**Supporting Information**

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**Metabolic Correlations of *Salvia* *dugesii* Fernald and *Salvia gesneriflora* Lindl. *&* Paxton with Native *Salvia* Plants from Four Continents Using Essential Oils Compositions**

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# **Table S1.** Chemical composition of essential oils of the twelve analyzed *Salvia* plants

|  |  |  |  |
| --- | --- | --- | --- |
| **Number** | **Compound** | **Structural****Skeleton** | **Composition (%)** |
| A | B | C | D | E | F | G | H | I | J | K | L |
| **1** | Spathulenol | IX | 7.63 | 4.74 |  |  |  |  |  |  |  |  |  |  |
| **2** | *β*-Bourbonene | XVII | 1.60 | 1.01 | 5.60 |  | 2.90 |  | 0.29 |  |  |  |  |  |
| **3** | *δ*-Cadinene | X | 4.80 |  | 0.80 |  |  |  | 0.45 | 2.30 | 1.70 |  |  |  |
| **4** | 9-Methoxy calamenene | X | 0.73 |  |  |  |  |  |  |  |  |  |  |  |
| **5** | Aromadendrene | IX | 2.95 | 1.09 |  |  | 0.10 |  | 0.08 |  |  |  |  | 1.22 |
| **6** | Bornyl acetate | XXII | 3.35 | 5.80 |  |  |  |  | 1.05 |  |  |  |  | 0.50 |
| **7** | Camphor | XXII |  | 1.00 |  |  |  | 6.80 | 25.14 |  |  |  |  | 0.08 |
| **8** | Caryophyllene | V | 10.04 | 15.68 | 27.70 | 2.00 |  |  | 3.30 |  |  | 11.55 | 14.00 | 0.88 |
| **9** | Caryophyllene oxide | V | 5.84 | 2.54 | 4.20 |  | 2.00 | 1.10 | 0.06 | 3.00 | 0.20 | 3.38 |  | 15.54 |
| **10** | *cis*-1-Methyl-4-(1-methylethyl)-2-cyclohexen-1-ol | XXIII |  | 0.73 |  |  |  |  |  |  |  |  |  |  |
| **11** | *cis*-*β*-Farnesene | XV | 1.47 |  |  |  |  |  |  |  |  |  |  |  |
| **12** | Diepicedrene-1-oxide | XVI | 2.24 |  |  |  |  |  |  |  |  |  |  |  |
| **13** | Elixene | XIV |  | 1.59 |  |  |  |  |  |  |  |  |  |  |
| **14** | *endo*-Borneol | XXII | 1.06 | 1.40 |  | 0.90 |  | 7.60 | 2.81 |  |  | 1.66 |  | 0.55 |
| **15** | Eugenol | XXIX |  | 1.96 |  |  |  |  | 0.28 |  |  |  |  | 0.78 |
| **16** | Geranyl-*α*-terpinene | XXV |  | 5.49 |  |  |  |  |  |  |  |  |  |  |
| **17** | Germacrene D | XI | 4.97 |  | 19.50 |  | 7.90 |  | 0.17 | 0.20 |  | 4.37 |  |  |
| **18** | Guaiol | IX |  | 2.73 | 1.50 |  |  |  |  |  |  |  |  |  |
| **19** | Hedycaryol | XI |  | 7.57 |  |  |  |  |  |  |  |  |  |  |
| **20** | Humulene | V | 4.62 |  | 2.30 | 10.70 | 3.60 |  | 2.48 | 3.60 | 0.40 | 1.28 |  |  |
| **21** | Isoalloaromadendrene epoxide | IX | 2.23 |  |  |  |  |  |  |  |  |  |  |  |
| **22** | Isoaromadendrene epoxide | IX | 3.38 |  |  |  |  |  |  |  |  |  |  |  |
| **23** | Ledol | IX |  | 3.20 |  |  |  |  |  |  |  |  |  | 5.14 |
| **24** | Phenyl ethyl alcohol | XXIX |  | 2.06 |  |  |  |  |  |  |  |  |  |  |
| **25** | Podocarp-7-en-3-one,13*β*-methyl-13-vinyl | XXVI | 0.62 |  |  |  |  |  |  |  |  |  |  |  |
| **26** | Sandaracopimaradiene | XXVI | 4.89 |  |  |  |  |  |  |  |  |  |  |  |
| **27** | Rimuene | XXVI | 0.65 |  |  |  |  |  |  |  |  |  |  |  |
| **28** | Sclareol oxide | XXVII | 0.84 |  |  |  |  |  |  |  |  |  |  |  |
| **29** | Terpinen-4-ol | XXIII |  | 1.06 |  |  | 0.30 |  | 0.74 |  |  |  |  |  |
| **30** | Valeranone | XIII |  | 6.26 |  |  |  |  |  |  |  |  |  |  |
| **31** | Viridiflorol | IX | 0.81 |  | 0.50 | 32.40 | 0.10 |  | 7.98 | 2.20 | 33.00 |  |  |  |
| **32** | *α*-Cedrene | XVI | 1.13 |  |  |  |  |  |  |  |  |  |  |  |
| **33** | *α*-Copaen-11-ol | VI |  | 3.66 |  |  |  |  |  |  |  |  |  |  |
| **34** | *α*-Copaene | VI | 1.74 |  | 1.70 |  | 1.10 |  | 0.07 |  |  |  |  | 5.70 |
| **35** | *α*-Pinene | XXI |  | 1.45 | 0.50 | 0.50 | 2.10 | 6.80 | 0.84 | 3.10 | 4.20 |  |  |  |
| **36** | *β*-Bisabolene | IV | 1.48 |  |  |  |  |  |  |  |  |  |  |  |
| **37** | *β*-Cadinene | X |  | 1.20 |  |  |  |  |  |  |  |  |  |  |
| **38** | *β*-Cubebene | XII | 0.81 | 3.56 |  |  | 0.30 |  |  |  |  |  |  | 0.62 |
| **39** | *β*-Eudesmane | VIII | 0.95 |  |  |  |  |  |  |  |  |  |  |  |
| **40** | *7-epi-α-*Eudesmol | VIII |  | 3.66 |  | 0.70 |  |  |  | 12.30 | 0.30 |  |  |  |
| **41** | *γ*-Cadinene | X | 1.39 |  |  |  | 2.00 |  | 0.12 |  |  |  |  | 5.30 |
| **42** | *γ*-Elemene | XIV |  | 7.54 |  |  |  |  |  |  |  |  |  |  |
| **43** | *γ*-Muurolene | X | 8.31 |  |  |  | 0.80 |  |  |  |  |  |  | 1.84 |
| **44** | *γ*-Terpinene | XXIII |  | 1.03 |  |  | 0.20 | 5.40 | 0.61 |  |  |  |  |  |
| **45** | (*E*)-Nerolidol | XV |  |  | 1.20 |  |  |  |  | 0.20 | 2.00 |  |  |  |
| **46** | (*E*)-*β*-Ocimene | XIX |  |  |  |  | 3.00 |  |  |  |  |  |  |  |
| **47** | (*Z*)-Caryophyllene | V |  |  |  |  | 0.10 | 3.30 |  |  |  |  |  | 0.91 |
| **48** | (*Z*)-*β*-Ocimene | XIX |  |  |  |  | 1.50 |  |  |  |  |  |  |  |
| **49** | 1,8-Cineole | XXIII |  |  | 0.80 | 3.10 |  | 40.10 | 14.14 | 1.80 | 4.80 |  |  | 0.18 |
| **50** | 14-Hydroxy-*δ*-Cadinene | X |  |  |  |  | 0.20 |  |  |  |  |  |  |  |
| **51** | 14-Hydroxy-*δ*-Muurolene | X |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **52** | 1-*epi*-Cubenol | X |  |  |  |  | 0.70 |  |  |  |  |  |  |  |
| **53** | 1-Hydroxy-1,7-dimethyl-4-isopropyl-2,7-cyclodecadiene | XI |  |  |  |  |  |  |  |  |  | 0.98 |  |  |
| **54** | 2-Cyclohexen-1-one,5-methyl-2-(1-methylethyl)- | XXIII |  |  |  |  |  |  |  |  |  | 0.14 |  |  |
| **55** | 3-Cyclohexen-1-carboxaldehyde,3,4-dimethyl | XXIX |  |  |  |  |  |  |  |  |  | 2.04 |  |  |
| **56** | Acetophenone | XXIX |  |  |  |  |  |  |  |  |  |  |  | 0.21 |
| **57** | Allo-aromadendrene | IX |  |  |  |  | 0.30 |  | 0.06 |  |  |  |  |  |
| **58** | Benzaldehyde | XXIX |  |  |  | 0.60 |  |  |  |  |  |  |  |  |
| **59** | Benzene acetaldehyde | XXIX |  |  |  |  | 0.20 |  |  |  |  |  |  |  |
| **60** | Bicyclogermacrene | XI |  |  | 18.30 |  | 1.50 | 5.40 |  | 0.90 |  |  |  |  |
| **61** | Cadalene | X |  |  |  |  |  |  |  |  |  |  |  | 5.28 |
| **62** | Calarene | I |  |  |  |  |  |  | 0.14 |  |  |  |  |  |
| **63** | Camphene | XX |  |  |  |  | 0.20 | 3.00 | 0.78 |  |  | 1.63 |  |  |
| **64** | Carvacrol | XXIII |  |  |  |  |  |  | 0.18 |  |  |  | 1.20 |  |
| **65** | Caryophylla-(14),8(15)-dien-5*α*-ol | V |  |  | 1.00 |  |  |  |  |  |  |  |  |  |
| **66** | Widdrol | XVIII |  |  |  |  |  |  |  |  |  | 3.54 |  |  |
| **67** | *cis*-Calamenene | X |  |  |  |  |  |  | 0.08 |  |  | 0.73 |  | 9.60 |
| **68** | *cis*-Linalool oxide | XIX |  |  |  |  |  |  |  |  |  |  |  | 0.19 |
| **69** | *cis*-Muurola-3,5-diene | X |  |  |  |  | 0.20 |  |  |  |  |  |  |  |
| **70** | *cis*-Sabinene hydrate | XXIV |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **71** | *cis*-Thujone | XXIV |  |  |  | 7.30 |  |  | 18.83 |  |  |  |  |  |
| **72** | Cubenol | X |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **73** | Cyclohexene, 3-acetoxy-4-(1-hydroxy-1-methylethyl) -1-methyl- | XXIII |  |  |  |  |  |  |  |  |  | 0.47 |  |  |
| **74** | Cyclosativene | IV |  |  |  |  |  |  |  |  |  |  |  | 0.11 |
| **75** | Dehydroabietan | XXVIII |  |  |  |  |  |  |  |  |  | 0.56 |  |  |
| **76** | Elemol | XIV |  |  | 0.70 |  |  |  |  |  |  |  |  | 1.16 |
| **77** | *ent*-Pimara-8,15-diene | XXVI |  |  |  |  |  |  | 0.13 |  |  |  |  |  |
| **78** | *epi*-13-Manoyl oxide | XXVI |  |  |  |  | 0.20 |  |  |  |  |  |  |  |
| **79** | *epi*-Manool | XXVII |  |  |  |  |  |  | 1.18 |  |  |  |  |  |
| **80** | *epi*-Zonarene | X |  |  |  |  | 0.80 |  |  |  |  |  |  |  |
| **81** | Farnesyl acetone | XV |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **82** | Fenchone | XXII |  |  |  |  |  |  |  |  |  |  |  | 0.16 |
| **83** | Geranyl acetate | XXV |  |  |  |  |  |  |  |  |  |  | 7.20 |  |
| **84** | Germacrene A | XI |  |  | 1.20 |  |  |  |  |  |  |  |  |  |
| **85** | Germacrene B | XI |  |  | 0.40 |  | 0.20 |  |  |  |  |  |  | 0.27 |
| **86** | Hexahydrofarnesyl acetone | XV |  |  |  | 3.50 | 0.10 |  |  |  |  |  |  |  |
| **87** | Humulene epoxide II | V |  |  |  | 2.30 | 0.70 |  |  |  |  |  |  |  |
| **88** | Isophytol | XXV |  |  |  |  |  |  |  |  |  | 1.64 |  |  |
| **89** | Limonene | XXIII |  |  | 0.90 |  |  | 0.20 | 1.43 | 3.20 | 17.30 |  |  |  |
| **90** | Linalool | XIX |  |  |  |  | 0.10 | 0.40 | 0.39 |  |  | 0.65 | 38.00 | 0.48 |
| **91** | Linalyl acetate | XIX |  |  |  |  |  |  |  |  |  |  | 3.60 |  |
| **92** | Longibornene | II |  |  |  |  |  |  | 0.04 |  |  |  |  |  |
| **93** | Manool | XXVII |  |  |  | 14.60 |  |  |  |  |  |  |  |  |
| **94** | Mintsulfide | XI |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **95** | Myrtenol | XXI |  |  |  |  |  |  | 0.30 |  |  |  |  |  |
| **96** | Naphtalene | XXIX |  |  |  |  |  |  | 0.20 |  |  |  |  |  |
| **97** | Neointermedol | VIII |  |  |  |  | 1.60 |  |  |  |  |  |  |  |
| **98** | *o*-Xylene | XXIX |  |  |  |  |  |  |  |  |  | 0.26 |  |  |
| **99** | *p*-Cymene | XXIII |  |  |  |  | 0.10 | 0.10 |  |  |  |  |  |  |
| **100** | Phytol | XXV |  |  |  | 1.20 |  |  |  |  |  | 1.57 |  |  |
| **101** | Pinocarvone | XXI |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **102** | *p*-Mentha-1(7),8-diene | XXIII |  |  |  |  | 0.20 |  |  |  |  |  |  |  |
| **103** | Sabinene | XXIV |  |  |  |  |  |  | 0.30 |  |  |  |  |  |
| **104** | Selina-3,7(11)-diene | VIII |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **105** | Sinularene | VII |  |  |  |  |  |  | 0.17 |  |  |  |  |  |
| **106** | Spathulenol | IX |  |  | 2.40 | 4.00 |  |  |  | 0.70 | 0.30 |  |  | 0.21 |
| **107** | Terpinolene | XXIII |  |  |  |  | 0.20 |  | 0.52 |  |  | 0.10 |  |  |
| **108** | Thujyl alcohol | XXIV |  |  |  |  |  |  | 0.17 |  |  |  |  |  |
| **109** | τ-Muurolol | X |  |  |  |  |  |  | 0.09 |  |  |  |  |  |
| **110** | *trans*-Calamenen-10-ol | X |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **111** | *trans*-Muurola-4(14),5-diene | X |  |  |  |  | 9.00 |  |  |  |  |  |  |  |
| **112** | *trans*-Pinocarveol | XXI |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **113** | *trans*-Thujone | XXIV |  |  |  | 1.70 |  |  | 4.46 |  |  |  |  |  |
| **114** | Valencenne | III |  |  |  |  |  |  | 0.05 |  |  |  |  |  |
| **115** | Valerianol | VIII |  |  |  |  |  |  |  | 3.10 | 0.10 |  |  |  |
| **116** | Ylangene | VI |  |  |  |  | 0.20 |  |  |  |  |  |  | 0.24 |
| **117** | Zonarene | X |  |  |  |  | 3.80 |  |  |  |  |  |  |  |
| **118** | *α*-Amorphene | X |  |  |  |  |  |  | 0.30 |  |  |  |  |  |
| **119** | *α*-Bisabolol | IV |  |  |  |  |  |  |  | 0.20 | 0.50 |  |  |  |
| **120** | *α*-Bourbonene | XVII |  |  |  |  |  |  | 0.12 |  |  |  |  |  |
| **121** | *α*-Cadinene | X |  |  |  |  | 0.20 |  |  |  |  |  |  |  |
| **122** | *α*-Cadinol | X |  |  | 1.50 |  | 1.40 |  |  |  |  |  |  | 5.08 |
| **123** | *α*-Calacorene | X |  |  |  |  | 0.50 |  | 0.23 |  |  |  |  | 2.75 |
| **124** | *α*-Cubebene | XII |  |  |  |  | 0.50 |  |  |  |  |  |  | 3.76 |
| **125** | *α*-Eudesmol | VIII |  |  |  |  |  |  |  | 12.4 | 0.40 |  |  |  |
| **126** | *α*-Gurjenene | IX |  |  |  |  |  |  | 0.17 |  |  |  |  |  |
| **127** | *α*-Muurolene | X |  |  |  |  |  |  |  |  |  |  |  | 5.19 |
| **128** | *α*-Terpinene | XXIII |  |  |  |  | 0.10 |  | 0.30 |  |  |  |  |  |
| **129** | *α*-Terpineol | XXIII |  |  |  |  |  | 0.50 | 1.33 |  |  | 0.81 |  |  |
| **130** | *α*-Thujene | XXIV |  |  |  |  | 0.20 | 0.50 | 0.36 |  |  |  |  |  |
| **131** | *β*-(*E*)-Ionone | XXIX |  |  |  | 1.00 |  |  |  |  |  | 1.27 |  |  |
| **132** | *β*-Calacorene | X |  |  |  |  | 0.10 |  |  |  |  |  |  |  |
| **133** | *β*-Copaene | VI |  |  |  |  | 13.30 |  |  |  |  |  |  |  |
| **134** | *β*-Cyclocitral | XXIII |  |  |  |  | 0.30 |  |  |  |  |  |  |  |
| **135** | *β*-Elemene | XIV |  |  | 0.50 |  | 0.50 |  |  |  |  |  |  |  |
| **136** | *β*-Himachalene | II |  |  |  |  |  |  | 0.95 |  |  |  |  |  |
| **137** | *β*-Myrcene | XIX |  |  |  |  | 0.40 |  | 1.93 | 3.00 | 1.50 |  |  | 0.11 |
| **138** | *β*-Patchoulene | IX |  |  |  |  |  |  | 0.42 |  |  |  |  |  |
| **139** | *β*-Phellandrene | XXIII |  |  |  |  | 1.30 |  |  | 1.60 | 2.10 |  |  |  |
| **140** | *β*-Pinene | XXI |  |  | 1.10 |  | 26.4 |  | 0.85 |  |  |  |  |  |
| **141** | *γ*-Eudesmol | VIII |  |  |  |  |  |  |  |  |  |  |  | 14.04 |
| **142** | *γ*-Terpineol | XXIII |  |  |  |  | 0.20 |  |  |  |  |  |  |  |
| **143** | *γ*-Vanillin | XXIX |  |  |  |  |  |  |  |  |  | 0.35 |  |  |
| **144** | *δ*-3-Carene | XXIV |  |  |  |  |  | 1.20 | 6.50 |  |  |  |  |  |
| **145** | *δ*-Amorphene | X |  |  |  |  | 0.20 |  |  |  |  |  |  |  |
| **146** | τ-Cadinol | X |  |  |  |  |  |  |  | 7.60 | 2.20 |  |  | 10.21 |

A) *S. dugesii*, B) *S. gesneriflora*, C) *Salvia angulata*, D) *Salvia argentea*, E) *Salvia viridis*, F) *Salvia lavandulifolia*, G) *Salvia officinalis*, H) *Salvia africana-lutea*, I) *Salvia chamelaeagnea*, J) *Salvia miltiorrhiza*, K) *Salvia sclarea* and L) *Salvlia plebeia*

# **Table S2.** Chemical composition of essential oils of the twelve analyzed *Salvia* plants, according to their structural skeleton

|  |  |
| --- | --- |
|  | Composition (%) |
| StructuralSkeleton | A | B | C | D | E | F | G | H | I | J | K | L |
| I | 8.3 | 1.2 | 1.5 |  |  |  | 0.5 |  |  | 0.7 |  |  |
| II |  |  |  |  |  |  | 1.0 |  |  |  |  |  |
| III |  | 6.3 |  |  |  |  |  |  |  |  |  |  |
| IV | 1.5 |  |  |  |  |  |  | 0.2 | 0.5 |  |  |  |
| V | 10.0 | 15.7 | 27.7 | 10.7 | 3.6 | 1.1 | 3.3 | 3.6 | 0.4 | 8.3 | 14.0 | 15.4 |
| VI | 1.7 | 3.7 | 0.1 |  | 13.3 |  |  |  |  |  |  | 5.7 |
| VII |  |  |  |  |  |  | 0.2 |  |  |  |  |  |
| VIII | 1.0 | 3.7 |  | 0.7 | 1.6 |  |  | 12.4 | 0.4 |  |  | 14.0 |
| IX | 7.6 | 4.7 | 2.4 | 32.4 | 0.3 |  | 8.0 | 2.2 | 33.0 |  |  | 5.1 |
| X |  |  |  |  | 9.0 |  |  | 7.6 | 2.2 |  |  | 10.2 |
| XI | 5.0 | 7.6 | 19.5 |  | 7.9 | 5.4 | 0.2 | 0.9 |  | 4.4 |  | 0.3 |
| XII | 0.8 | 3.6 |  |  | 0.5 |  |  |  |  |  |  | 2.9 |
| XIII |  |  |  |  |  |  |  |  |  |  |  |  |
| XIV |  | 7.5 | 0.7 |  | 0.5 |  |  |  |  |  |  | 1.2 |
| XV | 1.5 |  | 1.2 | 3.5 | 0.2 |  |  |  |  |  |  |  |
| XVI | 2.2 |  |  |  |  |  |  |  |  |  |  |  |
| XVII | 1.6 | 1.0 | 5.6 |  | 2.9 |  | 0.3 |  |  |  |  |  |
| XVIII |  |  |  |  |  |  |  |  |  | 2.7 |  |  |
| XIX |  |  |  |  | 0.4 | 0.4 | 1.9 | 3.0 | 1.5 | 0.7 | 38.0 | 0.5 |
| XX |  |  |  |  | 0.2 | 3.0 | 0.8 |  |  | 1.6 |  |  |
| XXI |  | 1.5 | 0.5 | 0.5 | 26.4 | 6.8 | 0.9 | 3.1 | 42.0 |  |  |  |
| XXII | 3.4 | 5.8 |  | 0.9 |  | 7.6 | 25.1 |  |  | 1.1 |  | 0.6 |
| XXIII | 1.1 | 1.0 | 0.9 | 3.1 | 1.3 | 40.1 | 14.1 | 10.1 | 17.3 | 0.8 | 1.2 | 0.2 |
| XXIV |  |  |  | 7.3 | 0.2 | 0.5 | 18.8 | 1.2 | 6.5 |  |  |  |
| XXV |  | 5.5 |  | 1.2 |  |  |  |  |  | 1.6 | 7.2 |  |
| XXVI | 4.9 |  |  |  | 0.2 |  | 0.1 |  |  |  |  |  |
| XXVII | 0.8 |  |  | 14.6 |  |  | 1.2 |  |  |  |  |  |
| XXVIII |  |  |  |  |  |  |  |  |  | 0.6 |  |  |
| XXVIX |  | 2.1 |  | 1 |  |  | 0.3 |  |  | 2.0 |  | 0.8 |