Supporting Information

***Rec. Nat. Prod.* X:X (202X) XX-XX**

A New Diphenyl Ether Derivative Isolate from an Endolichenic Fungus *Preussia africana*

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S1. ^{1}H and ^{13}C NMR data for compounds 2–6

Barceloneic lactone B (**2**), ^{1}H NMR (600 MHz, DMSO-d_6) of compound **2**: δ_H 7.09 (1H, d, J = 2.4 Hz, H-4), 7.57 (1H, t, J = 8.3 Hz, H-5), 6.79 (1H, d, J = 8.3 Hz, H-6), 6.92 (1H, s, H-10), 5.05 (1H, s, H-14), 4.35 (1H, d, J = 8.3 Hz, H-15), 3.86 (3H, s, H-3a), 9.71 (1H, br s, OH-9), 5.15 (1H, t, J =5.7 Hz, OH-15); ^{13}C NMR (600 MHz, DMSO-d_6): 166.8 (C-1), 115.6 (C-2), 157.2 (C-3), 110.0 (C-4), 134.3 (C-5), 114.7 (C-6), 152.8 (C-7), 142.8 (C-8), 149.1 (C-9), 116.2 (C-10), 139.7 (C-11),117.8 (C-12), 68.9 (C-14),62.6 (C-15),56.7 (C-3a).

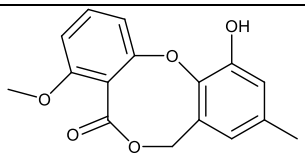
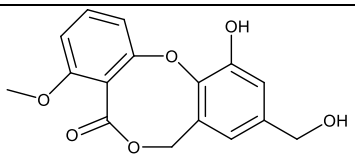
Quercilolin (**3**), ^{1}H NMR (600 MHz, Aceton-d_6) of compound **3**: δ_H 6.34 (1H, d, J = 1.8 Hz, H-2), 6.21 (1H, d, J = 2.0 Hz, H-6), 6.28 (1H, s, H-2′), 6.12 (1H, s, H-4′), 6.02 (1H, s, H-6′), 3.74 (1H, s, 4-OMe), 2.17 (1H, s, 5′-Me), 2.02 (1H, s, 5-Me); ^{13}C NMR (150 MHz, Aceton-d_6) δ**:** 134.0 (C-1), 100.1 (C-2), 150.6 (C-3), 157.3 (C-4), 133.4 (C-5), 106.7 (C-6), 139.9 (C-1′), 99.1 (C-2′), 159.5 (C-3′), 106.8 (C-4′), 158.4 (C-5′),109.3 (C-6′), 54.7 (4-OMe),20.7 (5′-Me),15.6 (5-Me).

3-hydroxy-5-methylphenyl ether (**4**), ^{1}H NMR (600 MHz, DMSO-d_6) of compound **4**: δ_H 6.39 (1H, d, J = 2.5 Hz, H-3′), 6.31 (1H, s, H-4), 6.29 (1H, d, J = 2.5 Hz, H-5′), 6.26 (1H, s, H-6), 6.10 (1H, s, H-2), 2.21(3H, s, 4′-Me), 2.01 (3H, s, 3-Me); ^{13}C NMR (600 MHz, DMSO-d_6) δ: 159.6 (C-5), 158.2 (C-1′), 157.6 (C-6′), 150.4 (C-2′), 139.7 (C-3), 134.1 (C-1), 130.2 (C-4′), 109.4 (C-4), 107.0 (C-6), 107.0 (C-2), 100.2 (C-3′), 99.0 (C-5′), 21.7 (3-Me), 16.5 (4′-Me).

2,2′,3,4′-tetrahydroxy-5,6′-dimethyldiphenyl ether (**5**), ^{1}H NMR (600 MHz, DMSO-d_6) of compound **5**: δ_H 6.35 (1H, d, J = 3.0 Hz, H-3′), 6.29 (1H, d, J = 3.0 Hz, H-5′), 6.21 (1H, d, J = 1.2 Hz, H-6), 5.62 (1H, d, J = 1.2 Hz, H-4), 3.69 (3H, s, 4′-OMe), 2.00 (3H, s, 6′-Me), 1.97 (3H, s, 5-Me); ^{13}C NMR (600 MHz, DMSO-d_6) δ: 156.2 (C-4′), 150.6 (C-2′), 146.8 (C-3), 146.1 (C-1), 134.4 (C-1′), 132.3 (C-6′), 131.6 (C-2), 126.8 (C-5), 109.8 (C-6), 106.0 (C-5′), 104.9 (C-4), 100.4 (C-3′), 55.0 (4′-OMe), 20.8 (5-Me), 16.1 (6′-Me).

1,3,6-trihydroxy-8-methyl-9H-xanthen-9-one (**6**), ^{1}H NMR (600 MHz, DMSO-d_6) of compound **6**: δ_H 6.64 (1H, d, J = 2.3 Hz, H-5), 6.62 (1H, dd, J = 1.1, 2.4 Hz, H-7), 6.26 (1H, d, J = 2.2 Hz, H-4), 6.11 (1H, d, J = 2.2 Hz, H-2), 2.72 (3H, s, 8-Me); ^{13}C NMR (600 MHz, DMSO-d_6) δ: 181.8 (C-9), 165.5 (C-3), 163.7 (C-1), 163.5 (C-6), 159.3 (C-10a), 157.0 (C-4a), 143.2 (C-8), 116.8 (C-7), 111.1 (C-8a), 102.5 (C-9a), 100.1 (C-5), 98.3 (C-2), 93.7 (C-4), 23.5 (8-Me).

Table S1: Comparison of NMR data between compound **1** and barceloneic lactone B in DMSO-d_6

No.	 **1**		 barceloneic lactone B	
	δ_H (integral, mult., J in Hz)	δ_C	δ_H (integral, mult., J in Hz)	δ_C
1	-	166.3	-	166.8
2	-	115.1	-	115.6
3	-	156.7	-	157.2
4	7.07 (1H, d, J = 8.4 Hz)	109.5	7.09 (1H, d, J = 8.3 Hz)	110.0
5	7.54 (1H, t, J = 8.4 Hz)	133.8	7.57 (1H, t, J = 8.3 Hz)	134.3
6	6.77 (1H, d, J = 8.4 Hz, overlapped)	114.3	6.79 (1H, d, J = 8.3 Hz)	114.7
7	-	152.3	-	152.8
8	-	141.6	-	142.8
9	-	148.5	-	149.1
10	6.77 (1H, br s)	118.2	6.92 (1H, s)	116.2
11	-	134.0	-	139.7
12	6.41 (1H, br s)	119.9	6.56 (1H, s)	117.8
13	-	127.3		127.7
14	5.01 (2H, s)	68.4	5.05 (2H, s)	68.9
15	2.15 (3H, s)	20.4	4.35 (2H, d, J = 5.7 Hz)	62.6
3-OMe	3.85 (3H, s)	56.2	3.86 (3H, s)	56.7
9-OH	9.65 (s)	-	9.71 (br s)	-
15-OH	-	-	5.15 (t, J = 5.7 Hz)	-

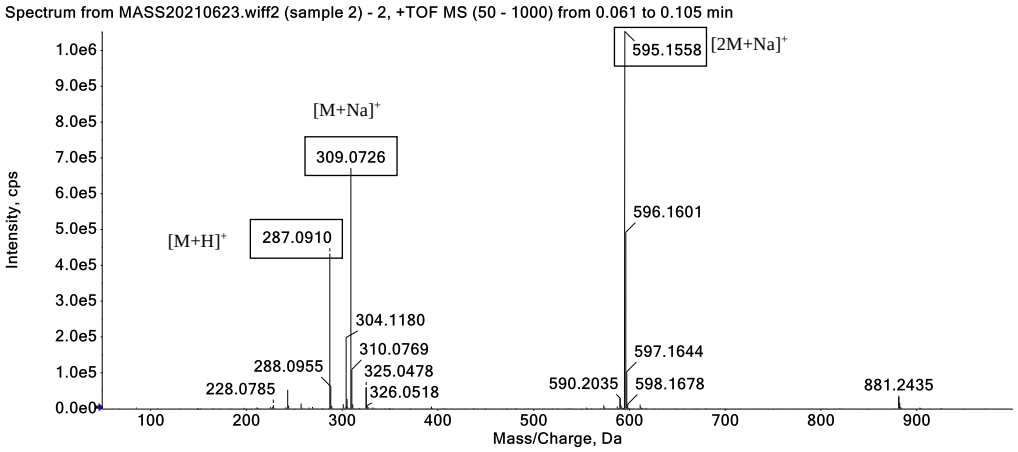
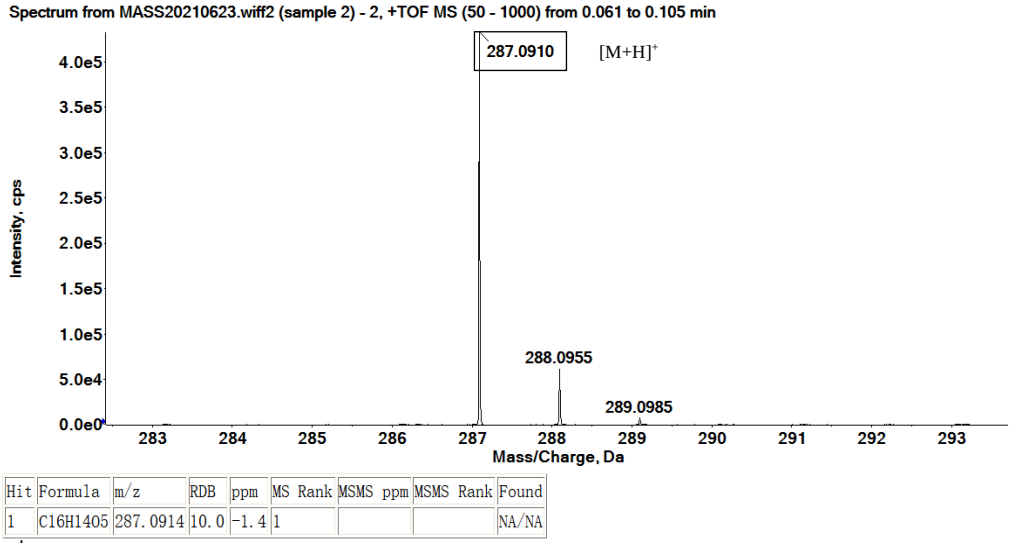


Figure S1: HR-ESI-MS spectrum of **1** (barceloneic lactone D) (From 100 Da to 900 Da)



Hit	Formula	m/z	RDB	ppm	MS Rank	MSMS ppm	MSMS Rank	Found
1	C16H14O5	287.0914	10.0	-1.4	1			NA/NA

Figure S2: HR-ESI-MS spectrum of **1** (barceloneic lactone D) (From 283 Da to 293 Da)

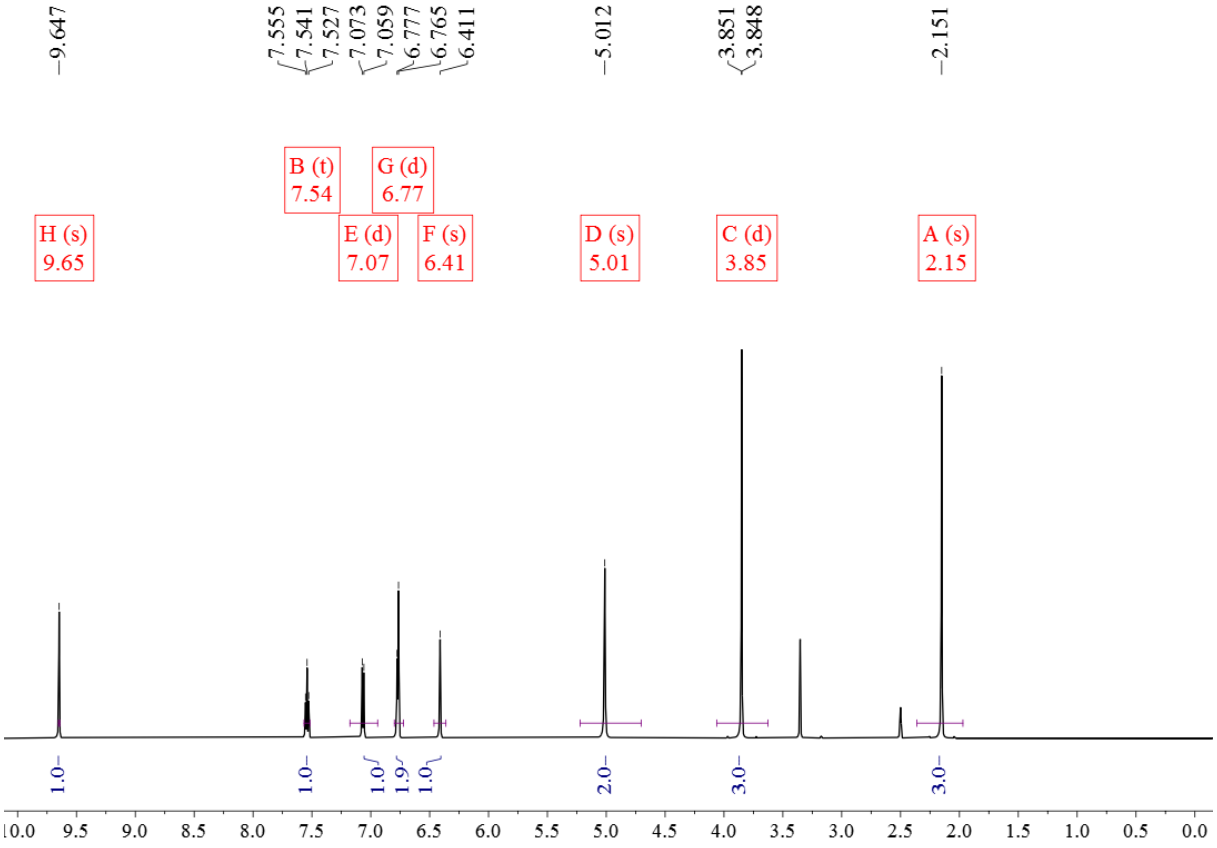


Figure S3: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **1** (barceloneic lactone D)

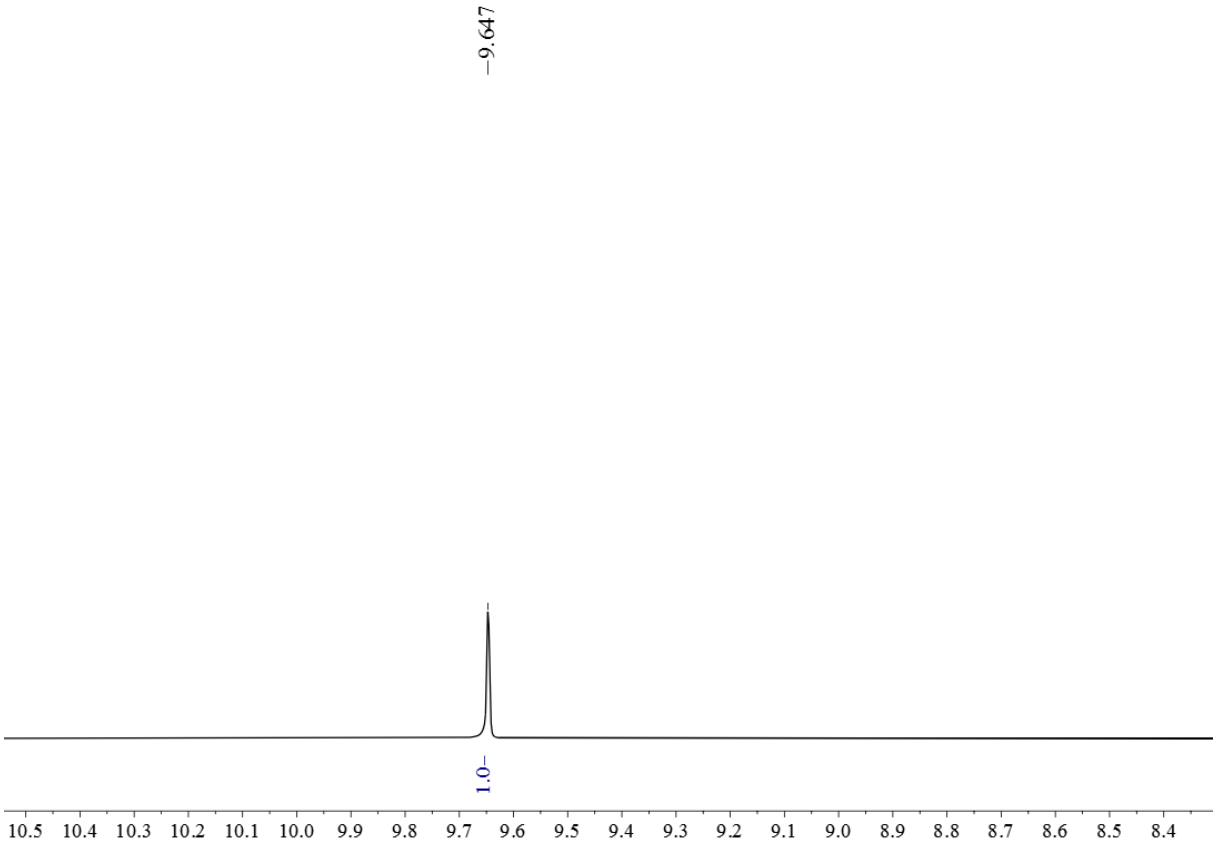


Figure S4: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **1** (barceloneic lactone D) (From δ_H 8.4 ppm to 10.5 ppm)

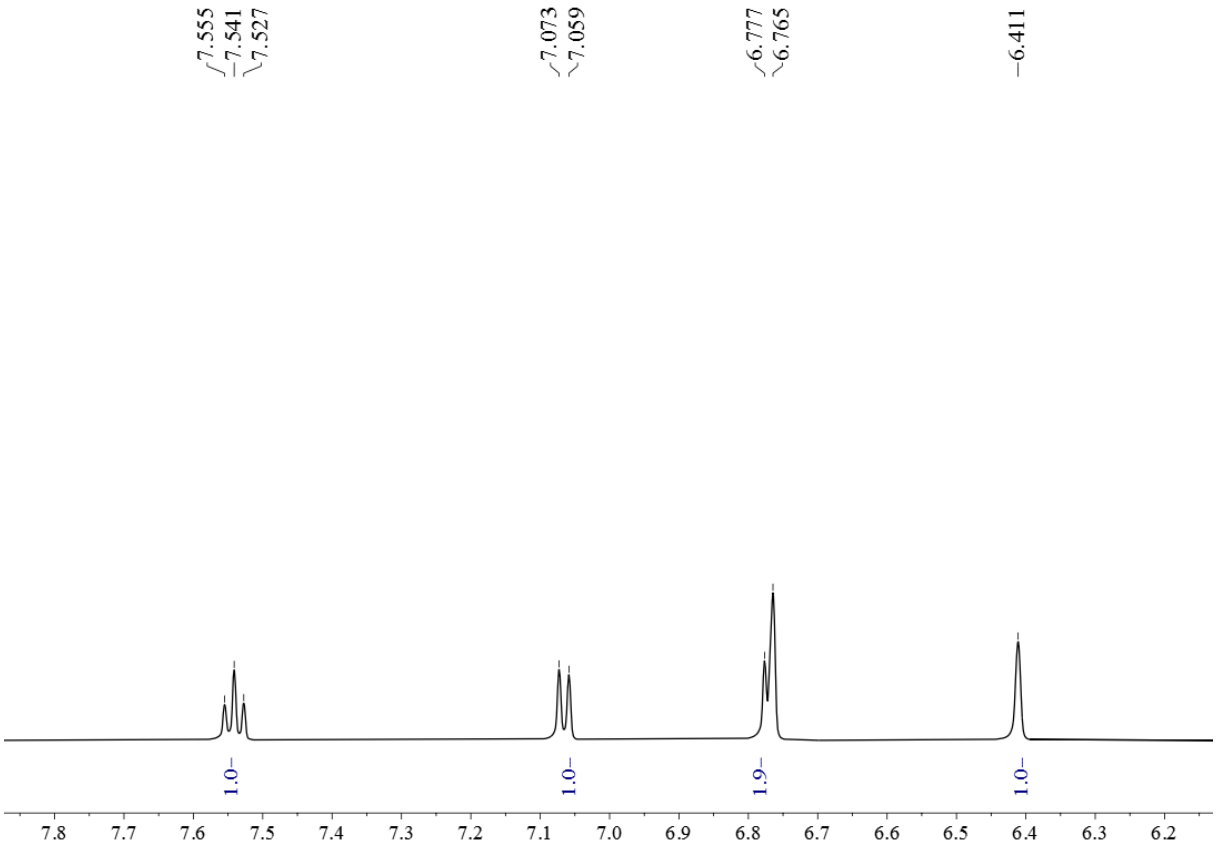


Figure S5: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **1** (barceloneic lactone D) (From δ_H 6.2 ppm to 7.8 ppm)

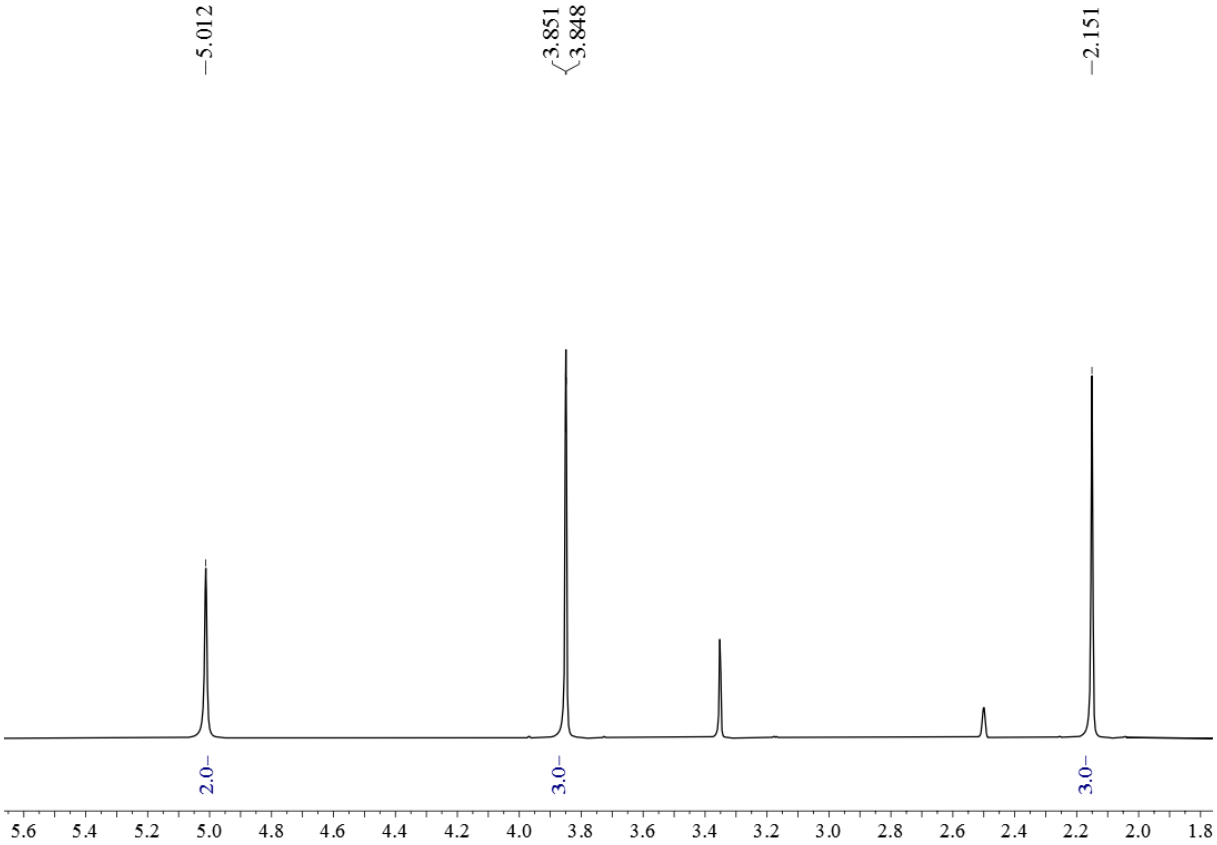


Figure S6: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **1** (barceloneic lactone D) (From δ_H 1.8 ppm to 5.6 ppm)

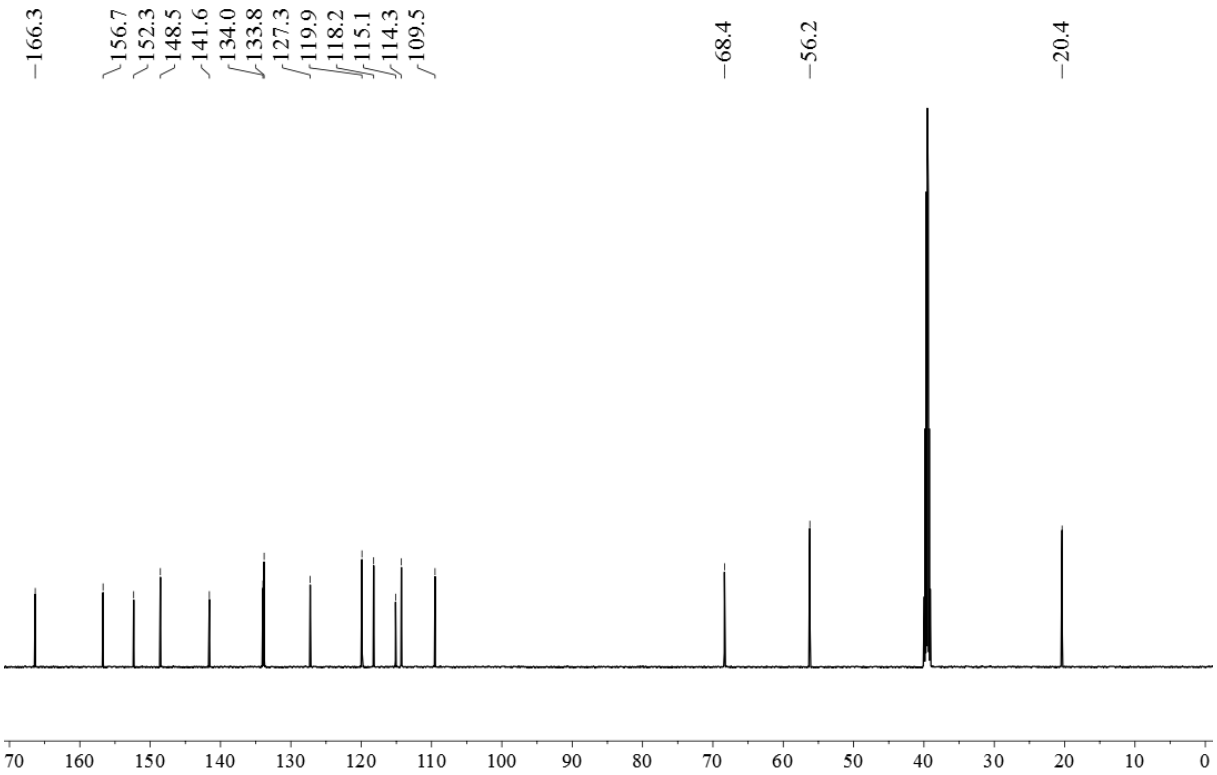


Figure S7: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of **1** (barceloneic lactone D)

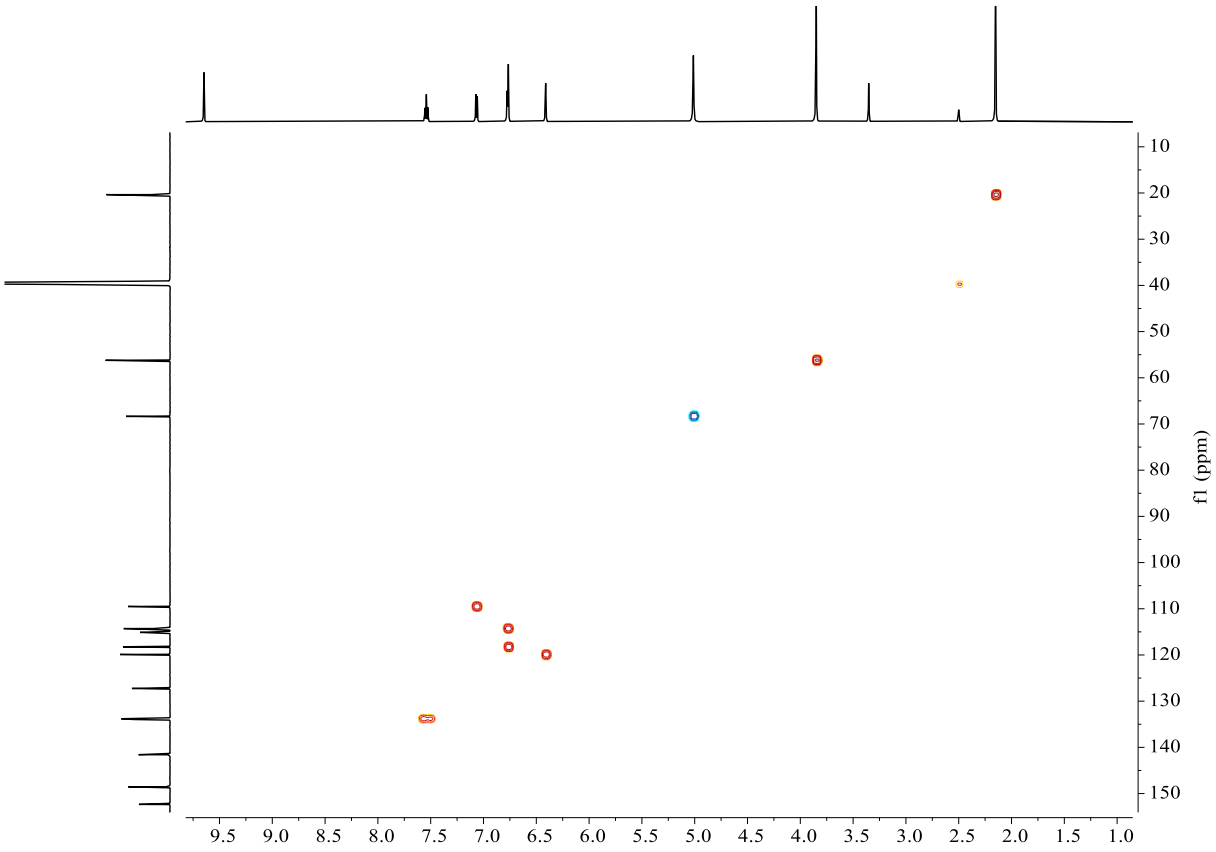


Figure S8: HSQC spectrum of **1** (barceloneic lactone D)

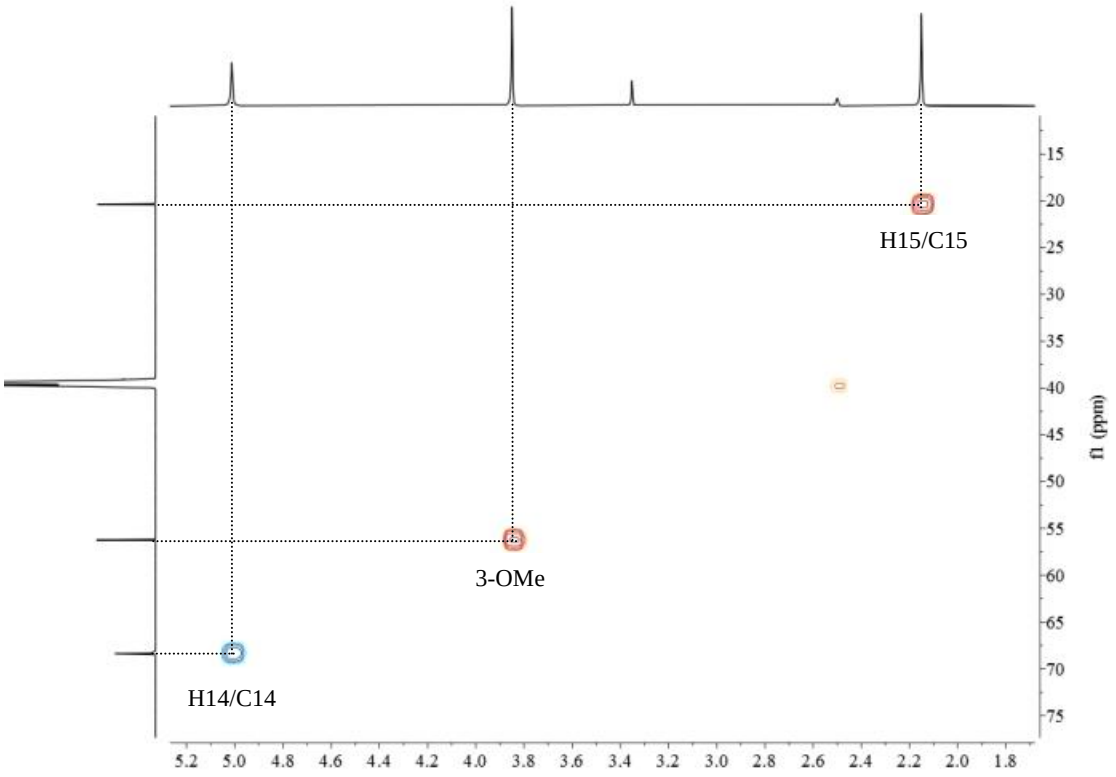


Figure S9: HSQC spectrum of **1** (barceloneic lactone D) (From δ_C 15 ppm to 75 ppm)

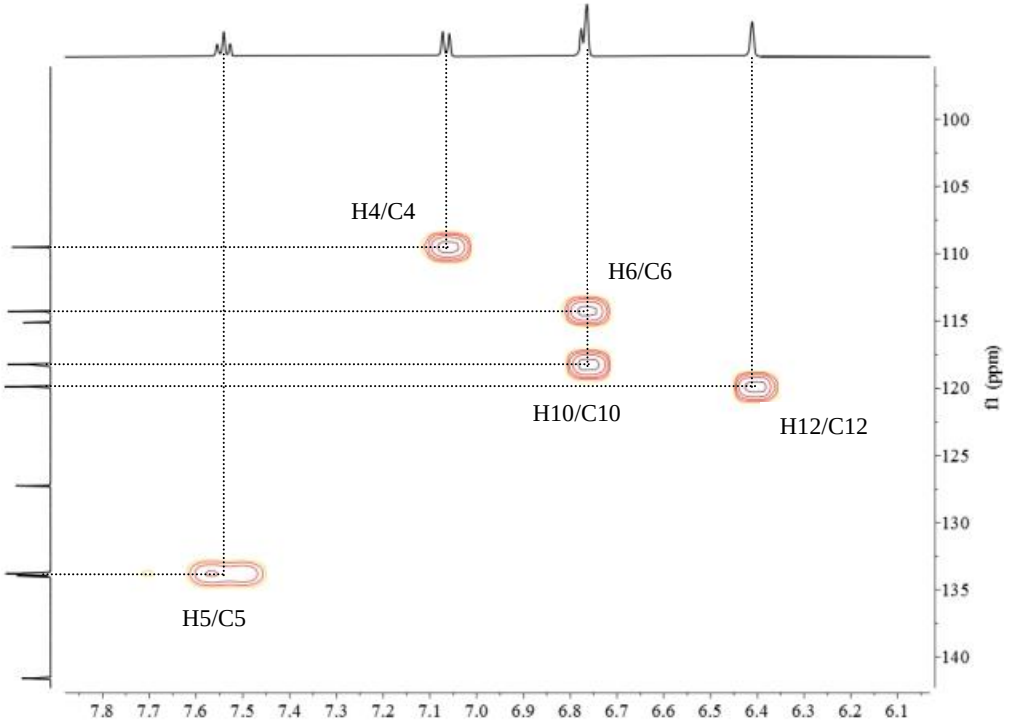


Figure S10: HSQC spectrum of **1** (barceloneic lactone D) (From δ_C 100 ppm to 140 ppm)

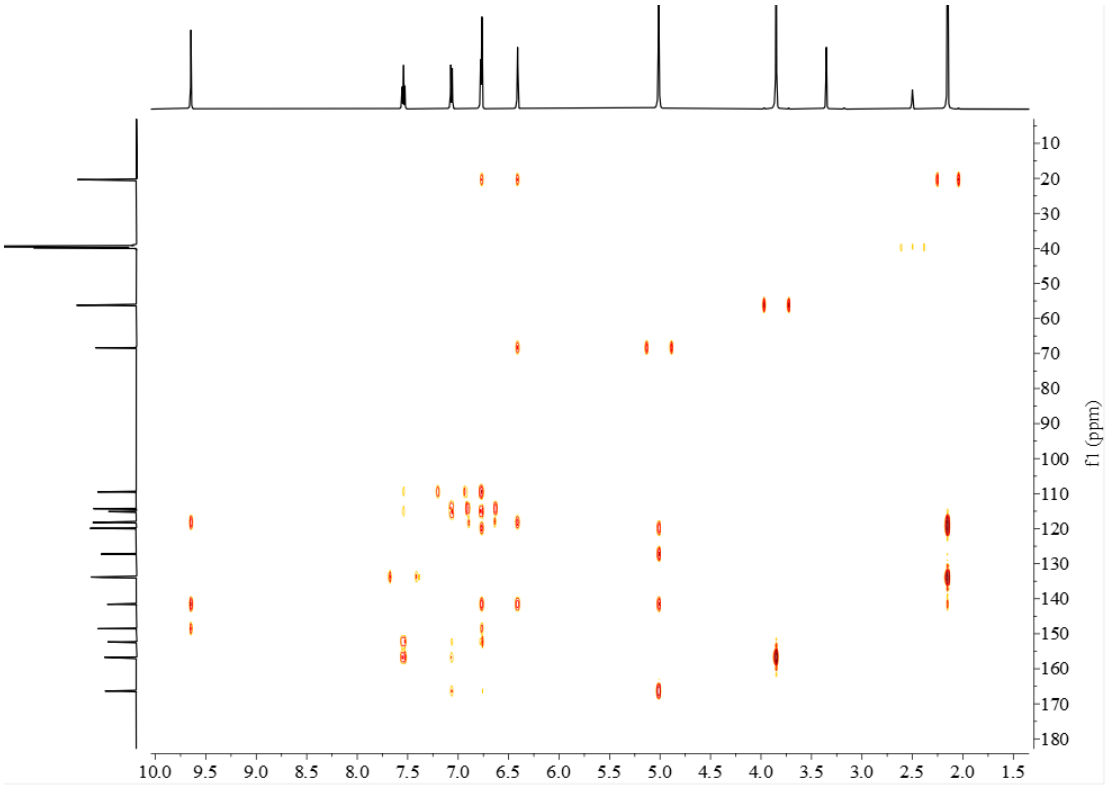


Figure S11: HMBC spectrum of **1** (barceloneic lactone D)

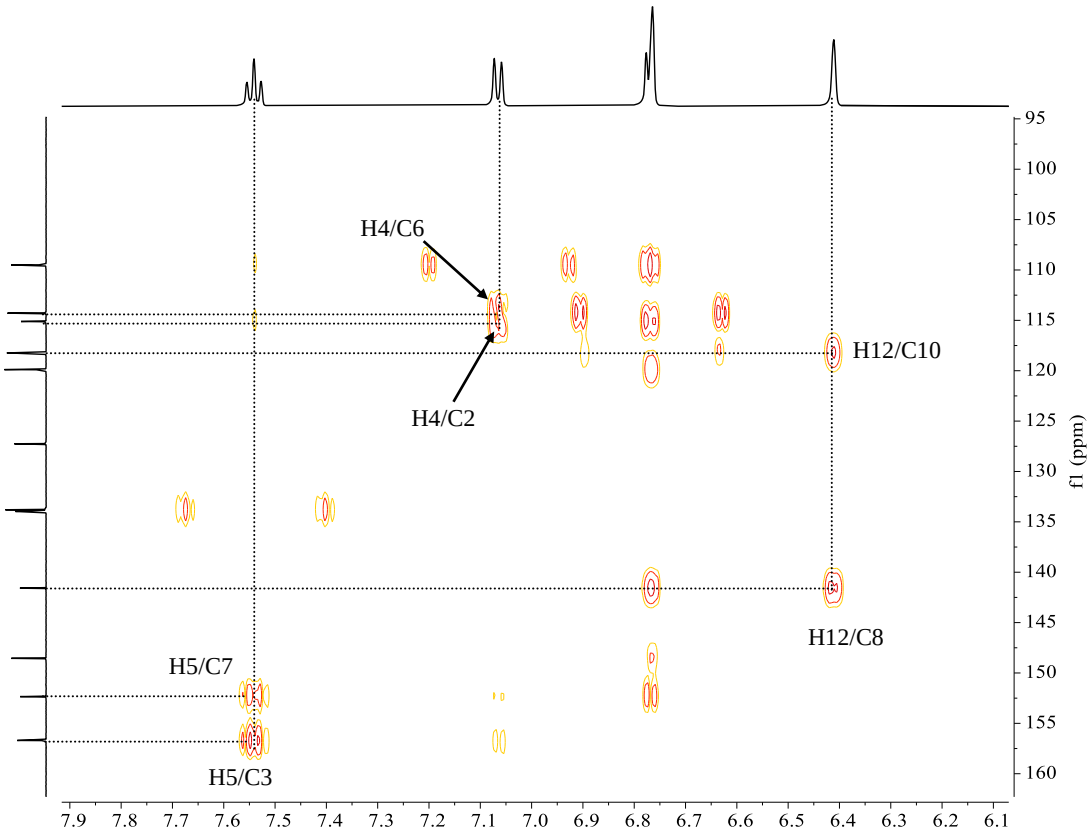


Figure S12: HMBC spectrum of **1** (barceloneic lactone D) (From δ_C 95 ppm to 160 ppm)

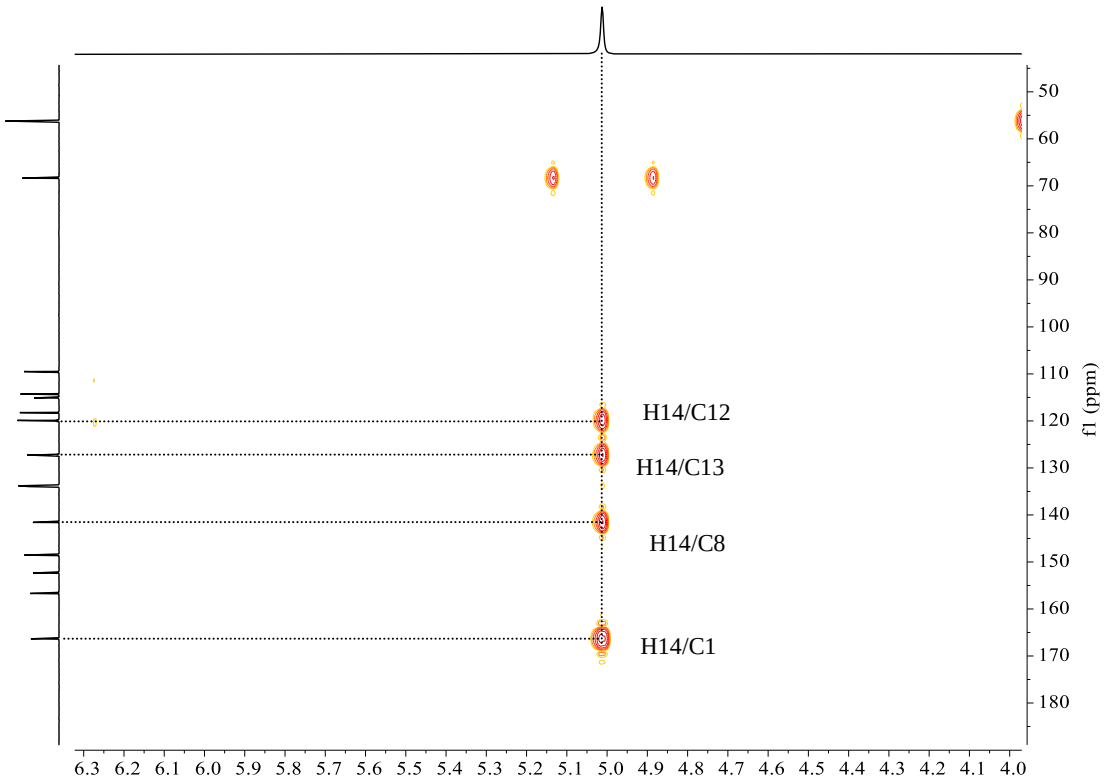


Figure S13: HMBC spectrum of **1** (barceloneic lactone D) (From δ_C 50 ppm to 180 ppm)

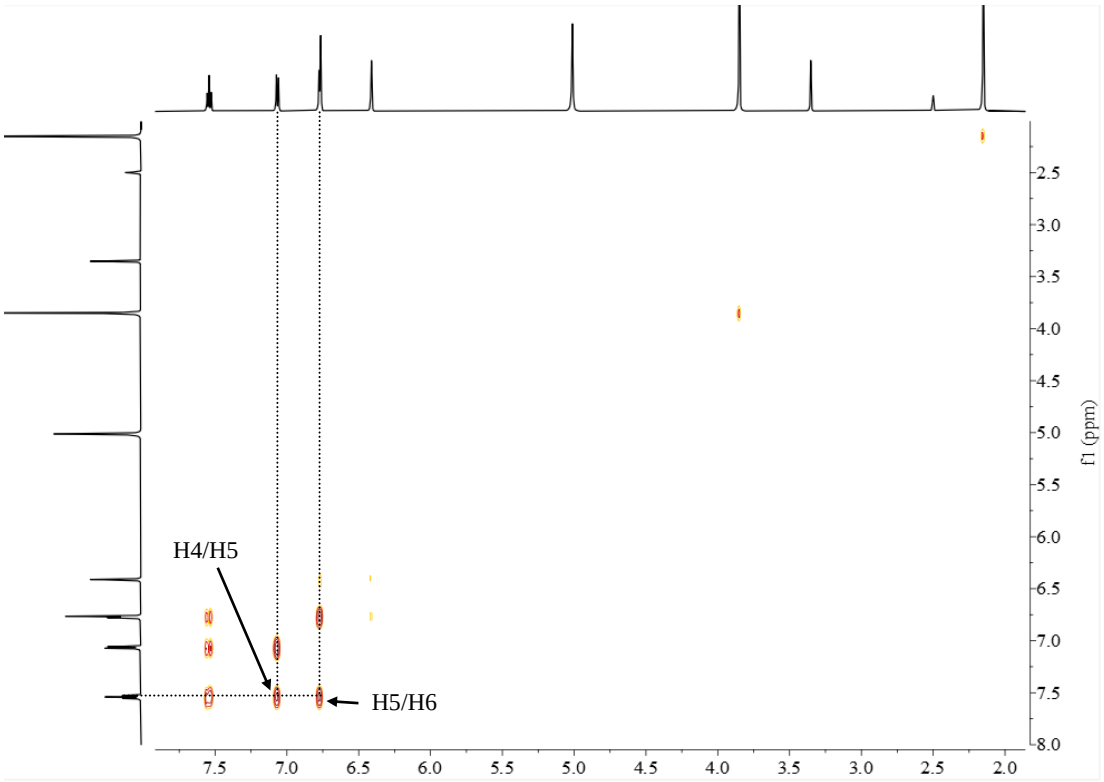


Figure S14: ^{1}H-^{1}H COSY spectrum of **1** (barceloneic lactone D)

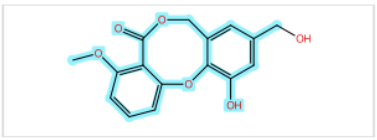
CAS SciFinder^{n}

Substances (7)

View in SciFinder^{n}

1 Similarity Score: **96**

1443221-26-8



$C_{16}H_{14}O_6$

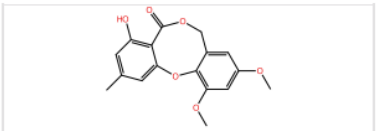
11-Hydroxy-9-(hydroxymethyl)-4-methoxy-5*H*,7*H*-dibenzo[*b*,*g*][1,5]dioxocin-5-one

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	302.28	-
Boiling Point (Predicted)	604.2±55.0 °C	Press: 760 Torr
Density (Predicted)	1.396±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	8.21±0.20	Most Acidic Temp: 25 °C
Spectra		

2 Similarity Score: **94**

2824125-39-3



$C_{17}H_{16}O_6$

5*H*,7*H*-Dibenzo[*b*,*g*][1,5]dioxocin-5-one, 4-hydroxy-9,11-dimethoxy-2-methyl-

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	316.31	-
Boiling Point (Predicted)	568.3±50.0 °C	Press: 760 Torr
Density (Predicted)	1.302±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	7.34±0.20	Most Acidic Temp: 25 °C

Figure S15: SciFinder search report for the non dimer version of compound **1** with 90-98 % similarity.