Supplementary Materials

Aviculin Isolated from *Lespedeza cuneata* Induce Apoptosis in Breast Cancer Cells through Mitochondria-Mediated Caspase Activation Pathway

Dahae Lee [1,†], Yong Hoon Lee [2,†], Kwang Ho Lee [2,†], Bum Soo Lee [2], Akida Alishir [2], Yoon-Joo Ko [3], Ki Sung Kang [1,*] and Ki Hyun Kim [2,*]

[1] College of Korean Medicine, Gachon University, Seongnam 13120, Korea; pjsldh@naver.com
[2] School of Pharmacy, Sungkyunkwan University, Suwon 16419, Korea; yhl2090@naver.com (Y.H.L.); sholaly@naver.com (K.H.L.); kosboybs@naver.com (B.S.L.); akida.alishir@gmail.com (A.A.)
[3] Laboratory of Nuclear Magnetic Resonance, National Center for Inter-University Research Facilities (NCIRF), Seoul National University, Gwanak-gu, Seoul 08826, Korea; yjko@snu.ac.kr
* Correspondence: kkang@gachon.ac.kr (K.S.K.); khkim83@skku.edu (K.H.K.); Tel.: +82-31-750-5402 (K.S.K.); +82-31-290-7700 (K.H.K.)
† These authors contributed equally to this work

Figure S1. ^{1}H-NMR data of compound **1**.

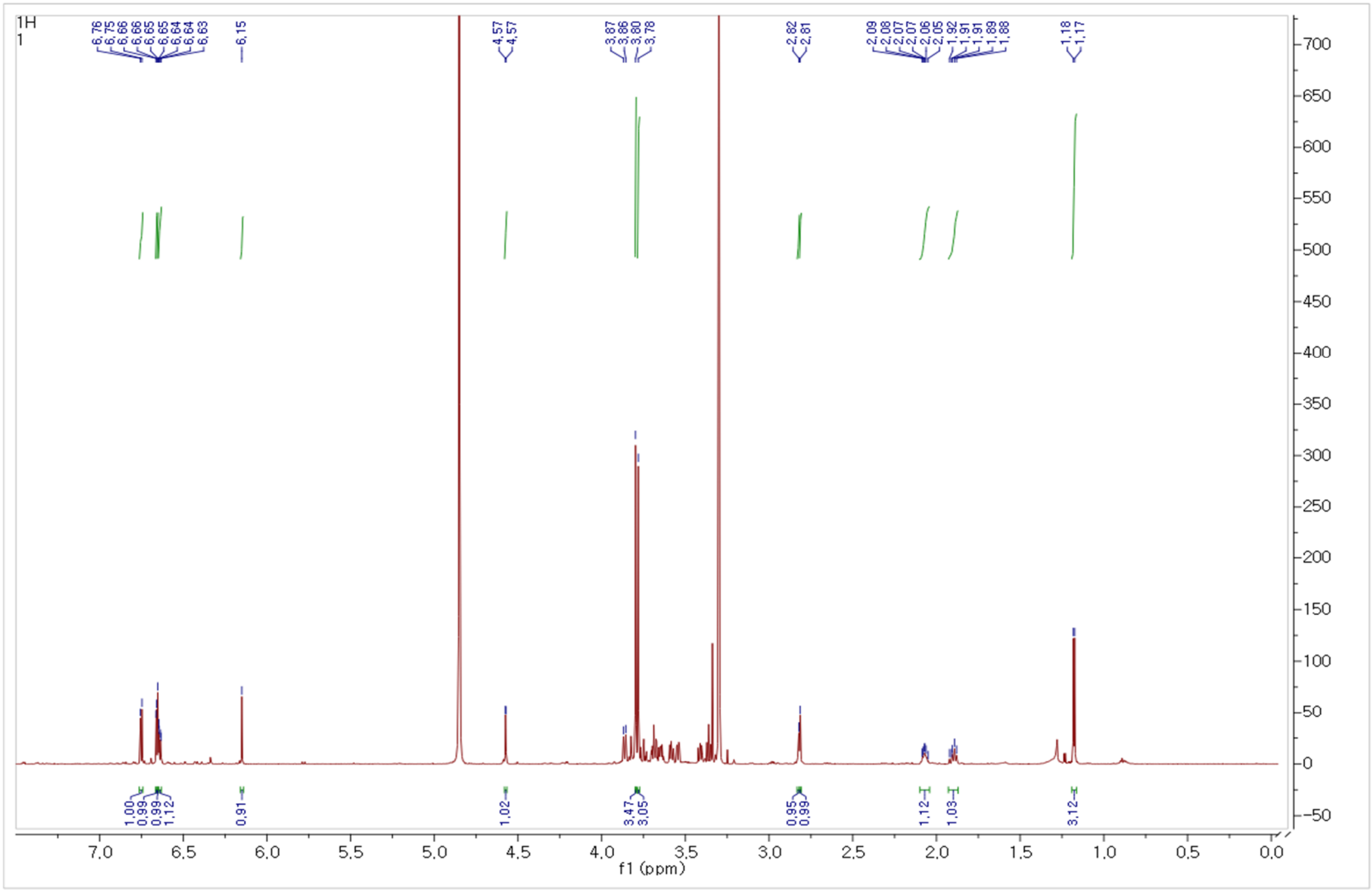


Figure S2. ^{1}H-NMR data of compound **2**.

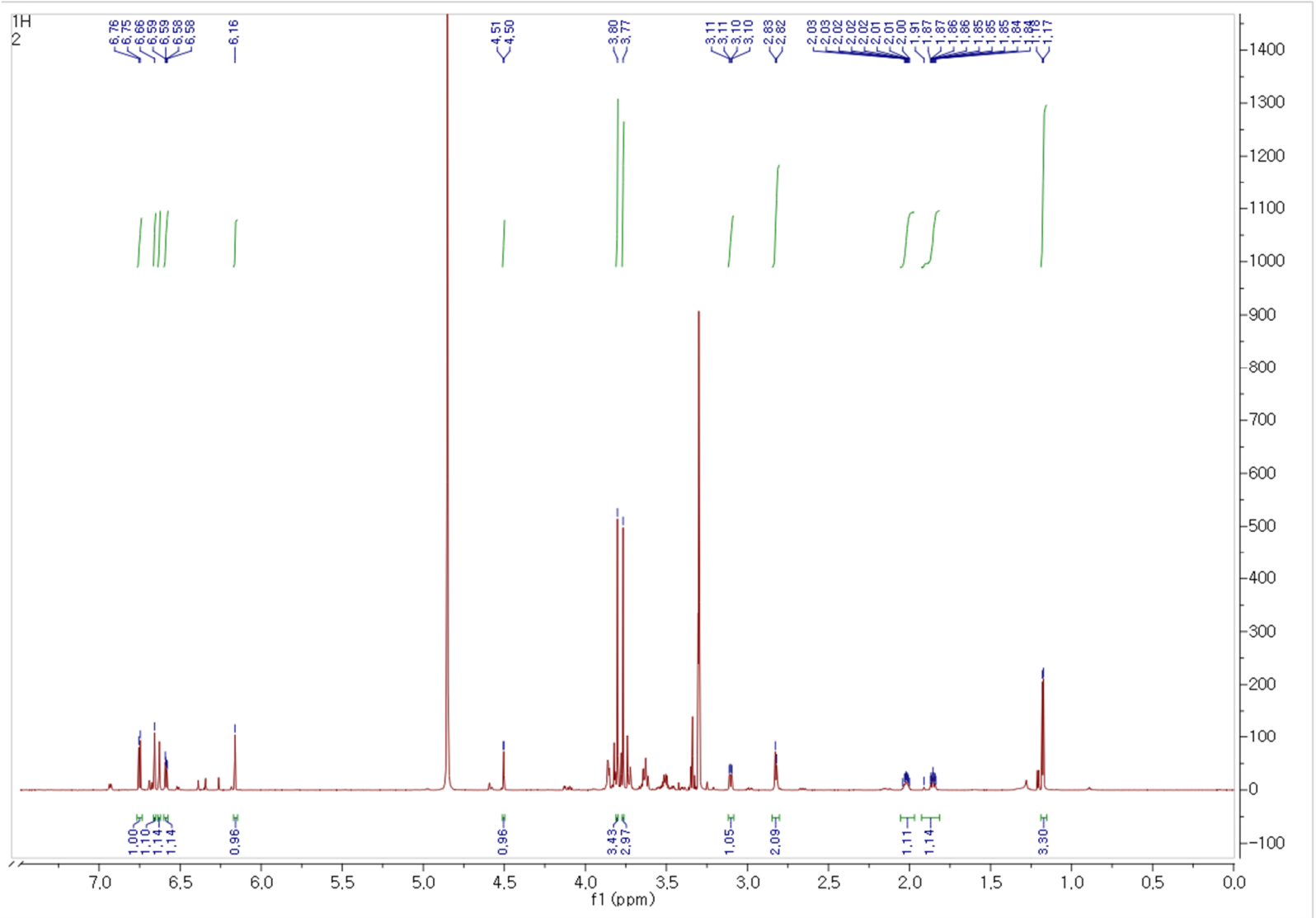


Figure S3. ^{1}H-NMR data of compound **3**.

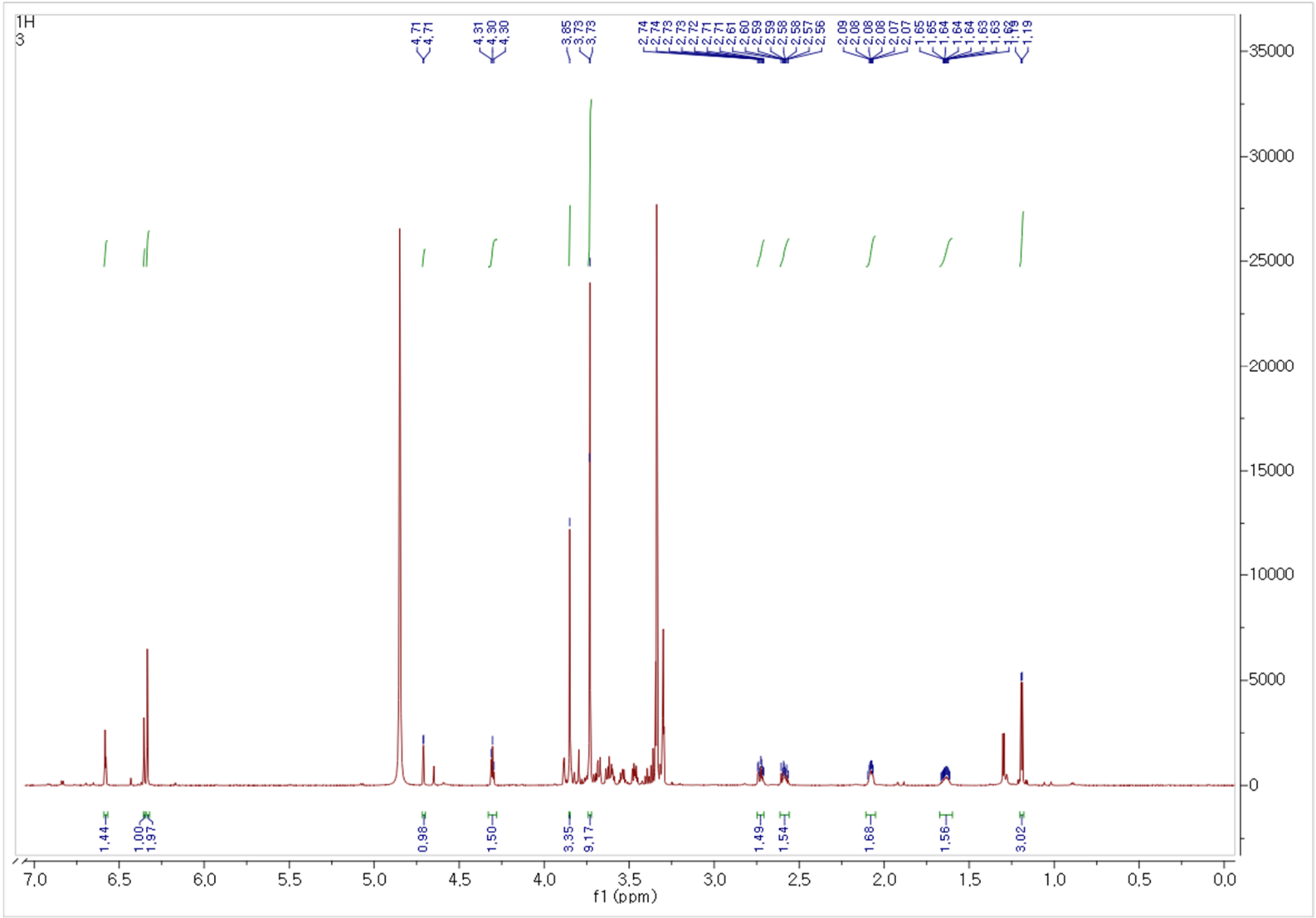


Figure S4. ^{1}H-NMR data of compound **4**.

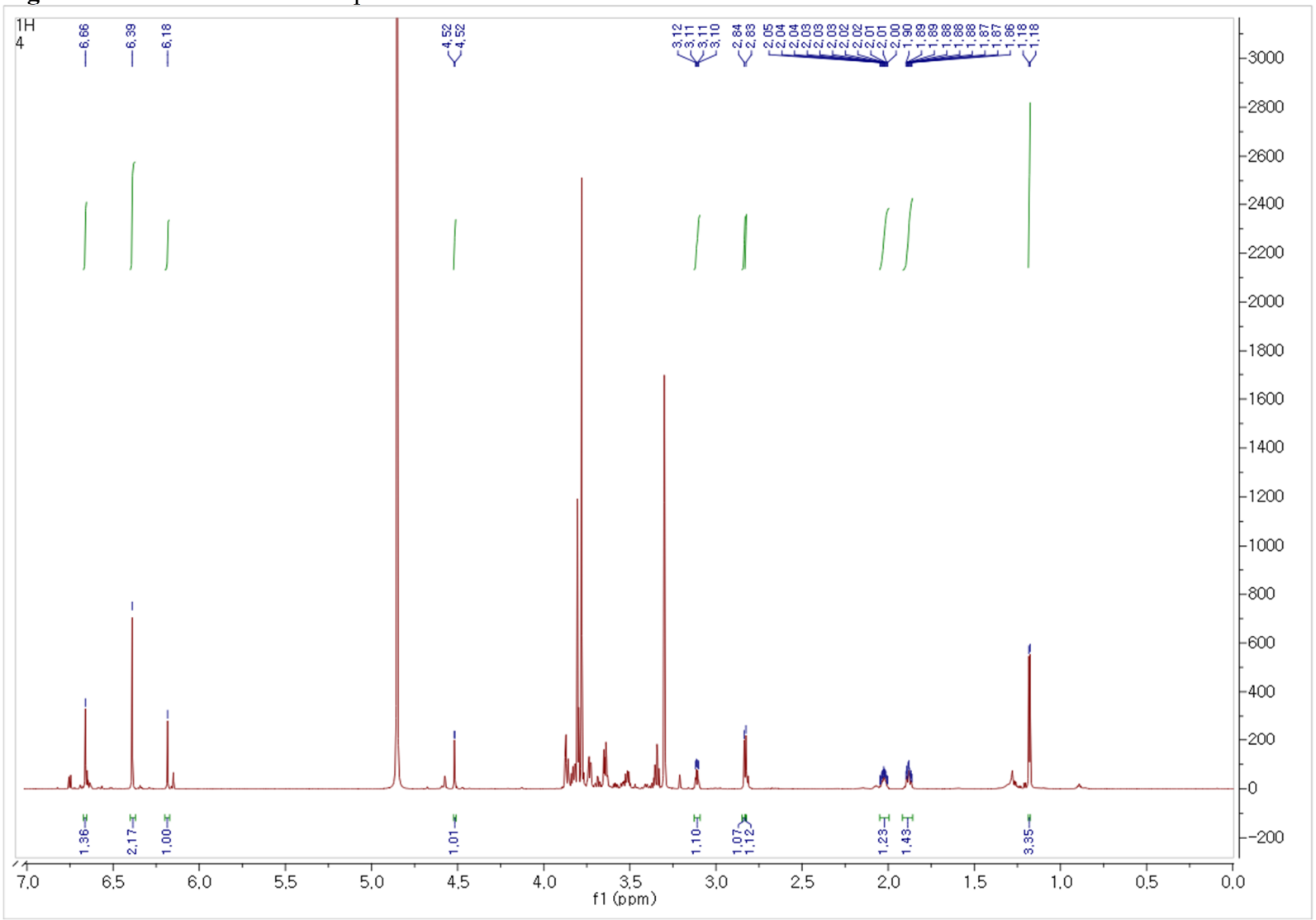


Figure S5. ^{1}H-NMR data of compound **5**.

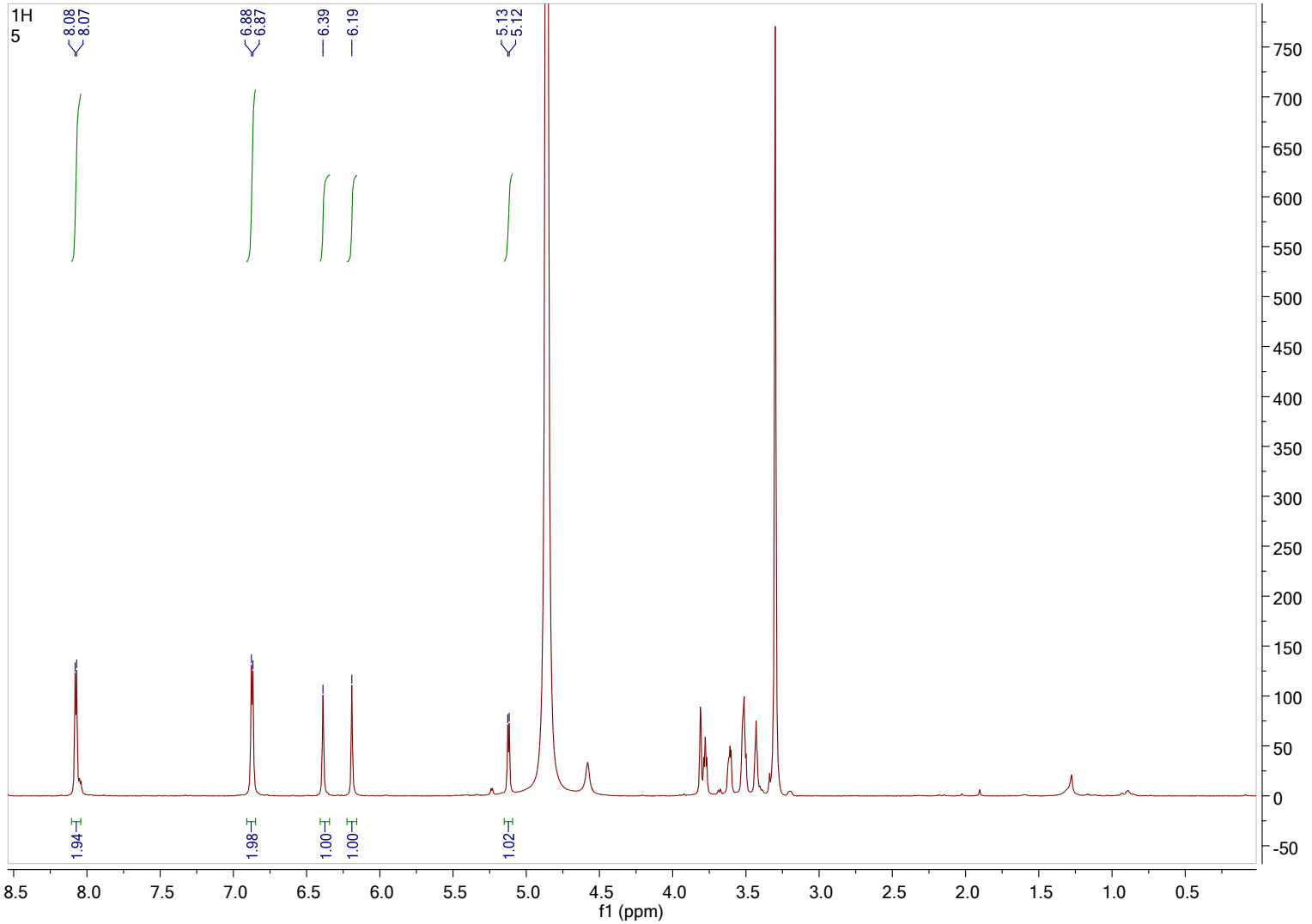


Figure S6. ^{1}H-NMR data of compound **6**.

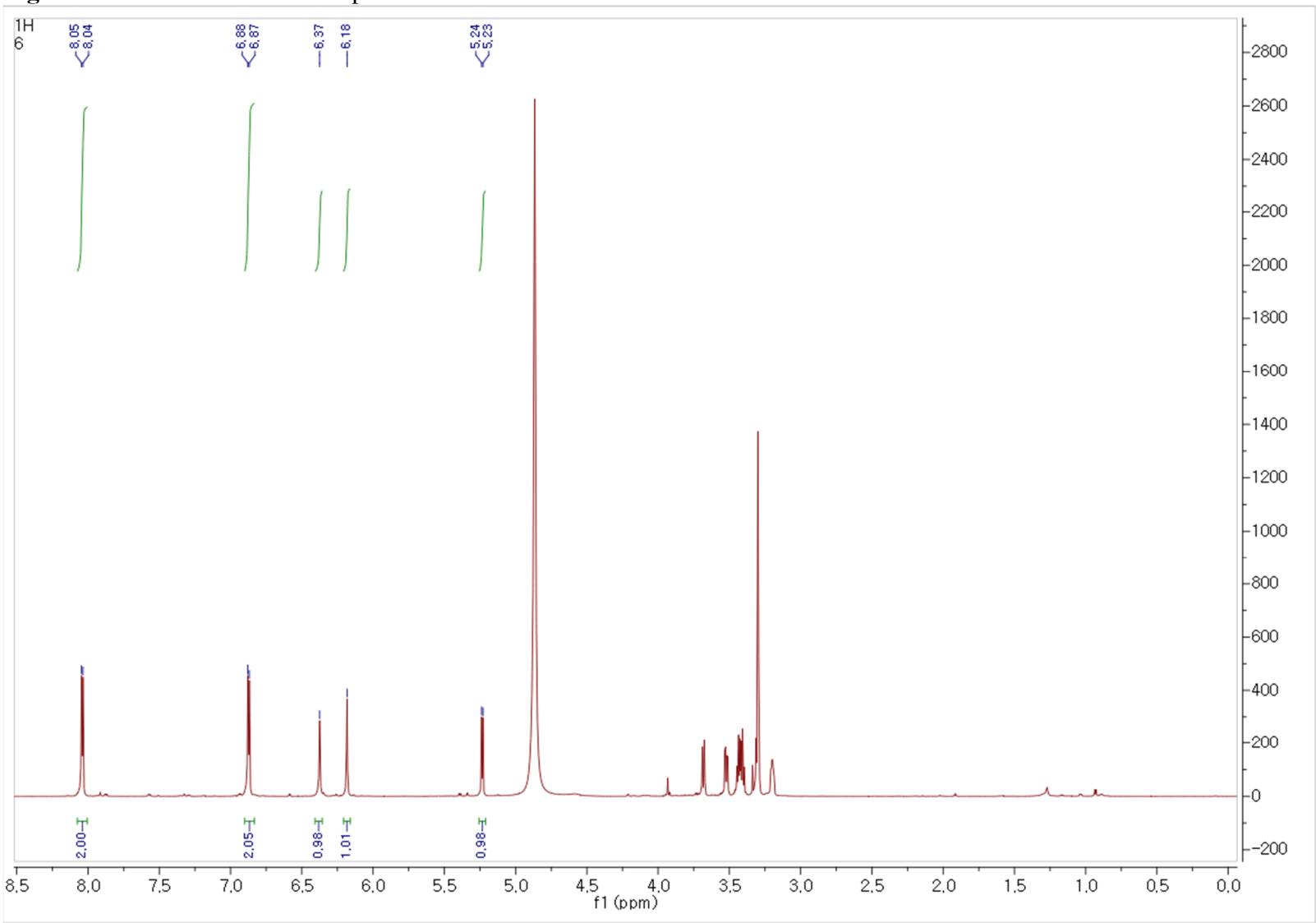


Figure S7. ^{1}H-NMR data of compound **7**.

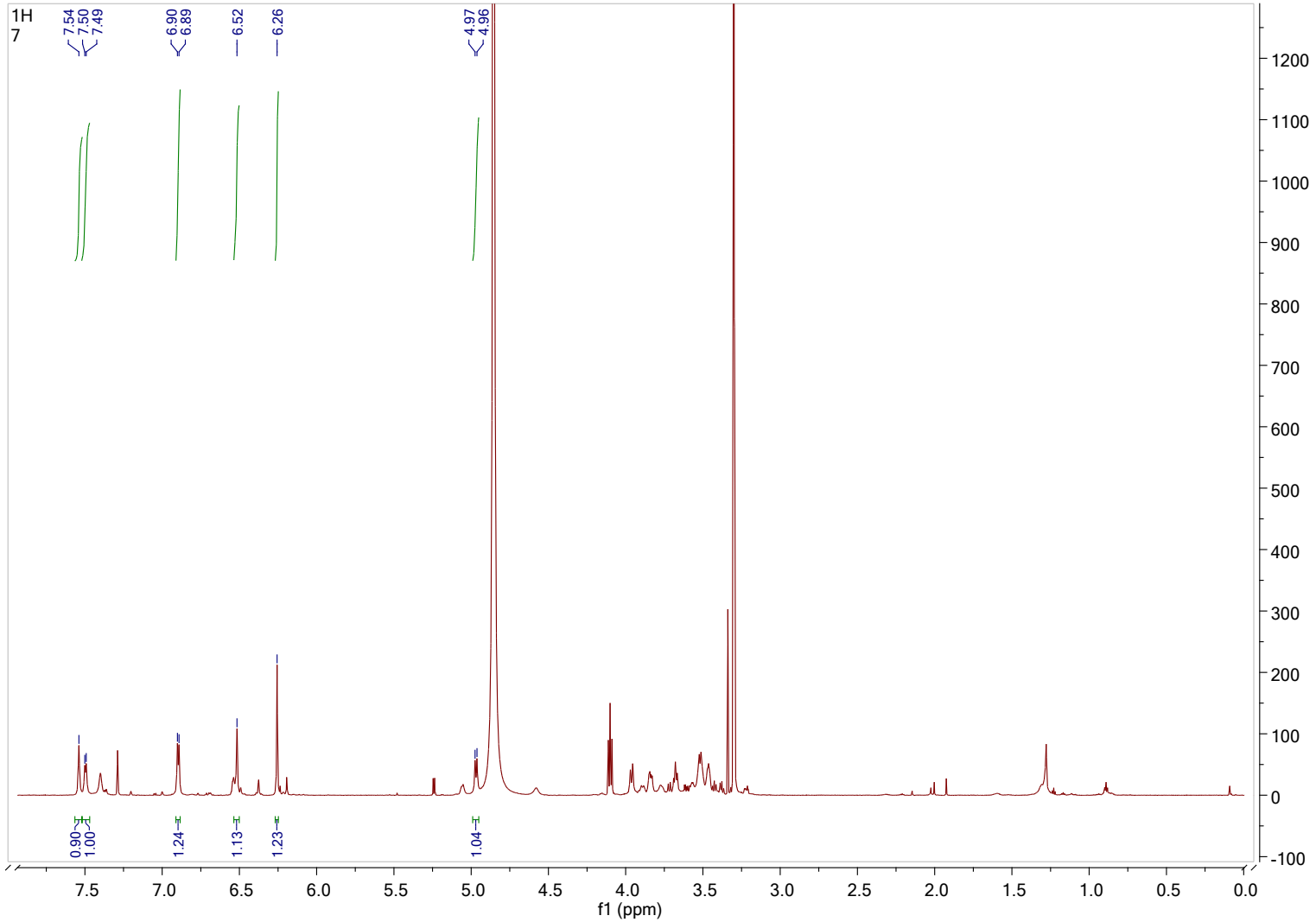


Figure S8. ^{1}H-NMR data of compound **8**.

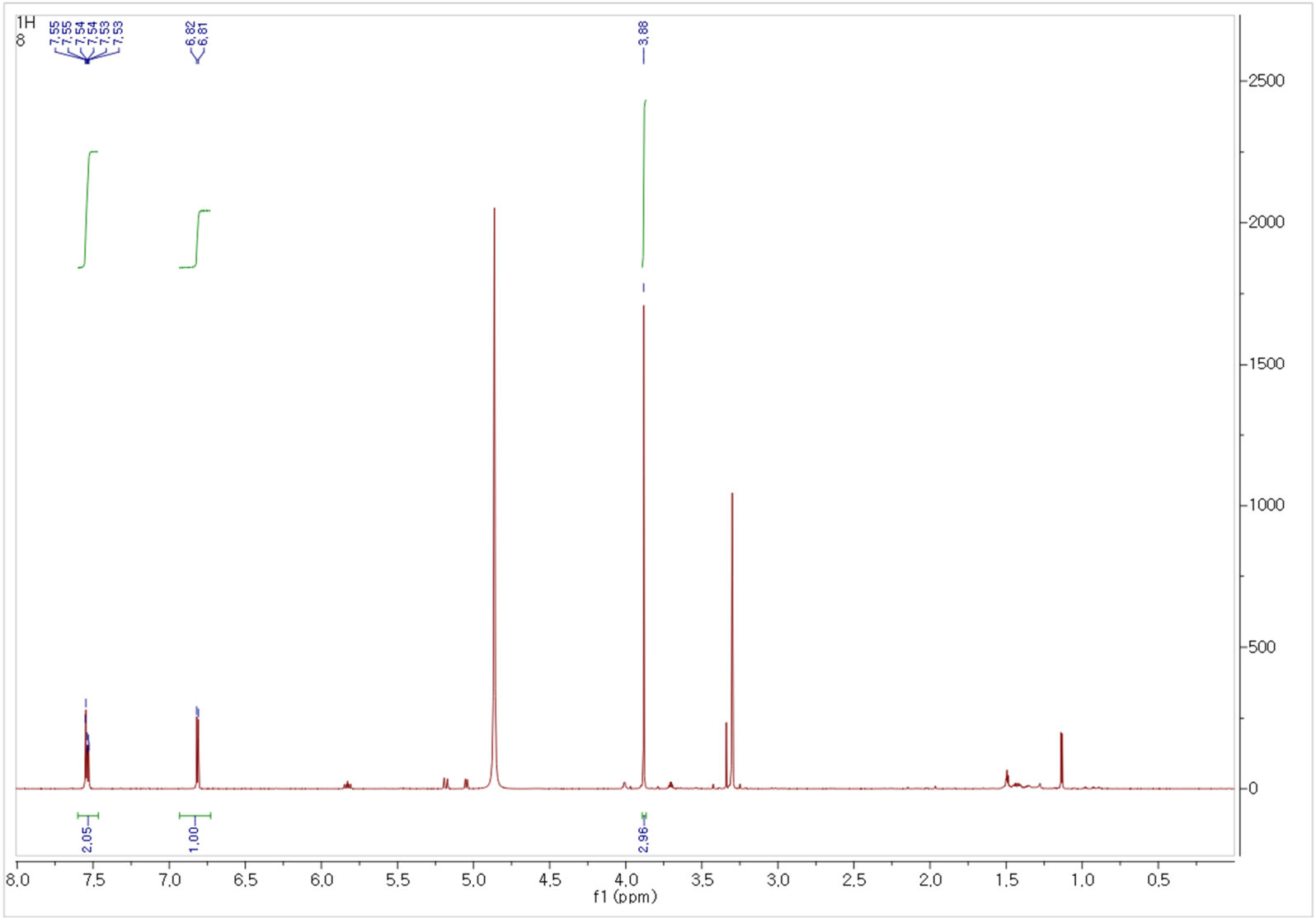


Figure S9. ^{1}H-NMR data of compound **9**.

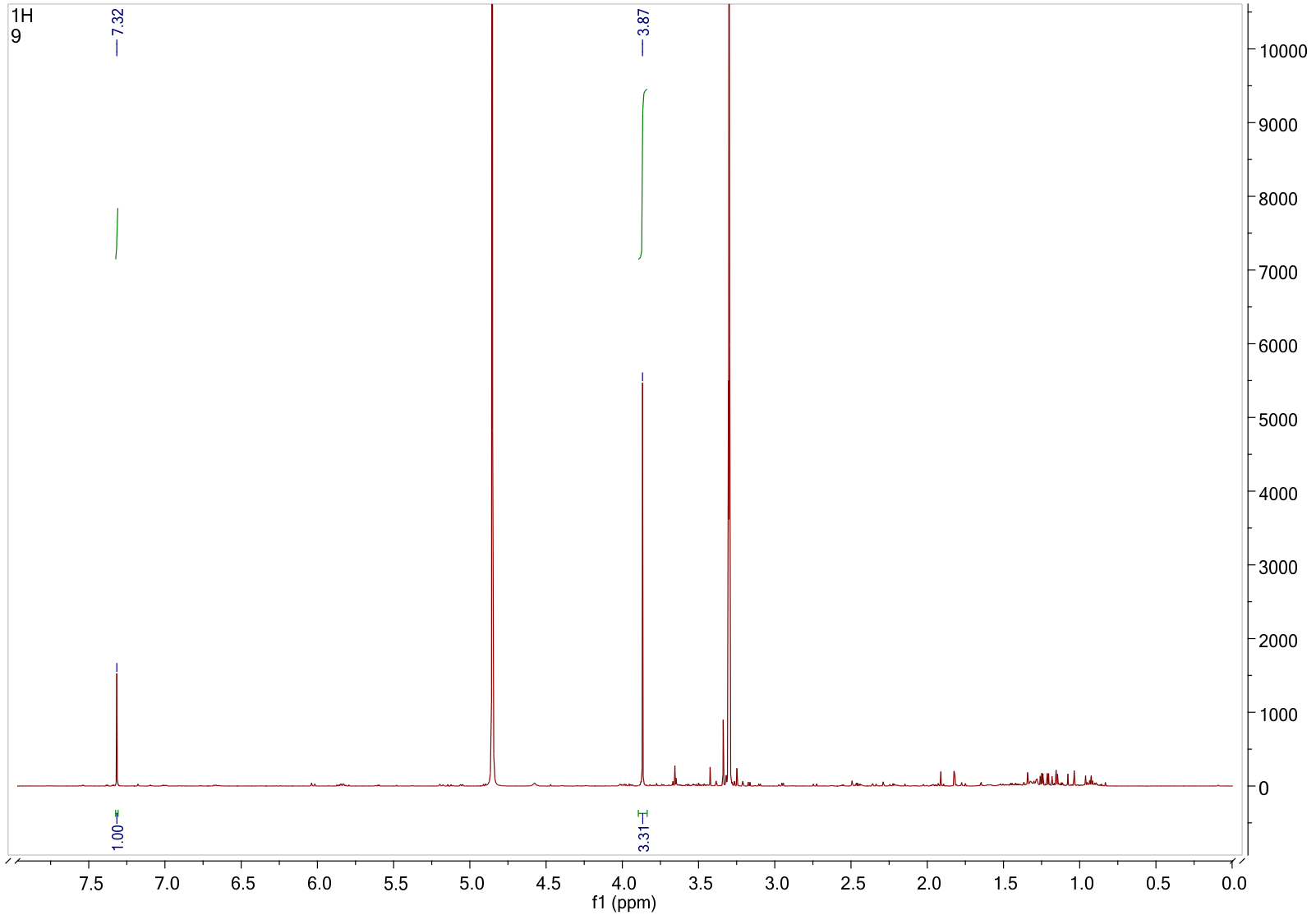
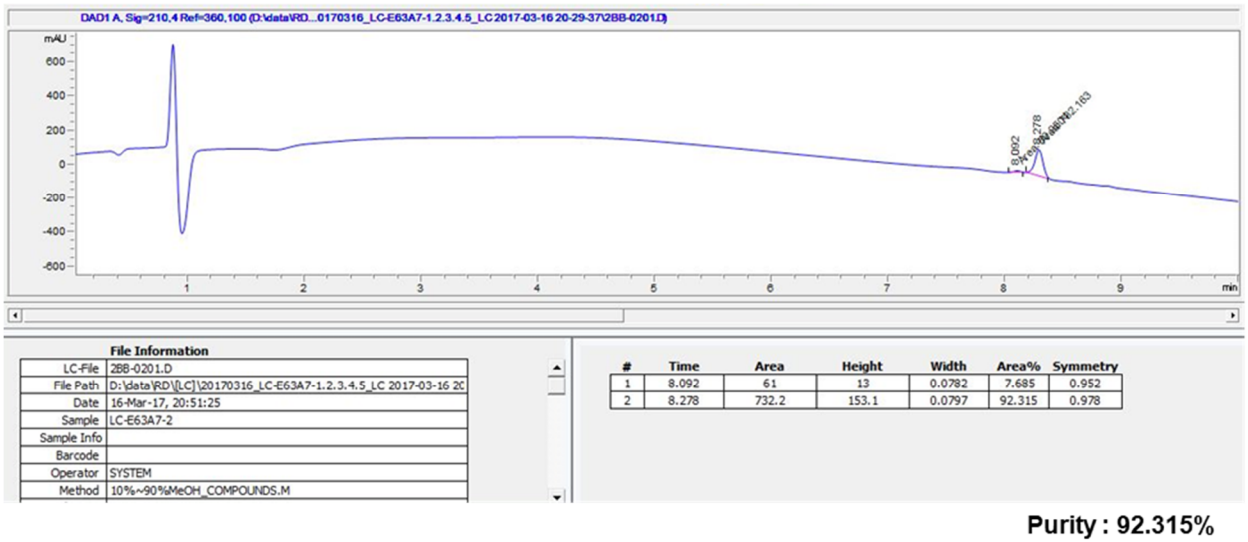


Figure S10. LC/MS analysis for purity of compounds **1-9**.

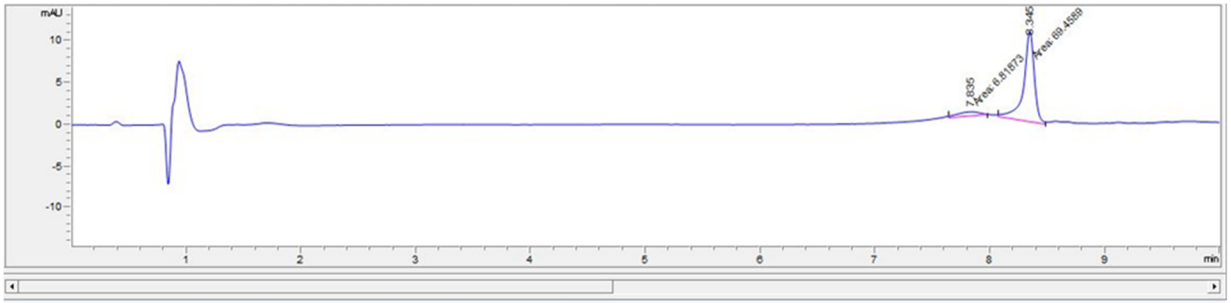


Purity : 92.315%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (210 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 1



File Information

LC-File	2DD-0301.D
File Path	D:\data\RD\[LC]\20170306_LC-E63725-1.2.3_LC 2017-03-06 17-0
Date	06-Mar-17, 17:48:55
Sample	LC-E63725-3
Sample Info	
Barcode	
Operator	SYSTEM
Method	10%~90%MeOH_COMPOUNDS.M

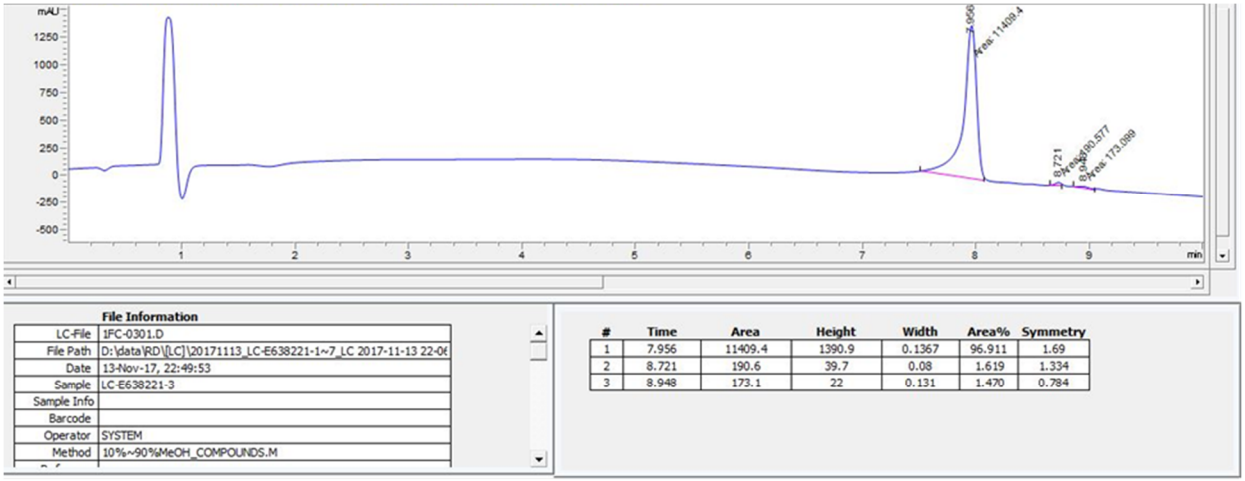
#	Time	Area	Height	Width	Area%	Symmetry
1	7.835	6.8	5E-1	0.2281	8.939	1.882
2	8.345	69.5	10.8	0.1072	91.061	1.342

Purity : 91.061%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (315 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 2



File Information

LC-File	1FC-0301.D
File Path	D:\data\RD\[LC]\20171113_LC-E638221-1~7_LC 2017-11-13 22-0(
Date	13-Nov-17, 22:49:53
Sample	LC-E638221-3
Sample Info	
Barcode	
Operator	SYSTEM
Method	10%~90%MeOH_COMPOUNDS.M

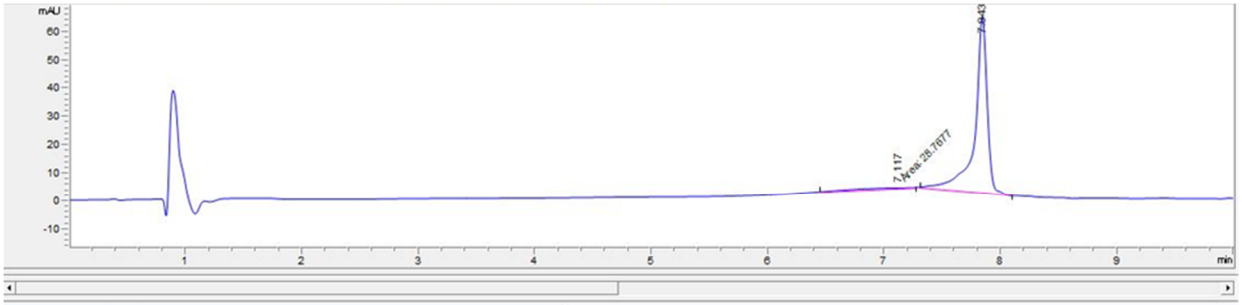
#	Time	Area	Height	Width	Area%	Symmetry
1	7.956	11409.4	1390.9	0.1367	96.911	1.69
2	8.721	190.6	39.7	0.08	1.619	1.334
3	8.948	173.1	22	0.131	1.470	0.784

Purity : 96.911%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (210 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 3



File Information	
LC-File	2FG-0201.D
File Path	D:\data\RD\[LC]\20170428_LC-E637222-1.2.3_LC 2017-04-28 18-3
Date	28-Apr-17, 18:53:03
Sample	LC-E637222-2
Sample Info	
Barcode	
Operator	SYSTEM
Method	10%~90%MeOH_COMPOUNDS.M

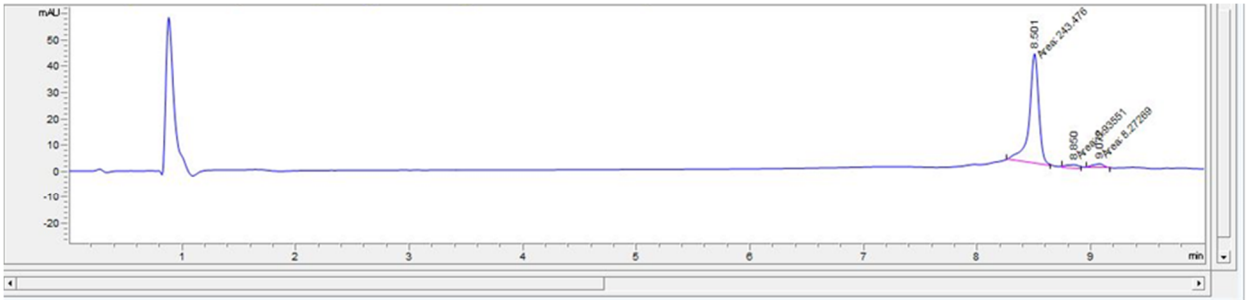
#	Time	Area	Height	Width	Area%	Symmetry
1	7.117	28.8	6.7E-1	0.5359	5.706	3.867
2	7.843	475.4	62.6	0.1086	94.294	1.695

Purity : 94.294%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (254 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 4



File Information

LC-File	1FF-0601.D
File Path	D:\data\RD\[LC]\20171113_LC-E638221-1~7_LC 2017-11-13 22-0(
Date	13-Nov-17, 23:53:02
Sample	LC-E638221-6
Sample Info	
Barcode	
Operator	SYSTEM
Method	10%~90%MeOH_COMPOUNDS.M

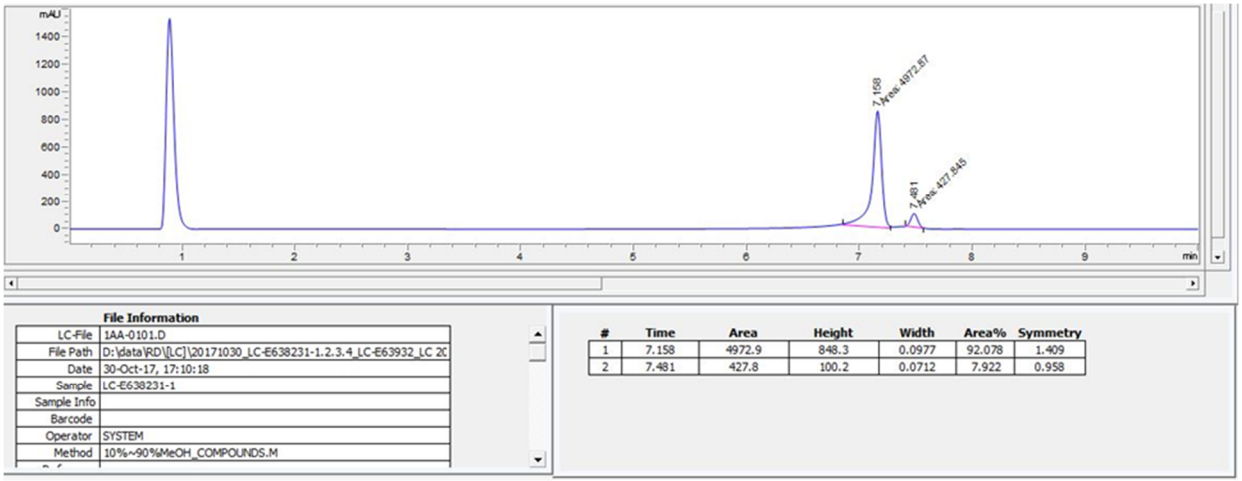
#	Time	Area	Height	Width	Area%	Symmetry
1	8.501	243.5	41.6	0.0974	93.399	1.259
2	8.85	8.9	1.2	0.1243	3.428	1.271
3	9.072	8.3	1.3	0.1045	3.173	1.622

Purity : 93.399%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (254 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 5



File Information	
LC-File	1AA-0101.D
File Path	D:\data\RD\[LC]\20171030_LC-E638231-1.2.3.4_LC-E63932_LC 2(
Date	30-Oct-17, 17:10:18
Sample	LC-E638231-1
Sample Info	
Barcode	
Operator	SYSTEM
Method	10%~90%MeOH_COMPOUNDS.M

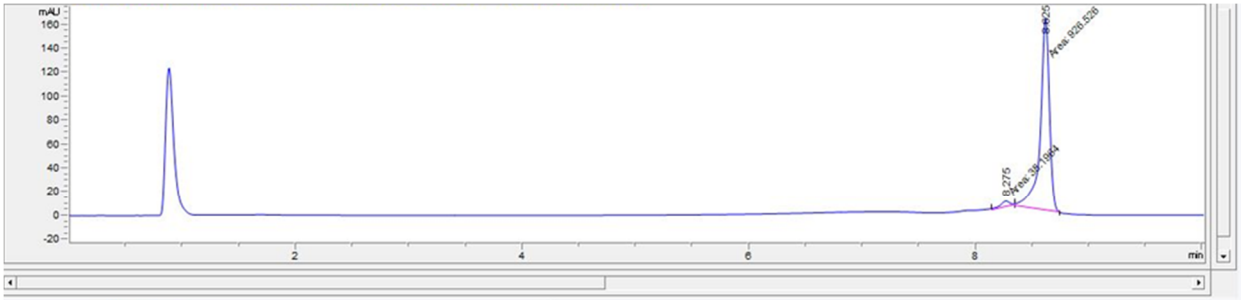
#	Time	Area	Height	Width	Area%	Symmetry
1	7.158	4972.9	848.3	0.0977	92.078	1.409
2	7.481	427.8	100.2	0.0712	7.922	0.958

Purity : 92.078%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (254 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 6



File Information

LC-File	1AC-0301.D
File Path	D:\data\RD\[LC]\20171030_LC-E638231-1.2.3.4_LC-E63932_LC 2(
Date	30-Oct-17, 17:52:20
Sample	LC-E638231-3
Sample Info	
Barcode	
Operator	SYSTEM
Method	10%~90%MeOH_COMPOUNDS.M

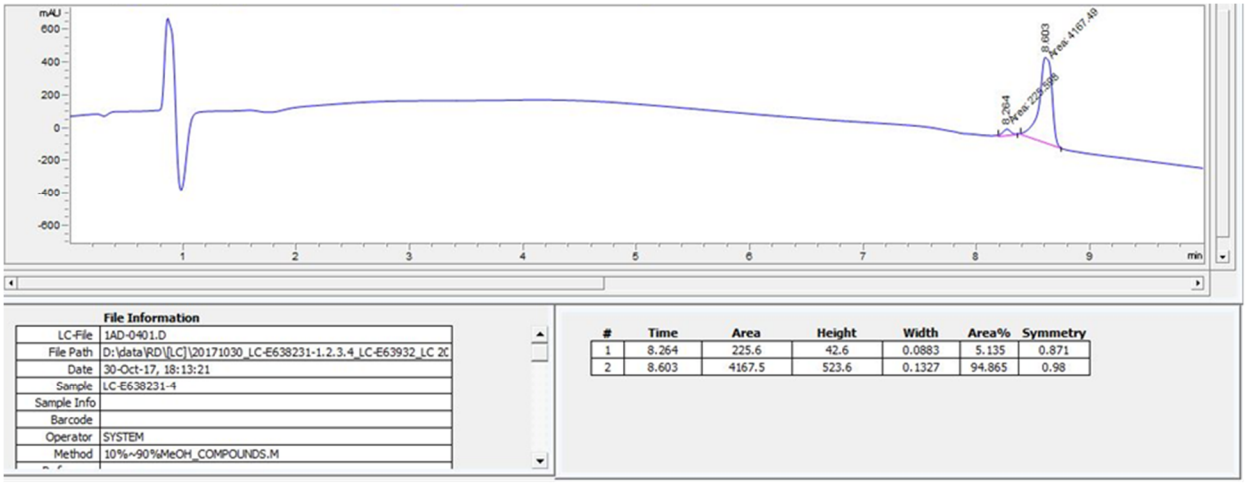
#	Time	Area	Height	Width	Area%	Symmetry
1	8.275	38.2	5.5	0.1157	3.959	1.533
2	8.625	926.5	162.1	0.0953	96.041	1.38

Purity : 96.041%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (315 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 7



File Information

LC-File	1AD-0401.D
File Path	D:\data\RD\[LC]\20171030_LC-E638231-1.2.3.4_LC-E63932_LC 2(
Date	30-Oct-17, 18:13:21
Sample	LC-E638231-4
Sample Info	
Barcode	
Operator	SYSTEM
Method	10%~90%MeOH_COMPOUNDS.M

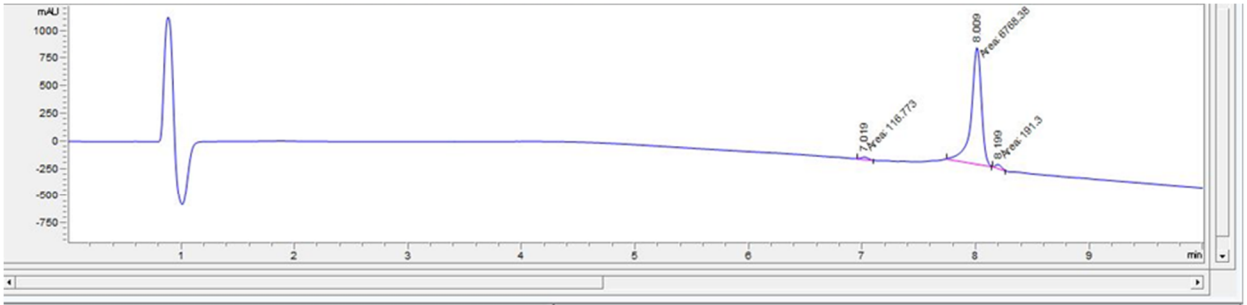
#	Time	Area	Height	Width	Area%	Symmetry
1	8.264	225.6	42.6	0.0883	5.135	0.871
2	8.603	4167.5	523.6	0.1327	94.865	0.98

Purity : 94.865%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (210 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 8



File Information

LC-File	2CA-0101.D
File Path	D:\data\RD\[LC]\20171026_LCE29_LC 2017-10-27 15-14-54
Date	27-Oct-17, 15:15:57
Sample	LCE29
Sample Info	
Barcode	
Operator	SYSTEM
Method	10%~90%MeOH_COMPOUNDS.M

#	Time	Area	Height	Width	Area%	Symmetry
1	7.019	116.8	24.8	0.0785	1.650	0.892
2	8.009	6768.4	1065.8	0.1058	95.646	1.303
3	8.199	191.3	44.5	0.0716	2.703	0.464

Purity : 95.646%

Conditions for LC-MS/MS analysis
- Agilent Technologies 1200s
- Column: Phenomenex Kinetex 5 μm C18 100A 100 x 2.1 mm
- Flow: 0.3 mL/min
- Detector: PDA detector (210 nm)
- Mobile phase: Water-MeOH gradient

Time	MeOH
0.0	10
10	90

Compound 9