SUPPLEMENTARY MATERIAL

Licochalcone L, an undescribed retrochalcone from *Glycyrrhiza inflata* roots

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ABSTRACT: *Glycyrrhiza inflata* Batalin is among the three glycyrrhizin producing *Glycyrrhiza* species and can be distinguished from other species with regard to its retrochalcone contents. Seven retrochalcones, echinatin and licochalcones A, C, D, E, K, and L were isolated and characterized from the chloroform extract of *G. inflata* roots. Among the isolates, licochalcone L was found to be previously undescribed. Structure elucidation of these specialized metabolites was achieved through NMR and mass spectroscopic data analyses.

Keywords: Licorice/liquorice, *Glycyrrhiza inflata*, licorice root, retrochalcone, licochalcone L, marker compounds

Contents

Table S1. ^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) data of licochalcone L recorded in acetone-d_6.

No.	δ_C, mult.	δ_H, mult. (*J* in Hz)
CO	187.3, C	-
α	118.4, CH	7.71, d (15.7)
β	138.4, CH	8.12, d (15.7)
1	116.6, C	-
2	160.1, C	-
3	93.9, CH	6.51, s
4	162.0, C	-
5	130.3, C	-
6	121.9, CH	7.73, s
1'	130.9, C	-
2', 6'	130.6, CH	8.02, d (8.8)
3', 5'	115.1, CH	6.95, d (8.8)
4'	161.4, C	-
1"	42.4, C	-
2"	94.0, CH	4.41, t (6.0)
3"	60.8, CH_2	3.86, m
4"	27.3, CH_3	1.43, s
5"	22.4, CH_3	1.24, s
OMe	55.4, CH_3	3.91, s

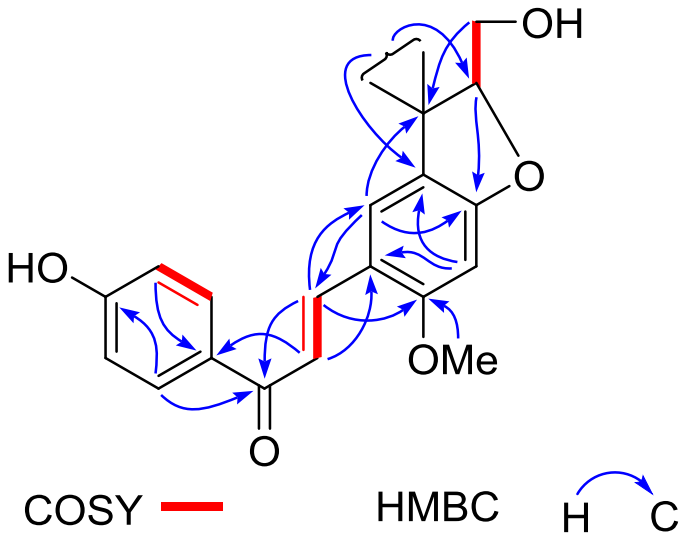

Figure S1. Key COSY and HMBC correlations for licochalcone L.

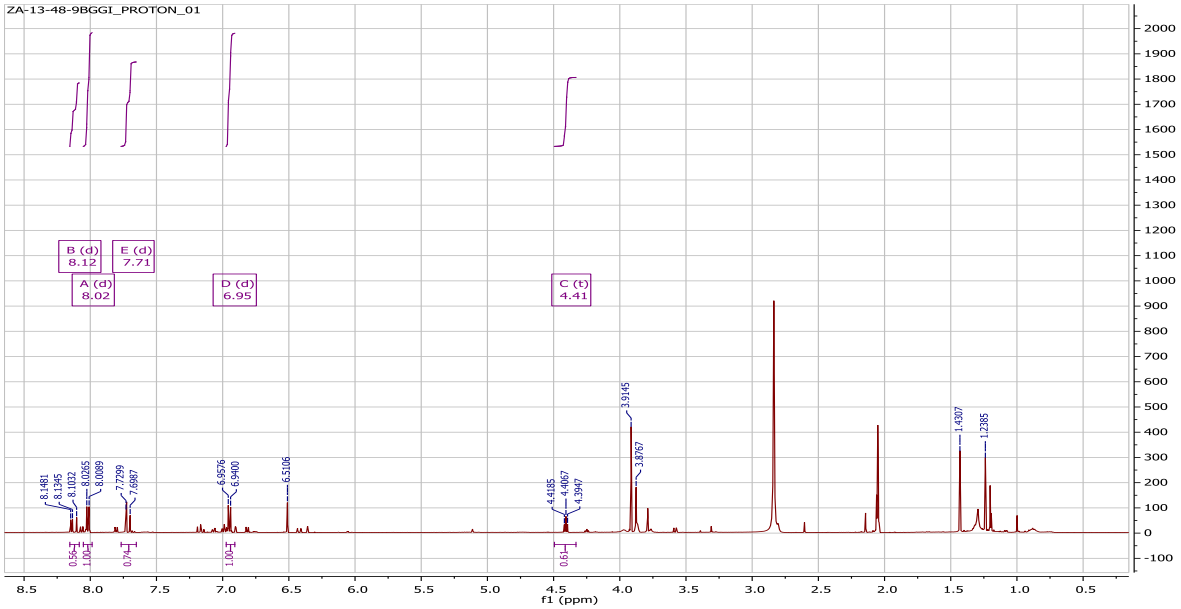

Figure S2. ^{1}H NMR spectrum of licochalcone L.

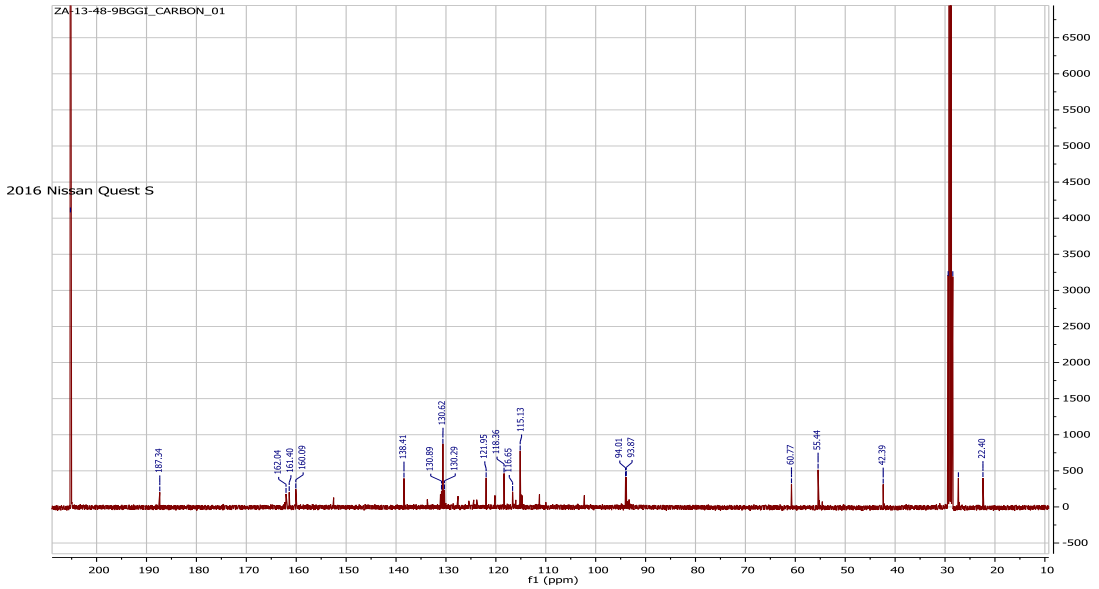

Figure S3. ^{13}C NMR spectrum of licochalcone L.

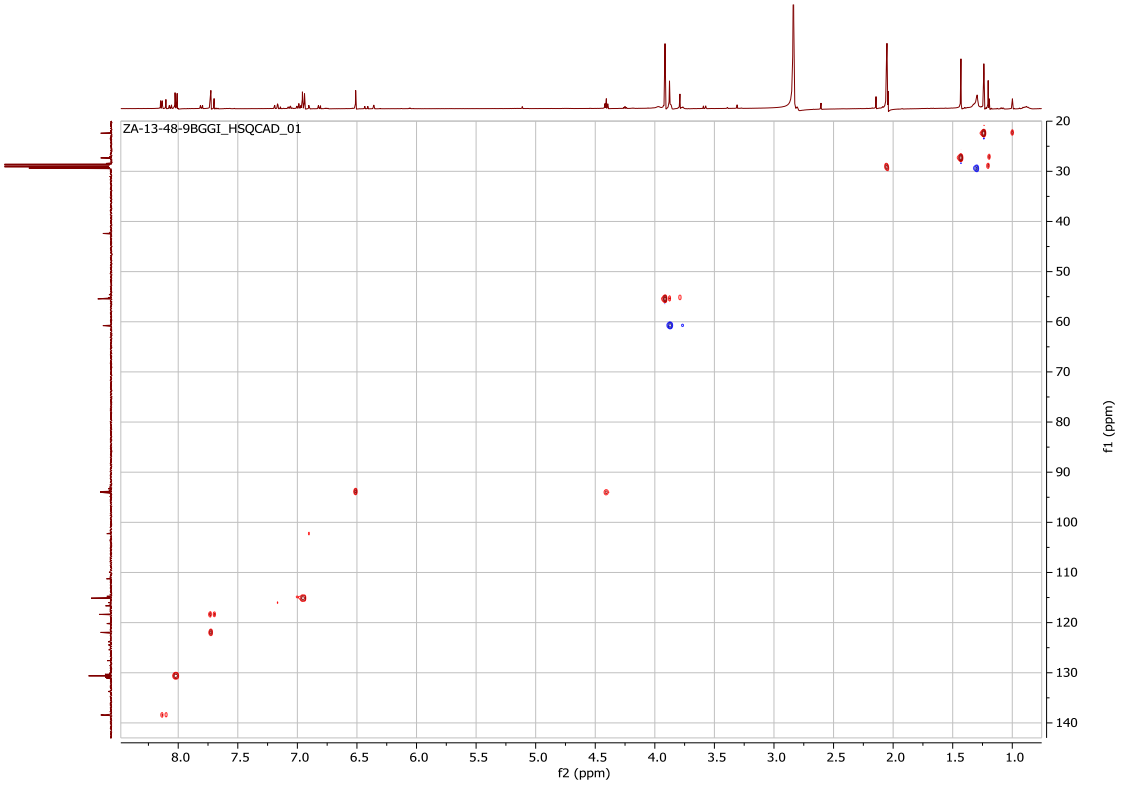

Figure S4. HSQC spectrum of licochalcone L.

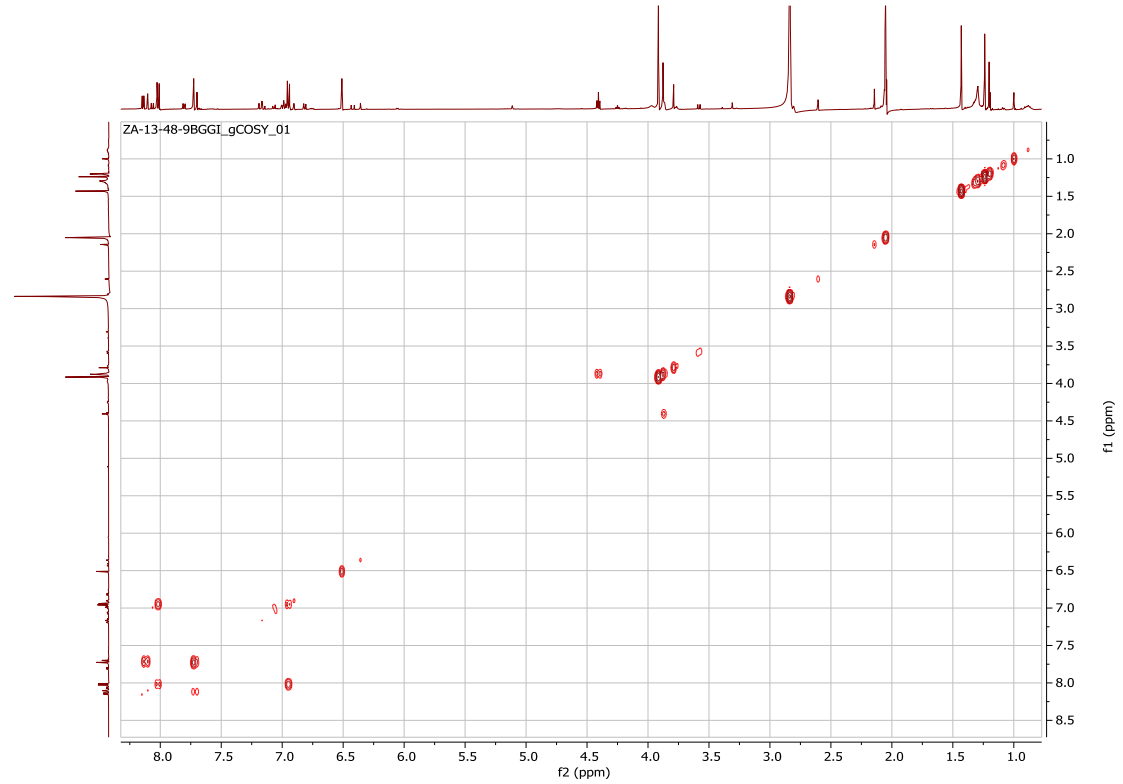

Figure S5. COSY spectrum of licochalcone L.

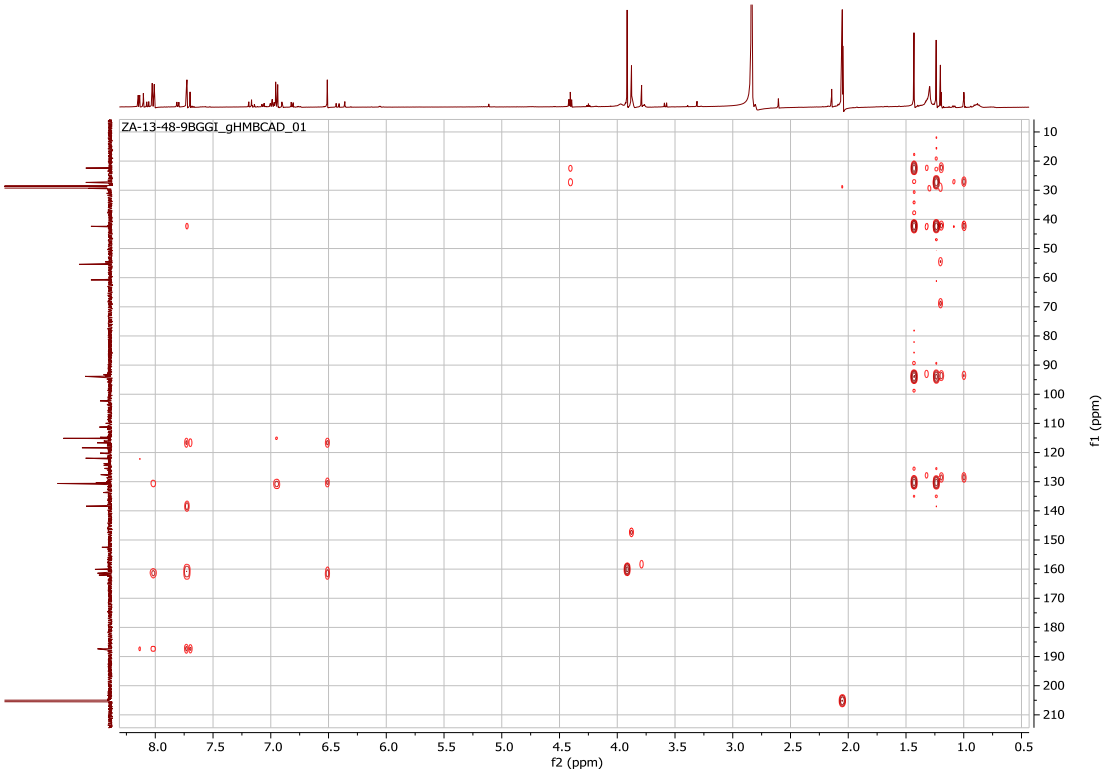

Figure S6. HMBC spectrum of licochalcone L.

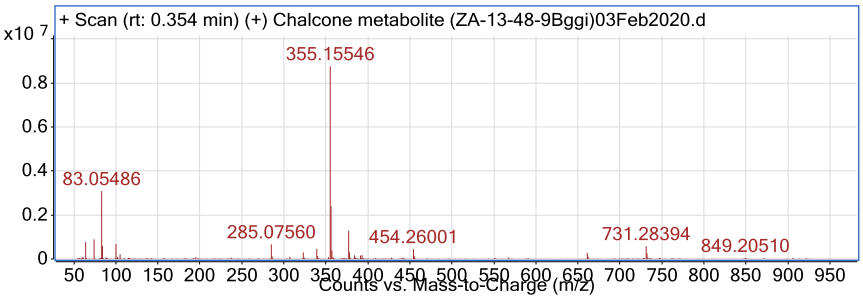

Figure S7. HRESIMS of licochalcone L.

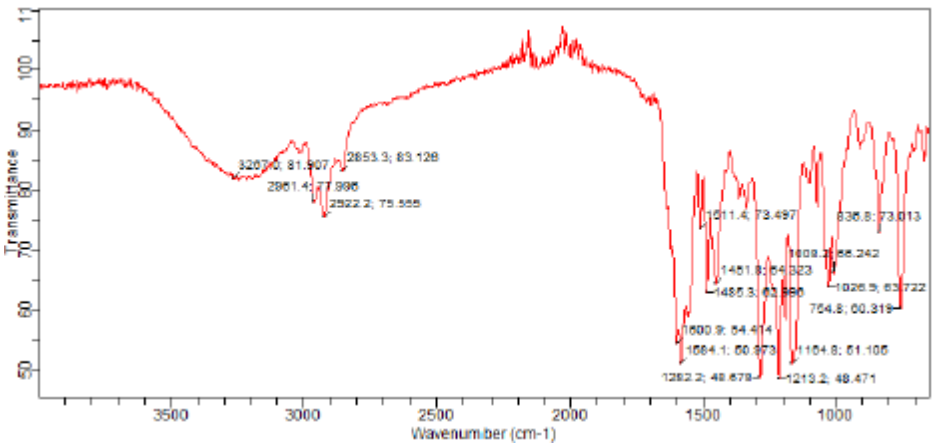

Figure S8. IR spectrum of licochalcone L.