Supporting Information

Noonindoles G–L: Indole terpene glycosides from the Australian marine-derived fungus *Aspergillus noonimiae* CMB-M0339

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List of contents

List of figures

List of tables

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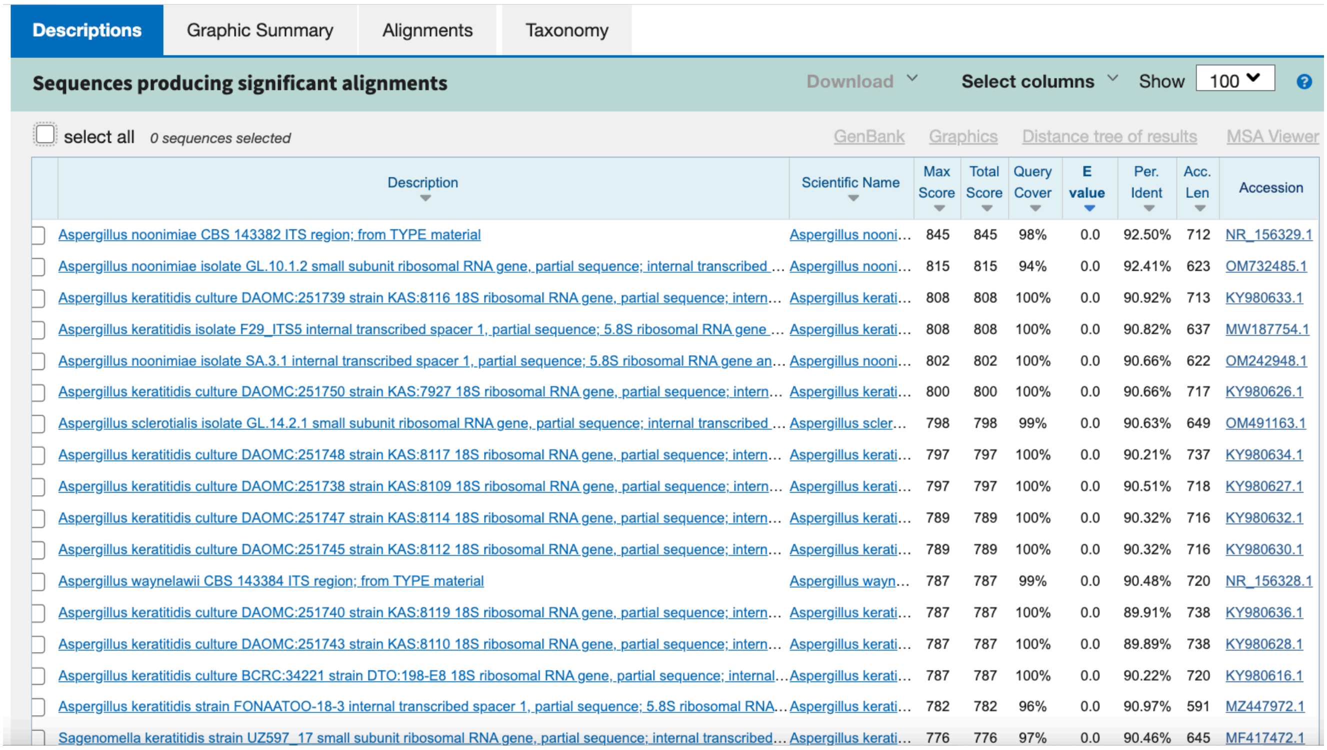
Figure S1.ITS gene sequence of CMB-M0339



Descriptions | Graphic Summary | Alignments | Taxonomy

Sequences producing significant alignments Download Select columns Show 100

select all *0 sequences selected* GenBank Graphics Distance tree of results MSA Viewer

Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
Aspergillus noonimiae CBS 143382 ITS region; from TYPE material	Aspergillus nooni...	845	845	98%	0.0	92.50%	712	NR_156329.1
Aspergillus noonimiae isolate GL.10.1.2 small subunit ribosomal RNA gene, partial sequence; internal transcribed ...	Aspergillus nooni...	815	815	94%	0.0	92.41%	623	OM732485.1
Aspergillus keratitidis culture DAOMC:251739 strain KAS:8116 18S ribosomal RNA gene, partial sequence; intern...	Aspergillus kerati...	808	808	100%	0.0	90.92%	713	KY980633.1
Aspergillus keratitidis isolate F29_ITS5 internal transcribed spacer 1, partial sequence; 5.8S ribosomal RNA gene ...	Aspergillus kerati...	808	808	100%	0.0	90.82%	637	MW187754.1
Aspergillus noonimiae isolate SA.3.1 internal transcribed spacer 1, partial sequence; 5.8S ribosomal RNA gene an...	Aspergillus nooni...	802	802	100%	0.0	90.66%	622	OM242948.1
Aspergillus keratitidis culture DAOMC:251750 strain KAS:7927 18S ribosomal RNA gene, partial sequence; intern...	Aspergillus kerati...	800	800	100%	0.0	90.66%	717	KY980626.1
Aspergillus sclerotialis isolate GL.14.2.1 small subunit ribosomal RNA gene, partial sequence; internal transcribed ...	Aspergillus scler...	798	798	99%	0.0	90.63%	649	OM491163.1
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Aspergillus keratitidis culture DAOMC:251738 strain KAS:8109 18S ribosomal RNA gene, partial sequence; intern...	Aspergillus kerati...	797	797	100%	0.0	90.51%	718	KY980627.1
Aspergillus keratitidis culture DAOMC:251747 strain KAS:8114 18S ribosomal RNA gene, partial sequence; intern...	Aspergillus kerati...	789	789	100%	0.0	90.32%	716	KY980632.1
Aspergillus keratitidis culture DAOMC:251745 strain KAS:8112 18S ribosomal RNA gene, partial sequence; intern...	Aspergillus kerati...	789	789	100%	0.0	90.32%	716	KY980630.1
Aspergillus waynelawii CBS 143384 ITS region; from TYPE material	Aspergillus wayn...	787	787	99%	0.0	90.48%	720	NR_156328.1
Aspergillus keratitidis culture DAOMC:251740 strain KAS:8119 18S ribosomal RNA gene, partial sequence; intern...	Aspergillus kerati...	787	787	100%	0.0	89.91%	738	KY980636.1
Aspergillus keratitidis culture DAOMC:251743 strain KAS:8110 18S ribosomal RNA gene, partial sequence; intern...	Aspergillus kerati...	787	787	100%	0.0	89.89%	738	KY980628.1
Aspergillus keratitidis culture BCRC:34221 strain DTO:198-E8 18S ribosomal RNA gene, partial sequence; internal...	Aspergillus kerati...	787	787	100%	0.0	90.22%	720	KY980616.1
Aspergillus keratitidis strain FONAATOO-18-3 internal transcribed spacer 1, partial sequence; 5.8S ribosomal RNA...	Aspergillus kerati...	782	782	96%	0.0	90.97%	591	MZ447972.1
Sagenomella keratitidis strain UZ597_17 small subunit ribosomal RNA gene, partial sequence; internal transcribed...	Aspergillus kerati...	776	776	97%	0.0	90.46%	645	MF417472.1

Figure S2. NCBI-BLAST search of ITS sequence of CMB-M0339

Aspergillus noonimiae CBS 143382 ITS region; from TYPE material

Sequence ID: NR_156329.1 Length: 712 Number of Matches: 1

See 1 more title(s) See all Identical Proteins(IPG)

Range 1: 52 to 642 GenBank Graphics ▼ Next Match ▲ Previous Match

Score	Expect	Identities	Gaps	Strand
845 bits(457)	0.0	555/600(93%)	15/600(2%)	Plus/Plus

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Aspergillus noonimiae CBS 143382 ITS region; from TYPE material

NCBI Reference Sequence: NR_156329.1

FASTA Graphics

Go to:

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VERSION     NR_156329.1
DBLINK      BioProject: PRJNA177353
KEYWORDS    RefSeq.
SOURCE      Aspergillus noonimiae
  ORGANISM  Aspergillus noonimiae
            Eukaryota; Fungi; Dikarya; Ascomycota; Pezizomycotina;
            Eurotiomycetes; Eurotiomycetidae; Eurotiales; Aspergillaceae;
            Aspergillus; Aspergillus subgen. Polypaecilum.
REFERENCE   1  (bases 1 to 712)
  AUTHORS   Tanney,J.B., Visagie,C.M., Yilmaz,N. and Seifert,K.A.
  TITLE     Aspergillus subgenus Polypaecilum from the built environment
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  JOURNAL   Submitted (21-APR-2017) Biodiversity (Mycology), Agriculture and
            Agri-Food Canada, 960 Carling Avenue, Ottawa, Ontario K1A0C6,
            Canada
```

Figure S3. Blast search (closet match) for CMB-M0339

1 Phylogenetic tree

Phylogenetic tree obtained by PhyML Maximum Likelihood analysis was constructed using the top similar ITS sequences displayed after BLAST on Refseq RNA NCBI database using CMB-M0339 ITS as queries. The JC69 model was used to infer phylogeny sequences[1]. Sequences alignments were produced with the MUSCLE program[2]. Phylogenetic tree was constructed using the UGENE program using the aforementioned models and visualized using Ugene's tree view[3].

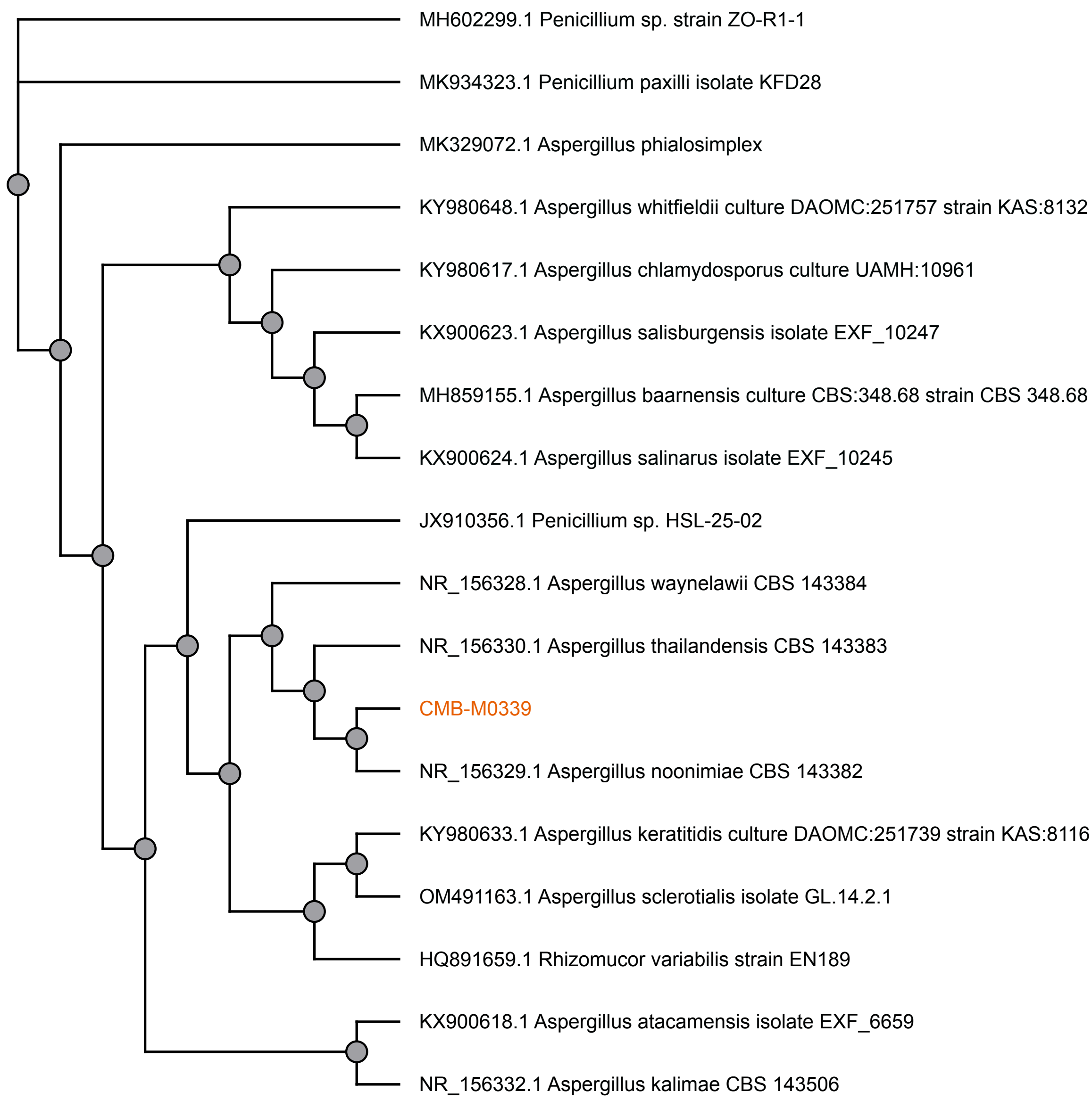

Figure S4. Phylogenetic tree by PhyML Maximum Likehood analysis of ITS sequences showing the relationship of CMB-M0339 among selected reference strains (RefSeq GenBank) with the accession numbers

Figure S5. CMB-M0339 cultivated on M1 agar (supplemented with 3.3% artificial sea salt)

2 MATRIX cultivation of CMB-M0339

CMB-M0339 was cultivated in 24-well MBR plate (×11) including solid, broth shaking and static to generate 33 different cultivation media composition / conditions. The fungal spores from M1 agar plate were transformed using a sterile loop to inoculate MBR deep well plate (containing 1.5 mL broth or 2.0 mL agar). M1 media served as negative controls. MBR cultures were incubated at 190 rpm at 27 °C (broth shaking), at 30 °C (broth static and solid) for 10-14 days with continuous monitoring for fungal growth.

The culture (×33) per strain were extracted *in situ* with EtOAc (2 mL per well) followed by filtration or centrifugation at 13,000 rpm for 3 min and dried under N_2 at 40 °C to yield 33 crude extracts. The extracts were dissolved in 30 µL of MeOH with calibrant (50 ng/mL) to generate 0.1 mg/ mL. An aliquot (10 µL) of crude extract was analysed with UHPLC-DAD, UHPLC-QTOF and HPLC-DAD-ESIMS.

a) b) c)

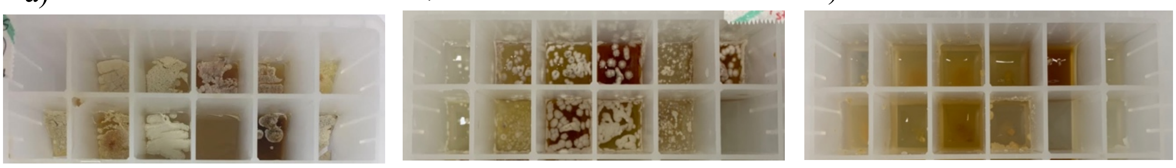

Figure S6. CMB-M0339 cultivated under MATRIX conditions. (a) solid (b) broth static (c) broth shaking

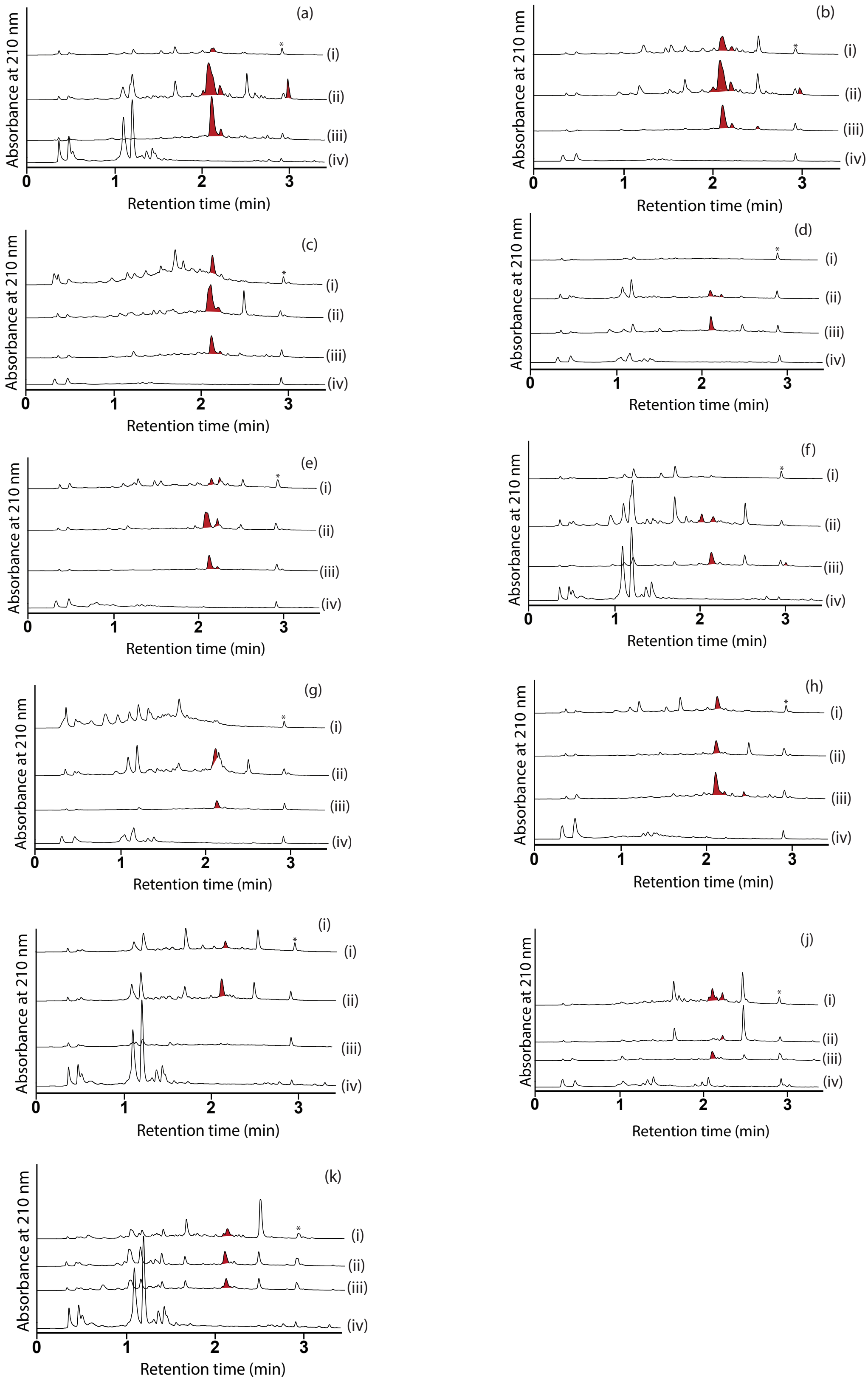

Figure S7. UPLC-DAD chromatograms of MATRIX extracts of CMB-M0339 showing the production of **1-3** (highlighted in red) in different media and culture conditions; (a) D400, (b) GY, (c) IM ,(d) M1, (e) M2, (f) SGG, (g) YEME, (h) YES, (i) 333, (j) PD, (k) SD, (i) Liquid shaking, (ii) Liquid static, (iii) solid, (iv) Media blank, * Internal calibrant

Table S1. **Composition of media used for cultivation profiling**

Medium	Composition (per Litre)
M1	Peptone (2.0 g), yeast extract (4.0 g), starch (10.0 g), artificial sea salt (33.0 g), agar (18.0 g)
M2	Mannitol (40.0 g), maltose (40.0 g), yeast extract (10.0 g), K_2HPO_4 (2.0 g), $MgSO_4.7H_2O$ (0.5 g), $FeSO_4.7H_2O$ (0.01 g), agar (18.0 g),
IM	Yeast extract (Difco) (4.0 g), malt extract (Difco) (10.0 g), glucose (country brewers) (4.0 g), mannitol (Amyl) 40.0 g, agar (Amyl) (18.0 g)
Modified YEME	Bacto peptone (Difco) (5.0 g), yeast extract (Difco) (3.0 g), Oxoin malt extract (3.0 g), glucose (10.0 g), sucrose (170.0 g), agar (18.0 g)
GY	Yeast extract (Difco) (4.0 g), malt extract (Difco) (10.0 g), glucose (country brewers) (4.0 g), $CaCO_3$ (Univar Ajax) (2.0 g), soluble starch (Difco) (20.0 g), agar (Amyl) (18.0 g)
YES	Sucrose (150 g), yeast extract (20 g), $MgSO_4.7H_2O$ (0.5 g), $ZnSO_4.7H_2O$ (0.01 g), $CuSO_4.5H_2O$ (0.005 g), agar (18.0 g)
D400	Glucose (10.0 g), malt extract (3.0 g), peptone (3.0 g), soluble starch (20.0 g), yeast extract (5.0 g), $CaCO_3$ (3.0 g), agar (18.0 g).
SGG	Glucose (10.0 g), glycerol (10.0 g), cornsteep powder (2.5 g), peptone (5.0 g), soluble starch 10.0 g), yeast extract (2.0 g), $CaCO_3$ (3.0 g), NaCl (1.0 g), agar (18.0 g).
333	Glucose (5.0 g), peptone (3.0 g), soluble starch (10.0 g), yeast extract (3.0 g), $CaCO_3$ (2.0 g), agar (18.0 g).
PD	Potato extract (4.0 g), dextrose (20.0 g), agar (18 g)
SD	Peptic digest of animal tissue (5.0 g), pancreatic digest of casein (5.0 g), dextrose (40.0 g), agar (18 g)

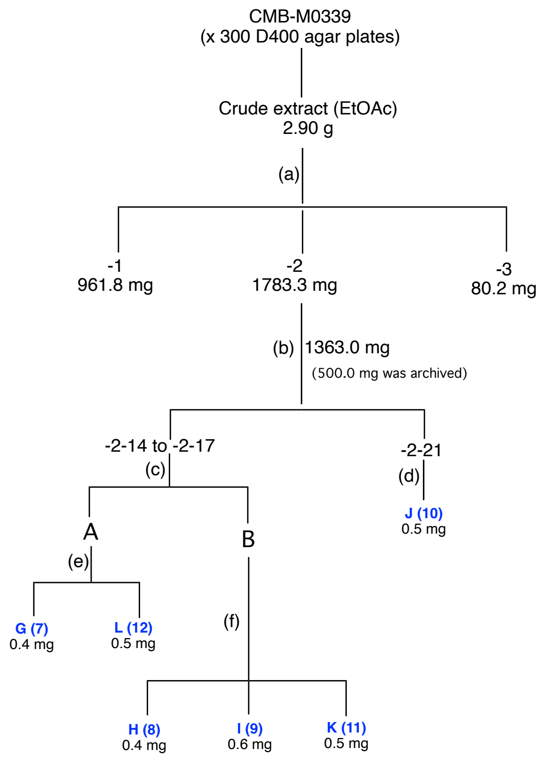

Figure S8. Isolation scheme of noonindoles G – L (**7-12**) from CMB-M0339. (a) Trituration [hexane (-1), DCM (-2), MeOH (-3)]. (b) Preparative reversed phase HPLC (Phenomenex Luna-C_8 10 µm, 21.2 × 250 mm column, with gradient elution at 20 mL/min over 20 min from 90% H_2O/MeCN to 100% MeCN with constant 0.1% TFA/MeCN modifier). (c) Column chromatography: Sep-Pak (Agilent Bond Elut C_{18} column, 5 g) gradient elution from 90% H_2O/MeCN to 100% MeCN (d) Semi preparative HPLC (Zorbax C_{18} 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 85% MeCN/H_2O over 15 min with constant 0.1% TFA modifier. (e) Semi preparative HPLC (Zorbax C_{18} 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 45% MeCN/H_2O over 35 min with constant 0.1% TFA modifier. (f) Semi preparative HPLC (Zorbax C_{18} 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 45% MeCN/H_2O over 25 min with constant 0.1% TFA modifier

3 Spectroscopic characterization of metabolites G-L (7-12)

3.1 Noonindole G (7)

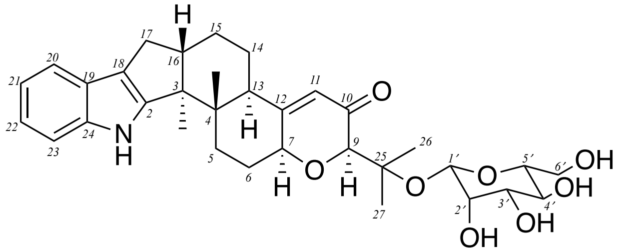

Table S2. 1D and 2D NMR (600 MHz, methanol-d_4) data for noonindole G (**7**)

Pos.	$\delta_{H,}$ mult. (*J* in Hz)	δ_C	COSY	^1H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	151.2	-	-	-
3	-	51.8	-	-	-
4	-	50.6[a]	-	-	-
5	*a* 2.12, ddd (*13.8, 13.8, 3.7*)	33.0	6*a*, 6*b*, 5*b*	13, 4-Me	-
	b 2.04, m		5*a*, 6*b*	6, 7, 13	-
6	*a* 2.31, m	31.1	6*b*, 7	4/16, 7	-
	b 1.93, ddd (*13.8, 13.5, 4.4*)		5*b*, 6*a*, 7	5	-
7	4.41, dd (*7.9, 7.9)*	77.0	6*a*, 6*b*	6, 11	9
9	4.01, br s	85.0	-	7, 10, 25, 26, 27	7
10	-	196.5	-	-	-
11	5.77, br s	122.8	-	7, 9, 13	-
12	-	169.2	-		-
13	2.58, br d (*11.6*)	43.8	14*a*, 14*b*	4/16, 11, 12, 4-Me	3-Me
14	*a* 1.71, d (*13.0)*	27.0	14*b*, 13	13, 15, 4/16	-
	b 1.60, dd (*13.0, 4.7*)		15*a*, 15*b*, 14*a*, 13	13, 4/16	-
15	*a* 1.83, m	25.4	15*b*, 16, 14*a*,14*b*	3, 13, 14	-
	b 1.76, dd (*13.0, 3.4*)		15*a*, 14*a*,14*b*,16	4/16	-
16	2.84, m	50.6[a]	17*a*, 17*b*, 15*b*	-	4-Me
17	*a* 2.68, dd (*12.6*, *6.4*)	28.2	17*b*, 16	2, 3, 18	-
	b 2.38, dd (*12.6*, *10.8*)		17*a*, 16	2, 4/16, 18	-
18	-	118.2	-	-	-
19	-	126.3	-	-	-
20	7.30, d (*8.3*)	119.0	21	22, 24	-
21	6.93, dd (*8.3*, *7.3*)	120.0	20, 22	19, 23	-
22	6.97, dd (*8.2*, *7.3*)	121.1	21, 23	20, 24	-
23	7.28, d (*8.2*)	112.8	22	19, 21	-
24	-	142.2	-	-	-
25	-	79.3	-	-	-
26	1.41, s	21.5	-	9, 25, 27	-
27	1.48, s	26.1	-	9, 25, 26	-
1′	4.96, br s	97.0	2′	2′, 25	5′, 3′
2′	3.81, d (*3.0*)	73.7	3′	3′, 4′	-
3′	3.43, dd (*9.4*, *3.0*)	75.7	2′, 4′	4′	1′, 5′
4′	3.57, t (*9.4*)	68.5	3′, 5′	6′, 5′	-
5′	3.17, ddd (*9.4*, *5.6*, *2.1*)	78.1	6′ *b*, 4′	-	1′, 3′
6′	*a* 3.84, dd (*11.7*, *2.1*)	63.0	5′, 6′ *b*	4′	-
	b 3.69, dd (*11.7*, *5.6*)		5′, 6′ *a*	4′, 5′	-
3-Me	1.09, s	14.9	-	2, 3, 4/16	13
4-Me	0.99, s	16.4	-	3, 4/16, 5, 13	16

[a] Resonances with the same superscript within a column are overlapping and assignments may be interchanged

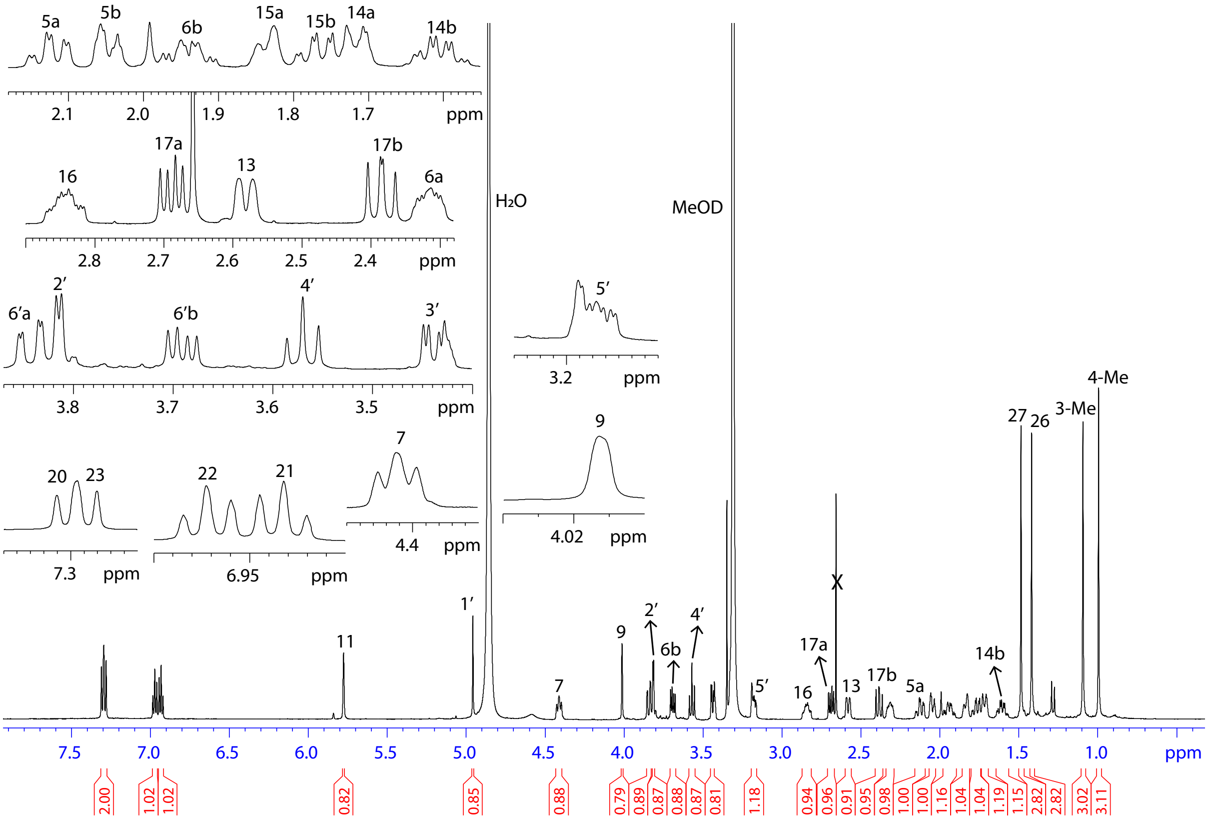

Figure S9. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of noonindole G (**7**)

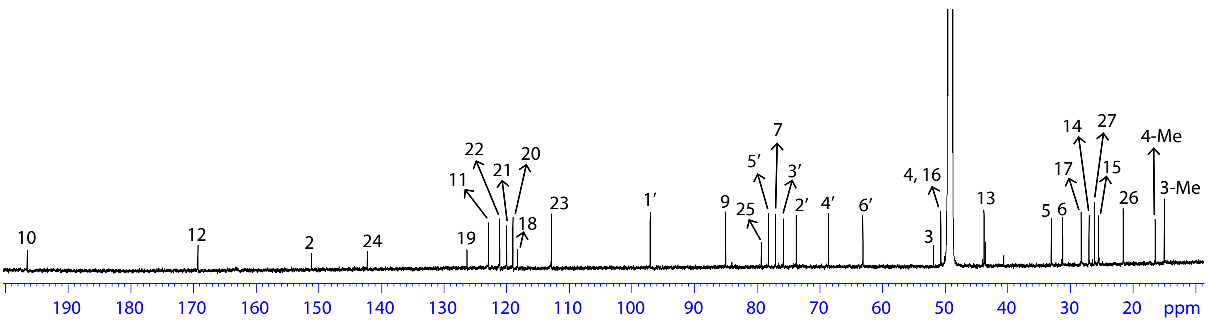

Figure S10. ^{13}C NMR (150 MHz, methanol-d_4) spectrum of noonindole G (**7**)

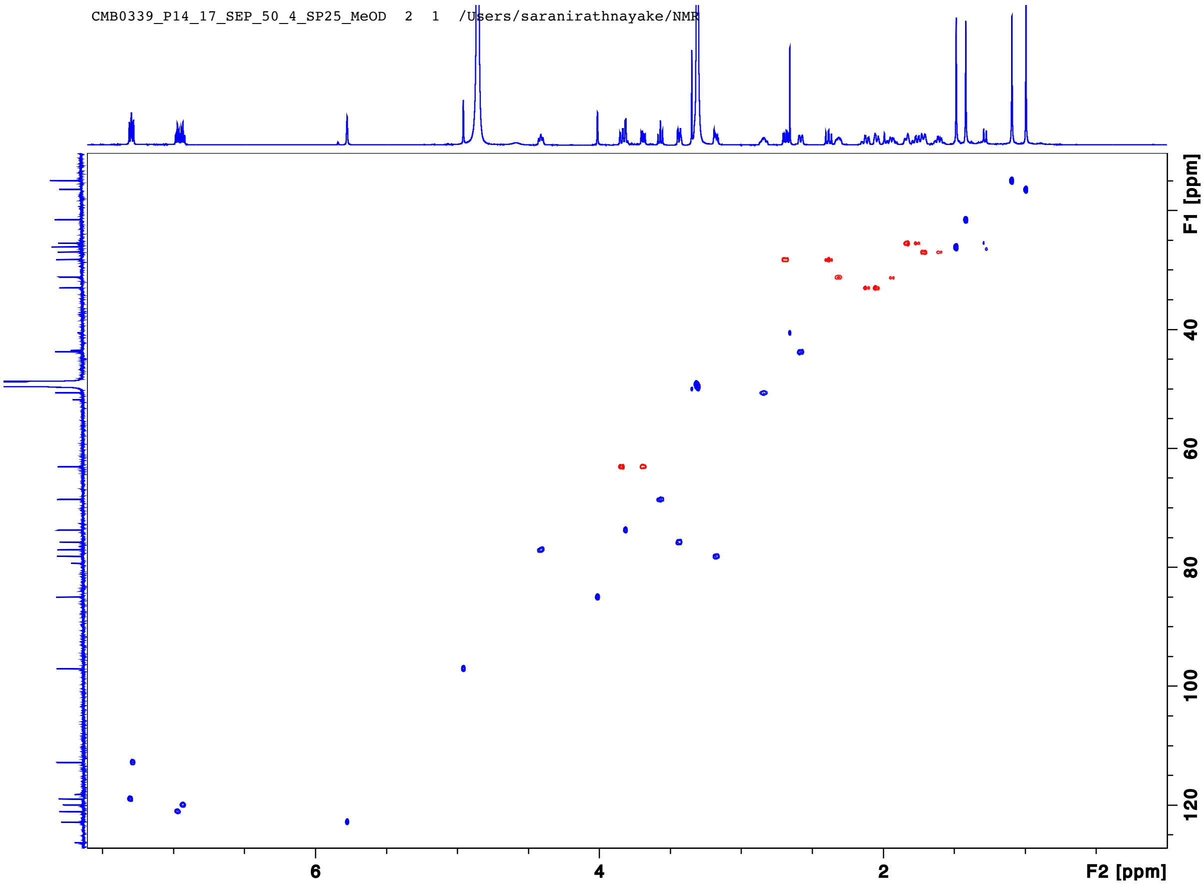

Figure S11. HSQC (methanol-d_4) spectrum of noonindole G (**7**)

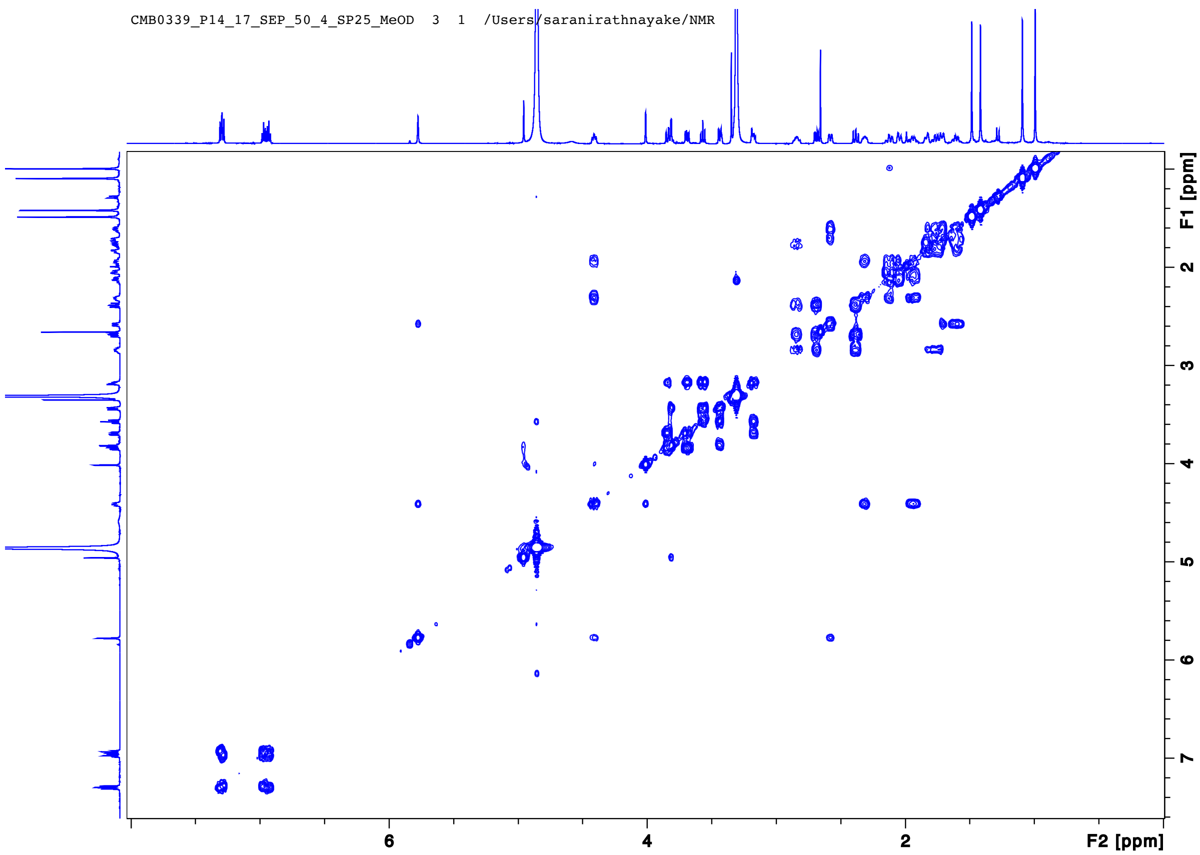

Figure S12. COSY (methanol-d_4) spectrum of noonindole G (**7**)

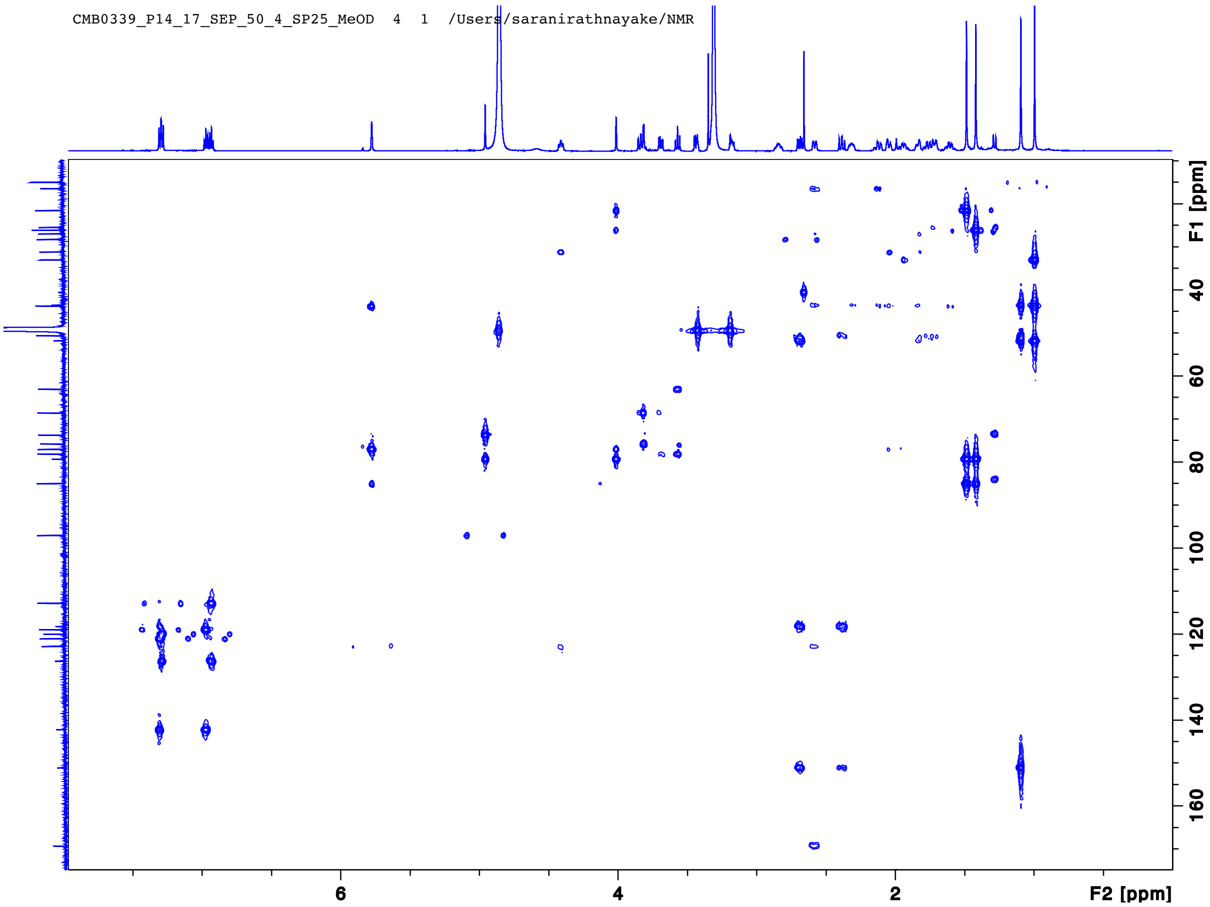

Figure S13. HMBC (methanol-d_4) spectrum of noonindole G (**7**)

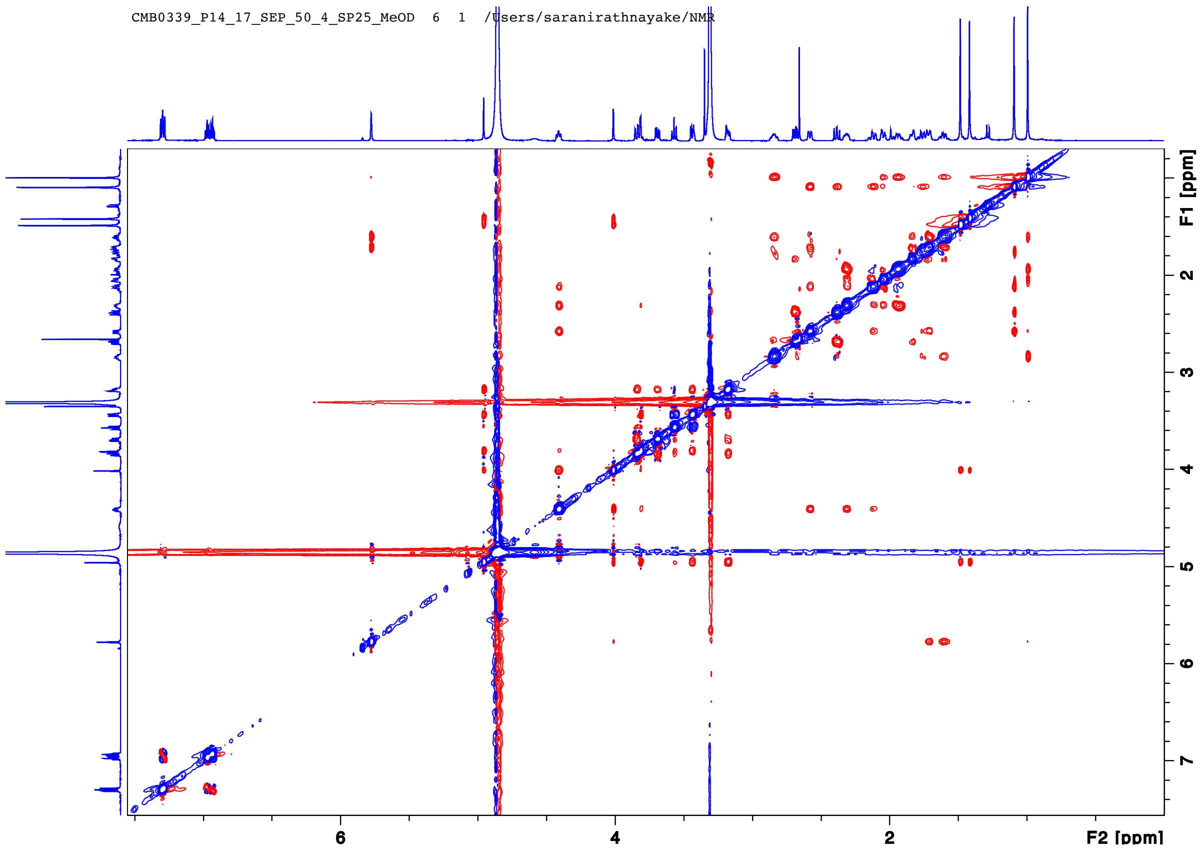

Figure S14. ROESY (methanol-d_4) spectrum of noonindole G (**7**)

Mass Spectrum Molecular Formula Report

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Comment			

Acquisition Parameter

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Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.			
Formula, max.			
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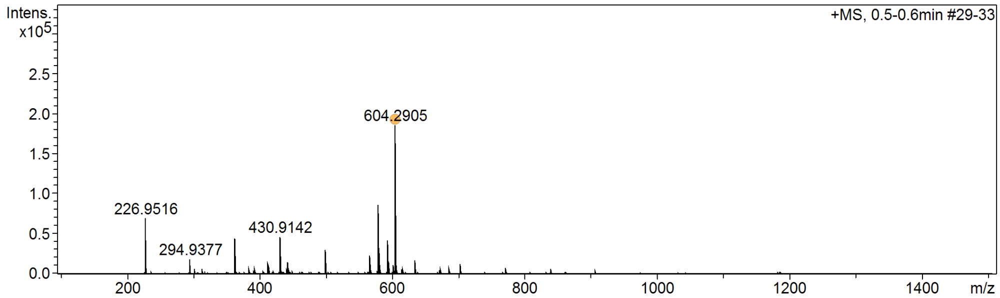
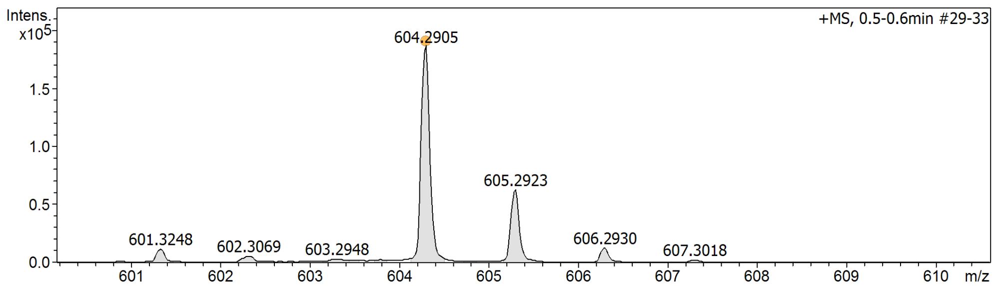
Estimate Carbon			





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
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	2	C30H35N11NaO2	604.2867	-6.2	16.3	2	12.47	18.5	even	ok
	3	C33H43NNaO8	604.2881	-3.9	17.6	3	45.53	12.5	even	ok
	4	C26H47NNaO13	604.2940	-5.8	21.0	4	14.58	3.5	even	ok
	5	C34H39N5NaO4	604.2894	1.7	28.6	5	91.65	17.5	even	ok
	6	C35H35N9Na	604.2908	-0.5	40.1	6	100.00	22.5	even	ok
	7	C39H39N3NaO2	604.2934	4.9	52.8	7	10.62	21.5	even	ok

Bruker Compass DataAnalysis 4.1 printed: 5/23/2022 10:34:30 AM Page 1 of 1

Figure S15. HRMS spectrum of noonindole G (**7**)

3.2 Noonindole H (8)

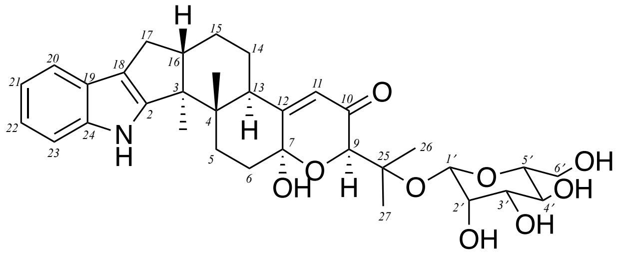


Table S3. 1D and 2D NMR (600 MHz, methanol-d_4) data for noonindole H (**8**)

Pos.	δ_H, mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	151.1	-	-	-
3	-	51.8	-	-	-
4	-	44.0	-	-	-
5	*a* 2.27, m	32.0	6, 5*b*	7, 13, 4-Me	-
	b 1.93, m		6, 5*a*	7, 13, 4-Me	
6	2.17, m	37.2	5*a*, 5*b*	4, 7	-
7	-	95.5	-	-	-
9	4.50, s	78.6	-	7, 10, 25, 26, 27	-
10	-	197.1	-	-	-
11	5.68, br s	123.3	-	7, 9, 13	-
12	-	166.3	-	-	-
13	2.83, dd (*12.8, 2.4*)	43.1	14*a*, 14*b*	12	3-Me
14	*a* 1.67, m	26.9	13, 14*b*, 15*b*	-	-
	b 1.57, dd (*12.8, 4.3*)		15*a*, 15*b*, 14*a*, 13	-	-
15	*a* 1.84, m	25.5	14*a*,14*b*, 15*b*, 16	13	-
	b 1.76, dd (*12.8, 3.4*)		15*a*, 14*a*,14*b*,16	-	-
16	2.85, m	50.8	17*a*, 17*b*, 15*a*	-	4-Me
17	*a* 2.68, dd (*13.3, 6.5*)	28.3	17*b*, 16	2, 3, 18	-
	b 2.38, dd (*13.3*, *11.0*)		17*a*, 16	18	-
18	-	118.2	-	-	-
19	-	126.3	-	-	-
20	7.30, d (*8.1*)	118.9	21	18, 22, 24	-
21	6.93, dd (*8.1*, *7.3*)	120.6	20, 22	19, 23	-
22	6.97, dd (*8.1*, *7.3*)	121.1	21, 23	20, 24	-
23	7.28, d (*8.1*)	112.8	22	19, 21	-
24	-	142.3	-	-	-
25	-	79.3	-	-	-
26	1.31, s	22.3	-	9, 25, 27	-
27	1.49, s	25.9	-	9, 25, 26	-
1′	4.94, s	96.9	2′	25, 2′	5′, 3′
2′	3.85, d (*3.2*)	73.7	1′, 3′	3′, 4′	-
3′	3.44, dd (*9.4*, *3.2*)	75.7	2′, 4′	4′	1′
4′	3.54, t (*9.4*)	68.5	3′, 5′	3′, 5′, 6′	-
5′	3.18, m	78.1	6′ *a*, 6′*b*, 4′	-	1′
6′	*a* 3.84, dd (*11.8, 1.6*)	63.1	5′, 6′*b*	-	-
	b 3.68, dd (*11.8, 5.9*)		5′, 6′*a*	5′	-
3-Me	1.10, s	15.1	-	2, 3, 4, 16	13
4-Me	0.99, s	15.8	-	3, 4, 5, 13	16

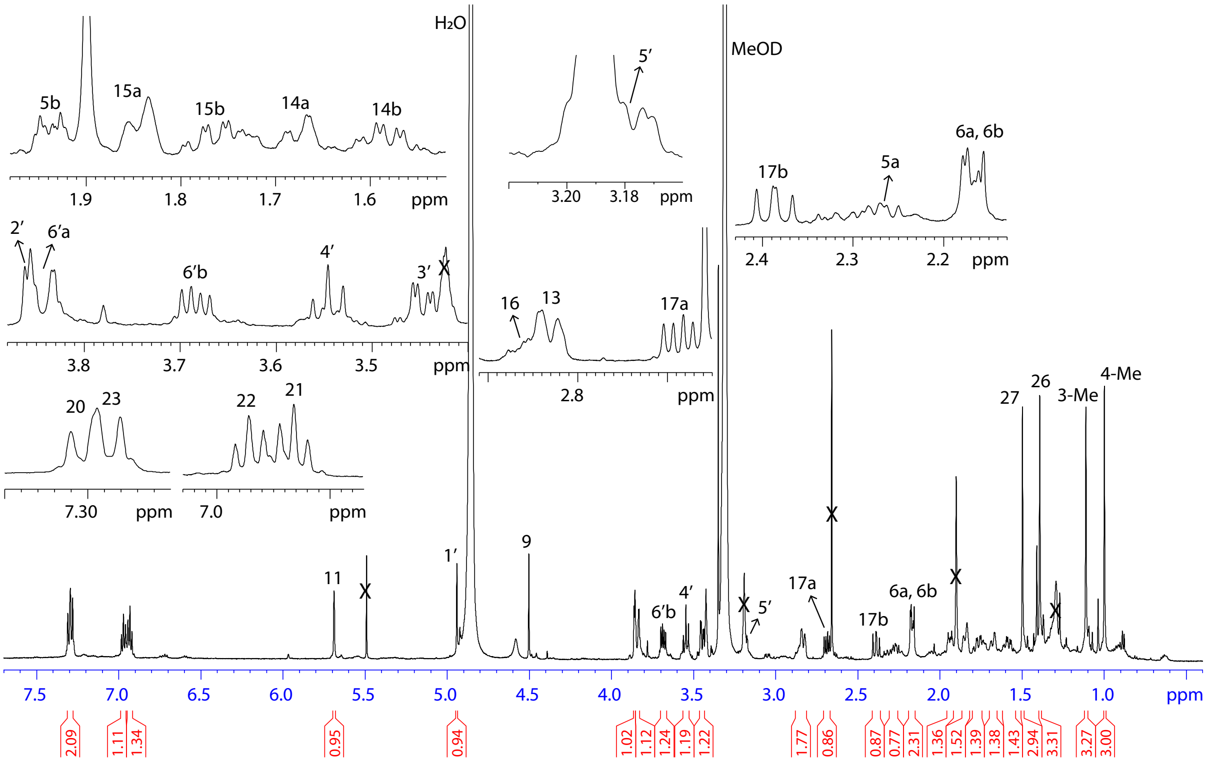


Figure S16. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of noonindole H (**8**)

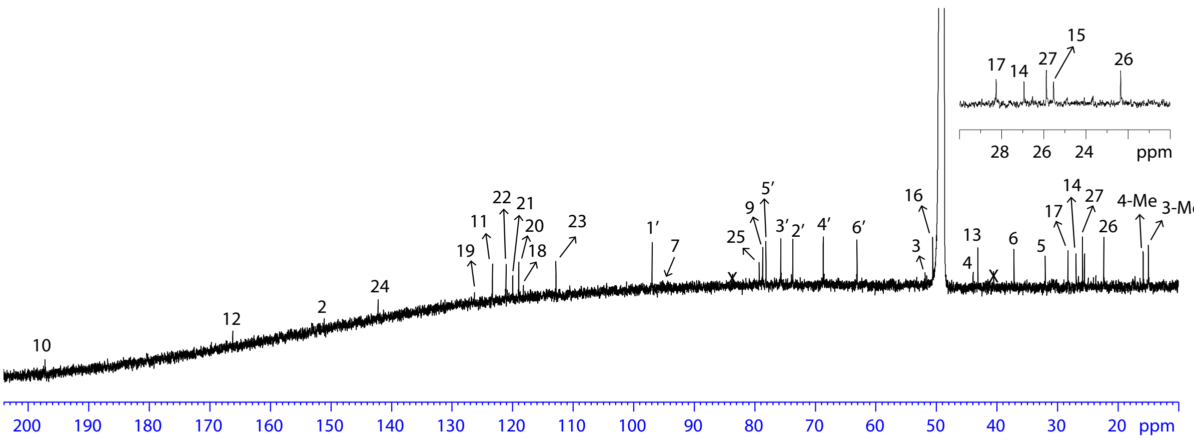


Figure S17. ^{13}C NMR (150 MHz, methanol-d_4) spectrum of noonindole H (**8**)

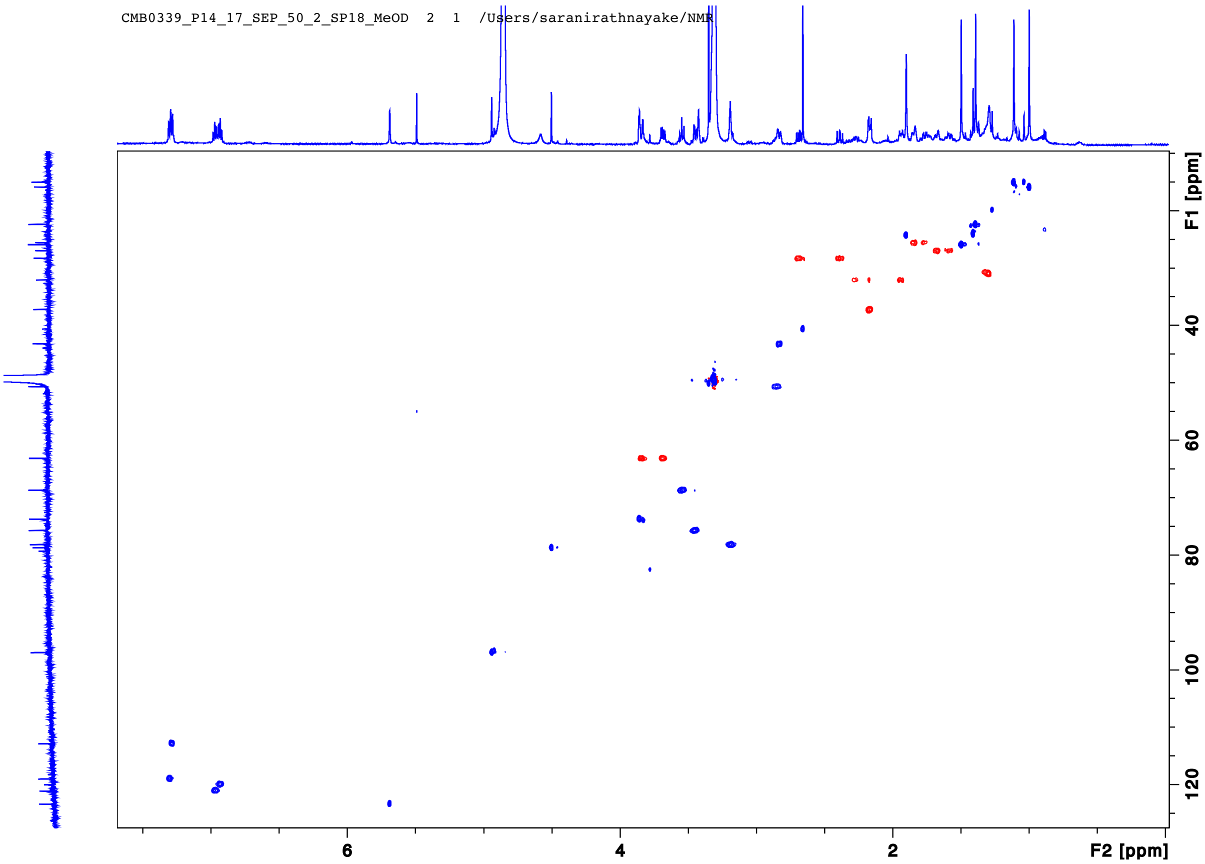


Figure S18. HSQC (methanol-d_4) spectrum of noonindole H (**8**)

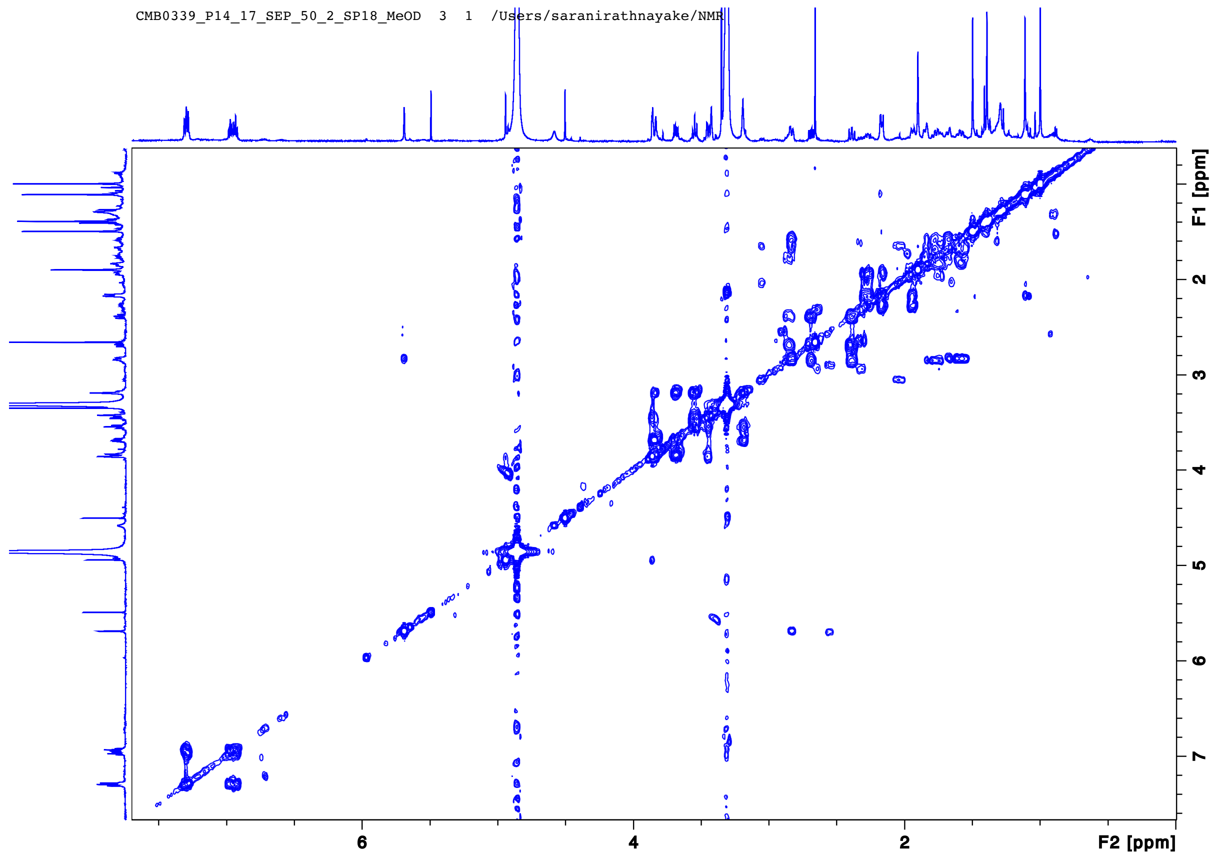


Figure S19. COSY (methanol-d_4) spectrum of noonindole H (**8**)

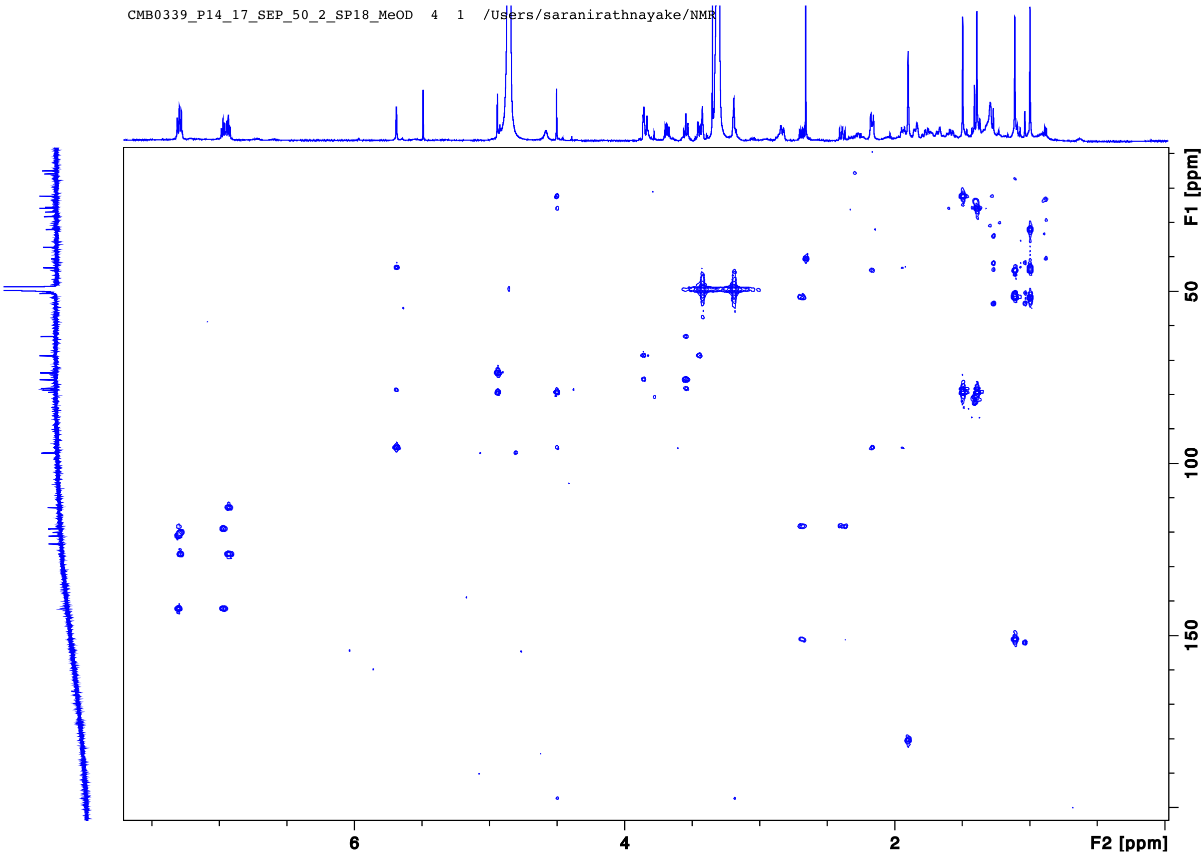


Figure S20. HMBC (methanol-d_4) spectrum of noonindole H (**8**)

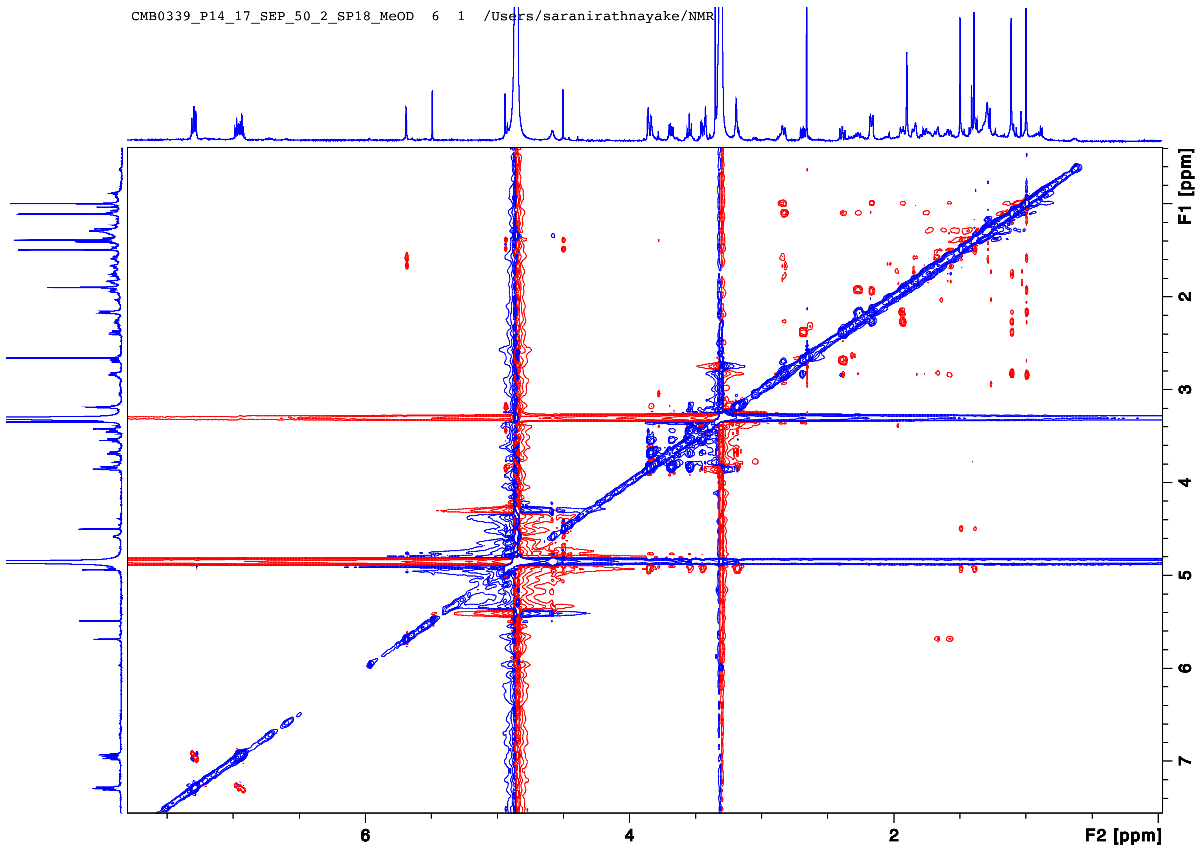


Figure S21. ROESY (methanol-d_4) spectrum of noonindole H (**8**)

Mass Spectrum Molecular Formula Report

Analysis Info

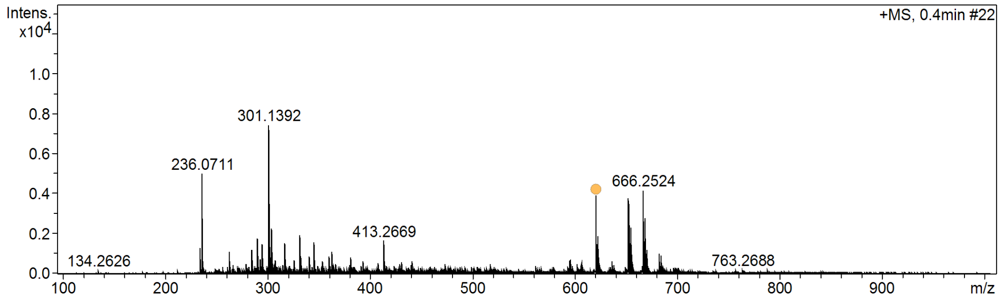
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_SEP_50_2_SP18_again.d	Acquisition Date	11/2/2021 2:36:11 PM
Method	tune-med_AP.m	Operator	a.salim
Sample Name	CMB0339_D400_SEP_50_2_SP18_again	Instrument / Ser#	micrOTOF 213750.00232
Comment			

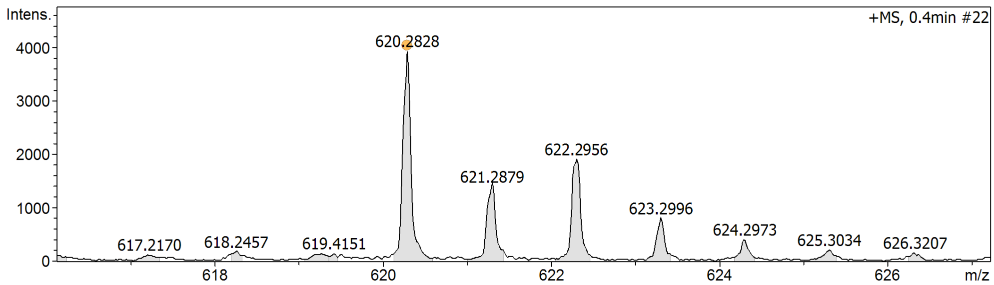
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	5.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.					
Formula, max.					
Measured m/z		Tolerance		Charge	
Check Valence		Minimum		Maximum	
Nirogen Rule		Electron Configuration			
Filter H/C Ratio		Minimum		Maximum	
Estimate Carbon					





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
620.2828	1	C33H43NNaO9	620.2830	-0.4	222.7	1	100.00	12.5	even	ok
	2	C34H39N5NaO5	620.2843	2.5	223.3	2	45.26	17.5	even	ok
	3	C35H35N9NaO	620.2857	4.7	224.3	3	13.98	22.5	even	ok
	4	C29H39N7NaO7	620.2803	4.0	228.8	4	13.42	13.5	even	ok
	5	C28H43N3NaO11	620.2790	-6.1	228.9	5	3.48	8.5	even	ok
	6	C30H35N11NaO3	620.2817	1.8	229.0	6	34.48	18.5	even	ok
	7	C26H31N17NaO	620.2790	6.1	235.0	7	1.90	19.5	even	ok

Bruker Compass DataAnalysis 4.1 printed: 11/2/2021 2:40:22 PM Page 1 of 1

Figure S22. HRMS spectrum of noonindole H (**8**)

3.3 Noonindole I (9)

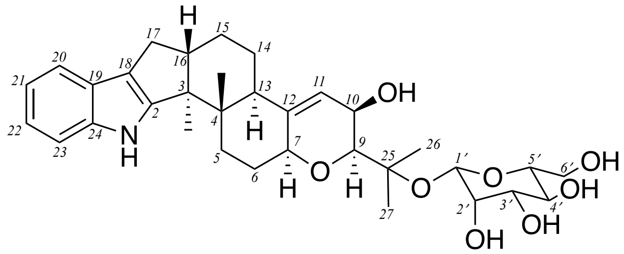


Table S4. 1D and 2D NMR (600 MHz, methanol-d_4) data for noonindole I (**9**)

Pos.	$\delta_{H,}$ mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	151.9	-	-	-
3	-	51.6	-	-	-
4	-	42.2	-	-	-
5	*a* 1.98, d (*13.2*)	33.3	-	-	-
	b 1.96[a], m				
6	*a* 2.12, m	30.5	5[a], 7	4, 5, 7, 12	-
	b 1.95[a], m		-	-	-
7	4.01, m	78.5	6*a*	6, 11, 12	9
9	3.39, br s	84.2	10	7, 10, 25, 26	7
10	4.08, br d (*6.0*)	64.4	9, 11	9, 11, 12	11, 9
11	5.55, br d (*6.0*)	120.2	10	7, 9, 13	-
12	-	146.6	-	-	-
13	2.28, br d (*12.8*)	42.6	14*a*, 14*b*	4, 11, 12, 14, 4-Me	3-Me
14	*a* 1.65, m	27.4	13, 14*b*, 15*a*, 15*b*	15, 16	-
	b 1.57, dd (*12.3, 4.7*)		15*b*, 14*a*, 13	15, 13	-
15	*a* 1.79, m	25.8	15*b*, 16	13, 14, 16	-
	b 1.72, ddd (*15.5, 12.3, 3.1*)		15*a*, 14*a*,14*b*,16	14, 16	-
16	2.82, m	50.8	17*a*, 17*b*, 15*b*	3	4-Me
17	*a* 2.65, dd (*13.5, 6.3*)	28.3	17*b*, 16	2, 3, 18	-
	b 2.36, dd (*13.5, 11.3*)		17*a*, 16	16	-
18	-	118.1	-	-	-
19	-	126.4	-	-	-
20	7.29, d (*7.1*)	118.9	21	18, 22, 24	-
21	6.92, dd (*8.0, 7.1*)	119.8	20, 22	19, 23	-
22	6.95, dd (*8.0, 7.0*)	120.8	21, 23	20, 24	-
23	7.27, d (*7.0*)	112.8	22	19, 21	-
24	-	142.1	-	-	-
25	-	80.6	-	-	-
26	1.45, s	23.6	-	9, 25, 27	-
27	1.39, s	24.5	-	9, 25, 26	-
1′	4.99, br s	96.6	2′	2′, 25	5′, 3′
2′	3.78, d (*3.1*)	74.1	1′, 3′	1′, 3′, 4′	-
3′	3.46, dd (*9.6, 3.1*)	75.7	2′, 4′	4′	1′, 5′
4′	3.57, dd (*9.7, 9.6*)	68.6	3′, 5′	5′, 3′, 6′	-
5′	3.20, ddd (*9.7, 5.8, 2.0*)	78.1	6′ *b*, 4′	1′, 4′, 6′	1′, 3′
6′	*a* 3.84, dd (*11.9, 2.0*)	63.0	5′, 6′ *b*	4′, 5′	-
	b 3.70, dd (*11.9, 5.8*)		5′, 6′ *a*	4′, 5′	-
3-Me	1.05, s	14.9	-	2, 3, 4, 16	13
4-Me	0.99, s	16.1	-	3, 4, 5, 13	16

[a] Resonances with the same superscript within a column are overlapping and assignments may be interchanged

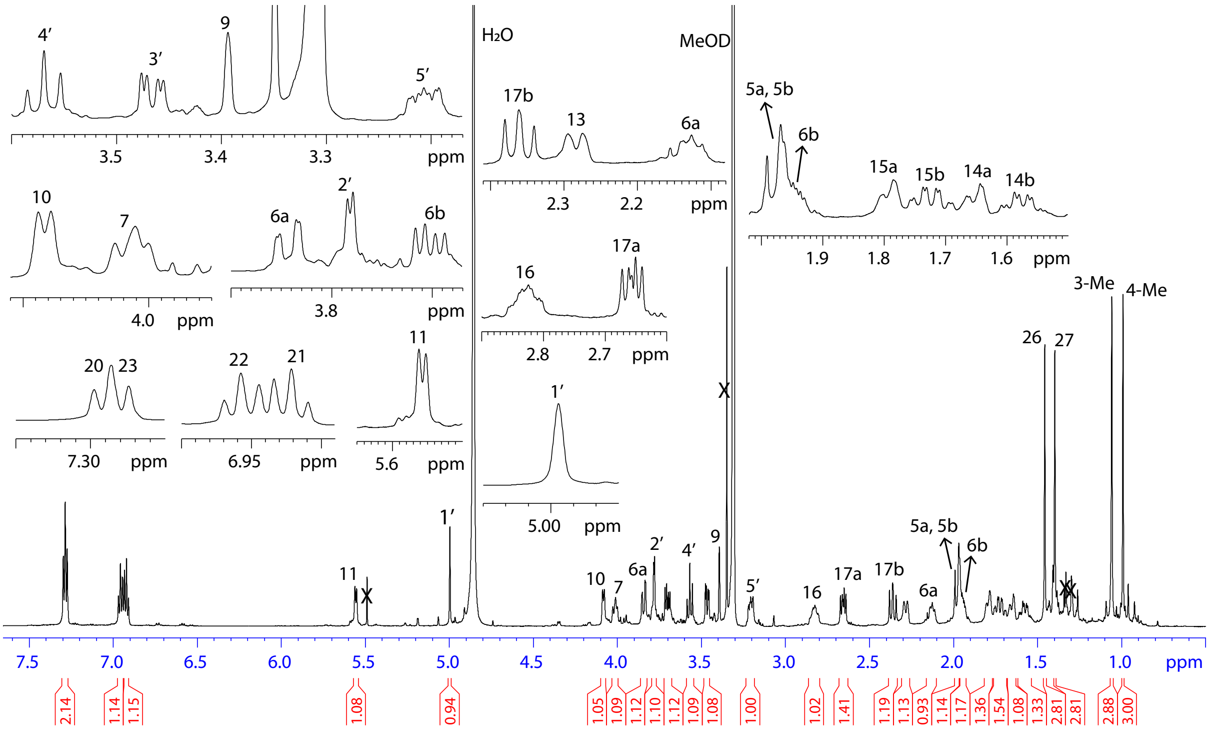


Figure S23. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of noonindole I (**9**)

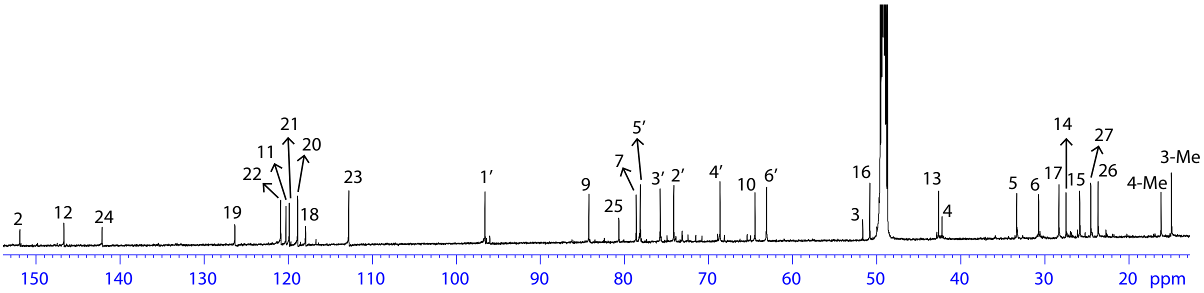


Figure S24. ^{13}C NMR (150 MHz, methanol-d_4) spectrum of noonindole I (**9**)

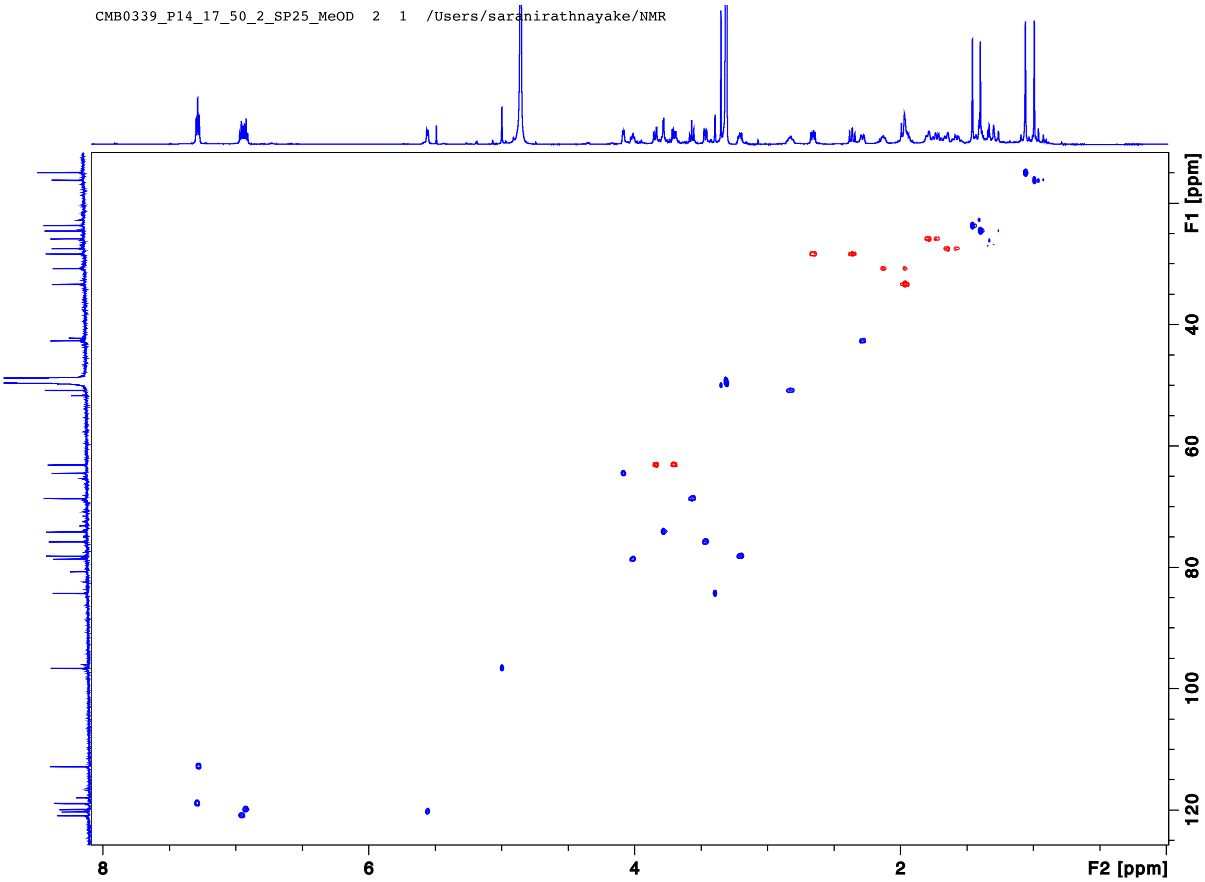


Figure S25. HSQC (methanol-d_4) spectrum of noonindole I (**9**)

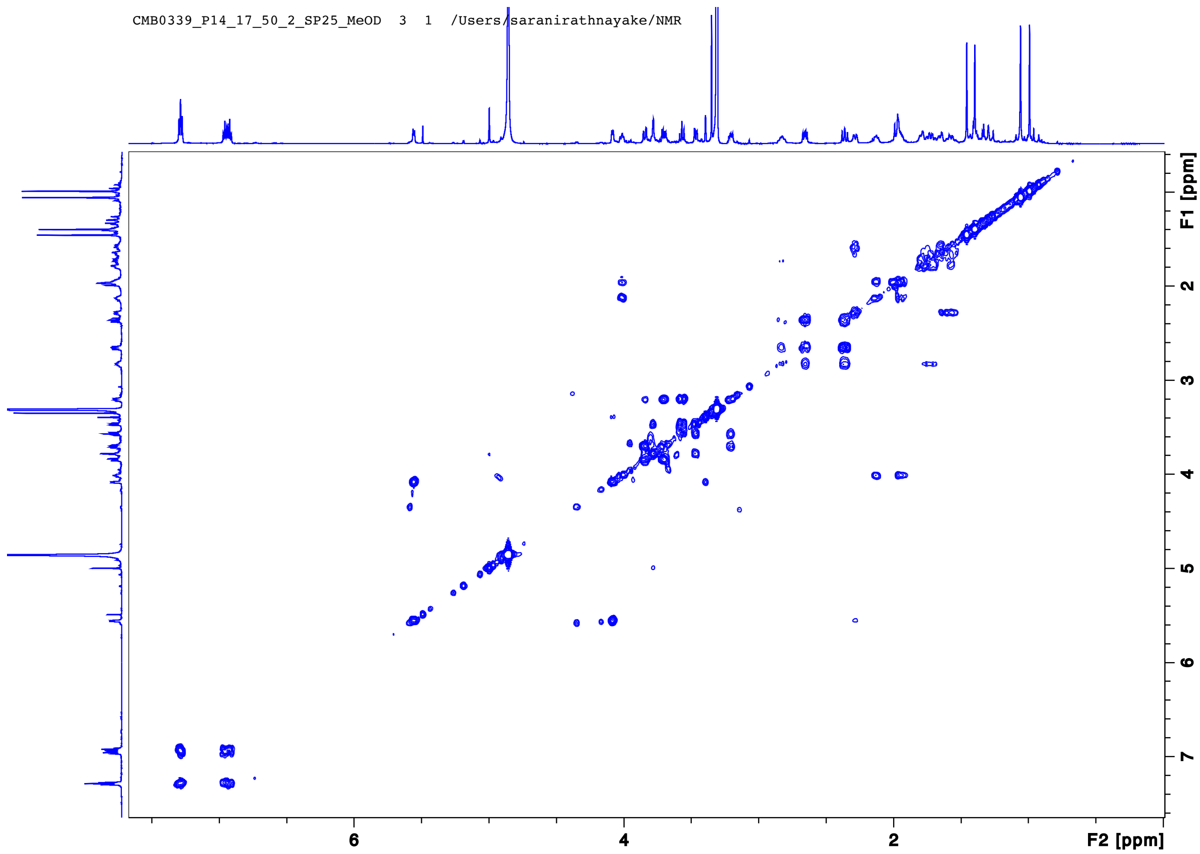


Figure S26. COSY (methanol-d_4) spectrum of noonindole I (**9**)

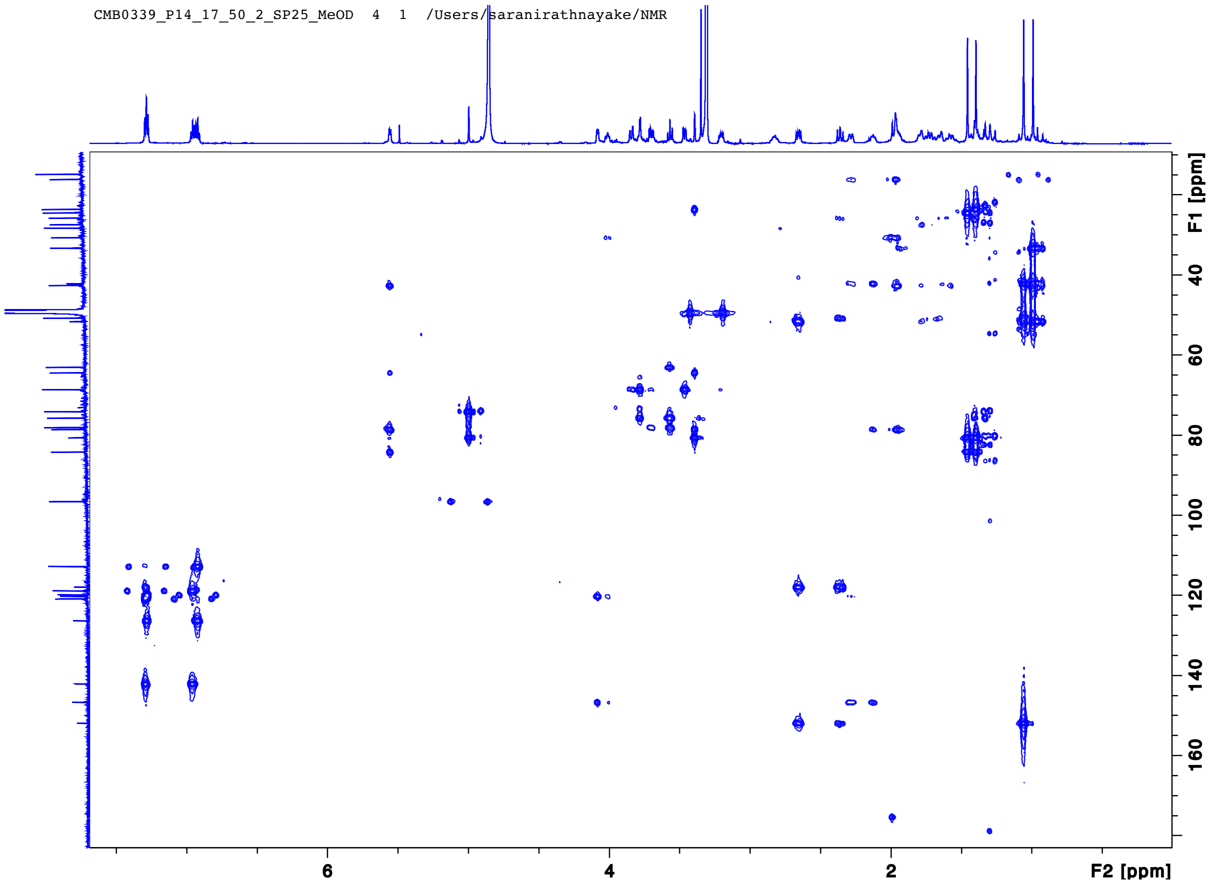


Figure S27. HMBC (methanol-d_4) spectrum of noonindole I (**9**)

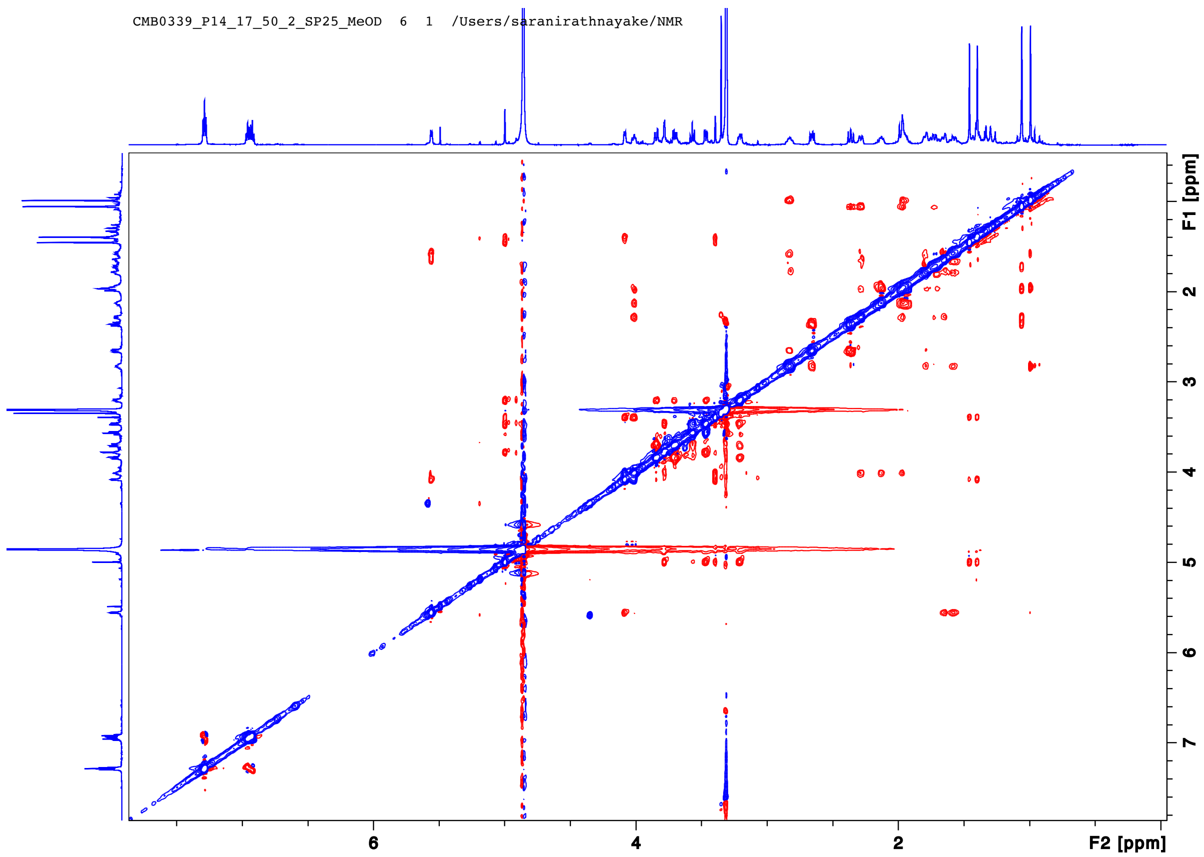


Figure S28. ROESY (methanol-d_4) spectrum of noonindole I (**9**)

Mass Spectrum Molecular Formula Report

Analysis Info

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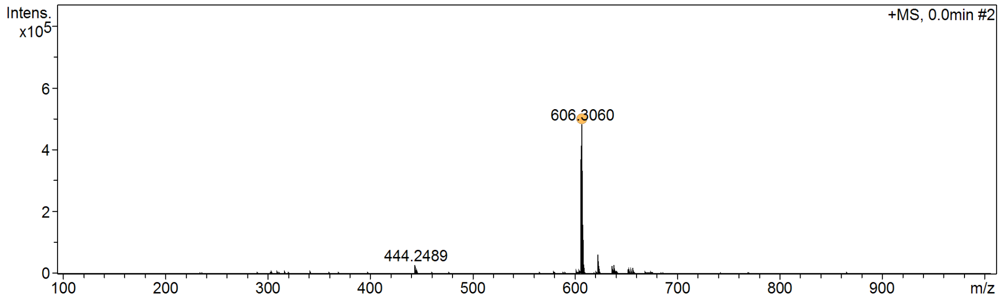
Method	tune-med_AP.m	Operator	a.salim
Sample Name	CMB0339_SEP_50_2_SP25_A	Instrument / Ser#	micrOTOF 213750.00232
Comment			

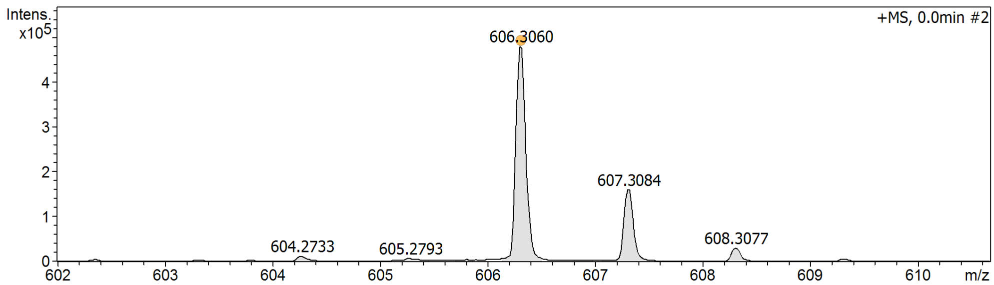
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	5.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.		
Formula, max.		
Measured m/z	Tolerance	Charge
Check Valence	Minimum	Maximum
Nirogen Rule	Electron Configuration	
Filter H/C Ratio	Minimum	Maximum
Estimate Carbon		





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
606.3060	1	C24H37N15NaO3	606.3096	-6.0	7.0	1	17.78	13.5	even	ok
	2	C23H41N11NaO7	606.3083	3.8	18.1	2	52.03	8.5	even	ok
	3	C26H49NNaO13	606.3096	-6.0	18.9	3	13.95	2.5	even	ok
	4	C30H37N11NaO2	606.3024	5.9	19.3	4	15.10	17.5	even	ok
	5	C33H45NNaO8	606.3037	-3.7	21.3	5	51.96	11.5	even	ok
	6	C34H41N5NaO4	606.3051	1.5	32.0	6	100.00	16.5	even	ok
	7	C35H37N9Na	606.3064	-0.7	43.3	7	92.32	21.5	even	ok
	8	C39H41N3NaO2	606.3091	-5.2	56.1	8	8.88	20.5	even	ok

Bruker Compass DataAnalysis 4.1 printed: 8/4/2022 4:02:55 PM Page 1 of 1

Figure S29. HRMS spectrum of noonindole I (**9**)

3.4 Noonindole J (10)

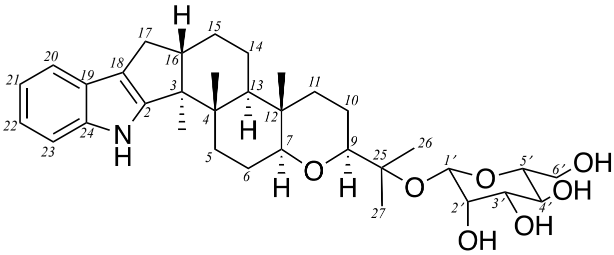


Table S5. 1D and 2D NMR (600 MHz, methanol-d_4) data for noonindole J (**10**)

Pos.	$\delta_{H,}$ mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	152.5	-	-	-
3	-	54.3	-	-	-
4	-	41.2	-	-	-
5	1.92, m	34.3	6*a*, 6*b*[a]	4, 7, 13, 4-Me	-
6	*a* 1.82, dd (*12.7, 3.8*)	26.0	5*a*, 5*b*, 7	5, 4	-
	b 1.67[a], m		-	-	-
7	3.06, dd (*11.7*, *3.8*)	87.6	6*a*, 6*b*[a]	6, 12-Me	9
9	3.38, dd (*12.0*, *2.6*)	86.5	10*b*[b]	25	7
10	*a* 1.65[a], m	23.5	-	-	-
	b 1.55[b], m		-	-	-
11	*a* 1.85, m	39.1	11*b*	7, 9	-
	b 1.19, dd (*15.3, 12.7, 4.6*)		11*a*, 10*b*[b]	12-Me	-
12	-	37.8	-		-
13	1.55[b], m	48.0	-	-	-
14	*a* 1.72, dd (*12.6, 2.6)*	23.2	14*b*	4, 16	-
	b 1.43, ddd (*16.7, 12.6, 4.2*)		15*a*, 14*a*, 13[b]	13	-
15	*a* 1.78, br d (*12.6*)	26.6	15*b*[a], 14*b*, 16	13	-
	b 1.63[a], m		-	-	-
16	2.77, m	50.3	17*a*, 17*b*, 15*b*[a]	-	4-Me
17	*a* 2.61, dd (*13.0*, *6.5*)	28.4	17*b*, 16	2, 3, 16, 18	-
	b 2.28, dd (*13.0*, *10.8*)		17*a*, 16	2, 16, 18	-
18	-	118.2	-	-	-
19	-	126.5	-	-	-
20	7.27[c], d (*7.4*)	118.8	-	-	-
21	6.91, dt (*7.4, 1.0*)	119.8	20[c], 22	19, 23	-
22	6.95, dt (*7.4, 1.0*)	120.8	21, 23[c]	20, 24	-
23	7.27[c], d (*7.4*)	112.8	-	-	-
24	-	142.2	-	-	-
25	-	80.3	-	-	-
26	1.33, s	21.5	-	9, 25, 27	-
27	1.24, s	24.5	-	9, 25, 26	-
1′	4.91, br s	96.8	2′	2′, 5′, 25	5′, 3′
2′	3.79, d (*3.1*)	73.9	1′, 3′	3′, 4′	-
3′	3.44, dd (*9.5*, *3.1*)	75.7	2′, 4′	4′	1′, 5′
4′	3.56, t (*9.5*)	68.7	3′, 5′	6′, 3′, 5′	-
5′	3.18, ddd (*9.5*, *5.6*, *2.3*)	78.0	6′ *a*, 6′ *b*, 4′	-	1′, 3′
6′	*a* 3.83, dd (*11.7*, *2.3*)	63.1	5′, 6′ *b*	4′	-
	b 3.69, dd (*11.7*, *5.6*)		5′, 6′ *a*	4′, 5′	-
3-Me	1.03, s	15.0	-	2, 3, 4, 16	-
4-Me	1.15, s	20.3	-	3, 4, 5, 13	16, 12-Me
12-Me	0.92, s	13.4	-	7, 11, 12, 13	4-Me

[a-c] Resonances with the same superscript within a column are overlapping and assignments may be interchanged

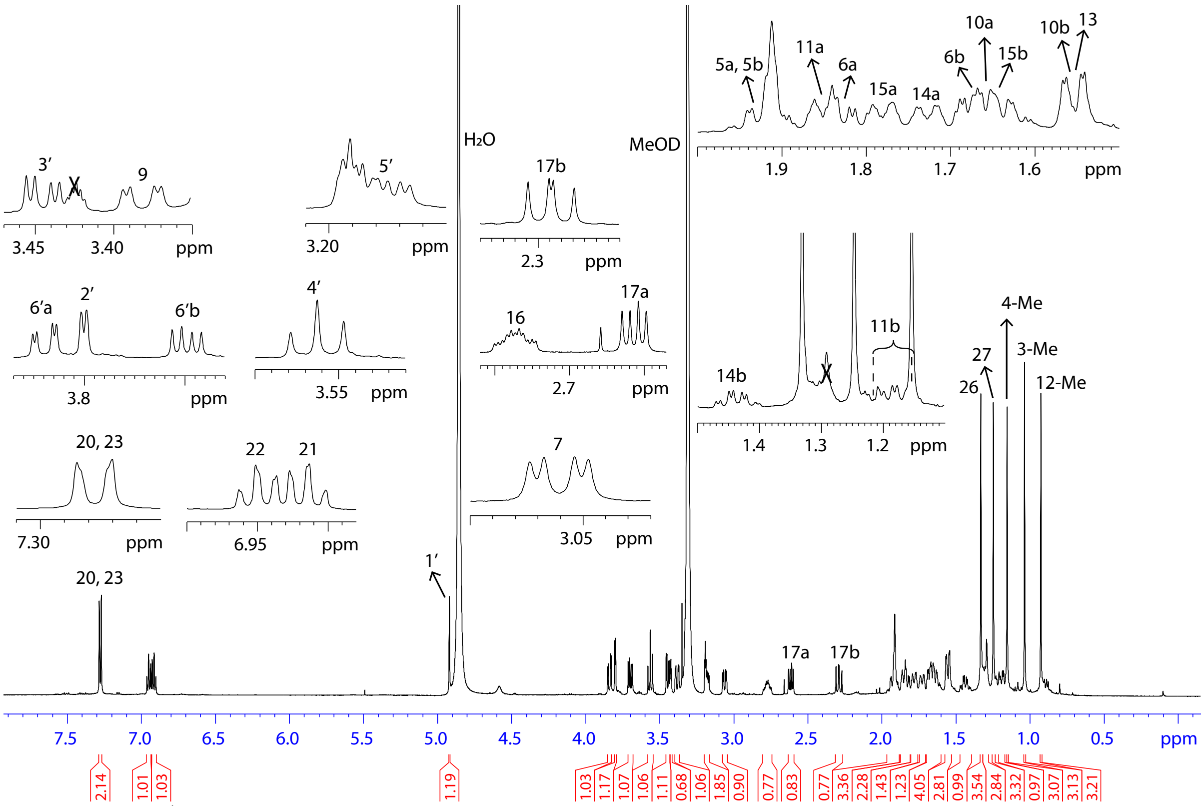


Figure S30. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of noonindole J (**10**)

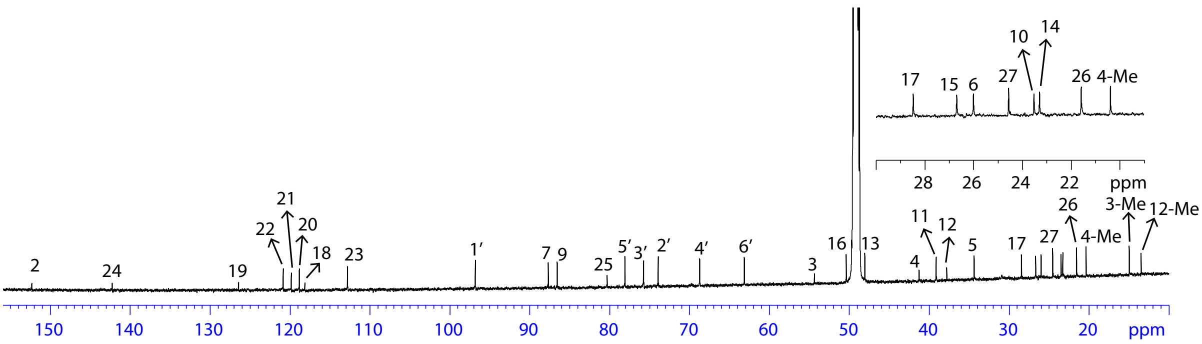


Figure S31. ^{13}C NMR (150 MHz, methanol-d_4) spectrum of noonindole J (**10**)

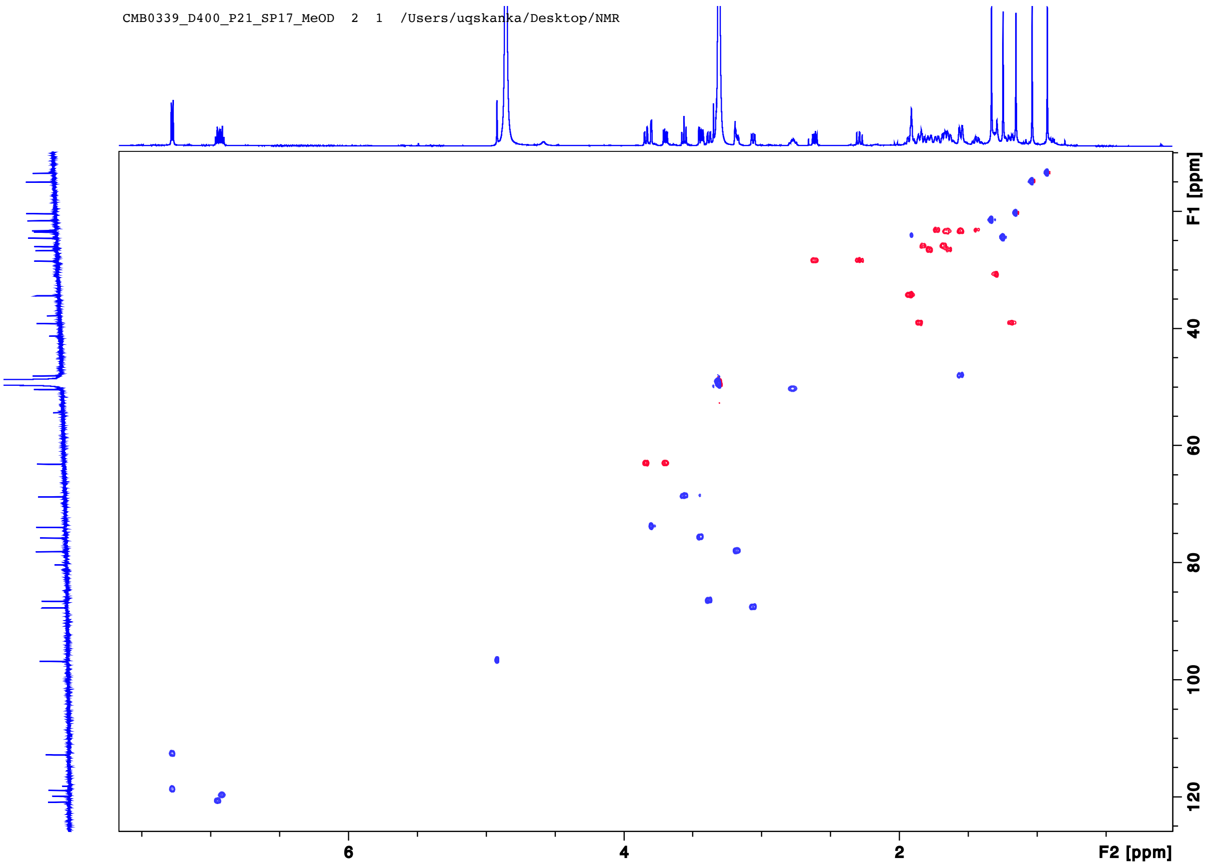


Figure S32. HSQC (methanol-d_4) spectrum of noonindole J (**10**)

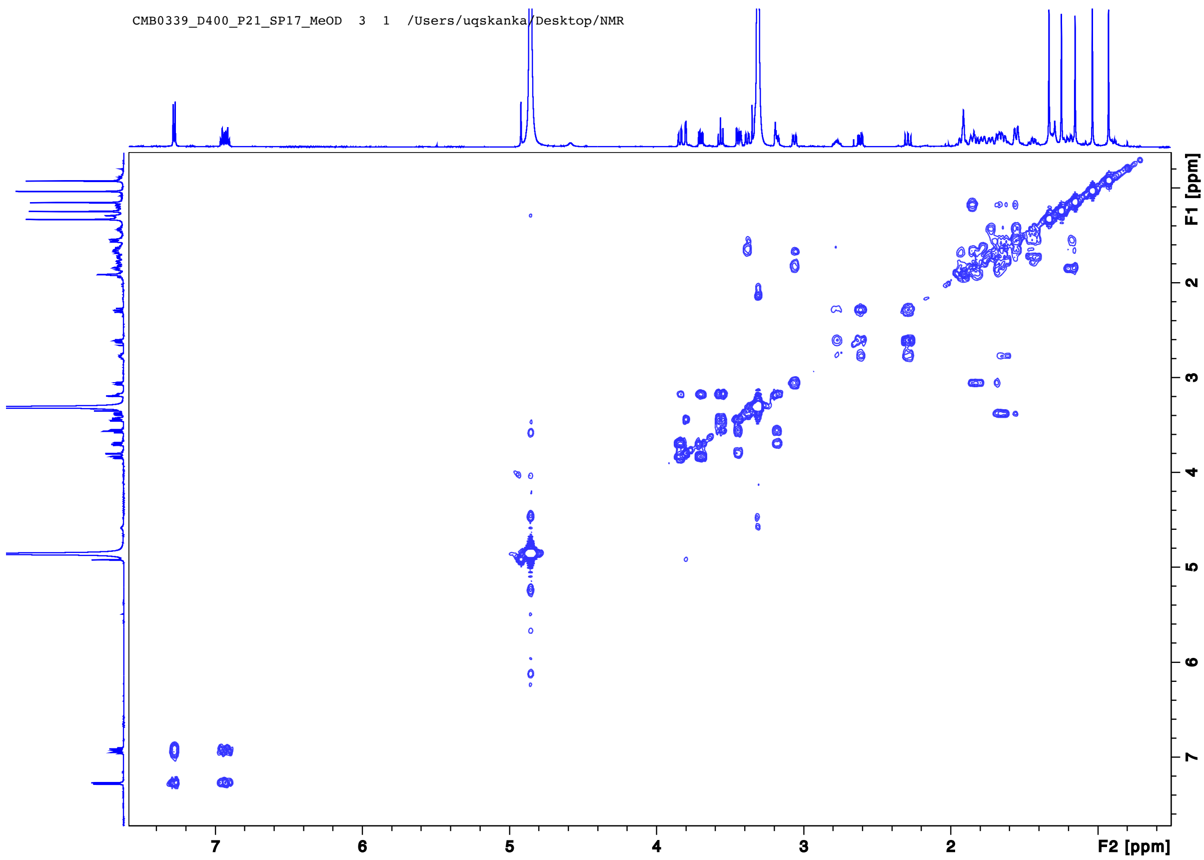


Figure S33. COSY (methanol-d_4) spectrum of noonindole J (**10**)

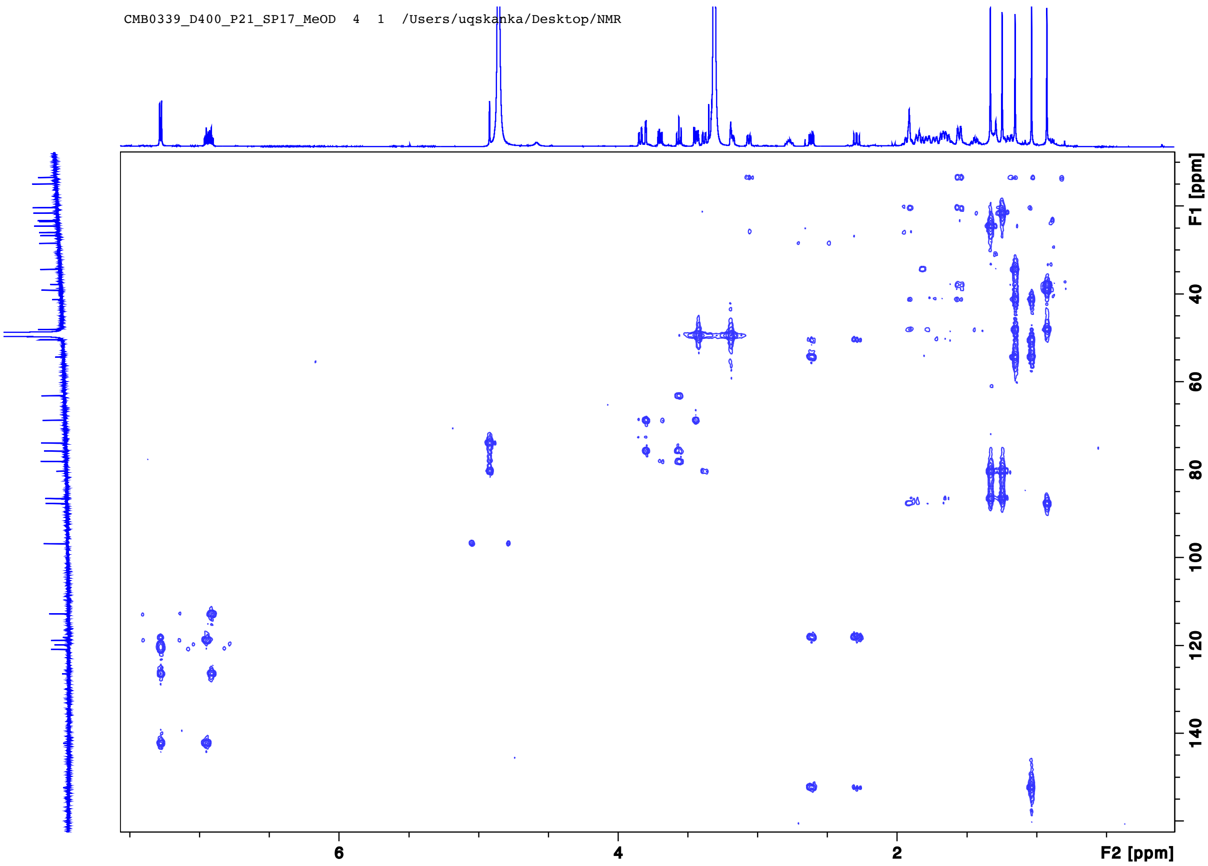


Figure S34. HMBC (methanol-d_4) spectrum of noonindole J (**10**)

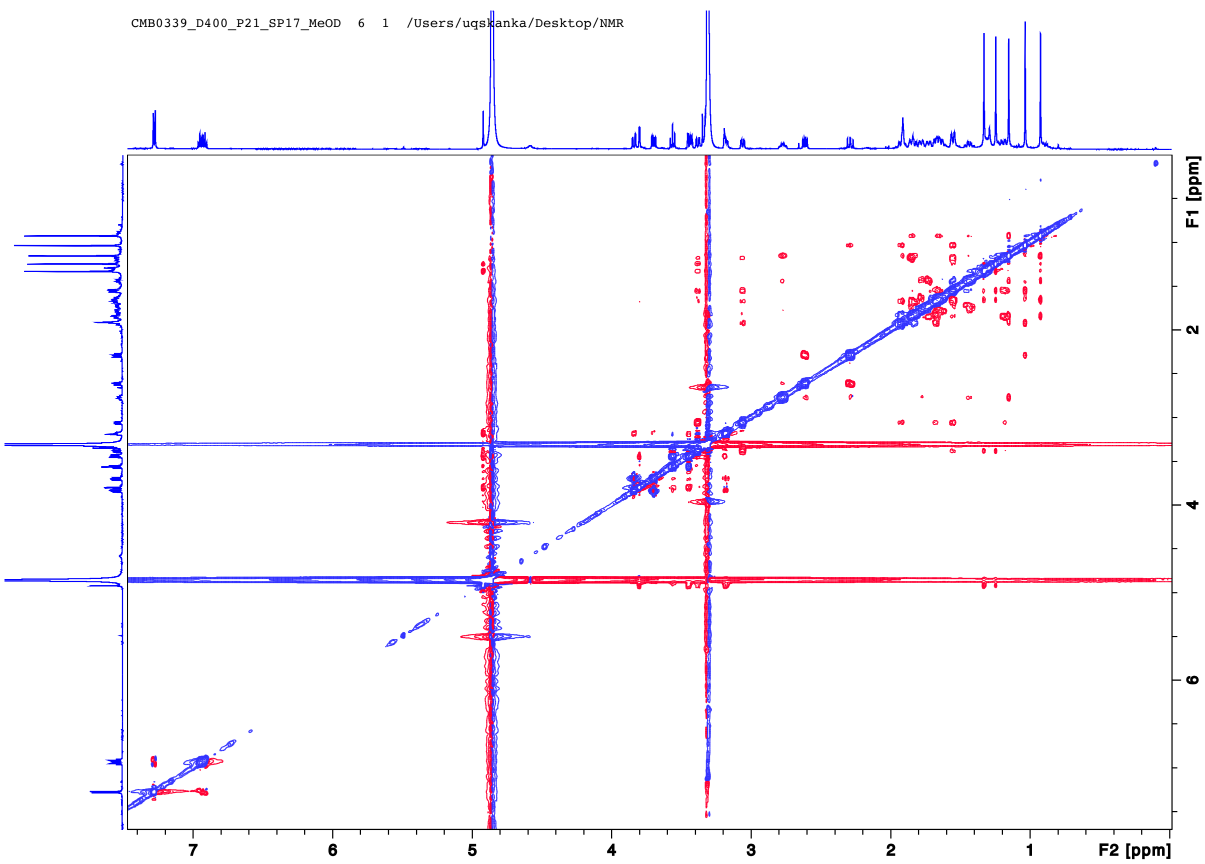


Figure S35. ROESY (methanol-d_4) spectrum of noonindole J (**10**)

Mass Spectrum Molecular Formula Report

Analysis Info

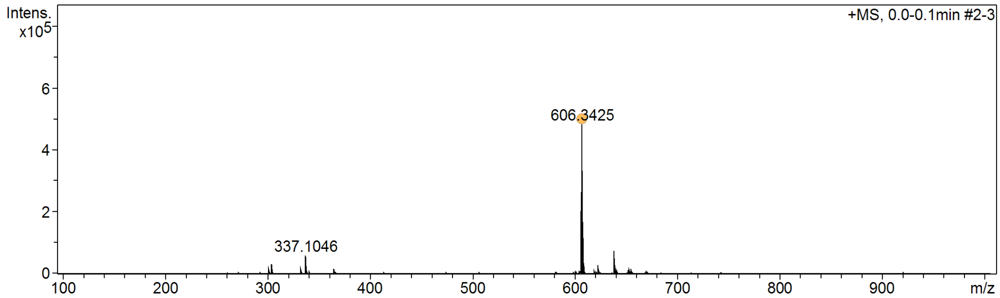
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_P21_SP17_again2.d	Acquisition Date	11/2/2021 2:29:13 PM	
Method	tune-med_AP.m	Operator	a.salim	
Sample Name	CMB0339_D400_P21_SP17_again2	Instrument / Ser#	micrOTOF	213750.00232
Comment				

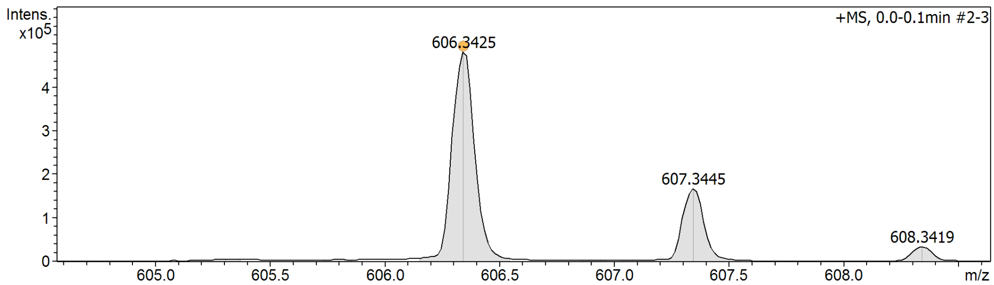
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	5.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.		
Formula, max.		
Measured m/z	Tolerance	Charge
Check Valence	Minimum	Maximum
Nirogen Rule	Electron Configuration	
Filter H/C Ratio	Minimum	Maximum
Estimate Carbon		





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
606.3425	1	C25H41N15NaO2	606.3460	-5.8	10.4	1	19.23	12.5	even	ok
	2	C31H41N11NaO	606.3388	6.1	16.9	2	13.85	16.5	even	ok
	3	C34H49NNaO7	606.3401	3.9	18.1	3	50.26	10.5	even	ok
	4	C27H53NNaO12	606.3460	-5.8	20.4	4	15.55	1.5	even	ok
	5	C24H45N11NaO6	606.3446	3.6	20.8	5	54.66	7.5	even	ok
	6	C35H45N5NaO3	606.3415	1.7	29.2	6	100.00	15.5	even	ok
	7	C40H45N3NaO	606.3455	-5.0	53.4	7	11.00	19.5	even	ok

Bruker Compass DataAnalysis 4.1 printed: 11/2/2021 2:33:11 PM Page 1 of 1

Figure S36. HRMS spectrum of noonindole J (**10**)

3.5 Noonindole K (11)

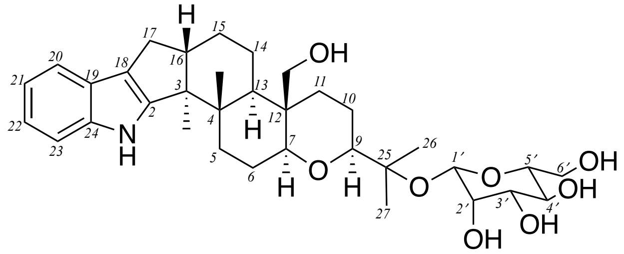


Table S6. 1D and 2D NMR (600 MHz, methanol-d_4) data for noonindole K (**11**)

Pos.	δ_{H}, mult. (J in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	152.4	-	-	-
3	-	54.6	-	-	-
4	-	41.3	-	-	-
5	1.93, dd (*13.2, 3.7*)	34.3	6*b*	6, 7, 13, 4-Me	-
6	*a* 1.74[a], m	25.8	-	-	-
	b 1.64, m		5, 7	-	-
7	3.15, dd (*12.6, 2.9*)	87.3	6*b*	12-<u>C</u>H$_2$OH	9
9	3.42, m	86.6	10*b*	25, 11	7
10	*a* 1.74[a], m	23.5	-	-	-
	b 1.57, m		11*a*, 11*b*, 9	12	-
11	*a* 2.46, br d (*13.0*)	33.5	11*b*, 10*b*	9, 12	-
	b 1.00, m		11*a*, 10*b*	12, 12-<u>C</u>H$_2$OH	-
12	-	41.8	-		-
13	1.54[b], m	48.6	-	-	-
14	*a* 1.83, m	25.2	14*b*, 15*b*[b]	4, 13, 15, 16	-
	b 1.77, m		14*a*, 15*b*[b]	13, 16	-
15	*a* 1.74[a], m	27.1	-	-	-
	b 1.55[b], m		-	-	-
16	2.77, m	50.6	17*a*, 17*b*, 15*b*[b]	4	-
17	*a* 2.61, dd (*13.4*, *6.5*)	28.5	17*b*, 16	2, 3, 16, 18	-
	b 2.28, dd (*13.4*, *10.5*)		17*a*, 16	2, 16, 18	-
18	-	118.3	-	-	-
19	-	126.4	-	-	-
20	7.28[c], d (*8.0*)	118.8	-	-	-
21	6.91, t (*8.0*)	119.8	20[c], 22	19, 23	-
22	6.95, t (*8.0*)	120.8	21, 23[c]	20, 24	-
23	7.28[c], d (*8.0*)	112.7	-	-	-
24	-	142.3	-	-	-
25	-	80.5	-	-	-
26	1.32, s	21.7	-	9, 25, 27	-
27	1.26[d], s	24.5	-	-	-
1′	4.91, br s	96.8	2′	2′, 25	5′, 3′
2′	3.79, d (*3.1*)	73.9	1′, 3′	3′, 4′	-
3′	3.43, m	75.7	2′, 4′	4′	1′, 5′
4′	3.56, t (*9.5*)	68.7	3′, 5′	6′, 3′, 5′	-
5′	3.18, m	78.0	6′ *b*, 4′	-	1′, 3′
6′	*a* 3.83, dd (*11.7*, *2.3*)	63.1	5′, 6′ *b*	4′	-
	b 3.69, dd (*11.7*, *5.6*)		5′, 6′ *a*	4′, 5′	-
3-Me	1.03, s	15.1	-	2, 3, 4, 16	-
4-Me	1.26[d], s	20.2	-	-	-
12-C<u>H</u>$_2$OH	*a* 4.08, d (*12.0*)	61.0	12-C<u>H</u>$_2$OH-*a*	11, 13	-
	b 3.93, d (*12.0*)	61.0	12-C<u>H</u>$_2$OH-*b*	11, 12, 7	-

[a-d] Resonances with the same superscript within a column are overlapping and assignments may be interchanged

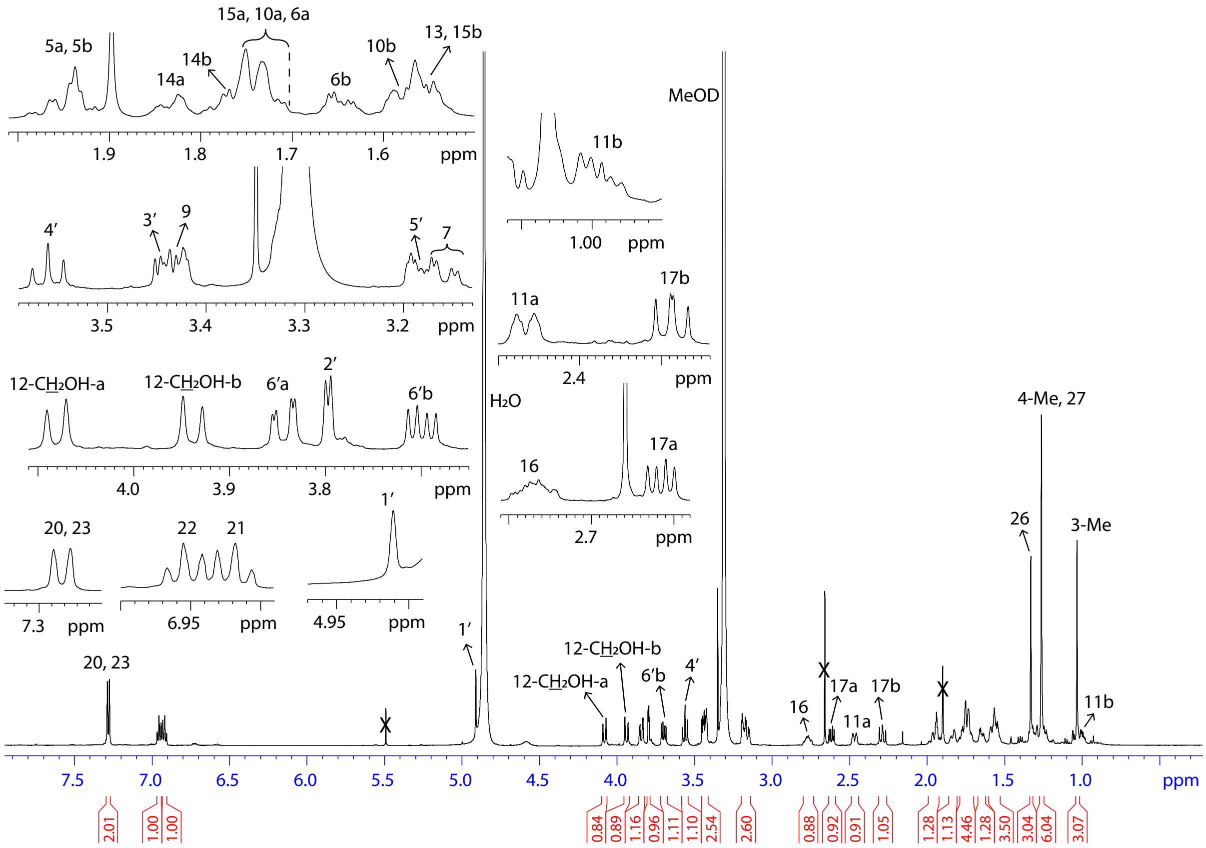


Figure S37. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of noonindole K (**11**)

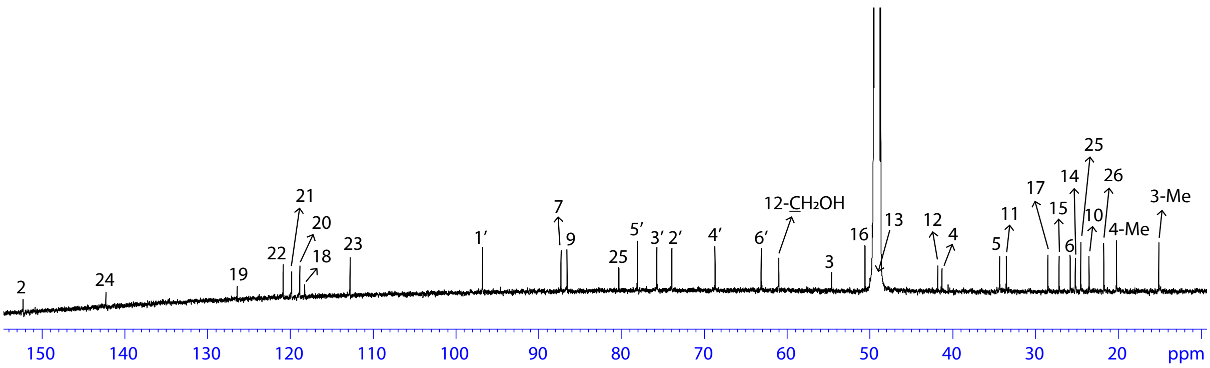


Figure S38. ^{13}C NMR (150 MHz, methanol-d_4) spectrum of noonindole K (**11**)

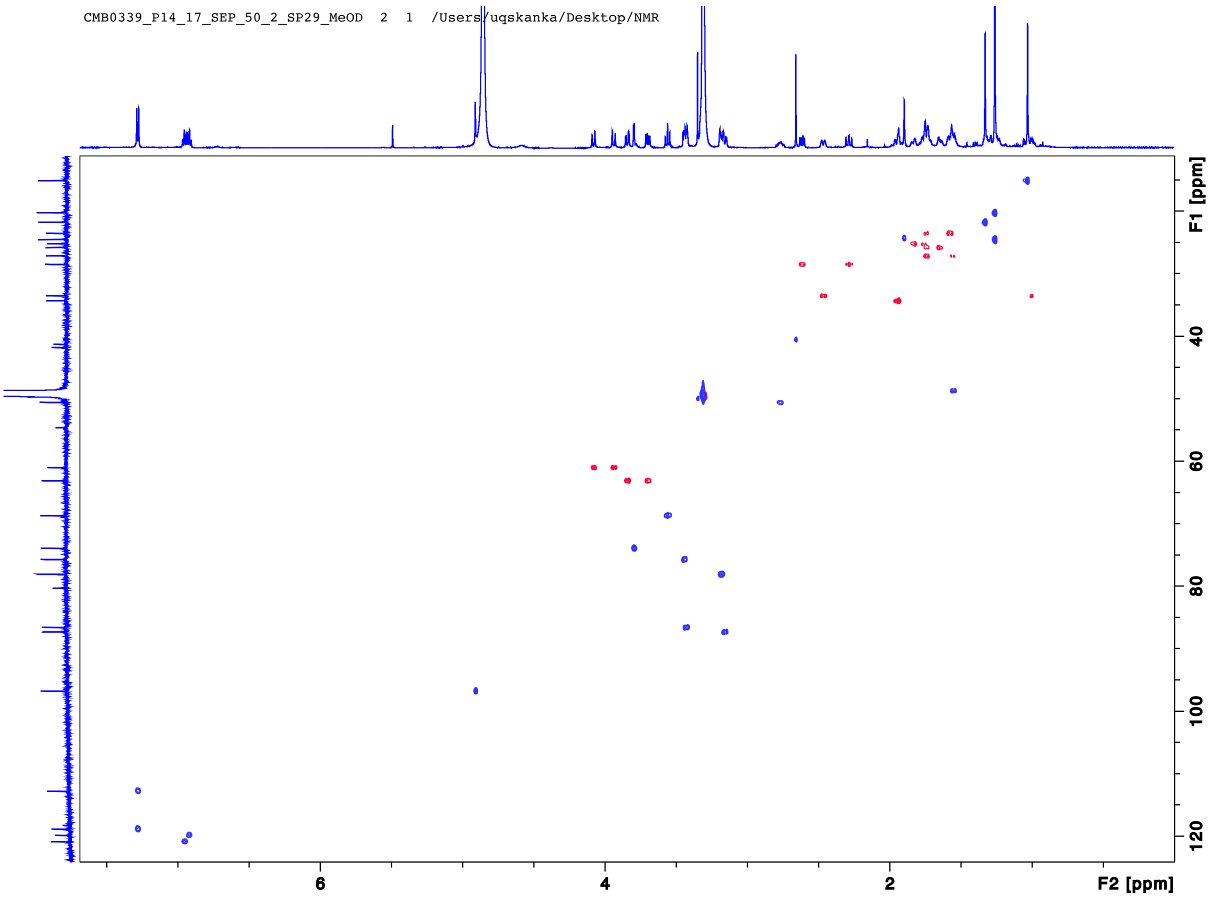


Figure S39. HSQC (methanol-d_4) spectrum of noonindole K (**11**)

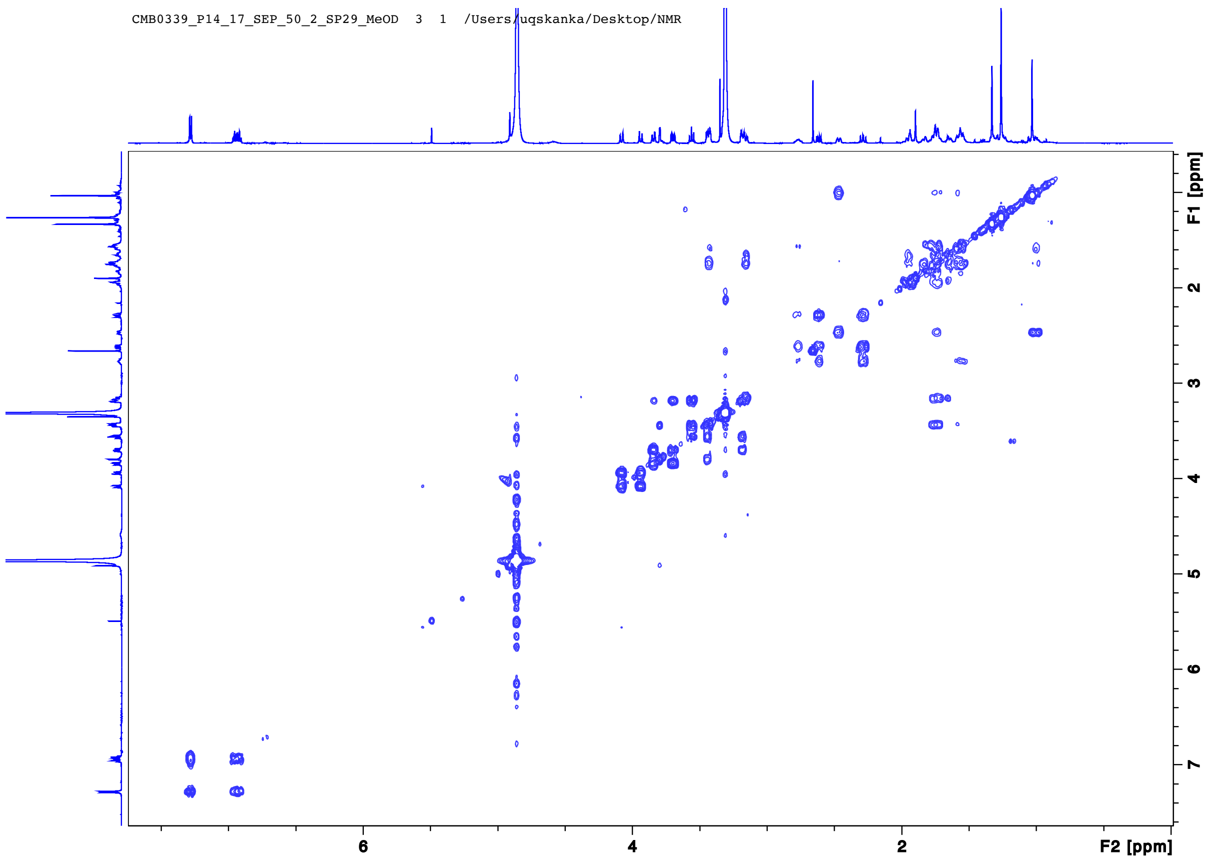


Figure S40. COSY (methanol-d_4) spectrum of noonindole K (**11**)

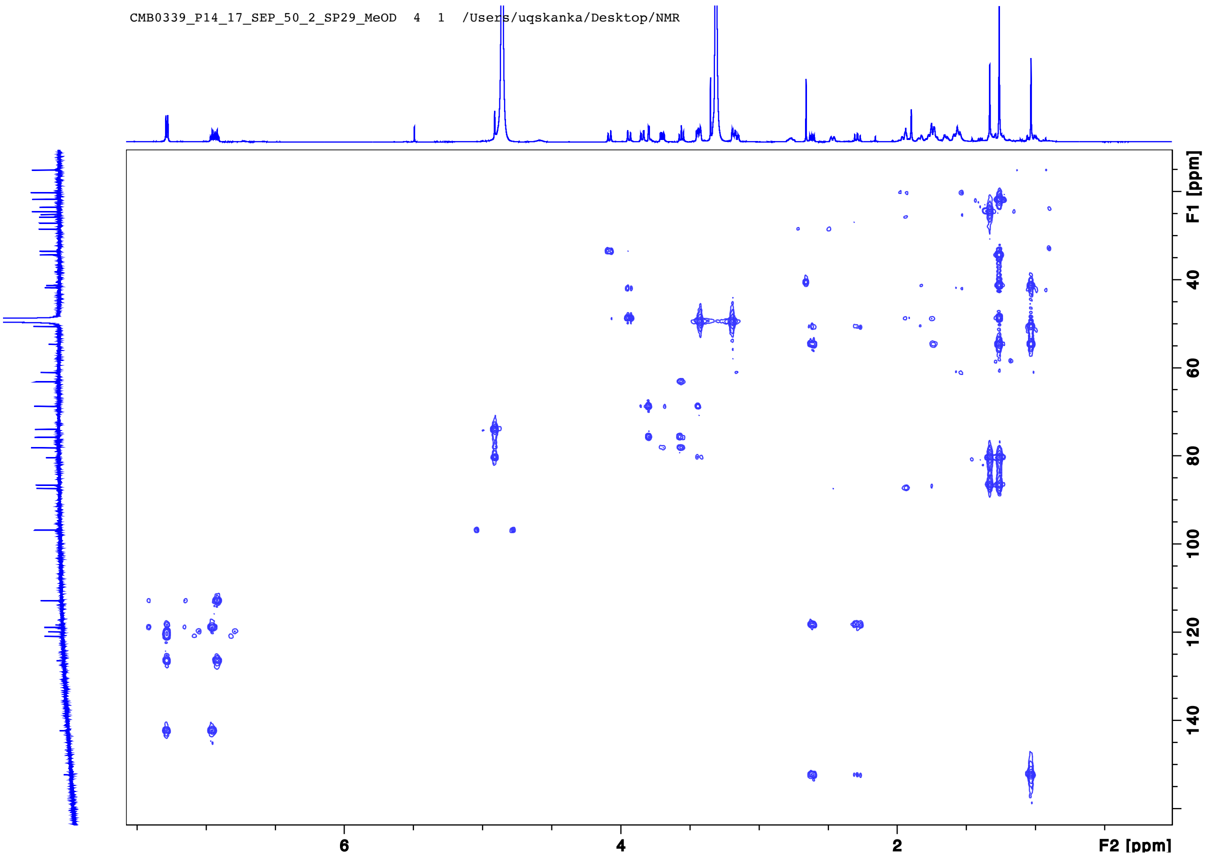


Figure S41. HMBC (methanol-d_4) spectrum of noonindole K (**11**)

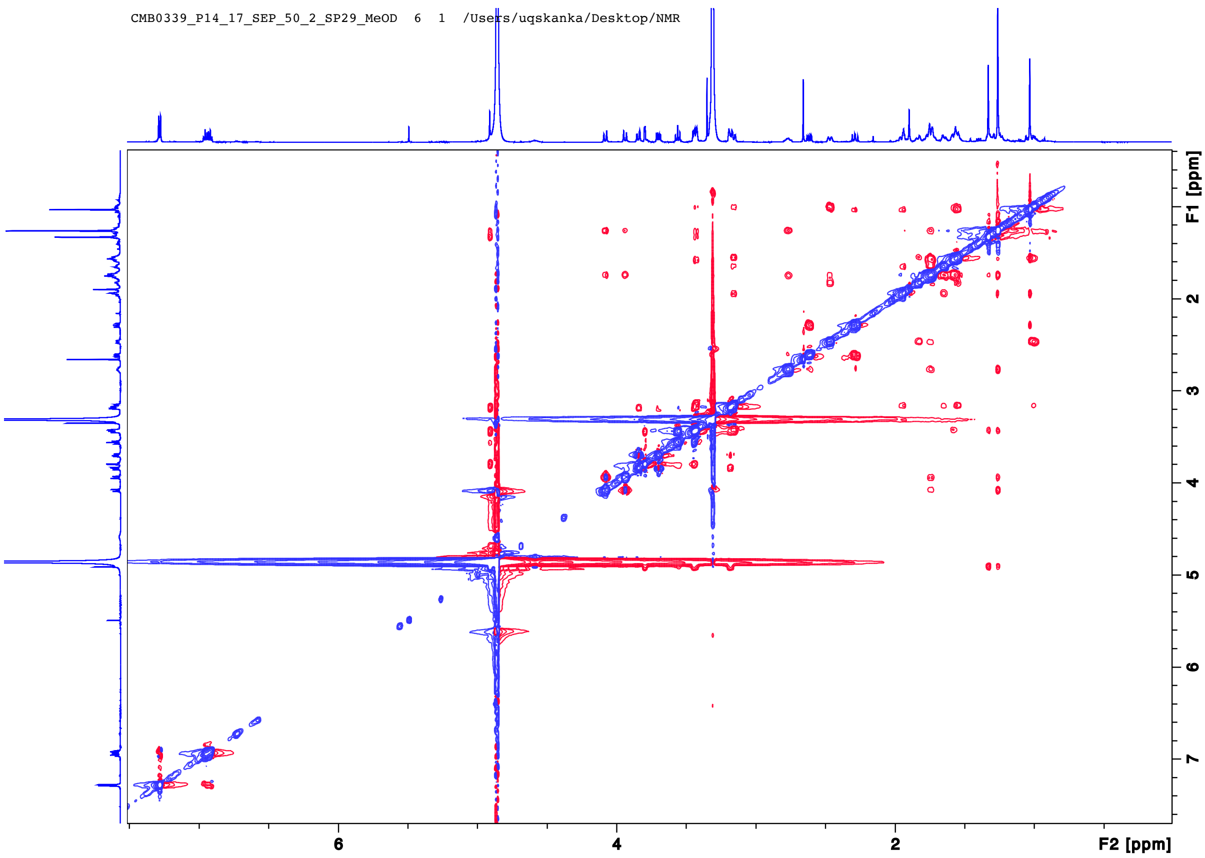


Figure S42. ROESY (methanol-d_4) spectrum of noonindole K (**11**)

Mass Spectrum Molecular Formula Report

Analysis Info

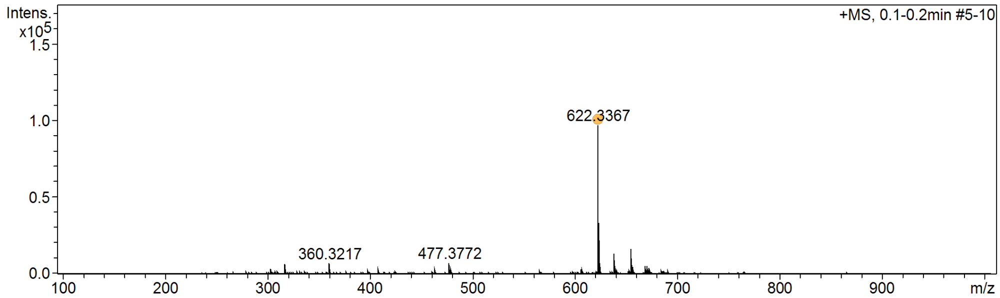
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_50_2_SP29_B.d	Acquisition Date	8/4/2022 11:48:47 AM
Method	tune-med_AP.m	Operator	a.salim
Sample Name	CMB0339_D400_50_2_SP29_B	Instrument / Ser#	micrOTOF 213750.00232
Comment			

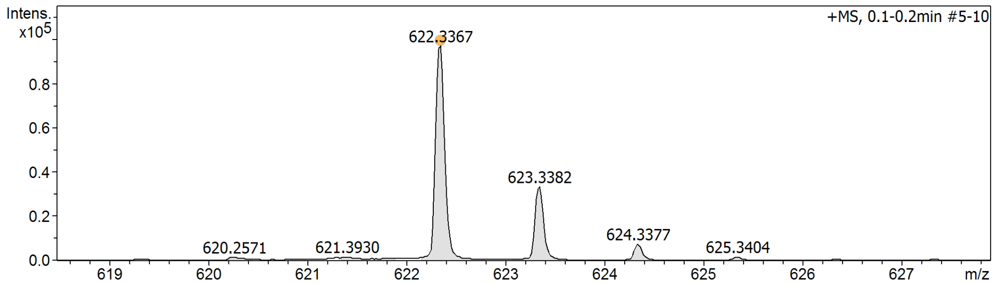
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	5.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.		
Formula, max.		
Measured m/z	Tolerance	Charge
Check Valence	Minimum	Maximum
Nirogen Rule	Electron Configuration	
Filter H/C Ratio	Minimum	Maximum
Estimate Carbon		





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
622.3367	1	C34H49NNaO8	622.3350	-2.7	19.2	1	59.79	10.5	even	ok
	2	C35H45N5NaO4	622.3364	0.6	30.6	2	100.00	15.5	even	ok
	3	C36H41N9Na	622.3377	1.6	42.2	3	54.21	20.5	even	ok

Bruker Compass DataAnalysis 4.1 printed: 8/4/2022 11:51:21 AM Page 1 of 1

Figure S43. HRMS spectrum of noonindole K (**11**)

3.6 Noonindole L (12)

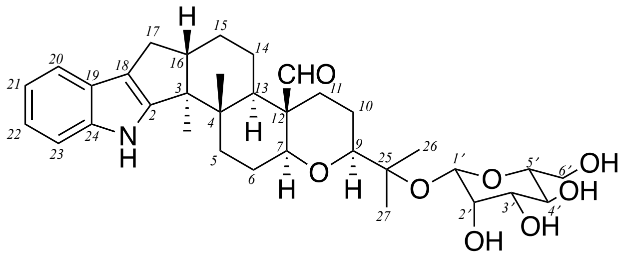


Table S7. 1D and 2D NMR (600 MHz, methanol-d_4) data for noonindole L (**12**)

Pos.	$\delta_{H,}$ mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	151.7	-	-	-
3	-	53.3	-	-	-
4	-	50.3	-	-	-
5	2.02, m	33.5	6*a*[a]	4, 7, 13, 4-Me	-
6	*a* 2.29[a], m	26.1	-	-	-
	b 1.97, m		6*a*[a], 7	4, 7	-
7	3.38, dd (*12.6*, *4.5*)	85.3	6*a*[a], 6*b*	6, 9, 11, 12-CHO	-
9	3.44[b], m	86.1	-	-	-
10	*a* 1.65, dd (*13.3, 3.7*)	24.8	10*b*[c], 11*b*[c], 11*a*, 9[b]	12	-
	b 1.25[c], m		-	-	-
11	*a* 2.44, m	34.9	10*a*, 10*b*[c],11*b*[c]	7, 9, 10, 12	-
	b 1.25[c], m		-	-	-
12	-	52.1	-	-	-
13	1.81, dd (*13.0, 3.1*)	49.0	14*a*, 14*b*	4, 12, 14, 4-Me, 12-CHO	3-Me
14	*a* 1.89, m	23.7	14*b*, 13	15, 16	-
	b 1.51, dd (*13.0, 4.5*)		15*a*, 15*b*, 14*a*, 13	13	-
15	*a* 1.76, m	26.2	14*a*,14*b*, 15*b*, 16	3, 13, 14	-
	b 1.62, dd (*13.0, 3.3*)		15*a*, 14*a*,14*b*,16	-	-
16	2.68, m	50.7	17*a*, 17*b*[a], 15*a*, 15*b*	17, 18	4-Me
17	*a* 2.61, dd (*13.0*, *6.4*)	28.3	16, 17*b*[a]	2, 3, 16, 18	-
	b 2.29[a], m		-	-	-
18	-	118.2	-	-	-
19	-	126.3	-	-	-
20	7.27[d], br d (*8.0*)	118.9	-	-	-
21	6.91, dd (*8.0*, *7.3*)	119.9	20[d], 22	19, 23	-
22	6.95, dd (*8.0*, *7.3*)	121.0	21, 23[d]	20, 24	-
23	7.27[d], br d (*8.0*)	112.8	-	-	-
24	-	142.2	-	-	-
25	-	80.0	-	-	-
26	1.29, s	21.9	-	9, 25, 27	-
27	1.20, s	23.9	-	9, 25, 26	-
1′	4.89, br s	96.6	2′	2′, 25	5′
2′	3.77, d (*3.1*)	74.1	1′, 3′	1′, 3′, 4′	-
3′	3.44[b], m	75.8	-	-	-
4′	3.55, t (*9.4*)	68.7	3′, 5′	6′, 3′, 5′	-
5′	3.17, m	78.2	6′ *b*, 4′	1′, 4′	1′
6′	*a* 3.83, dd (*11.8*, *1.9*)	63.1	5′, 6′*b*	4′	-
	b 3.69, dd (*11.8*, *5.4*)		5′, 6′*a*	4′, 5′	-
3-Me	1.03, s	15.1	-	2, 3, 4, 16	13
4-Me	0.93, s	19.9	-	3, 4, 5, 13	16, 12-CHO
12-CHO	10.16, s	210.2	-	12	4-Me

[a-d] Resonances with the same superscript within a column are overlapping and assignments may be interchanged

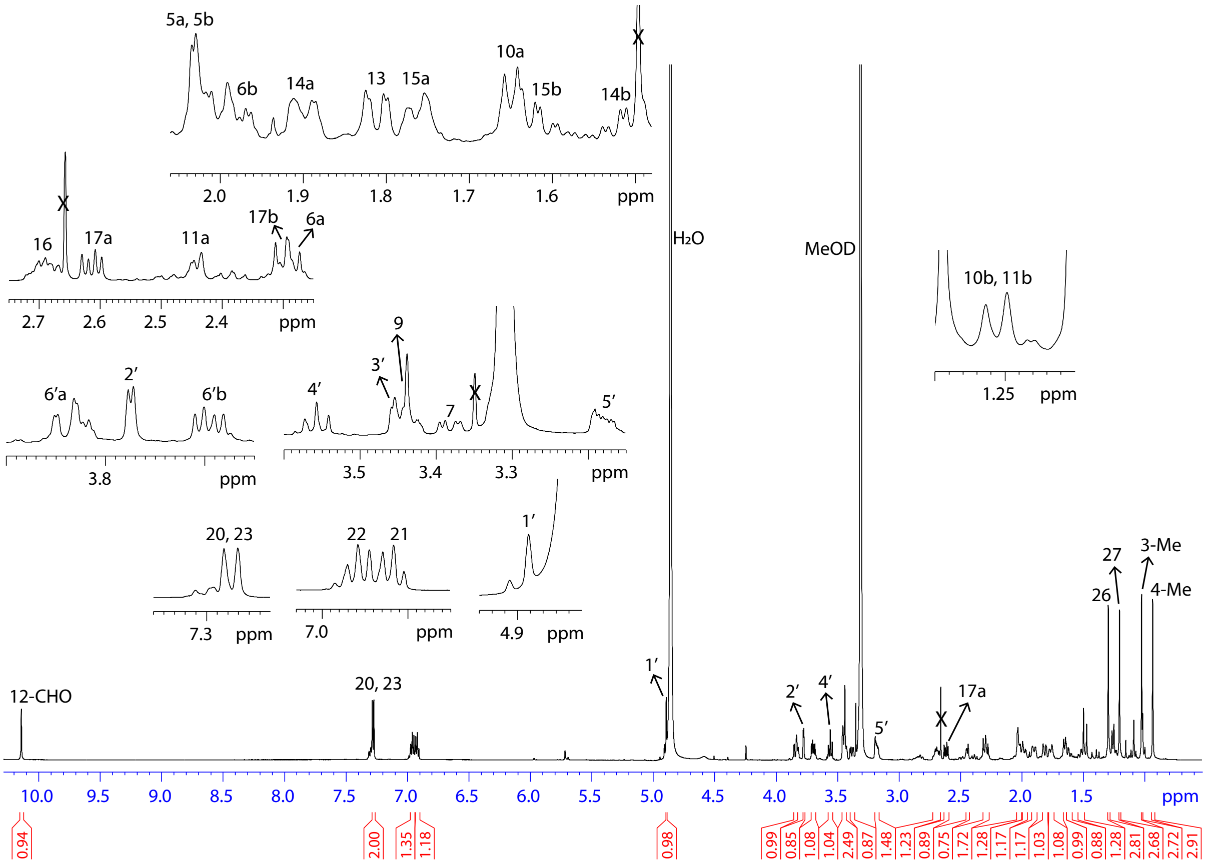


Figure S44. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of noonindole L (**12**)

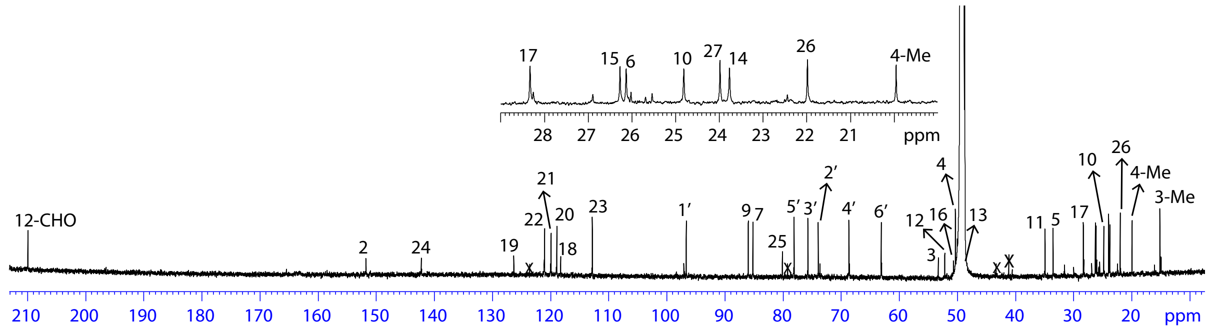


Figure S45. ^{13}C NMR (150 MHz, methanol-d_4) spectrum of noonindole L (**12**)

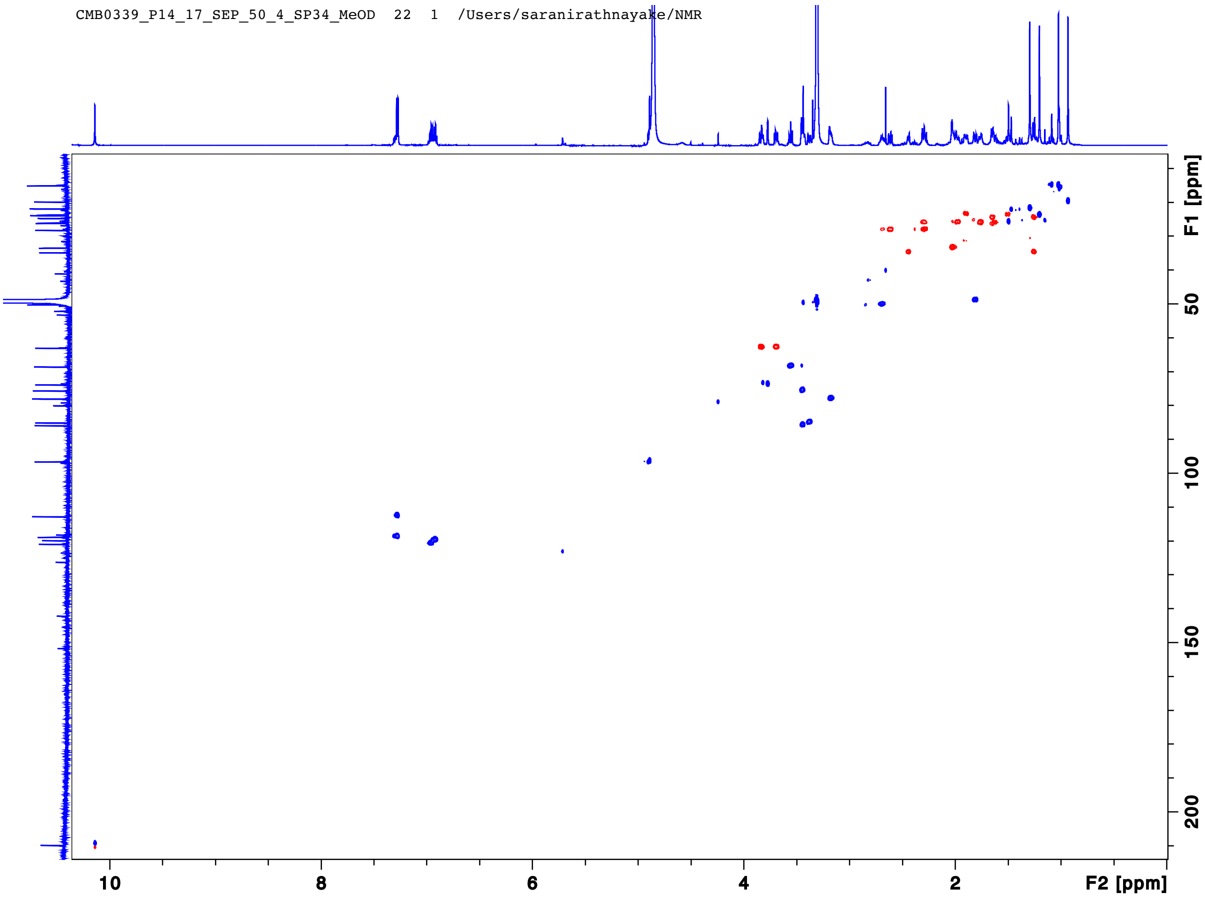


Figure S46. HSQC (methanol-d_4) spectrum of noonindole L (**12**)

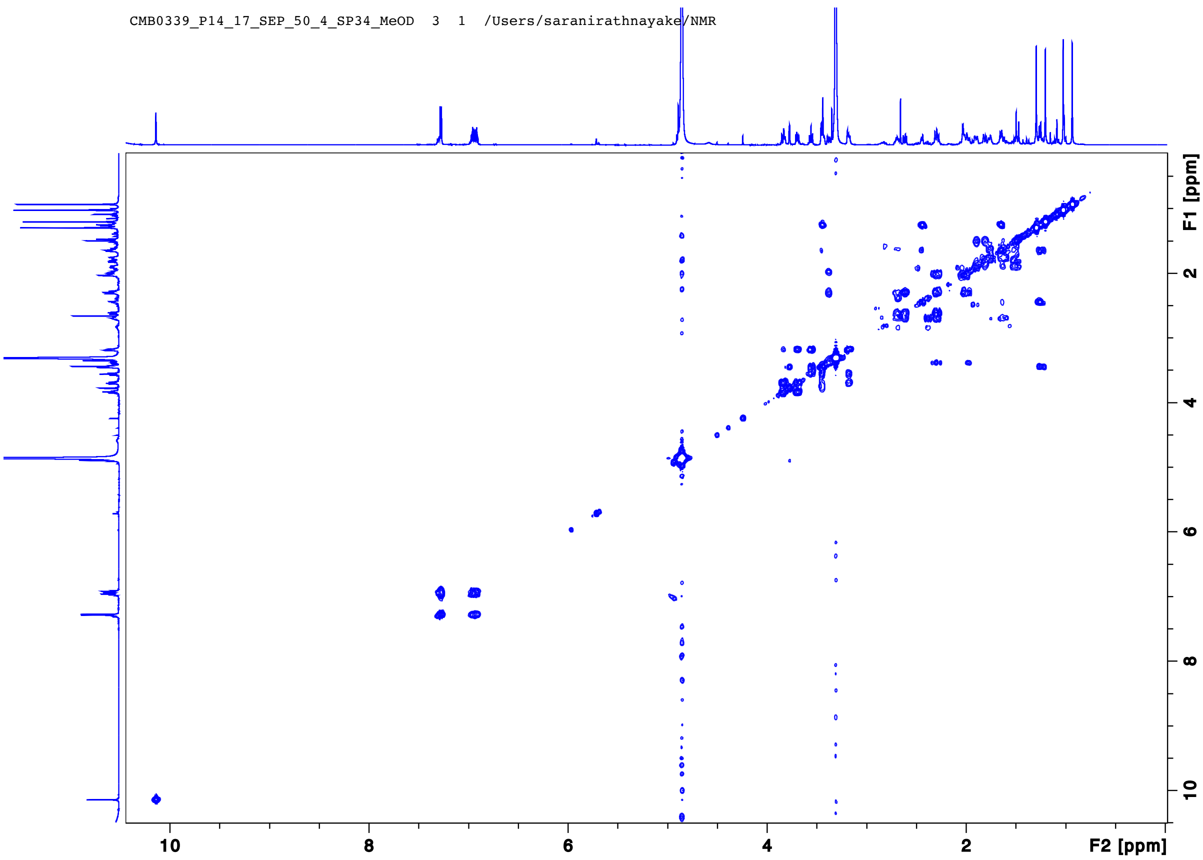


Figure S47. COSY (methanol-d_4) spectrum of noonindole L (**12**)

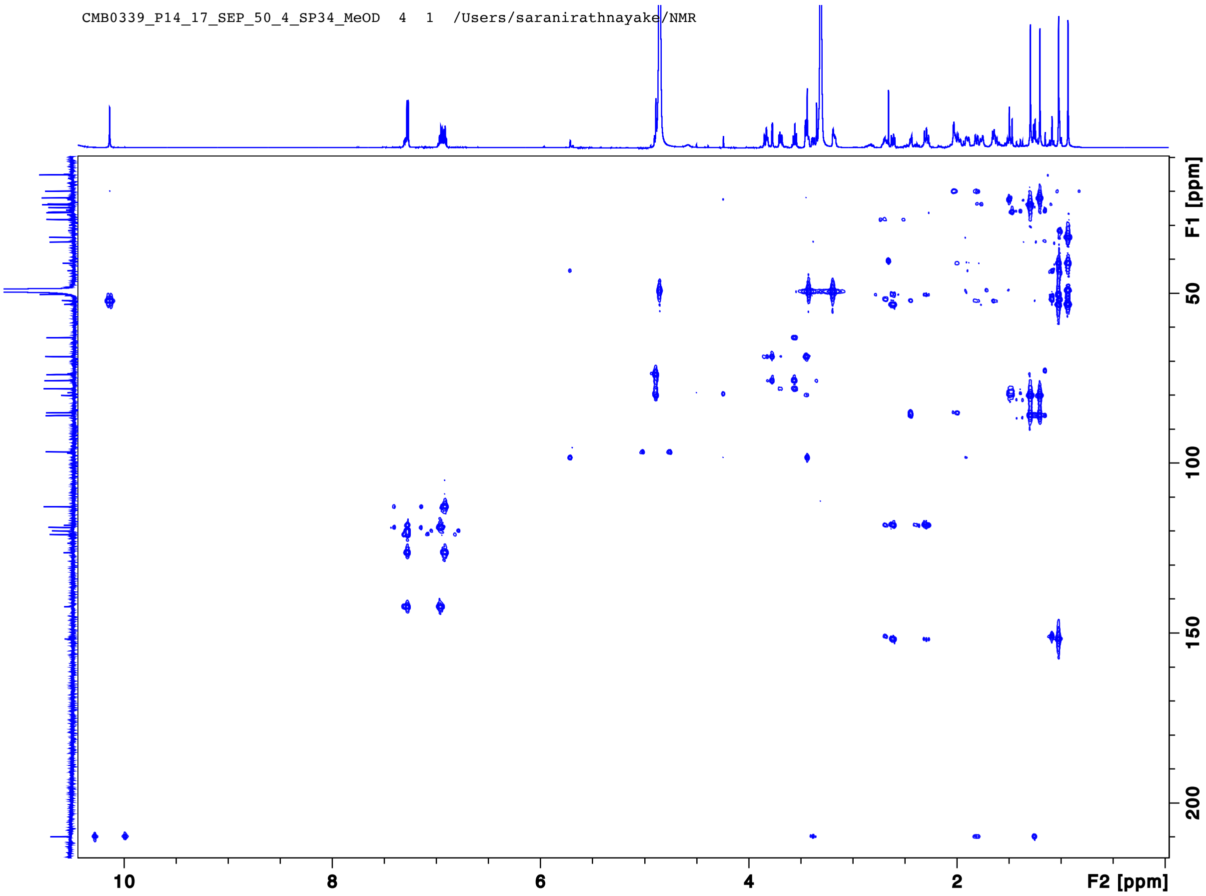


Figure S48. HMBC (methanol-*d*4) spectrum of noonindole L (**12**)

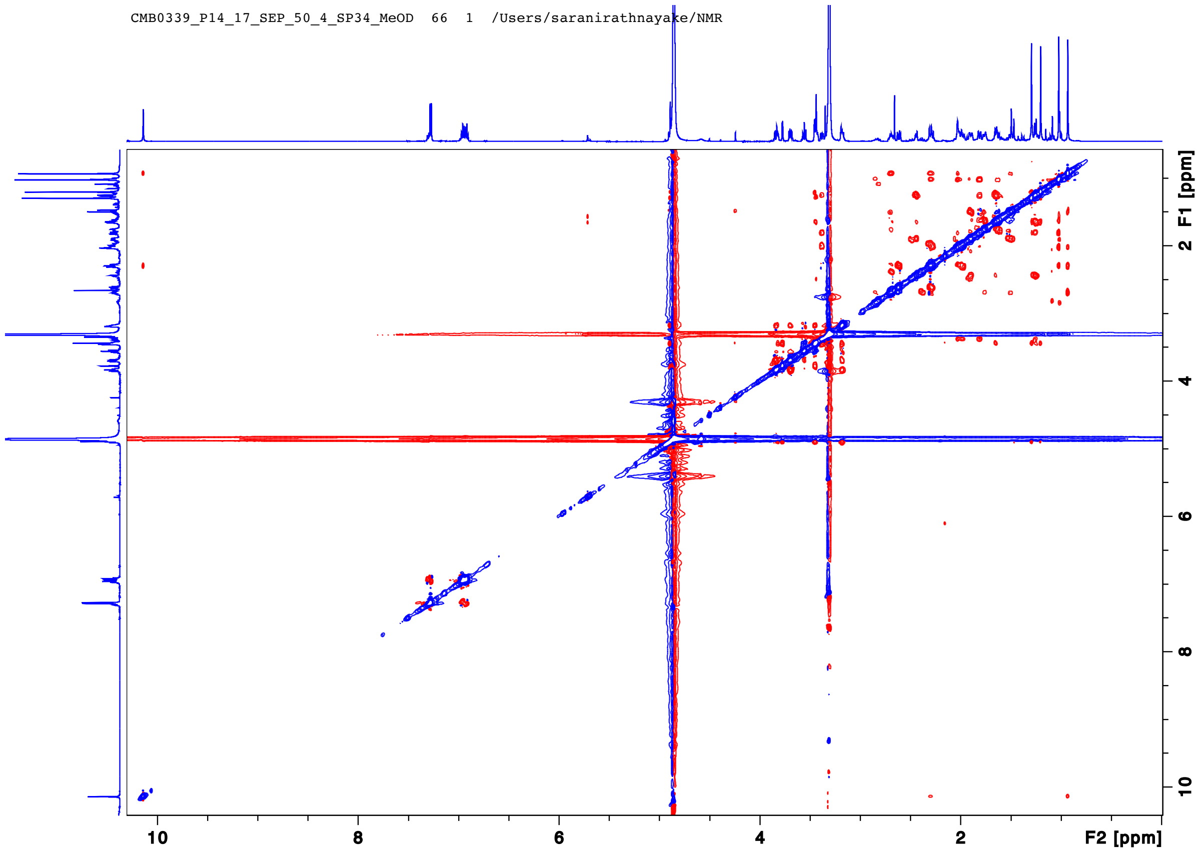


Figure S49. ROESY (methanol-*d*4) spectrum of noonindole L (**12**)

Mass Spectrum Molecular Formula Report

Analysis Info

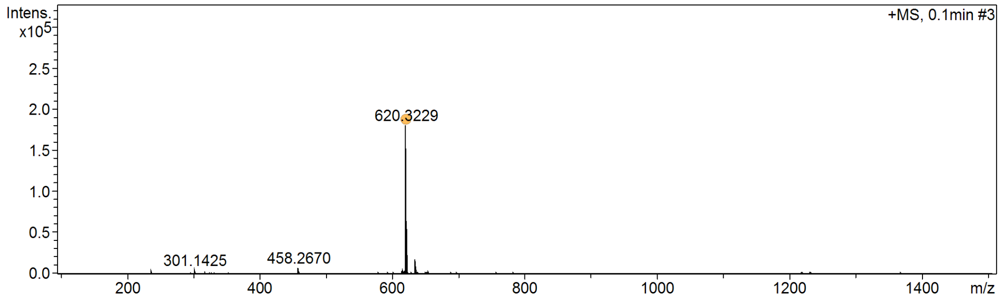
Analysis Name	D:\Data\s.kankanamge\CMB0339_P14_17_SEP_50_4_SP34.d	Acquisition Date	10/11/2021 3:53:51 PM	
Method	tune-medhigh_AP.m	Operator	a.salim	
Sample Name	CMB0339_P14_17_SEP_50_4_SP34	Instrument / Ser#	micrOTOF	213750.00232
Comment				

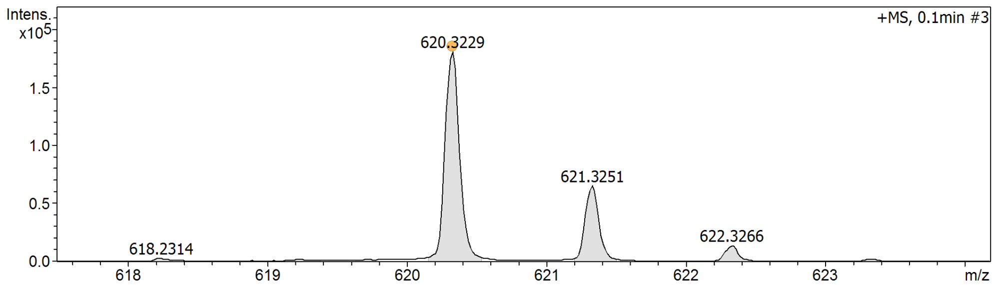
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	5.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.		
Formula, max.		
Measured m/z	Tolerance	Charge
Check Valence	Minimum	Maximum
Nirogen Rule	Electron Configuration	
Filter H/C Ratio	Minimum	Maximum
Estimate Carbon		





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
620.3229	1	C27H41N12NaO4	620.3266	-6.0	9.9	1	14.08	13.0	odd	ok
	2	C34H47NNaO8	620.3194	5.6	12.1	2	17.10	11.5	even	ok
	3	C28H47N5NaO9	620.3266	-6.0	14.9	3	12.70	7.5	even	ok
	4	C25H39N15NaO3	620.3253	3.8	16.2	4	46.29	13.5	even	ok
	5	C33H41N8NaO3	620.3194	5.6	16.6	5	15.55	17.0	odd	ok
	6	C26H45N8NaO8	620.3253	3.8	20.9	6	41.78	8.0	odd	ok
	7	C35H43N5NaO4	620.3207	-3.5	22.9	7	47.65	16.5	even	ok
	8	C27H51NNaO13	620.3253	3.8	26.6	8	36.60	2.5	even	ok

Bruker Compass DataAnalysis 4.1 printed: 10/20/2021 1:54:00 PM Page 1 of 2

Figure S50. HRMS spectrum of noonindole L (**12**)

4 Grain based MATRIX

Figure S51. CMB-M0339 growing in grain MATRIX

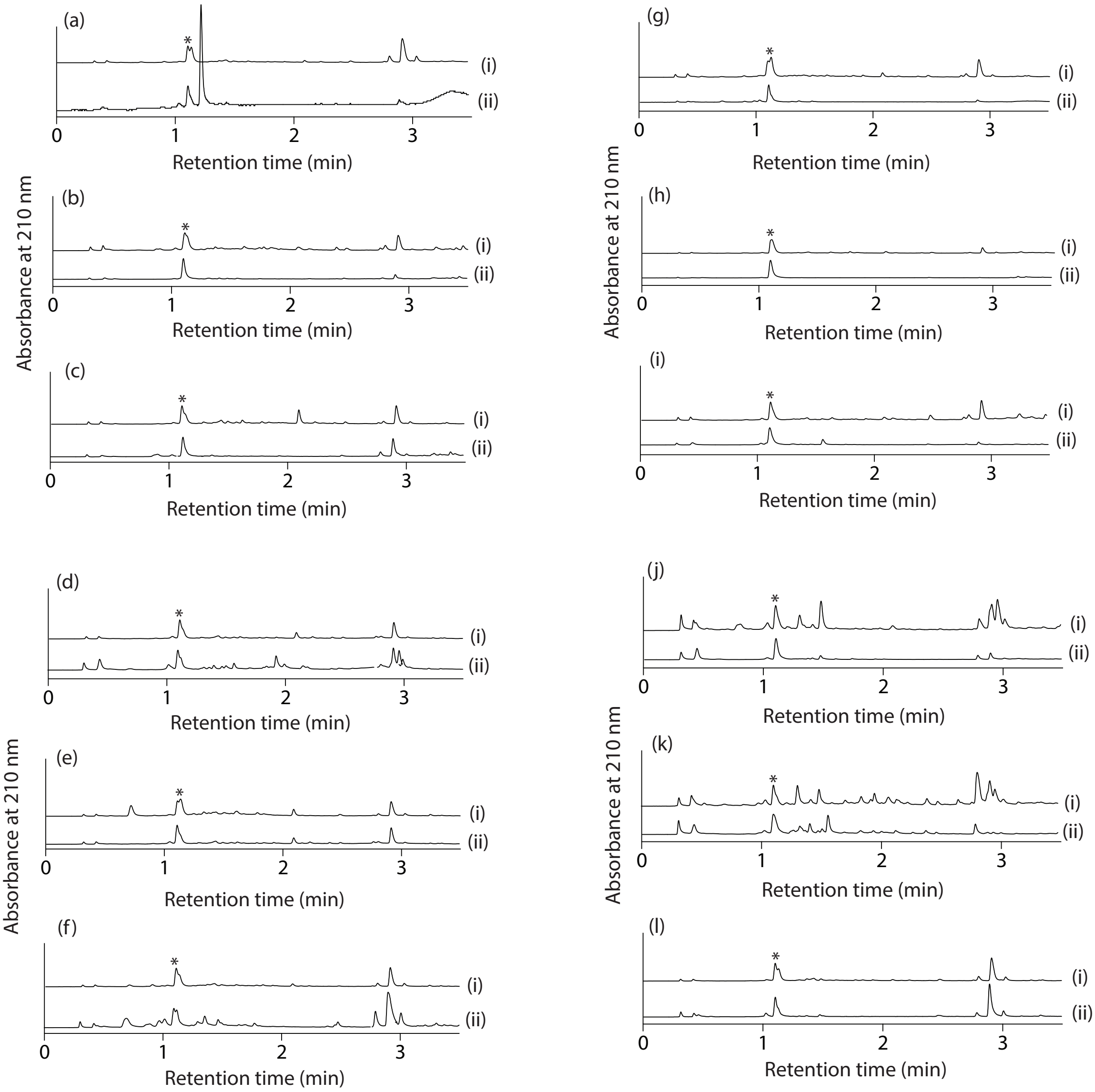


Figure S52. UPLC-DAD chromatograms of MATRIX extracts of CMB-M0339 cultivated in grain MATRIX, (a) Mung beans with shell, (b) Cous Cous, (c) Barley, (d) Jasmine rice, (e) Black rice, (f) Red rice, (g) Rice flour, (h) Noodles, (i) Semolina, (j) Lentils, (k) Black gram without shell, (l) Basmati rice, (i) Extract from CMB-M0339, (ii) Media blank, * Internal calibrant

Table S8. Composition of media used for grain-based MATRIX

Grains	Composition (per well)
Red rice	Red rice (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Black rice	Black rice (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Jasmine rice	Jasmine rice (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Basmati rice	Basmati rice (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Barley	Barley (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Cous cous (Wheat)	Cous cous (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Noodles	Noodles (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Mung bean with shell	Mung bean (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Black gram without shell	Black gram (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Lentils	Lentils (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Semolina (Wheat)	Semolina (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water
Rice flour	Rice flour (1.0 g), peptone (0.0045 g), yeast extract (0.0045 g), monosodium glutamate (0.0015 g) and 1.5 mL distilled water

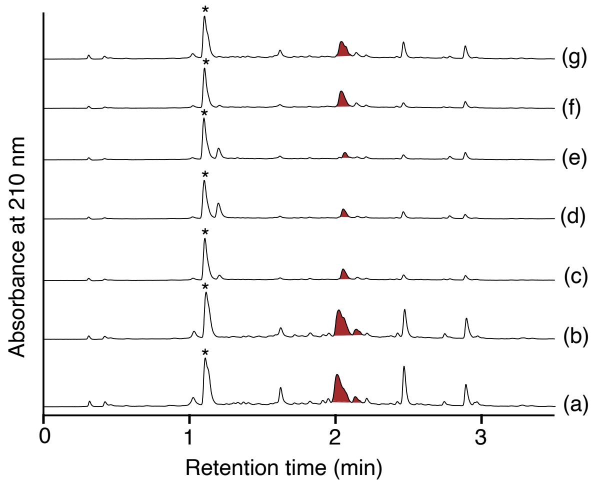


Figure S53. UPLC-DAD chromatograms of CMB-M0339 cultivated in D400 agar supplemented with D-mannose (4, 2, 1 mg/mL, b-d, respectively) and D-glucosamine (4, 2, 1 mg/mL, e-g, respectively) (a) Control. (Production of **1-3** are highlighted in red). * Internal calibrant

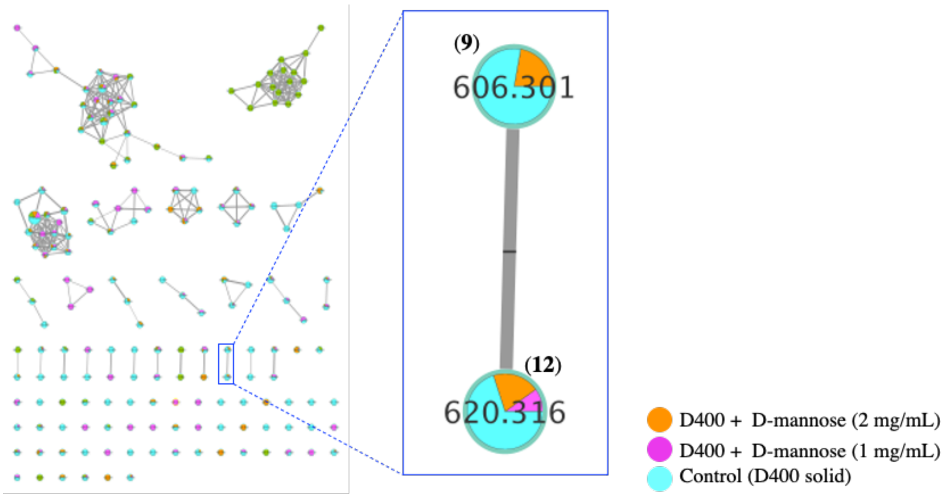


Figure S54. GNPS molecular network of CMB-M0339 cultivated in D400 agar supplemented with D-mannose. Expanded cluster showing the presence of **9** and **12**

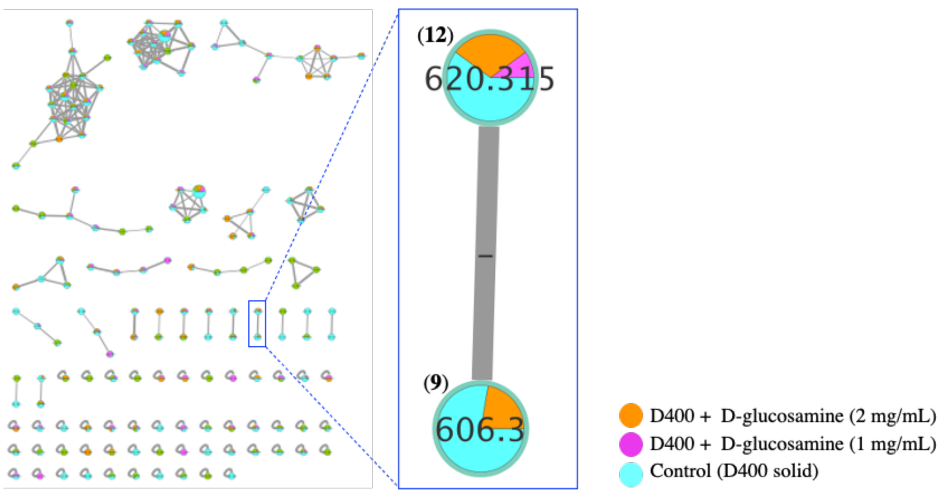


Figure S55. GNPS molecular network of CMB-M0339 cultivated in D400 agar supplemented with D-glucosamine. Expanded cluster showing the presence of **9** and **12**

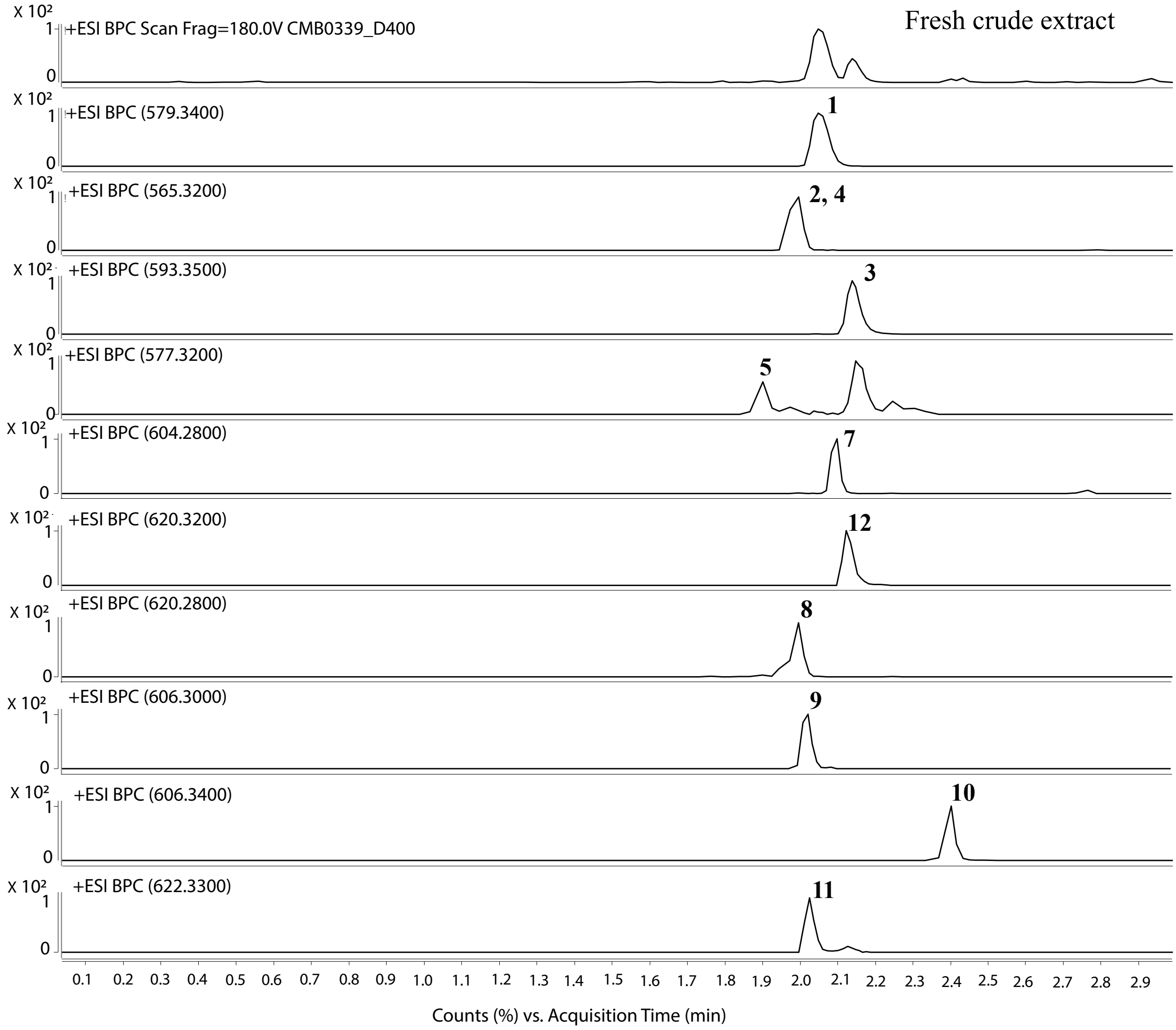


Figure S56.Single ion extraction of CMB-M0339 fresh crude extract to show the presence of **1-12**

5 Biological screening

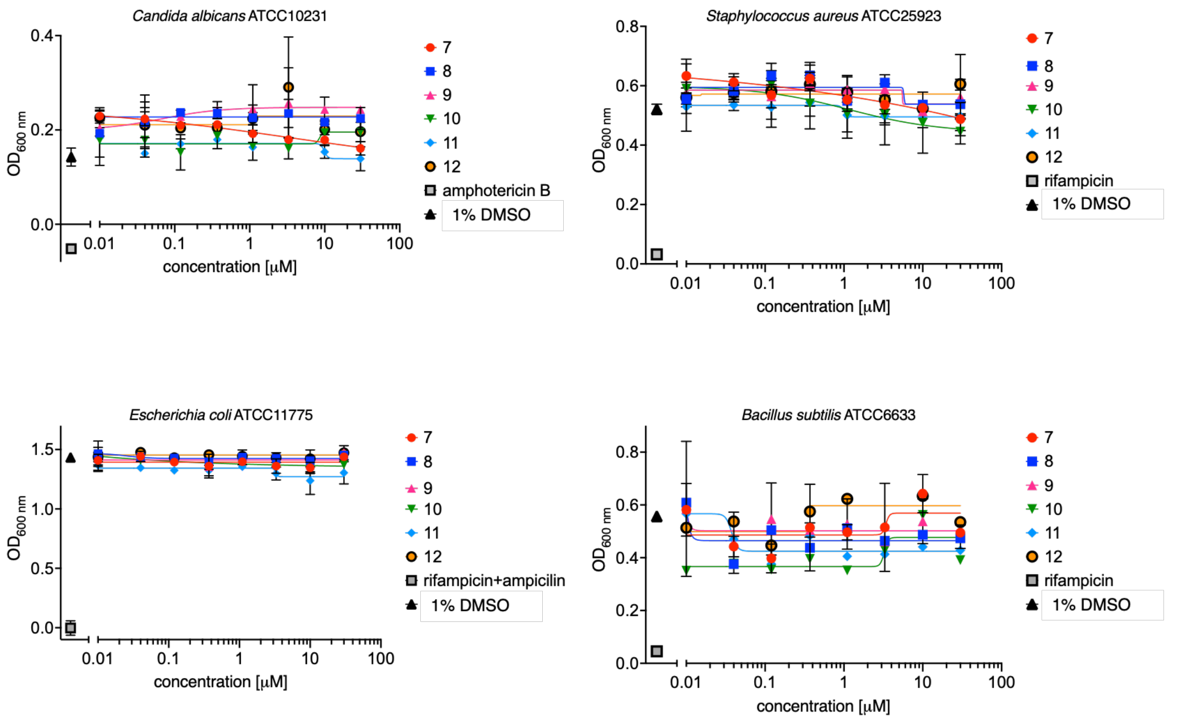


Figure S57. Antimicrobial activity of metabolites **7-12** against *S. aureus*, *E. coli*, *B. subtilis* and *C. albicans*

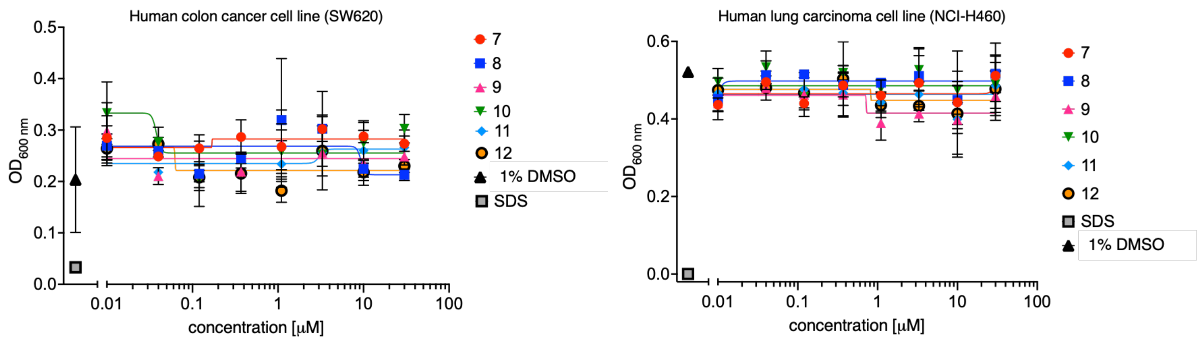


Figure S58. Cytotoxicity of metabolites **7-12** against human colon cancer (SW620) and human lung carcinoma (NCI-H460) cell lines

6 References

1. Yang, Z. G., N.; Friday, A. Comparison of Models for Nucleotide Substitution Used in Maximum-Likelihood Phylogenetic Estimation. *Mol. Biol. Evol.* **1994**, *11* (2), 316-324.

2. Edgar, R. C. MUSCLE: a multiple sequence alignment method with reduced time and space complexity. *BMC Bioinformatics* **2004**, *5*.

3. Okonechnikov, K. G., O.; Fursov, M. Unipro UGENE: a unified bioinformatics toolkit. *Bioinformatics* **2012**, *28* (8), 1166-1167.