

SUPPORTING INFORMATION

Furylated flavonoids: biobased building blocks produced by condensed tannins depolymerization

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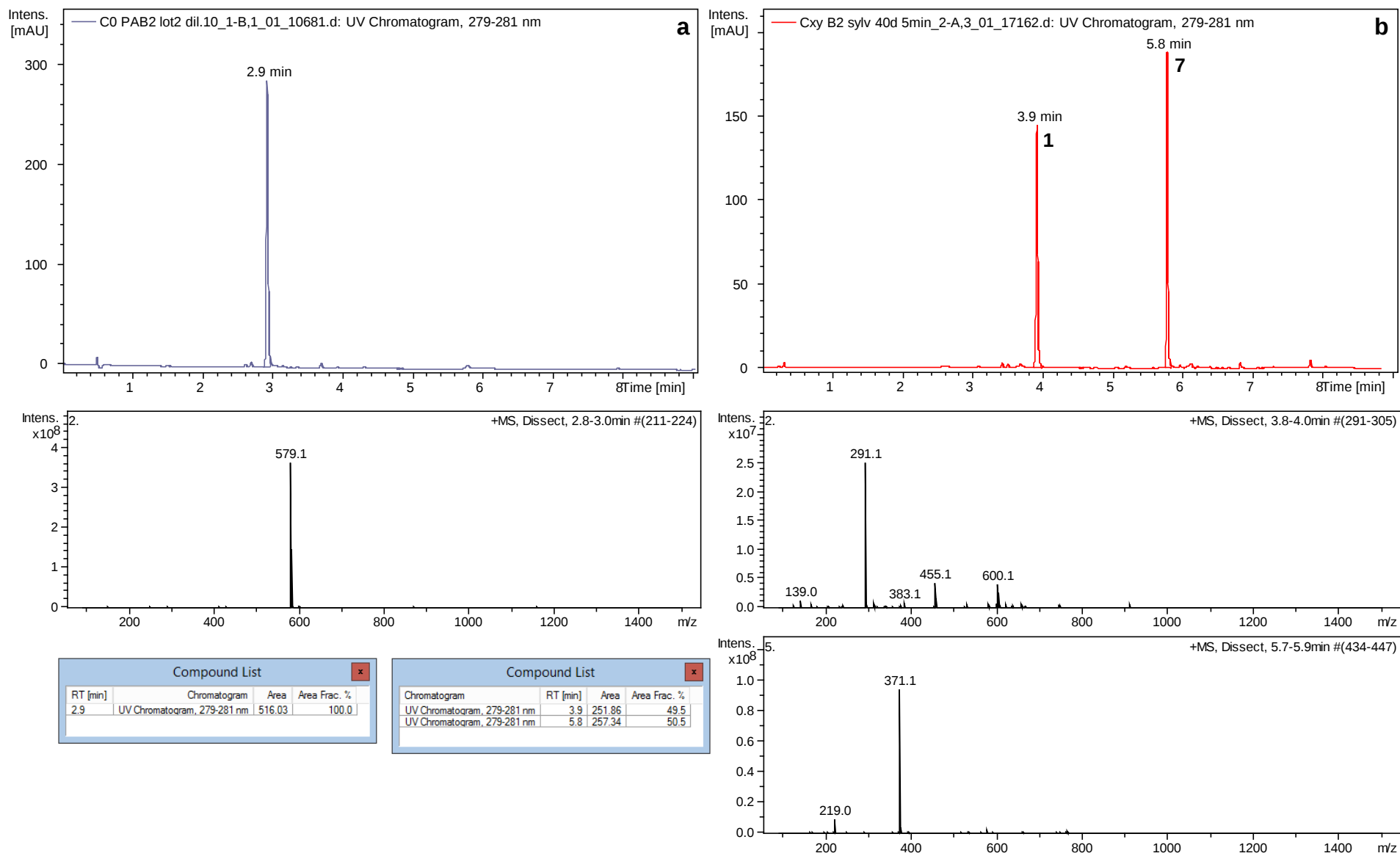
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Number of figures : 6



Figures S1. UV chromatograms at 280 nm and matching MS(+) spectra of integrated peaks of procyanidin B2 at 0 min (a) and products after 10 min of complete B2 sylvanolsysis at 40°C (b). The peak area are displayed in the tables referred to as “Compound List”.

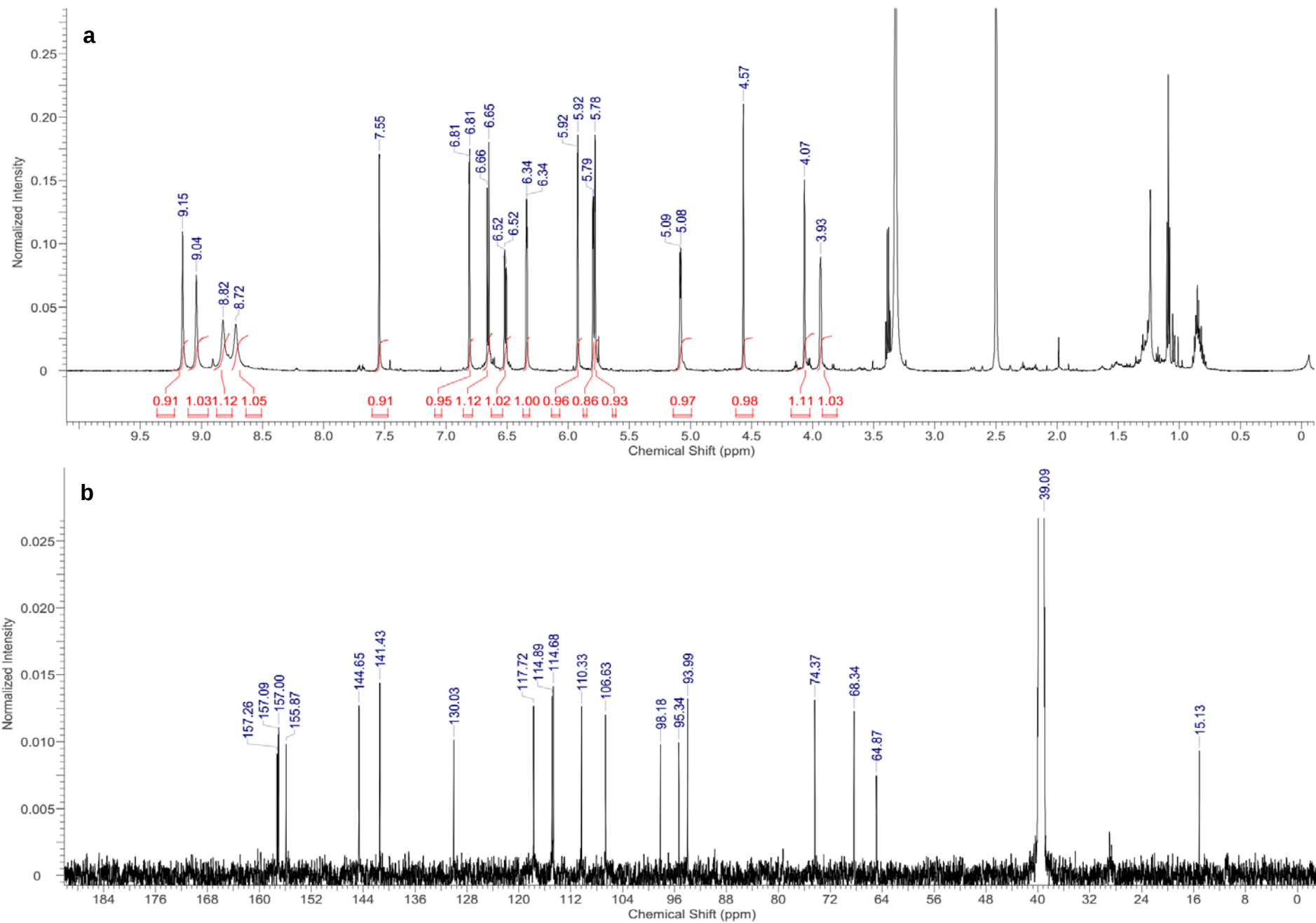
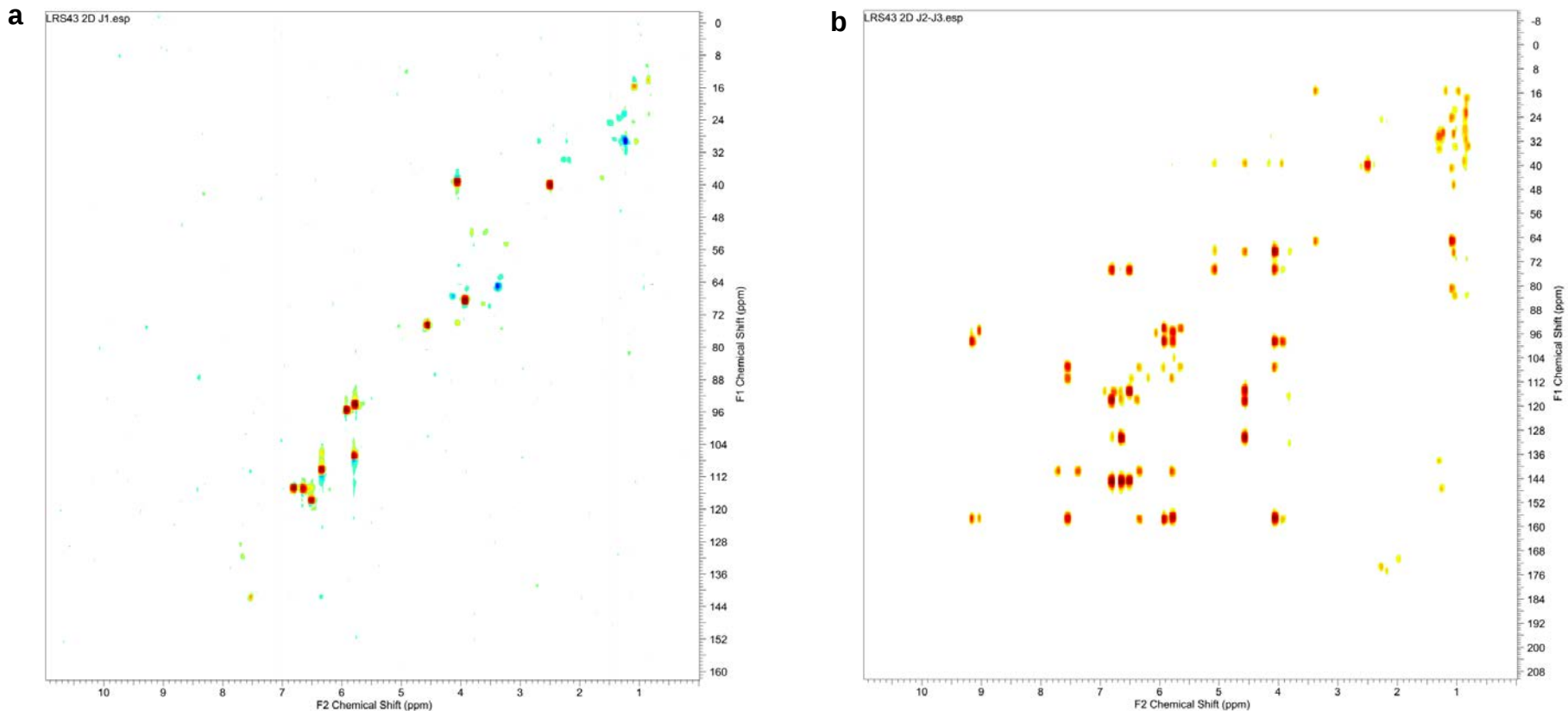


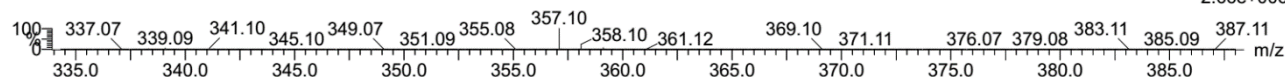
Figure S2. (a) ^1H and (b) ^{13}C NMR chemical shifts of 4-(furan-2-yl)-(epi)catechin (**5**).



c Monoisotopic Mass, Even Electron Ions
 863 formula(e) evaluated with 2 results within limits (up to 20 closest results for each mass)
 Elements Used:
 C: 1-150 H: 1-200 N: 0-30 O: 0-50
 SYNAPT G2-S#UEB205
 Y-HF15022302 4 (0.155) Cm (1:5)

LS108

23-Feb-2015
 1: TOF MS ES+
 2.66e+006



Minimum:
 Maximum:

-1.5
 1.0 1.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
357.0976	357.0974	0.2	0.6	11.5	1855.8	0.004	99.55	C19 H17 O7
	357.0979	-0.3	-0.8	4.5	1861.2	5.408	0.45	C4 H13 N12 O8

Figure S3. (a) HSQC-DEPT, (b) HMBC and (c) HMRS spectra of 4-(furan-2-yl)-(epi)catechin (**5**)

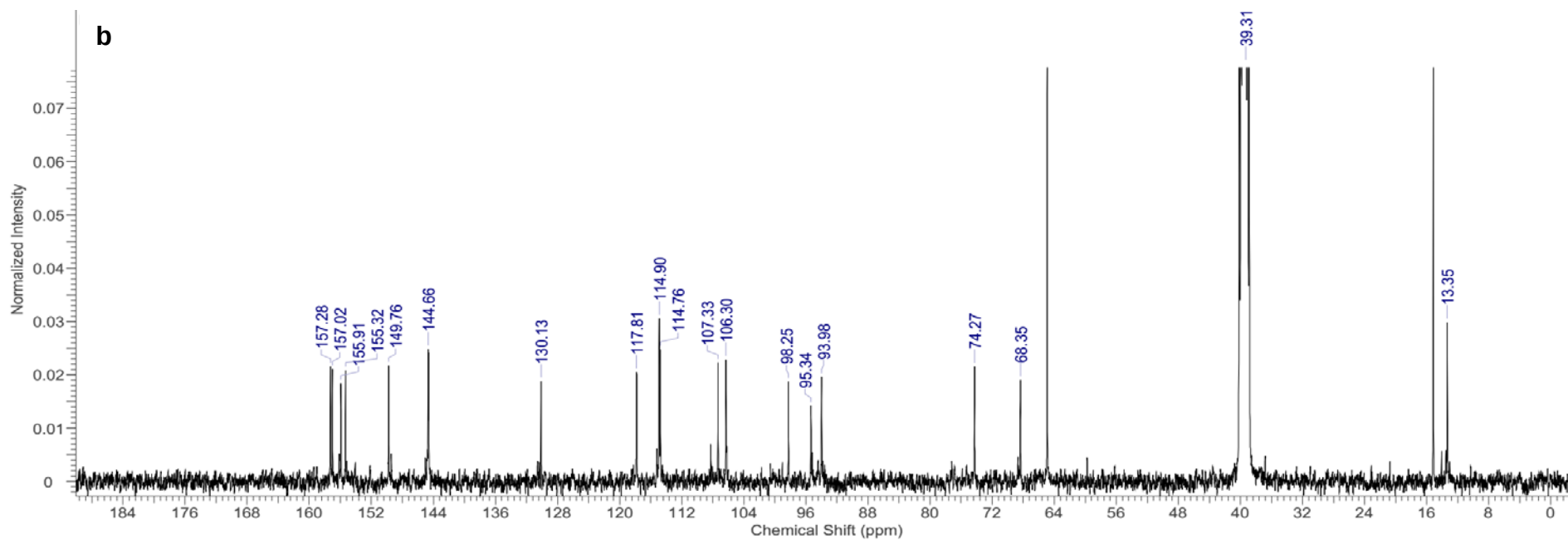
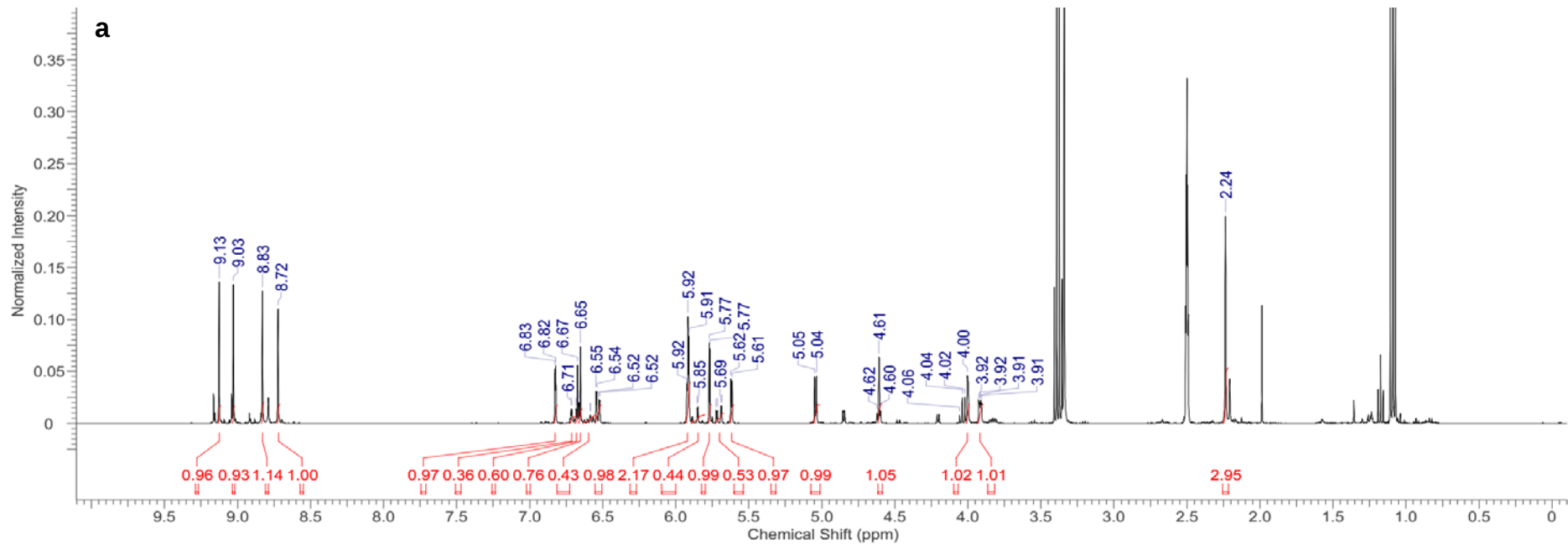
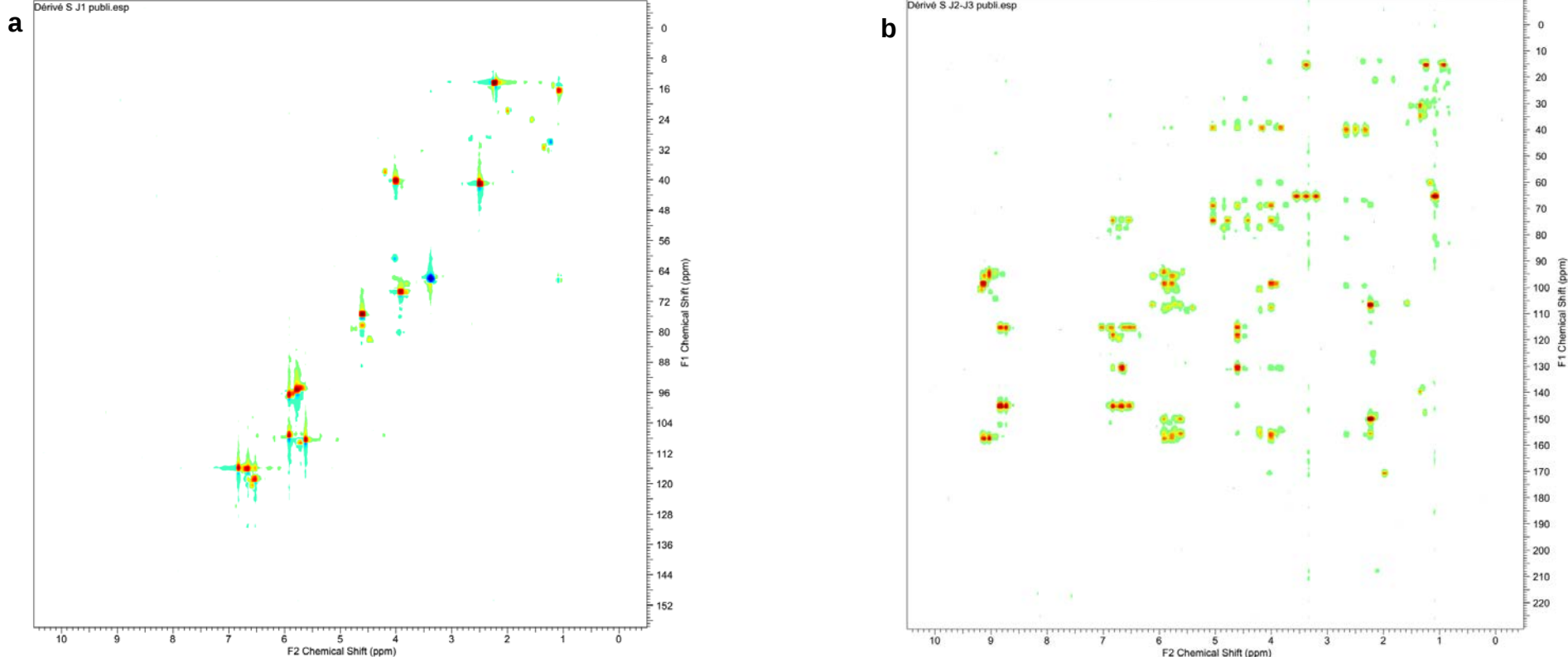


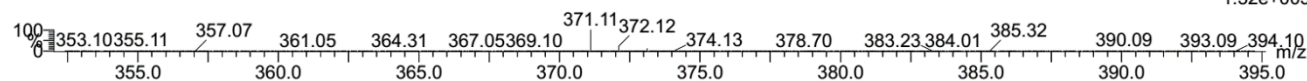
Figure S4. (a) ^1H and (b) ^{13}C NMR chemical shifts of 4-(5-methylfuran-2-yl)-(epi)catechin (**7**).



c Monoisotopic Mass, Even Electron Ions
 79 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
 Elements Used:
 C: 1-100 H: 1-150 O: 1-50
 SYNAPT G2-S#NotSet
 Y-HF14060301 53 (0.970)

LR

03-Jun-2014
 1: TOF MS ES+
 1.52e+005



Minimum: -5.0
 Maximum: 1.0 1.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
371.1128	371.1131	-0.3	-0.8	11.5	1243.2	n/a	n/a	C20 H19 O7

Figure S5. (a) HSQC-DEPT, (b) HMBC and (c) HMRS spectra of 4-(5-methylfuran-2-yl)-(epi)catechin (**7**).

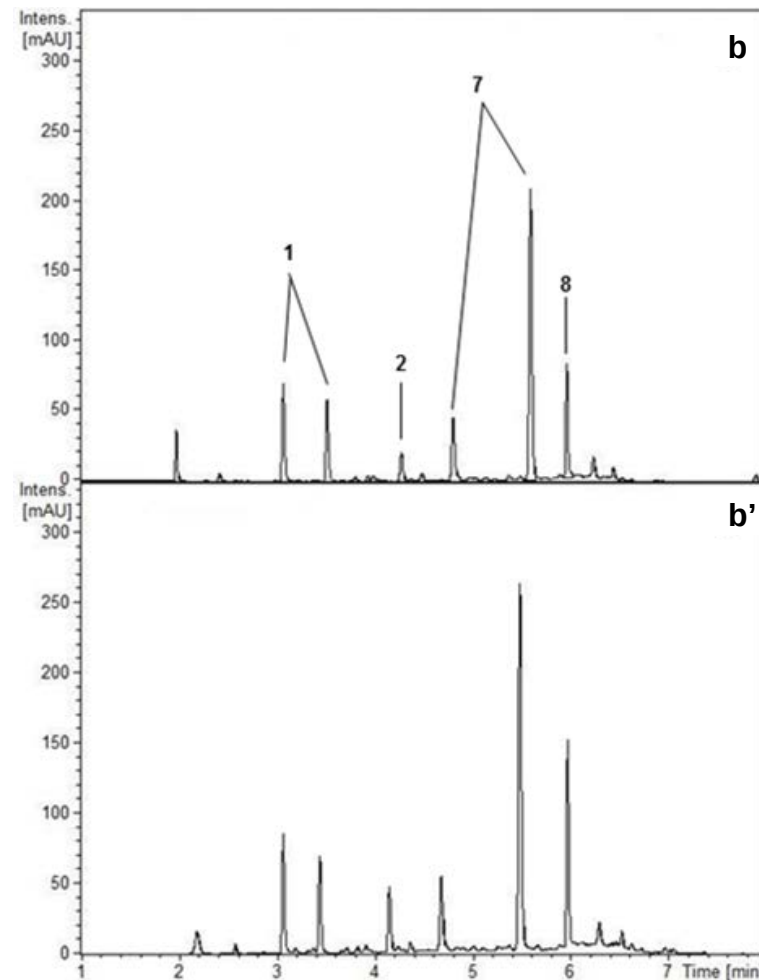
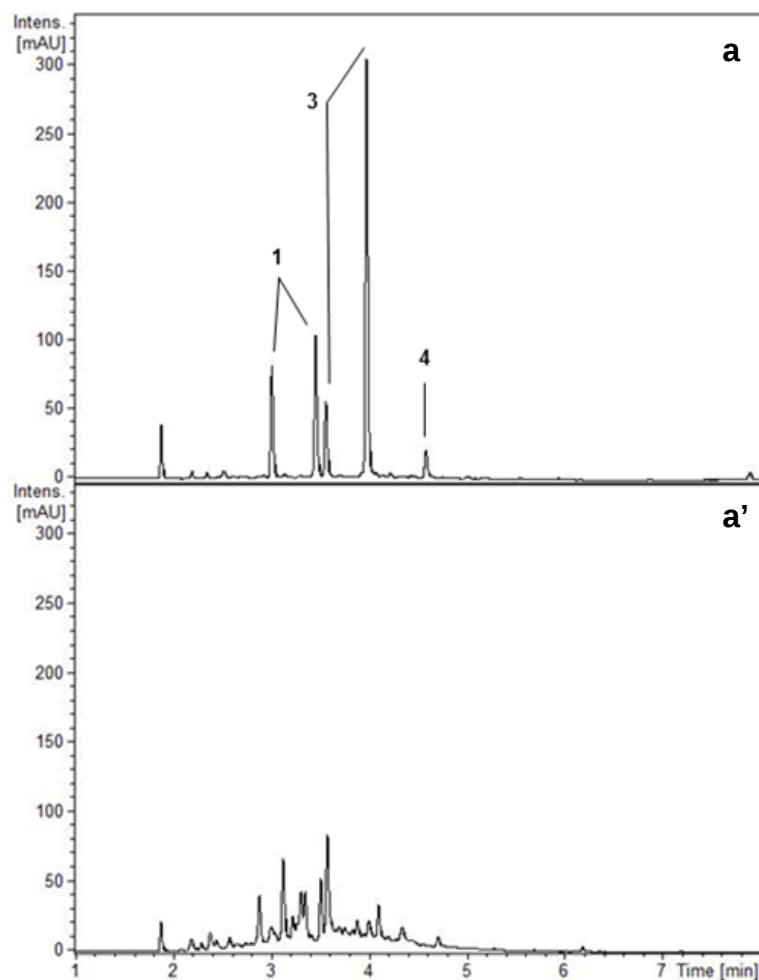


Figure S6. UV chromatograms at 280 nm of the isolated products from tannin preparative mercaptolysis (left) and sylvanols (right) before (a and b, respectively) and after (a' and b', respectively) 19 h at RT in borate buffer, pH 9.0, showing the low stability of the mercaptolysis products and the high stability of the furylated derivatives