

(Z)-5-Benzylidene-4-phenyl-2-(p-tolyl)-4,5-dihydrooxazole

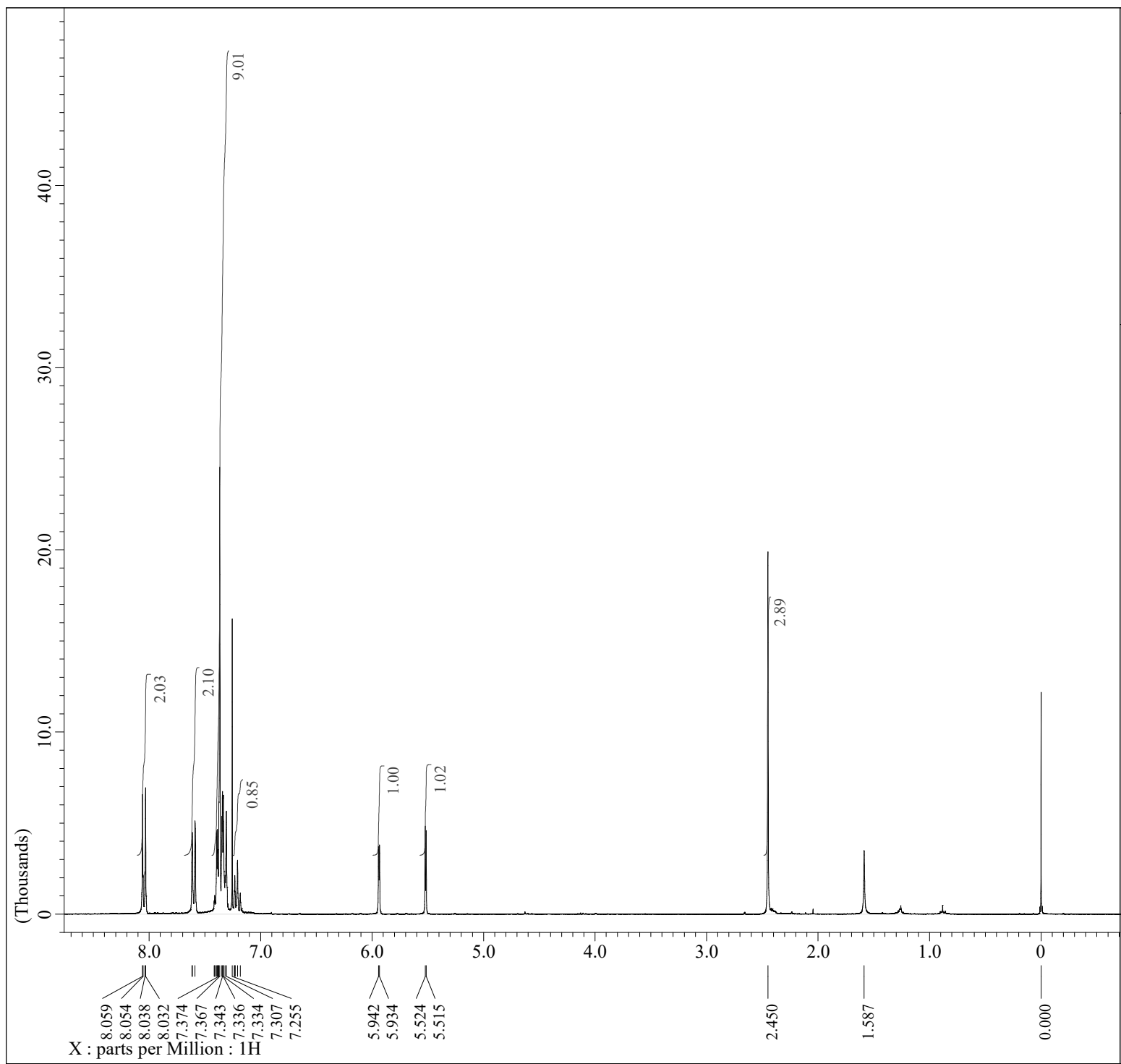
Supporting Information

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Contents

¹H NMR, ¹³C NMR, IR, and HRMS of oxazoline **15**



---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sext(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm

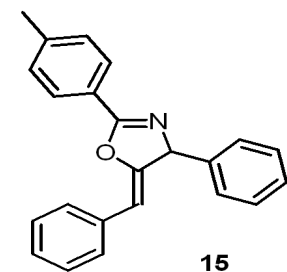
以下に由来: Morita_3060-1.jdf

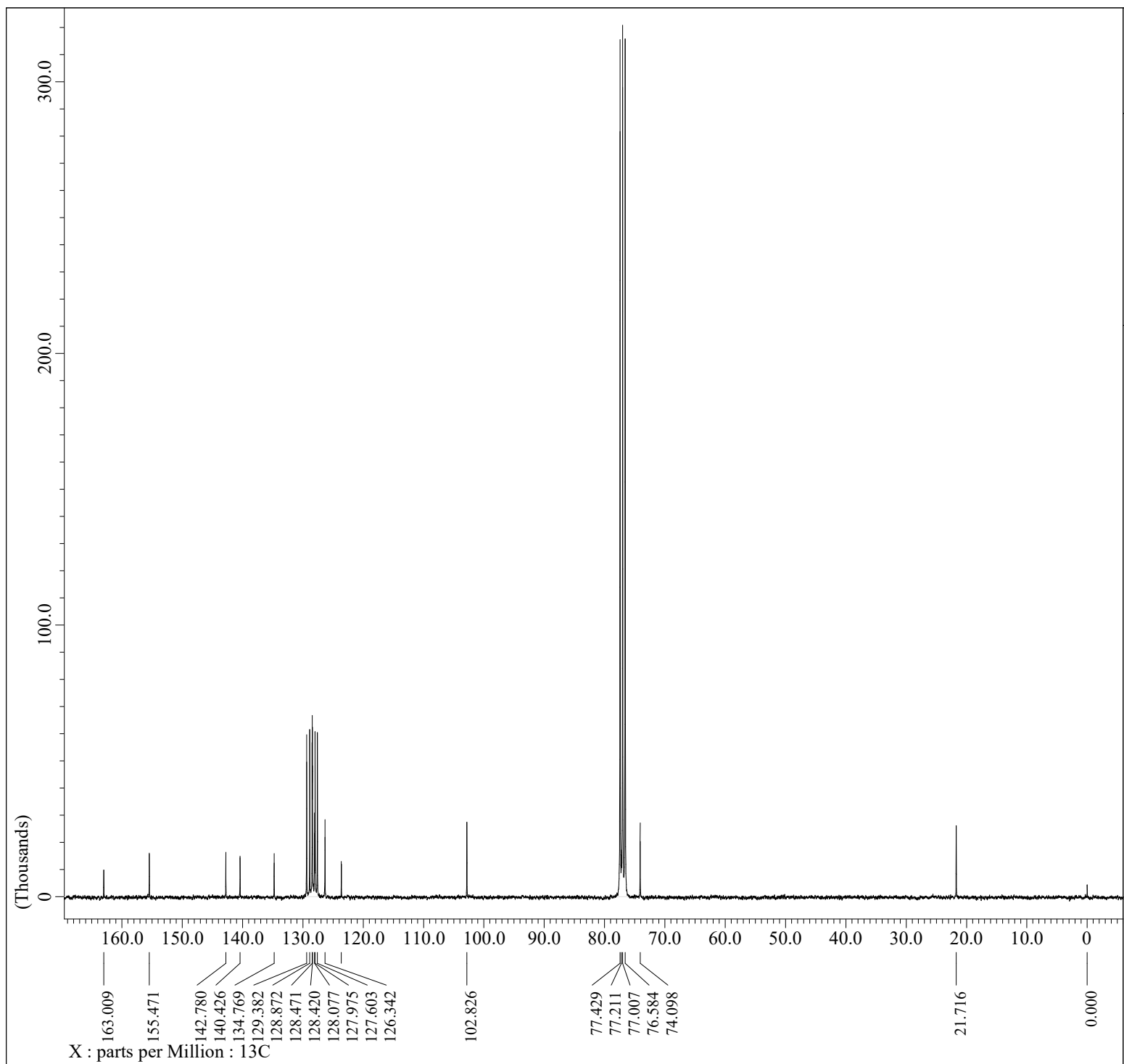
Filename = Morita_3060-3.jdf
Author = Administrator
Experiment = zg30
Sample_Id = NM1074_Fr13
Solvent = CHLOROFORM-D
Creation_Time = 30-JAN-2023 18:41:17
Revision_Time = 30-JAN-2023 20:59:58
Current_Time = 30-JAN-2023 21:00:12

Comment = NM1074_Fr13
Data_Format = 1D COMPLEX
Dim_Size = 32768
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Spectrometer = BRUKER_DMX_NMR

Field_Strength = 7.0492145[T] (300[MHz])
X_Domain = 1H
X_Freq = 300.13185343[MHz]
X_Freq_Flip = TRUE
X_Offset = 1.85342561[kHz]
X_Points = 32768
X_Prescans = 2
X_Sweep = 6.18811881[kHz]
Scans = 16

Temp_Get = 294.46[K]
Filter_Factor = 3232





---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexf(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm

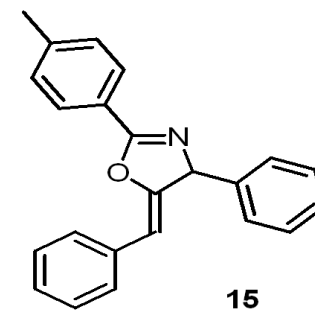
以下に由来: Morita_3090-1.jdf

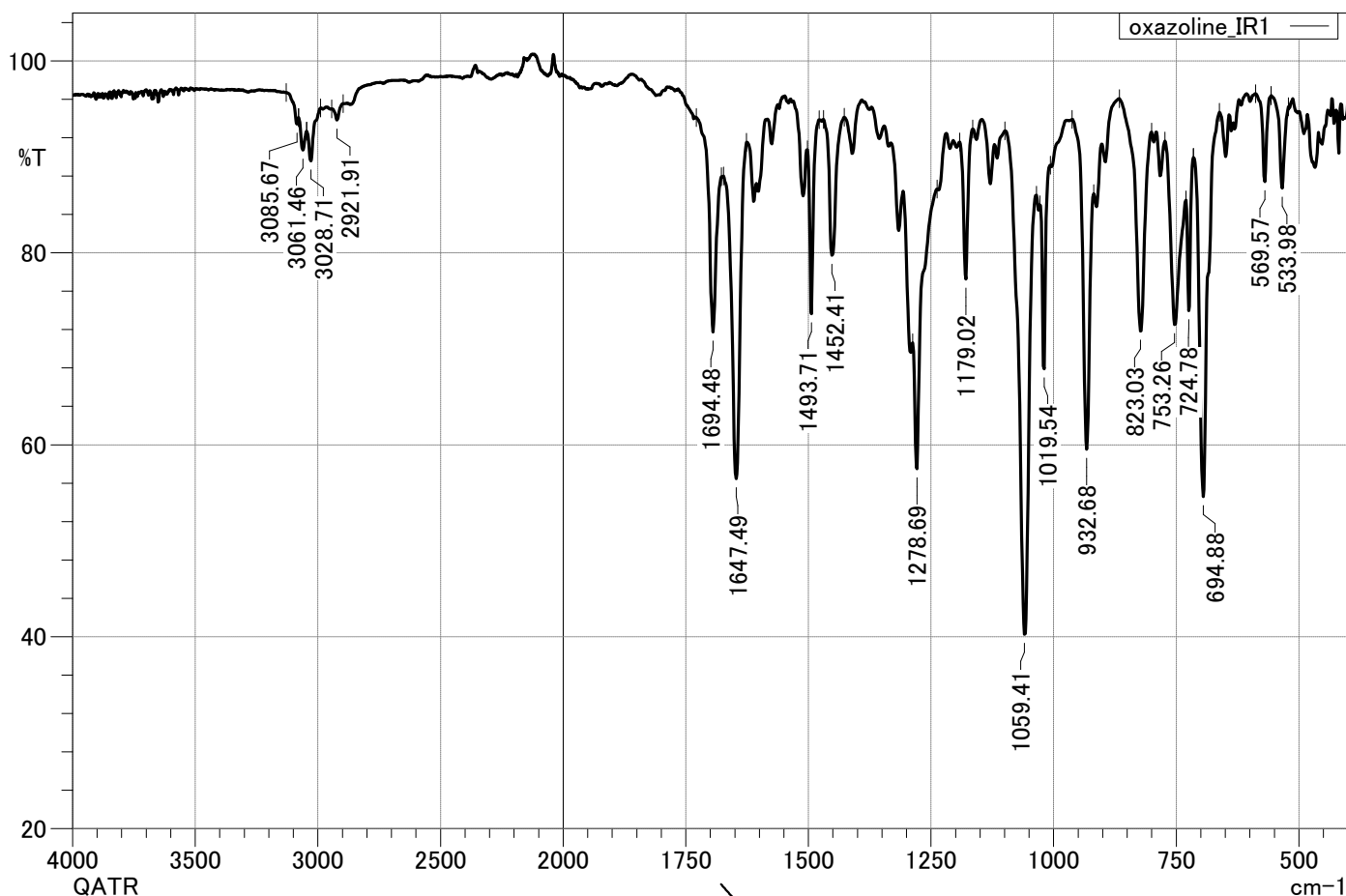
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Author = Administrator
Experiment = zgpg30
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Solvent = CHLOROFORM-D
Creation_Time = 31-JAN-2023 10:24:48
Revision_Time = 31-JAN-2023 10:25:03
Current_Time = 31-JAN-2023 10:26:41

Comment = NM1074_Fr13
Data_Format = 1D COMPLEX
Dim_Size = 32768
Dim_Title = ¹³C
Dim_Units = [ppm]
Dimensions = X
Spectrometer = BRUKER_DMX_NMR

Field_Strength = 7.0492145[T] (300[MHz])
X_Domain = ¹³C
X_Freq = 75.4752953[MHz]
X_Freq_Flip = TRUE
X_Offset = 7.54630085[kHz]
X_Points = 32768
X_Prescans = 4
X_Sweep = 18.02884615[kHz]
Scans = 10000

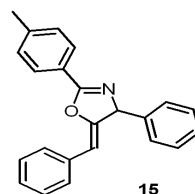
Temp_Get = 296.06[K]
Filter_Factor = 1109





C:\Users\admin\Desktop\2018\千秋\oxazoline_IR1.ispd

QATR



	パラメータ	値
2	サンプル名	
3	サンプルID	
4	オプション	
5	測定モード	透過率
6	アボタイズ関数	SqrTriangle
9	積算回数	45
10	分解	4 cm ⁻¹

	ピーク	高さ	補正高さ	ベース (H)	ベース (L)	面積	補正面積	コメント
1	533.98	86.73	8.91	556.76	521.16	245.694	96.497	
2	569.57	87.43	9.05	588.08	556.76	192.310	82.710	
3	694.88	54.62	37.10	714.81	662.13	1072.487	666.028	
4	724.78	73.99	13.10	730.48	714.81	272.852	80.224	
5	753.26	72.53	16.25	773.20	730.48	802.422	314.049	
6	823.03	71.86	21.94	865.75	800.25	829.453	458.242	
7	932.68	59.52	29.15	962.58	918.44	833.930	394.455	
8	1019.54	67.92	18.74	1028.08	1006.72	399.332	123.223	
9	1059.41	40.26	48.29	1099.28	1035.20	1771.336	1089.857	
10	1179.02	77.28	14.91	1191.83	1164.78	354.269	144.003	
11	1278.69	57.51	15.87	1287.24	1237.40	1167.891	103.300	
12	1452.41	79.74	14.27	1469.50	1426.78	469.036	214.224	
13	1493.71	73.65	18.20	1502.25	1478.04	318.202	132.026	
14	1647.49	56.46	33.46	1673.12	1626.13	1093.803	612.787	
15	1694.48	71.74	18.24	1728.66	1677.39	718.269	257.490	
16	2921.91	93.85	1.41	2943.27	2897.71	239.085	24.118	
17	3028.71	89.59	3.81	3045.80	2988.84	419.096	70.782	
18	3061.46	90.72	2.64	3078.55	3045.80	259.278	42.875	
19	3085.67	93.44	1.04	3129.81	3078.55	231.974	-3.003	

[Elemental Composition]

Data : Yakukagaku-Morita-004

Date : 01-Feb-2023 09:38

Sample: NM1074-Fr13

Note : -

Inlet : Reserv.

Ion Mode : EI+

RT : 0.90 min

Scan#: 28

Elements : C 40/0, H 49/0, N 1/1, O 1/1

Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5

Unsaturation (U.S.) : -0.5 - 20.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
325.1473	100.0	+2.0 / +0.6	15.0	C 23 H 19 N O

