

Supporting Information to

Screening of Panamanian Plant Extracts for Pesticidal Properties and HPLC-Based Identification of Active Compounds

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Table of Contents

- Tab. S1.** List of the 19 active extracts from the extract screening
- Fig. 1S.** Profiles of the MeOH stem extracts of *Bocconia frutescens* for the plant pathogenic fungi *Botryotinia fuckeliana* (A), *Phytophthora infestans* (B), and *Septoria tritici* (C)
- Fig. 2S.** HPLC-DAD chromatograms of the crude extract and its polyamide fractions (PA1–PA5) of *Myrcia splendens*.
- Fig. 3S.** HPLC-DAD chromatograms of the crude extract and its polyamide fractions (PA1–PA5) of *Combretum aff. laxum*.
- Fig. 4S.** HPLC-DAD chromatograms of the crude extract and its polyamide fractions (PA1–PA5) of *Erythroxylum macrophyllum*.
- Tab. 2S.** ^1H and ^{13}C NMR data (500 MHz) of compounds **1–5**
- Tab. 3S.** ^1H and ^{13}C NMR data (500 MHz) of compound **6** in DMSO- d_6
- Tab. 4S.** ^1H and ^{13}C NMR data (500 MHz) of compounds **12** and **25**
- Tab. 5S.** ^1H and ^{13}C NMR (500 MHz) of compound **7** and **10**
- Tab. 6S.** ^1H and ^{13}C NMR data (500 MHz) of compound **8** in DMSO- d_6
- Tab. 7S.** ^1H and ^{13}C NMR (500 MHz) of compounds **13** and **14** in CD $_3$ OD
- Tab. 8S.** ^1H and ^{13}C NMR (500 MHz) of compounds **15–17** in CD $_3$ OD
- Tab. 9S.** ^1H and ^{13}C NMR (500 MHz) of compounds **19** and **26** in DMSO- d_6
- Tab. 10S.** ^1H and ^{13}C NMR (500 MHz) of compounds **20–23** in CD $_3$ OD
- Tab. 11S.** ^1H and ^{13}C NMR (500 MHz) of compounds **24** in DMSO- d_6
- Tab. 12S.** ^1H and ^{13}C NMR (500 MHz) of compounds **27–29** in DMSO- d_6

Tab. S1. List of the 19 active extracts from the extract screening

Plant name	Extract	Indication
<i>Bocconia frutescens</i>	MeOH (stem)	Fungicide
<i>Miconia affinis</i>	EtOAc (stem)	Fungicide
<i>Bocconia frutescens</i>	EtOAc (stem)	Fungicide
<i>Miconia ligulata</i>	EtOAc (leaves)	Fungicide
<i>Piper gatunense</i>	EtOAc (stem)	Fungicide
<i>Clusia uvitana</i>	EtOAc (leaves)	Fungicide
<i>Salvia alvajaca</i>	MeOH (root)	Insecticide
<i>Simaba cedron</i>	MeOH (stem)	Insecticide
<i>Myrcia splendens</i>	MeOH (leaves)	Insecticide
<i>Psychotria erecta</i>	MeOH (stem)	Insecticide
<i>Psychotria suerrensii</i>	MeOH (root)	Insecticide
<i>Rollinia pittieri</i>	EtOAc (leaves)	Insecticide
<i>Rollinia mucosa</i>	EtOAc (leaves)	Insecticide
<i>Myrcia splendens</i>	MeOH (branch)	Insecticide
<i>Ocotea glaucosericea</i>	EtOAc (stem)	Insecticide
<i>Trichilia hirta</i>	MeOH (stem)	Herbicide
<i>Combretum aff. laxum</i>	MeOH (leaves)	Herbicide
<i>Erythroxylum macrophyllum</i>	MeOH (leaves)	Herbicide
<i>Picramnia antidesma</i>	MeOH (root)	Herbicide

Fig. 1S. Profiles of the MeOH stem extracts of *Bocconia frutescens* for the plant pathogenic fungi *Botryotinia fuckeliana* (A), *Phytophthora infestans* (B), and *Septoria tritici* (C)

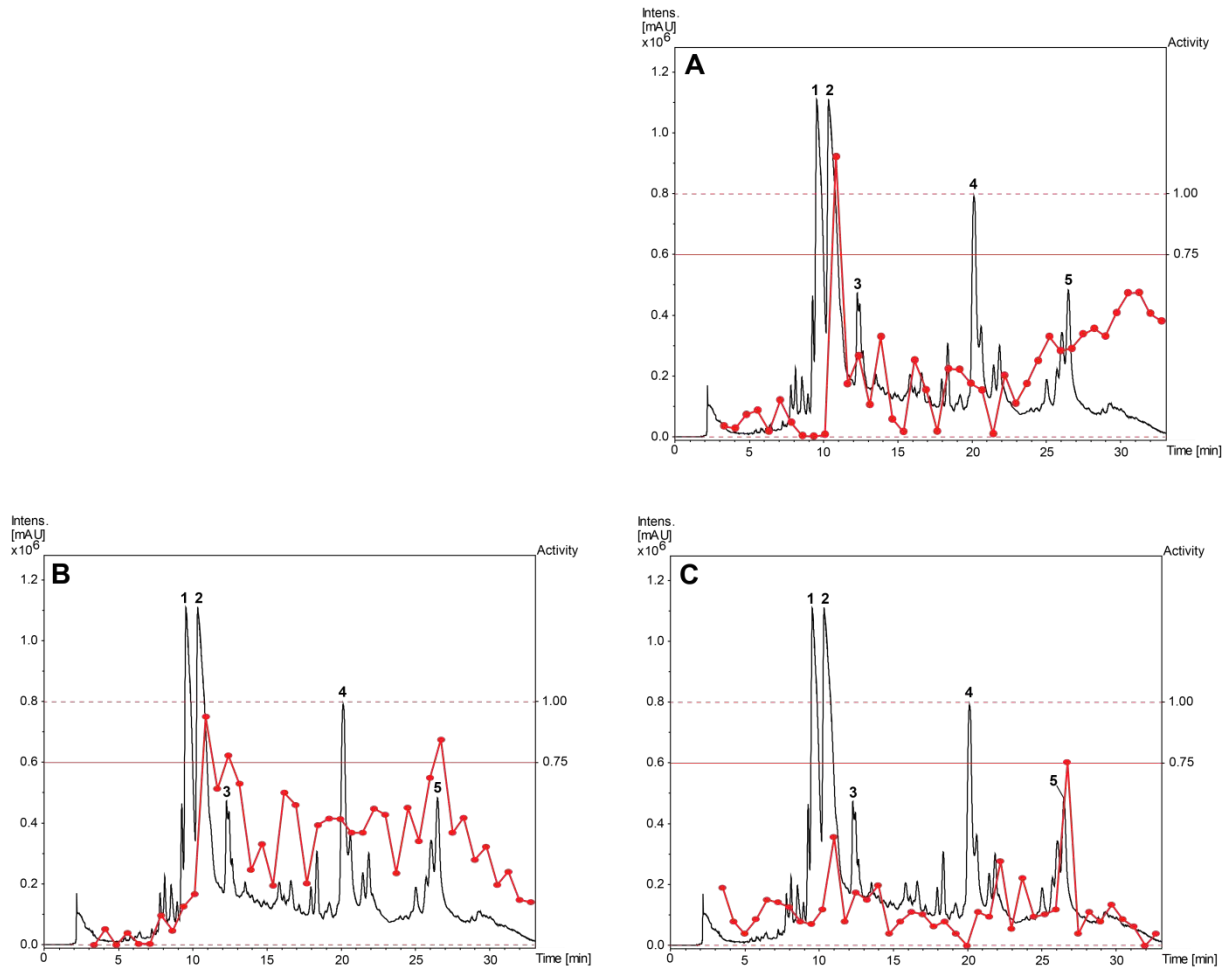


Fig. 2S. HPLC-DAD chromatograms of the crude extract and its polyamide fractions (PA1–PA5) of *Myrcia splendens*. SunFire C18 column (150 x 3 mm i.d., 3.5 μ m); 5–100% MeCN/0.1% aqueous formic acid in 30min, 0.4 mL/min; detection: 210–700nm, maxplot.

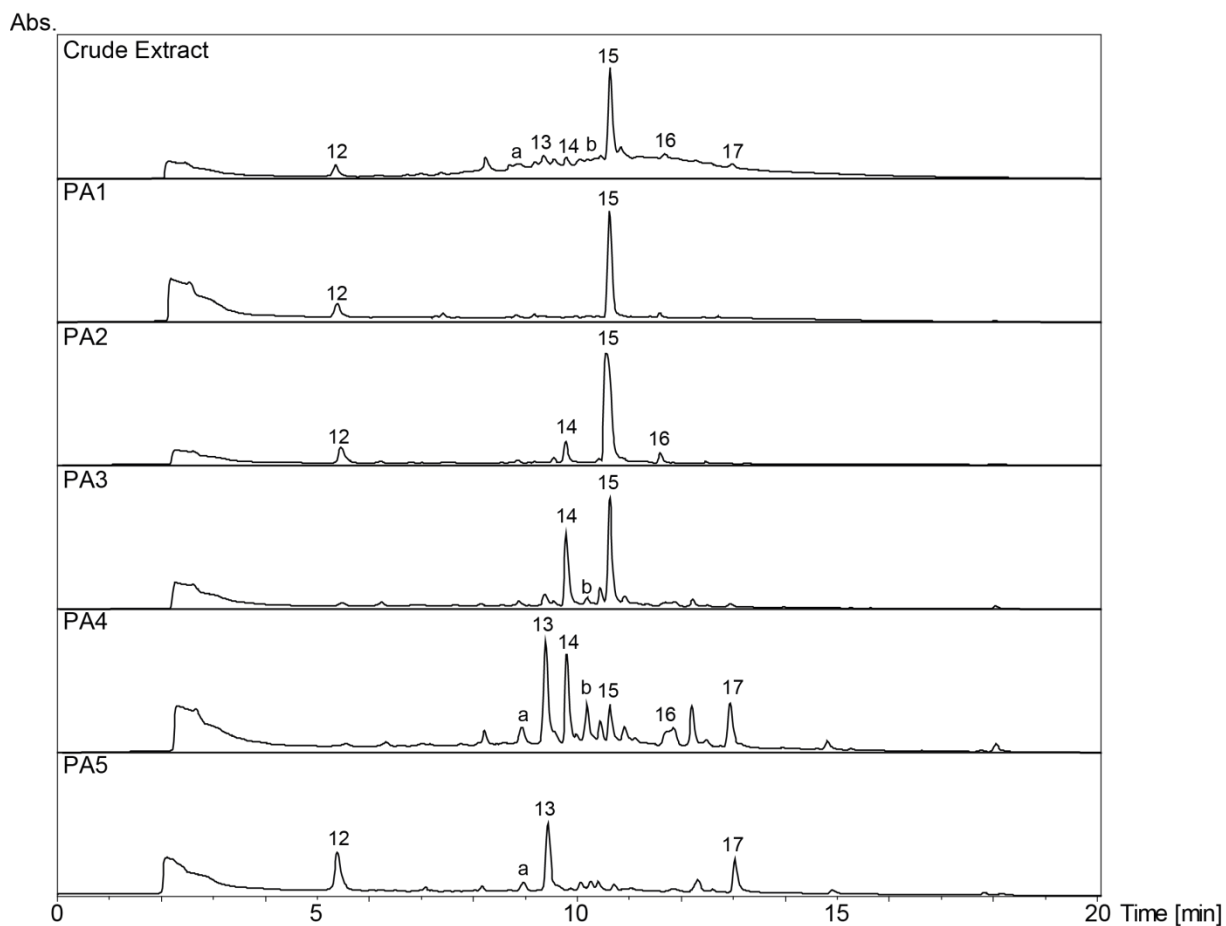


Fig. 3S. HPLC-DAD chromatograms of the crude extract and its polyamide fractions (PA1–PA5) of *Combretum aff. laxum*. SunFire C18 column (150 x 3 mm i.d., 3.5 μ m); 5–100% MeCN/0.1% aqueous formic acid in 30min, 0.4 mL/min; detection: 210–700nm, maxplot.

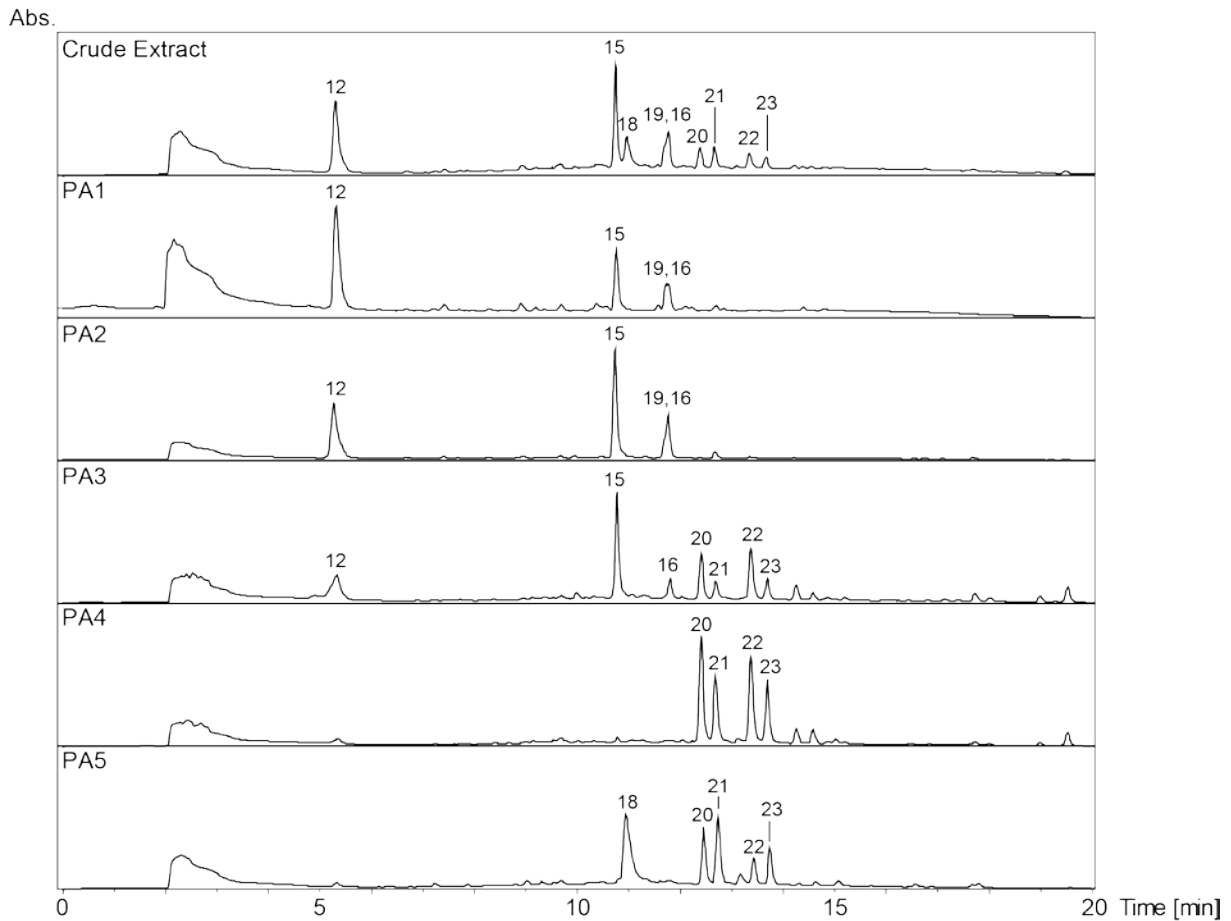
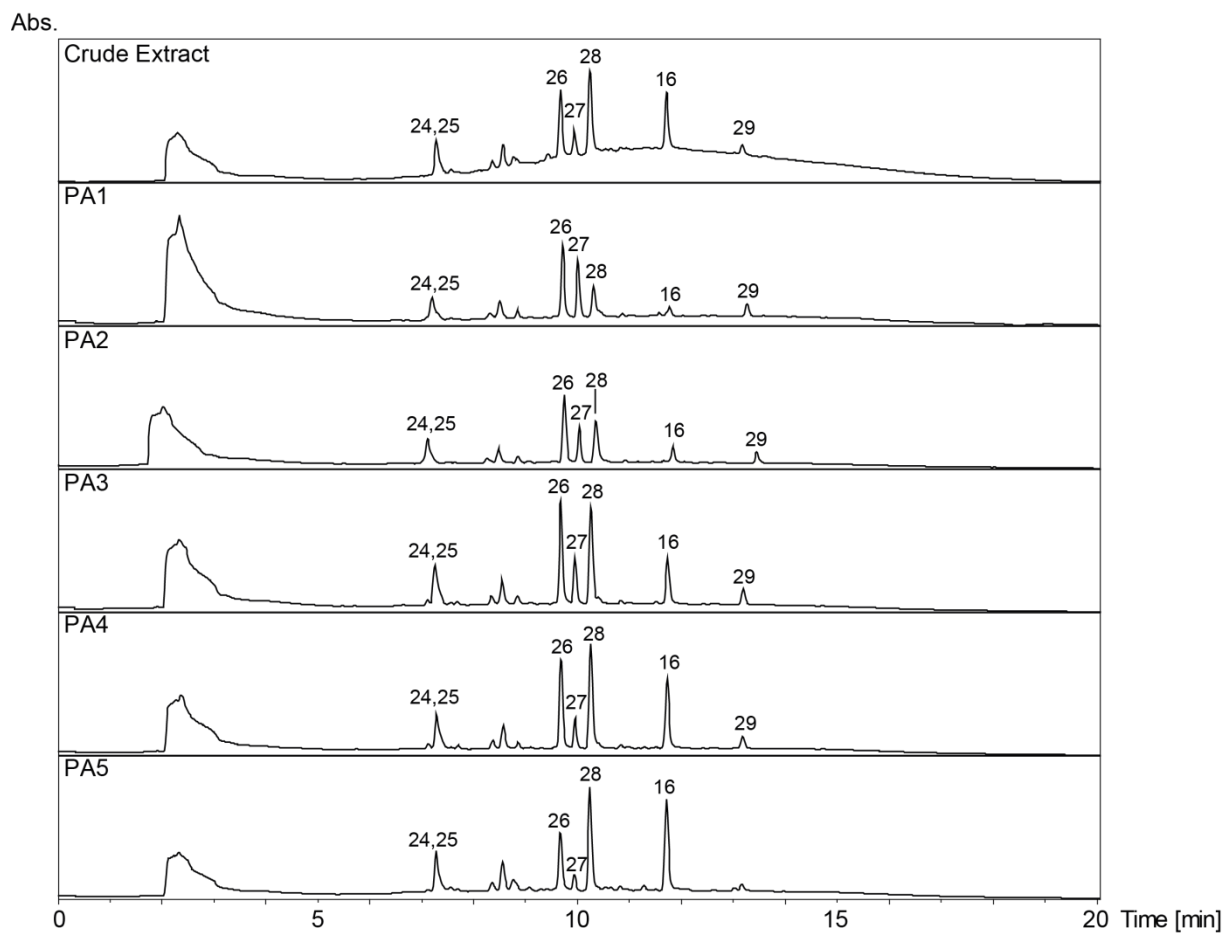


Fig. 4S. HPLC-DAD chromatograms of the crude extract and its polyamide fractions (PA1–PA5) of *Erythroxyllum macrophyllum*. SunFire C18 column (150 x 3 mm i.d., 3.5 μ m); 5–100% MeCN/0.1% aqueous formic acid in 30min, 0.4 mL/min; detection: 210–700nm, maxplot.



Tab. 2S. ^1H and ^{13}C NMR^a data (500 MHz) of compounds 1–5

Position	1 ^b		2 ^b		3 ^c		4 ^d		5 ^c	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	7.51 (s)	106.9	7.43 (s)	106.7	7.61 (s)	98.8	7.14 (s)	104.5	7.31 (s)	104.0
2	—	150.6	—	150.6	—	148.6	—	147.8	—	147.2
3	—	150.6	—	150.6	—	148.6	—	147.8	—	147.8
4	8.11 (s)	104.8	8.07 (s)	104.6	8.06 (s)	104.0	7.55 (s)	102.2	7.53 (s)	99.4
4a	—	121.4	—	121.5	—	120.7	—	118.9	—	124.9
4b	—	132.8	—	132.9	—	126.2	—	136.2	—	141.0
6	9.90 (s)	150.3	9.85 (s)	151.1	9.72 (s)	145.7	—	162.8	4.16 (s)	47.7
6a	—	110.9	—	120.6	—	109.8	—	111.1	—	112.3
7	—	147.8	—	147.1	—	139.0	—	146.6	—	144.2
8	—	149.2	—	151.6	—	147.5	—	146.6	—	146.6
9	7.93 (d, 8.8)	121.0	8.12 (d, 9.1)	127.2	7.83 (s)	103.8	7.22 (d, 8.6)	113.0	6.95 (d, 8.1)	107.1
10	8.47 (d, 8.8)	118.1	8.52 (d, 9.1)	119.4	—	152.8	7.74 (d, 8.6)	115.2	7.40 (d, 8.1)	116.1
10a	—	128.7	—	129.8	—	113.9	—	133.6	—	126.2
10b	—	127.3	—	126.6	—	123.5	—	115.9	—	123.7
11	8.56 (d, 8.9)	119.4	8.48 (d, 9.0)	119.1	8.71 (s)	99.6	7.96 (d, 8.6)	118.4	7.77 (d, 8.6)	120.0
12	8.16 (d, 8.9)	132.7	8.08 (d, 9.0)	132.2	—	155.0	7.51 (d, 8.6)	123.5	7.57 (d, 8.6)	123.9
12a	—	133.5	—	134.0	—	123.0	—	129.8	—	130.2
2,3-OCH ₂ O	6.28 (s)	104.0	6.24 (s)	103.8	6.32 (s)	102.3	6.08 (s)	101.1	6.14 (s)	100.9
5-NCH ₃	4.93 (s)	52.7	4.94 (s)	52.8	4.78 (s)	51.5	3.89 (s)	40.7	2.53 (s)	41.1
7,8-OCH ₂ O	6.53 (s)	106.2	—	—	6.51 (s)	103.6	6.25 (s)	102.7	6.10 (s)	101.1
7-OCH ₃	—	—	4.27 (s)	62.6	—	—	—	—	—	—
8-OCH ₃	—	—	4.11 (s)	57.4	—	—	—	—	—	—
10-OCH ₃	—	—	—	—	4.17 (s)	57.5	—	—	—	—
12-OCH ₃	—	—	—	—	4.12 (s)	55.7	—	—	—	—

^a ^{13}C NMR data derived from HSQC and HMBC experiments; ^b recorded in CD₃OD; ^c recorded in DMSO-d₆; ^d recorded in CDCl₃.

Tab. 3S. ^1H and ^{13}C NMR^a data (500 MHz) of compound **6** in DMSO- d_6

6		
Position	δ_{H}	δ_{C}
1	—	196.7
2	3.04 (t, 6.4)	40.6
3	3.76 (t, 6.4)	57.0
1'	—	127.6
2'	7.43 (d, 1.7)	110.9
3'	—	147.5
4'	—	152.6
5'	6.84 (d, 8.3)	114.8
6'	7.49 (dd, 8.3, 1.7)	123.1
3'-OCH ₃	3.81 (s)	55.3

^a ^{13}C NMR data derived from HSQC and HMBC experiments.

Tab. 4S. ^1H and ^{13}C NMR^a data (500 MHz) of compounds **12** and **25**

Position	12 ^b		25 ^c	
	δ_{H}	δ_{C} ^a	δ_{H}	δ_{C}
1	—	119.4	—	123.2
2	7.09 (s)	107.8	7.36 (s)	116.6
3	—	143.9	—	144.6
4	—	136.7	—	149.1
5	—	143.9	6.77 (d, 8.1)	114.8
6	7.09 (s)	107.8	7.28 (d, 8.1)	121.4
7	—	167.4	—	168.3

^a ^{13}C NMR data derived from HSQC and HMBC experiments; ^brecorded in CD_3OD ; ^crecorded in DMSO-d_6 .

Tab. 5S. ^1H and ^{13}C NMR^a (500 MHz) of compound **7** and **10**

Position	7 ^b		10 ^c	
	δ_{H}	δ_{C} ^a	δ_{H}	δ_{C}
1	—	n.d.	—	114.5
2	—	n.d.	—	132.4
3	—	138.3	—	138.8
4	—	150.2	—	151.3
5	7.44 (s)	103.3	7.57 (s)	105.0
6	—	n.d.	—	115.7
7	—	n.d.	—	158.6
1'	—	108.5	—	113.0
2'	—	n.d.	—	137.9
3'	—	141.4	—	147.6
4'	—	n.d.	—	148.6
5'	7.47 (s)	113.2	—	154.3
6'	—	n.d.	—	105.9
7'	—	n.d.	—	154.9
3,4-OCH ₂ O	6.34 (s)	103.6	6.27 (s)	104.2
3'-OCH ₃	4.04 (s)	60.2	4.25 (s)	62.3
4'-OCH ₃	—	—	4.00 (s)	62.3
5'-OCH ₃	—	—	4.02 (s)	62.6

^a ^{13}C NMR data derived from HSQC and HMBC experiments; ^brecorded in DMSO-*d*₆; ^crecorded in CDCl₃; n.d.: not detected.

Tab. 6S. ^1H and ^{13}C NMR data (500 MHz) of compound **8** in DMSO-d_6

8		
Position	δ_{H}	δ_{C}
1a	0.73 (m)	
1b	1.75 (dd, 12.5, 4.4)	46.7
2	3.49 (ddd, 11.0, 9.3, 4.4)	67.4
3	3.18 (d, 9.3)	75.5
4	—	42.5
5	1.22 (m)	46.0
6a	1.24 (m)	
6b	1.41 (m)	17.5
7a	1.19 (m)	
7b	1.44 (m)	31.9
8	—	38.9
9	1.55 (t, 8.8)	47.1
10	—	37.4
11	1.84 (m)	23.0
12	5.18 (t, 3.3)	121.5
13	—	143.9
14	—	41.4
15a	0.99 (m)	
15b	1.68 (m)	27.2
16a	1.49 (m)	
16b	1.91 (td, 13.5, 3.7)	22.6
17	—	45.4
18	2.76 (dd, 13.7, 3.9)	40.8
19a	1.07 (m)	
19b	1.62 (m)	45.7
20	—	30.4
21a	1.14 (m)	
21b	1.32 (td, 13.6, 3.6)	33.3
22a	1.44 (m)	
22b	1.63 (m)	32.1
23a	3.06 (d, 10.6)	
23b	3.32 (d, 10.6)	63.9
24	0.56 (s)	13.7
25	0.93 (s)	16.8
26	0.72 (s)	16.9
27	1.10 (s)	25.7
28	—	178.6
29	0.88 (s)	32.9
30	0.88 (s)	23.4

Tab. 7S. ^1H and ^{13}C NMR^a (500 MHz) of compounds **13** and **14** in CD_3OD

Position	13		14	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
2	—	158.8	—	n.d.
3	—	135.9	—	135.8
4	—	n.d.	—	n.d.
5	—	n.d.	—	162.7
6	6.17 (d, 1.8)	99.8	6.17 (s)	99.5
7	—	n.d.	—	165.7
8	6.35 (d, 1.8)	94.6	6.35 (s)	94.3
9	—	n.d.	—	158.3
10	—	n.d.	—	105.5
1'	—	121.5	—	121.3
2'	7.34 (s)	110.0	7.37 (s)	109.7
3'	—	146.3	—	145.8
4'	—	139.8	—	137.8
5'	—	146.3	—	145.8
6'	7.34 (s)	110.0	7.37 (s)	109.7
1''	5.15 (d, 7.9)	105.2	5.13 (d, 7.8)	105.2
2''	3.87 (dd, 9.5, 7.9)	73.0	3.85 (dd, 9.5, 7.8)	72.9
3''	3.62 (dd, 9.5, 2.9)	74.8	3.61 (m)	74.6
4''	3.91 (d, 2.9)	69.9	3.89 (d, 2.5)	69.6
5''	3.81 (t, 6.4)	74.3	3.52 (t, 6.1)	76.6
6''a	4.25 (dd, 11.1, 5.9)	63.6	3.61 (m)	61.6
6''b	4.33 (dd, 11.1, 6.9)		3.67 (dd, 11.2, 5.9)	
1'''	—	121.1	—	—
2'''	6.91	110.0	—	—
3'''	—	146.3	—	—
4'''	—	138.2	—	—
5'''	—	146.3	—	—
6'''	6.91	110.0	—	—
7'''	—	167.8	—	—

^a ^{13}C NMR data derived from HSQC and HMBC experiments; n.d.: not detected.

Tab. 8S. ^1H and ^{13}C NMR^a (500 MHz) of compounds **15–17** in CD_3OD

Position	15		16		17	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}
2	—	158.9	—	158.9	—	n.d.
3	—	135.9	—	135.8	—	n.d.
4	—	179.2	—	n.d.	—	n.d.
5	—	163.2	—	163.6	—	n.d.
6	6.20 (d, 2.0)	99.6	6.20 (d, 1.7)	99.7	6.18 (s)	99.2
7	—	165.5	—	165.4	—	n.d.
8	6.36 (d, 2.0)	94.5	6.36 (d, 1.7)	94.6	6.37 (s)	94.2
9	—	158.0	—	158.2	—	n.d.
10	—	105.4	—	105.6	—	n.d.
1'	—	121.5	—	n.d.	—	123.3
2'	6.95 (s)	109.3	7.34 (d, 2.1)	116.9	7.35 (s)	108.5
3'	—	146.4	—	146.2	—	147.5
4'	—	137.4	—	149.1	—	137.1
5'	—	146.4	6.92 (d, 6.3)	116.2	—	147.5
6'	6.95 (s)	109.3	7.30 (dd, 6.3, 2.1)	122.7	7.35 (s)	108.5
1''	5.32 (d, 1.5)	103.4	5.36 (d, 1.3)	103.3	—	—
2''	4.23 (dd, 3.3, 1.5)	71.7	4.23 (dd, 3.1, 1.3)	71.7	—	—
3''	3.79 (dd, 9.5, 3.3)	71.9	3.76 (dd, 9.3, 3.1)	72.1	—	—
4''	3.35 (t, 9.6)	73.2	3.35 (9.4)	73.2	—	—
5''	3.52 (dq, 9.7, 6.2)	71.8	3.43 (dq, 9.6, 6.1)	71.8	—	—
6''	0.97 (d, 6.2)	17.6	0.95 (d, 6.1)	17.5	—	—

^a ^{13}C NMR data derived from HSQC and HMBC experiments; n.d.: not detected.

Tab. 9S. ^1H and ^{13}C NMR^a (500 MHz) of compounds **19** and **26** in DMSO- d_6

Position	19		26	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
2	—	157.1	—	n.d.
3	—	n.d.	—	135.0
4	—	n.d.	—	n.d.
5	—	n.d.	—	n.d.
6	6.24 (d, 1.2)	98.5	6.44 (d, 1.6)	99.1
7	—	n.d.	—	n.d.
8	6.44 (d, 1.2)	93.2	6.75 (d, 1.6)	94.1
9	—	n.d.	—	n.d.
10	—	104.2	—	105.6
1'	—	n.d.	—	n.d.
2'	6.86 (s)	107.8	7.36 (d, 1.8)	115.5
3'	—	150.7	—	145.0
4'	—	137.9	—	148.1
5'	—	150.7	6.89 (d, 8.2)	115.2
6'	6.86 (s)	107.8	7.30 (dd, 8.2, 1.8)	120.9
1''	5.16 (d, 1.0)	101.8	5.28 (s)	101.6
2''	4.00 (m)	69.7	4.00 (bs)	69.8
3''	3.56 (m)	70.1	3.55 (dd, 9.2, 3.1)	70.2
4''	3.16 (m)	71.0	3.18 (m)	71.0
5''	3.22 (m)	70.0	3.28 (m)	70.2
6''	0.83 (d, 6.1)	17.1	0.85 (d, 6.1)	17.3
1'''	—	—	5.55 (s)	98.2
2'''	—	—	3.86 (bs)	69.5
3'''	—	—	3.65 (dd, 9.2, 3.0)	70.0
4'''	—	—	3.32 (m)	71.4
5'''	—	—	3.46 (m)	69.8
6'''	—	—	1.14 (d, 6.1)	17.6
4'-OCH ₃	3.75 (s)	59.3	—	—

^a ^{13}C NMR data derived from HSQC and HMBC experiments; n.d.: not detected.

Tab. 10S. ^1H and ^{13}C NMR^a (500 MHz) of compounds **20–23** in CD_3OD

Position	20		21		22		23	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}
2	—	158.7	—	158.9	—	158.9	—	159.3
3	—	135.1	—	135.7	—	135.2	—	135.9
4	—	178.9	—	n.d.	—	178.7	—	n.d.
5	—	163.3	—	163.6	—	163.4	—	163.9
6	6.18 (d, 1.8)	99.3	6.21 (s)	99.3	6.19 (d, 1.9)	99.6	6.21 (s)	99.8
7	—	165.5	—	165.3	—	165.2	—	165.8
8	6.35 (d, 1.8)	94.2	6.37 (s)	94.2	6.36 (d, 1.9)	94.4	6.38 (s)	94.7
9	—	157.9	—	157.8	—	158.0	—	158.3
10	—	105.4	—	105.6	—	105.4	—	106.0
1'	—	121.6	—	121.7	—	n.d.	—	n.d.
2'	7.00 (s)	109.3	7.02 (s)	109.3	7.37 (d, 2.0)	116.7	7.40 (m)	116.9
3'	—	146.2	—	146.4	—	146.0	—	146.5
4'	—	137.2	—	137.5	—	149.3	—	149.6
5'	—	146.2	—	146.4	6.94 (d, 8.3)	116.2	6.96 (d, 8.7)	116.5
6'	7.00 (s)	109.3	7.02 (s)	109.3	7.33 (dd, 8.3, 2.0)	122.6	7.40 (m)	123.0
1''	5.51 (d, 1.1)	100.0	5.34 (d, 1.1)	103.0	5.50 (d, 1.5)	100.2	5.41 (bs)	103.3
2''	5.64 (dd, 3.1, 1.1)	73.0	4.51 (dd, 2.8, 1.1)	69.5	5.64 (dd, 3.2, 1.5)	73.3	4.49 (m)	69.9
3''	4.08 (dd, 8.9, 3.1)	70.2	5.27 (dd, 8.9, 2.8)	75.0	4.04 (dd, 8.9, 3.2)	70.5	5.24 (9.7, 3.0)	75.3
4''	3.50 (m)	73.4	3.70 (m)	70.5	3.47 (m)	73.5	3.69 (t, 9.7)	70.9
5''	3.53 (m)	71.7	3.70 (m)	71.8	3.47 (m)	71.9	3.59 (m)	72.2
6''	1.05 (d, 5.6)	17.2	1.02 (d, 4.5)	17.1	1.04 (d, 5.4)	17.4	1.01 (d, 6.1)	17.6
1'''	—	120.8	—	121.2	—	121.0	—	121.7
2'''	7.09 (s)	110.0	7.19 (s)	110.1	7.09 (s)	110.2	7.19 (s)	110.5
3'''	—	145.6	—	145.8	—	146.0	—	146.3
4'''	—	139.3	—	139.5	—	139.4	—	139.9
5'''	—	145.6	—	145.8	—	146.0	—	146.3
6'''	7.09 (s)	110.0	7.19 (s)	110.1	7.09 (s)	110.2	7.19 (s)	110.5
7'''	—	166.9	—	168.2	—	167.1	—	168.4

^a ^{13}C NMR data derived from HSQC and HMBC experiments; n.d.: not detected.

Tab. 11S. ^1H and ^{13}C NMR^a (500 MHz) of compounds **24** in DMSO- d_6

24		
Position	δ_{H}	δ_{C}
1	—	n.d.
2a	1.71 (d, 12.8)	37.2
2b	1.89 (m)	68.1
3	3.76 (m)	70.6
4	3.63 (m)	70.4
5	5.26 (bs)	35.6
6a	1.85 (m)	165.6
6b	1.93 (m)	114.6
1'	—	144.1
2'	6.20 (d, 15.9)	125.2
3'	7.47 (d, 15.9)	114.4
4'	—	145.3
5'	7.04 (s)	147.6
6'	—	115.6
7'	—	120.7
8'	6.78 (d, 7.9)	n.d.
9'	6.96 (d, 7.9)	n.d.
1-COOH	—	n.d.

^a ^{13}C NMR data derived from HSQC and HMBC experiments; n.d.: not detected.

Tab. 12S. ^1H and ^{13}C NMR (500 MHz) of compounds **27–29** in DMSO-d_6

Position	27		28		29	
	δ_{H}	δ_{C}	δ_{H}	$\delta_{\text{C}}^{\text{a}}$	δ_{H}	$\delta_{\text{C}}^{\text{a}}$
2	—	154.7	—	156.2	—	n.d.
3	—	136.0	—	n.d.	—	n.d.
4	—	173.2	—	n.d.	—	n.d.
5	—	158.4	—	160.9	—	n.d.
6	6.86 (s)	102.4	6.19 (s)	98.5	6.35 (s)	97.5
7	—	163.8	—	163.9	—	164.6
8	—	95.7	—	93.3	—	91.6
9	—	157.7	—	156.0	—	n.d.
10	—	109.0	—	103.5	—	n.d.
1'	—	122.5	—	120.9	—	121.8
2'	7.57 (s)	115.8	7.54 (m)	116.0	7.56 (s)	115.3
3'	—	145.9	—	144.4	—	145.5
4'	—	150.0	—	147.6	—	149.7
5'	7.03 (d, 8.5)	111.3	6.85 (d, 7.8)	114.9	7.04 (d, 8.7)	110.9
6'	7.74 (d, 8.5)	121.5	7.54 (m)	121.2	7.72 (d, 8.7)	120.9
1''	5.25 (d, 6.9)	101.4	5.34 (bd)	101.0	5.39 (d, 6.6)	100.6
2''	3.26 (m)	74.1	3.25 (m)	73.8	3.22 (m)	73.5
3''	3.27 (m)	75.7	3.24 (m)	76.1	3.23 (m)	75.8
4''	3.12 (m)	69.8	3.30 (m)	70.3	3.10 (m)	69.4
5''	3.28 (m)	76.5	3.26 (m)	75.6	3.25 (m)	75.4
6''a	3.34 (m)	66.9	3.30 (m)	66.8	3.31 (m)	66.4
6''b	3.71 (d, 11.1)	66.9	3.72 (d, 10.8)	66.8	3.69 (m)	66.4
1'''	4.42 (bs)	100.8	4.40 (s)	100.4	4.39 (s)	100.3
2'''	3.42 (m)	70.4	3.42 (m)	70.1	3.41 (m)	69.9
3'''	3.33 (m)	70.7	3.08 (m)	69.8	3.29 (m)	70.1
4'''	3.10 (m)	71.9	3.09 (m)	71.6	3.08 (m)	71.3
5'''	3.30 (m)	68.3	3.29 (m)	67.8	3.27 (m)	67.8
6'''	0.99 (d, 5.9)	17.9	1.00 (d, 4.4)	17.5	0.97 (d, 6.0)	17.4
1''''	4.84 (d, 7.4)	103.7	—	—	—	—
2''''	3.42 (m)	73.6	—	—	—	—
3''''	3.34 (m)	75.9	—	—	—	—
4''''	3.21 (m)	69.9	—	—	—	—
5''''	3.41 (m)	77.7	—	—	—	—
6''''a	3.53 (dd, 11.1, 6.0)	60.9	—	—	—	—
6''''b	3.77 (d, 11.1)	60.9	—	—	—	—
7-OCH ₃	3.89 (s)	56.2	—	—	3.86 (s)	55.3
4'-OCH ₃	3.86 (s)	55.7	—	—	3.86 (s)	55.3

^a ^{13}C NMR data derived from HSQC and HMBC experiments; n.d.: not detected.