

## Supporting Information

### **Pitfalls in the structural elucidation of small molecules. A critical analysis of a decade of structural missassignments of marine natural products**

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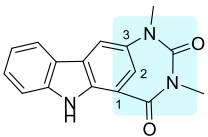
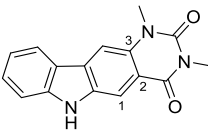
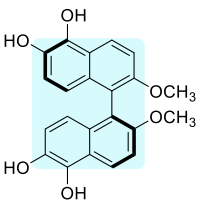
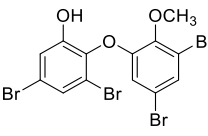
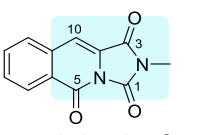
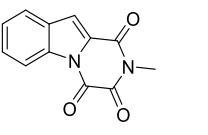
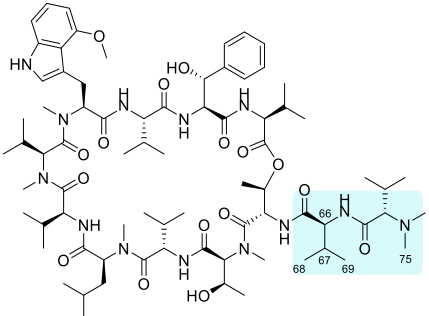
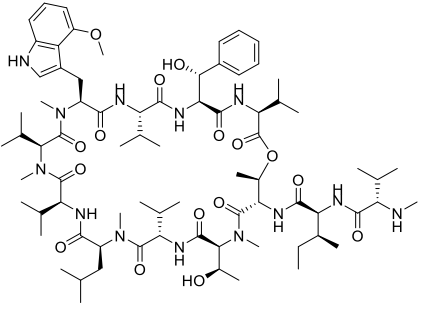
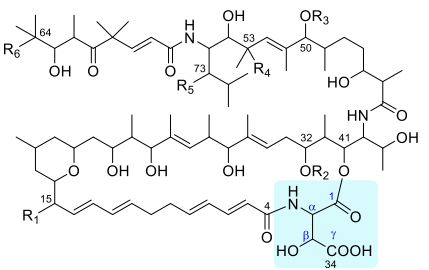
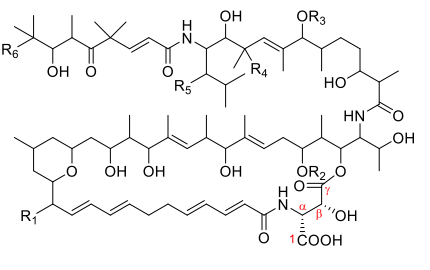
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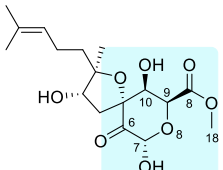
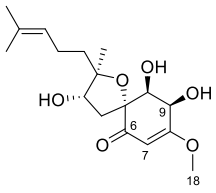
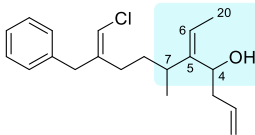
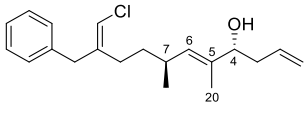
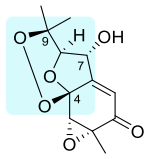
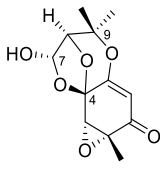
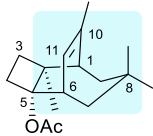
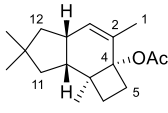
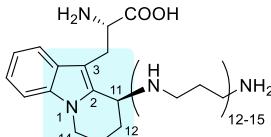
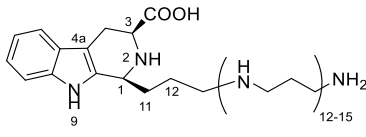
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**Table S1.** Wrong carbon-carbon connectivity assignment of MNPs (2010–2021).

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
1	 <p>antipathine A<sup>1</sup> coral (2009)</p>	HMBC		total synthesis (2013) <sup>2</sup>
2	 <p>(<i>S</i>)-2,2'-dimethoxy-1,1'-binaphthyl-5,5',6,6'-tetraol<sup>3</sup> sponge (2007)</p>	HRESIMS; NMR	 <p>= 3,5-dibromo-2-(3,5-dibromo-2-methoxyphenoxy)phenol</p>	total synthesis; X-ray; re-evaluation NMR and MS (2012) <sup>4</sup>
3	 <p>2-methylimidazo[1,5-<i>b</i>]isoquinoline-1,3,5(2<i>H</i>)-trione<sup>5</sup> fungus (2011)</p>	EIMS; NMR		total synthesis; X-ray (2017) <sup>6</sup>
4	 <p>ohmyungsamycin B<sup>7</sup> bacterial strain (2013)</p>	NMR comparison; 2D NMR; derivatization; Marfey's method; Mosher's method		total synthesis (2018) <sup>8</sup>
5–8	 <p>poecillastrin C<sup>10</sup>: R<sub>1</sub> = OMe, R<sub>2</sub> = R<sub>3</sub> = R<sub>4</sub> = R<sub>5</sub> = R<sub>6</sub> = H poecillastrin B<sup>10</sup>: R<sub>1</sub> = OMe, R<sub>2</sub> = R<sub>3</sub> = R<sub>5</sub> = R<sub>6</sub> = H, R<sub>4</sub> = Me poecillastrin D<sup>11</sup>: R<sub>1</sub> = OMe, R<sub>2</sub> = R<sub>4</sub> = R<sub>5</sub> = R<sub>6</sub> = H, R<sub>3</sub> = Me 73-deoxychondropsin A<sup>12</sup>: R<sub>1</sub> = R<sub>3</sub> = R<sub>4</sub> = R<sub>5</sub> = H, R<sub>2</sub> = COCH<sub>2</sub>CH(OH)CO<sub>2</sub>H, R<sub>6</sub> = CO<sub>2</sub>Me sponge (2007, 2004)</p>	NMR comparison		re-evaluation NMR; acid hydrolysis; chemical transformation; Marfey's analysis (2017) <sup>9</sup>

**Table S1 (continued)**

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
9	 <p>aspersiropene A<sup>13</sup> fungus (2017)</p>	HRESIMS 1D and 2D NMR computer-aided		HRESIMS; re-evaluation NMR; UV; IR; Snatzke's method; TDDFT-ECD (2021) <sup>14</sup>
10	 <p>trichotoxin<sup>15</sup> cyanobacterium (2011)</p>	COSY; HMBC	 <p>trichotoxin = trichotoxin A</p>	NMR analysis; biosynthesis (2016) <sup>16</sup>
11	 <p>acremine P<sup>17</sup> fungus (2013)</p>	HMBC; chemical transformation		re-evaluation NMR; computer-aided (2017) <sup>18</sup>
12	 <p>paesslerin A<sup>19</sup> coral (2001)</p>	NMR		re-evaluation NMR; total synthesis (2019) <sup>20</sup>
13	 <p>protoaculeine B<sup>21</sup> sponge (2014)</p>	MALDI-TOFMS; 2D NMR; chemical transformation		total synthesis (2020, 2021) <sup>22, 23</sup>

Only the structure elucidation methods used for the erroneous structure element are mentioned in this table.

**Table S2.** Wrong constitution of a heterocyclic ring scaffold of MNPs (2010–2021).

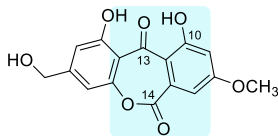
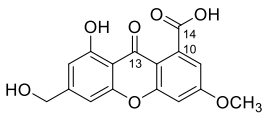
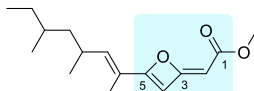
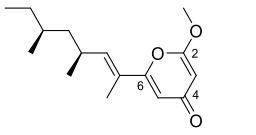
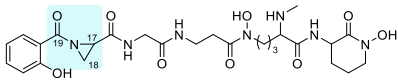
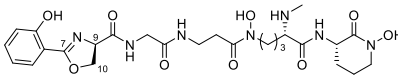
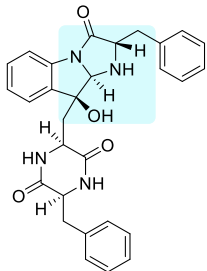
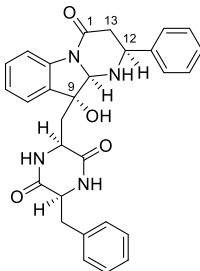
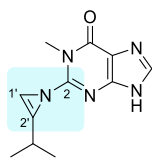
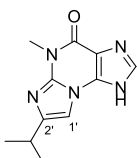
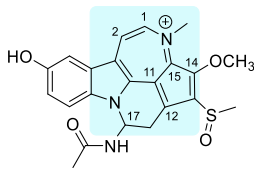
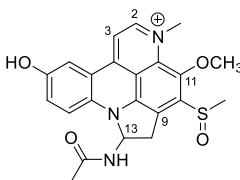
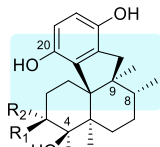
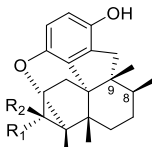
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
1	 <p>wentiquinone C<sup>24</sup> fungus (2014)</p>	NMR comparison		NMR; chemical transformation; X-ray (2019) <sup>25</sup>
2	 <p>fusariumin D<sup>26</sup> strain (2019)</p>	chemical shifts; COSY; HMBC	 <p>fusariumin D = fusarester C</p>	NMR comparison; computer-aided (2019) <sup>27</sup>
3	 <p>madurastatin C<sup>128</sup> fungus (2012)</p>	NMR		partial synthesis; NMR reanalysis (2017) <sup>29</sup>
4	 <p>citreindole<sup>30</sup> strain (1991)</p>	COSY; HMBC; acid hydrolysis; chiral HPLC		chiral HPLC; C <sub>3</sub> Marfey's analysis (2016) <sup>31</sup>
5	 <p>acremolin<sup>32</sup> fungus (2012)</p>	COSY; HMBC		NMR reanalysis (2012) <sup>33</sup> ; total synthesis; <sup>1</sup> H- <sup>15</sup> N HMBC; J-based (2013) <sup>34</sup>
6	 <p>pseudocerosine<sup>35</sup> flatworm (2009)</p>	<sup>1</sup> H- <sup>13</sup> C HMBC; <sup>1</sup> H- <sup>15</sup> N HMBC		synthesis (2020) <sup>36</sup>
7–9	 <p>dysiherbol A<sup>37</sup>: R<sub>1</sub> = R<sub>2</sub> = H dysiherbol B<sup>37</sup>: R<sub>1</sub> = OH, R<sub>2</sub> = H dysiherbol C<sup>37</sup>: R<sub>1</sub> = R<sub>2</sub> = O sponge (2016)</p>	HRESIMS; HMBC; NMR comparison		total synthesis; X-ray (2021) <sup>38, 39</sup>

Table S2 (continued)

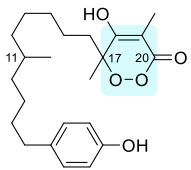
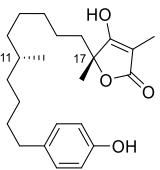
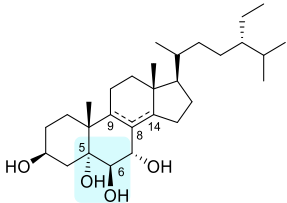
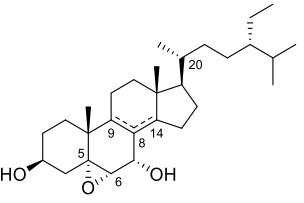
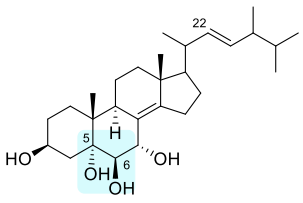
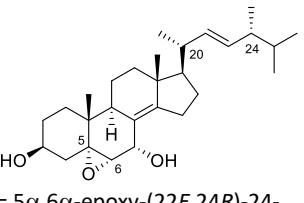
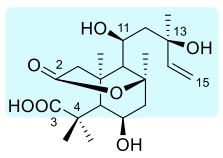
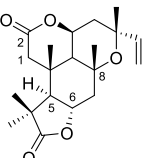
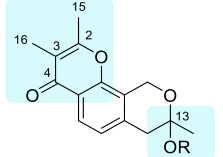
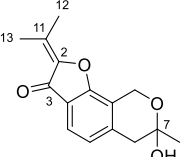
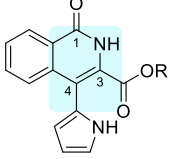
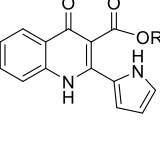
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
10	 <p>plakinidone<sup>40</sup> sponge (1991)</p>	HRMS; NMR		synthesis (2015, 2016) <sup>41, 42</sup> ; computer-aided (2016) <sup>42</sup>
11&12	 <p>(24S)-24-ethylcholest-8-ene-3β,5α,6β,7α-tetraol<sup>43</sup>; <math>\Delta^{8,9}</math> (24S)-24-ethylcholest-8(14)-ene-3β,5α,6β,7α-tetraol<sup>43</sup>; <math>\Delta^{8,14}</math> sponge (1995)</p>	HRMS; NMR; NMR comparison	 <p>= (24S)-5α,6α-epoxy-24-ethylcholest-8-ene-3β,7α-diol<sup>44</sup>; <math>\Delta^{8,9}</math> = (24S)-5α,6α-epoxy-24-ethylcholest-8(14)-ene-3β,7α-diol<sup>44</sup>; <math>\Delta^{8,14}</math></p>	MS reanalysis; NMR comparison (2015) <sup>44</sup>
13	 <p>(22E)-24-methylcholesta-8(14),22-diene-3β,5α,6β,7α-tetraol<sup>45</sup> fungus (2006)</p>	HRFABMS; NMR	 <p>= 5α,6α-epoxy-(22E,24R)-24-methylcholesta-8(14),22-diene-3β,7α-diol</p>	NMR comparison (2016) <sup>46</sup>
14	 <p>rhizophorin A<sup>47</sup> mangrove (2001)</p>	CIMS; NMR	 <p>rhizophorin A = excolide A</p>	NMR; CD; X-ray; chemical derivatization (2015) <sup>48</sup>
15&16	 <p>aspergione E<sup>49</sup>: R = Me aspergione F<sup>49</sup>: R = H fungus (2003)</p>	NMR comparison; HRESIMS	 <p>aspergione E = pergillin and MeOH (1:1) aspergione F = pergillin</p>	synthesis (2015) <sup>50</sup>
17&18	 <p>marinamide<sup>51</sup>: R = H marinamide methyl ester<sup>51</sup>: R = CH<sub>3</sub> fungi (2006)</p>	COSY; HMBC; NMR comparison		chemical transformation (2013) <sup>52</sup>

Table S2 (continued)

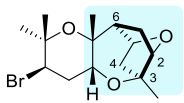
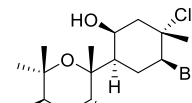
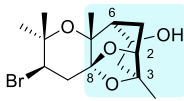
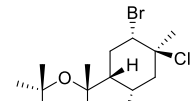
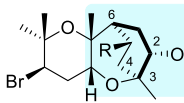
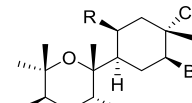
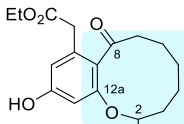
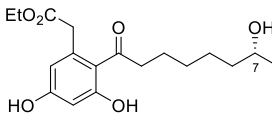
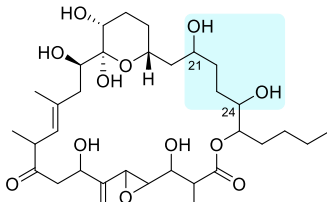
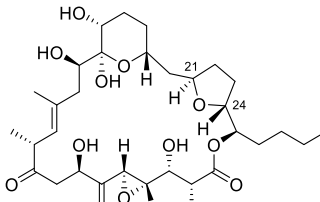
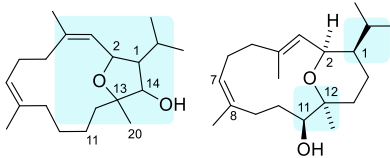
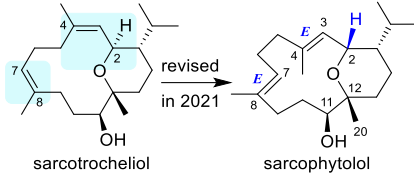
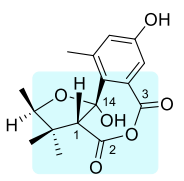
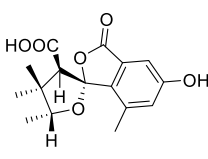
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
19	 aldingenin A <sup>53</sup> alga (2003)	HREIMS; COSY; HMBC	 aldingenin A = 5-(S)-hydroxycaespitol	computer-aided (2015) <sup>54</sup>
20	 aldingenin B <sup>55</sup> alga (2006)	HREIMS; NMR comparison	 aldingenin B = hemiacetal	total synthesis (2012) <sup>56</sup> ; computer-aided (2015) <sup>54</sup>
21&22	 aldingenin C <sup>55</sup> : R = H aldingenin D <sup>55</sup> : R = OAc alga (2006)	HREIMS; NMR comparison	 aldingenin C = caespitol: R = H aldingenin D = 5-(S)-acetoxycespitol: R = OAc	synthesis (2014) <sup>57</sup> ; computer-aided (2015) <sup>54</sup>
23	 phomopsis B <sup>58</sup> fungus (2008)	HREIMS; HMBC; NMR comparison	 phomopsis B = dothiorelone A	total synthesis (2011) <sup>59</sup>
24	 amphidinolide N <sup>60</sup> dinoflagellate (1994)	HRFABMS; 2D NMR; J-based		ESIMS; NMR solvents; HMBC; J-based; NOESY (2013) <sup>61</sup>
25	 sarcophytol sarcotrocheliol sarcophytol <sup>62</sup> (sarcotrocheliol <sup>63</sup> ) coral (2014, 2015)	COSY; HMBC	 sarcotrocheliol sarcophytol	X-ray (2019) <sup>64</sup> NMR comparison; reanalysis X-ray results (2021) <sup>65</sup>
26	 cereoanhydride <sup>66</sup> fungus (2012)	HMBC		total synthesis; X-ray (2016) <sup>67</sup> ; computer-aided (2017) <sup>68</sup>

Table S2 (continued)

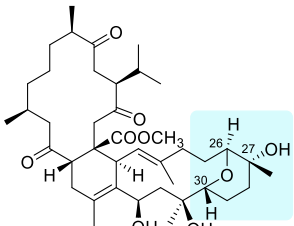
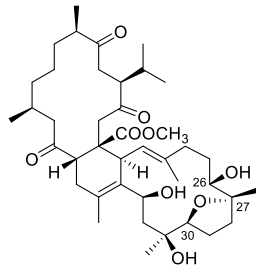
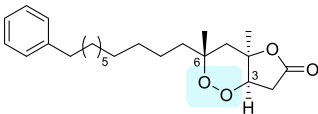
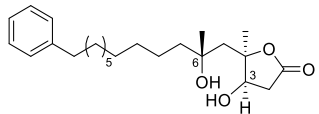
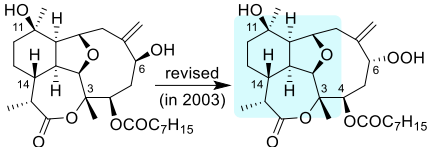
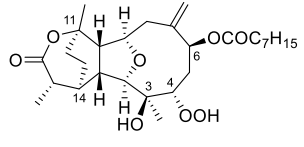
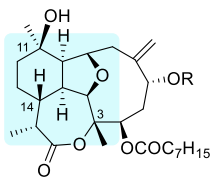
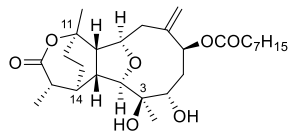
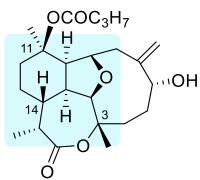
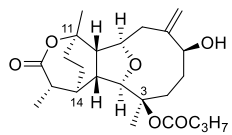
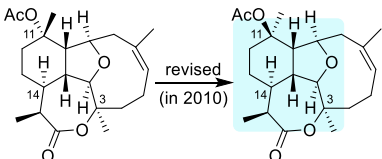
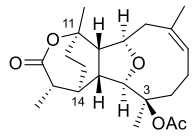
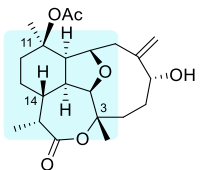
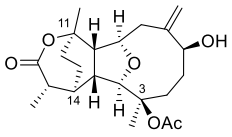
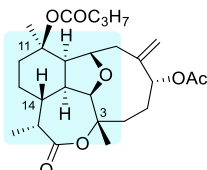
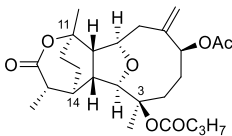
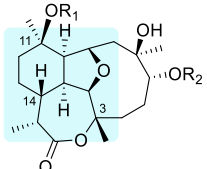
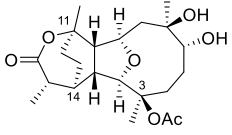
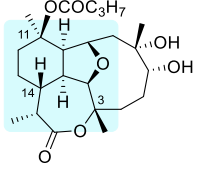
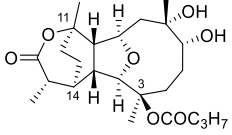
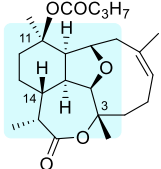
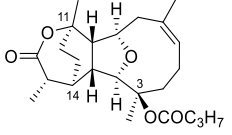
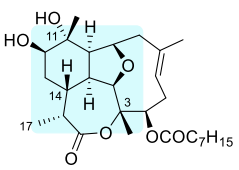
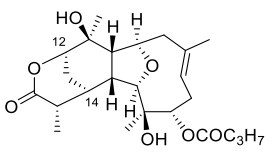
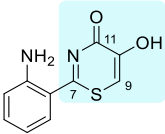
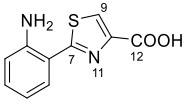
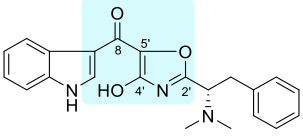
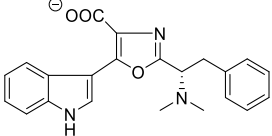
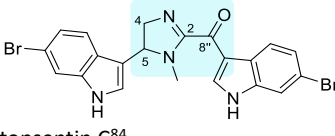
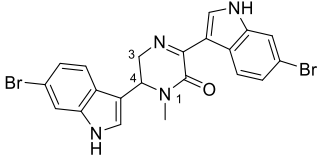
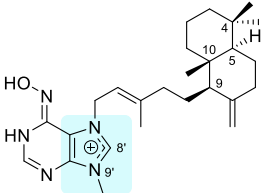
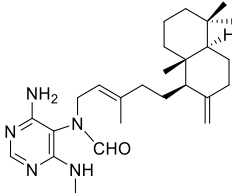
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
27	 <p>methyl tortuoate D<sup>69</sup> coral (2009)</p>	COSY; HMBC		re-evaluation NMR (2013) <sup>70</sup>
28	 <p>plakortolide E<sup>71</sup> sponge (1995)</p>	HREIMS; NMR; chemical transformation	 <p>plakortolide E = <i>seco</i>-plakortolide E</p>	NMR comparison (2011) <sup>72</sup> ; total synthesis (2012) <sup>73</sup>
29	 <p>briarellin A<sup>74,75</sup> coral (1995, 2003)</p>	HREIMS; NMR comparison		computer-aided (2020) <sup>76</sup>
30	 <p>briarellin B<sup>74</sup>: R = H briarellin C<sup>74</sup>: R = COC<sub>3</sub>H<sub>7</sub> coral (1995)</p>	NMR comparison	 <p>briarellin B</p>	computer-aided (2020) <sup>76</sup>
31	 <p>briarellin D<sup>74</sup> coral (1995)</p>	NMR comparison		computer-aided (2020) <sup>76</sup>
32	 <p>briarellin J<sup>75,77</sup> coral (2003)</p>	2D NMR; NMR comparison <sup>75</sup> ; total synthesis <sup>77</sup>		computer-aided (2020) <sup>76</sup>



Table S2 (continued)

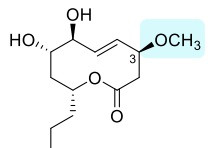
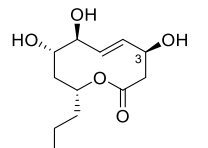
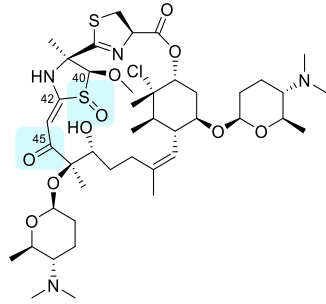
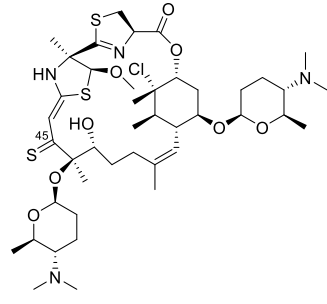
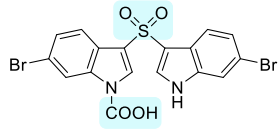
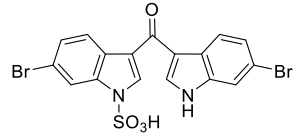
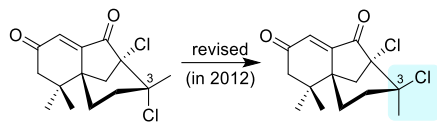
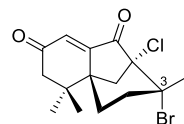
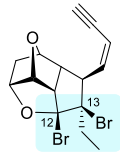
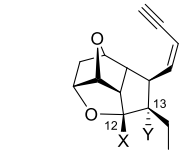
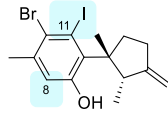
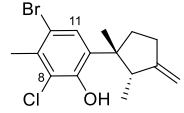
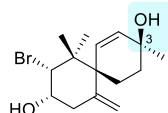
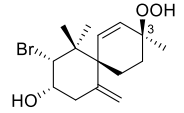
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
33	 <p>briarellin K<sup>75</sup> coral (2003)</p>	NMR comparison		computer-aided (2020) <sup>76</sup>
34	 <p>briarellin L<sup>75</sup> coral (2003)</p>	NMR comparison		computer-aided (2020) <sup>76</sup>
35	 <p>briarellin M<sup>75</sup>: R<sub>1</sub> = Ac, R<sub>2</sub> = OH briarellin N<sup>75</sup>: R<sub>1</sub> = Ac, R<sub>2</sub> = OCH<sub>3</sub> briarellin O<sup>75</sup>: R<sub>1</sub> = COC<sub>3</sub>H<sub>7</sub>, R<sub>2</sub> = OH briarellin P<sup>75</sup>: R<sub>1</sub> = COC<sub>3</sub>H<sub>7</sub>, R<sub>2</sub> = OCH<sub>3</sub> coral (2003)</p>	NMR comparison	 <p>briarellin M</p>	computer-aided (2020) <sup>76</sup>
36	 <p>briarellin Q<sup>78</sup> coral (2006)</p>	NMR comparison		computer-aided (2020) <sup>76</sup>
37	 <p>briarellin R<sup>78</sup> coral (2006)</p>	NMR comparison		computer-aided (2020) <sup>76</sup>
38	 <p>briarellin H<sup>79</sup> coral (1995)</p>	NMR comparison		computer-aided (2020) <sup>76</sup>

**Table S2 (continued)**

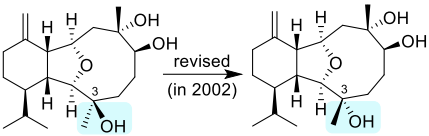
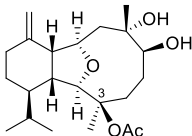
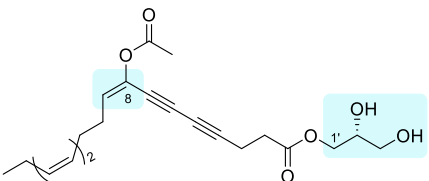
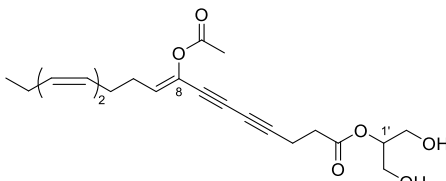
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
39	 <p>thiasporine A<sup>80</sup> bacterium (2015)</p>	NMR comparison; HMBC; chemical transformation		total synthesis; X-ray (2016) <sup>81</sup>
40	 <p>almazole D<sup>82</sup> alga (1996)</p>	NMR comparison		synthesis (2010) <sup>83</sup>
41	 <p>topsentin C<sup>84</sup> sponge (1990)</p>	NMR comparison; chemical shifts; IR		total synthesis (2017) <sup>85</sup>
42	 <p>(-)-ageloxime D<sup>86</sup> sponge (2010)</p>	NMR comparison		total synthesis (2019) <sup>87</sup>

Only the structure elucidation methods used for the erroneous structure element are mentioned in this table.

**Table S3.** Functional group misidentification of MNPs (2010–2021).

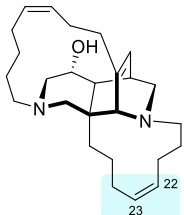
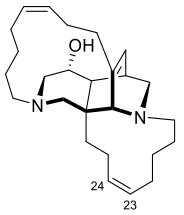
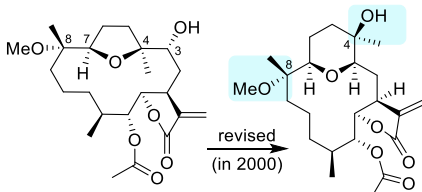
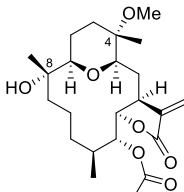
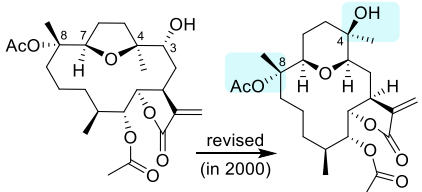
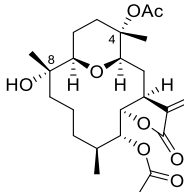
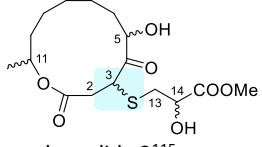
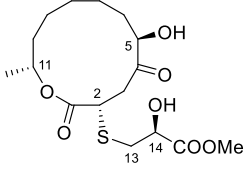
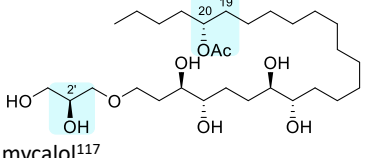
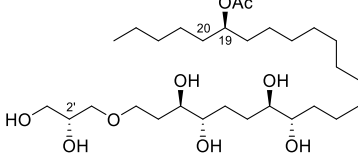
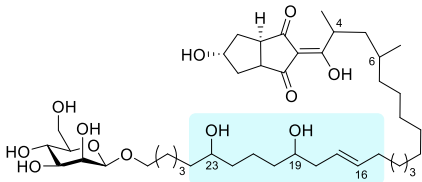
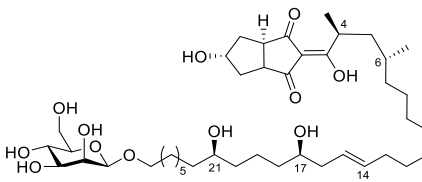
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
1	 <p>phomolide H<sup>88</sup> fungus (2010)</p>	HRMS; NMR comparison		total synthesis; X-ray (2017) <sup>89</sup>
2	 <p>forazoline A<sup>90</sup> strain (2014)</p>	MS isotopic analysis; NMR; <sup>13</sup> C- <sup>13</sup> C gCOSY NMR		isotopic fine structure analysis; X-ray (2020) <sup>91</sup>
3	 <p>echinosulfone A<sup>92</sup> sponge (1999)</p>	NMR comparison		NMR; decomposition; MS fragmentation; SDP4+ analysis; X-ray (2020) <sup>93</sup> ; MS; NMR reanalysis (2020) <sup>94</sup> ; total synthesis (2020) <sup>95</sup>
4	 <p>gomerone B<sup>96, 97</sup> alga (2008)</p>	NMR comparison <sup>96</sup> ; total synthesis <sup>97</sup>		computer-aided (2017) <sup>98</sup>
5	 <p>lembyne B<sup>99</sup> alga (2001)</p>	HREIMS; NMR	 <p>X = Cl, Y = Br or X = Br, Y = Cl</p>	computer-aided (2017) <sup>98</sup>
6	 <p>10-bromo-7-hydroxy-11-iodolaurene<sup>100</sup> alga (1979)</p>	MS; NMR comparison		computer-aided (2017) <sup>98</sup>
7	 <p>rigidol<sup>101</sup> alga (1997)</p>	HRMS; IR; chemical shifts		computer-aided (2017) <sup>98</sup>

**Table S3 (continued)**

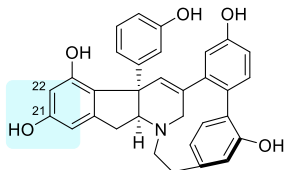
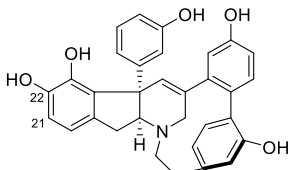
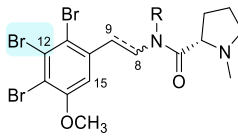
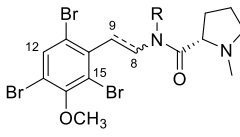
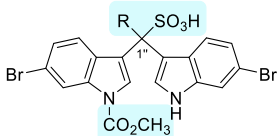
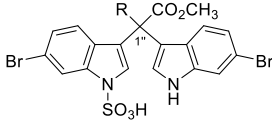
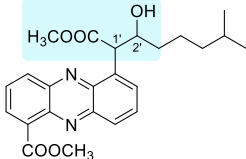
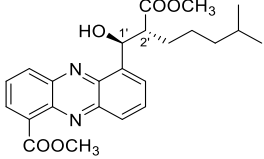
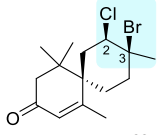
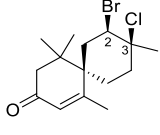
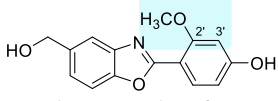
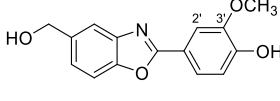
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
8	 <p>sclerophytin F<sup>102, 103</sup> coral (1989)</p>	EIMS; NMR comparison	 <p>sclerophytin F = sclerophytin E</p>	total synthesis (2015) <sup>104</sup>
9	 <p>peyssonenyne B<sup>105</sup> alga (2004)</p>	NMR comparison; 2D NMR		total synthesis (2011) <sup>106</sup>

Only the structure elucidation methods used for the erroneous structure element are mentioned in this table.

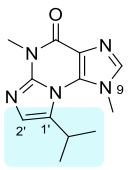
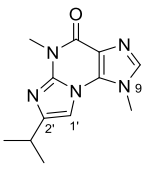
**Table S4.** Functional group mispositioning of MNPs (2010–2021).

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
1	 <p>xestocyclamine A<sup>107</sup>,<sup>108</sup> sponge (1993)</p>	HMBC; <sup>1</sup> H- <sup>1</sup> H COSY	 <p>xestocyclamine A = <i>ent</i>-ingenamine</p>	total synthesis (2020) <sup>109</sup>
2	 <p>uprolide G acetate<sup>110,111</sup> coral (1995)</p>	NMR comparison; NOESY <sup>110</sup> ; revised by partial synthesis <sup>111</sup>		total synthesis (2015) <sup>112,113</sup> ; X-ray (2015) <sup>112</sup>
3	 <p>uprolide F diacetate<sup>110,111</sup> coral (1995)</p>	NMR comparison; NOESY <sup>110</sup> ; revised by partial synthesis <sup>111</sup>		total synthesis (2015) <sup>114</sup>
4	 <p>pandangolide 3<sup>115</sup> fungus (2001)</p>	HMBC		NMR comparison; HMBC; NOESY; ECD (2019) <sup>116</sup>
5	 <p>mycalol<sup>117</sup> sponge (2013)</p>	NMR; chemical and chiroptical methods; Snatzke's and Frelek's method		total synthesis (2015) <sup>118-120</sup>
6	 <p>burnettramic acid A<sup>121</sup> fungus (2019)</p>	<sup>1</sup> H- <sup>1</sup> H COSY; HMBC		NMR; chemical derivatization; Mosher's method; Marfey's analysis (2020) <sup>122</sup>

**Table S4 (continued)**

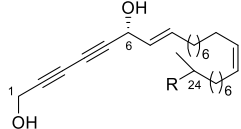
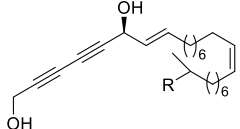
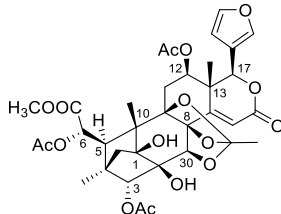
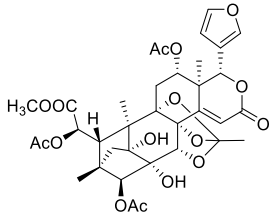
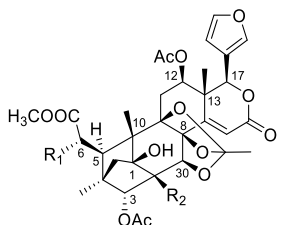
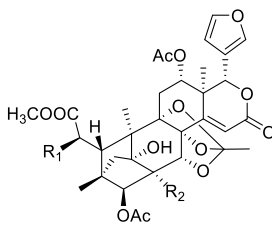
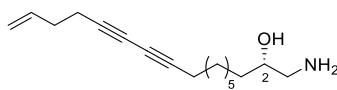
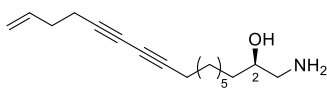
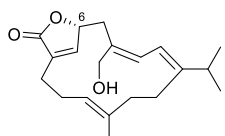
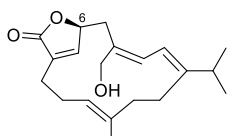
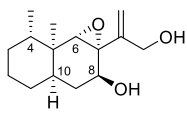
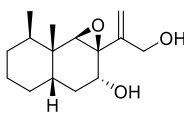
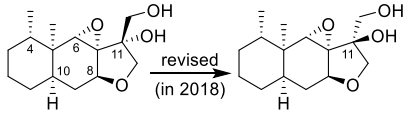
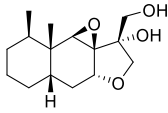
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
7	 <p>haouamine B<sup>123</sup> ascidian (2003)</p>	NMR comparison; HMBC; biosynthetic analysis		total synthesis (2012, 2014) <sup>124, 125</sup>
8– 11	 <p>amathamide C<sup>126</sup>: <math>\Delta^{8,9}</math> 8E, R = CH<sub>3</sub> amathamide D<sup>126</sup>: R = H amathamide E<sup>126</sup>: <math>\Delta^{8,9}</math> 8E, R = H amathamide F<sup>126</sup>: <math>\Delta^{8,9}</math> 8Z, R = H bryozoan (1987)</p>	NMR comparison		chemical shifts (2011) <sup>127</sup> total synthesis (2012) <sup>128</sup> total synthesis (2015) <sup>129</sup>
12– 15	 <p>echinosulfonic acid A<sup>92</sup>: R = OEt echinosulfonic acid B<sup>92</sup>: R = OCH<sub>3</sub> echinosulfonic acid C<sup>92</sup>: R = OH echinosulfonic acid D<sup>130</sup>: R = H sponge (1999, 2005)</p>	NMR comparison <sup>92</sup> ; MS/MS analysis <sup>130</sup>		decomposition; NMR comparison (2020) <sup>93</sup> ; MS; NMR reanalysis (2020) <sup>94</sup> ; biogenetic consideration (2020) <sup>95</sup>
16	 <p>streptophenazine A<sup>131</sup> strain (2008)</p>	COSY; HMBC		total synthesis (2011) <sup>132</sup>
17	 <p>tristichone C<sup>133</sup> alga (2016)</p>	COSY; HMBC		computer-aided (2017) <sup>98</sup>
18	 <p>nocarbenoxazole G<sup>134</sup> strain (2015)</p>	NMR comparison; HMBC		total synthesis (2019) <sup>135</sup>

**Table S4** (continued)

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
19	 acremolin C <sup>136</sup> fungus (2018)	NMR comparison; NOESY; HMBC	 acremolin C = acremolin B	NMR comparison; computer-aided (2019) <sup>137</sup>

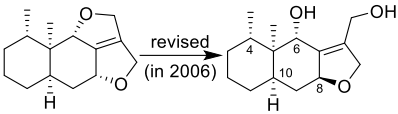
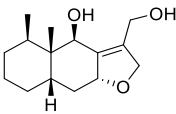
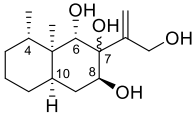
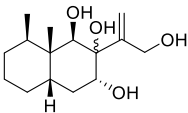
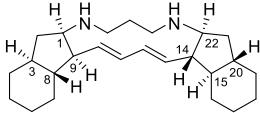
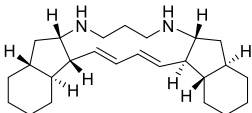
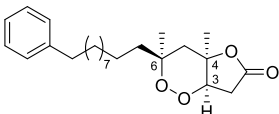
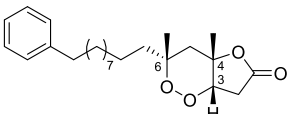
Only the structure elucidation methods used for the erroneous structure element are mentioned in this table.

**Table S5.** Structural revisions of absolute configuration of MNPs (2010–2021).

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
1&2	 <p>strongylodiol H<sup>138</sup>: R = H strongylodiol I<sup>138</sup>: R = CH<sub>3</sub> sponge (2005)</p>	Mosher's method		total synthesis; Mosher's method (2018) <sup>139</sup>
3	 <p>xyloccensin Q<sup>140</sup> mangrove (2005)</p>	Mosher's method; ECD analysis		X-ray; TDDFT-ECD (2014) <sup>141</sup>
4–8	 <p>xyloccensin O<sup>140</sup>: R<sub>1</sub> = OAc, R<sub>2</sub> = H xyloccensin P<sup>140</sup>: R<sub>1</sub> = R<sub>2</sub> = OAc xyloccensin R<sup>140</sup>: R<sub>1</sub> = R<sub>2</sub> = OH xyloccensin S<sup>140</sup>: R<sub>1</sub> = OH, R<sub>2</sub> = OAc xyloccensin V<sup>140</sup>: R<sub>1</sub> = H, R<sub>2</sub> = OAc mangrove (2005)</p>	Mosher's method; ECD analysis		ECD analysis (2014) <sup>141</sup>
9	 <p>distaminolyne A<sup>142</sup> ascidian (2016)</p>	dibenzoate exciton coupled CD		total synthesis; OR; chiral derivatizing agents (2017) <sup>143</sup>
10	 <p>ehrenbergol D<sup>144</sup> coral (2015)</p>	empirical helicity rule		TDDFT-ECD (2019) <sup>145</sup>
11	 <p>peribysin A<sup>146-148</sup> sea hare (2004, 2005)</p>	chemical conversion <sup>147</sup> ; total synthesis; X-ray (Mo K $\alpha$ ) <sup>148</sup>		enantiospecific total synthesis; X-ray (Cu K $\alpha$ ) (2020) <sup>149</sup>
12	 <p>peribysin B<sup>146, 148</sup> sea hare (2004)</p>	total synthesis; X-ray (Mo K $\alpha$ ) <sup>148</sup>		enantiospecific total synthesis (2020) <sup>149</sup>

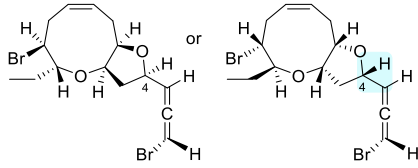
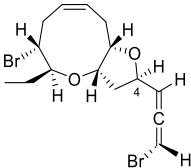
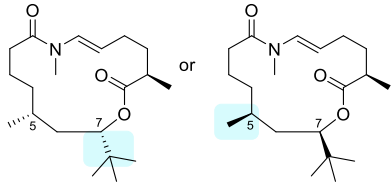
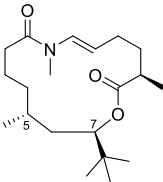
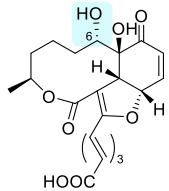
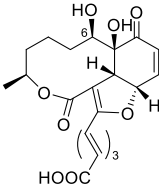
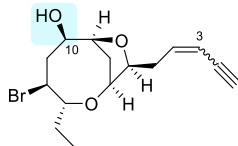
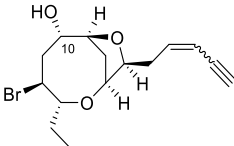
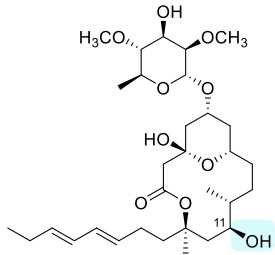
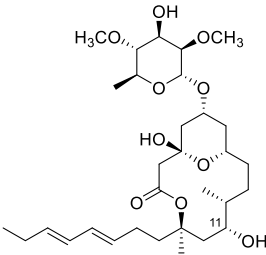
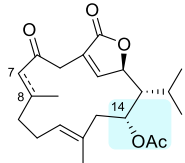
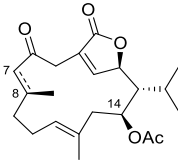


**Table S5 (continued)**

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
13	 <p>peribysin C<sup>146, 150</sup> sea hare (2004)</p>	computer-aided <sup>150</sup>		enantiospecific total synthesis (2020) <sup>149</sup>
14& 15	 <p>peribysin F<sup>147</sup>: 7<math>\alpha</math>-OH peribysin G<sup>147</sup>: 7<math>\beta</math>-OH sea hare (2005)</p>	chemical transformation; ECD	 <p>peribysin F: 7<math>\beta</math>-OH peribysin G: 7<math>\alpha</math>-OH</p>	enantiospecific total synthesis (2020) <sup>149</sup>
16	 <p>haliclonadamine<sup>151, 152</sup> sponge (1988)</p>	total synthesis <sup>152</sup>		X-ray; calculated ECD (2020) <sup>153</sup>
17	 <p>plakortolide I<sup>154</sup> sponge (2003)</p>	OR comparison		total synthesis; OR (2012) <sup>73</sup>

Only the structure elucidation methods used for the erroneous structure element are mentioned in this table.

**Table S6.** Single stereocenter misidentification of MNPs (2010–2021).

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
1	 <p>(+)-itomanallene A<sup>155</sup> alga (2002)</p>	NOESY; Lowe's rule		total synthesis (2010) <sup>156</sup>
2	 <p>palmyrolide A<sup>157</sup> cyanobacteria (2010)</p>	NOESY; <i>J</i> -based; selective hydrolysis		total synthesis (2012) <sup>158-160</sup>
3	 <p>(+)-dictyosphaeric acid A<sup>161</sup> fungus (2004)</p>	NOESY; ROESY; <i>J</i> -based		total synthesis (2010) <sup>162</sup>
4&5	 <p>laurefurenyne E<sup>163</sup>: 3<i>Z</i> laurefurenyne F<sup>163</sup>: 3<i>E</i> alga (2010)</p>	NOESY; NMR comparison		total synthesis (2020) <sup>164</sup>
6	 <p>lyngbouillose<sup>165</sup> cyanobacterium (2002)</p>	ROESY; <i>J</i> -based		total synthesis (2012) <sup>166</sup>
7&8	 <p>isosarcophytonolide D<sup>167</sup>: Δ<sup>7,8</sup> sarcophytonolide J<sup>168</sup> coral (2007)</p>	NOESY; NMR comparison		total synthesis (2016, 2018) <sup>169, 170</sup>

**Table S6 (continued)**

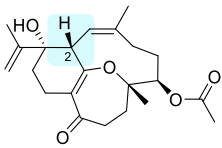
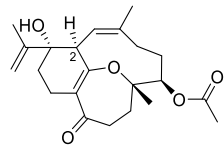
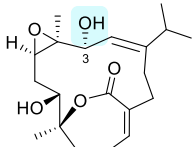
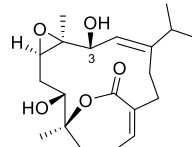
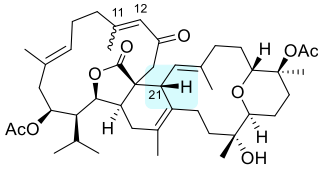
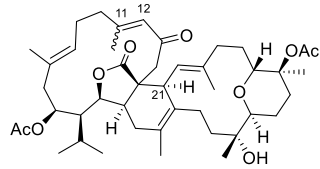
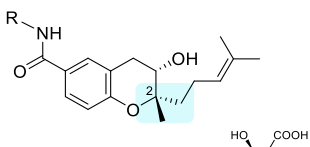

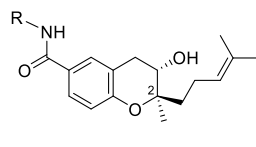
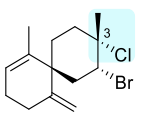
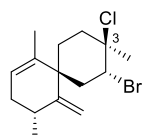
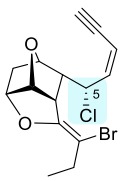
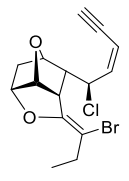
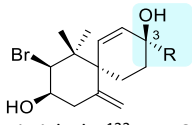
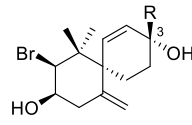
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
9	 <p>sarsolenone<sup>171</sup> coral (1995)</p>	NOESY		NOESY reanalysis; TDDFT ECD (2014) <sup>172</sup>
10	 <p>sartrolide C<sup>173</sup> coral (2013)</p>	NOESY		NMR comparison; computer-aided (2018) <sup>174</sup>
11& 12	 <p>bislatumlide A<sup>167</sup>: 11E bislatumlide B<sup>167</sup>: 11Z coral (2007)</p>	NOESY; NMR comparison		NMR comparison; TDDFT-ECD (2013) <sup>175</sup>
13& 14	 <p>xiamenmycin A<sup>176</sup>: R =  xiamenmycin C: R<sup>177</sup> = H strains (2012, 2013)</p>	NOESY; Mosher's method; Marfey's reagent; QM calculations <sup>176</sup> biosynthetic; CD comparison <sup>177</sup>		total synthesis (2016) <sup>178, 179</sup>
15	 <p>laurokamin A<sup>180</sup> alga (2012)</p>	NOESY		chemical shifts; NOESY reanalysis (2018) <sup>181</sup>
16	 <p>12E-lembyne A<sup>182</sup> alga (2001)</p>	NMR comparison		computer-aided (2017) <sup>98</sup>
17& 18	 <p>tristichol A<sup>133</sup>: R = CHBr<sub>2</sub> tristichol B<sup>133</sup>: R = CH<sub>2</sub>OH alga (2016)</p>	NOESY; NMR comparison		computer-aided (2017) <sup>98</sup>

Table S6 (continued)

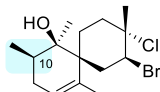
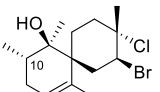
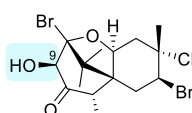
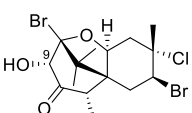
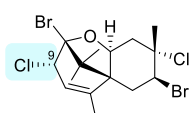
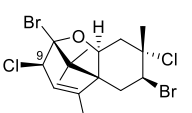
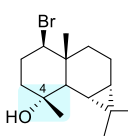
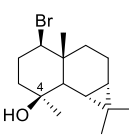
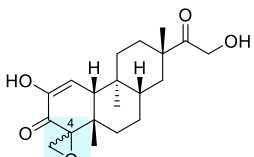
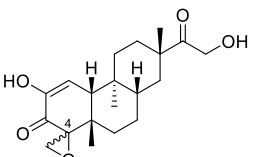
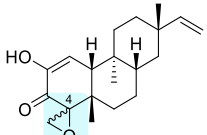
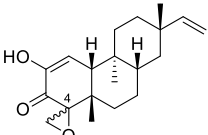
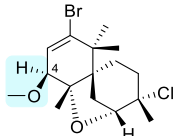
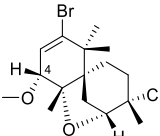
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
19	 compositacin A <sup>181</sup> alga (2017)	ROESY; NMR comparison		computer-aided (2017) <sup>98</sup>
20	 kimura-cmpd 14 <sup>183</sup> alga (1999)	NMR; chemical transformation		computer-aided (2017) <sup>98</sup>
21	 compositacin L <sup>181</sup> alga (2017)	ROESY; NMR comparison		computer-aided (2017) <sup>98</sup>
22	 1(R)-Br-ent-maaliol <sup>184</sup> alga (1989)	NOESY		computer-aided (2017) <sup>98</sup>
23& 24	 tagalene I <sup>185</sup> : 4 $\alpha$ -CH <sub>2</sub> , 4S 4-epitagalene I <sup>186</sup> : 4 $\beta$ -CH <sub>2</sub> , 4R mangrove (2016, 2017)	NOESY	 tagalene I: 4 $\beta$ -CH <sub>2</sub> , 4R 4-epitagalene I: 4 $\alpha$ -CH <sub>2</sub> , 4S	X-ray; NOESY reanalysis (2018) <sup>187</sup>
25& 26	 tagalsin A <sup>188</sup> : 4 $\alpha$ -CH <sub>2</sub> , 4S tagalsin B <sup>188</sup> : 4 $\beta$ -CH <sub>2</sub> , 4R mangrove (2005)	NOESY	 tagalsin A: 4 $\beta$ -CH <sub>2</sub> , 4R tagalsin B: 4 $\alpha$ -CH <sub>2</sub> , 4S	NOESY reanalysis; NMR comparison (2018) <sup>187</sup>
27	 cycloelatanene A <sup>189</sup> alga (2011)	1D NOE		crystalline sponge method (2018) <sup>190</sup>

Table S6 (continued)

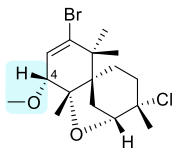
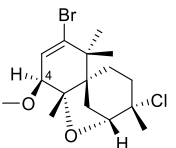
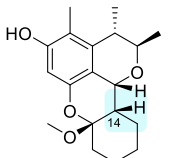
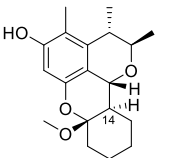
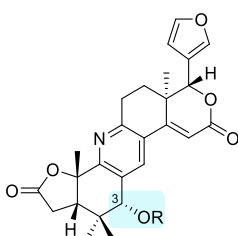
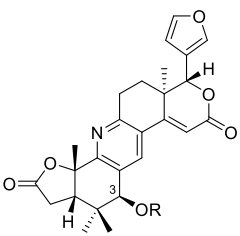
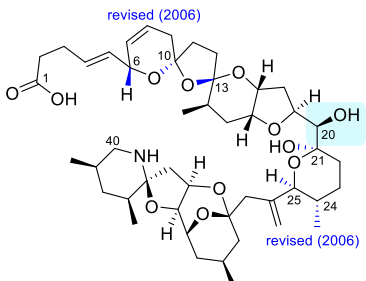
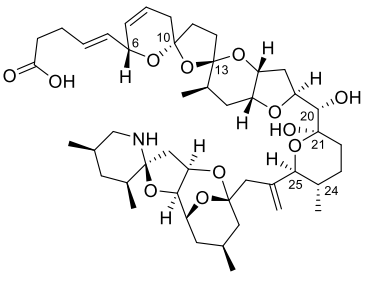
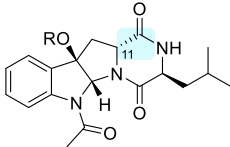
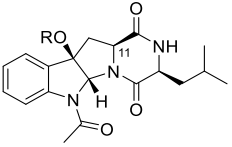
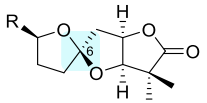
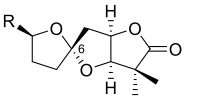
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
28	 <p>cycloelatanene B<sup>189</sup> alga (2011)</p>	1D NOE; NMR comparison;		crystalline sponge method (2017) <sup>190</sup>
29	 <p>penicitol A<sup>191</sup> fungus (2015)</p>	NOESY; TDDFT-ECD		DP4+ analysis; calculated ECD spectra; analogue comparison (2021) <sup>192</sup>
30& 31	 <p>(+)-xylogranatin F<sup>193</sup>: R = H; (+)-xylogranatin G<sup>193</sup>: R = Ac mangrove (2008)</p>	NOESY; chemical transformation; Mosher's method		total synthesis; X-ray (2019) <sup>194</sup> DU8+ calculation (2020) <sup>195</sup>
32	 <p>azaspiracid-3<sup>196, 197</sup> mussel (1999)</p>	ROESY; NMR comparison <sup>196</sup> ; total synthesis <sup>197</sup>		total synthesis (2018) <sup>198, 199</sup>
33& 34	 <p>(-)-protubonine A<sup>200</sup>: R = H; (-)-protubonine B<sup>200</sup>: R = Ac fungus (2010)</p>	NOESY		total synthesis (2014) <sup>201</sup>
35& 36	 <p>cephalosporolide I<sup>202</sup>: R = (CH<sub>2</sub>)<sub>3</sub>COOH; cephalosporolide H<sup>202</sup>: R = (CH<sub>2</sub>)<sub>6</sub>CH<sub>3</sub> fungus (2007)</p>	NOESY; NMR comparison		total synthesis (2016) <sup>203</sup> ; NMR method (2016) <sup>204</sup>

Table S6 (continued)

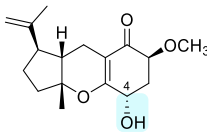
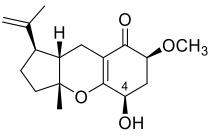
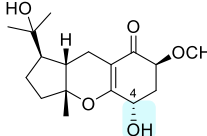
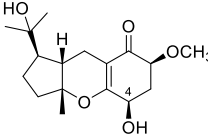
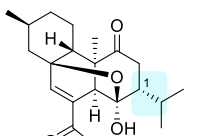
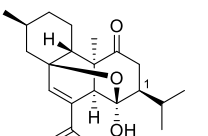
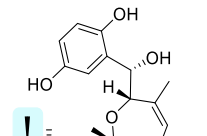
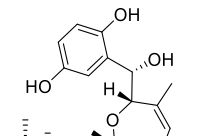
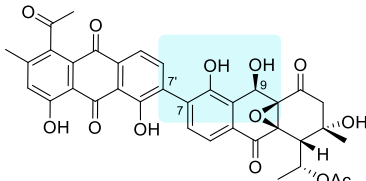
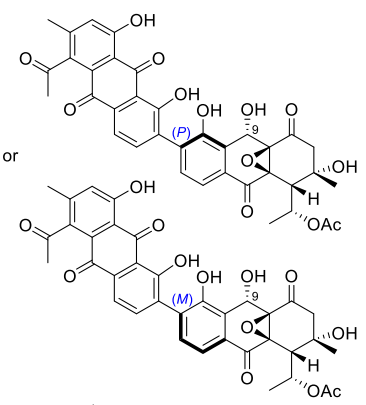
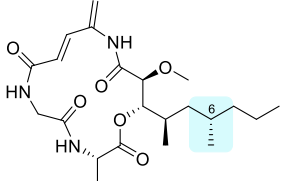
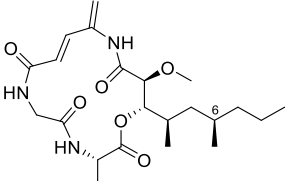
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
37	 guignardone H <sup>205</sup> fungus (2012)	ROESY; NMR comparison	 Guignardone H is a racemic mixture or includes impurities <sup>206</sup> .	asymmetric synthesis (2019) <sup>206</sup>
38	 (-)-guignardone I <sup>205</sup> fungus (2012)	ROESY; NMR comparison		asymmetric synthesis (2019) <sup>206</sup>
39	 (-)-isosarcophytin <sup>207</sup> coral (1999)	NMR comparison	 (-)-isosarcophytin = (-)-3-oxochatancin	total synthesis (2019) <sup>208</sup>
40	 halioxepine <sup>209</sup> (Only the relative configuration was proposed.) sponge (2011)	NOESY		total synthesis (2021) <sup>210</sup>
41	 julichrome Q <sub>3.5</sub> <sup>211</sup> fungus (1970)	NMR comparison	 or	X-ray (2020) <sup>212</sup>
42	 boholamide A <sup>213</sup> bacteria (2020)	ROESY; Marfey's method; ECD		total synthesis (2021) <sup>214</sup>

Table S6 (continued)

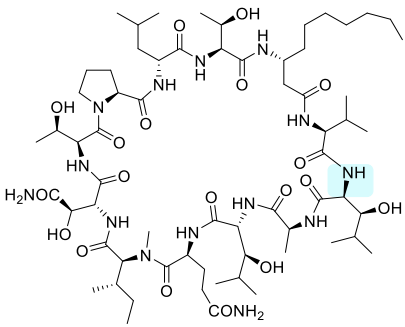
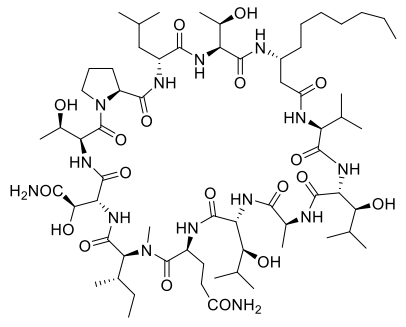
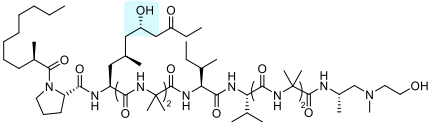
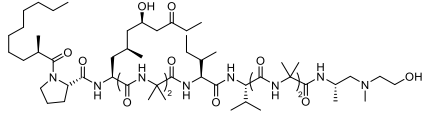
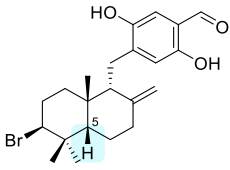
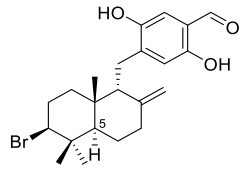
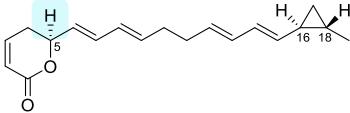
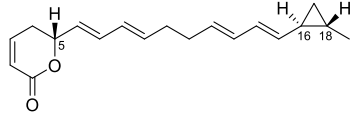
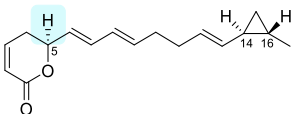
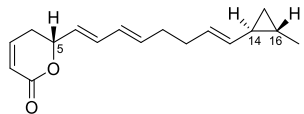
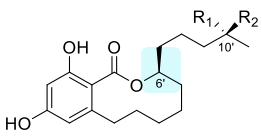
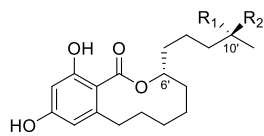
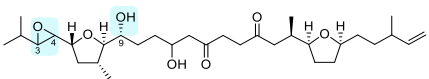
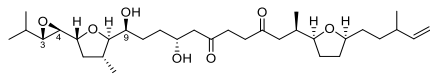
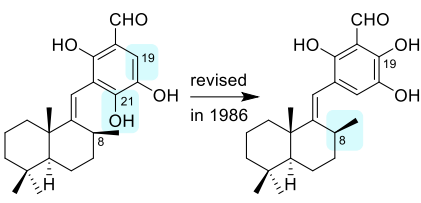
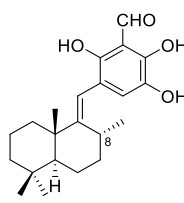
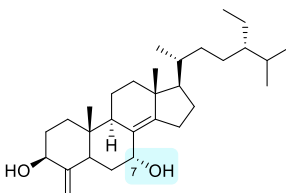
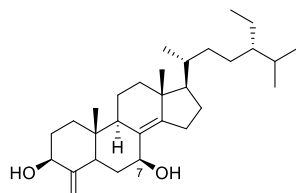
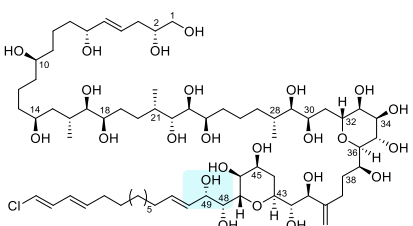
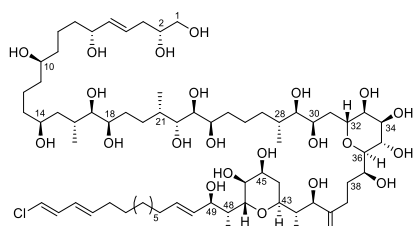
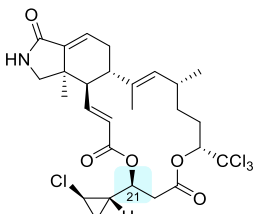
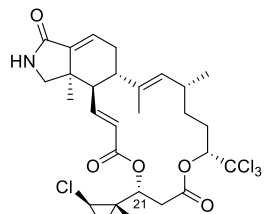
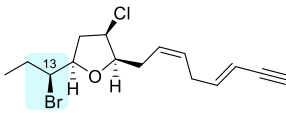
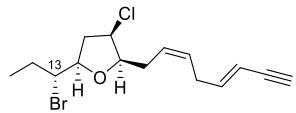
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
43	 <p>laxaphycin B<sup>215, 216</sup> alga (1992, 1997)</p>	Marfey's method; amino acid analysis		total synthesis; HPLC retention time; LCMS (2013) <sup>217</sup>
44	 <p>trichoderin A<sup>218</sup> fungus (2010)</p>	NOE; HPLC analysis		total synthesis (2016) <sup>219</sup>
45	 <p>peyssonol A<sup>220</sup> alga (1994)</p>	chemical shifts		total synthesis; X-ray (2010) <sup>221</sup>
46	 <p>coibacin A<sup>222</sup> cyanobacterium (2012)</p>	CD analysis; NOESY; J-based		total synthesis (2014) <sup>223</sup>
47	 <p>coibacin B<sup>222</sup> cyanobacterium (2012)</p>	NMR comparison		total synthesis (2014) <sup>223</sup>
48& 49	 <p>relgro<sup>224</sup>: R<sub>1</sub> = H, R<sub>2</sub> = OH 10'-oxorelgro<sup>225</sup>: R<sub>1</sub> = R<sub>2</sub> = O fungus (2011, 2016)</p>	CD comparison; Mosher's method		total synthesis (2019) <sup>226</sup>
50	 <p>amphirionin-5<sup>227</sup> strain (2014)</p>	J-based; NOESY		stereodivergent synthesis (2016) <sup>228, 229</sup>

Table S6 (continued)

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
51	 <p>siphonodictyal B<sup>230, 231</sup> sponge (1981, 1986)</p>	<i>J</i> -based		total synthesis; NOESY (2015) <sup>232</sup>
52	 <p>7<math>\alpha</math>-hydroxytheonellasterol<sup>233</sup> sponge (2000)</p>	<i>J</i> -based; chemical shifts	 <p>7<math>\beta</math>-hydroxytheonellasterol</p>	chemical conversion; NOESY; X-ray (2020) <sup>234</sup>
53	 <p>karlotoxin 2 dinoflagellate (2010)<sup>235</sup></p>	<i>J</i> -based; NOESY; chemical degradation; Mosher's method		DP4 chemical-shift analysis (2015) <sup>236</sup>
54	 <p>(+)-muironolide A<sup>237</sup> sponge (2009)</p>	<i>J</i> -based; chemical degradation; chiral LC-MS; NOESY	 <p>(+)-muironolide A = <i>ent</i>-muironolide A</p>	total synthesis (2015) <sup>238</sup>
55	 <p>(-)-bisezakyne A<sup>239</sup> alga (1999)</p>	NOESY; biogenetic consideration		total synthesis; biogenetic consideration (2016) <sup>240</sup>

Only the structure elucidation methods used for the erroneous structure element are mentioned in this table.



**Table S7.** Multiple stereocenters misidentification of MNPs (2010–2021).

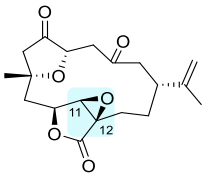
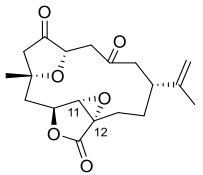
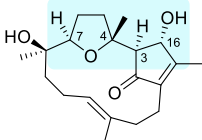
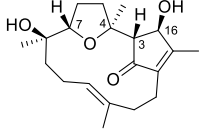
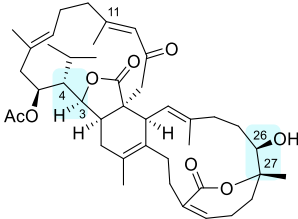
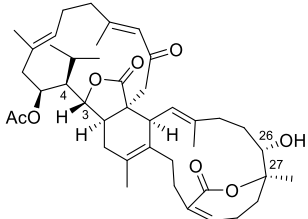
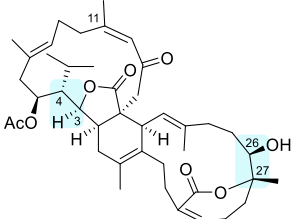
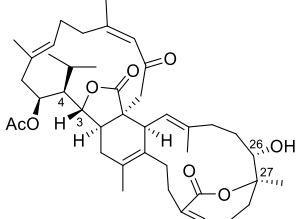
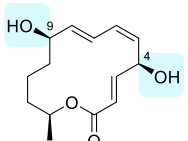
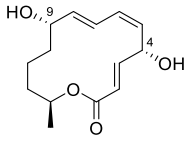
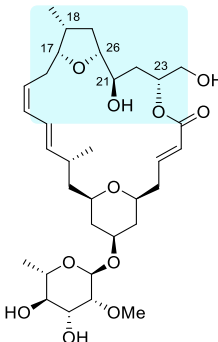
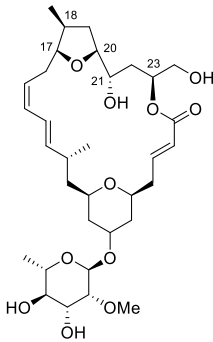
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
1	 scabrolide D <sup>241</sup> coral (2002)	NOESY	 scabrolide D = norcembrenolide C	total synthesis; X-ray (2011) <sup>242</sup>
2	 lobocrasol <sup>243</sup> coral (2009)	NOESY; Mosher's method		NMR comparison; X-ray (2021) <sup>244</sup>
3	 glaucumolide A <sup>245</sup> coral (2015)	NOESY; NMR comparison		NOESY; J-based; X-ray; TDDFT-ECD (2019) <sup>246</sup>
4	 glaucumolide B <sup>245</sup> coral (2015)	NOESY; NMR comparison		NOESY; NMR comparison; TDDFT-ECD (2019) <sup>246</sup>
5	 pesralotioprolide F <sup>247</sup> fungus (2016)	NMR comparison; NOESY		total synthesis (2018) <sup>248</sup>
6	 mandelalide A <sup>249</sup> ascidian (2012)	ROESY; J-based		total synthesis (2014, 2015) <sup>250-252</sup> ; computer-aided (2016) <sup>253</sup>

Table S7 (continued)

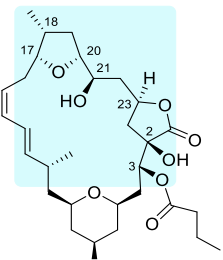
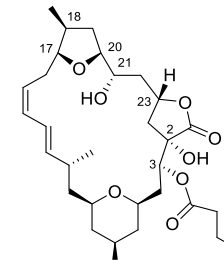
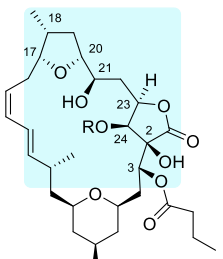
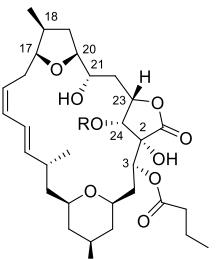
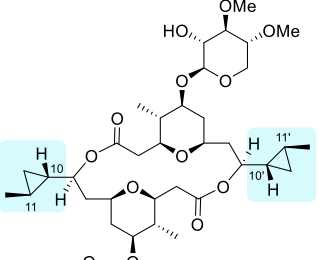
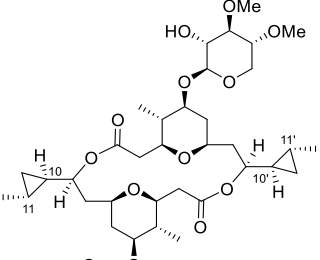
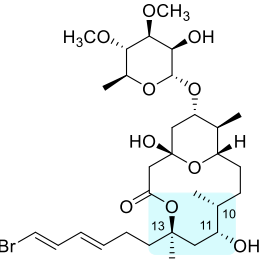
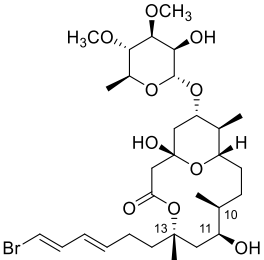
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
7	 mandelalide B <sup>249</sup> ascidian (2012)	ROESY; J-based		total synthesis (2015) <sup>252</sup>
8 & 9	 mandelalide C <sup>249</sup> : R = OH mandelalide D <sup>249</sup> : R = COCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> ascidian (2012)	ROESY; NMR comparison		total synthesis (2015) <sup>252</sup>
10	 clavosolide B <sup>254</sup> sponge (2002)	ROESY; NMR comparison		enantioselective total synthesis (2010) <sup>255</sup>
11	 (-)-lyngbyaloside B <sup>256</sup> cyanobacterium (2002)	ROESY		total synthesis (2015, 2016) <sup>257, 258</sup>

Table S7 (continued)

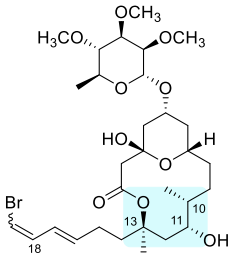
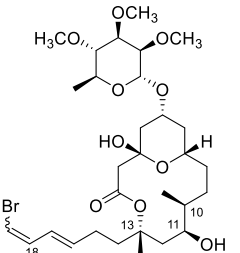
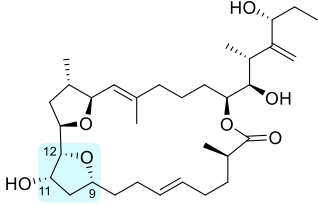
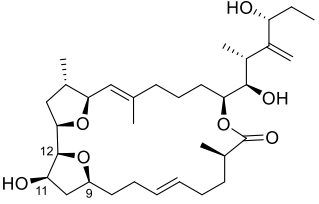
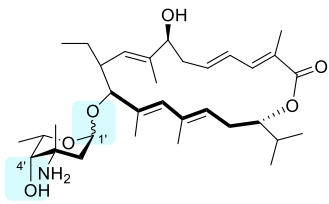
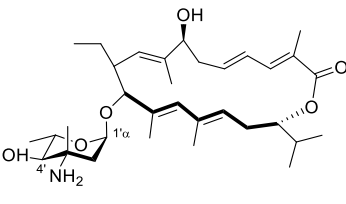
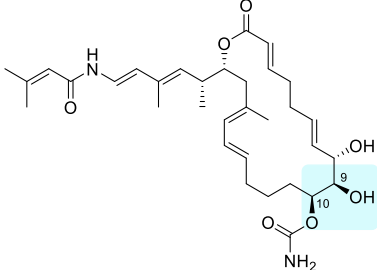
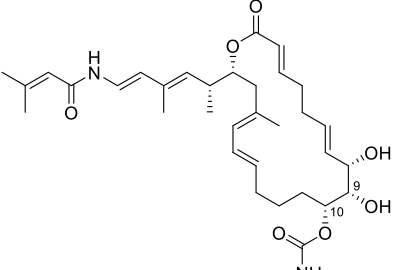
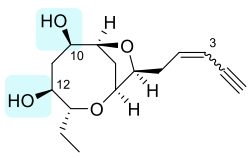
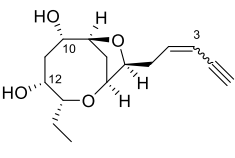
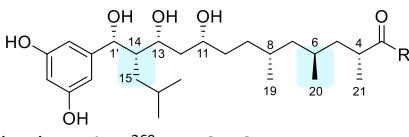
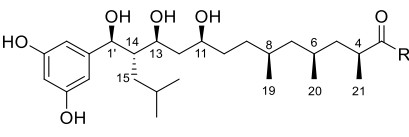
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12	 <p>18<i>E/Z</i>-lyngbyalide C<sup>259</sup> cyanobacterium (2010)</p>	<i>J</i> -based; NOESY		total synthesis (2015) <sup>260</sup>
13	 <p>iriomoteolide-2a<sup>261</sup> dinoflagellate (2015)</p>	ROESY; <i>J</i> -based; Mosher's method		total synthesis (2018, 2019) <sup>262, 263</sup>
14	 <p>mangrolide D<sup>264</sup> strain (2013)</p>	NMR		total synthesis (2019) <sup>265</sup>
15	 <p>palmerolide C<sup>266</sup> tunicate (2007)</p>	NOESY		total synthesis (2020) <sup>267, 268</sup>
16& 17	 <p>laurefurenyne C<sup>163</sup>: 3<i>Z</i> laurefurenyne D<sup>163</sup>: 3<i>E</i> alga (2010)</p>	NOESY; NMR comparison		total synthesis (2020) <sup>164</sup>
18& 19	 <p>baulamycin A<sup>269</sup>: R = CH<sub>2</sub>CH<sub>3</sub> baulamycin B<sup>269</sup>: R = CH<sub>3</sub> microbe (2014)</p>	<i>J</i> -based; (PS-DQF)-COSY; HOMO2DJ		total synthesis <sup>270-273</sup> ; DFT calculations <sup>270</sup> ; chemical transformation; ROESY (2017) <sup>270, 273</sup>

Table S7 (continued)

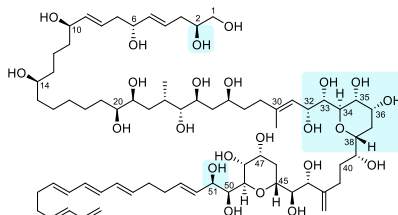
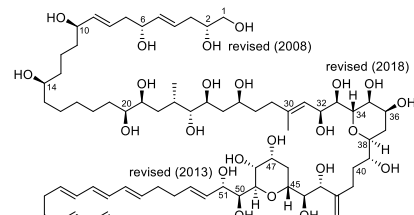
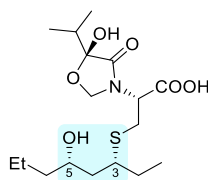
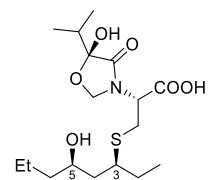
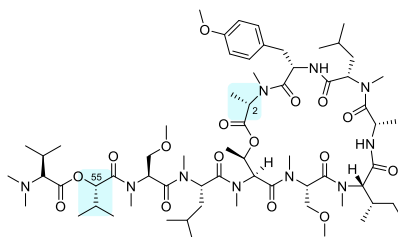
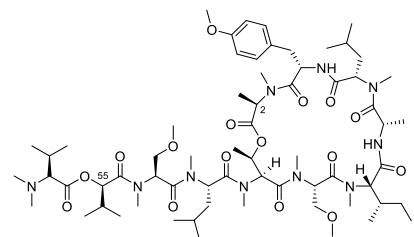
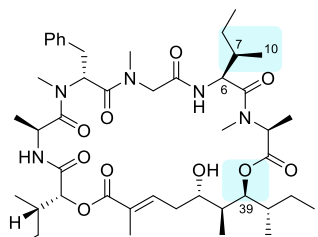
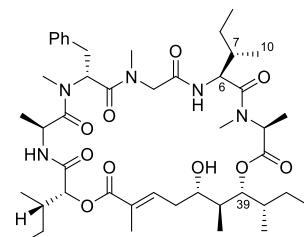
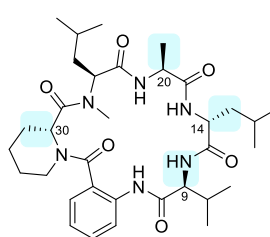
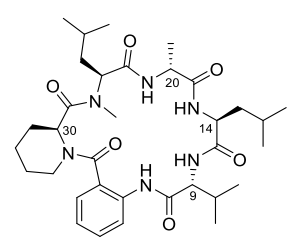
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
20	 <p>amphidinol 3<sup>274</sup> dinoflagellate (1999)</p>	<p><i>J</i>-based; Mosher's method; degradation; GC-MS</p>	 <p>OH revised (2008) revised (2018) revised (2013)</p>	<p>stereoselective synthesis (2013, 2018)<sup>275, 276</sup>; total synthesis (2020)<sup>277</sup></p>
21	 <p>thelepamide<sup>278</sup> worm (2014)</p>	<p>ROESY; <i>J</i>-based; computer-aided</p>		<p>total synthesis; computer-aided (2018)<sup>279</sup></p>
22	 <p>coibamide A<sup>280</sup> cyanobacterium (2008)</p>	<p>ROESY; acid hydrolysis; HPLC-MS; GC-MS</p>		<p>total synthesis (2014, 2015)<sup>281, 282</sup>; computer-aided (2016)<sup>253</sup></p>
23	 <p>lagunamide A<sup>283</sup> cyanobacterium (2010)</p>	<p>NOESY; ROESY; <i>J</i>-based; Marfey's method; Mosher's method</p>		<p>total synthesis (2012)<sup>284</sup></p>
24	 <p>similanamide<sup>285</sup> fungus (2015)</p>	<p>NOESY; acid hydrolysis; chiral HPLC analysis</p>		<p>total synthesis (2015)<sup>286</sup></p>

Table S7 (continued)

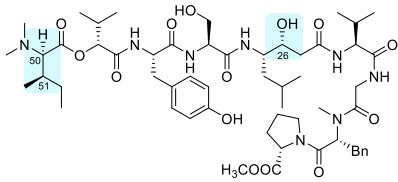
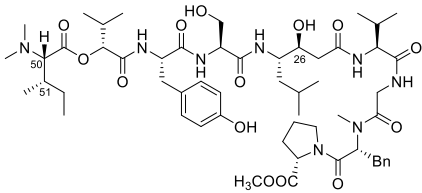
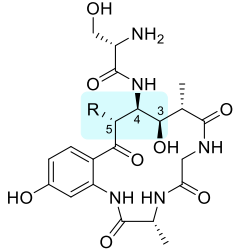
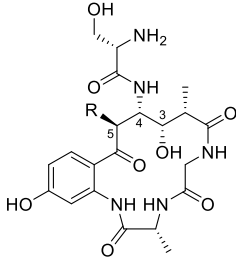
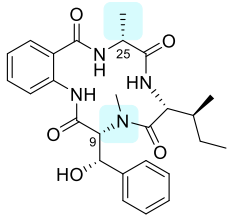
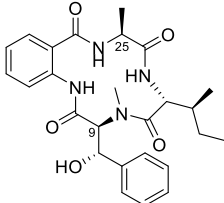
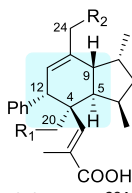
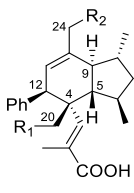
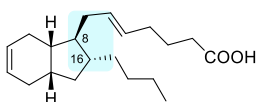
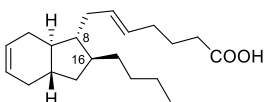
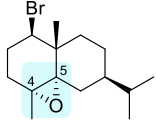
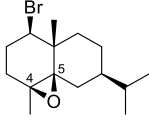
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
25	 <p>symplotin A<sup>287</sup> cyanobacterium (2012)</p>	acid hydrolysis; Marfey's method; HPLC analysis		total synthesis (2017) <sup>288</sup>
26& 27	 <p>solomonamide A<sup>289</sup>: R = OH solomonamide B<sup>289</sup>: R = H sponge (2011)</p>	ROESY; computer-aided; NMR comparison		total synthesis (2016, 2018) <sup>290, 291</sup>
28	 <p>asperterrestide A<sup>292</sup> fungus (2012)</p>	NOESY; J-based		total synthesis (2019) <sup>293</sup>
29– 31	 <p>plakotenin<sup>294</sup>: R<sub>1</sub> = Me, R<sub>2</sub> = H; <i>homo</i>-plakotenin<sup>295</sup>: R<sub>1</sub> = R<sub>2</sub> = Me; <i>nor</i>-plakotenin<sup>295</sup>: R<sub>1</sub> = R<sub>2</sub> = H sponge (1992, 1999)</p>	NOESY; NMR comparison; optical rotation		total synthesis; computer-aided (2012) <sup>296</sup>
32	 <p>(-)-mucosin<sup>297</sup> sponge (1997)</p>	NOESY; ROESY		total synthesis (2017, 2018) <sup>298, 299</sup>
33	 <p>1β-bromo-4α,5α-epoxyselinane<sup>300</sup> alga (2016)</p>	NOESY		computer-aided (2017) <sup>98</sup>

Table S7 (continued)

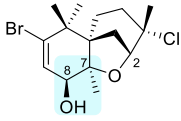
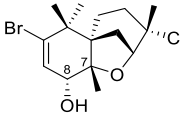
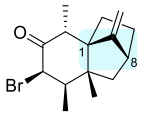
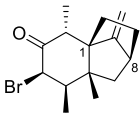
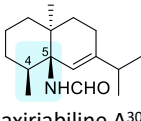
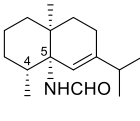
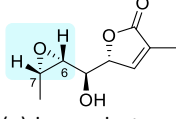
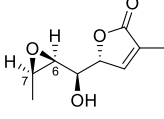
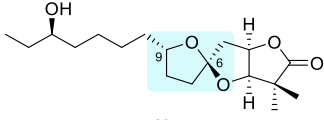
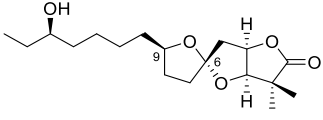
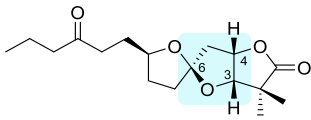
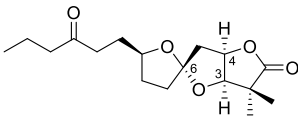
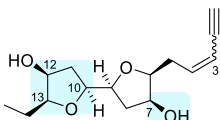
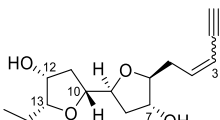
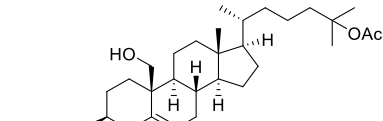
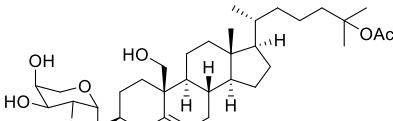
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
34	 <p>(8<math>\beta</math>)-10-bromo-3-chloro-2,7-epoxychamigr-9-en-8-ol<sup>301</sup> alga (2010)</p>	ROESY		computer-aided (2017) <sup>98</sup>
35	 <p>coll-compd 4<sup>302</sup> alga (1989)</p>	NMR comparison		computer-aided (2017) <sup>98</sup>
36	 <p>axiriabiline A<sup>303</sup> sponge (2017)</p>	ROESY		X-ray (2019) <sup>304</sup>
37	 <p>(+)-hypoxylactone<sup>305</sup> fungus (1999)</p>	NOESY		synthesis (2020) <sup>306</sup>
38	 <p>penisporolide A<sup>307</sup> fungus (2007)</p>	NOESY; NMR comparison		NMR method (2016) <sup>204</sup>
39	 <p>penisporolide B<sup>307</sup> fungus (2007)</p>	NMR comparison		total synthesis (2016) <sup>203</sup>
40& 41	 <p>laurefurenyne A<sup>163</sup>: 3Z laurefurenyne B<sup>163</sup>: 3E alga (2010)</p>	NOESY; NMR comparison		total synthesis (2013) <sup>308, 309</sup>
42	 <p>junceelloside C<sup>310</sup> coral (2005)</p>	NOESY		J-based; acid hydrolysis; HPLC analysis (2013) <sup>311</sup>

Table S7 (continued)

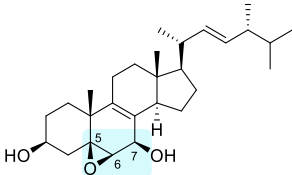
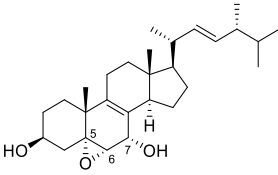
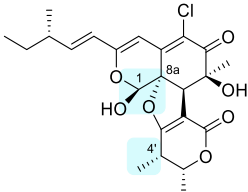
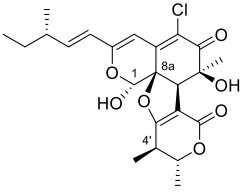
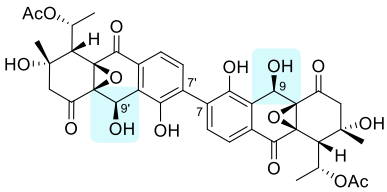
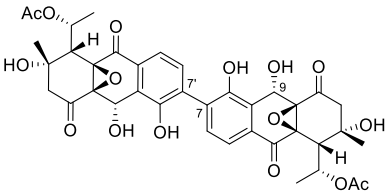
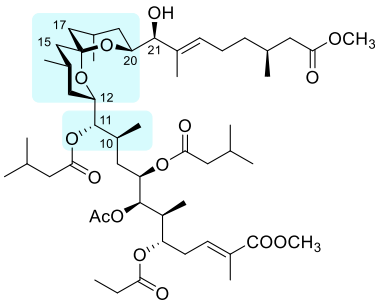
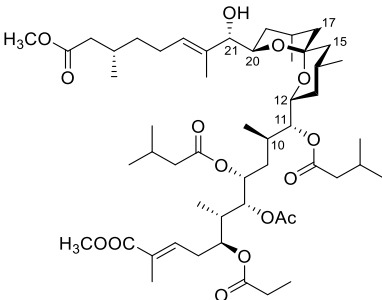
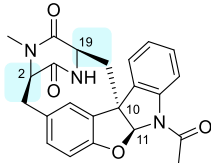
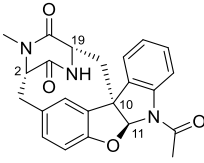
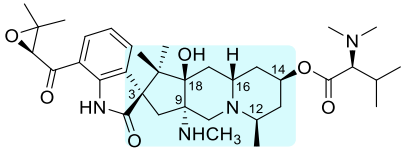
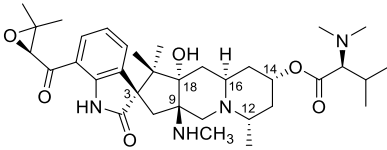
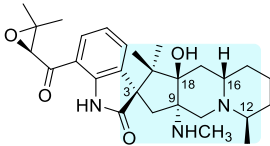
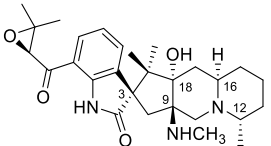
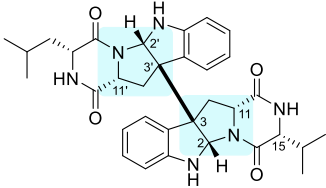
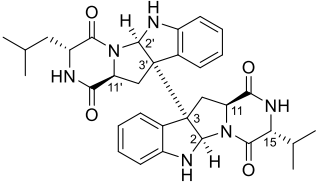
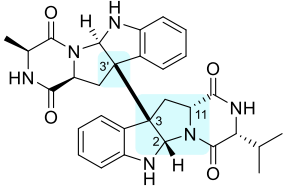
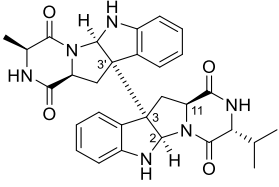
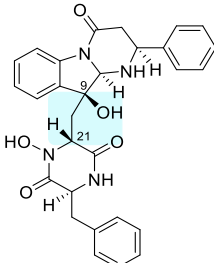
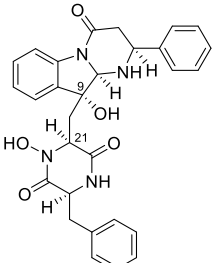
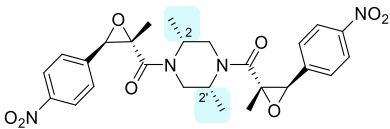
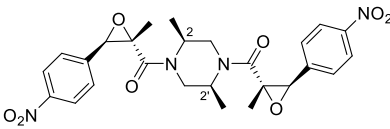
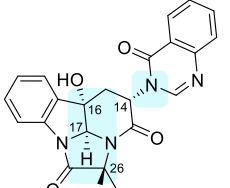
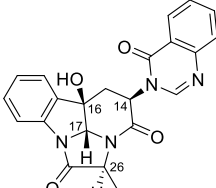
no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
43	 <p>5β,6β-epoxy-(22<i>E</i>,24<i>R</i>)-ergosta-8,22-diene-3β,7β-diol<sup>312</sup> coral (2016)</p>	NOESY; NMR comparison		re-examine NMR (2017) <sup>313</sup>
44	 <p>chaephilone C<sup>314</sup> fungus (2018)</p>	NOESY; TDDFT-ECD		NMR comparison; OR; X-ray (2019) <sup>315</sup>
45	 <p>julichrome Q<sub>3,3</sub><sup>316, 317</sup> strain (1970)</p>	NMR		NMR comparison (2020) <sup>212</sup>
46	 <p>didemnaketal B<sup>318</sup> ascidian (1991)</p>	NMR comparison		total synthesis (2013, 2014) <sup>319, 320</sup> , X-ray (2014) <sup>320</sup>
47	 <p>(+)-azonazine<sup>321</sup> fungus (2010)</p>	1D NOE; TDDFT-ECD		total synthesis (2013, 2014) <sup>322, 323</sup>
48	 <p>(-)-citrinadin A<sup>324, 325</sup> fungus (2004)</p>	ROESY <sup>324</sup> ECD; VCD comparison <sup>325</sup>		total synthesis (2013, 2014) <sup>326, 327</sup>

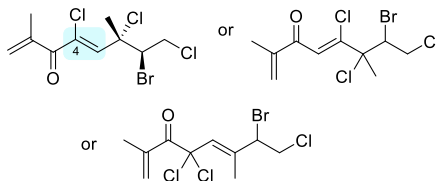
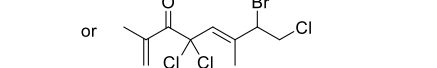
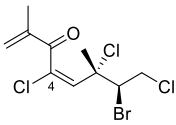
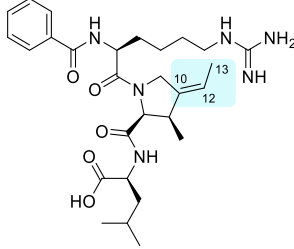
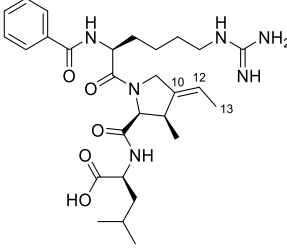
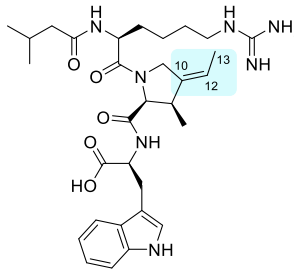
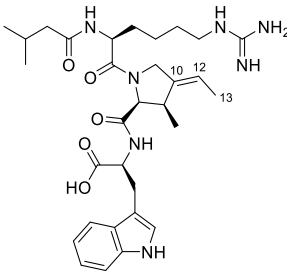
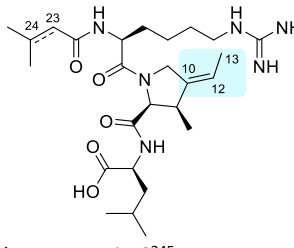
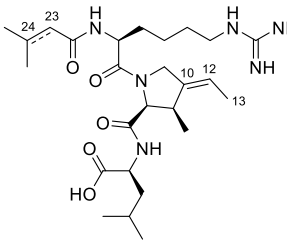
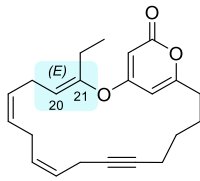
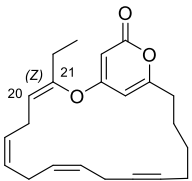
Table S7 (continued)

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
49	 <p>(+)-citrinadin B<sup>325</sup> fungus (2005)</p>	ROESY; ECD; VCD comparison		total synthesis (2013, 2014) <sup>327, 328</sup>
50	 <p>(+)-asperdimin<sup>329</sup> fungus (2004)</p>	NMR comparison; acid hydrolysis		total synthesis (2014) <sup>201</sup>
51	 <p>(+)-cristatumin C<sup>330</sup> fungus (2012)</p>	NOESY; acid hydrolysis; chiral HPLC analysis		total synthesis (2014) <sup>331</sup>
52	 <p>haenamindole<sup>332</sup> fungus (2015)</p>	ROESY; Marfey's method		ROESY; C <sub>3</sub> Marfey analysis (2016) <sup>31</sup>
53	 <p>chrysamide B<sup>333</sup> fungus (2016)</p>	X-Ray		total synthesis; NMR comparison; X-ray (2018) <sup>334</sup>
54	 <p>(-)-versiquinazoline H<sup>335</sup> fungus (2016)</p>	NOESY; ECD; Marfey's method; acid hydrolysis; HPLC analysis		total synthesis (2020) <sup>336</sup>

Only the structure elucidation methods used for the erroneous structure element are mentioned in this table.



**Table S8.** Structural revisions of double bond geometry of MNPs (2010–2021).

no.	Proposed structure	Methods used in initial assignment	Revised structure	Basis for revision
1	 <p>or</p>  <p>plocamenone<sup>337-343</sup> alga (1979, 1983, 1984, 1985, 1997, 2010)</p>	chemical shifts; no complete 2D NMR analysis		2D NMR (2012) <sup>344</sup>
2	 <p>lucentamycin A<sup>345</sup> strain (2007)</p>	ROESY		total synthesis (2009, 2012) <sup>346, 347</sup> ; X-ray (2012) <sup>347</sup> ; ROESY reanalysis (2012) <sup>348</sup>
3	 <p>lucentamycin B<sup>345</sup> strain (2007)</p>	NMR comparison		NMR comparison (2012) <sup>348</sup>
4&5	 <p>lucentamycin C<sup>345</sup> lucentamycin D<sup>345</sup>: <math>\Delta^{23,24}</math> strain (2007)</p>	NMR comparison		NMR comparison (2012) <sup>348</sup>
6	 <p>phacelocarpus 2-pyrone A<sup>349</sup> alga (1982)</p>	<i>J</i> -based		total synthesis; computer-aided (2015) <sup>350</sup>

Only the structure elucidation methods used for the erroneous structure element are mentioned in this table.

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