

Supporting Information

Rec. Nat. Prod. 15:6 (2021) 608-612

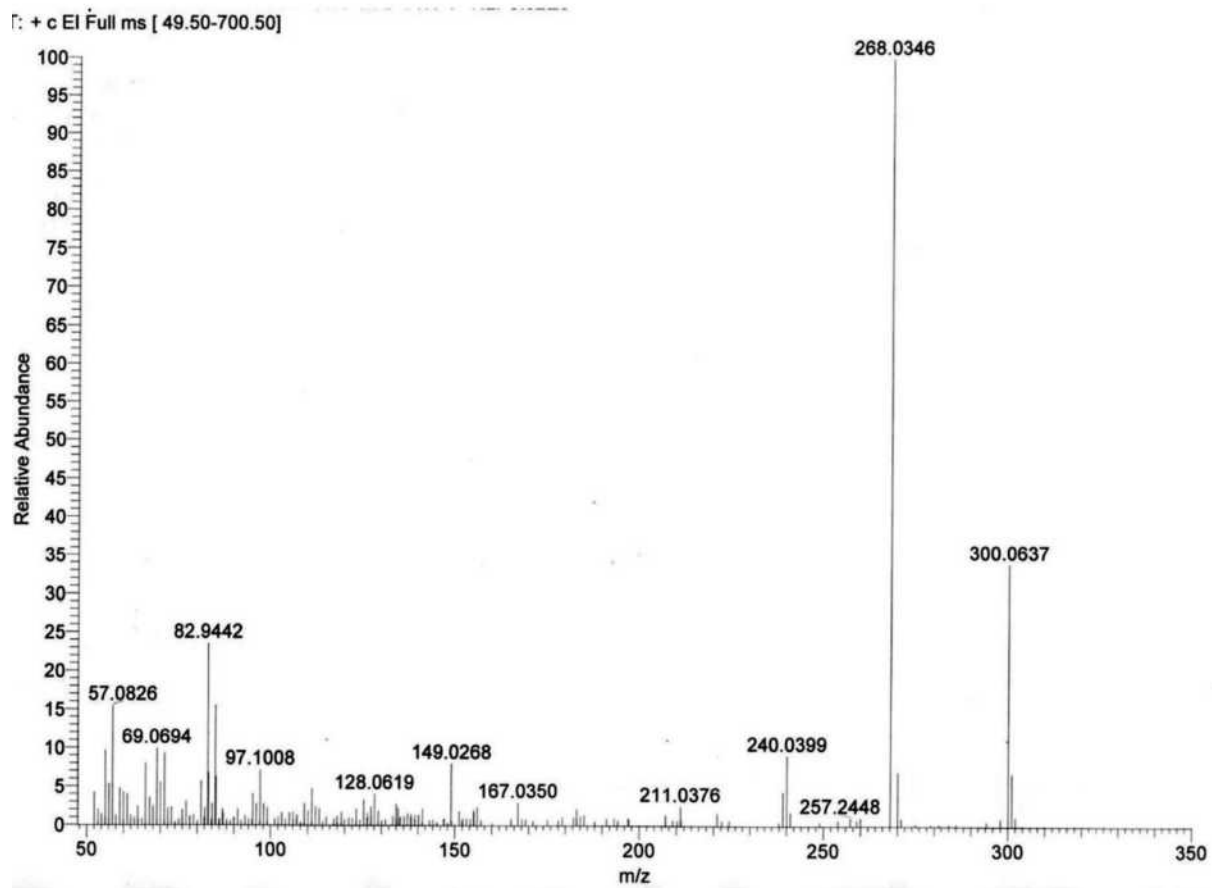
Bioactive Natural Products from Endophytic Fungus *Aspergillus nidulans* Associated with *Nyctanthes arbor-tristis* Linn.

Talea Sana¹, Bina S. Siddiqui^{1,*}, Majid Khan¹, Saleem Shahzad², Samia Sattar² and Sabira Begum¹

¹HEJ Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan

²Department of Agriculture & Agribusiness Management, University of Karachi

Table of Contents	Page
Figure S1: HR-EIMS spectrum of 1 (1,5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)	2
Figure S2: ¹ H-NMR (400 MHz, CDCl ₃) spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)	3
Figure S3: ¹ H-NMR (400 MHz, CDCl ₃) spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester) (From δ_H 6.0 ppm to δ_H 8.0 ppm)	4
Figure S4: ¹ H-NMR (400 MHz, CDCl ₃) spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester) (From δ_H 6.6 ppm to δ_H 7.5 ppm)	5
Figure S5: ¹³ C-NMR (150 MHz, CDCl ₃) spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)	6
Figure S6: DEPT135 (150 MHz, CDCl ₃) spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)	7
Figure S7: HSQC spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)	8
Figure S8: HSQC spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester) (From δ_C 20 ppm to δ_C 130 ppm)	9
Figure S9: HMBC spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)	10
Figure S10: HMBC spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester) (From δ_C 70 ppm to δ_C 180 ppm)	11
Figure S11: HMBC spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester) (From δ_C 20 ppm to δ_C 90 ppm)	12
Figure S12: NOESY spectrum of 1 (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)	13
Figure S13: NMR comparison table for the new compound and similar structures from Scifinder search	14
S1. Scifinder search reports	15



Scan No.	Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [amu]	RDB	Composition
1 of 1	300.0637	7.6	300.0634	1.2	0.4	11.0	C ₁₄ H ₁₂ O ₆
			300.0693	-18.4	-5.5	2.0	C ₈ H ₁₆ O ₁₁
			300.0575	20.8	6.2	20.0	C ₂₃ H ₈ O ₇
			300.0786	-49.6	-14.9	15.0	C ₂₀ H ₁₂ O ₈

Figure S1:HR-EIMS spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)

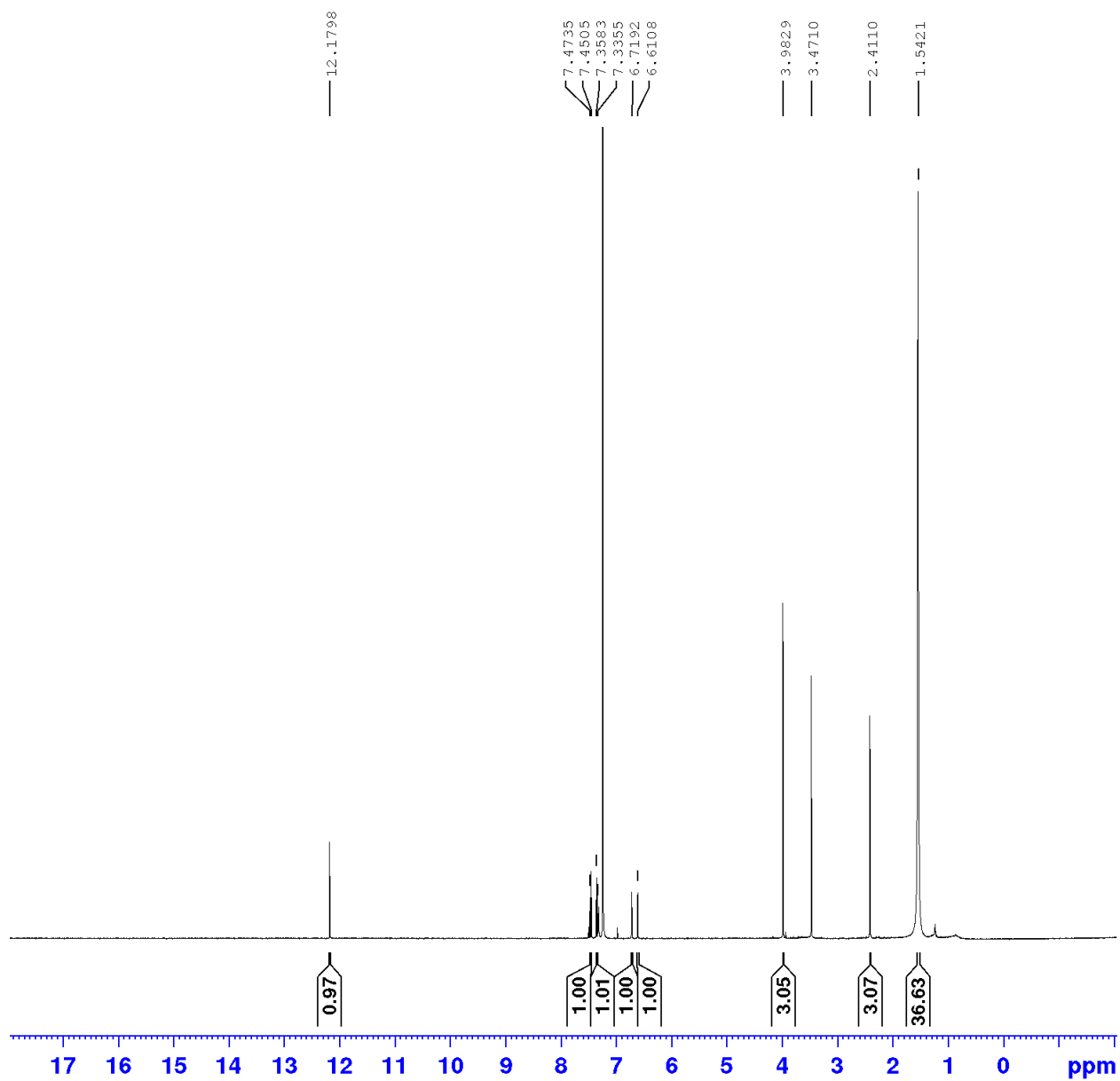


Figure S2: $^1\text{H-NMR}$ (400 MHz, CDCl_3) spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)

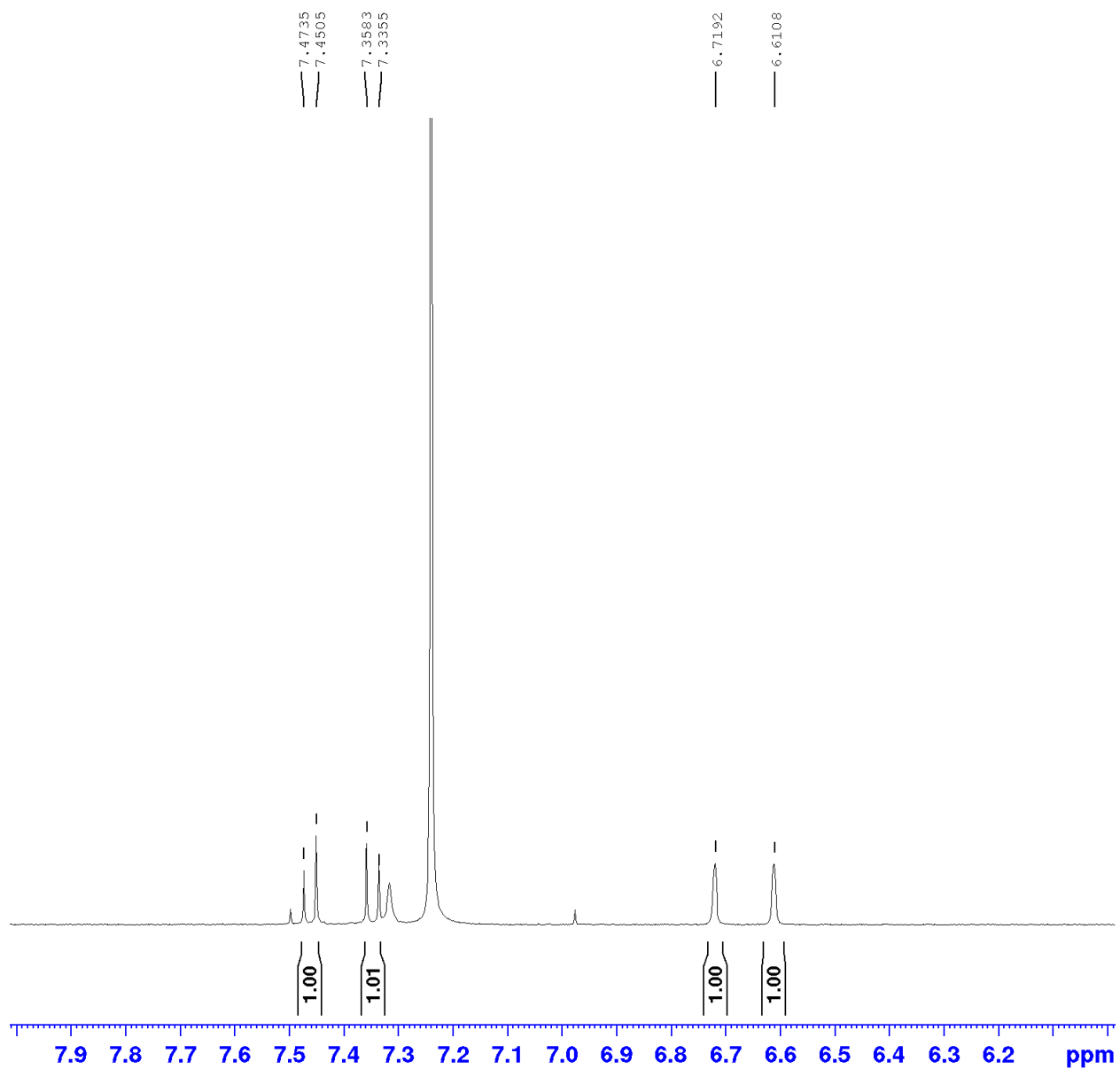


Figure S3: ¹H-NMR (400 MHz, CDCl₃) spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)(From δ_{H} 6.0 ppm to δ_{H} 8.0 ppm)

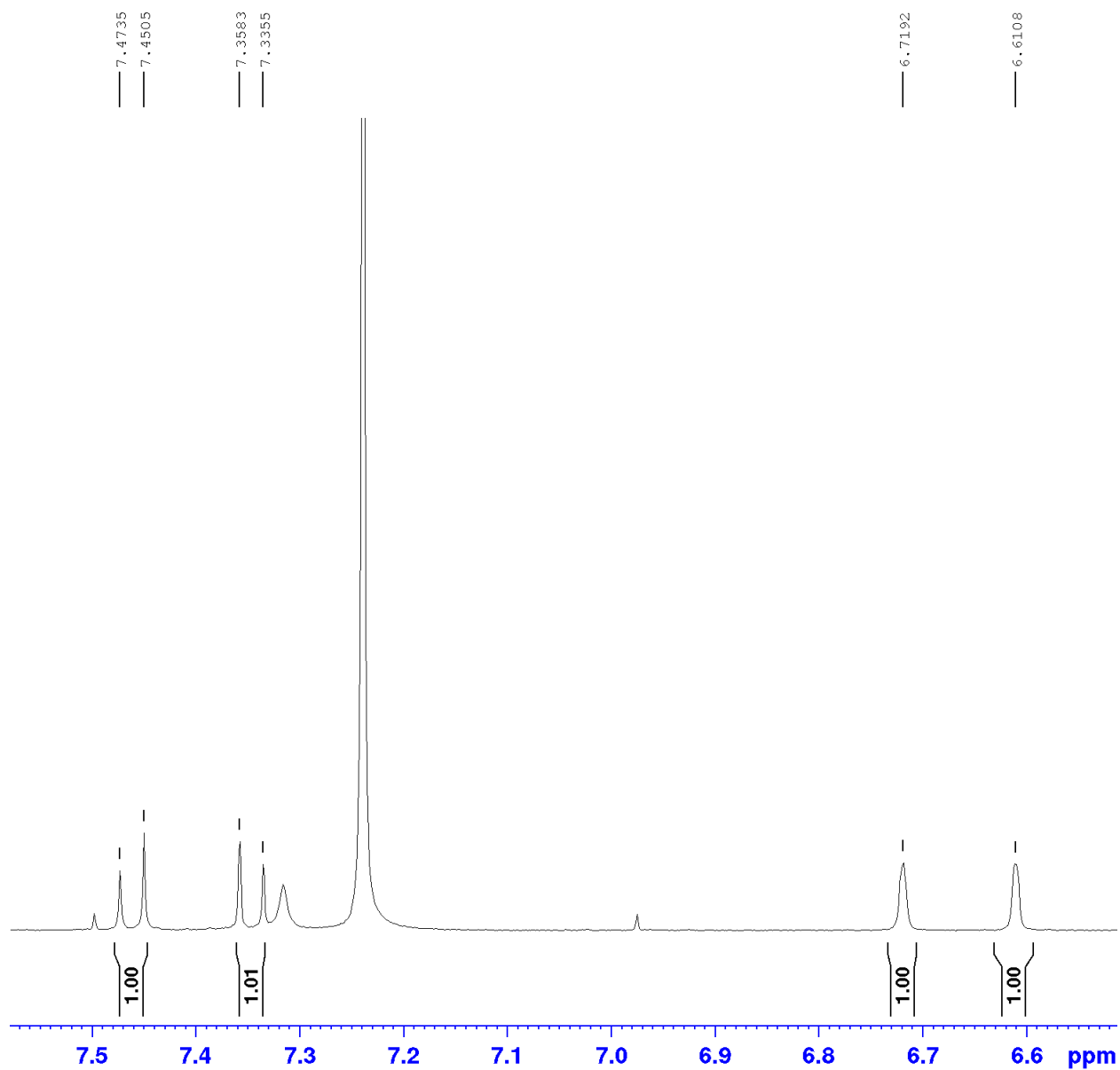


Figure S4: ¹H-NMR (400 MHz, CDCl₃) spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester) (From δ_{H} 6.6 ppm to δ_{H} 7.5 ppm)

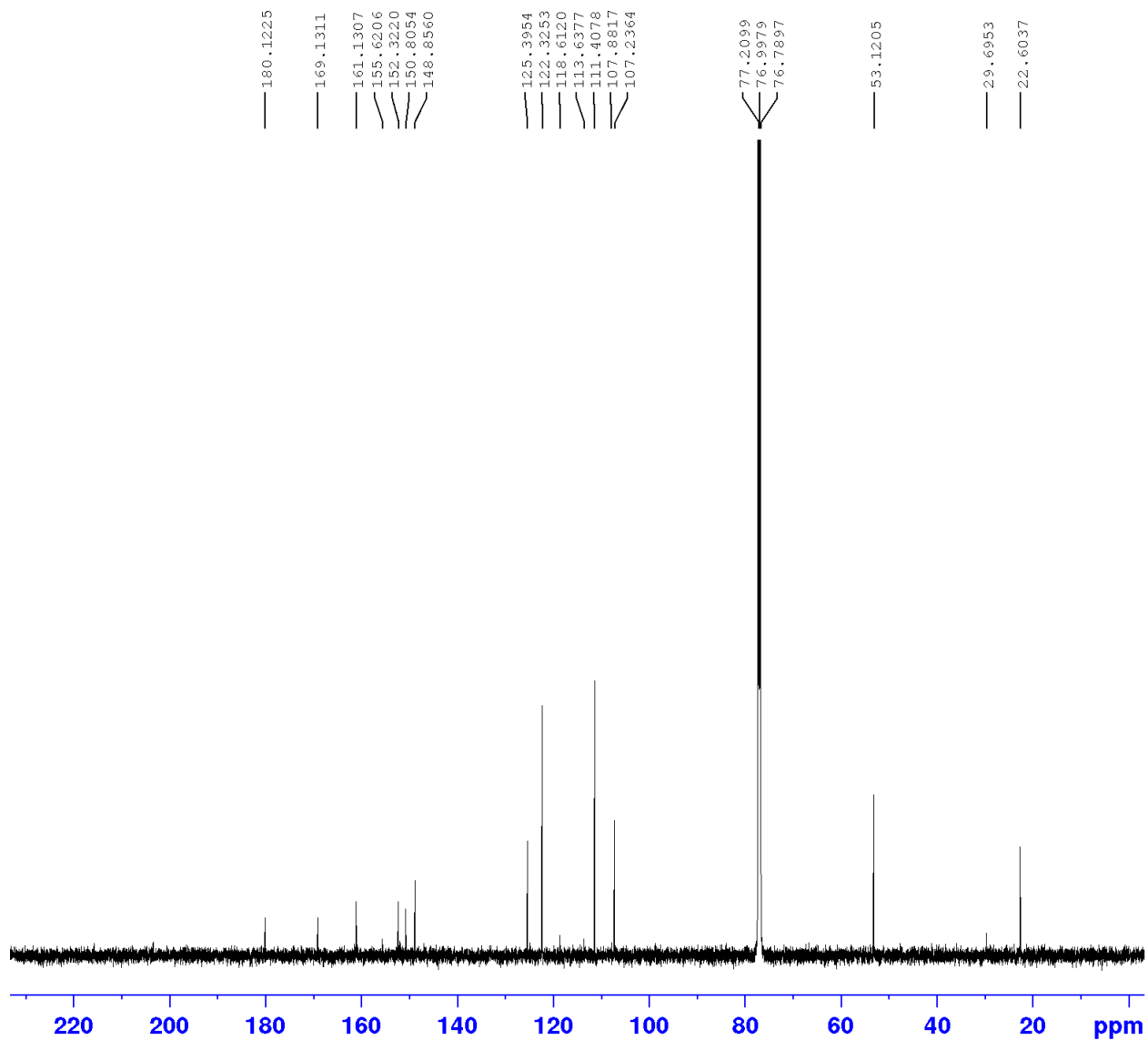


Figure S5: ^{13}C -NMR (150 MHz, CDCl_3) spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)

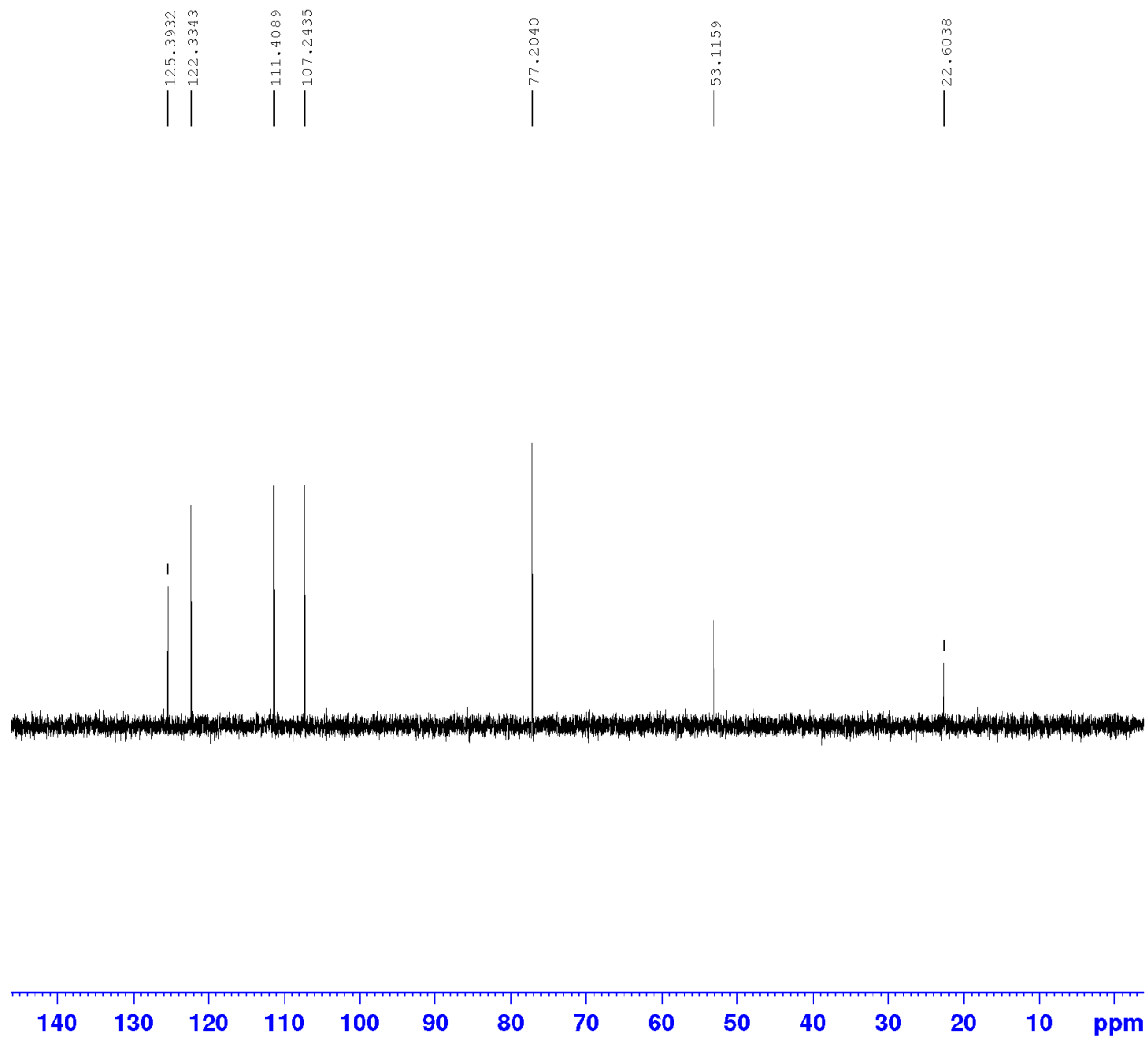


Figure S6: DEPT135 (150 MHz, CDCl₃) spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)

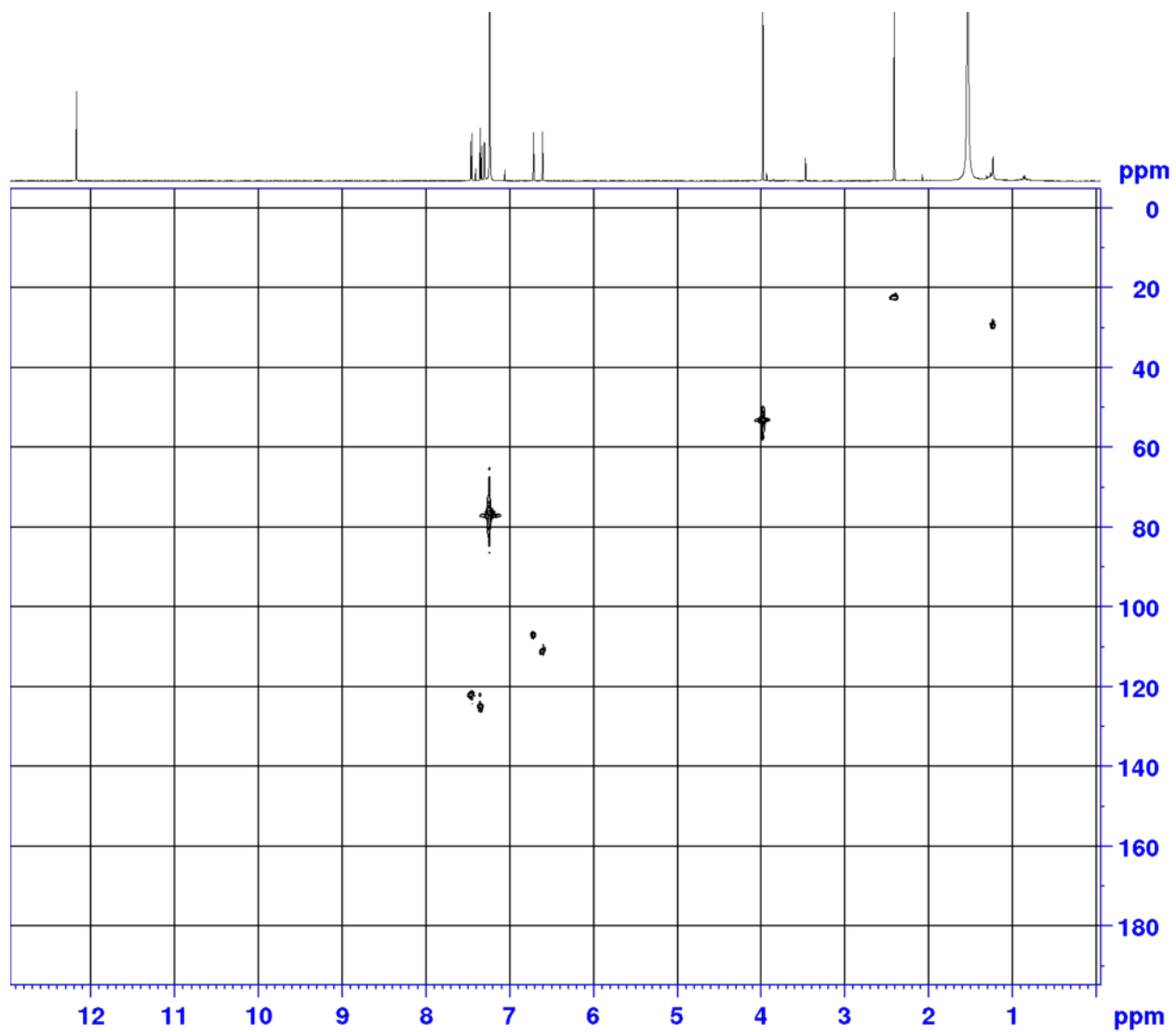


Figure S7: HSQC spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)

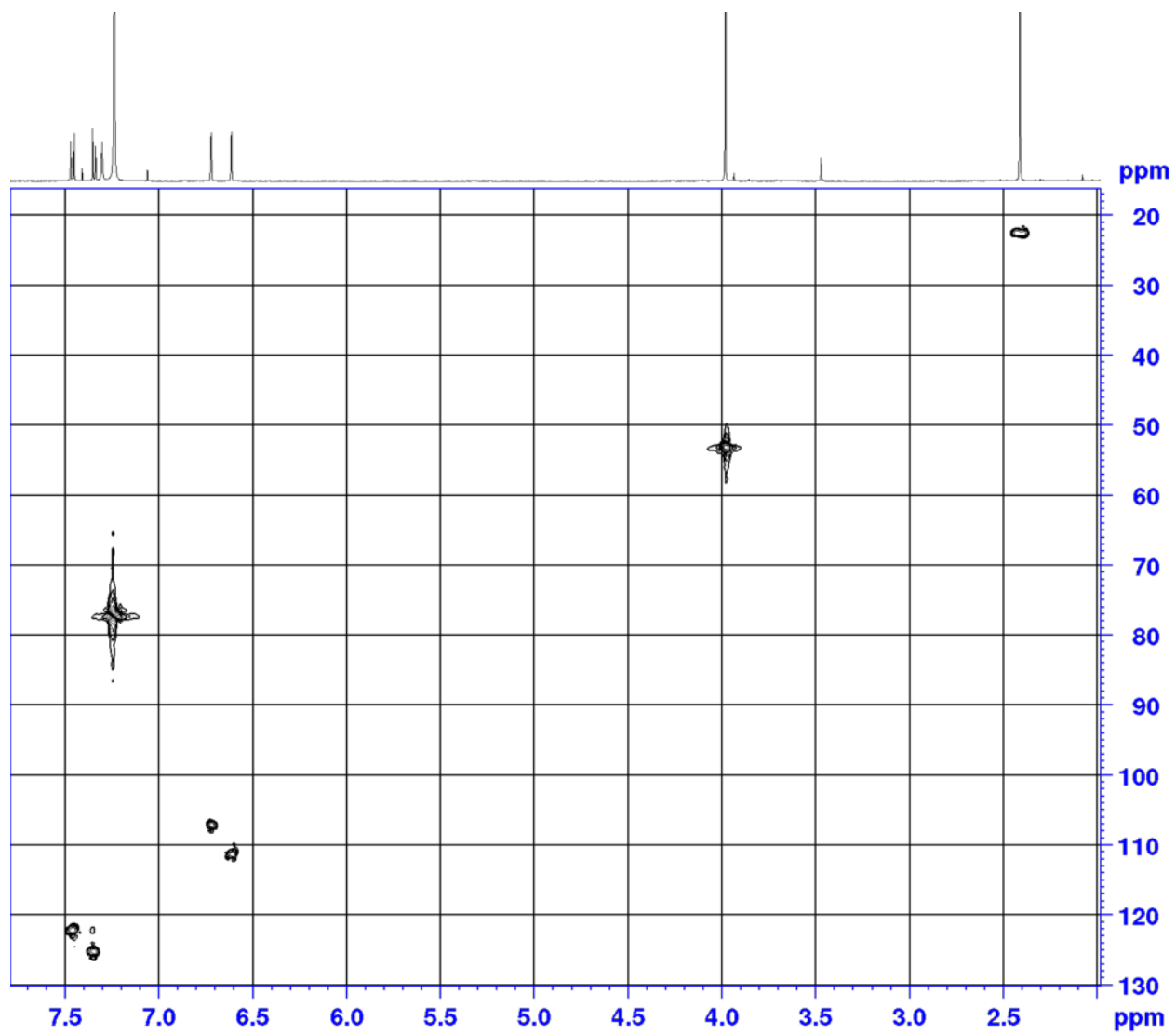


Figure S8: HSQC spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)
 (From δ_c 20 ppm to δ_c 130 ppm)

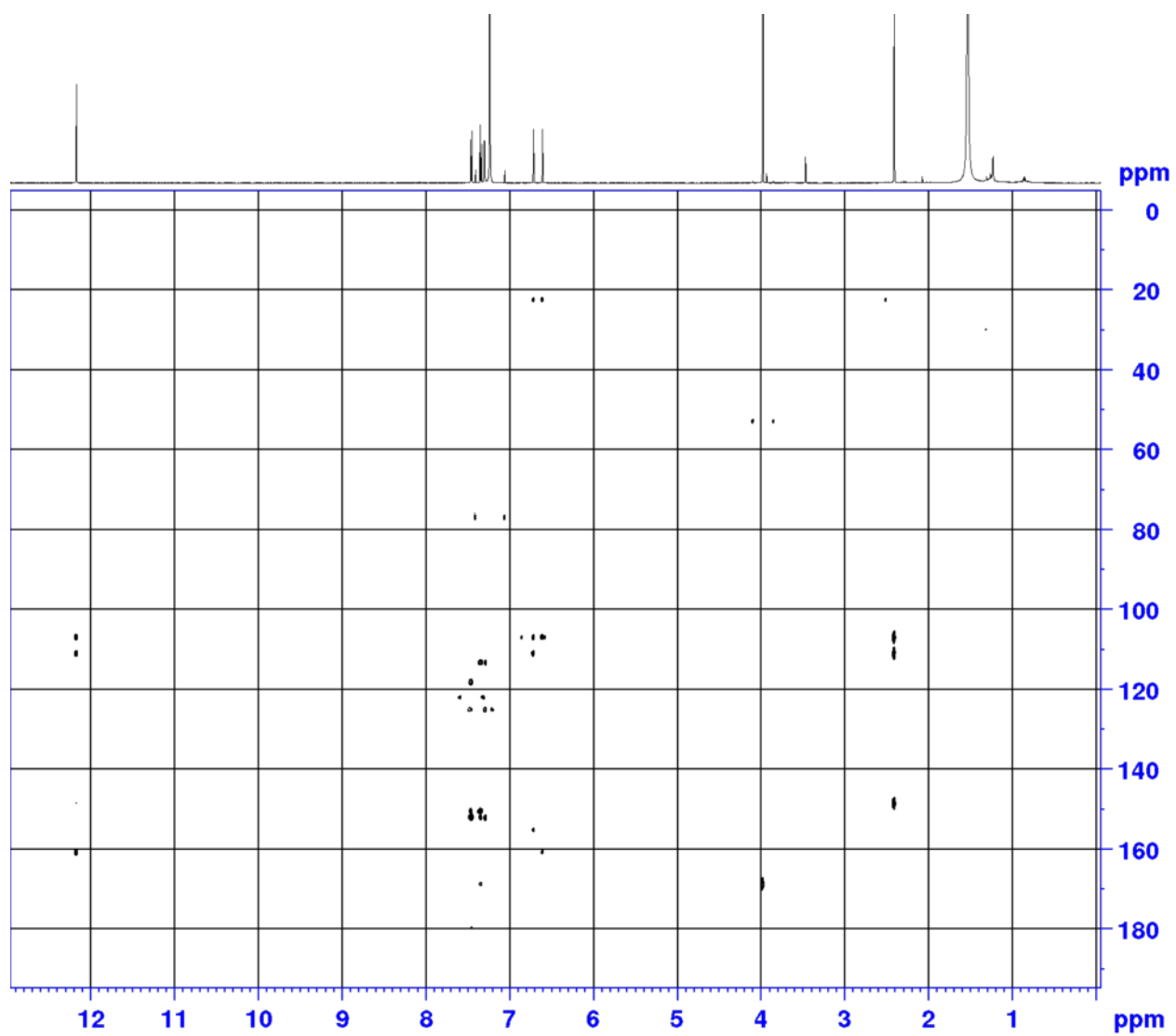


Figure S9: HMBC spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)

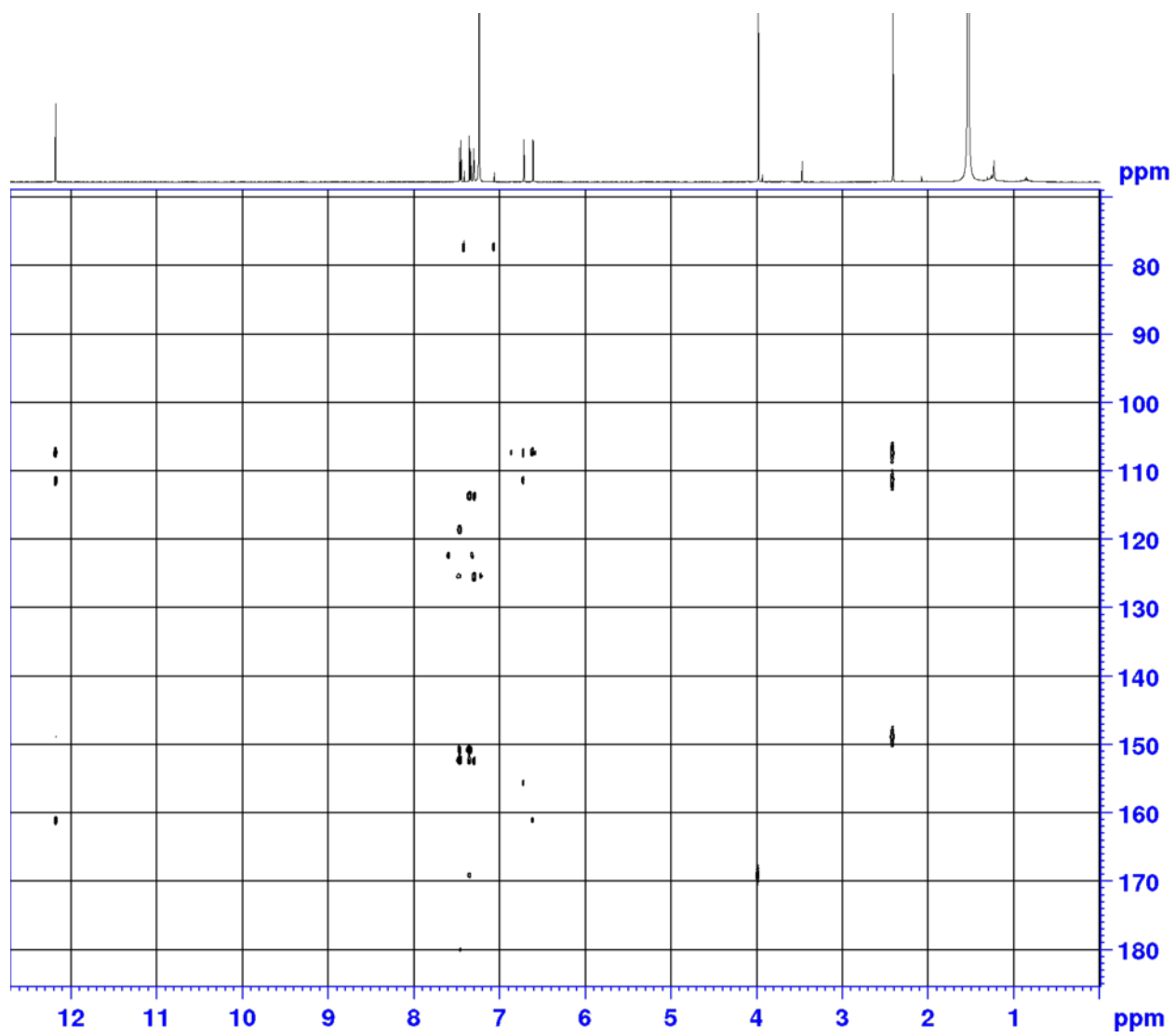


Figure S10: HMBC spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)
(From δ_c 70 ppm to δ_c 180 ppm)

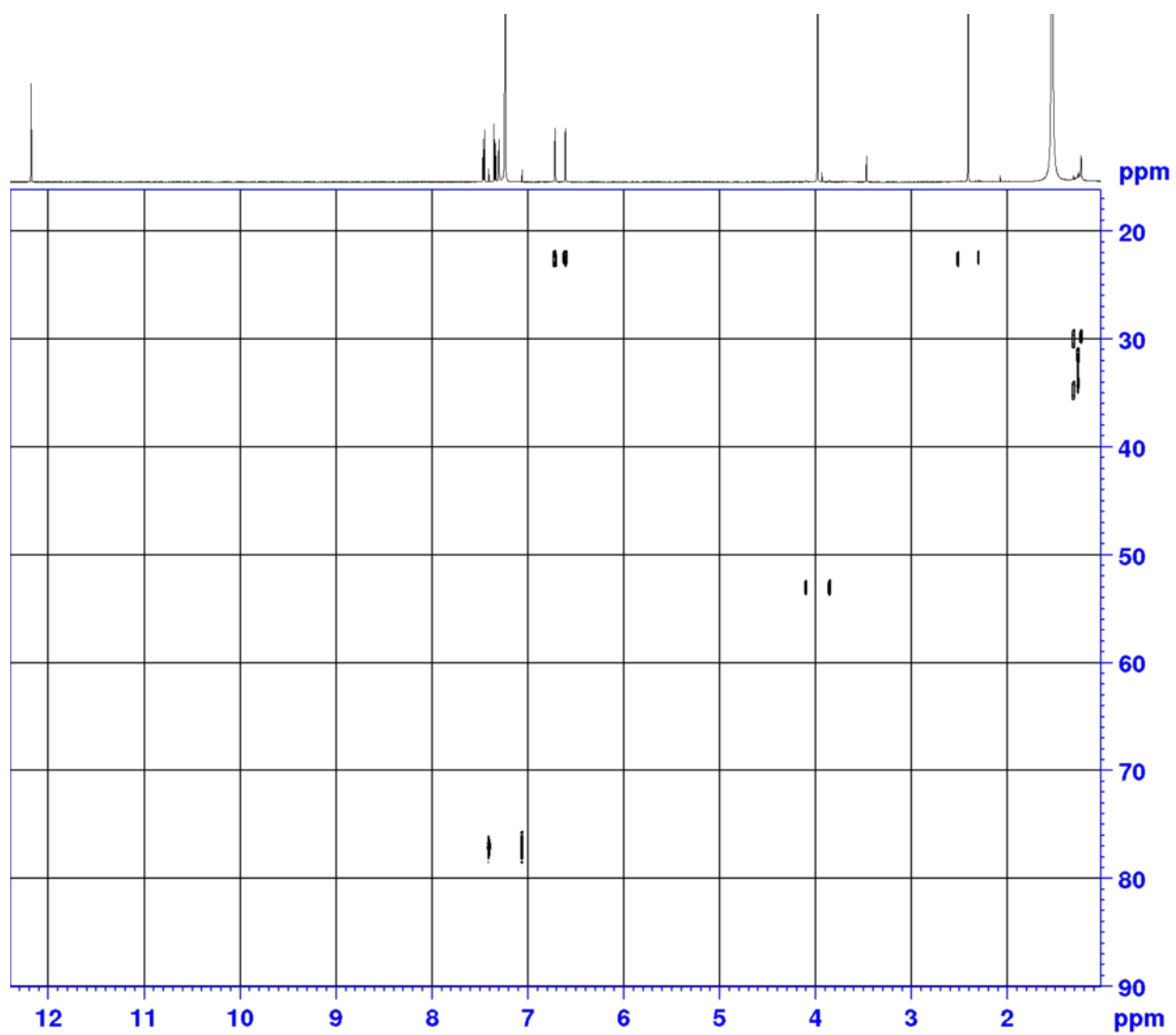


Figure S11: HMBC spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)
 (From δ_c 20 ppm to δ_c 90 ppm)

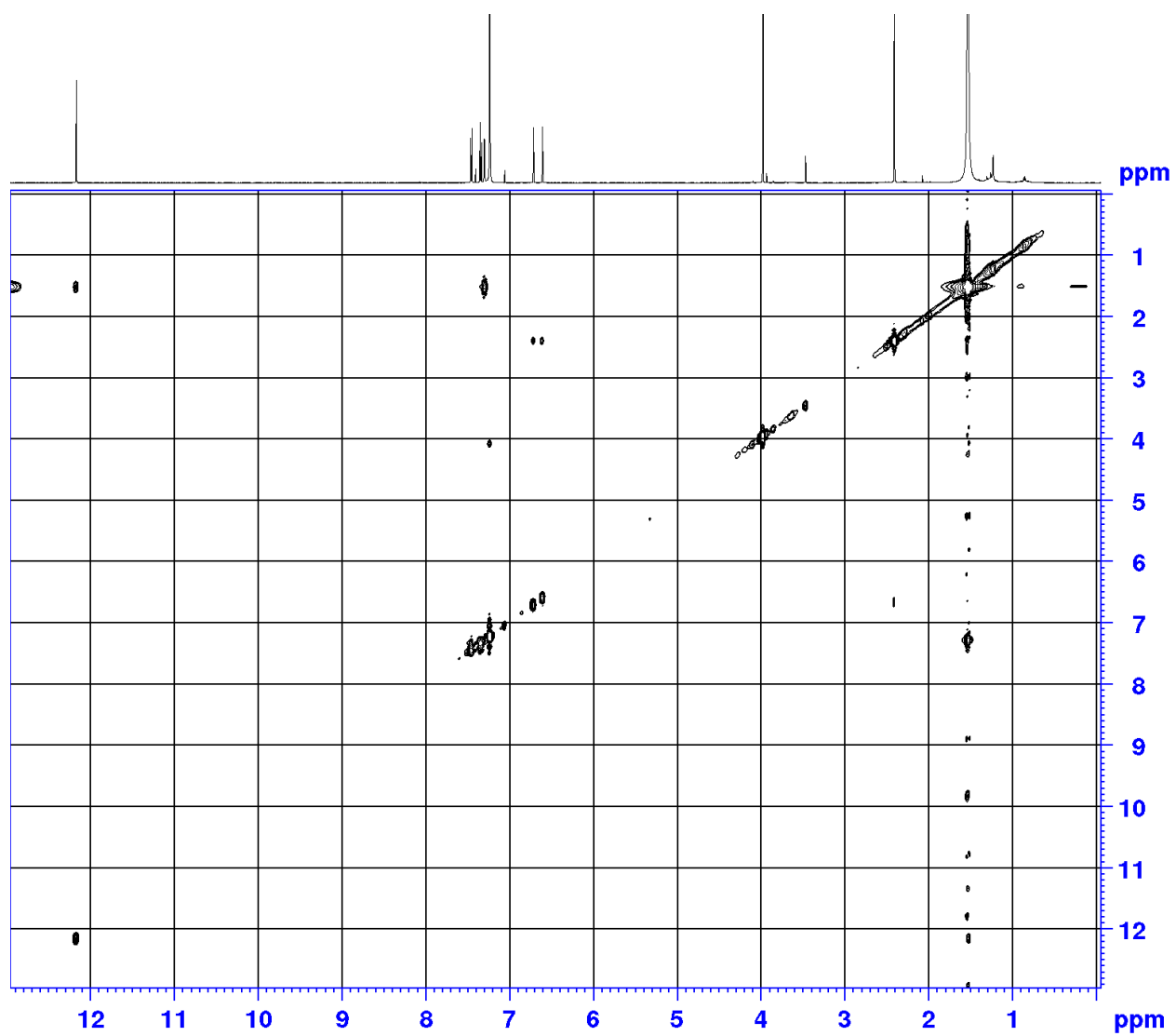
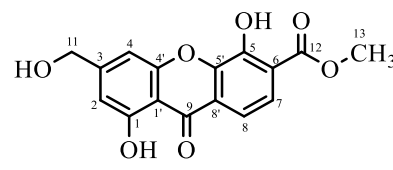
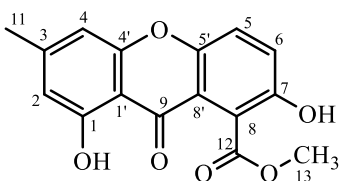
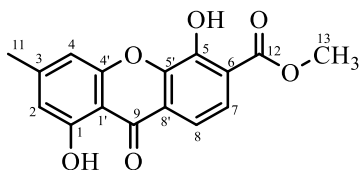


Figure S12: NOESY spectrum of **1** (1, 5-dihydroxy-3-methylxanthone-6-carboxylic acid methyl ester)

Table S1: NMR comparison for the new compound and similar structures from Scifinder search¹H-NMR (CDCl₃, 400 MHz) ;¹H-NMR (CDCl₃, 400 MHz) ;¹H-NMR (DMSO-d₆, 500 MHz) ;¹³C-NMR (CDCl₃, 150 MHz)¹³C-NMR (CDCl₃, 100 MHz)¹³C-NMR (DMSO-d₆, 125 MHz)

No	New compound		Pinselin		Fischexanthone	
	δ_H (mult. <i>J</i> in Hz)	δ_C	δ_H (mult. <i>J</i> in Hz)	δ_C	δ_H (mult. <i>J</i> in Hz)	δ_C
1		161.1, C		155.7, C		160.6, C
1-OH	12.17, s		12.23, s		12.19, s	
1'		107.8, C		114.7, C		106.8, C
2	6.61, d (1.2)	111.4, CH	6.75 (s)	107.2, CH	6.72 (br s)	107.3, CH
3		148.8, C		151.9, C		154.3, C
4	6.72, d (1.2)	107.2, CH	6.64 (s)	111.3, CH	6.96 (br s)	104.2, CH
4'		155.6, C		161.2, C		155.8, C
5		150.8, C	7.45, d (9.0)	121.7, CH		150.9, C
5'		152.3, C		150.5, C		149.2, C
6		118.6, C	7.40, d (9.0)	125.4, CH		117.5, C
7	7.33, d (9.2)	125.4, CH		155.7, C	7.45, d (7.6)	125.5, CH
8	7.45, d (9.2)	122.3, CH		148.8, C	7.58, d (7.6)	120.3, CH
8'		113.6, C		118.5, C		117.3, C
9		180.1, C		180.3, C		180.6, C
11	2.41, s	22.6, CH ₃	2.45, s	22.6, CH ₃	4.57, s	62.5, CH ₂ OH
12		169.1, C		168.9, C		167.1, C
13	3.98, s	53.1, OCH ₃	4.03, s	53.1, OCH ₃	3.85, s	52.4, OCH ₃

S1: Scifinder search reports

SciFinder - Explore

scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

SciFinder[®] is here! Learn more about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore | Saved Searches | SciPlanner

Chemical Structure similarity > substances (2)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java | Non-Java

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

ChemDraw

Launch a SciFinder/SciFinder[®] substance or reaction search directly from the latest version of ChemDraw. Learn More

SAVED ANSWER SETS

Autosaved Substance Set

Learn how to:
Create Saved Answer Sets

View All | Import

KEEP ME POSTED

You have no profiles.

Learn how to:
Create Keep Me Posted

Type here to search

3:45 PM 5/3/2021

SciFinder - Substance Answer Set

scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

CAS Solutions

SciFinder[®] A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome TALEA SANA

SciFinder[®] is here! Learn more about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore | Saved Searches | SciPlanner

Explore Substances resulted in 0 substances [Return](#)

Chemical Structure exact > substances (0)

SUBSTANCES

Analyze | Refine

Analyze by:
No substances available

Create Keep Me Posted Alert

Contact Us | Legal

Copyright © 2021 American Chemical Society. All Rights Reserved. | 京ICP備13047075号-3

Type here to search

3:46 PM 5/3/2021

SciFinder search report as 95-98 % similarity search

SciFinder - Explore

scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

SciFinder[®] is here! Learn more about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore Saved Searches SciPlanner

Chemical Structure similarity > substances (2)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Click image to change structure or view detail.

Import CXF

Search

Advanced Search

ChemDraw

Launch a SciFinder/SciFinder[®] substance or reaction search directly from the latest version of ChemDraw. Learn More

SAVED ANSWER SETS

Autosaved Substance Set

Learn how to:
Create Saved Answer Sets

View All | Import

KEEP ME POSTED

You have no profiles.

Learn how to:
Create Keep Me Posted

SciFinder - Similarity Candidates

scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

SCIFINDER[®] A CAS SOLUTION

Preferences | SciFinder Help | Sign Out

Welcome TALEA SAMA

SciFinder[®] is here! Learn more about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore Saved Searches SciPlanner

Chemical Structure similarity > substances (2)

SUBSTANCES

Select All Deselect All

1 of 8 Similarity Candidates Selected

Similarity Range	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input checked="" type="checkbox"/> 95-98	2
<input type="checkbox"/> 90-94	12
<input type="checkbox"/> 85-89	39
<input type="checkbox"/> 80-84	140
<input type="checkbox"/> 75-79	500
<input type="checkbox"/> 70-74	1863
<input type="checkbox"/> 65-69	4958
<input type="checkbox"/> 0-64 (least similar)	21183

Get Substances

Contact Us | Legal

Copyright © 2021 American Chemical Society. All Rights Reserved. | 京ICP备13047075号-3

SciFinder - Substance Answer Set x +

scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

SciFinderⁿ is here! Learn more about the power of n. Participating customers can access using their existing SciFinder credentials by clicking here: <https://scifinder-n.cas.org>

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Chemical Structure similarity > substances (2)

Get References Get Reactions Get Commercial Sources Tools ▾

Create Keep For Postcard Alert Send to SciPlanner

Analyze Refine

Sort by: Similarity Score ▾

0 of 2 Substances Selected

Analyze by: Substance Role

Biological Study 2

Occurrence 2

Preparation 2

Properties 2

Analytical Study 1

Formation, Nonpreparative 1

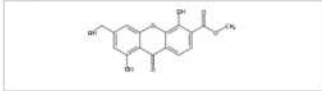
Reactant or Reagent 1

Uses 1

Show More

Score: 97

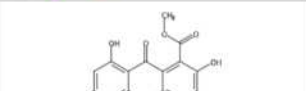
1. 1392484-49-9



C₁₈ H₁₂ O₇
 9H-Xanthene-3-carboxylic acid, 4,8-dihydroxy-5-(hydroxymethyl)-9-oxo-, methyl ester
 ▶ Key Physical Properties

Score: 95

2. 476-53-9



C₁₈ H₁₂ O₆
 9H-Xanthene-1-carboxylic acid, 2,8-dihydroxy-6-methyl-9-oxo-, methyl ester
 ▶ Key Physical Properties
 Spectra
 Experimental Properties

Type here to search

3:47 PM 3/3/2021

Two compounds were found on search

1. 1392484-49-9 (Similarity Score: 97 %)
2. 476-53-9 (Similarity Score: 95 %)