Supporting Information

Rec. Nat. Prod. 17:3 (2023) 561-565

Phenolic Bisabolanes from the Marine-Derived Fungus

Aspergillus sp. MEA11

Xin Liu^{1#}, Wenzhen Lin^{3,4,#}, Ruzhen Liu^{2,3,4}, Minghuang Ling³,

Chiming Guo⁴, Hongyan Meng⁴, Ying Guo⁴, Wei Xu^{1,3}

and Xiaona Du^{2,*}

¹School of Life Sciences, Anhui Agricultural University, Hefei 230036, China

²Sanquan College of Xinxiang Medical University, Xinxiang, Henan 453000, China

³Key Laboratory of Marine Biogenetic Resources, Third Institute of Oceanography, Ministry of Natural Resources, 178 Daxue Road, Xiamen 361005, China

⁴Fujian Key Laboratory of Subtropical Plant Physiology and Biochemistry, Fujian Institute of

Subtropical Botany, Xiamen 361006, China

Table of Contents	Page
Figure S1: ¹ H NMR spectrum of 1 in CD ₃ OD (400 MHz)	2
Figure S2: ¹³ C NMR spectrum of 1 in CD ₃ OD (100 MHz)	2
Figure S3: HSQC spectrum of 1 in CD ₃ OD	3
Figure S4: ¹ H- ¹ H COSY spectrum of 1 in CD ₃ OD	3
Figure S5: HMBC spectrum of 1 in CD ₃ OD	4
Figure S6: ¹ H NMR spectrum of 2 in CD ₃ OD (400 MHz)	4
Figure S7: ¹³ C NMR spectrum of 2 in CD ₃ OD (100 MHz)	5
Figure S8: ¹ H NMR spectrum of 3 in CD ₃ OD (400 MHz)	5
Figure S9: ¹³ C NMR spectrum of 3 in CD ₃ OD (100 MHz)	6
Figure S10: ¹ H NMR spectrum of 4 in CD ₃ OD	6
Figure S11: ¹³ C NMR spectrum of 4 in CD ₃ OD	7
Figure S12: ¹ H NMR spectrum of 5 in CD ₃ OD	7
Figure S13: ¹ H NMR spectrum of 6 in CD ₃ OD	8
Figure S14: ¹ H NMR spectrum of 7 in CD ₃ OD	8
Figure S15: ¹ H NMR spectrum of 8 in CD ₃ OD	9
Figure S16: HRESIMS spectrum of 1	9
Figure S17: Search report of SciFinder for compound 1	10
Figure S18: ECD spectra of 8a and 8b.	11

© 2023 ACG Publications. All rights reserved.



© 2023 ACG Publications. All rights reserved.



Figure S3:HSQC spectrum of 1 in DMSO-*d*₆



Figure S4:¹H-¹H COSY spectrum of 1 in CD₃OD

© 2023 ACG Publications. All rights reserved.



© 2023 ACG Publications. All rights reserved.

5



© 2023 ACG Publications. All rights reserved.



© 2023 ACG Publications. All rights reserved.



© 2023 ACG Publications. All rights reserved.

Figure S12:¹H NMR spectrum of 5 in CD₃OD



© 2023 ACG Publications. All rights reserved.



© 2023 ACG Publications. All rights reserved.

	ucture exact > su	ostances (0)	
RECORNE	S	UBSTANCES: CHEMICAL STRUCTU	URE 🛛
Besearch T	Topic		
Author Nam	me		
Company N	Name	Structure Editor:	Sauch Turan
Document J	Identifier	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	Exact Structure
Journal		, ,	Substructure
Patent		ÍÍ	Similarity
Tags			
+ SUBSTANC	ICES		Show precision analysis
Chemical St	Structure	Click image to change	
Markush		structure or view detail.	
Molecular F	Formula	Import CYE	Chembraw
Substance I	Identifier	Import ext-	Launch a SciFinder/SciFinder Substance of reaction search directly from the latest version of Chempraw. Learn More
		Connet	
REACTION	NS	Search	
Reaction St	Structure	Search	
Explore ¥	Saved Sear	ches SciDlanner	
Explore Sul	+ Saveu Seal		
 Explore Sul 	ubstances resulted	n o substances <u>Return</u>	
hemical Struc	icture exact > sub	stances (0)	
UBSTANCES	s		
nalyze Ref	efine		
nalyze by:			
lo substànces	s available		
omical Churt	turo cimilarity		
iemical Structi	ture similarity		
REFERENCES	ES	STANCES: CHEMICAL STRUCTURE	E U
Research Top	pic		
Author Name	9	Structure Editor:	
Company Nan Document Ide	ime Iontifior		Search Type:
Journal			Exact Structure
Patent		(([^])	Substructure Similarity
Tags			- onmony
SUBSTANCE	ES		Show precision analysis
Chemical Stru	ucture	Click image to change	
Markush		structure or view detail.	
Molecular For			
Property	rmula	Import CVE	O ChemDraw
Substance Ide	rmula	Import CXF	OcenDraw Launch a SciFinder/SciFinder ^D substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide	rmula lentifier	Import CXF	OverDeav Launch a SciFinder/SciFinder ^D substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide	rmula lentifier S	Import CXF Search	OkenDeaw Launch a SciFinder/SciFinder ^D substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide REACTIONS Reaction Strue	rmula Ientifier S ucture	Import CXF Search Search	OkamDaw Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide REACTIONS Reaction Strue	rmula lentifier <u>S</u>	Import CXF Search Search	OkenDew Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Structure sin	rmula Ientifier S ucture	Import CXF Search & Advanced Search	OkenDew Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide REACTIONS Reaction Structure sin CALSES	rmula lentifier s ucture imilarity	Import CXF Search Search	OkenDew Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Structure sin cal Structure sin TANCES	rmula lentifier s ucture imilarity Select All C	Import CXF Search Search	ChemDew SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Structure sin TANCES	Imilarity Select All C 0 of 7 Similar	Import CXF Search Search Advanced Search reselect All ity Candidates Selected	Combow Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Structure sin TANCES	Interfier S Lucture S Select All C O of 7 Simila C 2 99 (r	Import CKF Search Search Advanced Search reselect All ity Candidates Selected not similar)	Combow Launch a SciFinder/SciFinder ^{II} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Structure sin CANCES	Image: Select All C Select All C 0 of 7 similar > 299 (r 95.98 90.04	Import CXF Search S Advanced Search reselect All try Candidates Selected nest similar)	Combow Launch a SciFinder/SciFinder ^{III} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Structure sin CANCES	Implicit and the second seco	Import CXF Search Search Advanced Search eselect All ity Candidates Selected nost similar)	ChemDow Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Stru- cal Structure sin IANCES	rmula lentifier s	Import CKF Search Search Advanced Search reselect All ity Candidates Selected nost similar)	Chembow Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide REACTIONS Reaction Stru- cal Structure sin IANCES	rmula lentifier S Lucture Select All C S Select All C S Select All C S Select All C S Select Select Select S Select Select Select S Select Se	Import CXF Search CANADAC Search CANADAC Search Reselect All ty Candidates Selected nost similar)	Combow Launch a SciFinder/SciFinder ^{II} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide REACTIONS Reaction Stru- cal Structure sin IANCES	rmula lentifier S imilanty Select All C 0 of 7 smala 0 ≥ 95 88 9 90-84 8 8589 9 80-84 8 8589 9 0-64 (k) 0 65-69 0 -64 (k)	Import CXF Search C Advanced Search reselect All ity Candidates Selected nost similar)	Chambow Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Stru- cal Structure sin <u>IANCES</u>	rmula lentifier S cuture Select All C 9 of 7 Simila 2 99 (1 9 59-98 9 09-94 8 88-89 8 88-89 9 73-74 8 66-69 9 70-74 6 65-69 9 0 0-64 (1) 6 65-69	Import CXF Search Search Advanced Search reselect All ity Candidates Selected root similar) act similar)	ChemDow Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Stru- cal Structure sin TANCES	rmula lentifier S jucture 0 of 7 Simila 0 of 7 Simila 0 0 of 7 Simila 0 90.94 88.99 80.84 1 75.79 1 70.74 1 65.69 0 0.64 (li 6.549 0 0.64 (li 6.549) 0 0.65 (li 6.549) 0 0.64	Import CXF Search Search Advanced Search reselect All thy candidates Selected nost similar) test similar)	Chembow Launch a SciFinder/SciFinder ^{In} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide <u>REACTIONS</u> Reaction Stru- cal Structure sin <u>FANCES</u>	rmula lentifier s_ imilanty Select All [0 of 7 Simila ≥ 99 (8 90.94 88.99 80.94 87.579 70.74 85.89 80.94 75.79 0.6-64 (k Get Subst: ure subst:	Import CXF Search Search Advanced Search weselect All ity Candidates Selected most similar) at similar) mores ances (4)	Combow Launch a SciFinder/SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More
Substance Ide REACTIONS Reaction Struc- cal Structure sin TANCES	rmula lentifier s jucture 0 of 7 simila ≥ 90 (95-58 90-54 85-59 80-64 (lu € 65-69 0 - 0-64 (lu € 65-69) - 0-66 (lu € 65-69) - 0-66 (lu)	Import CXF Search Search Advanced Search esselect All ity Candidates Selected nost similar) ances (4) effect Commercial [#, Tools*	Create Keep Me Sed Sub
Substance Ide <u>REACTIONS</u> Reaction Stru- tal Structure sin TANCES hemical Structur UBSTANCES nalyze	rmula lentifier S initianity Select All [0 of 7 similar 2 99 (0 8 569) 8 859) 8 80-84 8 859) 8 90-94 0 -64 (li Get Substr References 1 Seterences 1 Seter	Import CXF Search Advanced Search Advanced Search reselect All ity Candidates Selected reselect All ity Candidates Selected ast similar) ances (4) reselect All All Advanced Search Advanced Search A	Create Keep Ne Sub Create Keep Ne Create Keep N
Substance Ide <u>REACTIONS</u> Reaction Stru- cal Structure sin <u>FANCES</u> hemical Structure <u>UBSTANCES</u> nalyze <u>eBope</u> by •	select All E 0 of 7 Similar 2 > 90 9 > 98 9 > 98 9 > 98 9 > 90 88-89 88-89 0 of 7 Similar 55-59 0 - 0.44 (tr) Get substration 9 - 0.44 (tr) 55-69 0 - 0.45 (tr) 56 9 - 0.44 (tr) 57 - 97 9 - 0.44 (tr) 56 9 - 0.44 (tr)	Import CXF Search Advanced Search Advanced Search ity Candidates Selected ity Candidates Selected ity Candidates Selected more similar) ast similar) ast similar) ast similar) ast similar) ast similar) ast similar) arces arces (4) if Candidates Selected if Candidates Selected	Create Keep Me
hemical Structure hemical Structure hemical Structure ubstances nalyze effyee by: • ubstance R •	select All [0 of 7 Similar 2 >90 (9 > 98 9 > 98 9 > 98 9 > 98 9 > 98 9 > 98 9 > 90 9 > 91 9 > 92 9 > 94 9 > 95 0 > 64 (II 75.74 65.69 0 > 64 (II 70.74 65.69 0 > 64 Substr 5 of 4 Substr	Import CXF Search Search Advanced Search esclect All ty Candidates Selected nost similar) ances (a) intersity of the commercial (# Tools* Sources Selected 3 %	Contrology Launch a SciFinder ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More Sub
Nubstance Ide REACTIONS Reaction Stru- cal Structure sin FANCES hemical Structure UBSTANCES halfyze by: by: by: by: course tor tor tor tor tor tor tor tor	rmula lentifier S scicture Select All C 0 of 7 smla 0 > 508 9 0.04 9 558 9 0.04 8 859 0 0.64 1 75.79 0 0.64 1 80.64 1 75.79 0 0.64 1 80.64 1 75.79 0 0.64 1 80.64 1 50.64 1 50.64 1 50.64 1 50.64 1 50.64 1 22072-63 1 2	Import CXF Search CANADACE Search Conditional Search Advanced Search	Control over Launch a SciFinder [®] substance or reaction search directly from the latest version of ChemDraw. Learn More Sub Sub Sub Sub Sub Sub Sub Sub
Substance Ide REACTIONS Reaction Stru- cal Structure sin TANCES hemical Structur UBSTANCES nalyze efforts for e biostance R + iccurrenc 4 roperties 4	rmula lentifier S cuture Select All C O of 7 Similar Select All C O of 7 Similar S 2 90 (1 S 30 54 S 509 0 0 - 64 (1) Get Substa References 4 (1) S of 4 Substa Store 10 of 4 Substa Store 2 1 122/073-63 A 1 ~ 1 ²	Import CXF Search Search Advanced Search reselect All ity Candidates Selected road similar) ances (4) let sources ances (4) ances	Create New More Subtrace or reaction search directly from the latest version of ChemDraw. Learn More Sub
hemical Structure sin TANCES hemical Structure sin tances hemical Structure hemical Structure ubstance R • courses 4 iological 2 5 1 1 1 1 1 1 1 1 1 1 1 1 1	mula lentifier S Licture S Select All C 0 of 7 Similar 0 of 7 Similar 0 of 7 Similar 0 99 98 0 90 94 0 88 89 0 0 44 (http://www.select.org/selec	Import CXF Search ⊯ Advanced Search wedetect All ity Candidates Selected more similar) mores ats similar) more similar) ats second ats similar) ats similar)	Cheadow Launch a SciFinder/SciFinder [®] substance or reaction search directly from the latest version of ChemDraw. Learn More Sub Sub Sub Sub Sub Sub Sub Sub
benical Structure sin TANCES	select All [0 of 7 Similar 2 99 (9 0.94 88.89 90.94 88.89 80.84 75.79 70.74 65.69 0.64 (lt 75.79 70.74 65.69 0.64 (lt 75.79 5.61 0.64 (lt 75.79 0.64 (lt 75.79 0.64 (lt 75.79 0.64 (lt 75.79 1.1227073-63 4 ~1*	Import CXF Search Search Advanced Search Reselect All ty Candidates Selected nost similar) ances (a) ist imported in the selection of	Conclose Launch a SciFinder/SciFinder [®] substance or reaction search directly from the latest version of ChemDraw. Learn More Sub S
hemical Structure sin rANCES hemical Structure sin rANCES hemical Structure ubstance R viccurrenc roperties iological reparation rep	rmula lentifier S inilanty Select All C 0 of 7 simila 2 Select All C 0 of 7 simila 2 Select All C 9 568 9 9.04 8 8589 9 0.04 8 8589 9 0.04 Cet Substr Cet Substr Cet Substr Soft by: Similarty S Soft by: Similarty S Soft by: Similarty S 1.1227073-03 -4 ⁸ ~1 ⁸	Import CXF Search Carch Advanced Search reselect All rity Candidates Selected notes similar) ances (4) iet constrained in Tools* Sources ore $\neg $ (ces Selected 3 *	Subtract lines a SciFinder/SciFinder [®] substance or reaction search directly from the latest version of ChemDraw. Learn More sub • Create Keep Me * Southon • Create Keep Me
Animical Structure sin TANCES	rmula lentifier S intianty Select All C 0 of 7 Simila 0 of 64 0 of 7 Similar 0 of 64 0 of 7 Similar 0 of 7 Similar 0 of 7 Similar 0 of 7 Similar 0 of 64 0 of 7 Similar 0 of 64 0 of 7 Similar 0 of 64 0 of 7 Similar 0 of 4 Substar Score 92 0 1 2 Similar 0 of 4 Substar Score 92 0 1 2 Similar 0 of 7 of 4 0 of 7 of 4 0 of 7 of 4 0 of 7 of 7 0 of 7 0 of 7 of 7 0 of 7 0 of 7 of 7 0 of 7	Import CXF Search Search Advanced Search Reselect All ity Candidates Selected not similar) ances (4) iet searchons Sources $r \rightarrow \phi$ ces Selected 3 \sim $r \rightarrow \phi$ Rotation (+), Absolute stare SCS-64 aretylony-1 Hydrowy 1, -U-thmathalawa	Events Keep He SciPinder ¹ substance or reaction search directly from the latest version of ChemDraw. Learn More sub Sub Sub Sub Sub Sub Sub Sub
hemical Structure sin TANCES hemical Structure sin tances hemical Structure hemical Structure hemical Structure structure hemical Structure structure hemical Structure structure structure hemical Structure structure hemical Structure structure hemical Structure hemical Structure structure hemical Structure hemical Structure structure hemical Structure hemical Structure structure hemical Structure hemical Structure hemi	rmula lentifier S Licture Select All C 0 of 7 Similar 0 of 7 Similar 0 of 7 Similar 0 0 of 7 Similar 0 0 of 7 Similar 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Import CXF Search We Advanced Search We Advanced Search We consider the search we select All thy Candidates Selected nost similar) measures ances (4) interest ances (4) interest Sources $T \to 0$ C = Selected 3 *	Launch a SciFinder/SciFinder [®] substance or reaction search directly from the latest version of ChemDraw. Learn More Sub
Americal Structure sin TANCES	rmula lentifier S Lcture Select All C O f 7 simla D 0	Import CXF Search Advanced Search Heredect All thy Candidates Selected needs similar) acts similar) acts similar) acts similar) act	Lunch a SciFinder/SciFinde ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More sub Sub Sub Sub Sub Sub Sub Sub
Substance Ide REACTIONS Reaction Stru- cal Structure sin TANCES temical Structure ubstance R structure structure temical Structure temical Structure temic	mula lentifier S cuture Select All C 0 of 7 Simila 2 99 (0 9 958) 8 8589 8 8589 0 0-64 (li Get Substr References 1 Sort by: Similarly S Sort by: S S Sort by: S S S S S S S S S S S S S S	Import CXF Search Search Advanced Search reselect All ity Candidates Selected not similar) antes (4) iet strimar) rese iet commercial [# Tools" reserved at similar) reserved at similar) rese	Launch a SciFinder/SciFinder [®] substance or reaction search directly from the latest version of ChemDraw. Learn More Sub Sub Sub Sub Sub Sub Sub Sub
Substance Ide REACTIONS Reaction Stru- cal Structure sin TANCES Ammical Structure malyze	mula lentifier S Licture Select All C 0 of 7 Simila 0 of 7 Simila 0 of 7 Simila 0 99.98 0 0 4 Substar Score: 92 = 1.1227073-63 - 4 ³ ~ 1 ⁶ Benzoic acid, 4-{(11 Score: 92 = 3.2293120-59 - 2 ³	Import CXF Search Search Advanced Search Reselect All ity Candidates Selected most similar) acts similar) acts similar) ity Candidates Selected most similar) ity Candidates Selected most similar) acts s	Launch a SciFinder/SciFinder [®] substance or reaction search directly from the latest version of ChemDraw. Learn More sub Sub sub su
Substance Ide REACTIONS Reaction Stru- cal Structure sin TANCES hemical Structure UBSTANCES advantage by: • Substance R • Courrenc 4 roperties 4 idogical 2 sees 2 2 Show Hore	rmula lentifier S Licture Select All [0 of 7 Similar 0 of 7 Similar 0 of 7 Similar 0 of 7 Similar 0 0 of 7 Similar 0 99 (8 99 0 0 0 0 0	Import CXF Search We Advanced Search We Advanced Search We condicates Selected inty Candidates Selected most similar) most similar)	Launch a SciFinder ¹ substance or reaction search directly from the latest version of ChemDraw. Learn More Sub Sub Sub Sub Sub Sub Sub Sub
Above the second	mula lentifier S inilarity Select All C 0 of 7 simila ○ 20 of 7 simila ○ 5000 9 5500 0 95500 0 955000 0 9550000 0 9550000 0 955000 0 955000 0 955000 0 9550000000 0 9550000000000000000000000000000000000	Import CXF Search Search Advanced Search reselect All rity Candidates Selected reselect All rity Candidates Selected reselections ances (4) refer Commercial $ = Tools^+$ reselections reselected 3 • $q_{+} = f_{+} $	Lunch a SciFinder/SciFinde ^{IN} substance or reaction search directly from the latest version of ChemDraw. Learn More Sub Sub Constant Keepy Ne SciPinde S
Americal Structure sin Americal Structure sin ANCES hemical Structure sin ANCES hemical Structure ubstance R • coursec 4 opperties 4 iological 3 reparatio 2 ses 2 show More	rmula lentifier S intianty Select All C 0 of 7 Simila ○ 2 99 (○ 55-98 ○ 0-64 () ○ 65-60 ○ 6-64 () ○ 64 Substar Score 92 ○ 1, 122707-63- Clar 4 (Clar 4 () Clar 4 () Cla	Import CXF Search Search Advanced Search Heselect All ity Candidates Selected food similar) ances (4) Section & Commercial A Tools ⁻ ord Sources $a_{a_{a_{a_{a_{a_{a_{a_{a_{a_{a_{a_{a_{a$	Launch a SciFinder/SciFinder [®] substance or reaction search directly from the latest version of ChemDraw. Learn More sub

Figure S17: Search report of SciFinder for compound 1.

© 2023 ACG Publications. All rights reserved.



Figure S18: ECD spectra of 8a and 8b.