

Total Synthesis of the Proposed Structure of Indolyl 1,2-Propanediol Alkaloid, 1-(1*H*-Indol-3-yloxy)propan-2-ol

Momoko Kimata, and Takumi Abe*

Graduate School of Medicine, Dentistry and Pharmaceutical Sciences, Okayama University, 1-1-1 Tsushima-naka, Kita-ku, Okayama 7008530, Japan

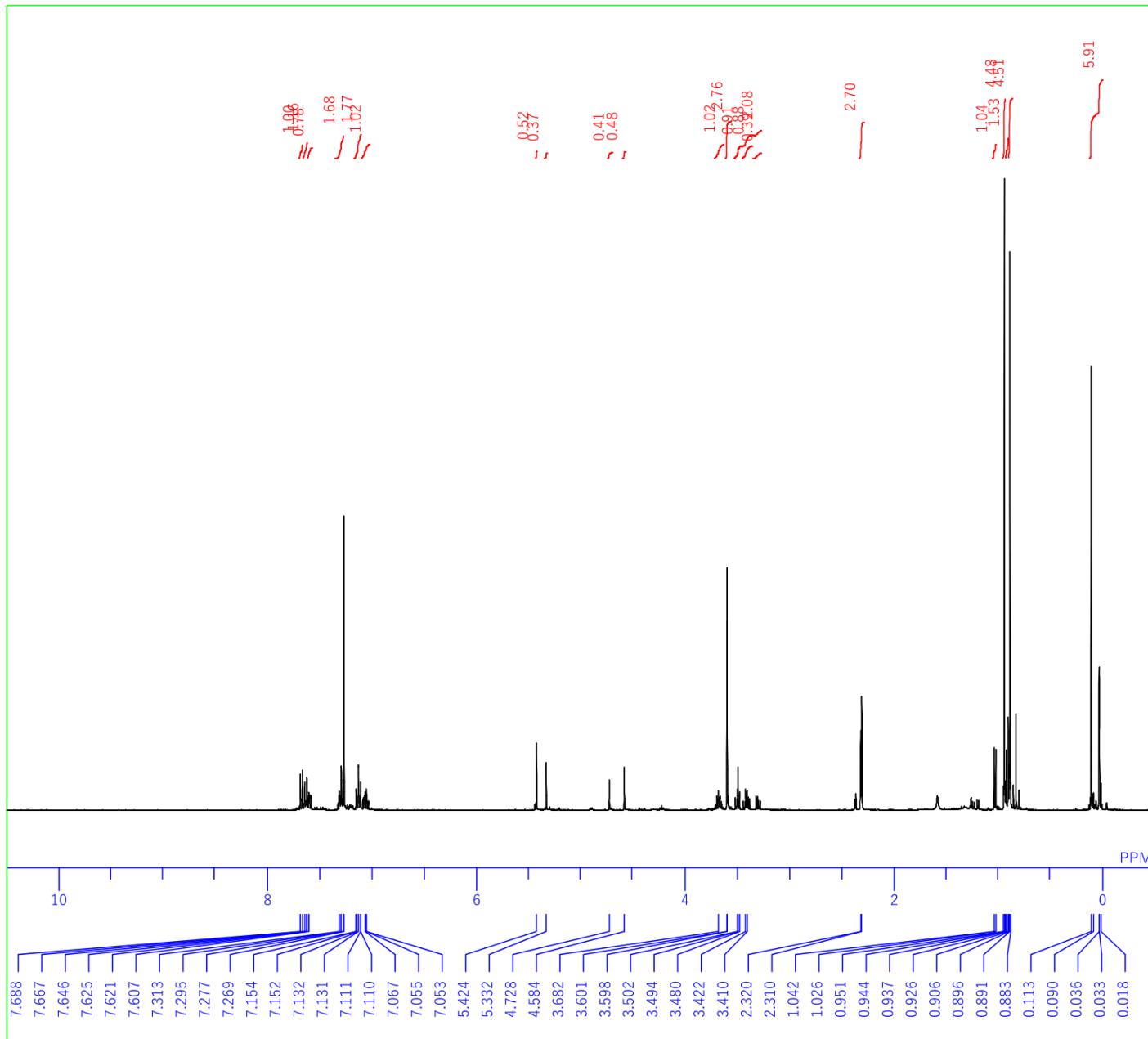
E-mail: t-abe@okayama-u.ac.jp

SUPPORTING INFORMATION

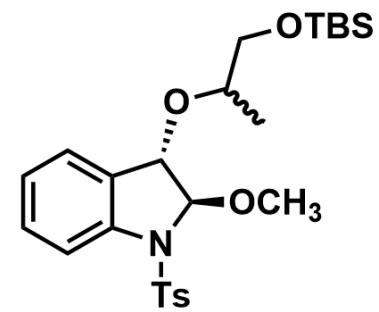
Table of Contents		Page No
Copies of ^1H and $^{13}\text{C}\{\text{H}\}$ NMR spectra of TBS-5	Figures S1-S2	S2-3
Copies of ^1H and $^{13}\text{C}\{\text{H}\}$ NMR spectra of 5	Figures S3-S4	S4-5
Copies of ^1H and $^{13}\text{C}\{\text{H}\}$ NMR spectra of 6	Figures S5-S6	S6-7
Copies of ^1H and $^{13}\text{C}\{\text{H}\}$ NMR spectra of TBS-7	Figures S7-S8	S8-9
Copies of ^1H and $^{13}\text{C}\{\text{H}\}$ NMR spectra of 7	Figures S9-S10	S10-11
Copies of ^1H and $^{13}\text{C}\{\text{H}\}$ NMR spectra of 3	Figures S11-S12	S12-13
Copies of ^1H and $^{13}\text{C}\{\text{H}\}$ NMR spectra of 1	Figures S13-S14	S14-15

Figure S1. $^1\text{H-NMR}$ of TBS-5

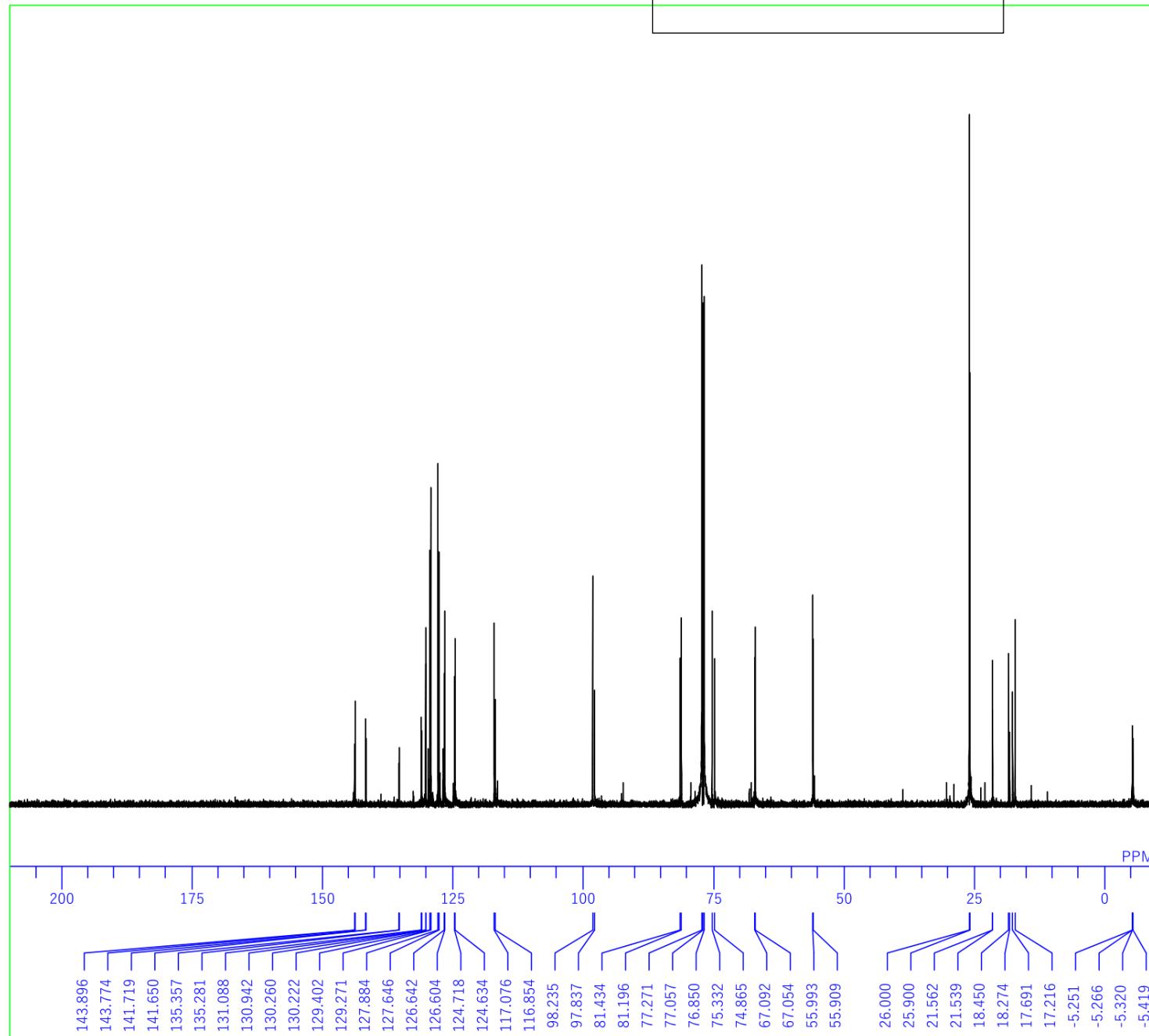
D:\\$1H NMR \B\YM7-46-sankaime-cdcl3.fid\YM7-46-sankaime-cdcl3.als



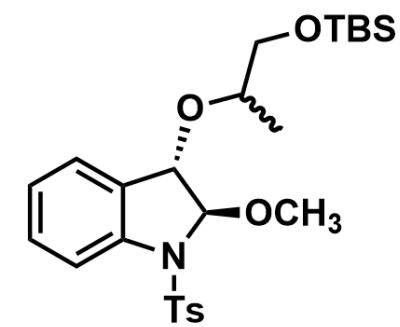
DFILE	M7-46-sankaime-cdcl3.als
COMNT	
DATIM	2023-08-23 11:34:15
OBNUC	H1
EXMOD	s2pul
OBFRQ	399.91 MHz
OBSET	1.99 KHz
OBFIN	2.00 Hz
POINT	32768
FREQU	6410.26 Hz
SCANS	32
ACQTM	3.5000 sec
PD	1.0000 sec
PW1	7.15 usec
IRNUC	
CTEMP	37.0 c
SLVNT	cdcl3
EXREF	0.00 ppm
BF	0.10 Hz
RGAIN	36



TBS-5

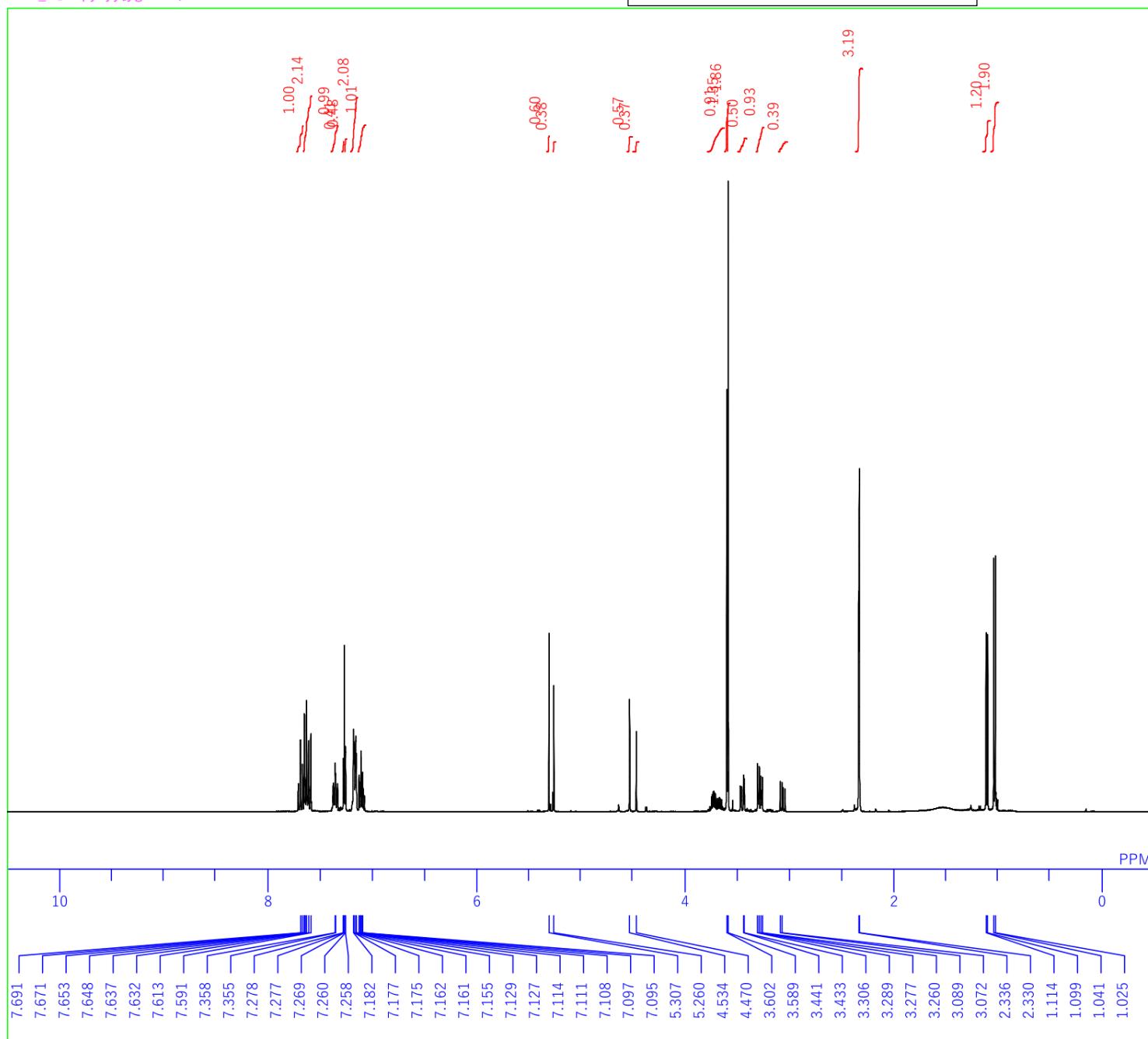
Figure S2. ^{13}C -NMR of TBS-5

DFILE 13C-M7-46-sankaime-cdcl3.als
 COMNT
 DATIM 2023-08-23 12:47:06
 OBNUC C13
 EXMOD s2pul
 OBFRQ 150.82 MHz
 OBSET 6.72 KHz
 OBFIN 8.70 Hz
 POINT 32768
 FREQU 37878.79 Hz
 SCANS 64
 ACQTM 0.8651 sec
 PD 1.0000 sec
 PW1 6.10 usec
 IRNUC
 CTEMP 15.0 c
 SLVNT cdcl3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 60

**TBS-5**

D:\Y_\¶—pf`ff[fg¥‰»‡•“7”5¥M7-52-1-cdcl3.fid¥M7-52-1-cdcl3.als

Figure S3. ^1H -NMR of 5



DFILE	M7-52-1-cdcl3.als
COMNT	
DATIM	2023-08-25 15:23:20
OBNUC	H1
EXMOD	s2pul
OBFRQ	399.91 MHz
OBSET	1.99 KHz
OBFIN	2.00 Hz
POINT	32768
FREQU	6410.26 Hz
SCANS	32
ACQTM	3.5000 sec
PD	1.0000 sec
PW1	7.15 usec
IRNUC	
CTEMP	37.0 c
SLVNT	cdcl3
EXREF	0.00 ppm
BF	0.10 Hz
RGAIN	36

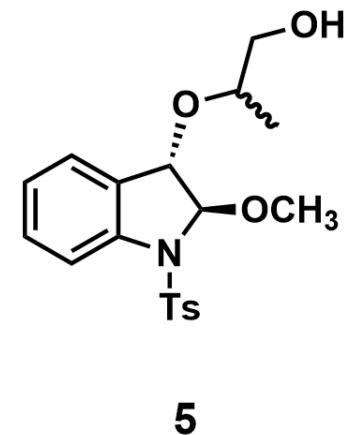
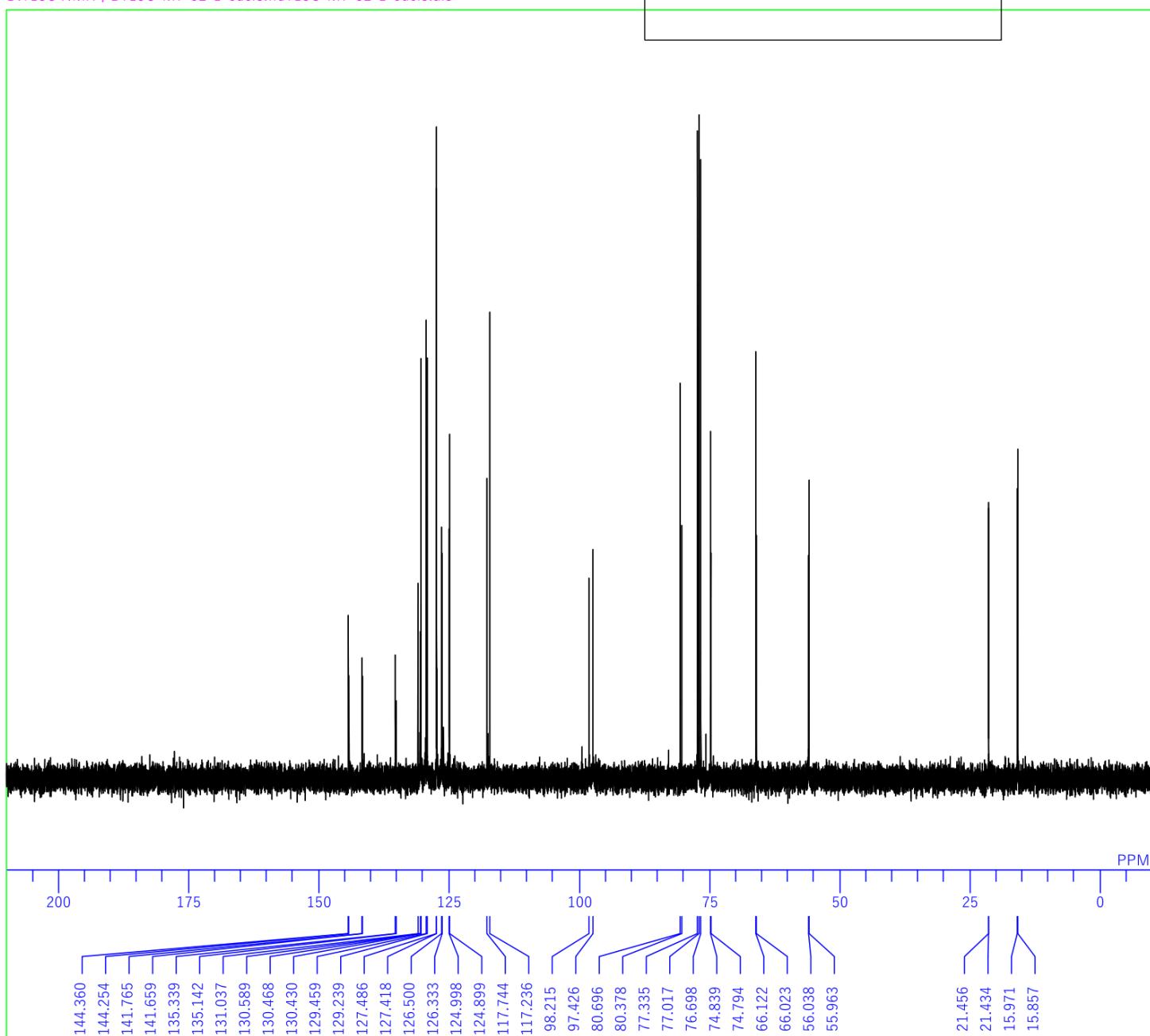


Figure S4. ^{13}C -NMR of 5

DFILE 13C-M7-52-1-cdcl3.als
 COMNT
 DATIM 2023-08-25 15:36:13
 OBNUC C13
 EXMOD s2pul
 OBFRQ 100.56 MHz
 OBSET 8.40 KHz
 OBFIN 8.30 Hz
 POINT 32768
 FREQU 25000.00 Hz
 SCANS 64
 ACQTM 1.3107 sec
 PD 1.0000 sec
 PW1 5.95 usec
 IRNUC
 CTEMP 37.0 c
 SLVNT cdcl3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 54

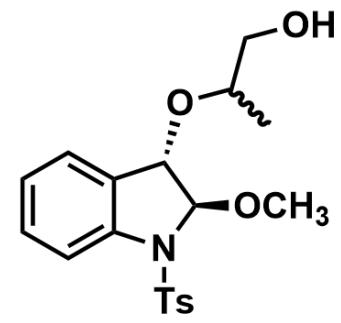
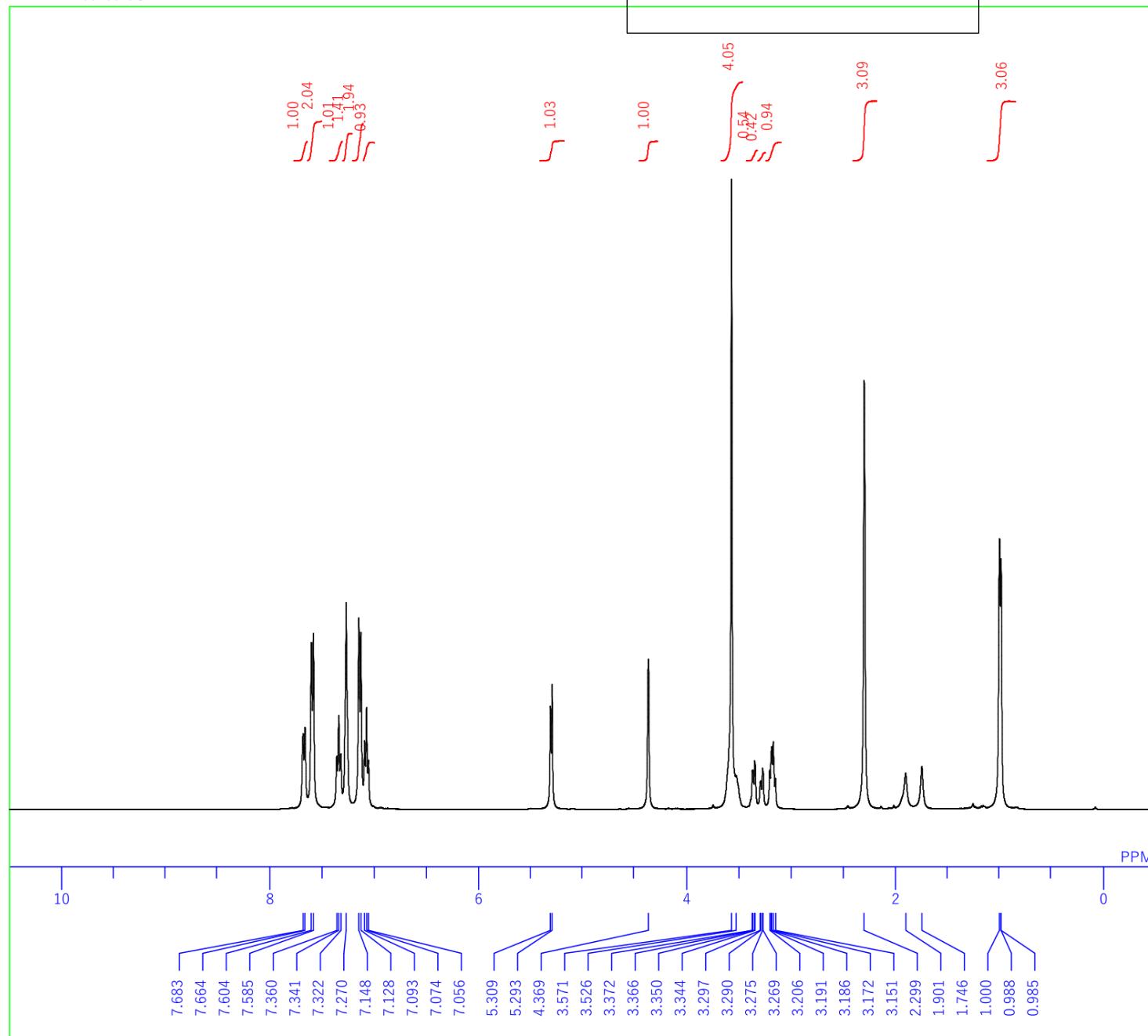
**5**

Figure S5. ^1H -NMR of 6

DFILE M7-16-1-cdcl3.als
 COMNT STANDARD PHOSPHORUS PARAMETERS
 DATIM 2023-08-07 21:52:01
 OBNUC H1
 EXMOD s2pul
 OBFRQ 399.91 MHz
 OBSET 1.99 kHz
 OBFIN 2.00 Hz
 POINT 32768
 FREQU 6410.26 Hz
 SCANS 32
 ACQTM 3.5000 sec
 PD 1.0000 sec
 PW1 7.15 usec
 IRNUC
 CTEMP 37.0 c
 SLVNT cdcl3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 24

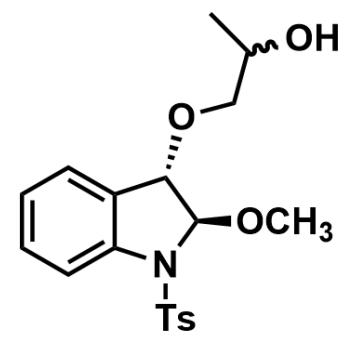
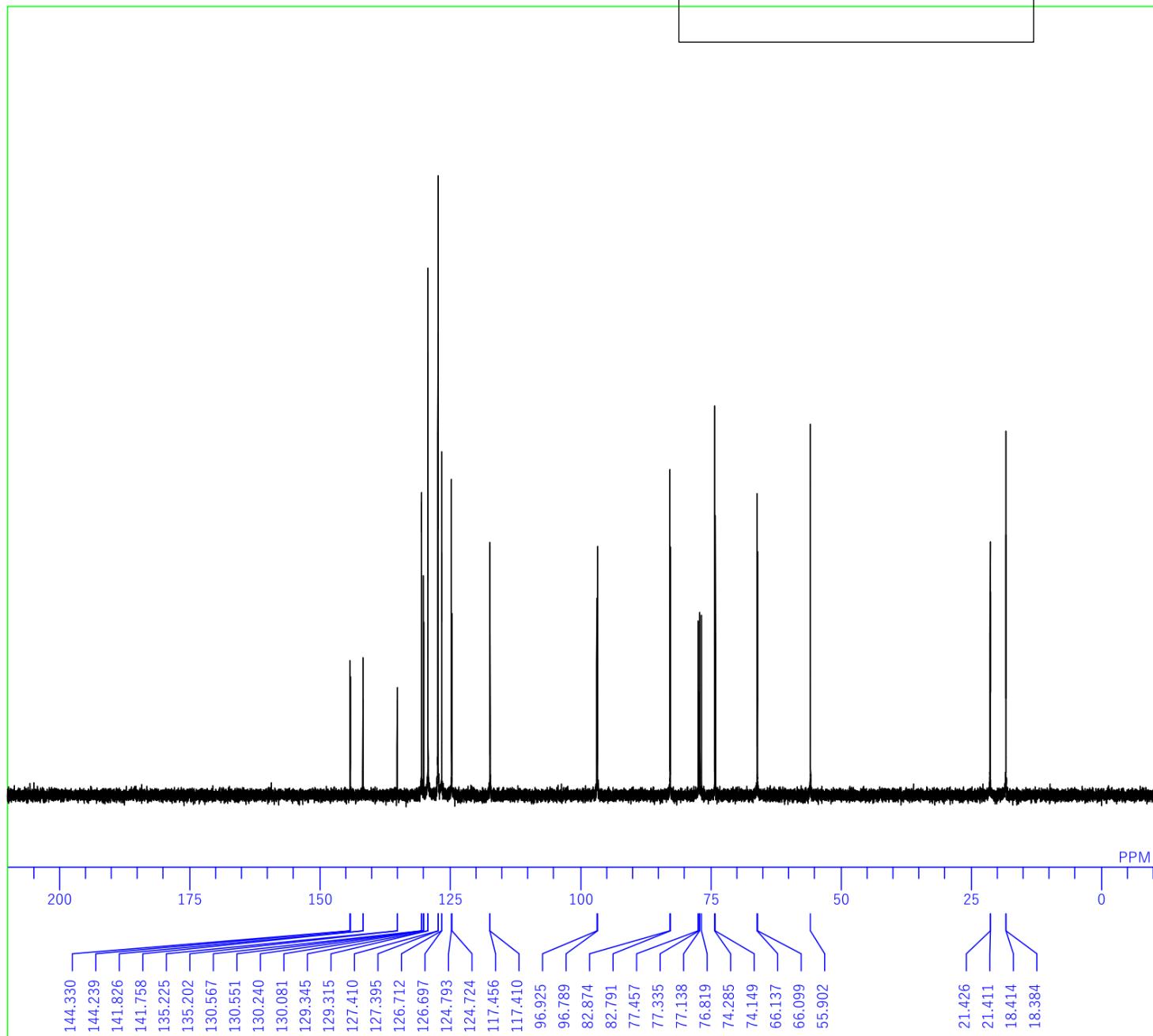
**6**

Figure S6. ^{13}C -NMR of 6

DFILE 13C-M7-16-1-cdcl3.als
 COMNT STANDARD PHOSPHORUS PARAMETERS
 DATIM 2023-08-07 22:05:53
 OBNUC C13
 EXMOD s2pul
 OBFRQ 100.56 MHz
 OBSET 8.40 KHz
 OBFIN 8.30 Hz
 POINT 32768
 FREQU 25000.00 Hz
 SCANS 64
 ACQTM 1.3107 sec
 PD 1.0000 sec
 PW1 5.95 usec
 IRNUC
 CTEMP 37.0 c
 SLVNT cdcl3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 54

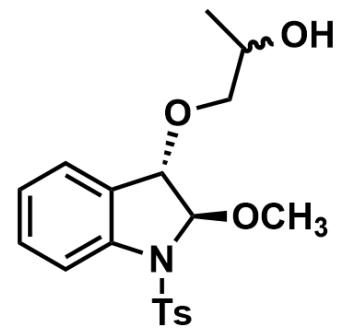
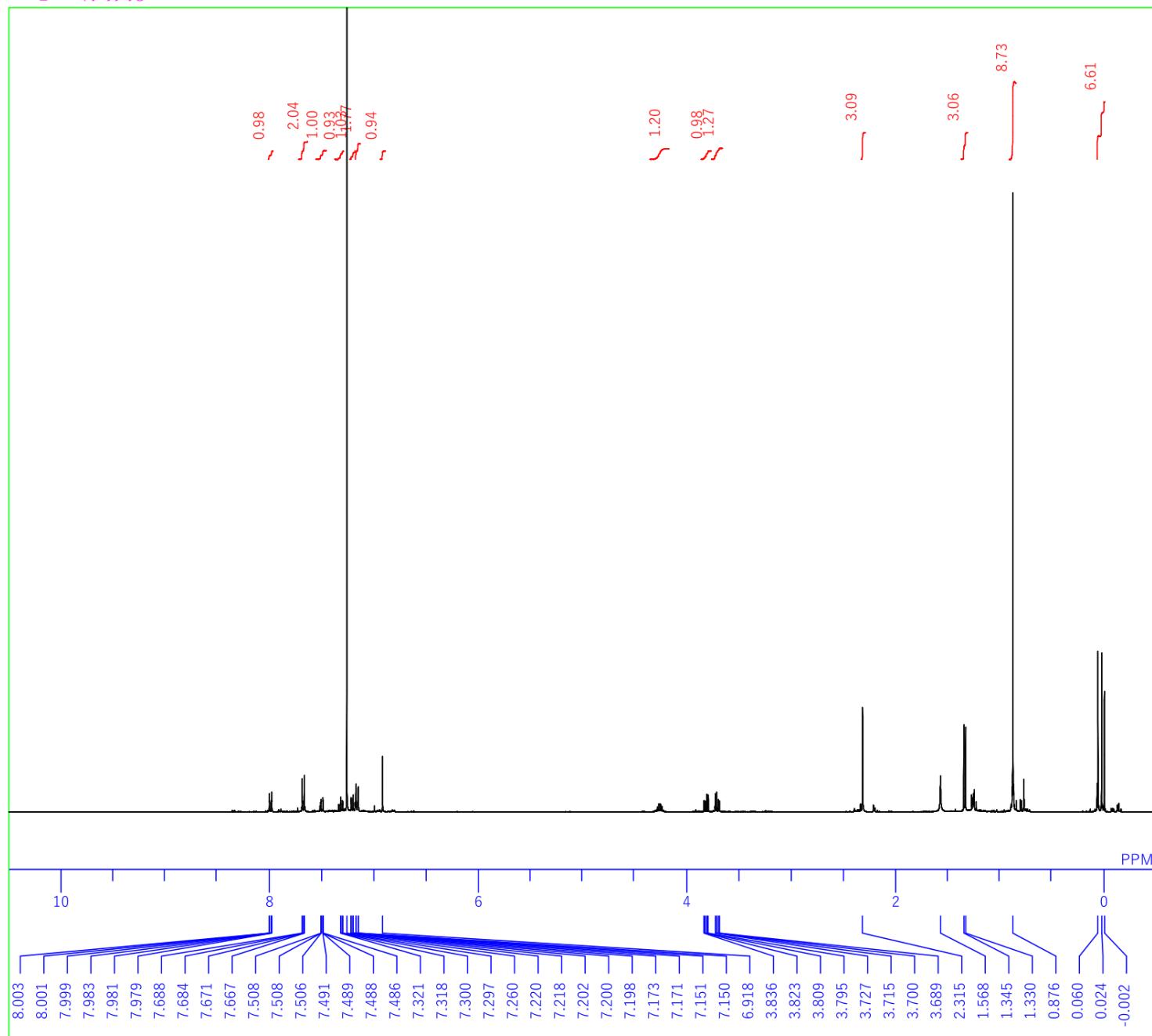
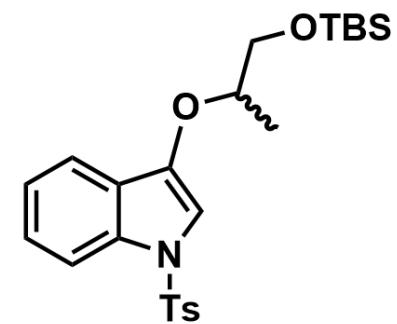


Figure S7. ^1H -NMR of TBS-7

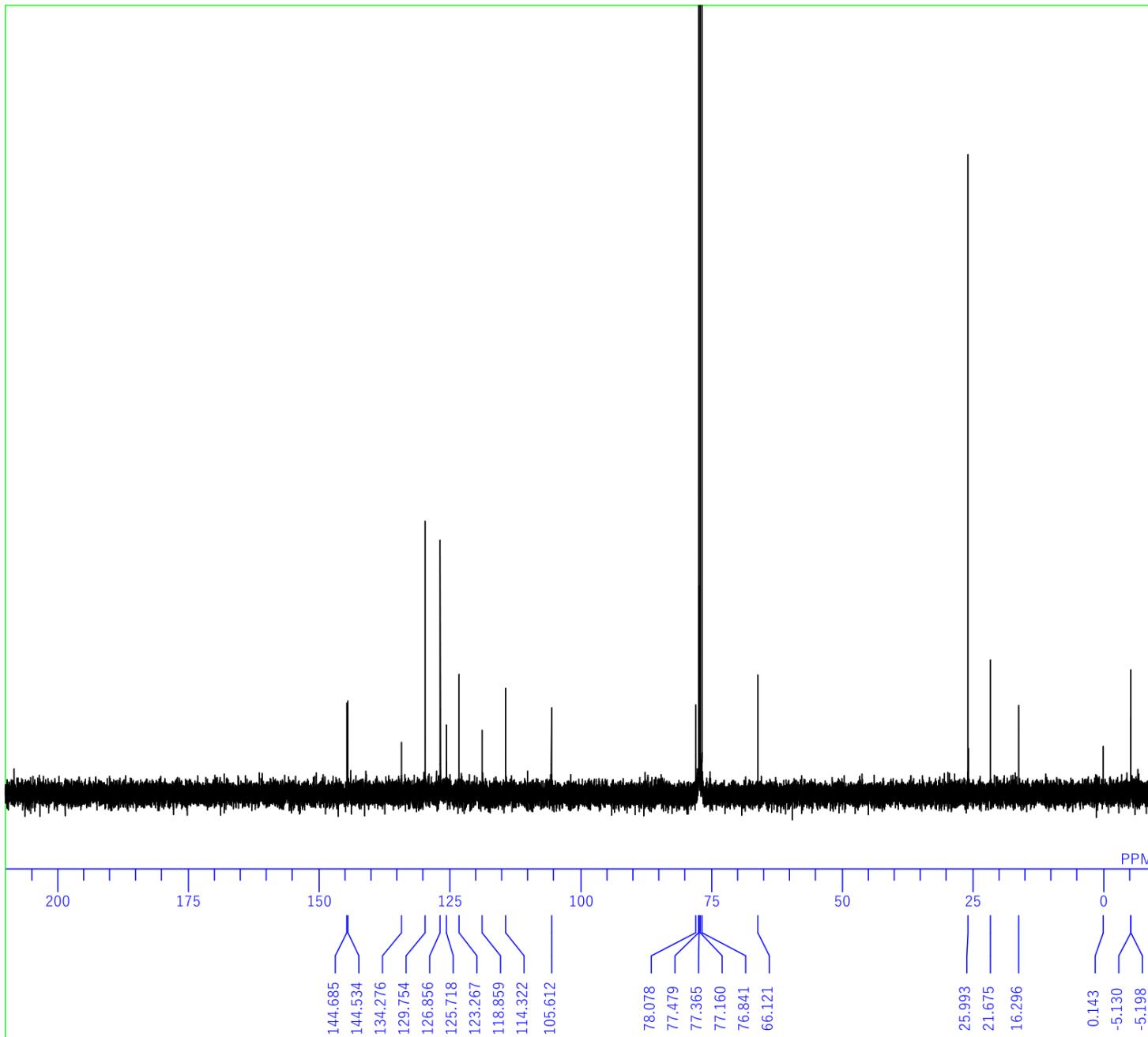
D:\Y_\•¶—pf`ff[fg¥‰»‡•“TBS-9”9YM5-79-2-nikaime-cdcl3.fidYM5-79-2-nikaime-cdcl3.als



DFILE M5-79-2-nikaime-cdcl3.als
 COMNT TK-II-70-b
 DATIM 2023-02-24 11:03:51
 OBNUC H1
 EXMOD s2pul
 OBFRQ 399.91 MHz
 OBSET 1.99 KHz
 OBFIN 2.00 Hz
 POINT 32768
 FREQU 6410.26 Hz
 SCANS 32
 ACQTM 3.5000 sec
 PD 1.0000 sec
 PW1 7.15 usec
 IRNUC
 CTEMP 37.0 c
 SLVNT cdcl3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 48



TBS-7

Figure S8. ^{13}C -NMR of TBS-7

DFILE 13C-M5-79-2-nikaime-cdcl3.als
 COMNT TK-II-70-b
 DATIM 2023-02-24 11:11:00
 OBNUC C13
 EXMOD s2pul
 OBFRQ 100.56 MHz
 OBSET 8.40 KHz
 OBFIN 8.30 Hz
 POINT 32768
 FREQU 25000.00 Hz
 SCANS 64
 ACQTM 1.3107 sec
 PD 1.0000 sec
 PW1 5.95 usec
 IRNUC
 CTEMP 37.0 c
 SLVNT cdcl3
 EXREF 77.16 ppm
 BF 0.10 Hz
 RGAIN 42

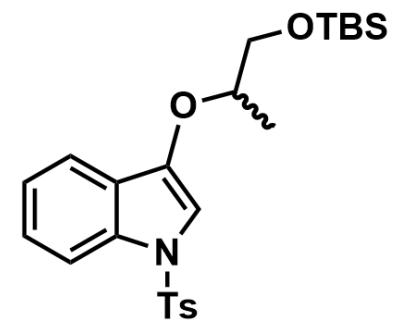
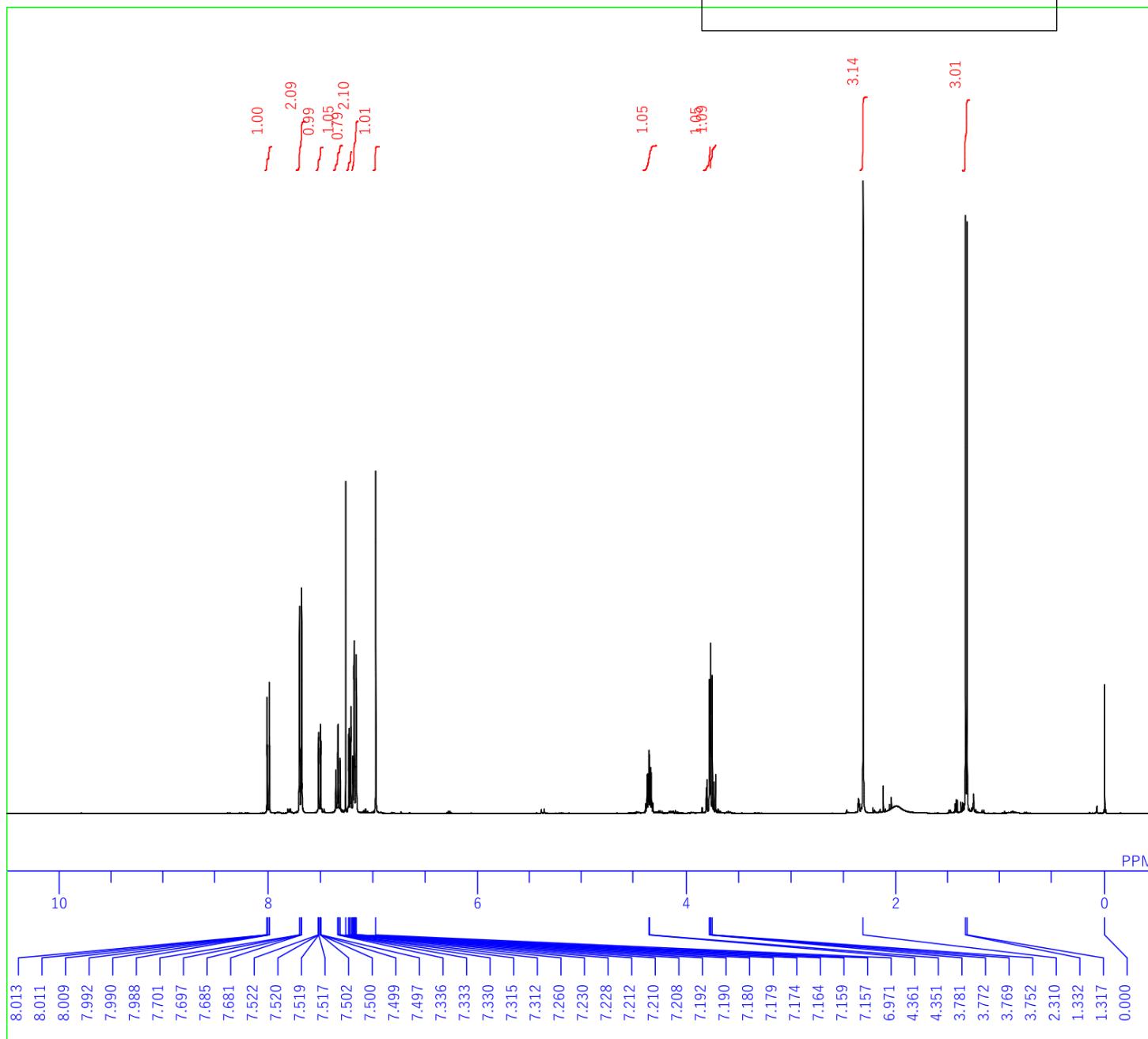


Figure S9. ^1H -NMR of 7

D:\Y1H NMR\@YM5-81-1-cdcl3.fid\YM5-81-1-cdcl3.als



DFILE M5-81-1-cdcl3.als
COMNT TK-II-70-b
DATIM 2023-02-24 10:08:56
OBNUC H1
EXMOD s2pul
OBFRQ 399.91 MHz
OBSET 1.99 KHz
OBFIN 2.00 Hz
POINT 32768
FREQU 6410.26 Hz
SCANS 32
ACQTM 3.5000 sec
PD 1.0000 sec
PW1 7.15 usec
IRNUC
CTEMP 37.0 c
SLVNT cdcl3
EXREF 7.26 ppm
BF 0.10 Hz
RGAIN 38

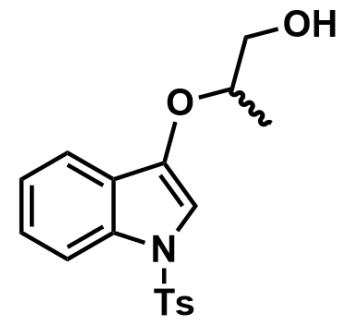
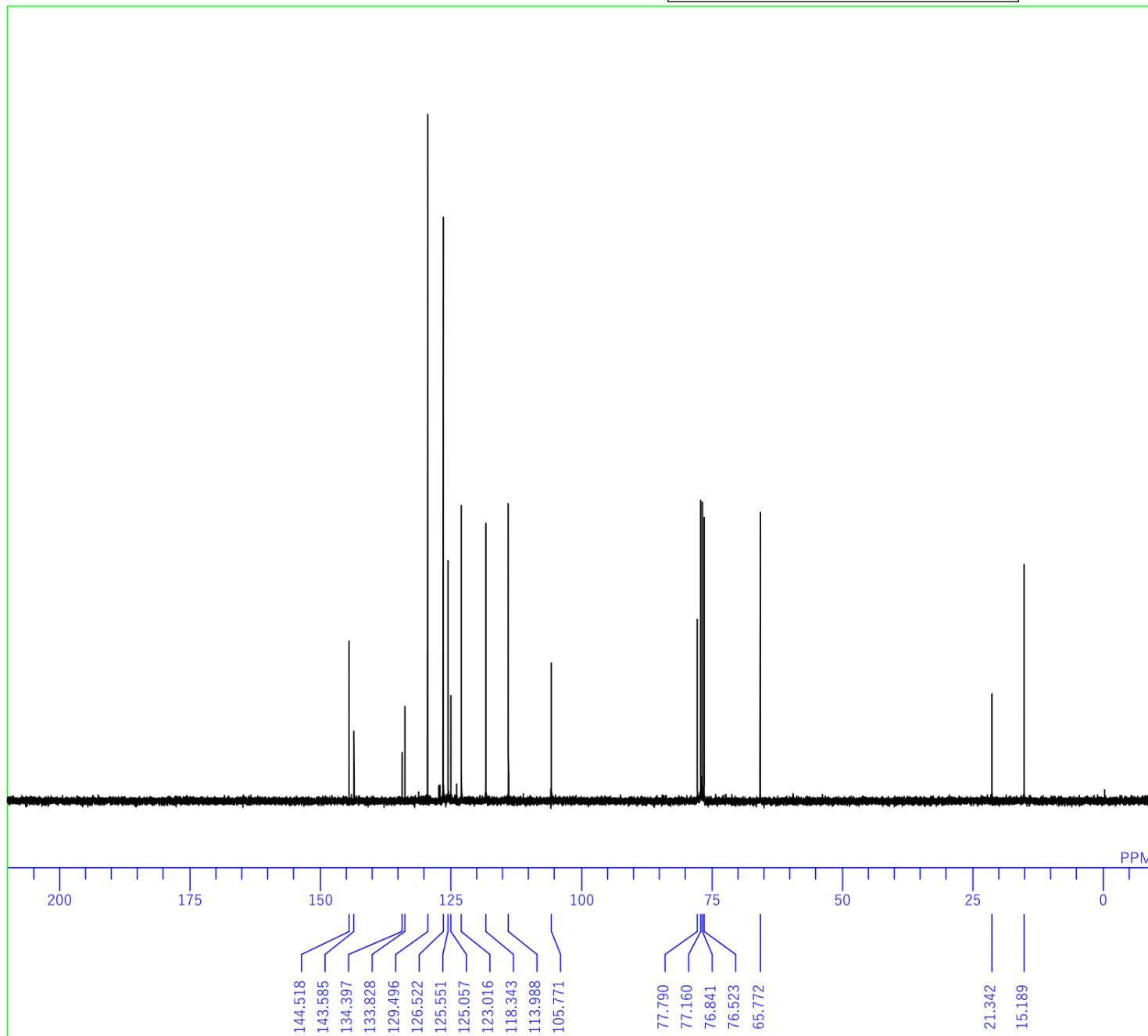
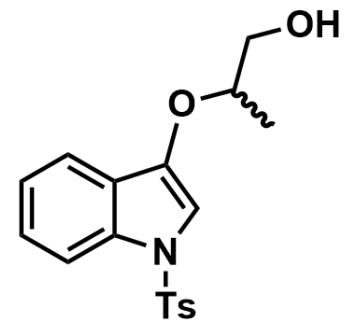
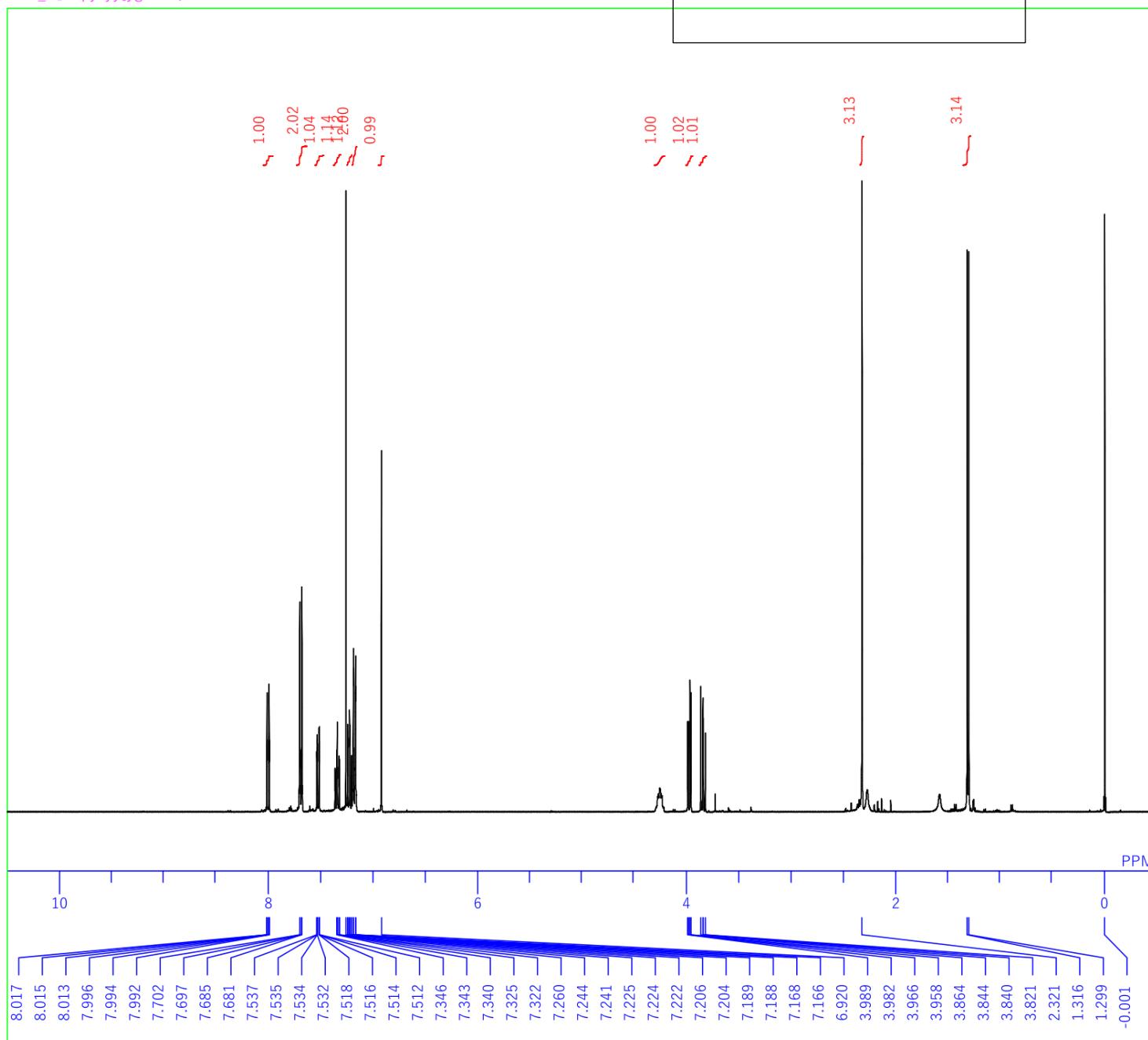


Figure S10. ^{13}C -NMR of 7

DFILE 13C-M5-81-1-cdcl3.als
 COMNT TK-II-70-b
 DATIM 2023-02-24 10:14:36
 OBNUC C13
 EXMOD s2pul
 OBFRQ 100.56 MHz
 OBSET 8.40 KHz
 OBFIN 8.30 Hz
 POINT 32768
 FREQU 25000.00 Hz
 SCANS 64
 ACQTM 1.3107 sec
 PD 1.0000 sec
 PW1 5.95 usec
 IRNUC
 CTEMP 37.0 c
 SLVNT cdcl3
 EXREF 77.16 ppm
 BF 0.10 Hz
 RGAIN 48



7

Figure S11. ^1H -NMR of 3

DFILE M5-71-2-sankaime-cdcl3.als
 COMNT
 DATIM 2023-02-22 12:19:40
 OBNUC H1
 EXMOD s2pul
 OBFRQ 399.91 MHz
 OBSET 1.99 KHz
 OBFIN 2.00 Hz
 POINT 32768
 FREQU 6410.26 Hz
 SCANS 32
 ACQTM 3.5000 sec
 PD 1.0000 sec
 PW1 7.15 usec
 IRNUC
 CTEMP 37.0 c
 SLVNT cdcl3
 EXREF 7.26 ppm
 BF 0.10 Hz
 RGAIN 42

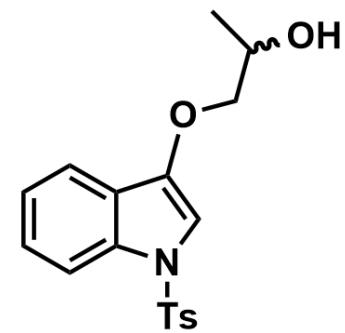
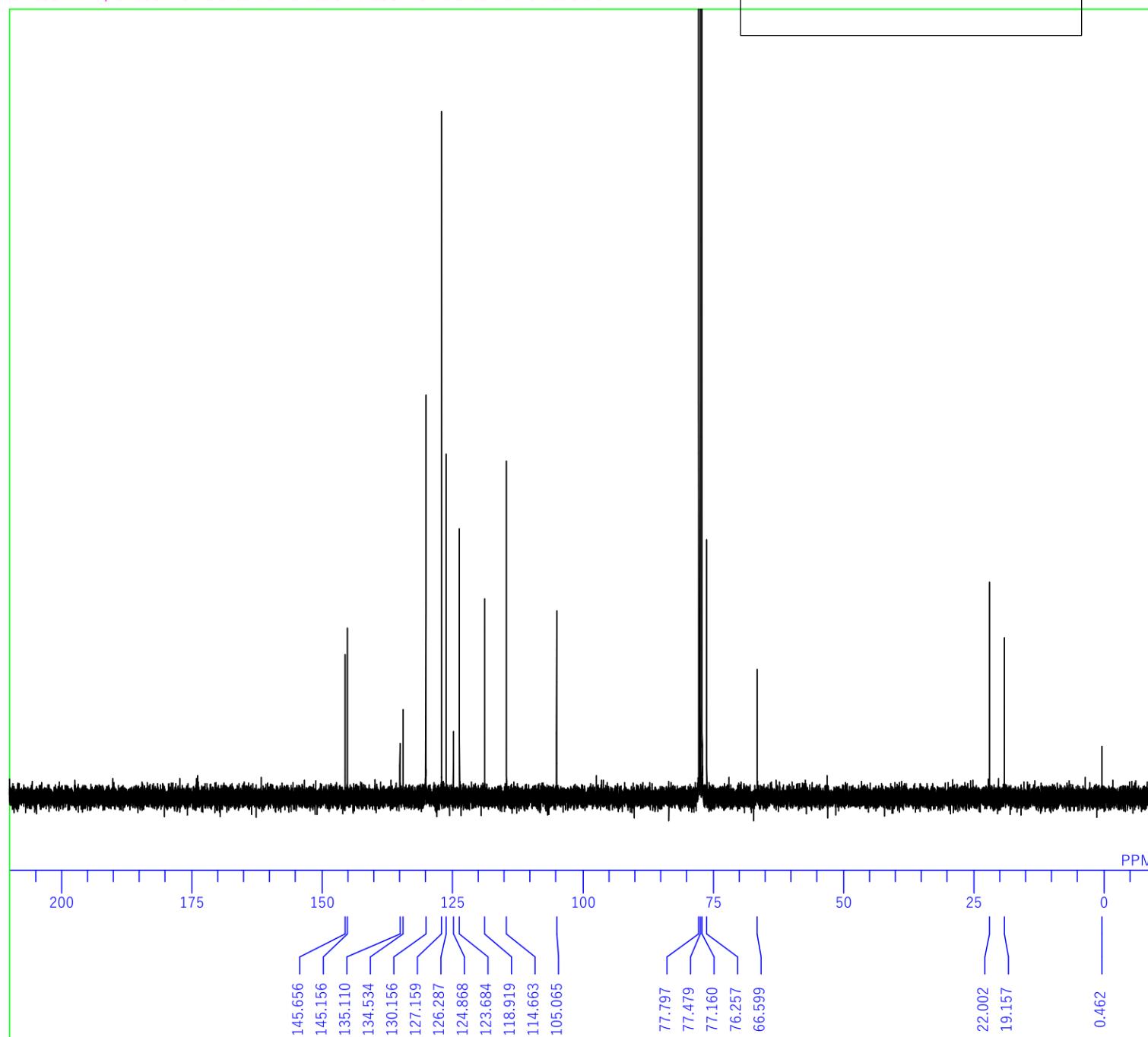
**3**

Figure S12. ^{13}C -NMR of 3

DFILE 13C-M5-71-2-sankaime-cdcl3.als
 COMNT
 DATIM 2023-02-22 12:25:38
 OBNUC C13
 EXMOD s2pul
 OBFRQ 100.56 MHz
 OBSET 8.40 KHz
 OBFIN 8.30 Hz
 POINT 32768
 FREQU 25000.00 Hz
 SCANS 64
 ACQTM 1.3107 sec
 PD 1.0000 sec
 PW1 5.95 usec
 IRNUC
 CTEMP 37.0 c
 SLVNT cdcl3
 EXREF 77.16 ppm
 BF 0.10 Hz
 RGAIN 54

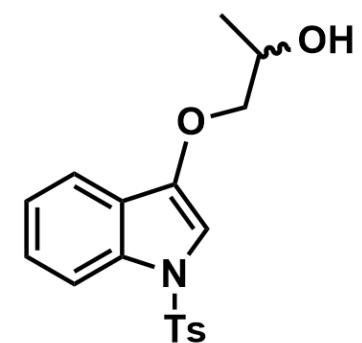
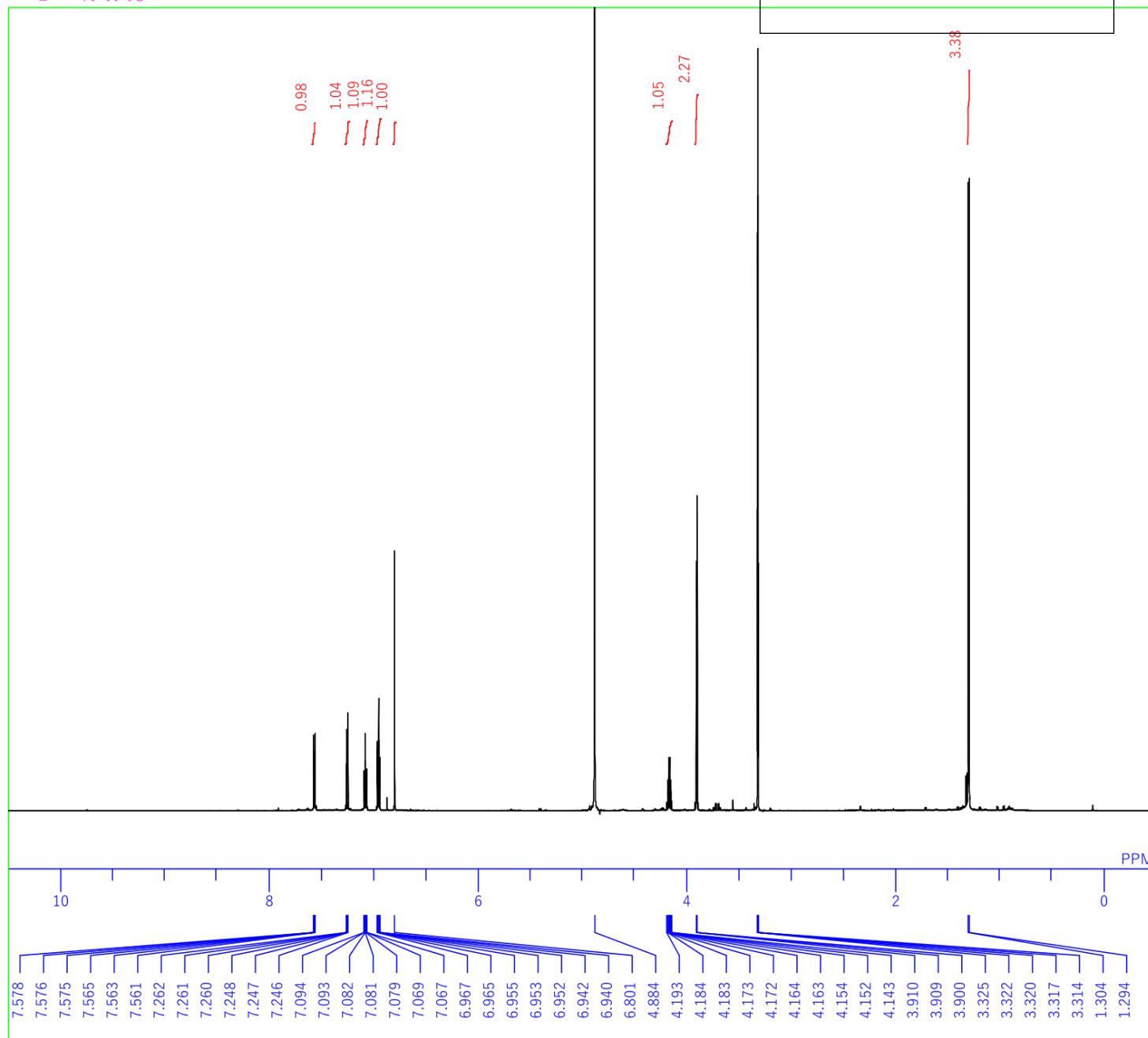
**3**

Figure S13. ^1H -NMR of 1

DFILE M7-36-1-nikaime-meod.als
 COMNT
 DATIM 2023-08-10 18:00:19
 OBNUC H1
 EXMOD s2pul
 OBFRQ 599.76 MHz
 OBSET 7.42 KHz
 OBFIN 3.60 Hz
 POINT 32768
 FREQU 9615.38 Hz
 SCANS 32
 ACQTM 3.4079 sec
 PD 1.0000 sec
 PW1 5.65 usec
 IRNUC
 CTEMP 15.0 c
 SLVNT cd3od
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 46

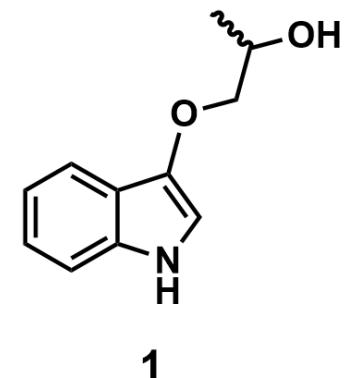
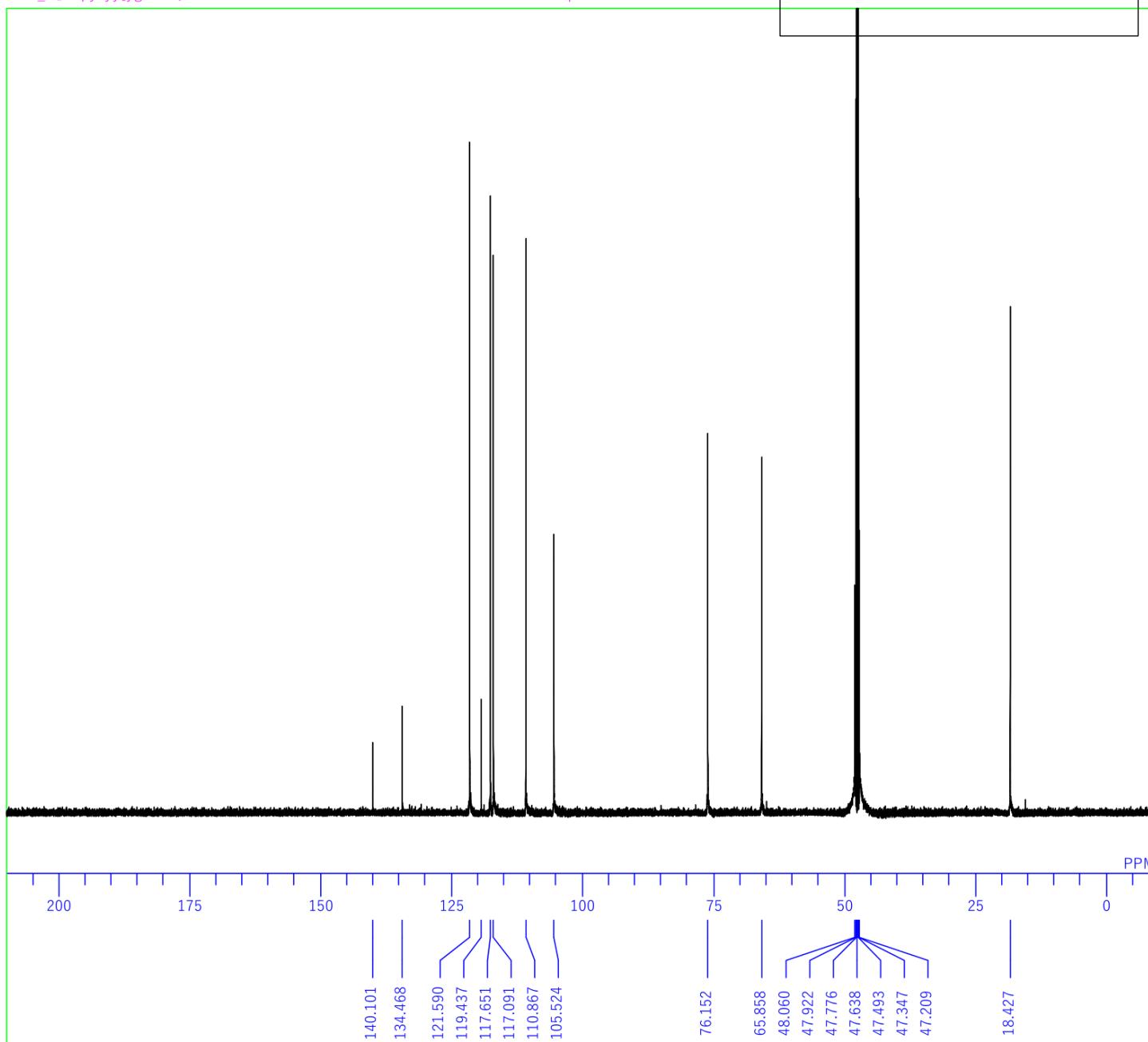


Figure S14. ^{13}C -NMR of 1

DFILE 13C-M7-38-2-mead-2-power.als
 COMNT
 DATIM 2023-08-11 15:21:29
 OBNUC C13
 EXMOD s2pul
 OBFRQ 150.82 MHz
 OBSET 7.32 kHz
 OBFIN 2.90 Hz
 POINT 32768
 FREQU 37878.79 Hz
 SCANS 64
 ACQTM 0.8651 sec
 PD 1.0000 sec
 PW1 6.10 usec
 IRNUC
 CTEMP 15.0 c
 SLVNT cd3od
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 60

