

Table S1 ¹H NMR data of Cy3Gal

Isolated compound in CD ₃ OD			Cy3Gal in CD ₃ OD and DCl ⁽¹⁾		Cy3Gal in CD ₃ OD ⁽²⁾		Cy3Gal in CD ₃ OD:CF ₃ COOD (20:1) ⁽³⁾		Cy3Gal in acidified CD ₃ OD ⁽⁴⁾		
position	oH (ppm)		HMBC	oH (ppm)		oH (ppm)		oH (ppm)		oH (ppm)	
4	9.03	s	2, 3, 4a	8.98	s	9.113	d, <i>J</i> = 1.0 Hz	9.11	d, <i>J</i> = 0.9 Hz	8.96	s
6	6.65	d, <i>J</i> = 1.0 Hz	4a, 8	6.67	d, <i>J</i> = 1.5 Hz	6.738	d, <i>J</i> = 2.0 Hz	6.74	d, <i>J</i> = 2.0 Hz	6.62	d, <i>J</i> = 2.0 Hz
8	6.9	d, <i>J</i> = 1.0 Hz		6.92	d, <i>J</i> = 1.5 Hz	6.982	dd, <i>J</i> = 2.0, 1.0 Hz	6.98	dd, <i>J</i> = 2.0, 0.9 Hz	6.84	d, <i>J</i> = 2.0 Hz
2'	8.03	d, <i>J</i> = 2.4 Hz	4', 6'	8.04	d, <i>J</i> = 2.5 Hz	8.158	d, <i>J</i> = 2.3 Hz	8.17	d, <i>J</i> = 2.4 Hz	8.01	d, <i>J</i> = 2.0 Hz
5'	7.01	d, <i>J</i> = 8.8 Hz	1', 3'	7.01	d, <i>J</i> = 8.7 Hz	7.105	d, <i>J</i> = 8.8 Hz	7.11	d, <i>J</i> = 8.8 Hz	6.97	d, <i>J</i> = 8.9 Hz
6'	8.27	dd, <i>J</i> = 8.8, 2.4 Hz	2, 2', 4'	8.23	dd, <i>J</i> = 8.7, 2.5 Hz	8.358	dd, <i>J</i> = 8.8, 2.3 Hz	8.34	dd, <i>J</i> = 8.8, 2.4 Hz	8.2	dd, <i>J</i> = 8.9, 2.0 Hz
1''	5.25	d, <i>J</i> = 7.8 Hz		5.43	d, <i>J</i> = 7.3 Hz	5.35	d, <i>J</i> = 7.7 Hz	5.34	d, <i>J</i> = 7.7 Hz	5.27	d, <i>J</i> = 7.5 Hz
2''	3.98	dd, <i>J</i> = 9.5, 7.8 Hz		4.03	dd, <i>J</i> = 11.8, 6.2 Hz	4.08	dd, <i>J</i> = 9.6, 7.7 Hz	4.08	m	4.01	dd, <i>J</i> = 9.6, 7.5 Hz
3''	3.65	dd, <i>J</i> = 9.5, 3.5 Hz		3.62	dd, <i>J</i> = 11.8, 1.5 Hz	3.76	dd, <i>J</i> = 9.6, 3.4 Hz	3.76	dd, <i>J</i> = 9.9, 3.3 Hz	3.7	dd, <i>J</i> = 9.6, 3.4 Hz
4''	3.94	d, <i>J</i> = 3.5 Hz		3.81	dd, <i>J</i> = 11.8, 6.2 Hz	4.04	dd, <i>J</i> = 3.4, 0.5 Hz	4.04	t, <i>J</i> = 3.3 Hz	3.97	br dd, <i>J</i> = 3.4Hz
5''	3.76	m		3.64		3.89	m	3.89	m	3.83	br dd, <i>J</i> = 8.2 Hz, 3.0Hz
6''a	3.82	m		3.71	dd, <i>J</i> = 9.0, 7.6 Hz	3.89	m	3.87	m	3.81	dd, <i>J</i> = 11.3, 8.2 Hz
6''b	3.76-3.78	m		3.64	m	3.86	m	3.87	m	3.78	dd, <i>J</i> = 11.3, 2.3 Hz
methanol 3.31 ppm as internal reference											

Table S2 Sample Materials

Material	Leaves			Galls		
Starting material (g)	133.4	395.3	358.0	78.9	305.3	416.1
After ODS column chromatography (mg)	346.7	112.1	66.3	301.0	108.1	204.1
After HPLC (mg)	5.1	1.0	8.6	36.5	71.6	22.3

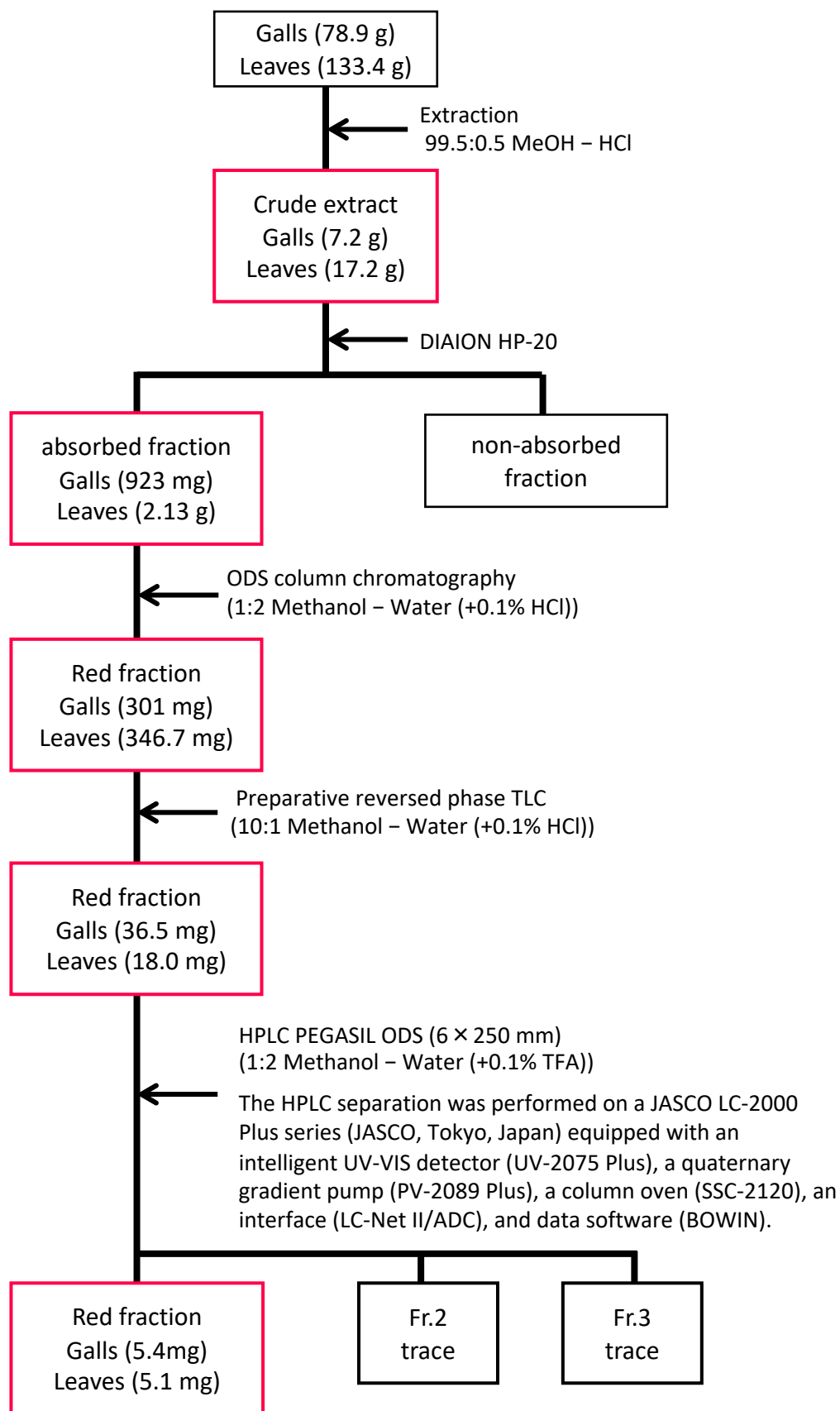


Fig. S1 Isolation scheme for cyanidin-3-O-β-galactoside

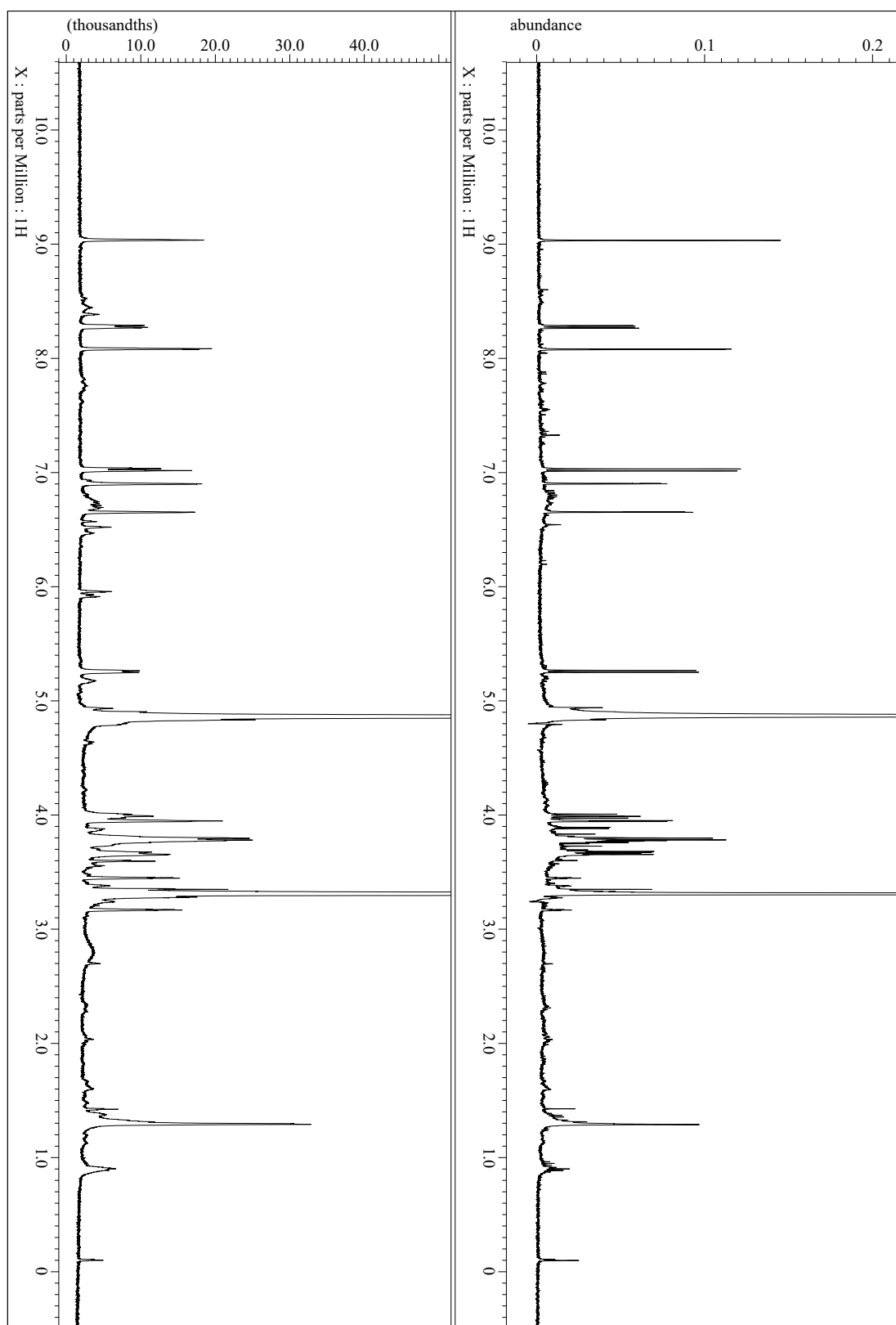


Fig. S2 ^1H NMR Spectra of Isolated compounds

Cy3Gal from Gall tissue (upper) and leaves (lower).

^1H NMR (500 MHz, CD_3OD), Methanol 3.31 ppm as internal reference.

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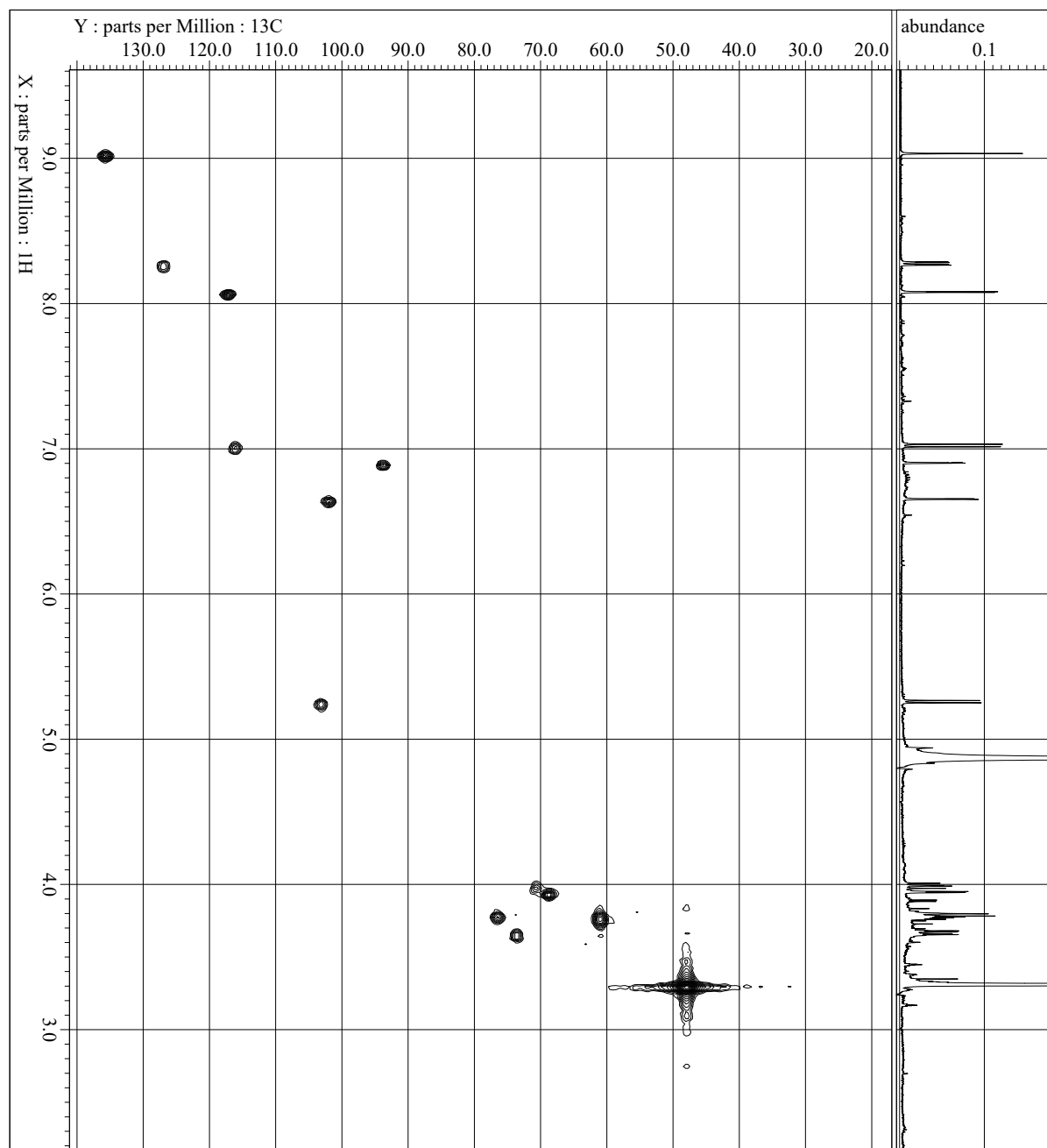


Fig. S3 HMQC NMR Spectrum of Isolated compound from gall tissue

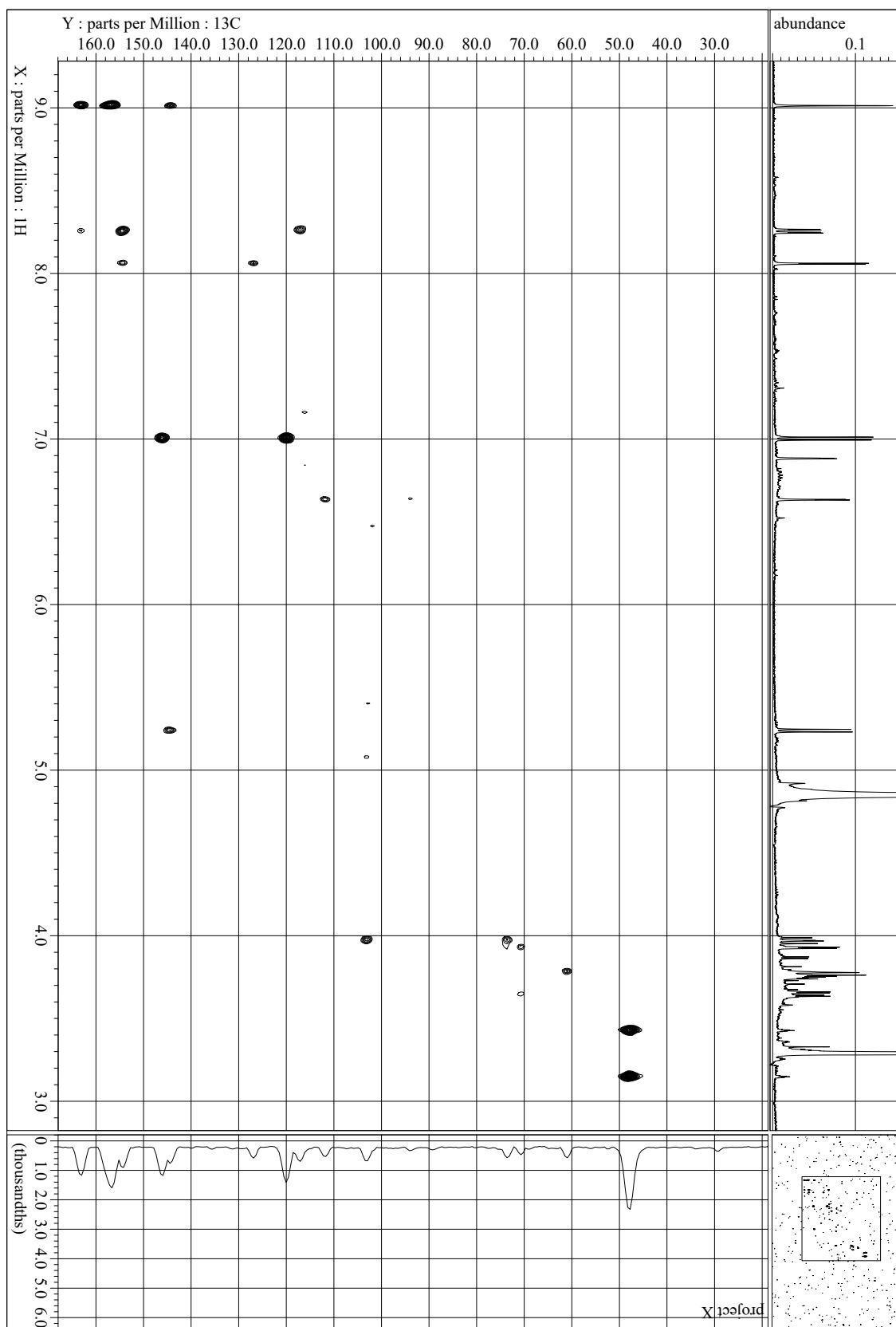


Fig. S4 HMBC NMR Spectrum of Isolated compound from gall tissue

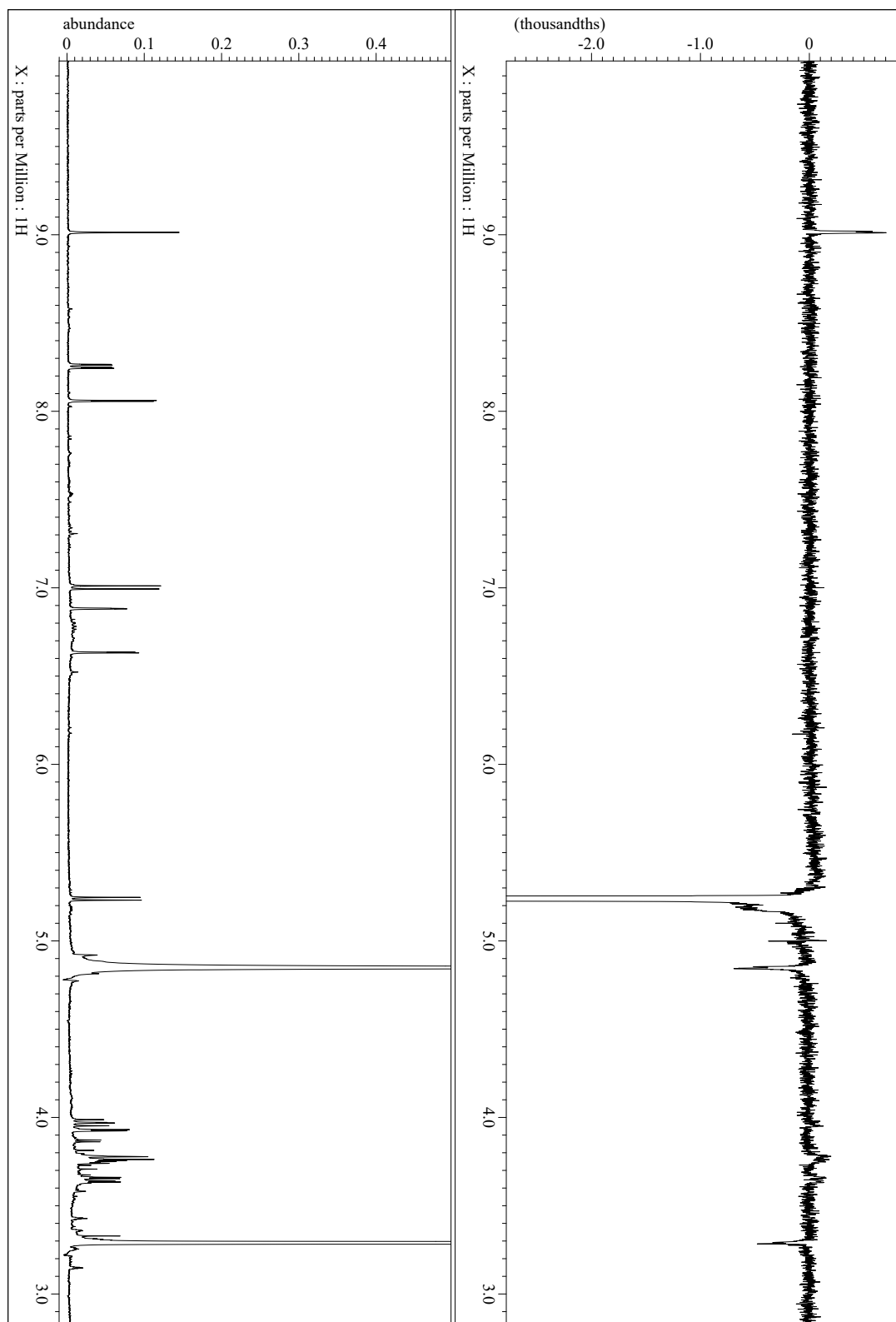


Fig. S5 NOE NMR Spectrum of Isolated compound from gall tissue

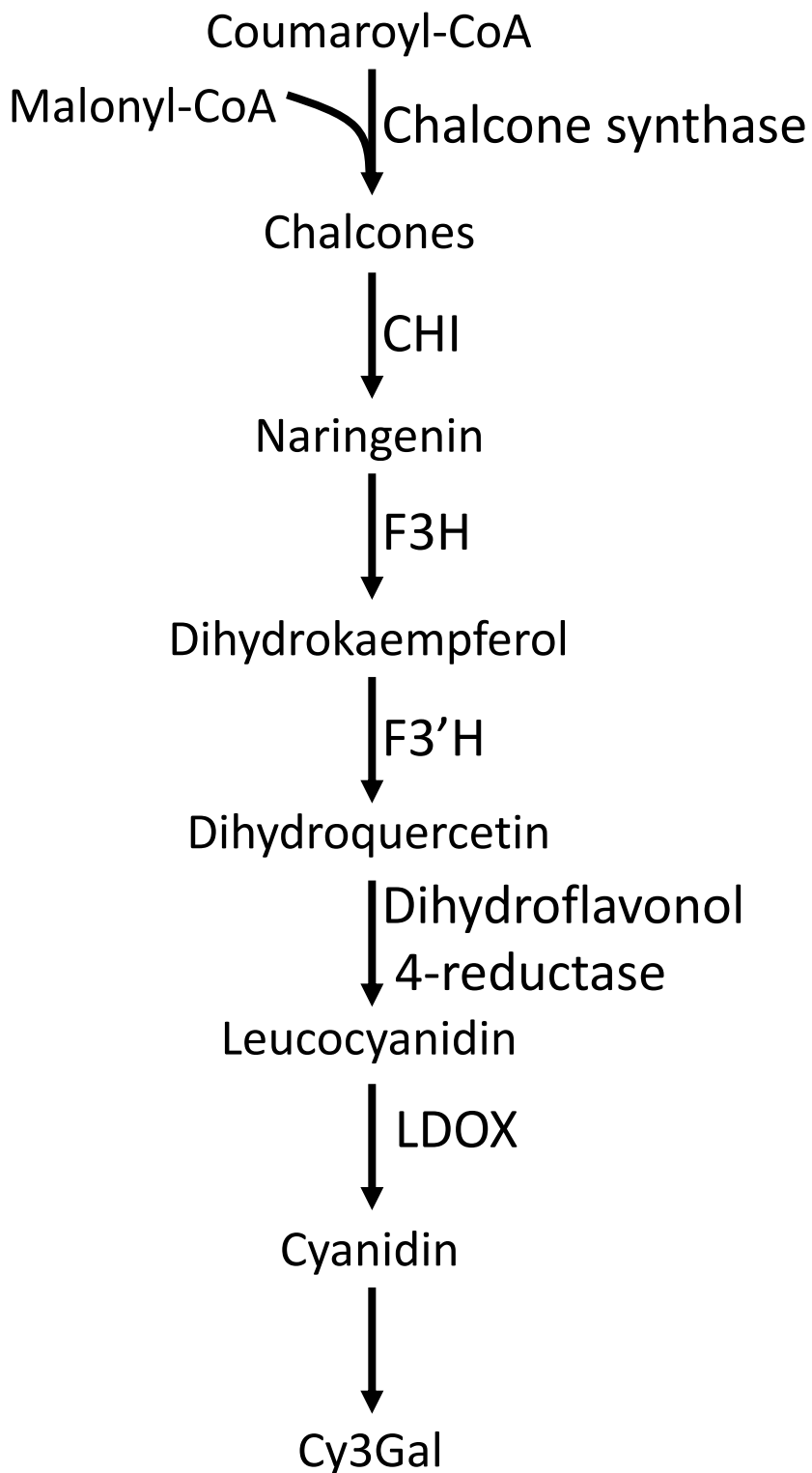


Fig. S6 Anthocyanin biosynthetic pathway