

Figure S1. Length distribution of contigs and unigenes in the *Lavandula pubescens* transcriptome.

| | | |
|---|------|--|
| A | 17 | RNA processing and modification |
| B | 38 | Chromatin Structure and dynamics |
| C | 874 | Energy production and conversion |
| D | 192 | Cell cycle control, cell division, chromosome partitioning |
| E | 968 | Amino acid transport and metabolism |
| F | 371 | Nucleotide transport and metabolism |
| G | 1590 | Carbohydrate transport and metabolism |
| H | 616 | Coenzyme transport and metabolism |
| I | 852 | Lipid transport and metabolism |
| J | 1799 | Translation, ribosomal structure and biogenesis |
| K | 795 | Transcription |
| L | 601 | Replication, recombination and repair |
| M | 725 | Cell wall/membrane/envelope biogenesis |
| N | 90 | Cell motility |
| O | 1464 | Post-translational modification, protein turnover, chaperones |
| P | 621 | Inorganic ion transport and metabolism |
| Q | 593 | Secondary metabolite biosynthesis, transport and catabolism |
| R | 1441 | General functional prediction only |
| S | 339 | Function unknown |
| T | 1330 | Signal transduction mechanisms |
| U | 96 | Intracellular trafficking, secretion, and vesicular transport |
| V | 272 | Defense mechanisms |
| W | 3 | Extracellular structures |
| X | 129 | Phage-derived proteins, transposases and other mobilome components |
| Y | 0 | Nuclear structure |
| Z | 22 | Cytoskeleton |

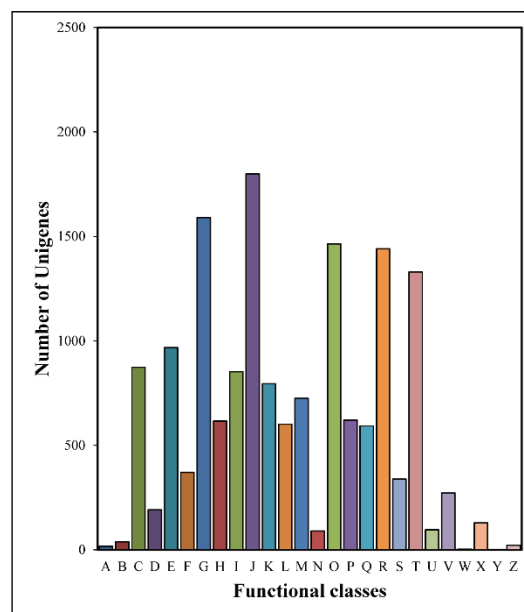


Figure S2. COG functional classification of the *Lavandula pubescens* unigenes.

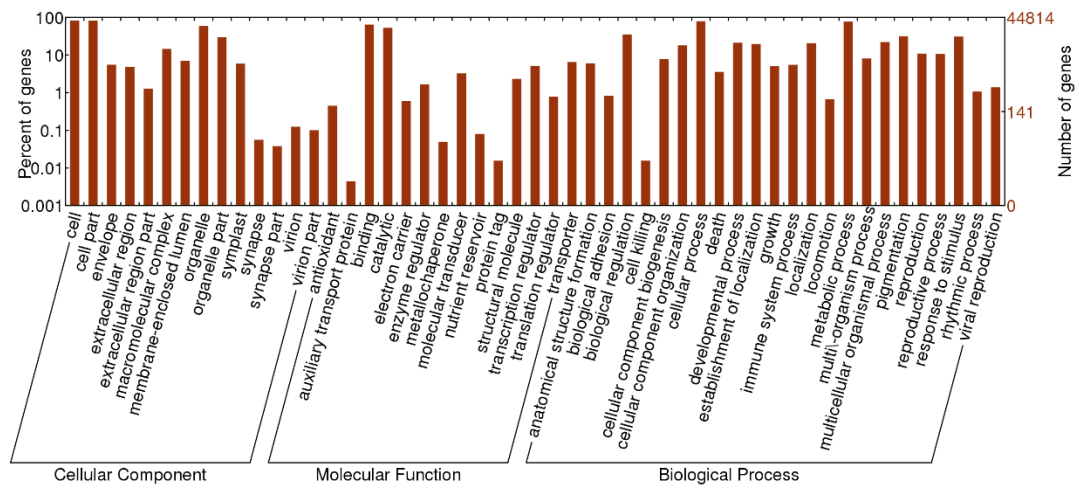


Figure S3. GO annotation of the *Lavandula pubescens* unigenes.

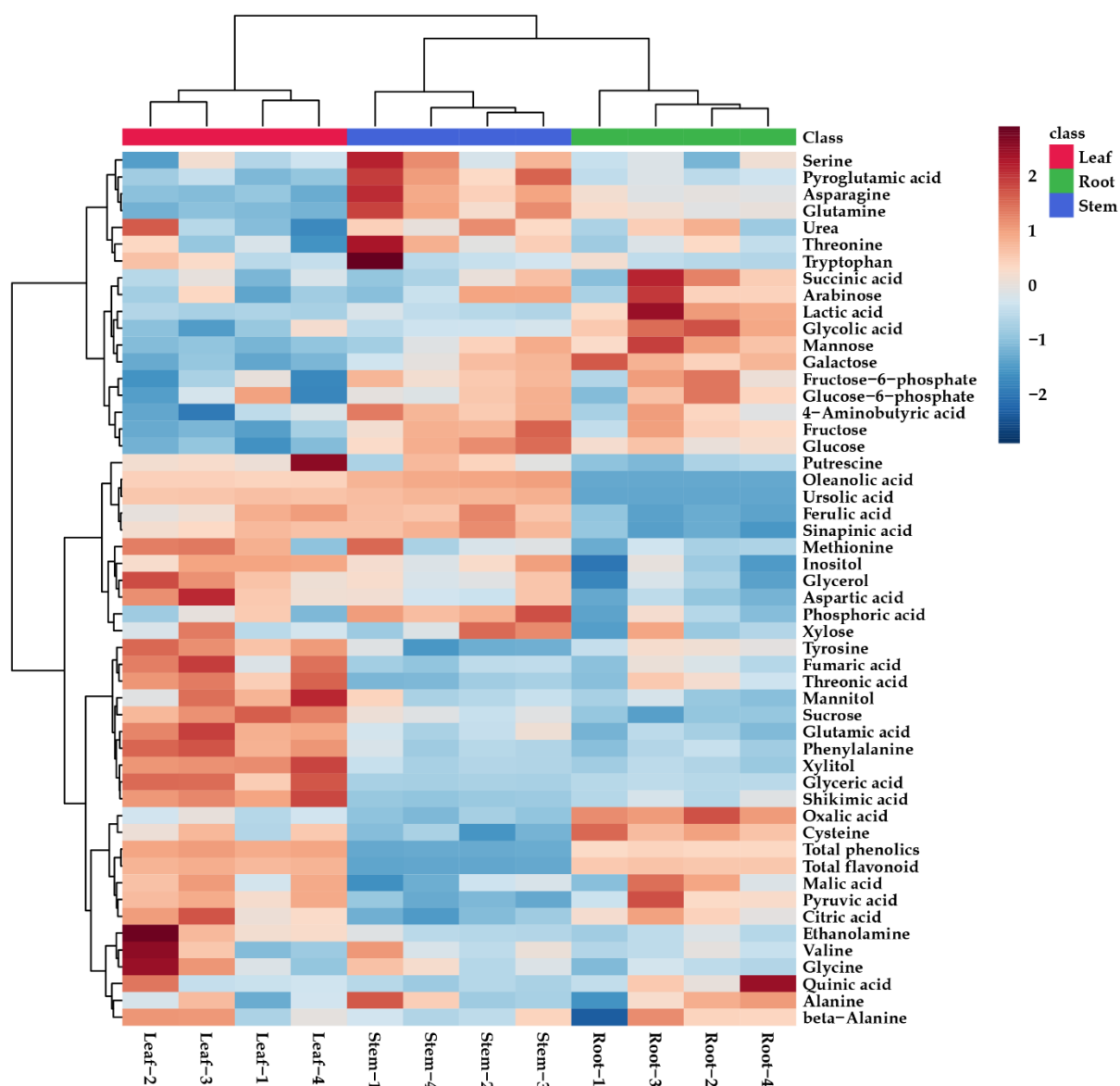


Figure S4. Heatmap representing differences in relative metabolite concentrations of roots, leaves, and stems of *Lavandula pubescens*. Increasing and decreasing the contents of metabolites are shown by red and blue color, respectively.

Table S1. Summary of unigenes in the *Lavandula pubescens*

| | Raw reads | Contigs | Unigenes |
|---------------------------------|---------------|------------|------------|
| Total length (bp ¹) | 9,476,122,928 | 86,598,482 | 58,431,429 |
| Number of sequences | 124,685,828 | 180,249 | 124,233 |
| Average length (bp) | 76 | 480 | 470 |
| Median length (bp) | 76 | 322 | 319 |
| Maximum length (bp) | 76 | 11,308 | 11,308 |
| Minimum length (bp) | 76 | 224 | 224 |
| N50 (bp) | 76 | 545 | 522 |

¹bp, basepair

Table S2. Summary of the annotation of *Lavandula pubescens* unigenes

| | Number of BLASTed unigenes | Ratio (%) |
|-------------------------------------|----------------------------|-----------|
| All unigenes | 124,233 | 100 |
| Unigenes BLASTed against Nr | 64,993 | 52.32 |
| Unigenes BLASTed against Nt | 20,947 | 16.86 |
| Unigenes BLASTed against SWISS-PROT | 45,750 | 36.83 |
| Unigenes BLASTed against BRAD | 57,951 | 46.65 |
| Unigenes BLASTed against TAIR | 56,604 | 45.56 |
| Unigenes BLASTed against COG | 16,019 | 12.89 |
| Unigenes BLASTed against GO | 44,814 | 36.07 |
| All annotated unigenes | 68,695 | 55.30 |

Table S3. Comparison of terpene biosynthetic genes of *Lavandula pubescens* with orthologous genes and proteins showing the highest identity

| Genes | Orthologous genes (Accession no.) | Identity (%) | Orthologous proteins (Accession no.) | Identity (%) |
|---------|---|-----------------|--|-----------------|
| LpDXS2 | <i>Lavandula angustifolia</i> (JX630150.1) | 86 | <i>Lavandula angustifolia</i> (AGQ04154.1) | 87 |
| | <i>Isodon rubescens</i> (KT831764.1) | 81 | <i>Isodon rubescens</i> (AMM72794.1) | 85 |
| | <i>Prunella vulgaris</i> (MK272806.1) | 82 | <i>Plectranthus barbatus</i> (ALE19960.1) | 85 |
| LpMCT | <i>Isodon rubescens</i> (MK192294.1) | 93 | <i>Isodon rubescens</i> (QCZ24926.1) | 96 |
| | <i>Prunella vulgaris</i> (MK272812.1) | 87 | <i>Salvia miltiorrhiza</i> (AEZ55666.1) | 92 |
| | <i>Pogostemon cablin</i> (KF926080.1) | 86 | <i>Prunella vulgaris</i> (QEV81819.1) | 91 |
| LpMCS | <i>Isodon rubescens</i> (KT948057.1) | 92 | <i>Salvia miltiorrhiza</i> (AFQ95411.1) | 83 |
| | <i>Prunella vulgaris</i> (MK272815.1) | 89 | <i>Isodon rubescens</i> (AMW77341.1) | 81 |
| | <i>Plectranthus barbatus</i> (KF749265.1) | 88 | <i>Phlomis umbrosa</i> (QEN91944.1) | 76 |
| LpHDR | <i>Lavandula angustifolia</i> (JX630153.1) | 90 | <i>Lavandula angustifolia</i> (AGQ04157.1) | 94 |
| | <i>Isodon rubescens</i> (KT948058.1) | 88 | <i>Isodon rubescens</i> (AMW77342.1) | 89 |
| | <i>Salvia miltiorrhiza</i> (JX233817.1) | 84 | <i>Salvia miltiorrhiza</i> (AEZ55670.1) | 84 |
| LpIDI | <i>Isodon rubescens</i> (KT948056.1) | 88 | <i>Salvia miltiorrhiza</i> (ABV08818.1) | 94 |
| | <i>Salvia miltiorrhiza</i> (EF635967.1) | 87 | <i>Prunella vulgaris</i> (QEV81828.1) | 91 |
| | <i>Prunella vulgaris</i> (MK272820.1) | 87 | <i>Scutellaria barbata</i> (QEY10174.1) | 81 |
| LpAACT | <i>Isodon rubescens</i> (KR154220.1) | 92 | <i>Isodon rubescens</i> (ALG00700.1) | 93 |
| | <i>Prunella vulgaris</i> (MK272796.1) | 89 | <i>Prunella vulgaris</i> (QEV81803.1) | 91 |
| | <i>Scutellaria barbata</i> (MK035028.1) | 85 | <i>Sesamum indicum</i> (XP_011095902.1) | 88 |
| LpHMGS | <i>Lavandula angustifolia</i> (JX630154.1) | 92 | <i>Lavandula angustifolia</i> (AGQ04158.1) | 98 |
| | <i>Isodon rubescens</i> (KX151718.1) | 90 | <i>Isodon rubescens</i> (ANW07497.1) | 97 |
| | <i>Salvia miltiorrhiza</i> (FJ785326.1) | 87 | <i>Salvia miltiorrhiza</i> (ACV65039.1) | 92 |
| LpHMGR | <i>Lavandula angustifolia</i> (JX630155.1) | 86 | <i>Lavandula angustifolia</i> (AGQ04159.1) | 93 |
| | <i>Salvia miltiorrhiza</i> (JN831102.1) | 82 | <i>Prunella vulgaris</i> (QEV81808.1) | 86 |
| | <i>Osmanthus fragrans</i> (KY451762.1) | 79 | <i>Sesamum indicum</i> (XP_011095902.1) | 84 |
| LpMVK | PREDICTED: <i>Ananas comosus</i> transcript X1 (XM_020245820.1) | 73 | <i>Salvia miltiorrhiza</i> (AEZ55674.1) | 92 |
| | PREDICTED: <i>Ananas comosus</i> transcript X2 (XM_020245821.1) | 73 | <i>Prunella vulgaris</i> (QEV81809.1) | 91 |
| | PREDICTED: <i>Ananas comosus</i> transcript X3 (XM_020245822.1) | 73 | <i>Picrorhiza kurroa</i> (AGS18028.1) | 86 |
| LpPMK | <i>Scutellaria barbata</i> (MK035034.1) | 85 | <i>Salvia miltiorrhiza</i> (AEZ55665.1) | 86 |
| | <i>Prunella vulgaris</i> (MK272803.1) | 85 | <i>Scutellaria barbata</i> (QEY10159.1) | 82 |
| | <i>Osmanthus fragrans</i> (KY451764.1) | 77 | <i>Sesamum indicum</i> (XP_011074642.1) | 81 |
| LpMVD | <i>Isodon rubescens</i> (MK344321.1) | 93 | <i>Isodon rubescens</i> (QDQ03532.1) | 96 |
| | <i>Prunella vulgaris</i> (MK272804.1) | 91 | <i>Phlomis umbrosa</i> (APU50937.1) | 94 |
| | <i>Phlomis umbrosa</i> (KU317504.1) | 90 | <i>Scutellaria barbata</i> (QEY10160.1) | 94 |
| LpGPPS | <i>Salvia officinalis</i> (KY399788.1) | 84 | <i>Salvia officinalis</i> (KY399788.1) | 89 |
| | <i>Salvia miltiorrhiza</i> (JX090100.1) | 83 | <i>Pogostemon cablin</i> (AHK06506.1) | 89 |
| | <i>Lavandula x intermedia</i> (MN641908.1) | 82 | <i>Handroanthus impetiginosus</i> (PIN08988.1) | 87 |
| LpSQS | <i>Prunella vulgaris</i> (MK272831.1) | 89 | <i>Prunella vulgaris</i> (QEV81838.1) | 91 |
| | <i>Osmanthus fragrans</i> (KY992860.1) | 84 | <i>Sesamum indicum</i> (XP_011092839.1) | 92 |
| | <i>Camellia oleifera</i> (JX914592.1) | 83 | <i>Phtheirospermum japonicum</i> (GFP85929.1) | 88 |
| LpGGPPS | <i>Plectranthus barbatus</i> (KP889114.1) | 83 | <i>Salvia miltiorrhiza</i> (ACR19637.1) | 86 |
| | <i>Salvia sclarea</i> (MK442922.1) | 82 | <i>Plectranthus barbatus</i> (ALE19959.1) | 89 |
| | <i>Lavandula x intermedia</i> (MN064858.1) | 85 | <i>Salvia sclarea</i> (QEH04692.1) | 86 |
| LpActin | <i>Lavandula angustifolia</i> (KY596032.1) | 90 | <i>Prunella vulgaris</i> (AHY94895.1) | 99 |
| | <i>Prunella vulgaris</i> (KJ010818.1) | 90 | <i>Striga asiatica</i> (AAC49652.1) | 99 |

Table S4. Primers designed based on terpene biosynthetic gene sequences

| Genes | Sequence of forward primer (5'–3') | Sequence of reverse primer (5'–3') | Amplicon length (bp ¹) |
|----------------|---------------------------------------|---------------------------------------|--|
| <i>LpDXS</i> | AGAGAGGGTGGCTCTACTGG | CCACCAACTGACCCTTCCTC | 195 |
| <i>LpMCT</i> | AATTTGCATTGCCCCGGAAG | CCTAGTACAGCTGCACCGAC | 172 |
| <i>LpMCS</i> | TCGACCTTCATCGACTCGAAC | TCGGTGTCTGGAAAGATCTGC | 175 |
| <i>LpHDR</i> | ATCCTAGTTGTTGGCGGATGG | TGTCTCCACCAACTCACCATG | 159 |
| <i>LpIDI</i> | CAAACACCTGCTGCAGTCATC | TGTAGAGCATACGCCCCAAAG | 165 |
| <i>LpAACT</i> | GGTGTTTGTGCAGAGCTGTG | TGGCTTTCCTTGCTACCAG | 162 |
| <i>LpHMGS</i> | TGACCCGAAGCAGATTGGAC | AATAGTGCTGCAGTCCCACC | 165 |
| <i>LpHMGR</i> | CACAGTTGGAGGTGGGACTC | GCCGACATCAGAGAGAGCTC | 159 |
| <i>LpMVK</i> | GCAGTGCCATGAATTCCGTC | TGGCTGACCCCCATTGATTG | 169 |
| <i>LpPMK</i> | AGCCAATTGGGATCATGAGAGG | ACGTTTCAAGGGCATTGAGG | 155 |
| <i>LpMVD</i> | TGCTTGAGAGAACTCCGCTC | AAAACGAGGCATGCCAAACC | 170 |
| <i>LpGPPS</i> | GGCGTTTCAGTTGATCGACG | TGCCGGATTATCGAAGCCTC | 172 |
| <i>LpSQS</i> | CGTGAAAATGAGACGCGGTC | ATGCACCAGAGTCTCTGCAG | 188 |
| <i>LpGGPPS</i> | GTCGAGAAGTTGCGGGTTTTTC | TTCTCCAATCCGAGCAGCTTC | 161 |
| <i>LpActin</i> | TGAGCCACACAGTCCCAATC | TCCCTCACAATTTCCCGCTC | 157 |

¹bp, basepair