

13C DEPT135 F5(2)
C13DEPT135 CDC13 C:\PFSF USM

Current Data Parameters
NAME DRAMIN_LOIYELSIR
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120610
Time_ 17.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135
TD 65536
SOLVENT CDC13
NS 1000
DS 4
SWH 20161.291 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 188.56
DW 24.800 usec
DE 6.50 usec
TE 294.3 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.25 usec
P13 2000.00 usec
PLW0 0 W
PLW1 74.00000000 W
SFO1 125.7678486 MHz
SPNAM5 Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 11.87899971 W

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 14.80 usec
P4 29.60 usec
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.51337999 W
SFO2 500.1315995 MHz

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

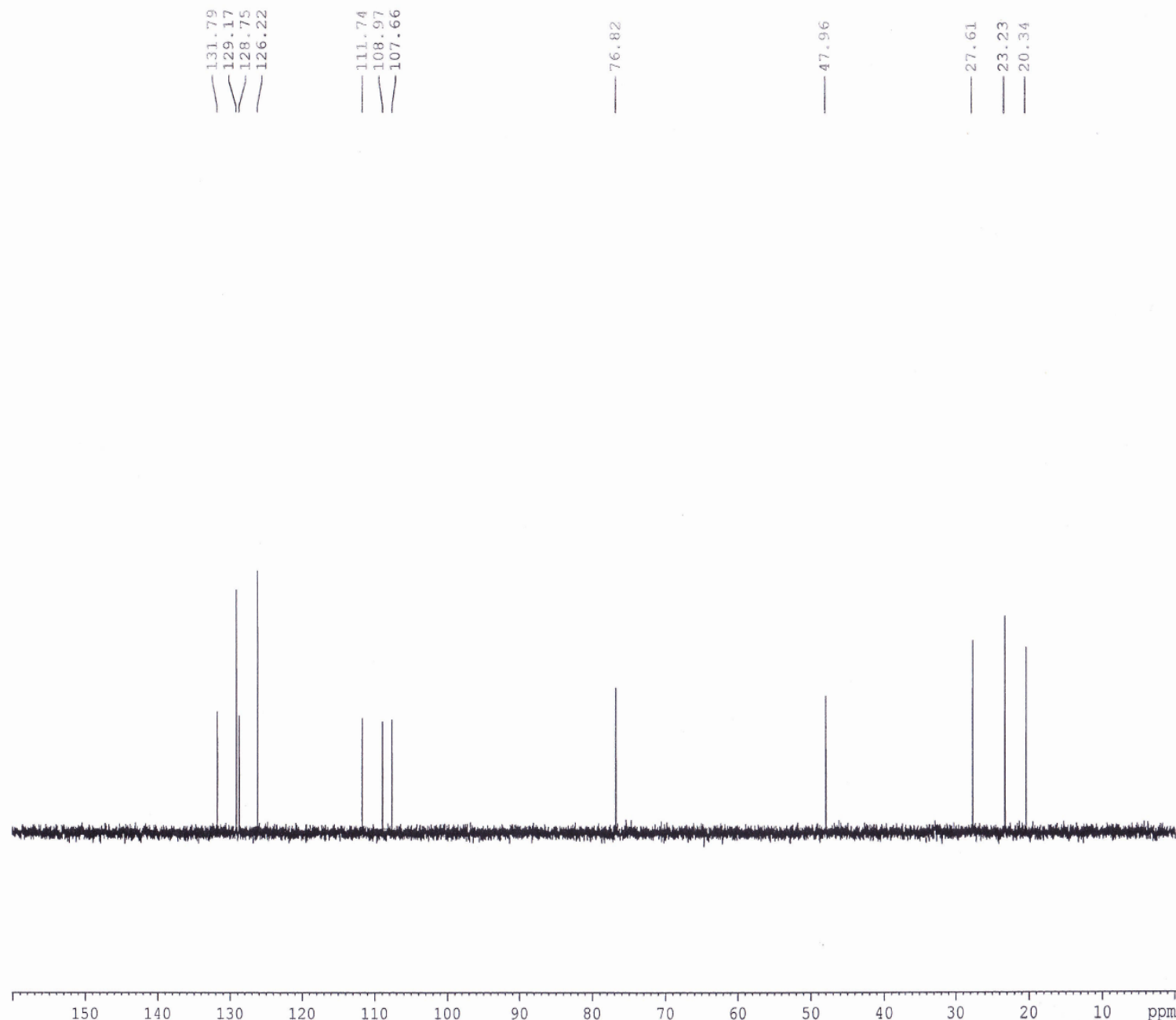


Figure S1: ^{13}C DEPT135 NMR spectrum of (-)-pseudosemiglabrin collected in CDCl_3 at ambient temperature (125.7 MHz).

13C DEPT45 F5(2)
C13DEPT45 CDC13 C:\PPSF USM

Current Data Parameters
NAME DRAMIN_LOIYELSIR
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120610
Time_ 16.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept45
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 188.56
DW 16.800 usec
DE 6.50 usec
TE 294.3 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.25 usec
P2 20.50 usec
PLW1 74.00000000 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 14.80 usec
P4 29.60 usec
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.51337999 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

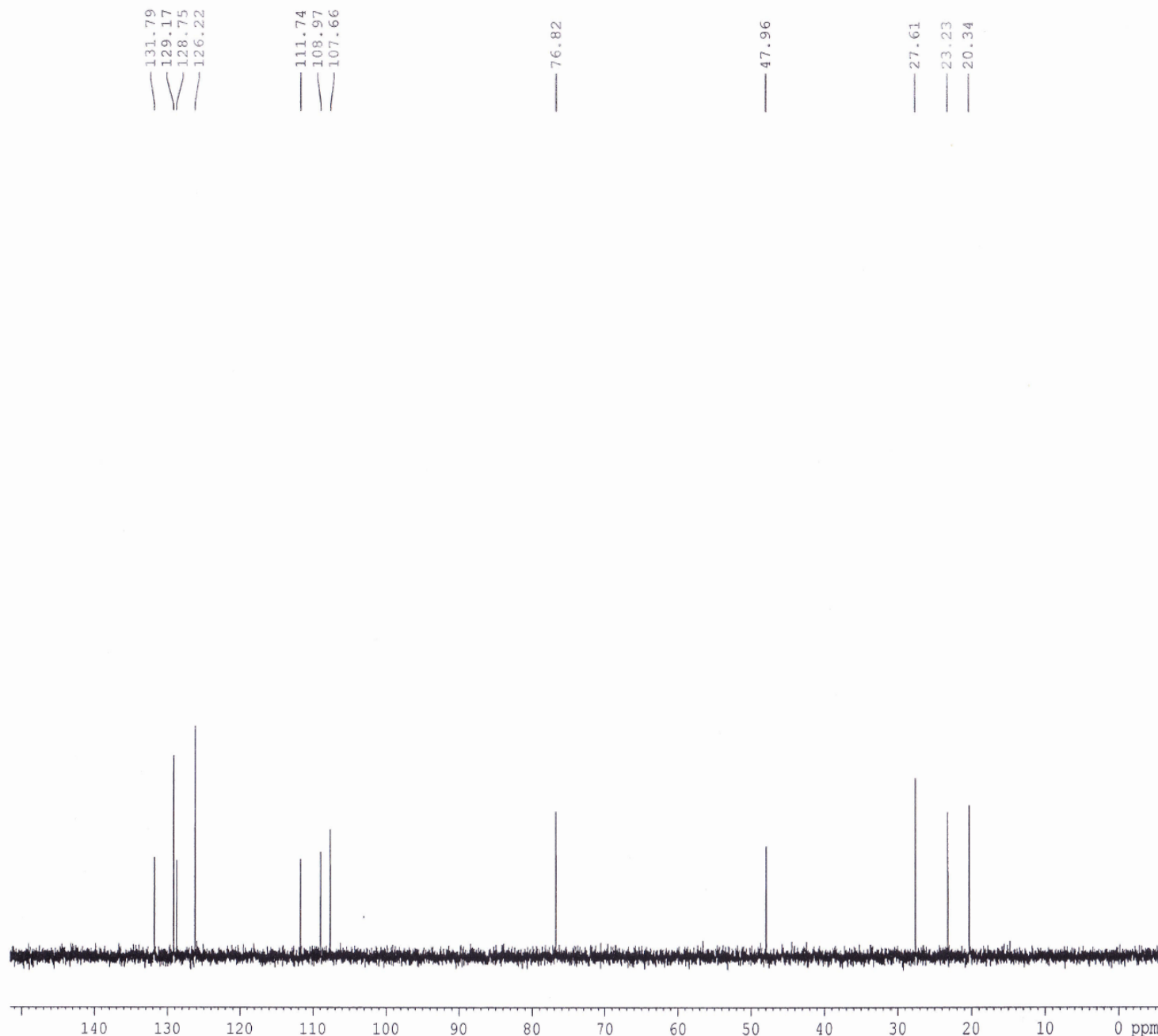


Figure S2: ^{13}C DEPT145 NMR spectrum of (-)-pseudosemiglabrin collected in CDCl_3 at ambient temperature (125.7 MHz).

C-H

DRAMIN_LOIYELSIR 27 1 C:\PPSF\data\USM\nmr

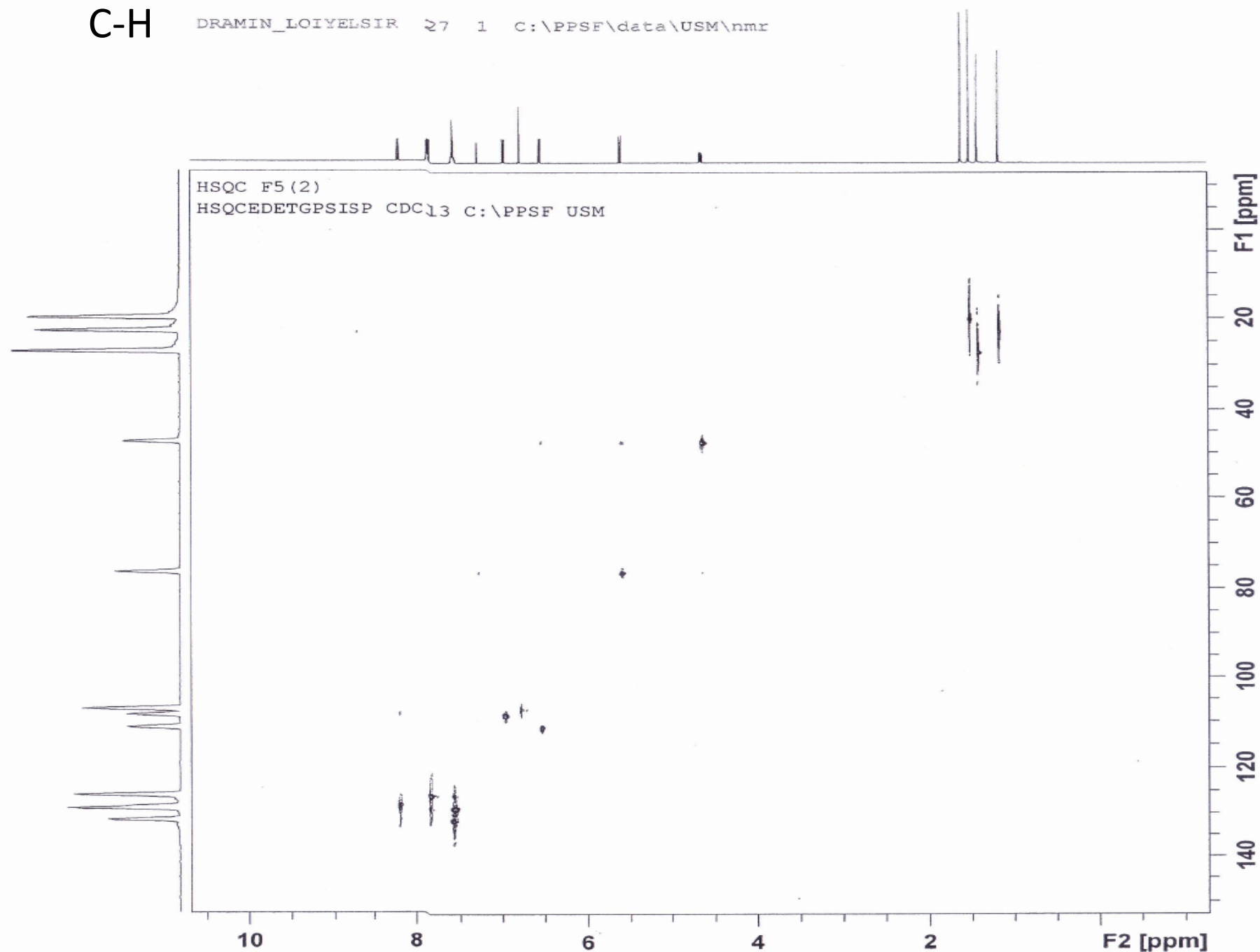


Figure S3: 2D HSQC (Heteronuclear single quantum coherence spectroscopy) NMR spectrum of (-)-pseudosemiglabrin collected in CDCl₃ at ambient temperature.

C-(-)_nH

DRAMIN_LOIYELSIR 28 1 C:\PPSF\data\USM\nmr

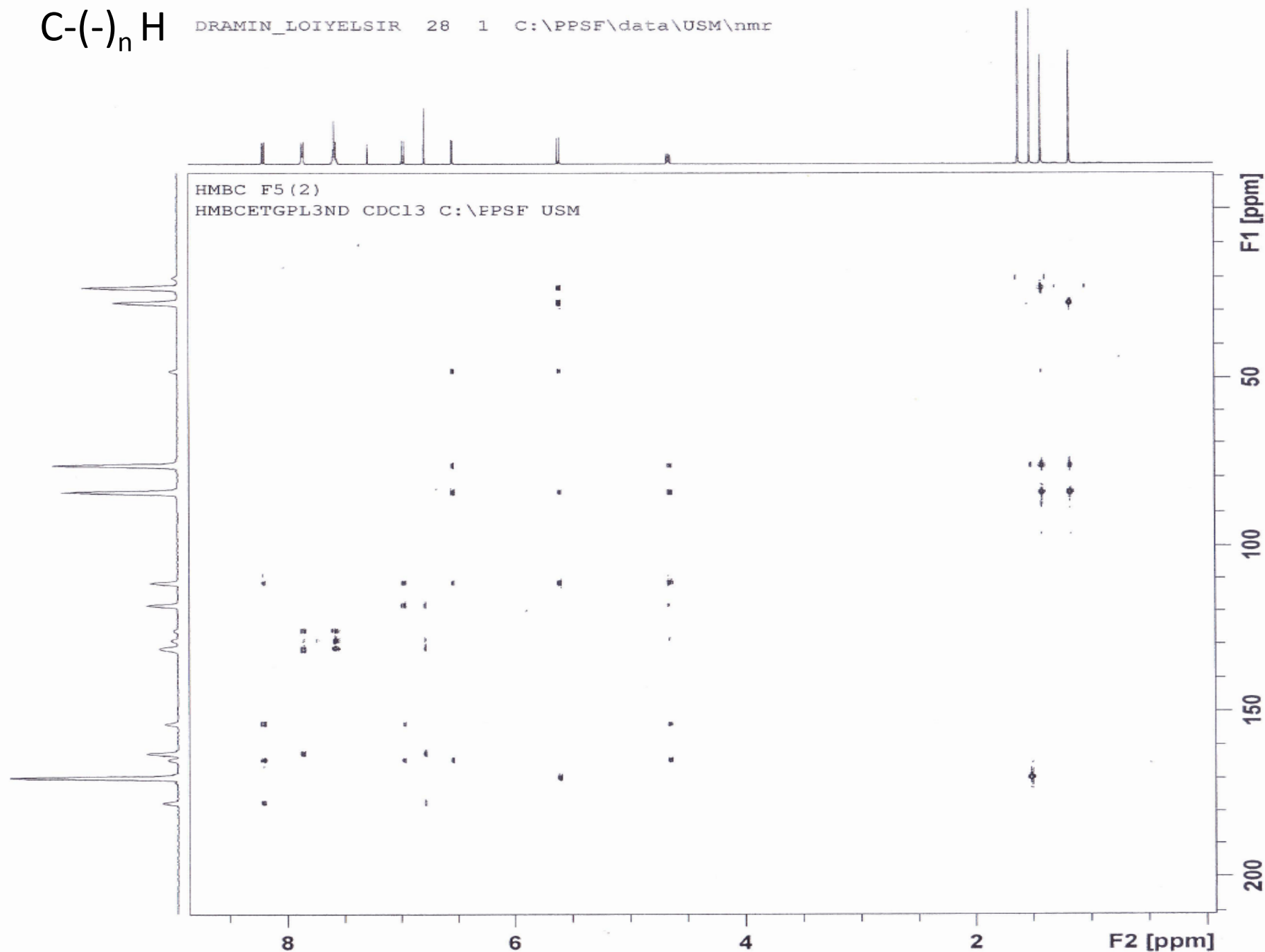
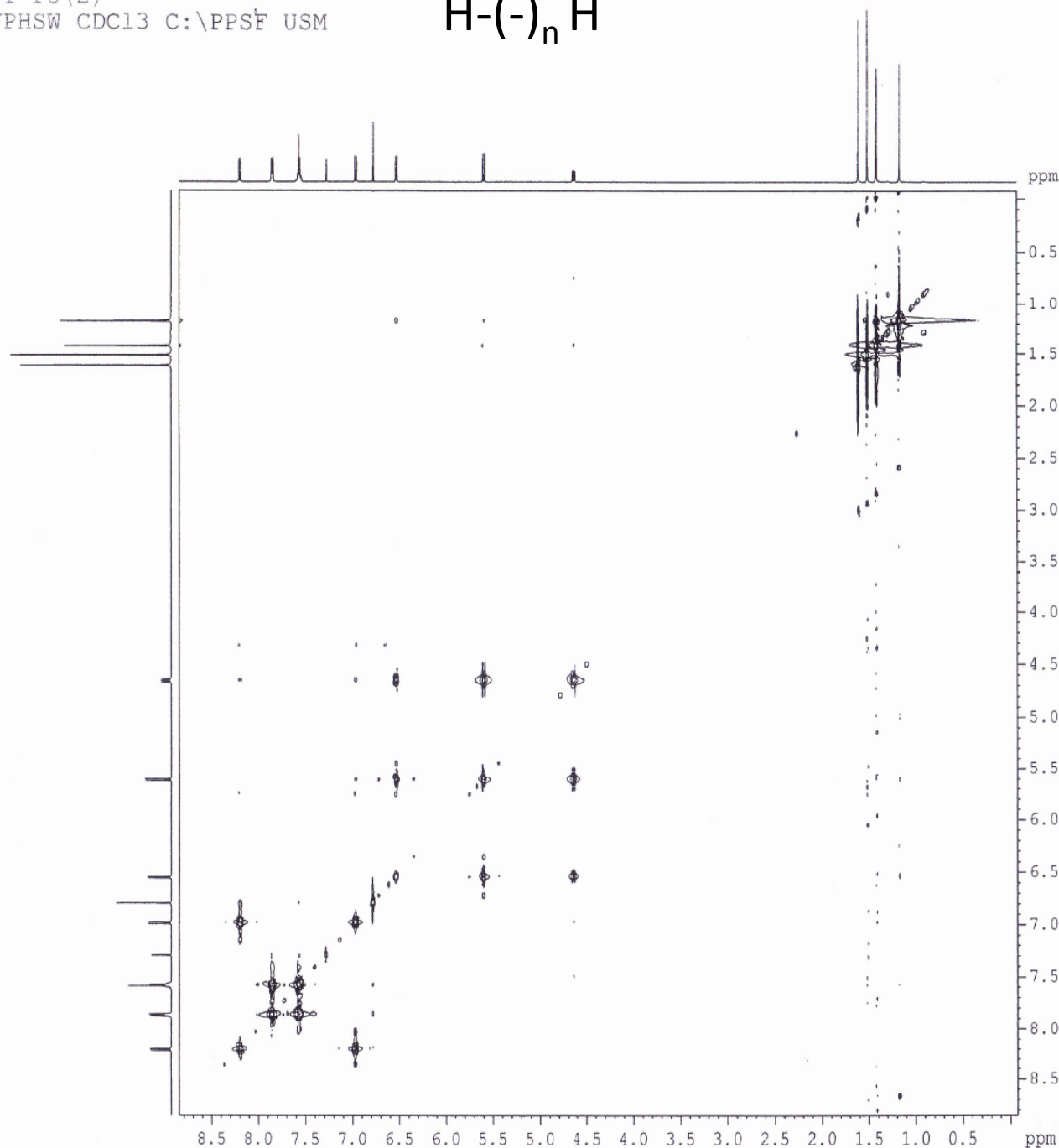
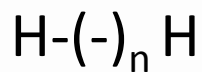


Figure S4: 2D HMBC (heteronuclear multiple-bond correlation spectroscopy) NMR spectrum of (-)-pseudosemiglabrin collected in CDCl₃ at ambient temperature.



Current Data Parameters
NAME DRAMIN_LOIYELSIR
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120611
Time_ 0.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG mlevphpp
TD 2048
SOLVENT CDC13
NS 20
DS 16
SWH 4464.286 Hz
FIDRES 2.179827 Hz
AQ 0.2294260 sec
RG 188.56
DW 112.000 usec
DE 6.50 usec
TE 295.2 K
D0 0.00009858 sec
D1 1.97132802 sec
D9 0.08000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
IN0 0.00022400 sec
L1 42

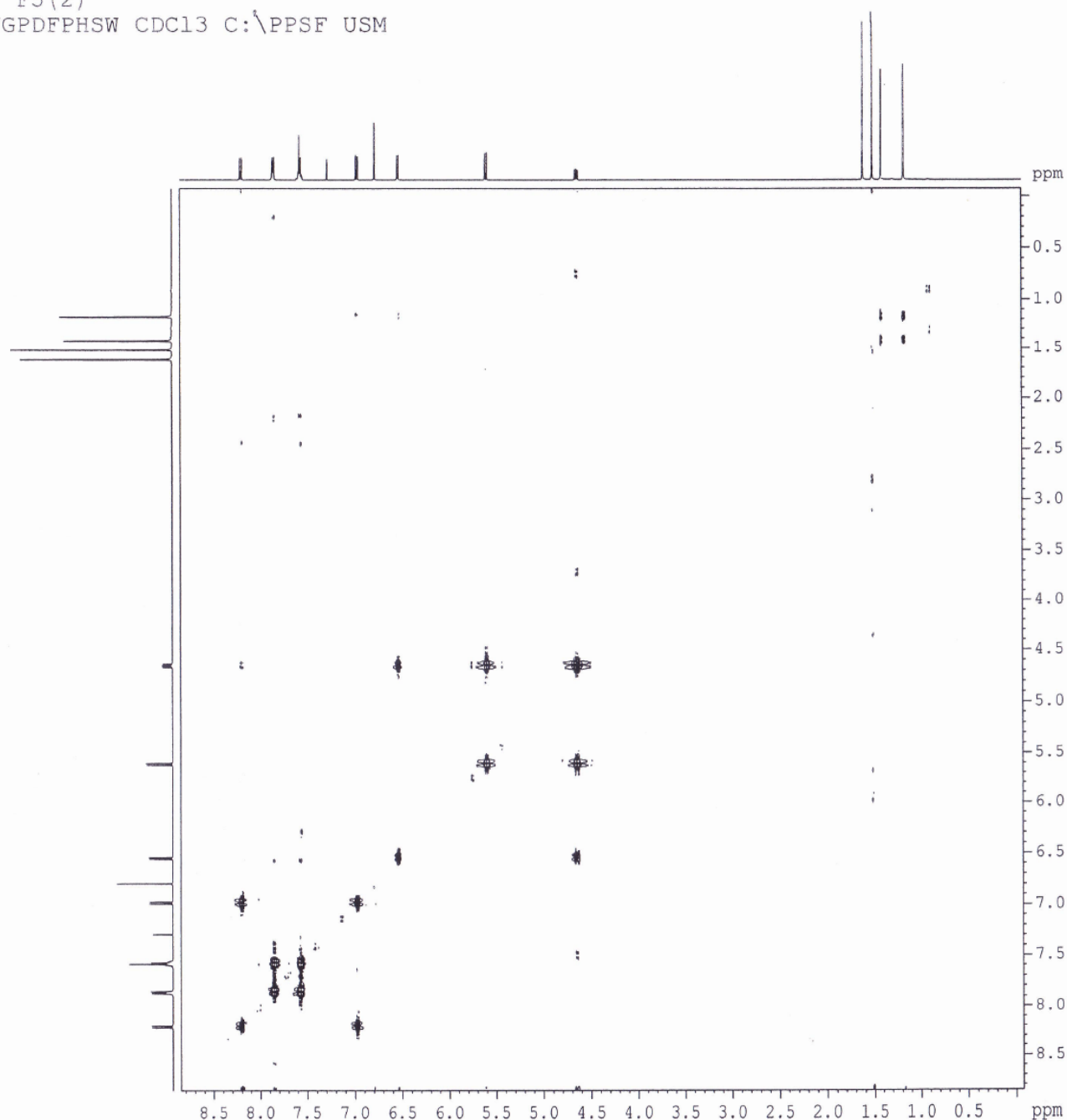
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P5 17.34 usec
P6 26.00 usec
P7 52.00 usec
P17 2500.00 usec
PLW1 15.00000000 W
PLW10 4.86040020 W
SFO1 500.1321938 MHz

F1 - Acquisition parameters
TD 256
SFO1 500.1322 MHz
FIDRES 17.438616 Hz
SW 8.926 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 500.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

Figure S5: 2D TOCSY (total correlation spectroscopy) NMR spectrum of (-)-pseudosemiglabrin collected in CDCl₃ at ambient temperature.

COSY F5(2)
COSYGPDPFPHSW CDCl3 C:\PPSF USM



Current Data Parameters
NAME DRAMIN_LOIYELSIR
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120610
Time_ 17.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfphpp
TD 2048
SOLVENT CDCl3
NS 20
DS 4
SWH 4464.286 Hz
FIDRES 2.179827 Hz
AQ 0.2294260 sec
RG 188.56
DW 112.000 usec
DE 6.50 usec
TE 293.9 K
D0 0.00009316 sec
D1 1.93719494 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00022400 sec

===== CHANNEL f1 =====
NUC1 1H
P1 14.80 usec
P2 29.60 usec
P17 2500.00 usec
PLW1 15.00000000 W
PLW10 4.86040020 W
SFO1 500.1321938 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SMSQ10.100
GPNAM2 SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 500.1322 MHz
FIDRES 17.438616 Hz
SW 8.926 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 500.1300000 MHz
WDW QSINE
SSB 2

Figure S6: 2D COSY (correlation spectroscopy) NMR spectrum of (-)-pseudosemiglabrin collected in CDCl₃ at ambient temperature.

H-Bonding

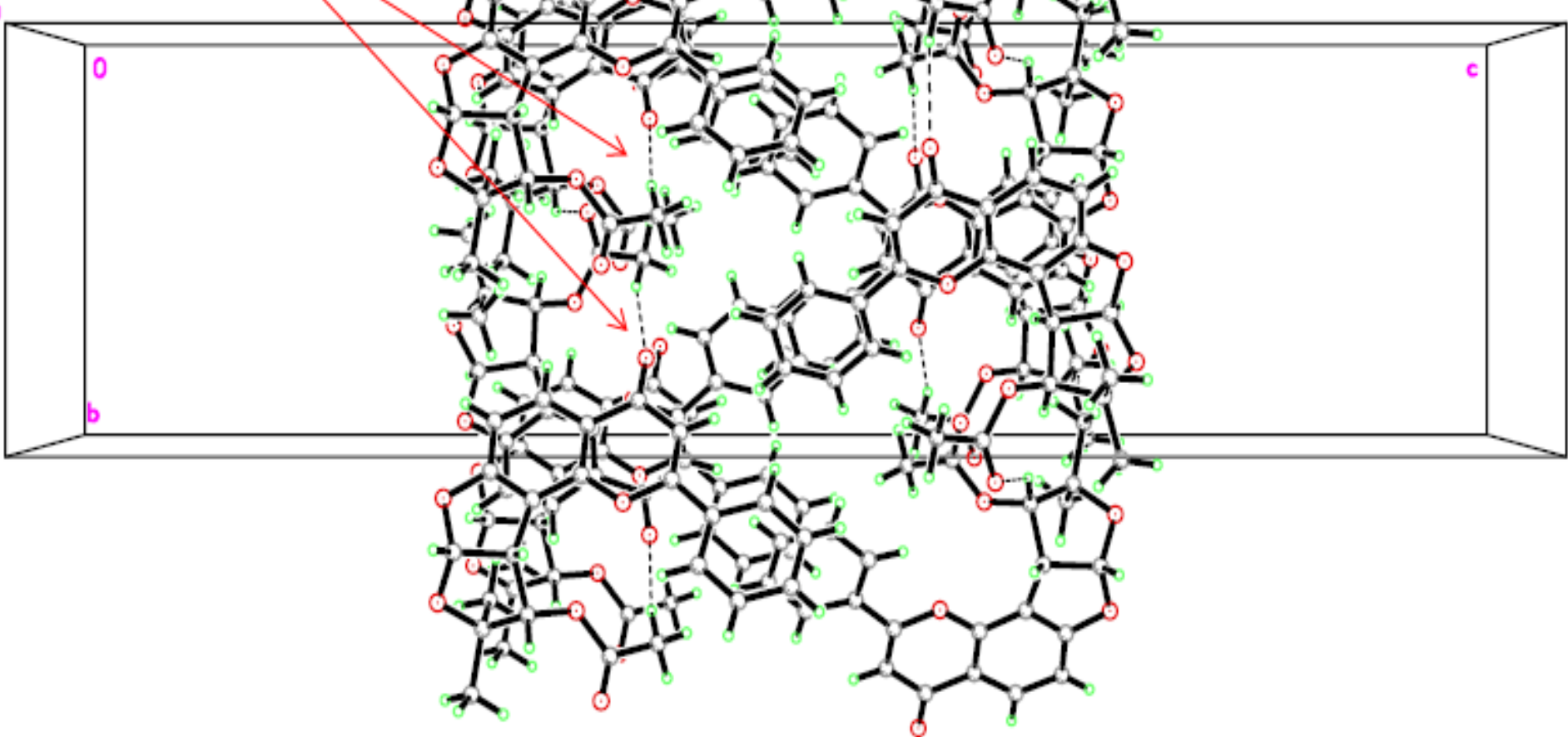


Figure S7: Crystal packing of (-)-Pseudosemiglabrin. The molecules packed in orthorhombic crystal system through intermolecular hydrogen bonds (C=O---H), shown as dashed lines.

Table S1: Selected Bond Lengths (Å) and Angles (°) of (-)-Pseudosemiglabrin
(Crystal Structure Unit A).

C15A-O3A	1.461(2)	C9A-O5A	1.237(3)	C17A-C18A	1.505(3)
O3A-C14A	1.393(2)	C22A-O6A	1.197(3)	C14A-C17A	1.551(3)
C14A-O2A	1.461(2)	C7A-C6A	1.462(12)		
O2A-C13A	1.369(2)	C6A-C5A	1.475(3)		
C19A-O1A	1.370(2)	C6A-C1A	1.402(3)		
O1A-C7A	1.367(2)	C16A-C17A	1.539(3)		
O2A-C14A-O3A	110.73(15)		C14A-O2A-C13A	108.27(14)	
C18A-C17A-C16A	116.54(16)		C15A-O3A-C14A	110.58(14)	
C21A-C15A-C20A	110.57(16)		C19A-O1A-C7A	118.93(15)	
C13A-C12A-C11A	116.49(18)		C16A-O4A-C22A	117.41(15)	
C10A-C9A-C8A	114.25(17)		O4A-C22A-C23A	110.29(16)	
C1A-C6A-C5A	118.72(18)				

Table S2: Selected Bond Lengths (Å) and Angles (°) of (-)-Pseudosemiglabrin
(Crystal Structure Unit B).

C15B-O3B	1.456(2)	C9B-O5B	1.237(2)	C17B-C18B	1.504(3)
O3B-C14B	1.392(2)	C22B-O6B	1.202(3)	C14B-C17B	1.552(3)
C14B-O2B	1.471(2)	C7B-C6B	1.472(3)		
O2B-C13	1.364(2)	C6B-C5B	1.403(3)		
C19B-O1B	1.373(2)	C6B-C1B	1.396(3)		
O1B-C7B	1.368(2)	C16B-C17B	1.549(3)		
O2B-C14B-O3B	110.58(15)		C14B-O2B-C13B	108.53(14)	
C18B-C17B-C16B	116.18(16)		C15B-O3B-C14B	111.24(14)	
C21B-C15B-C20B	111.06(16)		C19B-O1B-C7B	118.96(15)	
C13B-C12B-C11B	116.63(18)		C16B-O4B-C22B	117.07(15)	
C10B-C9B-C8B	114.32(17)		O4B-C22B-C23B	110.94(16)	
C1B-C6B-C5B	118.67(18)				