SUPPLEMENTARY MATERIAL

A new isoflavone glycoside from *Pueraria alopecuroides*

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One new isoflavone glycoside, (-)-tuberosin-3-*O*-*β*-D-glucopyranoside (**1**), along with ten known compounds **1a**-**10**, were isolated from *Pueraria alopecuroides*. Their structures were determined on the basis of spectral data including 1D and 2D NMR and HREIMS. These compounds were isolated from this plant for the first time.

Keywords: *Pueraria alopecuroides*; isoflavone glycoside;

(-)-tuberosin-3-*O*-*β*-D-glucopyranoside

Table S1. [13]C and [1]H NMR chemical shift data (at 600 MHz in CD_3OD) of compounds **1**and **1a**.

	1			**1a**	
position	*δ*(H) (*J*, Hz)	*δ*(C)	**position**	*δ*(H) (*J*, Hz)	*δ*(C)
1	7.39 (*d*,*J*= 8.4)	133.34	**1**	7.38 (*d*,*J*=8.4)	133.42
1a		116.12	**1a**		113.06
2	6.80 (*dd*, *J* = 8.4, 2.4)	112.21	**2**	6.80(*dd*,*J*=11.4,2.4)	111.26
3		160.39	**3**		160.31
4	6.63 (*d*, *J* = 2.4)	105.91	**4**	6.63(*d*,*J*=2.4)	104.19
4a		157.33	**4a**		157.03
Ha-6	4.14(*d*,*J*=11.5)	70.89	Ha-6	4.13(*d*,*J*=9.6)	70.98
Hb-6	3.99(*d*,*J*=11.5)		Hb-6	3.99(*d*,*J*=9.6)	

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6a		77.80	6a		77.27
7	7.02 (*s*)	122.56	**7**	7.02(*s*)	123.42
8		116.95	**8**		116.85
9		157.33	**9**		157.50
10	6.18 (*s*)	100.27	**10**	6.18(*s*)	100.25
10a		161.86	**10a**		161.85
11a	5.23 (s)	86.01	**11a**		86.20
1′	6.35 (*d*, *J* = 9.8)	123.39	**1′**	6.34(*d*,*J*=9.6)	122.49
2′	5.54 (*d*, *J* = 9.8)	129.08	**2′**	5.54(*d*,*J*=9.6)	128.99
3′		77.82	**3′**		77.27
4′	1.37(*s*)	28.30	**4′**	1.38(*s*)	28.30
5′	1.35(*s*)	28.28	**5′**	1.36(*s*)	28.28
1"	4.89	102.10			
2"	3.38 (*m*)	74.96			
3"	3.37 (*m*)	78.29			
4"	3.45(*td*,*J*=9.5, 5.9)	71.41			
5"	4.17(*d*,*J*=9.5)	78.04			
6"	3.88 (*d*, *J* = 12.1),	62.54			
	3.69 (*d*, *J* = 12.1)				

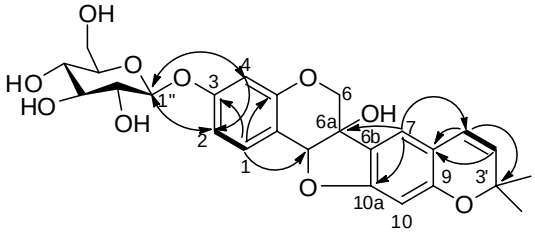
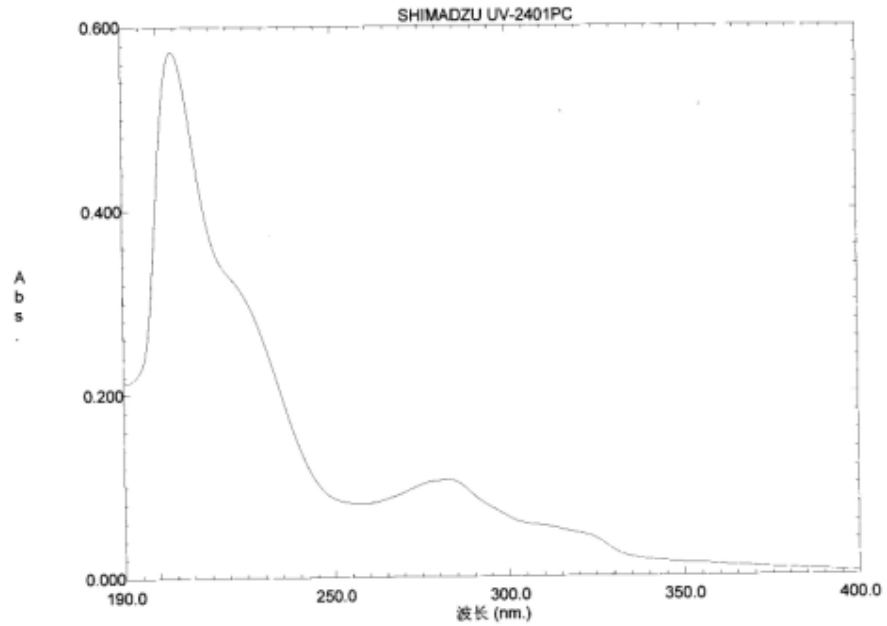


Figure S1. Key COSY (H—H), HMBCs(H→C) and ROESY(H↔H) of compound **1**

Original spectra of new isolated compound **1**



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创建于: 17:50 14-10-25
数据: 原始

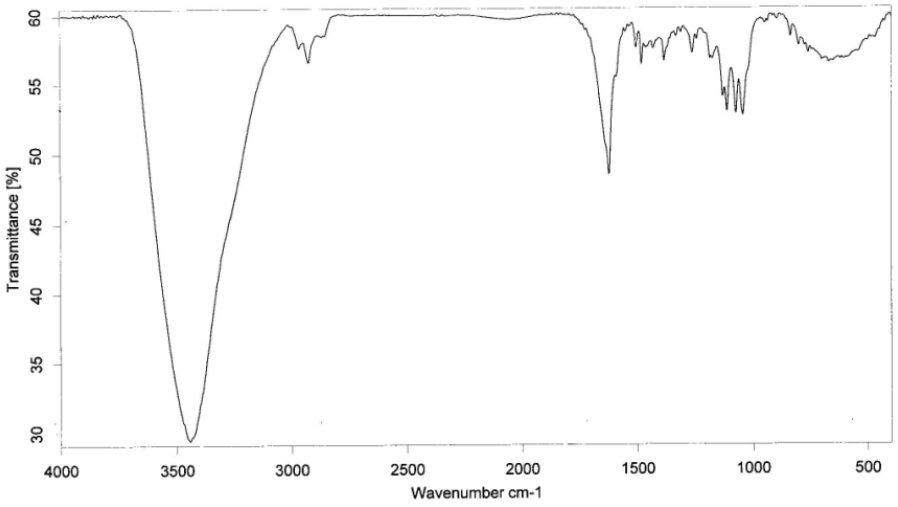
测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	282.60	0.1056
2	204.40	0.5736

SYJL-28

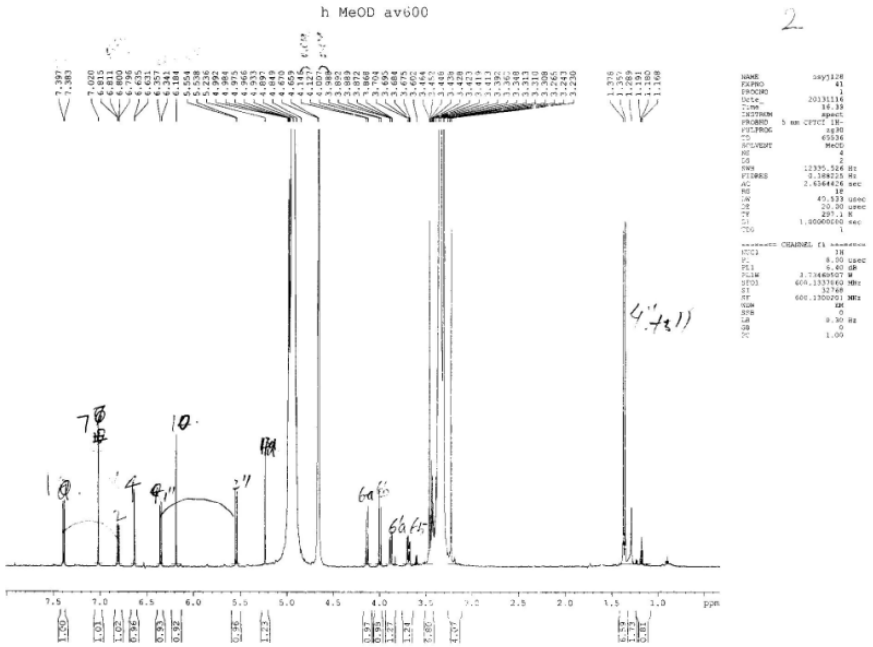
样品浓度：0.0031毫克/毫升
溶剂：甲醇

UV of compound **1**

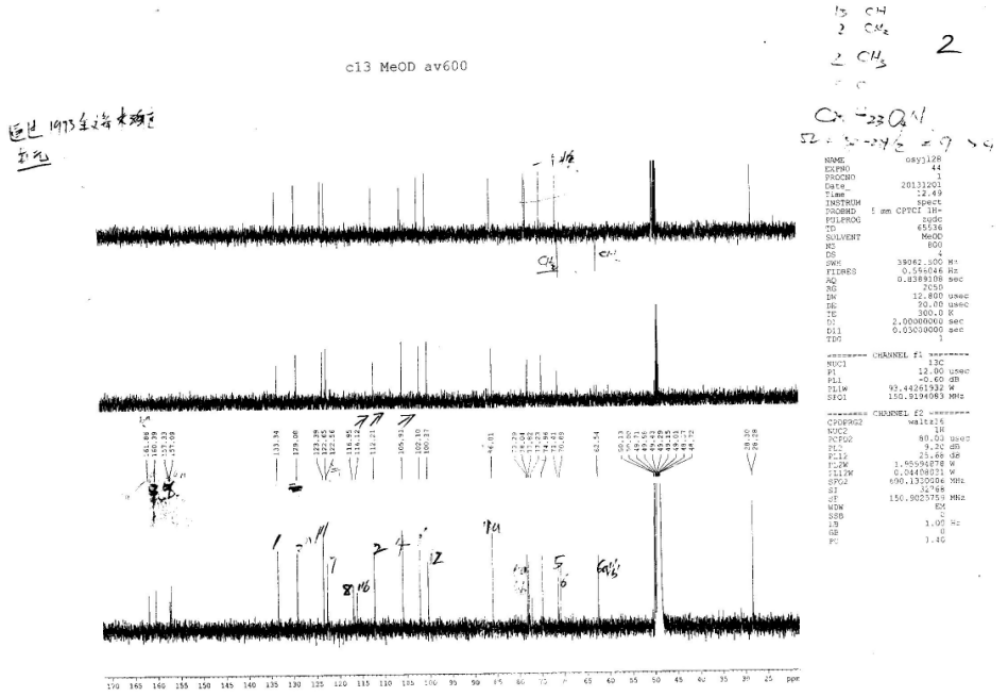


Sample : syjl-28	Frequency Range : 399.246 - 3996.32	Measured on : 24/11/2014	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 141124IR2	Zerofilling : 2	Acquisition : Double Sided,For	

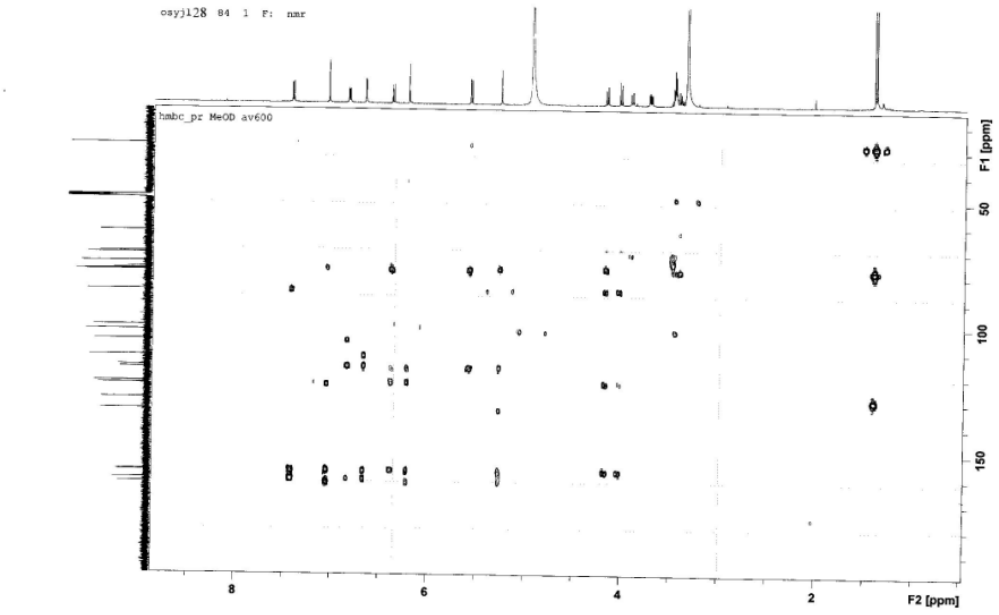
IR of compound **1**



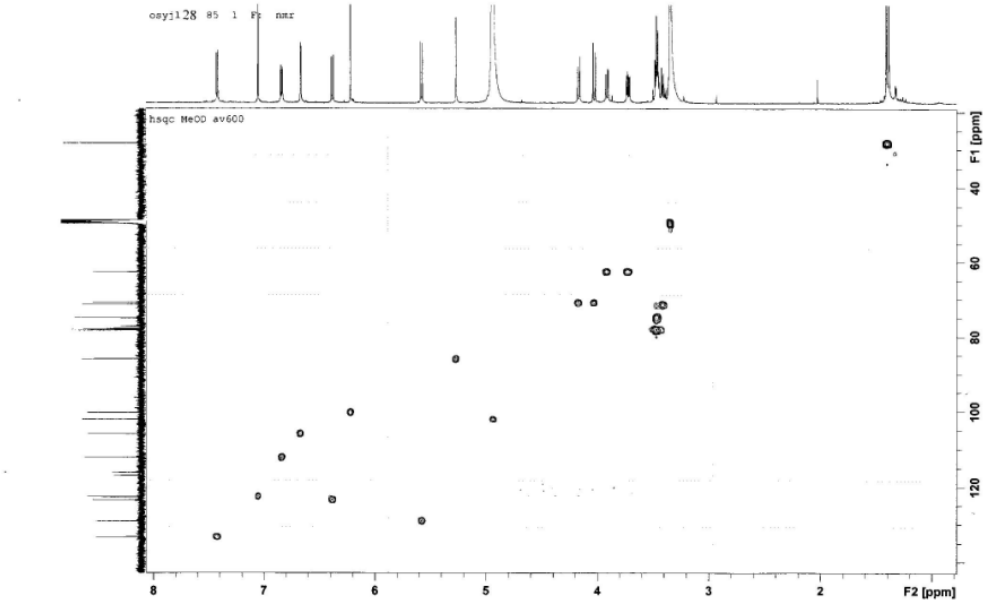
HNMR of compound **1**



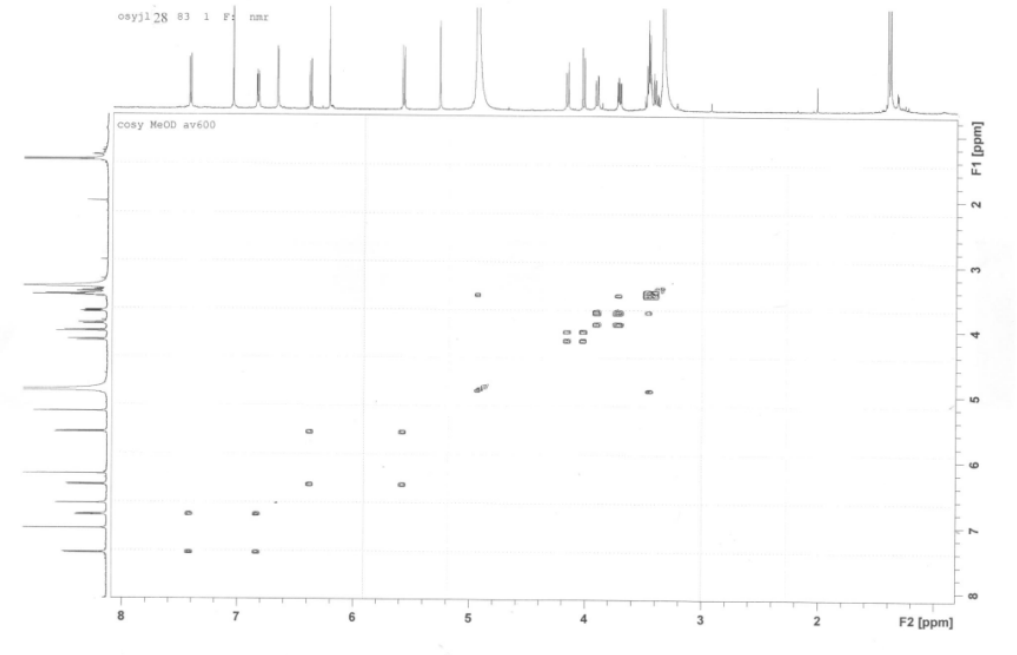
DEPT of compound **1**



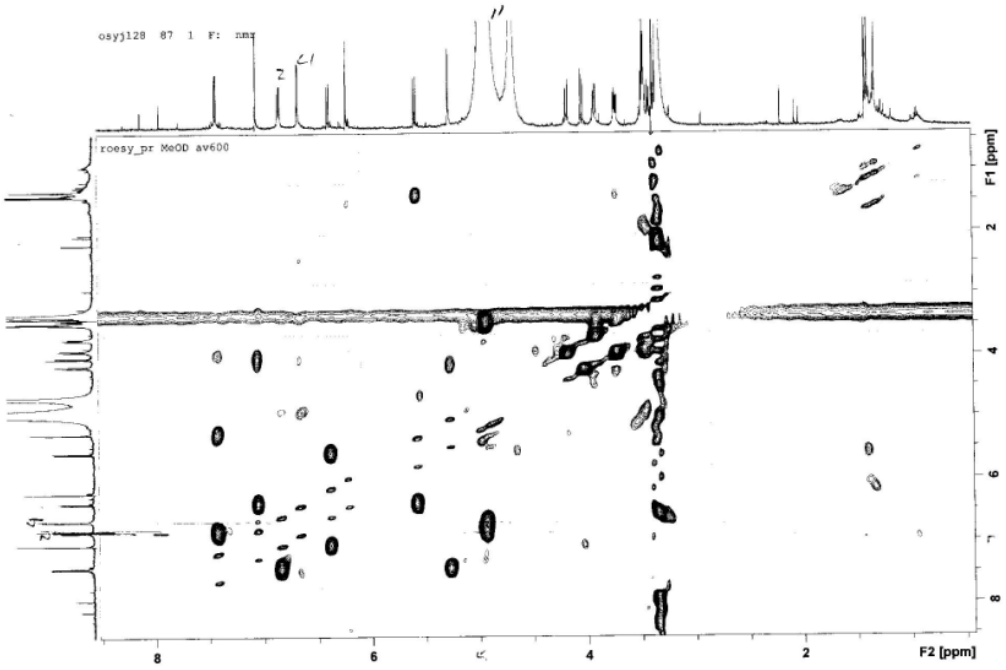
HMBC of compound **1**



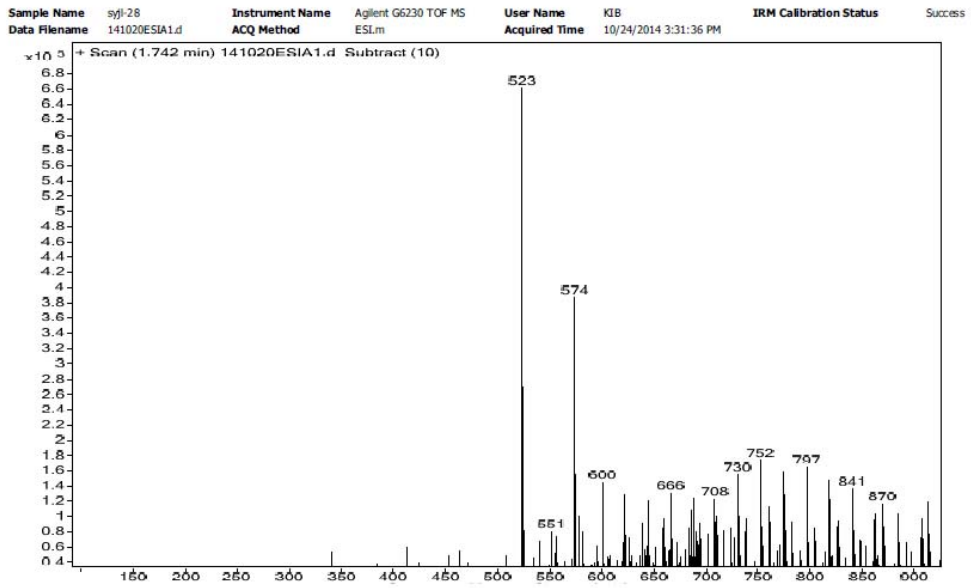
HSQC of compound **1**



COSY of compound **1**



ROESY of compound **1**



ESI of compound **1**

Qualitative Analysis Report

Data Filename	141020ESIA1.d	**Sample Name**	syjl-28
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	10/24/2014 3:31:36 PM
IRM Calibration Status	Success	**DA Method**	demo.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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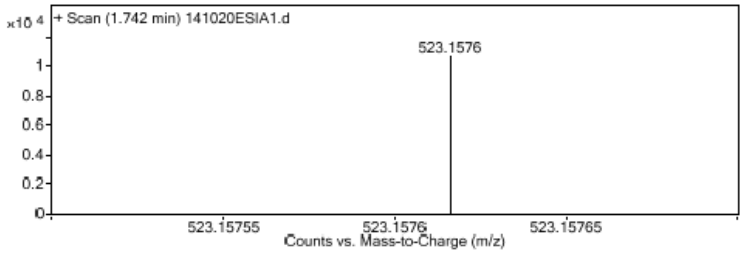

Peak List

m/z	z	Abund
922.0098	1	84557.8

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	16
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C26 H28 Na O10	523.1580	523.1576	0.4	0.8	12.5

--- End Of Report ---

HRESI of compound **1**