Supporting Information

Noonindoles A–F: Rare indole diterpene amino acid conjugates from a marine-derived fungus, *Aspergillus noonimiae* CMB-M0339

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CGGCACCCTCGCGGTGCCAACCTCCCATCCTTGTCTATTGTTACCGTCGTTGCTTCGGCGGG

CCCGTTCCTCCTCCCCCGGGGGGAGGGCCGTCGGGGGGCATTCGCCCCCGGGCGAGCGCCCG

CCGGAGACCCCAACACGAACTCTGAGTGAAAGACTGTCGTCTGAGTGGGCTTTTTGAATCAG

TTAAAACTTTCAACAACGGATCTCTTGGTTCCGGCATCGATGAAGAACGCAGCGAACTGCGA

TAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAGTCTTTGAACGCATATTGCGCCCCC

TGGTATTCCGGGGGGCATGCCTGTCCGAGCGTCATTGCTACCCTCAAGCACGGCTTGTGTGT

TGGGTCGGCGTCCCCGGGGAGTCCCCGGGGACGGGCCCGAAAGGCAGCGGCGGCACCGCGTC

CTGGTCCTCGAGCGTATGGGGCTCTGTCACCCGCTCTGAGGGGCCGGCCGGCGCCTTTGGCC

AACCTGTTTATGGGCCCTTCCGGGGGACCGAAACACCATTTTTTTCTCAGGTTGACCTCGGA

TCAGGTAGGGATACCCGCTGAACTTAAGCATATCAATAAGGCGGAGGA (**606 bp**)

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
Aspergillus keratitidis culture DAOMC:251748 strain KAS:8117 18S ribosomal RNA gene, partial sequence; intern…	Aspergillus kerati…	797	797	100%	0.0	90.21%	737	KY980634.1
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 18S rRNA 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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Query  13   GGTGCCAACCTCCCATCCTTGTCTATTGTTACCGTCGTTGCTTCGGCGGGCCCGTTCCTC  72
            |||||||||||||||||| ||||||||| |||| |||||||||||||||||||||| |||
Sbjct  52   GGTGCCAACCTCCCATCCGTGTCTATTG-TACCTTCGTTGCTTCGGCGGGCCCGTTTCTC  110

Query  73   CT---CCCCCGGG-GGGAGGGCCGTCGGGGGGCATTCGCCCCCGGGCGAGCGCCCGCCGG  128
            ||   ||||||||  |||||||||||||||||||   ||||||||||| | |||||||||
Sbjct  111  CTTCCCCCCCGGGAAGGAGGGCCGTCGGGGGGCAGCTGCCCCCGGGCGTGTGCCCGCCGG  170

Query  129  AGACCCCAACACGAACTCTGAGTGAAAGACTGTCGTCTGAGTGGGCTTTT-TGAATCAGT  187
            ||||||||||||||||||||  ||||||||||||||||||||||| ||||  | ||||| |
Sbjct  171  AGACCCCAACACGAACTCTGTCTGAAAGACTGTCGTCTGAGTGGGTTTTTATAAATCATT  230

Query  188  TAAAACTTTCAACAACGGATCTCTTGGTTCCGGCATCGATGAAGAACGCAGCGAACTGCG  247
            ||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||
Sbjct  231  TAAAACTTTCAACAACGGATCTCTTGGTTCCGGCATCGATGAAGAACGCAGCGAACTGCG  290

Query  248  ATAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAGTCTTTGAACGCATATTGCGCC  307
            ||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||
Sbjct  291  ATAAGTAATGTGAATTGCAGAATTCAGTGAATCATCGAGTCTTTGAACGCATATTGCGCC  350

Query  308  CCCTGGTATTCCGGGGGGCATGCCTGTCCGAGCGTCATTGCTACCCTCAAGCACGGCTTG  367
            ||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||
Sbjct  351  CCCTGGTATTCCGGGGGGCATGCCTGTCCGAGCGTCATTGCTACCCTCAAGCACGGCTTG  410

Query  368  TGTGTTGGGTCGGCGTCCCCGGGGAGT-CCCCGGGGACGGGCCCGAAAGGCAGCGGCGGC  426
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Sbjct  411  TGTGTTGGGTCGGCGTCCCTGGGGCTCCCCCCGGGGACGGGCCCGAAAGGCAGCGGCGGC  470

Query  427  ACCGCGTCCTGGTCCTCGAGCGTATGGGGCTCTGTCACCCGCTCTGAGGGGCCGGCCGGC  486
            |||||||||||||||||||||||||||||||||||||||||||| |||||||||||||||
Sbjct  471  ACCGCGTCCTGGTCCTCGAGCGTATGGGGCTCTGTCACCCGCTCGGAGGGGCCGGCCGGC  530

Query  487  GCCTTTGGCCAACCTGTTTATGGGCCCTTCCGGGGGACCGAAACACCAtttttttCTCAG  546
            |||||||||||   | ||| ||| |  ||| |||  | ||||| ||  ||  ||||| ||
Sbjct  531  GCCTTTGGCCATTATTTTTCTGGTC--TTCTGGG--ATCGAAAAAC--TTC-TTTCTTAG  583

Query  547  GTTGACCTCGGATCAGGTAGGGATACCCGCTGAACTTAAGCATATCAATAAGGCGGAGGA  606
            |||||||||||||||||||||||||||||||||||||||||||||||||||| |||||||
Sbjct  584  GTTGACCTCGGATCAGGTAGGGATACCCGCTGAACTTAAGCATATCAATAAG-CGGAGGA  642
```

Aspergillus noonimiae CBS 143382 ITS region; from TYPE material

NCBI Reference Sequence: NR_156329.1

FASTA Graphics

Go to:

```
LOCUS       NR_156329                712 bp    DNA     linear   PLN 27-JUN-2018
DEFINITION  Aspergillus noonimiae CBS 143382 ITS region; from TYPE material.
ACCESSION   NR_156329
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
  JOURNAL   Stud. Mycol. 88, 237-267 (2018)
REFERENCE   2  (bases 1 to 712)
  CONSRTM   NCBI RefSeq Targeted Loci Project
  TITLE     Direct Submission
  JOURNAL   Submitted (01-MAY-2018) National Center for Biotechnology
            Information, NIH, Bethesda, MD 20894, USA
REFERENCE   3  (bases 1 to 712)
  AUTHORS   Tanney,J.B., Visagie,C.M., Yilmaz,N. and Seifert,K.A.
  TITLE     Direct Submission
  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

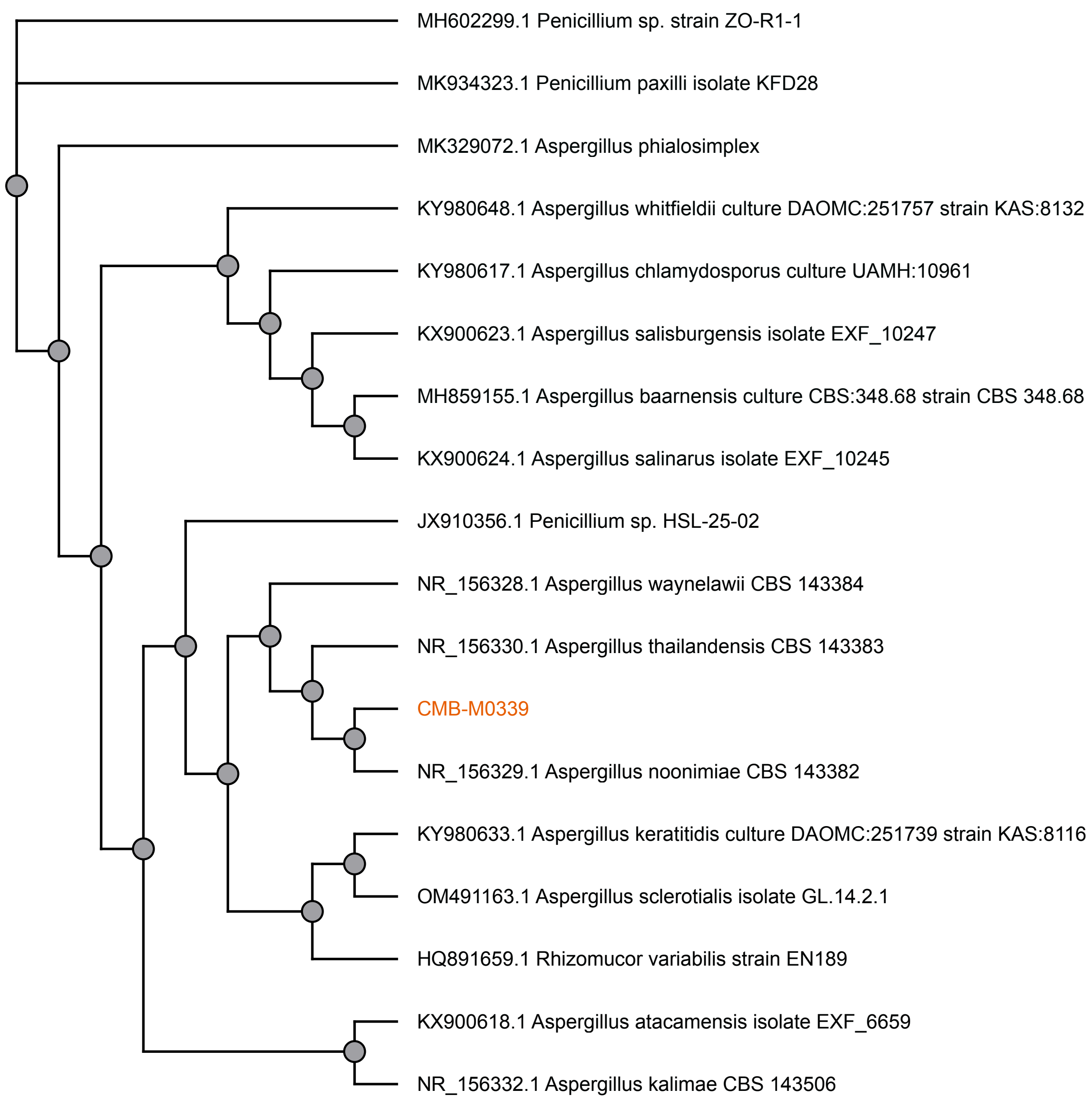

Figure S4. Phylogenetic tree by PhyML Maximum Likehood analysis of 18s rRNA sequences showing the relationship of CMB-M0339 among selected reference strains (RefSeq GenBank) with the accession numbers

Figure S5. CMB-M0339 cultivated on SD agar

2 Chemical investigation of CMB-M0339

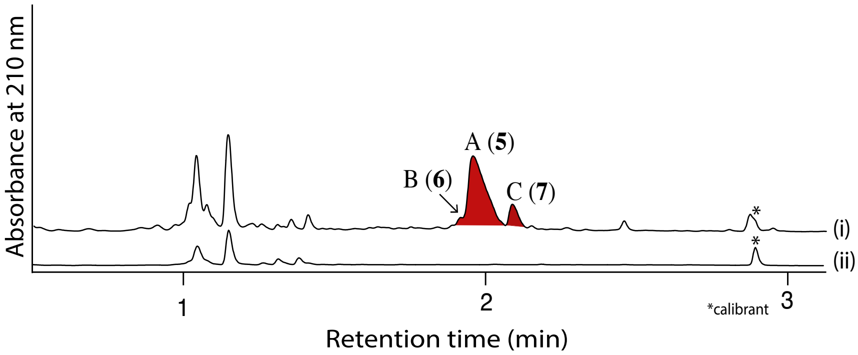

Figure S6. UPLD-DAD chromatograms of (i) crude extract of CMB-M0339 cultivated on M1 agar (supplemented with 3.3% artificial sea salt) (ii) Media blank

The crude extract of *Aspergillus* sp. CMB-M0339 cultivated on M1 agar (supplemented with 3.3% artificial sea salt) was subjected to UPLC-DAD analysis which revealed the production of one major metabolite, noonindole A (**5**) and two minor metabolites, noonindoles B (**6**) and C (**7**) sharing similar UV-Vis chromophore.

3 MATRIX cultivation profiling of CMB-M0339

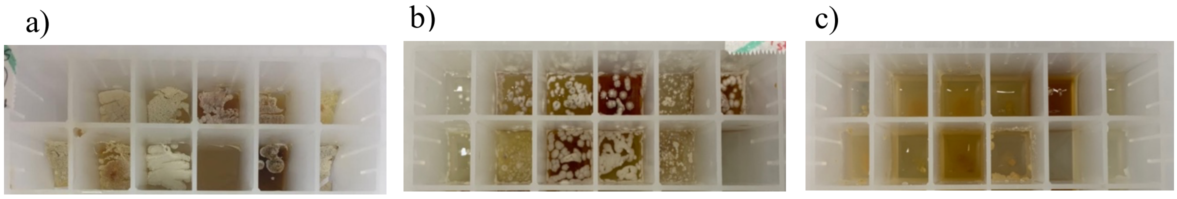

Figure S7. CMB-M0339 cultivated under MATRIX conditions. (a) agar (b) static broth (c) shaken broth

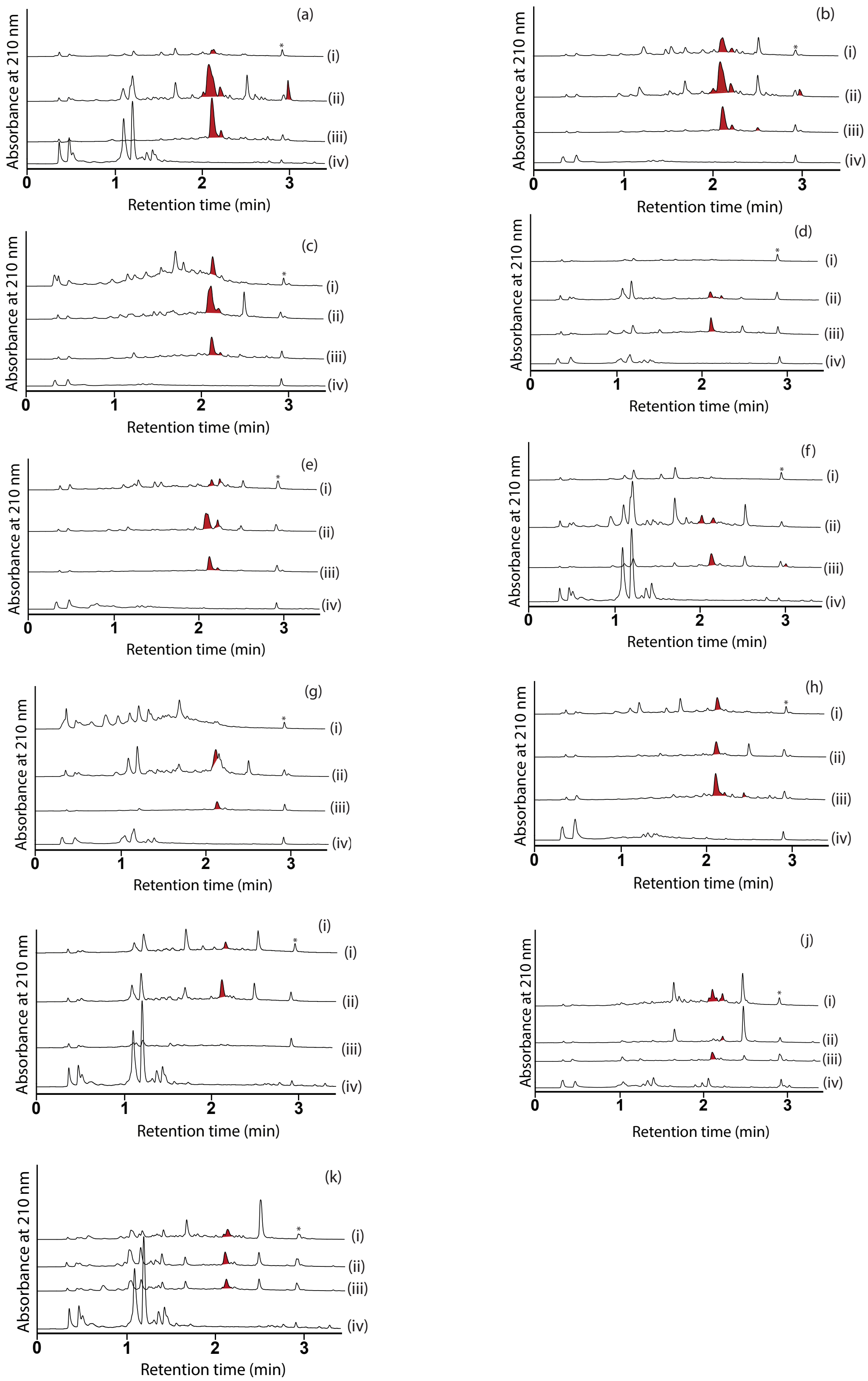

Figure S8. UPLC-DAD chromatograms of MATRIX extracts of CMB-M0339 showing the production of noonindoles A–C **(5–7)** (highlighted in red) in different media and culture conditions; (a) D400, (b) GY, (c) IM ,(d) M1, (e) M2, (f) SGG, (g) YEME, (h) YES, (i) 333, (j) PD, (k) SD, (i) shaken broth, (ii) static broth, (iii) agar, (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)

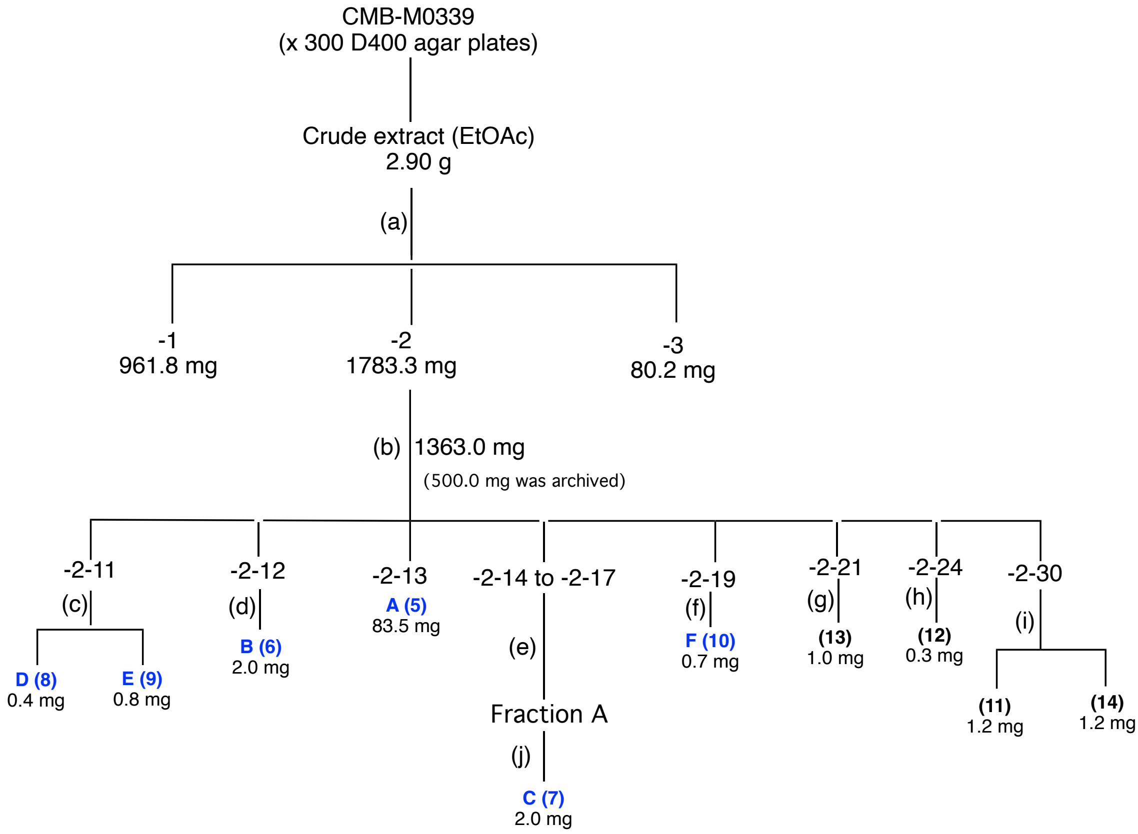

Figure S9. Isolation scheme for **5-14** from CMB-M0339. (a) Trituration [hexane (-1), DCM (-2), MeOH (-3)]. (b) Preparative HPLC (Phenomenex Luna-C_8 10 µm, 21.2 × 250 mm column, 20 mL/min gradient elution from 90% H_2O/MeCN to 100% MeCN over 20 min with constant 0.1% TFA modifier). (c) Semi preparative HPLC (Zorbax C_{18} 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 40% MeCN/H_2O over 30 min with constant 0.1% TFA modifier. (d) Semi preparative HPLC (Zorbax C_8 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 37% MeCN/H_2O over 20 min with constant 0.1% TFA modifier. (e) Column chromatography: Sep-Pak (Agilent Bond Elut C_{18} column, 5 g) gradient elution from 90% H_2O/MeCN to 100% MeCN (f) Semi preparative HPLC (Agilent C_8-Ep 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 50% MeCN/H_2O over 25 min with constant 0.1% TFA modifier. (g) 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. (h) Semi preparative HPLC (Agilent C_8-Ep 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 60% MeCN/H_2O over 25 min with constant 0.1% TFA modifier. (i) Semi preparative HPLC (Agilent CN 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 60% MeCN/H_2O over 20 min with constant 0.1% TFA modifier. (j) Zorbax C_8 5µm column, 9.4 × 250 mm, 3 mL/min isocratic elution of 40% MeCN/H_2O over 20 min with constant 0.1% TFA modifier

4 Noonindole A (5)

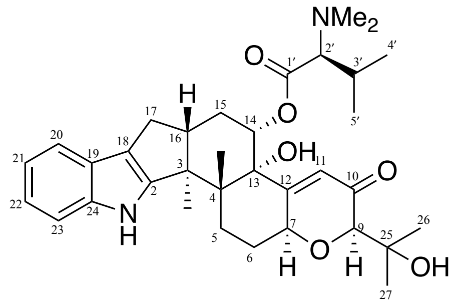

Table S2. 1D and 2D NMR (methanol-d_4, 600 MHz) data for noonindole A (**5**)

Pos.	δ_H, mult. (J in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	152.4	-	-	-
3	-	52.0	-	-	-
4	-	46.4	-	-	-
5	*a* 2.87 (ddd, 1H, J =*13.6, 13.6, 5.2* Hz)	28.1	5*b*, 6*a*, 6*b*	4, 6, 13, 3	3-Me
	b 1.81 (br dd, 1H, J =*13.6, 5.2* Hz)		5*a*, 6*b*	4, 6, 7, 13	
6	*a* 2.38 (m, 1H)	30.6	5*a*, 6*b*, 7	5, 7, 4, 12	-
	b 1.91 (m, 1H)		5*a*, 6*a*, 7	5, 7	
7	4.91 (m, 1H)	74.6	6, 9, 11	6, 11, 12	9
9	3.68 (d, 1H, J = *1.9* Hz)	84.0	7	7, 25, 26, 27, 10	7, 27
10	-	198.5	-	-	-
11	5.62 (d, 1H, J =*1.9* Hz)	122.4	7	7, 9, 13	-
12	-	165.9	-	-	-
13	-	80.0	-	-	-
14	5.53 (dd, 1H, J = *10.2, 5.3* Hz)	77.9	15*a*, 15*b*	15, 1′	16
15	*a* 2.24 (dd, 1H, J = *11.1, 10.2* Hz)	28.5	14, 15*b*, 16	3, 13, 14, 16	3-Me
	b 2.21 (m, 1H)		14, 15*a*, 16	3, 13, 14, 16	
16	2.92 (m, 1H)	47.4	15*a*, 15*b*, 17*a*	17, 3-Me, 3	14
17	*a* 2.73 (dd, 1H, J = *13.0, 6.2* Hz)	27.6	16, 17*b*[a]	2, 3, 15, 16, 18	-
	b 2.47[a] (m, 1H)		-	-	
18	-	117.4	-	-	-
19	-	126.2	-	-	-
20	7.31 (d, 1H, J = *7.5* Hz)	119.0	21	18, 22, 24	-
21	6.94 (ddd, 1H, J = *7.5, 7.5, 1.1* Hz)	120.1	20, 22	19, 23	-
22	6.98 (ddd, 1H, J = *7.5, 7.5, 1.1* Hz)	121.1	21, 23	20, 24	-
23	7.27 (d, 1H, J = *7.5* Hz)	112.7	22	19, 21	-
24	-	141.8	-	-	-
25	-	73.3	-		-
26	1.28 (s, 3H)	25.4	-	9, 25, 27	-
27	1.26 (s, 3H)	26.2	-	9, 25, 26	9
1′	-	167.4	-	-	-
2′	3.86 (d, 1H, J = *5.5* Hz)	74.8	3′[a]	1′, 3′, 4′ [b], 5′, NMe_2	NMe_2
3′	2.47[a] (m, 1H)	28.4	-	-	-
4′	1.05[b]	19.4	3′[a]	5′	-
5′	1.03 (d, 1H, J = *7.1* Hz)	17.0	3′[a]	4′[b]	-
3-Me	1.37 (s, 3H)	16.7	-	2, 3, 4, 16	15*a*, 5*a*
4-Me	1.04[b]	19.4	-	13, 3, 4	-
NMe_2	2.90 (s, 6H)	43.0	-	2′, NMe_2	2′

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

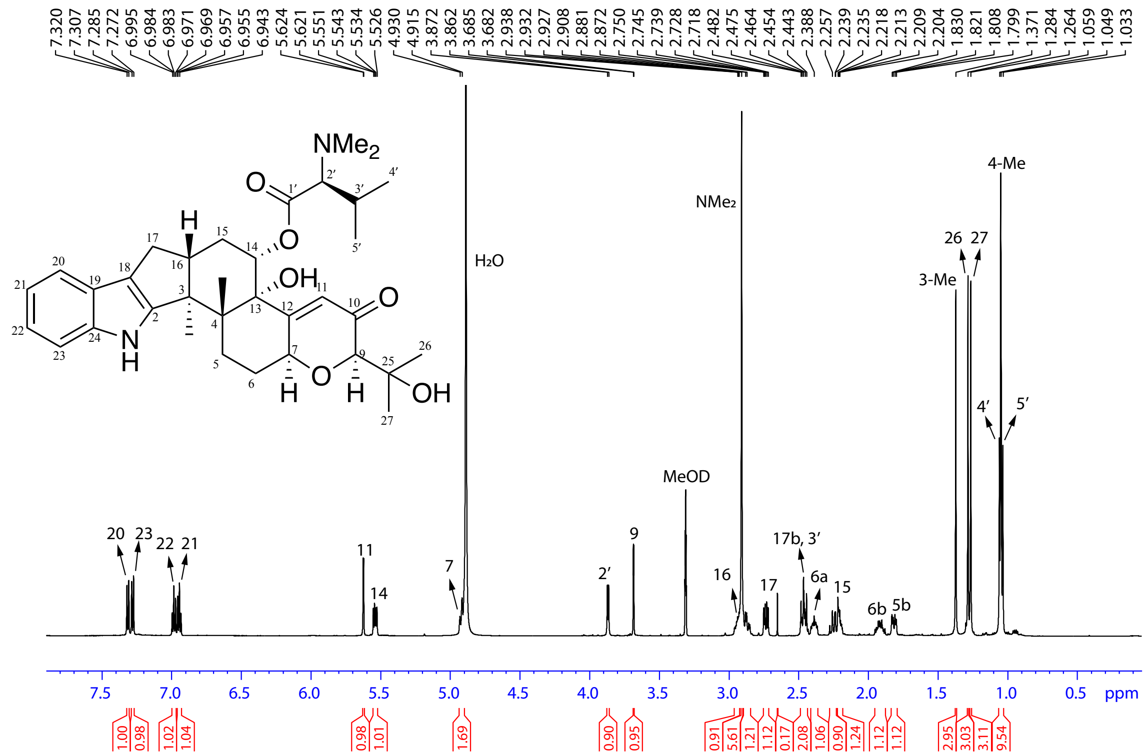

Figure S10. ^{1}H NMR (600 MHz, methanol-d_4) spectrum of noonindole A (**5**)

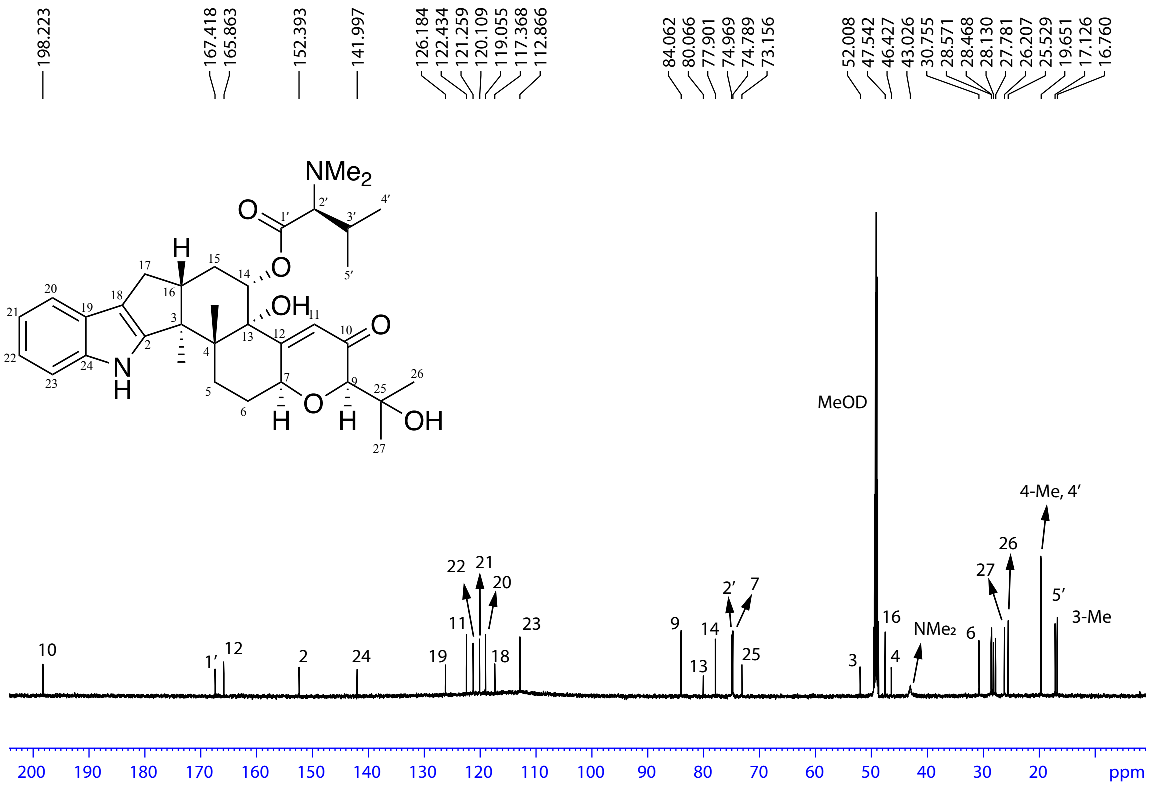

Figure S11. ^{13}C NMR (150 MHz, methanol-d_4) spectrum of noonindole A (**5**)

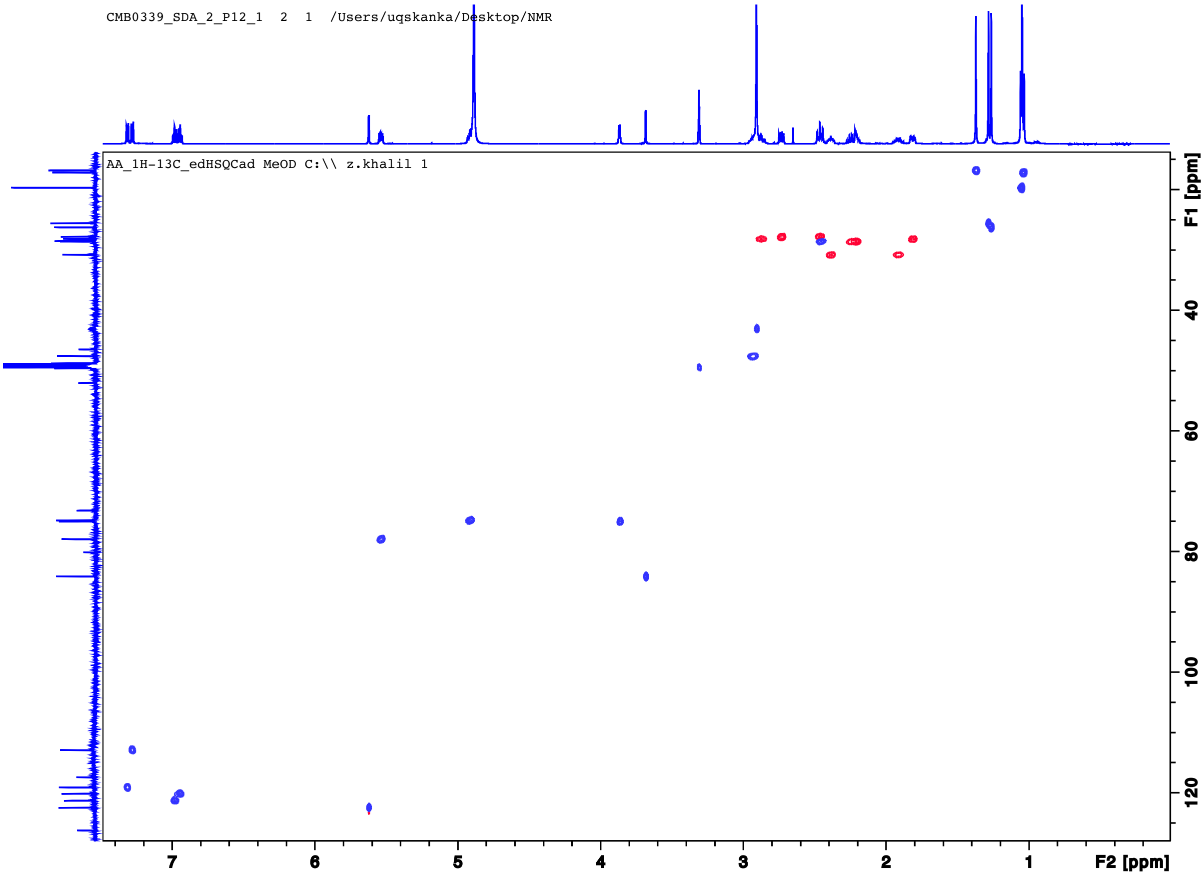

Figure S12. HSQC (methanol-d_4) spectrum of noonindole A (**5**)

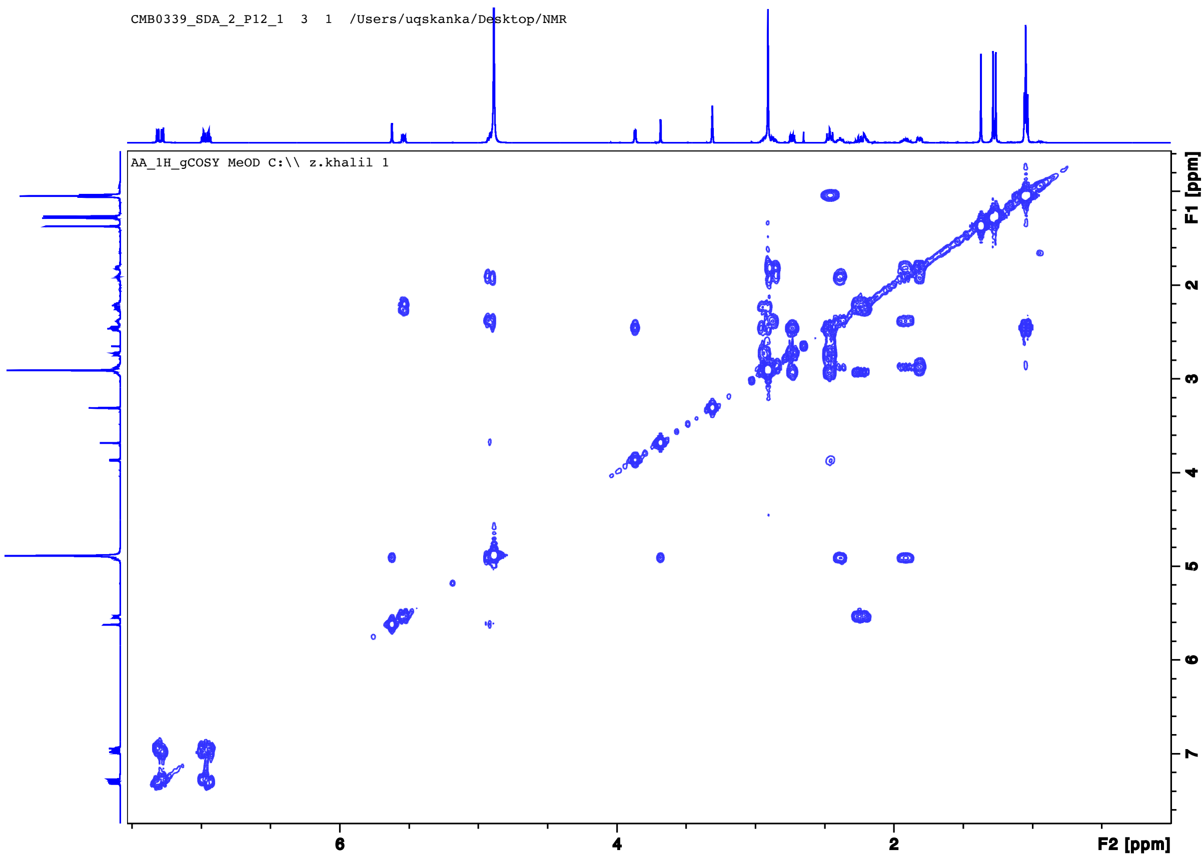

Figure S13. COSY (methanol-d_4) spectrum of noonindole A (**5**)

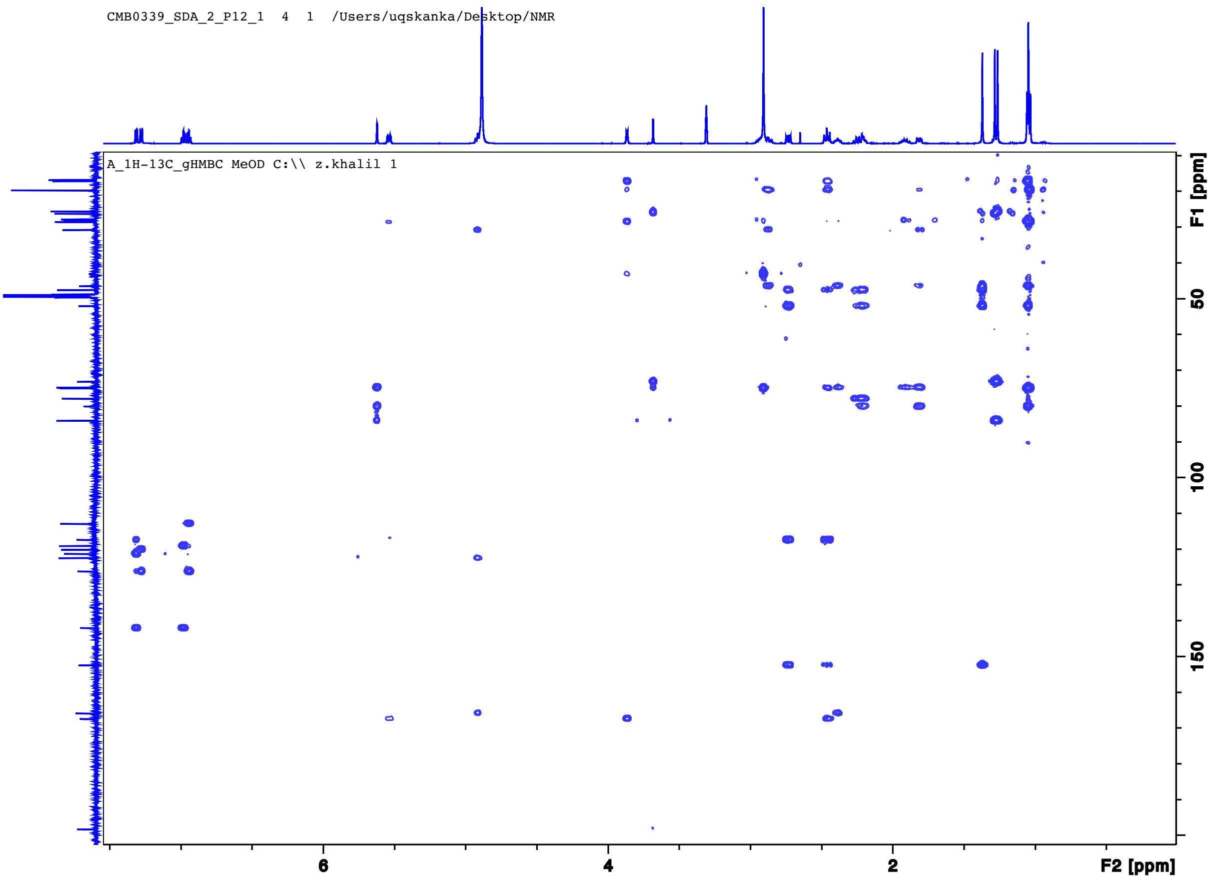

Figure S14. HMBC (methanol-d_4) spectrum of noonindole A (**5**)

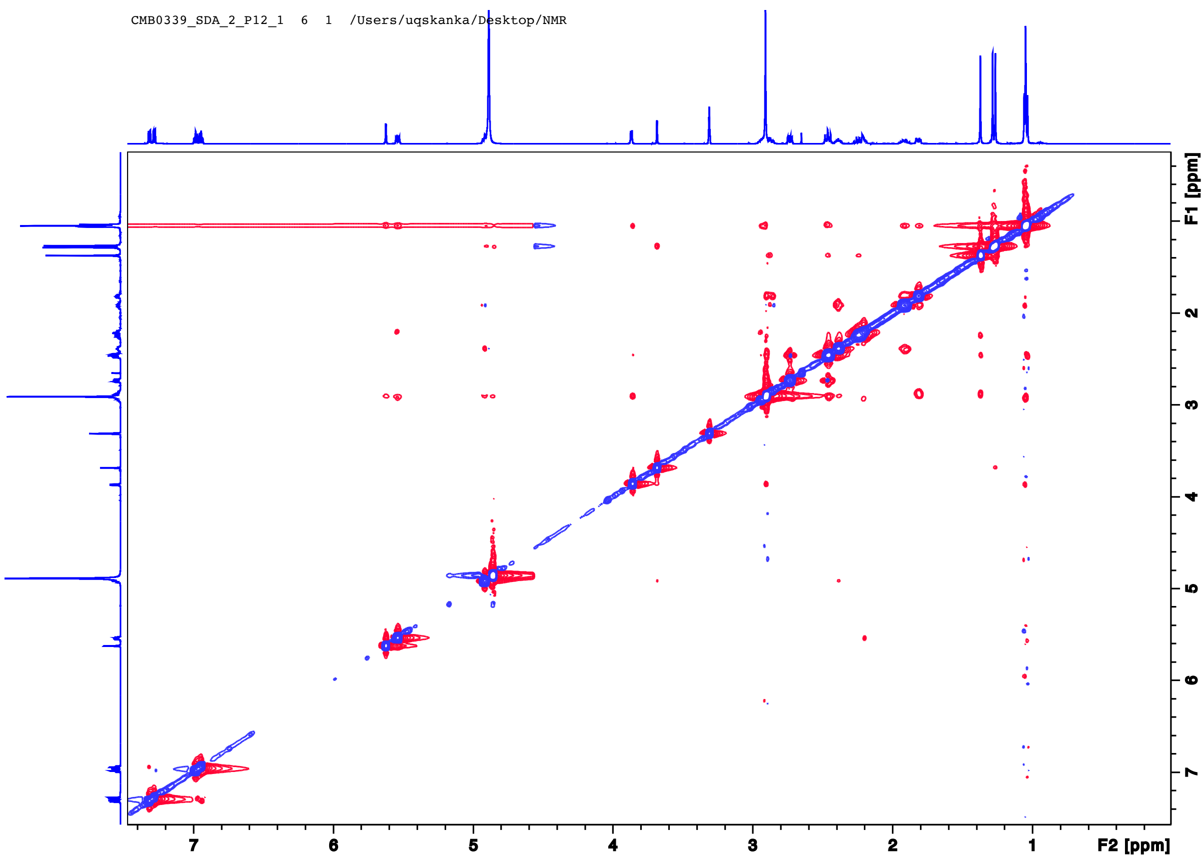

Figure S15. ROESY (methanol-d_4) spectrum of noonindole A (**5**)

Mass Spectrum Molecular Formula Report

Analysis Info

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Method	tune-medhigh_AP.m	Operator	a.salim	
Sample Name	CMB0339_SDA_2_P12	Instrument / Ser#	micrOTOF	213750.00232
Comment				

Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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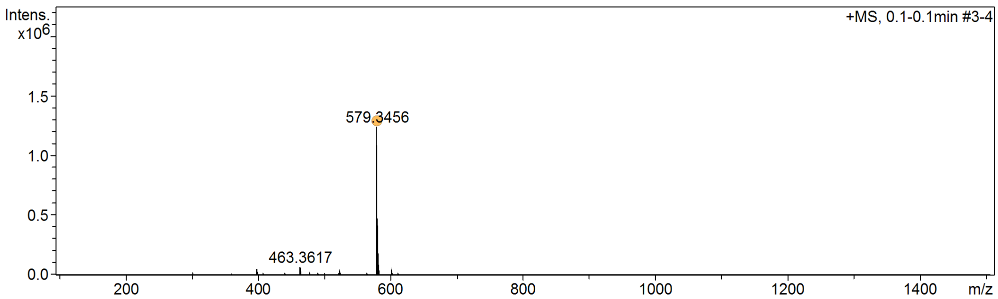
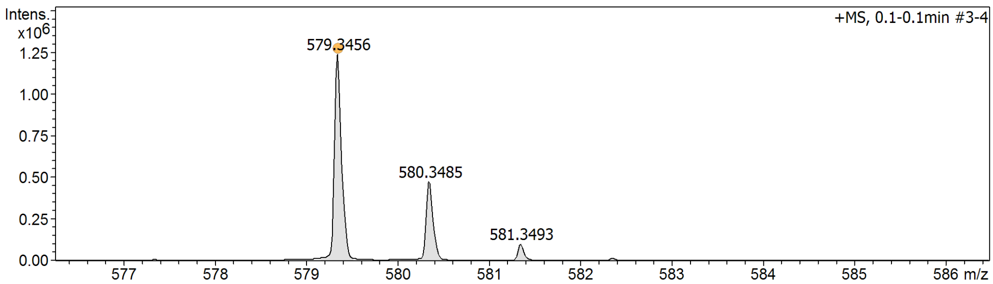
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.		
Formula, max.		
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
579.3456	1	C33H47N4O5	579.3541	-14.6	1.8	1	0.01	12.5	even	ok
	2	C34H47N2O6	579.3429	-4.8	2.0	2	41.79	12.5	even	ok
	3	C31H39N12	579.3415	-7.1	4.4	3	9.52	18.5	even	ok
	4	C34H43N8O	579.3554	-16.9	10.0	4	0.00	17.5	even	ok
	5	C30H43N8O4	579.3402	-9.4	11.9	5	1.34	13.5	even	ok
	6	C35H43N6O2	579.3442	2.5	12.1	6	100.00	17.5	even	ok
	7	C32H51O9	579.3528	12.3	13.5	7	0.08	7.5	even	ok
	8	C29H43N10O3	579.3514	10.0	14.4	8	0.80	13.5	even	ok

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Figure S16. HRMS spectrum of noonindole A (**5**)

5 Noonindole B (6)

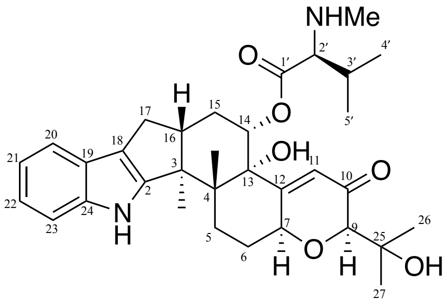

Table S3. 1D and 2D NMR (methanol-d_4, 600 MHz) data for noonindole B (**6**)

Pos.	δ_H, mult. (*J* in Hz)	δ_C	COSY	^1H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	152.3	-	-	-
3	-	51.9	-	-	-
4	-	46.2	-	-	-
5	*a* 2.88 (ddd, 1H, J = *13.5, 13.5, 5.1* Hz)	28.0	5*b*, 6*a*, 6*b*	3, 4, 6, 13, 4-Me	3-Me
	b 1.83 (br dd, 1H, J = *13.5, 5.1* Hz)		5*a*, 6*a*, 6*b*	4, 6, 7, 13, 4-Me	-
6	*a* 2.39 (m, 1H)	30.5	5*a*, 6*b*, 7	5, 7, 4, 12	-
	b 1.93 (m, 1H)		5*a*, 5*b*, 6*a*, 7	4, 5, 7	
7	4.90 (m, 1H)	74.8	6, 9, 11	6, 11, 12	-
9	3.72 (d, 1H, J = *1.5* Hz)	83.9	7	7, 25, 26, 27	26, 27
10	-	198.1	-	-	-
11	5.57 (d, 1H, J = *1.5* Hz)	122.0	7	7, 9, 13	-
12	-	165.8	-	-	-
13	-	80.0	-	-	-
14	5.50 (dd, 1H, J = *10.4, 5*.0 Hz)	77.3	15*a*, 15*b*	15, 1′	16, 4-Me
15	*a* 2.25 (dd, 1H, J = *13.0, 10.4* Hz)	28.3	14, 15*b*, 16	3, 13, 14, 16	3-Me
	b 2.17 (m, 1H)		14, 15*a*, 16	3, 13, 14, 16	-
16	2.98 (m, 1H)	47.5	15*a*, 17*a*, 17*b*	14, 17, 3-Me, 3	14, 4-Me
17	*a* 2.74 (dd, 1H, J = *13.1, 6.3* Hz)	27.6	16, 17*b*	2, 3, 16, 18	3-Me
	b 2.47 (dd, 1H, J = *13.1, 11.1* Hz)		16, 17*a*	2, 15, 16, 18	-
18	-	117.3	-	-	-
19	-	126.0	-	-	-
20	7.30 (d, 1H, J = *7.9* Hz)	118.8	21	18, 22, 24	-
21	6.93 (br dd, 1H, J = *7.9,7.7* Hz)	119.9	20, 22	19, 23	-
22	6.97 (ddd, 1H, J = *7.9,7.9, 0.9* Hz)	121.1	21, 23	20, 24	-
23	7.28 (d, 1H, J = *7.9* Hz)	112.7	22	19, 21	-
24	-	141.9	-	-	-
25	-	73.0	-		-
26	1.28 (s, 3H)	25.3	-	9, 25, 27	9
27	1.26 (s, 3H)	26.4	-	9, 25, 26	9
1′	-	168.9	-	-	-
2′	3.90 (br s, 1H)	68.7	3′	-	-
3′	2.31 (m, 1H)	30.7	2′, 4′, 5′	-	-
4′	1.09 (br d, 1H, J = *5.3* Hz)	18.7	3′	2′, 3′, 5′	-
5′	0.99 (d, 1H, J = *7.0* Hz)	17.7	3′	2′, 3′, 4′	-
3-Me	1.37 (s, 3H)	16.6	-	2, 3, 4, 16	5*a*, 15*a*, 17*a*
4-Me	1.10 (s, 3H)	19.5	-	3, 4, 5, 13	16, 14
NMe	2.72 (s, 3H)	33.8	-	2′	-

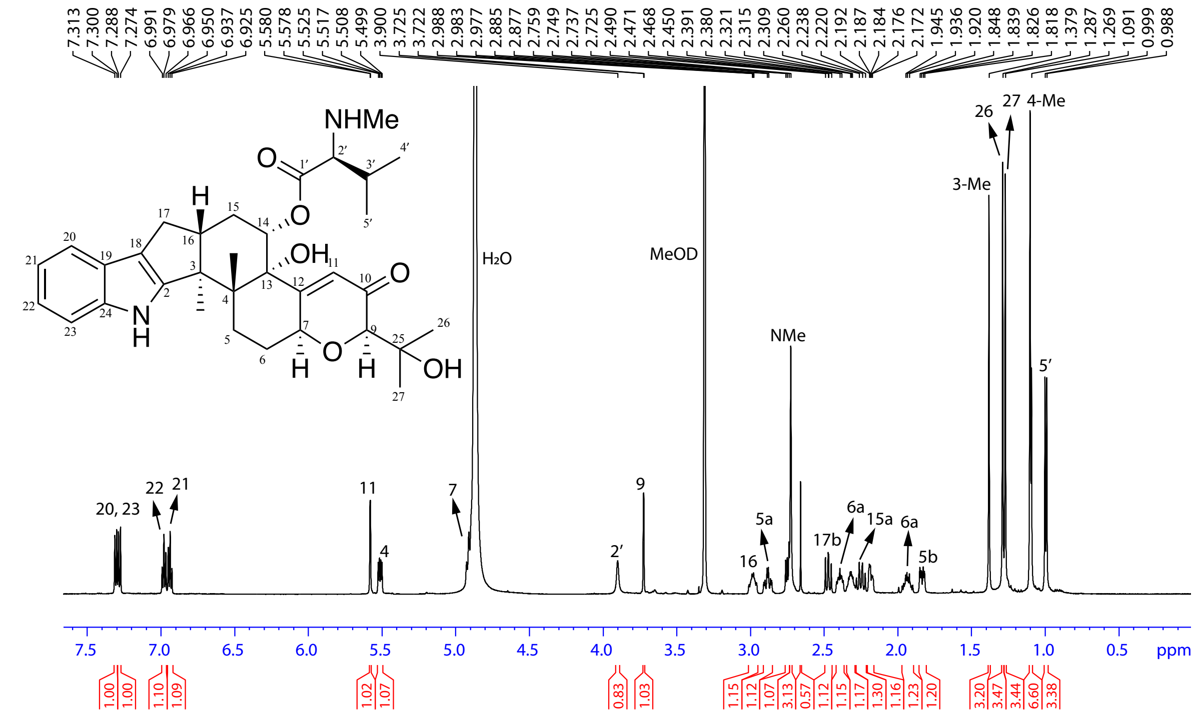

Figure S17.[1]H NMR (600 MHz, methanol-d_4) spectrum of noonindole B (**6**)

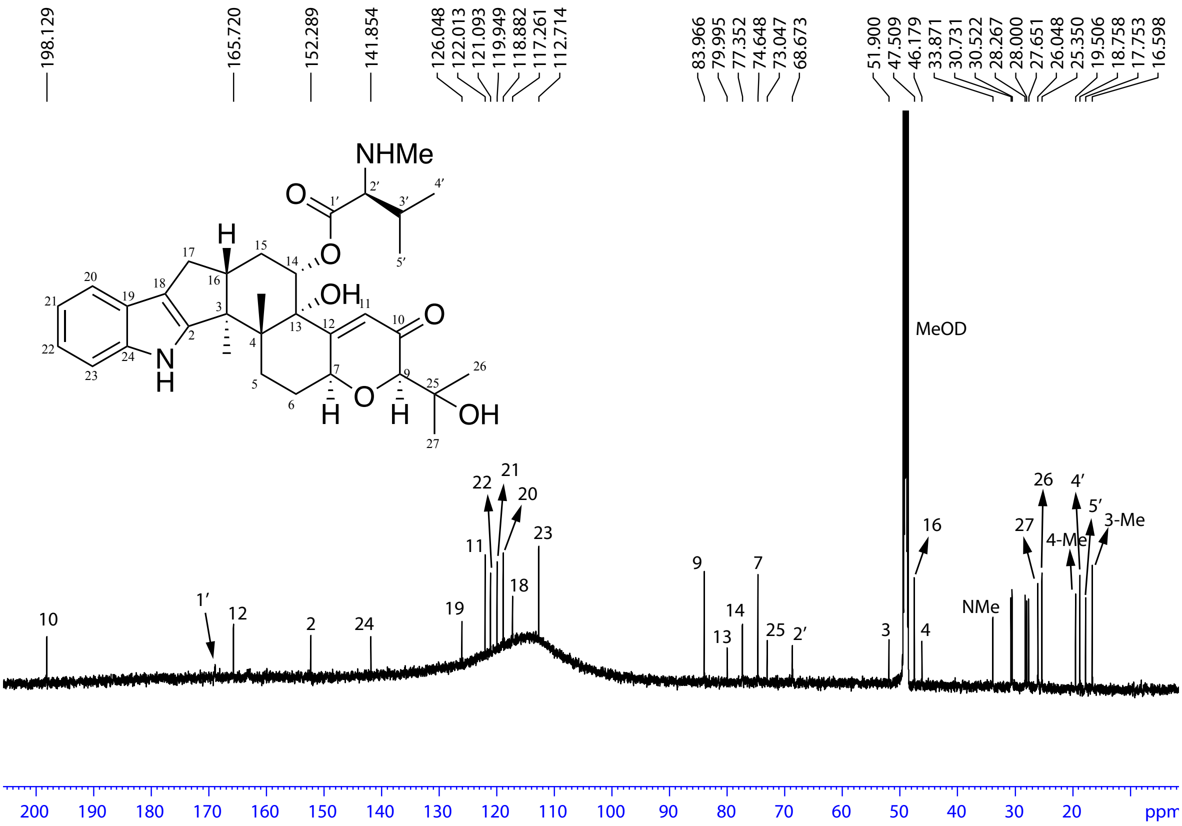

Figure S18. [13]C NMR (150 MHz, methanol-d_4) spectrum of noonindole B (**6**)

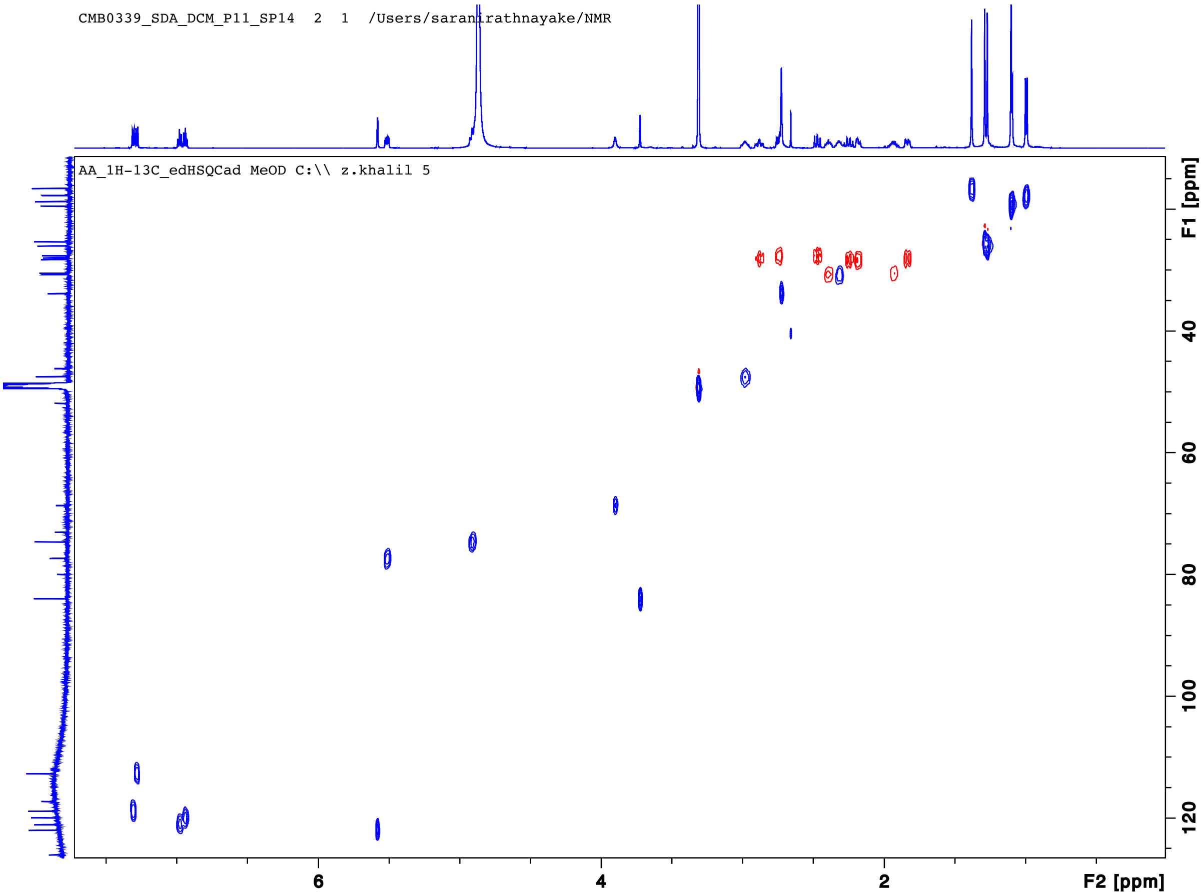

Figure S19. HSQC (methanol-d_4) spectrum of noonindole B (**6**)

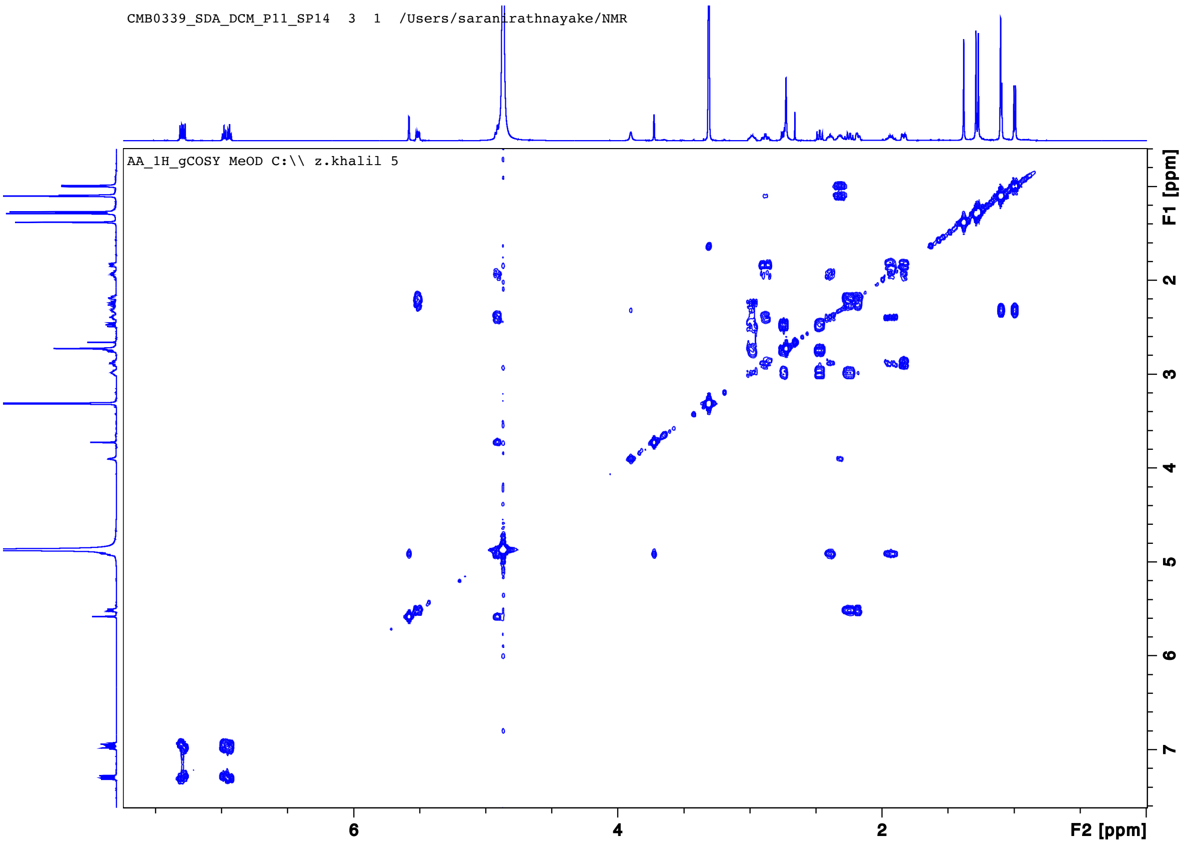

Figure S20. COSY (methanol-d_4) spectrum of noonindole B (**6**)

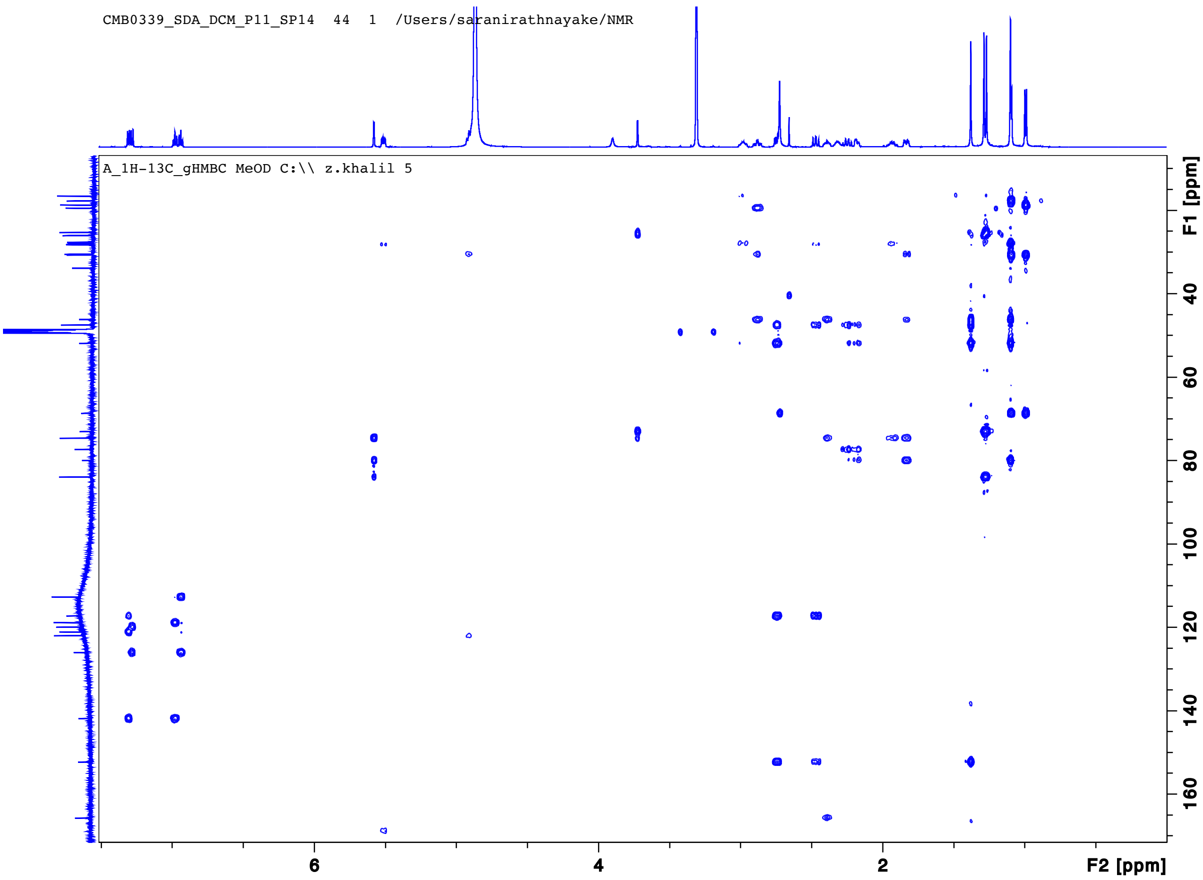

Figure S21. HMBC (methanol-d_4) spectrum of noonindole B (**6**)

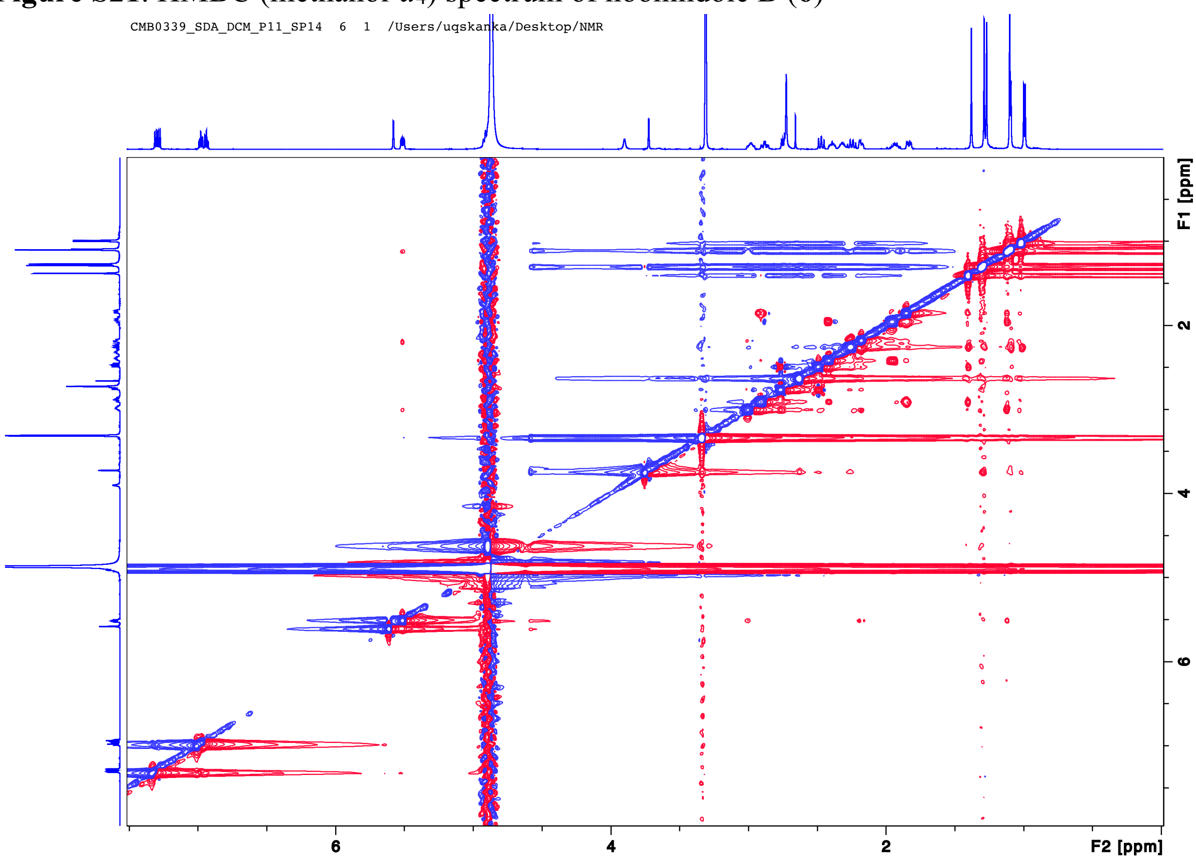

Figure S22. ROESY (methanol-d_4) spectrum of noonindole B (**6**)

Mass Spectrum Molecular Formula Report

Analysis Info

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Method	tune-med_AP.m	Operator	a.salim
Sample Name	CMB0339_SDA_P11_SP14_E	Instrument / Ser#	micrOTOF 213750.00232
Comment			

Acquisition Parameter

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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.		
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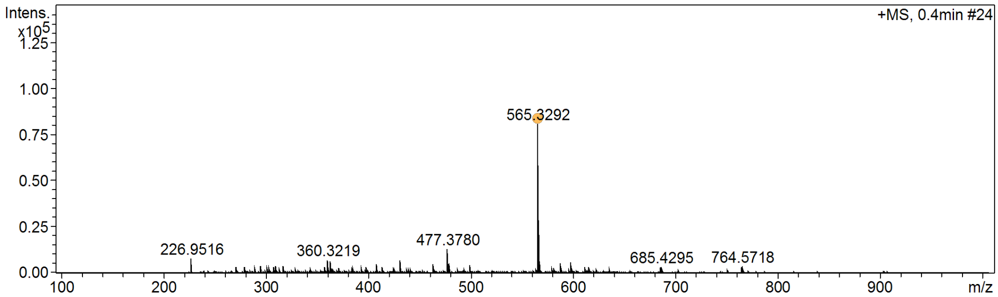

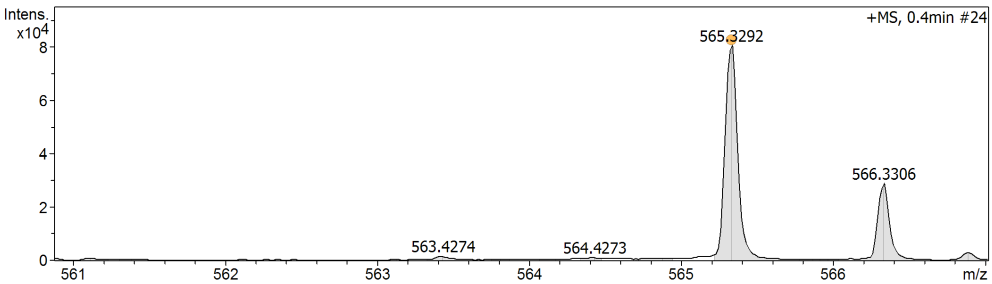

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
565.3292	1	C33H45N2O6	565.3272	3.5	7.0	1	53.94	12.5	even	ok
	2	C34H41N6O2	565.3286	1.1	18.5	2	100.00	17.5	even	ok
	3	C38H45O4	565.3312	3.6	30.9	3	30.65	16.5	even	ok

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Figure S23. HRMS spectrum of noonindole B (**6**)

6 Noonindole C (7)

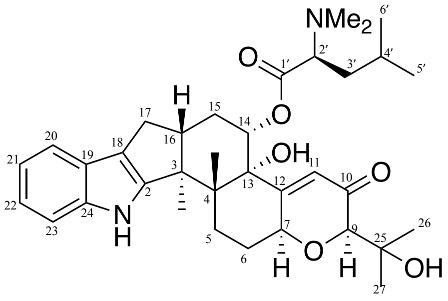


Table S4.1D and 2D NMR (in methanol-d_4, 600 MHz) data for noonindole C (**7**)

Pos.	$\delta_{H,}$ mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	152.2	-	-	-
3	-	51.8	-	-	-
4	-	46.2	-	-	-
5	*a* 2.87 (ddd, 1H, J = *13.8, 13.8, 5.4* Hz)	27.9	5*b*, 6*a*, 6*b*	4, 6, 4-Me	-
	b 1.84 (br dd, 1H, J = *13.8, 5.4* Hz)		5*a*, 6*a*, 6*b*	4, 6, 7, 4-Me, 13	-
6	*a* 2.39 (m, 1H)	30.5	5*a*, 6*b*, 7	7, 4, 12	-
	b 1.93 (m, 1H)		5*a*, 6*a*, 6*b*, 7	4, 5, 7	-
7	4.92 (br t, 1H, J = *8.5* Hz)	74.8	6, 9, 11	6, 11	9
9	3.71 (br s, 1H)	84.0	7	7, 25, 26	7
10	-	197.9	-	-	-
11	5.57 (d, 1H, J = *1.9* Hz)	121.8	7	7, 9, 13	-
12	-	165.0	-	-	-
13	-	80.1	-	-	-
14	5.51 (dd, 1H, J =*10.4, 5.1* Hz)	77.5	15*a*, 15*b*	1′	4-Me, 16
15	*a* 2.25 (dd, 1H, J = *13.2, 10.4* Hz)	28.1	14, 15*b*, 16	3, 14, 16	3-Me
	b 2.20 (m, 1H)		14, 15*a*, 16	3, 14, 13, 16	-
16	2.97 (m, 1H)	47.5	15, 17*b*	15	4-Me, 14
17	*a* 2.74 (dd, 1H, J = *13.0, 6.3* Hz)	27.6	16, 17*b*	2, 3, 16, 18	3-Me
	b 2.47 (dd, 1H, J = *13.0, 10.8* Hz)		16, 17*a*	2, 16, 18	-
18	-	117.2	-	-	-
19	-	126.1	-	-	-
20	7.30 (d, 1H, J = *7.8* Hz)	118.9	21	18, 22, 24	-
21	6.93 (ddd, 1H, J = *7.8, 7.8, 1.1* Hz)	119.9	20, 22	19, 23	-
22	6.98 (ddd, 1H, J = *7.8, 7.8, 1.1* Hz)	121.1	21, 23	20, 24	-
23	7.28 (d, 1H, J = *7.8* Hz)	112.7	22	19, 21	-
24	-	141.9	-	-	-
25	-	73.0	-		-
26	1.30 (s, 3H)	25.5	-	9, 25, 27	-
27	1.27 (s, 3H)	25.8	-	9, 25, 26	-
1′	-	168.9	-	-	-
2′	4.02 (m, 1H)	67.5	3′	-	6′
3′	*a* 1.90 (m, 1H)	37.4	2′, 3′ *b*, 4′	4′	5′
	b 1.69, (m, 1H)		2′, 3′ *a*, 4′	-	5′, 6′, NMe_2
4′	1.56 (m, 1H)	26.2	3′, 5′, 6′	-	-
5′	0.97 (d, 3H, J = *6.4* Hz)	23.4	4′	3′, 4′, 6′	3′ b, 3′ *a*
6′	0.91 (d, 3H, J = *6.4* Hz)	21.4	4′	3′, 4′, 5′	2′, 3′ b
3-Me	1.38 (s, 3H)	16.6	-	2, 3, 4, 16	17*a*, 15*a*
4-Me	1.09 (br s, 3H)	19.4	-	3, 4, 5, 13	14, 16
NMe_2	2.93 (s, 6H)	42.1	-	2′, NMe_2	3′ *b*

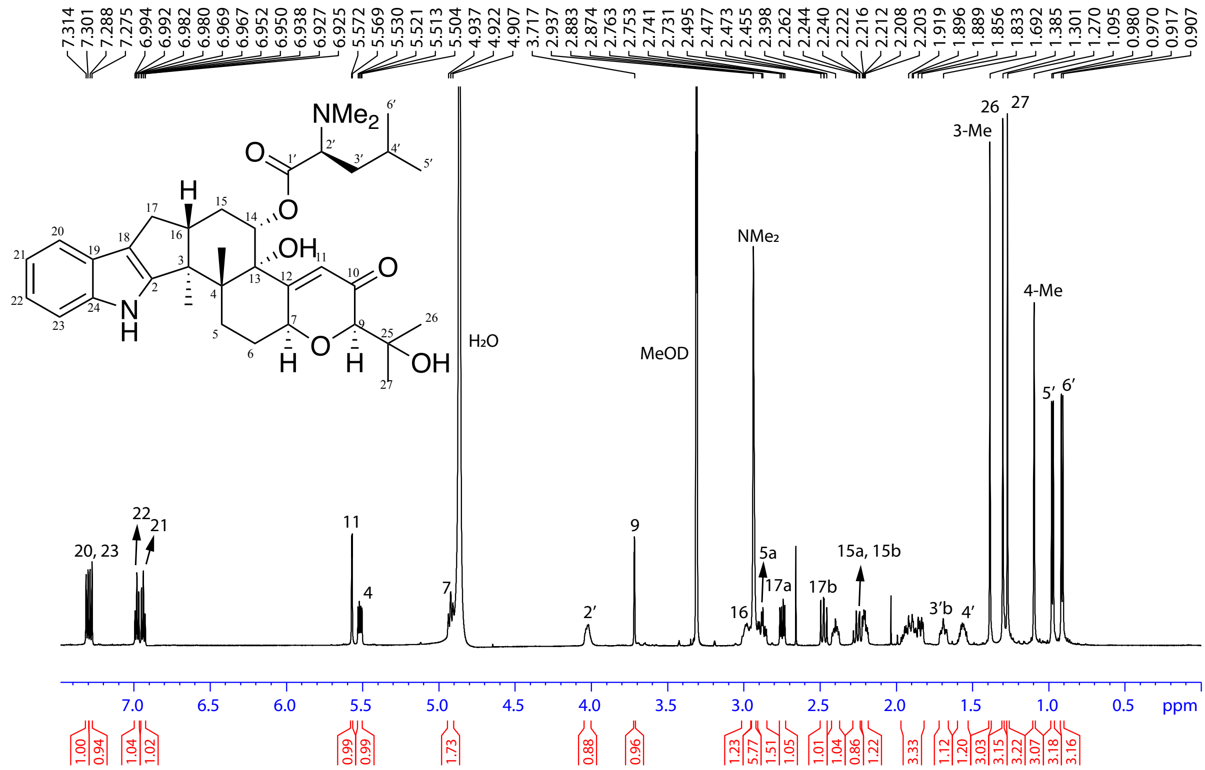


Figure S24. [1]H NMR (600 MHz, methanol-d_4) spectrum of noonindole C (**7**)

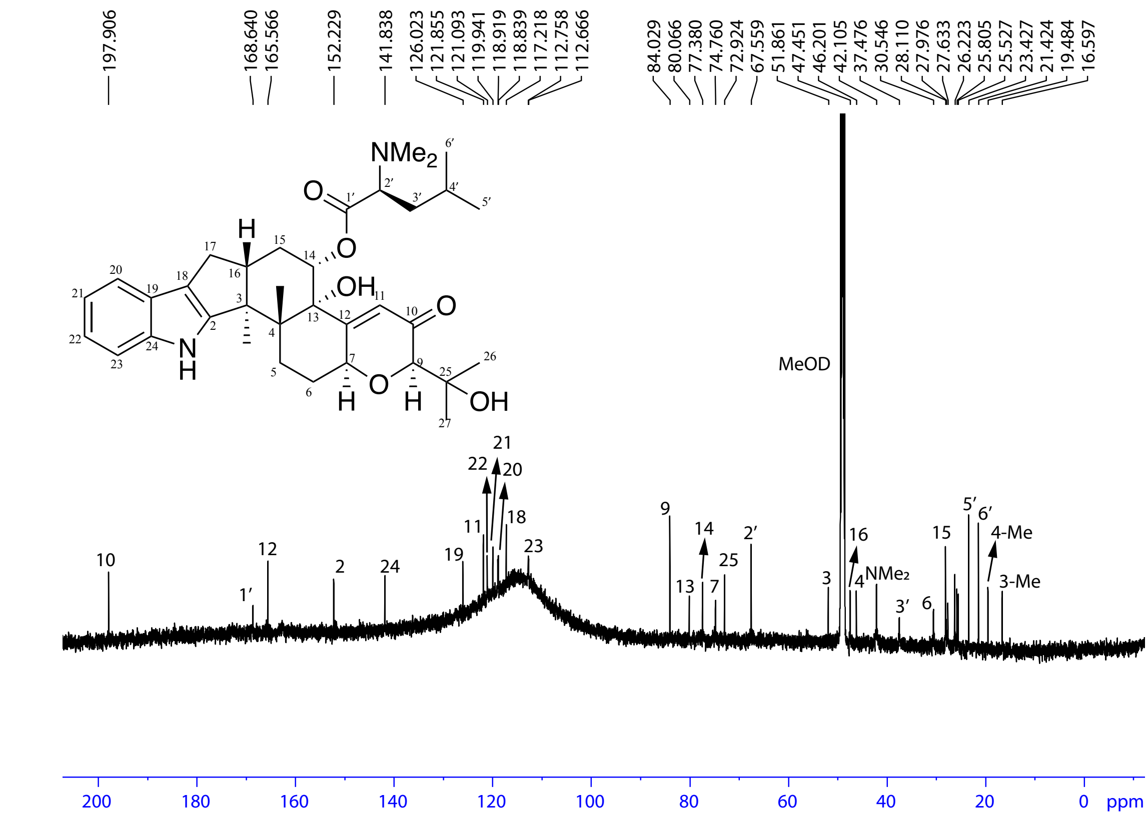


Figure S25. [13]C NMR (150 MHz, methanol-d_4) spectrum of noonindole C (**7**)

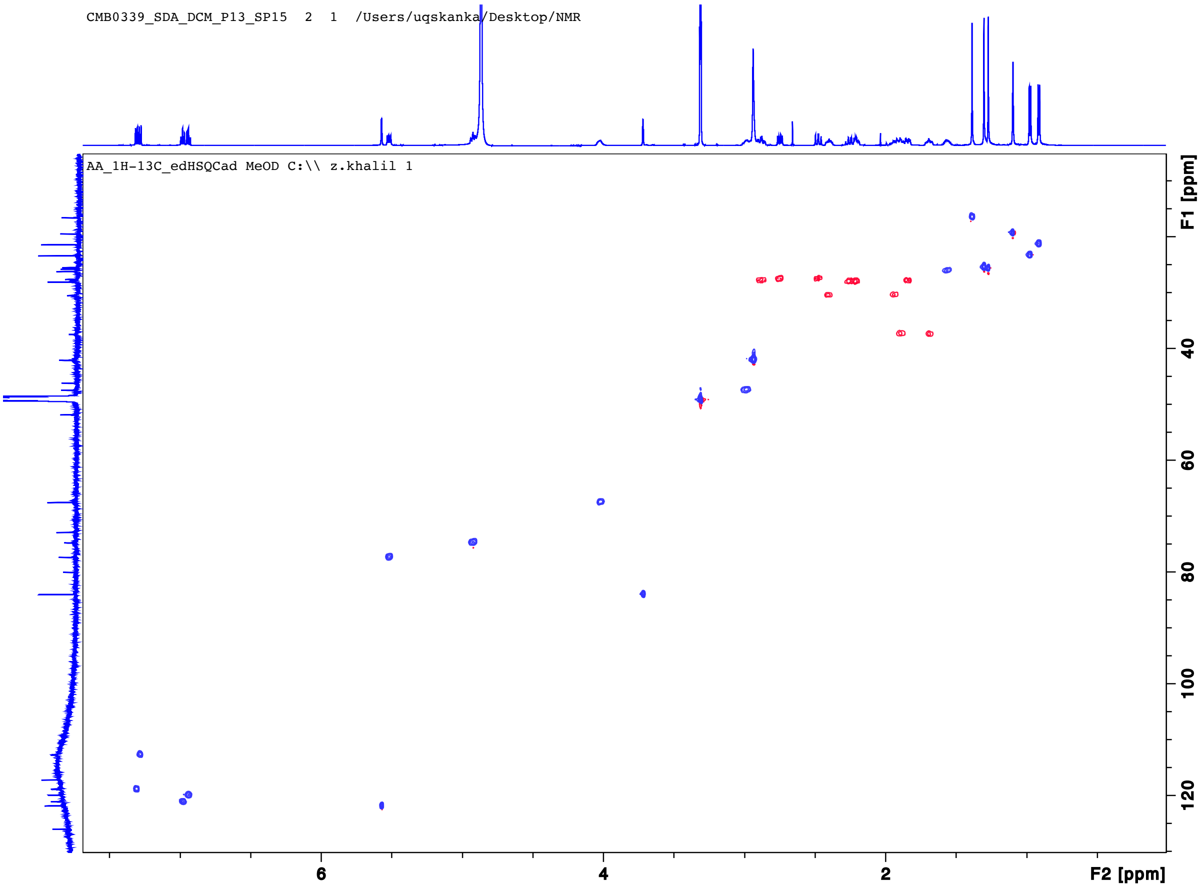


Figure S26. HSQC (methanol-d_4) spectrum of noonindole C (**7**)

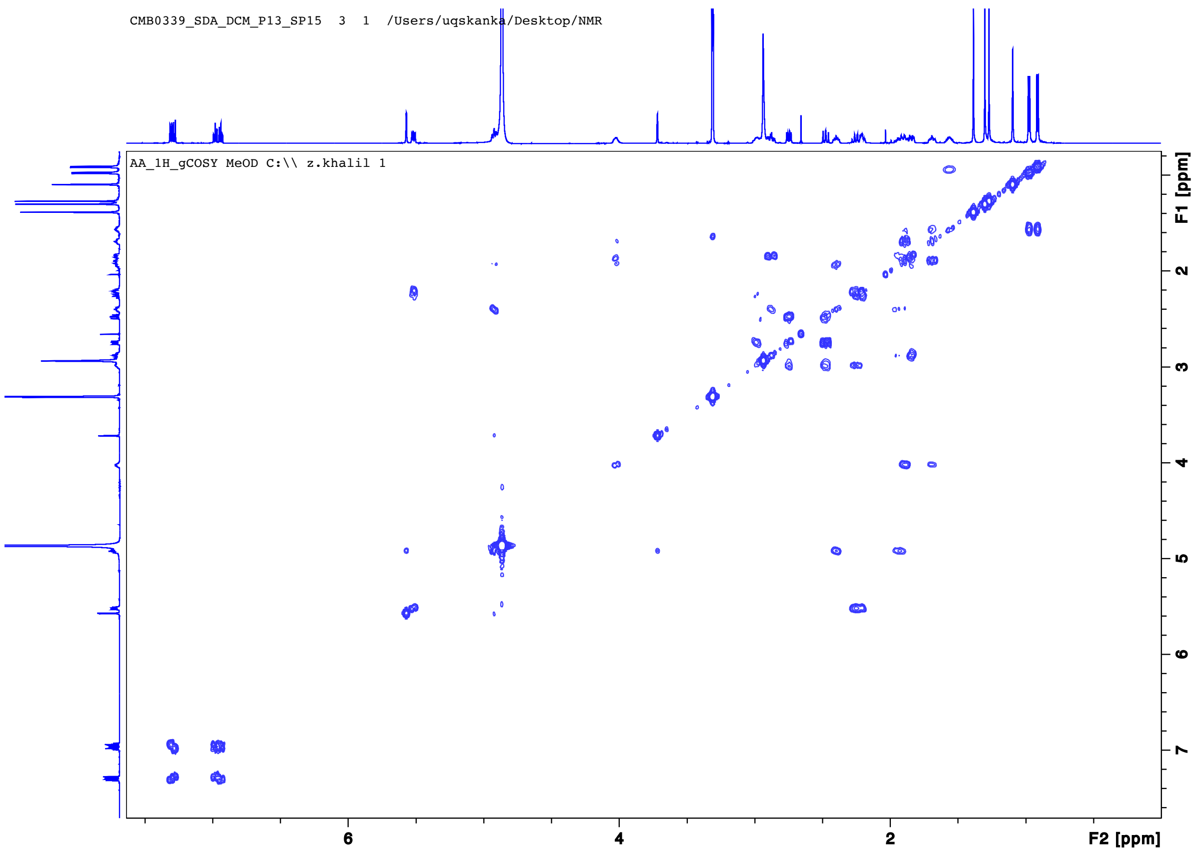


Figure S27. COSY (methanol-d_4) spectrum of noonindole C (**7**)

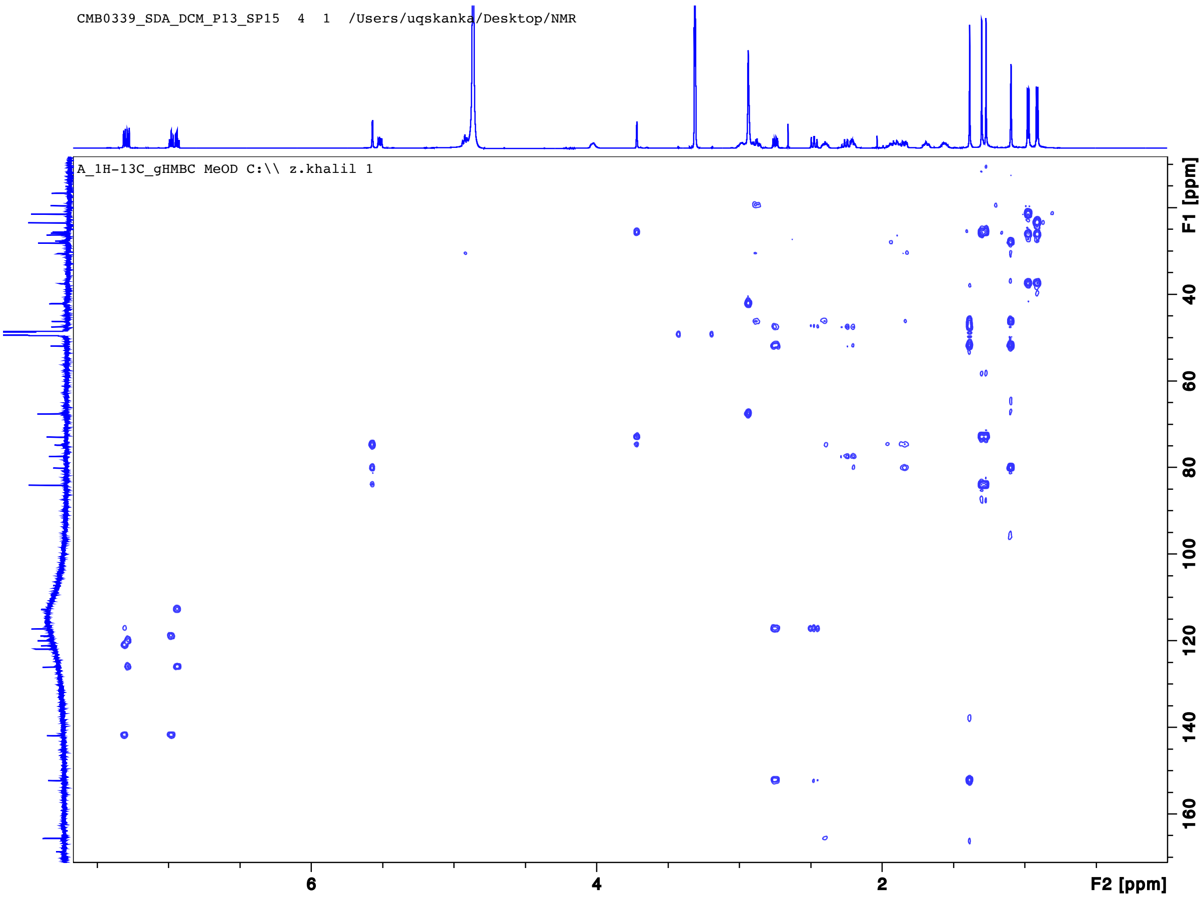


Figure S28. HMBC (methanol-d_4) spectrum of noonindole C (**7**)

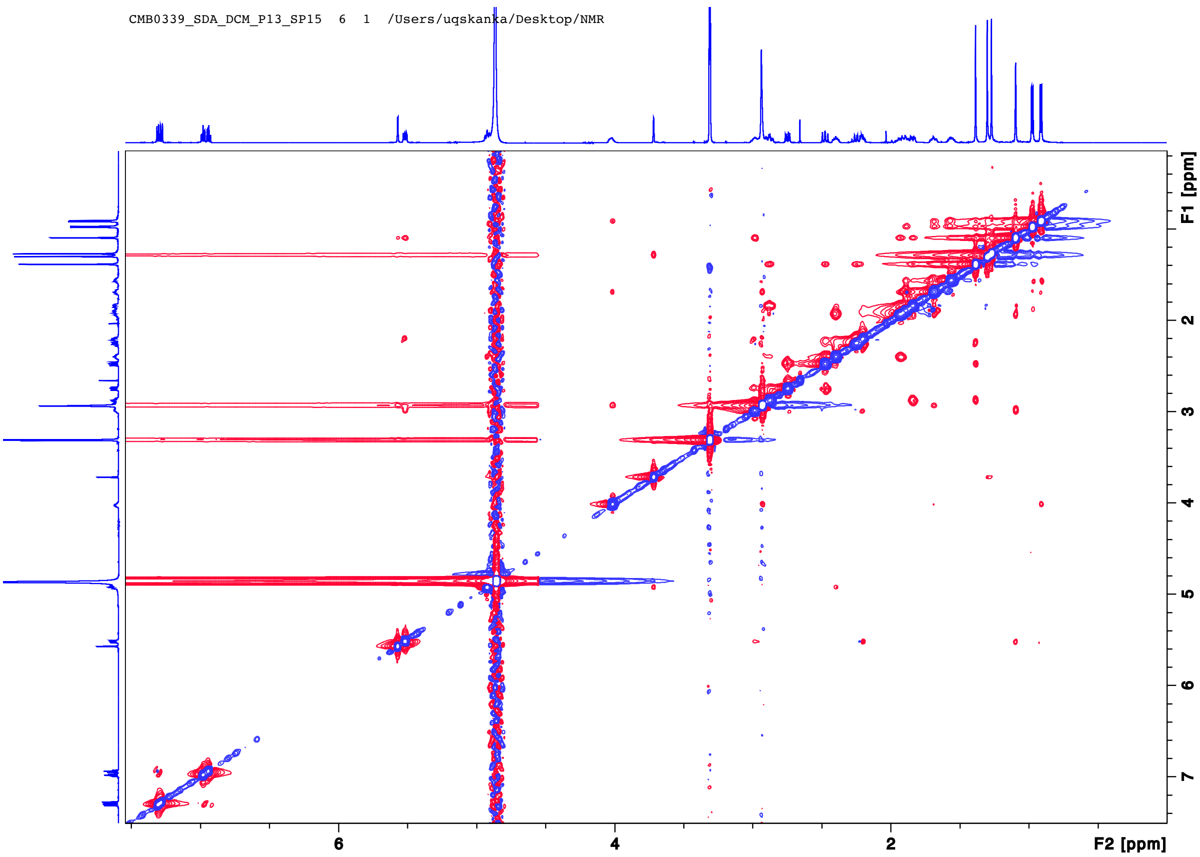


Figure S29. ROESY (methanol-d_4) spectrum of noonindole C (**7**)

Mass Spectrum Molecular Formula Report

Analysis Info

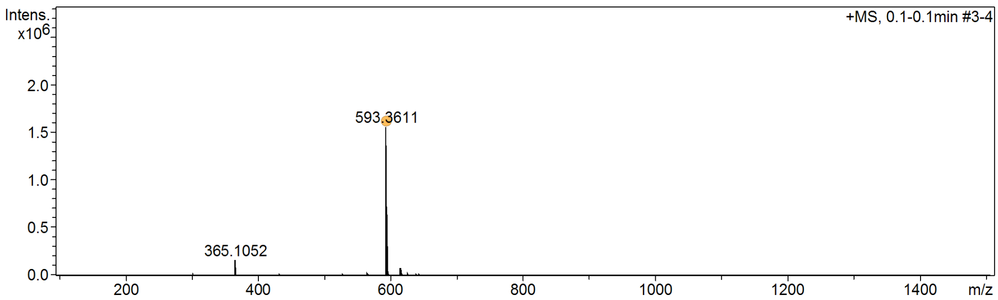
Analysis Name	D:\Data\s.kankanamge\CMB0339_SDA_DCM_P13_SP15_2.d	Acquisition Date	10/27/2020 3:48:30 PM
Method	tune-medhigh_AP.m	Operator	a.salim
Sample Name	CMB0339_SDA_DCM_P13_SP15_2	Instrument / Ser#	micrOTOF 213750.00232
Comment			

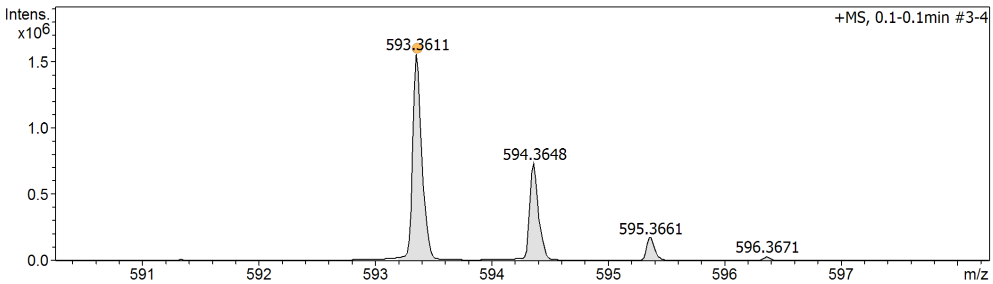
Acquisition Parameter

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
593.3611	1	C41H45N4	593.3639	-4.6	2.7	1	43.33	21.5	even	ok
	2	C40H49O4	593.3625	2.4	14.0	2	100.00	16.5	even	ok
	3	C36H45N6O2	593.3599	-2.2	26.8	3	82.09	17.5	even	ok
	4	C35H49N2O6	593.3585	-4.4	38.1	4	22.59	12.5	even	ok
	5	C32H41N12	593.3572	-6.7	39.9	5	5.36	18.5	even	ok
	6	C31H45N8O4	593.3558	-8.9	50.8	6	0.66	13.5	even	ok
	7	C33H53O9	593.3684	12.3	51.9	7	0.02	7.5	even	ok
	8	C30H45N10O3	593.3671	10.0	53.3	8	0.23	13.5	even	ok

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Figure S30. HRMS spectrum of noonindole C (**7**)

7 Noonindole D (8)

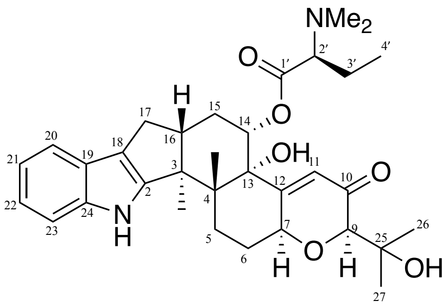


Table S5. 1D and 2D NMR (methanol-d_4, 600 MHz) data for noonindole D (**8**)

Pos.	δ_H, mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	151.1	-	-	-
3	-	50.5	-	-	-
4	-	44.6	-	-	-
5	*a* 2.87[a] (m, 1H)	28.0	-	-	-
	b 1.80, (m, 1H)	28.0	5*a*[a], 6*b*	-	-
6	*a* 2.37 (m, 1H)	30.4	5*a*[a], 6*b*, 7	-	-
	b 1.91 (m, 1H)	30.4	5*b*, 6*a*	-	-
7	4.90 (m, 1H)	74.6	6*a*, 6*b*, 9, 11	-	-
9	3.71 (d, 1H, J = *1.9* Hz)	83.7	7	25	27
10	-	nd	-	-	-
11	5.58 (d, 1H, J = *1.9* Hz)	121.7	7	7, 9, 13	14
12	-	nd	-	-	-
13	-	78.9	-	-	-
14	5.37 (dd, 1H, J = *10.6, 5.1* Hz)	74.4	15*a*, 15*b*	-	11, 16, 4-Me
15	*a* 2.16 (m, 1H)	28.4	14, 15*b*, 16	-	-
	b 2.04 (ddd, 1H, J = *7.1, 5.1, 2.3* Hz)	28.4	15*a*, 14, 16	-	-
16	2.95 (m, 1H)	47.0	15*a*, 17*a*, 17*b*	-	14, 4-Me
17	*a* 2.72 (dd, 1H, J = *13.1, 6.4* Hz)	27.5	16, 17*b*	2, 3, 18	-
	b 2.45 (dd, 1H, J = *13.1, 10.7* Hz)	27.5	17*a*, 16	18	-
18	-	116.8	-	-	-
19	-	124.7	-	-	-
20	7.30 (d, 1H, J = *7.7* Hz)	118.6	21	18, 22, 24	-
21	6.92 (ddd, 1H, J = *7.7, 7.3, 0.9* Hz)	119.6	20, 22	19, 23	-
22	6.97 (ddd, 1H, J = *8.1, 7.3, 0.9* Hz)	120.7	21, 23	20, 24	-
23	7.27 (d, 1H, J = *8.1* Hz)	112.4	22	19, 21	-
24	-	140.4	-	-	-
25	-	71.6	-	-	-
26	1.28 (s, 3H)	25.1	-	9, 25, 27	-
27	1.26 (s, 3H)	25.9	-	9, 25, 26	9
1′	-	nd	-	-	-
2′	2.87[a] (m, 1H)	72.9	-	-	-
3′	*a* 1.77 (m, 1H)	23.8	2′[a], 4′	-	-
	b 1.69 (m, 1H)		2′[a], 4′	-	-
4′	0.91 (t, 1H, J = *7.4* Hz)	10.1	3′*a*, 3′*b*	2′, 3′	-
3-Me	1.37 (s, 3H)	16.3	-	2, 3, 4, 16	-
4-Me	1.08 (s, 3H)	19.4	-	3, 4, 5, 13	14, 16
NMe_2	2.26 (s, 6H)	43.4	-	2′, NMe_2	-

[nd] not detected

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

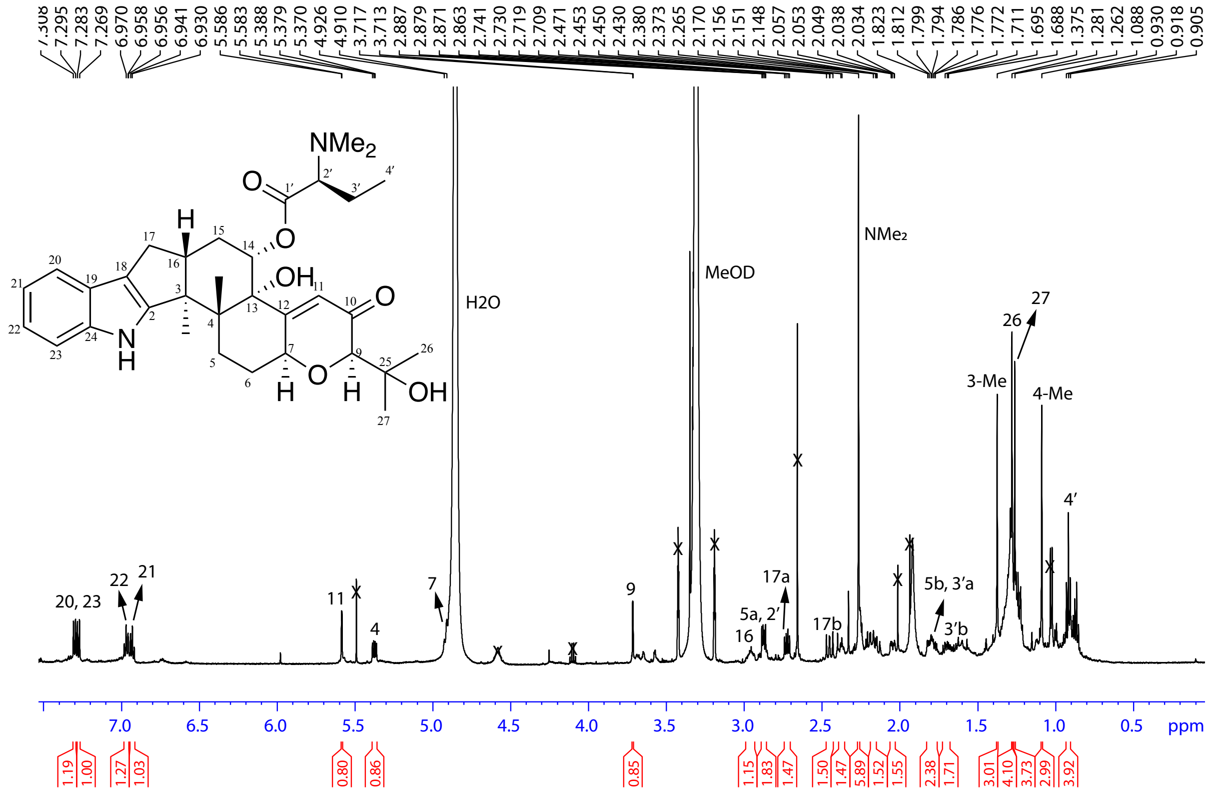


Figure S31. ^{1}H NMR (methanol-d_4) spectrum of noonindole D (**8**)

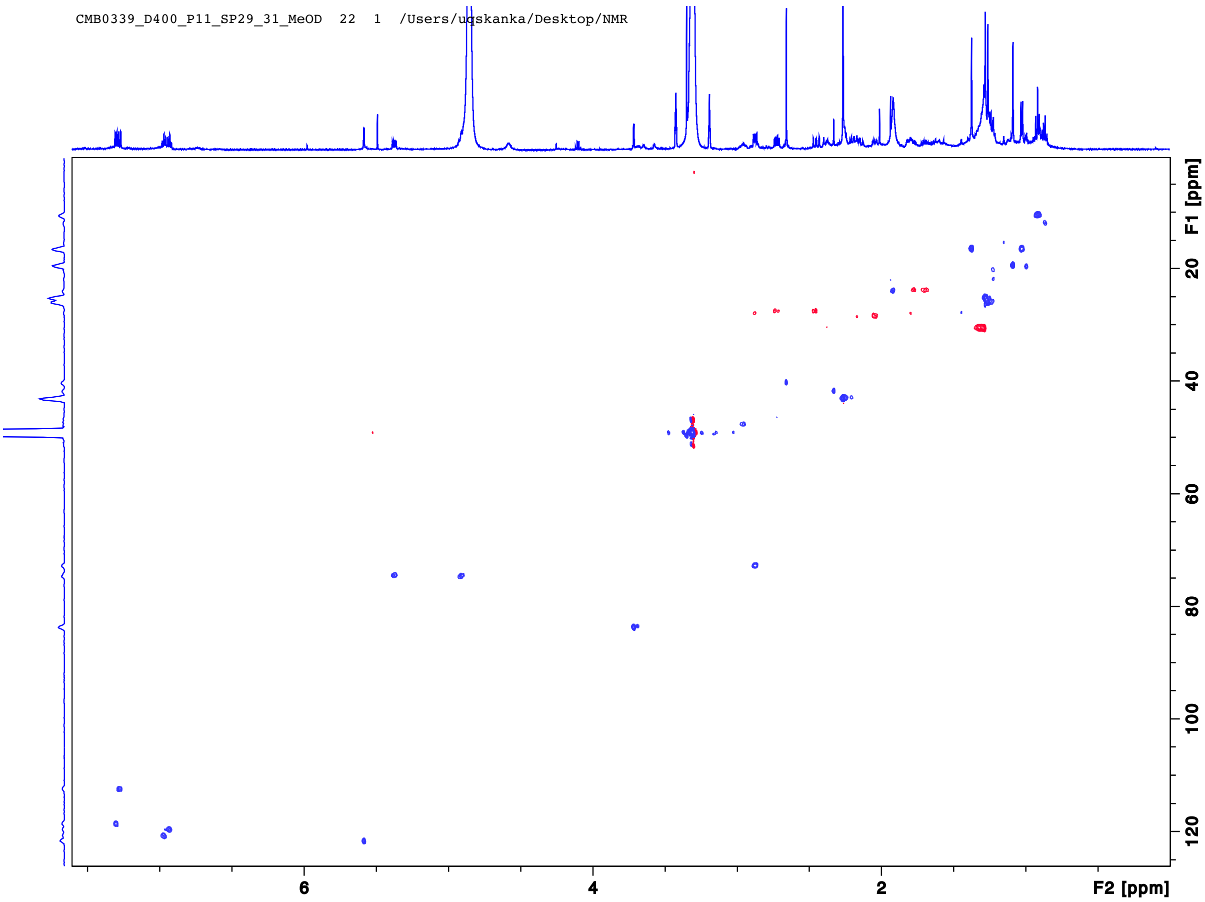


Figure S32. HSQC (methanol-d_4) spectrum of noonindole D (**8**)

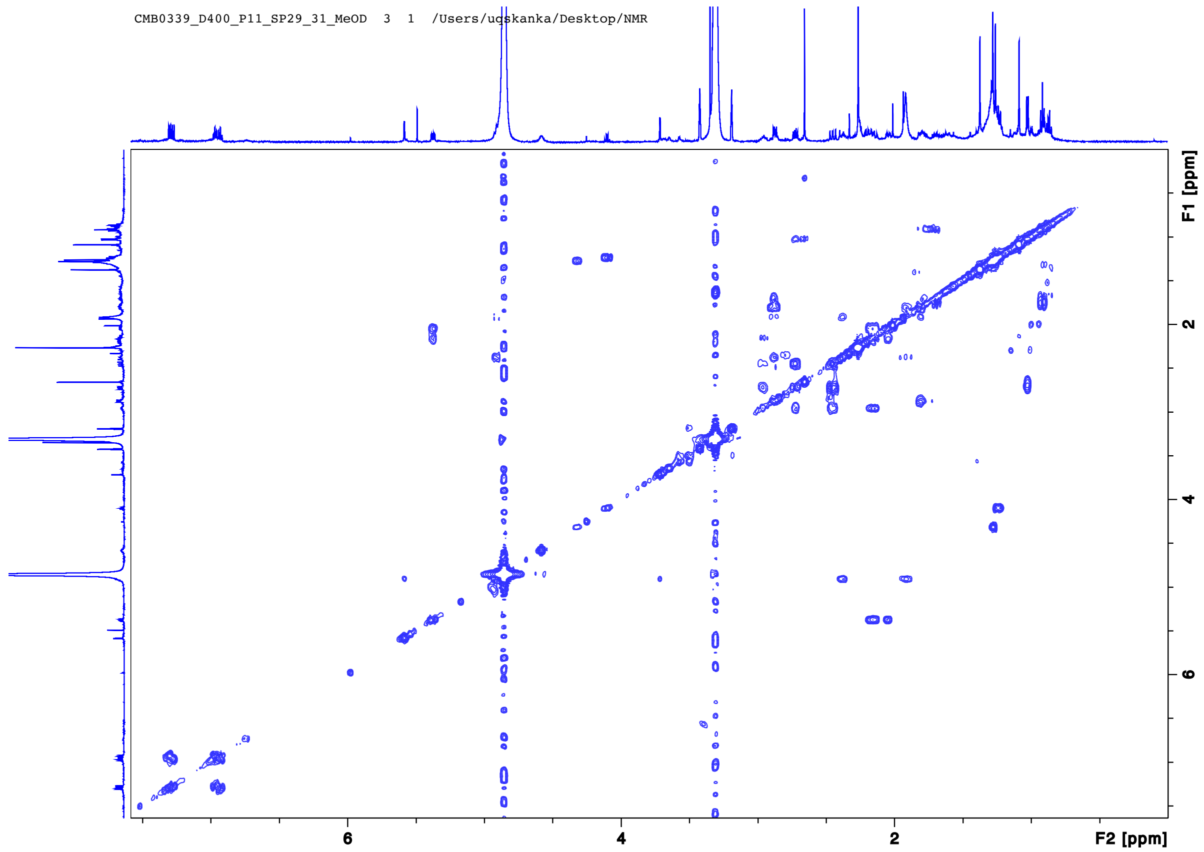


Figure S33. COSY (methanol-d_4) spectrum of noonindole D (**8**)

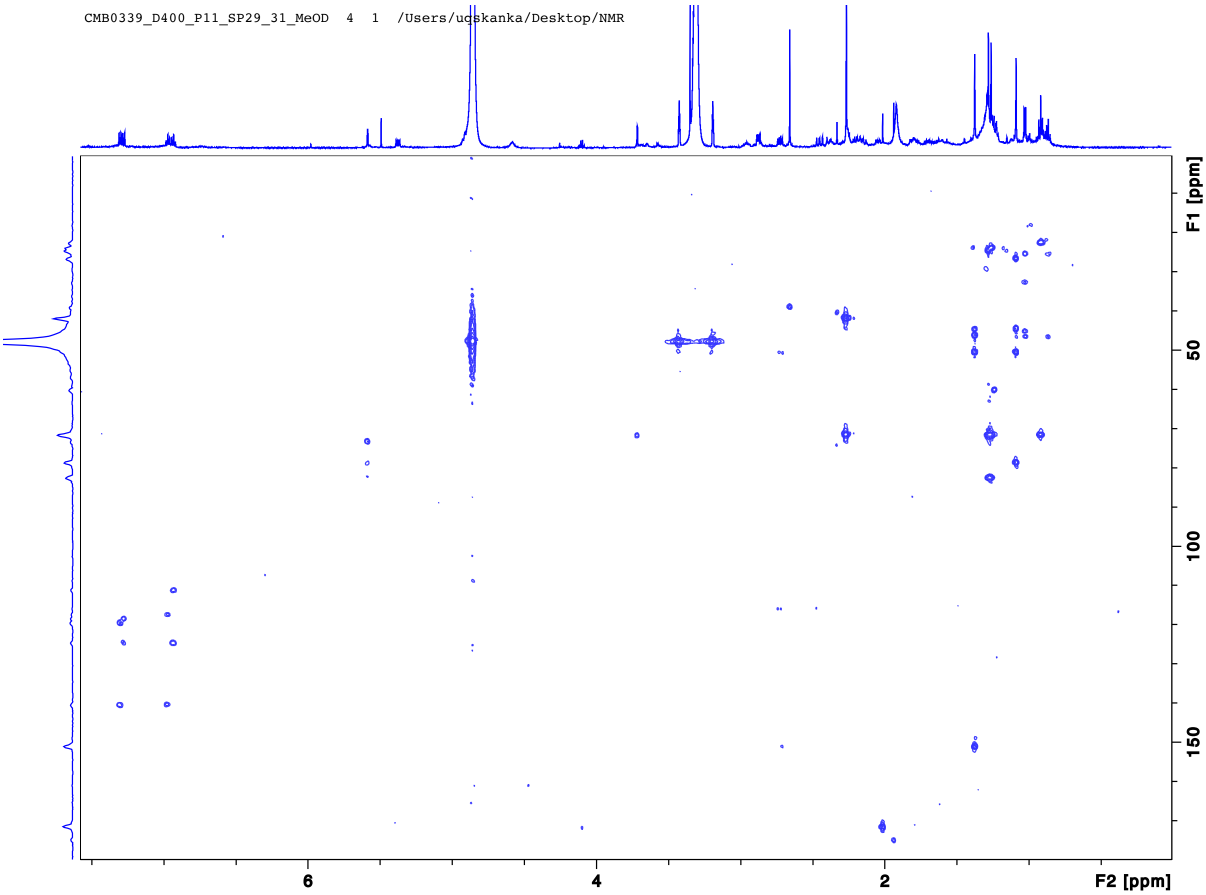


Figure S34. HMBC (methanol-d_4) spectrum of noonindole D (**8**)

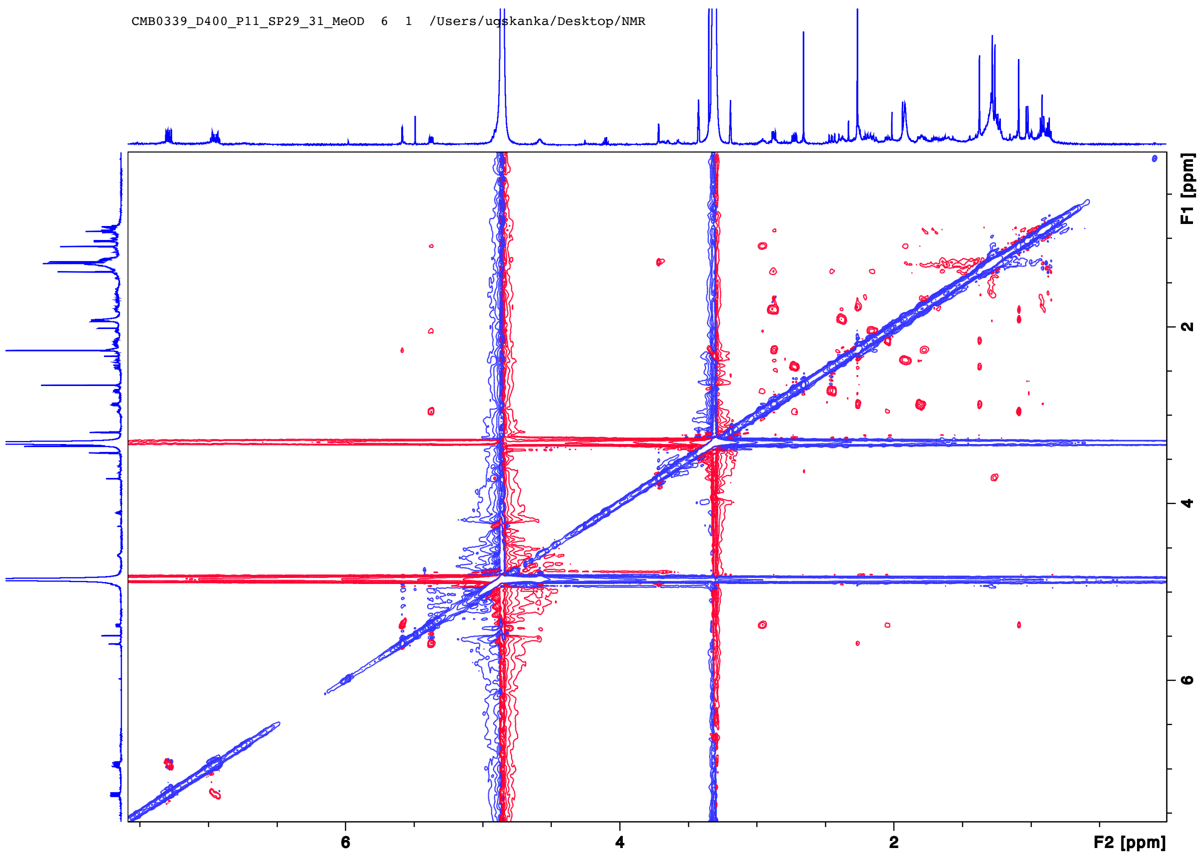


Figure S35. ROESY (methanol-d_4) spectrum of noonindole D (**8**)

Mass Spectrum Molecular Formula Report

Analysis Info

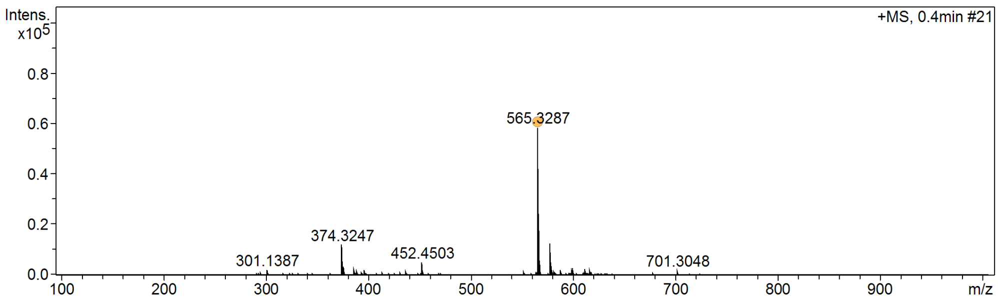
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_P11_SP29_31_again.d	Acquisition Date	11/2/2021 1:56:53 PM
Method	tune-med_AP.m	Operator	a.salim
Sample Name	CMB0339_D400_P11_SP29_31_again	Instrument / Ser#	micrOTOF 213750.00232
Comment			

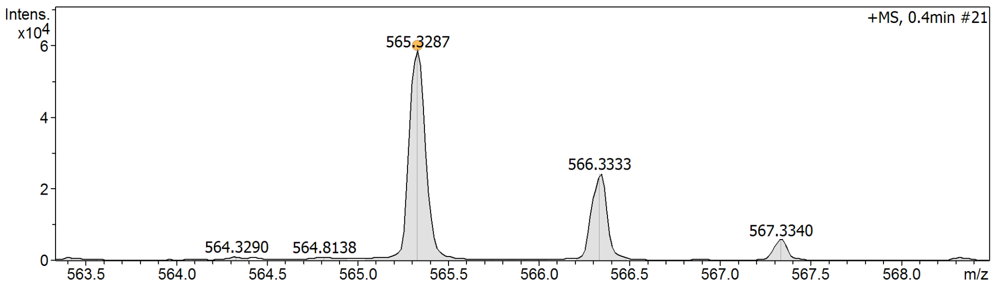
Acquisition Parameter

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
565.3287	1	C38H45O4	565.3312	-4.5	3.7	1	25.45	16.5	even	ok
	2	C39H41N4	565.3326	-6.9	13.5	2	5.45	21.5	even	ok
	3	C34H41N6O2	565.3286	-0.2	13.9	3	100.00	17.5	even	ok
	4	C33H45N2O6	565.3272	-2.6	23.7	4	39.72	12.5	even	ok
	5	C30H37N12	565.3259	-5.0	26.6	5	12.80	18.5	even	ok

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Figure S36. HRMS spectrum of noonindole D (**8**)

8 Noonindole E (9)

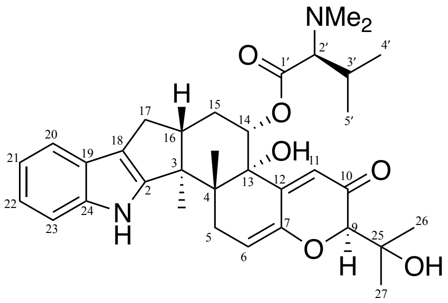


Table S6. 1D and 2D NMR (methanol-d_4, 600 MHz) data for noonindole E (**9**)

Pos.	$\delta_{H,}$ mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	152.5	-	-	-
3	-	51.9	-	-	-
4	-	46.2	-	-	-
5	*a* 3.28*	33.0	5*b*, 6	6, 7, 4-Me	-
	b 2.36 (d, 1H, J = *6.3* Hz)		5*a*, 6	6, 7	-
6	5.74 (m, 1H)	113.5	5*a*, 5*b*	-	-
7	-	146.4	-	-	-
9	4.09 (s, 1H)	87.6	-	7, 26[a], 27[a], 10	26, 27
10	-	196.8	-	-	-
11	5.71 (br s, 1H)	119.5	-	7, 9, 13	14
12	-	nd	-	-	-
13	-	77.8	-	-	-
14	5.41 (dd, 1H, J = *9.8, 5.8* Hz)	75.5	15	-	11, 16, 4-Me
15	2.18 (m, 1H)	30.0	14, 16	3, 13, 16	-
16	2.90 (m, 1H)	47.5	15, 17*a*, 17*b*	-	14, 4-Me
17	*a* 2.72 (dd, 1H, J = *13.0, 6.5* Hz)	28.0	16, 17*b*	2, 3, 18	-
	b 2.44 (dd, 1H, J = *13.0, 10.8* Hz)		16, 17*a*	18	-
18	-	117.4	-	-	-
19	-	126.2	-	-	-
20	7.30 (d, 1H, J = *7.2* Hz)	119.1	21	18, 22, 24	-
21	6.93 (m, 1H)	120.0	20, 22	19, 23	-
22	6.97 (m, 1H)	121.2	21, 23	20, 24	-
23	7.27 (d, 1H, J = *7.5* Hz)	112.8	22	19, 21	-
24	-	142.1	-	-	-
25	-	75.6	-	-	-
26	1.33 (s, 3H)	27.1[a]	-	9, 25, 27[a]	9
27	1.26 (s, 3H)	27.1[a]	-	9, 25, 26[a]	9
1′	-	nd	-	-	-
2′	2.86 (d, 1H, J = *9.4* Hz)	76.0	3′	NMe_2	-
3′	2.11 (m, 1H)	28.7	2′, 4′/5′	-	-
4′/5′	0.97 (t, 6H, J = *7.4* Hz)	19.9	3′	2′, 3′, 4′/5′	-
3-Me	1.40 (s, 3H)	16.9	-	2, 3, 4, 16	-
4-Me	1.14 (s, 3H)	21.0	-	3, 4, 5, 13	14, 16
NMe_2	2.34 (s, 6H)	42.4	-	2′, NMe_2	-

[a] Resonances with the same superscript within a column are overlapping and assignments may be interchanged
*Obscured by residual MeOD signal
[nd] not detected

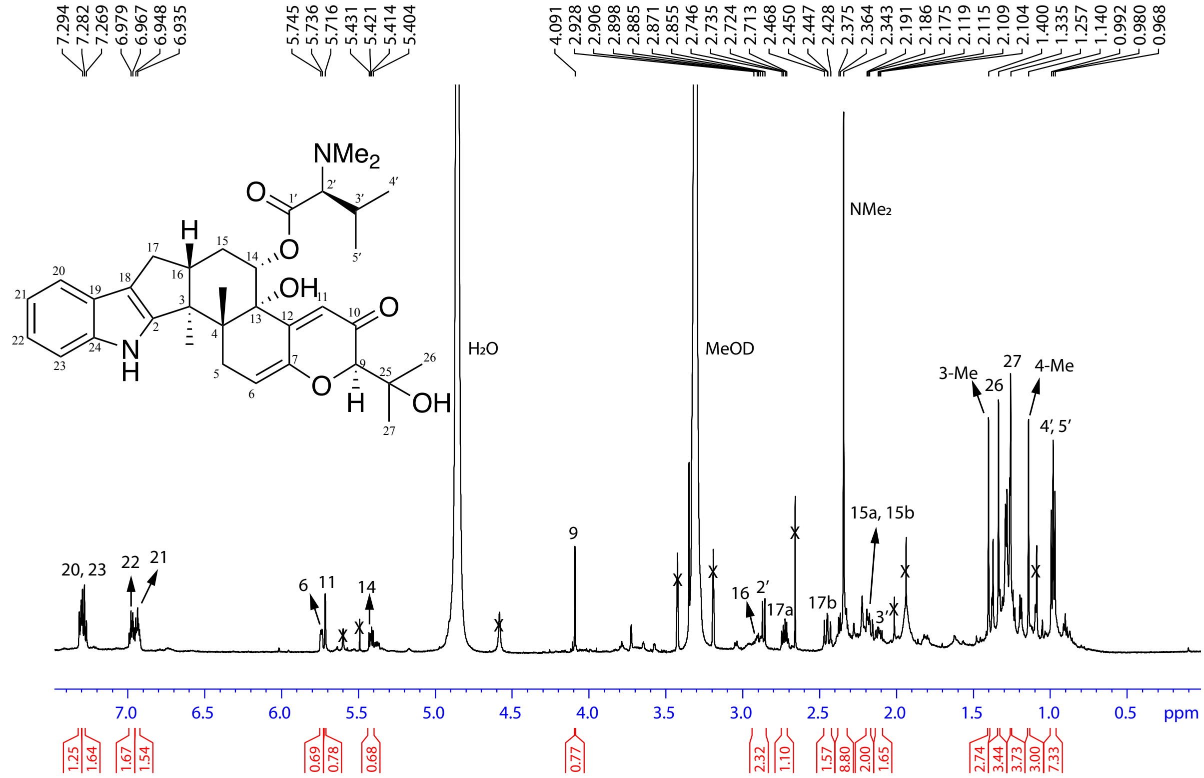


Figure S37. [1]H NMR (methanol-d_4) spectrum of noonindole E (**9**)

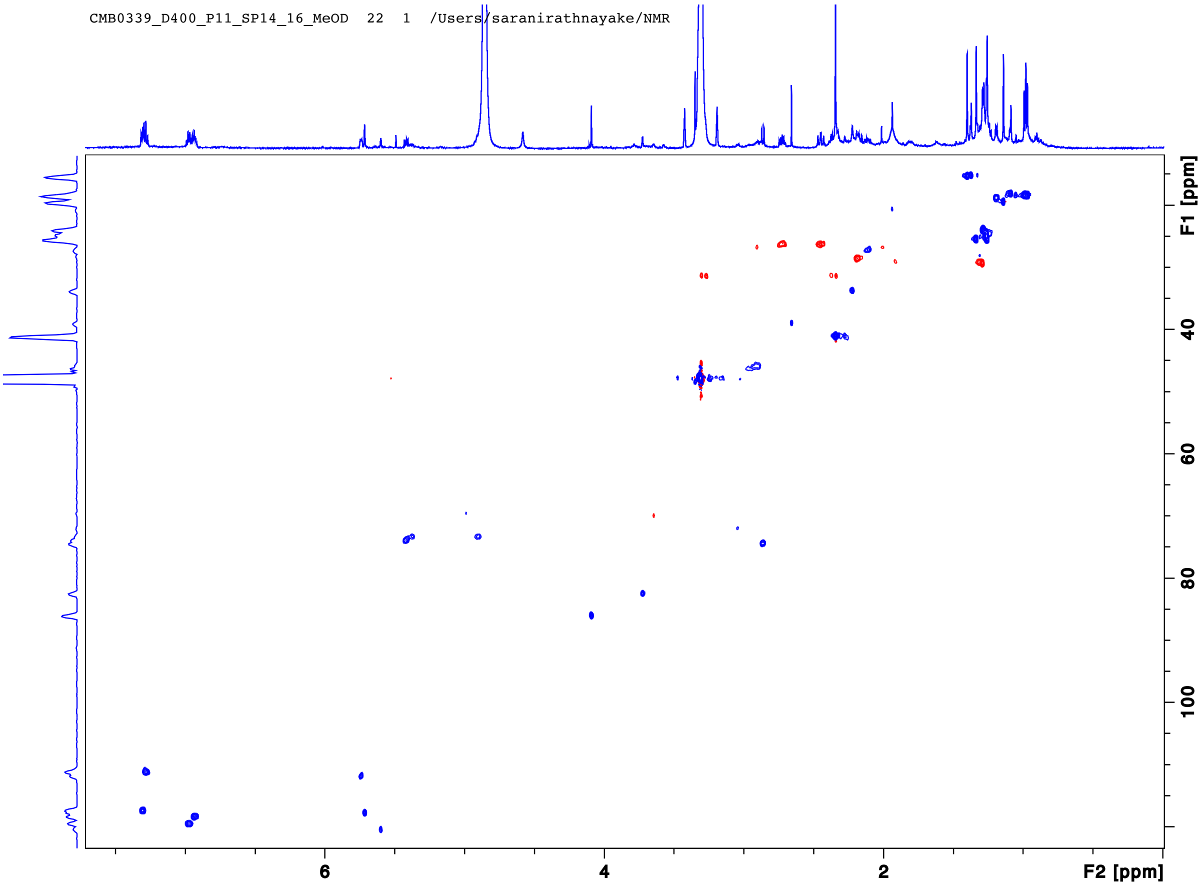


Figure S38. HSQC (methanol-*d*4) spectrum of noonindole E (**9**)

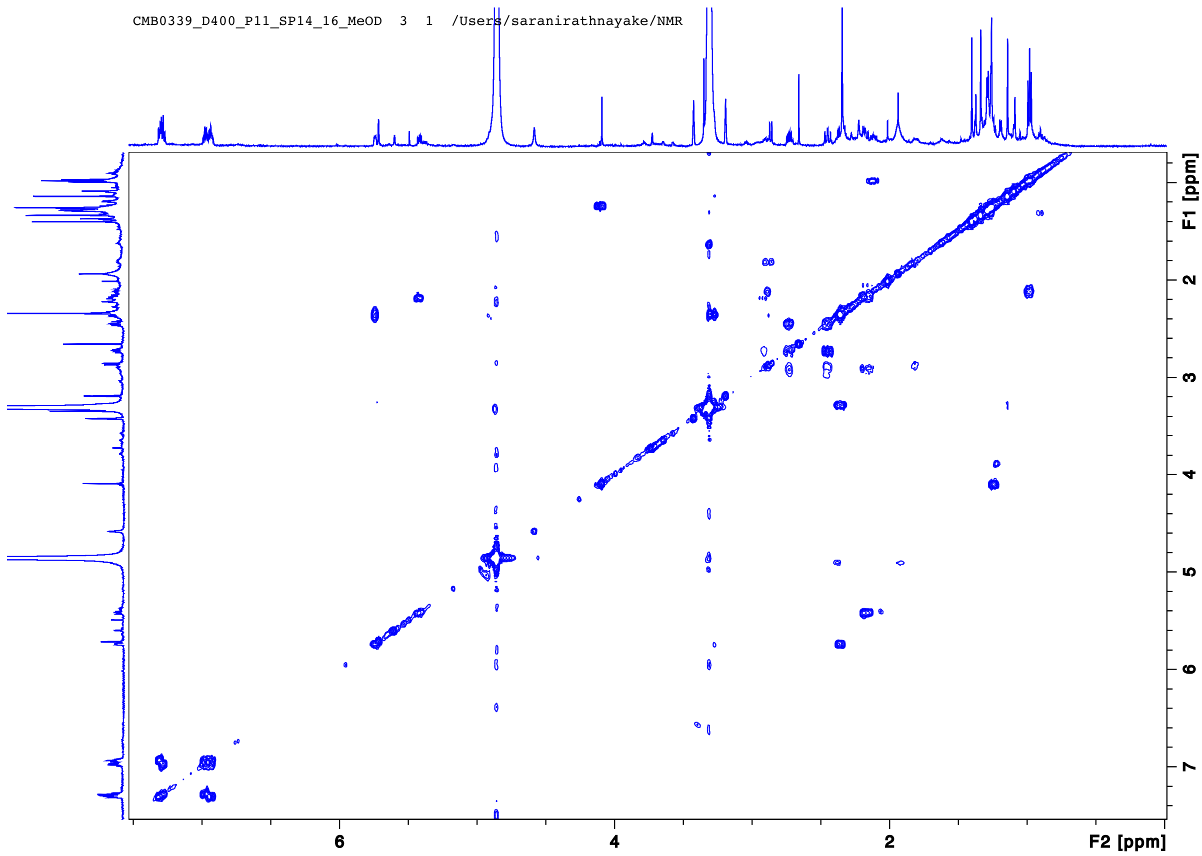


Figure S39. COSY (methanol-*d*4) spectrum of noonindole E (**9**)

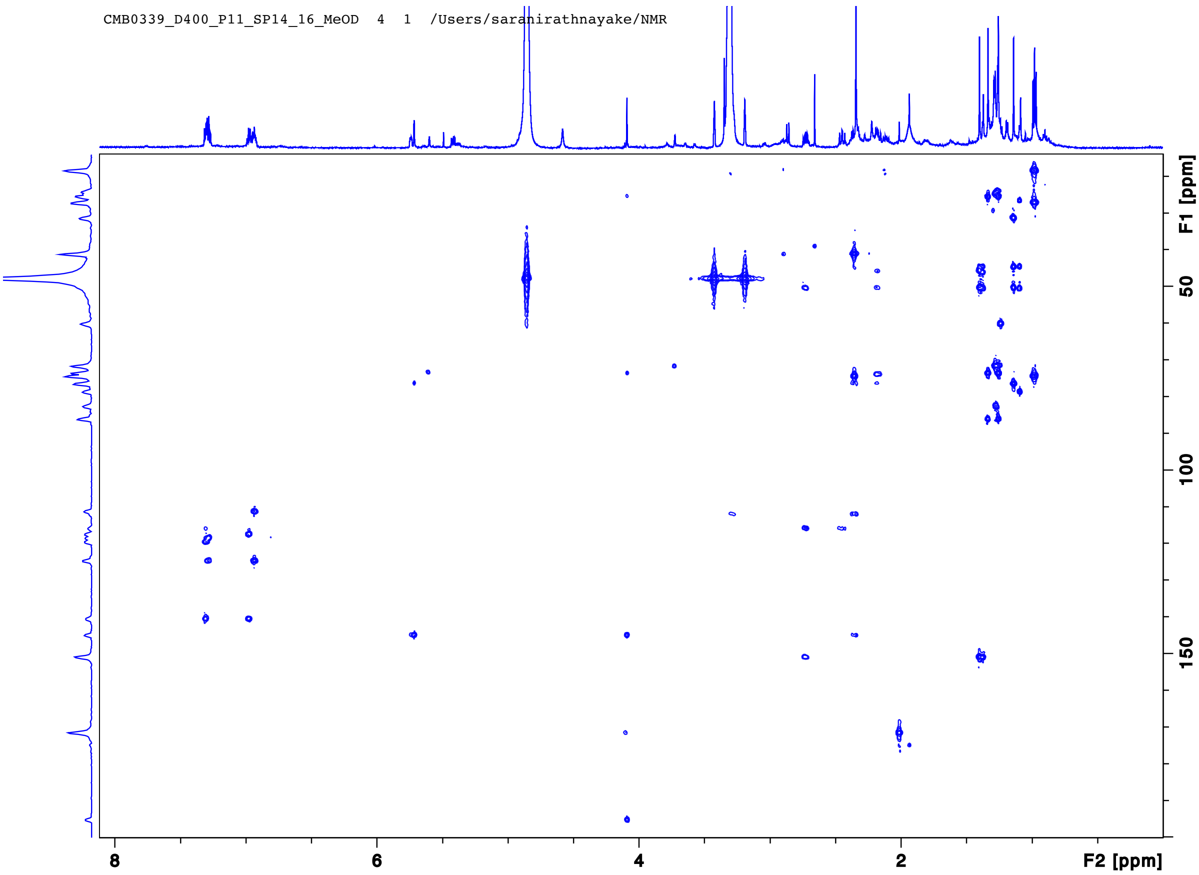


Figure S40. HMBC (methanol-d_4) spectrum of noonindole E (**9**)

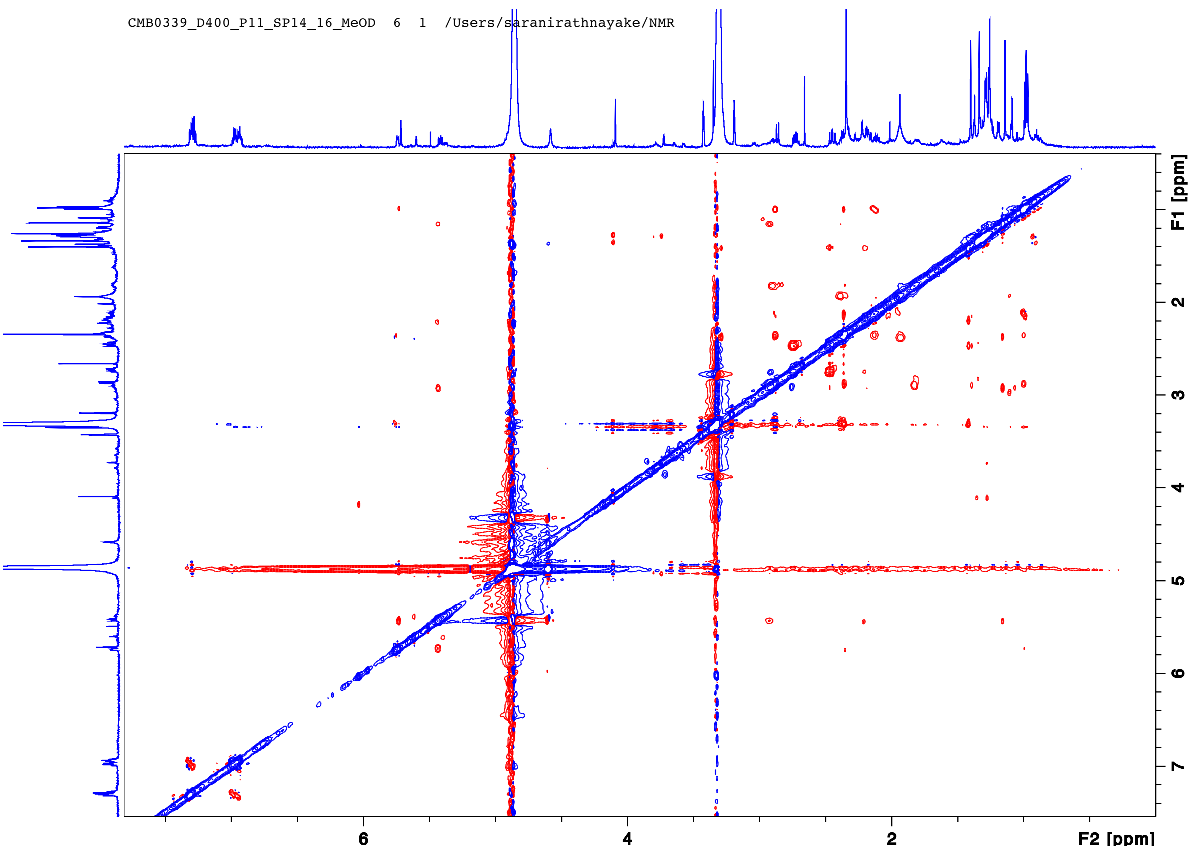


Figure S41. ROESY (methanol-d_4) spectrum of noonindole E (**9**)

Mass Spectrum Molecular Formula Report

Analysis Info

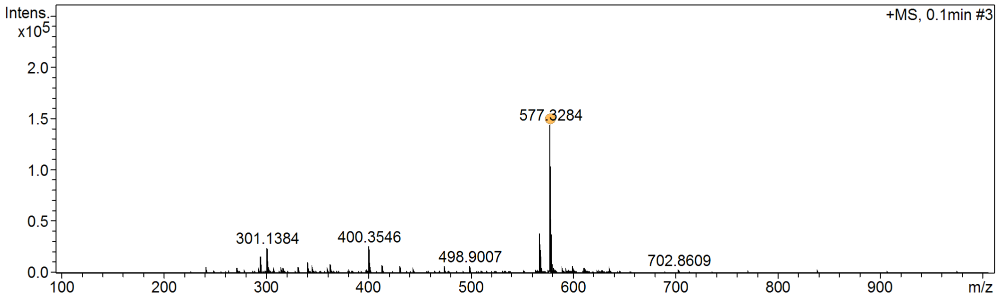
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_P11_SP14_16_again.d	Acquisition Date	11/2/2021 2:06:04 PM
Method	tune-med_AP.m	Operator	a.salim
Sample Name	CMB0339_D400_P11_SP14_16_again	Instrument / Ser#	micrOTOF 213750.00232
Comment			

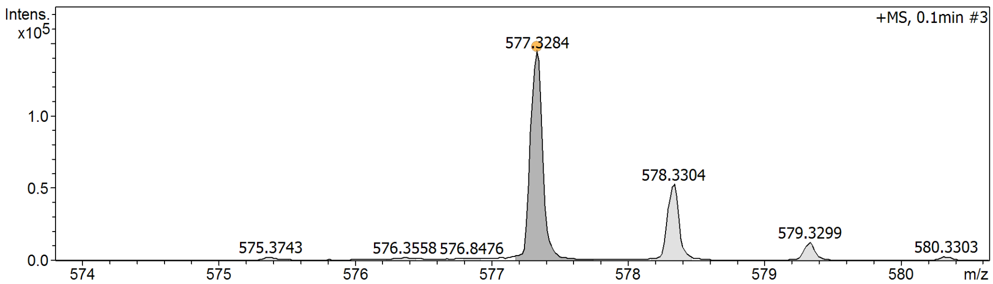
Acquisition Parameter

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
577.3284	1	C30H41N8O4	577.3245	-6.7	8.0	1	7.33	14.5	even	ok
	2	C34H45N2O6	577.3272	-2.0	9.0	2	74.87	13.5	even	ok
	3	C31H37N12	577.3259	4.4	12.1	3	26.28	19.5	even	ok
	4	C35H41N6O2	577.3286	0.3	20.7	4	100.00	18.5	even	ok
	5	C39H45O4	577.3312	4.9	32.5	5	12.57	17.5	even	ok

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Figure S42. HRMS spectrum of noonindole E (**9**)

9 Noonindole F (10)

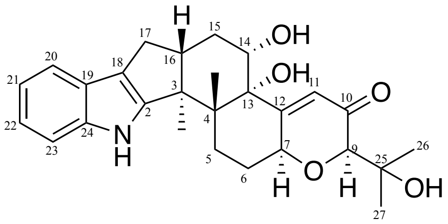


Table S7. 1D and 2D NMR (in methanol-d_4, 600 MHz) data for noonindole F (**10**)

Pos.	$\delta_{H,}$ mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	ROESY
1-NH	-	-	-	-	-
2	-	152.9	-	-	-
3	-	51.8	-	-	-
4	-	44.7	-	-	-
5	*a* 2.80 (ddd, 1H, J = *13.5,13.5, 5.1* Hz)	28.1	5*b*, 6*a*	4, 6, 4-Me	3-Me
	b 1.79 (dd, 1H, J = *13.5, 5.1* Hz)		5*a*, 6*b*	6, 7, 13	-
6	*a* 2.33 (m, 1H)	30.2	5*a*, 6*b*, 7	7, 5, 4, 12	3-Me
	b 1.90 (m, 1H)		6*a*, 5*b*, 7	5, 7	-
7	4.88 (m, 1H)	74.7	6*a*, 6*b*, 9, 11	11, 12	9
9	3.78 (d, 1H, J = *1.5* Hz)	84.0	7	7, 25, 26, 27	7, 26, 27
10	-	200.0	-	-	-
11	6.01 (br s, 1H)	122.9	7	7, 9, 13	14
12	-	167.5	-	-	-
13	-	80.8	-	-	-
14	4.16 (dd, 1H, J = *10.5, 4.9* Hz)	70.3	15*a*, 15*b*	-	4-Me, 16, 11
15	*a* 2.08 (dd, 1H, J = *13.3, 10.5* Hz)	31.7	14, 15*b*, 16	14, 16	-
	b 1.93 (m, 1H)		15*a*, 14	14, 16	4-Me
16	2.90 (m, 1H)	48.0	15*a*, 15*b*, 17*a*, 17*b*	3-Me	14, 4-Me
17	*a* 2.68 (dd, 1H, J = *13.0, 6.1* Hz)	27.8	16, 17*b*	2, 3, 16, 18	-
	b 2.42 (dd, 1H, J = *13.0, 10.0* Hz)		16, 17*a*	16, 18	-
18	-	117.4	-	-	-
19	-	126.2	-	-	-
20	7.29 (d, 1H, J = *7.6* Hz)	118.8	21	18, 22, 24	-
21	6.92 (br dd, 1H, J = *7.6, 7.2* Hz)	119.8	20, 22	19, 23	-
22	6.95 (br dd, 1H, J = *7.4, 7.2* Hz)	120.9	21, 23	20, 24	-
23	7.26 (d, 1H, J = *7.4* Hz)	112.7	22	19, 21	-
24	-	141.8	-	-	-
25	-	73.2	-		-
26	1.29 (s, 3H)	25.2	-	9, 25, 27	9
27	1.27 (s, 3H)	26.2	-	9, 25, 26	9
3-Me	1.32 (s, 3H)	16.5	-	2, 3, 4, 16	5*a*, 6*a*
4-Me	1.04 (s, 3H)	19.6	-	3, 4, 5, 13	14, 15b, 16

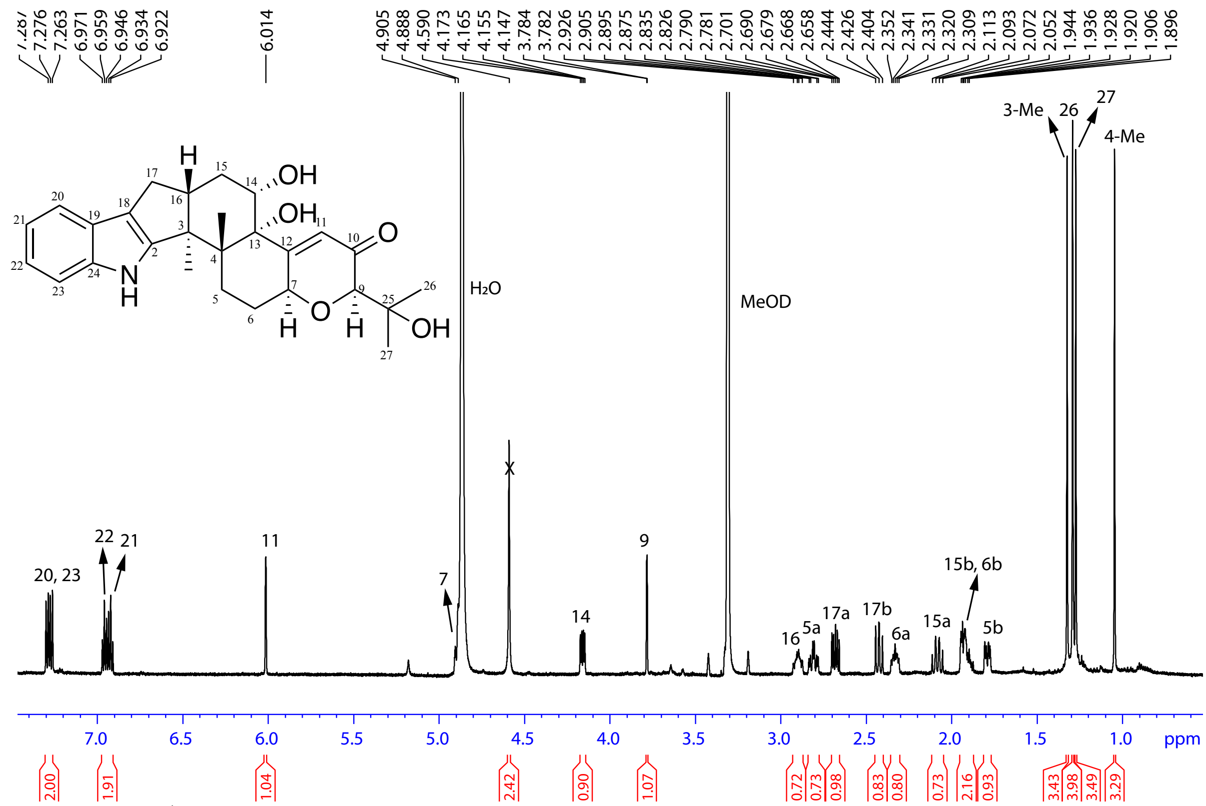


Figure S43. [1]H NMR (methanol-d_4) spectrum of noonindole F (**10**)

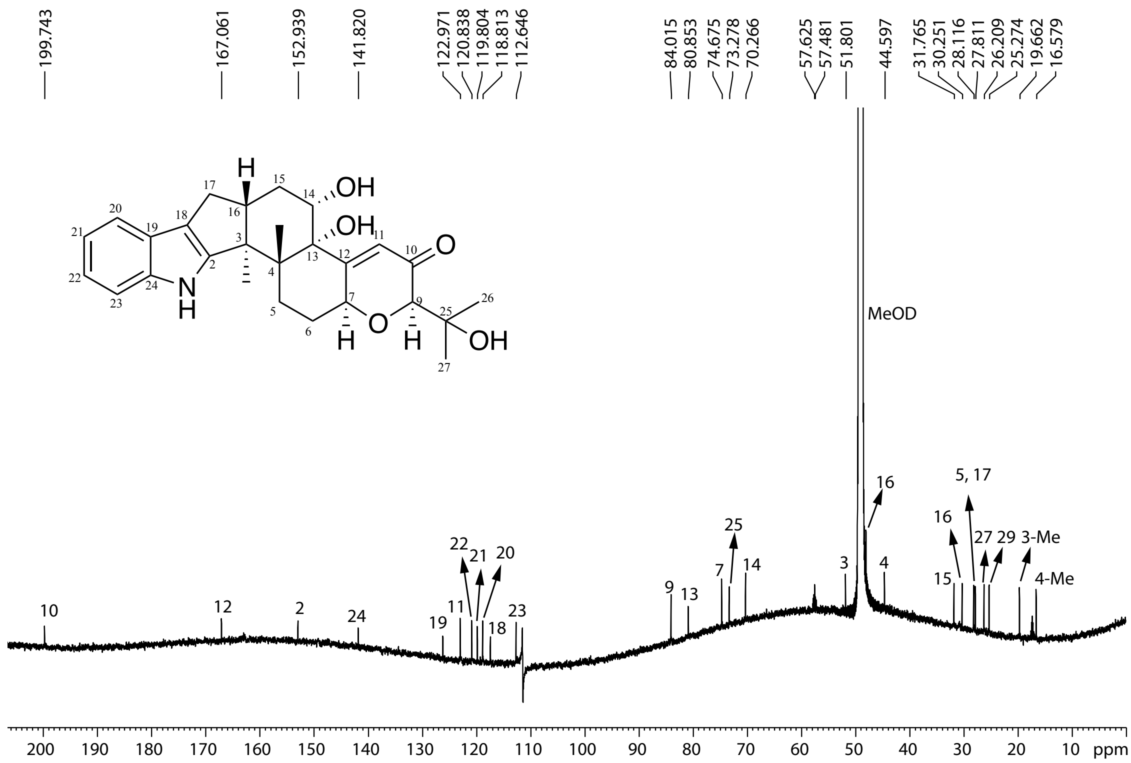


Figure S44. [13]C NMR (methanol-d_4) spectrum of noonindole F (**10**)

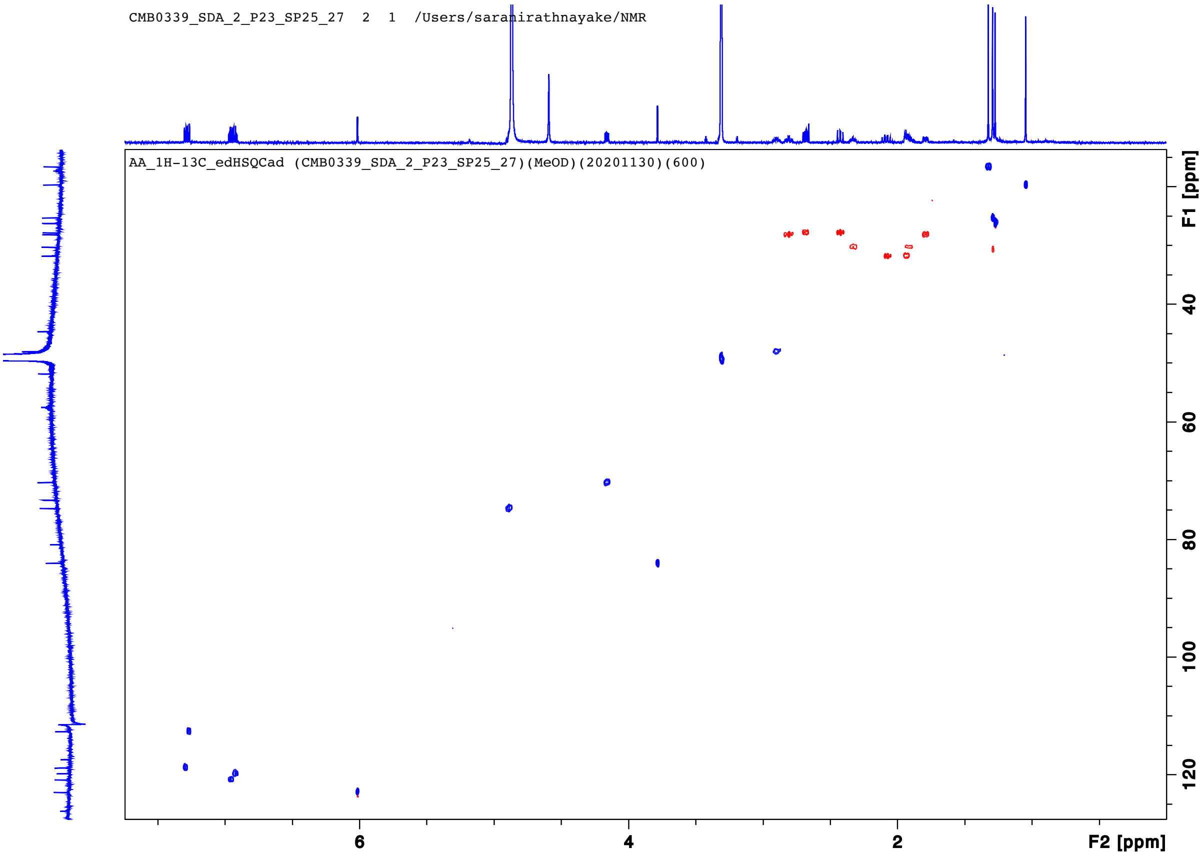


Figure S45. HSQC (methanol-d_4) spectrum of compound noonindole F (**10**)

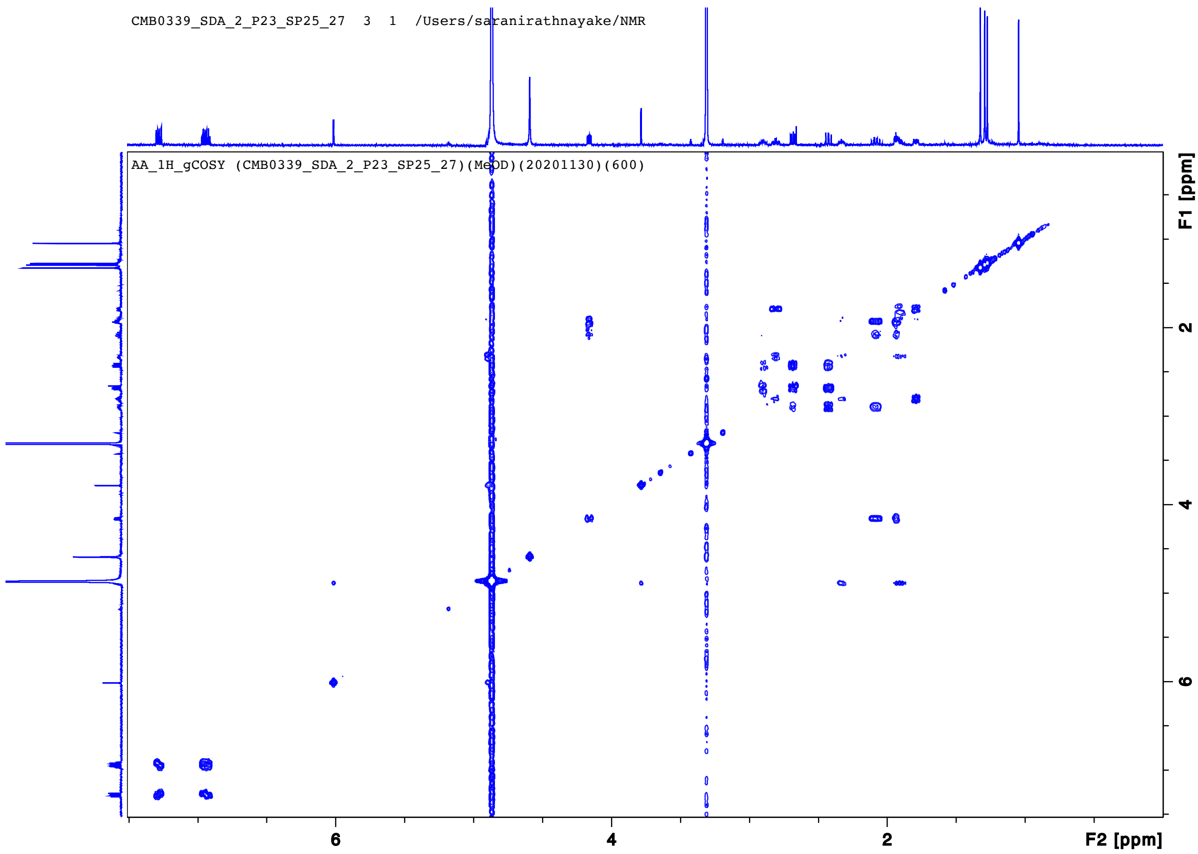


Figure S46. COSY (methanol-d_4) spectrum of compound noonindole F (**10**)

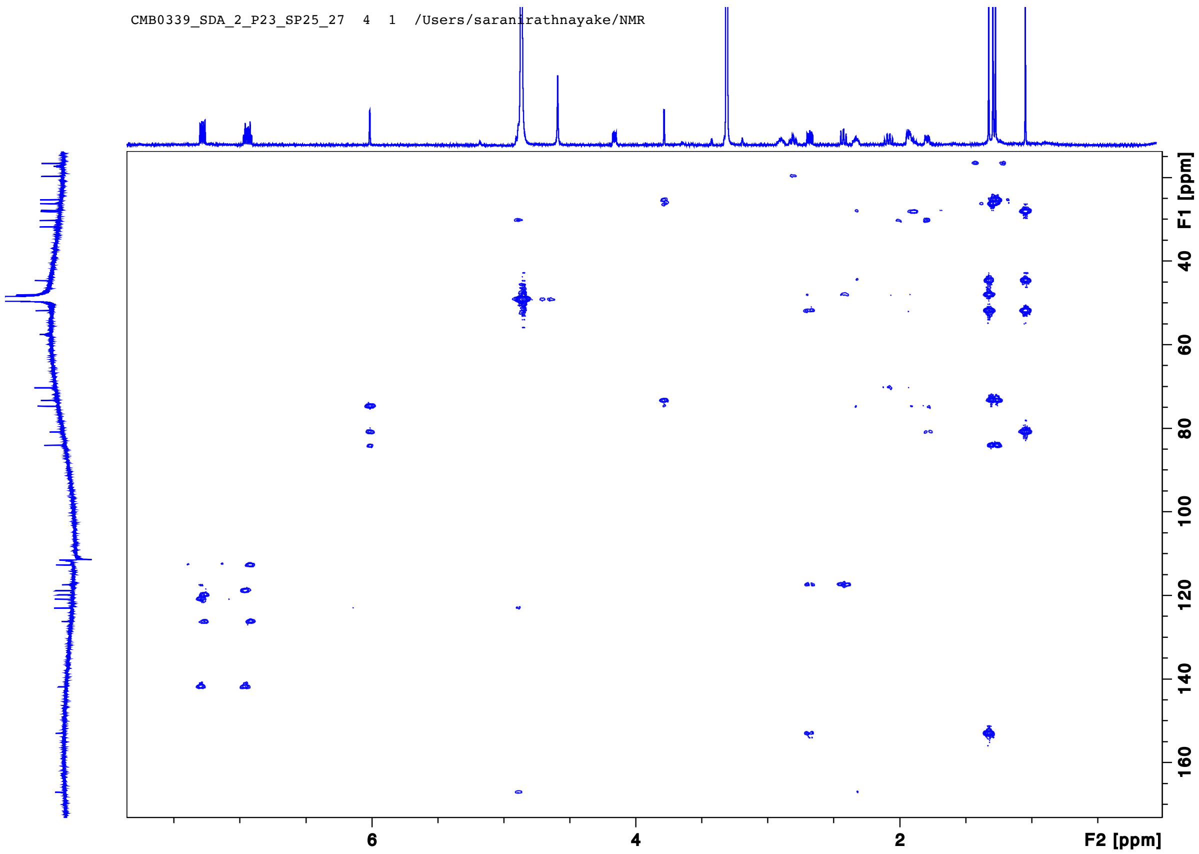


Figure S47. HMBC (methanol-d_4) spectrum of compound noonindole F (**10**)

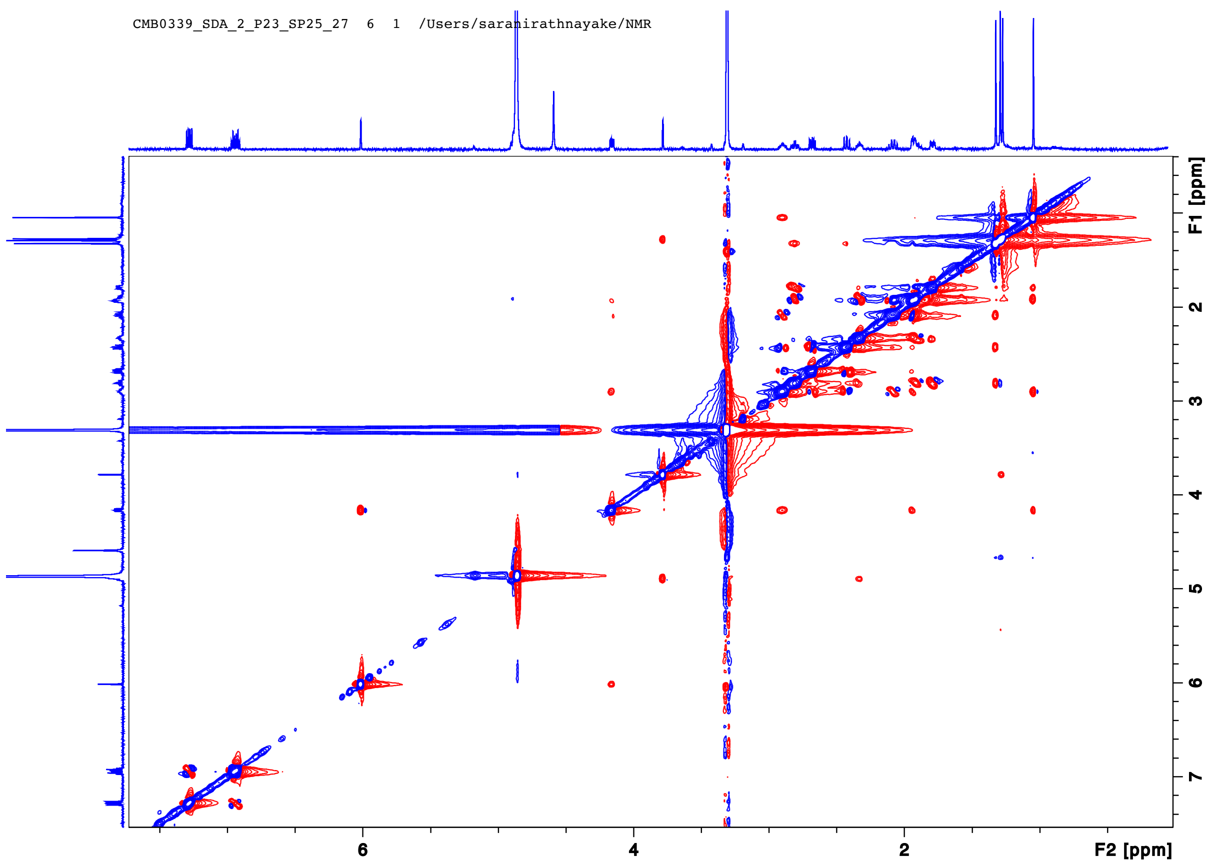


Figure S48. ROESY (methanol-d_4) spectrum of compound noonindole F (**10**)

Mass Spectrum Molecular Formula Report

Analysis Info

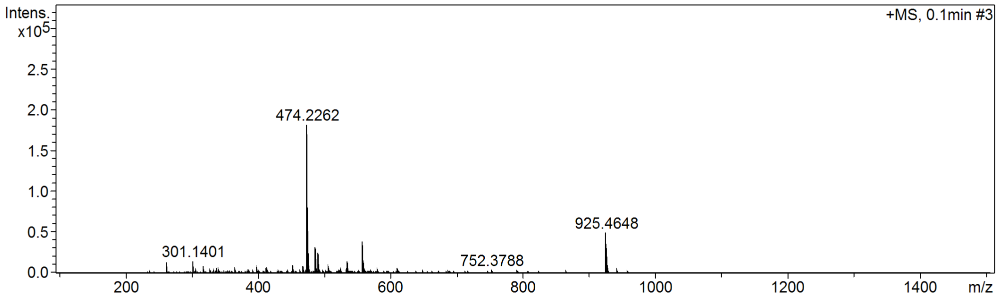
Analysis Name	D:\Data\s.kankanamge\CMB0339_SDA_2_P23_SP25_27.d	Acquisition Date	11/30/2020 10:43:26 AM
Method	tune-medhigh_AP.m	Operator	a.salim
Sample Name	CMB0339_SDA_2_P23_SP25_27	Instrument / Ser#	micrOTOF 213750.00232
Comment			

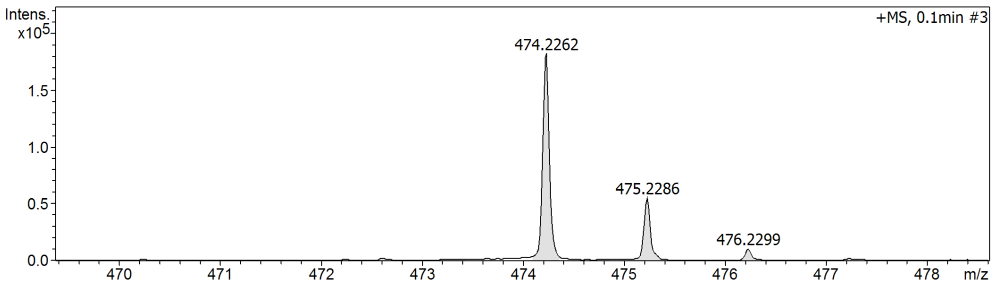
Acquisition Parameter

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
474.2262	1	C27H33NNaO5	474.2251	-2.4	1.3	1	74.93	11.5	even	ok
	2	C28H29N5NaO	474.2264	0.4	12.0	2	100.00	16.5	even	ok
	3	C23H29N7NaO3	474.2224	-8.1	12.7	3	6.01	12.5	even	ok
	4	C17H29N11NaO4	474.2296	7.1	37.8	4	5.43	8.5	even	ok
	5	C16H33N7NaO8	474.2283	4.3	48.8	5	13.44	3.5	even	ok
	6	C13H25N17NaO2	474.2269	-1.5	57.5	6	18.24	9.5	even	ok
	7	C12H29N13NaO6	474.2256	-1.3	70.0	7	12.21	4.5	even	ok
	8	C9H21N23Na	474.2242	4.2	71.4	8	4.97	10.5	even	ok

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Figure S49. HRMS spectrum of noonindole F (**10**)

10 Paspaline (11)

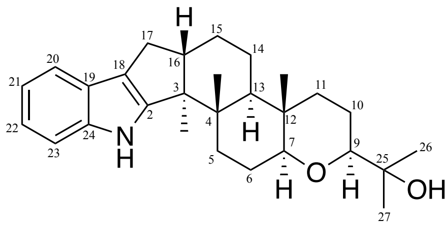


Table S8.1D and 2D NMR (DMSO-d_6, 600 MHz) data of paspaline (**11**)
(Reported data are shaded in grey)

Pos.	δ_H, mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	δ_H, mult. (*J* in Hz) [1]	δ_C [1]
1-NH	10.56, s	-	-	2, 18, 19, 24	-	-
2	-	151.6	-	-	-	151.2
3	-	52.9	-	-	-	52.6
4	-	39.9	-	-	-	39.2
5	*a* 1.92 (m, 1H)	32.1	5*b*	4, 7, 13, 4-Me	1.91 (m, 1H)	31.1
	b 1.78 (m, 1H)		5*a*	4, 7, 4-Me	1.60 (m, 1H)	31.1
6	*a* 1.69[a] (m, 1H)	24.3	-	-	1.78 (m, 1H)	24.7
	b 1.55[b] (m, 1H)		-	-	1.72 (m, 1H)	24.7
7	2.97 (dd, 1H, J = *11.6, 3.4* Hz)	84.9	-	5, 9, 11, 12-Me	2.94 (dd, 1H, J = *11.5, 2.4* Hz)	85.4
9	3.08 (dd, 1H, J = *11.5, 1.8* Hz)	84.2	-	7, 25, 26, 27	3.09 (dd, 1H, J = *11.7, 2.2* Hz)	84.7
10	*a* 1.54[b] (m, 1H)	20.9	-	-	1.68 (m, 1H)	21.2
	b 1.47[c] (m, 1H)		-	-	1.44 (m, 1H)	21.2
11	*a* 1.75 (m, 1H)	37.0	11b	10, 12	1.30 (m, 1H)	37.4
	b 1.10 (m, 1H)		11*a*, 10b[c]	-	1.27 (m, 1H)	37.4
12	-	36.6	-		-	36.2
13	1.46[c] (m, 1H)	45.6	-	-	1.42 (m, 1H)	46.1
14	*a* 1.63 (br d, 1H, J = *12.6* Hz)	21.2	14*b*	4, 13, 15, 16	1.55 (m, 1H)	21.6
	b 1.33 (ddd, 1H, J = *16.5, 12.6, 4.1* Hz)		14*a*	4, 13, 15	1.28 (m, 1H)	21.6
15	*a* 1.70[a] (m, 1H)	24.8	-	-	1.77 (m, 1H)	25.3
	b 1.54[b] (m, 1H)		-	-	1.53 (m, 1H)	25.3
16	2.64 (m, 1H)	48.3	17*a*, 17*b*	3, 17, 3-Me	2.72 (t, 1H, J = *6.4* Hz)	48.7
17	*a* 2.55 (dd, 1H, J = *13.2*, *6.3* Hz)	26.8	17*b*, 16	2, 3, 16, 18	2.60 (m, 1H)	28.7
	b 2.23 (dd, 1H, J = *13.2*, *11.3* Hz)		17*a*, 16	2, 15, 16, 18	2.53 (m, 1H)	28.7
18	-	116.2	-	-	-	115.9
19	-	124.9	-	-	-	124.5
20	7.25[d] (dd, 1H, J = *7.4, 2.5* Hz)	117.2	-	-	7.25 (d, 1H, J = *7.9* Hz)	117.7
21	6.88 (dd, 1H, J = *7.9, 7.4* Hz)	118.0	20[d], 22	19, 23	6.92 (t, 1H, J = *6.7* Hz)	118.5
22	6.92 (dd, 1H, J = *7.9, 7.4* Hz)	118.9	21, 23[d]	20, 24	6.90 (t, 1H, J = *6.7* Hz)	119.4
23	7.25[d] (dd, 1H, J = *7.4, 2.5* Hz)	111.5	-	-	7.26 (d, 1H, J = *7.9* HZ)	112.0
24	-	140.8	-	-	-	140.4
25	-	70.9	-	-	-	70.5
26	1.04[e] (s, 3H)	24.4	-	-	1.03 (s, 3H)	26.8
27	1.09 (s, 3H)	26.7	-	9, 25, 29	1.05 (s, 3H)	28.9
12-Me	0.82 (s, 3H)	12.4	-	7, 11, 12, 13	0.81 (s, 3H)	14.0
3-Me	0.95 (s, 3H)	14.3	-	2, 3, 4, 16	1.10 (s, 3H)	14.6
4-Me	1.04[e] (s, 3H)	19.2	-	-	0.81 (s, 3H)	22.2
25-OH	4.07 (s, 1H)	-	-	9, 25, 26, 27	-	-

[a-e] Resonances with the same superscript within a column are overlapping and assignments may be interchanged
*Literature data were recorded (^{1}H NMR in 600 MHz and ^{13}C NMR in 150 MHz) in DMSO-d_6

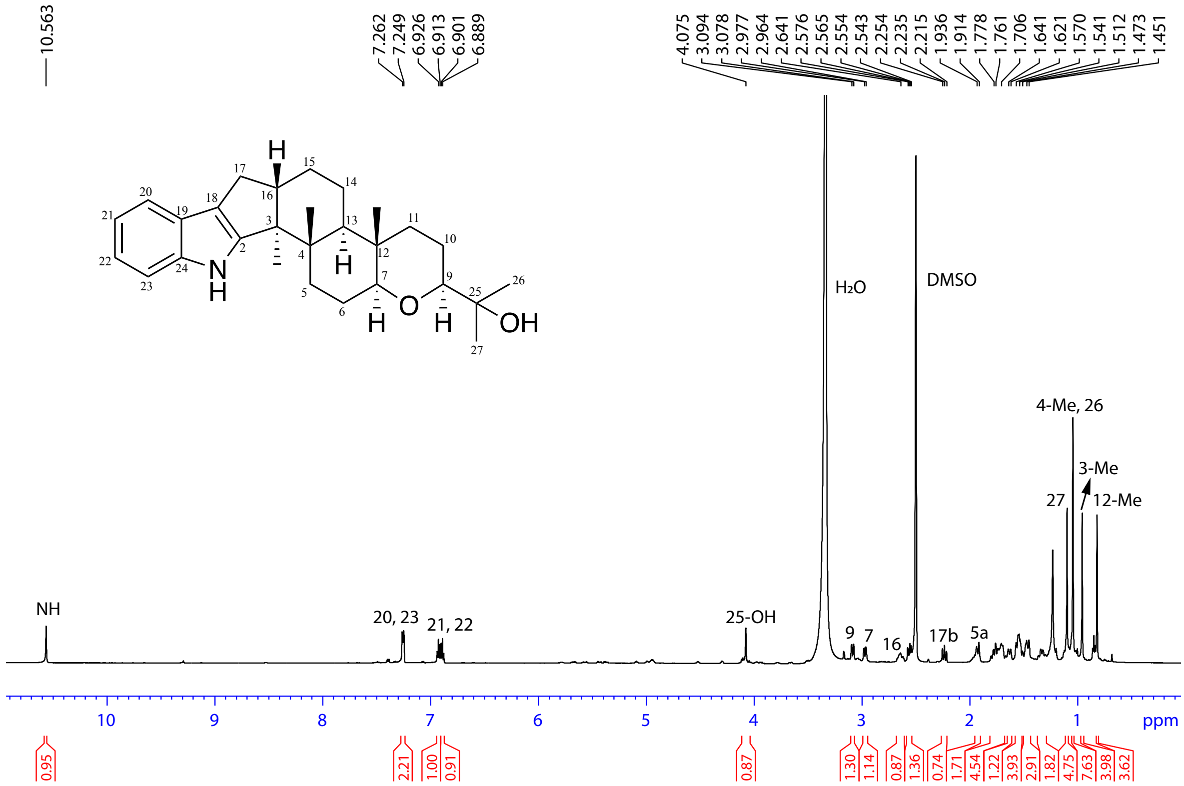


Figure S50.[1]H NMR (DMSO-d_6) spectrum of paspaline (**11**)

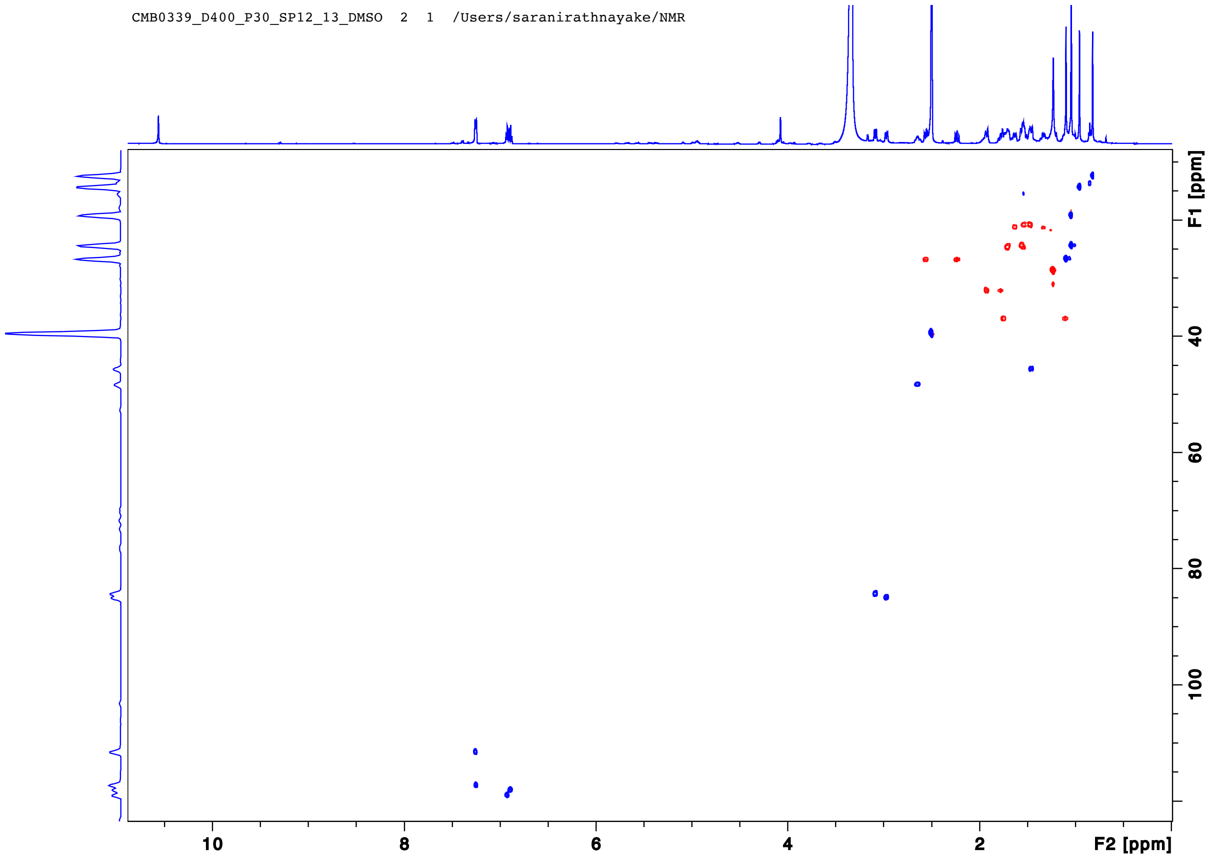


Figure S51. HSQC (DMSO-d_6) spectrum of paspaline (**11**)

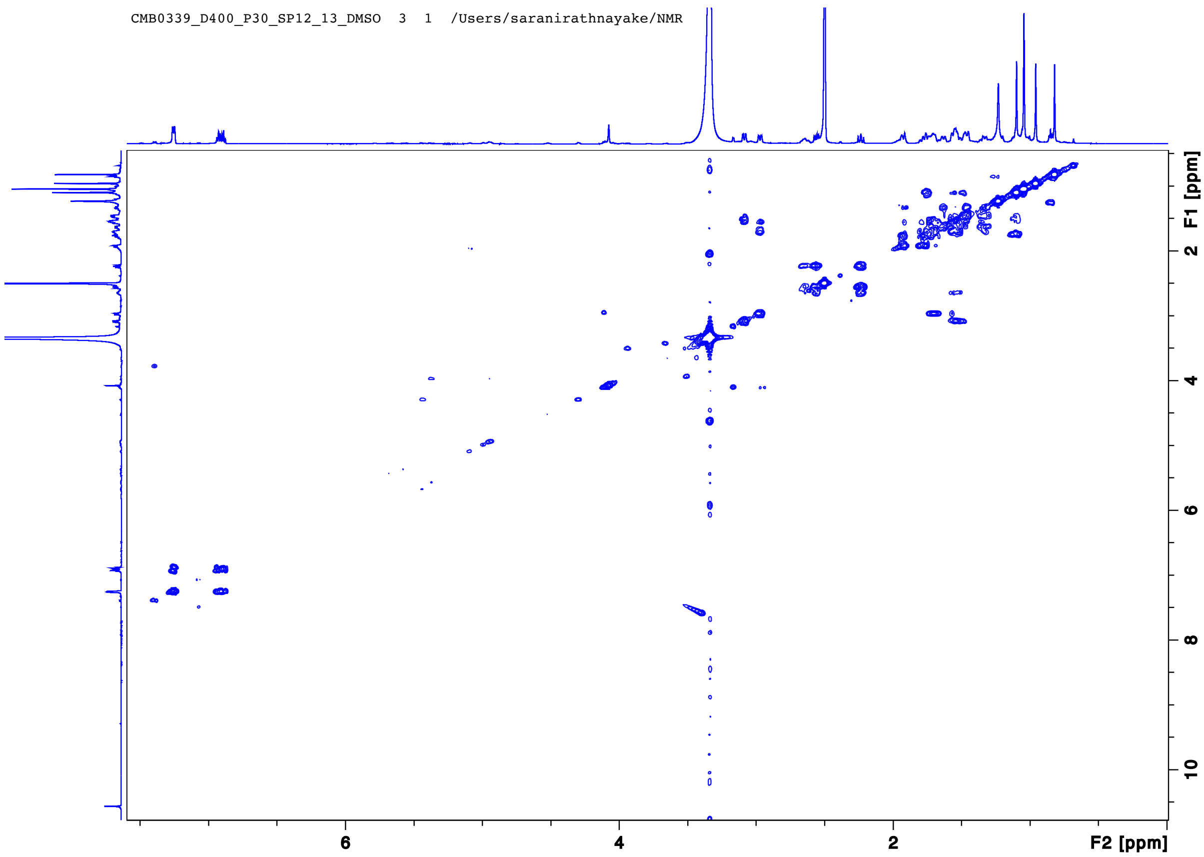


Figure S52. COSY (DMSO-d_6) spectrum of paspaline (**11**)

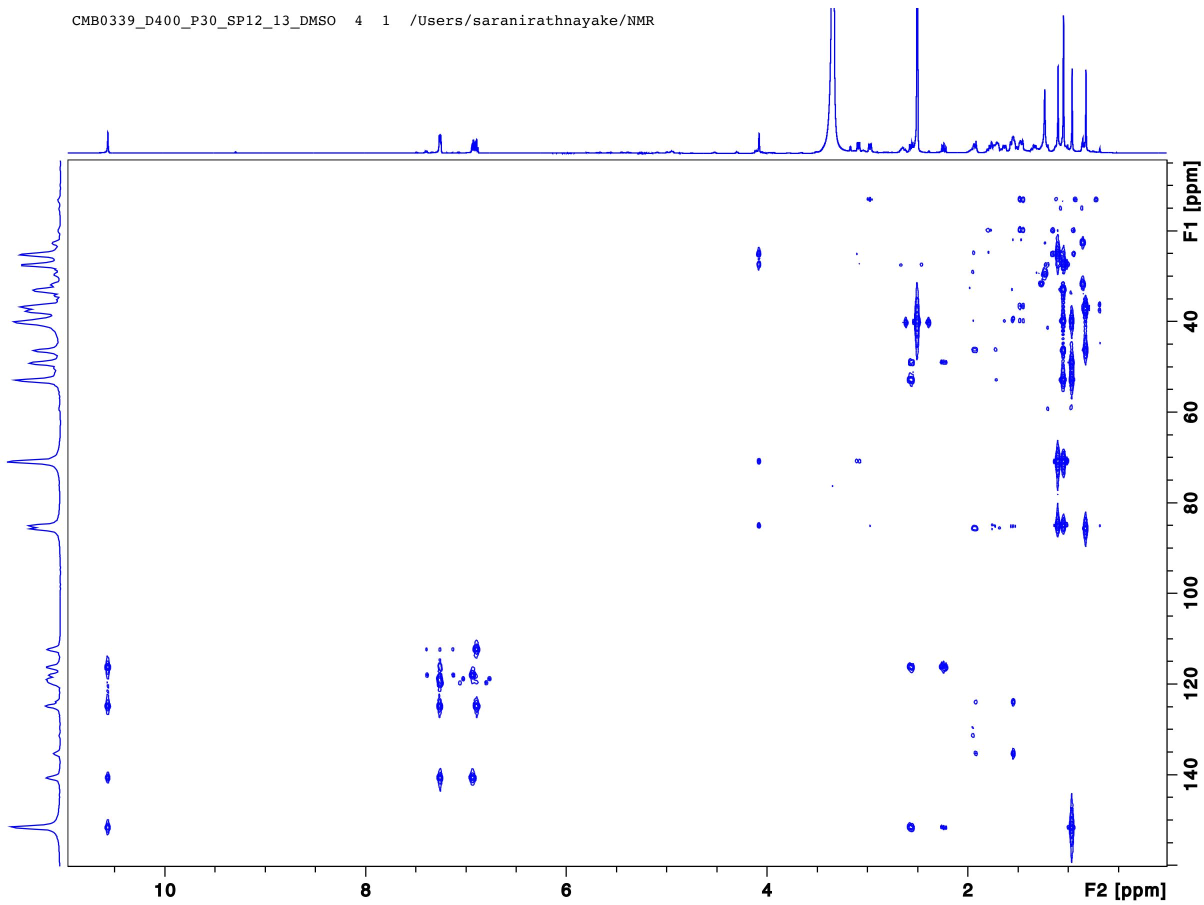


Figure S53. HMBC (DMSO-d_6) spectrum of paspaline (**11**)

Mass Spectrum Molecular Formula Report

Analysis Info

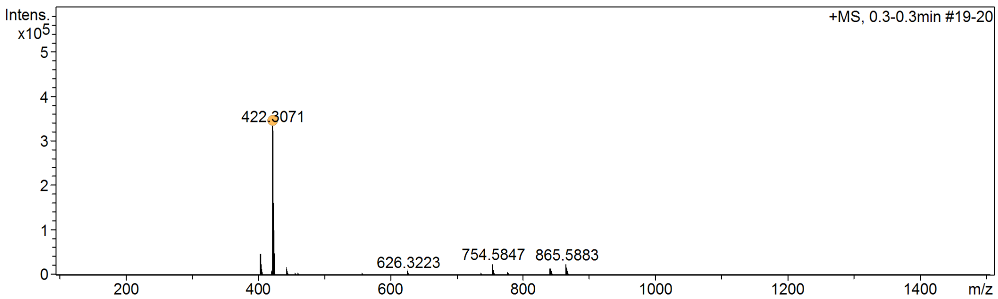
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_P30_SP12_13.d	Acquisition Date	9/8/2021 4:50:26 PM
Method	tune-medhigh_AP.m	Operator	a.salim
Sample Name	CMB0339_D400_P30_SP12_13	Instrument / Ser#	micrOTOF 213750.00232
Comment			

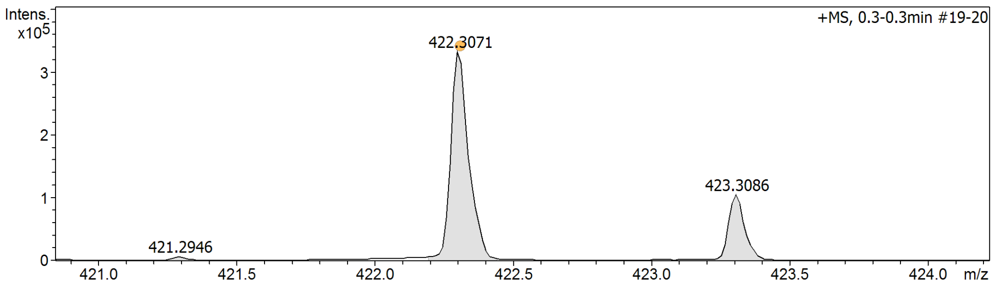
Acquisition Parameter

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
422.3071	1	C28H40NO2	422.3054	4.1	3.0	1	100.00	9.5	even	ok

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Figure S54. HRMS spectrum of paspaline (**11**)

11 Paspaline B (12)

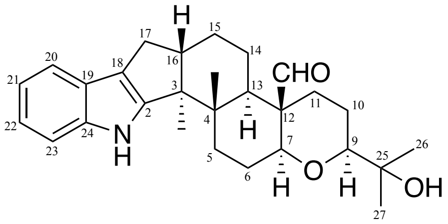


Table S9. 1D and 2D NMR ($CDCl_3$, 600 MHz) data of paspaline B (**12**)
(Reported data are shaded in grey)

Pos.	δ_H, mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	δ_H, mult. (*J* in Hz) [2]	δ_C[2]
1-NH	7.67 (s, 1H)	-	-	18, 19, 24	7.69, s	-
2	-	149.9	-	-	-	150.0
3	-	51.9	-	-	-	52.0
4	-	39.9	-	-	-	39.9
5	*a* 2.02 (dd, 1H, J = *13.1, 3.9* Hz)	33.2	6*a*, 5*b*, 6*b*		2.07	33.2
	b 1.71 (dd, 1H, J = *10.2, 3.8* Hz)		5*a*	-	1.72	33.2
6	*a* 2.24 (dd, 1H, J = *12.3, 3.8* Hz)	24.8	7, 6*b*, 5*b*	-	2.04	24.9
	b 1.99 (m, 1H)		7, 6*a*	-	1.24	24.9
7	3.30 (dd, 1H, J = *12.3, 4.6* Hz)	83.6	6*a*, 6*b*	-	3.32	83.6
9	3.25 (dd, 1H, J = *11.7, 2.4* Hz)	84.8	10*b*	25	3.28	85.0
10	*a* 1.52*	23.1	-	-	1.55	23.4
	b 1.27 (m, 1H)		7	-	1.29	23.4
11	*a* 2.47 (m, 1H)	34.1	11*b*	-	2.49	33.9
	b 1.17 (m, 1H)		11*a*	9	1.22	33.9
12	-	50.6	-		-	50.7
13	1.68 (dd, 1H, J = *12.2, 3.5* Hz)	47.6	-	-	1.69	47.6
14	*a* 1.86 (m, 1H)	22.4	13	16	1.90	22.4
	b 1.52*		-	-	1.55	22.4
15	*a* 1.76 (m, 1H)	24.7	15*b*	-	1.80	24.9
	b 1.56*		-		1.55	24.9
16	2.68[a] (m, 1H)	48.7	-	-	2.70	48.7
17	*a* 2.66[a] (m, 1H)	27.3	-	2, 18, 16	2.68	27.4
	b 2.31 (m, 1H)		17*a*	18	2.32	27.4
18	-	118.4	-	-	-	118.0
19	-	125.7	-	-	-	125.7
20	7.40 (dd, 1H, J = *7.5, 1.6* Hz)	118.5	21[b]	22, 24	7.41	118.6
21	7.05[b] (m, 1H)	119.6	-	-	7.07	119.7
22	7.06[b] (m, 1H)	120.6	-	-	7.06	120.7
23	7.26 (dd, 1H, J = *7.8, 1.6* Hz)	111.4	22[b]	21, 19	7. 29	111.5
24	-	140.0	-		-	140.0
25	-	-	-		-	71.9
26	1.10 (s, 3H)	23.7	-	9, 25, 26	1.12	23.8
27	1.14 (s, 3H)	25.7		9, 25, 27	1.17	25.8
3-Me	0.98 (s, 3H)	14.8	-	2, 3, 4, 16	1.01	14.8
4-Me	0.91 (s, 3H)	19.6	-	3, 4, 5, 13	0.94	19.7
12-CHO	10.11 (s, 1H)	207.2	-	12	10.13	207.3

[a-b] Resonances with the same superscript within a column are overlapping and assignments may be interchanged
* Obscured by H_2O signal
**Literature data were recorded (^{1}H NMR in 300 MHz and ^{13}C NMR in 75 MHz) in $CDCl_3$

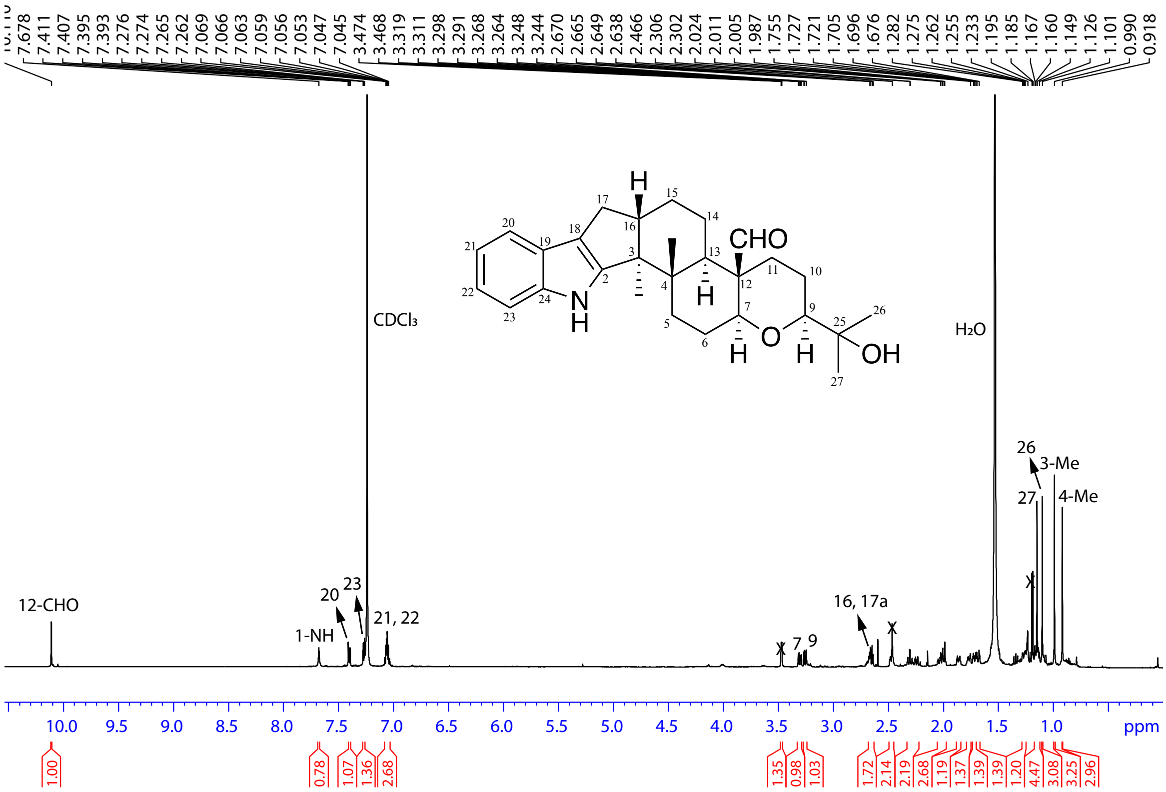


Figure S55. ^{1}H NMR ($CDCl_3$) spectrum of paspaline B (**12**)

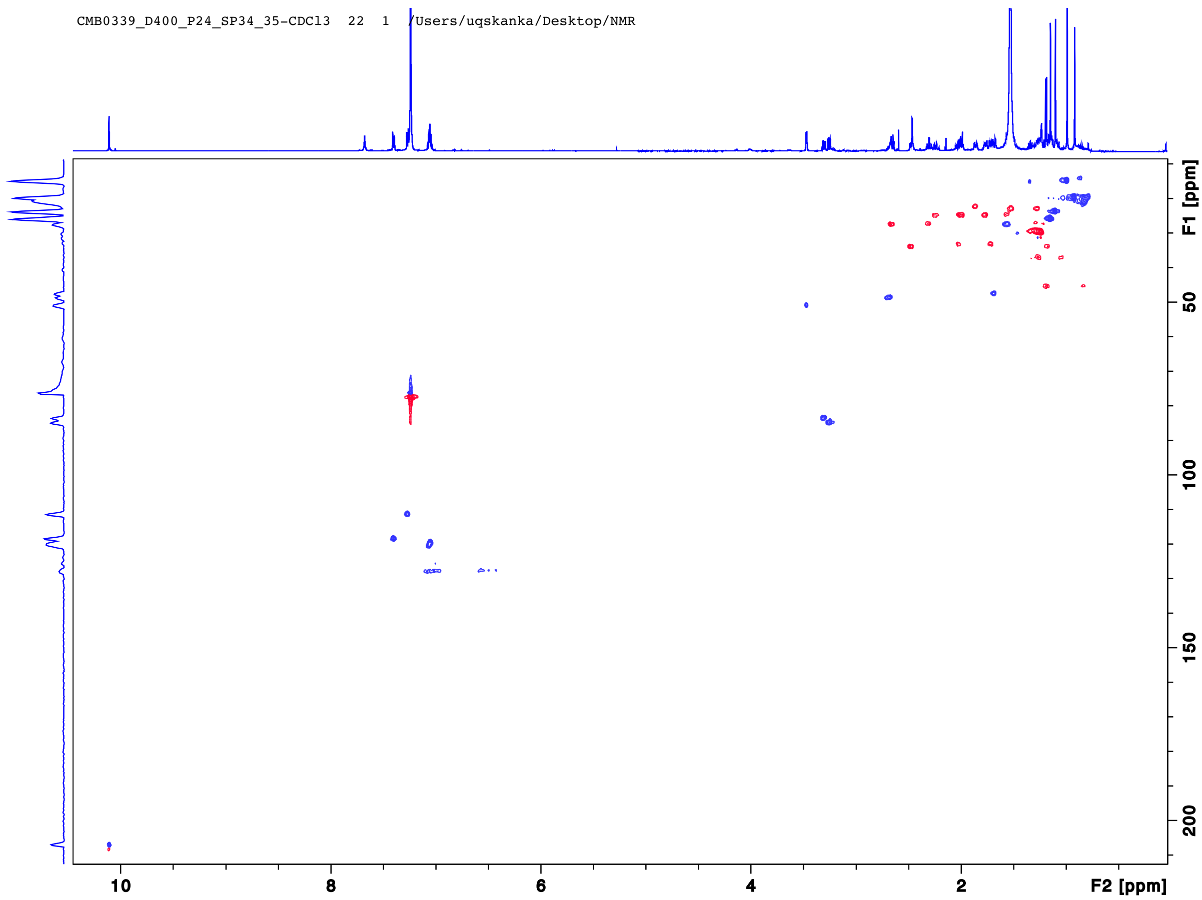


Figure S56. HSQC ($CDCl_3$) spectrum of paspaline B (**12**)

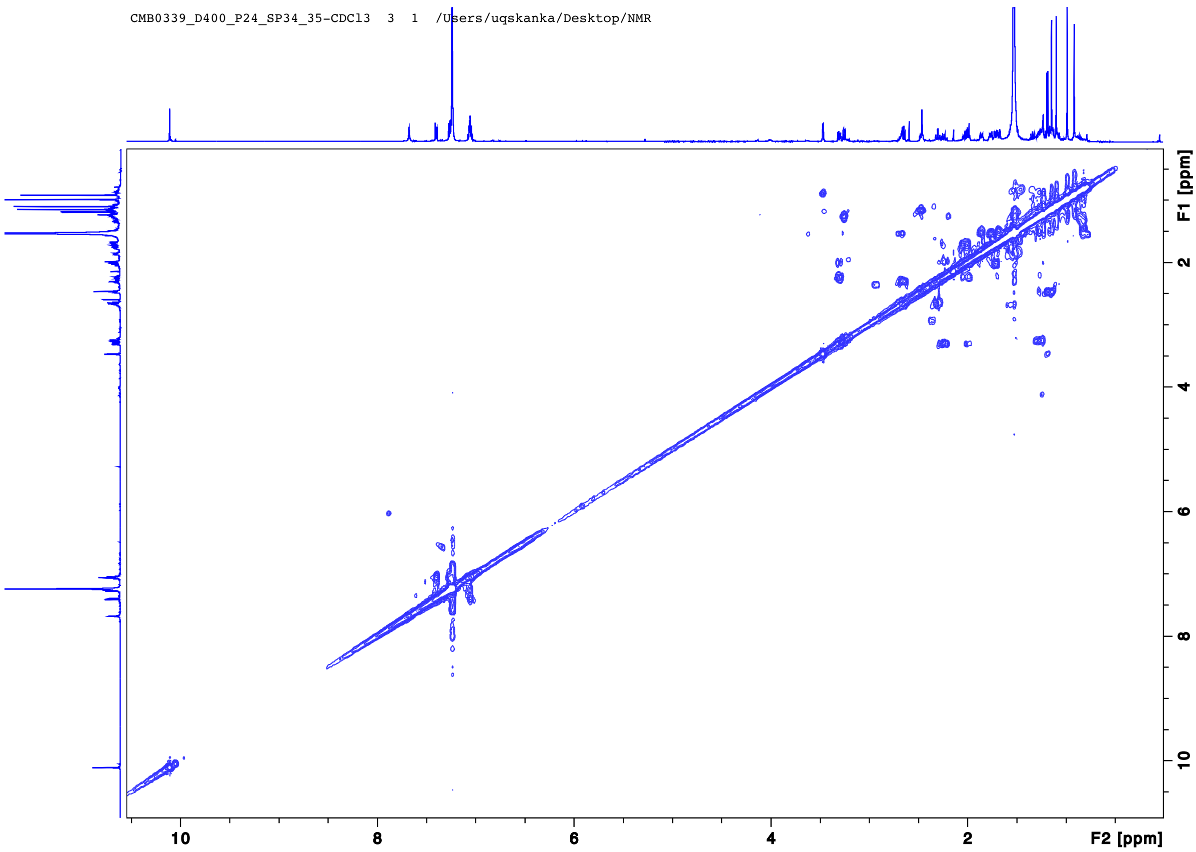


Figure S57. COSY ($CDCl_3$) spectrum of paspaline B (**12**)

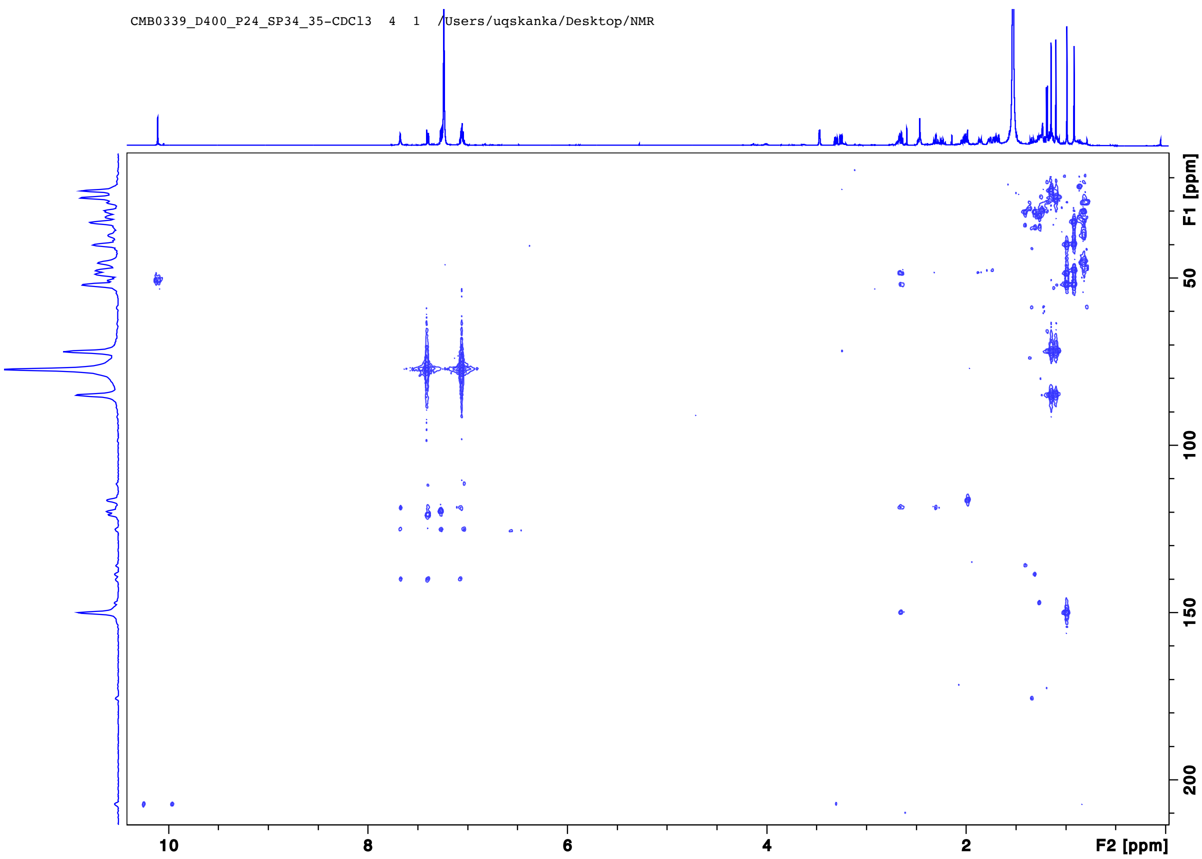


Figure S58. HMBC ($CDCl_3$) spectrum of paspaline B (**12**)

Mass Spectrum Molecular Formula Report

Analysis Info

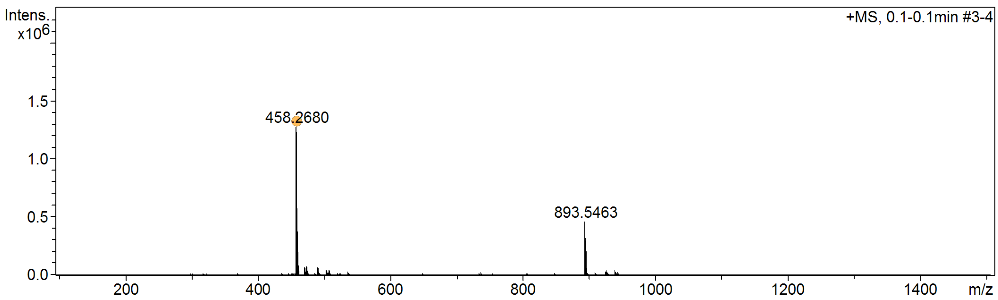
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_P24_SP34_35.d	Acquisition Date	9/8/2021 11:13:58 AM
Method	tune-medhigh_AP.m	Operator	a.salim
Sample Name	CMB0339_D400_P24_SP34_35	Instrument / Ser#	micrOTOF 213750.00232
Comment			

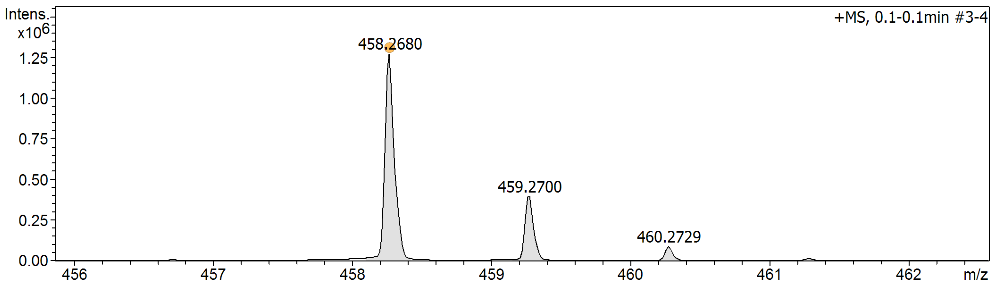
Acquisition Parameter

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
458.2680	1	C28H37NNaO3	458.2666	-3.2	8.1	1	100.00	10.5	even	ok

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Figure S59. HRMS spectrum of paspaline B (**12**)

12 12-demethylpaspaline-12-carboxylic acid (13)

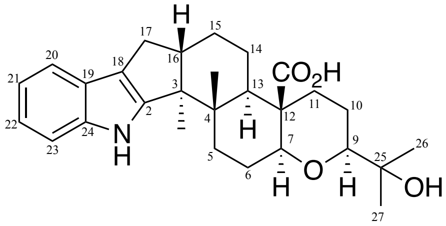


Table S10. 1D and 2D NMR (DMSO-d_6, 600 MHz) data of 12-demethylpaspaline-12-carboxylic acid (**13**) (Reported data are shaded in grey)

Pos.	δ_H, mult. (J in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	δ_H (mult., J (Hz) [1]	δ_C [1]
1-NH	10.58 (s, 1H)	-	-	2, 18, 19, 24	-	-
2	-	151.4	-	-	-	151.0
3	-	52.1	-	-	-	51.7
4	-	40.0	-	-	-	40.2
5	*a* 1.98 (br d, 1H, J = *12.7* Hz)	32.2	6*a*, 5b[a]	4, 6, 7, 13, 4-Me	*a* 1.97 (dt, 1H, J= *12.6, 3.1* Hz)	32.4
	b 1.82[a] (m, 1H)		-	-	*b* 1.83 (m, 1H)	
6	*a* 1.61[b] (m, 1H)	25.0	-	-	*a* 1.61 (m, 1H)	25.2
	b 2.55[c] (m, 1H)		-	-	*b* 2.54 (m, 1H)	
7	3.11[d] (br d, 1H, J = *11.3* Hz)	83.9[g]	10*b*	-	3.10 (dd, 1H, J = *11.0, 2.3* Hz)	83.7
9	3.11[d] (br d, 1H, J = *11.3 Hz*)	83.9[g]	10*b*	-	3.12 (dd, 1H, J = *11.1, 2.2* Hz)	84.3
10	*a* 1.62[b] (m, 1H)	22.5	-	-	*a* 1.65 (m, 1H)	22.8
	b 1.19 (m, 1H)		11*a*	9[d], 11	*b* 1.18 (m, 1H)	
11	*a* 2.36 (br d, 1H, J = *11.6* Hz)	35.0	11*b*, 10*a* [b]	10, 12, 7[d], 9[d], 12-CO_2H	*a* 2.35 (d, 1H, J = *11.4* Hz)	35.3
	b 1.24 (m, 1H)		11a	12, 10, 12-<u>C</u>O_2H	*b* 1.23 (m, 1H)	
12	-	47.8	-	-	-	47.3
13	1.67[e] (m, 1H)	45.8	-	-	1.67 (m, 1H)	46.1
14	*a* 1.68[e] (m, 1H)	23.1	-	-	*a* 1.61 (m, 1H)	21.6
	b 1.82[a] (m, 1H)		-	-	*b* 1.81 (m, 1H)	
15	*a* 1.68[e] (m, 1H)	24.5	-	-	*a* 1.69 (m, 1H)	24.8
	b 1.50 (m, 1H)		16	14, 16	*b* 1.50 (m, 1H)	
16	2.62 (m, 1H)	48.4	15*b*, 17*b*	3, 17, 3-Me	2.61 (m, 1H)	48.7
17	*a* 2.57[c] (m, 1H)	26.7	-	-	*a* 2.57 (dd, 1H, J= *12.9, 6.4* Hz)	27.0
	b 2.24 (dd, 1H, J = *12.6*, *11.0* Hz)		16, 17*a*[c]	2, 15, 16, 18	*b* 2.24 (dd, 1H, J= *12.9, 10.6* Hz)	
18	-	116.2	-	-	-	115.9
19	-	124.9	-	-	-	124.4
20	7.25[f] (dd, 1H, J = *7.4, 2.6* Hz)	117.3	-	-	7.24 (d, 1H, J = *7.9* Hz)	117.7
21	6.89 (t, 1H, J = *7.4* Hz)	118.1	20[f], 22	19, 23	6.89 (t, 1H, J = *7.9* Hz)	118.5
22	6.93 (t, 1H, J = *7.4* Hz)	119.0	21, 23[f]	20, 24	6.93 (t, 1H, J = *7.9* Hz)	119.4
23	7.25[f] (dd, 1H, J = *7.4, 2.6* Hz)	111.6	-	-	7. 26 (d, 1H, J = *7.9* Hz)	111.9
24	-	140.7	-	-	-	140.3
25	-	70.8	-	-	-	70.4
26	0.99 (s, 3H)	24.7	-	9[d], 25, 27	0.99 (s, 3H)	24.5
27	1.08 (s, 3H)	26.7	-	9[d], 25, 26	1.09 (s, 3H)	27.0
12-CO_2H	-	175.7	-	-	-	175.4
3-Me	0.93 (s, 3H)	14.1	-	2, 3, 4, 16	0.92 (s, 3H)	14.5
4-Me	0.97 (s, 3H)	15.7	-	3, 4, 5, 13	0.97 (s, 3H)	16.2
25-O<u>H</u>	4.04 (s, 1H)	-	-	9[d], 25, 26, 27	-	-

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

*Literature data were recorded (^{1}H NMR in 600 MHz and ^{13}C NMR in 150 MHz) in DMSO-d_6

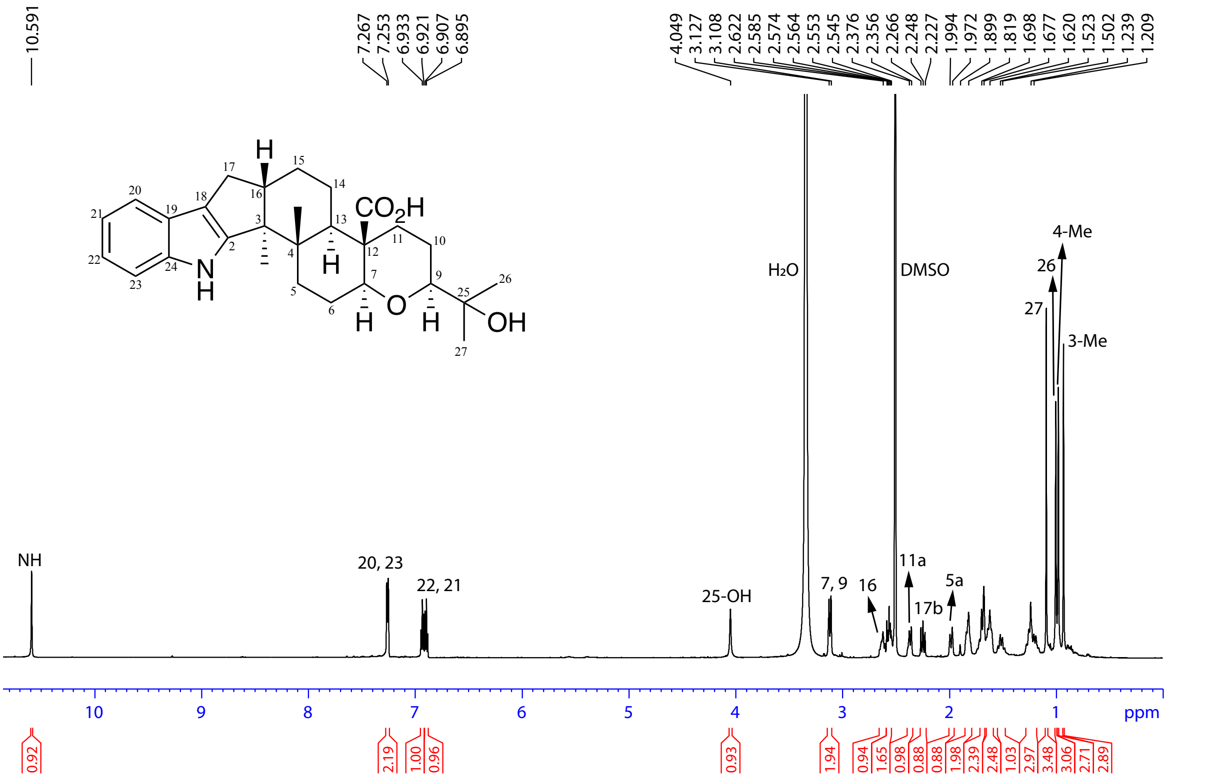


Figure S60. ^{1}H NMR (DMSO-d_6) spectrum of 12-demethylpaspaline-12-carboxylic acid (**13**)

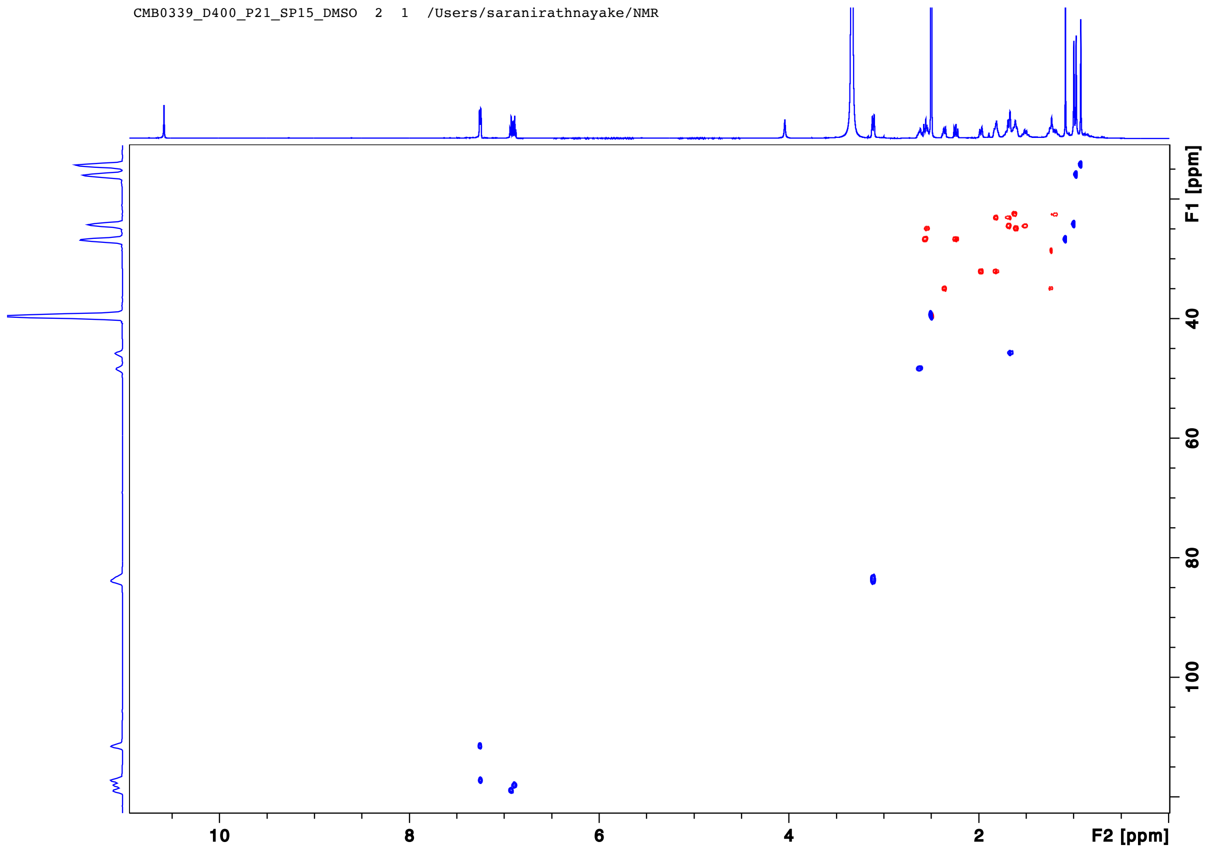


Figure S61. HSQC (DMSO-d_6) spectrum of 12-demethylpaspaline-12-carboxylic acid (**13**)

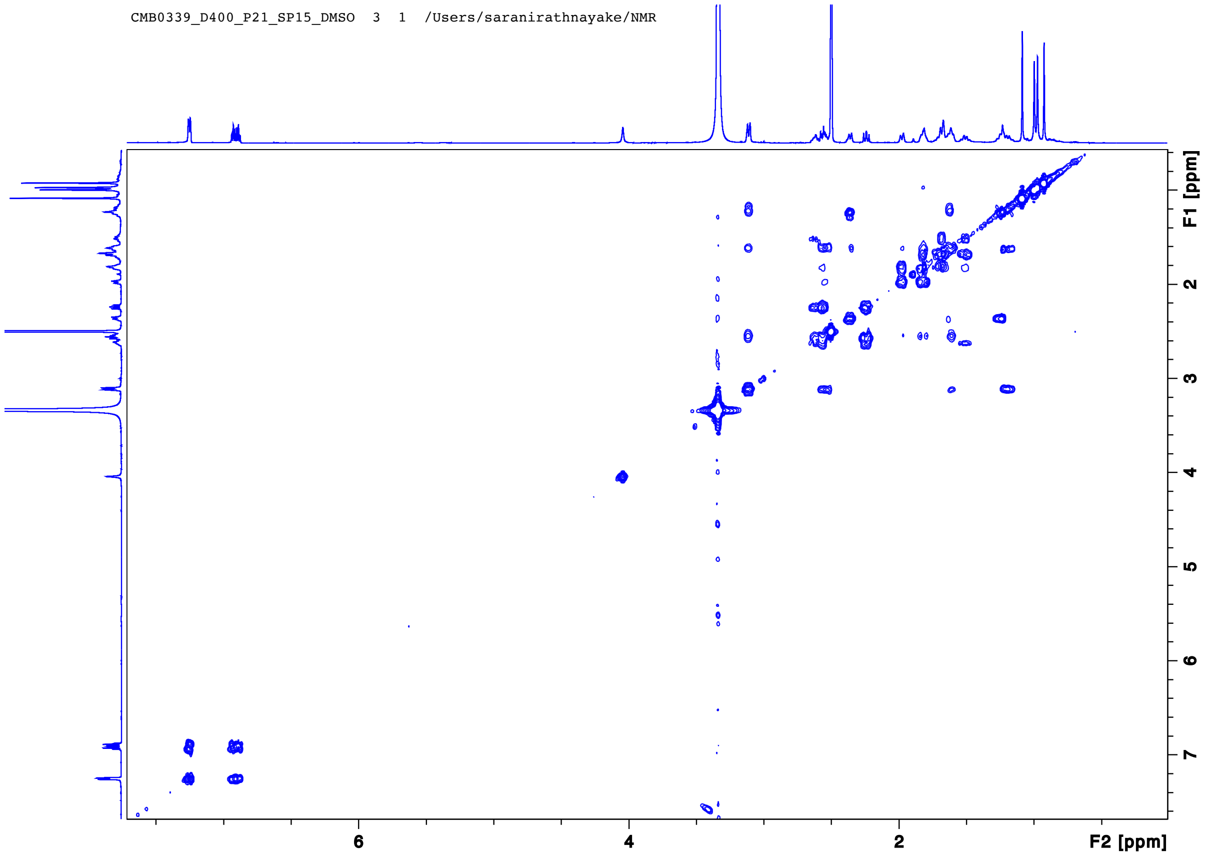


Figure S62. COSY (DMSO-d_6) spectrum of 12-demethylpaspaline-12-carboxylic acid (**13**)

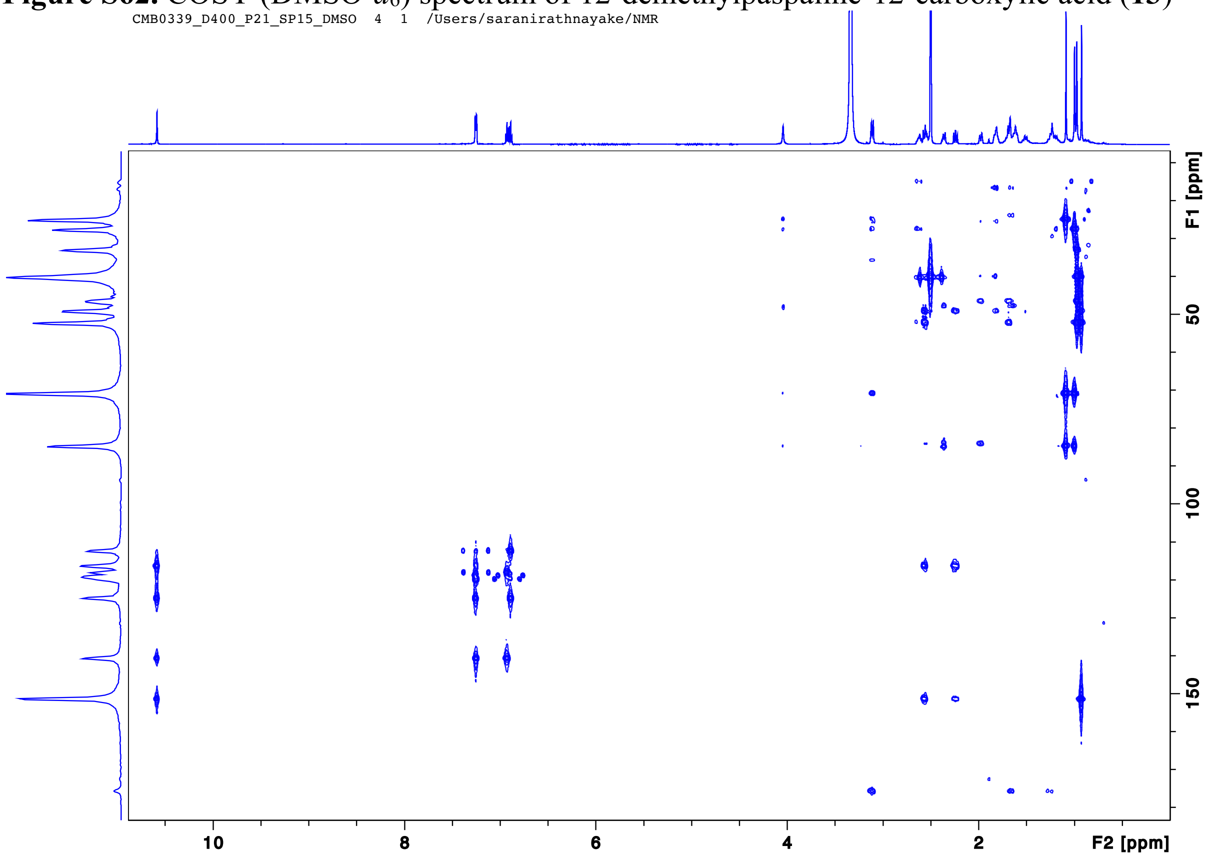


Figure S63. HMBC (DMSO-d_6) spectrum of 12-demethylpaspaline-12-carboxylic acid (**13**)

Mass Spectrum Molecular Formula Report

Analysis Info

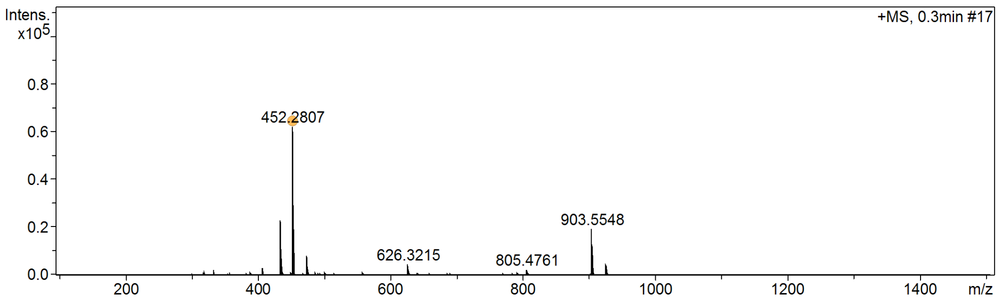
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_P21_SP15.d	Acquisition Date	9/8/2021 4:57:44 PM
Method	tune-medhigh_AP.m	Operator	a.salim
Sample Name	CMB0339_D400_P21_SP15	Instrument / Ser#	micrOTOF 213750.00232
Comment			

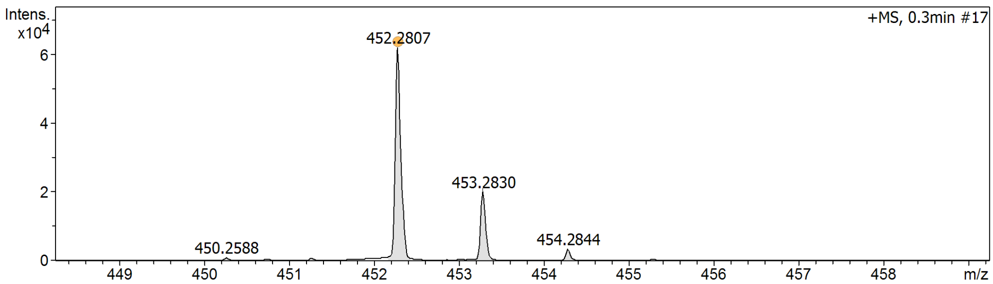
Acquisition Parameter

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
452.2807	1	C28H38NO4	452.2795	2.7	4.7	1	61.14	10.5	even	ok
	2	C29H34N5	452.2809	-0.3	7.6	2	100.00	15.5	even	ok
	3	C26H36N4O3	452.2782	5.6	10.0	3	20.62	11.0	odd	ok
	4	C31H36N2O	452.2822	3.3	13.7	4	43.26	15.0	odd	ok
	5	C24H34N7O2	452.2768	8.6	16.1	5	4.69	11.5	even	ok
	6	C25H40O7	452.2769	8.6	21.7	6	4.19	6.0	odd	ok

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Figure S64. HRMS spectrum of 12-demethylpaspaline-12-carboxylic acid (**13**)

13 Emindole SB (14)

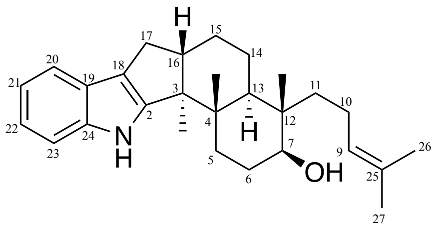


Table S11. 1D and 2D NMR (DMSO-d_6, 600 MHz) data of emindole SB (**14**)
(Reported data are shaded in grey)

Pos.	δ_H, mult. (*J* in Hz)	δ_C	COSY	^{1}H-^{13}C HMBC	δ_H (mult., *J* (Hz) [1]	δ_C [1]
1-NH	10.55 (s, 1H)	-	-	2, 18, 19, 24	10.55 (s, 1H)	-
2	-	151.8		-	-	151.3
3	-	52.9		-	-	52.6
4	-	39.2		-	-	40.8
5	*a* 1.85 (m, 1H)	31.7	-	4, 7, 4-Me	*a* 1.84 (m, 1H)	32.0
	b 1.68[a] (m, 1H)		-	-	*b* 1.68 (m, 1H)	
6	*a* 1.68[a] (m, 1H)	27.0	-	-	*a* 1.67 (m, 1H)	27.4
	b 1.62 (m, 1H)		-	-	*b* 1.52 (m, 1H)	
7	3.38 (m, 1H)	71.0	7-OH	-	3.38 (m, 1H)	71.4
9	5.09 (t, 1H, J = *7.0* Hz)	124.9	10*a*, 10*b*	26, 27, 10	5.10 (t, 1H, J = *7.4* Hz)	125.2
10	*a* 1.92 (m, 1H)	20.7	10*b*, 9, 11*b*	9, 11, 25	*a* 1.92 (m, 1H)	21.1
	b 1.8 (m, 1H)		10*a*, 9	-	*b* 1.85 (m, 1H)	
11	*a* 1.56[b] (m, 1H)	36.9	-	-	*a* 1.54 (m, 1H)	37.2
	b 1.10 (ddd, 1H, J = *14.0, 12.6, 4.9* Hz)		10*a*, 10*b*	-	*b* 1.11 (m, 1H)	
12	-	41.3			-	38.7
13	1.66[a] (m, 1H)	39.1	-	-	1.67 (m, 1H)	39.6
14	*a* 1.52 (m, 1H)	22.1	14*b*, 15*a*	13, 16	*a* 1.51 (m, 1H)	22.4
	b 1.36 (ddd, 1H, J = *15.1, 13.5, 4.7* Hz)		14*a*	-	*b* 1.36 (m, 1H)	
15	*a* 1.70 (m, 1H)	24.7	14*a*, 16	-	*a* 1.69 (m, 1H)	25.0
	b 1.54[b] (m, 1H)		-	-	*b* 1.53 (m, 1H)	
16	2.64 (m, 1H)	48.2	17*a*, 17*b*	-	2.62 (m, 1H)	48.7
17	*a* 2.56 (dd, 1H, J = *13.0, 6.4* Hz)	26.7	17*b*, 16	2, 3, 16, 18	2.56 (dd, 1H, J = (*13.0, 6.4* Hz)	27.1
	b 2.23 (dd, 1H, J = *13.0, 10.8* Hz)		17*a*, 16	2, 16, 18	2.23 (m, 1H)	27.1
18	-	116.4	-	-	-	115.9
19	-	124.9		-	-	124.5
20	7.25 (d, 1H, J = *7.5* Hz)	117.2	21	22, 24	7.25 (d, 1H, J = *7.8* Hz)	117.6
21	6.88 (dt, 1H, J = *7.5, 1.3* Hz)	118.0	20, 22	19, 23	6.89 (td, 1H, J = *7.0, 1.2* Hz)	118.4
22	6.92 (dt, 1H, J = *7.5, 0.8* Hz)	118.9	21, 23	20, 24	6.93 (td, 1H, J = *7.0, 1.3* Hz)	119.3
23	7.26 (d, 1H, J = *7.5* Hz)	111.4	22	19, 21	7. 26 (d, 1H, J = *7.7* Hz)	111.9
24	-	140.7	-		-	140.3
25	-	130.4	-		-	129.9
26	1.58 (s, 3H)	17.2	-	9, 25, 26	1.59 (s, 3H)	17.5
27	1.64 (s, 3H)	25.2		9, 25, 27	1.65 (s, 3H)	25.6
12-Me	0.71 (s, 3H)	16.6	-	7, 11, 12, 13	0.71 (s, 3H)	16.9
3-Me	0.94 (s, 3H)	14.4	-	2, 3, 4, 16	0.93 (s. 3H)	14.6
4-Me	1.01 (s, 3H)	18.4	-	3, 4, 5, 13	1.01 (s, 3H)	18.7
7-OH	4.32 (d, 1H, J = *5.0* Hz)	-	7	-	4.36 (d, 1H, J = *5.2* Hz)	-

[a-b] Resonances with the same superscript are overlapping and assignments may be interchanged
*Literature data were recorded (^{1}H NMR in 600 MHz and ^{13}C NMR in 150 MHz) in DMSO-d_6

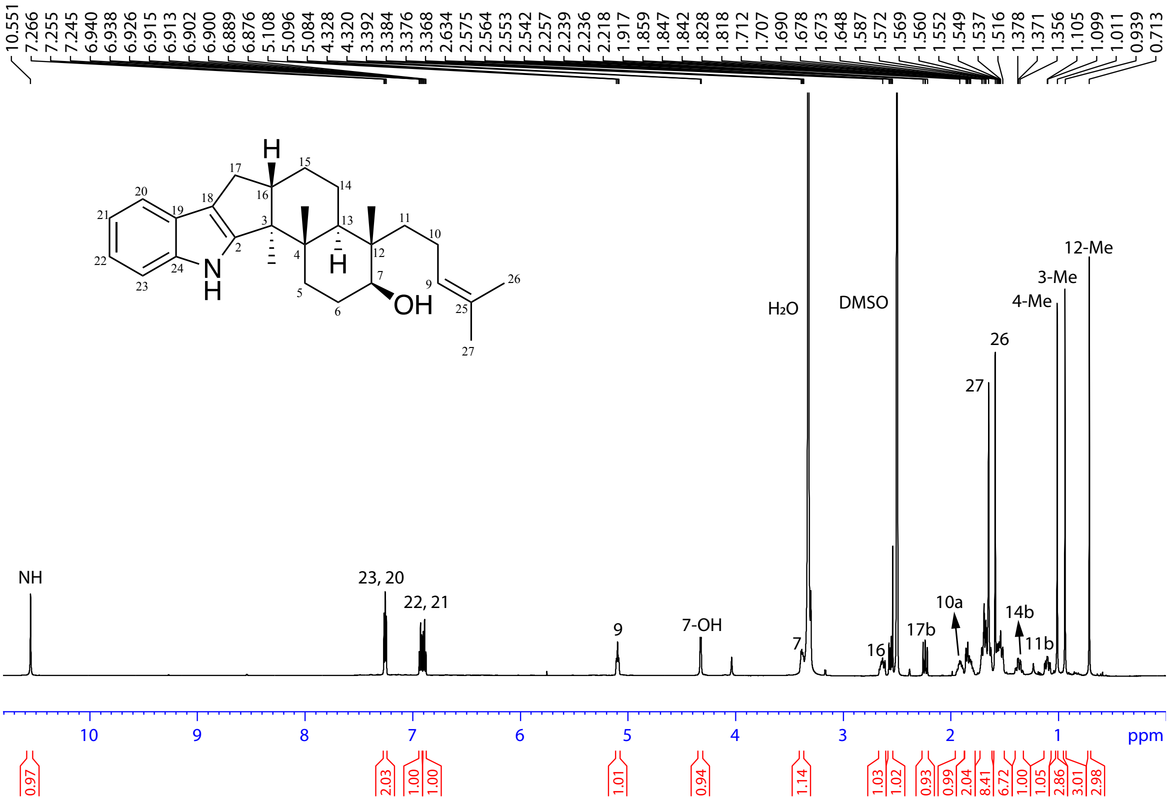


Figure S65. ^{1}H NMR (DMSO-d_6) spectrum of emindole SB (**14**)

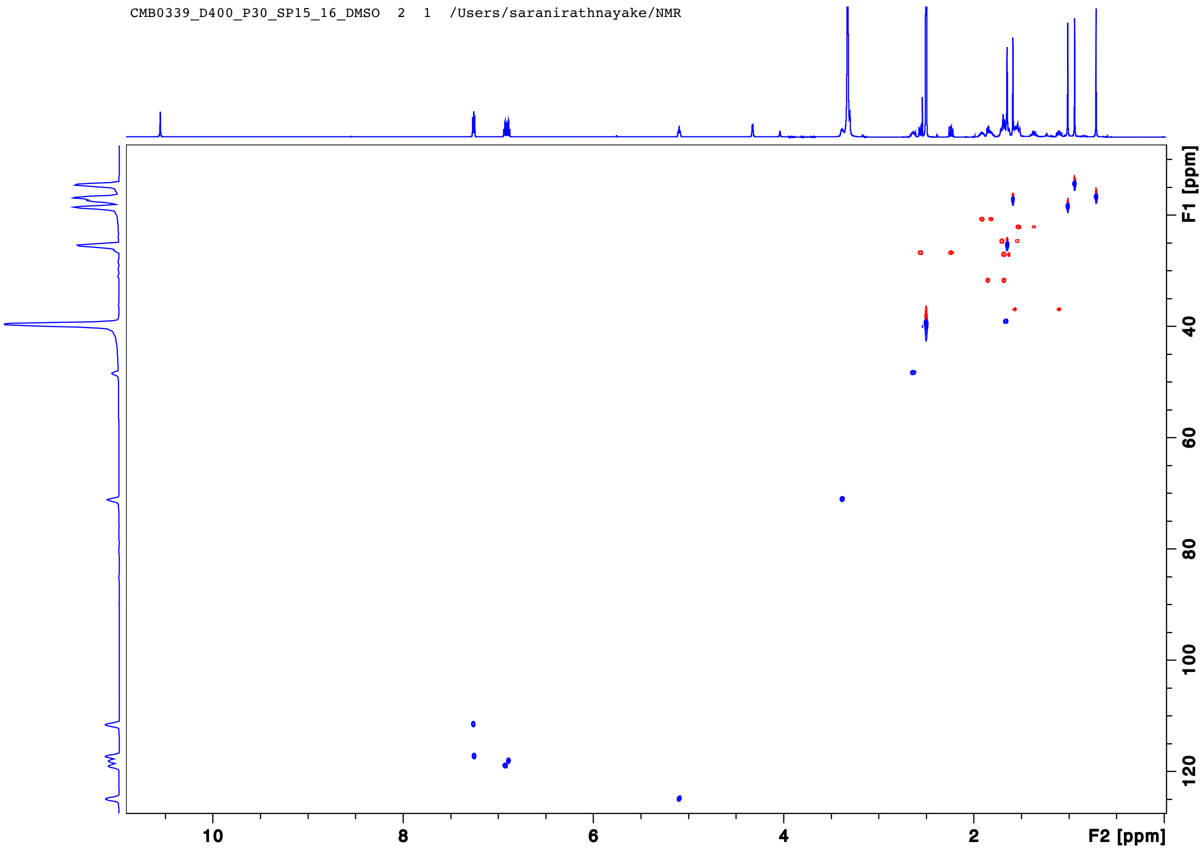


Figure S66. HSQC (DMSO-d_6) spectrum of emindole SB (**14**)

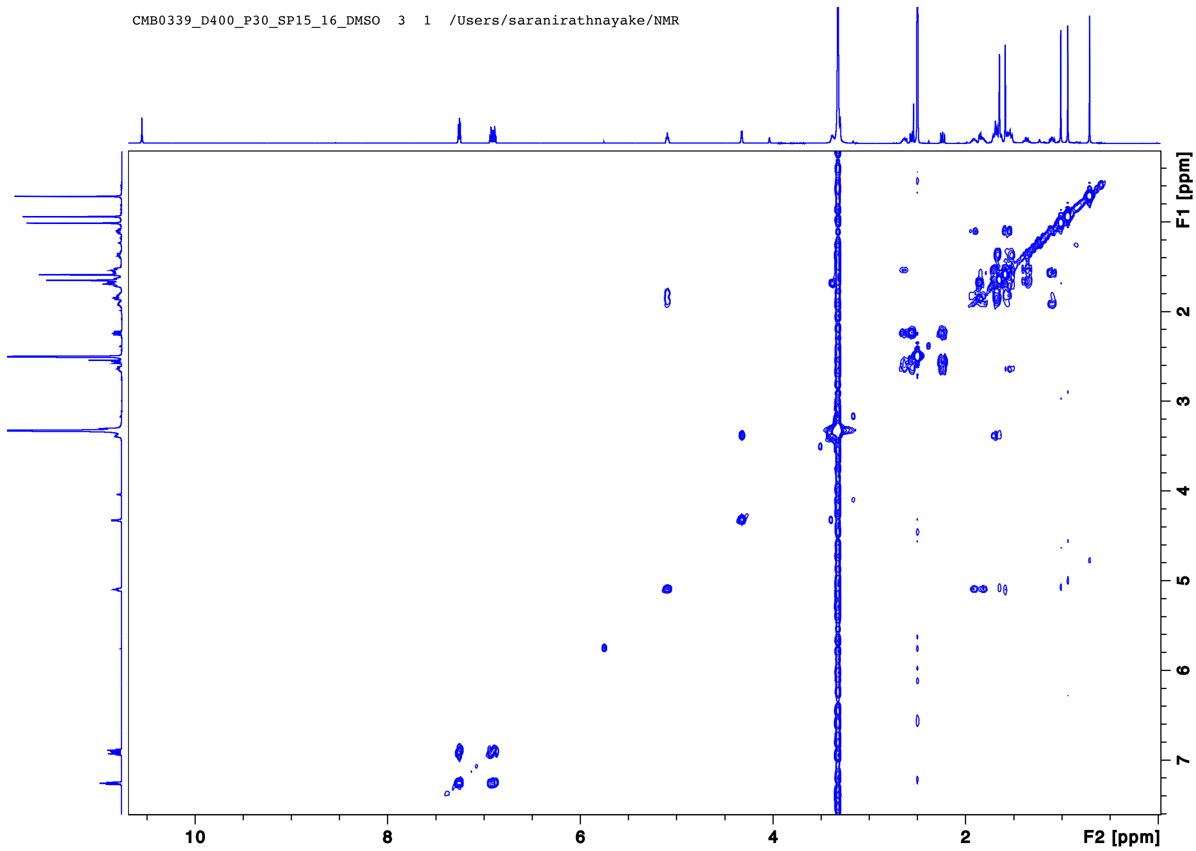


Figure S67. COSY (DMSO-d_6) spectrum of emindole SB (**14**)

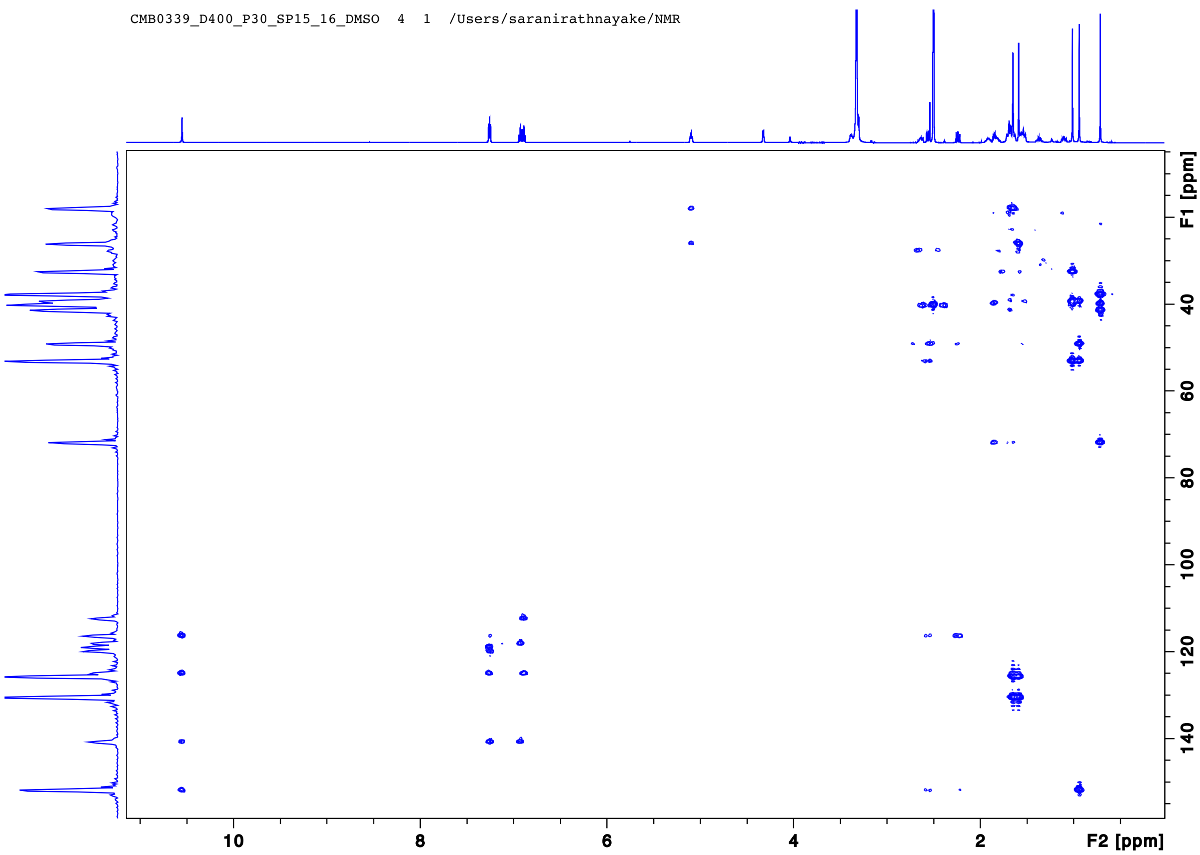


Figure S68. HMBC (DMSO-d_6) spectrum of emindole SB (**14**)

Mass Spectrum Molecular Formula Report

Analysis Info

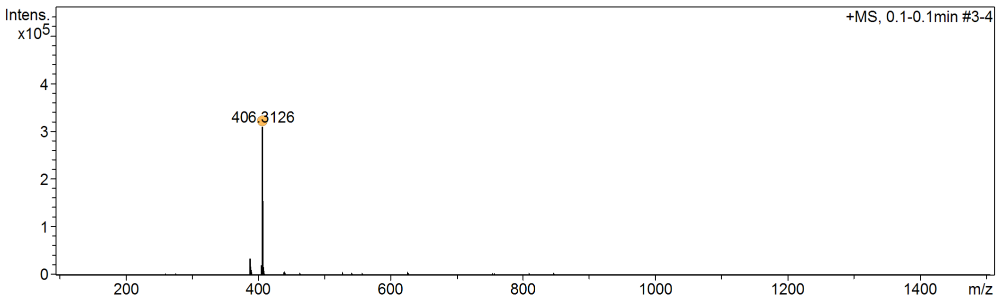
Analysis Name	D:\Data\s.kankanamge\CMB0339_D400_P30_SP15_16.d	Acquisition Date	9/8/2021 4:54:59 PM
Method	tune-medhigh_AP.m	Operator	a.salim
Sample Name	CMB0339_D400_P30_SP15_16	Instrument / Ser#	micrOTOF 213750.00232
Comment			

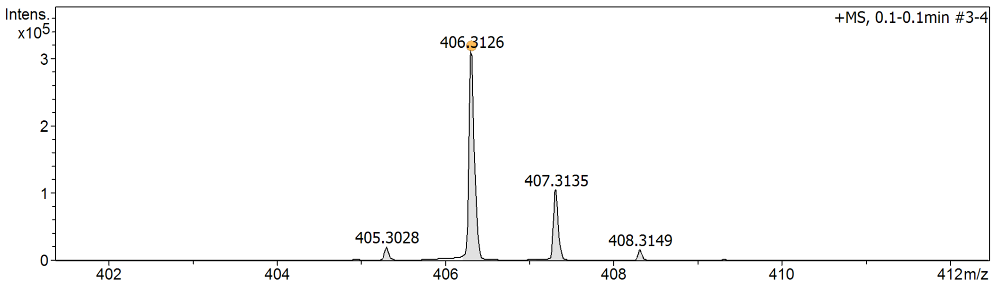
Acquisition Parameter

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
406.3126	1	C28H40NO	406.3104	5.3	12.5	1	100.00	9.5	even	ok

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Figure S69. HRMS spectrum of emindole SB (**14**)

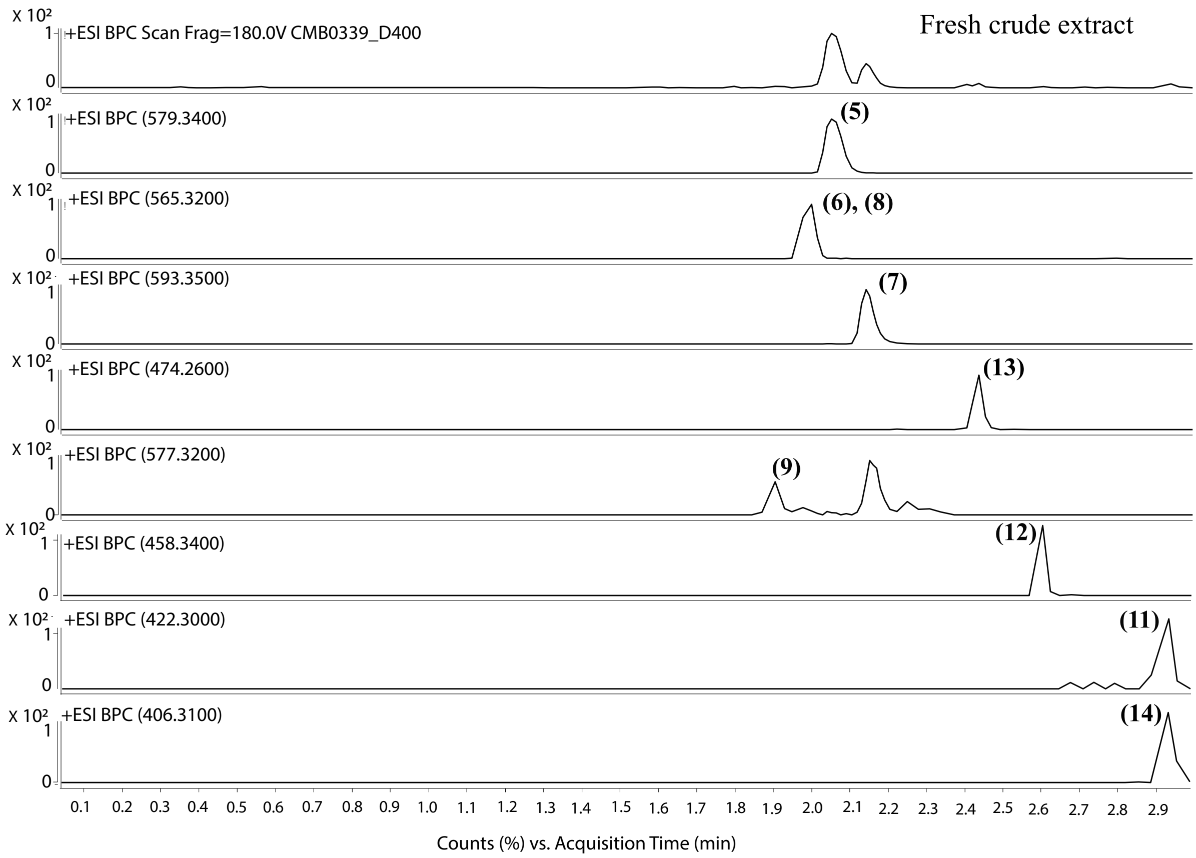

Figure S70. Single ion extraction of CMB-M0339 fresh crude extract to show the presence of isolated metabolites

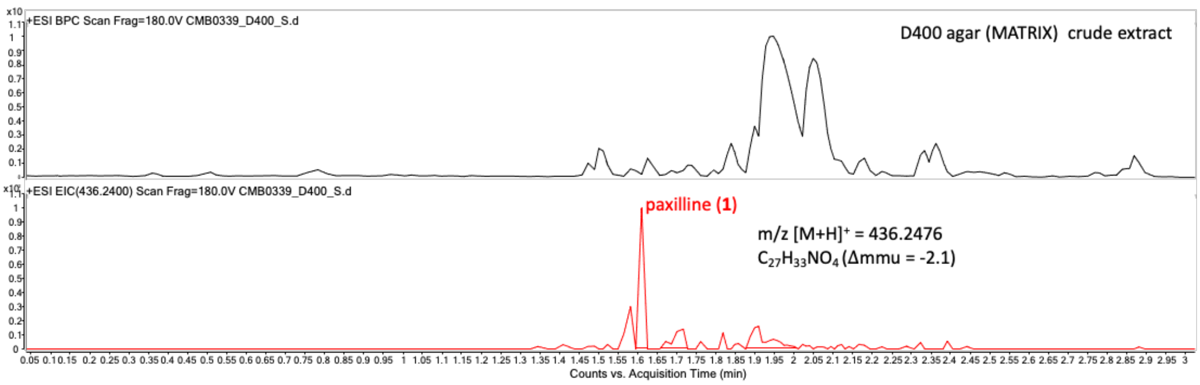

Figure S71. Single ion extraction of crude extract of CMB-M0339 grown on D400 agar (MATRIX) to show the presence of paxilline (**1**)

14 MS/MS fragmentation patterns of 5 - 9 and i-v

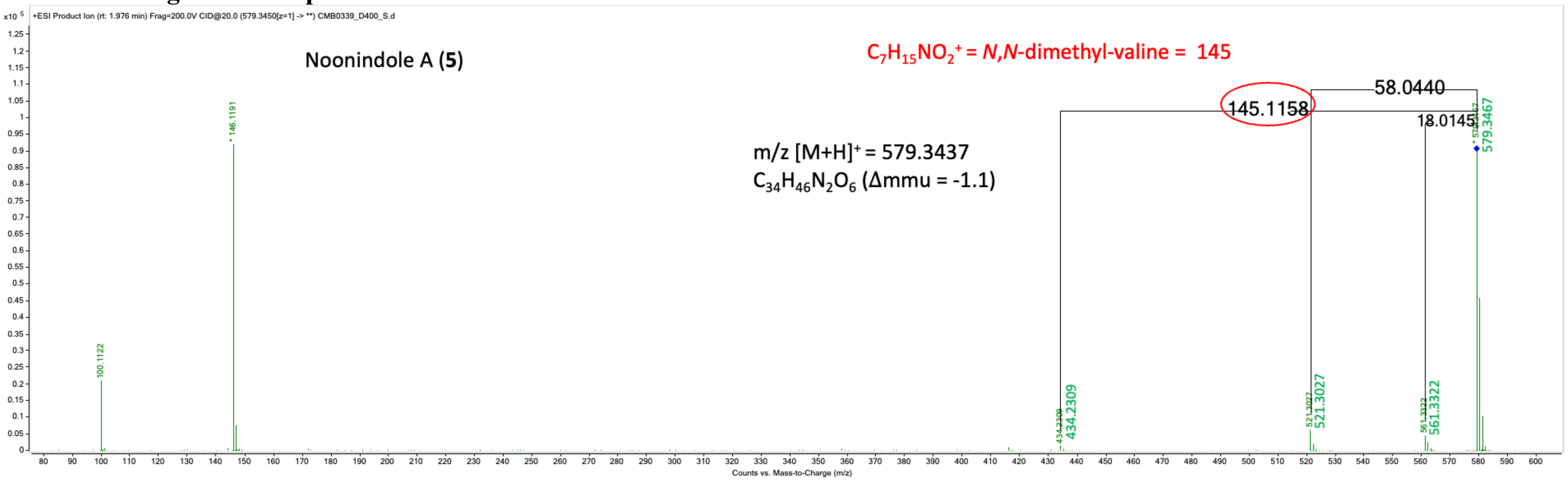

Figure S72. MS/MS fragmentation pattern of (**5**)

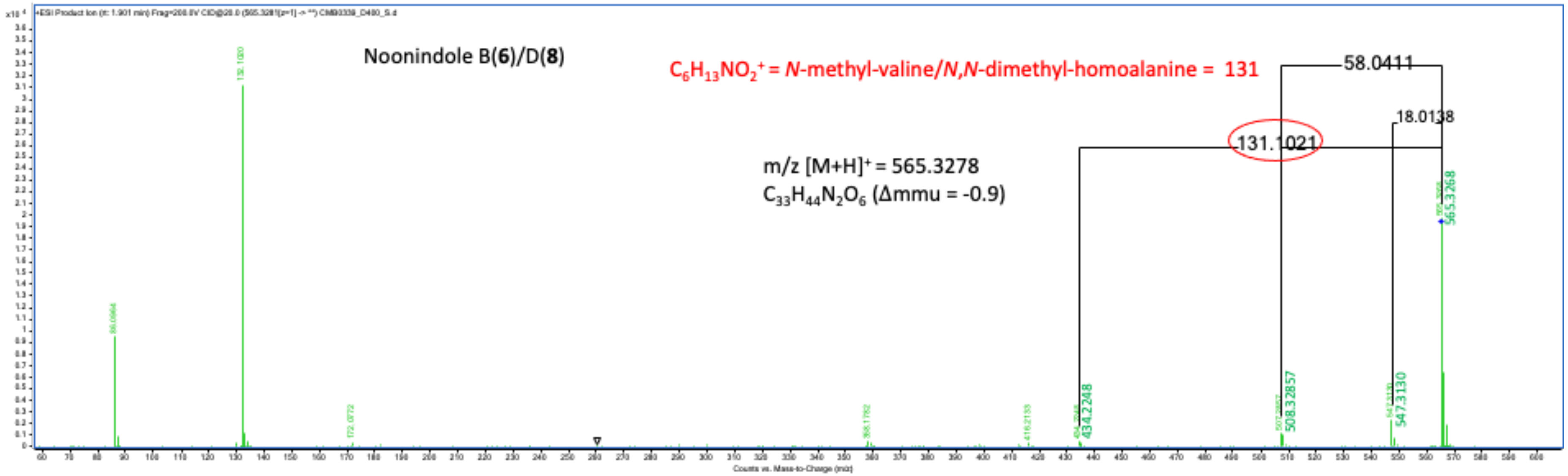

Figure S73. MS/MS fragmentation pattern of (**6**)/(**8**)

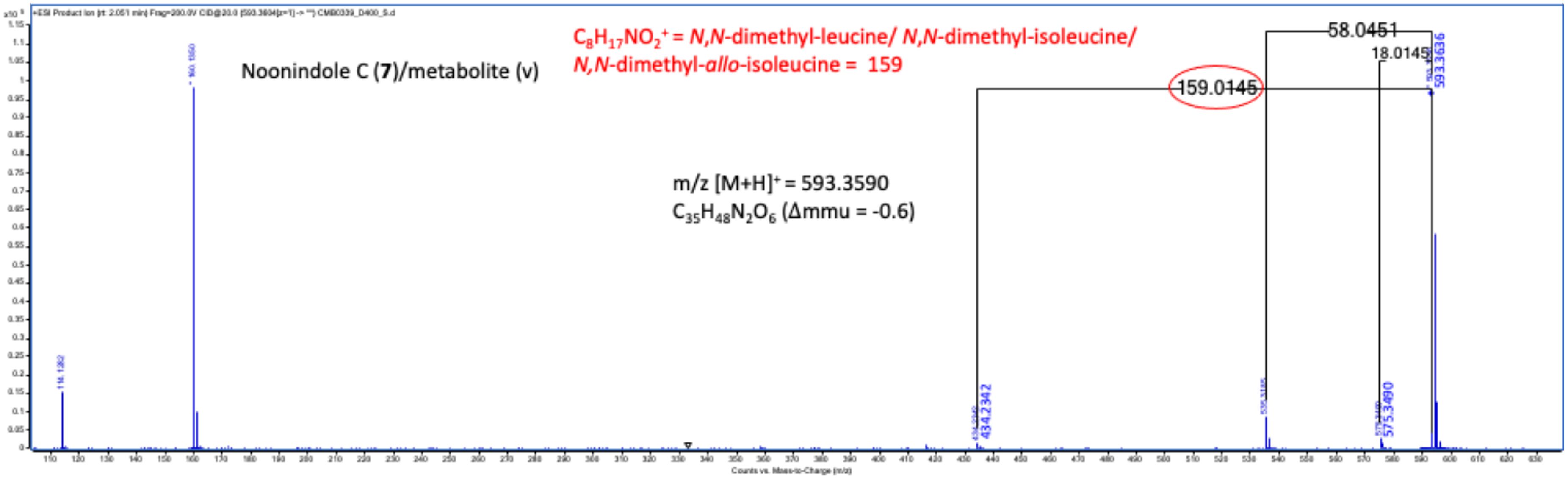

Figure S74. MS/MS fragmentation pattern of (**7**)/v

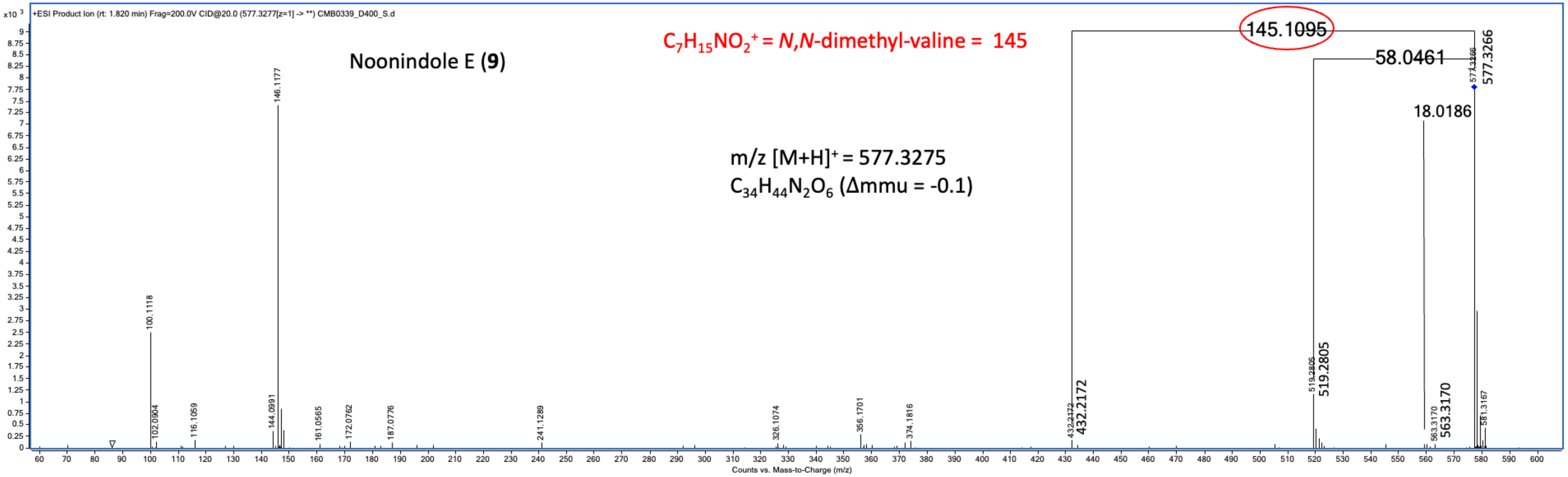

Figure S75. MS/MS fragmentation pattern of (**9**)

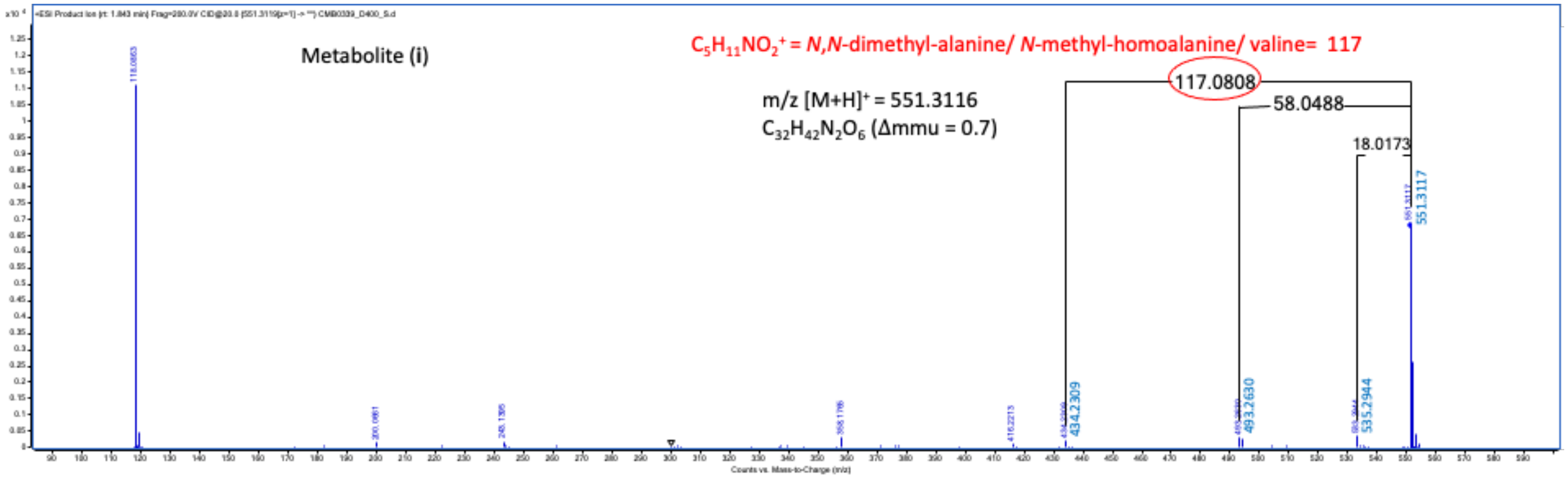

Figure S76. MS/MS fragmentation pattern of i

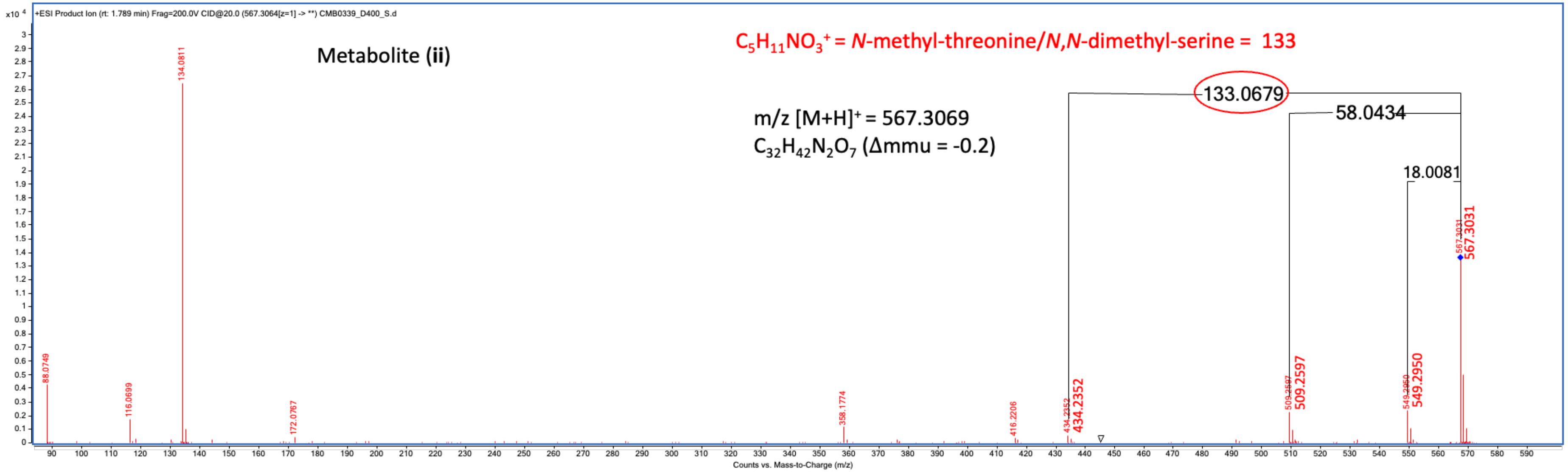

Figure S77. MS/MS fragmentation pattern of ii

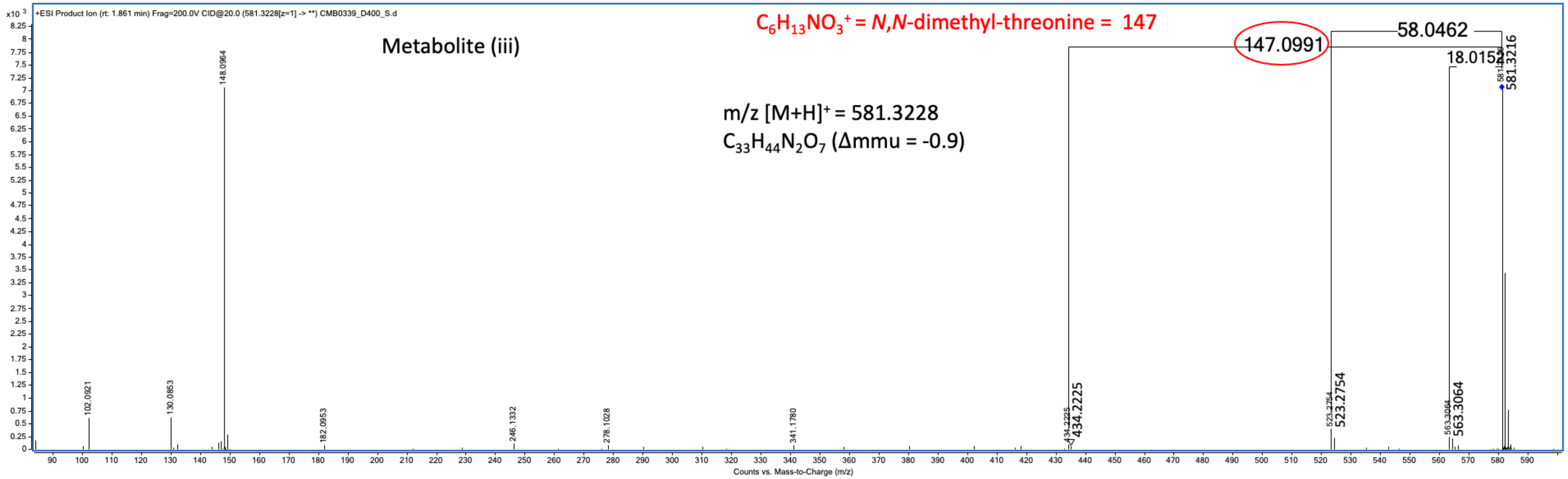

Figure S78. MS/MS fragmentation pattern of iii

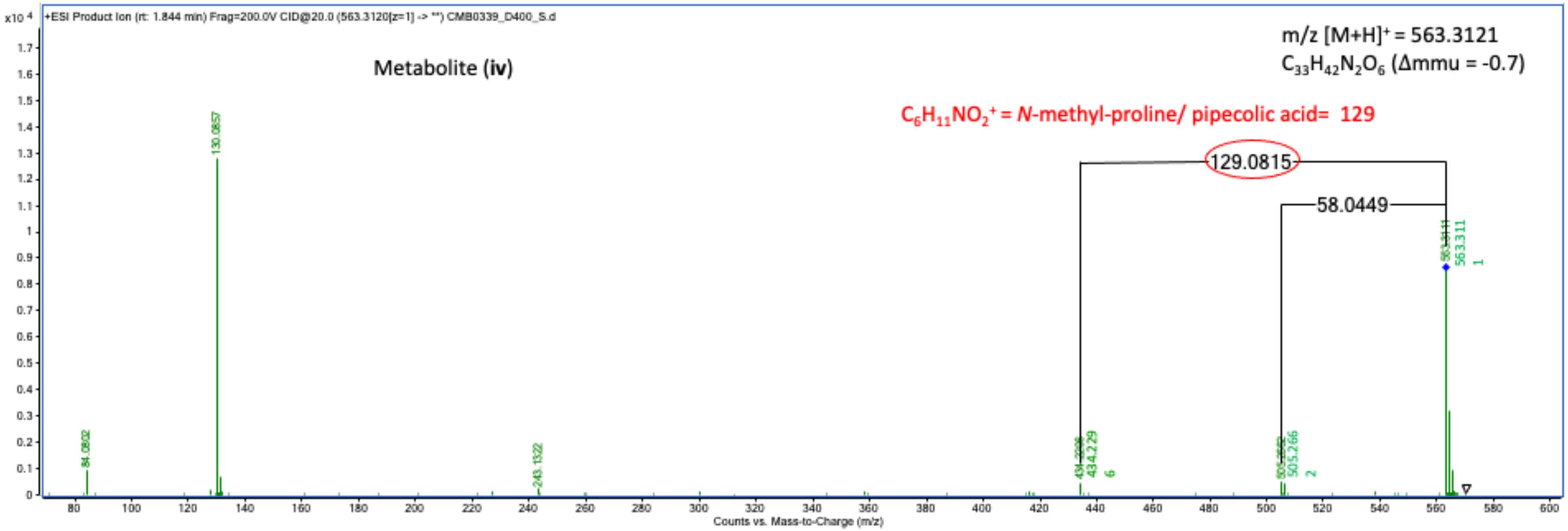

Figure S79. MS/MS fragmentation pattern of iv

Table S12. Molecular formulas generated for noonindoles A (**5**) -E (**9**) and predicted molecular formulas for minor metabolites (**i**) – (**viii**) observed in GNPS cluster

Metabolites		**HRESI m/z [M+H]$^+$**	**HRESI MW**	**Predicted MF**	**ΔmDa**
Isolated metabolites	**Minor metabolites detected in GNPS cluster**				
(**5**)		579.3437	578.3363	$C_{34}H_{46}N_2O_6$	-1.1
(**6**)/(**8**)		565.3278	564.3205	$C_{33}H_{44}N_2O_6$	-0.9
(**7**)		593.3590	592.3516	$C_{35}H_{48}N_2O_6$	-0.6
(**9**)		577.3275	576.3200	$C_{34}H_{44}N_2O_6$	-0.1
	(i)	551.3116	550.3051	$C_{32}H_{42}N_2O_6$	0.7
	(ii)	567.3069	566.2993	$C_{32}H_{42}N_2O_7$	-0.2
	(iii)	581.3228	580.3154	$C_{33}H_{44}N_2O_7$	-0.9
	(iv)	563.3121	562.3052	$C_{33}H_{42}N_2O_6$	-0.7
	(v)	593.3590	592.3516	$C_{35}H_{48}N_2O_6$	-0.6
	(vi)	609.3545	608.3472	$C_{35}H_{48}N_2O_7$	-1.7
	(vii)	591.3434	590.3362	$C_{35}H_{46}N_2O_6$	-0.9
	(viii)	595.3383	594.3309	$C_{34}H_{46}N_2O_7$	-0.6

15 Crystal data and structure refinement for noonindole A (5).

Identification code	2100_0339_p12	
Empirical formula	$C_{36}H_{46}F_3N_2O_8.3H_2O$	
Formula weight	746.80	
Temperature	190(2) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	$P\ 2_1\ 2_1\ 2_1$	
Unit cell dimensions	a = 11.0176(2) Å	α= 90°.
	b = 19.8910(3) Å	β= 90°.
	c = 20.5726(2) Å	γ = 90°.
Volume	4508.51(12) Å^3	
Z	4	
Density (calculated)	1.100 Mg/m^3	
Absorption coefficient	0.750 mm^{-1}	
F(000)	1592	
Crystal size	0.200 x 0.200 x 0.200 mm^3	
Theta range for data collection	4.298 to 61.601°.	
Index ranges	-12<=h<=12, -22<=k<=22, -23<=l<=16	
Reflections collected	6976	
Independent reflections	6976 [R(int) = 0.0399]	
Completeness to theta = 61.602°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6976 / 6 / 475	

Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0332, wR2 = 0.0845
R indices (all data)	R1 = 0.0365, wR2 = 0.0863
Absolute structure parameter	-0.06(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.112 and -0.145 e.Å^{-3}

Table S13. Bond lengths [Å] and angles [°] for X-ray crystal structure of noonindole A (**5**)

C(1)-C(2)	1.379(3)	C(19)-C(20)	1.340(3)
C(1)-C(6)	1.392(3)	C(20)-C(21)	1.458(3)
C(2)-C(3)	1.396(4)	C(21)-O(2)	1.223(3)
C(3)-C(4)	1.378(3)	C(21)-C(22)	1.508(4)
C(4)-C(5)	1.399(3)	C(22)-O(1)	1.423(3)
C(5)-C(6)	1.427(3)	C(22)-C(23)	1.552(4)
C(5)-C(7)	1.427(3)	C(23)-O(5)	1.430(4)
C(6)-N(1)	1.382(3)	C(23)-C(24)	1.503(7)
C(7)-C(11)	1.363(3)	C(23)-C(25)	1.517(6)
C(7)-C(8)	1.508(3)	C(26)-O(4)	1.199(3)
C(8)-C(9)	1.548(3)	C(26)-O(3)	1.341(3)
C(9)-C(12)	1.511(3)	C(26)-C(27)	1.512(3)
C(9)-C(10)	1.565(3)	C(27)-N(2)	1.502(3)
C(10)-C(11)	1.512(3)	C(27)-C(28)	1.550(3)
C(10)-C(33)	1.542(3)	C(28)-C(30)	1.517(4)
C(10)-C(15)	1.562(3)	C(28)-C(29)	1.519(4)
C(11)-N(1)	1.376(3)	C(32)-N(2)	1.492(3)

C(12)-C(13)	1.524(3)	C(35)-O(8)	1.215(3)
C(13)-O(3)	1.466(2)	C(35)-O(7)	1.238(3)
C(13)-C(14)	1.530(3)	C(35)-C(36)	1.507(6)
C(14)-O(6)	1.428(3)	C(36)-F(3)	1.318(4)
C(14)-C(19)	1.526(3)	C(36)-F(1)	1.319(4)
C(14)-C(15)	1.589(3)	C(36)-F(2')	1.320(4)
C(15)-C(34)	1.537(3)	C(36)-F(1')	1.320(4)
C(15)-C(16)	1.539(3)	C(36)-F(2)	1.325(4)
C(16)-C(17)	1.543(3)	C(36)-F(3')	1.326(4)
C(17)-C(18)	1.535(3)	N(2)-C(31)	1.502(3)
C(18)-O(1)	1.435(3)	C(16)-C(15)-C(10)	112.06(16)
C(18)-C(19)	1.509(3)	C(34)-C(15)-C(14)	110.28(16)
C(2)-C(1)-C(6)	117.5(2)	C(16)-C(15)-C(14)	106.00(17)
C(1)-C(2)-C(3)	121.7(2)	C(10)-C(15)-C(14)	110.05(16)
C(4)-C(3)-C(2)	121.2(2)	C(15)-C(16)-C(17)	112.10(18)
C(3)-C(4)-C(5)	119.0(2)	C(18)-C(17)-C(16)	114.0(2)
C(4)-C(5)-C(6)	118.78(19)	O(1)-C(18)-C(19)	111.4(2)
C(4)-C(5)-C(7)	136.0(2)	O(1)-C(18)-C(17)	103.41(19)
C(6)-C(5)-C(7)	105.17(18)	C(19)-C(18)-C(17)	112.64(19)
N(1)-C(6)-C(1)	129.4(2)	C(20)-C(19)-C(18)	119.72(19)
N(1)-C(6)-C(5)	108.79(17)	C(20)-C(19)-C(14)	125.7(2)
C(1)-C(6)-C(5)	121.81(19)	C(18)-C(19)-C(14)	114.48(18)
C(11)-C(7)-C(5)	108.14(19)	C(19)-C(20)-C(21)	121.4(2)
C(11)-C(7)-C(8)	111.31(18)	O(2)-C(21)-C(20)	121.0(3)
C(5)-C(7)-C(8)	140.3(2)	O(2)-C(21)-C(22)	121.6(2)
C(7)-C(8)-C(9)	98.48(17)	C(20)-C(21)-C(22)	117.3(2)
C(12)-C(9)-C(8)	121.56(18)	O(1)-C(22)-C(21)	110.4(2)
C(12)-C(9)-C(10)	111.31(18)	O(1)-C(22)-C(23)	107.0(2)
C(8)-C(9)-C(10)	106.60(16)	C(21)-C(22)-C(23)	113.4(3)
C(11)-C(10)-C(33)	106.18(15)	O(5)-C(23)-C(24)	109.8(3)
C(11)-C(10)-C(15)	119.45(17)	O(5)-C(23)-C(25)	107.4(3)
C(33)-C(10)-C(15)	113.48(18)	C(24)-C(23)-C(25)	111.4(4)
C(11)-C(10)-C(9)	96.36(16)	O(5)-C(23)-C(22)	107.8(3)
C(33)-C(10)-C(9)	111.32(17)	C(24)-C(23)-C(22)	110.9(3)
C(15)-C(10)-C(9)	108.78(15)	C(25)-C(23)-C(22)	109.4(3)
C(7)-C(11)-N(1)	110.21(17)	O(4)-C(26)-O(3)	124.3(2)
C(7)-C(11)-C(10)	112.63(18)	O(4)-C(26)-C(27)	123.4(2)
N(1)-C(11)-C(10)	135.9(2)	O(3)-C(26)-C(27)	112.2(2)

C(9)-C(12)-C(13)	105.98(17)	N(2)-C(27)-C(26)	110.95(19)
O(3)-C(13)-C(12)	107.95(16)	N(2)-C(27)-C(28)	113.1(2)
O(3)-C(13)-C(14)	106.76(16)	C(26)-C(27)-C(28)	110.63(17)
C(12)-C(13)-C(14)	114.24(17)	C(30)-C(28)-C(29)	111.1(2)
O(6)-C(14)-C(19)	106.77(17)	C(30)-C(28)-C(27)	114.7(2)
O(6)-C(14)-C(13)	109.50(16)	C(29)-C(28)-C(27)	110.1(2)
C(19)-C(14)-C(13)	113.66(16)	O(8)-C(35)-O(7)	127.7(3)
O(6)-C(14)-C(15)	107.63(15)	O(8)-C(35)-C(36)	115.2(3)
C(19)-C(14)-C(15)	106.78(16)	O(7)-C(35)-C(36)	116.9(2)
C(13)-C(14)-C(15)	112.20(16)	F(3)-C(36)-F(1)	109.6(9)
C(34)-C(15)-C(16)	108.71(18)		
C(34)-C(15)-C(10)	109.67(17)		
F(2')-C(36)-F(1')	99.9(9)		
F(3)-C(36)-F(2)	111.6(13)		
F(1)-C(36)-F(2)	101.3(10)		
F(2')-C(36)-F(3')	110.5(13)		
F(1')-C(36)-F(3')	116.4(13)		
F(3)-C(36)-C(35)	114.0(6)		
F(1)-C(36)-C(35)	116.8(6)		
F(2')-C(36)-C(35)	111.4(5)		
F(1')-C(36)-C(35)	108.8(7)		
F(2)-C(36)-C(35)	102.5(8)		
F(3')-C(36)-C(35)	109.5(8)		
C(11)-N(1)-C(6)	107.67(17)		
C(32)-N(2)-C(31)	108.6(2)		
C(32)-N(2)-C(27)	111.9(2)		
C(31)-N(2)-C(27)	111.8(2)		
C(22)-O(1)-C(18)	115.32(18)		
C(26)-O(3)-C(13)	116.59(17)		

16 Biological activity of 5-14

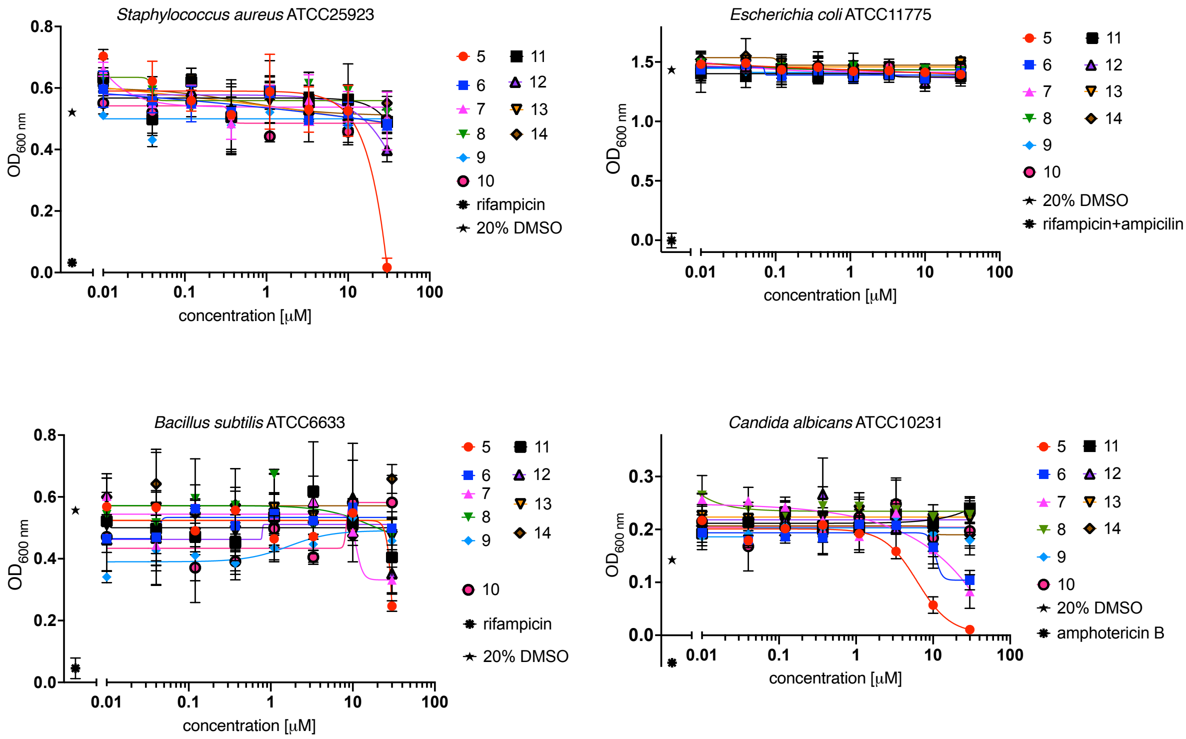

Figure S80. Antimicrobial activity of metabolites **5–14** against *S. aureus*, *E. coli*, *B. subtilis* and *C. albicans*

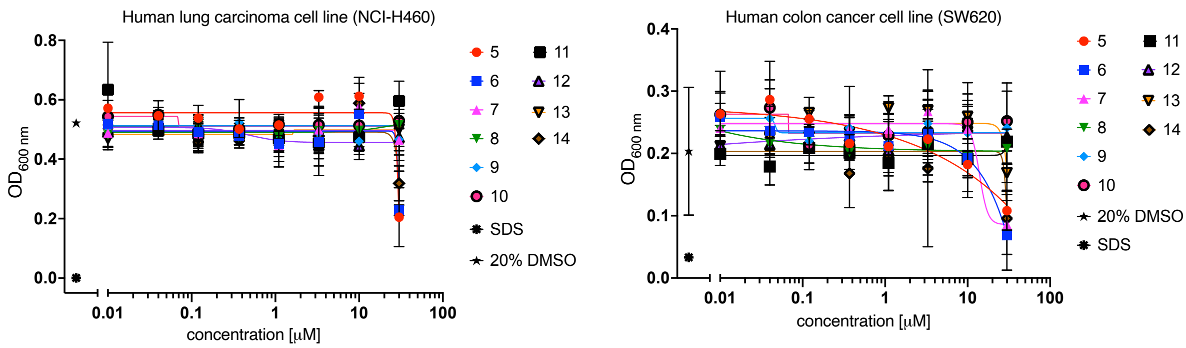

Figure S81. Cytotoxicity of metabolites **5–14** against human colon cancer (SW620) and human lung carcinoma (NCI-H460) cell lines

17 References

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