

Sesterterpenoids: Chemistry, Biology, and Biosynthesis

Keke Li,^a Kirk R. Gustafson^{*b}

Affiliation

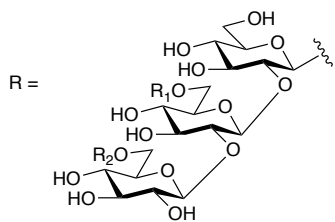
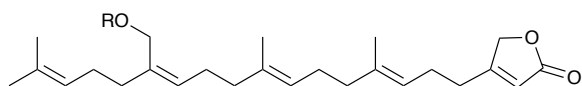
^a*College of Life Science, Dalian Minzu University, Dalian 116600, China*

^b*Molecular Targets Program, Center for Cancer Research, National Cancer Institute, Frederick, Maryland 21702-1201, United States*

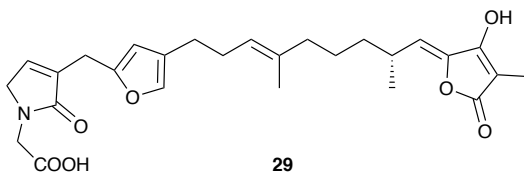
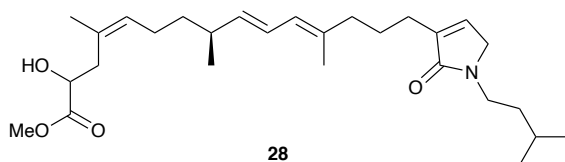
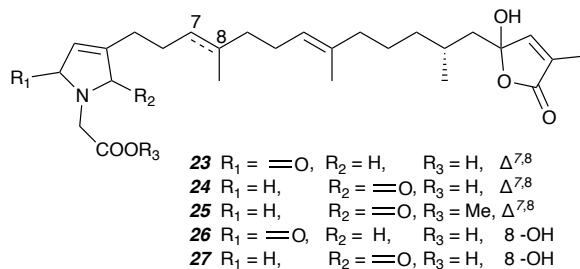
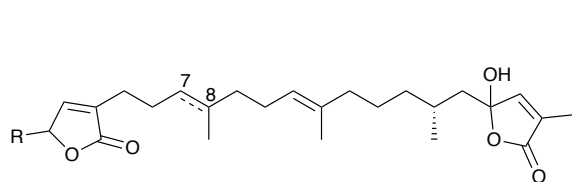
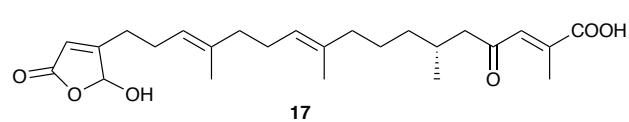
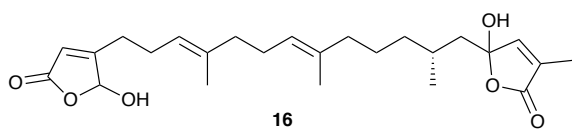
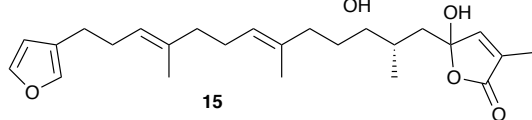
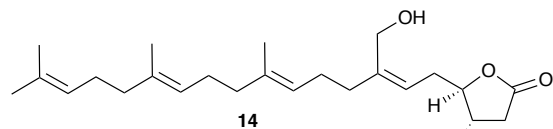
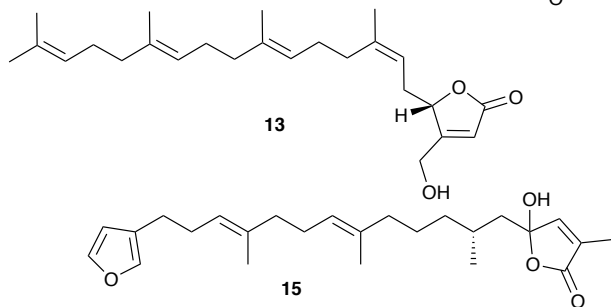
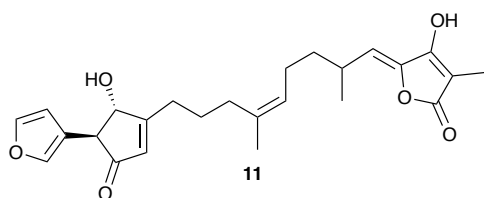
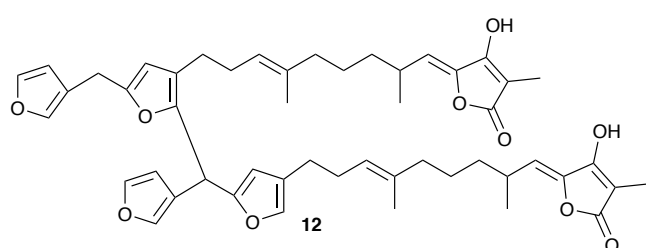
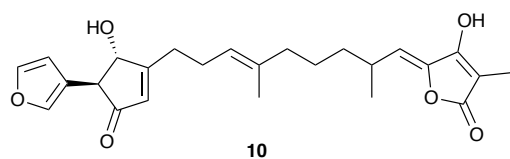
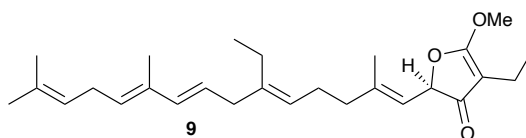
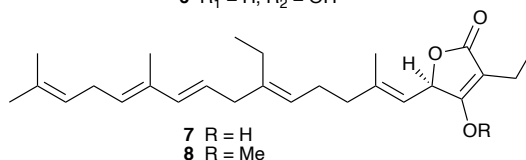
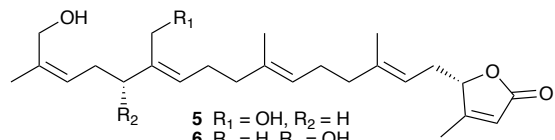
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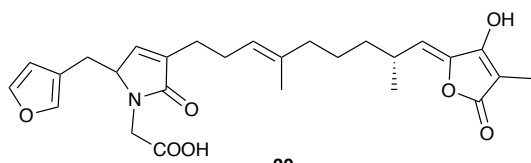
Supporting Information

Contents – Compilation of all the sesterterpenoid structures

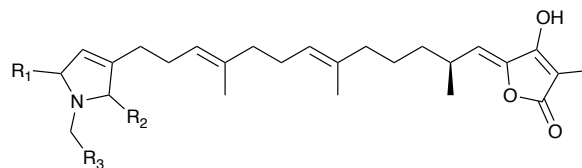


- 1** $R_1 = H, R_2 = H$
2 $R_1 = Ac, R_2 = H$
3 $R_1 = H, R_2 = Ac$
4 $R_1 = Ac, R_2 = Ac$



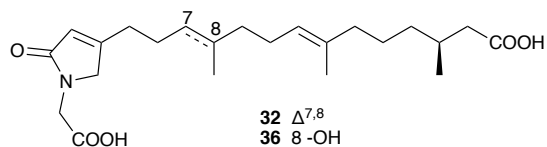


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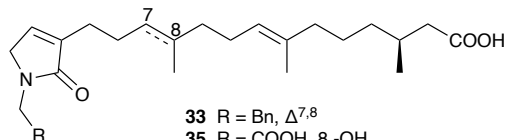
31 $R_1 = \text{O}, R_2 = \text{H}_2, R_3 = \text{COOH}$

34 $R_1 = \text{H}_2, R_2 = \text{O}, R_3 = \text{Bn}$



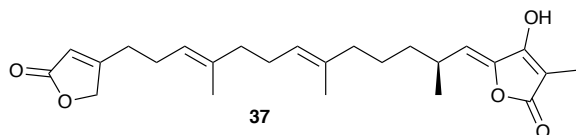
32 $\Delta^{7,8}$

36 8-OH

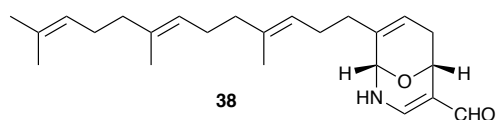


33 $R = \text{Bn}, \Delta^{7,8}$

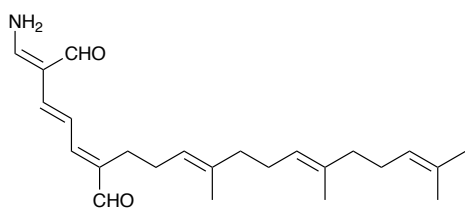
35 $R = \text{COOH}, 8\text{-OH}$



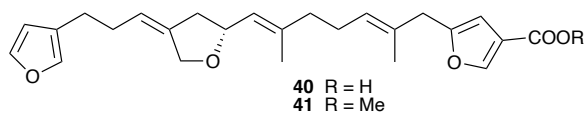
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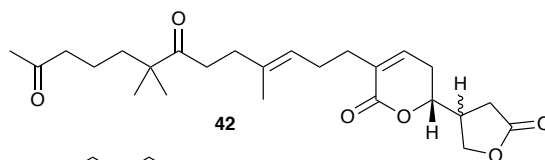
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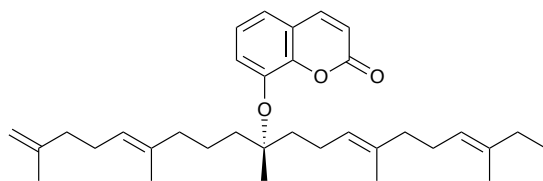
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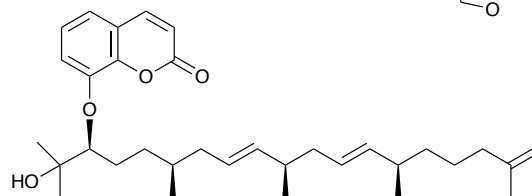
40 $R = \text{H}$
41 $R = \text{Me}$



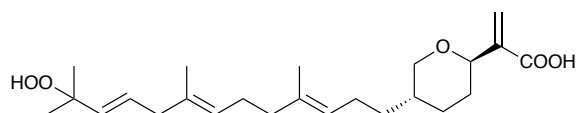
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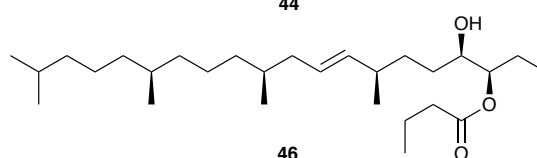
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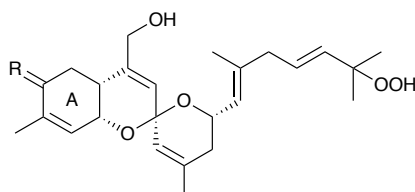
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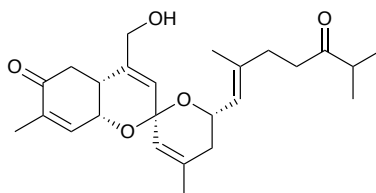
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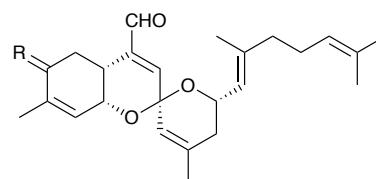
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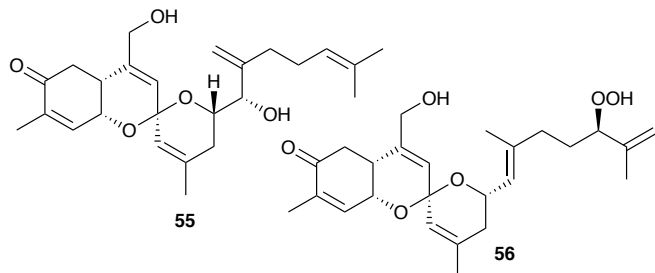
47 $R = \text{O}$
49 $R = R\text{-OAc}$
50 $R = S\text{-OAc}$



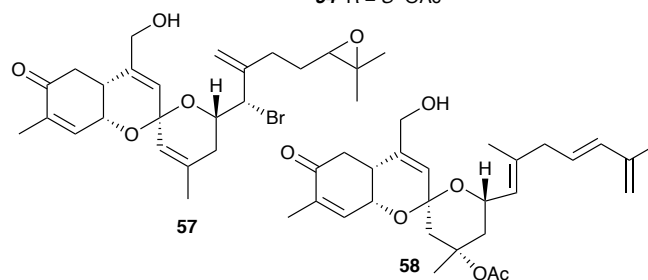
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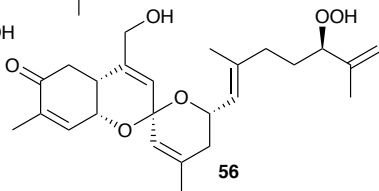
51 $R = R\text{-OH}$
52 $R = \text{O}$
53 $R = R\text{-OAc}$
54 $R = S\text{-OAc}$



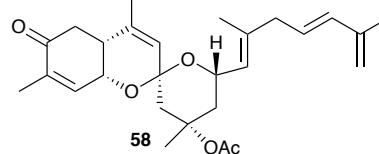
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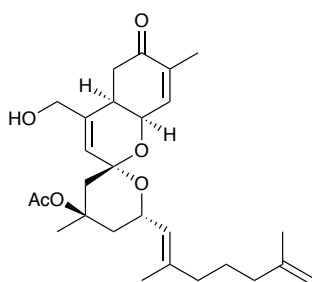
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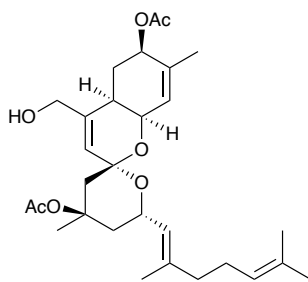
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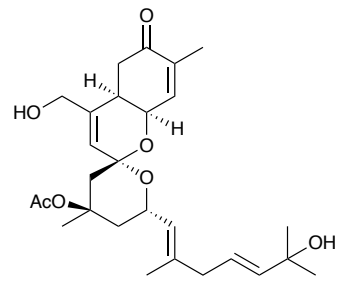
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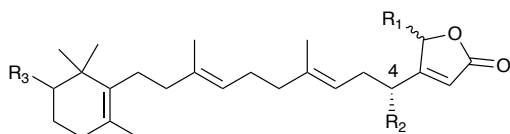
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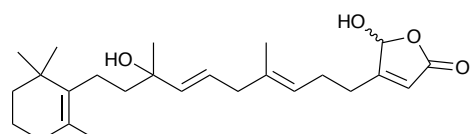


62 $R_1 = H, R_2 = OH, R_3 = \equiv O$

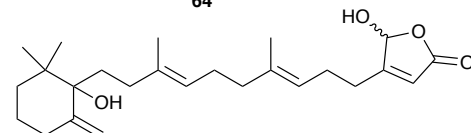
63 $R_1 = OH, R_2 = H, R_3 = \equiv O$

66 $R_1 = H, R_2 = OH, R_3 = H$

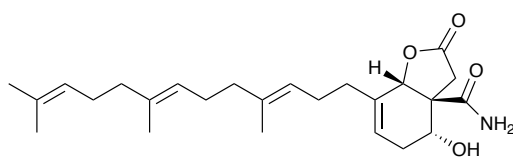
67 $R_1 = H, R_2 = OAc, R_3 = \equiv O$



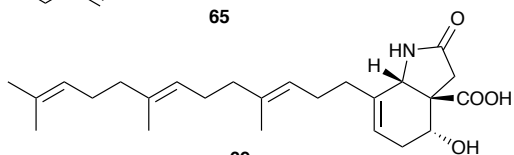
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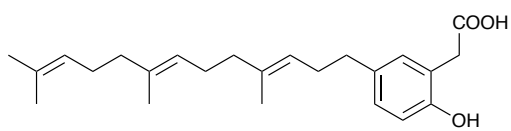
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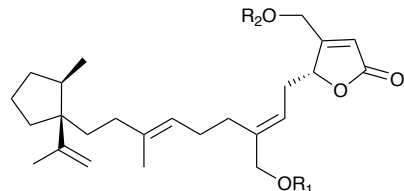
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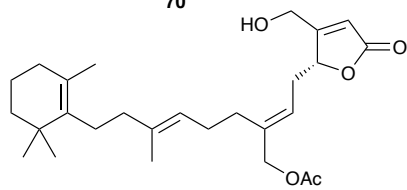
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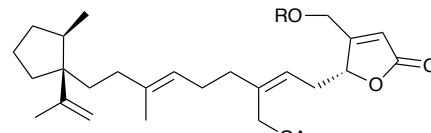
71 $R_1 = Ac, R_2 = H$

72 $R_1 = Ac, R_2 = Ac$

73 $R_1 = H, R_2 = H$

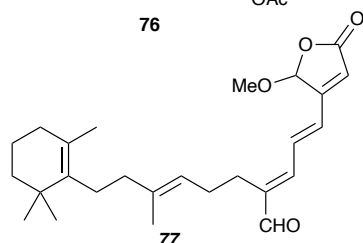


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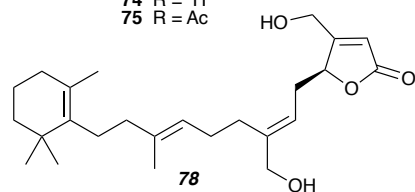


74 $R = H$

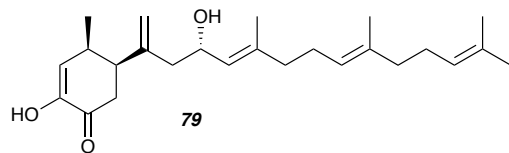
75 $R = Ac$



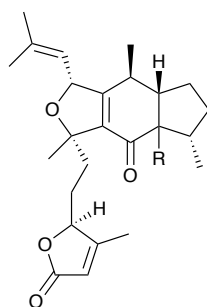
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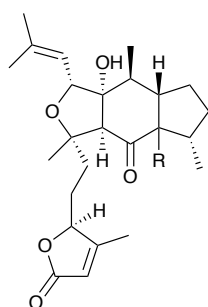


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80 $R = \beta-OH$

81 $R = \alpha-OH$

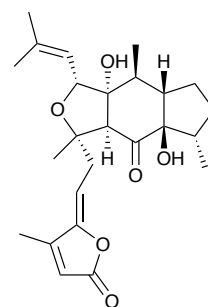


82 $R = \beta-OH$

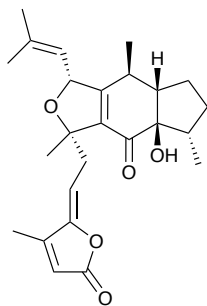
83 $R = \alpha-OH$

84 $R = \beta-H$

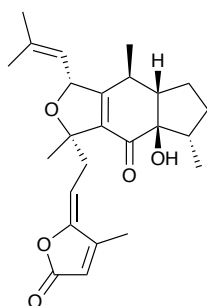
85 $R = \alpha-H$



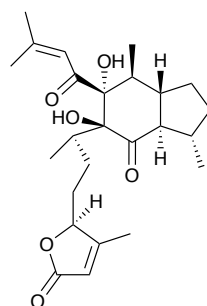
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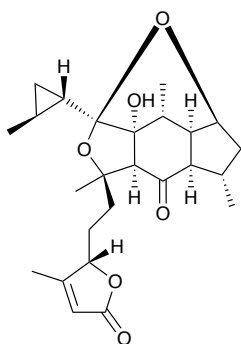
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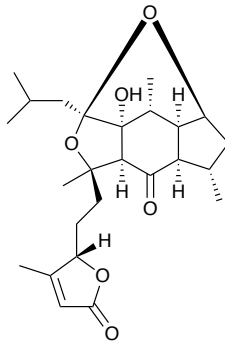
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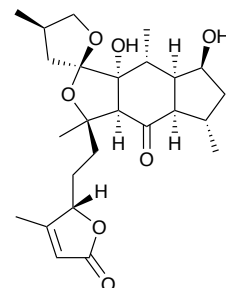
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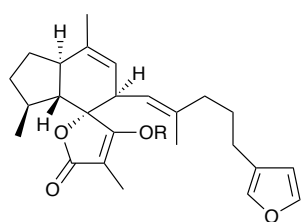
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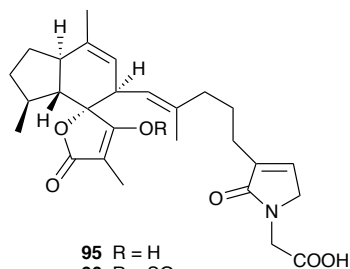
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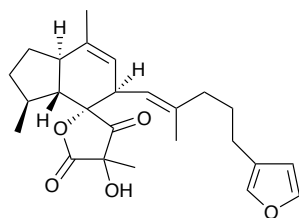
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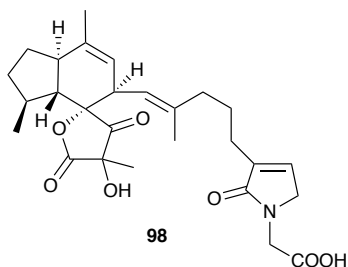
93 R = H
94 R = SO₃⁻



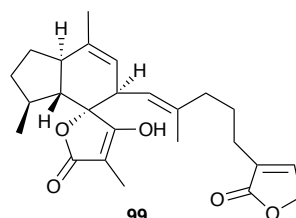
95 R = H
96 R = SO₃⁻



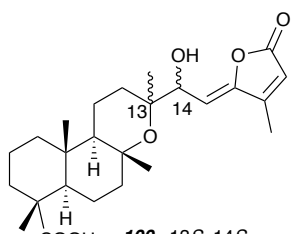
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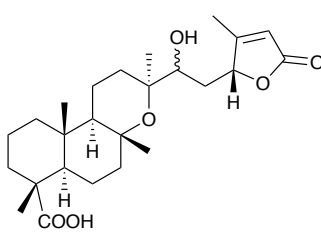
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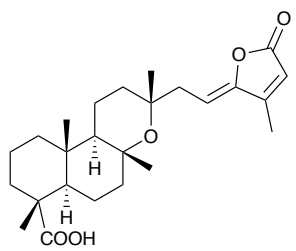
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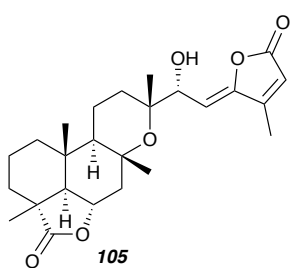
100 13S, 14S
101 13R, 14S
102 13S, 14R



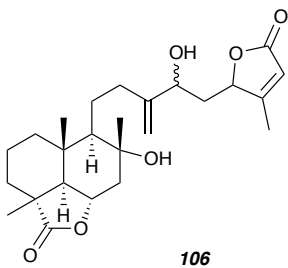
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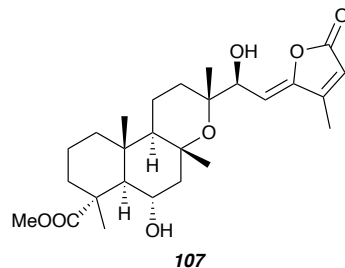
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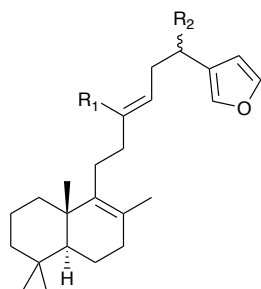
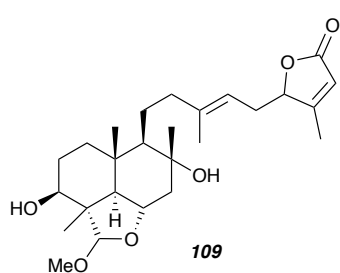
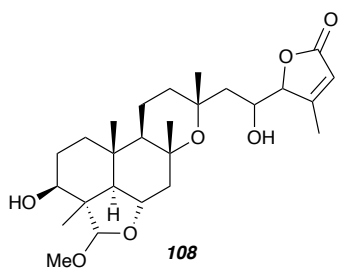
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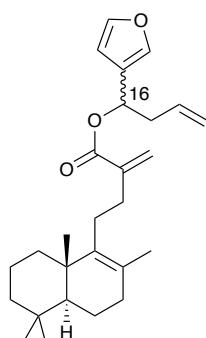
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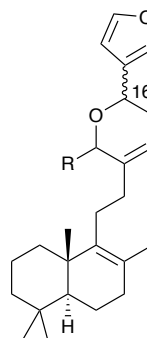
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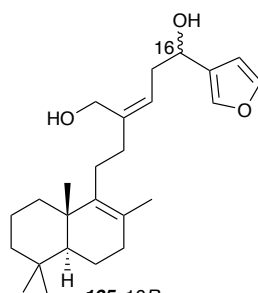
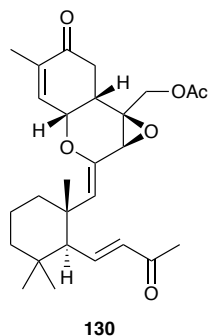
- 110** $R_1 = \text{CH}_2\text{OH}$, $R_2 = S\text{-OAc}$
111 $R_1 = \text{CH}_2\text{OH}$, $R_2 = R\text{-OAc}$
112 $R_1 = \text{CHO}$, $R_2 = S\text{-OAc}$
113 $R_1 = \text{CHO}$, $R_2 = R\text{-OAc}$
114 $R_1 = \text{COOH}$, $R_2 = S\text{-OAc}$
115 $R_1 = \text{COOH}$, $R_2 = R\text{-OAc}$
116 $R_1 = \text{COOH}$, $R_2 = S\text{-OH}$
117 $R_1 = \text{COOH}$, $R_2 = R\text{-OH}$
118 $R_1 = \text{COOMe}$, $R_2 = \equiv\text{O}$
119 $R_1 = \text{COOMe}$, $R_2 = R\text{-OH}$
120 $R_1 = \text{CH}_2\text{OH}$, $R_2 = R\text{-OH}$



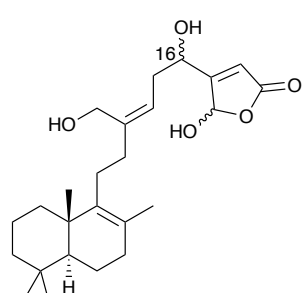
122 $16S$



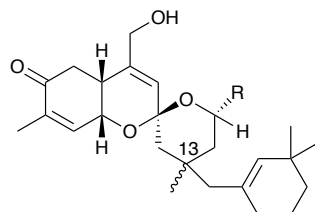
124 $16S$, $R = \equiv\text{O}$
129 $16S$, $R = \text{OH}$



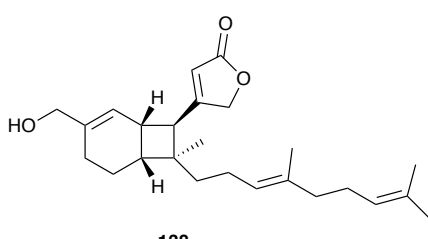
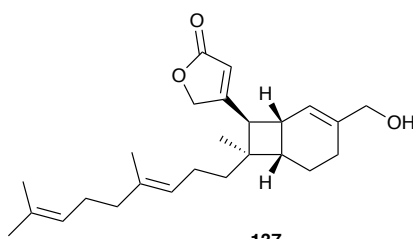
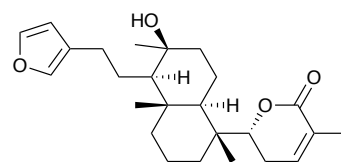
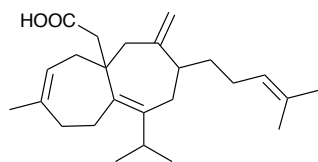
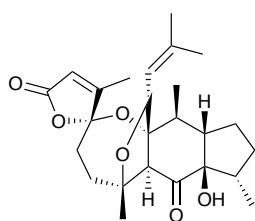
126 $16S$

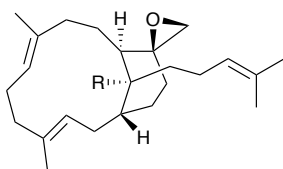


128 $16S$

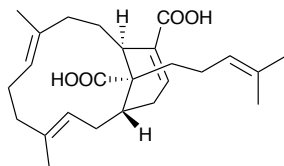


132 $R = \text{OMe}$, $13S$
133 $R = \text{OH}$, $13R$

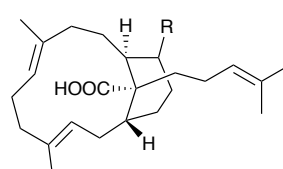




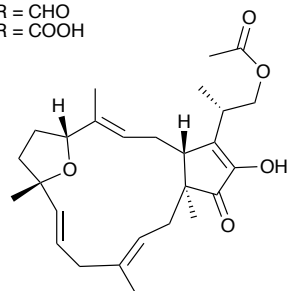
139 R = CHO
140 R = COOH



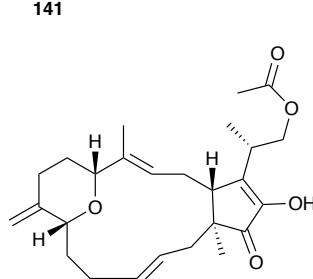
141



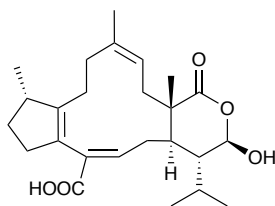
142 R = α -CHO
143 R = β -CHO



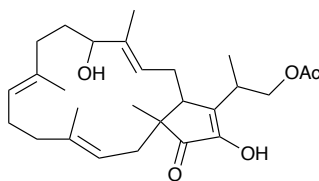
144



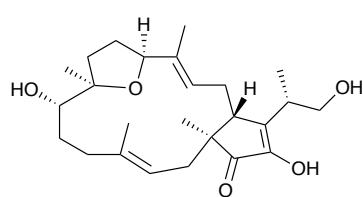
145



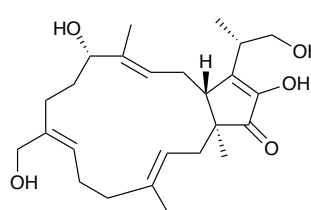
146



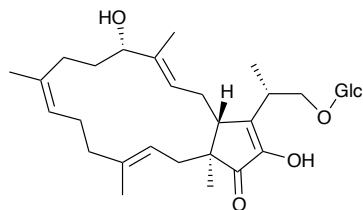
147



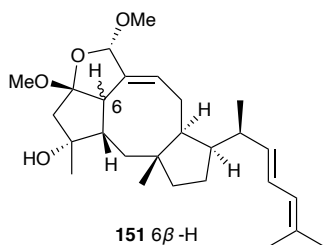
148



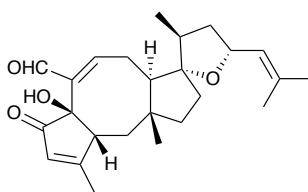
149



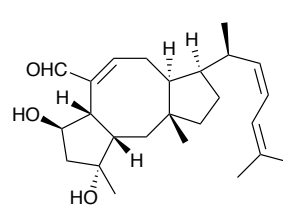
150



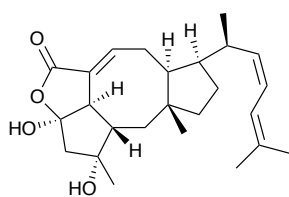
151 6 β -H
152 6 α -H



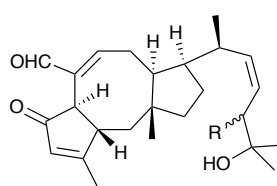
153



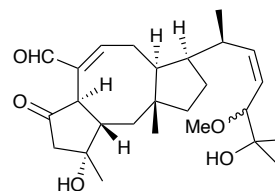
154



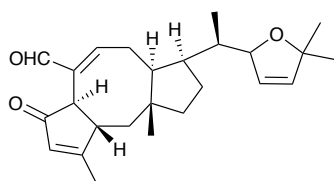
155



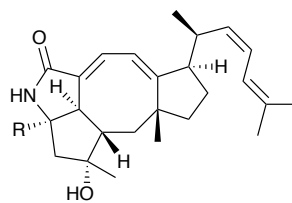
156 R = α -OH
157 R = OMe



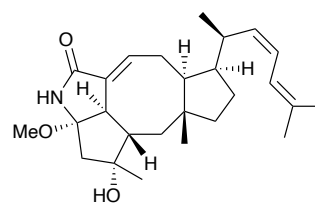
158



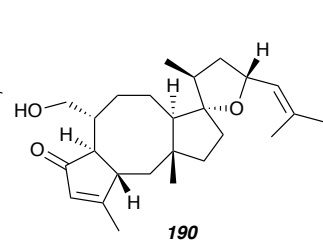
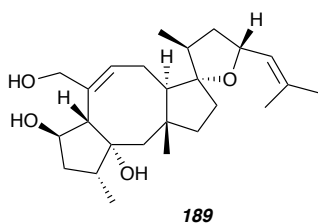
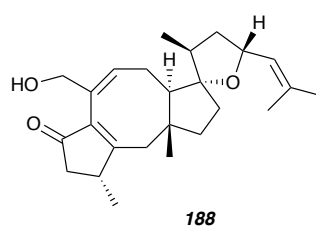
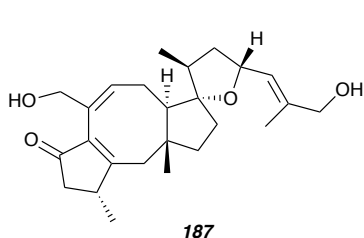
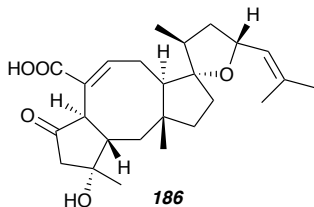
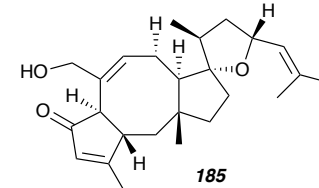
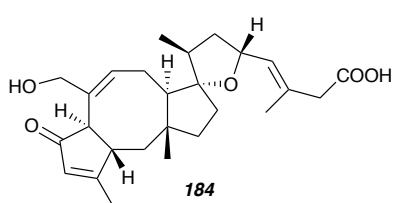
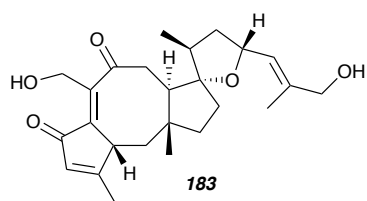
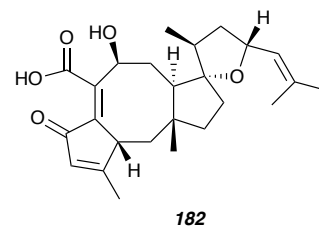
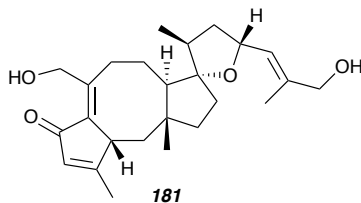
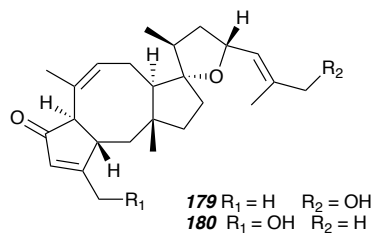
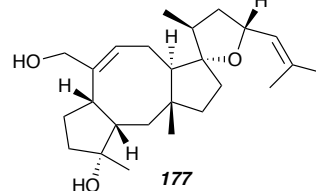
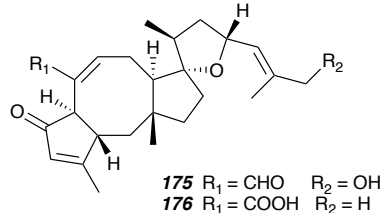
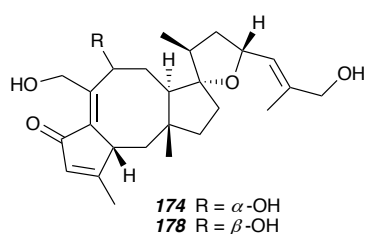
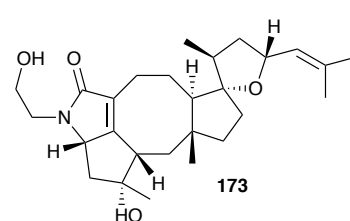
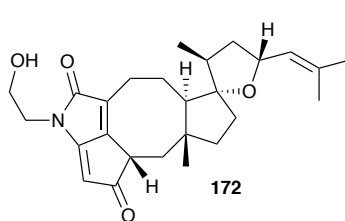
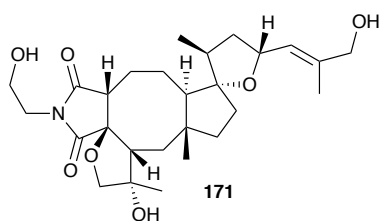
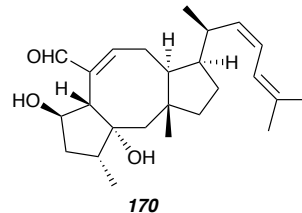
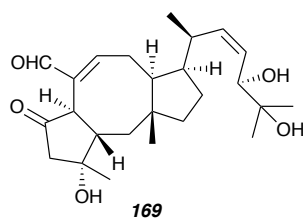
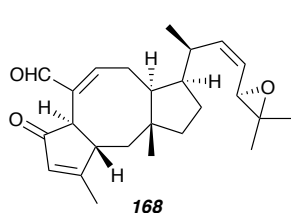
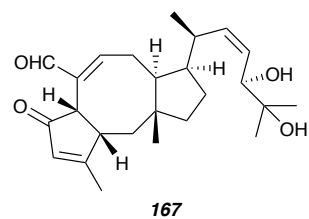
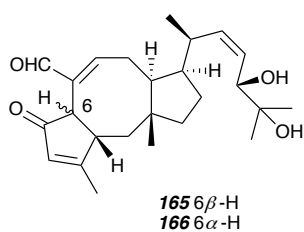
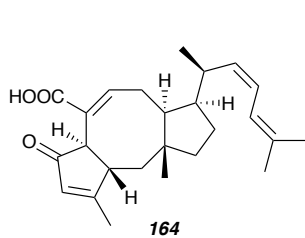
159

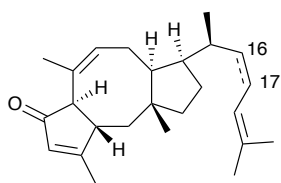


160 R = OCH₃
161 R = OH
162 R = H

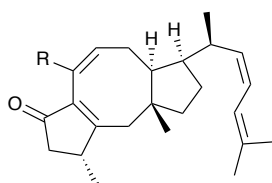


163

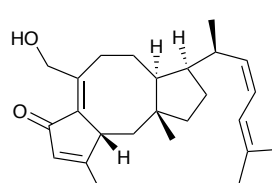




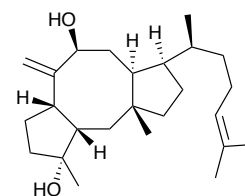
191 $\Delta^{16,17}$
192



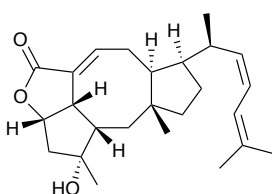
193 R = CH₂OH
196 R = CHO



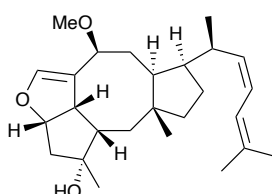
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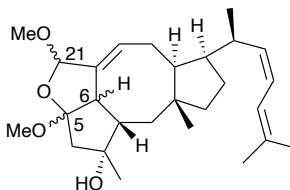
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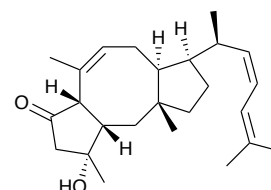
197



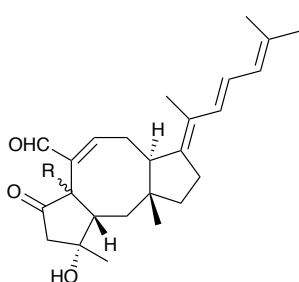
198



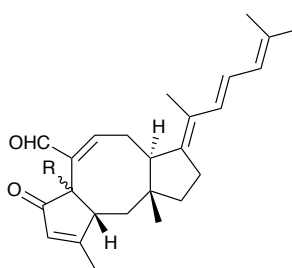
199 5 α , 6 α , 21 β
200 5 α , 6 α , 21 α
201 5 β , 6 β , 21 β



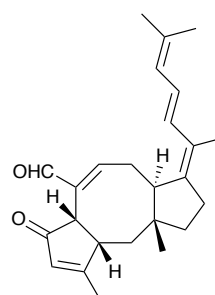
202



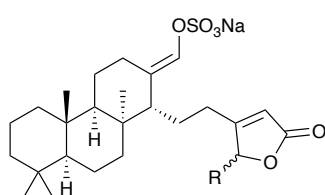
203 R = α -H
204 R = β -H



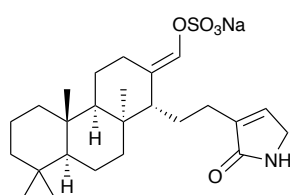
205 R = α -H
206 R = β -H



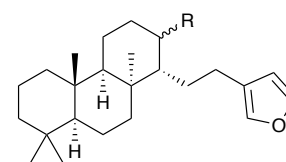
207



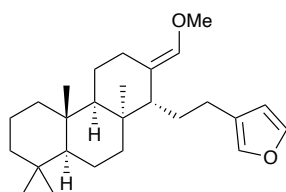
208 R = OH
210 R = OAc



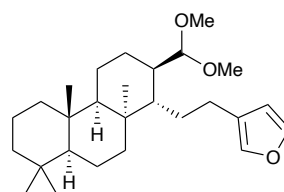
209



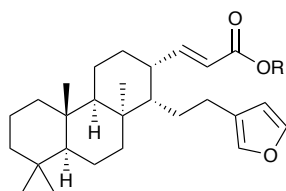
211 R = β -CHO
212 R = α -CHO
213 R = β -CH₂OH
214 R = β -COOH
215 R = =O
216 R = α -OH



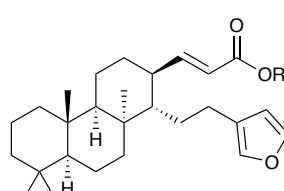
217



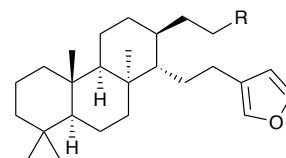
218



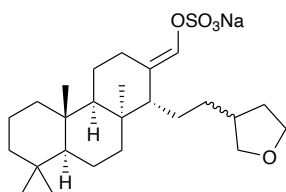
219 R = H
220 R = Et



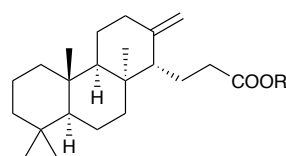
221 R = H
222 R = Et



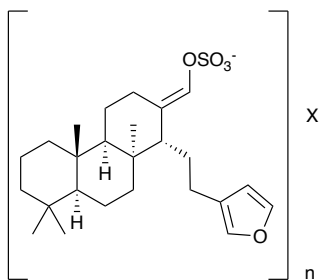
223 R = COOMe
224 R = COOH
225 R = CH₂OH



226
227

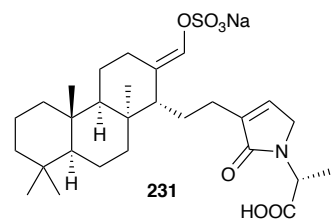
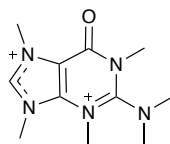


228 R = H
229 R = Me

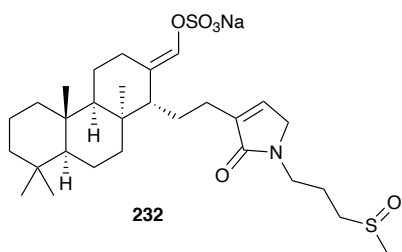


230

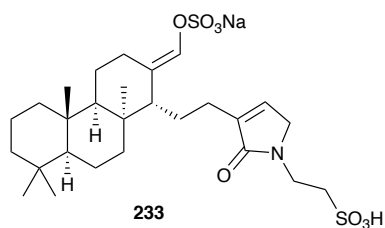
$n = 2, X =$



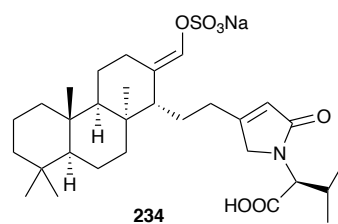
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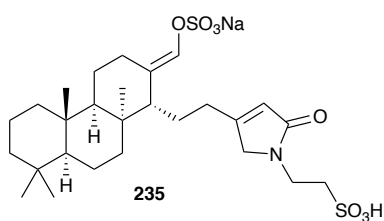
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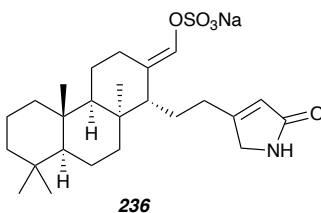
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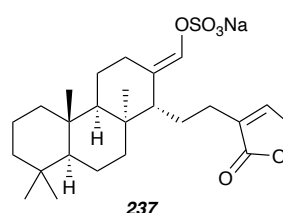
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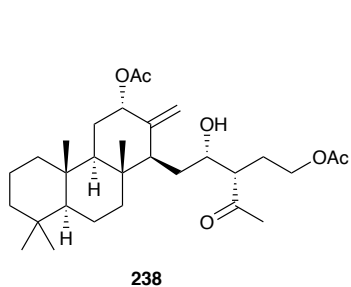
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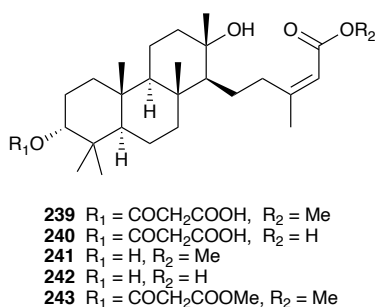
236



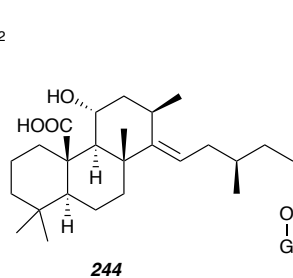
237



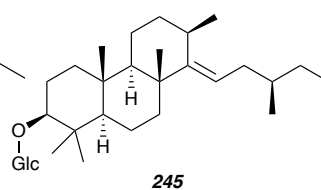
238



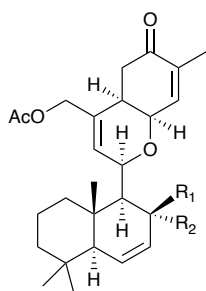
239 $R_1 = \text{COCH}_2\text{COOH}, R_2 = \text{Me}$
 240 $R_1 = \text{COCH}_2\text{COOH}, R_2 = \text{H}$
 241 $R_1 = \text{H}, R_2 = \text{Me}$
 242 $R_1 = \text{H}, R_2 = \text{H}$
 243 $R_1 = \text{COCH}_2\text{COOMe}, R_2 = \text{Me}$



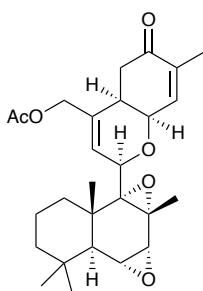
244



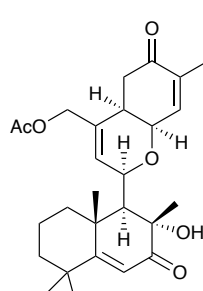
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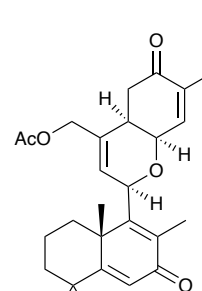
246 $R_1 = \text{Me}, R_2 = \text{OMe}$
 247 $R_1 = \text{OH}, R_2 = \text{Me}$



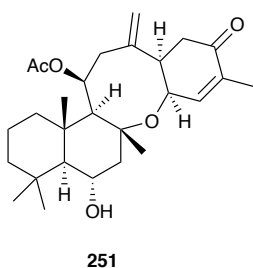
248



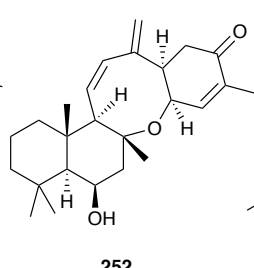
249



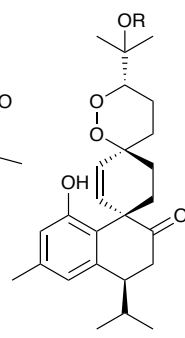
250



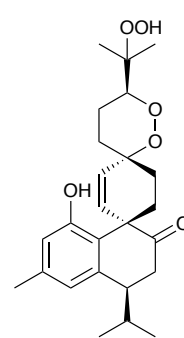
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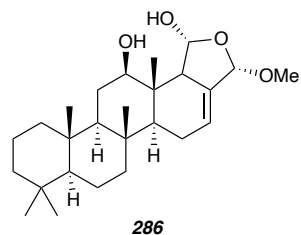
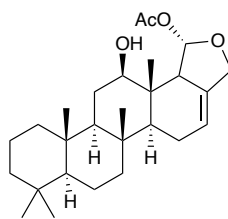
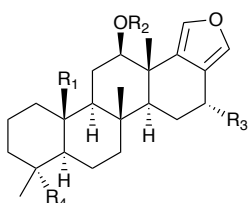
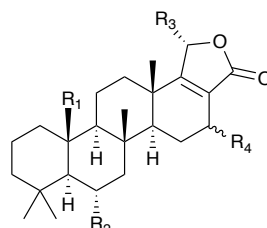
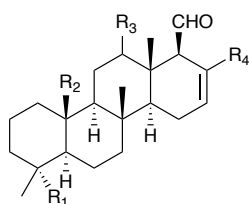
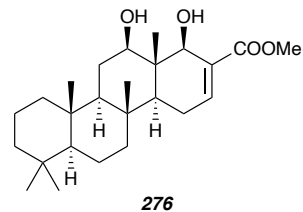
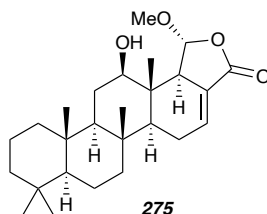
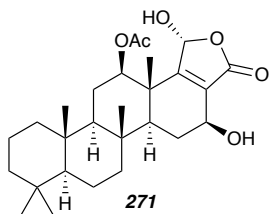
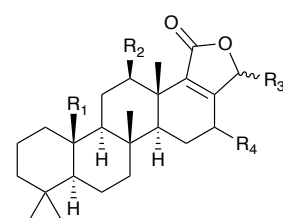
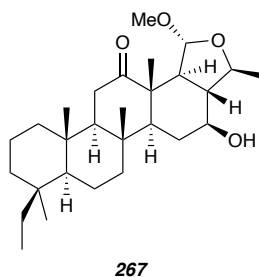
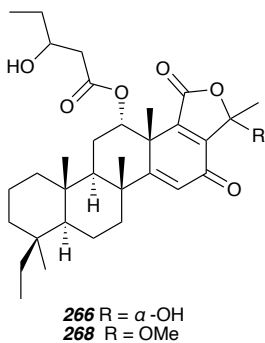
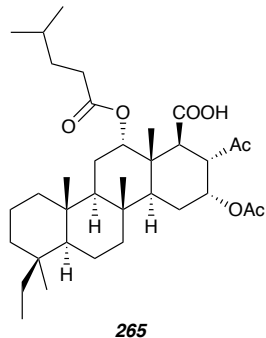
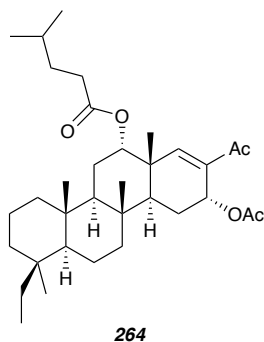
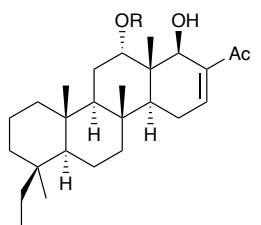
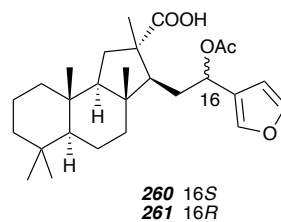
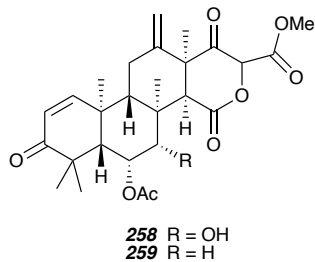
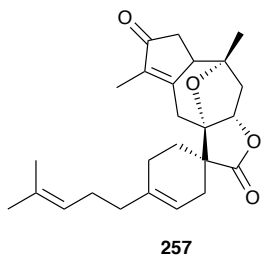
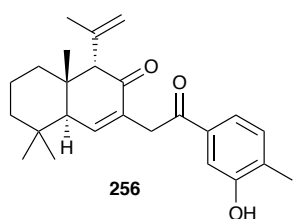
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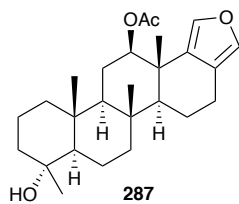


253 $R = \text{OH}$
 255 $R = \text{H}$

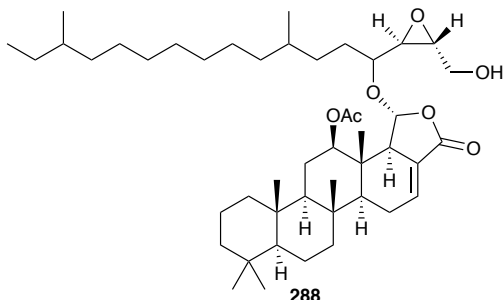


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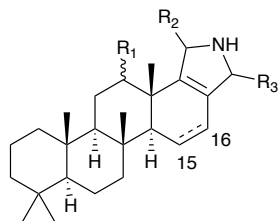




287



288



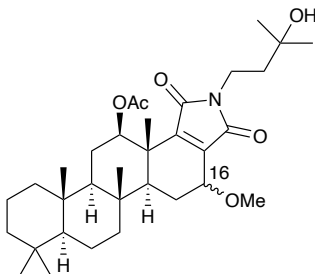
289 $R_1 = \alpha\text{-OAc}$, $R_2 = \text{O}$, $R_3 = \alpha\text{-OMe}$, $16\alpha\text{-OMe}$

290 $R_1 = \beta\text{-OH}$, $R_2 = R_3 = \text{O}$

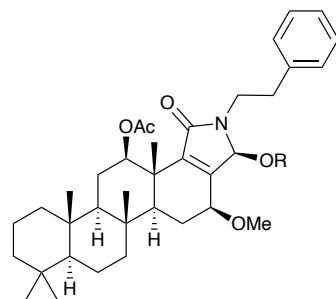
291 $R_1 = \beta\text{-OH}$, $R_2 = \text{H}_2$, $R_3 = \text{O}$, $\Delta^{15,16}$

292 $R_1 = \beta\text{-OH}$, $R_2 = \text{H}_2$, $R_3 = \text{O}$

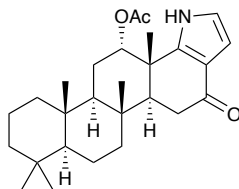
293 $R_1 = \beta\text{-OAc}$, $R_2 = \text{O}$, $R_3 = \alpha\text{-OH}$, $16\alpha\text{-OMe}$



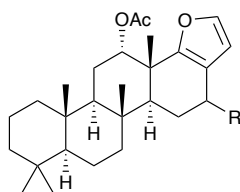
294 16S
295 16R



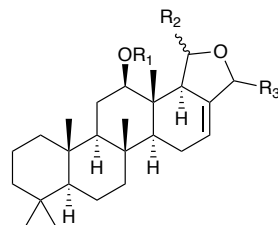
296 $R = \text{Me}$
297 $R = \text{H}$



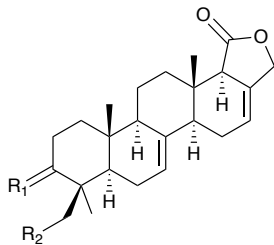
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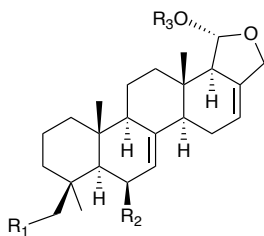
299 $R = \alpha\text{-OMe}$
300 $R = \beta\text{-OMe}$



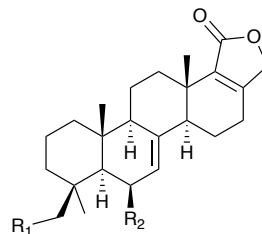
301 $R_1 = \text{Me}$, $R_2 = \alpha\text{-OAc}$, $R_3 = \beta\text{-OH}$
302 $R_1 = \text{H}$, $R_2 = \beta\text{-OH}$, $R_3 = \text{O}$



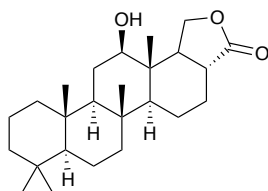
303 $R_1 = \text{H}_2$, $R_2 = \text{H}$
304 $R_1 = \text{O}$, $R_2 = \text{H}$
312 $R_1 = \text{H}_2$, $R_2 = \text{OAc}$



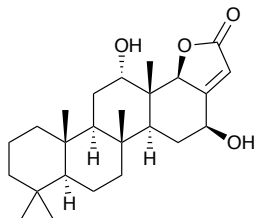
305 $R_1 = R_2 = R_3 = \text{H}$
306 $R_1 = \text{OH}$, $R_2 = R_3 = \text{H}$
307 $R_1 = \text{OAc}$, $R_2 = R_3 = \text{H}$
308 $R_1 = R_3 = \text{H}$, $R_2 = \text{OAc}$



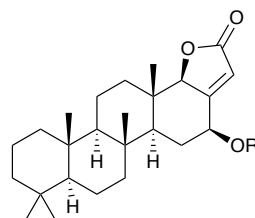
309 $R_1 = R_2 = \text{H}$
310 $R_1 = \text{OAc}$, $R_2 = \text{H}$
311 $R_1 = \text{H}$, $R_2 = \text{OAc}$



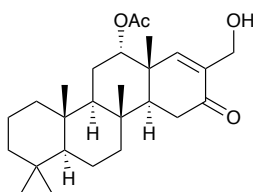
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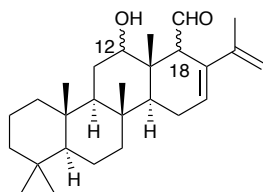
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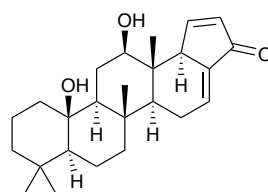
315 $R = \text{Ac}$
316 $R = \text{H}$



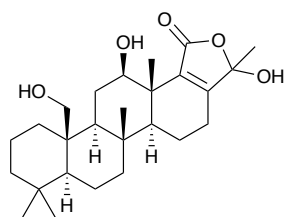
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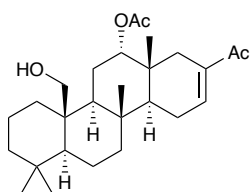
318 $12\alpha\text{-OH}$, $18\alpha\text{-CHO}$
319 $12\beta\text{-OH}$, $18\beta\text{-CHO}$



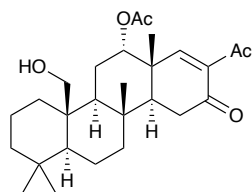
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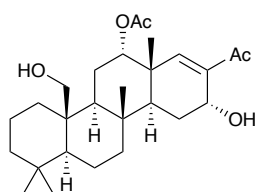
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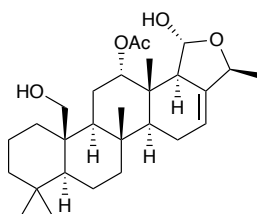
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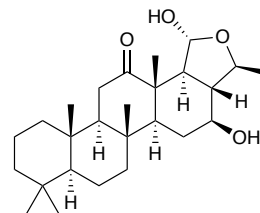
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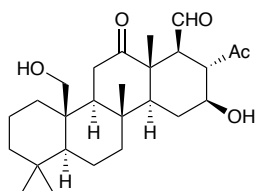
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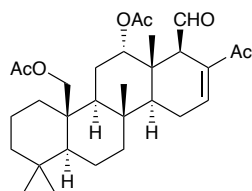
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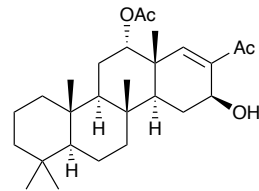
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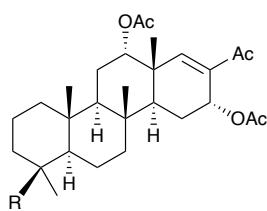
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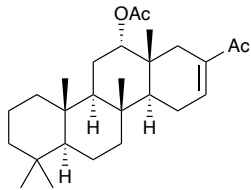
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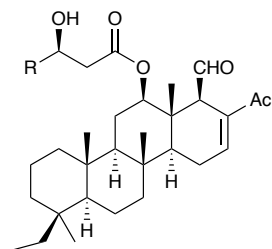
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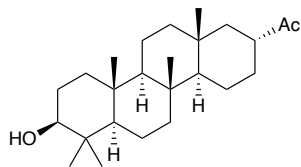
330 R = Me
331 R = Et



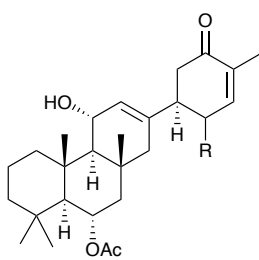
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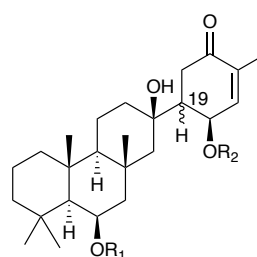
333 R = Me
334 R = Et



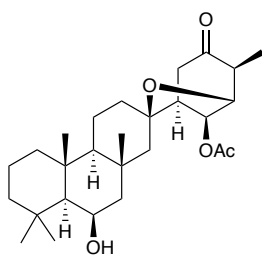
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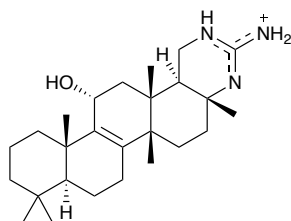
336 R = H
337 R = S-OAc



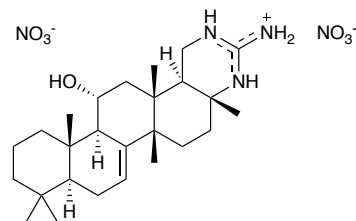
338 R₁ = H, R₂ = Ac, 19 α -H
339 R₁ = Ac, R₂ = H, 19 β -H



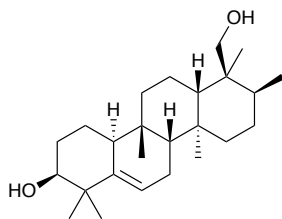
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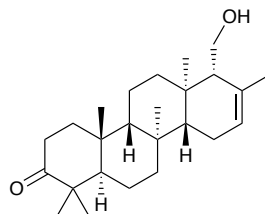
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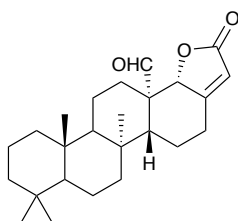
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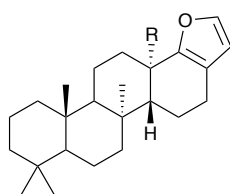
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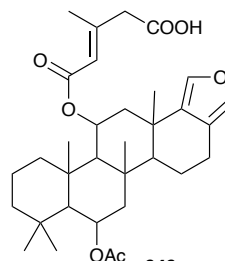
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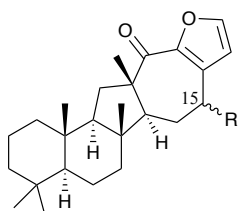
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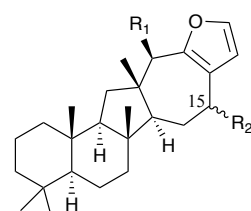
346 R = CHO
347 R = CH₂OH



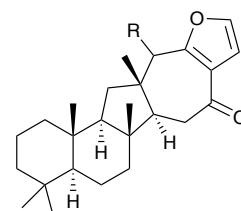
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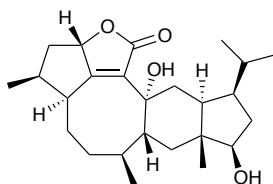
349 R = S-OAc
350 R = R-OAc
351 R = S-OH
352 R = R-OH



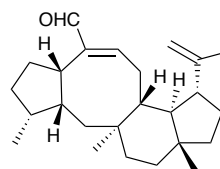
353 R₁ = OAc, R₂ = S-OH
354 R₁ = OAc, R₂ = R-OH
355 R₁ = OH, R₂ = S-OH



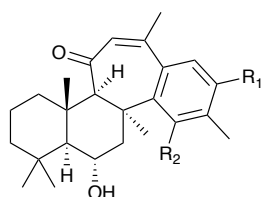
356 R = =O
357 R = S-OH
358 R = R-OAc
359 R = R-OH



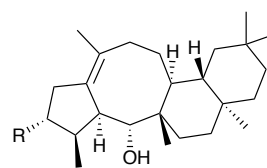
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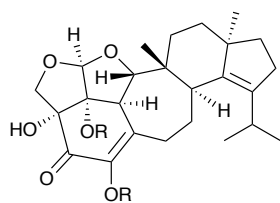
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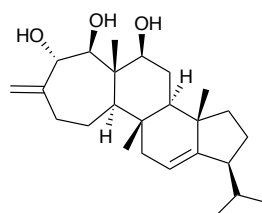
362 R₁ = OH, R₂ = H
363 R₁ = H, R₂ = OH
364 R₁ = H, R₂ = OMe



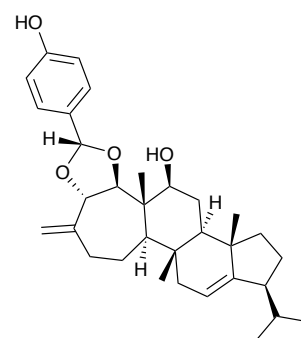
365 R = H
366 R = OH



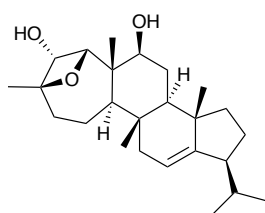
367 R = H
368 R = Ac



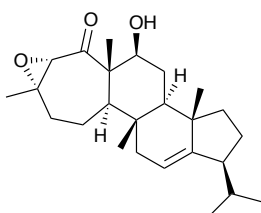
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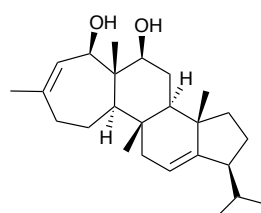
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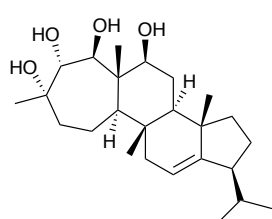
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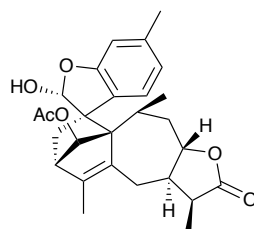
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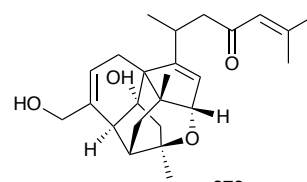
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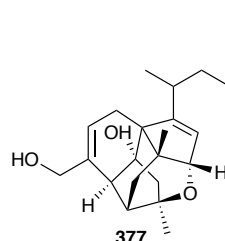
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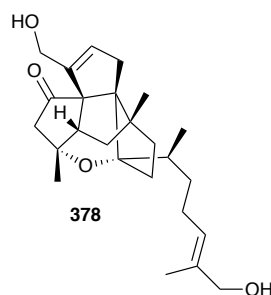
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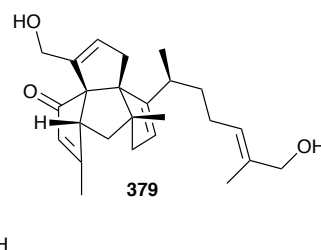
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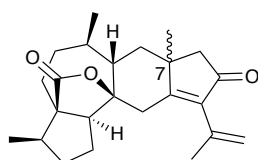
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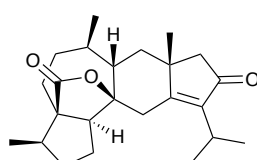
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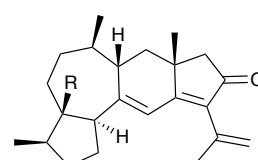
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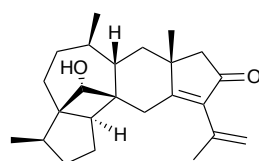
380 7 β -Me
381 7 α -Me



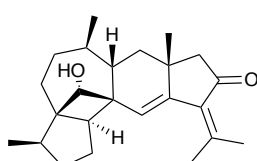
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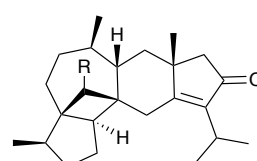
383 R = COOEt
384 R = CHO



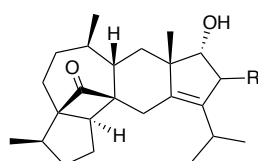
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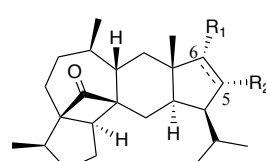
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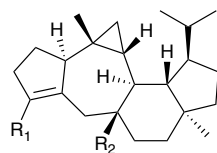
387 R = α -OH
388 R = =O



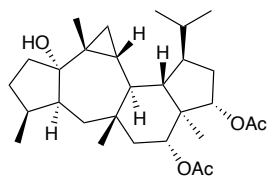
389 R = α -OH
390 R = =O



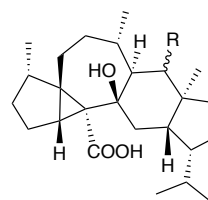
391 R₁ = R₂ = OH
392 $\Delta^{5,6}$



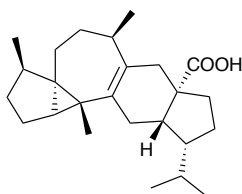
393 $R_1 = \text{COOH}$, $R_2 = \text{CH}_2\text{OH}$



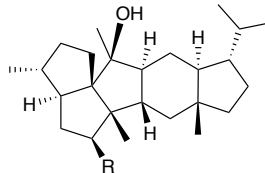
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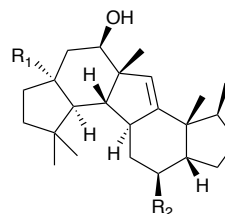
395 $R = S\text{-OAc}$
396 $R = R\text{-OH}$



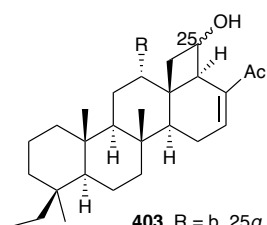
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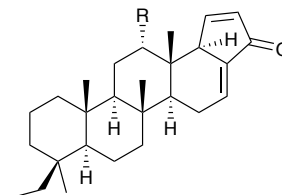
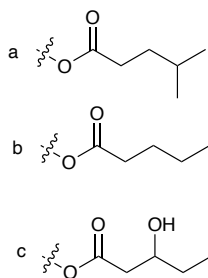
398 $R = \text{H}$
399 $R = \text{OH}$



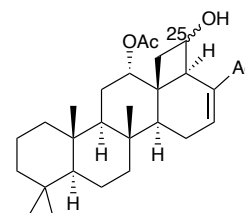
400 $R_1 = \text{Me}$, $R_2 = \text{OH}$
401 $R_1 = \text{Me}$, $R_2 = \text{Me}$
402 $R_1 = \text{OH}$, $R_2 = \text{Me}$



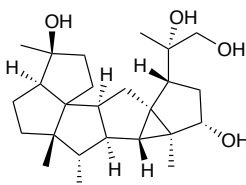
403 $R = b$, $25\alpha\text{-OH}$
404 $R = b$, $25\beta\text{-OH}$
405 $R = a$, $25\alpha\text{-OH}$
406 $R = a$, $25\beta\text{-OH}$



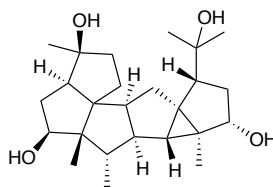
407 $R = c$



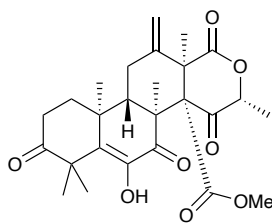
408 $25\beta\text{-OH}$
409 $25\alpha\text{-OH}$



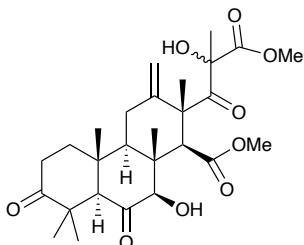
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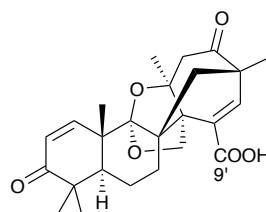
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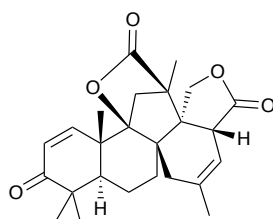
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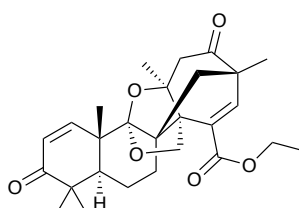
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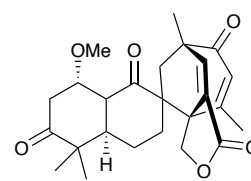
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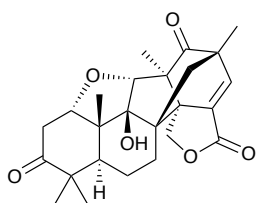
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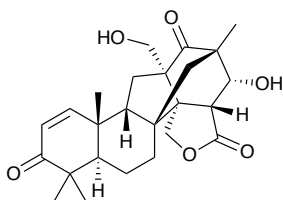
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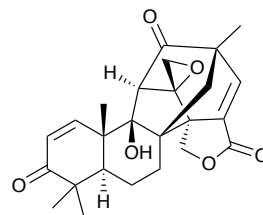
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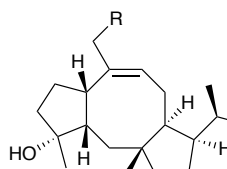
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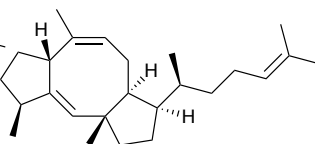
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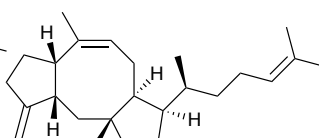
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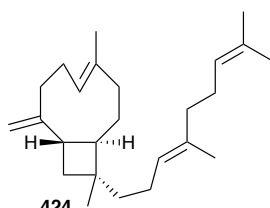
421 R = H
425 R = OH



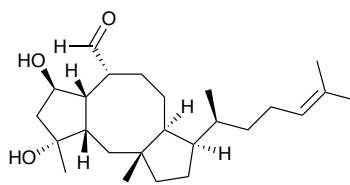
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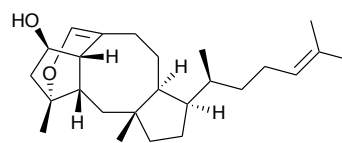
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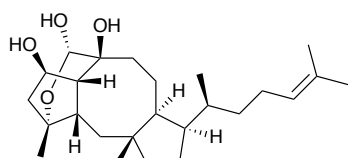
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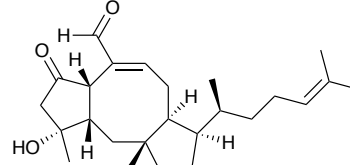
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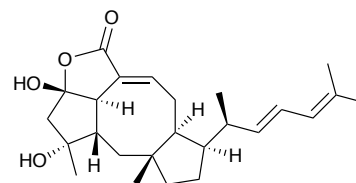
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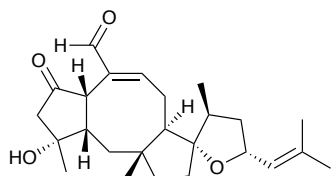
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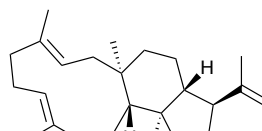
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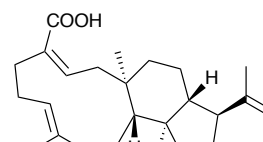
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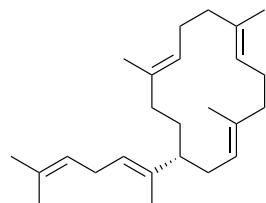
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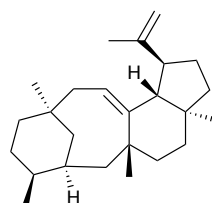
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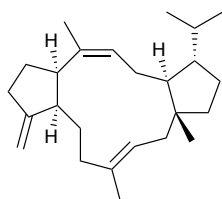
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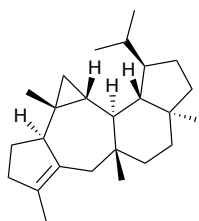
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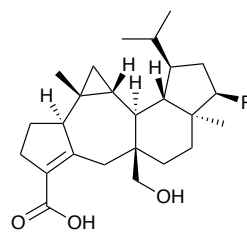
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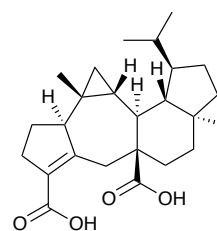
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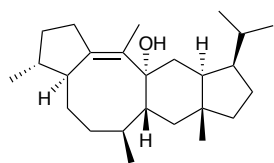
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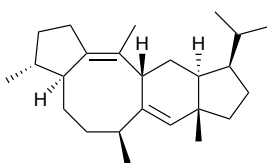
438 R = H
440 R = OH



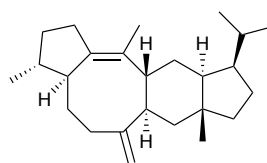
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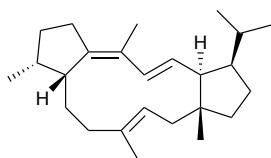
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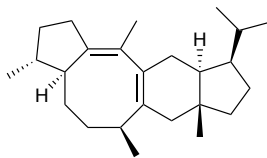
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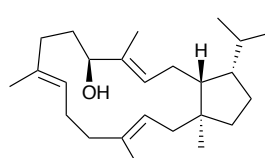
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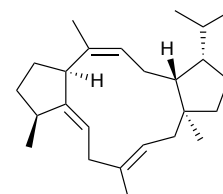
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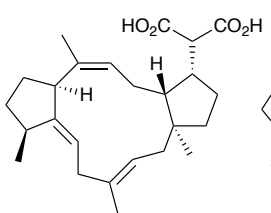
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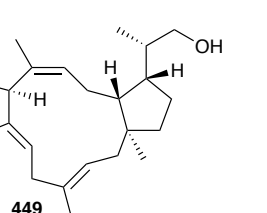
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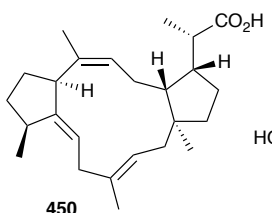
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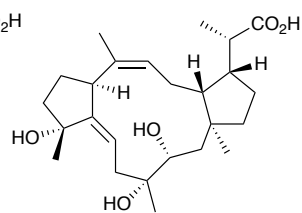
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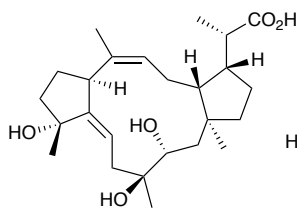
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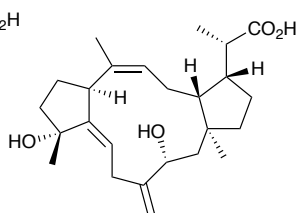
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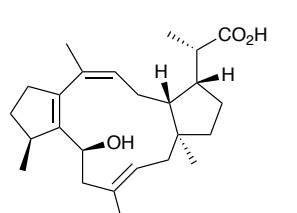
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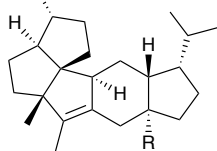
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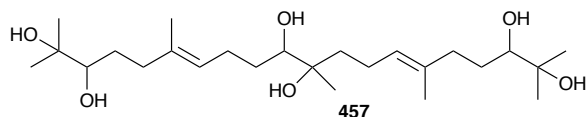


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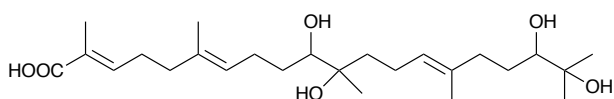


455 R = CH₃

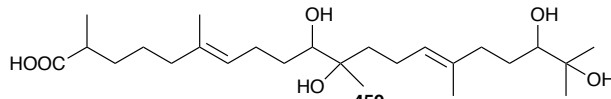
456 R = COOH



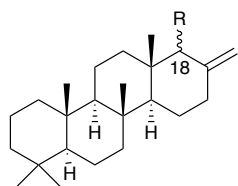
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458



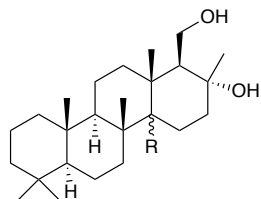
459



460 R = β-CH₂OH

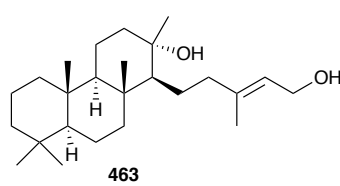
465 R = α-CH₂OH

471 R = β-CH₂OAc

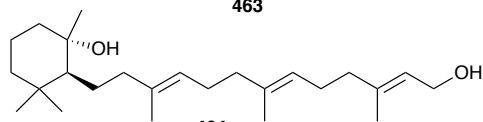


461 R = β-H

462 R = α-H



463



464

