

## Supporting Information

# New Benzofuran Oligomers from the Roots of *Eupatorium heterophyllum* Collected in China

Yiming Hu <sup>1</sup>, Yoshinori Saito <sup>1,\*</sup>, Yosuke Matsuo <sup>1</sup>, Xun Gong <sup>2</sup> and Takashi Tanaka <sup>1,\*</sup>

<sup>1</sup> Graduate School of Biomedical Sciences, Nagasaki University, 1-14 Bunkyo-machi, Nagasaki 852-8521, Japan

<sup>2</sup> Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, China

\* Correspondence: saiyoshi@nagasaki-u.ac.jp (Y.S.); t-tanaka@nagasaki-u.ac.jp (T.T.);  
Tel.: +81-95-819-2433 (Y.S.); +81-95-819-2432 (T.T.)

## Index

<b>Figure S1.</b> <sup>1</sup> H NMR spectrum of <b>1</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	1
<b>Figure S2.</b> <sup>13</sup> C NMR spectrum of <b>1</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	2
<b>Figure S3.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>1</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	3
<b>Figure S4.</b> HSQC spectrum of <b>1</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	4
<b>Figure S5.</b> HMBC spectrum of <b>1</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	5
<b>Figure S6.</b> NOESY spectrum of <b>1</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	6
<b>Figure S7.</b> <sup>1</sup> H NMR spectrum of <b>2</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	7
<b>Figure S8.</b> <sup>13</sup> C NMR spectrum of <b>2</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	8
<b>Figure S9.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>2</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	9
<b>Figure S10.</b> HSQC spectrum of <b>2</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	10
<b>Figure S11.</b> HMBC spectrum of <b>2</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	11

<b>Figure S12.</b> NOESY spectrum of <b>2</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	12
<b>Figure S13.</b> <sup>1</sup> H NMR spectrum of <b>3</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	13
<b>Figure S14.</b> <sup>13</sup> C NMR spectrum of <b>3</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	14
<b>Figure S15.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>3</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	15
<b>Figure S16.</b> HSQC spectrum of <b>3</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	16
<b>Figure S17.</b> HMBC spectrum of <b>3</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	17
<b>Figure S18.</b> NOESY spectrum of <b>3</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	18
<b>Figure S19.</b> Experimental ECD spectra of <b>29</b> and calculated ECD spectra of <i>2S,3R-29</i> and <i>2R,3R-29</i> . .....	19
<b>Figure S20.</b> Optimized structures (B3LYP/6-31G(d,p) in MeOH (PCM)) and calculated ECD spectra (CAM-B3LYP/6-31G(d,p) in MeOH (PCM)) for each conformer of <b>29</b> ( <b>29A–29F</b> ). .....	20
<b>Figure S21.</b> <sup>1</sup> H NMR spectrum of <b>4</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	21
<b>Figure S22.</b> <sup>13</sup> C NMR spectrum of <b>4</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	22
<b>Figure S23.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>4</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	23
<b>Figure S24.</b> HSQC spectrum of <b>4</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	24
<b>Figure S25.</b> HMBC spectrum of <b>4</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	25
<b>Figure S26.</b> NOESY spectrum of <b>4</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	26
<b>Figure S27.</b> <sup>1</sup> H NMR spectrum of <b>5</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	27
<b>Figure S28.</b> <sup>13</sup> C NMR spectrum of <b>5</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	28
<b>Figure S29.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>5</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	29
<b>Figure S30.</b> HSQC spectrum of <b>5</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	30
<b>Figure S31.</b> HMBC spectrum of <b>5</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	31
<b>Figure S32.</b> NOESY spectrum of <b>5</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	32
<b>Figure S33.</b> Experimental and calculated ECD spectra and chiral HPLC analysis of <b>4</b> and <b>5</b> . .....	33

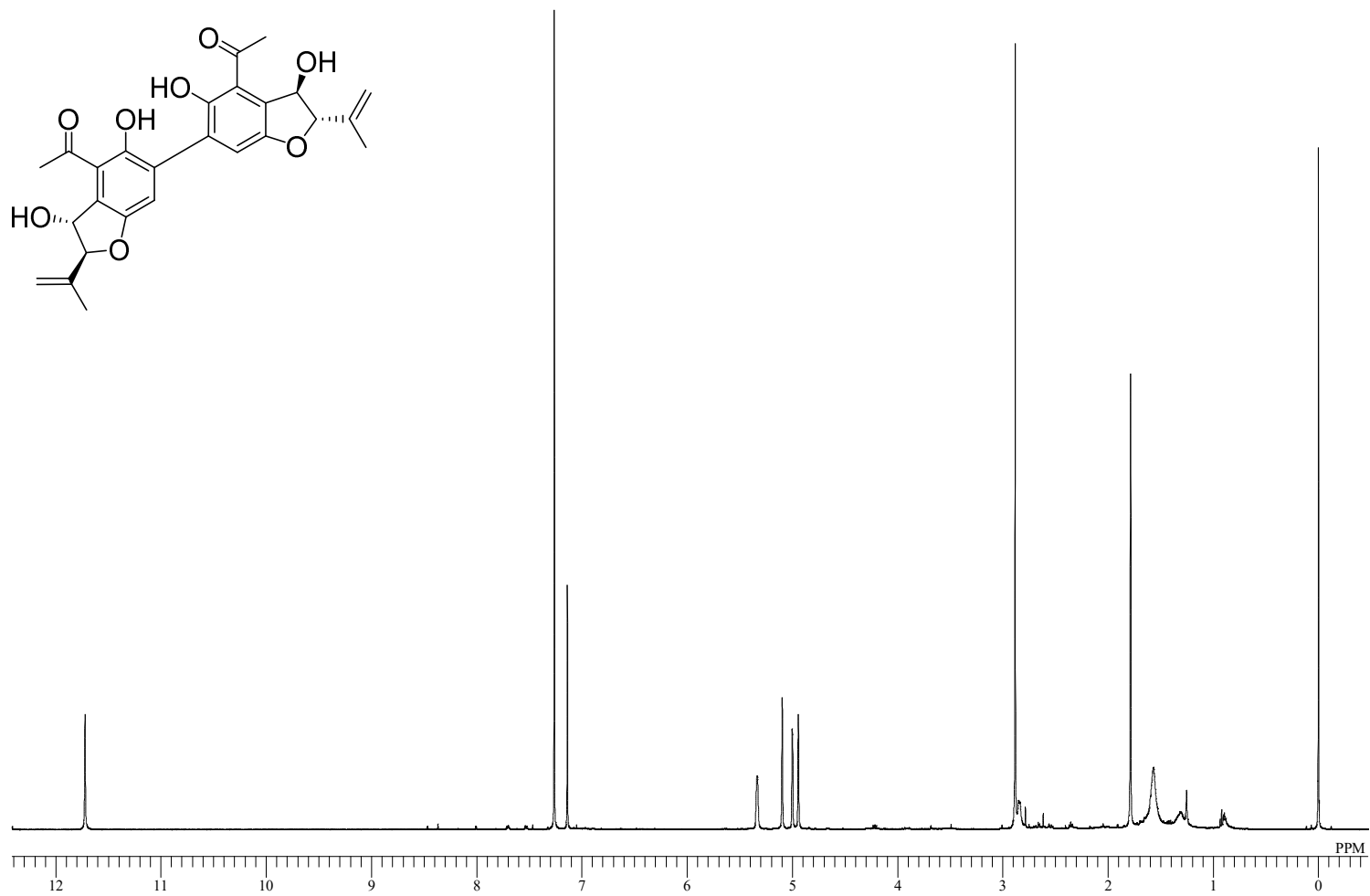
<b>Figure S34.</b> $^1\text{H}$ NMR spectrum of <b>14</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	34
<b>Figure S35.</b> $^{13}\text{C}$ NMR spectrum of <b>14</b> (measured in $\text{CDCl}_3$ , 126 MHz). .....	35
<b>Figure S36.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>14</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	36
<b>Figure S37.</b> HSQC spectrum of <b>14</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	37
<b>Figure S38.</b> HMBC spectrum of <b>14</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	38
<b>Figure S39.</b> NOESY spectrum of <b>14</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	39
<b>Figure S40.</b> $^1\text{H}$ NMR spectrum of <b>17</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	40
<b>Figure S41.</b> $^{13}\text{C}$ NMR spectrum of <b>17</b> (measured in $\text{CDCl}_3$ , 126 MHz). .....	41
<b>Figure S42.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>17</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	42
<b>Figure S43.</b> HSQC spectrum of <b>17</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	43
<b>Figure S44.</b> HMBC spectrum of <b>17</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	44
<b>Figure S45.</b> NOESY spectrum of <b>17</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	45
<b>Figure S46.</b> $^1\text{H}$ NMR spectrum of <b>21</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	46
<b>Figure S47.</b> $^{13}\text{C}$ NMR spectrum of <b>21</b> (measured in $\text{CDCl}_3$ , 126 MHz). .....	47
<b>Figure S48.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>21</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	48
<b>Figure S49.</b> HSQC spectrum of <b>21</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	49
<b>Figure S50.</b> HMBC spectrum of <b>21</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	50
<b>Figure S51.</b> NOESY spectrum of <b>21</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	51
<b>Figure S52.</b> $^1\text{H}$ NMR spectrum of <b>25</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	52
<b>Figure S53.</b> $^{13}\text{C}$ NMR spectrum of <b>25</b> (measured in $\text{CDCl}_3$ , 126 MHz). .....	53
<b>Figure S54.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>25</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	54
<b>Figure S55.</b> HSQC spectrum of <b>25</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	55
<b>Figure S56.</b> HMBC spectrum of <b>25</b> (measured in $\text{CDCl}_3$ , 500 MHz). .....	56

<b>Figure S57.</b> NOESY spectrum of <b>25</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	57
<b>Figure S58.</b> <sup>1</sup> H NMR spectrum of <b>26</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	58
<b>Figure S59.</b> <sup>13</sup> C NMR spectrum of <b>26</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	59
<b>Figure S60.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>26</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	60
<b>Figure S61.</b> HSQC spectrum of <b>26</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	61
<b>Figure S62.</b> HMBC spectrum of <b>26</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	62
<b>Figure S63.</b> NOESY spectrum of <b>26</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	63
<b>Figure S64.</b> <sup>1</sup> H NMR spectrum of <b>31</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	64
<b>Figure S65.</b> <sup>13</sup> C NMR spectrum of <b>31</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	65
<b>Figure S66.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>31</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	66
<b>Figure S67.</b> HSQC spectrum of <b>31</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	67
<b>Figure S68.</b> HMBC spectrum of <b>31</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	68
<b>Figure S69.</b> NOESY spectrum of <b>31</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	69
<b>Figure S70.</b> <sup>1</sup> H NMR spectrum of <b>32</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	70
<b>Figure S71.</b> <sup>13</sup> C NMR spectrum of <b>32</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	71
<b>Figure S72.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>32</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	72
<b>Figure S73.</b> HSQC spectrum of <b>32</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	73
<b>Figure S74.</b> HMBC spectrum of <b>32</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	74
<b>Figure S75.</b> NOESY spectrum of <b>32</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	75
<b>Figure S76.</b> <sup>1</sup> H NMR spectrum of <b>34</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	76
<b>Figure S77.</b> <sup>13</sup> C NMR spectrum of <b>34</b> (measured in CDCl <sub>3</sub> , 126 MHz). .....	77
<b>Figure S78.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>34</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	78
<b>Figure S79.</b> HSQC spectrum of <b>34</b> (measured in CDCl <sub>3</sub> , 500 MHz). .....	79

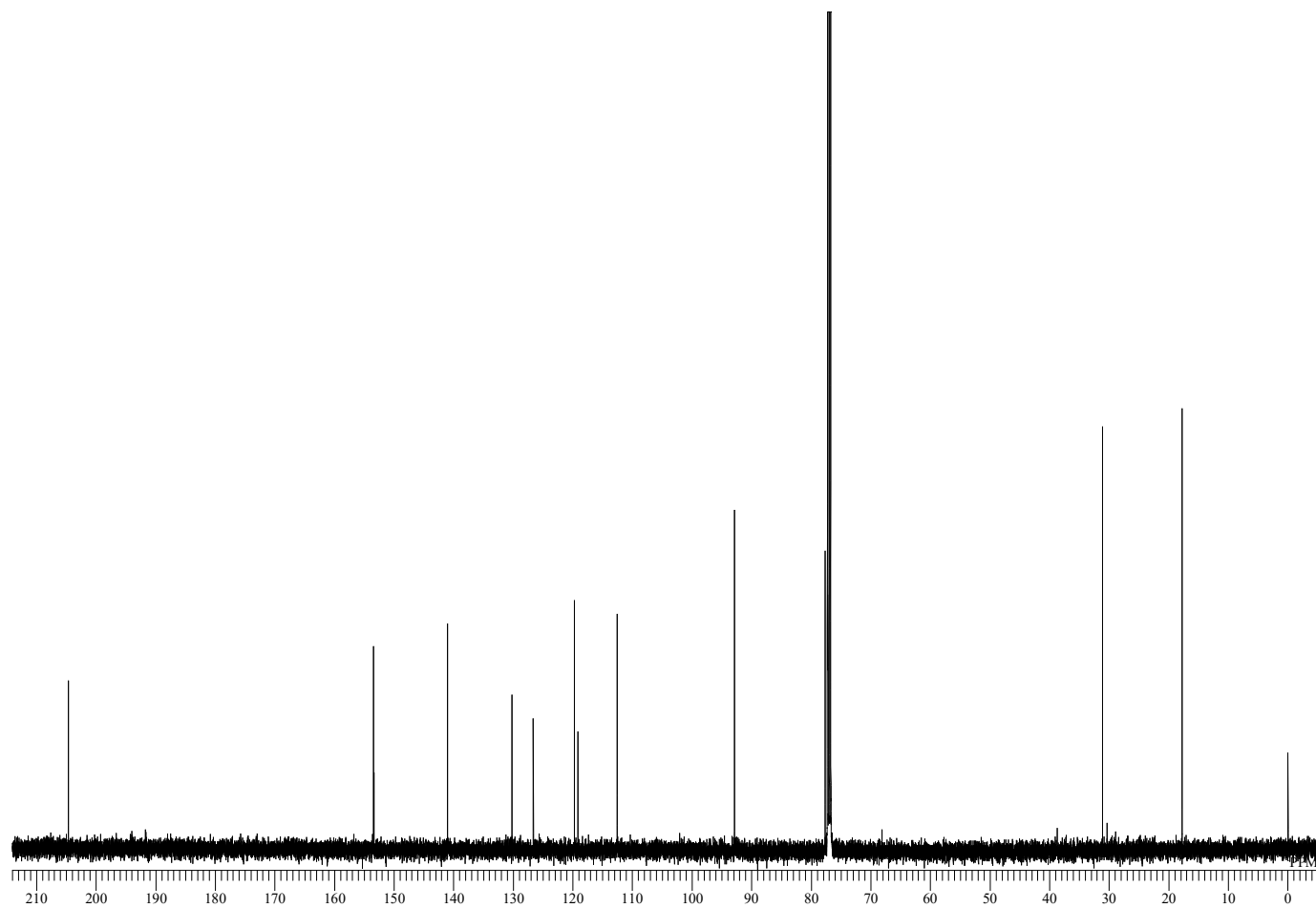


<b>Figure S80.</b> HMBC spectrum of <b>34</b> (measured in CDCl <sub>3</sub> , 500 MHz).	80
<b>Figure S81.</b> NOESY spectrum of <b>34</b> (measured in CDCl <sub>3</sub> , 500 MHz).	81
<b>Figure S82.</b> <sup>1</sup> H NMR spectrum of <b>36</b> (measured in CDCl <sub>3</sub> , 500 MHz).	82
<b>Figure S83.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>36</b> (measured in CDCl <sub>3</sub> , 500 MHz).	83
<b>Figure S84.</b> NOESY spectrum of <b>36</b> (measured in CDCl <sub>3</sub> , 500 MHz).	84
<b>Figure S85.</b> <sup>1</sup> H NMR spectrum of <b>39</b> (measured in CDCl <sub>3</sub> , 500 MHz).	85
<b>Figure S86.</b> <sup>13</sup> C NMR spectrum of <b>39</b> (measured in CDCl <sub>3</sub> , 126 MHz).	86
<b>Figure S87.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>39</b> (measured in CDCl <sub>3</sub> , 500 MHz).	87
<b>Figure S88.</b> HSQC spectrum of <b>39</b> (measured in CDCl <sub>3</sub> , 500 MHz).	88
<b>Figure S89.</b> HMBC spectrum of <b>39</b> (measured in CDCl <sub>3</sub> , 500 MHz).	89
<b>Figure S90.</b> NOESY spectrum of <b>39</b> (measured in CDCl <sub>3</sub> , 500 MHz).	90
<b>Figure S91.</b> <sup>1</sup> H NMR spectrum of <b>20</b> (measured in CDCl <sub>3</sub> , 500 MHz).	91
<b>Figure S92.</b> <sup>13</sup> C NMR spectrum of <b>20</b> (measured in CDCl <sub>3</sub> , 126 MHz).	92
<b>Figure S93.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>20</b> (measured in CDCl <sub>3</sub> , 500 MHz).	93
<b>Figure S94.</b> HSQC spectrum of <b>20</b> (measured in CDCl <sub>3</sub> , 500 MHz).	94
<b>Figure S95.</b> HMBC spectrum of <b>20</b> (measured in CDCl <sub>3</sub> , 500 MHz).	95
<b>Figure S96.</b> NOESY spectrum of <b>20</b> (measured in CDCl <sub>3</sub> , 500 MHz).	96
<b>Figure S97.</b> <sup>1</sup> H NMR spectrum of <b>28</b> (measured in CDCl <sub>3</sub> , 500 MHz).	97
<b>Figure S98.</b> <sup>13</sup> C NMR spectrum of <b>28</b> (measured in CDCl <sub>3</sub> , 126 MHz).	98
<b>Figure S99.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>28</b> (measured in CDCl <sub>3</sub> , 500 MHz).	99
<b>Figure S100.</b> HSQC spectrum of <b>28</b> (measured in CDCl <sub>3</sub> , 500 MHz).	100
<b>Figure S101.</b> HMBC spectrum of <b>28</b> (measured in CDCl <sub>3</sub> , 500 MHz).	101
<b>Figure S102.</b> NOESY spectrum of <b>28</b> (measured in CDCl <sub>3</sub> , 500 MHz).	102

**Figure S1.**  $^1\text{H}$  NMR spectrum of **1** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S2.**  $^{13}\text{C}$  NMR spectrum of **1** (measured in  $\text{CDCl}_3$ , 126 MHz).

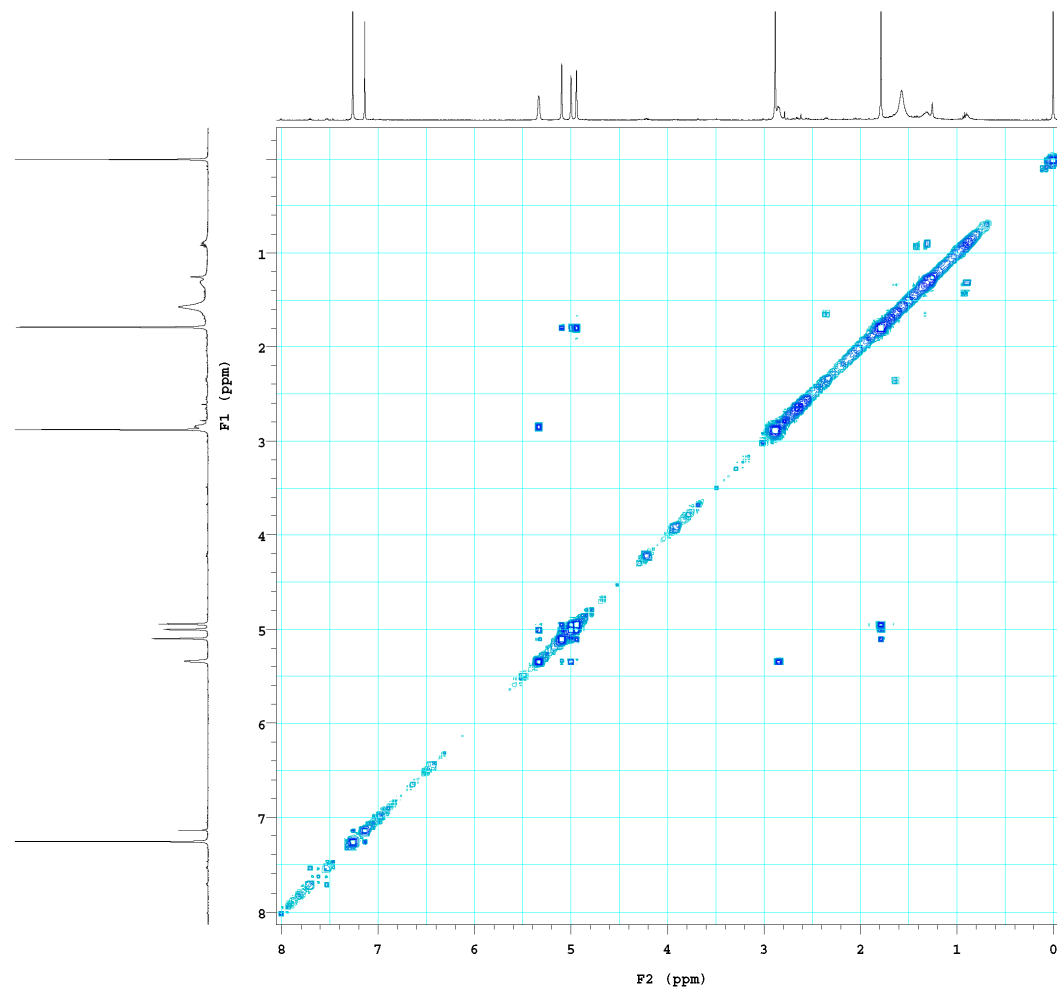


**Figure S3.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** (measured in  $\text{CDCl}_3$ , 500 MHz).

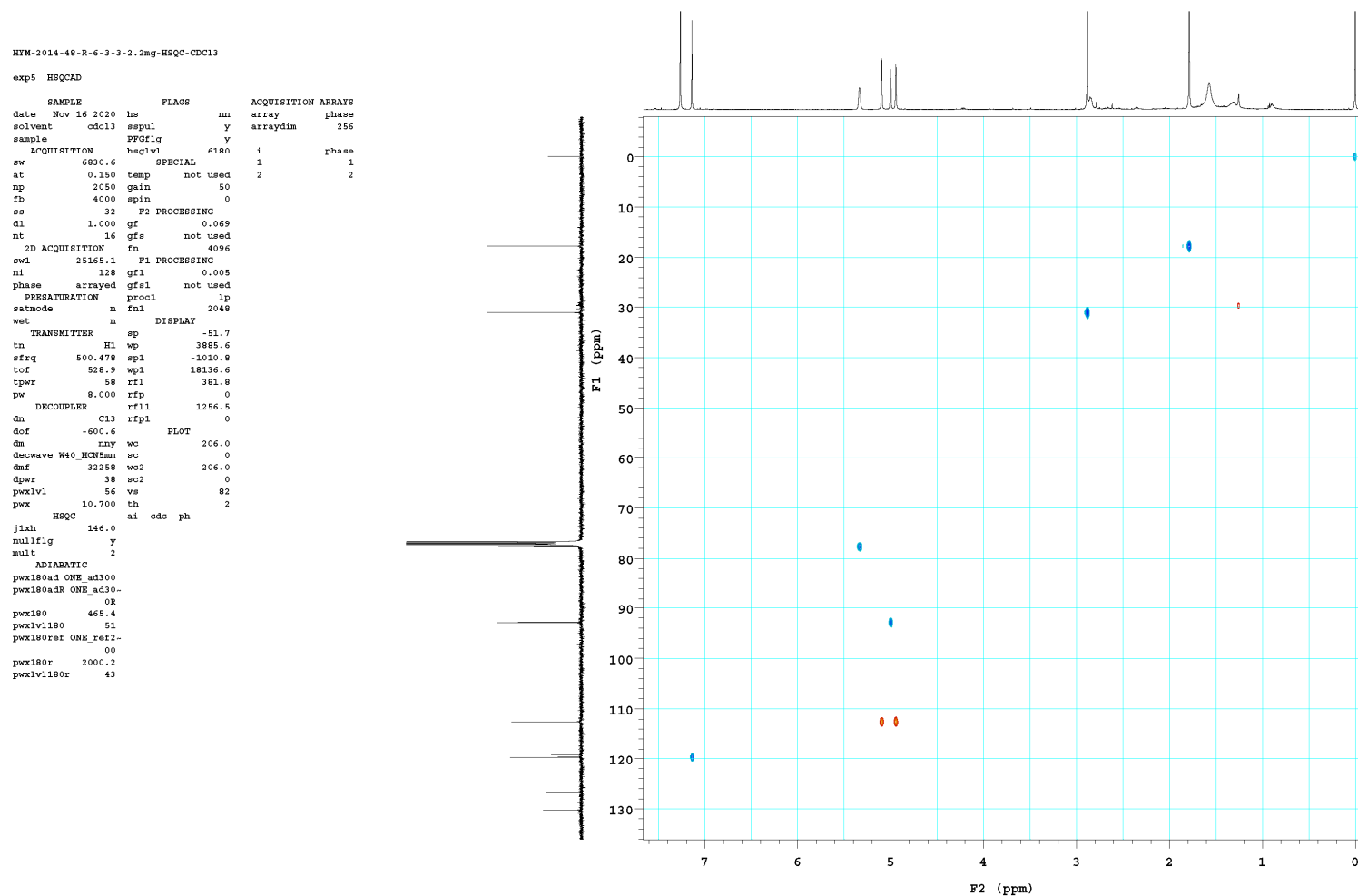
HYM-2014-48-R-6-3-3-2.2mg-COSY- $\text{CDCl}_3$

exp4 gCOSY

SAMPLE		FLAGS	
date	Nov 16 2020	hs	nn
solvent	cdcl3	espul	y
sample	hsglvi		6180
ACQUISITION		SPECIAL	
sw	6830.6	temp	not used
at	0.150	gain	50
np	2050	spin	0
fb	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	16	fn	4096
2D ACQUISITION		F1 PROCESSING	
sw1	6830.6	sbl	-0.019
n1	128	sbs1	not used
d2	0	proc1	lp
PRESATURATION		fml	
satmode	n	DISPLAY	4096
wet	n	sp	-95.0
TRANSMITTER		wp	
tn	H1	sp1	-165.1
sfrq	500.478	wp1	4232.4
tof	528.9	rf1	381.8
tpwr	58	rfp	0
pw	8.000	rf11	381.8
GRADIENTS		rfp1	
gr1v1s	5154	PLOT	0
gtE	0.001000	wc	206.0
EDratio	1.000	sc	0
gstab	0.000500	wc2	206.0
DECOUPLER		sc2	
dn	C13	vs	82
dm	nmn	th	5
	ai	cdc	av



**Figure S4.** HSQC spectrum of **1** (measured in CDCl<sub>3</sub>, 500 MHz).

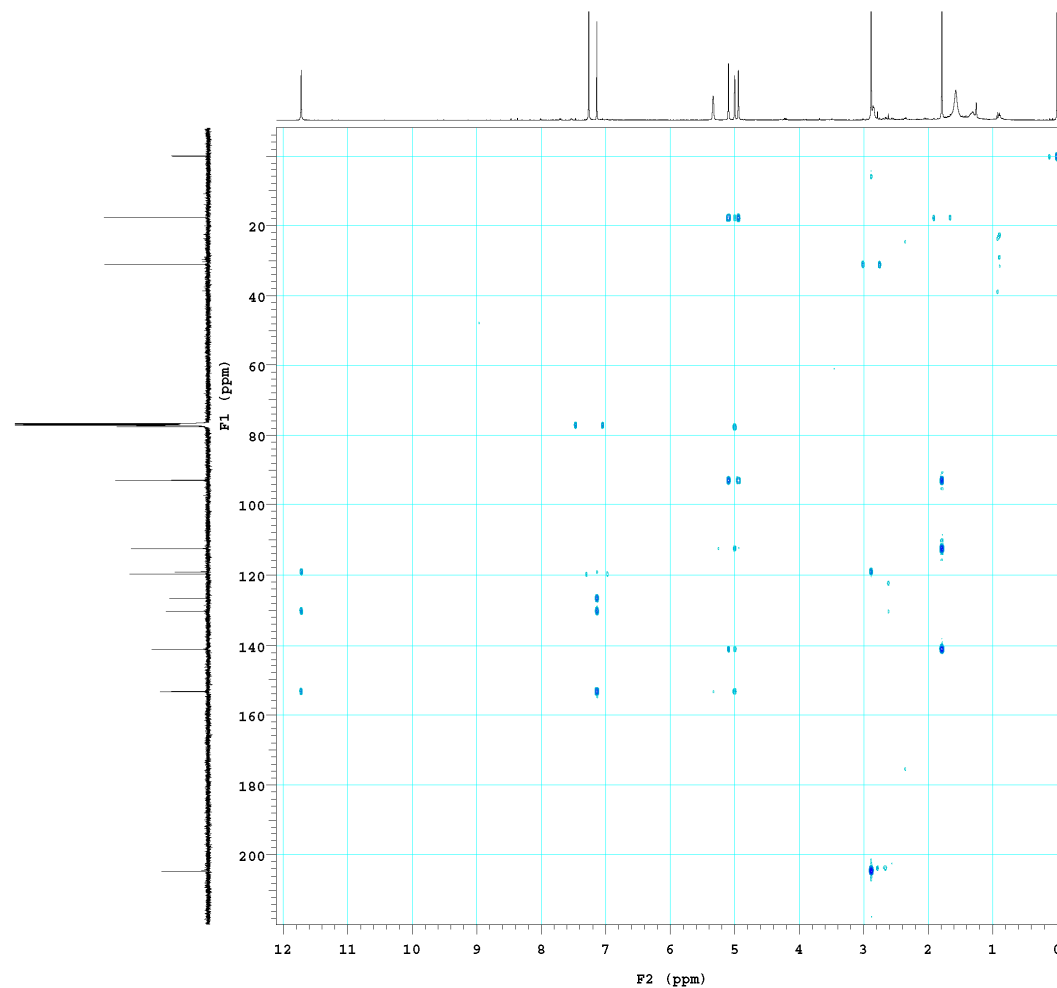


**Figure S5.** HMBC spectrum of **1** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-3-3-2.2mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Nov 16 2020	hs		mn	
solvent	cdcl3	spul	y	array	phase
sample		ppgflg	y	arraydim	256
ACQUISITION		huglvi	6180	1	phase
sw	6830.6	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2050	gain	50		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	grlvi1	409		
nt	32	gt1	0.001000		
2D ACQUISITION		grlvi3	1227		
sw1	30200.1	gt3	0.001000		
ni	228	gstab	0.000500		
phase		arrayed	F2 PROCESSING		
PRESATURATION		sb	-0.075		
satmode		n	sbs	not used	
wet		n	fn	4096	
TRANSMITTER		F1 PROCESSING			
tn		hl	gr1	0.004	
sfrq	500.478	grf1	not used		
tof	528.9	procl	lp		
tpwr	58	fn1	2048		
pw	8.000	DISPLAY			
DECOUPLER		sp	-111.7		
dn	C13	wp	6170.2		
dof	1287.0	sp1	-1001.6		
dm	nmn	wp1	28637.0		
decwave	W40_HCM5mm	r1	381.8		
dmf	32258	rfp	0		
dpwr	38	rf11	1886.4		
pxzlv1	56	rfp1	0		
pxz	10.700	PLOT			
HMBC		wc	206.0		
j1xh	146.0	sc	0		
jnxh	8.0	wc2	206.0		
ADIBATIC		sc2	0		
pxz180ad	ONE_ad300	vs	82		
pxzlv180	51	th	2		
pxz180	465.4	ai	cdc	av	

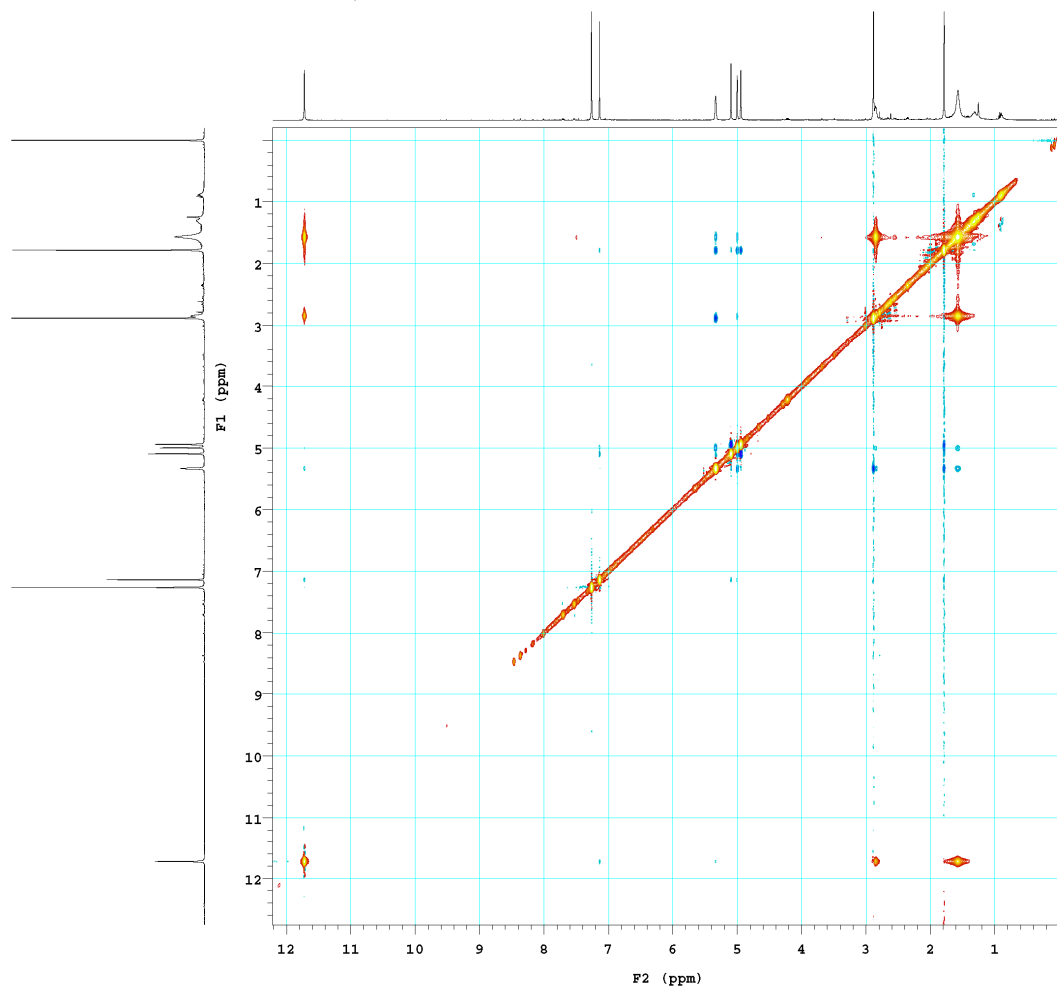


**Figure S6.** NOESY spectrum of **1** (measured in CDCl<sub>3</sub>, 500 MHz).

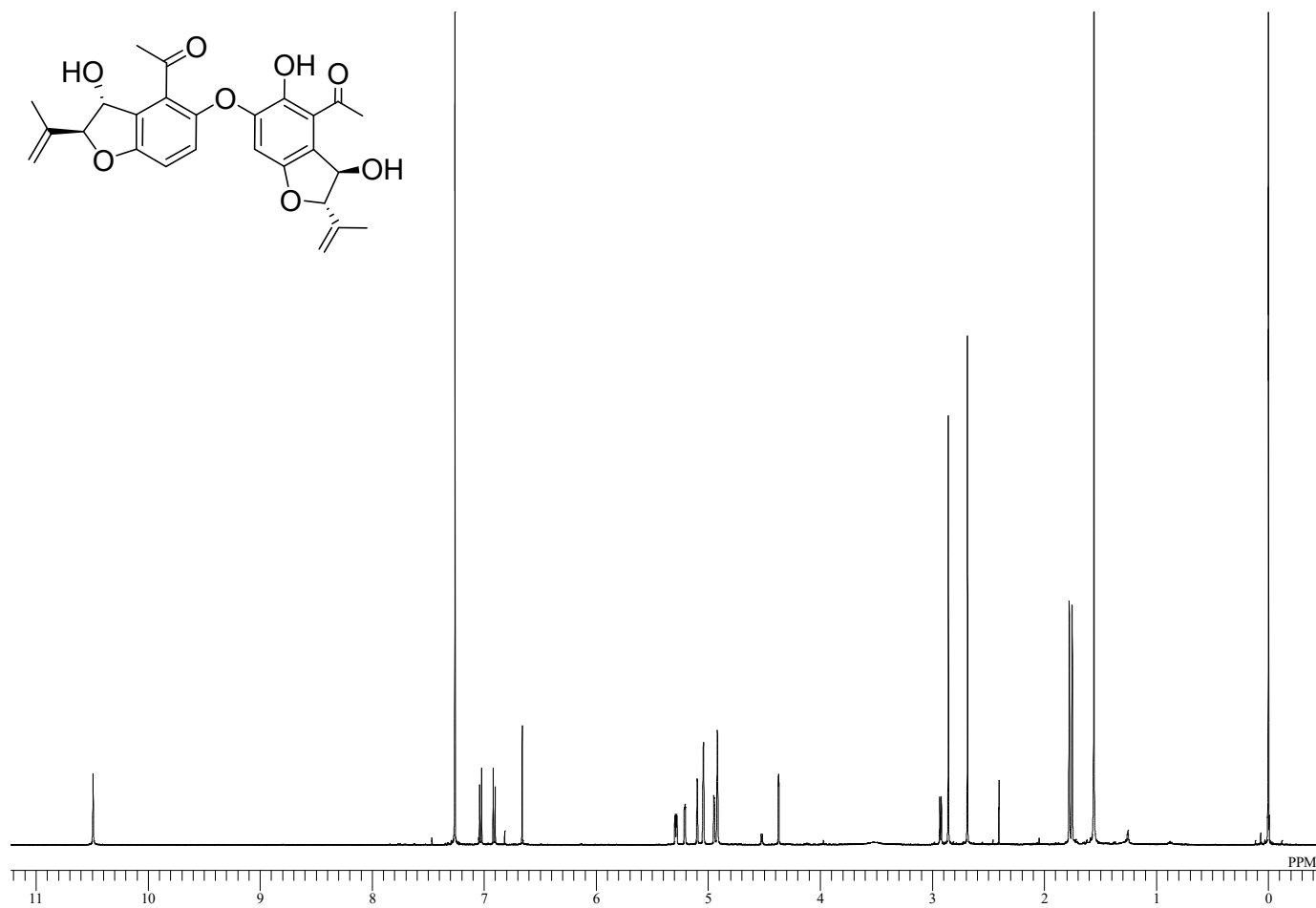
HYM-2014-48-R-6-3-3-2.2mg-NOESY-CDCl3

exp7 NOESY

SAMPLE		FLAGS	
date	Nov 16 2020	hs	nn
solvent	cdcl3	sspul	y
sample	PPGflg	y	
ACQUISITION		hsglvl	6180
sw	6830.6	SPECIAL	
at	0.150	temp	not used
np	2050	gain	50
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION		fn	4096
sw1	6830.6	F1 PROCESSING	
ni	128	gtl	0.017
TRANSMITTER		gtsl	not used
tn	H1	procl	lp
stfq	500.478	tnl	4096
tof	528.9	DISPLAY	
tpwr	58	sp	-65.0
pw	8.000	wp	6176.9
NOESY		sp1	-98.4
mixN	0.500	wp1	6480.4
PRESATURATION		rfl	381.8
satmode	n	rfp	0
wet	n	rfl1	381.8
DECOUPLER		rfl1	0
dn	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	82
		th	1
		ai	ph

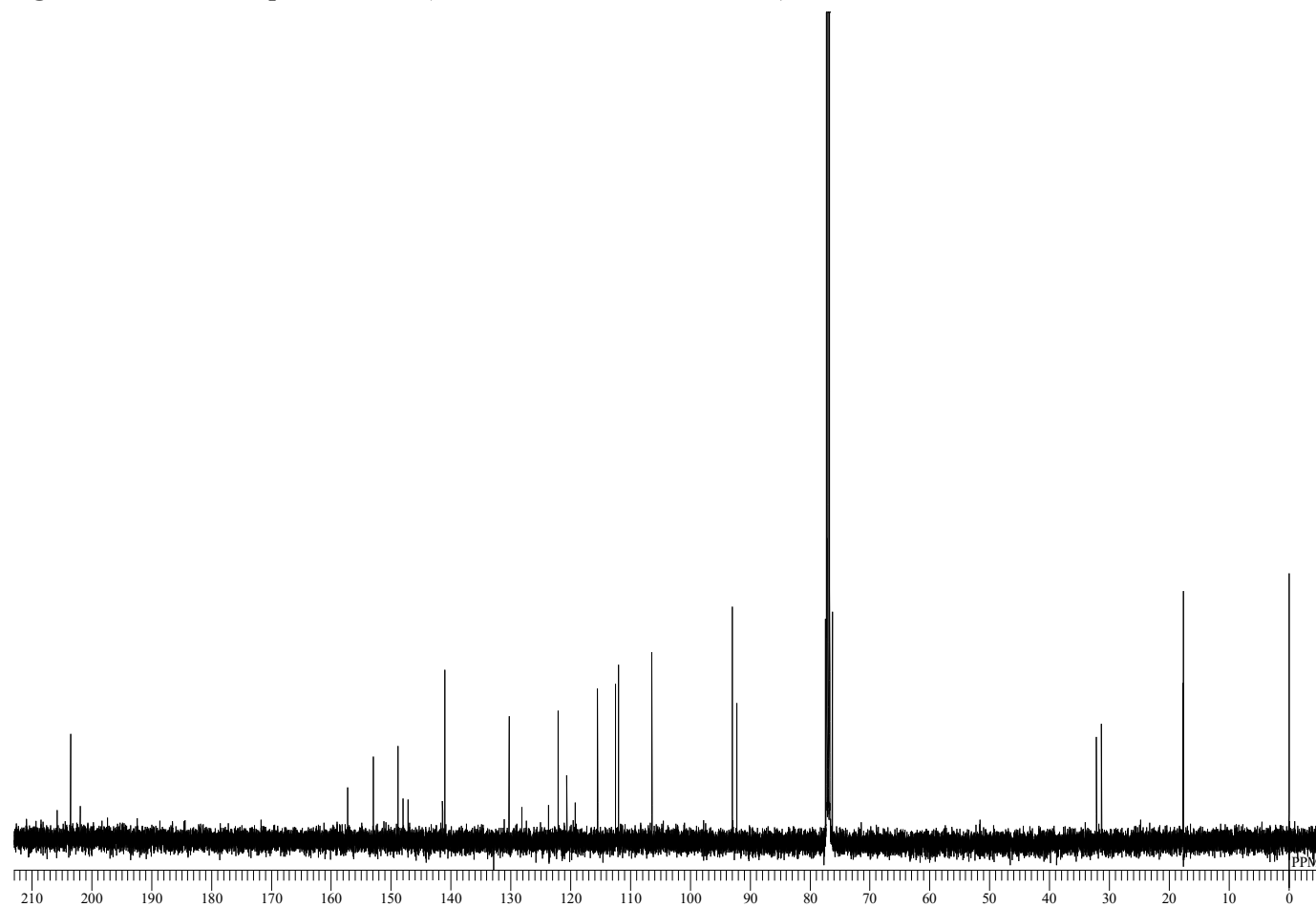


**Figure S7.**  $^1\text{H}$  NMR spectrum of **2** (measured in  $\text{CDCl}_3$ , 500 MHz).





**Figure S8.**  $^{13}\text{C}$  NMR spectrum of **2** (measured in  $\text{CDCl}_3$ , 126 MHz).

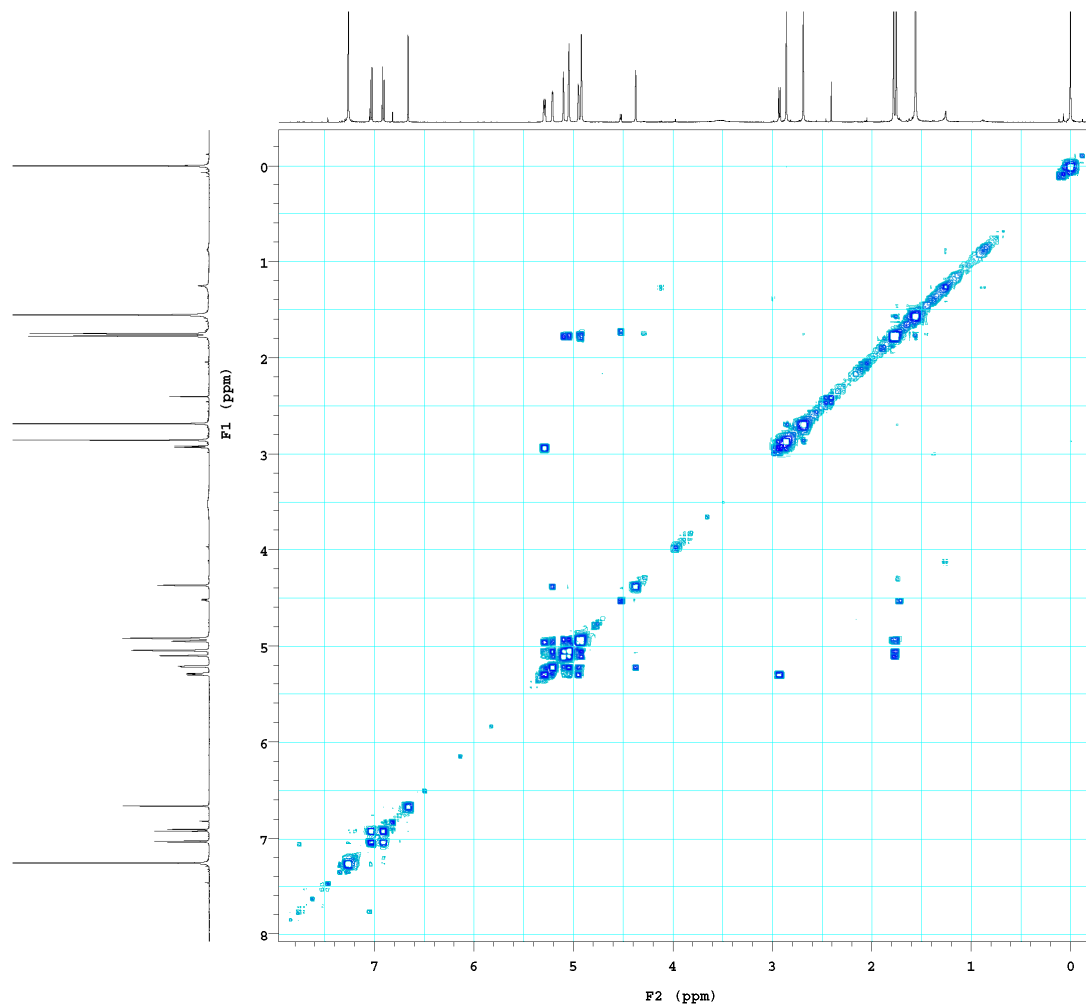


**Figure S9.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-6-3-2-1-1.lmg-COSY-CDCl3

exp4 gCOSY

SAMPLE		FLAGS	
date	Dec 16 2020	hs	nn
solvent	cdcl3	sspul	y
sample	hsglv1		6180
ACQUISITION		SPECIAL	
sw	6097.6	temp	not used
at	0.150	gain	46
np	1830	spin	0
fb	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	16	fn	2048
2D ACQUISITION		F1 PROCESSING	
sw1	6097.6	sb1	-0.021
ni	128	sbel	not used
d2	0	procl	1p
PRESATURATION		fml	
satmode	n		2048
TRANSMITTER		DISPLAY	
wet	n	sp	-89.0
tn	H1	sp1	4073.0
sfrq	500.478	wp1	-184.3
tof	276.8	rfl	4227.8
tpwr	58	rfl	267.7
pw	8.000	rfl1	267.7
GRADIENTS		rfl1	
gslvie	5154		0
gtE	0.001000	wc	206.0
Edratio	1.000	sc	0
getab	0.000500	wo2	206.0
DECOUPLER		sc2	
dn	C13	vs	132
dm	nmn	th	6
	ai	cdc	av

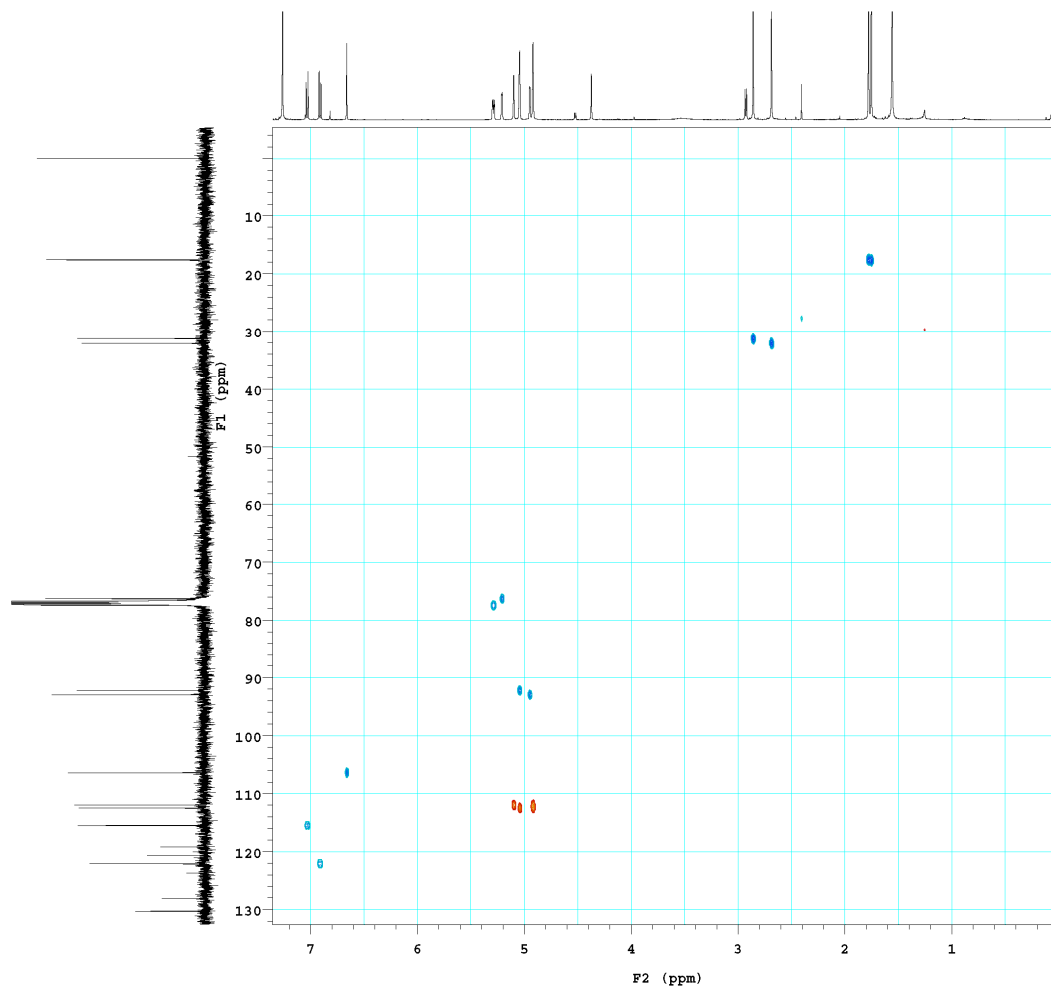


**Figure S10.** HSQC spectrum of **2** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-3-2-1-1.img-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Dec 16 2020	hs	nm	array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample		PFGflg	y		
ACQUISITION	hsglvt	6180	i	phase	
sv	6097.6	SPECIAL	1	1	
at	0.150	temp	not used	2	2
np	1830	gain	46		
fb	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	32	gfs	not used		
2D ACQUISITION		fn	2048		
sw1	25165.1	F1 PROCESSING			
ni	229	gfl	0.005		
phase	arrayed	gfl	not used		
PRESATURATION	procl	lp			
satmode	n	fnl	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	-41.4		
tn	H1	wp	3721.7		
sfrq	500.478	sp1	-666.7		
tof	276.8	wp1	17350.2		
tpwr	58	rfl	267.7		
pw	8.000	rpf	0		
DECOUPLER		rfl1	1256.5		
dn	C13	rfl1	0		
dof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pxxlvl	56	vs	132		
pxx	10.700	th	3		
HSQC		ai	odc	ph	
j1xh	146.0				
multiflg	y				
mult	2				
ADIABATIC					
pxxl80ad	ONE_ad300				
pxxl80adR	ONE_ad30-				
or					
pxxl80	465.4				
pxxlvl80	51				
pxxl80ref	ONE_ref2-				
00					
pxxl80r	2000.2				
pxxlvl80r	43				

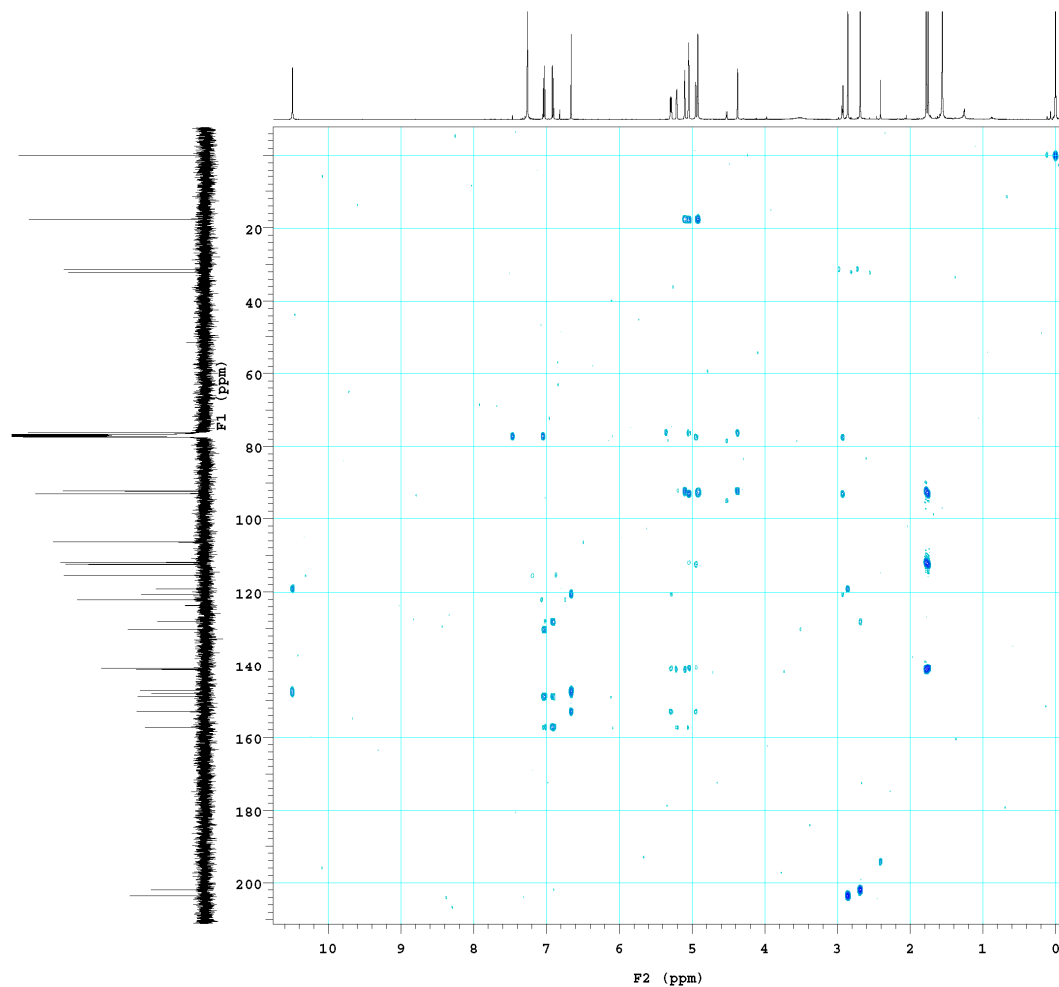


**Figure S11.** HMBC spectrum of **2** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-49-R-6-3-2-1-1.1mg-HMBC-CDCl3

exp6 gHMCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Dec 16 2020	hs		array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample		PFGflg	y		
ACQUISITION		hsglvt	6180	i	phase
sw	6097.6	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	1830	gain	46		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlvt1	409		
nt	64	gt1	0.001000		
2D ACQUISITION		gzlvt3	1227		
sw1	30200.1	gt3	0.001000		
ni	129	gstab	0.000500		
phase		arrayed	F2 PROCESSING		
PRESATURATION		sb	-0.075		
satmode		n	sbs	not used	
wet		n	fn	2048	
TRANSMITTER		F1 PROCESSING			
tn	H1	gt1	0.004		
sfrq	500.478	gtel	not used		
tof	276.8	procl	lp		
tpwr	58	fnl	2048		
pw	8.000	DISPLAY			
DECOUPLER		sp	-89.0		
dn	C13	wp	5472.3		
dof	1287.0	ep1	-972.1		
dm	nmn	wp1	27545.8		
decwave	W40_HCN5mm	rfl	267.7		
dmf	32258	rfp	0		
dpwr	38	rfl1	1886.4		
pxlvt1	56	rflp1	0		
pxw	10.700	PLOT			
HMBC		wc	206.0		
j1xh	146.0	sc	0		
jnxh	8.0	wc2	206.0		
ADIABATIC		sc2	0		
pxl180ad	ONE_ad300	vs	132		
pxlvt180	51	th	3		
pxl180	465.4	ai	cdc	av	

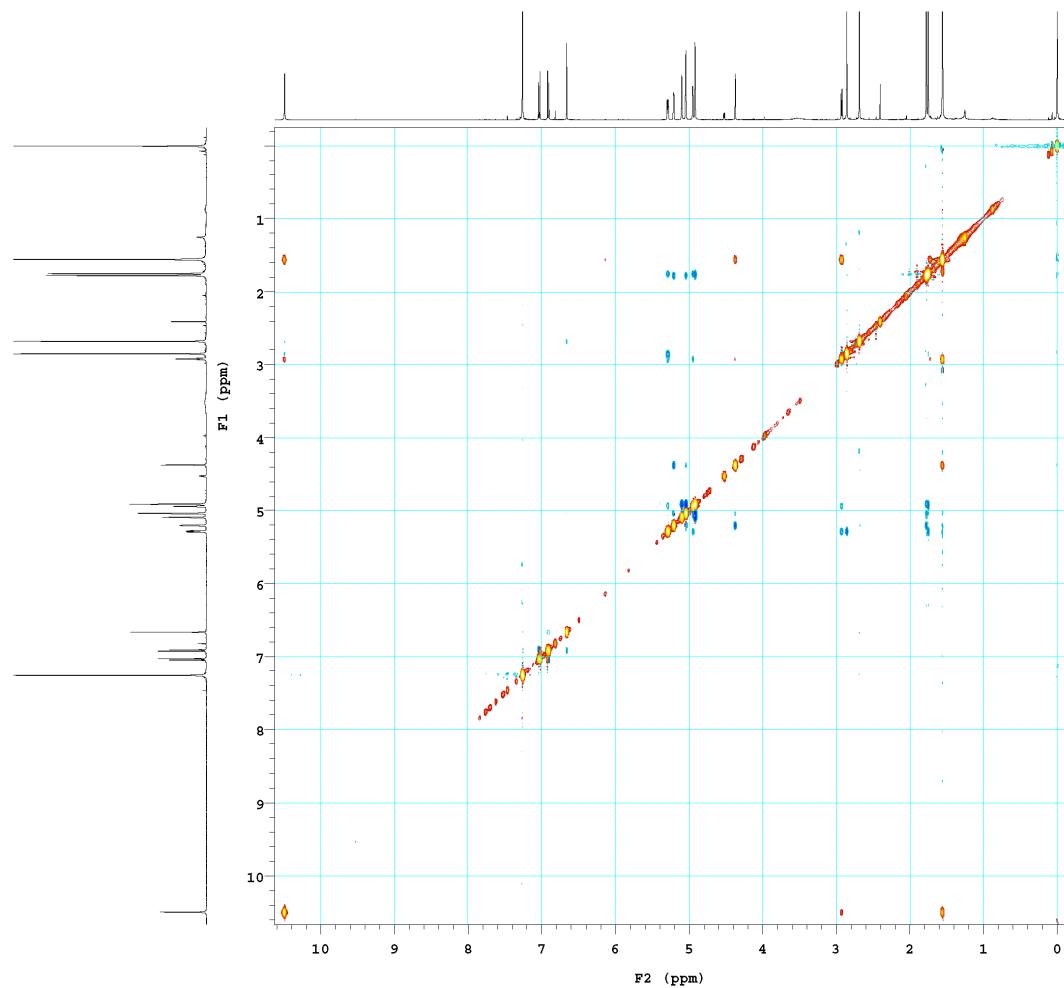


**Figure S12.** NOESY spectrum of **2** (measured in CDCl<sub>3</sub>, 500 MHz).

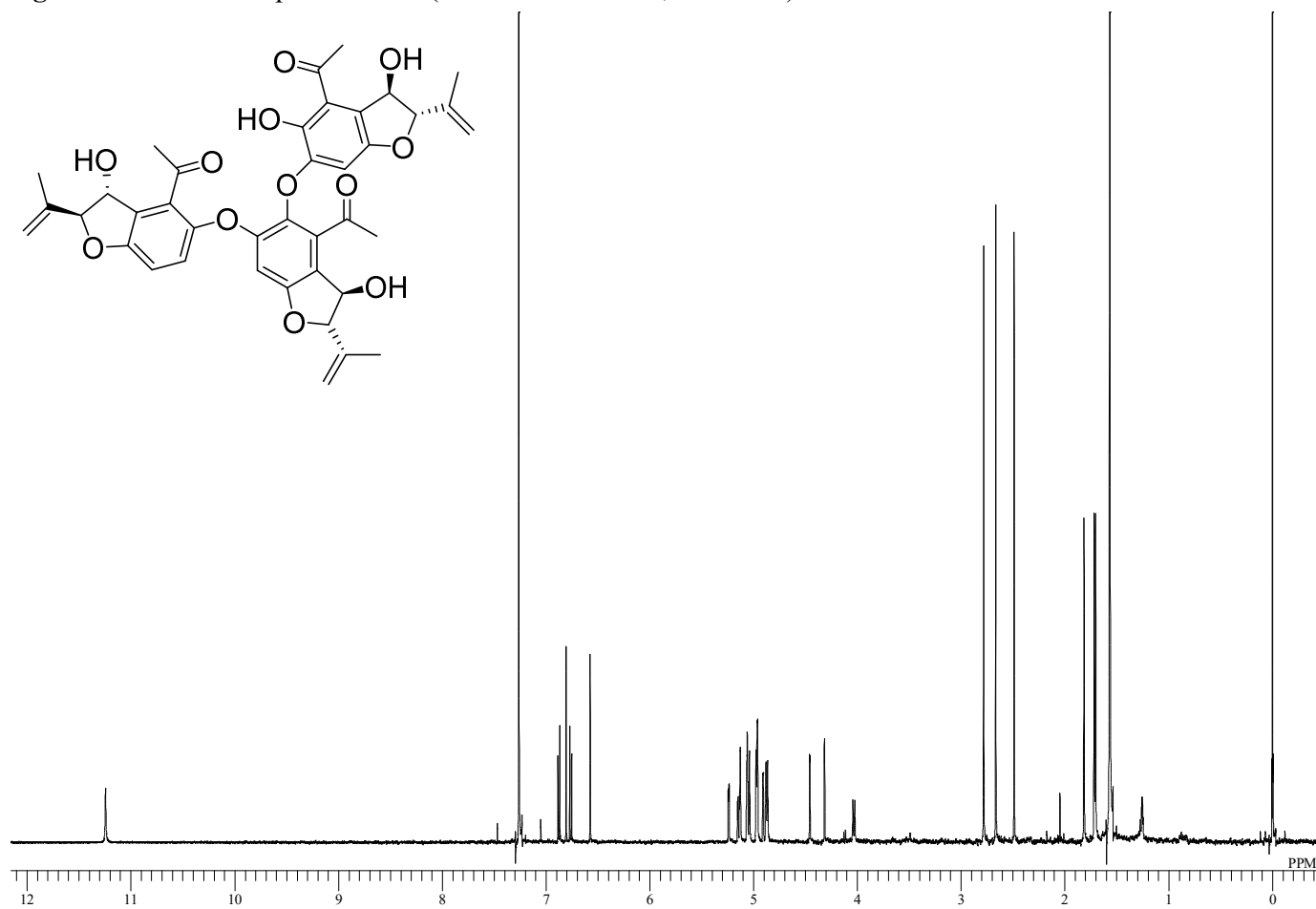
HYM-2014-48-R-6-3-2-1-1.lmg-NOESY-CDCl3

exp7 NOESY

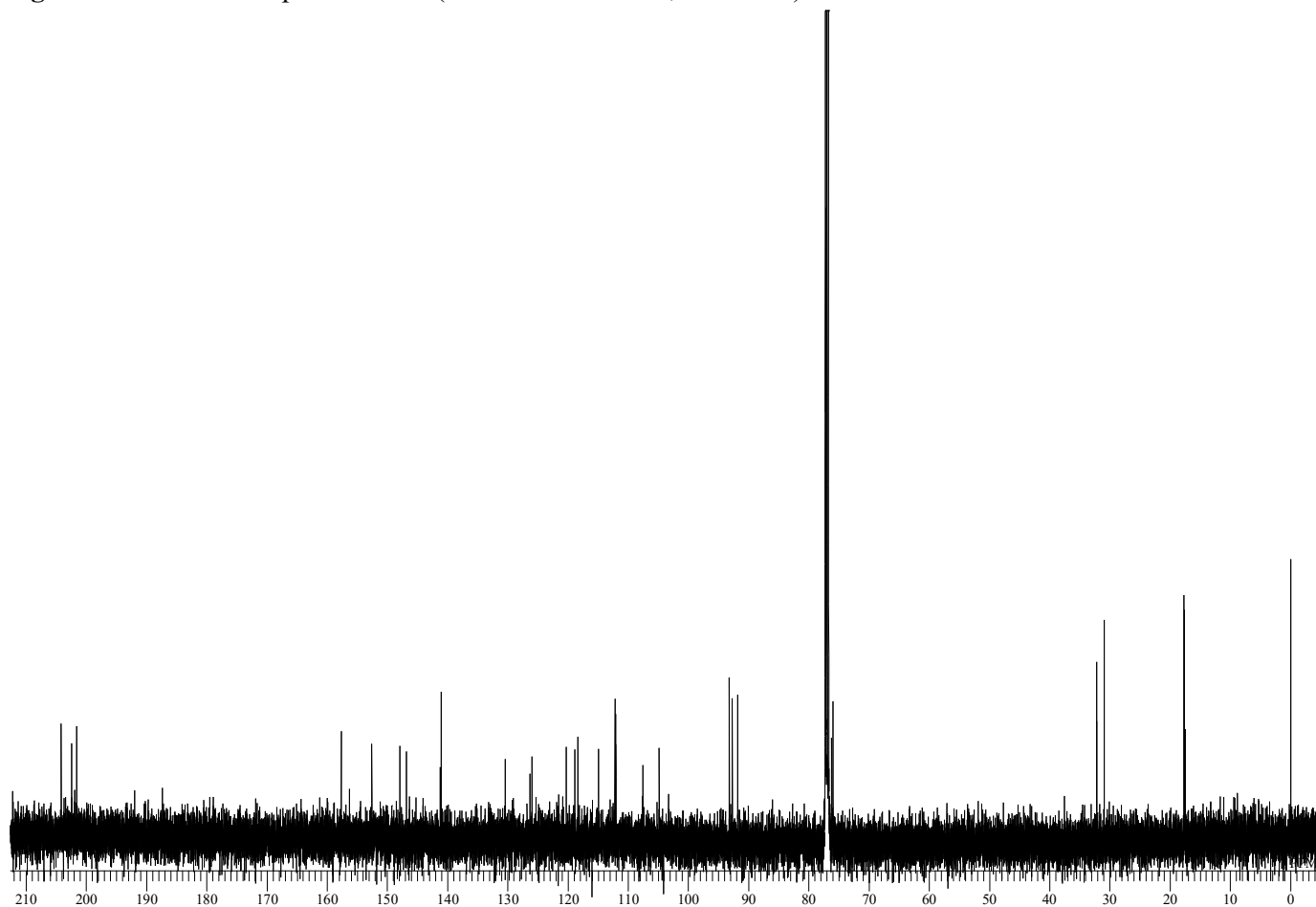
SAMPLE		FLAGS	
date	Dec 16 2020	hs	nn
solvent	cdcl3	spul	y
sample	PFGf1g	y	
ACQUISITION		haglvl	6180
sw	6097.6	SPECIAL	
at	0.150	temp	not used
np	1830	gain	46
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	8	gfs	not used
2D ACQUISITION		fn	2048
sw1	6097.6	F1 PROCESSING	
ni	128	gfl	0.019
TRANSMITTER		gfs1	not used
tn	H1	procl	lp
sfrq	500.478	fnl	2048
tof	276.8	DISPLAY	
tpwr	58	sp	-83.1
pw	8.000	wp	5400.9
NOESY		sp1	-124.8
mixN	0.500	wp1	5460.4
PRESATURATION		rf1	267.7
satmode	n	rpf	0
wet	n	rf11	267.7
DECOUPLER		rfpl	0
dm	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	132
		th	1
		ai	ph



**Figure S13.**  $^1\text{H}$  NMR spectrum of **3** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S14.**  $^{13}\text{C}$  NMR spectrum of **3** (measured in  $\text{CDCl}_3$ , 126 MHz).



**Figure S15.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** (measured in  $\text{CDCl}_3$ , 500 MHz).



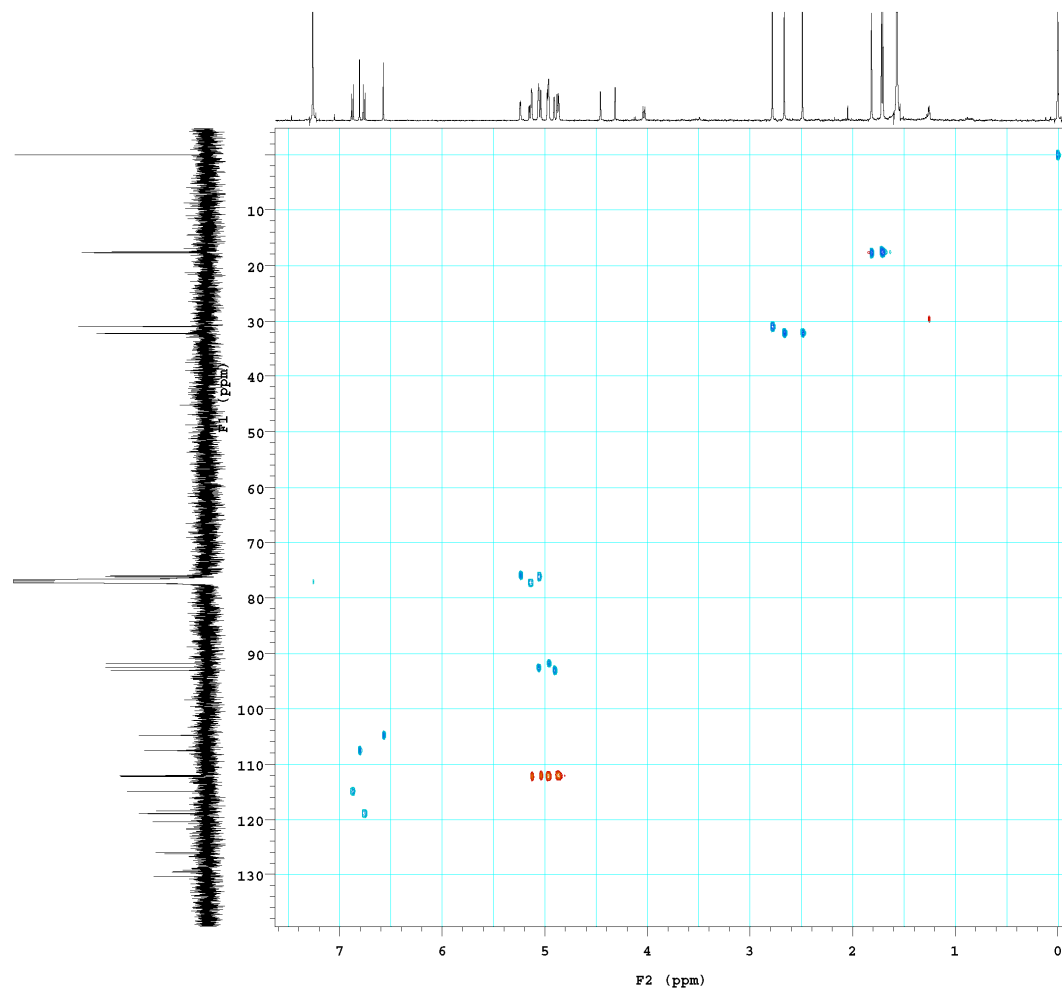


**Figure S16.** HSQC spectrum of **3** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-R-6-6-4-2-0.8mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Jun 3 2021	hs	nm	array	phase
solvent	cdcl3	sspl	y	arraydim	256
sample		ppcf1g	y		
ACQUISITION	haglv1	6024	1	phase	
sw	6510.4	SPECIAL	1	1	
at	0.150	temp	not used	2	2
np	1954	gain	50		
fb	4000	spin	0		
ss	32	P2 PROCESSING			
d1	1.000	gf	0.069		
nt	32	gfs	not used		
2D ACQUISITION	fn	2048			
sw1	25165.1	P1 PROCESSING			
nl	128	gf1	0.005		
phase	arrayed	gfs1	not used		
PRESSATURATION	procl	1p			
satmode	n	fn1	2048		
wet	n	DISPLAY			
TRANSMITTER	sp	-66.9			
tn	H1	vp	3884.6		
sfrq	500.478	sp1	-593.0		
tof	327.6	vp1	18136.6		
tpwr	58	rfl	423.0		
pw	8.100	rfp	0		
DECOUPLER	rfl1	1256.5			
dn	Cl3	rflp1	0		
dof	-600.6	FLOT			
ds	nmv	sc	206.0		
decwave	W40_HCNsm	sc	0		
dmf	32258	sc2	206.0		
dpwr	38	sc2	0		
pwxlvl	56	va	249		
pw	10.500	th	4		
j1xh	HSQC	ai	cdc ph		
j1xh	146.0				
mult1g	y				
mult	2				
ADIABATIC					
pwxl80ad	ONE_ad300				
pwxl80adr	ONE_ad300				
pwxl80	465.4				
pwxlvl180	51				
pwxl80ref	ONE_ref2-				
pwxl80r	2000.2				
pwxlvl180r	43				

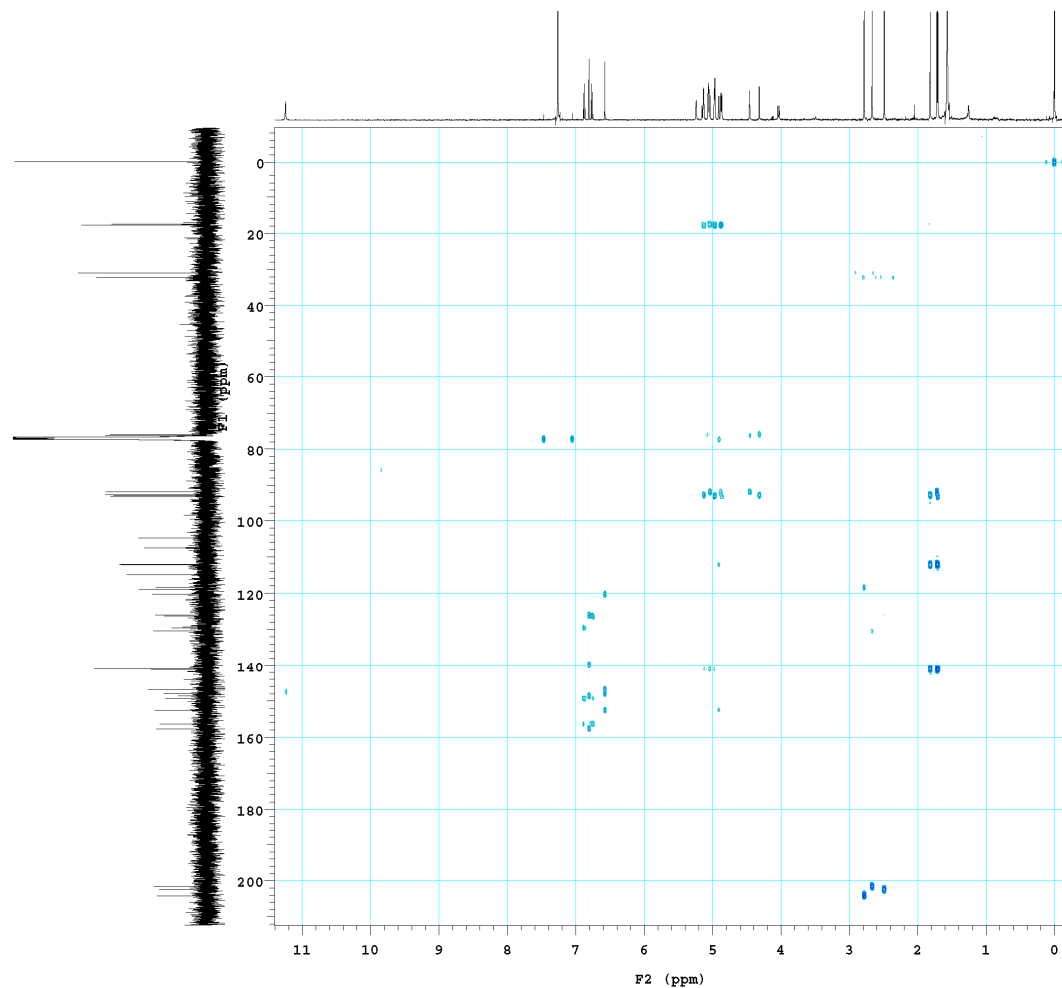


**Figure S17.** HMBC spectrum of **3** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-R-6-6-4-2-0.8mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Jun 3 2021	hs		nm	array
solvent	cdcl3	sspul	y	arraydim	256
sample		pfgrlg	y		
ACQUISITION		hsplv1	6024	1	phase
sw	6510.4	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	1954	gain	50		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlv11	409		
nt	64	gt1	0.001000		
2D ACQUISITION		gzlv13	1227		
sw1	30200.1	gt3	0.001000		
ni	128	gstab	0.000500		
phase		arrayed	P2 PROCESSING		
PRESATURATION		sb	-0.075		
satmode	n	sbs	not used		
wet	n	fn	2048		
TRANSMITTER		f1	PROCESSING		
tn	H1	gt1	0.004		
sfrq	500.478	gt#1	not used		
tof	327.6	procl	lp		
tpwr	58	fn1	2048		
pw	8.100	DISPLAY			
DECOUPLER		sp	-117.8		
dn	C13	vp	5923.8		
dof	1287.0	sp1	-1178.6		
da	nmn	vp1	27899.7		
decwave	W40_HCN5mm	rfl	423.0		
daf	32258	rfl	0		
dpr	38	rfl1	1886.4		
pwkiv1	56	rfl1	0		
pwk	10.500	PLOT			
HMB		wc	206.0		
j1xh	146.0	sc	0		
jnxh	8.0	wc2	206.0		
ADIABATIC		sc2	0		
pwk180ad	ONE_ad300	vs	249		
pwk1v180	51	th	4		
pwk180	465.4	ai	cdc av		

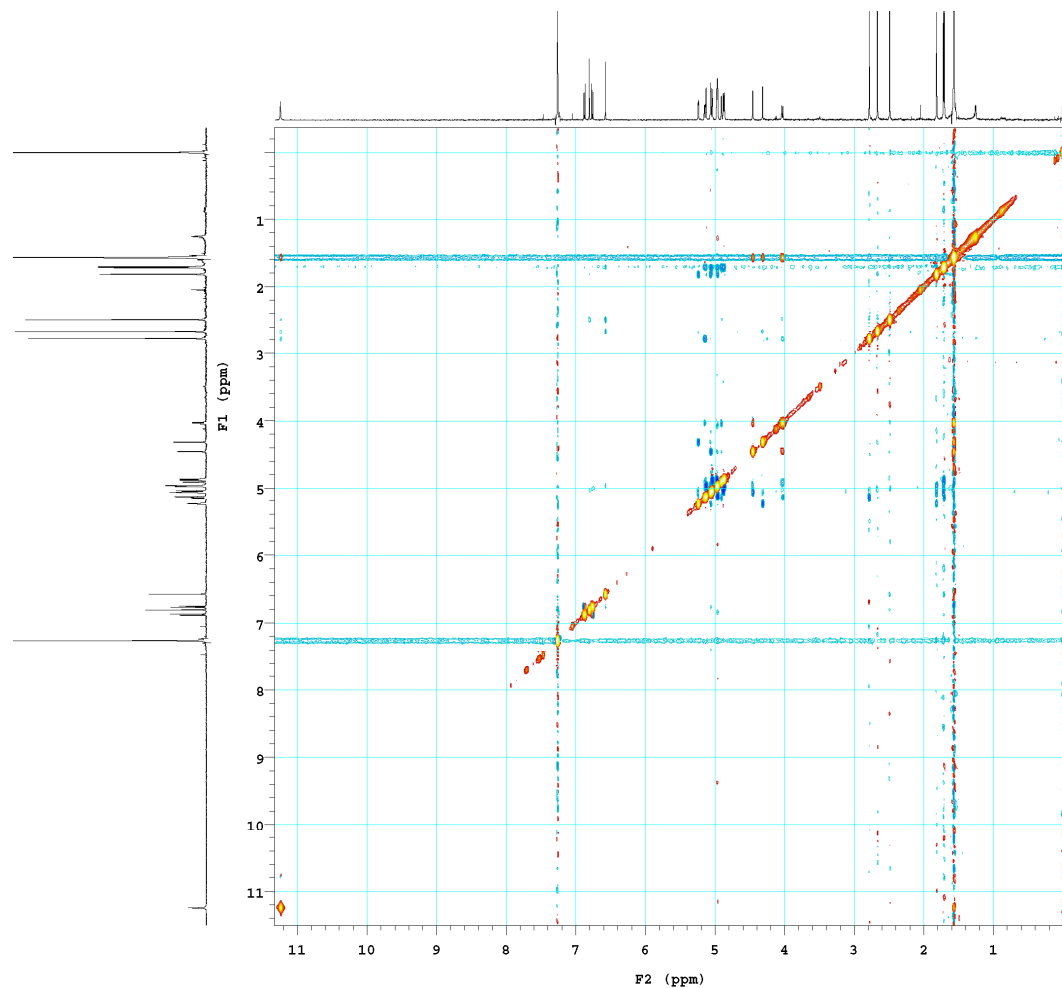


**Figure S18.** NOESY spectrum of **3** (measured in CDCl<sub>3</sub>, 500 MHz).

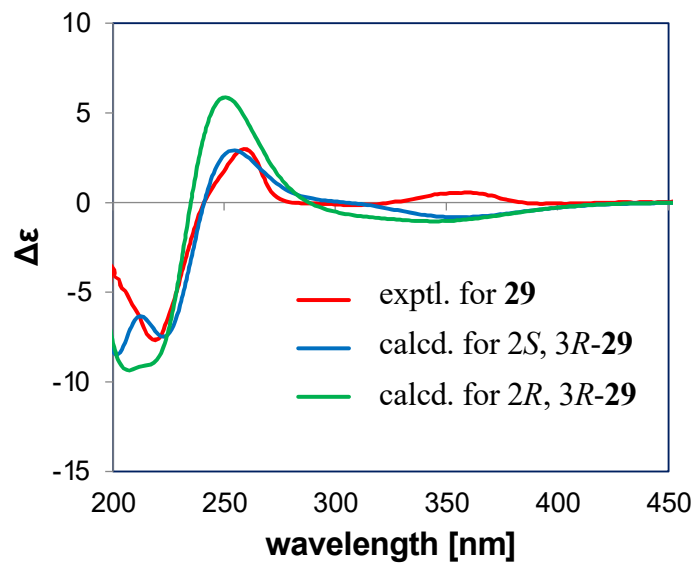
HYM-2014-R-6-6-4-2-0.8mg-NOESY-CDCl3

exp4 NOESY

SAMPLE		FLAGS	
date	Jun 3 2021	hs	nn
solvent	cdcl3	sspl	y
sample	PF061g	y	
ACQUISITION		hsplv1	6024
sw	6510.4	SPECIAL	
at	0.150	temp	not used
np	1954	gain	50
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gt	0.069
nt	8	gfs	not used
2D ACQUISITION		fn	2048
sw1	6510.4	F1 PROCESSING	
ni	128	gf1	0.018
TRANSMITTER		gfsl	not used
tn	H1	procl	lp
sfrq	500.478	fn1	2048
tof	327.6	DISPLAY	
tpw	58	sp	-54.2
pw	8.100	wp	5722.0
NOESY		sp1	-181.4
mixn	0.500	wp1	5938.2
PRESATURATION		rf1	423.0
satmode	n	rfl	0
wet	n	rfl1	423.0
DECOUPLER		rfpl	0
dn	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	249
		th	1
		ai	ph

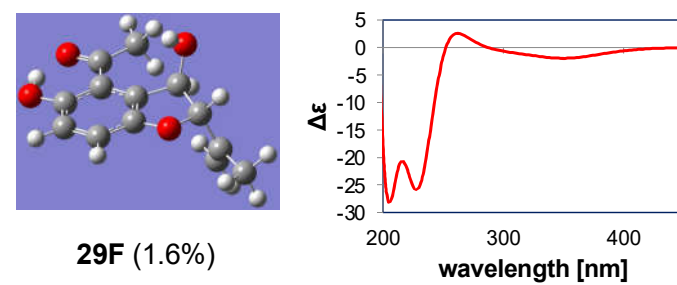
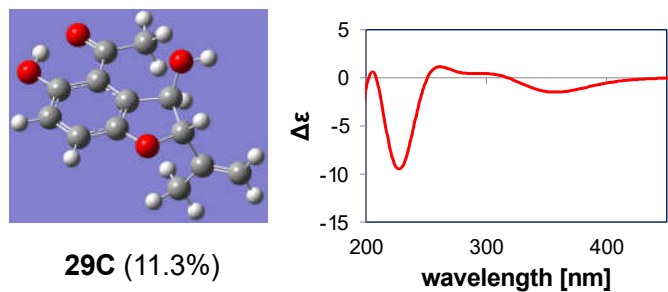
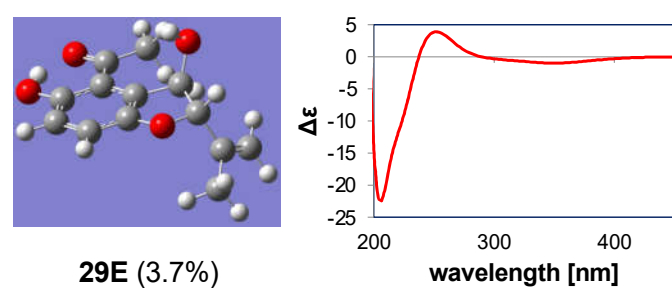
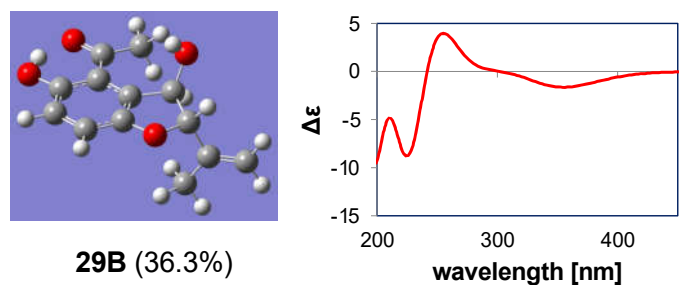
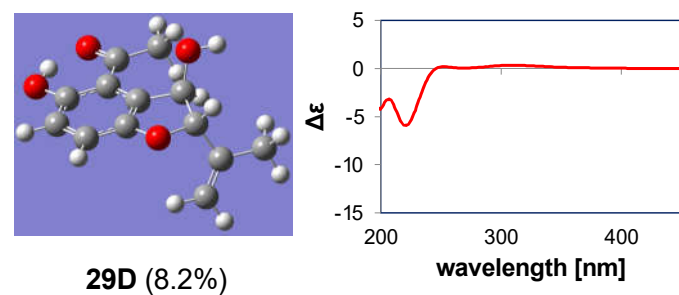
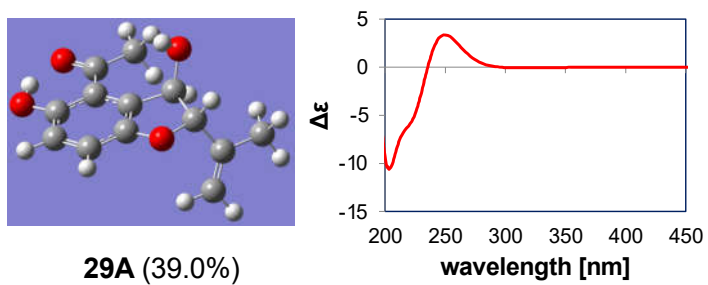


**Figure S19.** Experimental ECD spectrum of **29** and calculated ECD spectra of 2*S*,3*R*-**29** and 2*R*,3*R*-**29**.

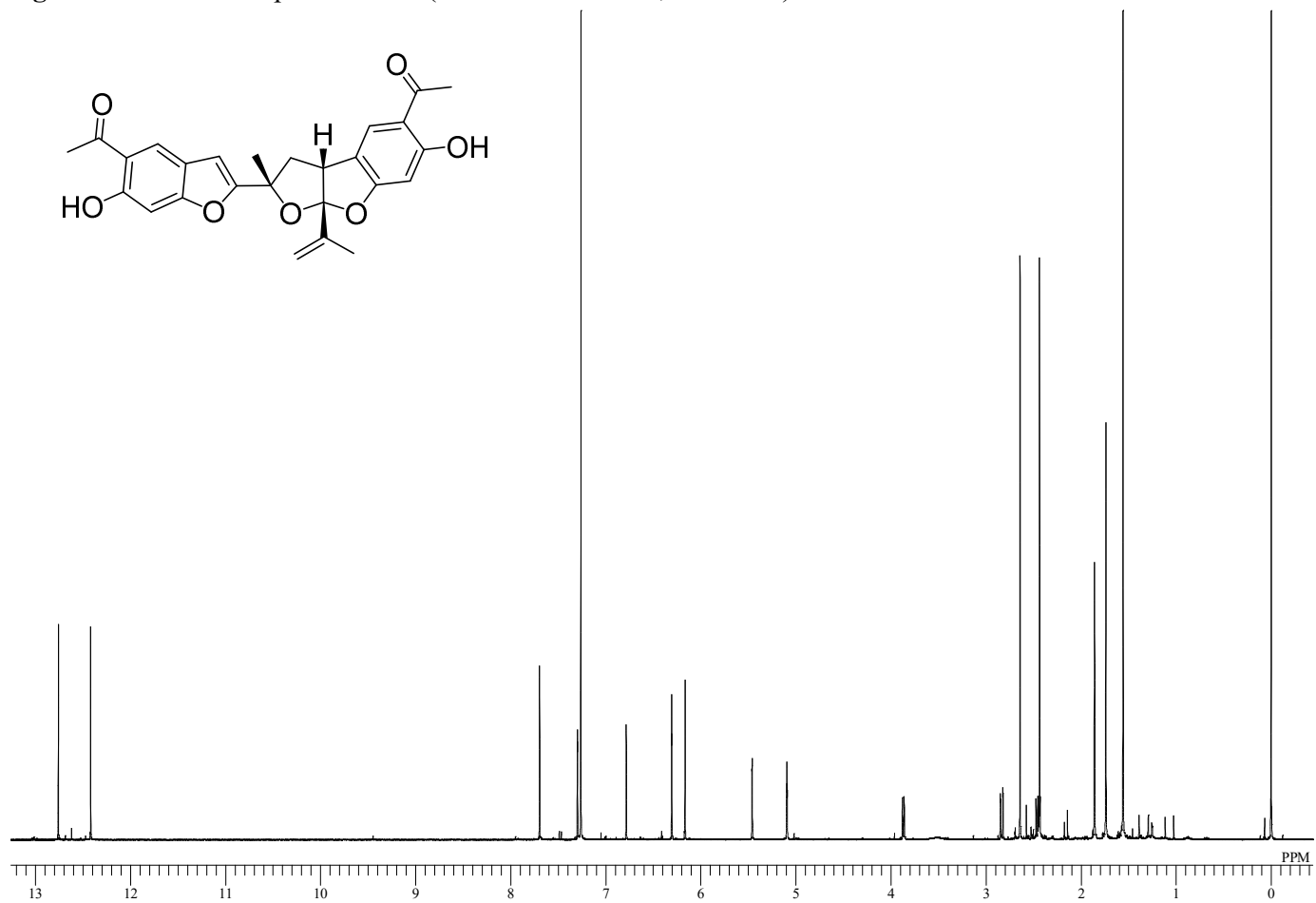


Calculated ECD spectra of 2*S*,3*R*-**29** and 2*R*,3*R*-**29** are very similar to each other. The Cotton effect around 350 nm is derived from torsion angle between benzofuran and olefin moieties (see Figure S20). Disagreement on this band between experimental and calculated ECD spectra may be due to the presence of some intermolecular interaction.

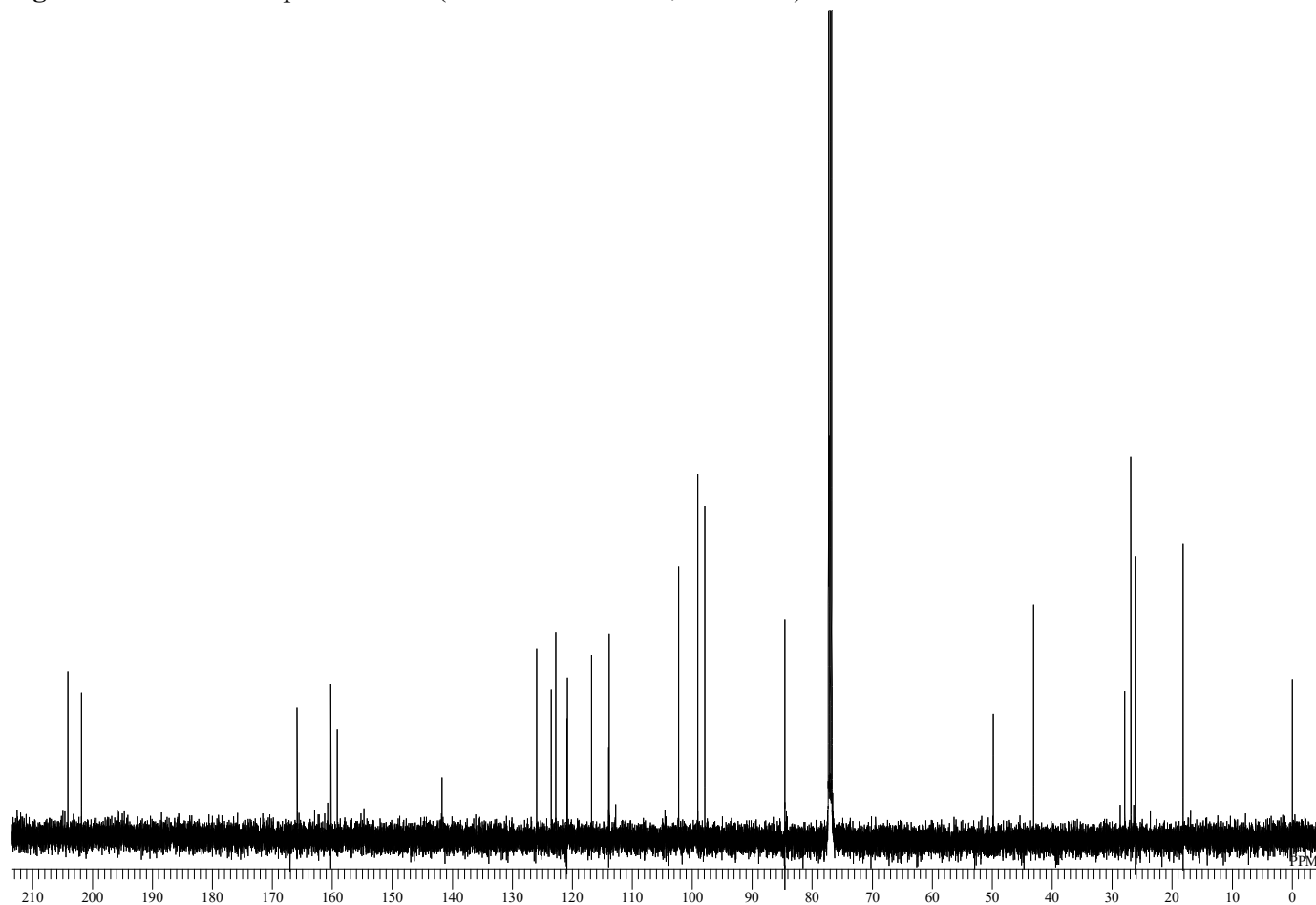
**Figure S20.** Optimized structures (B3LYP/6-31G(d,p) in MeOH (PCM)) and calculated ECD spectra (CAM-B3LYP/6-31G(d,p) in MeOH (PCM)) for each conformer of **29** (**29A–29F**).



**Figure S21.**  $^1\text{H}$  NMR spectrum of **4** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S22.**  $^{13}\text{C}$  NMR spectrum of **4** (measured in  $\text{CDCl}_3$ , 126 MHz).

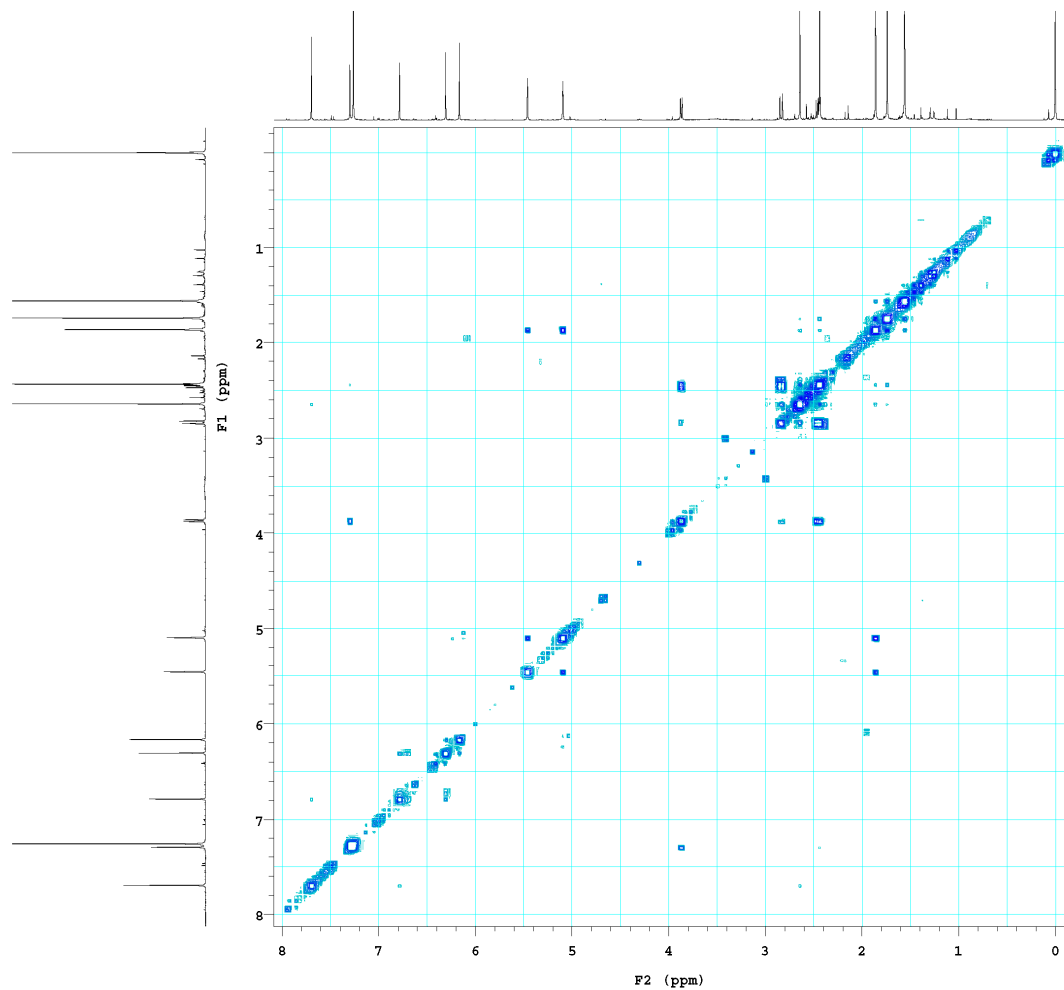


**Figure S23.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-6-2-1-3-1.3mg-COSY-CDCl3

exp4 gCOSY

SAMPLE		FLAGS	
date	Dec 12 2020	hs	nm
solvent	cdcl3	sspul	y
sample	hsglvl		6180
ACQUISITION		SPECIAL	
sw	7183.9	temp	not used
at	0.150	gain	48
hp	2156	spin	0
fd	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	16	fn	4096
2D ACQUISITION		F1 PROCESSING	
sw1	7183.9	sb1	-0.018
ni	128	sbs1	not used
d2	0	procl	lp
PRESATURATION		fml	
satmode	n	DISPLAY	
wet	n	sp	-76.3
TRANSMITTER		wp	
tn	H1	sp1	-128.9
sfrq	500.478	wp1	4195.3
tof	649.8	rfl	437.6
tpwr	58	rpf	0
pw	8.000	rfl1	437.6
GRADIENTS		rflp1	
gzlvie	5154	PLOT	
gte	0.001000	wc	206.0
EDratio	1.000	sc	0
gstab	0.000500	wc2	206.0
DECOUPLER		sc2	
dn	C13	vs	94
dm	nmn	th	6
	al	odc	av



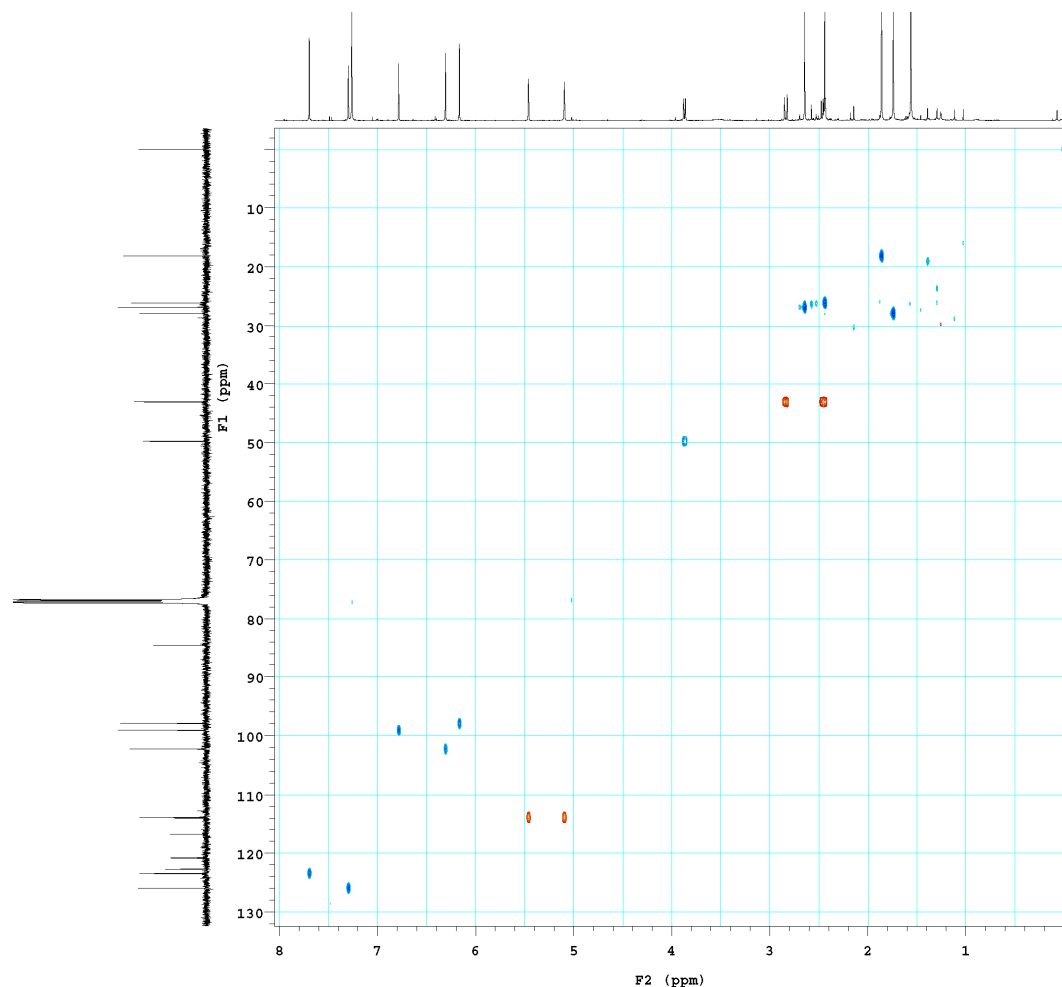


**Figure S24.** HSQC spectrum of **4** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-2-1-3-1.3mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Dec 12 2020	hs	nm	array	phase
solvent	cdcl3	sspl	y	arraydim	256
sample		ppgflg	y		
ACQUISITION	haglv1	6180	1	phase	
sw	7183.9	SPECIAL	1	1	
at	0.150	temp	not used	2	2
np	2156	gain	48		
fb	4000	spin	0		
ss	32	P2 PROCESSING			
d1	1.000	gf	0.069		
nt	16	gfs	not used		
2D ACQUISITION	fn	4096			
sw1	25165.1	P1 PROCESSING			
nl	128	gf1	0.005		
phase	arrayed	gfs1	not used		
PRESSATURATION	procl	1p			
satmode	n	fn1	2048		
wet	n	DISPLAY			
TRANSMITTER	sp	-34.2			
tn	H1	wp	4062.0		
sfrq	500.478	sp1	-445.6		
tof	649.8	wp1	17104.4		
tpwr	58	rfl	437.6		
pw	8.000	rfp	0		
DECOUPLER	rfl1	1256.5			
dn	Cl3	rflp1	0		
sof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pwxlvl	56	va	94		
pw	10.700	th	3		
j1xh	HSQC	al	cdc ph		
multflg	y				
mult	2				
ADIBATIC					
pwxl80ad	ONE ad300				
pwxl80adr	ONE ad30-				
or					
pwxl80	465.4				
pwxlvl180	51				
pwxl80ref	ONE ref2-				
00					
pwxl80r	2000.2				
pwxlvl180r	43				

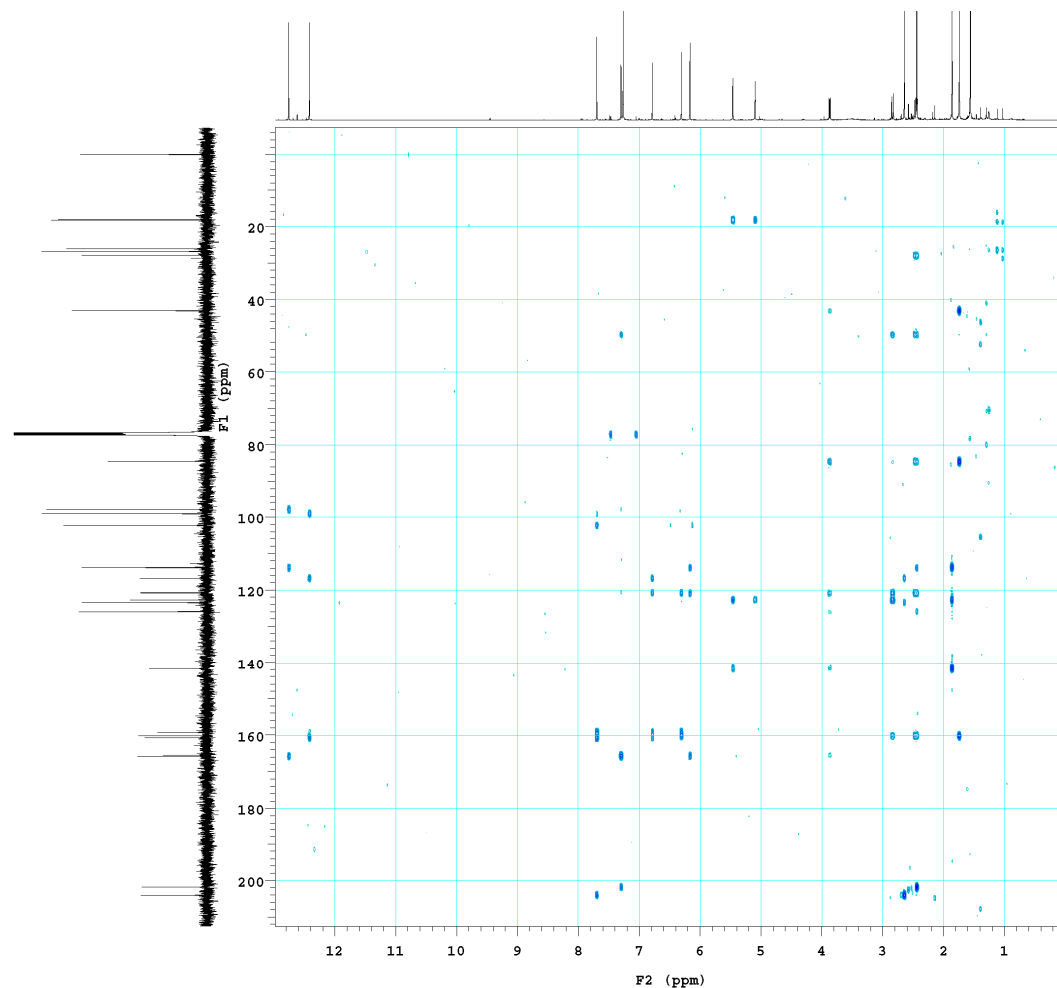


**Figure S25.** HMBC spectrum of **4** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-2-1-3-1.3mg-HMBC-CDCl<sub>3</sub>

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Dec 12 2020	hs		mn	
solvent	cdcl3	sspul	y	array	phase
sample		PFGflg	y	arraydim	256
ACQUISITION		hsglvi	6180	1	phase
sw	7183.9	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2156	gain	48		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlvi1	409		
nt	64	gt1	0.001000		
2D ACQUISITION		gzlvi3	1227		
sw1	30200.1	gt3	0.001000		
nl	128	gstab	0.000500		
phase	arrayed	F2 PROCESSING			
PRESATURATION	sb	-0.075			
satmode	n	sbs	not used		
wet	n	fn	4096		
TRANSMITTER		F1 PROCESSING			
tn	H1	gt1	0.004		
strq	500.478	gfal	not used		
tof	649.8	procl	lp		
tpwr	58	fn1	2048		
pw	8.000	DISPLAY			
DECOUPLER		sp	-48.2		
dm	C13	wp	6542.0		
dof	1287.0	sp1	-913.2		
dm	mm	wp1	27653.7		
decwave	W40_HCM5mm	rf1	437.6		
dma	32258	rfp	0		
dpr	38	rf11	1886.4		
pcxlv1	56	rfp1	0		
pcw	10.700	PLOT			
HMB		wc	206.0		
j1xh	146.0	sc	0		
j1xh	8.0	wc2	206.0		
ADDITIONAL		sc2	0		
pcx180ad	ONE	ad300	vs	94	
pcx1v1180	51	th		3	
pcx180	465.4	ai	odc	av	

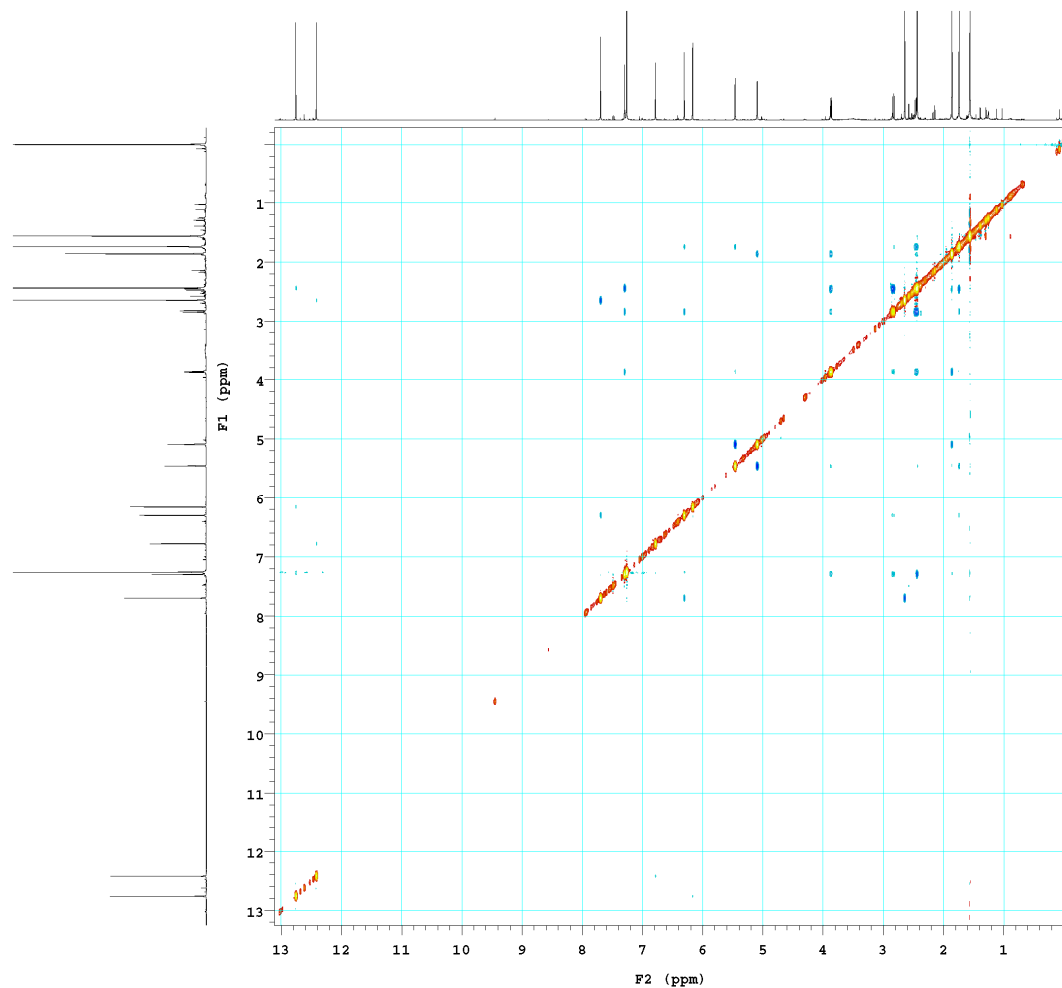


**Figure S26.** NOESY spectrum of **4** (measured in CDCl<sub>3</sub>, 500 MHz).

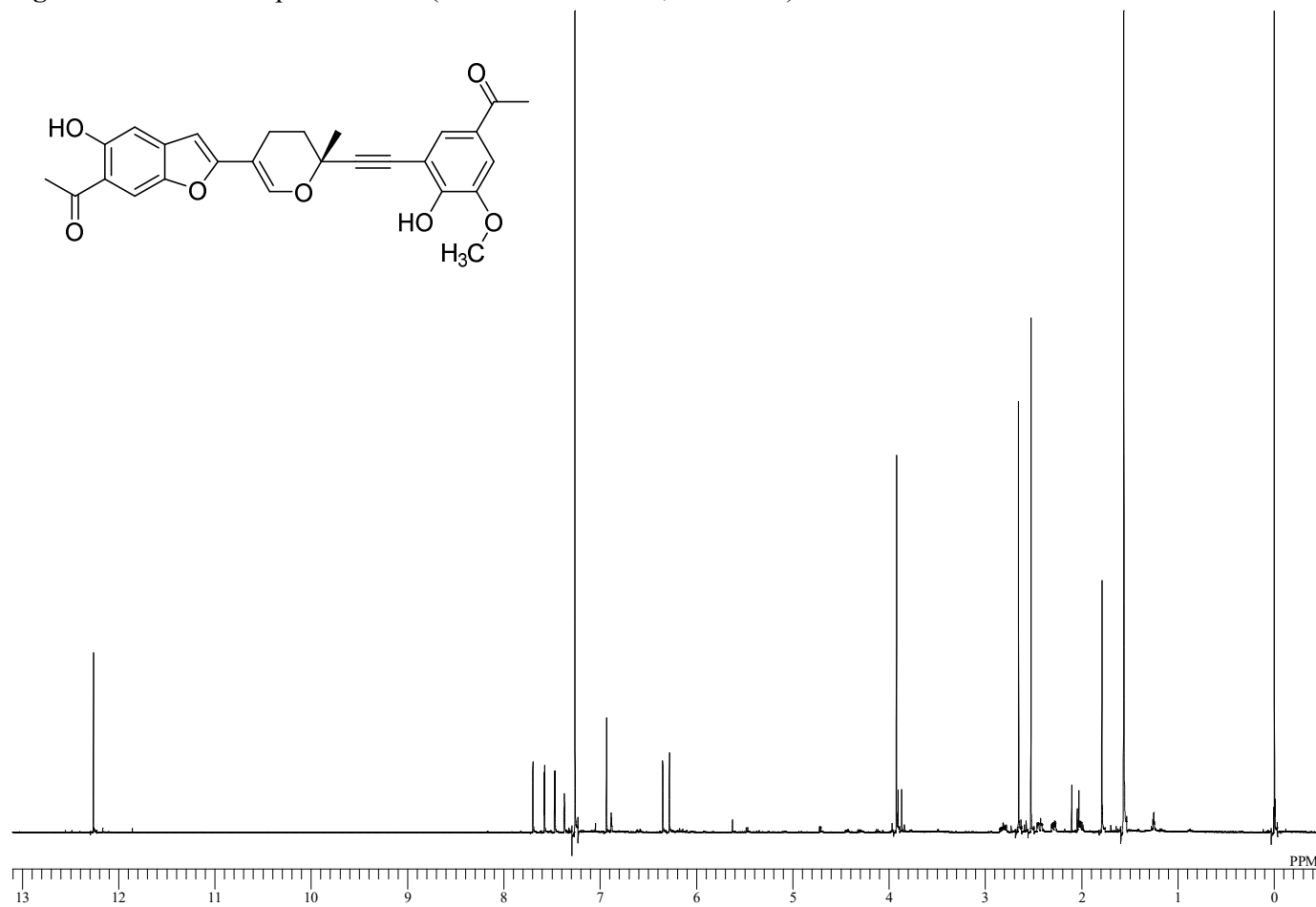
HYM-2014-48-R-6-2-1-3-1.3mg-NOESY-CDCl3

exp7 NOESY

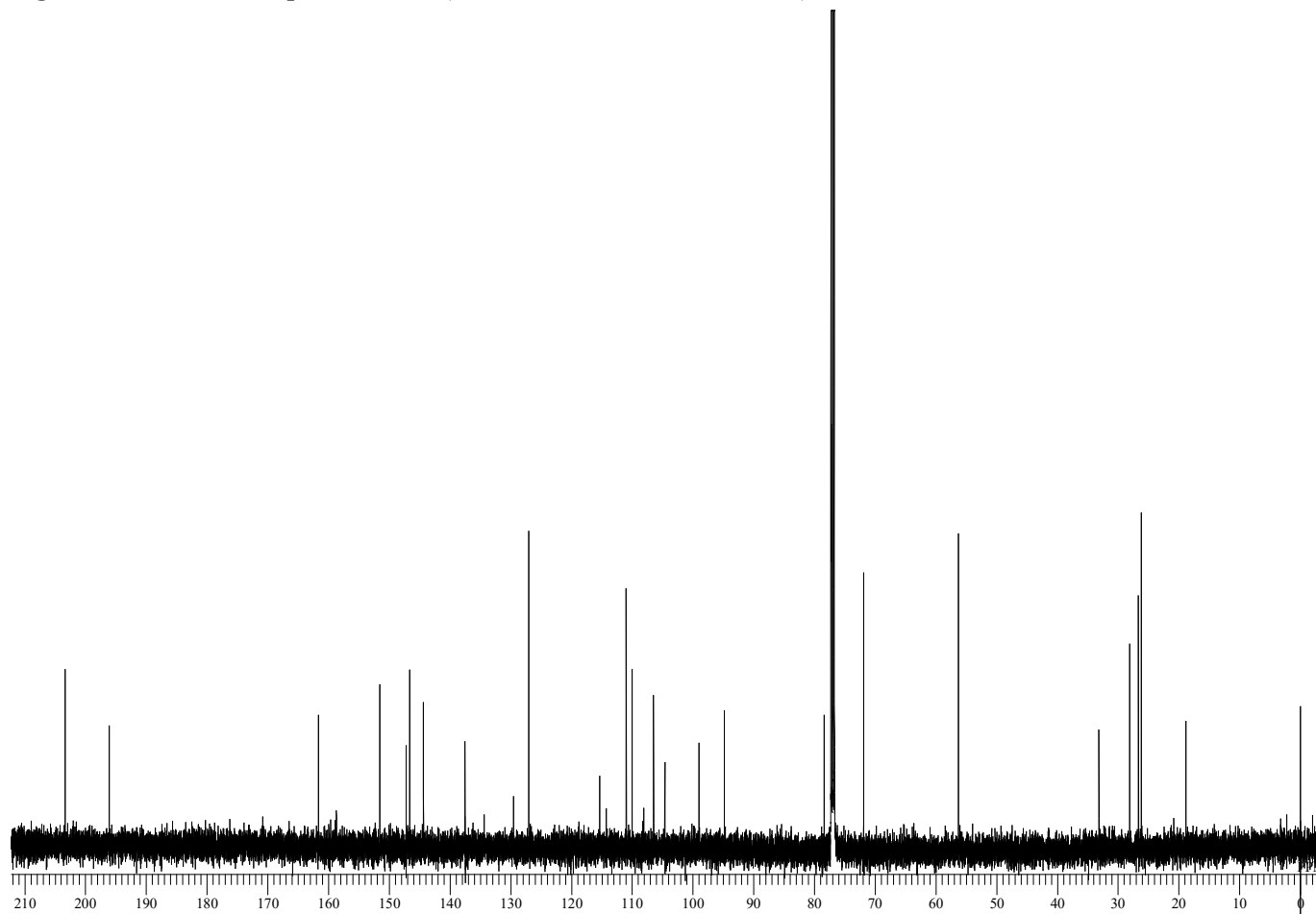
SAMPLE		FLAGS	
date	Dec 12 2020	hs	nn
solvent	cdcl3	#pul	y
sample		ppoflg	y
ACQUISITION		haglvi	6100
sw	7183.9	SPECIAL	
at	0.150	temp	not used
np	2156	gain	48
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION		fn	4096
sw1	7183.9	F1 PROCESSING	
ni	128	gfl	0.016
TRANSMITTER		gfs1	not used
tn	H1	procl	lp
sfrq	500.478	fn1	4096
tof	649.8	DISPLAY	
tpwr	58	sp	-55.3
pw	8.000	vp	6615.6
NOESY		sp1	-139.4
mixd	0.500	vp1	6770.0
PRESATURATION		rf1	437.6
satmode	n	rtp	0
wet	n	rf11	437.6
DECOUPLER		rtp1	0
dm	Cl3	PLOT	
dm	nmn	wd	206.0
		sc	0
		wd2	206.0
		sc2	0
		va	94
		th	1
	ai	ph	



**Figure S27.**  $^1\text{H}$  NMR spectrum of **5** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S28.**  $^{13}\text{C}$  NMR spectrum of **5** (measured in  $\text{CDCl}_3$ , 126 MHz).

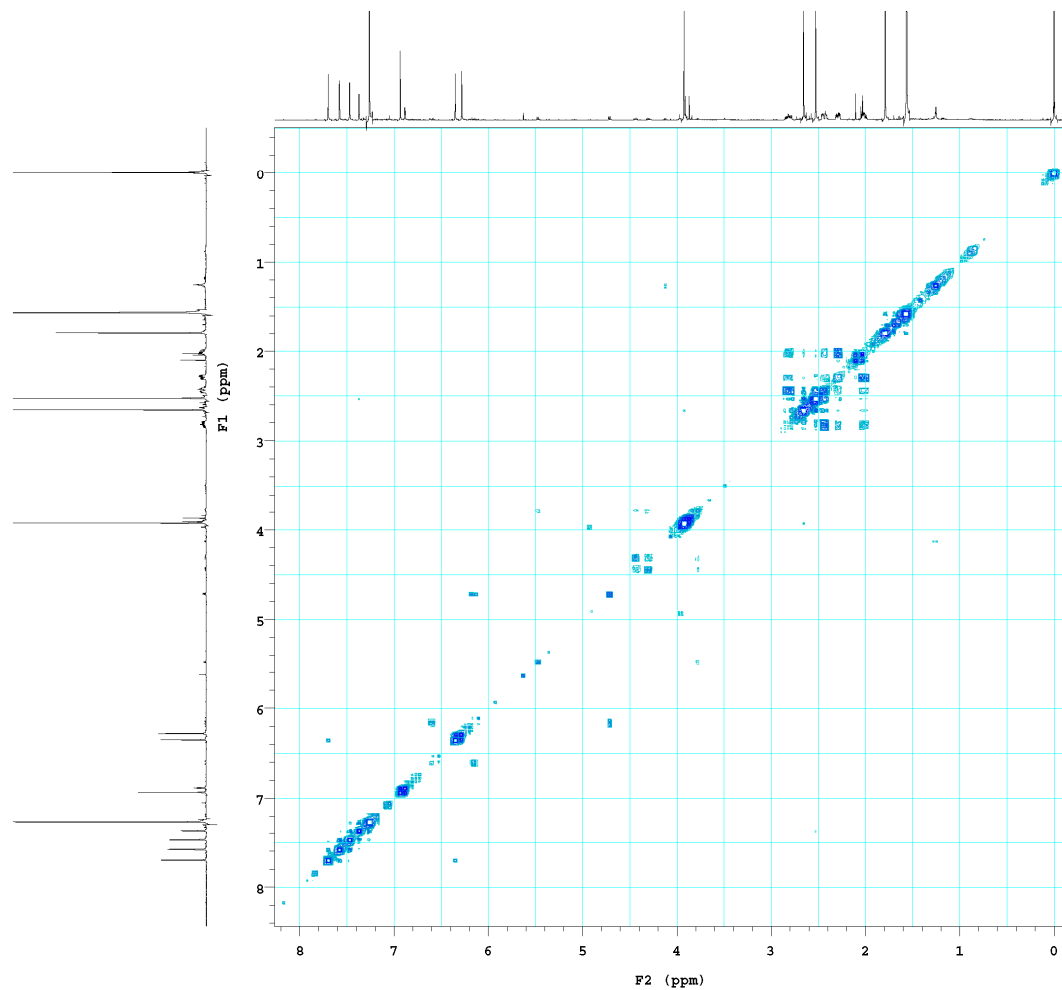


**Figure S29.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **5** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-6-6-1-1-1.tmg-COSY-CDCl3

exp4 gcOSY

SAMPLE		FLAGS		
date	Jun 5 2021	hs		nn
solvent	cdcl3	sspul		y
sample	haglv1			6024
ACQUISITION		SPECIAL		
sw	7062.1	temp		not used
at	0.150	gain		50
np	2118	spin		0
fb	4000	F2 PROCESSING		
ss	32	sb		-0.075
d1	1.000	sbs		not used
nt	8	fn		4096
2D ACQUISITION		F1 PROCESSING		
sw1	7062.1	sb1		-0.018
n1	128	sbs1		not used
d2	0	procl		lp
PRESATURATION		fml <td>4096</td>		4096
satmode	n			
wet	n	sp		-87.9
TRANSMITTER		vp <td>4224.2</td>		4224.2
tn	H1	sp1		-253.4
sfrq	500.478	vp1		4475.9
tof	497.5	rf1		529.3
tpwr	58	rfp		0
pw	8.100	rf11		529.3
GRADIENTS		rfp1 <td>0</td>		0
gslvie	5025			PLOT
gse	0.001000	wc		206.0
EDratio	1.000	sc		0
gstab	0.000500	wc2		206.0
DECOUPLER		sc2 <td>0</td>		0
dn	C13	vs		39
dm	nm	th		7
		ai	cdc	av

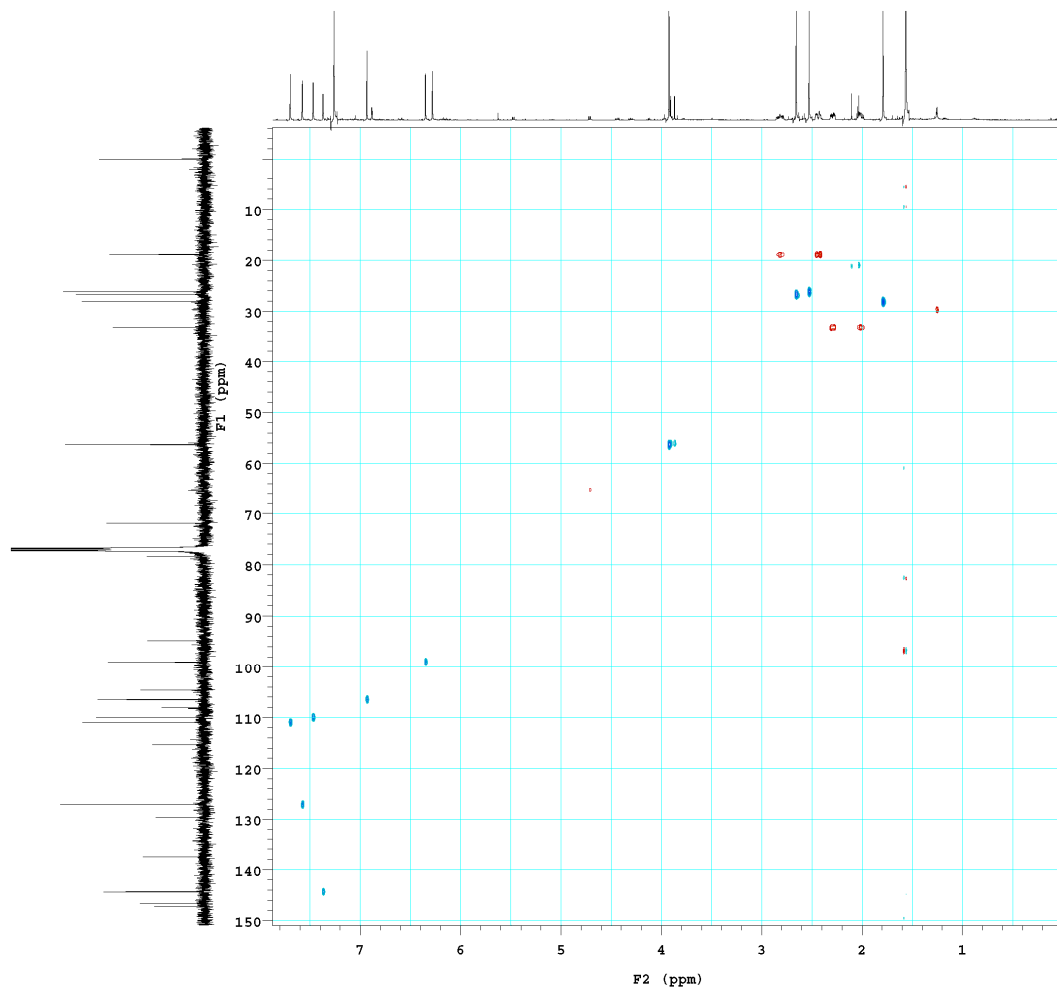


**Figure S30.** HSQC spectrum of **5** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-6-1-1-1.4mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Jun 5 2021	hs		nm	
solvent	cdcl3	sspul		array	phase
sample		PFGflg	Y	arraydia	256
ACQUISITION		hsqivl	6024	1	phase
sw	7062.1	SPECIAL		1	1
at	0.150	temp	not used	2	2
hp	2118	gain	50		
fd	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	16	gfs	not used		
2D ACQUISITION		fn	4096		
sw1	25165.1	F1 PROCESSING			
ni	128	gf1	0.005		
phase	arrayed	gfsl	not used		
PRESATURATION		procl	lp		
satmode	n	fn1	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	-29.3		
tn	H1	wp	3969.0		
sfrq	500.478	sp1	-765.0		
tof	497.5	wp1	19758.6		
tpwr	58	rf1	529.3		
pw	8.100	rfp	0		
DECOUPLER		rf11	1256.5		
dn	Cl3	rfpl	0		
dof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pxivl	56	vs	39		
pxw	10.500	th	3		
HSQC		ai	odc ph		
jlxb	146.0				
multfig	y				
mult	2				
ADDITIONAL					
pxv180ad	ONE ad300				
pxv180adr	ONE ad30-				
	OR				
pxv180	465.4				
pxv1v180	51				
pxv180ref	ONE ref2-				
	30				
pxv180r	2000.2				
pxv1v180r	43				

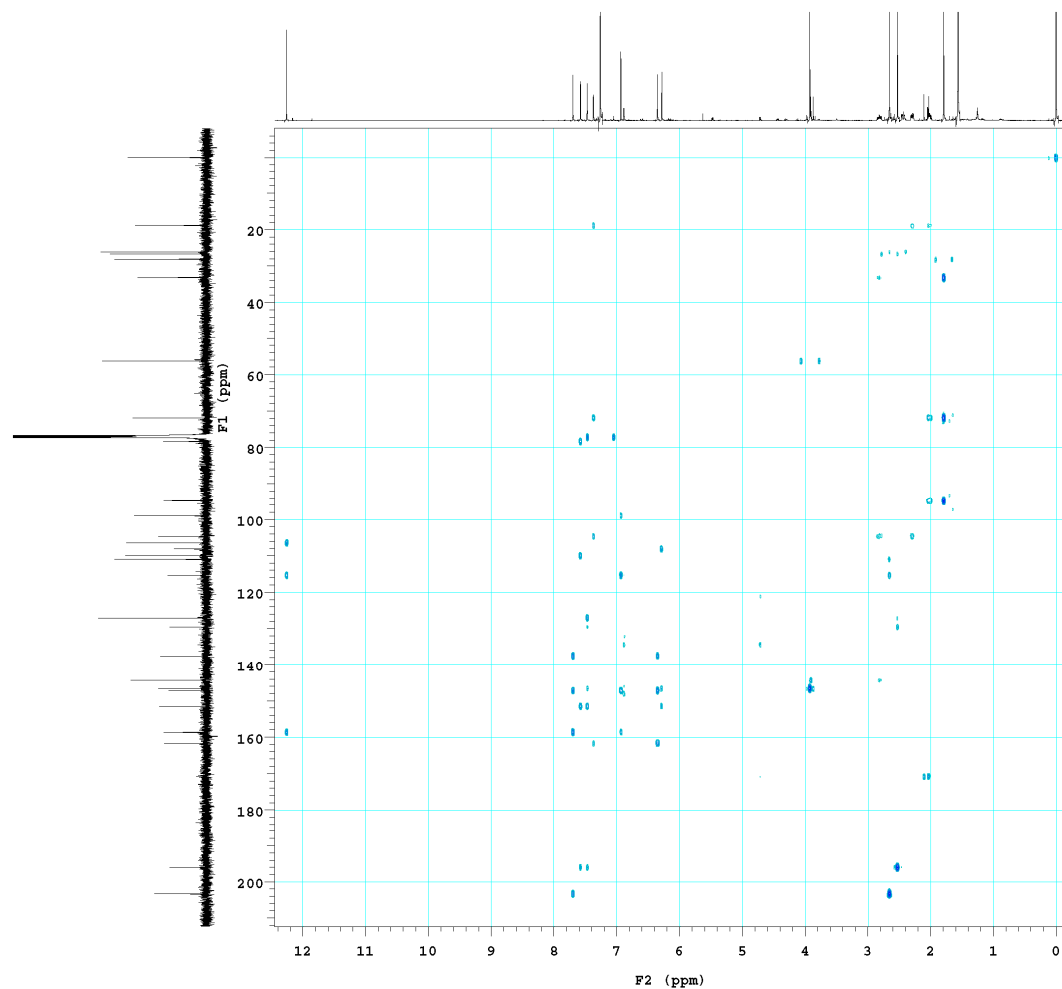


**Figure S31.** HMBC spectrum of **5** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-6-1-1-1, 4mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Jun 5 2021	hs	nm	array	phase
solvent	cdcl3	sspl	y	arraydim	256
sample		ppcf1g			
ACQUISITION		haglv1	6024	1	phase
sw	7062.1	SPECIAL		1	1
at	0.150	temp	not used	2	2
rp	2118	gain	50		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlv11	409		
nt	64	gt1	0.001000		
2D ACQUISITION		gzlv13	1227		
sw1	30200.1	gt3	0.001000		
nl	128	gstab	0.000500		
phase		arrayed	F2 PROCESSING		
PRESSATURATION		sb	-0.075		
satmode	n	sbs	not used		
wet	n	fn	4096		
TRANSMITTER		F1 PROCESSING			
tn	H1	gt1	0.004		
strq	500.478	grs1	not used		
tof	497.5	procl	1p		
tpwr	58	fn1	2048		
pw	8.100	DISPLAY			
DECOUPLER		sp	-115.5		
dn	Cl3	wp	6344.9		
dof	1287.0	sp1	-1001.6		
ds	nm	wp1	27722.7		
decwave	w40_HCNsm	rf1	529.3		
daf	32258	rfp	0		
dpwr	38	rf11	1886.4		
pwkvl1	56	rfp1	0		
pwk	10.500	PLOT			
HMB		wd	206.0		
j1xh	146.0	sc	0		
jnxh	8.0	wd2	206.0		
ADIABATIC		sc2	0		
pwk180ad ONE_ad300	vs		39		
pwkvl180	51	th	3		
pwk180	465.4	ai	cdc av		



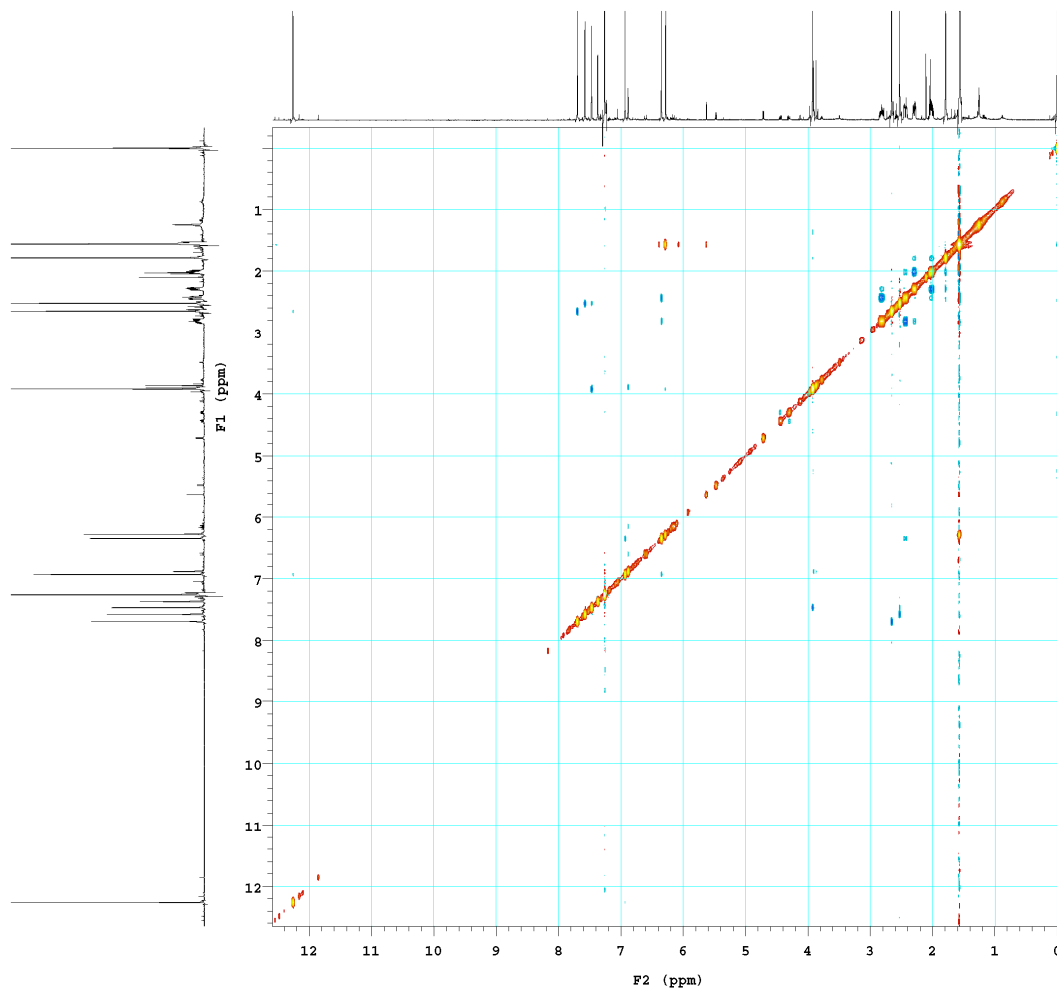


**Figure S32.** NOESY spectrum of **5** (measured in CDCl<sub>3</sub>, 500 MHz).

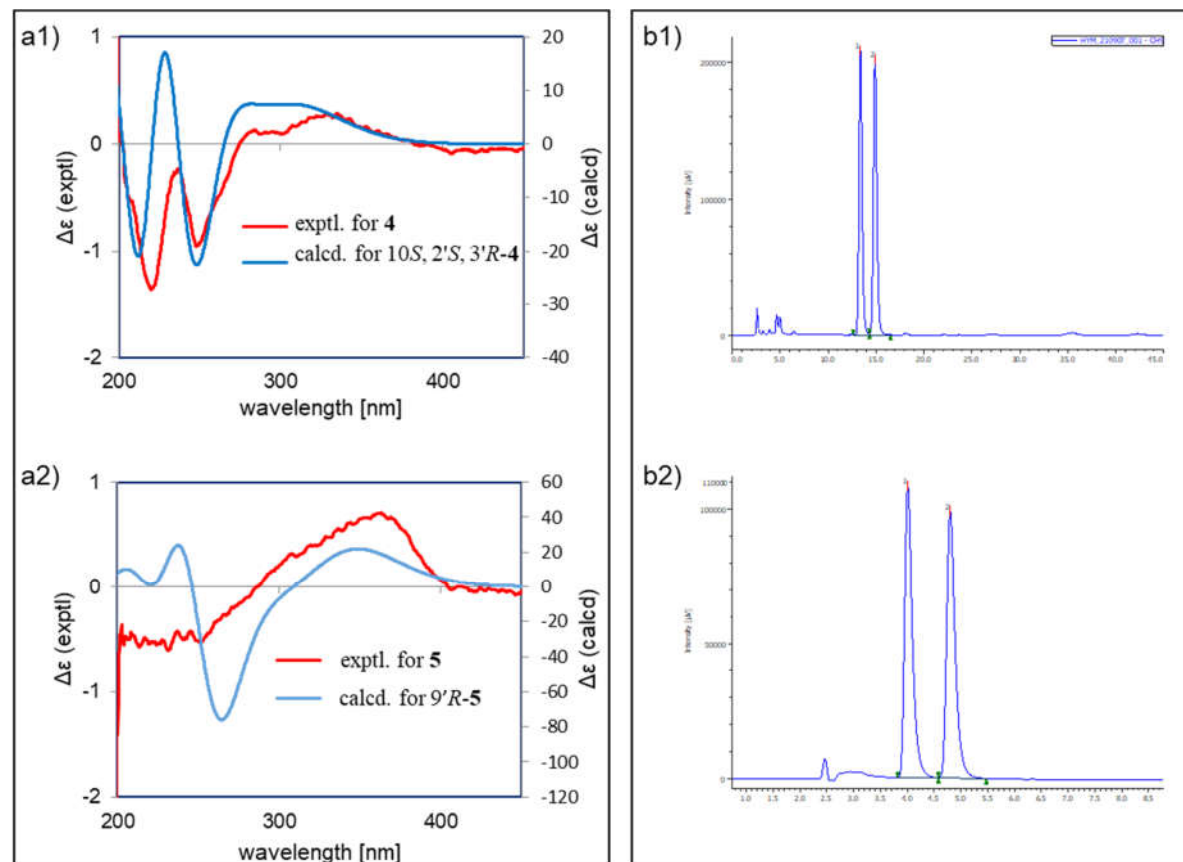
HYM-2014-48-R-6-6-1-1-1.4mg-NOESY-CDCl3

exp7 NOESY

SAMPLE		FLAGS	
date	Jun 5 2021	hs	nn
solvent	cdcl3	#spul	y
sample	PPG1g	y	
acqmethod	hag1v1	6034	
sw	7062.1	SPECIAL	
at	0.150	temp	not used
np	2118	gain	50
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION		fn	4096
sw1	7062.1	F1 PROCESSING	
ni	128	gf1	0.017
TRANSMITTER		gf1	not used
tn	H1	proc1	1p
sfrq	500.478	fn1	4096
tof	497.5	DISPLAY	
tpwr	58	sp	-91.3
pw	8.100	wp	6389.7
NOESY		sp1	-163.7
mixN	0.500	wpl	6493.2
PRESATURATION		rf1	529.3
satmode	n	rfp	0
wet	n	rf11	529.3
DECOUPLER		rfp1	0
dn	Cl3	PLOT	
dm	mm	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	39
		th	1
		al	ph

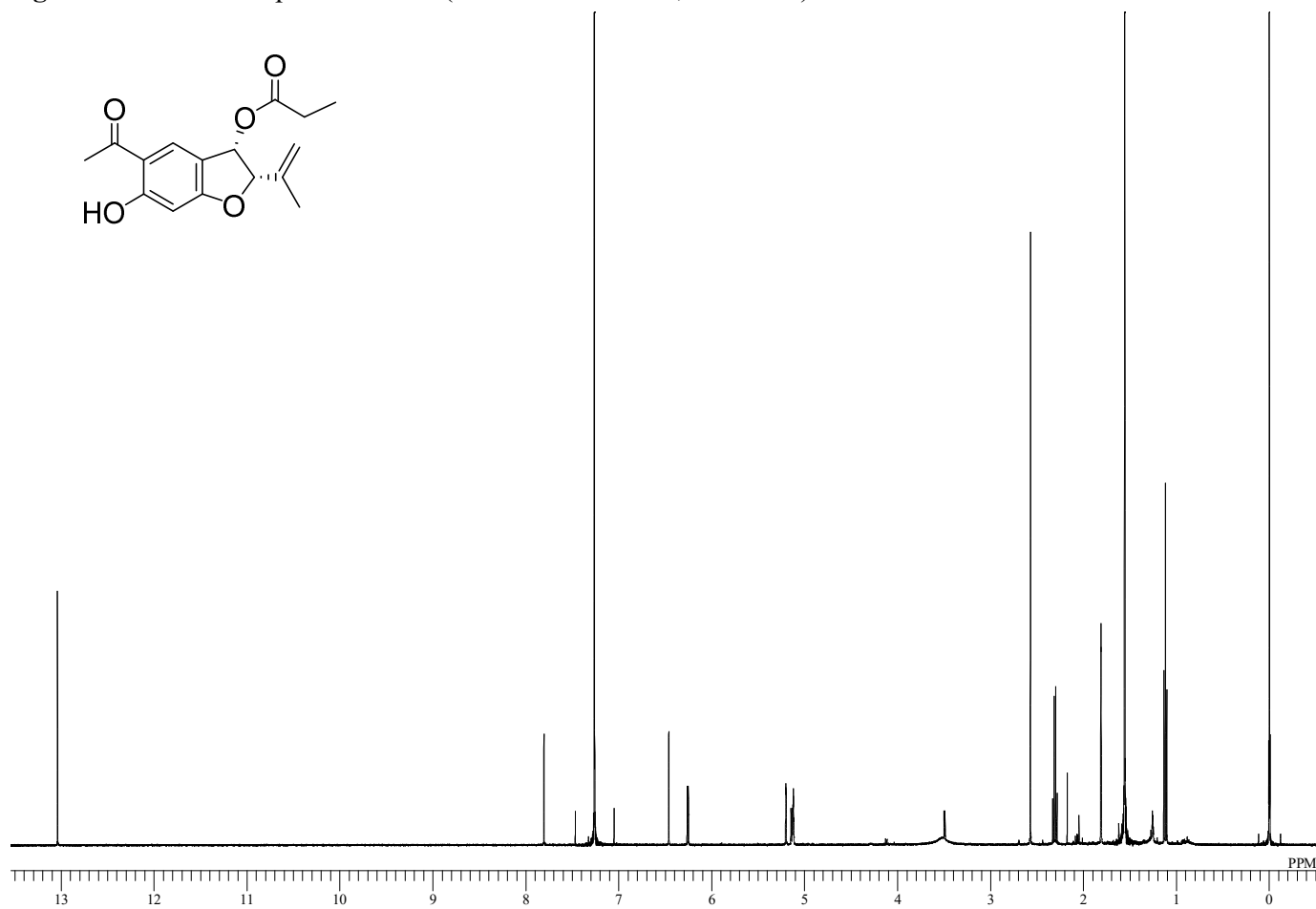


**Figure S33.** Experimental and calculated ECD spectra and chiral HPLC analysis of **4** and **5**.

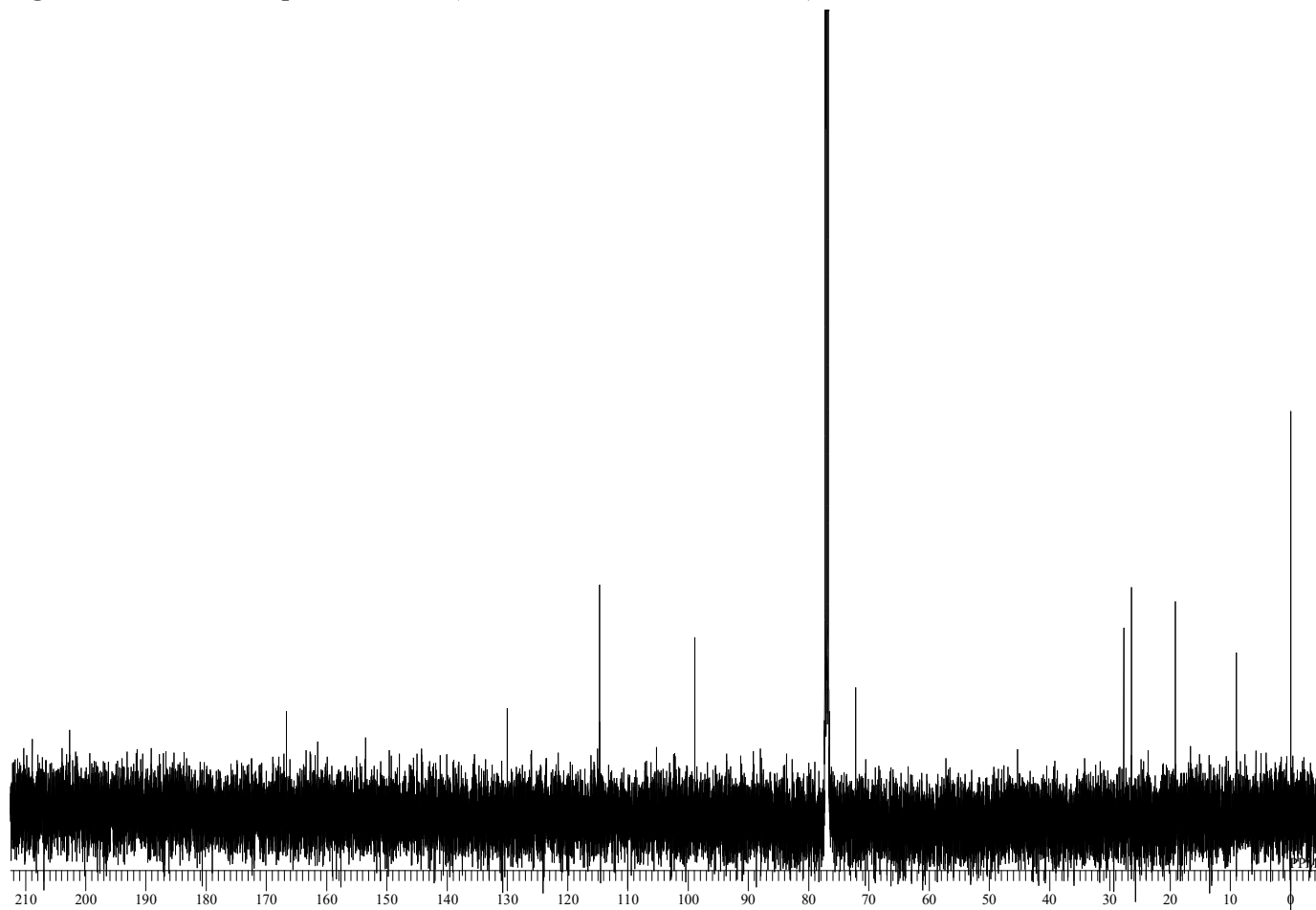


a) Experimental and calculated ECD spectra of **4** (a1,  $c = 5.98 \times 10^{-5}$  mol/L in MeOH) and **5** (a2,  $c = 4.87 \times 10^{-5}$  mol/L in MeOH). Left and right axes represent  $\Delta\epsilon$  values of experimental and calculated spectra, respectively; b) Chiral HPLC analysis of **4** (b1) and **5** (b2).

**Figure S34.**  $^1\text{H}$  NMR spectrum of **14** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S35.**  $^{13}\text{C}$  NMR spectrum of **14** (measured in  $\text{CDCl}_3$ , 126 MHz).

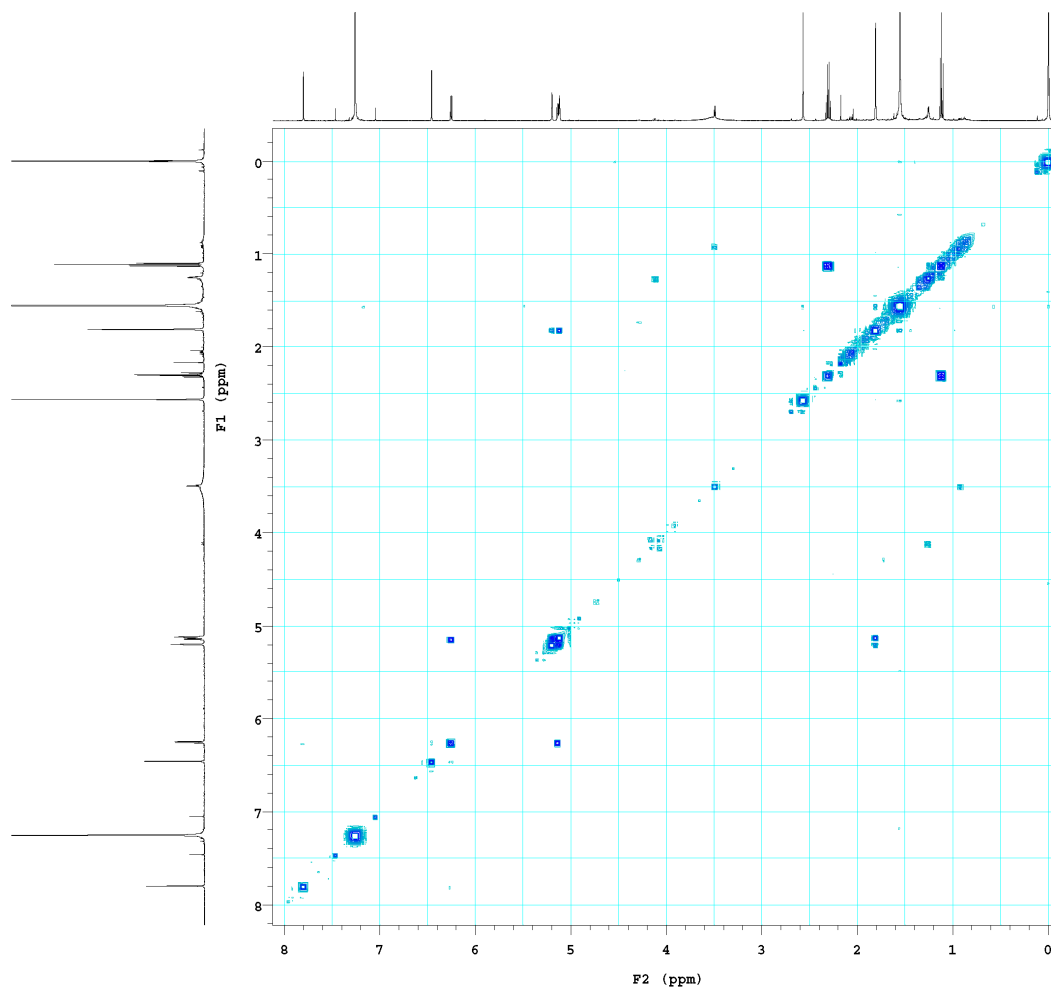


**Figure S36.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **14** (measured in  $\text{CDCl}_3$ , 500 MHz).

2014-48-R-4-2-1-1-0.4mg-COSY- $\text{CDCl}_3$

exp4 gCOSY

SAMPLE		FLAGS		nm
date	Dec 3 2020	hs		
solvent	$\text{cdcl}_3$	sspul		y
sample	hsplvl			6180
ACQUISITION		SPECIAL		
sw	7530.1	temp	not used	
at	0.150	gain	36	
np	2260	spin	0	
fb	4000	F2 PROCESSING		
ss	32	sb	-0.075	
d1	1.000	sbs	not used	
nt	16	fn	4096	
2D ACQUISITION		F1 PROCESSING		
sw1	7530.1	sb1	-0.017	
ni	128	sbs1	not used	
d2	0	procl	lp	
PRESATURATION		fml		4096
satmode	n		DISPLAY	
wet	n	sp	-101.5	
TRANSMITTER		wp		4165.8
tn	H1	sp1	-175.0	
sfrq	500.478	wp1	4287.2	
tof	751.3	rf1	509.6	
tpwr	58	rfp	0	
pw	8.000	rf11	509.6	
GRADIENTS		rfp1		0
gzlvie	5154		PLOT	
gte	0.001000	wc	206.0	
EDratio	1.000	sc	0	
gstab	0.000500	wc2	206.0	
DECOUPLER		sc2		0
dn	$\text{Cl}_3$	vs	1784	
dm	nnn	th	6	
	al	odc	av	

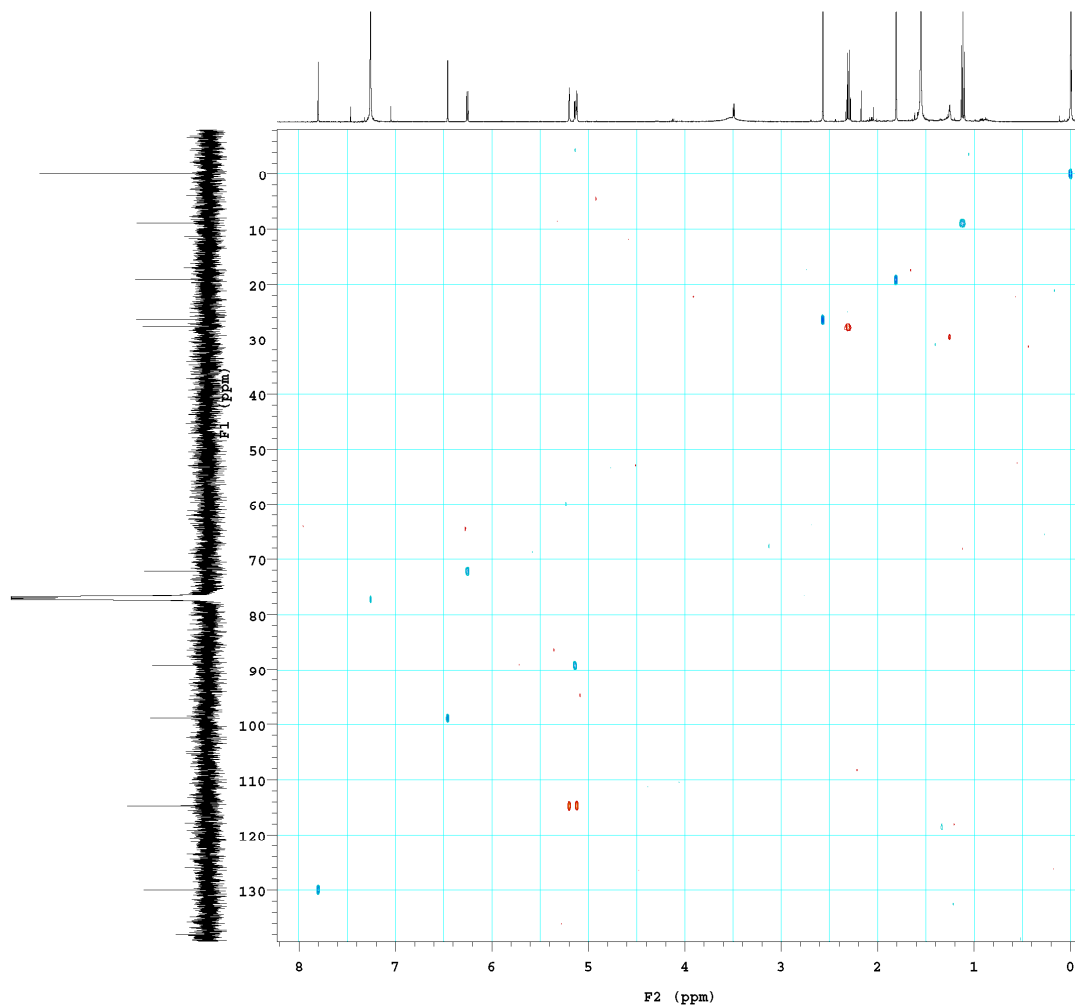


**Figure S37.** HSQC spectrum of **14** (measured in CDCl<sub>3</sub>, 500 MHz).

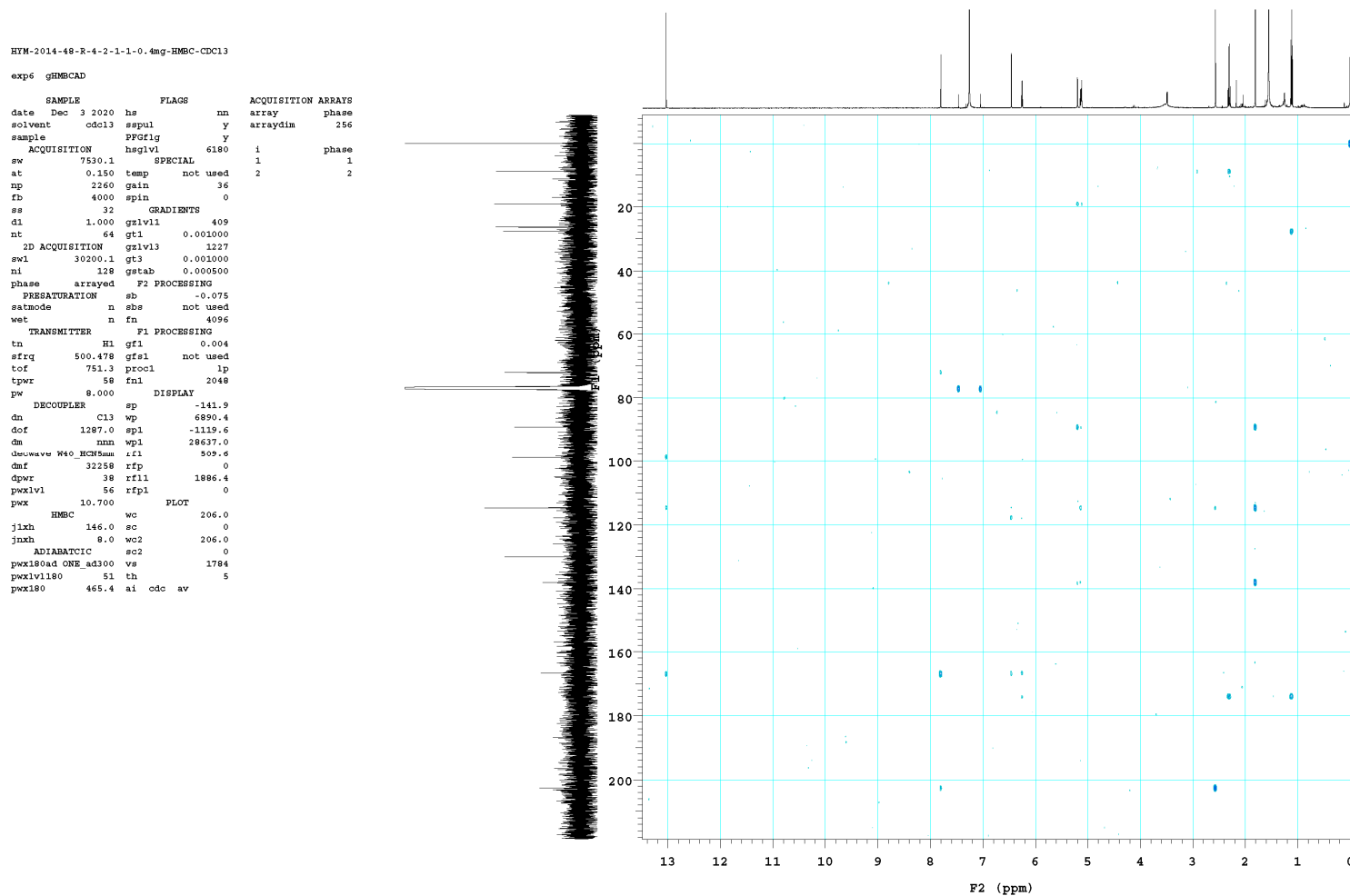
HYM-2014-48-R-4-2-1-1-0.4mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS	ACQUISITION ARRAYS	
date	Dec 3 2020	hs	nm	phase
solvent	cdcl3	sspul	y	256
sample		PPGflg	y	
ACQUISITION		hsq1v1	6180	i
sw	7530.1	SPECIAL	1	1
at	0.150	temp	not used	2
np	2260	gain	36	
fb	4000	spin	0	
ss	32	F2 PROCESSING		
d1	1.000	gf	0.069	
nt	32	gf#	not used	
2D ACQUISITION		fn	4096	
sw1	25165.1	F1 PROCESSING		
ni	128	gf1	0.005	
phase	arrayed	gfsl	not used	
PRESATURATION		procl	1p	
satmode	n	fn1	2048	
wet	n	DISPLAY		
TRANSMITTER		sp	-86.8	
tn	H1	wp	4202.6	
sfrq	500.478	sp1	-1010.8	
tofr	751.3	wp1	18529.8	
tpwr	58	rf1	509.6	
pw	8.000	rtp	0	
DECOUPLER		rf11	1256.5	
dn	C13	rfp1	0	
dof	-600.6	PLOT		
dm	mnx	wc	206.0	
dcwave	W40_HCN5mm	sc	0	
dmf	32258	wc2	206.0	
dpwr	38	sc2	0	
pw1v1	56	vs	1784	
pw1	10.700	th	4	
HSQC		ai	cdc	ph
j1xh	146.0			
multiflg	y			
mult	2			
ADIABATIC				
pw180ad	ONE ad300			
pw180adr	ONE ad300			
or				
pw180	465.4			
pw1v1180	51			
pw180ref	ONE_ref2-			
or				
pw180r	2000.2			
pw1v1180r	43			



**Figure S38.** HMBC spectrum of **14** (measured in CDCl<sub>3</sub>, 500 MHz).

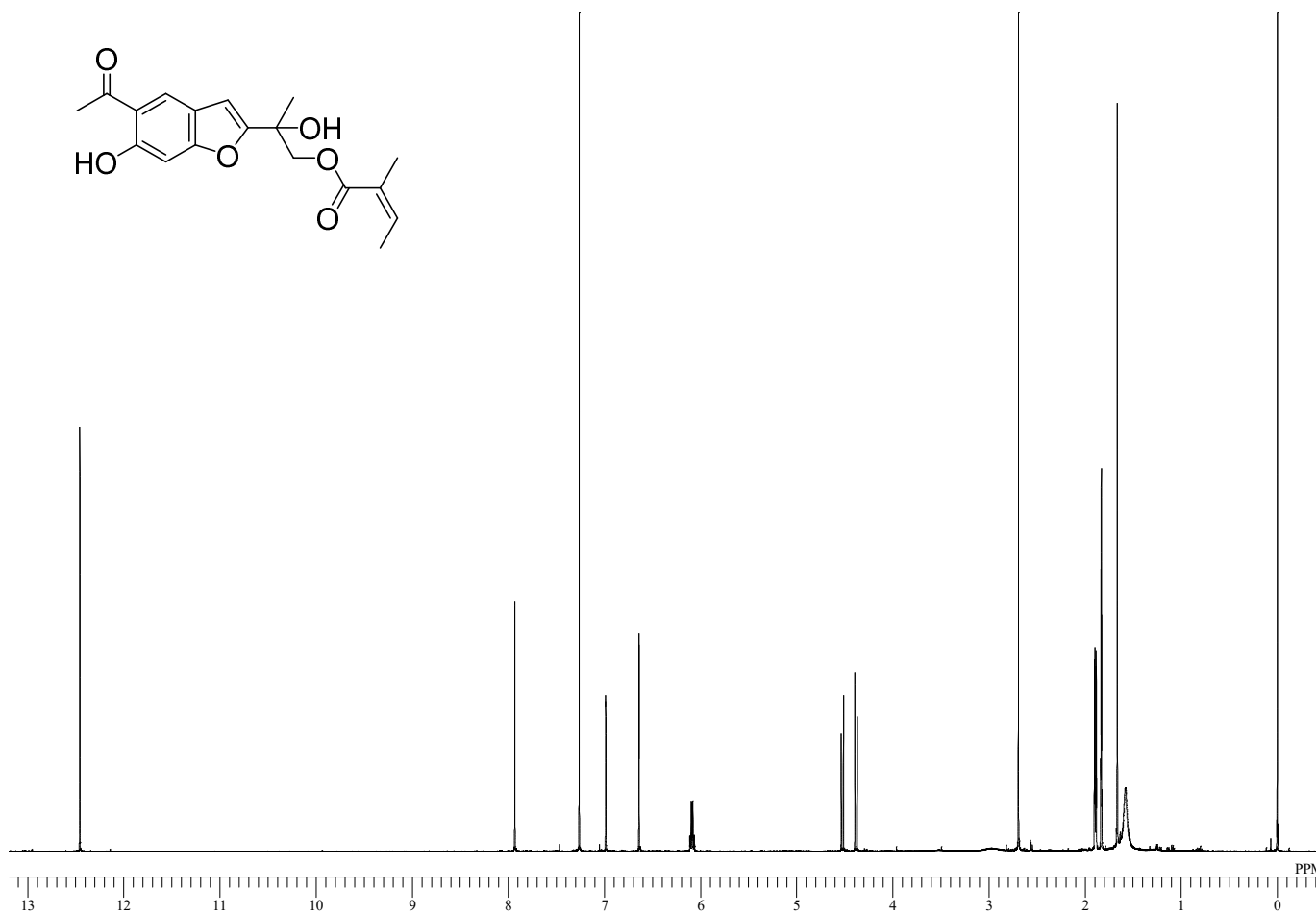


**Figure S39.** NOESY spectrum of **14** (measured in CDCl<sub>3</sub>, 500 MHz).

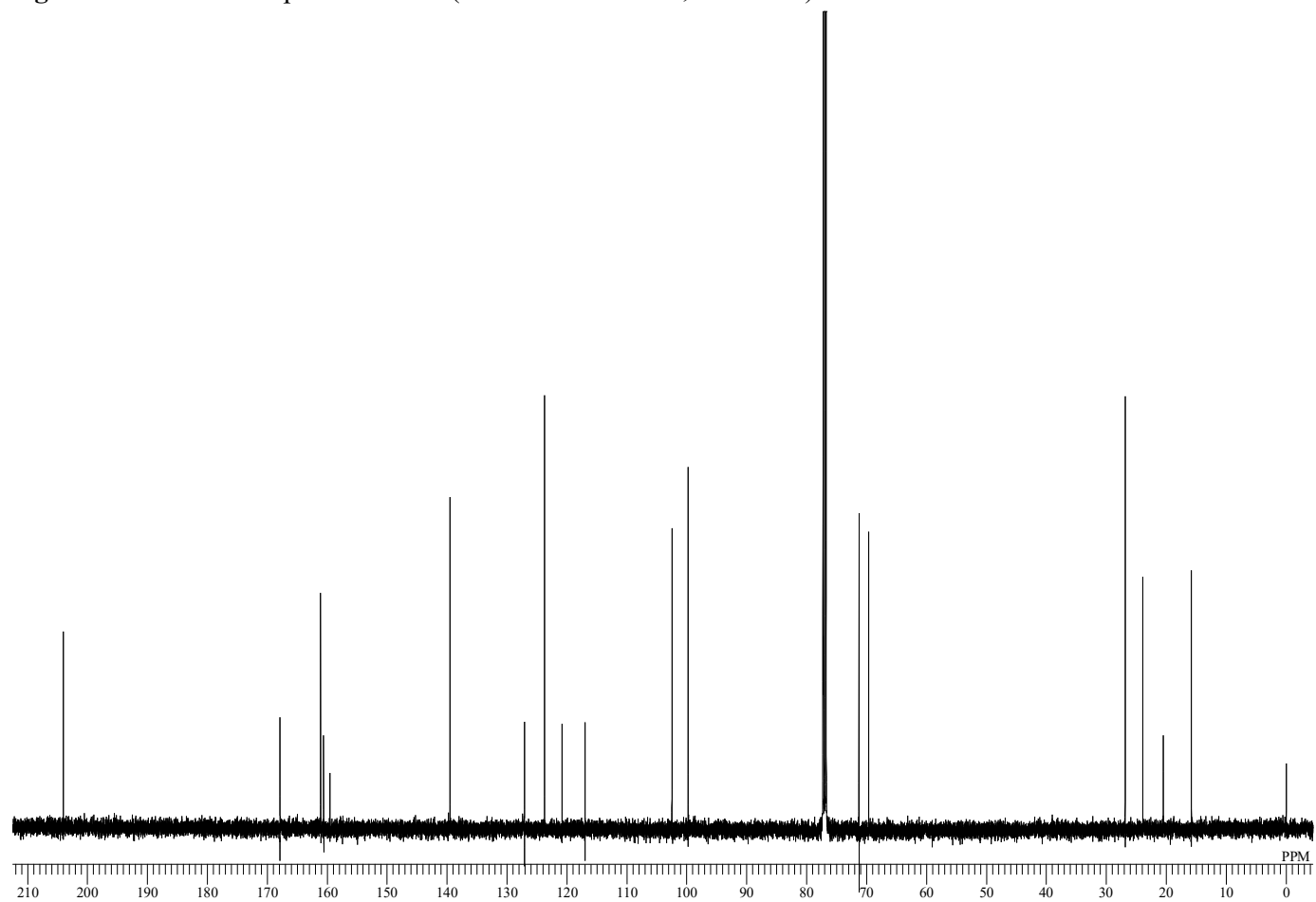




**Figure S40.**  $^1\text{H}$  NMR spectrum of **17** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S41.**  $^{13}\text{C}$  NMR spectrum of **17** (measured in  $\text{CDCl}_3$ , 126 MHz).

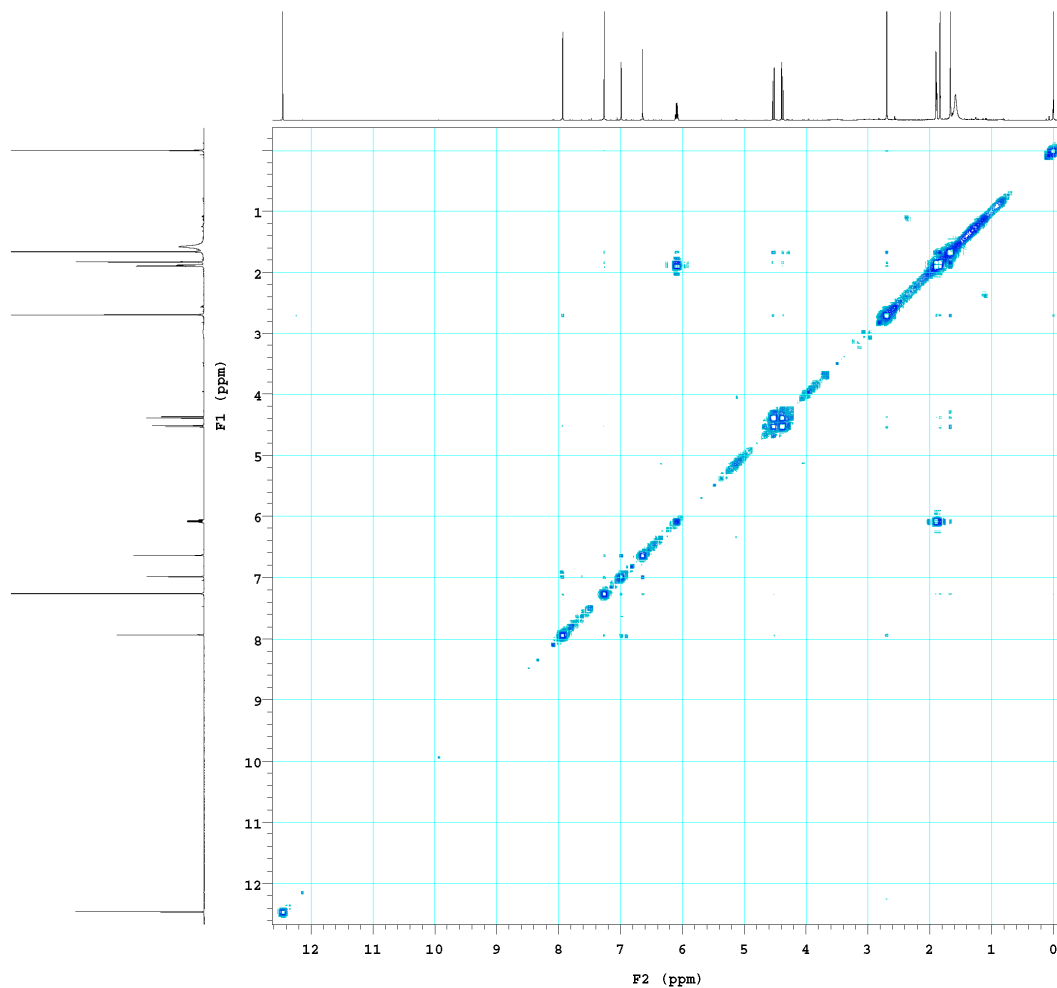


**Figure S42.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **17** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-6-3-1-3-2.0mg-COSY-CDCl3

exp4 gCOSY

SAMPLE		FLAGS	
date	Nov 24 2020	hs	nn
solvent	cdcl3	sspul	y
sample	hsq1v1		6180
ACQUISITION		SPECIAL	
sw	7309.9	temp	not used
at	0.150	gain	20
np	2192	spin	0
fb	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	16	fn	4096
2D ACQUISITION		F1 PROCESSING	
sw1	7309.9	sb1	-0.018
ni	128	sbs1	not used
d2	0	prool	lp
PRESATURATION		f1	
satmode	n	fn1	4096
wet		DISPLAY	
transmitter	n	sp	-114.6
tn	H1	wp	6431.9
sfrq	500.478	wpl	6517.6
tof	664.6	rf1	485.8
tpwr	58	rfl	0
pw	8.000	rf11	485.8
GRADIENTS		rfpl	
g1v1e	5154		0
gtE	0.001000	wc	206.0
EDratio	1.000	sc	0
gstab	0.000500	wc2	206.0
DECOUPLER		sc2	
dn	C13	vs	894
dm	nm	th	5
	ai	cdc	av

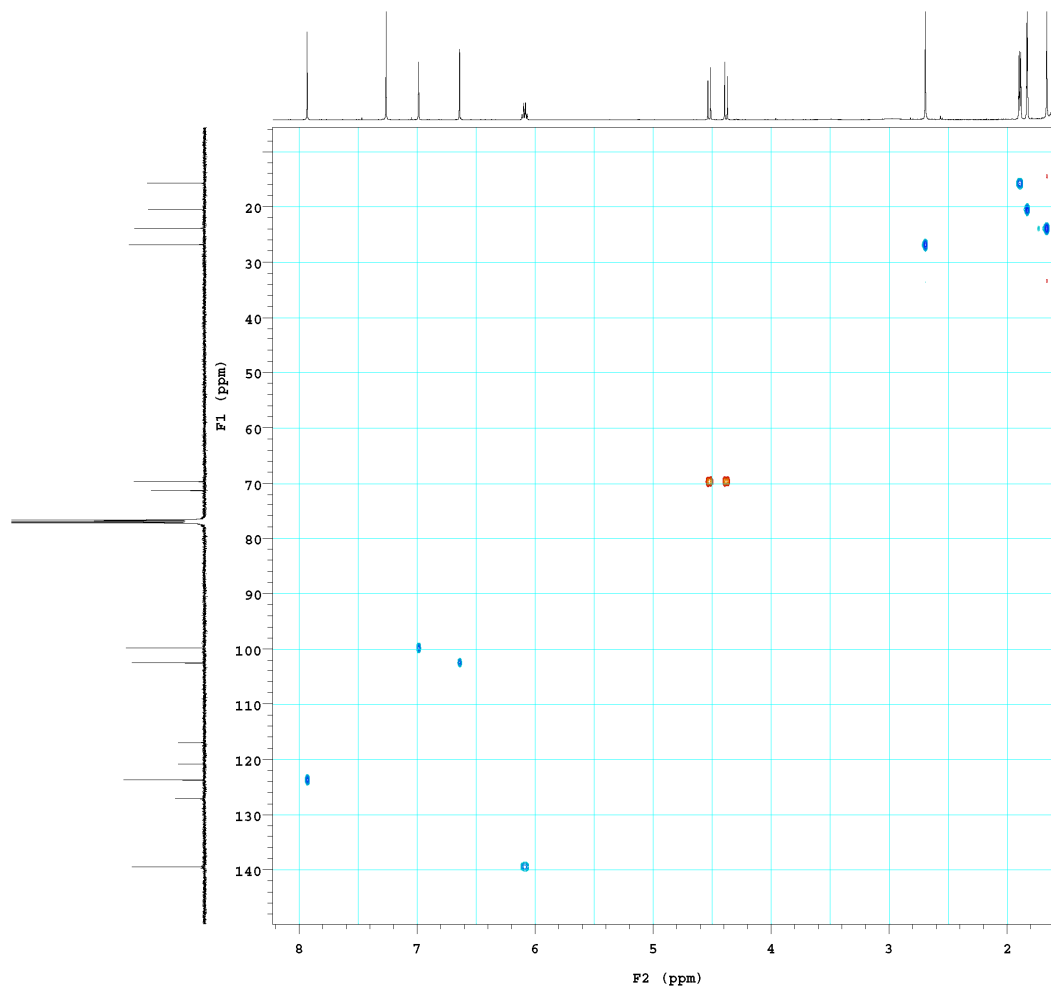


**Figure S43.** HSQC spectrum of **17** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-3-1-3-2.0mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Nov 24 2020	hs		array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample		PFGflg	y		
ACQUISITION		hsqvlvl	6180	i	phase
sv	7309.9	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2192	gain	20		
fb	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	32	gfs	not used		
2D ACQUISITION		fn	4096		
sw1	25165.1	F1 PROCESSING			
ni	229	gfl	0.005		
phase	arrayed	gfs1	not used		
PRESATURATION		procl	1p		
satmode	n	fnl	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	745.6		
tn	H1	wp	3369.4		
sfrq	500.478	sp1	709.5		
tof	664.6	wp1	18136.6		
tpwr	58	rfl	485.8		
pw	8.000	rpf	0		
DECOUPLER		rfl1	1256.5		
dn	Cl3	rfl1	0		
dof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pxxlvl	56	vs	894		
pxx	10.700	th	2		
HSQC		ai	odc	ph	2
j1xh	146.0				
multifig	y				
mult	2				
ADIABATIC					
pxxl80ad	ONE_ad300				
pxxl80adR	ONE_ad30-				
OR					
pxxl80	465.4				
pxxlvl180	51				
pxxl80ref	ONE_ref2-				
00					
pxxl80r	2000.2				
pxxlvl180r	43				

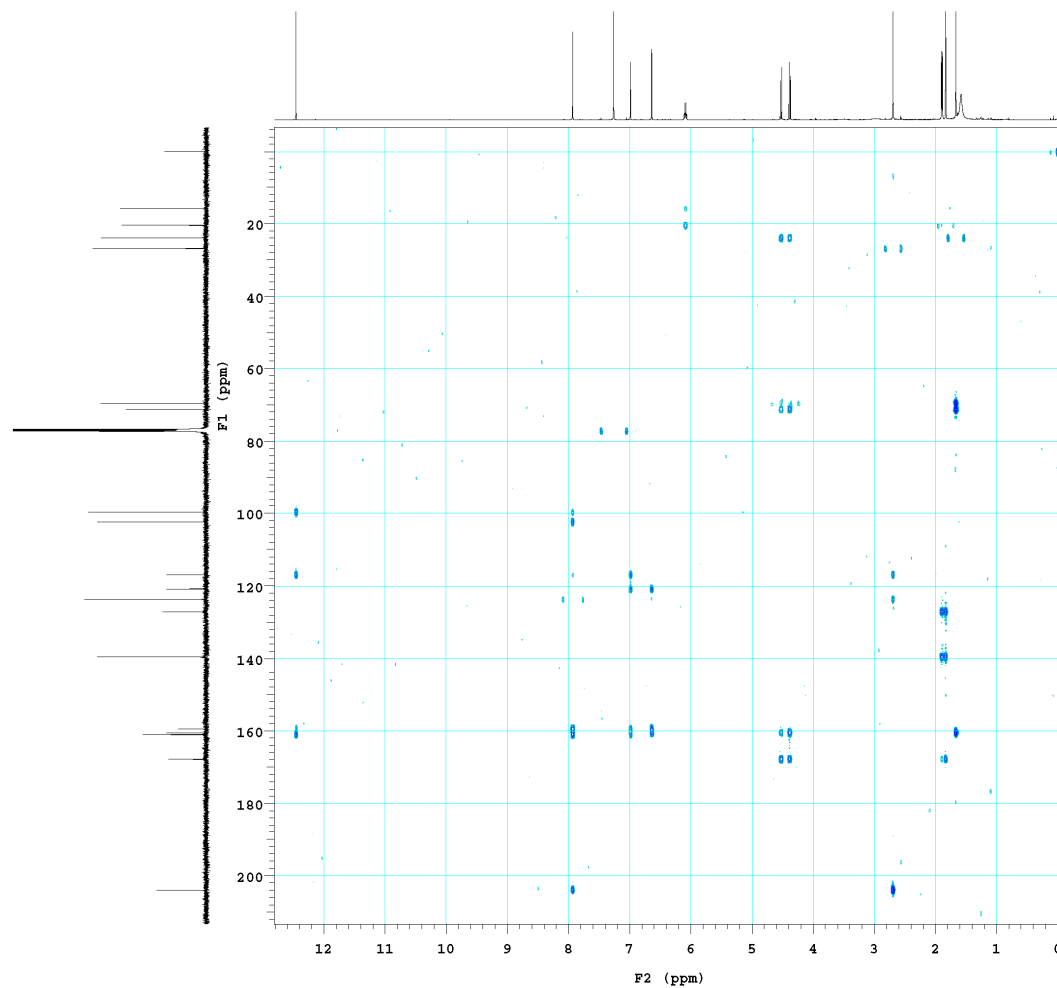


**Figure S44.** HMBC spectrum of **17** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-3-1-3-2.0mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Nov 24 2020	hs	mn	array	phase
solvent	cdcl3	sspul	y	arraydia	256
sample	PFG1g	y			
ACQUISITION		hsglvi	6180	i	phase
sw	7309.9	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2192	gain	20		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlvi1	409		
nt	32	gt1	0.001000		
2D ACQUISITION		gzlvi3	1227		
sw1	30200.1	gt3	0.001000		
ni	128	gstab	0.000500		
phase		arrayed	F2 PROCESSING		
PRESATURATION		sb	-0.075		
satmode		n	sbs	not used	
wet		n	fn	4096	
TRANSMITTER		F1 PROCESSING			
tn	H1	gf1	0.004		
sfrq	500.478	gf1	not used		
tof	664.6	procl	lp		
tpwr	58	fn1	2048		
pw	8.000	DISPLAY			
DECOUPLER		sp	-96.7		
dn	C13	wp	6506.8		
dof	1287.0	sp1	-824.7		
dm	mmn	wp1	27663.7		
decwave	W40_HCN2mm	rf1	485.8		
dmf	32258	rfp	0		
dpr	38	rf11	1886.4		
pxlvi	56	rfp1	0		
pxw	10.700	PLOT			
HMB		wc	206.0		
jlkh	146.0	sc	0		
jnxh	8.0	wc2	206.0		
ADDITIONAL		sc2	0		
pxw180ad	ONE_ad300	vs	894		
pxw180	51	th	2		
pxw180	465.4	ai	cdc	av	

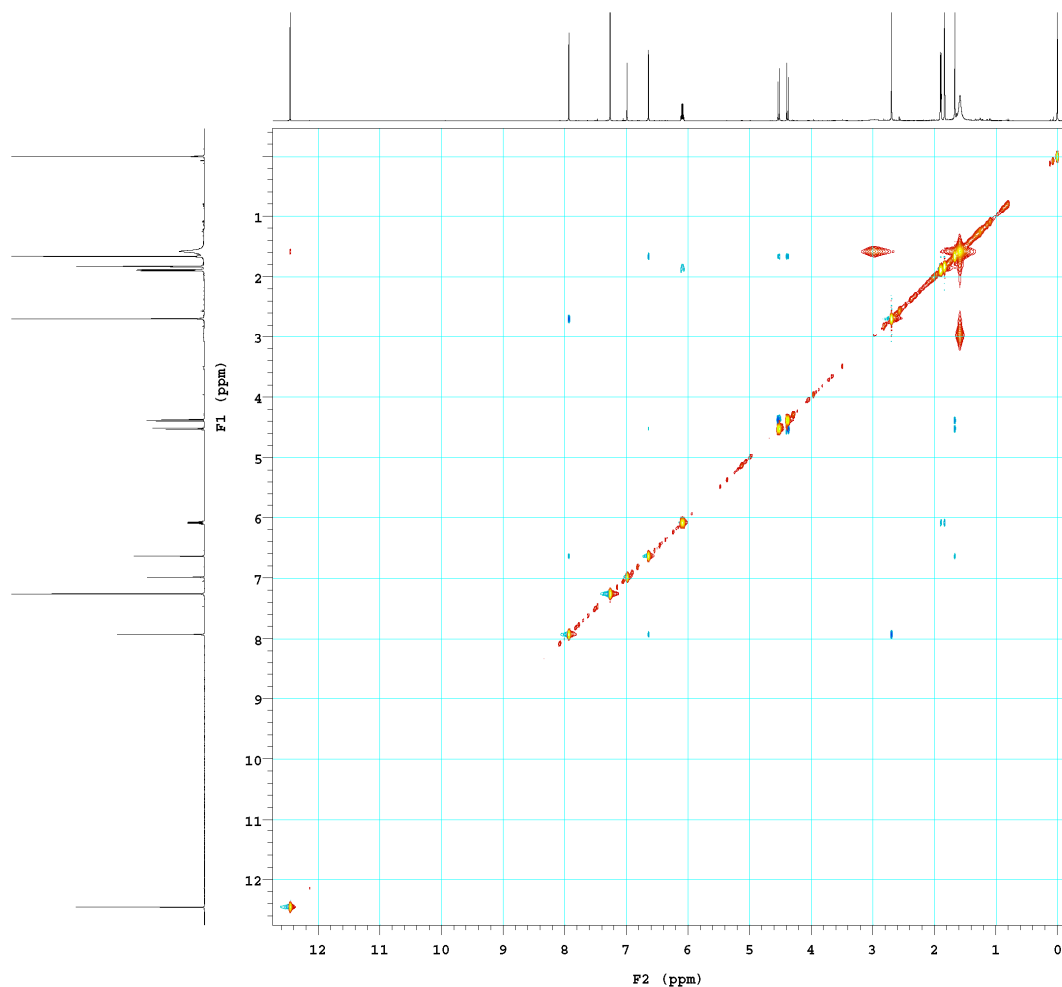


**Figure S45.** NOESY spectrum of **17** (measured in CDCl<sub>3</sub>, 500 MHz).

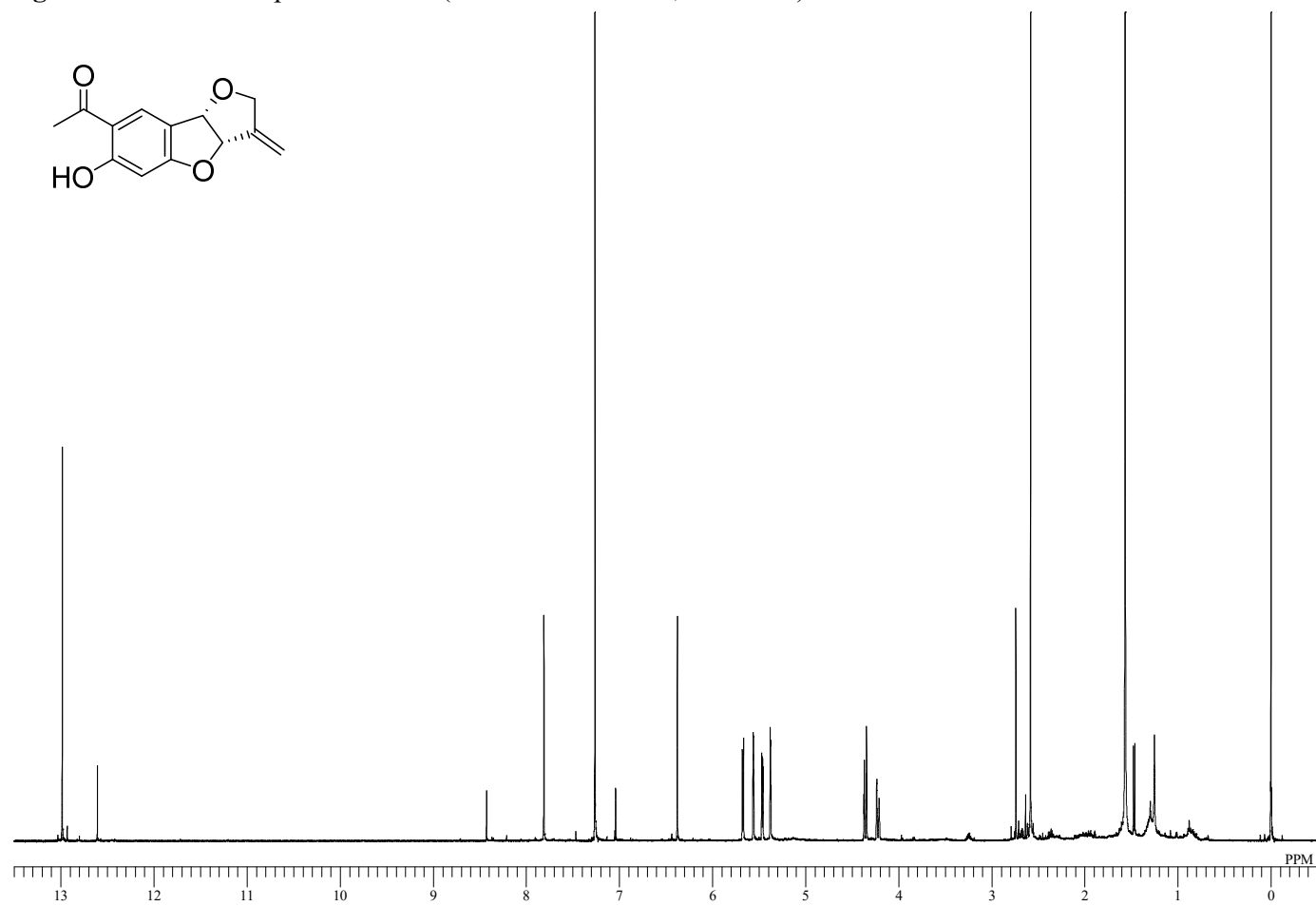
HTM-2014-48-R-6-3-1-3-2\_0mg-NOESY-CDCl3

exp7 NOESY

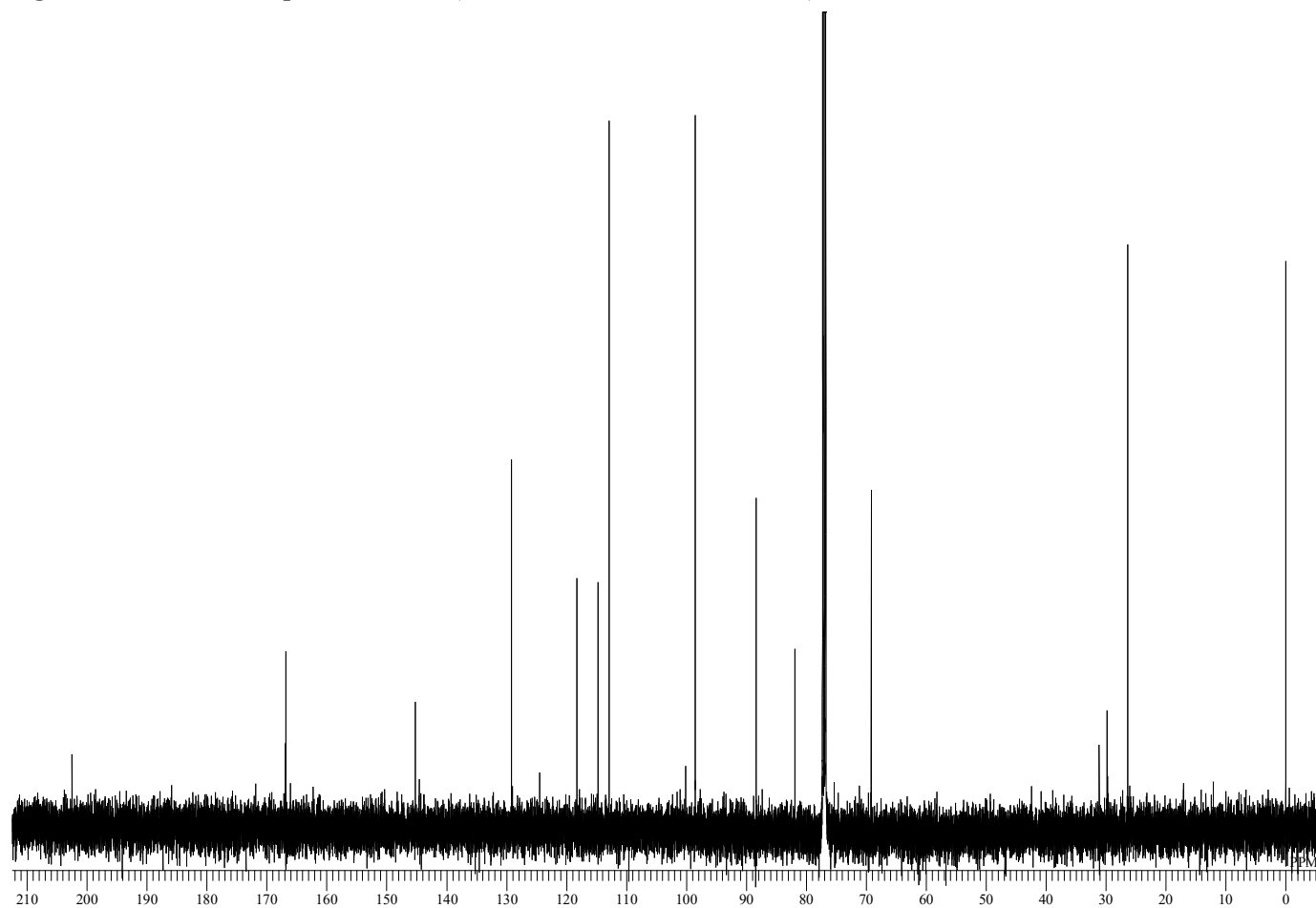
SAMPLE		FLAGS	
date	Nov 24 2020	hs	nn
solvent	cdcl3	sspl	y
sample		ppfig	y
ACQUISITION		haglv1	6180
sw	7309.9	SPECIAL	
at	0.150	temp	not used
rp	2192	gain	20
fn	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION		fn	4096
sw1	7309.9	F1 PROCESSING	
ni	128	gf1	0.016
TRANSMITTER		gfsl	not used
tn	H1	procl	lp
sfrq	500.478	fn1	4096
tof	664.6	DISPLAY	
tpwr	58	sp	-82.5
pw	8.000	wp	6456.9
	NOESY	wp1	-228.8
mixN	0.500	wp1	6610.4
PRESATURATION		rf1	485.8
satmode	n	rfl	0
wet	n	rfl1	485.8
DECOUPLER		rfl1	0
dn	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		ve	894
		th	1
		ai	ph



**Figure S46.**  $^1\text{H}$  NMR spectrum of **21** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S47.**  $^{13}\text{C}$  NMR spectrum of **21** (measured in  $\text{CDCl}_3$ , 126 MHz).



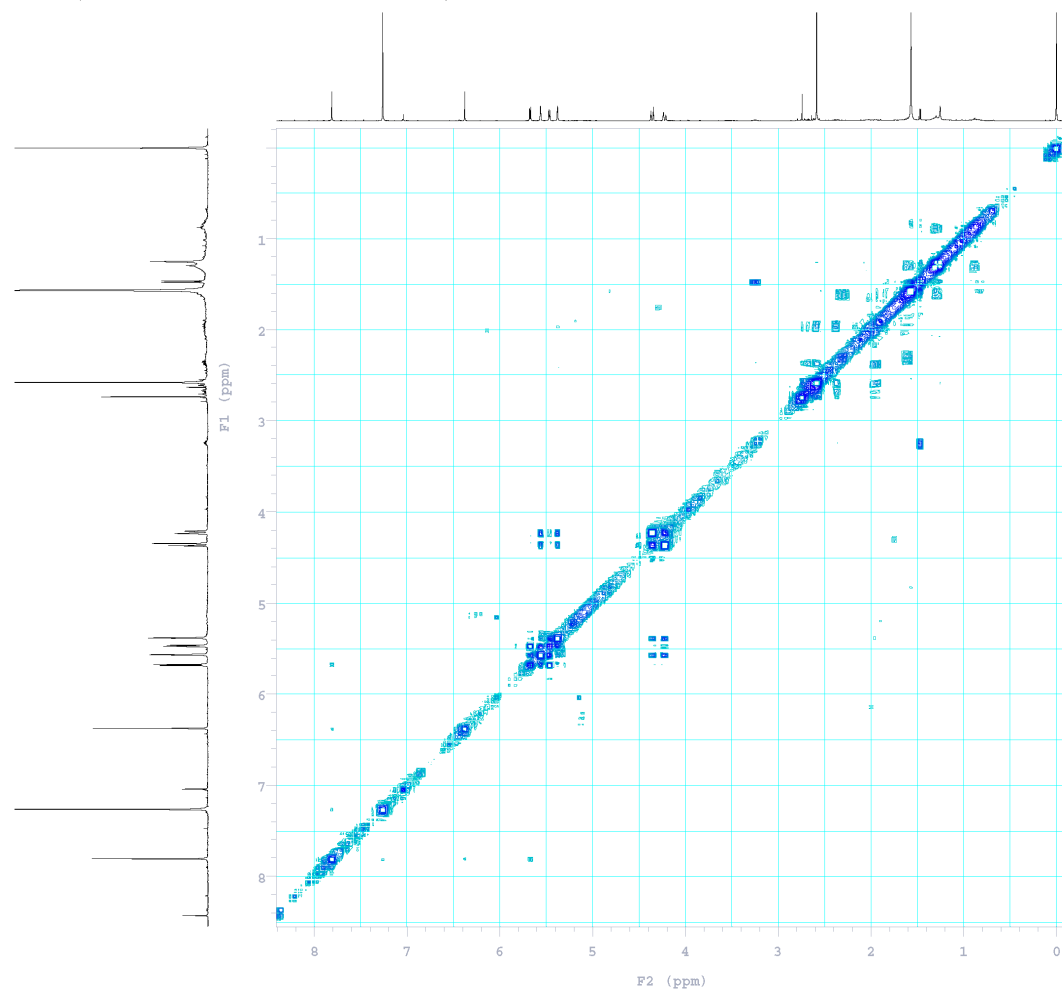


**Figure S48.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **21** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-5-6-1.6mg-COSY- $\text{CDCl}_3$

exp4 gCOSY

SAMPLE		FLAGS		nm
date	Sep 19 2020	hs		
solvent	$\text{cdcl}_3$	sspul		y
sample	hag1v1			6180
ACQUISITION		SPECIAL		
sw	7530.1	temp	not used	
at	0.150	gain	38	
np	2260	spin	0	
fb	4000	F2 PROCESSING		
ss	32	sb	-0.075	
d1	1.000	sbs	not used	
nt	8	fn	4096	
2D ACQUISITION		F1 PROCESSING		
sw1	7530.1	sb1	-0.017	
n1	128	sb1	not used	
d2	0	procl	1p	
PRESATURATION		fml <th>4096</th>		4096
satmode	n		DISPLAY	
wet	n	sp	-86.8	
TRANSMITTER		vp <th>4294.5</th>		4294.5
tn	H1	sp1	-105.2	
sfreq	500.478	wp1	4382.8	
tof	747.2	rfl	513.3	
tpwr	58	rpf	0	
pw	8.000	rfl1	513.3	
GRADIENTS		rflp1 <th>0</th>		0
gslv1s	5154		PLOT	
gtE	0.001000	wc	206.0	
EDratio	1.000	sc	0	
getab	0.000500	wc2	206.0	
DECOUPLER		sc2 <th>0</th>		0
dm	$\text{Cl}_3$	vs	231	
dm	nmn	th	7	
	ai	cdc	av	

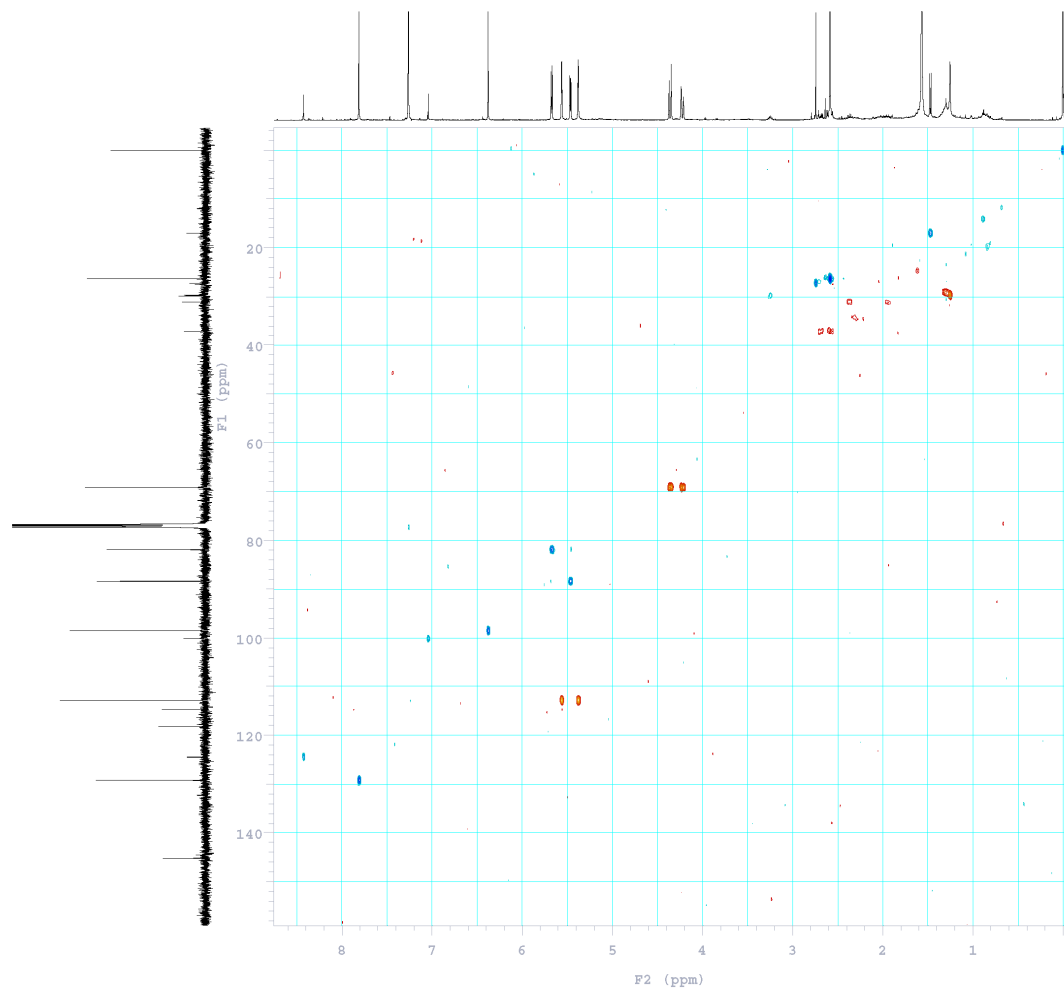


**Figure S49.** HSQC spectrum of **21** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-5-6-1.6mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Sep 19 2020	hs	nm	array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample		DPGflg	y		
ACQUISITION		hscvl1	6180	1	phase
sv	7530.1	SPECIAL		1	1
at	0.150	temp	not used	2	2
hp	2260	gain	38		
fd	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	16	gfs	not used		
2D ACQUISITION		fn	4096		
sw1	25165.1	F1 PROCESSING			
ni	128	gfl	0.005		
phase	arrayed	gfl	not used		
PRESATURATION		procl	1p		
satmode	n	fnl	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	-39.0		
tn	H1	wp	4419.5		
sfrq	500.478	spl	-568.4		
torf	747.2	wpl	20569.6		
tpwr	58	rfl	513.3		
pw	8.000	rpf	0		
DECOUPLER		rfl1	1256.5		
dm	C13	rfl1	0		
dof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pxxlvl	56	vs	231		
pxx	10.700	th	3		
HSQC		ai	cdc	ph	
j1xh	146.0				
multifig	y				
mult	2				
ADIABATIC					
pxxl80ad	ONE_ad300				
pxxl80adR	ONE_ad30-				
or					
pxxl80	465.4				
pxxlvl180	51				
pxxl80ref	ONE_ref2-				
00					
pxxl80r	2000.2				
pxxlvl180r	43				

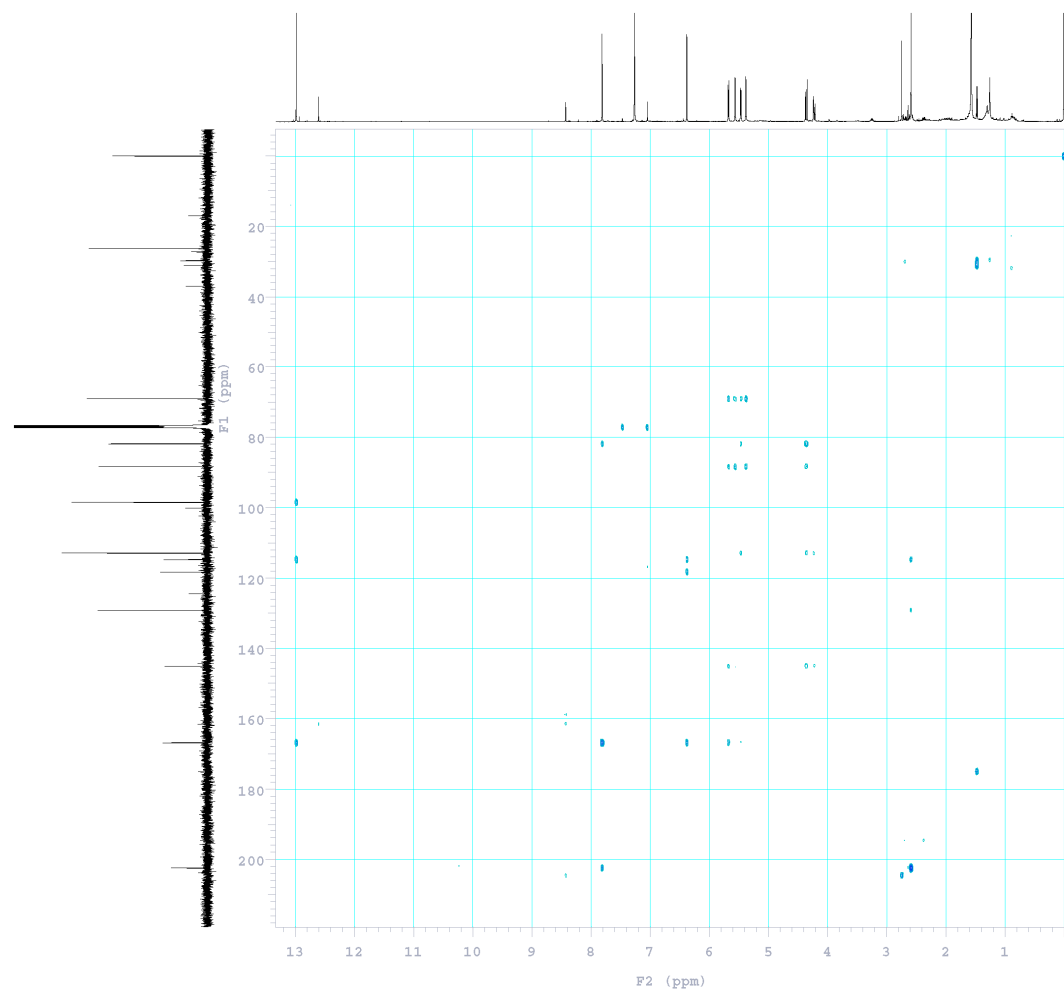


**Figure S50.** HMBC spectrum of **21** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-5-6-1.6mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Sep 19 2020	hs	nn	array	phase
solvent	cdcl3	sspl	y	arraydim	256
sample	PPGflg	y			
ACQUISITION		haglvl	6190	i	phase
sw	7530.1	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2260	gain	38		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlvi1	409		
nt	16	gtl	0.001000		
2D ACQUISITION		gzlvi3	1227		
sw1	30200.1	gt3	0.001000		
ni	128	gstab	0.000500		
phase		arrayed	F2 PROCESSING		
PERSATURATION		sb	-0.075		
satmode	n	sbs	not used		
wet	n	fn	4096		
TRANSMITTER		F1 PROCESSING			
tn	H1	gt1	0.004		
sfrq	500.478	gtf1	not used		
tof	747.2	procl	lp		
tpwr	58	fnl	2048		
pw	8.000	DISPLAY			
DECOUPLER		sp	-64.7		
dn	C13	wp	6735.9		
dof	1287.0	sp1	-942.7		
dn	nmn	wp1	28519.0		
decwave	W40	HCN5mm	rf1	513.3	
dmf	32258	rfp	0		
dpwr	38	rf11	1886.4		
pw1v1	56	rfp1	0		
pw1	10.700	PLOT			
HMBC		wd	206.0		
j1xh	146.0	sc	0		
j1xh	8.0	wd2	206.0		
ADIABATIC		sc2	0		
pw180ad	ONE	ad300	vs	231	
pw1v1180	51	th	4		
pw180	465.4	ai	cdc	av	

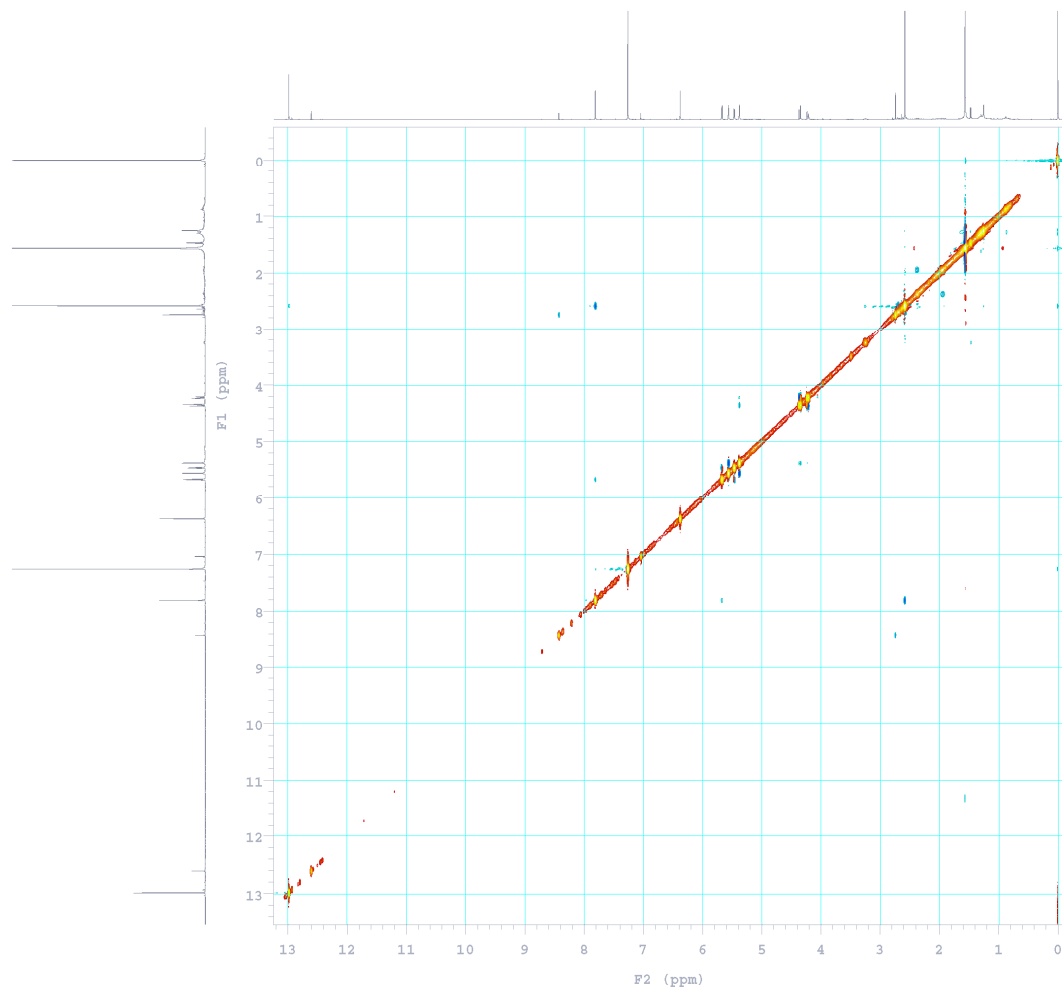


**Figure S51.** NOESY spectrum of **21** (measured in CDCl<sub>3</sub>, 500 MHz).

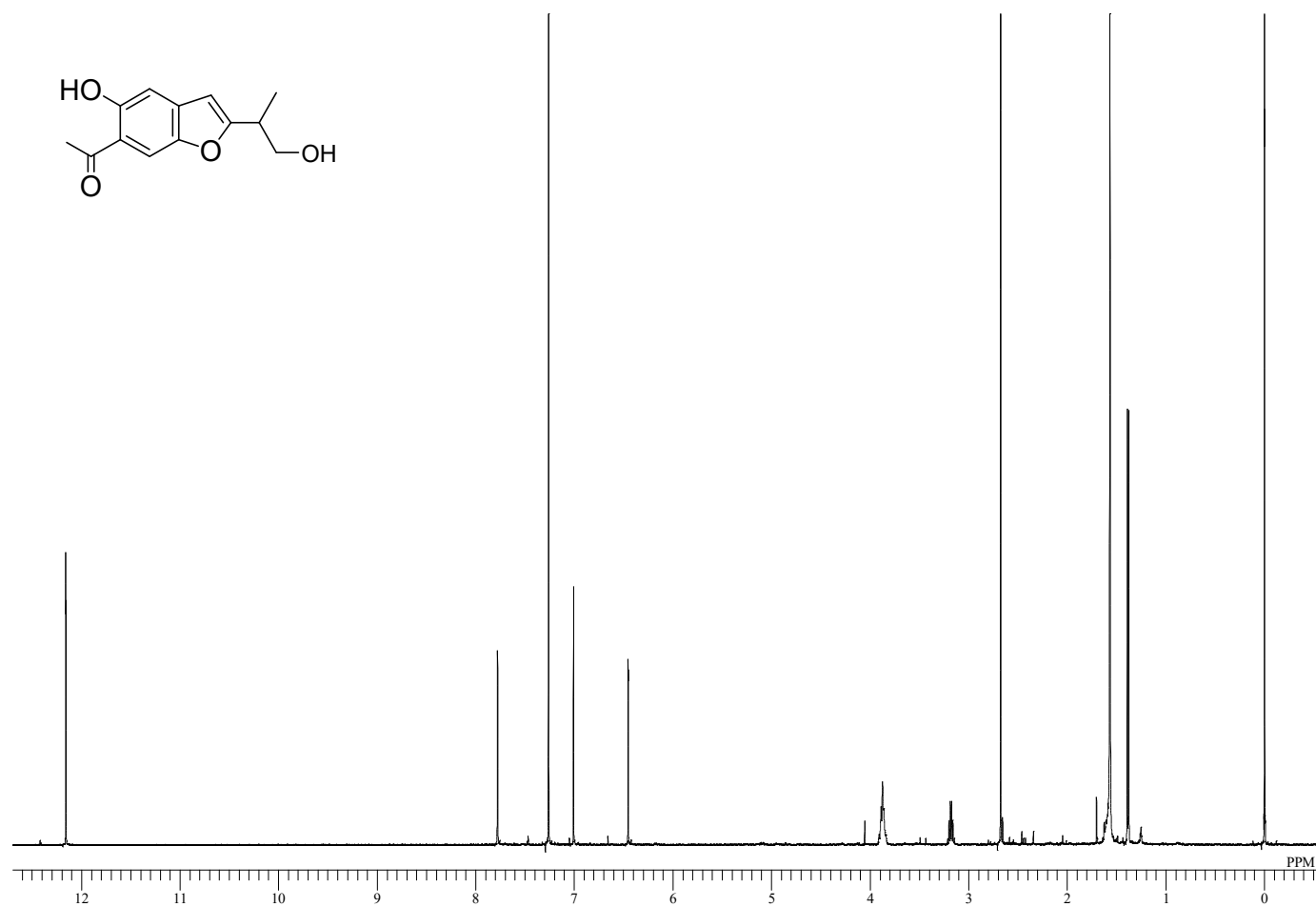
HYM-2014-48-R-5-6-1.6mg-NOESY-CDCl3

exp7 NOESY

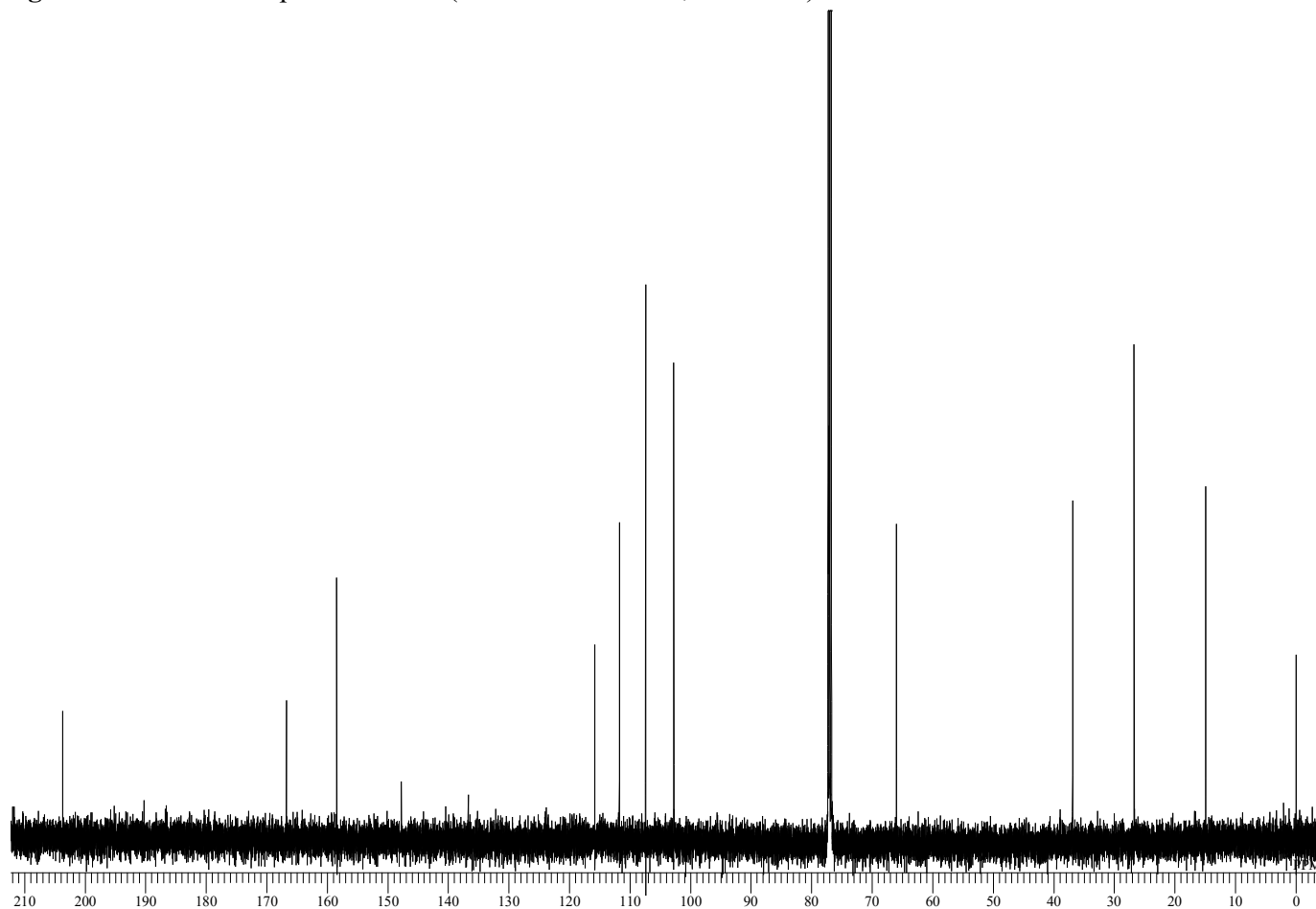
SAMPLE		FLAGS	
date	Dec 28 2020	hs	nn
solvent	cdcl3	spul	y
sample		ppgflg	y
ACQUISITION		haglvi	c190
sw	7142.9	SPECIAL	
at	0.150	temp	not used
np	2142	gain	38
rb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gt	0.069
nt	32	gfs	not used
2D ACQUISITION		fn	4096
sw1	7142.9	F1 PROCESSING	
ni	128	gt1	0.016
TRANSMITTER		gfs1	not used
tn	H1	procl	lp
sfrq	500.478	fn1	4096
tof	724.4	DISPLAY	
tpwr	58	sp	-98.3
pw	8.000	wp	6724.3
	NOESY	sp1	-290.2
mixN	0.500	wp1	7062.6
PRESATURATION		rf1	342.5
satmode	n	rfp	0
wet	n	rf11	342.5
DECOUPLER		rfpl	0
dn	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	219
		th	1
		ai	ph



**Figure S52.**  $^1\text{H}$  NMR spectrum of **25** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S53.**  $^{13}\text{C}$  NMR spectrum of **25** (measured in  $\text{CDCl}_3$ , 126 MHz).

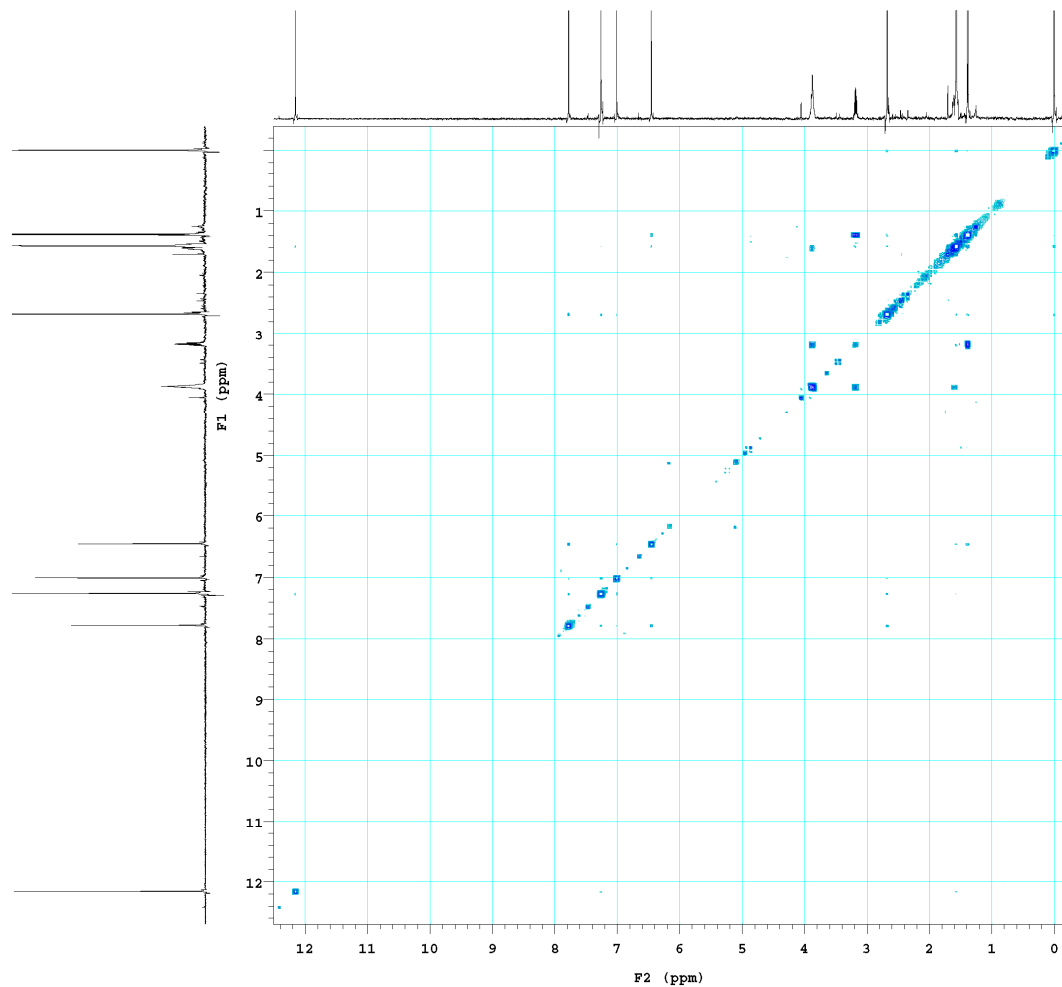


**Figure S54.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **25** (measured in  $\text{CDCl}_3$ , 500 MHz).

HTM-2014-48-R-6-5-3-1-0.8mg-COSY-CDCl3

exp4 gCOSY

SAMPLE		FLAGS	
date	May 31 2021	hs	nn
solvent	cdcl3	sspul	y
sample	hsglvl	6024	
ACQUISITION		SPECIAL	
sw	7102.3	temp	not used
at	0.150	gain	46
np	2130	spin	0
fb	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	8	fn	4096
2D ACQUISITION		F1 PROCESSING	
sw1	7102.3	sb1	-0.018
nl	128	sbs1	not used
d2	0	procl	1p
PERSATURATION		fml	
satmode	n	fnl	4096
TRANSMITTER		DISPLAY	
wet	n	sp	-123.3
tn	H1	wp	6380.9
sfrq	500.478	wp1	-192.6
tof	506.9	rfl	6547.4
tpwr	58	rfl	539.4
pw	8.100	rfl1	0
GRADIENTS		rfpl	
gslv1e	5025	rfpl	0
g1e	0.001000	wc	206.0
EDratio	1.000	sc	0
getab	0.000500	wc2	206.0
DECOUPLER		sc2	
dm	C13	vs	116
dm	nmn	th	7
	ai	cdc	av

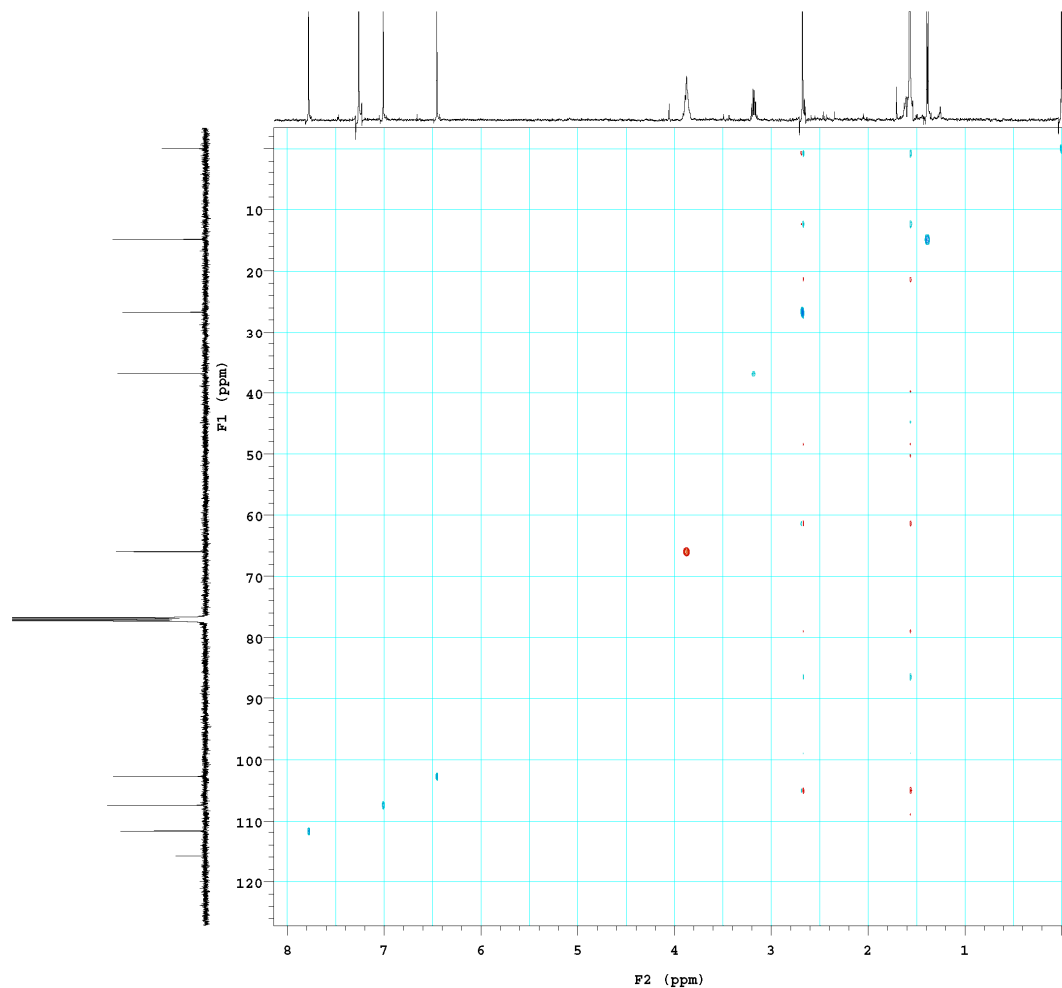


**Figure S55.** HSQC spectrum of **25** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-5-3-1-0.8mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	May 31 2021	hs	nn	array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample		ppgflg	y		
ACQUISITION		hsclvl	6024	1	phase
sw	7102.3	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2130	gain	46		
fb	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	16	gfs	not used		
2D ACQUISITION		fn	4096		
sw1	25165.1	F1 PROCESSING			
ni	228	gfl	0.005		
phase	arrayed	gfs1	not used		
PRESATURATION		procl	lp		
satmode	n	fnl	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	-43.5		
tn	H1	wp	4116.4		
sfrq	500.478	sp1	-421.0		
tof	506.9	wp1	16416.3		
tpwr	58	rfl	539.4		
pw	8.100	rfp	0		
DECOUPLER		rfl1	1256.5		
dm	Cl3	rfpl	0		
dof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pwxlvl	56	vs	116		
pw	10.500	th	3		
HSQC		ai	cdc	ph	
j1kh	146.0				
nullflg	y				
mult	2				
ADDITIONAL					
pwxl80ad	ONE ad300				
pwxl80adr	ONE ad300	or			
pwxl80	465.4				
pwxlvl80	51				
pwxl80ref	ONE ref2-				
	00				
pwxl80r	2000.2				
pwxlvl80r	43				



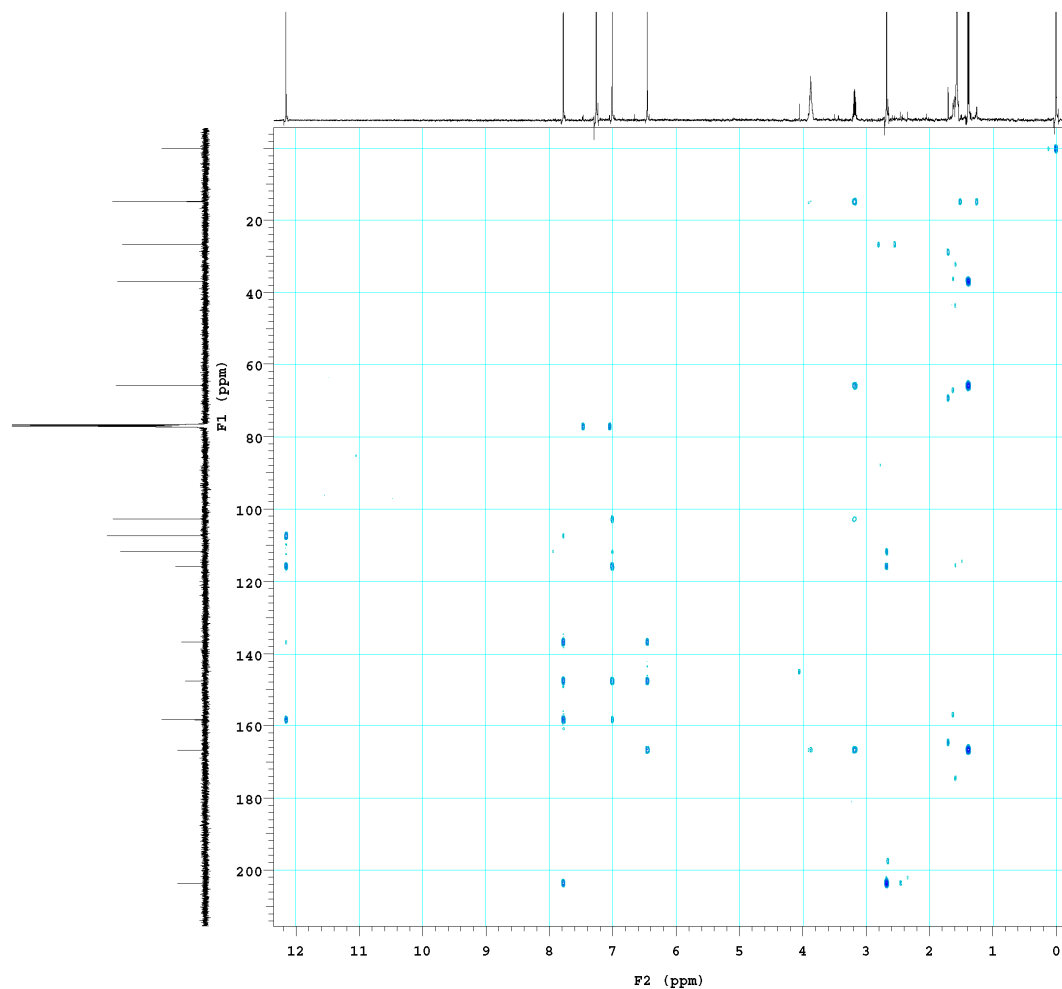


**Figure S56.** HMBC spectrum of **25** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-5-3-1-0.8mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	May 31 2021	hs	nm	array	phase
solvent	cdcl3	spul	y	arraydim	256
sample		ppgfig			
ACQUISITION	hagivl	6024	i	phase	
sw	7102.3	SPECIAL	1	1	
at	0.150	temp	not used	2	2
np	2130	gain	46		
fn	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlvi1	409		
nt	64	gt1	0.001000		
2D ACQUISITION	gzlvi3	1227			
sw1	30200.1	gt3	0.001000		
ni	128	gstab	0.000500		
phase	arrayed	P2 PROCESSING			
PRESSATURATION	sb	-0.075			
satmode	n	sbs	not used		
wet	n	fn	4096		
TRANSMITTER		P1 PROCESSING			
tn	H1	gt1	0.004		
sfrq	500.478	gtf1	not used		
tof	506.9	procl	1p		
tpwr	58	fn1	2048		
pw	8.100	DISPLAY			
DECOUPLER	sp	-106.0			
dm	C13	wp	6287.3		
dof	1287.0	sp1	-706.7		
dm	nm	wp1	27811.2		
decwave	W40 HCN5mm	rfl	539.4		
dmf	32258	rfl	0		
dpwr	38	rfl1	1886.4		
pwrlv1	56	rfl1	0		
pw	10.500	PLOT			
HMBC	wd	206.0			
j1kh	146.0	sc	0		
j1xh	8.0	wd2	206.0		
ADIABATIC	sc2	0			
pwrl80ad ONE_ad300	vs	116			
pwrlv1180	51	th	3		
pwrl80	465.4	ai	cdc av		

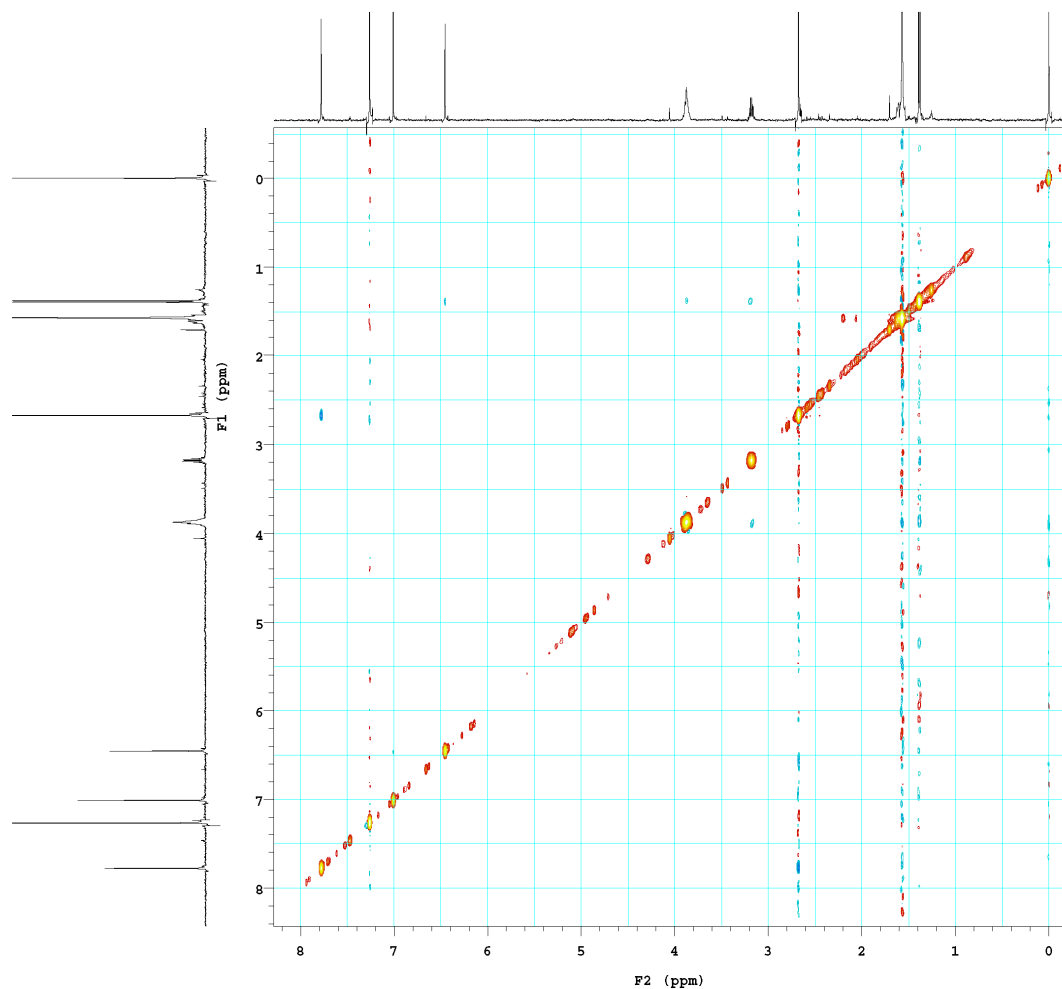


**Figure S57.** NOESY spectrum of **25** (measured in CDCl<sub>3</sub>, 500 MHz).

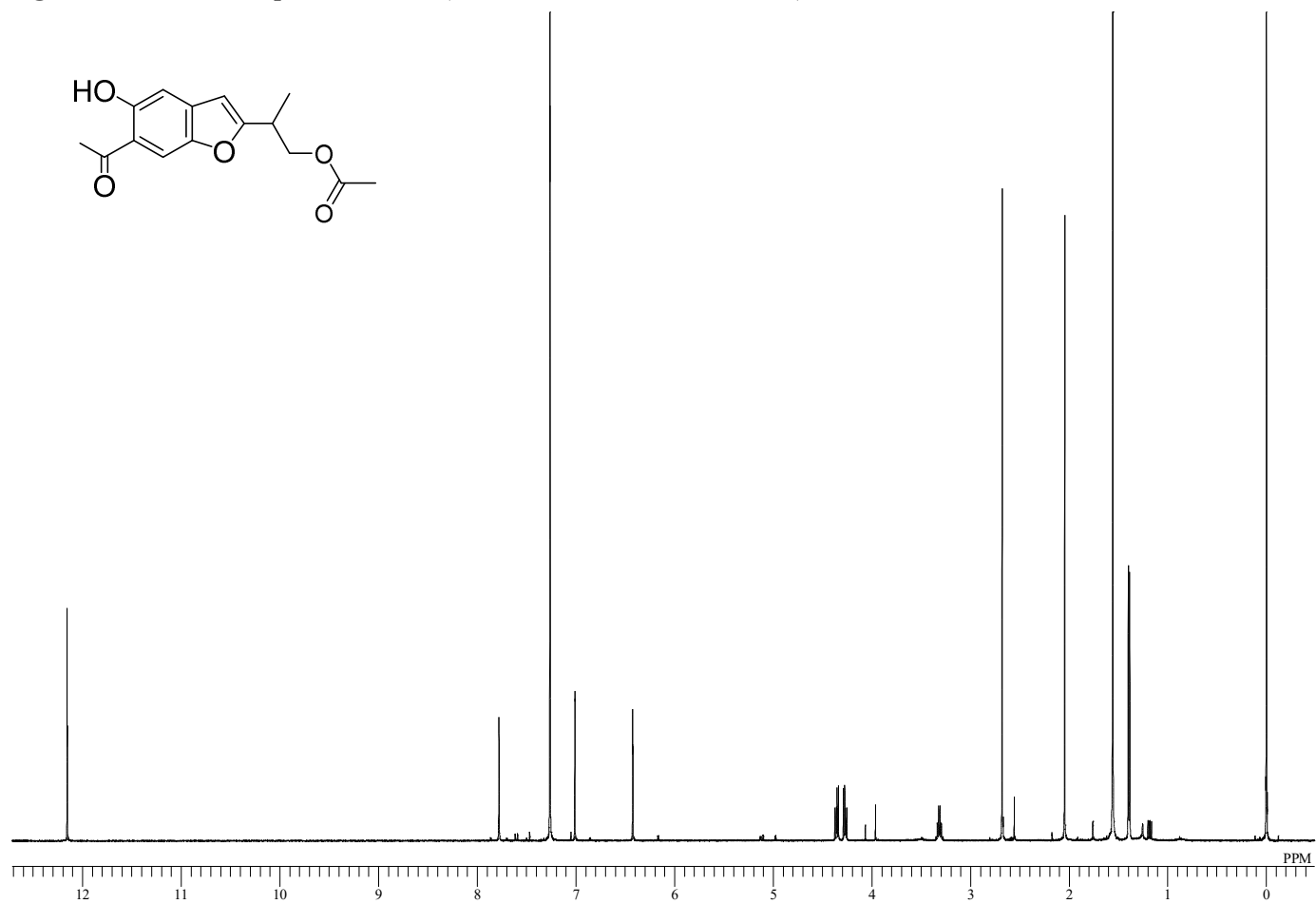
HYM-2014-48-R-6-5-3-1-0.8mg-NOESY-CDCl3

exp7 NOESY

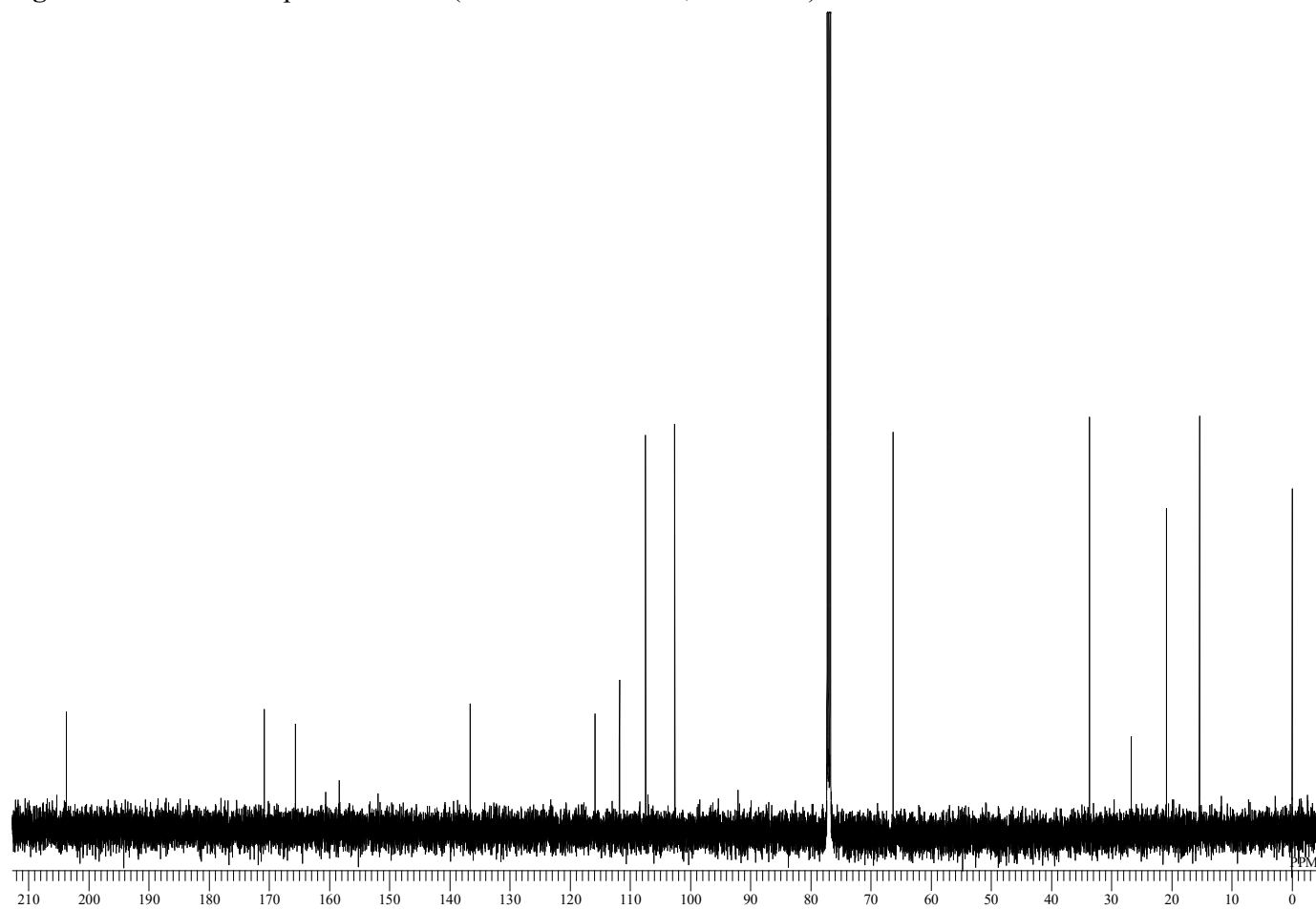
SAMPLE		FLAGS	
date	May 31 2021	hs	nn
solvent	cdcl3	espul	y
sample		ppgfig	y
acq	7102.3	hagivl	6024
sw	7102.3	SPECIAL	
at	0.150	temp	not used
np	2130	gain	46
fn	4000	spin	0
ss	32	P2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION		fn	4096
sw1	7102.3	P1 PROCESSING	
ni	128	gf1	0.017
TRANSMITTER		gfs1	not used
tn	H1	proc1	lp
sfrq	500.478	fn1	4096
tof	506.9	DISPLAY	
tpwr	58	sp	-112.9
pw	8.100	wp	4258.6
NOESY		sp1	-286.3
mixN	0.500	wp1	4501.3
PRESATURATION		rf1	539.4
satmode	n	rfp	0
wet	n	rf11	539.4
DECOUPLER		rfp1	0
dn	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	116
		th	1
		ai	ph



**Figure S58.**  $^1\text{H}$  NMR spectrum of **26** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S59.**  $^{13}\text{C}$  NMR spectrum of **26** (measured in  $\text{CDCl}_3$ , 126 MHz).

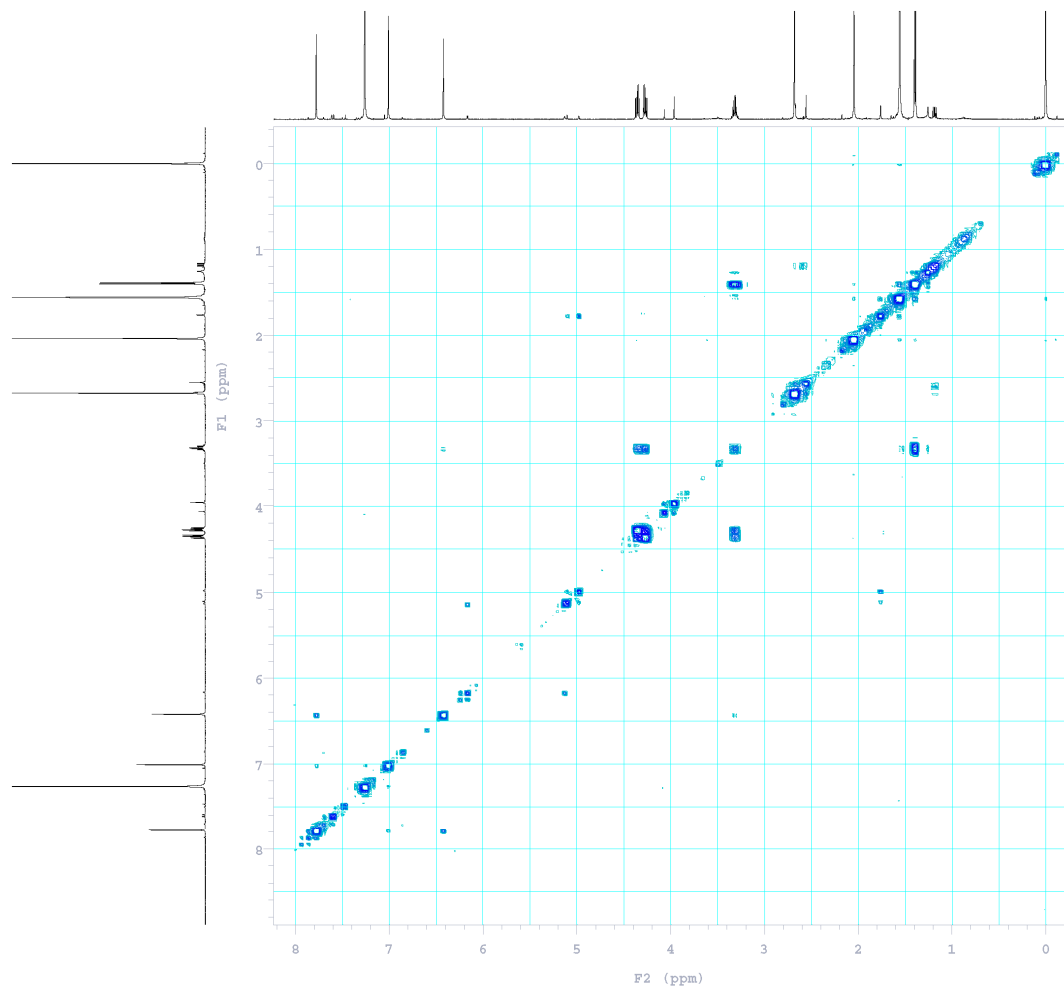


**Figure S60.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **26** (measured in  $\text{CDCl}_3$ , 500 MHz).

HVM-2014-48-R-4-2-4-3-0.8mg-COSY-CDCl3

exp4 gCOSY

SAMPLE		FLAGS	
date	Oct 27 2020	hs	nm
solvent	cdcl3	sspul	y
sample	hs91v1		6180
ACQUISITION		SPECIAL	
sw	6720.4	temp	not used
at	0.150	gain	50
np	2016	spin	0
fb	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	16	fn	2048
2D ACQUISITION		F1 PROCESSING	
sw1	6720.4	sb1	-0.019
ni	128	sbs1	not used
d2	0	procl	1p
PRESATURATION		fml	
satmode	n	fnl	2048
TRANSMITTER		DISPLAY	
wet	n	sp	-126.3
tn	H1	wp	4246.2
sfrq	500.478	wp1	4659.7
tor	513.0	rf1	342.9
tpwr	58	rfp	0
pw	8.000	rf11	342.9
GRADIENTS		rfp1	
g1v1e	5154		0
gtE	0.001000	wc	206.0
EDratio	1.000	sc	0
gstab	0.000500	wc2	206.0
DECOUPLER		sc2	
dn	C13	vs	61
dm	nmn	th	6
	ai	odc	av

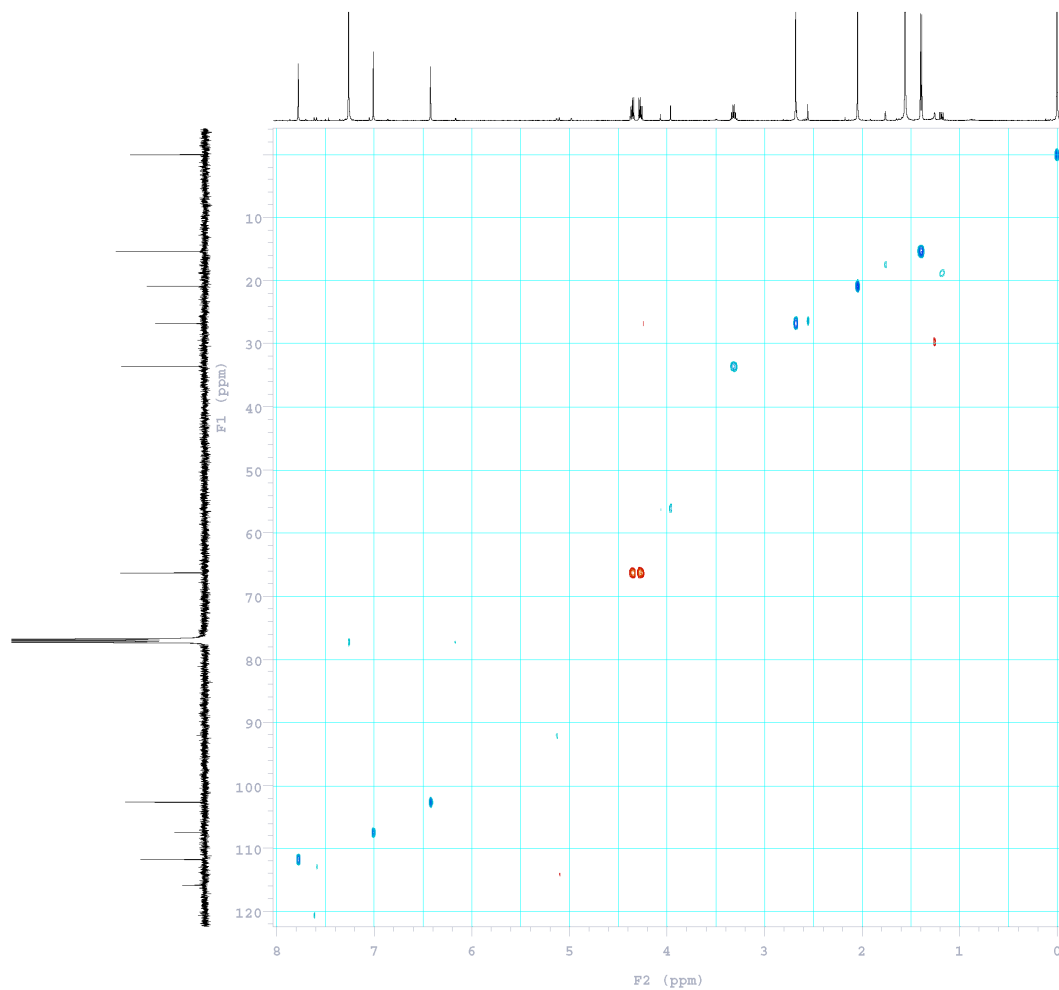


**Figure S61.** HSQC spectrum of **26** (measured in CDCl<sub>3</sub>, 500 MHz).

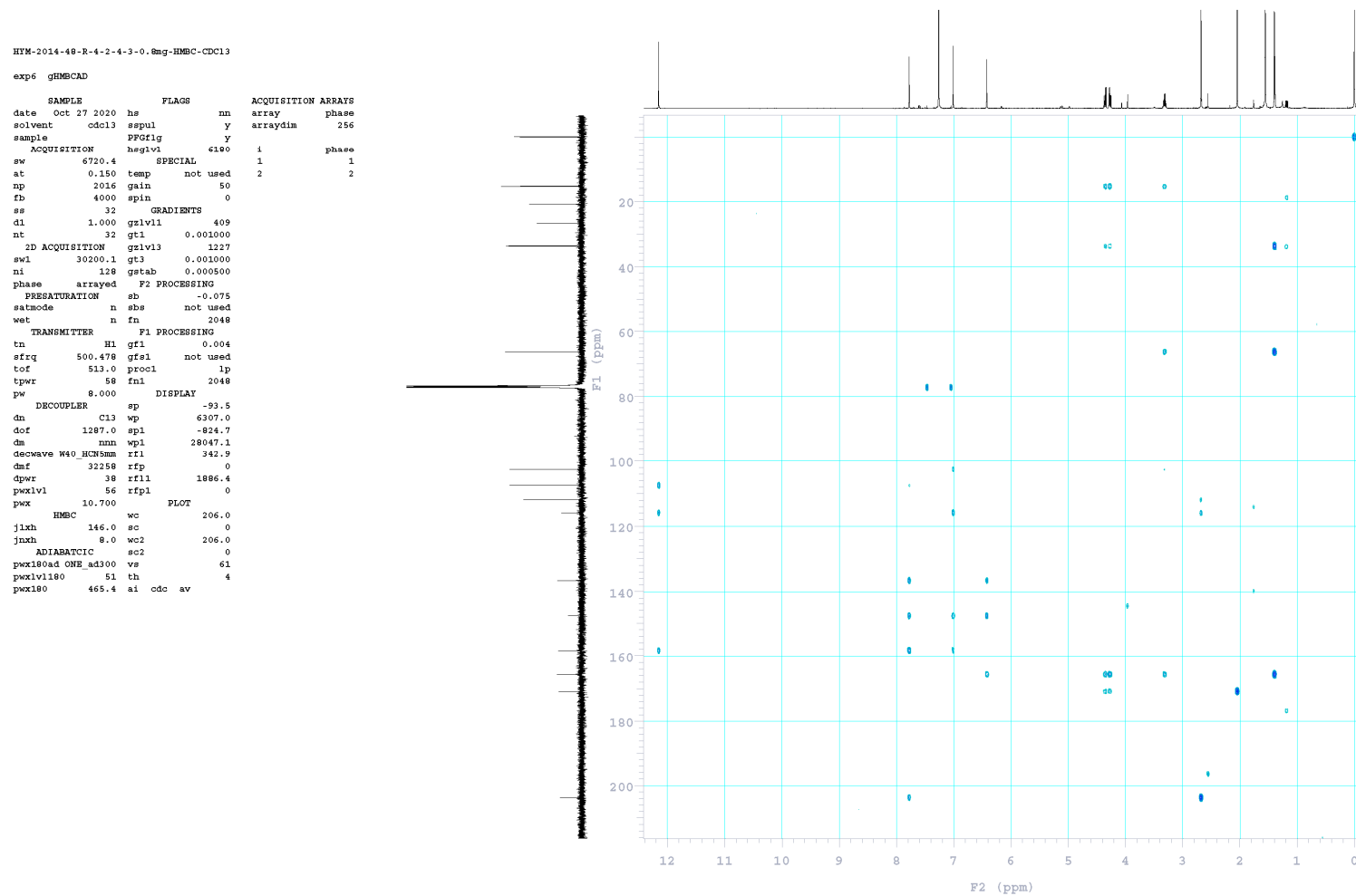
HTM-2014-48-R-4-2-4-3-0.8mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Oct 27 2020	hs	nn	array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample		PPGflg	y		
ACQUISITION		hsgivl	6180	1	phase
sw	6720.4	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2016	gain	50		
fb	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	16	gfs	not used		
2D ACQUISITION		fn	2048		
sw1	25165.1	F1 PROCESSING			
ni	128	gf1	0.005		
phase	arrayed	gfsl	not used		
PRESATURATION		procl	1p		
satmode	n	fn1	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	-60.7		
tn	H1	wp	4082.1		
sfrq	500.478	sp1	-519.3		
tof	513.0	vp1	15924.8		
tpwr	58	rfl	342.9		
pw	8.000	rfp	0		
DECOUPLER		rfl1	1256.5		
dn	Cl3	rfp1	0		
dof	-600.6	PLOT			
dm	rny	wc	206.0		
decwave	W40_MCHSum	vc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pw1v1	56	vs	61		
pw1	10.700	th	4		
HSQC		ai	cdc ph		
j1xh	146.0				
nullflg	y				
mult	2				
ADIABATIC					
pw180ad	ONE_ad300				
pw180adr	ONE_ad30-				
	OR				
pw180	465.4				
pw1v180	51				
pw180ref	ONE_ref2-				
	00				
pw180r	2000.2				
pw1v180r	43				



**Figure S62.** HMBC spectrum of **26** (measured in CDCl<sub>3</sub>, 500 MHz).

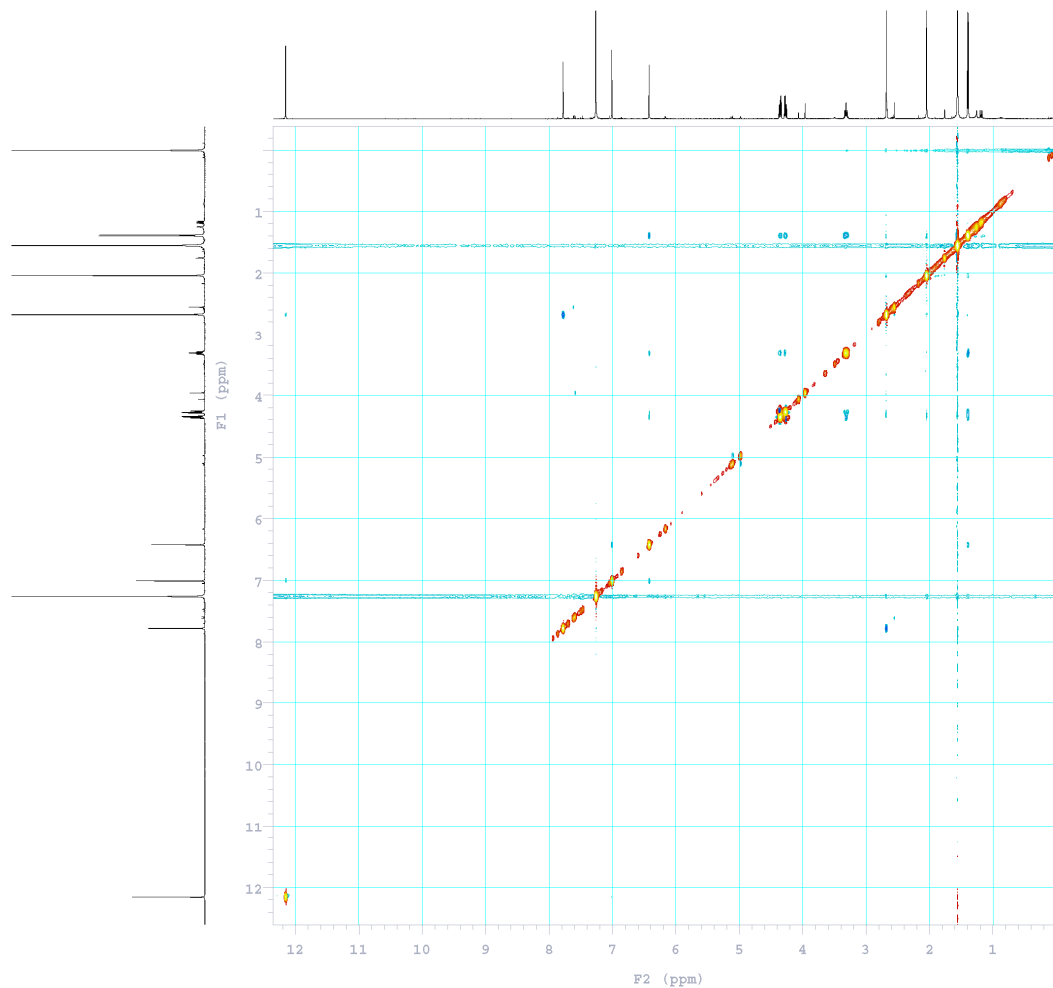


**Figure S63.** NOESY spectrum of **26** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-4-2-4-3-0.8ag-NOEST-CDCl3

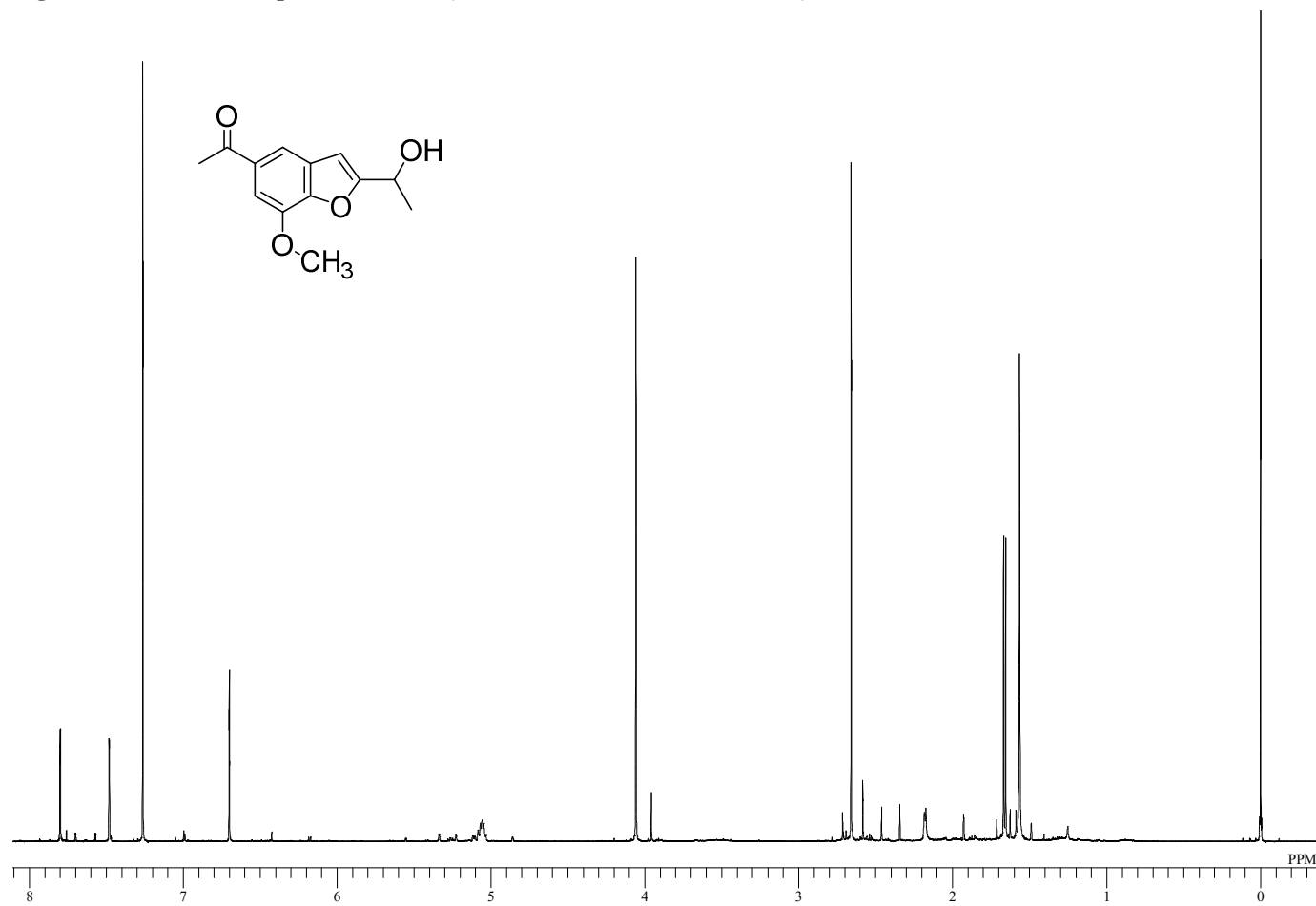
exp7 NOESY

SAMPLE		FLAGS	
date	Oct 27 2020	hs	nm
solvent	cdcl3	sspul	y
sample		PFGLg	y
ACQUISITION		hsq1v1	6180
sw	6720.4	SPECIAL	
at	0.150	temp	not used
np	2016	gain	50
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION		fn	2048
sw1	6720.4	F1 PROCESSING	
ni	128	gf1	0.018
TRANSMITTER		gf1	not used
tn	H1	proc1	lp
sfrq	500.478	fn1	2048
tof	513.0	DISPLAY	
tpwr	58	sp	-100.1
pw	8.000	wp	6280.7
NOESY		sp1	-192.0
mixN	0.500	vp1	6497.3
PRESATURATION		rf1	342.9
satmode	n	rpf	0
wet	n	rf11	342.9
DECOUPLER		rfp1	0
dn	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	22
		th	1
		ai	ph

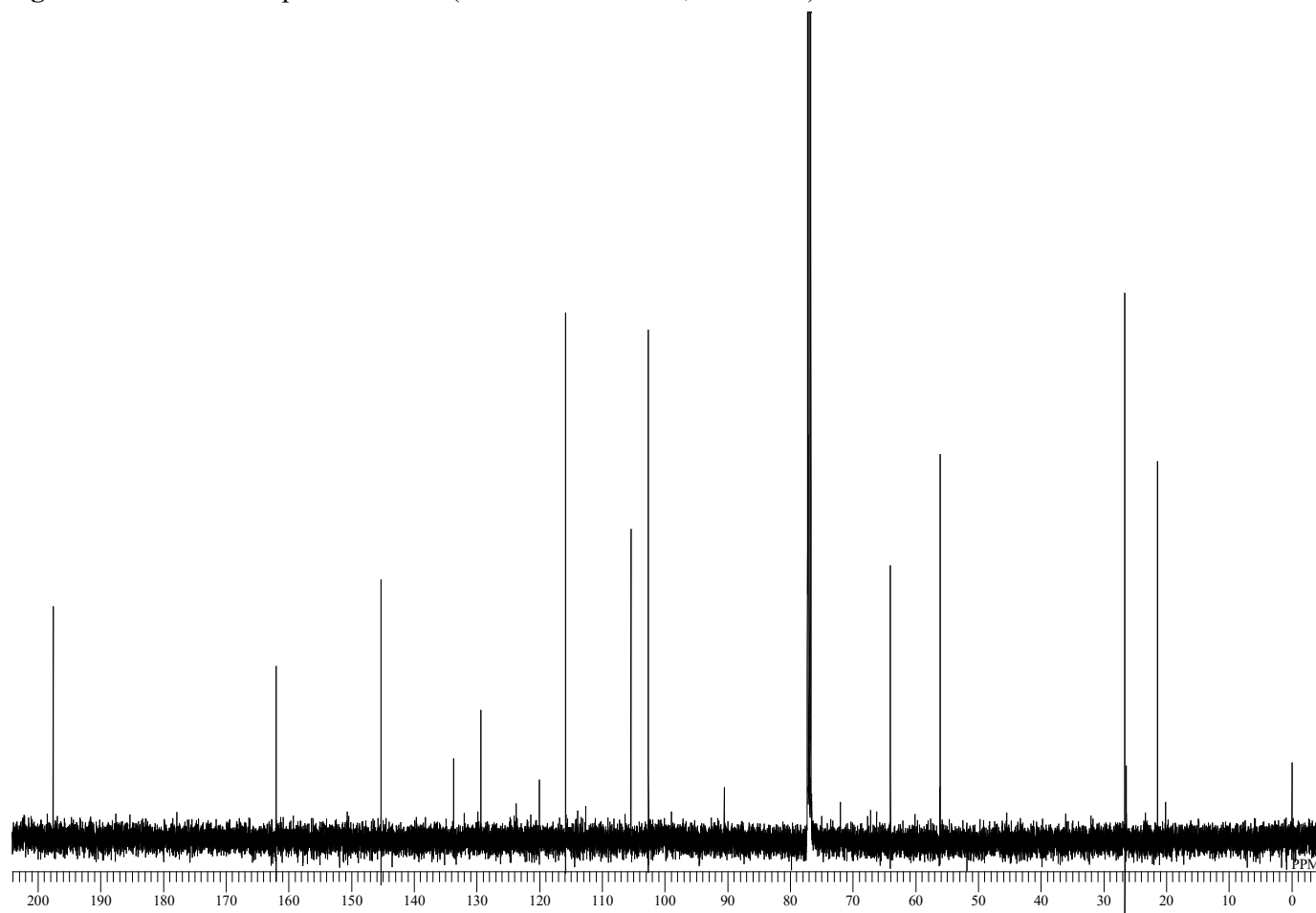




**Figure S64.**  $^1\text{H}$  NMR spectrum of **31** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S65.**  $^{13}\text{C}$  NMR spectrum of **31** (measured in  $\text{CDCl}_3$ , 126 MHz).

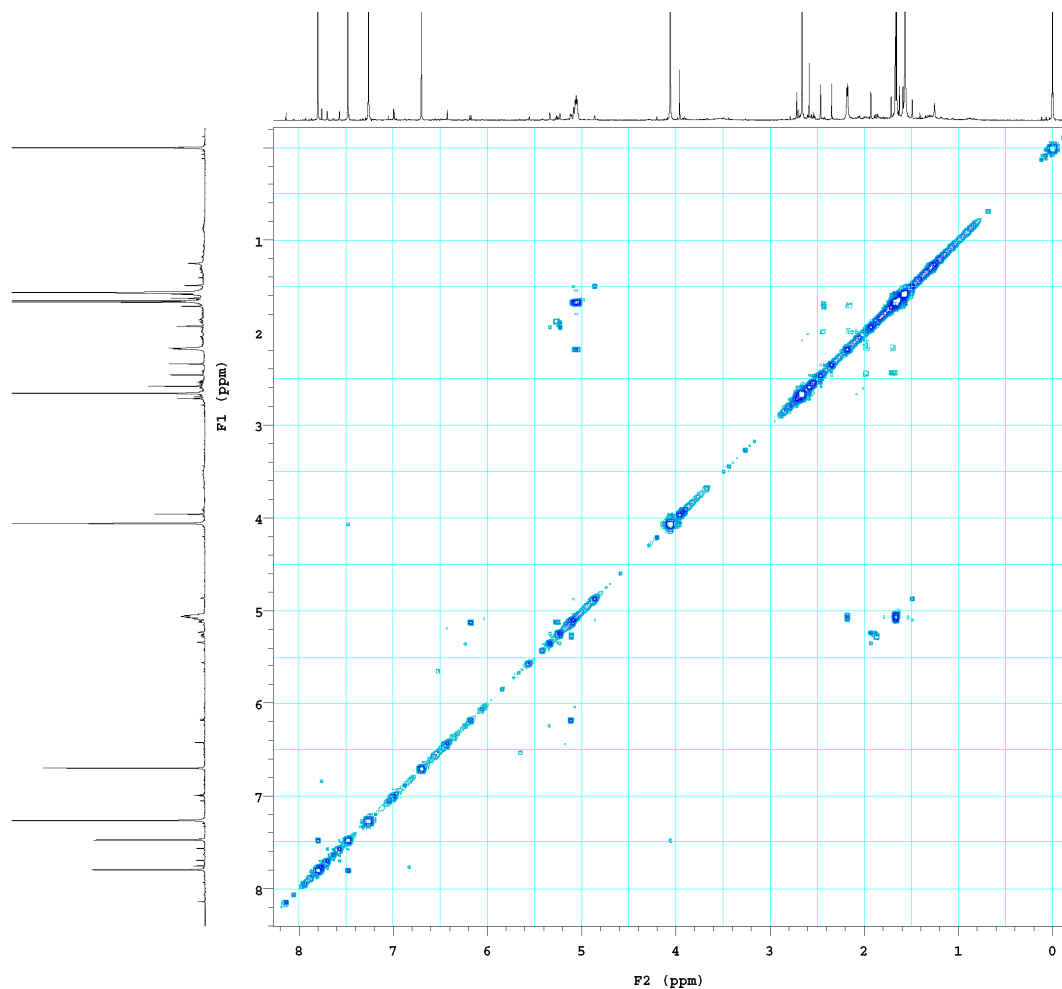


**Figure S66.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **31** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-6-6-3-1.4mg-COSY- $\text{CDCl}_3$

exp4 gCOSY

SAMPLE		FLAGS	
date	Nov 22 2020	hs	nn
solvent	$\text{cdcl}_3$	espul	y
sample		hsqvl	6180
ACQUISITION		REPROTAT.	
sw	4734.8	temp	not used
at	0.150	gain	48
np	1420	spin	0
fn	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	16	fn	2048
2D ACQUISITION		F1 PROCESSING	
sw1	4734.8	sb1	-0.027
ni	128	sbs1	not used
d2	0	procl	lp
PRESATURATION		fn1	
satmode	n	2048	
wet	n	sp	-87.2
TRANSMITTER		wp	
tn	H1	sp1	-105.7
sfrq	500.477	wp1	4309.5
tof	-483.0	rf1	346.1
tpwr	58	rfp	0
pw	8.000	rf11	346.1
GRADIENTS		rfp1	
gslvie	5154	PLOT	
gtb	0.001000	wc	206.0
EDratio	1.000	sc	0
gstab	0.000500	wc2	206.0
DECOUPLER		sc2	
dn	$\text{Cl}_3$	vs	126
dm	nnn	th	6
	ai	cdc	av

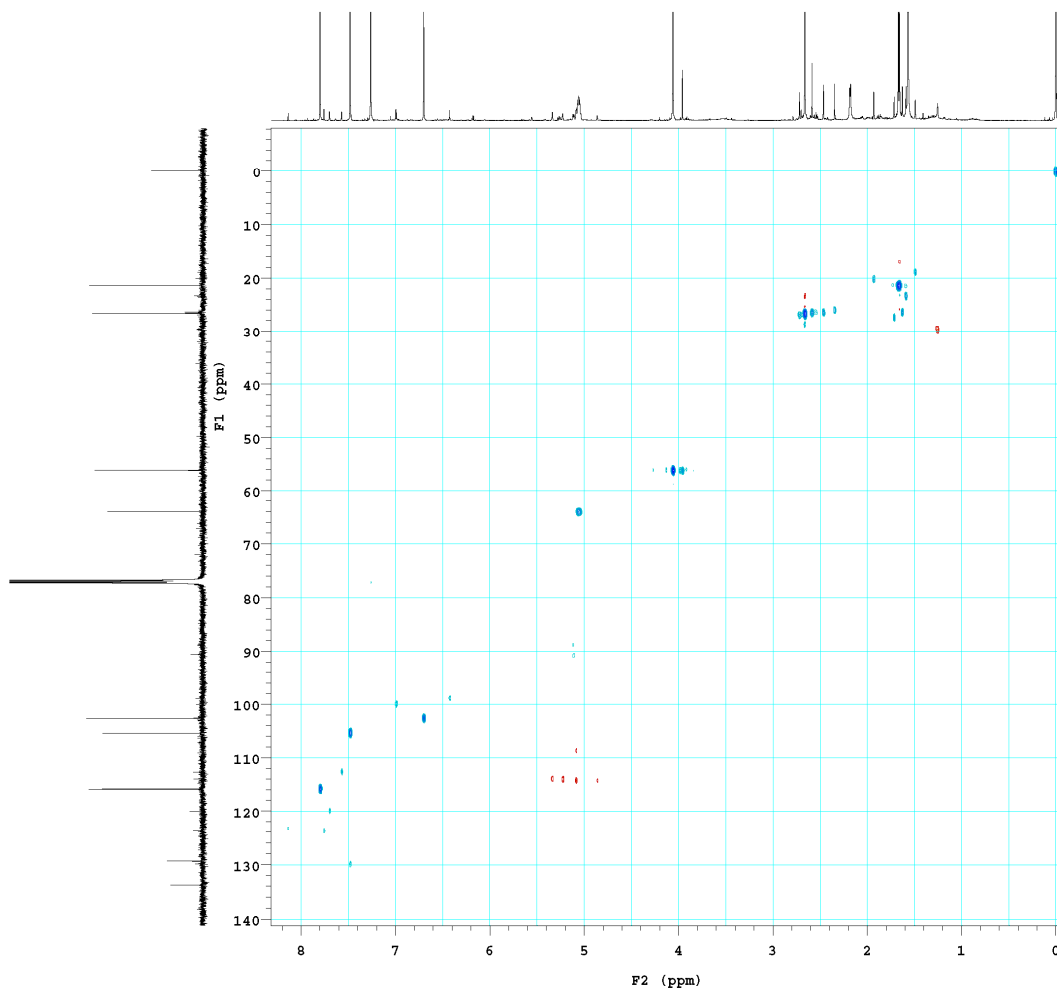


**Figure S67.** HSQC spectrum of **31** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-6-3-1.4mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Nov 22 2020	hs		nm	array
solvent	cdcl3	sspul	y	arraydim	256
sample		PFGrig	y		
ACQUISITION	hsqivl		6180	1	phase
sw	4734.8	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	1450	gain	48		
fd	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	32	gfs	not used		
2D ACQUISITION	fn		2048		
sw1	25165.1	F1 PROCESSING			
ni	128	gf1	0.005		
phase	arrayed	gfs1	not used		
PRESSATURATION	procl	lp			
satmode	n	fn1	2048		
wet	n	DISPLAY			
TRANSMITTER	sp		-59.4		
tn	H1	wp	4221.6		
sfrq	500.477	sp1	-1010.8		
tof	-483.0	wp1	18775.6		
tpwr	58	rfl	346.1		
pw	8.000	rfp	0		
DECOUPLER	rfl1		1256.5		
dm	C13	rflp1	0		
dof	-600.6	PLOT			
dm	nny	wc	206.0		
deuwave	W40	sc	0		
dmf	32258	wc2	206.0		
dpr	38	sc2	0		
pwivl	56	vs	126		
pwk	10.700	th	3		
HSQC	ai	cdc	ph		
j1xh	146.0				
nullflg	y				
mult	2				
ADABATIC					
pw180ad	ONE	ad300			
pw180adr	ONE	ad300			
OR					
pw180	465.4				
pw1v1180	51				
pw180ref	ONE	ref2			
OR					
pw180r	2000.2				
pw1v1180r	43				

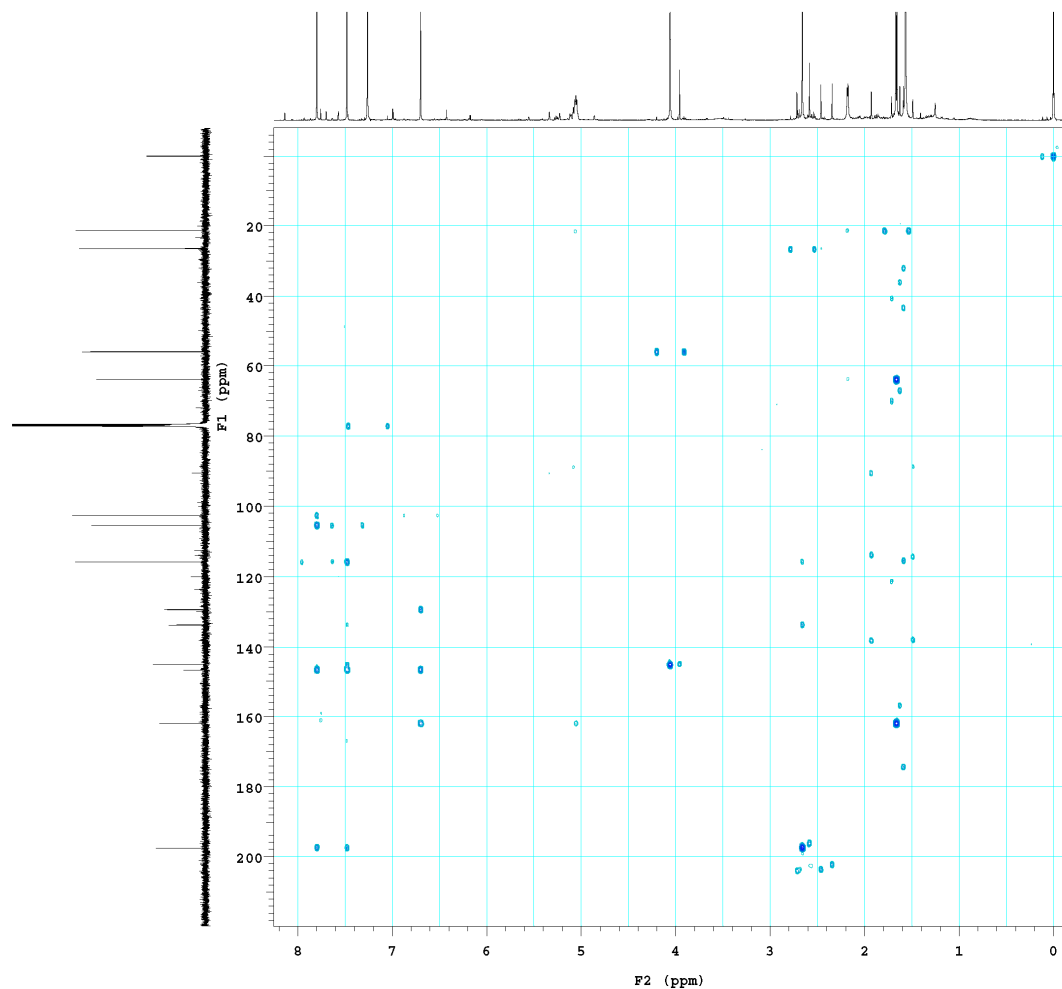


**Figure S68.** HMBC spectrum of **31** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-6-3-1.4mg-HMBC-CDCl<sub>3</sub>

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Nov 22 2020	hs	nn	array	phase
solvent	cdcl3	ssul	y	arraydim	256
sample		ppdfig	y		
acq	4734.8	hagivl	6180	i	phase
sw	4734.8	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	1420	gain	48		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlvi1	409		
nt	32	gt1	0.001000		
2D ACQUISITION		gzlvi3	1227		
sw1	30200.1	gt3	0.001000		
ni	128	gstab	0.000500		
phase	arrayed	P2 PROCESSING			
PRESATURATION	sb	-0.075			
satmode	n	sbs	not used		
wet	n	fn	2048		
TRANSMITTER		F1 PROCESSING			
tn	H1	gf1	0.004		
sfrq	500.477	gfs1	not used		
tof	-483.0	procl	lp		
tpwr	58	fn1	2048		
pw	8.000	DISPLAY			
DECOUPLER		sp	-87.2		
dm	C13	wp	4217.0		
dof	1287.0	sp1	-1001.6		
dm	nmn	wp1	28637.0		
decwave	W40	HCN5mm	rfl	346.1	
dmf	32258	rfl	0		
dpwr	38	rfl1	1886.4		
pwrlvl	56	rfl1	0		
pw	10.700	PLOT			
HMBC		wd	206.0		
j1kh	146.0	sc	0		
j1xh	8.0	wd2	206.0		
ADIABATIC		sc2	0		
pwrlvl180ad	ONE	ad300	vs	126	
pwrlvl180	51	th	3		
pwrlvl80	465.4	ai	cdc	av	

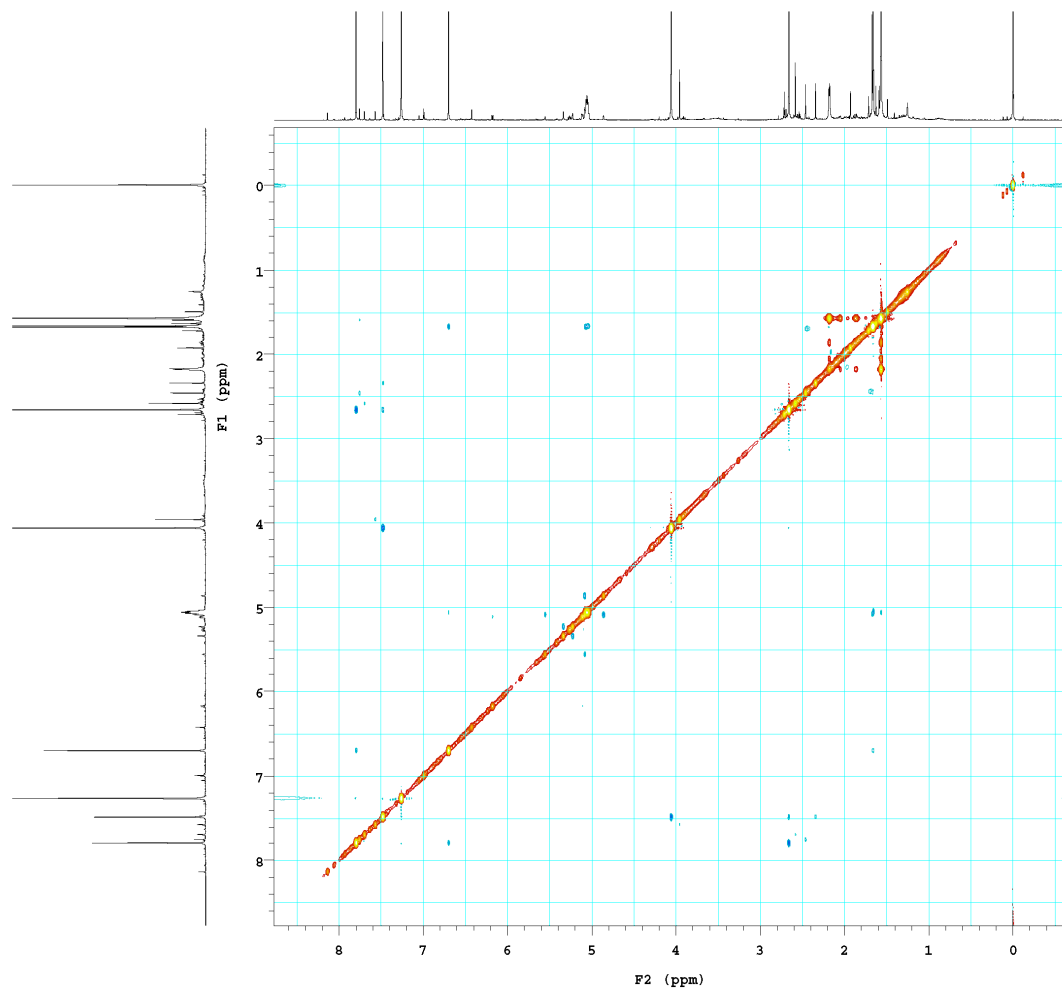


**Figure S69.** NOESY spectrum of **31** (measured in CDCl<sub>3</sub>, 500 MHz).

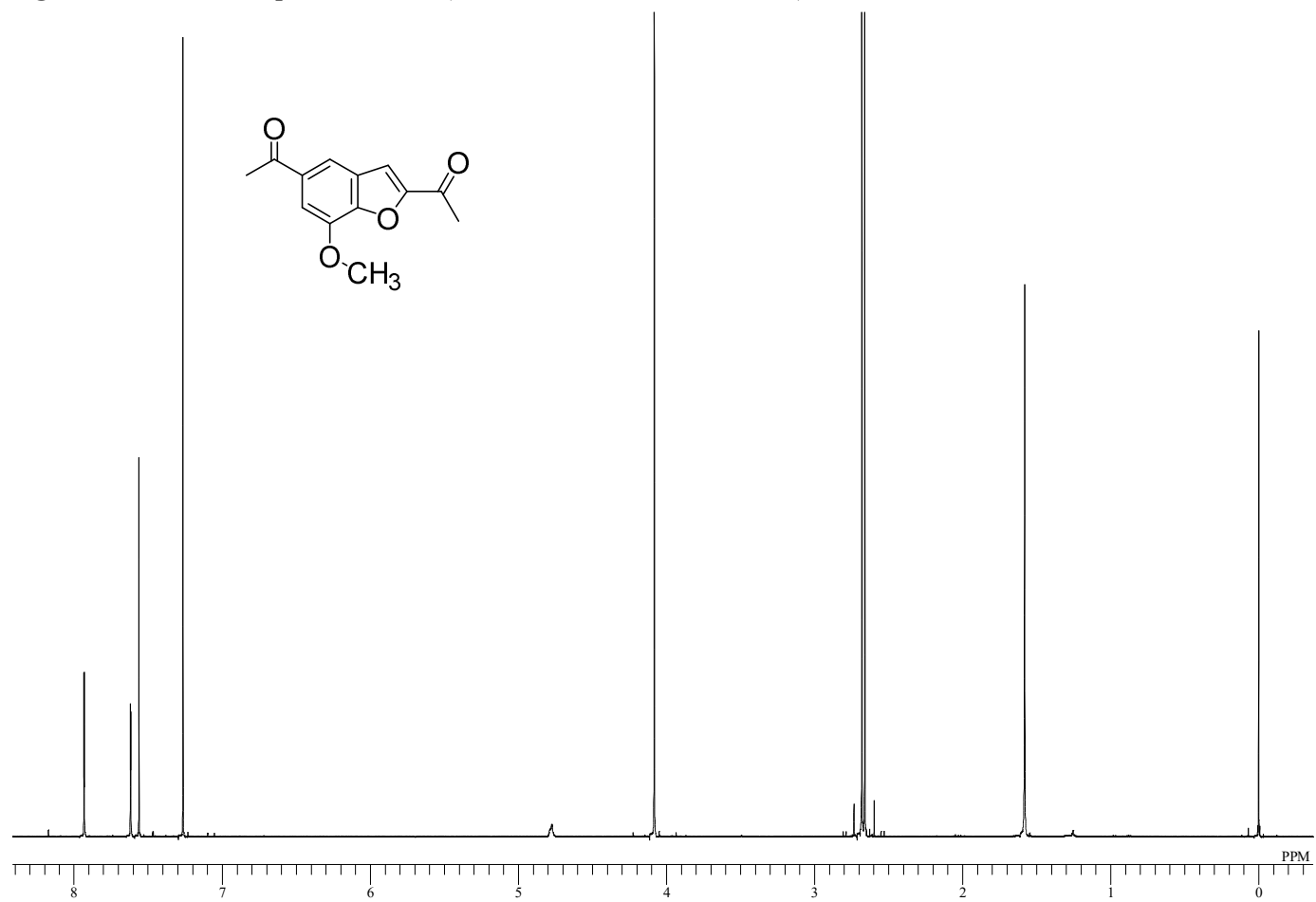
HYM-2014-48-R-6-6-3-1.4mg-NOESY-CDCl3

exp7 NOESY

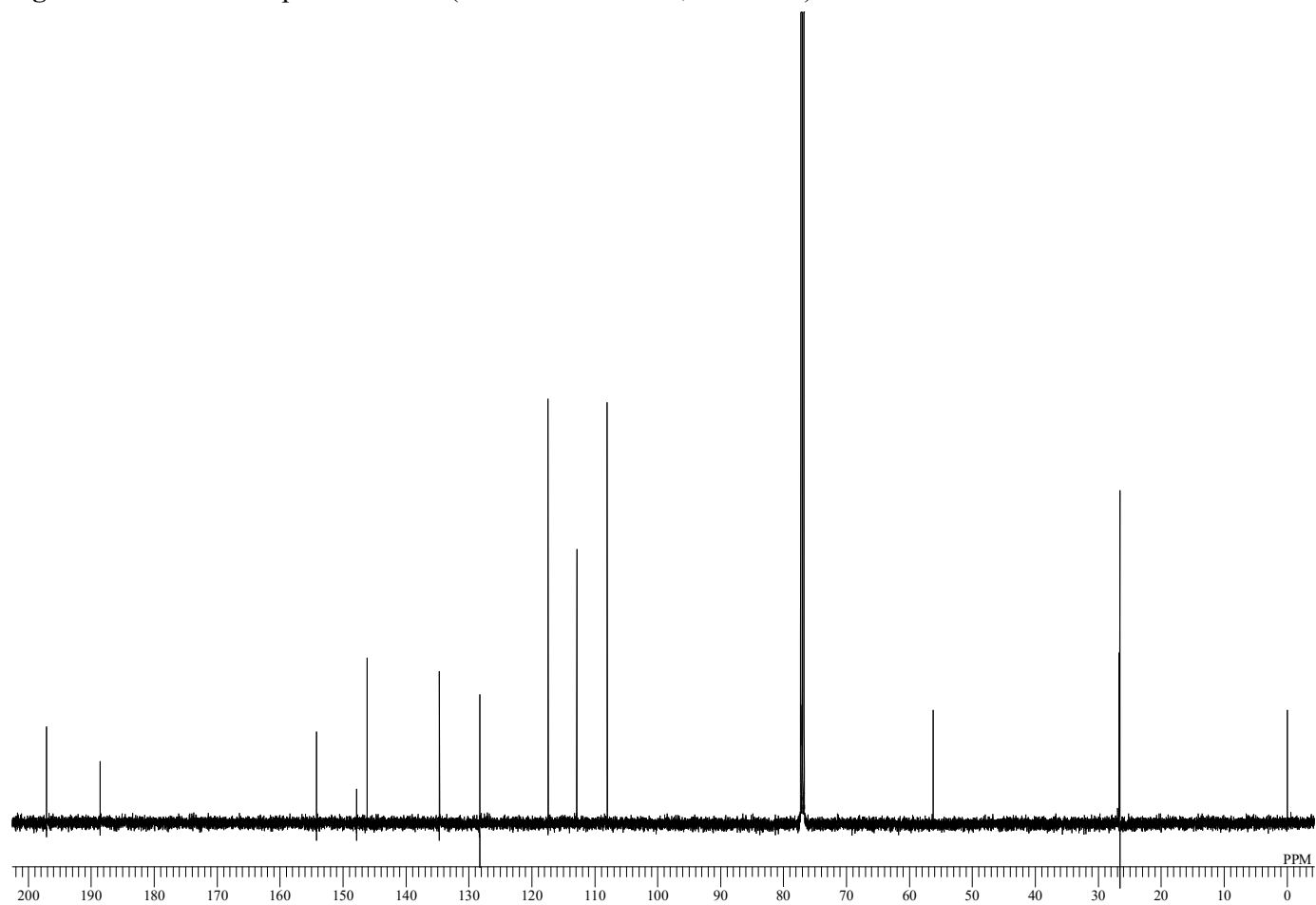
SAMPLE		FLAGS	
date	Nov 22 2020	hs	nn
solvent	cdcl3	sspul	y
sample		PFGflg	y
ACQUISITION	hsclv1		6180
sw	4734.8	SPECIAL	
at	0.150	temp	not used
np	1420	gain	48
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION	fn		2048
sw1	4734.8	F1 PROCESSING	
ni	128	gfl	0.025
TRANSMITTER	gfs1		not used
tn	H1	procl	lp
sfrq	500.477	fn1	2048
tof	-483.0	DISPLAY	
tpwr	58	sp	-341.5
pw	8.000	wp	4730.2
NOESY	sp1		-341.5
mixN	0.500	vp1	4730.2
PRESATURATION	rf1		346.1
satmode	n	rpf	0
wet	n	rf11	346.1
DECOUPLER	rfpl		0
dm	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	126
		th	1
	ai	ph	



**Figure S70.**  $^1\text{H}$  NMR spectrum of **32** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S71.**  $^{13}\text{C}$  NMR spectrum of **32** (measured in  $\text{CDCl}_3$ , 126 MHz).



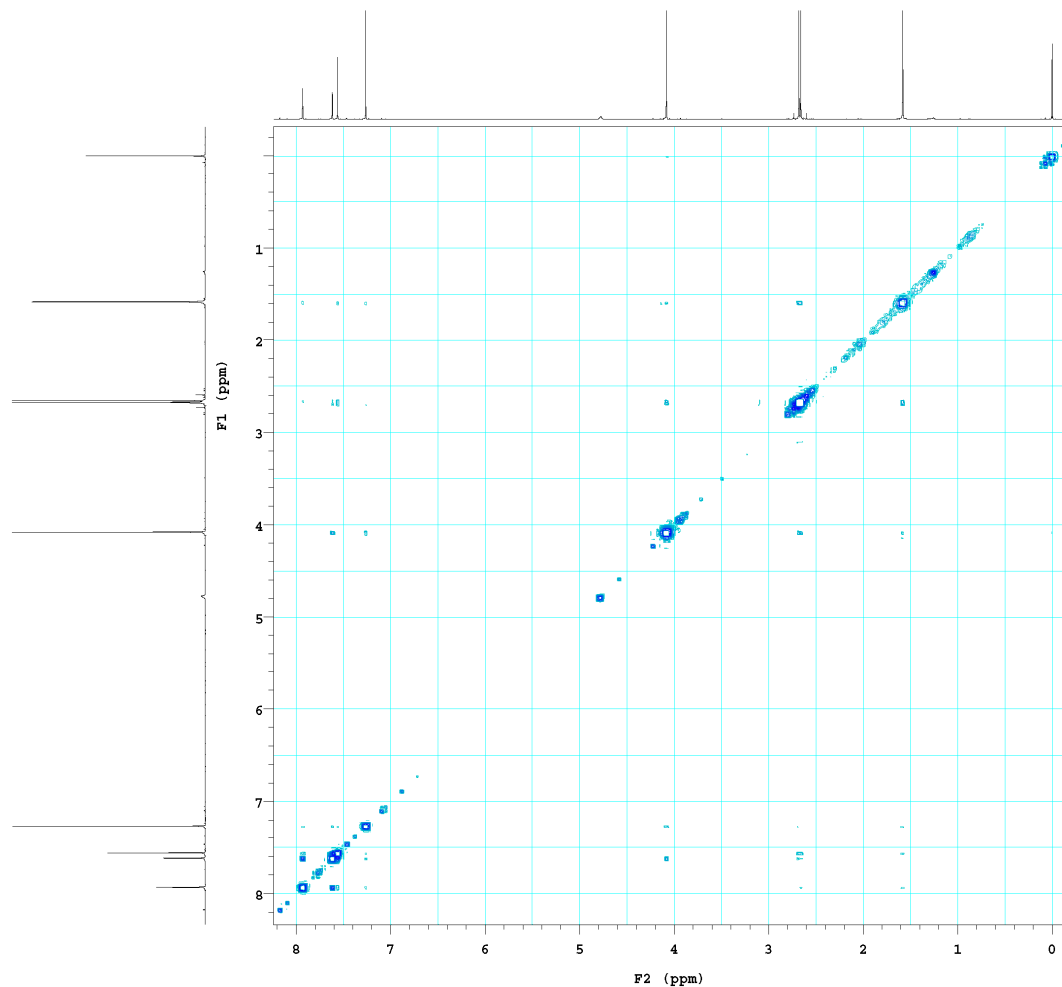


**Figure S72.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **32** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-6-4-1-2-2.2mg-COSY-CDCl3

exp4 gCOSY

SAMPLE		FLAGS		nn
date	Jun 6 2021	hs		y
solvent	cdcl3	sspul		
sample	hsgl1			6024
ACQUISITION		SPECIAL		
sw	4960.3	temp	not used	
at	0.150	gain	46	
np	1488	spin	0	
fb	4000	F2 PROCESSING		
ss	32	sb	-0.075	
d1	1.000	sbs	not used	
nt	4	fn	2048	
2D ACQUISITION		F1 PROCESSING		
sw1	4960.3	sb1	-0.026	
n1	128	sb1	not used	
d2	0	procl	1p	
PRESATURATION		fml		2048
satmode	n	DISPLAY		
wet	n	sp	-92.3	
TRANSMITTER		vp		4214.3
tn	H1	sp1	-155.3	
sfrq	500.477	wp1	4325.7	
tof	-534.0	rf1	508.9	
tpwr	58	rpf	0	
pw	8.100	rf11	508.9	
GRADIENTS		rfp1		0
gplv1e	5025	PLOT		
gte	0.001000	wc	206.0	
EDratio	1.000	sc	0	
gatab	0.000500	wc2	206.0	
DECOUPLER		sc2		0
dm	C13	vs	63	
dm	nm	th	7	
	ai	cdc	av	

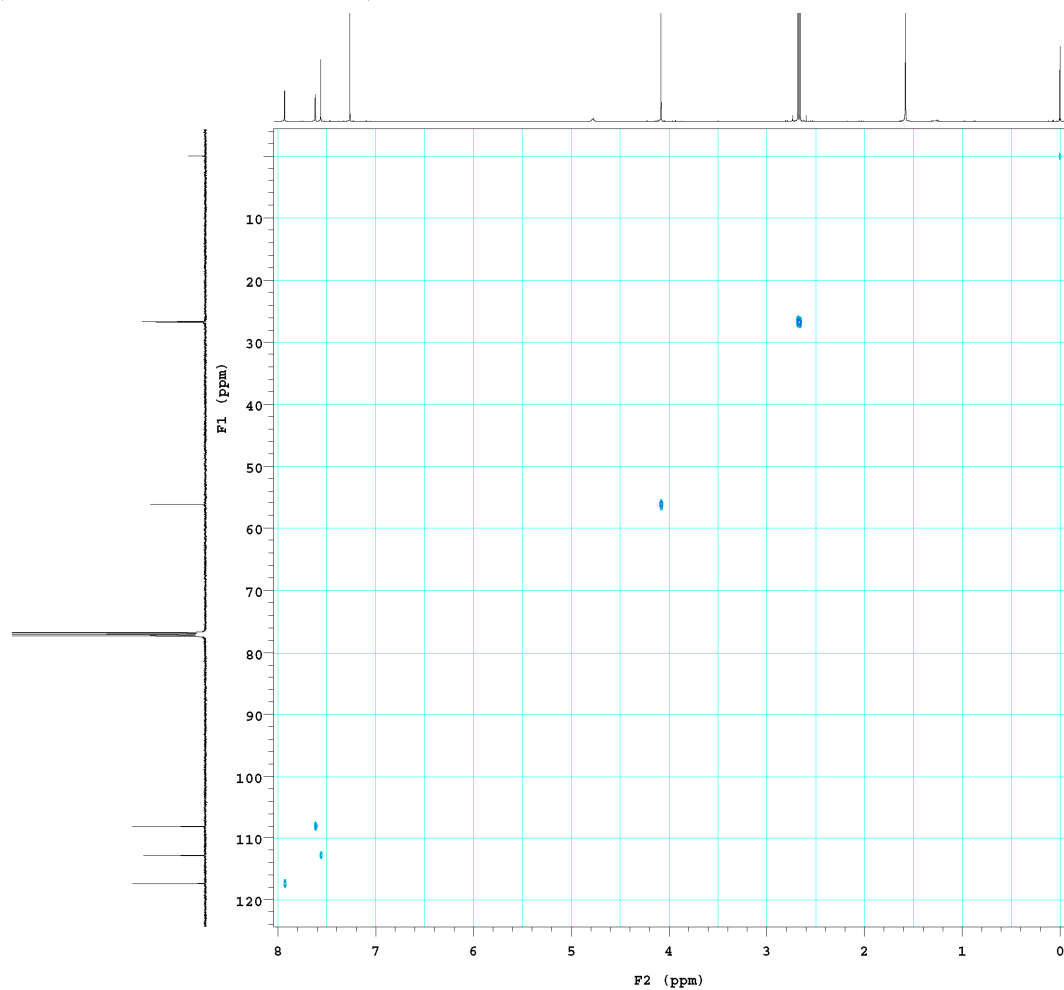


**Figure S73.** HSQC spectrum of **32** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-4-1-2-2.2mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Jun 6 2021	hs	nm	array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample		PFGflg	y		
ACQUISITION		hsglvl	6024	i	phase
sw	4960.3	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	1488	gain	46		
fb	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	8	gfs	not used		
2D ACQUISITION		fn	2048		
sw1	25165.1	F1 PROCESSING			
ni	128	gf1	0.005		
phase	arrayed	gf1	not used		
PRESATURATION		procl	1p		
satmode	n	fn1	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	-48.7		
tn	H1	wp	4073.9		
sfrq	500.477	spl	-543.9		
torf	-534.0	wpl	16195.1		
tpwr	58	rfl	508.9		
pw	8.100	rfp	0		
DECOUPLER		rfl1	1256.5		
dn	C13	rfl1	0		
dof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pxl1vl	56	vs	63		
pxx	10.500	th	2		
HSQC		ai	cdc	ph	2
j1xh	146.0				
multifig	y				
mult	2				
ADIABATIC					
pxl180ad	ONE_a3300				
pxl180adR	ONE_a330-				
	OR				
pxl180	465.4				
pxl1vl180	51				
pxl180ref	ONE_ref2-				
	00				
pxl180r	2000.2				
pxl1vl180r	43				

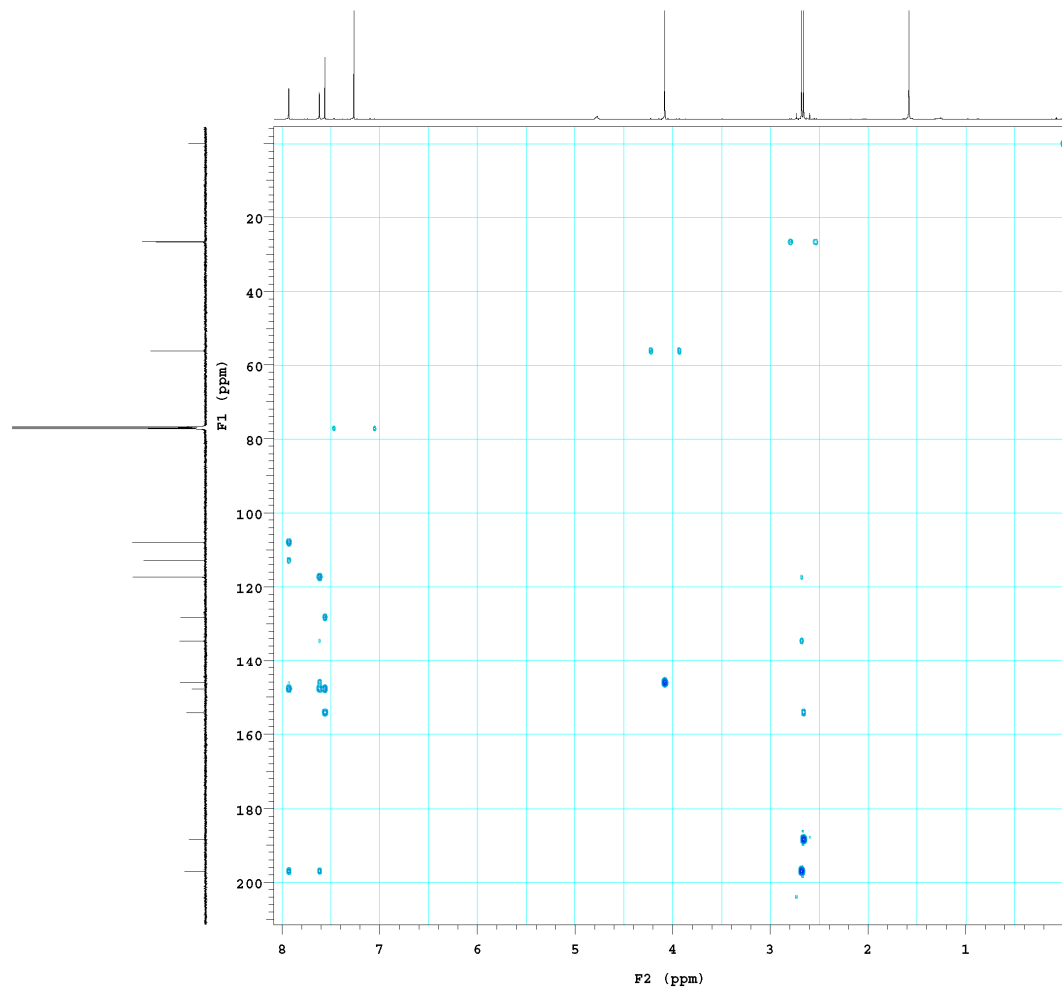


**Figure S74.** HMBC spectrum of **32** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-6-4-1-2-2.2mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Jun 6 2021	hs	nn	array	phase
solvent	cdcl3	spul	y	arraydim	256
sample		PPGflg	y		
ACQUISITION		hscvl1	6024	1	phase
sw	4960.3	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	1498	gain	46		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlvi1	409		
nt	16	gtl1	0.001000		
2D ACQUISITION		gzlvi3	1227		
sw1	30200.1	gt3	0.001000		
ni	228	gstab	0.000500		
phase		arrayed	P2 PROCESSING		
PRESATURATION		sb	-0.075		
satmode	n	sbs	not used		
wet	n	fn	2048		
TRANSMITTER		F1 PROCESSING			
tn	H1	gt1	0.004		
sfrq	500.477	gtcl	not used		
tof	-534.0	procl	lp		
tpwr	58	fnl	2048		
pw	8.100	DISPLAY			
DECOUPLER		sp	-34.2		
dn	Cl3	wp	4078.7		
dof	1287.0	sp1	-559.3		
dm	nmn	wp1	27162.4		
decwave	W40_HCN5mm	rfl	508.9		
dmf	32258	rfp	0		
dpwr	38	rfl1	1886.4		
pwzvl1	56	rfl1	0		
pwz	10.500	PLOT			
HMBC		wc	206.0		
j1kh	146.0	sc	0		
j1xh	8.0	wc2	206.0		
ADIABATIC		sc2	0		
pwz180ad	CN300	vs	63		
pwzvl180	51	th	3		
pwz180	465.4	ai	cdc av		

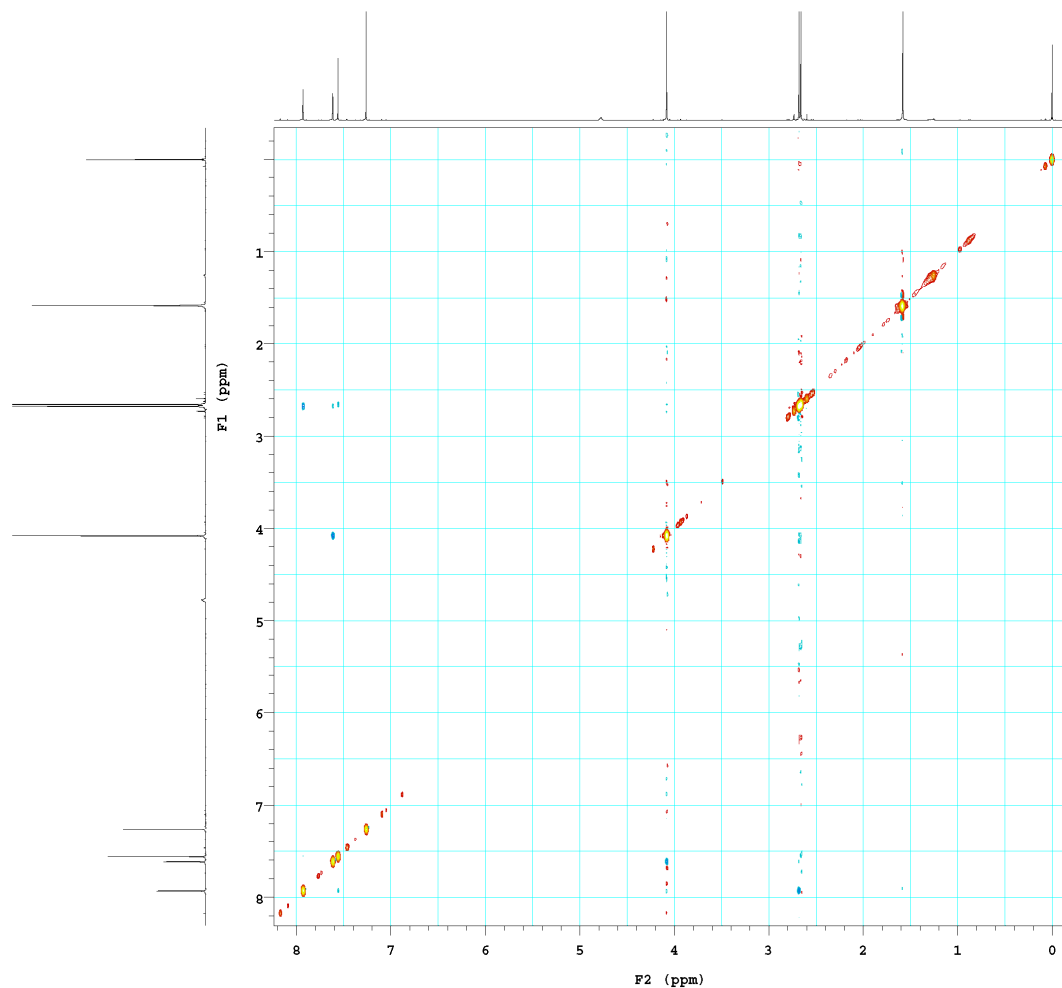


**Figure S75.** NOESY spectrum of **32** (measured in CDCl<sub>3</sub>, 500 MHz).

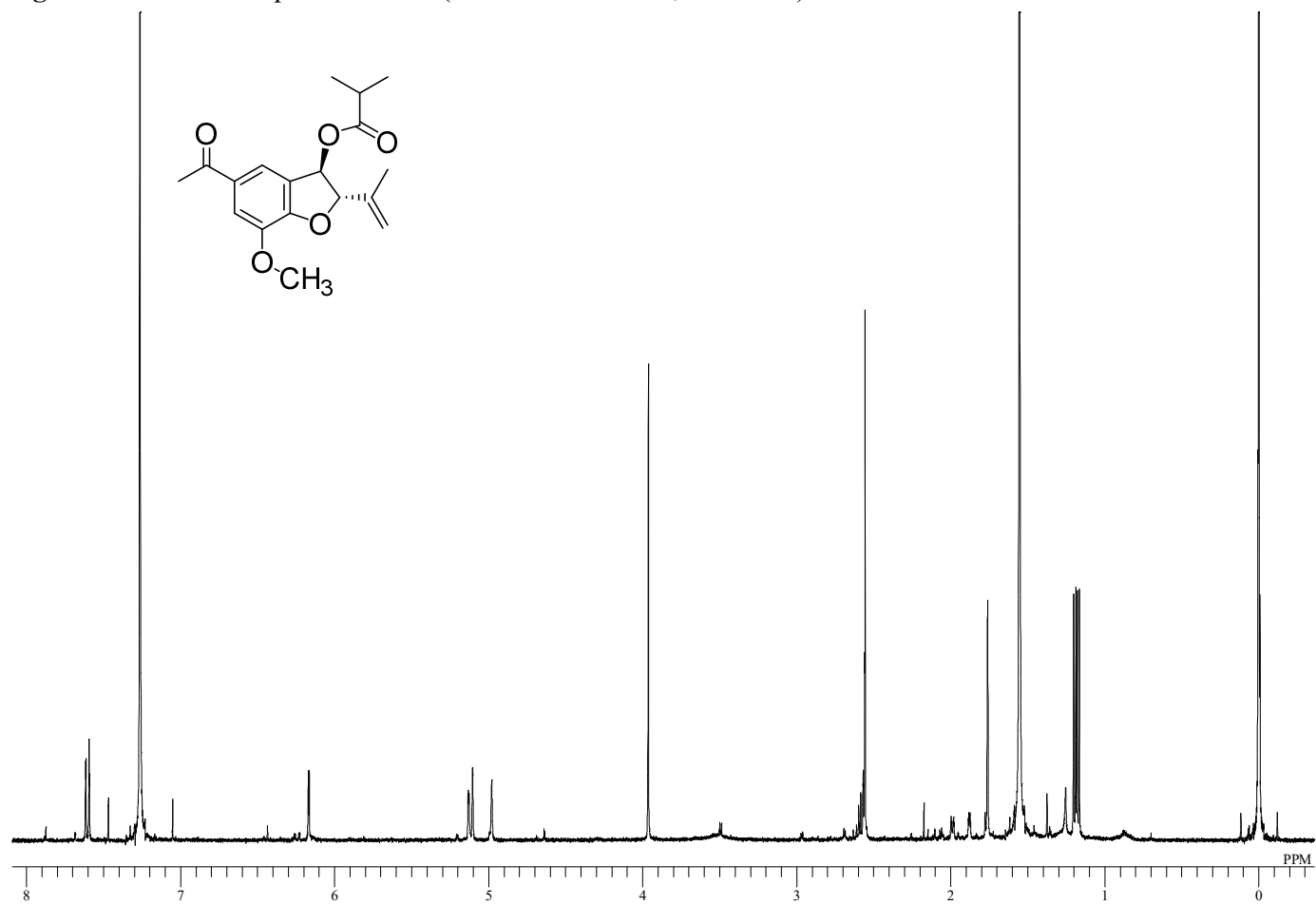
HYM-2014-48-R-6-4-1-2-2.2mg-NOESY-CDCl3

exp7 NOESY

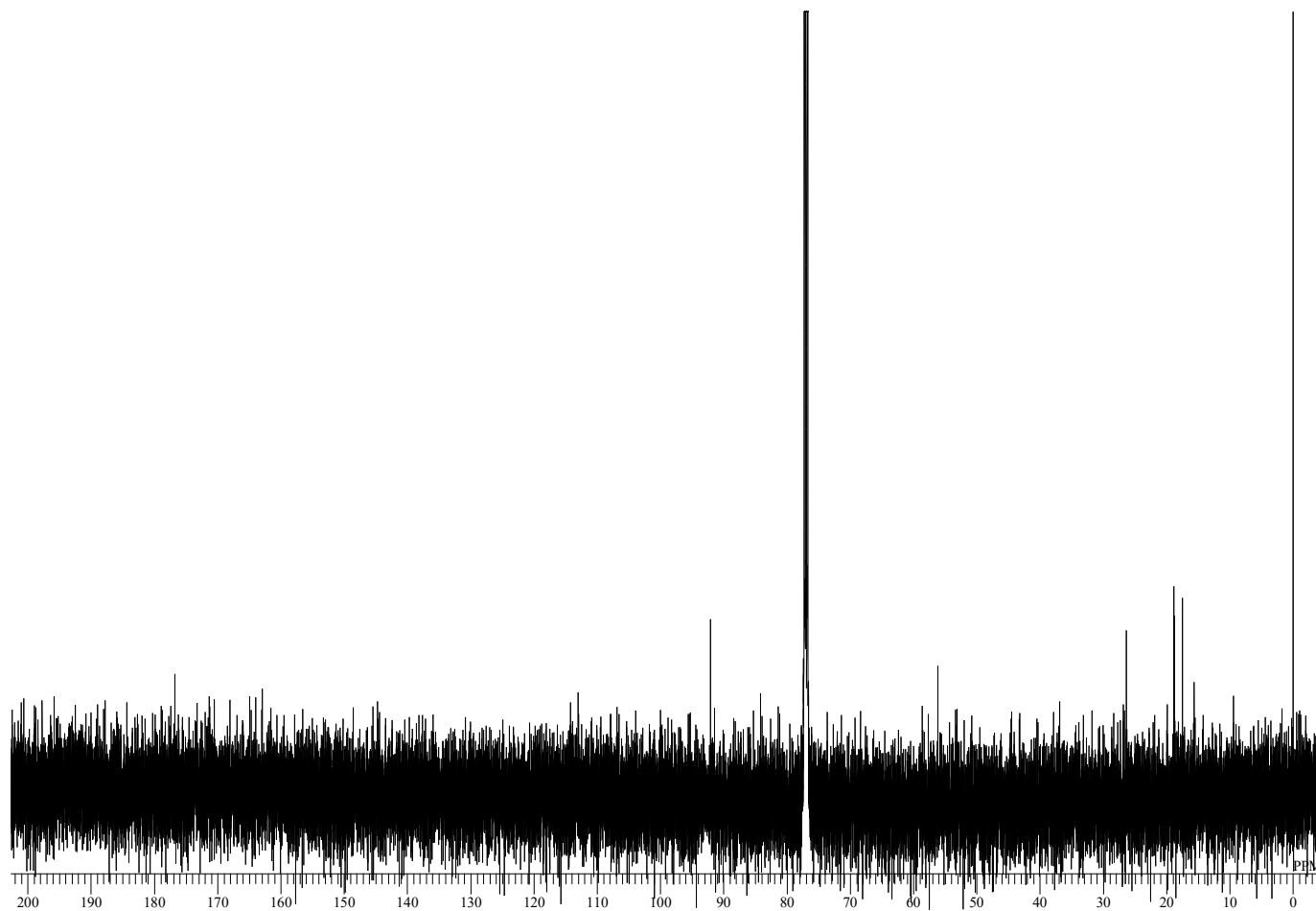
SAMPLE		FLAGS	
date	Jun 6 2021	hs	nn
solvent	cdcl3	sspul	y
sample		PFGflg	y
ACQUISITION		hsclvl	6024
sw	4960.3	SPECIAL	
at	0.150	temp	not used
np	1488	gain	46
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	8	gfs	not used
2D ACQUISITION		fn	2048
sw1	4960.3	F1 PROCESSING	
ni	128	gfl	0.024
TRANSMITTER		gfs1	not used
tn	H1	procl	lp
sfrq	500.477	fn1	2048
tof	-534.0	DISPLAY	
tpwr	58	sp	-97.1
pw	8.100	wp	4219.2
NOESY		sp1	-169.8
mixN	0.500	vp1	4325.7
PRESATURATION		rfl	508.9
satmode	n	rfp	0
wet	n	rfl1	508.9
DECOUPLER		rfpl	0
dm	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	63
		th	1
		ai	ph



**Figure S76.**  $^1\text{H}$  NMR spectrum of **34** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S77.**  $^{13}\text{C}$  NMR spectrum of **34** (measured in  $\text{CDCl}_3$ , 126 MHz).

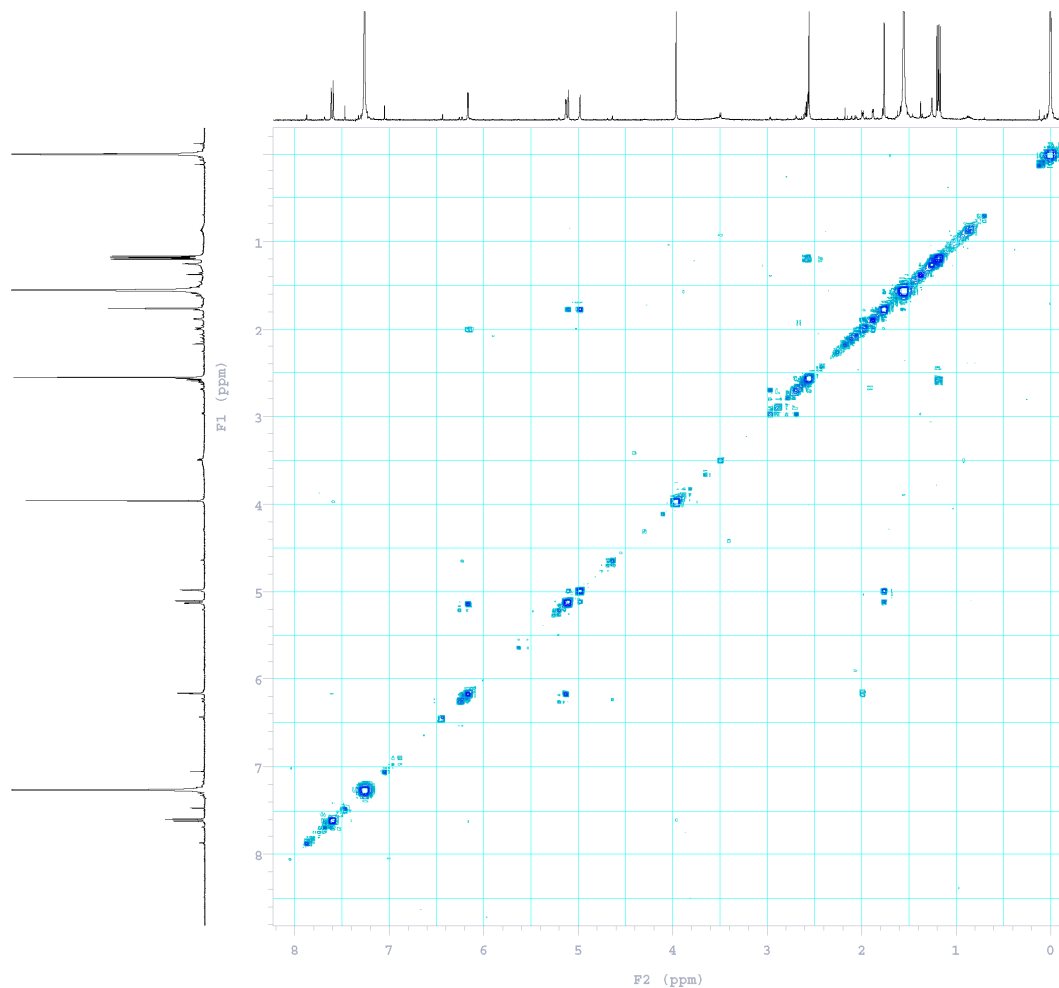


**Figure S78.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **34** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-4-2-4-2-0.2mg-COSY-CDCl3

exp4 gCOSY

SAMPLE		FLAGS		
date	Oct 30 2020	hs		nm
solvent	cdcl3	sepul		y
sample	heglvl			6180
ACQUISITION		SPECIAL		
sw	5060.7	temp		not used
at	0.150	gain		54
rp	1518	spin		0
fd	4000	F2 PROCESSING		
ss	32	sb		-0.075
d1	1.000	sbs		not used
nt	16	fn		2048
2D ACQUISITION		F1 PROCESSING		
sw1	5060.7	sb1		-0.025
nl	128	sbs1		not used
d2	0	procl		lp
PRESATURATION		fml <th>2048</th>		2048
satmode	n	DISPLAY		
wet	n	sp		-98.0
TRANSMITTER		H1		sp1
tn	H1	wp		4215.6
sfrq	500.477	wp1		4556.6
tof	-511.8	rfl		537.9
tpwr	58	rfl		0
pw	8.000	rfl1		537.9
GRADIENTS		rfl1		0
gzlvis	5154	PLOT		
gte	0.001000	wc		206.0
EDratio	1.000	sc		0
gstab	0.000500	wc2		206.0
DECOUPLER		sc2		0
dn	Cl3	vs		34
dm	nmn	th		6
	ai	cdc		av

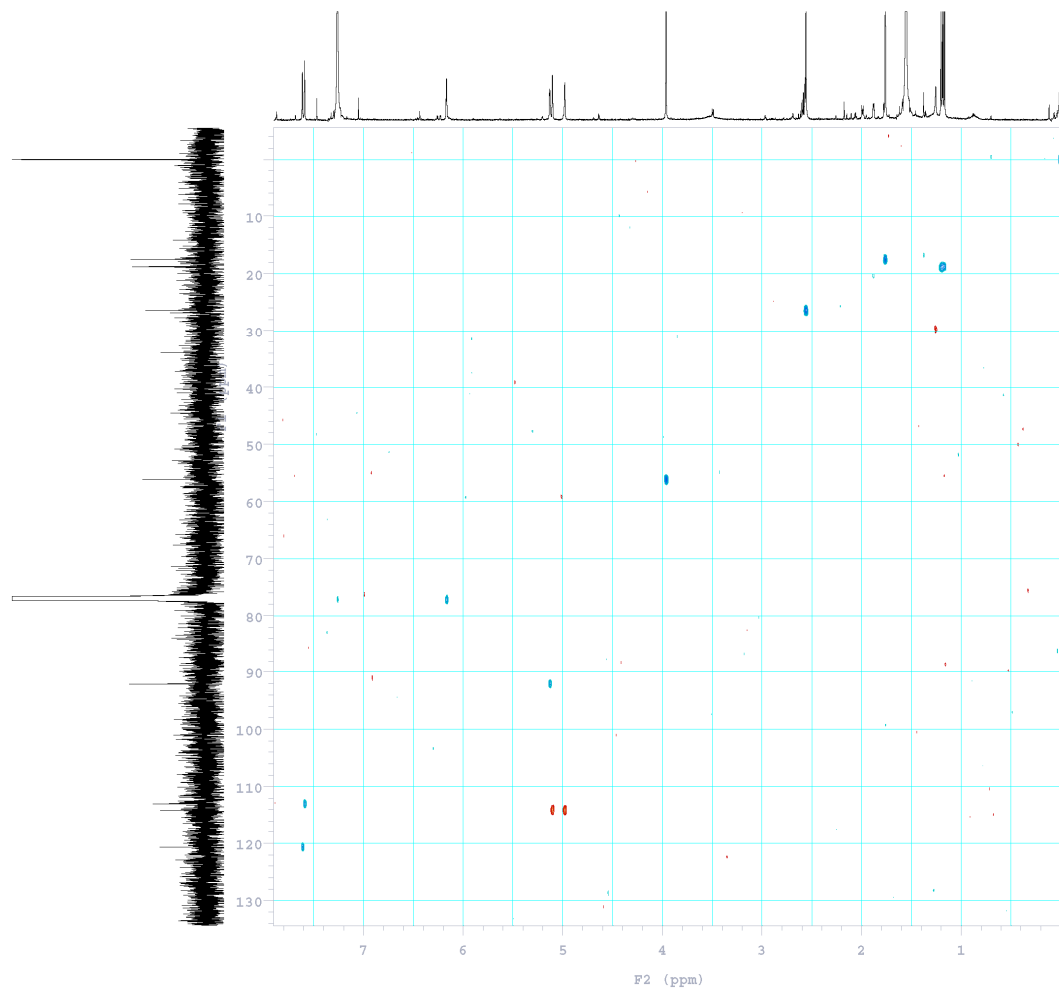


**Figure S79.** HSQC spectrum of **34** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-4-2-4-2-0.2mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Oct 30 2020	hs	nm	array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample		DPGflg	y		
ACQUISITION		hscvlvl	6180	i	phase
sw	5060.7	SPECIAL		1	1
at	0.150	temp	not used	2	2
hp	1518	gain	54		
fb	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	32	gfs	not used		
2D ACQUISITION		fn	2048		
sw1	25165.1	F1 PROCESSING			
ni	128	gfl	0.005		
phase	arrayed	gfl	not used		
PRESATURATION		procl	1p		
satmode	n	fnl	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	-43.6		
tn	H1	wp	3998.2		
sfrq	500.477	spl	-691.1		
tor	-511.8	wpl	17595.9		
tpwr	58	rfl	537.9		
pw	8.000	rfl	0		
DECOUPLER		rfl1	1256.5		
dm	C13	rfl1	0		
dof	-600.6	PLOT			
dm	nmr	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pwxlvl	56	vs	34		
pwex	10.700	th	3		
HSQC		ai	cdc	ph	
j1xh	146.0				
multifig	y				
mult	2				
ADIABATIC					
pwxl80ad	ONE_ad300				
pwxl80adR	ONE_ad30-				
	or				
pwxl80	465.4				
pwxlvl180	51				
pwxl80ref	ONE_ref2-				
	00				
pwxl80r	2000.2				
pwxlvl180r	43				



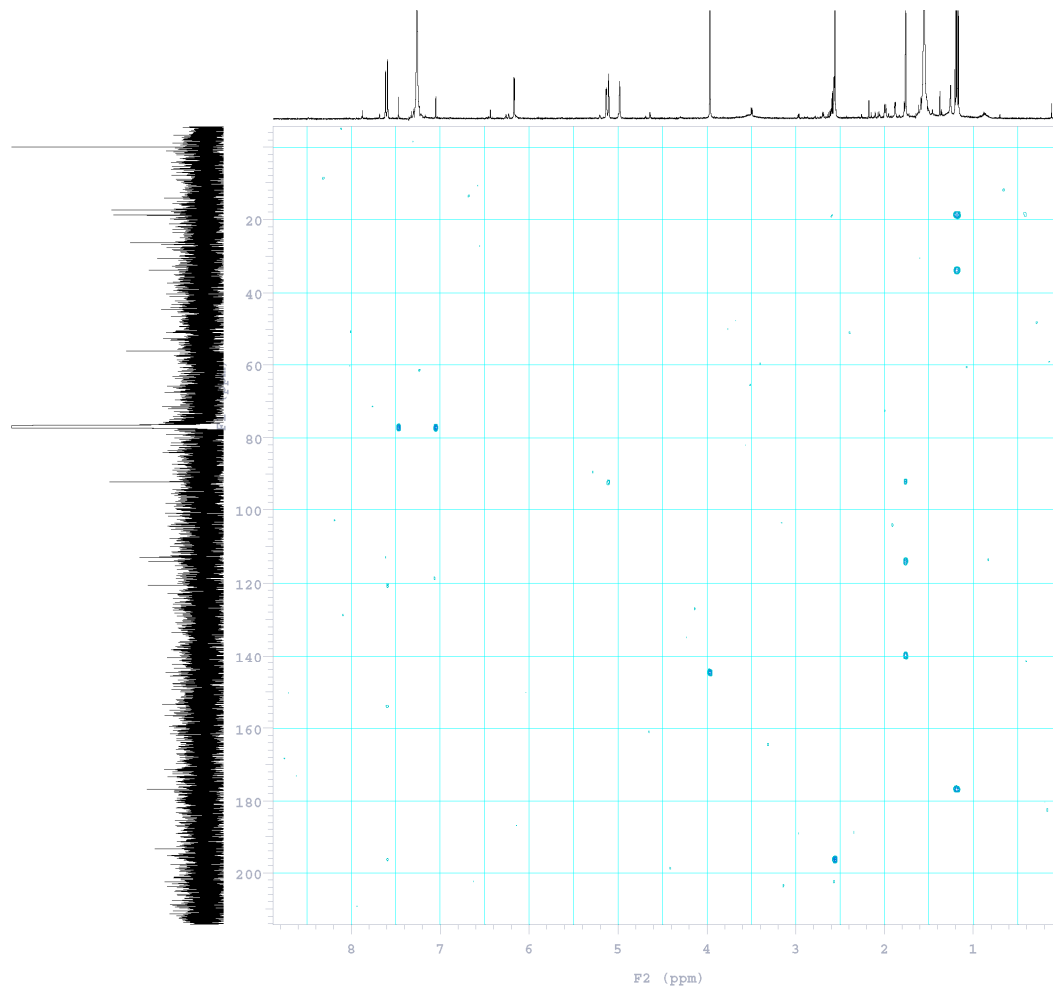


**Figure S80.** HMBC spectrum of **34** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-49-R-4-2-4-2-0.2mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Oct 30 2020	hs	nm	array	phase
solvent	cdcl3	sspul	y	arraydim	256
sample	cdcl3	PPGflg	y		
ACQUISITION	hsqivl	6180	1	phase	
sw	5060.7	SPECIAL	1	1	
at	0.150	temp	not used	2	2
np	1518	gain	54		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlv11	409		
nt	32	gt1	0.001000		
2D ACQUISITION	gzlv13	1227			
sw1	30200.1	gt3	0.001000		
ni	128	gstab	0.000500		
phase	arrayed	F2 PROCESSING			
PRESATURATION	sb	-0.075			
satmode	n	sbs	not used		
wet	n	fn	2048		
TRANSMITTER	H1	F1 PROCESSING			
tn	500.477	gf1	0.004		
stf	-511.8	gfal	not used		
tof	58	procl	lp		
tpwr	8.000	fnl	2048		
pw		DISPLAY			
DECOUPLER	sp	-38.7			
dn	C13	wp	4482.5		
dof	1287.0	ep1	-706.7		
dm	nmn	wpl	27663.7		
decwave	M40_HCNsm	rfl	537.9		
dmf	32258	rpf	0		
dpwr	38	rfl1	1886.4		
pwxlvl	56	rfpl	0		
pwk	10.700	PLOT			
HMBC	sc	206.0			
j1xh	146.0	sc	0		
jnxh	8.0	wc2	206.0		
ADIABATIC	sc2	0			
pwxl80ad ONE_ad300	vs	34			
pwxlvl180	51	th	5		
pwxl80	465.4	ai cdc av			

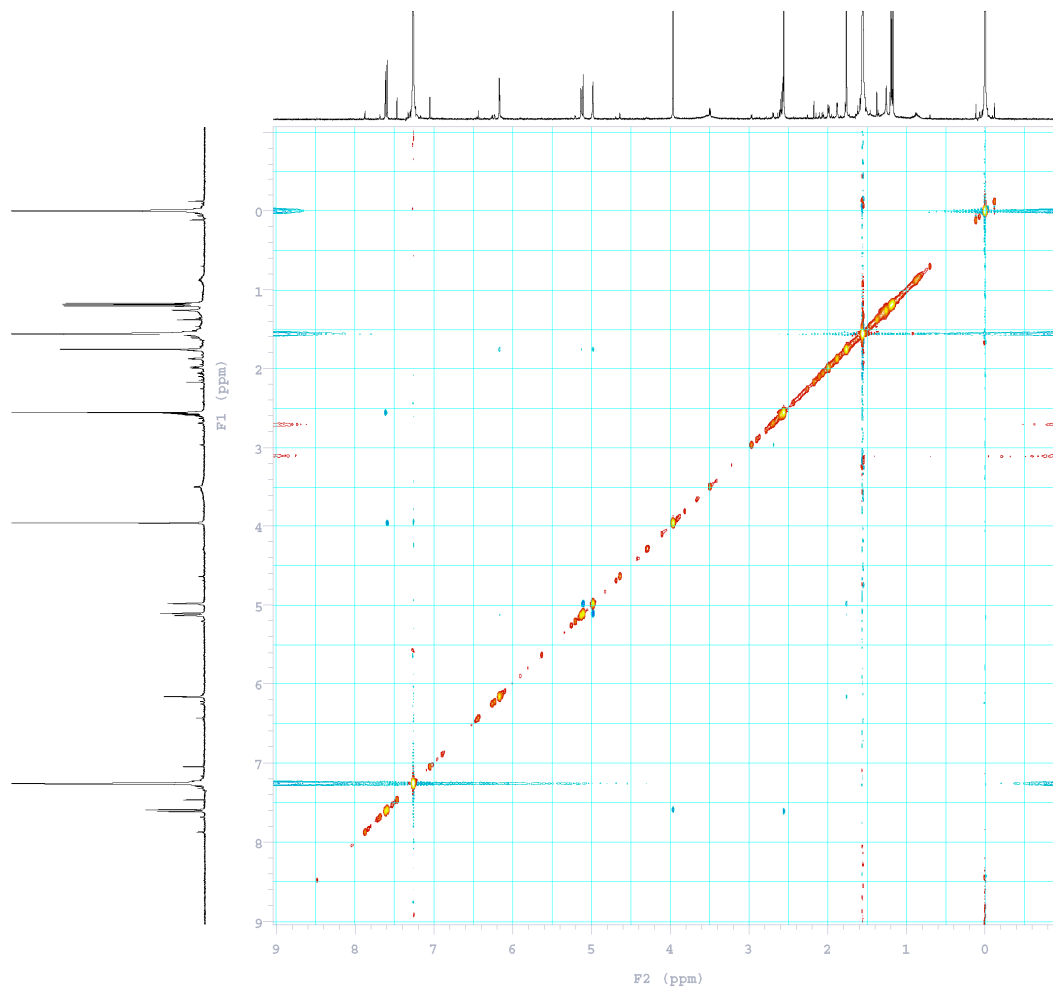


**Figure S81.** NOESY spectrum of **34** (measured in CDCl<sub>3</sub>, 500 MHz).

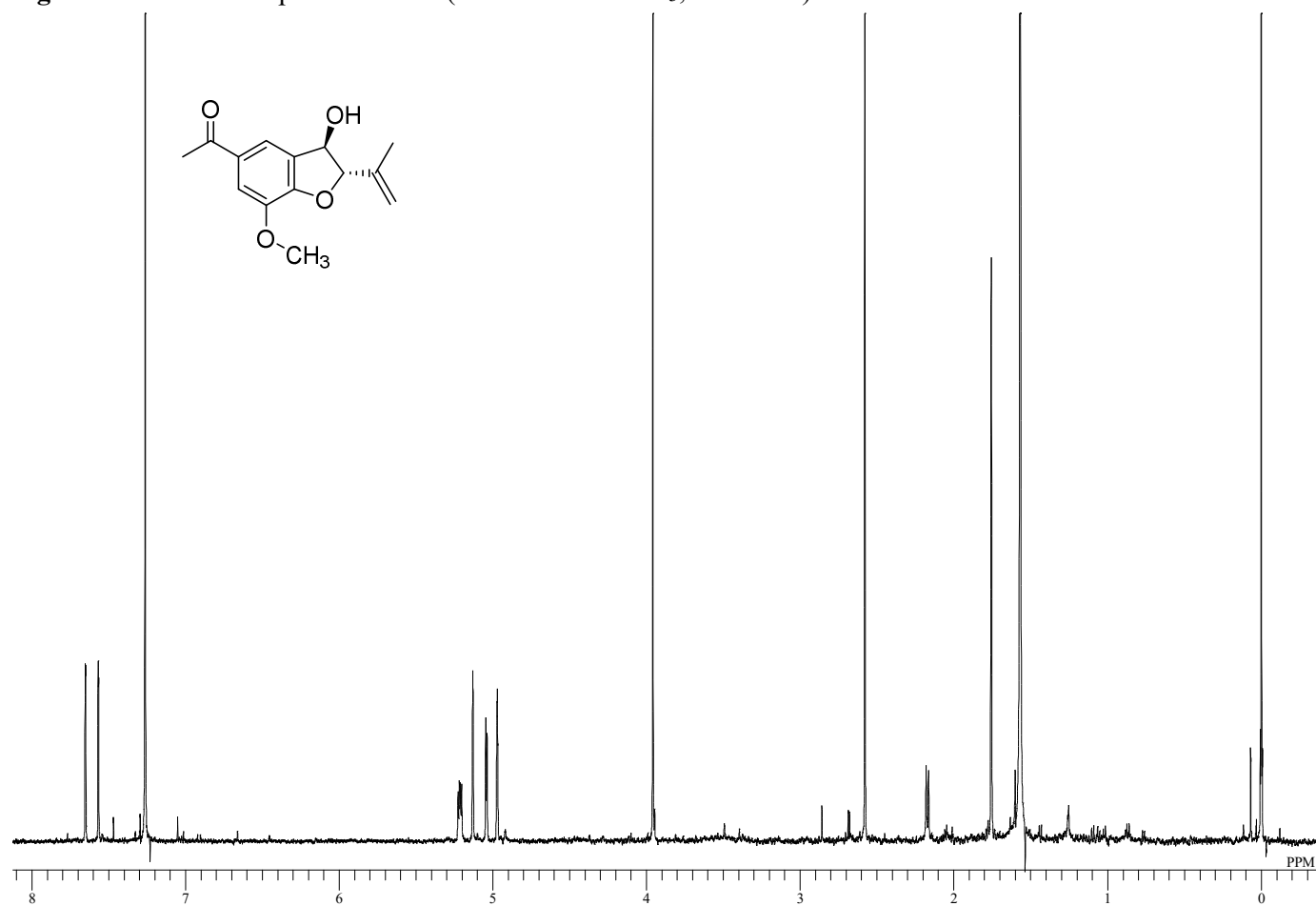
HYM-2014-48-R-4-2-4-2-0.2mg-NOESY-CDCl3

exp7 NOESY

SAMPLE		FLAGS	
date	Oct 30 2020	hs	nm
solvent	cdcl3	sspul	y
sample	PFGflg	y	
ACQUISITION		hsq1v1	6180
sw	5060.7	SPECIAL	
at	0.150	temp	not used
np	1518	gain	54
fb	4000	spin	0
ss	32	F2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION		fn	2048
sw1	5060.7	F1 PROCESSING	
ni	128	gf1	0.023
TRANSMITTER		gfsl	not used
tn	H1	procl	lp
sfrq	500.477	fn1	2048
tof	-511.8	DISPLAY	
tpwr	58	ep	-532.9
pw	8.000	wp	5055.8
NOESY		ep1	-532.9
mixN	0.500	vp1	5055.8
PRESSATURATION		rfl	537.9
satmode	n	rpf	0
wet	n	rfl1	537.9
DECOUPLER		rfpl	0
dm	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	34
		th	1
		ai	ph



**Figure S82.**  $^1\text{H}$  NMR spectrum of **36** (measured in  $\text{CDCl}_3$ , 500 MHz).

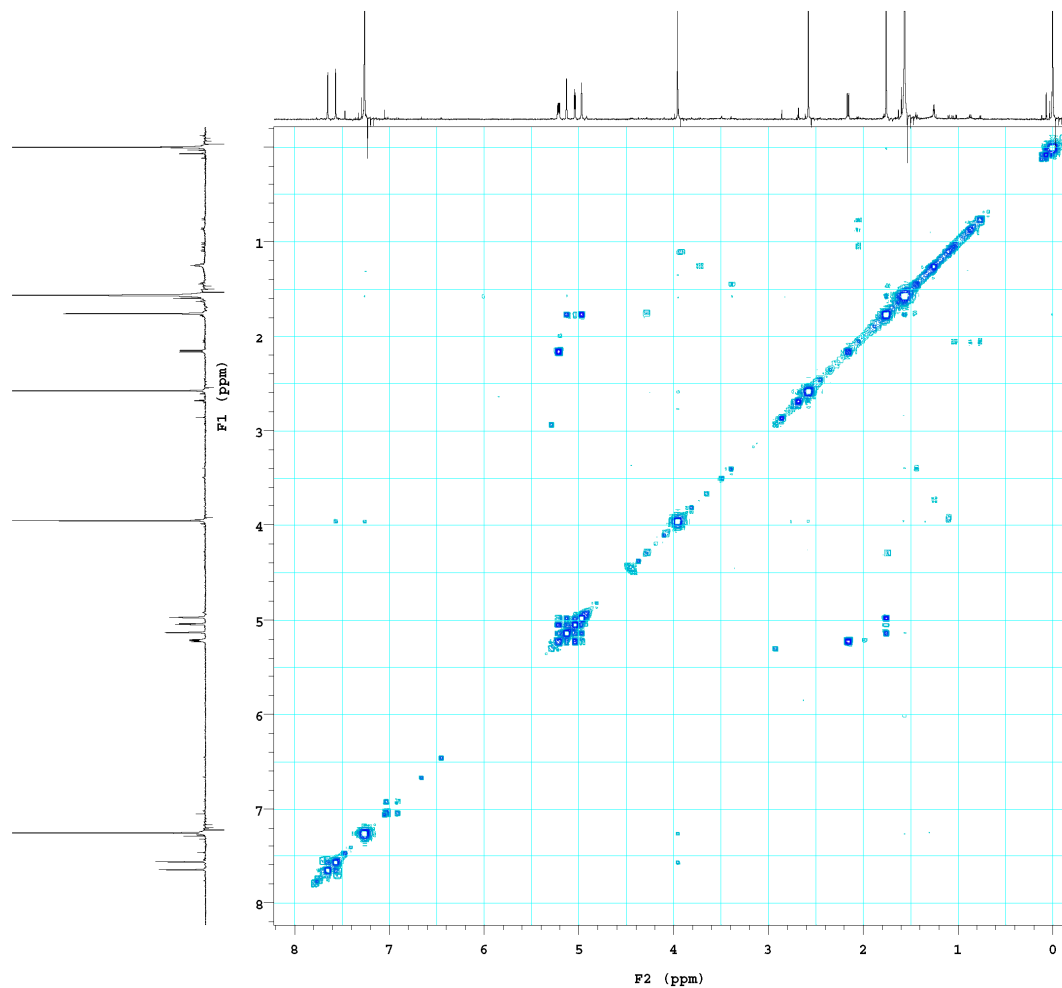


**Figure S83.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **36** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-48-R-6-6-4-1-0.4mg-COSY-CDCl3

exp4 gcOSY

SAMPLE		FLAGS		nn
date	Jul 16 2021	hs		nn
solvent	cdcl3	spul	y	
sample	hsglv1		6024	
ACQUISITION		SPECIAL		
sw	4699.2	temp	not used	
at	0.150	gain	52	
np	1410	spin	0	
fb	4000	F2 PROCESSING		
ss	32	sb	-0.075	
d1	1.000	sbs	not used	
nt	16	fn	2048	
2D ACQUISITION		F1 PROCESSING		
sw1	4699.2	sb1	-0.027	
n1	128	sbs1	not used	
d2	0	procl	lp	
PRESATURATION		fn1 <th>2048</th>		2048
satmode	n			
wet	n	sp	-91.2	
TRANSMITTER		vp <th>4203.6</th>		4203.6
tn	H1	sp1	-105.0	
sfrq	500.477	wp1	4226.6	
tof	-650.0	rf1	495.1	
tpwr	58	rfl	0	
pw	8.100	rfl1	495.1	
GRADIENTS		rfl1 <th>0</th>		0
gplv1e	5025			
gTE	0.001000	wc	206.0	
EDratio	1.000	sc	0	
getab	0.000500	wc2	206.0	
DECOUPLER		sc2 <th>0</th>		0
dm	C13	vs	407	
dm	nm	th	6	
	ai	cdc	av	

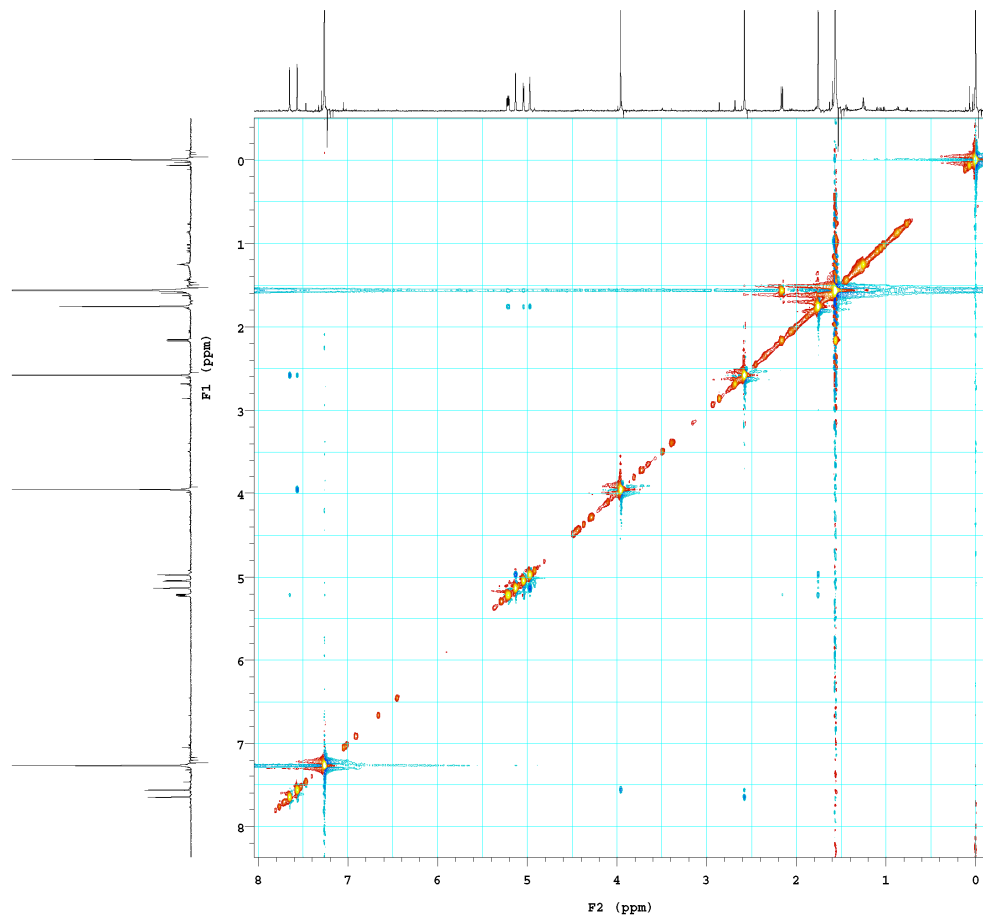


**Figure S84.** NOESY spectrum of **36** (measured in CDCl<sub>3</sub>, 500 MHz).

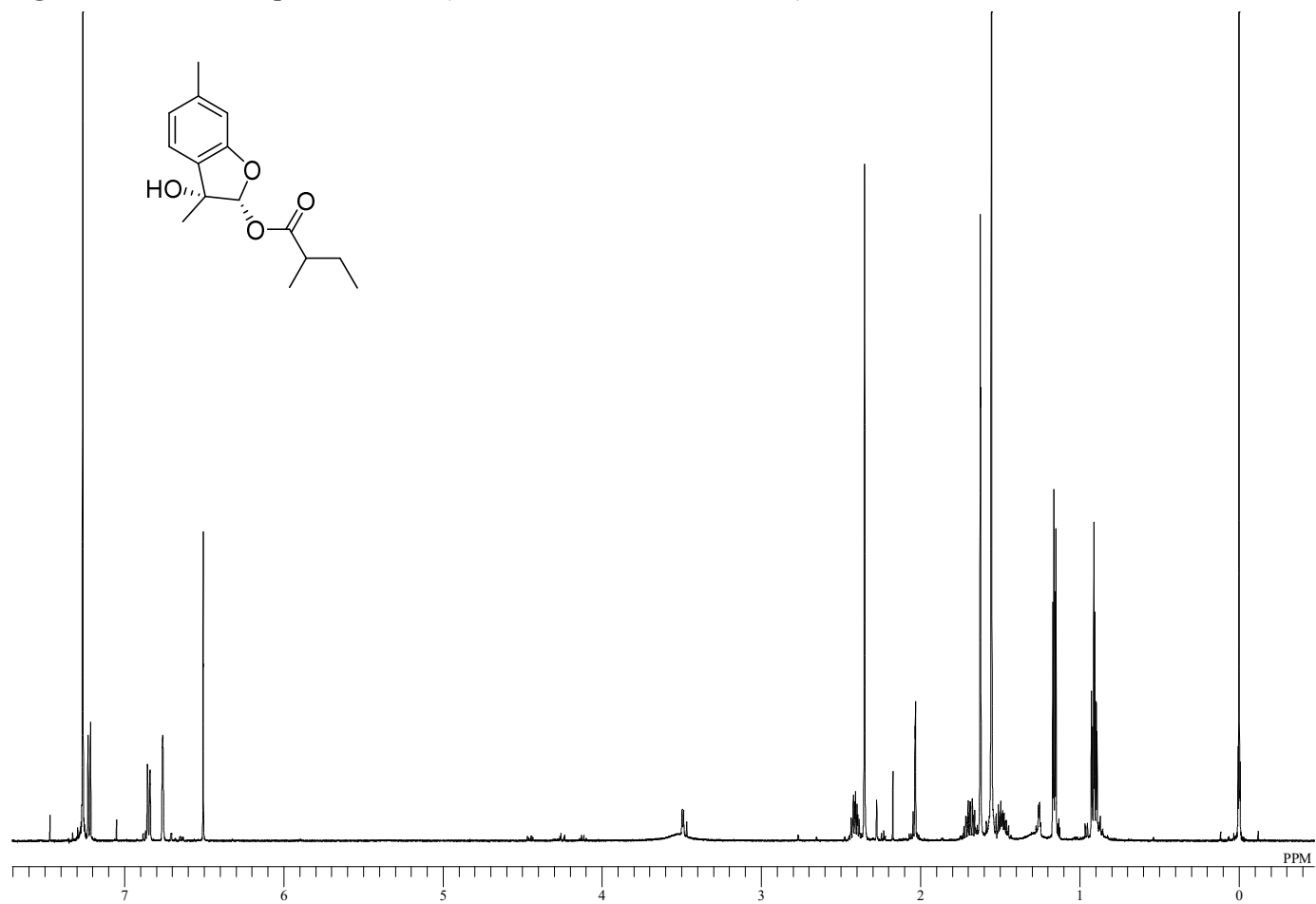
HYM-48-R-6-4-1-0.4mg-NOESY-CDCl3

exp7 NOESY

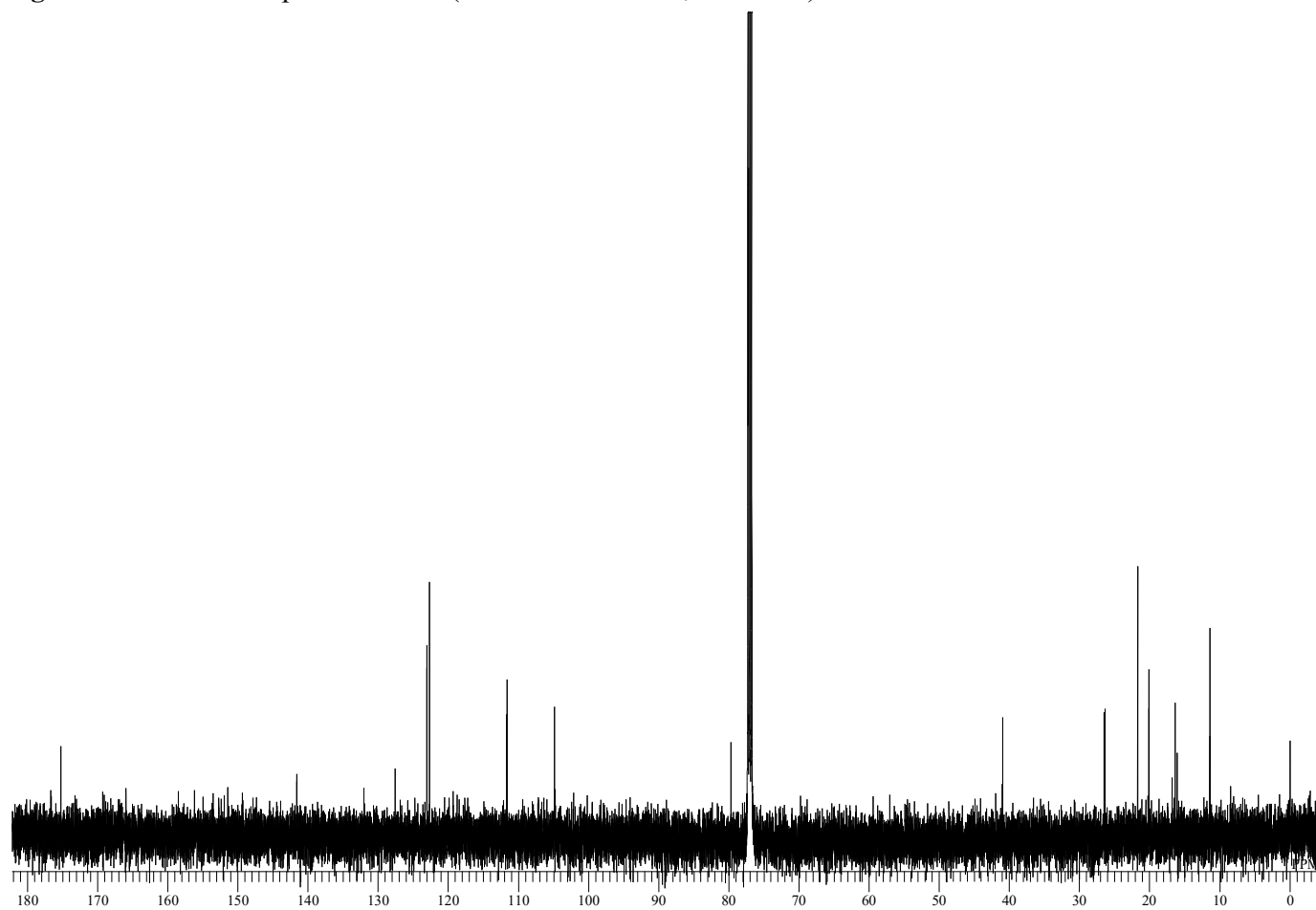
SAMPLE		FLAGS	
date	Jul 16 2021	hs	nn
solvent	odcl3	sspl	y
sample	PFGClg	y	
Acquisition	hcg1v4	4024	
sv	4699.2	SPECIAL	
at	0.150	temp	not used
np	1410	gain	52
fb	4000	spin	0
ss	32	F2 PROCESSING	
dl	2.000	gf	0.069
nt	32	gfs	not used
2D ACQUISITION	rn	2048	
sw1	4699.2	F1 PROCESSING	
ni	128	gf1	0.025
TRANSMITTER	gfsl	not used	
tn	h1	procl	lp
strq	500.477	fn1	2048
tof	-650.0	DISPLAY	
tpwr	58	sp	-86.6
pw	8.100	wp	4111.8
NOESY	sp1	-251.8	
mixN	0.500	wp1	4437.7
PRESATURATION	rf1	495.1	
satmode	n	rfp	0
wet	n	rf11	495.1
DECOUPLER	rfp1	0	
dm	Cl3	PLOT	
dm	nmn	wc	206.0
	sc	0	
	wc2	206.0	
	sc2	0	
	vs	407	
	th	1	
	ai	ph	



**Figure S85.**  $^1\text{H}$  NMR spectrum of **39** (measured in  $\text{CDCl}_3$ , 500 MHz).



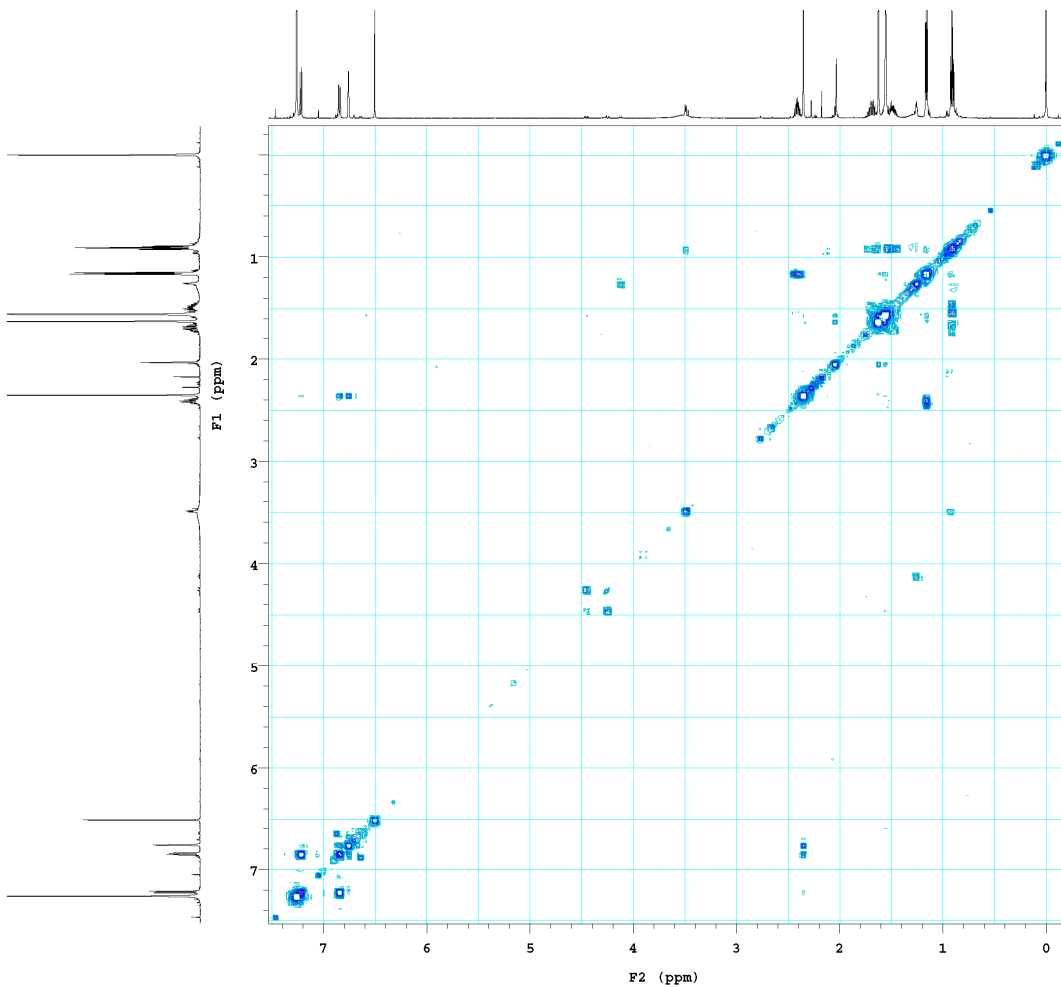
**Figure S86.**  $^{13}\text{C}$  NMR spectrum of **39** (measured in  $\text{CDCl}_3$ , 126 MHz).



**Figure S87.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **39** (measured in  $\text{CDCl}_3$ , 500 MHz).



SAMPLE				PLAGE	
date	Dec 9 2020	hs		nn	
solvent	cdc13	sepul			6180
sample		hagvlv			
ACQUISITION			SPECIAL		
sw	4370.6	temp	not used		
at	0.150	gain		52	
np	1312	asp			
fb		F2	PROCESSING	0	
as	32	sb		-0.075	
ni	1.000	abs	not used		
nt	16	fn		2048	
2D ACQUISITION			F1 PROCESSING		
sw1	4370.6	sbl		-0.029	
ni1	128	sbs1	not used		
ds		o precl		1p	
PRESATURATION			fn1		
satsmode			DISPLAY		
wet	n	sp		-88.7	
		wp		3958.4	
tn		HL		-139.9	
tsq	500.477	rpl		3909	
tof	-625.4	rfl		306.4	
twpr		rf1			
	8.000	rfl1		306.4	
GRADIENTS			rf1		
gvlve	5154				
gTE	0.001000	wc		206.0	
EDratio	1.000	ac			
gstab	0.000500	wc2		206.0	
DECOUPLER					
dm	C13	se		74.6	
q1	nmn	th		6	
		ai	cdc av		



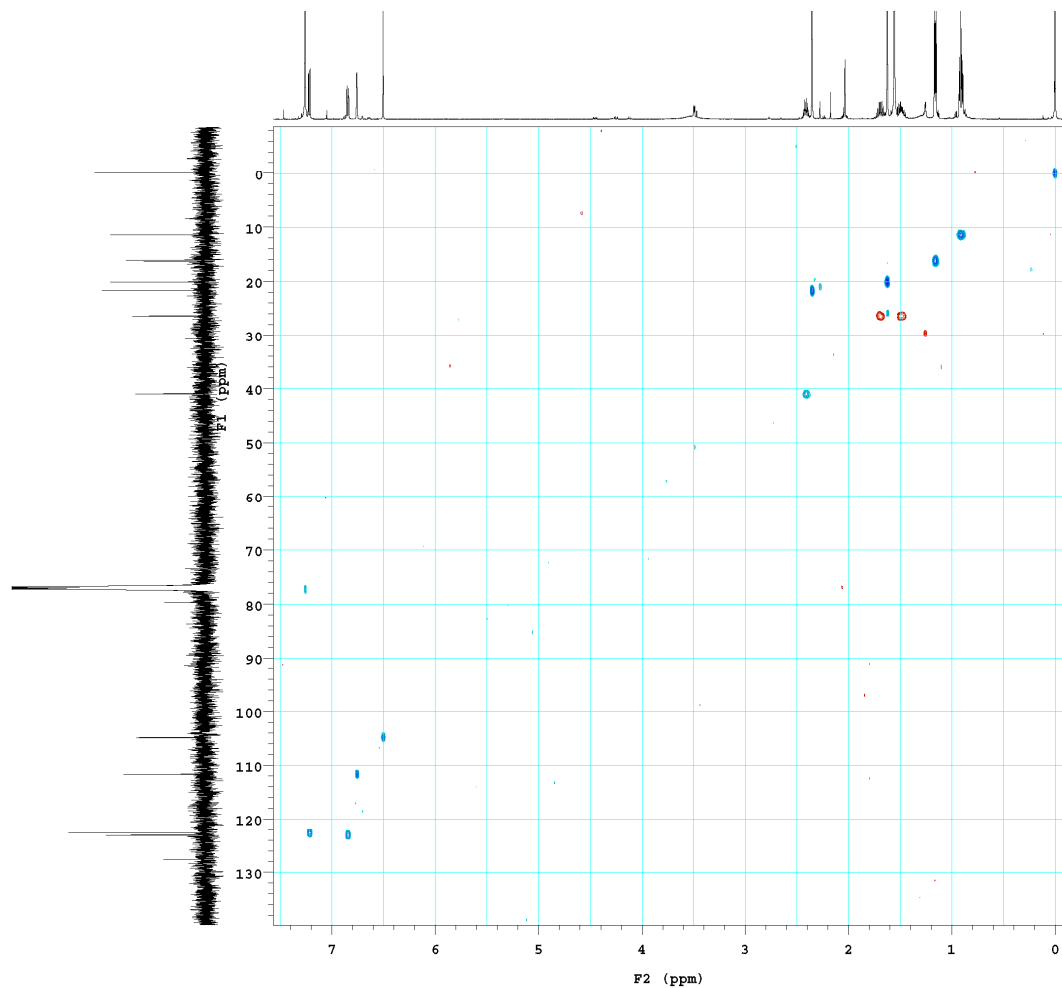


**Figure S88.** HSQC spectrum of **39** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-10-R-4-2-5-0.3mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Dec 9 2020	hs		nn	array
solvent	cdcl3	spul	y	arraydim	256
sample		PFGflg	y		
ACQUISITION	haglvl	6180	1	phase	
sw	4370.6	SPECIAL	1	1	
at	0.150	temp	not used	2	2
np	1312	gain	52		
fb	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	32	gfs	not used		
2D ACQUISITION	fn	2048			
sw1	25165.1	F1 PROCESSING			
ni	128	gf1	0.005		
phase	arrayed	gfs1	not used		
PRESATURATION	procl	lp			
satmode	n	fn1	2048		
wet	n	DISPLAY			
TRANSMITTER	sp	-67.4			
tn	H1	wp	3884.2		
sfrq	500.477	sp1	-1084.5		
tof	-625.4	wp1	18677.3		
tpwr	58	rfl	306.4		
pw	8.000	rfp	0		
DECOUPLER	rfl1	1256.5			
dm	C13	rfpl	0		
dof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dmf	32258	wc2	206.0		
dpwr	38	sc2	0		
pwxlvl	56	va	74		
pwz	10.700	th	3		
HSQC	ai	cdc	ph		
j1kh	146.0				
multflg	y				
mult	2				
ADJABATIC					
pwxl80ad ONE	ad300				
pwxl80adr ONE	ad30-				
OR					
pwxl80	465.4				
pwxlvl180	51				
pwxl80ref ONE	ref2-				
OR					
pwxl80r	2000.2				
pwxlvl180r	43				

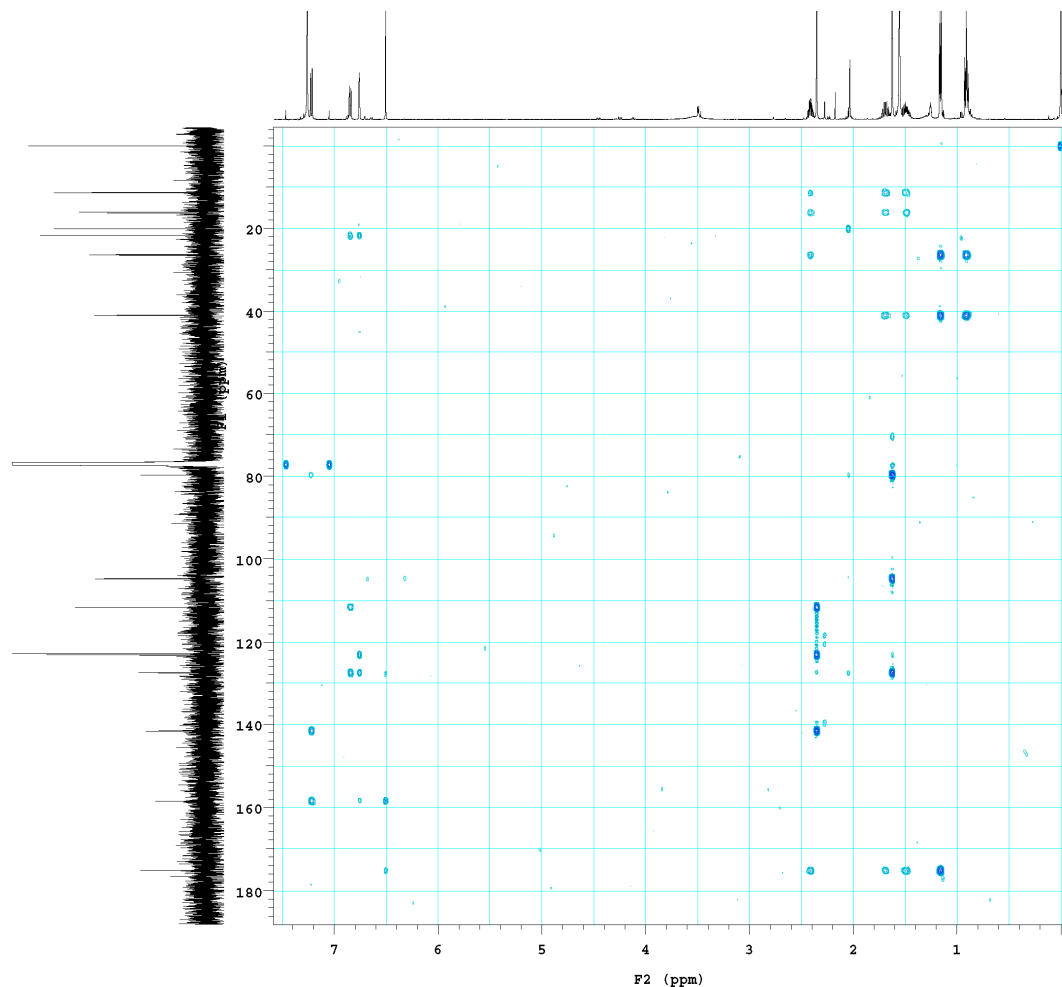


**Figure S89.** HMBC spectrum of **39** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-10-R-4-2-5-0.3mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Dec 9 2020	hs		nm	array
solvent	cdcl3	spul	y	arraydim	256
sample		PPGf1g	y		
ACQUISITION		haglv1	6180	i	phase
sw	4370.6	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	1312	gain	52		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gzlv11	409		
nt	64	gt1	0.001000		
2D ACQUISITION		gzlv13	1227		
sw1	30200.1	gt3	0.001000		
ni	128	gstab	0.000500		
phase	arrayed	F2 PROCESSING			
PRESATURATION	sb	-0.075			
satmode	n	sbs	not used		
wet	n	fn	2048		
TRANSMITTER		F1 PROCESSING			
tn	H1	gt1	0.004		
sfrq	500.477	gtel	not used		
tof	-625.4	procl	lp		
tpwr	58	fnl	2048		
pw	8.000	DISPLAY			
DECOUPLER		sp	-41.8		
dn	C13	wp	3837.1		
dof	1287.0	sp1	-559.3		
dm	nnm	wp1	24213.1		
decwave	W40_HCN5mm	zfl	306.4		
dmf	32258	rpf	0		
dpr	38	rf11	1886.4		
pxlv1	56	rfpl	0		
pxw	10.700	PLOT			
HMBC		vc	206.0		
j1kh	146.0	sc	0		
jmxh	8.0	vc2	206.0		
ADIABATIC		sc2	0		
pxv180ad	CNE_ad300	ve	74		
pxv1180	si	th	4		
pxv180	465.4	ai	cdc	av	

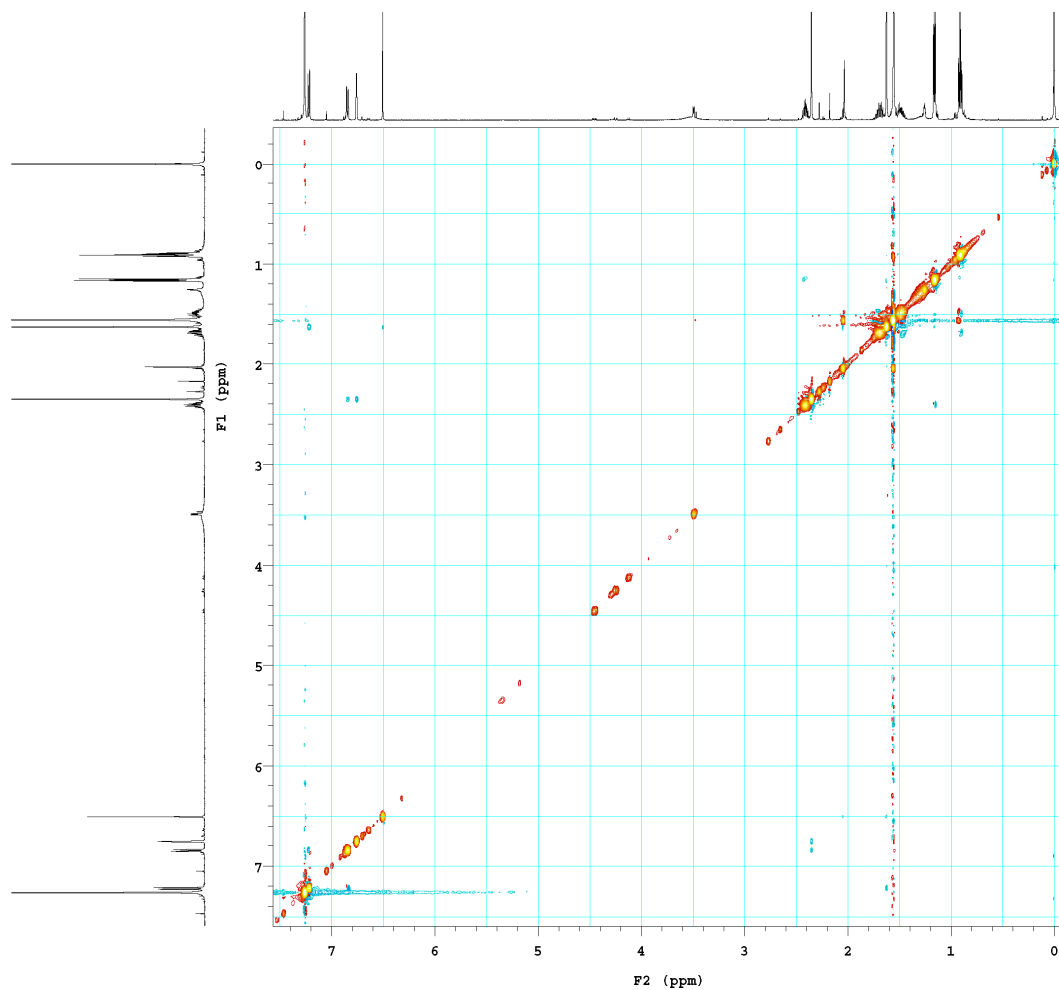


**Figure S90.** NOESY spectrum of **39** (measured in CDCl<sub>3</sub>, 500 MHz).

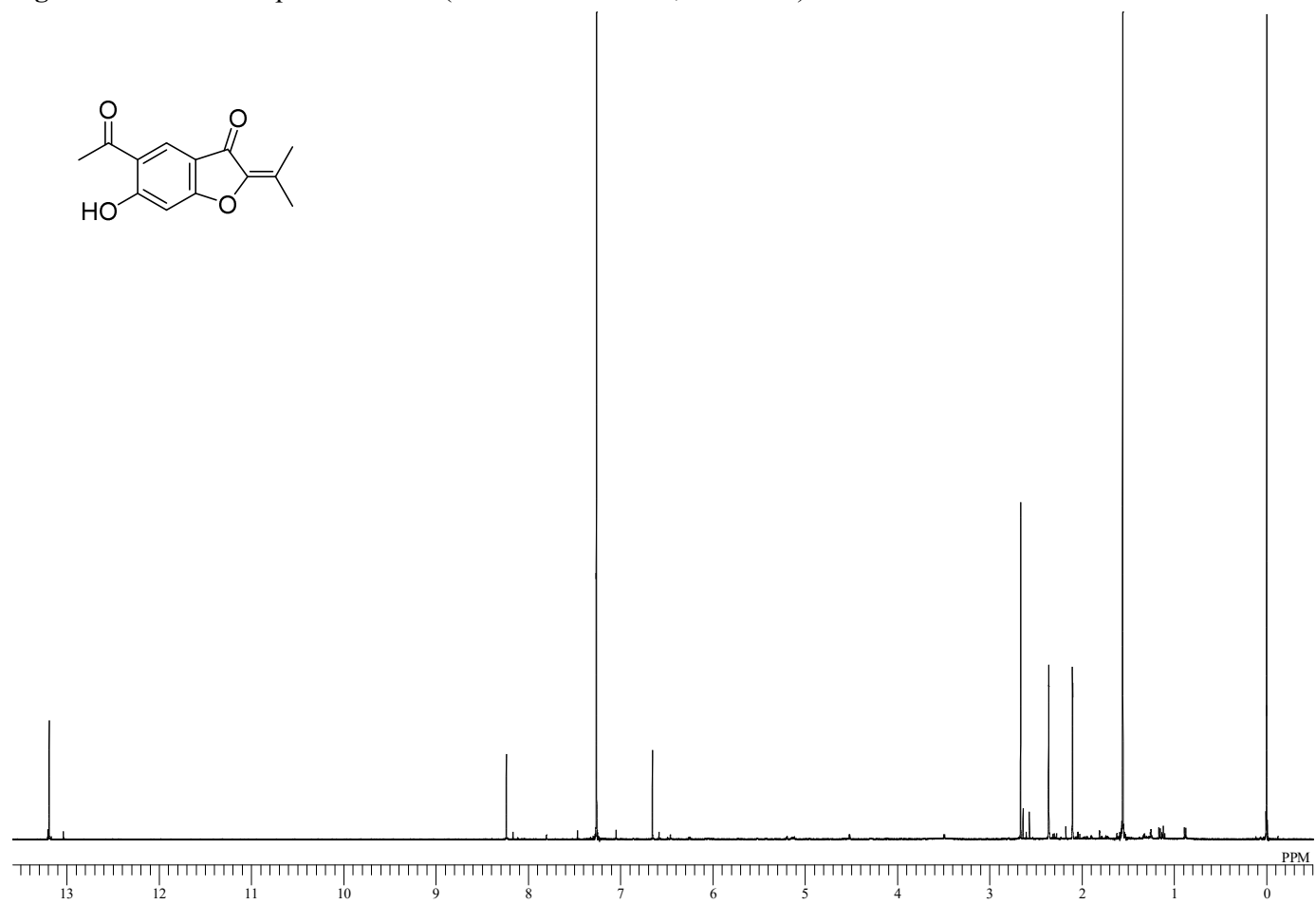
HYM-2014-10-R-4-2-5-0.3mg-NOESY-CDCl3

exp7 NOESY

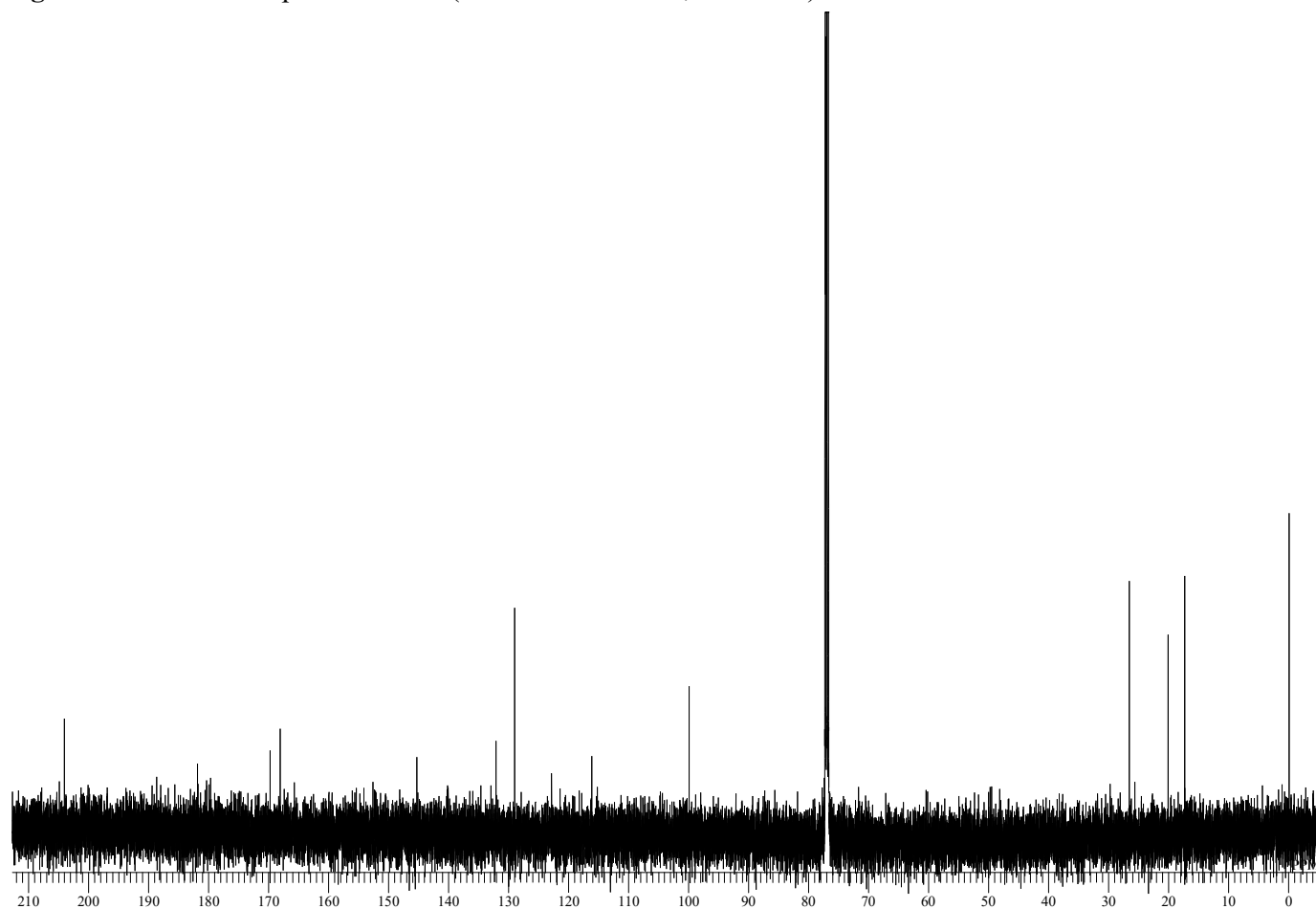
SAMPLE		FLAGS	
date	Dec 9 2020	hs	nn
solvent	cdcl3	sspul	y
sample		ppcrlg	y
ACQUISITION		hcg1v1	6100
sw	4370.6	SPECIAL	
at	0.150	temp	not used
np	1312	gain	52
fb	4000	spin	0
ss	32	F2	PROCESSING
d1	2.000	gf	0.069
nt	8	gfs	not used
2D ACQUISITION		fn	2048
sw1	4370.6	F1	PROCESSING
ni	128	gf1	0.027
TRANSMITTER		gfs1	not used
tn	H1	procl	lp
sfrq	500.477	fn1	2048
tof	-625.4	DISPLAY	
tpwr	58	sp	-71.7
pw	8.000	wp	3858.4
mixN NOESY		sp1	-179.4
PRESATURATION		wp1	3978.0
satmode		rf1	306.4
wet		n rfp	0
DECOUPLER		n rfl1	306.4
		rfp1	0
dn	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	74
		th	1
		ai	ph



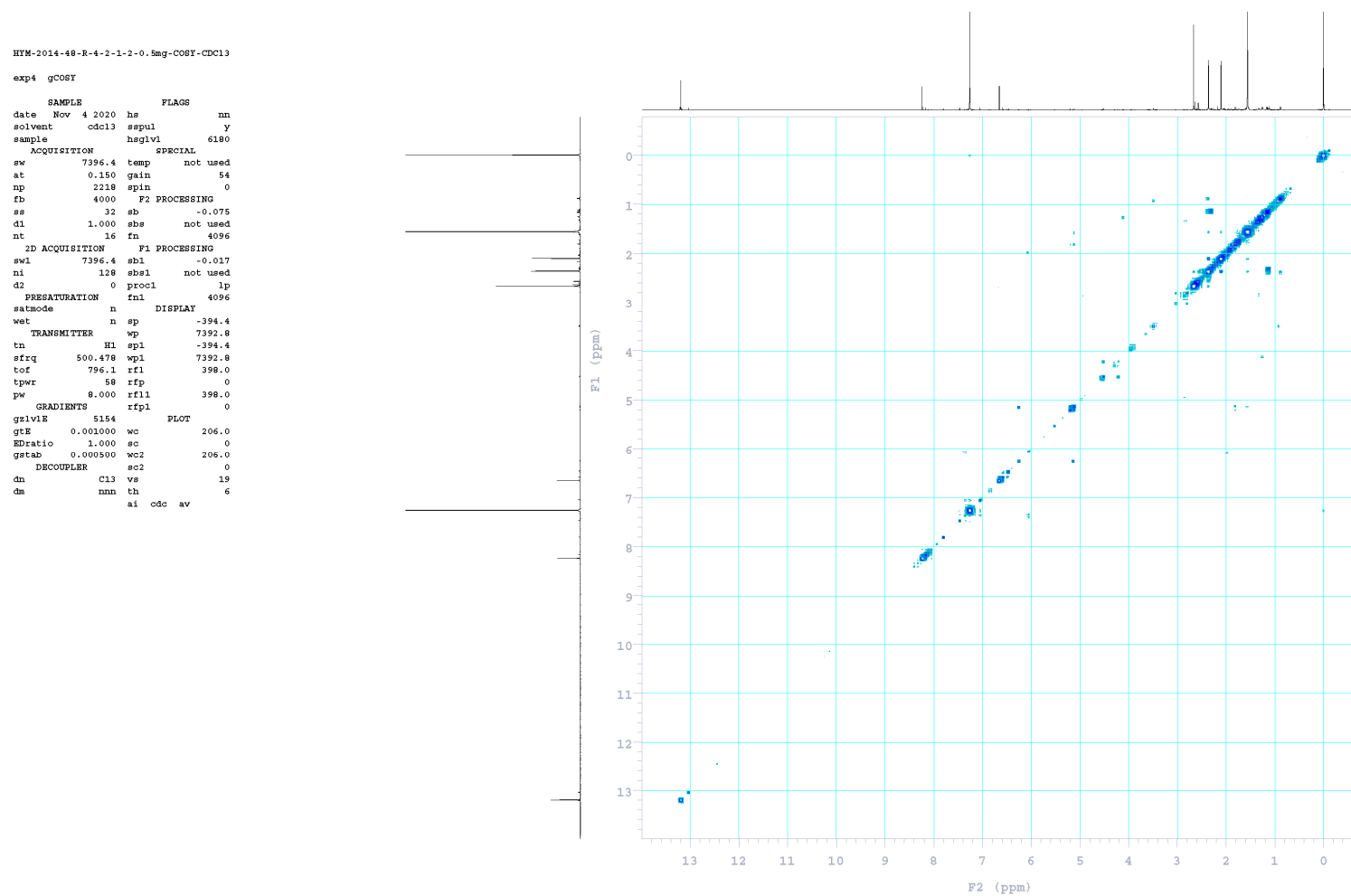
**Figure S91.**  $^1\text{H}$  NMR spectrum of **20** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S92.**  $^{13}\text{C}$  NMR spectrum of **20** (measured in  $\text{CDCl}_3$ , 126 MHz).



**Figure S93.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **20** (measured in  $\text{CDCl}_3$ , 500 MHz).

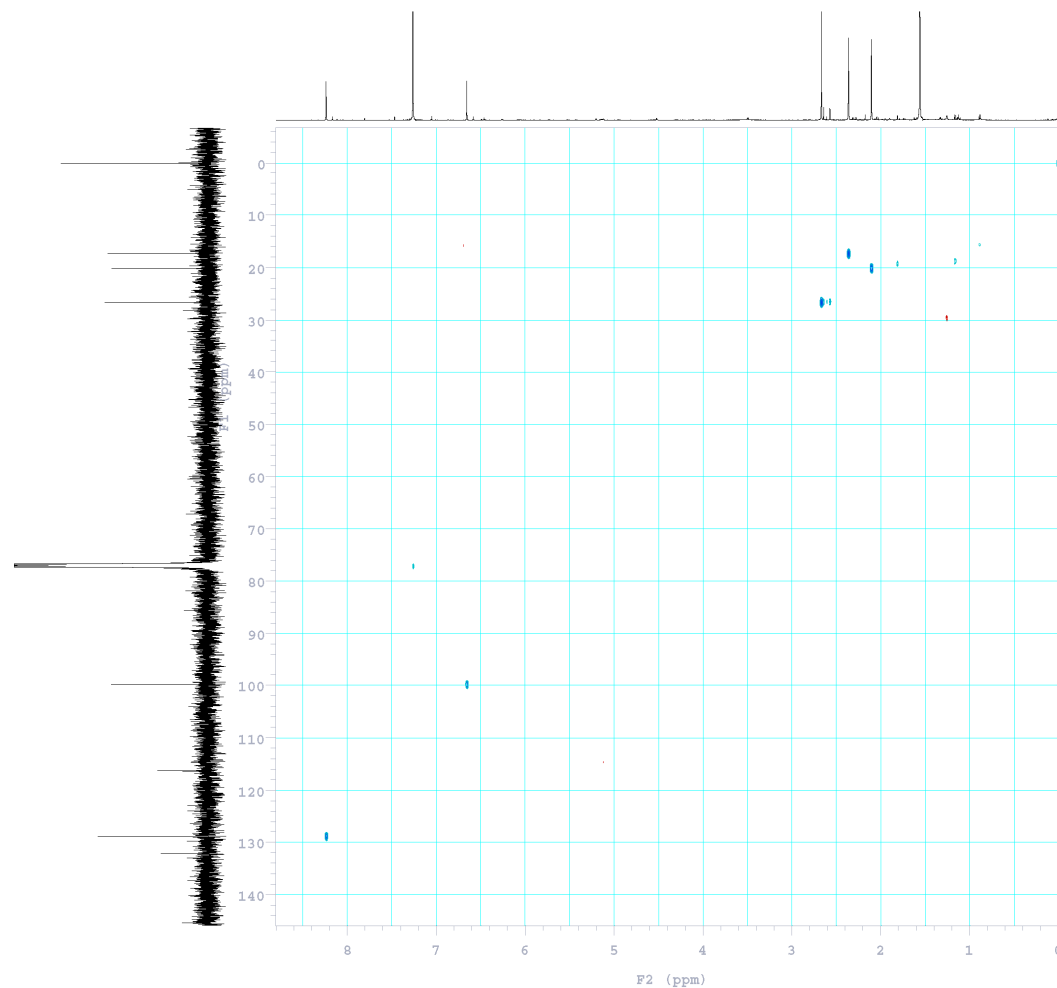


**Figure S94.** HSQC spectrum of **20** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-4-2-1-2-0.5mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Nov 4 2020	hs	nn	array	phase
solvent	cdcl3	sspul	y	arraydia	256
sample		pfqflg	y		
ACQUISITION		hsqvlv	6180	1	phase
sw	7396.4	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2218	gain	54		
fb	4000	spin	0		
ss	32	F2 PROCESSING			
d1	1.000	gf	0.069		
nt	32	gfs	not used		
2D ACQUISITION		fn	4096		
sw1	25165.1	F1 PROCESSING			
nl	128	gf1	0.005		
phase	arrayed	gfsl	not used		
PRESATURATION		proc1	lp		
satmode	n	fn1	2048		
wet	n	DISPLAY			
TRANSMITTER		sp	-76.5		
tn	H1	wp	4481.9		
strq	500.478	sp1	-838.8		
tof	796.1	wp1	19193.3		
tpwr	58	rf1	398.0		
pw	8.000	rfp	0		
DECOUPLER		rf11	1256.5		
dm	Cl3	rfp1	0		
dof	-600.6	PLOT			
dm	nmv	wc	206.0		
decwave	W40_HCN5mm	sc	0		
dma	32258	wc2	206.0		
dpr	38	sc2	0		
pxlvi	56	vs	19		
pxw	10.700	th	4		
HSQC		ai	cdc	ph	
j1xh	146.0				
multflg	y				
mult	2				
ADDITIONAL					
pxl180ad	ONE_ad300				
pxl180adr	ONE_ad300				
pxl180	465.4				
pxl1v1180	51				
pxl180ref	ONE_ref2-				
pxl180r	2000.2				
pxl1v1180r	43				

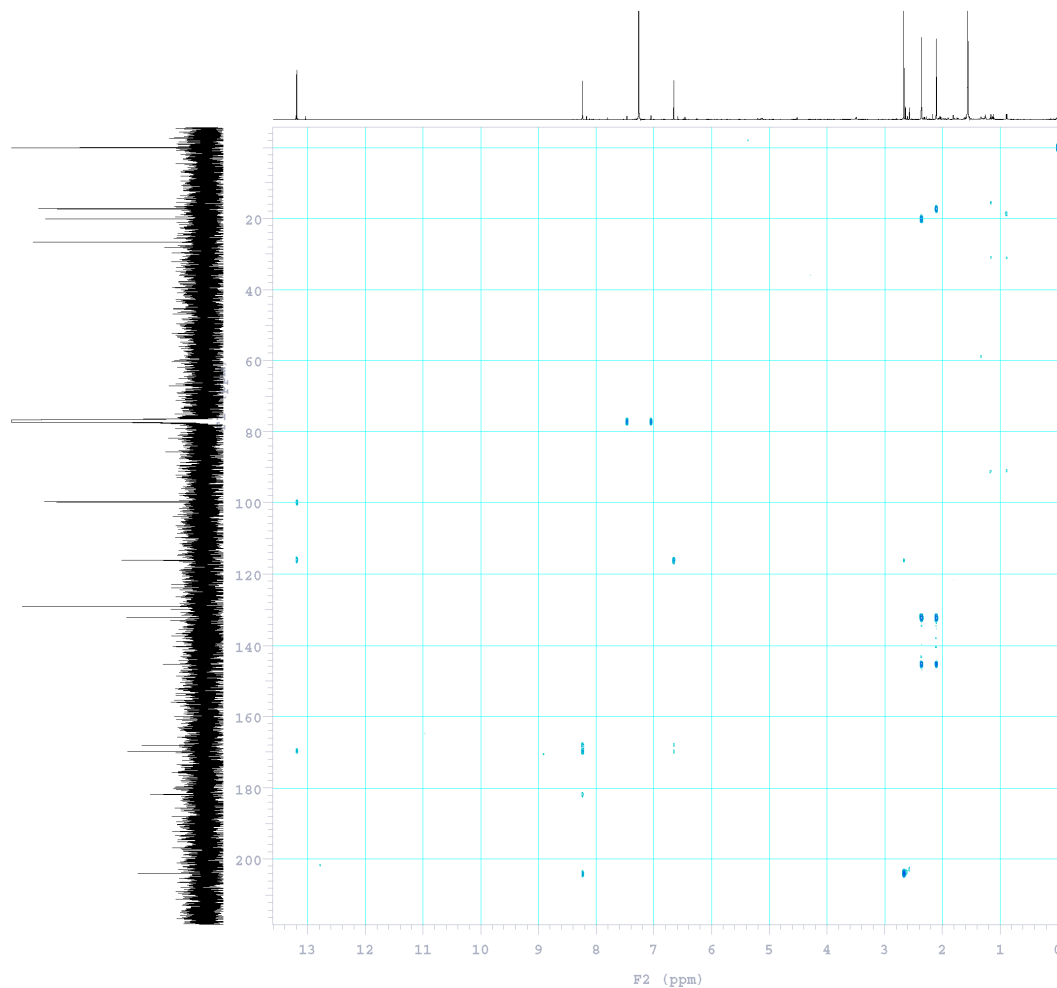


**Figure S95.** HMBC spectrum of **20** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-4-2-1-2-0.5mg-HMBC-CDCl3

exp6 gHMBCAD

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Nov 4 2020	hs	nm	array	phase
solvent	cdcl3	sapul	y	arraydim	256
sample		PPdrlg	y		
ACQUISITION		heglvl	6180	i	phase
sw	7396.4	SPECIAL		1	1
at	0.150	temp	not used	2	2
np	2218	gain	54		
fb	4000	spin	0		
ss	32	GRADIENTS			
d1	1.000	gs1vl1	409		
nt	32	gt1	0.001000		
2D ACQUISITION		gs1vl3	1227		
sw1	30200.1	gt3	0.001000		
nl	128	gstab	0.000500		
phase		arrayed	F2 PROCESSING		
PRESATURATION		sb	-0.075		
satmode	n	sbs	not used		
wet	n	fn	4096		
TRANSMITTER		F1 PROCESSING			
tn	H1	gt1	0.004		
sfrq	500.478	gtf1	not used		
tof	796.1	procl	lp		
tpwr	58	fn1	2048		
pw	8.000	DISPLAY			
DECOUPLER		sp	-94.6		
dn	C13	wp	6901.7		
dof	1287.0	sp1	-706.7		
dm	nnn	vp1	28135.6		
decwave	w40	HCNsm	rl1	398.0	
daf	32258	rfl	0		
dpwr	38	rfl1	1886.4		
pw1vl1	56	rflp1	0		
pw1	10.700	PLOT			
j1xh	146.0	sc	0		
jnxh	8.0	wc2	206.0		
ADIABATIC		sc2	0		
pw180ad	ONE	vs	19		
pw1vl180	51	th	5		
pw180	465.4	ai	cdc av		



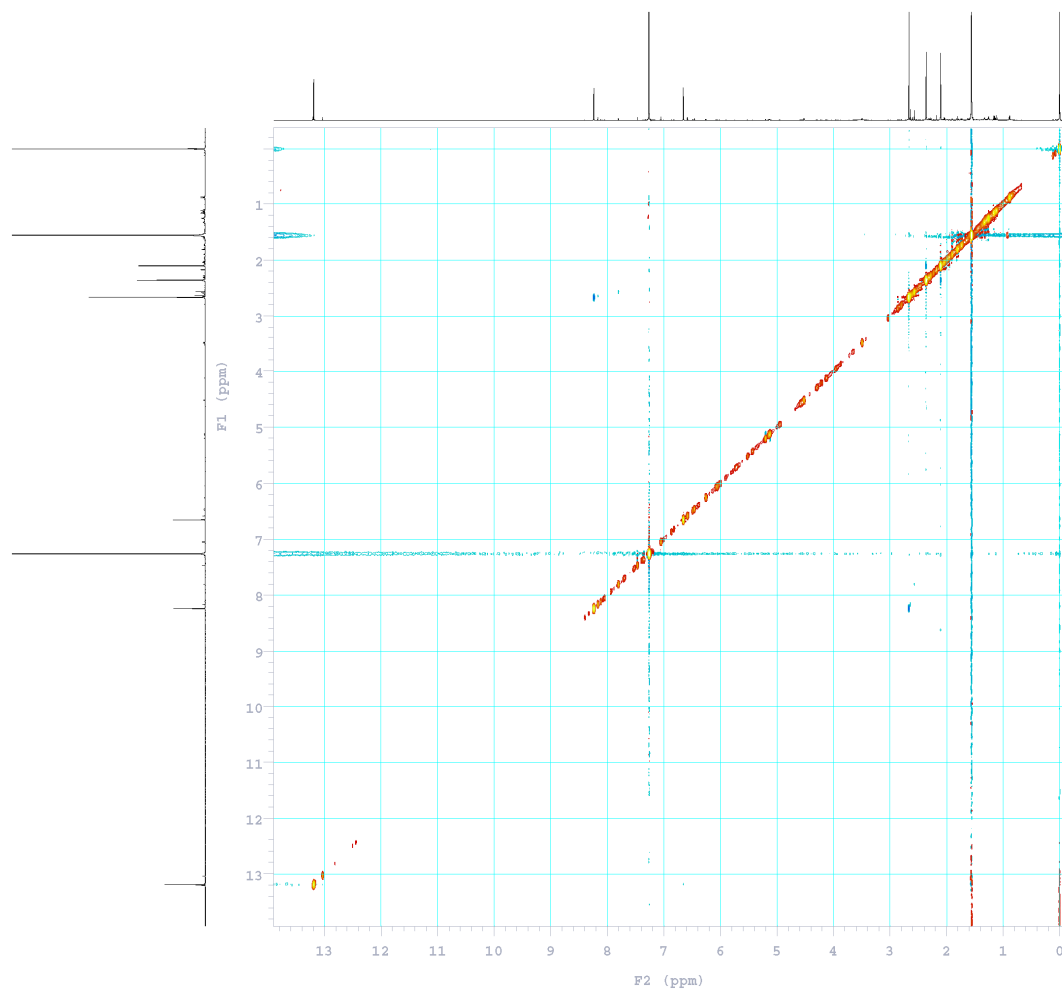


**Figure S96.** NOESY spectrum of **20** (measured in CDCl<sub>3</sub>, 500 MHz).

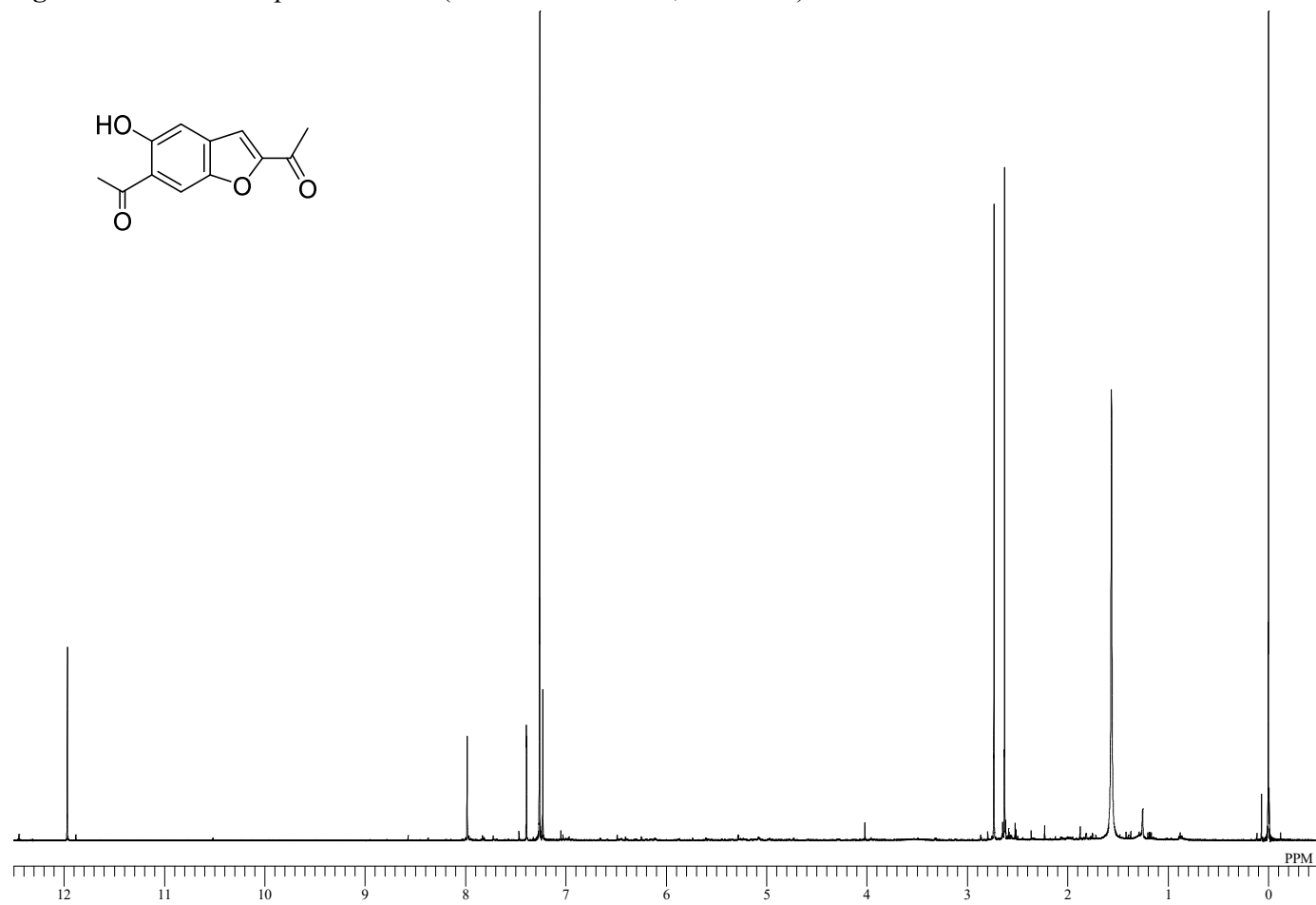
HYM-2014-48-R-4-2-1-2-0. Smg-NOESY-CDCl3

exp7 NOESY

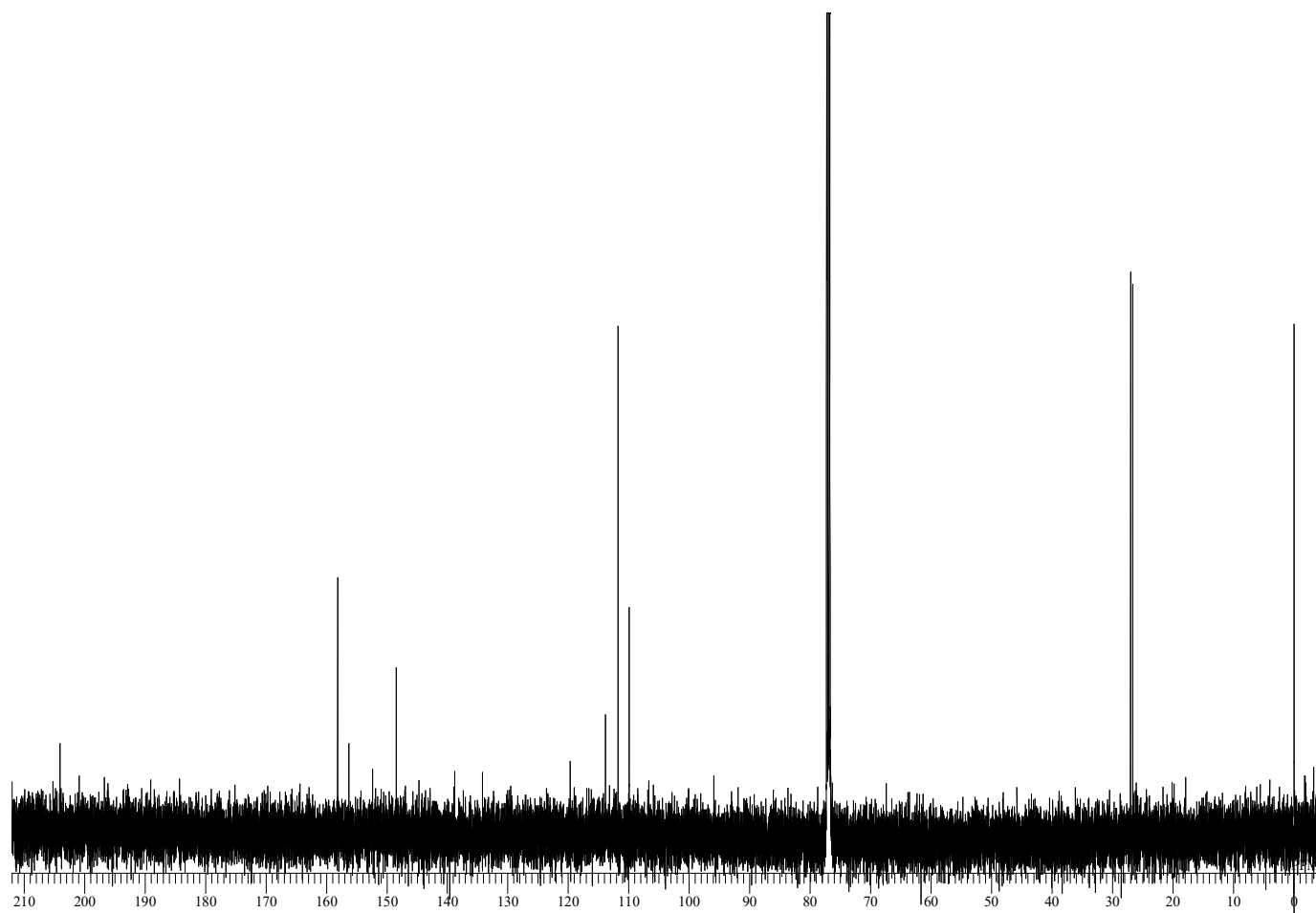
SAMPLE		FLAGS	
date	Nov 4 2020	hs	nn
solvent	cdcl3	espul	y
sample		ppdfig	y
acq	hagiv1	atn	
sw	7396.4	SPECIAL	
at	0.150	temp	not used
np	2218	gain	54
fn	4000	spin	0
ss	32	P2 PROCESSING	
d1	2.000	gf	0.069
nt	16	gfs	not used
2D ACQUISITION		fn	4096
sw1	7396.4	P1 PROCESSING	
ni	128	gf1	0.016
TRANSMITTER		gfsl	not used
tn	H1	procl	lp
sfrq	500.478	fnl	4096
tof	796.1	DISPLAY	
tpwr	58	sp	-87.4
pw	8.000	wp	7042.5
NOESY		wp1	-184.9
mixN	0.500	wp1	7154.5
PRESATURATION		rf1	398.0
satmode	n	rfl	0
wet	n	rfl1	398.0
DECOUPLER		rfpl	0
dn	C13	PLOT	
dm	nmn	wc	206.0
		sc	0
		wc2	206.0
		sc2	0
		vs	19
		th	1
		ai	ph



**Figure S97.**  $^1\text{H}$  NMR spectrum of **28** (measured in  $\text{CDCl}_3$ , 500 MHz).



**Figure S98.**  $^{13}\text{C}$  NMR spectrum of **28** (measured in  $\text{CDCl}_3$ , 126 MHz).

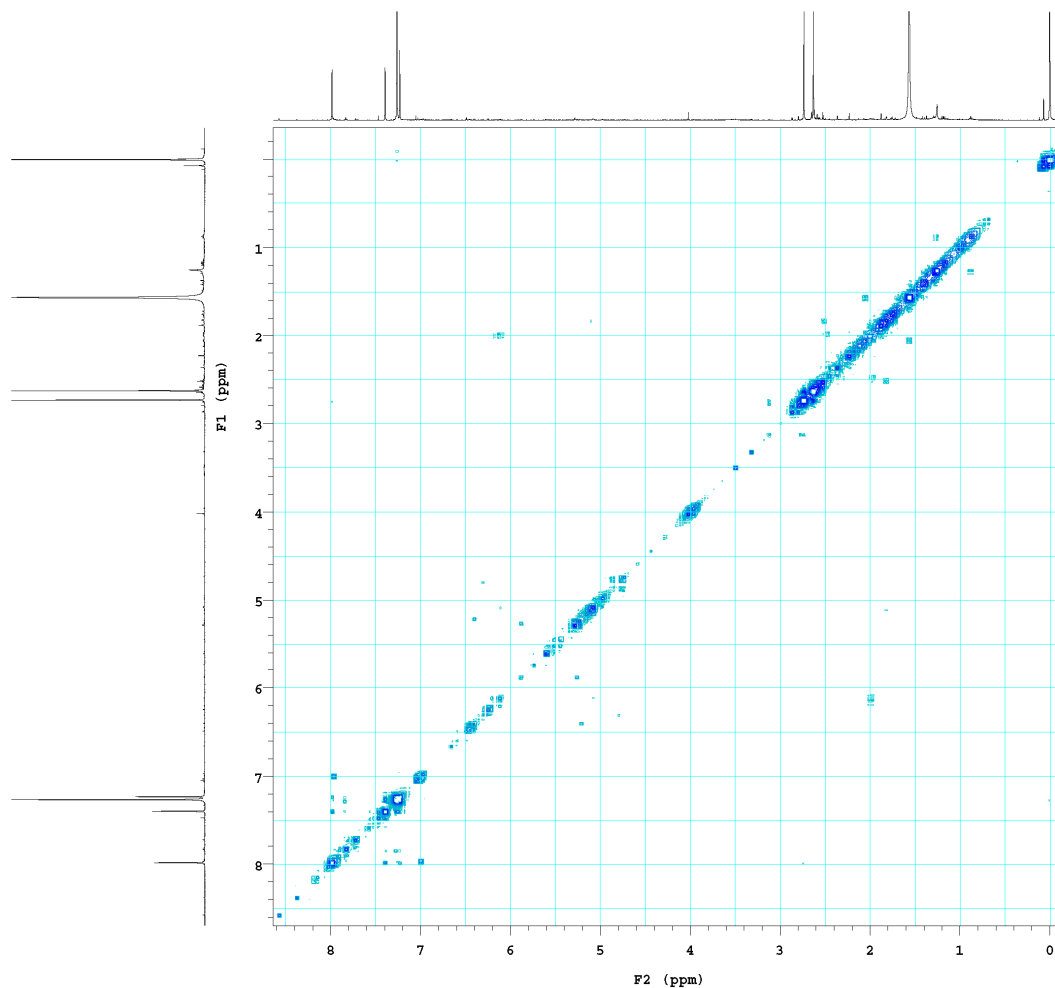


**Figure S99.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **28** (measured in  $\text{CDCl}_3$ , 500 MHz).

HYM-2014-48-R-5-3-3-1-0.6mg-COSY- $\text{CDCl}_3$

exp4 gCOSY

SAMPLE		FLAGS	nm
date	Jan 6 2021	hs	y
solvent	odcl3	espul	6180
sample	hscvlv		
ACQUISITION		SPECIAL	
sw	6944.4	temp	not used
st	0.150	gain	40
np	2084	spin	0
fb	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	8	fn	4096
2D ACQUISITION		F1 PROCESSING	
sw1	6944.4	sb1	-0.018
n1	128	sb1	not used
d2	0	procl	lp
PRESATURATION		fn1	4096
satmode	n	DISPLAY	
wet	n	sp	-109.3
TRANSMITTER		wp	4431.8
tn	H1	sp1	-177.2
sfrq	500.478	wp1	4526.8
tof	441.5	rf1	526.4
tpwr	58	rfp	0
pw	8.000	rf11	526.4
GRADIENTS		rfp1	0
gvlv1E	5154	PLOT	
gtE	0.001000	wc	206.0
EDratio	1.000	sc	0
gstab	0.000500	wc2	206.0
DECOUPLER		sc2	0
dn	C13	vs	137
dm	nmn	th	7
	ai	cdc	av

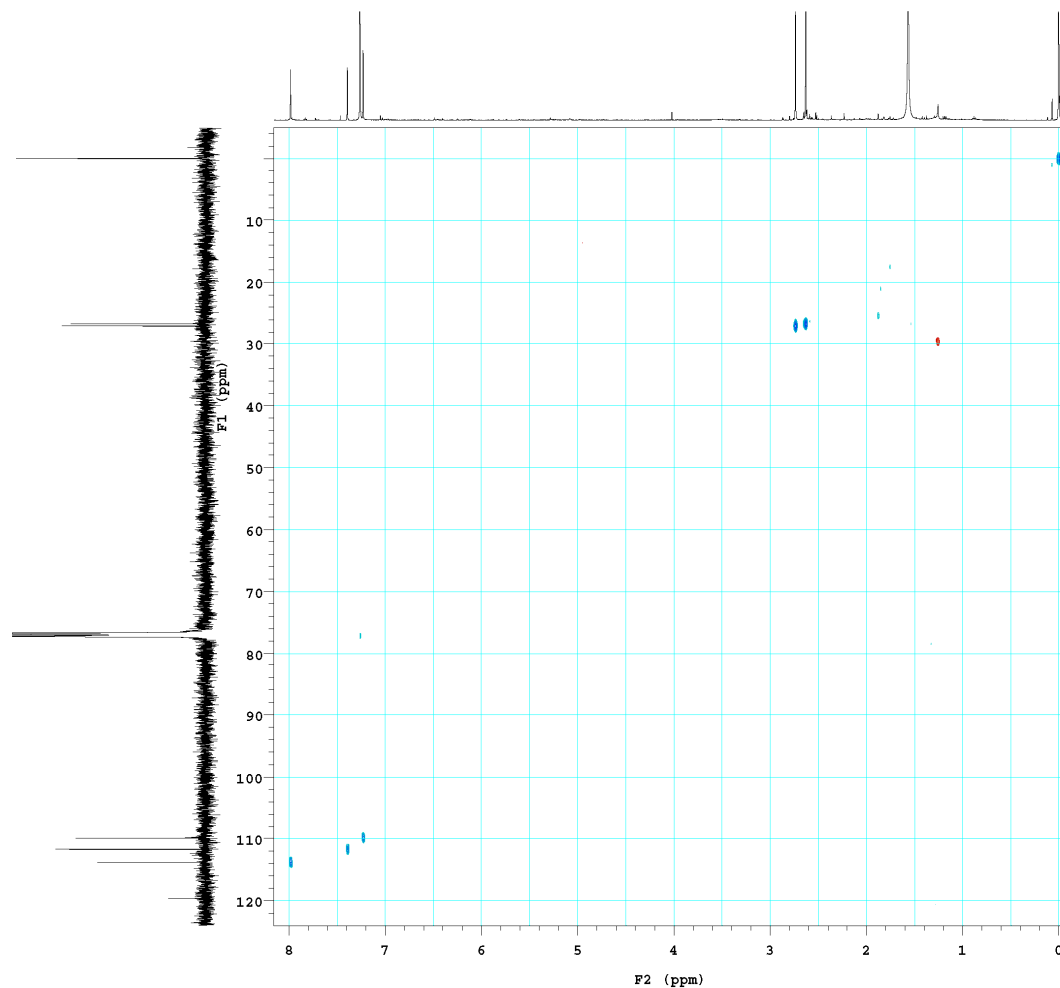


**Figure S100.** HSQC spectrum of **28** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-5-3-3-1-0.6mg-HSQC-CDCl3

exp5 HSQCAD

SAMPLE		FLAGS	ACQUISITION ARRAYS	
date	Jan 6 2021	hs	mn	array
solvent	cdcl3	sapul	y	arraydim
sample	PPGf1q	y		256
ACQUISITION		hsglvt	6180	1
sw	6944.4	SPECIAL	1	1
at	0.150	temp	not used	
np	2084	gain	40	2
fb	4000	spin	0	
ss	32	F2 PROCESSING		
dl	1.000	gf	0.069	
nt	16	gfs	not used	
2D ACQUISITION		fn	4096	
sw1	25165.1	F1 PROCESSING		
nl	128	gtl	0.005	
phase	arrayed	gfs1	not used	
PRESATURATION	procl	lp		
satmode	n	fnl	2048	
wet	n	DISPLAY		
TRANSMITTER		sp	-58.5	
tn	H1	wp	4140.2	
sfrq	500.478	sp1	-617.6	
tof	441.5	wp1	16219.7	
tpwr	58	rfl	526.4	
pw	8.000	rtp	0	
DECOUPLER		rfl1	1256.5	
dn	C13	rflp1	0	
dof	-600.6	PLOT		
dm	nny	wc	206.0	
decwave	W40_HCN5mm	sc	0	
dmf	32258	wc2	206.0	
dpwr	38	sc2	0	
pw1vt1	56	vs	137	
pw1	10.700	th	4	
HSQC		ai	cdc	ph
j1kh	146.0			
nullflg	y			
mult	2			
ADIABATIC				
pw180ad	ONE	ad300		
pw180adr	ONE	ad300		
OR				
pw180	465.4			
pw1vt180	51			
pw180ref	ONE	ref2		
OR				
pw180r	2000.2			
pw1vt180r	43			

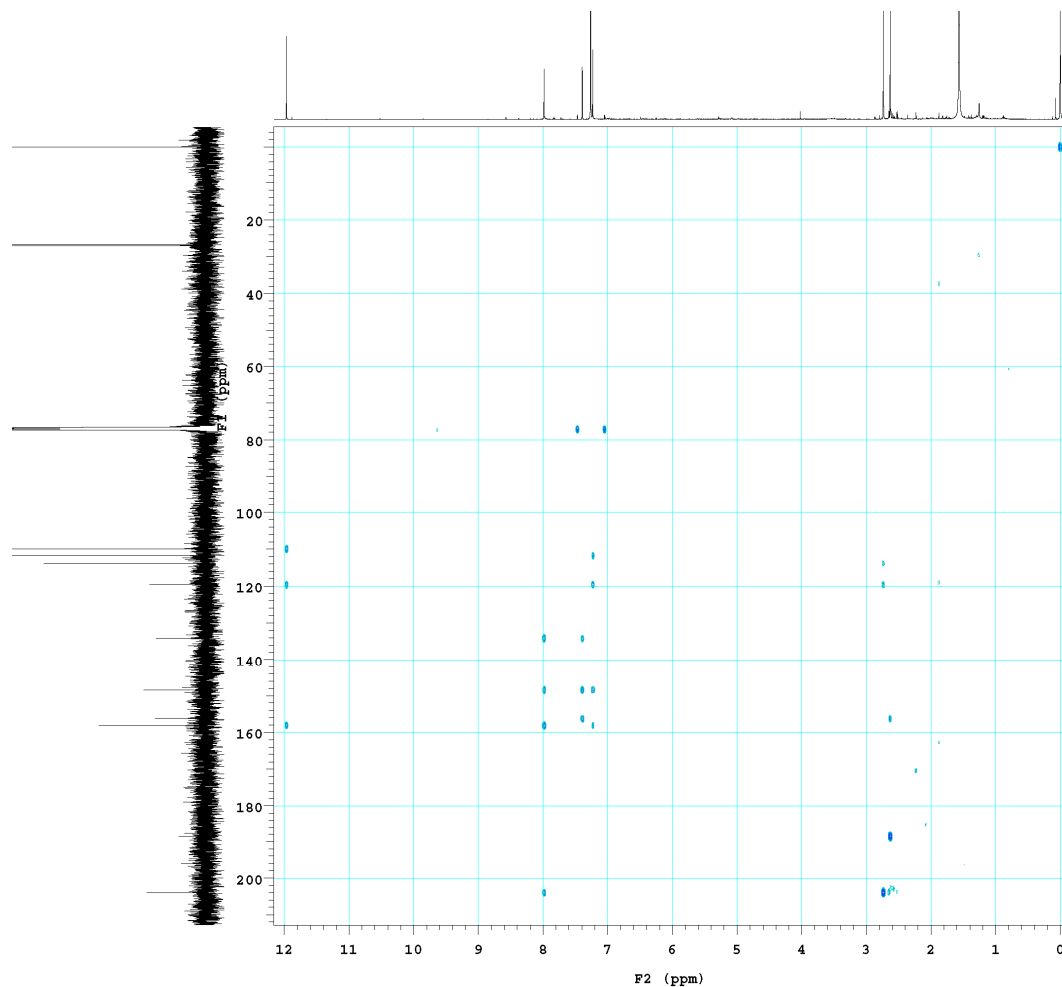


**Figure S101.** HMBC spectrum of **28** (measured in CDCl<sub>3</sub>, 500 MHz).

HYM-2014-48-R-5-3-3-1-0.6mg-HMBC-CDCl3

exp6 gRMBSCAD

SAMPLE		FLAGS	ACQUISITION ARRAYS	
date	Jan 6 2021	hs	nm	array phase
solvent	cdcl3	sspul	y	arraydim 256
sample		PPGflg	y	
ACQUISITION		hsglvi	6180	i phase
sw	6944.4	SPECIAL	1	1
at	0.150	temp	not used	
np	2084	gain	40	2
fb	4000	spin	0	
ss	32	GRADIENTS		
d1	1.000	gzlvi1	409	
nt	64	gt1	0.001000	
2D ACQUISITION		gzlvi3	1227	
sw1	30200.1	gt3	0.001000	
ni	128	gstab	0.000500	
phase	arrayed	F2 PROCESSING		
PRESATURATION		sb	-0.075	
satmode	n	sbs	not used	
wet	n	fn	4096	
TRANSMITTER		F1 PROCESSING		
tn	H1	gt1	0.004	
strq	500.478	gtsl	not used	
tof	441.5	procl	lp	
tpwr	58	fnl	2048	
pw	8.000	DISPLAY		
DECOUPLER		sp	-75.4	
dn	C13	wp	6161.2	
dof	1287.0	sp1	-677.2	
dn	nm	wp1	27457.3	
decwave	W40_HCN5mm	rfl	526.4	
dmf	32258	rfp	0	
dpr	38	rfl1	1886.4	
pxwlv1	56	rflp1	0	
pxw	10.700	PLOT		
HMBC		wc	206.0	
jlxh	146.0	sc	0	
jmxh	8.0	wc2	206.0	
ADIABATIC		sc2	0	
pxw180ad	ONE_ad300	vs	137	
pxwlv180	51	th	4	
pxw180	465.4	ai	cdc	av



**Figure S102.** NOESY spectrum of **28** (measured in CDCl<sub>3</sub>, 500 MHz).



SAMPLE				PLAGE	
date	6 of 2021	hs		nn	
solvent	cdcl3	apul		y	
sample		PGFqlv		y	
ACQUISITION		hagvlv		6180	
sw	6944.4				
at	0.150	temp	not used		
nb	2084	gain		40	
fp	4000	spin			
ns	22	P2 PROCESSING			
d1	2.000	gf	0.069		
nt	16	gfs	not used		
		fn	4096		
2D ACQUISITION		F1 PROCESSING			
sw1	6944.4				
nt1	128	gr1	0.017		
tn		gfs1	not used		
TRANSMITTER	H1	procl		lp	
sfrq	500.478	fn1		4096	
cos	441.5				
tpwr	58	sp	-34.7		
pw	8.000	wp	4353.8		
	NOE5Y	sp1	-139.9		
mixN	0.500	wpl	4970.9		
SATURATION		r1	526.4		
satmode	n	rtp	0		
wet	n	rfl1	526.4		
DECOUPLER		rflp1	0		
dn					
C13					
	sc		206.0		
	wc		206.0		
	wc2		206.0		
	sc2		137.4		
	vs		137.4		
	th		1		
	ai	ph			

