Supporting Information

Bioactive Trimeric and Tetrameric Type A Proanthocyanidins from Cinnamon (*Cinnamomum cassia*)

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9 S2. ^{13}C DEPTQ NMR spectrum of **4**, C and CH^2 down, CH and CH^3 up (methanol-d_4, 150 MHz, 280K)

10 S3. ^{13}C DEPTQ NMR spectrum of **4**, C only (methanol-d_4, 150 MHz, 280K)

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12 S5. PS-DQFCOSY spectrum of **4** (methanol-d_4, 600 MHz, 280K)

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15 S8. Multiplicity Edited HSQC spectrum of **4** (methanol-d_4, 600 MHz, 280K)

16 S9. HMBC spectrum of **4** (methanol-d_4, 600 MHz, 280K)

17 S10. ^{1}H NMR spectrum of **4** (dmso-d_6, 700 MHz, 298K)

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19 S12. Multiplicity Edited HSQC spectrum of **4** (dmso-d_6, 700 MHz, 298K)

20 S13. HMBC spectrum of **4** (dmso-d_6, 700 MHz, 298K)

21 S14. PS-DQFCOSY spectrum of **4** (dmso-d_6, 700 MHz, 298K)

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23 S16. +HR-ESIMS of **1**

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25 S18. -HR-ESIMS of **3**

26 S19. +HR-ESIMS of **3**

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Table 1S. ^{1}H and ^{13}C NMR Data of Compounds **1** and **2** With HMBC Correlations (methanol-d4, AVIII-600, 298 K)
(* 4-bond correlation)

		1			**2**		
ring	no.	◊C m	◊H m (J/HZ)	HMBC (Unit: C#)	◊C m	◊H m (J/HZ)	HMBC (Unit: C#)
unit I							
C	2	100.0, C			100.0, C		
	3	67.2, CH	3.28, d (3.4)	I: 10	67.2, CH	3.45, d (3.5)	I: 10
	4	28.9, CH	4.14, d (3.4)	I: 2,3,5,9,10 II: 7,8,9	28.8, CH	4.00, d (3.5)	I: 2,3,5,9,10 II: 7,8,9
A	5	156.8, C			156.6, C		
	6	98.3, CH	5.96, d (2.3)	I: 8,10	98.3, CH	5.93, d (2.2)	I: 8,10
	7	157.9, C			157.8, C		
	8	96.6, CH	6.01, d (2.3)	I: 6,7,10	96.5, CH	6.00, d (2.2)	I: 6,7,10
	9	154.2, C			154.2, C		
	10	105.0, C			105.0, C		
B	1'	132.5, C			132.5, C		
	2'	115.8, CH	7.02, d (2.1)	I: 2,4',6'	115.8, CH	7.08, d (1.9)	I: 2,4',6'
	3'	145.5, C			145.5, C		
	4'	146.6, C			146.7, C		
	5'	115.8, CH	6.81, d (8.2)	I: 1',3'	115.7, CH	6.85, d (8.2)	I: 1',3'
	6'	119.9, CH	6.84, dd (8.2, 2.1)	I: 2,4'	120.0, CH	6.94, dd (8.2, 1.9)	I: 2,4'
unit II							
F	2	78.9, CH	5.69, brs	II: 3,4,1',2',6'	78.7, CH	5.50, brs	II: 3,4,1',2',6'
	3	72.6, CH	4.12, m		72.5, CH	4.04, brm	
	4	38.3, CH	4.55, brs	II: 2,3,5,9,10 III: 7,8,9	38.3, CH	4.52, brs	II: 2,3,5,9,10 III: 7,8,9
D	5	155.8, C			155.9, C		
	6	96.1, C	5.80, s	II: 4*,5,7,8,10, I: 4*	96.0, C	5.83, s	II: 4*,5,7,8,10, I: 4*
	7	151.1, C			151.1, C		
	8	106.6, C			106.2, C		
	9	151.8, C			151.8, C		
	10	106.8, C			106.5, C		
E	1'	131.8, C			131.5, C		
	2'	116.8, CH	7.30, d (2.0)	II: 2,4',6'	116.5, CH	7.23, d (1.7)	II: 2,4',6'
	3'	145.9, C			146.0, C		
	4'	146.3, C			146.3, C		
	5'	116.2, CH	6.83, d (8.2)	II: 1',3'	116.2, CH	7.08, d (8.3)	II: 1',3'
	6'	121.4, CH	7.18, dd (8.2, 2.0)	II: 2,4'	121.1, CH	7.08, dd (8.3, 1.7)	II: 2,4'
unit III							
L	2	80.4, CH	4.37, brs	III: 3,4,1',2',6'	83.3, CH	3.94, d (9.2)	III: 3,4,1',2',6'
	3	67.6, CH	3.85, m		70.1, CH	3.66, ddd (10.1, 9.2, 6.0)	
	4	29.9, CH2	2.82, m	III: 2,3,5,9,10	30.7, CH2	3.04, dd (16.2, 6.0)	III: 2,3,5,9,10
	4	29.9, CH2	2.82, m	III: 2,3,5,9,10	30.7, CH2	2.41, dd (16.2, 10.1)	III: 2,3,5,9,10
J	5	156.8, C			155.4, C		
	6	96.5, CH	6.09, s	III: 4*,5,7,8,10, II: 4*	96.5, CH	6.09, s	III: 4*,5,7,8,10, II: 4*
	7	155.6, C			155.6, C		
	8	108.9, C			108.8, C		
	9	156.1, C			155.5, C		
	10	100.1, C			100.1, C		
K	1'	132.2, C			132.7, C		
	2'	115.5, CH	6.82, d (1.8)	III: 2,4',6'	115.8, CH	6.74, d (1.6)	III: 2,4',6'
	3'	145.8, C			146.0, C		
	4'	145.4, C			145.9, C		
	5'	116.0, CH	6.74, d (8.2)	III: 1',3'	116.2, CH	6.75, d (8.1)	III: 1',3'
	6'	119.5, CH	6.72, dd (8.2, 1.8)	III: 2,4'	120.0, CH	6.66, dd (8.2, 1.6)	III: 2,4'

Table 2S. ^{1}H and ^{13}C NMR Data of Compounds **3** and **4** With HMBC Correlations (methanol-d4, AVIII-600, 280 K) (* 4-bond correlation)

		3			**4**		
Ring	no.	C m	H m (J/HZ)	HMBC (Unit: C#)	C m	H m (J/HZ)	HMBC (Unit: C#)
Unit I							
C	2	100.1, C			100.3, C		
	3	66.7, CH	3.27, d (3.6)	I: 10	66.9, CH	3.51, d (3.7)	I: 10
	4	28.8, CH	4.23, d (3.6)	I: 2,3,5,9,10 II: 7,8,9	28.9, CH	4.03, d (3.7)	I: 2,3,5,9,10 II: 7,8,9
A	5	156.7, C			156.5, C		
	6	98.2, CH	5.97, d (2.3)	I: 8,10	98.4, CH	5.94, d (2.4)	I: 8,10
	7	157.9, C			157.9, C		
	8	96.5, CH	6.04, d (2.3)	I: 6,7,10	96.6, CH	6.02, d (2.4)	I: 6,7,10
	9	154.2, C			154.2, C		
	10	104.9, C			105.1, C		
B	1'	132.3, C			132.2, C		
	2'	115.8, CH	7.14, d (1.7)	I: 2,4',6'	115.7, CH	7.15, d (2.1)	I: 2,4',6'
	3'	145.5, C			145.5, C		
	4'	146.7, C			146.7, C		
	5'	116.1, CH	6.88, d (8.2)	I: 1',3'	116.0, CH	6.86, d (8.4)	I: 1',3'
	6'	119.9, CH	6.90, dd (8.2, 1.7)	I: 2,4'	120.2, CH	6.98, dd (8.4, 2.1)	I: 2,4'
Unit II							
F	2	78.8, CH	5.64, brs	II: 3,4,1',2',6'	78.5, CH	5.54, brs	II: 3,4,1',2',6'
	3	72.4, CH	4.04, m		72.2, CH	4.00, m	
	4	38.4, CH	4.42, brs	II: 2,3,5,9,10 III: 7,8,9	38.3, CH	4.41, brs	II: 2,3,5,9,10 III: 7,8,9
D	5	154.2, C			154.2, C		
	6	107.6, C			108.1, C		
	7	148.4, C			148.4, C		
	8	106.9, C			106.7, C		
	9	150.3, C			150.4, C		
	10	107.2, C			107.1, C		
E	1'	131.7, C			131.2, C		
	2'	116.7, CH	7.30, d (1.5)	II: 2,4',6'	116.6, CH	7.24, d (2.1)	II: 2,4',6'
	3'	145.9, C			145.9, C		
	4'	146.3, C			146.4, C		
	5'	116.1, CH	6.82, d (8.3)	II: 1',3'	116.0, CH	67.11, d (8.1)	II: 1',3'
	6'	121.4, CH	7.21, dd (8.3, 1.5)	II: 2,4'	121.3, CH	7.11, dd (8.1, 2.1)	II: 2,4'
Unit III							
L	2	80.1, CH	4.09, d (9.0)	III: 3,4,1',2',6'	83.4, CH	3.95, d (9.4)	III: 3,4,1',2',6'
	3	67.4, CH	3.60, m		70.1, CH	3.65, ddd (10.8, 9.4, 6.5)	
	4	29.8, CH2	2.88, dd (16.2, 5.7)	III: 2,3,5,9,10	30.7, CH2	3.05, dd (16.5, 6.5)	III: 2,3,5,9,10
	4	29.8, CH2	2.77, dd (16.2, 10.1)	III: 2,3,5,9,10	30.7, CH2	2.43, dd (16.5, 10.8)	III: 2,3,5,9,10
J	5	156.1, C			155.6, C		
	6	96.4, CH	6.07, s	III: 4*,5,7,8,10, II: 4*	96.6, CH	6.06, s	III: 4*,5,7,8,10, II: 4*
	7	155.5, C			155.2, C		
	8	108.8, C			108.7, C		
	9	155.6, C			155.3, C		
	10	99.7, C			101.7, C		
K	1'	132.8, C			131.2, C		
	2'	115.4, CH	6.63, d (1.7)	III: 2,4',6'	115.7, CH	6.69, d (1.9)	III: 2,4',6'
	3'	145.7, C			144.4, C		
	4'	145.4, C			145.9, C		
	5'	115.8, CH	6.70, d (8.1)	III: 1',3'	116.0, CH	6.76, d (8.2)	III: 1',3'
	6'	119.2, CH	6.24, dd (8.1, 1.7)	III: 2,4'	1120.1, CH	6.48, dd (8.2, 1.9)	III: 2,4'
Unit II'							
I	2	76.5, CH	4.73, brs	II': 3,4,1',2',6'	77.2, CH	4.80, brs	II': 3,4,1',2',6'
	3	71.2, CH	4.09, brs	II': 10	72.5, CH	4.06, brs	II': 10
	4	37.6, CH	4.36, brs	II': 2,3,5,9,10 II: 5,6,7	37.2, CH	4.45, brs	II': 2,3,5,9,10 II: 5,6,7
G	5	157.9, C			15779, C		
	6	96.0, CH	5.91, d (2.2)	II': 5',8',10'	95.9, CH	5.92, d (2.4)	II': 5',8',10'
	7	159.5, C			159.4, C		
	8	96.6 CH	5.87, d (2.2)	II': 6',10'	96.7 CH	5.86, d (2.4)	II': 6',10'
	9	159.4, C			159.4, C		
	10	99.1, C			99.1, C		
H	1'	131.6, C			131.9, C		
	2'	116.8, CH	7.10, d (1.6)	II': 2,4',6'	116.2, CH	7.13, d (2.0)	II': 2,4',6'
	3'	146.2, C			146.2, C		
	4'	146.3, C			146.1, C		
	5'	115.9, CH	6.90, d (8.2)	II': 1',3'	116.2, CH	6.90, d (8.3)	II': 1',3'
	6'	120.8, CH	6.91, dd (8.2, 1.6)	II': 2,4'	120.4, CH	6.87, dd (8.3, 2.0)	II': 2,4'

Table 3S. ^{1}H and ^{13}C NMR Data of the conformational isomers of Compounds **1** and **2** With HMBC Correlations (dmso-d6, AVIII-700, 298 K) (* 4 bond correlation)

		1a		**1b**			**2a**		**2b**		
Ring	no.	C m	H m (J/HZ)	C m	H m (J/HZ)	HMBC (unit: C#)	C m	H m (J/HZ)	C m	H m (J/HZ)	HMBC (unit: C#)
unit I											
C	2	98.5, C		98.4, C			98.4, C		98.5, C		
	3	66.4, CH	3.85, m	65.0, CH	3.43, m	I: 10	66.4, CH	3.84, m	64.8, CH	3.51, m	I: 10
	3		5.31 d (4.0) OH		4.34 br OH	I: 2,3,4		5.32 d (3.4) OH			
	4	28.0, CH	4.29, d (3.5)	27.5, CH	4.06, d (3.4)	I: 2,3,5,9,10 II: 7,8,9	28.0, CH	4.28, d (3.1)	27.3, CH	3.84, brs	I: 2,3,5,9,10 II: 7,8,9
A	5	156.0, C	7.90 s OH	155.5, C	7.39 s OH	I: 5,6,10	156.3, C		155.4, C		I: 5,6,10
	5										
	6	96.6, CH	5.90, d (2.2)	96.8, CH	5.79, d (2.2)	I: 5,7,10	96.6, CH	5.90, d (2.2)	96.8, CH	5.76, d (2.2)	I: 5,7,10
	7	156.5, C		156.3, C			156.5, C		156.3, C		
	8	94.8, CH	5.89, d (2.2)	94.8, CH	5.84, d (2.2)	I: 6,7,10	94.7, CH	5.89, d (2.2)	94.8, CH	5.84, d (2.2)	I: 6,7,10
	9	152.7, C		152.6, C			152.8, C		152.7, C		
	10	103.1, C		103.9, C			103.0, C		104.0, C		
B	1'	131.0, C		130.9, C			131.0, C		130.8, C		
	2'	114.7, CH	7.03, d (2.1)	115.7, CH	6.97, d (1.8)	I: 2,4',6'	114.7, CH	7.03, d (1.8)	114.9, CH	7.00, d (1.7)	I: 2,4',6'
	3'	144.4, C		144.2, C			144.3, C		144.2, C		
	4'	145.4, C		144.2, C			145.5, C		144.2, C		
	5'	114.7, CH	6.77, d (8.3)	114.9, CH	6.76, d (8.2)	I: 1',3'	114.7, CH	6.77, d (8.3)	114.9, CH	6.80, d (8.2)	I: 1',3'
	6'	117.9, CH	6.88, dd (8.3, 2.1)	117.9, CH	6.70, dd (8.2, 1.8)	I: 2,4'	117.9, CH	6.88, dd (8.2, 1.8)	118.1, CH	6.79, dd (8.2, 1.7)	I: 2,4'
unit II											
F	2	76.6, CH	5.13, brs	76.3, CH	5.41, brs	II: 3,4,1',2',6'	76.7, CH	5.21, brs	76.3, CH	5.26, brs	II: 3,4,1',2',6'
	3	71.0, CH	3.78, m	69.6, CH	3.92, m		70.5, CH	3.80, m	69.5, CH	3.90, m	
	4	36.7, CH	4.48, brs	37.1, CH	4.30, brs	II: 2,3,5,9,10 III: 7,8,9	36.4, CH	4.46, brs	37.1, CH	4.26, brs	II: 2,3,5,9,10 III: 7,8,9
D	5	155.0, C	8.86, s OH	154.0, C	8.56, s OH	II: 5,6,10	154.9, C		154.0, C		II: 5,6,10
	6	94.1, CH	5.95, s	94.0, C	5.67 s	II: 4*,5,7,8,10 I: 4*	94.1, CH	5.95, s	94.0, C	5.68 s	II: 4*,5,7,8,10 I: 4*
	7	150.0, C		148.9, C			149.9, C		148.8, C		
	8	104.5, C		104.2, C			104.4, C		104.1, C		
	9	151.0, C		150.4, C			152.7, C		150.4, C		
	10	105.2, C		105.4, C			105.4, C		105.1, C		
E	1'	130.1, C		130.1, C			130.2, C		129.8, C		
	2'	114.9, CH	6.94, d (1.8)	115.9, CH	7.19, d (1.8)	II: 2,4',6'	115.09, CH	6.97, d (2.1)	115.7, CH	7.14, d (1.4)	II: 2,4',6'
	3'	144.7, C		144.8, C			144.4, C		144.5, C		
	4'	144.7, C		144.7, C			144.7, C		145.3, C		
	5'	115.2, CH	6.72, d (8.4)	114.9, CH	6.73, d (8.2)	II: 1',3'	115.15, CH	6.73, d (8.3)	114.8, CH	6.72, d (8.2)	II: 1',3'
	6'	118.4, CH	6.93, dd (8.4, 1.8)	119.7, CH	7.00, dd (8.2, 1.8)	II: 2,4'	119.0, CH	6.94, dd (8.3, 2.1)	119.6, CH	7.00, dd (8.2, 1.4)	II: 2,4'
unit III											
L	2	77.5, CH	4.95, brs	78.5, CH	4.25, brs	III: 3,4,1',2',6'	80.1, CH	4.48, d (5.1)	81.6, CH	3.81, d (8.7)	III: 3,4,1',2',6'
	3	64.7, CH	4.19, m	64.8, CH	3.70, m		66.1, CH	3.94, m	67.5, CH	3.50, m	
	4	27.5, CH2	2.70, dd (16.4, 4.4)	28.8, CH2	2.64, dd (16.4, obs)	III: 2,3,5,9,10	25.8, CH2	2.44, dd (16.2, 4.6)	29.9, CH2	2.82, dd (15.8, 5.4)	III: 2,3,5,9,10
	4	27.5, CH2	2.37, dd (16.4, 4.6)	28.8, CH2	2.50, dd (16.4, 4.4)	III: 2,3,5,9,10	25.8, CH2	2.39, dd (16.2, 5.4)	29.9, CH2	2.27, dd (15.8, 9.8)	III: 2,3,5,9,10
J	5	154.0, C		154.2, C		III: 5,10	153.8, C		154.0, C		III: 5,10
	6	95.7, CH	5.81, s	94.9, CH	6.07, s	III: 4*,5,7,8,10, II: 4*	95.7, CH	5.80, s	95.2, CH	6.06, s	III: 4*,5,7,8,10, II: 4*
	7	152.6, C	8.36 s OH	153.8, C		III: 6,7,8	154.3, C	8.36 s OH	153.8, C		III: 6,7,8
	8	106.8, C		107.2, C			106.7, C		107.3, C		
	9	154.0, C		154.0, C			152.5, C		153.6, C		
	10	98.8, C		98.4, C			98.5, C		99.7 C		
K	1'	130.1, C		131.2, C			131.2, C		130.9, C		
	2'	114.9, CH	6.94,d (1.8)	114.7, CH	6.70, d (1.8)	III: 2,4',6'	113.5, CH	6.76,d (1.8)	114.6, CH	6.61, d (1.4)	III: 2,4',6'
	3'	144.7, C		144.2, C			144.7, C		144.5, C		
	4'	144.7, C		143.9, C			144.4, C		144.2, C		
	5'	115.2, CH	6.72, d (8.4)	114.4, CH	6.68, d (8.1)	III: 1',3'	115.2, CH	6.65, d (8.1)	114.8, CH	6.70, d (8.2)	III: 1',3'
	6'	118.9, CH	6.93, dd (8.4,1.8)	117.6, CH	6.53, dd (8.1, 1.8)	III: 2,4'	117.5, CH	6.81, dd (8.1,1.8)	118.0, CH	6.47, dd (8.2, 1.4)	III: 2,4'

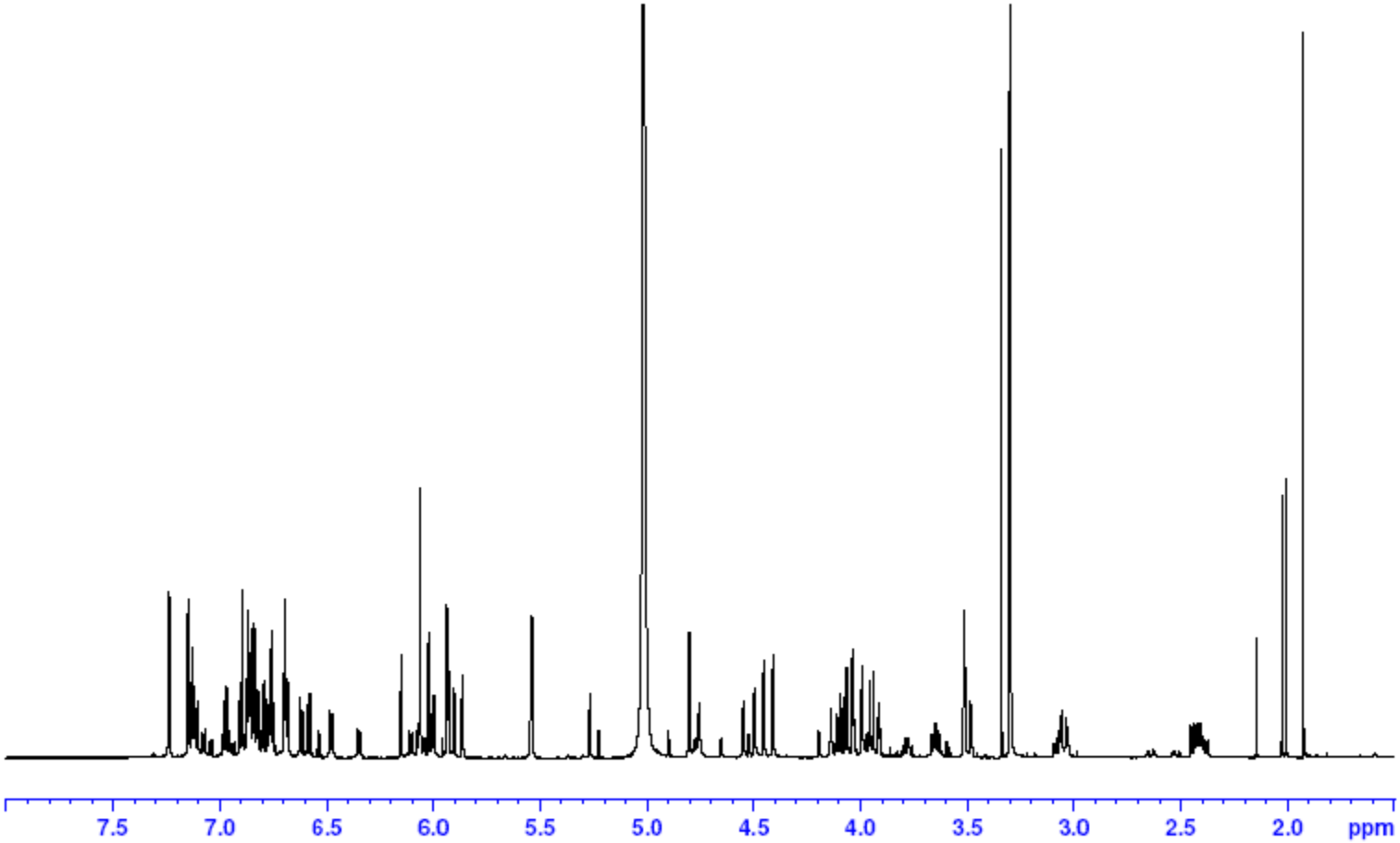
Table 4S. ^{1}H and ^{13}C NMR Data of the conformational isomers of Compounds **3** and **4** With HMBC Correlations (dmso-d6, AVIII-700, 298 K) (* 4-bond correlation)

		3a		**3b**			**4a**		**4b**		
Ring	no.	C m	H m (J/HZ)	C m	H m (J/HZ)	HMBC (unit: C#)	C m	H m (J/HZ)	C m	H m (J/HZ)	HMBC (unit: C#)
unit I											
C	2	98.6, C		98.8, C			98.8, C		98.8, C		
	3	64.7, CH	3.58, m	65.8, CH	3.89, m	I: 10	65.0, CH	3.49, m	65.9, CH	3.88, m	I: 10
	3					I: 2,3,4			5.33	d (4.0) OH	I: 2,3,4
	4	27.4, CH	4.10, bs	28.0, CH	4.37, bs	I: 2,3,5,9,10 II: 7,8,9	27.4, CH	3.83, d (3.5)	28.1, CH	4.35, d (3.4)	I: 2,3,5,9,10 II: 7,8,9
A	5	155.4, C		155.7, C			155.3, C		155.7, C		
	5							7.16, s OH		7.72, s OH	I: 5,6,10
	6	96.8, CH	5.78, d (2.4)	96.7, CH	5.89, d (2.2)	I: 5,7,10	96.9, CH	5.75, d (2.3)	96.8, CH	5.89, d (2.2)	I: 5,7,10
	7	156.3, C		156.3, C			156.3, C		156.5, C		
	8	94.7, CH	5.87, d (2.4)	94.6, CH	5.90, d (2.2)	I: 6,7,10	94.7, CH	5.87, d (2.3)	94.6, CH	5.91, d (2.2)	I: 6,7,10
	9	153.0, C		152.9, C			153.1, C		153.1, C		
	10	103.8, C		103.4, C			103.9, C		103.3, C		
B	1'	130.7, C		130.7, C			130.7, C		130.6, C		
	2'	115.6, CH	7.04, d (1.8)	115.6, CH	7.07, d (1.9)	I: 2,4',6'	115.5, CH	7.07, d (1.7)	115.7, CH	7.08, d (1.9)	I: 2,4',6'
	3'	144.8, C		144.7, C			144.9, C		144.8, C		
	4'	145.1, C		144.9, C			145.1, C		145.4, C		
	5'	114.9, CH	6.69, d (8.1)	115.1, CH	6.70, d (8.0)	I: 1',3'	115.0, CH	6.76, d (8.2)	115.2, CH	6.71, d (8.3)	I: 1',3'
	6'	117.9, CH	6.73, dd (8.1, 1.8)	118.0, CH	6.93, dd (8.0, 1.9)	I: 2,4'	118.2, CH	6.84, dd (8.2, 1.7)	118.0, CH	6.92, dd (8.3, 1.9)	I: 2,4'
unit II											
F	2	76.2, CH	5.40, brs	76.6, CH	6.00, brs	II: 3,4,1',2',6'	76.1, CH	5.30, brs	76.8, CH	5.06, brs	II: 3,4,1',2',6'
	3	69.3, CH	3.91, m	70.8, CH	3.81, m		69.2, CH	3.87, m	70.4, CH	3.88, m	
	3					II: 2,3,4		4.96, d (4.2) OH		4.50, d (5.2) OH	II: 2,3,4
	4	37.1, CH	4.14, brs	37.1, CH	4.31, brs	II: 2,3,5,9,10 III: 7,8,9	37.0, CH	4.14, brs	36.8, CH	4.23, brs	II: 2,3,5,9,10 III: 7,8,9
D	5	152.1, C		153.1, C			152.0, C		153.1, C		
	6	106.3, C		107.5, C			106.7, C		106.9, C		
	7	146.2, C		147.0, C			146.3, C		146.8, C		
	8	105.1, C		105.2, C			105.0, C		105.2, C		
	9	148.6, C		148.9, C			148.7, C		149.2, C		
	10	106.0, C		105.5, C			105.8, C		106.2, C		
E	1'	129.7, C		129.6, C			129.5, C		129.8, C		
	2'	115.9, CH	7.20, d (1.7)	115.2, CH	6.95, d (1.8)	II: 2,4',6'	115.9, CH	7.15, d (1.6)	115.3, CH	6.97, d (1.8)	II: 2,4',6'
	3'	144.7, C		144.8, C			144.9, C		144.9, C		
	4'	144.9, C		144.6, C			145.0, C		145.0, C		
	5'	115.2, CH	6.73, d (8.1)	115.2, CH	6.71, d (8.2)	II: 1',3'	115.9, CH	6.76, d (8.1)	115.1, CH	6.73, d (8.2)	II: 1',3'
	6'	119.7, CH	7.03, dd (8.1, 1.7)	119.1, CH	6.91, dd (8.2, 1.8)	II: 2,4'	119.8, CH	7.01, dd (8.1, 1.6)	119.3, CH	6.93, dd (8.2, 1.8)	II: 2,4'

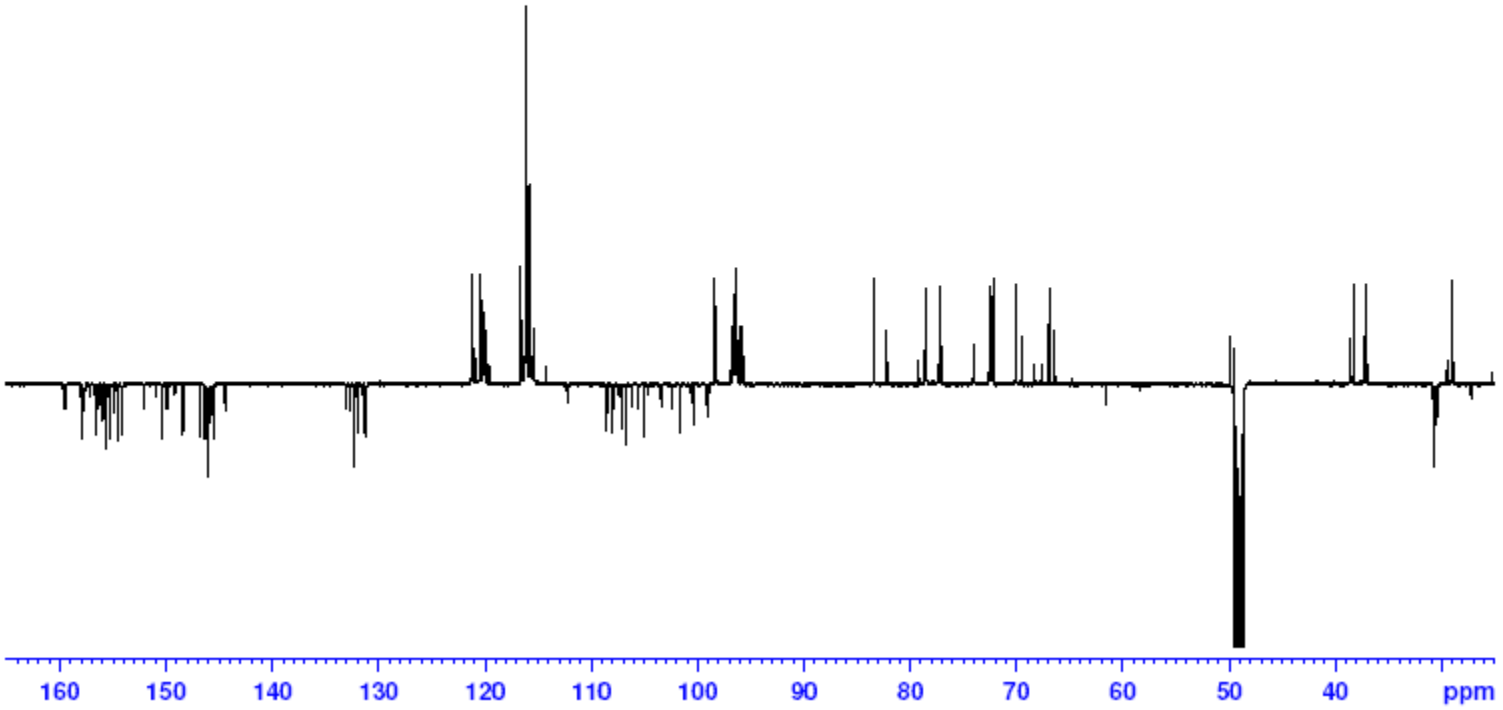
Table 4S. ^{1}H and ^{13}C NMR Data of the conformational isomers of Compounds **3** and **4** With HMBC Correlations (dmso-d6, AVIII-700, 298 K) (* 4-bond correlation)

		3a		**3b**			**4a**		**4b**		
Ring	no.	δC m	δH m (J/HZ)	δC m	δH m (J/HZ)	HMBC (unit: C#)	δC m	δH m (J/HZ)	δC m	δH m (J/HZ)	HMBC (unit: C#)
unit III											
L	2	78.6, CH	4.10, brs	77.4, CH	4.79, brs	III: 3,4,1',2',6'	81.7, CH	3.85, d (9.1)	80.5, CH	4.63, d (8.3)	III: 3,4,1',2',6'
	3	64.7, CH	3.58, m	64.4, CH	4.13, m		67.2, CH	3.51, m	66.3, CH	3.80, d m	
	3							4.73, d (3.7) OH		4.90, d (4.6) OH	III: 2,3,4
	4	29.0, CH2	2.54, m	28.4, CH2	2.67, dd (16.2, 5.1)	III: 9,10	30.1, CH2	2.87, dd (16.1, 5.8)	27.3, CH2	2.49, dd (16.1, 6.8)	III: 2,3,5,9,10
	4	29.0, CH2	2.54, m	28.4, CH2	2.44, dd (16.2, 7.1)	III: 9,10	30.1, CH2	2.22, dd (16.1, 10.1)	27.3, CH2	2.35, dd (16.1, 5.0)	III: 2,3,5,9,10
J	5	154.4, C		154.9, C			153.8, C	9.11, s OH	153.9, C	8.98, s OH	III: 5,10
	6	95.2, CH	6.03, s	95.5, CH	5.99, s	III: 4*,5,7,8,10, II: 4*	95.4, CH	6.04, s	95.5, CH	5.82, s	III: 4*,5,7,8,10, II: 4*
	7	153.6, C		154.3, C			153.8, C	9.08, s OH	154.4, C	8.37, s OH	III: 6,7,8
	8	106.7, C		105.7, C			106.8, C		106.1, C		
	9	153.8, C		152.9, C			153.7, C		152.7, C		
	10	98.2, C		99.6, C			99.7, C		99.1, C		
K	1'	130.4, C		130.9, C			130.6, C		130.8, C		
	2'	114.1, CH	6.99,d (1.7)	114.6, CH	6.61, brs	III: 2,4',6'	114.5, CH	6.58, d (1.4)	113.7, CH	6.72, d (1.6)	III: 2,4',6'
	3'	144.4, C		144.4, C			144.4, C		144.7, C		
	4'	143.9, C		144.0, C			145.0, C		144.3, C		
	5'	115.0, CH	6.56, d (8.0)	114.3, CH	6.61, d (8.2)	III: 1',3'	115.5, CH	6.75, d (8.0)	115.0, CH	6.48, d (8.1)	III: 1',3'
	6'	117.7, CH	6.69, dd (8.0,1.7)	117.1, CH	6.14, brd (8.2))	III: 2,4'	118.4, CH	6.29, dd (8.0,1.4)	117.9, CH	6.60, dd (8.1, 1.6))	III: 2,4'
unit II'											
I	2	75.4, CH	4.55, brs	76.0, CH	4.80, d (7.0)	II': 3,4,1',2',6'	76.0, CH	4.71, brs	76.0, CH	4.63, brs	II': 3,4,1',2',6'
	3	70.1, CH	3.75, m	72.3, CH	3.67, m	II': 10	70.9, CH	3.82, m	72.1, CH	3.69, m	II': 10
	3							4.63, d (5.8) OH			
	4	35.5, CH	4.25, brs	35.3, CH	4.48, brs	II': 2,3,5,9,10 II: 5,6,7	35.3, CH	4.32, brs	35.5, CH	4.47, brs	II': 2,3,5,9,10 II: 5,6,7
G	5	157.7, C	9.23, s OH	157.5, C		II': 5',6',10'	157.6, C	9.22, s OH	157.9, C	9.37, s OH	II': 5',6',10'
	6	95.6, CH	5.82, d (2.2)	95.5, CH	5.83, d (2.4)	II': 5',8',10'	95.7, CH	5.80, d (2.2)	95.7, CH	5.90, d (2.2)	II': 5',8',10'
	7	156.4, C		156.3, C			156.4, C		156.1, C		
	8	94.5, CH	5.77, d (2.2)	94.6, CH	5.78, d (2.2)	II': 6',10'	94.5, CH	5.78, d (2.2)	94.7, CH	5.86, d (2.2)	II': 6',10'
	9	156.2, C		156.3, C			156.1, C		156.3, C		
	10	97.7, C		98.5, C			97.9, C		97.5, C		
H	1'	130.1, C		130.7, C			130.5, C		130.3, C		
	2'	115.5, CH	6.94, d (1.6)	114.9, CH	6.92, d (1.7)	II': 2,4',6'	115.0, CH	6.93, d (1.6)	115.6, CH	7.06, d (1.6)	II': 2,4',6'
	3'	145.1, C		145.0, C			145.2, C		145.1, C		
	4'	144.7, C		144.7, C			144.7, C		144.8, C		
	5'	114.8, CH	6.77, d (8.2)	115.1, CH	6.72, d (8.1)	II': 1',3'	115.0, CH	6.70, d (8.2)	115.1, CH	6.76, d (8.2)	II': 1',3'
	6'	118.1, CH	6.50, dd (8.2, 1.6)	118.4, CH	6.51, dd (8.1, 1.7)	II': 2,4'	118.5, CH	6.50, dd (8.2, 1.6)	118.3, CH	6.57, dd (8.2, 1.6)	II': 2,4'

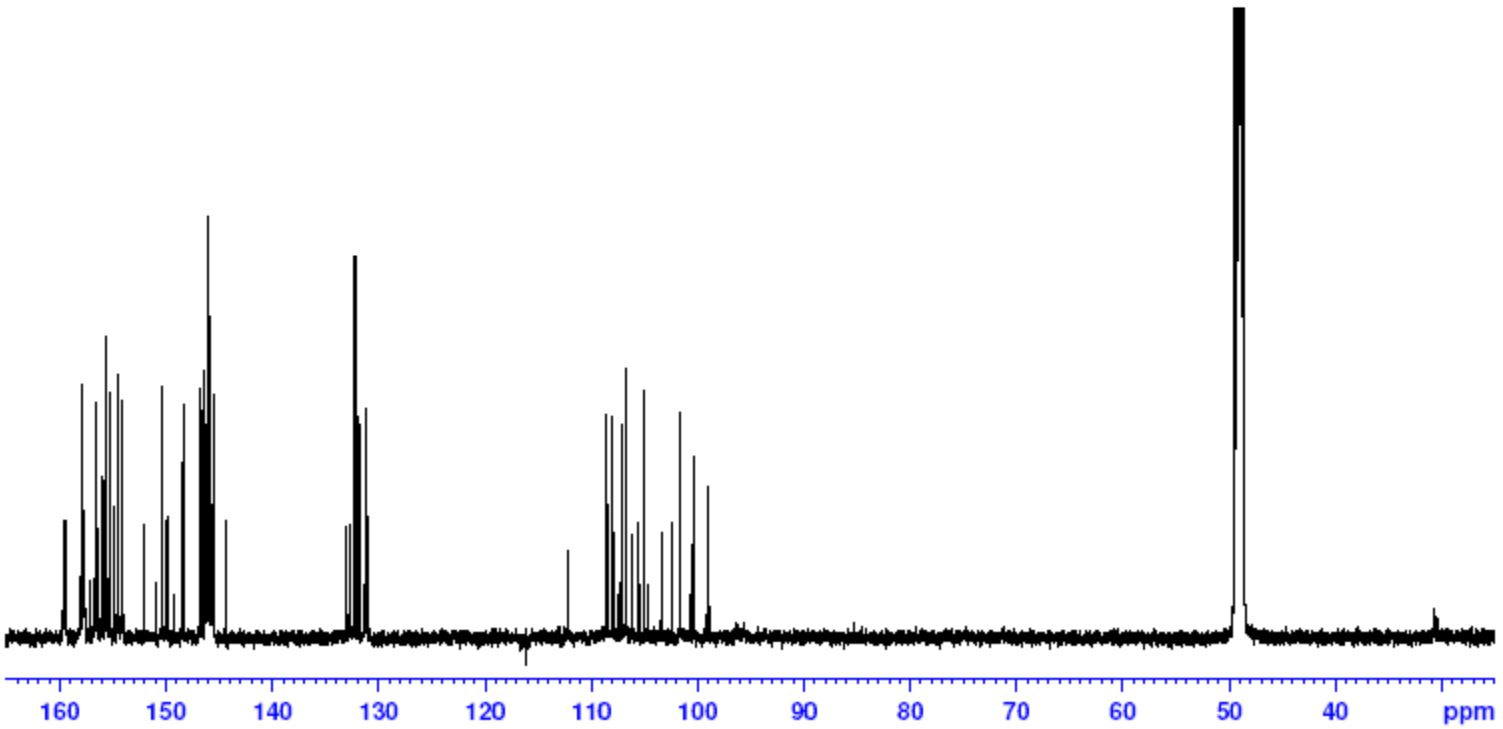
S1. ^{1}H NMR spectrum of **4** (methanol-d_4, 600 MHz, 280K)



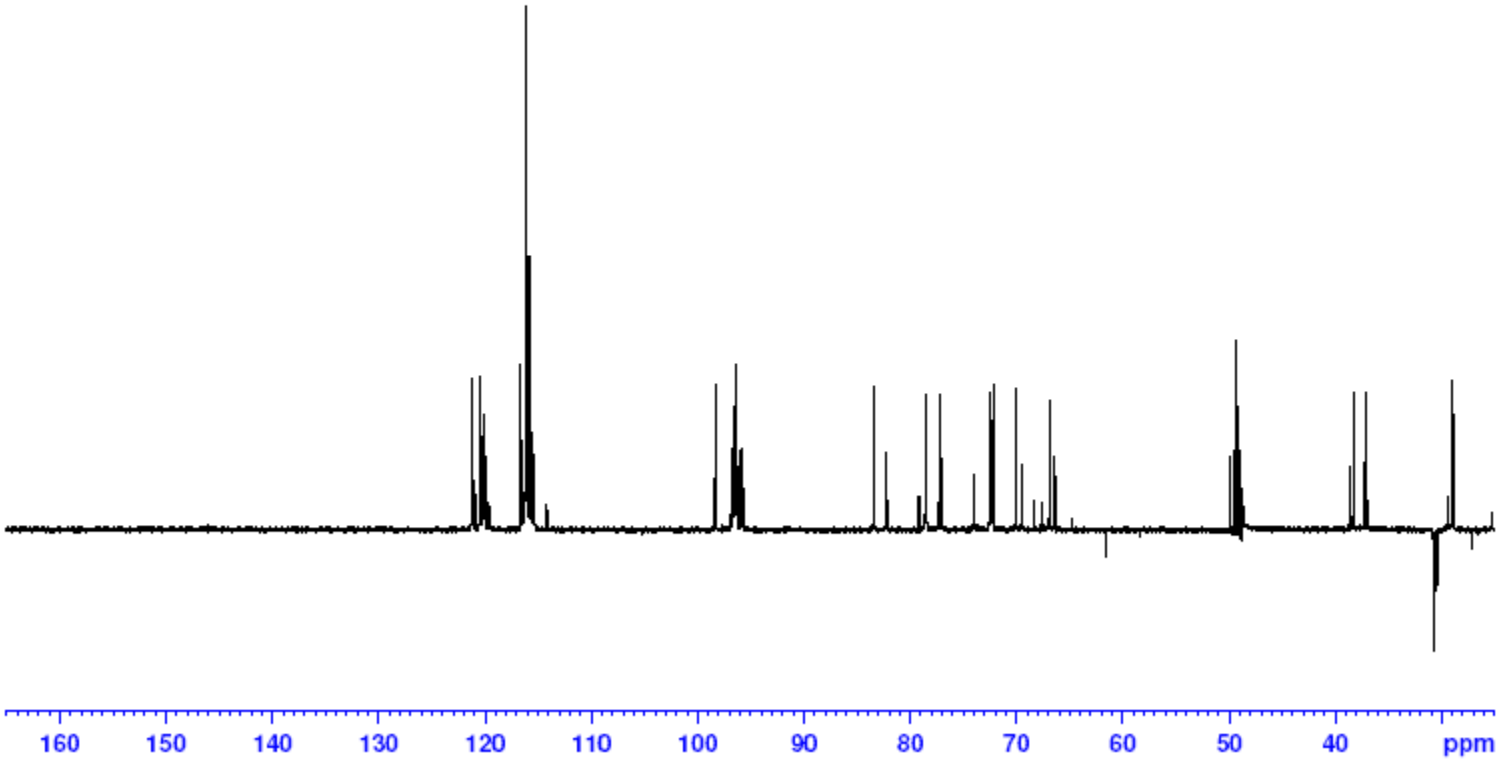
S2. ^{13}C DEPTQ NMR spectrum of **4**, C and CH^2 down, CH and CH^3 up (methanol-d_4, 150 MHz, 280K)



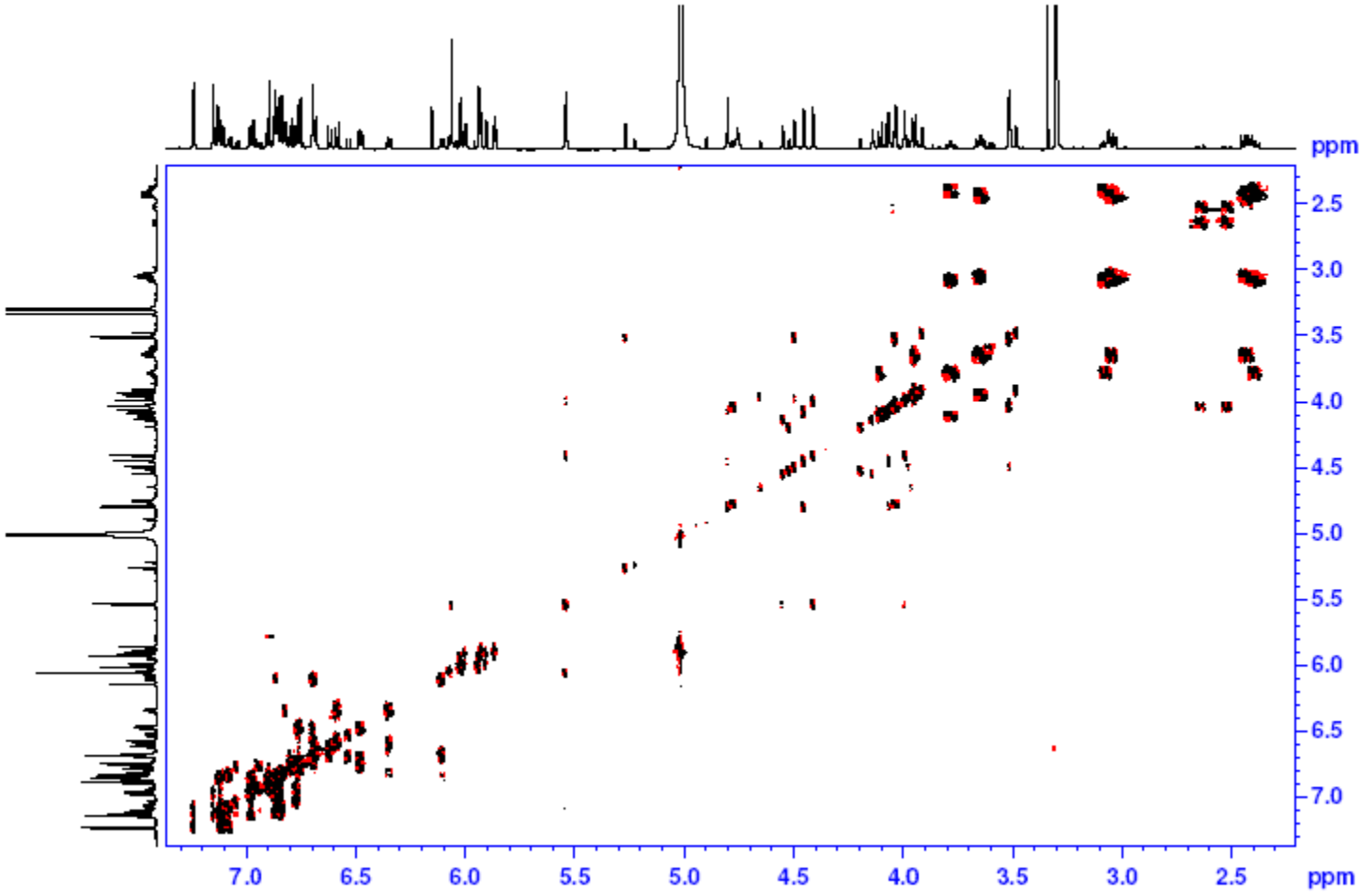
S3. ^{13}C DEPTQ NMR spectrum of **4**, C only (methanol-d_4, 150 MHz, 280K)



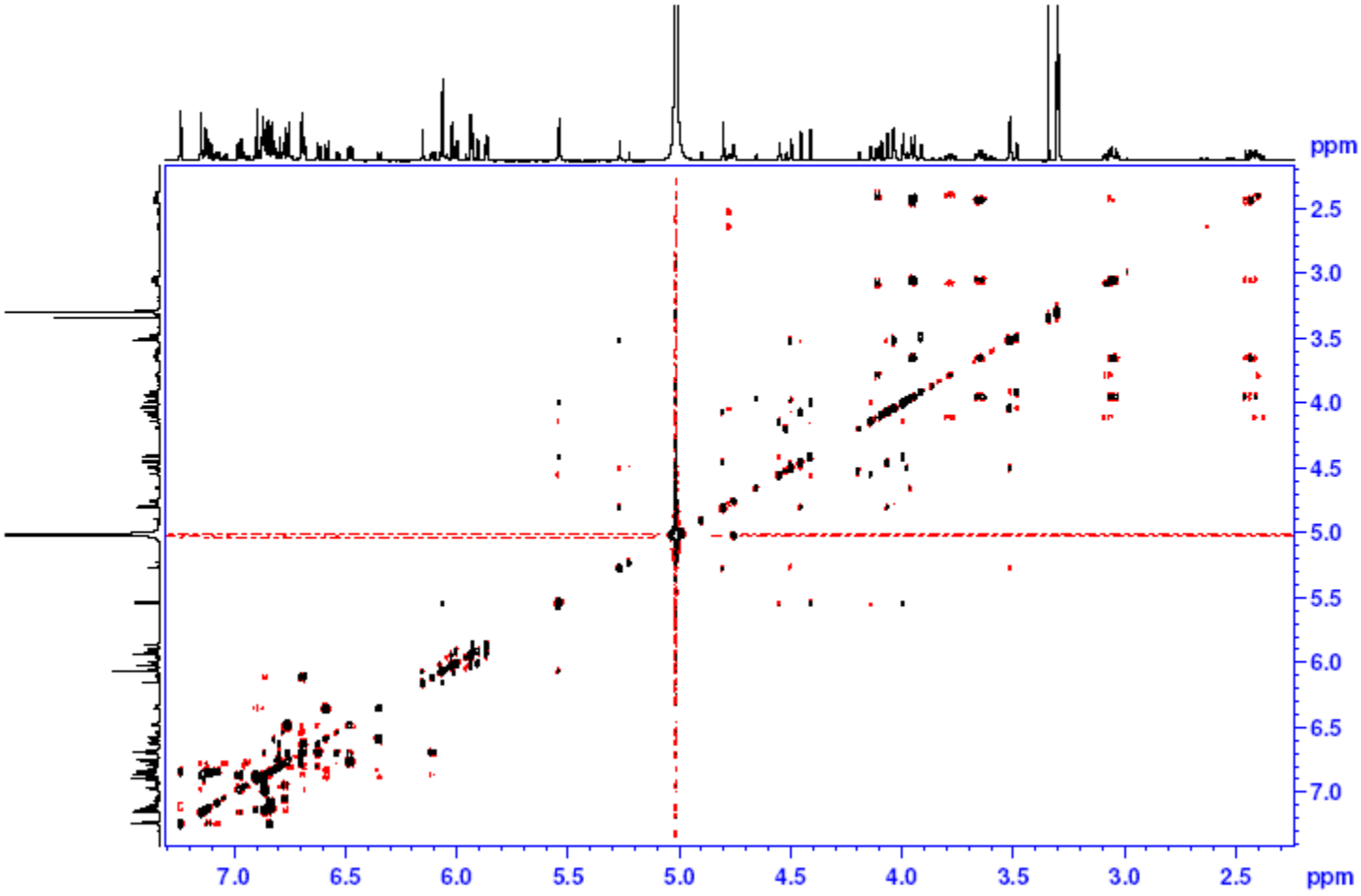
S4. ^{13}C DEPTQ NMR spectrum of **4**, CH^2 down, CH and CH^3 up (methanol-d_4, 150 MHz, 280K)



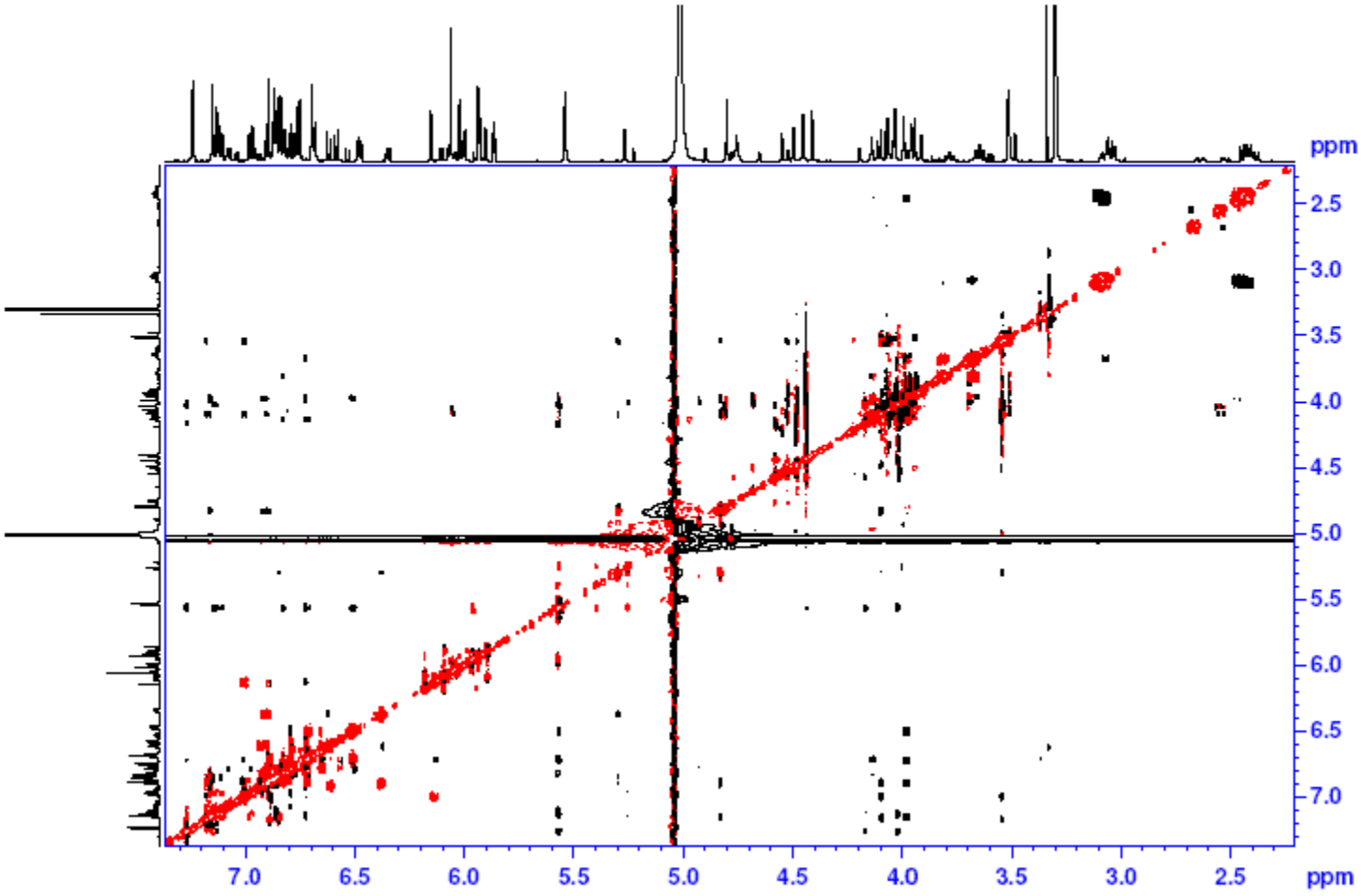
S5. PS-DQFCOSY spectrum of **4** (methanol-d_4, 600 MHz, 280K)



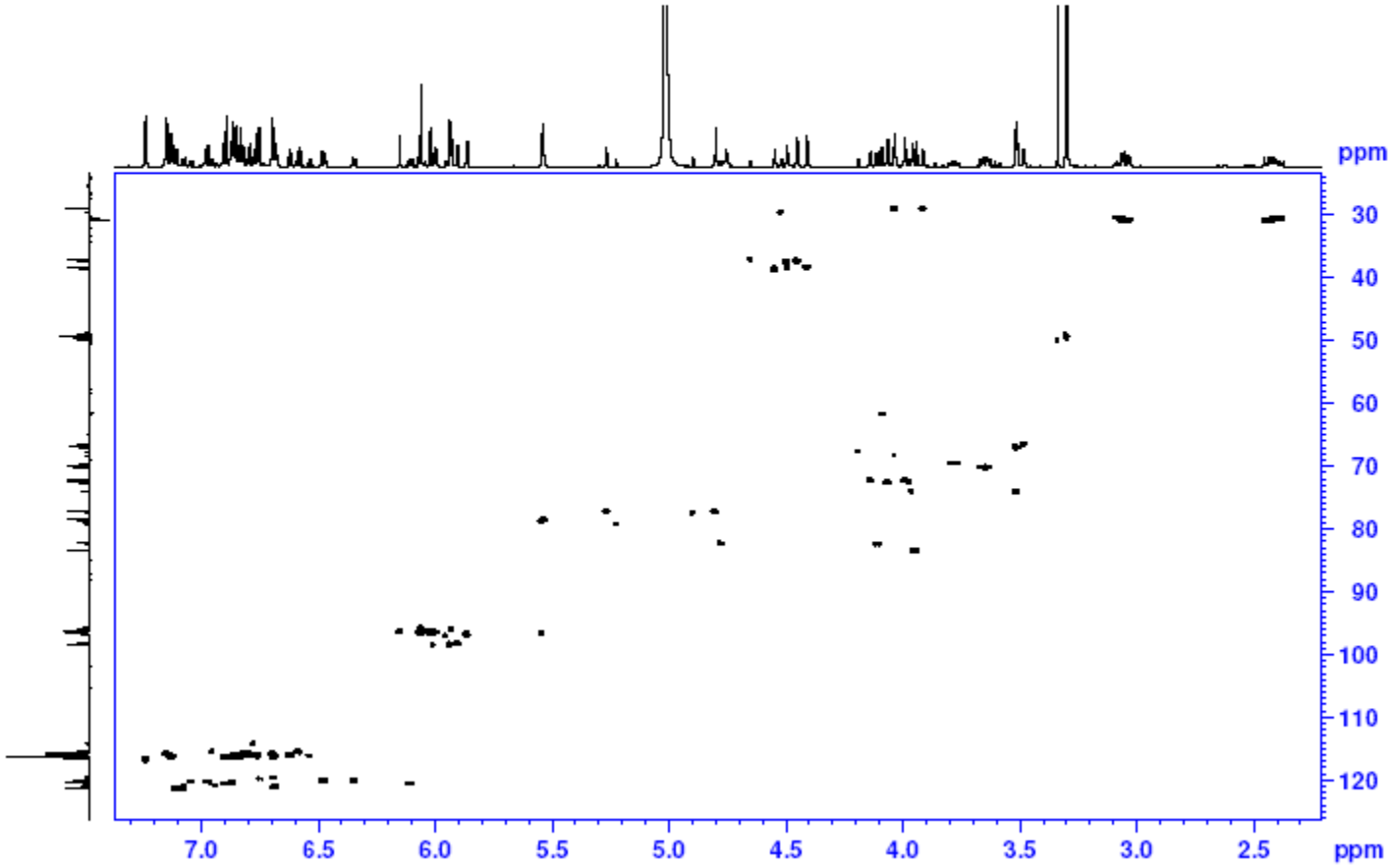
S6. TOCSY spectrum of **4** (methanol-d_4, 600 MHz, 280K)



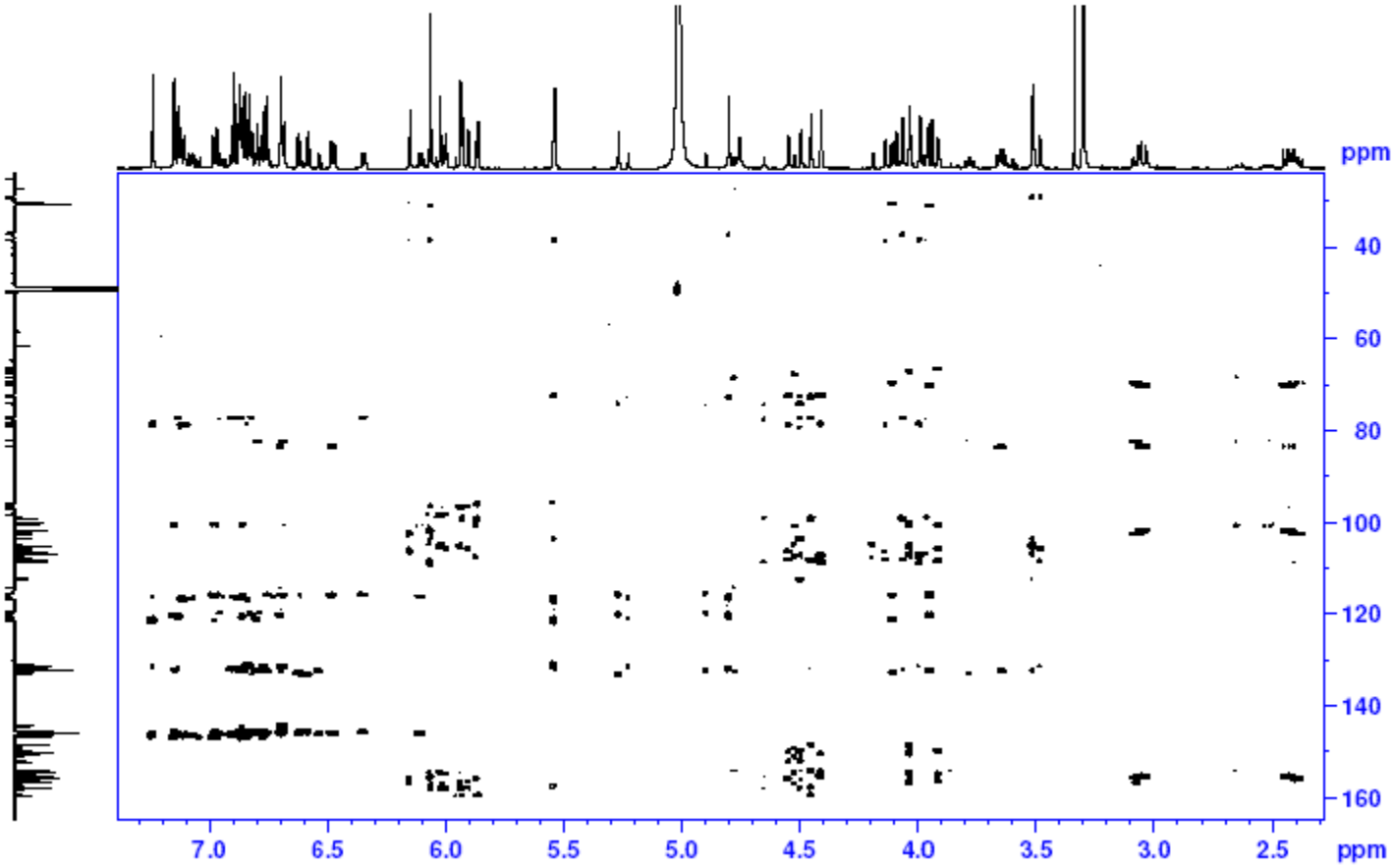
S7. ROESY spectrum of **4** (methanol-d_4, 600 MHz, 280K)



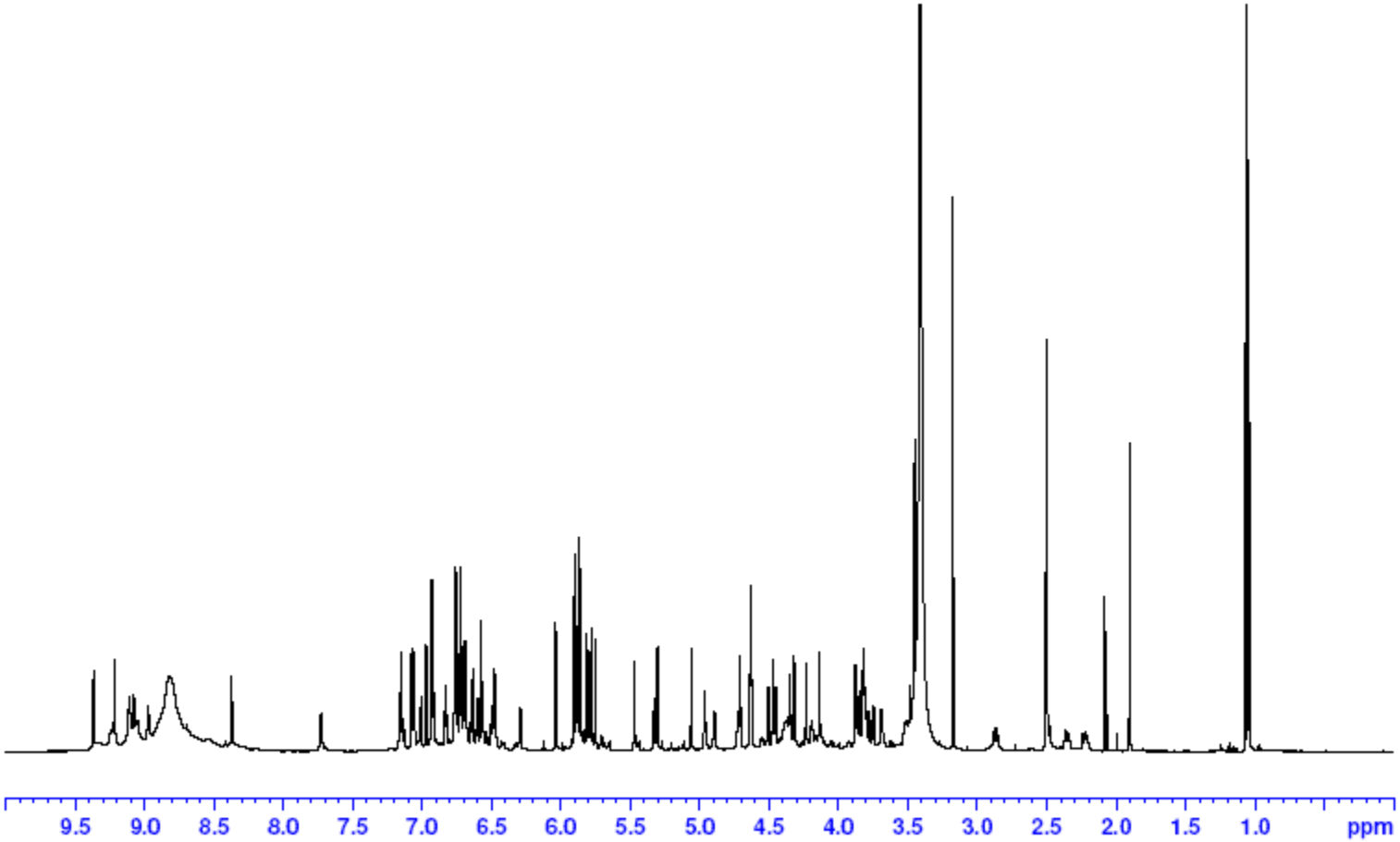
S8. Multiplicity Edited HSQC spectrum of **4** (methanol-d_4, 600 MHz, 280K)



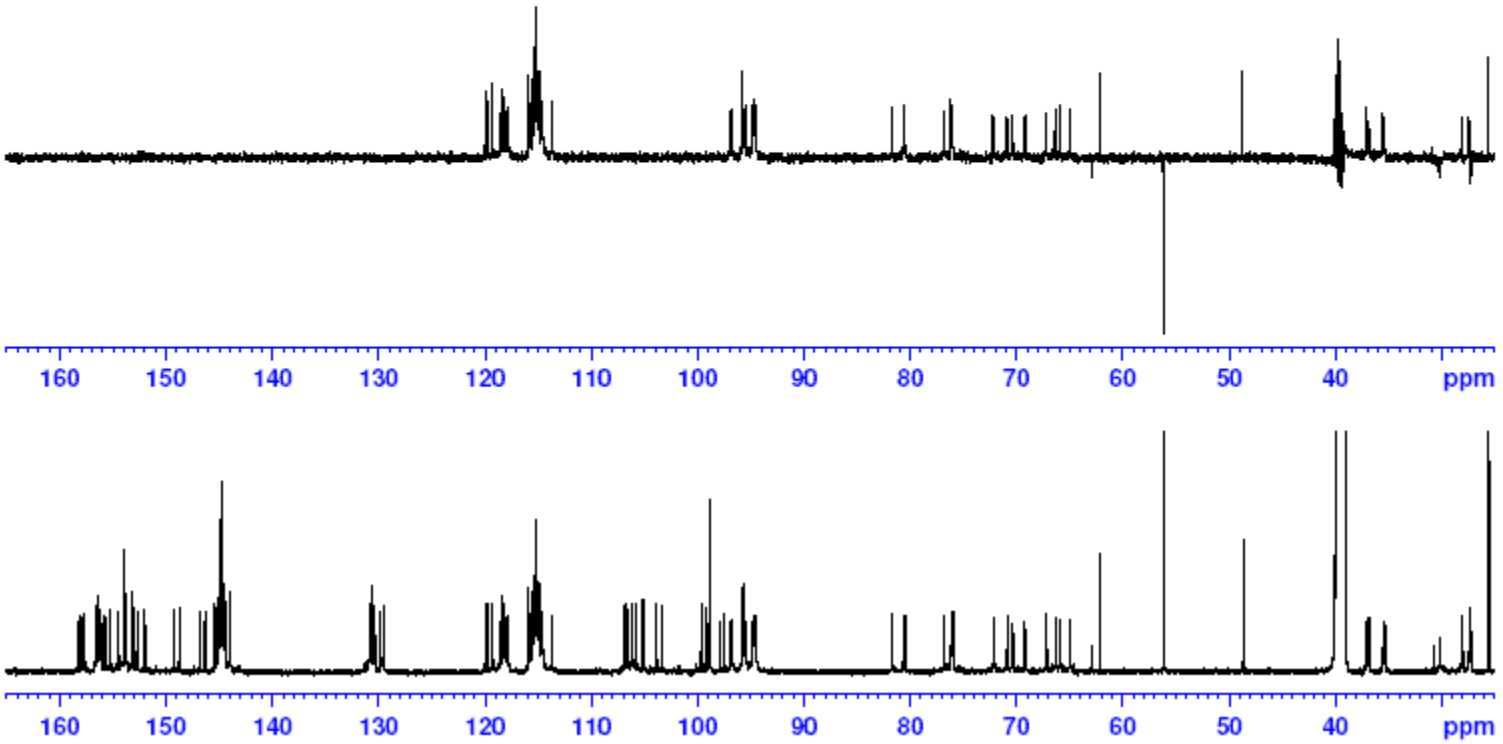
S9. HMBC spectrum of **4** (methanol-d_4, 600 MHz, 280K)



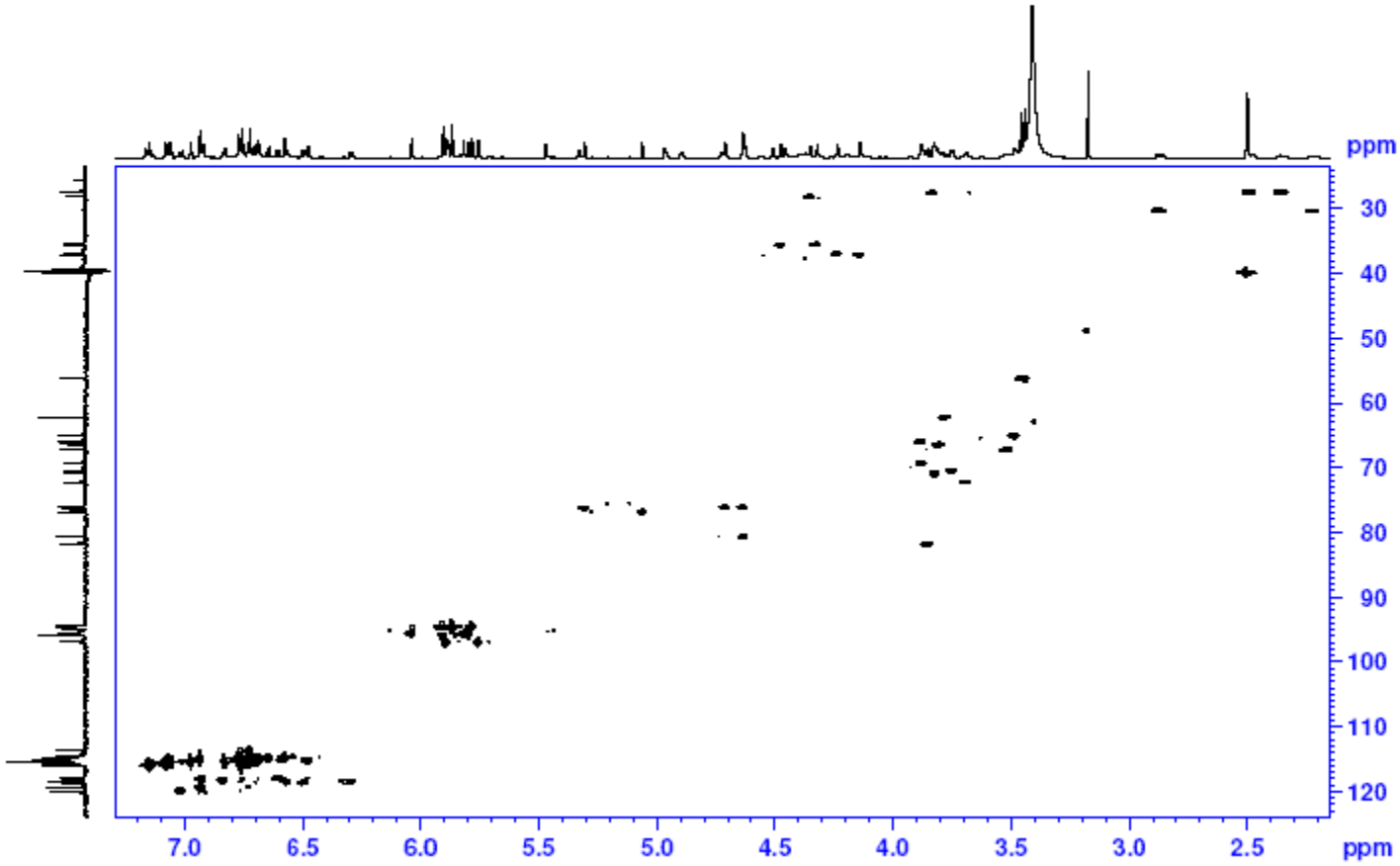
S10. ^{1}H NMR spectrum of **4** (dmso-d_6, 700 MHz, 298K)



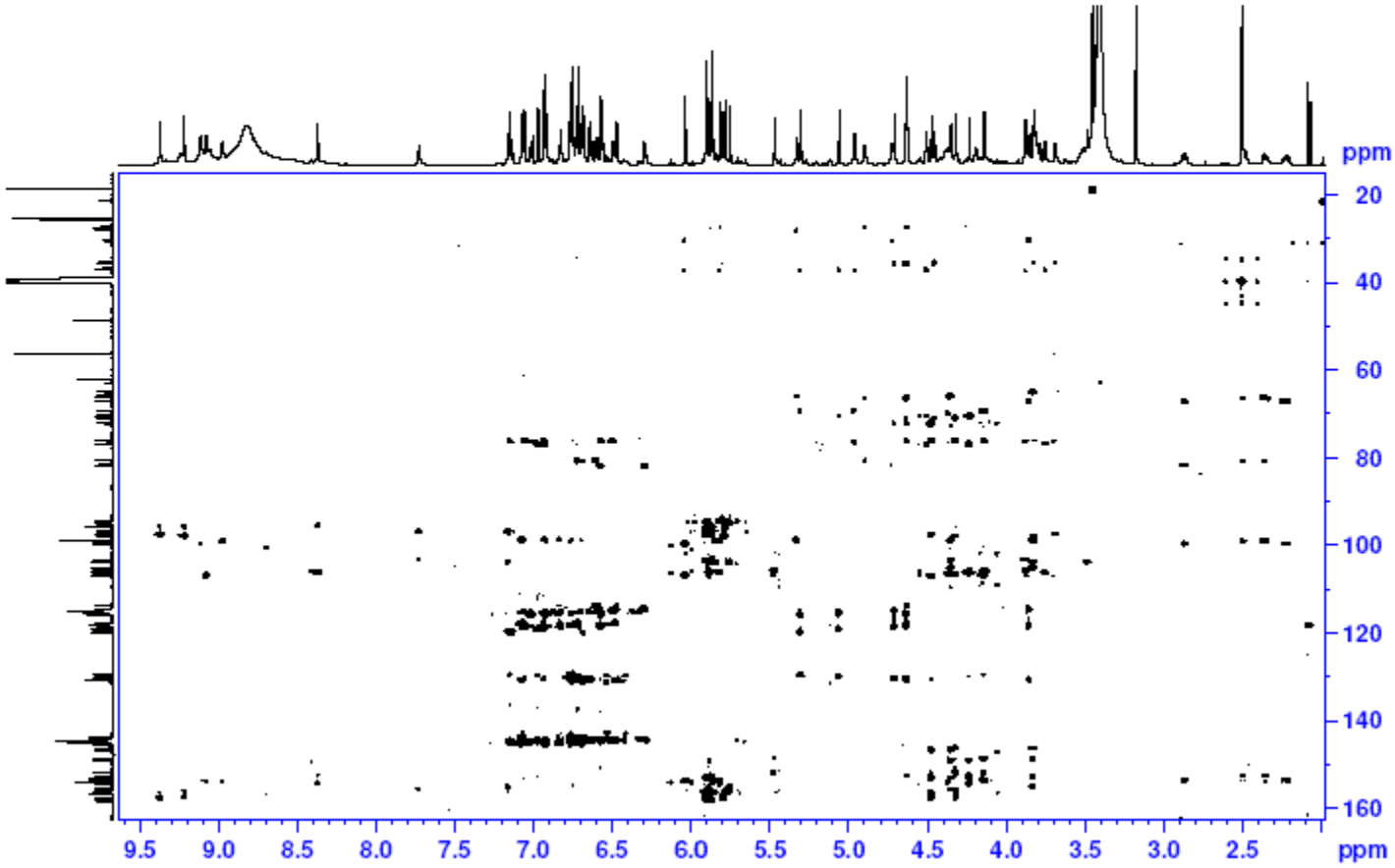
S11. ^{13}C and DEPT135 NMR spectrum of **4** (dmso-d_6, 150 MHz, 298K)



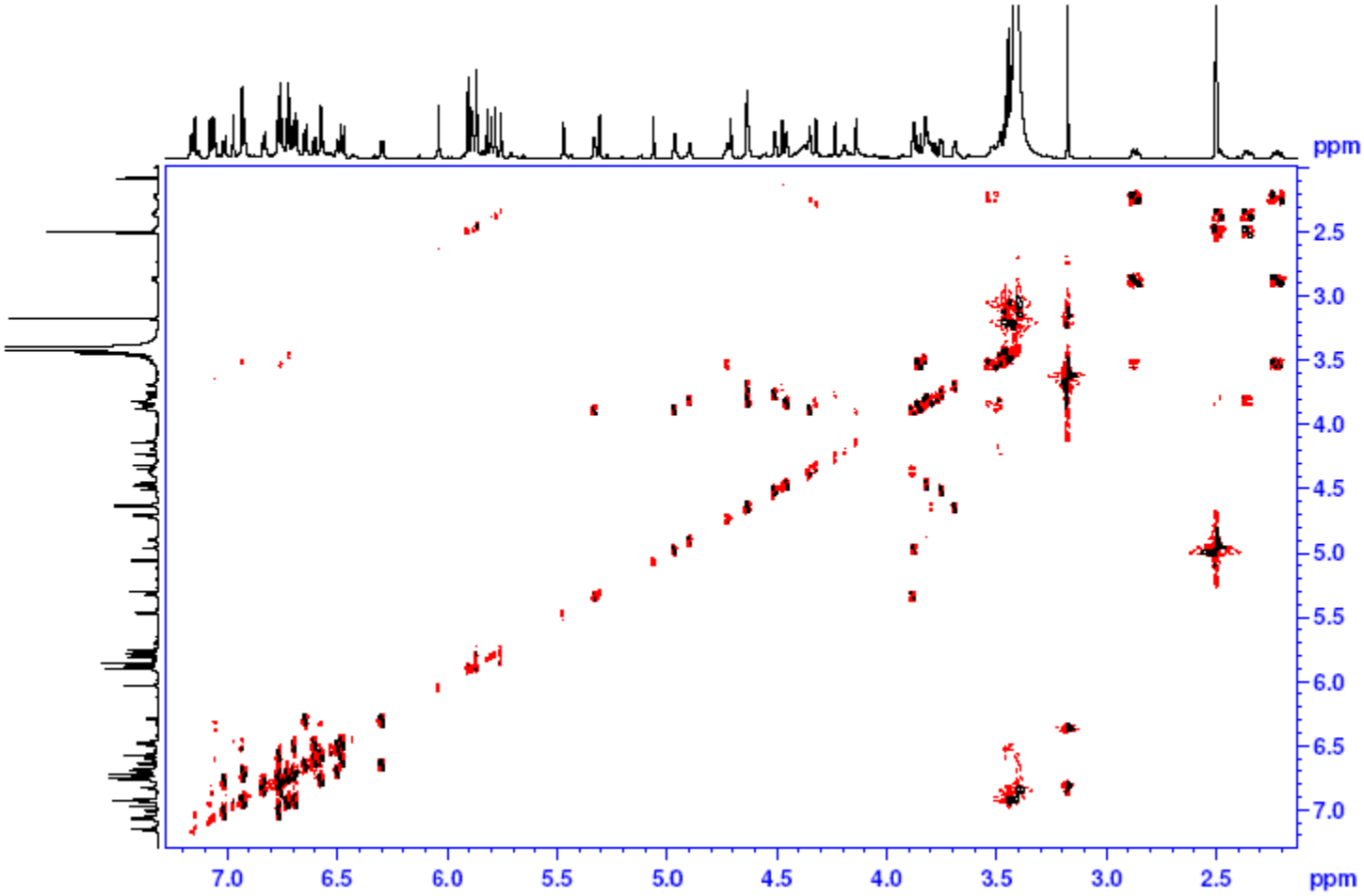
S12. Multiplicity Edited HSQC spectrum of **4** (dmso-d_6, 700 MHz, 298K)



S13. HMBC spectrum of **4** (dmso-d_6, 700 MHz, 298K)



S14. PS-DQFCOSY spectrum of **4** (dmso-d_6, 700 MHz, 298K)



S15. ROESY spectrum of **4** (dmso-d_6, 700 MHz, 298K)

