

## Supporting Information

### Unusual Tellurium(IV) mediated cyclisation of diols into dihydroxazoles with potential anticancer activity

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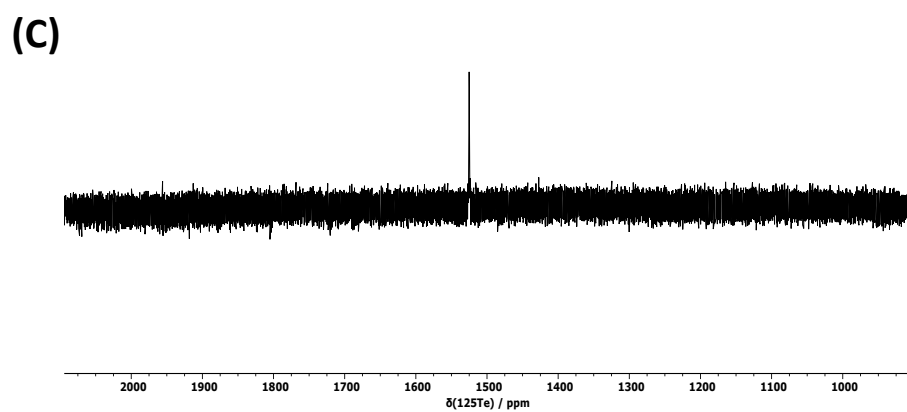
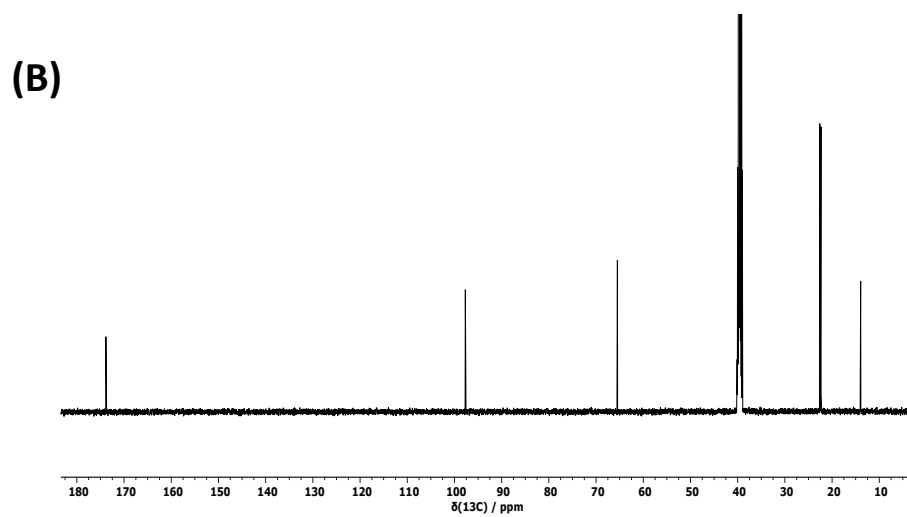
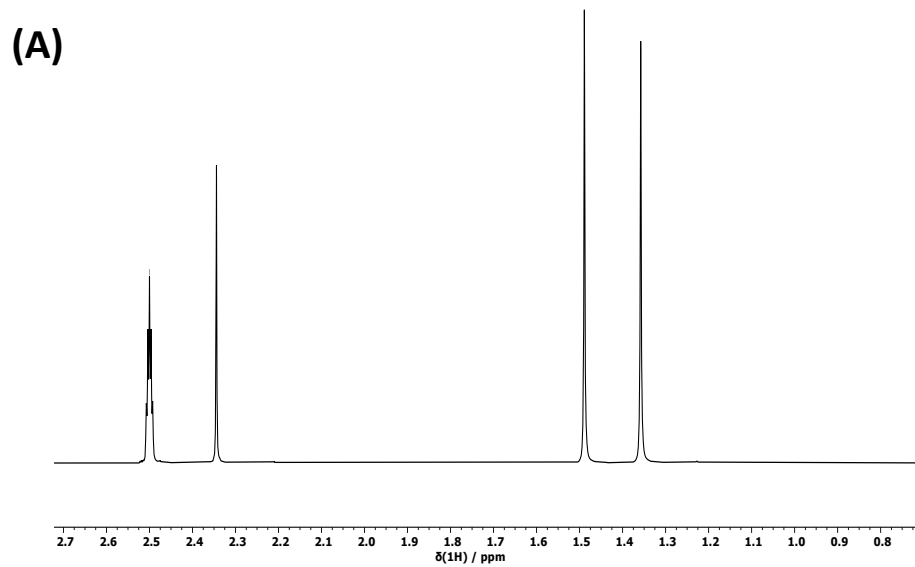
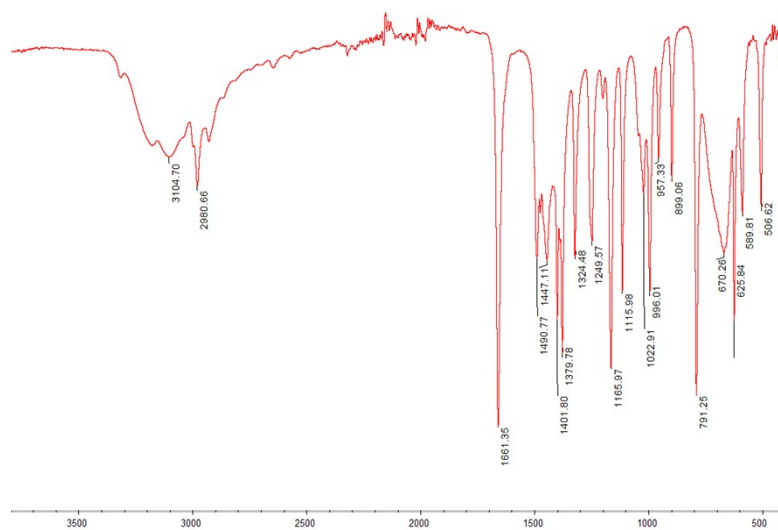
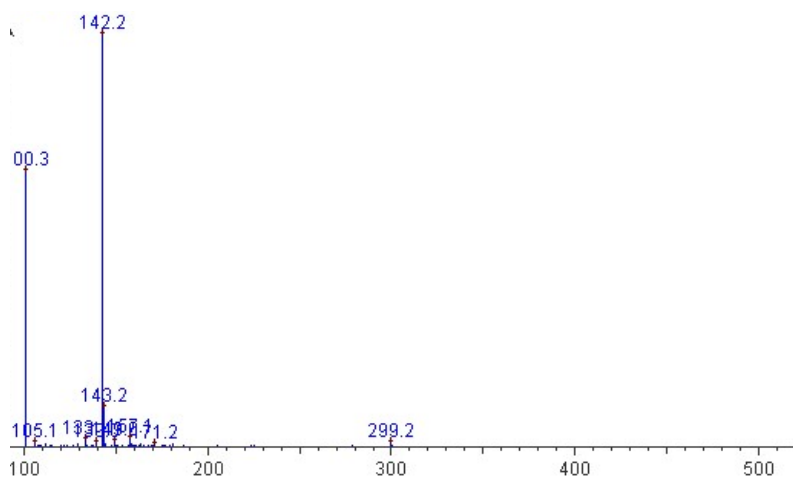


Figure S1. NMR Spectra of A)  $^1\text{H}$ , B)  $^{13}\text{C}$ , and C)  $^{125}\text{Te}$  NMR of compound **1** in  $\text{DMSO-}d_6$

(A)

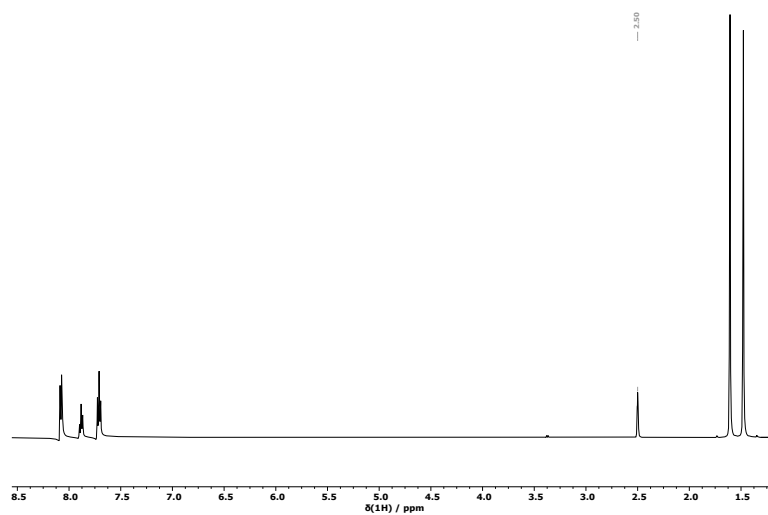


(B)

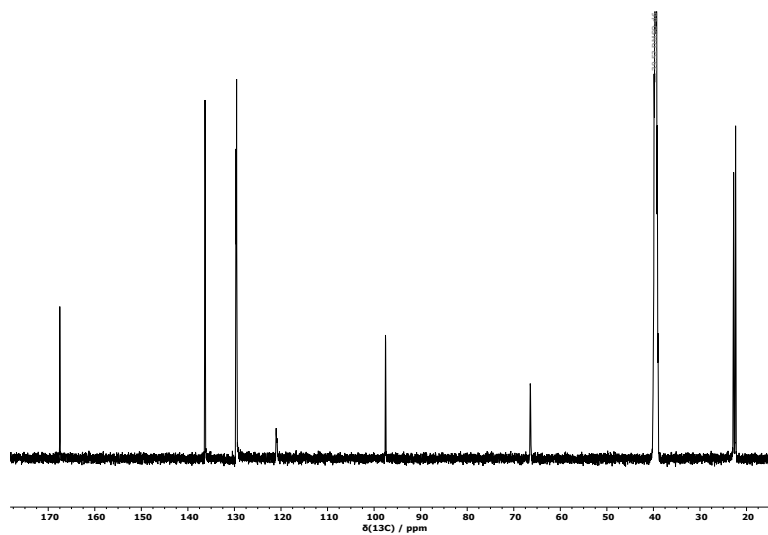


**Figure S2.** A) FTIR spectrum of compound **1**. Assignments ( $\text{cm}^{-1}$ ): 2980  $\rightarrow$  str. C-H ( $\text{CH}_3$ ); 1661  $\rightarrow$  str. C=N (ring); 1441  $\rightarrow$  oxazole ring vibr.; 1380  $\rightarrow$  sym. bend.  $\text{CH}_3\text{-C-CH}_3$ ; 1165  $\rightarrow$  str. C- $\text{CH}_3$ ; 1116  $\rightarrow$  str. -C-O-; 1023  $\rightarrow$  sym str. =C-O-; 996  $\rightarrow$  C-H oop vibr. ( $\text{CH}_3$ ); 791  $\rightarrow$  rocking  $\text{CH}_3\text{-C-CH}_3$ ; 670  $\rightarrow$  wagging  $\text{CH}_3\text{-C-C-CH}_3$ ; 590  $\rightarrow$  C-C skeleton vib.; 506  $\rightarrow$  C-C skeleton vib. B) ESI-MS (+) Mass spectrum of compound **1** (base peak:  $m/z$  142)

(A)



(B)



(C)

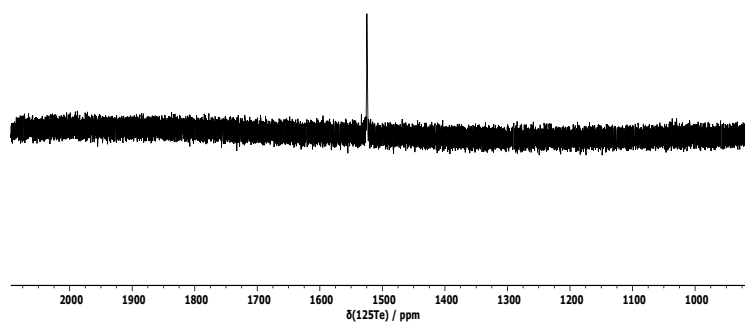
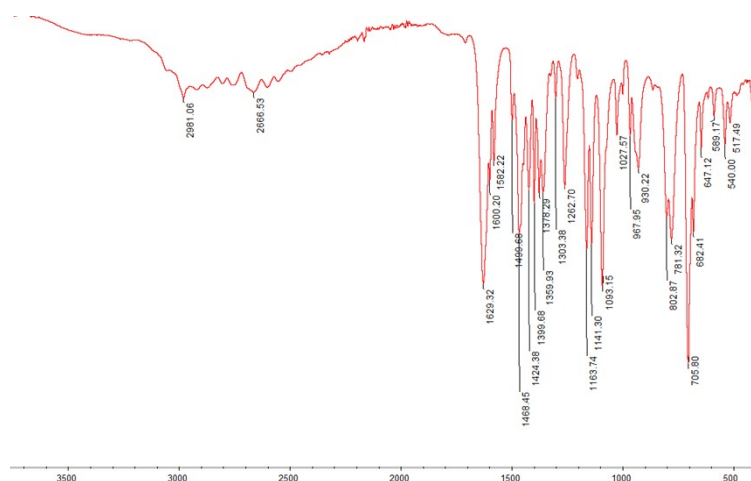
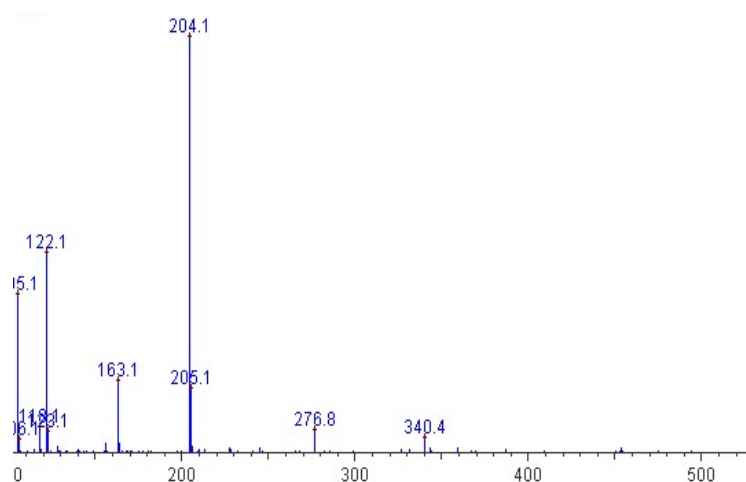


Figure S3. NMR Spectra of A)  $^1\text{H}$ , B)  $^{13}\text{C}$ , and C)  $^{125}\text{Te}$  NMR of compound **2** in  $\text{DMSO-}d_6$

(A)

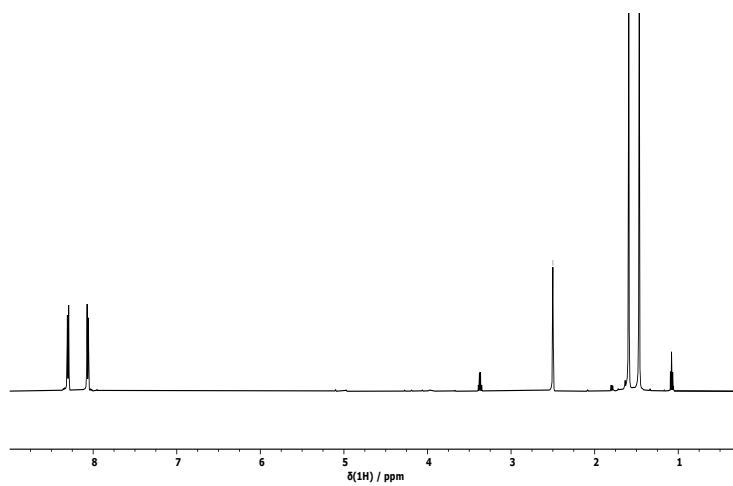


(B)



**Figure S4.** A) FTIR spectrum of compound **2**. Assignments ( $\text{cm}^{-1}$ ): 2981  $\rightarrow$  str. C-H ( $\text{CH}_3$ ); 1629  $\rightarrow$  str. C=N (ring); 1468  $\rightarrow$  oxazole ring vibr.; 1379  $\rightarrow$  sym. bend.  $\text{CH}_3\text{-C-CH}_3$ ; 1262  $\rightarrow$  Ph-C(=N)(-O) vib.; 1163  $\rightarrow$  str. C- $\text{CH}_3$ ; 1141  $\rightarrow$  str. -C-O-; 1093  $\rightarrow$  ip vibration C-H from benzene; 1027  $\rightarrow$  sym str. =C-O-; 930  $\rightarrow$  C-H oop vibr. ( $\text{CH}_3$ ); 780  $\rightarrow$  rocking  $\text{CH}_3\text{-C-CH}_3$ ; 705  $\rightarrow$  oop vibration benzene ring; 682  $\rightarrow$  wagging  $\text{CH}_3\text{-C-C-CH}_3$ ; 589  $\rightarrow$  C-C skeleton vib.; 540  $\rightarrow$  ip vibration benzene ring; 517  $\rightarrow$  C-C skeleton vib.; B) ESI-MS (+) Mass spectrum of compound **2** (base peak:  $m/z$  204)

(A)



(B)

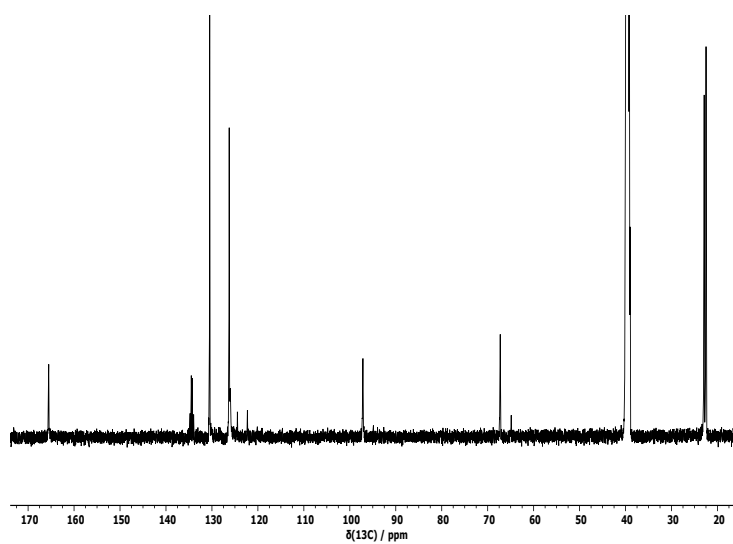
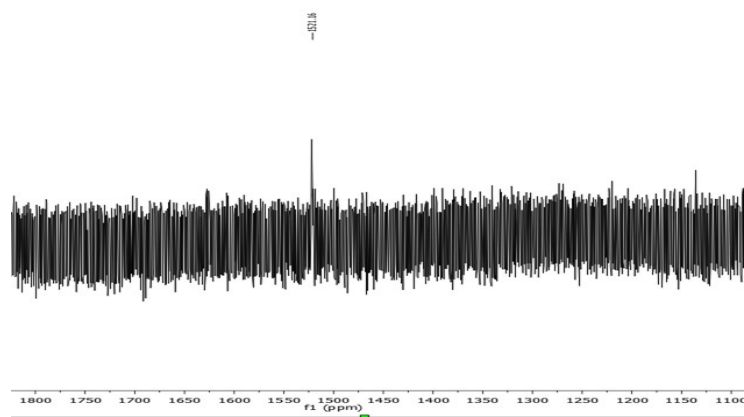


Figure S5. NMR Spectra of A)  $^1\text{H}$ , and B)  $^{13}\text{C}$  NMR of compound **3** in  $\text{DMSO-}d_6$

(A)



(B)

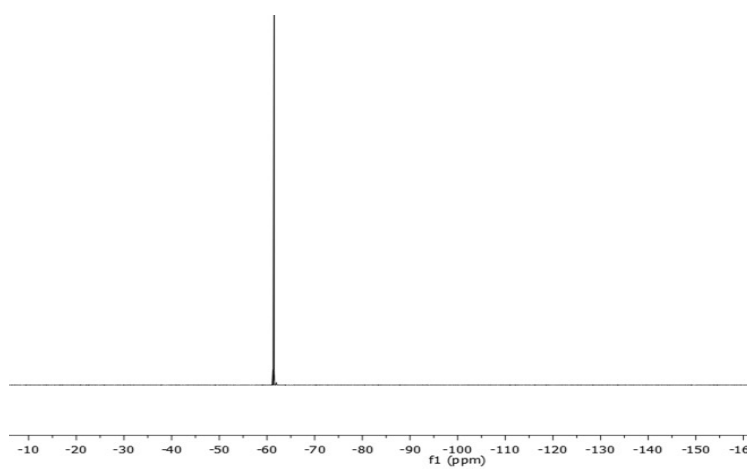
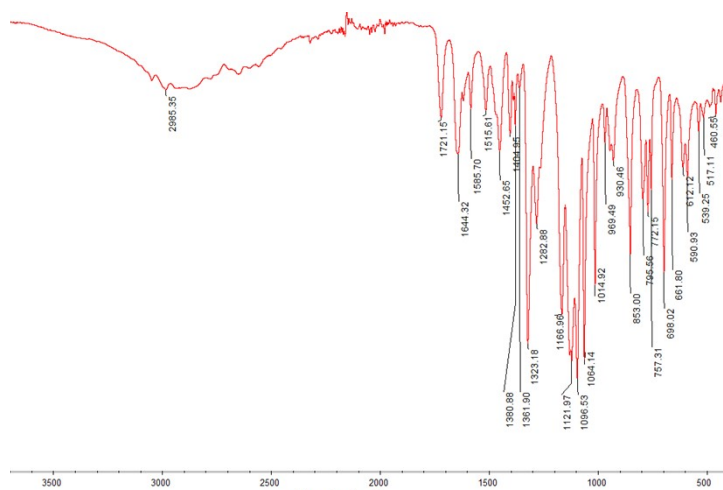
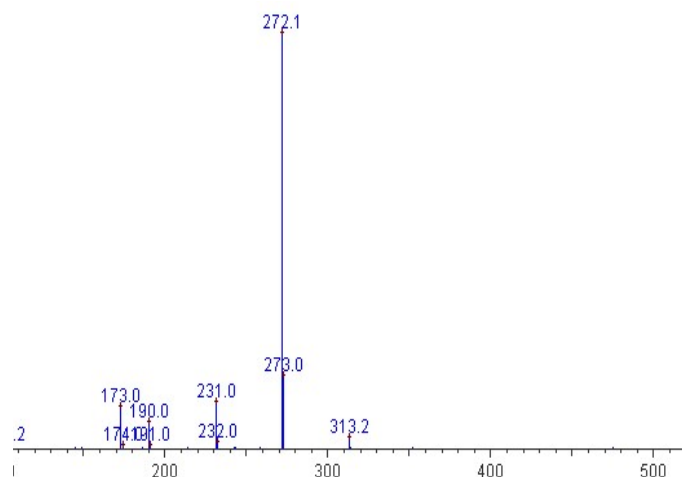


Figure S6. NMR Spectra of A)  $^{125}\text{Te}$ , and B)  $^{19}\text{F}$  NMR of compound **3** in  $\text{DMSO-}d_6$

(A)

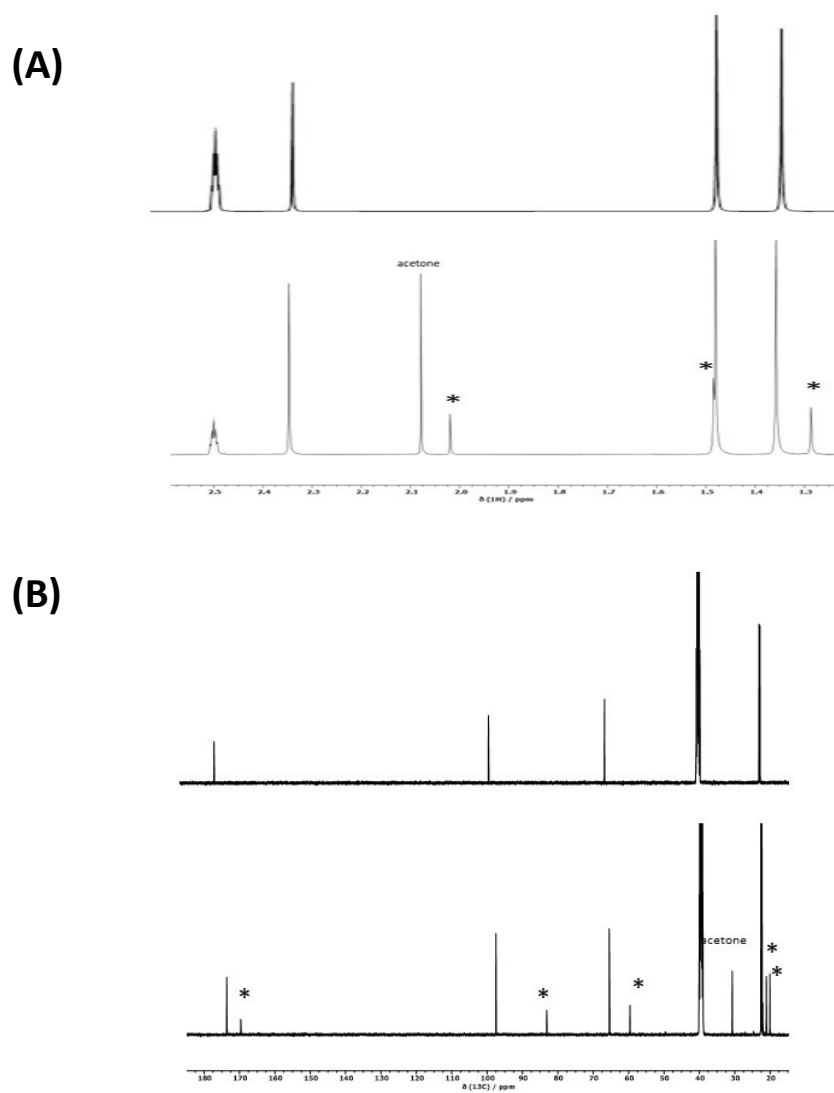


(B)

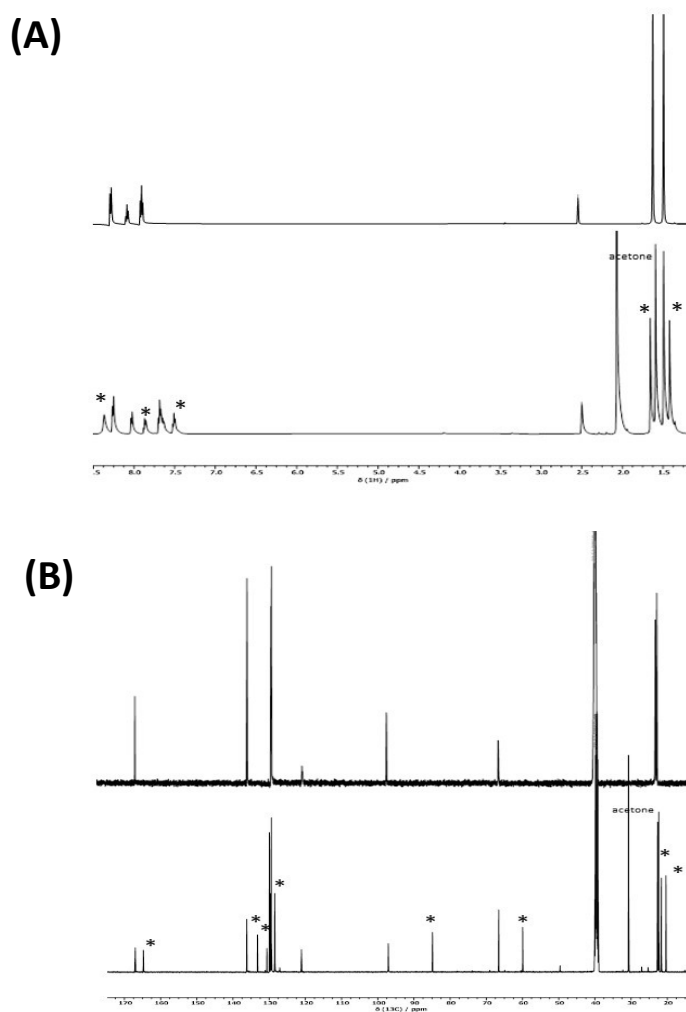


**Figure S7.** A) FTIR spectrum of compound **3**. Assignments ( $\text{cm}^{-1}$ ): 2985  $\rightarrow$  str. C-H ( $\text{CH}_3$ ); 1644  $\rightarrow$  str. C=N (ring); 1452  $\rightarrow$  oxazole ring vibr.; 1405  $\rightarrow$  sym. bend.  $\text{CH}_3\text{-C-CH}_3$ ; 1282  $\rightarrow$   $\text{CF}_3\text{Ph-C(=N)(-O)}$  vibr.; 1167  $\rightarrow$  str. C- $\text{CH}_3$ ; 1122  $\rightarrow$  str. -C-O-; 1096  $\rightarrow$  ip vibration C-H from benzene; 1014  $\rightarrow$  sym str. =C-O-; 969  $\rightarrow$  C-H oop vibr. ( $\text{CH}_3$ ); 853  $\rightarrow$  oop vibration benzene ring (H-C-C-H in 1,4-disubstituted benzenes); 795  $\rightarrow$  rocking  $\text{CH}_3\text{-C-CH}_3$ ; 772  $\rightarrow$  C-F; 757  $\rightarrow$  - $\text{CF}_3$ ; 698  $\rightarrow$  oop vibration benzene ring; 662  $\rightarrow$  wagging  $\text{CH}_3\text{-C-C-CH}_3$ ; 591  $\rightarrow$  C-C skeleton vibr.; 539  $\rightarrow$  ip vibration benzene ring; 517  $\rightarrow$  C-C skeleton vibr.; B) ESI-MS (+) Mass spectrum of compound **3** (base peak:  $m/z$  272)

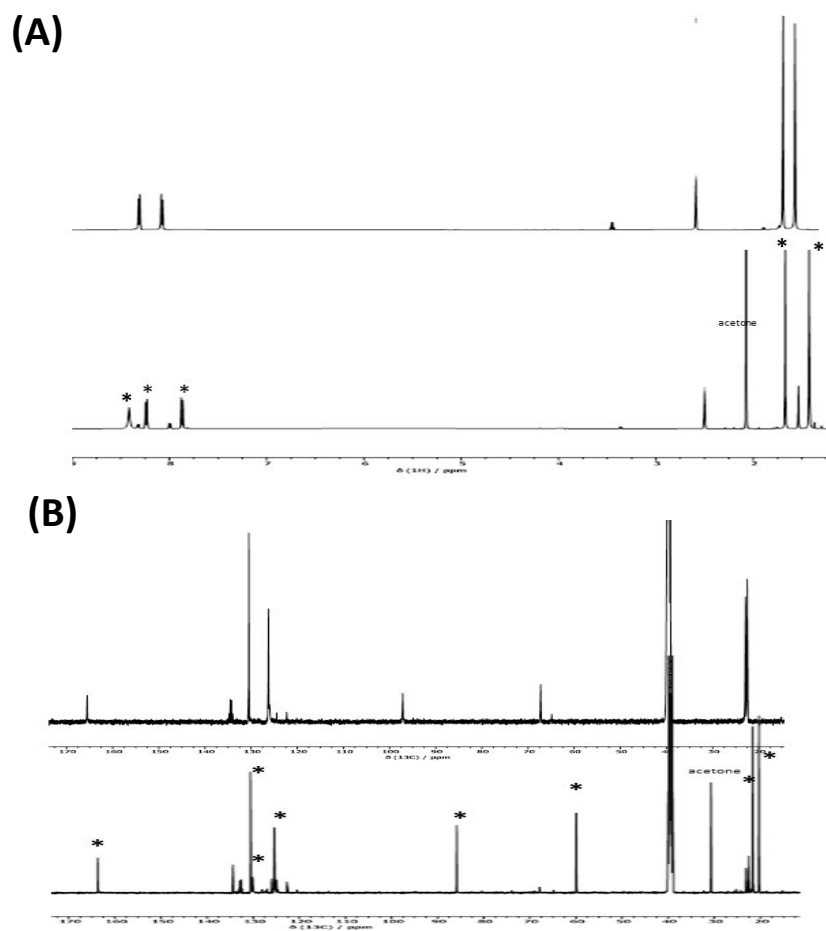




**Figure S8.** Decomposition experiment for compound **1** followed via  $^1\text{H}$  NMR (A) and  $^{13}\text{C}$  NMR (B) spectra in  $\text{DMSO-}d_6$ . For each analysis, the top spectra represent the initial situation, the bottom spectra are related to the compound after three days in water at room temperature. The peaks highlighted with \* indicate the decomposed product.

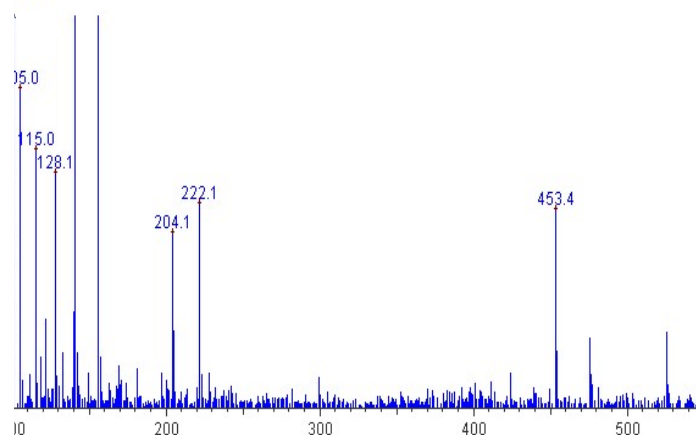


**Figure S9.** Decomposition experiment for compound **2** followed via  $^1\text{H}$  NMR (A) and  $^{13}\text{C}$  NMR (B) spectra in  $\text{DMSO-}d_6$ . For each analysis, the top spectra represent the initial situation, the bottom spectra are related to the compound after three days in water at room temperature. The peaks highlighted with \* indicate the decomposed product.

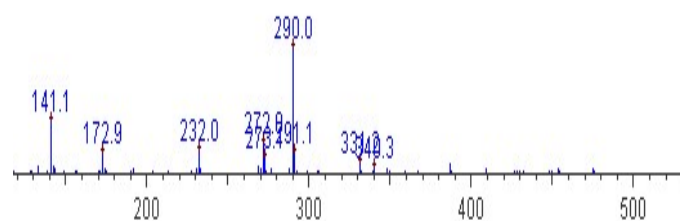


**Figure S10.** Decomposition experiment for compound **3** followed via  $^1\text{H}$  NMR (A) and  $^{13}\text{C}$  NMR (B) spectra in  $\text{DMSO-}d_6$ . For each analysis, the top spectra represent the initial situation, the bottom spectra are related to the compound after three days in water at room temperature. The peaks highlighted with \* indicate the decomposed product.

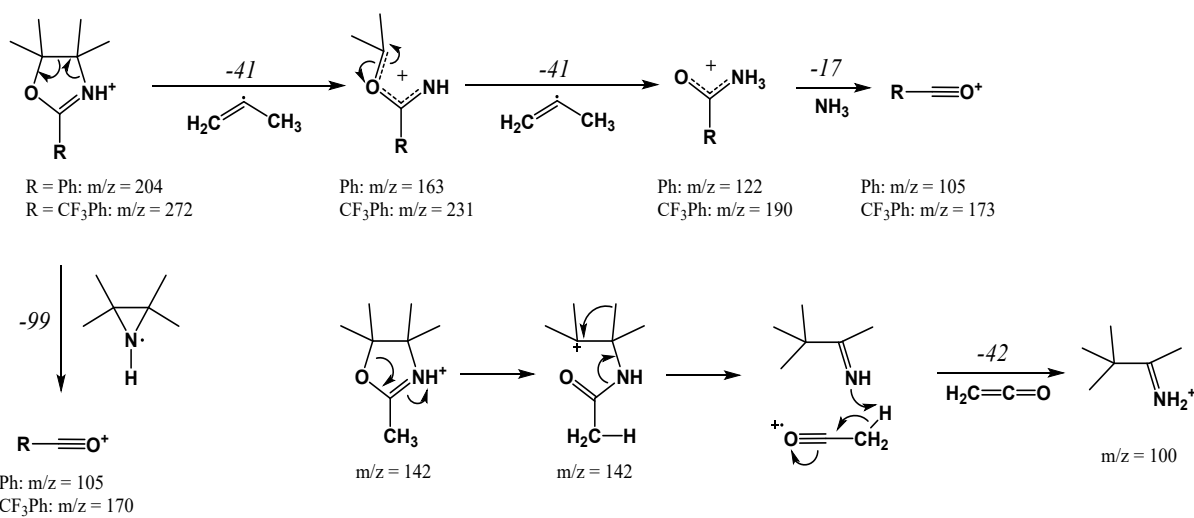
(A)



(B)



**Figure S11.** ESI-MS spectrum (+) of A) compound **2**, and B) compound **3** after decomposition.



**Figure S12.** Proposed fragmentation pattern for compounds **1-3** with the mass peaks assigned in the ESI-MS spectra reported in Figures **S2**, **S4** and **S7** (Ref.: S. Osman, C.J. Dooley, T.A. Foglia, and L.M. Gregory, *Org. Mass. Spectrom.* **1970**, *4*, 139-145).

**Table S1.** Selected distances [Å] of compounds **1**, **2** and **3**.

	<b>1</b>	<b>2</b>	<b>3</b>
Te1–Cl1	2.5431(4)	2.4557(4)	2.5271(3)
Te1–Cl2	2.5380(4)	2.5341(4)	2.5464(3)
Te1–Cl3	2.5494(4)	2.6432(4)	2.5385(3)
O1–C2	1.5111(17)	1.5063(15)	1.5035(13)
O1–C5	1.3191(17)	1.3138(16)	1.3120(14)
C2–C3	1.5577(19)	1.5548(18)	1.5609(16)
C2–C6	1.512(2)	1.5125(19)	1.5098(17)
C2–C7	1.519(2)	1.5184(18)	1.5146(17)
C3–N4	1.4817(17)	1.4938(16)	1.4841(14)
C3–C8	1.531(2)	1.5287(18)	1.5294(16)
C3–C9	1.520(2)	1.5189(17)	1.5248(16)
N4–C5	1.2887(19)	1.2953(17)	1.2946(15)
C5–C10	1.477(2)	1.4636(18)	1.4596(15)
C10–C11		1.4001(18)	1.3967(16)
C10–C15		1.3920(19)	1.3998(16)
C11–C12		1.3853(19)	1.3886(17)
C12–C13		1.3931(19)	1.3883(19)
C13–C14		1.3884(19)	1.3897(18)
C14–C15		1.3915(19)	1.3896(16)
C13–C16		1.5013(18)	
C16–F17		1.3304(16)	
C16–F18		1.3382(16)	
C16–F19		1.3380(16)	

**Table S2.** Selected angles [°] of compounds **1**, **2** and **3**.

	<b>1</b>	<b>2</b>	<b>3</b>
C5–O1–C2	107.36(10)	107.31(10)	107.67(9)
O1–C2–C3	101.41(10)	101.38(9)	101.46(9)
O1–C2–C6	107.73(11)	107.46(10)	106.98(10)
O1–C2–C7	104.63(11)	104.96(10)	104.98(9)
C6–C2–C3	115.25(12)	115.86(11)	116.09(10)
C6–C2–C7	111.61(12)	111.80(11)	111.91(11)
C7–C2–C3	114.82(12)	113.98(11)	113.94(10)
N4–C3–C2	99.64(11)	98.66(9)	99.61(9)
C9–C3–C2	114.01(12)	113.89(11)	114.25(10)
C8–C3–C2	114.06(12)	114.14(11)	113.42(10)
N4–C3–C9	110.06(12)	111.41(10)	111.06(10)
N4–C3–C8	107.37(11)	106.59(10)	107.37(10)
C9–C3–C8	110.89(12)	111.25(11)	110.47(10)
C5–N4–C3	111.31(12)	110.72(11)	110.79(10)
N4–C5–O1	114.03(13)	113.77(12)	114.25(10)
N4–C5–C10	127.05(13)	127.71(12)	127.07(10)
O1–C5–C10	118.92(13)	118.52(11)	118.66(10)
C15–C10–C11		121.03(12)	120.79(11)
C15–C10–C5		120.57(12)	120.11(10)
C11–C10–C5		118.40(12)	119.09(10)
C12–C11–C10		119.61(12)	119.21(11)
C11–C12–C13		119.15(12)	120.16(11)
C14–C13–C12		121.44(12)	120.61(11)
C13–C14–C15		119.58(13)	119.98(11)
C14–C15–C10		119.18(12)	119.24(11)
C14–C13–C16		120.22(12)	
C12–C13–C16		118.33(12)	