

Supplementary Material

Variation of the bromination site on the reaction of (*E*)-1-[5-methyl-1-(aryl)-1*H*-1,2,3-triazol-4-yl]-3-arylprop-2-en-1-ones with *N*-bromosuccinimide

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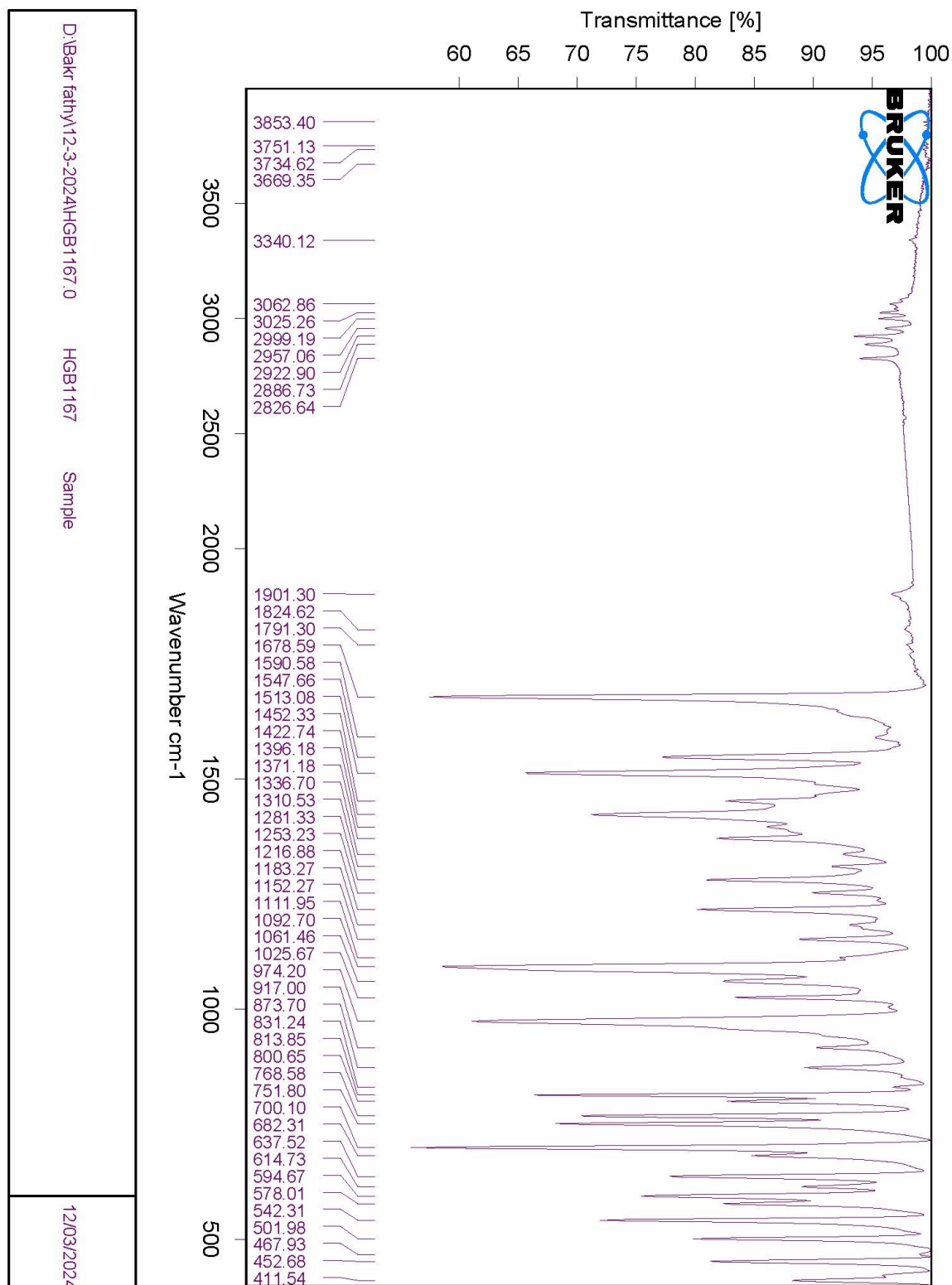


Figure S1. FTIR spectrum of 2.

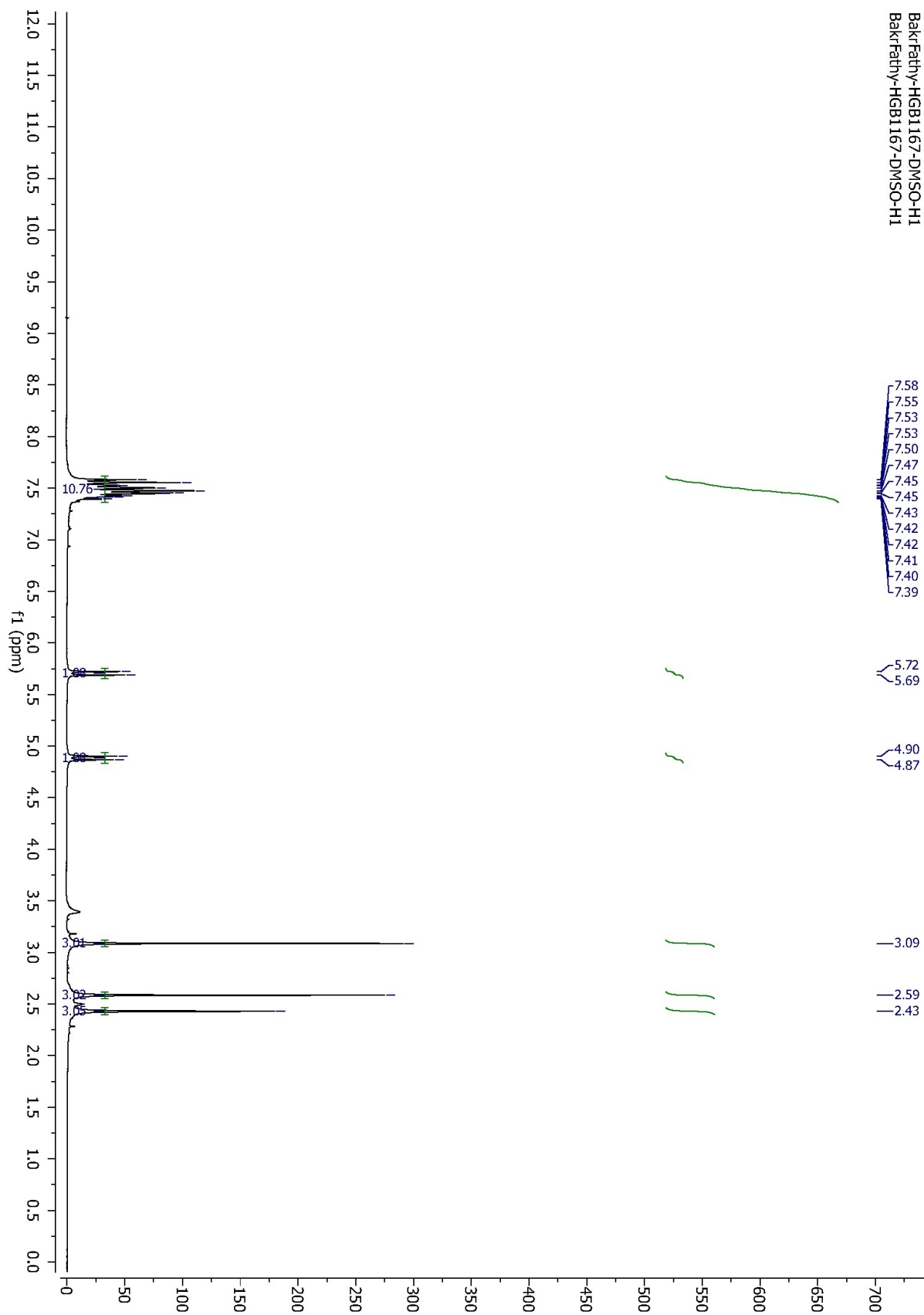
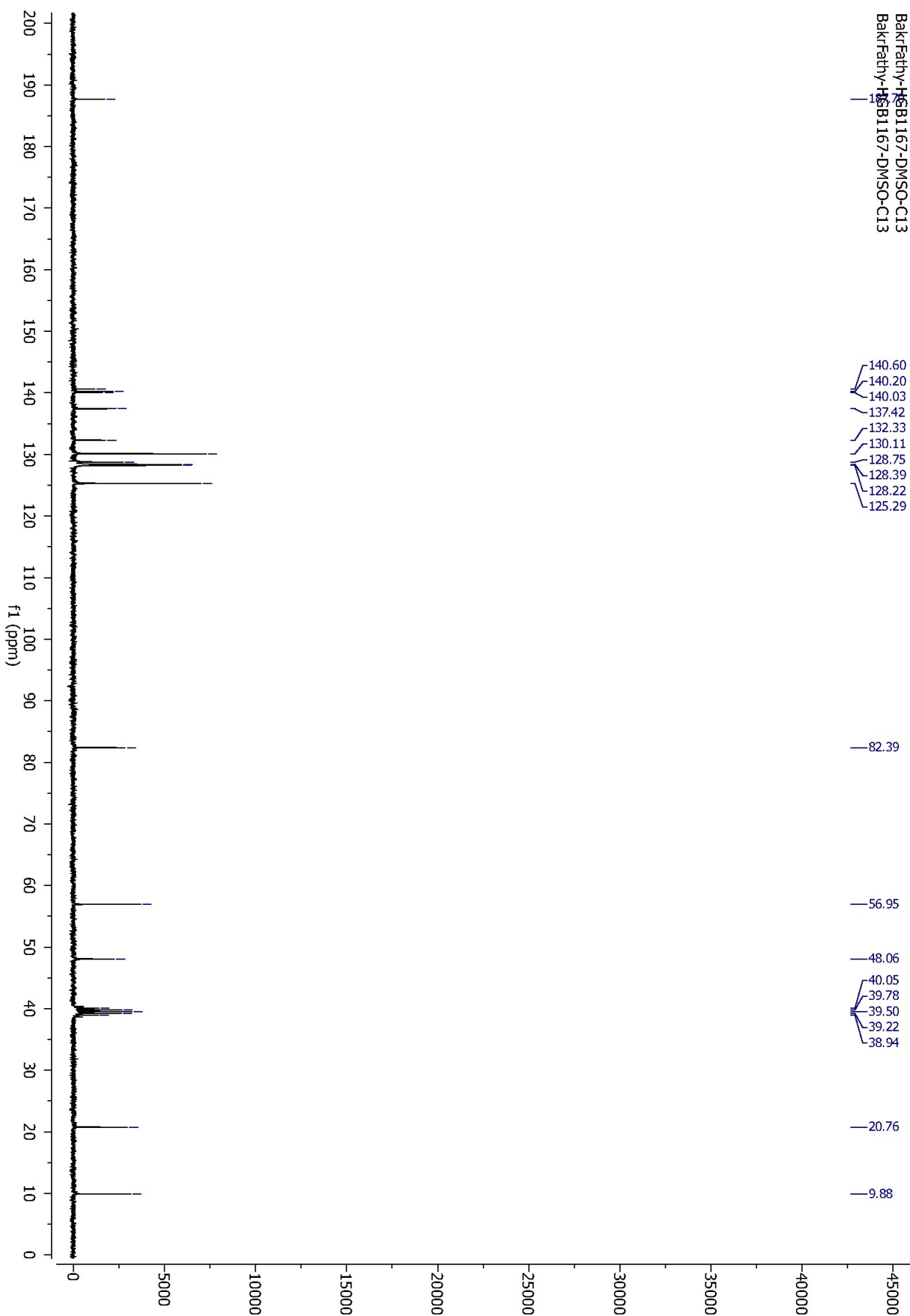


Figure S2. ^1H NMR spectrum of **2**.

Figure S3. ^{13}C NMR spectrum of 2.

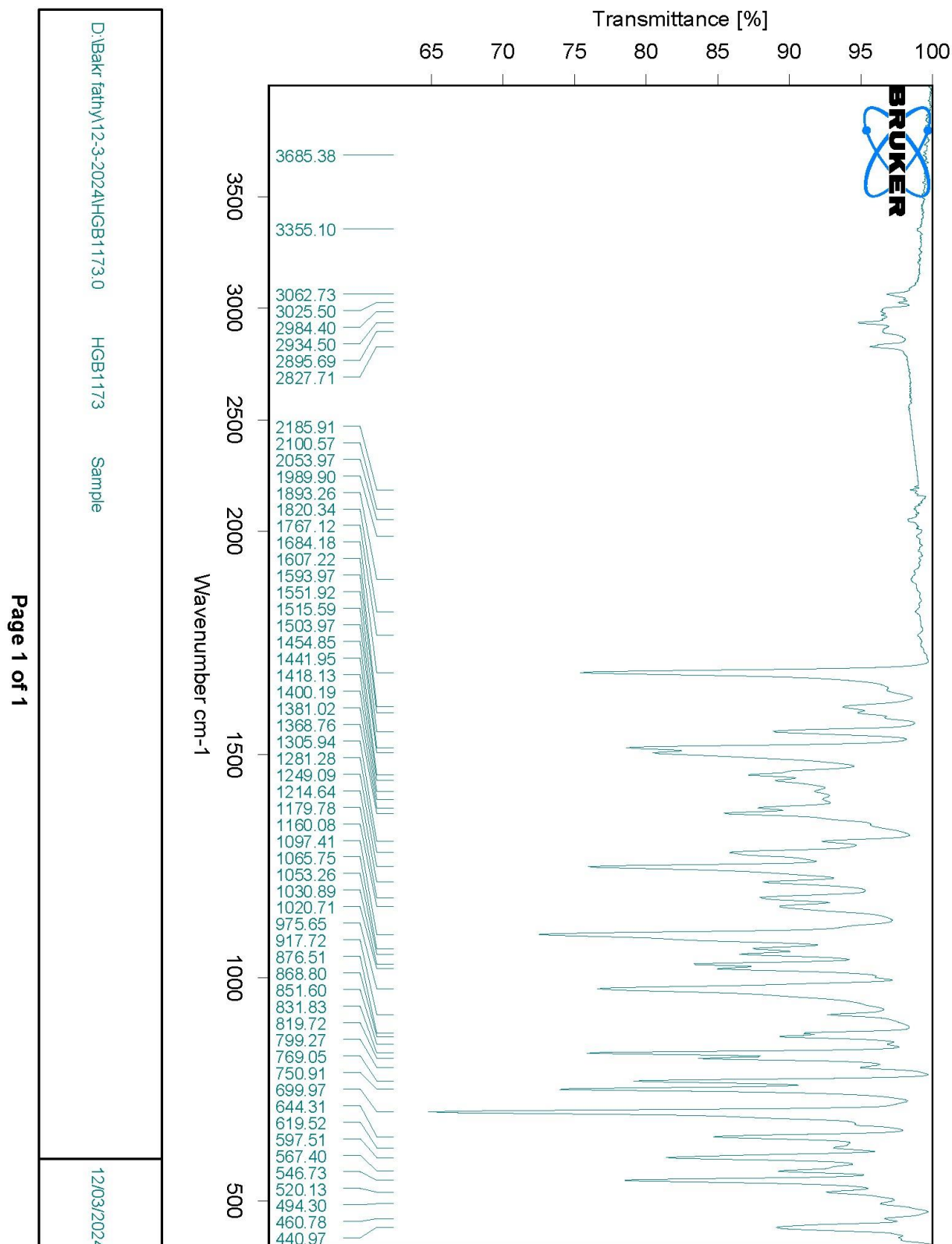
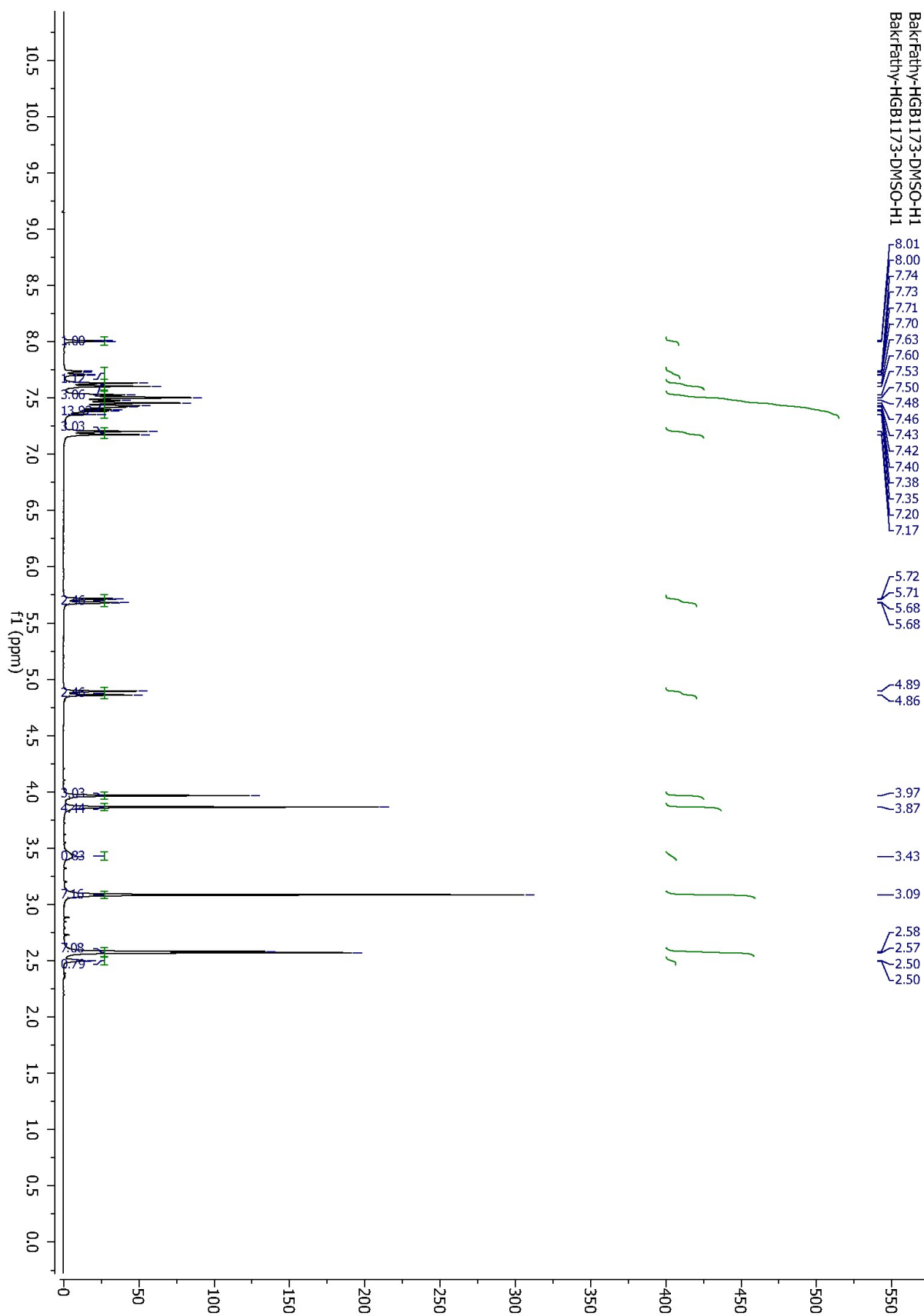
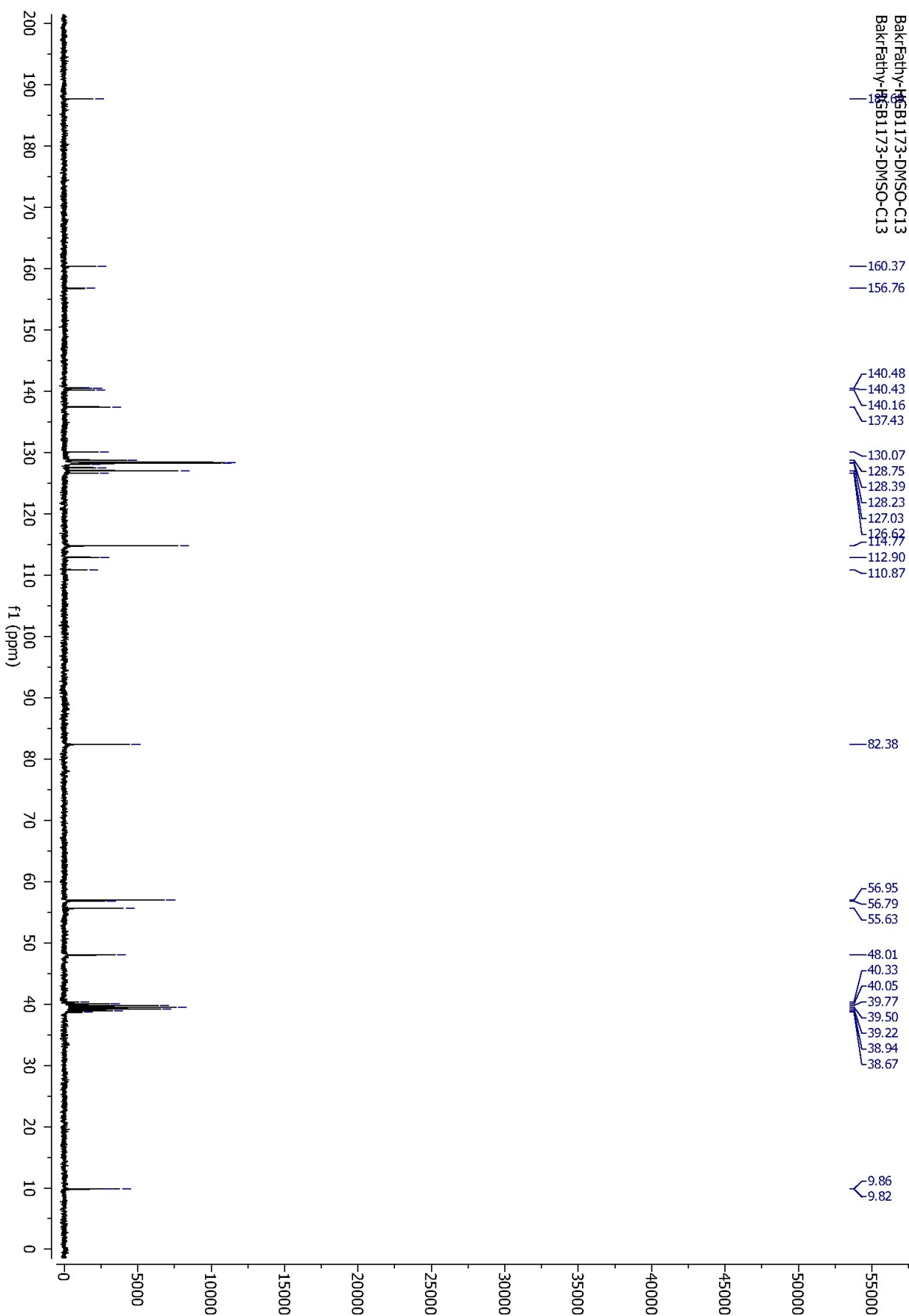


Figure S4. FTIR spectrum of 3.

Figure S5. ¹H NMR spectrum of 3.

Figure S6. ^{13}C NMR spectrum of **3**.

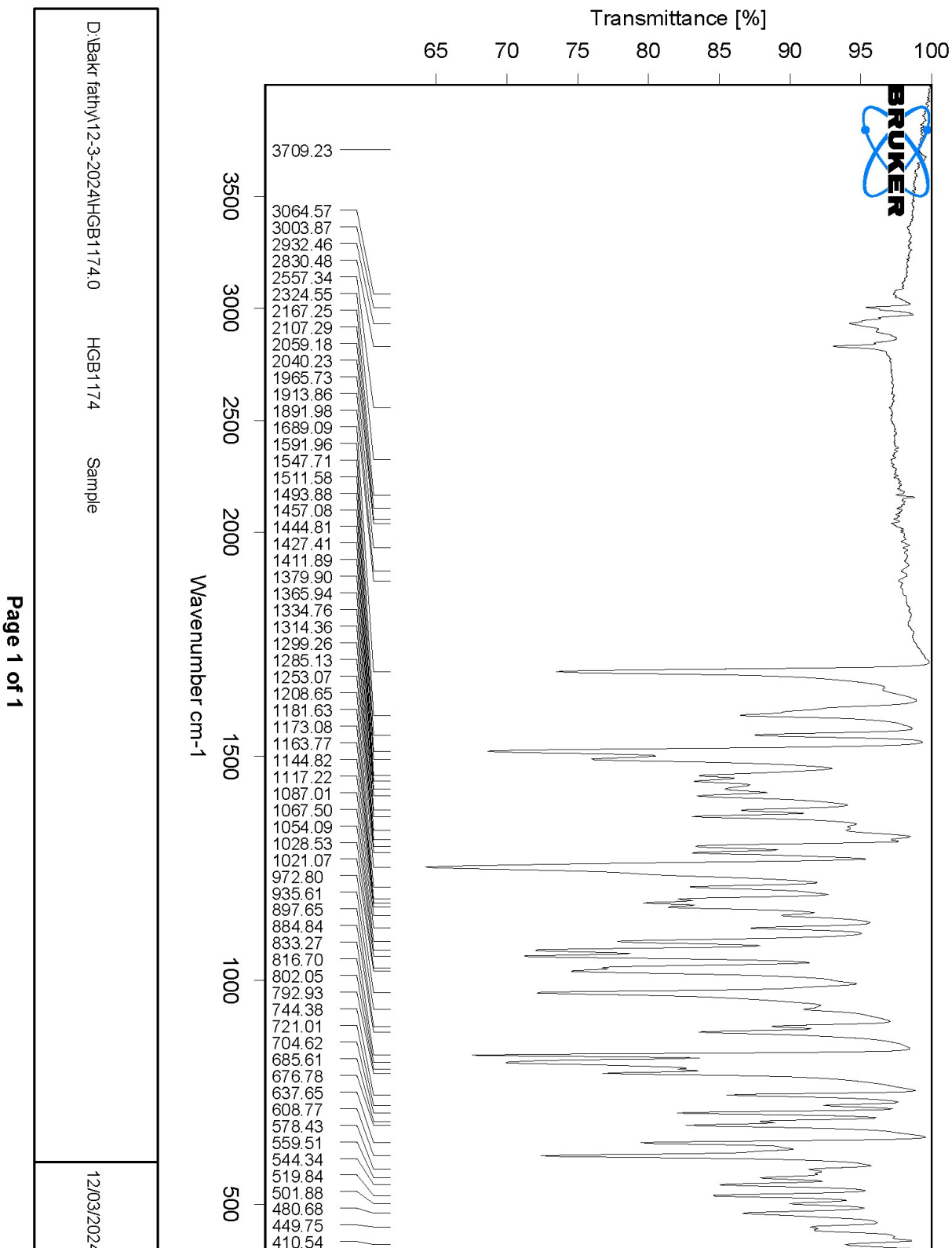
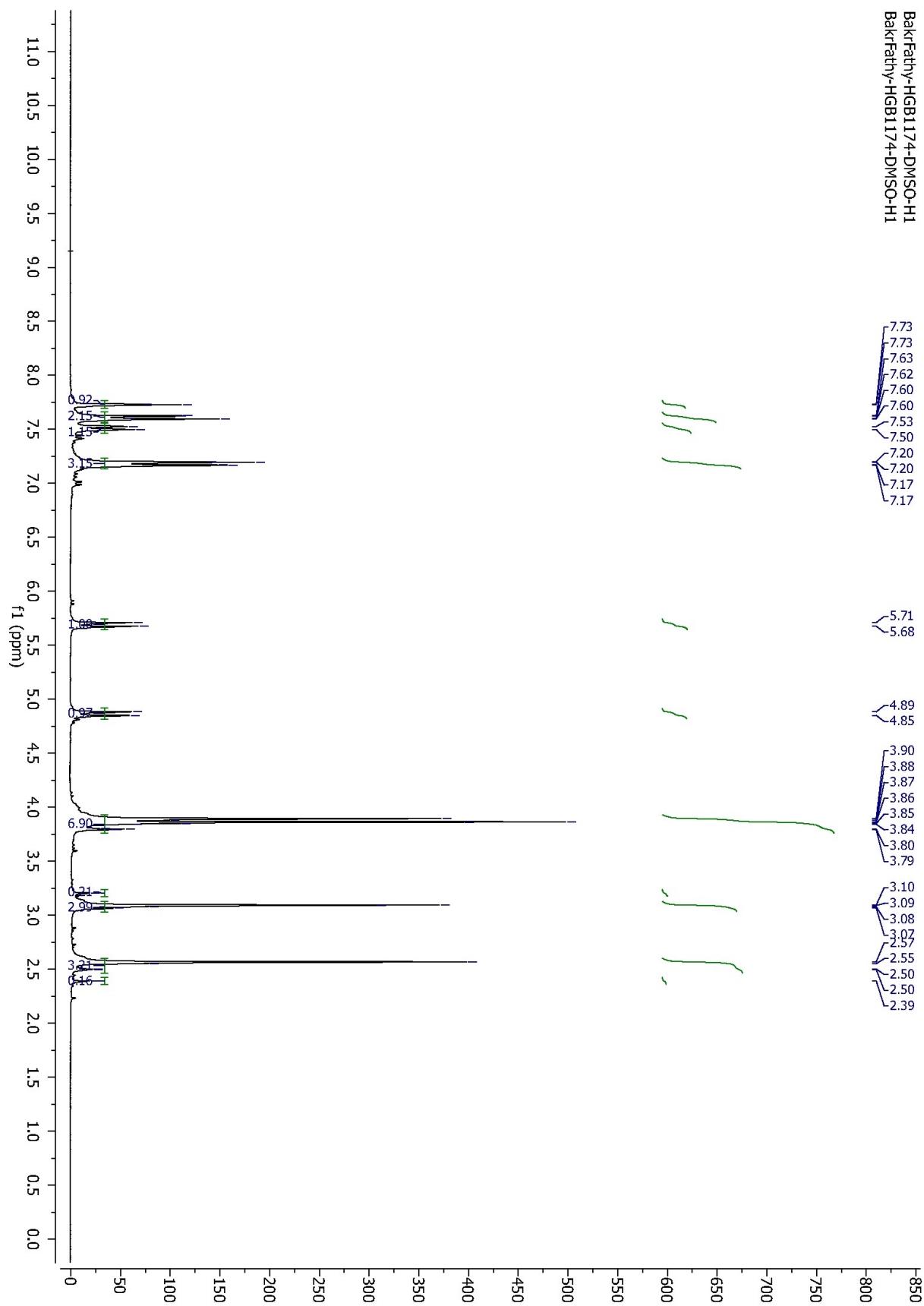
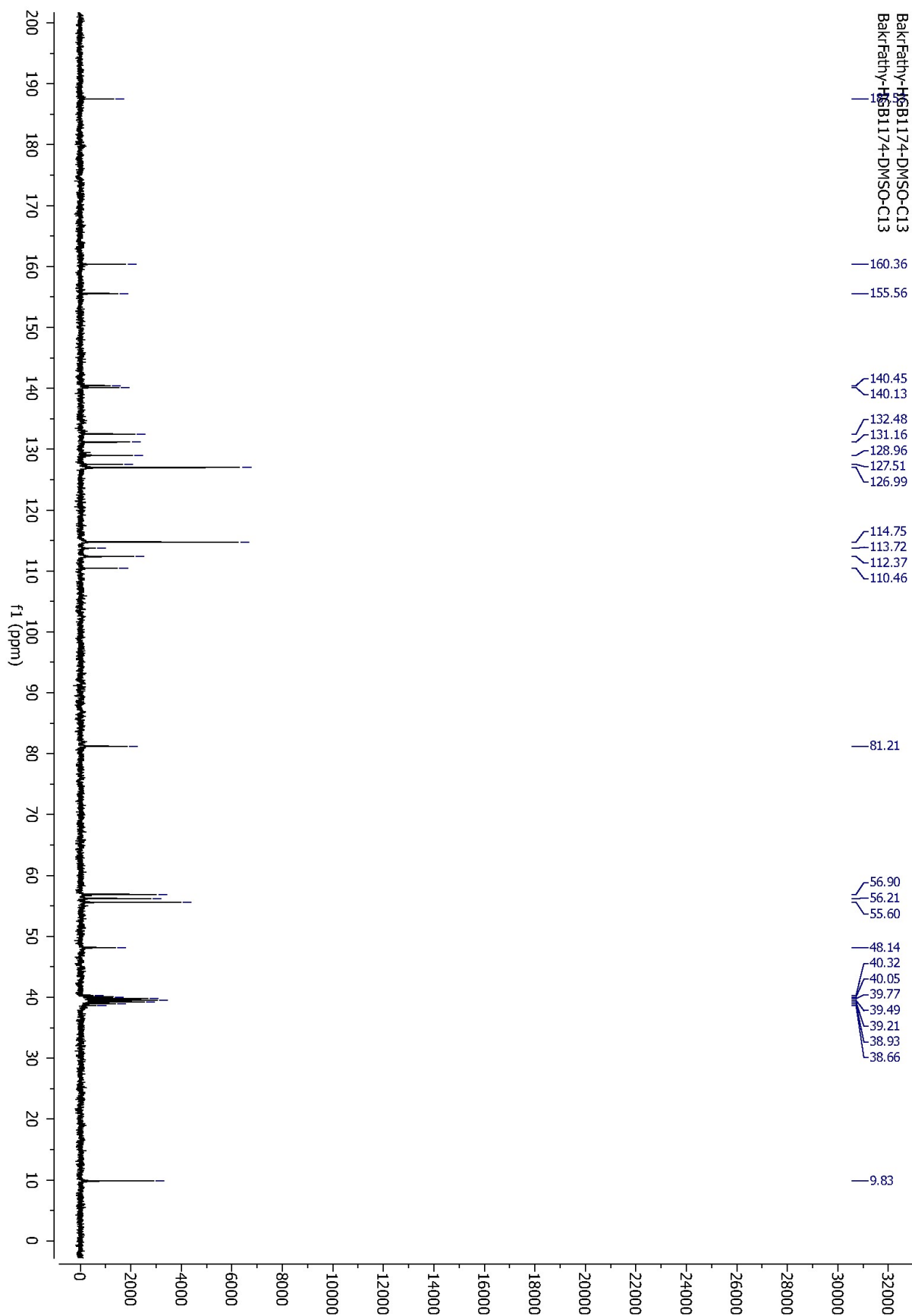


Figure S7. FTIR spectrum of 4.

Figure S8. ^1H NMR spectrum of **4**.

Figure S9. ¹³C NMR spectrum of 4.

CheckCIF of 2–4

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level C

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note
 1 1 0, 2 0 0, -1 0 1, -1 1 1, 0 1 1, 1 0 1,
 -2 0 2, 0 0 2,

Alert level G

PLAT480_ALERT_4_G Long H...A H-Bond Reported H6 ..BR1 . 3.09 Ang.
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 705 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.7 Low
 PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 2 Units
 PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 2 Units
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.33 Note
 Predicted wR2: Based on SigI**2 3.63 or SHELX Weight 11.73
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 8 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 1 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

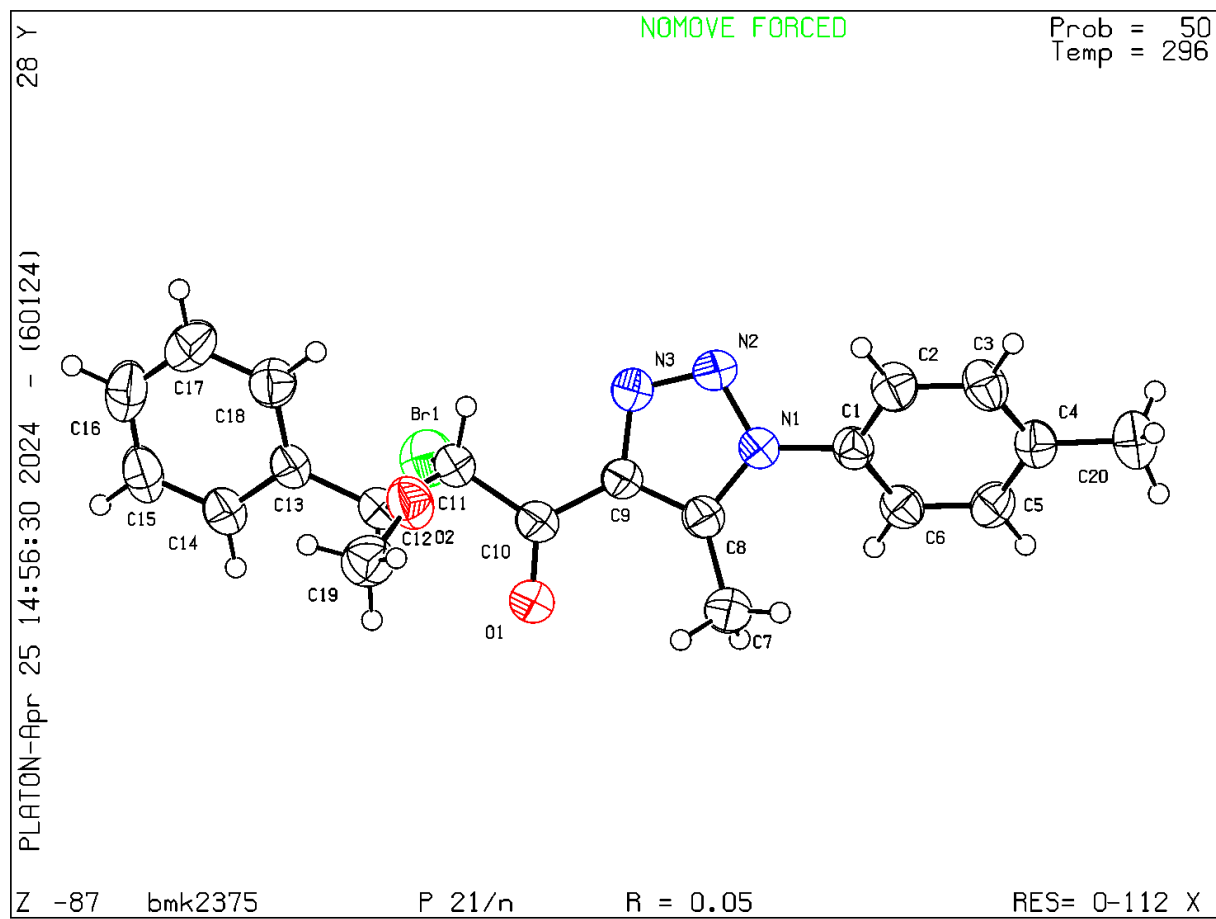
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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Datablock bmk2375 - ellipsoid plot



Check CIF of 3

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bmk2378

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: bmk2378

Bond precision:	C-C = 0.0054 A	Wavelength=0.71073	
Cell:	a=8.6657(6)	b=11.3808(7)	c=11.7740(8)
	alpha=66.237(6)	beta=77.532(6)	gamma=74.221(6)
Temperature:	293 K		
	Calculated	Reported	
Volume	1015.21(13)	1015.21(13)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C20 H19.58 Br1.42 N3 O3	?	
Sum formula	C20 H19.58 Br1.42 N3 O3	C20 H19.58 Br1.42 N3 O3	
Mr	463.09	463.44	
Dx, g cm ⁻³	1.515	1.516	
Z	2	2	
Mu (mm ⁻¹)	2.868	2.876	
F000	468.3	469.0	
F000'	467.65		
h, k, lmax	12, 15, 16	11, 15, 16	
Nref	5797	4833	
Tmin, Tmax	0.412, 0.563	0.546, 1.000	
Tmin'	0.264		

Correction method= # Reported T Limits: Tmin=0.546 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.834 Theta(max)= 29.759

R(reflections)= 0.0475(2992) wR2(reflections)=
0.1202(4833)
S = 1.017 Npar= 257

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.



Alert level C

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	9 Note
	1 0 0, 0 1 0, 1 1 0, 0 -1 1, -1 0 1, 0 0 1,	
	1 0 1, 0 1 1, 1 1 1,	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2 Report
	-7 7 3, 1 13 7,	



Alert level G

PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.006 Degree
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	5% Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	939 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.0 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.21 Note
	Predicted wR2: Based on SigI**2 5.44 or SHELX Weight 12.14	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info

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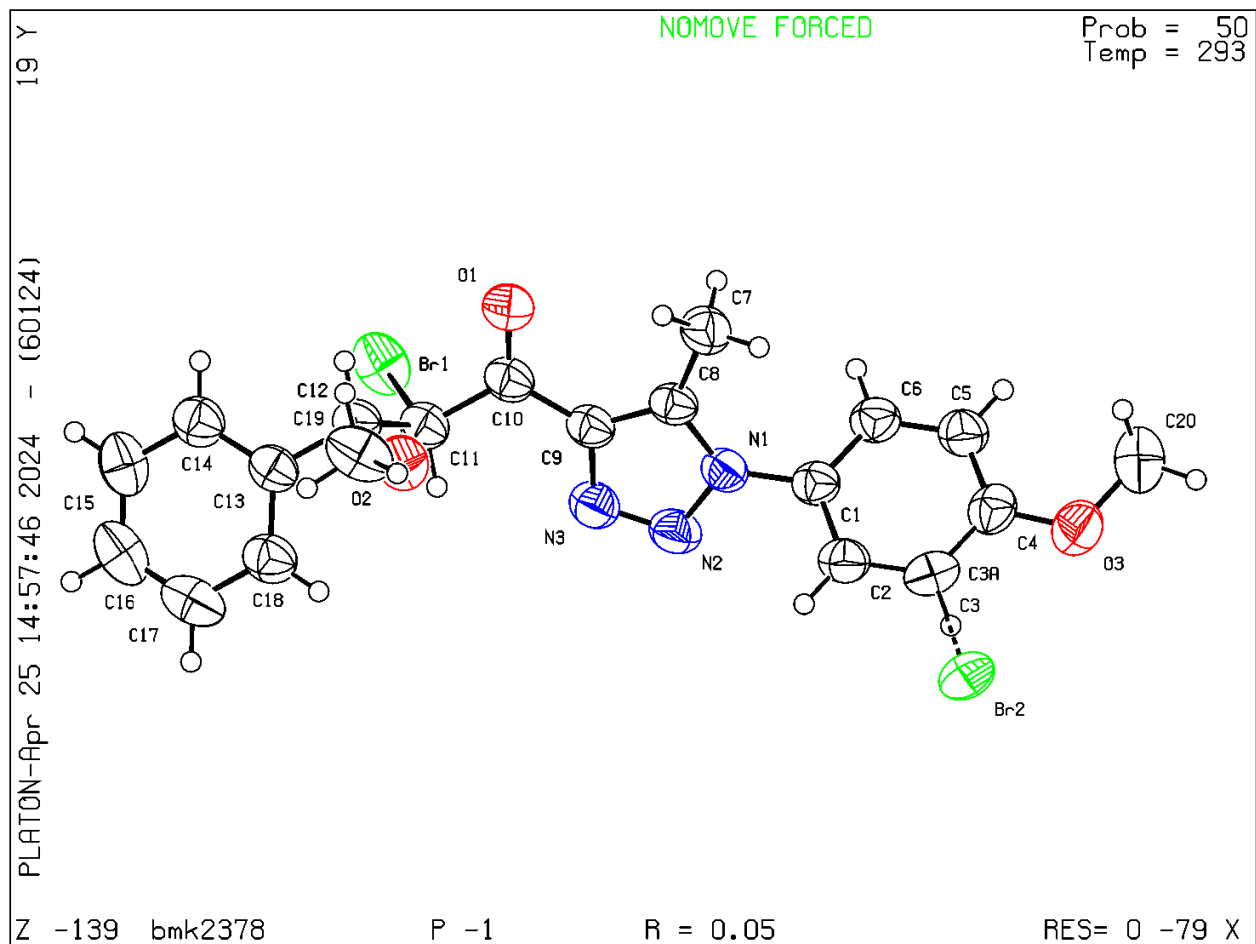
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Datablock bmk2378 - ellipsoid plot



CheckCIF of 4

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bmk2379

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: bmk2379

Bond precision: C-C = 0.0059 Å Wavelength=0.71073

Cell: a=7.9084 (7) b=9.6713 (6) c=14.9540 (12)
alpha=74.369 (6) beta=77.424 (7) gamma=86.856 (6)

Temperature: 293 K

	Calculated	Reported
Volume	1075.02 (15)	1075.02 (15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H21 Br2 N3 O4	?
Sum formula	C21 H21 Br2 N3 O4	C21 H21 Br2 N3 O4
Mr	539.21	539.23
Dx, g cm ⁻³	1.666	1.666
Z	2	2
Mu (mm ⁻¹)	3.803	3.803
F000	540.0	540.0
F000'	539.09	
h, k, lmax	11, 13, 20	10, 13, 20
Nref	6075	5107
Tmin, Tmax	0.176, 0.285	0.274, 1.000
Tmin'	0.087	

Correction method= # Reported T Limits: Tmin=0.274 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.841 Theta(max)= 29.654

R(reflections)= 0.0481 (3498) wR2(reflections)=
S = 1.047 Npar= 275 0.1367 (5107)

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note
 1 0 0, -1 1 0, 0 1 0, 0 -1 1, -1 0 1, 0 0 1,
 1 0 1, 0 1 1, 1 1 1, 0 0 2, 0 1 2,

Alert level G

PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.62 mm
 PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
 PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
 PLAT480_ALERT_4_G Long H...A H-Bond Reported H6 ..BR2 . 3.09 Ang.
 PLAT480_ALERT_4_G Long H...A H-Bond Reported H7C ..BR2 . 3.07 Ang.
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 954 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.0 Low
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.87 Note
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