



Supporting Information

for

Synthesis of benzo[*f*]quinazoline-1,3(2*H*,4*H*)-diones

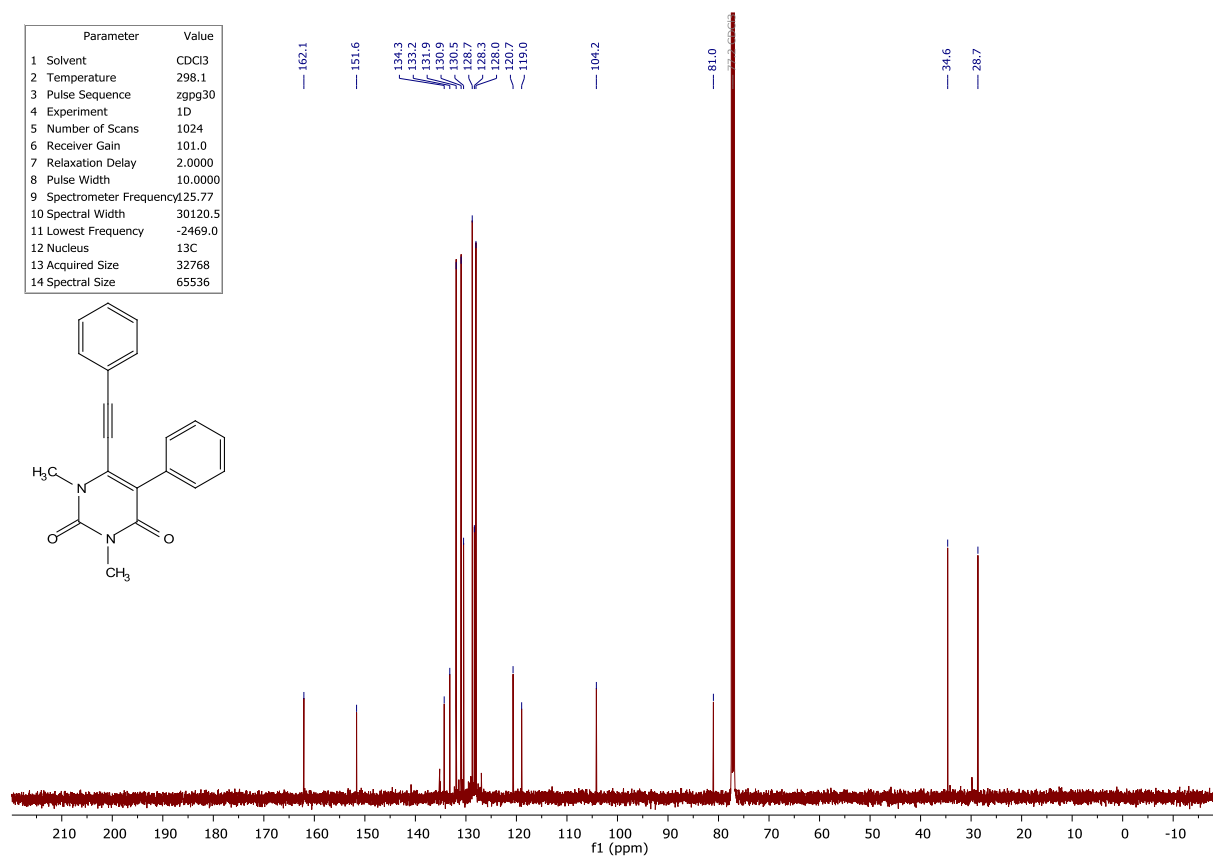
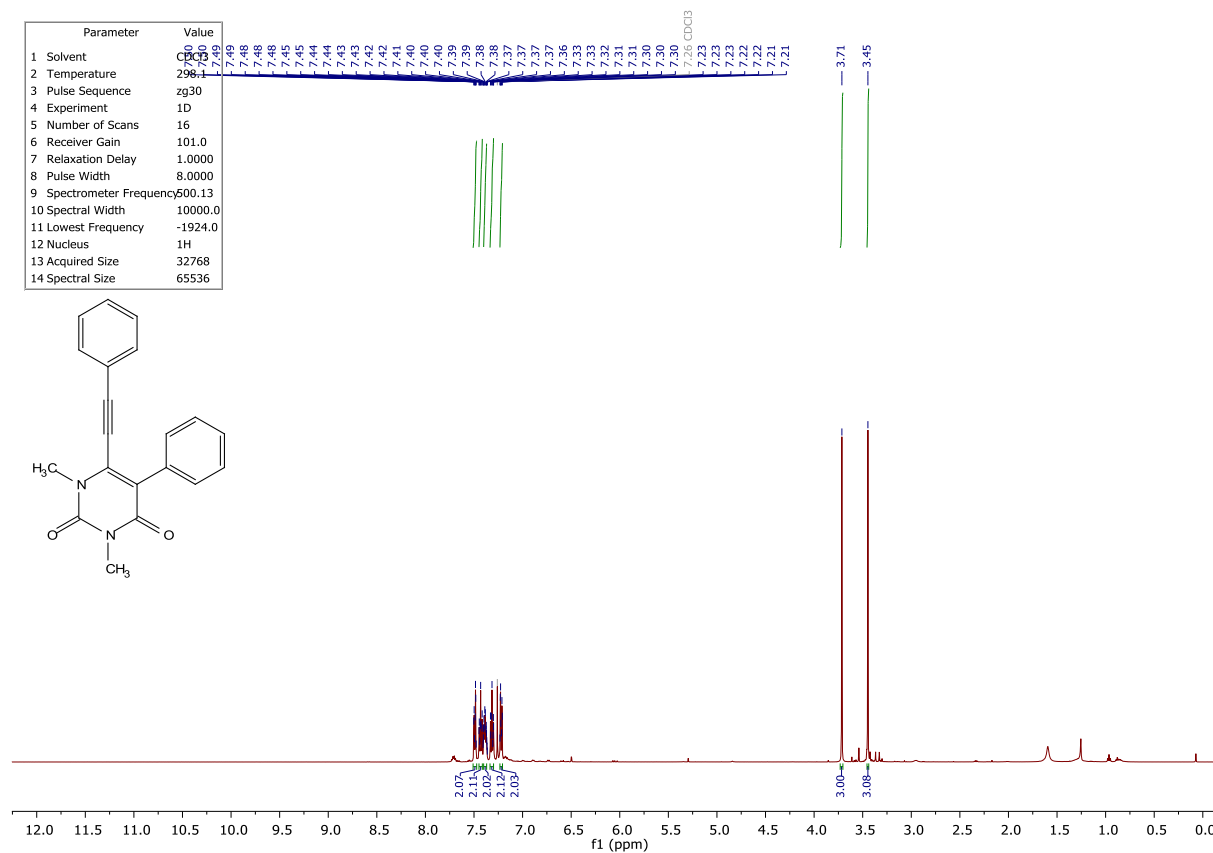
Ruben Manuel Figueira de Abreu, Peter Ehlers and Peter Langer

Beilstein J. Org. Chem. **2024**, *20*, 2708–2719. doi:10.3762/bjoc.20.228

Copies of NMR spectra

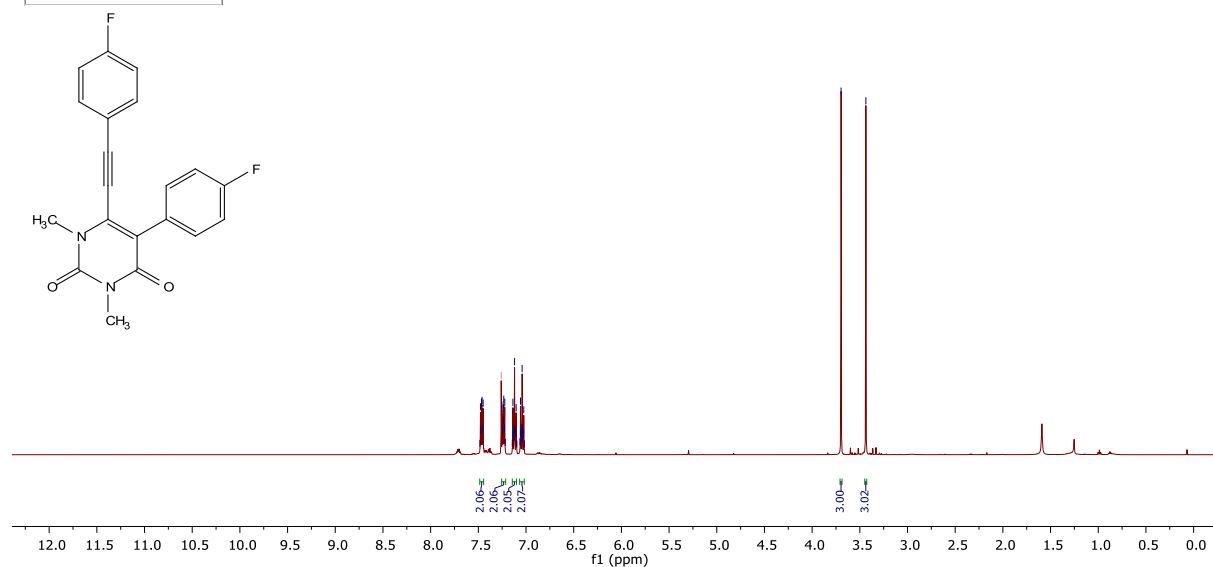
^1H , ^{13}C , and ^{19}F NMR spectra

1,3-Dimethyl-5-phenyl-6-(phenylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (4g).

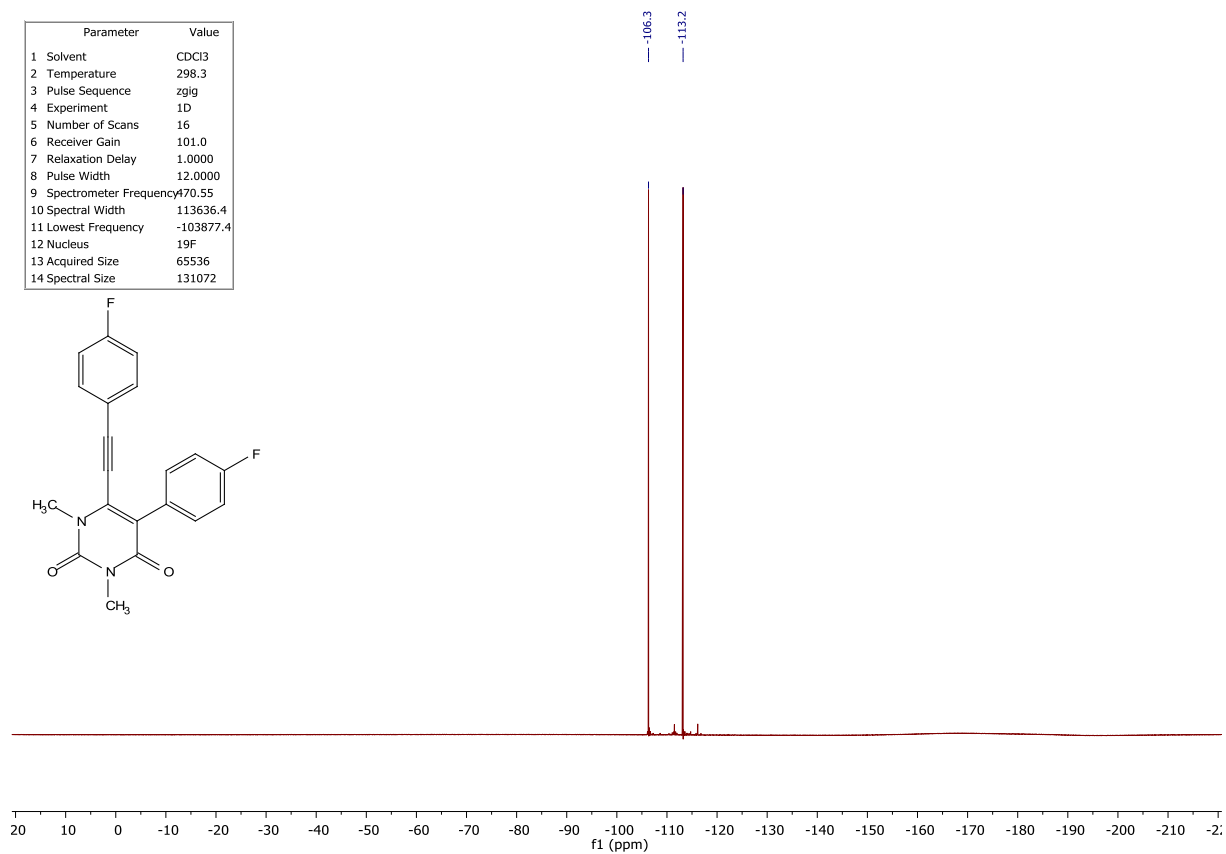


5-(4-Fluorophenyl)-6-((4-fluorophenyl)ethynyl)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione (4h)

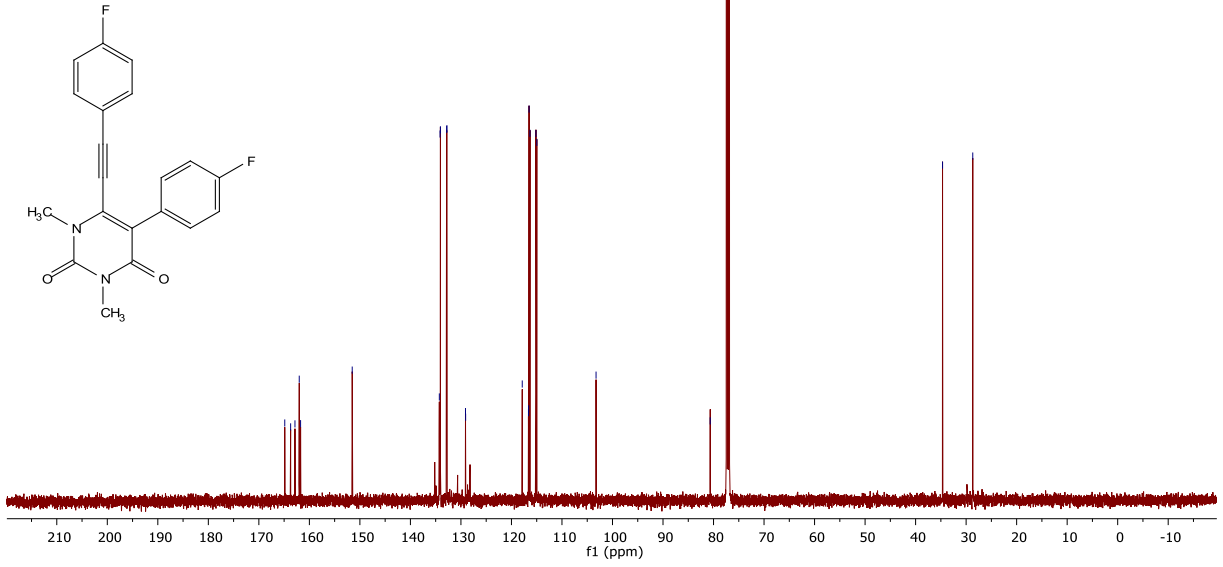
Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.1
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	8.0000
9 Spectrometer Frequency	500.13
10 Spectral Width	10000.0
11 Lowest Frequency	-1924.0
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



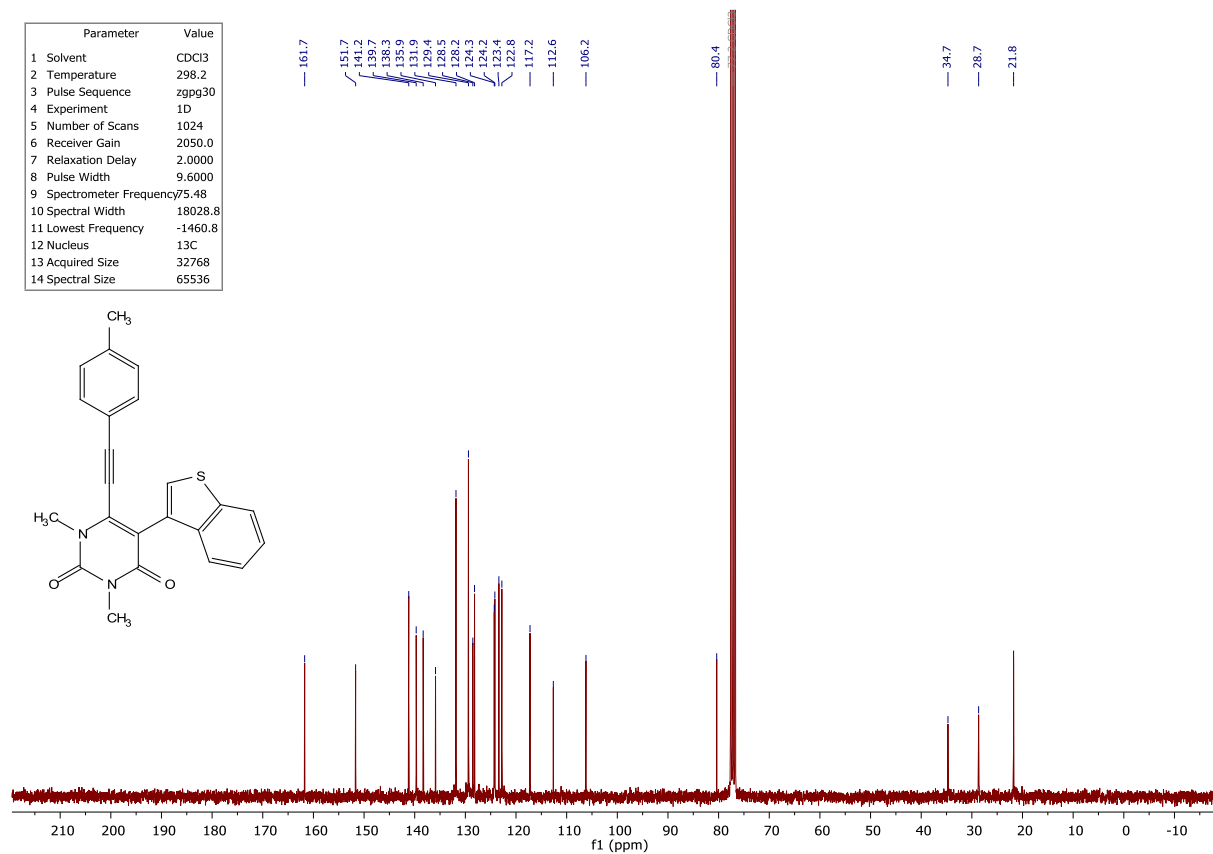
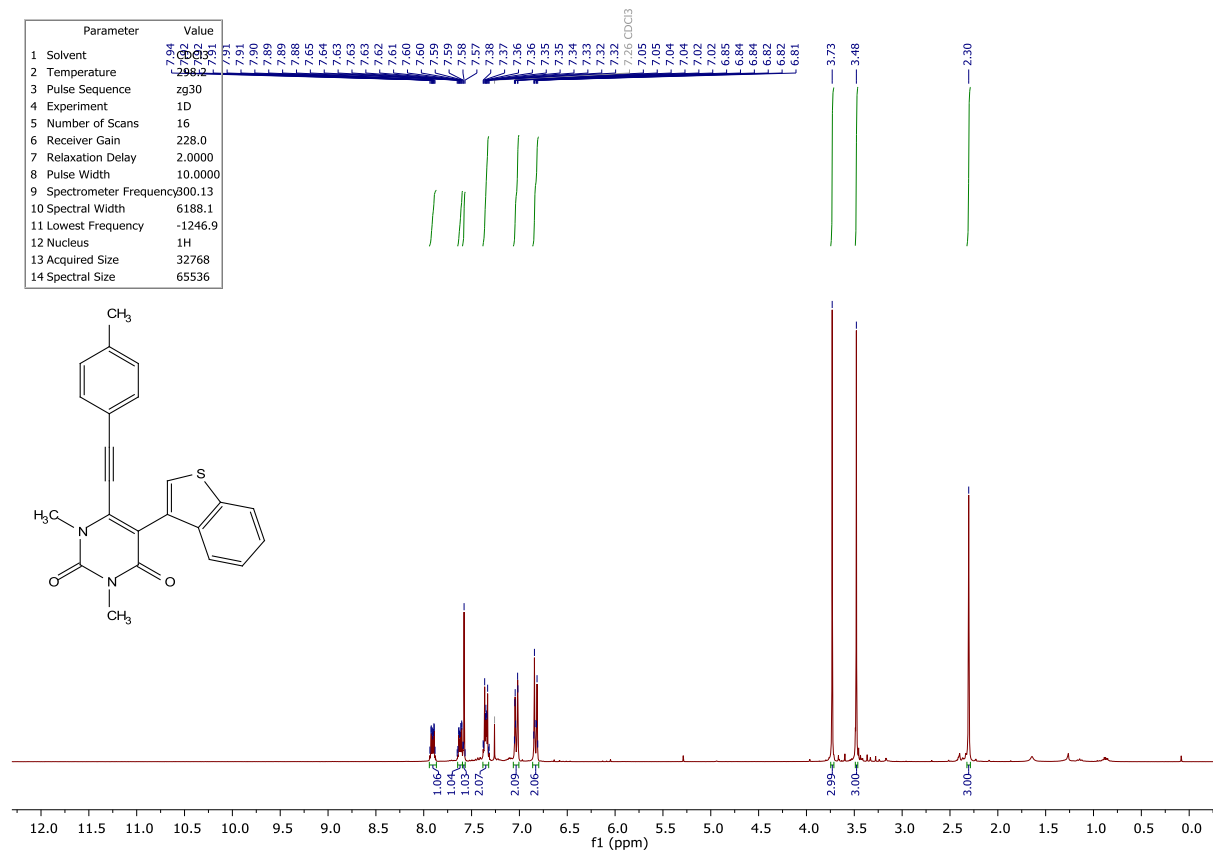
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1 Solvent	CDCl3
2 Temperature	298.3
3 Pulse Sequence	zgig
4 Experiment	1D
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	12.0000
9 Spectrometer Frequency	470.55
10 Spectral Width	113636.4
11 Lowest Frequency	-103877.4
12 Nucleus	19F
13 Acquired Size	65536
14 Spectral Size	131072



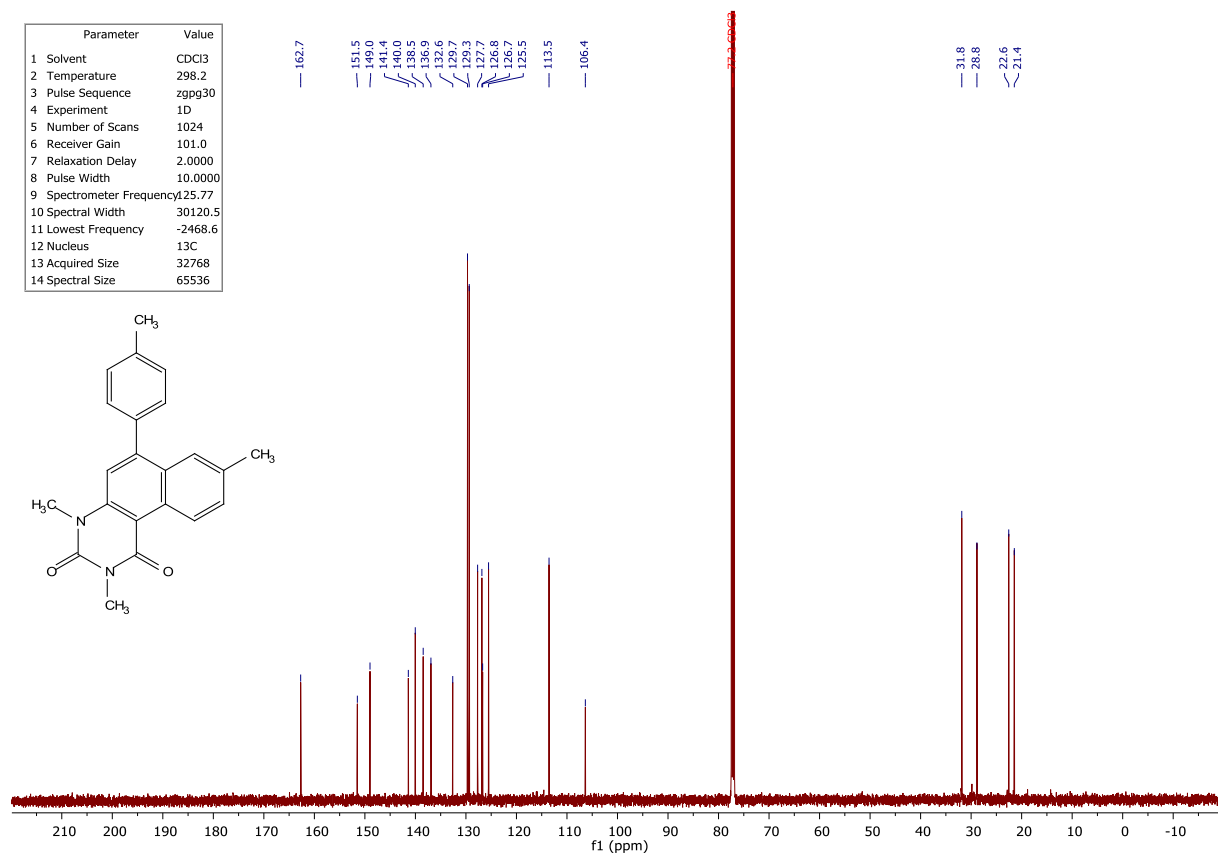
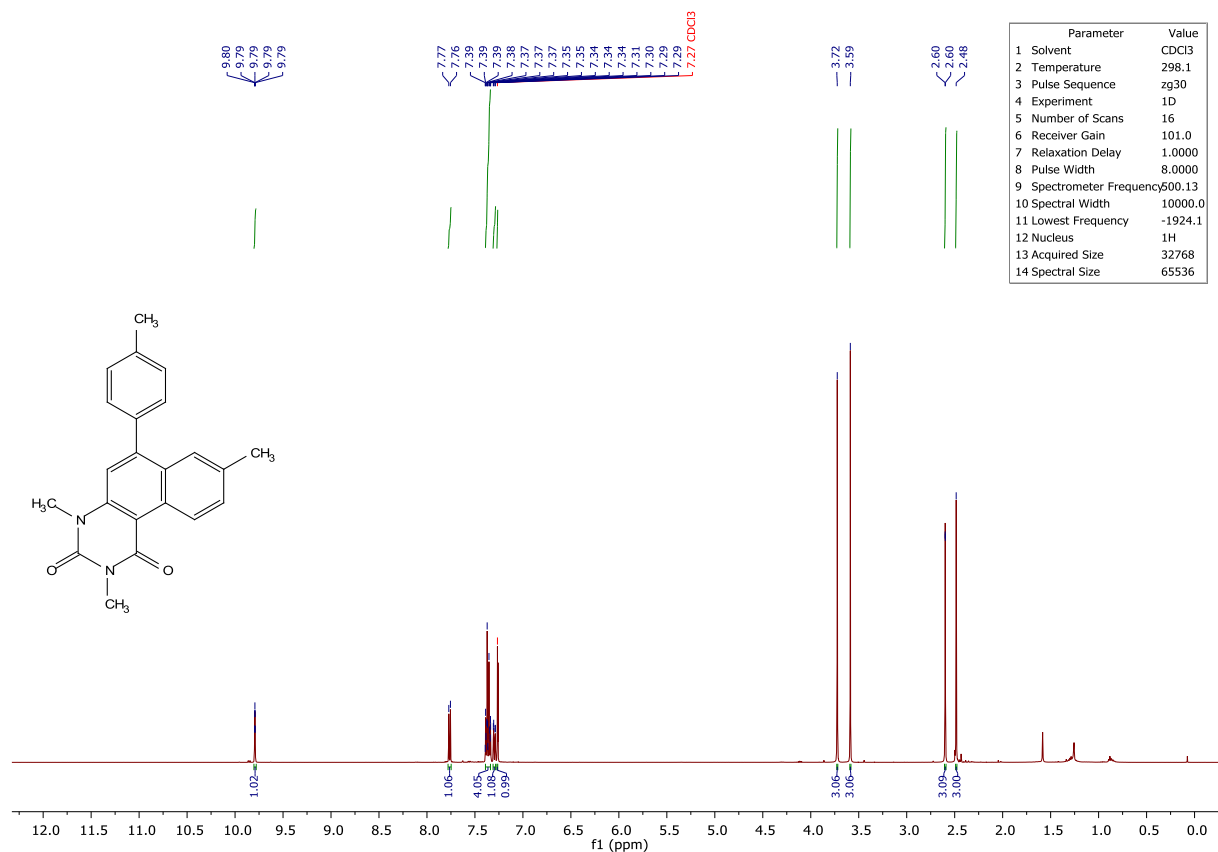
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1 Solvent	CDCl3
2 Temperature	298.2
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	2048
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.77
10 Spectral Width	30120.5
11 Lowest Frequency	-2468.6
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536



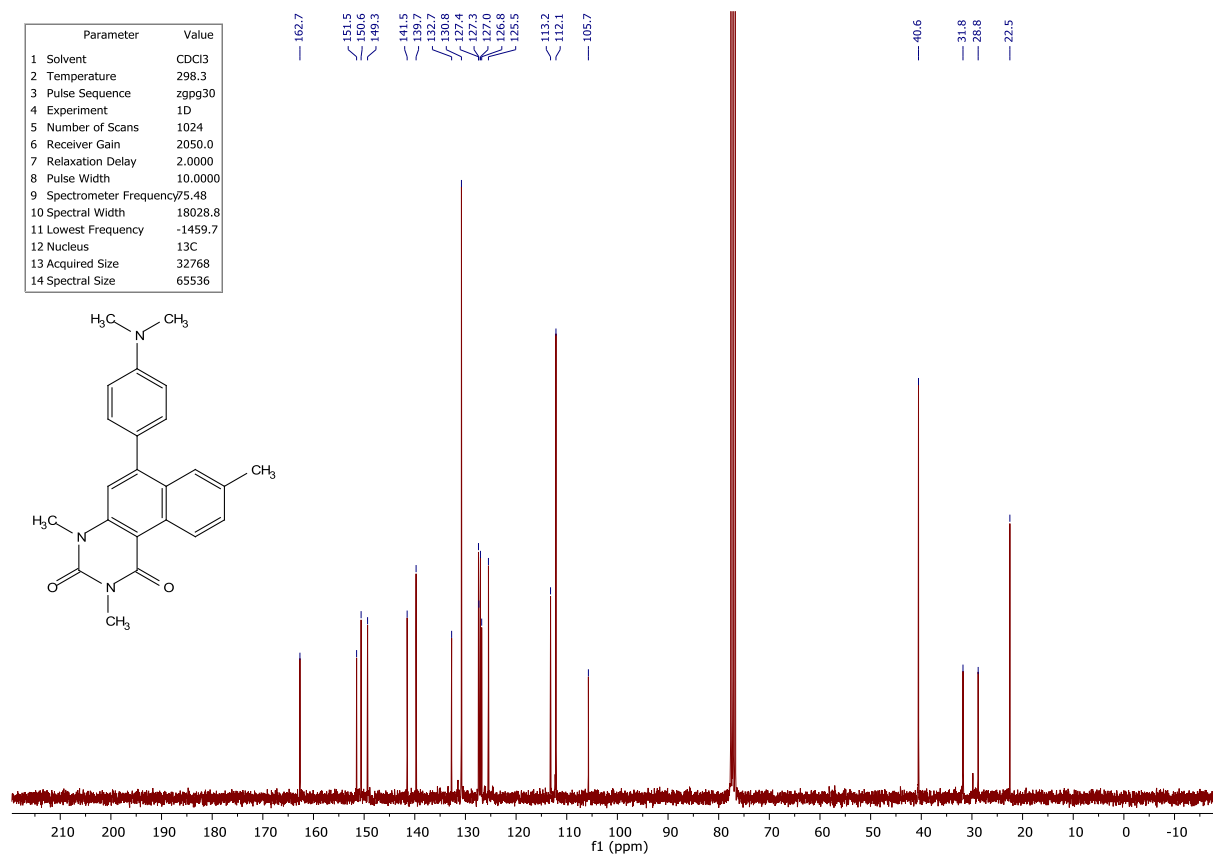
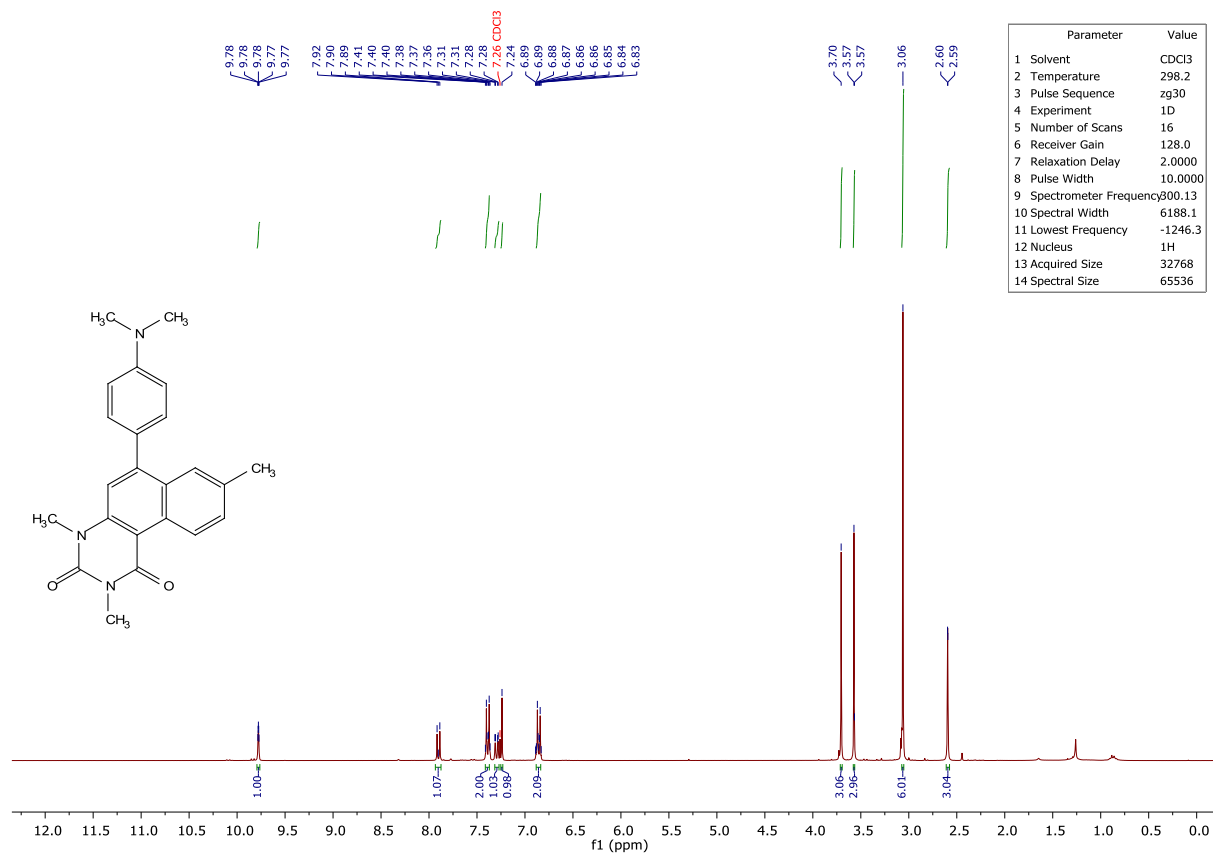
5-(Benzo[b]thiophen-3-yl)-1,3-dimethyl-6-(*p*-tolylethynyl)pyrimidine-2,4(1*H*,3*H*)-dione (4i)



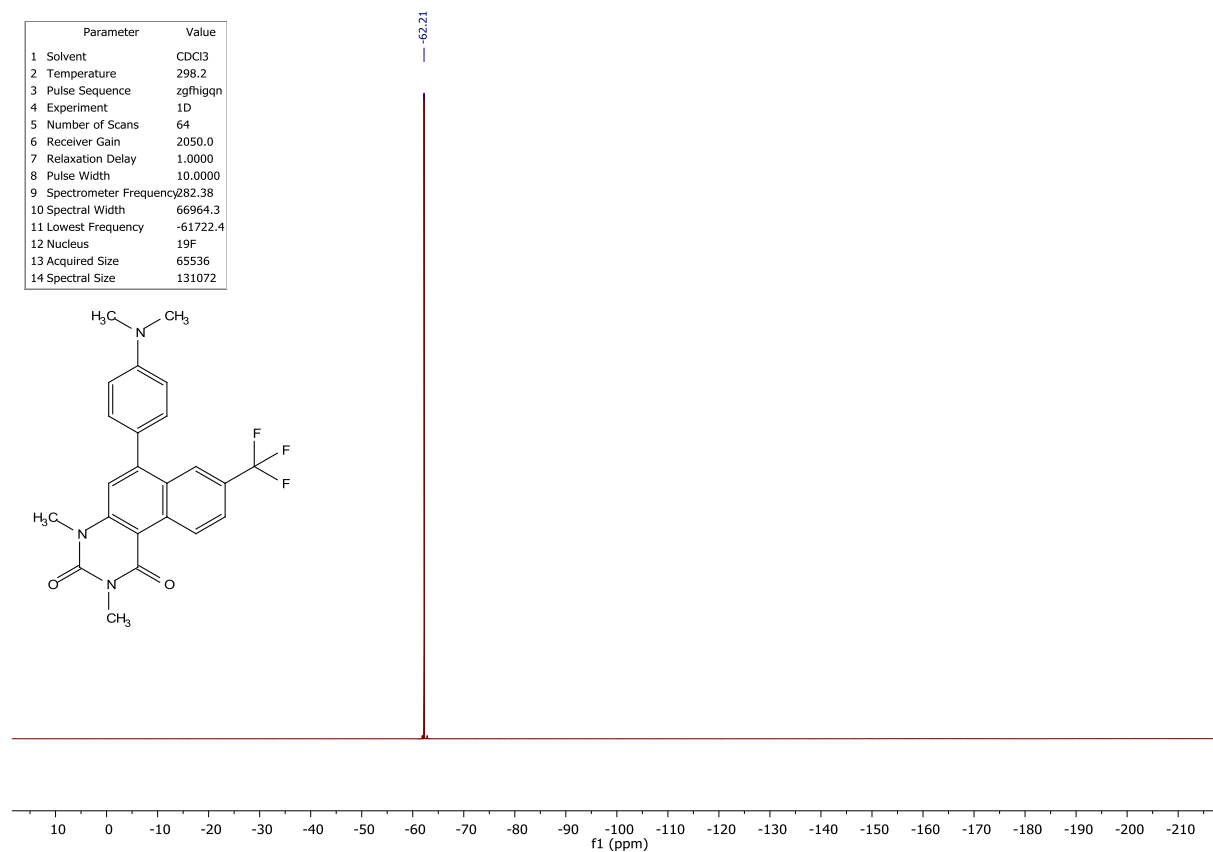
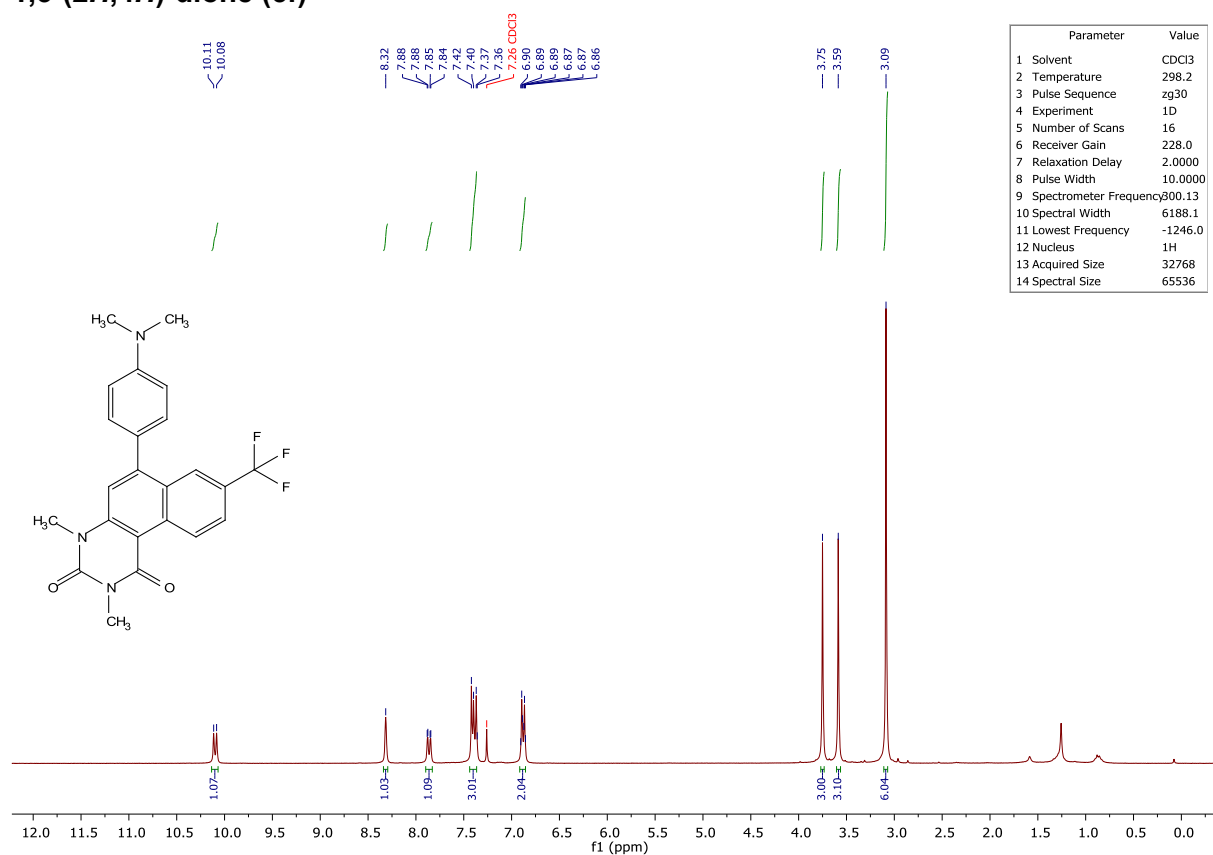
2,4,8-Trimethyl-6-(p-tolyl)benzo[f]quinazoline-1,3(2H,4H)-dione (5a)



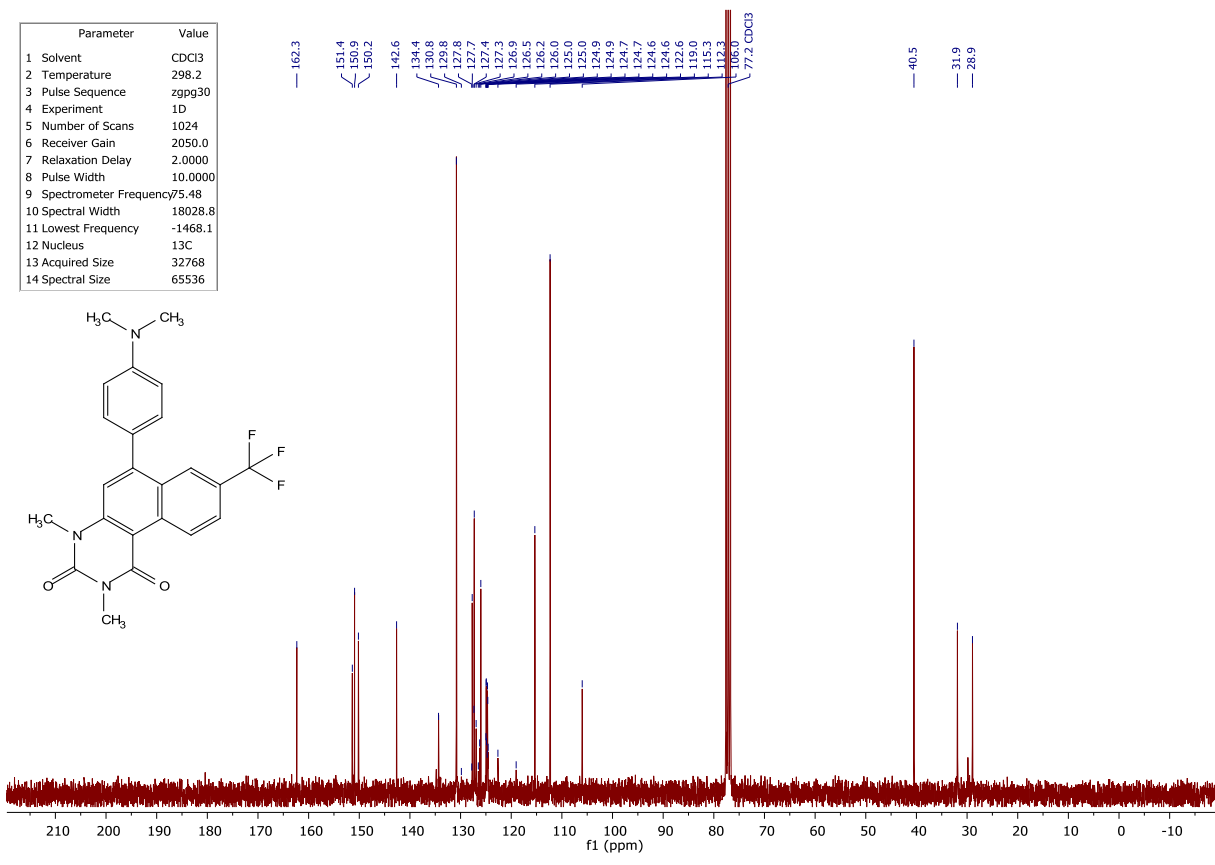
6-(4-(*N,N*-Dimethylamino)phenyl)-2,4,8-trimethylbenzo[*f*]quinazoline-1,3(2*H*,4*H*)-dione (5d)



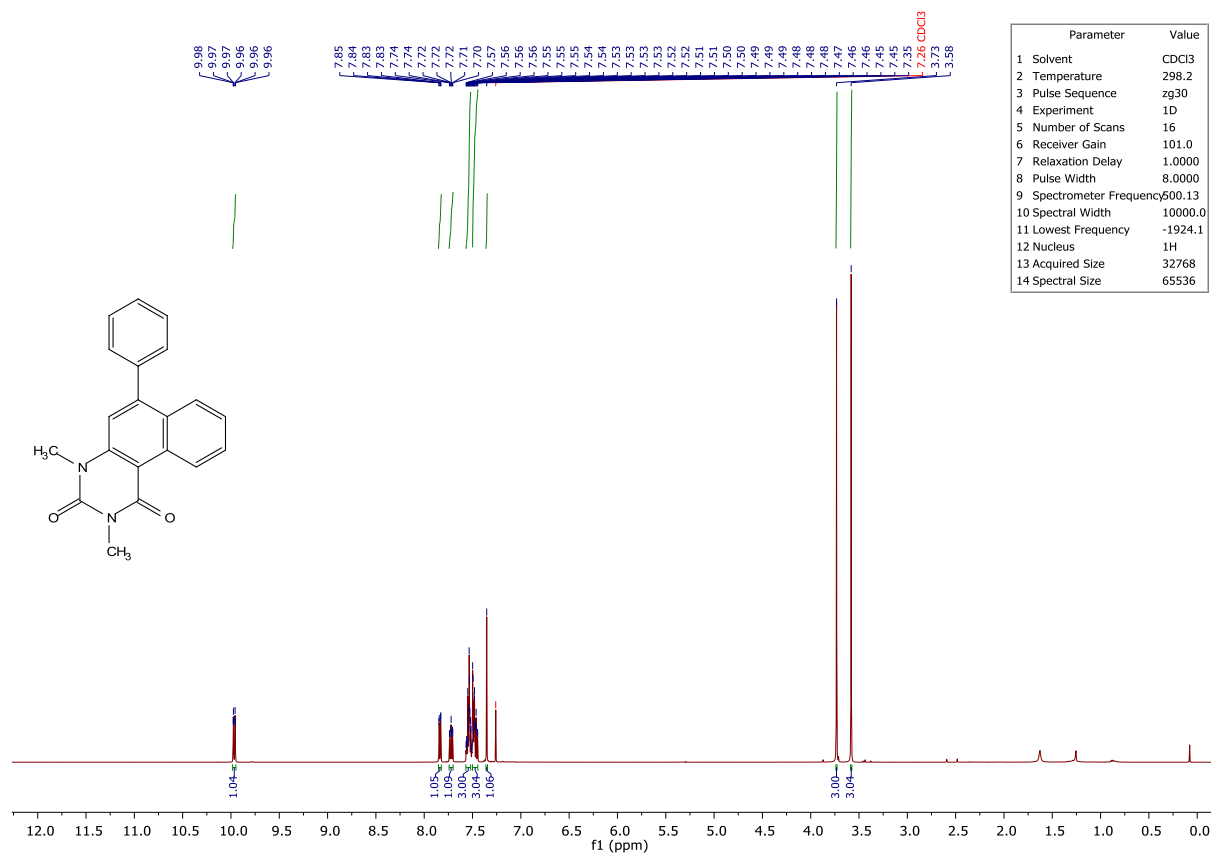
6-(4-(*N,N*-Dimethylamino)phenyl)-2,4-dimethyl-8-(trifluoromethyl)benzo[*f*]quinazoline-1,3-(2*H*,4*H*)-dione (5f)



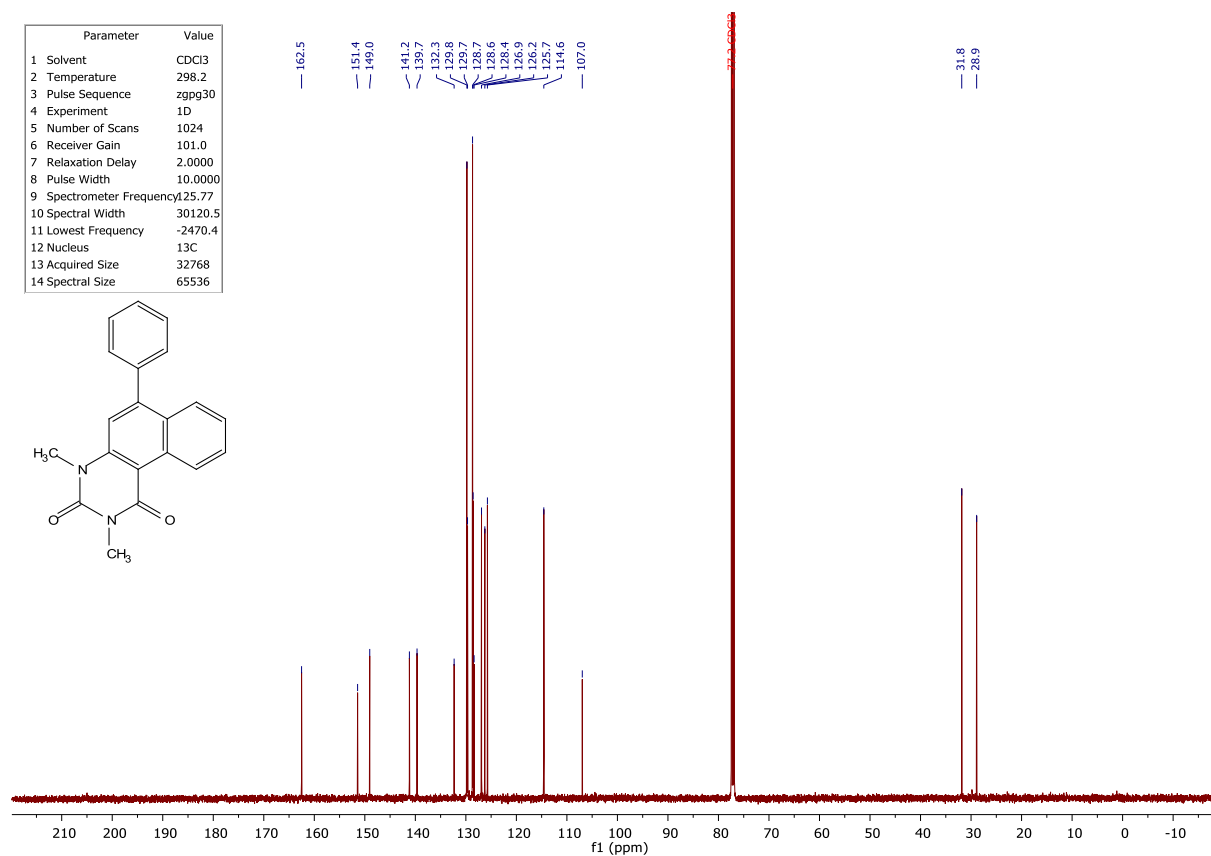
Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.2
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Receiver Gain	2050.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	75.48
10 Spectral Width	18028.8
11 Lowest Frequency	-1468.1
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536



2,4-Dimethyl-6-phenylbenzo[f]quinazoline-1,3(2H,4H)-dione (5g)

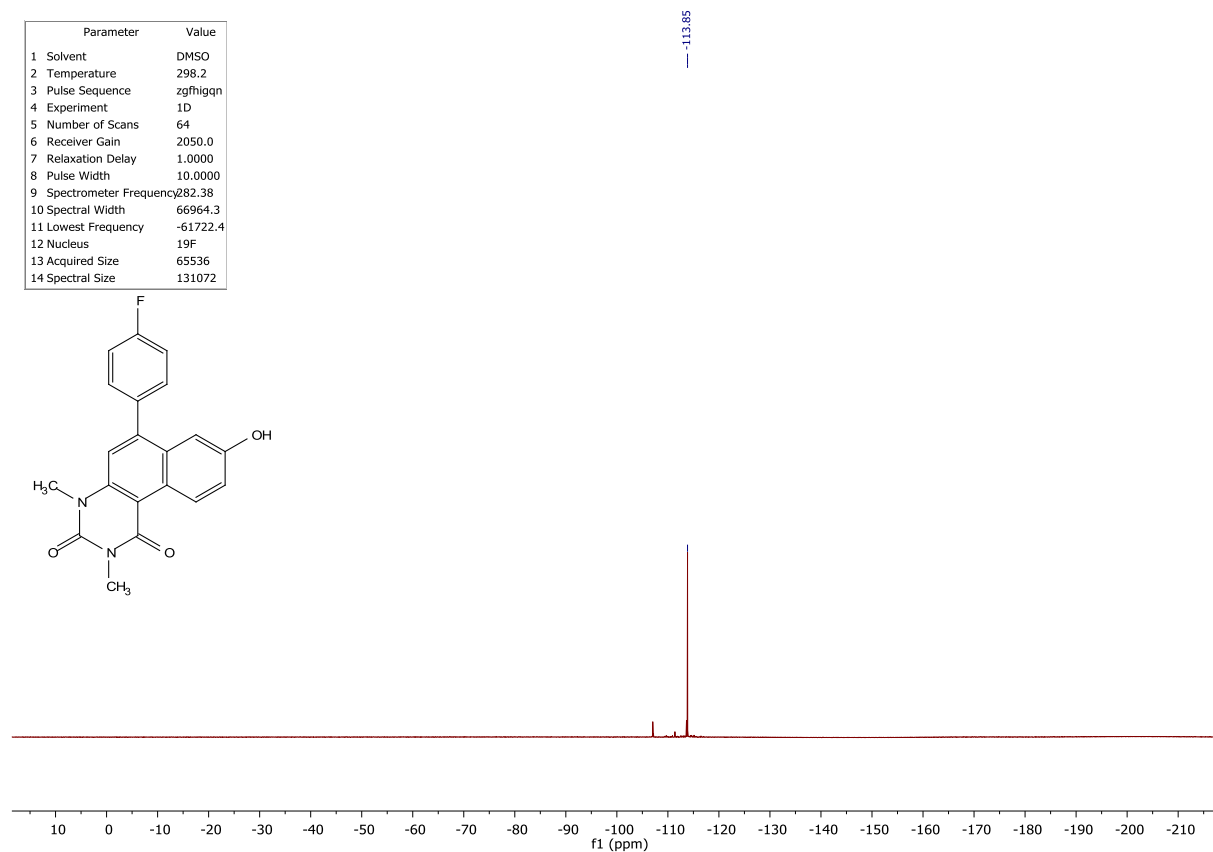
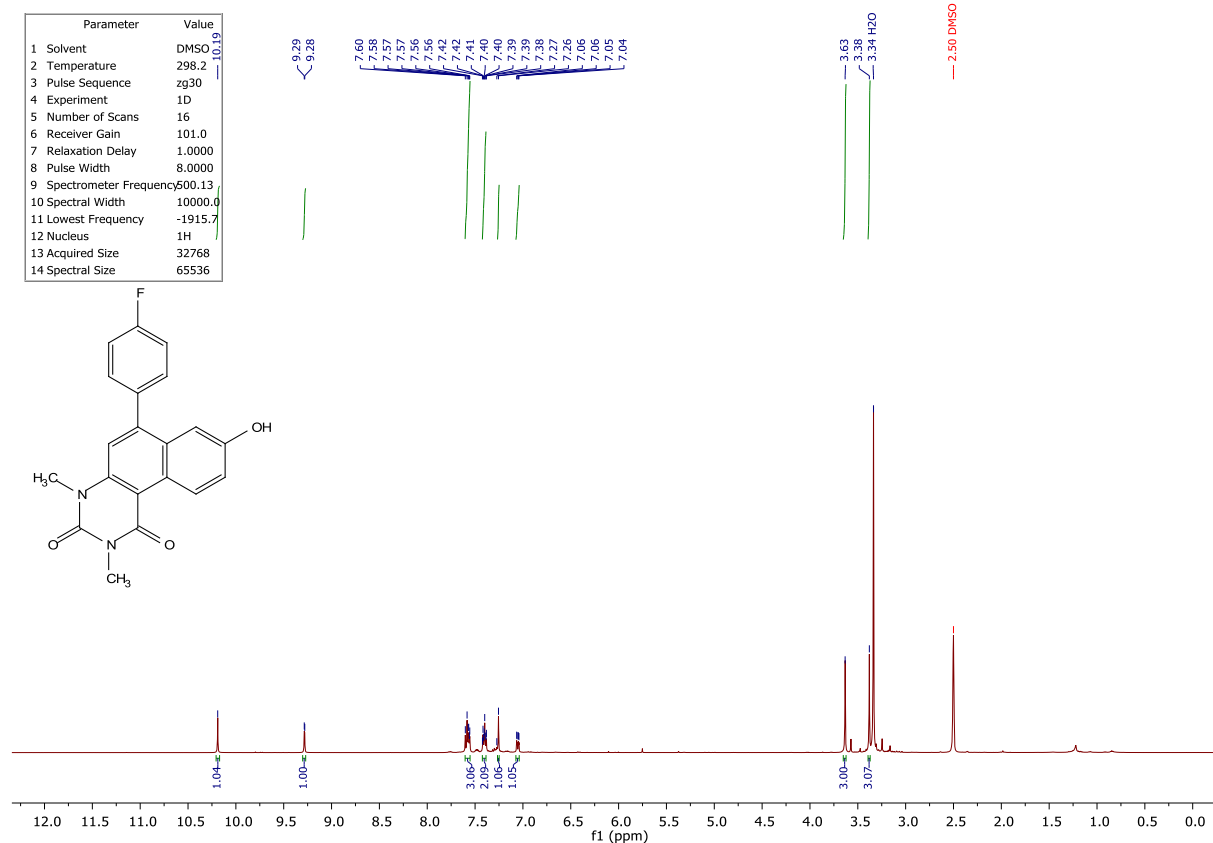


Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.2
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	8.0000
9 Spectrometer Frequency	500.13
10 Spectral Width	10000.0
11 Lowest Frequency	-1924.1
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536

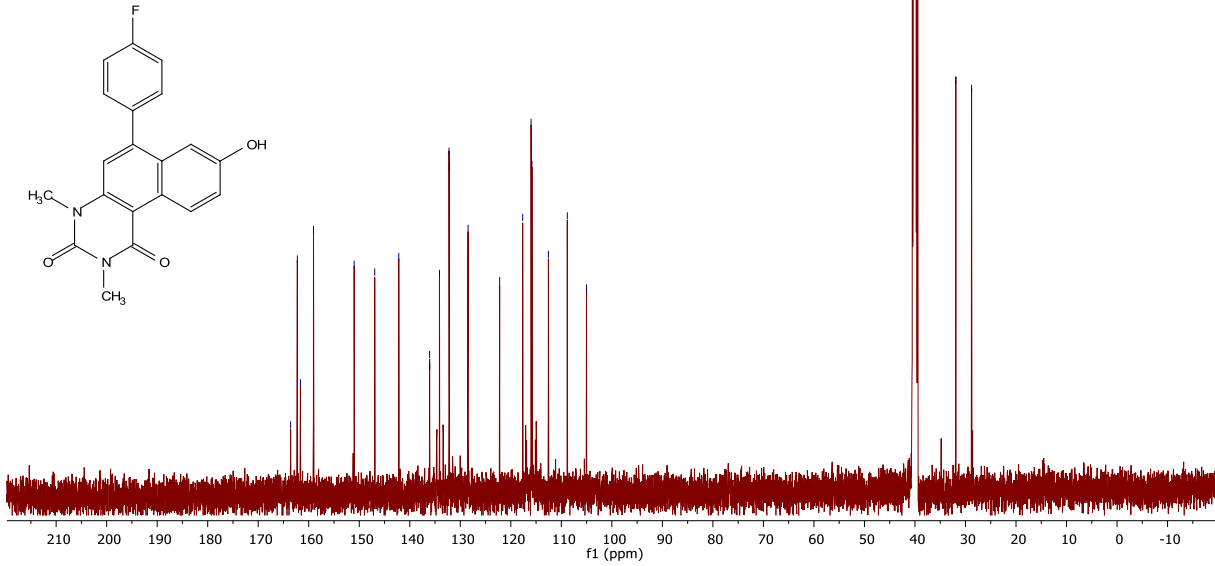


Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.2
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.77
10 Spectral Width	30120.5
11 Lowest Frequency	-2470.4
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

6-(4-Fluorophenyl)-8-hydroxy-2,4-dimethylbenzo[*f*]quinazoline-1,3(2*H*,4*H*)-dione (5h)

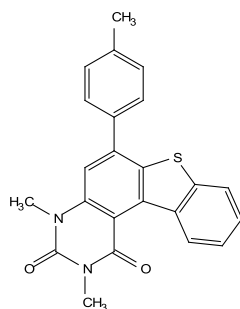
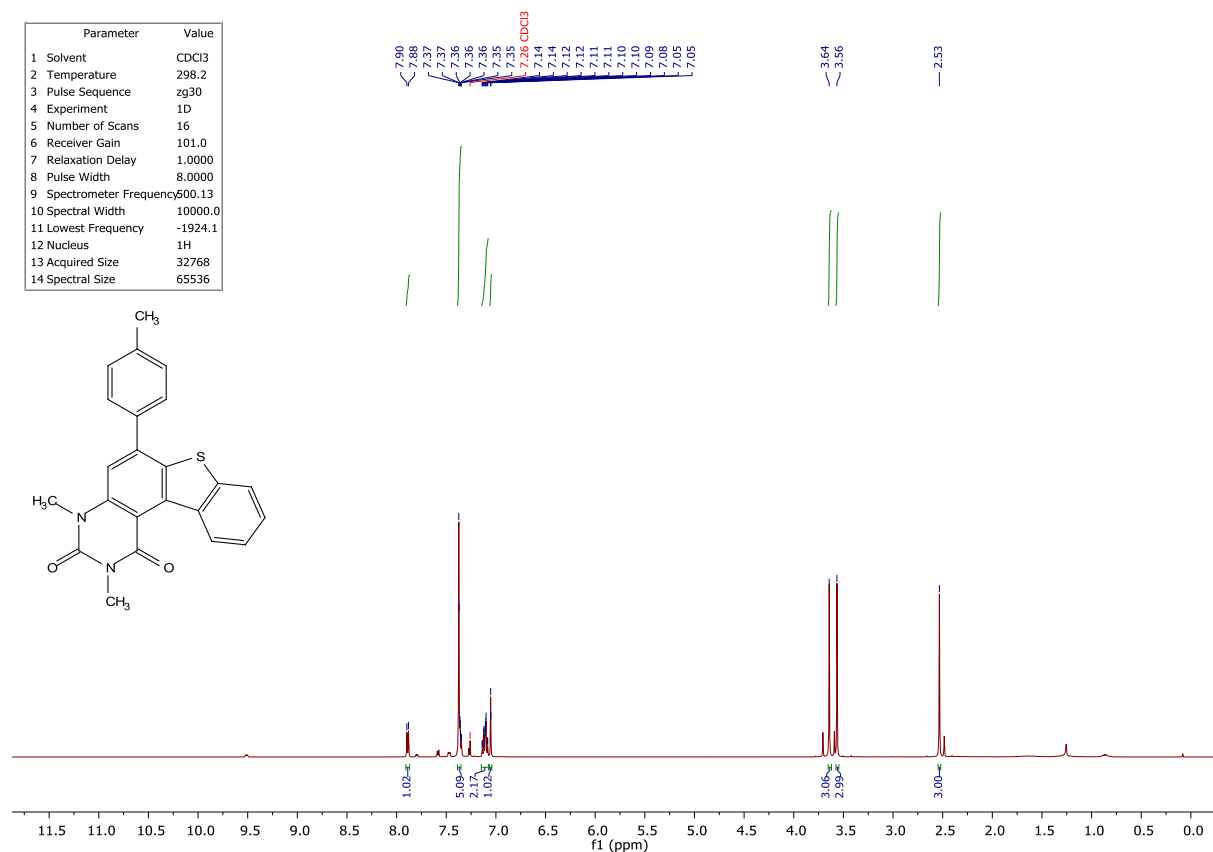


Parameter	Value
1 Solvent	DMSO
2 Temperature	298.2
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.77
10 Spectral Width	30120.5
11 Lowest Frequency	-2484.5
12 Nucleus	¹³ C
13 Acquired Size	32768
14 Spectral Size	65536



2,4-Dimethyl-6-(p-tolyl)benzo[4,5]thieno[3,2-f]quinazoline-1,3(2H,4H)-dione (5i)

Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.2
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	16
6 Receiver Gain	101.0
7 Relaxation Delay	1.0000
8 Pulse Width	8.0000
9 Spectrometer Frequency	500.13
10 Spectral Width	10000.0
11 Lowest Frequency	-1924.1
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.1
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	4096
6 Receiver Gain	101.0
7 Relaxation Delay	2.0000
8 Pulse Width	10.0000
9 Spectrometer Frequency	125.77
10 Spectral Width	30120.5
11 Lowest Frequency	-2471.4
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

