Supporting Information for

Exploring the energetic potential of 2,5-disubstituted tetrazoles: a case of 2,5-bis(oxadiazolyl)tetrazoles

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S1. Crystallographic data

Table S1. The main refinement details and crystallography data for **4** and **8**.

	4	**8**
Formula	$C_5H_4N_{10}O_2$	$C_{10}H_2N_{18}O_4$
Mass	236.18	438.30
T, K	120	120
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	P-1
Z (Z')	4 (1)	2 (2)
a, Å	6.754(2)	8.9657(4)
b, Å	9.061(3)	12.1892(5)
c, Å	14.743(4)	16.1224(7)
α, °	90	105.340(2)
β, °	98.556(9)	96.598(2)
γ, °	90	99.266(2)
V, $Å^3$	892.2(5)	1653.87(12)
d_{calc}, $g \cdot cm^{-3}$	1.758	1.760
μ, cm^{-1}	1.44	1.45
F(000)	480	880
$2\theta_{max}$, °	56	56
Number of reflections	5172	19245
Independent reflections	2037	7891
Reflections with I>2σ(I)	1253	5402
Number of parameters	170	594
R1	0.0504	0.0416
wR2	0.1617	0.1014
GOF	0.793	1.025
Residual electron density, $e \cdot Å^{-3}$ (d_{min}/d_{max})	0.234/-0.295	0.744/-0.285

S2. Computational details

A general formula used for the calculation of the enthalpies of formation was as follows:

$$\Delta_f H^0_{(g)} = \Sigma H_{atom} - \Sigma \Delta_{thermal} H_{atom} - \Sigma D_0$$

$$\Sigma D_0 = \Sigma CBS\text{-}4M(H_{atom}) - CBS\text{-}4M(H_{molecule})$$

Corrections on values of enthalpies of sublimation and enthalpies of vaporization were calculated according to empirical formulae:

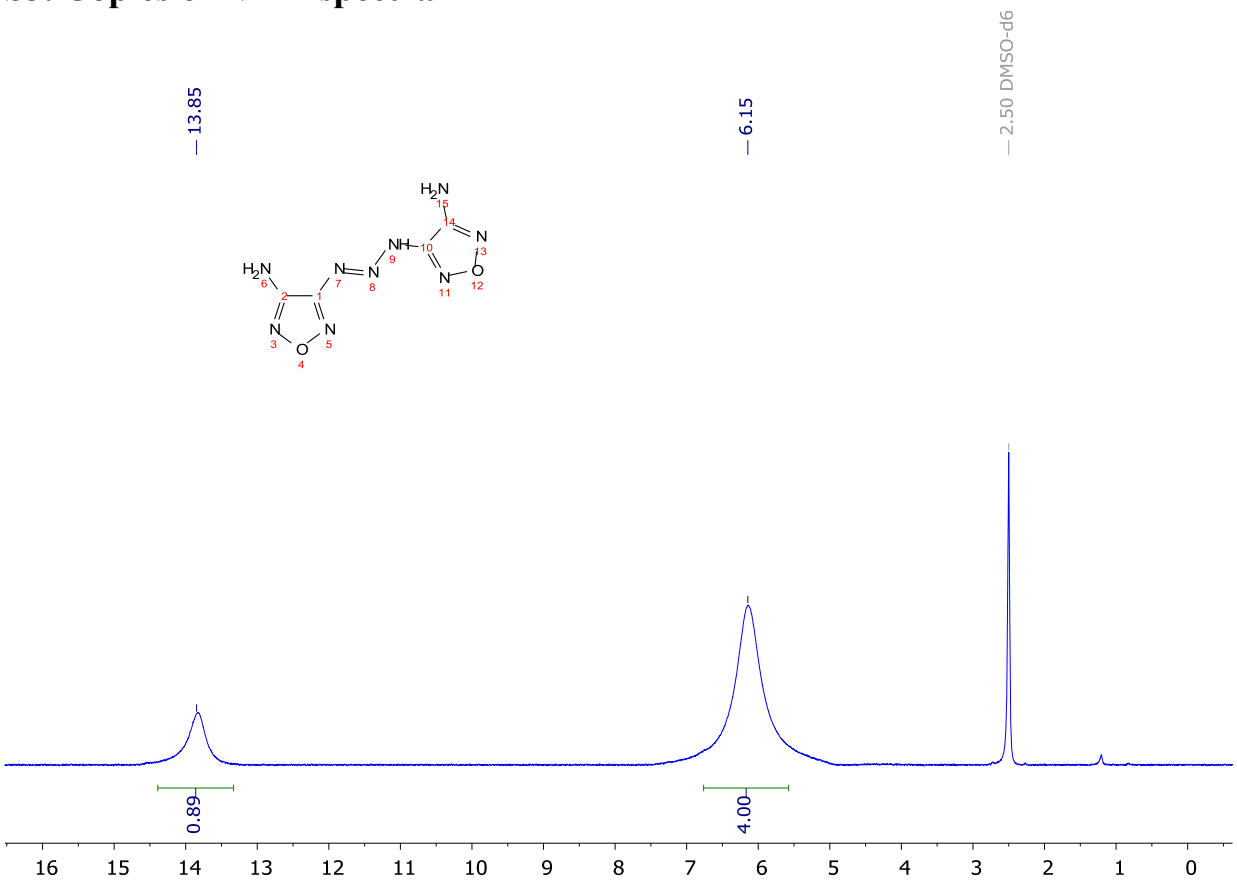
$$\Delta_f H^0_{(subl)} = 0.04476 \cdot T_m$$

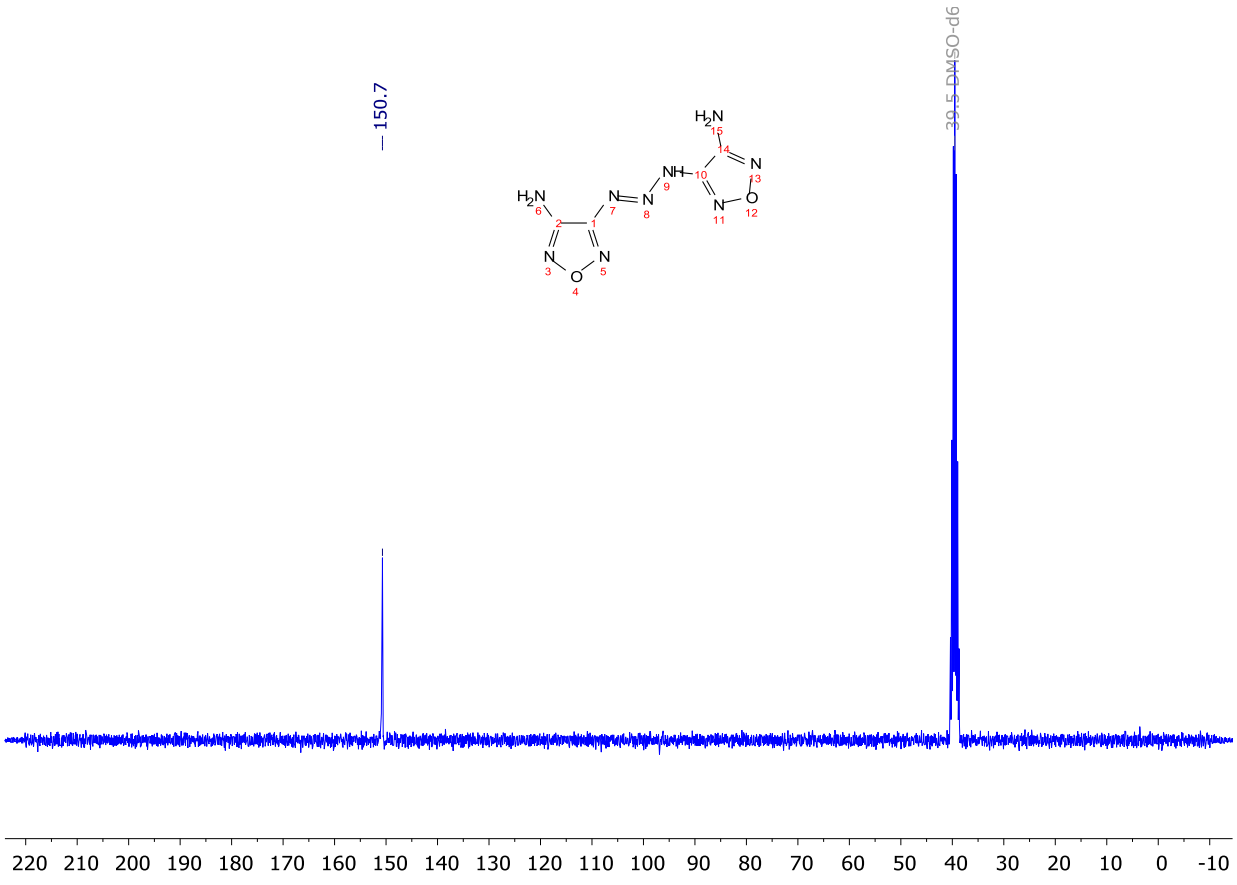
$$\Delta_f H^0_{(vap)} = 0.02095 \cdot T_{vap}$$

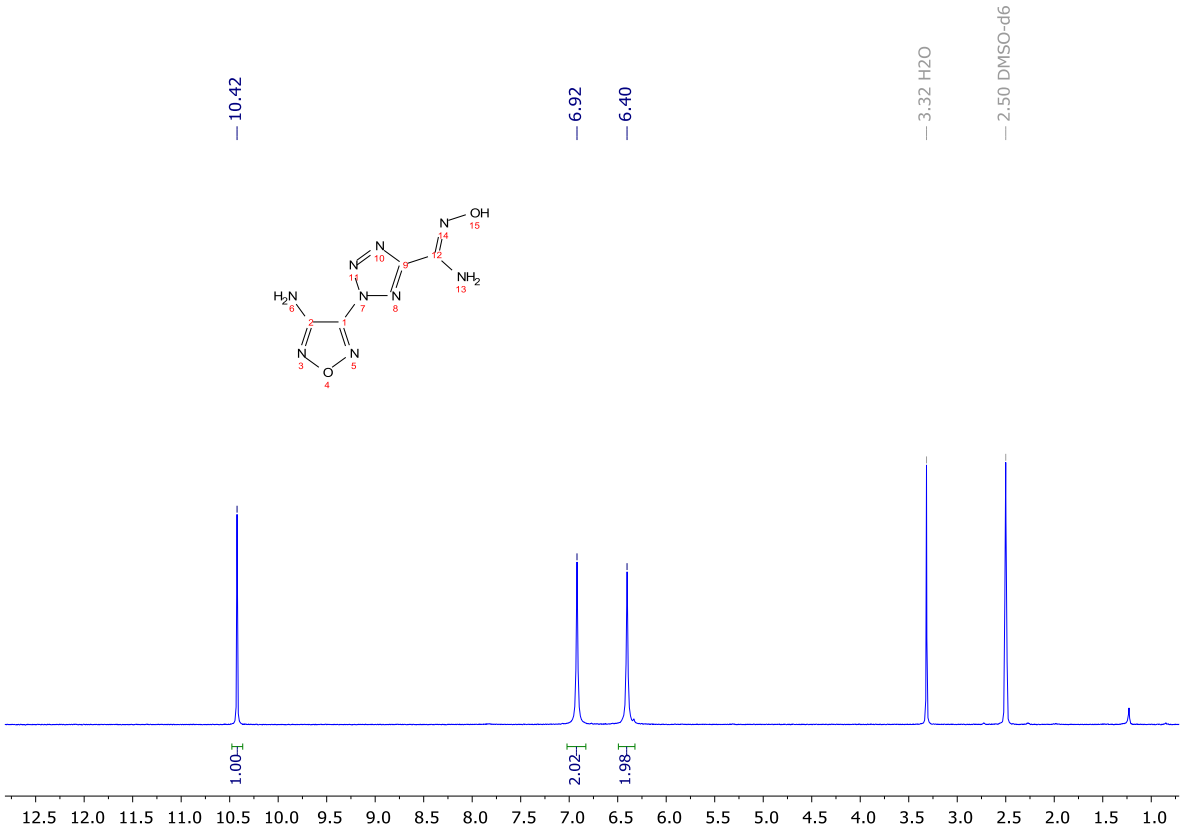
Table S2. Atomic contributions to the enthalpies of formation.

	multiplicity	$\Delta_f H^0$ (0K), kcal mol^{-1}	Thermal ΔΔH, kcal mol^{-1}	CBS-4M, hartree
H	2	51.63	1.01	-0.500991
C	3	169.98	0.25	-37.786156
N	4	112.53	1.04	-54.522462
O	3	58.99	1.04	-74.991202

S3. Copies of NMR spectra



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6.40
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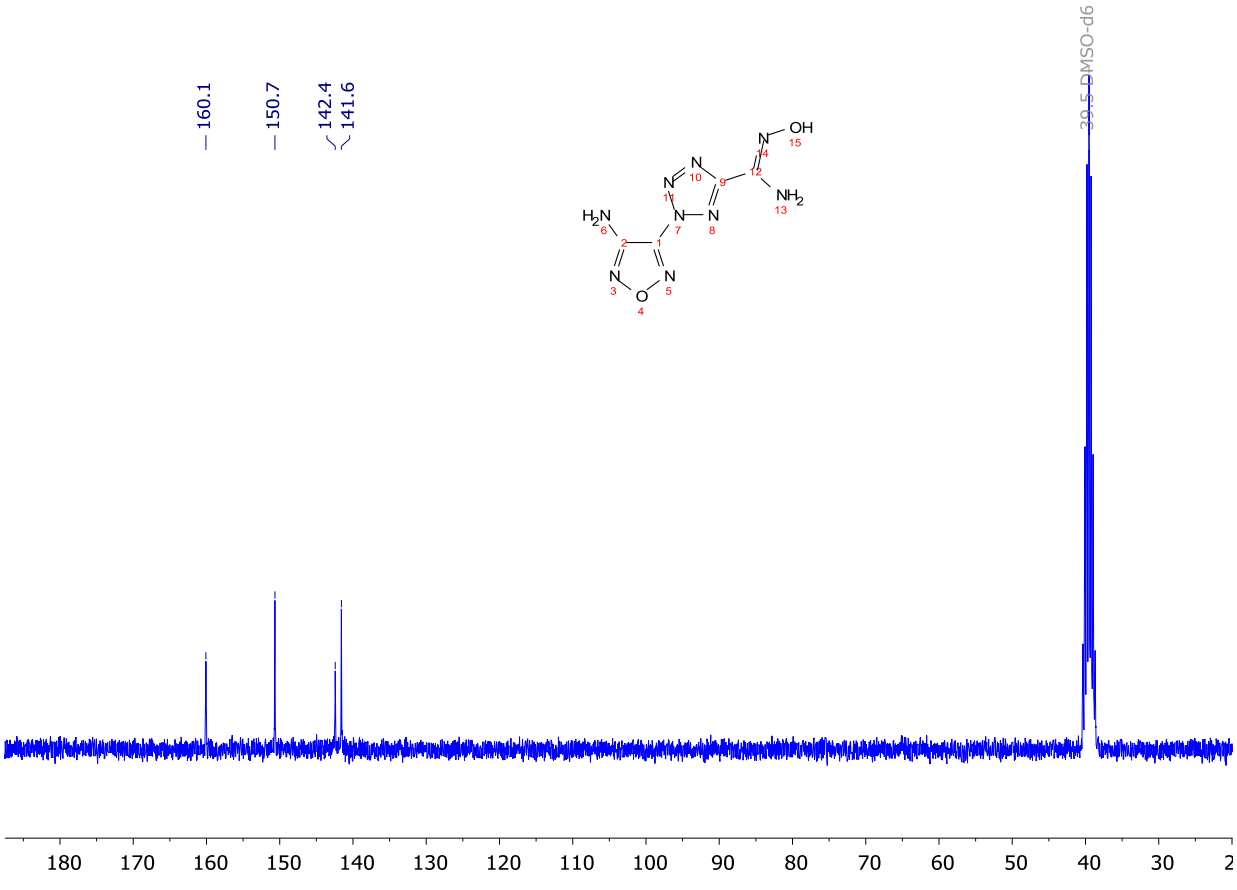
2.50 DMSO-d6
1.00
2.02
1.98
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0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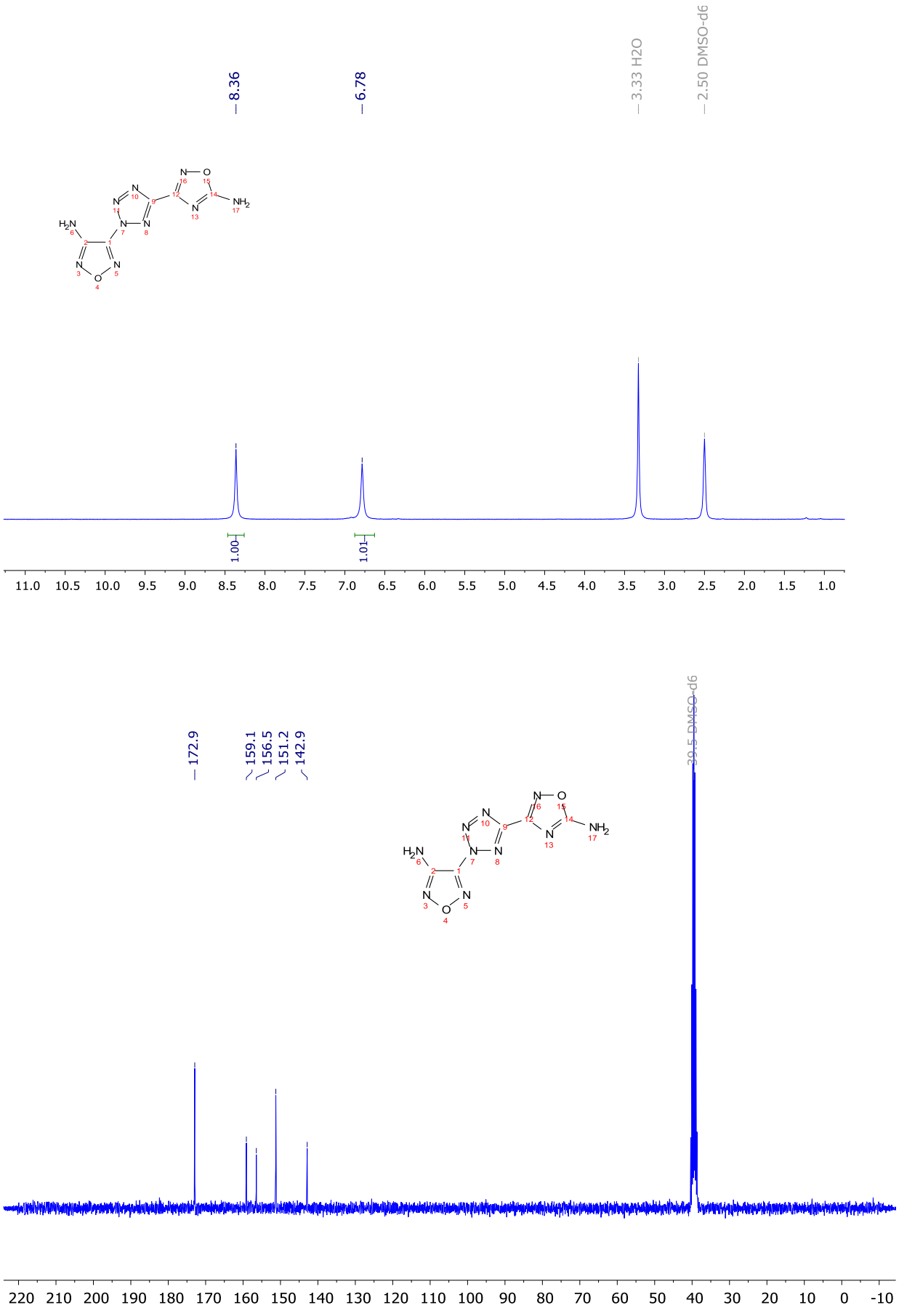
150.7
142.4
141.6
39.5 DMSO-d6
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 2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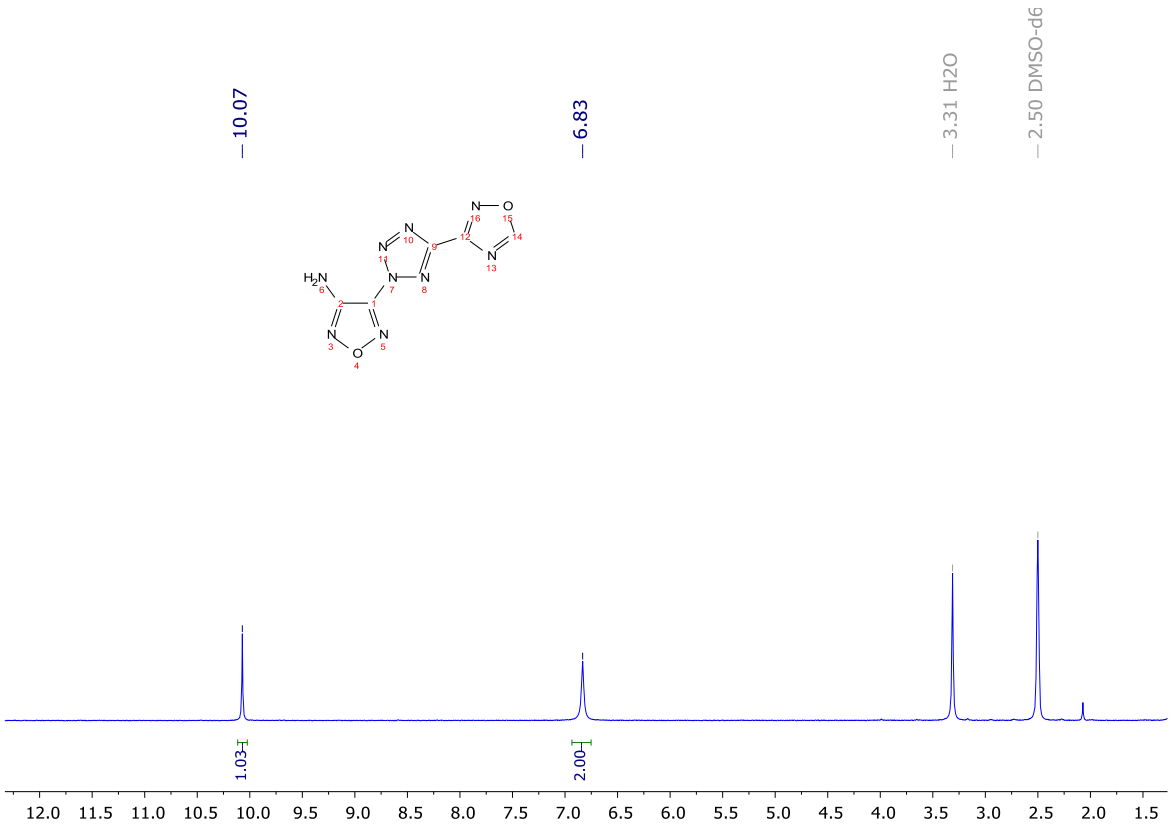
6.78
3.33 H2O
2.50 DMSO-d6
1.00
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
172.9
159.1
156.5
151.2
142.9
39.5 DMSO-d6
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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1.03
2.00
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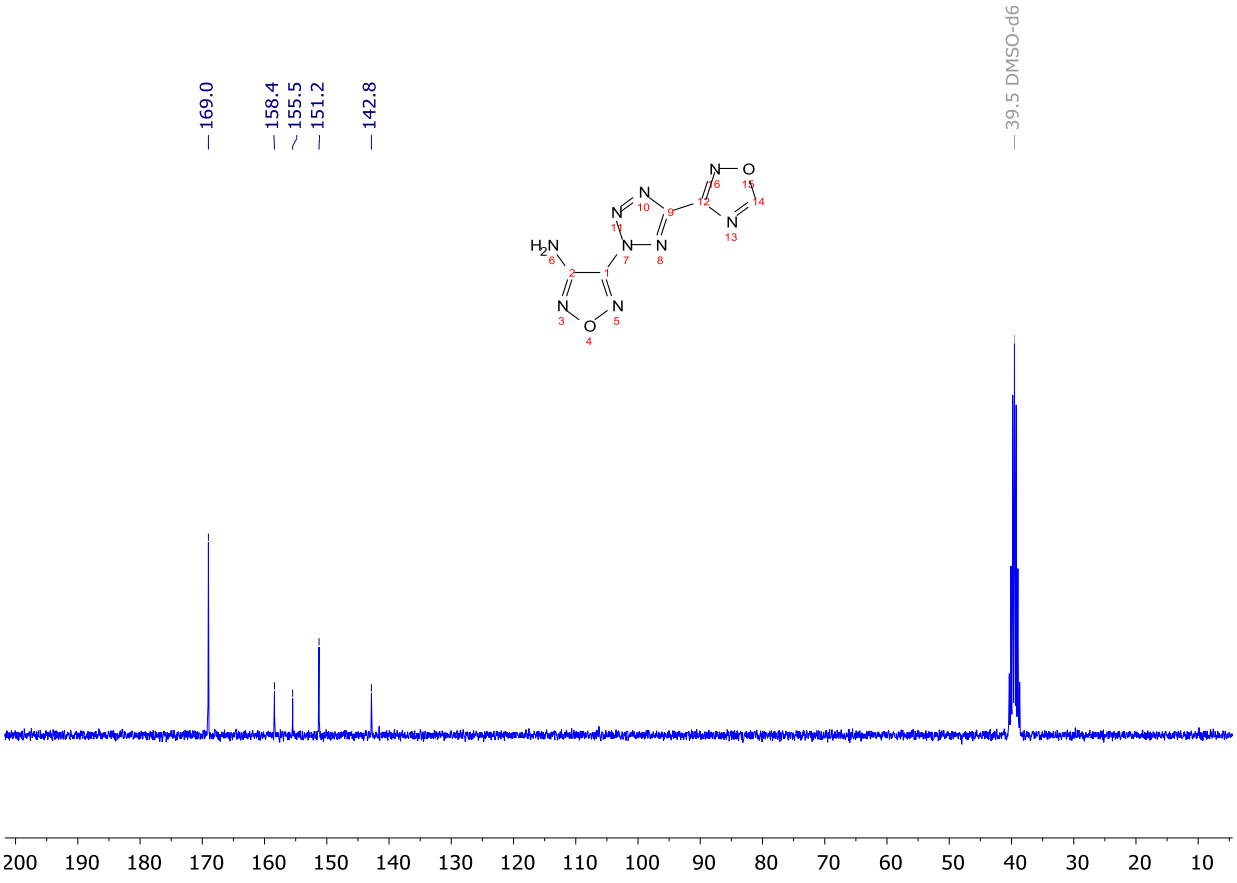
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158.4
155.5
151.2
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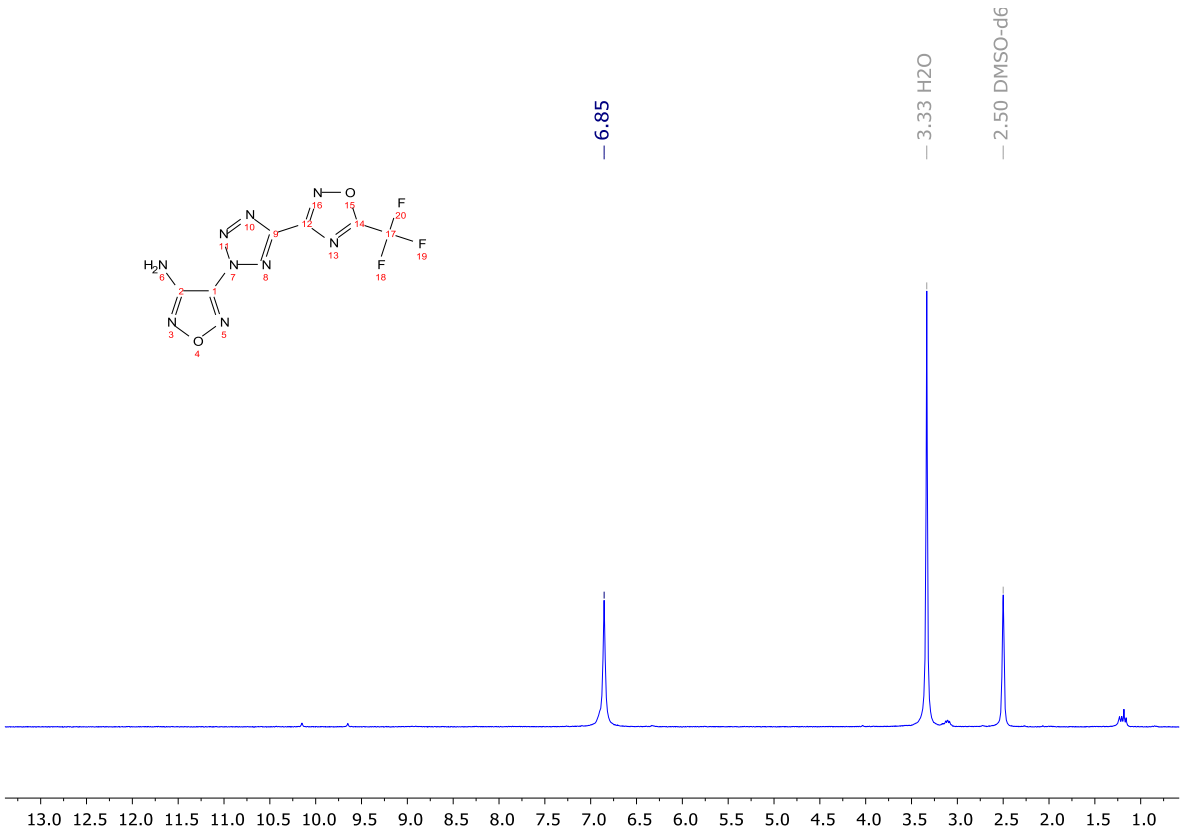
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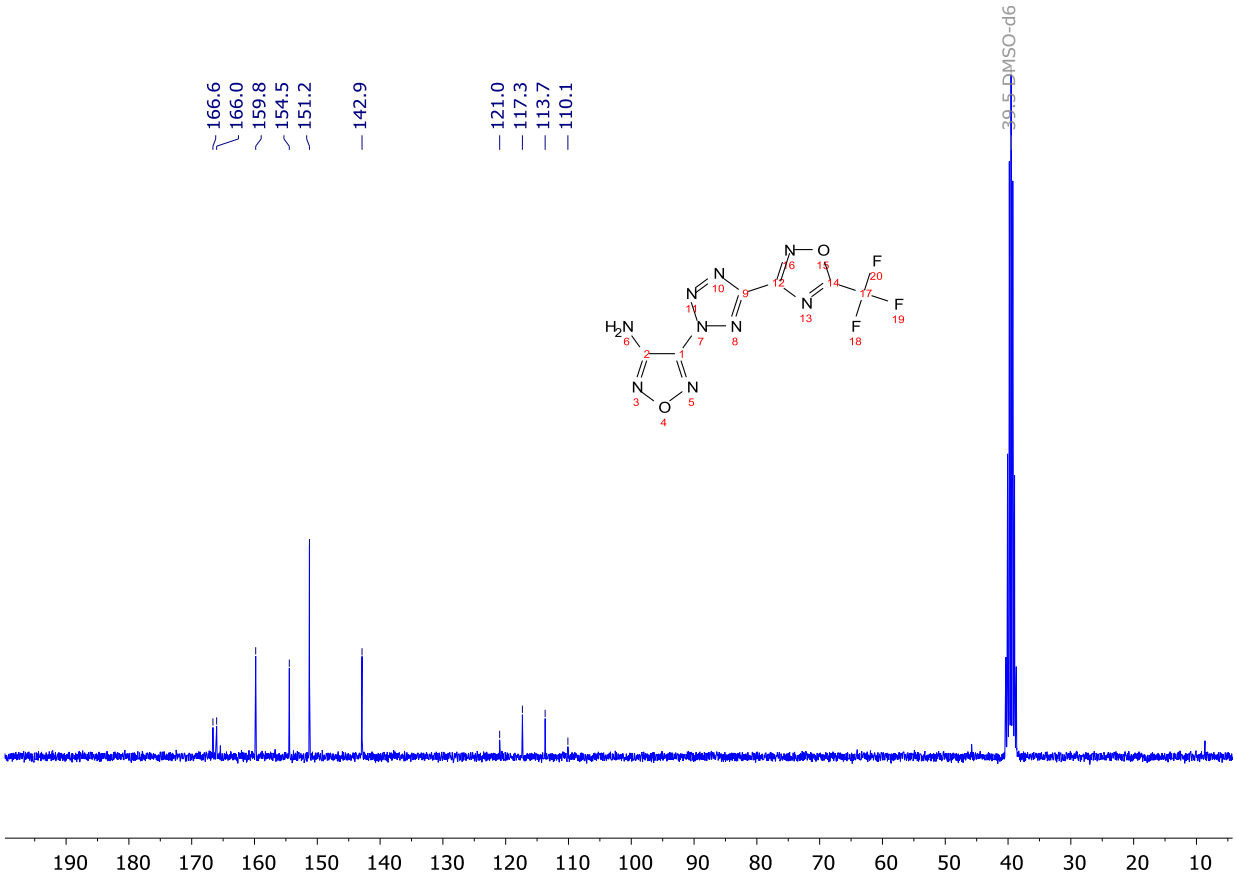
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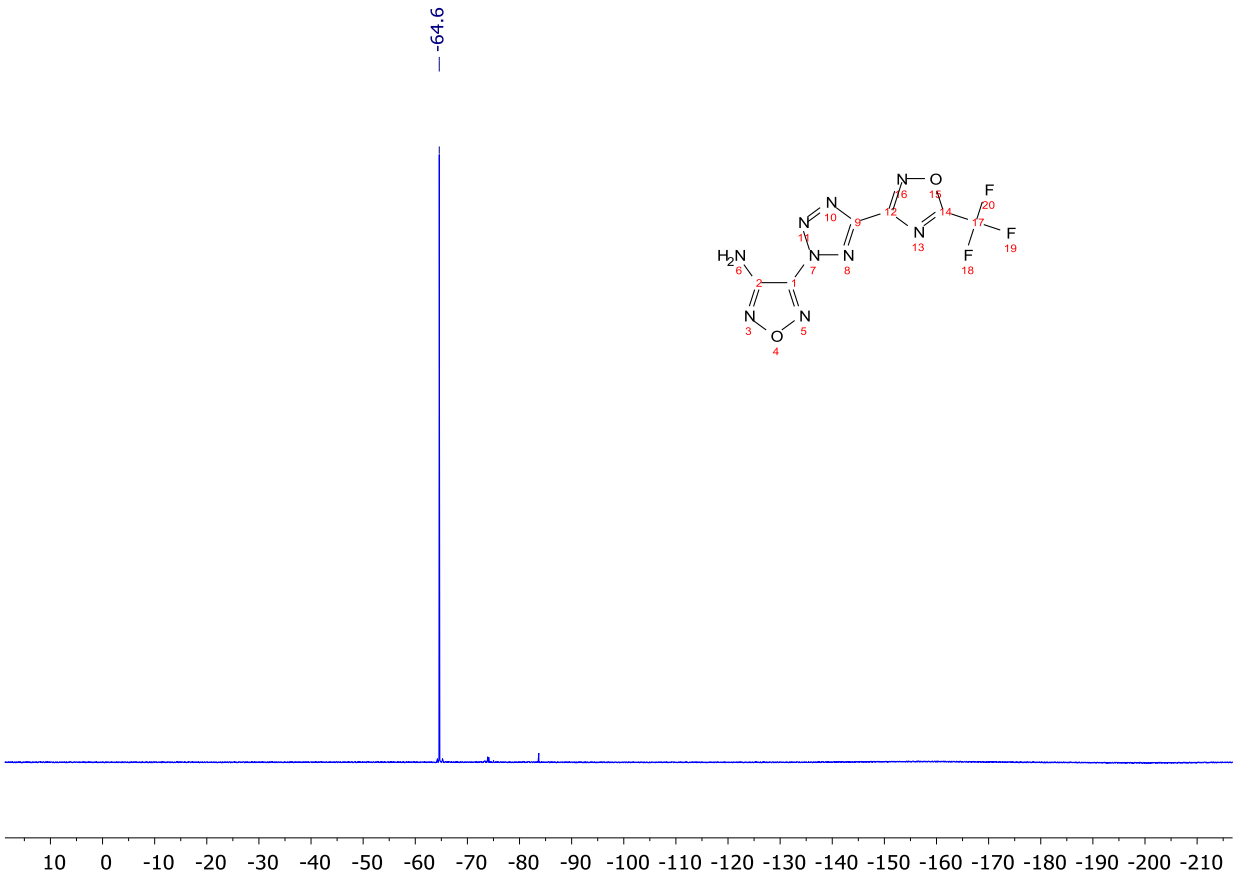
166.0
159.8
154.5
151.2
142.9
121.0
117.3
113.7
110.1
39.5 DMSO-d6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10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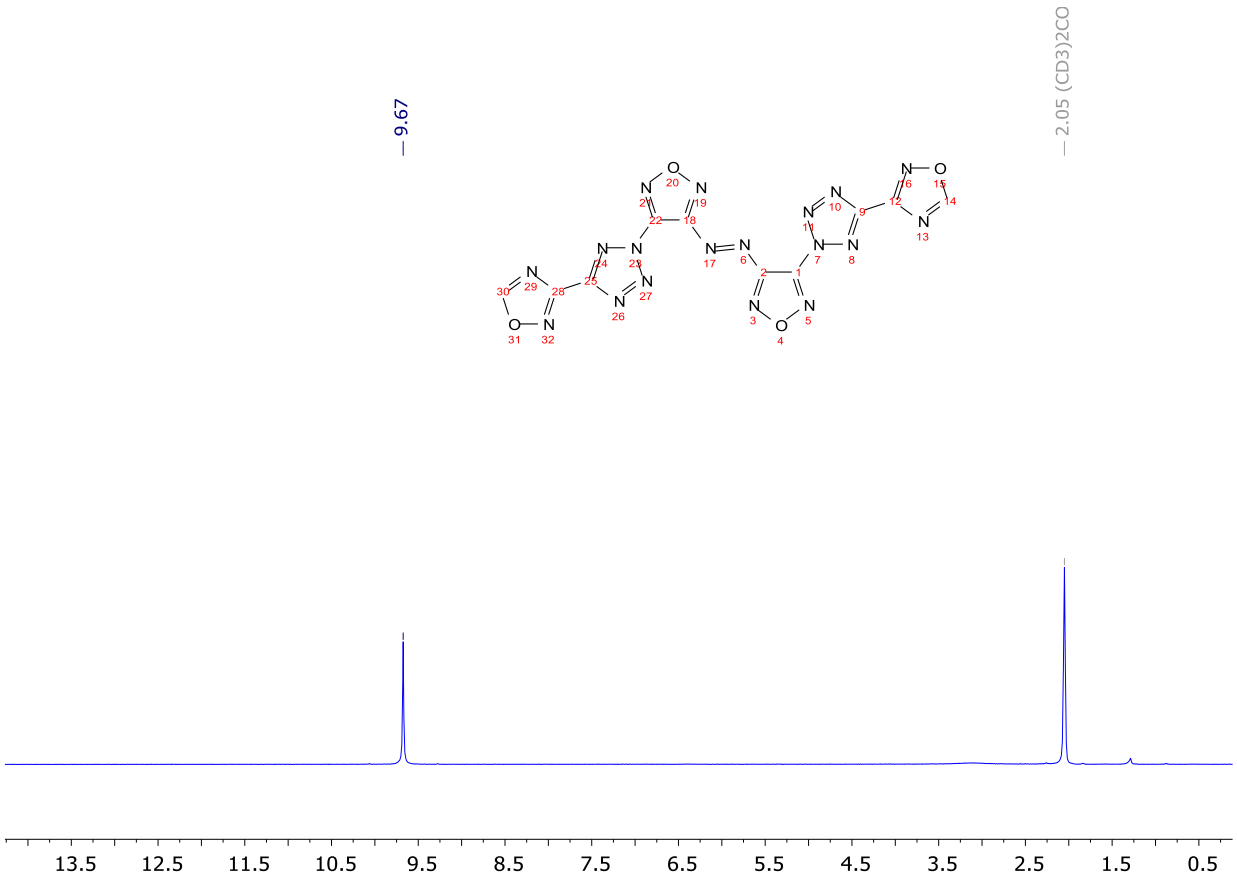
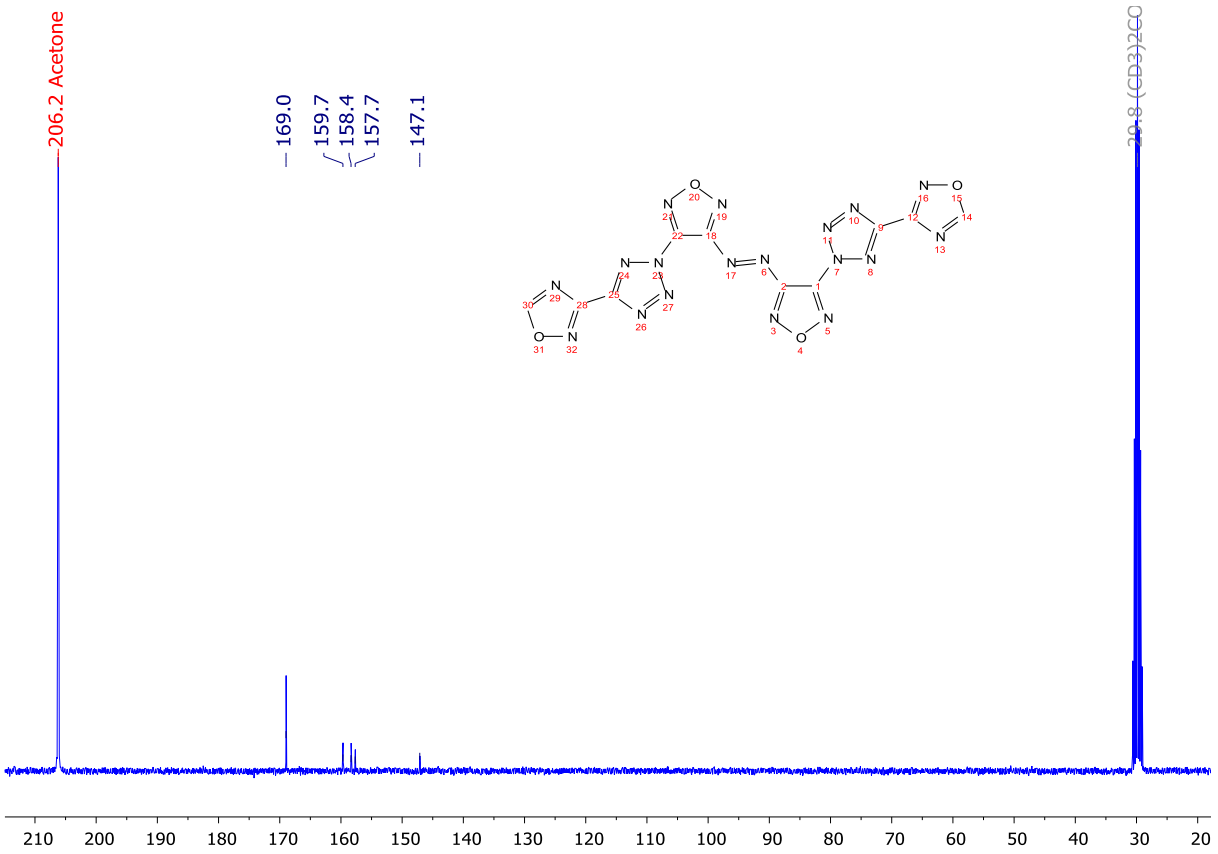
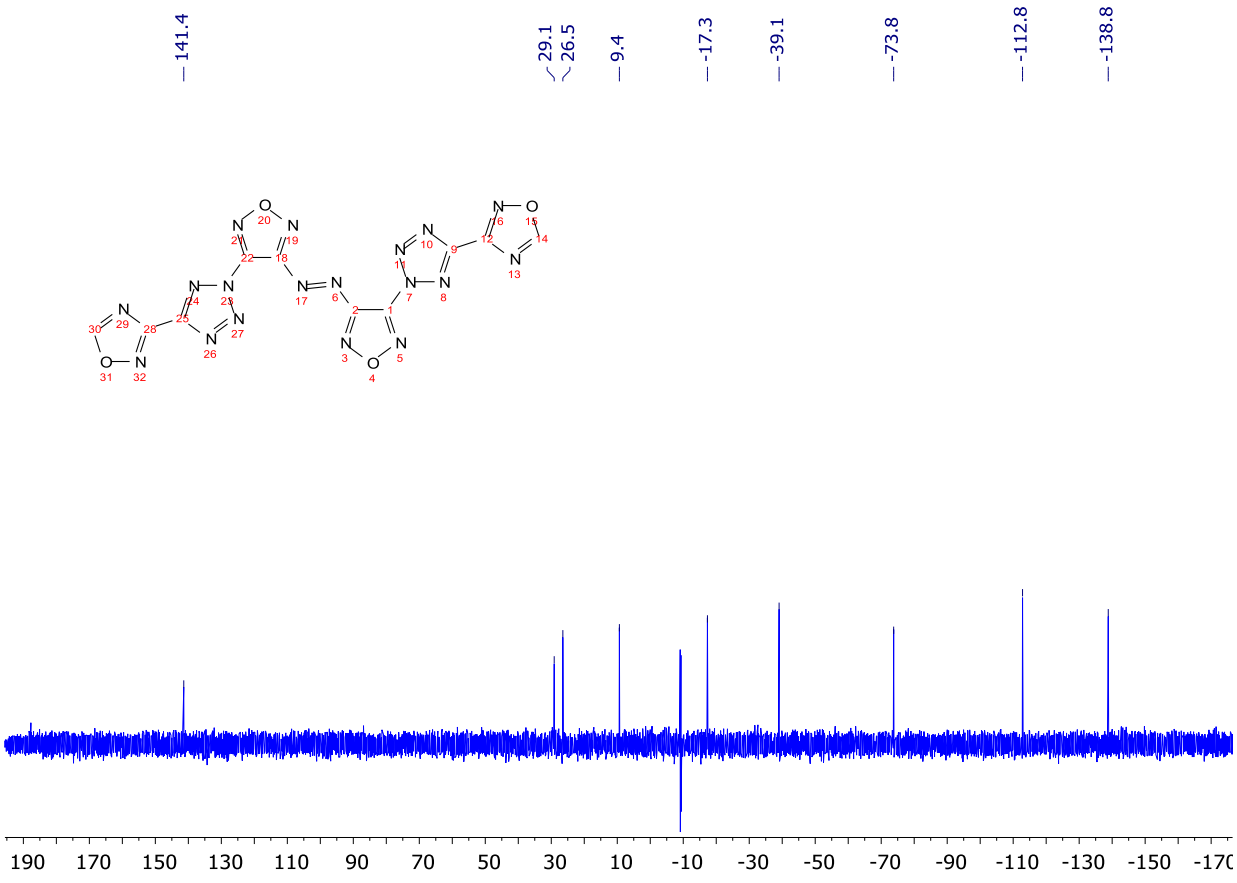
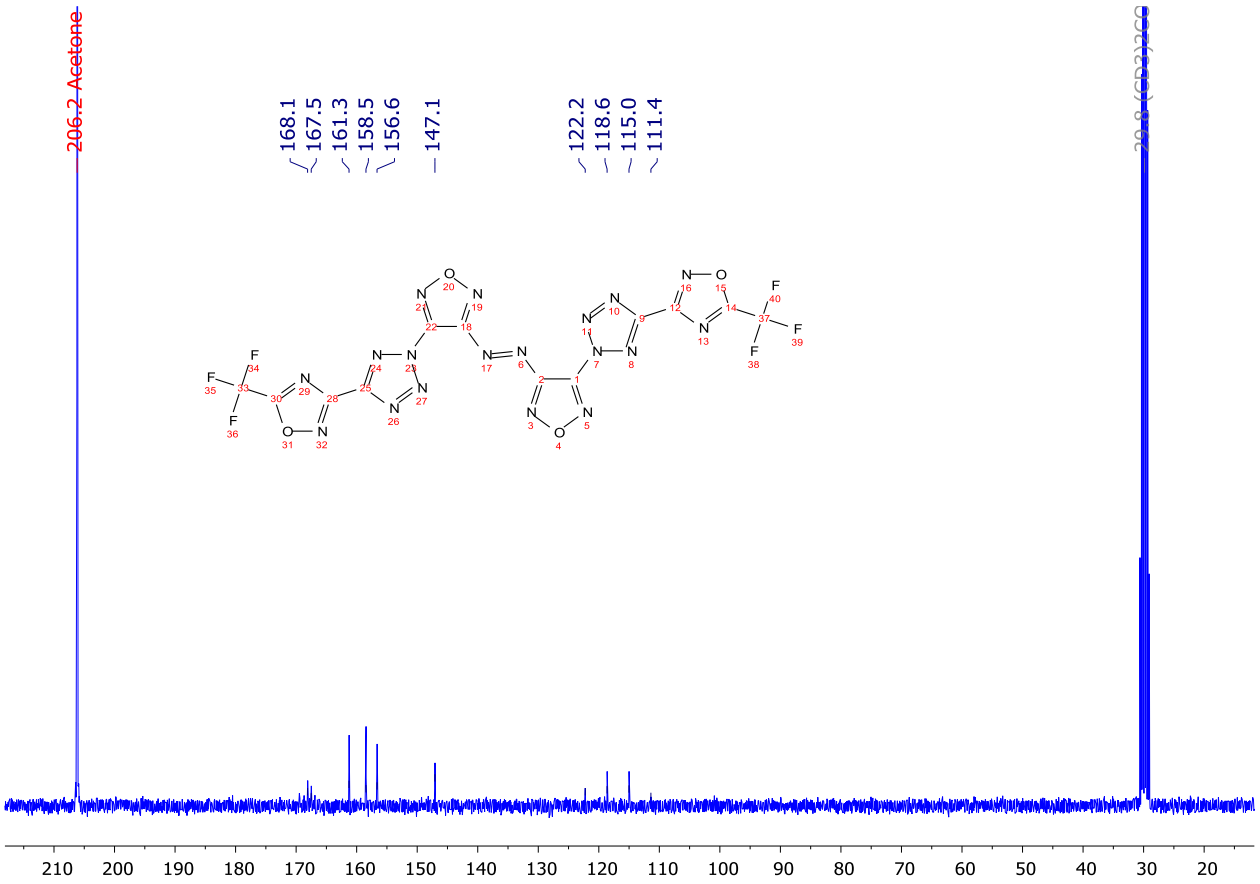
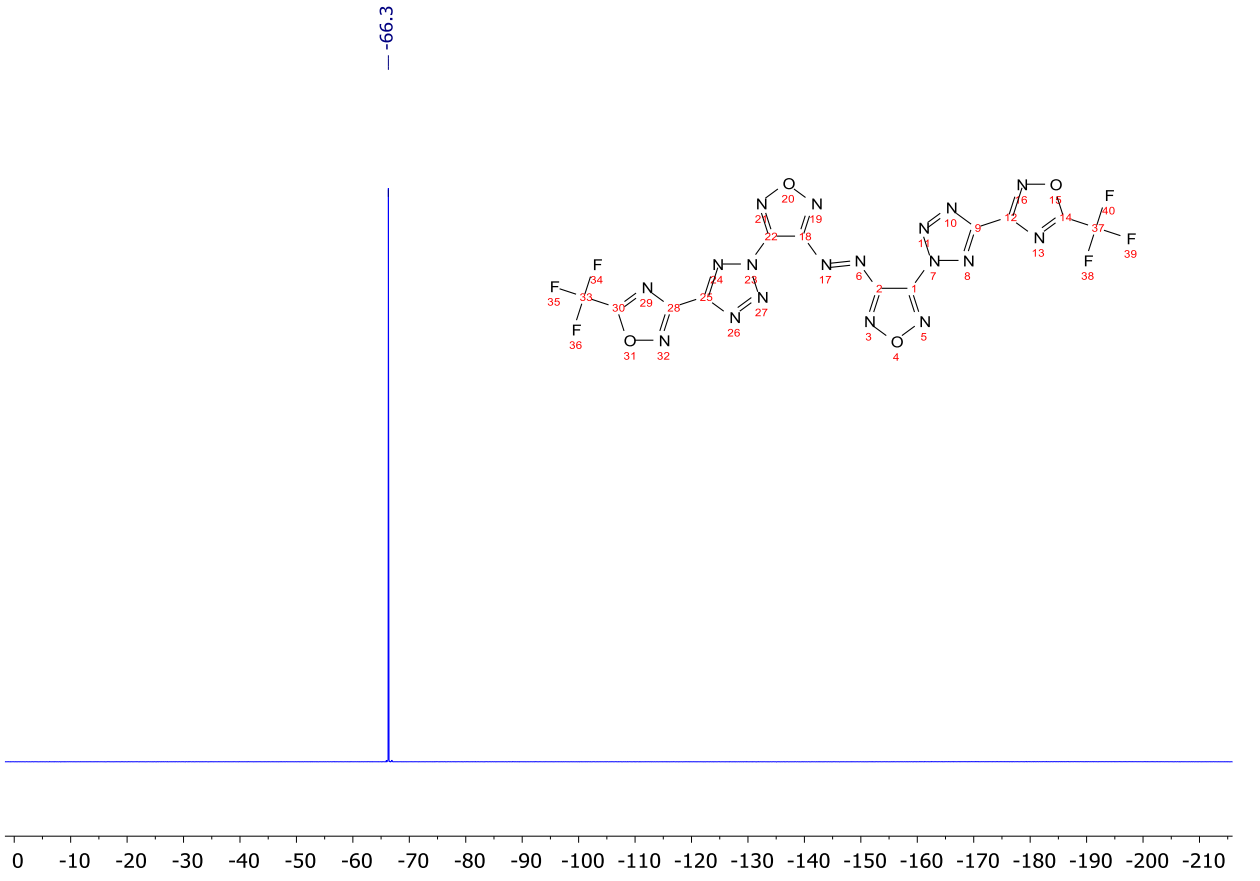

9.67
2.05 (CD3)2CO
13.5 12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5





Instrument artefact at -9.4 ppm


206.2 Acetone
168.1
167.5
161.3
158.5
156.6
147.1
122.2
118.6
115.0
111.4
30.8 (CD3)2CO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20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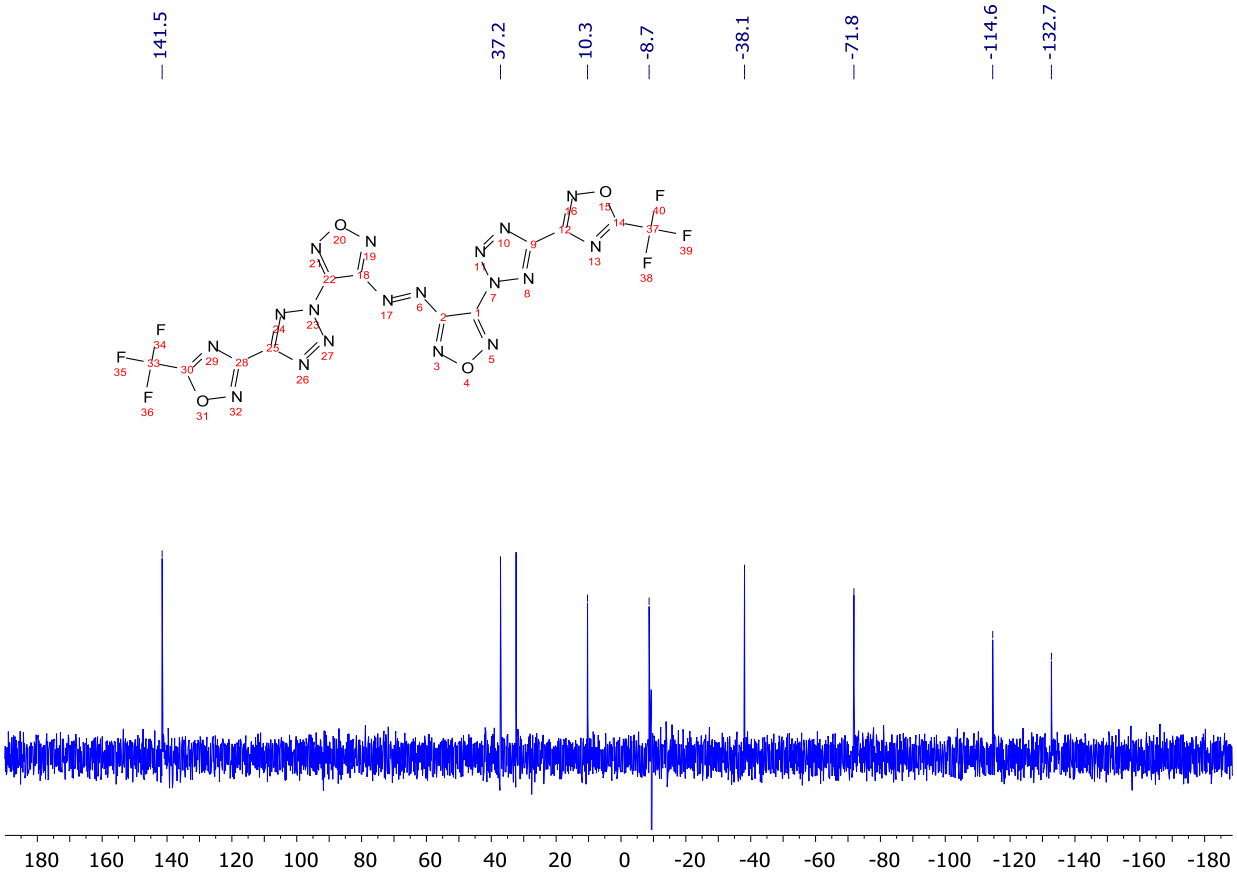
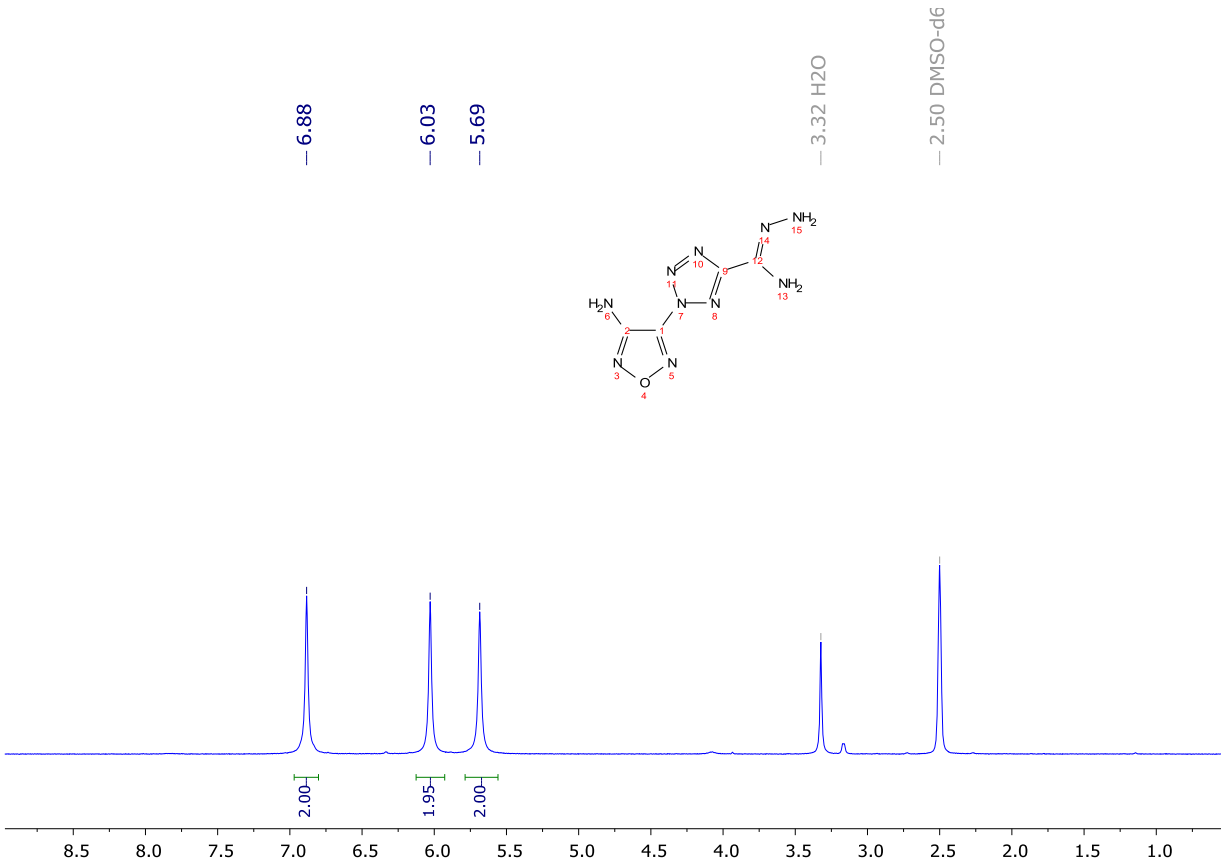
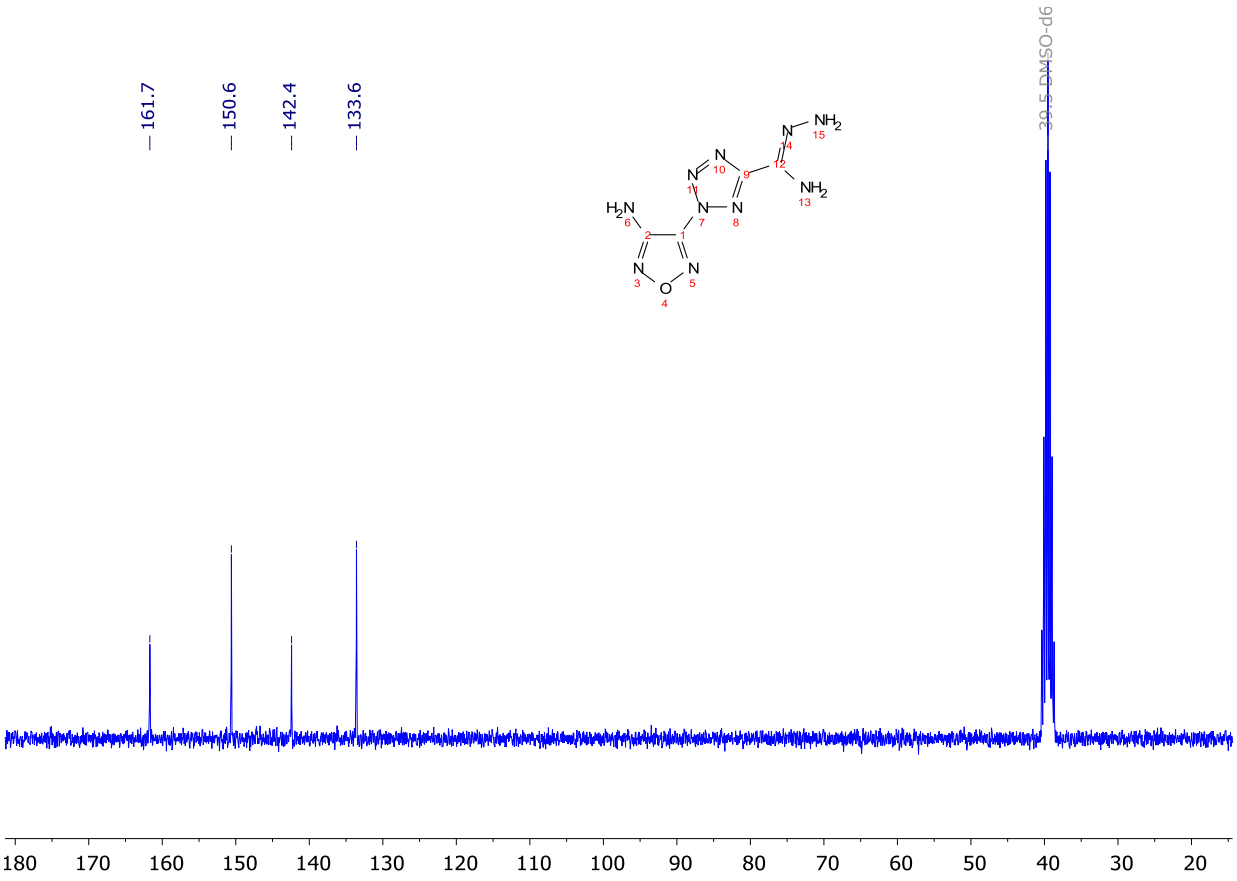


Instrument artefact at -9.4 ppm


6.88
6.03
5.69
3.32 H2O
2.50 DMSO-d6
2.00
1.95
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0


161.7
150.6
142.4
133.6
39.5 DMSO-d6
180
170
160
150
140
130
120
110
100
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80
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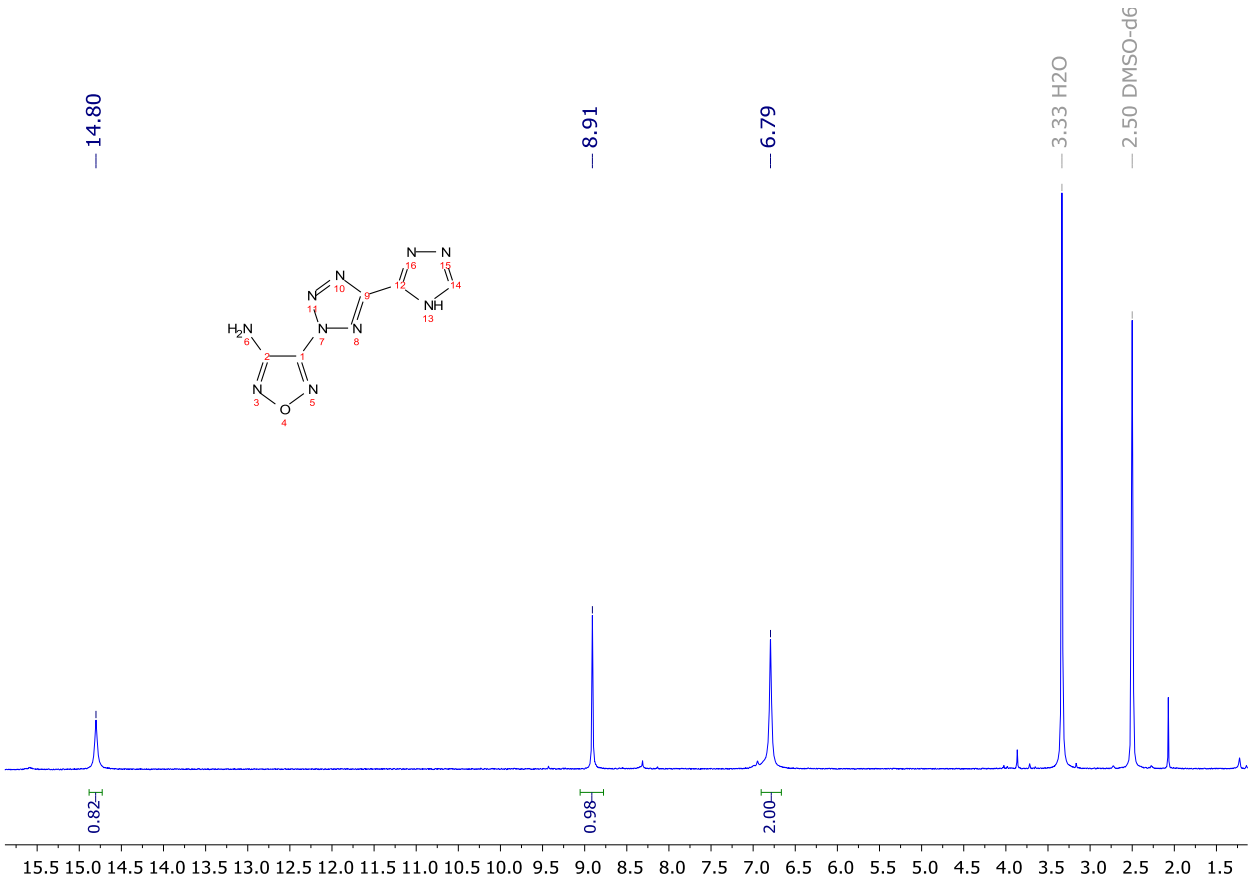
50
40
30
20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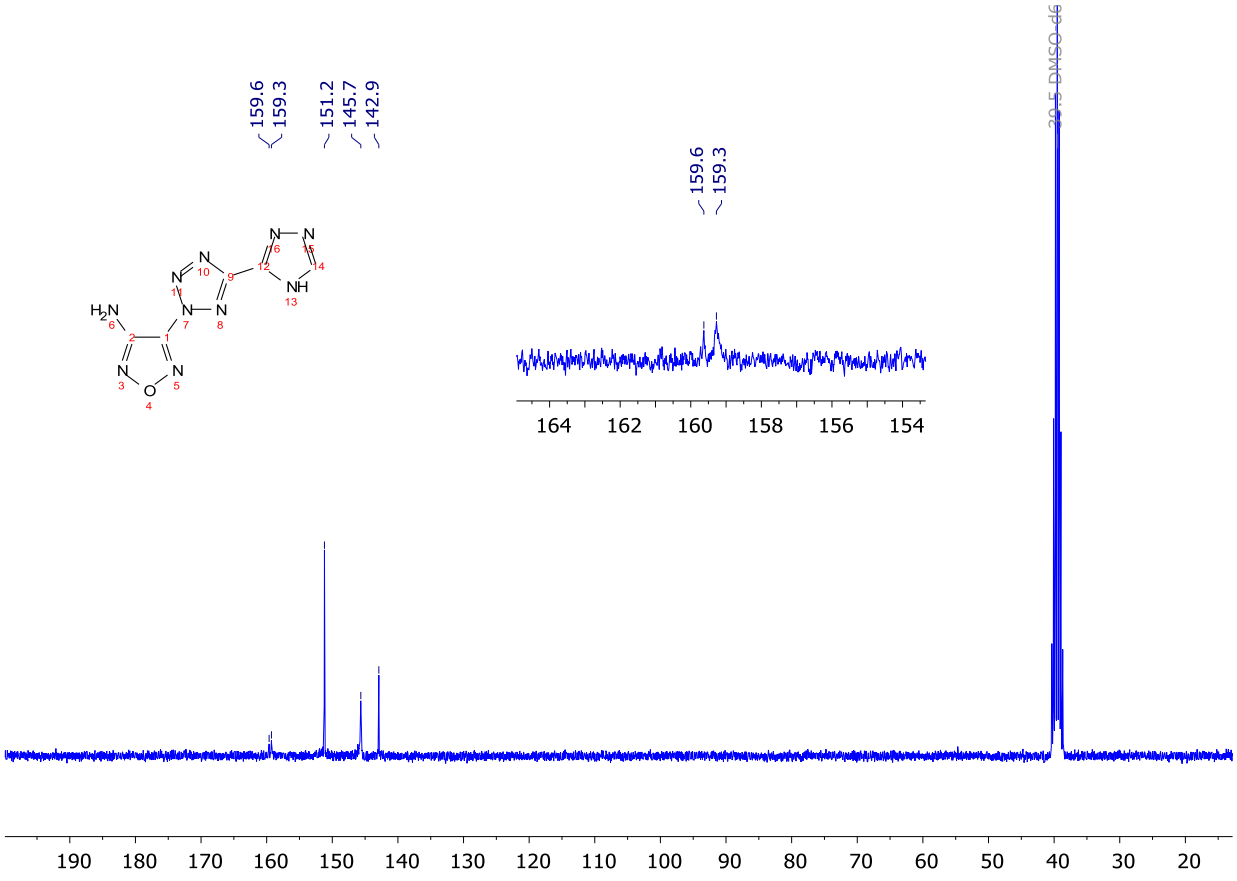
8.91
6.79
3.33 H2O
2.50 DMSO-d6
0.82
0.98
2.00
15.5 15.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5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159.3
151.2
145.7
142.9
39.5 DMSO-d6
159.6
159.3
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190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20