

Supplementary Information

Polar Compounds Isolated from the Leaves of *Calea prunifolia* H.B.K. and their Anti-Adrenergic Related Vasodilator Activity

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Quercetin 3-rutinoside (**1**)

Yellow amorphous solid. mp: 230-233 °C; ¹H NMR (CD₃OD, 200 MHz) δ 1.01(d, 3H, *J* 6.2 Hz), 3.05-3.80 (m, 10H), 4.40 (m, 1H), 5.0 (d, 1H, *J* 7.3 Hz), 6.08 (d, 1H, *J* 1.8 Hz), 6.27 (d, 1H, *J* 1.8 Hz), 6.76 (d, 1H, *J* 8.4 Hz), 7.54 (dd, 1H, *J* 2.2; 8.4 Hz), 7.77 (d, 1H, *J* 2.2 Hz); ¹³C NMR (CD₃OD, 50 MHz) δ 17.8, 68.4, 69.6, 71.3, 72.0, 72.1, 73.8, 75.6, 77.1, 78.1, 94.8, 99.9, 102.3, 104.6, 105.5, 115.9, 117.6, 123.0, 123.5, 135.5, 145.7, 149.7, 158.4, 159.2, 162.8, 165.9, 179.3.

3,5-di-O-[E]-caffeoylquinic acid (**2**)

Yellow oil. ¹H NMR (CD₃OD, 400 MHz) δ 2.79 (m, 2H), 2.94 (m, 2H), 4.50 (m, 1H), 5.97 (m, 1H), 6.05 (m, 1H), 6.96 (d, 1H, *J* 15.8 Hz), 7.04 (d, 1H, *J* 15.8 Hz), 7.54 (d, 1H, *J* 8.1 Hz), 7.55 (d, 1H, *J* 8.1 Hz), 7.73 (dd, 1H, *J* 1.9; 8.1 Hz), 7.81 (d, 1H, *J* 1.9 Hz), 8.21 (d, 1H, *J* 15.8 Hz), 8.25 (d, 1H, *J* 15.8 Hz); ¹³C NMR (DMSO, 100 MHz) δ 35.1, 36.3, 68.5, 71.2, 71.4, 73.2, 114.7, 114.9 (2), 115.3, 116.3 (2), 121.9, 122.1, 126.5, 126.6, 145.4 (2), 145.8, 146.0, 148.6, 148.7, 166.4, 167.0, 175.9

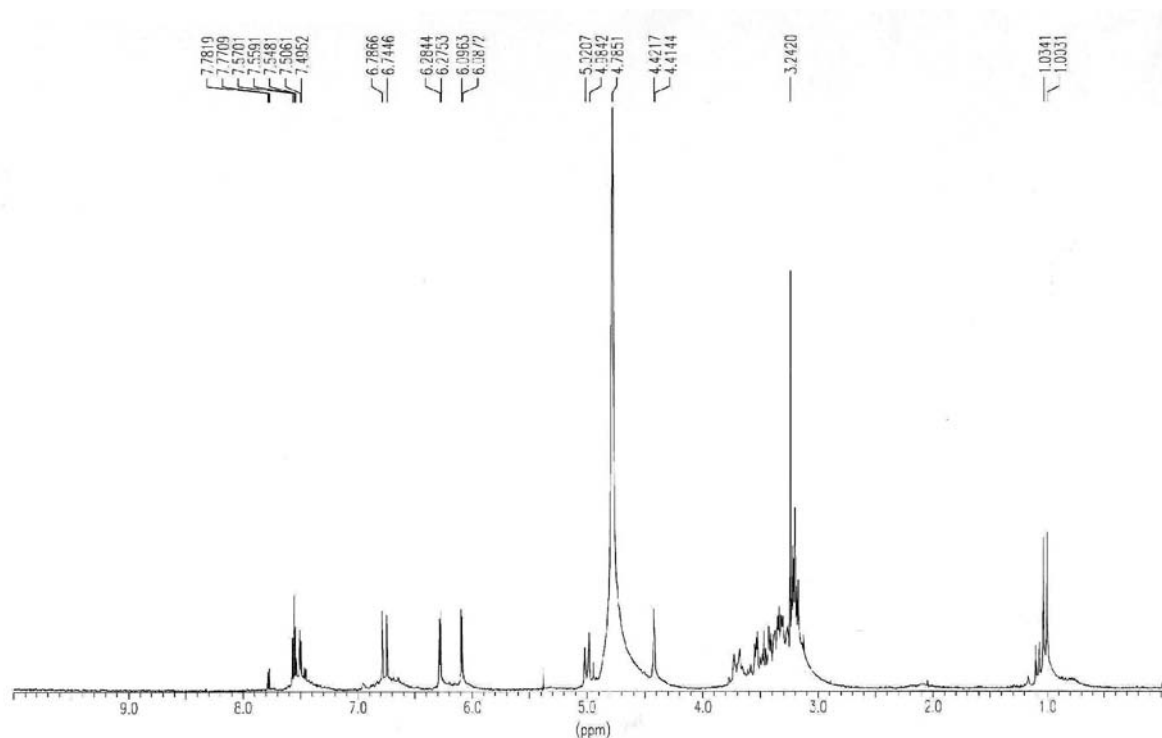


Figure S1. ¹H NMR (CD₃OD) spectrum of compound **1**.

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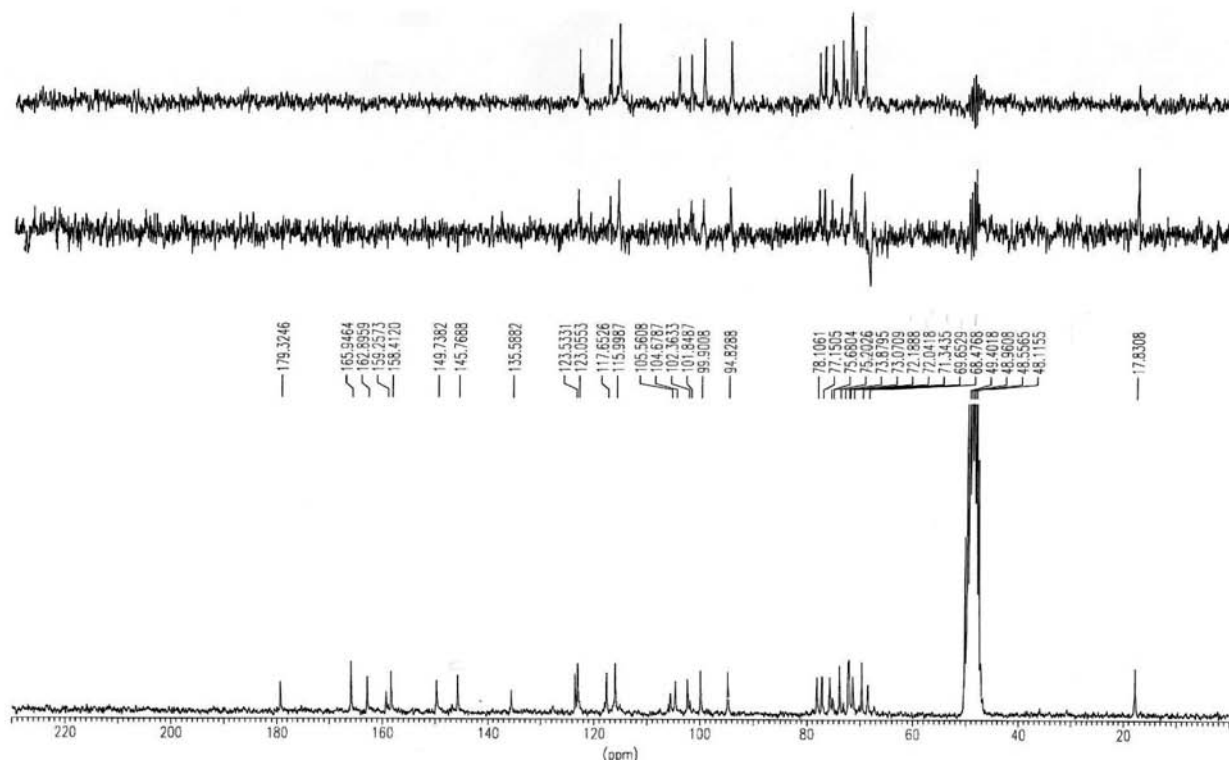


Figure S2. ^{13}C NMR (CD_3OD) spectrum of compound 1.

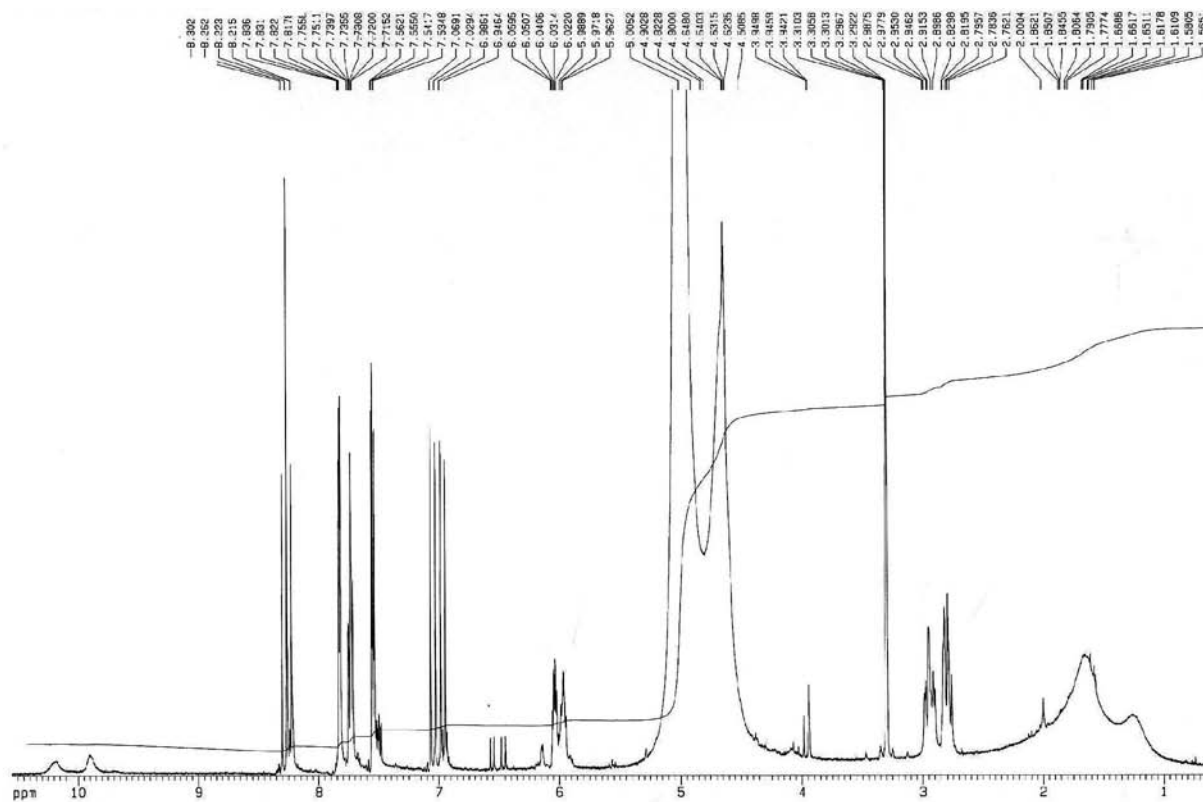


Figure S3. ^1H NMR (CD_3OD) spectrum of compound 2.

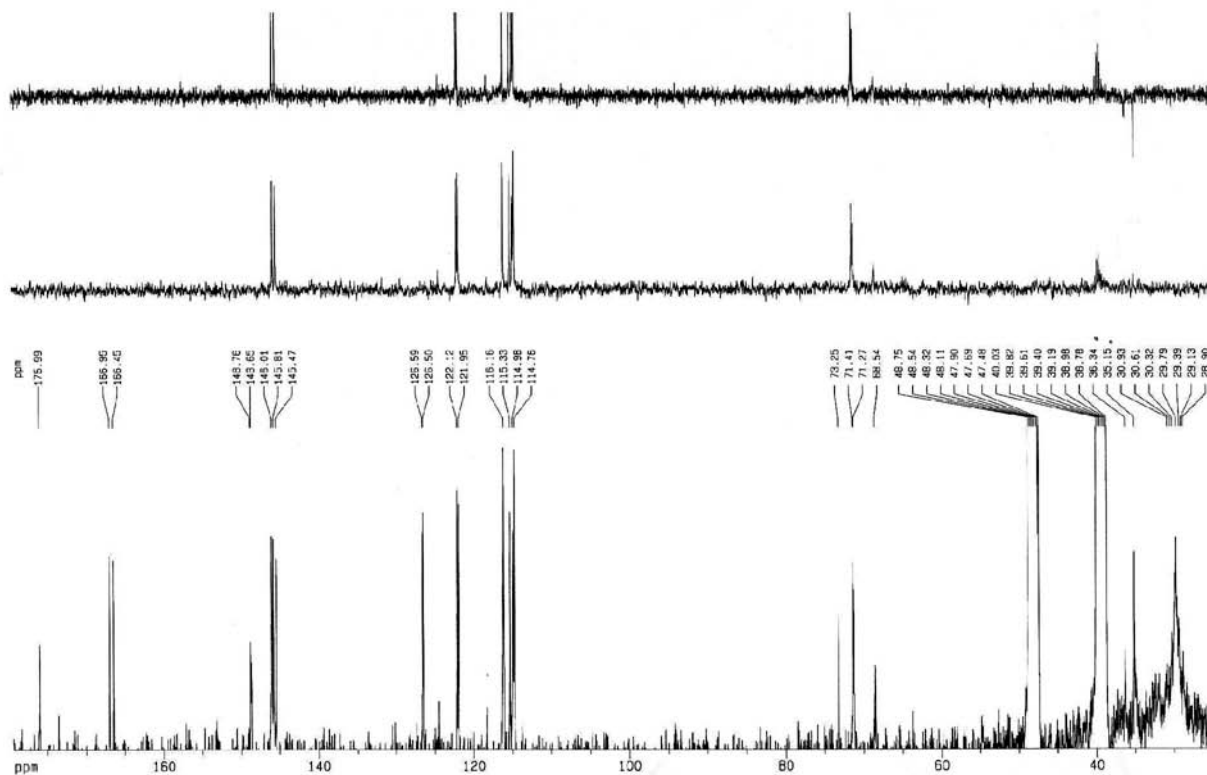
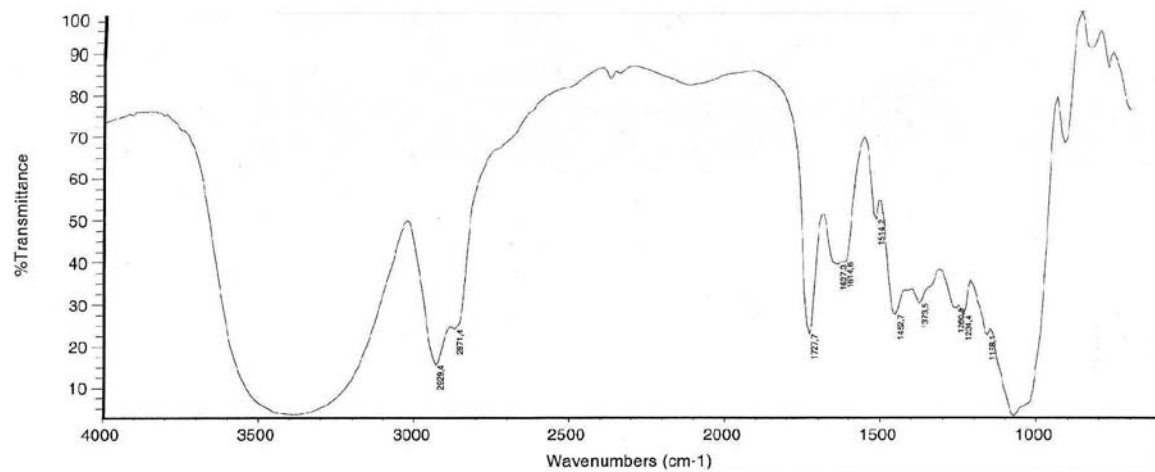


Figure S4. ^{13}C NMR (DMSO) spectrum of compound 2.



Collection time: Tue May 20 09:57:57 2008

Tue May 20 09:59:00 2008

FIND PEAKS:

Spectrum: *D-1 kaurano

Region: 4000.0 600.0

Absolute threshold: 51,532

Sensitivity: 50

Peak list:

Position	Intensity
1073.0	3,058
3390.6	3,457
2929.4	15,593
1158.1	22,644
1727.7	22,886
2871.4	24,078
1234.4	27,370
1452.7	27,575
1260.5	28,115
1373.5	30,277
1637.3	38,385
1614.6	38,929
1514.2	50,031

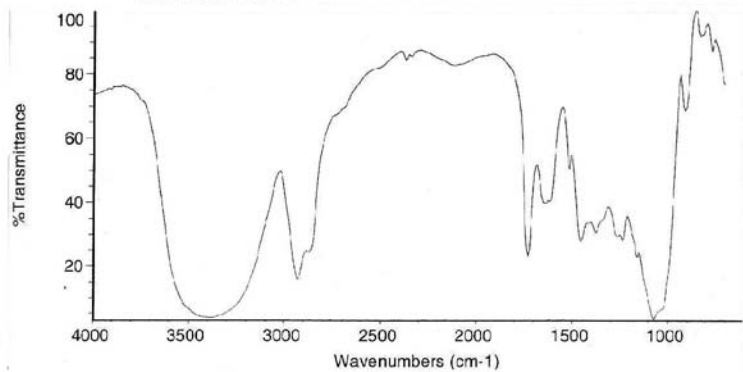
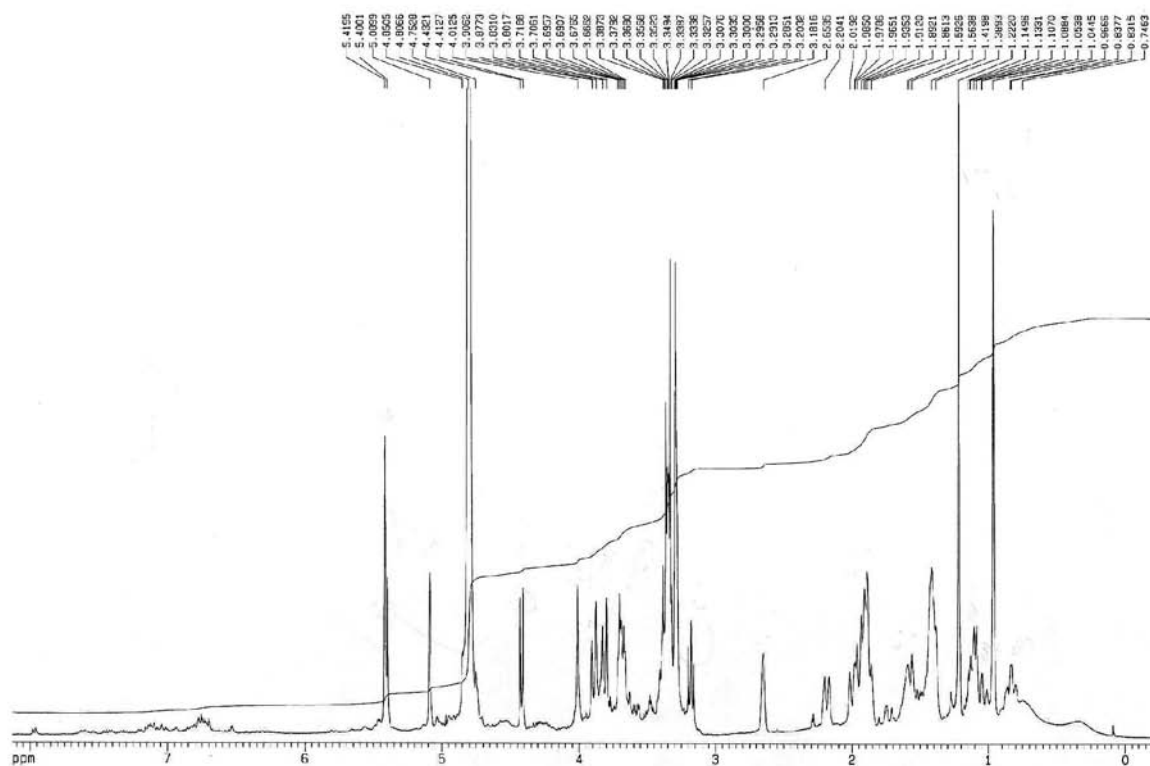
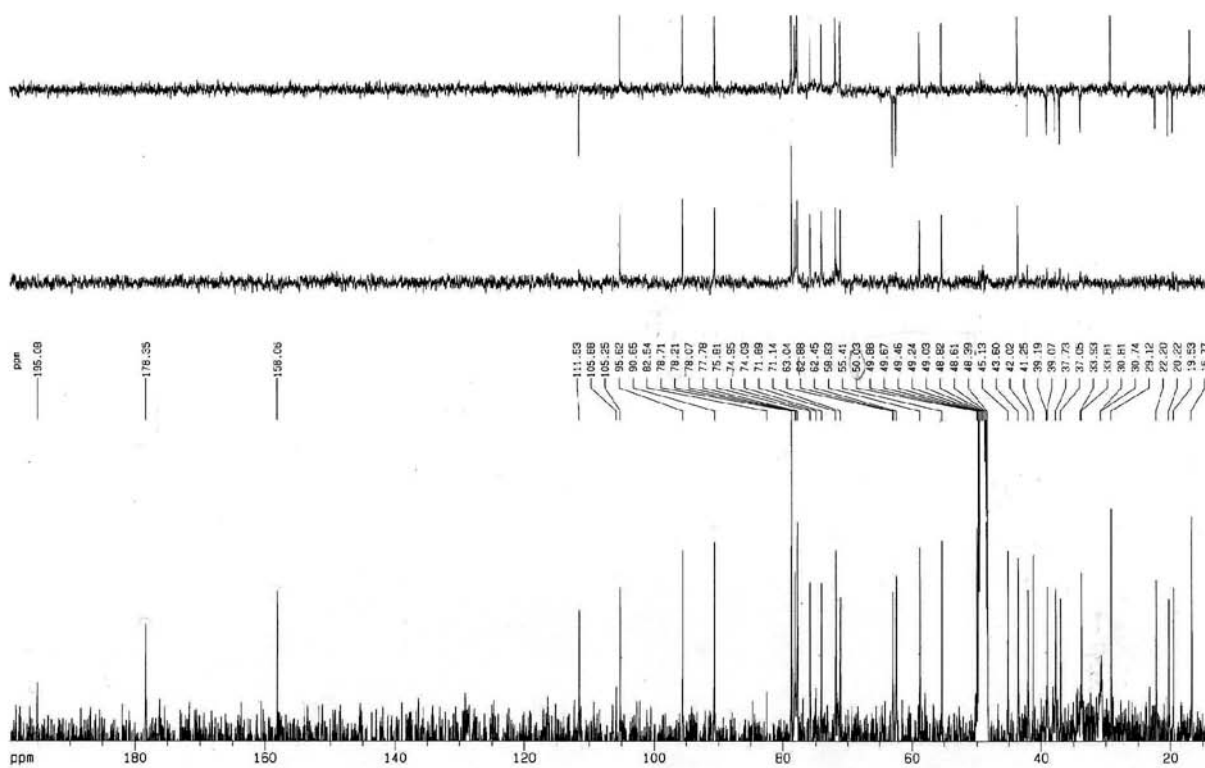


Figure S5. IR (film) spectrum of compound 3.

Figure S6. ^1H NMR (CD_3OD) spectrum of compound 3.Figure S7. ^{13}C NMR (CD_3OD) spectrum of compound 3.

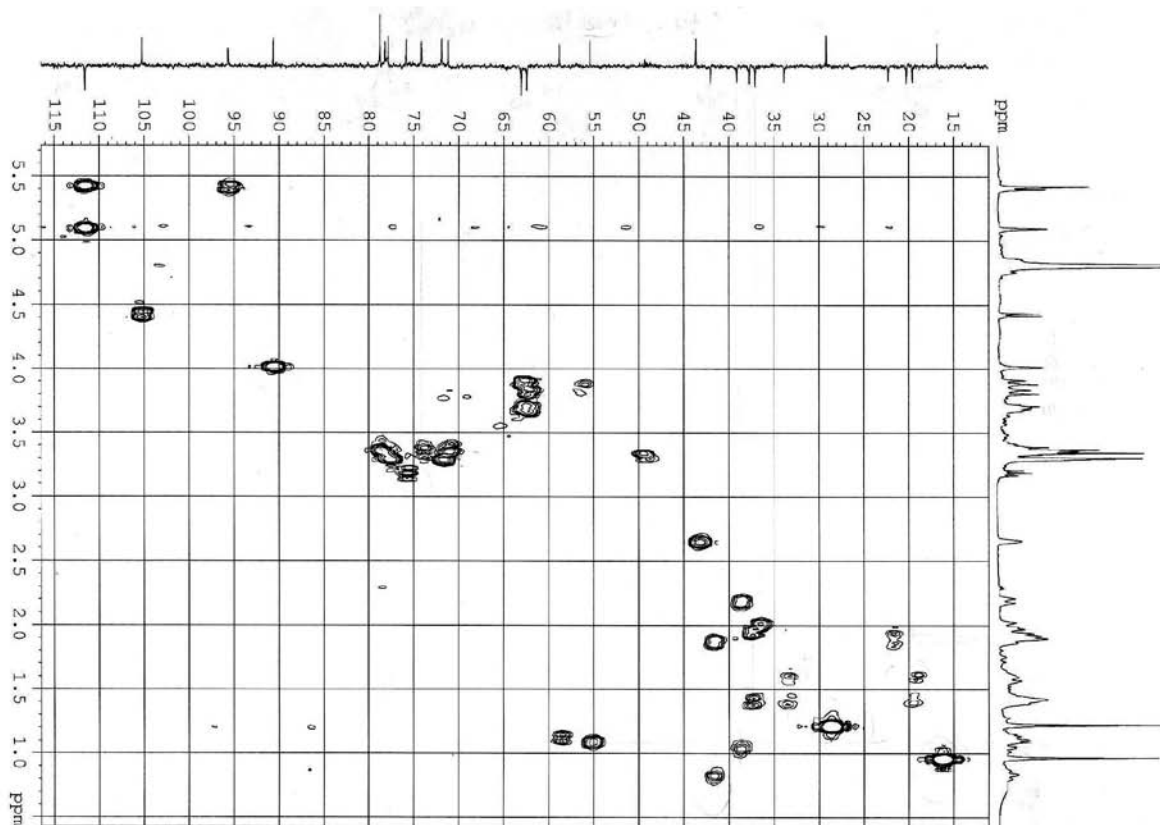


Figure S8. HMQC spectrum of compound 3.

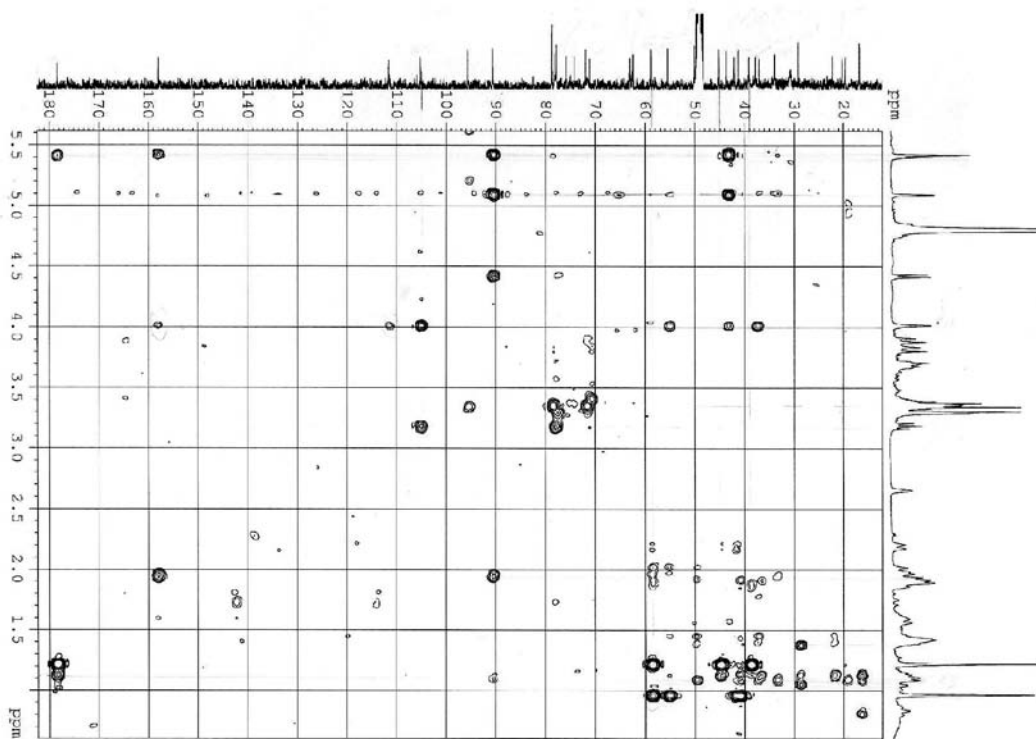


Figure S9. HMBC spectrum of compound 3.

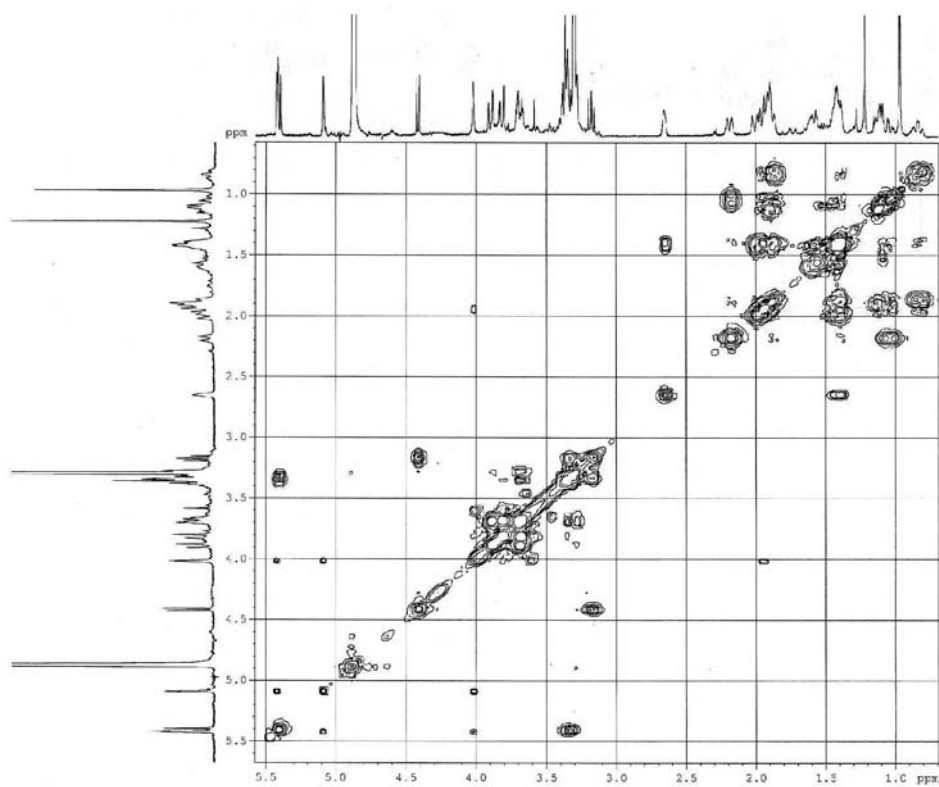


Figure S10. COSY spectrum of compound 3.

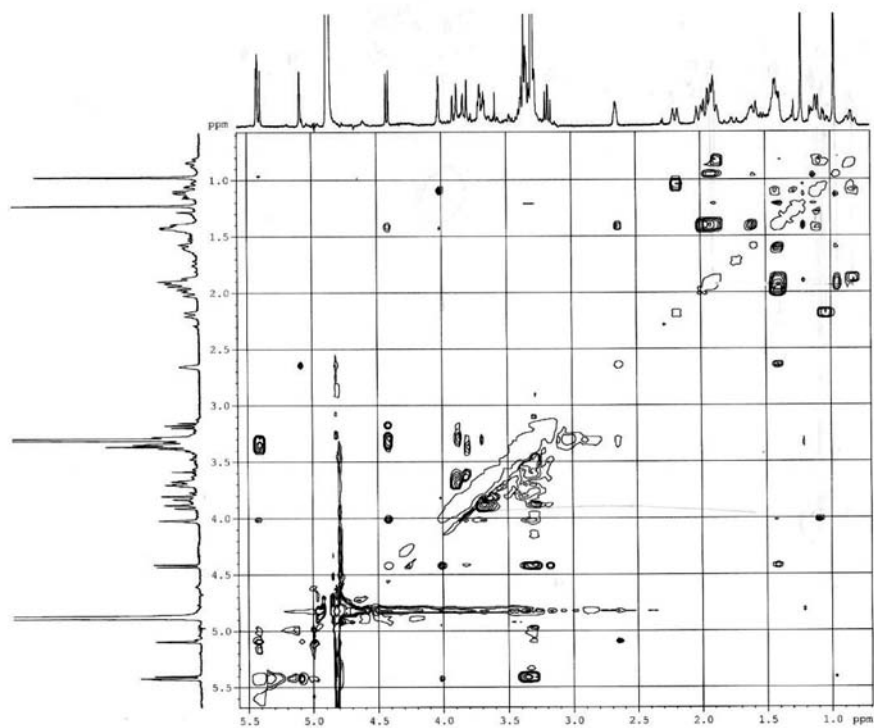
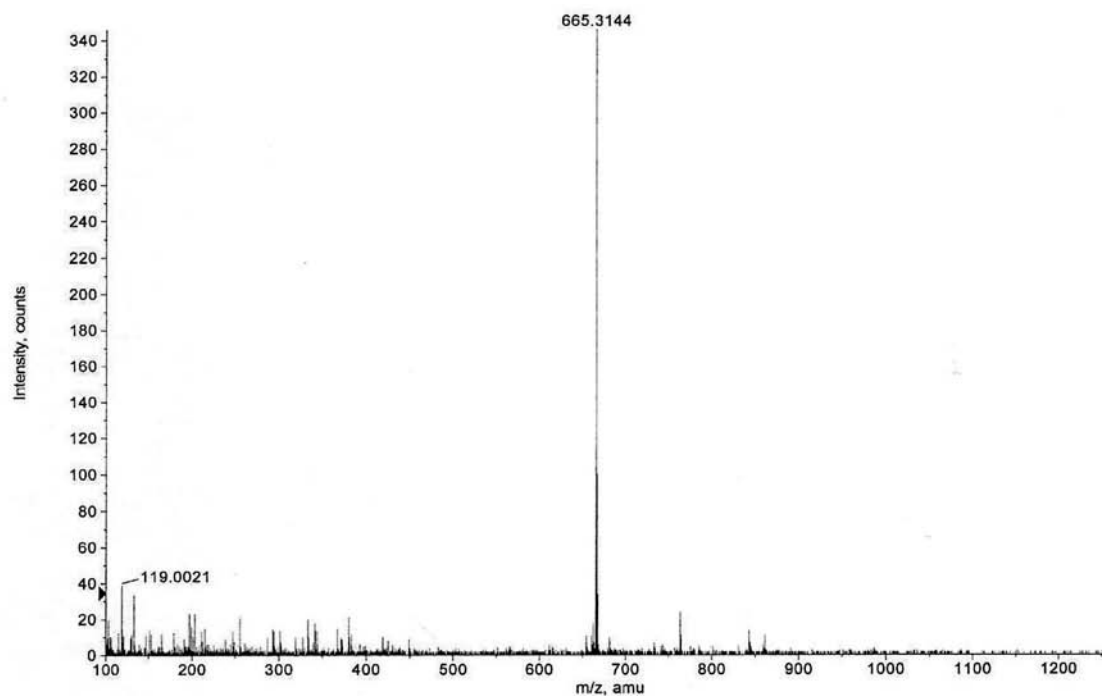


Figure S11. ROESY spectrum of compound 3.



Formula	CalculatedMass	mDaError	ppmError	RDB
C32 H50 O13 Na	665.314363	0.03656	0.054951	7.5
C30 H45 N6 O11	665.314083	0.316692	0.476003	11.5
C45 H42 N2 O2 Na	665.31385	0.549904	0.826532	25.5
C43 H37 N8	665.31357	0.830036	1.247584	29.5
C31 H41 N10 O7	665.315421	-1.02062	-1.53404	16.5
C33 H46 N4 O9 Na	665.315701	-1.300752	-1.955092	12.5
C29 H42 N10 O7 Na	665.313015	1.38464	2.08118	13.5
C29 H49 N2 O15	665.312746	1.654004	2.486047	6.5
C47 H41 N2 O2	665.316255	-1.855356	-2.788688	28.5
C42 H41 N4 O4	665.312233	2.167348	3.257627	24.5
C34 H49 O13	665.316769	-2.3687	-3.560269	10.5
C34 H42 N8 O5 Na	665.317038	-2.638064	-3.965136	17.5
C28 H46 N6 O11 Na	665.311678	2.721952	4.091223	8.5
C21 H50 N6 O16 Na	665.317551	-3.151408	-4.736716	-0.5
C41 H38 N8 Na	665.311165	3.235296	4.862804	26.5
C50 H42 Na	665.317873	-3.4728	-5.219784	29.5
C41 H45 O8	665.310895	3.50466	5.267671	19.5
C35 H45 N4 O9	665.318106	-3.706012	-5.570312	15.5
C27 H50 N2 O15 Na	665.310341	4.059264	6.101267	3.5
C25 H45 N8 O13	665.310061	4.339396	6.522319	7.5
C22 H46 N10 O12 Na	665.318889	-4.48872	-6.74676	4.5
C40 H42 N4 O4 Na	665.309827	4.572608	6.872847	21.5
C38 H37 N10 O2	665.309547	4.85274	7.293899	25.5

Figure S12. HRMS spectrum of compound 3.