

Supplementary Data

Abiesatrines A–J: anti-inflammatory and anti-tumor triterpenoids from *Abies georgei* Orr

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Legend for figures

Fig. S1. ¹³C NMR spectrum of abiesatrine A (**1**) in CDCl₃.

Fig. S2. ¹H NMR spectrum of abiesatrine A (**1**) in CDCl₃.

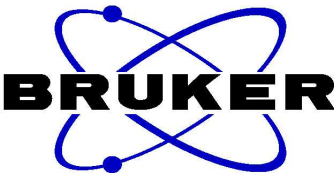
Fig. S3. HSQC NMR spectrum of abiesatrine A (**1**) in CDCl₃.

Fig. S4. ¹H–¹H COSY NMR spectrum of abiesatrine A (**1**) in CDCl₃.

Fig. S5. HMBC NMR spectrum of abiesatrine A (**1**) in CDCl₃.

Fig. S6. NOESY NMR spectrum of abiesatrine A (**1**) in CDCl₃.

Fig. S1. ¹³C NMR spectrum of abiesatrine A (1) in CDCl₃.



Current Data Parameters
NAME zhangwd-yagc2-39
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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Time 14.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 128
DS 2
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 sec
RG 32768
DW 11.000 usec
DE 6.00 usec
TE 301.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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P1 8.50 usec
PL1 2.00 dB
SFO1 150.9178988 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.00 dB
PL13 14.00 dB
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F2 - Processing parameters
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SF 150.9028138 MHz
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SSB 0
LB 3.00 Hz
GB 0
PC 1.40

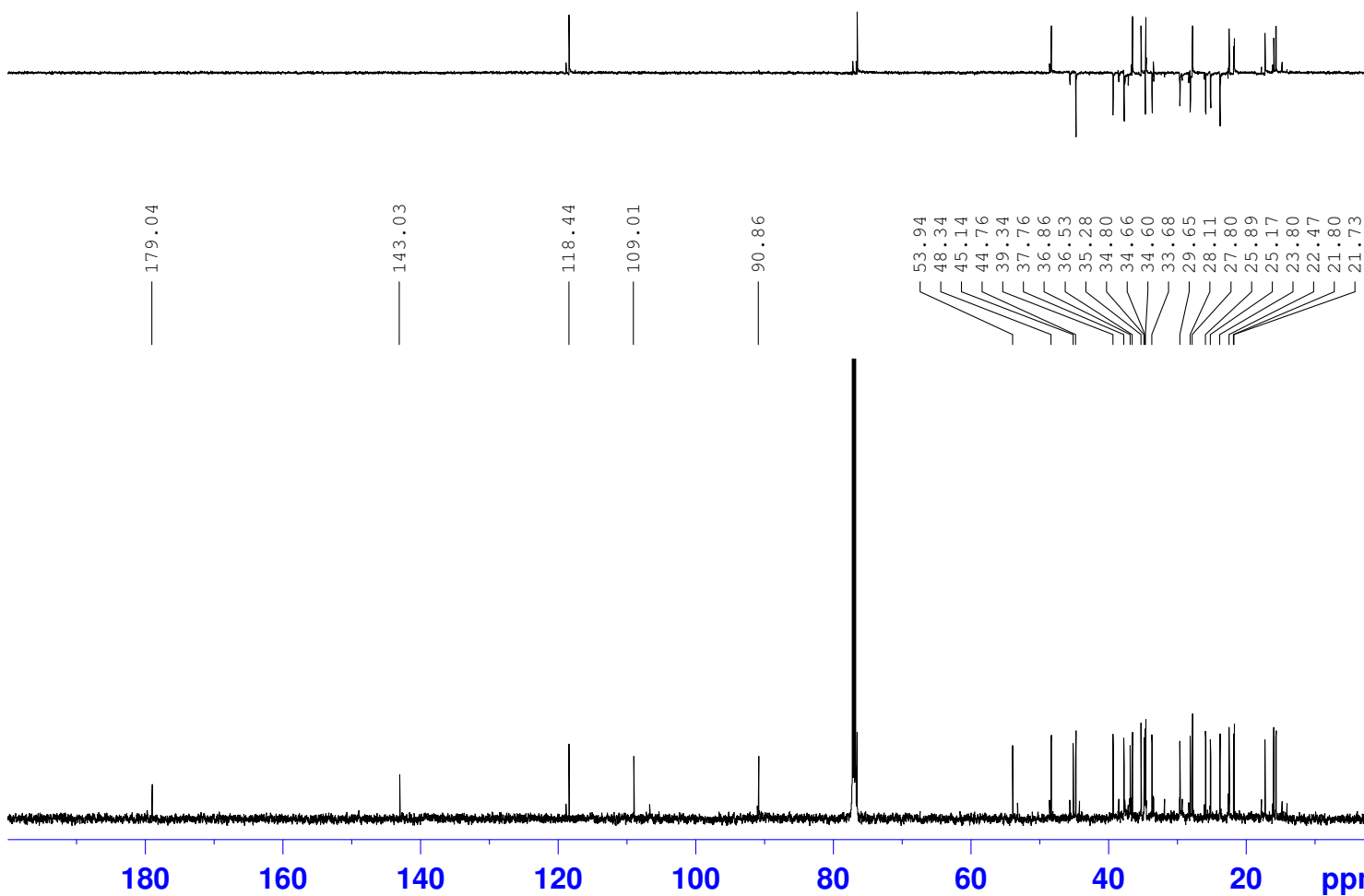
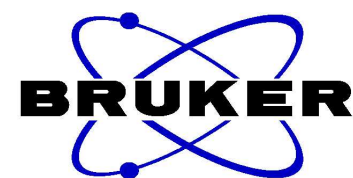
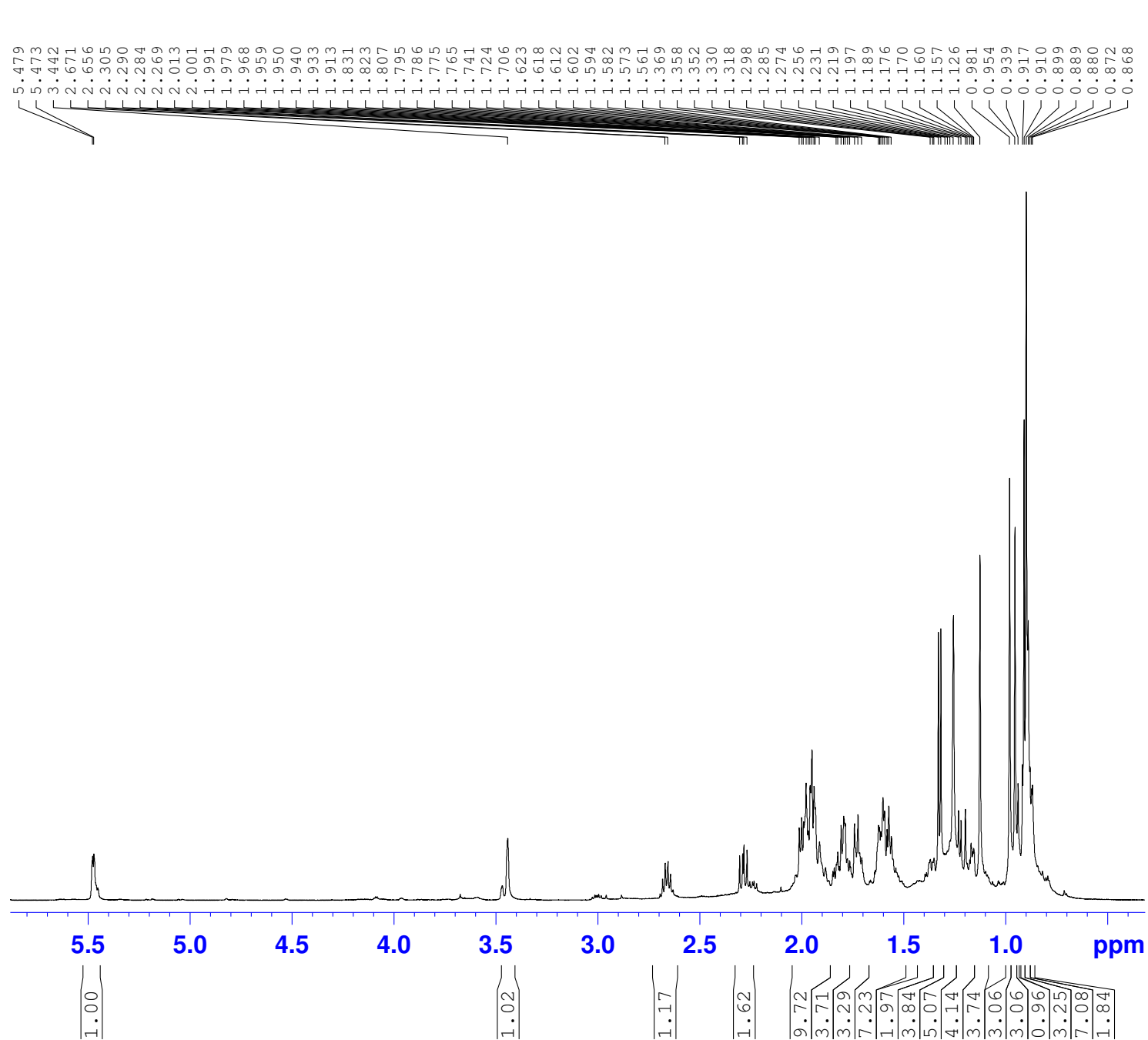


Fig. S2. ¹H NMR spectrum of abiesatrine A (1) in CDCl₃.



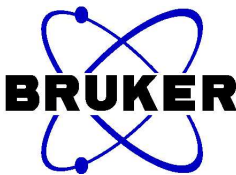
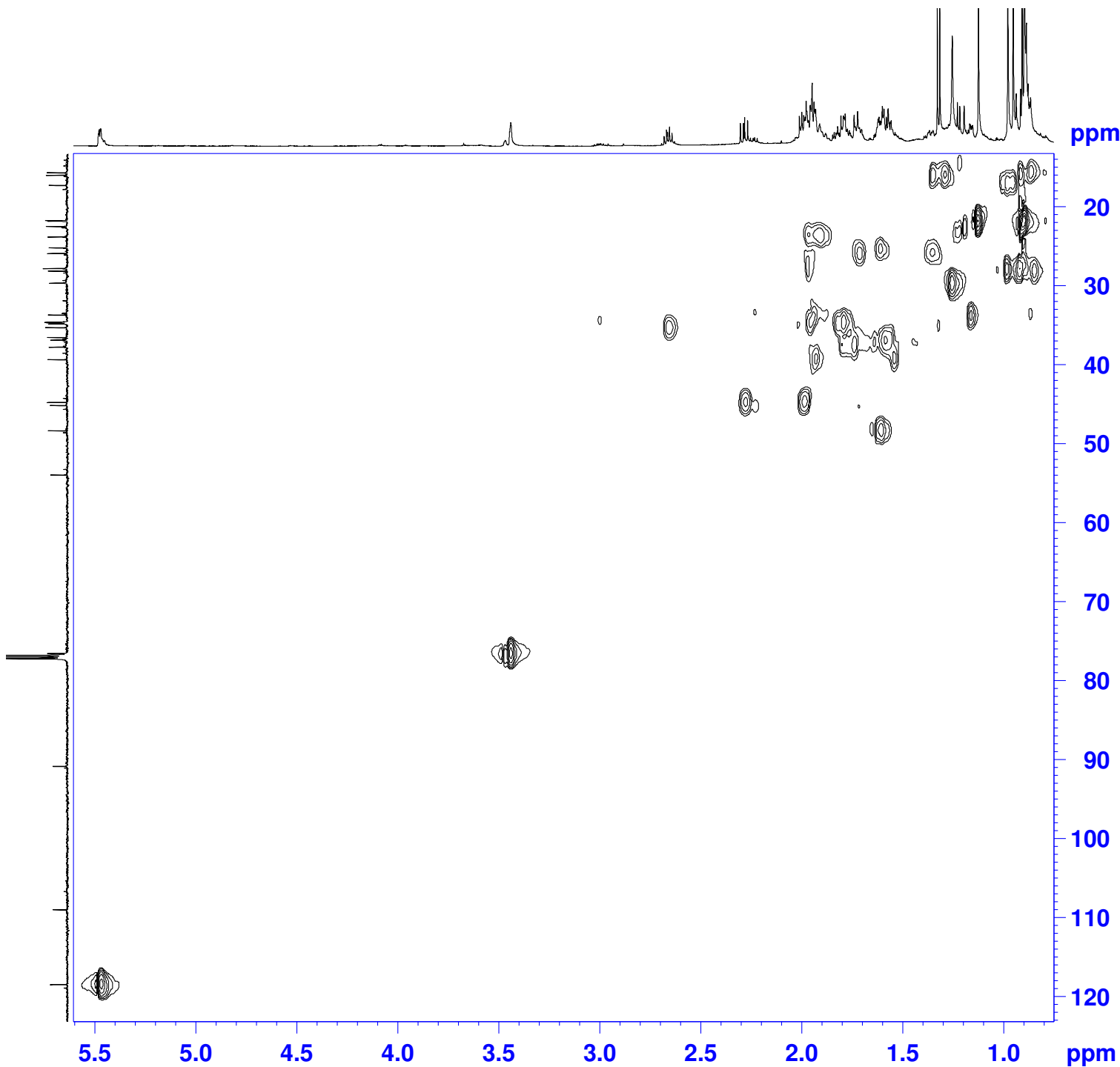
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PROCNO 1

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SOLVENT CDCl3
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DS 2
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FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 16
DW 55.467 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

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F2 - Processing parameters
SI 65536
SF 600.1300022 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Fig. S3. HSQC NMR spectrum of abiesatrine A (1) in CDCl3.



Current Data Parameters
NAME zhangwd-yagc2-39
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070902
Time 17.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgps12
TD 1024
SOLVENT CDCl3
NS 8
DS 16
SWH 4795.396 Hz
FIDRES 4.683004 Hz
AQ 0.1068191 sec
RG 2050
DW 104.267 usec
DE 6.00 usec
TE 300.1 K
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d11 0.03000000 sec
d13 0.00000400 sec
D16 0.00010000 sec
D24 0.00086207 sec
DELTA 0.00118340 sec
DELTA1 0.00110800 sec
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DELTA3 0.00062414 sec
IN0 0.00001840 sec
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ZGPTNS

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p2 27.40 usec
P28 1.00 usec
PL1 -1.00 dB
SFO1 600.1325750 MHz

===== CHANNEL f2 =====
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p4 19.60 usec
PCPD2 75.00 usec
PL2 2.00 dB
PL12 19.60 dB
SFO2 150.9178988 MHz

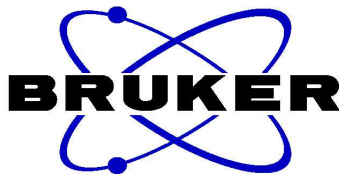
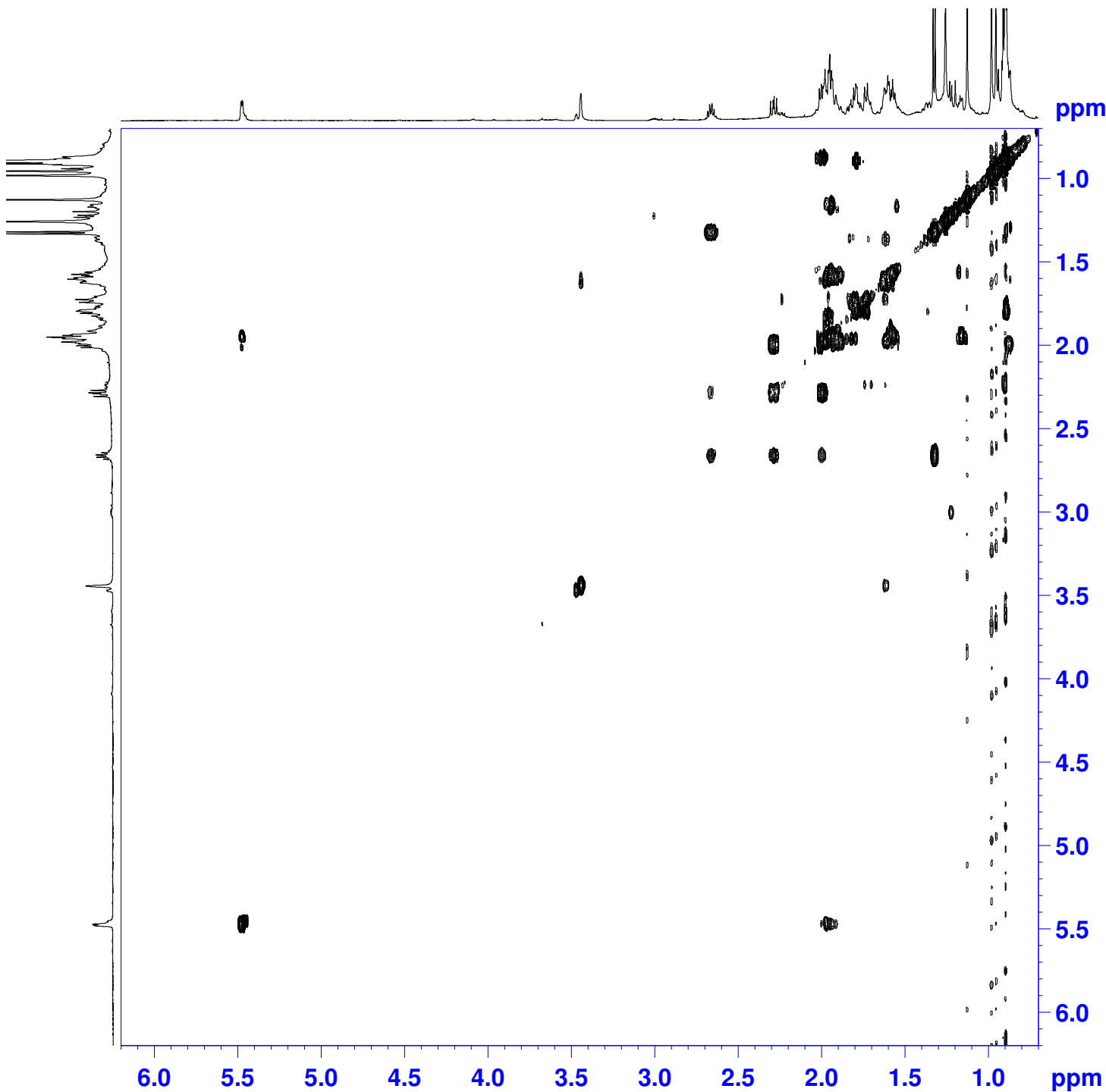
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GPNAM3 SINE.100
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GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 500.00 usec

F1 - Acquisition parameters
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FIDRES 169.836960 Hz
SW 180.058 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
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SF 600.1300020 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 150.9028138 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

Fig S4.1H-1H COSY NMR spectrum of abiesadine A (1) in CDCl3.



Current Data Parameters
NAME zhangwd-yagc2-39
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
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Time 16.52
INSTRUM spect
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PULPROG cosygpgf
TD 2048
SOLVENT CDCl3
NS 1
DS 16
SWH 4795.396 Hz
FIDRES 2.341502 Hz
AQ 0.2135881 sec
RG 128
DW 104.267 usec
DE 6.00 usec
TE 300.0 K
d0 0.00000300 sec
D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00010000 sec
IN0 0.00020855 sec

===== CHANNEL f1 =====
NUC1 1H
P0 13.70 usec
P1 13.70 usec
PL1 -1.00 dB
SFO1 600.1325750 MHz

===== GRADIENT CHANNEL =====
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GPNAM2 SINE.100
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
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TD 256
SFO1 600.1326 MHz
FIDRES 18.730520 Hz
SW 7.990 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.1300020 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 2048
MC2 QF
SF 600.1300020 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

Fig. S5. HMBC NMR spectrum of abiesatrine A (1) in CDCl3.

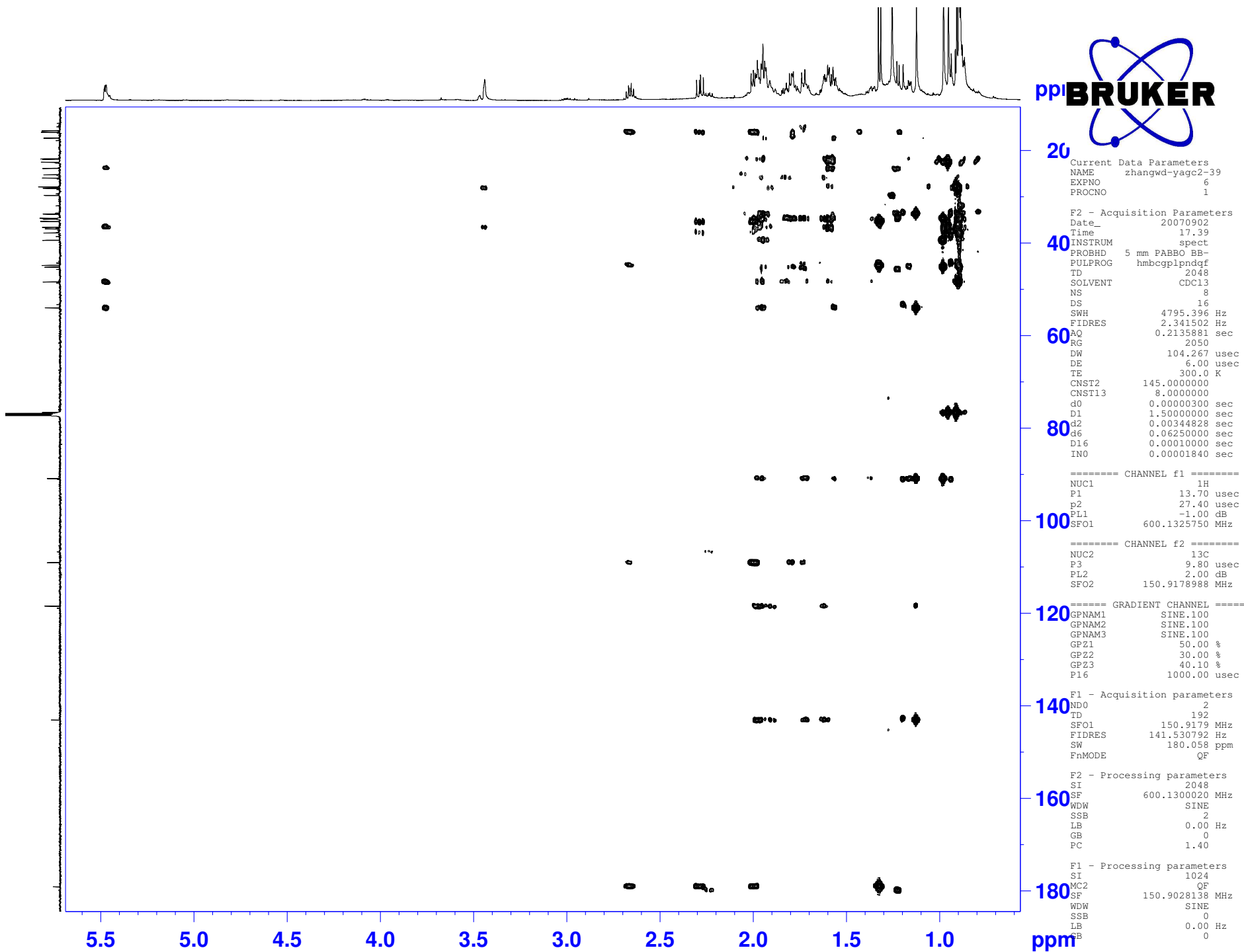


Fig. S6. NOESY NMR spectrum of abiesatrine A (1) in CDCl₃.

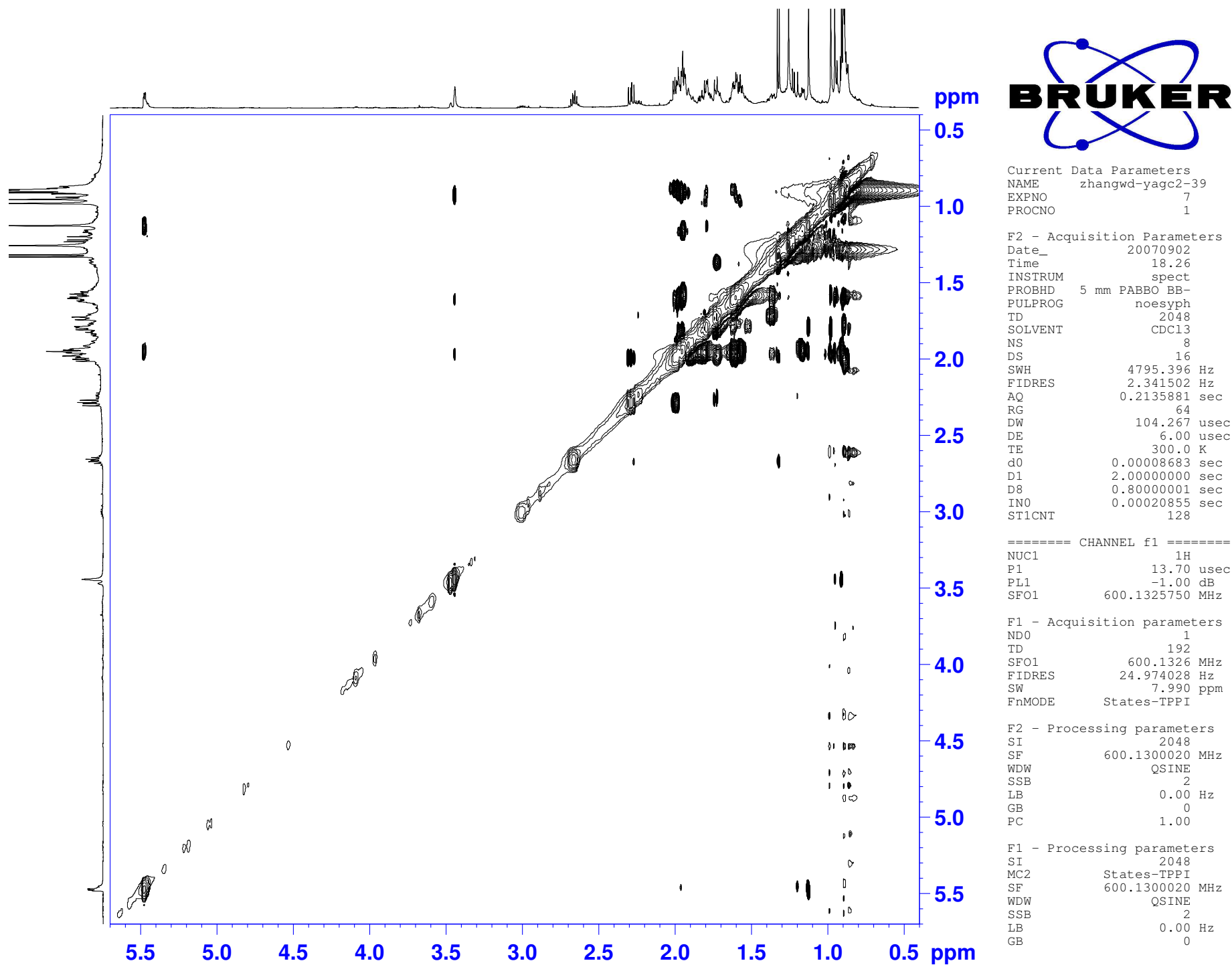


Table S1 ^1H NMR spectroscopic data for compounds **11**, **13–15**, and **17–20** (J in Hz within parentheses)

No.	11 ^a	13 ^b	14 ^b	15 ^a	17 ^a	18 ^b	19 ^b	20 ^b
1	1.61 m	2.05 m; 1.38 m	2.04 (dd, 12.9, 2.1); 1.99 m	2.45 m; 1.60 m	2.48 m; 1.75 m	1.94 m; 0.89 m	1.94 m; 0.88 m	1.69 m; 1.62 m
2	1.61 m; 1.57 m	2.50 m; 2.26 m	1.95 m; 1.56 m	2.51 m; 1.62 m	2.41 m; 1.89 m	3.78 m	3.69 (dt, 9.6, 4.8)	1.55 m; 0.97
3	3.22 (dd, 10.8, 4.8)		3.38 (t, 1.8)			3.05 (d, 9.0)	3.35 (d, 9.6)	3.15 (dd, 11.7, 4.5)
5	1.25 m	2.48 (dd, 11.4, 5.7)	1.46 m	1.46 m	1.48 m	0.94 m	1.27 m	0.74 (d, 11.7)
6	1.54 m; 0.79 m	1.48 m	1.92 m	1.92 m; 0.98 m	1.93 m; 1.81 m	1.61 m; 1.37 m	1.44 m; 1.33 m	1.53 m; 1.37 m
7	1.58 m; 1.03 m	1.32 m	5.66 (d, 6.0)	5.67 (dt, 7.5, 2.7)	5.69 (dt, 7.5, 2.8)	1.37 m; 1.31 m	1.64 m; 1.28 m	1.52 m; 1.32 m
8	1.49 (d, 4.5)	1.60 m						
9			1.42 m	2.25 m	2.27 m	1.59 m	1.63 m	1.55 m
11	1.31 m	2.17 m	2.21 m	1.67 m	1.65 m	1.93 m	1.95 m	1.92 (dd, 9.0, 3.6)
	1.06 m	1.32 m	1.83 (dt, 13.2, 2.4)	1.20 m	0.95 m	1.02 m	1.01 m	1.08 (brd, 13.8)
12	1.27 m	1.70 m	5.56 (dd, 8.4, 2.4)	2.52 m; 1.65 m	2.52 m; 1.67 m	5.23 (t, 3.3)	5.23 (t, 3.6)	5.22 (t, 3.6)
15	1.53 m; 1.27 m	1.33 m	1.40 m	1.42 m	1.63 m; 1.48 m	1.90 m; 1.06 m	1.03 m	0.98 m?
16	2.03 m; 1.09 m	1.92 m	1.93 m	1.28 m; 1.08 m	1.99 m; 1.33 m	2.03 (dt, 13.8, 4.2)	2.02 m	2.03 (dt, 12.6, 4.2)
						1.64 m	1.63 m	1.63 m
17	1.61 m	1.66 m		1.57 m	1.60 m			
18	0.97 s	1.01 s	0.96 s	0.83 s	0.86 s	2.20 (d, 11.4)	2.20 (d, 11.4)	2.19 (d, 11.7)
19	0.54 (d, 4.0)	0.76 (d, 4.5)	0.95 s	0.99 s	1.00 s	1.35 m	1.36 m	0.98 m
	0.33 (d, 4.0)	0.42 (d, 4.5)						
20	1.33 m	1.44 m	2.22 m	1.96 m; 1.26 m	2.03 m	0.95 m	0.95 m	0.95 m
21	0.88 (d, 7.2)	0.95 (d, 6.6)	0.89 (d, 6.6)	0.88 (d, 6.0)	0.90 (d, 6.3)	1.68 m; 1.57 m	1.48 m; 1.32 m	1.47 m; 1.29 m
22	1.79 (dt, 12.9, 3.0)	1.58 m	2.92 (dd, 15.0, 2.4)	2.62 m	2.65 (dd, 14.4, 2.7)	1.48 m	1.68 m	1.36 m
	0.97 m	1.19 m	2.30 (dd, 15.0, 10.2)	2.26 (dd, 15.9, 9.9)	2.24 m	1.34 m	1.57 m	1.00 m
23	1.90 m; 1.31 m	2.25 m; 2.12 m				1.22 s	0.69 s	0.95 s
24	3.16 (dd, 10.2, 1.5)	6.77 (t, 7.2)	6.94 brs	3.34 s	6.88 (d, 1.5)	4.02 (d, 11.4); 3.37 (d, 11.4)	3.50 (d, 10.8); 3.26 (d, 10.8)	0.77 s
25						0.99 s	1.04 s	0.95 s
26	1.14 s	1.81 s				0.82 s	0.84 s	0.84 s
27	0.92 s		2.15 (d, 1.2)	6.10 (d, 2.1); 5.45 m	2.19 (d, 1.5)	1.11 s	1.13 s	1.10 s
28	0.90 s	4.82 m	0.94 s	1.07 s	1.08 s			
		4.73 (t, 1.2)						
29	0.78 s	1.69 s	0.92 s	1.08 s	1.09 s	0.88 (d, 6.6)	0.88 (d, 6.6)	0.88 (d, 6.6)
30	1.13 s	0.99 s	1.20 s	1.05 s	1.06 s	0.94 (d, 6.6)	0.96 s	0.97 (d, 6.0)
OMe		3.62 s						

^a Measured at 300 MHz in CD₃OD. ^b Measured at 600 MHz in CDCl₃.

Table S2 ^{13}C NMR spectroscopic data for compounds **11–20**

No.	11 ^a	12 ^a	13 ^b	14 ^b	15 ^a	16 ^a	17 ^a	18 ^b	19 ^b	20 ^b
1	33.8 t	28.7 t	30.3 t	30.7 t	35.2 t	35.2 t	35.2 t	48.0 t	48.0 t	38.1 t
2	30.7 t	30.8 t	32.4 t	26.5 t	35.3 t	35.3 t	35.3 t	69.6 d	69.7 d	27.9 t
3	79.2 d	77.7 d	176.2 s	77.2 d	221.8 s	221.7 s	221.8 s	85.9 d	78.2 d	79.7 d
4	41.3 s	40.6 s	150.8 s	38.0 s	48.0 s	48.1 s	48.1 s	44.4 s	44.1 s	39.8 s
5	48.2 d	42.2 d	47.2 d	39.4 d	53.7 d	53.7 d	53.7 d	57.1 d	48.1 d	56.8 d
6	22.0 t	22.2 t	29.0 t	24.3 t	23.9 t	24.0 t	23.9 t	19.8 t	19.1 t	19.5 t
7	29.0 t	29.1 t	26.6 t	120.1 d	122.8 d	122.8 d	122.8 d	34.5 t	33.6 t	34.3 t
8	49.1 d	49.6 d	49.3 d	147.4 s	149.9 s	149.9 s	149.9 s	40.8 s	40.8 s	38.1 s?
9	20.8 s	20.9 s	22.7 s	52.6 d	46.8 d	46.8 d	46.8 d	49.1 d	48.8 d	48.9 d
10	27.0 s	27.8 s	28.4 s	36.0 s	37.0 s	37.0 s	37.0 s	39.0 s	39.0 s	40.8 s
11	26.9 t	27.4 t	28.1 t	29.1 t	21.8 t	21.9 t	21.8 t	24.7 t	24.4 t	24.4 t
12	36.4 t	34.9 t	34.3 t	123.8 d	35.5 t	35.6 t	35.5 t	126.6 d	126.7 d	126.9 d
13	46.1 s	46.4 s	46.4 s	157.4 s	45.2 s	45.2 s	45.3 s	139.7 s	139.8 s	139.6 s
14	49.6 s	50.1 s	50.2 s	51.2 s	53.2 s	53.2 s	53.2 s	43.2 s	43.4 s	43.3 s
15	32.9 t	36.7 t	36.8 t	37.9 t	34.2 t	34.2 t	34.2 t	29.2 t	29.1 t	29.2 t
16	27.3 t	26.9 t	29.1 t	39.3 t	29.3 t	29.5 t	29.4 t	25.3 t	25.3 t	25.3 t
17	53.3 d	53.7 d	53.5 d	47.6 s	54.3 d	54.7 d	54.5 d	49.1 s	49.1 s	54.4 s
18	18.6 q	18.6 q	18.7 q	25.3 q	22.9 q	22.9 q	22.9 q	54.3 d	54.3 d	54.4 d
19	30.7 t	33.6 t?	31.0 t	22.8 q	23.5 q	23.5 q	23.4 q	40.4 d	40.4 d	40.4 d
20	37.4 d	37.8 d	37.2 d	40.1 d	34.0 d	34.2 d	34.9 d	40.4 d	40.4 d	40.4 d
21	18.9 q	19.0 q	18.7 q	16.2 q	19.9 q	20.8 q	19.9 q	38.1 t	31.7 t	31.8 t
22	34.5 t	34.2 t	36.1 t	49.4 t	50.3 t	50.1 t	52.9 t	31.8 t	38.1 t	40.0 t
23	28.8 t	29.6 t	26.2 t	205.1 s	211.8 s	200.0 s	205.5 s	23.8 q	13.9 q	28.8 q
24	80.3 d	80.6 d	144.4 d	131.2 d	48.6 t	128.1 d	129.3 d	66.2 t	66.3 t	16.4 q
25	73.7 s	73.9 s	128.6 s	146.5 s	140.8 s	150.2 s	149.9 s	17.6 q	17.7 q	16.0 q
26	24.9 q	24.9 q	12.4 q	173.5 s	173.1 s	16.5 q	175.3 s	17.6 q	17.8 q	17.8 q
27	25.9 q	26.6 q	171.8 s	15.4 q	125.4 t	173.6 s	16.0 q	24.1 q	24.2 q	24.1 q
28	25.3 q	25.7 q	112.1 t	28.9 q	28.4 q	28.4 q	28.4 q	181.6 s	181.6 s	181.6 s
29	14.6 q	21.9 q	20.1 q	23.6 q	21.7 q	21.7 q	21.7 q	17.6 q	17.7 q	17.6 q
30	19.8 q	19.8 q	19.9 q	26.6 q	27.8 q	27.9 q	27.8 q	21.6 q	21.6 q	21.6 q
OMe			52.1 q							

^a Measured at 75 MHz in CD₃OD. ^b Measured at 150 MHz in CDCl₃.

(24R)-Cycloartane-3 β ,24,25-triol (11)

Amorphous powder; ^1H and ^{13}C NMR data, see Tables S1 and S2; ESIMS (positive) m/z 483 $[\text{M}+\text{Na}]^+$, 943 $[2\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 496 $[\text{M}+\text{Cl}]^-$.

(24R)-Cycloartane-3 α ,24,25-triol (12)

Amorphous powder; ^1H NMR (CD_3OD , 300 MHz) δ 3.39 (1H, t, $J = 2.1$ Hz, H-3), 3.16 (1H, dd, $J = 10.2, 1.5$ Hz, H-24), 1.16 (3H, s, Me-27), 1.12 (3H, s, Me-26), 1.01 (3H, s, Me-18), 0.95 (3H, s, Me-27), 0.92 (3H, s, Me-28), 0.91 (3H, d, $J = 6.3$ Hz, Me-21), 0.89 (3H, s, Me-29), 0.52 (1H, d, $J = 4.0$ Hz, H-19a), 0.36 (1H, d, $J = 4.0$ Hz, H-19b); ^{13}C NMR data, see Table S2; ESIMS (positive) m/z 483 $[\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 496 $[\text{M}+\text{Cl}]^-$.

Methyl (24E)-26-carboxy-3,4-seco-cycloartane-4(29),24-dien-3-oate (13)

Amorphous powder; ^1H and ^{13}C NMR (CDCl_3 , 150 MHz) spectroscopic data, see Tables S1 and S2; ESIMS (positive) m/z 485 $[\text{M}+\text{H}]^+$; 507 $[\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 483 $[\text{M}-\text{H}]^-$, 967 $[2\text{M}-\text{H}]^-$.

23-Oxo-mariesiic acid B (14)

Amorphous powder; $[\alpha]_{\text{D}}^{20} -125.9$ (c 0.50, MeOH); IR (KBr) ν_{max} 3441, 2965, 2851, 1688, 1621, 1563, 1453, 1373, 1282, 1063, 986 cm^{-1} ; for ^1H and ^{13}C NMR data, see Tables S1 and S2; ESIMS (positive) m/z 491 $[\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 467 $[\text{M}-\text{H}]^-$, 935 $[2\text{M}-\text{H}]^-$; HRESIMS (negative) $[\text{M}-\text{H}]^-$ m/z 467.3157, calcd for $\text{C}_{30}\text{H}_{43}\text{O}_4$, 467.3161.

Isofirmanoic acid (15)

Amorphous powder; for ^1H and ^{13}C NMR data, see Tables S1 and S2; ESIMS (positive) m/z 491 $[\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 491 $[\text{M}-\text{H}]^-$.

(24Z)-3,23-Dioxo-9 β -lanosta-7,24-dien-27-oic acid (16)

Amorphous powder; ^1H NMR (CD_3OD , 300 MHz) δ 5.67 (1H, dt, $J = 7.5, 2.7$ Hz, H-7), 1.94 (3H, d, $J = 1.2$ Hz, Me-26), 1.08 (3H, s, Me-29), 1.07 (3H, s, Me-28), 1.05 (3H, s, Me-30), 0.99 (3H, s, Me-19), 0.95 (3H, d, $J = 6.0$ Hz, Me-21), 0.82 (3H, s, Me-18); ^{13}C NMR spectroscopic data, see Table S2; ESIMS (positive) m/z 491 $[\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 467 $[\text{M}-\text{H}]^-$.

Firmanoic acid (17)

Amorphous powder; ^1H and ^{13}C NMR spectroscopic data, see Tables S1 and S2; ESIMS (positive) m/z 491 $[\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 467 $[\text{M}-\text{H}]^-$.

2 α ,3 β ,24-Trihydroxy-12-ursen-28-oic acid (18)

Amorphous powder; $[\alpha]_{\text{D}}^{20}$ +25.9 (c 0.50, MeOH); ^1H and ^{13}C NMR spectroscopic data, see Tables S1 and S2; ESIMS (positive) m/z 511 $[\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 487 $[\text{M}-\text{H}]^-$, 975 $[2\text{M}-\text{H}]^-$.

Dammarolic acid (19)

Amorphous powder; ^1H and ^{13}C NMR spectroscopic data, see Tables S1 and S2; ESIMS (positive) m/z 511 $[\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 487 $[\text{M}-\text{H}]^-$, 975 $[2\text{M}-\text{H}]^-$.

Ursolic acid (20)

Amorphous powder; ^1H and ^{13}C NMR spectroscopic data, see Tables S1 and S2; ESIMS (positive) m/z 479 $[\text{M}+\text{Na}]^+$, 935 $[2\text{M}+\text{Na}]^+$; ESIMS (negative) m/z 455 $[\text{M}-\text{H}]^-$, 911 $[2\text{M}-\text{H}]^-$.

Table S3. Crystal data and structure refinement for abiesatrine A, CH₃OH (**1**).

Identification code	abiesatrine A (1)
Empirical formula	C ₃₁ H ₅₀ O ₅
Formula weight	502.71
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 8.165(15) Å α = 90°. b = 13.02(3) Å β = 90°. c = 26.83(6) Å γ = 90°.
Volume	2852(10) Å ³
Z, Calculated density	4, 1.171 Mg/m ³
Absorption coefficient	0.077 mm ⁻¹
F(000)	1104
Crystal size	0.15 x 0.10 x 0.04 mm
Theta range for data collection	1.52 to 25.01°.
Limiting indices	-8 ≤ h ≤ 9, -15 ≤ k ≤ 14, -31 ≤ l ≤ 23
Reflections collected / unique	11872 / 5047 [R(int) = 0.2995]
Completeness to theta = 25.01	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9969 and 0.9885
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5047 / 0 / 327
Goodness-of-fit on F ²	0.948
Final R indices [I > 2σ(I)]	R ₁ = 0.0711, wR ₂ = 0.1422
R indices (all data)	R ₁ = 0.2828, wR ₂ = 0.1882
Absolute structure parameter	0(3)
Largest diff. peak and hole	0.166 and -0.180 e.Å ⁻³