

Supplementary Information

Structural revision of the Mcl-1 inhibitor MIM1. Synthesis and biological studies on ovarian cancer cells with evaluation of designed analogues.

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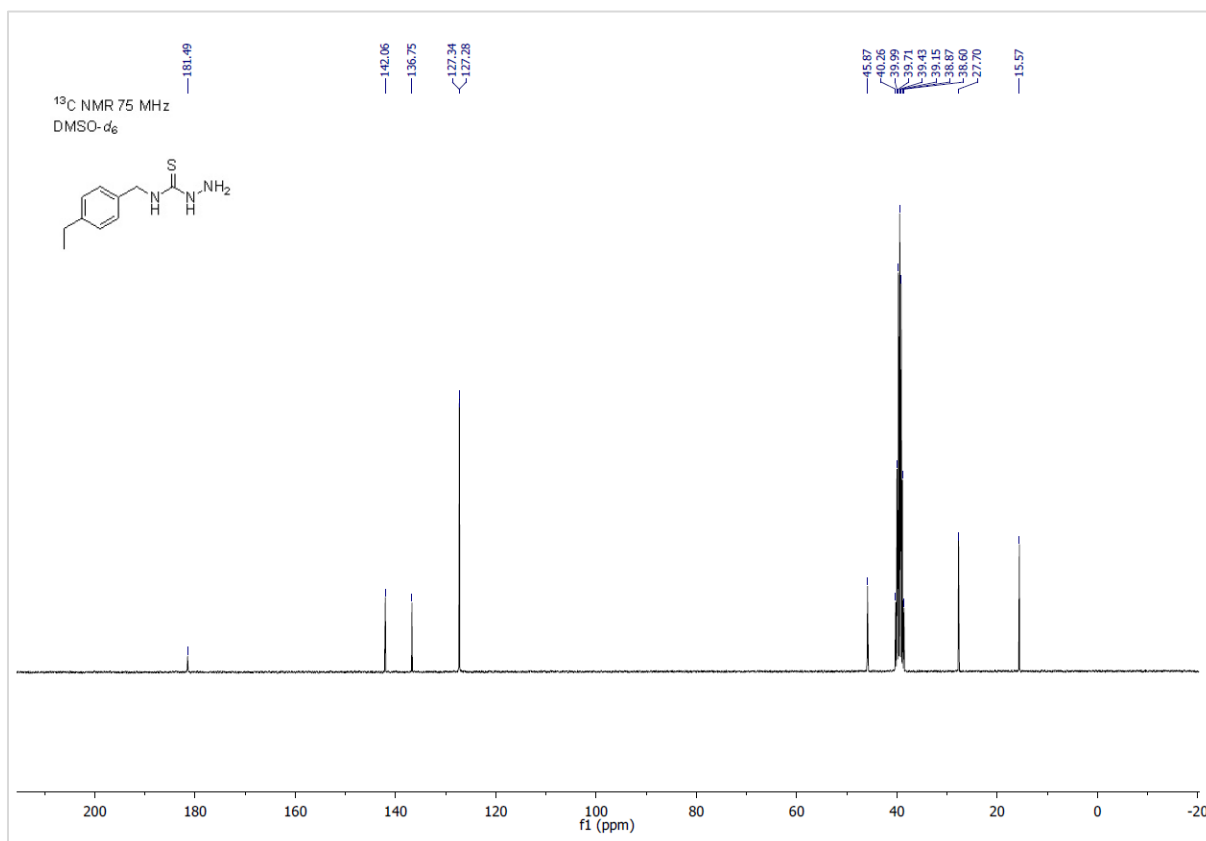
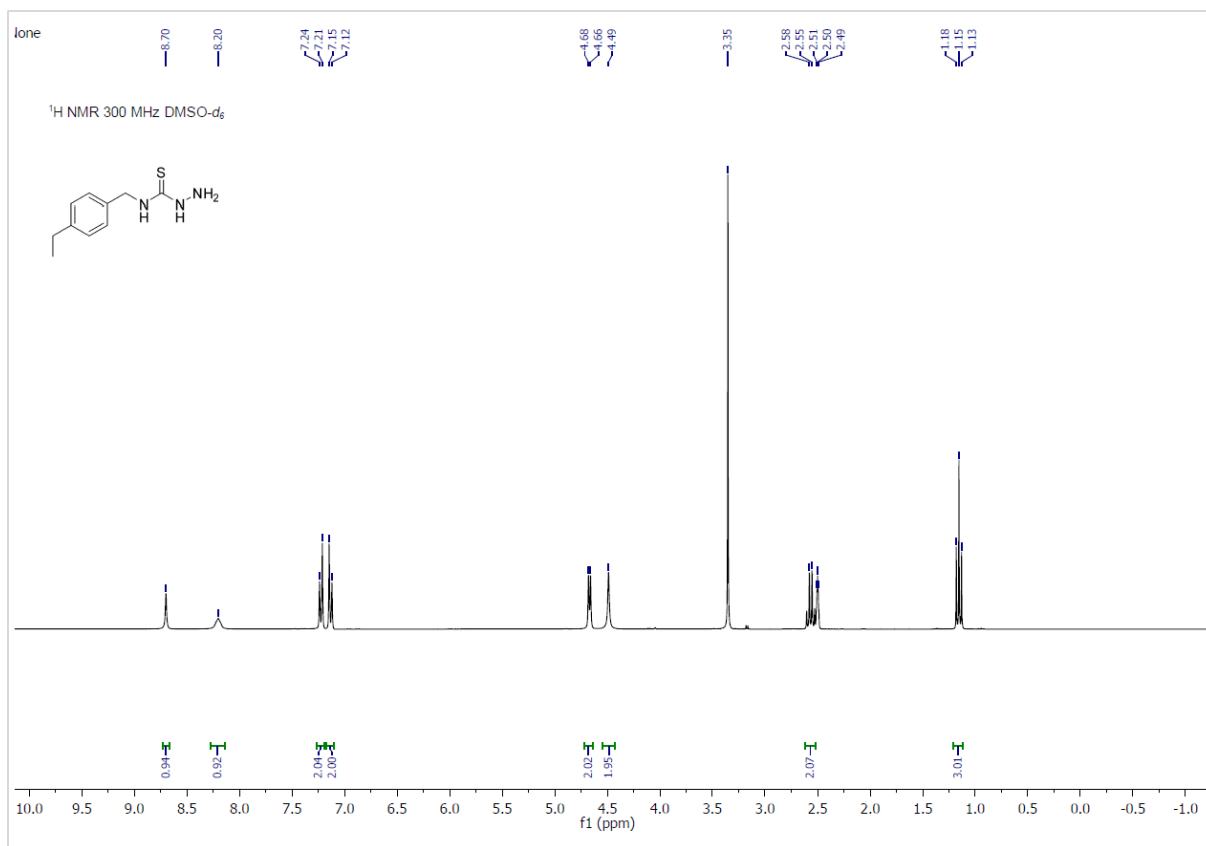
♦ Equal contribution to this work

*co-corresponding authors

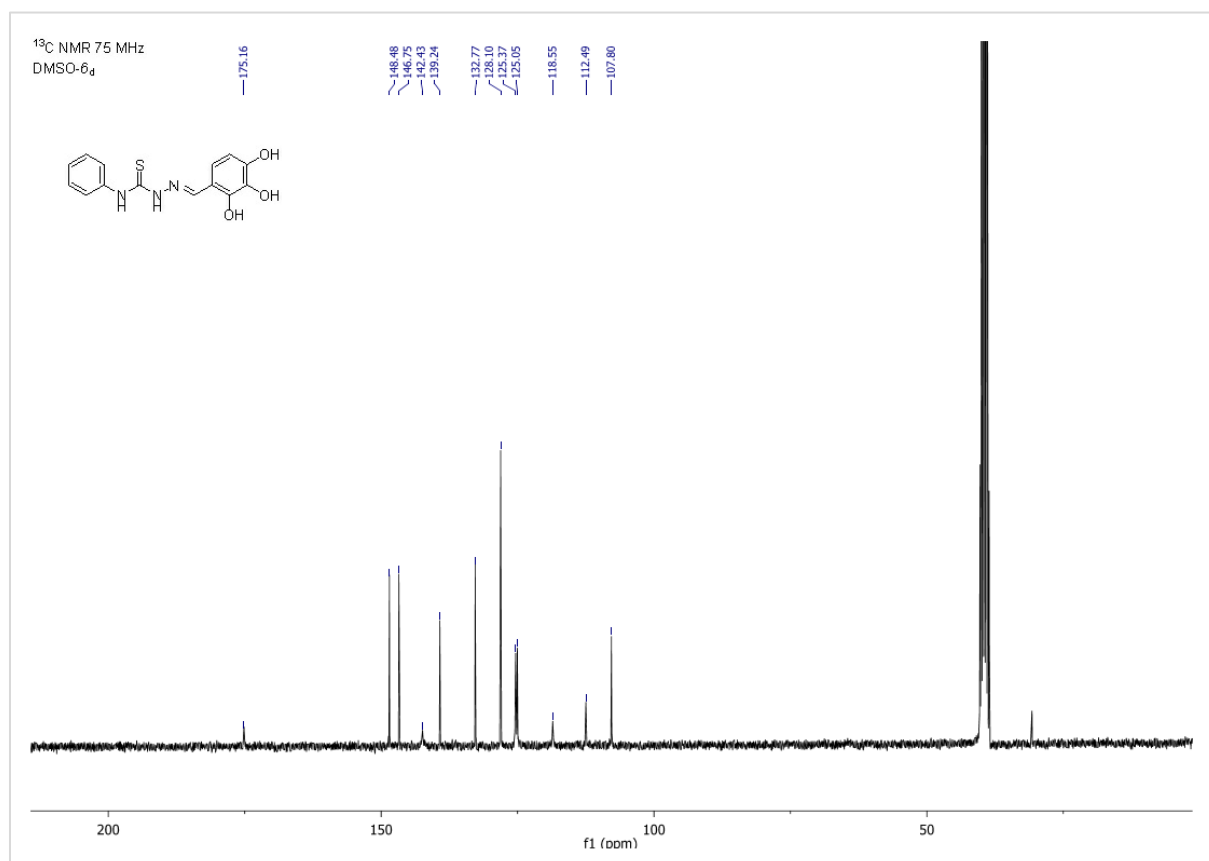
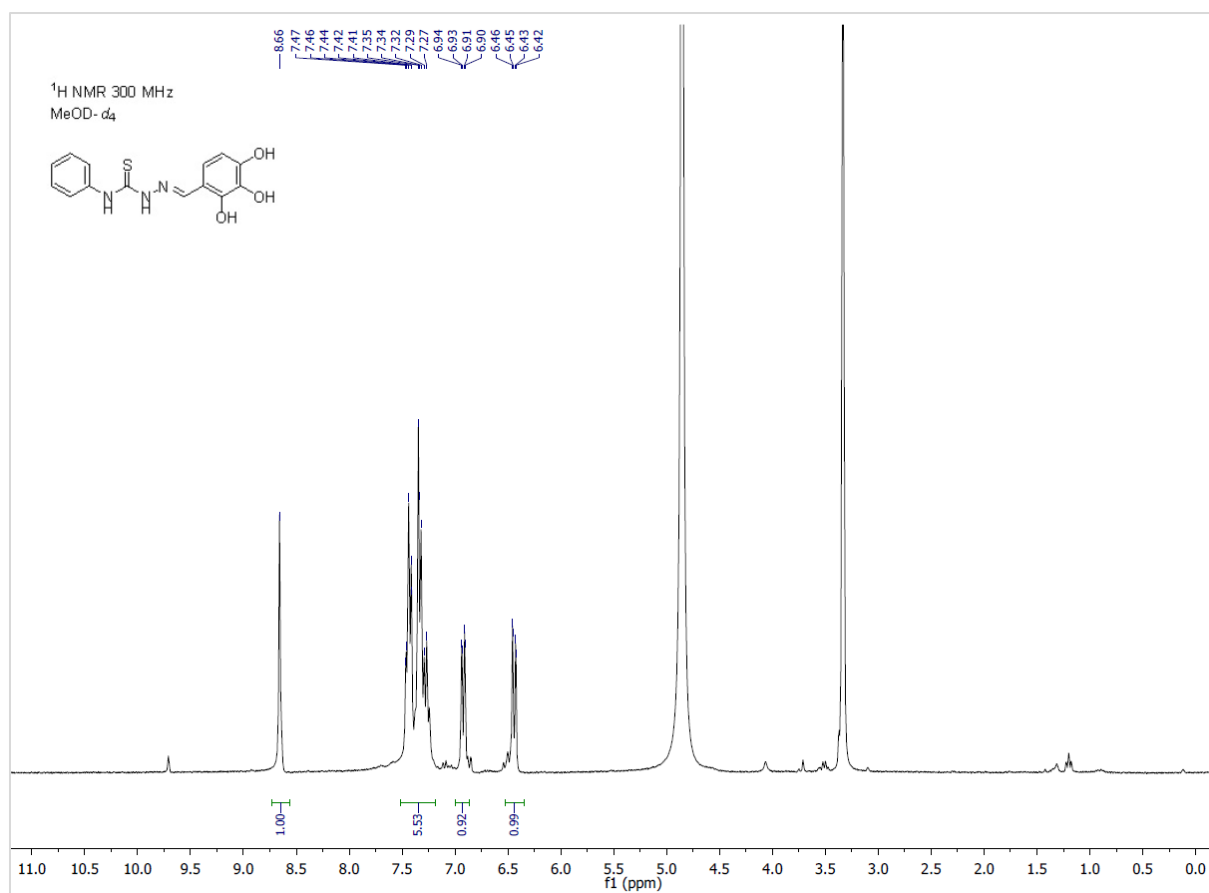
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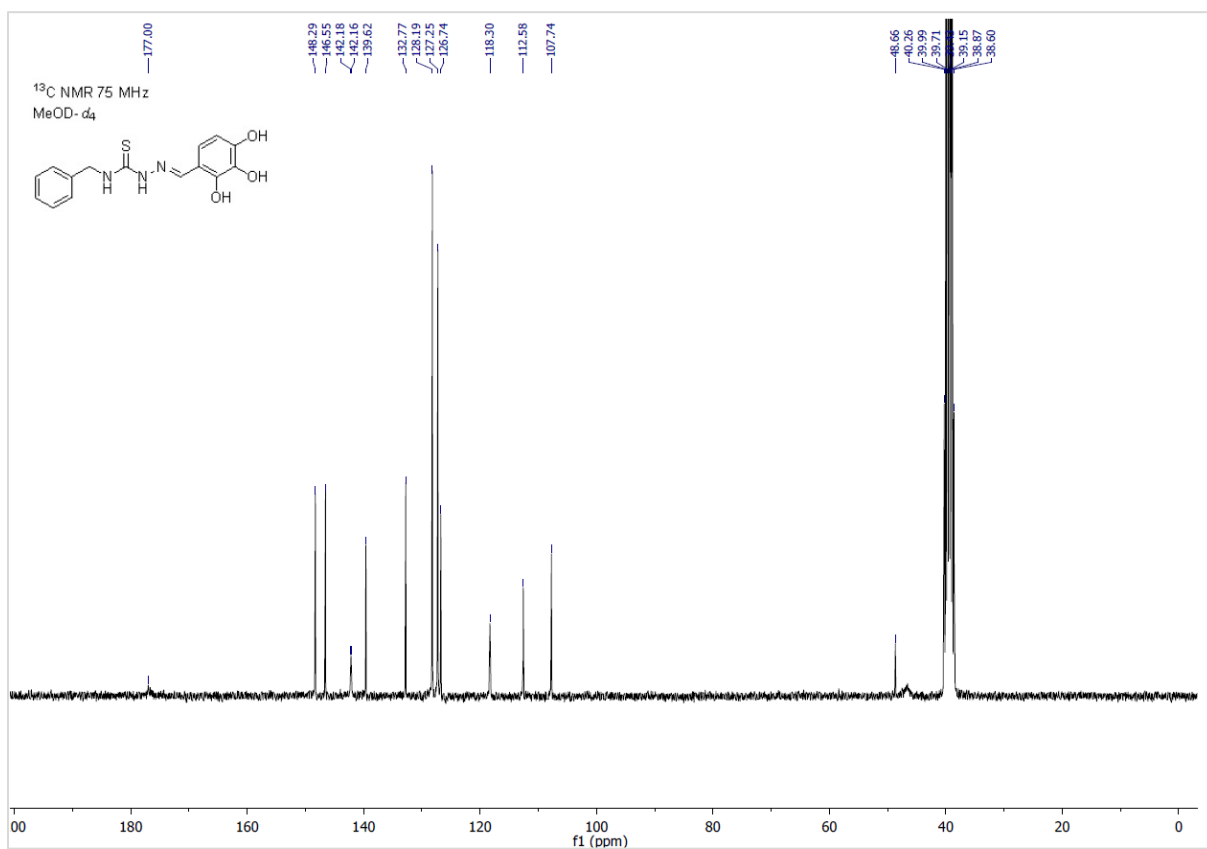
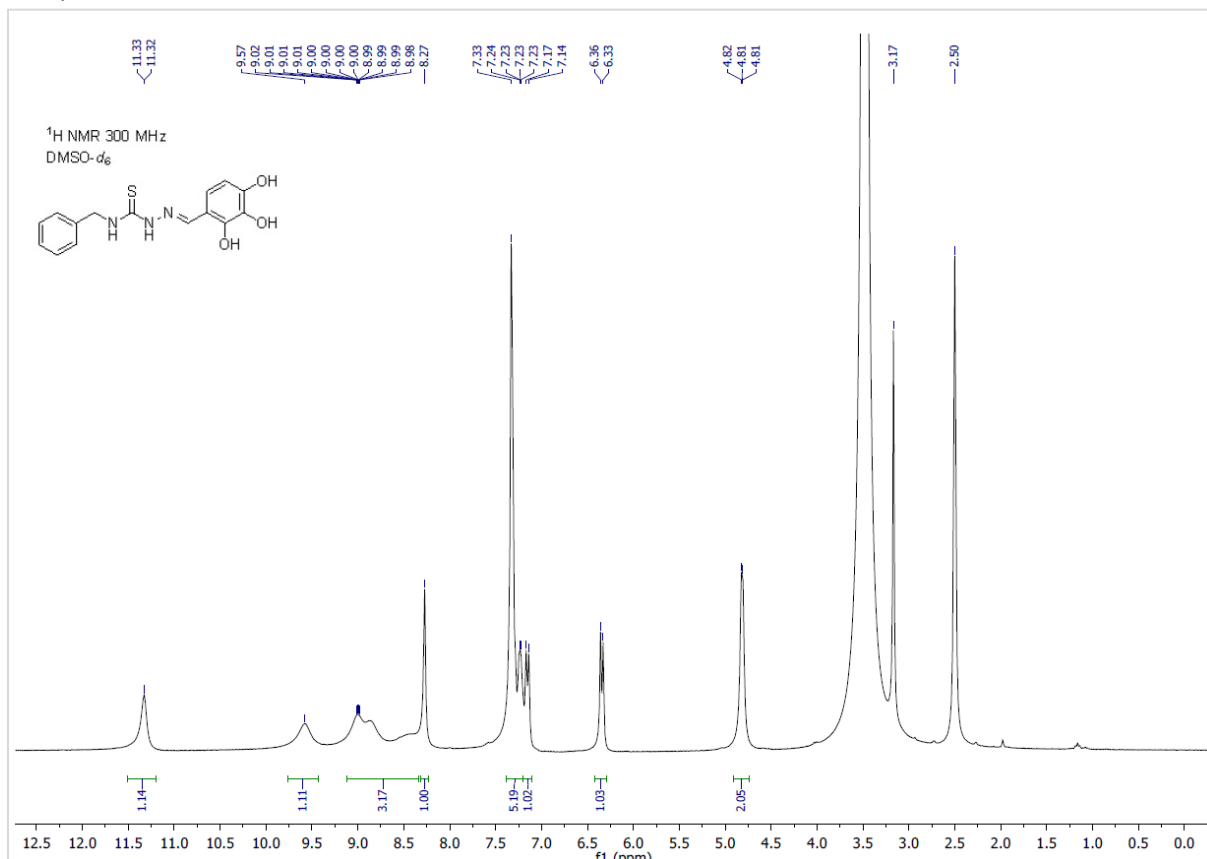
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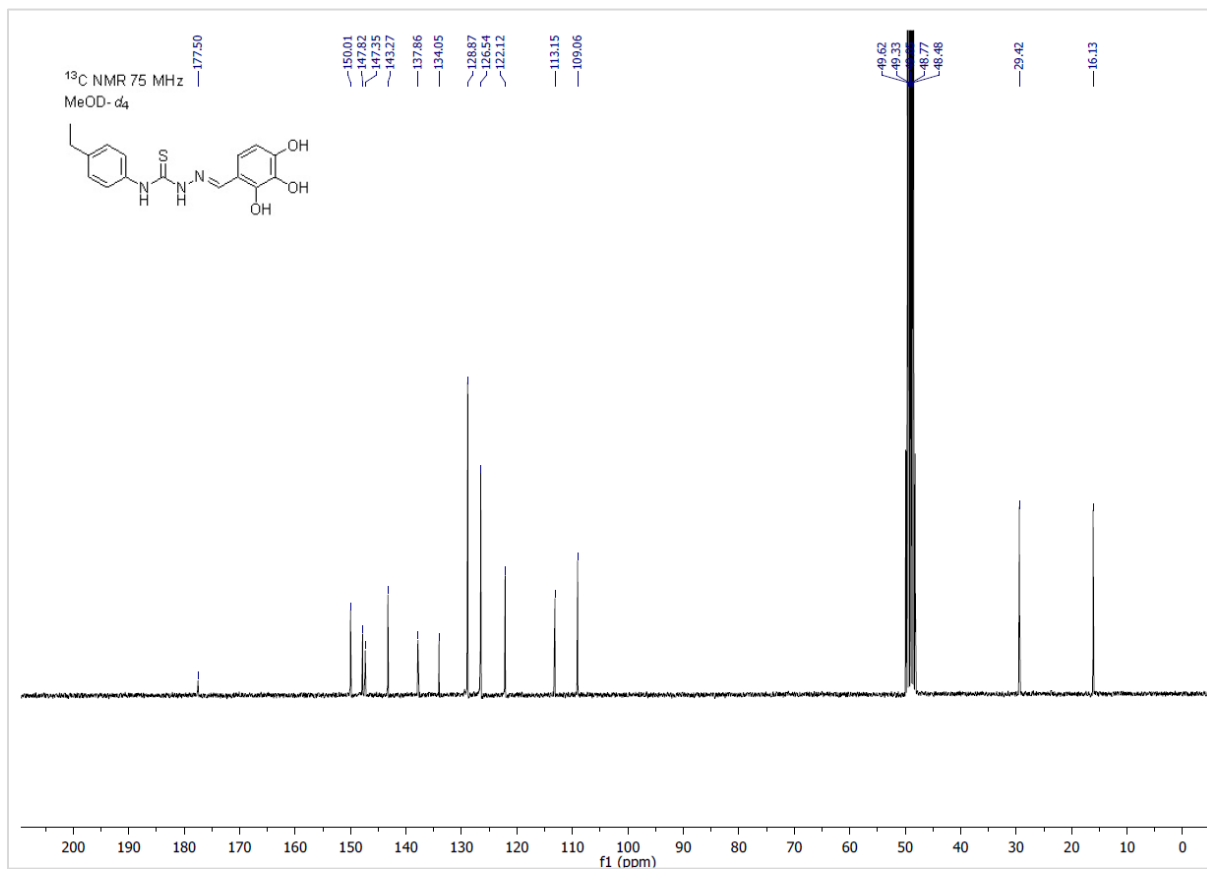
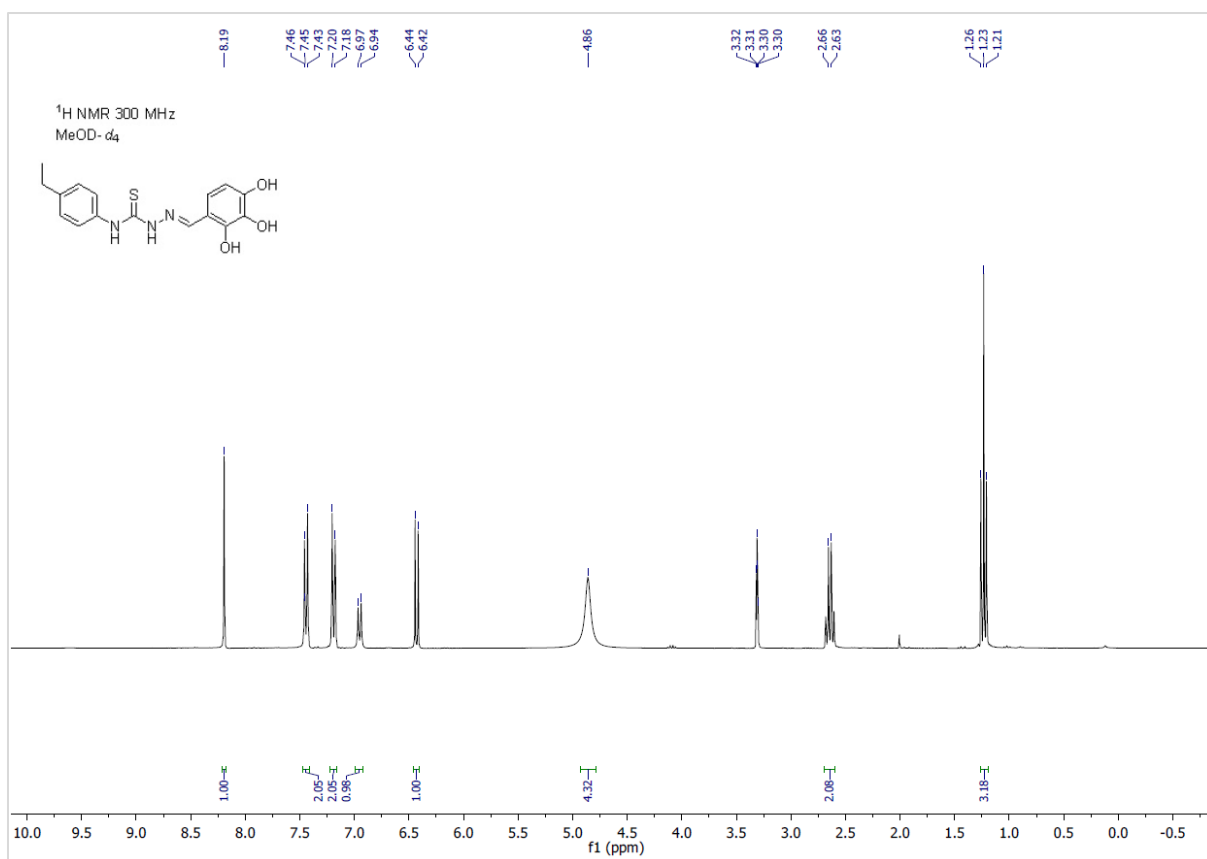
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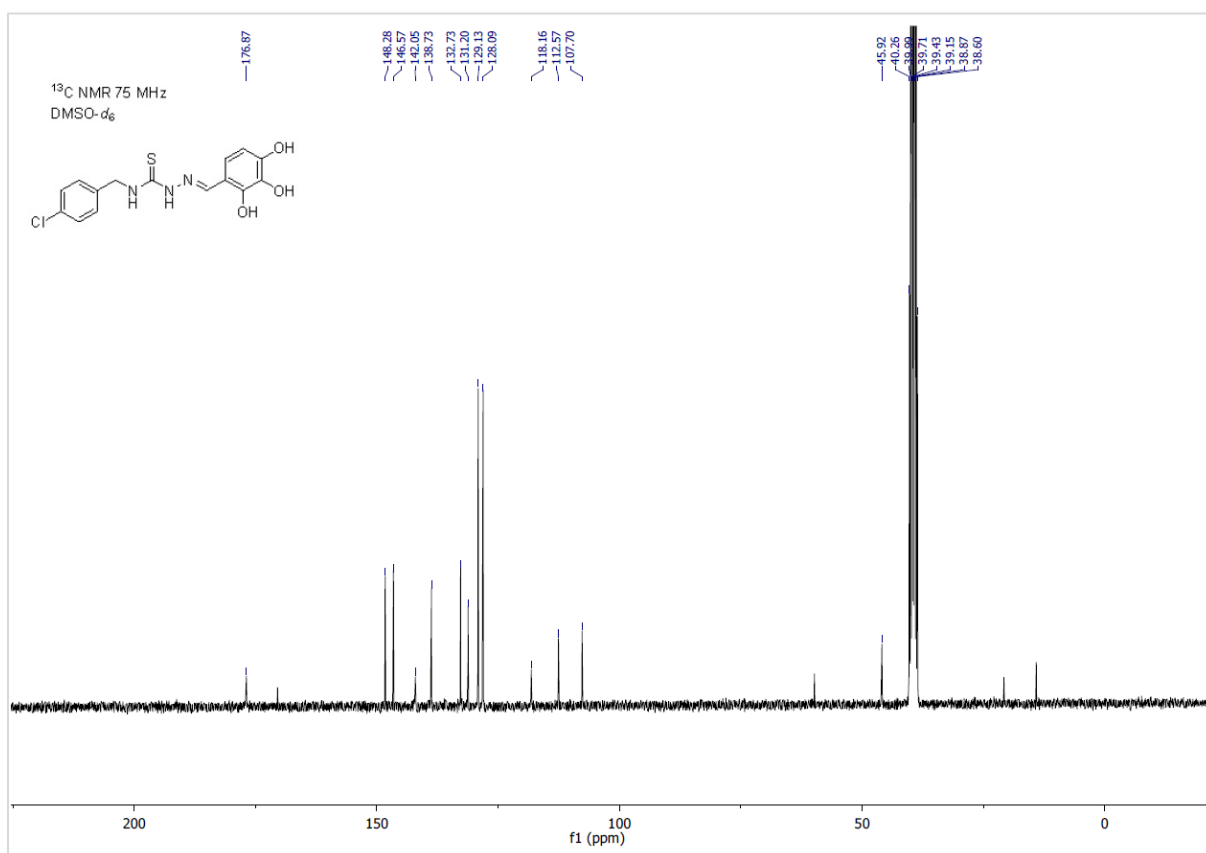
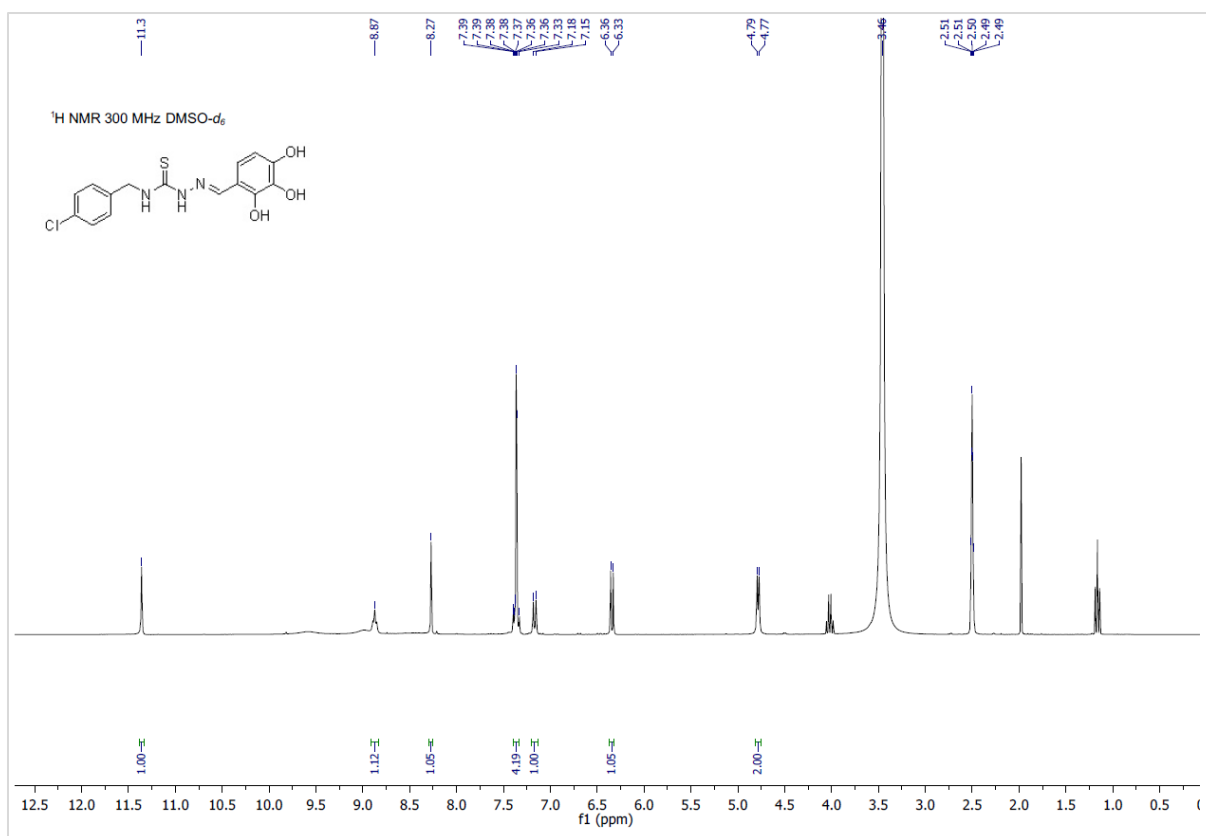
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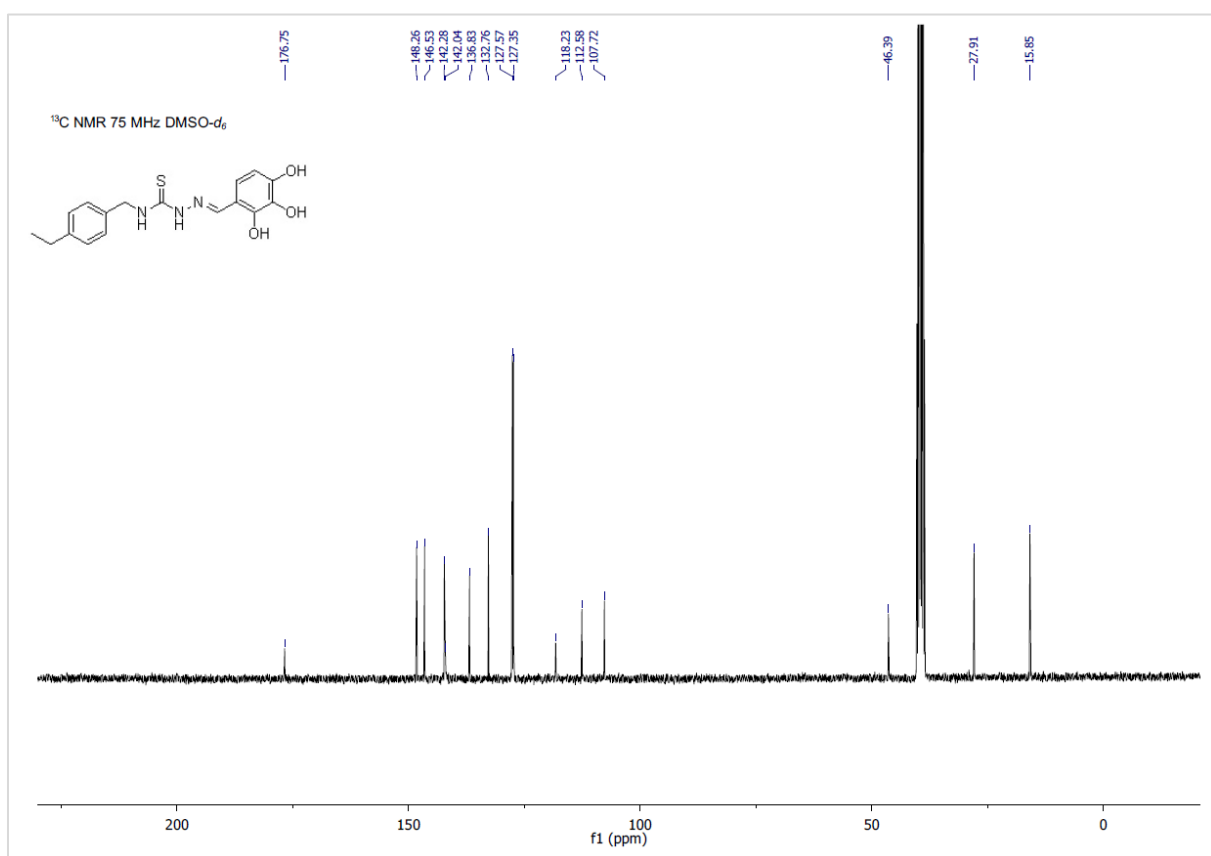
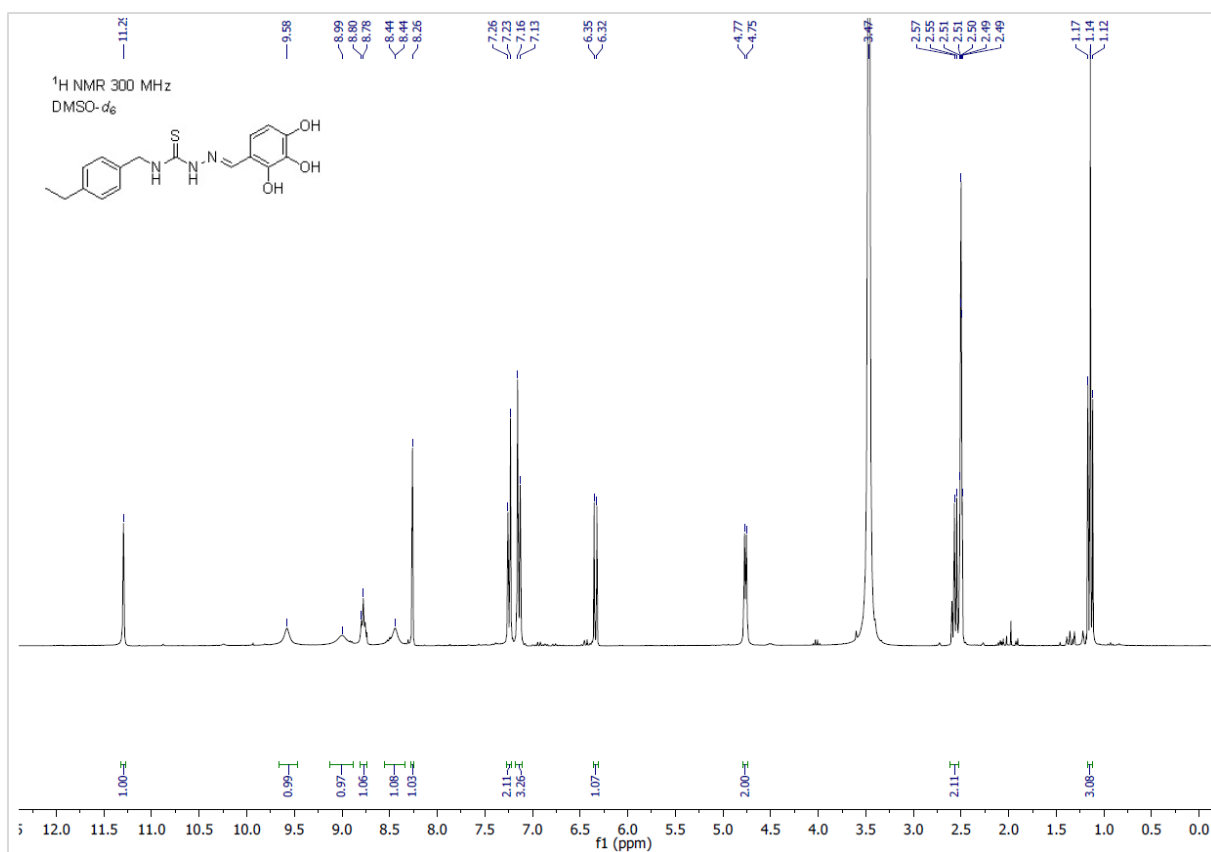
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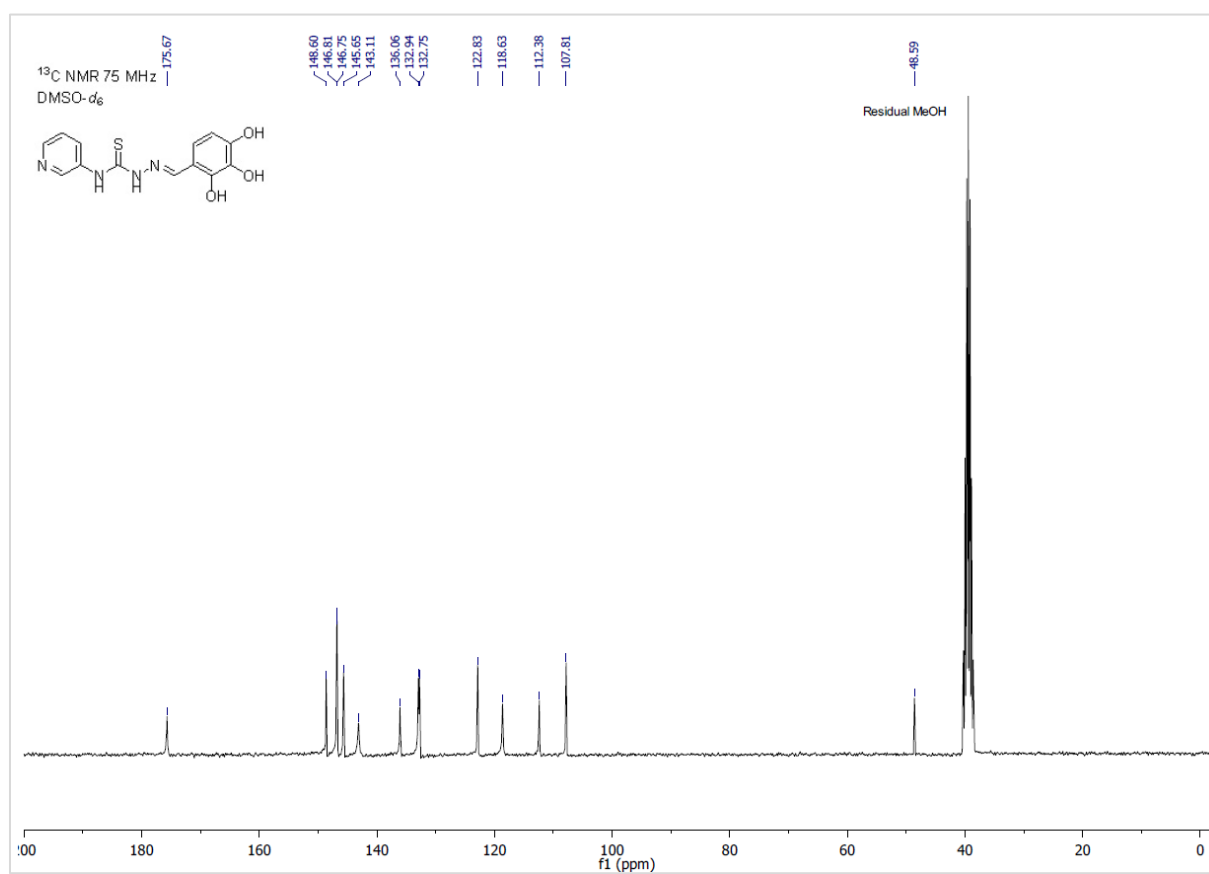
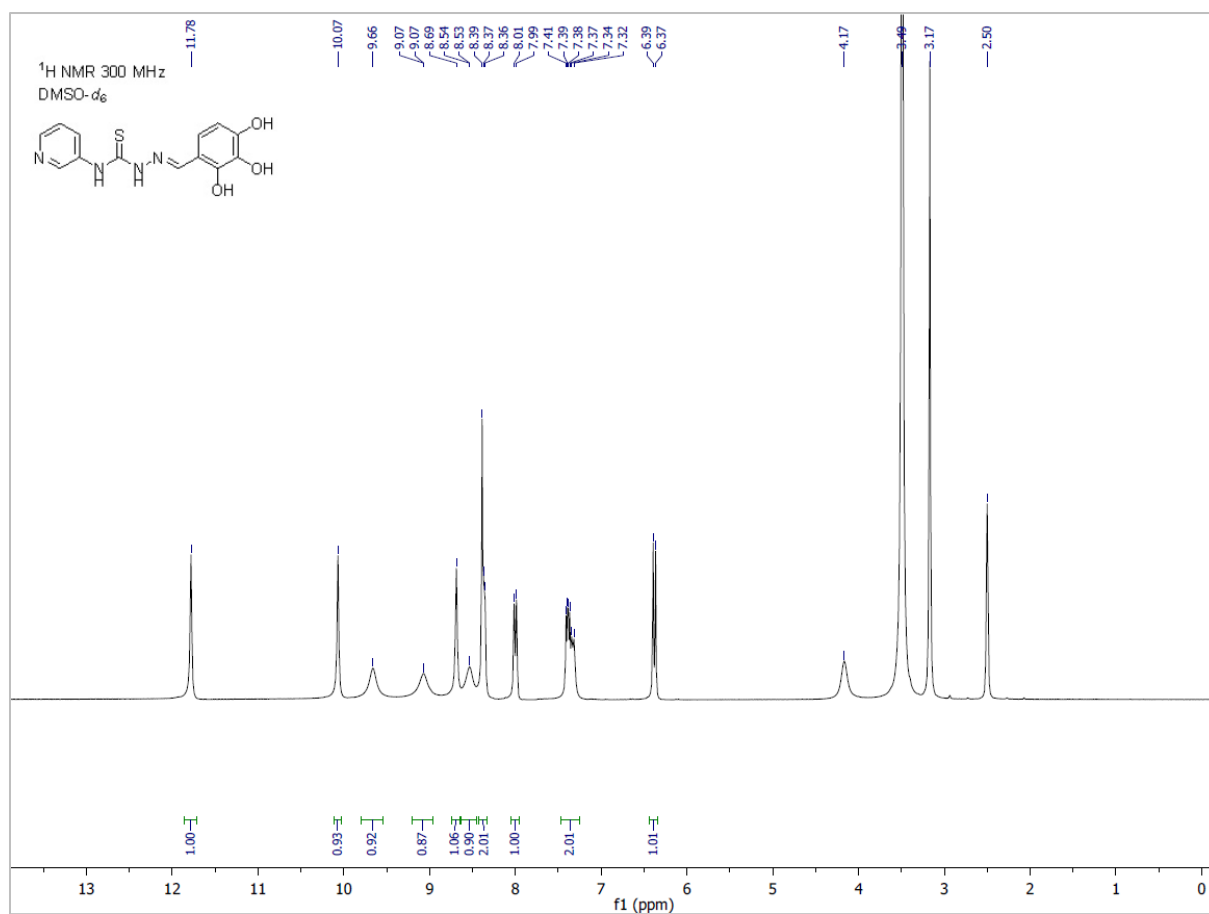
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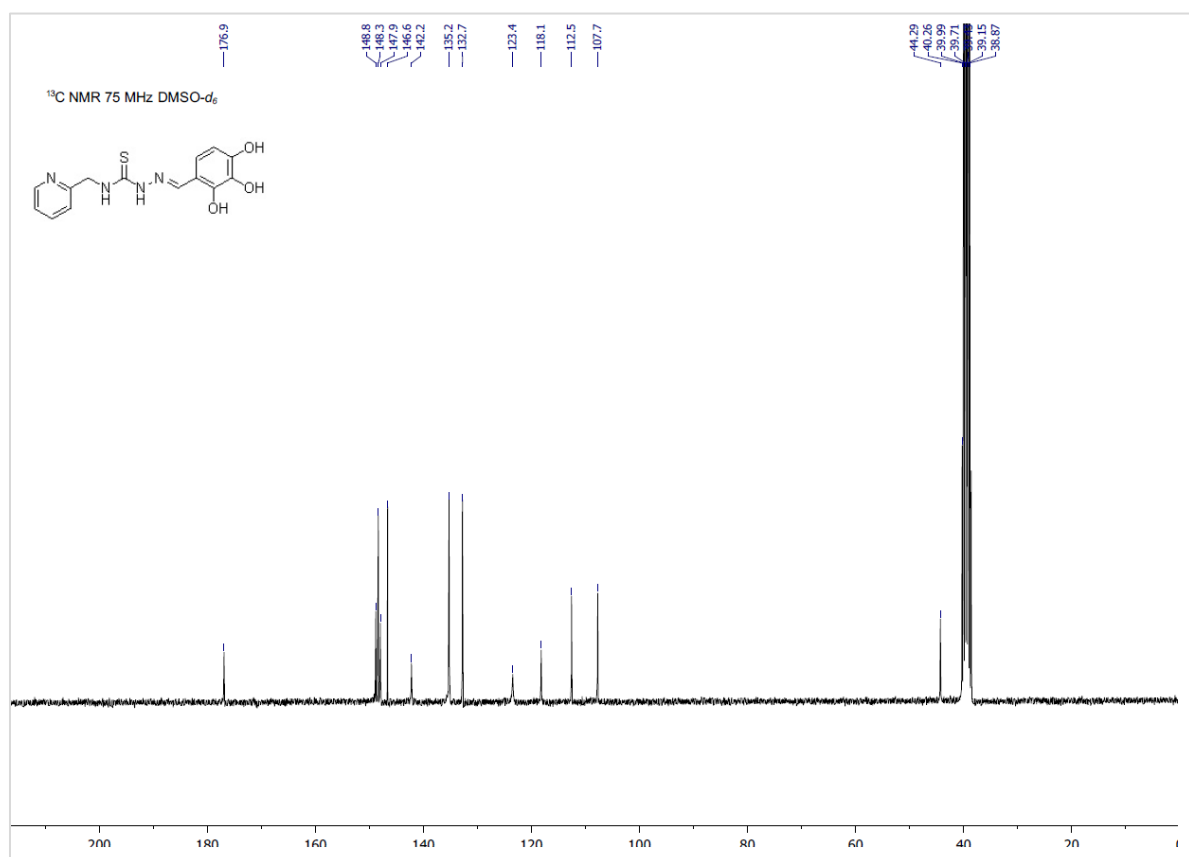
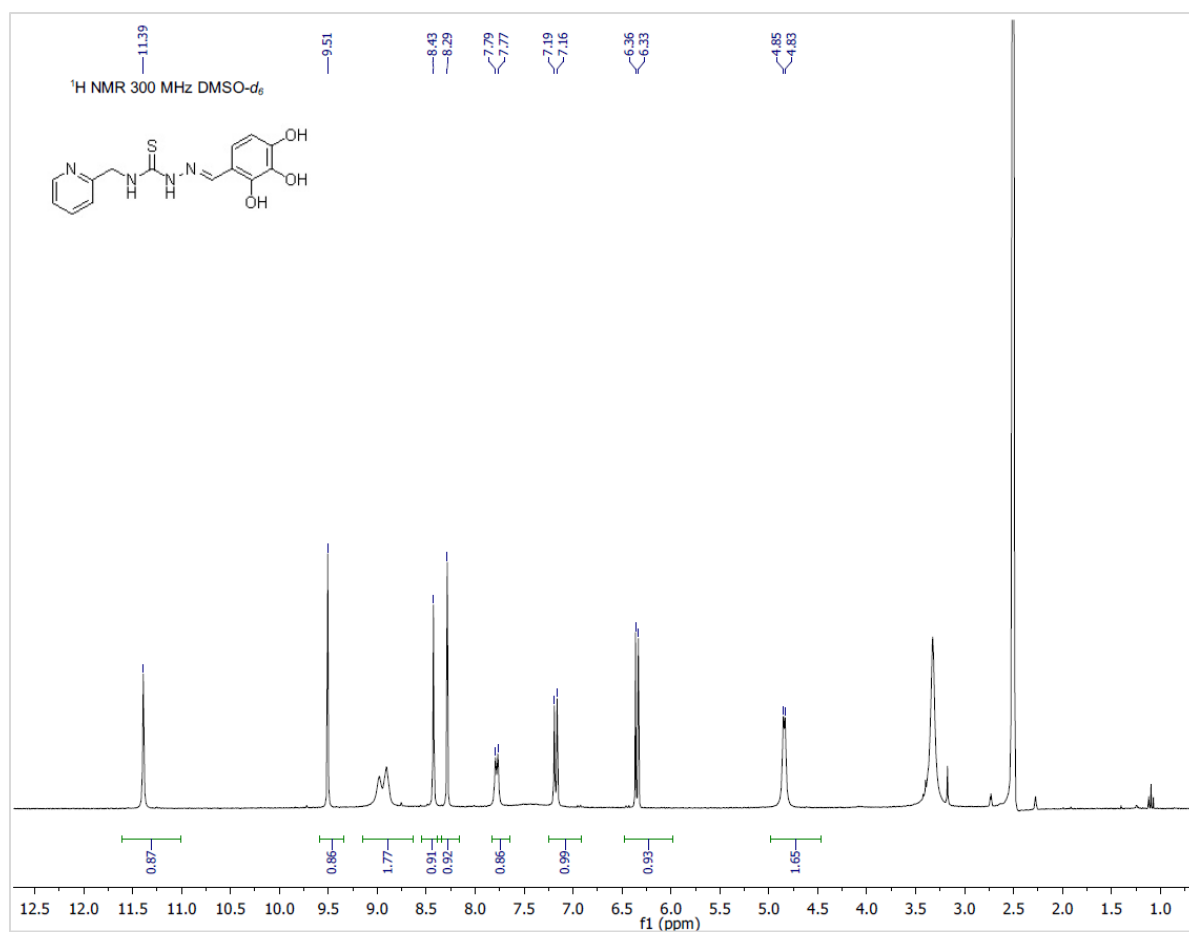
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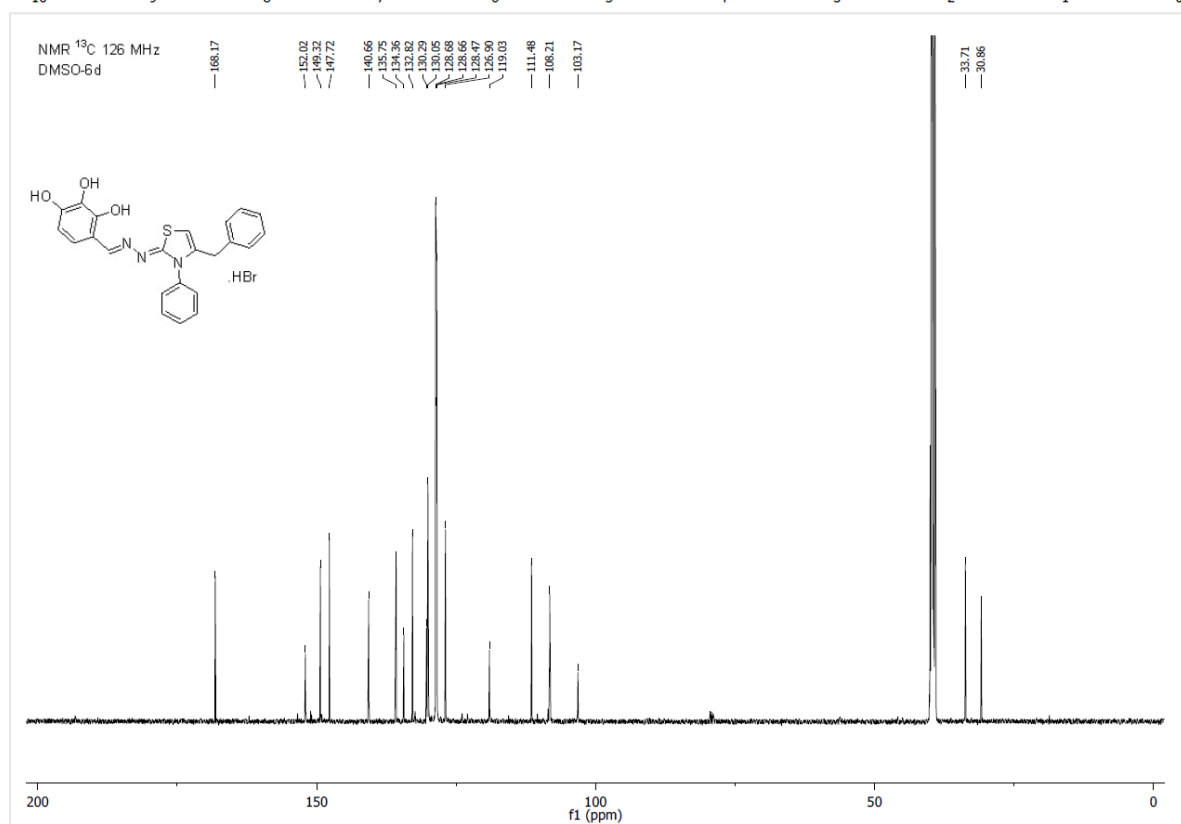
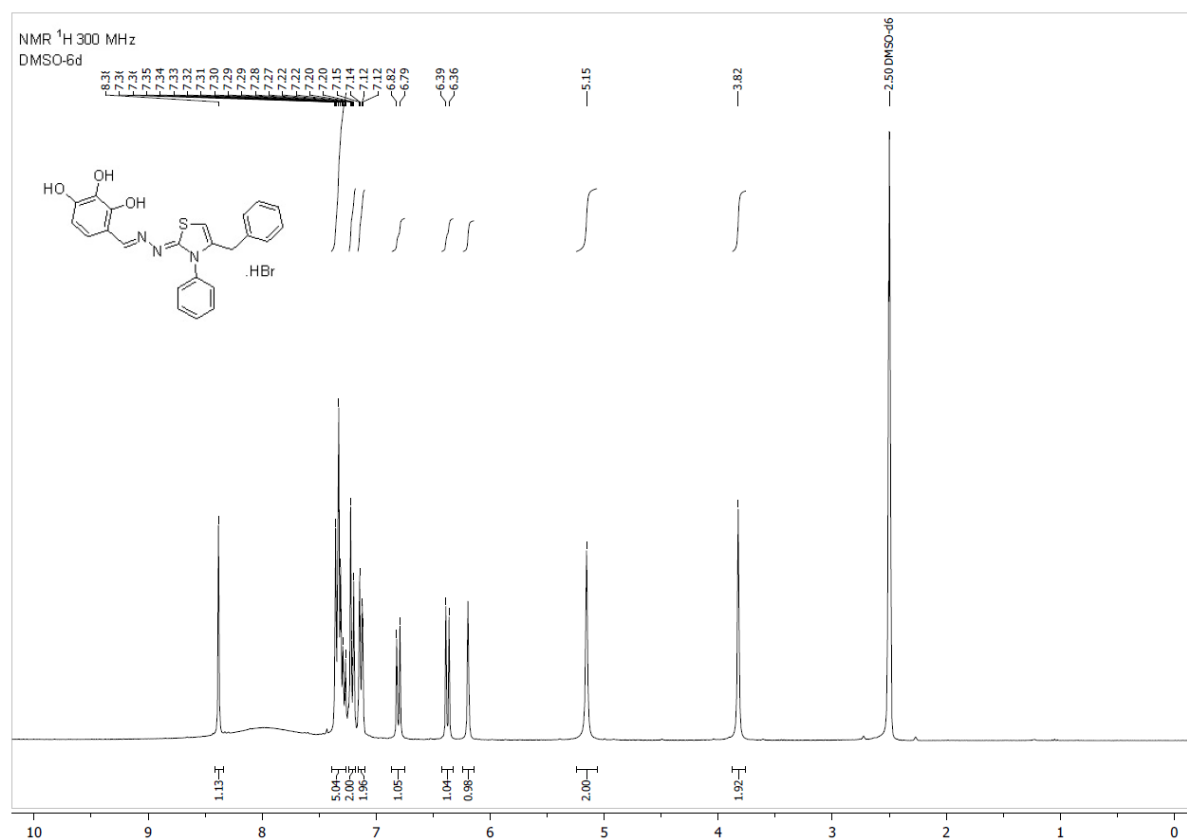
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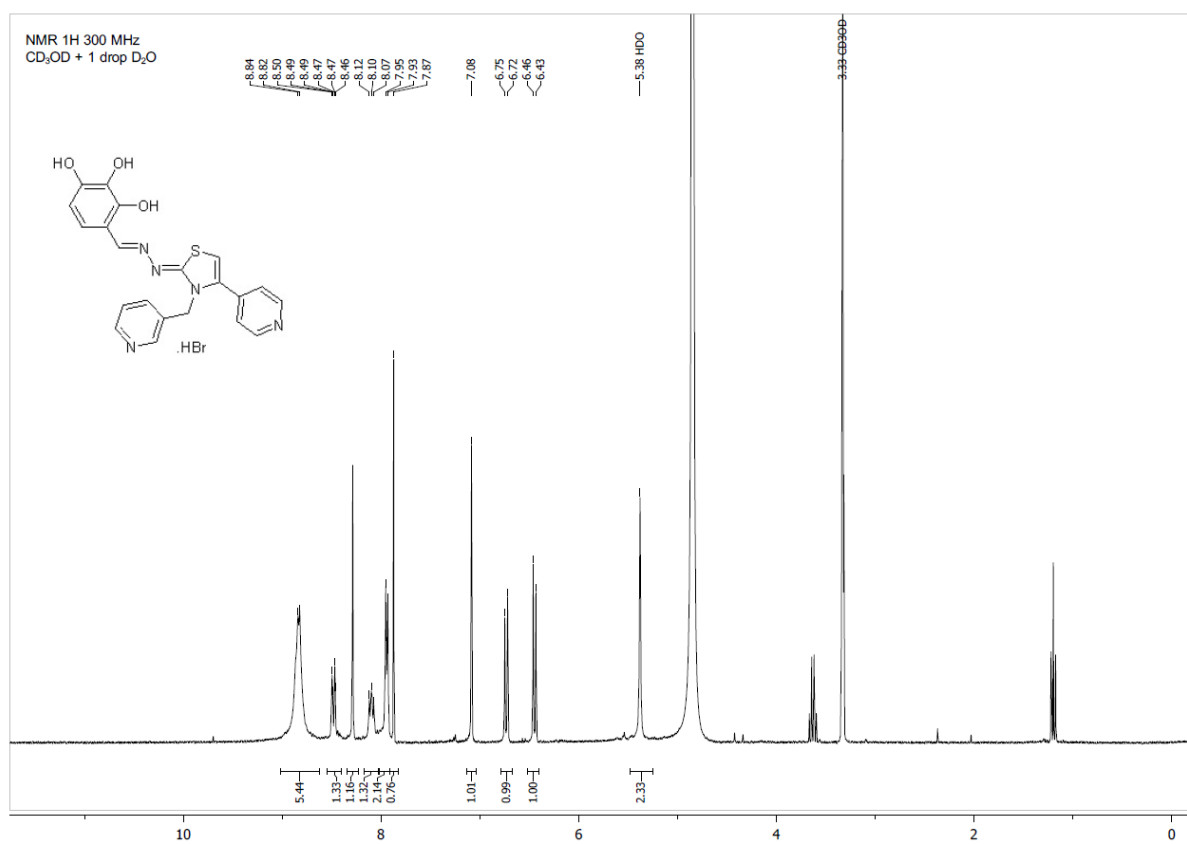
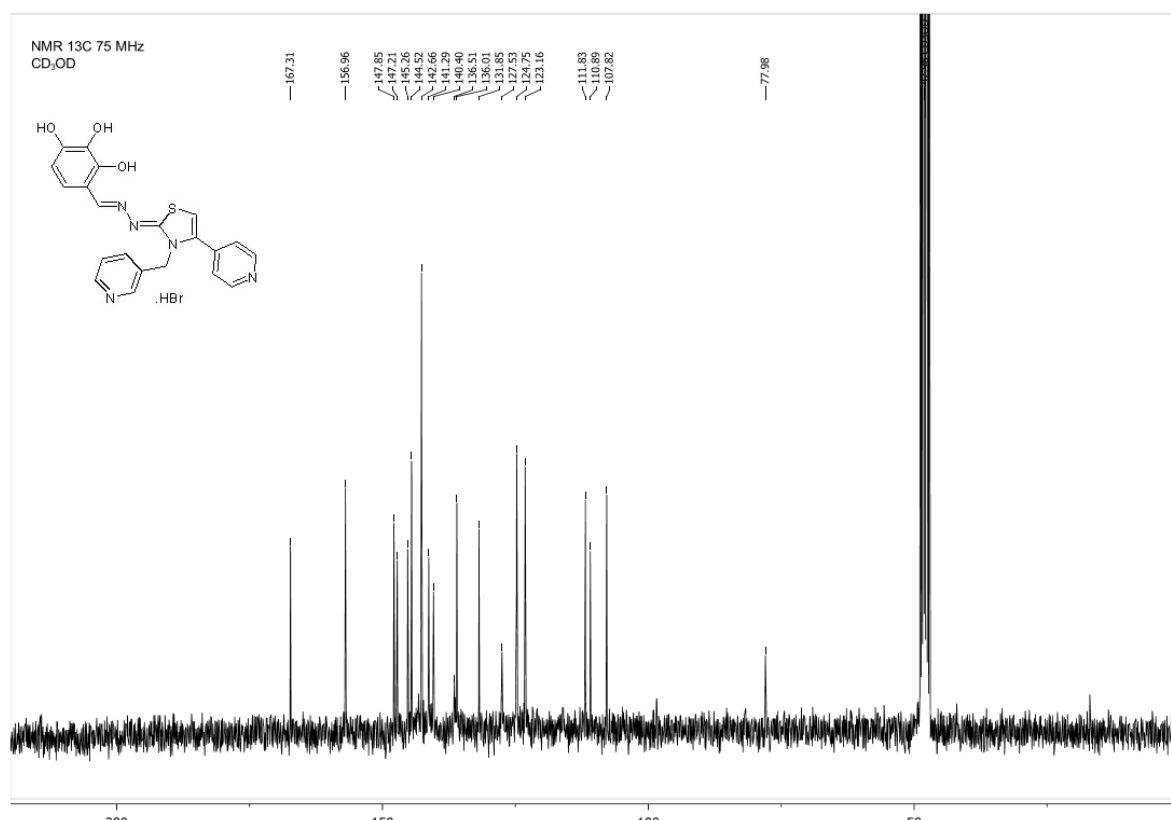
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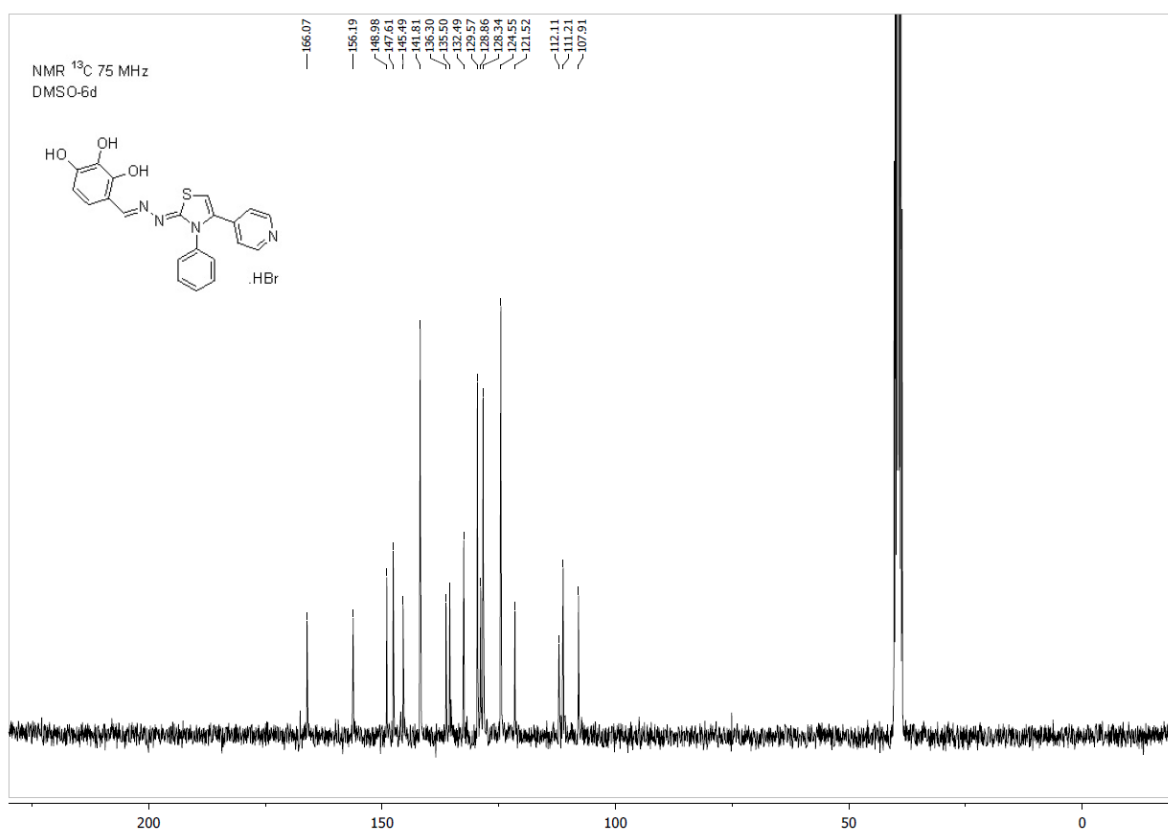
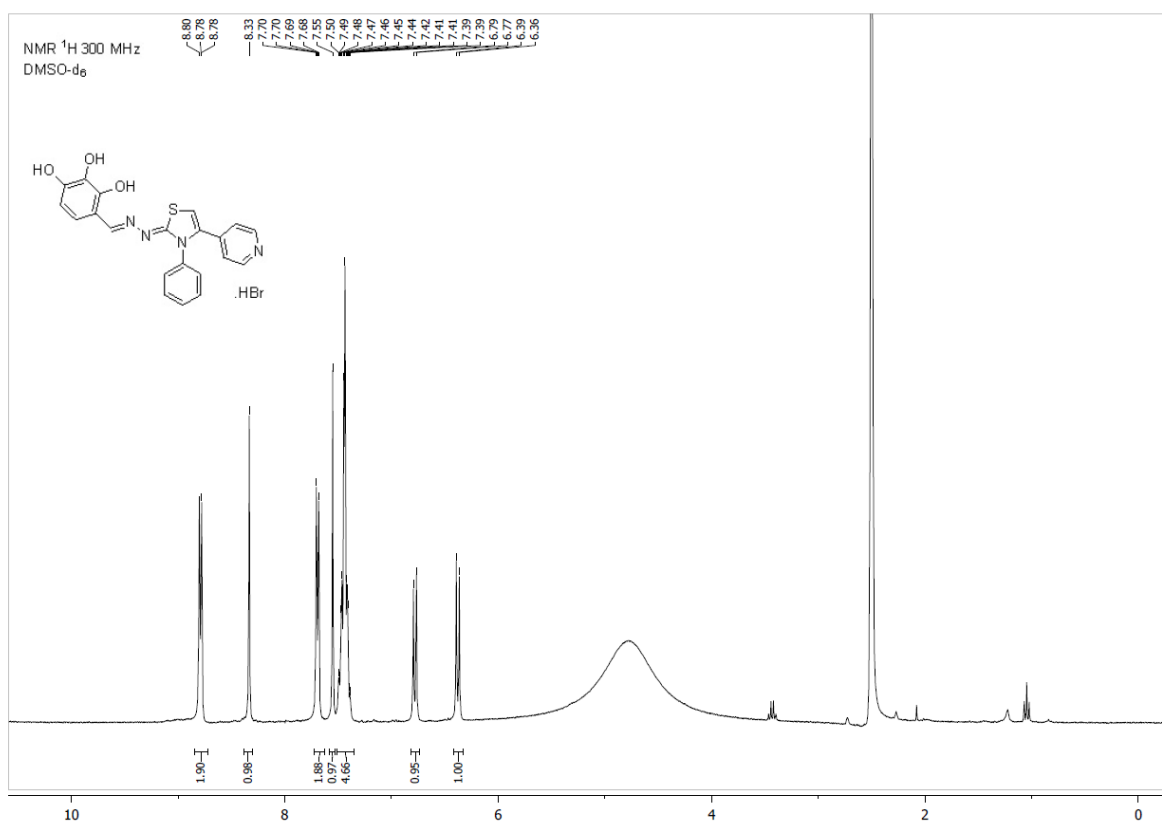
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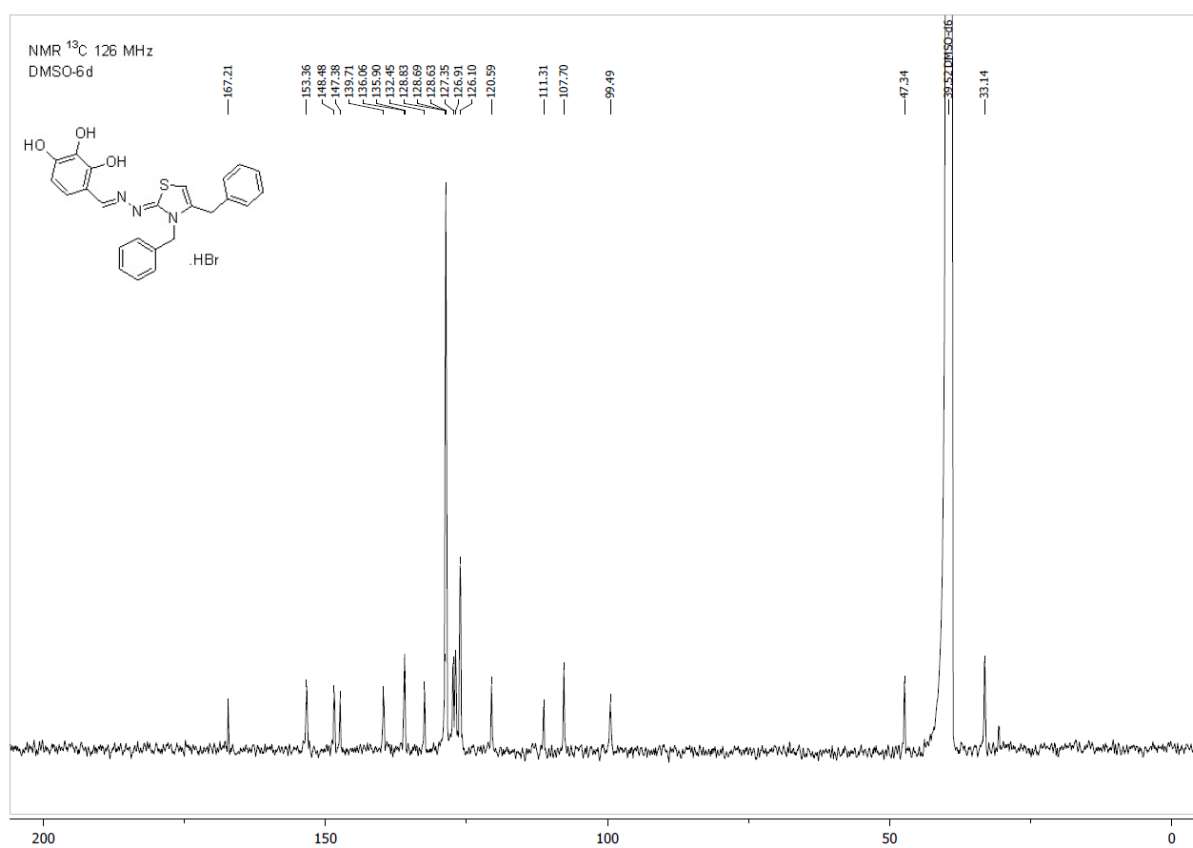
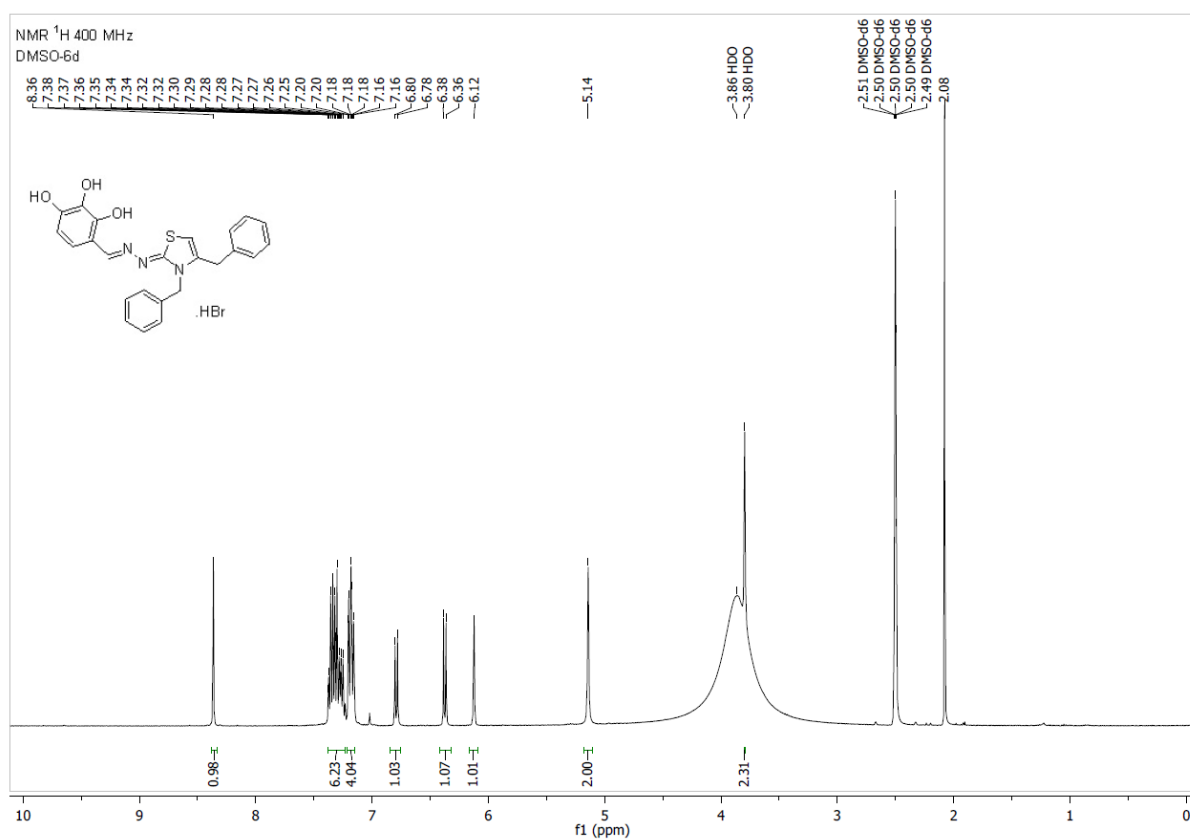
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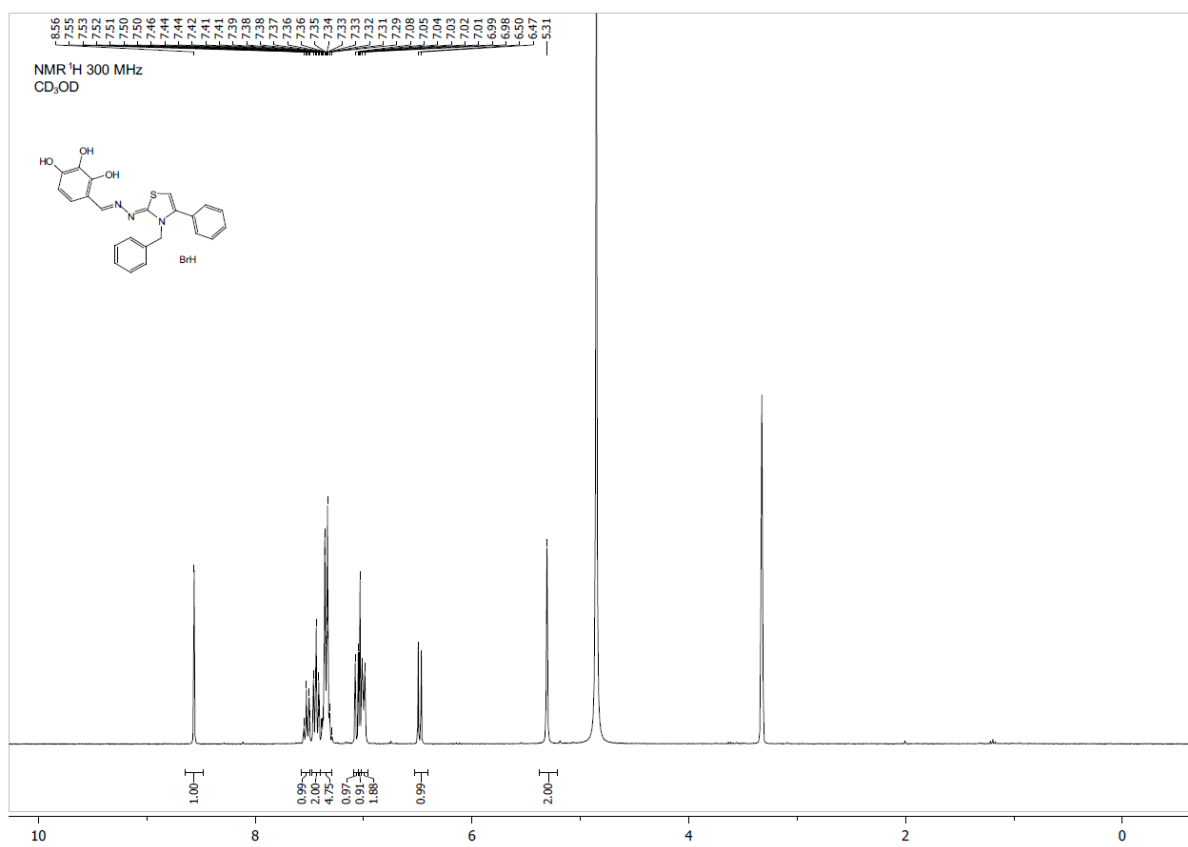
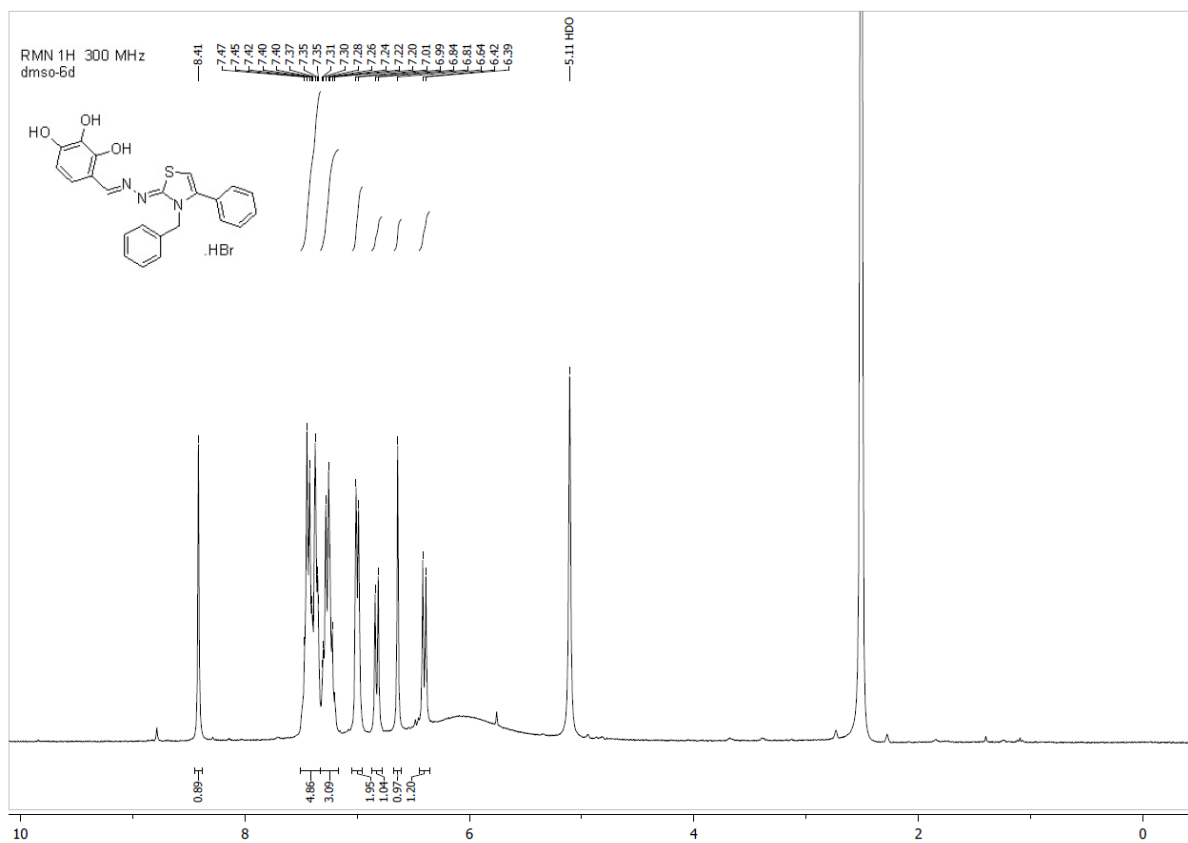
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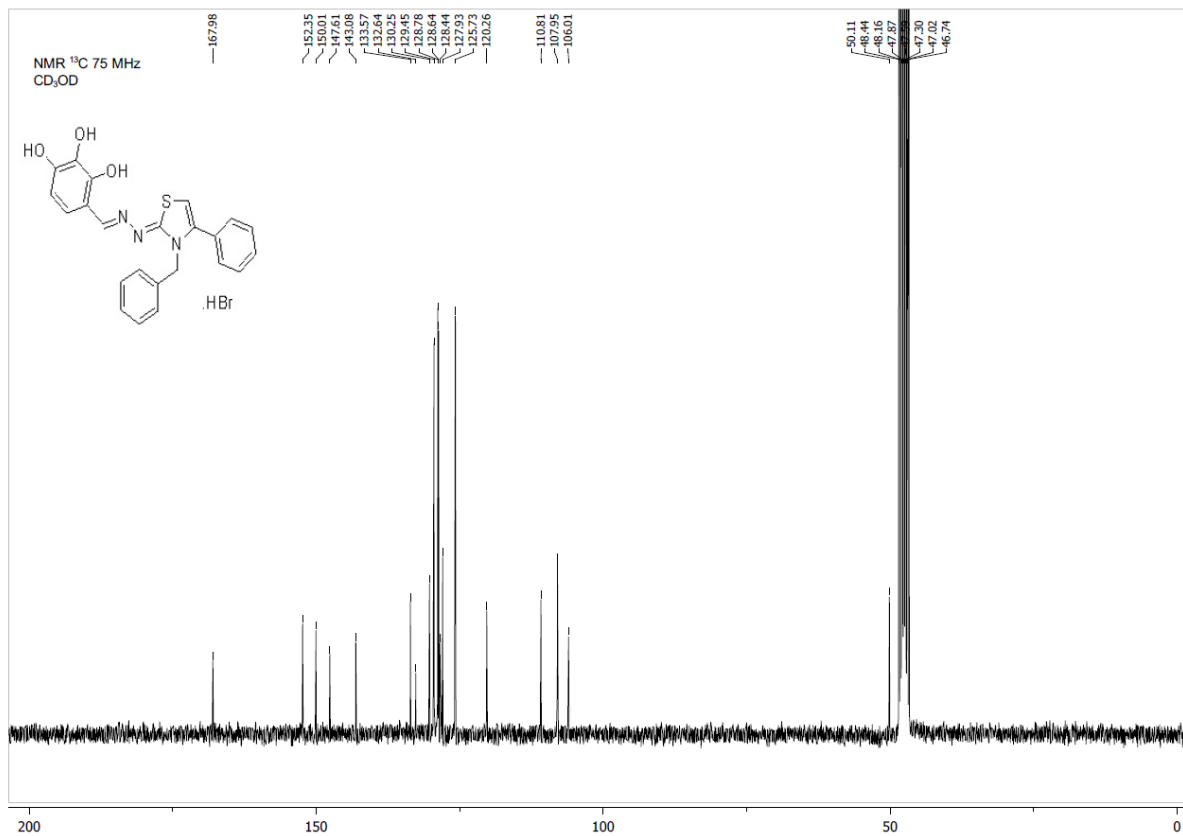


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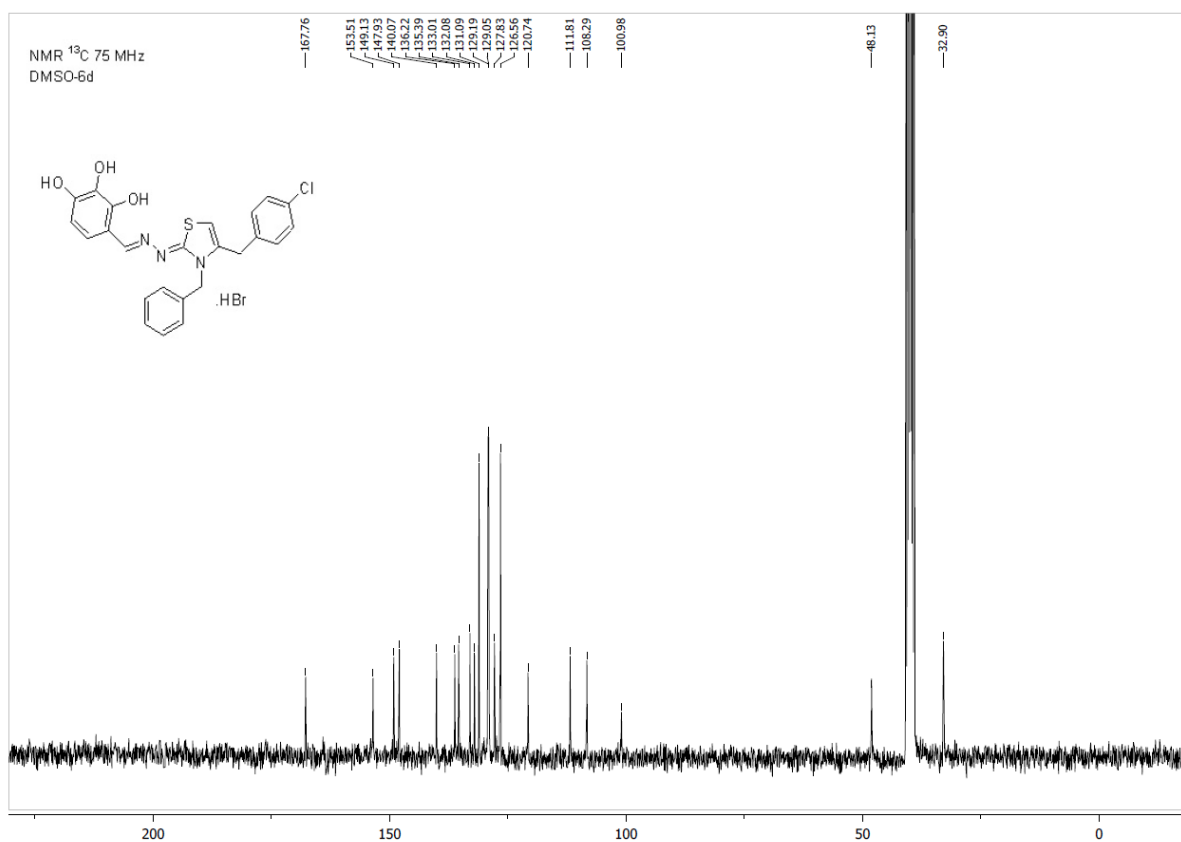
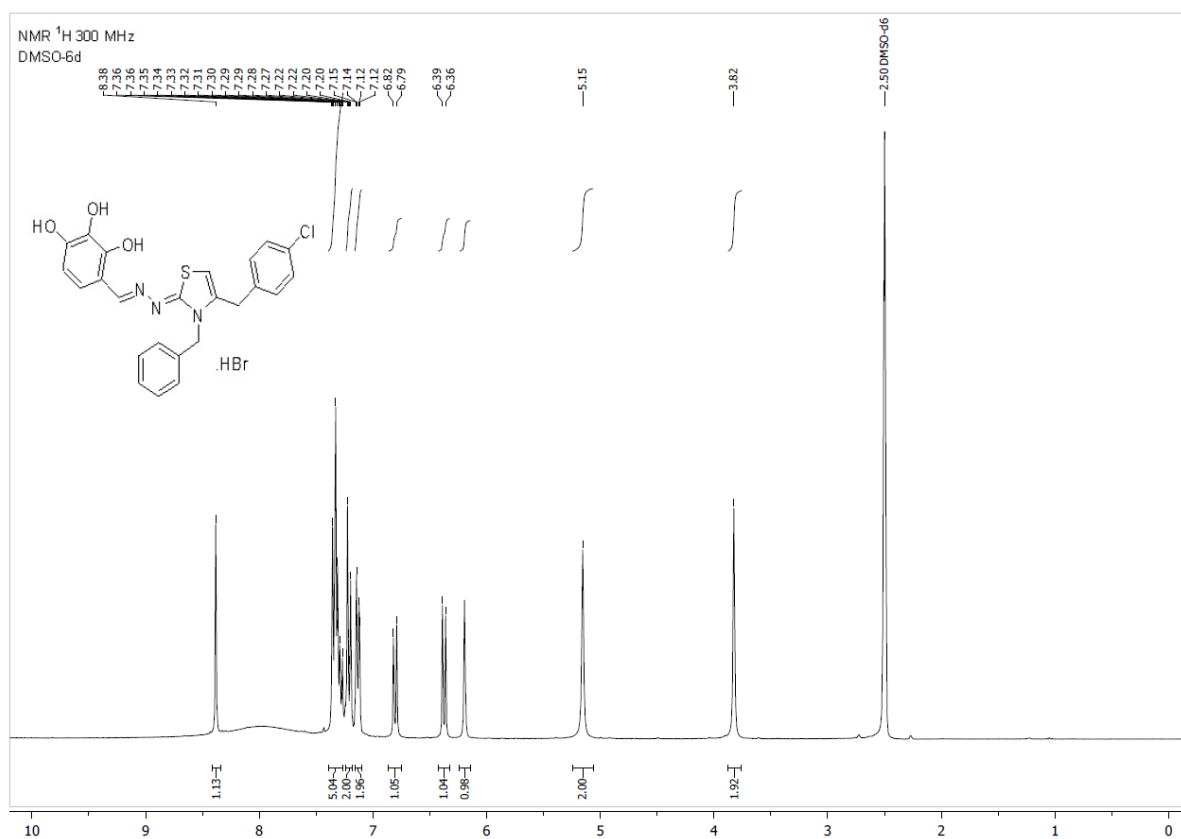


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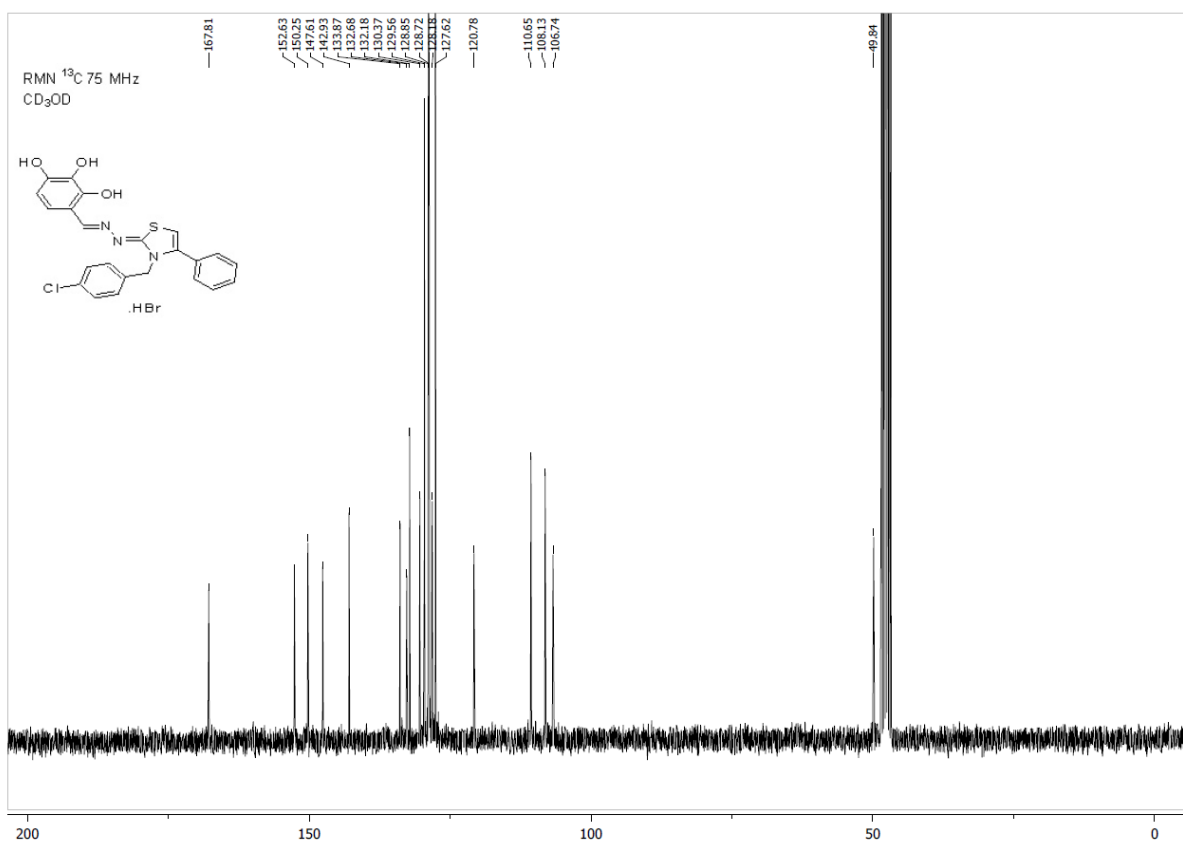
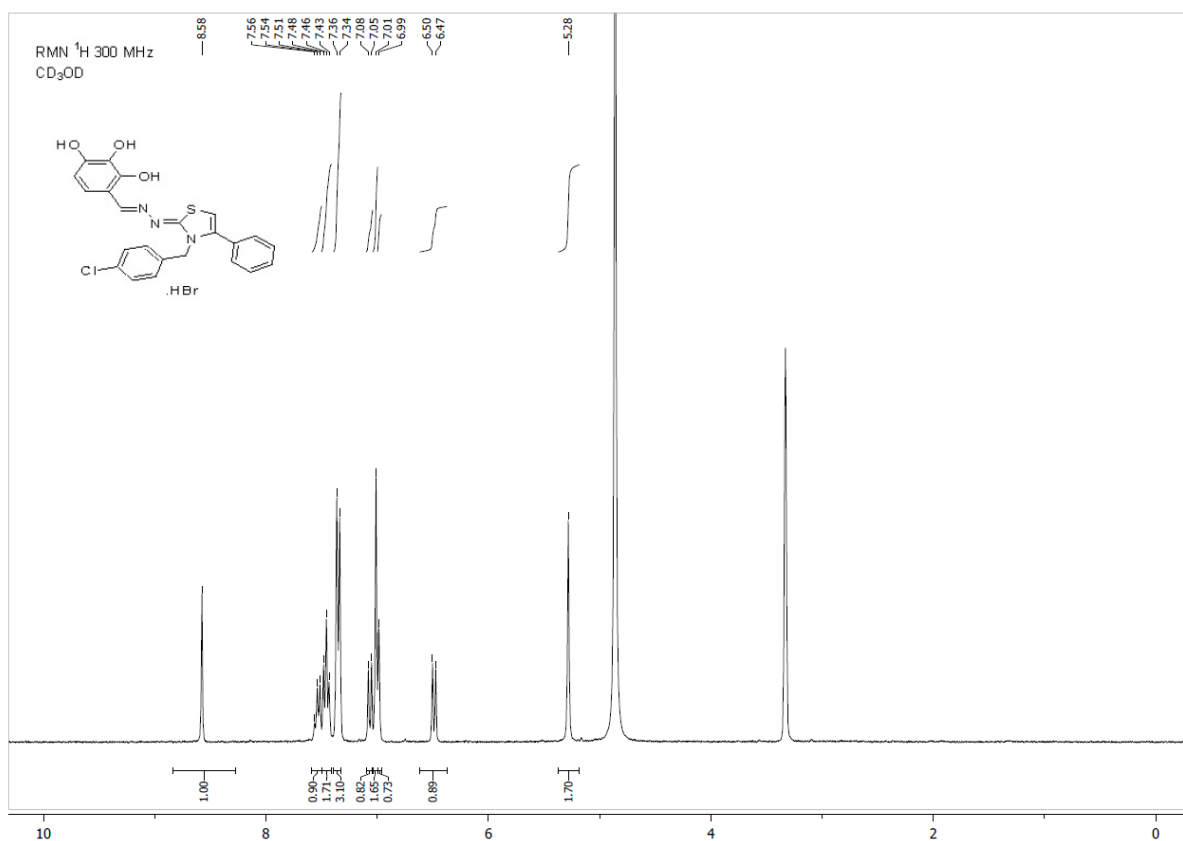




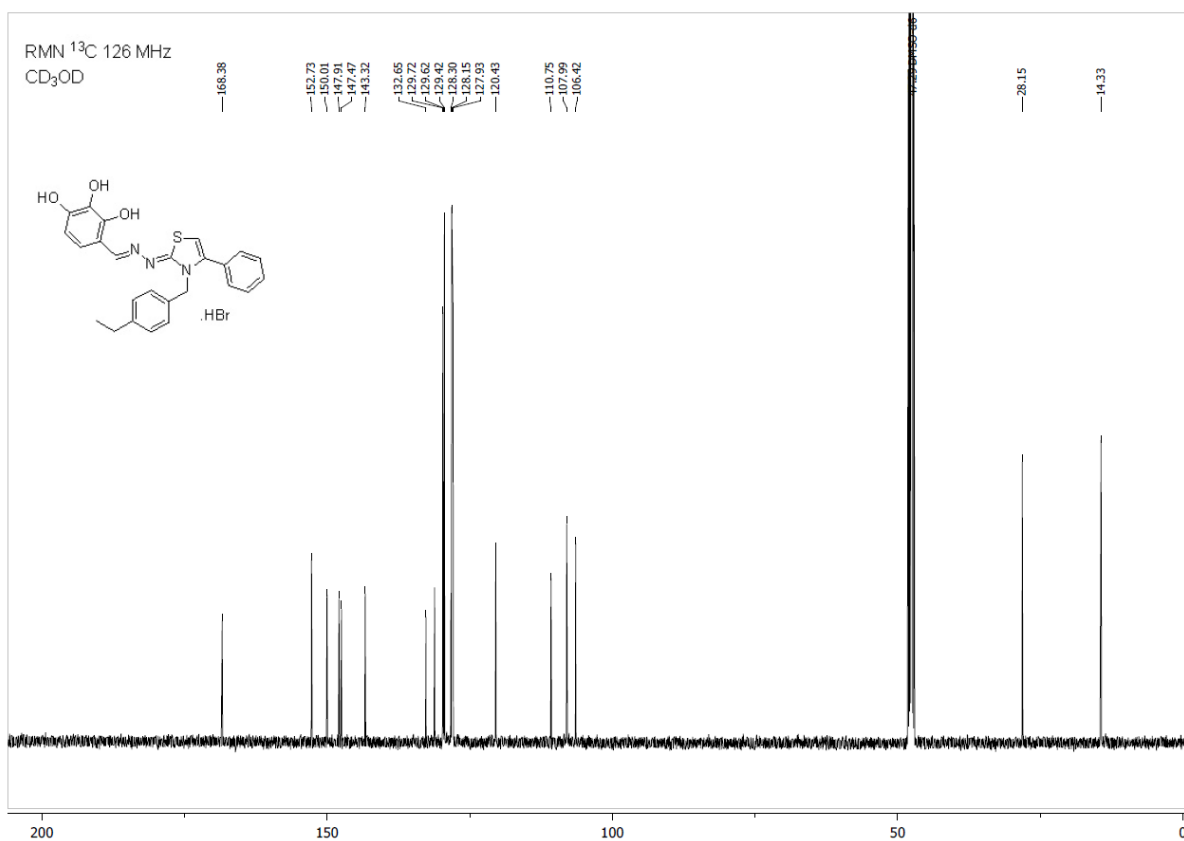
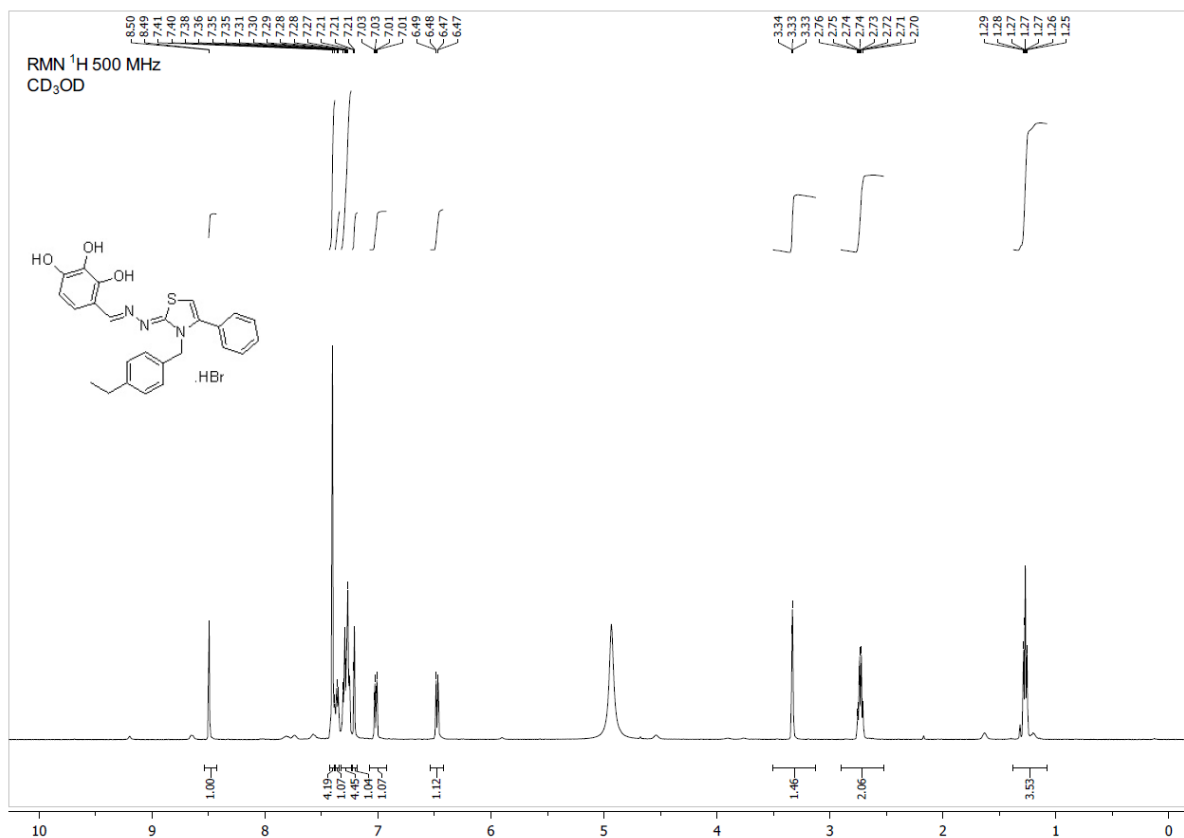
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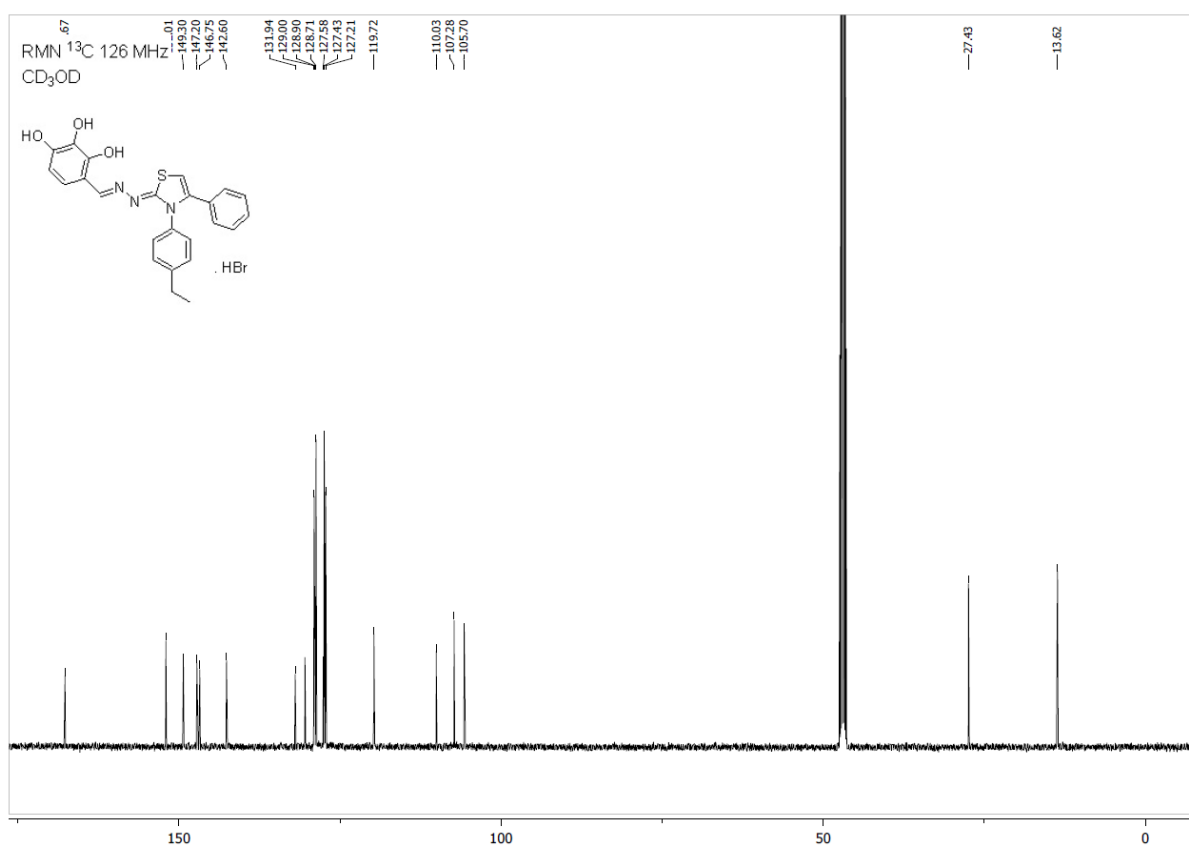
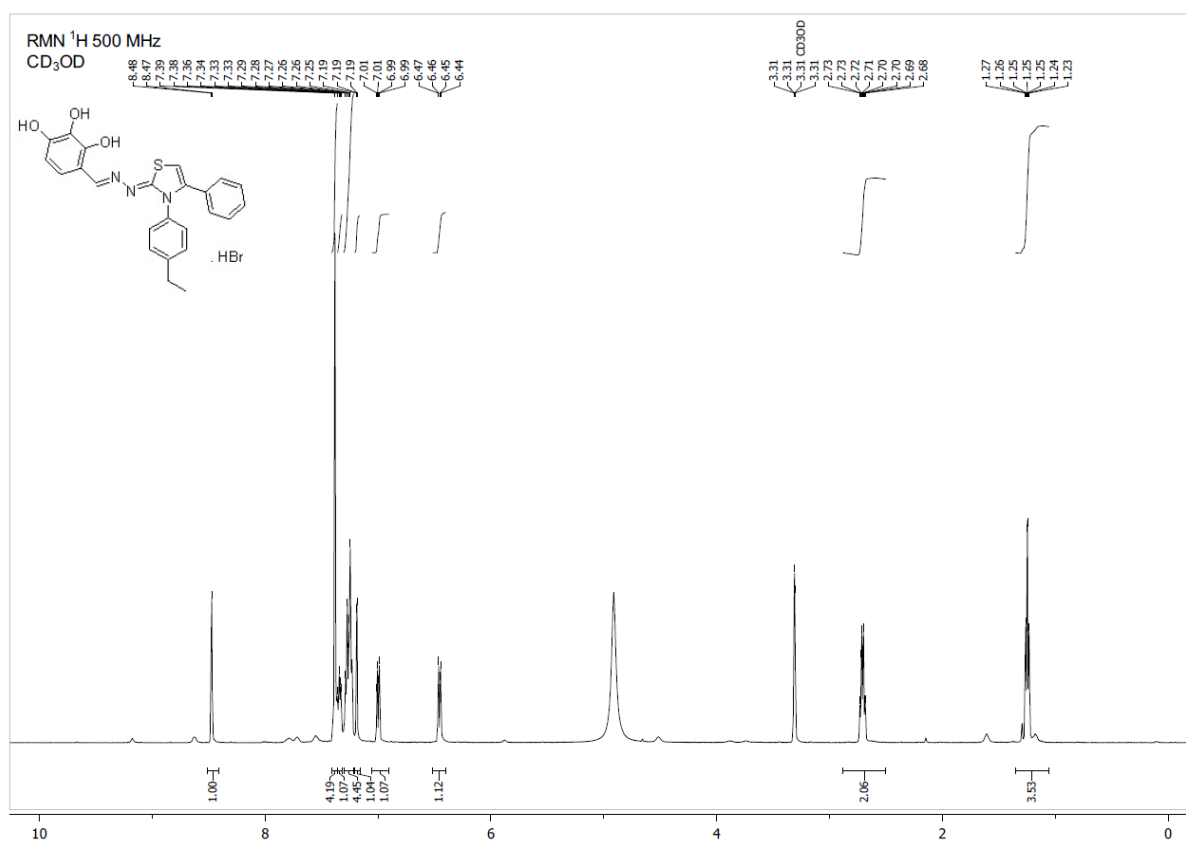
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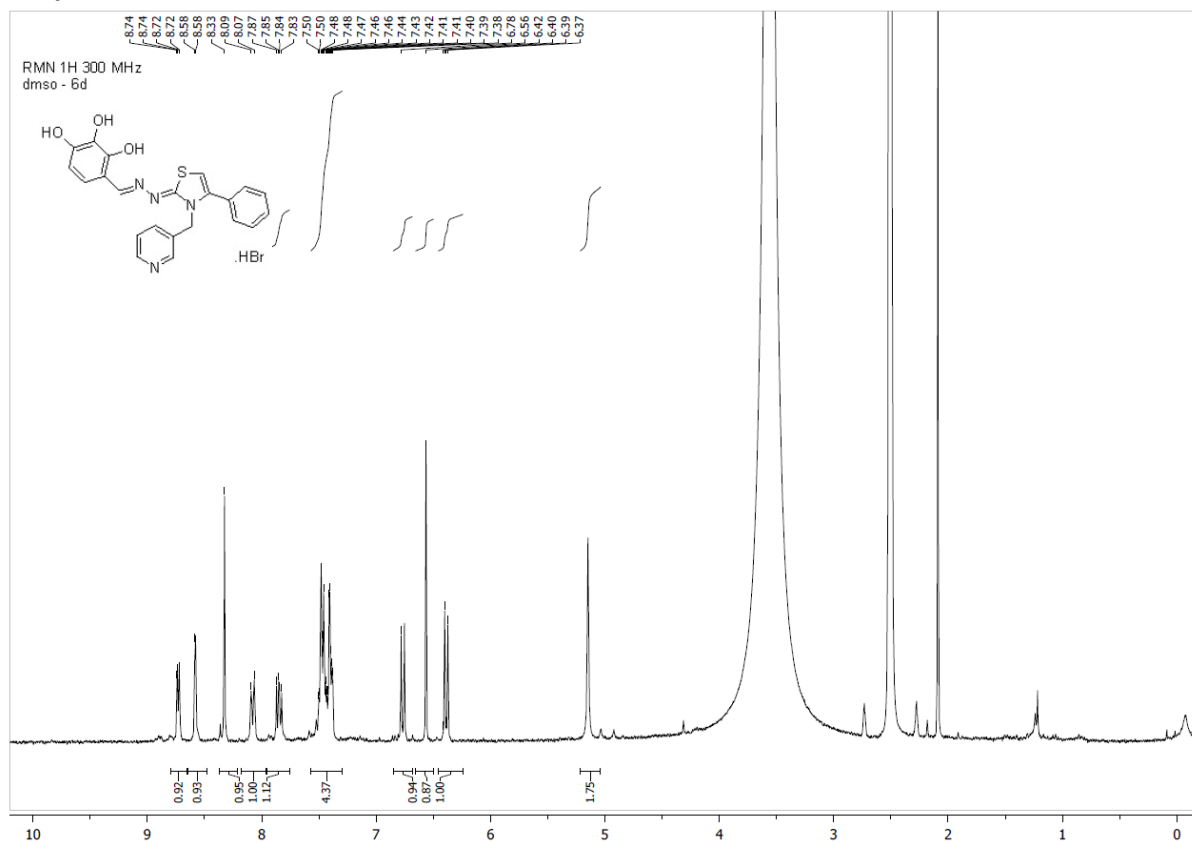
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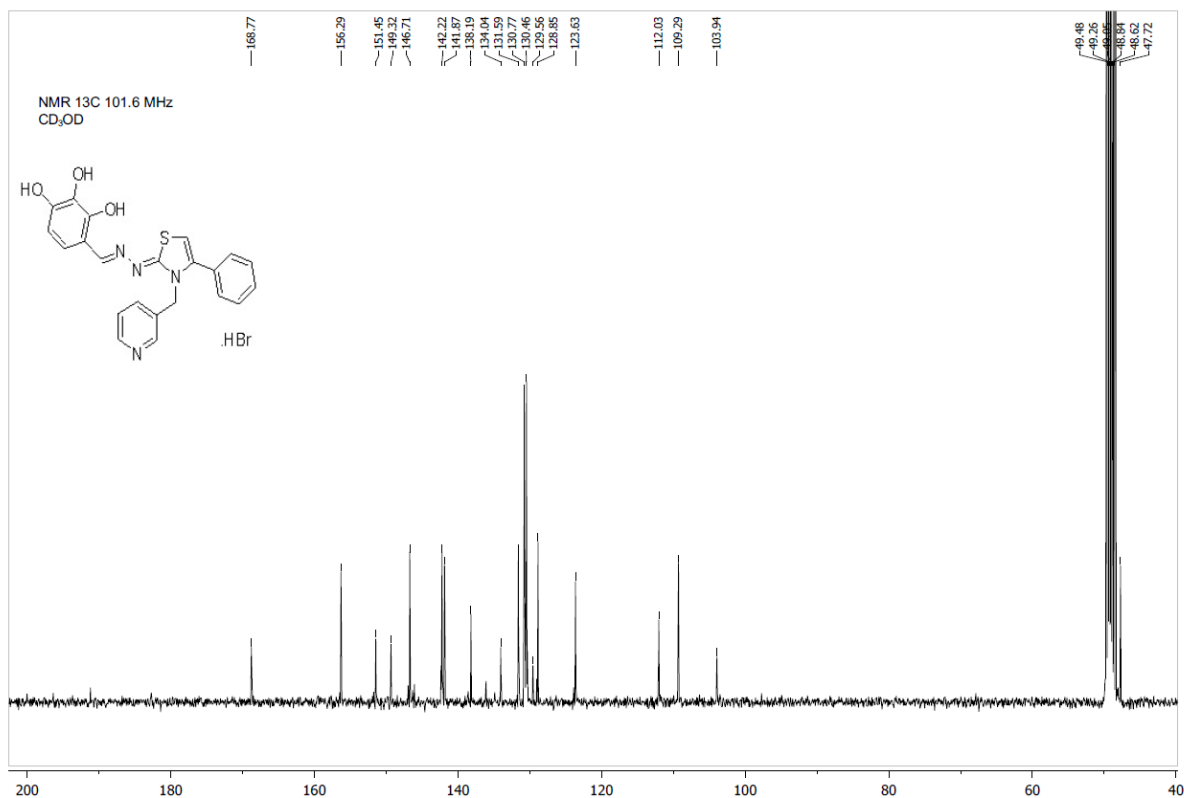
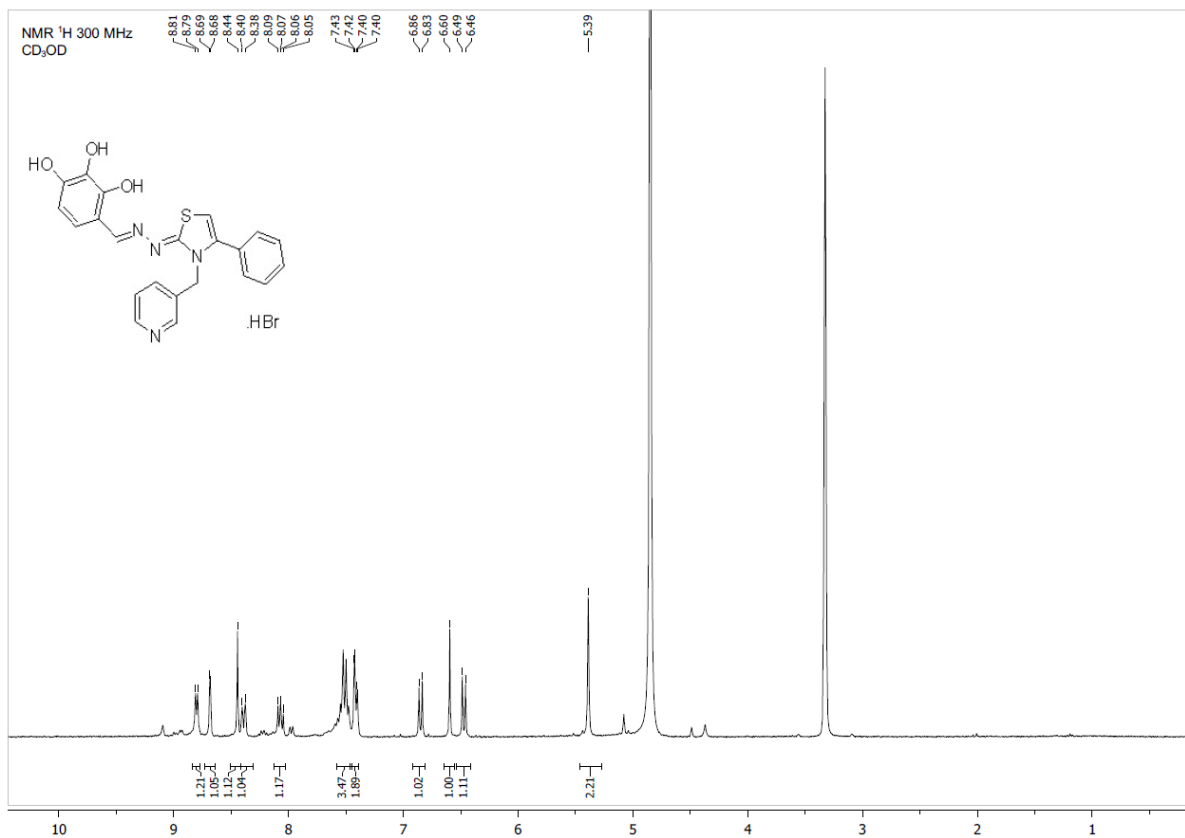


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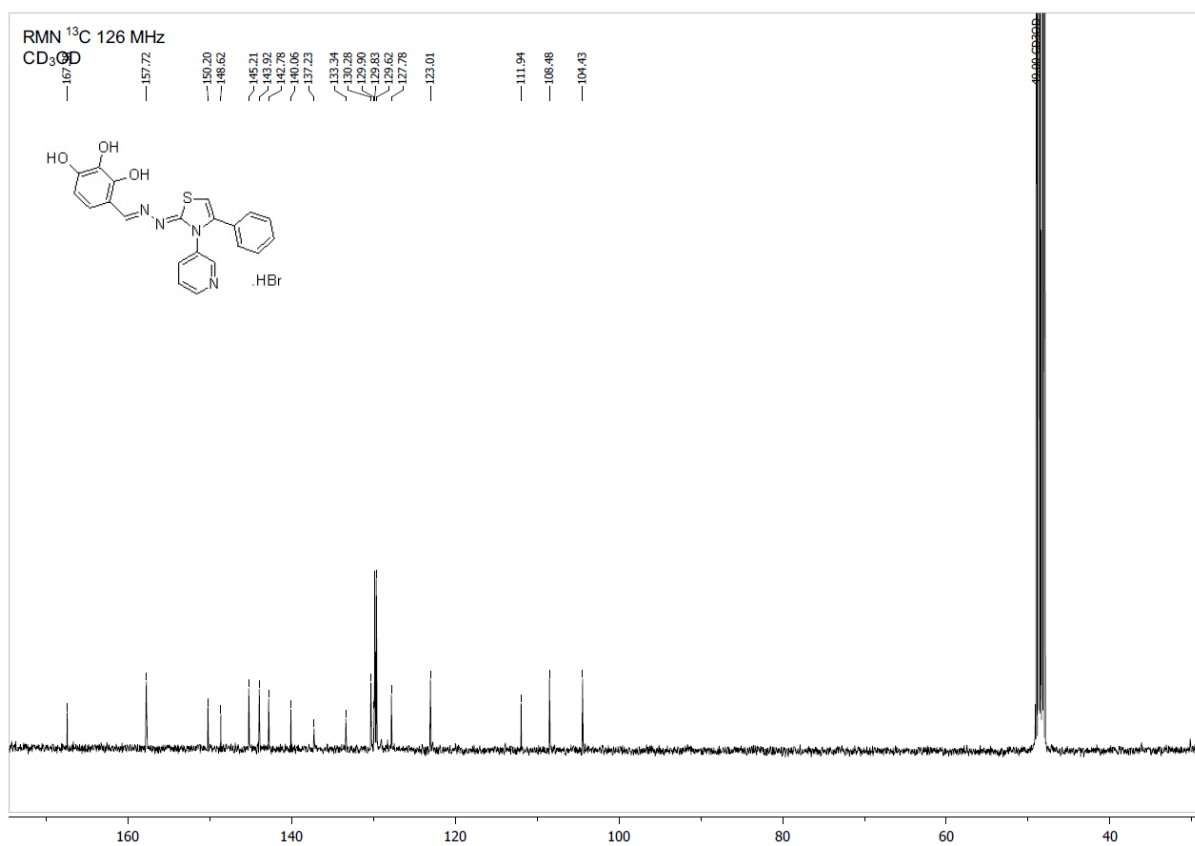
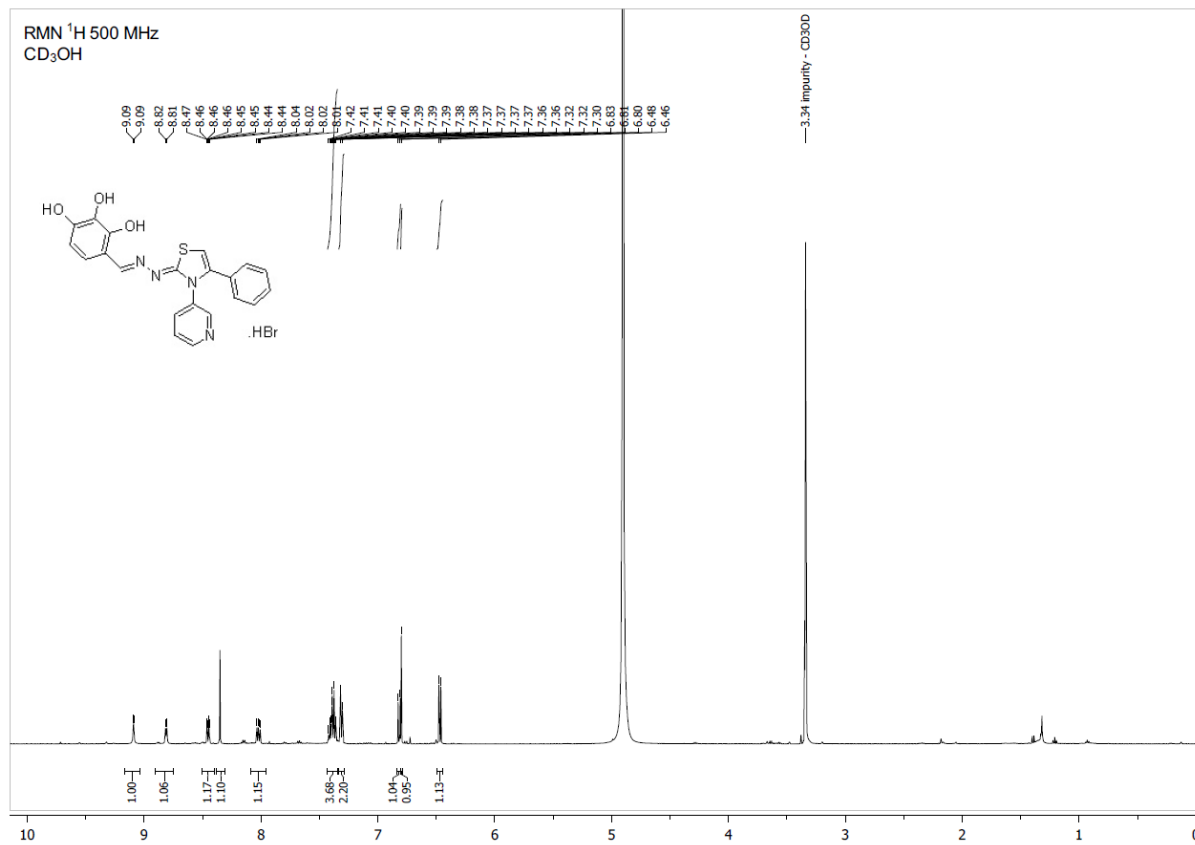


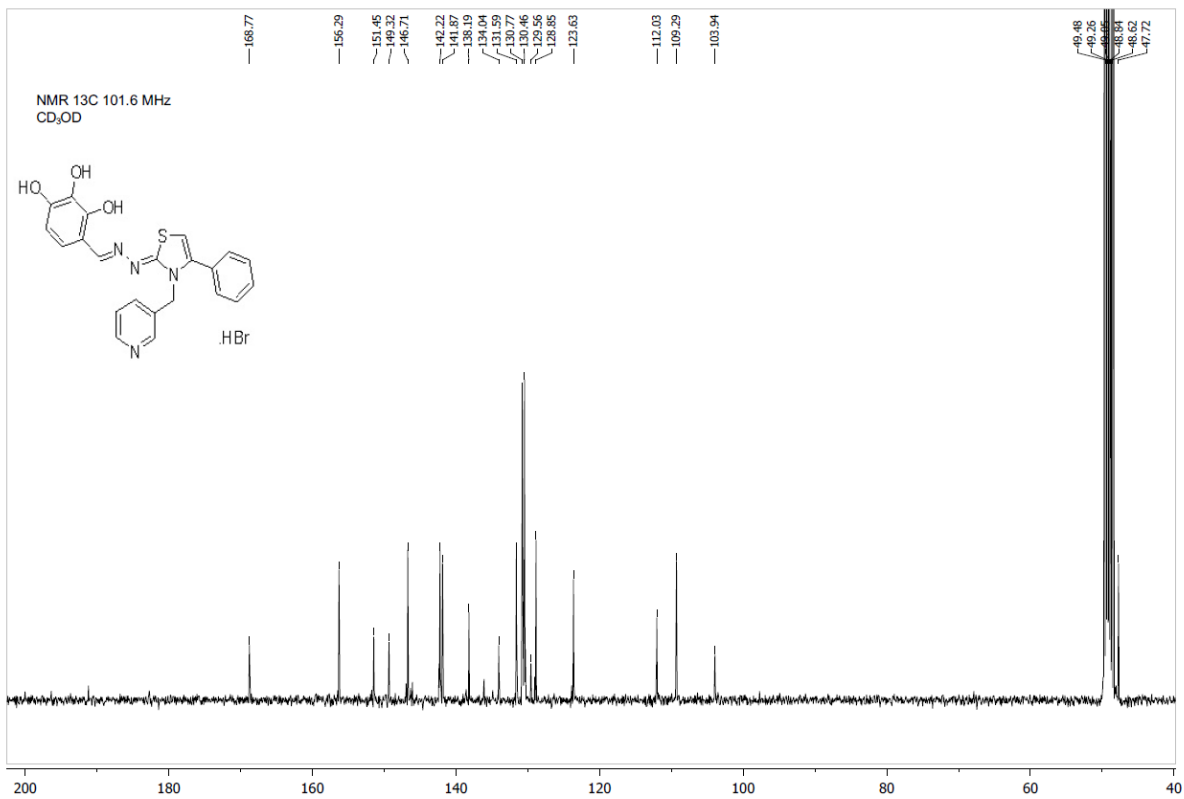
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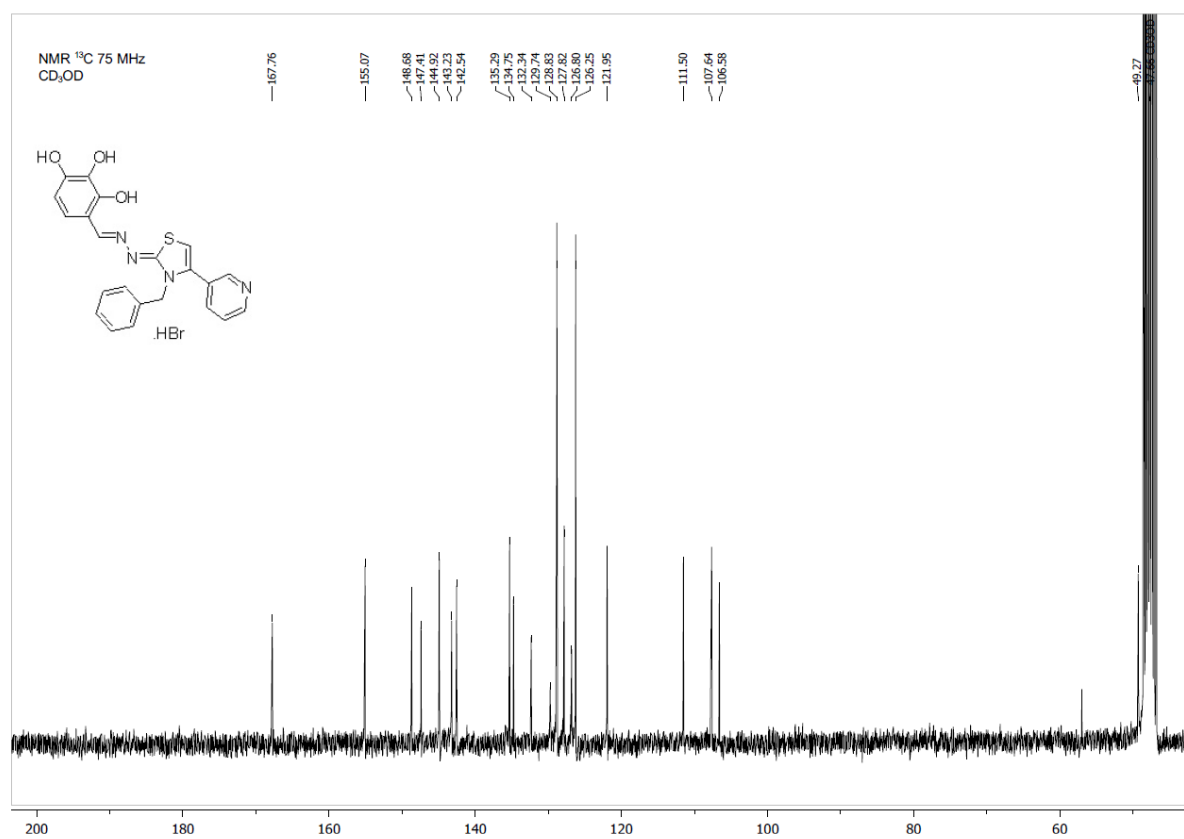
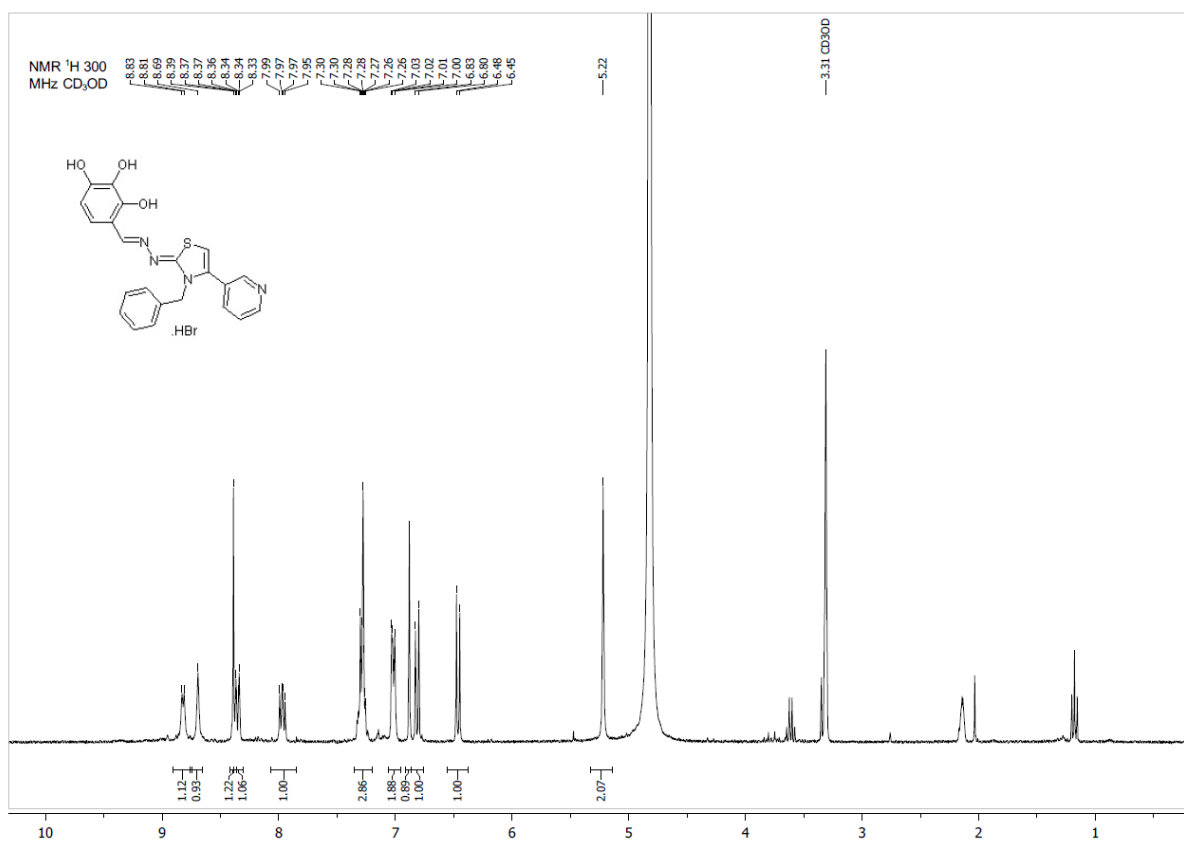


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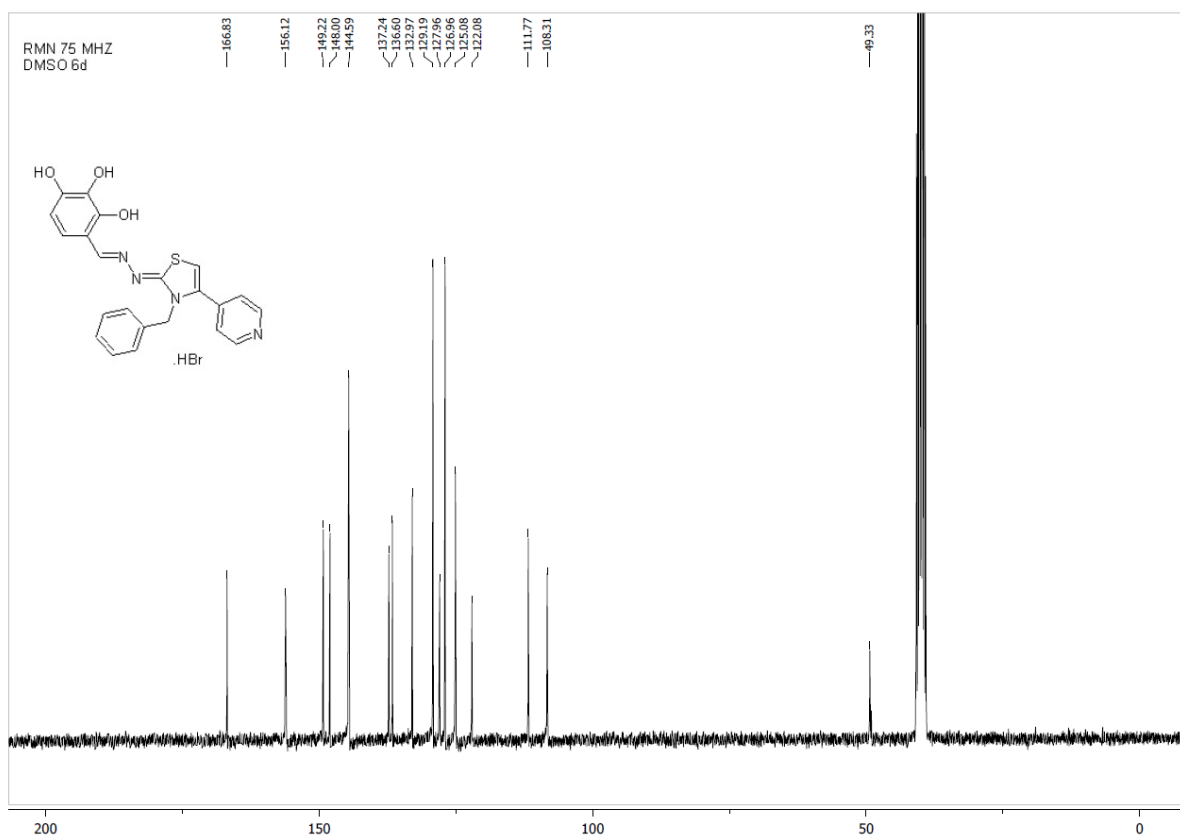
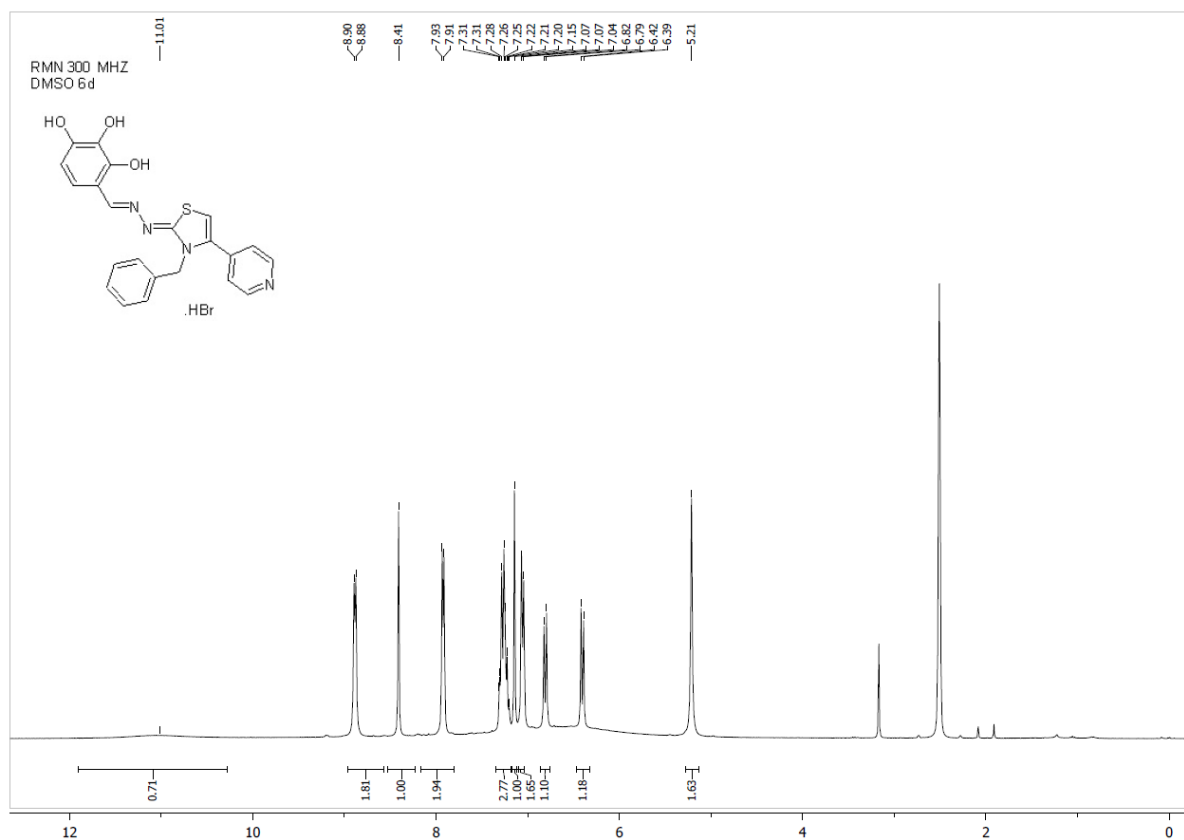




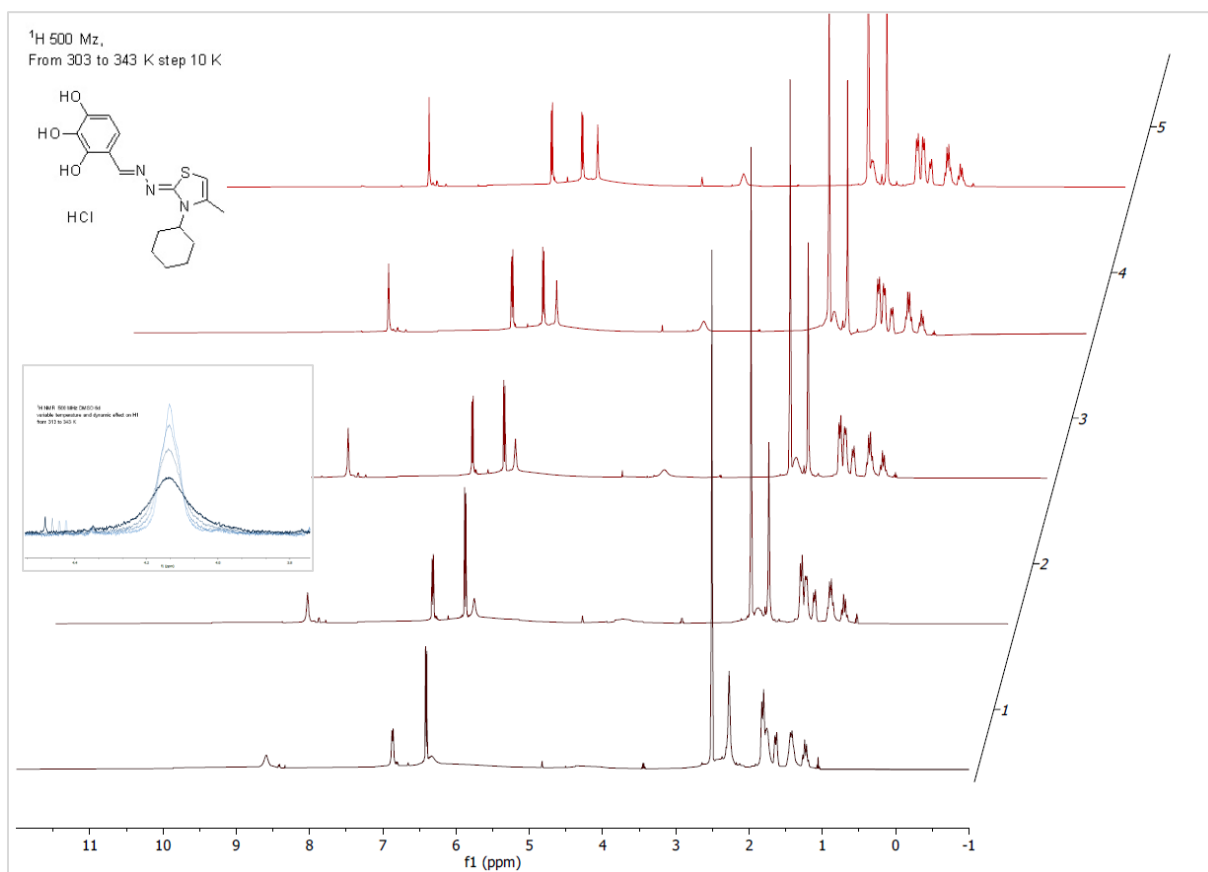
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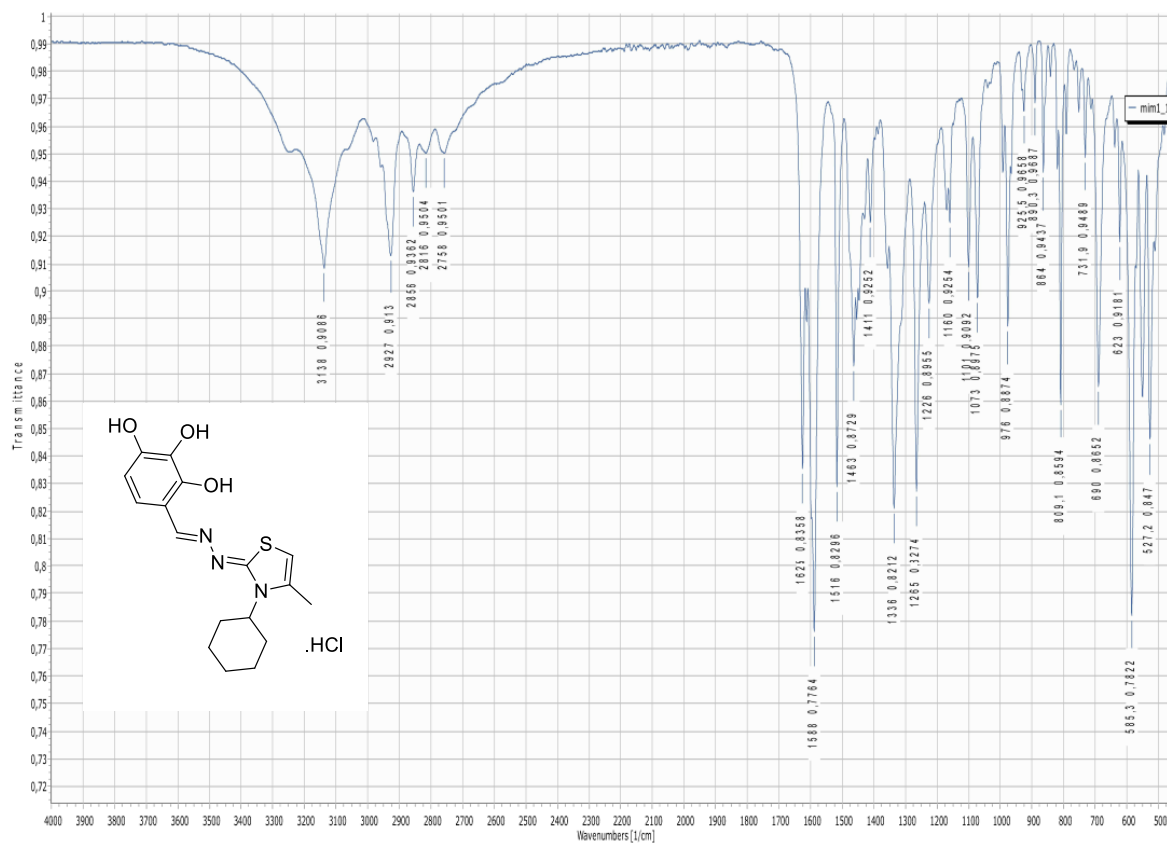
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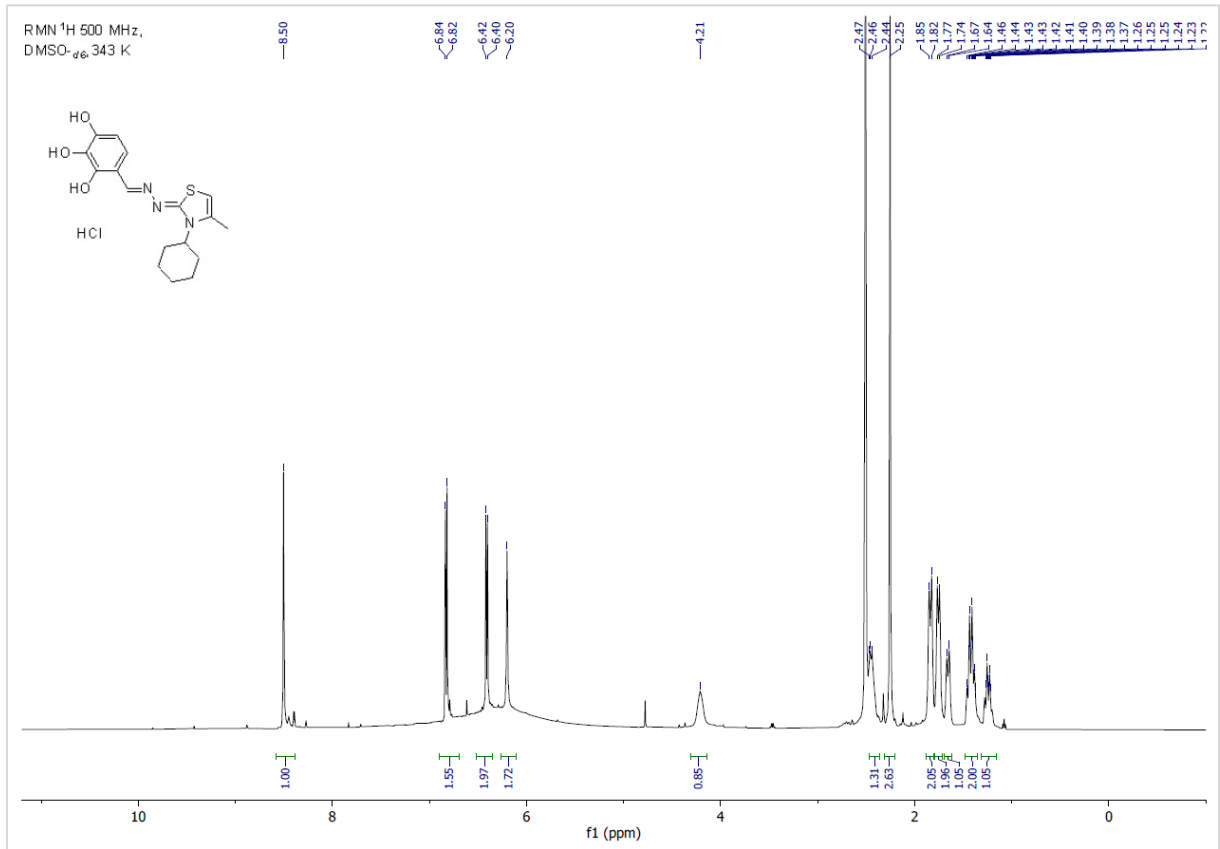
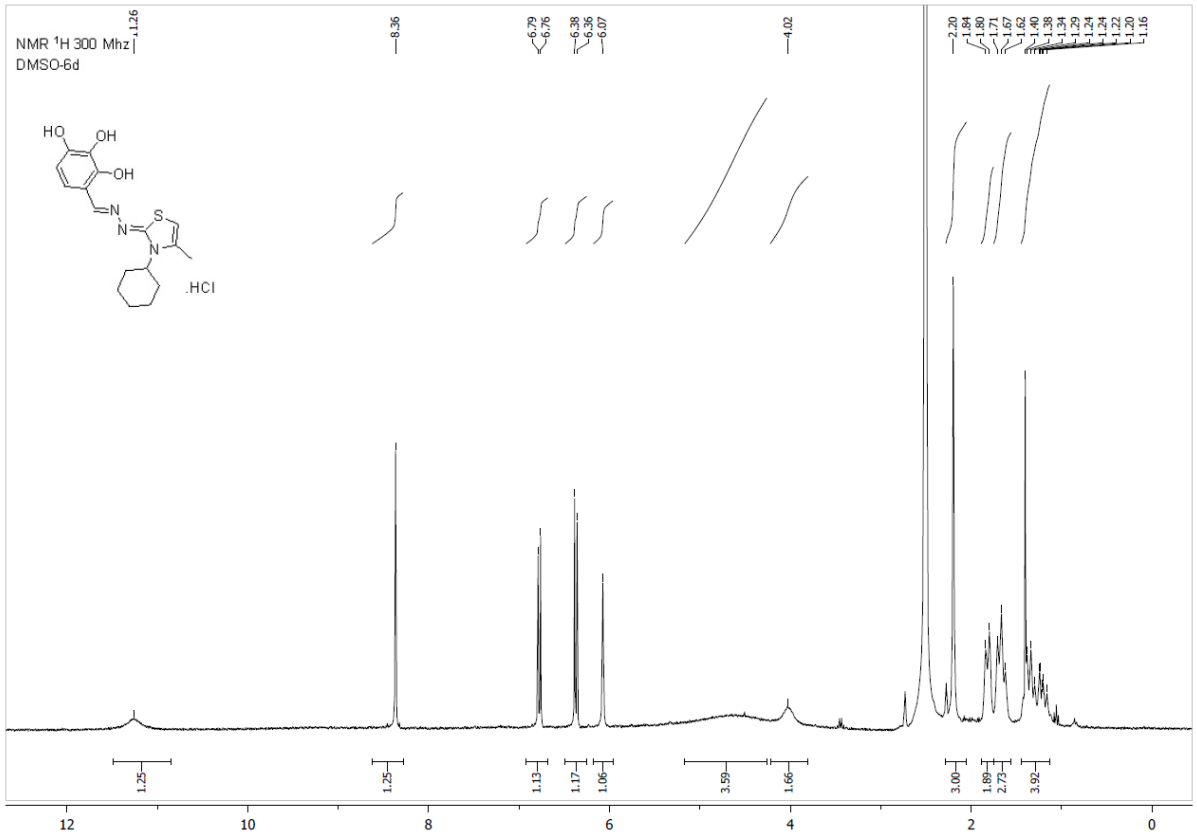
Compound 2 (MIM1 studies)

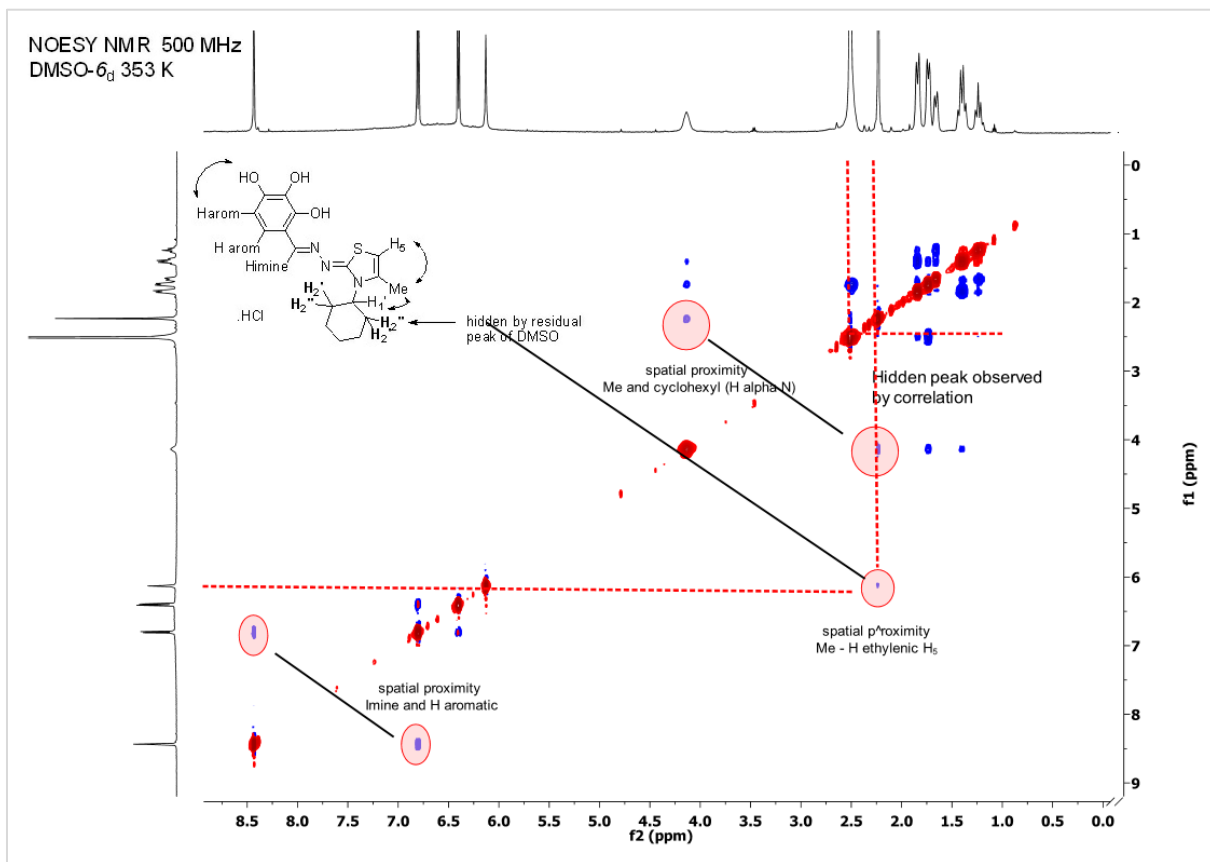
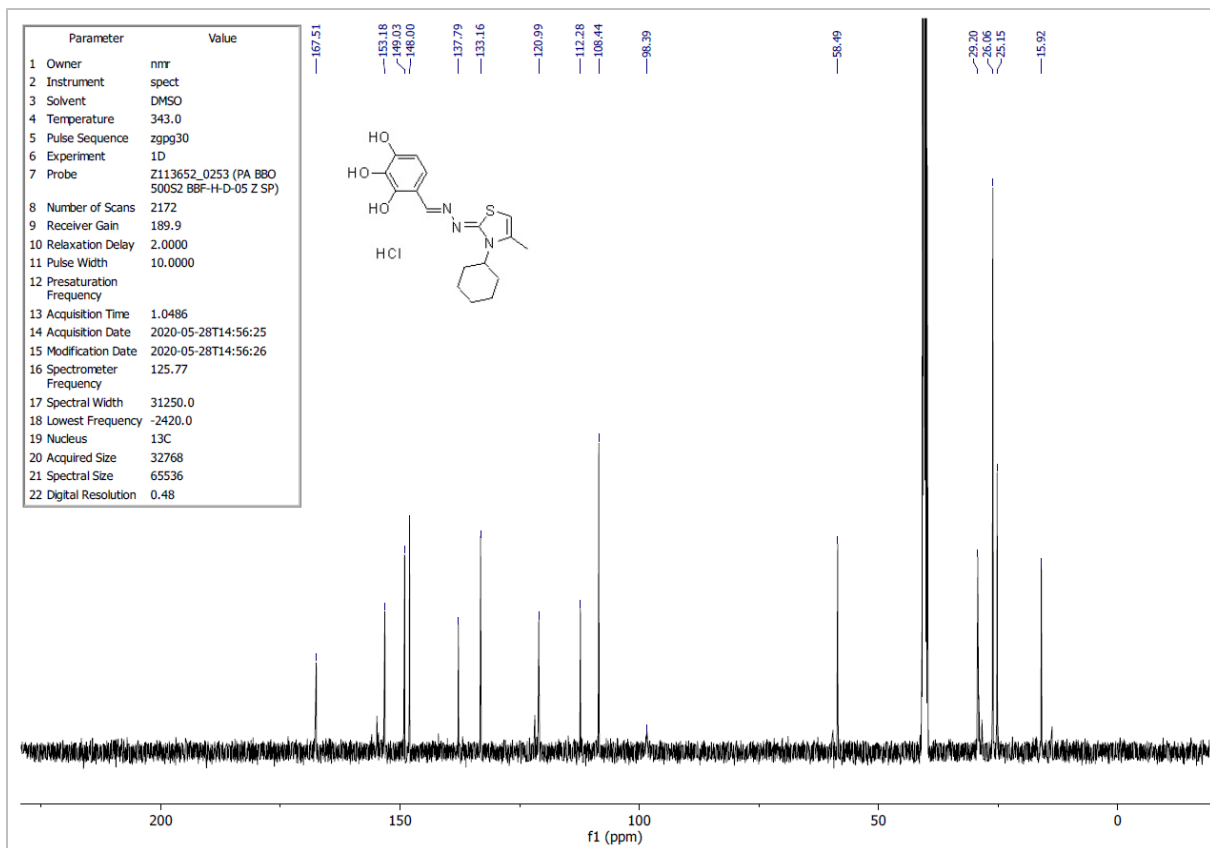


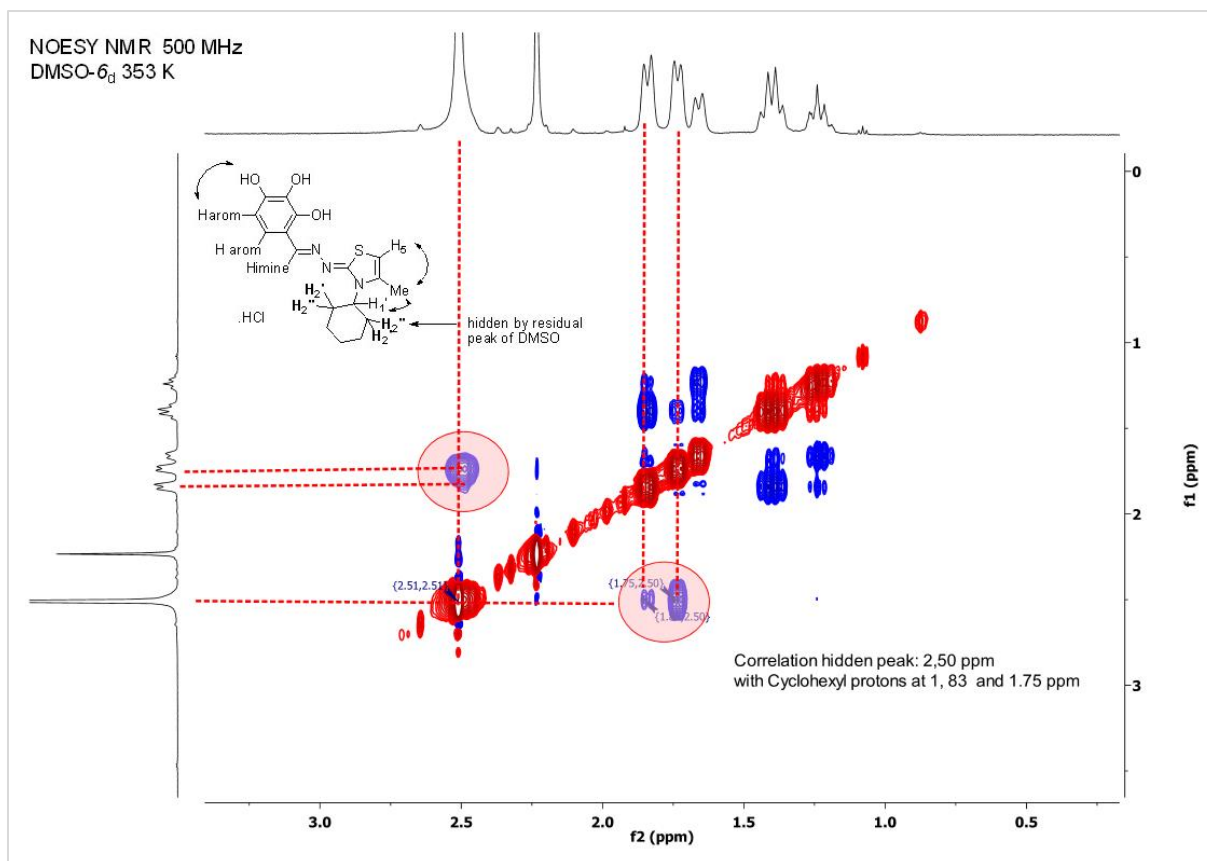
Supporting Information Figure 3: Dynamic Effect of ¹H NMR experiments with variations of temperature (step 10K)



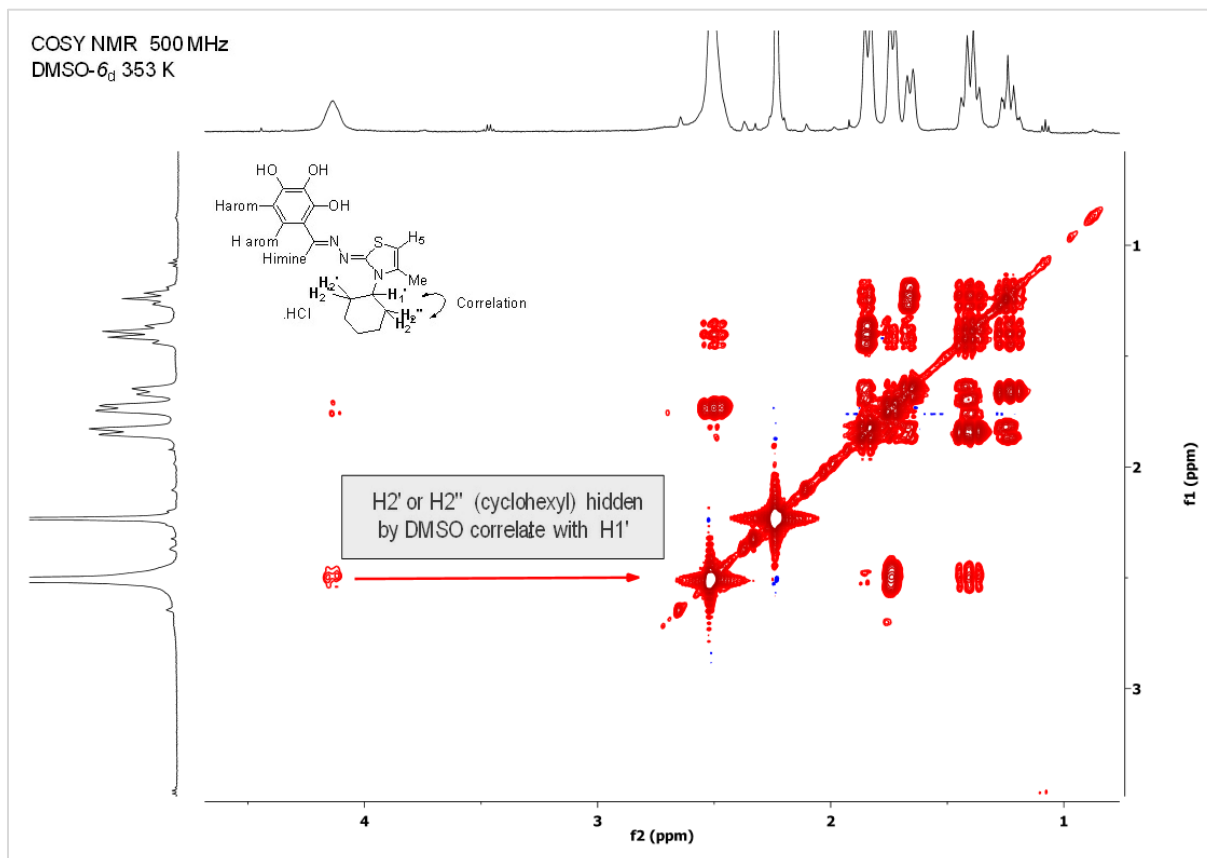
Supporting Information Figure 4: FT-IR of Compound 2



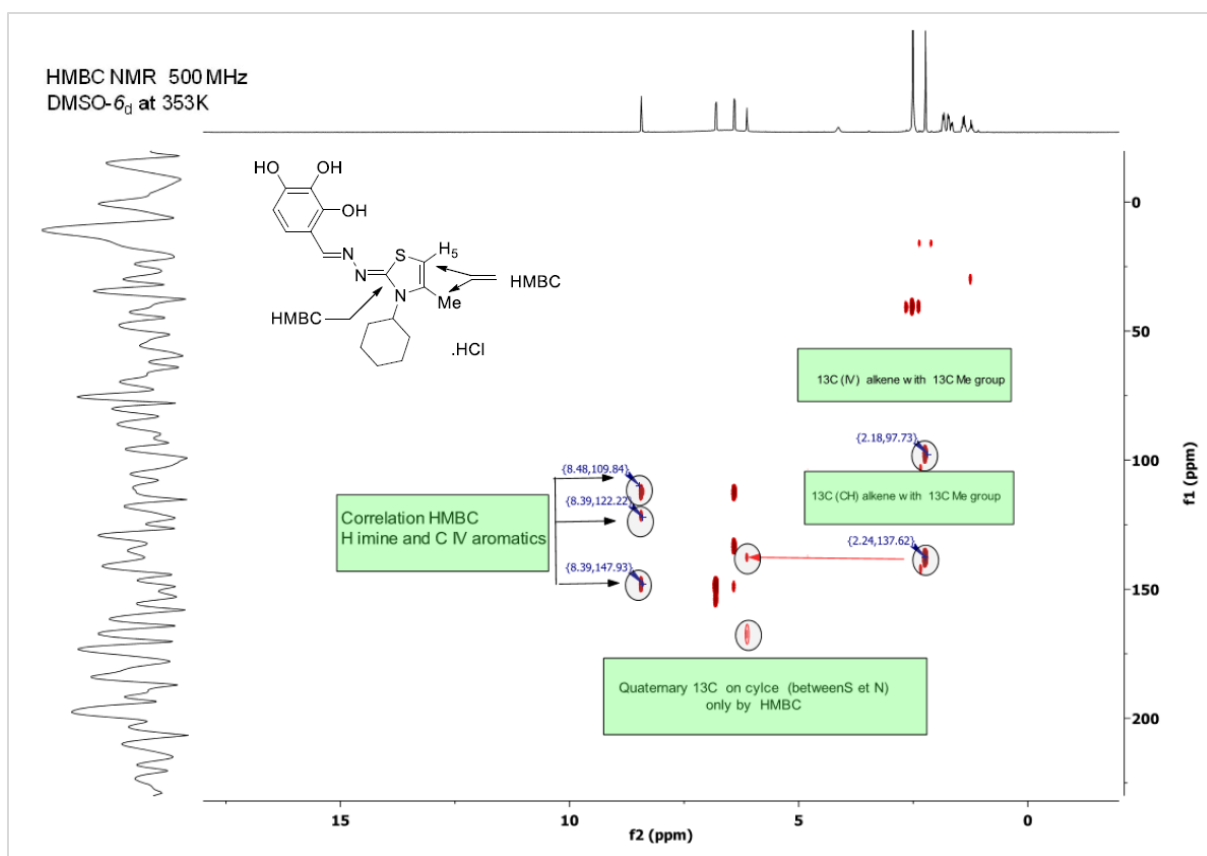
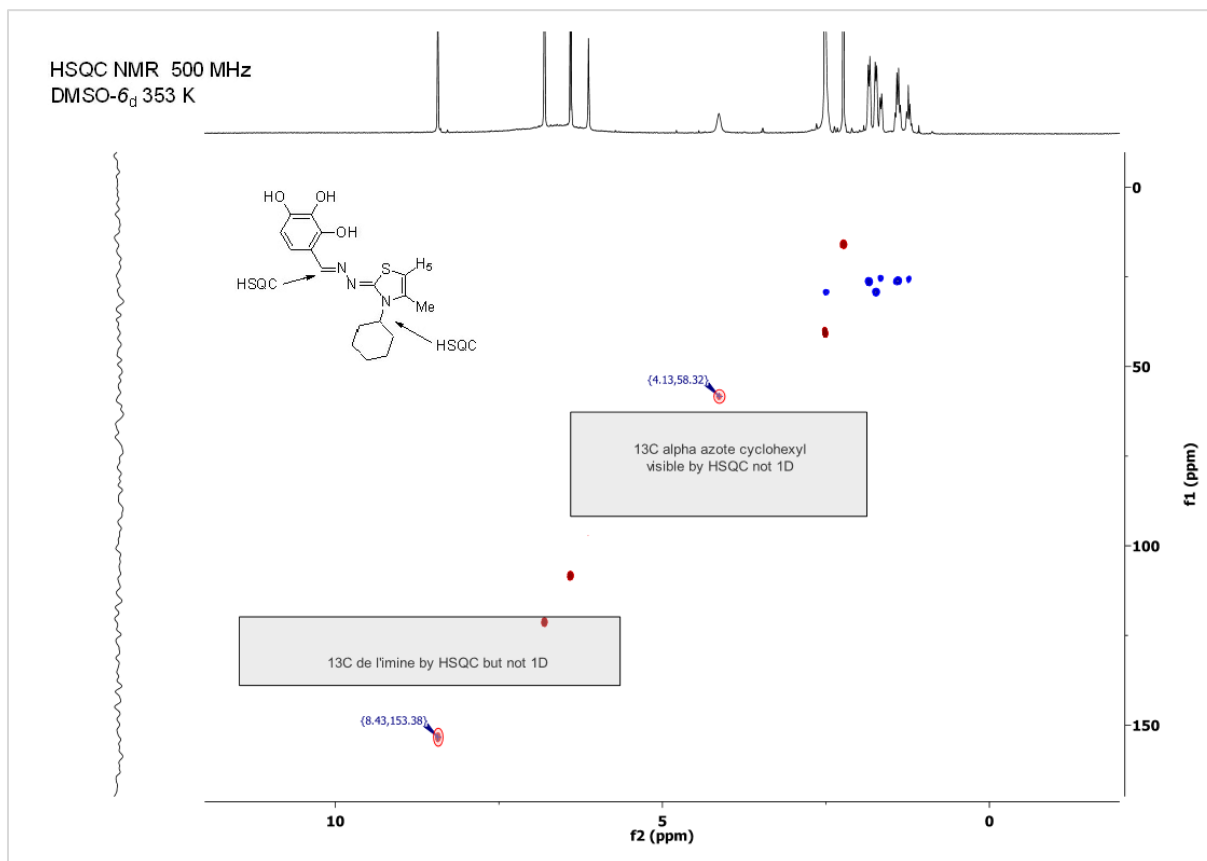




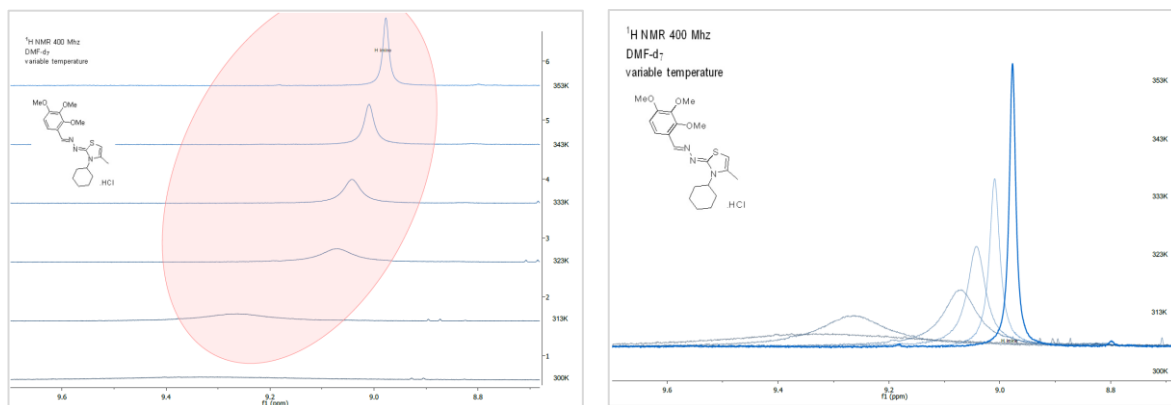
NOESY Experiment correlations: Me and H₅, Me and H₁', H₂''/2' cyclohexyl (hidden by DMSO -d) and H₂'/H₂'' (from cyclohexyl), Himine and Haromatic



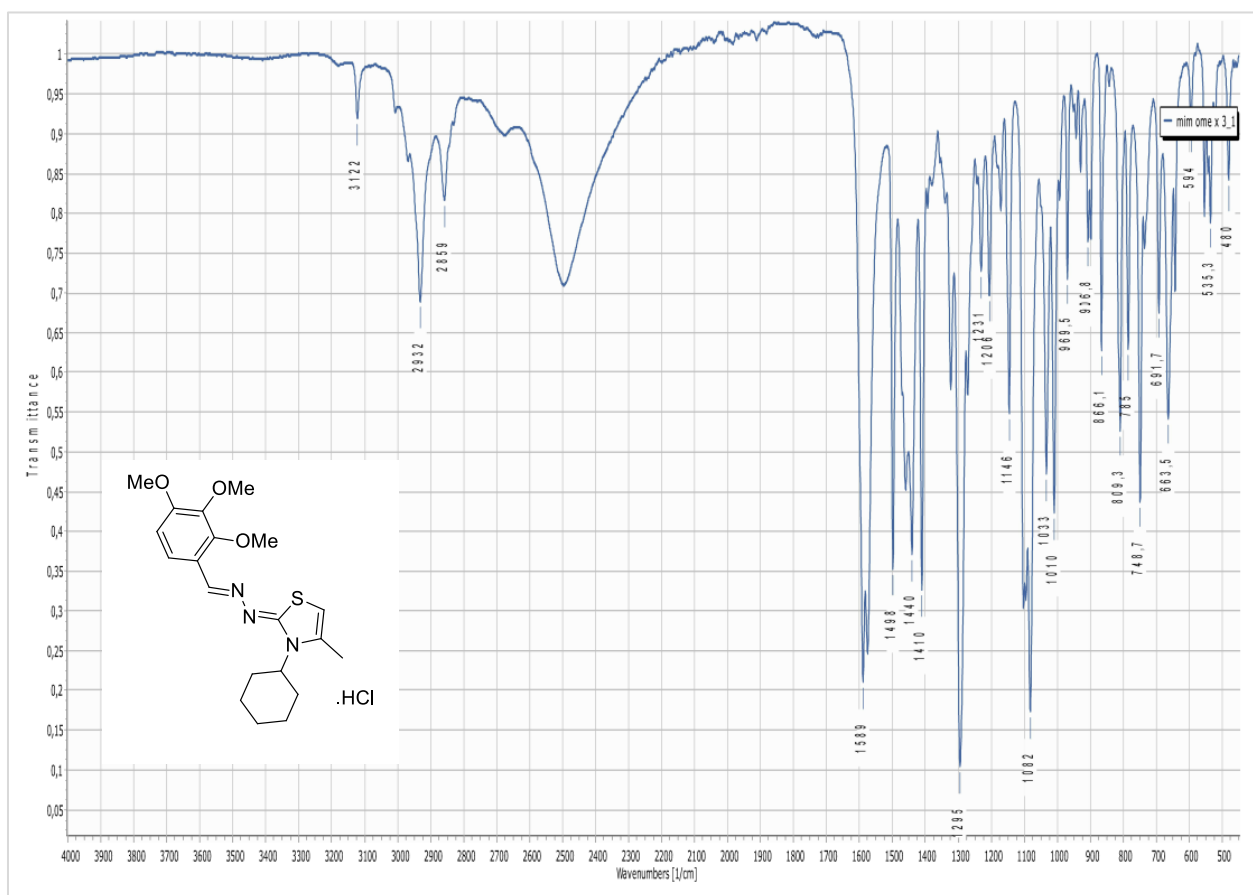
Correlation between H_{1'} and H₂/H_{2''} cyclohexyl hidden by DMSO-6d. (second proof)



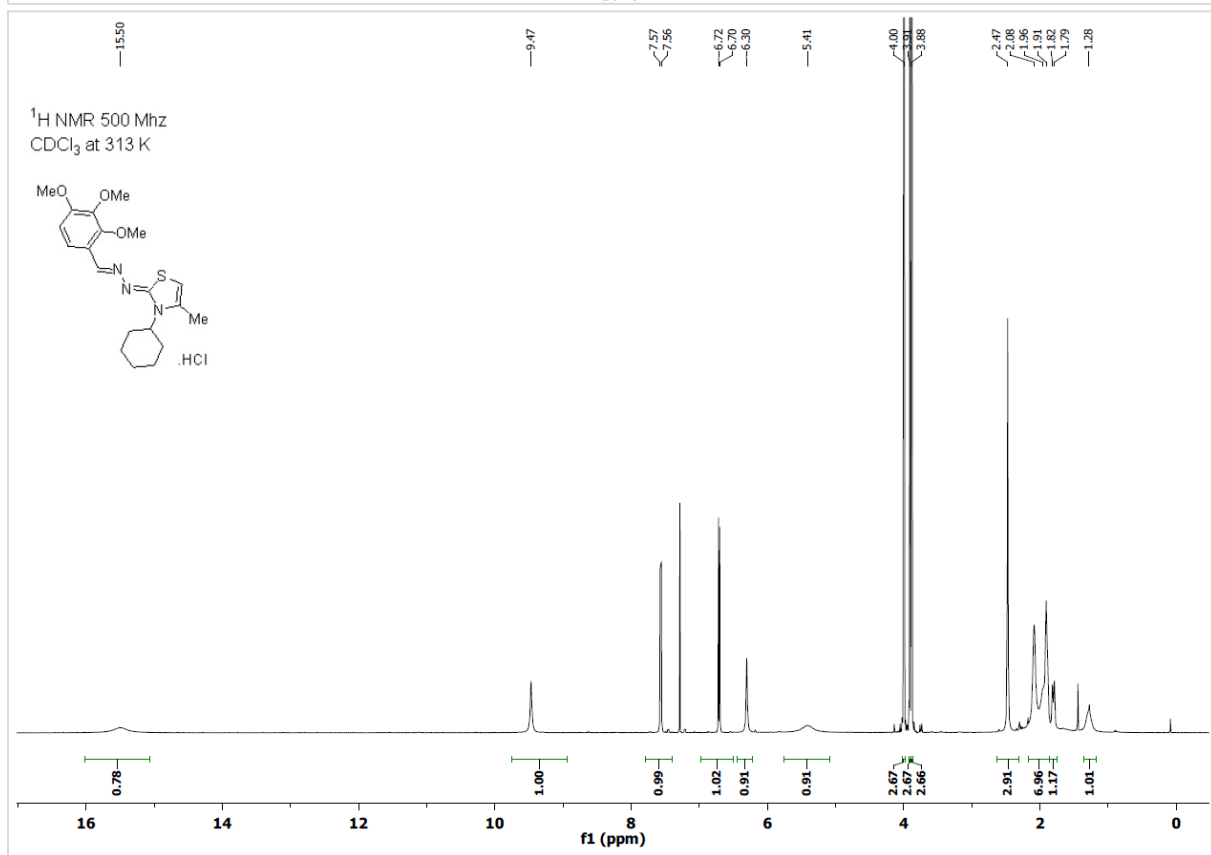
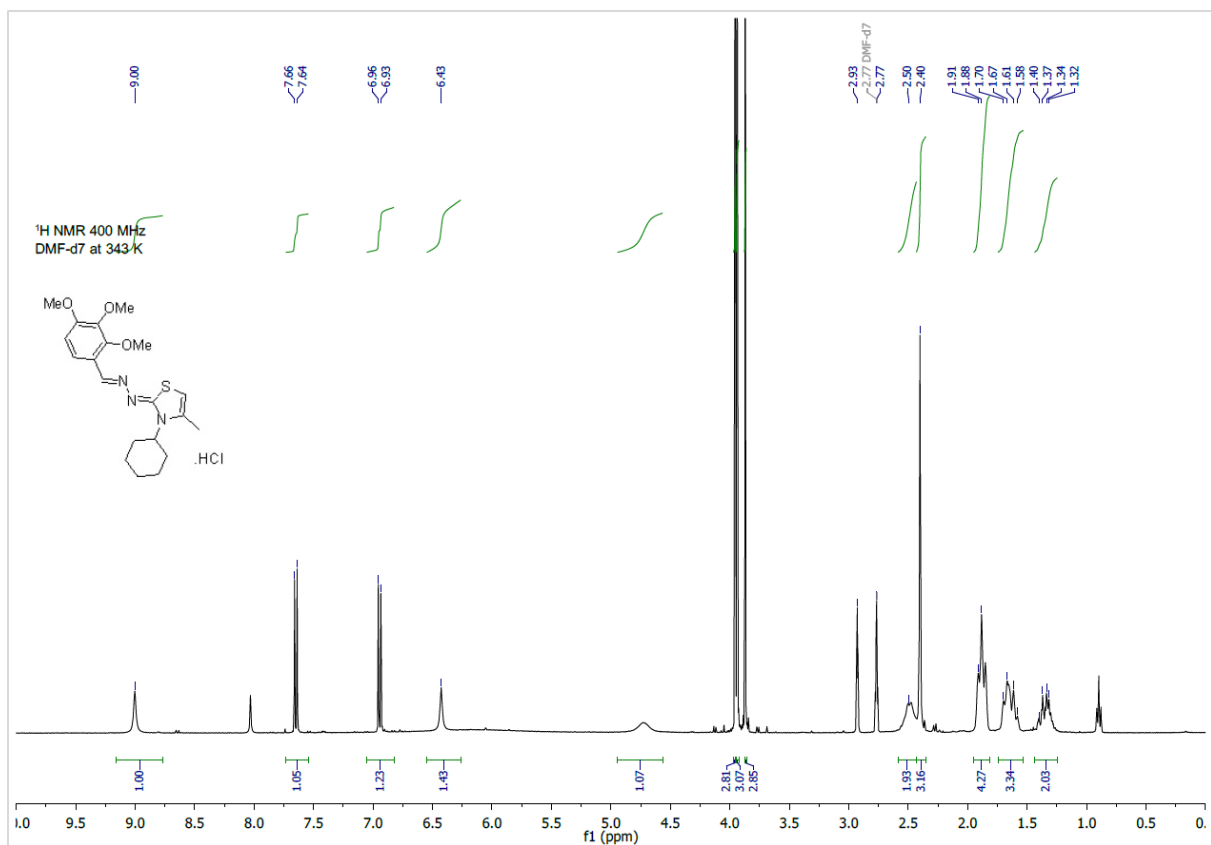
Compound 11 (analogue of MIM1 x OMe)

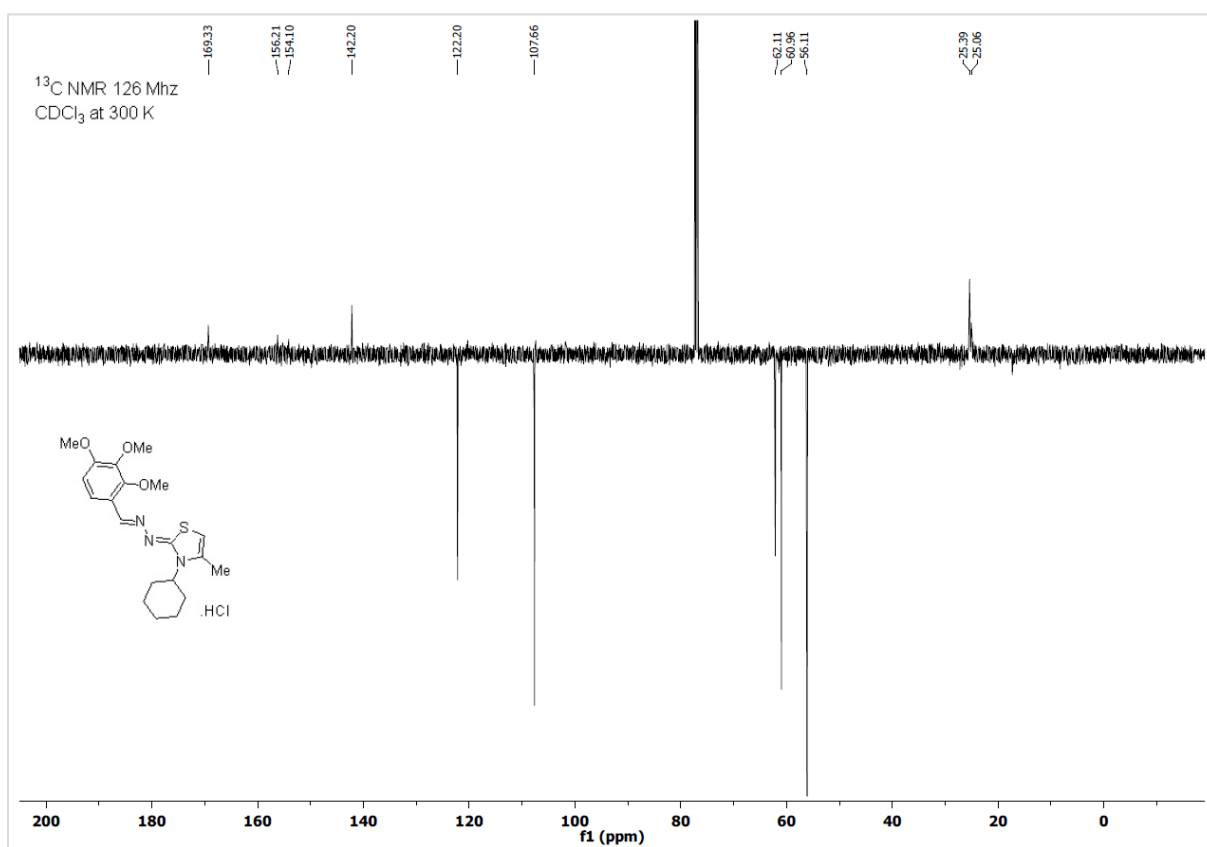
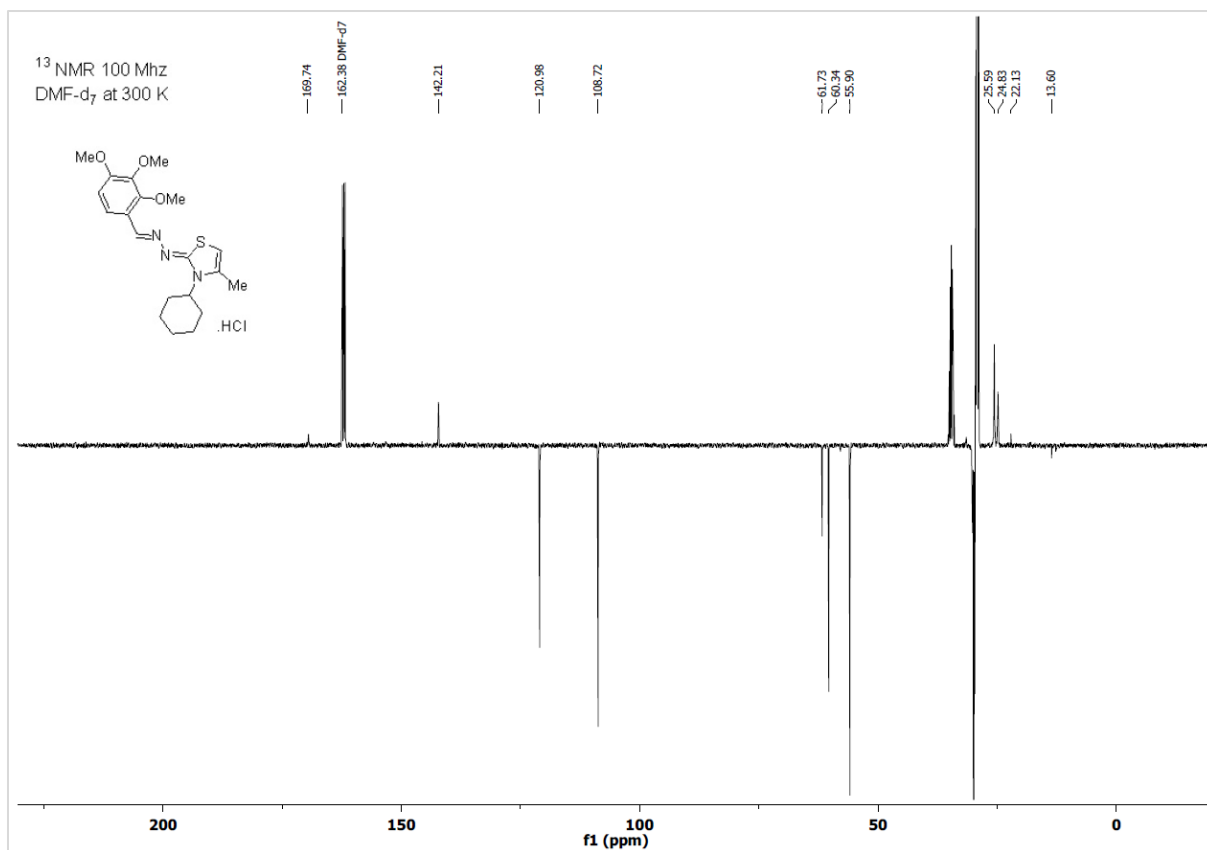


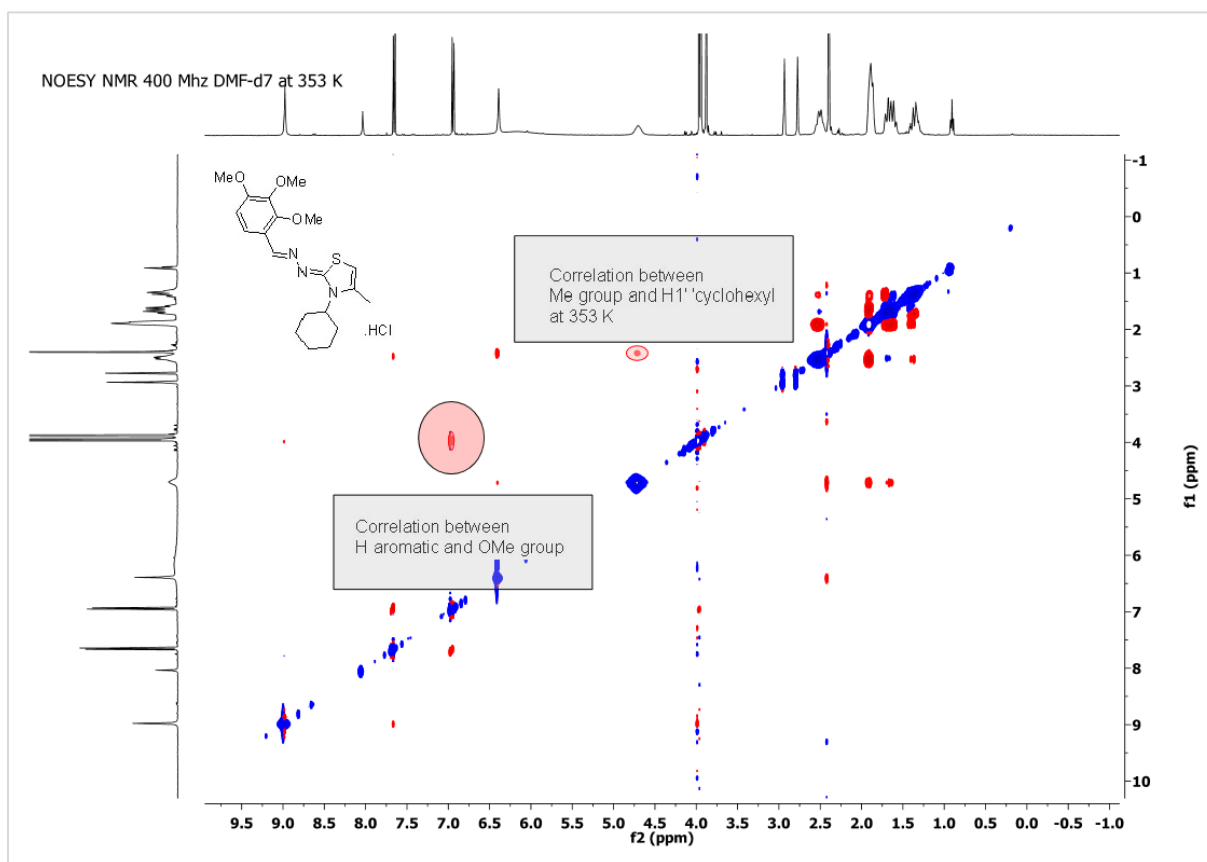
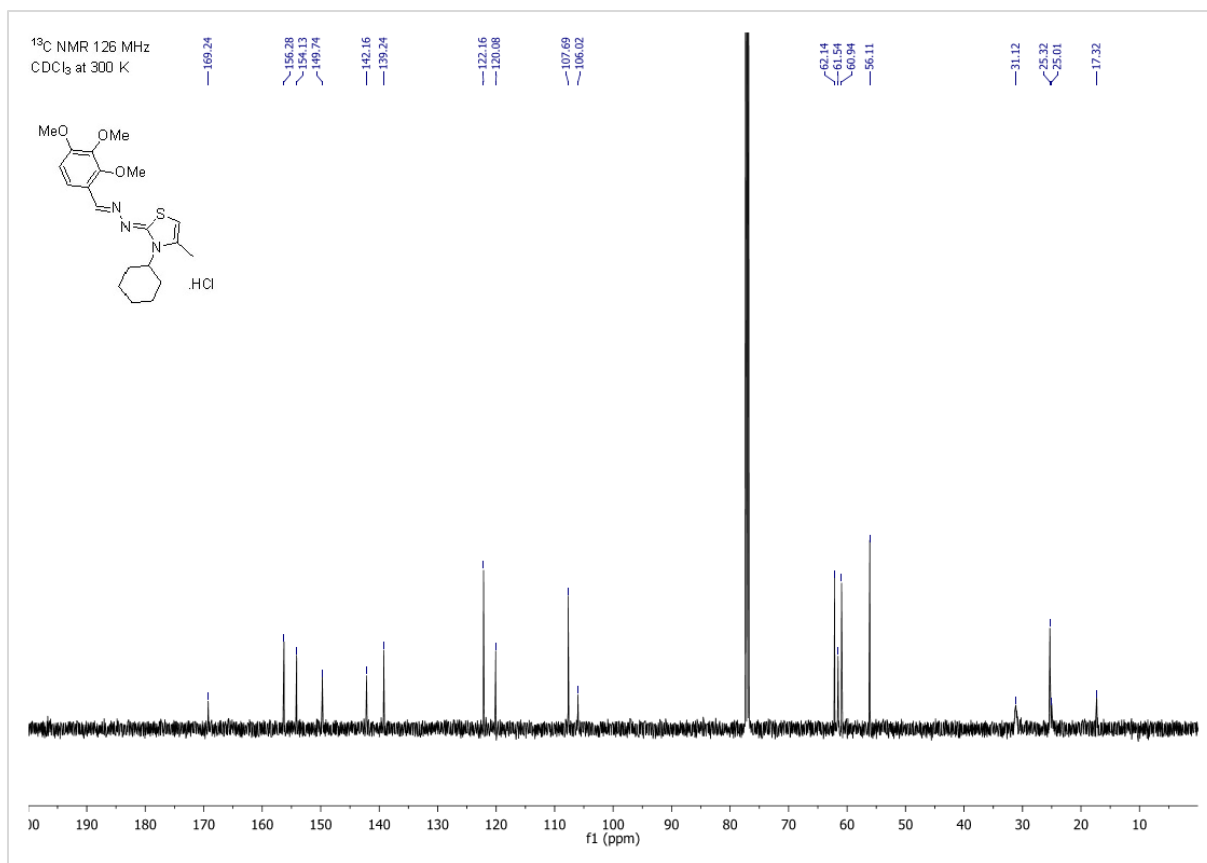
Supporting Information Figure 3: *H* imine proton of MIM1 (OMe x 3) relaxation upon temperature variation (copy of juxtaposition of ¹H NMR spectra)

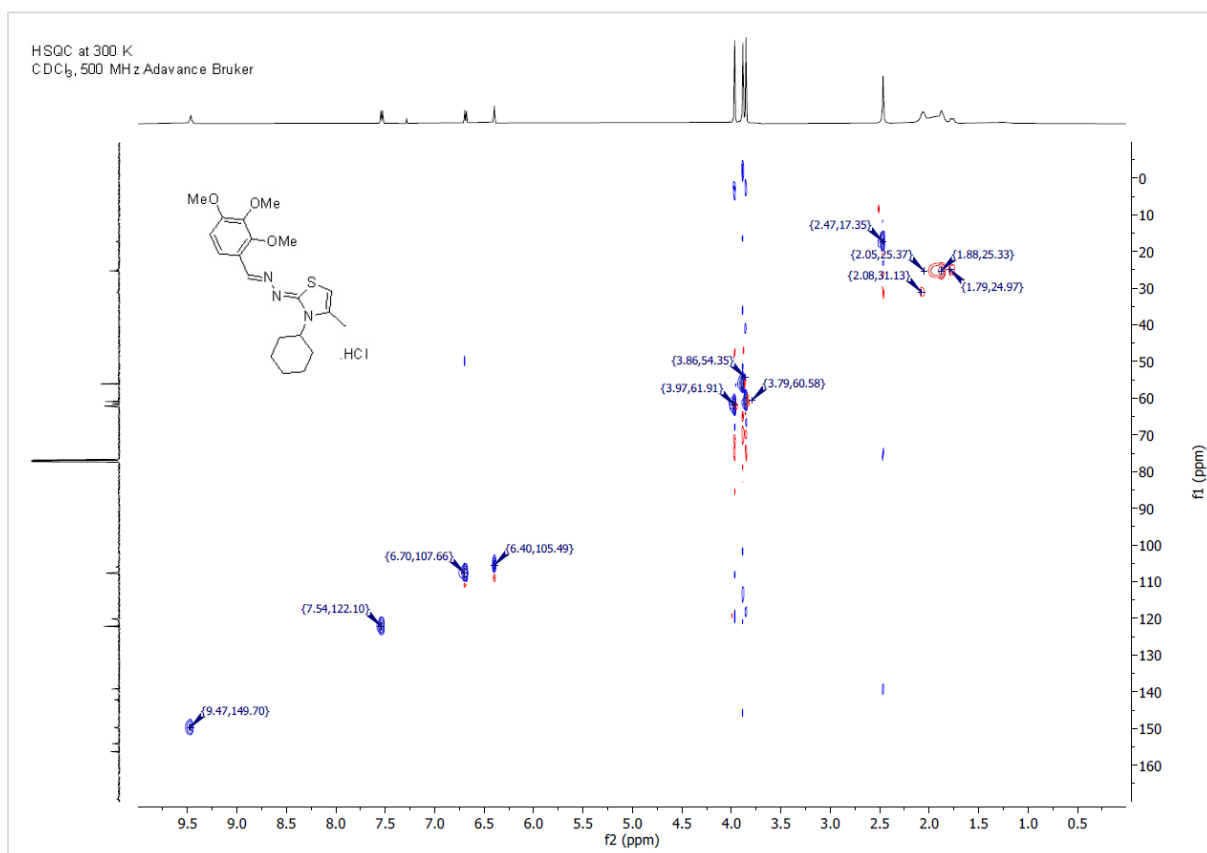
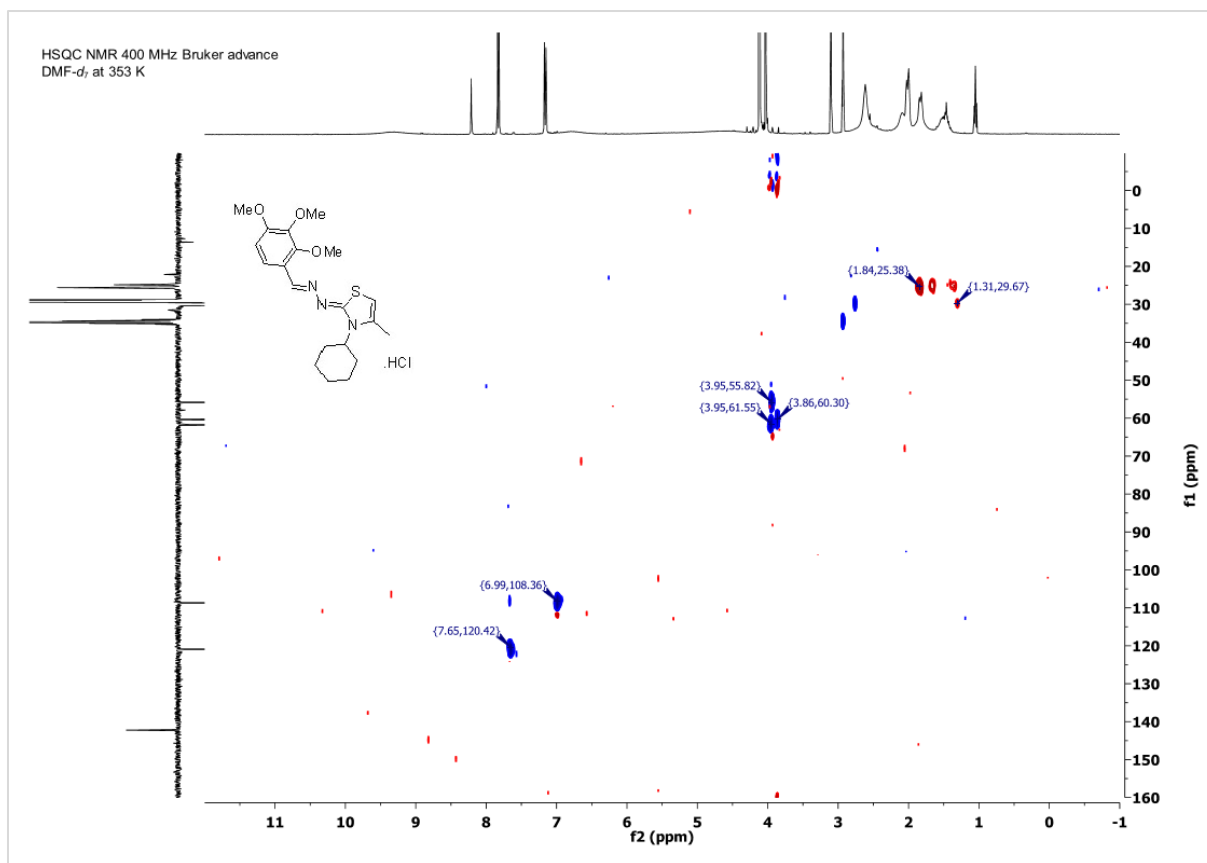


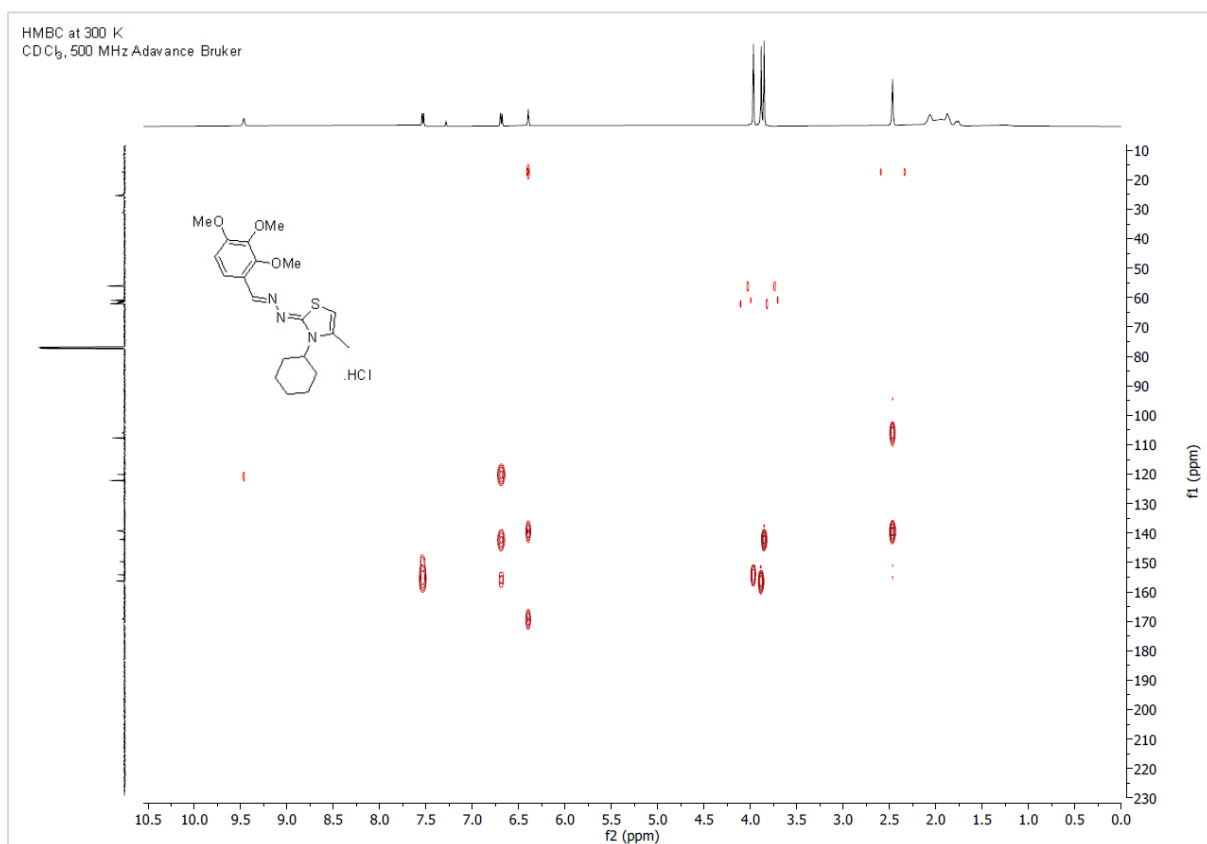
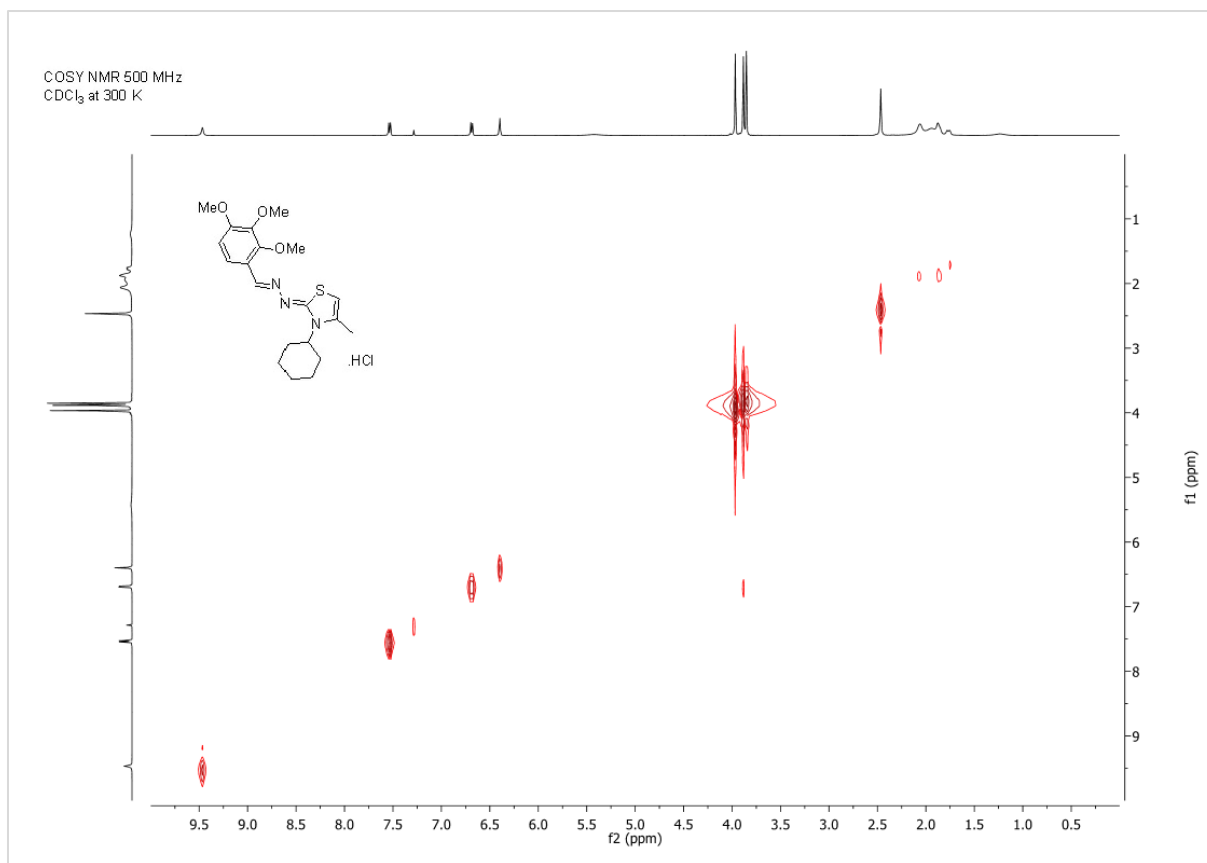
Supporting Information Figure 4: FT-IR compound 11



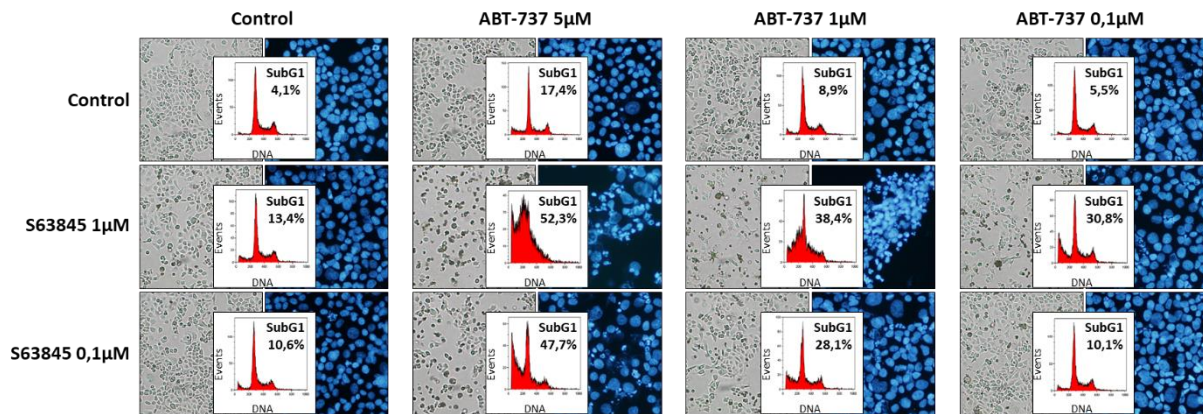






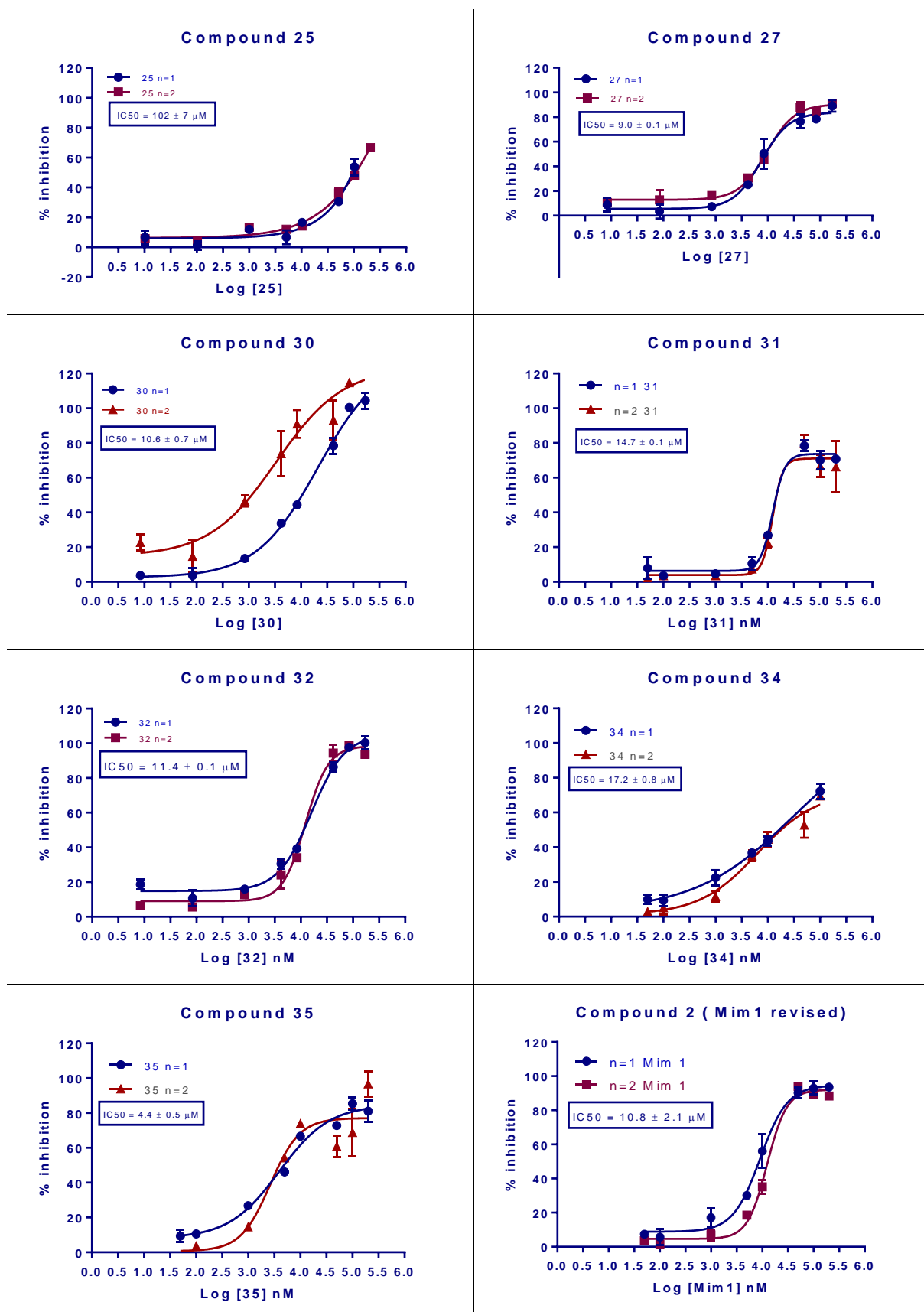


Supporting Information biological studies



Supporting Information Figure 5: Effect of ABT-737 and S63845 combination on IGROV1-R10 chemoresistant ovarian cancer cell line. Cellular morphology, DNA content and nuclear morphology were assessed after 24h exposure.

Supporting Information for Fluorescence Polarization Assays

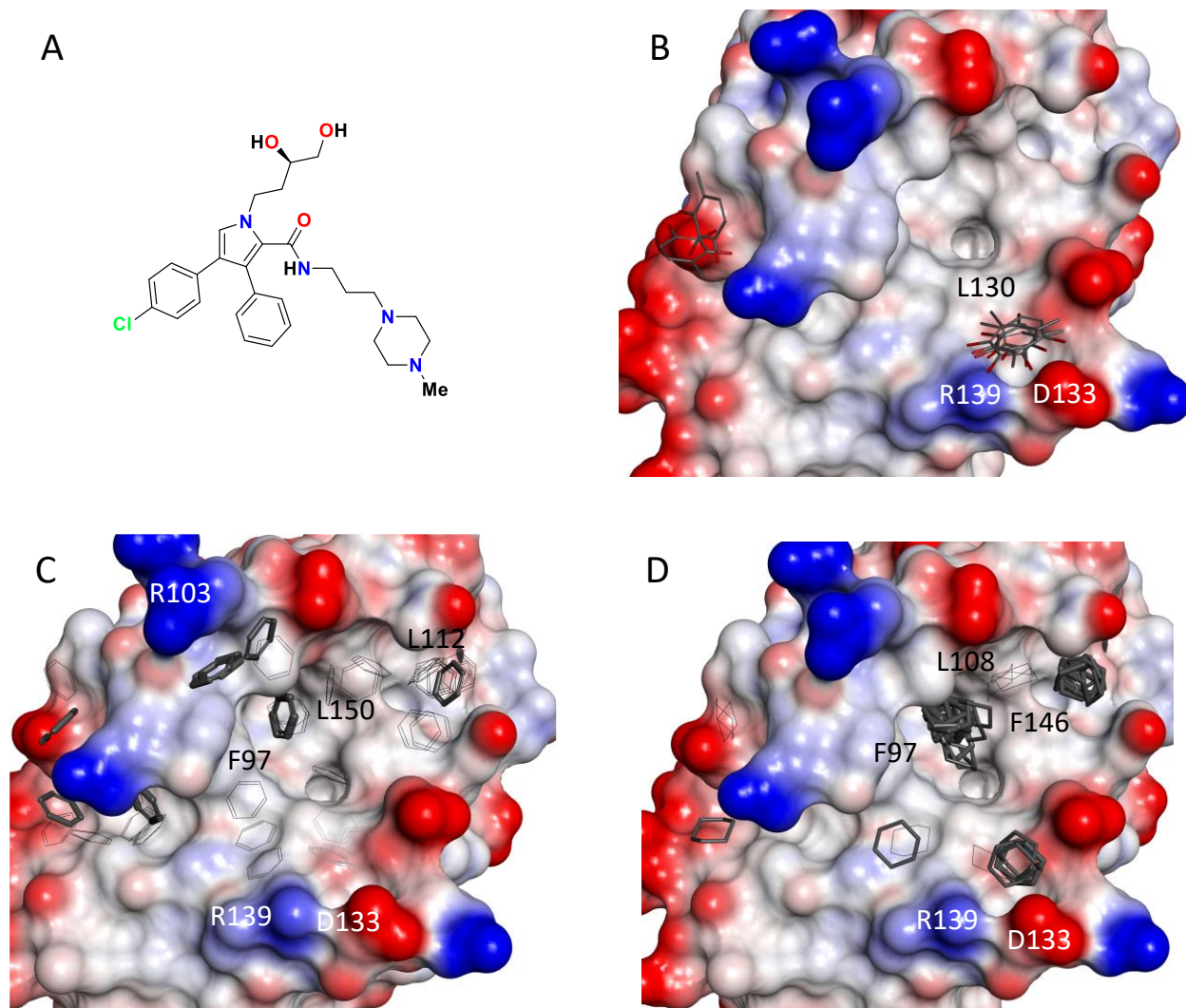


Supporting Information, Table 1. Competitive inhibition binding curves of MIM1 analogues.

Supporting Information for molecular docking

Determination of Bcl-x_L binding site by molecular modelling

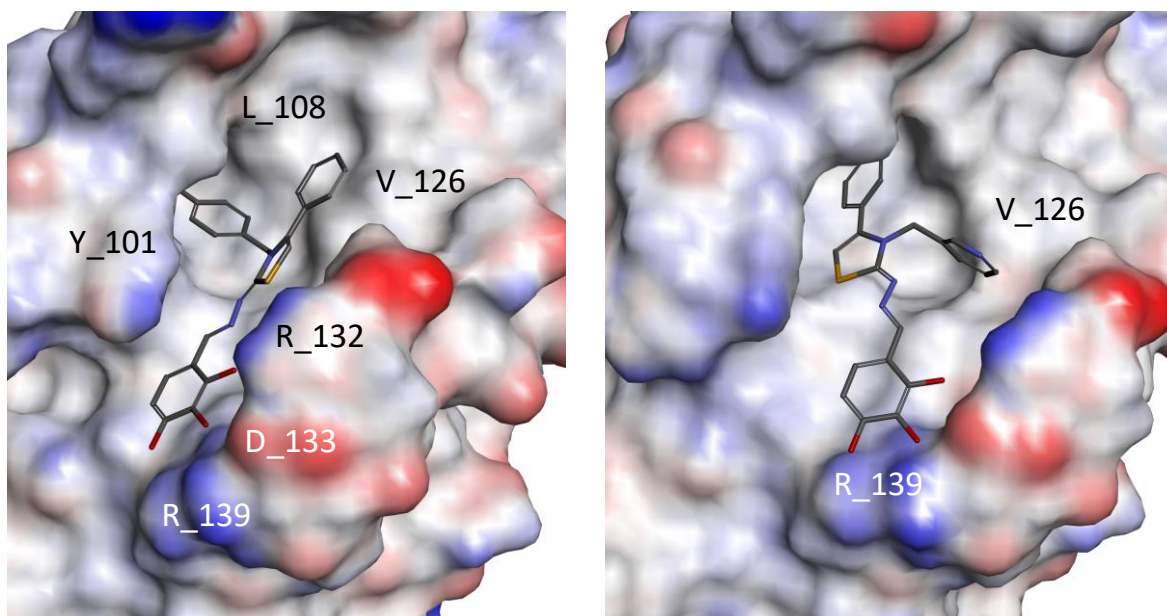
The structure of our compounds is, to our knowledge, completely new in the Bcl-x_L area. So, their binding site had to be deciphered. To this end, we investigated the 82 Bcl-x_L complexes available in the PDB to find the most similar ligand to our molecules. We found a diphenyl-pyrrole derivative with a somewhat similarity to our diphenyl-thiazole compounds (PDB: 3SPF)



Supporting Information, Fig. 6. (A) Chemical structure of the closest Bcl-x_L inhibitor found in the PDB. (B) Fragments docking at the surface of Bcl-x_L. Methyl-triphenol was mostly clustered in a cavity above R139/D133, with the highest calculated interaction energy: -44 kcal/mol. (C) Benzene was scattered on the protein surface, but much enriched in three cavities, one between F97 and L150 (-15.7 kcal/mol), the second beneath R103 (-14 kcal/mol), and the last near L112 (-11.6 kcal/mol). (D) Cyclohexane occupied essentially two deep cavities, the same as benzene (respectively -16.5 and -13.5 kcal/mol). The thickness of the fragments chemical bonds relates to the calculated interaction energy (the thickest, the highest).

To probe the possible binding sites and orientations of our ligands in this protein conformer, we first performed a multiple copy simultaneous search (MCSS) of different fragments: a triphenol and a benzene, directly related to our molecules, and a cyclohexane to identify the most hydrophobic binding site (more precisely, the site most prone to Van der Waals interactions). Clustering of the docked fragments and calculated interaction energy suggested that the triphenol might bind to a rather flat surface above L130, near the ionic pairs R139/D133 and R132/E129 (Fig. 6B). Benzene had more scattered binding sites, but the two most populated and highest affinity cavities were around F97, L150 and L112 (Fig. 6C). The cyclohexyl fragment predominated in the two central cavities (Fig. 6D). Interestingly, the predicted triphenol binding site corresponded to that of a co-crystallized glycerol (a trihydroxylated molecule), and the most favourable cyclohexane site to that of chlorophenyl of the co-crystallized inhibitor.

Independently of the MCSS experiment, we performed a flexible docking of compound **30**. The pose with the highest score suggests a binding mode where the triphenol forms extensive hydrogen bonds with ionic pairs R139/D133 and/or R132/E129 (Supporting Information Fig. 7). The thiazole is above V126, while the phenyl interacts with L108, V126 and L112, overhangs by Q111. The ethyl-benzyl is buried in the deep cavity, interacting with F146, L108, A104, Y101 and F97.

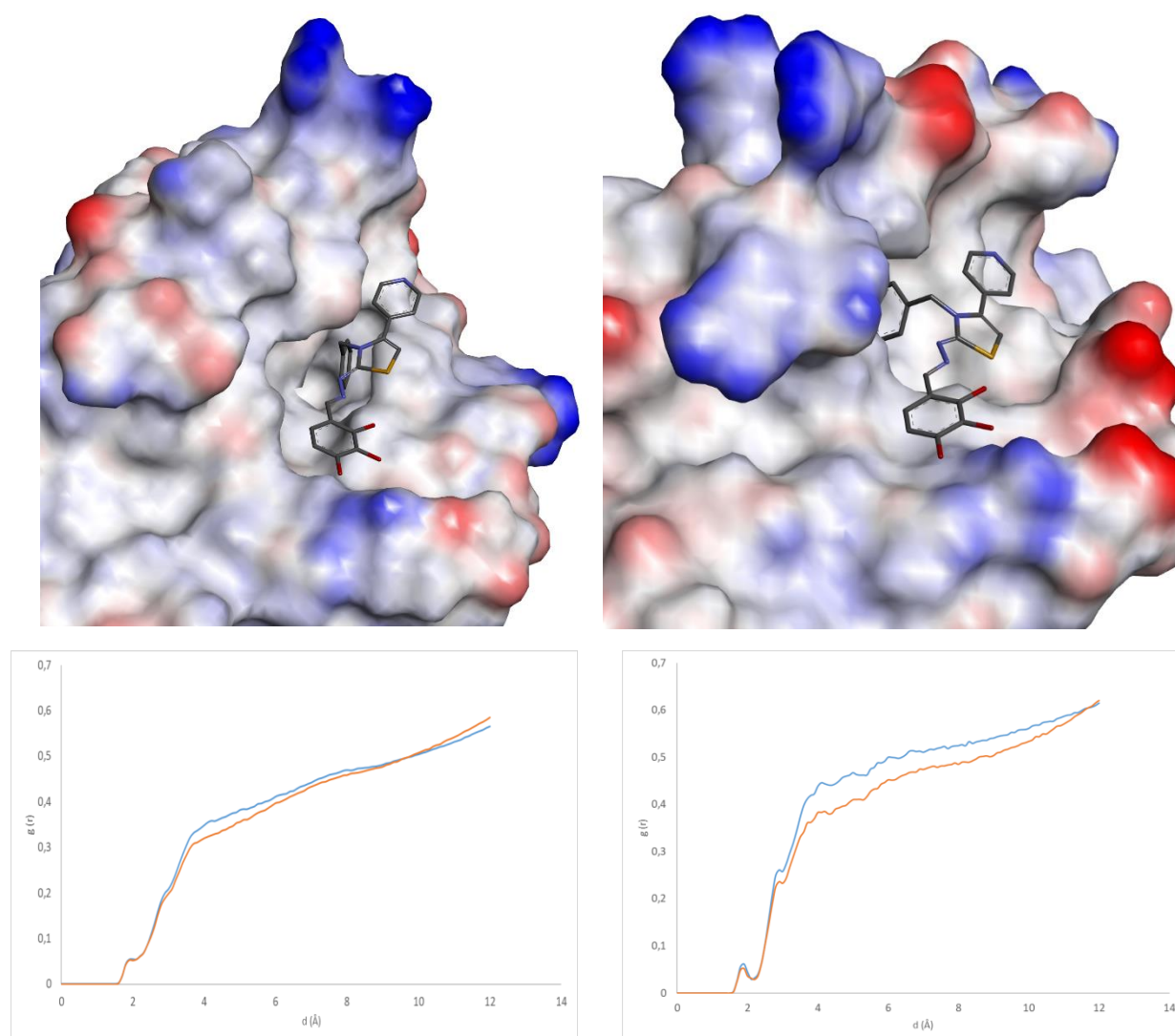


Supporting Information Fig. 7(left). Proposed binding mode of **30** in Bcl-xL. (B) (right) **32** docked in the same protein.

Computational studies of compound 35 onto Mcl-1 and Bcl-x_L

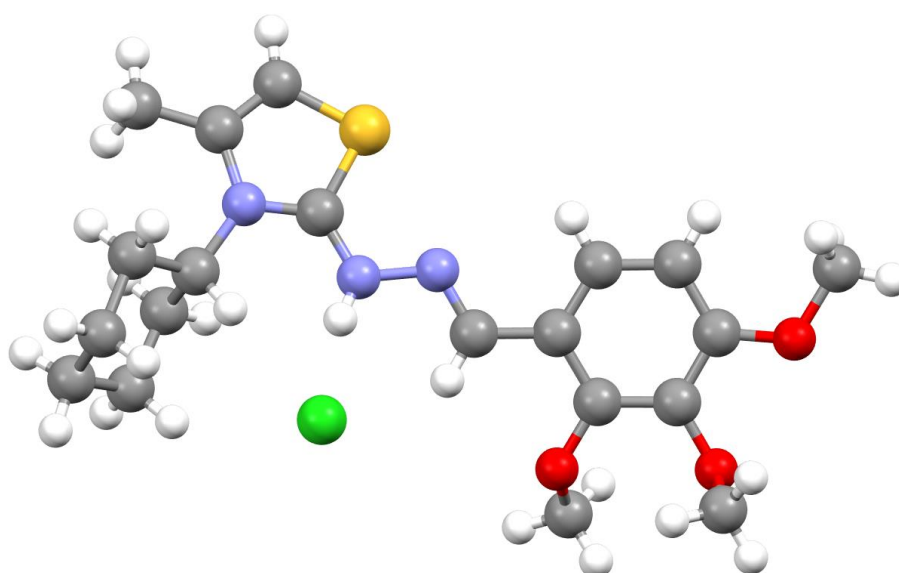
As already observed for Mcl-1, the ligand is able to flip in the binding site in order to minimize the solvent exposition of most hydrophobic parts. This was confirmed by molecular dynamics, showing that **35** is more solvated in Mcl-1 binding site than is Bcl-x_L (Supp. Info. Fig. 8), and explaining why **35** is selective for Mcl-1 in spite of a similar binding mode in both proteins.

This was confirmed by molecular dynamics, showing that **35** is more solvated in Mcl-1 binding site than is Bcl-x_L (Supporting Information Fig. 8), and explaining why **35** is selective for Mcl-1 in spite of a similar binding mode in both proteins.



Supporting Information, Fig. 8. (top) Compound 35 docked onto Mcl-1 (left) and Bcl-x_L (right). One can observe that the pyridine is much more solvent-exposed in the former. Radial distribution function $g(r)$ of water measured during molecular dynamics of full molecule 35 (bottom left) in Mcl-1 (blue) and Bcl-x_L (red), and only pyridine of 35 (bottom right).

Structure of **11** established by X-Ray analysis:



The details of X-Ray structural analysis of **11** have been deposited at CDDC with the number 2006656.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0026 A Wavelength=0.71073
Cell: a=7.8822(17) b=31.959(6) c=9.896(2)
alpha=90 beta=121.156(7) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	2133.3(8)	2133.2(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C20 H28 N3 O3 S, Cl	C20 H28 N3 O3 S, Cl
Sum formula	C20 H28 Cl N3 O3 S	C20 H28 Cl N3 O3 S
Mr	425.96	425.96
Dx,g cm-3	1.326	1.326
Z	4	4
Mu (mm-1)	0.303	0.303
F000	904.0	904.0
F000'	905.42	
h,k,lmax	10,41,12	10,41,12
Nref	4917	4862
Tmin,Tmax	0.897,0.982	0.822,0.982
Tmin'	0.891	

Correction method= # Reported T Limits: Tmin=0.822 Tmax=0.982
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 27.533

R(reflections)= 0.0407(4208) wR2(reflections)= 0.0972(4862)

S = 1.072 Npar= 260

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

PLAT213_ALERT_2_C	Atom C24	has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	5.2	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1 H	Uiso(max)/Uiso(min) Range	6.6	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	023	Check
PLAT414_ALERT_2_C	Short Intra	D-H..H-X	H6 ..H12	1.98	Ang.
			X,Y,Z =	1_555	Check
PLAT431_ALERT_2_C	Short Inter	HL..A Contact	Cl1 ..S1	3.31	Ang.
			-1+x,y,-1+z =	1_454	Check
PLAT906_ALERT_3_C	Large K Value	in the Analysis of Variance	2.647	Check
PLAT911_ALERT_3_C	Missing FCF Refl	Between Thmin & STh/L=	0.600	18	Report

Alert level G

PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	P21/n	P21/c	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			1
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		36
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.3
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			7

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

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

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing, _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and _publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

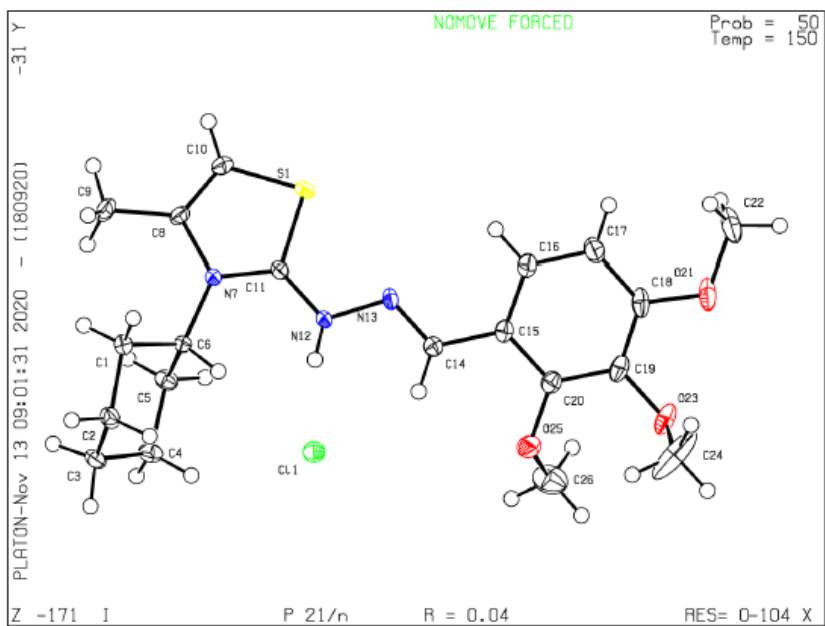
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

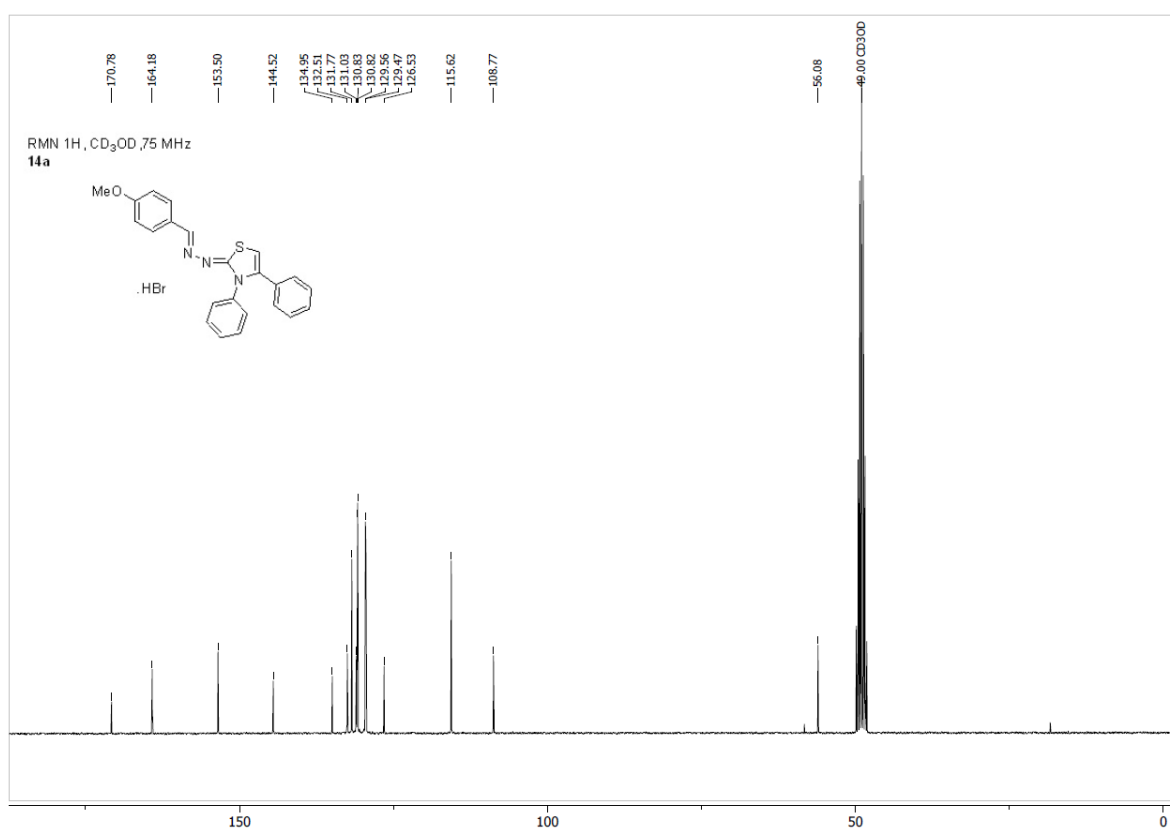
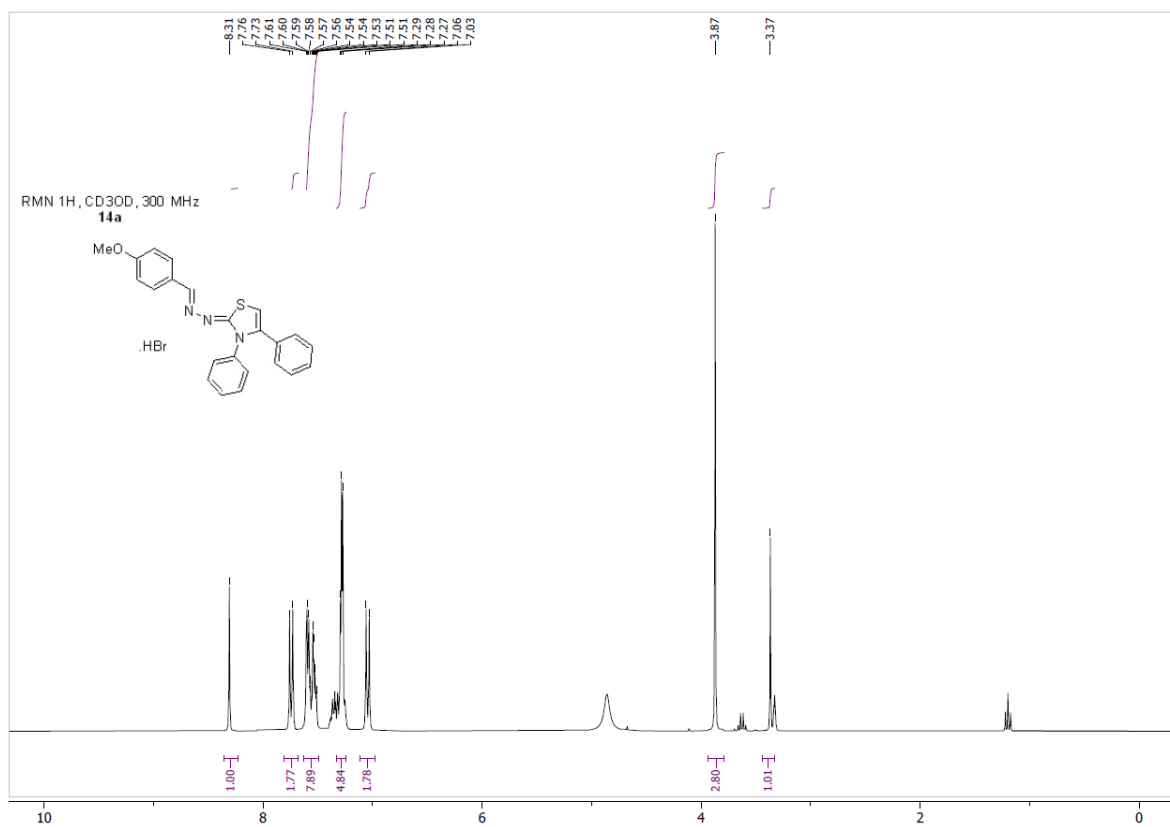
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 18/09/2020; check.def file version of 20/08/2020

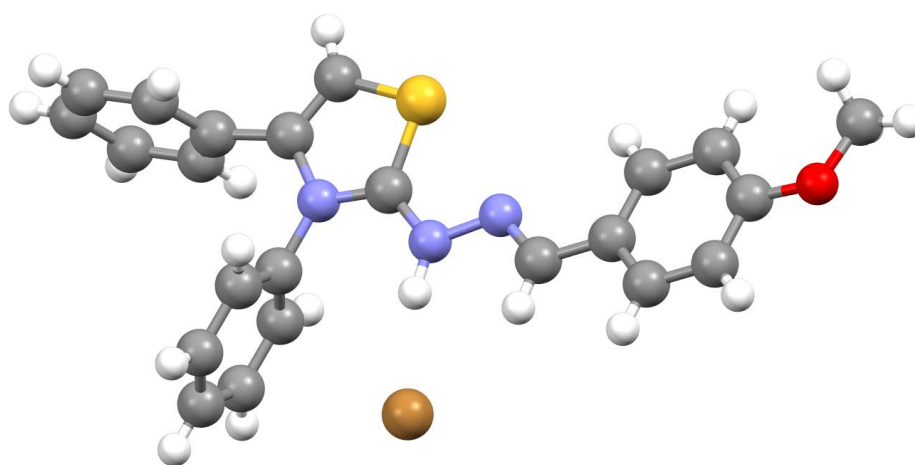
Datablock I - ellipsoid plot





NMR spectra of **14a**

Structure of **14a** established by X-Ray analysis:



The details of X-Ray structural analysis of **14a** have been deposited at CDDC with the number 2006657.

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
PLAT431_ALERT_2_C Short Inter HL..A Contact Br1 ..S1 . 3.44 Ang.
X,Y,L+Z = 1_556 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report

Alert level G
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 15.24 Why ?
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 116 A**3
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed 1 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A
PUBL004_ALERT_1 A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1 A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1 A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1 A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1 A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1 A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1 A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G
PUBL017_ALERT_1 G The _publ_section_references section is missing or
empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

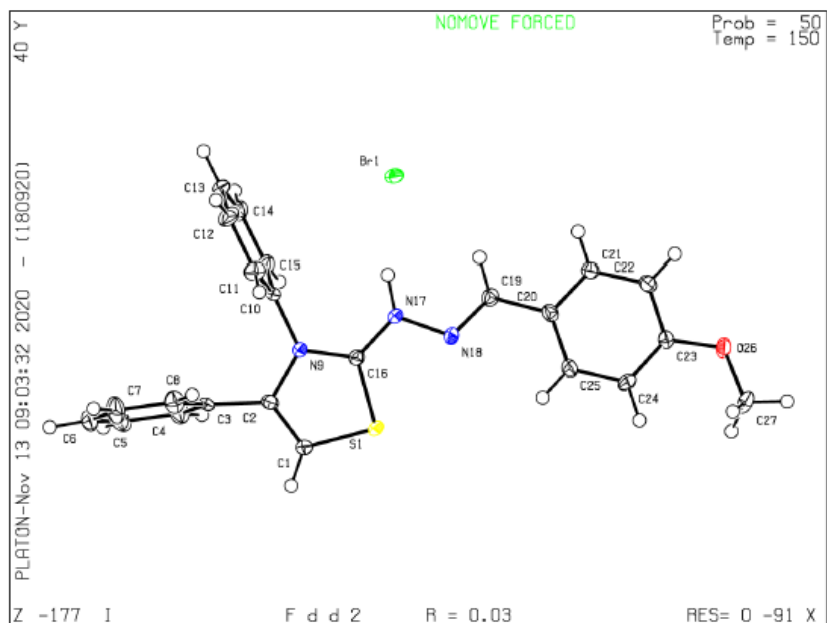
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
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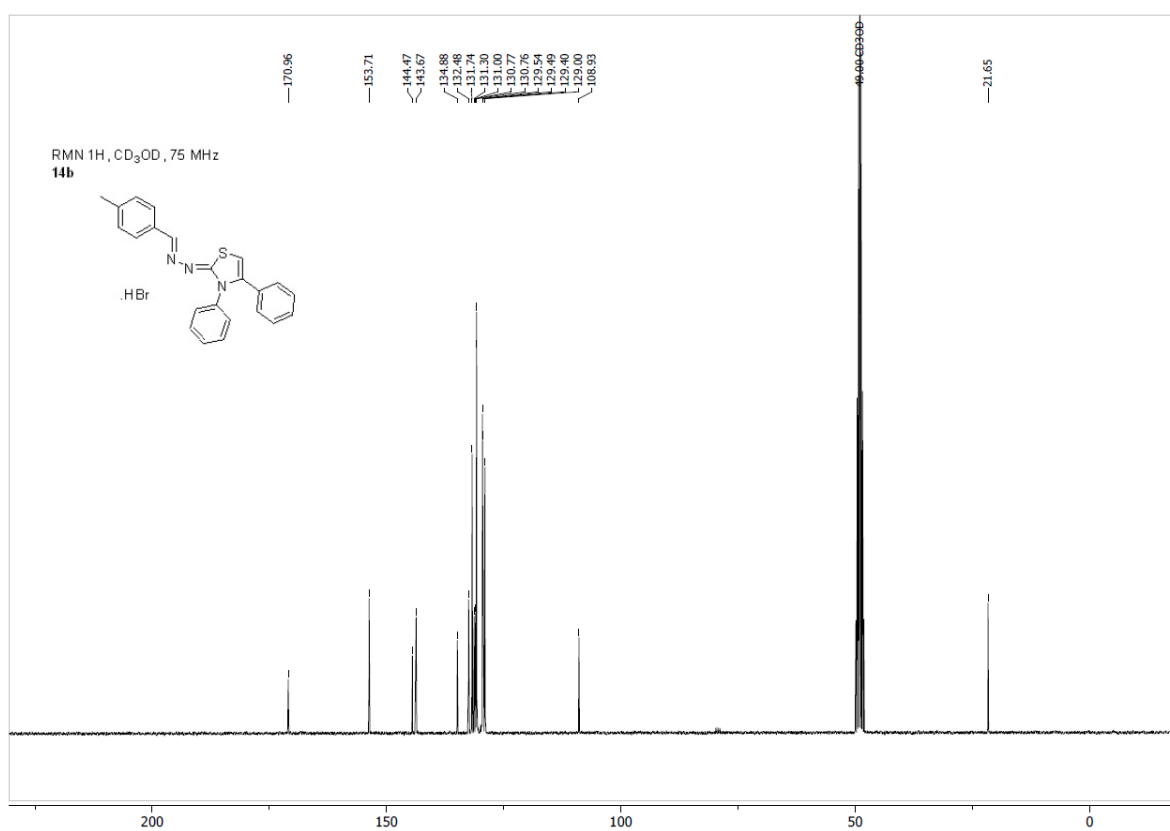
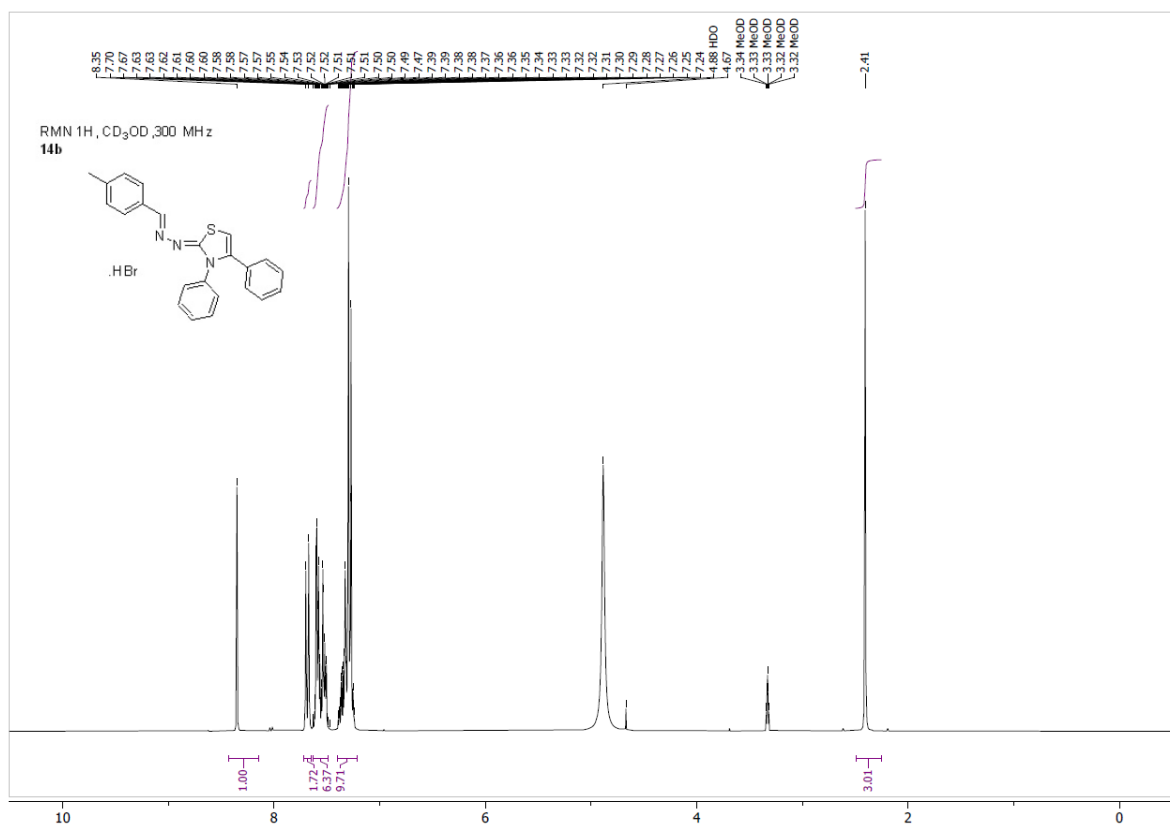
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 18/09/2020; check.def file version of 20/08/2020

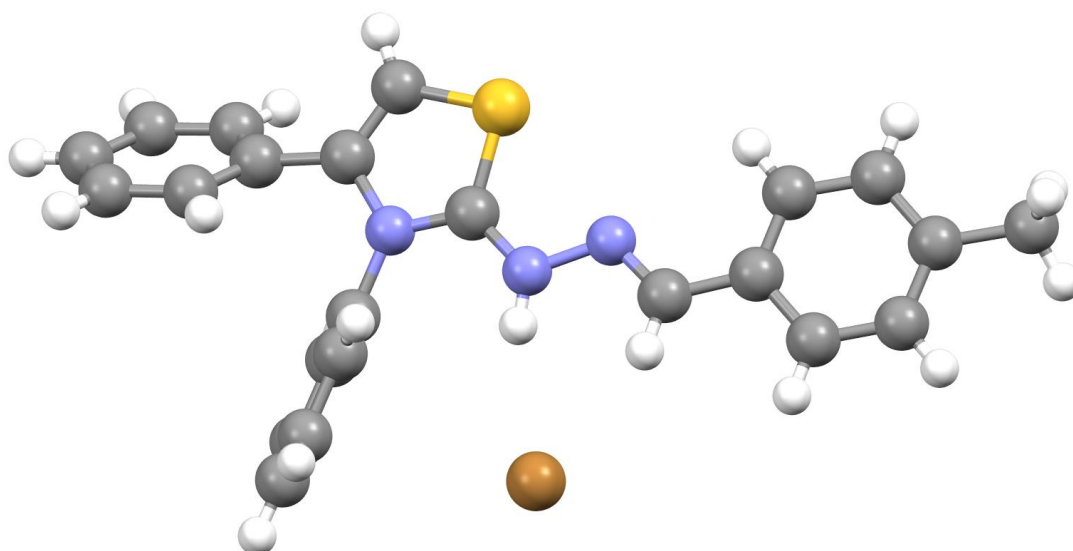
Datablock 1 - ellipsoid plot





NMR spectra of **14b**

Structure of **14b** established by X-Ray analysis:



The details of X-Ray structural analysis of **14b** have been deposited at CDDC with the number 2006655.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=9.087(1) b=10.0635(13) c=13.3909(17)
alpha=80.956(4) beta=81.422(4) gamma=65.230(4)

Temperature: 150 K

	Calculated	Reported
Volume	1093.3(2)	1093.3(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C23 H20 N3 S, Br, H2 O	C23 H20 N3 S, Br, H2 O
Sum formula	C23 H22 Br N3 O S	C23 H22 Br N3 O S
Mr	468.40	468.40
Dx,g cm-3	1.423	1.423
Z	2	2
Mu (mm-1)	1.994	1.994
F000	480.0	480.0
F000'	479.82	
h,k,lmax	11,13,17	11,13,17
Nref	5042	4926
Tmin,Tmax	0.555,0.772	0.592,0.772
Tmin'	0.437	

Correction method= # Reported T Limits: Tmin=0.592 Tmax=0.772
AbsCorr = MULTI-SCAN

Data completeness= 0.977 Theta(max)= 27.539

R(reflections)= 0.0264(4380) wR2(reflections)= 0.0595(4926)

S = 0.999 Npar= 272

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
PLAT431_ALERT_2_B Short Inter HL..A Contact Br1 ..S1 . 3.29 Ang.
1+x,y,z = 1_655 Check

Alert level C
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 63 Report

Alert level G
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.004 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 52 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 14 Info

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

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

checkCIF publication errors

Alert level A
PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G
PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
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Publication of your CIF

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Validation response form

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```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
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_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
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PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
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PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
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PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 18/09/2020; check.def file version of 20/08/2020

Datablock 1 - ellipsoid plot

