

Review

Alkaloids of the genus *Datura*: review of a rich resource for natural product discovery

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Electronic Supplementary Material

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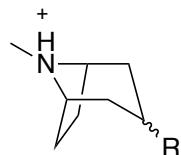
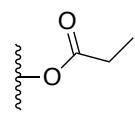


Table S1: Monosubstituted Tropane Alkaloids Described in *Datura*.

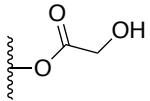
| R = | Stereochemistry at position 3 (and common name and number) | Species found in | References (see main text for reference numbers) |
|-----|--|--|---|
| OH | α (tropine, α -10) ^b | All (some variation in varieties), including some transformed root cultures | 22, 39, 40, 61, 64, 67, 68, 72, 73, 75, 76, 114-115, 118, 128, 130, 146, 152 |
| OH | β (Pseudotropine, β -10) | <i>D. inoxia</i> (including root cultures), <i>D. discolor</i> , <i>D. ferox</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> , <i>D. stramonium</i> (including hairy root cultures), <i>D. ceratocaula</i> , <i>D. quercifolia</i> (root cultures) | 22, 39, 40, 61, 64, 67, 68, 73, 113-114, 118, 130, 152 |
| OAc | α (α -24) | <i>D. inoxia</i> (including root cultures), <i>D. leichardtii</i> ssp. <i>pruinosa</i> (isomer unspecified), <i>D. stramonium</i> (isomer unspecified, including hairy root cultures), <i>D. quercifolia</i> (root cultures), <i>D. ceratocaula</i> (isomer unspecified). <i>D. wrightii</i> root cultures | 39, 40, 61, 64, 67, 68, 72, 73, 113-114, 118, 128, 146, 152 |
| OAc | β (β -24) | <i>D. inoxia</i> , <i>D. stramonium</i> (root cultures), <i>D. wrightii</i> root cultures | 39, 102, 128 |
| =O | N/A (tropinone, 19) | <i>D. leichhardtii</i> and ssp <i>pruinosa</i> , <i>D. metel</i> (var. <i>fastuosa</i>), <i>D. inoxia</i> (including root cultures), <i>D. stramonium</i> (including root cultures), <i>D. querifolia</i> (root cultures) | 22, 40, 61, 67, 68, 72, 75, 83, 89, 114, 118, 146 |



α (α -25)

D. inoxia

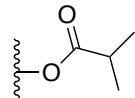
39



Unspecified, 26

D. inoxia, *D. stramonium*, *D. ferox*, *D. leichhardtii* (both ssp), *D. wrightii*,
D. metel (including var. *fastuosa*), *D. ceratocaula*,

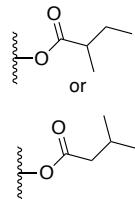
40, 63, 64, 113, 118, 146



α (α -27)

D. inoxia

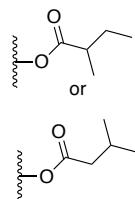
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α (α -28)^a

D. stramonium (isomer unspecified), *D. inoxia*

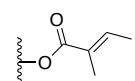
39, 64



β (β -29)^a

D. inoxia

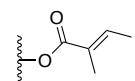
39



α (α -23)

D. stramonium (cultures, and plant, isomer unspecified), *D. inoxia* (plant
and root cultures), *D. ceratocaula*, *D. stramonium* (var. *tatula*, var.
godronii), *D. wrightii*, *D. leichhardtii* (both ssp), *D. metel* (including var.
fastuosa), *D. ferox*

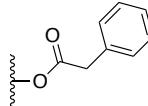
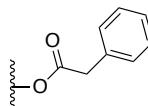
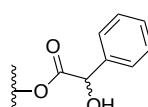
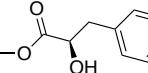
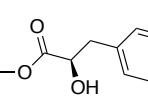
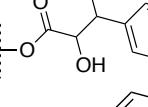
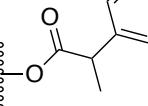
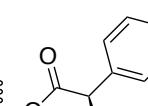
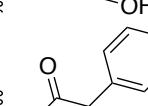
22, 37, 39, 40, 61, 64, 68, 72, 73, 75, 83, 91, 113-
115, 118, 128, 151-152



β (tigloidine), β -23

D. inoxia (including root cultures), *D. ceratocaula*, *D. ferox*, *D.*
leichhardtii ssp. *pruinosa*, *D. metel* (including *D. fastuosa*), *D.*
stramonium

22, 39, 40, 61, 64, 68, 72, 73, 83, 114

| | | | |
|---|--|---|--|
|  | α (or unspecified, α -30) | <i>D. inoxia</i> , (<i>isomer unspecified, including hairy root cultures</i>) <i>D. stramonium</i> (<i>multiple varieties and hairy root cultures</i>), <i>D. ferox</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> (<i>both ssp</i>), <i>D. metel</i> (<i>including var. <i>fastuosa</i></i>), <i>D. ceratocaula</i> , <i>D. quercifolia</i> (<i>root cultures</i>), | 22, 40, 61, 64, 67, 73, 68, 72, 83, 75, 91, 113-115, 140 |
|  | β (β -30) | <i>D. stramonium</i> | 68, 140 |
|  | Stereochemistry unspecified, described as just "homatropine" (31) | <i>D. metel</i> | 41 |
|  | α (littorine), 11 | All except <i>D. quercifolia</i> , including hairy root cultures | 32, 40, 64, 68, 72, 73, 89, 109, 118, 130, 146, 152 |
|  | α (presumably), 32 | <i>D. inoxia</i> , <i>D. stramonium</i> | 64, 113 |
|  | Unspecified, 33 | <i>D. inoxia</i> | 146 |
|  | Unspecified, 34 | <i>D. inoxia</i> , <i>D. stramonium</i> | 64, 68, 72 |
|  | α (hyoscyamine, or reported as "atropine"), (<i>S</i>)-1 or 1 | All species, including transformed root cultures | 22, 40, 36, 39, 61, 64, 68, 72, 73-75, 91, 115, 128, 130, 140, 146, 151-152 |
|  | Not specified, but presumably α , 35 | <i>D. stramonium</i> , <i>D. wrightii</i> , <i>D. ceratocaula</i> , <i>D. inoxia</i> | 40, 68, 73, 91, 146, 151. |

| | | | |
|--|---|--|---|
| | Not specified, but presumably α , 36 | <i>D. inoxia</i> (including hairy root cultures), <i>D. stramonium</i> | 61, 64, 68, 75, 113 |
| | Not specified, but presumably α , 37 | <i>D. stramonium</i> (multiple varieties), <i>D. ferox</i> , <i>D. inoxia</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> (both ssp), <i>D. metel</i> (including var. <i>fastuosa</i>), <i>D. ceratocaula</i> | 22, 32, 40, 64, 68, 72, 73, 114, 151 |
| | α (α - 38) | <i>D. quercifolia</i> | 73 |
| | Not specified, but presumably α (α - 39) | All except <i>D. discolor</i> , including multiple transformed root cultures | 22, 39, 40, 41, 61, 64, 67, 68, 72, 73, 75, 83, 91, 114-115, 118, 151-152 |
| | β (proposed), β - 39 | <i>D. stramonium</i> | 151 |
| | α (datumetine), 8 | <i>D. metel</i> | 45 |

^aSome references (e.g., 39) refer to separate isomers as “2-methylbutyryloxy”- and “methylbutyryloxy”. These are presumably valeroyl and isovaleroyl and are classified as such. ^b7-hydroxytropone is reported in reference 140 – there do not appear to be any other references to this compound.

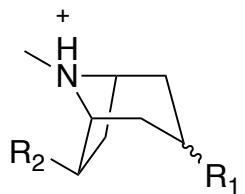
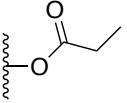
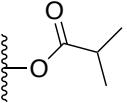
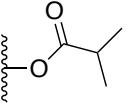
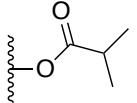
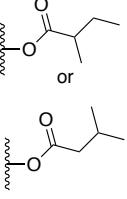
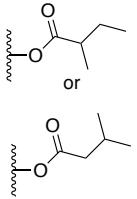
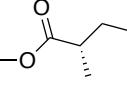
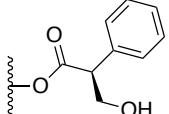
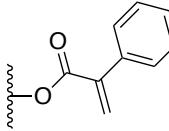
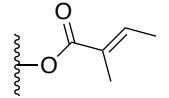
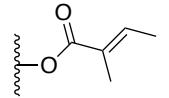
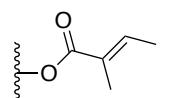


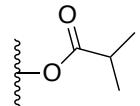
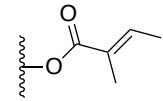
Table S2: Disubstituted Tropane Alkaloids from *Datura*.

| R ₁ = | R ₂ = | Stereochemistry at Position 3 and number | Species found in | References (see main text for reference numbers) |
|------------------|------------------|--|---|---|
| OH | OH | Not specified, 41 | <i>D. inoxia</i> , <i>D. metel</i> var. <i>fastuosa</i> , <i>D. ceratocaula</i> , <i>D. stramonium</i> | 22, 40, 64, 83, 113 |
| OAc | OH | Not specified, 44^b | <i>D. inoxia</i> (including root cultures), <i>D. stramonium</i> (multiple varieties, including root cultures), <i>D. ceratocaula</i> , <i>D. wrightii</i> (root cultures) | 61, 64, 68, 72, 73, 91, 113-115, 118, 128, 151 |
| OH | OAc | Not specified, specified as α in <i>D. metel</i> , 45 | <i>D. stramonium</i> , <i>D. metel</i> var. <i>fastuosa</i> , <i>D. quercifolia</i> (root cultures) | 40, 64, 68, 72, 128 |
| OAc | OAc | Not specified, 42 | <i>D. ceratocaula</i> , <i>D. stramonium</i> (including root cultures), <i>D. metel</i> (including var. <i>fastuosa</i>), <i>D. quercifolia</i> , <i>D. ferox</i> , <i>D. inoxia</i> , | 40, 64, 68, 72, 73, 113, 118, 128, |

| | | | | |
|-----|---|--------------------------------------|--|---|
| OH |  | Not specified, 46 | <i>D. metel</i> , including var. <i>fastuosa</i> | 40 |
| OH |  | Not specified, 47 | <i>D. stramonium</i> , <i>D. inoxia</i> | 64, 113 |
| OAc |  | Not specified, 48 | <i>D. stramonium</i> | 68, 72 |
| |  | OH | Not specified, 49^a | <i>D. inoxia</i> , <i>D. wrightii</i> |
| OH |  | Not specified, 50^a | <i>D. inoxia</i> (including hairy root cultures), <i>D. metel</i> var. <i>fastuosa</i> , <i>D. wrightii</i> , <i>D. ceratocaula</i> , <i>D. stramonium</i> | 40, 49, 61, 64, 68, 72, 73 |
| |  | OH | Not specified, 51 | <i>D. inoxia</i> , <i>D. metel</i> var. <i>fastuosa</i> , <i>D. ferox</i> , <i>D. stramonium</i> (multiple varieties) |
| OH |  | $\alpha, \alpha\text{-9}$ | <i>D. ceratocaula</i> | 49 |

| | | | | |
|--|----|--|---|--|
| | OH | Not specified, or α , 52 | <i>D. stramonium</i> (multiple varieties), <i>D. ferox</i> , <i>D. inoxia</i> (including hairy root cultures), <i>D. wrightii</i> , <i>D. ceratocaula</i> , <i>D. stramonium</i> hairy root cultures, <i>D. leichhardtii</i> (both ssp.), <i>D. metel</i> (including var. <i>fastuosa</i>) | 22, 40, 49, 61, 64, 68, 72, 73, 75, 91, 113-114, 118, 128, 140, 146, 151 |
| | OH | β , 52 | <i>D. ceratocaula</i> , <i>D. stramonium</i> | 68, 72, 73 |
| | OH | Not specified or α (53) | <i>D. inoxia</i> (including hairy root cultures), <i>D. stramonium</i> (multiple varieties), <i>D. ceratocaula</i> , <i>D. ferox</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> (both ssp.), <i>D. metel</i> (including var. <i>fastuosa</i>) | 22, 49, 61, 64, 68, 72, 73, 75, 91, 113-115, 128, 140, 151 |
| | OH | β (53) | <i>D. stramonium</i> (multiple varieties), <i>D. inoxia</i> | 22, 64, 113 |
| | | Not specified or α (54) | <i>D. stramonium</i> | 68 |
| | OH | Not specified, but presumably α (55) | <i>D. stramonium</i> , <i>D. inoxia</i> | 40, 64, 68, 72, 113 |
| | | α (56) | <i>D. stramonium</i> | 68 |

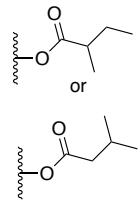
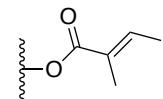
| | | | | |
|---|-----|--|--|--|
|  | OH | Not specified, but presumably α , 40 | <i>D. stramonium</i> (multiple varieties), <i>D. inoxia</i> (including transformed root cultures), <i>D. wrightii</i> , <i>D. leichhardtii</i> (both ssp.), <i>D. metel</i> (including var. <i>fastuosa</i>), <i>D. ceratocaula</i> , <i>D. ferox</i> | 36, 40, 61, 64, 68, 72, 73, 75, 91, 113-115, 128, 146, 151 |
|  | OH | Not specified, or α , 57 | <i>D. stramonium</i> , <i>D. ceratocaula</i> , <i>D. inoxia</i> (including hairy roots), <i>D. wrightii</i> , <i>D. leichhardtii</i> (both ssp), <i>D. metel</i> | 40, 61, 64, 68, 72, 73, 75, 83, 113 |
|  | OAc | α , α - 58 | <i>D. inoxia</i> , <i>D. metel</i> var. <i>fastuosa</i> , <i>D. leichhardtii</i> (both ssp.), <i>D. ceratocaula</i> , <i>D. stramonium</i> (including root cultures), <i>D. discolor</i> (possibly) | 40, 49, 64, 68, 72, 114, 118, |
|  | OAc | β , β - 58 | <i>D. ceratocaula</i> | 40 |
|  | | Not specified, or α , 59 | <i>D. inoxia</i> , <i>D. metel</i> (including var. <i>fastuosa</i>), <i>D. stramonium</i> (multiple varieties), <i>D. ferox</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> (both ssp.) | 22, 40, 49, 64, 68, 72, 114 |



Not specified, or
 α , **60**

D. stramonium (multiple varieties and hairy root cultures), *D. inoxia*,
D. ferox, *D. wrightii*, *D. leichhardtii* ssp. *pruinosa*, *D. metel* (including
var. *fastuosa*)

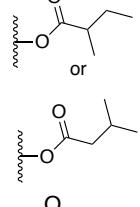
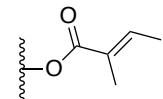
22, 64, 68, 72, 113-115, 118, 151



α , α -**61^a**

D. stramonium (multiple varieties and hairy root cultures), *D. ferox*, *D.*
inoxia, *D. wrightii*, *D. leichhardtii* (both ssp.), *D. metel* (including var.
fastuosa)

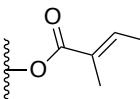
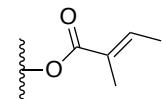
22, 32, 40, 49, 64, 68, 72, 114, 140, 151



β , β -**61^a**

D. stramonium

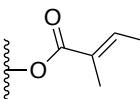
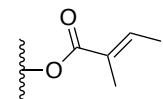
68



Not specified, or
 α , α -**43**

D. stramonium (multiple varieties and hairy root cultures), *D. ferox*, *D.*
inoxia (including hairy root cultures), *D. wrightii*, *D. leichhardtii* (both
ssp.), *D. metel* (including var. *fastuosa*), *D. ceratocaula*, *D. discolor*

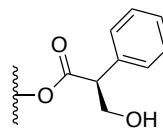
22, 40, 49, 61, 64, 68, 72, 113, 128, 140, 146,
151-152



β , β -**43**

D. inoxia (including hairy root cultures) *D. wrightii*, *D. stramonium*
(multiple varieties)

40, 61, 68, 72, 114

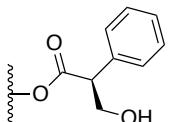
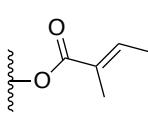
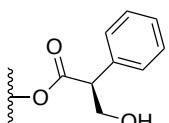
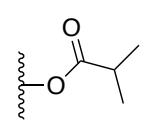
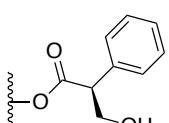
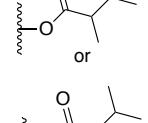
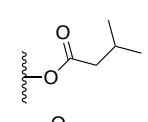
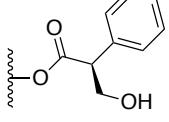
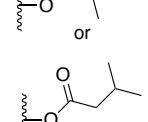
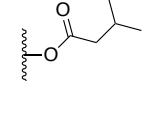


OAc

Not specified, but
presumably α , **62**

D. stramonium

64, 68, 72, 83

| | | | | |
|---|--|---|---|--|
|  |  | Not specified, but presumably α , 63 | <i>D. inoxia</i> (including hairy roots), <i>D. ceratocaula</i> , <i>D. stramonium</i> | 40, 49, 61, 64, 68, 73, 91, 113-114, 151 |
|  |  | Not specified, but presumably α , 64 | <i>D. stramonium</i> | 64 |
|  |  or  | Not specified, but presumably α , α - 65 | <i>D. inoxia</i> (including hairy root cultures), <i>D. metel</i> var. <i>fastuosa</i> , <i>D. stramonium</i> | 40, 49, 61, 64, 114 |
|  |  or  | β , β - 65 | <i>D. stramonium</i> | 64 |

^aSome references (e.g., 49) refer to separate isomers as "2-methylbutyryloxy"- and "methylbutyryloxy". These are presumably valeroyl and isovaleroyl and are classified as such.

^bSometimes referred to as "6-hydroxyacetoxyp propane (e.g., reference 72).

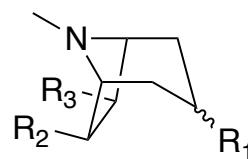
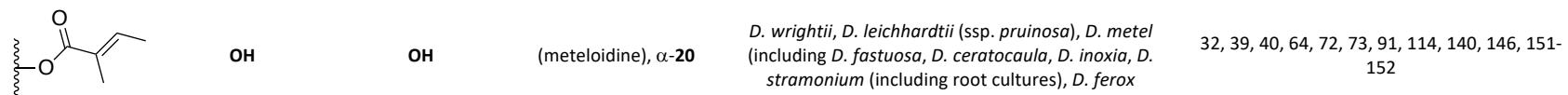
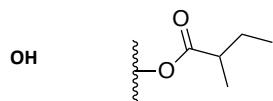


Table S3: 3,6,7-Trisubstituted Tropane Alkaloids from *Datura*.

| R ₁ = | R ₂ = | R ₃ = | Stereochemistry at Position 3 | Species found in | References (see main text for reference numbers) |
|------------------|------------------|------------------|--|--|---|
| OH | | OH | Not specified, 67 | <i>D. stramonium</i> | 64 |
| OAc | | OH | Not specified, 68 | <i>D. inoxia</i> | 113 |
| | | OH | Not specified, presumably α , α -69 | <i>D. stramonium</i> (including hairy root cultures), <i>D. ferox</i> , <i>D. inoxia</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> (both ssp), <i>D. metel</i> (including var. <i>fastuosa</i>), <i>D. ceratocaula</i> | 22, 40, 64, 68, 72, 73, 113, 118 |

| | | | | | |
|--|--|----|---|--|---|
| | | OH | Not specified, possibly β -69 | <i>D. inoxia, D. stramonium</i> | 68, 114 |
| | | OH | Not specified, 70 | <i>D. stramonium</i> | 64 |
| | | OH | α or unspecified, α -71 | <i>D. stramonium</i> (multiple varieties), <i>D. ferox, D. inoxia, D. wrightii, D. leichhardtii</i> (both ssp), <i>D. metel</i> var. <i>fastuosa, D. ceratocaula</i> | 22, 37, 40, 64, 68, 91, 113, 140 |
| | | OH | β , β -71 | <i>D. stramonium</i> (multiple varieties and hairy root cultures) | 22, 64, 68, 72, 91, 140, 151 |
| | | OH | α or unspecified (α -72) | <i>D. stramonium</i> (multiple varieties and hairy root cultures), <i>D. ceratocaula, D. ferox, D. inoxia</i> (including hairy root cultures), <i>D. wrightii, D. leichhardtii</i> (both ssp), <i>D. metel</i> (including <i>D. fastuosa</i>), <i>D. discolor, D. quercifolia</i> (hairy roots) | 22, 32, 39, 40, 61, 64, 68, 72, 73, 91, 114, 118, 128, 130, 140, 146, 152 |



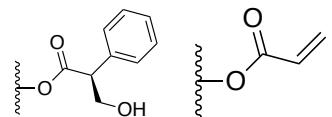


OH

Unspecified, **76**

D. stramonium

64

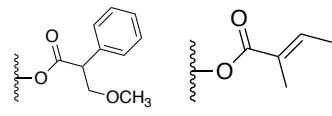


OH

α, α -**77**

D. ferox

37



OH

β, β -**7**

D. stramonium

48

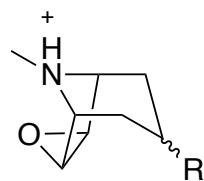


Table S4: 3-Substituted 6,7-Epoxytropane Alkaloids from *Datura*.

| $R_1 =$ | Stereochemistry at Position 3 and number | Species found in | References (see main text for reference numbers) |
|---------|--|------------------|--|
|---------|--|------------------|--|

| | | | |
|----|--------------------------------|---------------------------------|-------------------------|
| OH | α (scopine, 78) | <i>D. inoxia, D. stramonium</i> | 40, 64, 68, 75, 113-114 |
|----|--------------------------------|---------------------------------|-------------------------|

| | | | |
|-----|------------------------|------------------|-----|
| OAc | Unspecified, 79 | <i>D. inoxia</i> | 113 |
|-----|------------------------|------------------|-----|

| | | | |
|--|------------------------|------------------|-----|
| | Unspecified, 80 | <i>D. inoxia</i> | 113 |
|--|------------------------|------------------|-----|

| | | | |
|--|--|--|---|
| | α (Scopolamine, 2) | All species, including hairy root cultures | 22, 32, 37, 39, 40, 41, 61, 64, 67, 68, 72, 75, 81, 83, 89, 113-115, 118, 128, 130, 140, 146, 151 |
| | α (methylscopolamine, 81) | <i>D. metel</i> var. <i>fastuosa</i> , <i>D. stramonium</i> , <i>D. inoxia</i> (including hairy root cultures) | 40, 64, 68, 113, 151, |
| | Unspecified or α (aposcopamine, 82) | <i>D. ceratocaula</i> , <i>D. stramonium</i> (multiple varieties), <i>D. ferox</i> , <i>D. inoxia</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> ssp. <i>leichhardtii</i> , <i>D. metel</i> (including var. <i>fastuosa</i>) | 22, 31, 37, 40, 41, 64, 68, 72, 73, 75, 83, 113-114, 118 151 |
| | Unspecified or α , (anisodine, 22) | <i>D. wrightii</i> | 40 |
| | Unspecified or α , 83 | <i>D. inoxia</i> , <i>D. stramonium</i> | 64, 113 |
| | Unspecified or α (84) | <i>D. stramonium</i> (including root cultures), <i>D. inoxia</i> , <i>D. ferox</i> | 37, 40, 64, 68, 72, 75, 113, 118 |

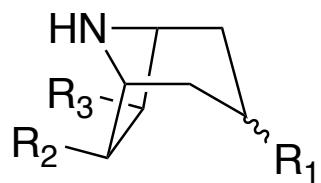


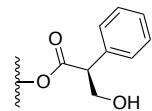
Table S5: Nortropanes Detected in *Datura*.

| R ₁ = | R ₂ = | R ₃ = | Stereochemistry at Position 3 | Species found in | References (see main text for reference numbers) |
|------------------|------------------|------------------|----------------------------------|------------------|---|
|------------------|------------------|------------------|----------------------------------|------------------|---|

| | | | | | |
|-----|---|---|--------------------------|---|---------|
| OAc | H | H | Not specified, 91 | <i>D. wrightii</i> (root cultures), <i>D. quercifolia</i> (root cultures) | 83, 128 |
|-----|---|---|--------------------------|---|---------|

| | | | | | |
|--|---|---|--------------------------|---|------------|
| | H | H | Not specified, 92 | <i>D. stramonium</i> , <i>D. inoxia</i> (including hairy roots) | 40, 61, 68 |
|--|---|---|--------------------------|---|------------|

| | | | | | |
|--|------------------|------------------|--|---|---------------------|
| | H | H | Not specified, presumably α , 93 | <i>D. stramonium</i> , <i>D. inoxia</i> , <i>D. ceratocaula</i> | 40, 68, 73, 113-114 |
| | H | H | Not specified, 94 | <i>D. stramonium</i> , <i>D. inoxia</i> | 68, 113 |
| | 6,7-epoxy | 6,7-epoxy | Not specified, 95 | <i>D. inoxia</i> | 113 |
| | 6,7-epoxy | 6,7-epoxy | Not specified, 96 | <i>D. stramonium</i> , <i>D. ferox</i> , <i>D. inoxia</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> spp. <i>leichhardtii</i> , <i>D. metel</i> , <i>D. ceratocaula</i> | 40, 68, 72 |
| | H | H | Not specified, 97 | <i>D. inoxia</i> , <i>D. stramonium</i> | 113 |
| | 6,7-epoxy | 6,7-epoxy | Not specified, 98 | <i>D. stramonium</i> , <i>D. inoxia</i> , <i>D. ferox</i> , <i>D. wrightii</i> , <i>D. leichhardtii</i> spp. <i>leichhardtii</i> , <i>D. metel</i> (including var. <i>fastuosa</i>), <i>D. ceratocaula</i> | 40, 64, 68, 72, 113 |



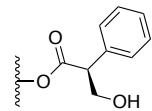
6,7-epoxy

6,7-epoxy

α or unspecified,
99

*D. stramonium, D. discolor, D. inoxia, D. ferox, D.
metel var. fastuosa, D. ceratocaula*

40, 68, 130, 151-152



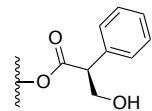
H

H

α or unspecified,
100

*D. stramonium, D. inoxia, D. metel var. fastuosa,
D. ceratocaula*

68, 73, 113, 146, 152



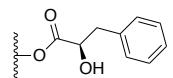
OH

H

α or unspecified,
101

D. inoxia

146



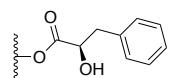
H

H

Unspecified, **102**

D. inoxia

146



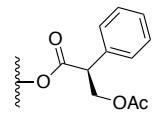
OH

H

Unspecified, **103**

D. inoxia

146



6,7-epoxy

6,7-epoxy

Unspecified, **104**

D. stramonium

68