HOKKAIDO UNIVERSITY

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Supplementary material

Isolation of rugosin A, B and related compounds as dipeptidyl peptidase-IV inhibitors from rose bud extract powder

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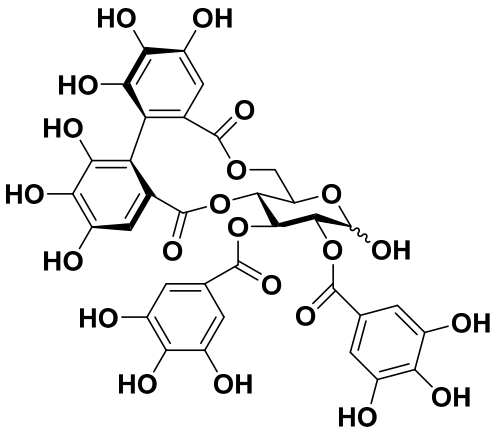
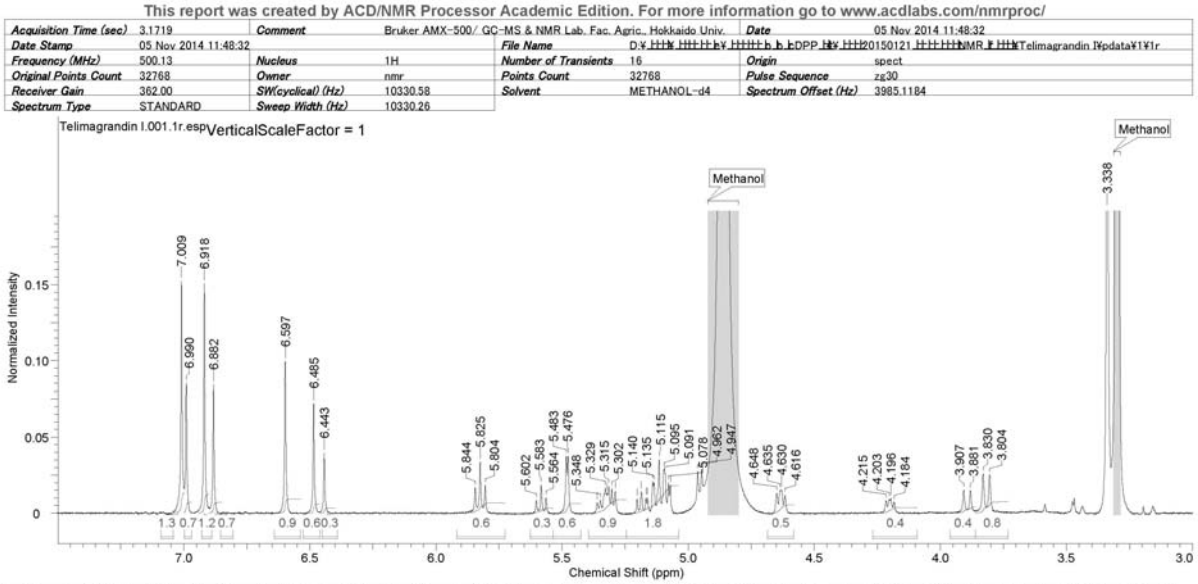
^{1}H NMR spectrum data of the isolated compounds in CD_3OD

Tellimagrandin I (**1**, mixture of α, β-anomer)



Tellimagrandin I (1)

^{1}H NMR (500 MHz, CD_3OD, rt) α-anomer: 3.82 (1H, d, J = 12.8 Hz), 4.63 (1H, dd, J = 6.9, 9.9 Hz), 5.09 (1H, dd, J = 3.7, 9.9 Hz), 5.12 (1H, dd, J = 9.9, 10.0 Hz), 5.31 (1H, dd, J = 6.9, 12.8 Hz), 5.48 (1H, d, J = 3.7 Hz), 5.83 (1H, dd, J = 9.9, 10.0 Hz), 6.49 (1H, s), 6.60 (1H, s), 6.92 (2H, s), 7.01 (2H, s) ppm; β-anomer: 3.89 (1H, d, J = 12.9 Hz), 4.20 (1H, dd, J = 6.3, 9.5 Hz), 4.95 (1H, d, J = 7.9 Hz), 5.14 (1H, t, J = 10.2 Hz), 5.19 (1H, t, J = 8.9 Hz), 5.34 (1H, dd, J = 6.3, 13.2 Hz), 5.58 (1H, t, J = 9.6 Hz), 6.44 (1H, s), 6.60 (1H, s), 6.88 (2H, s), 6.99 (2H, s) ppm



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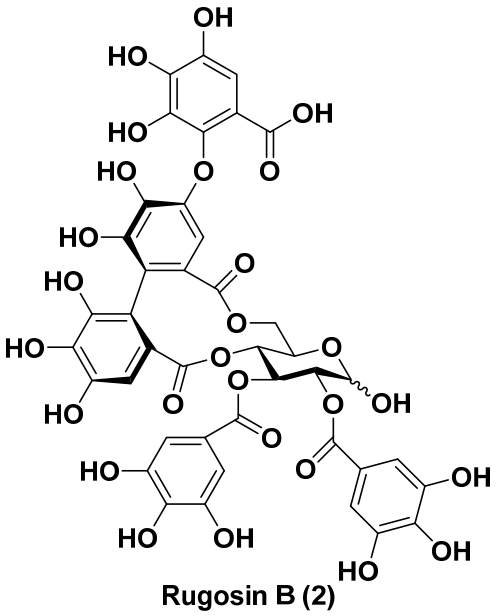
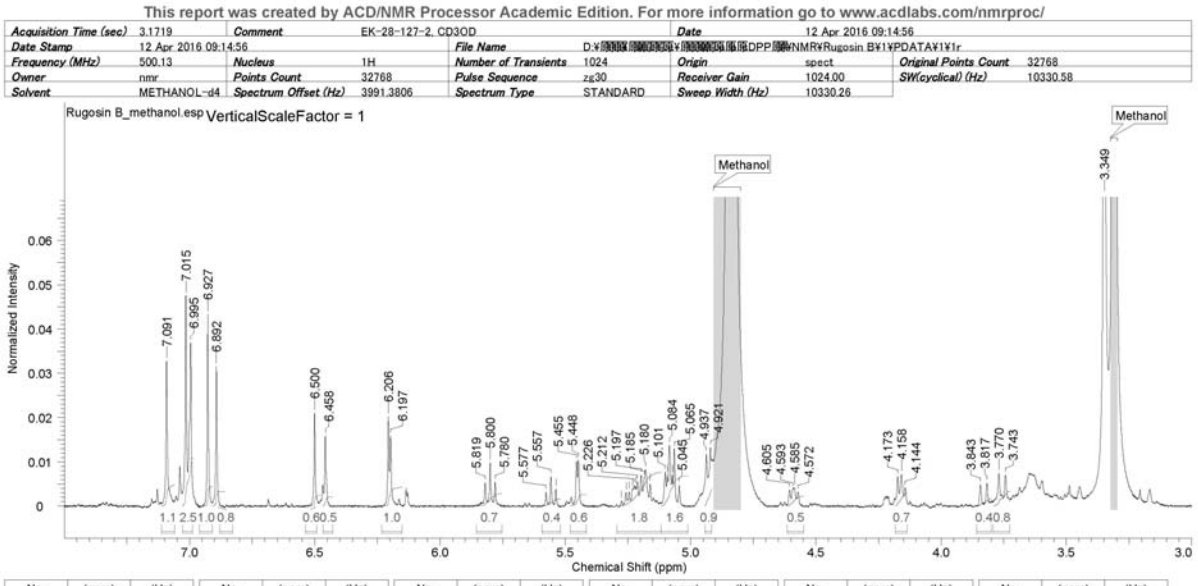
1	3.34	1669.7	10	4.62	2308.7	19	5.10	2548.3	28	5.30	2651.7	37	5.58	2792.0	46	6.92	3460.0
2	3.80	1902.6	11	4.63	2315.6	20	5.11	2558.1	29	5.32	2658.3	38	5.60	2801.8	47	6.99	3496.0
3	3.83	1915.6	12	4.64	2318.2	21	5.13	2568.2	30	5.32	2661.8	39	5.80	2903.0	48	7.01	3505.4
4	3.88	1941.1	13	4.65	2324.8	22	5.14	2570.7	31	5.33	2664.9	40	5.82	2913.1			
5	3.91	1954.0	14	4.95	2473.9	23	5.16	2581.1	32	5.35	2674.7	41	5.84	2922.8			
6	4.18	2092.4	15	4.96	2481.8	24	5.17	2584.2	33	5.36	2681.0	42	6.44	3222.3			
7	4.20	2098.7	16	5.07	2536.0	25	5.19	2593.4	34	5.48	2738.7	43	6.48	3243.1			
8	4.20	2101.9	17	5.08	2539.8	26	5.20	2601.9	35	5.48	2742.2	44	6.60	3299.6			
9	4.22	2108.2	18	5.09	2546.4	27	5.29	2645.1	36	5.56	2782.5	45	6.88	3441.8			

Rugosin B (**2**)



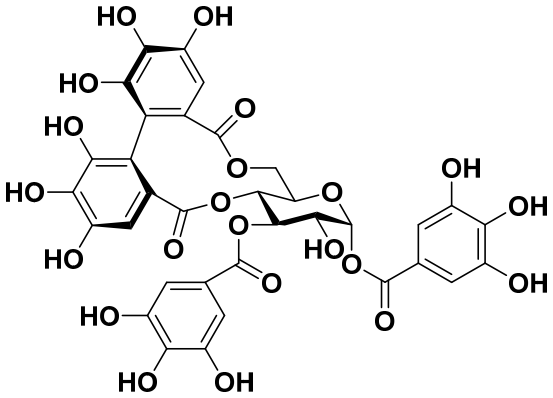
^{1}H NMR (500 MHz, CD_3OD, rt) α-anomer: 3.75 (1H, d, J = 13.2 Hz), 4.59 (1H, dd, J = 6.6, 10.1 Hz), 5.05-5.10 (2H, m), 5.16-5.27 (1H, m), 5.45 (1H, d, J = 3.8 Hz), 5.80 (1H, t, J = 9.9 Hz), 6.21 (1H, s), 6.50 (1H, s), 6.93 (2H, s), 7.02 (2H, s), 7.09 (1H, s) ppm;

β-anomer: 3.83 (1H, d, J = 13.2 Hz), 4.16 (1H, dd, J = 6.6, 10.1 Hz), 4.93 (1H, d, J = 8.2 Hz), 5.05-5.10 (1H, m), 5.16-5.27 (2H, m), 5.56 (1H, t, J = 9.8 Hz), 6.20 (1H, s), 6.46 (1H, s), 6.89 (2H, s), 7.00 (2H, s), 7.09 (1H, s) ppm



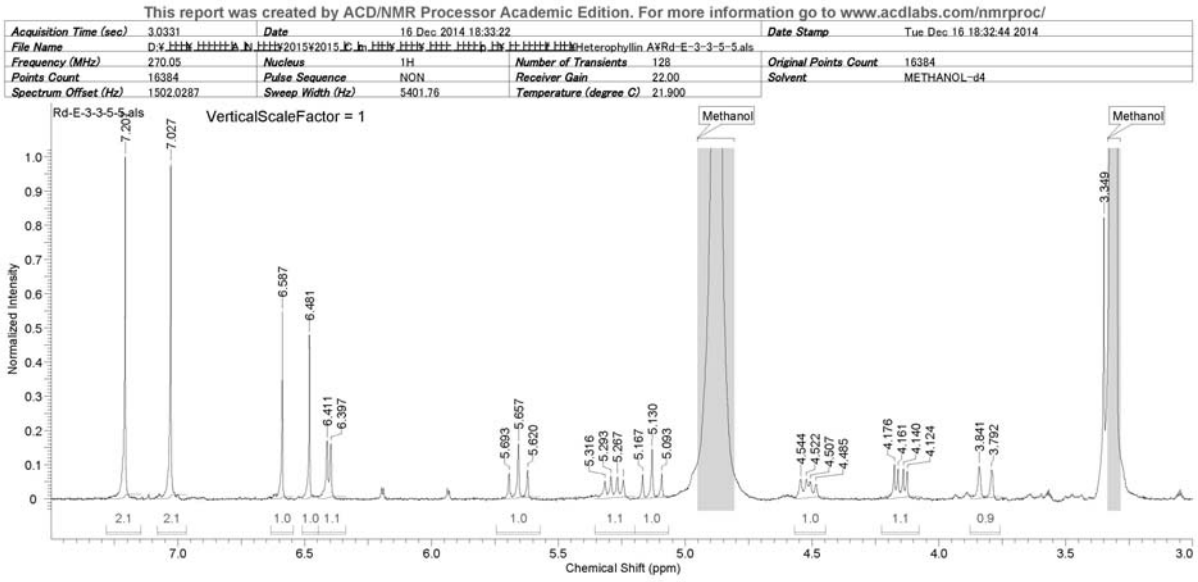
No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	3.35	1675.0	10	4.59	2293.2	19	5.09	2547.0	28	5.23	2616.7	37	5.78	2890.6	46	7.00	3498.5
2	3.74	1872.0	11	4.59	2297.0	20	5.10	2551.1	29	5.25	2623.3	38	5.80	2900.7	47	7.01	3508.2
3	3.77	1885.3	12	4.61	2303.3	21	5.16	2581.0	30	5.26	2629.3	39	5.82	2910.5	48	7.09	3546.4
4	3.82	1908.9	13	4.92	2460.9	22	5.18	2590.5	31	5.28	2638.4	40	6.20	3099.3			
5	3.84	1922.1	14	4.94	2469.1	23	5.18	2593.0	32	5.45	2724.5	41	6.21	3103.8			
6	4.14	2072.5	15	5.04	2523.0	24	5.20	2599.0	33	5.46	2728.3	42	6.46	3229.9			
7	4.16	2079.8	16	5.06	2533.1	25	5.21	2606.6	34	5.54	2769.6	43	6.50	3251.0			
8	4.17	2087.0	17	5.07	2536.9	26	5.22	2610.1	35	5.56	2779.3	44	6.89	3447.1			
9	4.57	2286.6	18	5.08	2542.6	27	5.23	2613.5	36	5.58	2789.1	45	6.93	3464.4			

Heterophyllin A (**3**)



Heterophyllin A (3)

^{1}H-NMR (270 MHz, CD_3OD, rt): 3.82 (1H, d, J = 13.3 Hz), 4.15 (1H, dd, J = 4.1, 9.9 Hz), 4.52 (1H, dd, J = 6.2, 10.2 Hz), 5.13 (1H, dd, J = 10.0, 10.2 Hz), 5.28 (1H, dd, J = 6.2, 13.3 Hz), 5.66 (1H, dd, J = 9.9, 10.0 Hz), 6.40 (1H, d, J = 4.1 Hz), 6.48 (1H, s), 6.59 (1H, s), 7.03 (2H, s), 7.21 (2H, s)



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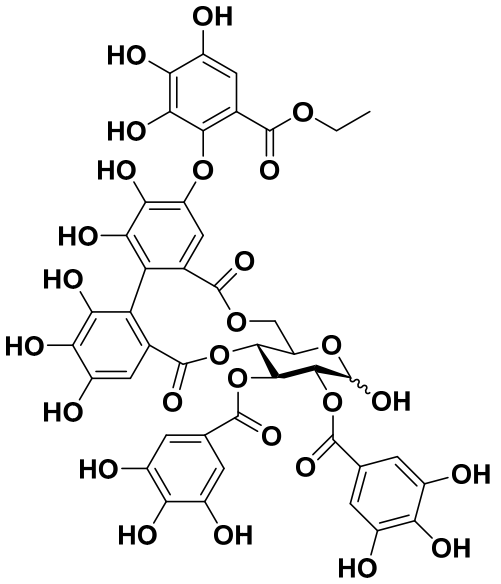
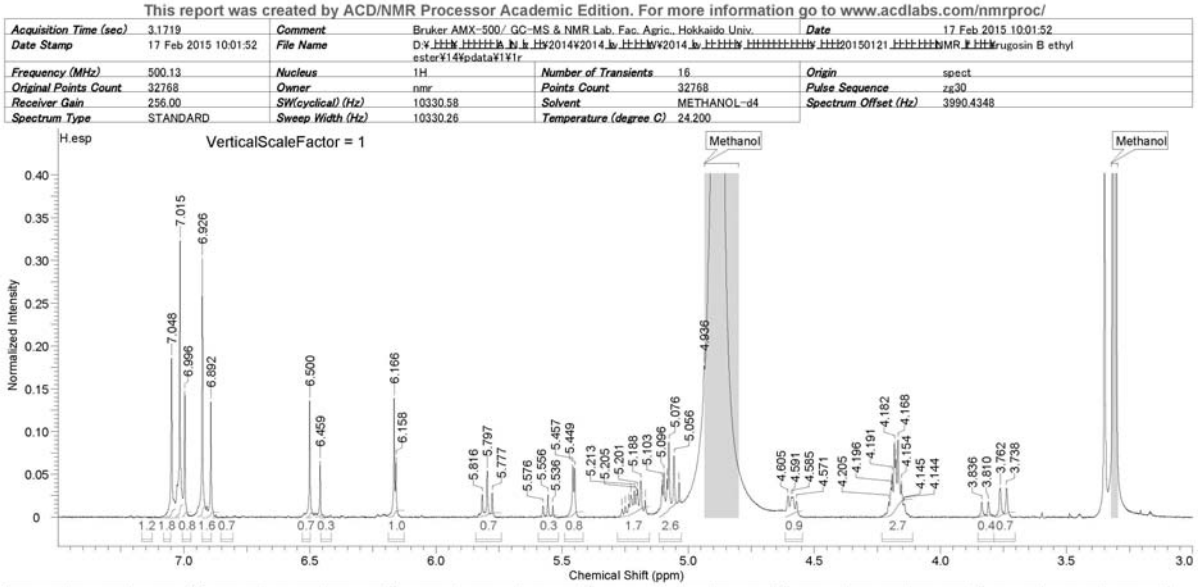
Points Count	16384	Pulse Sequence	NON	Receiver Gain	22.00	Solvent	METHANOL-d4
Spectrum Offset (Hz)	1502.0287	Sweep Width (Hz)	5401.76	Temperature (degree C)	21.900		

No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	3.35	904.4	6	4.16	1123.7	11	4.54	1227.2	16	5.27	1422.4	21	5.69	1537.5	26	7.03	1897.5
2	3.79	1024.1	7	4.18	1127.6	12	5.09	1375.3	17	5.29	1429.3	22	6.40	1727.4	27	7.21	1946.3
3	3.84	1037.3	8	4.48	1211.1	13	5.13	1385.5	18	5.32	1435.6	23	6.41	1731.3			
4	4.12	1113.8	9	4.51	1217.0	14	5.17	1395.4	19	5.62	1517.7	24	6.48	1750.1			
5	4.14	1118.1	10	4.52	1221.3	15	5.24	1415.8	20	5.66	1527.6	25	6.59	1778.8			

Rugosin B ethyl ester (**4**)



Rugosin B ethyl ester (4)



No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	1.18	590.5	11	4.15	2073.2	21	4.59	2296.0	31	5.19	2594.6	41	5.54	2768.9	51	6.89	3447.1
2	1.20	597.7	12	4.15	2077.6	22	4.60	2303.0	32	5.20	2601.2	42	5.56	2778.7	52	6.93	3463.8
3	1.21	604.0	13	4.17	2084.5	23	4.94	2468.8	33	5.20	2603.1	43	5.58	2788.5	53	7.00	3498.8
4	1.21	604.7	14	4.18	2088.9	24	5.04	2518.6	34	5.21	2607.2	44	5.78	2889.1	54	7.01	3508.2
5	1.22	611.0	15	4.18	2091.4	25	5.06	2528.7	35	5.23	2614.1	45	5.80	2899.1	55	7.05	3524.9
6	3.74	1869.5	16	4.19	2095.9	26	5.08	2538.8	36	5.24	2618.2	46	5.82	2908.9			
7	3.76	1881.5	17	4.20	2098.4	27	5.08	2542.3	37	5.25	2625.2	47	6.16	3079.8			
8	3.81	1905.4	18	4.21	2103.1	28	5.10	2548.9	38	5.26	2632.1	48	6.17	3083.6			
9	3.84	1918.4	19	4.57	2286.3	29	5.10	2552.4	39	5.45	2725.4	49	6.46	3230.2			
10	4.14	2072.5	20	4.59	2293.2	30	5.17	2585.8	40	5.46	2729.2	50	6.50	3251.0			

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

Acquisition Time (sec)	1.0027	*Comment*	Bruker AMX-500/ GC-MS & NMR Lab. Fac. Agric., Hokkaido Univ.	*Date*	17 Feb 2015 15:26:08		
Date Stamp	17 Feb 2015 15:26:08			*File Name*	D:¥ [illegible] ¥NMR¥Rugosin B ethyl ester¥C¥pdata¥1¥1r		
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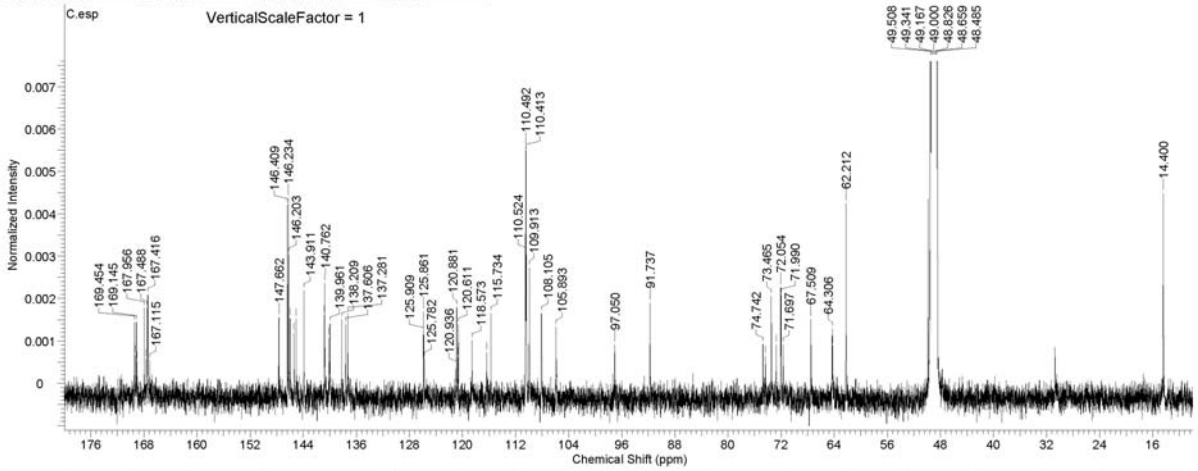
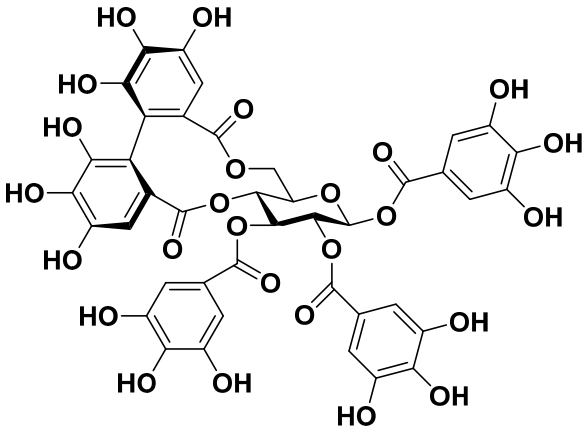
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	16384.00	*SW(cyclical) (Hz)*	32679.74	*Solvent*	METHANOL-d4	*Spectrum Offset (Hz)*	15267.0410
Spectrum Type	STANDARD	*Sweep Width (Hz)*	32678.74				



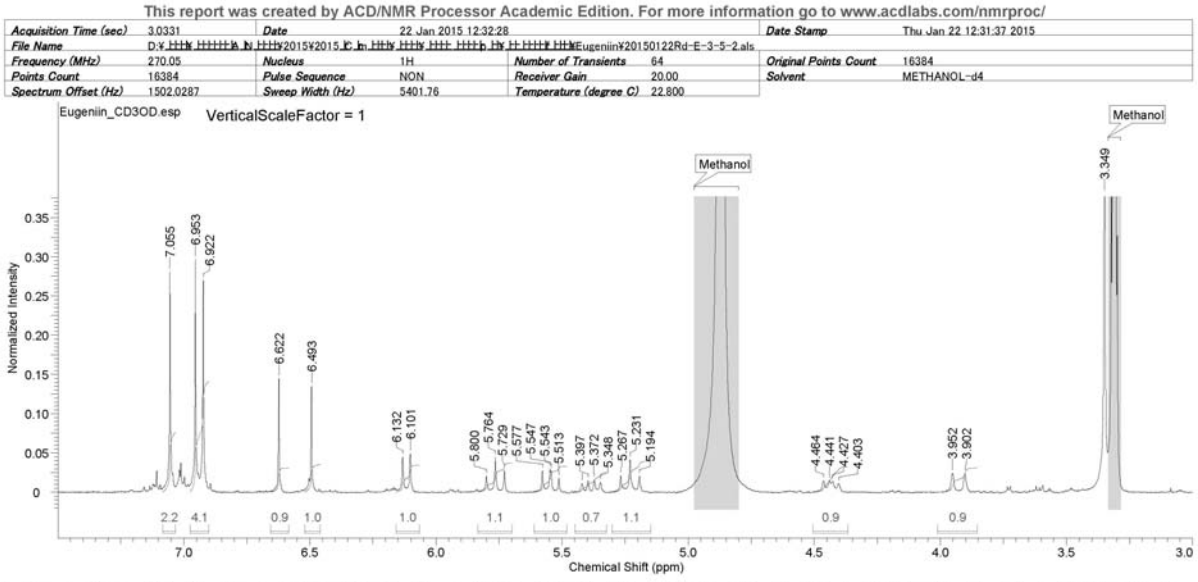
No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	14.40	1810.9	12	64.31	8086.9	23	105.89	13316.8	34	120.67	15174.8	45	140.76	17702.0	56	147.71	18575.6
2	14.44	1815.9	13	67.51	8489.8	24	108.11	13595.1	35	120.88	15201.7	46	140.83	17709.9	57	167.12	21016.0
3	48.48	6097.3	14	71.70	9016.4	25	109.91	13822.4	36	120.94	15208.7	47	143.91	18097.9	58	167.42	21053.9
4	48.66	6119.2	15	71.99	9053.3	26	110.37	13879.3	37	125.78	15818.1	48	145.07	18243.5	59	167.49	21062.9
5	48.83	6140.2	16	72.05	9061.3	27	110.41	13885.3	38	125.86	15828.0	49	145.40	18285.4	60	167.73	21092.8
6	49.00	6162.1	17	72.73	9146.1	28	110.49	13895.2	39	125.91	15834.0	50	145.99	18359.2	61	167.96	21121.7
7	49.17	6183.1	18	73.47	9238.8	29	110.52	13899.2	40	137.28	17264.1	51	146.20	18386.1	62	169.07	21261.4
8	49.34	6205.0	19	74.37	9352.5	30	115.73	14554.5	41	137.61	17305.0	52	146.23	18390.1	63	169.15	21271.3
9	49.51	6226.0	20	74.74	9399.4	31	116.33	14629.3	42	138.21	17380.8	53	146.39	18409.1	64	169.35	21297.3
10	62.21	7823.6	21	91.74	11536.6	32	118.57	14911.5	43	139.96	17601.2	54	146.41	18412.0	65	169.45	21310.2
11	64.22	8076.0	22	97.05	12204.8	33	120.61	15167.8	44	140.18	17628.2	55	147.66	18569.6			

Eugeniin (**5**)



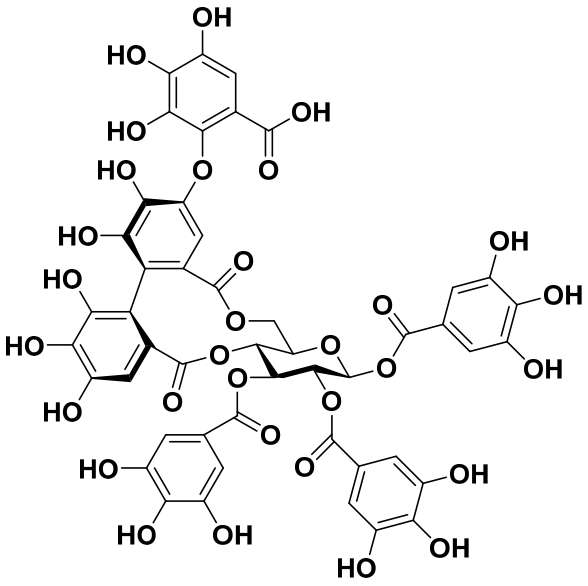
Eugeniin (5)

^{1}H-NMR (270 MHz, CD_3OD, rt): 3.93 (1H, d, J = 13.4 Hz), 4.43 (1H, dd, J = 6.6, 10.0 Hz), 5.23 (1H, dd, J = 9.5, 10.0 Hz), 5.38 (1H, dd, J = 6.6, 13.4 Hz), 5.55 (1H, dd, J = 8.2, 9.2 Hz), 5.76 (1H, dd, J = 9.2, 9.5 Hz), 6.11 (1H, d, J = 8.2 Hz), 6.49 (1H, s), 6.62 (1H, s), 6.92 (2H, s), 6.95 (2H, s), 7.06 (2H, s)



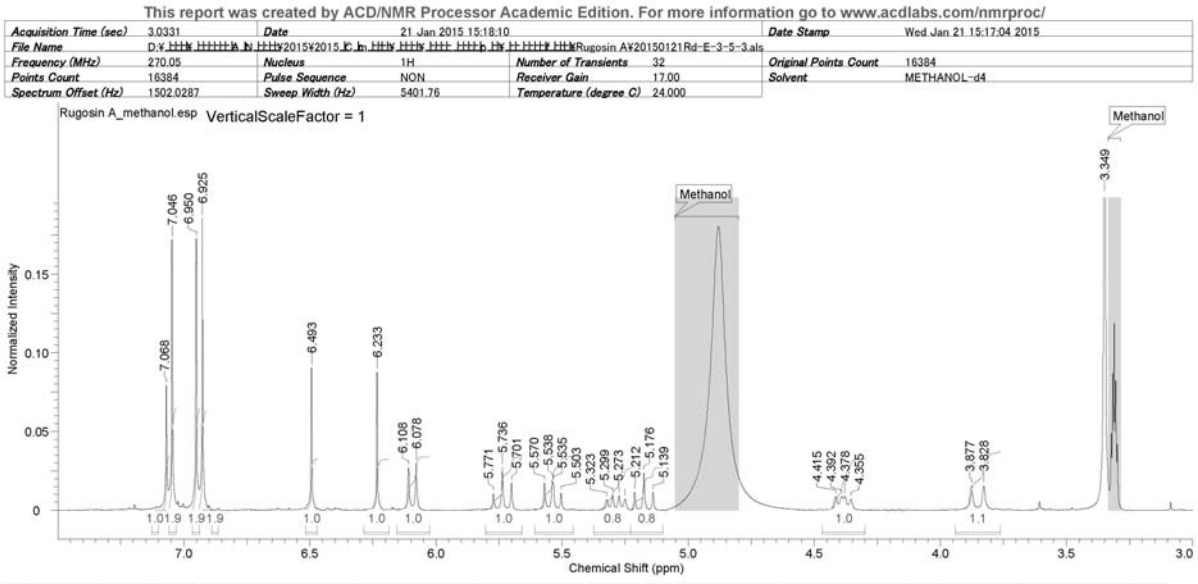
No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	3.35	904.4	6	4.44	1199.2	11	5.35	1444.2	16	5.54	1496.9	21	5.80	1566.2	26	6.92	1869.2
2	3.90	1053.8	7	4.46	1205.4	12	5.37	1450.8	17	5.55	1497.9	22	6.10	1647.6	27	6.95	1877.7
3	3.95	1067.3	8	5.19	1402.6	13	5.40	1457.4	18	5.58	1506.2	23	6.13	1655.8	28	7.05	1905.1
4	4.40	1189.0	9	5.23	1412.5	14	5.42	1463.9	19	5.73	1547.0	24	6.49	1753.4			
5	4.43	1195.6	10	5.27	1422.4	15	5.51	1488.7	20	5.76	1556.6	25	6.62	1788.4			

Rugosin A (**6**)



Rugosin A (6)

^{1}H-NMR (500 MHz, CD_3OD, rt): 3.85 (1H, d, J = 13.3 Hz), 4.38 (1H, dd, J = 6.4, 9.9 Hz), 5.18 (1H, dd, J = 9.5, 9.9 Hz), 5.29 (1H, dd, J = 6.4, 13.3 Hz), 5.54 (1H, dd, J = 8.4, 9.4 Hz), 5.74 (1H, dd, J = 9.4, 9.5 Hz), 6.09 (1H, d, J = 8.4 Hz), 6.23 (1H, s), 6.49 (1H, s), 6.93 (2H, s), 6.95 (2H, s), 7.05 (2H, s), 7.07 (1H, s)



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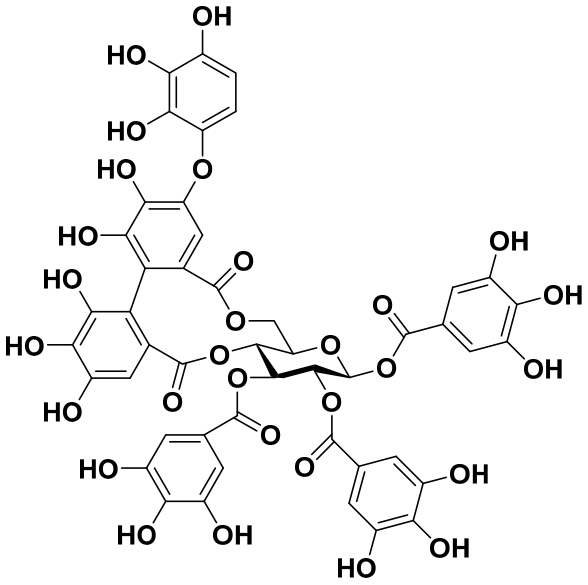
Points Count	16384	Pulse Sequence	NON	Receiver Gain	17.00	Solvent	METHANOL-d4
Spectrum Offset (Hz)	1502.0287	Sweep Width (Hz)	5401.76	Temperature (degree C)	24.000		

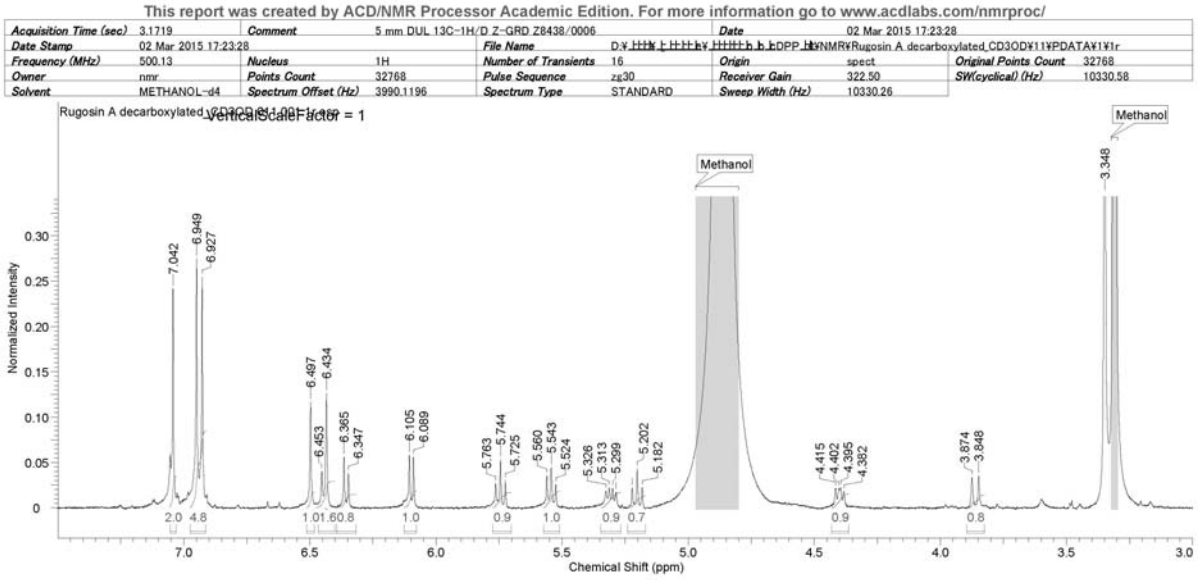
No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	3.35	904.4	6	4.39	1186.0	11	5.25	1417.8	16	5.53	1494.6	21	5.77	1558.6	26	6.93	1870.2
2	3.83	1033.7	7	4.41	1192.3	12	5.27	1424.1	17	5.54	1495.6	22	6.08	1641.3	27	6.95	1876.8
3	3.88	1046.9	8	5.14	1387.8	13	5.30	1431.0	18	5.57	1504.2	23	6.11	1649.6	28	7.05	1902.8
4	4.36	1176.1	9	5.18	1397.7	14	5.32	1437.6	19	5.70	1539.5	24	6.23	1683.2	29	7.07	1908.7
5	4.38	1182.4	10	5.21	1407.6	15	5.50	1486.0	20	5.74	1549.0	25	6.49	1753.4			

Rugosin A decarboxylated (**7**)



decarboxylated Rugosin A (7)

^{1}H-NMR (500 MHz, CD_3OD, rt): 3.86 (1H, d, J = 13.4 Hz), 4.40 (1H, dd, J = 6.3, 10.0 Hz), 5.20 (1H, dd, J = 9.8, 10.0 Hz), 5.31 (1H, dd, J = 6.3, 13.4 Hz), 5.54 (1H, dd, J = 8.6, 9.3 Hz), 5.74 (1H, dd, J = 9.3, 9.8 Hz), 6.09 (1H, d, J = 8.6 Hz), 6.36 (1H, d, J = 9.2 Hz), 6.43 (1H, s), 6.44 (1H, d, J = 9.2 Hz), 6.50 (1H, s), 6.93 (2H, s), 6.95 (2H, s), 7.04 (2H, s)

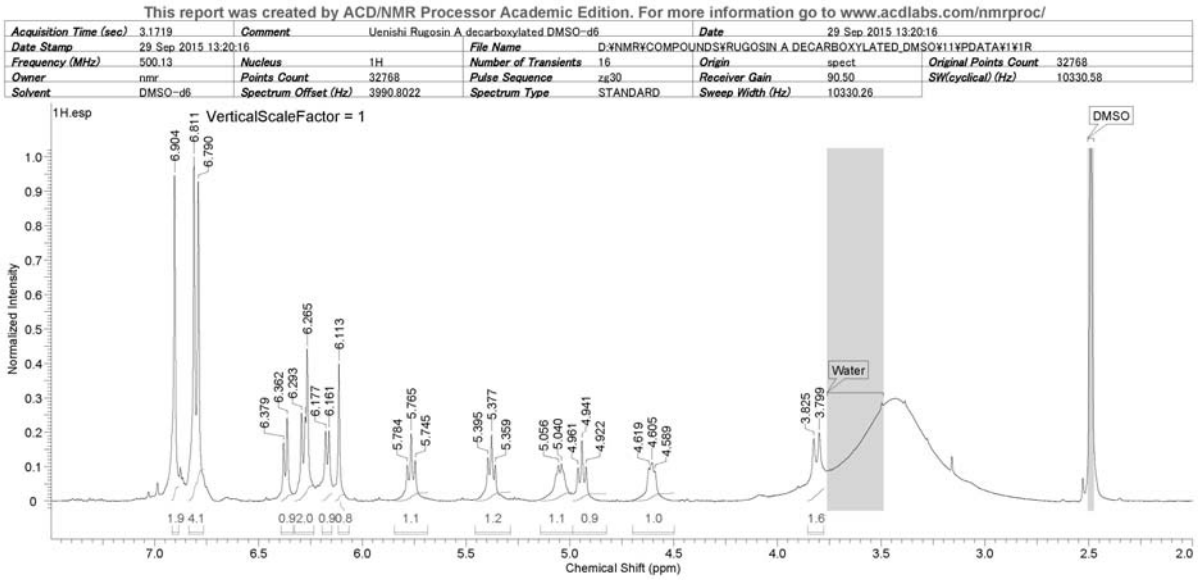


Acquisition Time (sec)	3.1719	Comment	5 mm DUL 13C-1H/D Z-GRD Z8438/0006	Date	02 Mar 2015 17:23:28		
Date Stamp	02 Mar 2015 17:23:28	File Name	D:¥ [illegible] ¥NMR¥Rugosin A decarboxylated_CD3OD¥11¥PDATA¥1¥1r				
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	16	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	322.50	SW(cyclical) (Hz)	10330.58
Solvent	METHANOL-d4	Spectrum Offset (Hz)	3990.1196	Spectrum Type	STANDARD	Sweep Width (Hz)	10330.26		

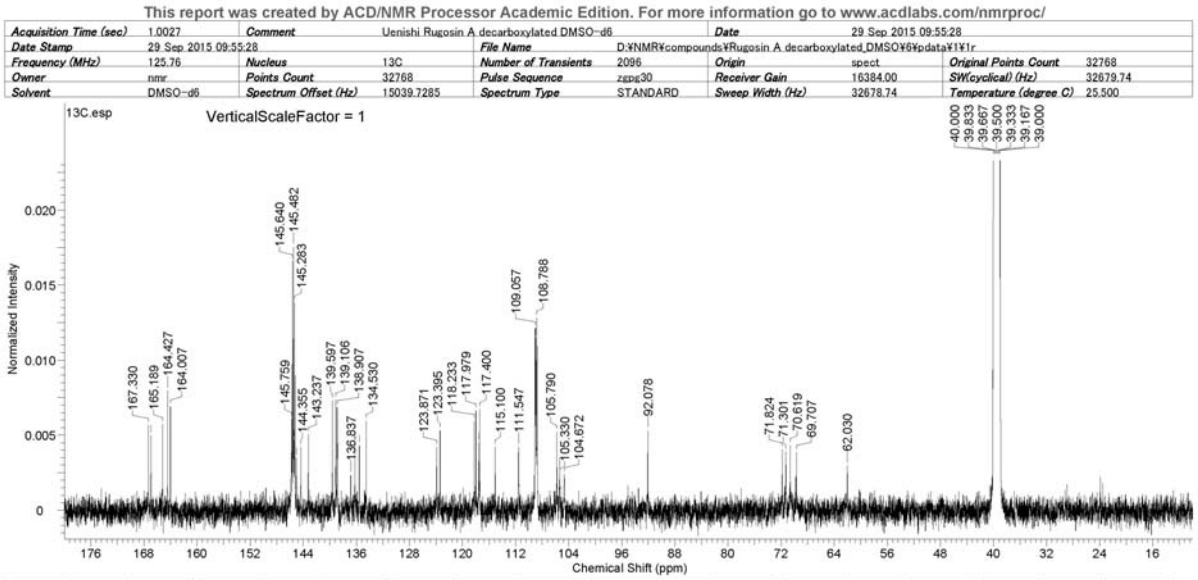
No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	3.35	1674.7	6	4.40	2201.5	11	5.29	2643.5	16	5.54	2772.1	21	6.09	3045.1	26	6.45	3227.3
2	3.85	1924.7	7	4.42	2208.1	12	5.30	2650.4	17	5.56	2780.9	22	6.11	3053.3	27	6.50	3249.4
3	3.87	1937.6	8	5.18	2591.8	13	5.31	2657.3	18	5.72	2863.2	23	6.35	3174.4	28	6.93	3464.4
4	4.38	2191.7	9	5.20	2601.9	14	5.33	2663.6	19	5.74	2872.7	24	6.36	3183.2	29	6.95	3475.5
5	4.40	2198.3	10	5.22	2611.6	15	5.52	2763.0	20	5.76	2882.4	25	6.43	3217.9	30	7.04	3522.1

NMR spectrums of rugosin A decarboxylated (**7**) in DMSO-d_6

^{1}H, ^{13}C spectrum in DMSO-d_6

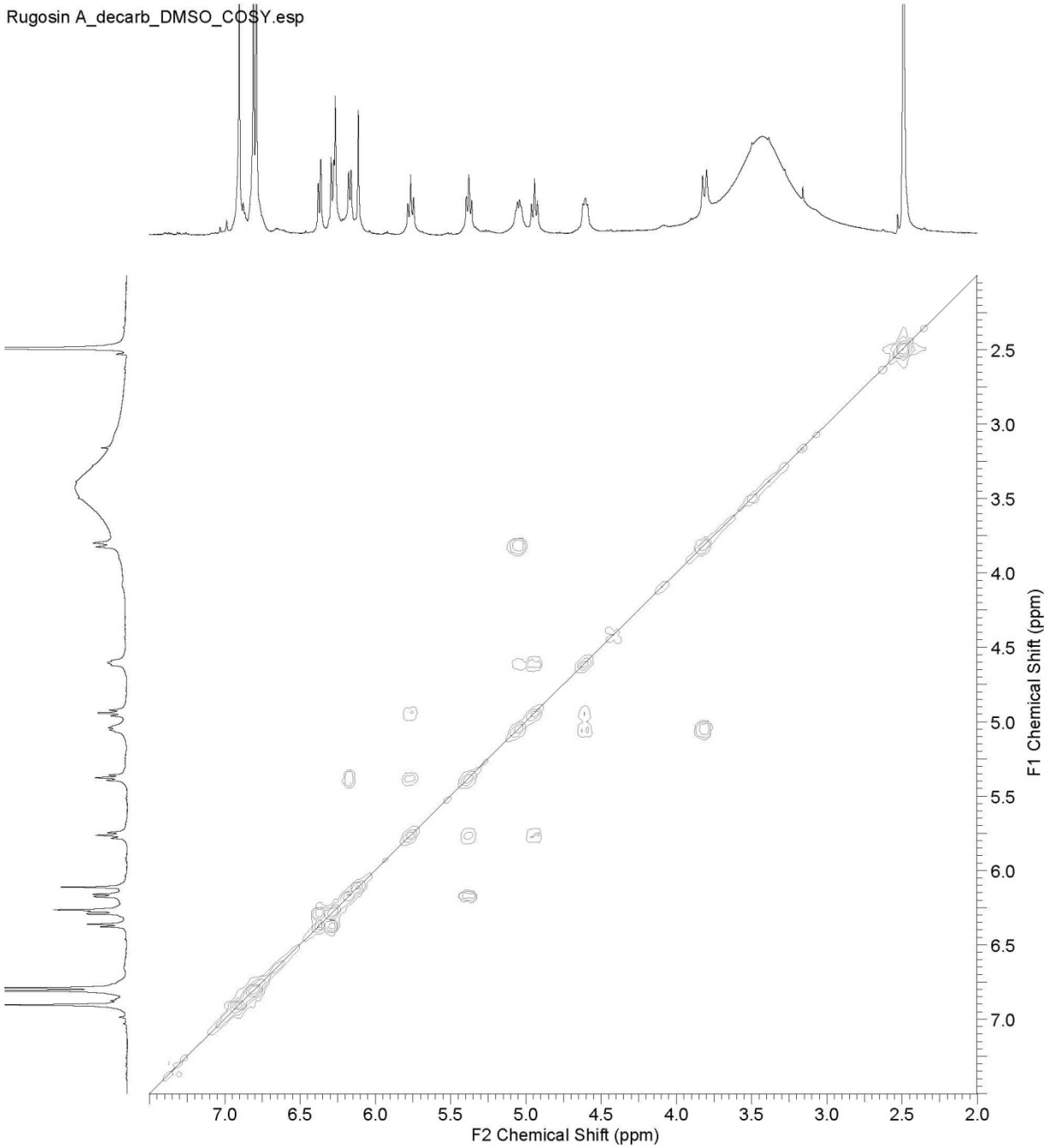


No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	3.80	1899.8	6	4.92	2461.6	11	5.36	2680.4	16	5.78	2892.6	21	6.27	3138.2	26	6.81	3406.5
2	3.83	1913.1	7	4.94	2471.4	12	5.38	2689.2	17	6.11	3057.1	22	6.29	3147.3	27	6.90	3453.1
3	4.59	2295.2	8	4.96	2481.2	13	5.39	2698.1	18	6.16	3081.1	23	6.36	3181.7			
4	4.60	2303.0	9	5.04	2520.9	14	5.75	2873.3	19	6.18	3089.3	24	6.38	3190.5			
5	4.62	2310.3	10	5.06	2528.4	15	5.76	2883.1	20	6.27	3133.4	25	6.79	3395.7			

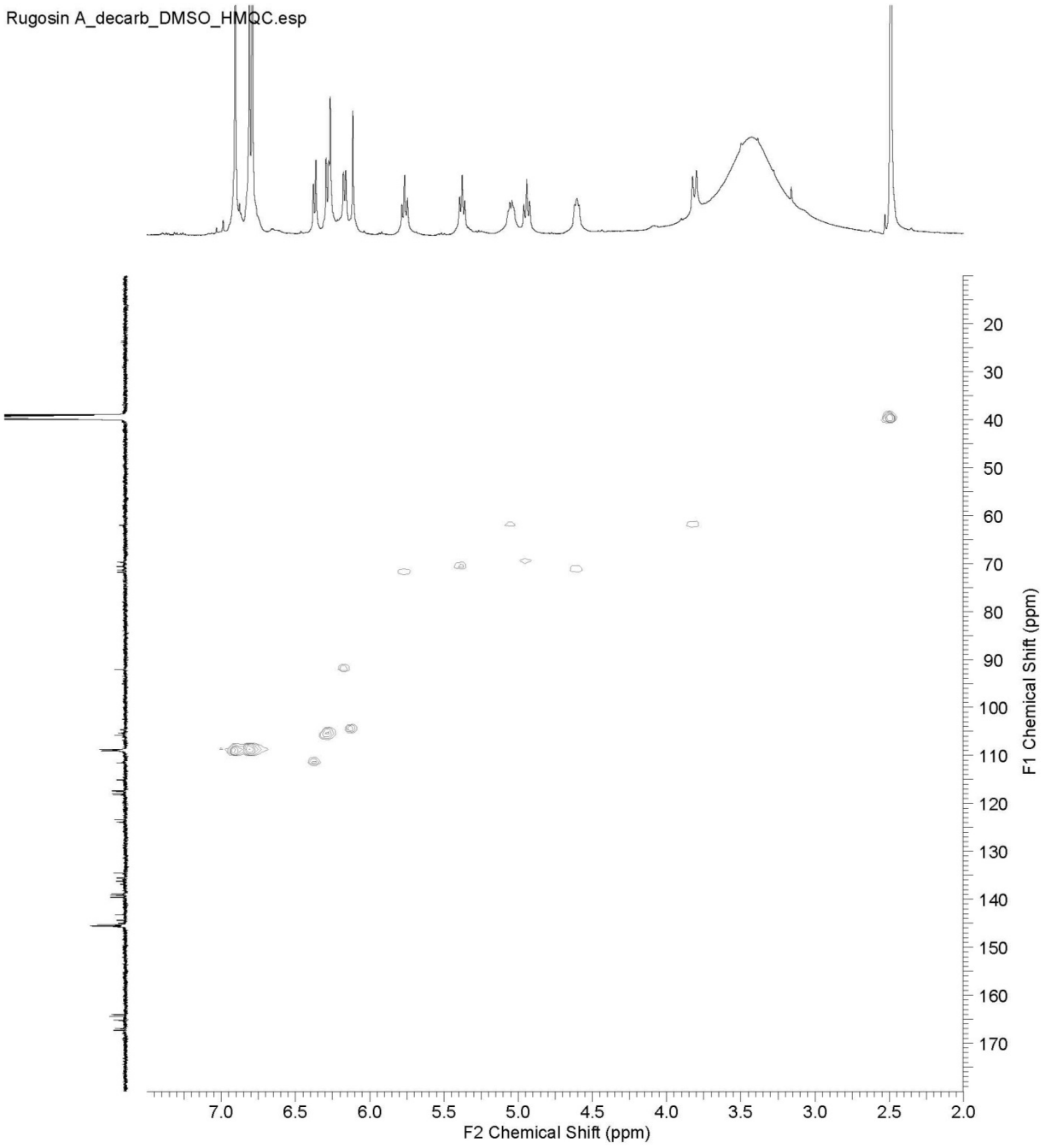


No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	No.	(ppm)	(Hz)
1	39.00	4904.6	10	70.62	8880.9	19	109.06	13714.8	28	134.53	16918.2	37	144.36	18153.8	46	165.19	20773.7
2	39.17	4925.5	11	71.30	8966.6	20	111.55	14028.0	29	135.56	17047.8	38	145.02	18237.6	47	166.93	20992.2
3	39.33	4946.5	12	71.82	9032.5	21	115.10	14474.8	30	136.20	17128.6	39	145.28	18270.5	48	167.33	21043.0
4	39.50	4967.4	13	92.08	11579.6	22	117.40	14764.0	31	136.84	17208.4	40	145.42	18287.5			
5	39.67	4988.4	14	104.67	13163.3	23	117.54	14781.9	32	138.86	17462.7	41	145.48	18295.4			
6	39.83	5009.3	15	105.33	13246.1	24	117.98	14836.8	33	138.91	17468.7	42	145.64	18315.4			
7	40.00	5030.3	16	105.79	13303.9	25	118.23	14868.7	34	139.11	17493.6	43	145.76	18330.3			
8	62.03	7800.8	17	108.79	13680.9	26	123.40	15517.9	35	139.60	17555.4	44	164.01	20625.1			
9	69.71	8766.2	18	108.95	13701.8	27	123.87	15577.8	36	143.24	18013.2	45	164.43	20678.0			

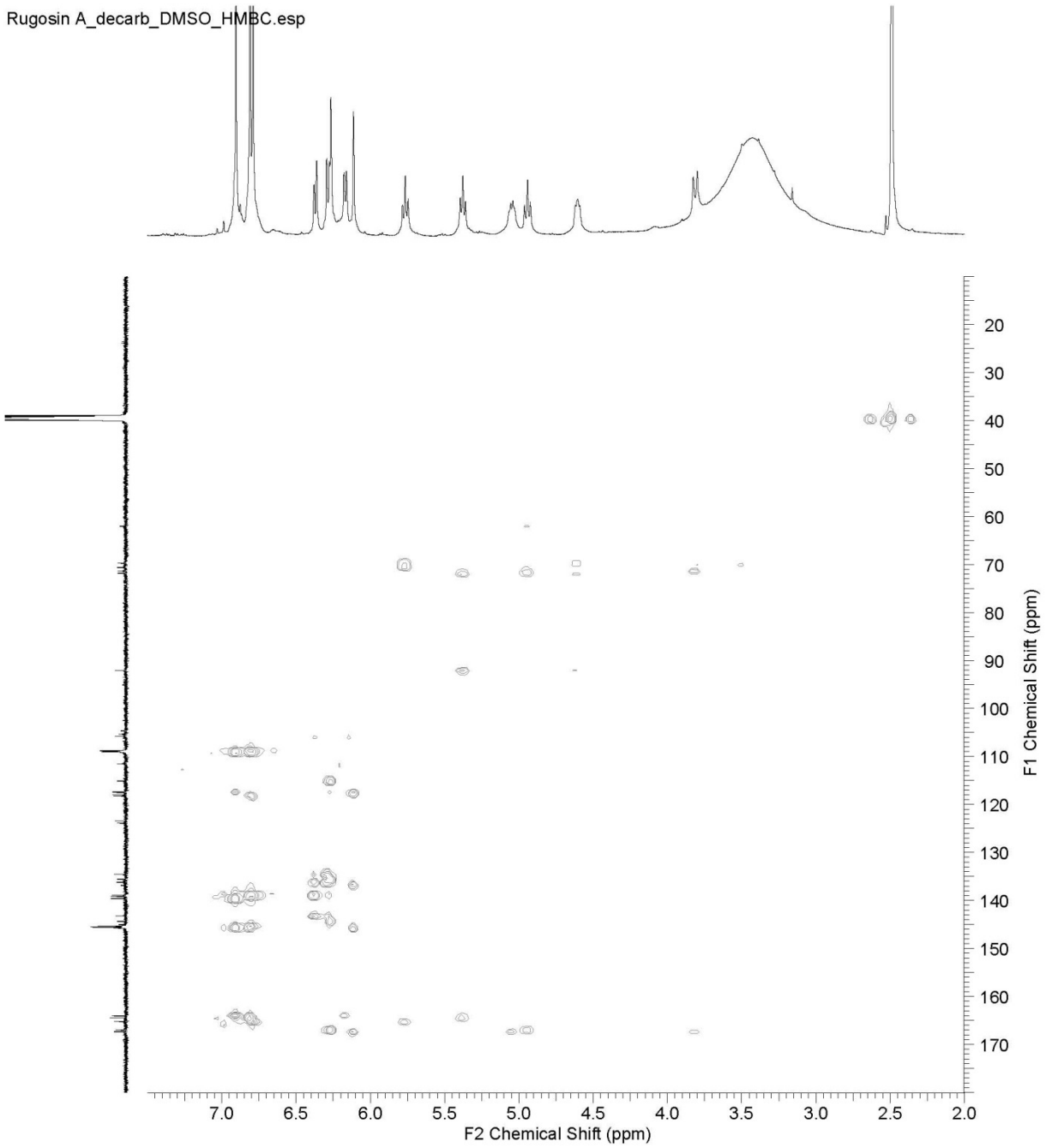
^{1}H-^{1}H COSY spectrum in DMSO-d_6



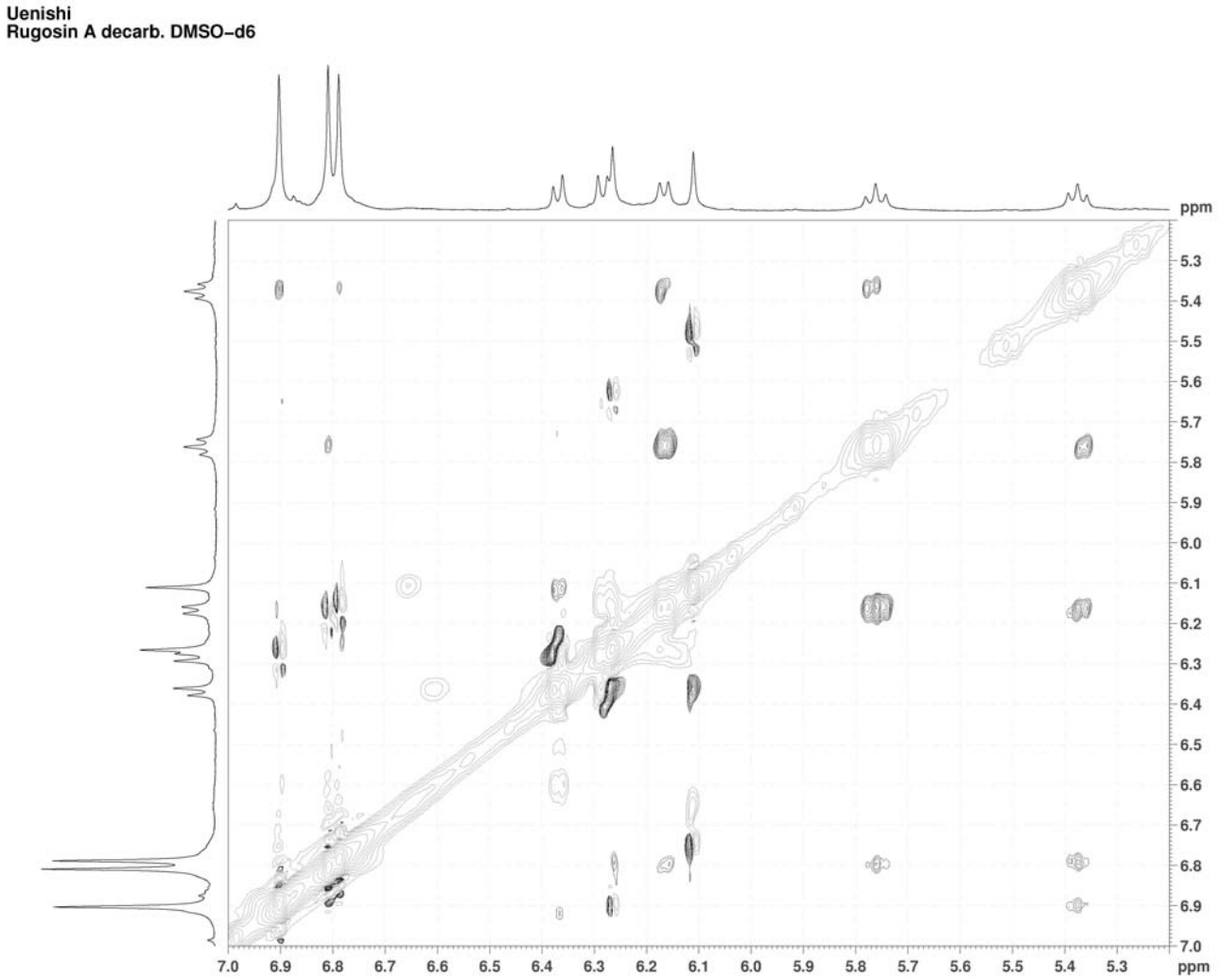
HMQC spectrum in DMSO-d_6



HMBC spectrum in DMSO-d_6



ROESY spectrum in DMSO-d_6



UPLC-MS quantitation of rugosin A, B in rose buds extract powder

Condition

Column: Inertsustain C18 (ϕ2.1×100 mm, GL Science Co.)

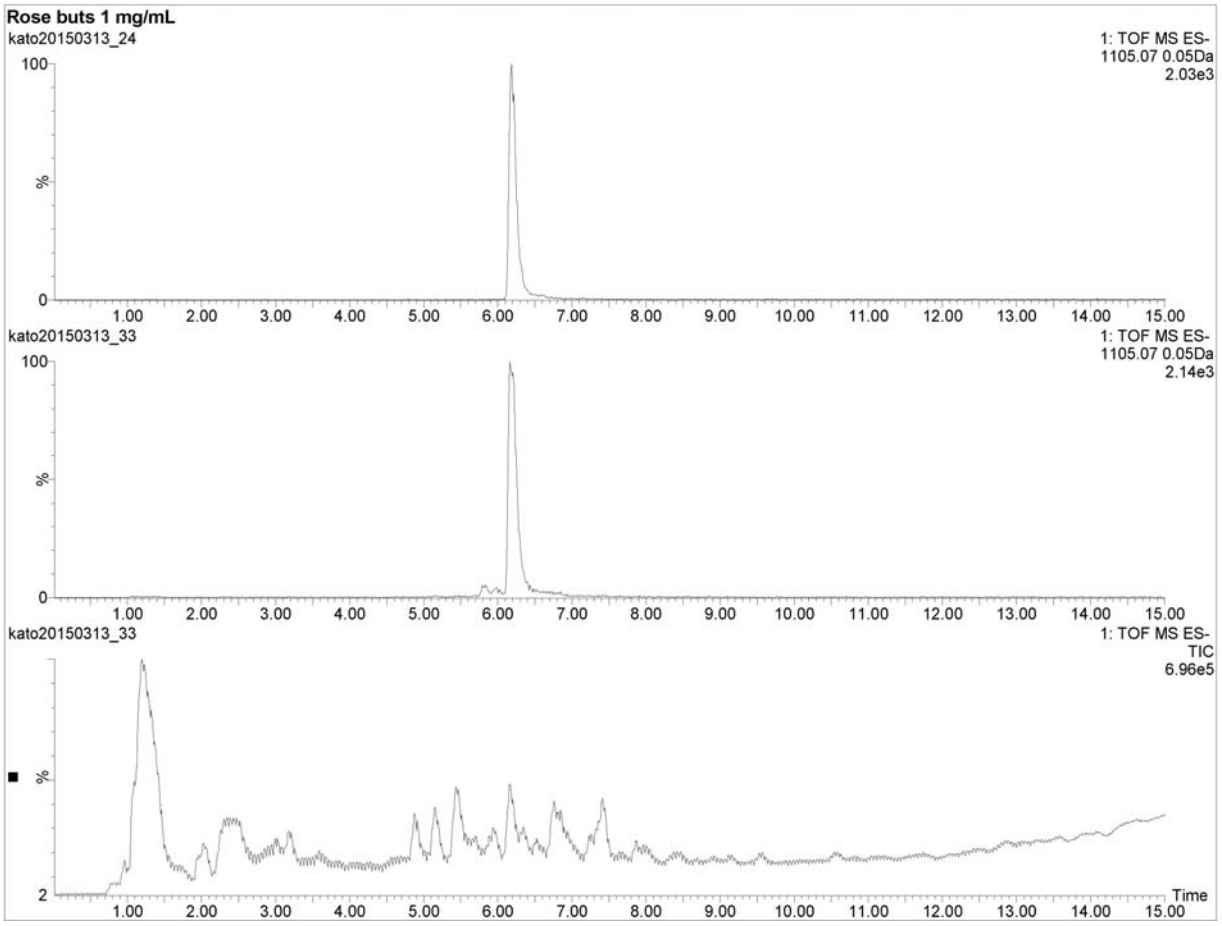
Mobile phase: gradient elution, 5% aq. MeCN with 0.1% TFA to 95% MeCN with 0.1% TFA (20 min)

Flow rate: 0.2 mL/min

Temperature: room temperature

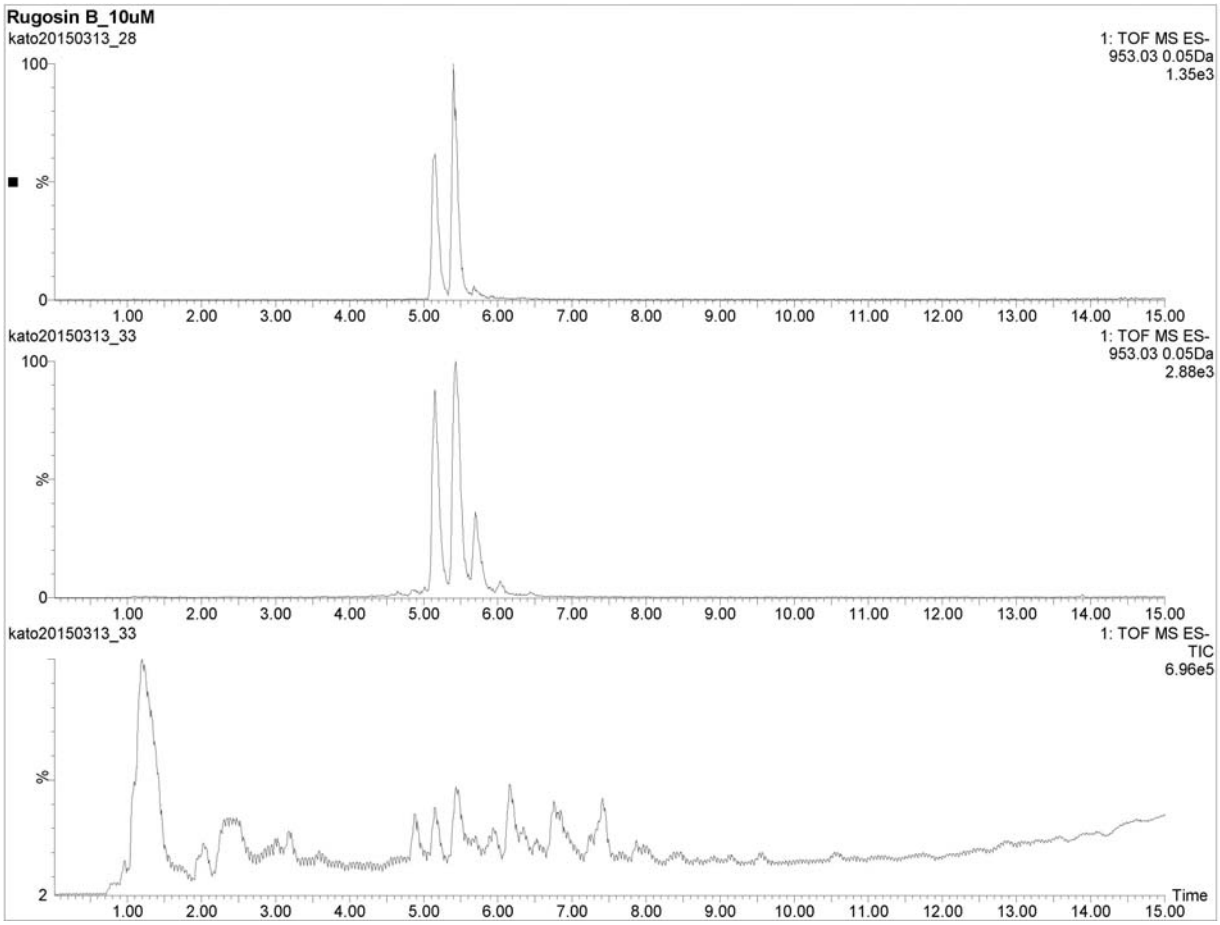
Detection: negative mode ([M-H]-)

Samples: 4 μL injection (Rose buds extract powder dissolved in water : 1 mg/mL)



Supplementary Figure 1. UPLC-MS analysis of rugosin A in the rose buts extract powder.

Top: Rugosin A (isolated sample); Middle: Selected ion chromatogram of rose buts extract powder; Bottom: Total ion chromatogram of rose buts extract powder.



Supplementary Figure 2. UPLC-MS analysis of rugosin B in the rose buts extract powder.

Top: Rugosin B (isolated sample); Middle: Selected ion chromatogram of rose buts extract powder; Bottom: Total ion chromatogram of rose buts extract powder.