

Supporting Information

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Bioassay-Guided Isolation of Topoisomerase I Poison from *Paphiopedilum callosum* (Rchb.f.) Stein

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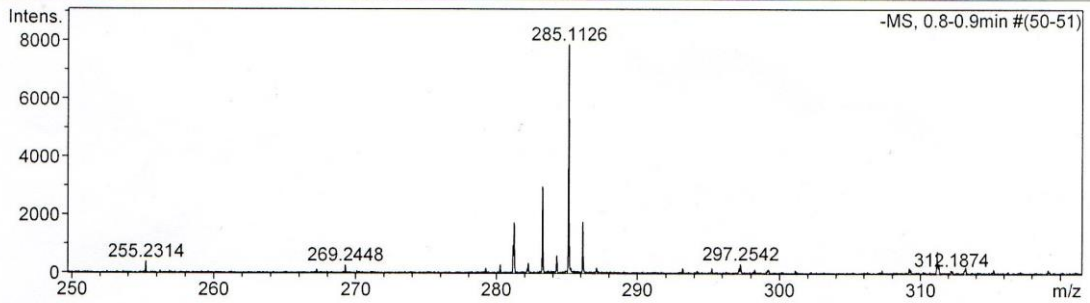
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Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 3000 m/z

Ion Polarity Negative
Capillary Exit -120.0 V
Hexapole RF 400.0 V
Skimmer 1 -50.0 V
Hexapole 1 -25.0 V

Set Corrector Fill 75 V
Set Pulsar Pull 372 V
Set Pulsar Push 372 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2295 V



#	m/z	I	I %	S/N	Res.
1	113.7204	52	0.7	4.0	4742
2	143.8712	52	0.7	4.1	4377
3	174.7592	44	0.6	3.2	7331
4	184.4298	32	0.4	2.3	7792
5	198.6564	38	0.5	2.6	6512
6	234.4761	35	0.4	2.3	8166
7	246.8008	48	0.6	3.0	7397
8	255.2314	370	4.7	23.2	6859
9	269.2448	252	3.2	15.4	4870
10	280.2592	273	3.5	16.4	5231
11	281.2405	1708	21.8	102.6	5369
12	283.2625	2956	37.7	177.0	5853
13	285.1126	7842	100.0	468.3	5885
14	286.1155	1741	22.2	103.8	5831
15	290.3796	29	0.4	1.7	9304
16	293.1758	159	2.0	9.4	5299
17	297.2542	296	3.8	17.3	3929
18	312.1874	104	1.3	5.9	3616
19	325.1859	1377	17.6	77.2	5559
20	339.2016	1584	20.2	85.5	5536
21	353.3313	348	4.4	18.2	4464
22	367.3583	821	10.5	41.2	5476
23	393.2770	1420	18.1	65.8	5728
24	411.3439	384	4.9	16.9	6184
25	421.1897	246	3.1	10.5	3451
26	437.1793	322	4.1	13.2	4734
27	443.2486	218	2.8	8.8	4178

Figure S1: ESI-MS spectrum of compound 1

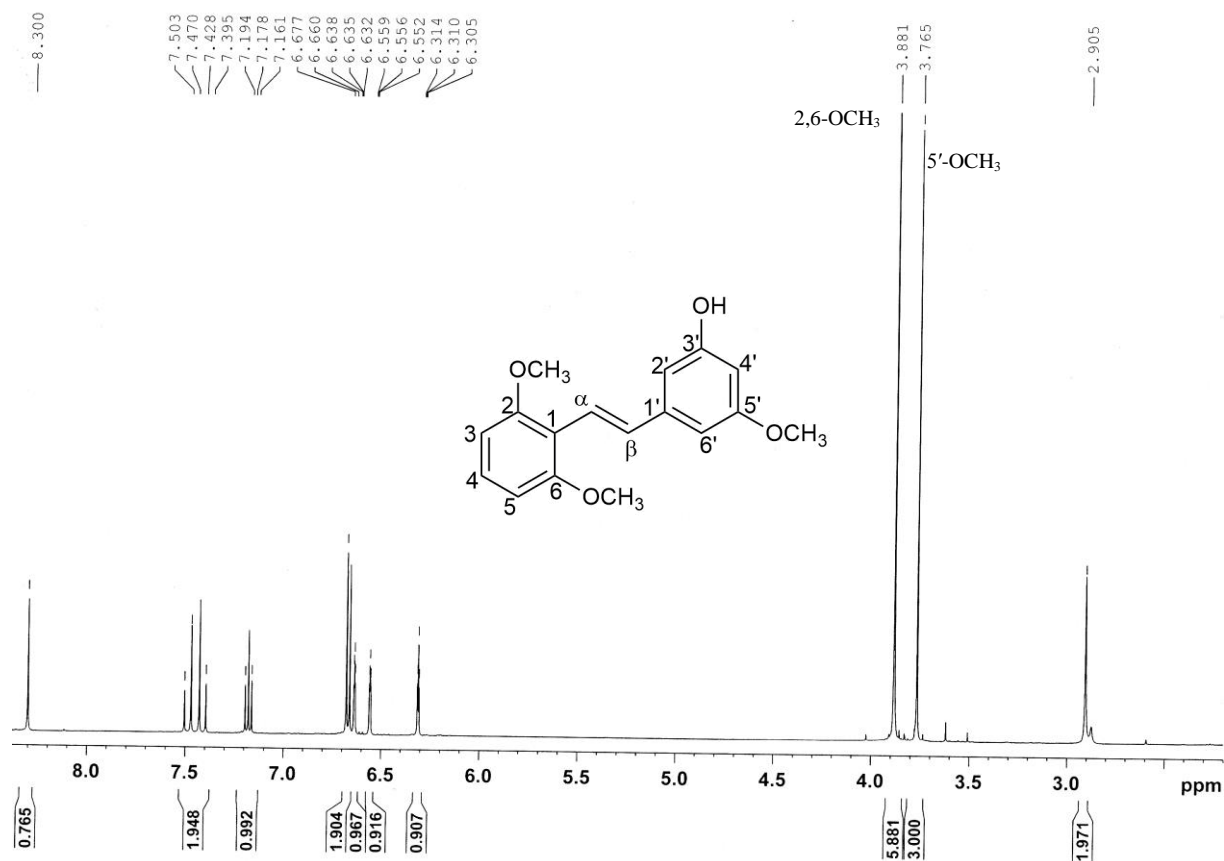


Figure S2: $^1\text{H-NMR}$ (500 MHz, Acetone- d_6) spectrum of compound **1**

3'-hydroxy-2,6,5'-trimethoxystilbene: yellowish brown semisolid. $^1\text{H-NMR}$ (Acetone- d_6 , 500 MHz), δ : 3.77 (1H, s, OCH_3 -5'), 3.88 (2H, s, OCH_3 -2/6), 6.31 (1H, t, H-4'), 6.56 (1H, t, H-6'), 6.64 (1H, t, H-2'), 6.67 (2H, d, H-3/5), 7.18 (1H, t, H-4), 7.41 (1H, d, H- α), 7.49 (1H, d, H- β), 8.30 (1H, s, OH-3'). $^{13}\text{C-NMR}$ (Acetone- d_6 , 125 MHz), δ : 55.4 (OCH_3 -5'), 56.1 (OCH_3 -2/6), 101.2 (C-4'), 104.5 (C-6'), 104.9 (C-3/5), 106.2 (C-2'), 115.1 (C-1), 120.8 (C- α), 129.3 (C-4), 132.9 (C- β), 142.4 (C-1'), 159.5 (C-3'), 159.6 (C-2/6), 162.1 (C-5'). ESIMS: m/z = 285.1126 [M] $^-$ for formula C₁₇H₁₈O₄.

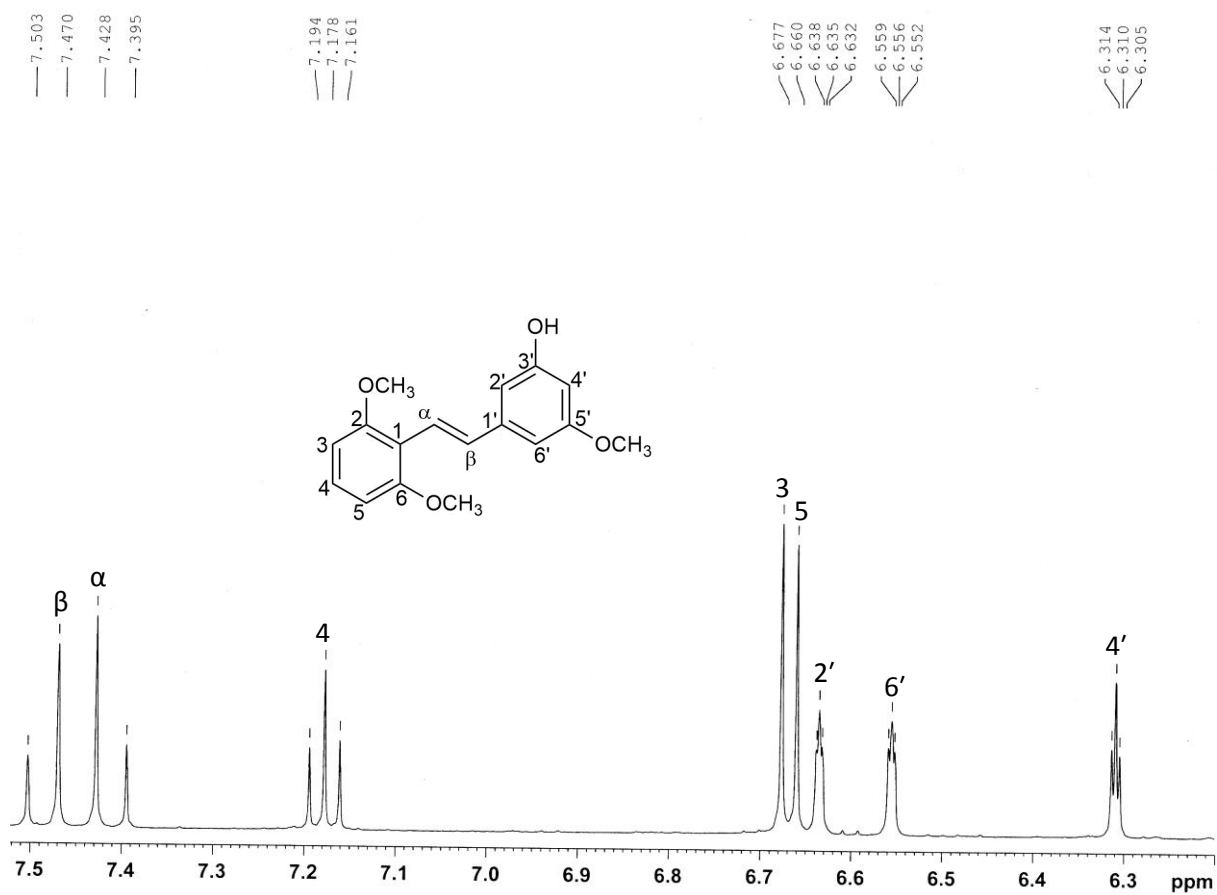


Figure S3: $^1\text{H-NMR}$ (500 MHz, Acetone- d_6) spectrum of compound **1** (from 6.3-7.5)

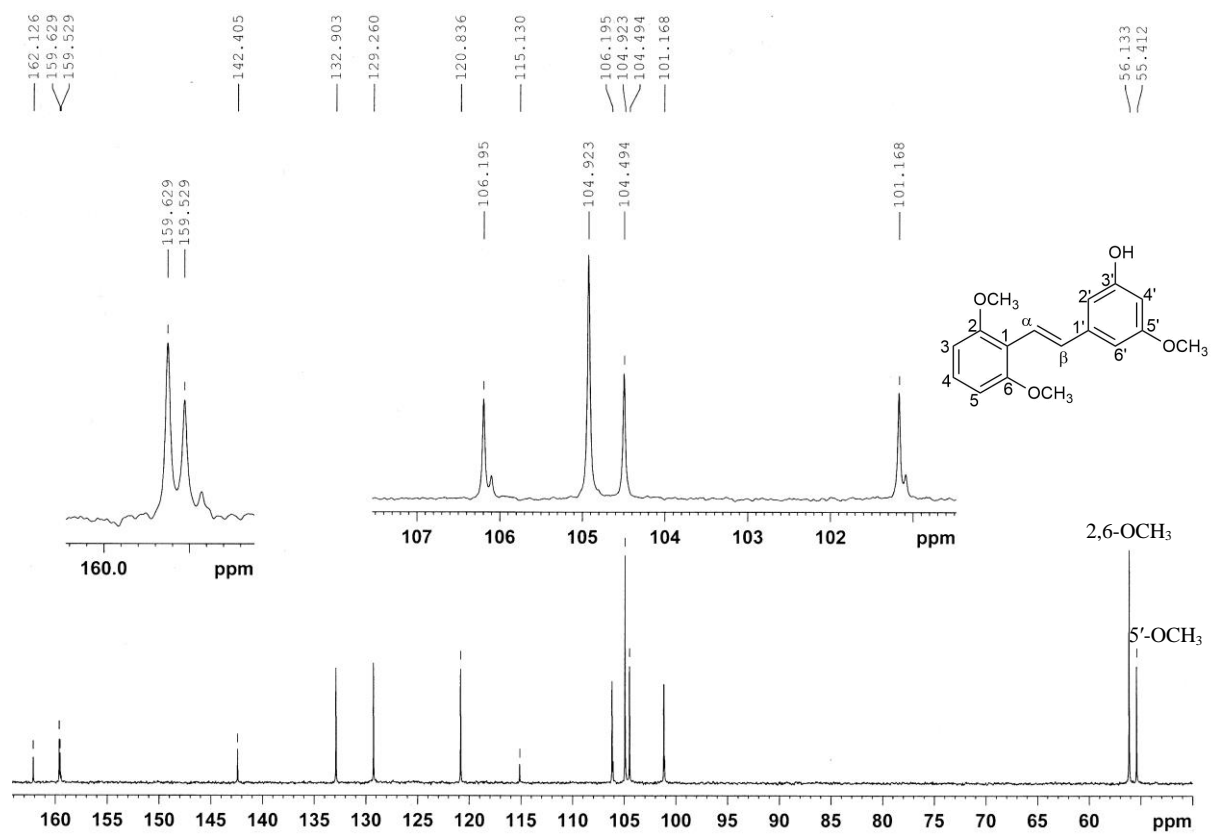


Figure S4: $^{13}\text{C-NMR}$ (125 MHz, Acetone- d_6) spectrum of compound 1

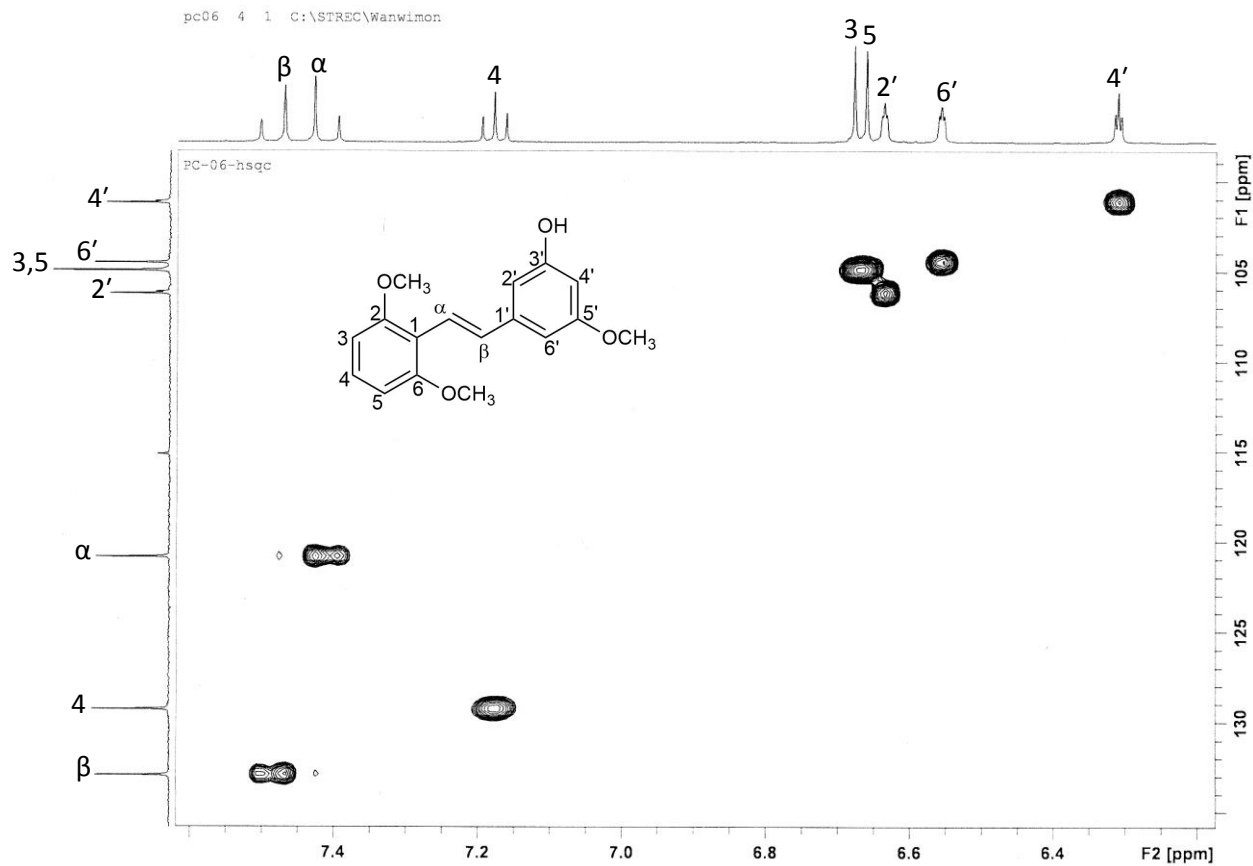
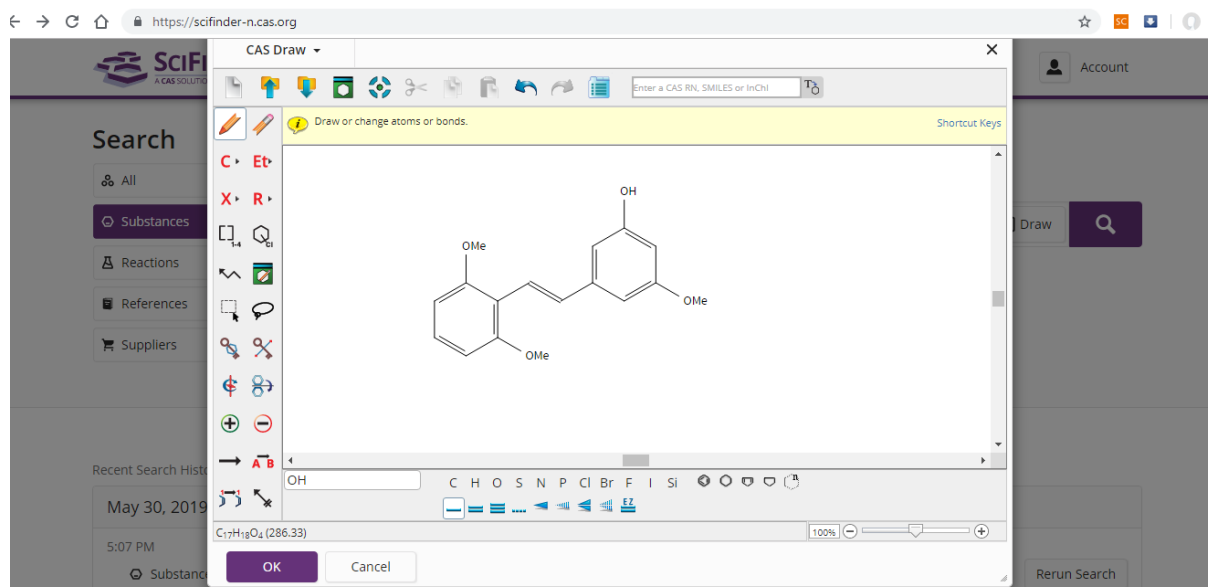


Figure S5: HSQC (500 MHz) spectrum of compound **1**



Substances (4)

Sort: Relevance View Partial

Structure Match: As Drawn (0), **Substructure (4)**, Similarity (56K)

Filter by: Commercial Availability (Not Available (4)), Reaction Role (Product (4), Reactant (2)), Reference Role (Biological Study (3), Preparation (4))

CAS Number	Chemical Name	References	Reactions	Suppliers
1445898-18-9	5-[(1E)-2-(2,6-Dimethoxyphenyl)ethenyl]-3-methoxy-2-(3-methyl-2-buten-1-yl)pheno...	2	9	0
1445896-86-5	Benzoic acid, 2-[(1E)-2-(2,6-dimethoxyphenyl)ethenyl]-6-hydroxy-4-methoxy-meth...	2	8	0
1445897-49-3	6-[(1E)-2-(2,6-Dimethoxyphenyl)ethenyl]-2-hydroxy-4-methoxy-3-(3-methyl-2-buten...	2	9	0
1445897-83-5				

Substances (0)

We couldn't find any results. Please update your search query and try again.

Figure S6: New compound search report of SciFinder