

**Supporting information**  
**for**

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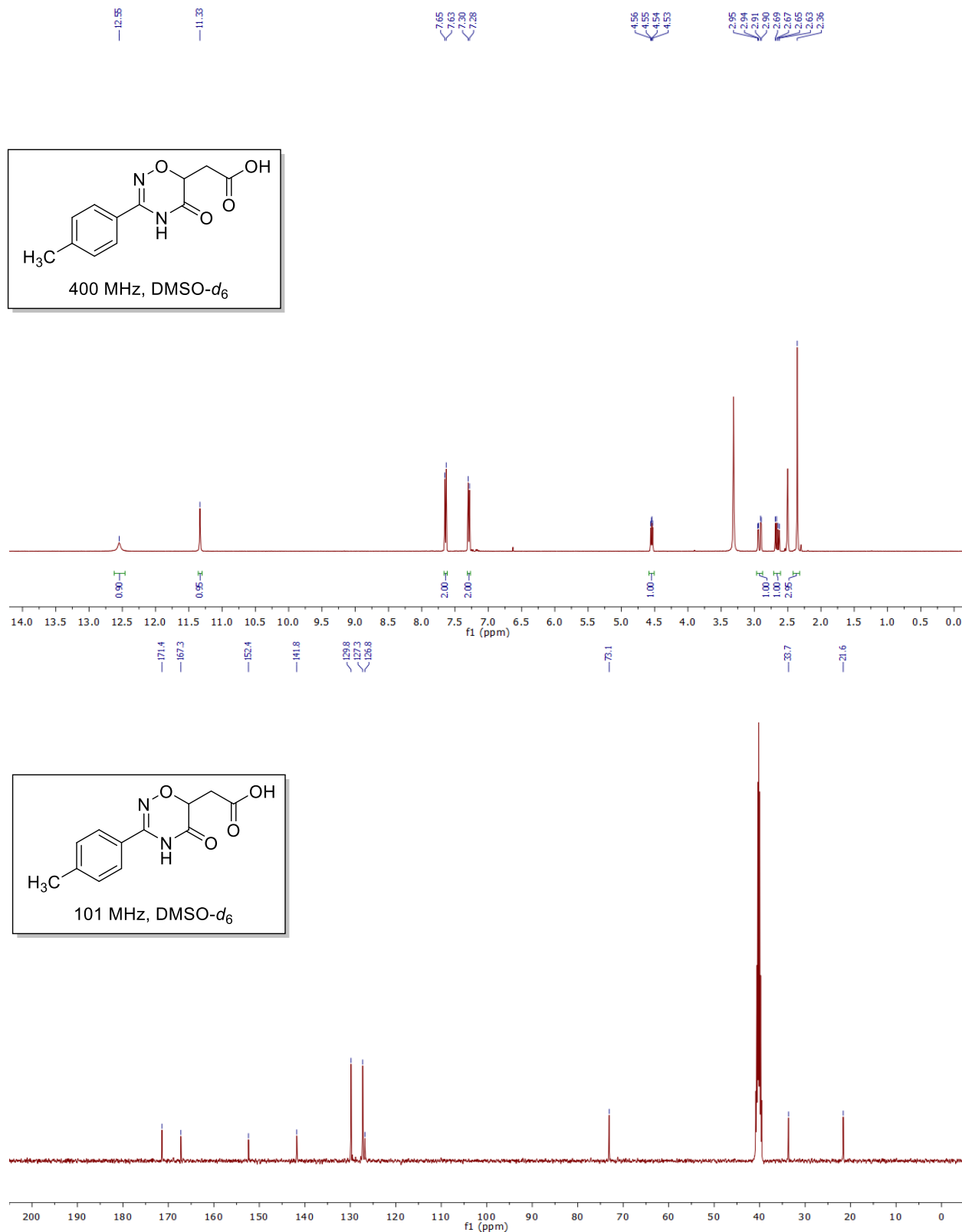
\*Corresponding authors: e-mail: v.boyarskii@spbu.ru.

## Content

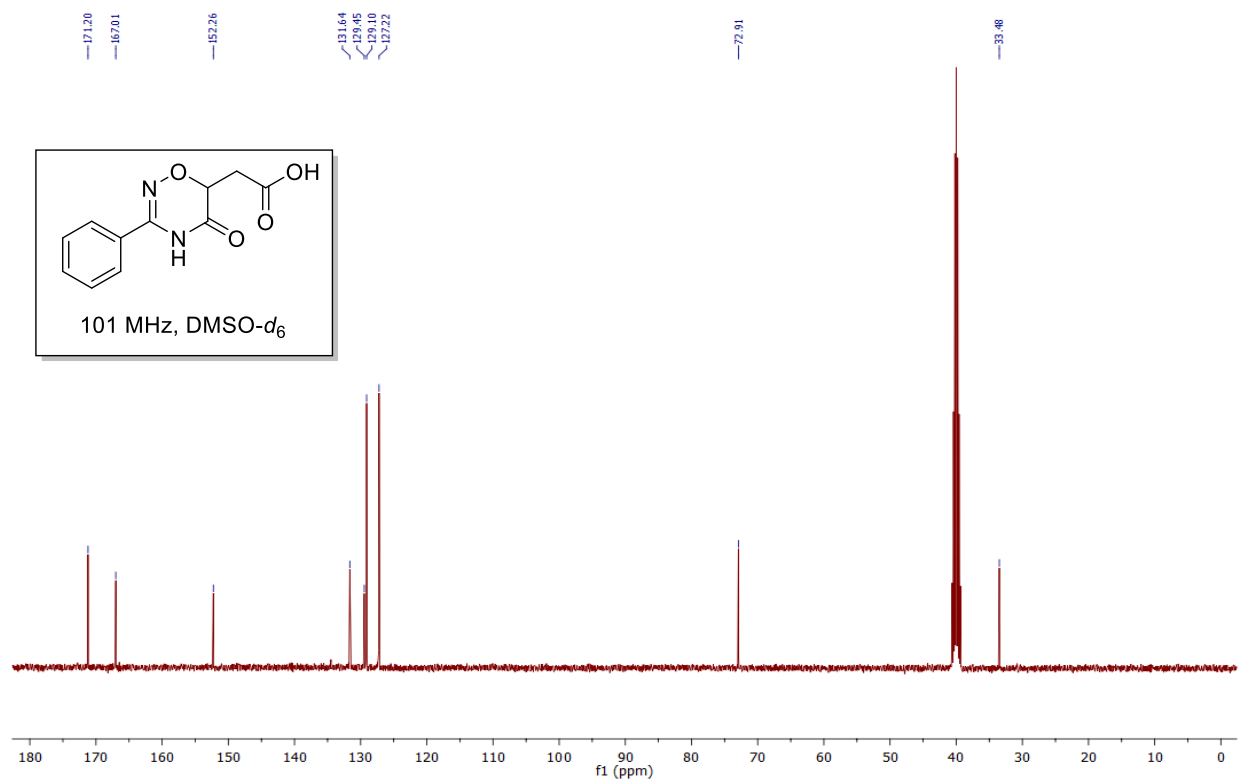
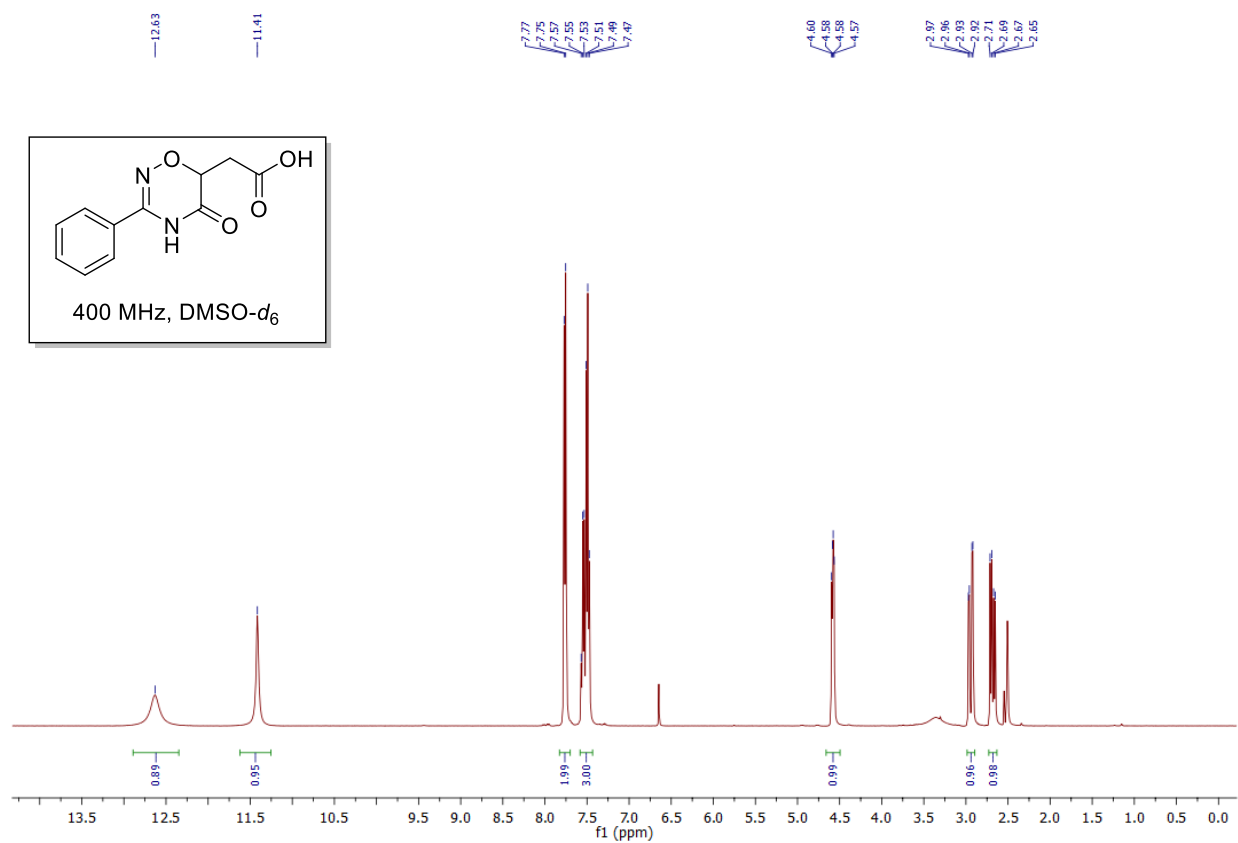
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# 1. Copies of $^1\text{H}$ , $^{13}\text{C}$ , and $^{19}\text{F}$ NMR spectra for compounds 3, 4, and 5

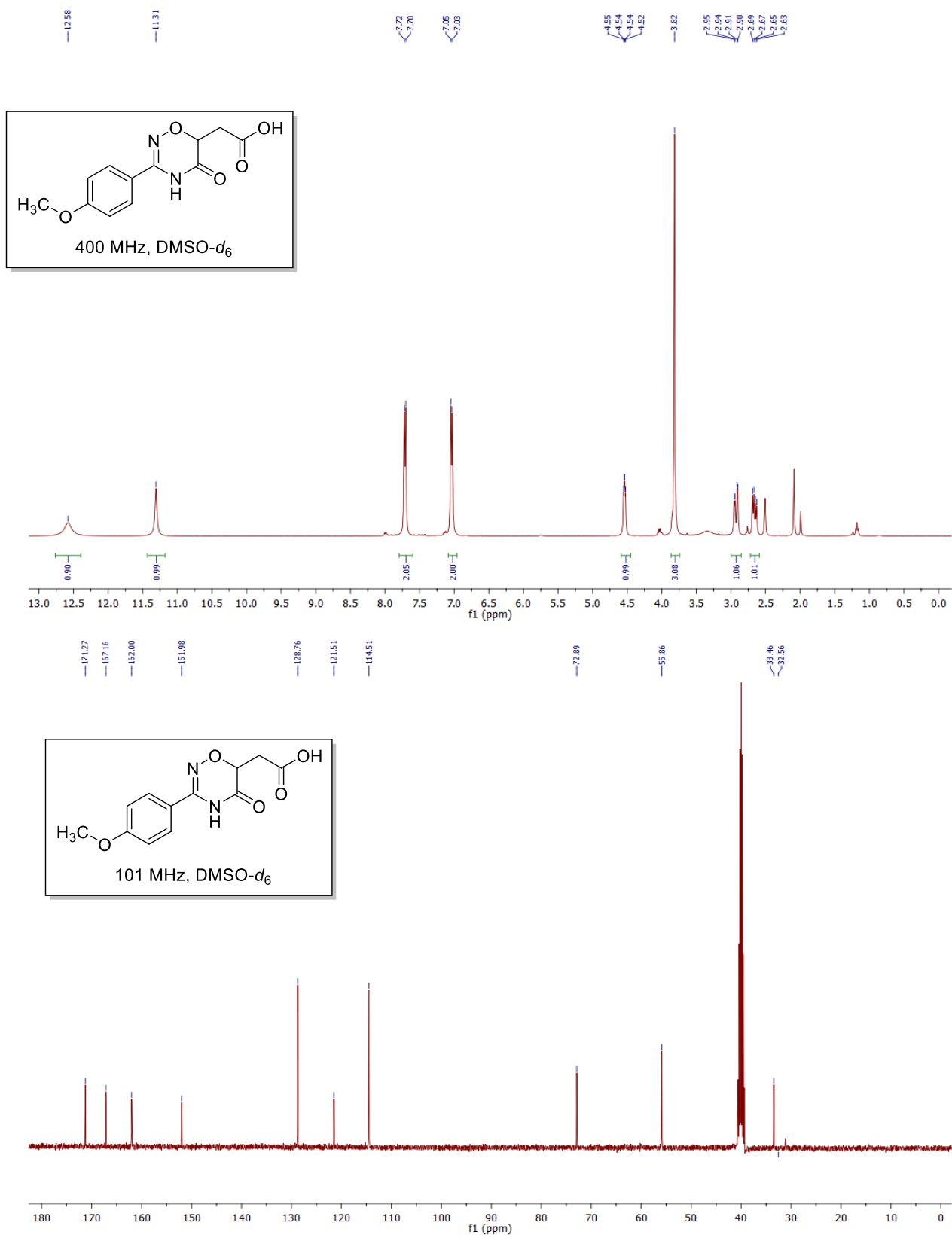
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(5-oxo-3-(4-methylphenyl)-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3a**



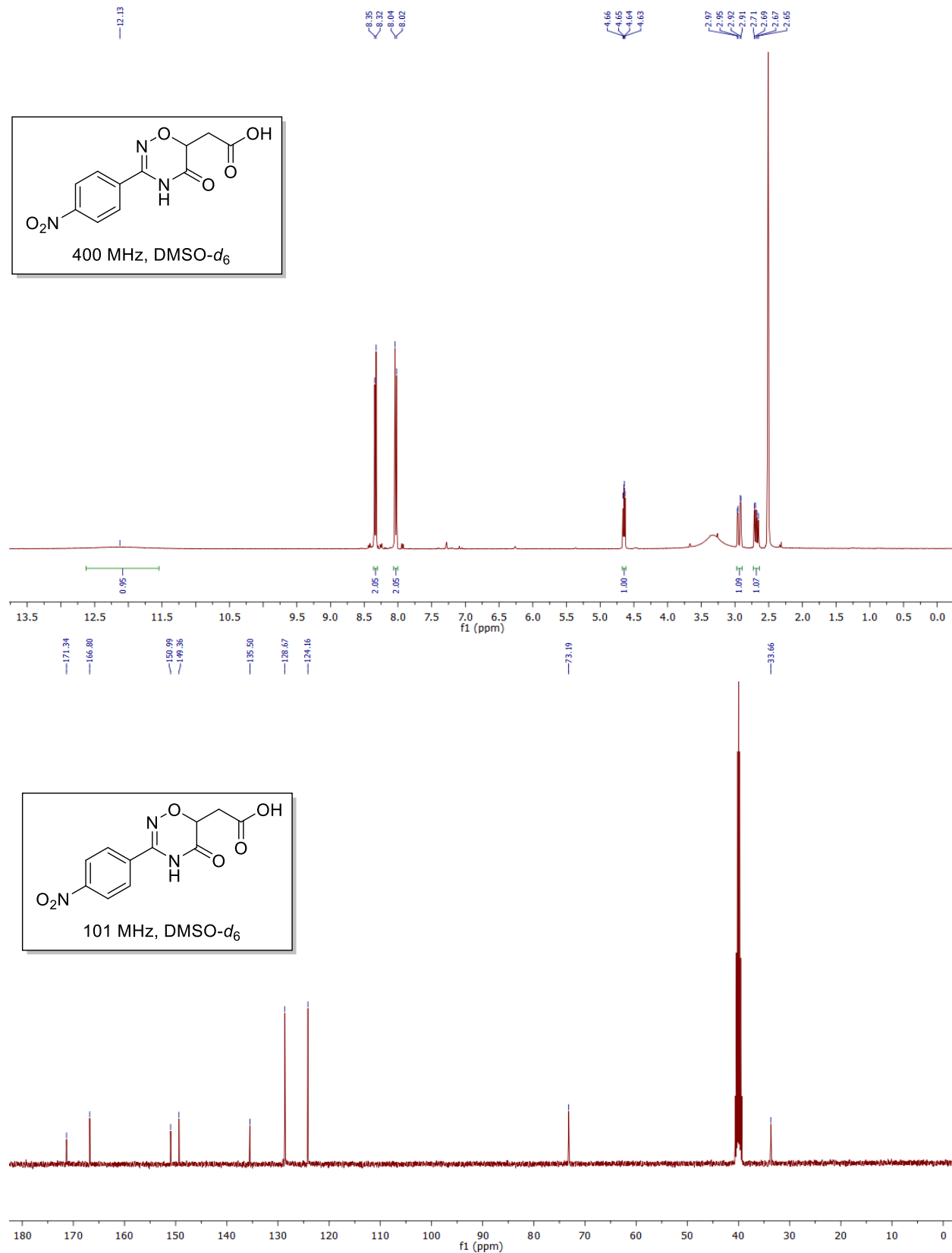
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(5-oxo-3-phenyl-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3b**



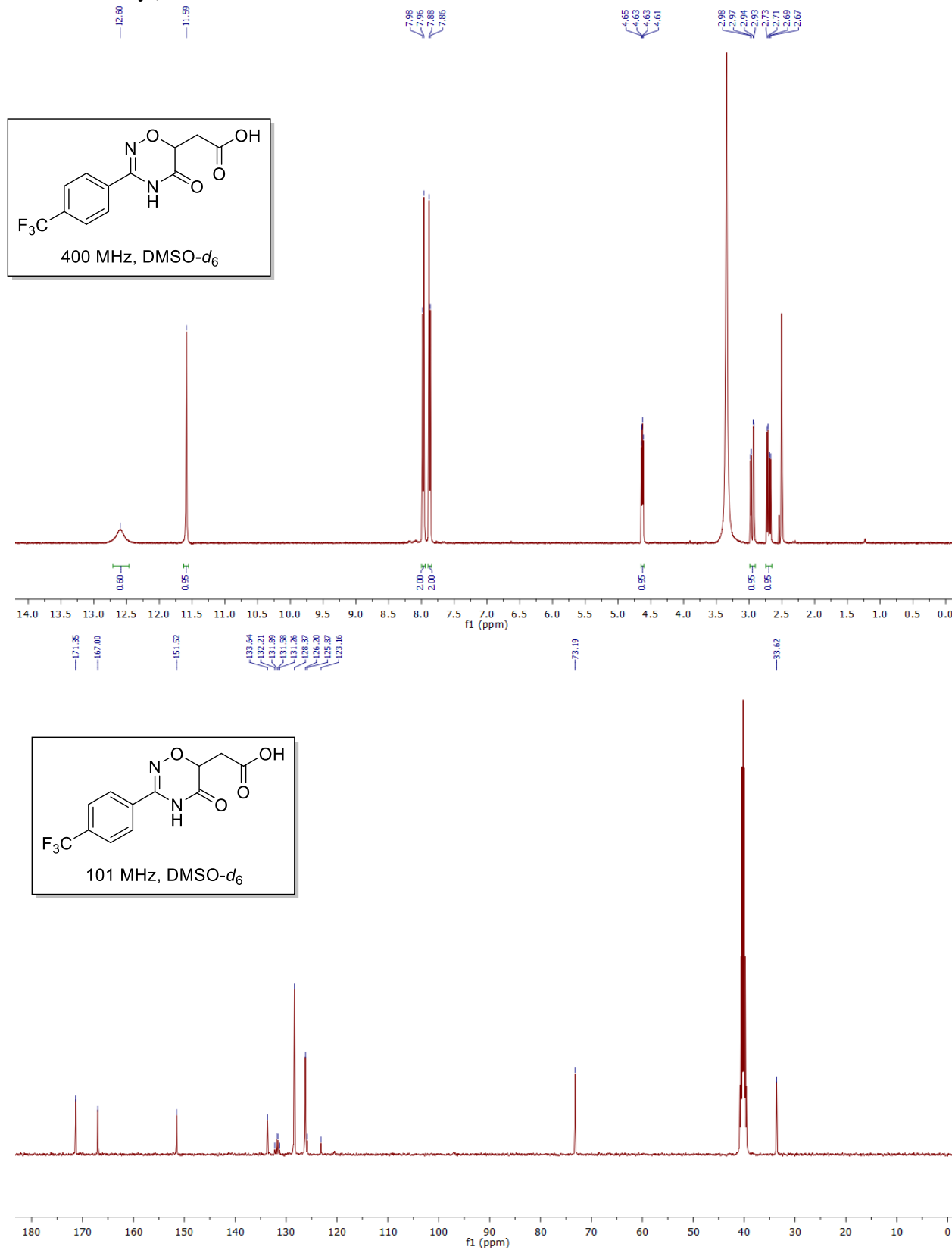
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(3-(4-methoxyphenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3c**

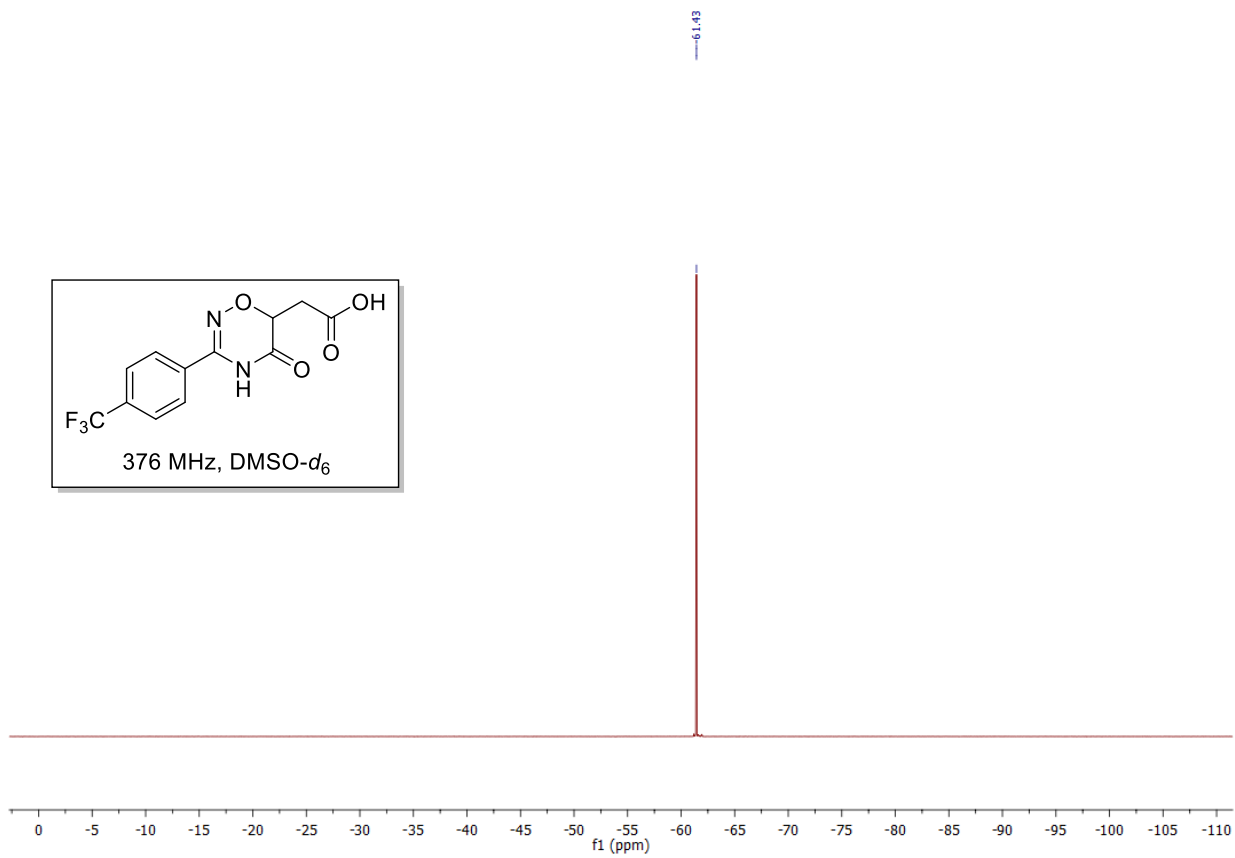


$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(3-(4-nitrophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3d**



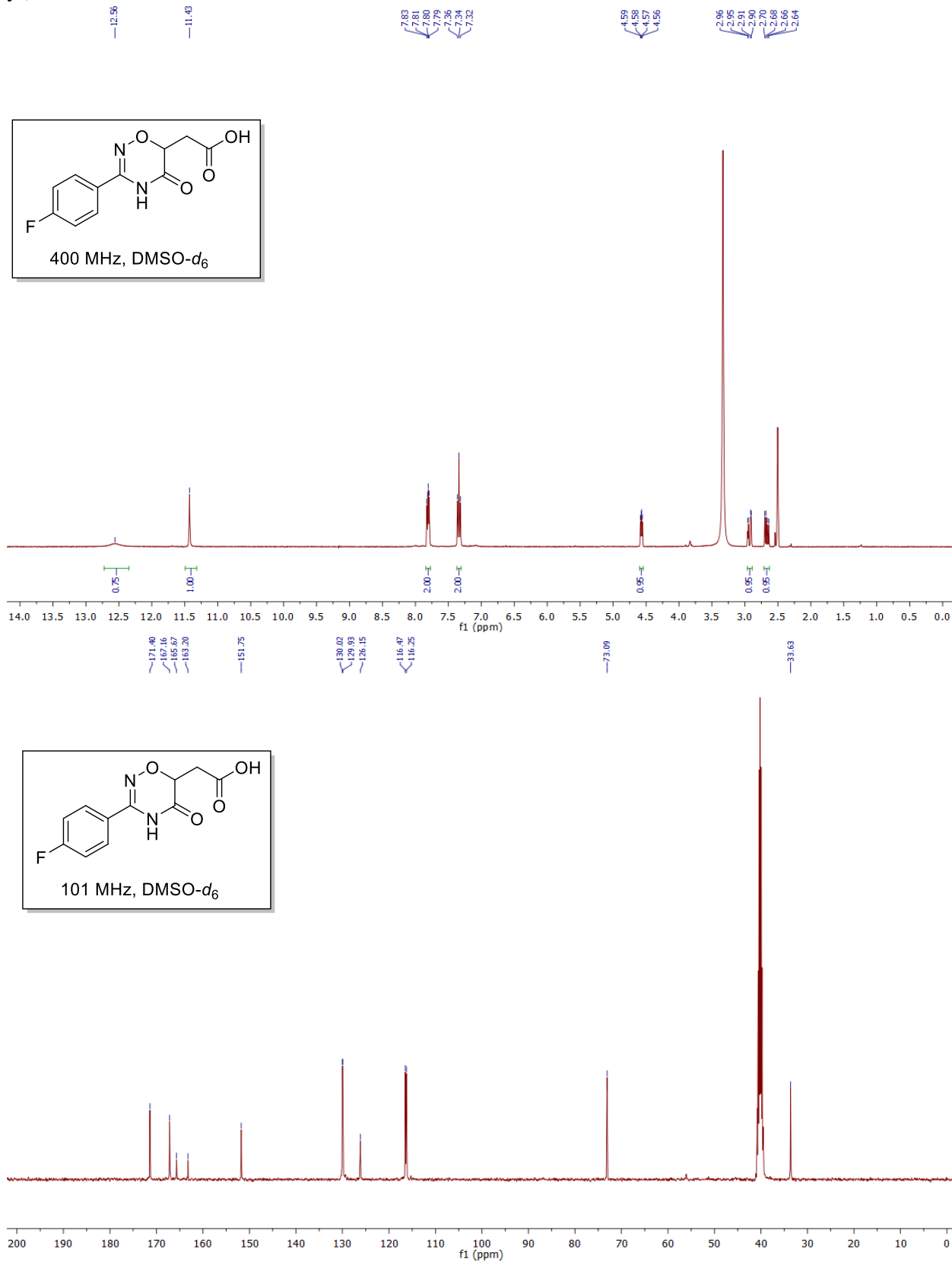
$^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  spectra of 2-(5-oxo-3-(4-(trifluoromethyl)phenyl)-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3e**

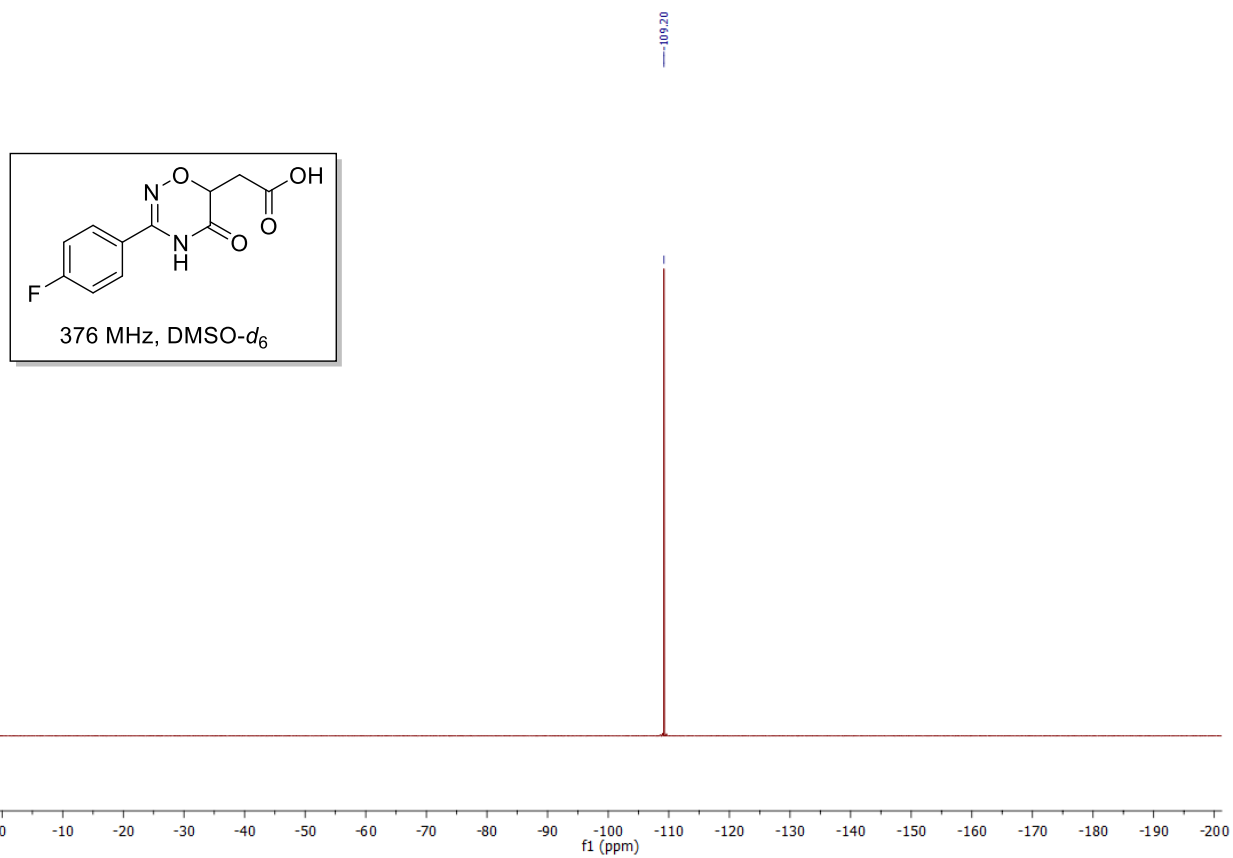




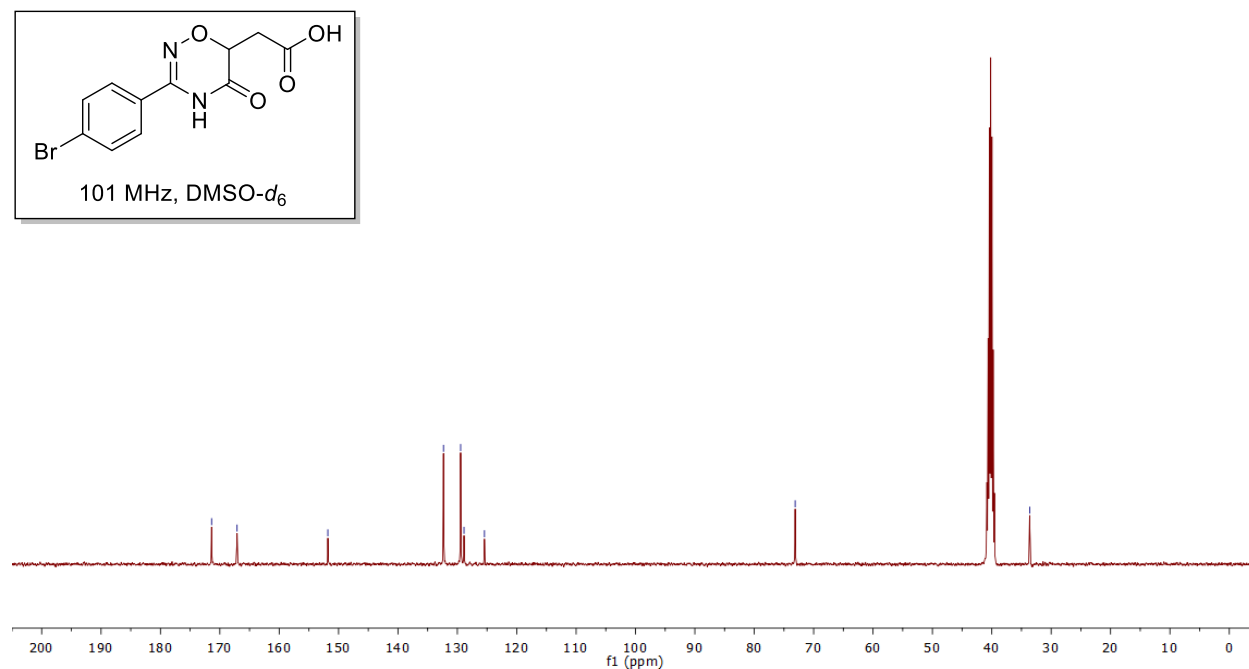
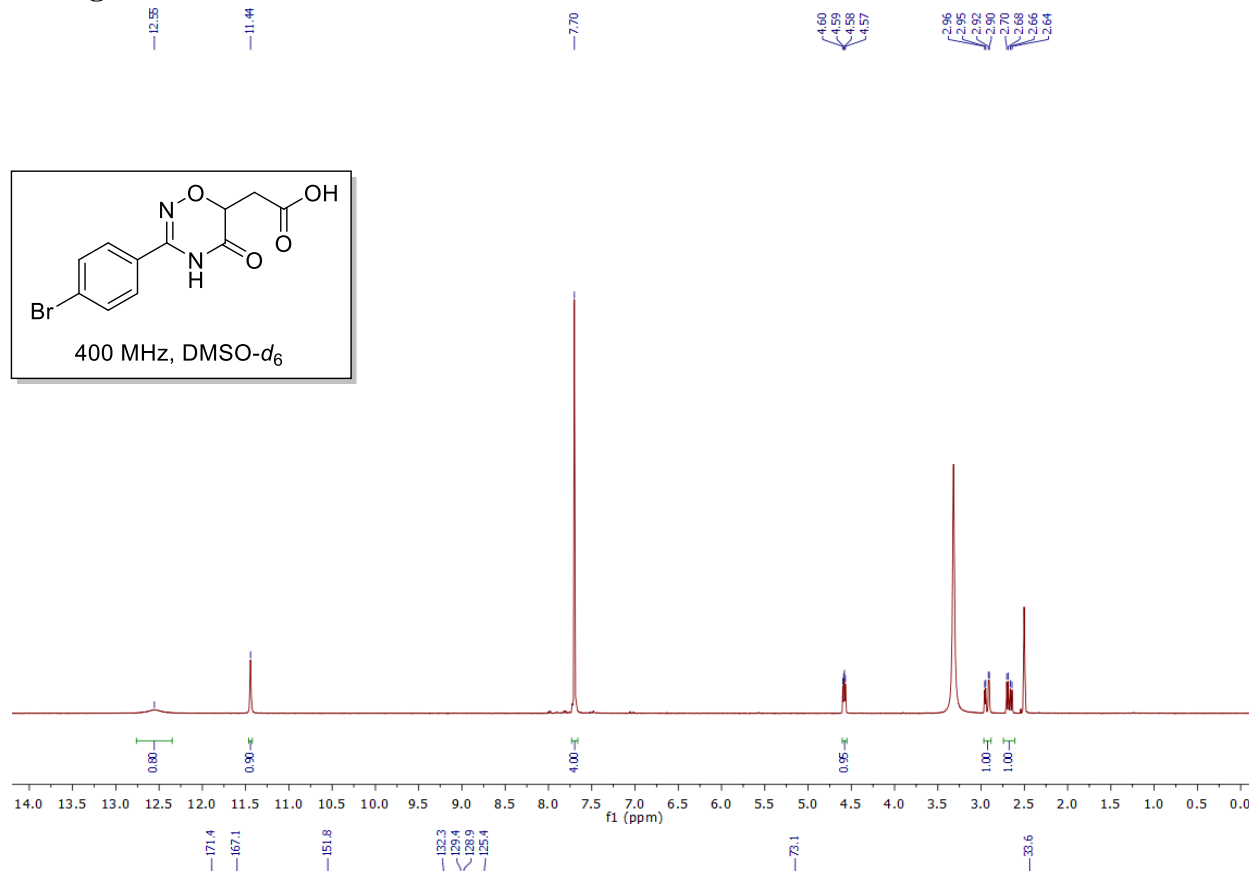


$^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  spectra of 2-(3-(4-fluorophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3f**

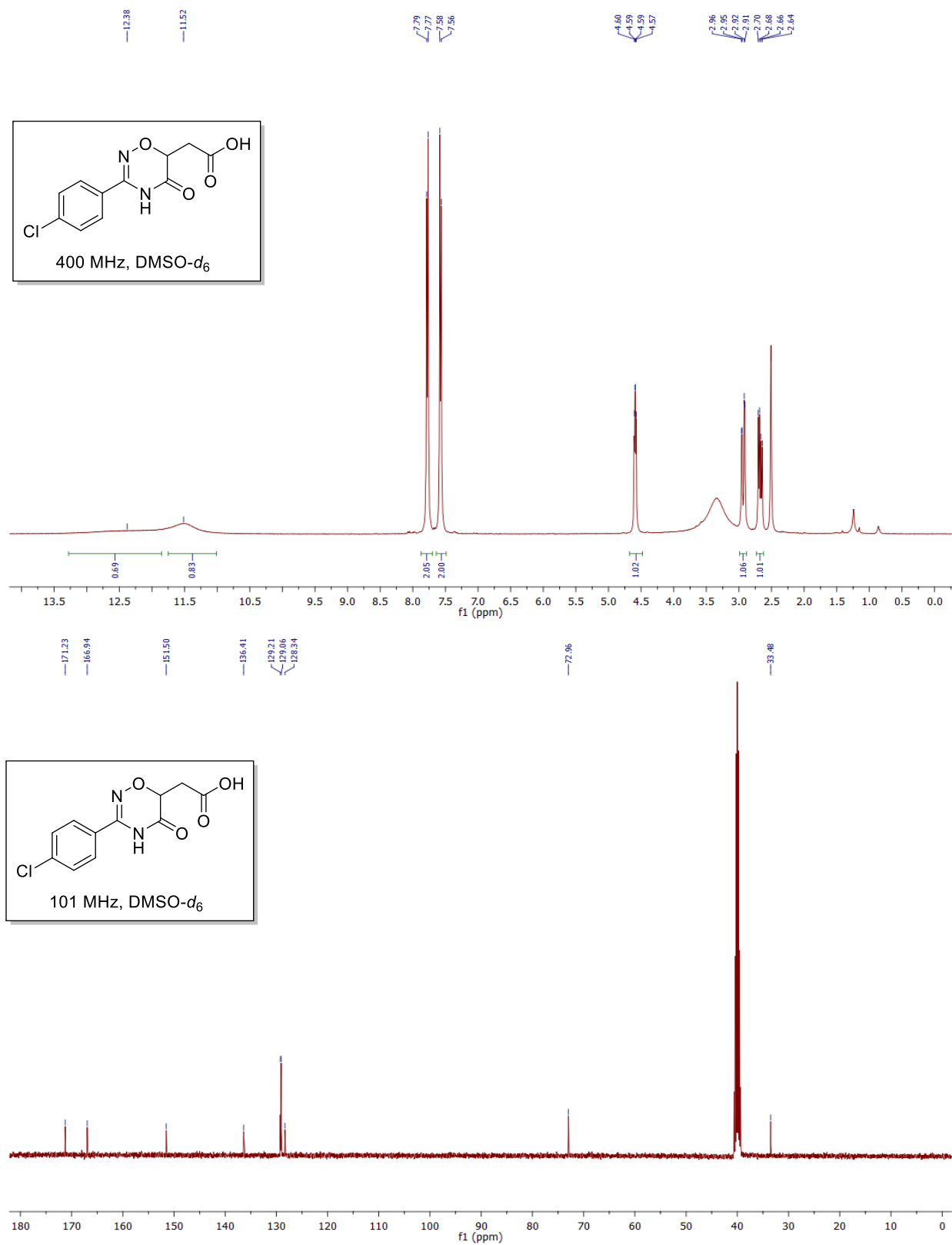




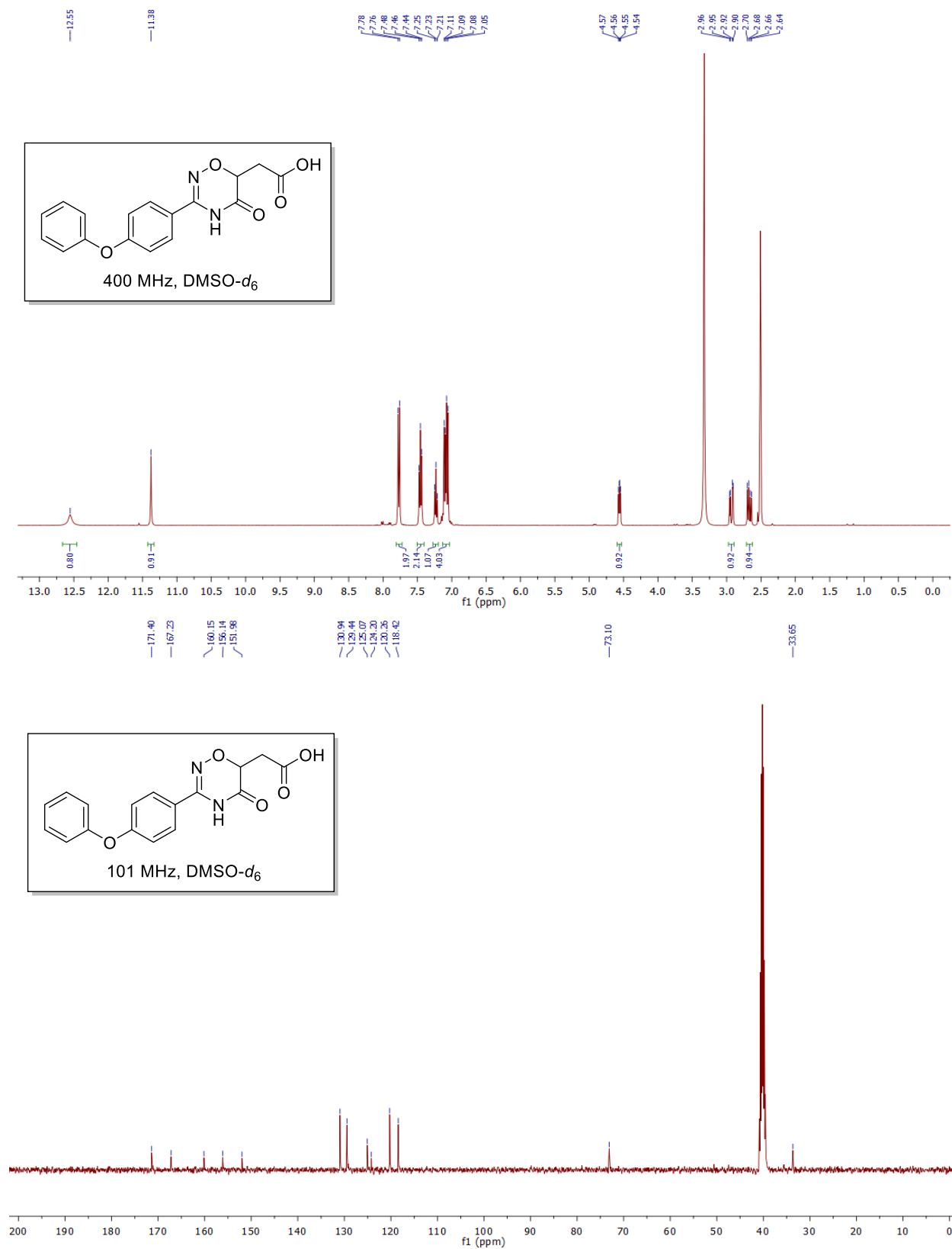
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(3-(4-bromophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3g**



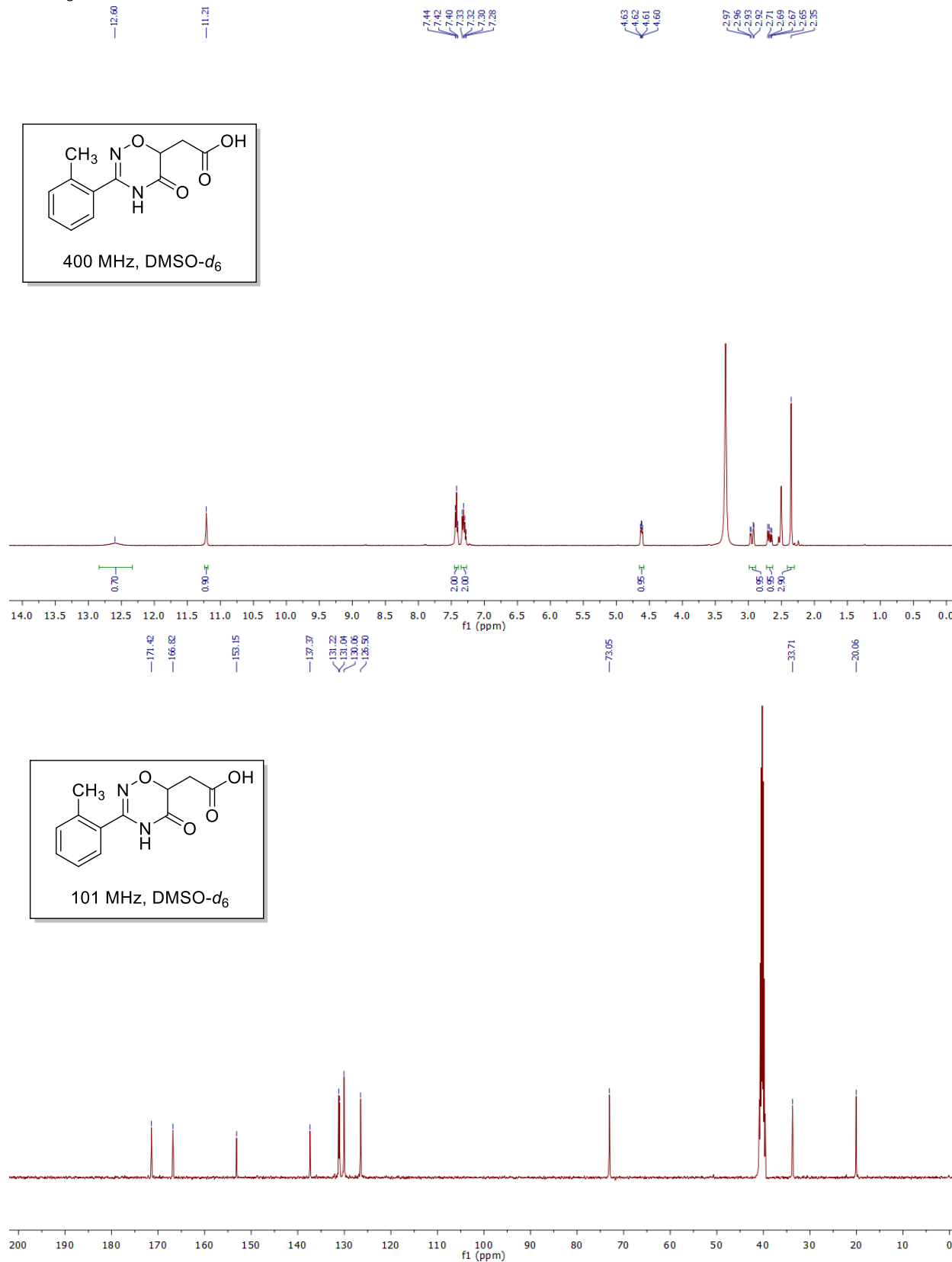
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(3-(4-chlorophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3h**



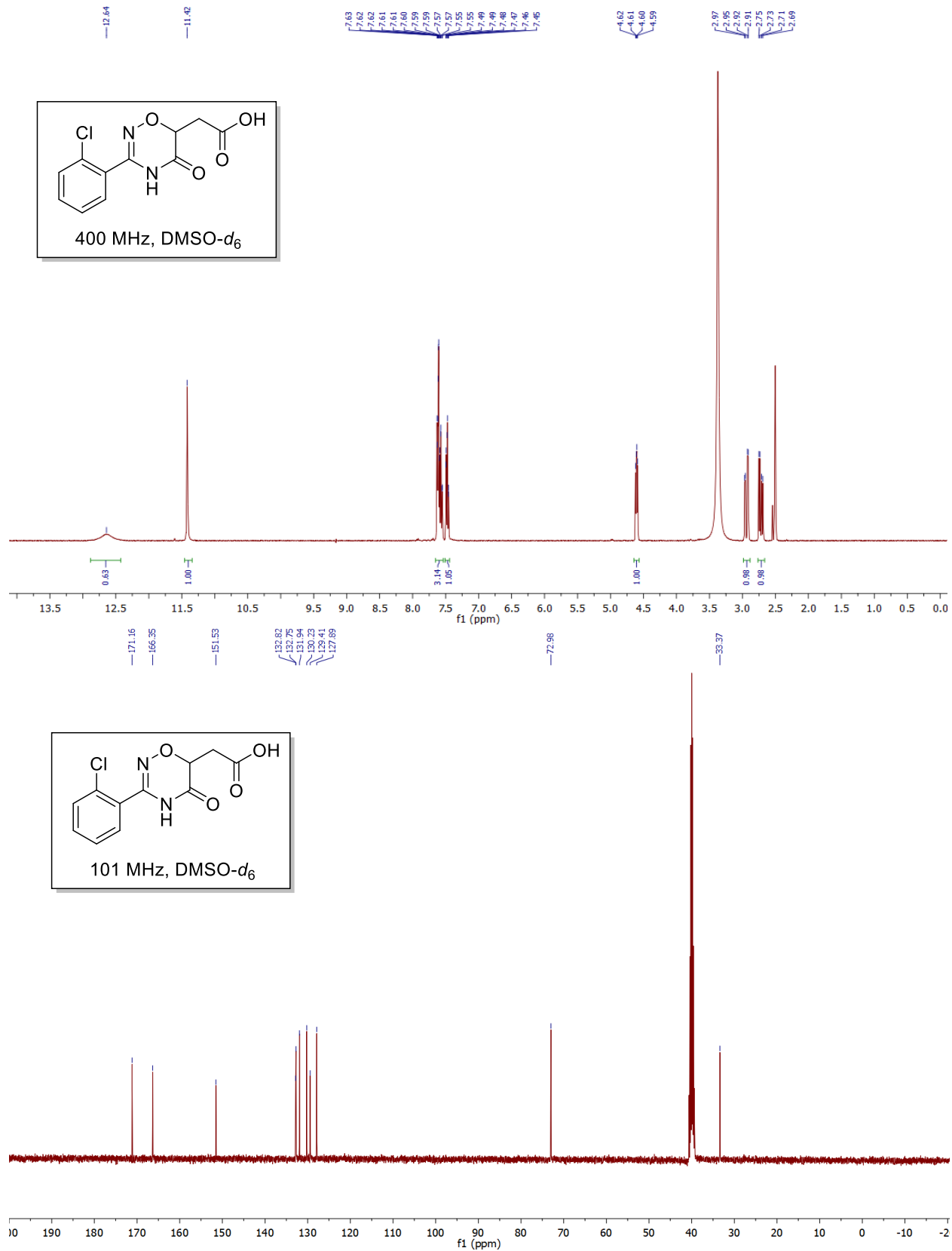
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(5-oxo-3-(4-phenoxyphenyl)-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3i**



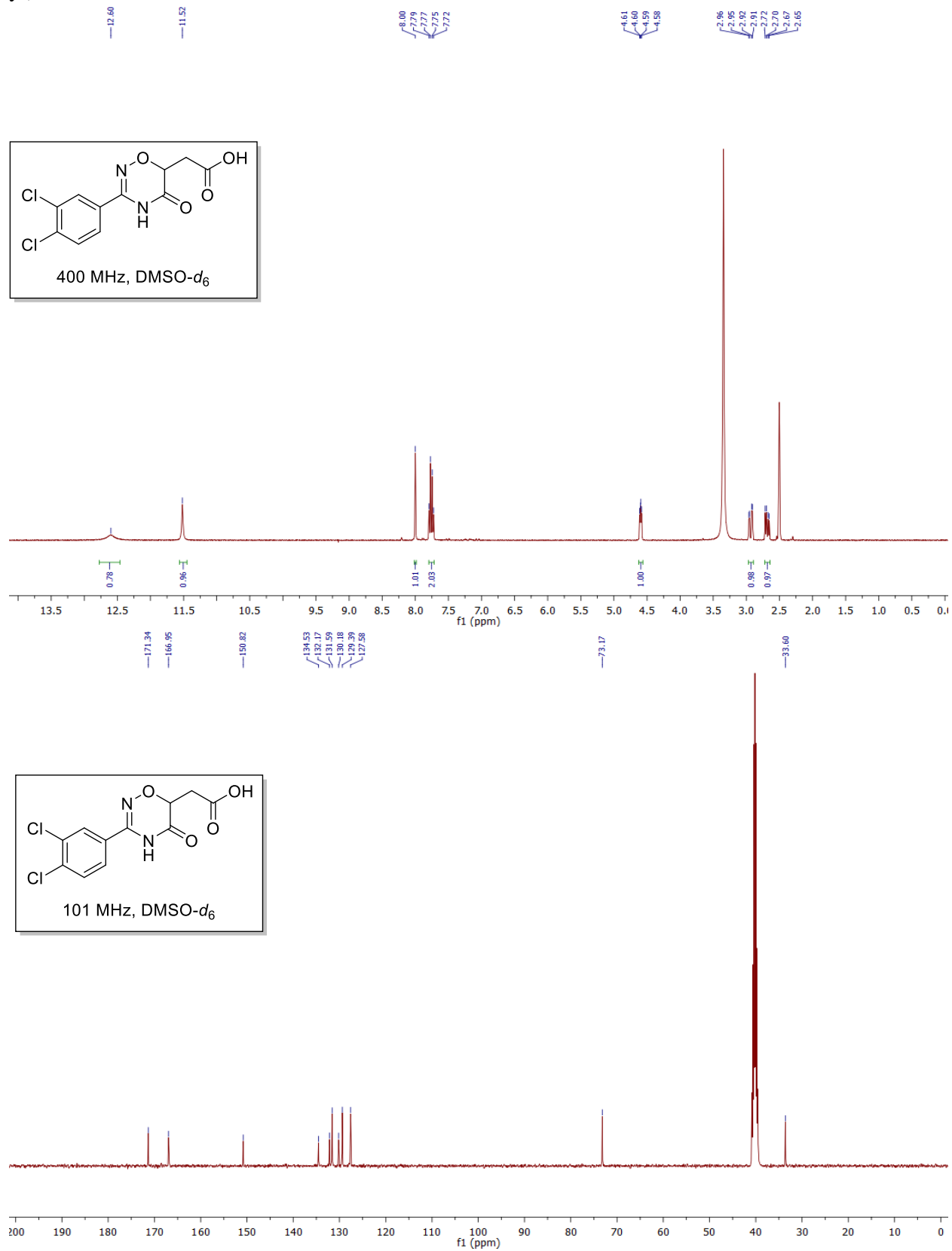
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(5-oxo-3-(2-methylphenyl)-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3j**



$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(3-(2-chlorophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **3k**

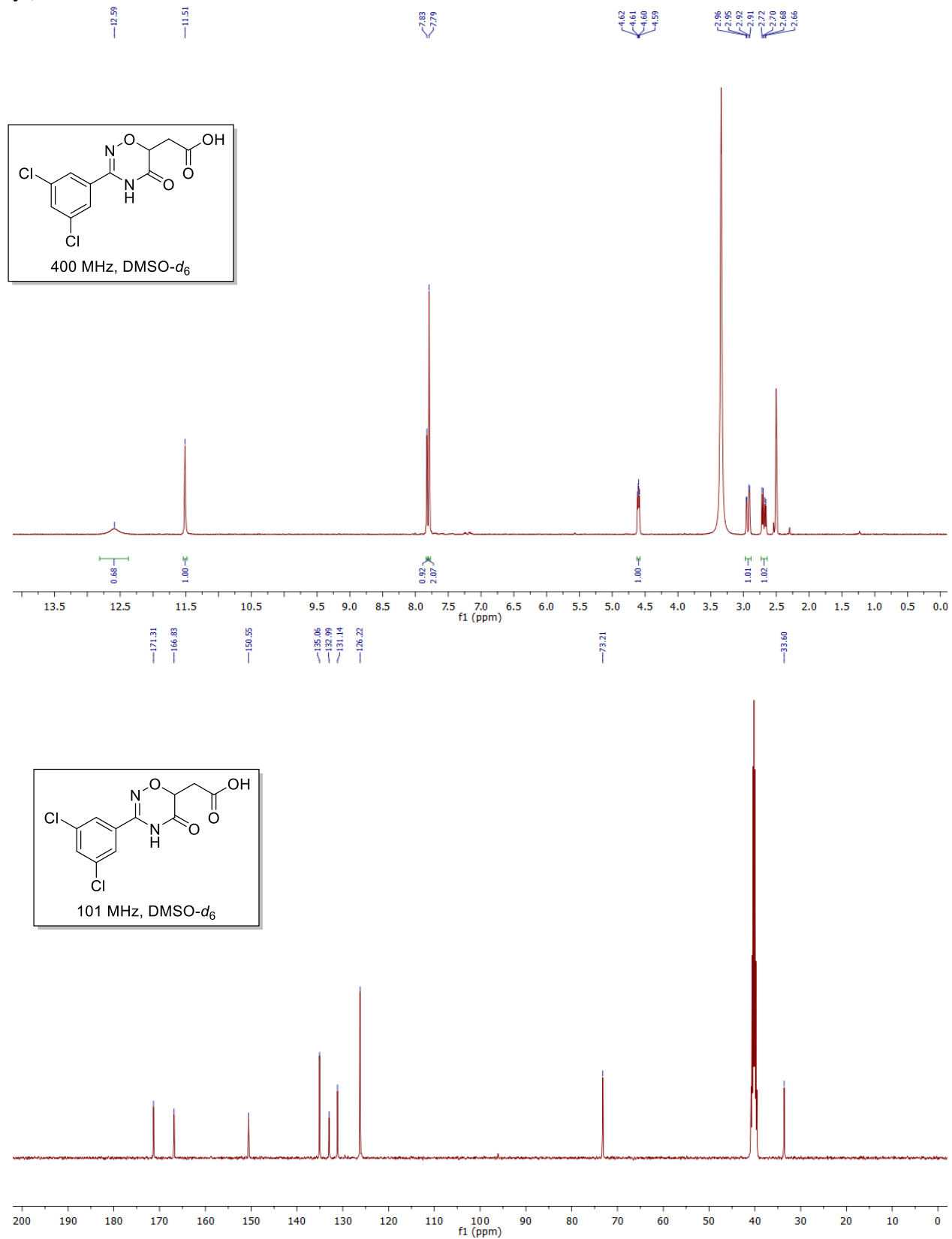


$^1\text{H}$  and  $^{13}\text{C}$  spectra of 2-(3-(3,4-Dichlorophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetic acid **31**

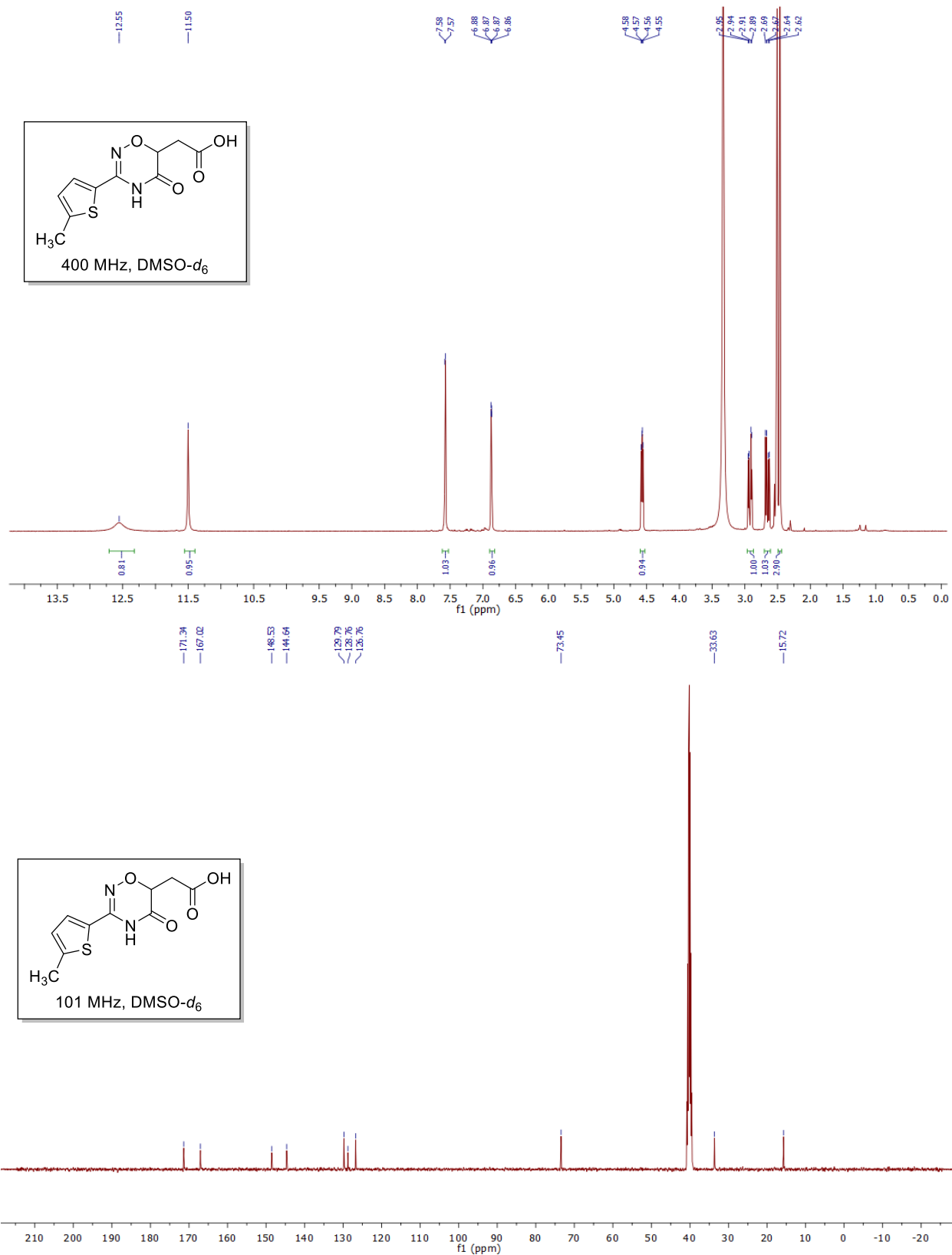




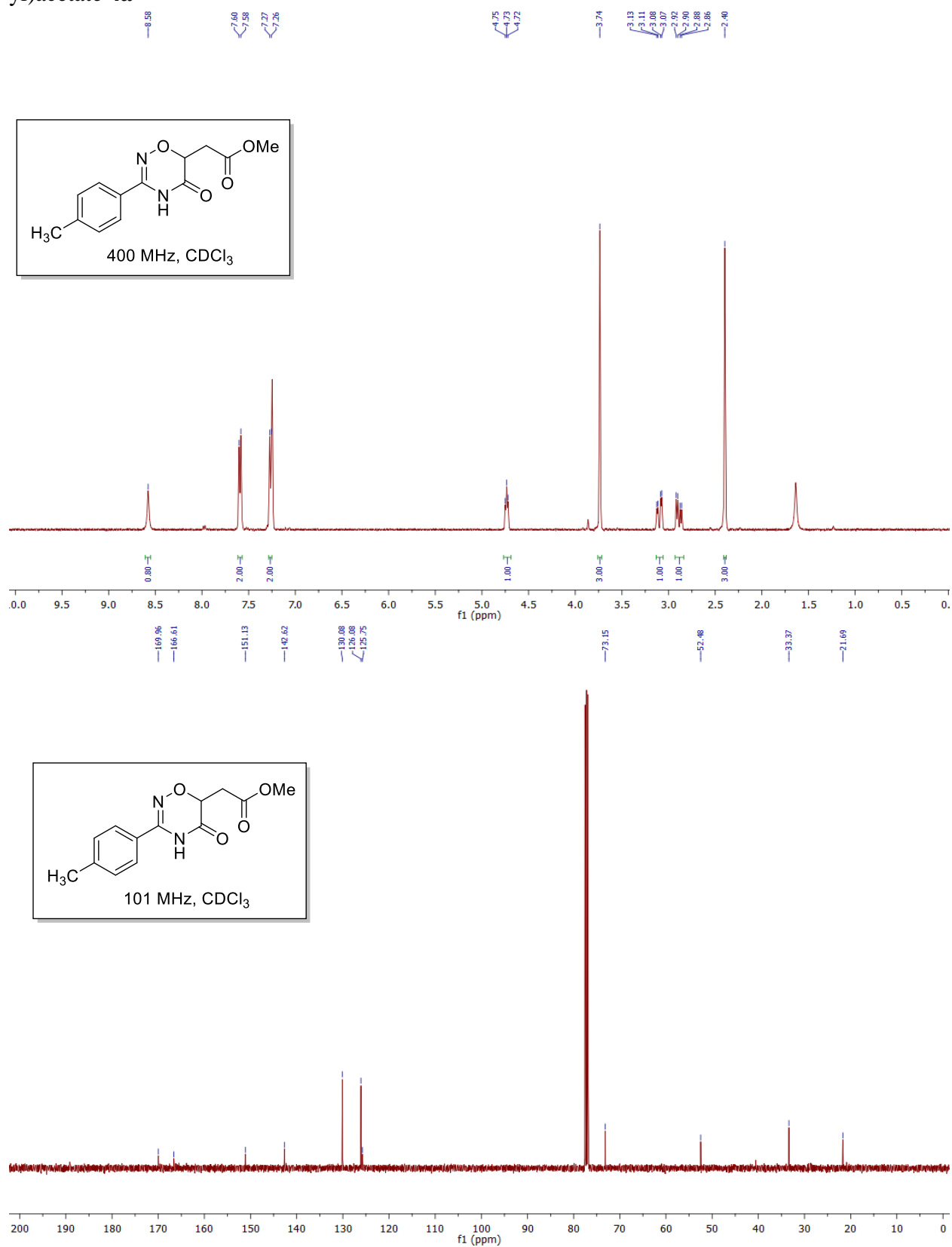
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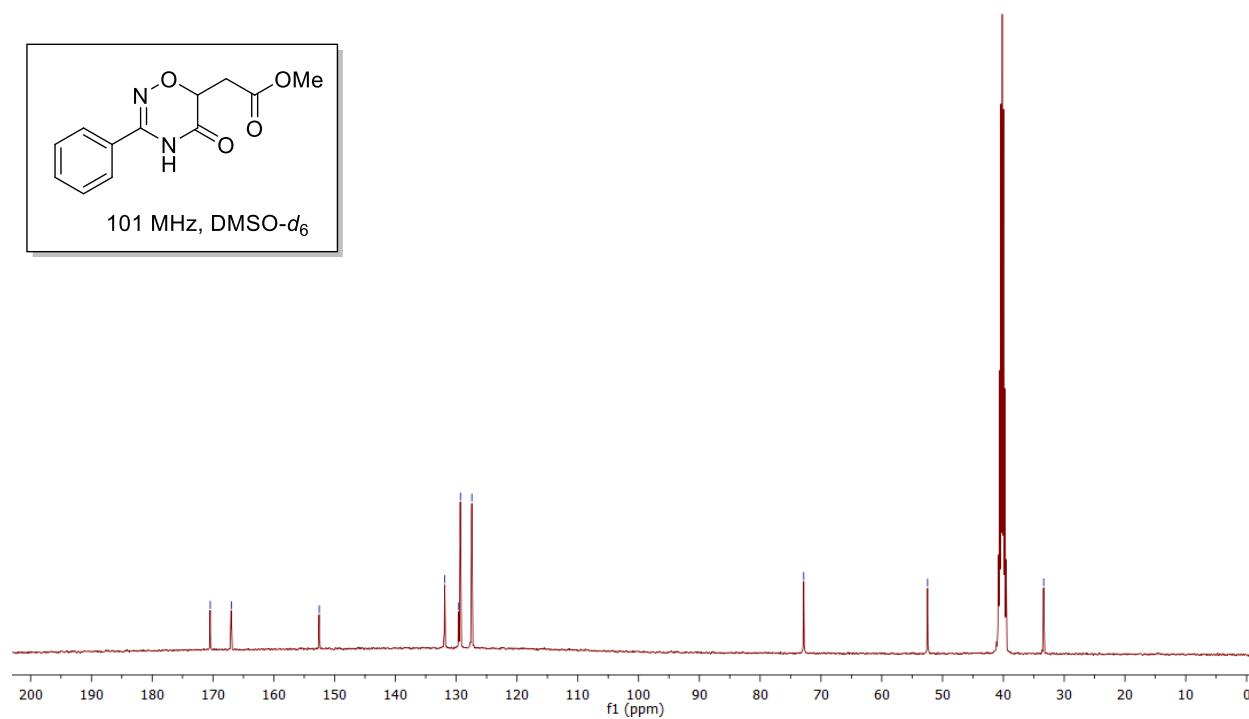
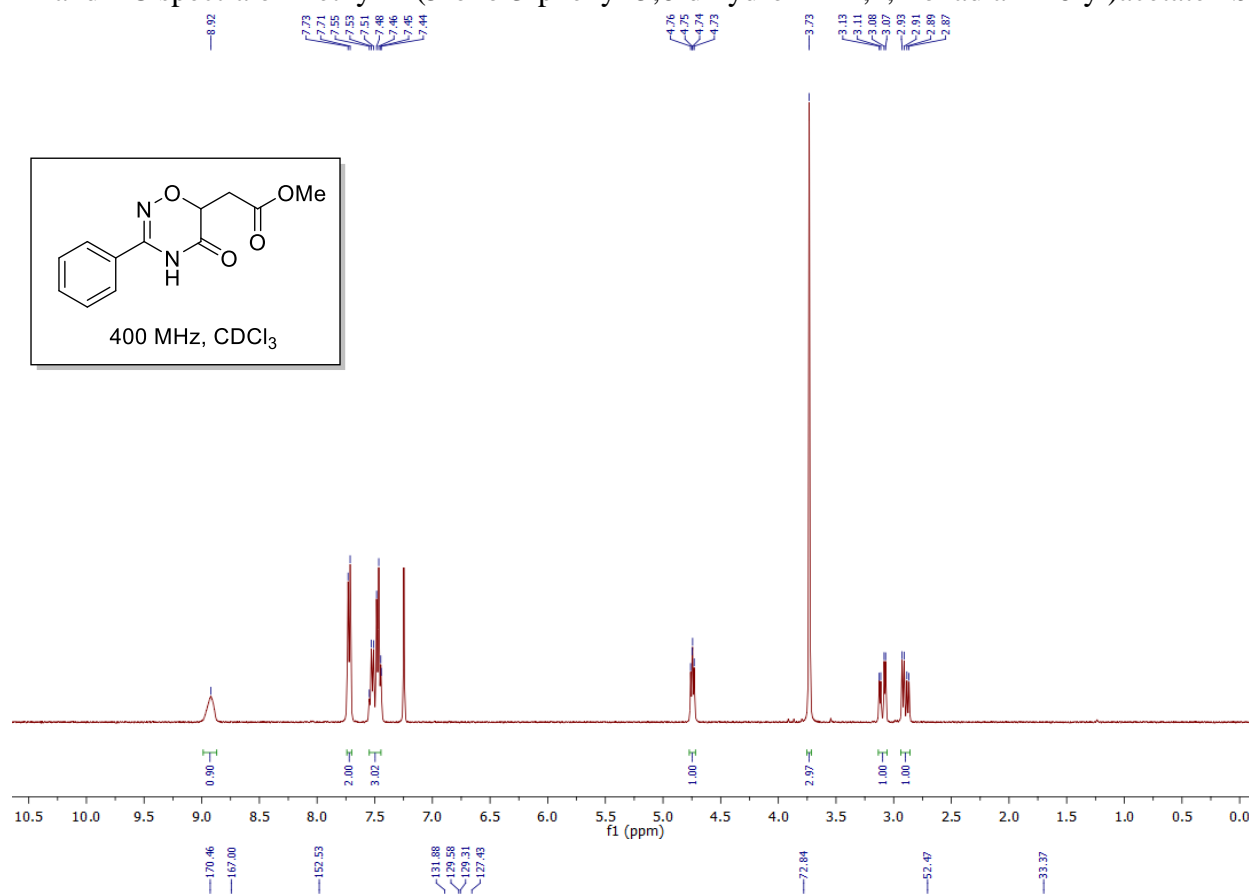
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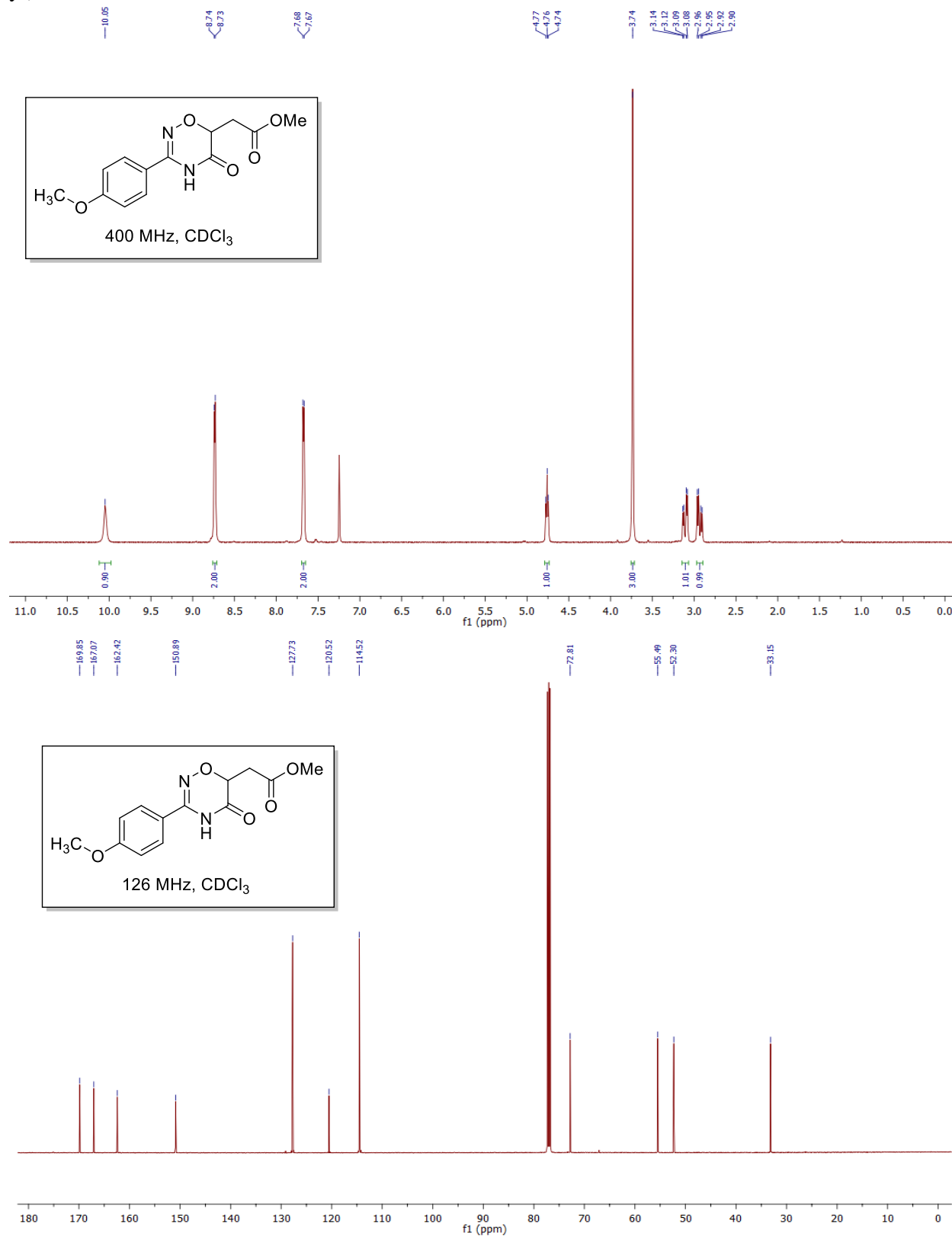
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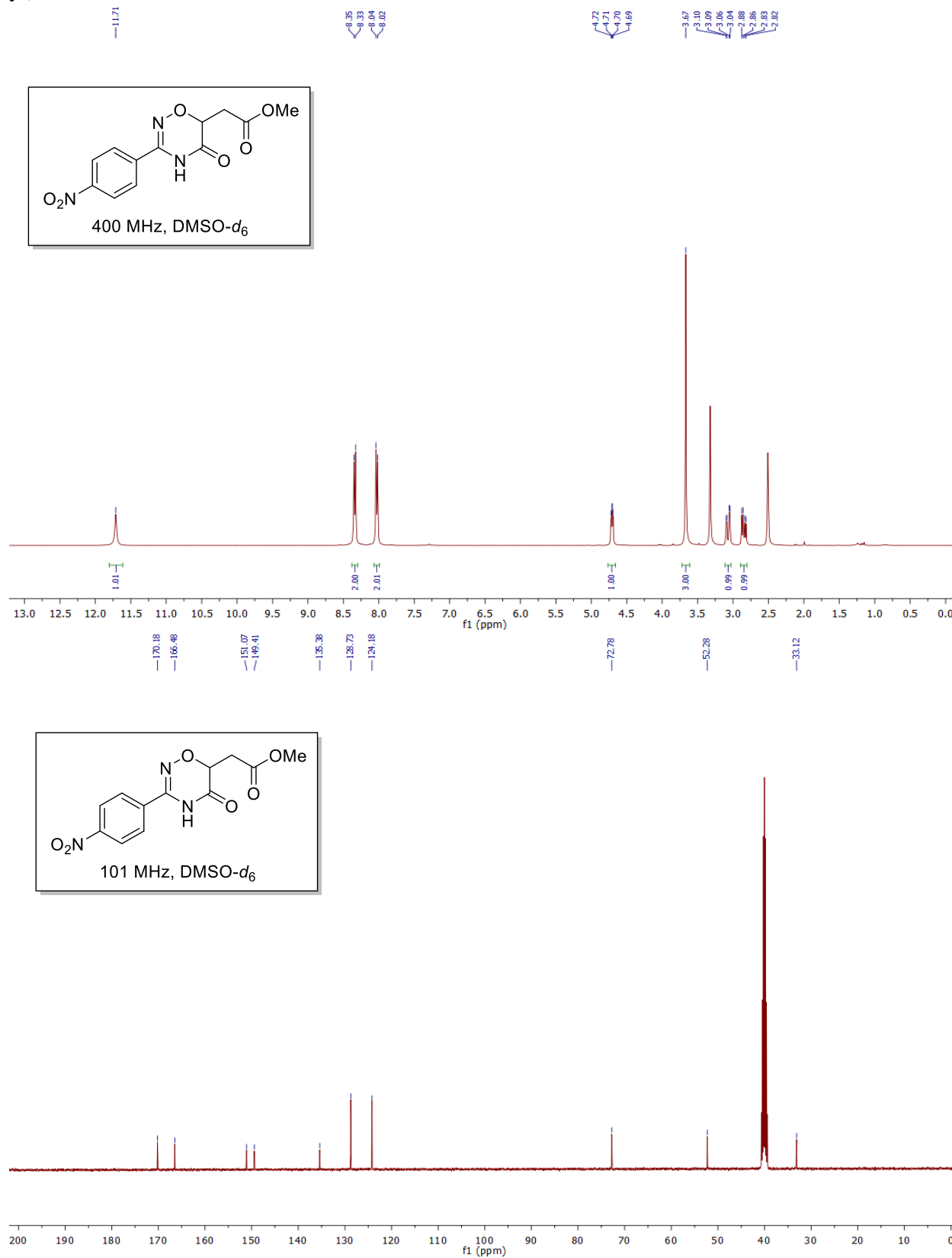
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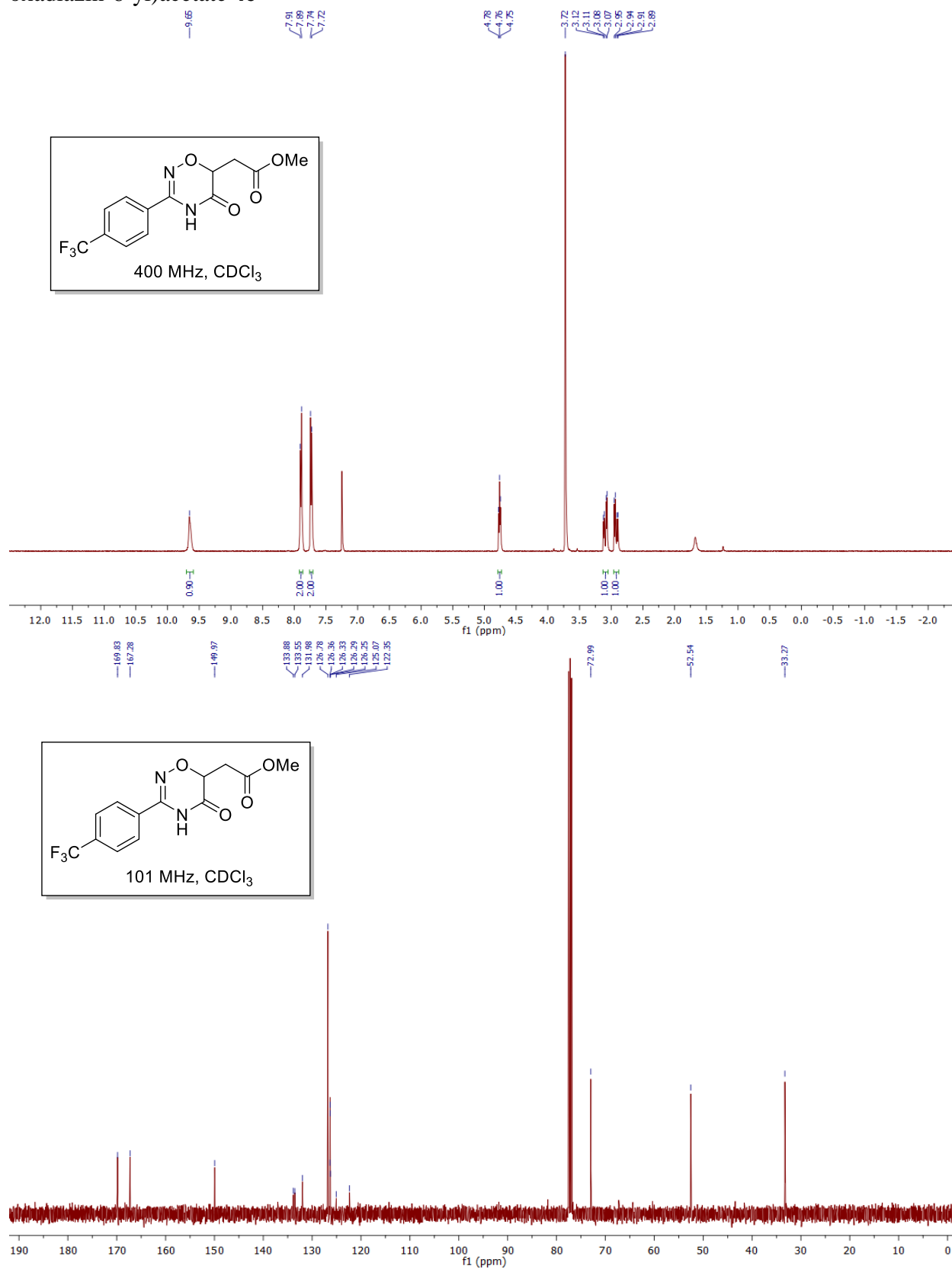
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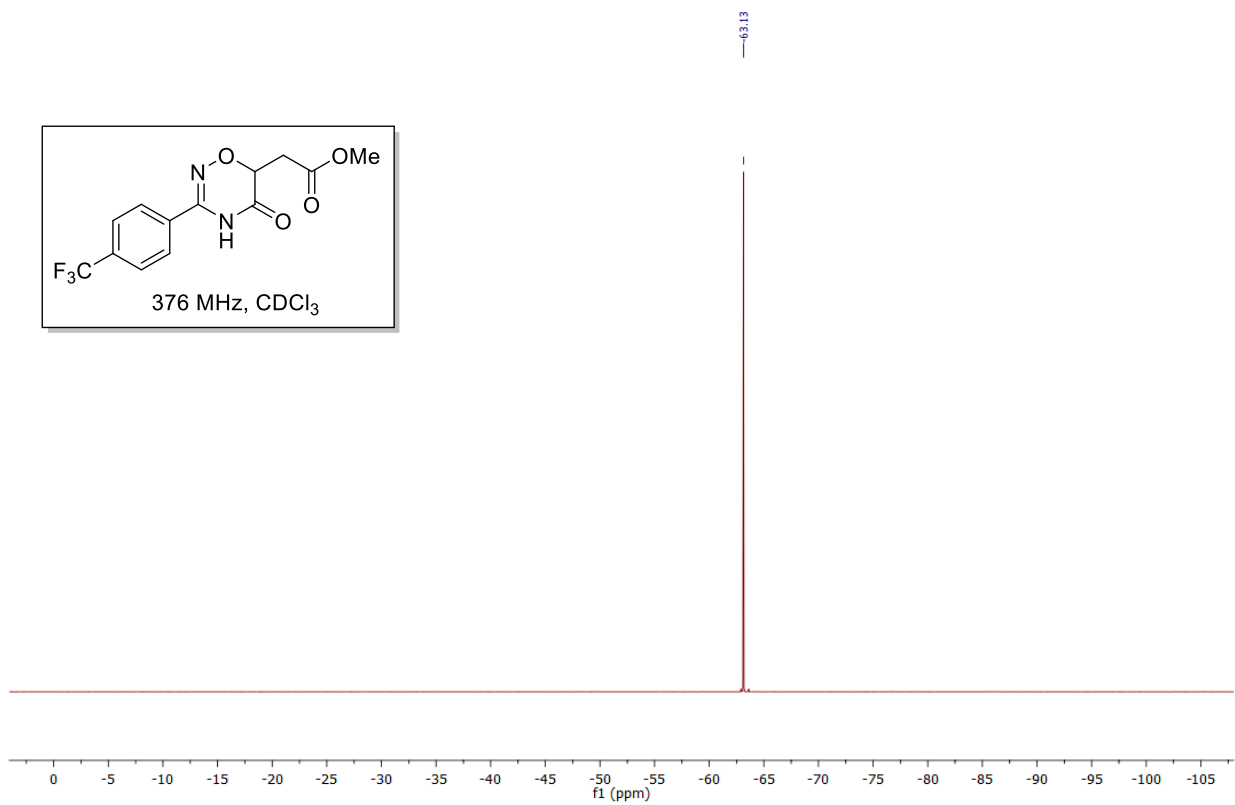


$^1\text{H}$  and  $^{13}\text{C}$  spectra of methyl 2-(3-(4-nitrophenyl)-5-oxo-5,6-dihydro-4H-1,2,4-oxadiazin-6-yl)acetate **4d**



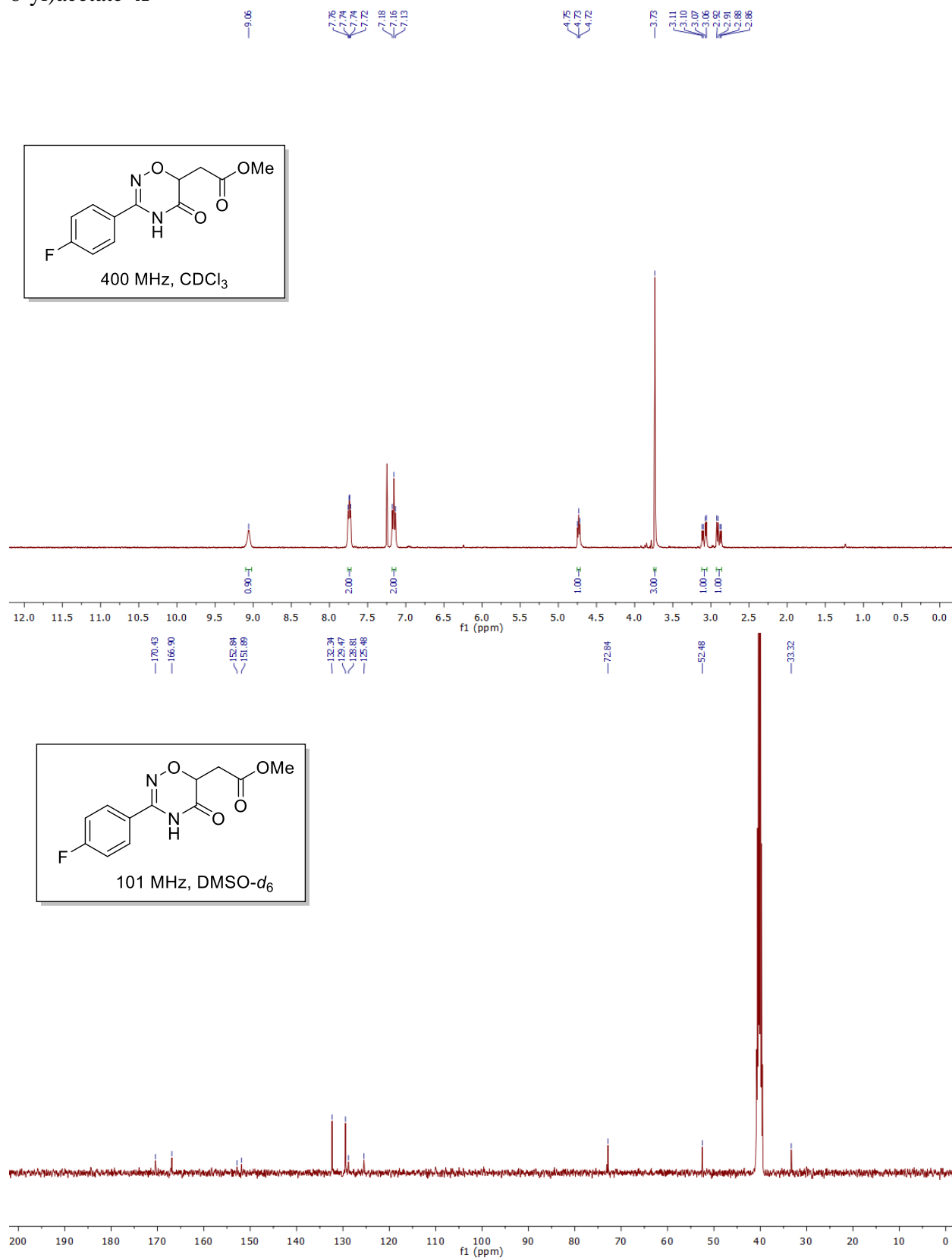
$^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  spectra of methyl 2-(5-oxo-3-(4-(trifluoromethyl)phenyl)-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetate **4e**

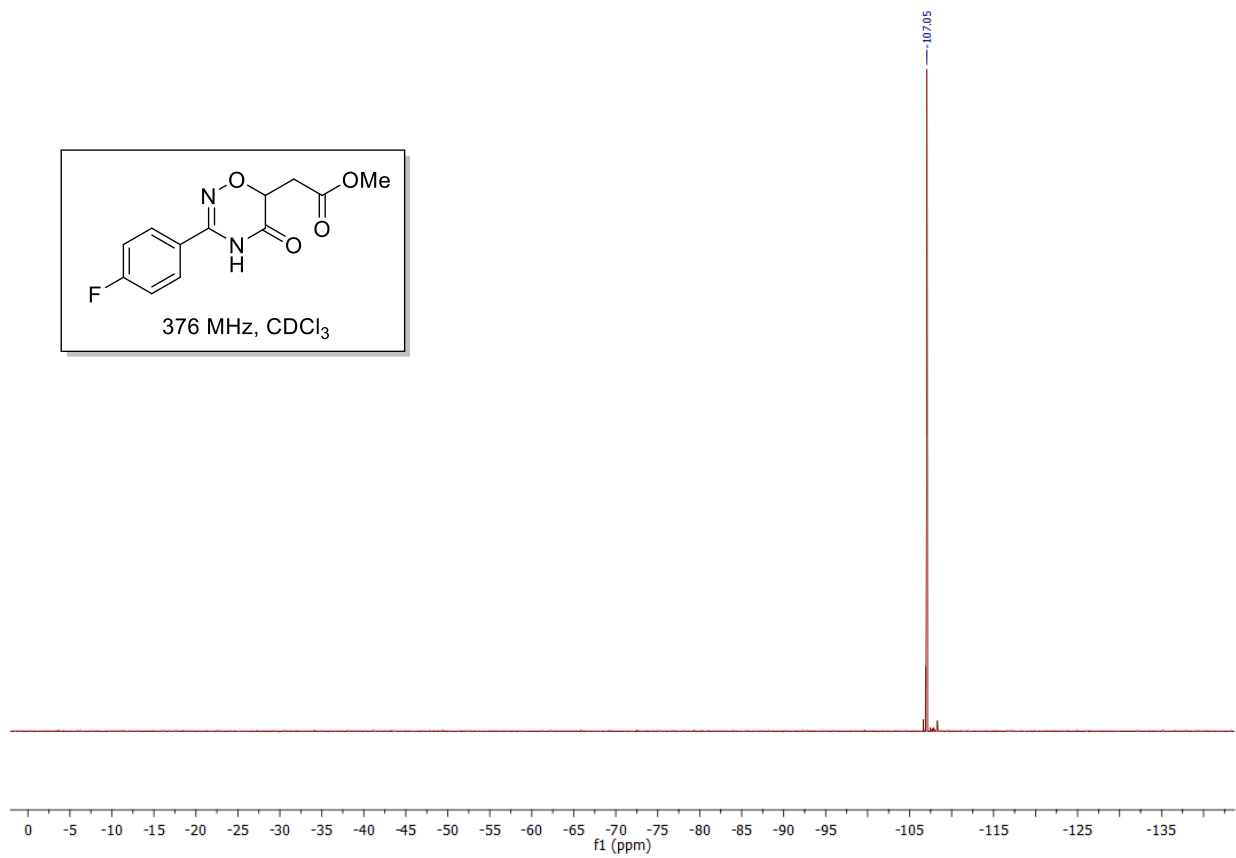
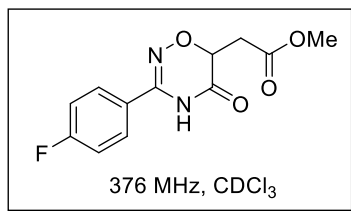




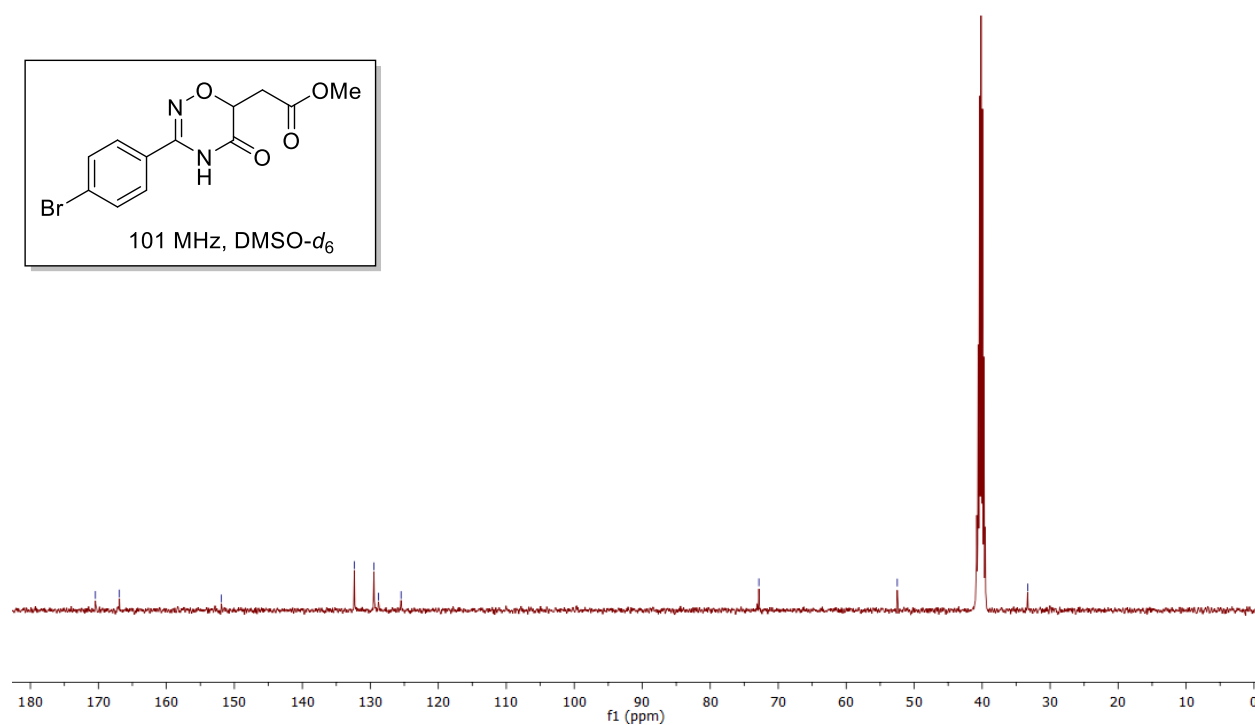
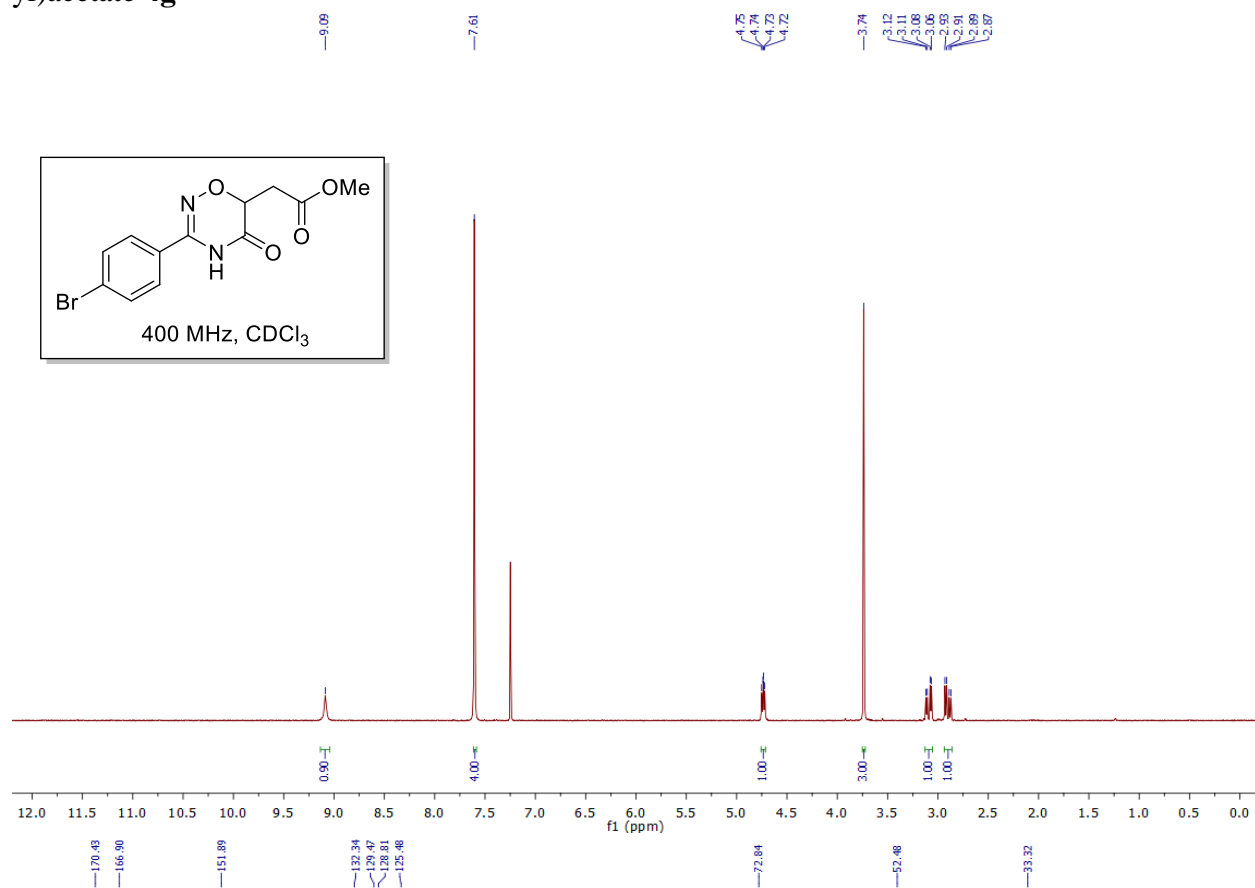


$^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  spectra of methyl 2-(3-(4-fluorophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetate **4f**

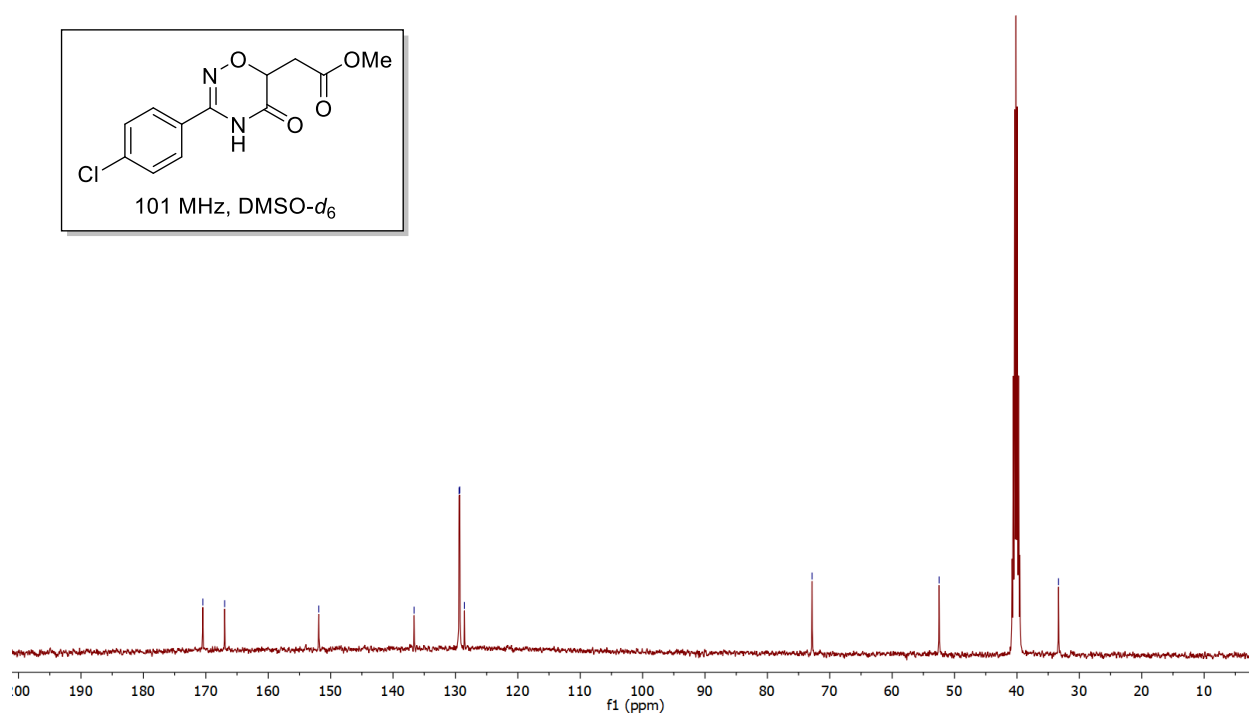
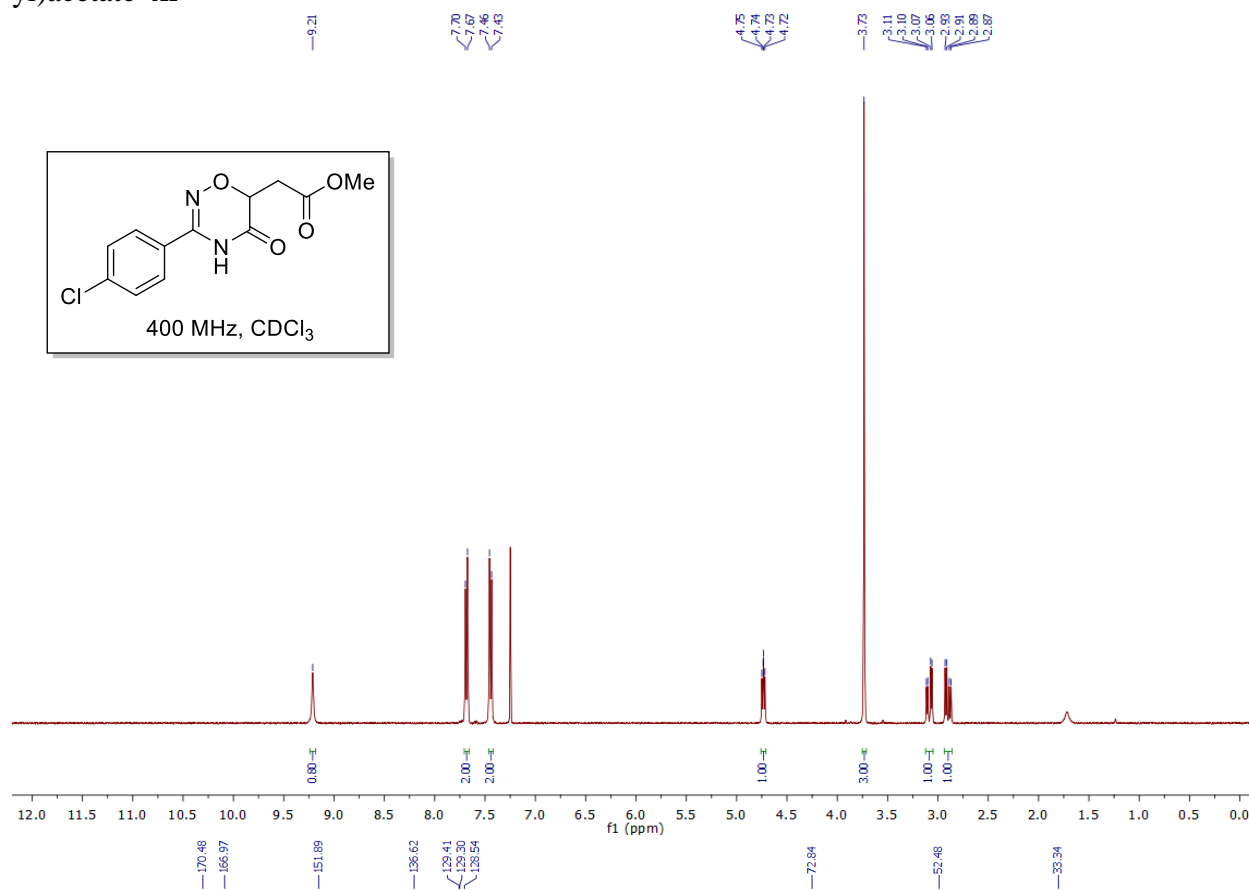




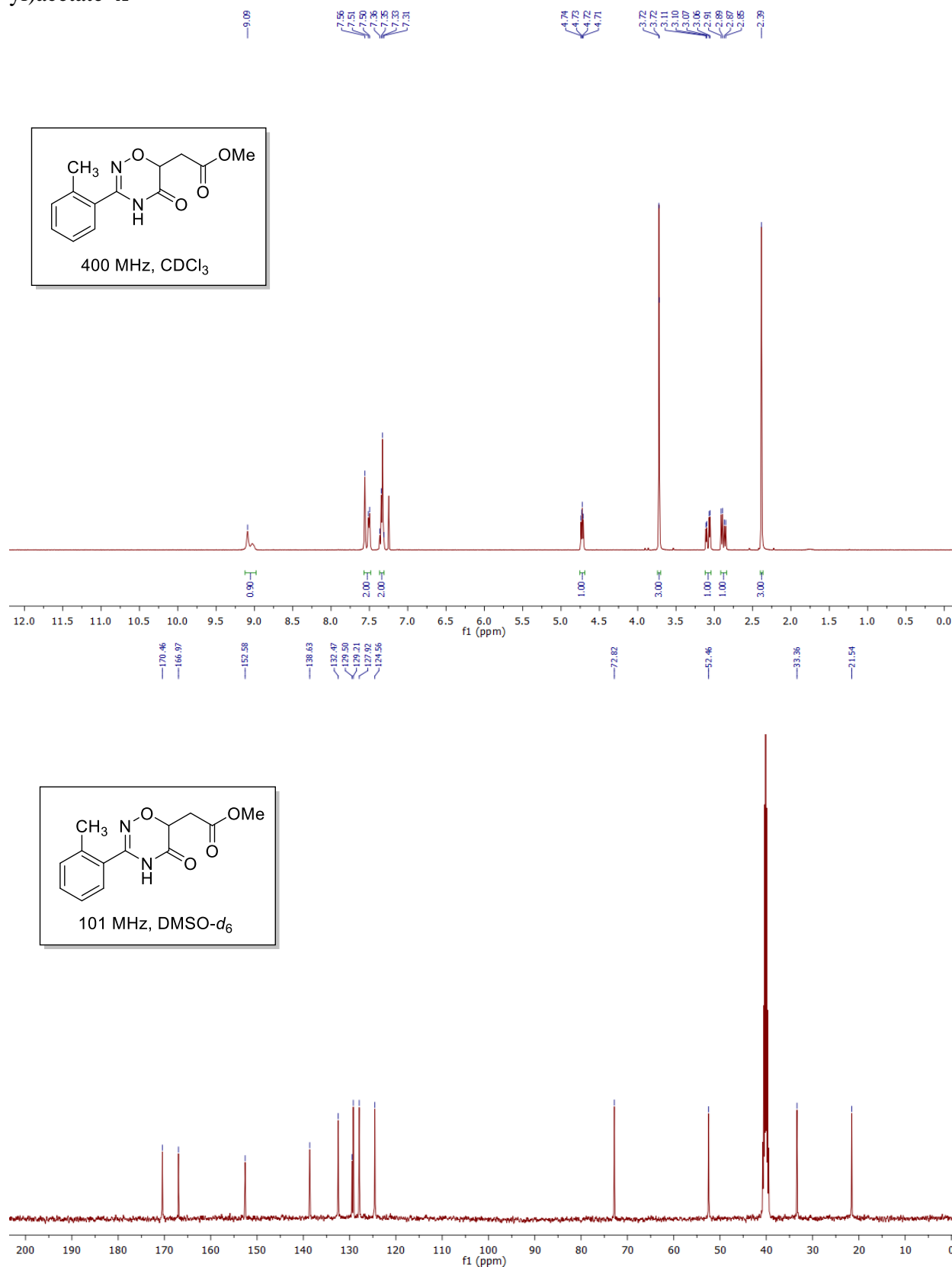
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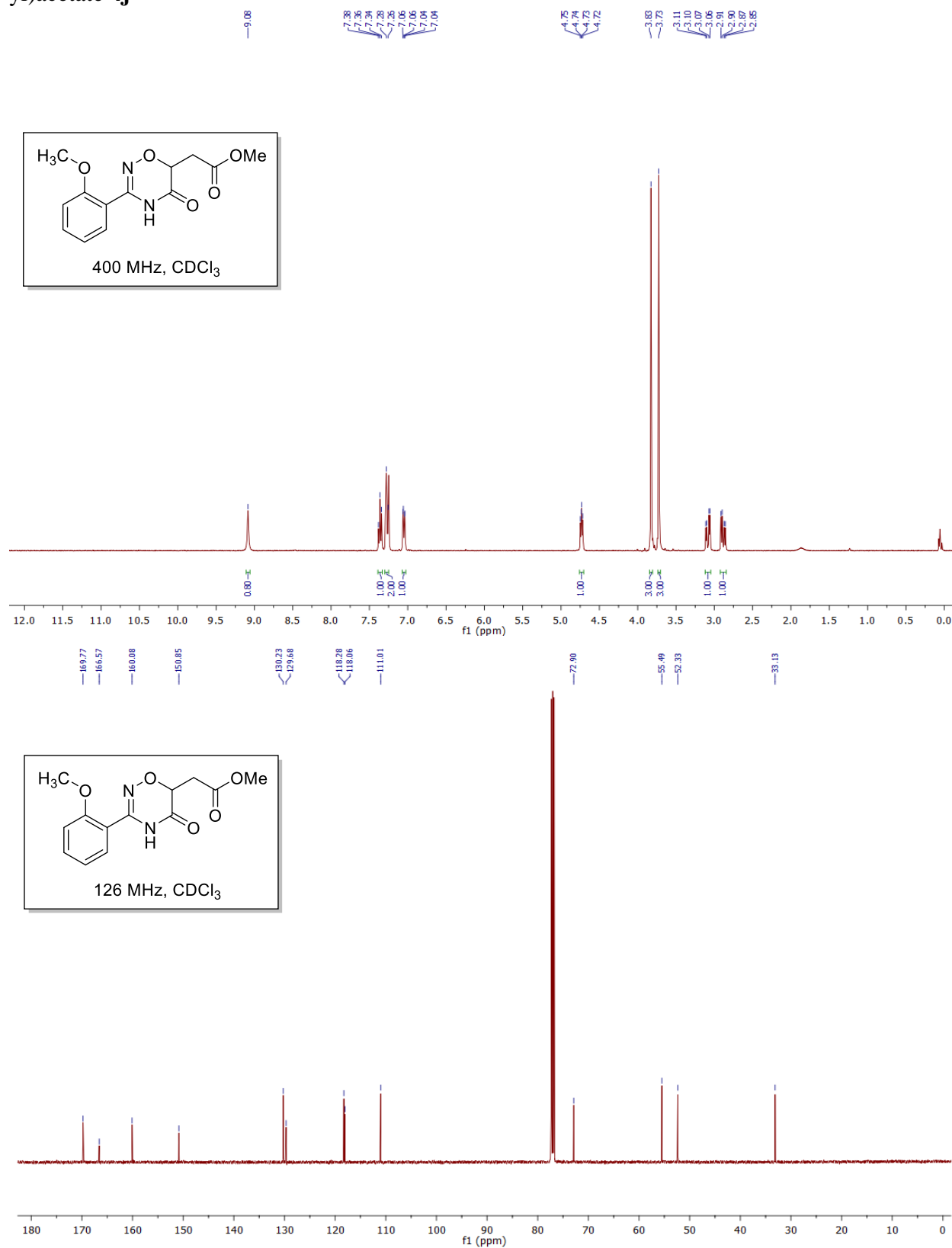
$^1\text{H}$  and  $^{13}\text{C}$  spectra of methyl 2-(3-(4-chlorophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetate **4h**



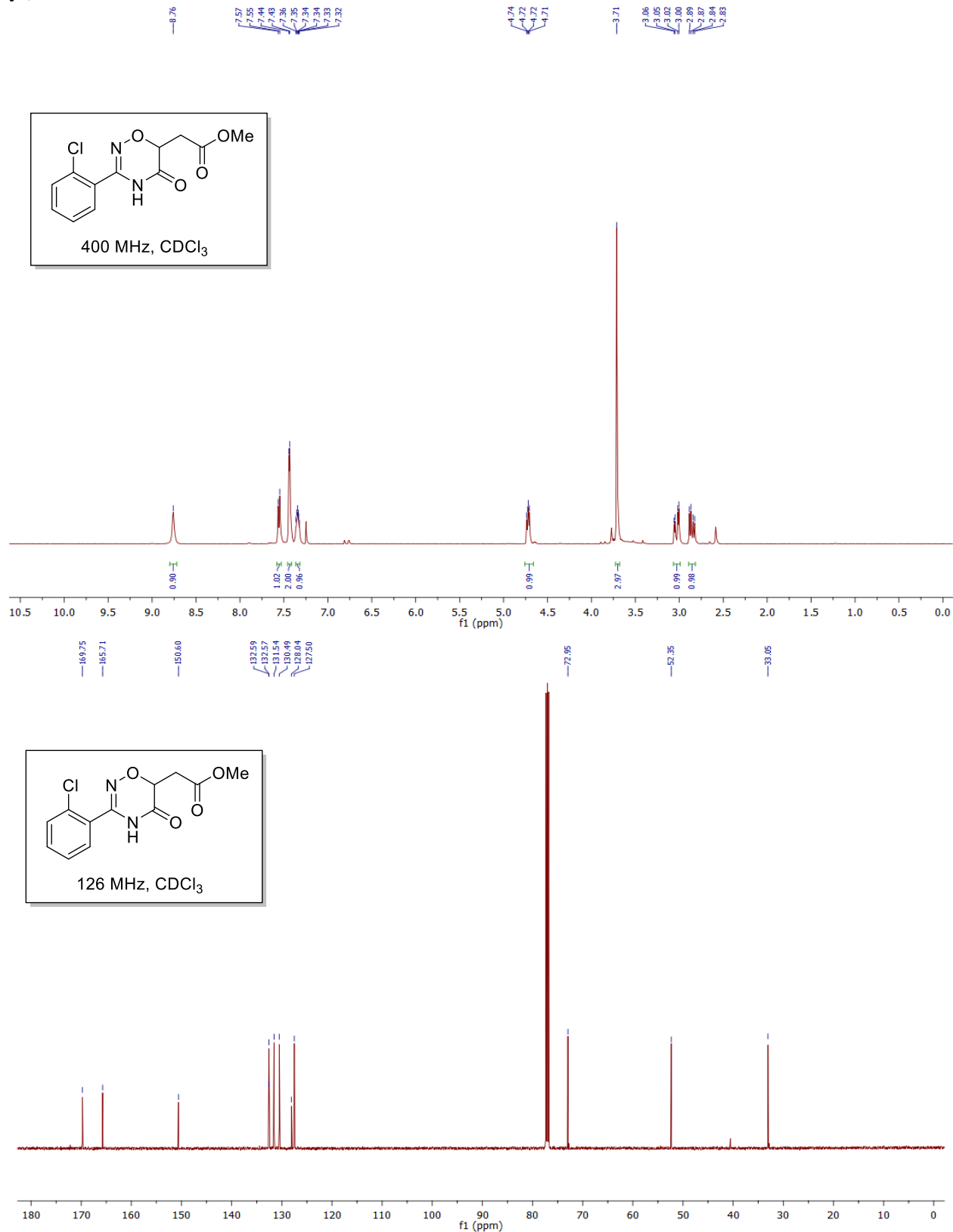
$^1\text{H}$  and  $^{13}\text{C}$  spectra of methyl 2-(3-(2-methylphenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetate **4i**



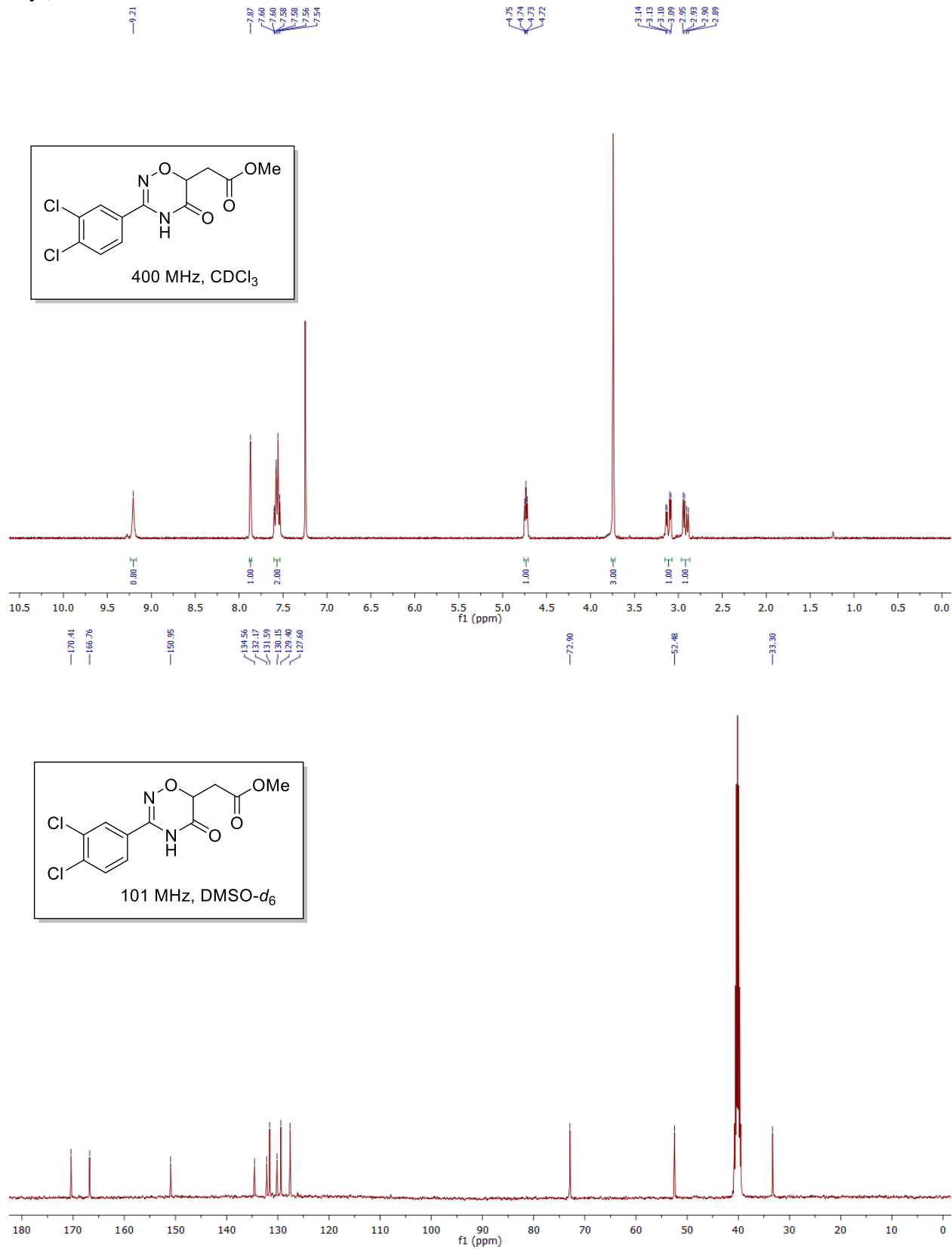
$^1\text{H}$  and  $^{13}\text{C}$  spectra of methyl 2-(3-(2-methoxyphenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetate **4j**



$^1\text{H}$  and  $^{13}\text{C}$  spectra of methyl 2-(3-(2-chlorophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetate **4k**

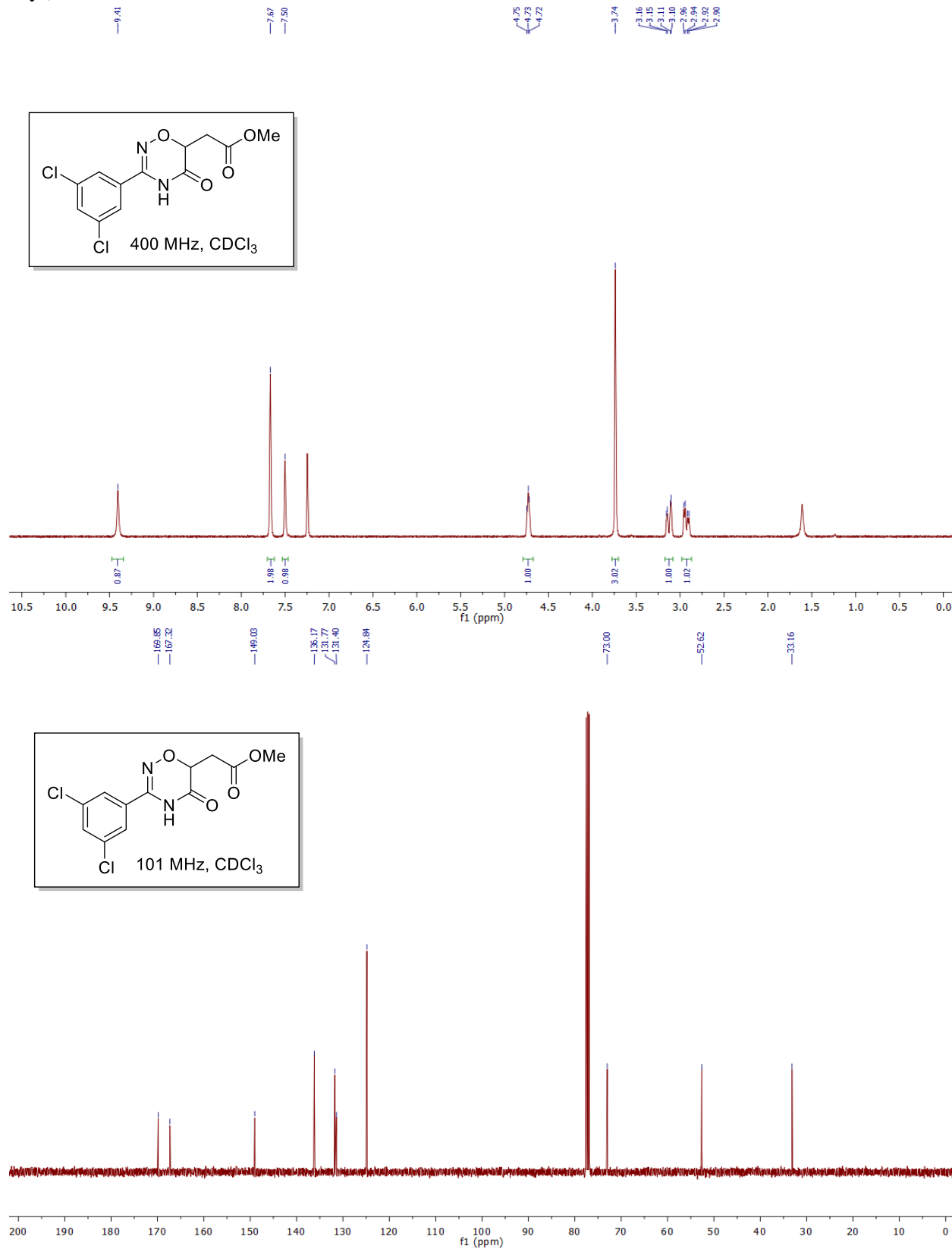


$^1\text{H}$  and  $^{13}\text{C}$  spectra of methyl 2-(3-(3,4-dichlorophenyl)-5-oxo-5,6-dihydro-4*H*-1,2,4-oxadiazin-6-yl)acetate **4l**

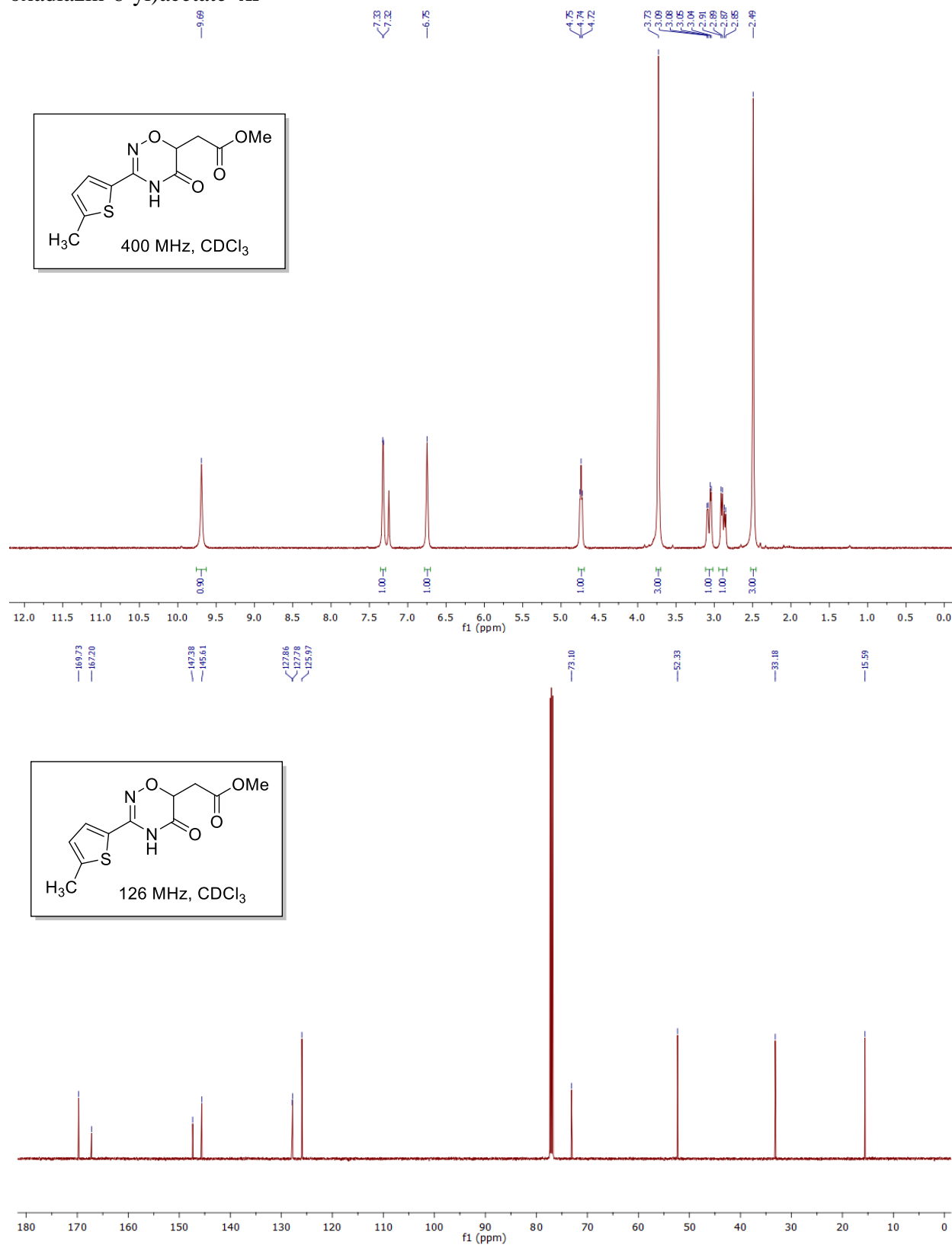




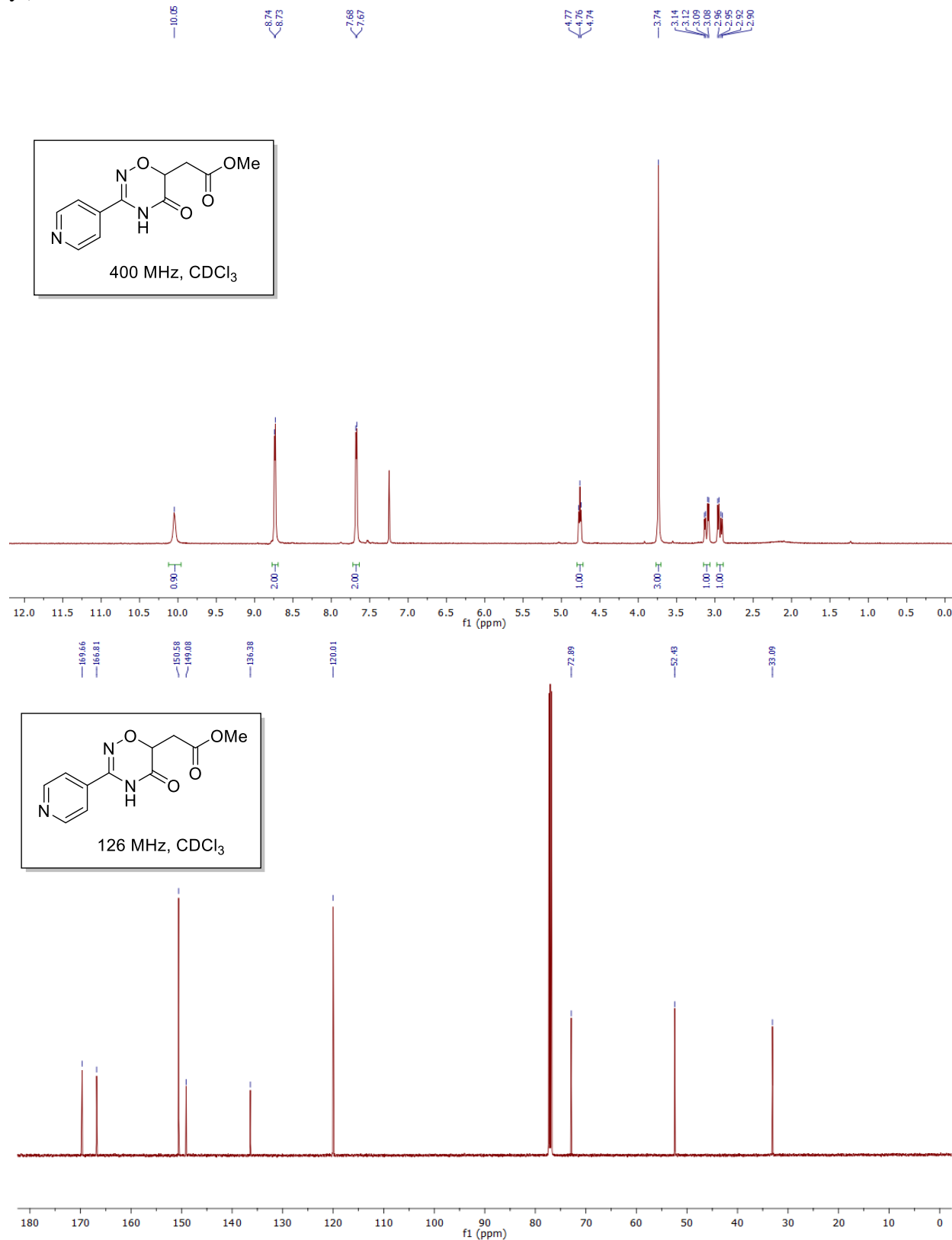
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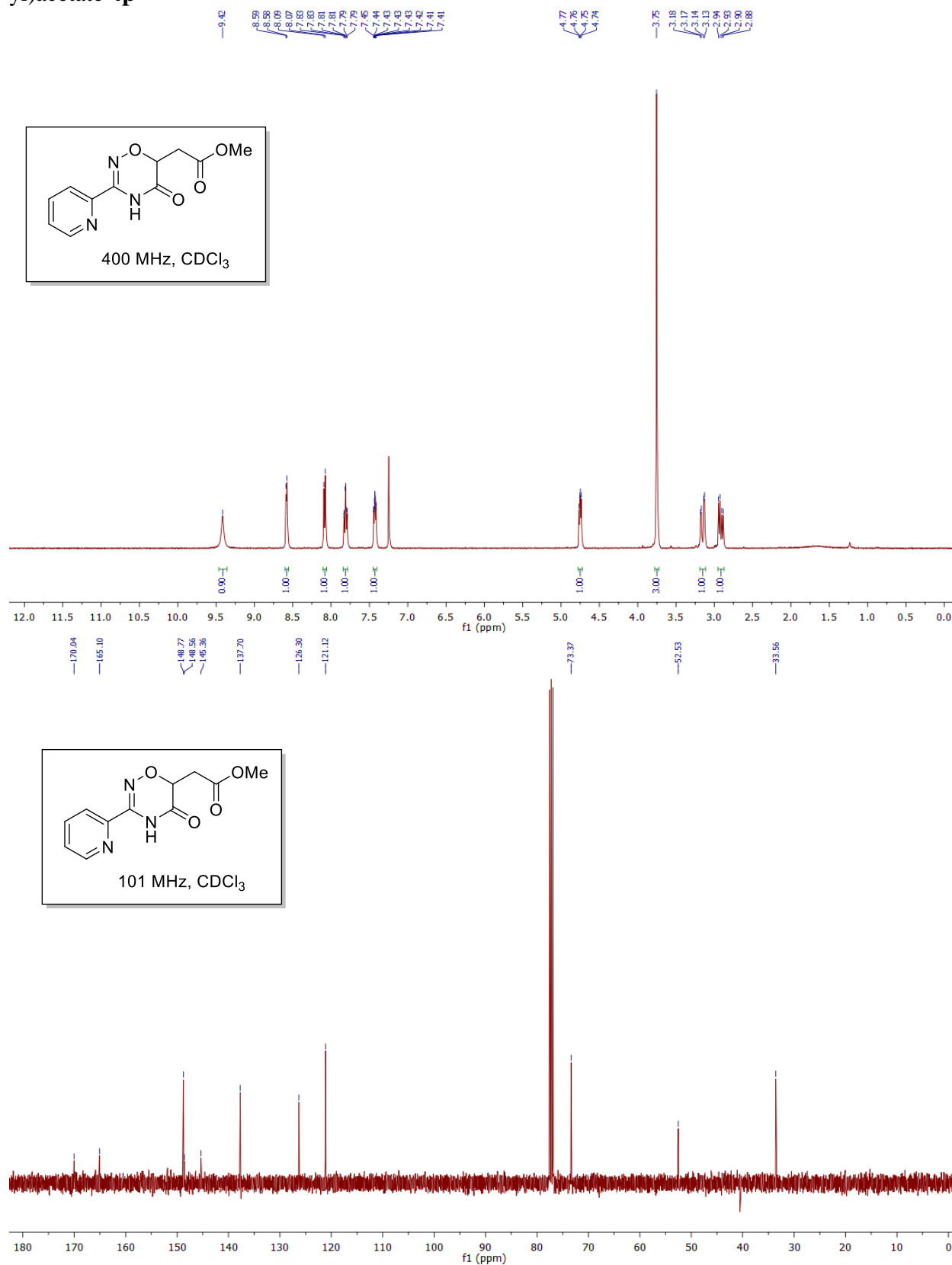
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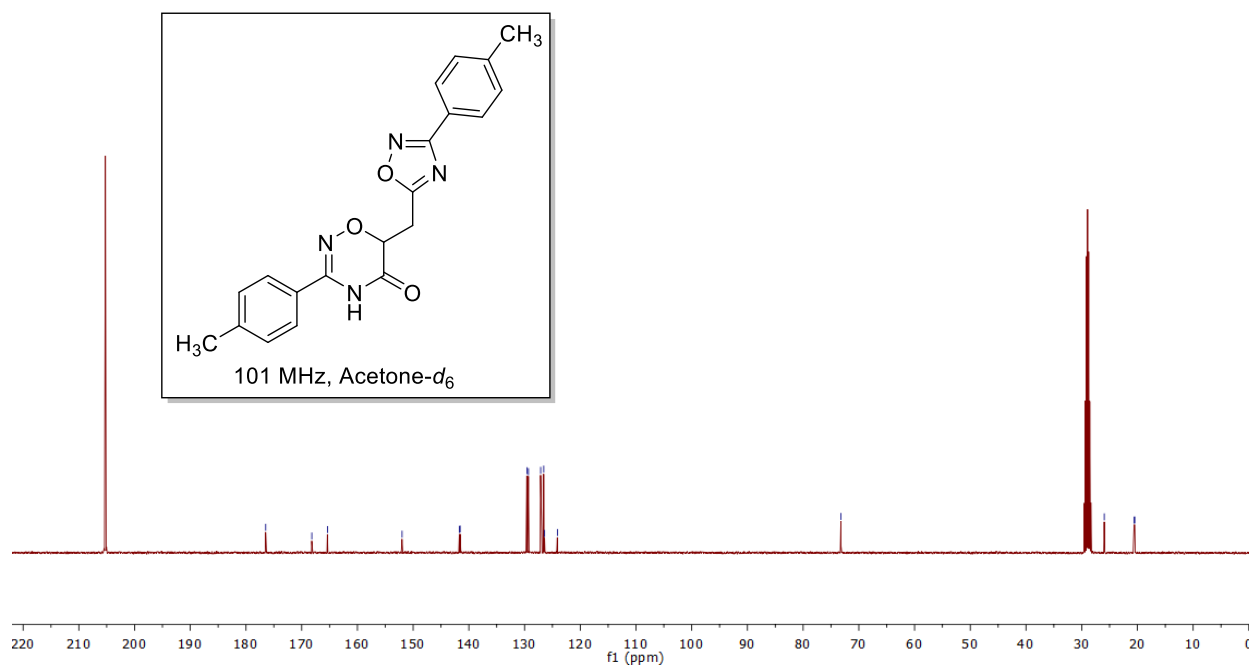
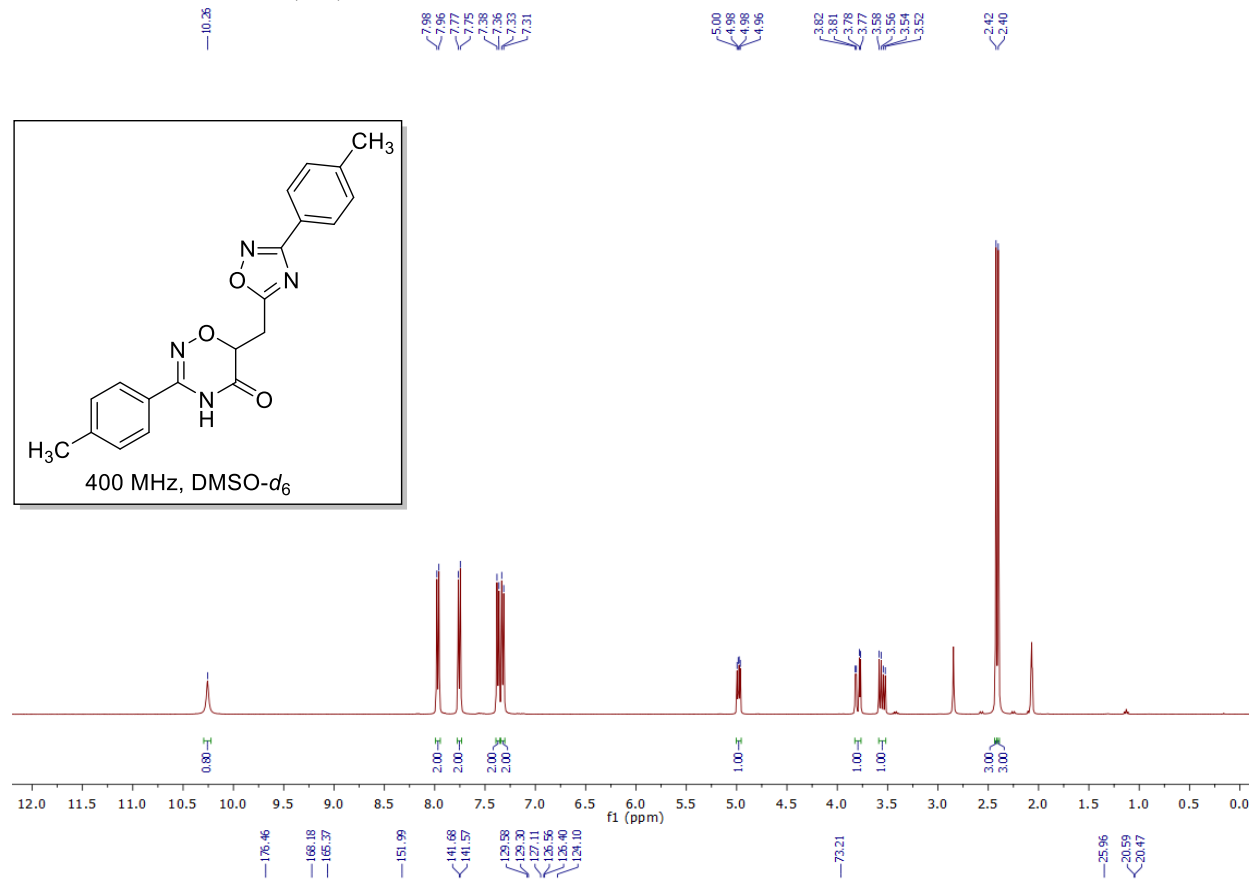
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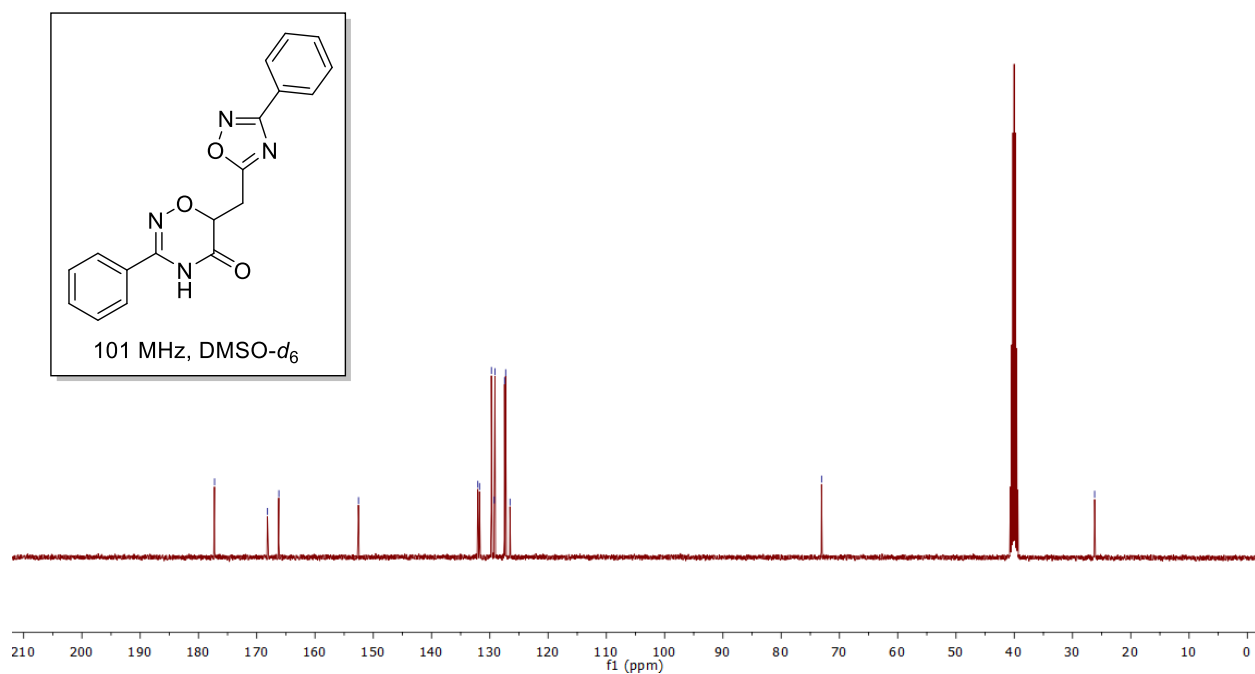
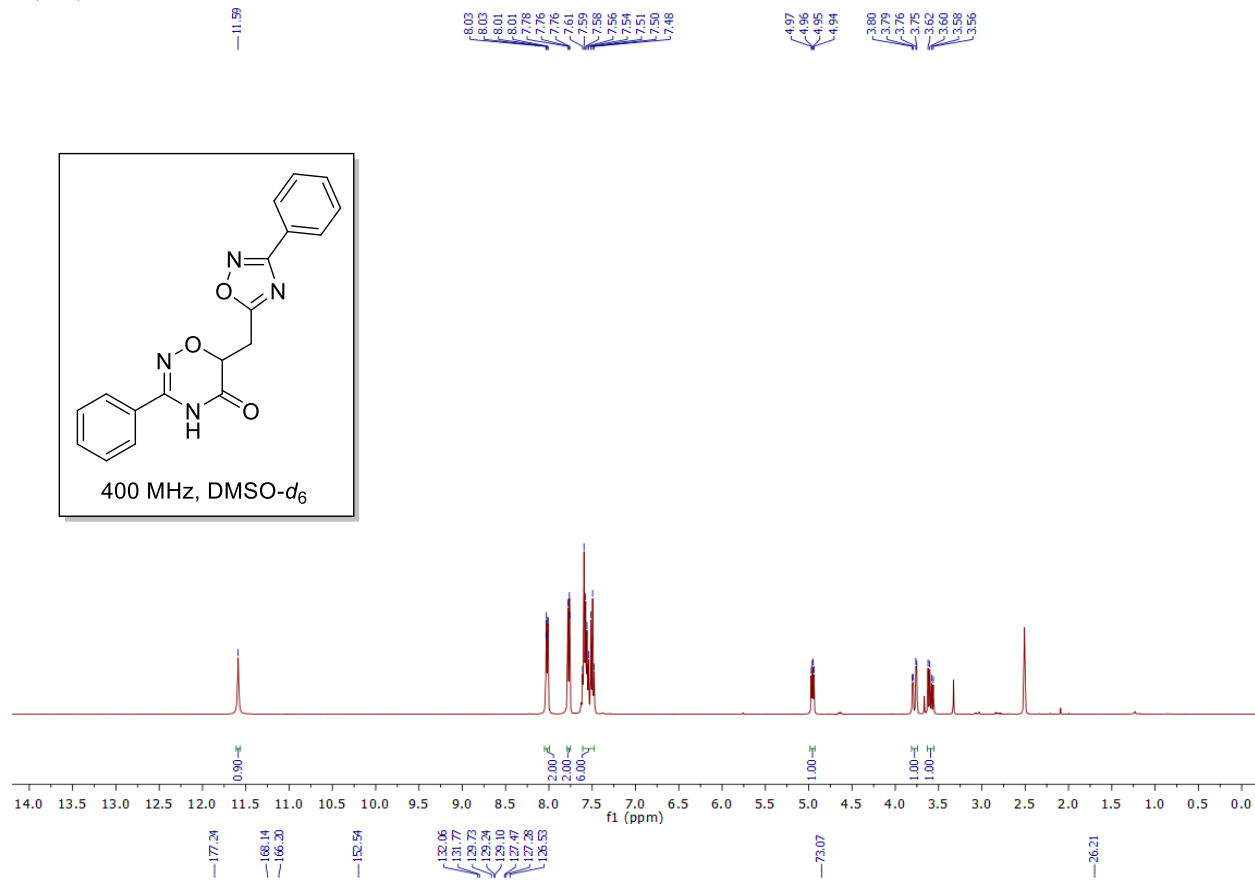
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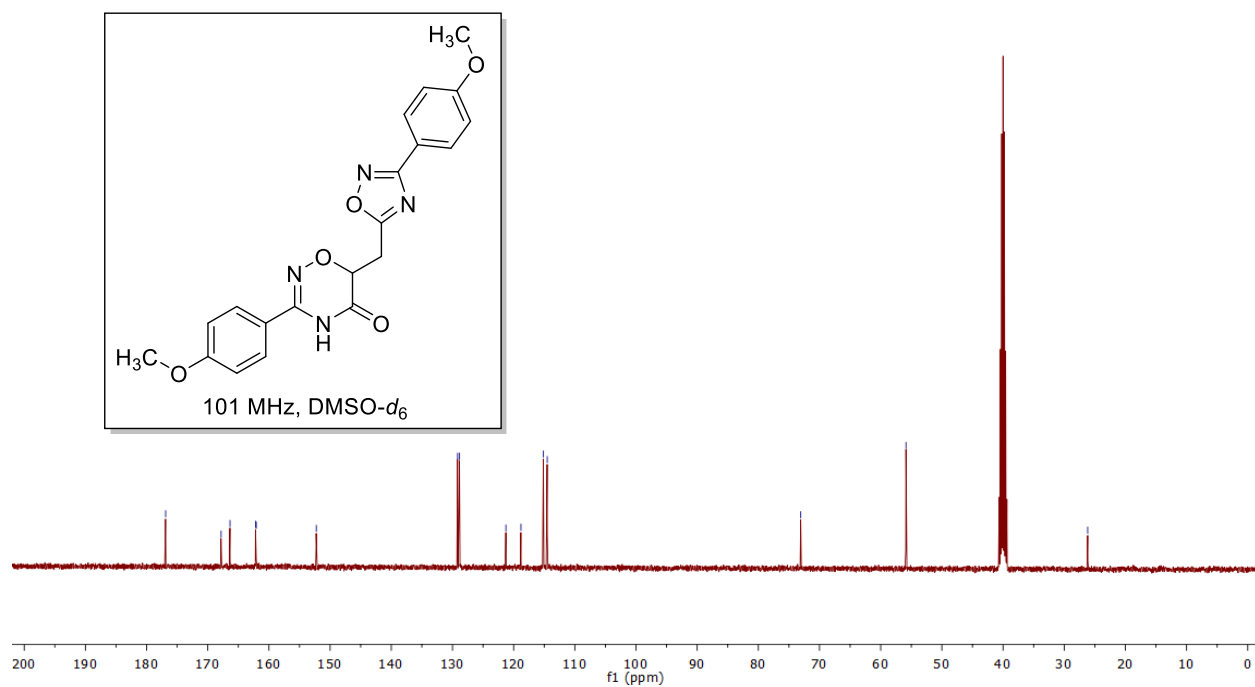
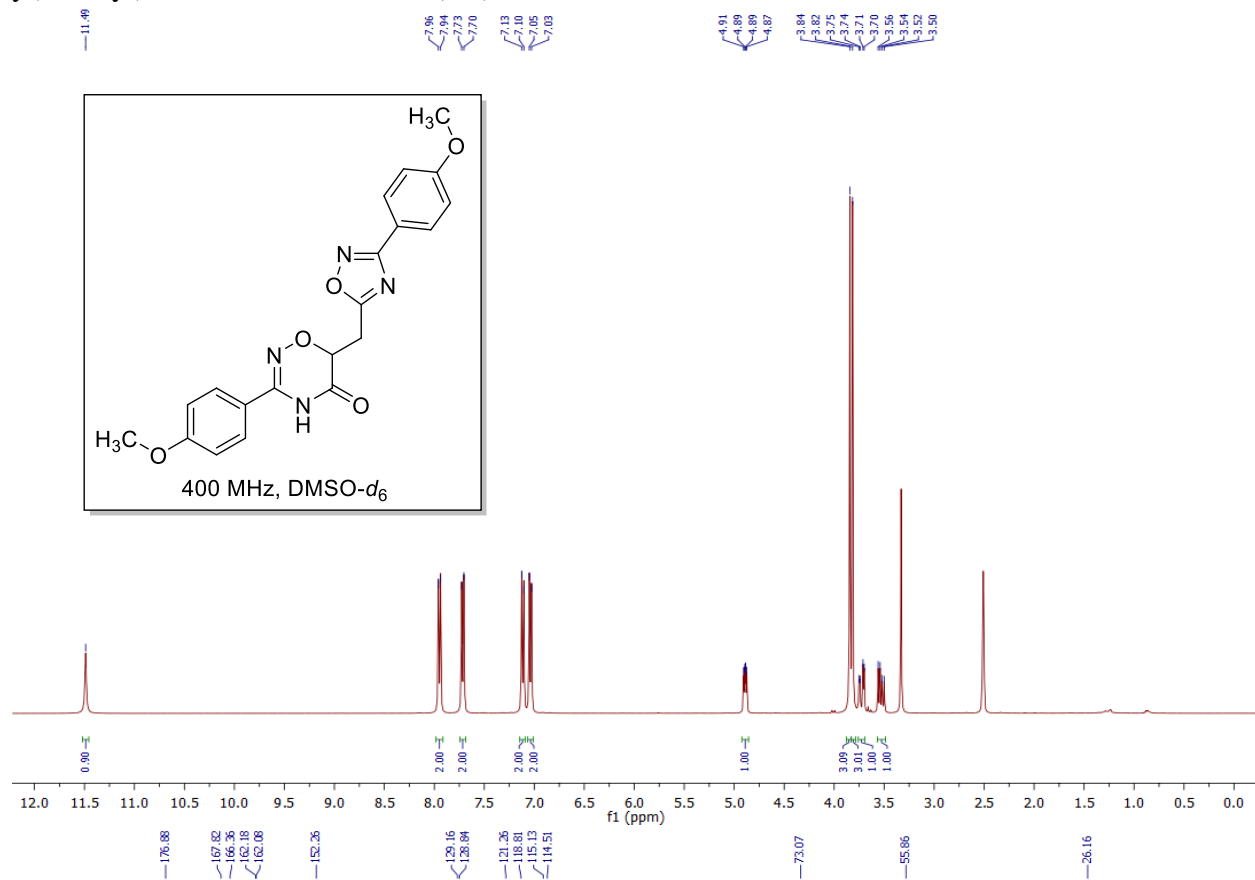
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(4-methylphenyl)-6-((3-(4-methylphenyl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5a**



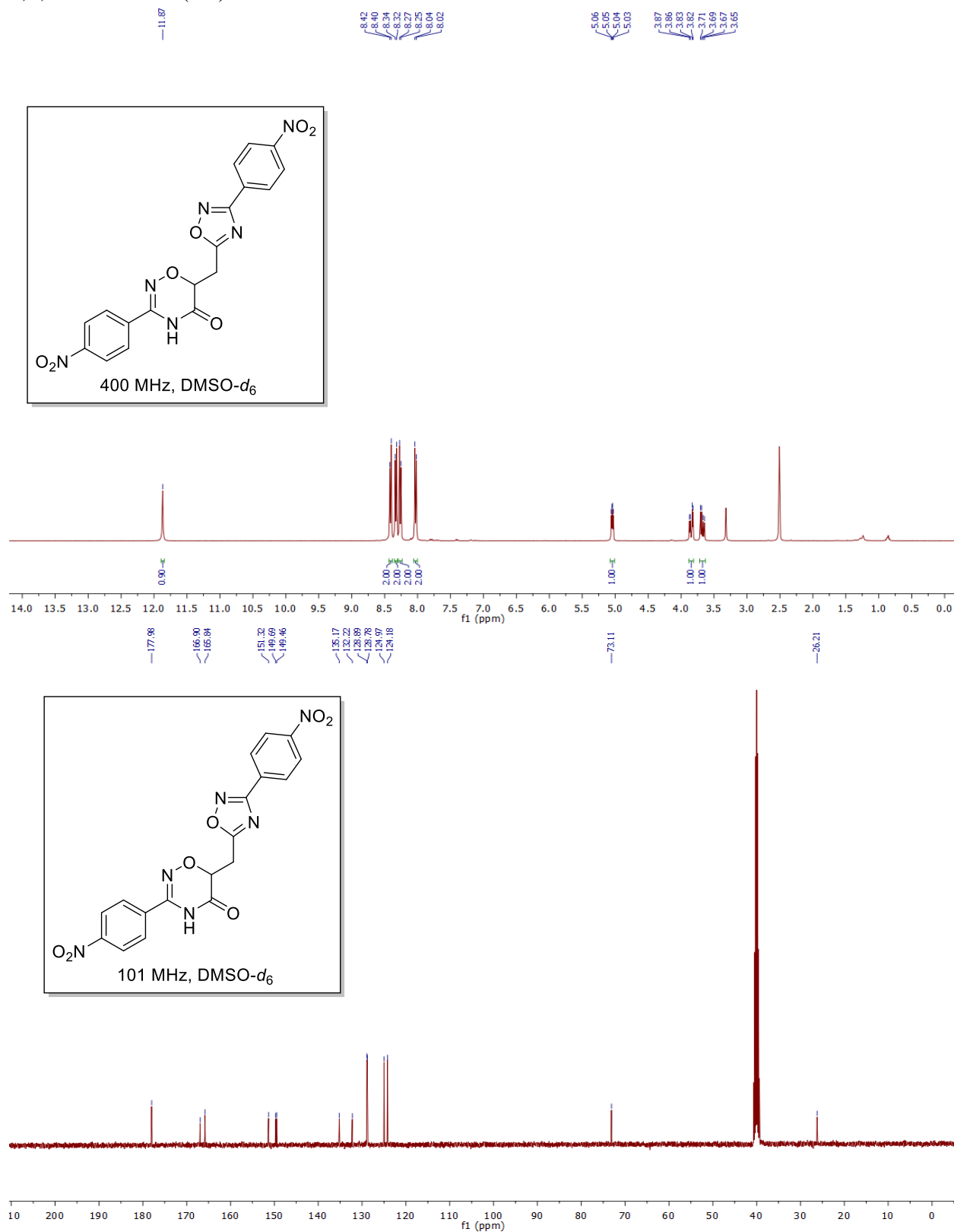
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$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(4-methoxyphenyl)-6-((3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5c**

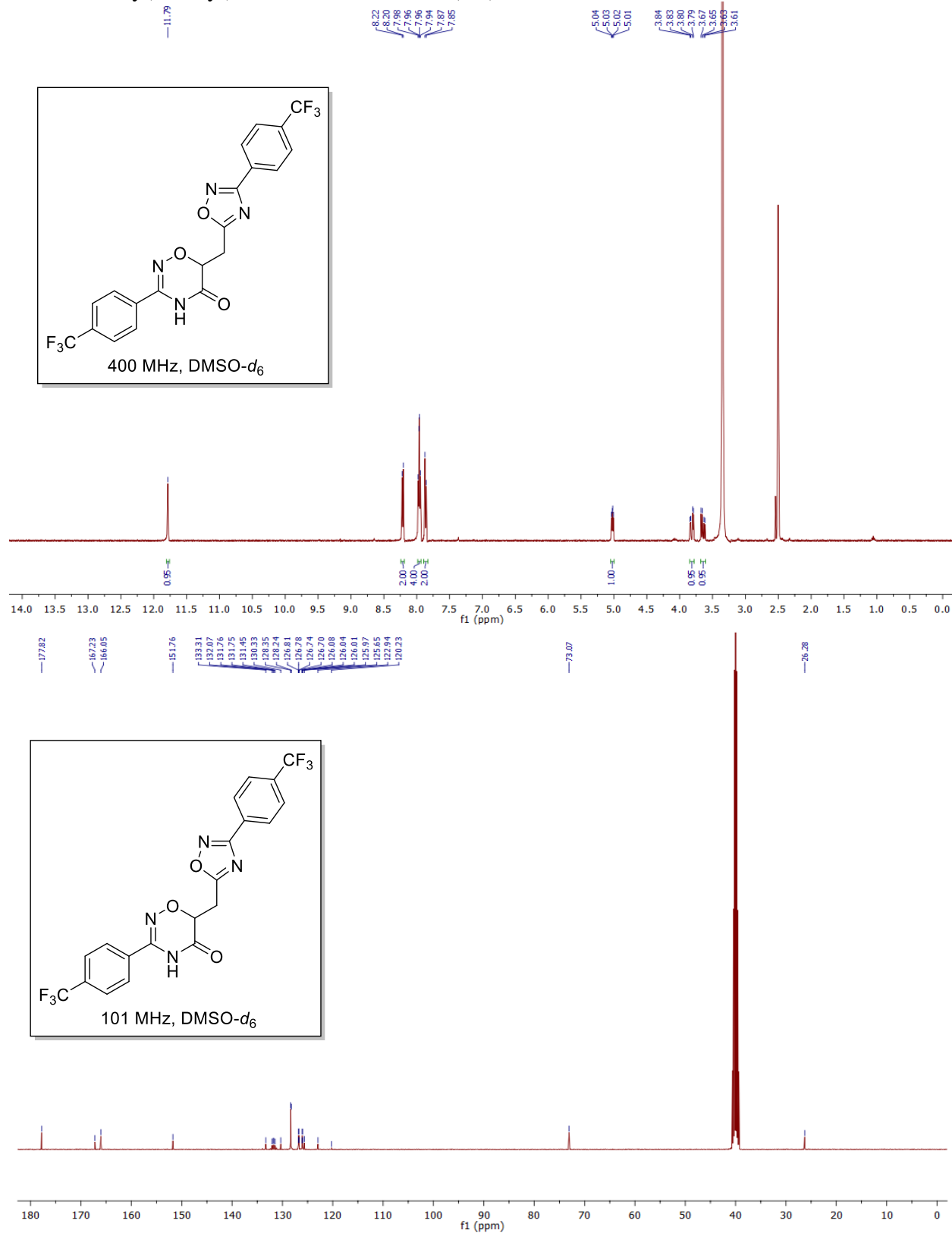


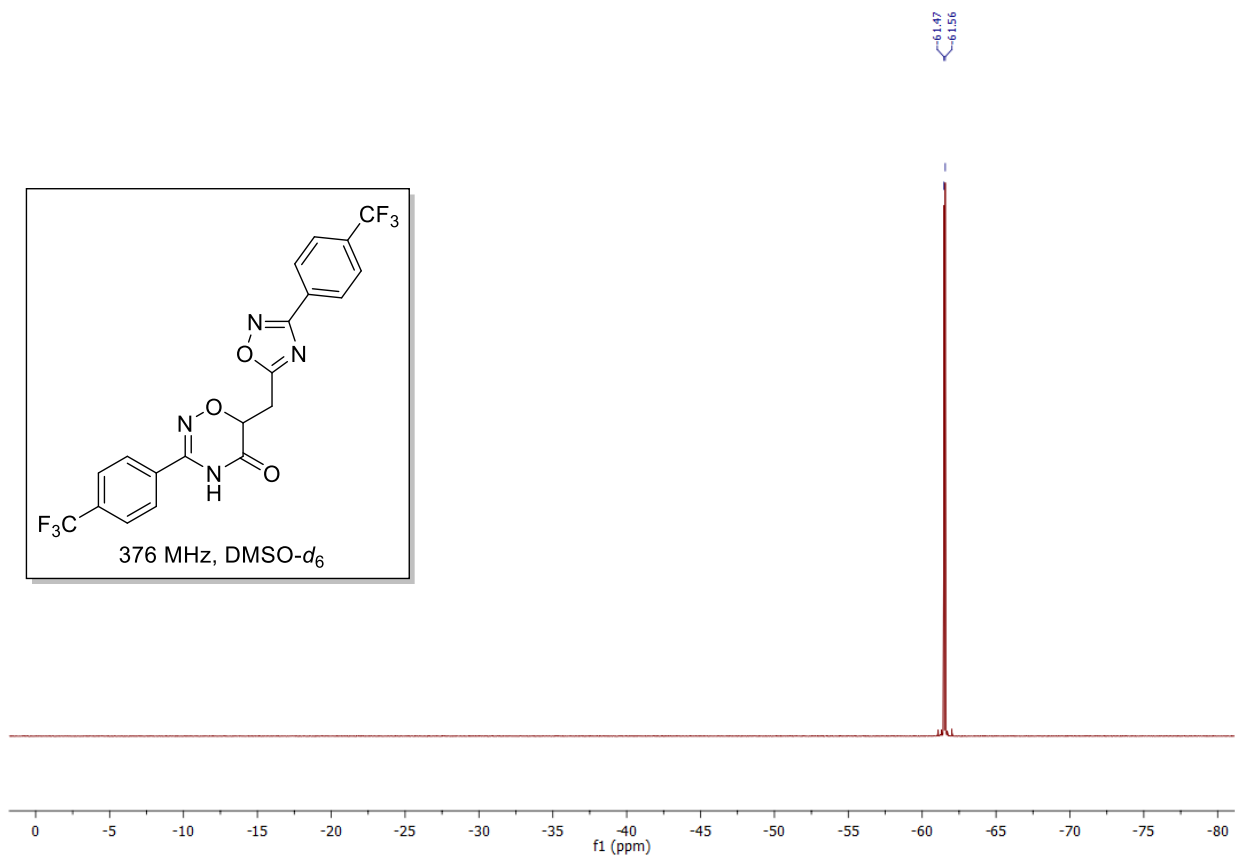
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(4-nitrophenyl)-6-((3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5d**



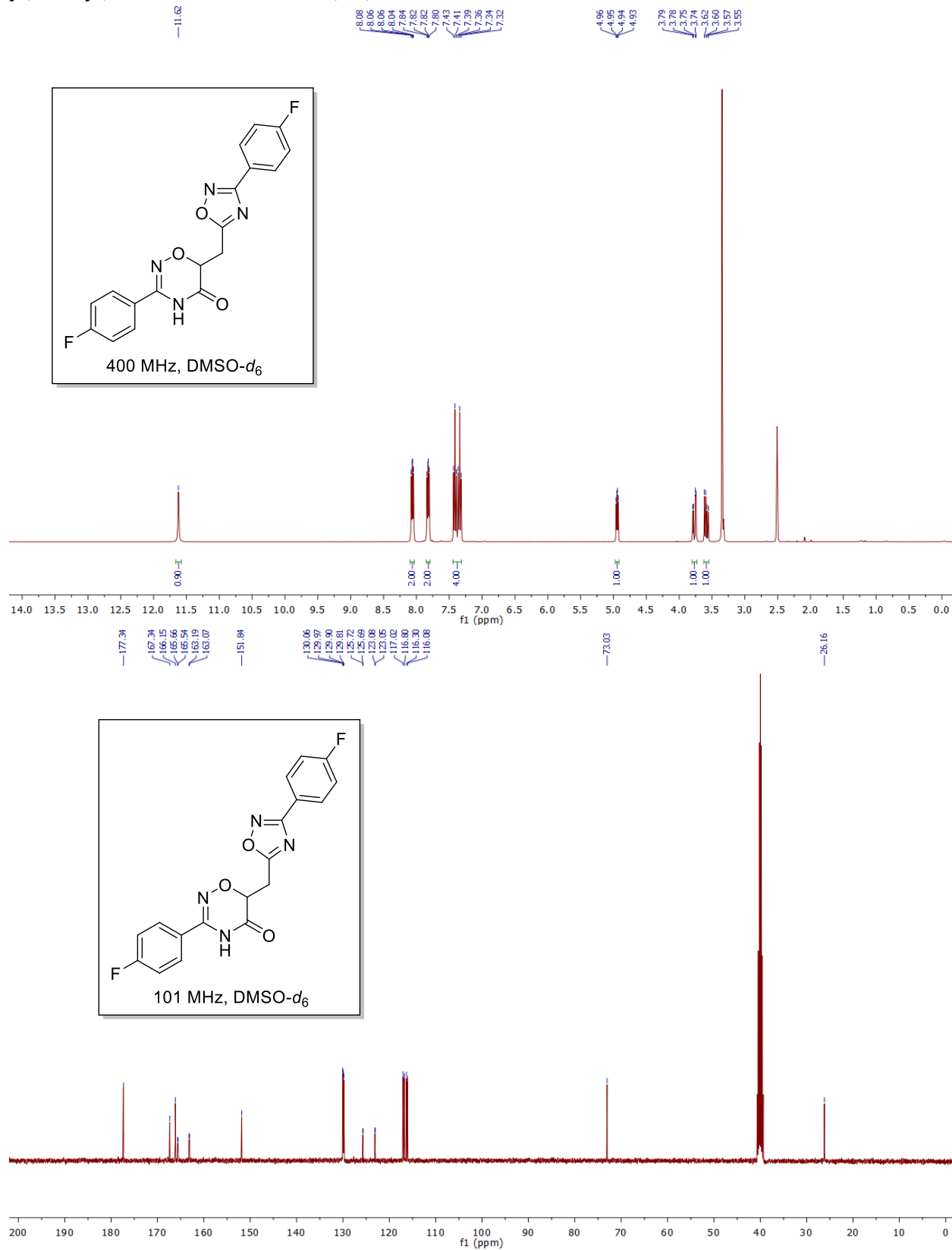


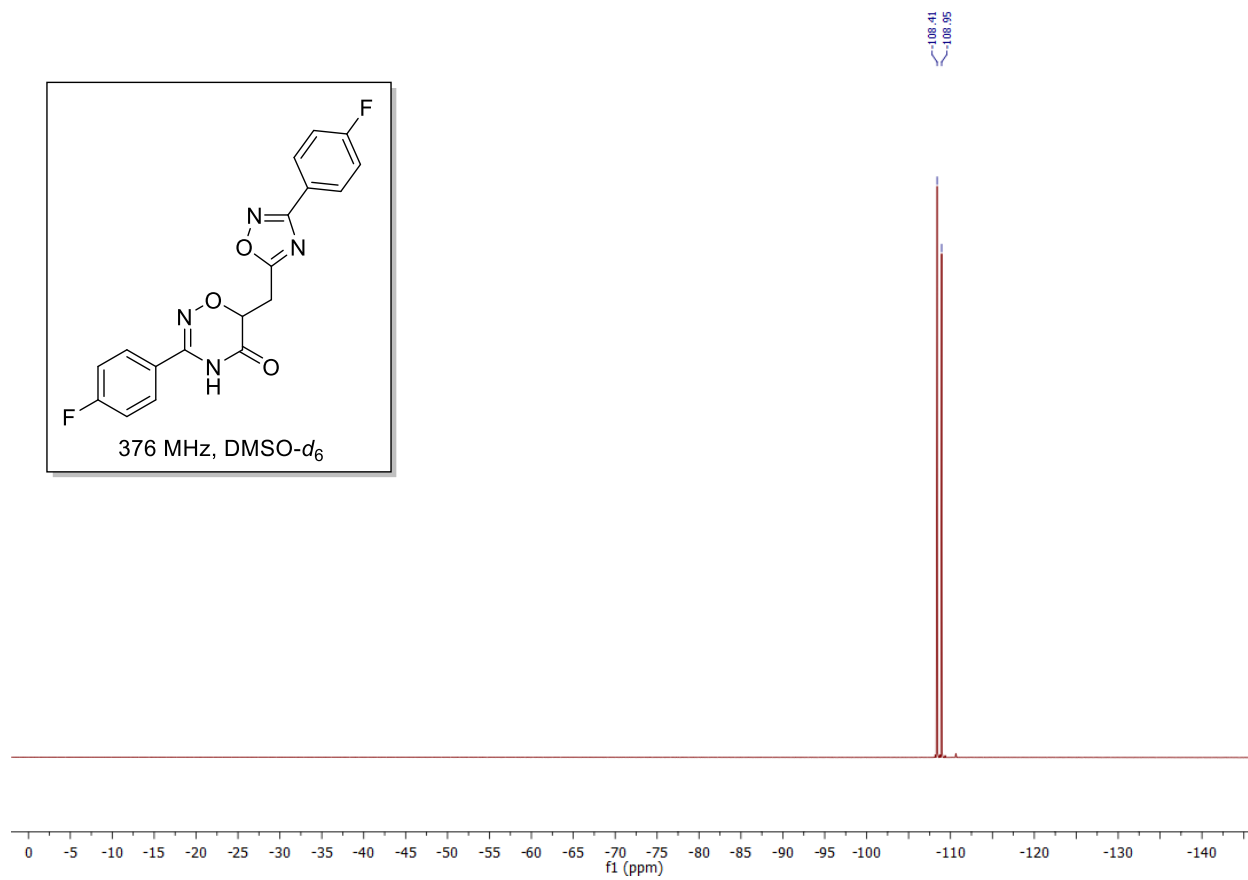
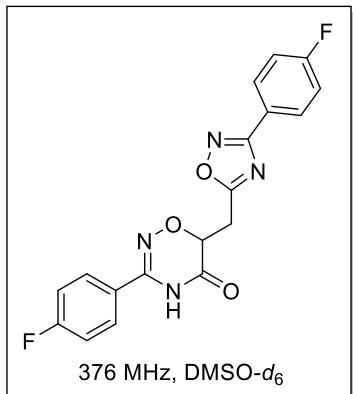
$^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  spectra of 3-(4-(trifluoromethyl)phenyl)-6-((3-(4-(trifluoromethyl)phenyl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5e**



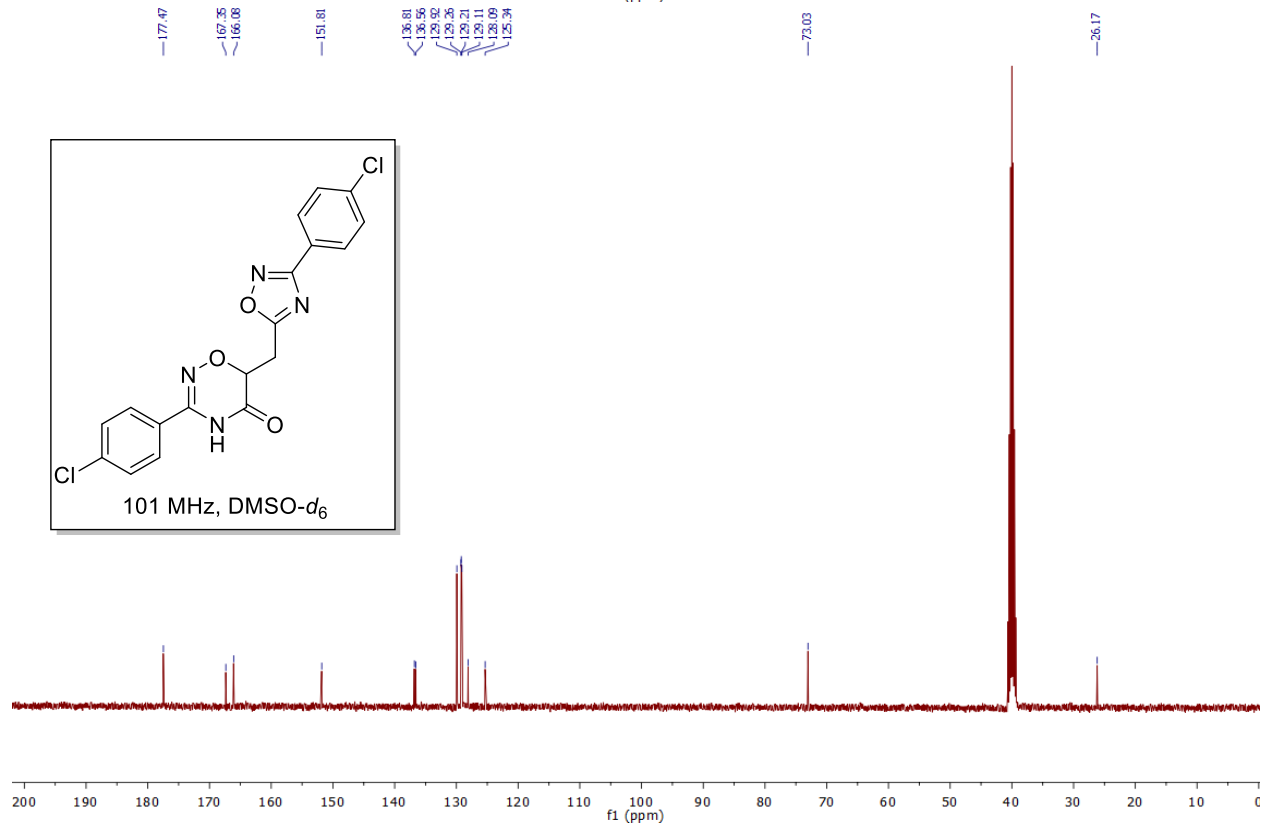
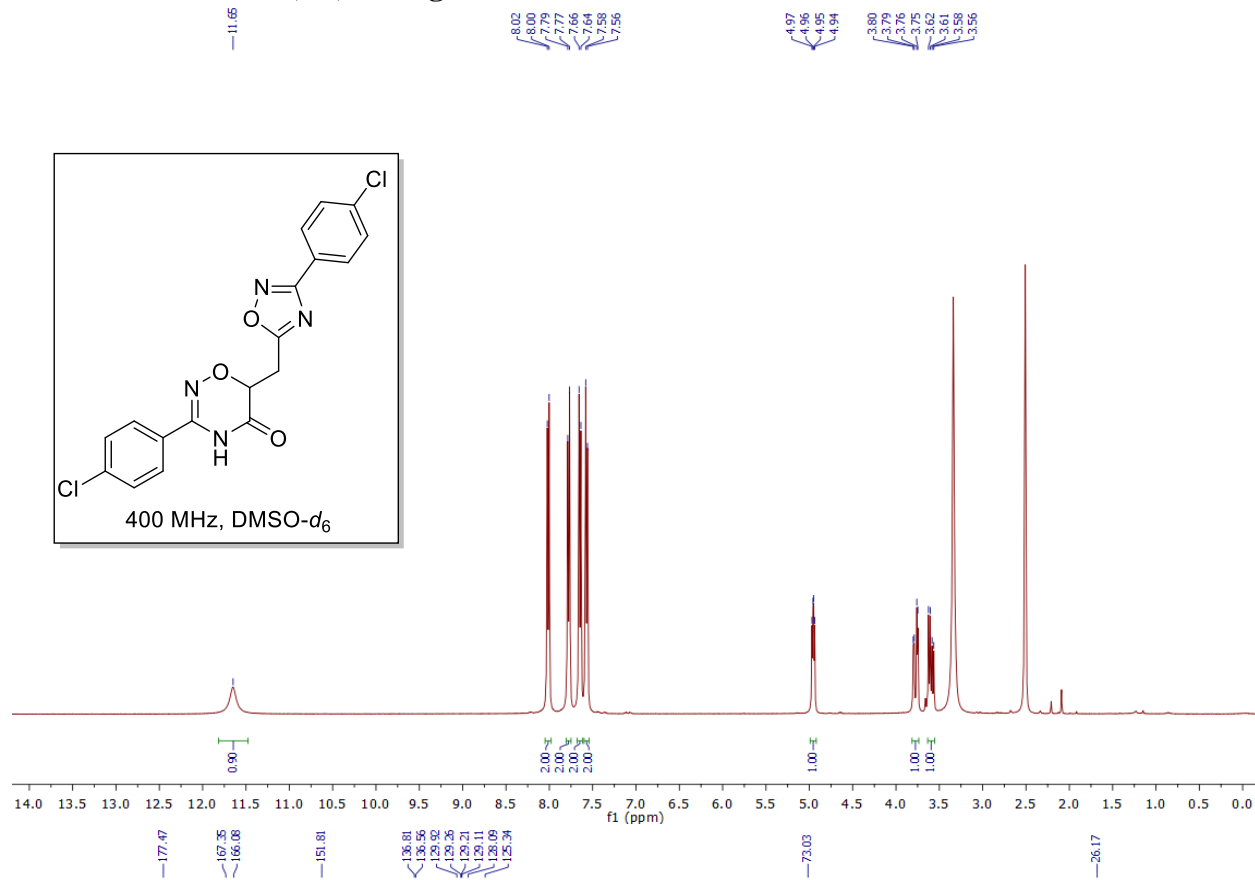


$^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  spectra of 3-(4-fluorophenyl)-6-((3-(4-fluorophenyl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5f**

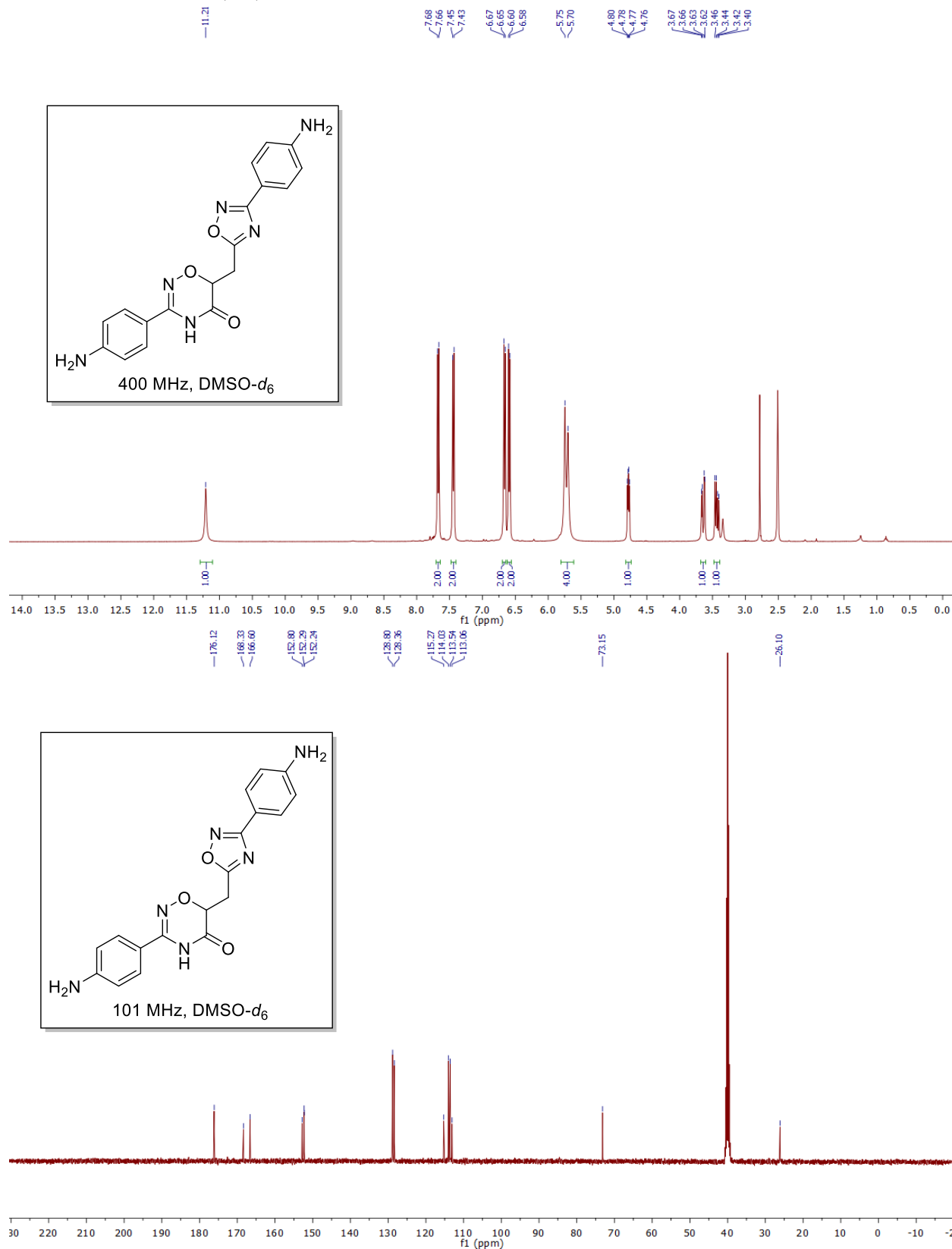




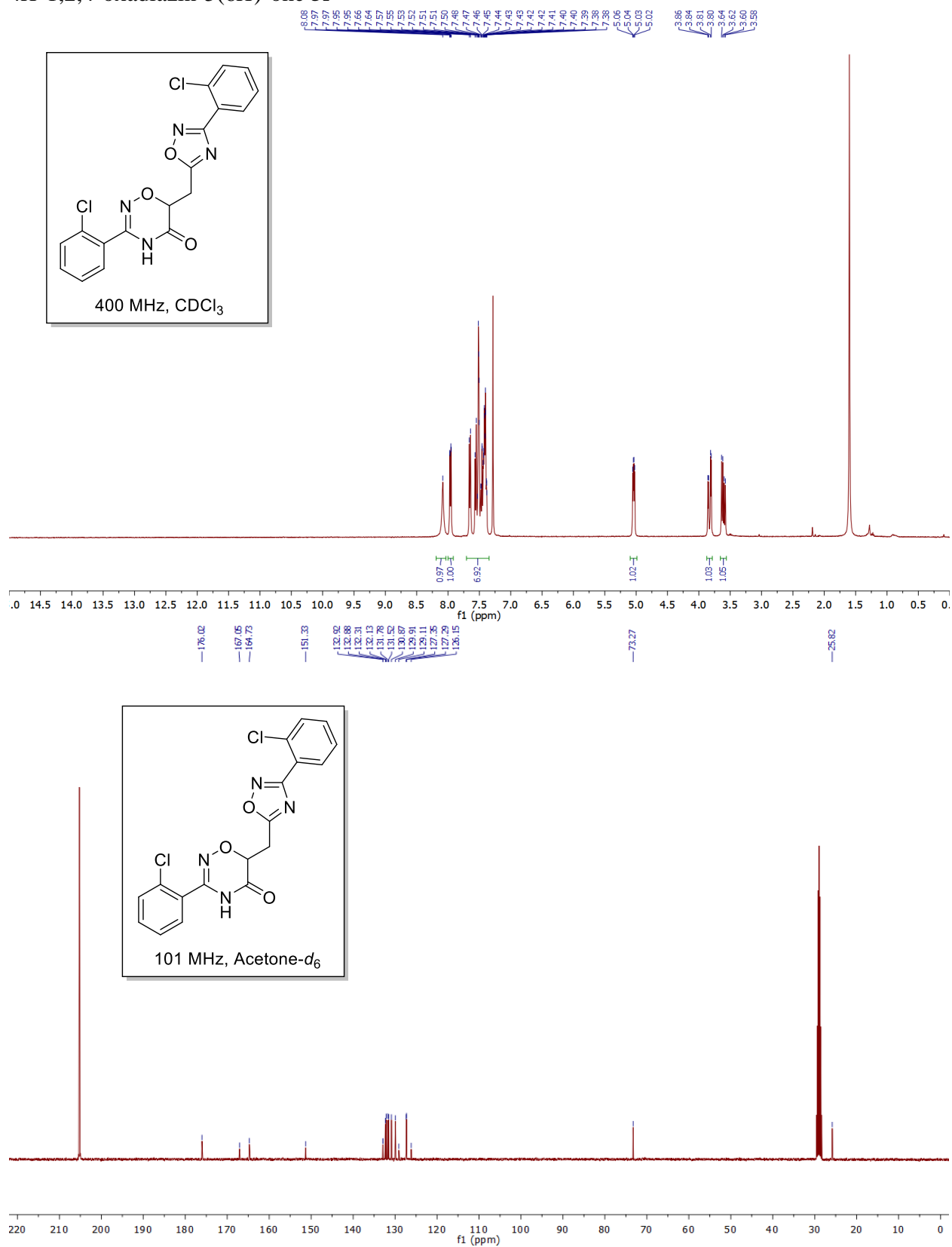
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(4-chlorophenyl)-6-((3-(4-chlorophenyl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5g**



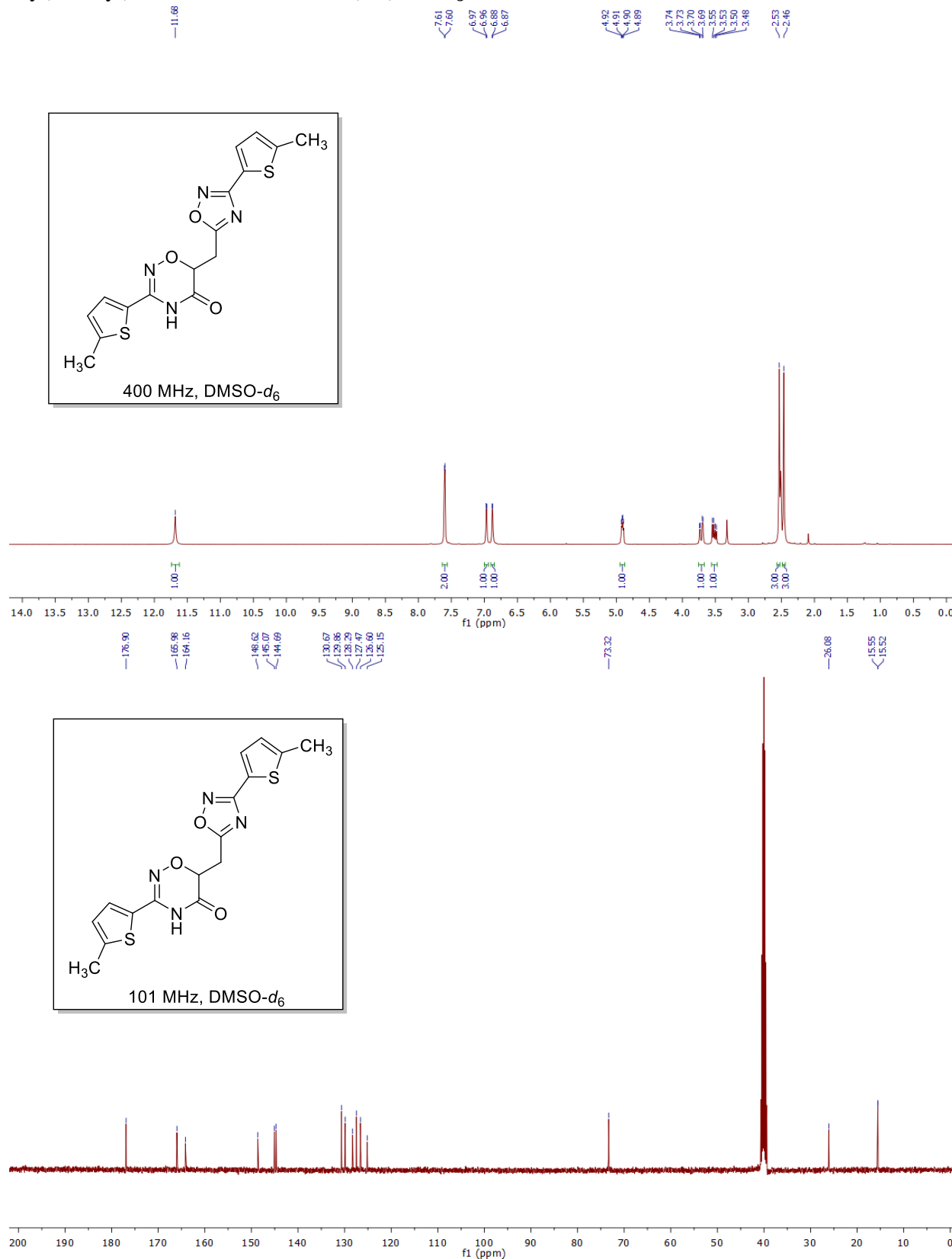
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(4-aminophenyl)-6-((3-(4-aminophenyl)-1,2,4-oxadiazol-5-yl)methyl)-4H-1,2,4-oxadiazin-5(6H)-one **5h**



$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(2-chlorophenyl)-6-((3-(2-chlorophenyl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5i**

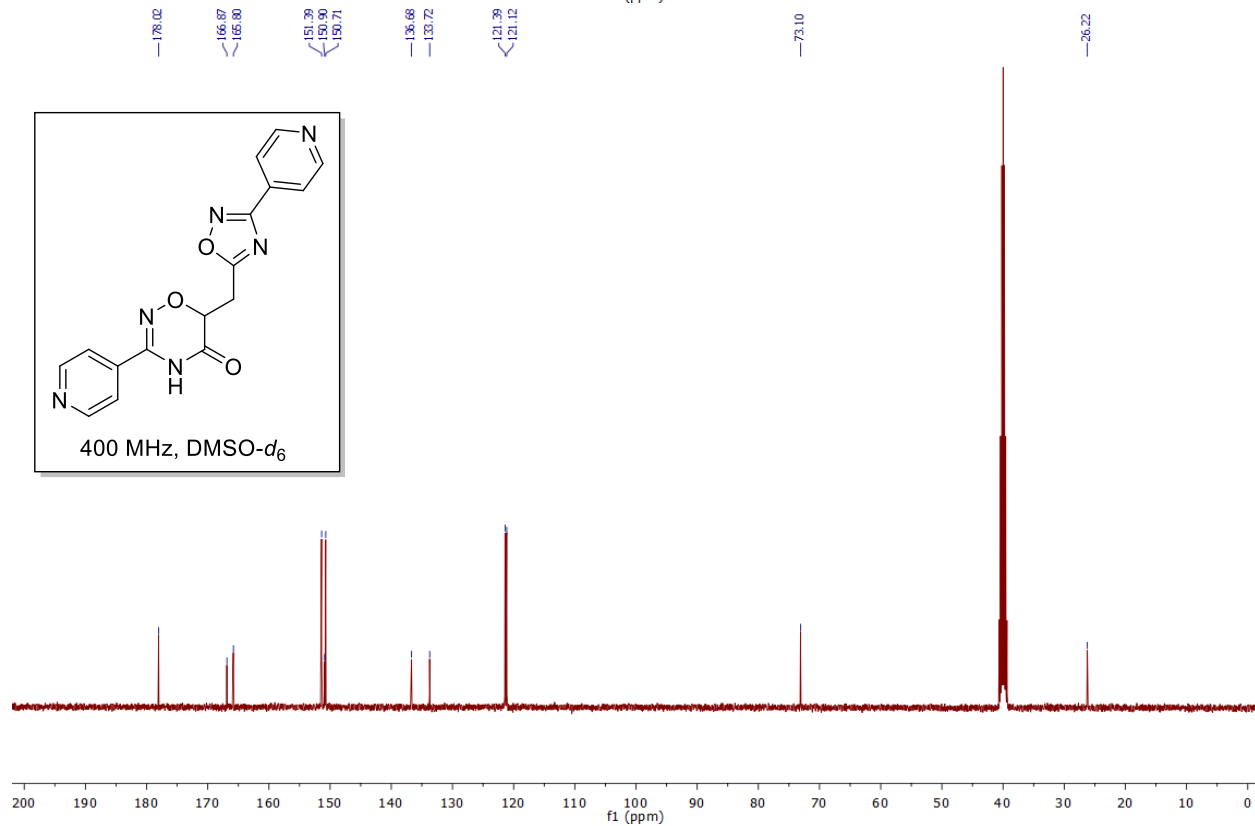
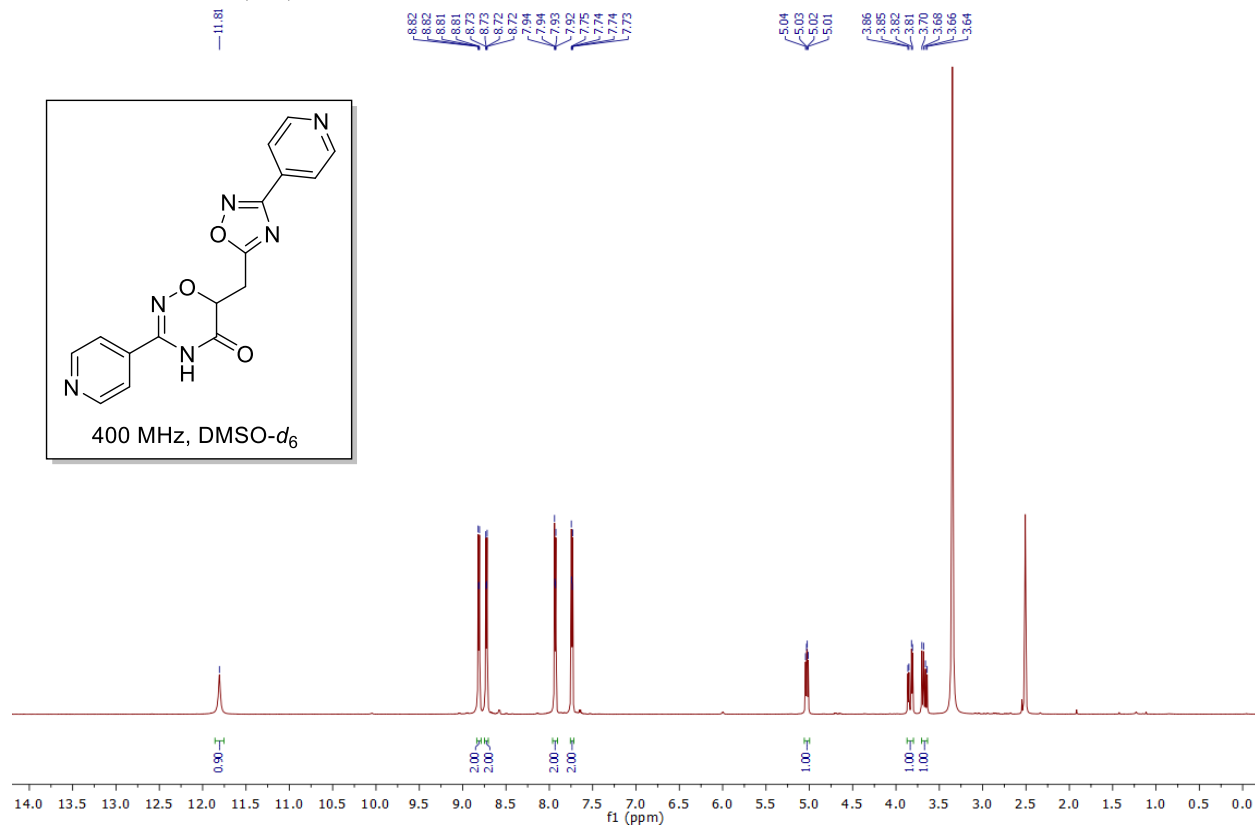


$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(5-methylthiophen-2-yl)-6-((3-(5-methylthiophen-2-yl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5j**

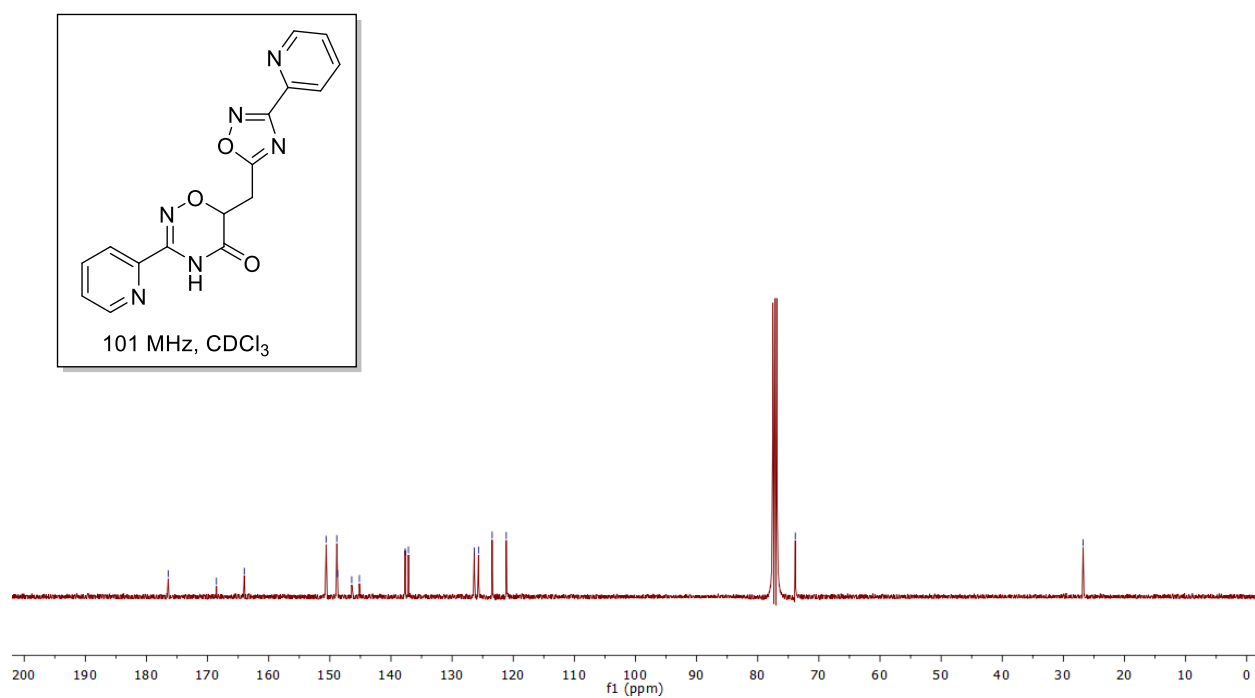
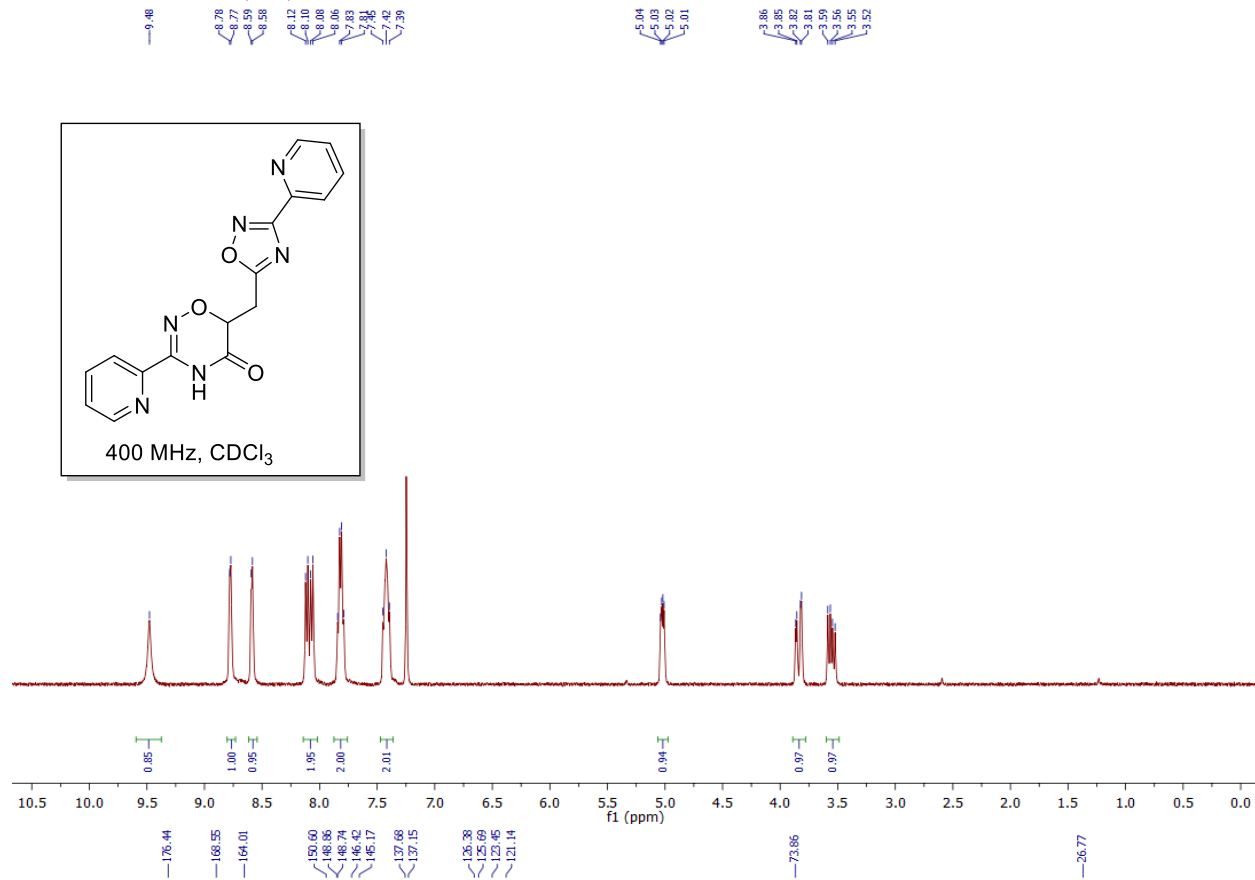




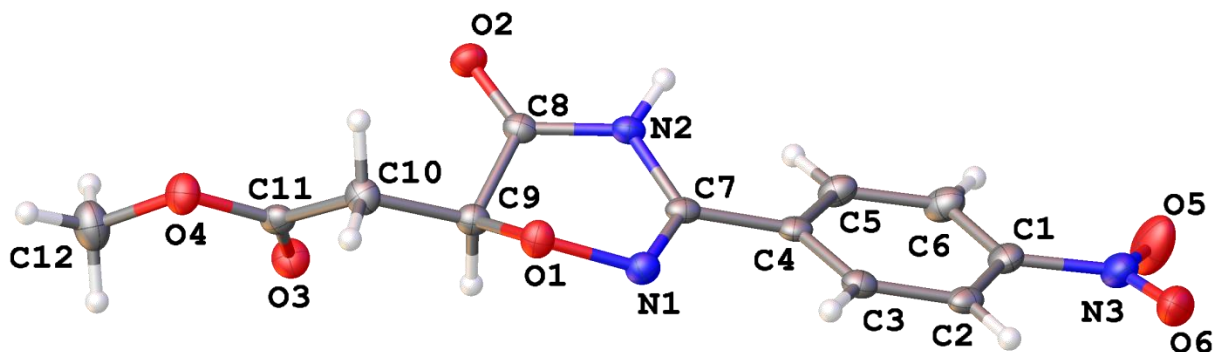
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(pyridin-4-yl)-6-((3-(pyridin-4-yl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **5k**



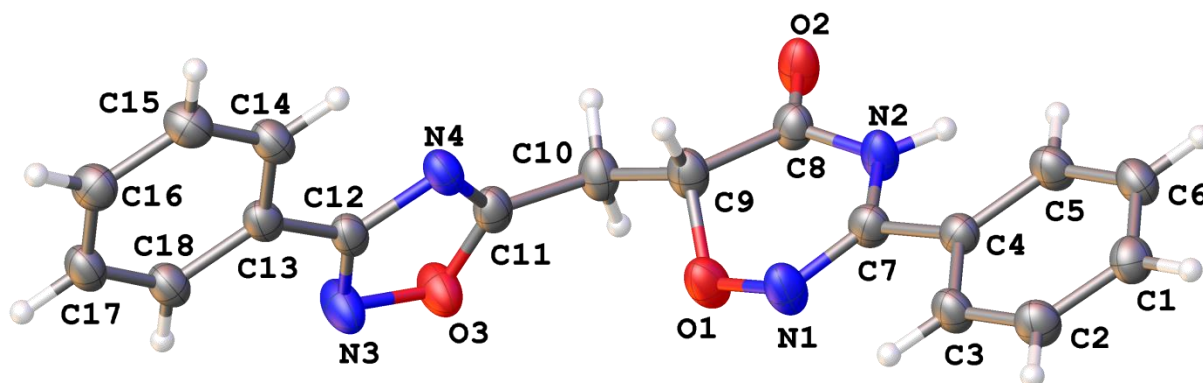
$^1\text{H}$  and  $^{13}\text{C}$  spectra of 3-(pyridin-2-yl)-6-((3-(pyridin-2-yl)-1,2,4-oxadiazol-5-yl)methyl)-4*H*-1,2,4-oxadiazin-5(6*H*)-one **51**



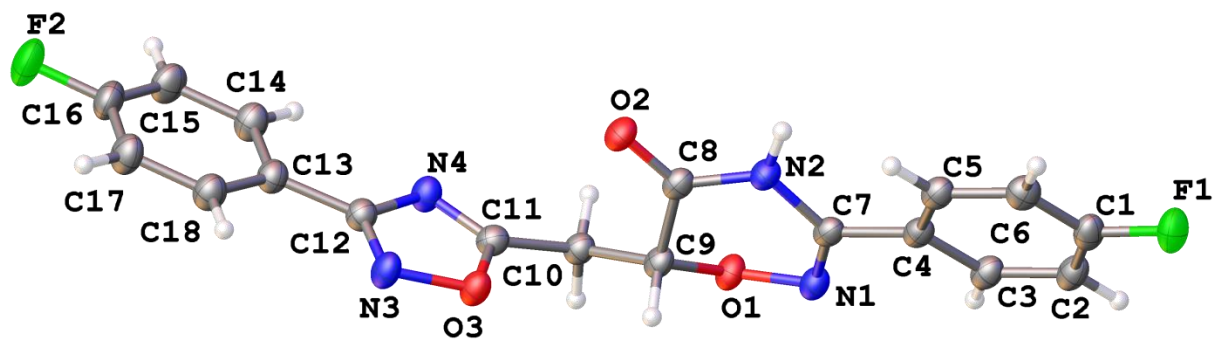
## 2. X-ray diffraction data



**Figure S1.** View of the molecular structure of **4d**. Thermal ellipsoids are drawn at the 50% probability level.



**Figure S2.** View of the molecular structure of **5b**. Thermal ellipsoids are drawn at the 50% probability level.



**Figure S3.** View of the molecular structure of **5f**. Thermal ellipsoids are drawn at the 50% probability level.

**Table S1.** Crystal data and structure refinement parameters for **4d**, **5b**, and **5f**.

Compound	<b>4d</b>	<b>5b</b>	<b>5f</b>
Identification code	SAV5	OZI-09	CJL-151
CCDC number	2210873	2210875	2210876
Empirical formula	C <sub>24</sub> H <sub>22</sub> N <sub>6</sub> O <sub>12</sub>	C <sub>18</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub>	C <sub>18</sub> H <sub>12</sub> F <sub>2</sub> N <sub>4</sub> O <sub>3</sub>
Formula weight	586.47	334.33	370.32
Temperature, K	100(2)	100(2)	100(2)
Crystal system	monoclinic	triclinic	triclinic
Space group	C2/c	P-1	P-1
a, Å	21.0394(11)	5.6292(2)	6.2398(2)
b, Å	6.8178(3)	9.9963(3)	7.9297(3)
c, Å	18.9521(10)	14.3394(4)	16.7543(4)
$\alpha$ , °	90	97.054(2)	78.848(2)
$\beta$ , °	98.851(5)	99.633(3)	80.191(2)
$\gamma$ , °	90	103.958(3)	89.581(3)
Volume, Å <sup>3</sup>	2686.2(2)	760.72(4)	801.17(4)
Z	4	2	2
$\rho_{\text{calc}}$ , g, cm <sup>3</sup>	1.450	1.460	1.535
$\mu$ , mm <sup>-1</sup>	0.119	0.850	1.055
F(000)	1216.0	348.0	380.0
Crystal size, mm <sup>3</sup>	0.16 × 0.14 × 0.13	0.18 × 0.16 × 0.13	0.15 × 0.14 × 0.12
Radiation	MoK $\alpha$ ( $\lambda$ = 0.71073)	CuK $\alpha$ ( $\lambda$ = 1.54184)	CuK $\alpha$ ( $\lambda$ = 1.54184)
2 $\Theta$ range for data collection, °	6.288 to 54.998	6.344 to 154.134	5.458 to 140.882
Index ranges	−27 ≤ h ≤ 27 −8 ≤ k ≤ 8, −24 ≤ l ≤ 24	−5 ≤ h ≤ 6, −12 ≤ k ≤ 12, −18 ≤ l ≤ 17	−7 ≤ h ≤ 7, −9 ≤ k ≤ 9, −20 ≤ l ≤ 20
Reflections collected	20491	21795	12627
Independent reflections	3015 [ $R_{\text{int}}$ = 0.0313, $R_{\text{sigma}}$ = 0.0188]	3132 [ $R_{\text{int}}$ = 0.0436 $R_{\text{sigma}}$ = 0.0236]	3026 [ $R_{\text{int}}$ = 0.0397, $R_{\text{sigma}}$ = 0.0375]
Data/restraints/parameters	3015/0/191	3132/0/226	3026/0/244
Goodness-of-fit on F <sup>2</sup>	1.060	1.077	1.043
Final R indexes [ $I \geq 2\sigma$ (I)]	$R_1$ = 0.0472 $wR_2$ = 0.1232	$R_1$ = 0.0462, $wR_2$ = 0.1303	$R_1$ = 0.0401, $wR_2$ = 0.1085
Final R indexes [all data]	$R_1$ = 0.0529 $wR_2$ = 0.1274	$R_1$ = 0.0505, $wR_2$ = 0.1345	$R_1$ = 0.0445, $wR_2$ = 0.1141
Largest diff. peak/hole/ eÅ <sup>-3</sup>	0.47/−0.24	0.85/−0.31	0.24/−0.24