Table: NMR data of ascomycin (COCON input file).

No.	an[a]	H[b]	δ(^{13}C) [ppm]	Atype[c]	^{1}H,^{1}H-COSY (52)[d]	^{1}H,^{13}C-HMBC (86)[e]	1,1-ADEQ. (59)[f]
1	6	0	169	11	---	---	---
2	6	1	57	67	3	1, 3, 4, 6, 7	1, 3
3	6	2	28	130	2, 4	5	2, 4
4	6	2	21	130	3	---	3, 5
5	6	2	24	130	6	---	4, 6
6	6	2	39	130	5	2, 4, 5, 7	5
7	6	0	165	11	---	---	---
8	6	0	196	11	---	---	---
9	6	0	97	4	---	---	---
10	6	1	35	67	11, 12	9, 11, 12	9, 11, 12
11	6	3	16	193	10	9, 10, 12	10
12	6	2	33	130	10, 13	9, 10, 13	10, 13
13	6	1	74	67	12, 15	---	12, 15
14	6	3	56	193	---	13	---
15	6	1	73	67	13, 16	9, 12, 13	13, 16
16	6	1	75	67	18	---	15, 18
17	6	3	57	193	---	16	---
18	6	2	33	130	16, 19	16	16, 19
19	6	1	26	67	18, 20, 21	22	18, 20, 21
20	6	3	20	193	19	18, 19, 21	19
21	6	2	49	130	19	18, 19, 20, 22, 23, 24	19, 22
22	6	0	139	11	---	---	---
23	6	3	16	193	---	21, 22, 24	22
24	6	1	123	74	25	21, 23, 25, 26	22, 25
25	6	1	55	67	24, 42	22, 24, 26, 42, 43	24, 26, 42
26	6	0	213	11	---	---	---
27	6	2	43	130	28	26, 28, 29	26, 28
28	6	1	70	67	27, 29	---	27, 29

29	6	1	40	67	28, 30, 31	28	28, 30, 31
30	6	3	10	193	29	28, 29, 31	29
31	6	1	77	67	29	1, 28, 29, 30, 32, 33, 34	29, 32
32	6	0	132	11	---	---	---
33	6	3	14	193	---	31, 32, 34	32
34	6	1	130	74	35	31, 33, 41	32, 35
35	6	1	35	67	34, 36, 41	---	34, 36, 41
36	6	2	35	130	35, 37	34, 37, 39	35, 37
37	6	1	84	67	36, 39	39	36, 39
38	6	3	57	193	---	37	---
39	6	1	74	67	37, 40	37	37, 40
40	6	2	31	130	39, 41	---	39, 41
41	6	2	31	130	35, 40	---	35, 40
42	6	2	25	130	25, 43	24, 25, 26, 43	25, 43
43	6	3	12	193	42	25, 42	42
44	7	0	0	3	---	---	---
45	8	0	0	2	---	---	---
46	8	0	0	2	---	---	---
47	8	0	0	2	---	---	---
48	8	0	0	2	---	---	---
49	8	0	0	9	---	---	---
50	8	0	0	9	---	---	---
51	8	0	0	9	---	---	---
52	8	0	0	9	---	---	---
53	8	0	0	9	---	---	---
54	8	1	0	65	---	8, 9, 10	---
55	8	1	0	65	---	---	---
56	8	1	0	65	---	---	---

[a] *an* stands for atomic number

[b] *H* stands for the number of protons attached to the atom.

[c] *Atype* stands for atom type which represents the hybridisation state of the atom.

[d] The COSY correlations are given for both sides of the diagonal. The number in parenthesis is the total number of correlations.

[e] The HMBC correlations are given from protons to carbons. The number in parenthesis is the total number of correlations.

[f] The 1,1-ADEQUATE correlations are theoretical data. The number in parenthesis is the total number of correlations.

1-222

1-271

1-228

1-256

1-227

1-270

1-223

1-257

1-335

1-282
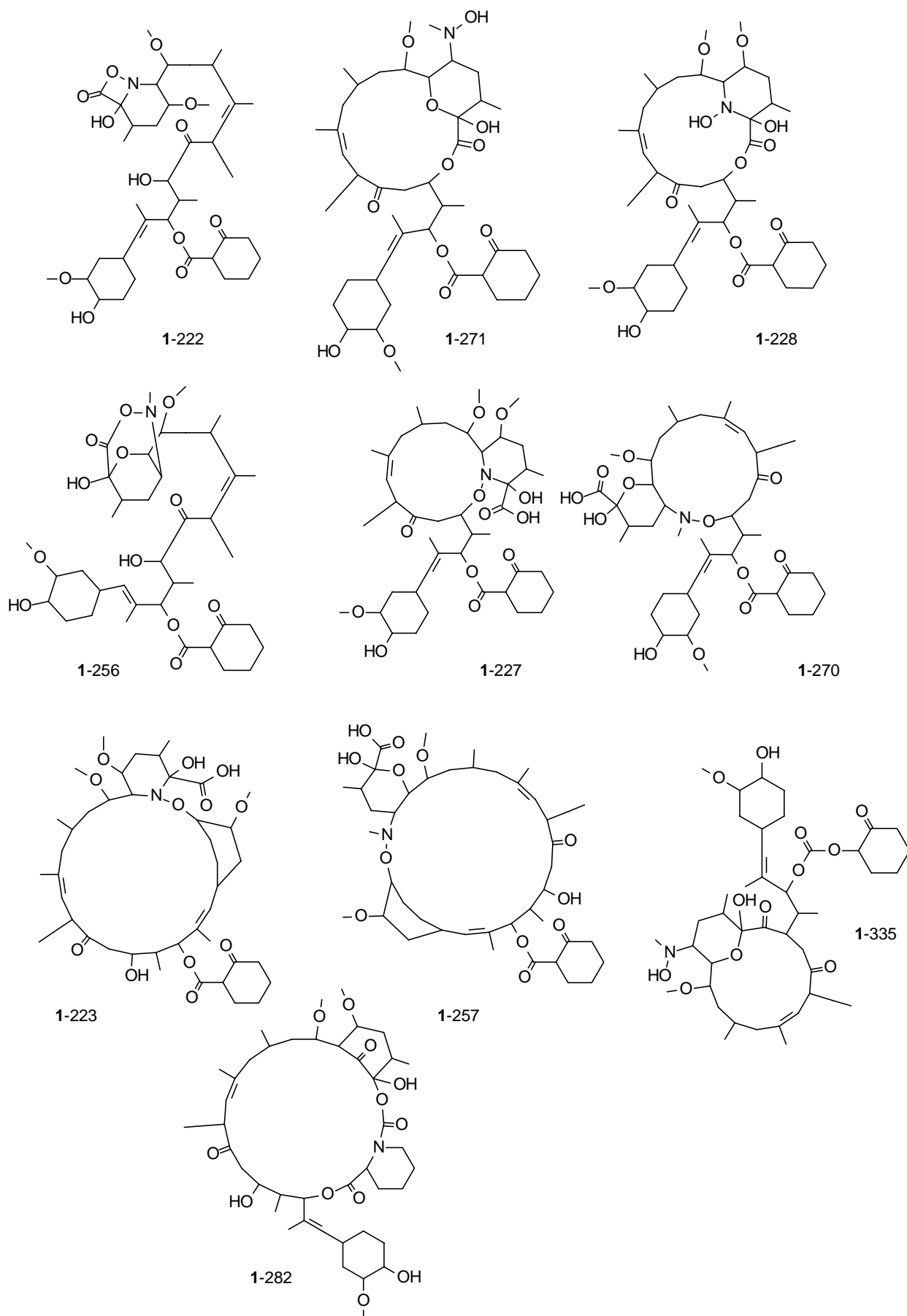
Figure (part 1): Structural proposals 1 to 10 for ascomycin generated by COCON. The structures are ordered according to the ranking of the SpecEdit calculation (e. g. **1**-222 is ranked first, **1**-257 is ranked eighth). Long straight lines represent more than one bond.

1-286

1-281

1-167

1-201

1-287

1-216

1-307

1-313

1-172

1-215
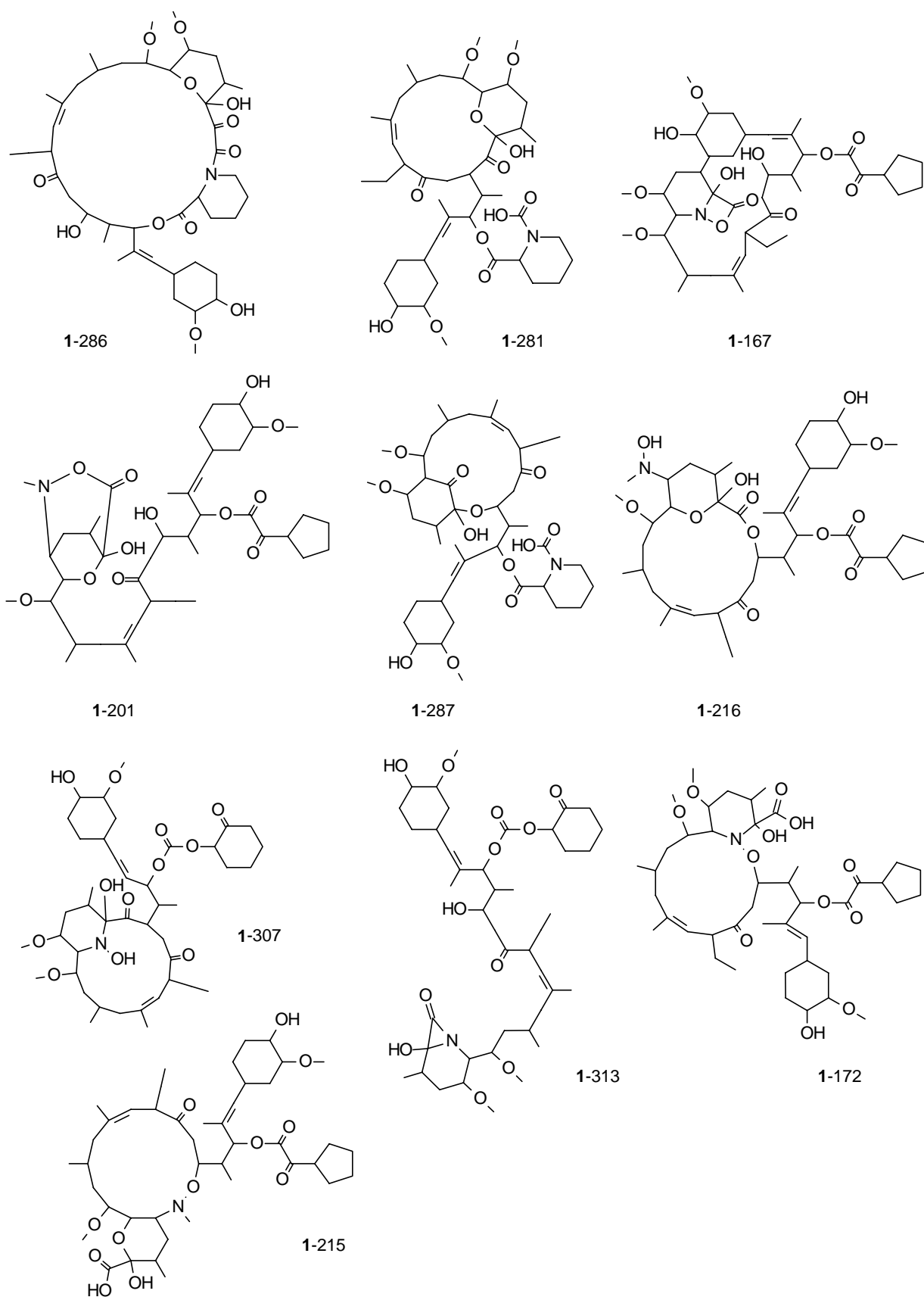
Figure (part 2): Structural proposals 11 to 20 for ascomycin generated by Cocon. The structures are ordered according to the ranking of the SpecEdit calculation.