Supplementary Materials

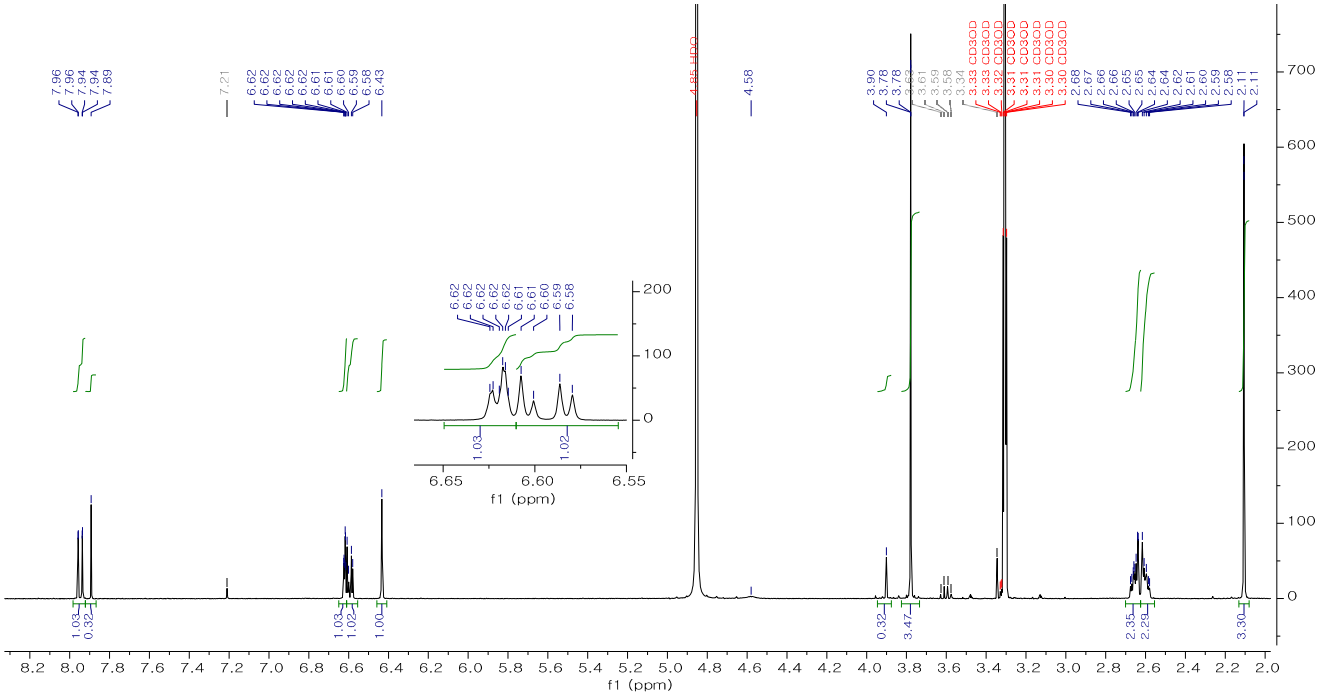


Figure S1. ^{1}H-NMR spectrum (400 MHz, CD_3OD) of **1**.

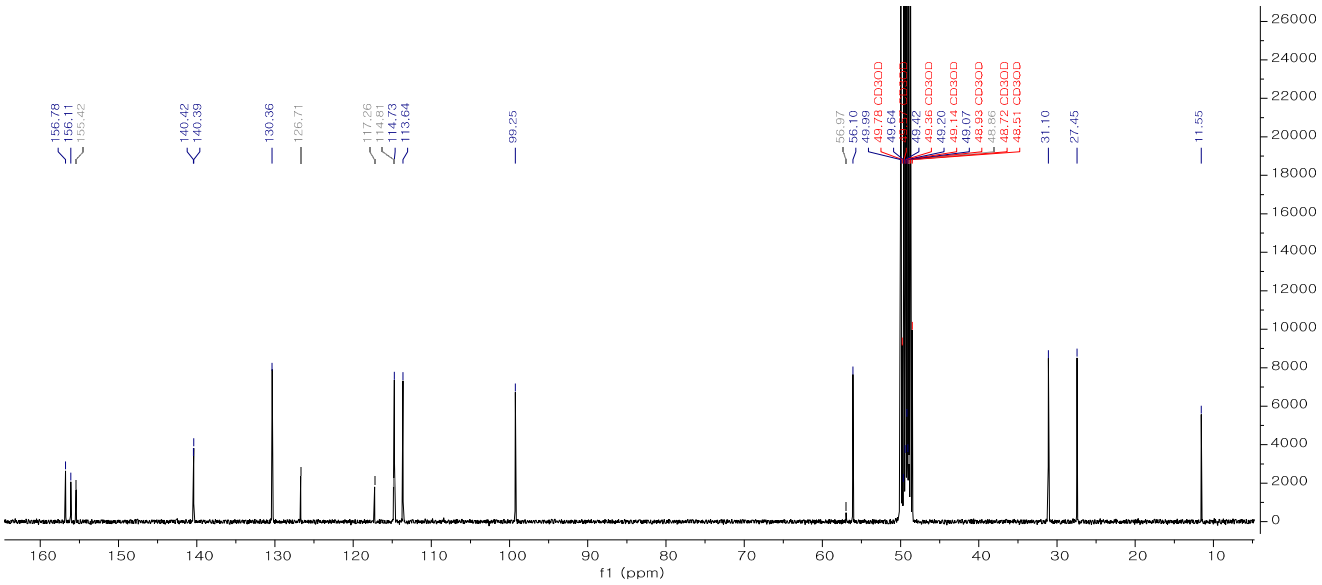


Figure S2. ^{13}C-NMR spectrum (100 MHz, CD_3OD) of **1**.

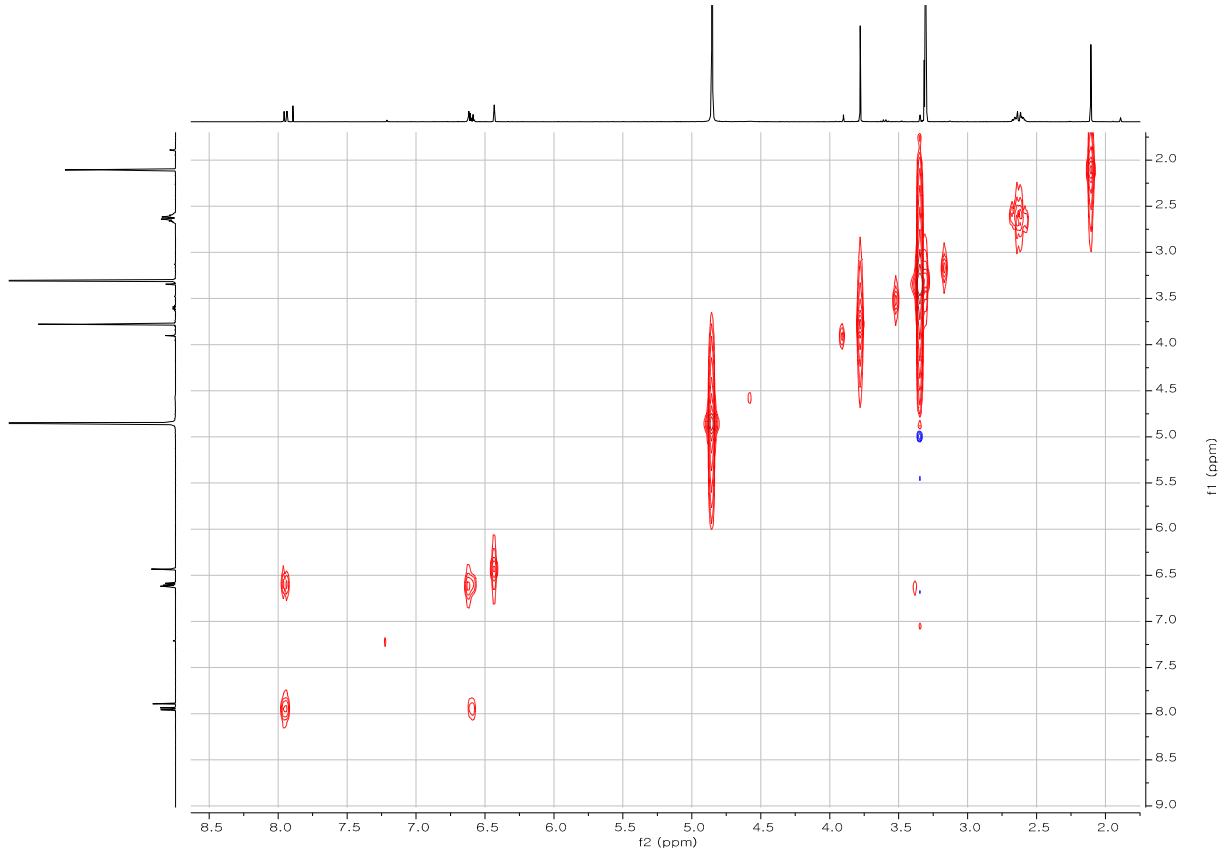


Figure S3. ^{1}H-^{1}H COSY NMR spectrum (CD_3OD) of **1**.

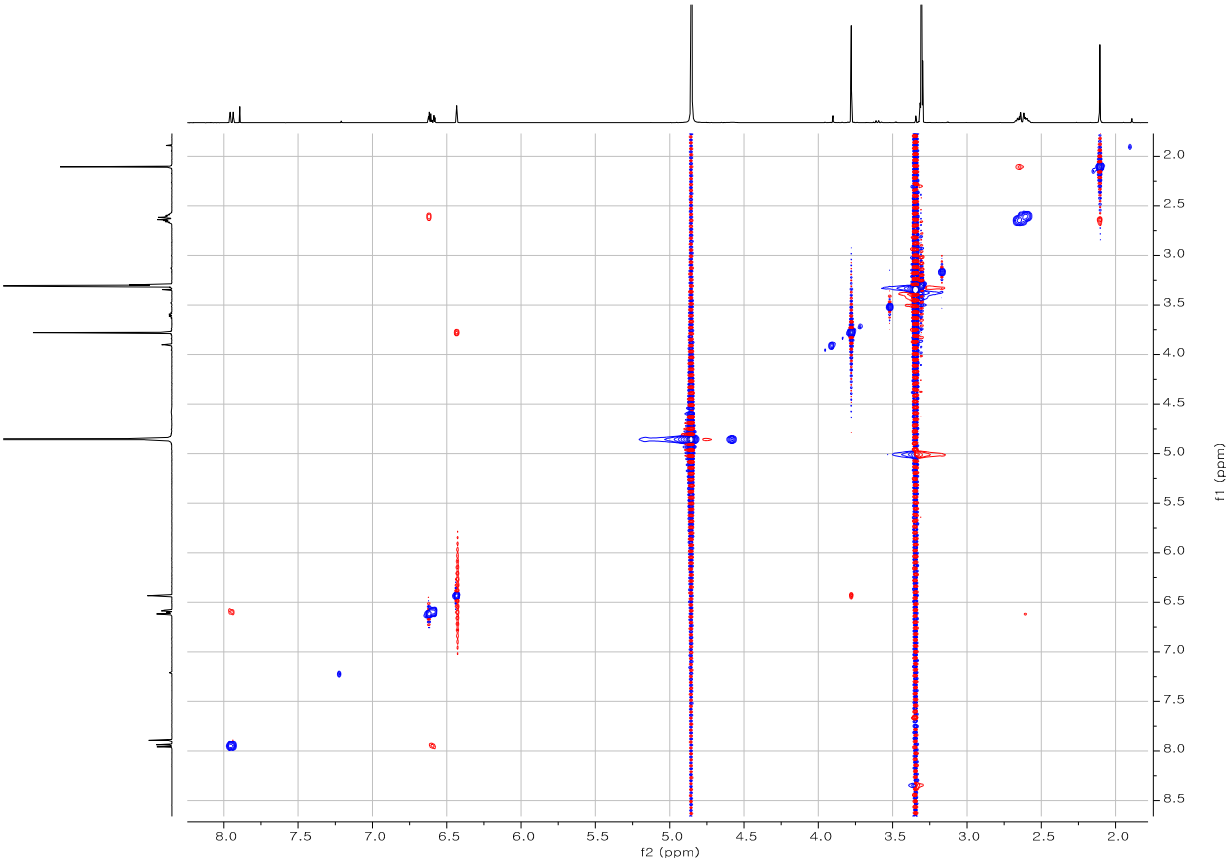


Figure S4. ^{1}H-^{1}H NOESY NMR spectrum (CD_3OD) of **1**.

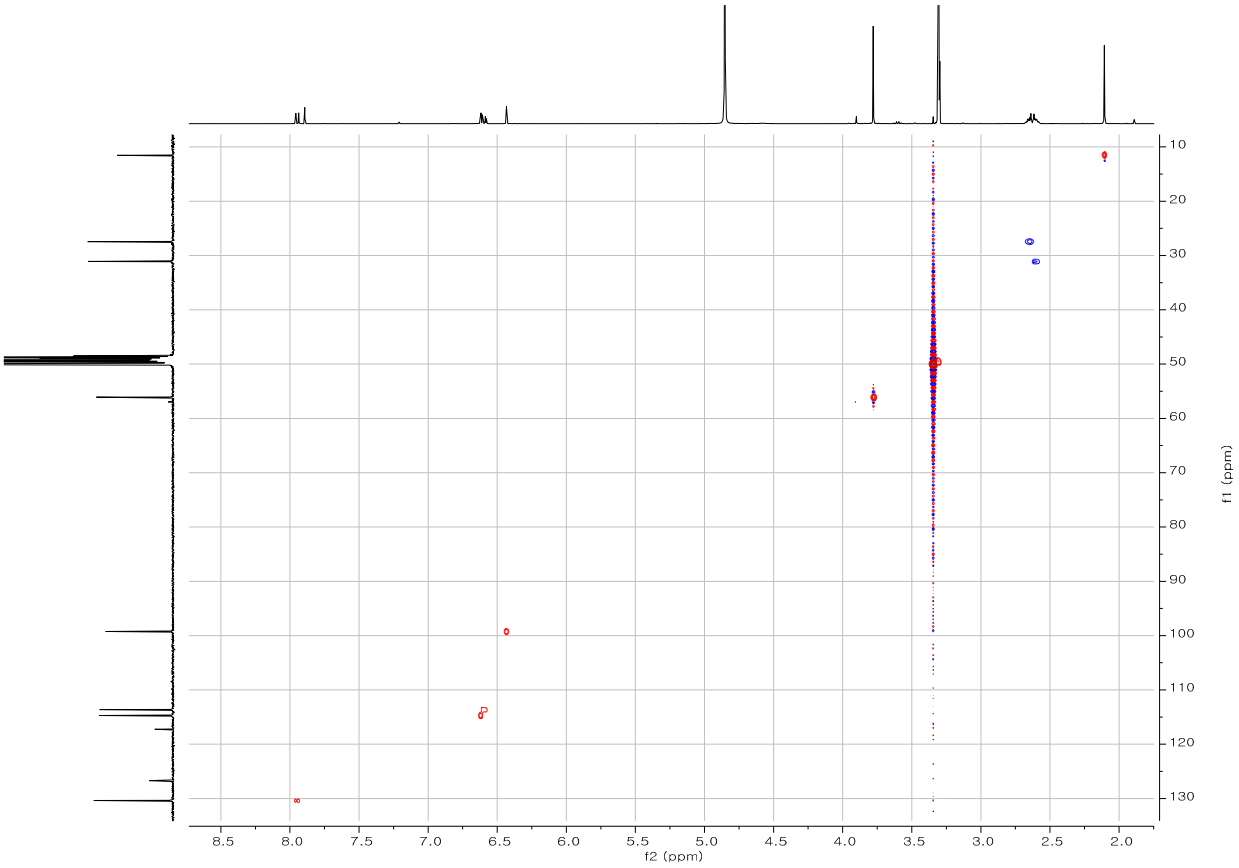


Figure S5. ^{1}H-^{13}C HSQC NMR spectrum (CD_3OD) of **1**.

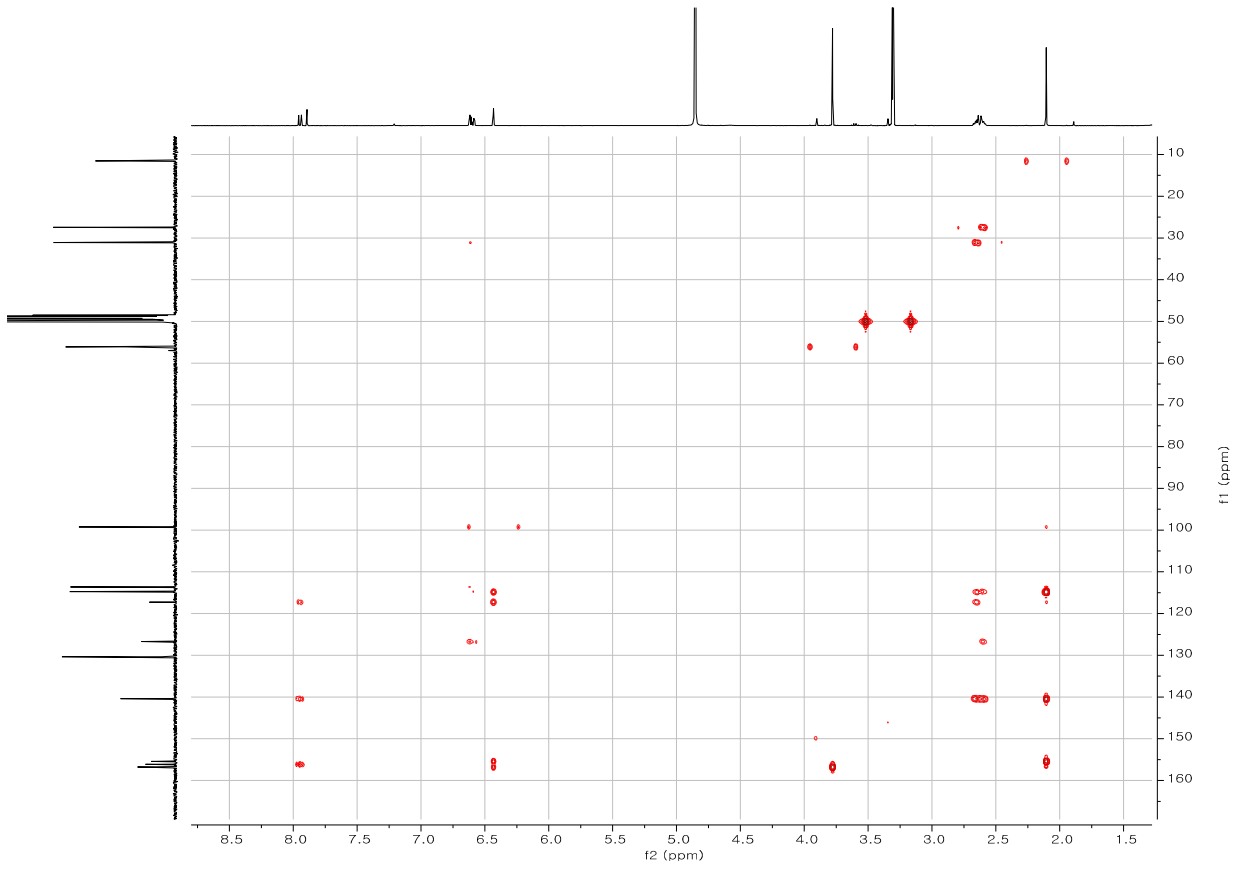


Figure S6. ^{1}H-^{13}C HMBC NMR spectrum (CD_3OD) of **1**.

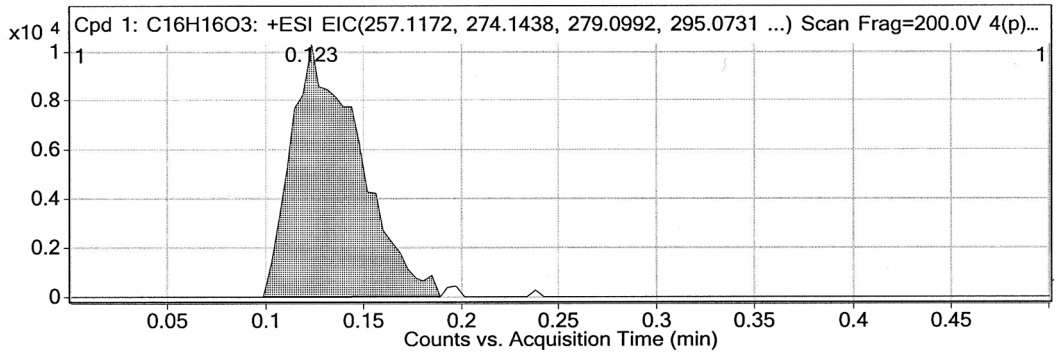
Qualitative Compound Report

Data File	4(p)02.d	**Sample Name**	SampleName
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	
Acq Method		**Acquired Time**	10/5/2012 11:22:42 AM
IRM Calibration Status	Success	**DA Method**	kikisil.m
Comment	vol. 0.01		

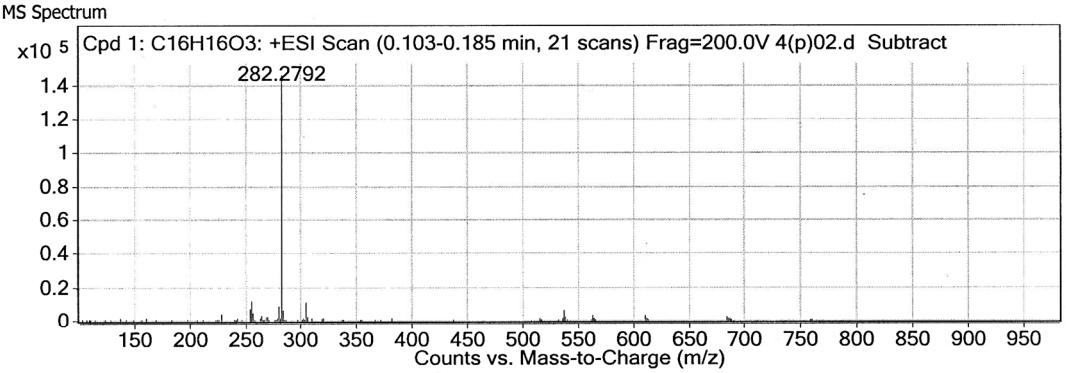
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C16H16O3	0.123	256.1099	4703	C16H16O3	256.1099	0.01

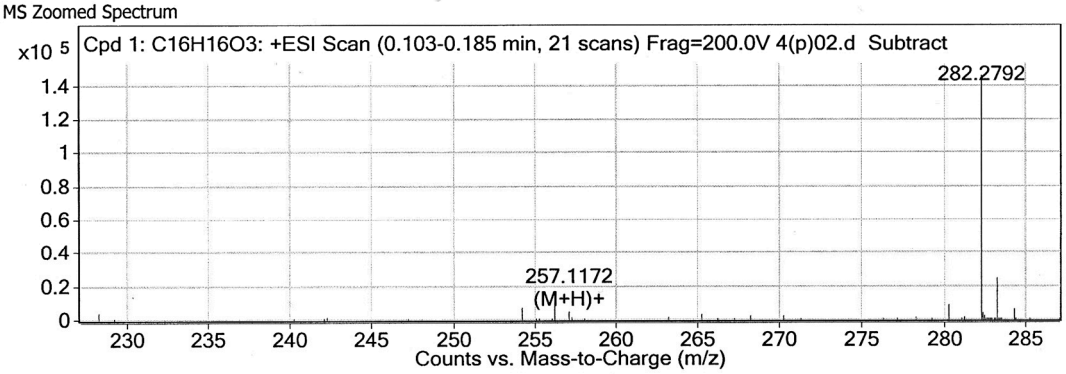
Compound Label	RT	Algorithm	Mass
Cpd 1: C16H16O3	0.123	Find By Formula	256.1099



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
257.1172	257.1172	-0.02	1	4703	C16 H17 O3	(M+H)+

Figure S7. HRESIMS spectrum of **1.**