The supporting information for

**Predicting the contents of polysaccharides and its monosugars in *Dendrobium huoshanense* by Partial Least Squares Regression Model Using attenuated total reflectance Fourier Transform Infra-red Spectroscopy**

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**S-Table 1**

The list of *Dendrobium huoshanense* samples

|  |  |  |
| --- | --- | --- |
| Samples | Collection place | Collection time |
| S1-S17 | Jinzhai Count, Anhui Province, China | January,2015-December,2015 |
| S18-S40 | Huoshan Count, Anhui Province, China | January,2015-December,2015 |
| S41-S52 | Yingshan Count, Anhui Province, China | January,2015-December,2015 |
| S53-S56 | Huoshan Count, Anhui Province, China | September,2015-December,2015 |
| S57-S60 | Huoshan Count, Anhui Province, China | September,2016-December,2017 |
| S61-S63 | Jinzhai Count, Anhui Province, China | October,2015-November,2015 |
| S64-S66 | Jinzhai Count, Anhui Province, China | October,2016-November,2016 |
| S67-S69 | Yingshan Count, Anhui Province, China | October,2015-December,2015 |
| S70-S72 | Yingshan Count, Anhui Province, China | October,2016-December,2016 |
| S73-S103 | Huoshan Count, Anhui Province, China | October,2018- November,2018 |
| S104-S132 | Jinzhai Count, Anhui Province, China | October,2018- November,2018 |

**S-Table 2**

The calibration curve, limit of detection (LOD), limit of quantification(LOQ) and precision (repeatability and reproducibility) of the monosaccharide standards detected by Gas Chromatography-Mass Spectrometry.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | Equation | Correalrion coefficient (r2) | Linea range (μg) | LOD(μg) | LOD(μg) | Reproducibility (%) | Repeatability (%) |
| Arabinose | *A*=0.607*C* | 0.985 | 0.5-1600 | 0.2 | 0.8 | 12 | 6 |
| Rhamnose | *A*=0.652*C* | 0.975 | 0.5-1600 | 0.2 | 0.5 | 9 | 11 |
| Xylose | *A*=0.547*C* | 0.989 | 0.5-600 | 0.1 | 0.5 | 7 | 6 |
| Mannose | *A*=0.811*C* | 0.993 | 2.5-1500 | 0.1 | 0.6 | 7 | 3 |
| Galactose | *A*=0.392*C* | 0.987 | 1.5-1500 | 0.3 | 0.7 | 7 | 5 |
| Glucose | *A*=0.913*C* | 0.998 | 1.0-1600 | 0.1 | 1.8 | 7 | 5 |
| Galacturonic acid | *A*=0.238*C* | 0.977 | 4.0-1300 | 0.1 | 5.0 | 9 | 7 |
| Fucose | *A*=0.566*C* | 0.969 | 0.5-550 | 0.4 | 1.2 | 12 | 9 |
| Inositol | *A*=0.954*C* | 0.993 | 1.0-1500 | 0.2 | 1.5 | 10 | 1 |

**S-Table 3**

The assignment of attenuated total reflectance Fourier transform infra-red spectroscopy signals relative to functional groups of polysaccharide

|  |  |  |
| --- | --- | --- |
| Absorption (cm–1) | Functional group | Structural characteristic |
| 3600-3200 | hydroxyl group (-OH) | stretching vibration of O-H |
| 3000-2800 | alkyl group (-CH2-) | stretching vibration of C-H |
| 1750-1600 | carboxyl group (-COOH), aldehyde group(-CHO) or esterfunction (-COOR) | stretching vibration of C=O |
| 1500-1400 | alkyl group (-CH2- or –CH3) | bending vibration of C-H |
| 1350-1290 | carboxyl group (-COOH) | symmetrical stretching vibration of C=O |
| 1280-1200 | carboxyl group (-COOH) | bending vibration of O-H |
| 1160-1070 | ether (-C-O-C-) | stretching vibration of C-O |
| 1060-970 | hydroxyl group (-OH) | bending vibration of O-H |
| 930-800 | D-glucopyranose ringα-type glycosidic linkageα-D-galactopyranose | antisymmetrical ring vibrationbending **v**ibration of C-H |



**S-Fig 1**. The representative attenuated total reflectance Fourier transform infra-red spectroscopy of the mannose and glucose samples.

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