Electronic Supplementary Information for:

Photocatalytic Conversion of CO_2 to CO using Rhenium Bipyridine Platforms Containing Ancillary Phenyl or BODIPY Moieties

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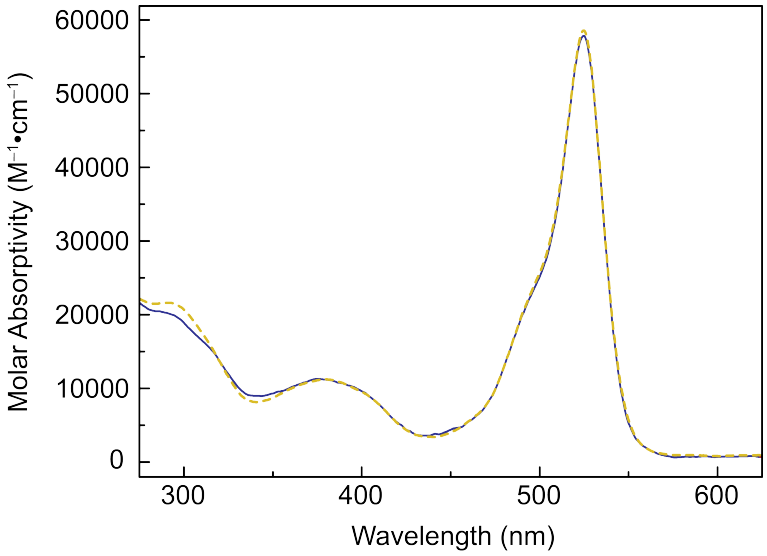


Figure S1. Overlay of the UV-vis absorption profile of complex **12** (blue) with the composite spectrum obtained for complexes **8** and **13** (gold dashed). Absorption data was recorded in DMF.

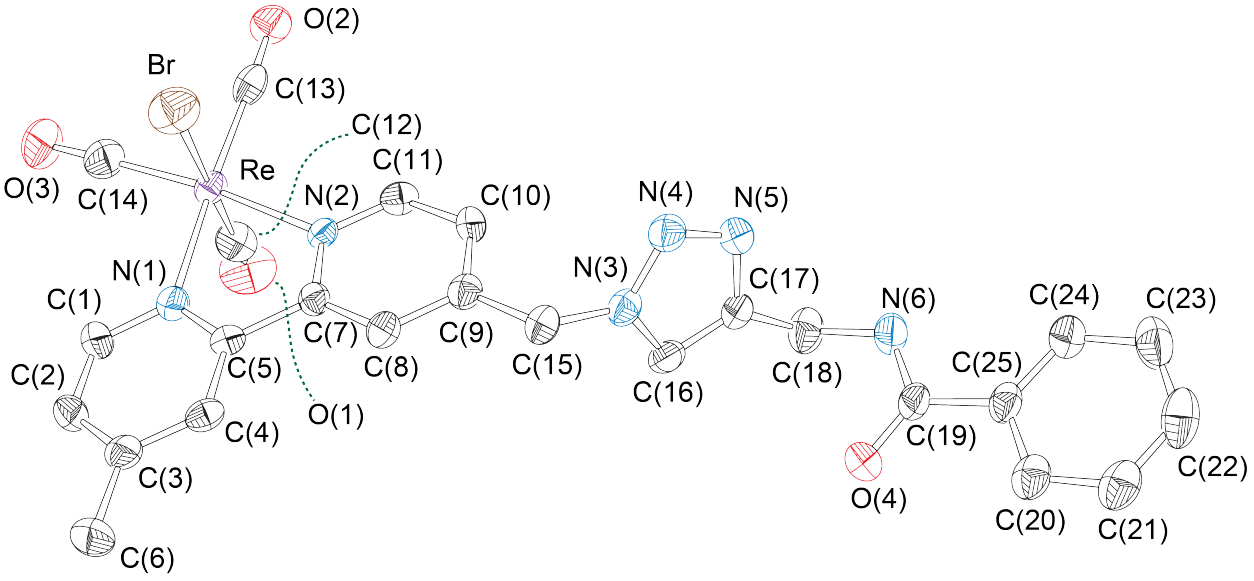


Figure S2. Fully labeled thermal ellipsoid plot for the bromide homologue of complex **8**. Ellipsoids are shown at the 50% probability level. Hydrogen atoms are removed for clarity.

Table S1. Crystallographic Data for the Bromide Homologue of Complex **8**.

Formula	$C_{25}H_{20}BrN_6O_4Re$
F_w	734.58
Crystal System	Monoclinic
Space Group	P 2_1/n
a	11.6786(9) Å
b	19.4125(16) Å
c	11.7398(9) Å
α	90°
β	104.9320(10)°
γ	90°
V	2571.7(4) Å^3
Z	4
Temp	200(2) K
D_{calcd}	1.897 g/cm^3
2θ range	55.18°
μ (Mo Kα)	6.322 mm^{-1}
Relections	33556
Unique	5946
R(int)	0.0587
R_1	0.0495
wR_2	0.1488

Table S2. Bond lengths (Å) for the Bromide Homologue of complex **8**.

Atom1	Atom2	Length (Å)
Re	C(14)	1.926(10)
Re	C(12)	1.933(10)
Re	C(13)	1.930(10)
Re	N(1)	2.171(7)
Re	N(2)	2.178(6)
Re	Br	2.5927(12)
N(1)	C(1)	1.339(10)
N(1)	C(5)	1.348(10)
N(2)	C(11)	1.345(10)
N(2)	C(7)	1.352(9)
N(3)	N(4)	1.322(10)
N(3)	C(16)	1.357(10)
N(3)	C(15)	1.447(10)
N(4)	N(5)	1.319(10)
N(5)	C(17)	1.341(11)
N(6)	C(19)	1.346(12)
N(6)	C(18)	1.472(11)
N(6)	H(6)	0.88(11)
O(1)	C(12)	1.103(12)
O(2)	C(13)	1.144(11)
O(3)	C(14)	1.143(12)
O(4)	C(19)	1.228(10)
C(1)	C(2)	1.364(12)
C(1)	H(1)	0.95
C(2)	C(3)	1.379(12)
C(2)	H(2)	0.95
C(3)	C(4)	1.374(12)
C(3)	C(6)	1.525(12)
C(4)	C(5)	1.394(10)
C(4)	H(4)	0.95
C(5)	C(7)	1.486(10)
C(6)	H(6A)	0.98
C(6)	H(6B)	0.98
C(6)	H(6C)	0.98
C(7)	C(8)	1.382(10)
C(8)	C(9)	1.398(11)
C(8)	H(8)	0.95
C(9)	C(10)	1.382(11)
C(9)	C(15)	1.509(11)
C(10)	C(11)	1.388(11)

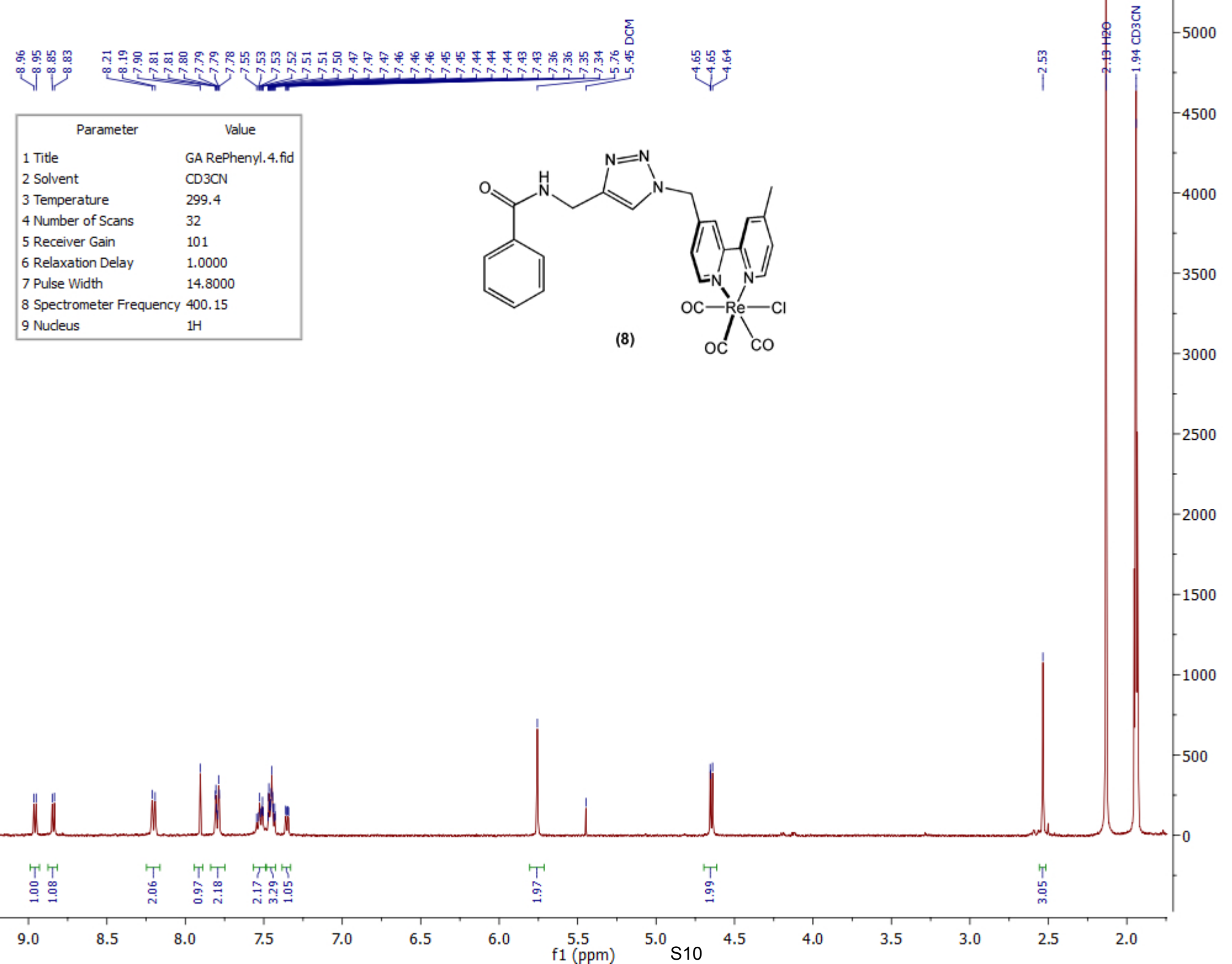
C(10)	H(10)	0.95
C(11)	H(11)	0.95
C(15)	H(15A)	0.99
C(15)	H(15B)	0.99
C(16)	C(17)	1.357(12)
C(16)	H(16)	0.95
C(17)	C(18)	1.498(12)
C(18)	H(18A)	0.99
C(18)	H(18B)	0.99
C(19)	C(25)	1.499(11)
C(20)	C(21)	1.395(13)
C(20)	C(25)	1.392(13)
C(20)	H(20)	0.95
C(21)	C(22)	1.340(15)
C(21)	H(21)	0.95
C(22)	C(23)	1.382(15)
C(22)	H(22)	0.95
C(23)	C(24)	1.395(14)
C(23)	H(23)	0.95
C(24)	C(25)	1.389(13)
C(24)	H(24)	0.95

Table S3. Bond angles (°) for the Bromide Homologue of complex **8**.

Atom1	Atom2	Atom3	Angle (°)
C(14)	Re	C(12)	89.4(4)
C(14)	Re	C(13)	87.5(4)
C(12)	Re	C(13)	90.7(4)
C(14)	Re	N(1)	97.4(3)
C(12)	Re	N(1)	94.2(3)
C(13)	Re	N(1)	173.2(3)
C(14)	Re	N(2)	170.5(3)
C(12)	Re	N(2)	94.8(3)
C(13)	Re	N(2)	100.9(3)
N(1)	Re	N(2)	73.9(2)
C(14)	Re	Br	91.2(3)
C(12)	Re	Br	179.2(3)
C(13)	Re	Br	89.9(2)
N(1)	Re	Br	85.23(19)
N(2)	Re	Br	84.54(16)
C(1)	N(1)	C(5)	118.5(7)
C(1)	N(1)	Re	123.5(6)
C(5)	N(1)	Re	118.0(5)
C(11)	N(2)	C(7)	118.6(6)
C(11)	N(2)	Re	123.9(5)
C(7)	N(2)	Re	117.4(5)
N(4)	N(3)	C(16)	110.0(7)
N(4)	N(3)	C(15)	120.7(7)
C(16)	N(3)	C(15)	129.3(7)
N(5)	N(4)	N(3)	107.7(7)
N(4)	N(5)	C(17)	108.9(7)
C(19)	N(6)	C(18)	119.7(8)
C(19)	N(6)	H(6)	119(7)
C(18)	N(6)	H(6)	121(7)
N(1)	C(1)	C(2)	122.4(8)
N(1)	C(1)	H(1)	118.8
C(2)	C(1)	H(1)	118.8
C(1)	C(2)	C(3)	120.0(8)
C(1)	C(2)	H(2)	120
C(3)	C(2)	H(2)	120
C(4)	C(3)	C(2)	118.3(7)
C(4)	C(3)	C(6)	121.6(8)
C(2)	C(3)	C(6)	120.1(8)
C(3)	C(4)	C(5)	119.4(7)
C(3)	C(4)	H(4)	120.3

C(5)	C(4)	H(4)	120.3
N(1)	C(5)	C(4)	121.4(7)
N(1)	C(5)	C(7)	114.6(6)
C(4)	C(5)	C(7)	124.0(7)
C(3)	C(6)	H(6A)	109.5
C(3)	C(6)	H(6B)	109.5
H(6A)	C(6)	H(6B)	109.5
C(3)	C(6)	H(6C)	109.5
H(6A)	C(6)	H(6C)	109.5
H(6B)	C(6)	H(6C)	109.5
N(2)	C(7)	C(8)	121.9(7)
N(2)	C(7)	C(5)	114.8(6)
C(8)	C(7)	C(5)	123.3(7)
C(9)	C(8)	C(7)	119.4(7)
C(9)	C(8)	H(8)	120.3
C(7)	C(8)	H(8)	120.3
C(10)	C(9)	C(8)	118.5(7)
C(10)	C(9)	C(15)	123.0(7)
C(8)	C(9)	C(15)	118.4(7)
C(9)	C(10)	C(11)	119.2(7)
C(9)	C(10)	H(10)	120.4
C(11)	C(10)	H(10)	120.4
N(2)	C(11)	C(10)	122.4(7)
N(2)	C(11)	H(11)	118.8
C(10)	C(11)	H(11)	118.8
O(1)	C(12)	Re	177.3(10)
O(2)	C(13)	Re	177.8(8)
O(3)	C(14)	Re	178.4(10)
N(3)	C(15)	C(9)	113.5(7)
N(3)	C(15)	H(15A)	108.9
C(9)	C(15)	H(15A)	108.9
N(3)	C(15)	H(15B)	108.9
C(9)	C(15)	H(15B)	108.9
H(15A)	C(15)	H(15B)	107.7
N(3)	C(16)	C(17)	105.1(7)
N(3)	C(16)	H(16)	127.4
C(17)	C(16)	H(16)	127.4
N(5)	C(17)	C(16)	108.3(7)
N(5)	C(17)	C(18)	120.5(8)
C(16)	C(17)	C(18)	131.2(8)
N(6)	C(18)	C(17)	112.1(8)
N(6)	C(18)	H(18A)	109.2
C(17)	C(18)	H(18A)	109.2

N(6)	C(18)	H(18B)	109.2
C(17)	C(18)	H(18B)	109.2
H(18A)	C(18)	H(18B)	107.9
O(4)	C(19)	N(6)	121.0(8)
O(4)	C(19)	C(25)	121.1(8)
N(6)	C(19)	C(25)	117.9(8)
C(21)	C(20)	C(25)	120.8(9)
C(21)	C(20)	H(20)	119.6
C(25)	C(20)	H(20)	119.6
C(22)	C(21)	C(20)	120.0(10)
C(22)	C(21)	H(21)	120
C(20)	C(21)	H(21)	120
C(21)	C(22)	C(23)	120.9(9)
C(21)	C(22)	H(22)	119.5
C(23)	C(22)	H(22)	119.5
C(22)	C(23)	C(24)	119.9(10)
C(22)	C(23)	H(23)	120
C(24)	C(23)	H(23)	120
C(25)	C(24)	C(23)	119.9(10)
C(25)	C(24)	H(24)	120
C(23)	C(24)	H(24)	120
C(24)	C(25)	C(20)	118.5(8)
C(24)	C(25)	C(19)	124.6(8)
C(20)	C(25)	C(19)	116.9(8)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4 Number of Scans
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9 Nucleus
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(8)
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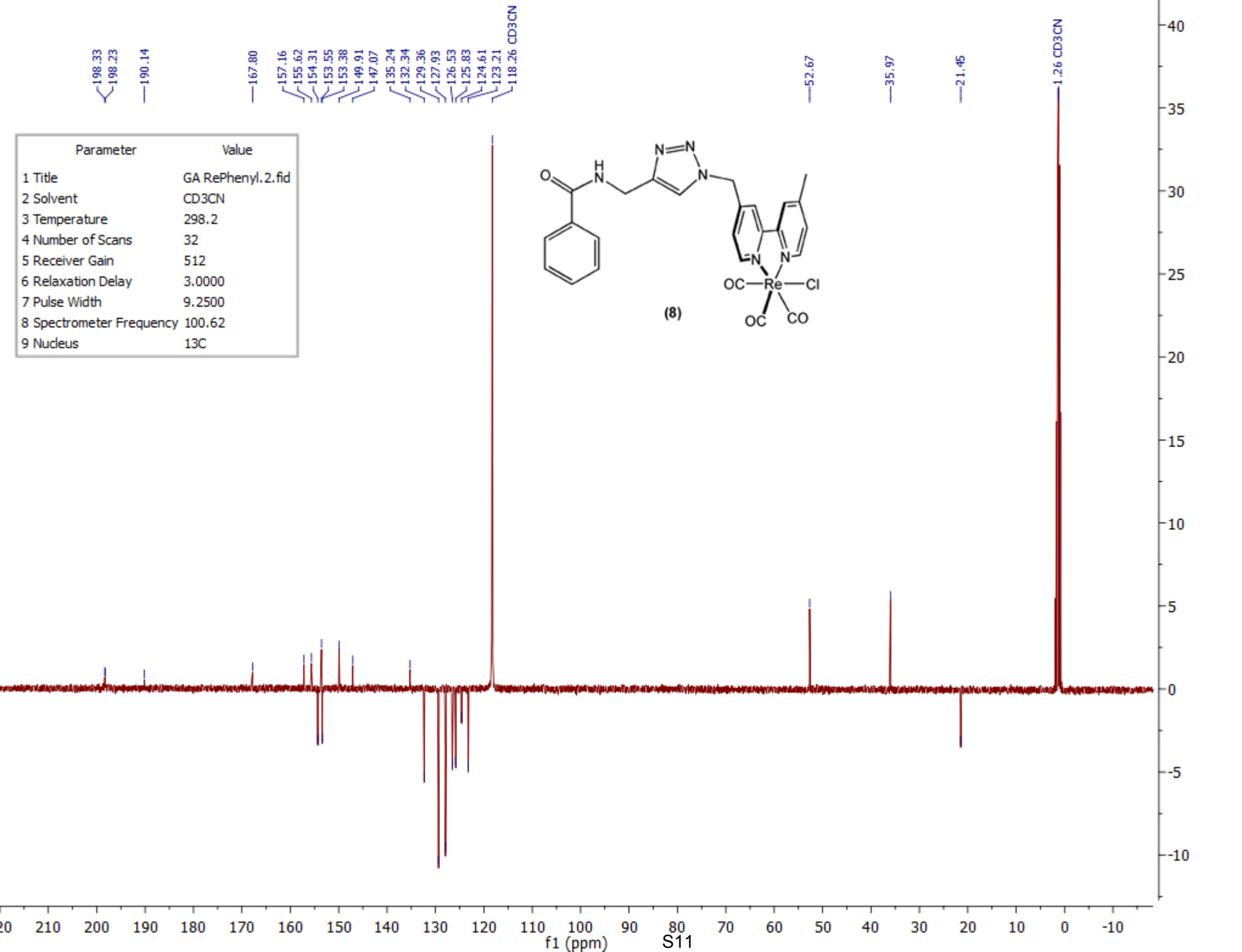
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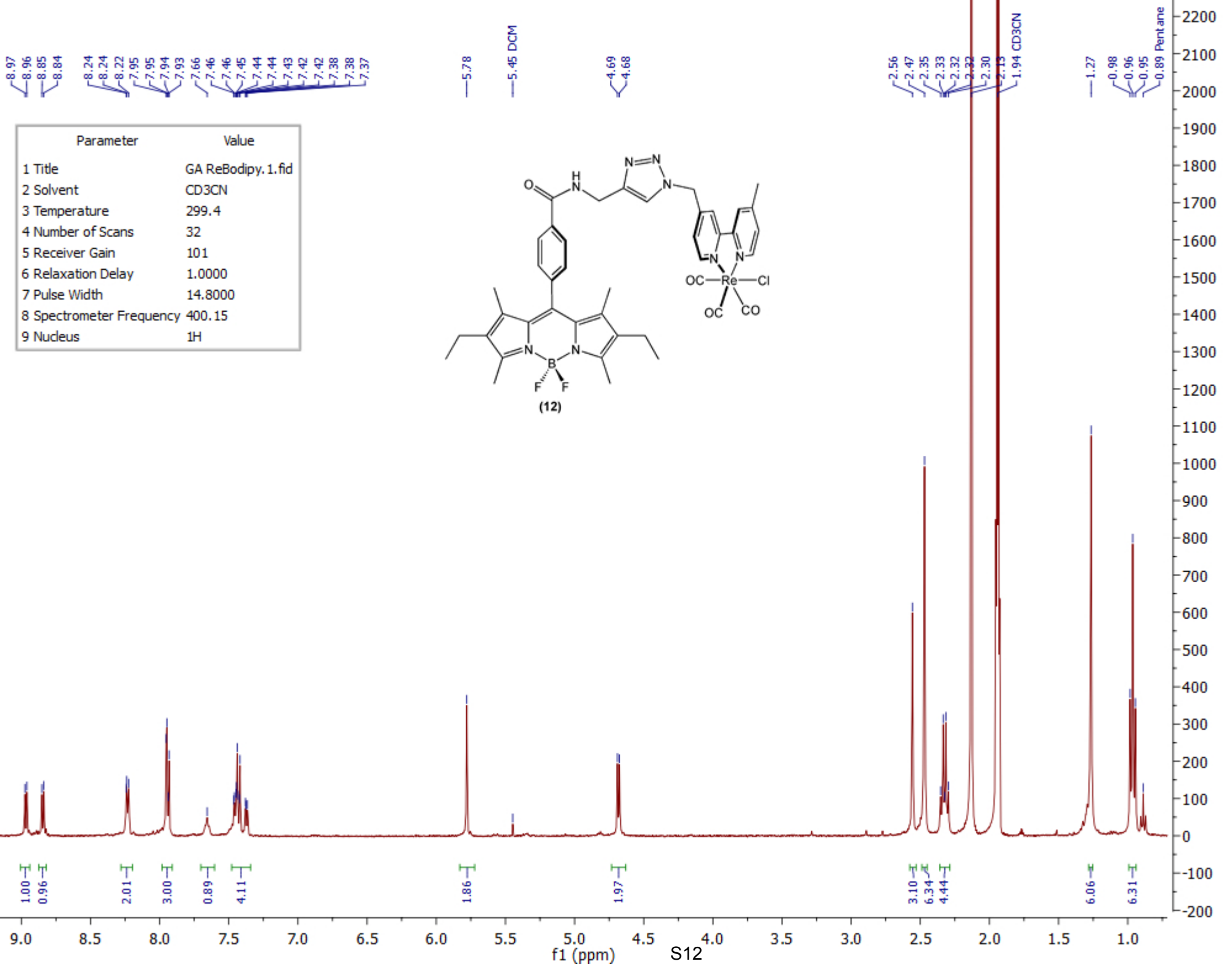
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4 Number of Scans 32
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8 Spectrometer Frequency 400.15
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(12)
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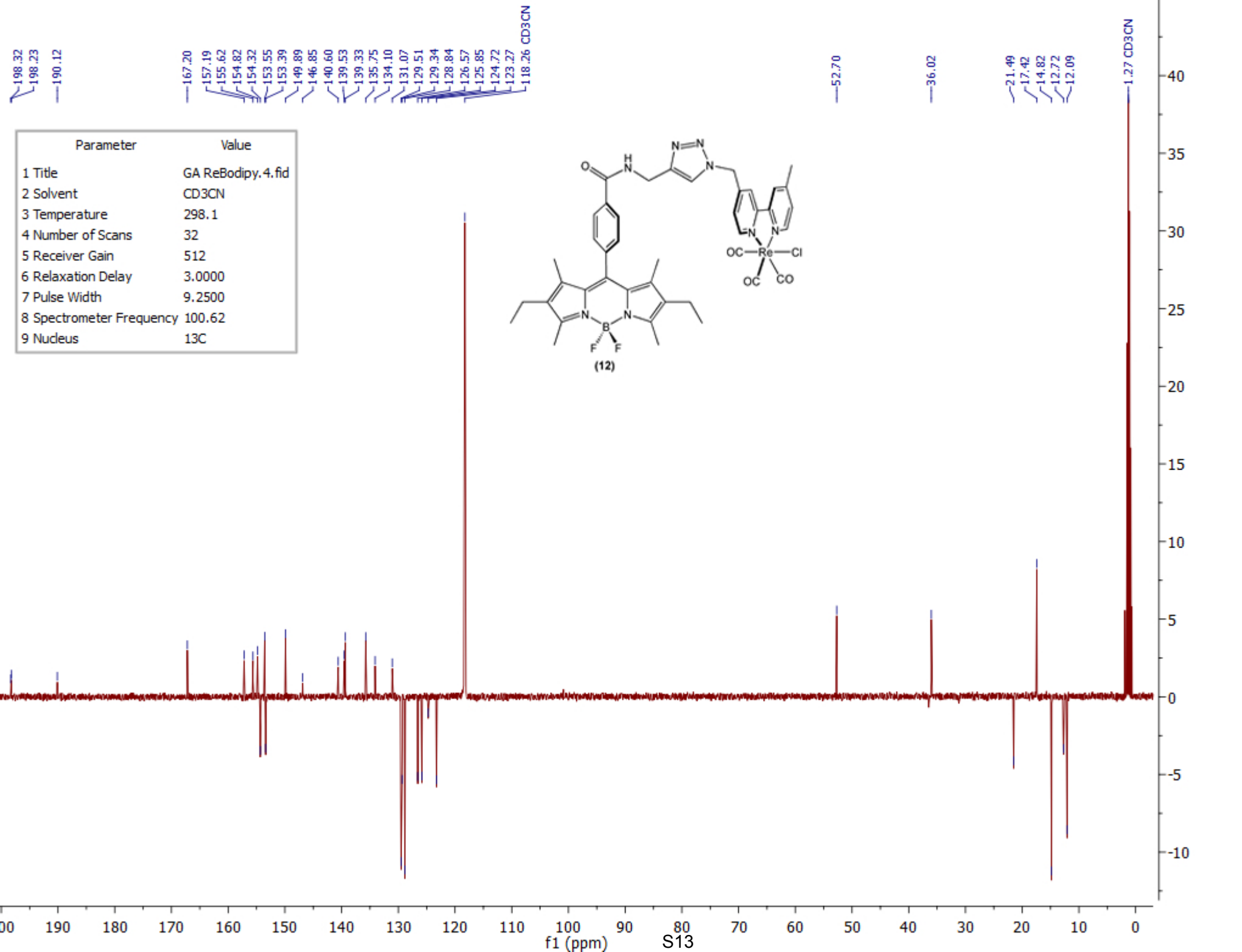
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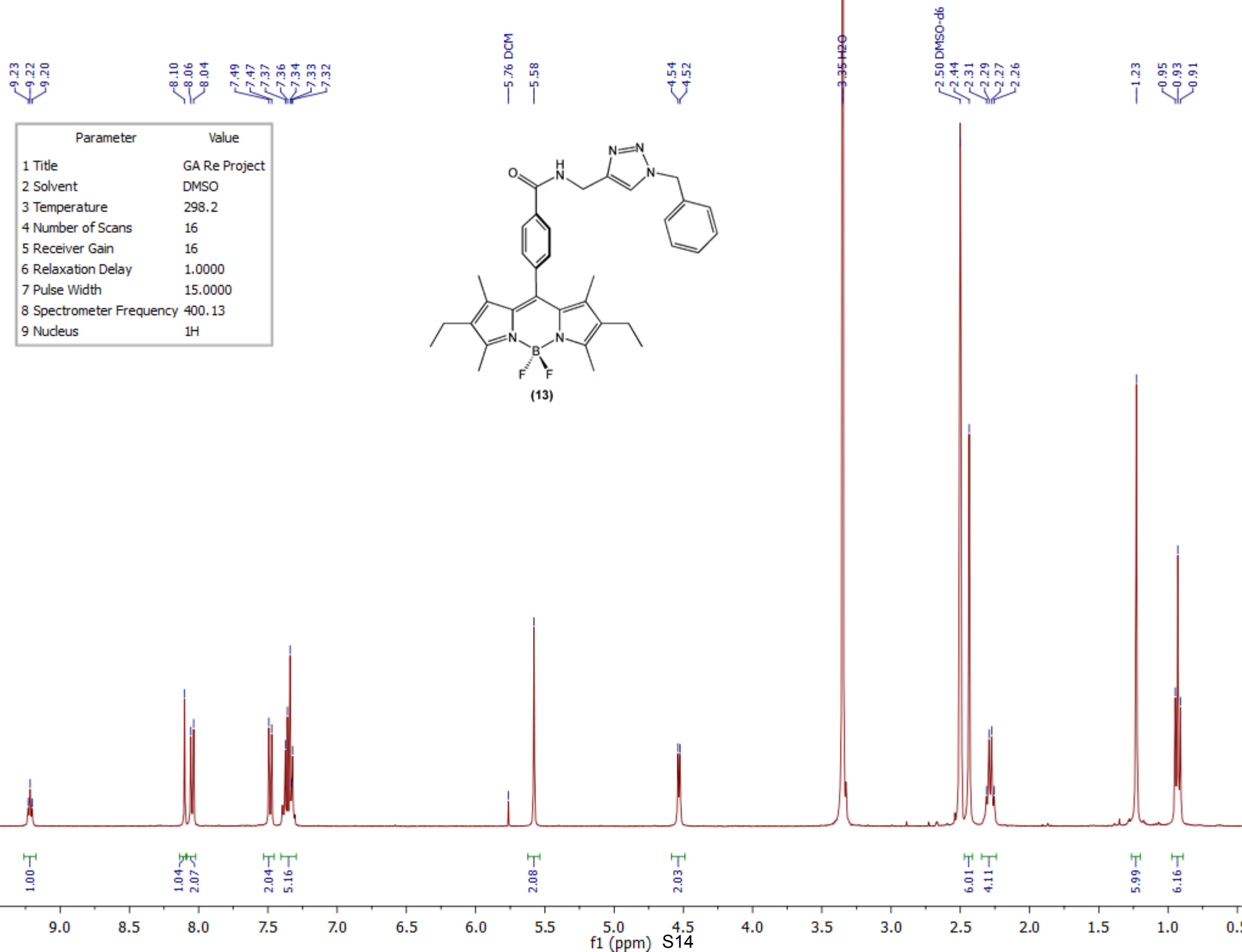
f1 (ppm)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4.52
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8 Spectrometer Frequency 400.13
9 Nucleus 1H
(13)
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2.07
2.04
5.16
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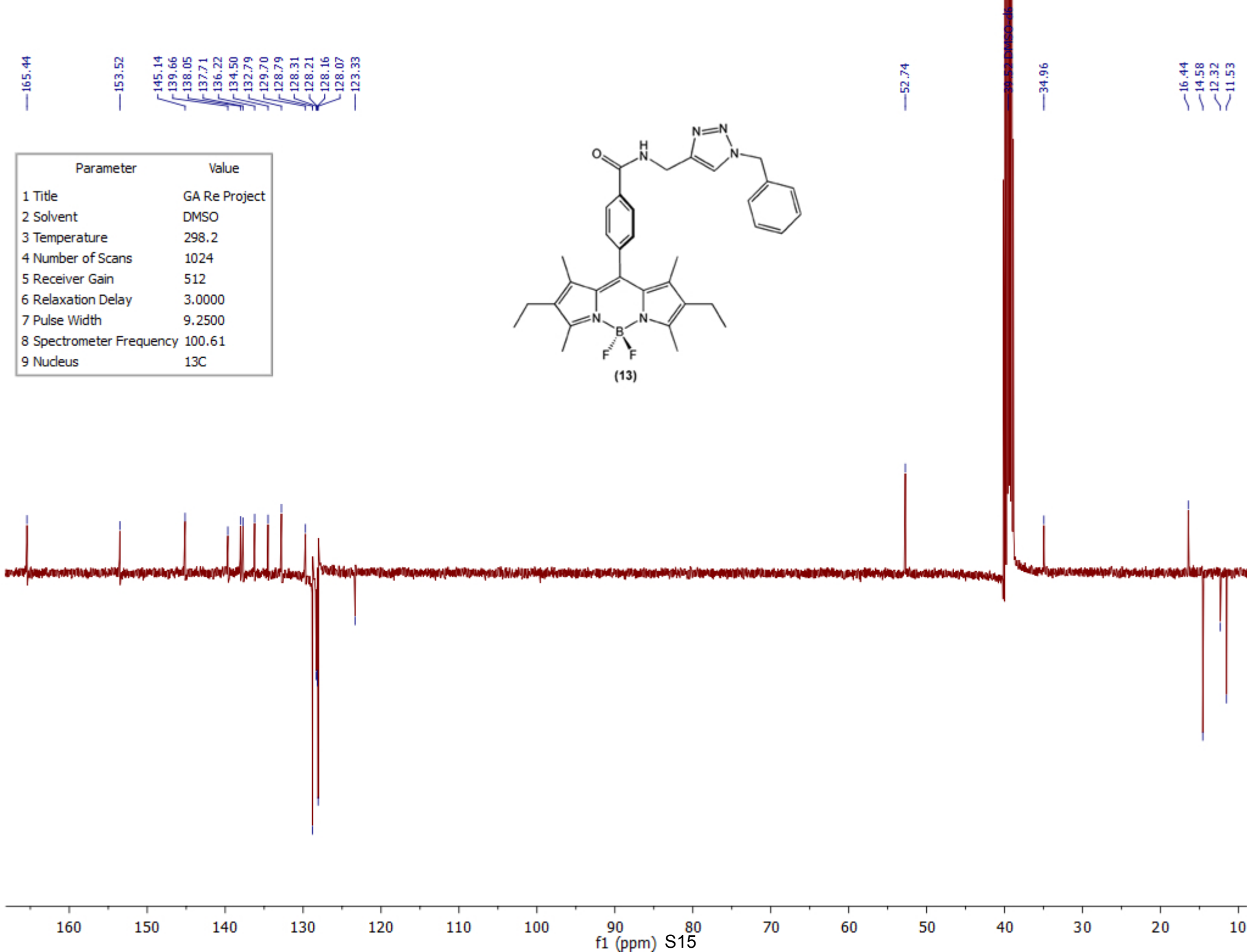
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128.16
128.07
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39.52 DMSO-d6
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14.58
12.32
11.53
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8 Spectrometer Frequency 100.61
9 Nucleus 13C
(13)
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150
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130
120
110
100
90
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70
60
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30
20
10
f1 (ppm)