SUPPLEMENTARY MATERIAL

Anti-cancer activity of di- and tri-organotin(IV) compounds with D-(+)-Galacturonic acid on human tumor cells.

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TABLE S1 Selected FT-IR bands (cm^{-1}) for the already synthesized $R_2SnGala$ (R=Me,n-Bu,Ph) compounds.[1]

Compound	ν(OH)	ν(COOH)	ν_{as}(COO)	ν_s(COO)	Δν	ν_{as}(Sn-C)	ν_s(Sn-C)
$H_2GalA-H_2O$	3441vw[a] 3364vw 3320vw	1713vw	--	--			
$Me_2Sn(D-GalA)$	3405m	--	1642ms	1370m	272	594m	527s
$Bu_2Sn(D-GalA)$	3391s	--	1613ms	1376m	237	584m	530m
$Ph_2Sn(D-GalA)$	3314m 3231m	--	1565m	1366m	199	278m	247s

[a]s=strong; ms=medium-strong; m=medium; w=weak; vw=very-weak

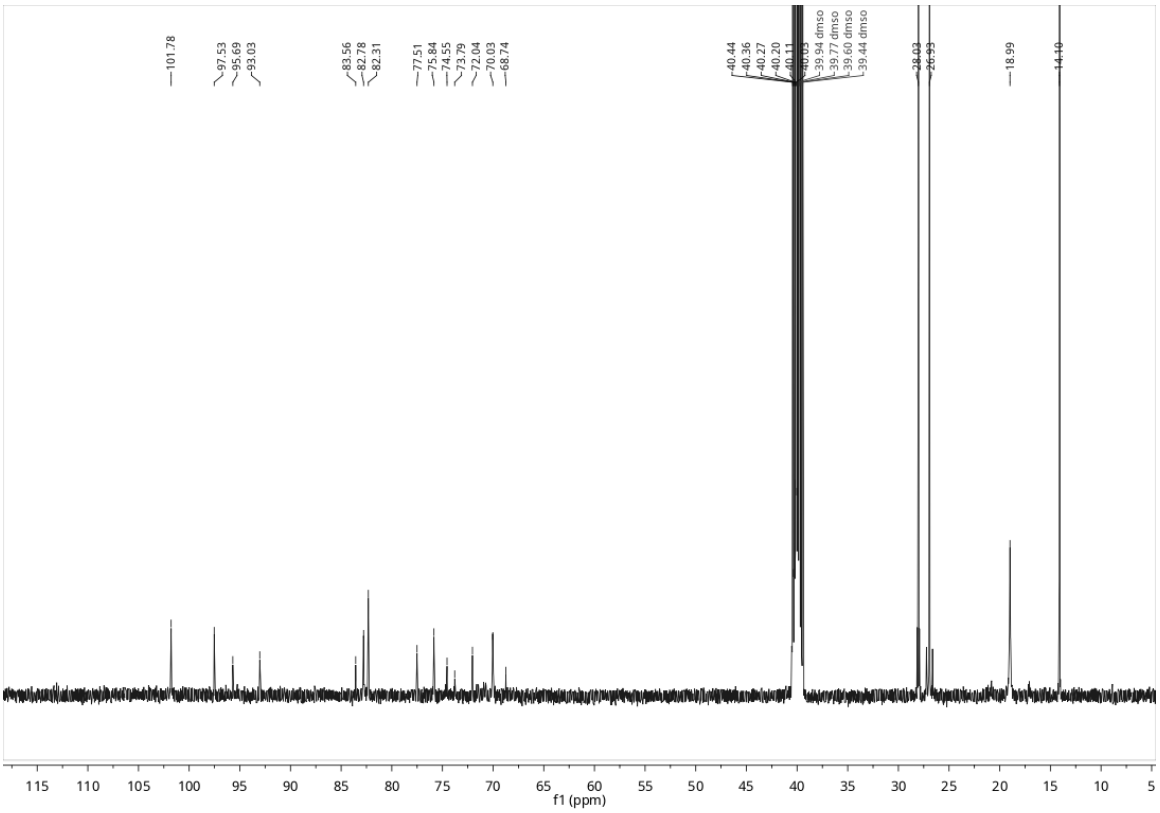

FIG. S1: $^{13}C\{^1H\}$ spectrum of n-$Bu_3SnGala$ (5) in DMSO-d_6 acquired at 125.73 MHz on a VARIAN 500 MHz Magnet with 16 scans. Concentration *ca.* 50 mM.

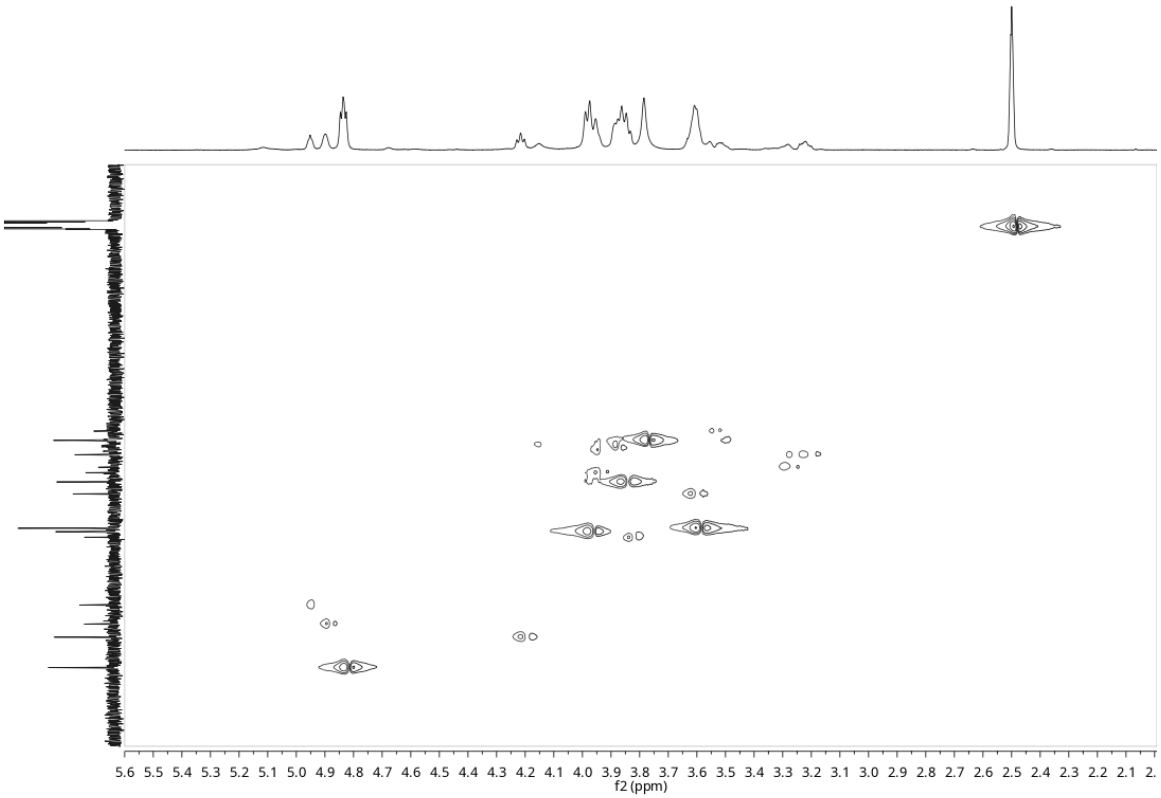

FIG. S2:[^{1}H,^{13}C]-gHSQCAD spectrum of n-Bu$_3$SnGala (5) in DMSO-d$_6$.

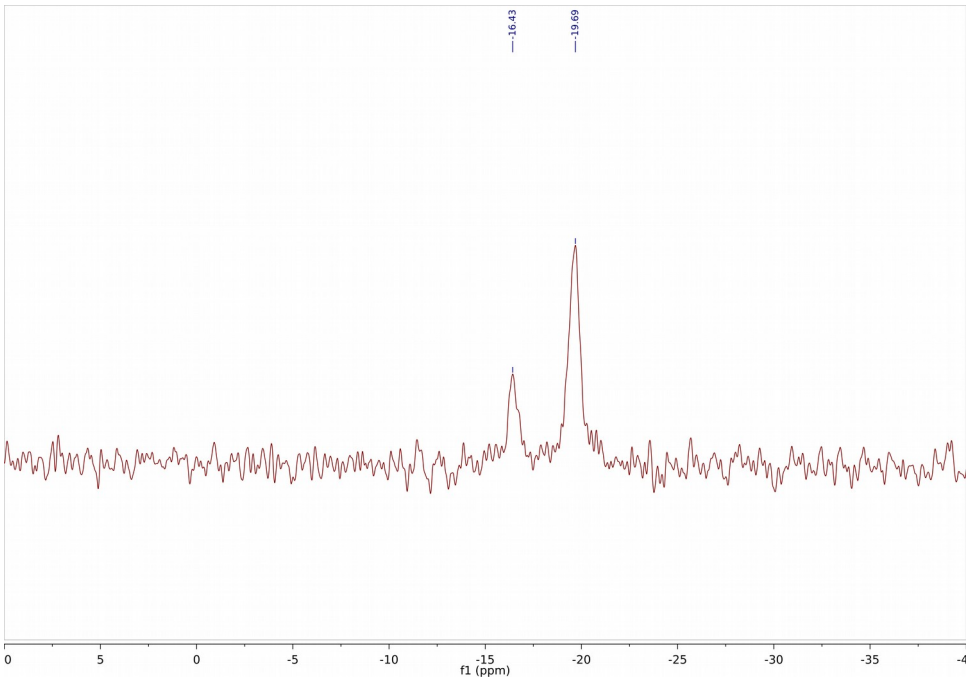

FIG. S3 ^{119}Sn{^{1}H} spectrum of n-Bu$_3$SnGala (5) in DMSO-d$_6$.

n-Bu$_3$SnGala (5) stability

Keeping in mind the tendency of $R_3Sn(IV)$ carboxylates to decompose, in some cases, in aqueous environment[2], for **5**, we also monitored its behavior DMSO-d_6, at 24, 48, and72 h, and after adding D_2O to the DMSO-d_6 solution at 24 h and 72 h. We monitored two DMSO-d_6/H_2O solutions: **(a)** *ca.* 1:4=D_2O:DMSO-d_6 (after 48 h) and **(b)** *ca.* 4:1=D_2O:DMSO-d_6 (after 72 h).

For DMSO-d_6 solution, the shape and the chemical shifts of the ^1H, ^{13}C and ^{119}Sn spectra in DMSO-d_6 remained unaffected during the monitoring time. NMR $^{119}Sn\{^1H\}$spectrum of **5** only in DMSO-d_6 is given in Figure S3. For solution **(a)** we observed in the ^1H spectrum, already after 48 h, the appearance of broad signals in the 3.4-4.7 ppm region. For the same solution, the NMR $^{119}Sn\{^1H\}$ spectrum (Figure S5) showed two more signals, caused by the presence of D_2O, at -15.33 ppm (LW ≈ 260 Hz) and -18.53 ppm (LW ≈ 180 Hz), besides the ones at -16.84 (LW ≈ 230 Hz) and -19.94 ppm (LW ≈ 130 Hz), already observed in DMSO-d_6. For solution **(b)**, after 72 h, in the ^1H spectrum, the small signals observed in solution **(a),** are almost prevalent and well resolved (Figure S4), and they resemble the already observed patterns in water for compounds **4** and **1** compounds[1], indicating that the ligand was still coordinated. Also a change in the isomeric/anomeric ratio was observed. Finally, the ^{119}Sn NMR spectrum (Figure S6), displayed only two signals at -2.74 ppm (LW ≈ 530 Hz), and -16.63 ppm (LW ≈ 700 Hz). The slight deshielded δ(^{119}Sn) values in solution b), compared with solution a), are in accord with a change of coordinated solvent to tin from DMSO-d_6 to D_2O. These findings, at the experimental conditions used, point only to a solvent effect, characterized by: i) a slight deshielding of the ^{119}Sn signlas, as a results of the (partial) displacement of DMSO_d_6 by D_2O in the tin coordination sphere, and ii) a broadening of the ^{119}Sn signals in the prevalent D_2O mixtures due to the different anomerization kinetics.

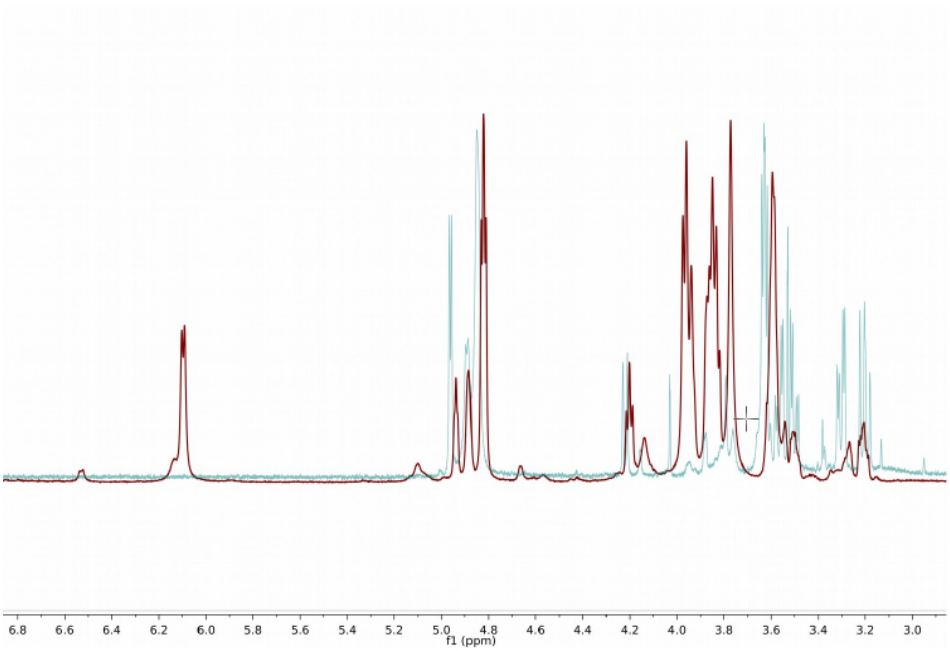

FIGURE S4: Superimposed presaturated spectra of n-Bu$_3$SnGala (5) in DMSO-d_6 (red spectrum) and DMSO-d_6/D_2O (*ca.* 1:4; solution (b) in the manuscript) after 72 h (cyan spectrum).

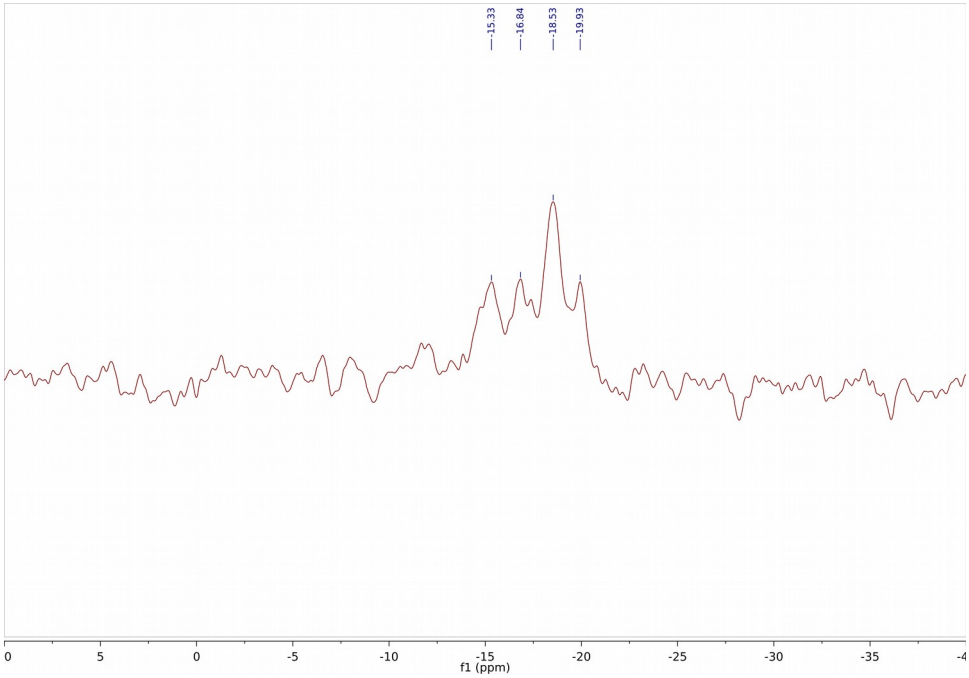

FIG. S5: $^{119}Sn\{^{1}H\}$ spectrum of n-$Bu_3SnGala$ (5) in DMSO-d_6/H_2O(ca. 4:1) after 72 h.

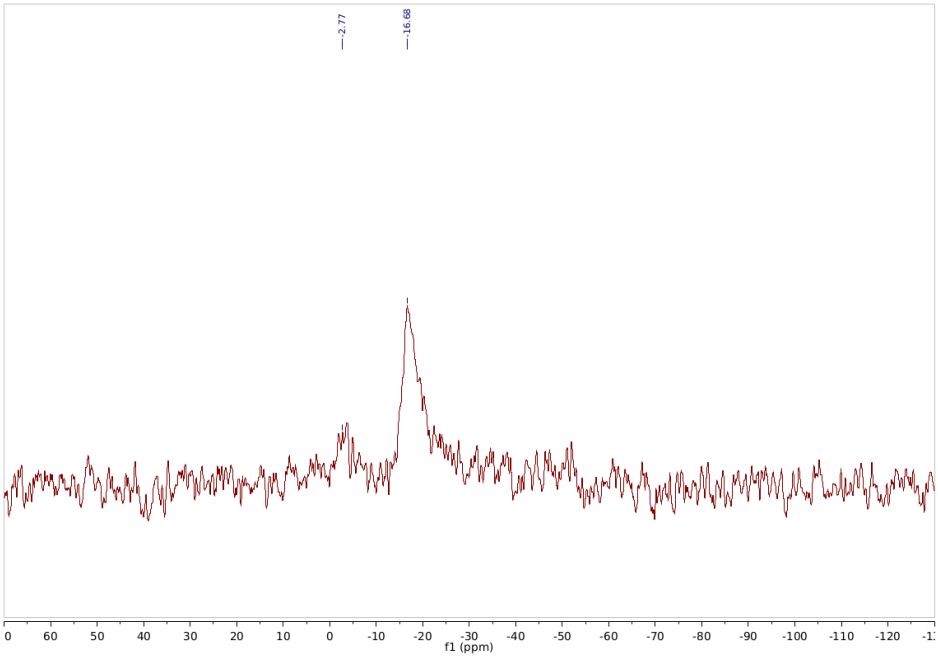

FIG. S6: $^{119}Sn\{^{1}H\}$ spectrum of n-$Bu_3SnGala$ (5) in DMSO-d_6/H_2Ov(ca. 1:4) after 72 h.

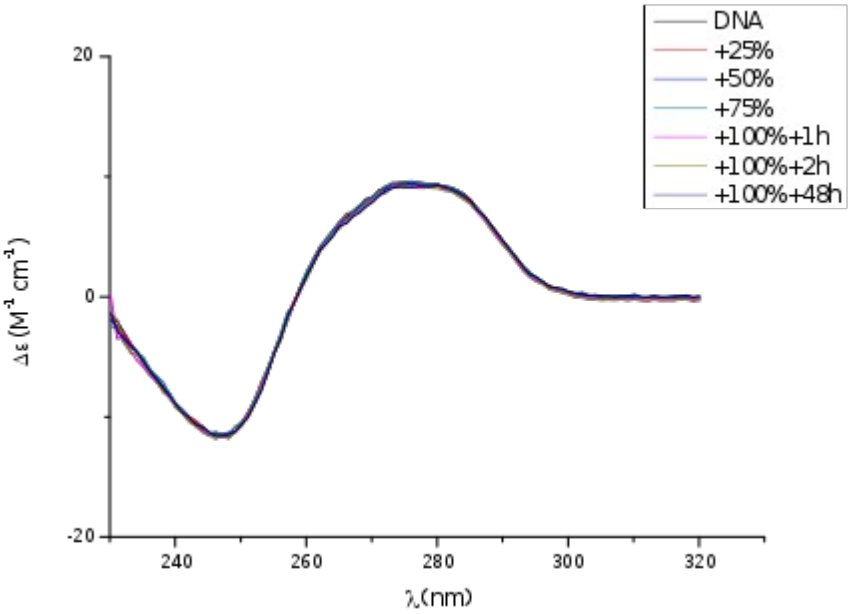

FIG. S7 The graph shows the typical signature of the presence of a B-type helix, unaffected by the incremental additions of n-Bu_3SnGALA up to 1 Sn every 2 P (phosphates) per base-pair.

REFERENCES

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