Supplementary Information

Chemotaxonomic Insights into *Erythrina* and *Sophora* Alkaloids Using Self-Organizing Maps

Adiel H. O. Pontes,*[a] Thalisson A. de Souza,[b] Marcus T. Scotti,[a] Mateus M. dos Santos,[a] Alan Ferreira Alves[a] and Luciana Scotti[a]

[a]Laboratório de Quimioinformática, Instituto de Pesquisa em Fármacos e Medicamentos, Universidade Federal da Paraíba, 58050-585 João Pessoa-PB, Brazil

[b]Laboratório Multiusuário de Caracterização e Análise (LMCA), Instituto de Pesquisa em Fármacos e Medicamentos, Universidade Federal da Paraíba, 58050-585 João Pessoa-PB, Brazil

*e-mail: adiel.pontes@academico.ufpb.br

Adiel H. O. Pontes: https://orcid.org/0009-0008-8690-8496
Thalisson A. de Sousa: https://orcid.org/0000-0002-6000-8747
Marcus T. Scotti: https://orcid.org/0000-0003-4863-8057
Mateus M. dos Santos: https://orcid.org/0009-0001-9447-5300
Alan Ferreira Alves: https://orcid.org/0000-0001-6042-1075
Luciana Scotti: https://orcid.org/0000-0003-1866-4107

Table S1. List of *Erythrina* alkaloids used in the SOM analysis with their corresponding SMILES representations. Duplicate molecular are highlighted in red

Name of molecule	SMILE
11-Hydroxyerysotinone-rhamnoside	[H]C1C(O)C2=C(C=C(OC)C(=C2)C2(O)OC(C)C(O)C(O)C2O)[C@]23CC(C(C)=O)C(=O)C=C2CCN13
(3*R*)-16-*O*-β-D-Glucopyranosyl erysodine *N*-oxide	COC1=C(O)C=CC([C@H](O)[C@H](CC2=CC=C(O)C=C2)ON[C@@H](CCC(O)=O)C=O)=C1OC
10, 11-Dioxo-6,7α-erythraline epoxide	CO[C@@H]1C[C@]23N(C[C@@H]4O[C@]24C=C1)C(=O)C(=O)C1=CC2=C(OCO2)C=C31
10,11-Dioxoerythraline	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)C1=O)C(=CC2)C=C[C@H](OC)C3
10,11-Dioxoepierythratidine	[H]C1CN2C(=O)C(=O)C3=C(C=C(OC)C(OC)=C3)C22CC(OC)[C@H](O)C=C12
10,11-Dioxoepierythratidine	CO[C@@H]1C[C@]23N(CCC2=C[C@H]1O)C(=O)C(=O)C1=C3C=C(OC)C(OC)=C1
10,11-Dioxoerysotramidine	COC1CC23N(C(=O)C=C2C=C1)C(=O)C(=O)C1=C3C=C(OC)C(OC)=C1
10,11-Dioxoerysotrine	O=C1N2[C@]3(C=4C(C1=O)=CC(OC)=C(OC)C4)C(=CC2)C=C[C@H](OC)C3
10,11-Dioxoerythraline	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)C1=O)C(=CC2)C=C[C@H](OC)C3
10,11-Dioxoerythraline	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)C1=O)C(=CC2)C=C[C@H](OC)C3
10,11-Dioxoerythratidinone	COC1CC23N(CCC2=CC1=O)C(=O)C(=O)C1=C3C=C(OC)C(OC)=C1
10,11-Dioxoerythratine	COC1CC23N(CCC2=C[C@H]1O)C(=O)C(=O)C1=C3C=C2OCOC2=C1
10-Hydroxy-11-erysotramidine	[H]C1[C@@H](O)N2C(=O)C=C3C=C[C@@H](C[C@]23C2=C1C=C(OC)C(OC)=C2)OC
10-Hydroxy-11-oxoerysotrine	O=C1N2[C@]3(C=4C([C@H]1O)=CC(OC)=C(OC)C4)C(=CC2)C=C[C@H](OC)C3
10-Hydroxy-erythratine	[H]C1CN2C(O)C([H])C3=C(C=C4OCOC4=C3)[C@@]22C[C@@H](OC)[C@H](O)C=C12
10-Oxoerythraline	CO[C@@H]1C[C@]23N(CC=C2C=C1)CC(=O)C1=CC(OC)=C(OC)C=C31
10-Oxoerythrinine	COC1CC23N(CC=C2C=C1)C(=O)[C@H](O)C1=C3C=C2OCOC2=C1
11-a-Hydroxyerysodine	COC1CC23N(CC=C2C=C1)C[C@@H](O)C1=C3C=C(OC)C(O)=C1
11-a-Hydroxyerysotrine	COC1CC23N(CC=C2C=C1)C[C@@H](O)C1=C3C=C(OC)C(OC)=C1
11-a-Hydroxyerysotrine-*N*-oxide	COC1CC23C(=CC[N+]2([O-])C[C@@H](O)C2=C3C=C(OC)C(O)=C2)C=C1
11-a-Hydroxyerythravine	COC1=CC2=C(C=C1OC)C13CC(O)C=CC1=CCN3C[C@H]2O
11-alfa-Hydroxyerysodine	[H]C1[C@@H](O)C2=C(C=C(OC)C(O)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
11-alfa-Hydroxyerysotrine	[H]C1[C@@H](O)C2=C(C=C(OC)C(OC)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13

11-alfa-Hydroxyerythravine	[H]C1[C@@H](O)C2=C(C=C(OC)C(OC)=C2)[C@]23C[C@@H](O)C=CC2=CC([H])([H])N13
11-a-Methoxyerysotramidine	COC1CC23N(C[C@@H](OC)C4=C2C=C(OC)C(OC)=C4)C(=O)C=C3C=C1
11-beta-Hydroxyerysodine-glucose	[H]C1[C@H](O)C2=C(C=C(OC)C(OC(=O)[C@@H](N)CCC(O)=O)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
11-beta-Hydroxyerysotramidine	[H]C1[C@H](O)C2=C(C=C(OC)C(OC)=C2)[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
11-beta-Hydroxyerysotrine	[H]C1[C@H](O)C2=C(C=C(OC)C(OC)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
11-b-Hydroxyerysodine	COC1CC23N(CC=C2C=C1)C[C@H](O)C1=C3C=C(OC)C(O)=C1
11-b-Hydroxyerysotramidine	COC1CC23N(C[C@H](O)C4=C2C=C(OC)C(OC)=C4)C(=O)C=C3C=C1
11-b-Hydroxyerysovine	COC1CC23N(CC=C2C=C1)C[C@H](O)C1=C3C=C(O)C(OC)=C1
11-b-Hydroxyerythratidine N-oxide	CO[C@@H]1CC23N(CCC2=C[C@@H]1O)C[C@H](O)C1=C3C=C(OC)C(OC)=C1
11-b-Methoxy-glucoerysodine	COC1C[C@]23N(CC=C2C=C1)C[C@H](OC)C1=C3C=C(OC)C(OC2OC(CO)C(O)C(O)C2O)=C1
11-b-Methoxy-10-oxoerysotramidine	[H]C1(OC)C(=O)N2C(=O)C=C3C=CC(CC23C2=C1C=C(OC)C(OC)=C2)OC
11-b-Methoxyerysodine	COC1CC23N(CC=C2C=C1)C[C@H](OC)C1=C3C=C(OC)C(O)=C1
11-b-Methoxyerysotramidine	COC1CC23N(C[C@H](OC)C4=C2C=C(OC)C(OC)=C4)C(=O)C=C3C=C1
11-b-Methoxyerysovine	COC1CC23N(CC=C2C=C1)C[C@H](OC)C1=C3C=C(O)C(OC)=C1
11-b-Methoxyerythraline	[H]C1[C@H](OC)C2=C(C=C3OCOC3=C2)C23CC(OC)C=CC2=CCN13
11-b-Methoxyerythraline-N-oxide	COC1CC23C(=CC[N+]2([O-])C[C@H](OC)C2=C3C=C3OCOC3=C2)C=C1
11-b-Methoxyglucoerysovine	COC1C[C@]23N(CC=C2C=C1)C[C@H](OC)C1=C3C=C(OC2OC(CO)C(O)C(O)C2O)C(OC)=C1
11-Ethoxy-18,19-dimethoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04,8]icosa-2,4(8),9,11,15,17-Hexaen-14-one	CCOC1=CN2C(=O)C=C3C=C(OC)C(CC23C2=CC3=C(OCO3)C=C12)OC
11-hydroxy-7-methoxy-2*H*,4*H*,5*H*,10*H*,11*H*-Indolo [7a,1-a] isoquinolin-2-one	CO[N+]12CCC3CCC(=O)CC13C1=C(CC(O)C=C1)C=C2
11-Hydroxy-8-methoxy-2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1-a] isoquinolin-2-one	COC1=CC2=C(C=CC(O)C2)C23CC(=O)CCC2CCN13
11-Hydroxyepierythratidine	O(C)[C@@H]1C[C@]23C=4C(C(O)CN2CCC3=C[C@H]1O)=CC(OC)=C(OC)C4
11-Hydroxyepierythratine	[H][C@]1(O)C=C2CCN3CC(O)C4=C(C=C5OCOC5=C4)C23CC1OC
11-Hydroxyerysodineglucuronicacid	[H]OC1CN2CC=C3C=CC(CC23C2=C1C=C(OC)C(OC)=C2)OC(=O)CC[C@H](N)C=O
11-Hydroxyerysosalvine	[H][C@@]1(O)C=C2CCN3CC(O)C4=C(C=C(O)C(OC)=C4)C23CC1OC
11-Hydroxyerysotine	[H][C@@]1(O)C=C2CCN3CC(O)C4=C(C=C(OC)C(O)=C4)C23CC1OC
11-Hydroxyerysotinone	O(C)[C@@H]1C[C@]23C=4C(C(O)CN2CCC3=CC1=O)=CC(O)=C(OC)C4

11-Hydroxyerythratidine	O(C)[C@@H]1C[C@]23C=4C(C(O)CN2CCC3=C[C@@H]1O)=CC(OC)=C(OC)C4
11-Hydroxyerythratidinone	[H]C1C(O)C2=C(C=C(OC)C(OC)=C2)[C@]23C[C@@H](OC)C(=O)C=C2CCN13
11-Hydroxyerythratine	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)C(O)CN2CCC3=C[C@H]1O
11-Methoxy-5-oxo-2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1-a] isoquinoline-7-carboxylic acid	COC1CC2=C(C=C1)C13CCCCC1C(=O)C[N+]3(C=C2)C(O)=O
11-Methoxyerysodine	[H]C1C2C([H])([H])C=C3C=C[C@@H](C[C@]23C2=C(C=C(O)C(OC)=C2)C1OC)OC
11-Methoxyerysopine	COC1CC23N(CC=C2C=C1)C[C@H](OC)C1=C3C=C(O)C(O)=C1
11-Methoxyerythratidine	O(C)[C@@H]1C[C@]23C=4C(C(OC)CN2CCC3=C[C@@H]1O)=CC(OC)=C(OC)C4
11-Methoxyerythratine	COC1CC23N(CCC2=C[C@H]1O)C[C@H](OC)C1=C3C=C2OCOC2=C1
11-O-b-Glucoerythraline	COC1CC23N(CC=C2C=C1)C[C@H](OC1OC(CO)C(O)C(O)C1O)C1=C3C=C2OCOC2=C1
11-Oxoerysodine	O(C)[C@@H]1C[C@]23C=4C(C(=O)CN2CC=C3C=C1)=CC(O)=C(OC)C4
11-Oxoerysopine	O(C)[C@@H]1C[C@]23C=4C(C(=O)CN2CC=C3C=C1)=CC(O)=C(O)C4
11-Oxoerysovine	O(C)[C@@H]1C[C@]23C=4C(C(=O)CN2CC=C3C=C1)=CC(OC)=C(O)C4
11α-Hydroxyerysotrine N-oxide	CO[C@@H]1C[C@@]23C(=CC[N+]2([O-])C=C(O)C2=C3C=C(OC)C(OC)=C2)C=C1
11β-Hydroxyerysotrine N-oxide	CO[C@@H]1C[C@@]23C(=CC[N+]2([O-])C=C(O)C2=C3C=C(OC)C(OC)=C2)C=C1
11β-Methoxy-10-oxoerysotramidine	CO[C@@H]1C[C@]23N(C(=O)C=C2C=C1)C(=O)[C@@H](OC)C1=C3C=C(OC)C(OC)=C1
11β-Methoxy-8-oxoerythraline	CO[C@@H]1C[C@@]23N(C[C@H](OC)C4=CC5=C(OCO5)C=C24)C(=O)C=C3C=C1
11β-Methoxyerysotramidine	[H]C1[C@@H](OC)C2=C(C=C(OC)C(OC)=C2)[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
11β-Methoxyerysotrine N-oxide	CO[C@@H]1C[C@@]23C(=CC[N+]2([O-])C=C(OC)C2=C3C=C(OC)C(OC)=C2)C=C1
11β-Methoxyerythraline	[H]C1([H])C=C2C=C[C@@H](C[C@]22N1C[C@H](OC)C1=CC3=C(OCO3)C=C21)OC
11β-Methoxyerythraline *N*-oxide	CO[C@@H]1C[C@@]23C(=CC[N+]2([O-])C[C@H](OC)C2=CC4=C(OCO4)C=C32)C=C1
11β-Methoxyglucoerysodine	[H]C1[C@@H](OC)C2=C(C=C(OC)C(OC(=O)[C@@H](N)CCC(O)=O)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
11β-Methoxyglucoerysovine	[H]C1[C@@H](OC)C2=C(C=C(OC(=O)CC[C@H](N)C=O)C(OC)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
15-beta-Glucoerysopine	[H]C1C([H])C2=C(C=C(OC(=O)[C@@H](N)CCC(O)=O)C(O)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])C13

15-*O*-b-Glucoerysopine	[H]OC1=CC2=C(C=C1OC(=O)[C@@H](N)CCC(O)=O)[C@]13C[C@@H](OC)C=CC1=CCN3CC2
16-beta-D-Glucoerysopine	[H]C1C([H])C2=C(C=C(O)C(OC(=O)[C@@H](N)CCC(O)=O)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
16-*O*-beta-Glucopyranosylcoccoline	[H]C1C([H])C2=C(C=C(OC)C(OC(=O)[C@@H](N)CCC(O)=O)=C2)[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
16-*O*-b-Glucococcoline	COC1CC23N(CCC4=C2C=C(OC)C(OC2OC(CO)C(O)C(O)C2O)=C4)C(=O)C=C3C=C1
16-*O*-β-D-Glucopyranosyl coccoline	CO[C@@H]1C[C@@]23N(CCC4=CC(OC(=O)[C@@H](N)CCC(O)=O)=C(OC)C=C24)C(=O)C=C3C=C1
18-Hydroxy-11,19-dimethoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04,8]Icosa-2,4(8),9,15,17-pentaen-14-one	COC1CC23N(CC(OC)C4=C2C=C2OCOC2=C4)C(=O)C=C3C=C1O
18-Hydroxy-19-methoxy-14-oxo-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04,8]icosa-2,4(8),9,11,15,17-hexaen-11-yl acetate	COC1CC23N(C=C(OC(C)=O)C4=CC5=C(OCO5)C=C24)C(=O)C=C3C=C1O
19-Methoxy-14-oxo-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04,8]icosa-2,4(8),9,11,15,17-hexaen-11-yl acetate	COC1CC23N(C=C(OC=O)C4=CC5=C(OCO5)C=C24)C(=O)C=C3C=C1O
19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04, 8]icosa-2,4(8),9,15-Tetraen-11-ol	COC1CC23N(CC=C2C=C1)CC(O)C1=CC2=C(OCO2)C=C31
19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04, 8]icosa-2,4(8),9,15-tetraen-18-ol	COC1CC23N(CC=C2C=C1O)CCC1=CC2=C(OCO2)C=C31
19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04, 8]icosa-2,4(8),9,16-tetraen-14-one	COC1CC=C2CC(=O)N3CCC4=CC5=C(OCO5)C=C4C23C1
19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04, 8]icosa-2,4(8),9,16-tetraen-18-one	CO[C@@H]1C[C@]23N(CCC2=CC1=O)CCC1=C3C=C2OCOC2=C1
19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,16.02,10.04, 8]icosa-2,4(8),9,16-tetraene-11,18-diol	COC1CC=C2CCN3CC(O)C4=CC5=C(OCO5)C=C4C23C1

19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,1⁶.02,1⁹.0⁴, ⁸]icosa-2,4 (8),9,17-tetraen-11-ol	COC1CC23C(CCN2CC(O)C2=CC(O)=C(O)C=C32)C=C1
19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,1⁶.02,1⁹.0⁴,⁸]icosa-2 (10),3,8,14,16-pentaen-18-one	COC1CC23N(CCC4=C2C=C2OCOC2=C4)C=CC3=CC1=O
19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,1⁶.02,1⁹.0⁴,⁸]icosa-2,4 (8),9,15,17-pentaen-11-one	COC1CC23N(CC=C2C=C1)CC(=O)C1=C3C=C2OCOC2=C1
19-Methoxy-5,7-dioxa-13-azapentacyclo [11.7.0.01,1⁶.02,1⁹.0⁴,⁸]icosa-2,4 (8),9,15,17-pentaen-14-one	CO[C@@H]1C[C@@]23N(CCC4=CC5=C(OCO5)C=C24)C(=O)C=C3C=C1
1*H*-Indole-3-propanamide	COC(CC1=CNC2=C1C=CC=C2)C(=O)N(C)C
1*H*-Indole-3-propanamide	COC(CC1=CNC2=C1C=CC=C2)C(=O)N(C)C
2-({11,12-Dihydroxy-5,8-dimethoxy-2*H*,4*H*,5*H*,10*H*,11*H*- indolo [7a,1-a]isoquinolin-7-yl}oxy)-6-(hydroxymethyl)oxane- 3,4,5-triol	COC1C[N+]2(OC3OC(CO)C(O)C(O)C3O)C(OC)=CC3=C(C=C(O)C(O)C3)C22CCCCC12
2-({5,12-Dihydroxy-7,11-dimethoxy-2*H*,4*H*,5*H*,10*H*,11*H*- indolo [7a,1-a]isoquinolin-8-yl}oxy)-6-(hydroxymethyl)oxane- 3,4,5-triol	COC1OC(OC2=CC3=C(C=C(O)C(C3)OC)C34CCCCC3C(O)C[N+]24OC)C(O)C(O)C1O
2-({5,12-Dihydroxy-8,11-dimethoxy-2*H*,4*H*,5*H*,10*H*,11*H*- indolo [7a,1-a]isoquinolin-7-yl}oxy)-6-(hydroxymethyl)oxane- 3,4,5-triol	COC1CC2=C(C=C1O)C13CCCCC1C(O)C[N+]3(OC1OC(CO)C(O)C(O)C1O)C(OC)=C2
2-({5,7-Dihydroxy-11-methoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,13a*H*- indolo [7a,1-a]isoquinolin-8-yl}oxy)-6-(hydroxymethyl)oxane- 3,4,5-triol	COC1CC2C=C(OC3OC(CO)C(O)C(O)C3O)[N+]3(O)CC(O)C4CCCCC34C2C=C1
2-({5,7-Dihydroxy-8-methoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,13a*H*- indolo [7a,1-a]isoquinolin-11-yl}oxy)-6-(hydroxymethyl) oxane-3,4,5-triol	COC1=CC2CC(OC3OC(CO)C(O)C(O)C3O)C=CC2C23CCCCC2C(O)C[N+]13O
2-({5,8-Dihydroxy-11-methoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,13a*H*- indolo [7a,1-a]isoquinolin-7-yl}oxy)-6-(hydroxymethyl)oxane- 3,4,5-triol	COC1CC2C=C(O)[N+]3(CC(O)C4CCCCC34C2C=C1)OC1OC(CO)C(O)C(O)C1O

2-({5,8-Dihydroxy-7-methoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,13a*H*- indolo [7a,1-a]isoquinolin-11-yl}oxy)-6-(hydroxymethyl) oxane-3,4,5-triol	COC1OC(OC2CC3C=C(O)[N+]4(CC(O)C5CCCCC45C3C=C2)OC)C(O)C(O)C1O
2-({5-Hydroxy-8,11-dimethoxy-4*H*,5*H*,10*H*,11*H*,13a*H*-indolo [7a,1-a]isoquinolin-7-yl}oxy)-6-(hydroxymethyl)oxane-3,4,5- triol	COC1CC2C=C(OC)[N+]3(CC(O)C4CC=CCC34C2C=C1)OC1OC(CO)C(O)C(O)C1O
2-({7-Hydroxy-5,11-dimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,13a*H*- indolo [7a,1-a]isoquinolin-8-yl}oxy)-6-(hydroxymethyl)oxane- 3,4,5-triol	COC1CC=C2CCN3CC(OC)C4=CC(O)=C(OC5OC(CO)C(O)C(O)C5O)C=C4C23C1
2-(Hydroxymethyl)-6-({7,8,11-trimethoxy- 2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1-a]isoquinolin-5-yl}oxy) oxane-3,4,5-triol	COC1CC2=C(C=C1)C13CCCCC1C(C[N+]3(OC)C(OC)=C2)OC1OC(CO)C(O)C(O)C1O
3-Demethoxyerythratidinone	O(C)C=1C=C2[C@]34C(CCN3CCC2=CC1OC)=CC(=O)CC4
5,7,8,10-Tetramethoxy-2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1-a] isoquinolin-2-one	COC1C[N+]2(OC)C(OC)=CC3=C(C=CCC3OC)C22CC(=O)CCC12
5,7,8-Trimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,12*H*-indolo [7a,1-a] isoquinoline-11,12-diol	COC1C[N+]2(OC)C(OC)=CC3=C(CC(O)C(O)C3)C22CCCCC12
5,7-Dihydroxy-8,11-dimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,12*H*- indolo [7a,1-a]isoquinolin-12-one (11-hydroxyerysotinone)	COC1CC2=C(CC1=O)C13CCCCC1C(O)C[N+]3(O)C(OC)=C2
5,8-Dihydroxy-7,11-dimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,12*H*- indolo [7a,1-a]isoquinolin-12-one (11-hydroxyerysosalvinone)	COC1CC2=C(CC1=O)C13CCCCC1C(O)C[N+]3(OC)C(O)=C2
6-*O*-b-Glucoerysopine	CO[C@@H]1C[C@]23N(CC=C2C=C1)CCC1=C3C=C(O)C(ON[C@@H](CCC(O)=O)C=O)=C1
7,11,12-Trimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,12*H*-indolo [7a,1- a]isoquinolin-8-ol	COC1CC23N(CCC2=CC1OC)CCC1=CC(OC)=C(O)C=C31
7,11-Dimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,13a*H*-indolo [7a,1-a] isoquinoline-5,8-diol	COC1CC23C(CCN2CC(O)C2=CC(OC)=C(O)C=C32)C=C1
7,11-Dimethoxy-2*H*,10*H*,11*H*-indolo [7a,1-a]isoquinolin-2-one	COC1CC2=C(C=C1)C13CC(=O)CC=C1C=C[N+]3(OC)C=C2

7,11-Dimethoxy-2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1-a] isoquinolin-2-one	COC1CC2=C(C=C1)C13CC(=O)CCC1CC[N+]3(OC)C=C2
7,11-Dimethoxy-4*H*,5*H*,10*H*,11*H*,13a*H*-indolo [7a,1-a] isoquinoline-5,8-diol (11-hydroxyerysovin (alpha or beta))	COC1CC23N(CC=C2C=C1)CC(O)C1=CC(OC)=C(O)C=C31
7,8,11,12-Tetramethoxy-2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1-a] isoquinolin-5-one	COC1CC2=C(C=C1OC)C13CCCCC1C(=O)C[N+]3(OC)C(OC)=C2
7,8,11-Trimethoxy-1*H*,2*H*,4*H*,5*H*,*10H*,11*H*,12*H*-indolo [7a,1-a] isoquinolin-12-ol (erythratidine)	CO[C@@H]1C[C@]23N(CCC2=C[C@@H]1O)CCC1=C3C=C(OC)C(OC)=C1
7,8,11-Trimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,12*H*-indolo [7a,1-a] isoquinoline-5,12-diol (11-hydroxyerythratidine or 11- hydroxyepie rythratidine)	COC1CC2=C(CC1O)C13CCCCC1C(O)C[N+]3(OC)C(OC)=C2
7,8,11-Trimethoxy-1*H*,2*H*,4*H*,5*H*,12*H*-indolo [7a,1-a] isoquinolin-12-ol	COC1=CC2=C(CC1O)C13CCCCC1CC[N+]3(OC)C(OC)=C2
7,8,11-Trimethoxy-2H,4H,5H,10*H*,11*H*-indolo [7a,1-a] isoquinoline-4,5-dione (10,11-dioxoerysotrine)	COC1CC23N(CC=[c]2cc1)C(=O)C(=O)C1=CC(OC)=C(OC)C=C31
7,8,11-Trimethoxy-4*H*,5*H*,10*H*,11*H*,12*H*-indolo [7a,1-a] isoquinoline-5,12-dione	COC1CC23N(CC(=O)C4=CC(OC)=C(OC)C=C24)C=CC3=CC1=O
7,8,12-Trimethoxy-10*H*,11*H*,12*H*,13*H*,13a*H*-indolo [7a,1-a] isoquinolin-11-ol	COC1CC2C(CC1O)C=C(OC)[N+]1(OC)C=CC3=CC=CCC213
7,8,12-Trimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,12*H*-indolo [7a,1-a] isoquinoline-5,11-diol	COC1CC2=C(CC1O)C=C(OC)[N+]1(CC(O)C3CCCCC213)OC
7,8-Dihydroxy-11-methoxy-2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1- a]isoquinolin-5-one	COC1CC2=C(C=C1)C13CCCCC1C(=O)C[N+]3(O)C(O)=C2
7,8-Dihydroxy-11-methoxy-4*H*,5*H*,10*H*,11*H*,12*H*-indolo [7a,1- a]isoquinolin-12-one	COC1CC2=C(CC1=O)C13CC=CCC1CC[N+]3(O)C(O)=C2
7-Hydroxy-8,11-dimethoxy-2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1- a]isoquinolin-5-one	COC1CC2=C(C=C1)C13CCCCC1C(=O)C[N+]3(O)C(OC)=C2

8,11,12-Trimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,12*H*-indolo [7a,1- a]isoquinolin-7-ol	COC1CC23N(CCC2=CC1OC)CCC1=CC(O)=C(OC)C=C31
8,11-Dimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,12*H*-indolo [7a,1-a] isoquinolin-12-one	COC1CC2=C(CC1=O)C13CCCCC1CCN3C(OC)=C2
8,11-Dimethoxy-1*H*,2*H*,4*H*,5*H*,10*H*,11*H*,13a*H*-indolo [7a,1-a] isoquinoline-5,7-diol	COC1CC2C=C(OC)[N+]3(O)CC(O)C4CCCCC34C2C=C1
8,11-Dimethoxy-2*H*,10*H*,11*H*-indolo [7a,1-a]isoquinolin-2-one	COC1CC2=C(C=C1)C13CC(=O)CC=C1C=CN3C(OC)=C2
8,11-Dimethoxy-2*H*,4*H*,5*H*,10*H*,11*H*-indolo [7a,1-a] isoquinolin-2-one	COC1CC=C2CC(=O)N3CCC4=CC=C(OC)C=C4C23C1
8-Oxo-11-b-methoxyerythraline	COC1CC23N(C[C@H](OC)C4=C2C=C2OCOC2=C4)C(=O)C=C3C=C1
8-Oxo-a-erythroidine	CO[C@@H]1CC23N(CCC4COC(=O)C=C24)C(=O)C=C3C=C1
8-Oxo-a-erythroidine epoxide	COC1CC23N(CCC4COC(=O)C=C24)C(=O)C=C3C2OC12
8-oxo-alfa-erythroidine	CO[C@@H]1C[C@@]23N(CCC4COC(=O)C=C24)C(=O)C=C3C=C1
8-oxo-alfa-erythroidineepoxide	CO[C@@H]1C[C@@]23N(CCC4COC(=O)C=C24)C(=O)C=C3[C@@H]2O[C@H]12
8-Oxo-b-erythroidine	CO[C@@H]1CC23N(CCC4=C2CC(=O)OC4)C(=O)C=C3C=C1
8-oxo-beta-erythroidine	CO[C@@H]1C[C@@]23N(CCC4=C2CC(=O)OC4)C(=O)C=C3C=C1
8-Oxoerysodine	[H]C1CN2C(=O)C=C3C=CC(CC23C2=C1C=C(O)C(OC)=C2)OC
8-Oxoerythraline	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)CC2)C(=C1)C=C[C@H](OC)C3
8-Oxoerythraline	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)CC2)C(=C1)C=C[C@H](OC)C3
8-Oxoerythraline	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)CC2)C(=C1)C=C[C@H](OC)C3
8-Oxoerythraline	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)CC2)C(=C1)C=C[C@H](OC)C3
8-Oxoerythraline epoxide	O=C1N2[C@@]3(C([C@]4([C@@]([C@H](OC)C3)(O4)[H])[H])=C1)C=5C(=CC6=C(C5)OCO6)CC2
8-Oxoerythraline epoxide	O=C1N2[C@@]3(C([C@]4([C@@]([C@H](OC)C3)(O4)[H])[H])=C1)C=5C(=CC6=C(C5)OCO6)CC2
8-Oxoerythrinine	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)[C@@H](O)C2)C(=C1)C=C[C@H](OC)C3
8-Oxoerythrinine	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)[C@@H](O)C2)C(=C1)C=C[C@H](OC)C3
8-Oxoerythrinine	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)[C@@H](O)C2)C(=C1)C=C[C@H](OC)C3
8α-(2-Oxopropyl)-11′-epi-*O*-methyl-erythrivarine A	[H][C@]1(C=C2C=C[C@@H](CC22N1C[C@@H](OC)C1=CC3=C(OCO3)C=C21)OC)C1=C2C=C[C@H](CC22N(C[C@H](O)C3=CC4=C(OCO4)C=C23)[C@@H]1CC(C)=O)OC
8α-(2-Oxopropyl)-11′-*O*-methyl-erythrivarine A	[H][C@]1(C=C2C=C[C@@H](CC22N1C[C@@H](OC)C1=CC3=C(OCO3)C=C21)OC)C1=C2C=C[C@@H](CC22N(C[C@H](O)C3=CC4=C(OCO4)C=C23)[C@@H]1CC(C)=O)OC

8α-(2-Oxopropyl)-11-methoxy-erythraline	CO[C@@H]1CC23N(C[C@H](OC)C4=CC5=C(OCO5)C=C24)[C@H](CC(C)=O)C=C3C=C1
8α-(2-Oxopropyl)-erythraline	[H]C1CN2[C@H](CC(C)=O)C=C3C=C[C@@H](CC23C2=CC3=C(OCO3)C=C12)OC
8α-(2-Oxopropyl)-erythrinine	CO[C@@H]1CC23N(C[C@H](O)C4=CC5=C(OCO5)C=C24)[C@H](CC(C)=O)C=C3C=C1
8α-(2-Oxopropyl)-erythrivarine A	[H][C@]1(C=C2C=C[C@@H](CC22N1C[C@H](O)C1=CC3=C(OCO3)C=C21)OC)C1=C2C=C[C@@H](CC22N(C[C@H](O)C3=CC4=C(OCO4)C=C23)[C@@H]1CC(C)=O)OC
8α-Acetatemethoxy-11β-methoxyerythraline	CO[C@@H]1CC23N(C[C@H](OC)C4=CC5=C(OCO5)C=C24)[C@H](CC(=O)OC)C=C3C=C1
8α-Acetatemethoxyerysotrine	[H]C1CN2[C@H](CC(=O)OC)C=C3C=C[C@@H](CC23C2=CC(OC)=C(OC)C=C12)OC
8α-Acetatemethoxyerythraline	[H]C1CN2[C@H](CC(=O)OC)C=C3C=C[C@@H](CC23C2=CC3=C(OCO3)C=C12)OC
8α-Acetatemethoxyerythrinine	CO[C@@H]1CC23N(C[C@H](O)C4=CC5=C(OCO5)C=C24)[C@H](CC(=O)OC)C=C3C=C1
8α-Acetylerythraline	CO[C@@H]1CC23N(CCC4=CC5=C(OCO5)C=C24)[C@H](CC(=O)OC)C=C3C=C1
8α-Acetylerythsotrine	CO[C@@H]1CC23N(CCC4=CC(OC)=C(OC)C=C24)[C@H](CC(=O)OC)C=C3C=C1
8α-Carbomethoxyerysotrine	[H]C1CN2[C@@H](C=C3C=C[C@@H](CC23C2=CC(OC)=C(OC)C=C12)OC)C(=O)OC
8α-Carbomethoxyerythrinine	CO[C@@H]1CC23N(C[C@H](O)C4=CC5=C(OCO5)C=C24)[C@@H](C=C3C=C1)C(=O)OC
Abrine	C([C@@H](C(O)=O)NC)C=1C=2C(NC1)=CC=CC2
Abrine	C([C@@H](C(O)=O)NC)C=1C=2C(NC1)=CC=CC2
a-Erythroidine	CO[C@@H]1CC23N(CC=C2C=C1)CCC1COC(=O)C=C31
Albomaculine	[H][C@@]12N(C)CCC1=CC[C@@]1([H])OC(=O)C3=C(C=C(OC)C(OC)=C3OC)[C@@]21[H]
alfa-erythroidine	[H]C1([H])C=C2C=C[C@@H](C[C@]22N1CCC1COC(=O)C=C21)OC
b-Erythroidine	CO[C@@H]1CC23N(CC=C2C=C1)CCC1=C3CC(=O)OC1
beta-Eerythroidine	[H]C1([H])C=C2C=C[C@@H](C[C@]22N1CCC1=C2CC(=O)OC1)OC
b-Glucoerysodine	[H]C1CN2CC=C3C=CC(C[C@]23C2=C1C=C(OC1OC(CO)C(O)C(O)C1O)C(OC)=C2)OC
Coreximine	OC=1C=C2[C@]3(N(CC=4C(C3)=CC(O)=C(OC)C4)CCC2=CC1OC)[H]
Coreximine	OC=1C=C2[C@]3(N(CC=4C(C3)=CC(O)=C(OC)C4)CCC2=CC1OC)[H]
Cristadine	OC1=CC=C(C=C1OC)CC2=NC=CC=3C=C(OC)C(O)=CC32
Cristanine	CO[C@@H]1C[C@@]23C(=CC[N+]2([O-])C=CC2=C3C=C3OCOC3=C2)C=C1
Cristanine A	O=N12[C@]3(C=4C(=CC5=C(C4)OCO5)CC1)C(=CC2)C=C[C@H](OC)C3
Cristanine A	O=N12[C@]3(C=4C(=CC5=C(C4)OCO5)CC1)C(=CC2)C=C[C@H](OC)C3

Cristanine B	[H]C1C([H])C2=C(C=C3OCOC3=C2)[C@]23C[C@@H](OC)[C@H](O)C=C2[C@@H](O)CN13
Cristanines B	O[C@@H]1C=2[C@]3(C=4C(=CC5=C(C4)OCO5)CCN3C1)C[C@@H](OC)[C@H](O)C2
Crystamidine	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)C=C2)C(=C1)C=C[C@H](OC)C3
Crystamidine	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)C=C2)C(=C1)C=C[C@H](OC)C3
Crystamidine	O=C1N2[C@]3(C=4C(=CC5=C(C4)OCO5)C=C2)C(=C1)C=C[C@H](OC)C3
Epi-erythraditinone	[H]C1C([H])C2=C(C=C(OC)C(OC)=C2)[C@]23C[C@@H](OC)C(=O)C=C2CCN13
Epierythratidine	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=C[C@H]1O)=CC(OC)=C(OC)C4
Epierythratidine	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=C[C@H]1O)=CC(OC)=C(OC)C4
Epierythratine	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CCC3=C[C@@H]1O
Erybidine	OC=1C=C2C(=CC1OC)C=3C=C(OC)C(OC)=CC3CCN(C)CC2
Erybidine	OC=1C=C2C(=CC1OC)C=3C=C(OC)C(OC)=CC3CCN(C)CC2
Erymelanthine	O=C(OC)C1=NC=C2C(=C1)C34C(C=CC(OC)C3)=CCN4CC2
Erymelanthine	O=C(OC)C1=NC=C2C(=C1)C34C(C=CC(OC)C3)=CCN4CC2
Erysodienone	O(C)C1=C[C@]23C=4C(CCN2CCC3=CC1=O)=CC(O)=C(OC)C4
Erysodine	[H]C1CN2CC=C3C=CC(CC23C2=C1C=C(O)C(OC)=C2)OC
Erysodine	[H]C1CN2CC=C3C=CC(CC23C2=C1C=C(O)C(OC)=C2)OC
Erysodine	[H]C1CN2CC=C3C=CC(CC23C2=C1C=C(O)C(OC)=C2)OC
Erysodine	[H]C1CN2CC=C3C=CC(CC23C2=C1C=C(O)C(OC)=C2)OC
Erysodine *N*-oxide	[H]C1=C[N+]2([O-])CC=C3C=C[C@@H](C[C@]23C2=C1C=C(O)C(OC)=C2)OC
Erysodine *N*-oxide	[H]C1=C[N+]2([O-])CC=C3C=C[C@@H](C[C@]23C2=C1C=C(O)C(OC)=C2)OC
Erysodinophorine hydroxide	O(C)[C@@H]1C[C@]23C=4C(=CC(OC([C@H](CC=5C=6C(NC5)=CC=CC6)[N@@+](C)(C)C)=O)=C(OC)C4)CCN2CC=C3C=C1.[OH-]
Erysoflorinone	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=CC1=O)=CC(O)=C(O)C4
Erysoline	[H]O[C@@H]1C[C@@]23N(C([H])C([H])C4=C2C=C(O[H])C(OC)=C4)C([H])([H])C=C3C=C1
Erysonine	[H]O[C@@H]1C[C@@]23N(C([H])C([H])C4=C2C=C(OC)C(O[H])=C4)C([H])([H])C=C3C=C1
Erysophorine chloride	CO[C@@H]1C[C@]23N(CC=C2C=C1)CCC1=CC(OC)=C(OC(=O)[C@H](CC2=CNC4=CC=CC=C24)[N+](C)(C)C)C=C31
Erysopine	[H]C1CN2CC=C3C=CC(CC23C2=C1C=C(O)C(O)=C2)OC
Erysopine	[H]C1CN2CC=C3C=CC(CC23C2=C1C=C(O)C(O)=C2)OC
Erysopine 15-*O*-sulfate	[H]OS(=O)(=O)OC1=CC2=C(CCN3CC=C4C=CC(C[C@]234)OC)C=C1O
Erysopine 15-*O*-sulfate	[H]OS(=O)(=O)OC1=CC2=C(CCN3CC=C4C=CC(C[C@]234)OC)C=C1O

Erysopinophorine hydroxide	O(C)[C@@H]1C[C@]23C=4C(=CC(OC([C@H](CC5=CC=6C(N5)=CC=CC6)[N+](C)(C)C)=O)=C(O)C4)CCN2CC=C3C=C1.[OH-]
Erysopitine	OC=1C=C2C(=CC1O)C34C(=CC(O)C(OC)C3)CCN4CC2
Erysosalvine	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=C[C@H]1O)=CC(OC)=C(O)C4
Erysosalvine	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=C[C@H]1O)=CC(OC)=C(O)C4
Erysosalvinone	CO[C@@H]1C[C@]23N(CCC2=CC1=O)CCC1=CC(OC)=C(O)C=C31
Erysosalvinone	CO[C@@H]1C[C@]23N(CCC2=CC1=O)CCC1=CC(OC)=C(O)C=C31
Erysothiopine	[H]C1C([H])C2=C(C=C(O)C(OS(=O)(=O)CC(O)=O)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
Erysothiopine	[H]C1C([H])C2=C(C=C(O)C(OS(=O)(=O)CC(O)=O)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
Erysothiovine	O(C)[C@@H]1C[C@]23C=4C(=CC(OC)=C(OS(CC(O)=O)(=O)=O)C4)CCN2CC=C3C=C1
Erysotine	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=C[C@H]1O)=CC(O)=C(OC)C4
Erysotine	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=C[C@H]1O)=CC(O)=C(OC)C4
Erysotinone	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=CC1=O)=CC(O)=C(OC)C4
Erysotramidine	O=C1N2[C@]3(C=4C(CC2)=CC(OC)=C(OC)C4)C(=C1)C=C[C@H](OC)C3
Erysotramidine	O=C1N2[C@]3(C=4C(CC2)=CC(OC)=C(OC)C4)C(=C1)C=C[C@H](OC)C3
Erysotrine	O(C)[C@@H]1C[C@]23C=4C(=CC(OC)=C(OC)C4)CCN2CC=C3C=C1
Erysotrine	O(C)[C@@H]1C[C@]23C=4C(=CC(OC)=C(OC)C4)CCN2CC=C3C=C1
Erysotrine	O(C)[C@@H]1C[C@]23C=4C(=CC(OC)=C(OC)C4)CCN2CC=C3C=C1
Erysotrine *N*-oxide	O=N12[C@]3(C=4C(CC1)=CC(OC)=C(OC)C4)C(=CC2)C=C[C@H](OC)C3
Erysotrine *N*-oxide	O=N12[C@]3(C=4C(CC1)=CC(OC)=C(OC)C4)C(=CC2)C=C[C@H](OC)C3
Erysotrine *N*-oxide	O=N12[C@]3(C=4C(CC1)=CC(OC)=C(OC)C4)C(=CC2)C=C[C@H](OC)C3
Erysovine	[H]C1CN2CC=C3C=CC(CC23C2=C1C=C(OC)C(O)=C2)OC
Erysovine	[H]C1CN2CC=C3C=CC(CC23C2=C1C=C(OC)C(O)=C2)OC
Erysovine *N*-oxide	[H]C1=C[N+]2([O-])CC=C3C=C[C@@H](C[C@]23C2=C1C=C(OC)C(O)=C2)OC
Erysovine *N*-oxide	[H]C1=C[N+]2([O-])CC=C3C=C[C@@H](C[C@]23C2=C1C=C(OC)C(O)=C2)OC
Erytharbine	O=C1N2[C@]3(C=4C(C=C2)=CC(OC)=C(OC)C4)C(=C1)C=C[C@H](OC)C3
Erytharbine	O=C1N2[C@]3(C=4C(C=C2)=CC(OC)=C(OC)C4)C(=C1)C=C[C@H](OC)C3
Erytharborine A	O(C)[C@@H]1C[C@]23C=4C(C5=C(N2CC=C3C=C1)OC(C)(C)O5)=CC(OC)=C(OC)C4
Erytharborine B	O(C)[C@@H]1C[C@]23C=4C(C5=C(N2CC=C3C=C1)OC(C)(C)O5)=CC6=C(C4)OCO6
Erytharborine C	CO[C@@H]1CC23N(C[C@H](C(Cl)Cl)C2=C\C1=N\O)CCC1=C3C=C(OC)C(OC)=C1
Erytharborine D	CO[C@H]1CC=C2[C@H](CN3CCC4=C(C=C(OC)C(OC)=C4)C23C1)C(Cl)Cl

Erytharborine E	CO[C@@H]1CC23N(C[C@@H]4O[C@]24C=C1)CCC1=C3C=C(OC)C(OC)=C1
Erytharborine F	COC1CC23N(C[C@@H](O)C2=C[C@H]1O)C(=O)C(=O)C1=C3C=C(OC)C(OC)=C1
Erytharborine G	COC1CC23N(CCC4=C2C=C(OC)C(OC)=C4)C(=O)[C@H](O)C3=C[C@@H]1O
Erytharborine H	[H]C1C=C2C=CC(CC22N1C(=O)C([H])(O)C1=C2C=C(OC)C(OC)=C1)OC
Erythbidin B	[H]C1([H])C=C2C=C[C@@H](C[C@]22N1[C@H](O)C(=O)C1=C2C=C2OCOC2=C1)OC
Erythrabine	CO[C@@H]1C[C@@]23N(C=CC4=C2C=C(OC)C(OC)=C4)C(=O)C=C3C=C1
Erythraline	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CC=C3C=C1
Erythraline	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CC=C3C=C1
Erythraline	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CC=C3C=C1
Erythraline	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CC=C3C=C1
Erythraline	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CC=C3C=C1
Erythraline *N*-oxide	CO[C@@H]1C[C@@]23C(CC[N+]2([O-])CCC2=C3C=C(OC)C(OC)=C2)=C[C@H]1O
Erythraline-11-beta-*O*-glucopyranoside	[H]C1[C@H](ON[C@@H](CCC(O)=O)C=O)C2=C(C=C3OCOC3=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
Erythramine	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CCC3=CC1
Erythramine	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CCC3=CC1
Erythrartine	O(C)[C@@H]1C[C@]23C=4C(=CC(OC)=C(OC)C4)[C@@H](O)CN2CC=C3C=C1
Erythrartine *N*-oxide	O=N12[C@]3(C=4C(=CC(OC)=C(OC)C4)[C@@H](O)C1)C(=CC2)C=C[C@H](OC)C3
Erythrascine	COC1C[C@]23N(CC=C2C=C1)C[C@H](OC(C)=O)C1=C3C=C(OC)C(OC)=C1
Erythratidine	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=C[C@@H]1O)=CC(OC)=C(OC)C4
Erythratidine	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=C[C@@H]1O)=CC(OC)=C(OC)C4
Erythratidinone	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=CC1=O)=CC(OC)=C(OC)C4
Erythratidinone	O(C)[C@@H]1C[C@]23C=4C(CCN2CCC3=CC1=O)=CC(OC)=C(OC)C4
Erythratine	[H]C1CN2C([H])C([H])C3=C(C=C4OCOC4=C3)[C@@]22C[C@@H](OC)[C@H](O)C=C12
Erythratinone	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CCC3=CC1=O
Erythravine	O[C@@H]1C[C@]23C=4C(=CC(OC)=C(OC)C4)CCN2CC=C3C=C1
Erythravine	O[C@@H]1C[C@]23C=4C(=CC(OC)=C(OC)C4)CCN2CC=C3C=C1
Erythrinarbine	O=C1N2CCC3=CC(OC)=C(O)C=C3C2CC1
Erythrinarbine	O=C1N2CCC3=CC(OC)=C(O)C=C3C2CC1

Erythrinine	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)[C@@H](O)CN2CC=C3C=C1
Erythrinine	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)[C@@H](O)CN2CC=C3C=C1
Erythrinine	O(C)[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)[C@@H](O)CN2CC=C3C=C1
Erythrinine *N*-oxide	O=N12[C@]3(C=4C(=CC5=C(C4)OCO5)[C@@H](O)C1)C(=CC2)C=C[C@H](OC)C3
Erythristemine	[H]C1[C@@H](OC)C2=C(C=C(OC)C(OC)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
Erythristemine-*N*-oxide	O=N12[C@]3(C=4C([C@@H](OC)C1)=CC(OC)=C(OC)C4)C(=CC2)C=C[C@H](OC)C3
Erythritol	COC1=C[C@]23N(CCC2=CC1O)CCC1=C3C=C(OC)C(OC)=C1
Erythrivarine A	CO[C@@H]1C[C@]23N(CC(C4C=C5C=C[C@@H](C[C@]55N4C[C@H](O)C4=C5C=C5OCOC5=C4)OC)=C2C=C1)C[C@H](O)C1=C3C=C2OCOC2=C1
Erythrivarine A1	[H][C@]1(C=C2C=C[C@@H](C[C@]22N1CCC1=CC3=C(OCO3)C=C21)OC)[C@]1([H])C=C2C=C[C@@H](C[C@]22N1C(=O)C(=O)C1=C2C=C2OCOC2=C1)OC
Erythrivarine A10	[H]C1CN2C(=O)C(=C3C[C@H](O)[C@@H](C[C@]23C2=CC(OC)=C(OC)C=C12)OC)[C@]1([H])C=C2C=C[C@@H](C[C@]22N1CCC1=CC(OC)=C(OC)C=C21)OC
Erythrivarine A11	[H]C1CN2C([H])([H])C(=C3C[C@H](O)[C@@H](C[C@]23C2=CC3=C(OCO3)C=C12)OC)[C@]1([H])C=C2C=C[C@@H](C[C@]22N1CCC1=CC3=C(OCO3)C=C21)OC
Erythrivarine A12	[H]C12C[C@](C)(O)O[C@@]1(C1=C[C@@H](O)[C@@H](C[C@]11N2CCC2=C1C=C1OCOC1=C2)OC)[C@]1([H])C=C2C=C[C@@H](C[C@]22N1CCC1=C2C=C2OCOC2=C1)OC
Erythrivarine A13	[H][C@@]1(CC2=CC3=C(OCO3)C=C2C23C[C@@H](OC)C=CC2=CCN13)C1=CN2\C(=C\C(C)=O)C=C3C=C[C@@H](C[C@]23C2=C1C=C1OCOC1=C2)OC
Erythrivarine A2	[H]C1([H])N2CCC3=C(C=C4OCOC4=C3)[C@@]22C[C@@H](OC)C(=O)C=C2[C@@]1([H])[C@@]1([H])CC2=CC3=C(OCO3)C=C2[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
Erythrivarine A3	[H][C@@]1(C(=O)N2CCC3=C(C=C4OCOC4=C3)[C@@]22C[C@@H](OC)[C@@H](O)C=C12)[C@@]1([H])CC2=CC3=C(OCO3)C=C2[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
Erythrivarine A4	[H]C1CN2[C@@]([H])(C=C3C=C[C@@H](C[C@]23C2=CC3=C(OCO3)C=C12)OC)C1=C2C=C[C@@H](C[C@]22N(C1)CCC1=C2C=C2OCOC2=C1)OC

Erythrivarine A5	[H][C@]1(C=C2C=C[C@@H](C[C@]22N1C[C@H](OC)C1=CC3=C(OCO3)C=C21)OC)C1=C2C=C[C@@H](C[C@]22N(C1)CCC1=C2C=C2OCOC2=C1)OC
Erythrivarine A6	[H]C1CN2[C@@]([H])(C=C3C=C[C@@H](C[C@]23C2=CC(OC)=C(OC)C=C12)OC)C1=C2C=C[C@@H](C[C@]22N(C1)CCC1=C2C=C2OCOC2=C1)OC
Erythrivarine A7	[H]C1CN2[C@@]([H])(C=C3C=C[C@@H](C[C@]23C2=CC3=C(OCO3)C=C12)OC)C1=C2C=C[C@@H](C[C@]22N(C1)CCC1=C2C=C(OC)C(OC)=C1)OC
Erythrivarine A8	[H]C1CC2=C(C(=O)N3CC([H])C4=CC5=C(OCO5)C=C4[C@]23C[C@H]1OC)[C@]1([H])C=C2C=C[C@@H](C[C@]22N1CCC1=CC3=C(OCO3)C=C21)OC
Erythrivarine A9	[H]C1CC2=C(C(=O)N3C[C@H](OC)C4=CC5=C(OCO5)C=C4[C@]23C[C@H]1OC)[C@]1([H])C=C2C=C[C@@H](C[C@]22N1CCC1=CC3=C(OCO3)C=C21)OC
Erythrivarine B	CO[C@@H]1C[C@@]23N(C[C@H](O)C4=CC5=C(OCO5)C=C24)C(C=C3C=C1)C1=CN2C[C@H](O)C3=C(C=C4OCOC4=C3)C3=C(OC)C=CC1=C23
Erythrivarine C	C(C(OC[C@H]1O[C@@H](O[C@@H]2C=3C([C@@]45N(C2=O)CC=C4C=C[C@H](OC)C5)=CC6=C(C3)OCO6)[C@H](O)[C@@H](O)[C@@H]1O)=O)[C@H]7N8[C@]9(C=%10C([C@@H](O)C8)=CC%11=C(C%10)OCO%11)C(=C7)C=C[C@H](OC)C9
Erythrivarine D	C(C(OC[C@H]1O[C@@H](O[C@@H]2C=3C([C@@]45N(C2=O)CC=C4C=C[C@H](OC)C5)=CC6=C(C3)OCO6)[C@H](O)[C@@H](O)[C@@H]1O)=O)[C@H]7N8[C@]9(C=%10C([C@@H](OC)C8)=CC%11=C(C%10)OCO%11)C(=C7)C=C[C@H](OC)C9
Erythrivarine E	O(C)[C@@H]1C[C@]23N([C@@H](C(=C2C=C1)[C@H]4N5[C@@]6(C(=C4)C=C[C@H](OC)C6)C=7C([C@@H](O)C5)=CC8=C(C7)OCO8)C9=C%10[C@@]%11(N(C9=O)C[C@H](O)C=%12C%11=CC%13=C(C%12)OCO%13)C[C@@H](OC)C=C%10)C[C@H](O)C=%14C3=CC%15=C(C%14)OCO%15
Erythrivarine F	O(C)[C@@H]1C[C@]23N([C@@H](C(=C2C=C1)[C@H]4N5[C@@]6(C(=C4)C=C[C@H](OC)C6)C=7C([C@@H](O)C5)=CC8=C(C7)OCO8)C9=C%10[C@@]%11(N(C9=O)C[C@H](O)C=%12C%11=CC%13=C(C%12)OCO%13)C[C@@H](OC)C=C%10)C[C@H](OC)C=%14C3=CC%15=C(C%14)OCO%15
Erythrivarine G	O=C1C[C@]23N([C@@H](C(=C2C=C1)[C@H]4N5[C@@]6(C(=C4)C=C[C@H](OC)C6)C=7C([C@@H](OC)C5)=CC8=C(C7)OCO8)C9=C%10[C@@]%11(N(C9=O)C[C@H](O)C=%12C%11=CC%13=C(C%12)OCO%13)C[C@@H](OC)C=C%10)C[C@H](O)C=%14C3=CC%15=C(C%14)OCO%15
Erythrivarine O	[H][C@]1(CC2=CC3=C(OCO3)C=C2[C@]23C[C@@H](OC)C=CC2=CCN13)C1=CN2C(=O)C=C3C=C[C@@H](C[C@]23C2=CC3=C(OCO3)C=C12)OC

Erythrivarine P	[H]C1CN2C[C@@]([H])(C3=C[C@@H](O)[C@@H](C[C@]23C2=C1C=C1OCOC1=C2)OC)[C@@]1([H])CC2=CC3=C(OCO3)C=C2[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
Erythrivarine Q	[H][C@@]1(CN2C[C@H](OC)C3=C(C=C4OCOC4=C3)[C@@]22C[C@@H](OC)[C@H](O)C=C12)[C@@]1([H])CC2=CC3=C(OCO3)C=C2[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
Erythrivarine R	[H]C1CN2C[C@@]([H])(C3=C[C@H](O)[C@@H](C[C@]23C2=C1C=C1OCOC1=C2)OC)[C@@]1([H])CC2=CC3=C(OCO3)C=C2[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
Erythrivarine S	[H][C@@]1(CN2C[C@H](OC)C3=C(C=C4OCOC4=C3)[C@@]22C[C@@H](OC)[C@@H](O)C=C12)[C@@]1([H])CC2=CC3=C(OCO3)C=C2[C@]23C[C@@H](OC)C=CC2=CC(=O)N13
Erythrivarine T	[H][C@@]1(CC2=CC3=C(OCO3)C=C2[C@]23C[C@@H](OC)C=CC2=CC(=O)N13)C1=CN2C=CC3=C(C=C4OCOC4=C3)[C@@]22C[C@@H](OC)C(=O)C=C12
Erythrivarine U	[H]C1([H])C=C2C=C[C@@H](C[C@]22N1[C@]([H])(CC1=CC3=C(OCO3)C=C21)C1=CN2C=CC3=C(C=C4OCOC4=C3)[C@@]22C[C@@H](OC)C(=O)C=C12)OC
Erythrivarine V	[H][C@]1(C=C2C=C[C@@H](C[C@]22N1CCC1=CC3=C(OCO3)C=C21)OC)C1=CN2CCC3=C(C=C4OCOC4=C3)C3=C2C1=CC=C3OC
Erythrivarine W	[H][C@]1(C=C2C=C[C@@H](C[C@]22N1CCC1=CC(OC)=C(OC)C=C21)OC)C1=CN2CCC3=C(C=C4OCOC4=C3)C3=C2C1=CC=C3OC
Erythrivarine X	[H][C@]1(C=C2C=C[C@@H](C[C@]22N1CCC1=CC3=C(OCO3)C=C21)OC)C1=CN2CCC3=C(C=C(OC)C(OC)=C3)C3=C2C1=CC=C3OC
Erythrivarine Y	COC1=CC2=C(C=C1OC)C1=C3N(CC2)C=CC3=CC=C1OC
Erythrivarine Z	CO[C@@H]1C[C@]23N(C=CC2=CC1=O)C=CC1=CC2=C(OCO2)C=C31
Erythrocarine	O[C@@H]1C[C@]23C=4C(=CC5=C(C4)OCO5)CCN2CC=C3C=C1
Erythromotidienone	[H]C1C[C@@]23N(C([H])C([H])C4=C2C=C(OC)C([H])=C4)C(=O)C=C3C=C1
Erythrosotidienone	[H]C1C[C@@]23N(C([H])C([H])C4=C2C=C2OCOC2=C4)C(=O)C=C3C=C1
Glucoerysodine	[H]C1C([H])C2=C(C=C(OC)C(OC(=O)[C@@H](N)CCC(O)=O)=C2)[C@]23C[C@@H](OC)C=CC2=CC([H])([H])N13
Glycoerysodine	[H]C1([H])C=C2C=C[C@@H](C[C@]22N1CCC1=C2C=C(OC)C(OC(=O)CC[C@H](N)C=O)=C1)OC
Hypaphorine	C([C@H]([N@+](C)(C)C)C([O-])=O)C=1C=2C(NC1)=CC=CC2
Hypaphorine	C([C@H]([N@+](C)(C)C)C([O-])=O)C=1C=2C(NC1)=CC=CC2
Hypaphorine	C([C@H]([N@+](C)(C)C)C([O-])=O)C=1C=2C(NC1)=CC=CC2
Hypaphorine	C([C@H]([N@+](C)(C)C)C([O-])=O)C=1C=2C(NC1)=CC=CC2
Hypaphorine	C([C@H]([N@+](C)(C)C)C([O-])=O)C=1C=2C(NC1)=CC=CC2
Hypaphorine	C([C@H]([N@+](C)(C)C)C([O-])=O)C=1C=2C(NC1)=CC=CC2
Hypaphorine	C([C@H]([N@+](C)(C)C)C([O-])=O)C=1C=2C(NC1)=CC=CC2

Hypaphorine methyl ester	C([C@@H](C(OC)=O)[N@@+](C)(C)C)C=1C=2C(NC1)=CC=CC2
Isoboldine	OC1=C2C=3[C@](CC=4C2=CC(OC)=C(O)C4)(N(C)CCC3C=C1OC)[H]
Isoerysopinophorin hydroxide	[OH-].COC1CC23N(CC=C2C=C1)CCC1=C3C=C(OC(=O)C(CC2=CNC3=CC=CC=C23)[N+](C)(C)C)C(O)=C1
Lycorine	[H][C@@]12N3CCC1=C[C@H](O)[C@@H](O)[C@@]2([H])C1=C(C3)C=C2OCOC2=C1
Melanacanthine (8-oxoerymelanthine)	CO[C@@H]1C[C@@]23N(CCC4=C2C=C(N=C4)C(=O)OC)C(=O)C=C3C=C1
N,N-Dimethyltryptophan methyl ester	C([C@@H](C(OC)=O)N(C)C)C=1C=2C(NC1)=CC=CC2
N-Nororientaline	C([C@@H]1C=2C(=CC(OC)=C(O)C2)CCN1)C3=CC(OC)=C(O)C=C3
N-Norprotosinomenine	COC1=CC=C(CC2NCCC3=CC(O)=C(OC)C=C23)C=C1O
Norisoorientaline	COC1=CC(CC2NCCC3=CC(O)=C(OC)C=C23)=CC=C1O
Nororientaline	COC1=C(O)C=CC(CC2NCCC3=CC(OC)=C(O)C=C23)=C1
Norreticuline	C([C@H]1C=2C(=CC(OC)=C(O)C2)CCN1)C3=CC(O)=C(OC)C=C3
O-Methyllycorenine	[H][C@@]12N(C)CCC1=CC[C@@]1([H])O[C@H](OC)C3=C(C=C(OC)C(OC)=C3)[C@@]21[H]
Protosinomenine	C([C@H]1C=2C(=CC(O)=C(OC)C2)CCN1C)C3=CC(O)=C(OC)C=C3
Reticuline	C([C@H]1C=2C(=CC(OC)=C(O)C2)CCN1C)C3=CC(O)=C(OC)C=C3
Retronccine	[H][C@@]12[C@H](O)CCN1CC=C2CO
Rhamnoerysodine	O(C)[C@@H]1C[C@]23C=4C(=CC(O[C@H]5[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O5)=C(OC)C4)CCN2CC=C3C=C1
Rhamnoerysodine	O(C)[C@@H]1C[C@]23C=4C(=CC(O[C@H]5[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O5)=C(OC)C4)CCN2CC=C3C=C1
Scoulerine	OC=1C=C2[C@]3(N(CC=4C(C3)=CC=C(OC)C4O)CCC2=CC1OC)[H]
Scoulerine	OC=1C=C2[C@]3(N(CC=4C(C3)=CC=C(OC)C4O)CCC2=CC1OC)[H]
Sodium erysovine 15-*O*-sulfate	COC1CC23N(CC=C2C=C1)CCC1=C3C=C(OS(=O)(=O)O[Na])C(OC)=C1
Sodium erysovine 15-*O*-sulfate	COC1CC23N(CC=C2C=C1)CCC1=C3C=C(OS(=O)(=O)O[Na])C(OC)=C1
Sodium erysovine *N*-oxy-15-*O*-sulfate	[H]C1=C[N+]2([O-])CC=C3C=C[C@@H](C[C@]23C2=C1C=C(OC)C(=C2)S(=O)(=O)O[Na])OC
Sodium erysovine *N*-oxy-15-*O*-sulfate	[H]C1=C[N+]2([O-])CC=C3C=C[C@@H](C[C@]23C2=C1C=C(OC)C(=C2)S(=O)(=O)O[Na])OC
Stachydrine	C([O-])(=O)[C@H]1[N+](C)(C)CCC1
Tazettine	[H][C@]12C[C@H](OC)C=C[C@]11C3=CC4=C(OCO4)C=C3CO[C@]1(O)CN2C

Table S2. List of *Sophora* alkaloids used in the SOM analysis with their corresponding SMILES representations. Duplicate molecular are highlighted in red

Name of molecule	SMILE
(−)-9α-Hydroxysophocarpine	[H]C1CN2CCC[C@@]3([H])CN4C(=O)C=CC[C@]4([H])[C@@]([H])(C1)[C@@]23[H]
(−)-*N*-methylcytisine	CN1CC2CC(C1)C1=CC=CC(=O)N1C2
(+)-5α-Hydroxyoxysophocarpine	[H]C1C[C@]2([H])[C@@]3([H])C([H])C=CC(=O)N3C[C@]3(O)CCC[N+]([O-])(C1)[C@]23[H]
(+)-Allomatrine	[H][C@]12CCCN3CCC[C@]([H])([C@@]4([H])CCCC(=O)N4C1)[C@@]23[H]
(+)-allo-sophoranol	[H][C@]12CCCN3CCC[C@](O)([C@@]4([H])CCCC(=O)N4C1)[C@@]23[H]
(+)-Isomatrine	[H][C@@]12CCCN3CCC[C@@]([H])([C@@]4([H])CCCC(=O)N4C1)[C@@]23[H]
(+)-Lehmannine	[H]C1CN2CCC[C@@]3([H])CN4C(=O)CC=C[C@]4([H])[C@@]([H])(C1)[C@@]23[H]
10-Oxy-5,6 dehydromatrine	[H][C@]12CCCC(=O)N1CC1=C3N(CCC1)C(=O)CC[C@]23[H]
10-Oxysophoridine	[H][C@@]12CCCN3C(=O)CC[C@]([H])([C@@]4([H])CCCC(=O)N4C1)[C@]23[H]
11-Allyl-cytisine	C=CCC1NCC2CC1CN1C(=O)C=CC=C21
11-Oxocytisine	O=C1NCC2CC1CN1C(=O)C=CC=C21
12 β-Hydroxy-sophocarpine	[H][C@@]1(O)C=CC(=O)N2C[C@]3([H])CCCN4CCC[C@@]([H])([C@]34[H])[C@@]12[H]
12α-Hydroxysophocarpine	[H][C@]12CCCN3CCC[C@]([H])([C@@]4([H])[C@@H](O)C=CC(=O)N4C1)[C@]23[H]
13-Methoxyanagyrine	[H][C@]12C[C@H](CCN1C[C@H]1C[C@@H]2CN2C(=O)C=CC=C12)OC
13α-Methoxy matrine	[H]C1N2C(=O)C[C@@H](C[C@]2([H])[C@@]2([H])CCCN3CCC[C@]1([H])[C@@]23[H])OC
13β-Hydroxyoxymatrine	[H]C1C[N+]2([O-])CCC[C@@]3([H])CN4C(C[C@H](O)CC4=O)[C@@]([H])(C1[H])[C@@]23[H]
14β-Hydroxylupanine	[H][C@@]12CC[C@H](O)CN1C[C@@H]1C[C@H]2CN2C(=O)CCC[C@]12[H]
14β-Hydroxymatrine	[H][C@@]12CCCN3CCC[C@@]([H])([C@]4([H])CC[C@@H](O)C(=C)N4C1)[C@@]23[H]
14β-Hydroxymatrine	[H][C@@]12CCCN3CCC[C@@]([H])([C@]4([H])CC[C@@H](O)C(=C)N4C1)[C@@]23[H]
5,6-Dehydrolupanine	[H][C@]12CCCCN1CC1CC2CN2C(=O)CCC=C12
5α,14β-Dihydroxymatrine	[H][C@]12CC[C@H](O)C(=O)N1C[C@]1(O)CCCN3CCC[C@@]2([H])[C@]13[H]

5α-Hydroxymatrine [(+)- Sophoranol]	[H][C@]12CCCC(=O)N1[C@@H](O)C1CCCN3CCC[C@@]2([H])[C@]13[H]
7 α -Hydroxysophoramine	[H][C@]12CCCN3CCC[C@](O)(C4=CC=CC(=O)N4C1)[C@]23[H]
7,11-Dehydromatrine	[H]C12CCCN3CCCC(=C4CCCC(=O)N4C1)C23[H]
7,11-Dehydro-oxymatrine	[H][C@]12CCC[N+]3([O-])CCCC(=C4CCCC(=O)N4C1)[C@]23[H]
7-epi-Sophoramine	[H][C@]12CCCN3CCC[C@@]([H])(C4=CC=CC(=O)N4C1)[C@]23[H]
7β-Sophoramine	[H][C@]12CCCN3CCC[C@]([H])(C4=CC=CC(=O)N4C1)[C@]23[H]
8α-Hydroxysophocarpine	[H]C1CN2CCC[C@@]3([H])CN4C(CC([H])=CC4=O)[C@@]([H])([C@@H]1O)[C@@]23[H]
9 α-Hydroxy- 7,11-dehydromatrine	[H][C@]12CCCN3C[C@@H](O)CC(=C4CCCC(=O)N4C1)[C@]23[H]
9 α-Hydroxysophocarpine	[H]C12C[C@H](O)CN3CCCC([H])([C@]4([H])CC=CC(=O)N4C1)C23[H]
9 α-Hydroxysophoramine	[H]C12C[C@H](O)CN3CCCC([H])(C4=CC=CC(=O)N4C1)C23[H]
9α-Acetoxymatrine	[H]C1CC2N(C[C@]3([H])CCCN4C[C@@H](OC(C)=O)C([H])[C@@]2([H])[C@]34[H])C(=O)C1
9α-Hydroxymatrine	OC1CC2C3CCCC(=O)N3CC3CCCN(C1)C23
Alopecine A	[H][C@]12CCCN3CCC[C@]([H])([C@@]4([H])C[C@H]5[C@@H](C(=O)C4C1)C5(Cl)Cl)[C@]23[H]
Alopecine B	[H][C@]12CCC[N+]3([O-])CCC[C@]([H])([C@@]4([H])C[C@H]5[C@@H](C(=O)N4C1)C5(Cl)Cl)[C@]23[H]
Alopecine C	[H][C@@]12CCCN3CCC[C@]([H])([C@@]4([H])C[C@H]5[C@@H](C(=O)N4C1)C5(Cl)Cl)[C@]23[H]
Alopecine D	[H][C@]12CCCN3CCC[C@]([H])([C@@]4([H])CC5=C(C(=O)N4C1)C5(Cl)Cl)[C@]23[H]
Alopecine E	[H][C@]12CCCN3CCC[C@]([H])([C@@]4([H])C[C@H](CC(=O)N4C1)C(Cl)(Cl)Cl)[C@]23[H]
Alopecurine A	[H][C@]12CCCC(=O)N1C[C@@]1(O)CCCN(CCCC2=O)C1=O
Alopecurine B	[H][C@]12CCCC(=O)N1CC(=O)CCCN1CCC[C@]2(O)C1=O
Aloperine	C1CCN2C[C@H]3C[C@H](C=C4CCCNC34)C2C1
Anagyrine	[H]C1CCN2CC3CC(CN4C(=O)C=CC=C34)[C@@]2([H])C1
Anagyrine	[H]C1CCN2CC3CC(CN4C(=O)C=CC=C34)[C@@]2([H])C1
Cytisine	O=C1C=CC=C2C3CNCC(C3)CN12
Epilamprolobin	[H]C12CCCCN1CCCC2CN1C(=O)CCCC1=O
Epilamprolobin-N-oxide	[H]C12CCCC[N+]1([O-])CCCC2CN1C(=O)CCCC1=O
Flavascensine	[H][C@]12CC(C)(C)NC1=C(C)C(=O)C(C)(C)N2
Flavesine G	OC(=O)CCCC1=NC=C2CCCN3CCCC1=C23
Flavesine H	[H][C@@]1(CCCC(O)=O)N=CC2=C3N(CCC2)CCC[C@@]13[H]
Flavesine I	OC(=O)CCCC1=NCC2CCCN3CCCC1=C23
Flavesine J	O=C(CCCC1=NC=C2CCCN3CCCC1=C23)N1CCCCC1
Isokurarimine	CN1C[C@H](CO)C[C@H](C1)C1=CC=CC(=O)N1
Isomatrine	[H][C@]12CCCN3CCC[C@]([H])(C4([H])CCCC(=O)N4C1)[C@]23[H]
Isosophoridine	[H][C@@]12CCCN3C(=O)CC[C@]([H])([C@@]4([H])CCCC(=O)N4C1)[C@@]23[H]

Kurarimine	CN1C[C@@H](CO)C[C@H](C1)C1=CC=CC(=O)N1
Lehmanine	[H]C12CCCN3CCCC([H])([C@@]4([H])C=CCC(=O)N4C1)C23[H]
Mamanine	[H]C12CCCCN1CC(CC2CO)C1=CC=CC(=O)N1
Mandarim	[H]C12CCCN3CCCC([H])([C@]4([H])CCCC(=O)N4C1)[C@]23[H]
Matrine	[H]C12CCCN3CCCC([H])([C@]4([H])CCCC(=O)N4C1)C23[H]
Matrine	[H]C12CCCN3CCCC([H])([C@]4([H])CCCC(=O)N4C1)C23[H]
Neosophoramine	[H]C1CN2CCC[C@]3([H])CN4C(=O)C=CC=C4[C@@]([H])(C1)[C@@]23[H]
N-Formyl cytosine	O=CN1CC2CC(C1)C1=CC=CC(=O)N1C2
N-Methyl cytosine	CN1CC2CC(C1)C1=CC=CC(=O)N1C2
Ochrocephalamines E	[H][C@]12CCC(=O)N1C[C@]1([H])CCCN3CCC[C@@]2([H])[C@]13[H]
Oxymatrine	[H]C12CCC[N+]3([O-])CCCC([H])([C@]4([H])CCCC(=O)N4C1)C23[H]
Oxymatrine	[H]C12CCC[N+]3([O-])CCCC([H])([C@]4([H])CCCC(=O)N4C1)C23[H]
Oxysophocarpine	[H][C@]12CCC[N+]3([O-])CCC[C@@]([H])([C@@]4([H])CC=CC(=O)N4C1)[C@]23[H]
Oxysophocarpine	[H][C@]12CCC[N+]3([O-])CCC[C@@]([H])([C@@]4([H])CC=CC(=O)N4C1)[C@]23[H]
Oxysophoridine	[H][C@@]12CCC[N+]3([O-])CCC[C@]([H])([C@@]4([H])CCCC(=O)N4C1)[C@]23[H]
Rhombifolin	C=CCN1CC2CC(C1)C1=CC=CC(=O)N1C2
Sophaline A	[H][C@@]12CCCN3CCC[C@@]([H])([C@]13[H])[C@@]1(CC)CC(=O)N1C2
Sophaline B	[H][C@@]12CC(=O)N3CCC[C@]([H])(CN4C(=O)CCC[C@]14[H])[C@@]23[H]
Sophaline C	[H][C@]12N3CCC[C@]1([H])CN1C(=O)CCC[C@]1([H])[C@@]2([H])C1=C3C=C(C=C1C)C(C)=O
Sophaline D	[H][C@]12N3CCC[C@@]1([H])CN1C(=O)CCC[C@]1([H])[C@@]2([H])C1=C3C=C(C=C1C)C(C)=O
Sophaline E	z[H][C@]12C[C@H](O)C[C@H](N1C[C@H]1C[C@@H]2CN2C(=O)C=CC=C12)C(=O)C1=CNC2=C1C=CC=C2
Sophaline G	[H][C@@]12CCCN[C@]1([H])[C@]([H])(CC1=CC3=C4N(CCCC4=C1)CCC3)[C@@]1([H])CCCC(=O)C1C2
Sophaline H	[H][C@]12CCCN[C@]1([H])[C@]([H])(CC1=CC3=C4N(CCCC4=C1)CCC3)[C@@]1([H])CCCC(=O)C1C2
Sophalode A	[H][C@]12CCCN3CCC[C@]([H])([C@]13[H])[C@]1(CCCC(=O)N1C2)OC
Sophalode B	[H][C@@]12CCC[N+]3([O-])CCC[C@@]([H])([C@]13[H])[C@]1(CCCC(=O)N1C2)OC
Sophalode C	[H][C@]12CCCN3CCC[C@]([H])([C@]13[H])[C@]1(O)CCCC(=O)N1C2
Sophalode D	[H][C@]12CCCN3CCC[C@@]([H])([C@]13[H])[C@]1(O)CCCC(=O)N1C2

Sophalode E	[H]C1CN2CC([H])C([H])[C@]3(O)[C@@]4([H])CCC([H])C(=O)N4C[C@@]([H])(C1)[C@]23[H]
Sophalode F	[H]C1CN2CC([H])[C@H](O)[C@]3([H])[C@@]4([H])CCC([H])C(=O)N4C[C@@]([H])(C1)[C@]23[H]
Sophalode G	[H]C1CN2C[C@@H](O)C([H])[C@]3([H])[C@@]4([H])CC[C@H](O)C(=O)N4C[C@]([H])(C1)[C@]23[H]
Sophalode H	[H]C1C[C@]2([H])C3=CC=CC(=O)N3C[C@@]3([H])CCC[N+]([O-])(C1)[C@]23[H]
Sophalode I	[H][C@@]12CCCN3CCC[C@@]([H])(C4=CC=CC(=O)N4C1)[C@]23[H]
Sophalode J	[H]C1C=C[C@@]2([H])N(C[C@]3([H])CCCN4C[C@@H](O)C[C@@]2([H])[C@]34[H])C1=O
Sophalode K	[H]C1CN2CCC[C@]3([H])CN4C(=O)[C@@H](O)C=C[C@]4([H])[C@@]([H])(C1)[C@@]23[H]
Sophalode L	[H][C@@]12CCCN3CCCC(=C4CCCC(=O)N4C1)[C@]23[H]
Sophaloseedline I	[H]C1CC[C@@]2([H])N(C[C@]34CCCN5CCC[C@]2(O3)[C@]45O)C1=O
Sophaloseedline J	[H][C@]12CC[C@H](O)C(=O)N1C[C@]13CCCN4CCC[C@]2(O1)[C@]34O
Sophaloseedline K	[H][C@]12CC[C@H](O)C(=O)N1C[C@@]13CCCN4CCC[C@@]2(O1)[C@@]34O
Sophaloseedline L	[H][C@]12CCCC(=O)N1C[C@]1([H])CCCN(CCC[C@H]2O)C1=O
Sophaloseedline M	[H][C@]12CC[C@@H](O)N3C(=O)CC[C@]([H])([C@@]4([H])CCCC(=O)N4C1)[C@]23[H]
Sophaloseedline N	[H]C1CC[C@@]2([H])CN3C(=O)CCC[C@]3([H])[C@@]3([H])CCC(=O)N1[C@@]23[H]
Sophaloseedline O	[H][C@@]12CCC[N+]3([O-])CCCC(=C4CCCC(=O)N4C1)[C@@]23[H]
Sophaloseedline P	[H][C@]12CCCC(=O)N1C[C@]1(O)CCCN3CCC[C@@]2(O)[C@@]13[H]
Sophaloseedline Q	[H][C@@]12N3CCC[C@@]1(O)CN1C(=O)CCC=C1[C@@]2(O)CCC3
Sophaloseedline R	[H][C@]12CCC[N+]3([O-])CCC[C@@]([H])([C@]13[H])[C@@]1(O)CCCC(=O)N1C2
Sophaloseedline S	[H]C1CC(=O)N2[C@H](O)[C@]3([H])CCCN4CCC[C@]([H])([C@@]2([H])C1)[C@]34[H]
Sophocarpine	[H]C12CCCN3CCCC([H])([C@]4([H])CC=CC(=O)N4C1)C23[H]
Sophocarpine	[H]C12CCCN3CCCC([H])([C@]4([H])CC=CC(=O)N4C1)C23[H]
Sophocarpine	[H]C12CCCN3CCCC([H])([C@]4([H])CC=CC(=O)N4C1)C23[H]
Sophocarpine	[H]C12CCCN3CCCC([H])([C@]4([H])CC=CC(=O)N4C1)C23[H]
Sophoramine	[H]C12CCCN3CCCC([H])(C4=CC=CC(=O)N4C1)C23[H]
Sophoranol *N*-oxide	[H]C1CC(=O)N2C([H])[C@]3(O)CCC[N+]4([O-])CCC[C@]([H])([C@@]2([H])C1)[C@]34[H]
Sophorasine A	[H]C(C)(O)C(=O)CN1C[C@]2([H])CN3C(=O)C=CC=C3[C@]([H])(C1)C2
Sophorasine B	[H]C(C)(O)C(=O)CN1C[C@]2([H])CN3C(=O)C=CC=C3[C@]([H])(C1)C2

Sophoridine	[H]C12CCCN3CCC[C@]([H])(C4([H])CCCC(=O)N4C1)[C@]23[H]
Sophoridine	[H]C12CCCN3CCC[C@]([H])(C4([H])CCCC(=O)N4C1)[C@]23[H]
Sophovicine A	[H][C@]12CCCN3CCC[C@]([H])([C@@]4([H])CC[C@@]([H])(N5C=NC6=C5N=CN=C6N)C(=O)N4C1)[C@]23[H]
Sophovicine B	[H][C@@]1(CC(=O)N2C[C@]3([H])CCCN4CCC[C@]([H])([C@@]2([H])C1)[C@]34[H])N1C=NC2=C1N=CN=C2N
Sophovicine C	[H][C@@]1(CC(=O)N2C[C@]3([H])CCC[N+]4([O-])CCC[C@]([H])([C@@]2([H])C1)[C@]34[H])N1C=NC2=C1N=CN=C2N
Sophtonkine C	[H]C1CC[C@@]2([H])N(C[C@@]34CCCN5CCC[C@@]2(O3)[C@@]45O)C1=O
sophtonrootine B	[H][C@]12CCC(=O)N1C[C@@]1([H])CCCN(CCCC2=O)C1=O
Sparteine	[H]C1([H])CCCC2([H])C3CC(CN12)[C@@]1([H])CCCCN1C3
Tsukushinamine A	C=CC[C@H]1[N@@]2CC3CC(C2)CN2C(=O)CC=C[C@]132
Tsukushinamine B	C=CCC1[N@@]2CC3CC(C2)CN2C(=O)CC=C[C@]132
Tsukushinamine C	C=CC[C@H]1[N@@]2CC3CC(C2)CN2C(=O)C=CC[C@]132

Table S3. Distribution of molecular descriptor values (nR10, nRC=N, and nCXr) for compounds from *Sophora* included in the SOM analysis

ID	nR10	nRC=N	nCXr	ID	nR10	nRC=N	nCXr
1	0	0	0	169	1	0	0
2	0	0	0	170	1	0	0
3	0	0	0	171	1	0	0
4	0	0	0	172	1	0	0
5	0	0	0	173	1	0	0
6	0	0	0	174	1	0	0
7	0	0	0	175	1	0	0
8	0	0	0	176	1	0	0
9	0	0	0	177	1	0	0
10	0	0	0	178	1	0	0
11	0	0	0	179	1	0	0
12	0	0	0	180	1	0	0
13	1	0	0	181	1	0	0
14	1	0	0	182	1	0	0
15	1	0	0	183	1	0	0
16	1	0	0	184	1	0	0
17	1	0	0	185	1	0	0
18	1	0	0	186	1	0	0
19	1	0	0	187	1	0	0
20	0	0	0	188	1	0	0
21	0	0	0	189	1	0	0
22	1	0	0	190	1	0	0
23	1	0	0	191	1	0	0
24	1	0	0	192	1	0	0
25	1	0	0	193	1	0	0
26	1	0	0	194	1	0	0
27	1	0	0	195	2	0	0
28	1	0	0	196	3	0	0
29	1	0	0	197	3	0	0
30	1	0	0	198	3	0	0
31	1	0	0	199	3	0	0
32	1	0	0	200	3	0	0
33	1	0	0	201	2	0	0
34	1	0	0	202	1	0	0
35	1	0	0	203	1	0	0
36	1	0	0	204	1	0	0
37	1	0	0	205	1	0	0
38	1	0	0	206	1	0	0

39	1	0	0	207	1	0	0
40	1	0	0	208	1	0	0
41	1	0	0	209	1	0	0
42	0	0	0	210	1	0	0
43	1	0	0	211	1	0	0
44	1	0	0	212	1	0	0
45	1	0	0	213	1	0	0
46	1	0	0	214	1	0	0
47	1	0	0	215	1	0	0
48	1	0	0	216	1	0	0
49	1	0	0	217	1	0	0
50	1	0	0	218	1	0	0
51	1	0	0	219	1	0	0
52	1	0	0	220	1	0	0
53	1	0	0	221	1	0	0
54	1	0	0	222	1	0	0
55	1	0	0	223	1	0	0
56	1	0	0	224	1	0	0
57	1	0	0	225	1	0	0
58	1	0	0	226	1	0	0
59	1	0	0	227	1	0	0
60	1	0	0	228	2	0	0
61	1	0	0	229	2	0	0
62	1	0	0	230	1	0	0
63	1	0	0	231	1	0	0
64	1	0	0	232	1	0	0
65	1	0	0	233	1	0	0
66	1	0	0	234	1	0	0
67	1	0	0	235	1	0	0
68	1	0	0	236	2	0	0
69	1	0	0	237	1	0	0
70	1	0	0	238	1	0	0
71	1	0	0	239	1	0	0
72	1	0	0	240	1	0	0
73	1	0	0	241	1	0	0
74	0	0	0	242	1	0	0
75	0	0	0	243	1	0	0
76	1	0	0	244	1	0	0
77	1	0	0	245	1	0	0
78	1	0	0	246	1	0	0
79	1	0	0	247	2	0	0
80	1	0	0	248	2	0	0

81	1	0	0	249	2	0	0
82	2	0	0	250	2	0	0
83	1	0	0	251	2	0	0
84	1	0	0	252	2	0	0
85	1	0	0	253	1	0	0
86	1	0	0	254	1	0	0
87	1	0	0	255	1	0	0
88	1	0	0	256	1	0	0
89	1	0	0	257	1	0	0
90	1	0	0	258	1	0	0
91	1	0	0	259	1	0	0
92	1	0	0	260	1	0	0
93	1	0	0	261	1	0	0
94	1	0	0	262	1	0	0
95	1	0	0	263	1	0	0
96	1	0	0	264	1	0	0
97	1	0	0	265	1	0	0
98	1	0	0	266	1	0	0
99	1	0	0	267	1	0	0
100	1	0	0	268	1	0	0
101	1	0	0	269	2	0	0
102	1	0	0	270	2	0	0
103	1	0	0	271	2	0	0
104	1	0	0	272	3	0	0
105	1	0	0	273	3	0	0
106	1	0	0	274	1	0	0
107	1	0	0	275	1	0	0
108	1	0	0	276	1	0	0
109	1	0	0	277	1	0	0
110	1	0	0	278	1	0	0
111	1	0	0	279	2	0	0
112	1	0	0	280	2	0	0
113	1	0	0	281	1	0	0
114	1	0	0	282	3	0	0
115	1	0	0	283	3	0	0
116	1	0	0	284	2	0	0
117	1	0	0	285	1	0	0
118	1	0	0	286	1	0	0
119	1	0	0	287	1	0	0
120	1	0	0	288	1	0	0
121	1	0	0	289	1	0	0
122	1	0	0	290	1	0	0

123	1	0	0	291	1	0	0
124	1	0	0	292	1	0	0
125	1	0	0	293	1	0	0
126	1	0	0	294	1	0	0
127	1	0	0	295	1	0	0
128	1	0	0	296	1	0	0
129	1	0	0	297	1	0	0
130	1	0	0	298	1	0	0
131	1	0	0	299	1	0	0
132	1	0	0	300	1	0	0
133	2	0	0	301	1	0	0
134	1	0	0	302	1	0	0
135	1	0	0	303	1	0	0
136	1	0	0	304	1	0	0
137	1	0	0	305	1	0	0
138	1	0	0	306	1	0	0
139	1	0	0	307	1	0	0
140	1	0	0	308	1	0	0
141	1	0	0	309	1	0	0
142	1	0	0	310	1	0	0
143	1	0	0	311	2	0	0
144	1	0	0	312	2	0	0
145	1	0	0	313	2	0	0
146	4	0	0	314	2	0	0
147	2	0	0	315	2	0	0
148	1	0	0	316	2	0	0
149	1	0	0	317	2	0	0
150	1	0	0	318	2	0	0
151	1	0	0	319	2	0	0
152	1	0	0	320	2	0	0
153	1	0	0	321	2	0	0
154	1	0	0	322	2	0	0
155	0	0	0	323	2	0	0
156	1	0	0	324	2	0	0
157	1	0	0	325	2	0	0
158	1	0	0	326	1	0	0
159	1	0	0	327	1	0	0
160	1	0	0	328	1	0	0
161	1	0	0	329	1	0	0
162	1	0	0	330	1	0	0
163	1	0	0	331	1	0	0
164	1	0	0	332	1	0	0

165	1	0	0	333	2	0	0
166	1	0	0	334	2	0	0
167	1	0	0	335	1	0	0
168	1	0	0	336	1	0	0

Table S4. Distribution of molecular descriptor values (nR10, nRC=N, and nCXr) for compounds from *Erythrina* included in the SOM analysis

ID	nR10	nRC=N	nCXr	ID	nR10	nRC=N	nCXr
1	0	0	0	61	4	0	0
2	1	0	0	62	4	0	0
3	1	0	0	63	4	0	0
4	3	0	0	64	4	0	0
5	3	1	0	65	4	0	0
6	3	1	0	66	4	0	0
7	0	0	0	67	4	0	0
8	0	0	0	68	4	0	0
9	1	0	0	69	4	0	0
10	1	0	0	70	4	0	0
11	4	0	0	71	4	0	0
12	4	0	0	72	4	0	0
13	1	0	0	73	4	0	0
14	1	0	0	74	4	0	0
15	1	0	0	75	4	0	0
16	3	0	0	76	4	0	0
17	2	0	0	77	4	0	0
18	2	0	0	78	4	0	0
19	1	0	0	79	4	0	0
20	1	0	0	80	4	0	0
21	1	0	0	81	4	0	0
22	4	0	0	82	4	0	0
23	1	0	0	83	2	0	0
24	4	0	2	84	2	0	0
25	3	0	0	85	4	0	0
26	1	0	0	86	6	0	0

27	1	0	0	87	6	0	0
28	1	0	0	88	1	0	0
29	1	0	0	89	4	0	0
30	4	0	0	90	4	0	0
31	4	0	0	91	5	0	0
32	4	0	0	92	5	0	0
33	4	0	0	93	3	0	0
34	4	0	0	94	4	0	0
35	4	0	0	95	4	0	0
36	4	0	0	96	4	0	0
37	4	0	0	97	4	0	0
38	4	0	0	98	4	0	0
39	4	0	0	99	4	0	0
40	4	0	0	100	4	0	0
41	2	0	0	101	4	0	0
42	4	0	2	102	4	0	0
43	4	0	2	103	4	0	0
44	4	0	2	104	4	0	0
45	6	0	0	105	4	0	0
46	6	0	0	106	4	0	0
47	1	0	0	107	4	0	0
48	1	0	0	108	4	0	0
49	1	0	0	109	4	0	0
50	2	0	0	110	4	0	0
51	2	0	0	111	4	0	0
52	4	0	0	112	4	0	0
53	4	0	0	113	4	0	0

54	4	0	0	114	4	0	0
55	4	0	0	115	4	0	0
56	4	0	0	116	2	0	0
57	4	0	0	117	2	0	0
58	4	0	0	118	2	0	0
59	4	0	0	119	2	0	0
60	4	0	0				