Supporting Information II

5-*exo*-Selective Asymmetric Bromolactonization of Stilbenecarboxylic Acids Catalyzed by Phenol-bearing Chiral Thiourea

Masayuki Sugano,[†] *Tsubasa Inokuma,*[†,‡] *Yousuke Yamaoka,*[§] *and Ken-ichi Yamada*[*,†,‡]

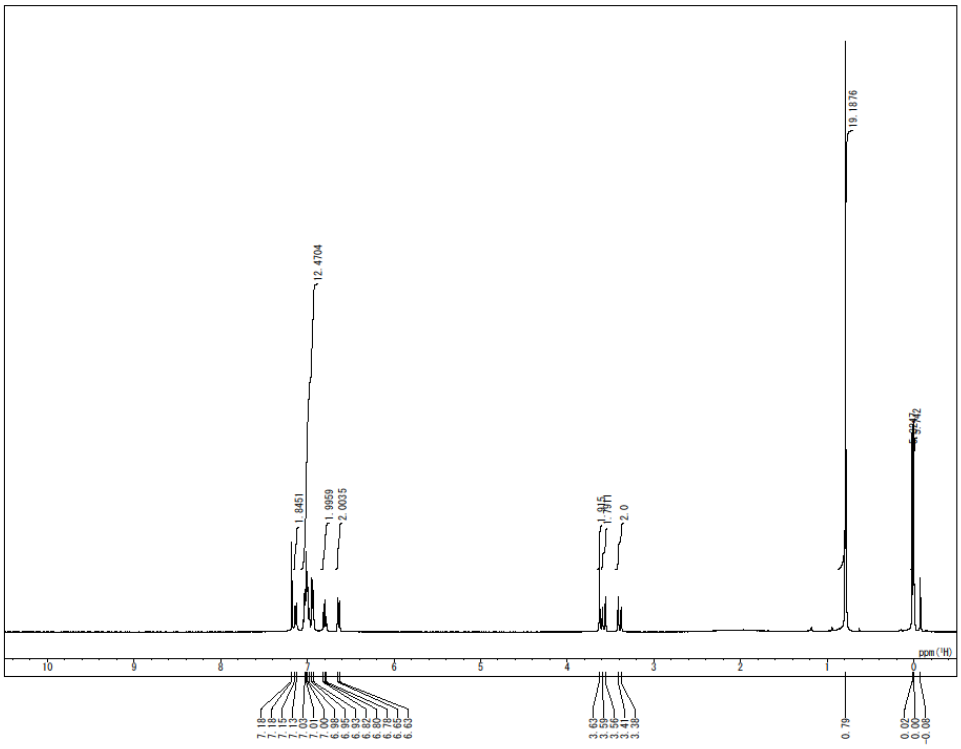
[†]Graduate School of Pharmaceutical Sciences, Tokushima University, Shomachi, Tokushima 770-8505, Japan. [‡]Research Cluster on "Key Material Development", Tokushima University, Shomachi, Tokushima 770-8505, Japan. [§]Graduate School of Pharmaceutical Sciences, Kyoto University, Yoshida, Sakyo-ku, Kyoto 606-8501, Japan.

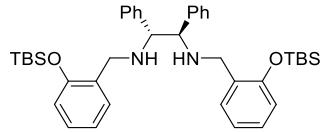
yamak@tokushima-u.ac.jp

Contents

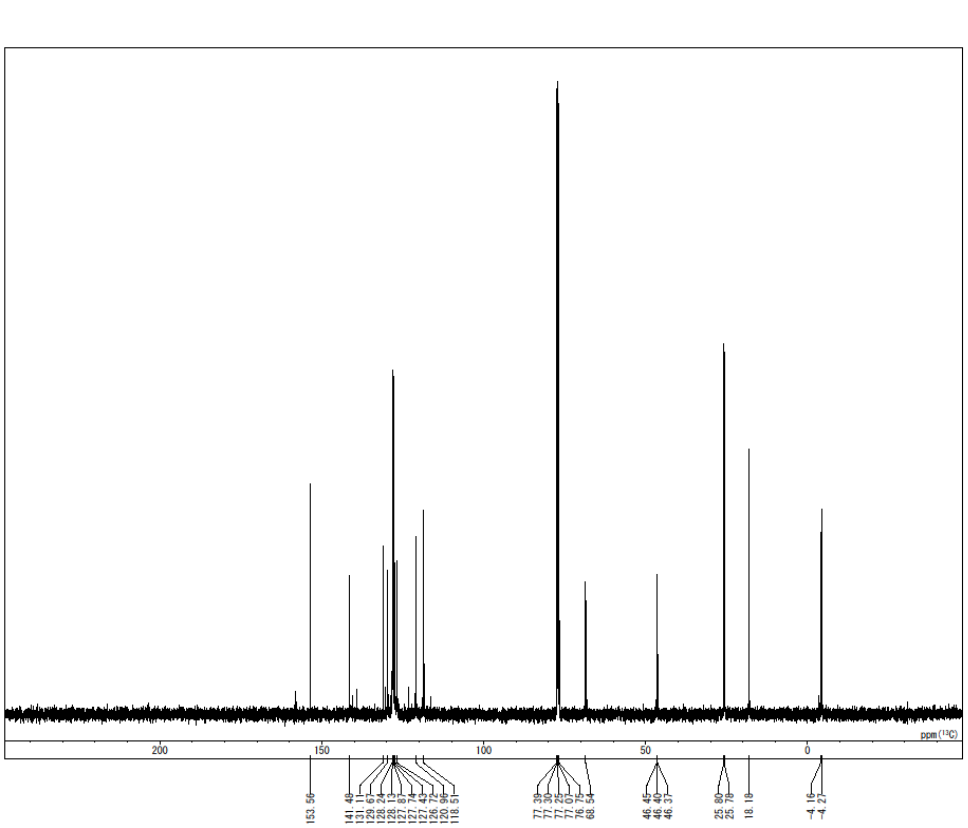
1. Copies of ^{1}H and ^{13}C NMR spectra.....S2
2. Copies of HPLC charts S72

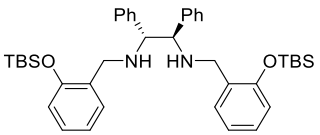
1. Copies of ^{1}H and ^{13}C NMR spectra



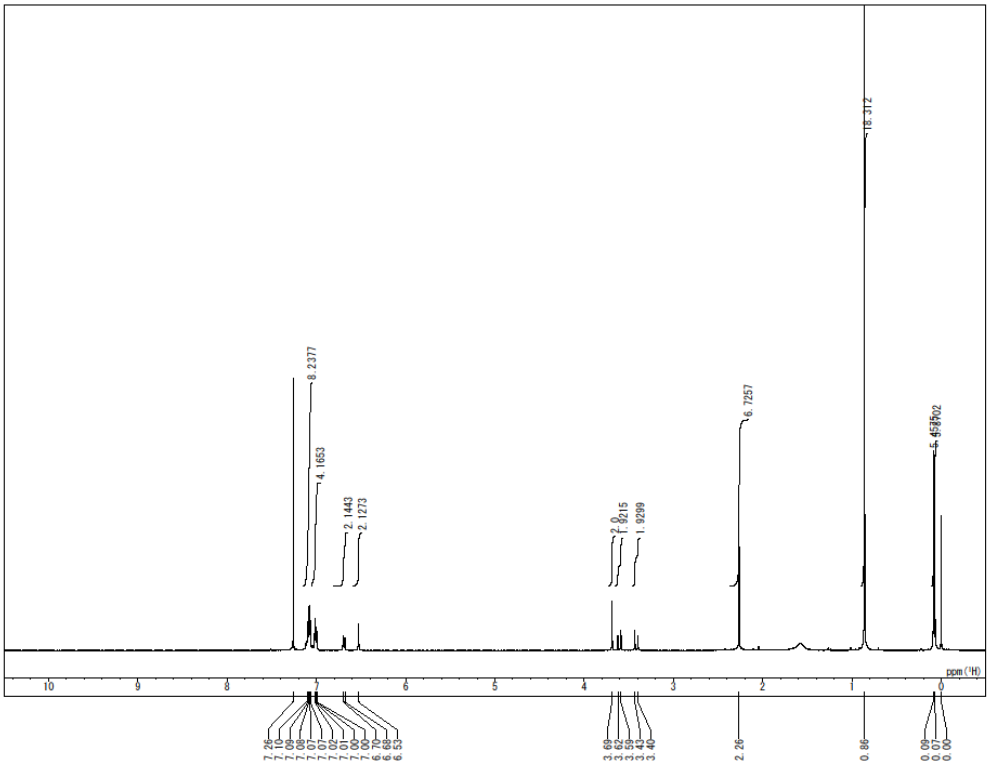


^{1}H NMR of **S2a**



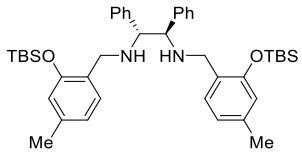


^{13}C NMR of **S2a**

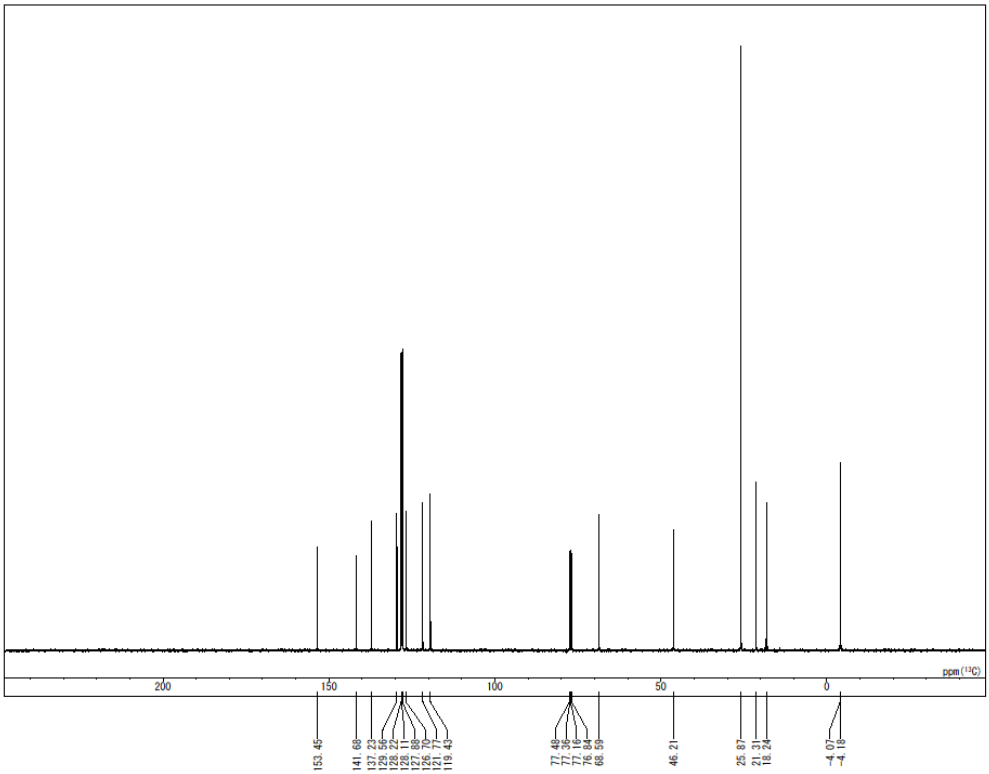


DFILE X:¥062ORGVDATA¥ORGVNMRVMS8177BV10¥PDAT
ORGFILE X:¥062ORGVDATA¥ORGVNMRVMS8177BV10¥PD
DATIM 06/Jun/2022 14:58:36
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	144
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.31 ℃
PRNT_DATE	2022/Jun/06 15:05:44

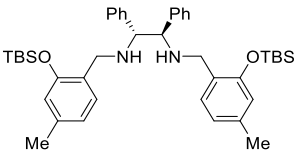


^{1}H NMR of **S2f**

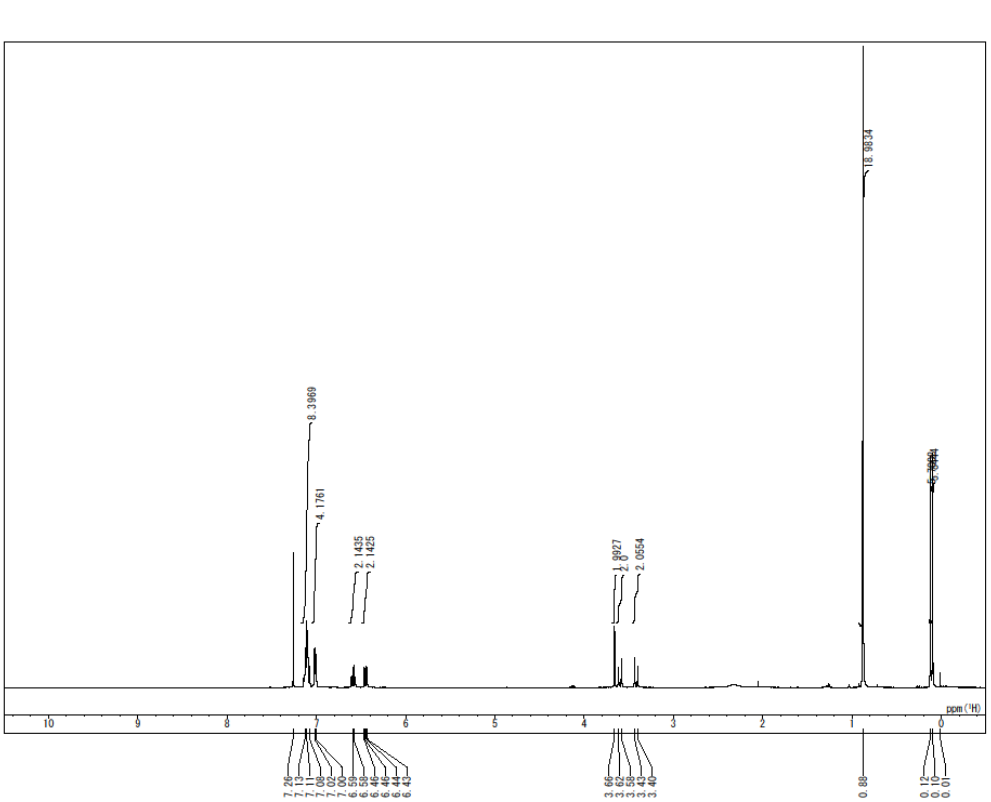


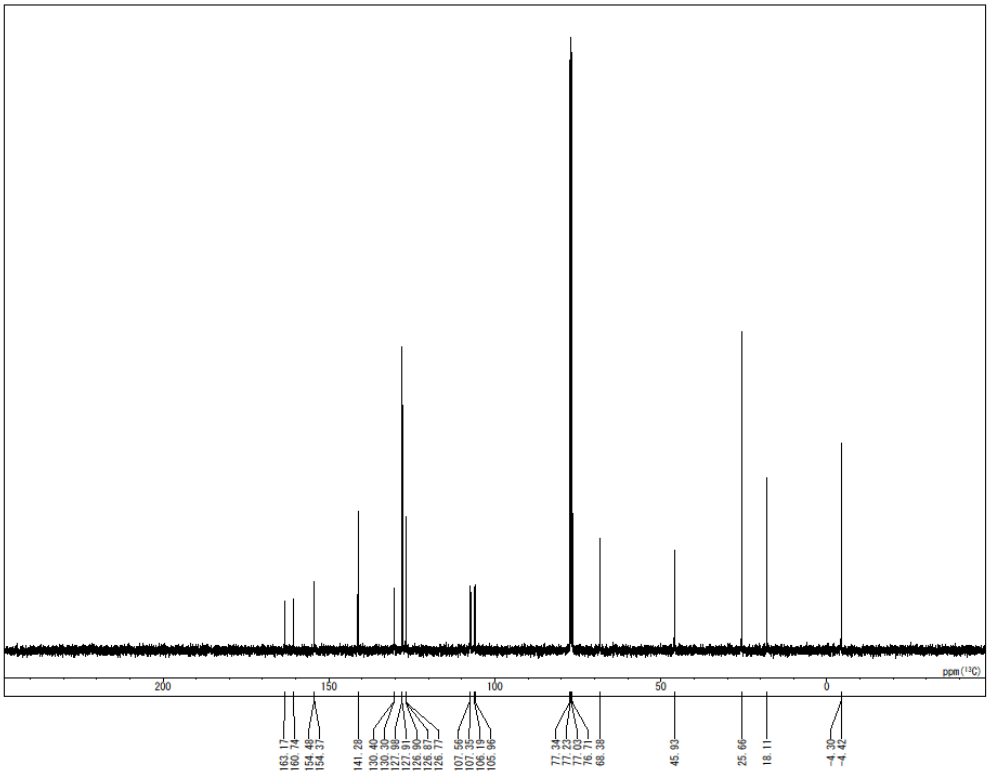
DFILE X:¥062ORGVDATA¥ORGVNMRVMS8177BC-NMRV10
ORGFILE X:¥062ORGVDATA¥ORGVNMRVMS8177BC-NMRV
DATIM 06/Jun/2022 15:30:46
COMNT

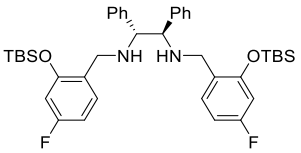
OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	26.21 ℃
PRNT_DATE	2022/Jun/06 15:42:32



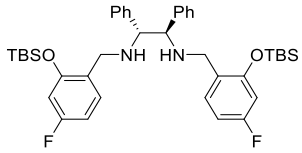
^{13}C NMR of **S2f**



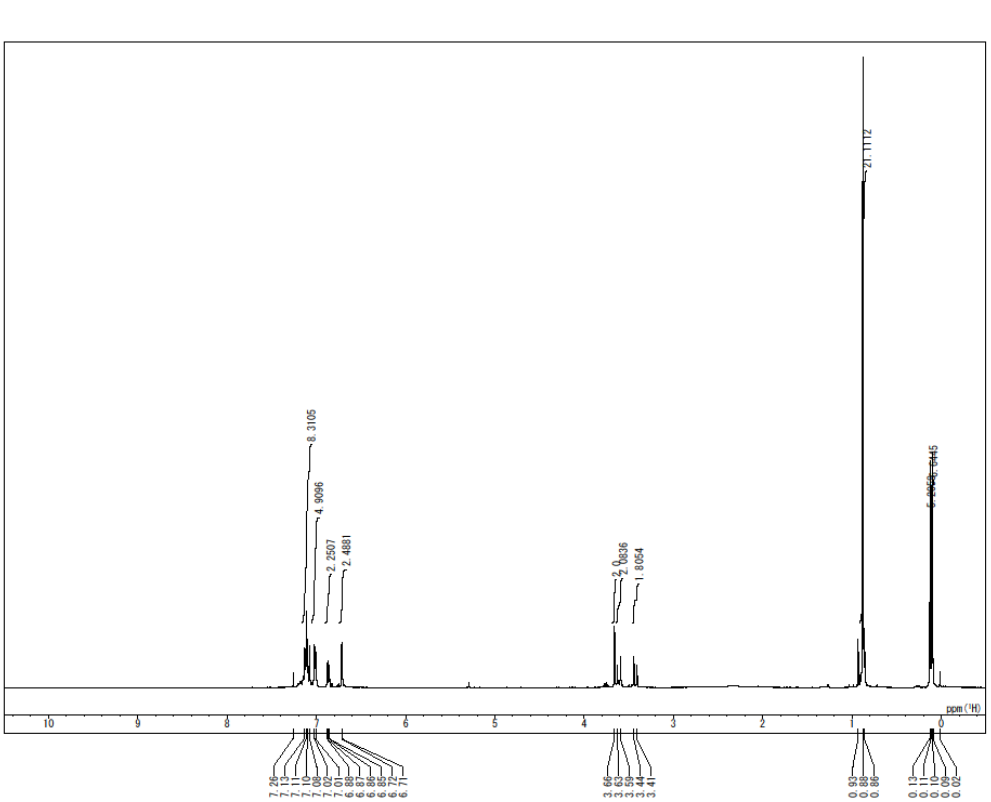




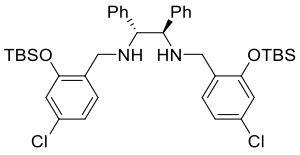
^{1}H NMR of **S2h**



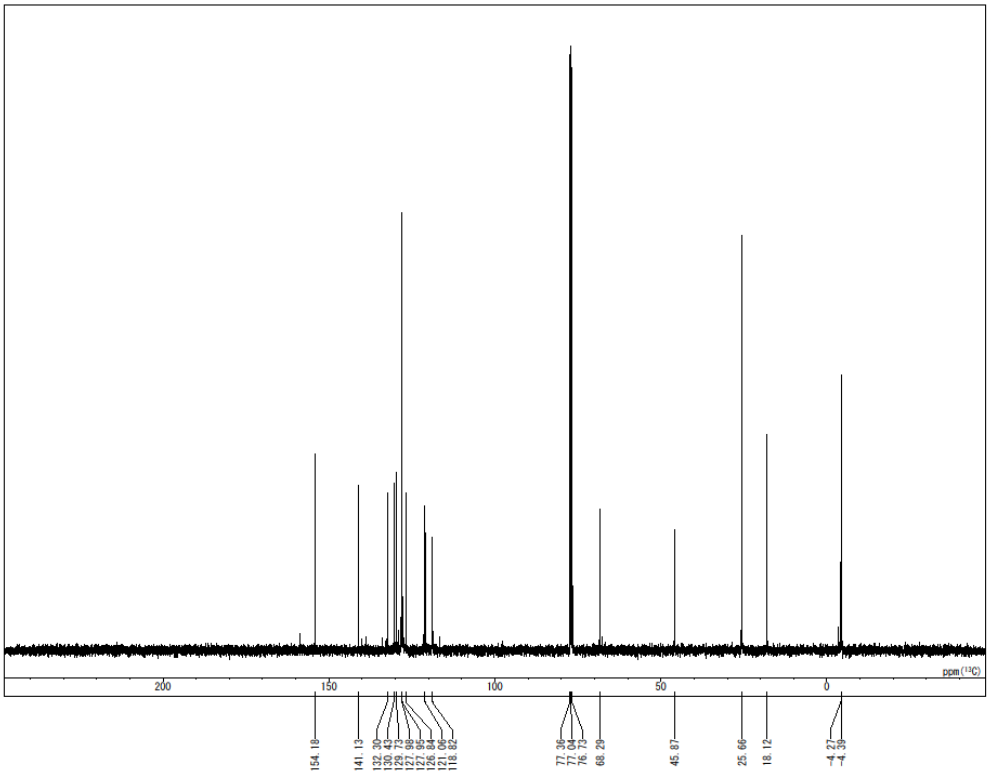
^{13}C NMR of **S2h**



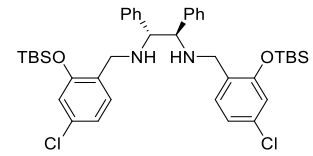
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	45
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	21.71 °C
PRNT_DATE	2022/Jun/02 21:59:47



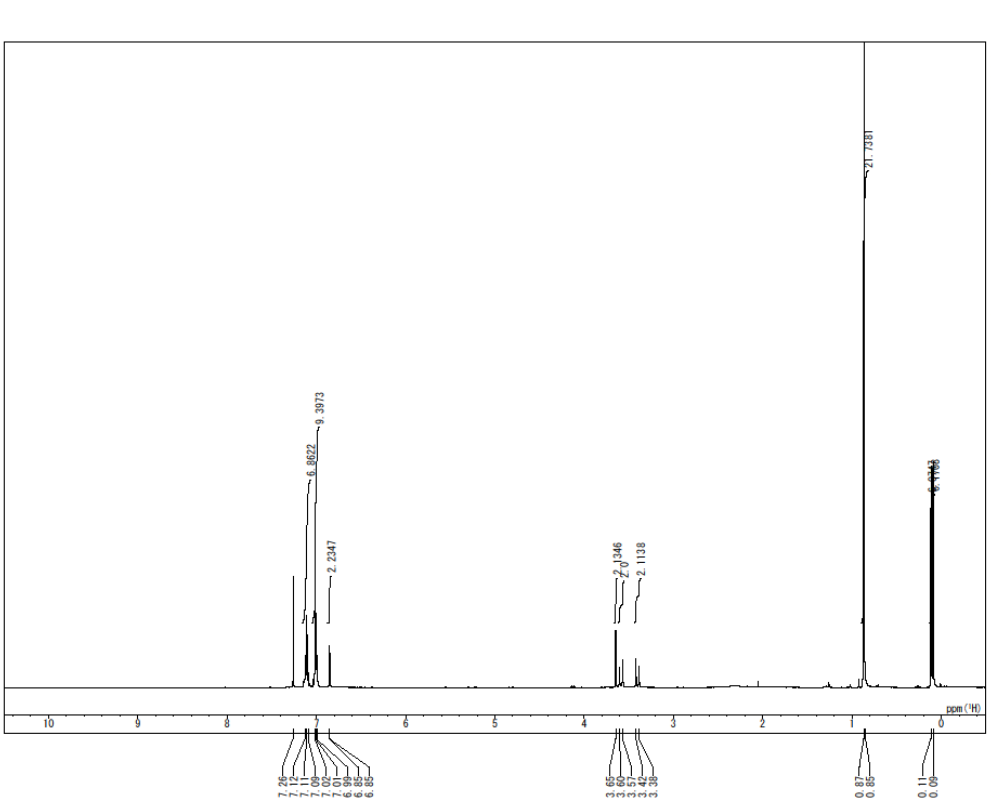
^{1}H NMR of **S2g**



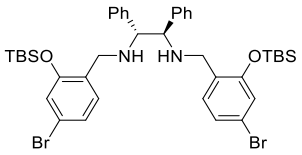
OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	114
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	22.01 °C
PRNT_DATE	2022/Jun/02 21:56:50



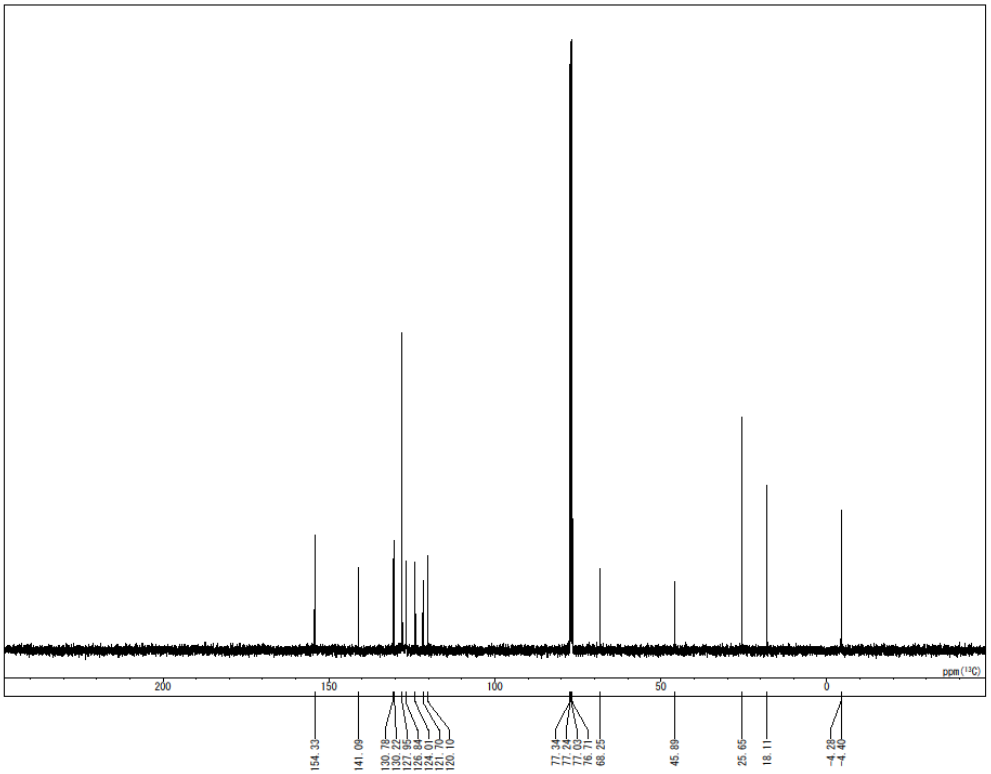
^{13}C NMR of **S2g**



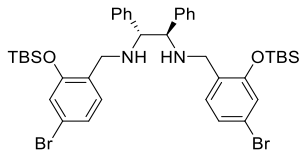
OBNUC	^{1}H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 μs
PW2	15.0 μs
PW3	30.0 μs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	64
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 μs
IRATN	0
CSPED	20.0 Hz
CTEMP	21.61 °C
PRNT_DATE	2022/Jun/02 22:05:44



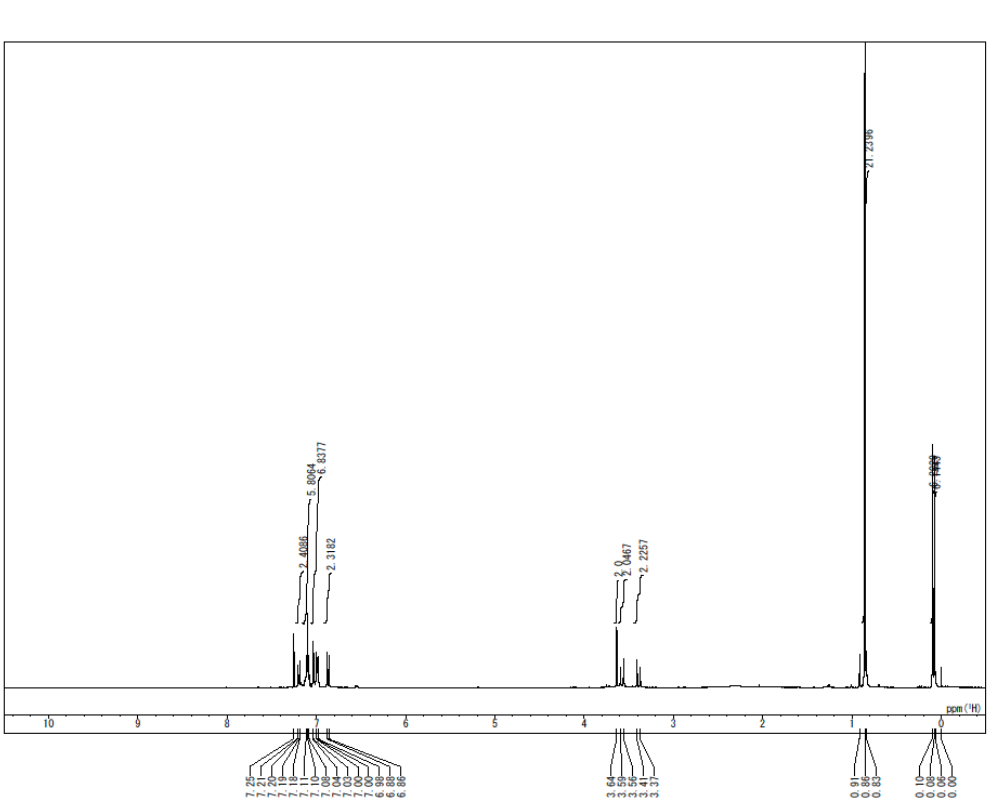
^{1}H NMR of **S2i**

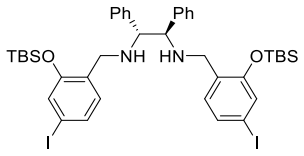


OBNUC	^{13}C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 μs
PW2	10.0 μs
PW3	20.0 μs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 μs
IRATN	0
CSPED	20.0 Hz
CTEMP	22.01 °C
PRNT_DATE	2022/Jun/02 22:02:29

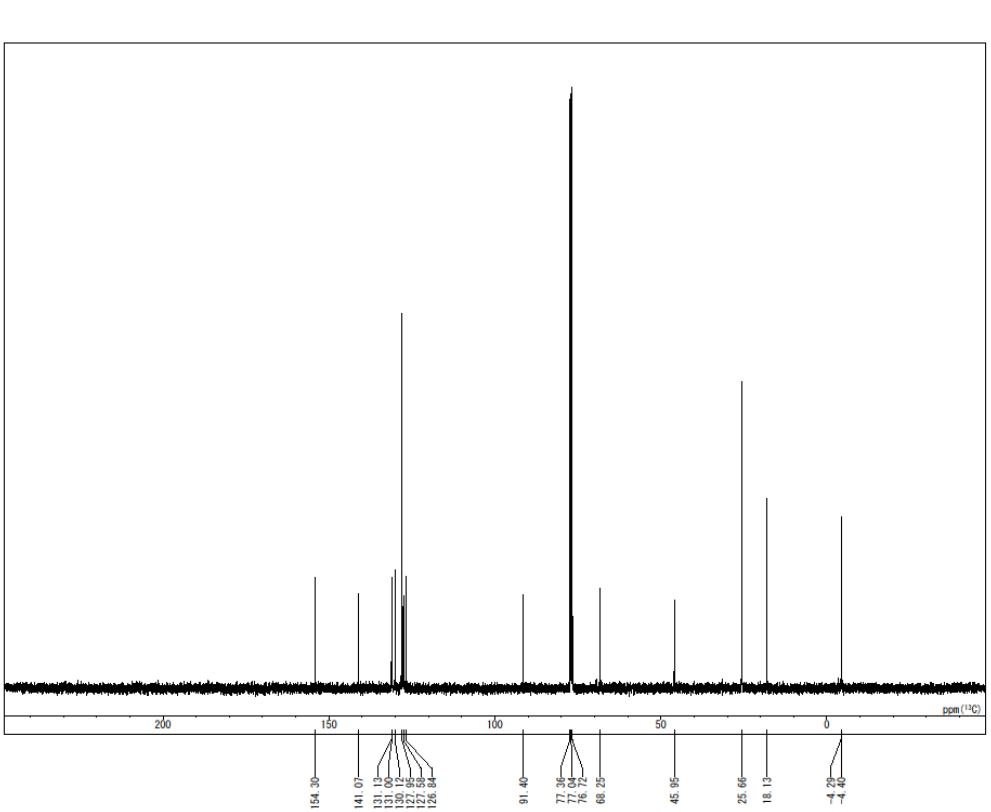


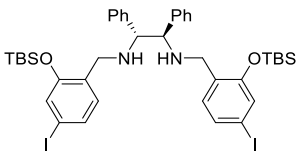
^{13}C NMR of **S2i**



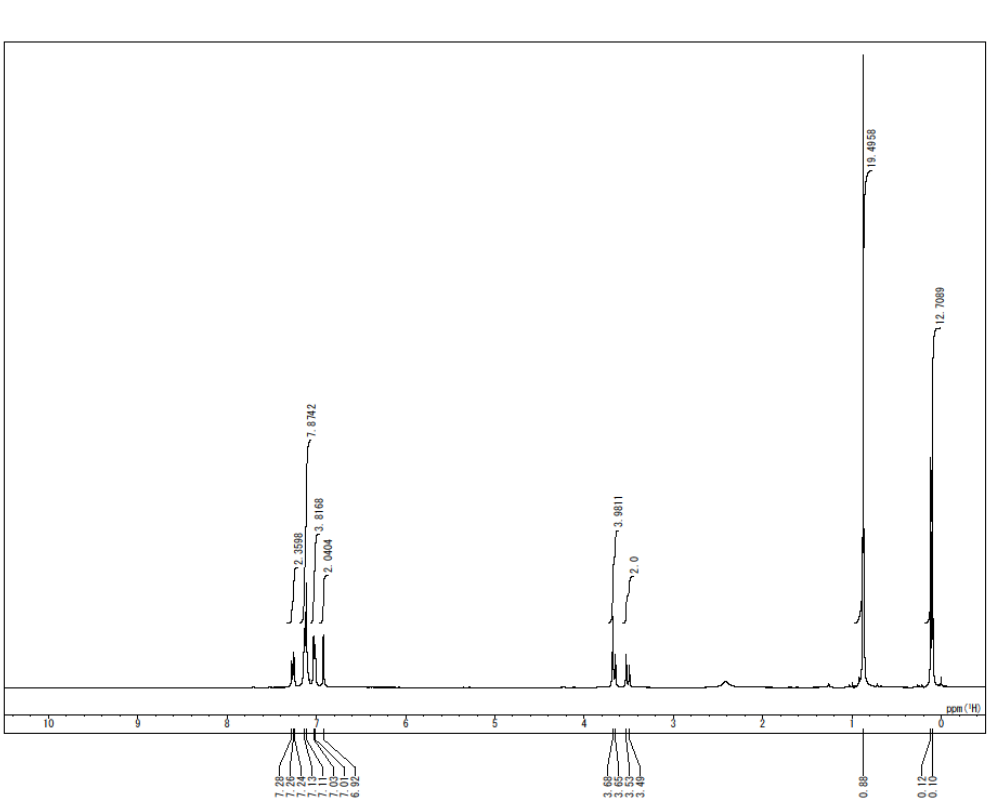


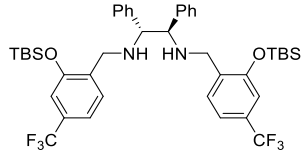
¹H NMR of **S2j**



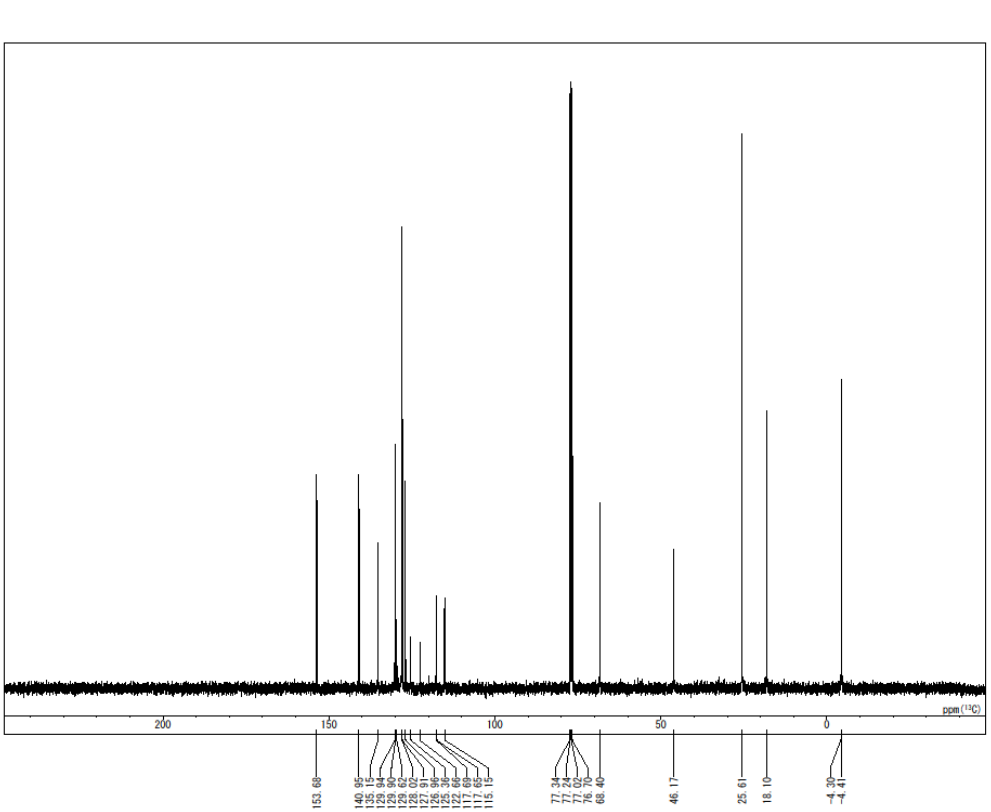


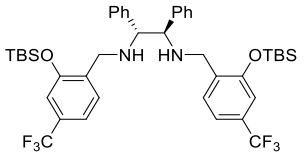
¹³C NMR of **S2j**



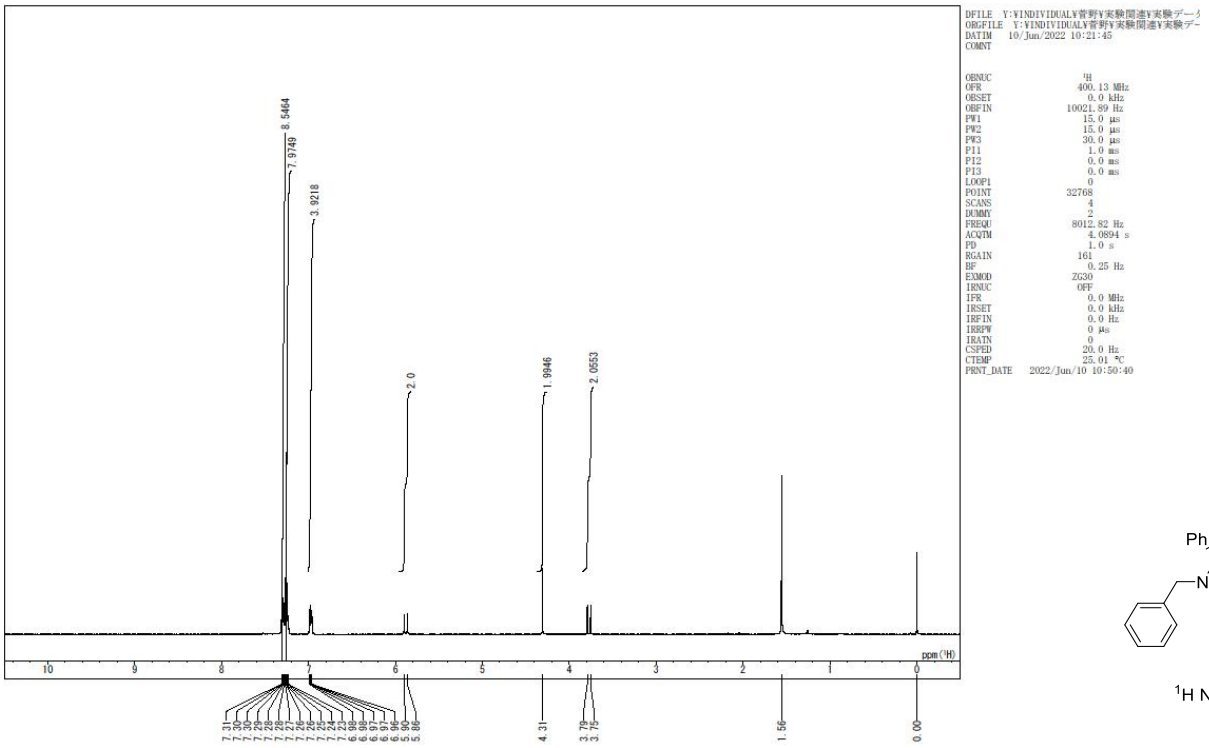


^{1}H NMR of **S2k**



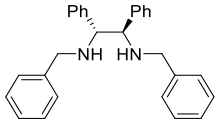


^{13}C NMR of **S2k**

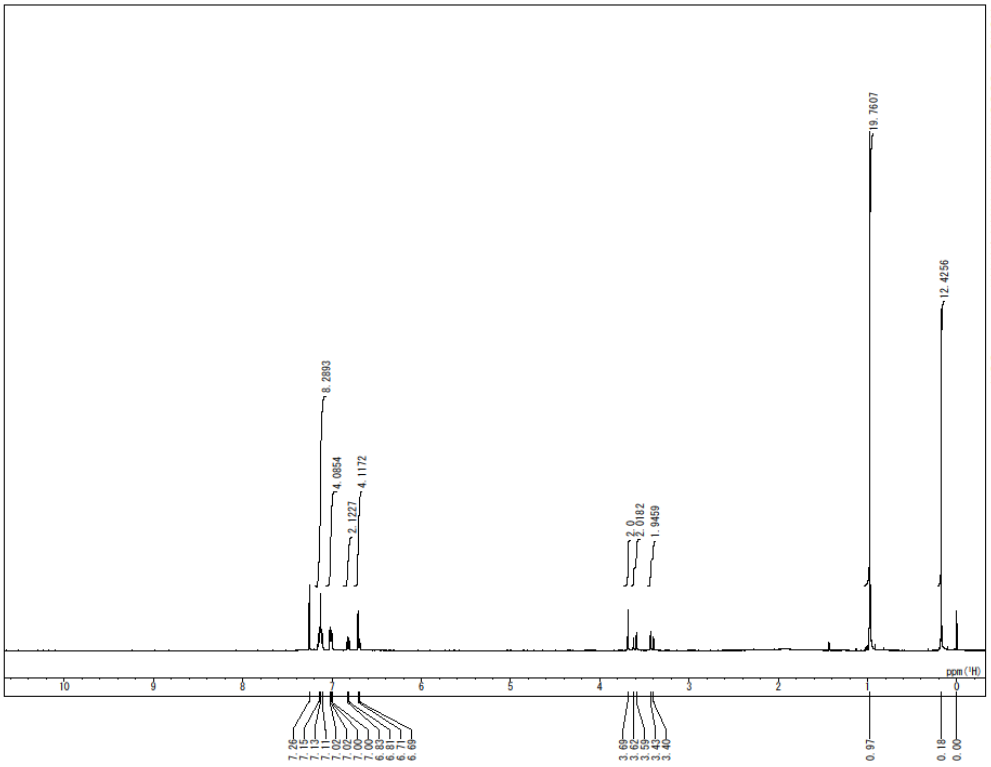


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 10/Jun/2022 10:21:45
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.01 °C
PRNT_DATE	2022/Jun/10 10:50:40

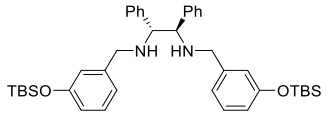


^{1}H NMR of **S1e**

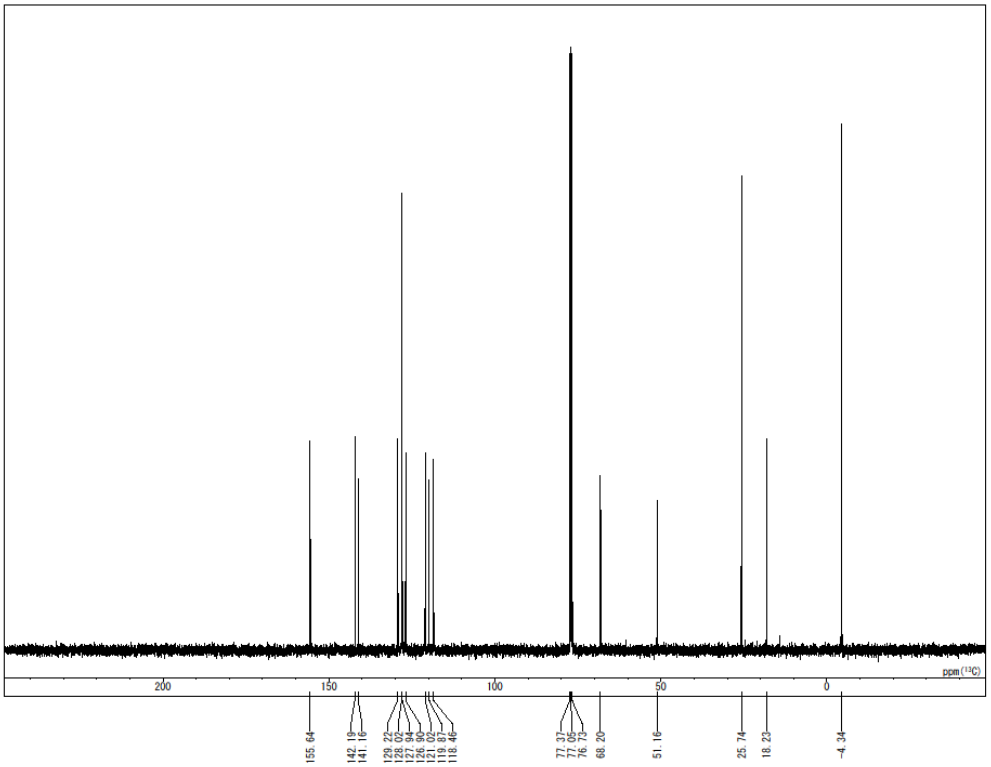


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 19/Jun/2022 16:03:40
COMNT

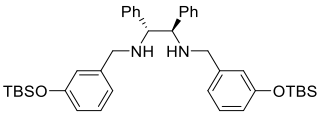
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	101
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRBPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.91 ℃
PRNT_DATE	2022/Jun/21 23:17:41



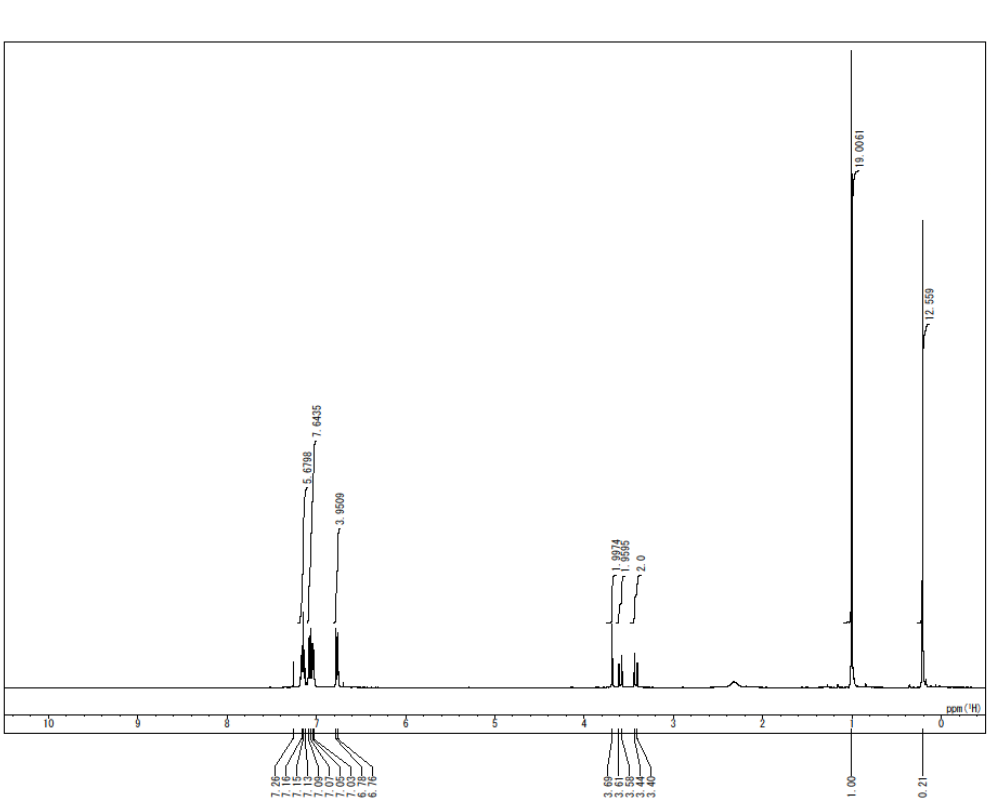
^{1}H NMR of **S2b**

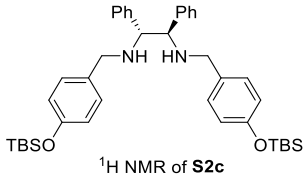


OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	114
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRBPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	22.31 ℃
PRNT_DATE	2022/Jun/02 21:33:23

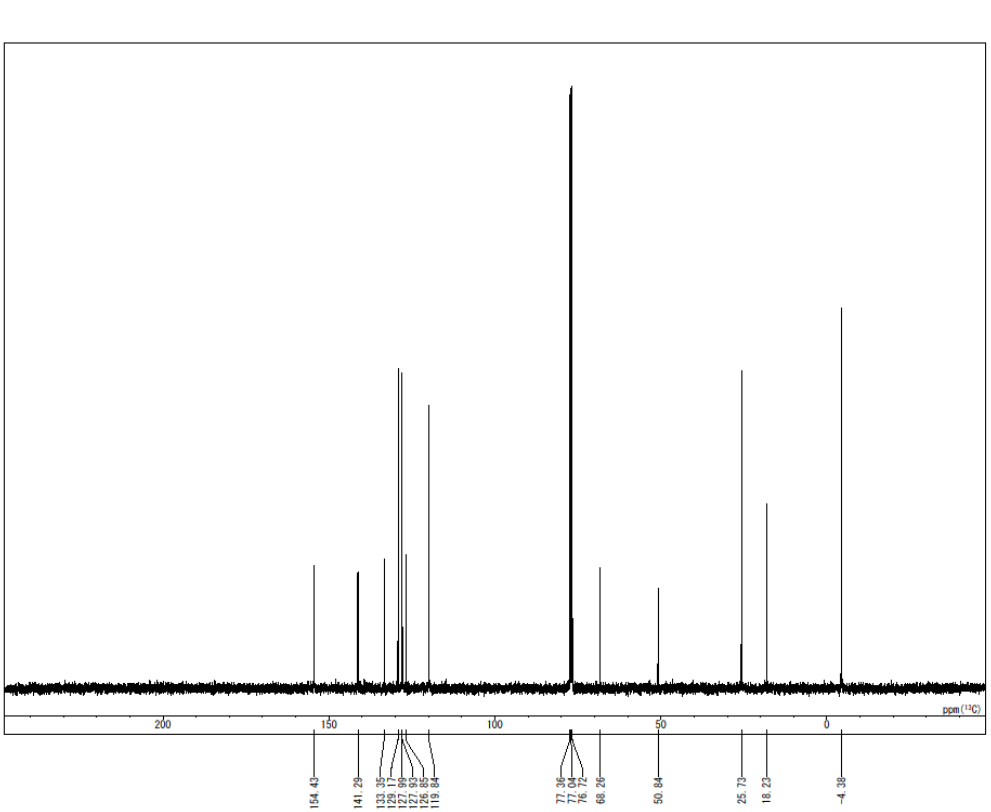


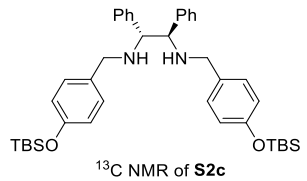
^{13}C NMR of **S2b**



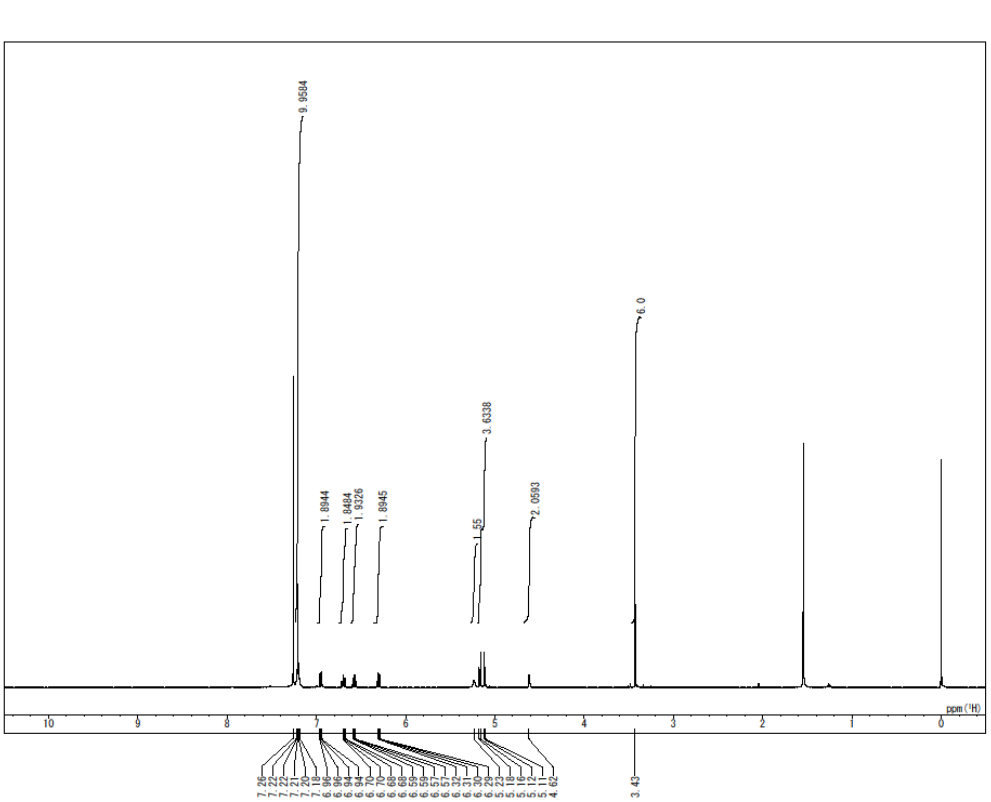


^{1}H NMR of **S2c**

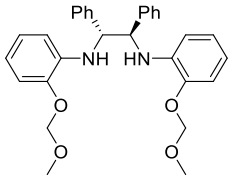




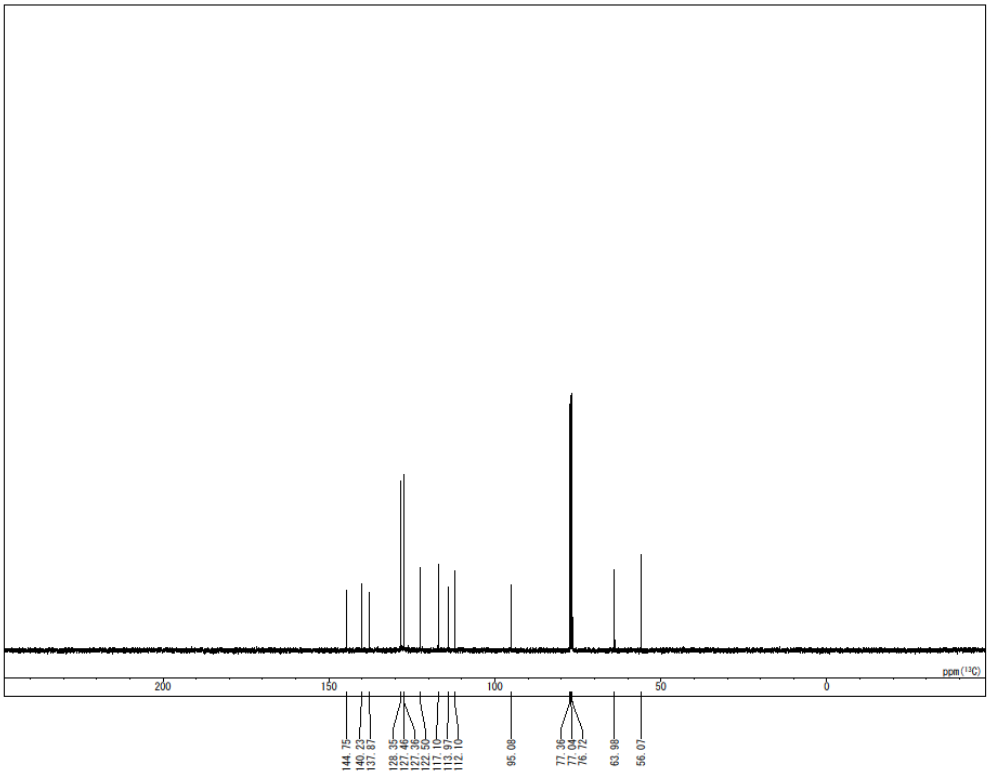
^{13}C NMR of **S2c**



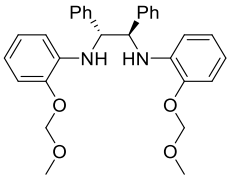
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.01 °C
PRNT_DATE	2022/Jun/05 18:03:23



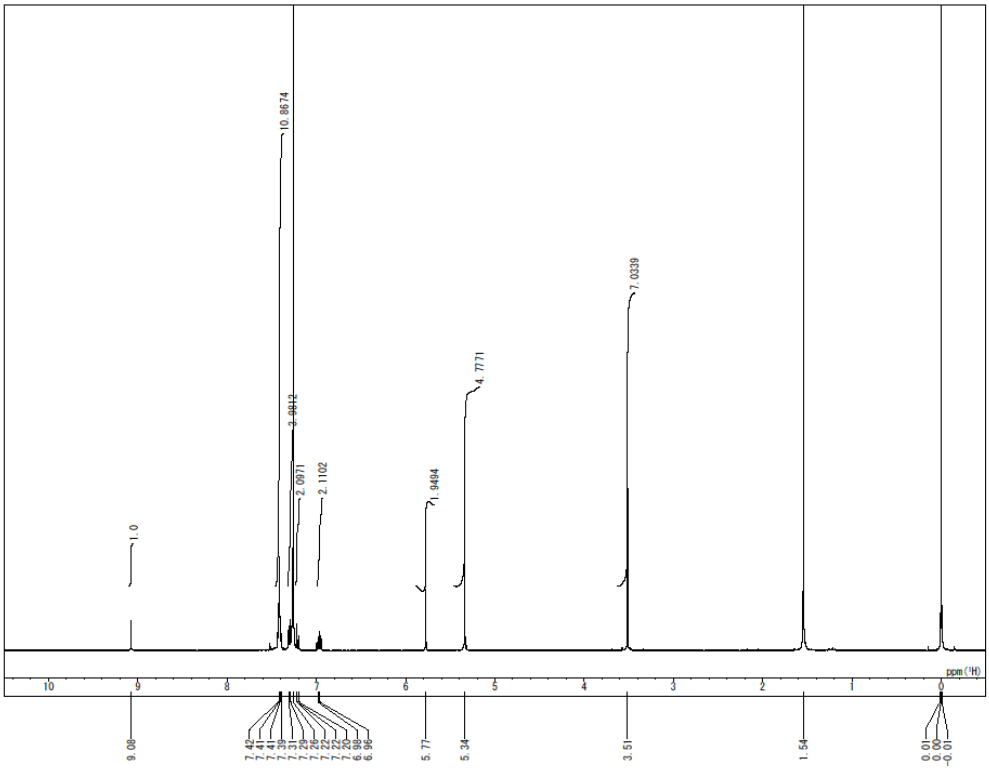
^{1}H NMR of **S2d**



OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.81 °C
PRNT_DATE	2022/Jun/05 18:19:51

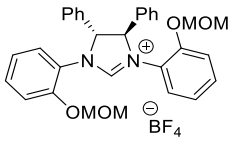


^{13}C NMR of **S2d**

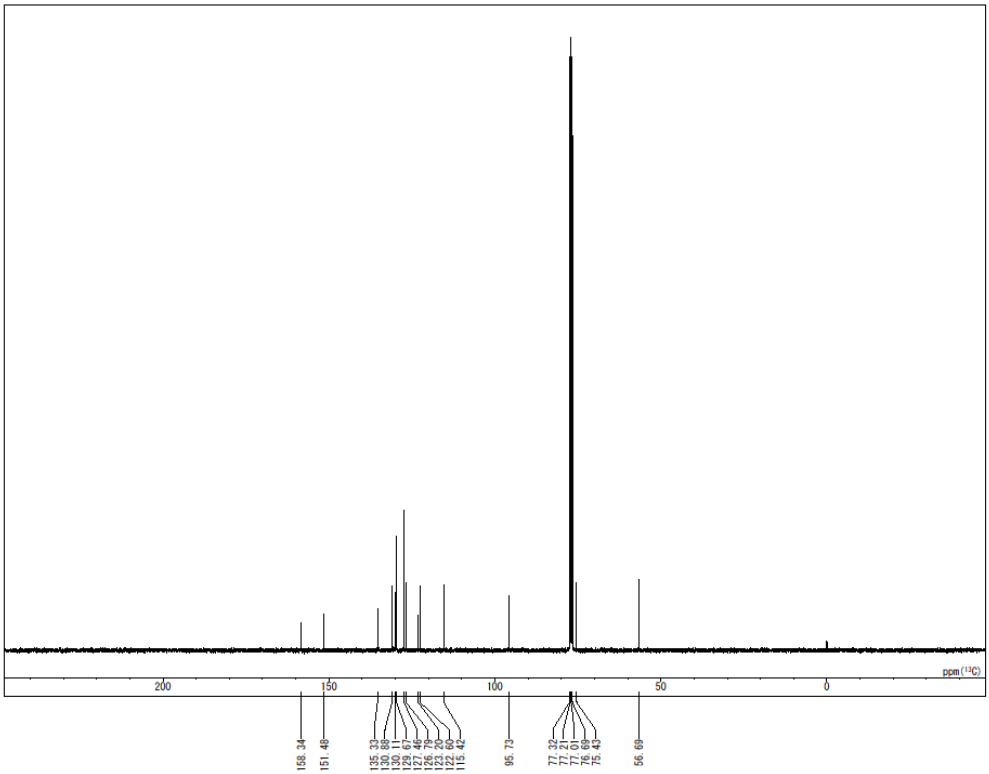


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 14/Jun/2022 23:17:56
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	24
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	181
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	24.91 ℃
PRNT_DATE	2022/Jun/15 10:08:48

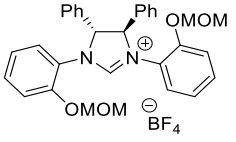


^{1}H NMR of **S2d'**

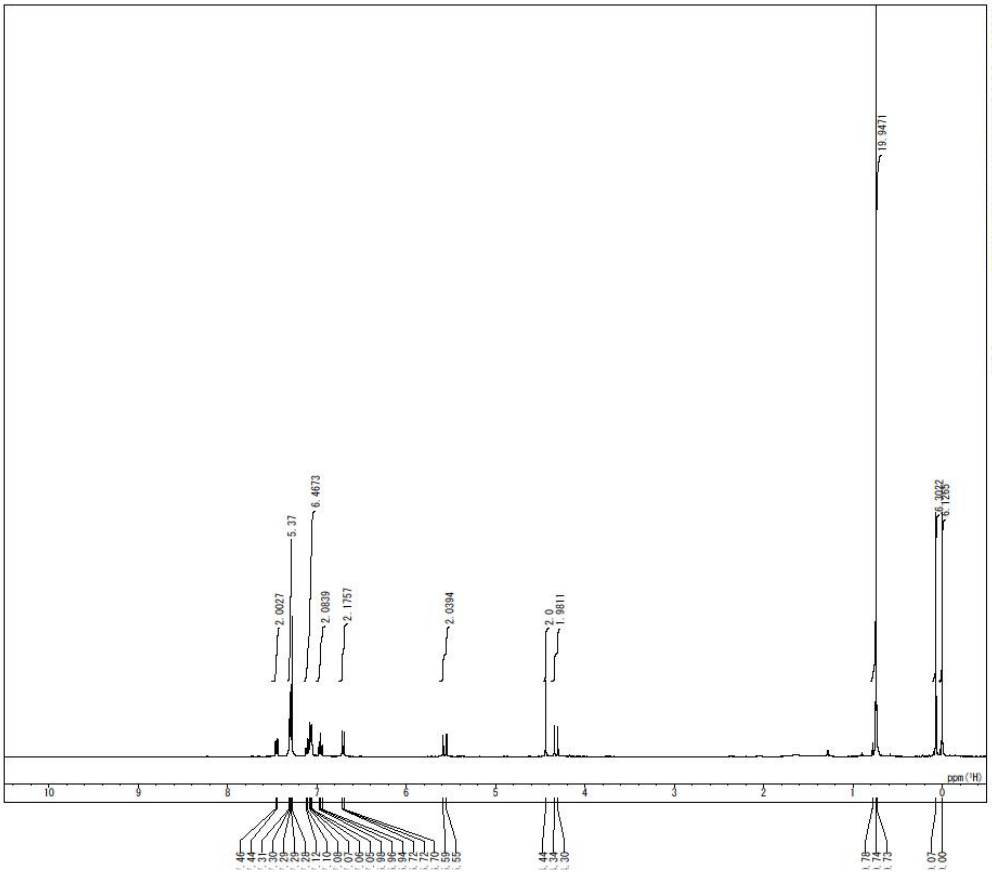


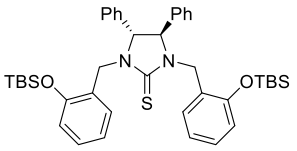
DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 15/Jun/2022 05:44:52
COMNT

OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
P11	2.0 ms
P12	0.0035 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	2048
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	26.01 ℃
PRNT_DATE	2022/Jun/15 09:55:58

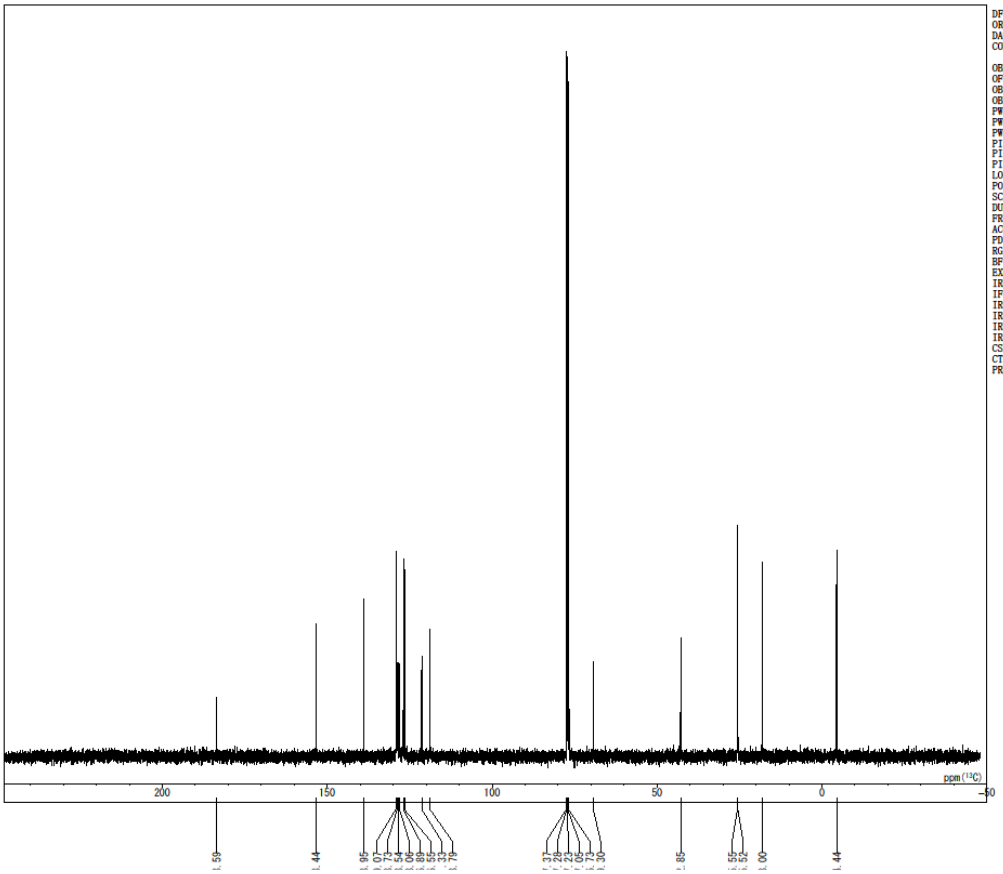


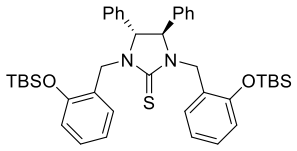
^{13}C NMR of **S2d'**



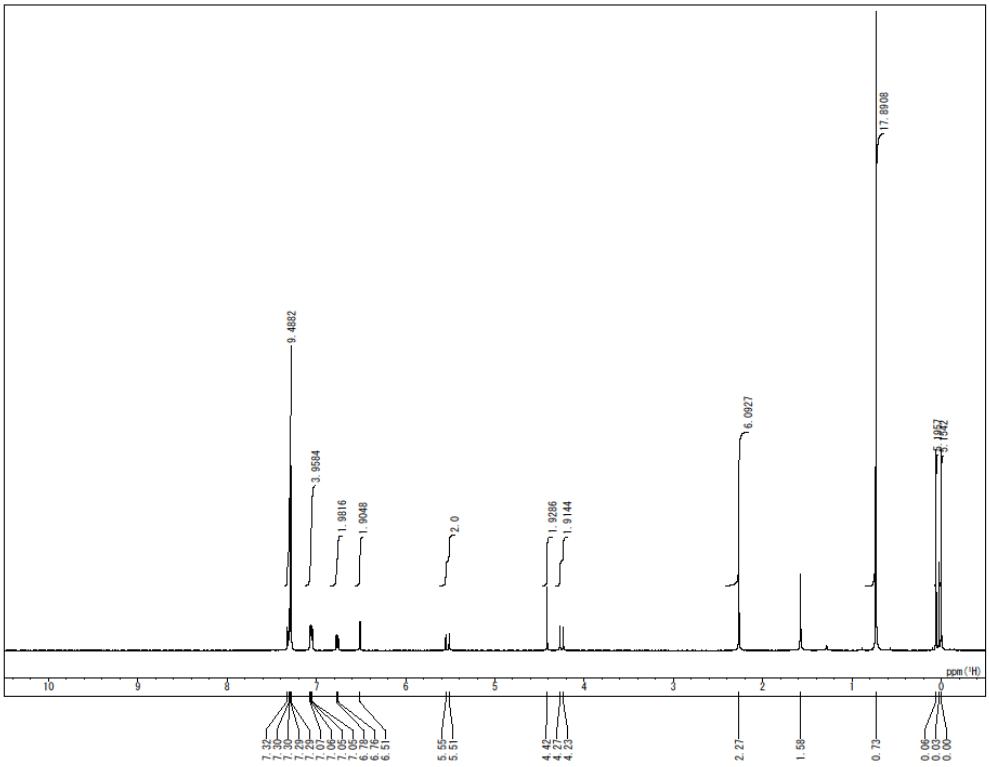


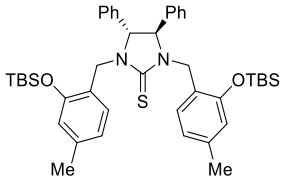
^{1}H NMR of **S3a**



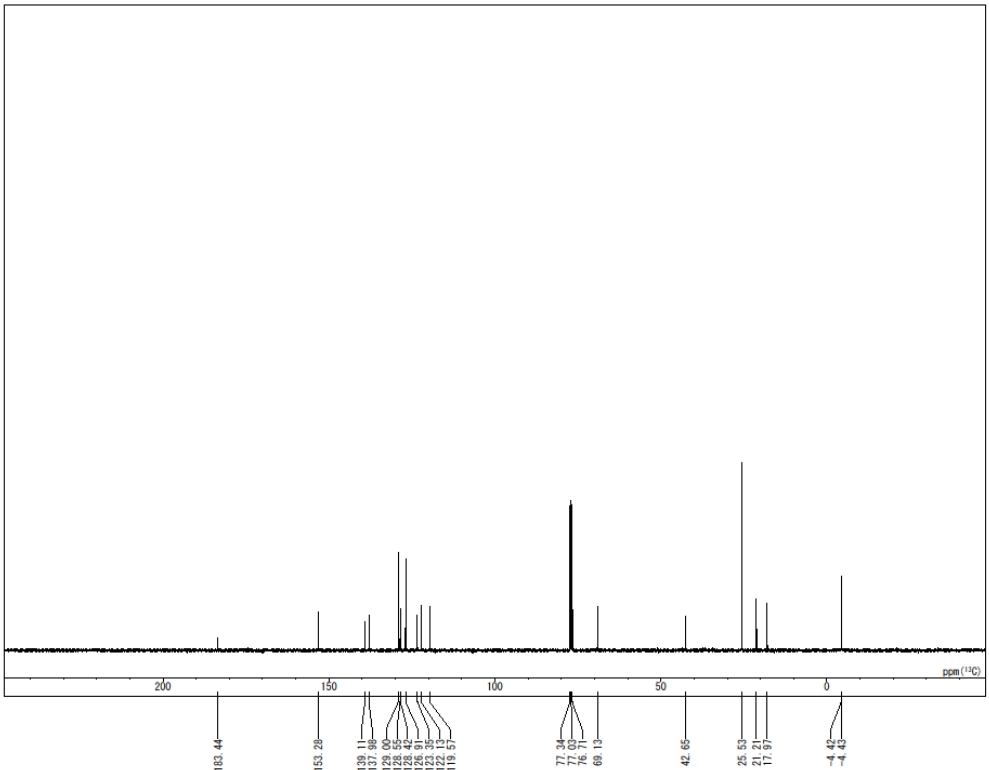


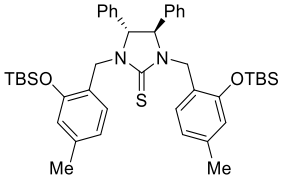
^{13}C NMR of **S3a**



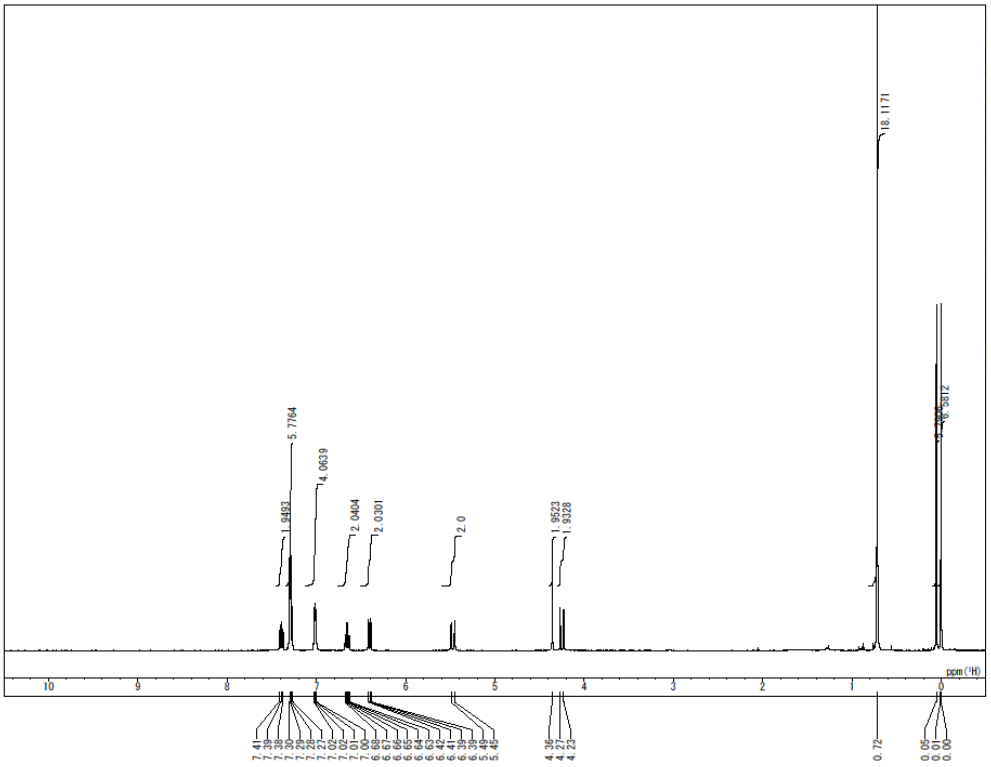


^{1}H NMR of **S3f**

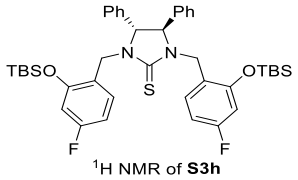




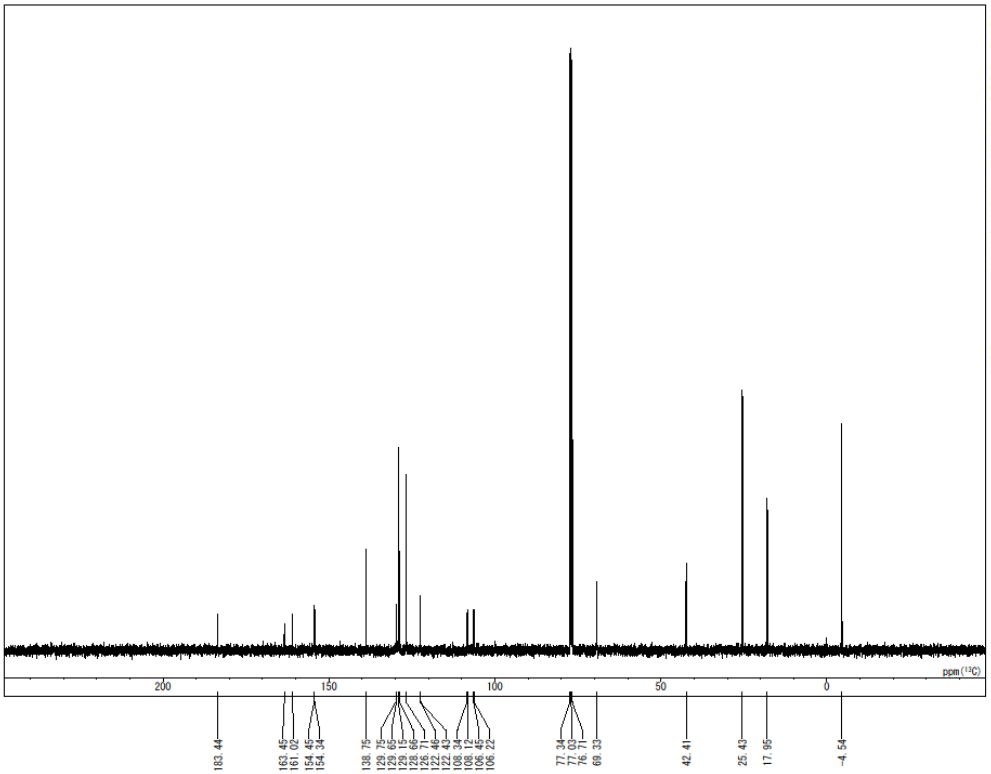
^{13}C NMR of **S3f**



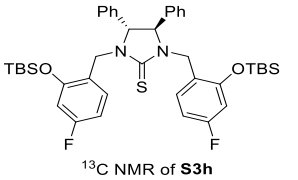

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM   01/Mar/2021 02:09:19
COMNT

OBNUC                  ¹H
OFR               400.13 MHz
OBSET               0.0 kHz
OBFIN            10021.89 Hz
PW1                15.0 µs
PW2                15.0 µs
PW3                30.0 µs
PI1                 1.0 ms
PI2                 0.0 ms
PI3                 0.0 ms
LOOP1                  0
POINT              32768
SCANS                  4
DUMMY                  2
FREQU            8012.82 Hz
ACQTM               4.0894 s
PD                  1.0 s
RGAIN                 81
BF                0.1223 Hz
EXMOD              ZG30
IRNUC              OFF
IFR                 0.0 MHz
IRSET               0.0 kHz
IRFIN               0.0 Hz
IRRPW               0 µs
IRATN                  0
CSPED              20.0 Hz
CTEMP              21.91 °C
PRNT_DATE   2022/Jun/22 00:17:31
```



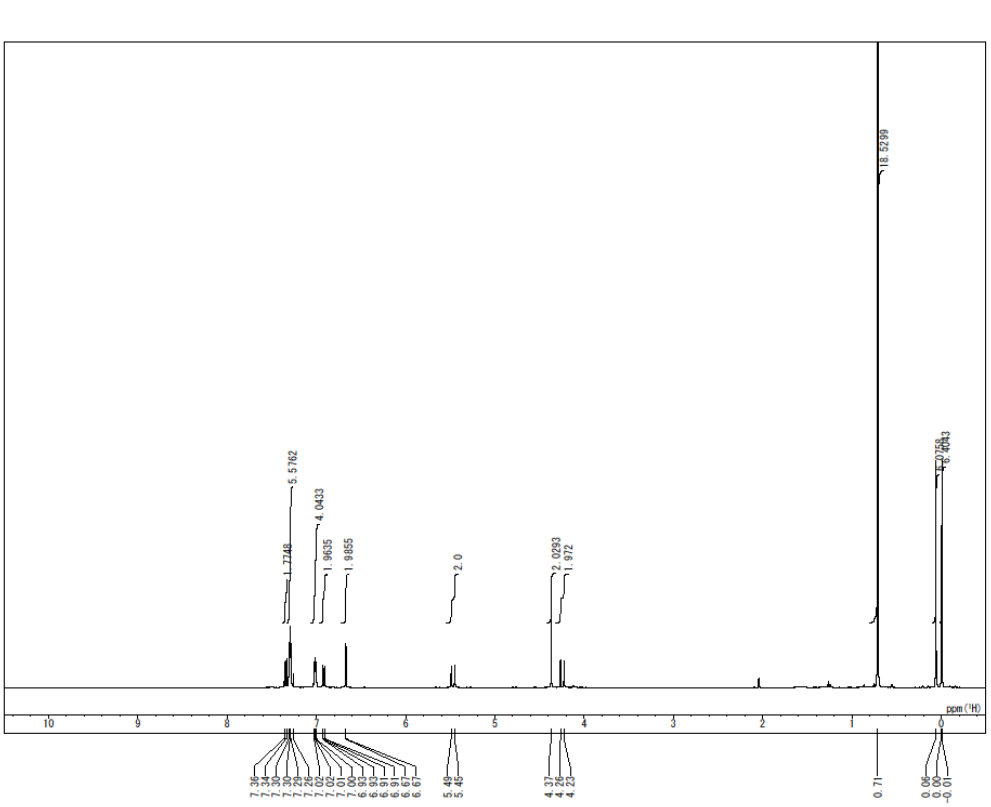
^{1}H NMR of **S3h**

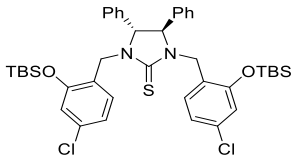



```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM   01/Mar/2021 02:24:33
COMNT

OBNUC                  ¹³C
OFR               100.61 MHz
OBSET               0.0 kHz
OBFIN            9999.159 Hz
PW1                10.0 µs
PW2                10.0 µs
PW3                20.0 µs
PI1                 2.0 ms
PI2                0.0035 ms
PI3                 0.0 ms
LOOP1                  0
POINT              32768
SCANS                256
DUMMY                  2
FREQU            29761.9 Hz
ACQTM               1.101 s
PD                  2.0 s
RGAIN                114
BF                0.4541 Hz
EXMOD            ZGPG30
IRNUC              OFF
IFR                 0.0 MHz
IRSET               0.0 kHz
IRFIN               0.0 Hz
IRRPW               0 µs
IRATN                  0
CSPED              20.0 Hz
CTEMP              22.41 °C
PRNT_DATE   2022/Jun/22 00:17:00
```

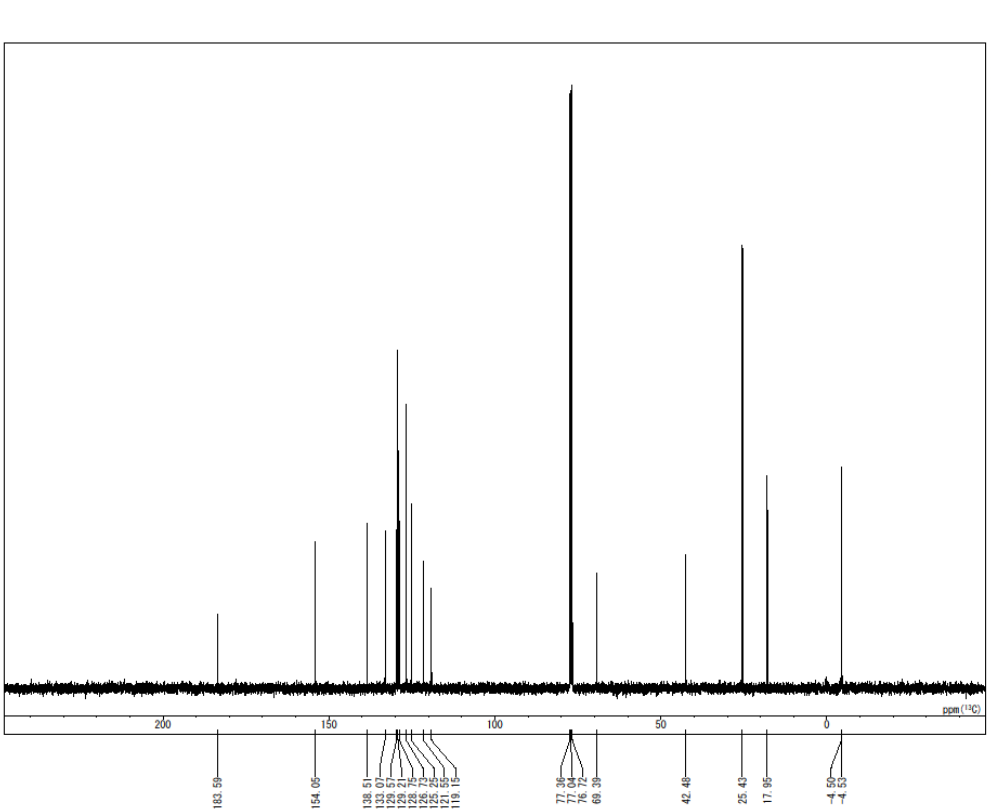


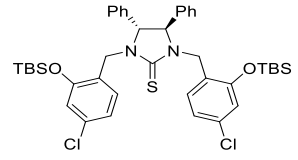
^{13}C NMR of **S3h**



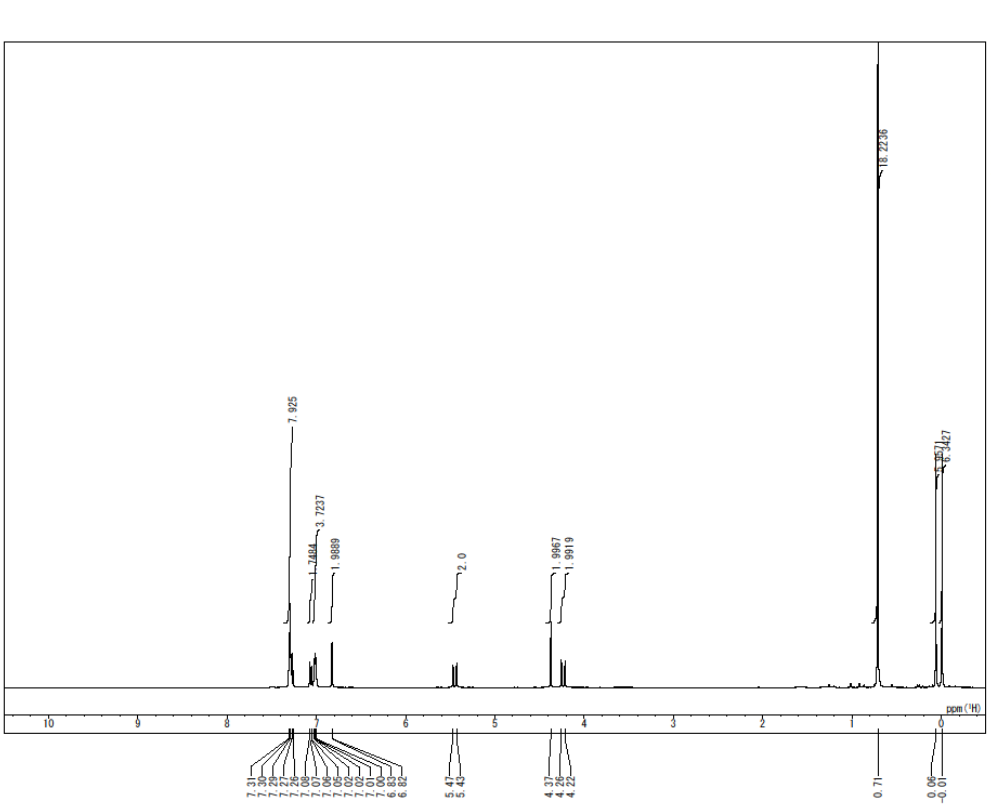


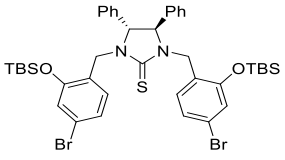
^{1}H NMR of **S3g**



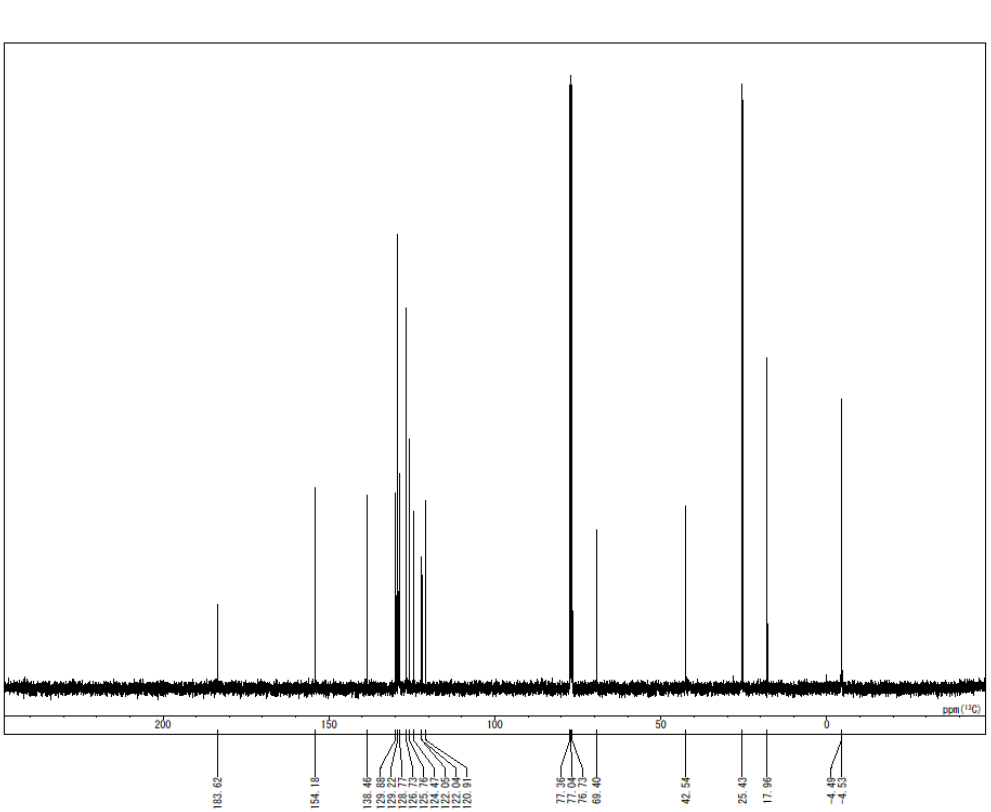


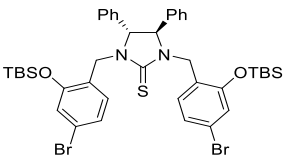
^{13}C NMR of **S3g**



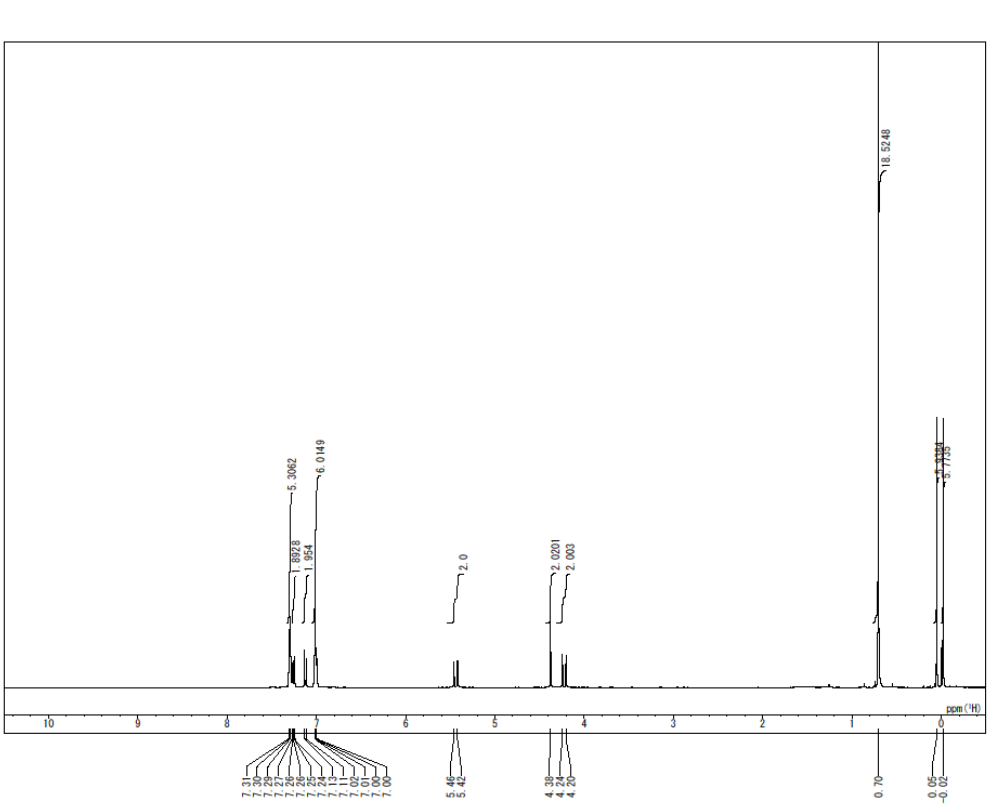


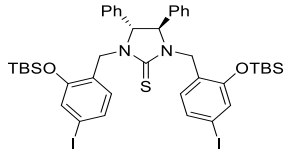
^{1}H NMR of **S3i**



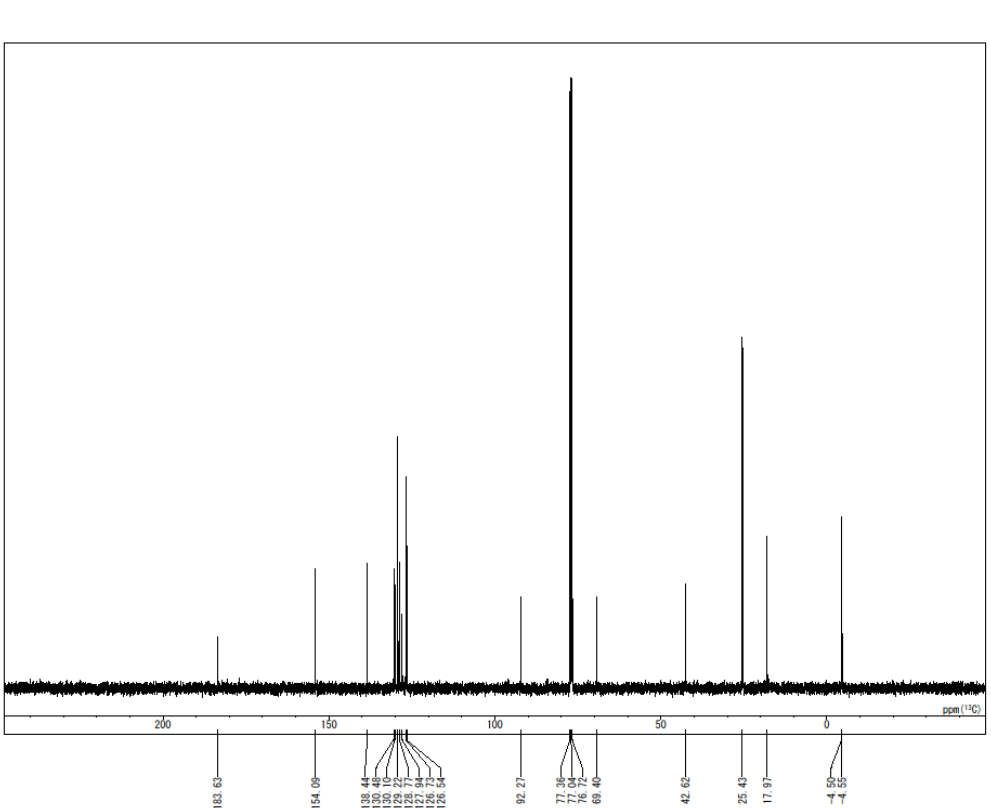


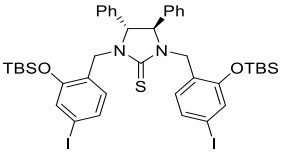
^{13}C NMR of **S3i**



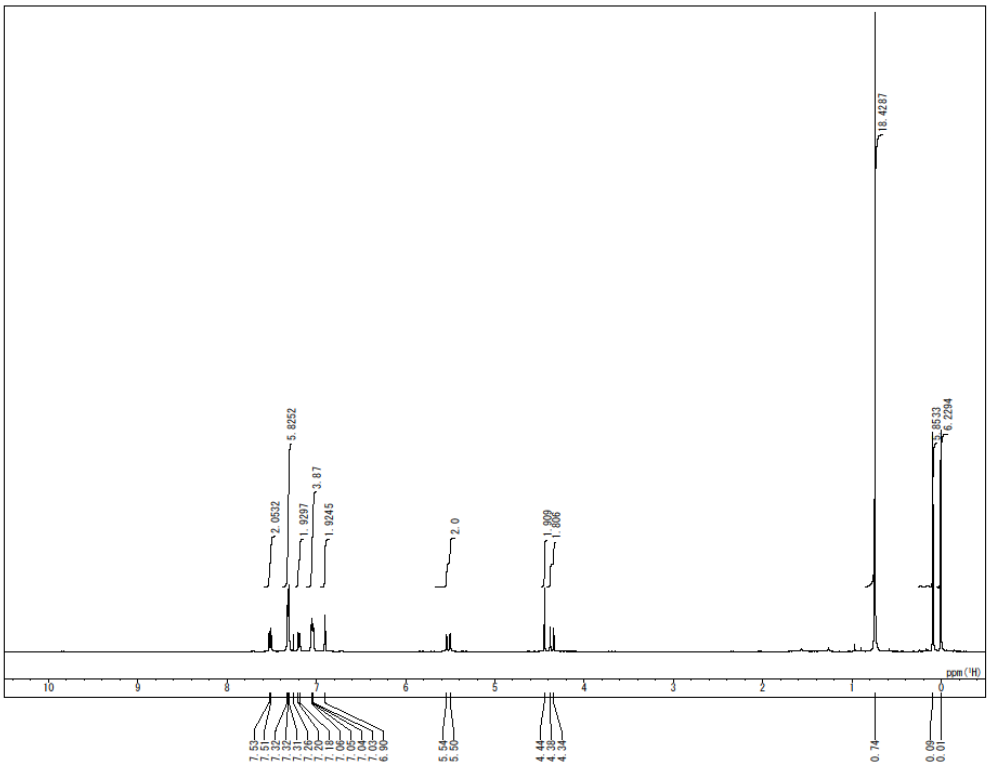


^{1}H NMR of **S3j**

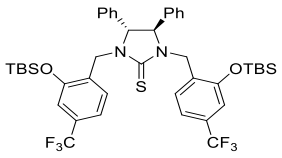




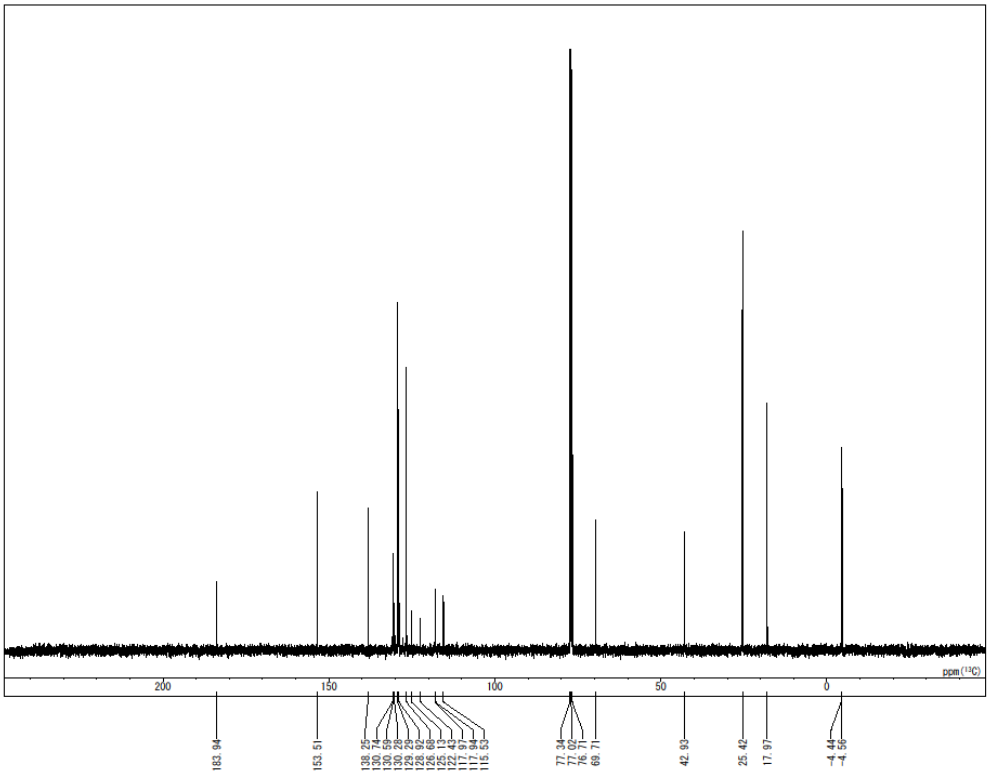
^{13}C NMR of **S3j**



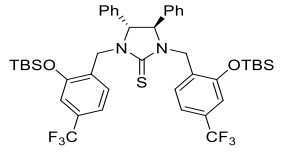
OBNUC ¹H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 57
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 22.41 °C
PRNT_DATE 2022/Jun/02 23:20:56



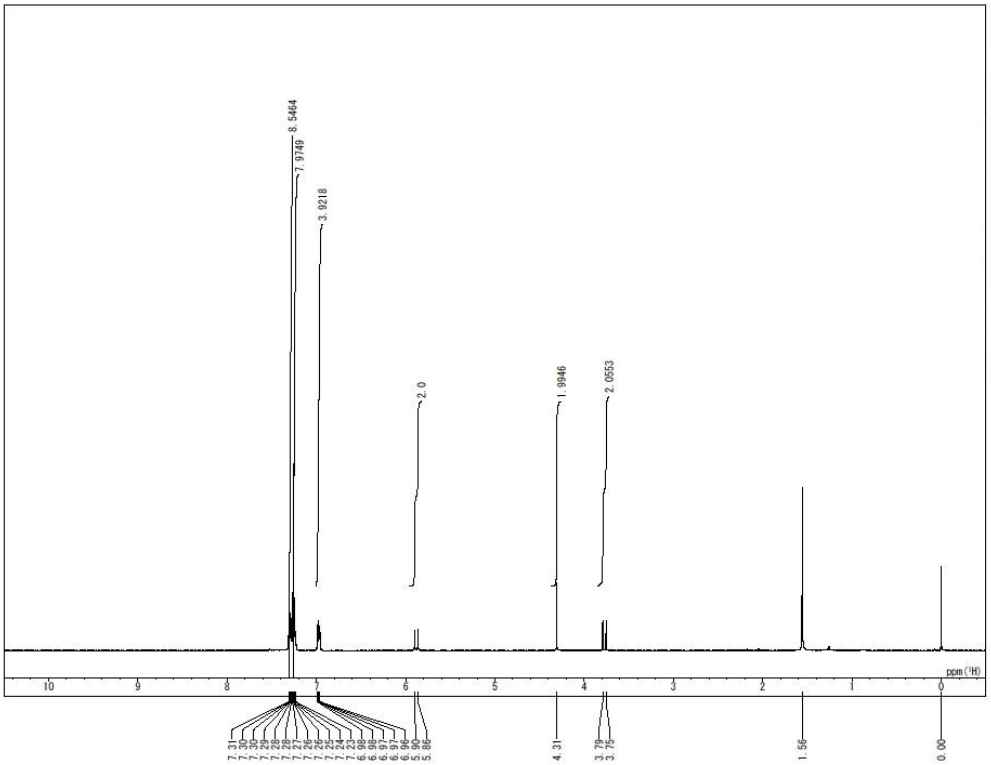
^{1}H NMR of **S3k**



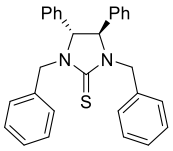
OBNUC ¹³C
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 9999.159 Hz
PW1 10.0 µs
PW2 10.0 µs
PW3 20.0 µs
PI1 2.0 ms
PI2 0.0035 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 256
DUMMY 2
FREQU 29761.9 Hz
ACQTM 1.101 s
PD 2.0 s
RGAIN 181
BF 0.25 Hz
EXMOD ZGPG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 22.81 °C
PRNT_DATE 2022/Jun/02 23:18:47



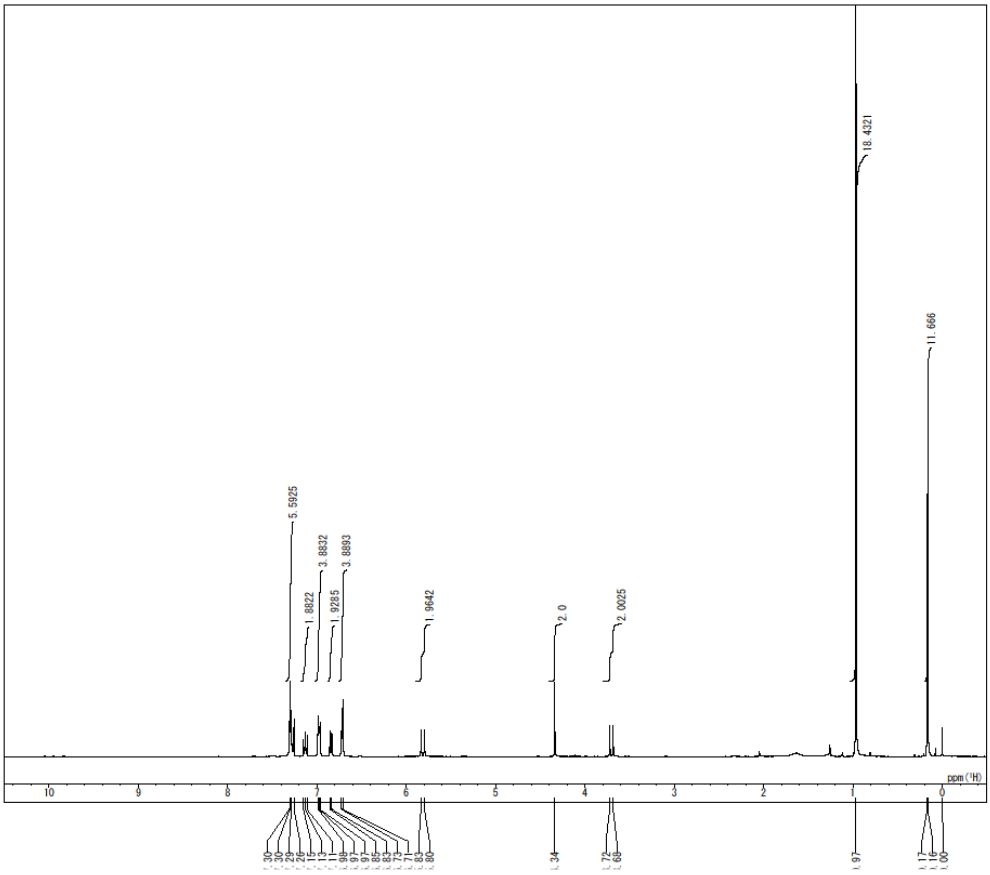
^{13}C NMR of **S3k**

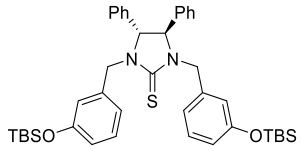



```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM    10/Jun/2022 10:21:45
COMNT


OBNUC                  ¹H
OFR                400.13 MHz
OBSET                0.0 kHz
OBFIN            10021.89 Hz
PW1                 15.0 µs
PW2                 15.0 µs
PW3                 30.0 µs
PI1                  1.0 ms
PI2                  0.0 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS                  4
DUMMY                  2
FREQU            8012.82 Hz
ACQTM               4.0894 s
PD                   1.0 s
RGAIN                161
BF                  0.25 Hz
EXMOD               ZG30
IRNUC               OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRPW                 0 µs
IRATN                  0
CSPED               20.0 Hz
CTEMP               25.01 ℃
PRNT_DATE    2022/Jun/10 10:50:40
```

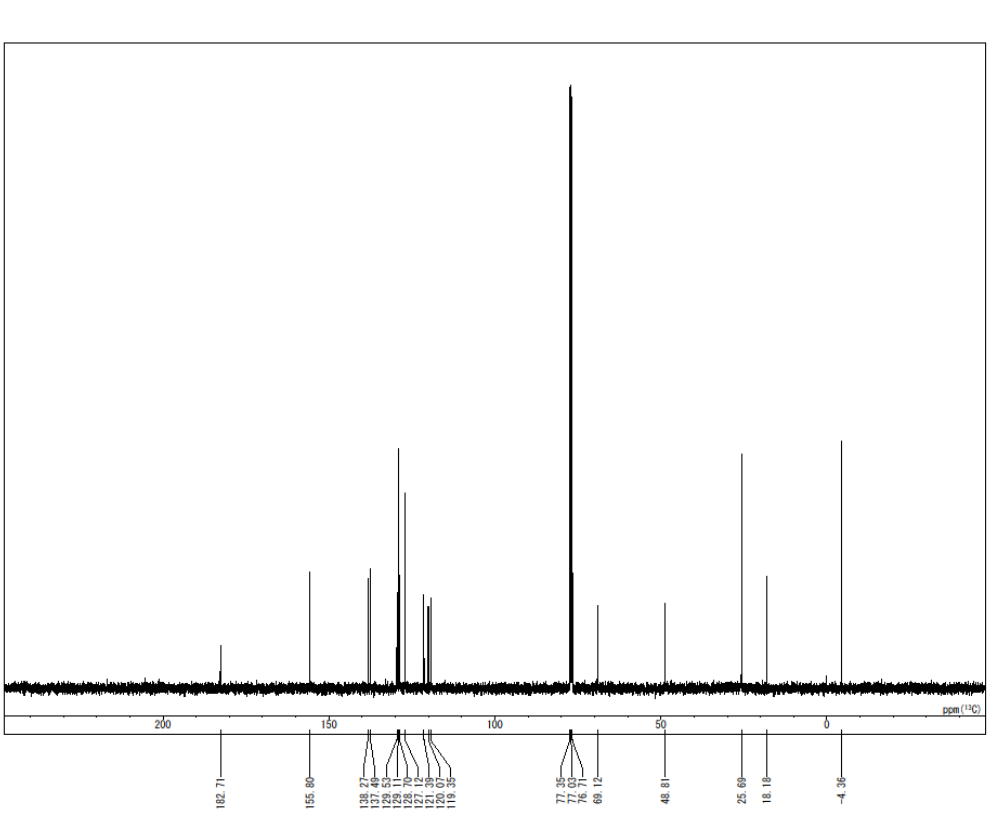


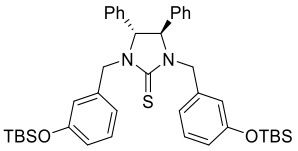
^{1}H NMR of **4e**



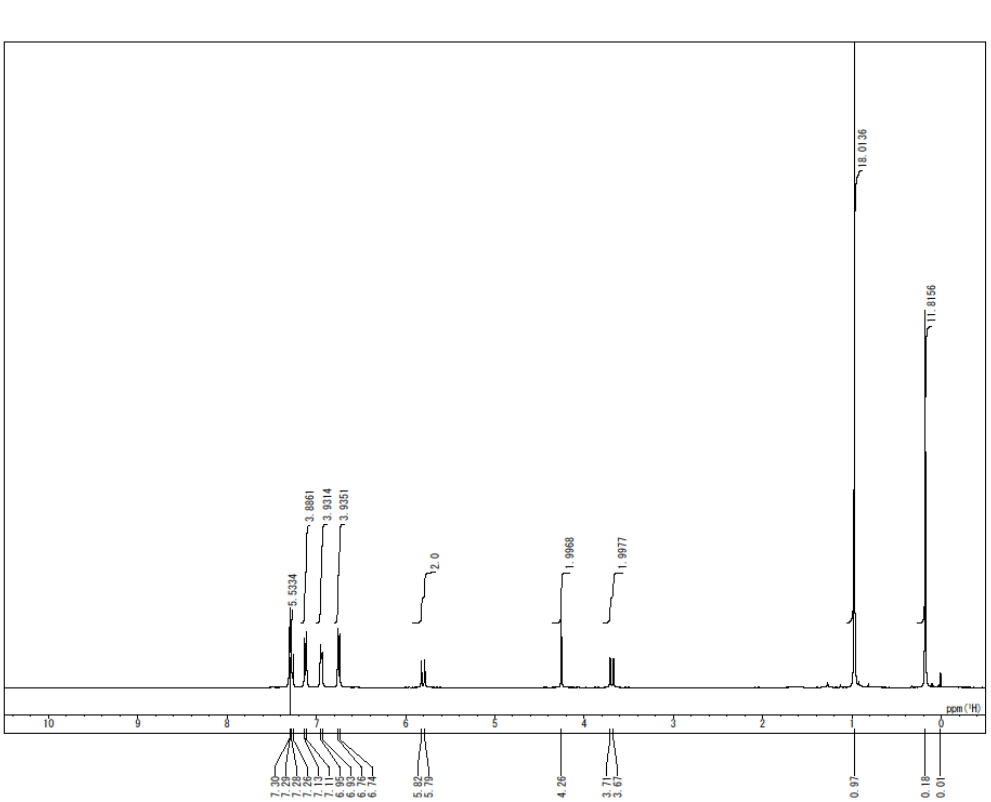


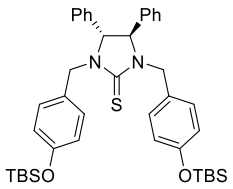
^{1}H NMR of **S3b**



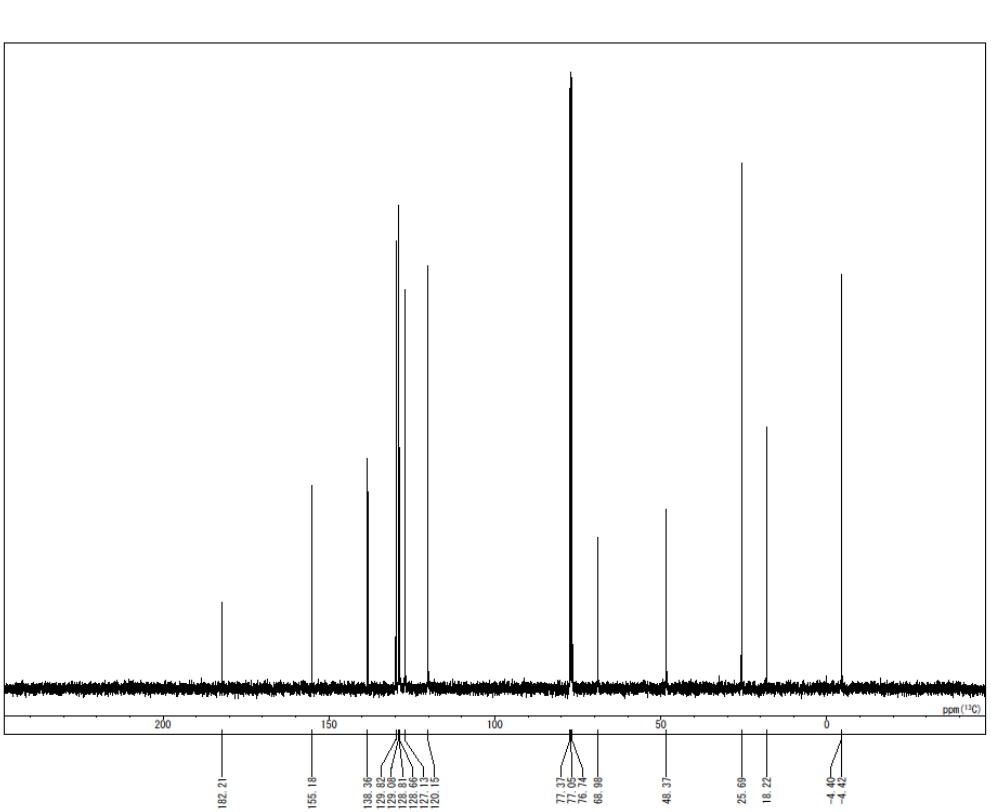


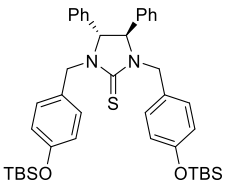
^{13}C NMR of **S3b**



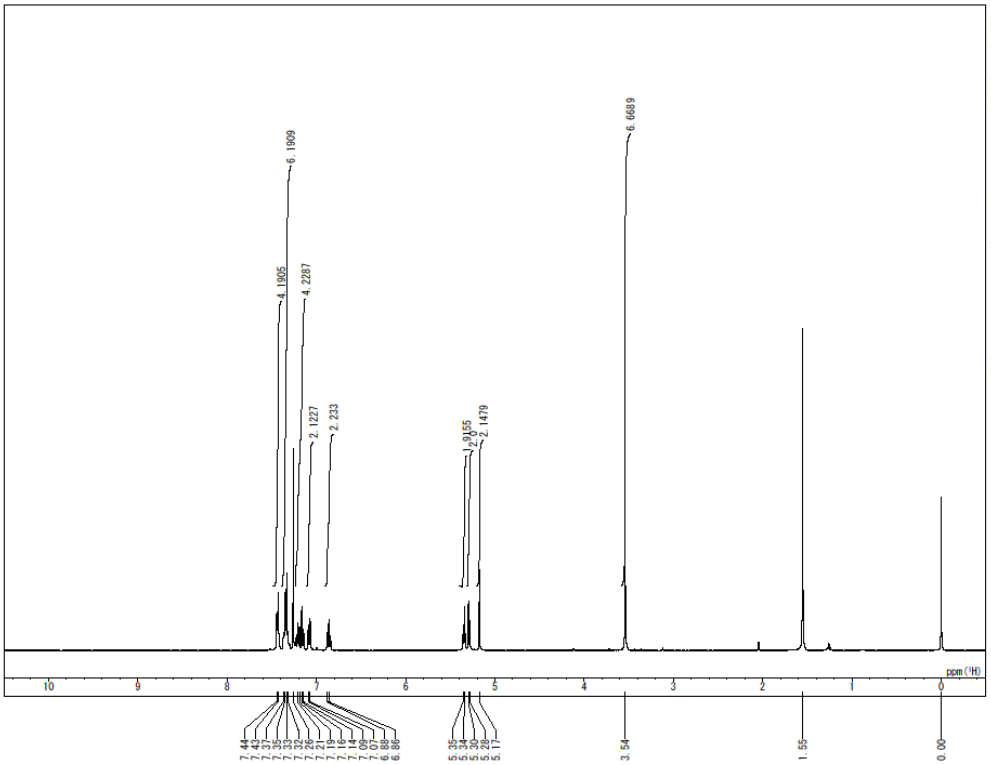


^{1}H NMR of **S3c**

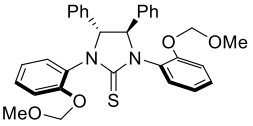




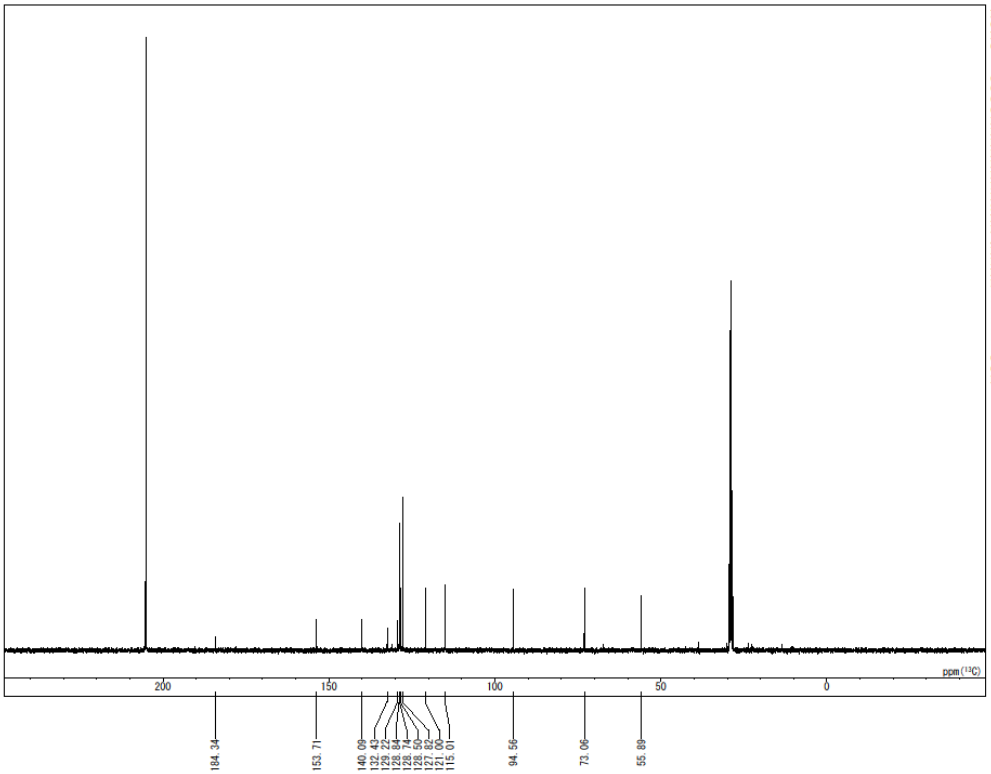
^{13}C NMR of **S3c**



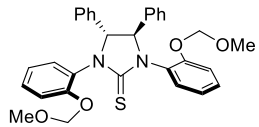

```
DFILE   X:¥062ORG¥ORG¥MS8193BV10¥PDATA¥1¥1I
ORGFILE   X:¥062ORG¥ORG¥MS8193BV10¥PDATA¥1¥1I
DATIM    20/Jun/2022 19:00:11
COMNT


OBNUC                  ¹H
OFR                400.03 MHz
OBSET                0.0 kHz
OBFIN            10009.24 Hz
PW1                2.6667 µs
PW2                  8.0 µs
PW3                 16.0 µs
PI1                  1.0 ms
PI2                  0.0 ms
PI3                  0.0 ms
LOOP1                  0
POINT              65536
SCANS                  4
DUMMY                  2
FREQU           7812.5 Hz
ACQTM              8.3886 s
PD                   1.0 s
RGAIN                101
BF                  0.25 Hz
EXMOD              ZG30
IRNUC              OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRRPW                0 µs
IRATN                0
CSPED                0.0 Hz
CTEMP             25.0126 °C
PRNT_DATE    2022/Jun/20 19:43:58
```



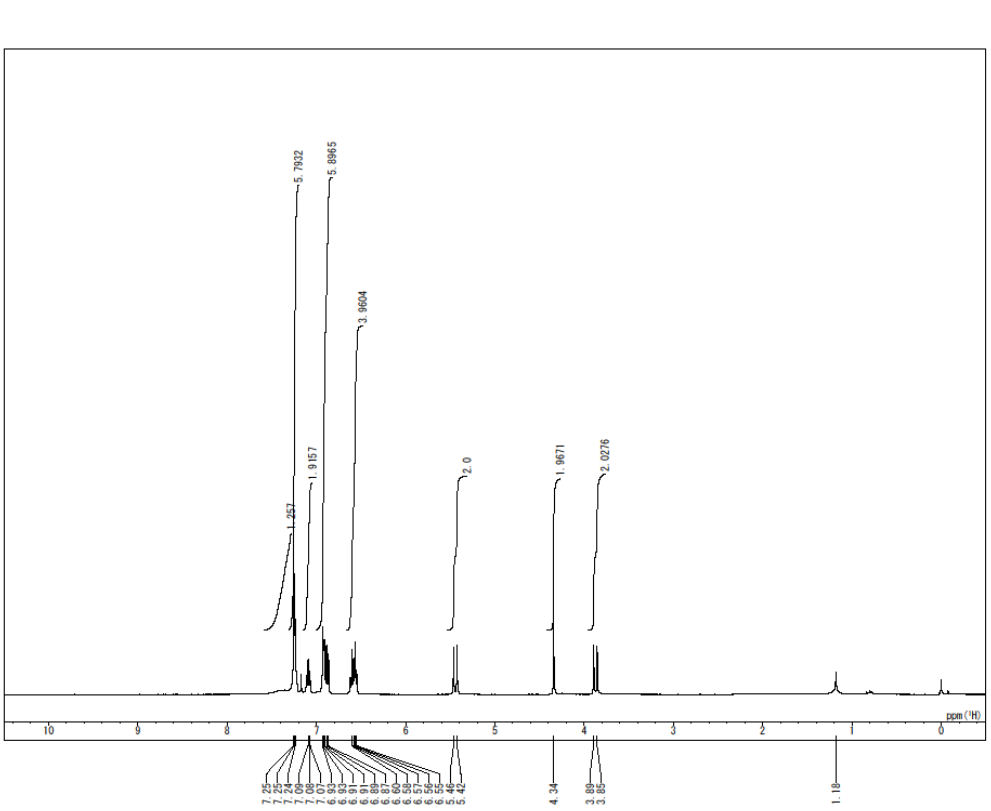
^{1}H NMR of **S3d**



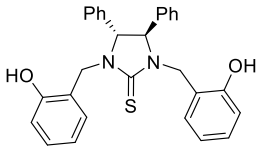

```
DFILE   X:¥062ORG¥DATA¥ORG¥NMR¥MS8201C-NMR¥10¥
ORGFILE   X:¥062ORG¥DATA¥ORG¥NMR¥MS8201C-NMR¥1
DATIM    01/Jul/2022 18:47:48
COMNT


OBNUC                  ¹³C
OFR               100.61 MHz
OBSET                0.0 kHz
OBFIN            9999.159 Hz
PW1                 10.0 µs
PW2                 10.0 µs
PW3                 20.0 µs
PI1                  2.0 ms
PI2                0.0035 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS                256
DUMMY                  2
FREQU           29761.9 Hz
ACQTM              1.101 s
PD                   2.0 s
RGAIN                203
BF                  0.25 Hz
EXMOD            ZGPG30
IRNUC              OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRRPW                0 µs
IRATN                0
CSPED               20.0 Hz
CTEMP             27.71 °C
PRNT_DATE    2022/Jul/01 20:35:57
```



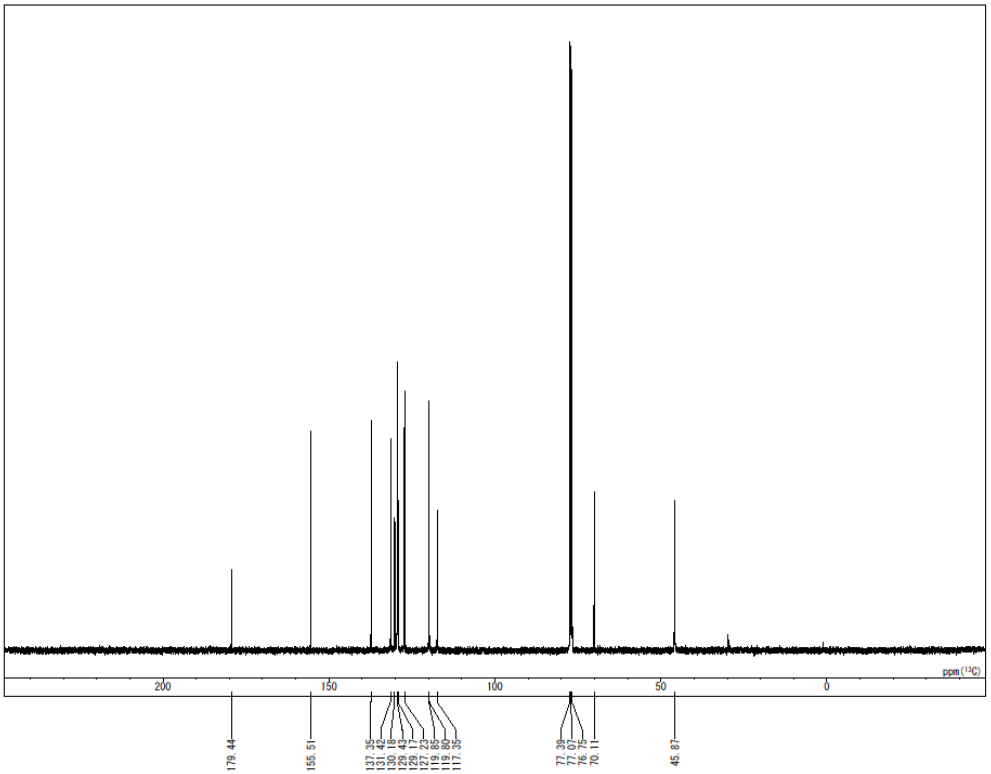
^{13}C NMR of **S3d**



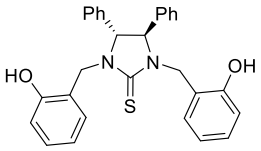
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	14.0 μs
PW2	14.0 μs
PW3	28.0 μs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	72
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 μs
IRATN	0
CSPED	20.0 Hz
CTEMP	23.01 °C
PRNT_DATE	2022/Jun/02 23:26:57



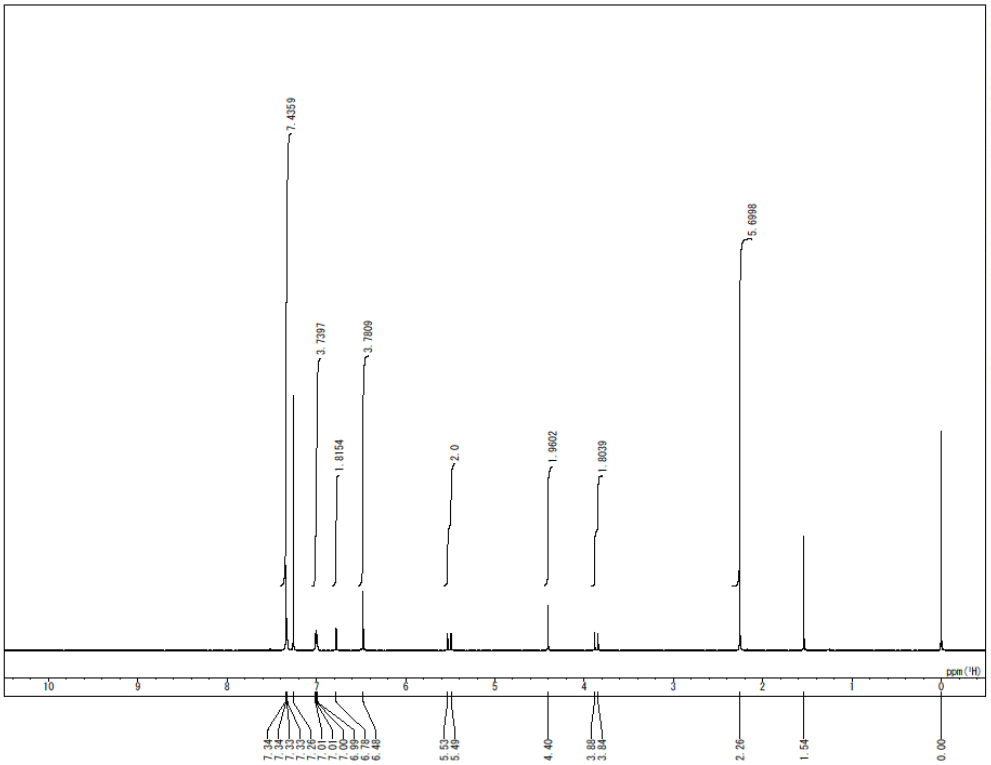
^{1}H NMR of **4a**



OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	8.6 μs
PW2	8.6 μs
PW3	17.2 μs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	1024
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	114
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 μs
IRATN	0
CSPED	20.0 Hz
CTEMP	24.01 °C
PRNT_DATE	2022/Jun/02 23:27:59

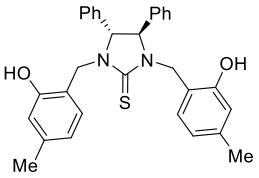


^{13}C NMR of **4a**

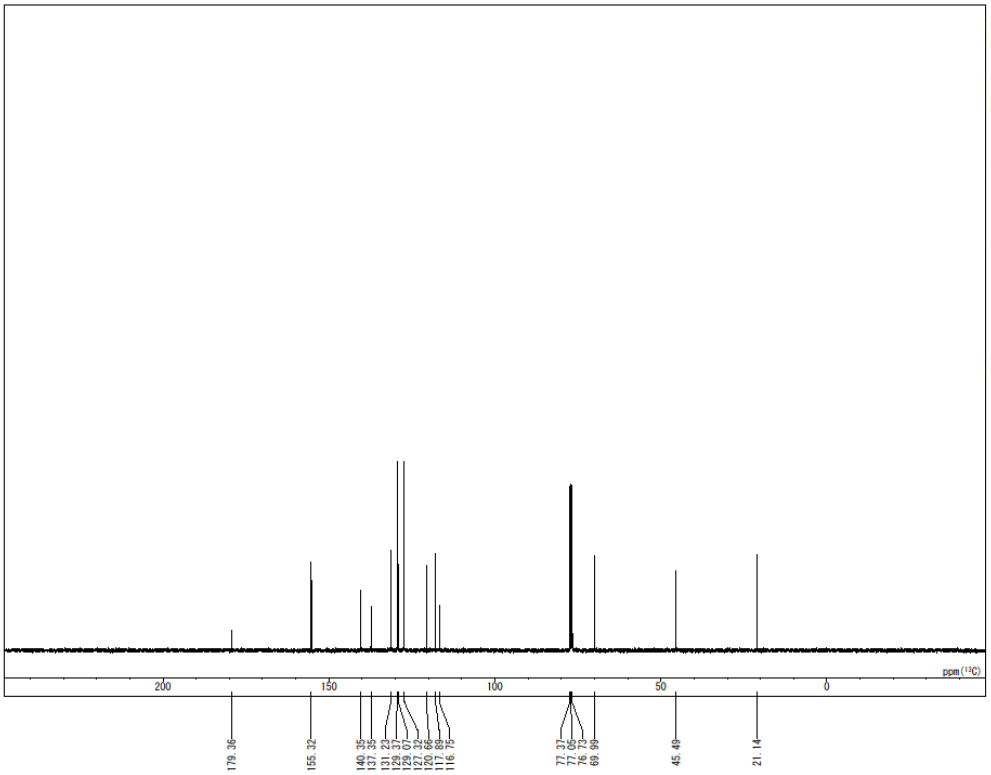


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 11/Jun/2022 15:53:41
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.01 ℃
PRNT_DATE	2022/Jun/11 16:27:29

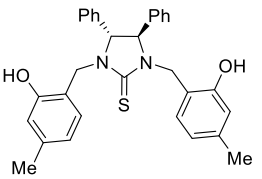


^{1}H NMR of **4f**

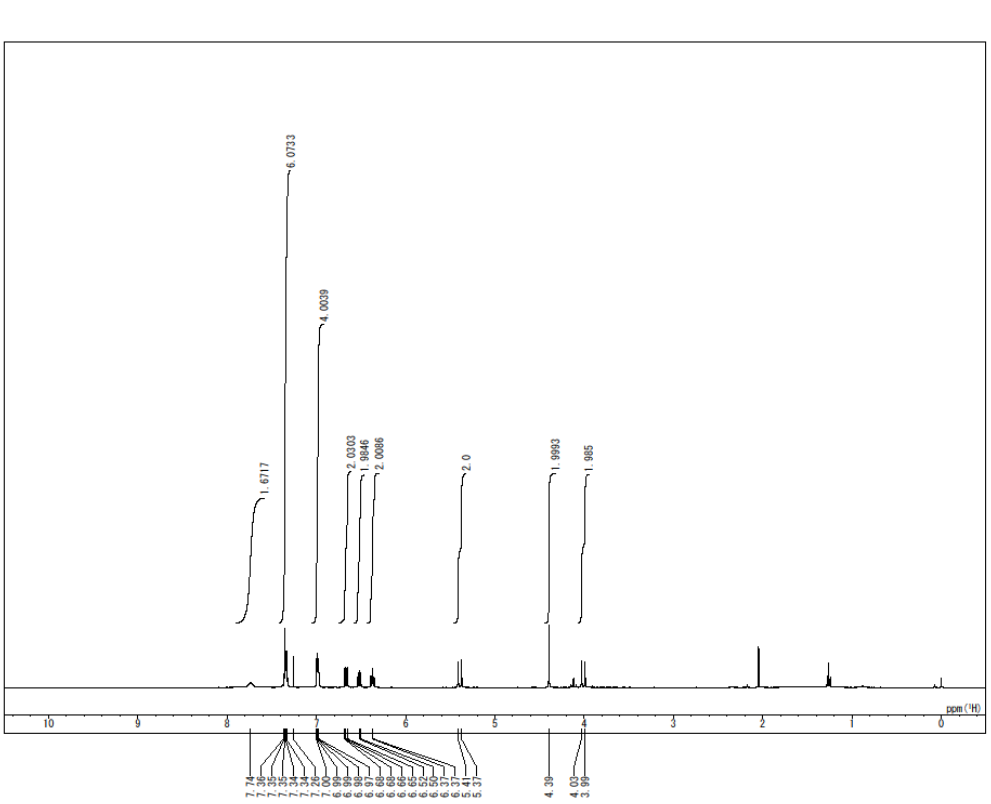


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 11/Jun/2022 16:17:28
COMNT

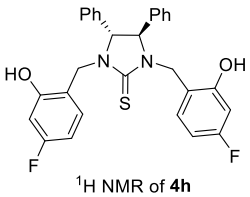
OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
P11	2.0 ms
P12	0.0035 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.81 ℃
PRNT_DATE	2022/Jun/11 16:33:54



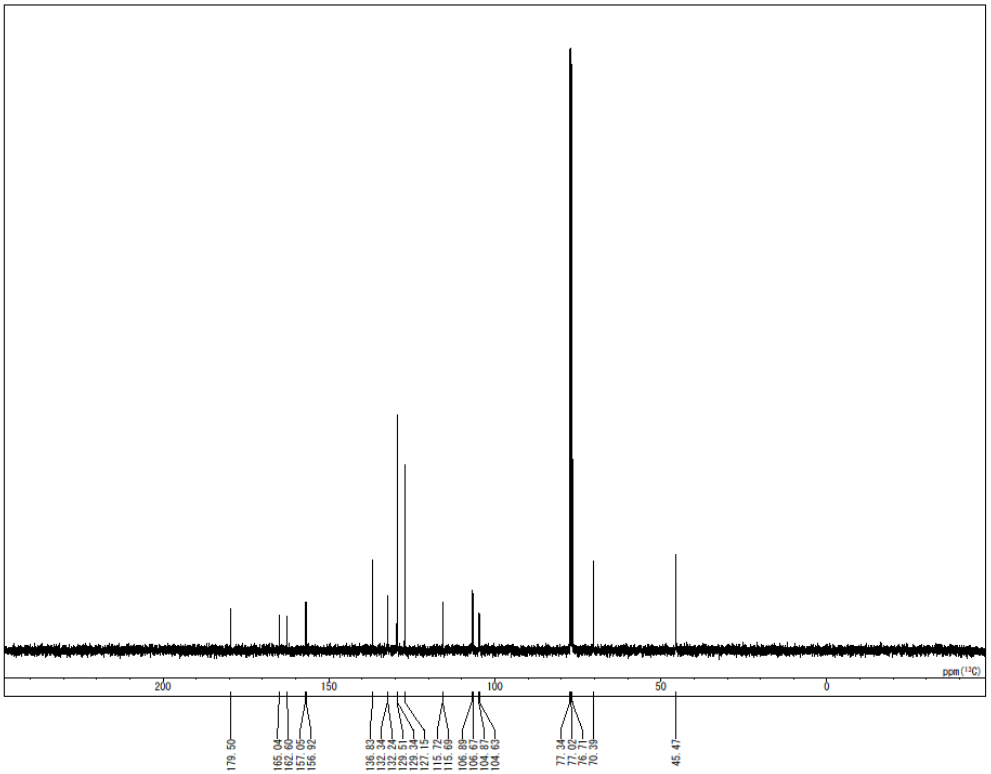
^{13}C NMR of **4f**



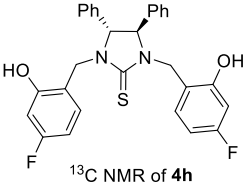
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	101
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	22.51 °C
PRNT_DATE	2022/Jun/02 23:52:54



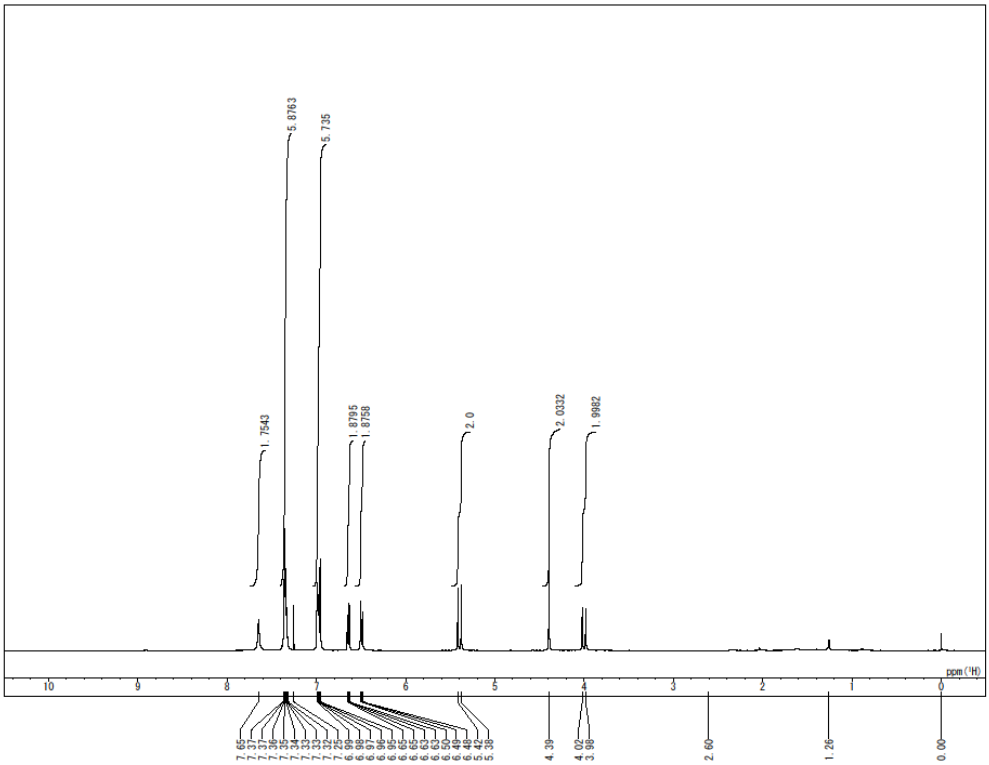
^{1}H NMR of **4h**

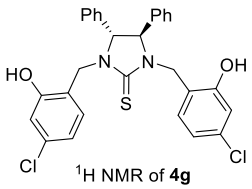


OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	23.01 °C
PRNT_DATE	2022/Jun/02 23:50:46

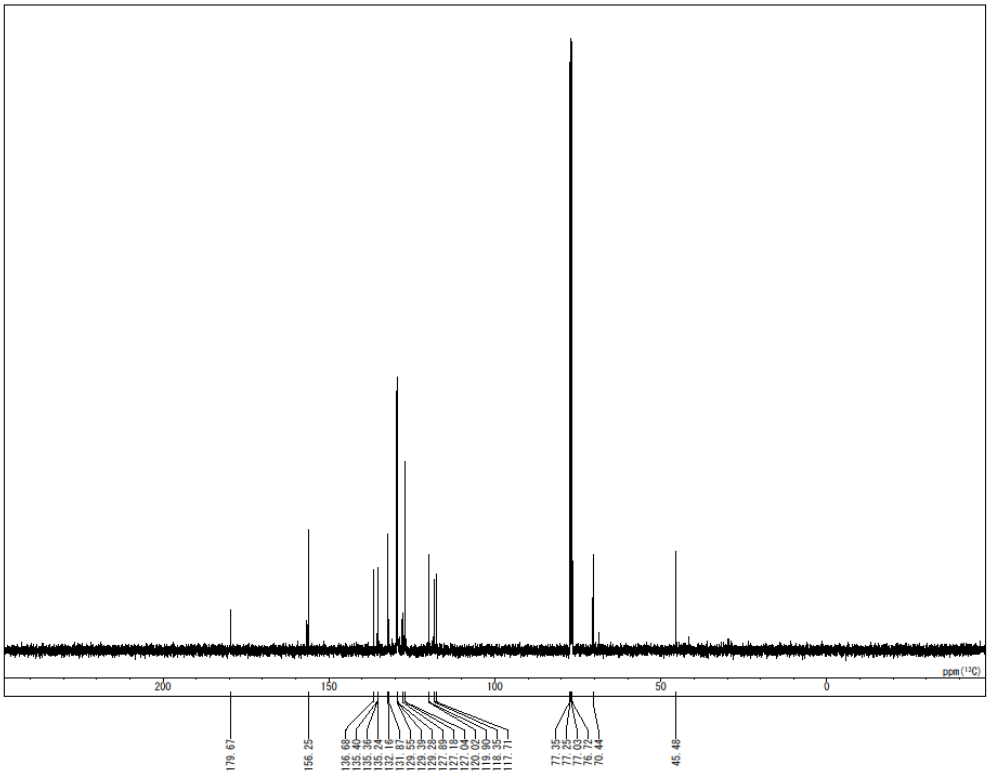


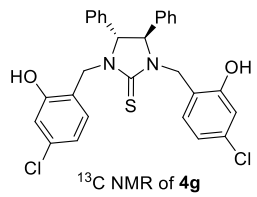
^{13}C NMR of **4h**



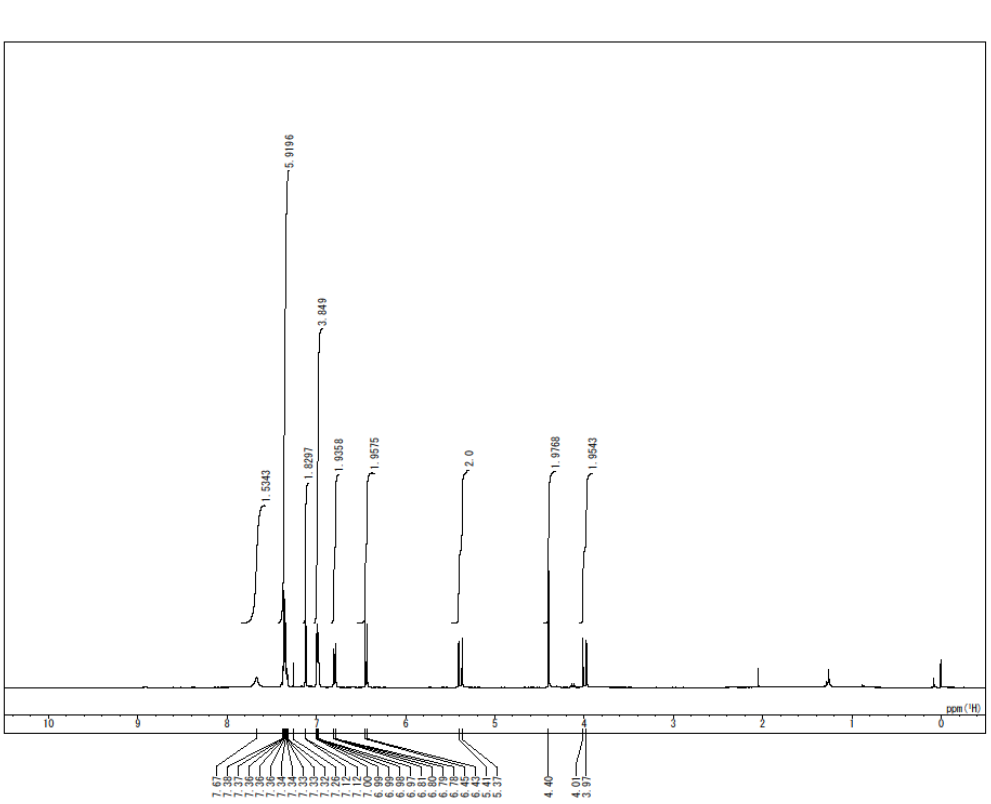


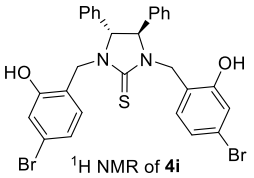
^{1}H NMR of **4g**



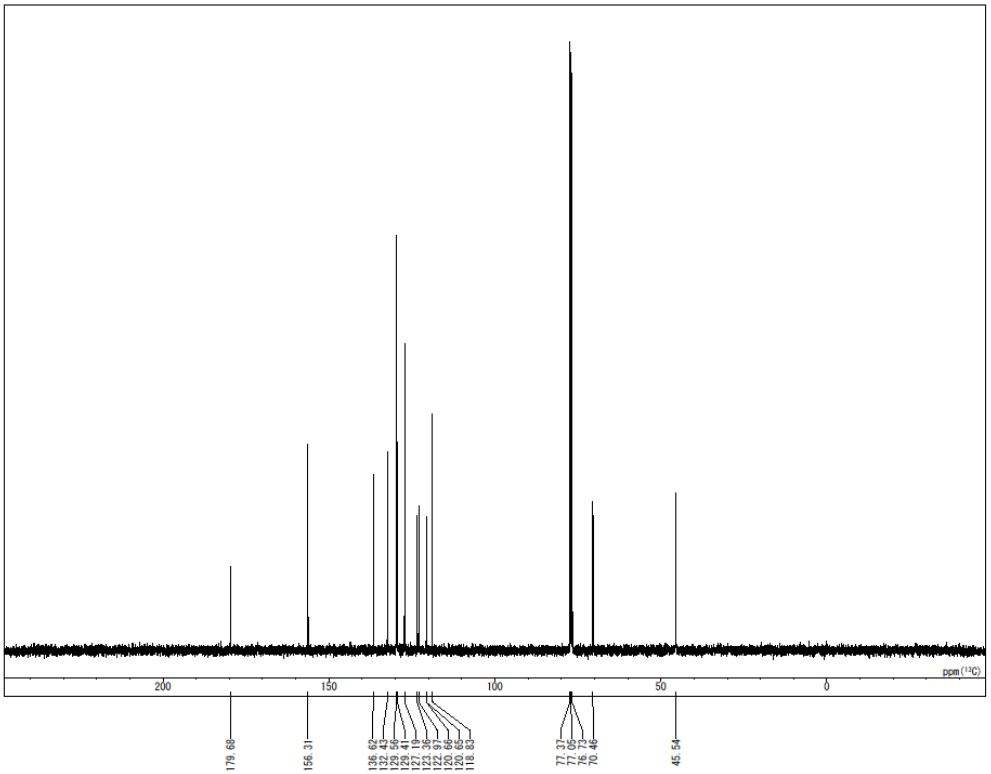


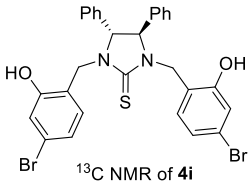
^{13}C NMR of **4g**



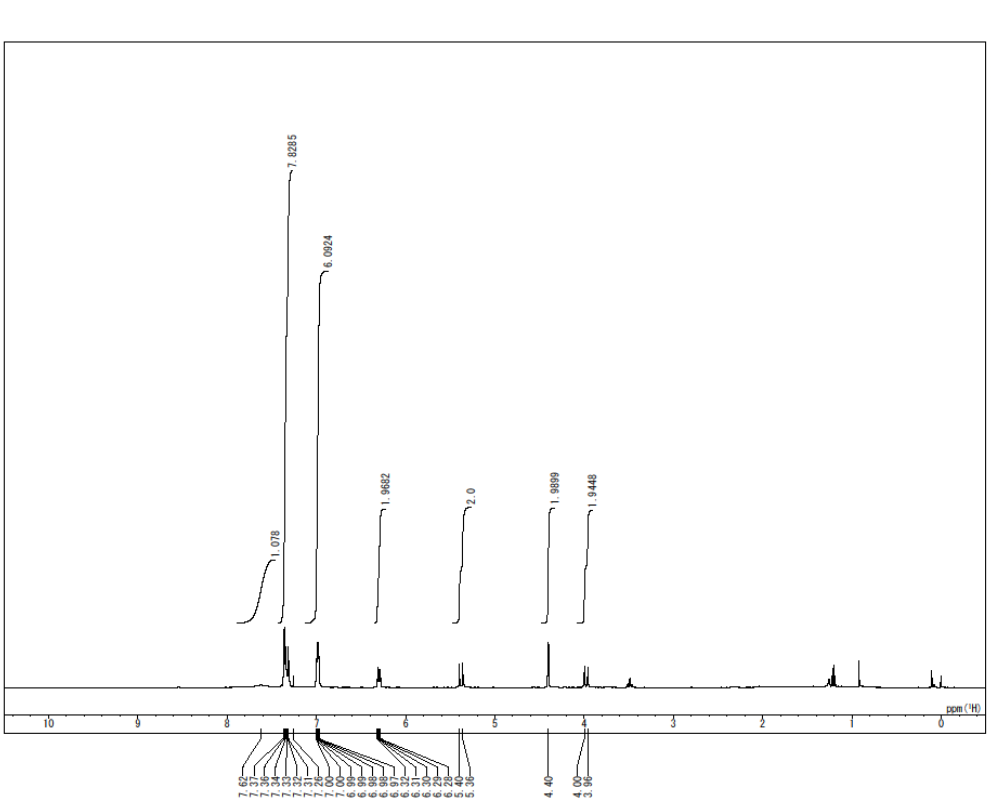


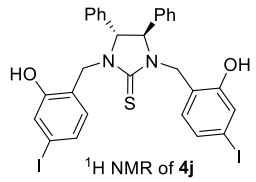
^{1}H NMR of **4i**



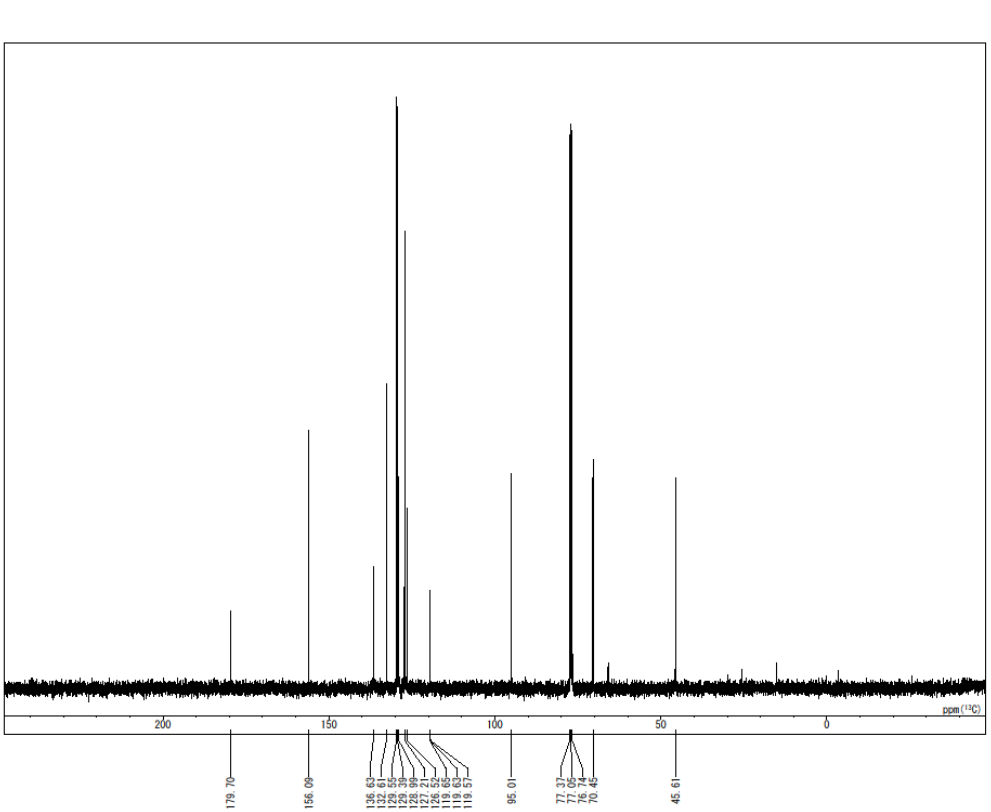


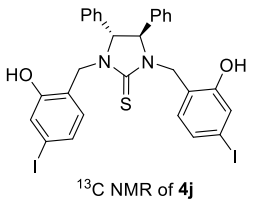
^{13}C NMR of **4i**



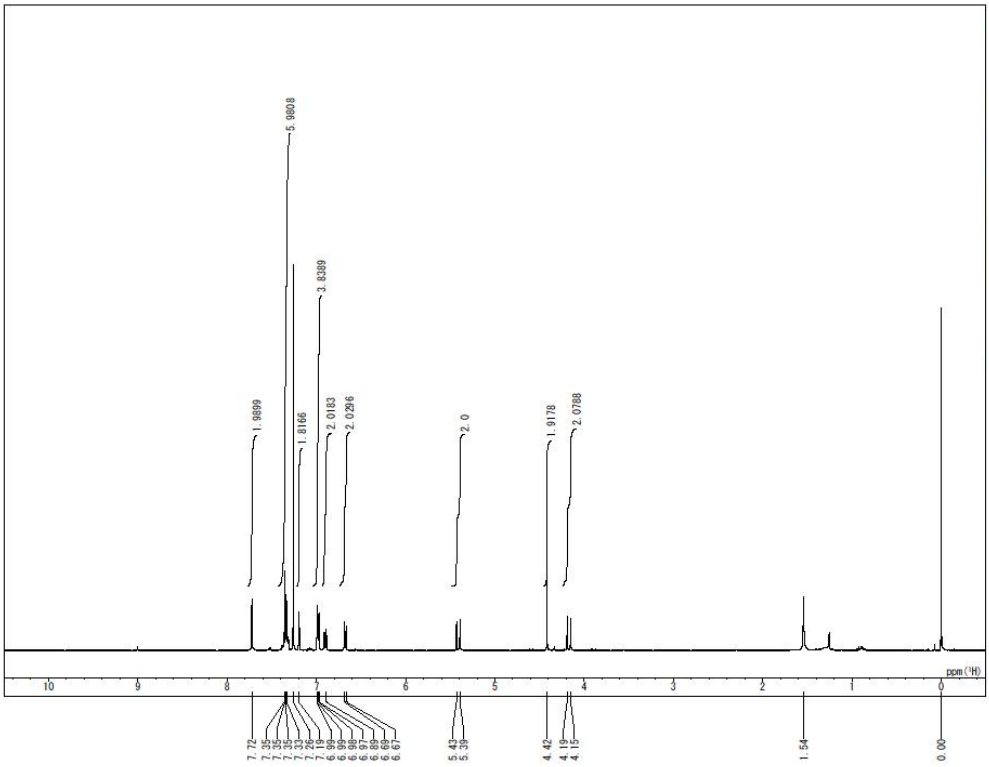


^{1}H NMR of **4j**



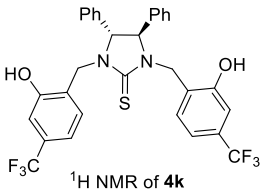


^{13}C NMR of **4j**

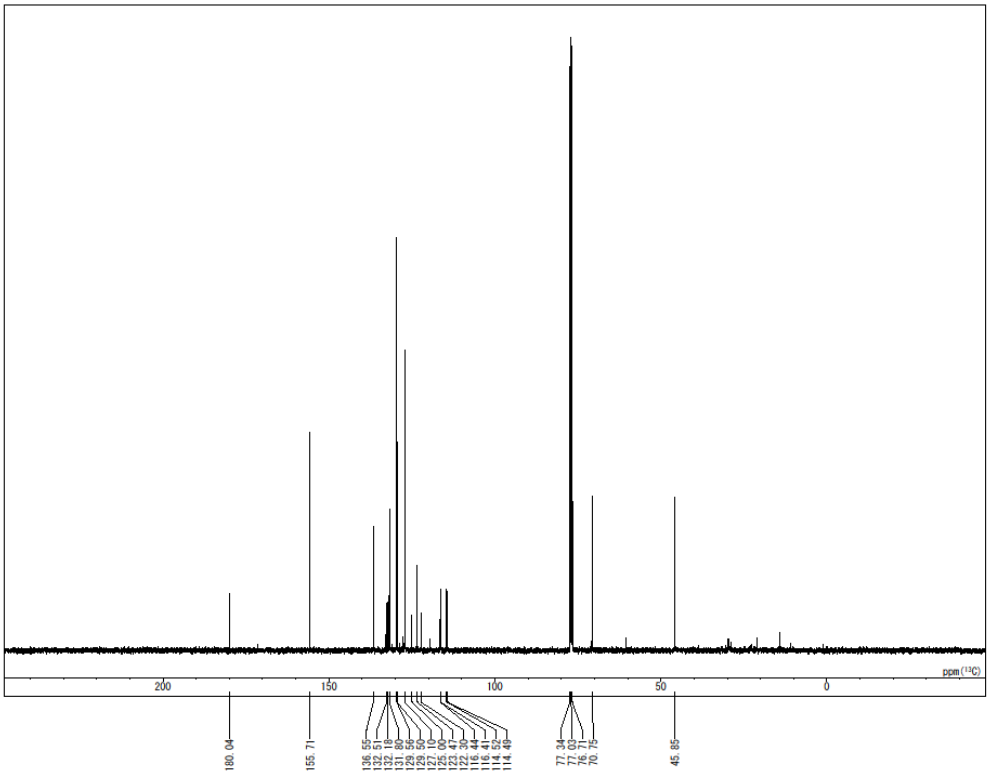


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 13/Jun/2022 15:54:42
COMNT

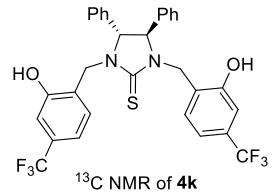
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.1223 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.11 °C
PRNT_DATE	2022/Jun/22 10:23:47



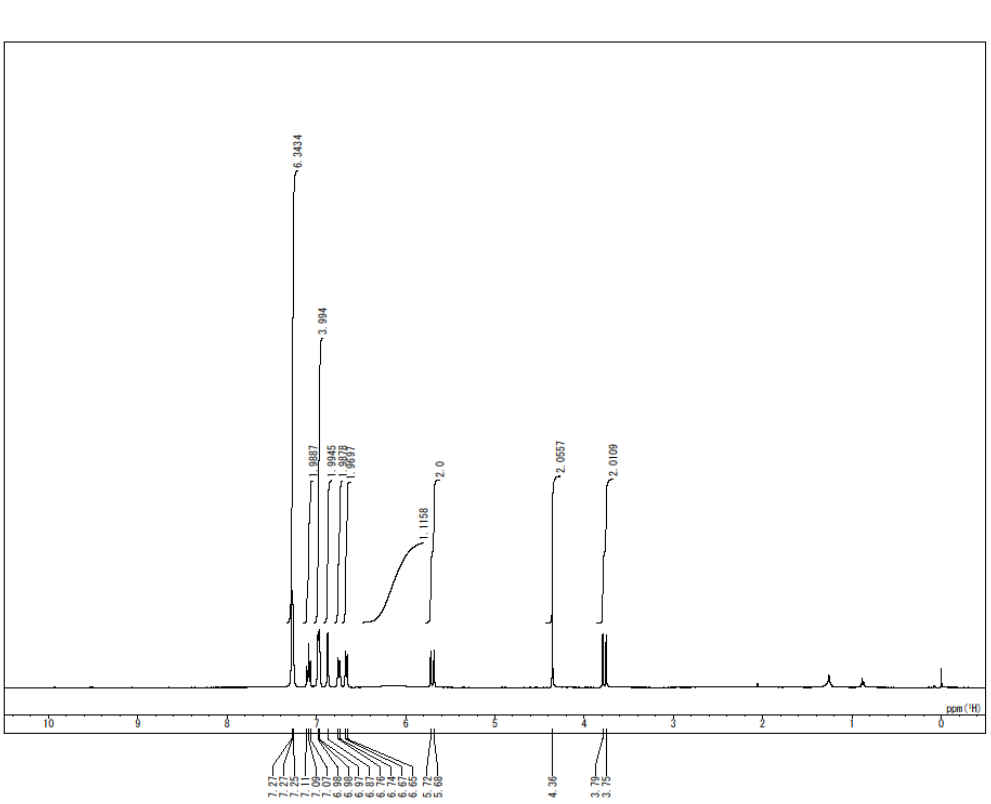
^{1}H NMR of **4k**



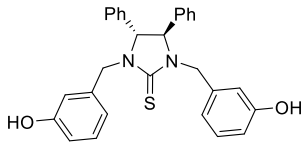
OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	1024
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	181
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	23.01 °C
PRNT_DATE	2022/Jun/03 00:12:07



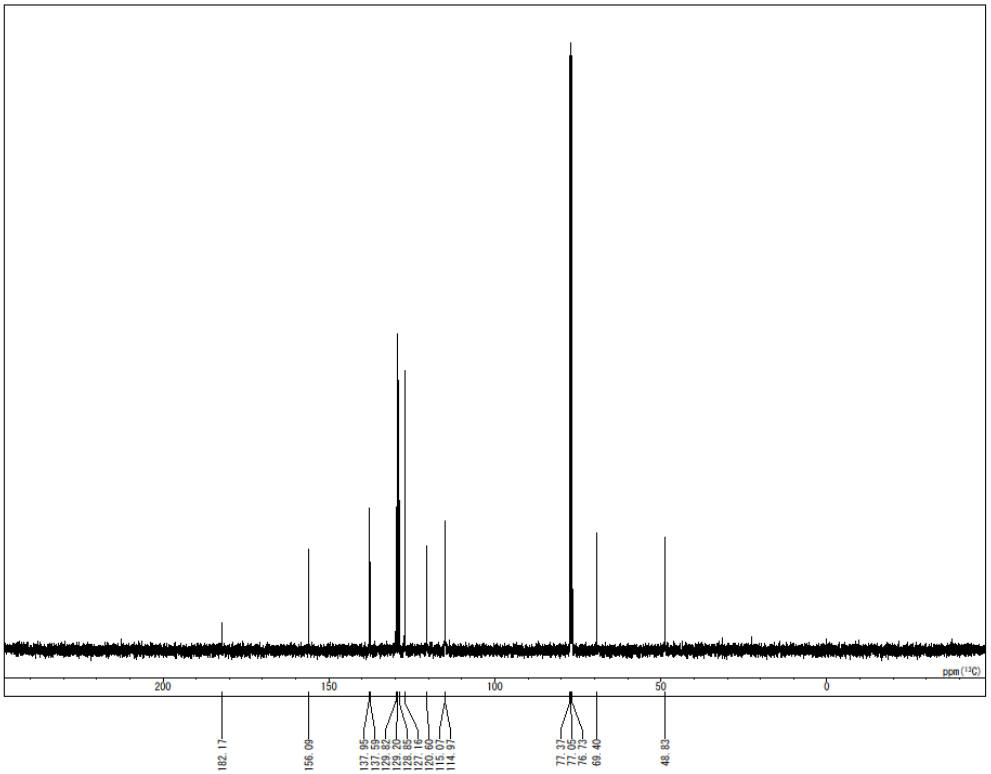
^{13}C NMR of **4k**



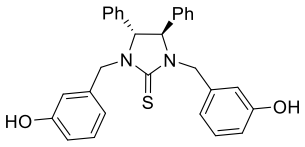
OBNUC ¹H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 81
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 22.41 °C
PRNT_DATE 2022/Jun/02 23:33:12



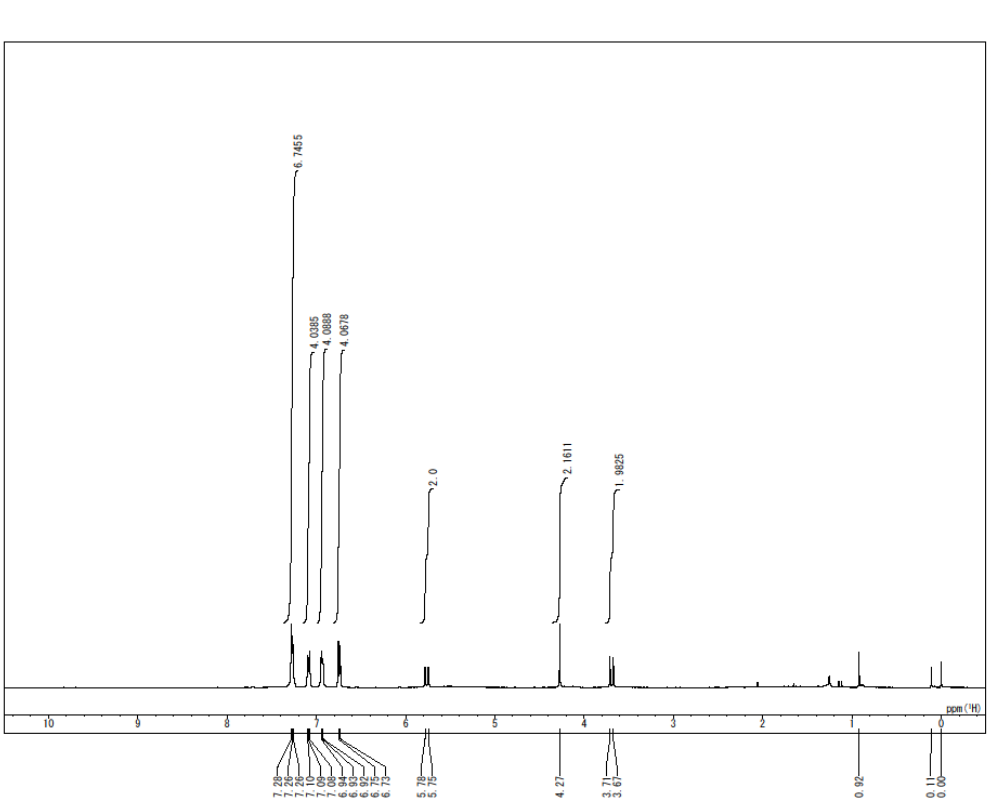
^{1}H NMR of **4b**



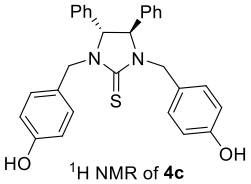
OBNUC ¹³C
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 9999.159 Hz
PW1 10.0 µs
PW2 10.0 µs
PW3 20.0 µs
PI1 2.0 ms
PI2 0.0035 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 256
DUMMY 2
FREQU 29761.9 Hz
ACQTM 1.101 s
PD 2.0 s
RGAIN 114
BF 0.25 Hz
EXMOD ZGPG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 23.01 °C
PRNT_DATE 2022/Jun/02 23:31:28



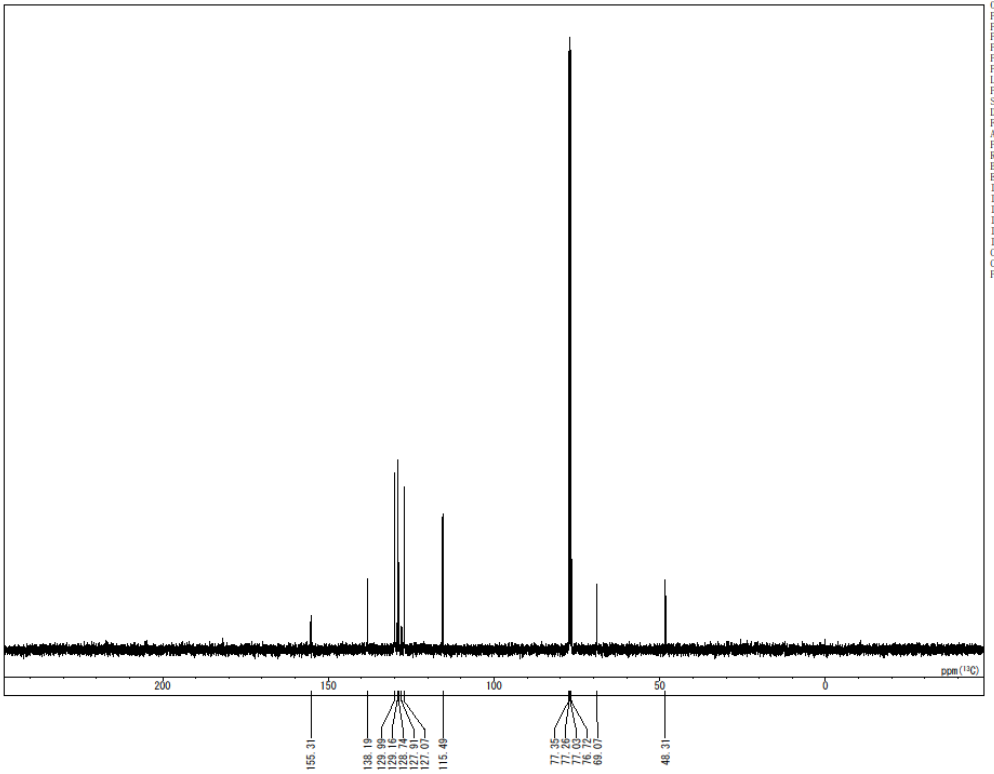
^{13}C NMR of **4b**



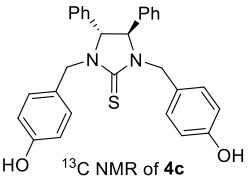
OBNUC ¹H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 90
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 22.61 °C
PRNT_DATE 2022/Jun/02 23:41:07



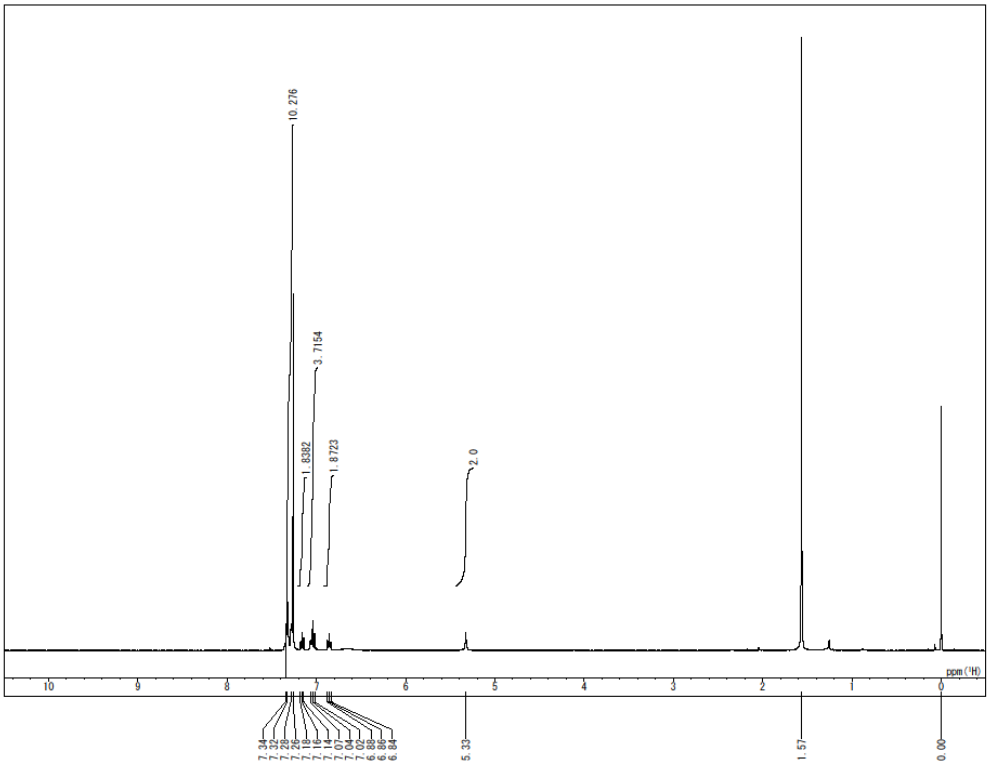
^{1}H NMR of **4c**



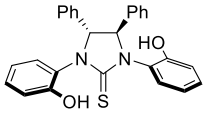
OBNUC ¹³C
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 9999.159 Hz
PW1 10.0 µs
PW2 10.0 µs
PW3 20.0 µs
PI1 2.0 ms
PI2 0.0035 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 256
DUMMY 2
FREQU 29761.9 Hz
ACQTM 1.101 s
PD 2.0 s
RGAIN 114
BF 0.25 Hz
EXMOD ZGPG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 22.81 °C
PRNT_DATE 2022/Jun/02 23:37:49



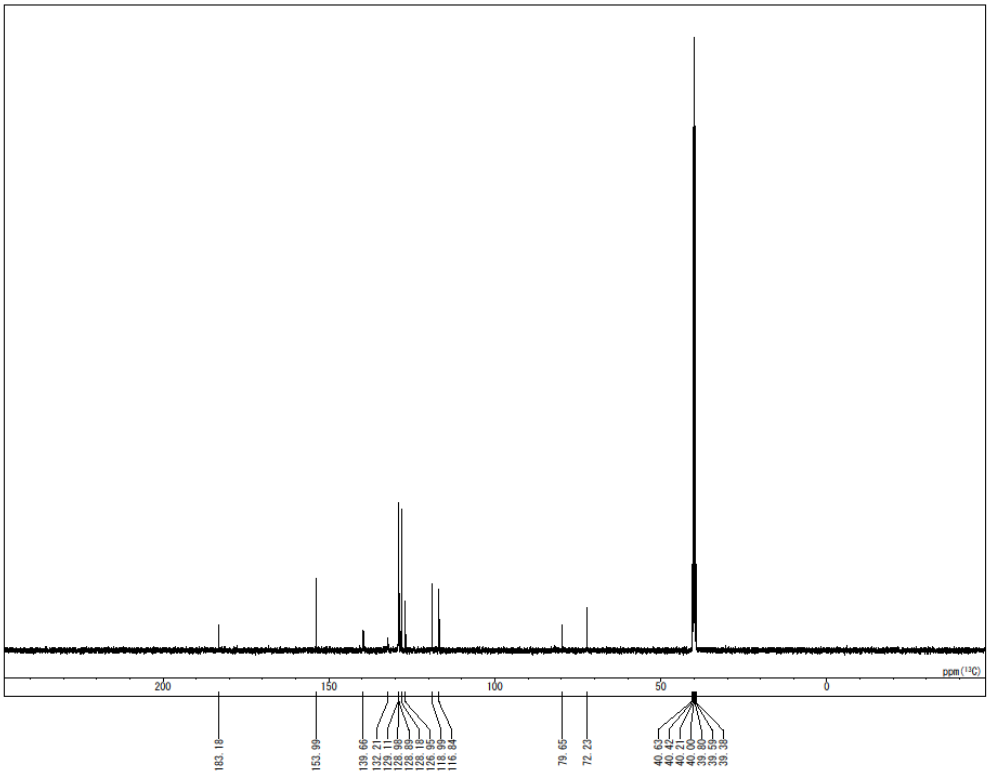
^{13}C NMR of **4c**



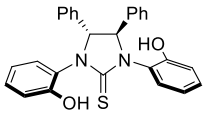

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM    22/Jun/2022 21:50:56
COMNT

OBNUC                  ¹H
OFR                400.03 MHz
OBSET                0.0 kHz
OBFIN            10009.25 Hz
PW1                2.6667 µs
PW2                8.0 µs
PW3                16.0 µs
PI1                1.0 ms
PI2                0.0 ms
PI3                0.0 ms
LOOP1                  0
POINT              65536
SCANS                  8
DUMMY                  2
FREQU            7812.5 Hz
ACQTM              8.3886 s
PD                 1.0 s
RGAIN                101
BF                 0.0596 Hz
EXMOD              ZG30
IRNUC              OFF
IFR                0.0 MHz
IRSET              0.0 kHz
IRFIN              0.0 Hz
IRRPW              0 µs
IRATN                  0
CSPED              0.0 Hz
CTEMP              24.9965 °C
PRNT_DATE    2022/Jun/22 22:05:53
```



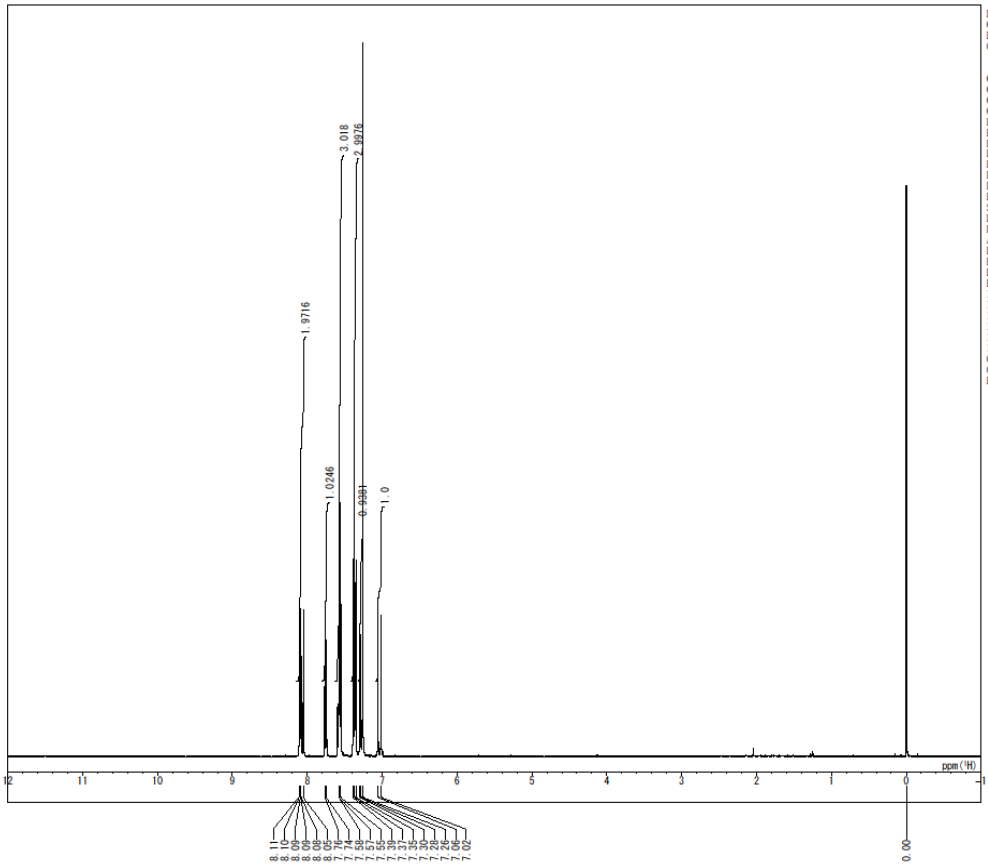
^{1}H NMR of **4d**




```
DFILE   X:¥062ORG¥DATA¥ORG¥NMR¥MS8196C-NMR-D-D
ORGFILE   X:¥062ORG¥DATA¥ORG¥NMR¥MS8196C-NMR-D
DATIM    22/Jun/2022 09:57:47
COMNT

OBNUC                  ¹³C
OFR                100.61 MHz
OBSET                0.0 kHz
OBFIN            9999.159 Hz
PW1                10.0 µs
PW2                10.0 µs
PW3                20.0 µs
PI1                2.0 ms
PI2                0.0035 ms
PI3                0.0 ms
LOOP1                  0
POINT              32768
SCANS                256
DUMMY                  2
FREQU            29761.9 Hz
ACQTM              1.101 s
PD                 2.0 s
RGAIN                203
BF                 0.25 Hz
EXMOD              ZGPG30
IRNUC              OFF
IFR                0.0 MHz
IRSET              0.0 kHz
IRFIN              0.0 Hz
IRRPW              0 µs
IRATN                  0
CSPED              20.0 Hz
CTEMP              26.81 °C
PRNT_DATE    2022/Jun/22 10:17:44
```

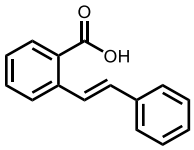


^{13}C NMR of **4d**

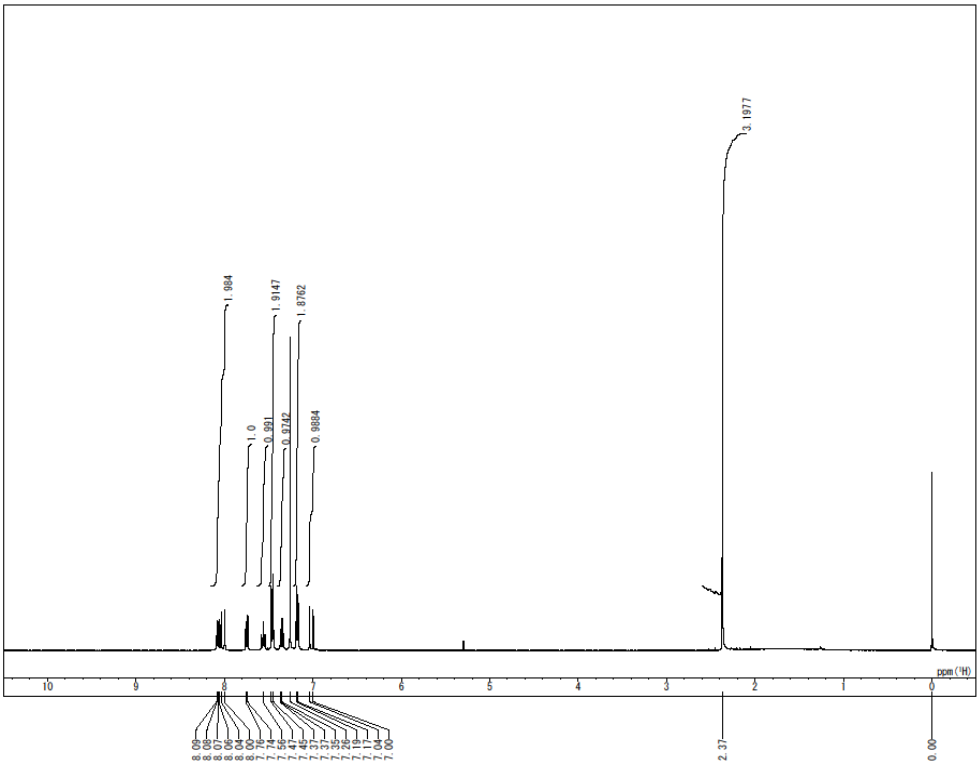


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 16/Aug/2021 15:38:57
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.91 ℃
PRNT_DATE	2022/Feb/22 21:38:55

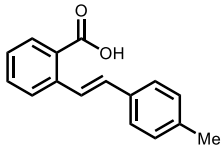


^{1}H NMR of **1a**

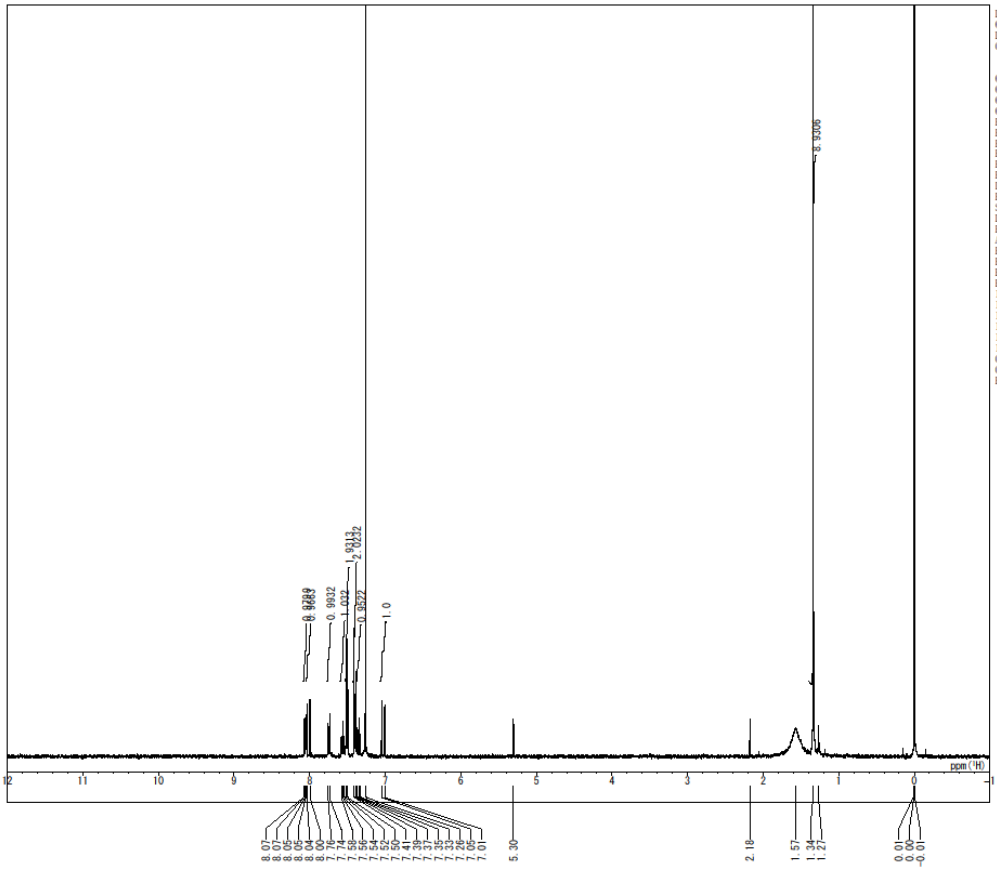


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 09/Jun/2022 20:56:30
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.31 ℃
PRNT_DATE	2022/Jun/09 21:16:47

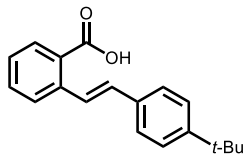


^{1}H NMR of **1b**

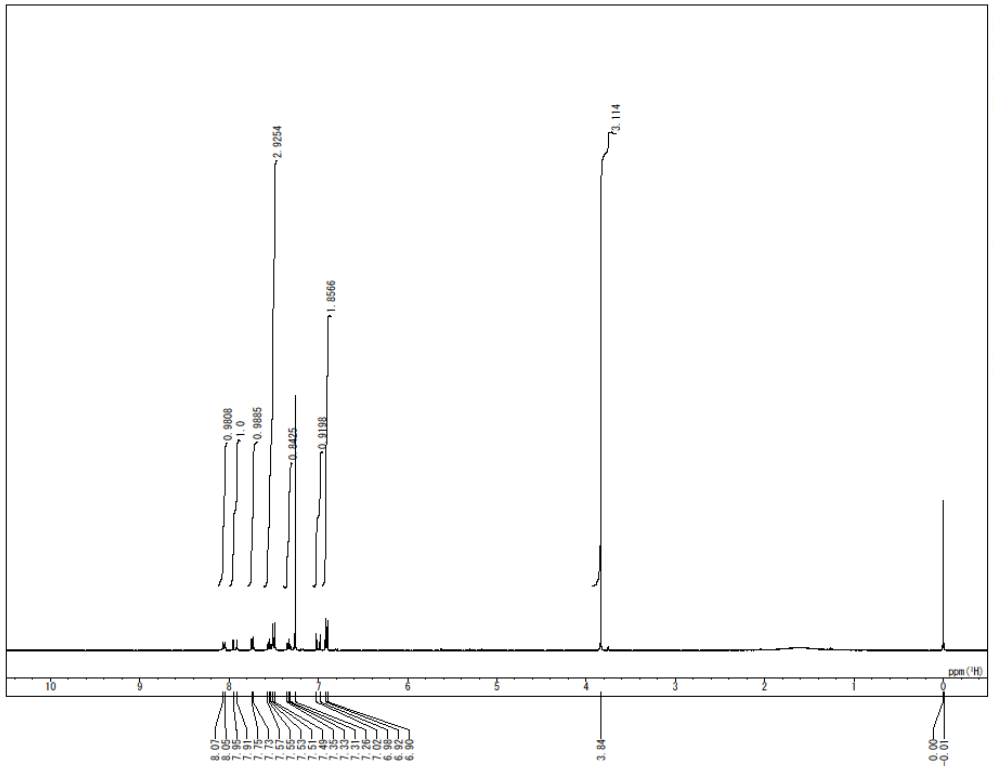


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 02/Feb/2022 09:26:43
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	21.01 °C
PRNT_DATE	2022/Feb/23 00:04:15

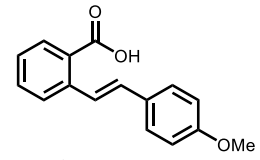


^{1}H NMR of **1c**

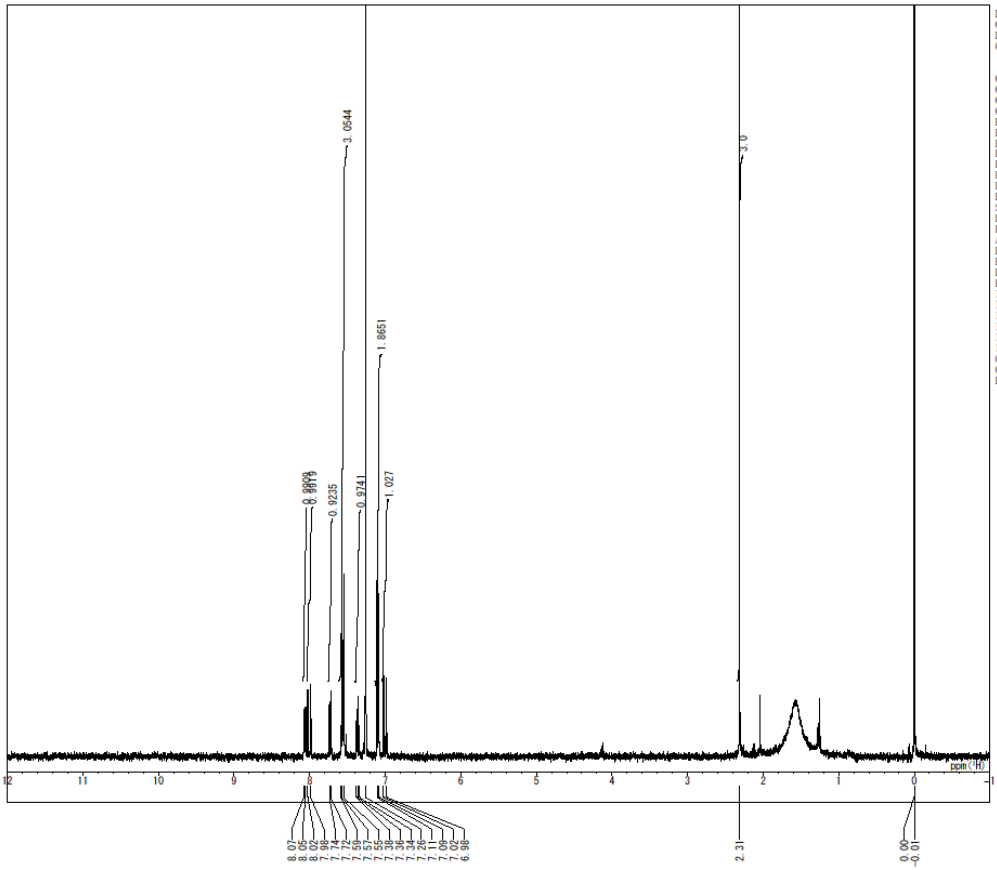


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 09/Jun/2022 21:01:14
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.41 °C
PRNT_DATE	2022/Jun/09 21:14:07

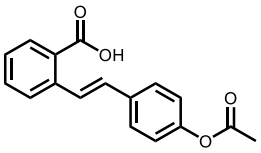


^{1}H NMR of **1d**

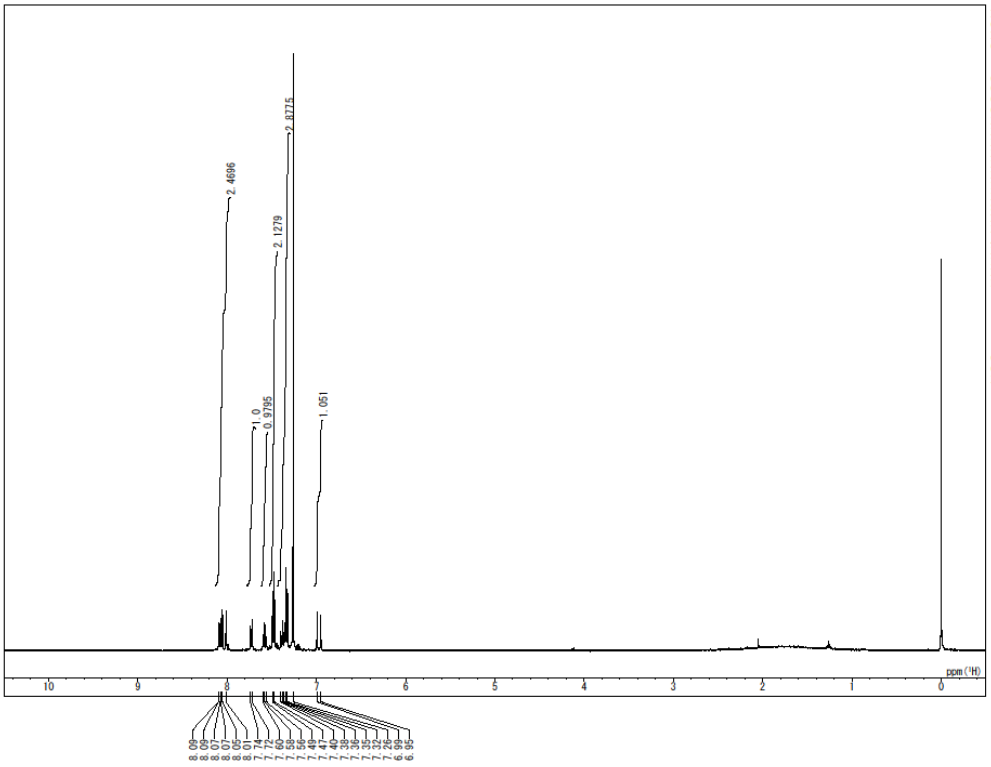


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 19/Aug/2021 15:18:05
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.91 °C
PRNT_DATE	2022/Feb/22 22:31:14

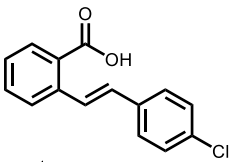


^{1}H NMR of **1e**

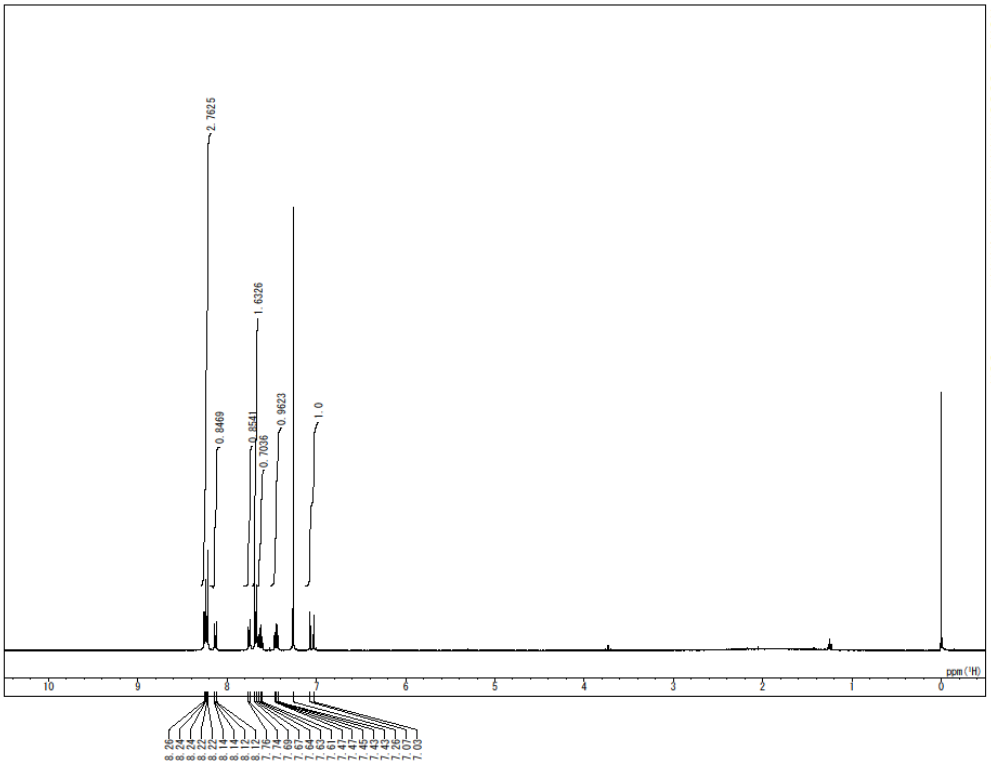


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 09/Jun/2022 21:05:54
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.41 °C
PRNT_DATE	2022/Jun/09 21:20:15

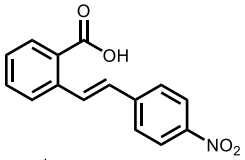


^{1}H NMR of **1f**

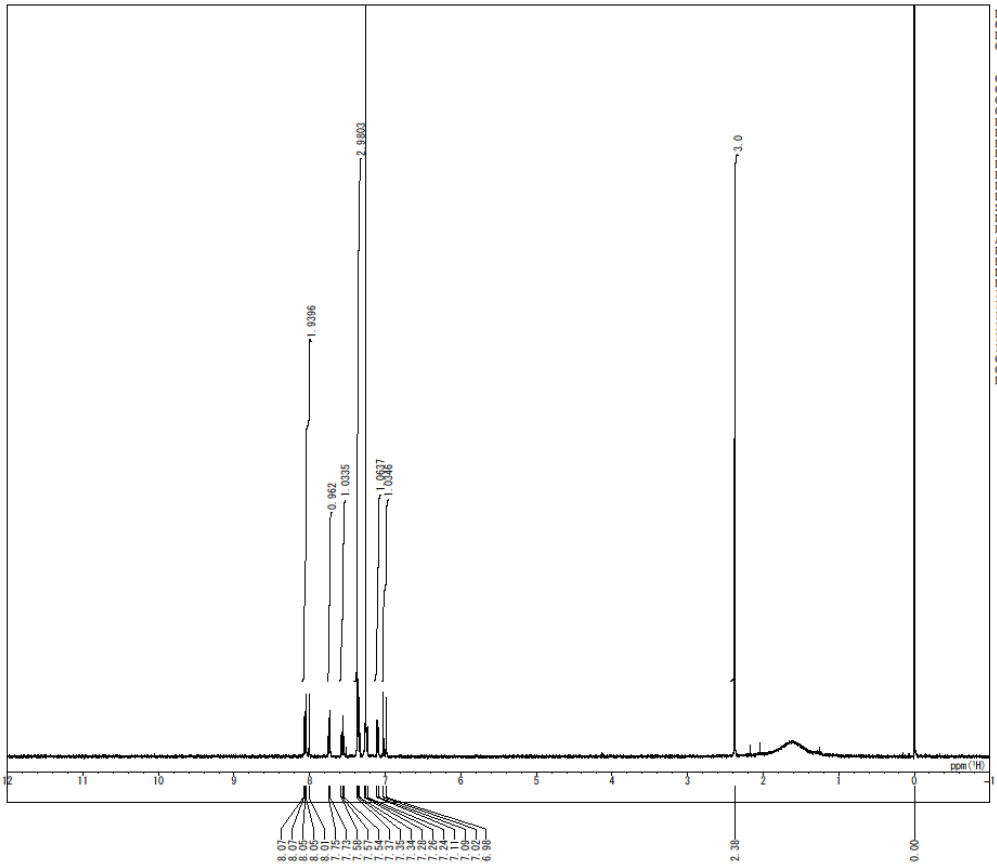


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 09/Jun/2022 23:25:06
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.31 ℃
PRNT_DATE	2022/Jun/09 23:40:25

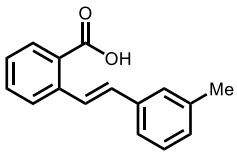


^{1}H NMR of **1g**

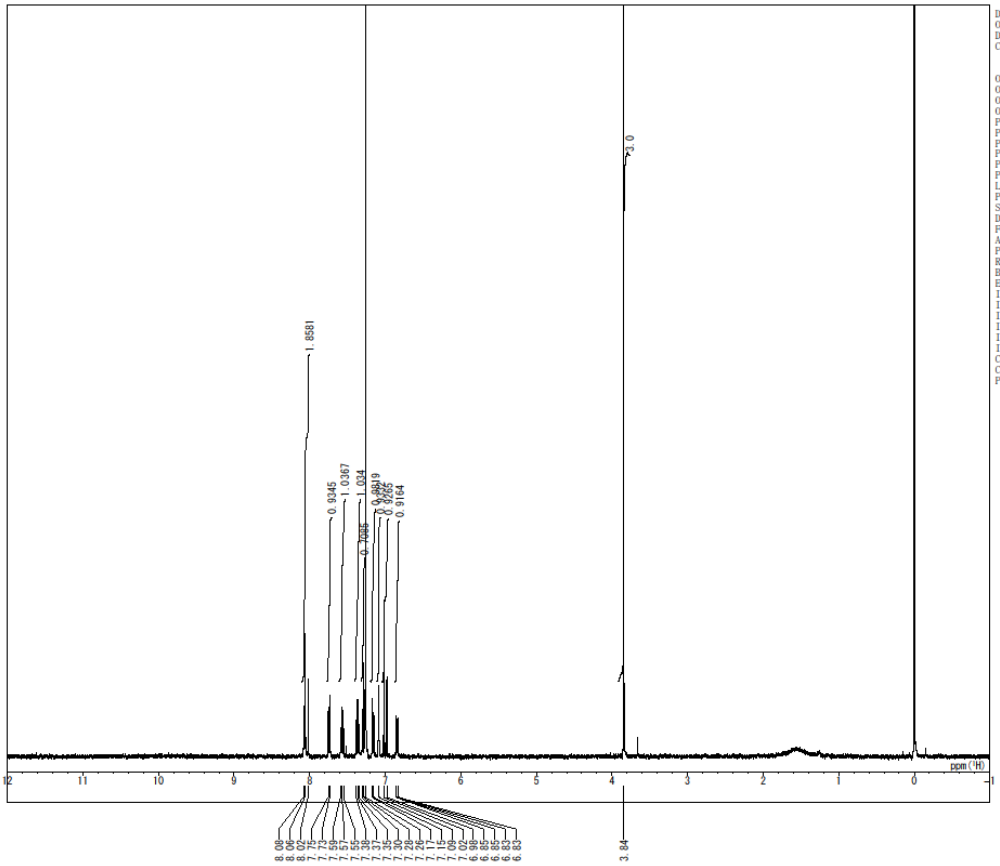


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 24/Jul/2021 16:18:21
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	26.21 ℃
PRNT_DATE	2022/Feb/23 00:27:06

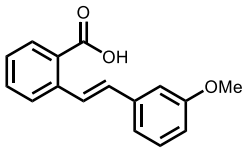


^{1}H NMR of **1h**

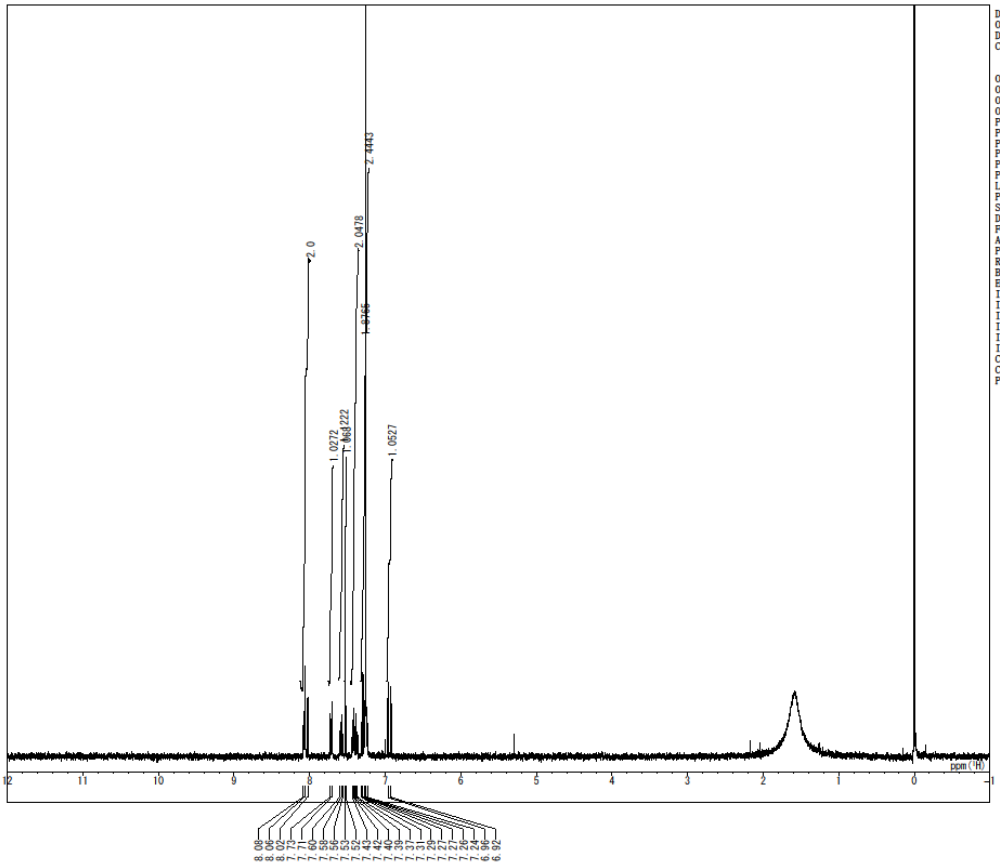


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 02/Aug/2021 17:13:49
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	27.21 °C
PRNT_DATE	2022/Feb/23 00:23:40

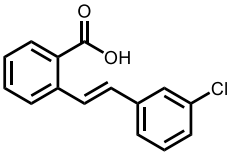


^{1}H NMR of **1i**

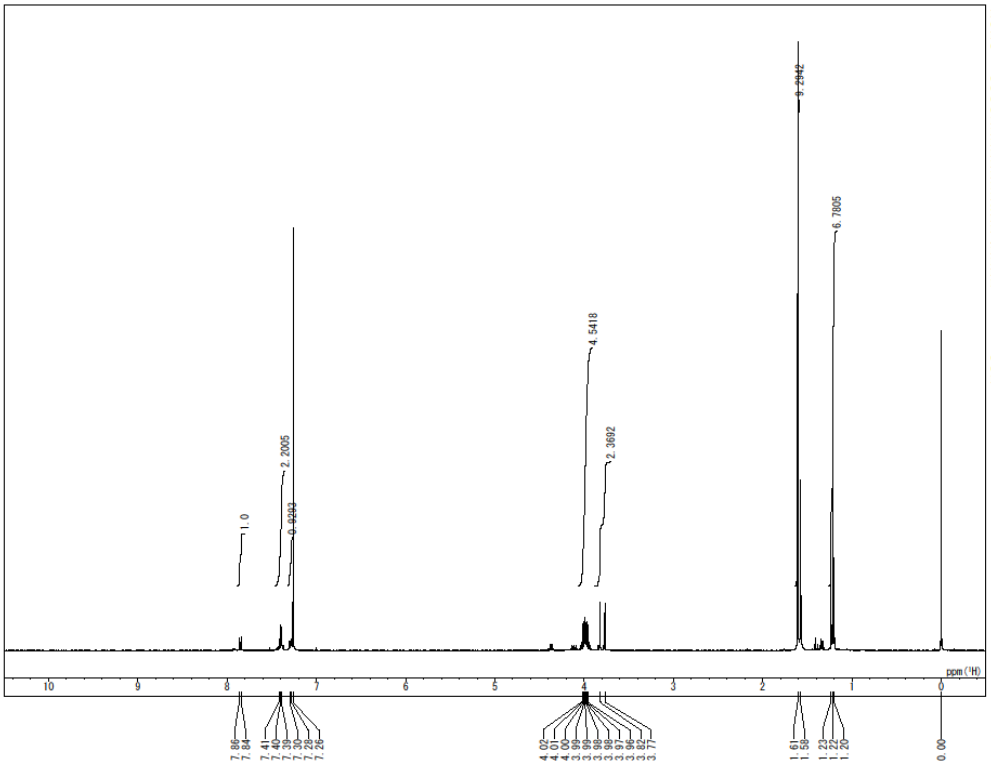


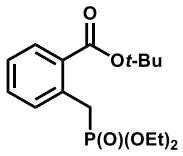
DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 13/Jul/2021 11:33:21
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.91 °C
PRNT_DATE	2022/Feb/22 22:12:30

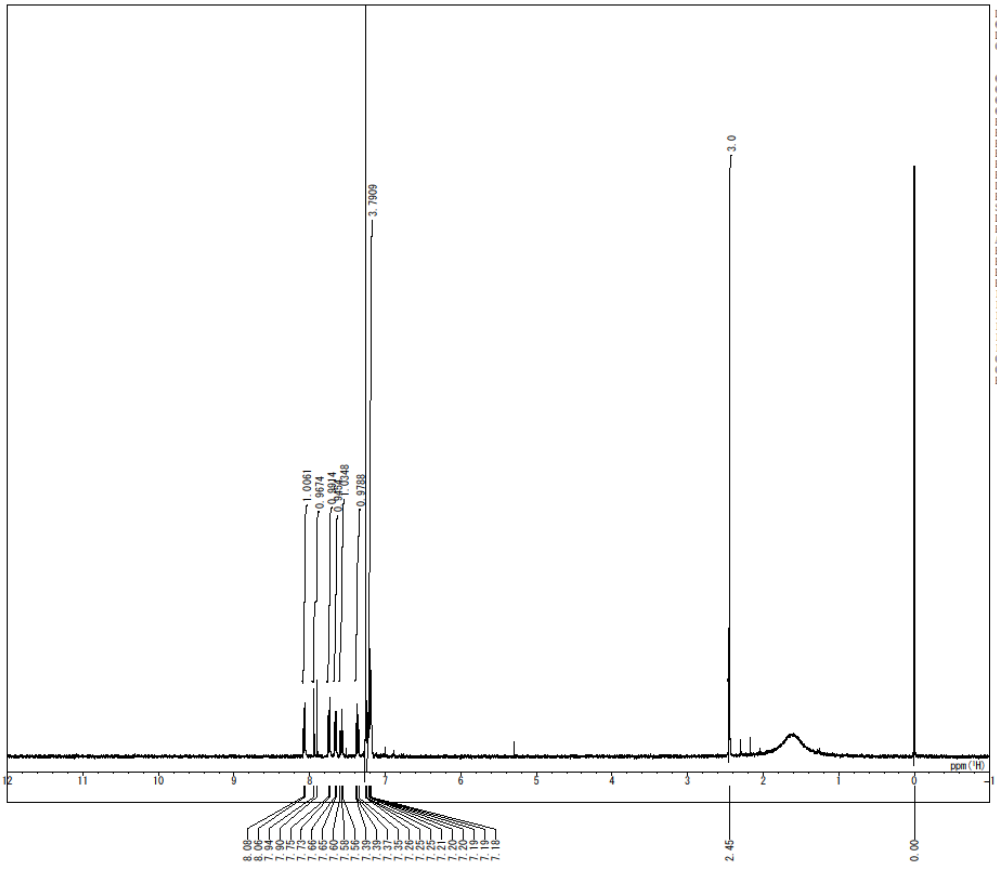


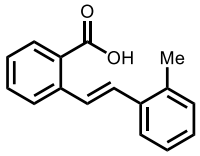
^{1}H NMR of **1j**



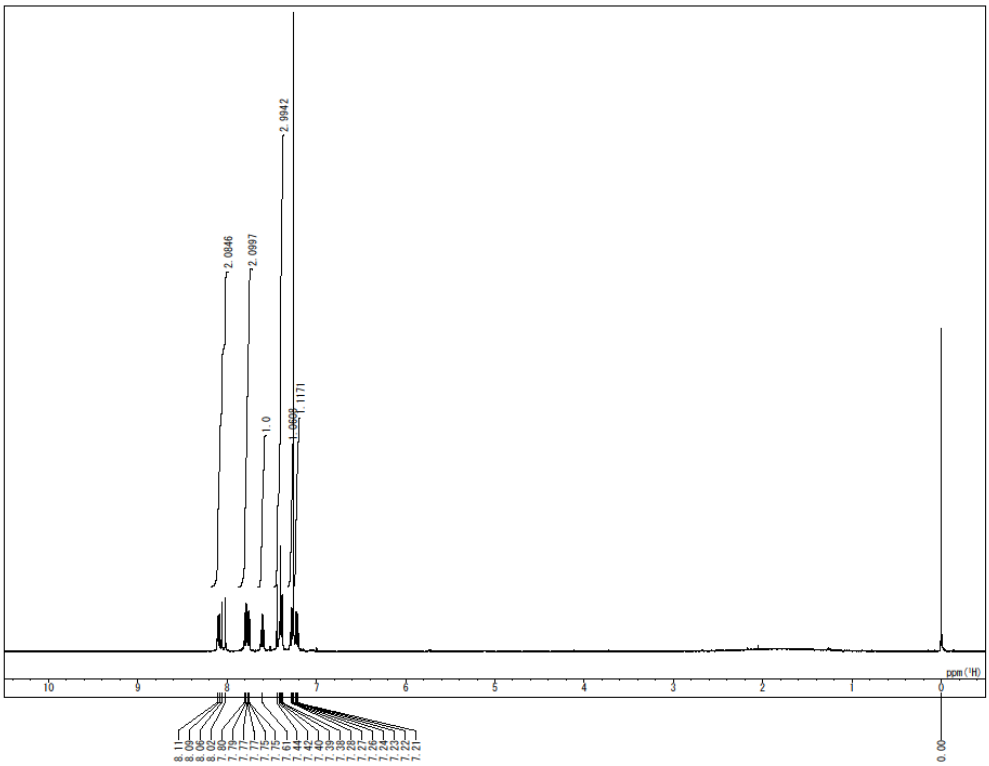


^{1}H NMR of **S4**

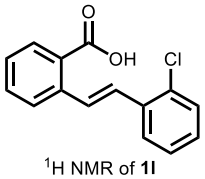




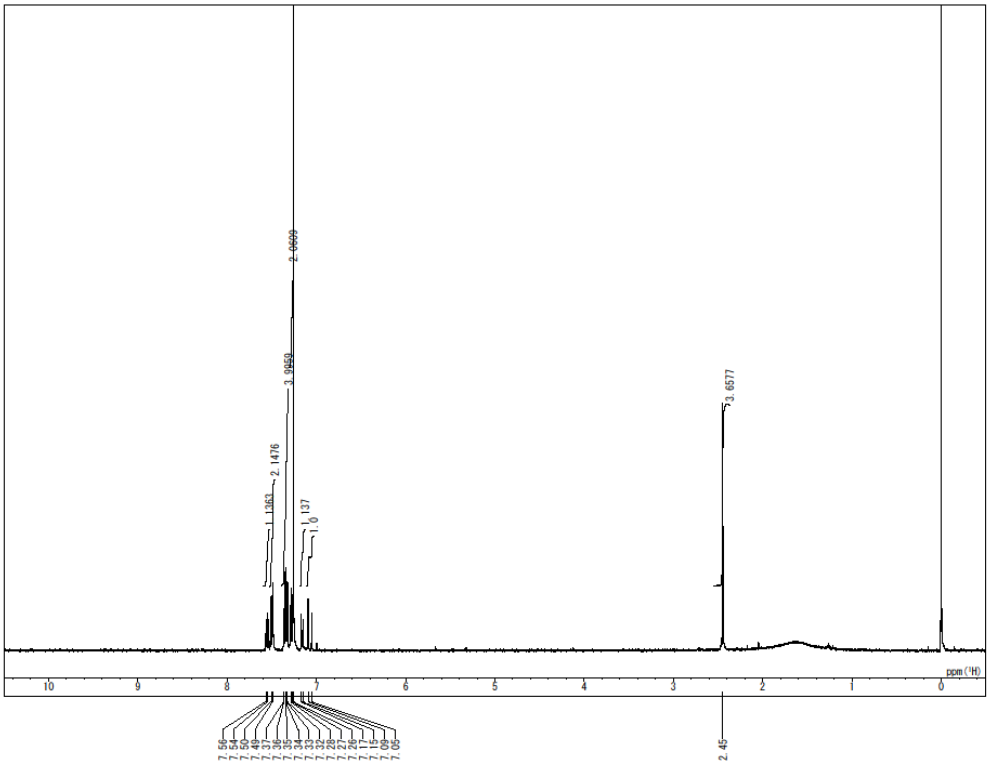
^{1}H NMR of **1k**



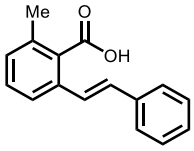

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM    09/Jun/2022 23:21:29
COMNT

OBNUC                  ¹H
OFR                400.13 MHz
OBSET                0.0 kHz
OBFIN            10021.89 Hz
PW1                 15.0 µs
PW2                 15.0 µs
PW3                 30.0 µs
PI1                  1.0 ms
PI2                  0.0 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS                  4
DUMMY                  2
FREQU             8012.82 Hz
ACQTM               4.0894 s
PD                   1.0 s
RGAIN                161
BF                  0.25 Hz
EXMOD               ZG30
IRNUC               OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRBFW                0 µs
IRATN                  0
CSPED               20.0 Hz
CTEMP               25.31 ℃
PRNT_DATE    2022/Jun/09 23:50:00
```



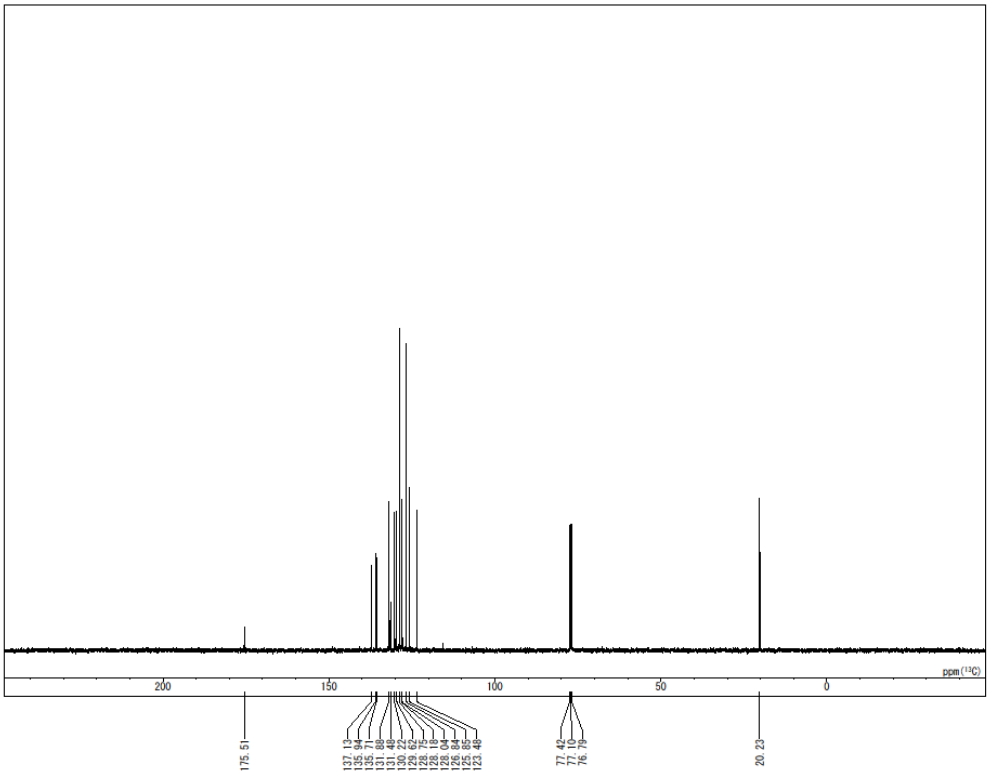
^{1}H NMR of **1l**



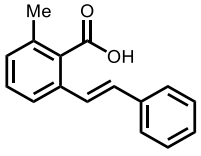

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM    15/Jun/2022 14:26:37
COMNT

OBNUC                  ¹H
OFR                400.13 MHz
OBSET                0.0 kHz
OBFIN            10021.89 Hz
PW1                 15.0 µs
PW2                 15.0 µs
PW3                 30.0 µs
PI1                  1.0 ms
PI2                  0.0 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS                  4
DUMMY                  2
FREQU            8012.82 Hz
ACQTM              4.0894 s
PD                   1.0 s
RGAIN                181
BF                  0.25 Hz
EXMOD              ZG30
IRNUC               OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRRPW                0 µs
IRATN                  0
CSPED               20.0 Hz
CTEMP               26.01 ℃
PRNT_DATE    2022/Jun/15 15:33:35
```



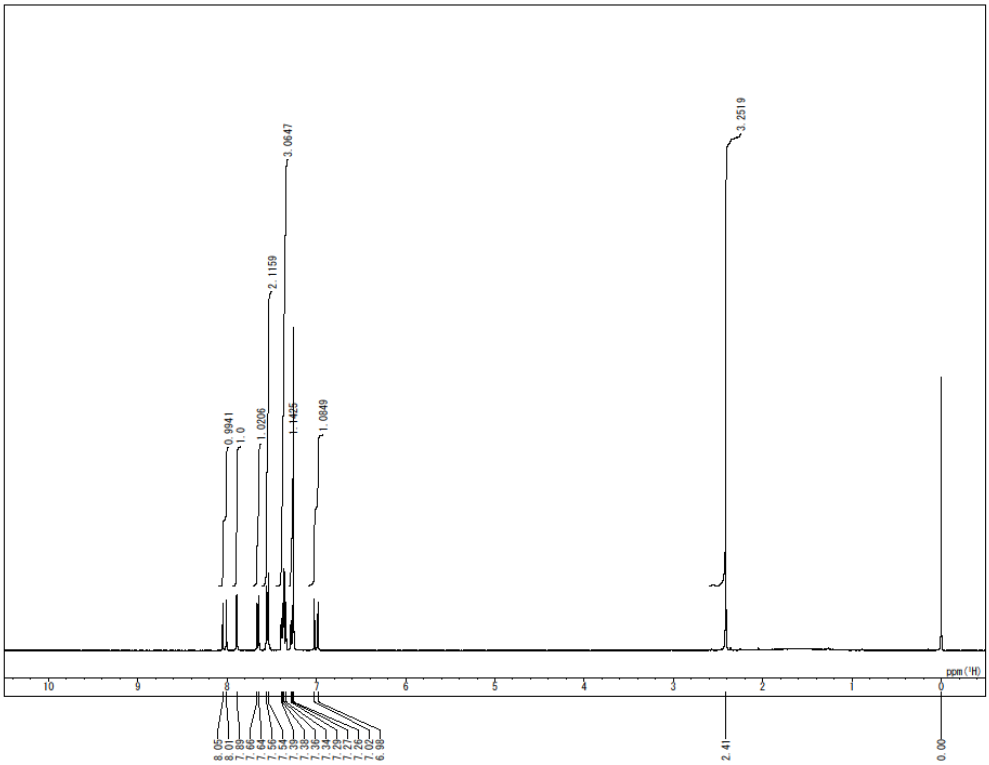
^{1}H NMR of **1m**

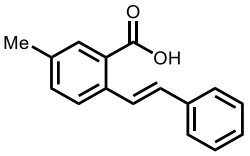



```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM    15/Jun/2022 16:25:32
COMNT

OBNUC                  ¹³C
OFR                100.61 MHz
OBSET                0.0 kHz
OBFIN            9999.159 Hz
PW1                 10.0 µs
PW2                 10.0 µs
PW3                 20.0 µs
PI1                  2.0 ms
PI2                0.0035 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS                256
DUMMY                  2
FREQU            29761.9 Hz
ACQTM              1.101 s
PD                   2.0 s
RGAIN                203
BF                  0.25 Hz
EXMOD            ZGPG30
IRNUC               OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRRPW                0 µs
IRATN                  0
CSPED               20.0 Hz
CTEMP               26.51 ℃
PRNT_DATE    2022/Jun/15 17:03:30
```

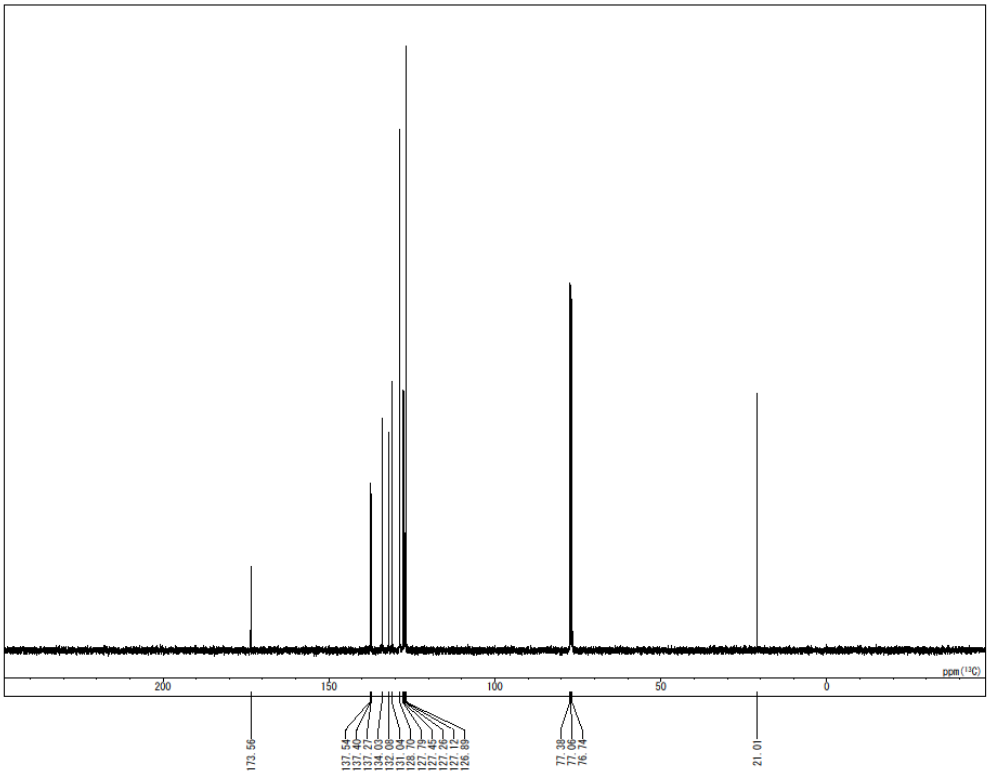


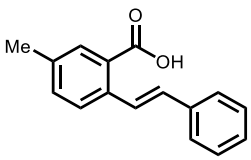
^{13}C NMR of **1m**



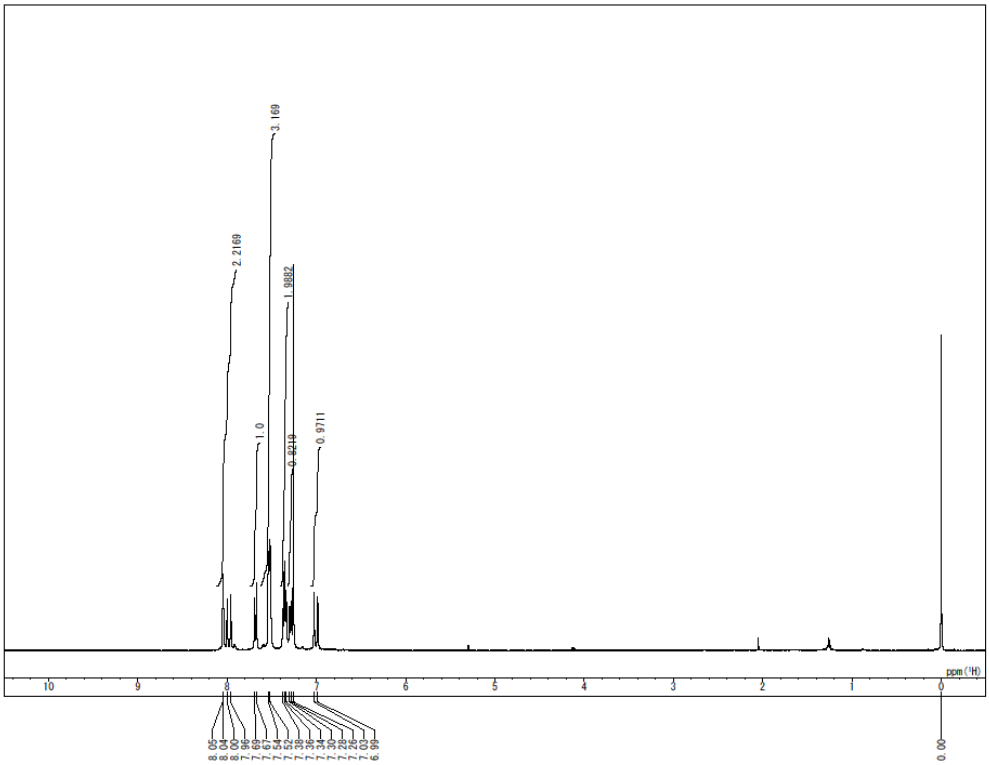


^{1}H NMR of **1n**

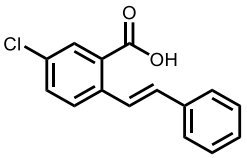




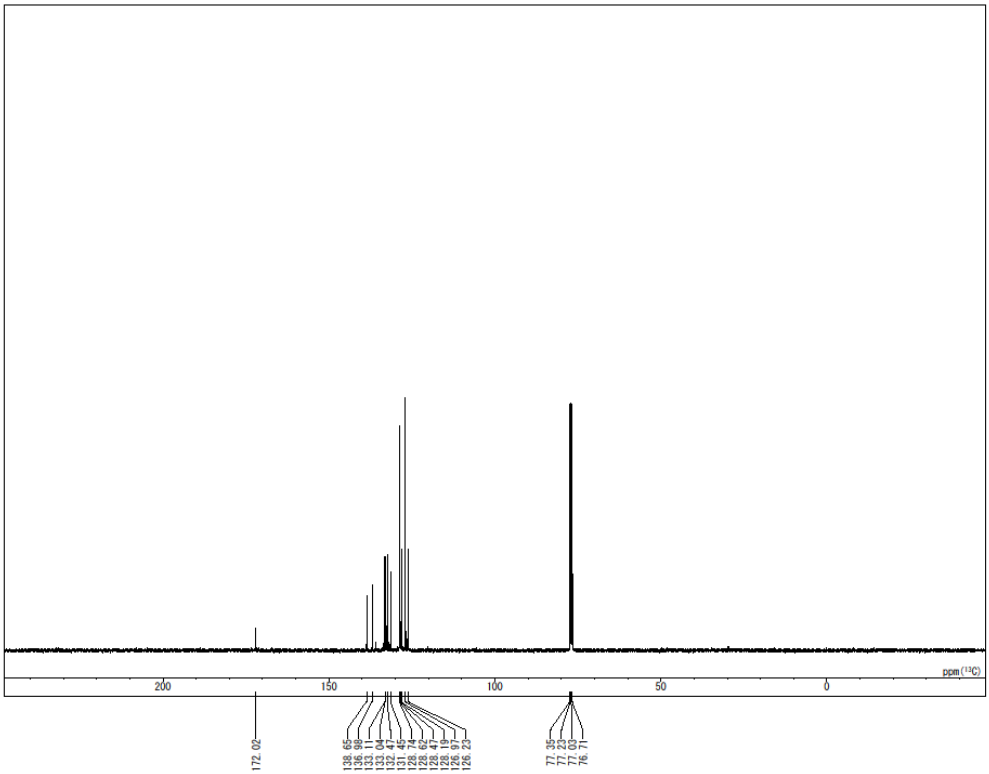
^{13}C NMR of **1n**



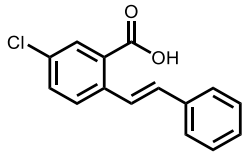

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM    14/Jun/2022 22:48:06
COMNT

OBNUC                  ¹H
OFR                400.03 MHz
OBSET                0.0 kHz
OBFIN            10009.24 Hz
PW1                2.6667 µs
PW2                  8.0 µs
PW3                 16.0 µs
PI1                  1.0 ms
PI2                  0.0 ms
PI3                  0.0 ms
LOOP1                  0
POINT              65536
SCANS                  4
DUMMY                  2
FREQU           7812.5 Hz
ACQTM              8.3886 s
PD                   1.0 s
RGAIN                101
BF                  0.25 Hz
EXMOD              ZG30
IRNUC              OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRRPW                0 µs
IRATN                0
CSPED                0.0 Hz
CTEMP             25.0126 ℃
PRNT_DATE    2022/Jun/15 10:58:58
```



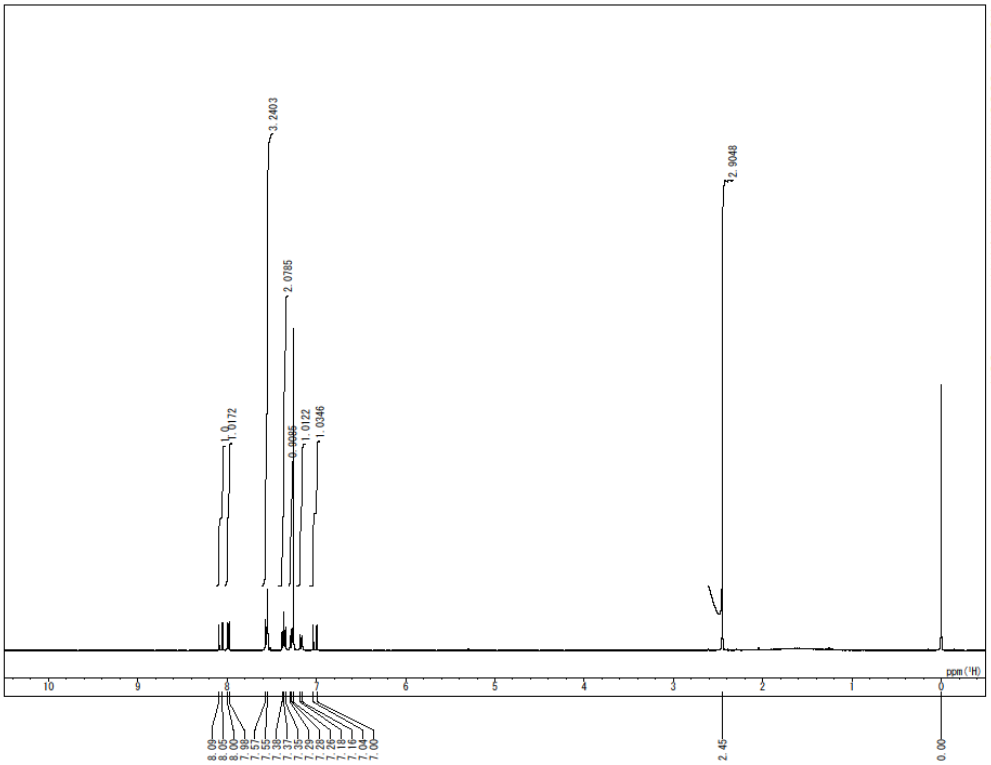
^{1}H NMR of **1o**




```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM    15/Jun/2022 01:24:42
COMNT

OBNUC                  ¹³C
OFR               100.61 MHz
OBSET                0.0 kHz
OBFIN            9999.159 Hz
PW1                 10.0 µs
PW2                 10.0 µs
PW3                 20.0 µs
PI1                  2.0 ms
PI2                0.0035 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS               1024
DUMMY                  2
FREQU           29761.9 Hz
ACQTM              1.101 s
PD                   2.0 s
RGAIN                203
BF                  0.25 Hz
EXMOD           ZGPG30
IRNUC              OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRRPW                0 µs
IRATN                0
CSPED               20.0 Hz
CTEMP             26.91 ℃
PRNT_DATE    2022/Jun/15 11:18:29
```

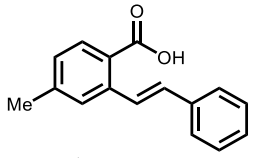


^{13}C NMR of **1n**

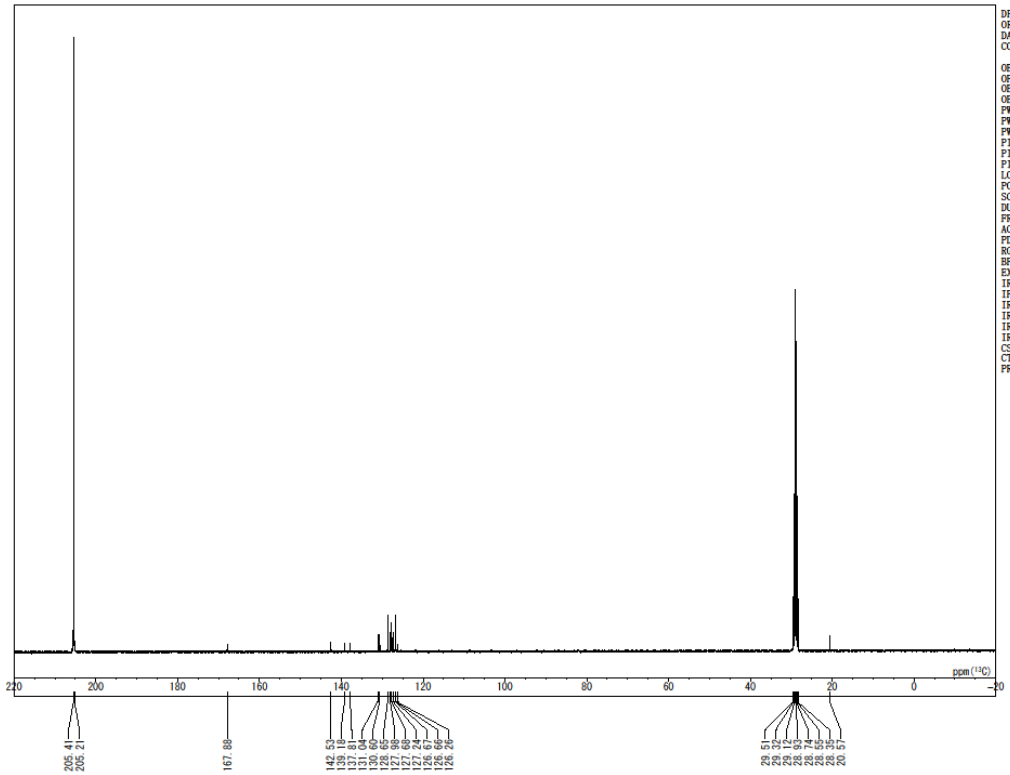


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 14/Jun/2022 22:52:57
COMNT

OBNUC	¹H
OFR	400.03 MHz
OBSET	0.0 kHz
OBFIN	10009.24 Hz
PW1	2.6667 µs
PW2	8.0 µs
PW3	16.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	65536
SCANS	4
DUMMY	2
FREQU	7812.5 Hz
ACQTM	8.3886 s
PD	1.0 s
RGAIN	101
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	0.0 Hz
CTEMP	25.005 ℃
PRNT_DATE	2022/Jun/15 10:32:27

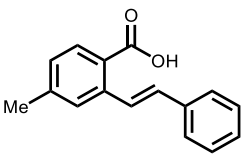


^{1}H NMR of **1p**

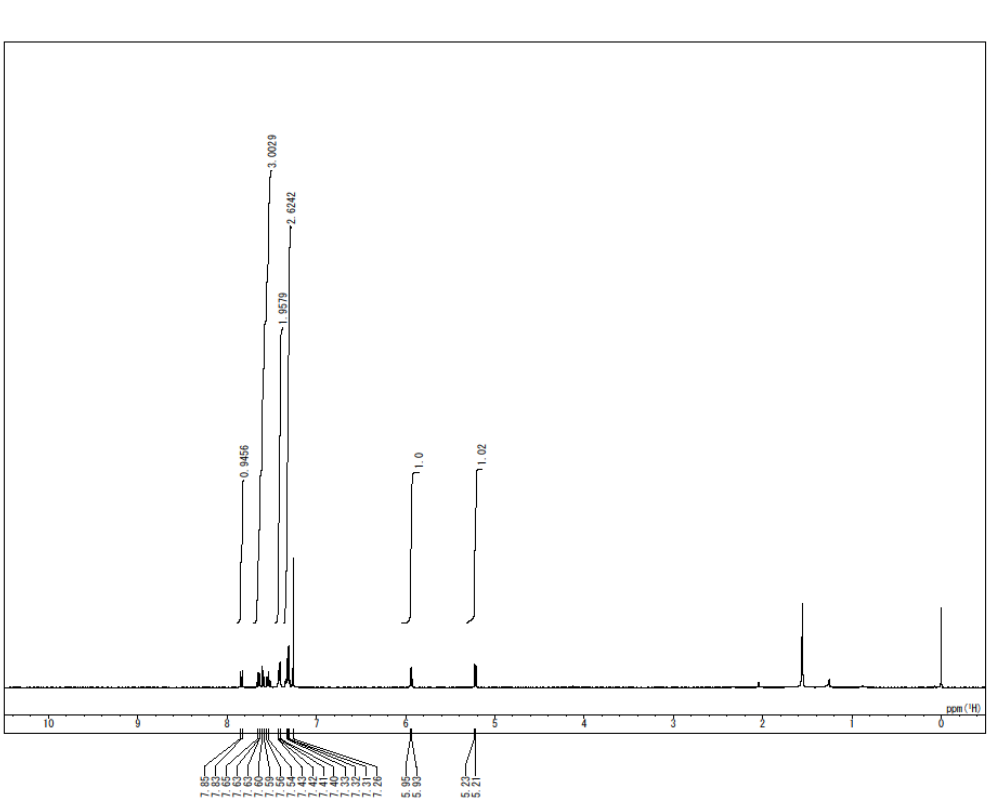


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 15/Jun/2022 02:54:59
COMNT

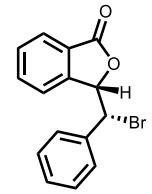
OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	10060.2 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	131072(ZeroFill:×4)
SCANS	1024
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	1.1 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	26.61 ℃
PRNT_DATE	2022/Jun/15 11:31:11



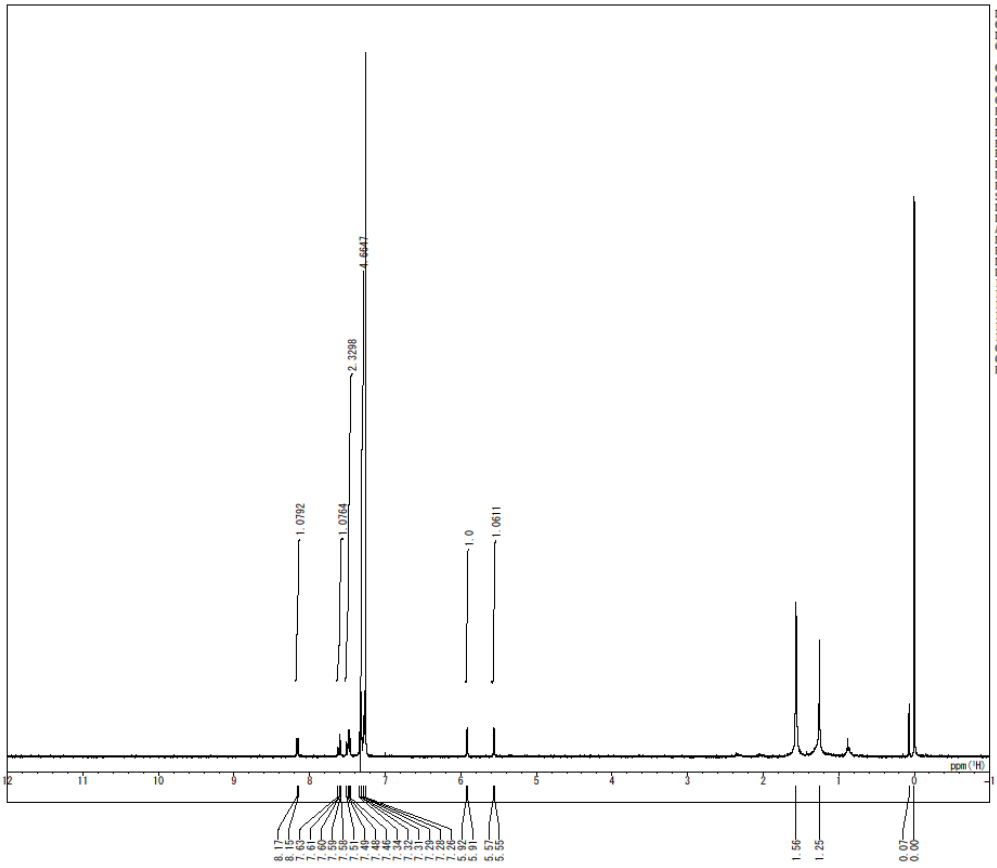
^{13}C NMR of **1p**



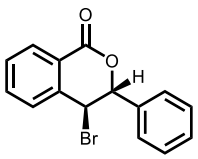
OBNUC	¹H
OFR	400.03 MHz
OBSET	0.0 kHz
OBFIN	10009.24 Hz
PW1	2.6667 µs
PW2	8.0 µs
PW3	16.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	65536
SCANS	4
DUMMY	2
FREQU	7812.5 Hz
ACQTM	8.3886 s
PD	1.0 s
RGAIN	101
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	0.0 Hz
CTEMP	25.0198 °C
PRNT_DATE	2022/Jun/03 00:22:24



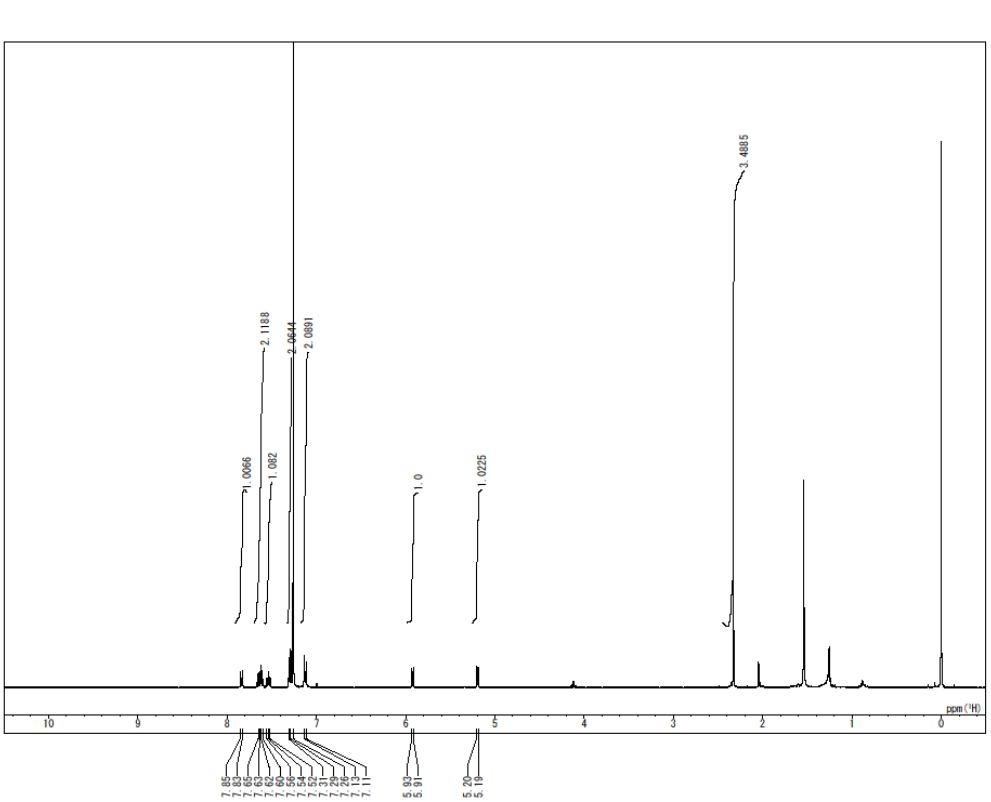
^{1}H NMR of **2a**



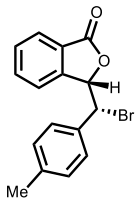
DFILE	Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
OBSFILE	Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM	02/Jul/2020 13:41:34
COMNT	
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	14.0 µs
PW2	14.0 µs
PW3	28.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	22.51 °C
PRNT_DATE	2022/Mar/01 20:59:33



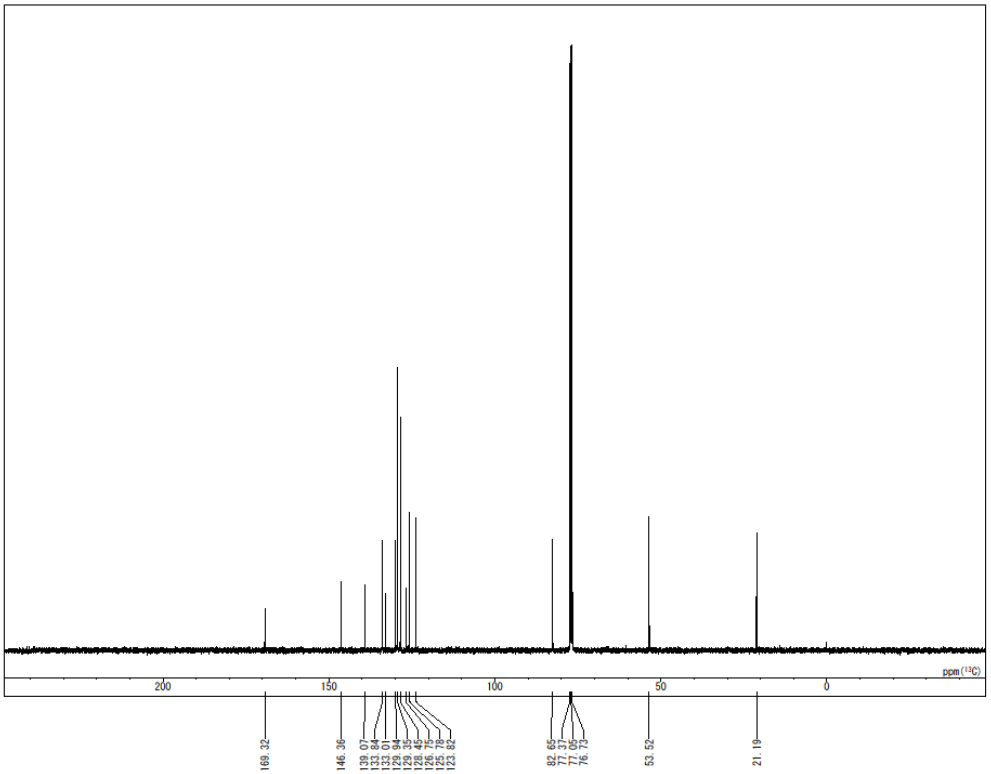
^{1}H NMR of **3a**



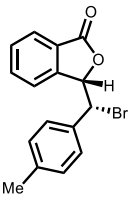
OBNUC	¹H
OFR	400.03 MHz
OBSET	0.0 kHz
OBFIN	10009.24 Hz
PW1	2.6667 µs
PW2	8.0 µs
PW3	16.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	65536
SCANS	4
DUMMY	2
FREQU	7812.5 Hz
ACQTM	8.3886 s
PD	1.0 s
RGAIN	101
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	0.0 Hz
CTEMP	24.9935 °C
PRNT_DATE	2022/Jun/03 00:30:57



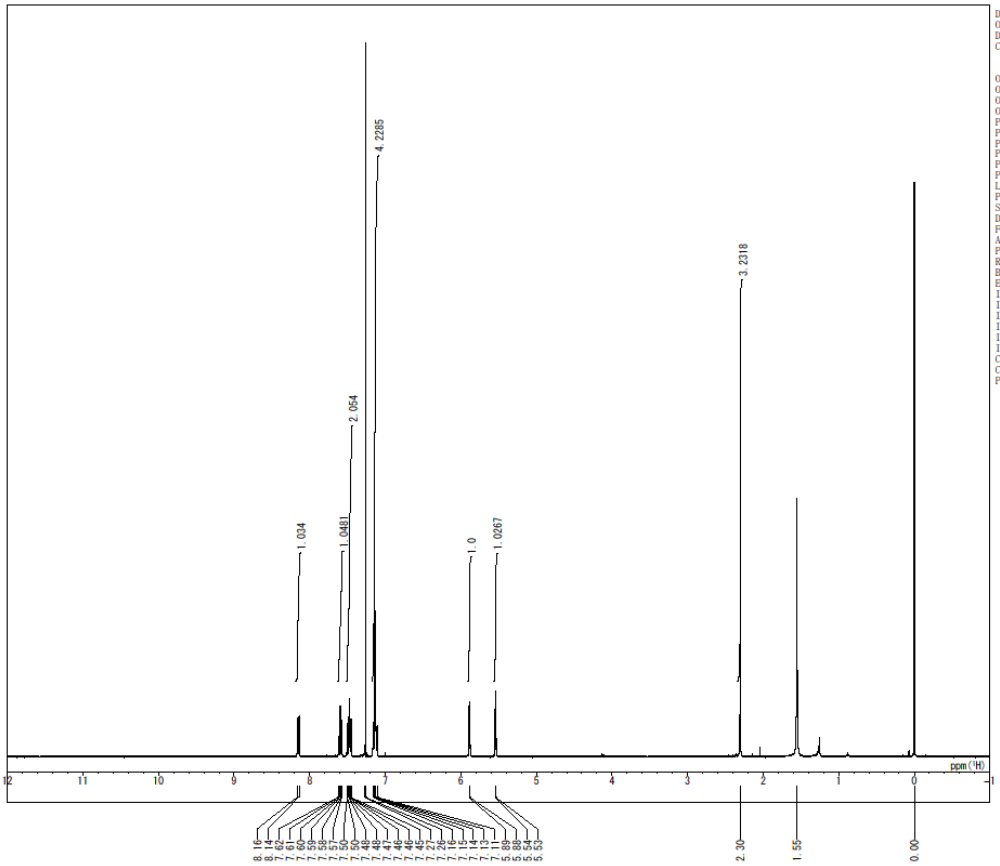
^{1}H NMR of **2b**

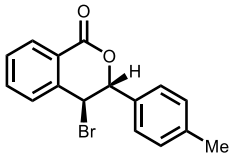


OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	1024
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	18.81 °C
PRNT_DATE	2022/Jun/03 00:26:31

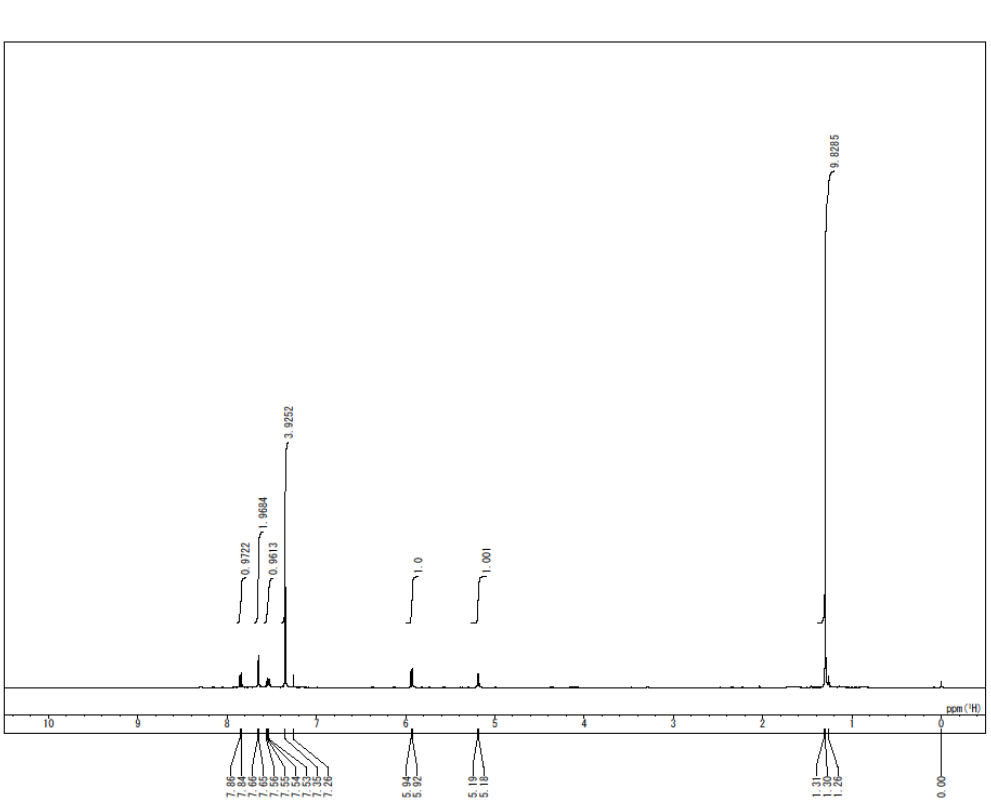


^{13}C NMR of **2b**

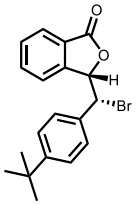

DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 21/Aug/2021 13:56:56
COMNT
OBNUC ¹H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 203
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRBFW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 25.81 ℃
PRNT_DATE 2022/Mar/01 21:29:39
1.034
1.0481
2.054
4.2285
1.0
1.0267
3.2318
ppm (¹H)
2.30
1.55
0.00


O
O
H
Br
Me

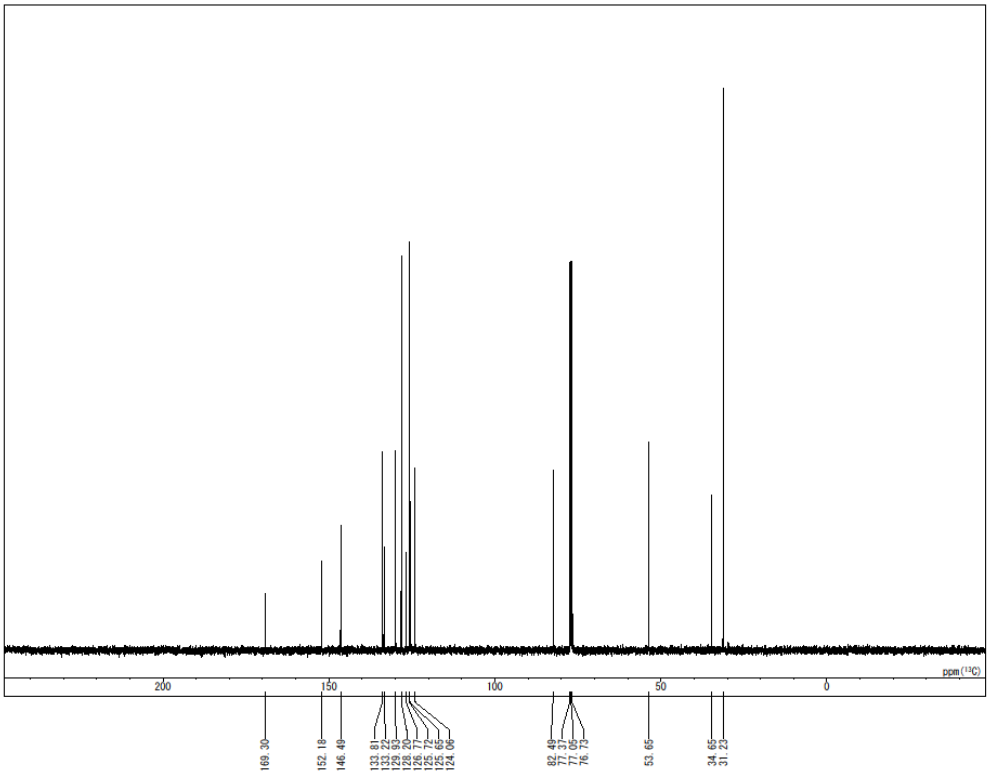
^{1}H NMR of **3b**



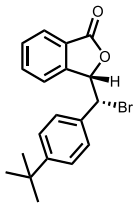
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 μs
PW2	15.0 μs
PW3	30.0 μs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	51
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 μs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.01 °C
PRNT_DATE	2022/Jun/03 00:35:16



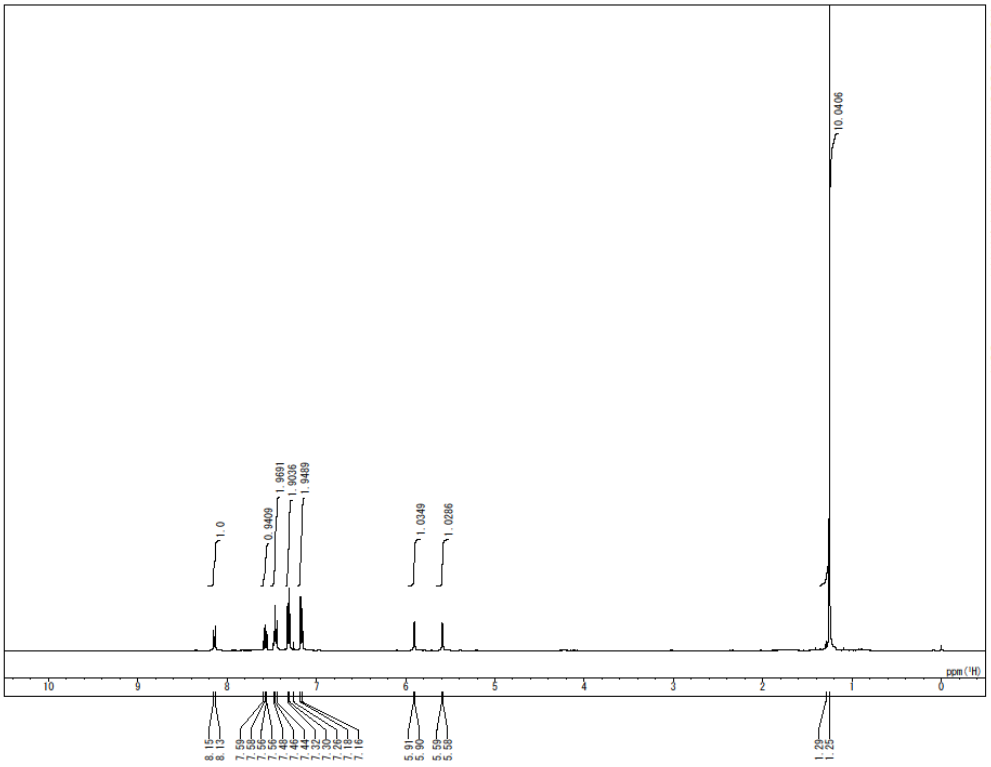
^{1}H NMR of **2c**



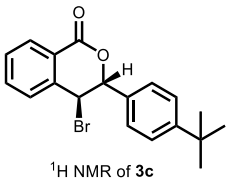
OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 μs
PW2	10.0 μs
PW3	20.0 μs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 μs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.41 °C
PRNT_DATE	2022/Jun/03 00:36:16



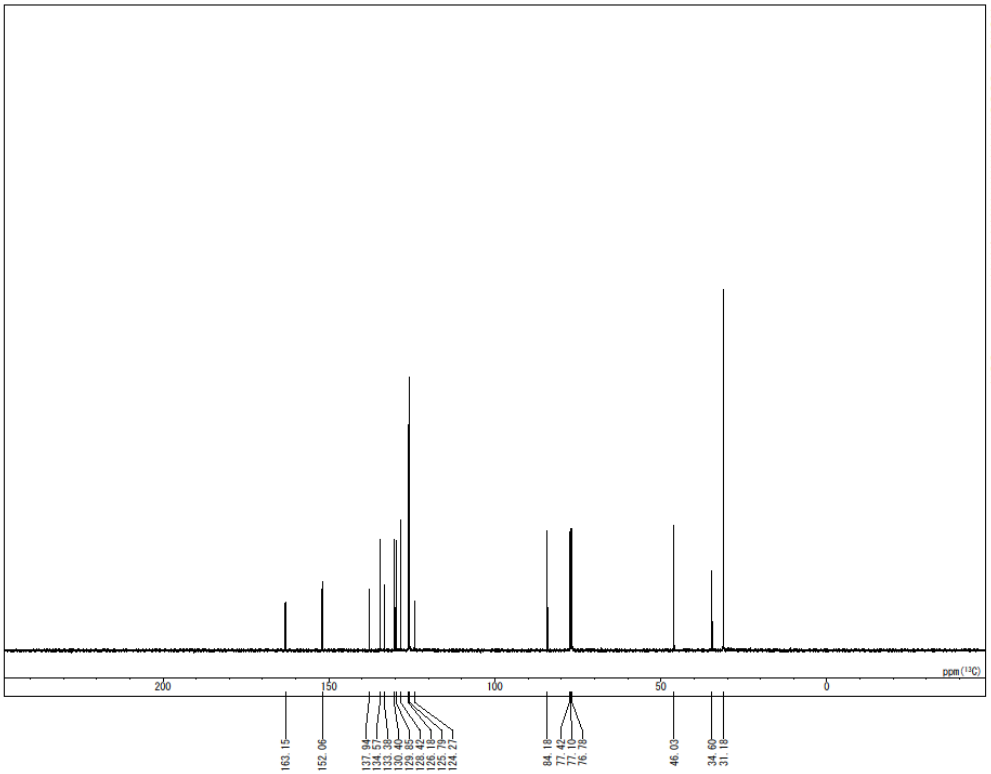
^{13}C NMR of **2c**



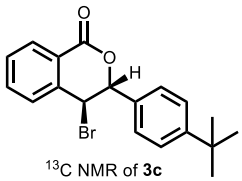

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM   11/Jun/2022 16:43:50
COMNT

OBNUC                 ¹H
OFR              400.13 MHz
OBSET              0.0 kHz
OBFIN           10021.89 Hz
PW1               15.0 µs
PW2               15.0 µs
PW3               30.0 µs
P11                1.0 ms
P12                0.0 ms
P13                0.0 ms
LOOP1                 0
POINT             32768
SCANS                 4
DUMMY                 2
FREQU          8012.82 Hz
ACQTM             4.0894 s
PD                1.0 s
RGAIN                28
BF                0.1223 Hz
EXMOD             ZG30
IRNUC              OFF
IFR                0.0 MHz
IRSET              0.0 kHz
IRFIN              0.0 Hz
IRPW               0 µs
IRATN                 0
CSPED             20.0 Hz
CTEMP             25.11 °C
PRNT_DATE   2022/Jun/21 21:49:07
```



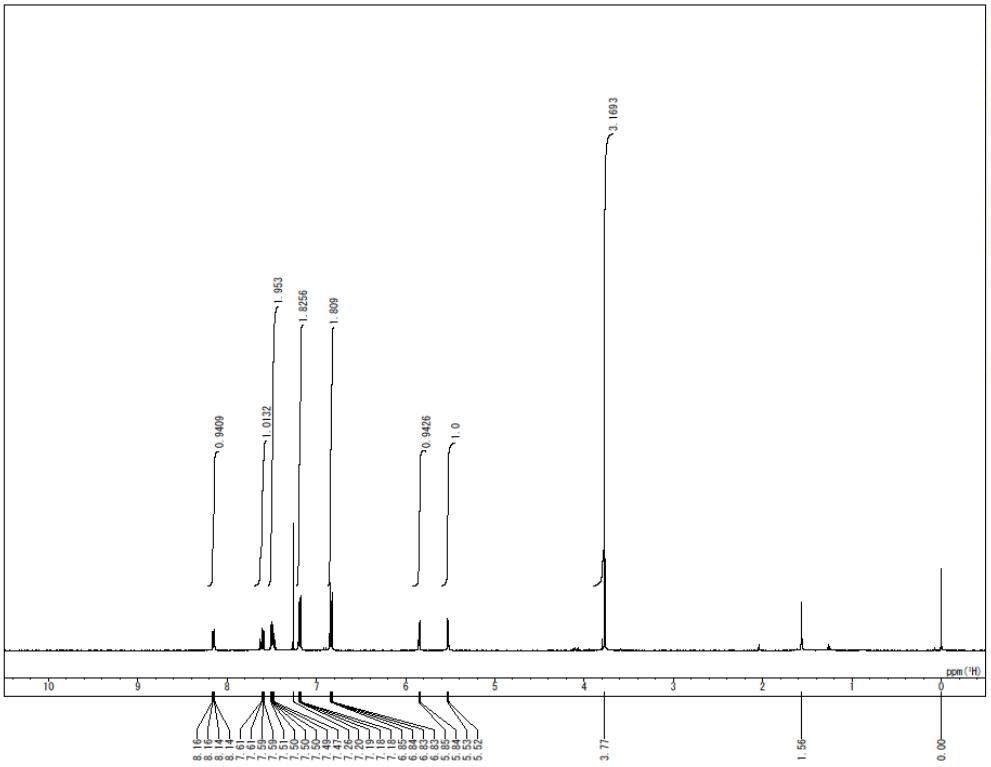
^{1}H NMR of **3c**



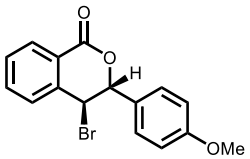

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM   11/Jun/2022 16:59:04
COMNT

OBNUC                 ¹³C
OFR              100.61 MHz
OBSET              0.0 kHz
OBFIN           9999.159 Hz
PW1               10.0 µs
PW2               10.0 µs
PW3               20.0 µs
P11                2.0 ms
P12             0.0035 ms
P13                0.0 ms
LOOP1                 0
POINT             32768
SCANS               256
DUMMY                 2
FREQU          29761.9 Hz
ACQTM             1.101 s
PD                2.0 s
RGAIN               203
BF                0.25 Hz
EXMOD           ZGPG30
IRNUC              OFF
IFR                0.0 MHz
IRSET              0.0 kHz
IRFIN              0.0 Hz
IRPW               0 µs
IRATN                 0
CSPED             20.0 Hz
CTEMP             25.94 °C
PRNT_DATE   2022/Jun/11 17:29:54
```



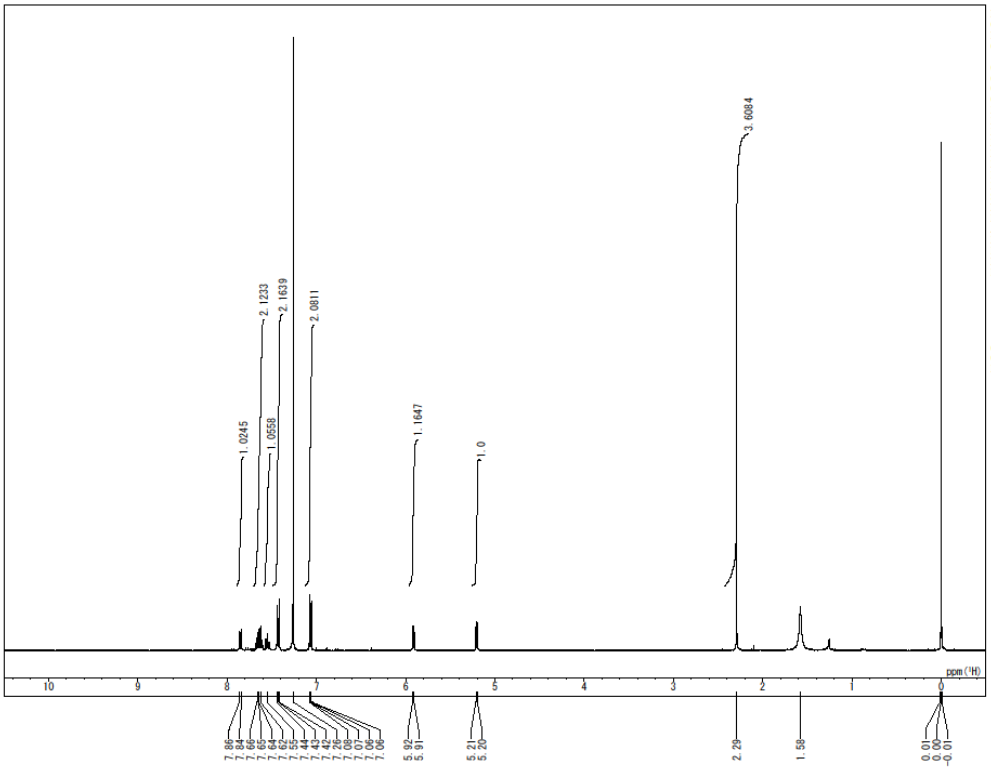
^{13}C NMR of **3c**




```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM     15/Jun/2022 14:22:17
COMNT


OBNUC                  ¹H
OFR                400.13 MHz
OBSET                0.0 kHz
OBFIN            10021.89 Hz
PW1                 15.0 µs
PW2                 15.0 µs
PW3                 30.0 µs
PI1                  1.0 ms
PI2                  0.0 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS                  4
DUMMY                  2
FREQU             8012.82 Hz
ACQTM                4.0894 s
PD                   1.0 s
RGAIN                144
BF                  0.25 Hz
EXMOD               ZG30
IRNUC               OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRBFW                0 µs
IRATN                  0
CSPED               20.0 Hz
CTEMP               26.01 ℃
PRNT_DATE     2022/Jun/15 15:57:27
```

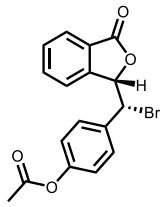


^{1}H NMR of **3d**

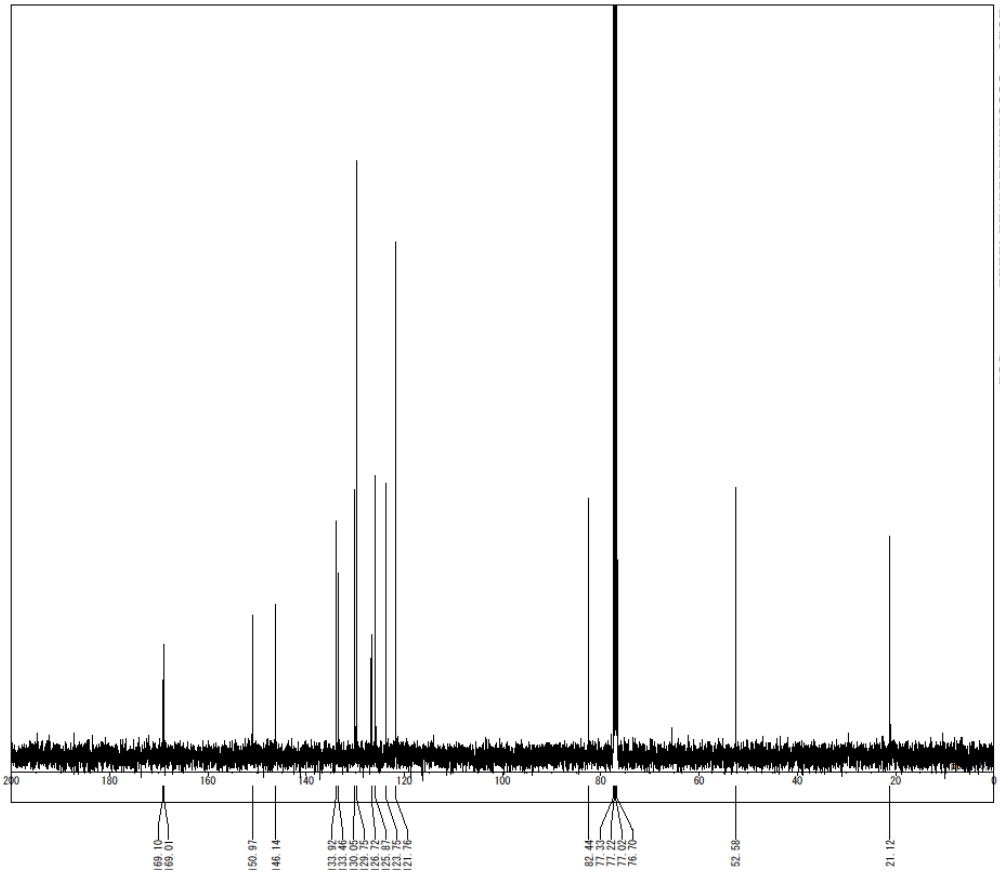


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 11/Jun/2022 23:15:28
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	181
BF	0.1223 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.31 °C
PRNT_DATE	2022/Jun/21 22:14:19

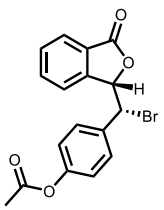


^{1}H NMR of **2e**

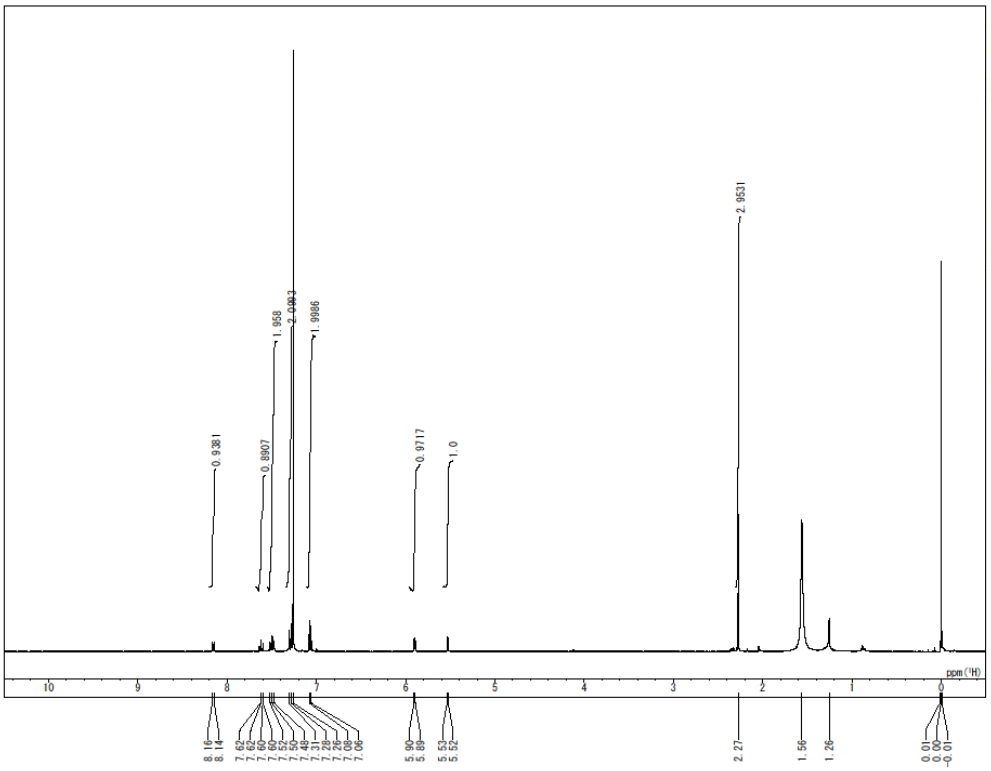


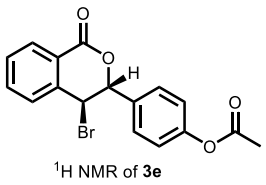
DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 24/May/2022 03:55:22
COMNT

OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
P11	2.0 ms
P12	0.0035 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.51 °C
PRNT_DATE	2022/Jun/02 09:18:52

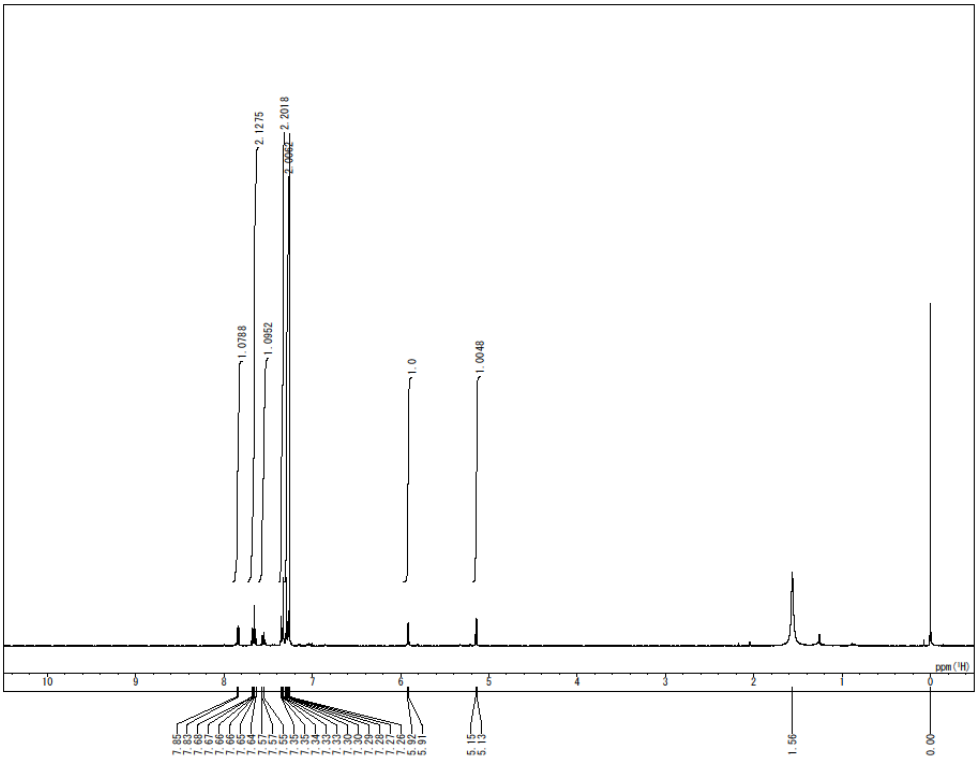


^{13}C NMR of **2e**

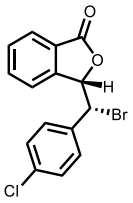

DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 23/Jun/2022 23:44:13
COMNT
OBNUC 1H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 16
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 181
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRBFW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 26.91 ℃
PRNT_DATE 2022/Jun/23 23:48:23
0.9381
0.8907
1.958
2.0003
1.9986
0.9717
1.0
2.9531
ppm (1H)
10
9
8
7
6
5
4
3
2
1
0
8.16
8.14
7.62
7.62
7.60
7.60
7.52
7.52
7.43
7.31
7.28
7.28
7.06
7.06
5.90
5.89
5.53
5.52
2.27
1.56
1.26
0.01
0.00
-0.01


O
O
H
Br
O
O

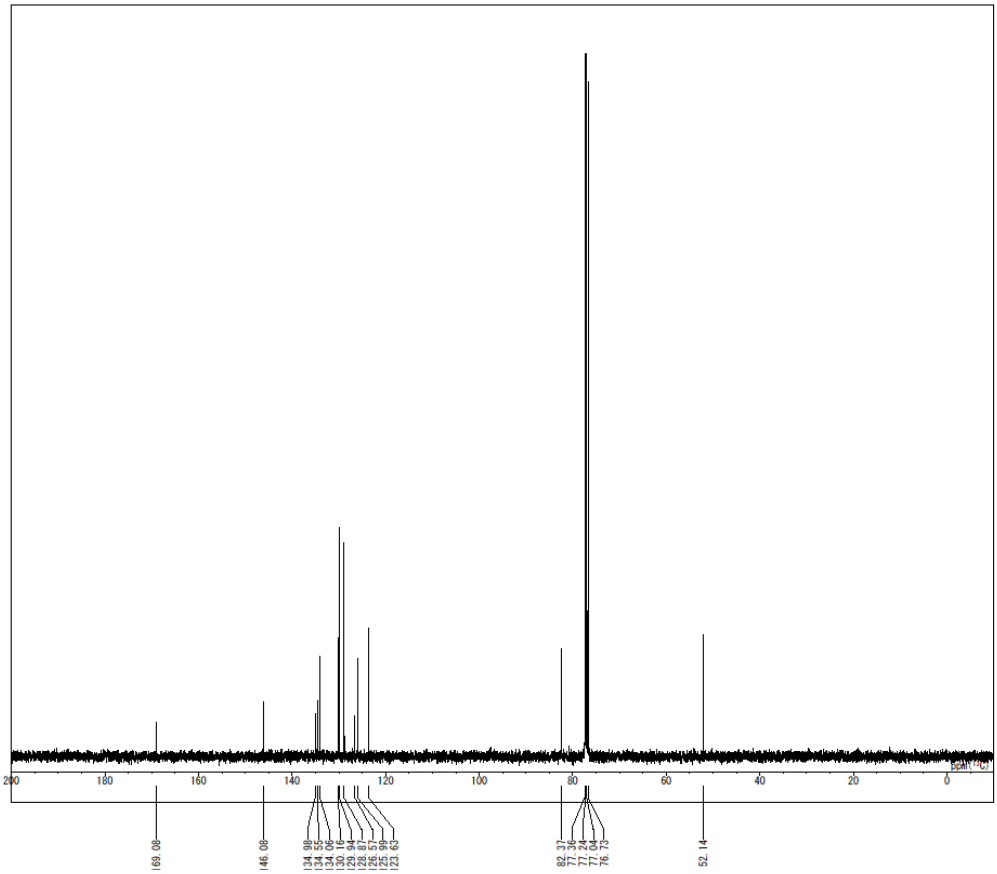
^{1}H NMR of **3e**



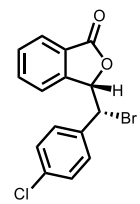

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM   23/Jun/2022 23:14:29
COMNT

OBNUC                  ¹H
OFR               400.13 MHz
OBSET               0.0 kHz
OBFIN            10021.89 Hz
PW1                15.0 µs
PW2                15.0 µs
PW3                30.0 µs
P11                 1.0 ms
P12                 0.0 ms
P13                 0.0 ms
LOOP1                  0
POINT              32768
SCANS                 16
DUMMY                  2
FREQU            8012.82 Hz
ACQTM               4.0894 s
PD                  1.0 s
RGAIN                161
BF                  0.1223 Hz
EXMOD              ZG30
IRNUC               OFF
IFR                 0.0 MHz
IRSET               0.0 kHz
IRFIN               0.0 Hz
IRRPW               0 µs
IRATN                  0
CSPED              20.0 Hz
CTEMP              27.11 ℃
PRNT_DATE    2022/Jun/23 23:29:32
```



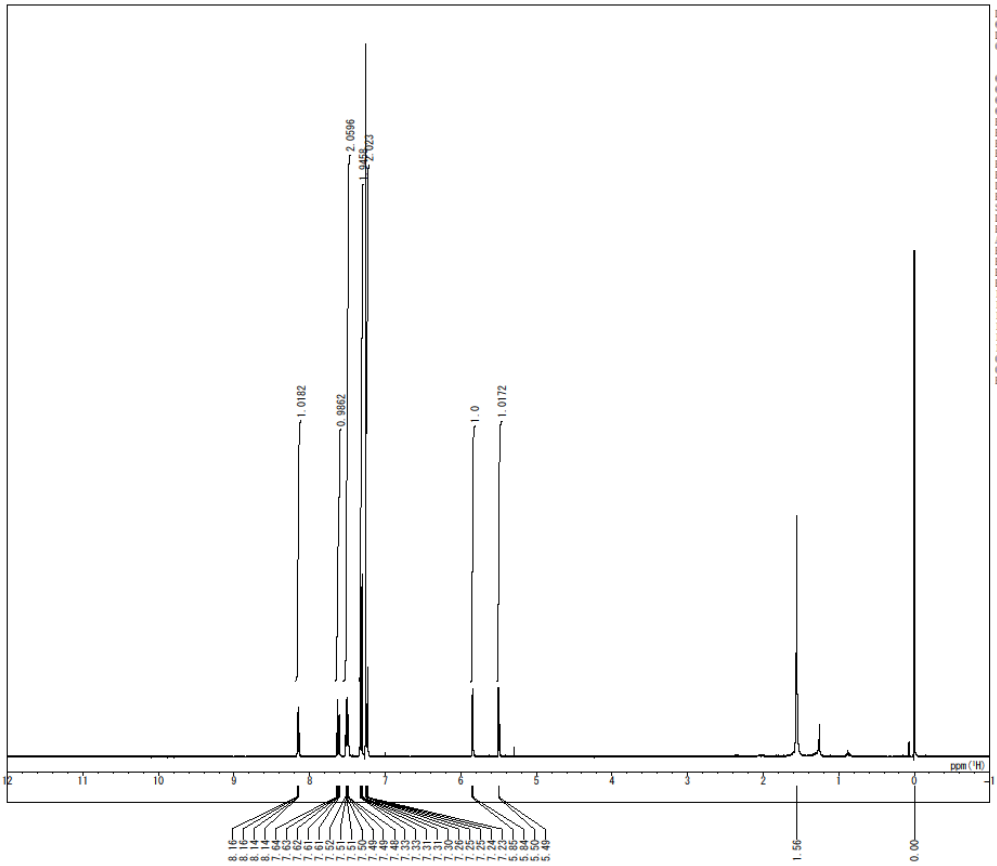
^{1}H NMR of **2f**

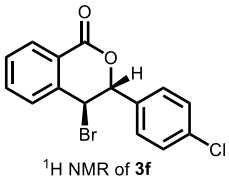



```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM   20/Jan/2022 11:48:17
COMNT

OBNUC                  ¹³C
OFR               100.61 MHz
OBSET               0.0 kHz
OBFIN            9999.159 Hz
PW1                10.0 µs
PW2                10.0 µs
PW3                20.0 µs
P11                 2.0 ms
P12                0.0035 ms
P13                 0.0 ms
LOOP1                  0
POINT              32768
SCANS                256
DUMMY                  2
FREQU            29761.9 Hz
ACQTM               1.101 s
PD                  2.0 s
RGAIN                161
BF                  0.25 Hz
EXMOD             ZGPG30
IRNUC               OFF
IFR                 0.0 MHz
IRSET               0.0 kHz
IRFIN               0.0 Hz
IRRPW               0 µs
IRATN                  0
CSPED              20.0 Hz
CTEMP              18.61 ℃
PRNT_DATE    2022/Mar/01 21:37:34
```

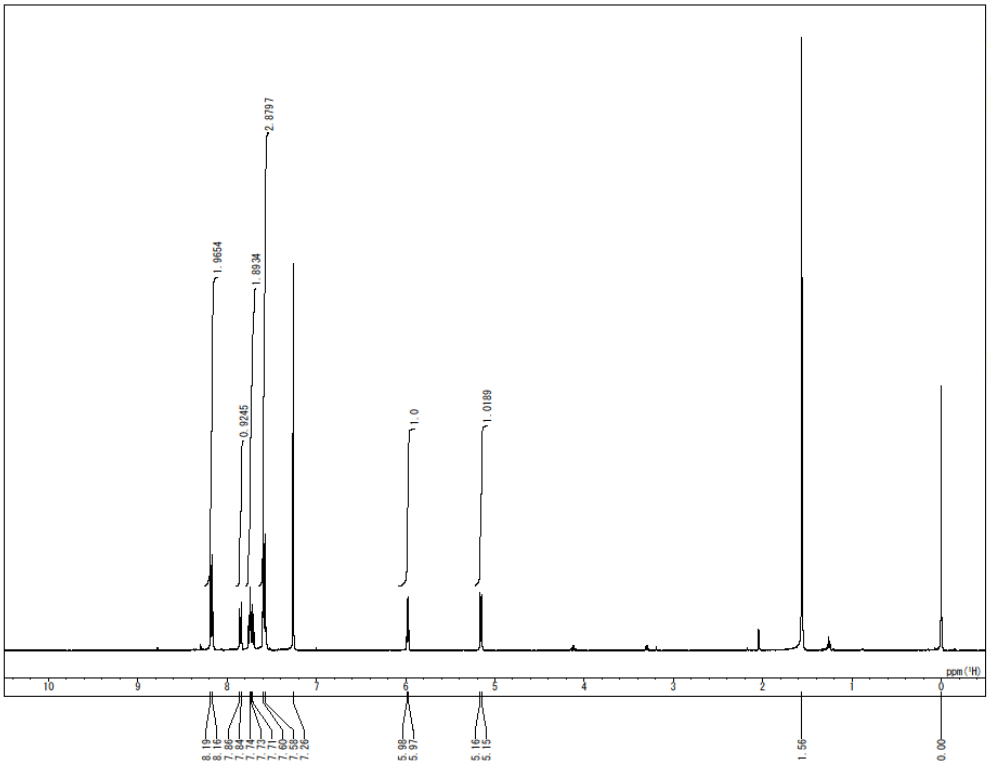


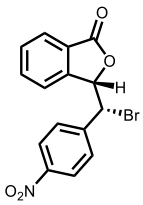
^{13}C NMR of **2f**



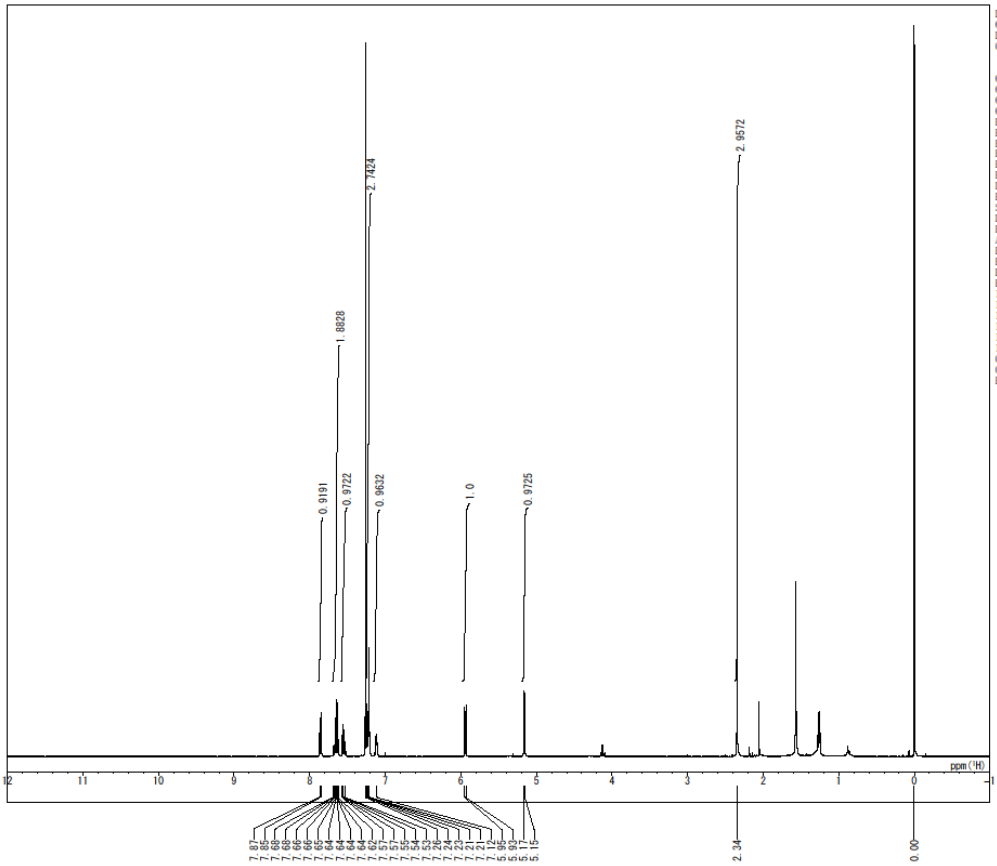


^{1}H NMR of **3f**



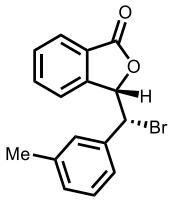


^{1}H NMR of **2g**

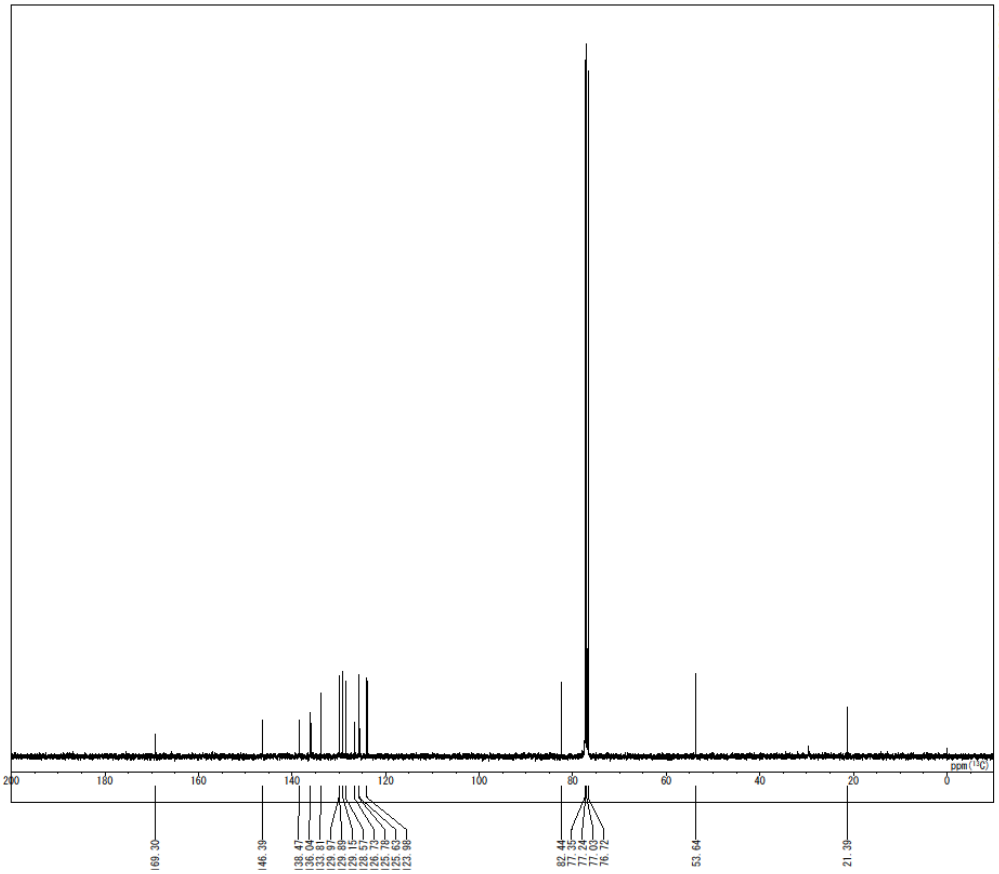


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 19/Jan/2022 02:17:46
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	16
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	18.01 °C
PRNT_DATE	2022/Mar/01 21:45:54

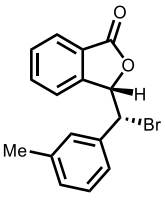


^{1}H NMR of **2h**

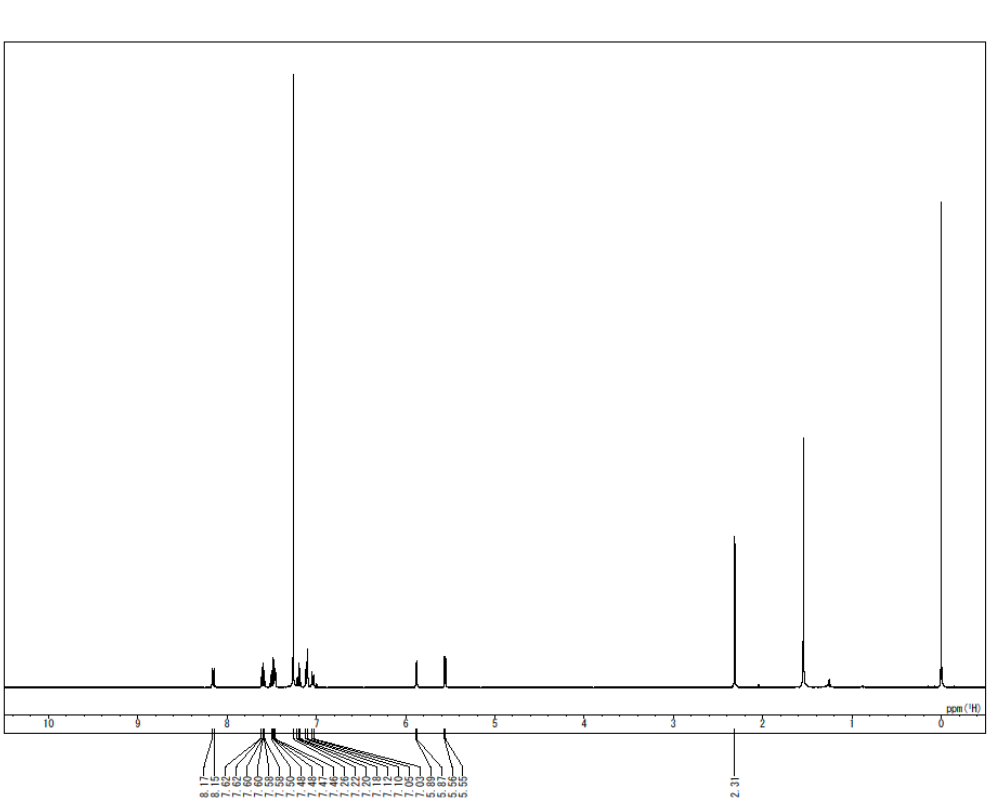


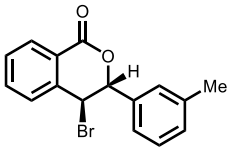
DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 19/Jan/2022 03:24:56
COMNT

OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
P11	2.0 ms
P12	0.0035 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	1024
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	144
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	18.91 °C
PRNT_DATE	2022/Mar/01 21:47:07

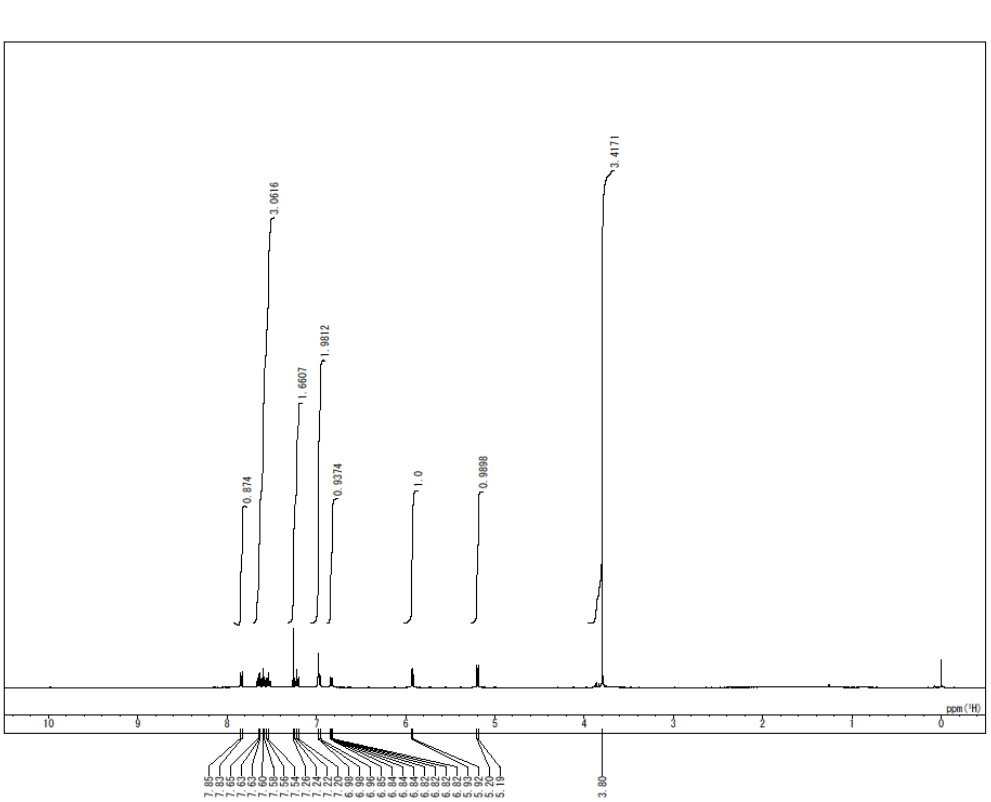


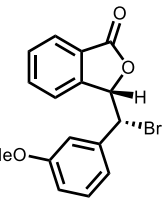
^{13}C NMR of **2h**


OBNUC 1H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 181
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 24.71 °C
PRNT_DATE 2022/Jun/03 10:59:16
ppm (1H)
10
9
8
7
6
5
4
3
2
1
0
2.31

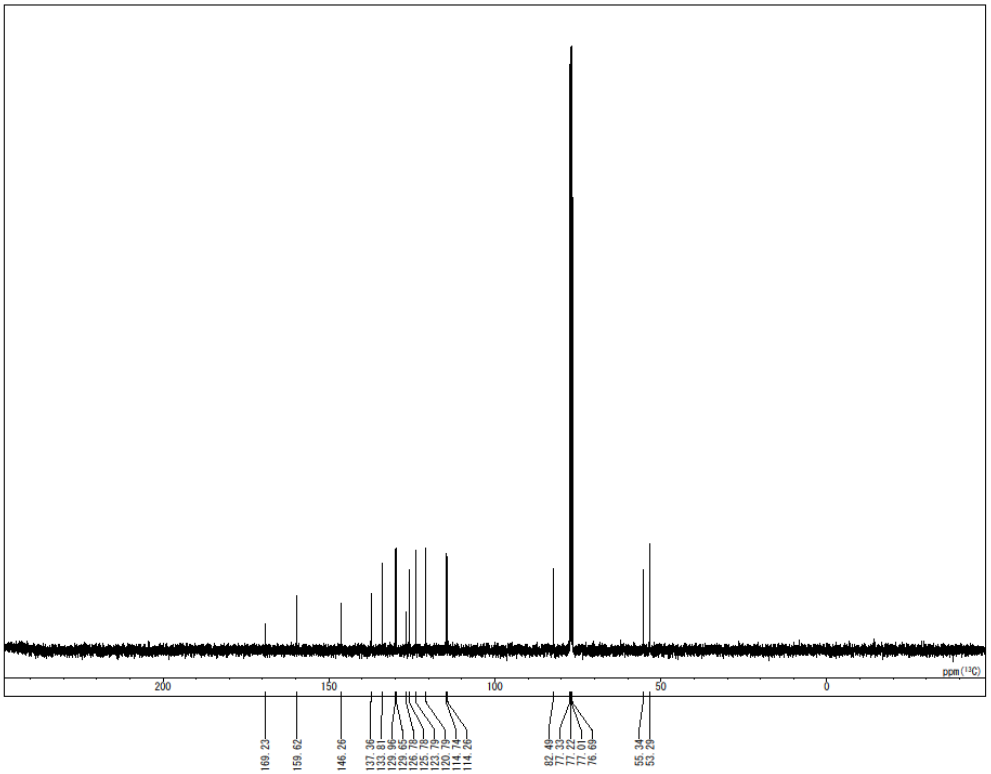

O
O
H
Me
Br

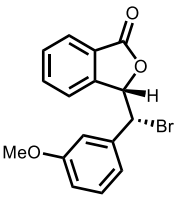
^{1}H NMR of **3h**



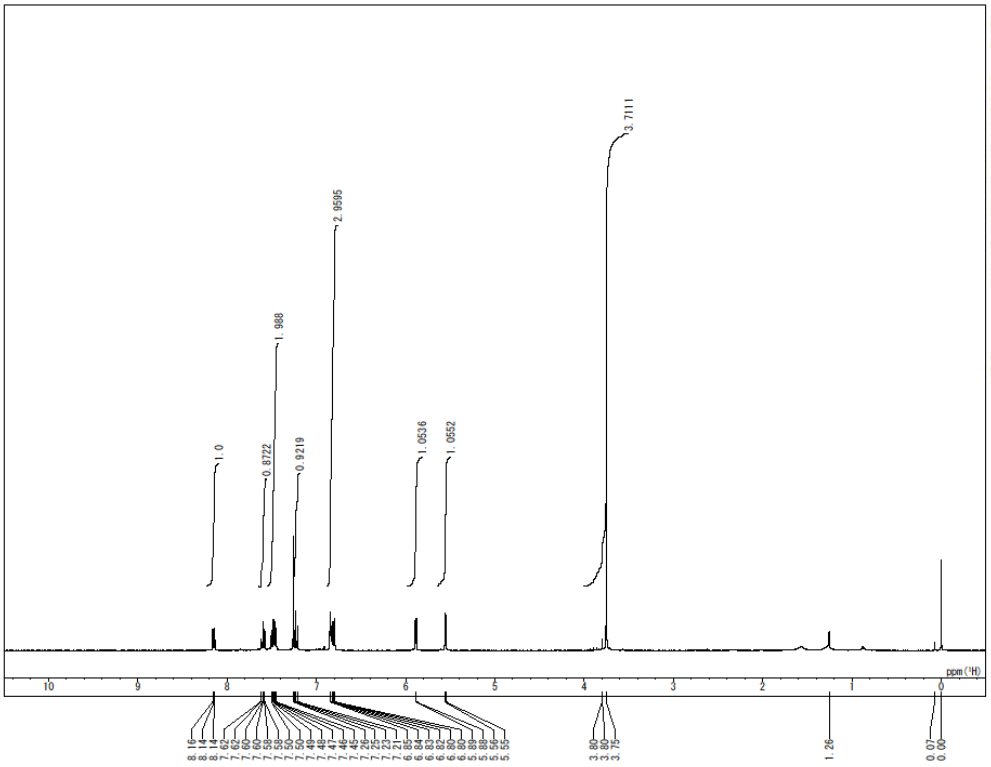


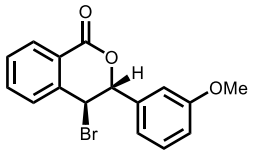
^{1}H NMR of **2i**



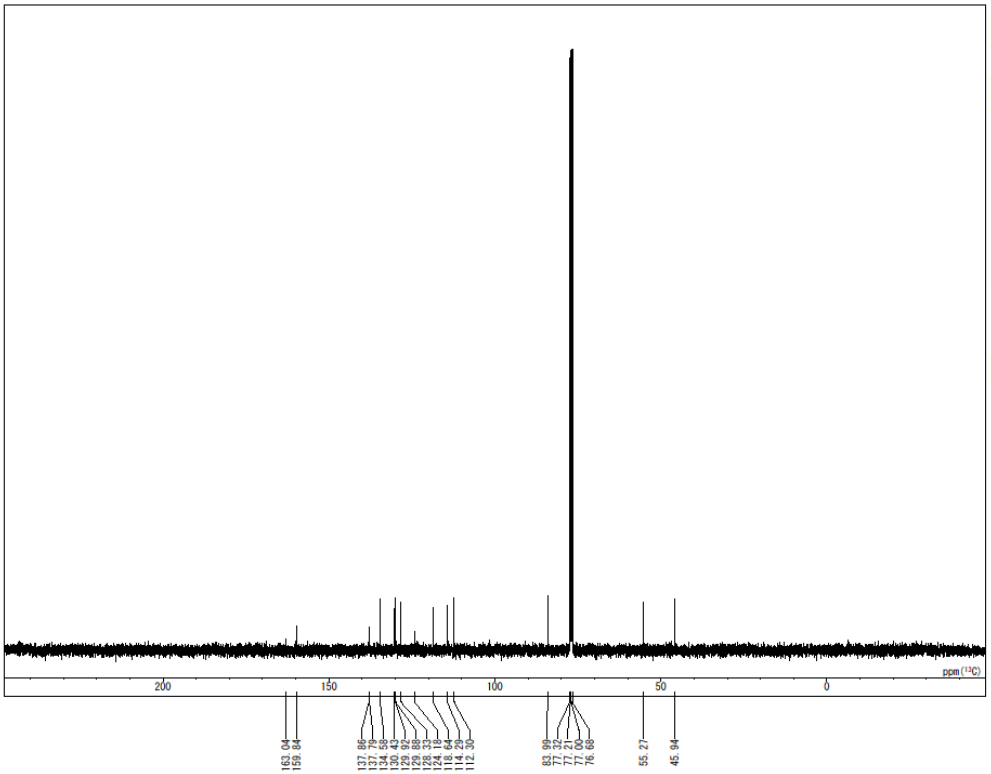


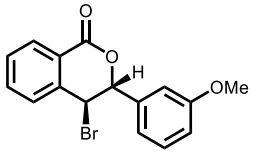
^{13}C NMR of **2i**



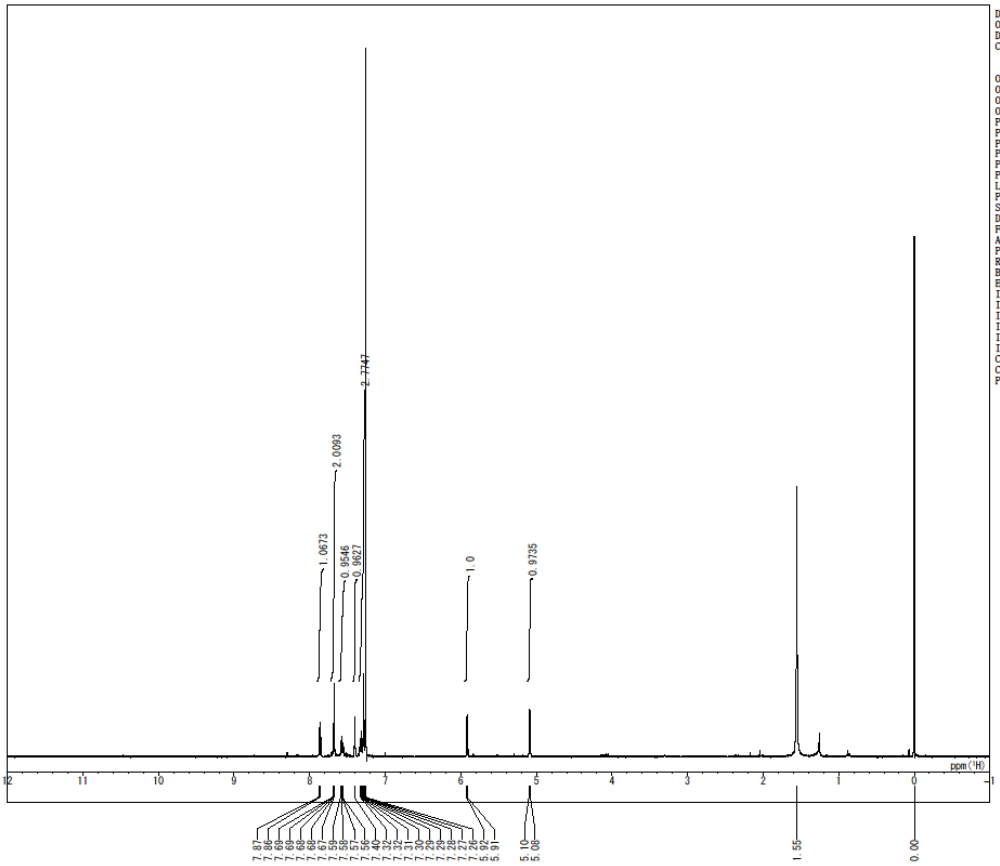


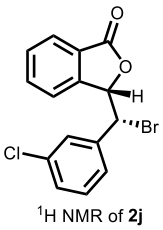
^{1}H NMR of **3i**



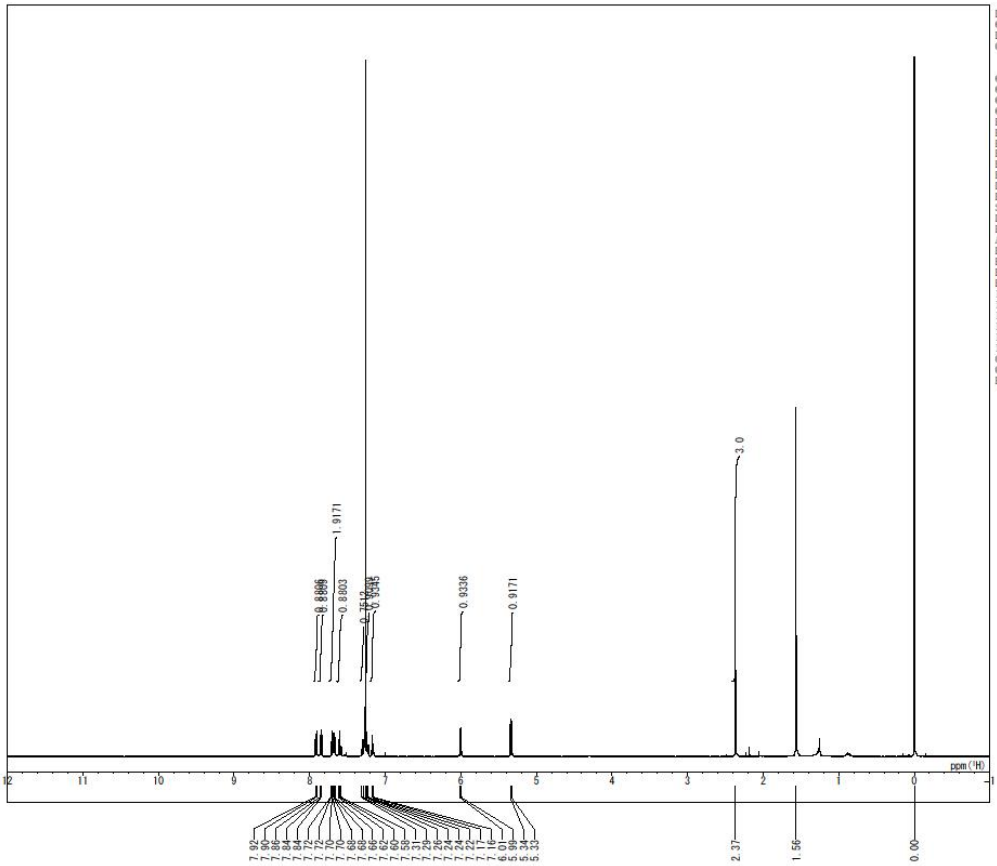


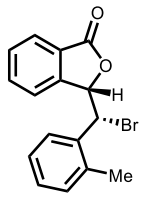
^{13}C NMR of **3i**


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 15/Jul/2021 13:09:47
COMNT
OBNUC ¹H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 203
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRBFW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 26.31 °C
PRNT_DATE 2022/Mar/01 21:41:39
1.0673
2.0093
0.9546
0.9627
2.7747
1.0
0.9735
ppm (¹H)
7.87
7.86
7.69
7.68
7.68
7.67
7.59
7.58
7.57
7.56
7.40
7.32
7.31
7.30
7.29
7.28
7.27
7.26
5.92
5.91
5.10
5.00
1.55
0.00

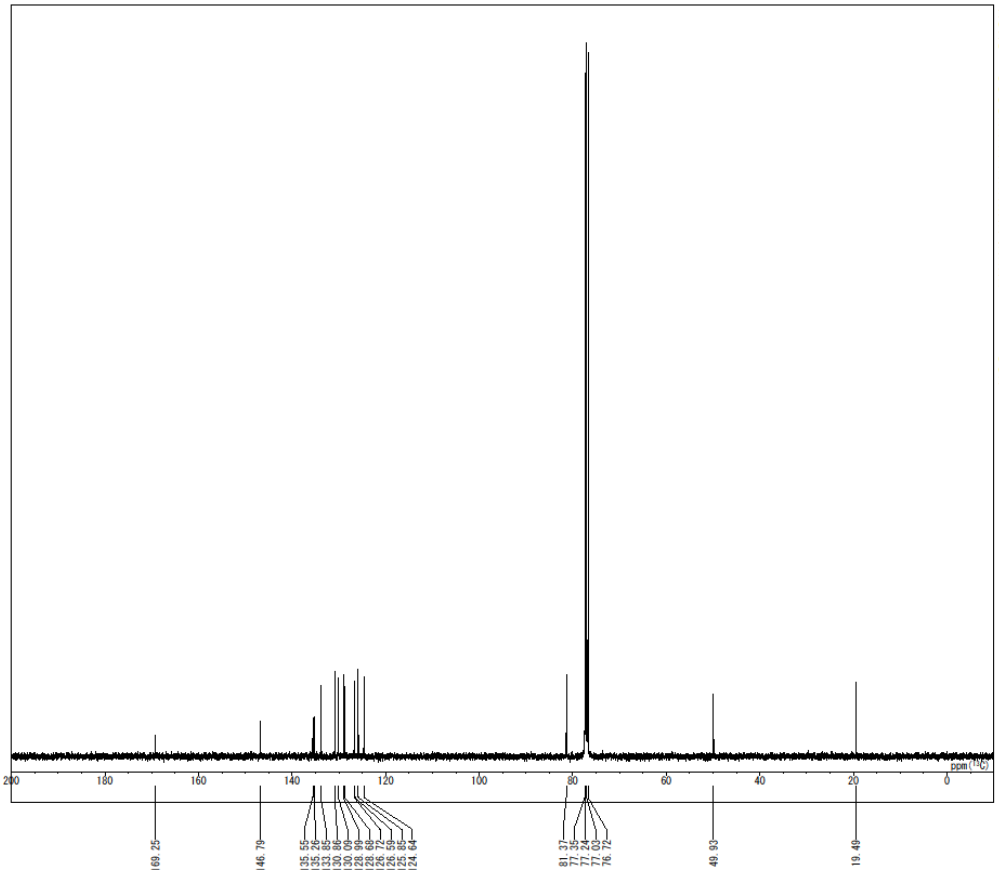

O
O
H
Br
Cl

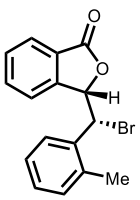
^{1}H NMR of **2j**



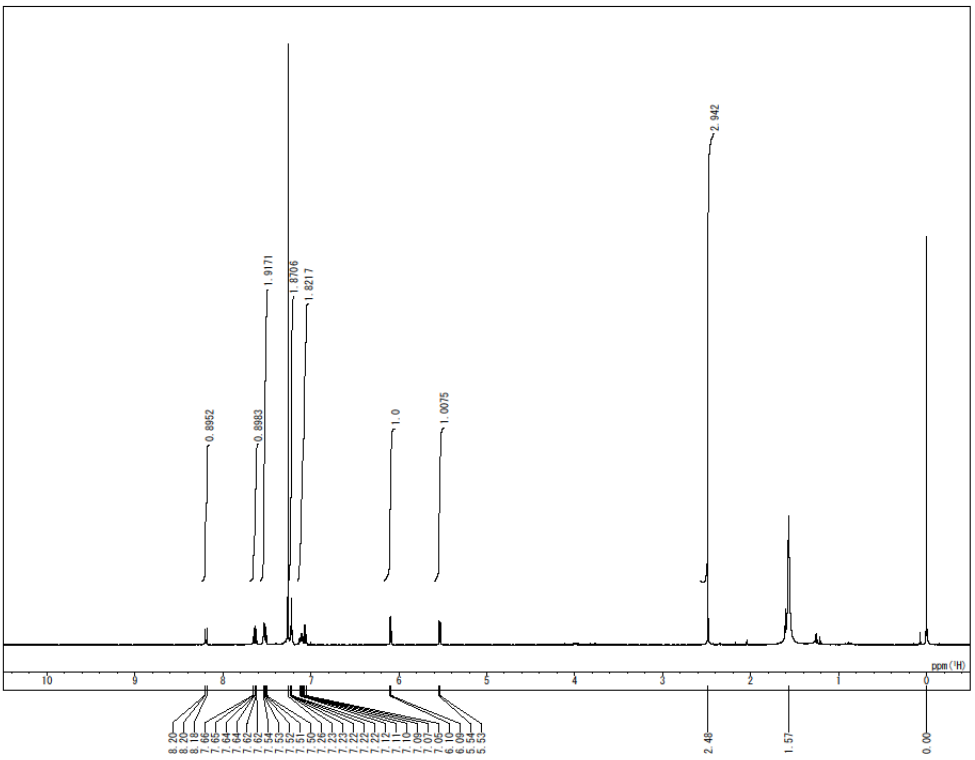


^{1}H NMR of **2k**



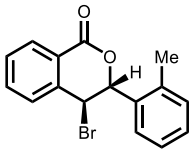


^{13}C NMR of **2k**

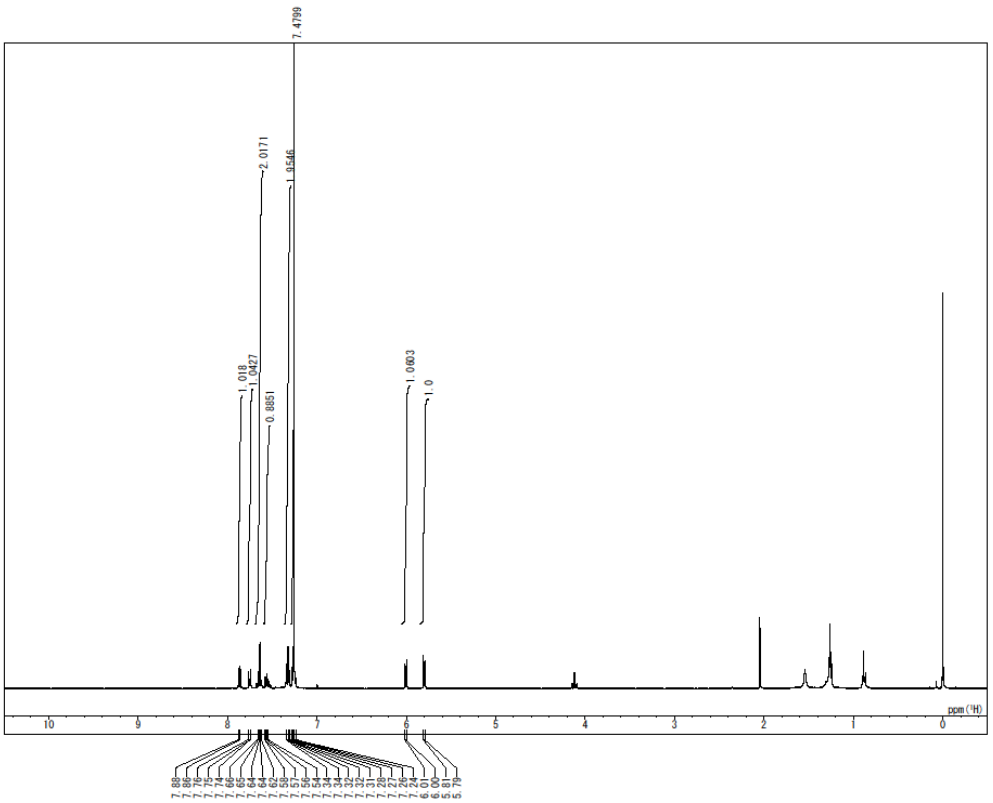


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
OBSFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 23/Jun/2022 23:20:05
COMNT

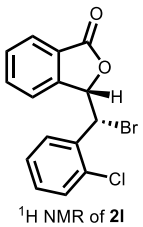
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	16
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	161
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	27.01 ℃
PRNT_DATE	2022/Jun/23 23:28:36



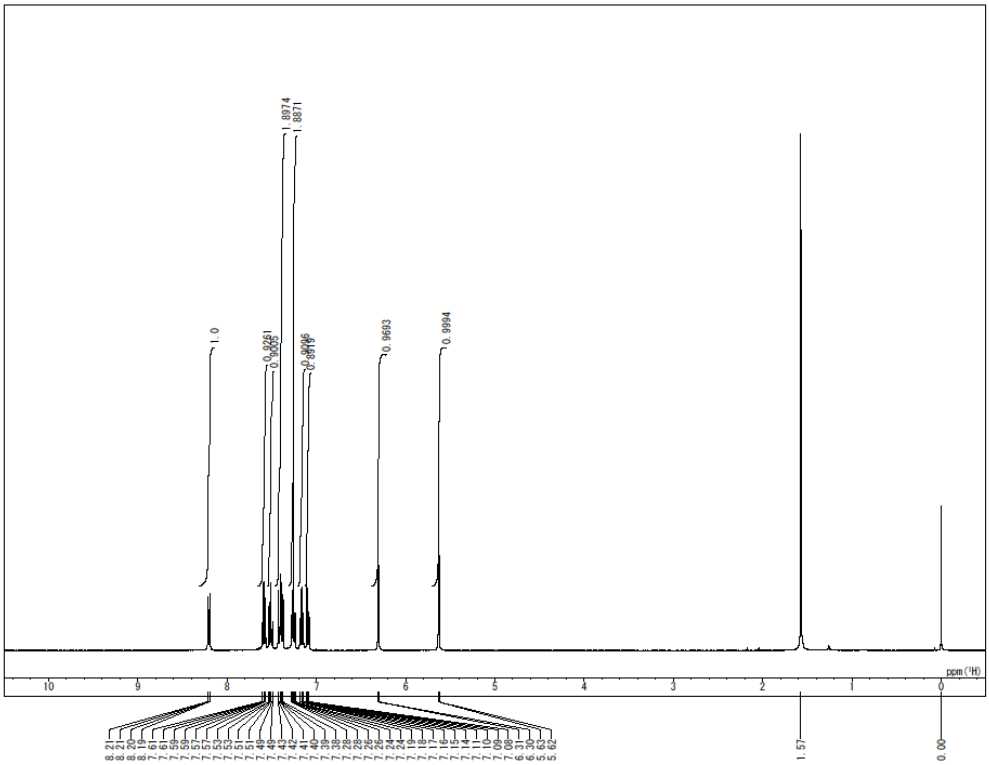
¹H NMR of **3k**



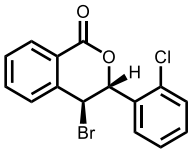
OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	24.91 ℃
PRNT_DATE	2022/Jun/03 01:12:22



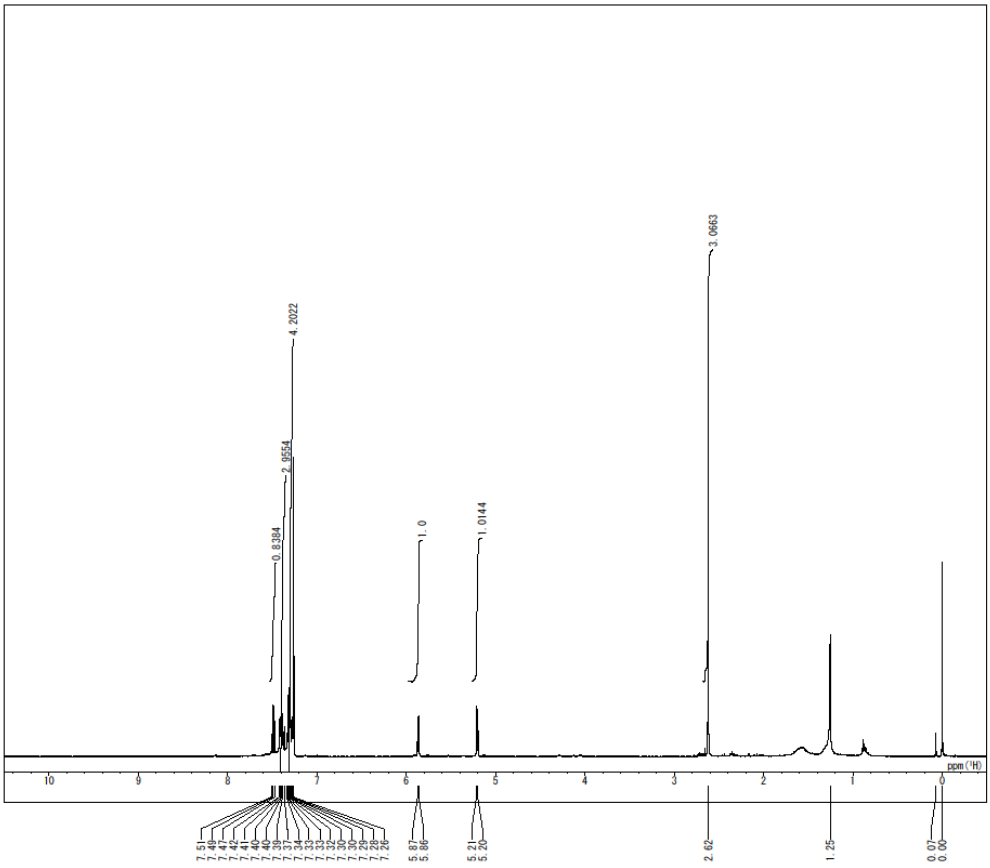
¹H NMR of **2l**



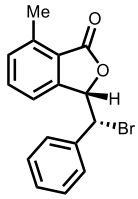

```
DFILE   X:¥062ORGVDATA¥ORGVNMR¥MSO-CL6-ENDO-H-
ORGFILE X:¥062ORGVDATA¥ORGVNMR¥MSO-CL6-ENDO-
DATIM   28/Jun/2022 10:44:44
COMNT

OBNUC                  ¹H
OFR               400.13 MHz
OBSET               0.0 kHz
OBFIN           10021.89 Hz
PW1                15.0 µs
PW2                15.0 µs
PW3                30.0 µs
PI1                 1.0 ms
PI2                 0.0 ms
PI3                 0.0 ms
LOOP1                  0
POINT              32768
SCANS                 16
DUMMY                  2
FREQU           8012.82 Hz
ACQTM              4.0894 s
PD                 1.0 s
RGAIN                144
BF                 0.25 Hz
EXMOD              ZG30
IRNUC              OFF
IFR                 0.0 MHz
IRSET               0.0 kHz
IRFIN               0.0 Hz
IRBPW               0 µs
IRATN                  0
CSPED              20.0 Hz
CTEMP              27.11 ℃
PRNT_DATE   2022/Jun/28 10:58:46
```



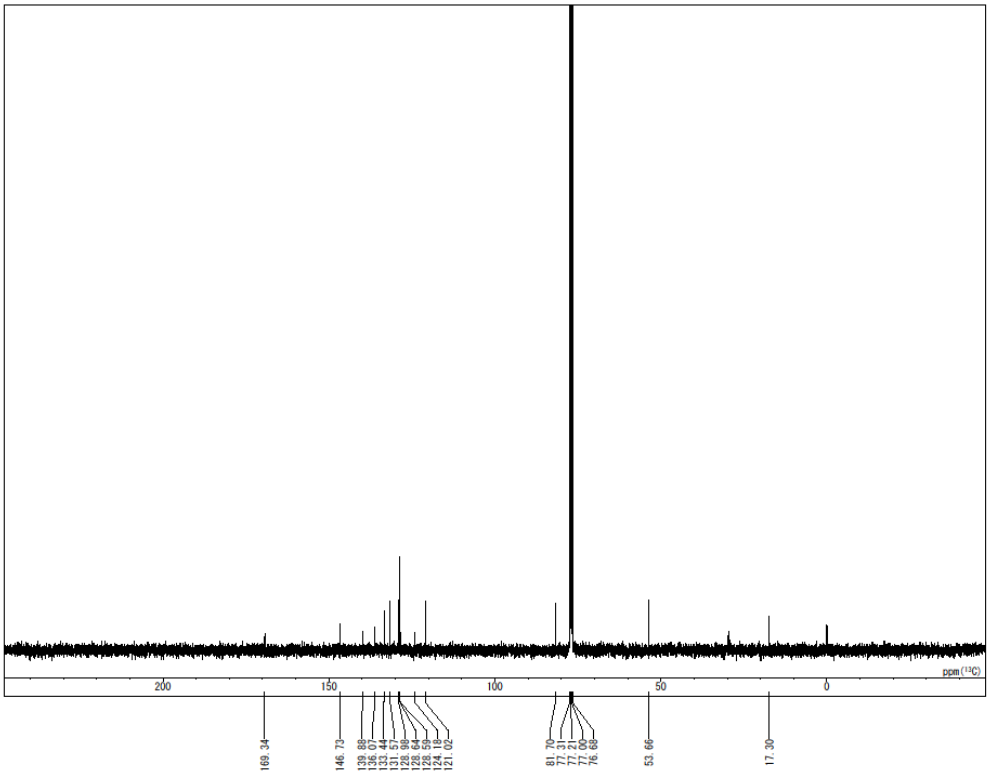
^{1}H NMR of **3l**



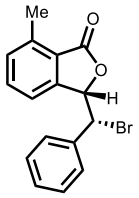

```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM   01/Jun/2022 02:21:47
COMNT

OBNUC                  ¹H
OFR                400.13 MHz
OBSET                0.0 kHz
OBFIN            10021.89 Hz
PW1                 15.0 µs
PW2                 15.0 µs
PW3                 30.0 µs
PI1                  1.0 ms
PI2                  0.0 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS                  4
DUMMY                  2
FREQU             8012.82 Hz
ACQTM              4.0894 s
PD                   1.0 s
RGAIN                161
BF                  0.25 Hz
EXMOD              ZG30
IRNUC              OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRPW                 0 µs
IRATN                  0
CSPED               20.0 Hz
CTEMP               25.01 °C
PRNT_DATE   2022/Jun/01 15:05:18
```



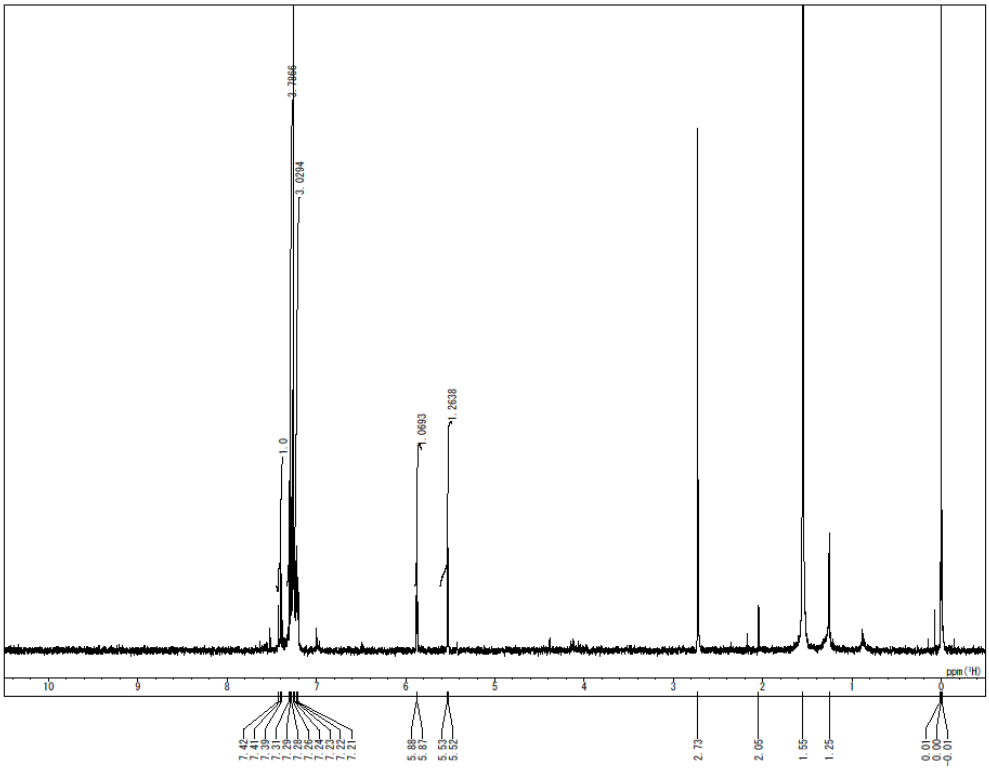
^{1}H NMR of **2m**




```
DFILE   Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM   01/Jun/2022 03:17:25
COMNT

OBNUC                  ¹³C
OFR                100.61 MHz
OBSET                0.0 kHz
OBFIN             9999.159 Hz
PW1                 10.0 µs
PW2                 10.0 µs
PW3                 20.0 µs
PI1                  2.0 ms
PI2                0.0035 ms
PI3                  0.0 ms
LOOP1                  0
POINT              32768
SCANS               1024
DUMMY                  2
FREQU             29761.9 Hz
ACQTM              1.101 s
PD                   2.0 s
RGAIN                203
BF                  0.4541 Hz
EXMOD            ZGPG30
IRNUC              OFF
IFR                  0.0 MHz
IRSET                0.0 kHz
IRFIN                0.0 Hz
IRPW                 0 µs
IRATN                  0
CSPED               20.0 Hz
CTEMP               25.91 °C
PRNT_DATE   2022/Jun/21 22:54:03
```

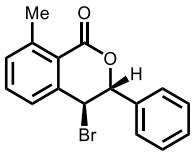


^{13}C NMR of **2m**

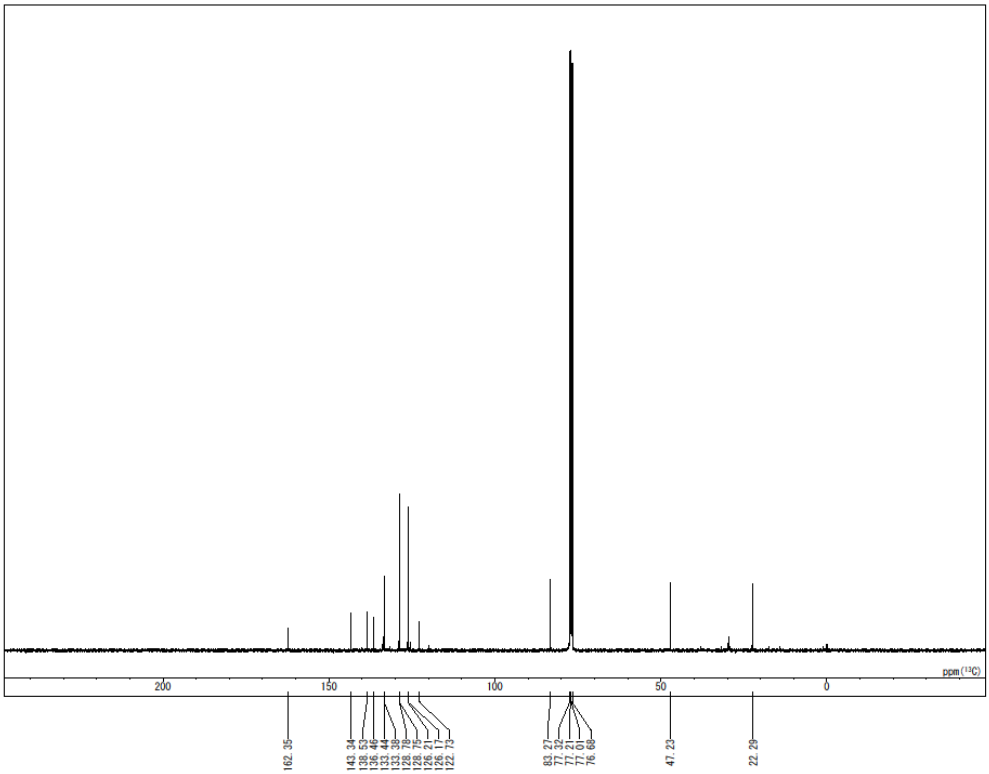


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 17/Jun/2022 23:50:43
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	181
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.81 ℃
PRNT_DATE	2022/Jun/18 00:19:37

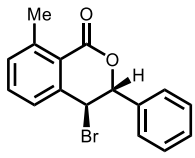


^{1}H NMR of **3m**

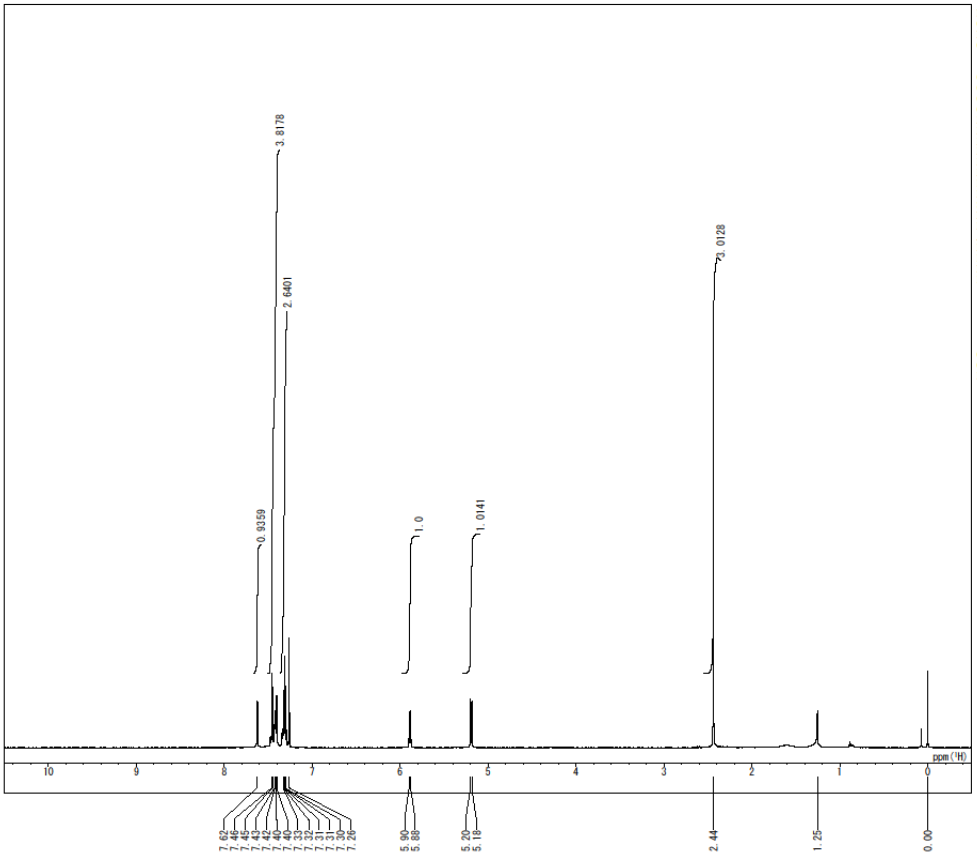


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 18/Jun/2022 05:58:31
COMNT

OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
P11	2.0 ms
P12	0.0035 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	6656
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	27.04 ℃
PRNT_DATE	2022/Jun/18 09:07:36

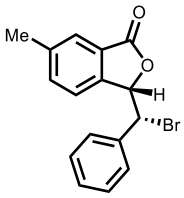


^{13}C NMR of **3m**

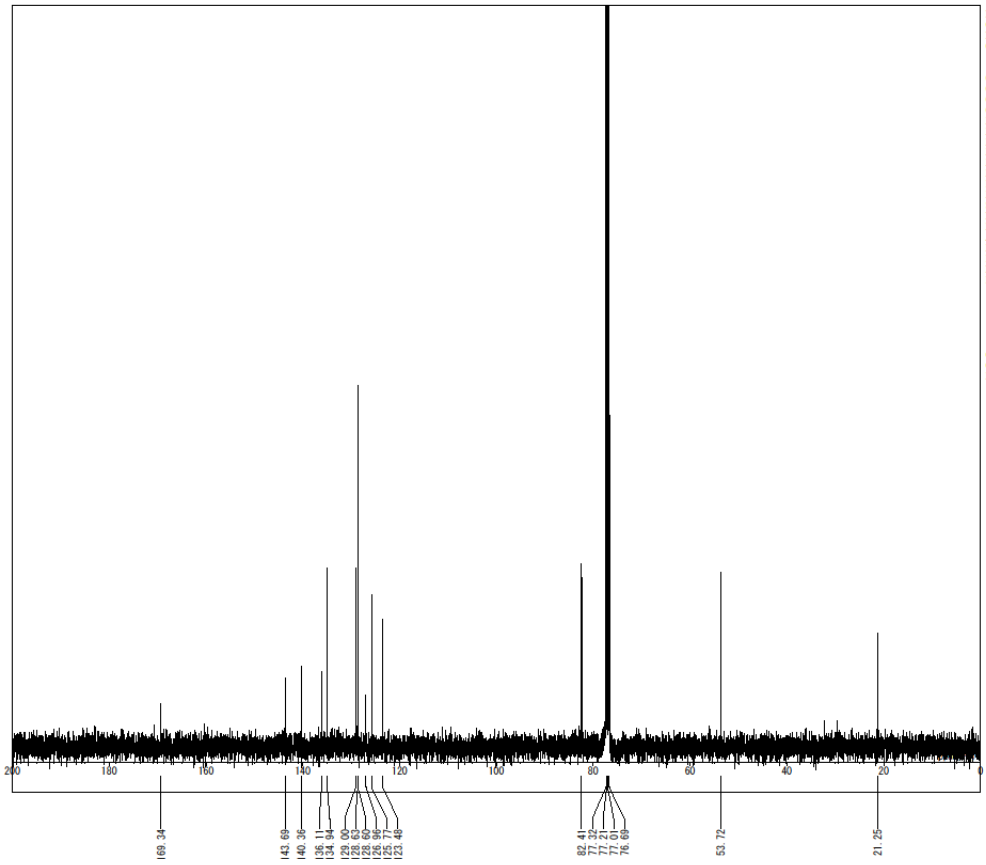


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 01/Jun/2022 01:12:21
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 μs
PW2	15.0 μs
PW3	30.0 μs
PI1	1.0 ms
PI2	0.0 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	114
BF	0.25 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 μs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.21 ℃
PRNT_DATE	2022/Jun/01 15:36:28

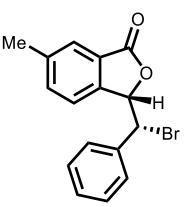


^{1}H NMR of **2n**

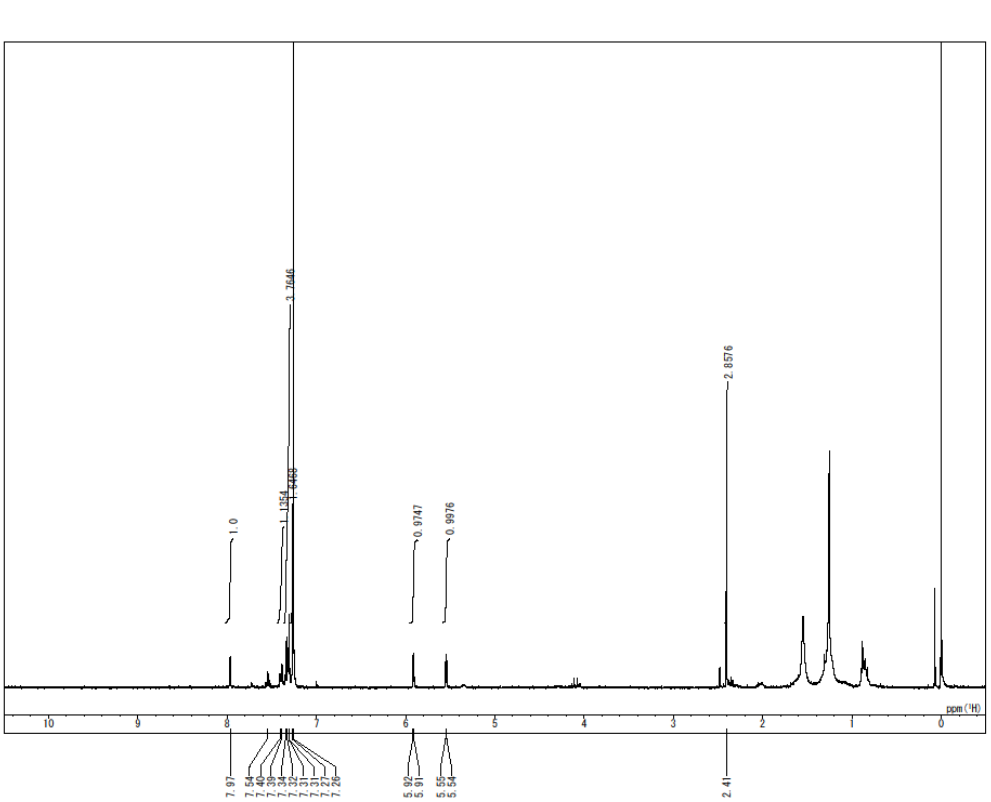


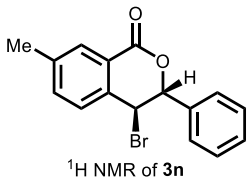
DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 01/Jun/2022 01:27:36
COMNT

OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 μs
PW2	10.0 μs
PW3	20.0 μs
PI1	2.0 ms
PI2	0.0035 ms
PI3	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRRPW	0 μs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.71 ℃
PRNT_DATE	2022/Jun/01 15:40:59

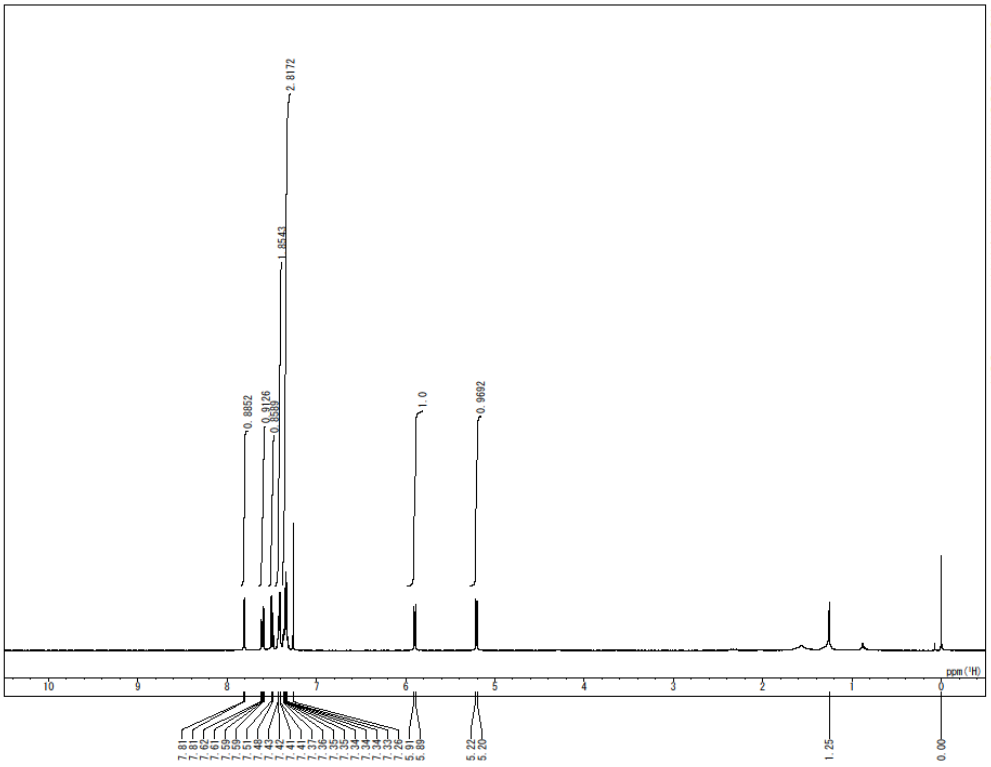


^{13}C NMR of **2n**


OBNUC 1H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 161
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 24.91 °C
PRNT_DATE 2022/Jun/03 11:22:36
1.0
1.1354
1.1440
3.7646
0.9747
0.9976
2.8576
ppm (1H)
7.97
7.54
7.49
7.39
7.34
7.33
7.31
7.31
7.27
7.20
5.92
5.91
5.55
5.54
2.41

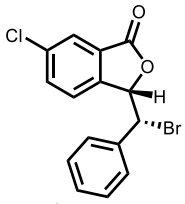

O
Me
O
H
Br

^{1}H NMR of **3n**

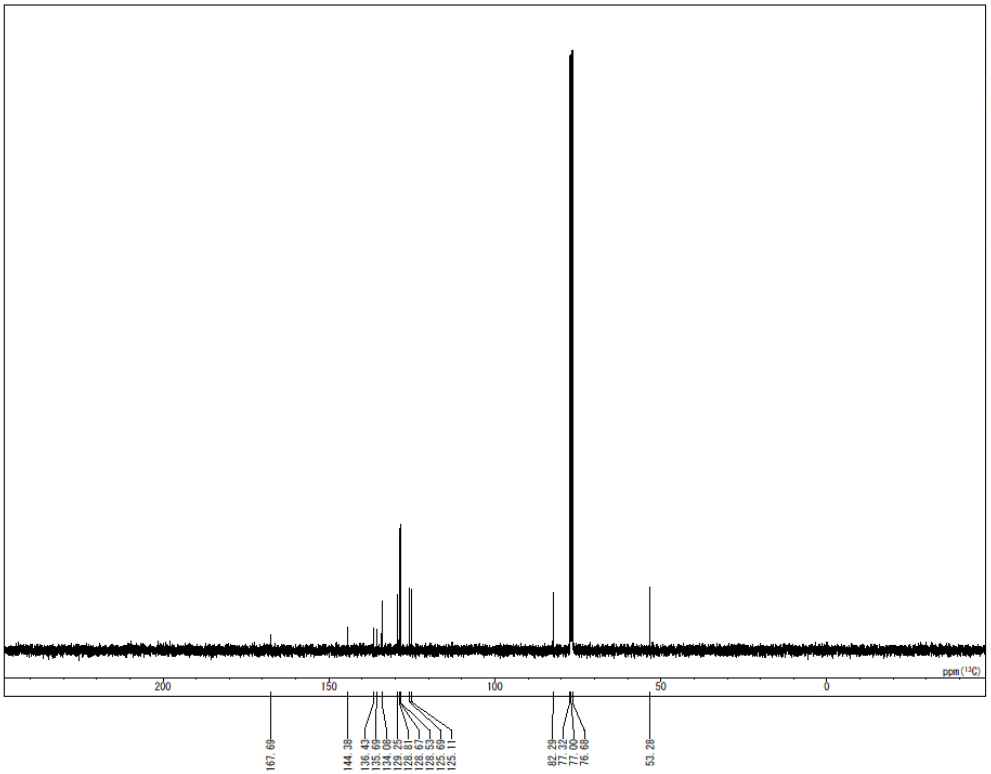


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 01/Jun/2022 01:46:35
COMNT

OBNUC ¹H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 128
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 25.11 ℃
PRNT_DATE 2022/Jun/11 22:56:22

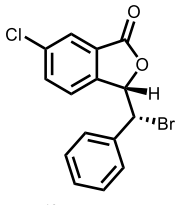


^{1}H NMR of **2o**

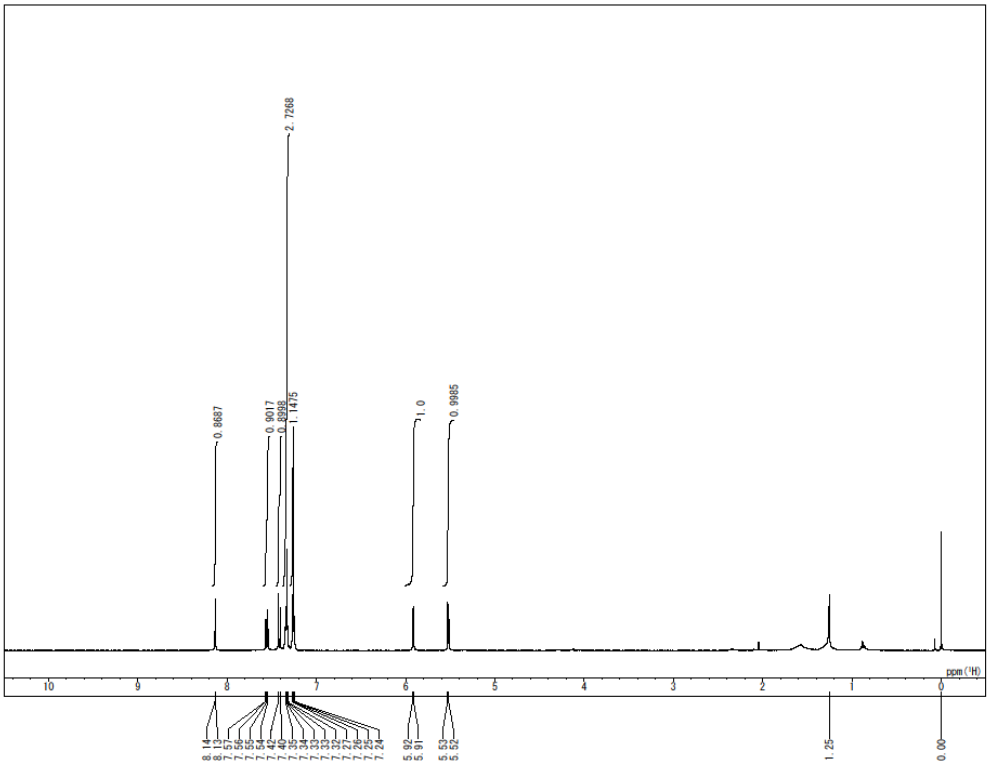


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 01/Jun/2022 02:01:43
COMNT

OBNUC ¹³C
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 9999.159 Hz
PW1 10.0 µs
PW2 10.0 µs
PW3 20.0 µs
PI1 2.0 ms
PI2 0.0035 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 256
DUMMY 2
FREQU 29761.9 Hz
ACQTM 1.101 s
PD 2.0 s
RGAIN 203
BF 0.25 Hz
EXMOD ZGPG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRRPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 25.81 ℃
PRNT_DATE 2022/Jun/11 22:58:37

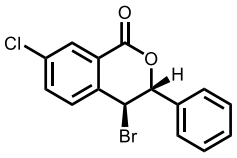


^{13}C NMR of **2o**

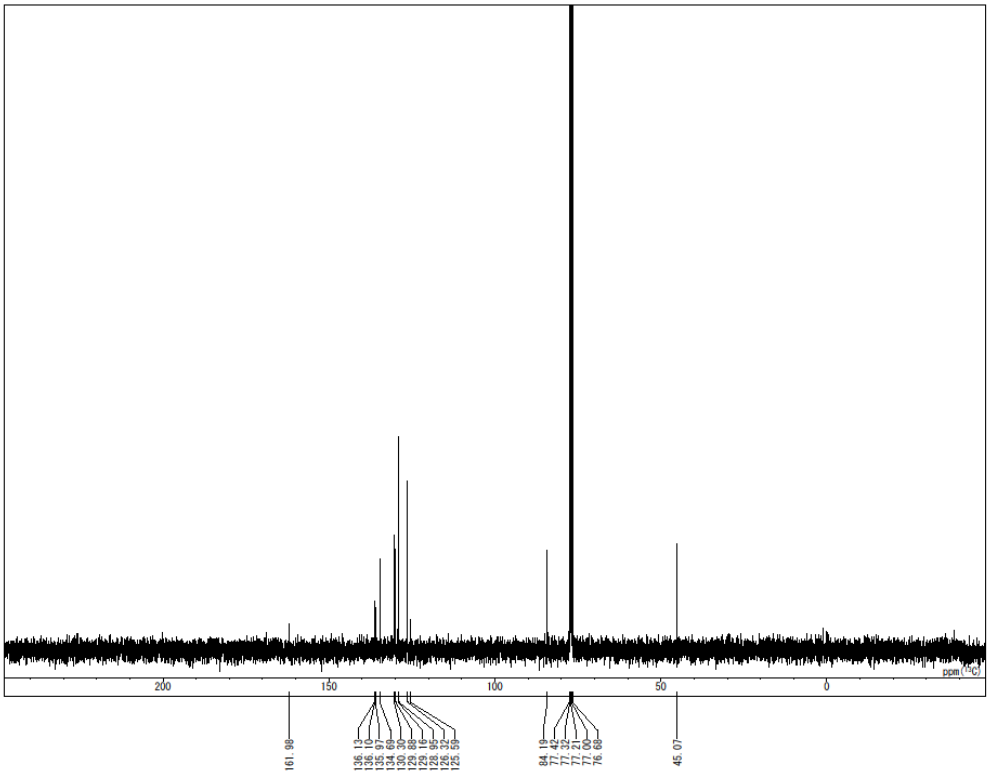


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 11/Jun/2022 19:23:05
COMNT

OBNUC ¹H
OFR 400.13 MHz
OBSET 0.0 kHz
OBFIN 10021.89 Hz
PW1 15.0 µs
PW2 15.0 µs
PW3 30.0 µs
PI1 1.0 ms
PI2 0.0 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 4
DUMMY 2
FREQU 8012.82 Hz
ACQTM 4.0894 s
PD 1.0 s
RGAIN 144
BF 0.25 Hz
EXMOD ZG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRBPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 25.21 ℃
PRNT_DATE 2022/Jun/11 20:05:17

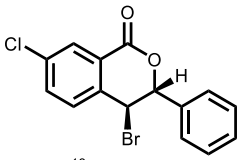


^{1}H NMR of **3o**

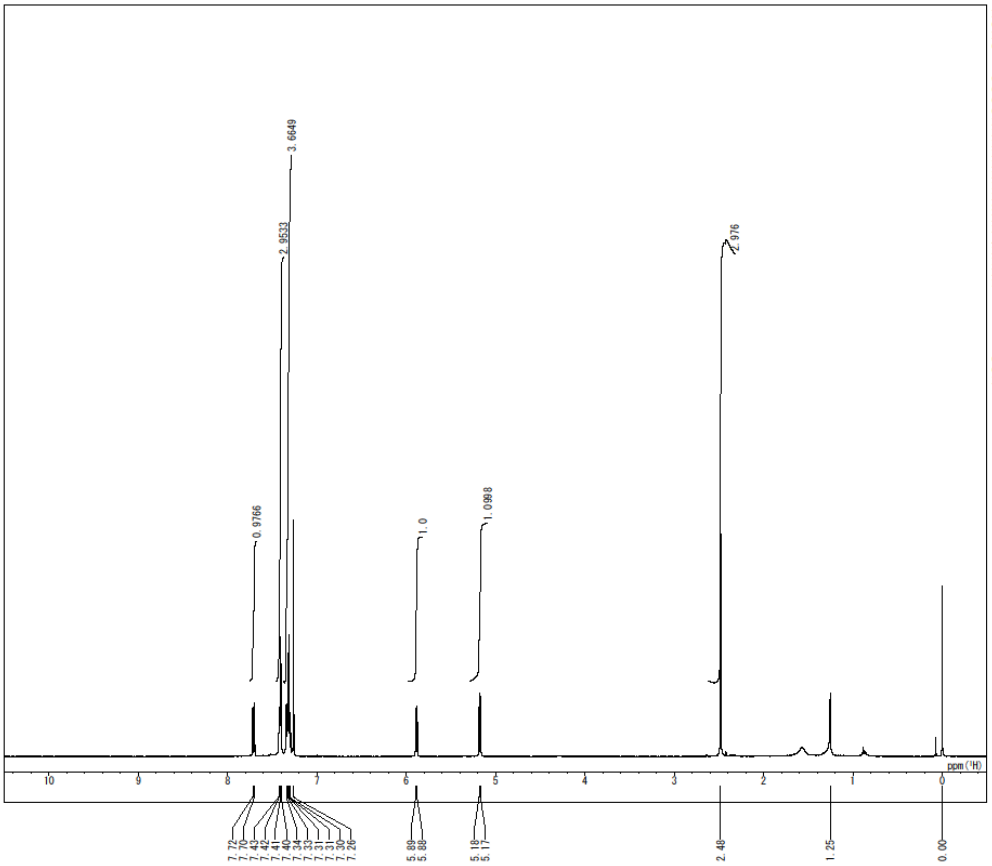


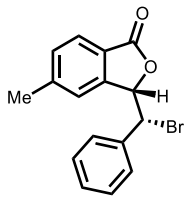
DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 11/Jun/2022 19:38:16
COMNT

OBNUC ¹³C
OFR 100.61 MHz
OBSET 0.0 kHz
OBFIN 9999.159 Hz
PW1 10.0 µs
PW2 10.0 µs
PW3 20.0 µs
PI1 2.0 ms
PI2 0.0035 ms
PI3 0.0 ms
LOOP1 0
POINT 32768
SCANS 256
DUMMY 2
FREQU 29761.9 Hz
ACQTM 1.101 s
PD 2.0 s
RGAIN 203
BF 0.25 Hz
EXMOD ZGPG30
IRNUC OFF
IFR 0.0 MHz
IRSET 0.0 kHz
IRFIN 0.0 Hz
IRBPW 0 µs
IRATN 0
CSPED 20.0 Hz
CTEMP 26.01 ℃
PRNT_DATE 2022/Jun/11 20:19:13

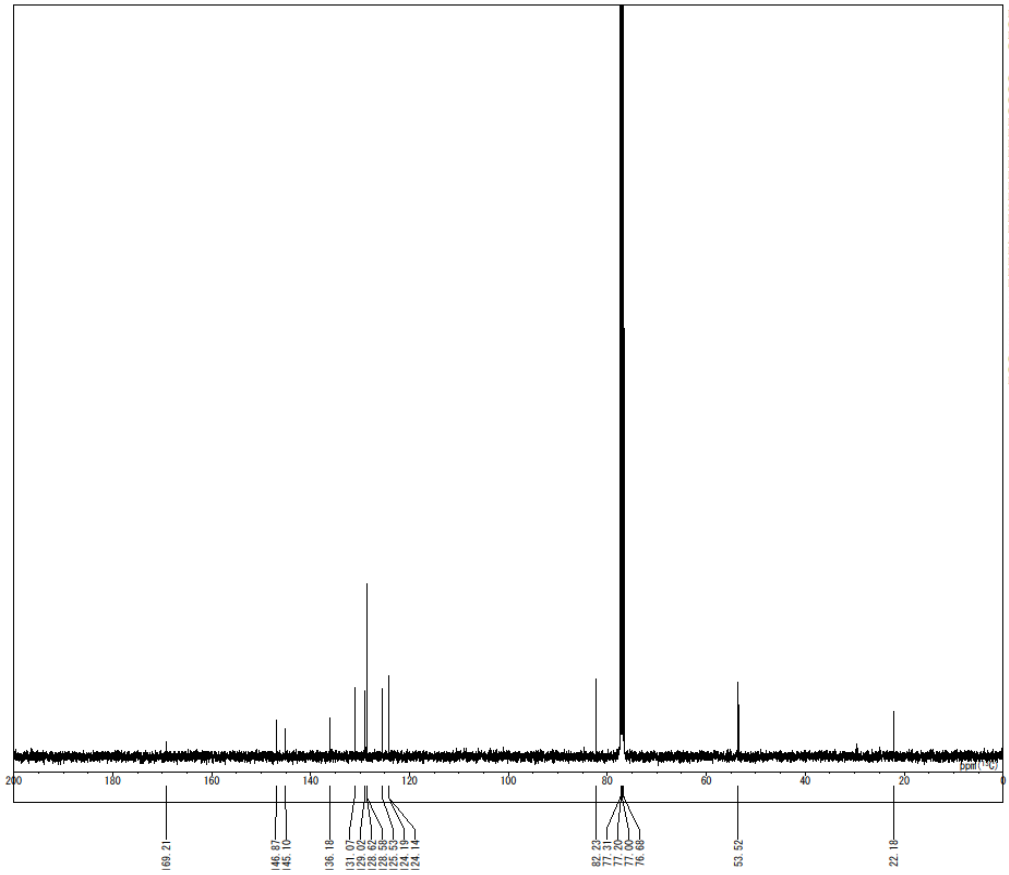


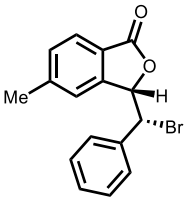
^{13}C NMR of **3o**



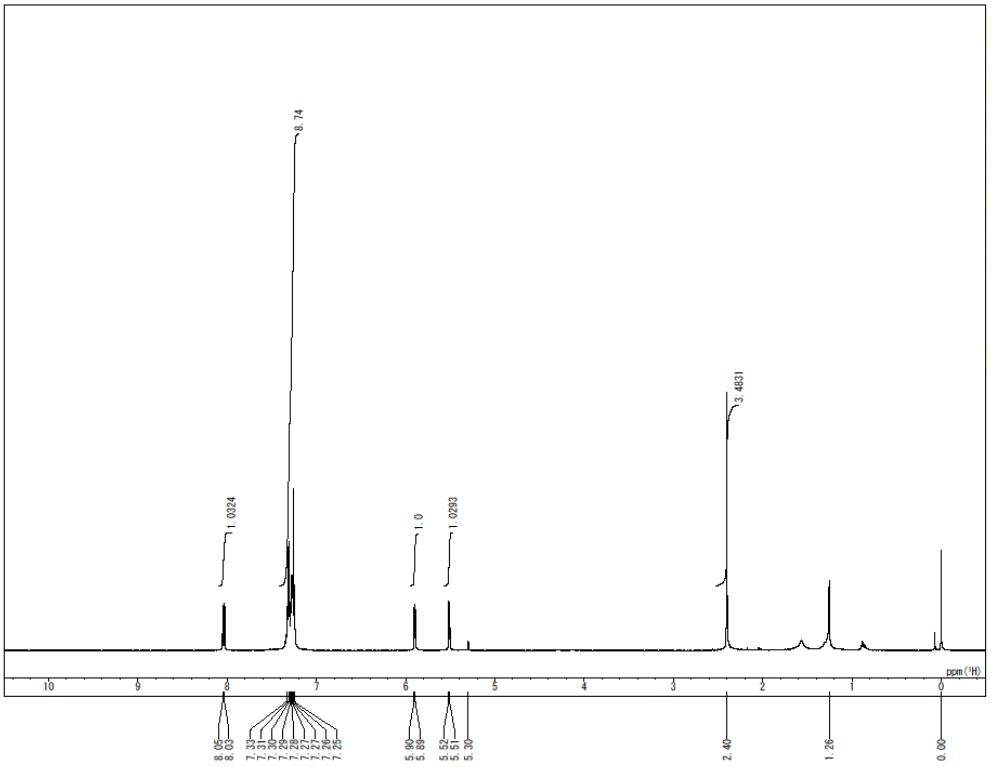


^{1}H NMR of **2p**



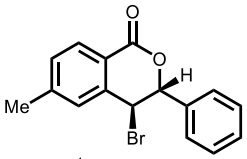


^{13}C NMR of **2p**

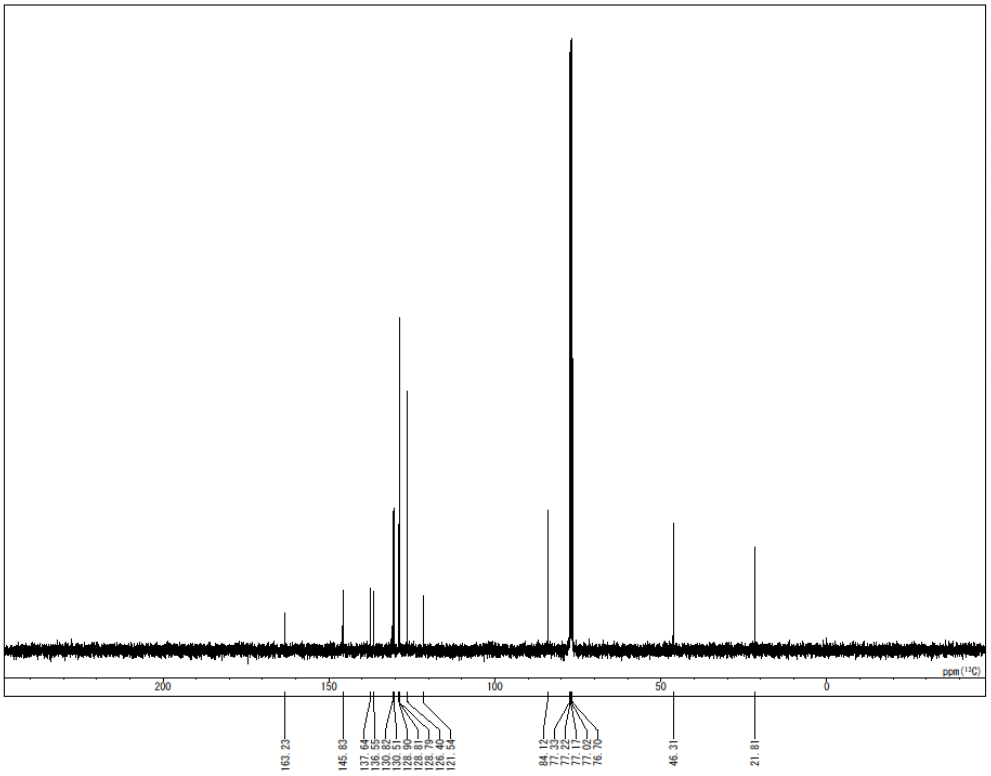


DFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験データ
ORGFILE Y:¥INDIVIDUAL¥菅野¥実験関連¥実験デー
DATIM 11/Jun/2022 21:42:47
COMNT

OBNUC	¹H
OFR	400.13 MHz
OBSET	0.0 kHz
OBFIN	10021.89 Hz
PW1	15.0 µs
PW2	15.0 µs
PW3	30.0 µs
P11	1.0 ms
P12	0.0 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	4
DUMMY	2
FREQU	8012.82 Hz
ACQTM	4.0894 s
PD	1.0 s
RGAIN	144
BF	0.1223 Hz
EXMOD	ZG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	25.51 °C
PRNT_DATE	2022/Jun/21 22:37:47

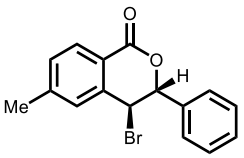


^{1}H NMR of **3p**



DFILE X:¥062ORG¥DATA¥ORG¥NMR¥MS4-ME6-ENDO-C-
ORGFILE X:¥062ORG¥DATA¥ORG¥NMR¥MS4-ME6-ENDO-
DATIM 18/Jun/2022 09:43:14
COMNT

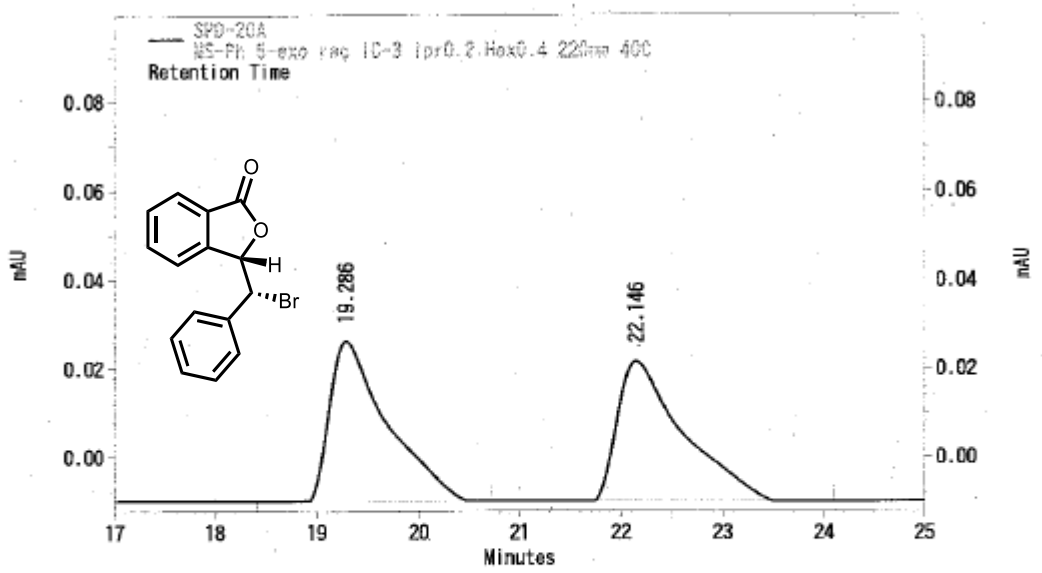
OBNUC	¹³C
OFR	100.61 MHz
OBSET	0.0 kHz
OBFIN	9999.159 Hz
PW1	10.0 µs
PW2	10.0 µs
PW3	20.0 µs
P11	2.0 ms
P12	0.0035 ms
P13	0.0 ms
LOOP1	0
POINT	32768
SCANS	256
DUMMY	2
FREQU	29761.9 Hz
ACQTM	1.101 s
PD	2.0 s
RGAIN	203
BF	0.25 Hz
EXMOD	ZGPG30
IRNUC	OFF
IFR	0.0 MHz
IRSET	0.0 kHz
IRFIN	0.0 Hz
IRPW	0 µs
IRATN	0
CSPED	20.0 Hz
CTEMP	26.91 °C
PRNT_DATE	2022/Jun/18 10:09:29



^{13}C NMR of **3p**

2.Copies of HPLC charts

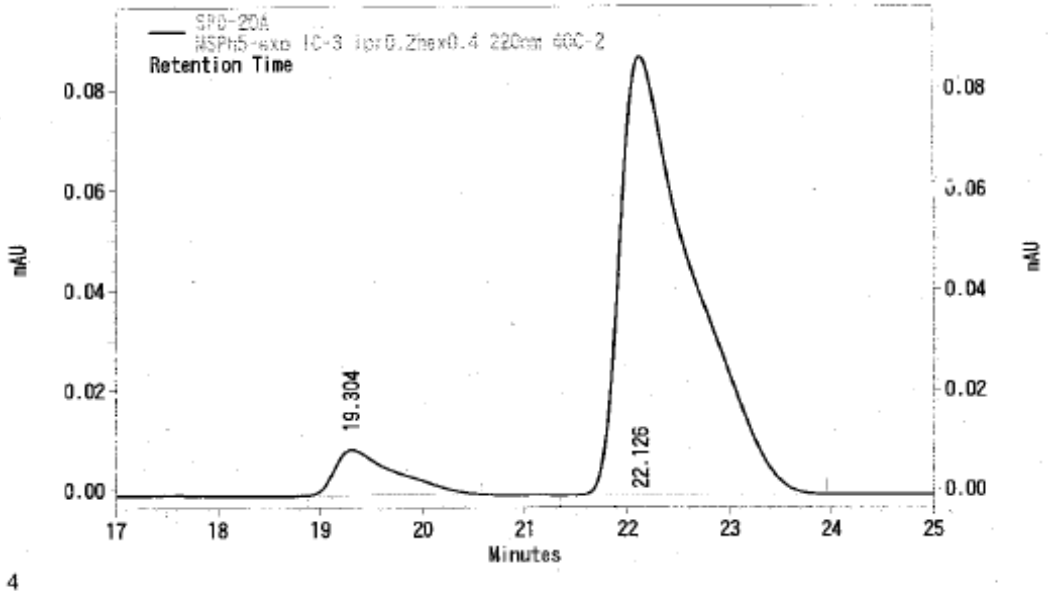
(±)-**2a**



4

	Name	Retention Time	Area	Area Percent	Height
1		19.286	1404296	50.062	36027
2		22.146	1400803	49.938	31468
Totals			2805099	100.000	67495

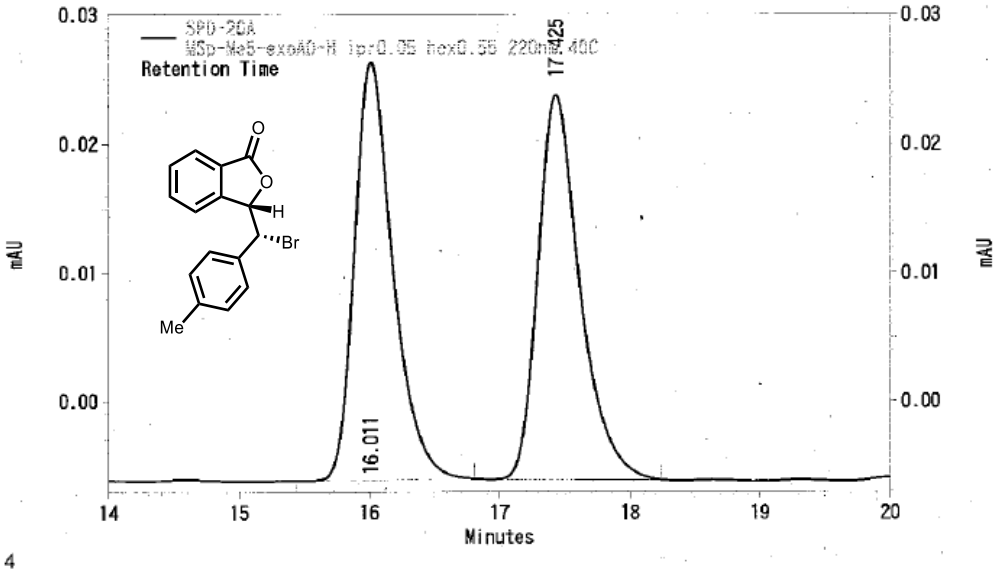
(3*R*,8*S*)-2a in Table 2, entry 10 (92:8 er)



4

	Name	Retention Time	Area	Area Percent	Height
1		19.304	376978	8.050	9098
2		22.126	4305967	91.950	87537
Totals			4682945	100.000	96635

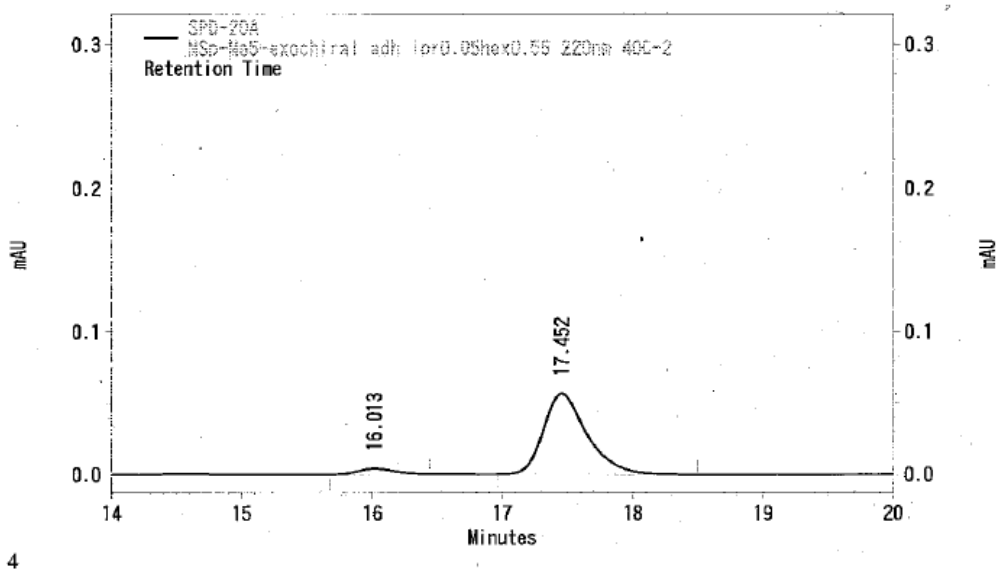
(±)-**2b**



4

Name	Retention Time	Area	Area Percent	Height
1	16.011	664650	49.875	32488
2	17.425	667984	50.125	29887
Totals		1332634	100.000	62375

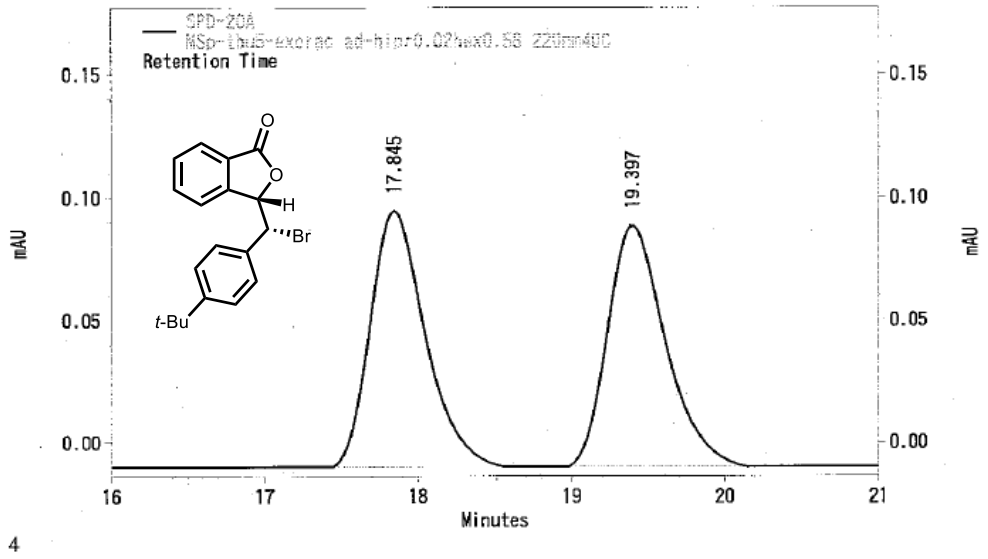
(3*R*,8*S*)-2b in Table 3, entry 1 (94:6 er)



4

Name	Retention Time	Area	Area Percent	Height
1	16.013	79162	5.736	4082
2	17.452	1300979	94.264	56566
Totals		1380141	100.000	60648

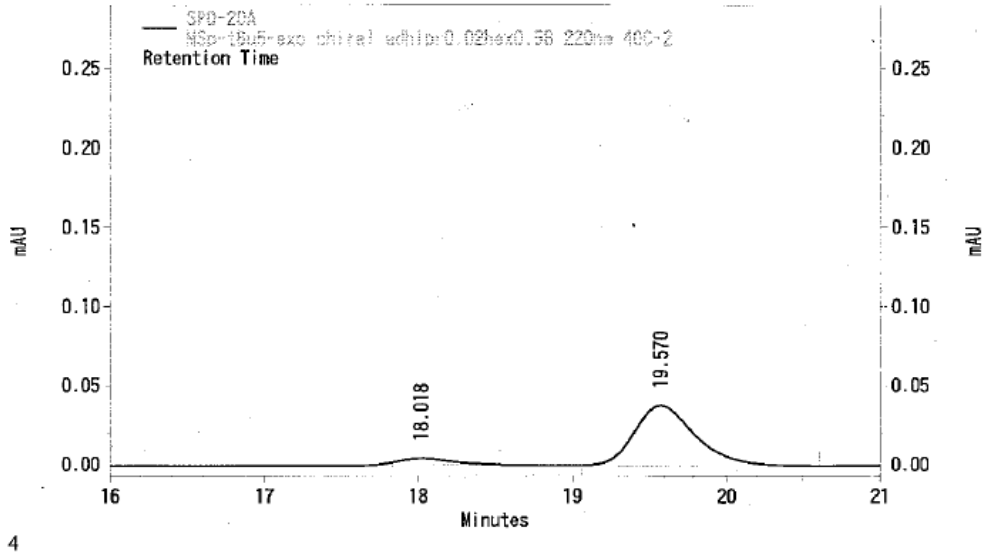
(±)-**2c**



4

	Name	Retention Time	Area	Area Percent	Height
1		17.845	2584956	49.948	104385
2		19.397	2590310	50.052	98285
Totals			5175266	100.000	202670

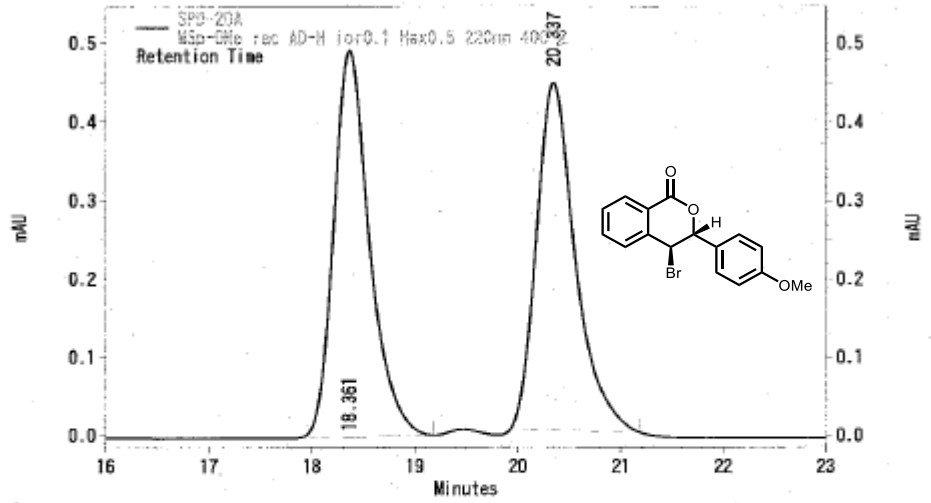
(3*R*,8*S*)-2c in Table 2, entry 2 (91:9 er)



4

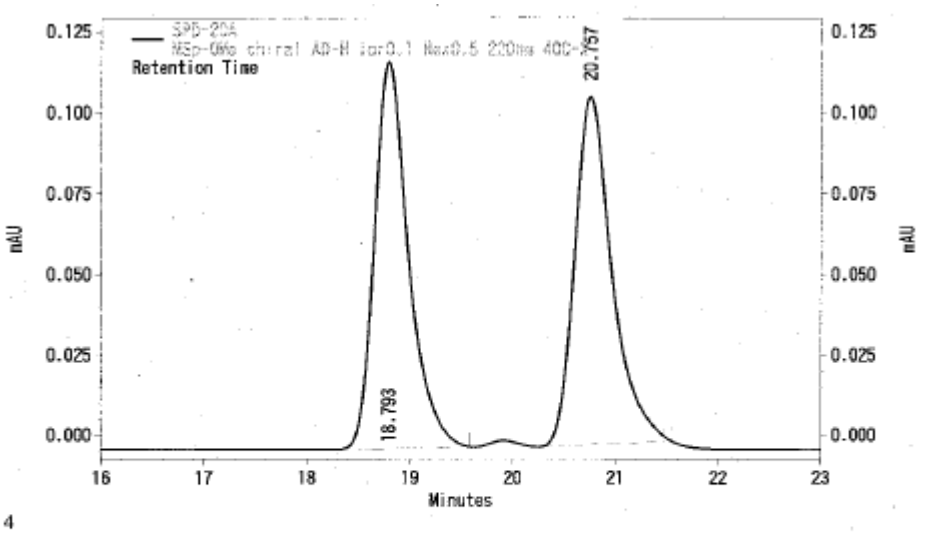
	Name	Retention Time	Area	Area Percent	Height
1		18.018	106549	9.314	4356
2		19.570	1037464	90.686	37965
Totals			1144013	100.000	42321

(±)-**2d**



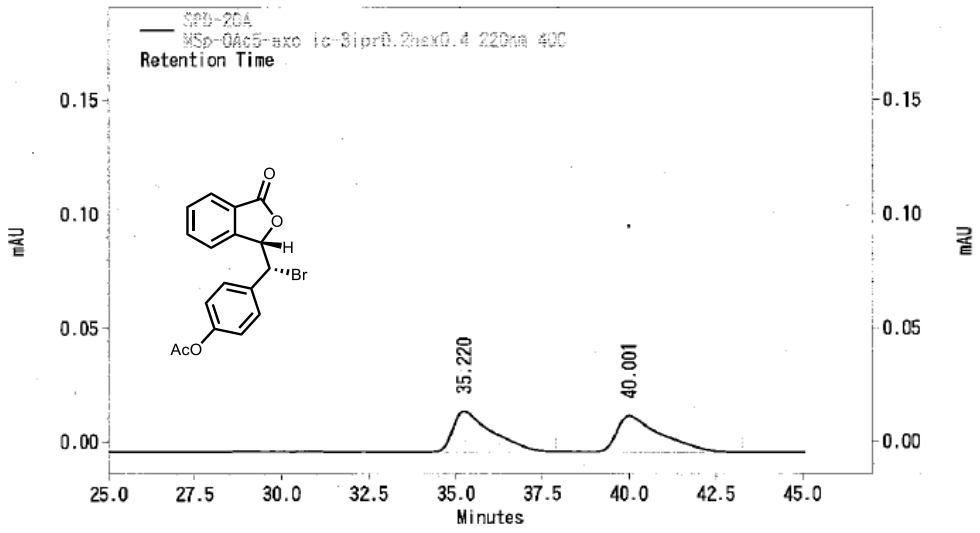
Name	Retention Time	Area	Area Percent	Height
1	18.361	11869990	50.599	492565
2	20.337	11588846	49.401	442718
Totals		23458836	100.000	935283

(3*SR*,8*RS*)-2d in Table 3, entry 3 (50:50 er)



Name	Retention Time	Area	Area Percent	Height
1	18.793	2761135	50.266	119724
2	20.757	2731954	49.734	107786
Totals		5493089	100.000	227510

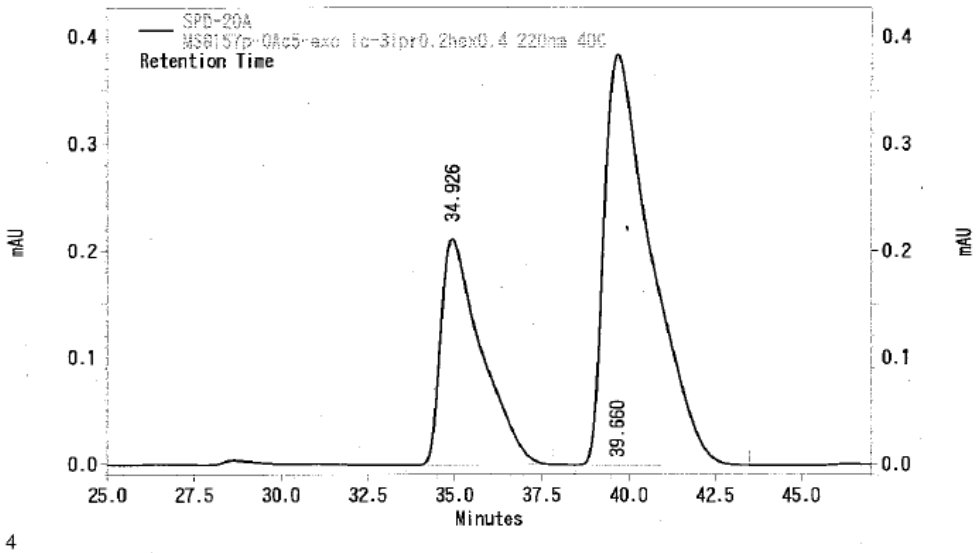
(±)-**2e**



4

Name	Retention Time	Area	Area Percent	Height
1	35.220	1377200	49.799	17834
2	40.001	1388336	50.201	15851
Totals		2765536	100.000	33685

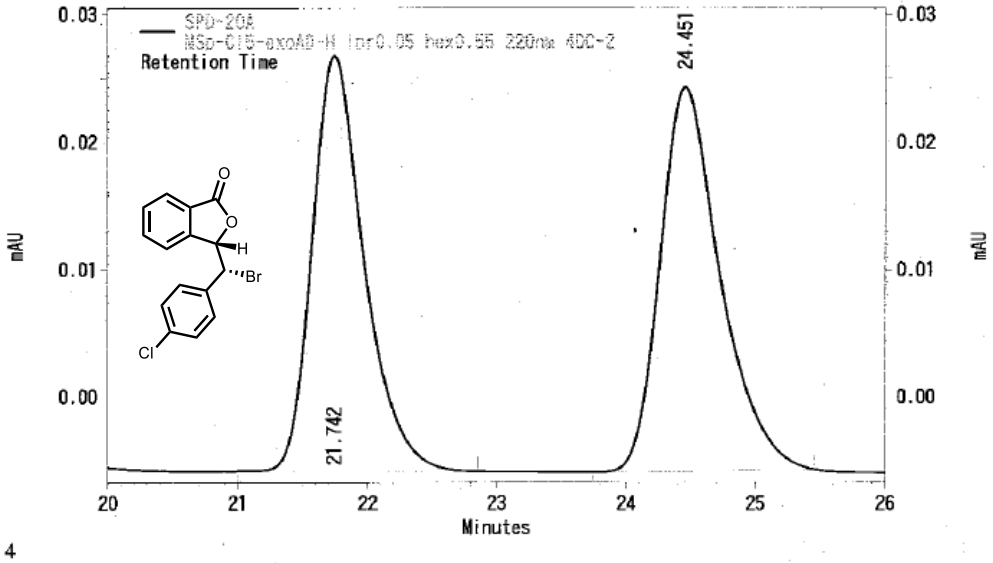
(3*R*,8*S*)-2e in Table 3, entry 4 (68:32 er)



4

Name	Retention Time	Area	Area Percent	Height
1	34.926	17152286	31.950	212094
2	39.660	36533271	68.050	383896
Totals		53685557	100.000	595990

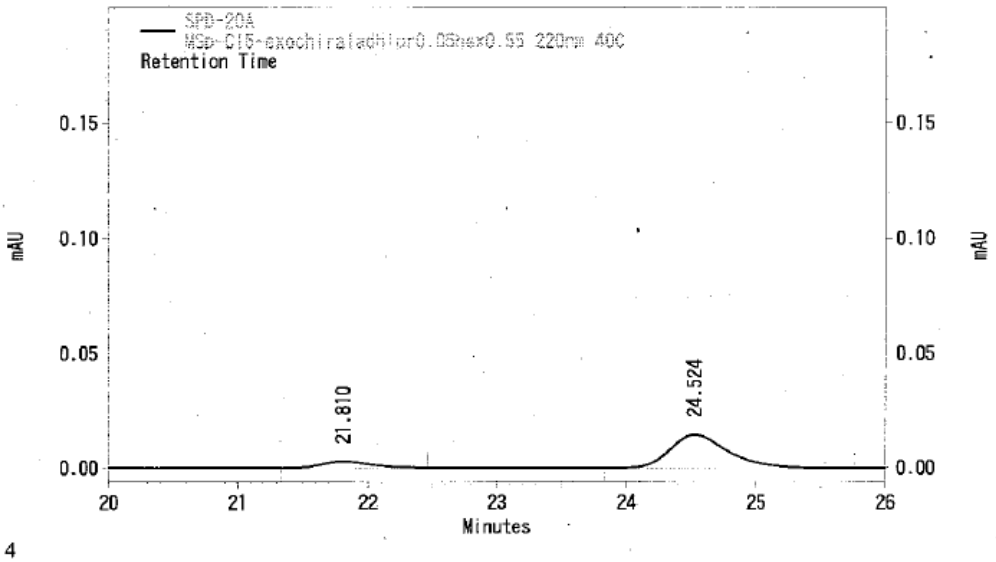
(±)-**2f**



4

	Name	Retention Time	Area	Area Percent	Height
1		21.742	910001	48.213	32651
2		24.451	977471	51.787	30212
Totals			1887472	100.000	62863

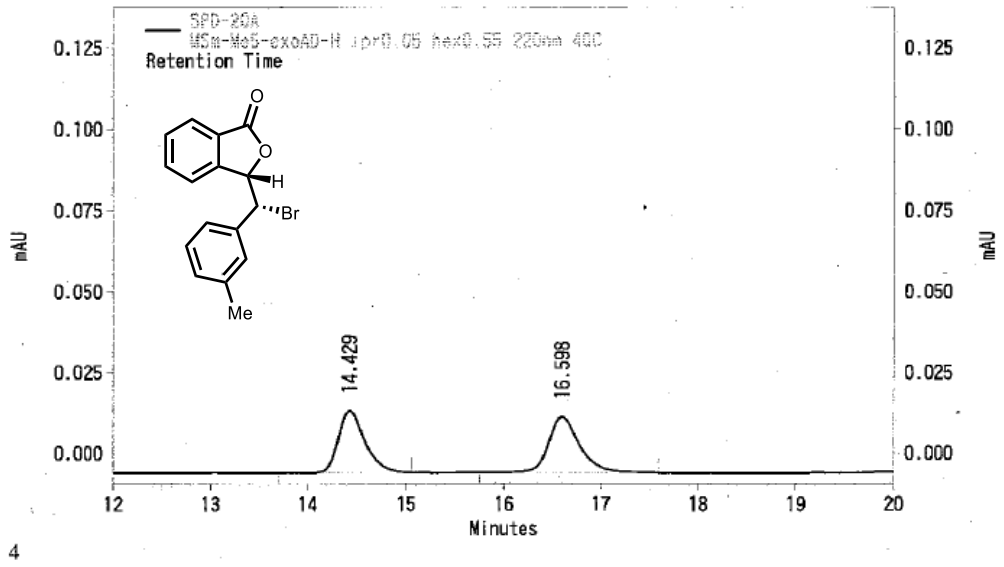
(3*R*,8*S*)-2f in Table 3, entry 5 (86:14 er)



4

	Name	Retention Time	Area	Area Percent	Height
1		21.810	74933	14.168	2872
2		24.524	453945	85.832	14593
Totals			528878	100.000	17465

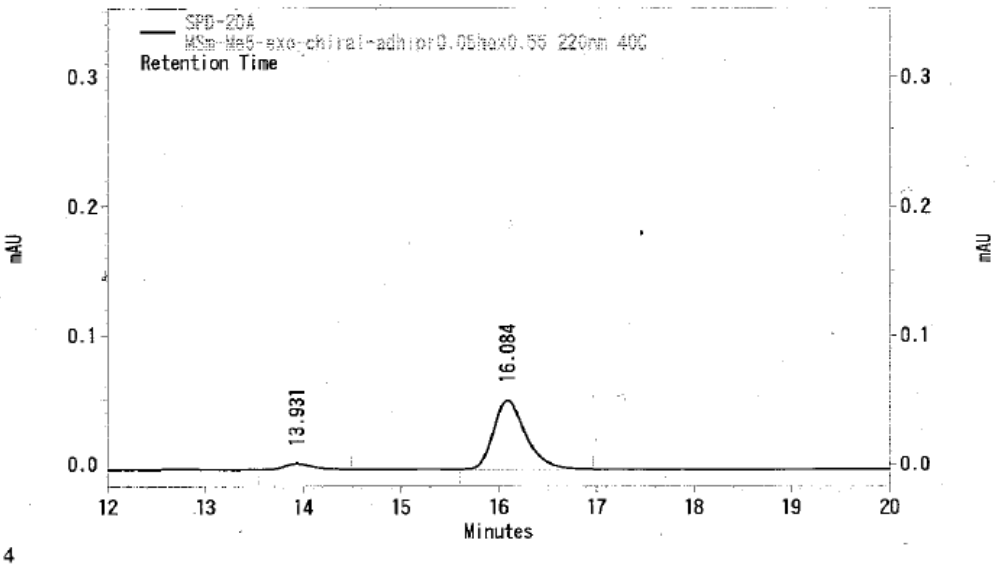
(±)-**2h**



4

Name	Retention Time	Area	Area Percent	Height
1	14.429	357460	48.449	19152
2	16.598	380353	51.551	17208
Totals		737813	100.000	36360

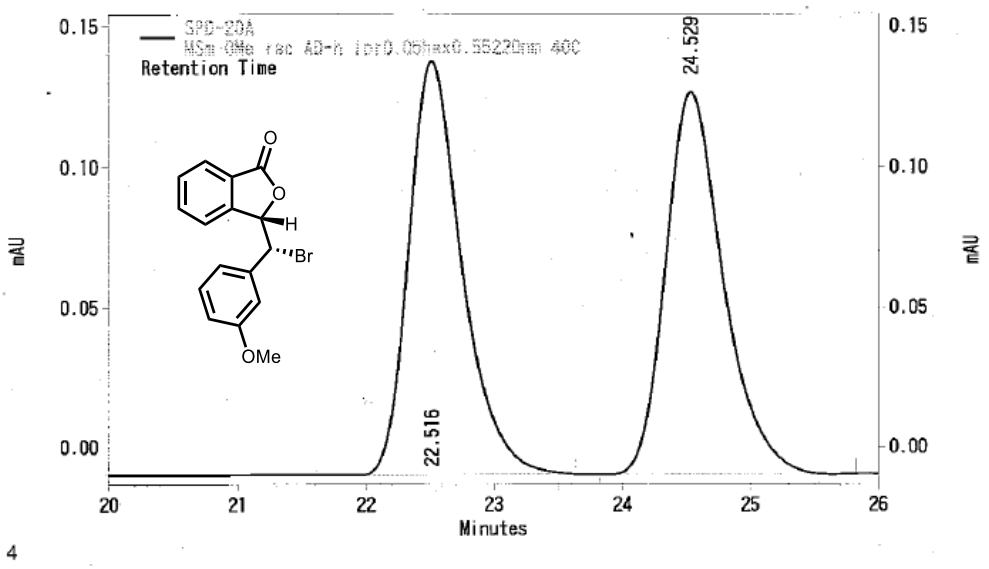
(3*R*,8*S*)-**2h** in Table 3, entry 7 (93:7 er)



4

Name	Retention Time	Area	Area Percent	Height
1	13.931	97786	7.338	4856
2	16.084	1234733	92.662	53815
Totals		1332519	100.000	58671

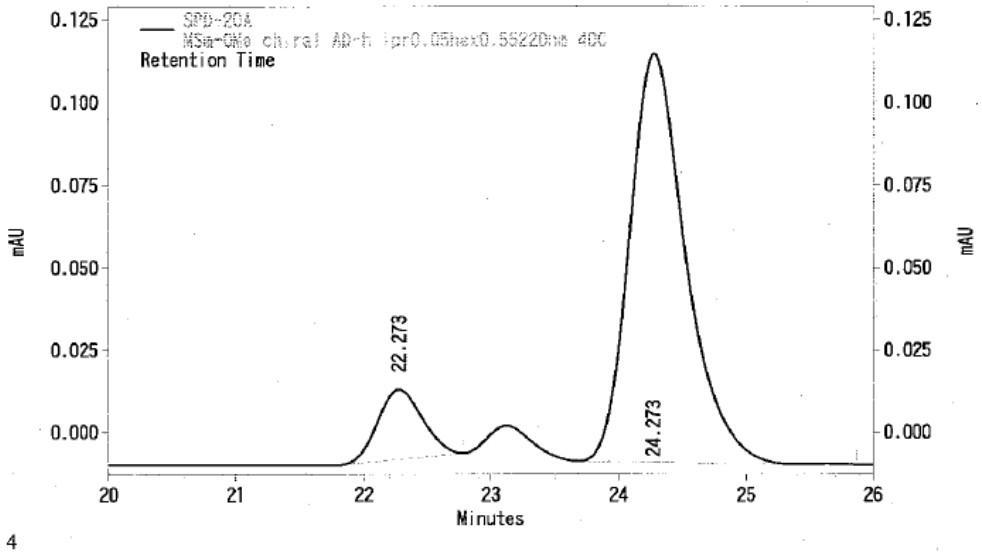
(±)-**2i**



4

Name	Retention Time	Area	Area Percent	Height
1	22.516	4267014	50.011	147336
2	24.529	4265156	49.989	136350
Totals		8532170	100.000	283686

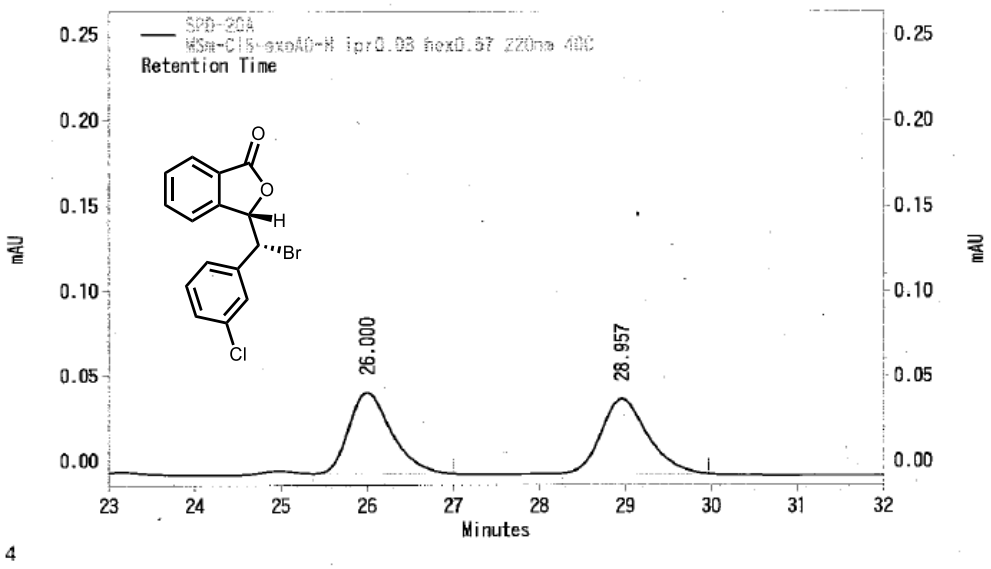
(3*R*,8*S*)-2i in Table 3, entry 8 (88:12 er)



4

Name	Retention Time	Area	Area Percent	Height
1	22.273	516421	12.027	21261
2	24.273	3777587	87.973	123736
Totals		4294008	100.000	144997

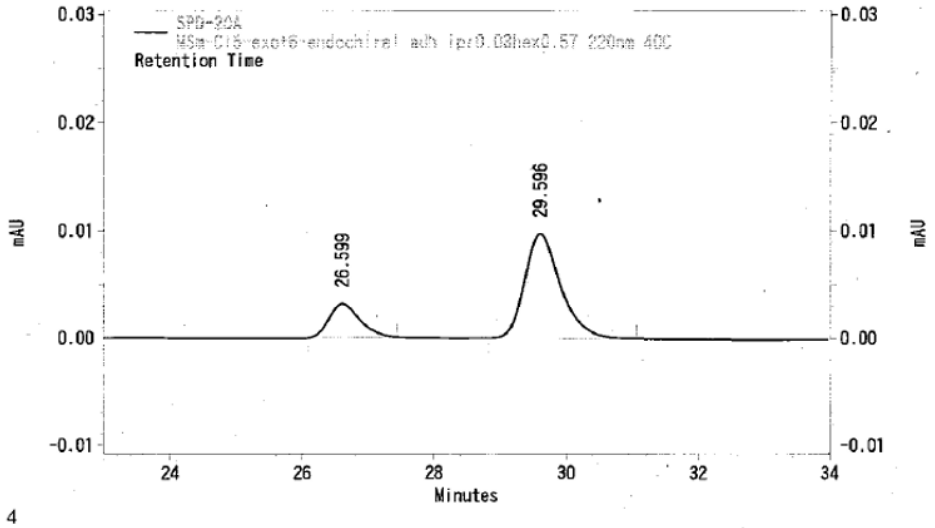
(±)-**2j**



4

Name	Retention Time	Area	Area Percent	Height
1	26.000	1628617	49.631	47907
2	28.957	1652858	50.369	43871
Totals		3281475	100.000	91778

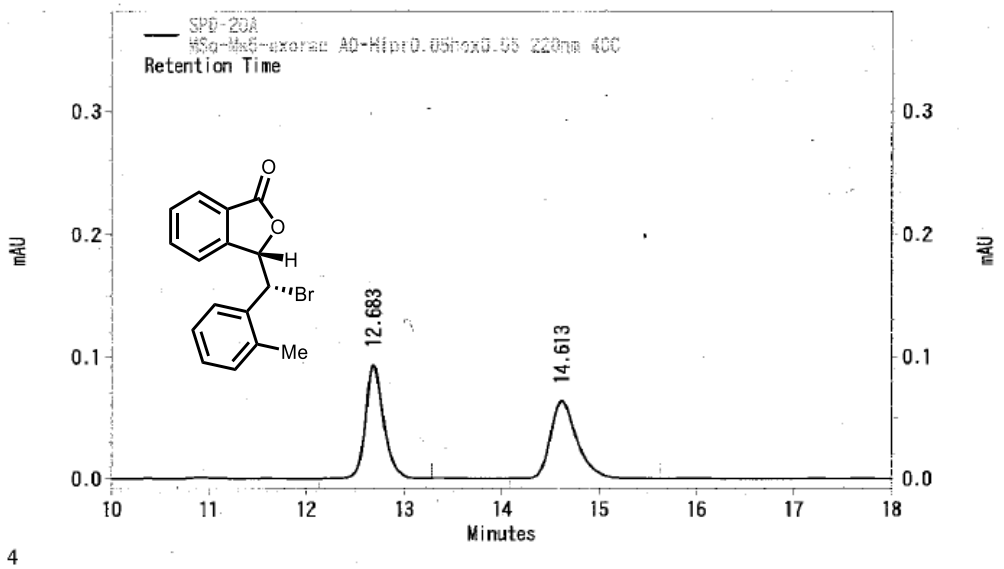
(3*R*,8*S*)-2j in Table 3, entry 9 (78:22 er)



4

Name	Retention Time	Area	Area Percent	Height	
1	26.599	102411	21.942	3148	MM
2	29.596	364331	78.058	9703	MM
Totals		466742	100.000	12851	

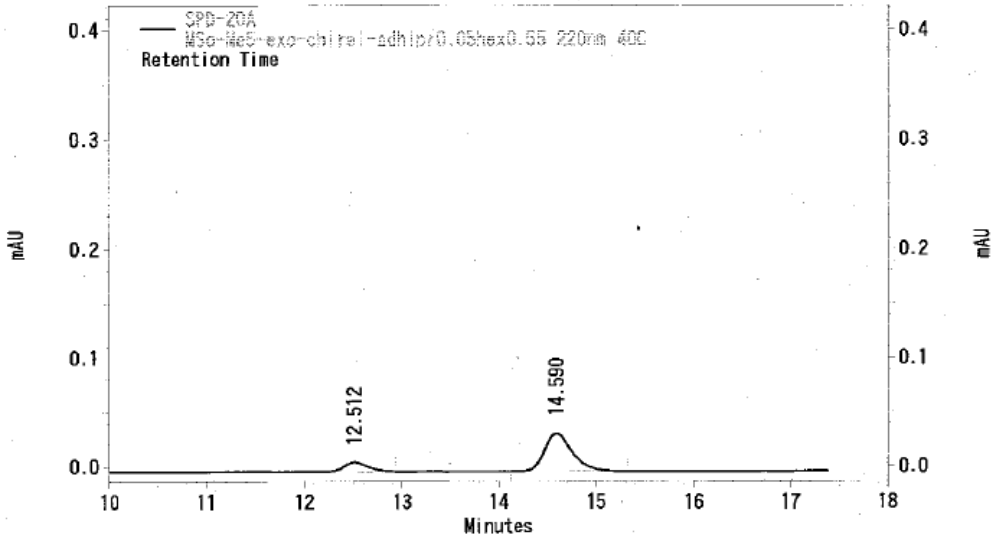
(±)-**2k**



4

	Name	Retention Time	Area	Area Percent	Height
1		12.683	1174011	49.403	93092
2		14.613	1202386	50.597	63417
Totals			2376397	100.000	156509

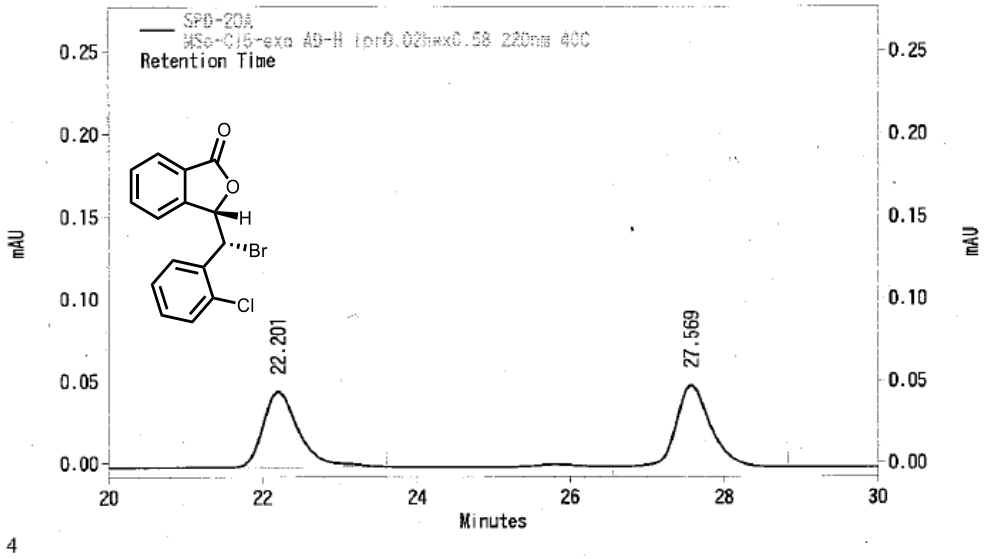
(3*R*,8*S*)-2k in Table 3, entry 10 (83:17 er)



4

	Name	Retention Time	Area	Area Percent	Height
1		12.512	141966	17.300	8388
2		14.590	678626	82.700	34852
Totals			820592	100.000	43240

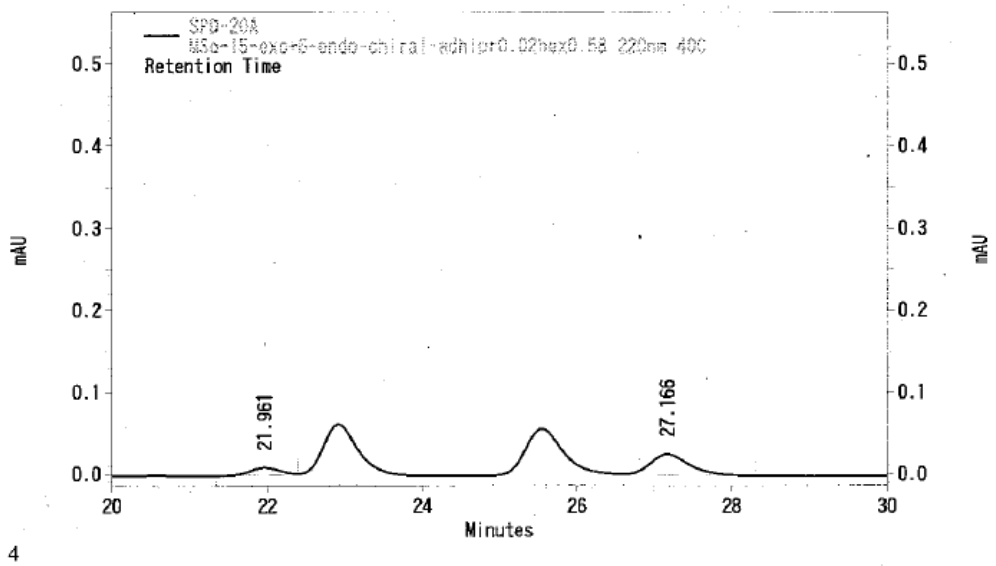
(±)-**2l**



4

Name	Retention Time	Area	Area Percent	Height
1	22.201	1487897	49.540	46204
2	27.569	1515517	50.460	49542
Totals		3003414	100.000	95746

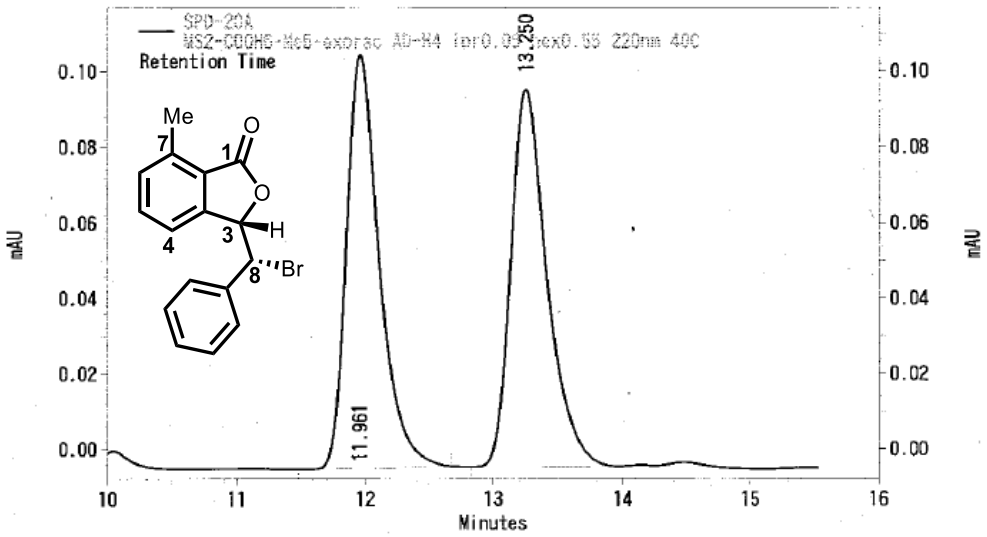
(3*R*,8*S*)-2l in Table 3, entry 11 (80:20 er)



4

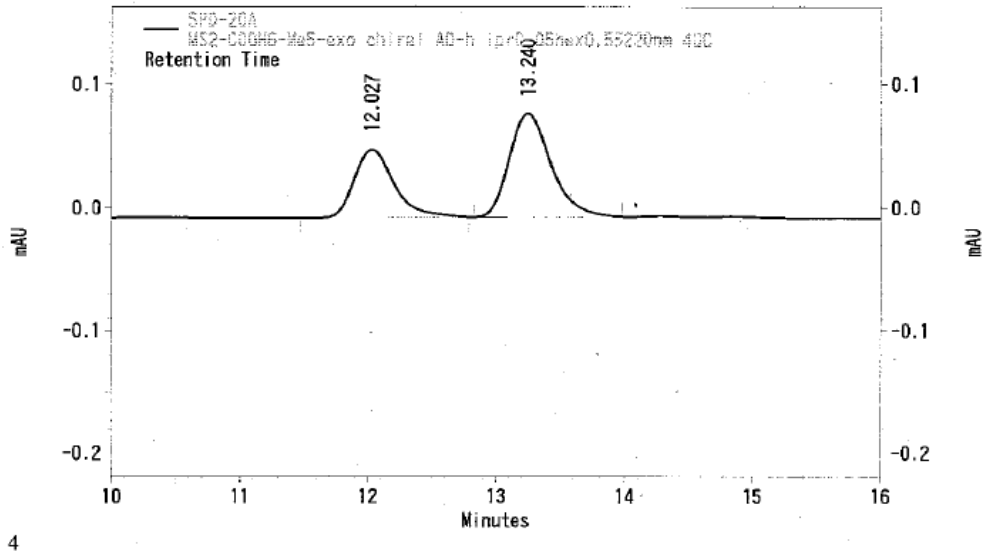
Name	Retention Time	Area	Area Percent	Height
1	21.961	212105	19.985	8399
2	27.166	849207	80.015	24902
Totals		1061312	100.000	33301

(±)-**2m**



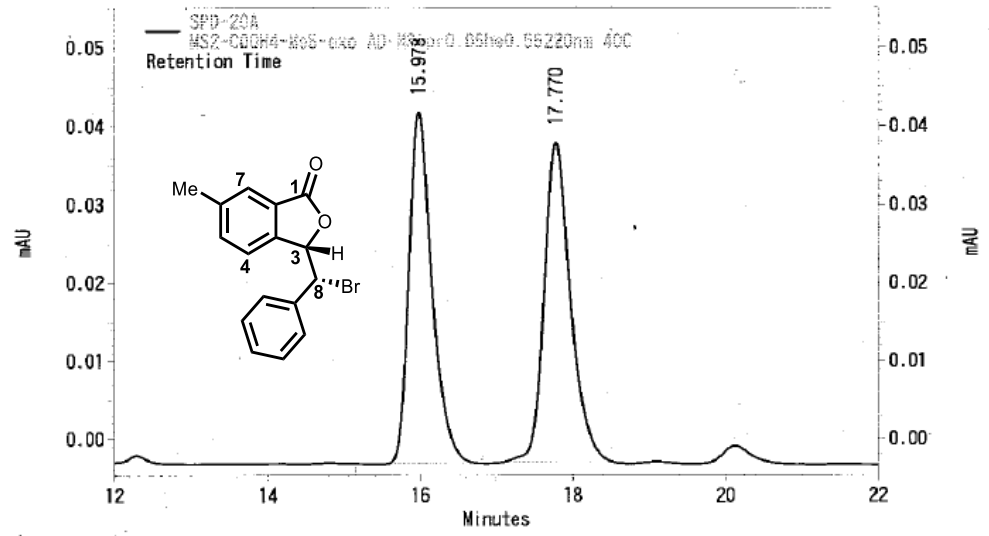
Name	Retention Time	Area	Area Percent	Height
1	11.961	1930358	49.920	109252
2	13.250	1936529	50.080	99796
Totals		3866887	100.000	209048

(3*R*,8*S*)-2m in Table 3, entry 12 (61:39 er)



Name	Retention Time	Area	Area Percent	Height
1	12.027	1178737	38.445	55111
2	13.240	1880780	61.343	83441
3	49.289	6505	0.212	195
Totals		3066022	100.000	138747

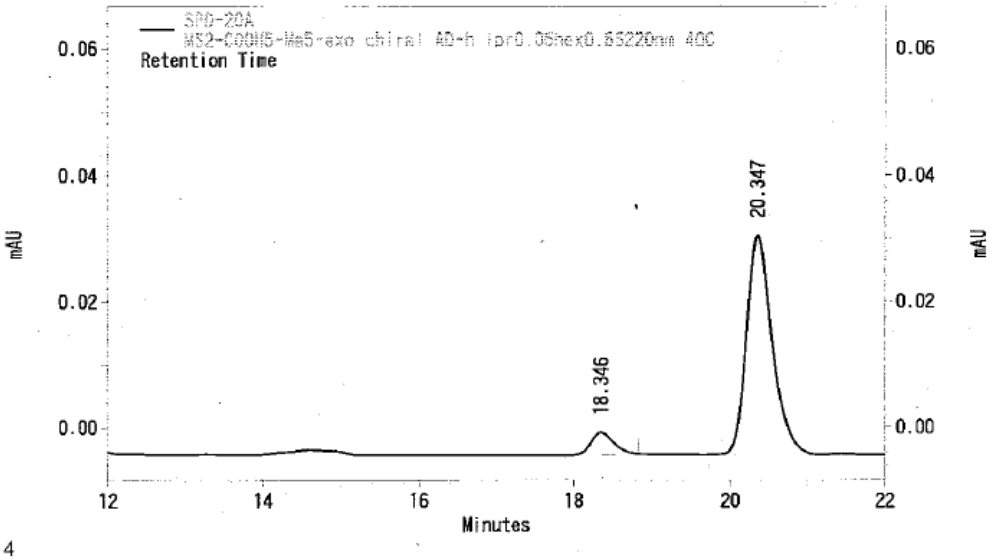
(±)-**2n**



4

Name	Retention Time	Area	Area Percent	Height
1	15.978	955418	49.410	44935
2	17.770	978219	50.590	40913
Totals		1933637	100.000	85848

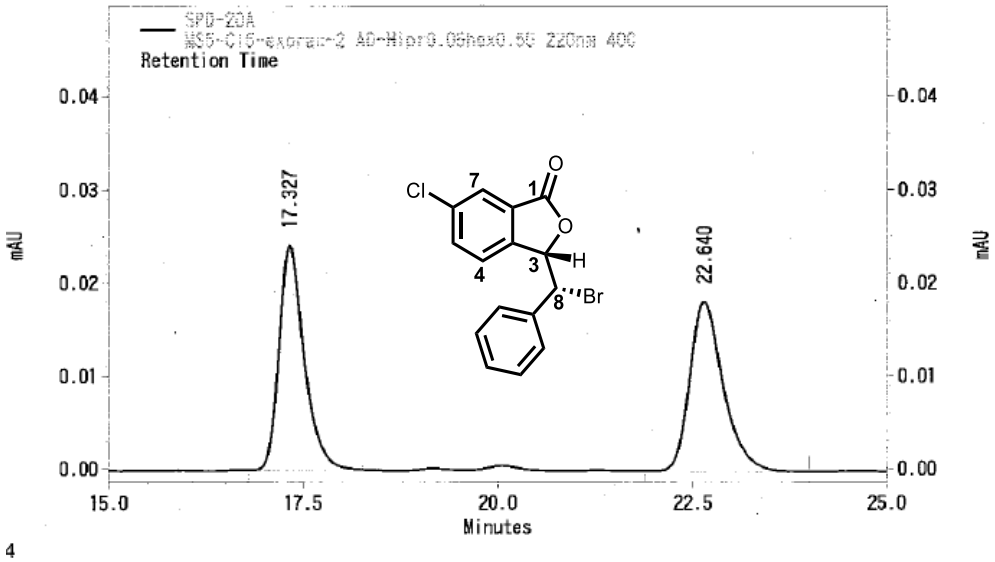
(3*R*,8*S*)-2n in Table 3, entry 13 (92:8 er)



4

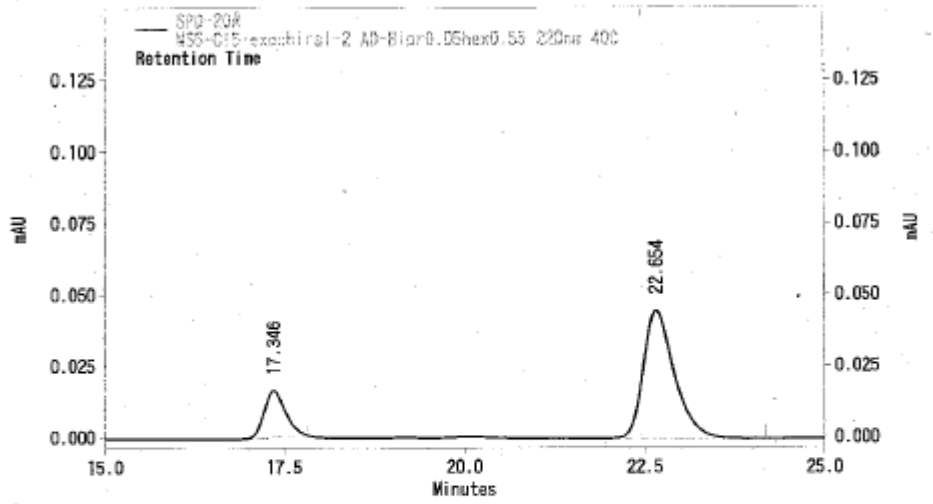
Name	Retention Time	Area	Area Percent	Height
1	18.346	69302	7.899	3492
2	20.347	808069	92.101	34795
Totals		877371	100.000	38287

(±)-**2o**



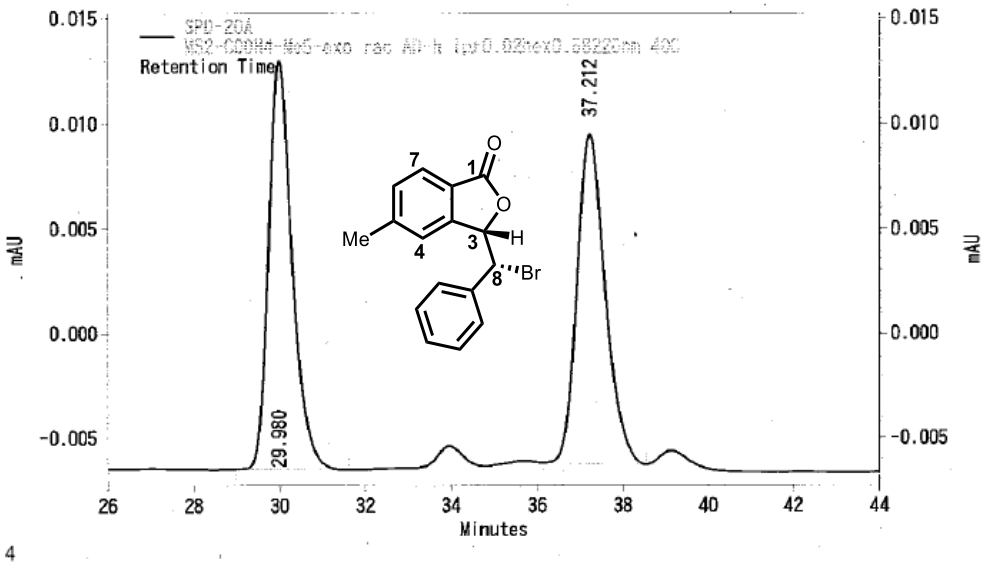
Name	Retention Time	Area	Area Percent	Height
1	17.327	542388	49.959	24091
2	22.640	543281	50.041	18260
Totals		1085669	100.000	42351

(3*R*,8*S*)-2o in Table 3, entry 14 (80:20 er)



Name	Retention Time	Area	Area Percent	Height
1	17.346	341775	20.387	16324
2	22.654	1334659	79.613	44828
Totals		1676434	100.000	61152

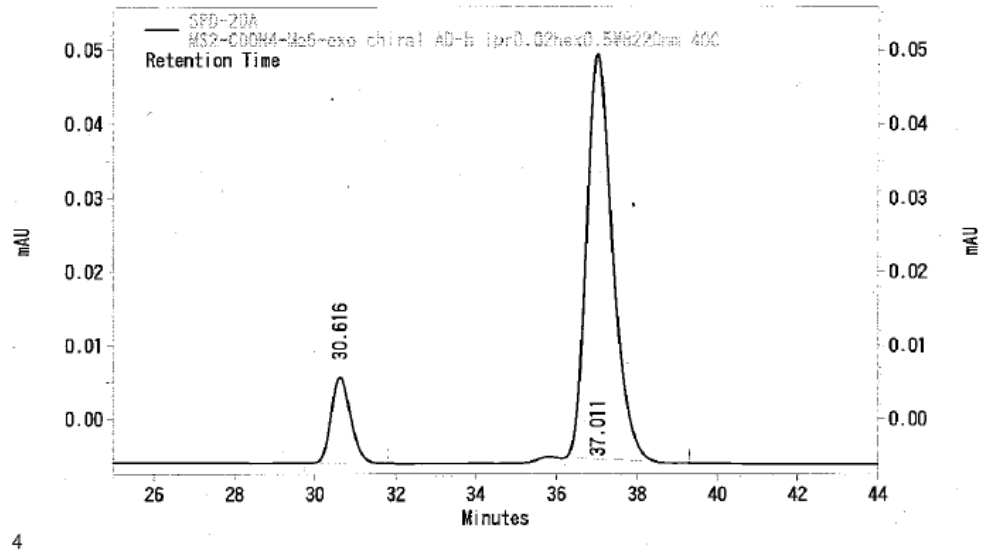
(±)-**2p**



4

Name	Retention Time	Area	Area Percent	Height
1	29.980	750806	51.057	19504
2	37.212	719726	48.943	15697
Totals		1470532	100.000	35201

(3*R*,8*S*)-2p in Table 3, entry 15 (86:14 er)



4

Name	Retention Time	Area	Area Percent	Height
1	30.616	394293	13.832	11636
2	37.011	2456376	86.168	54888
Totals		2850669	100.000	66524