Supporting Information

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Biotransformation of Perrottetin F by *Aspergillus niger*: New Bioactive Secondary Metabolites

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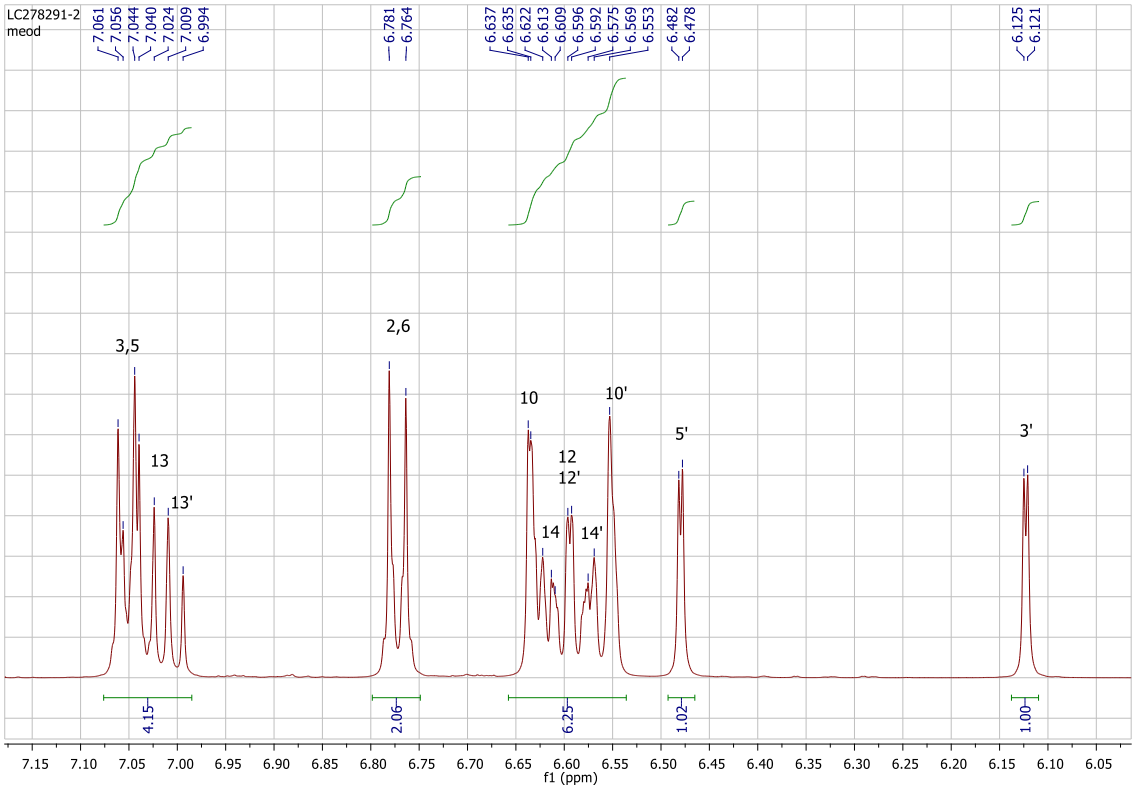


Figure S1: ^{1}H NMR spectrum of perrottetin F (**1**) (from δ_H 6.00 ppm to δ_H 7.20 ppm)

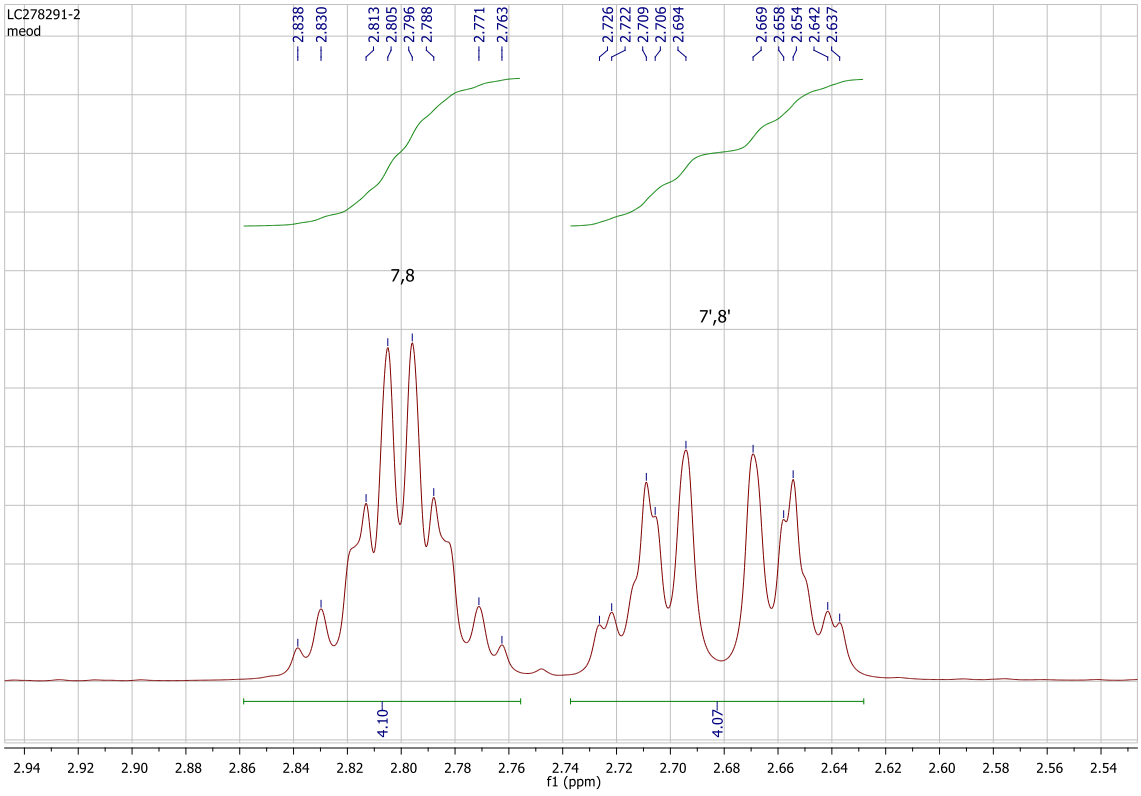


Figure S2: ^{1}H NMR spectrum of perrottetin F (**1**) (from δ_H 2.53 ppm to δ_H 2.95 ppm)

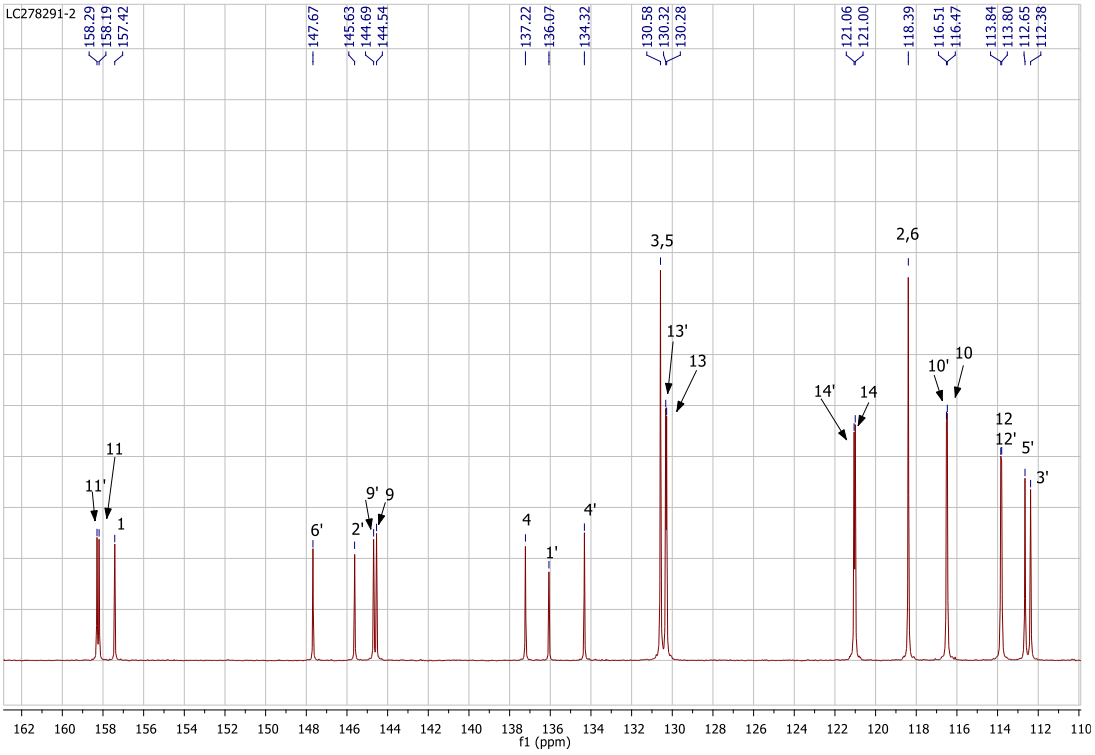


Figure S3: ^{13}C NMR spectrum of perrottetin F (**1**) (from δ_C 110 ppm to δ_C 163 ppm)

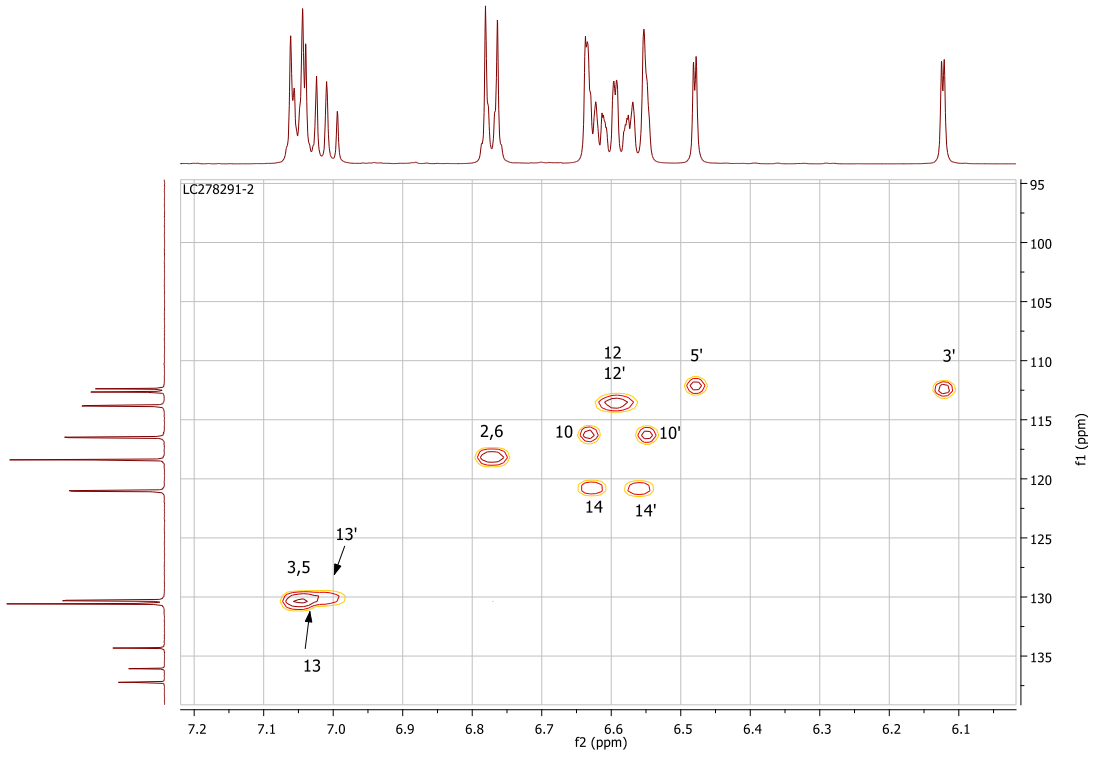


Figure S4: HSQC spectrum of perrottetin F (**1**) (from δ_C 95 ppm to δ_C 140 ppm and from δ_H 6.00 ppm to 7.22 ppm)

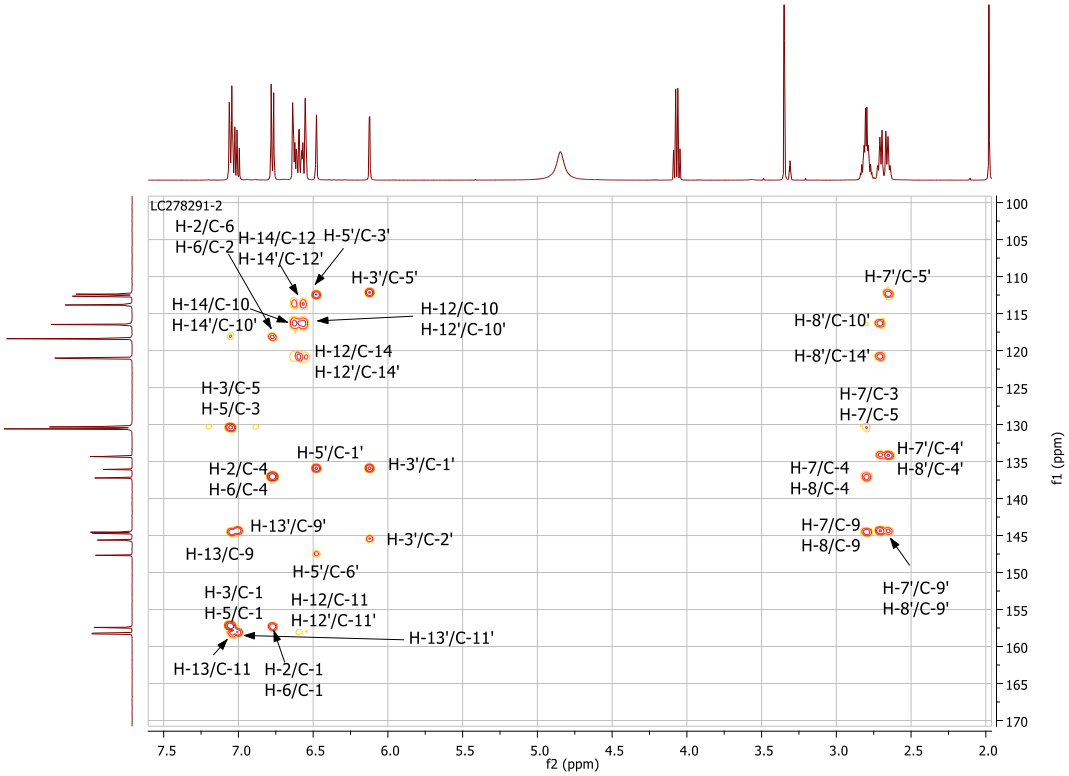


Figure S5: HMBC spectrum of perrottetin F (**1**) (from δ_C 100 ppm to δ_C 170 ppm and from δ_H 2.00 ppm to 7.55 ppm)

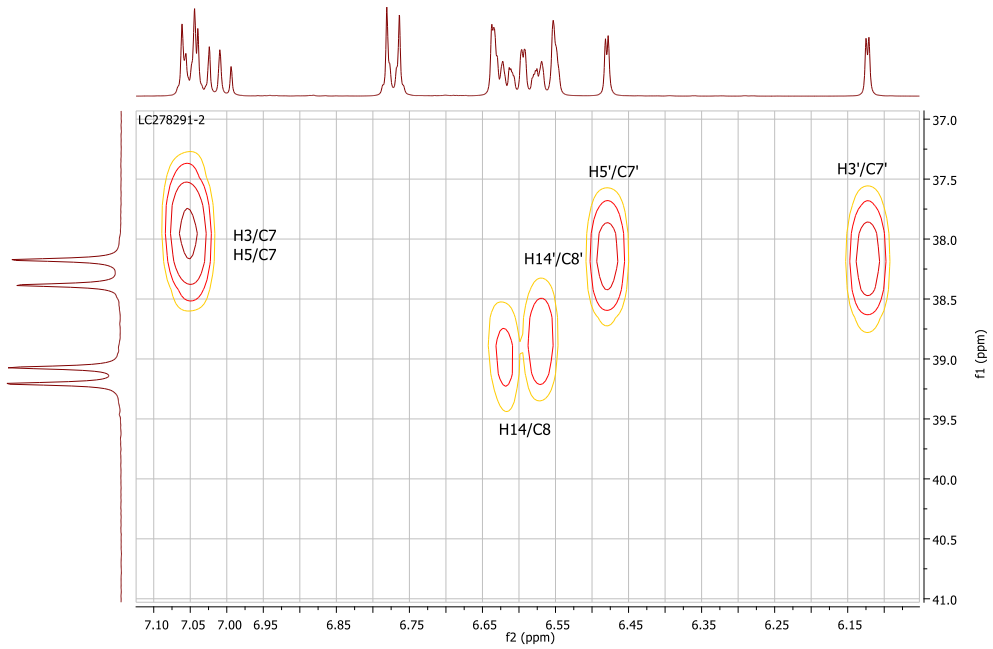
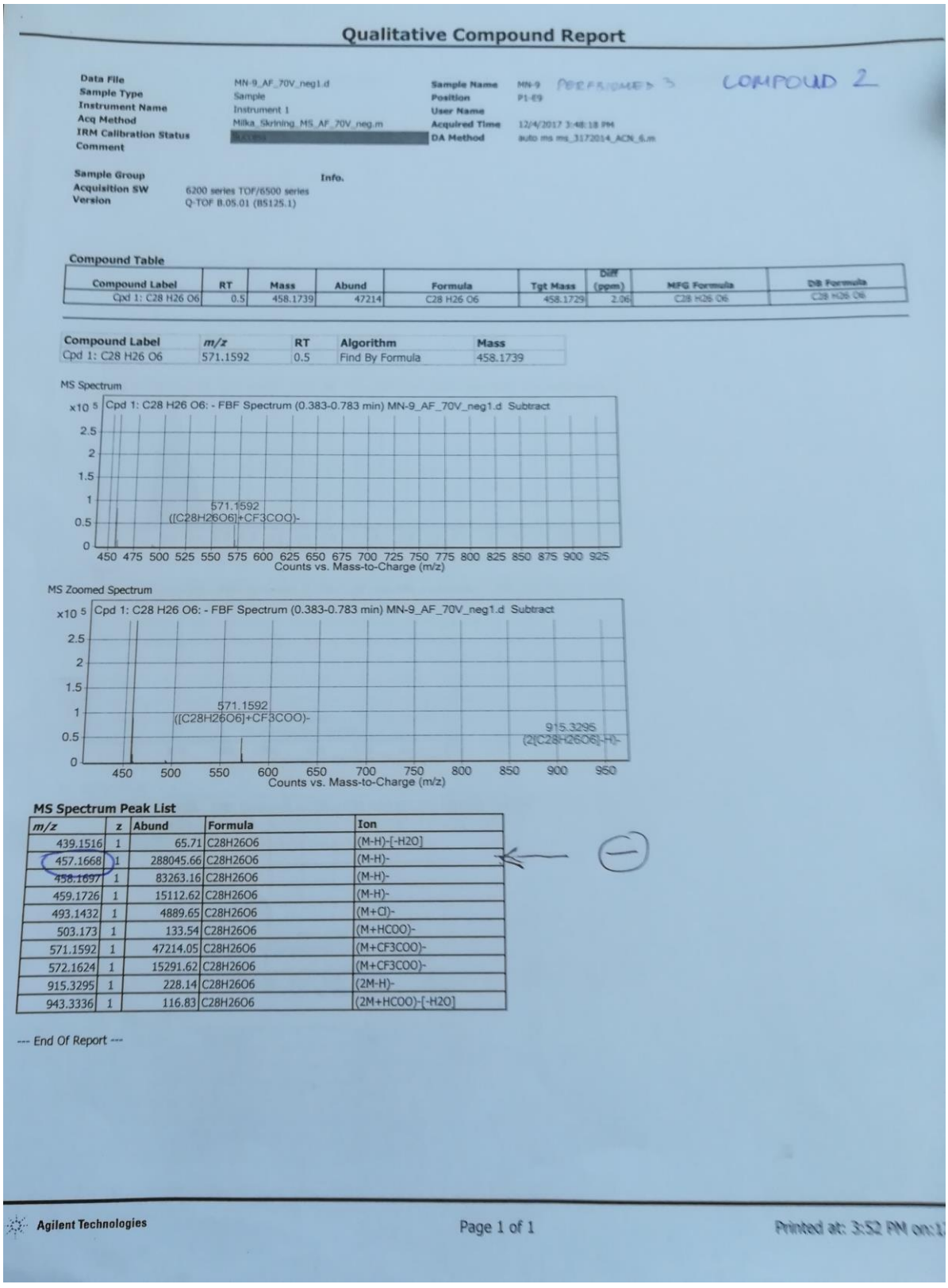


Figure S6: HMBC spectrum of perrottetin F (**1**) (from δ_C 37 ppm to δ_C 41 ppm and from δ_H 6.10 ppm to 7.15 ppm)



Qualitative Compound Report

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IRM Calibration Status	Success	DA Method	auto ms ms_3172014_ACN_6.m
Comment			
Sample Group	Info.		
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)		

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
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Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C28 H26 O6	571.1592	0.5	Find By Formula	458.1739

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
439.1516	1	65.71	C28H26O6	(M-H)-[-H2O]
457.1668	1	288045.66	C28H26O6	(M-H)-
458.1697	1	83263.16	C28H26O6	(M-H)-
459.1726	1	15112.62	C28H26O6	(M-H)-
493.1432	1	4889.65	C28H26O6	(M+Cl)-
503.173	1	133.54	C28H26O6	(M+HCOO)-
571.1592	1	47214.05	C28H26O6	(M+CF3COO)-
572.1624	1	15291.62	C28H26O6	(M+CF3COO)-
915.3295	1	228.14	C28H26O6	(2M-H)-
943.3336	1	116.83	C28H26O6	(2M+HCOO)-[-H2O]

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Figure S7: HRESIMS spectrum of compound **2**

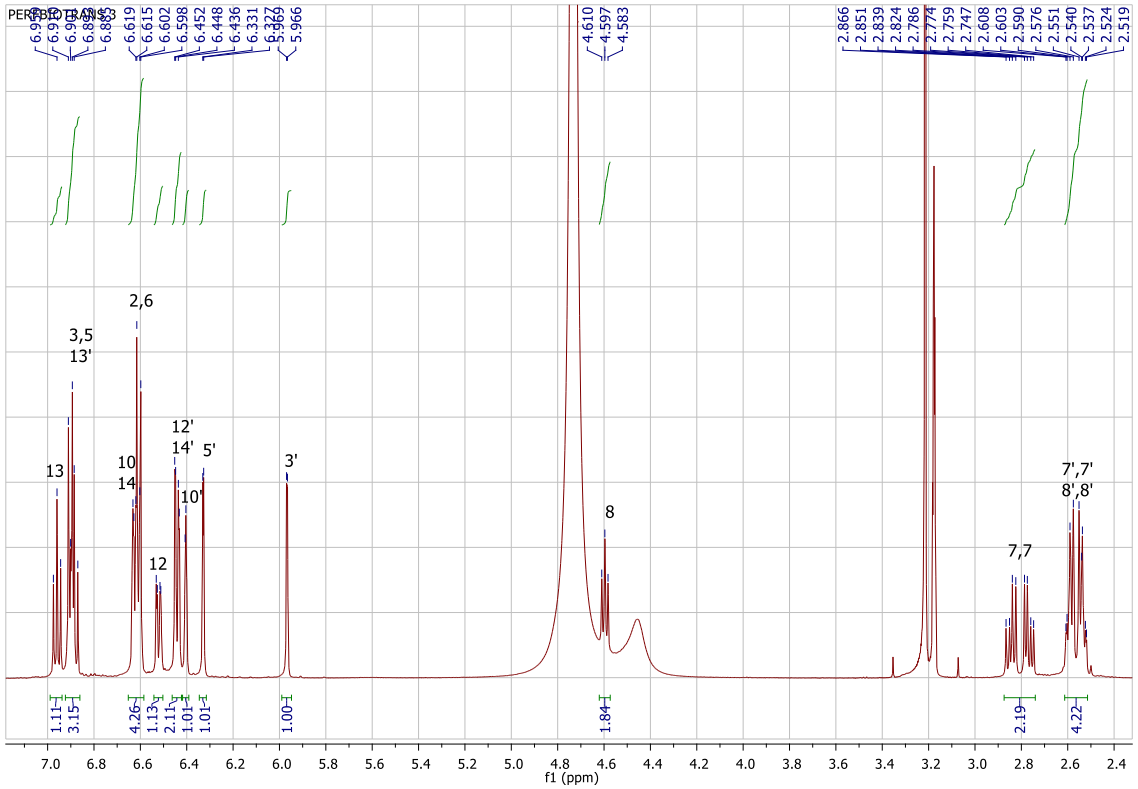


Figure S8: ^{1}H NMR spectrum of compound **2** (from δ_H 2.35 ppm to δ_H 7.20 ppm)

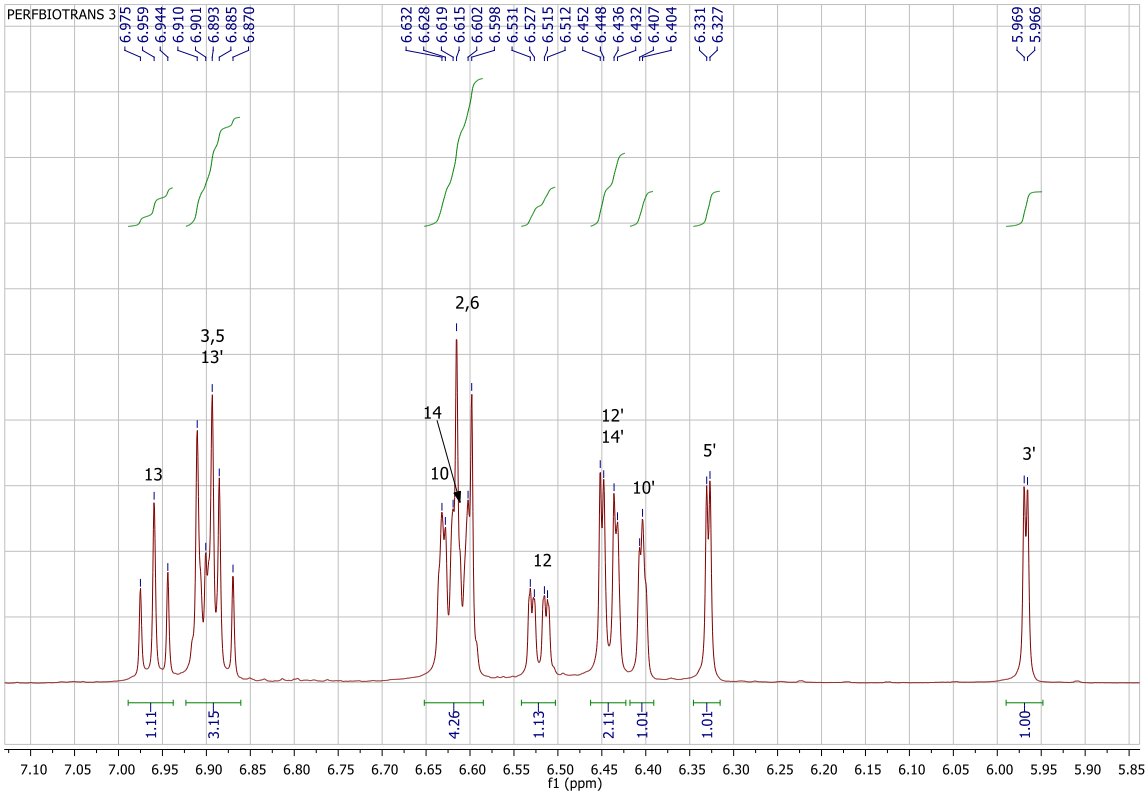


Figure S9: ^{1}H NMR spectrum of compound **2** (from δ_H 5.85 ppm to δ_H 7.15 ppm)

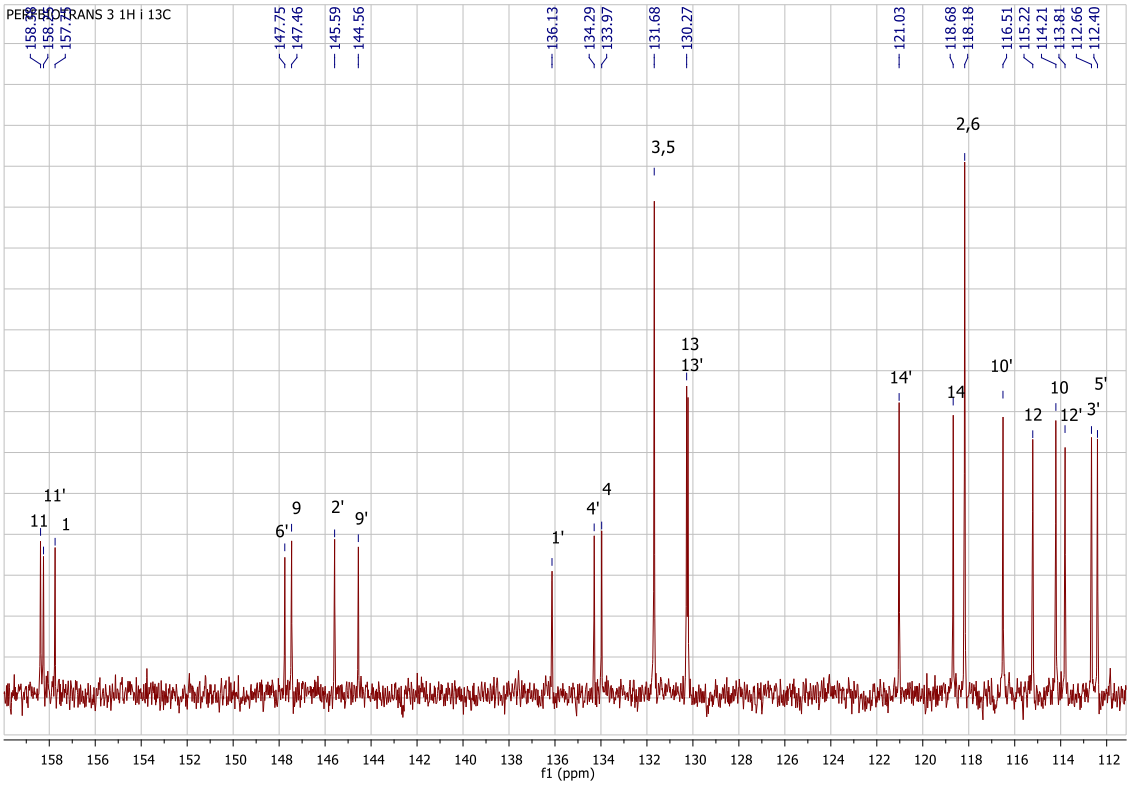


Figure S10: ^{13}C NMR spectrum of compound **2** (from δ_C 111 ppm to δ_C 160 ppm)

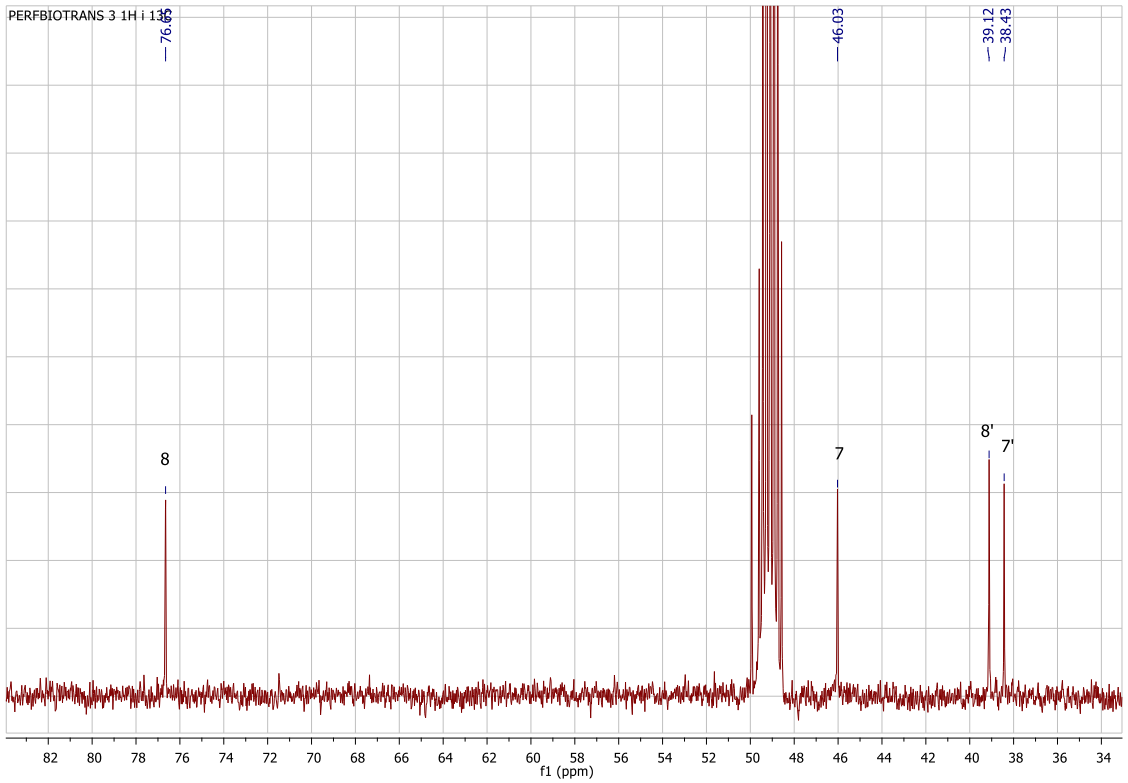


Figure S11: ^{13}C NMR spectrum of compound **2** (from δ_C 33 ppm to δ_C 84 ppm)

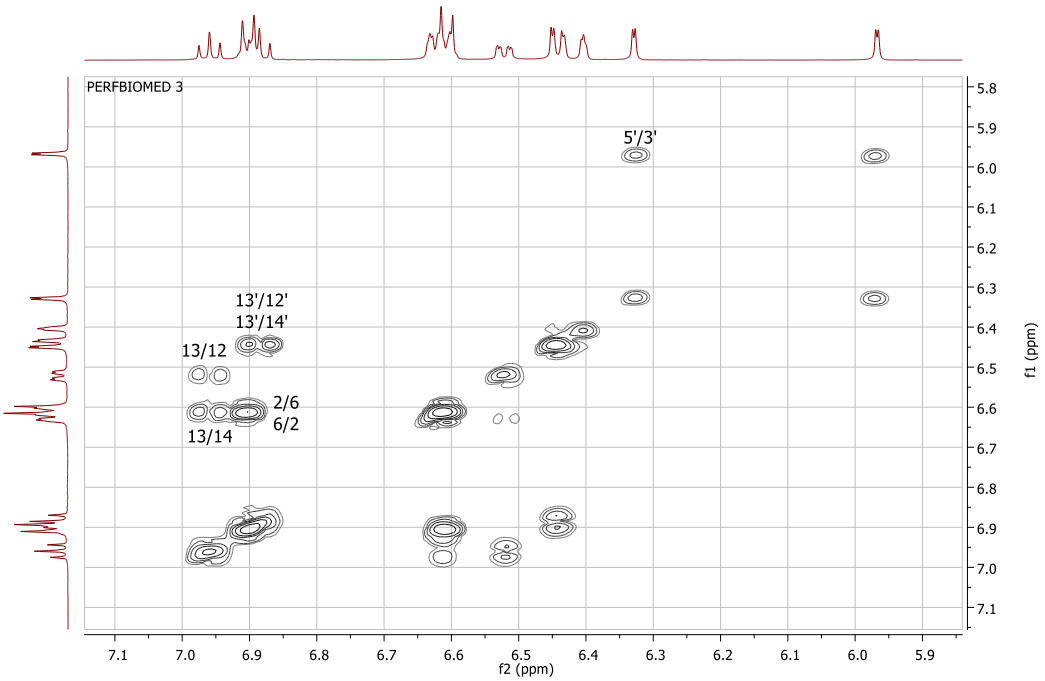


Figure S12: COSY spectrum of compound **2** (from δ_H 5.85 ppm to δ_H 7.15 ppm)

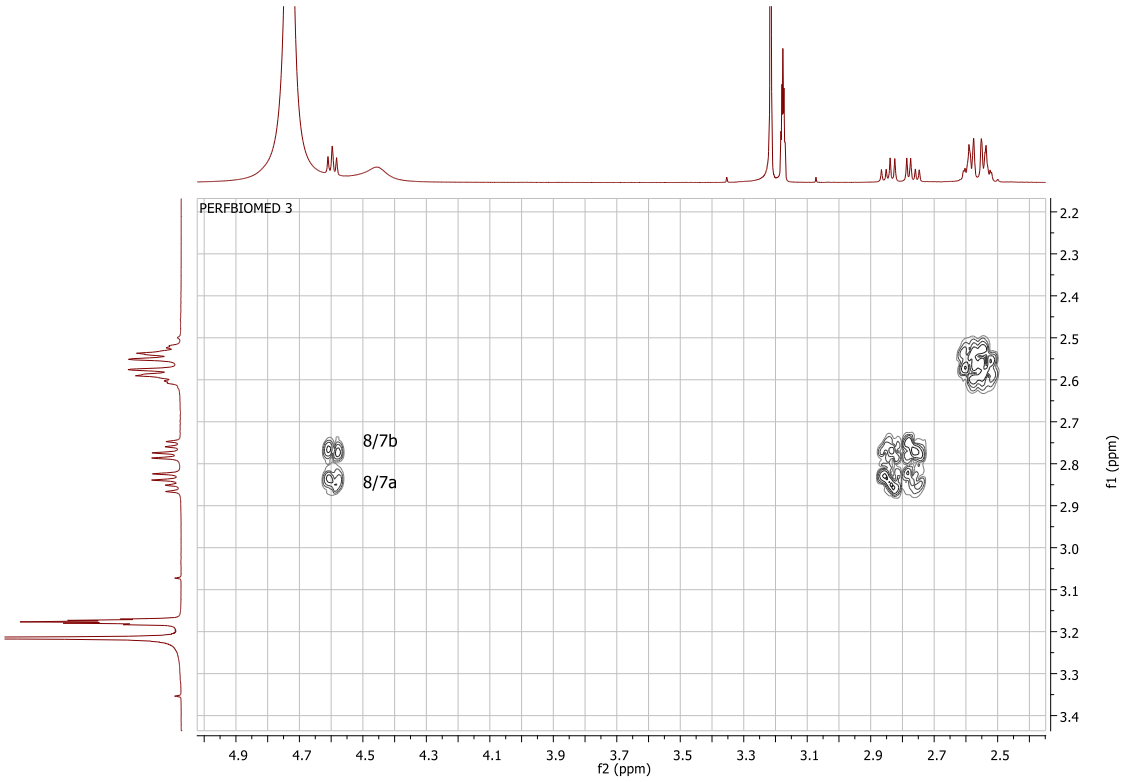


Figure S13: COSY spectrum of compound **2** (from δ_H 2.40 ppm to δ_H 5.00 ppm)

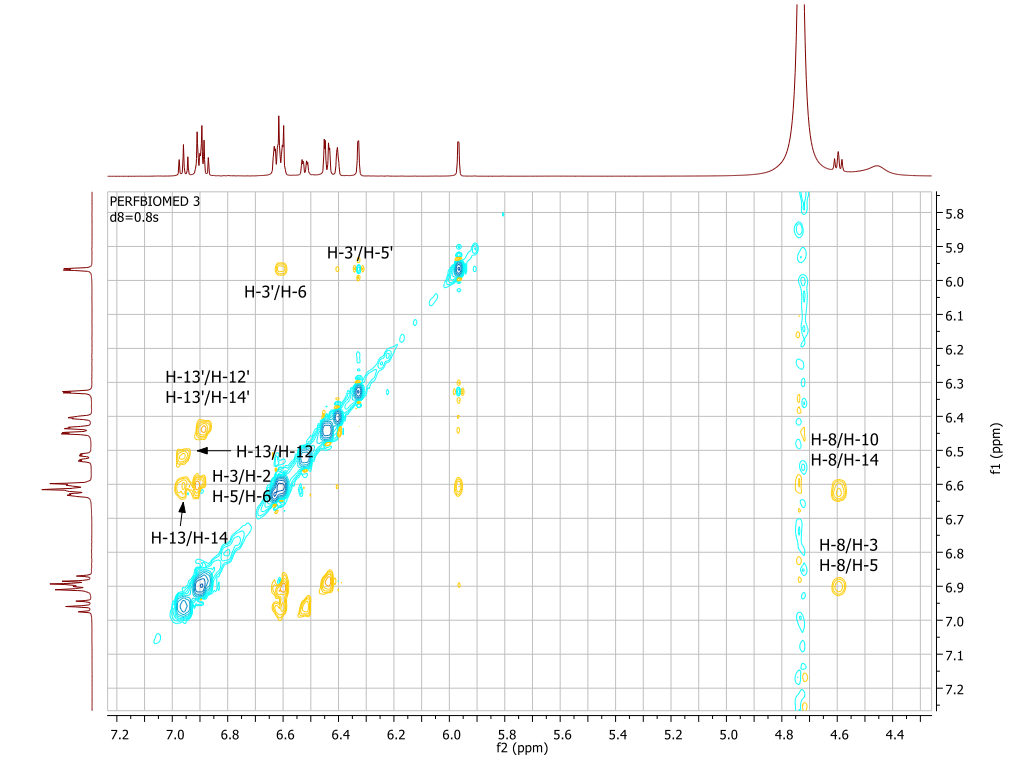


Figure S14: NOESY spectrum of compound **2** (from δ_H 4.30 ppm to δ_H 7.22 ppm)

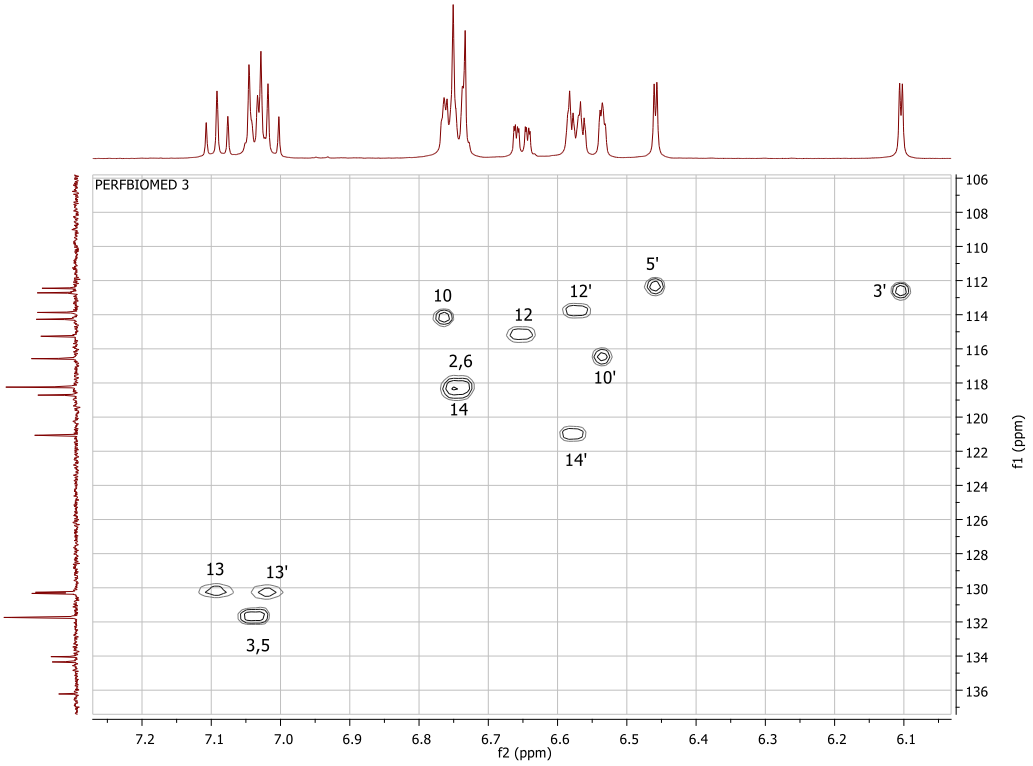


Figure S15: HSQC spectrum of compound **2** (from δ_C 106 ppm to δ_C 137 ppm and from δ_H 6.04 ppm to 7.27 ppm)

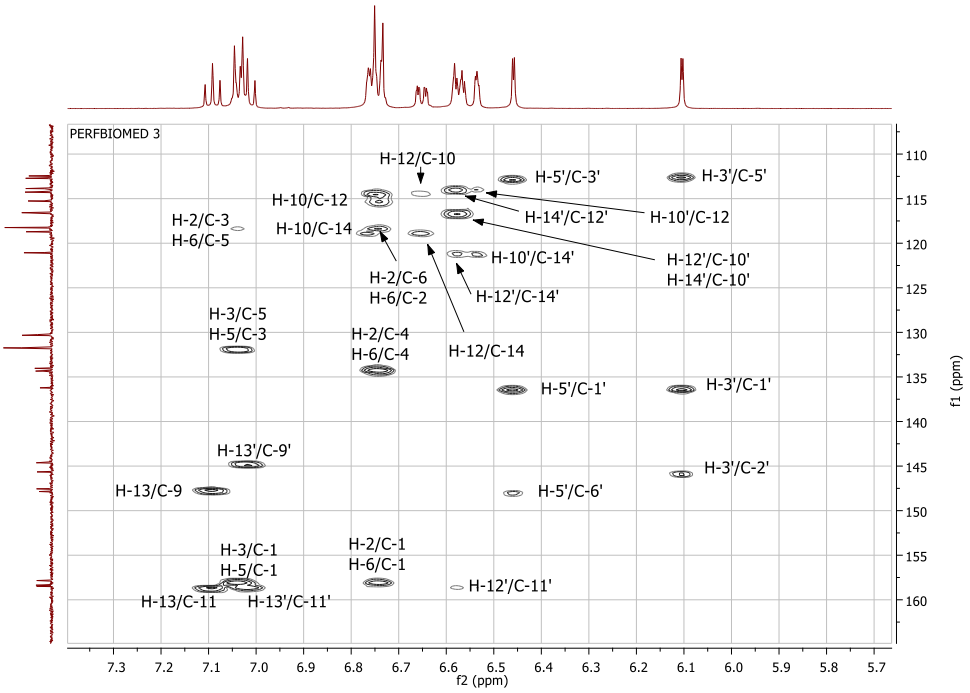


Figure S16: HMBC spectrum of compound **2** (from δ_C 104 ppm to δ_C 164 ppm and from δ_H 5.65 ppm to 7.40 ppm)

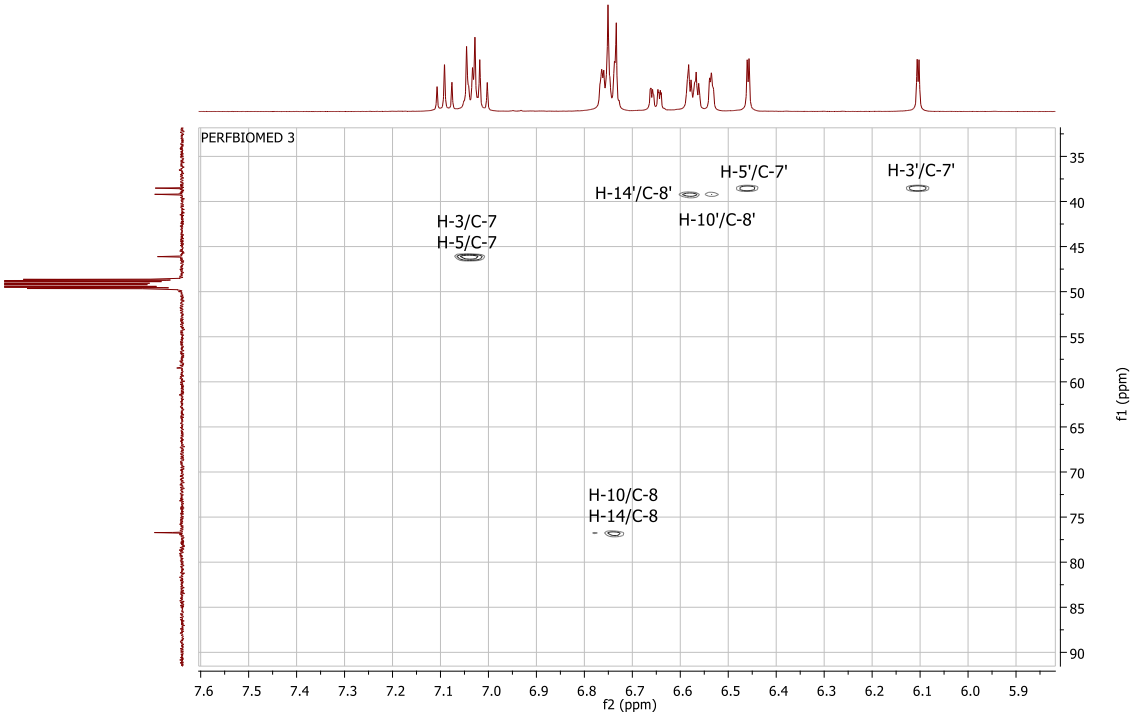


Figure S17: HMBC spectrum of compound **2** (from δ_C 32 ppm to δ_C 91 ppm and from δ_H 5.82 ppm to 7.60 ppm)

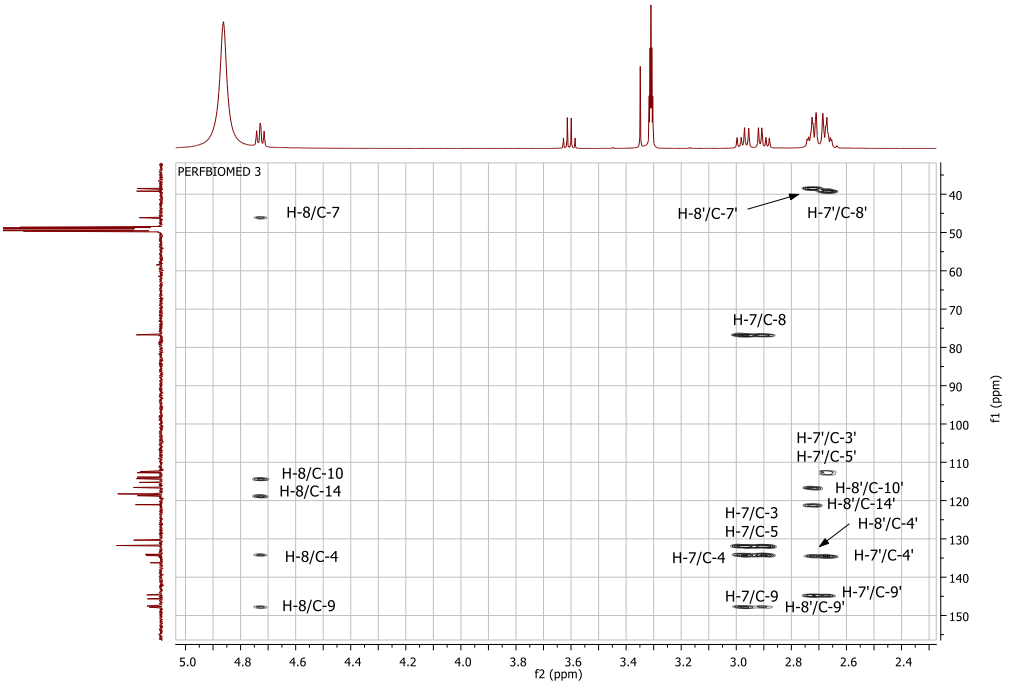


Figure S18: HMBC spectrum of compound **2** (from δ_C 34 ppm to δ_C 156 ppm and from δ_H 2.25 ppm to 5.05 ppm)

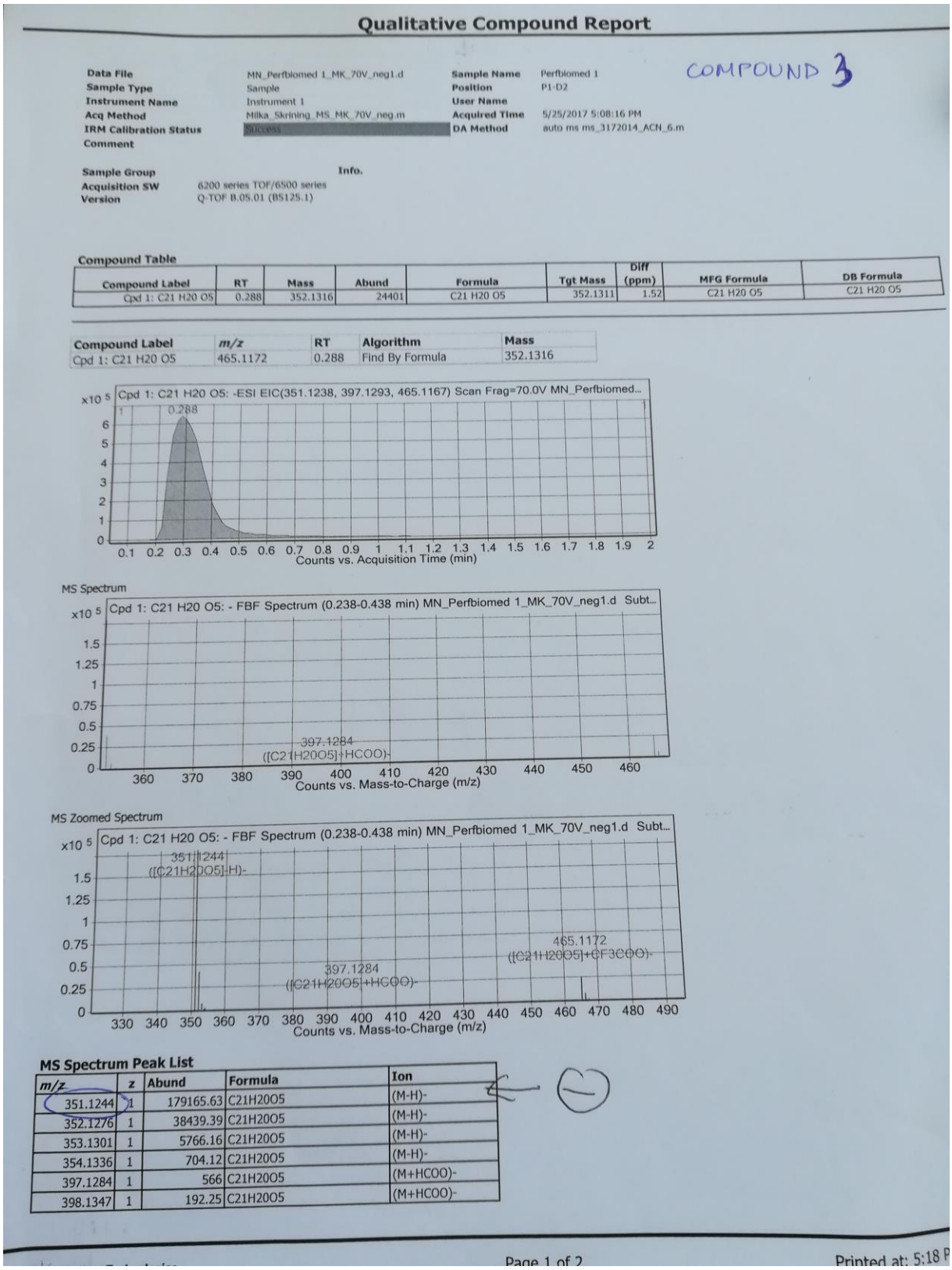


Figure S19: HRESIMS spectrum of compound **3**

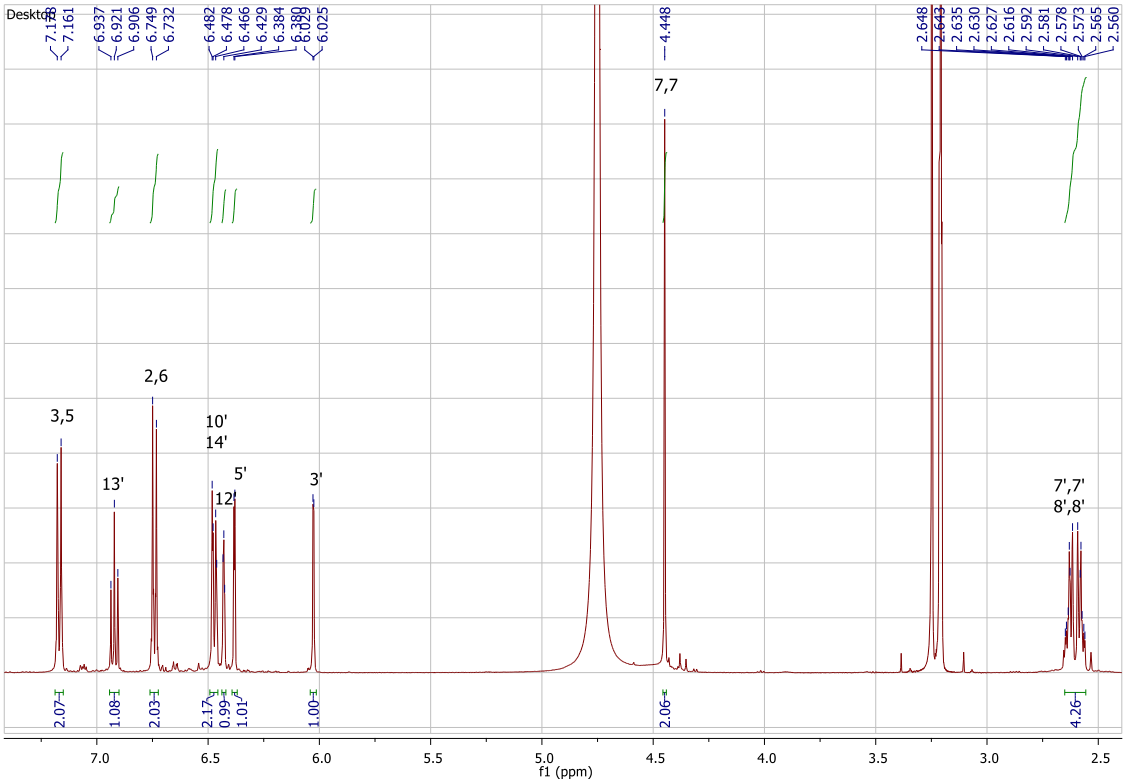


Figure S20: ^{1}H NMR spectrum of compound **3** (from δ_H 2.45 ppm to 7.35 ppm)

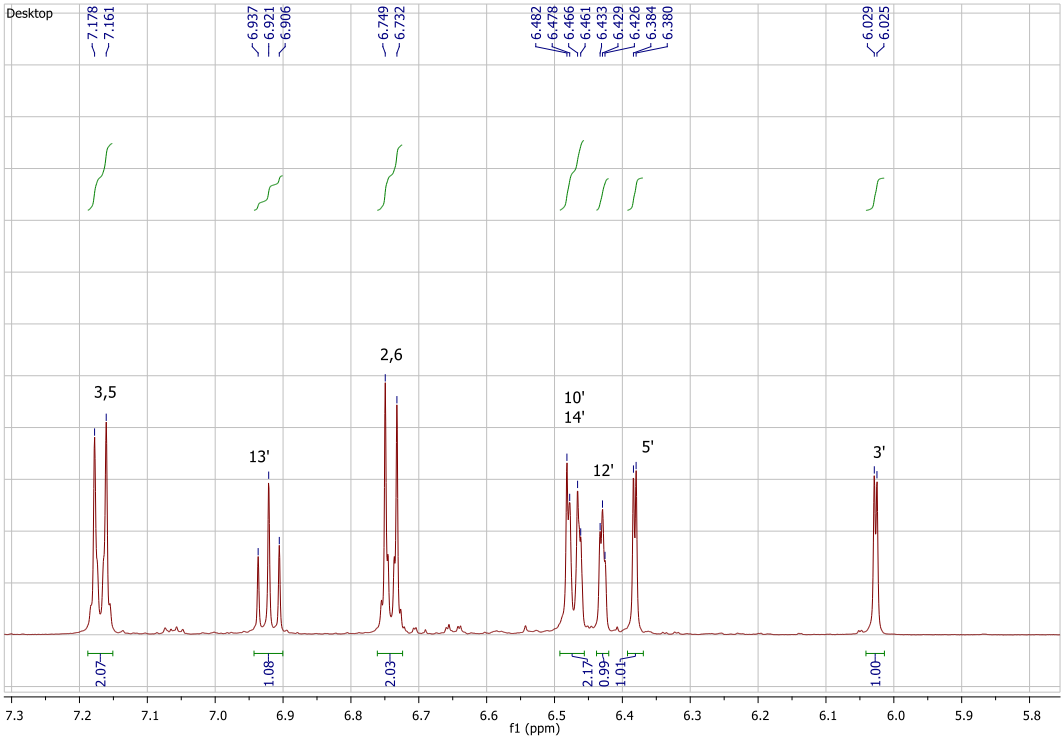


Figure S21: ^{1}H NMR spectrum of compound **3** (from δ_H 5.75 ppm to 7.31 ppm)

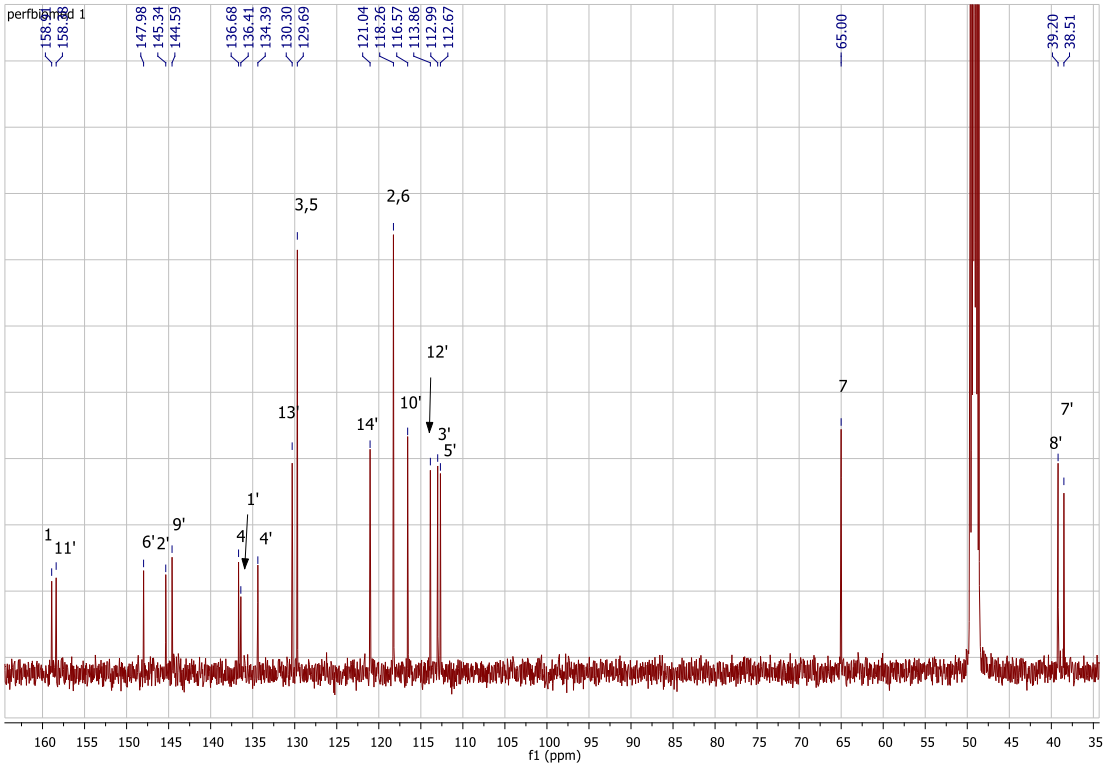


Figure S22: ^{13}C NMR spectrum of compound **3** (from δ_C 35 ppm to δ_C 165 ppm)

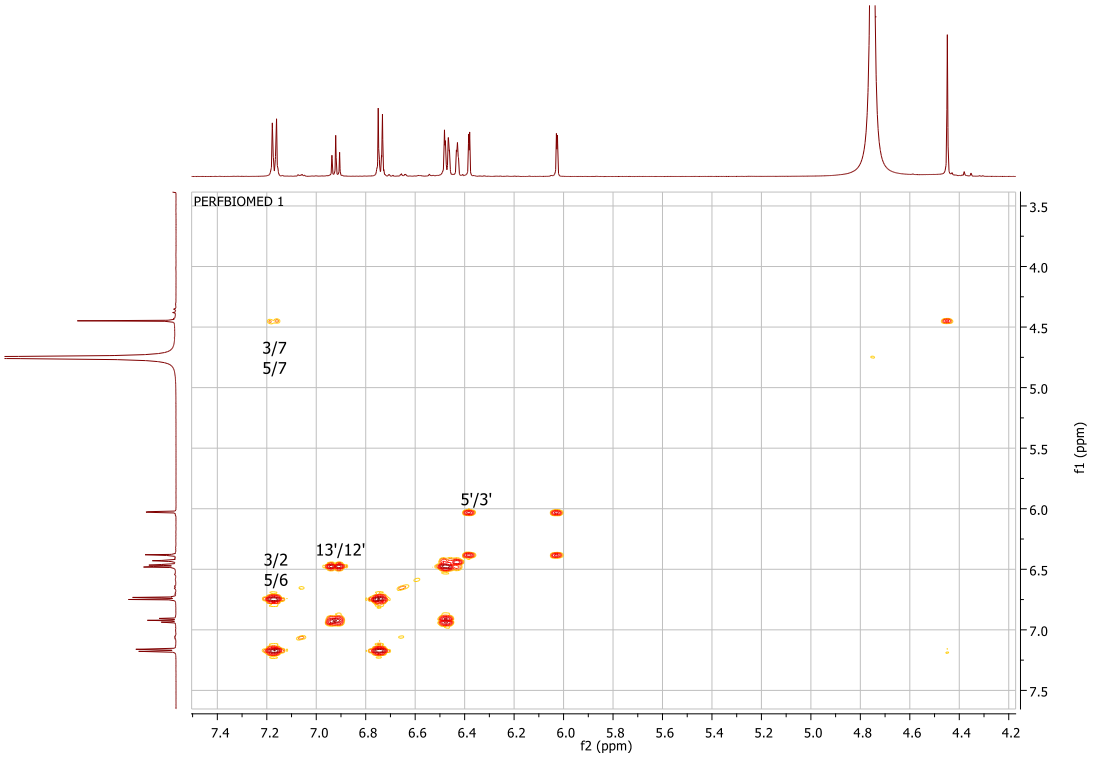


Figure S23: COSY spectrum of compound **3** (from δ_H 4.20 ppm to 7.50 ppm)

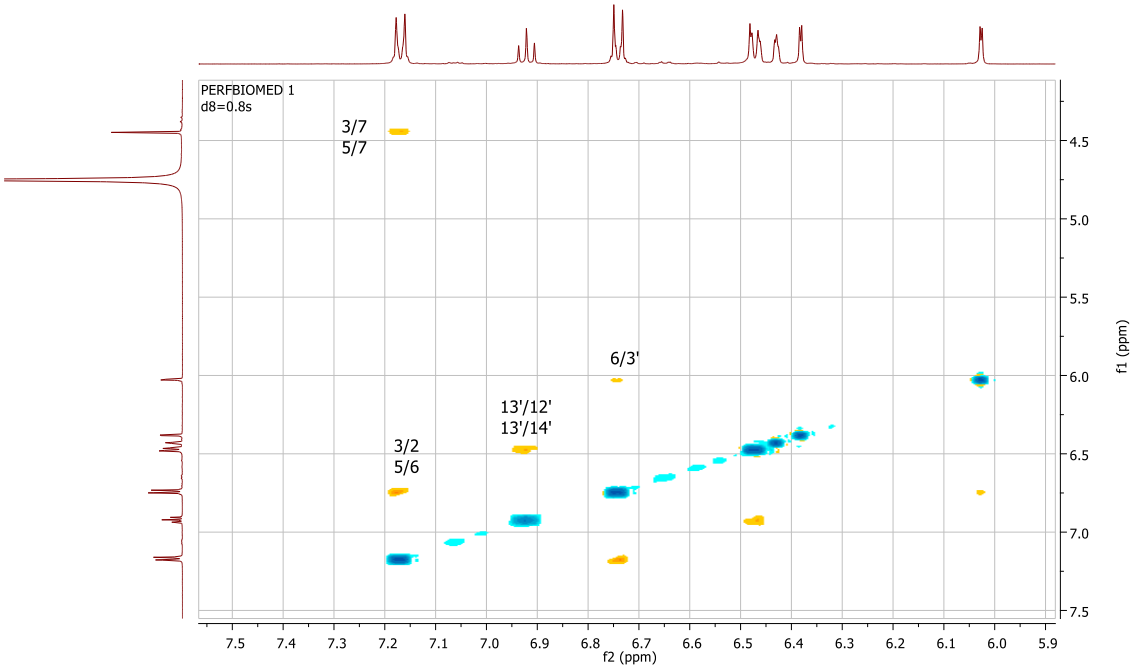


Figure S24: NOESY spectrum of compound **3** (from δ_H 5.90 ppm to 7.55 ppm)

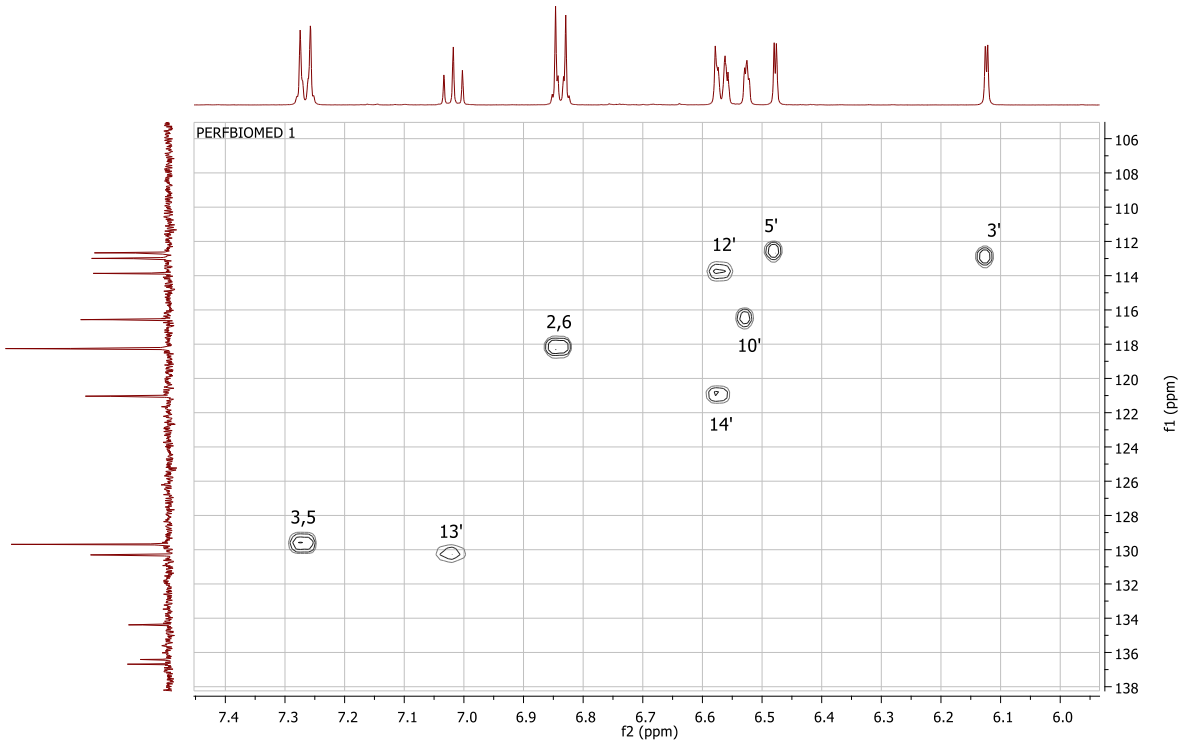


Figure S25: HSQC spectrum of compound **3** (from δ_C 105 ppm to δ_C 138 ppm and from δ_H 5.94 ppm to 7.45 ppm)

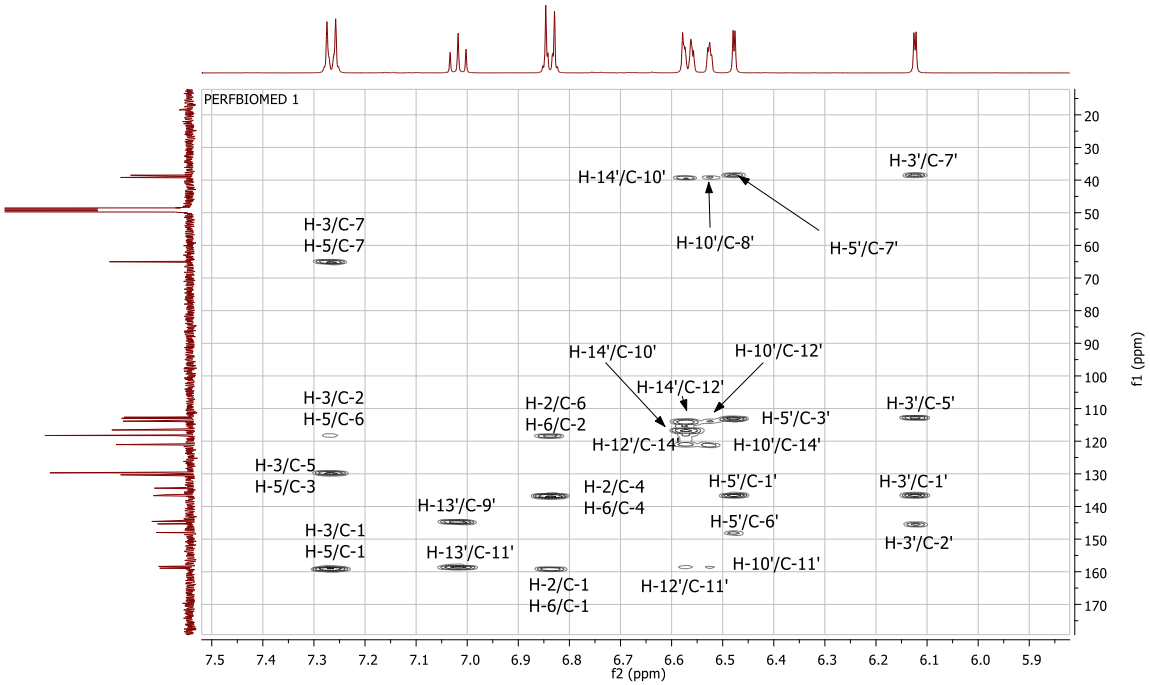


Figure S26: HMBC spectrum of compound **3** (from δ_C 14 ppm to δ_C 180 ppm and from δ_H 5.93 ppm to 7.52 ppm)

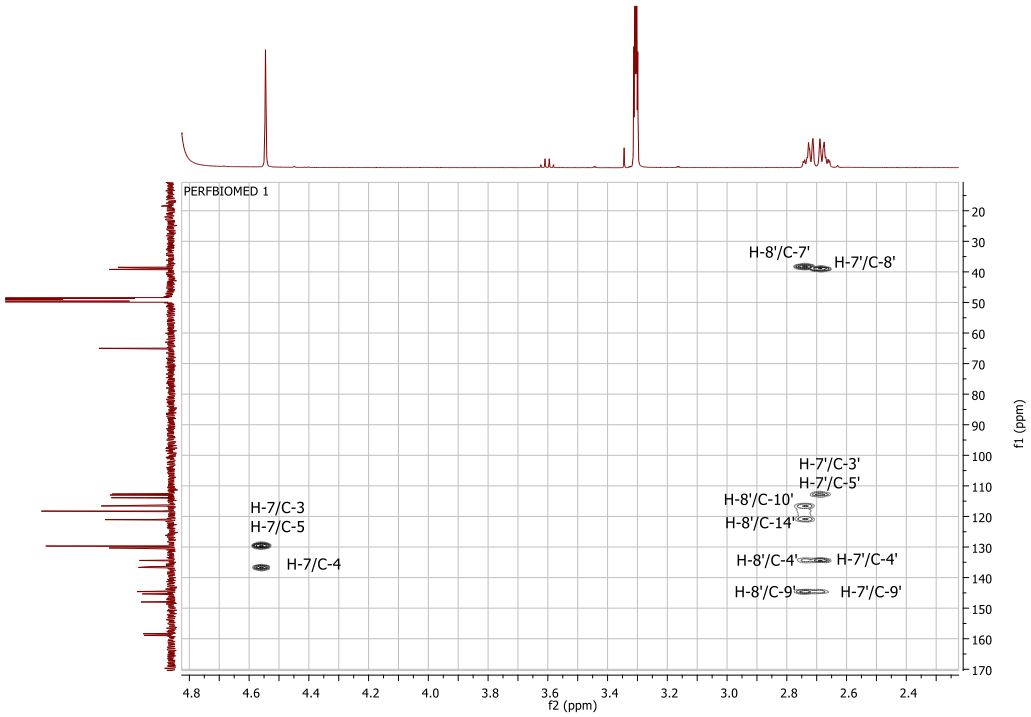
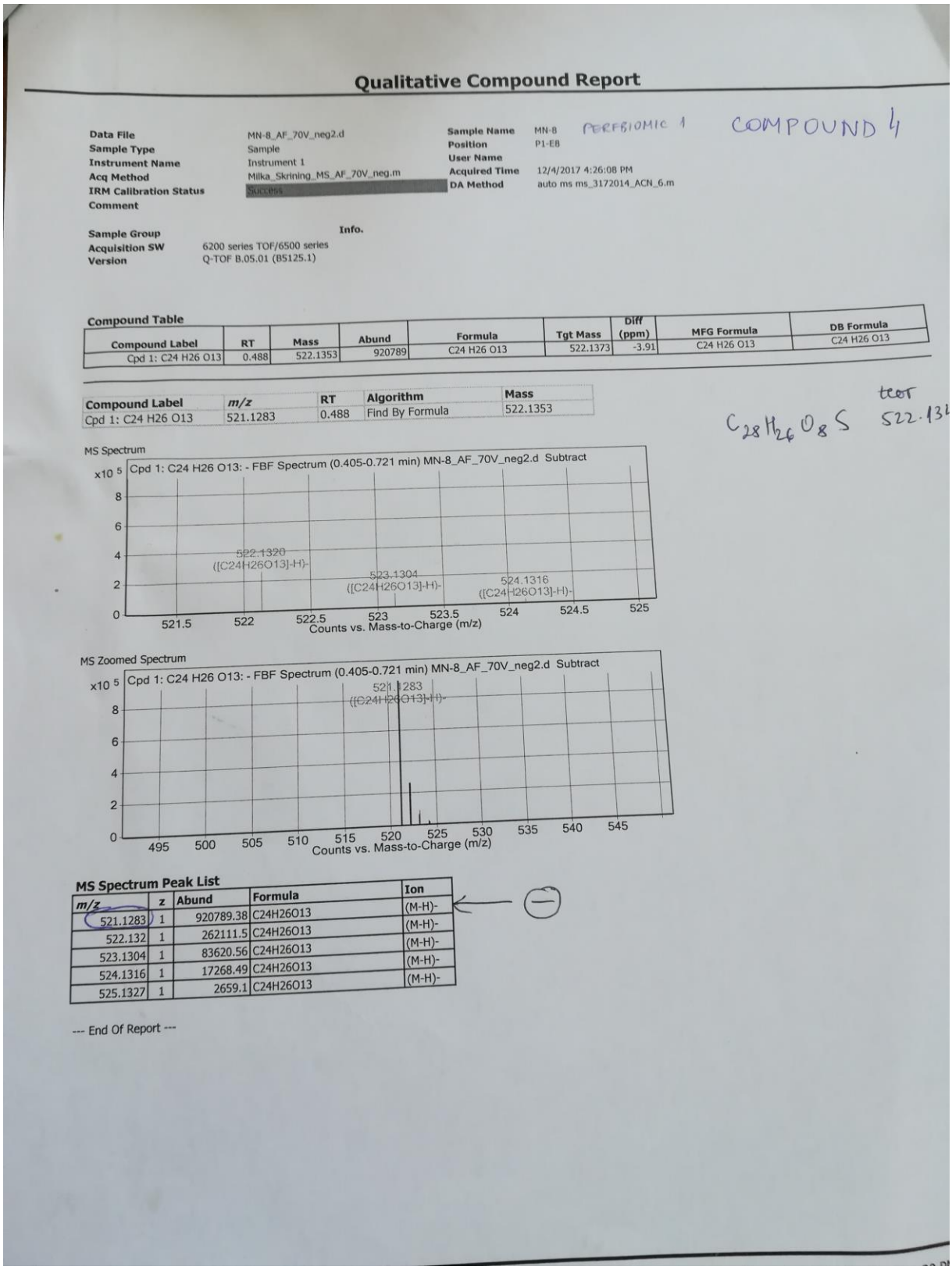


Figure S27: HMBC spectrum of compound **3** (from δ_C 12 ppm to δ_C 170 ppm and from δ_H 2.24 ppm to 4.81 ppm)



Qualitative Compound Report

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Acq Method Milka_Skrining_MS_AF_70V_neg.m
IRM Calibration Status Success
Comment

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Position P1-E8
User Name
Acquired Time 12/4/2017 4:26:08 PM
DA Method auto ms ms_3172014_ACN_6.m

Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
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Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C24 H26 O13	521.1283	0.488	Find By Formula	522.1353

$C_{28}H_{26}O_8S$ 522.134

MS Spectrum

MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
521.1283	1	920789.38	C24H26O13	(M-H)-
522.132	1	262111.5	C24H26O13	(M-H)-
523.1304	1	83620.56	C24H26O13	(M-H)-
524.1316	1	17268.49	C24H26O13	(M-H)-
525.1327	1	2659.1	C24H26O13	(M-H)-

--- End Of Report ---

Figure S28: HRESIMS spectrum of compound **4**

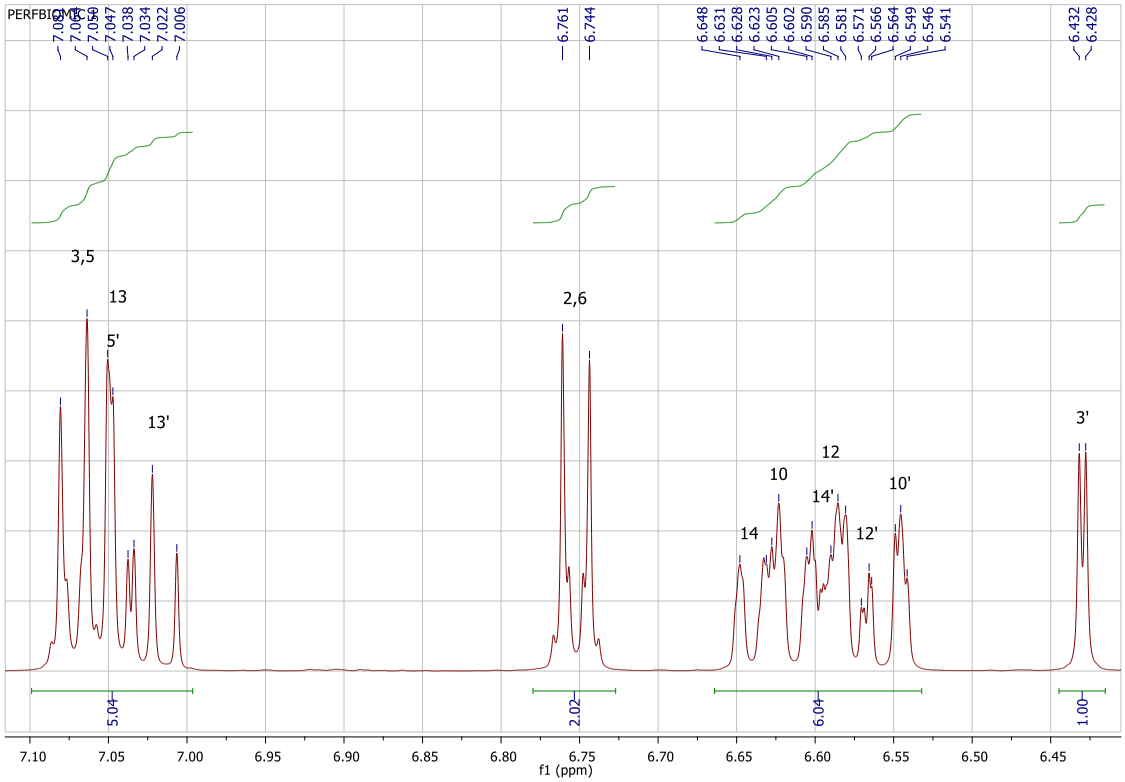

Figure S29: ^{1}H NMR spectrum of compound **4** (from δ_H 6.40 ppm to 7.12 ppm)

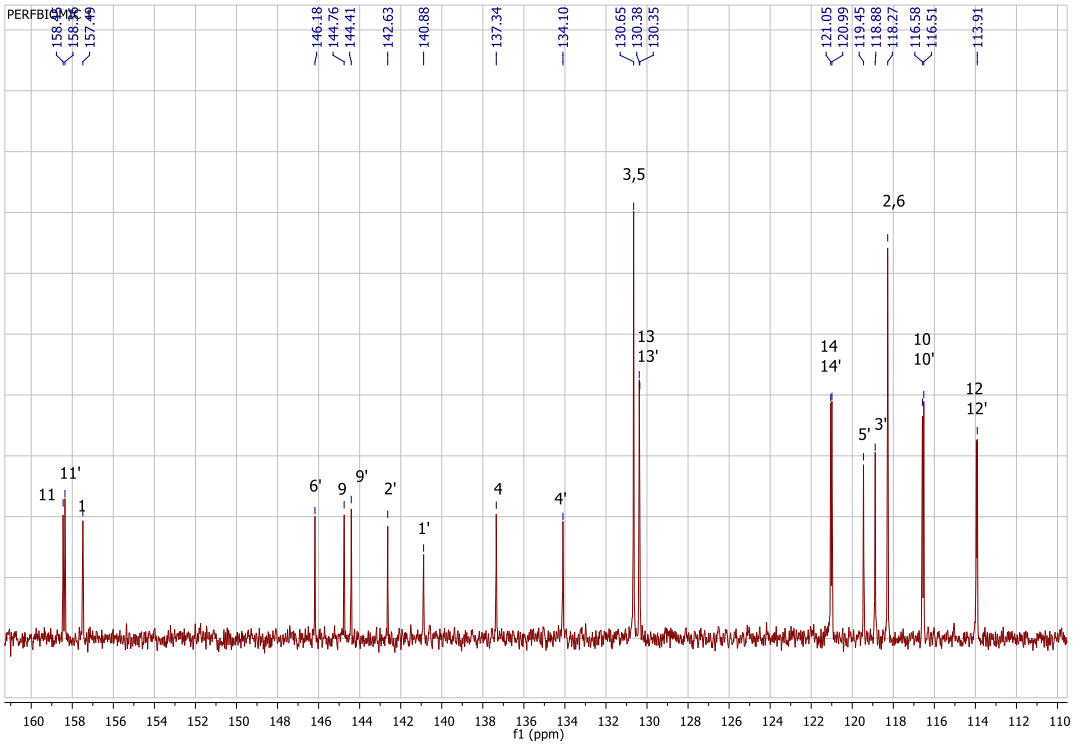

Figure S30: ^{13}C NMR spectrum of compound **4** (from δ_C 110 ppm to δ_C 161 ppm)

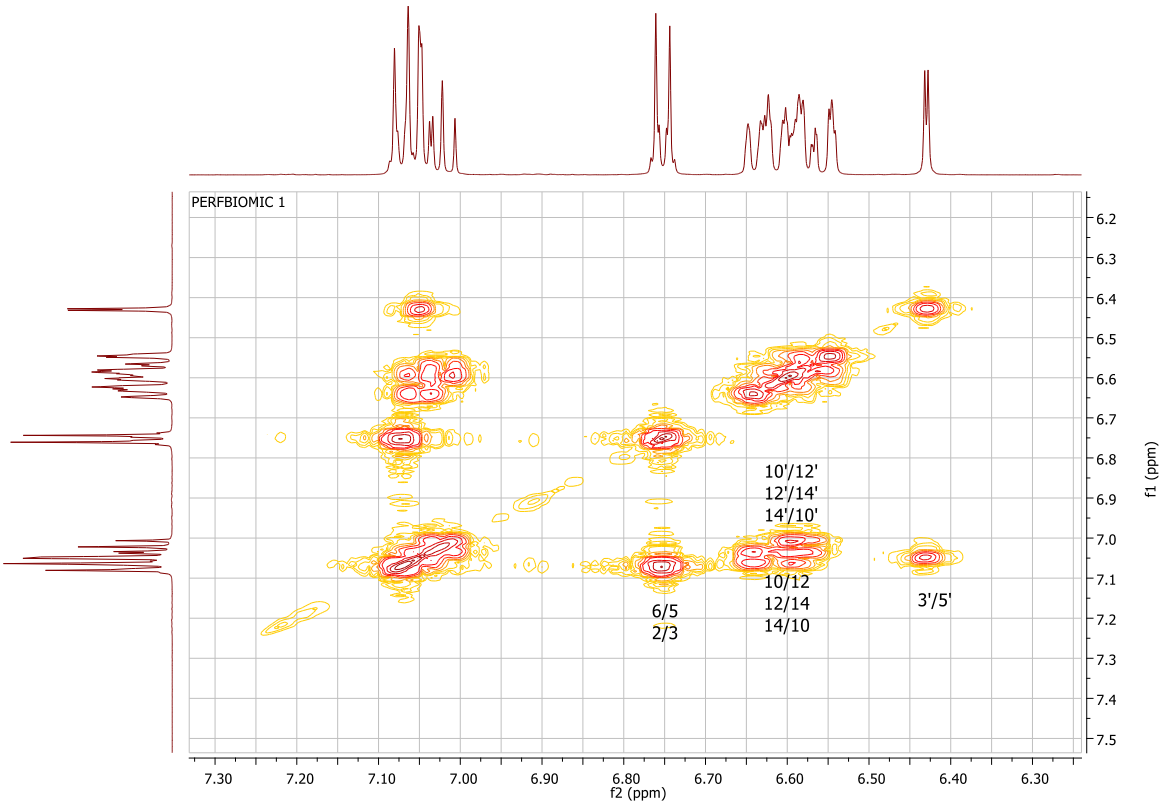

Figure S31: COSY spectrum of compound **4** (from δ_H 6.25 ppm to 7.33 ppm)

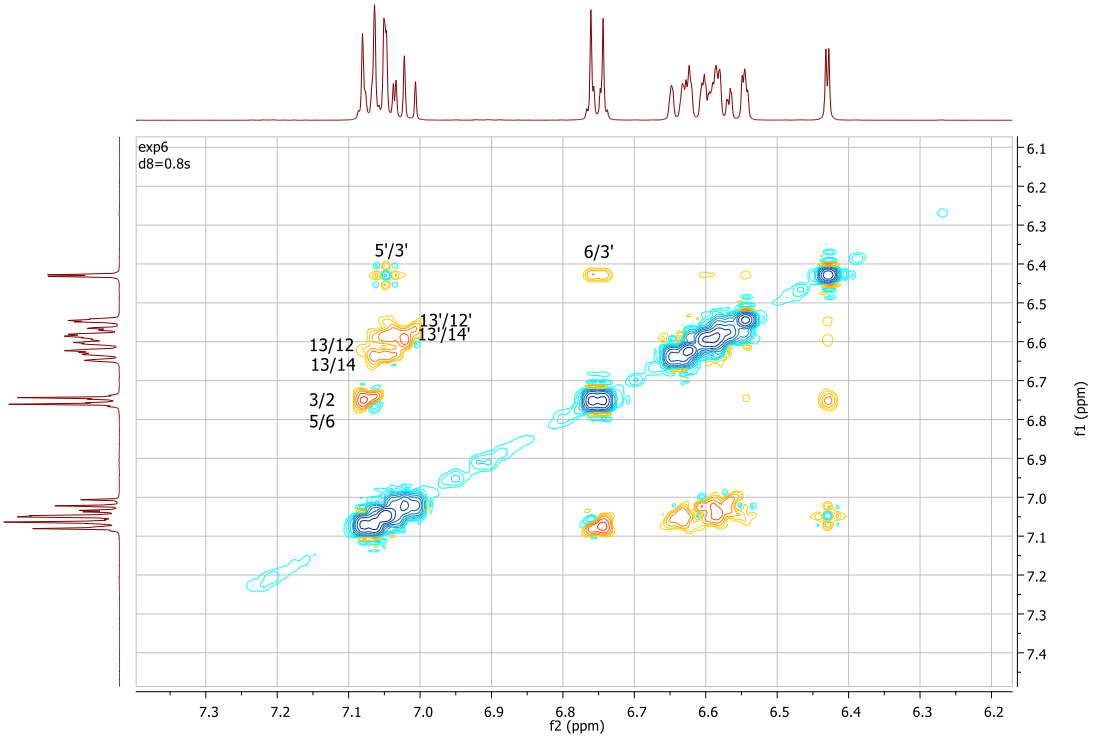

Figure S32: NOESY spectrum of compound **4** (from δ_H 6.18 ppm to 7.40 ppm)

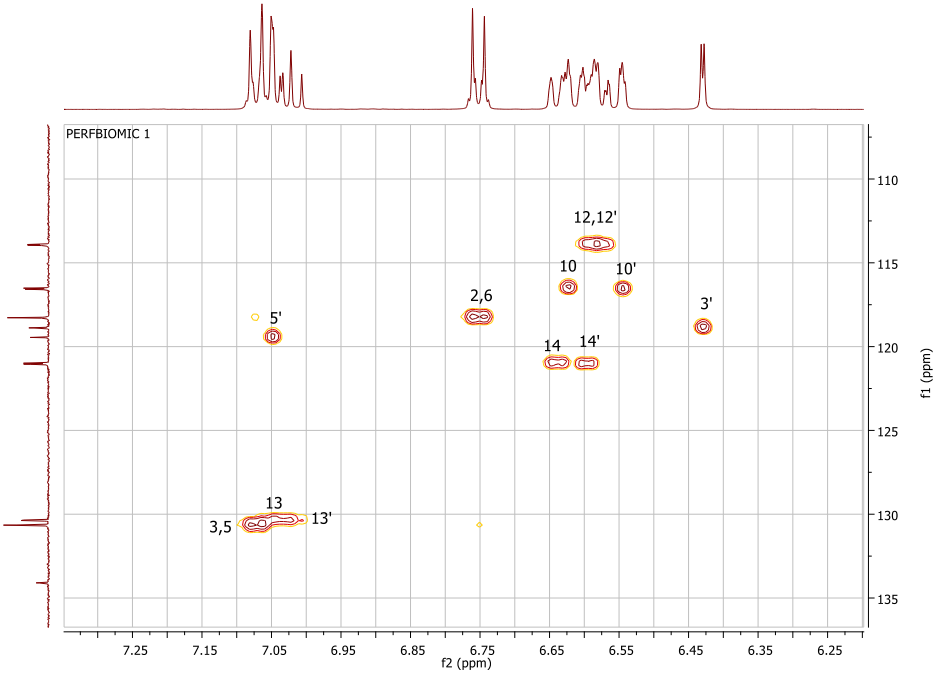

Figure S33: HSQC spectrum of compound **4** (from δ_C 107 ppm to δ_C 137 ppm and from δ_H 6.30 ppm to 7.35 ppm)

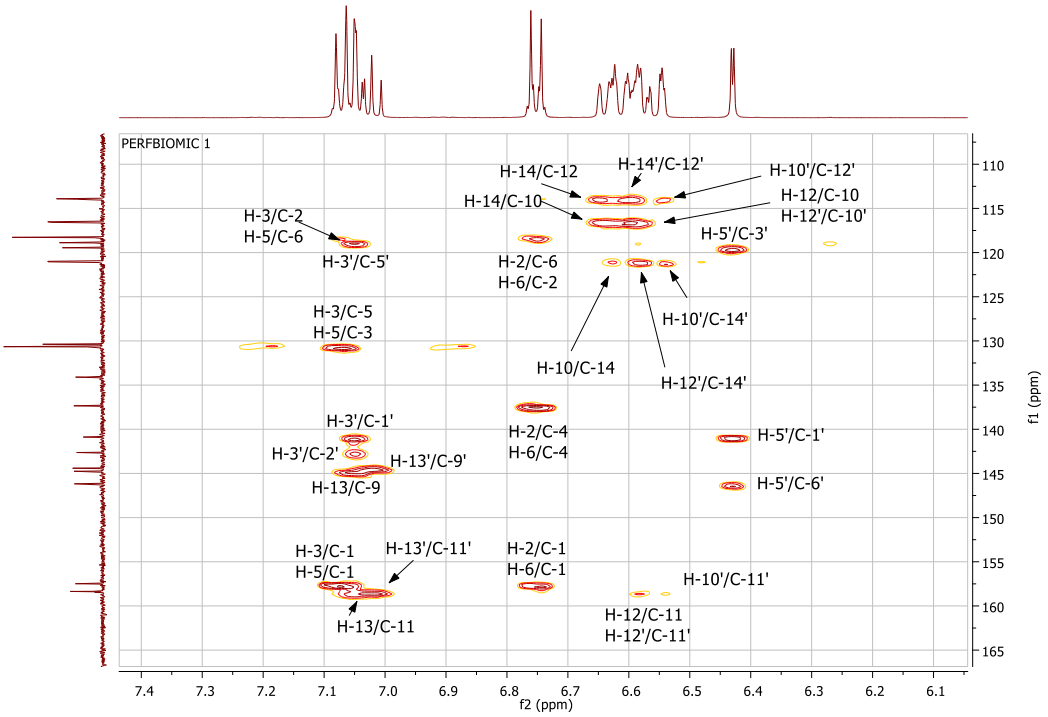

Figure S34: HMBC spectrum of compound **4** (from δ_C 107 ppm to δ_C 167 ppm and from δ_H 6.05 ppm to 7.45 ppm)

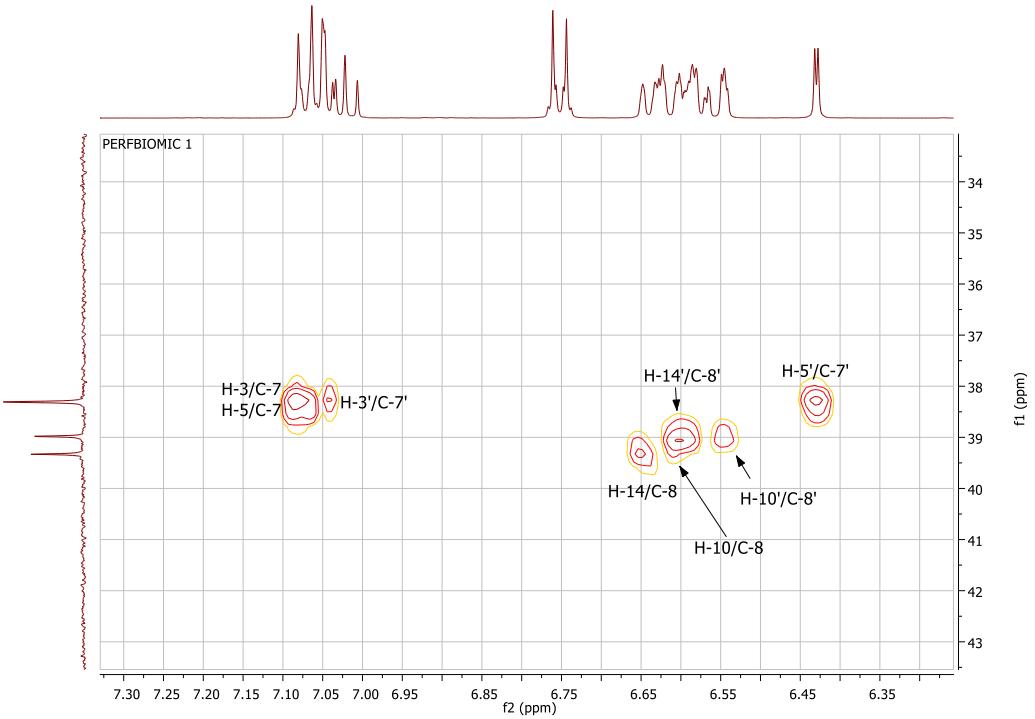

Figure S35: HMBC spectrum of compound **4** (from δ_C 33 ppm to δ_C 43.5 ppm and from δ_H 6.25 ppm to 7.32 ppm)

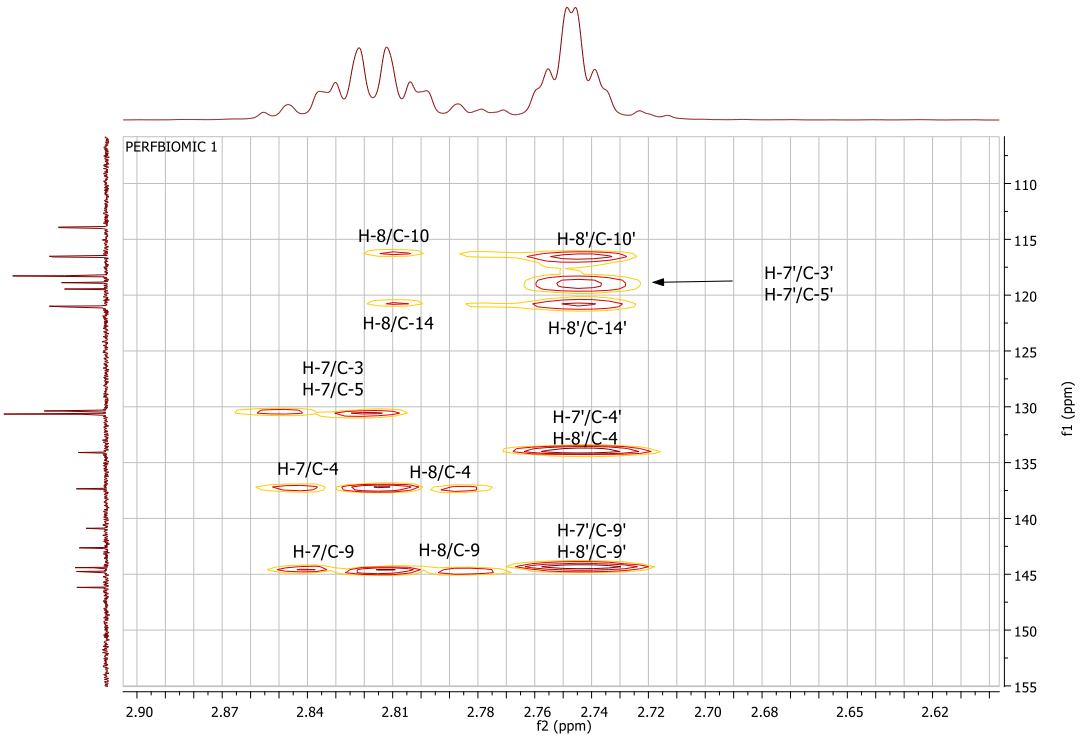

Figure S36: HMBC spectrum of compound **4** (from δ_C 106 ppm to δ_C 155 ppm and from δ_H 2.24 ppm to 4.81 ppm)

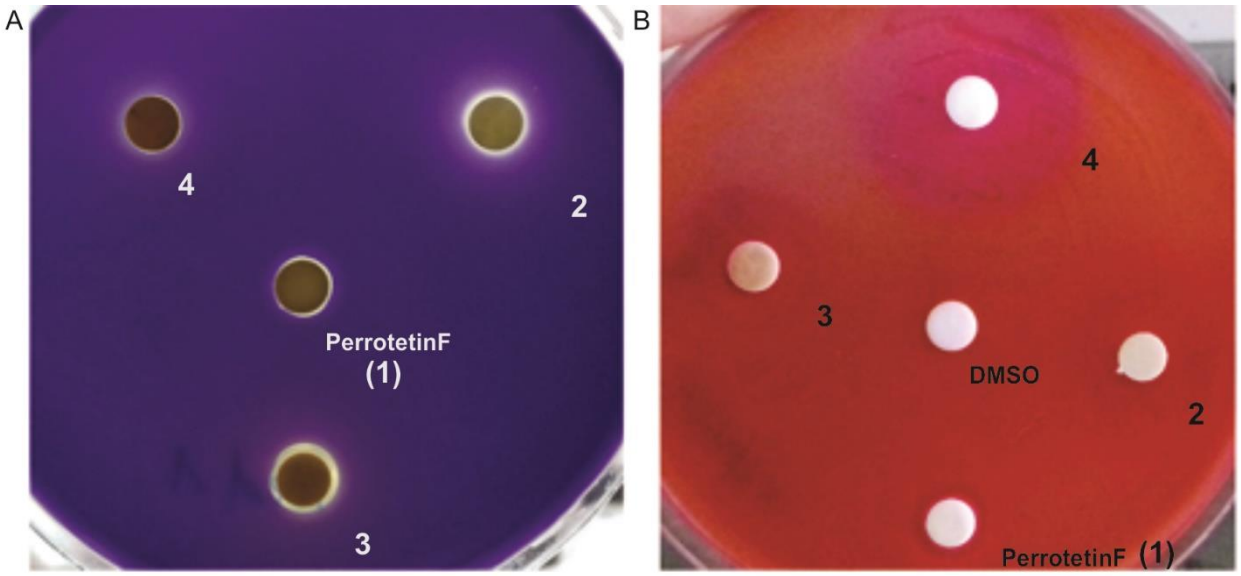

Figure S37: Effects of perrottetin F (**1**) and biotransformed products (250 µg/disc) on the production of violacein by *C. violaceum* CV026 (A) and prodigiosin by *S. marcescens* (B). The control in the bioassay was DMSO