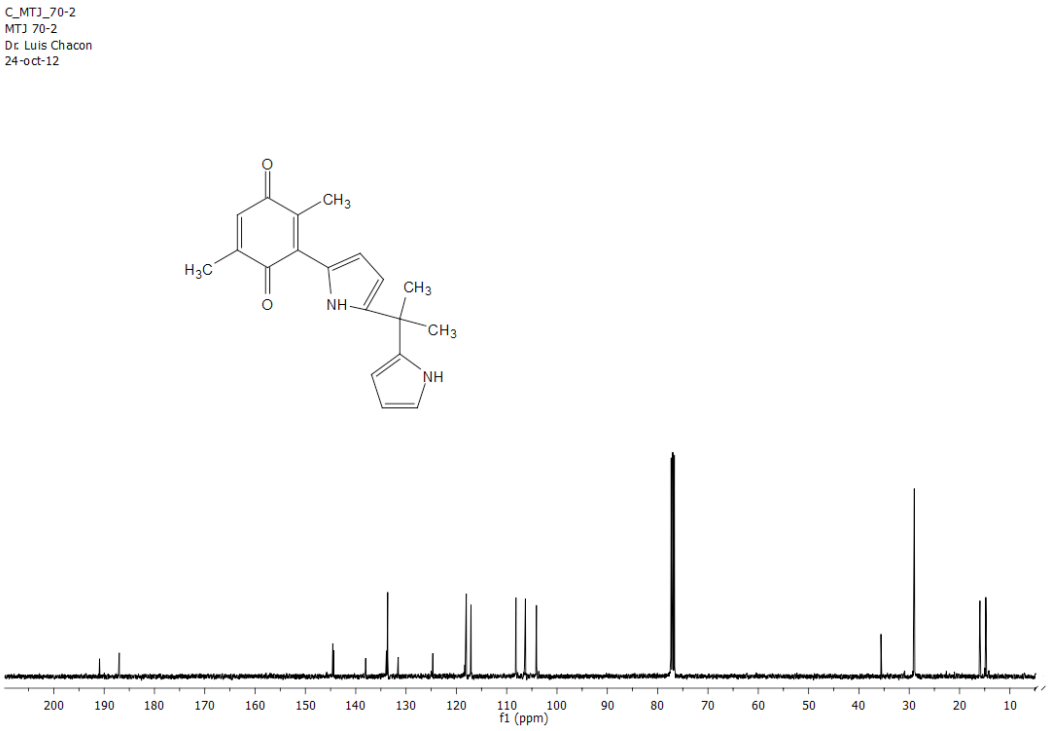
A new type of anion receptor: Pyrrolyl quinones

Melissa Tapia-Juárez,[a] J. Betzabe González-Campos,[a] Claudia Contreras-Celedón,[a] David Corona,[b] Erick Cuevas-Yañez,[b] and Luis Chacón-García *[a]

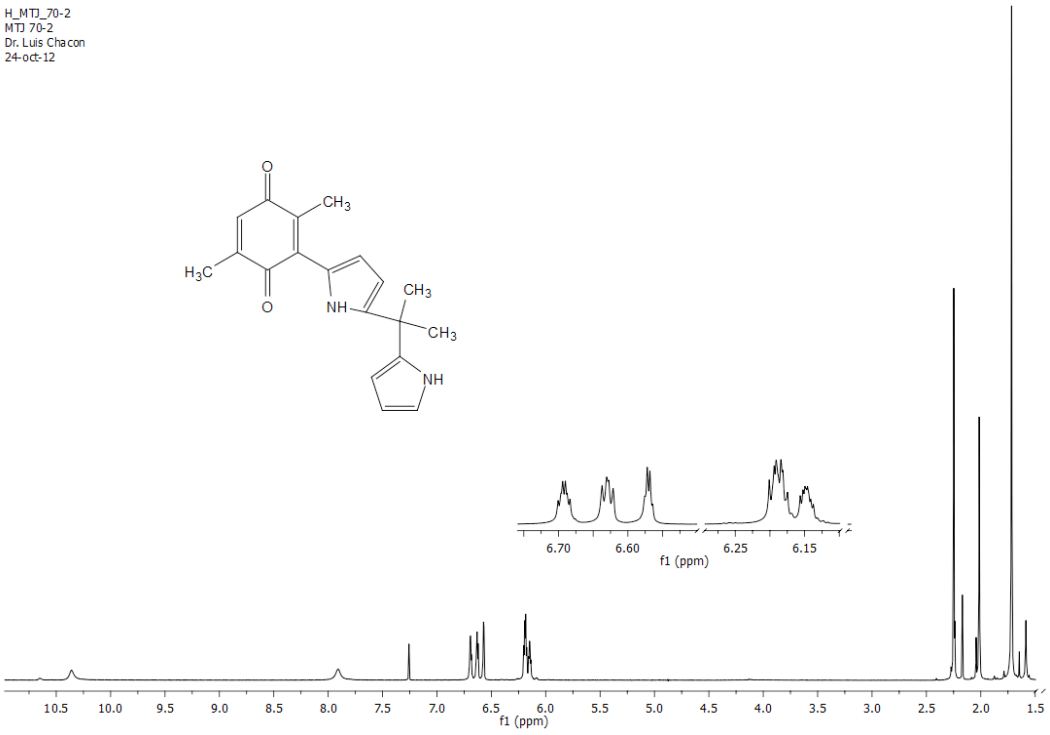
[a]Laboratorio de Diseño Molecular, Instituto de Investigaciones Químico BiológicasUniversidad Michoacana de San Nicolás de Hidalgo, Morelia, Mich., 58066, México

[b] Centro Conjunto de Investigación en Química Sustentable UAEM-UNAM, Carretera Toluca-Atlacomulco Km. 14.5, Toluca, Estado de México 52000, México

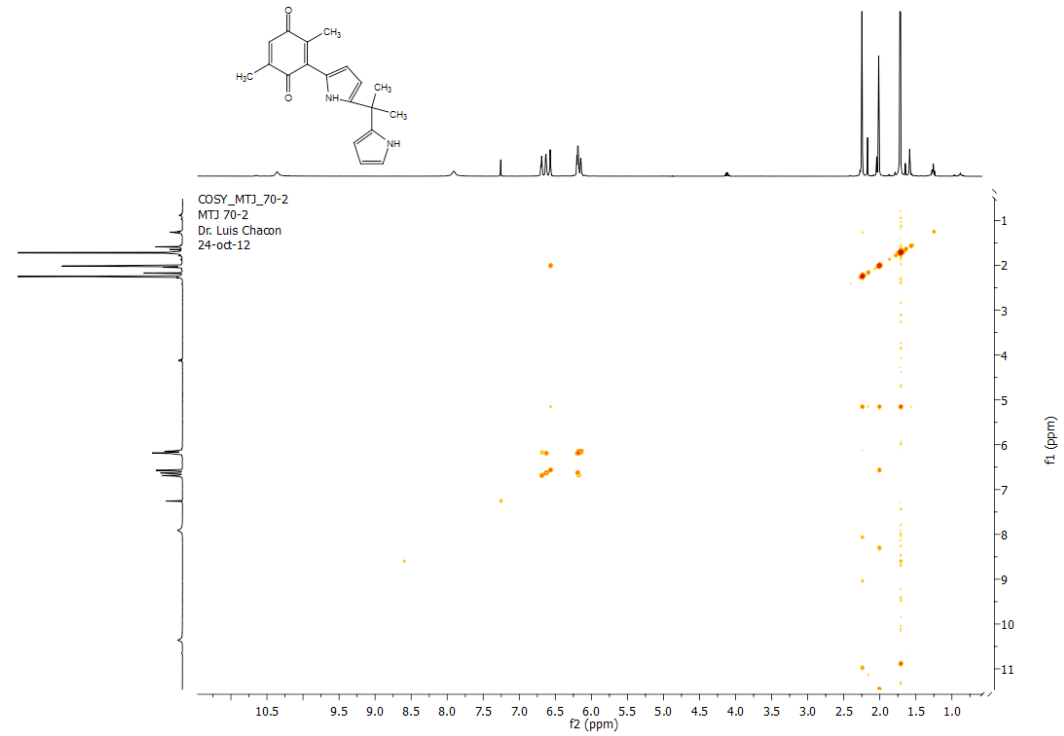
email: lchacon@umich.mx



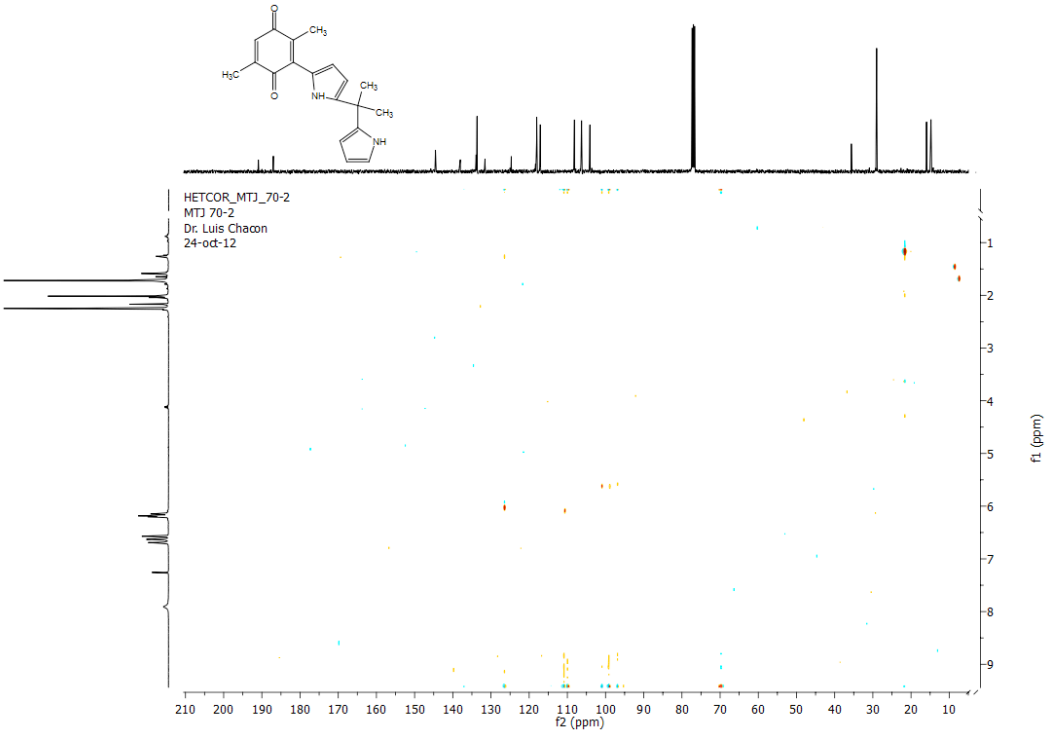
1.^{1}H NMR of 2 (400 MHz) in $CDCl_3$.



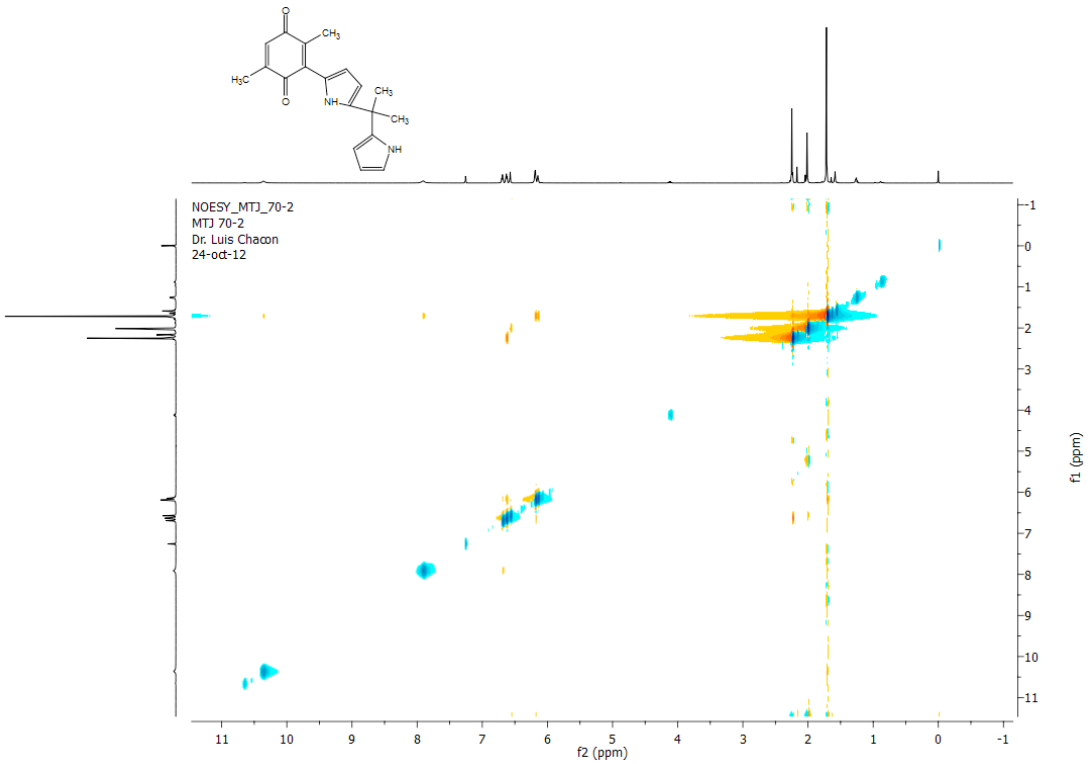
2. ^{13}C NMR of 2 (130MHz) in $CDCl_3$.



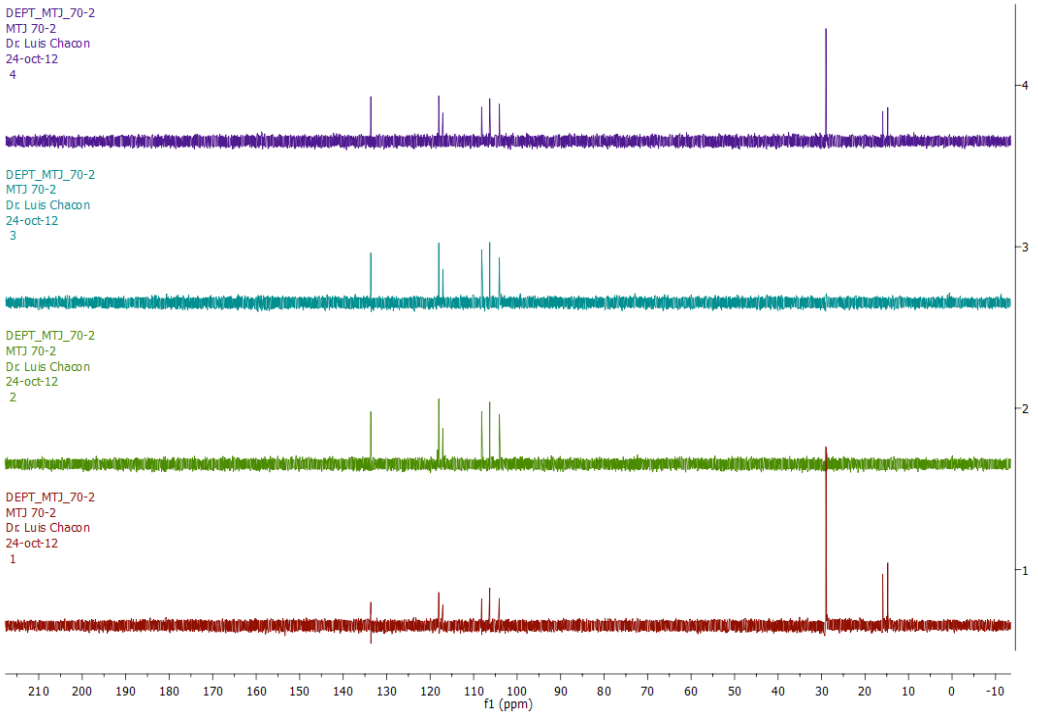
3.Cosy NMR (400 MHz) of 2 in $CDCl_3$.



4. Hetcor NMR of 2 in $CDCl_3$.

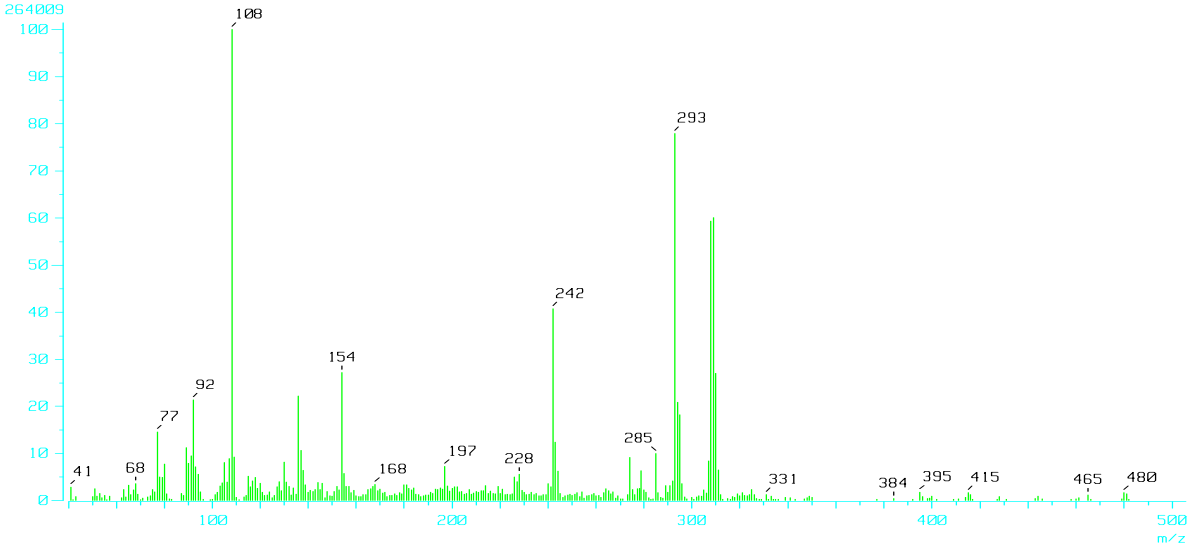


5. Noesy NMR of 2 in $CDCl_3$.



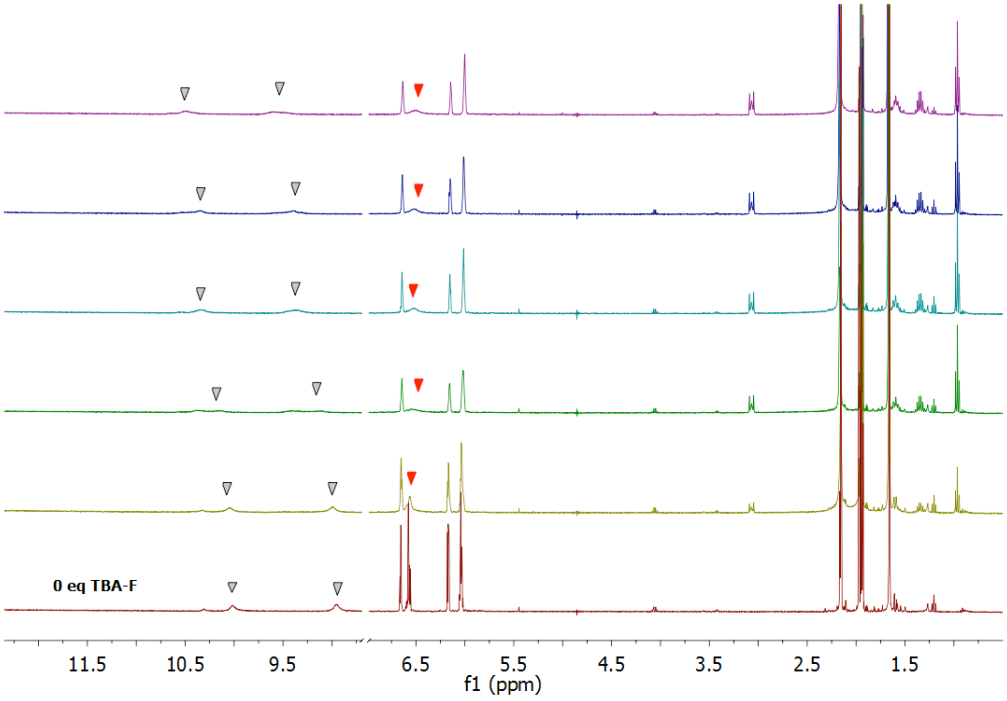
6. Dept NMR of 2 in $CDCl_2$

[Mass Spectrum]
Data : MOP259 Date : 04-Oct-2013 00:58
Sample: OJ-MT Operator name Ing.Victoria Labastida G.
Note : Dr.Mario Ordonez Centro de Investigaciones Quimicas UAEM
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.64 min Scan# : (6,7)
BP : m/z 108.0000 Int. : 24.82
Output m/z range : 40.0000 to 505.6973 Cut Level : 0.00 %

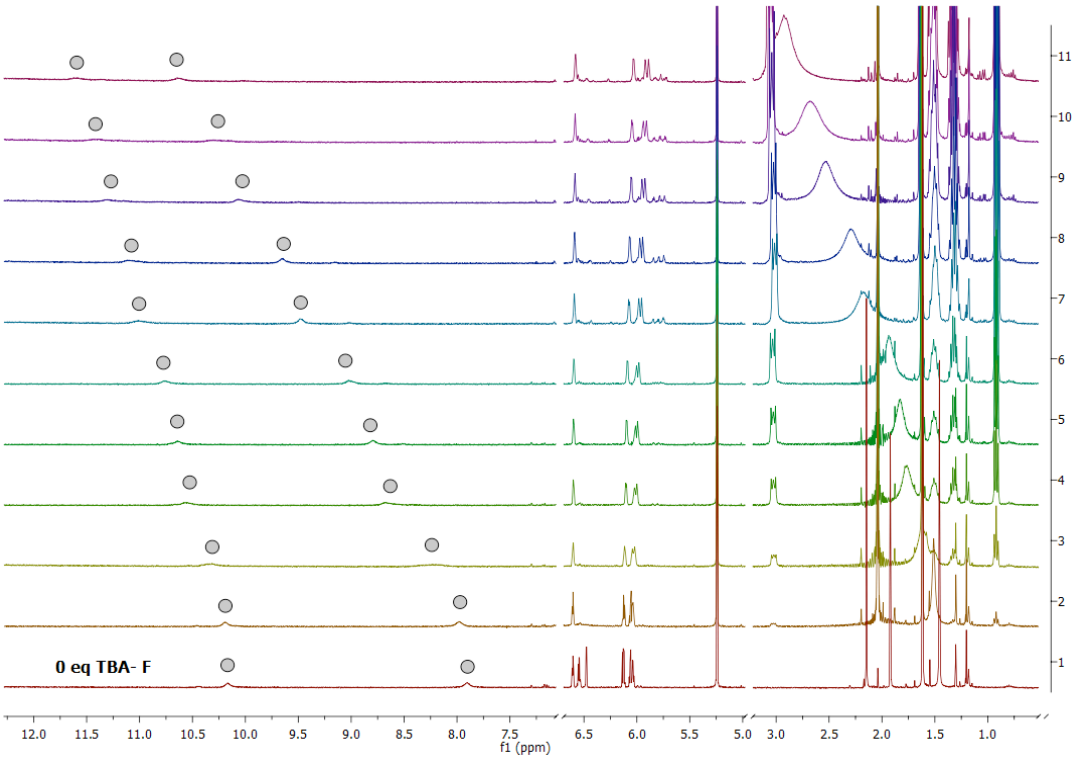


[Elemental Composition]
Data : MOP260 Date : 08-Oct-2013 00:53
Sample: OJ-MT Operate name:Ing.Victoria Labastida G.
Note : Dr.Mario Ordonez Centro de Investigaciones Quimicas UAEM
Inlet : Direct Ion Mode : FAB+
RT : 0.21 min Scan#: (2,8)+41
Elements : C 40/0, H 49/0, O 2/0, N 2/0
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 25mmu if m/z > 25
Unsaturation (U.S.) : 10.5 - 10.5

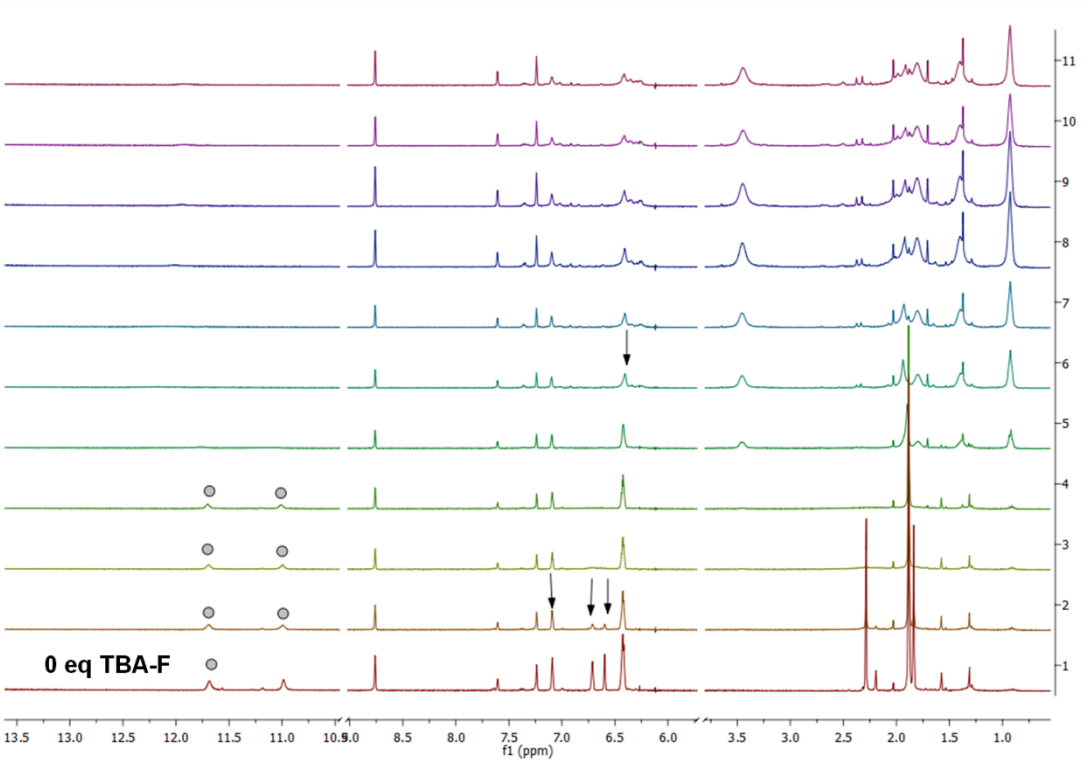
Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
309.1378	81.5	-72.8 / -22.5	10.5	C 19 H 21 O 2 N 2



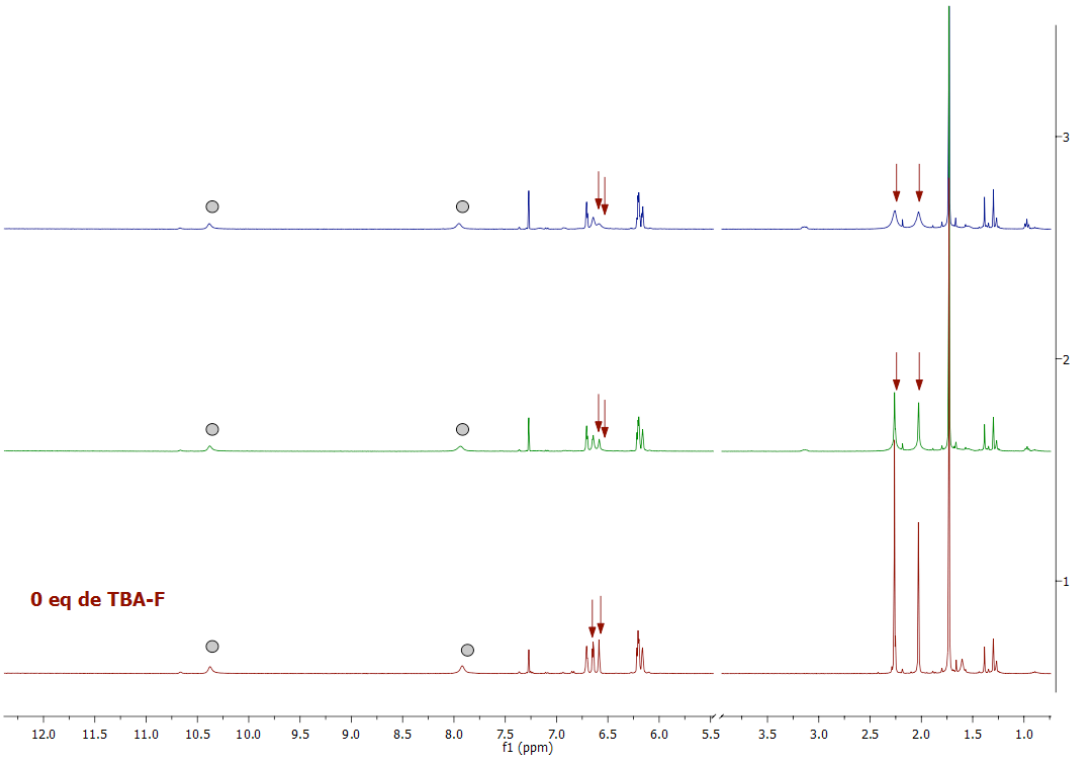
7. ^{1}H NMR spectra (400 MHz) for titration of compound 2 with TBA-F in CD_3CN.



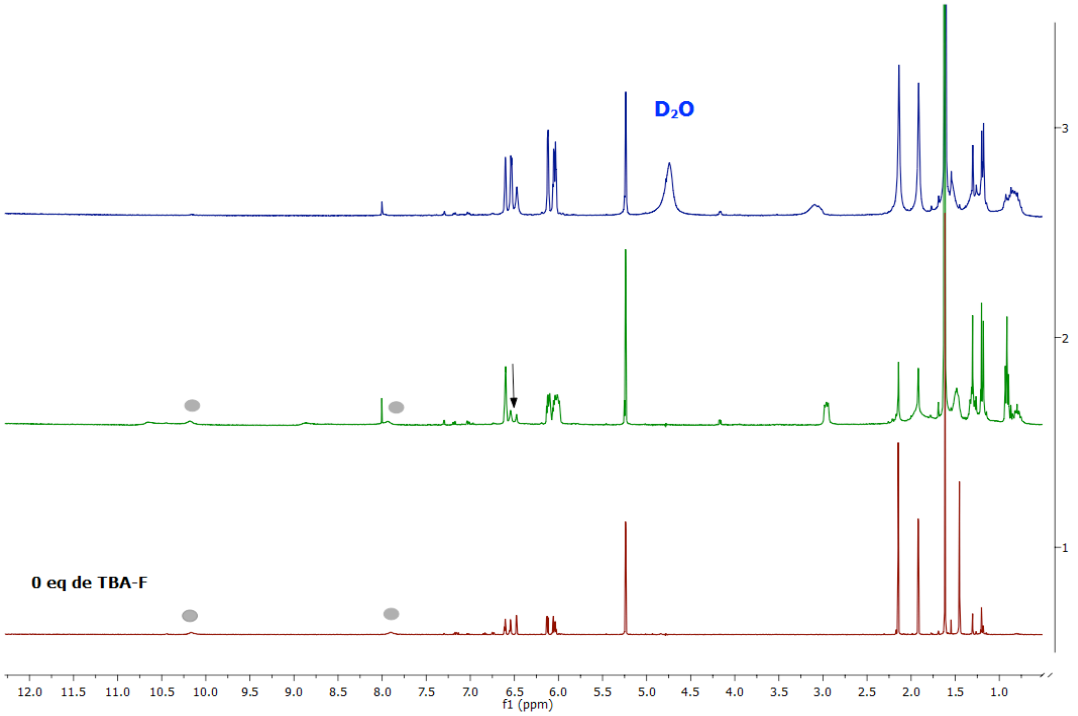
8.^{1}H NMR spectra (400 MHz) for titration of compound 2 with TBAF in CD_2Cl_2.



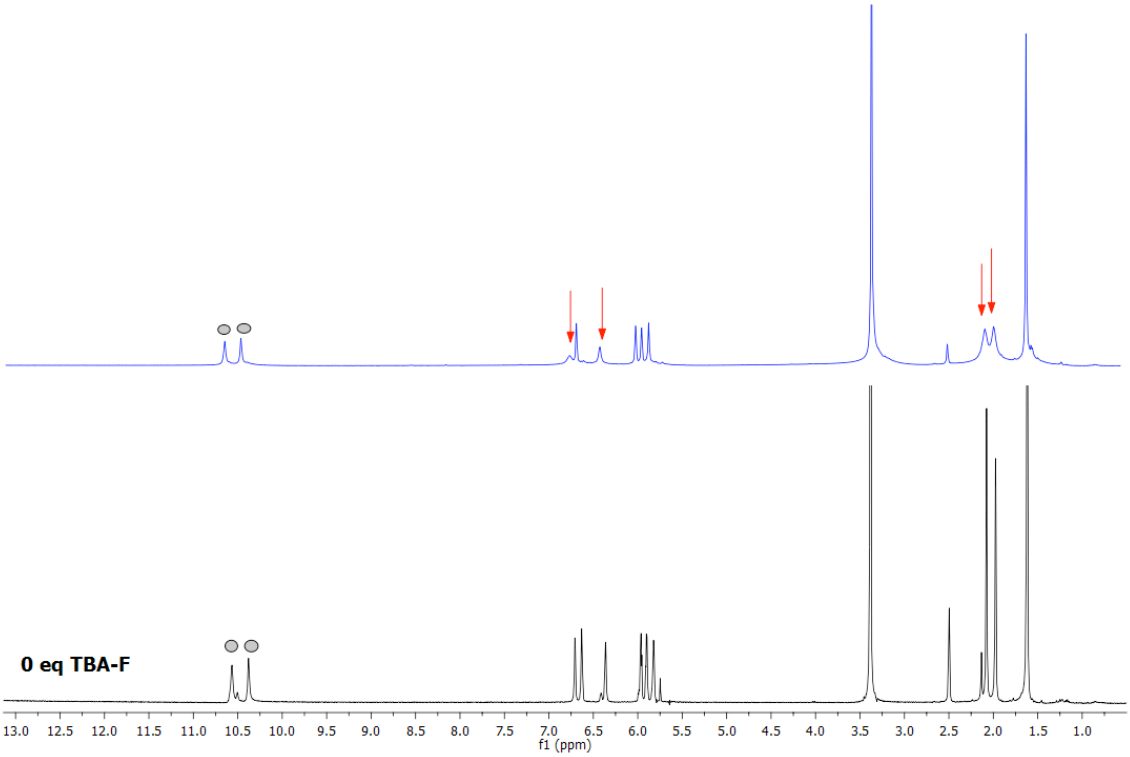
9.^{1}H NMR spectra (400 MHz) for titration of compound 2 with TBAF in C_5D_5N.



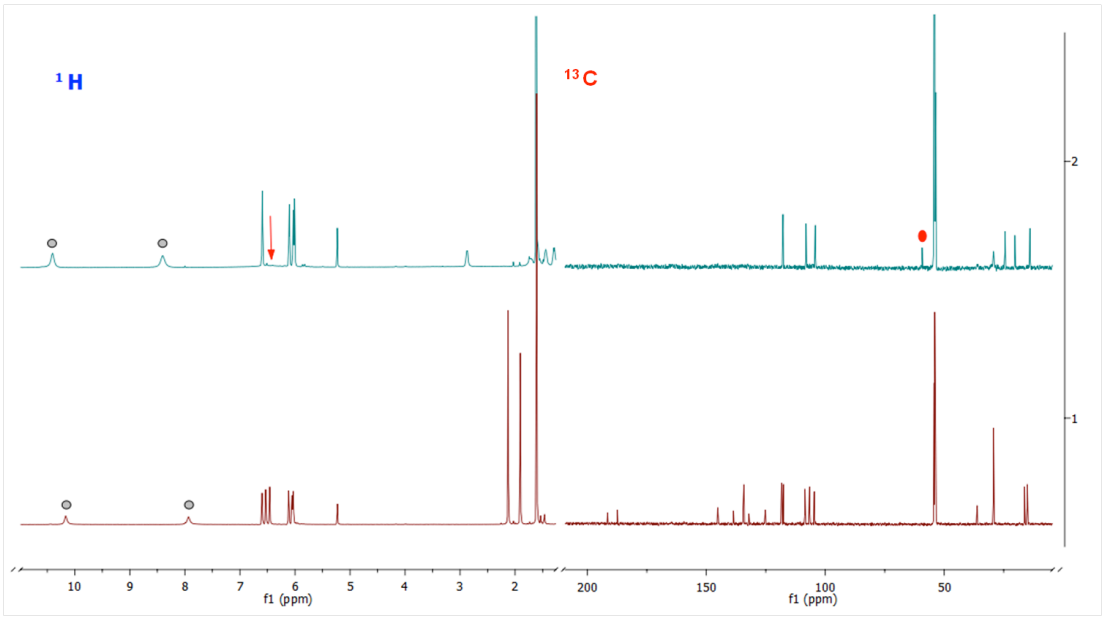
10. ^{1}H NMR spectra (400 MHz) for titration of compound 2 with TBAF in CD_3Cl_3.



11. ^{1} H NMR spectra (500 MHz) a) Compound 2. b) Compound 2- TBA- F c) Compound 2- TBA-F + D_2O

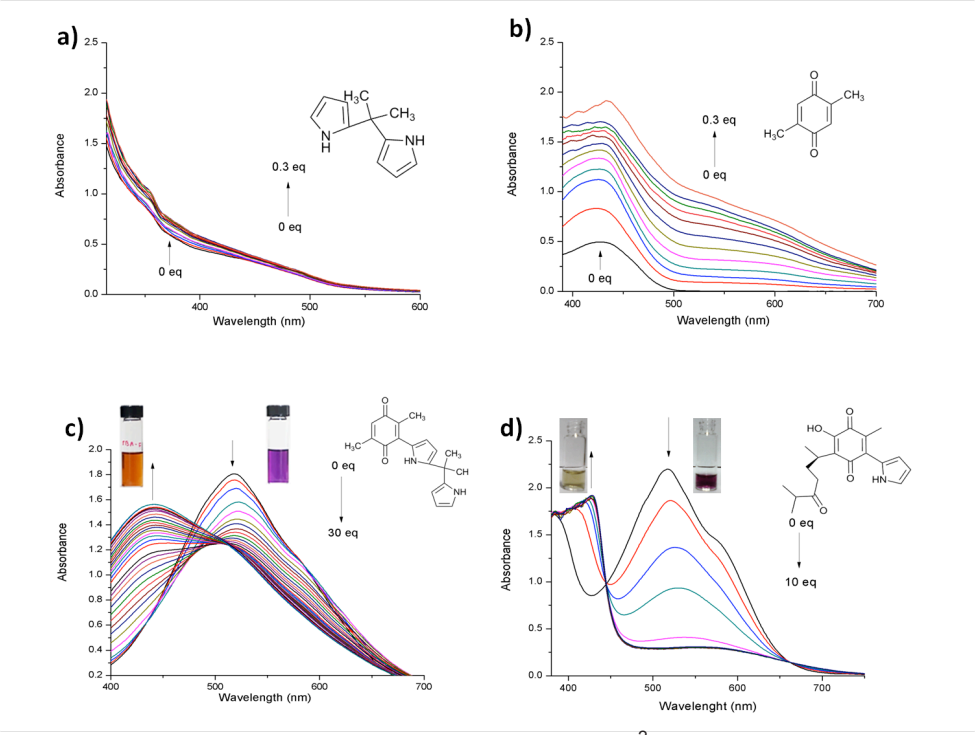


12. ^{1}H NMR spectra (500 MHz) a) Compound 2 in DMSO-d_6 b) compound 2 whit 0.08 eq of TBA-F in DMSO-d_6.



a) b)

13. ^{1}H NMR spectra (500 MHz) (a) of 2 (a-1) 2 with 0.08 eq TBA- F (a-2) in CD_2Cl_2. Red arrow: signal disappearance. ^{13}C NMR spectra (b) of 2 (b-1) 2 with 0.08 eq TBA- F (b-2).



14. a) UV-Vis titration of Dipirromethane in CH_3CN ($2x10^{-2}M$) solution upon addition of fluoride ion as TBA salt (equiv = 0 - 0.3 eq.) b) UV-Vis titration of 2,5- dimethyl-1,4- benzoquinone in CH_3CN ($2x10^{-2}M$) solution upon addition of fluoride ion as TBA salt (equiv = 0 - 0.3 eq.) c) UV-Vis titration of 2 in CH_3CN ($5x10^{-4}M$) solution upon addition of fluoride ion as TBA salt (equiv = 0-30 eq) d) UV-Vis titration of 1 in CH_3CN ($5x10^{-4}M$) solution upon addition of fluoride ion as TBA salt (equiv = 0-10 eq).