

(*E*)-5-[Bromo(phenyl)methylene]-4-phenyl-2-(*p*-tolyl)-4,5-dihydrooxazole

Supporting Information

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Yoshimitsu Hashimoto ¹, and Osamu Tamura ^{1*}

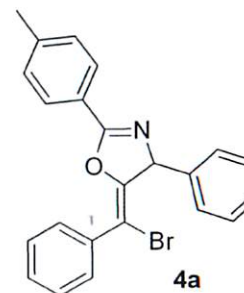
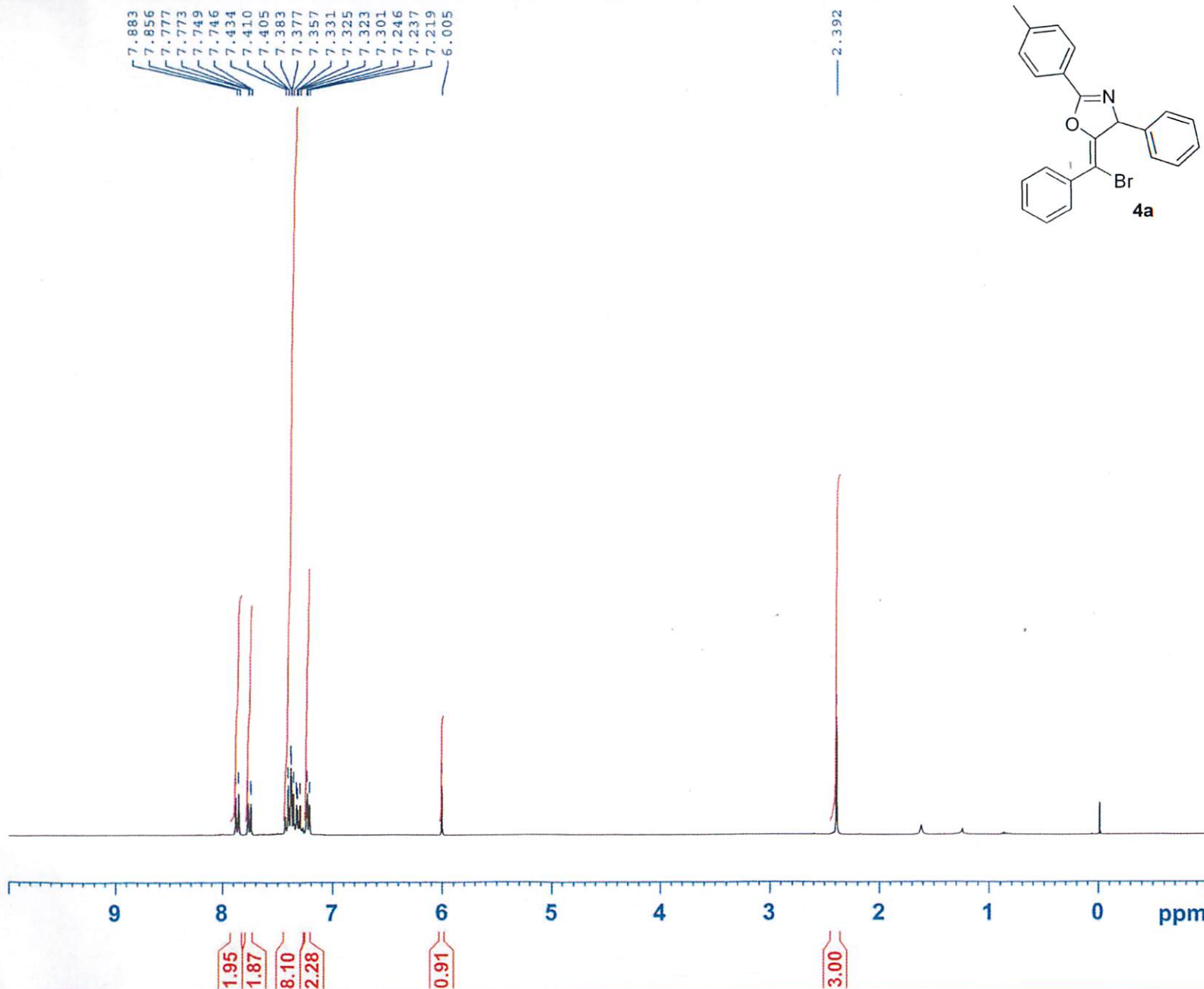
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¹H-NMR, ¹³C-NMR, IR, and HRMS of bromooxazoline **9**

X-ray Crystallographic data of bromooxazoline **9**

20180510KRM94_4



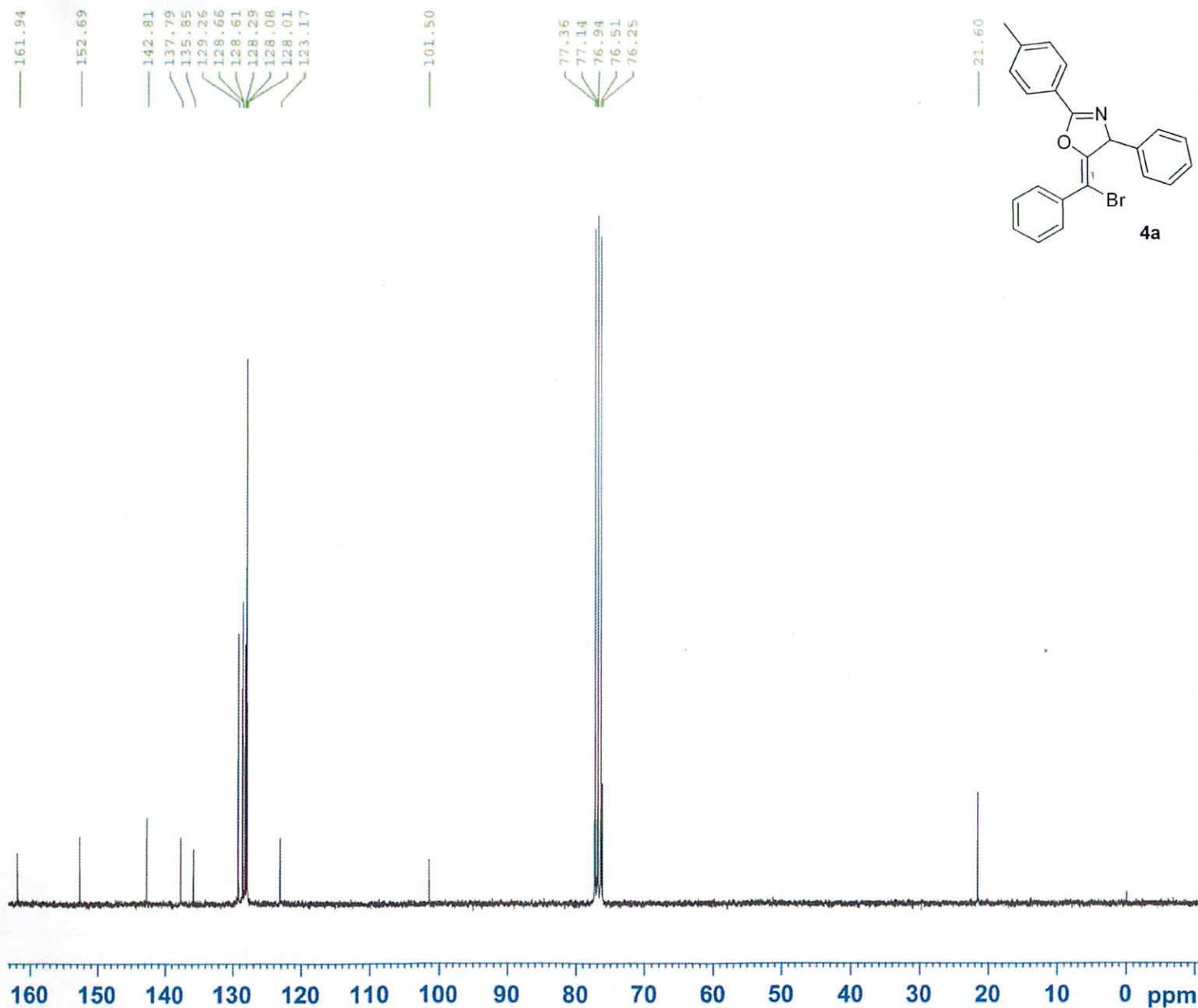
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EXPNO 1490
PROCNO 1

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Date_ 20180510
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PULPROG zg30
TD 65536
SOLVENT CDCl3
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DS 2
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RG 64
DW 80.800 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

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NUC1 1H
P1 14.75 usec
PLW1 6.19999981 W

F2 - Processing parameters
SI 32768
SF 300.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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 EXPNO 1491
 PROCNO 1

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 D11 0.03000000 sec
 TD0 1

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 PLW1 34.00000000 W

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 CPDPRG[2] waltz16
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 PLW12 0.21797000 W
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 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

[Elemental Composition]

Data : Yakukagaku-Morita-030

Date : 14-Mar-2023 14:32

Page: 1

Sample: MORITA_Bromoorazdiae

Note : -

Inlet : Reserv.

Ion Mode : EI+

RT : 1.07 min

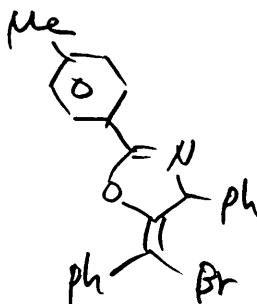
Scan#: 33

Elements : C 40/0, H 49/0, Br 1/1 (79Br 1/0, 81Br 1/0), N 1/1, O 1/1

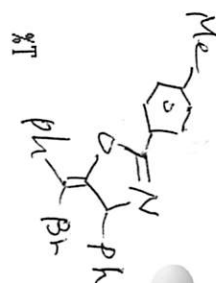
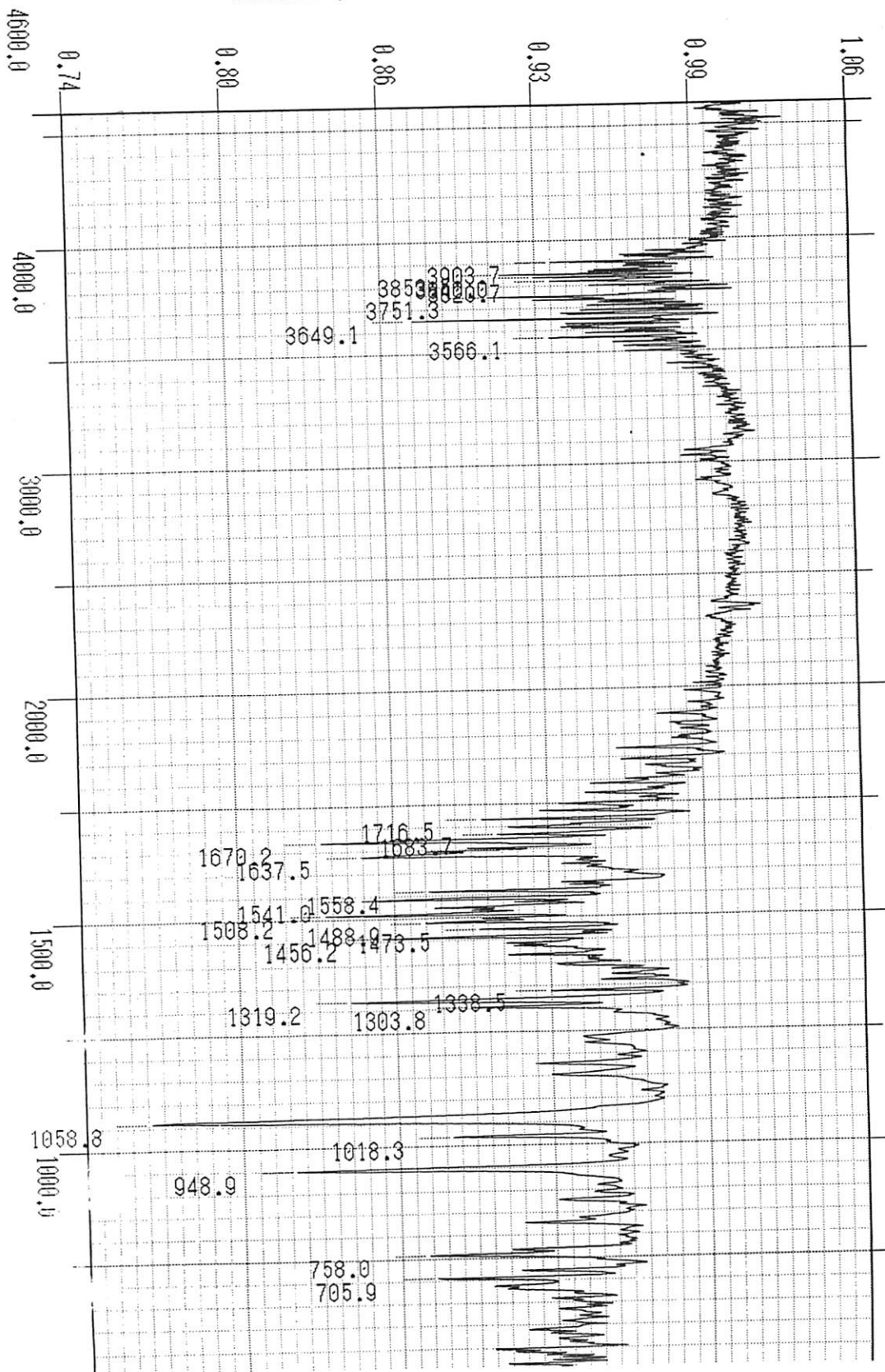
Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 10mmu if m/z > 10

Unsaturation (U.S.) : -0.5 - 30.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
403.0574	99.2	+0.5 / +0.2	15.0	C 23 H 18 79Br N O
405.0558	100.0	+1.5 / +0.6	15.0	C 23 H 18 81Br N O



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MEASURING MODE ; %T
RESOLUTION ; 4.0 cm-1
NO. OF SCAN ; 40
GAIN ; AUTO
DETECTOR ; DETECTOR 1 (2.8 mm/sec)
APODIZATION ; HAPP-GENZEL
REMARKS ; KRM121_1
ANALYST ; kurami
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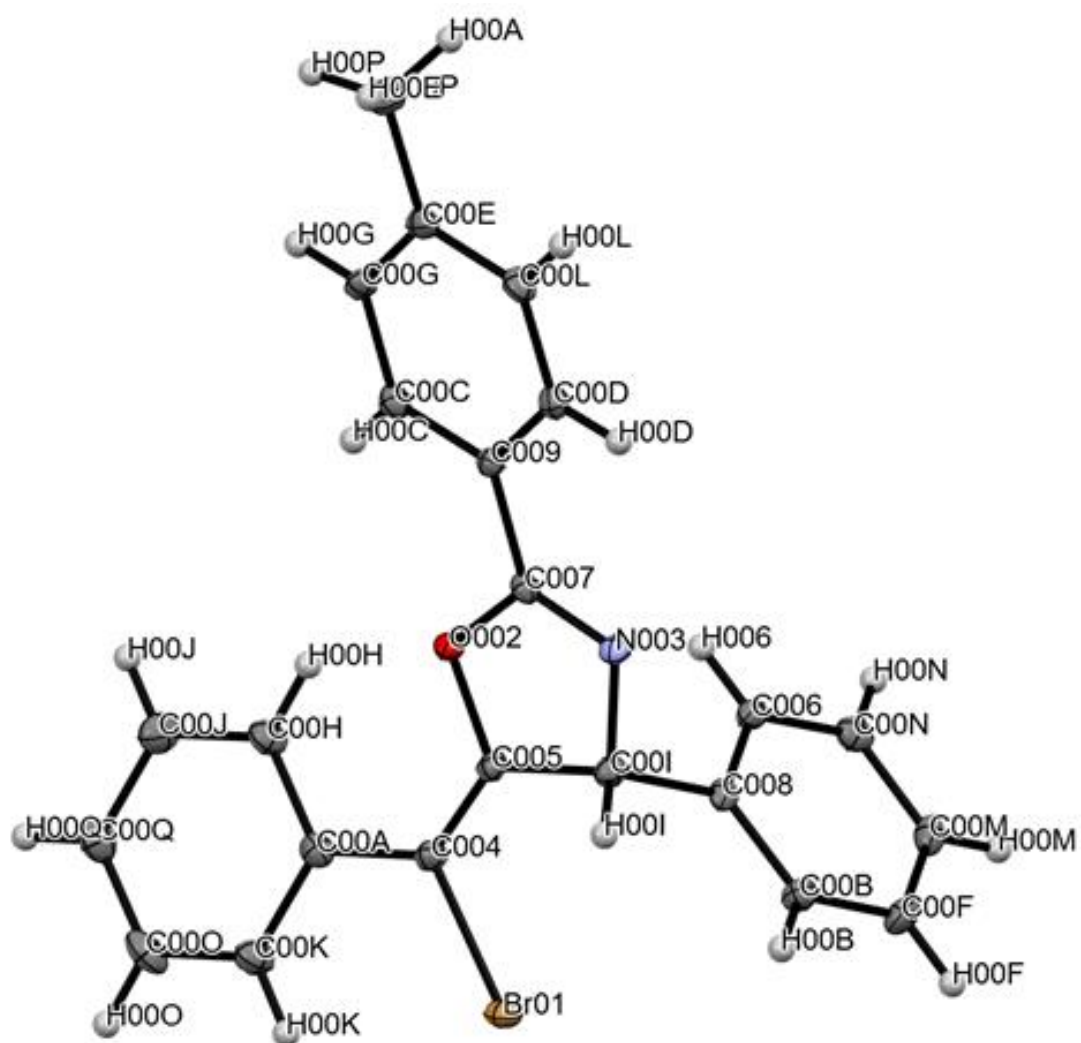


Table S1: Bond Lengths in Å for **exp_443_auto**.

Atom	Atom	Length/Å
Br01	C004	1.908(3)
O002	C005	1.391(3)
O002	C007	1.390(3)
N003	C007	1.269(4)
N003	C00I	1.474(4)
C004	C005	1.339(4)
C004	C00A	1.477(4)
C005	C00I	1.519(4)
C006	C008	1.390(4)
C006	C00N	1.390(4)
C007	C009	1.466(4)
C008	C00B	1.392(4)
C008	C00I	1.522(4)
C009	C00C	1.394(4)
C009	C00D	1.400(4)
C00A	C00H	1.402(4)
C00A	C00K	1.398(4)
C00B	C00F	1.394(4)
C00C	C00G	1.389(4)
C00D	C00L	1.384(4)
C00E	C00G	1.394(4)
C00E	C00L	1.397(4)
C00E	C00P	1.509(4)
C00F	C00M	1.386(5)
C00H	C00J	1.389(5)
C00J	C00Q	1.388(5)
C00K	C00O	1.385(5)
C00M	C00N	1.391(4)
C00O	C00Q	1.384(5)

Table S2: Bond Angles in ° for **exp_443_auto**.

Atom	Atom	Atom	Angle/°
C007	O002	C005	104.8(2)
C007	N003	C00I	107.1(2)
C005	C004	Br01	112.6(2)
C005	C004	C00A	130.1(3)
C00A	C004	Br01	117.2(2)
O002	C005	C00I	107.4(2)
C004	C005	O002	122.4(3)
C004	C005	C00I	130.2(3)
C008	C006	C00N	120.5(3)
O002	C007	C009	115.8(2)
N003	C007	O002	117.3(3)
N003	C007	C009	126.9(3)
C006	C008	C00B	119.5(3)
C006	C008	C00I	119.9(3)
C00B	C008	C00I	120.7(3)
C00C	C009	C007	121.3(3)
C00C	C009	C00D	119.5(3)
C00D	C009	C007	119.2(3)
C00H	C00A	C004	120.9(3)
C00K	C00A	C004	121.2(3)
C00K	C00A	C00H	117.9(3)
C008	C00B	C00F	120.1(3)
C00G	C00C	C009	120.0(3)
C00L	C00D	C009	119.6(3)
C00G	C00E	C00L	118.1(3)
C00G	C00E	C00P	121.4(3)
C00L	C00E	C00P	120.5(3)
C00M	C00F	C00B	120.0(3)
C00C	C00G	C00E	121.2(3)
C00J	C00H	C00A	120.5(3)
N003	C00I	C005	102.9(2)
N003	C00I	C008	111.0(2)
C005	C00I	C008	113.1(2)

Atom	Atom	Atom	Angle/°
C00Q	C00J	C00H	121.0(3)
C00O	C00K	C00A	121.1(3)
C00D	C00L	C00E	121.6(3)
C00F	C00M	C00N	120.1(3)
C006	C00N	C00M	119.8(3)
C00Q	C00O	C00K	120.7(3)
C00O	C00Q	C00J	118.9(3)