

Identification and Biological Characterization of the Pyrazolo[3,4-*d*]pyrimidine Derivative SI388 Active as Src Inhibitor

Claudia Contadini ^{1,2,†}, Claudia Cirotti ^{1,2,†}, Anna Carbone ³, Mehrdad Norouzi ^{1,2}, Annarita Cianciusi ³, Emmanuele Crespan ⁴, Cecilia Perini ⁴, Giovanni Maga ⁴, Daniela Barilà ^{1,2,*}, Francesca Musumeci ^{3,*} and Silvia Schenone ³

¹ Laboratory of Cell Signaling, IRCCS-Fondazione Santa Lucia, 00179 Rome, Italy; claudiacontadini@gmail.com (C.C.); claudiacirotti89@gmail.com (C.C.)

² Department of Biology, University of Rome "Tor Vergata", 00133 Rome, Italy

³ Department of Pharmacy, University of Genoa, Viale Benedetto XV, 3, 16132 Genoa, Italy; annar.cianciusi@gmail.com (A.C.); schenone@difar.unige.it (S.S.)

⁴ Institute of Molecular Genetics (IGM), IGM-CNR, Via Abbategrosso 207, 27100 Pavia, Italy; giovanni.maga@igm.cnr.it (G.M.)

* Correspondence: francesca.musumeci@unige.it (F.M.); daniela.barila@uniroma2.it (D.B.)

† These authors contributed equally to this work.

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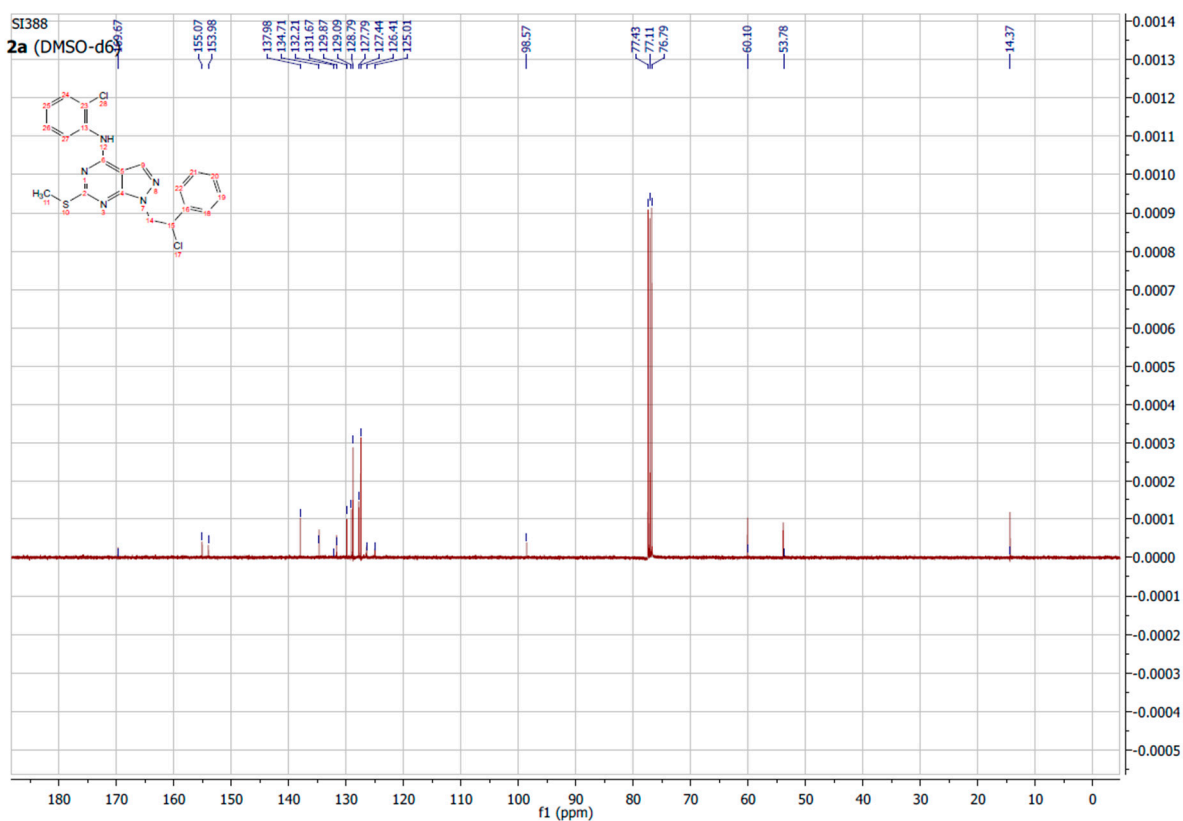
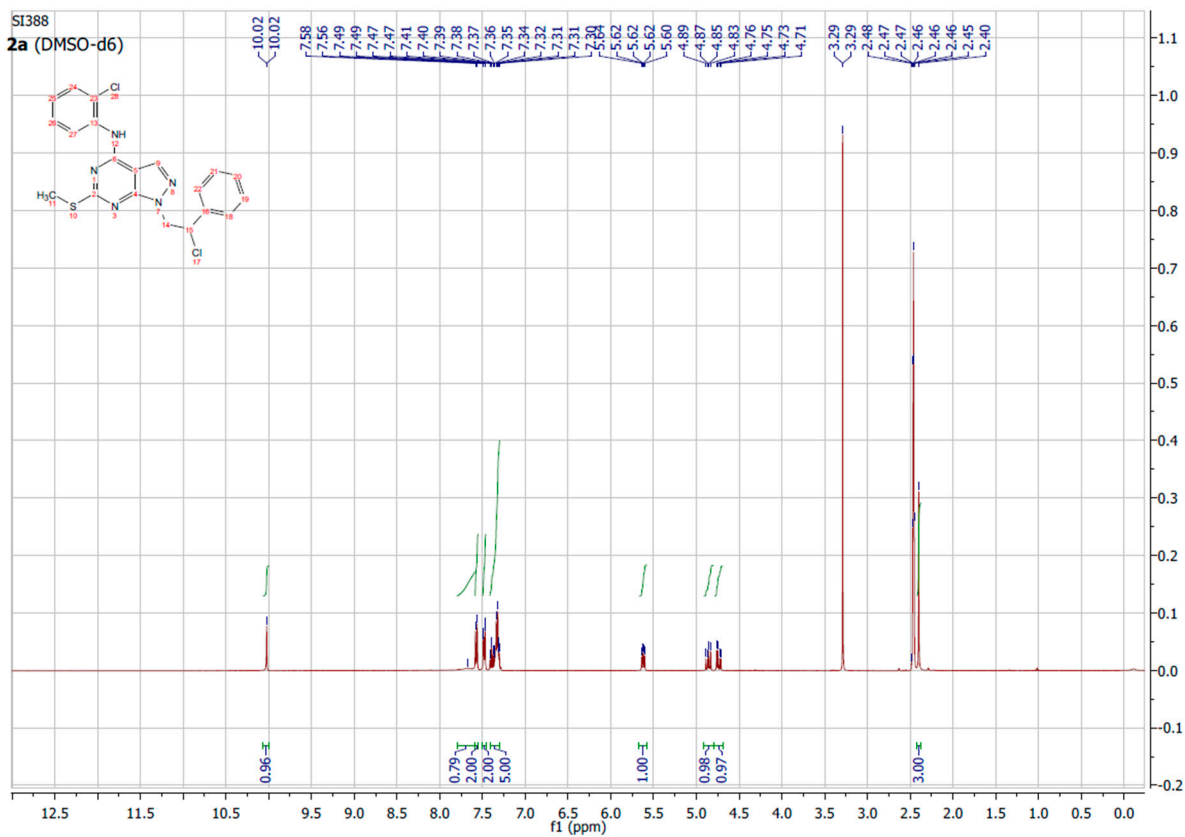
Table S1. Percentage of Src inhibition at 100, 10 and 1 μ M for compounds **2a-s**.

Cpd	% inhib Src			% inhib Fyn			% inhib Abl		
	100 μ M	10 μ M	1 μ M	100 μ M	10 μ M	1 μ M	100 μ M	10 μ M	1 μ M
2a	N.D.	90	N.D.	N.D.	90.7	x	N.D.	72	x
2b	N.D.	N.A.	24	N.D.	N.A.	N.A.	N.D.	23	N.A.
2c	N.D.	27	16	N.D.	64	33	N.D.	35	18
2d	99.5	34	N.D.	26	8	N.D.	N.D.	24	NA
2e	N.D.	N.A.	N.A.	N.D.	N.D.	N.D.	N.D.	26,3	NA
2f	N.D.	79	N.A.	N.D.	N.D.	N.D.	N.D.	67	3
2g	N.D.	93.6	43.3	N.D.	N.D.	N.D.	N.D.	83	33.5
2h	98.3	12	N.D.	82	57	N.D.	N.D.	N.A.	34
2i	98.8	56	N.D.	19	15	N.D.	N.D.	N.A.	N.A.
2j	95.3	5	N.D.	38	13	N.D.	N.D.	N.A.	39
2k	99.2	50.3	N.D.	66	47	N.D.	N.D.	39	N.A.
2l	N.D.	N.A.	N.A.	N.D.	10	19	N.D.	N.A.	40
2m	N.D.	67	N.A.	N.D.	20	2.50	N.D.	18	15
2n	N.D.	13	11	N.D.	23	16	N.D.	18	5
2o	N.D.	N.A.	N.A.	N.D.	8	N.A.	N.D.	N.A.	N.A.
2p	N.D.	55	14	N.D.	60	15	N.D.	12	N.A.
2q	N.D.	48	29	N.D.	78	24	N.D.	25	20
2r	N.D.	7.5	N.A.	N.D.	75	48	N.D.	N.A.	N.A.

2s	N.D.	19	24	N.D.	54	N.A.	N.D.	23	N.A.
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N.D. = Not determined

N.A. = Not Active



PM931 - 2b

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

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Pulse 28.8 degrees

Acq. time 2.000 sec

Width 4000.0 Hz

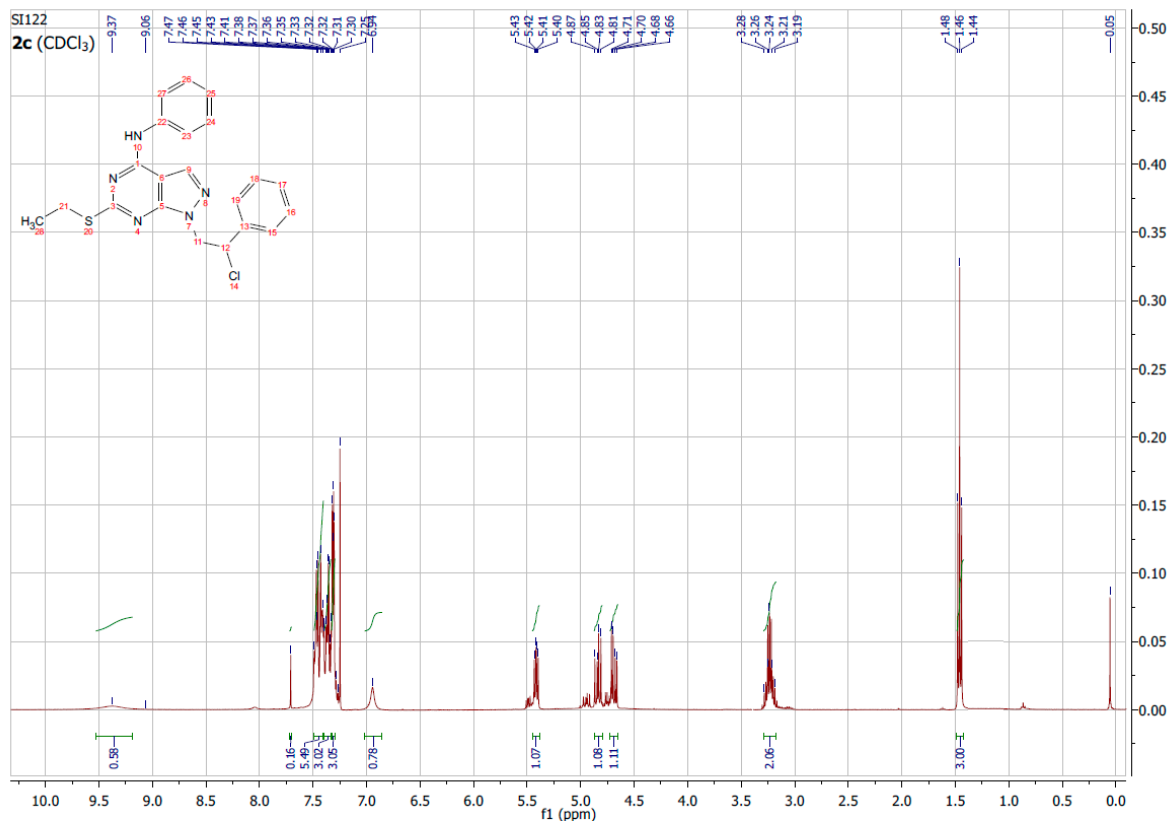
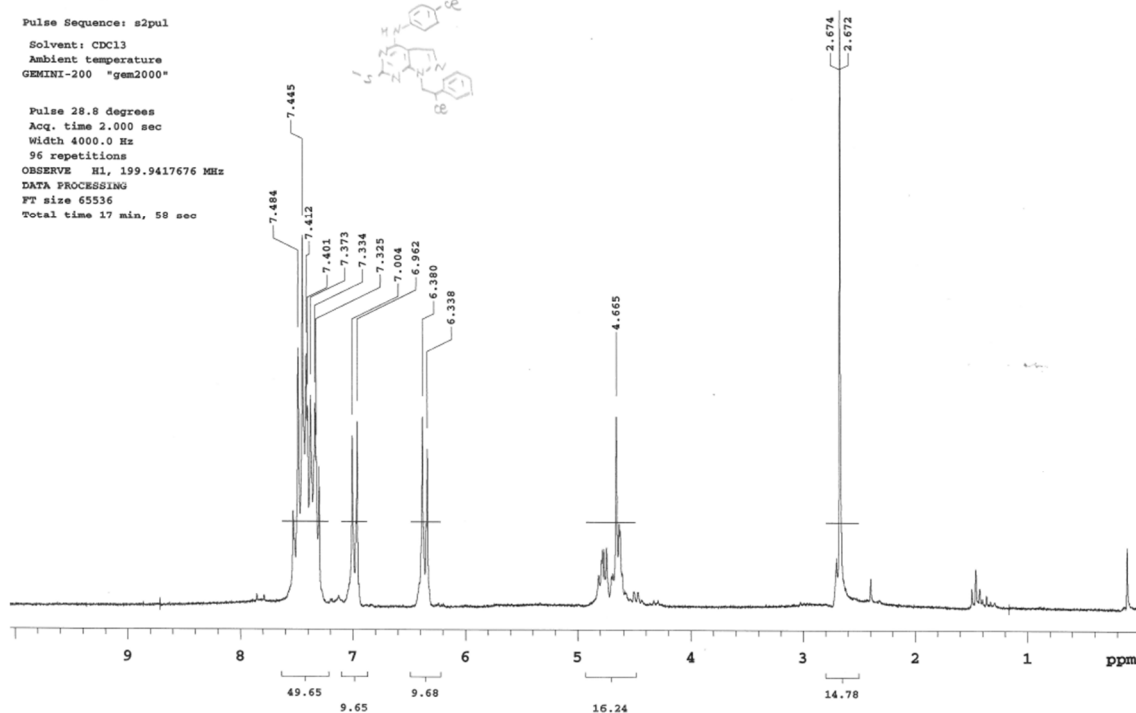
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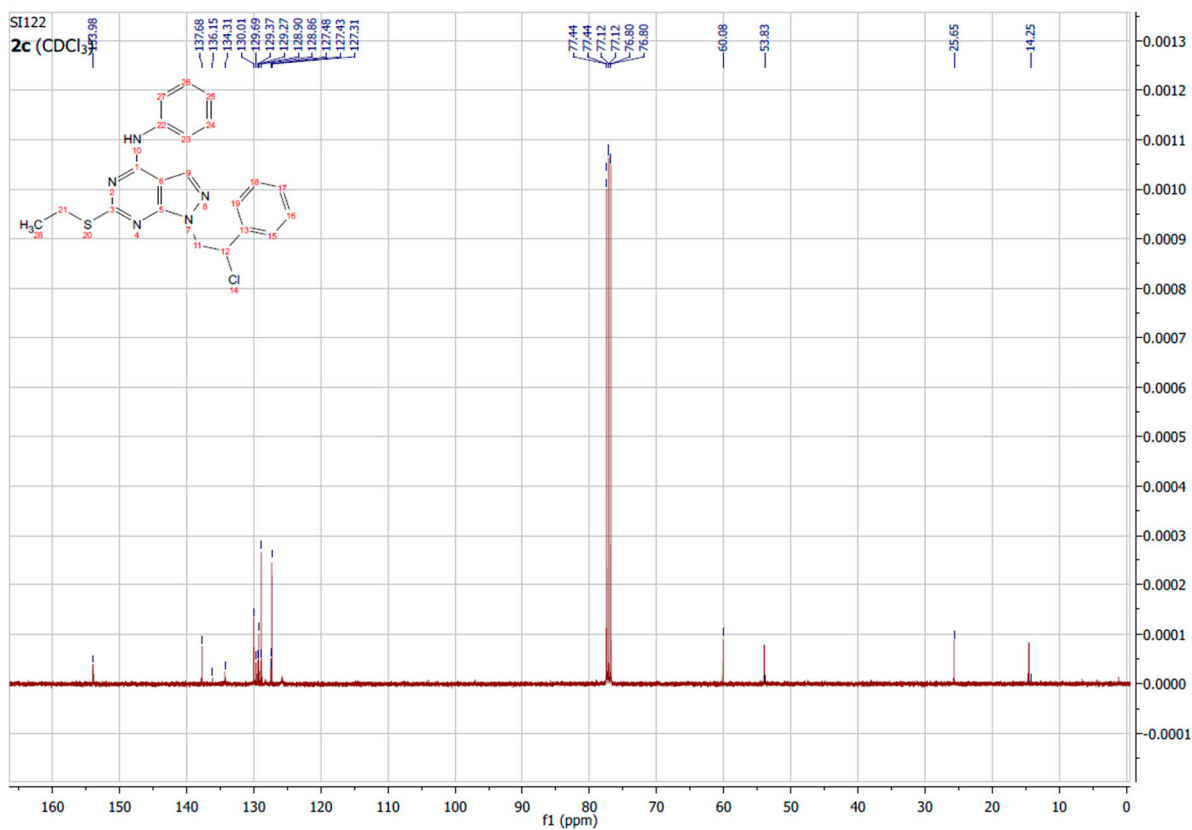
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DATA PROCESSING

FT size 65536

Total time 17 min, 58 sec





SI143 - 2b

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

GEMINI-200 "gem2000"

Pulse 28.8 degrees

Acq. time 2.000 sec

Width 4000.0 Hz

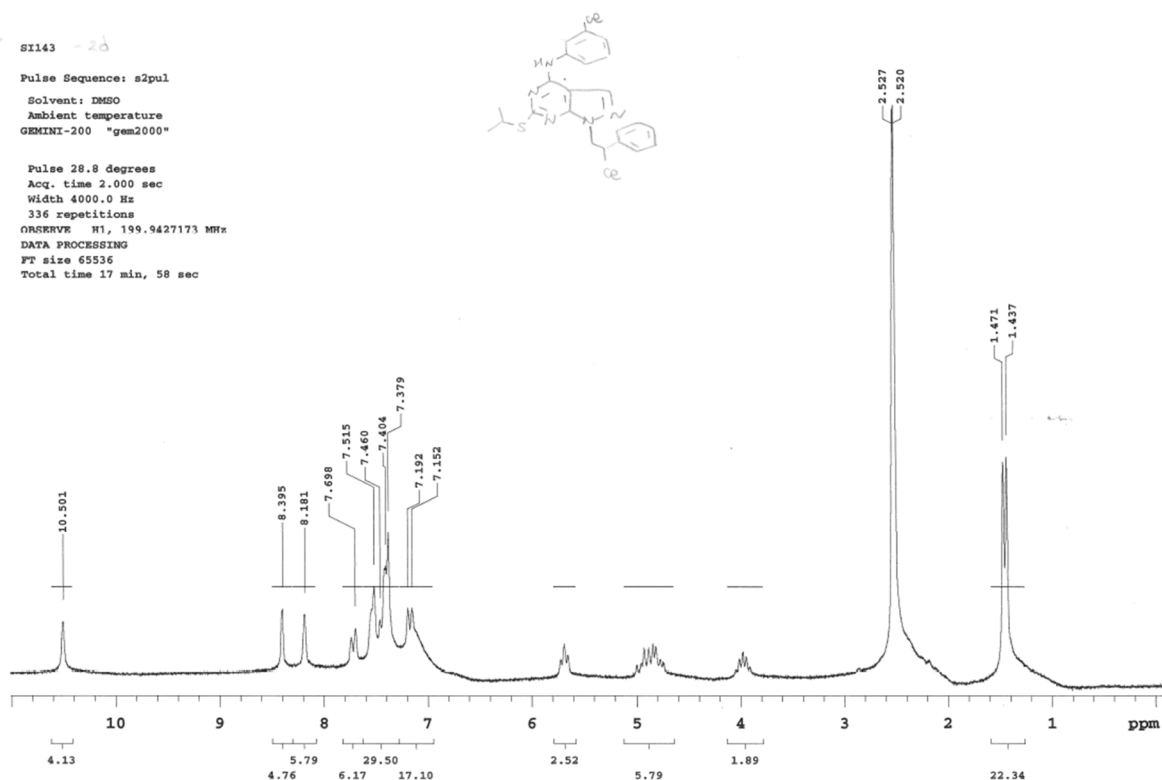
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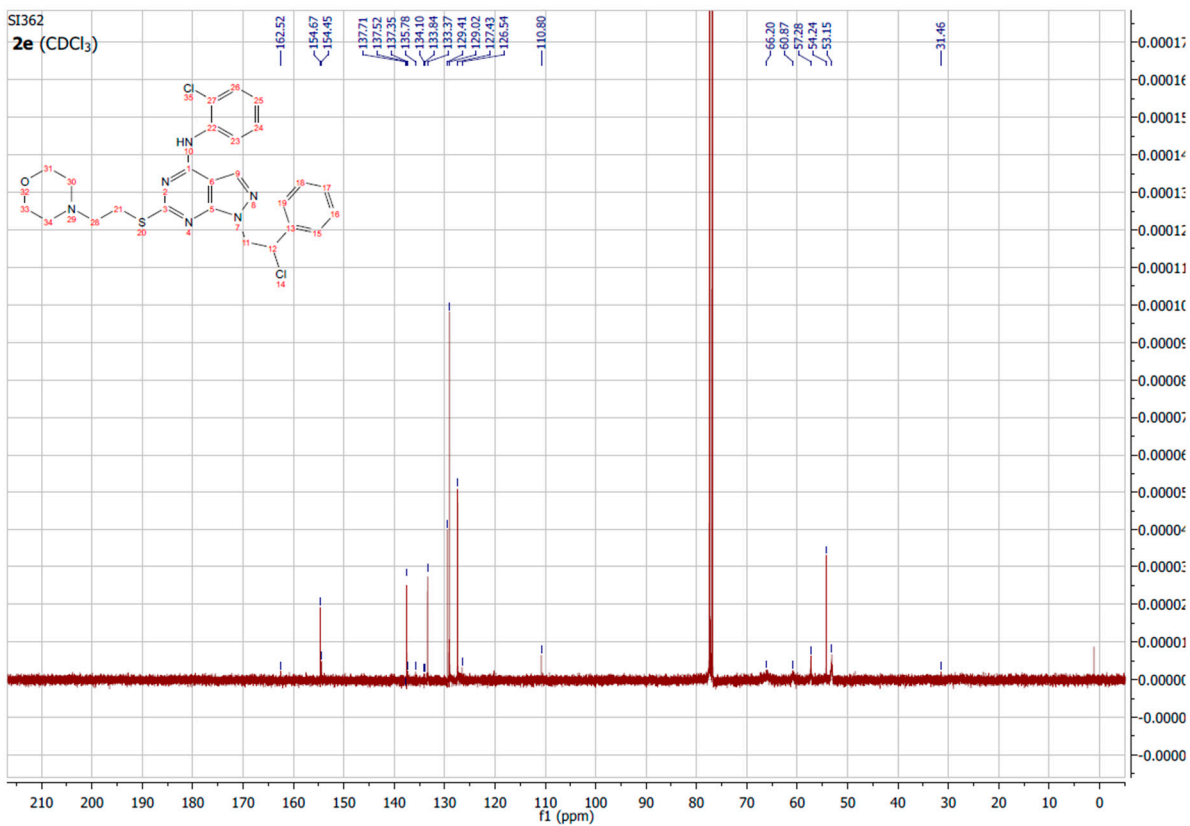
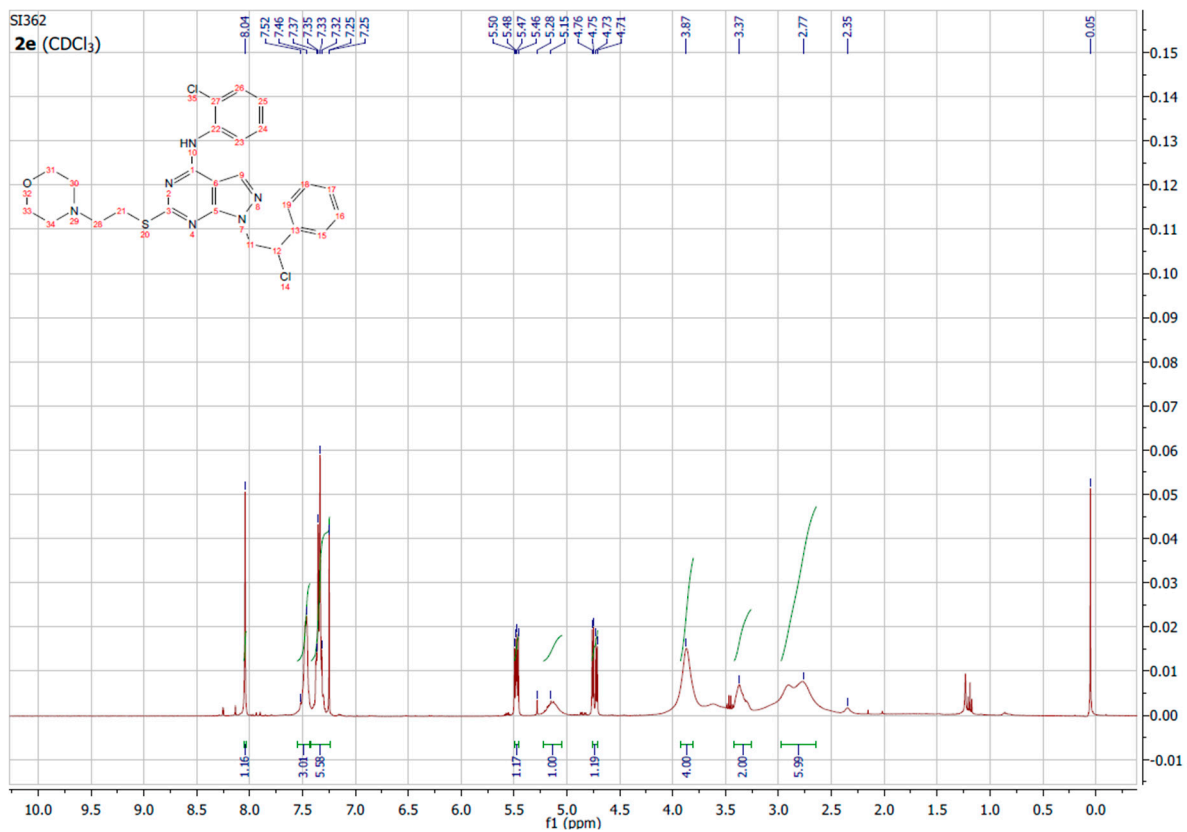
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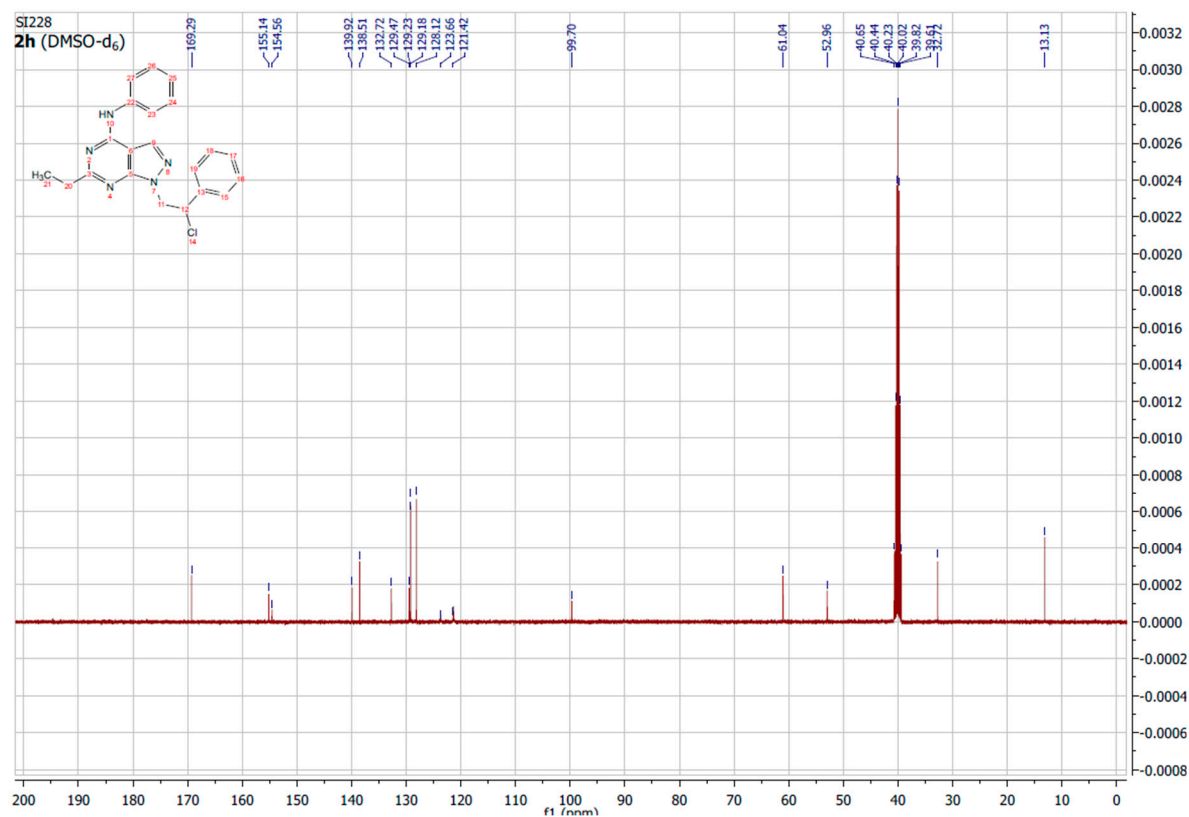
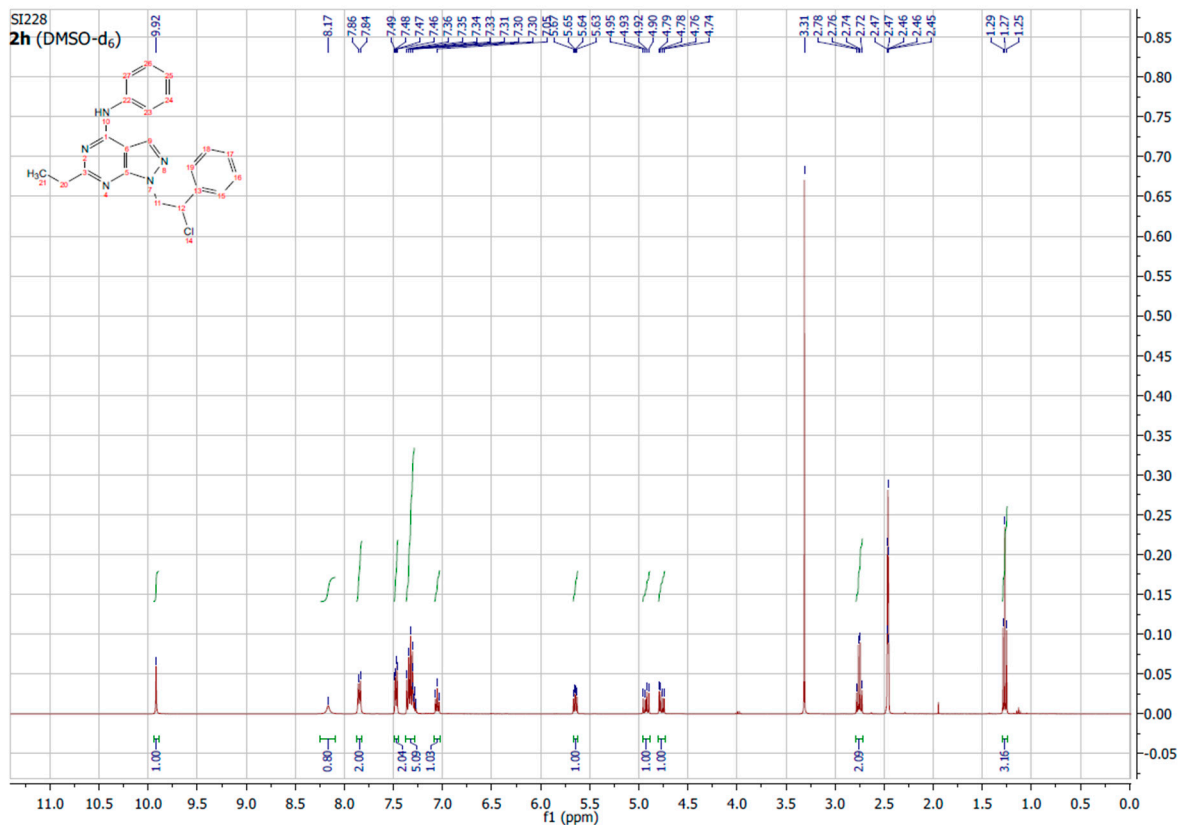
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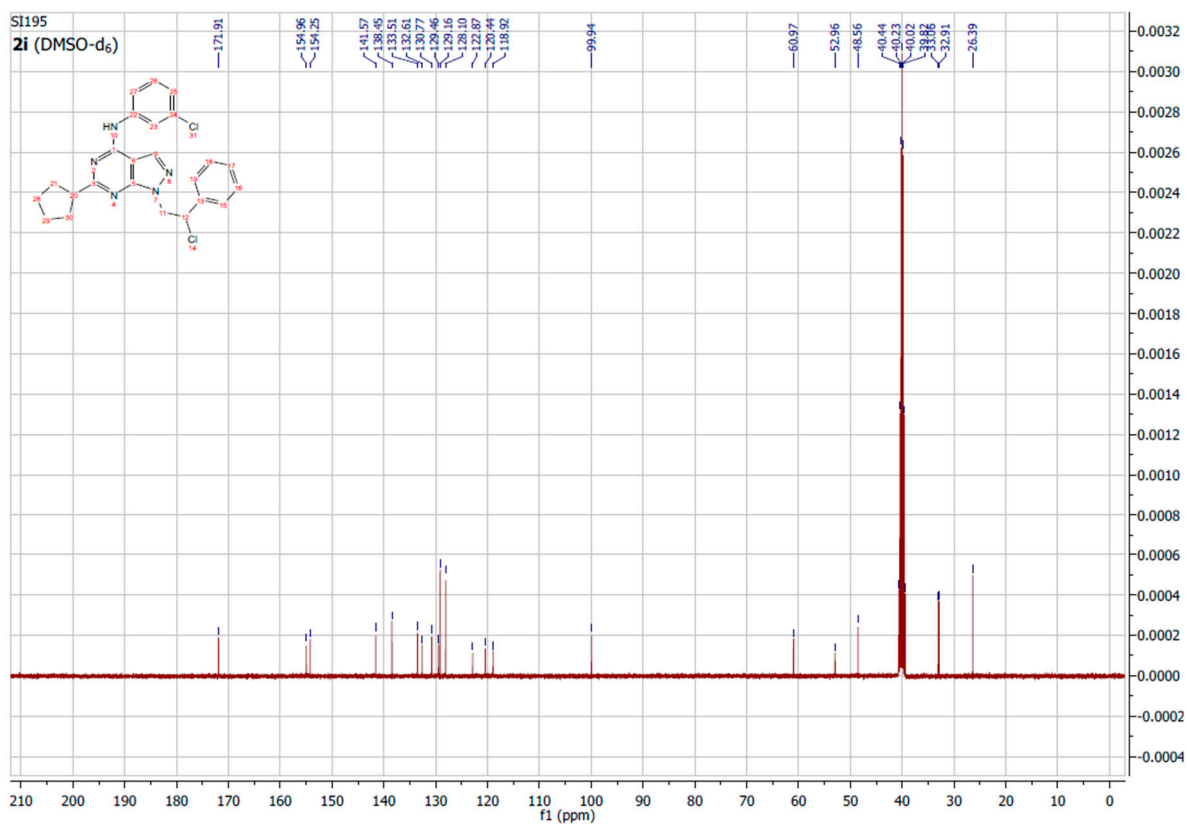
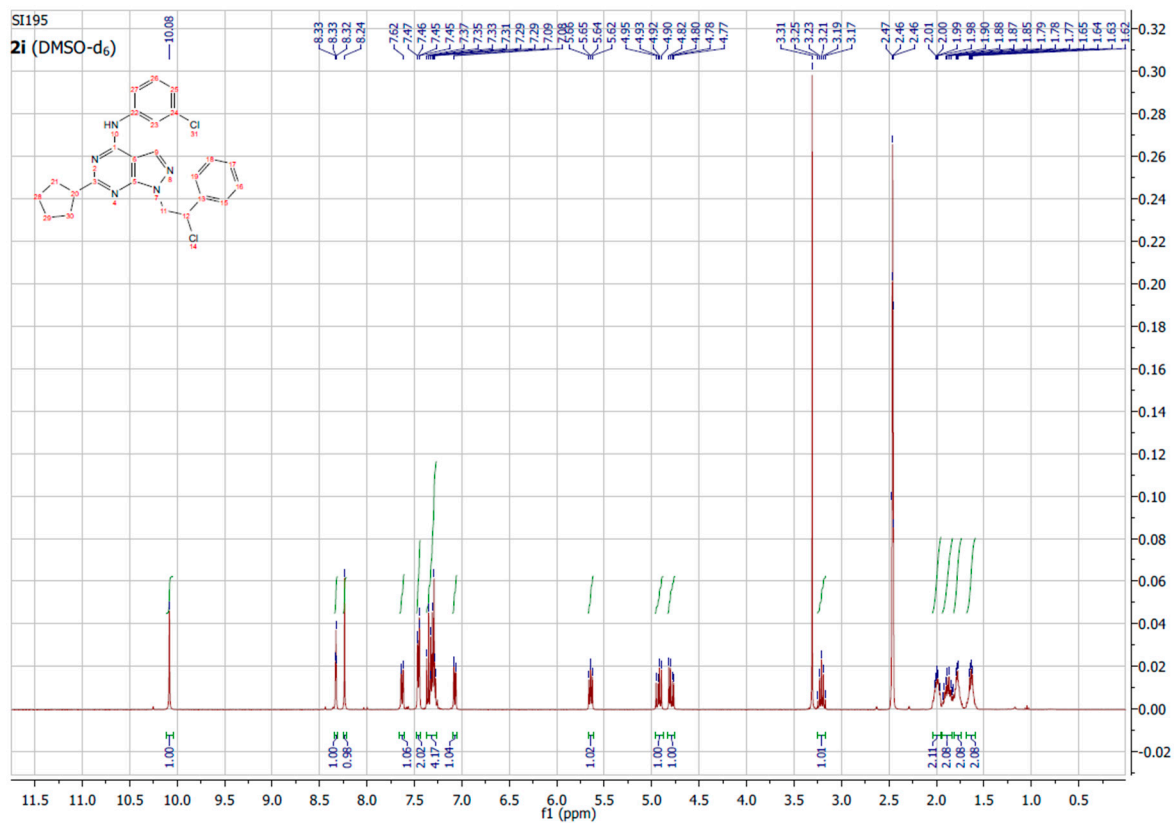
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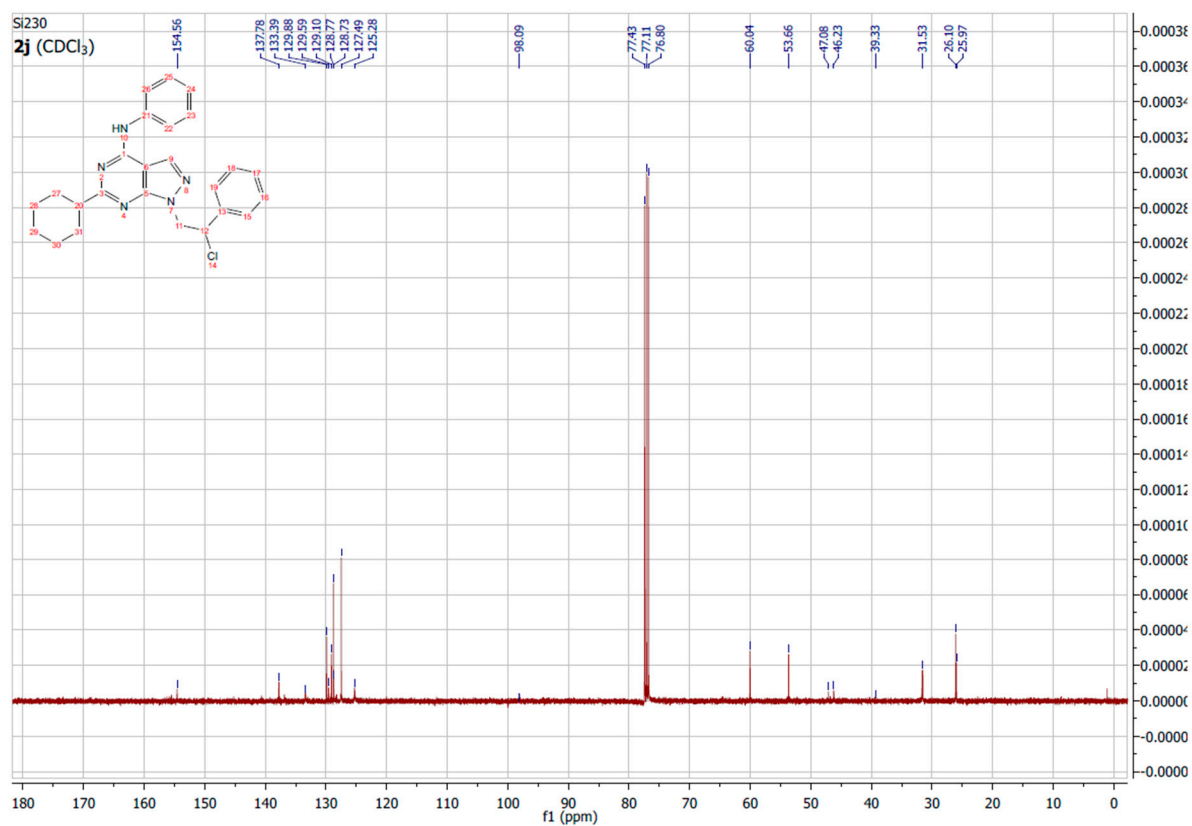
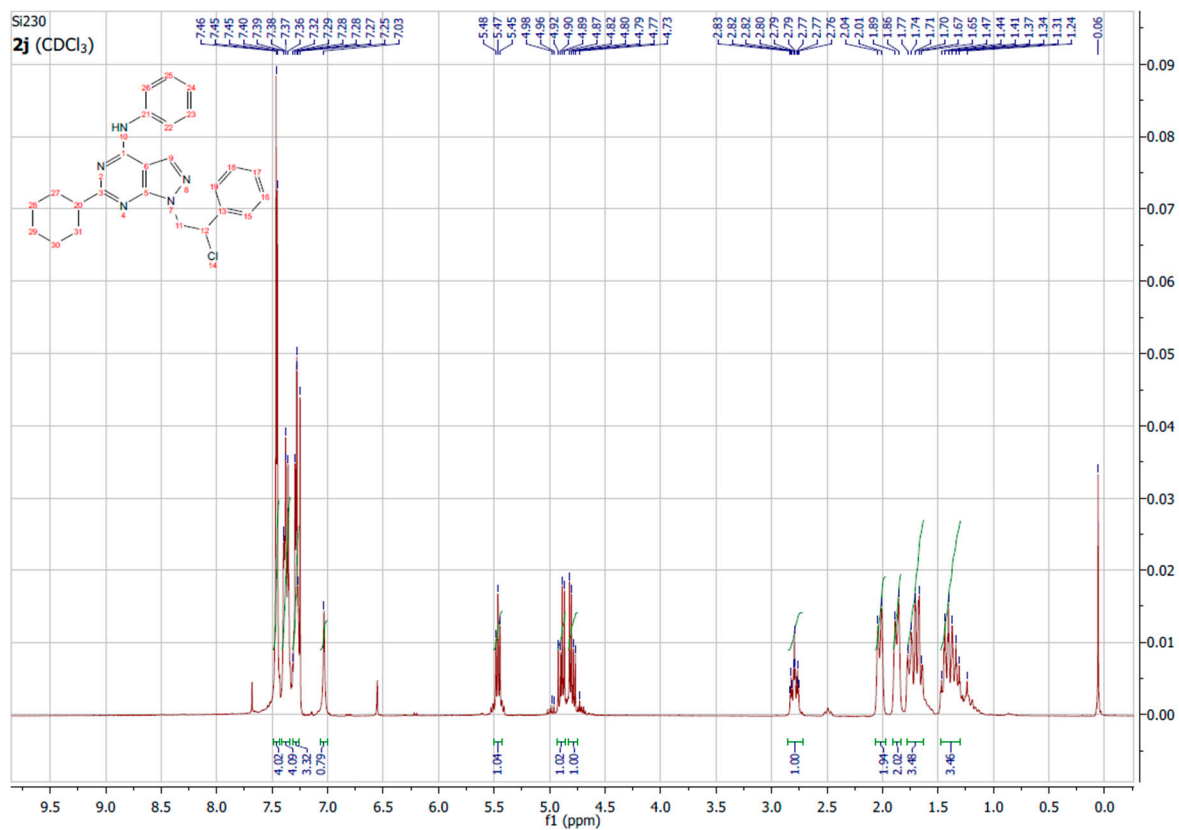
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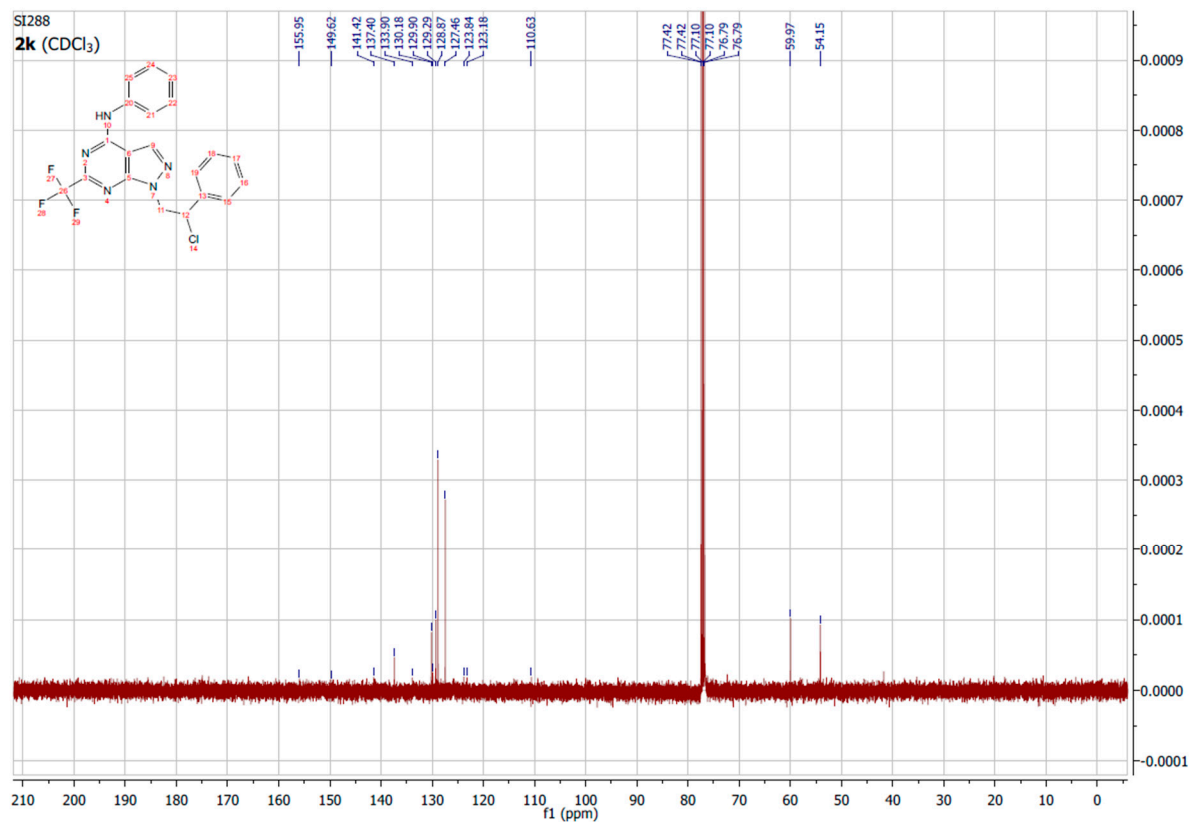
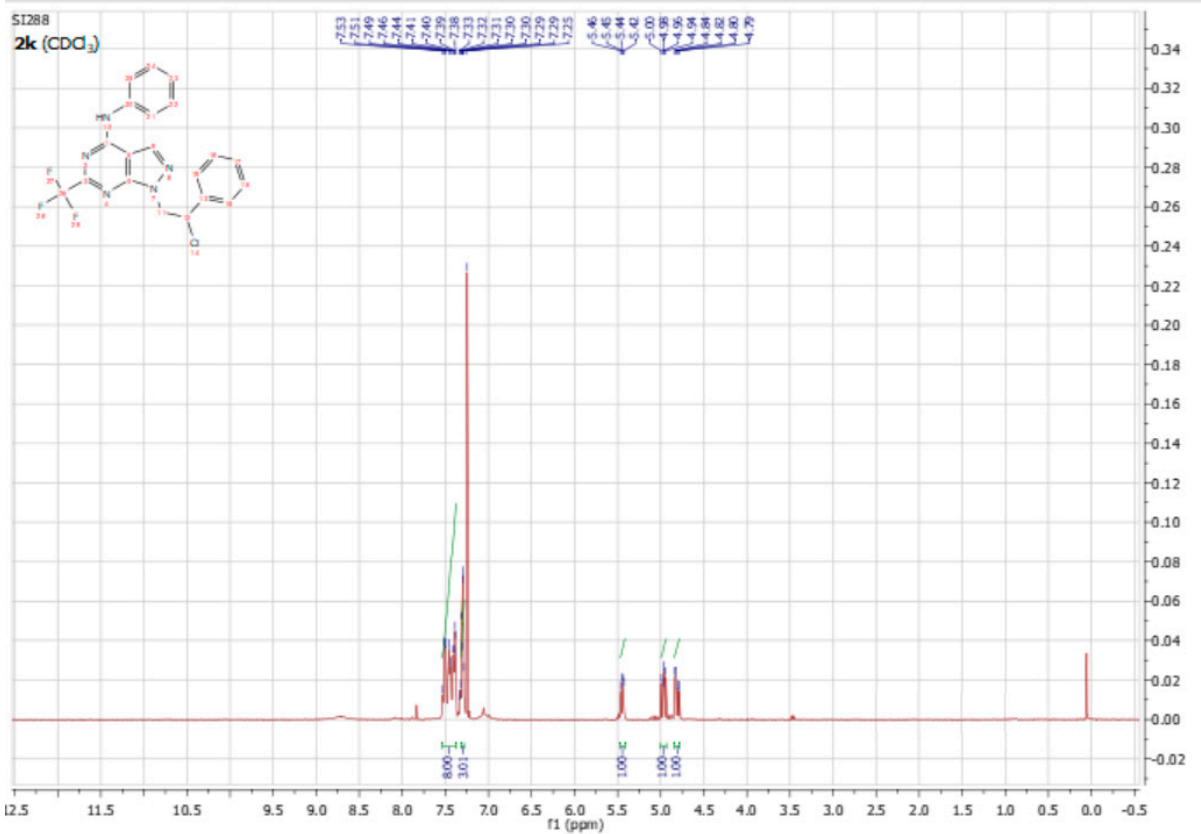


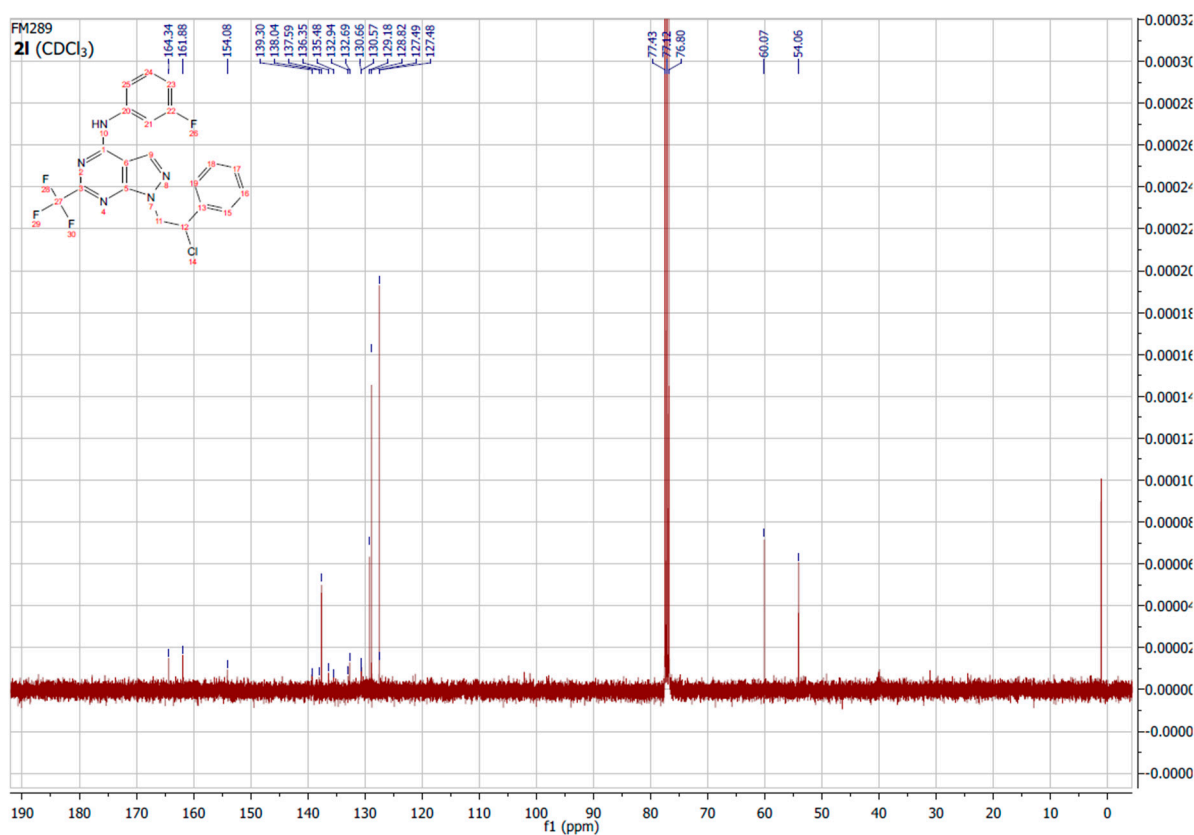
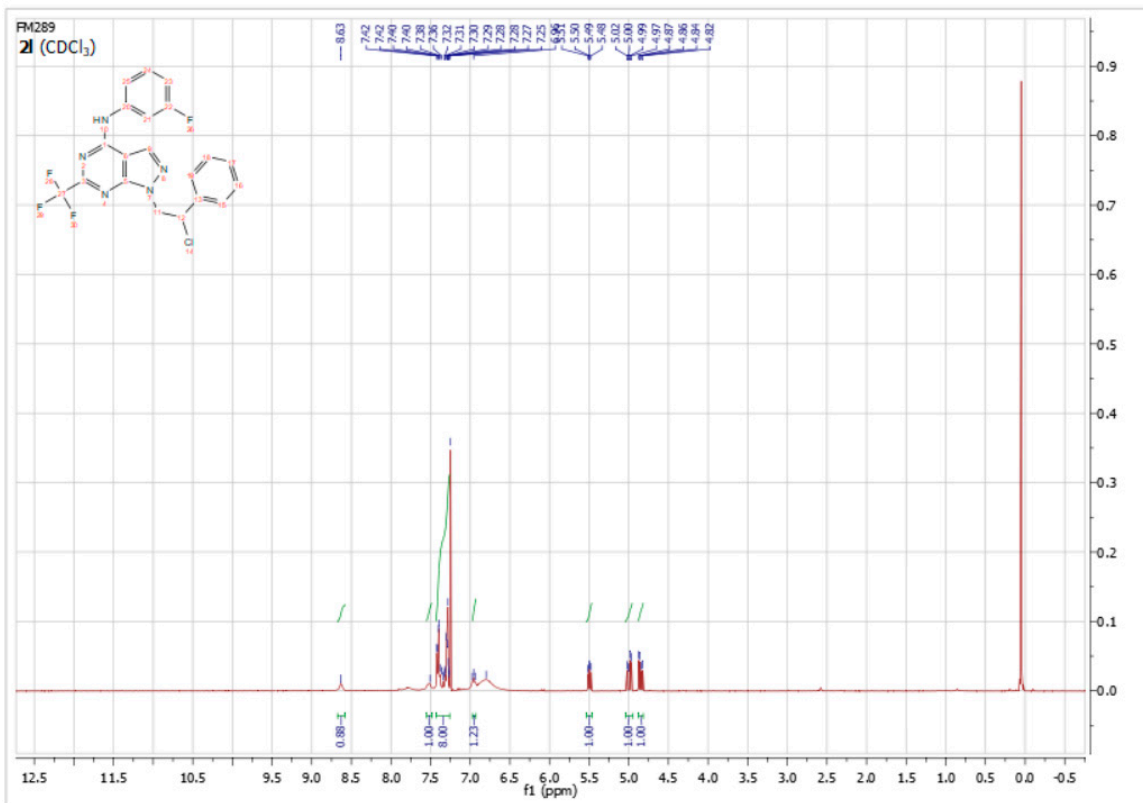


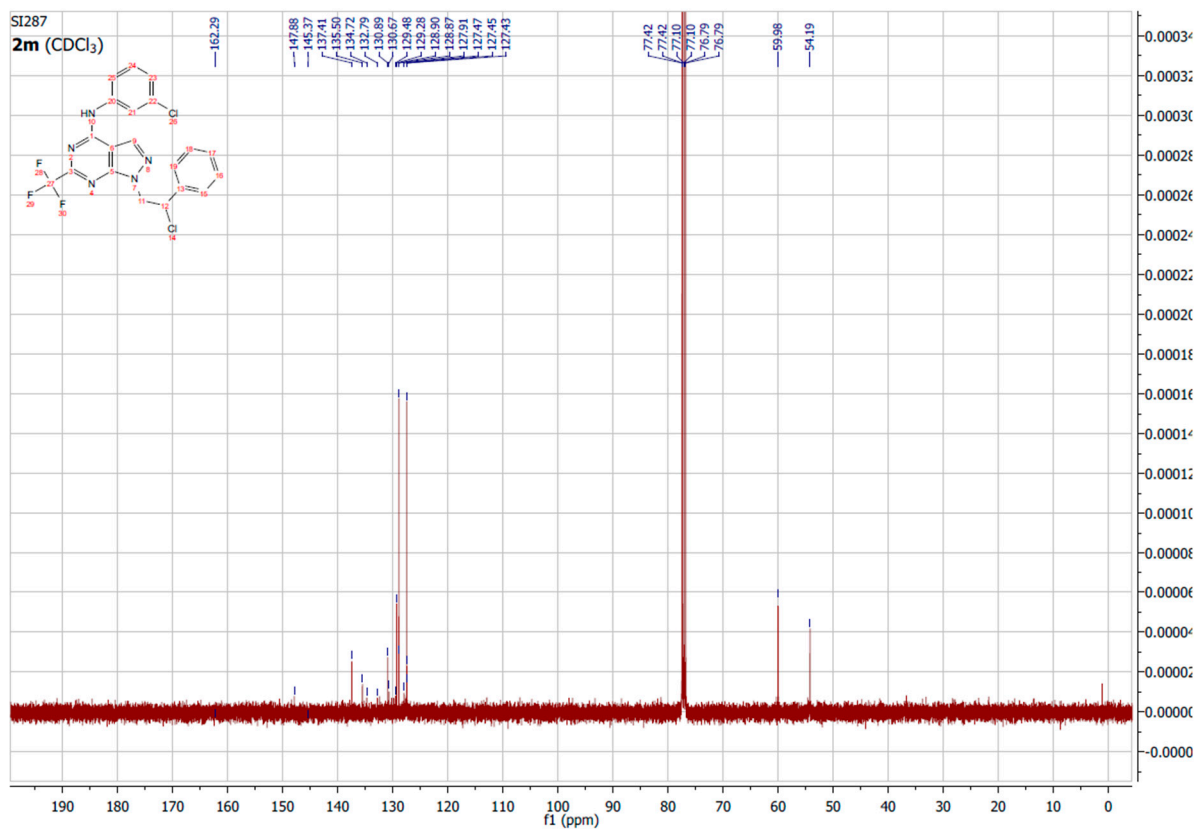
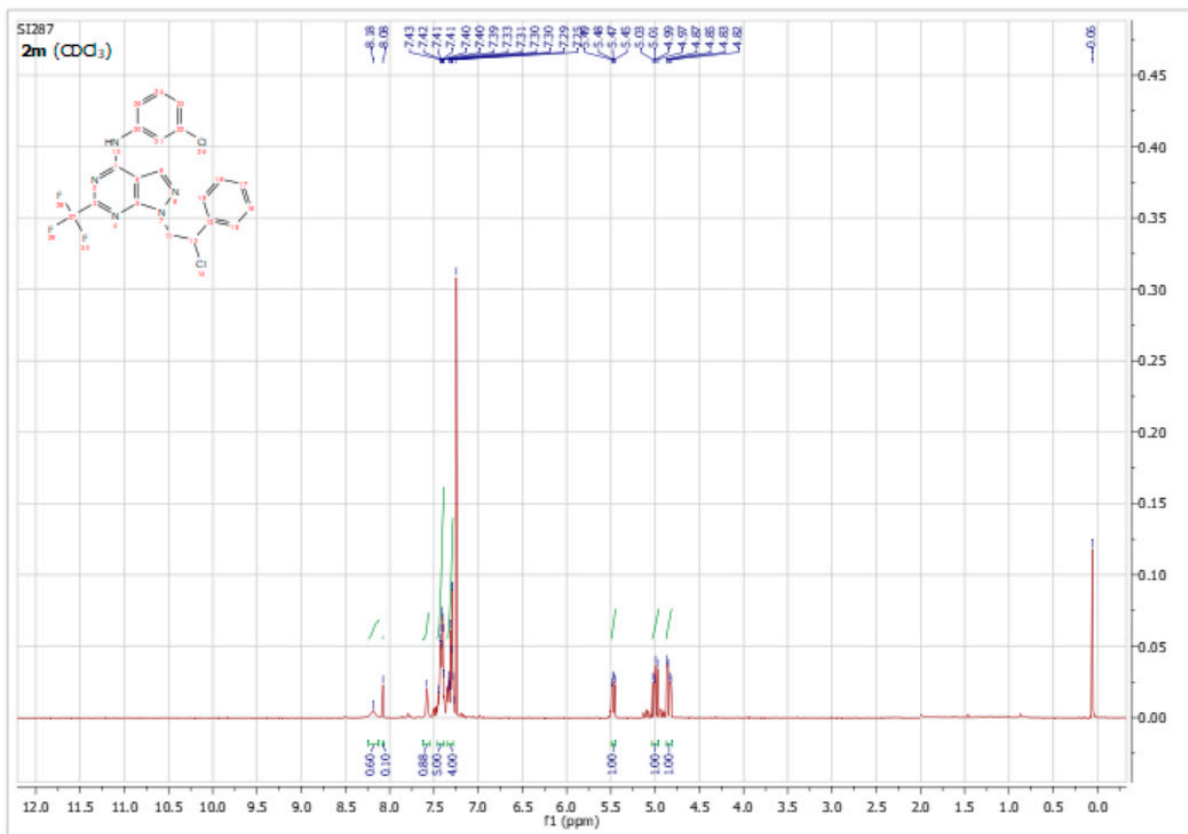


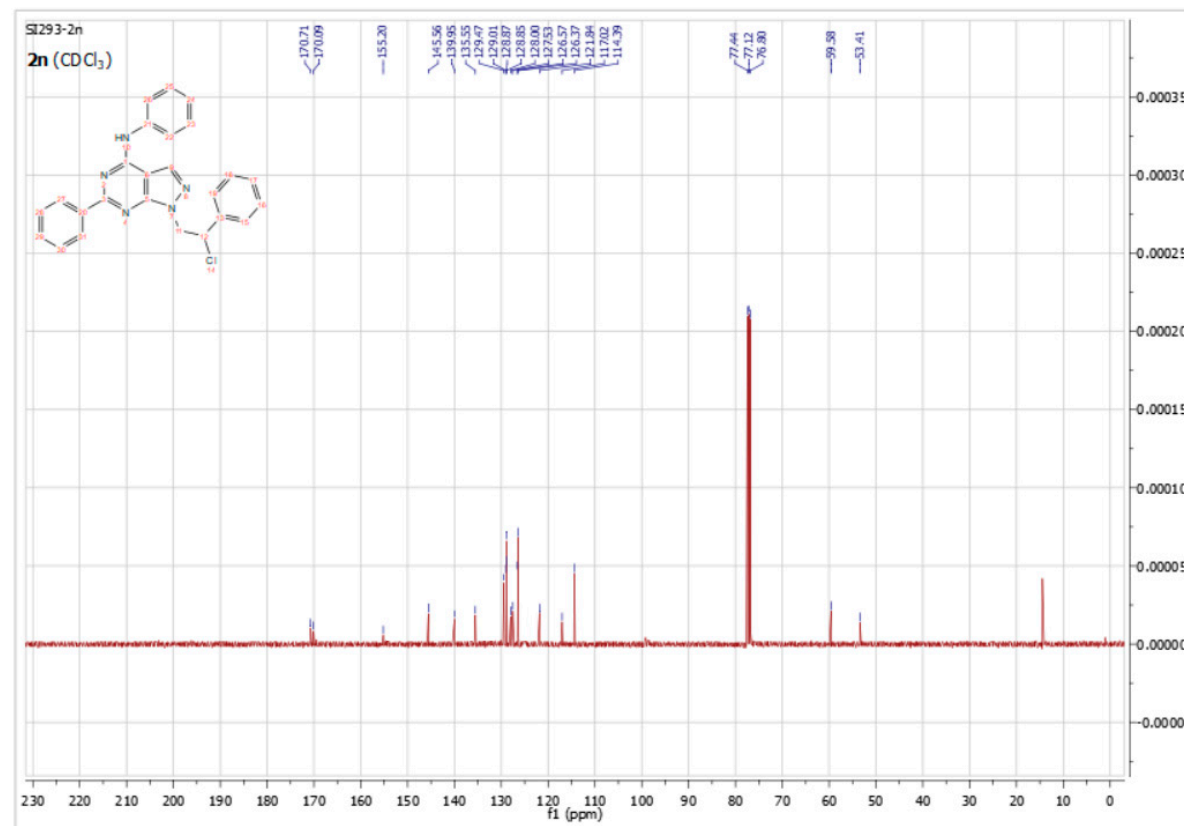
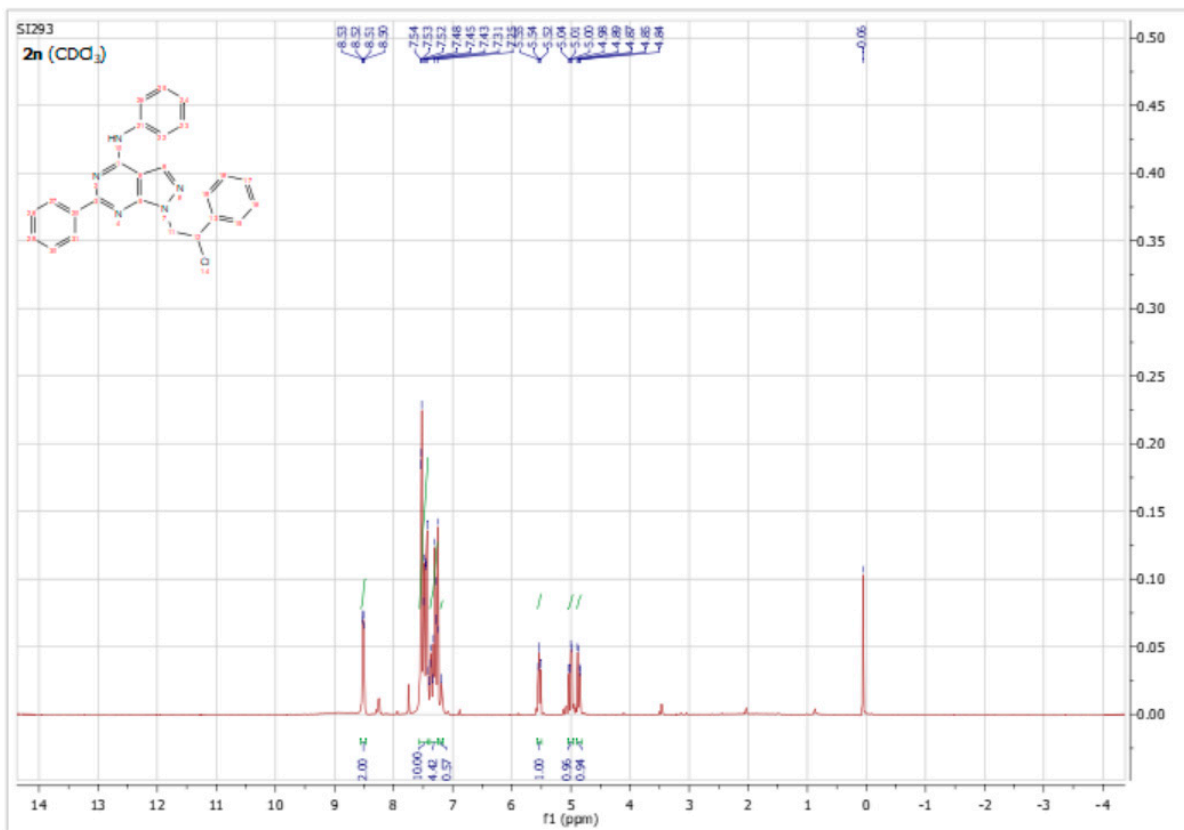


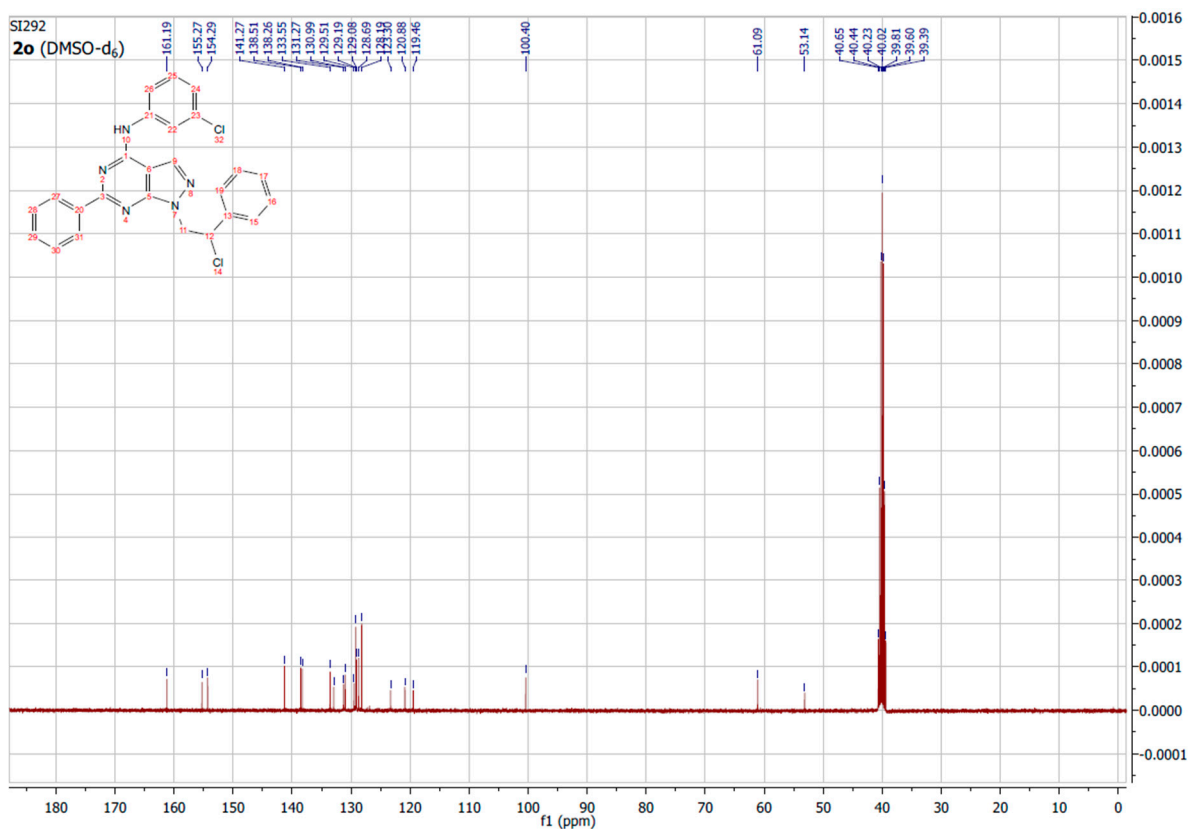
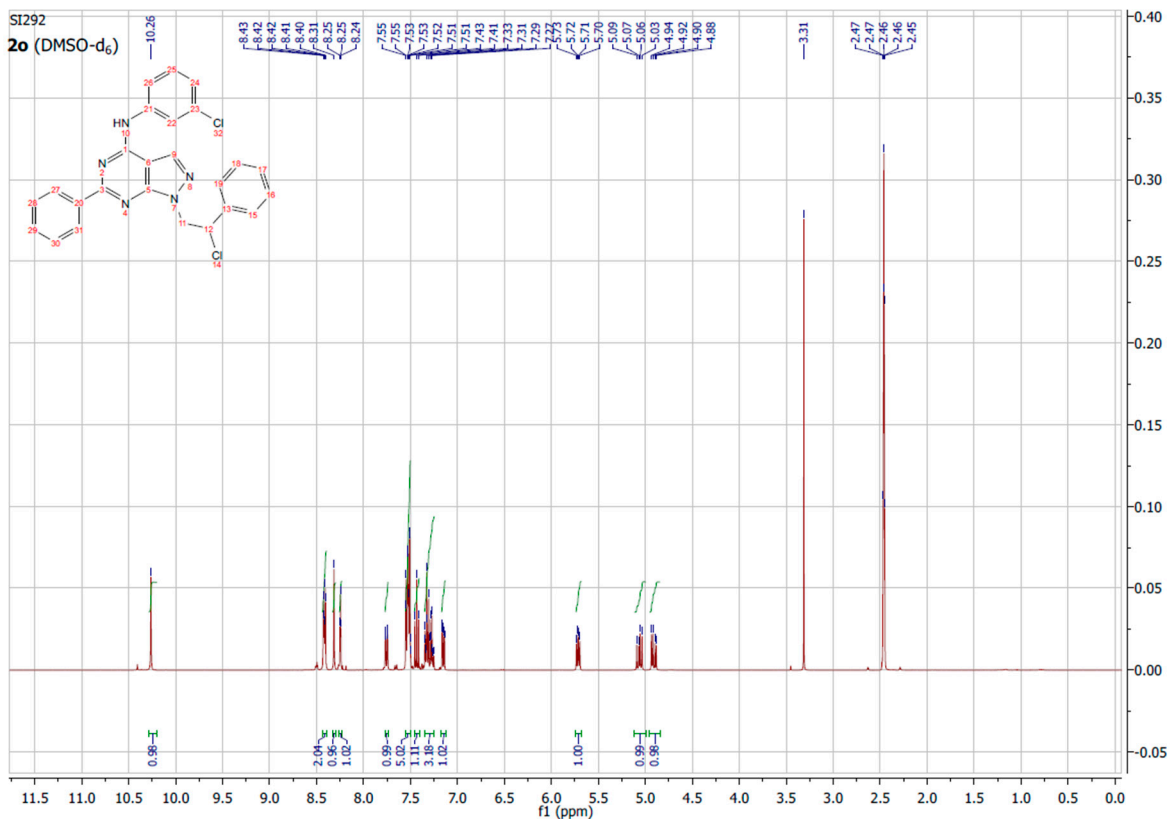


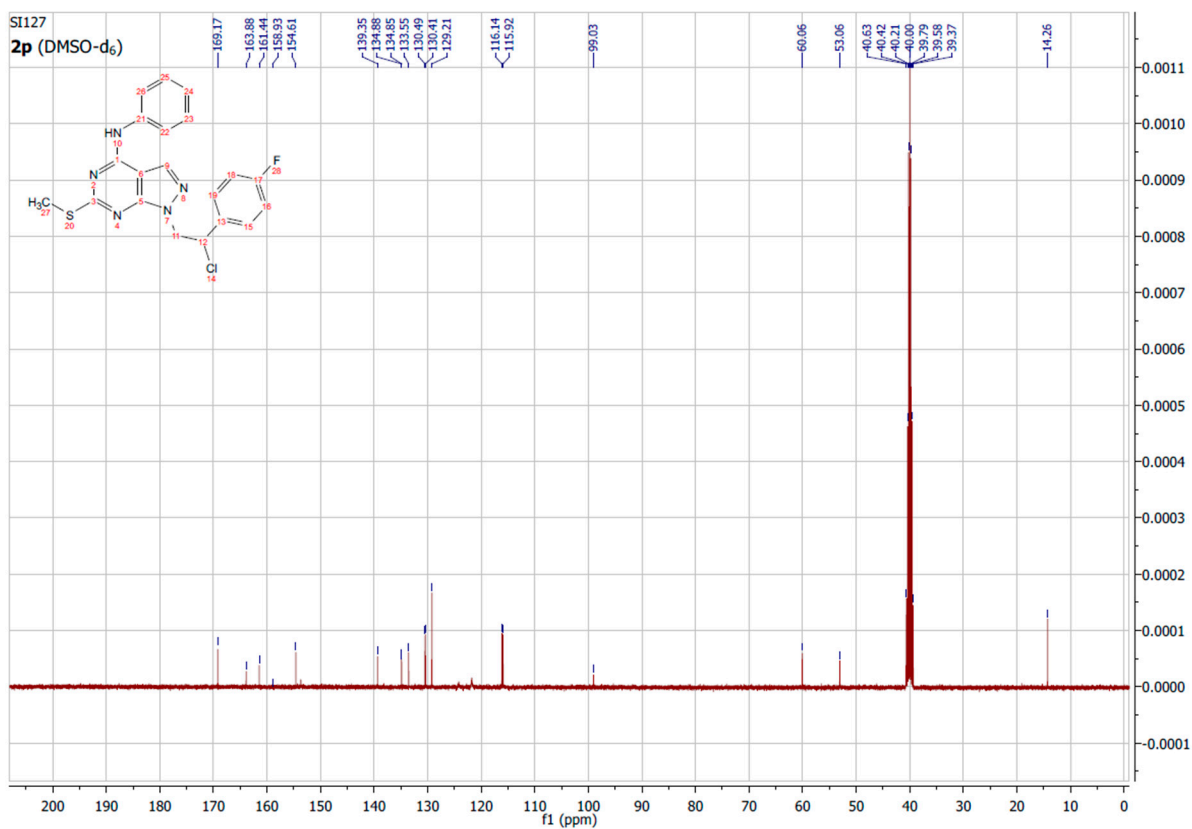
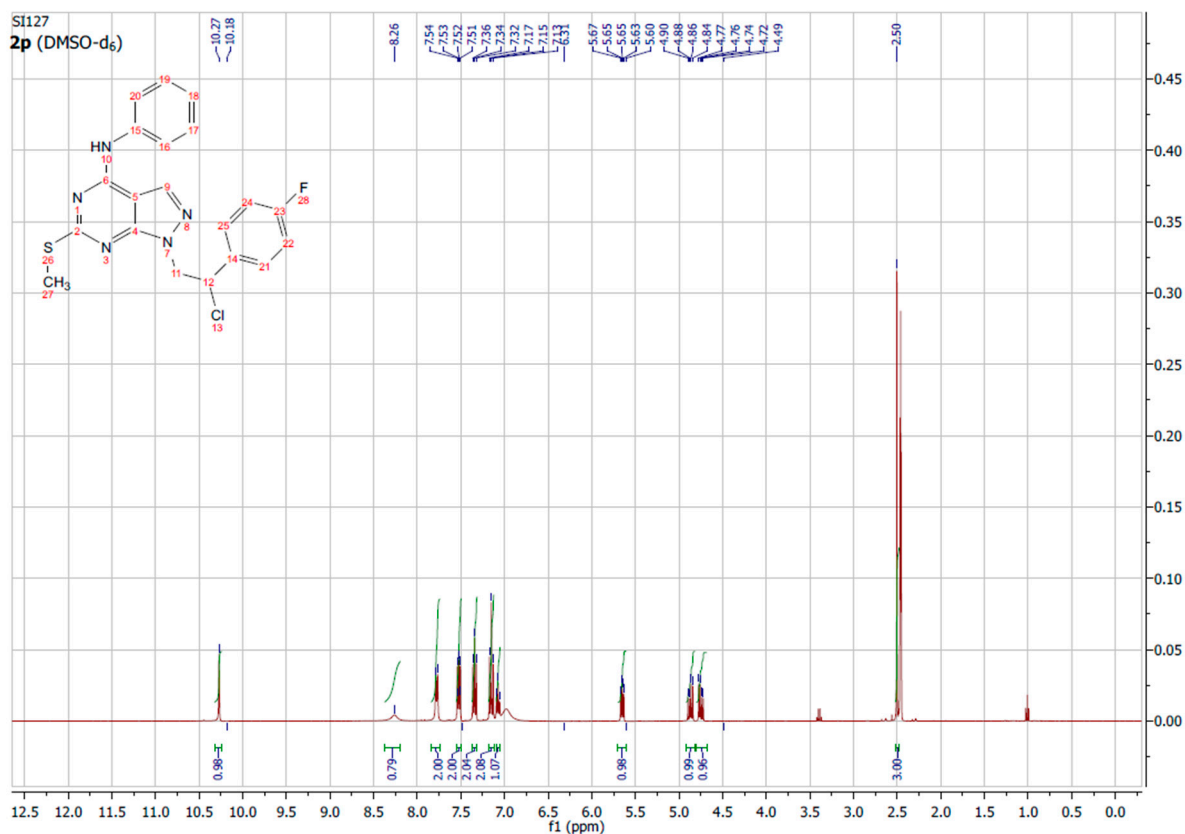


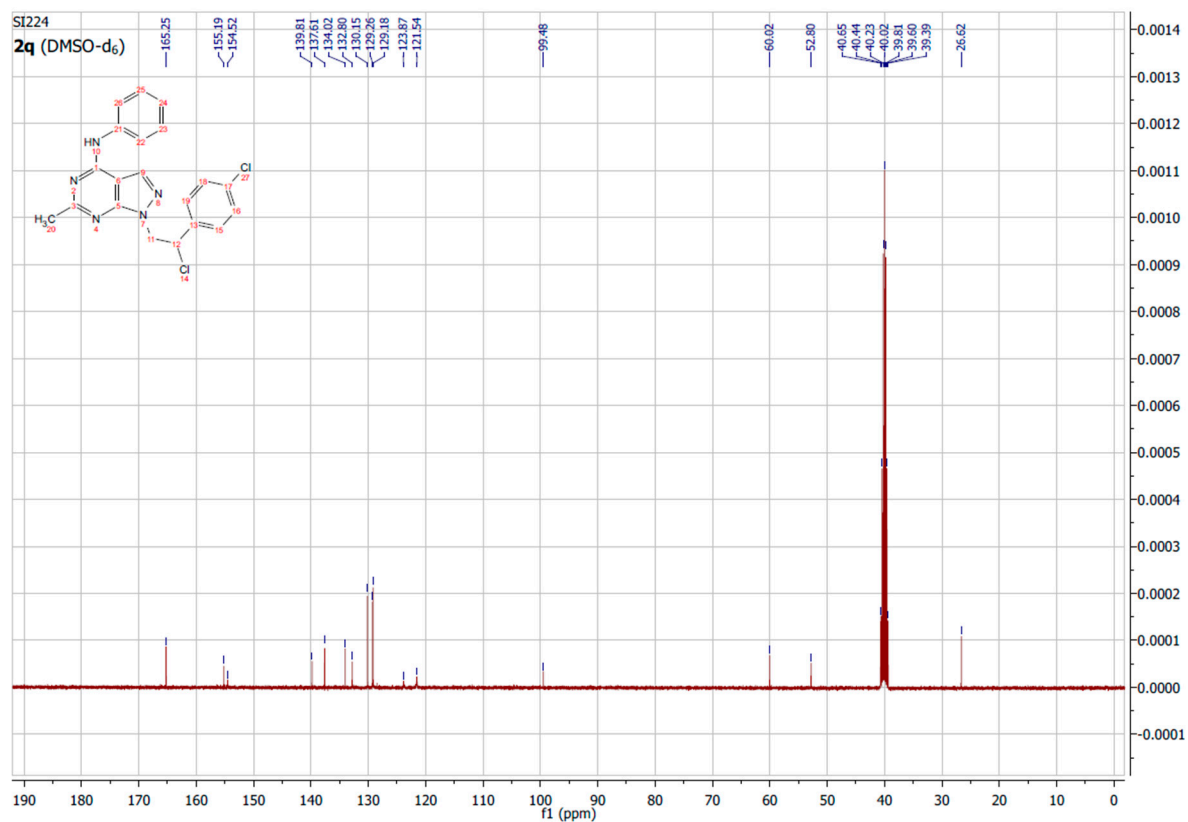
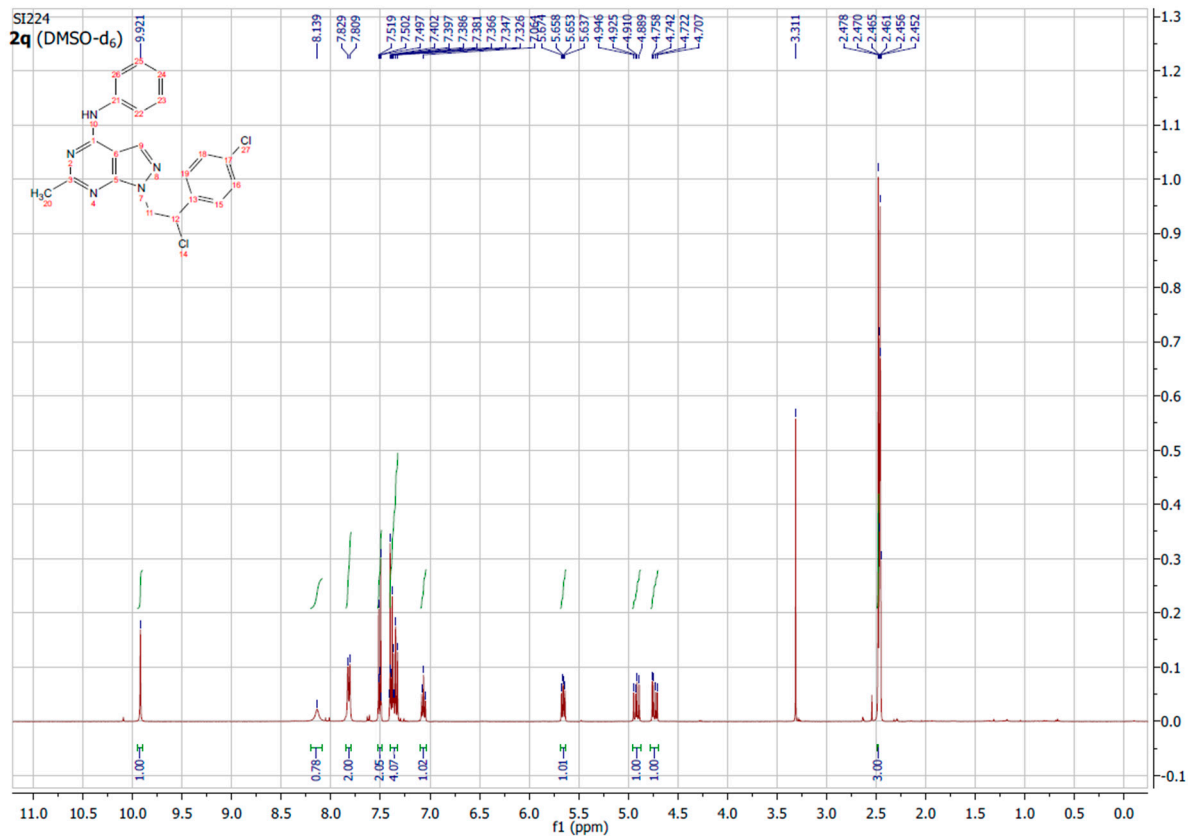


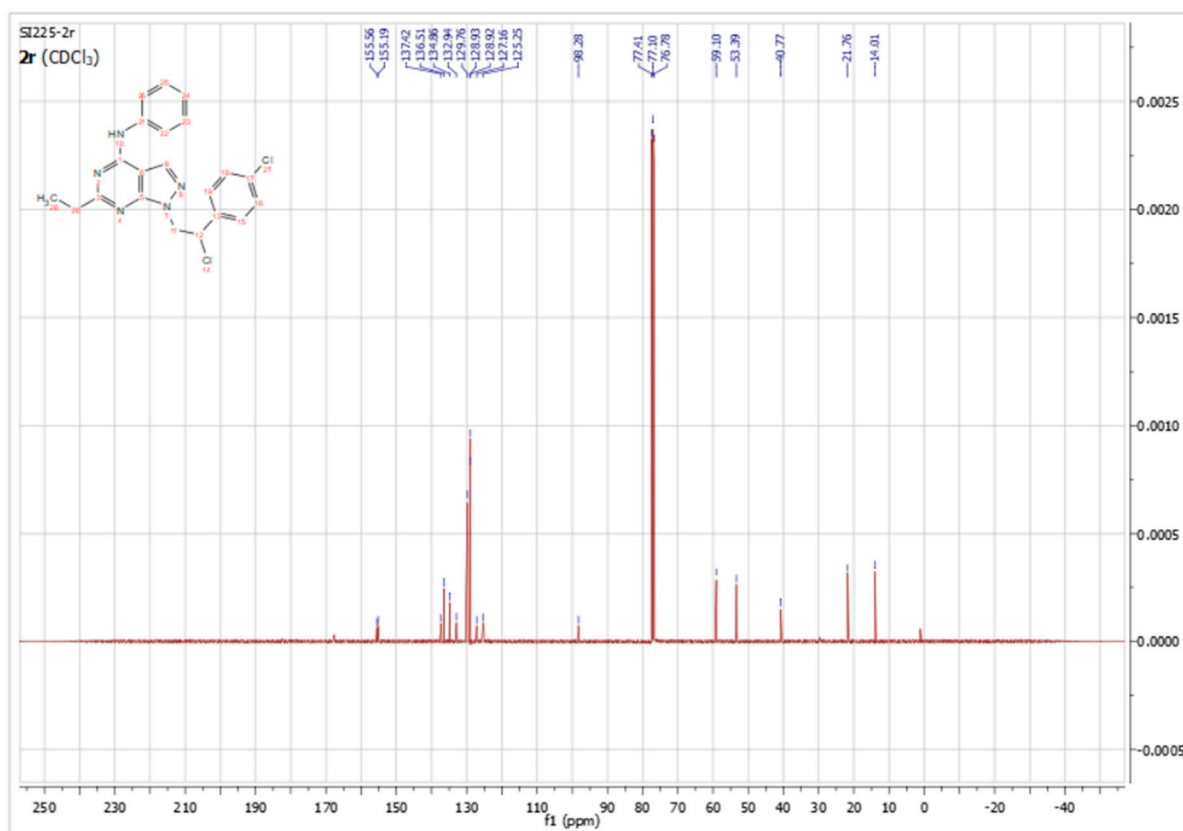
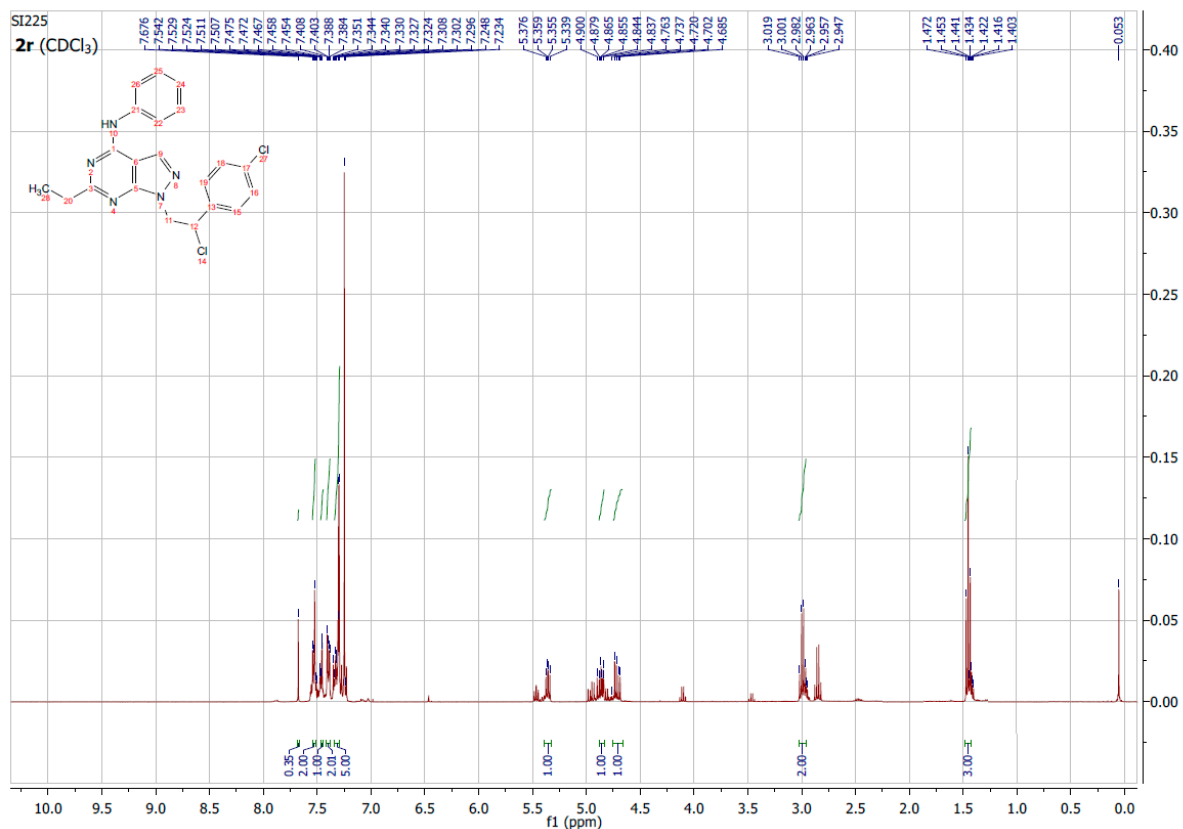


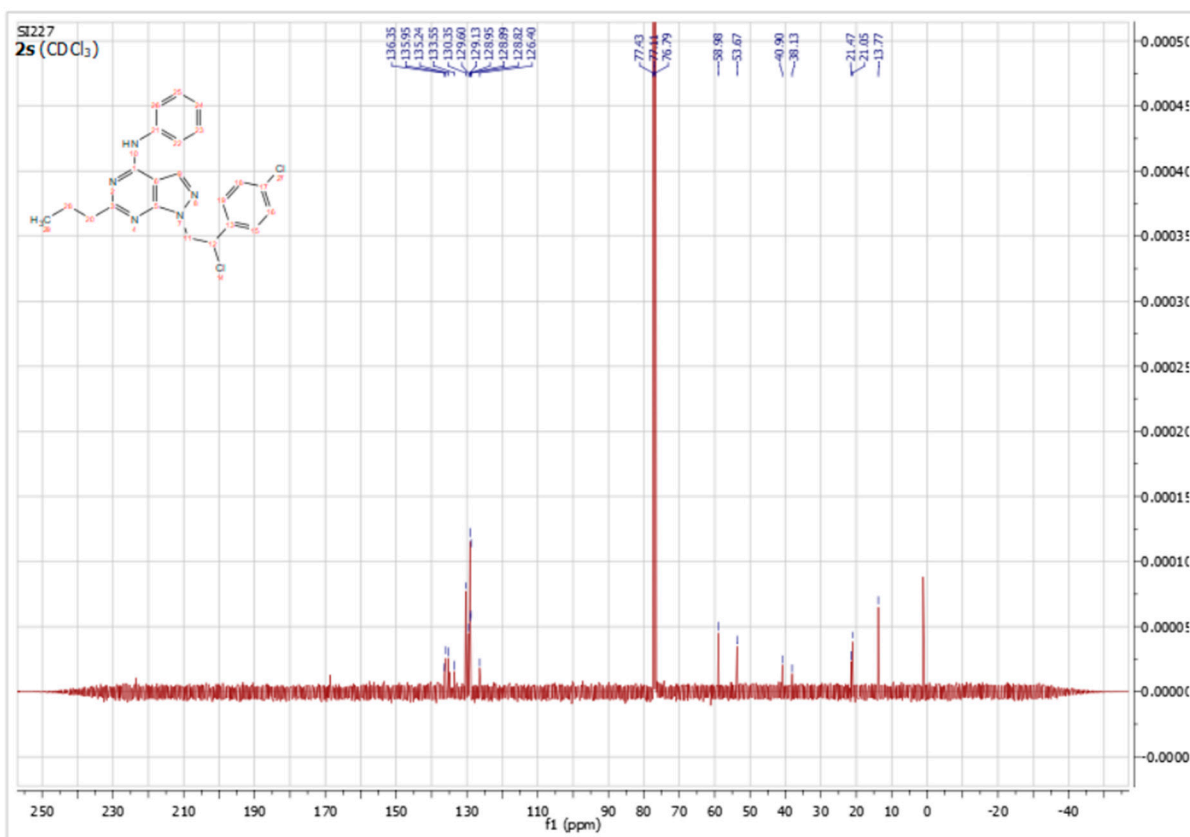
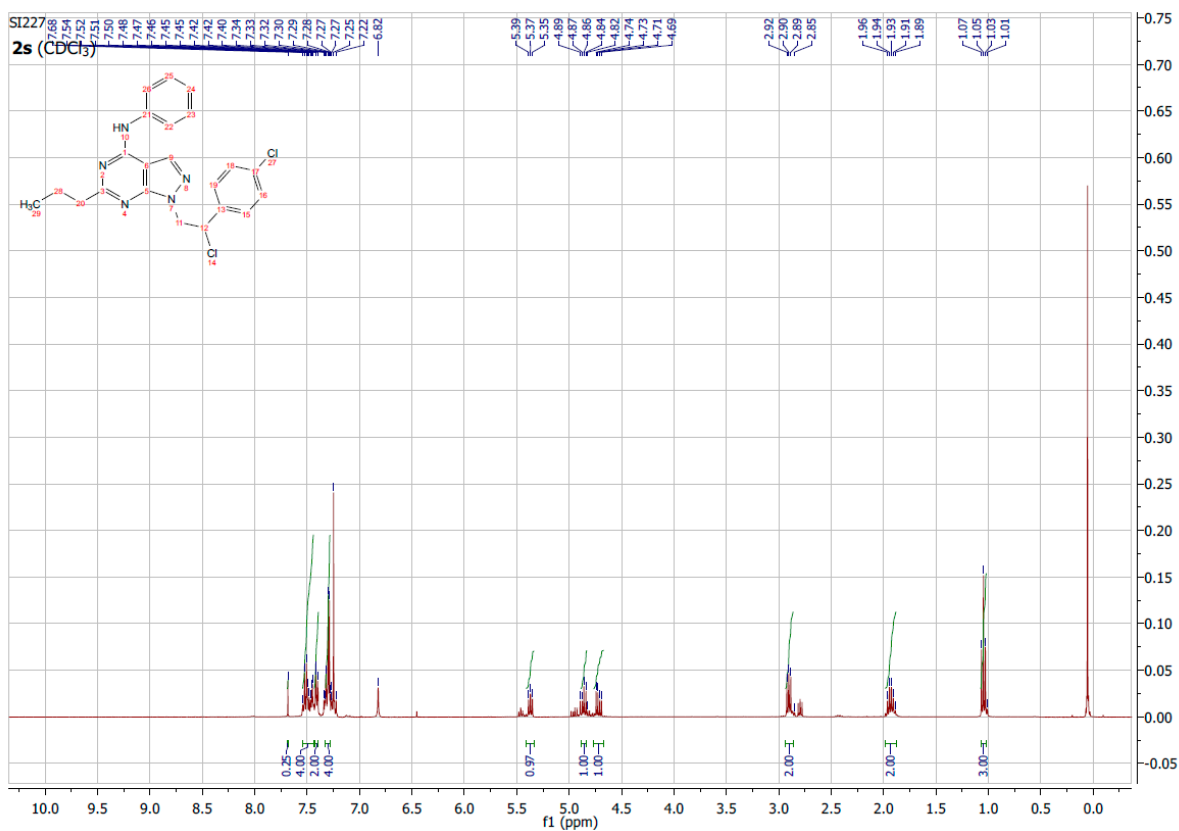


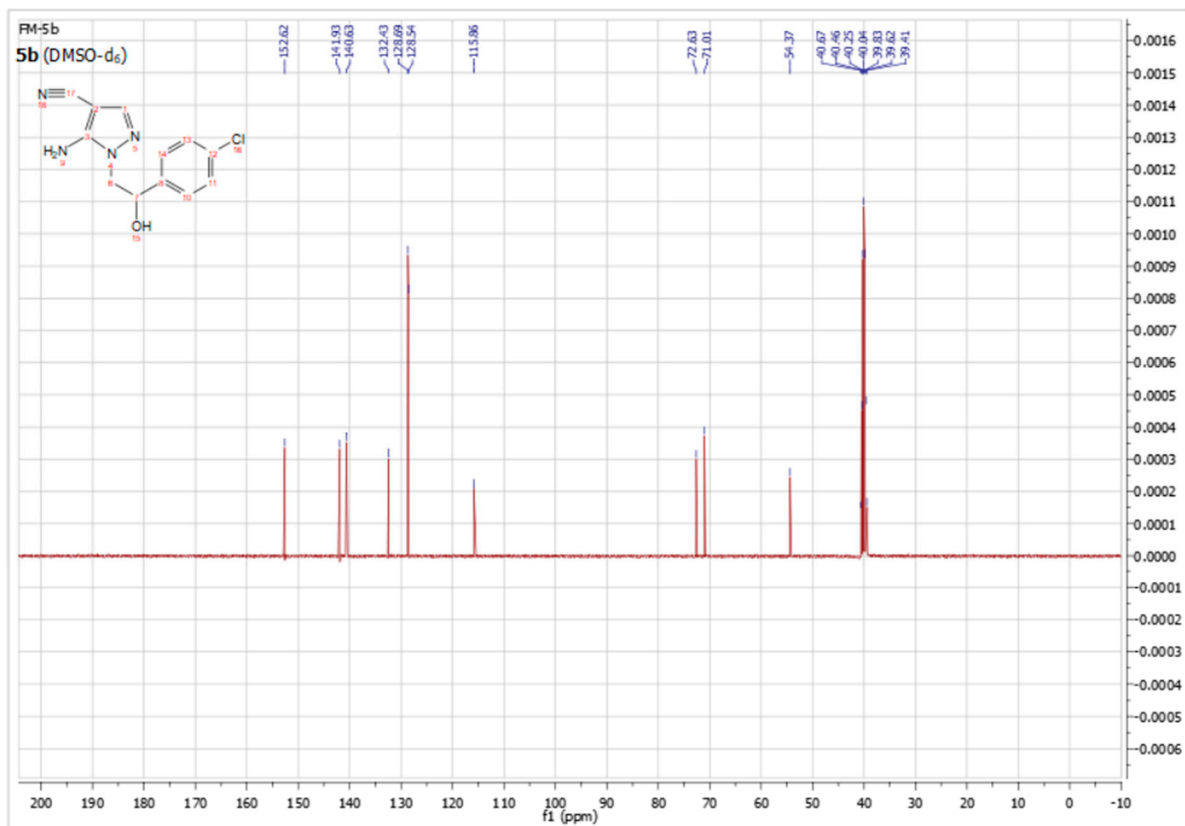
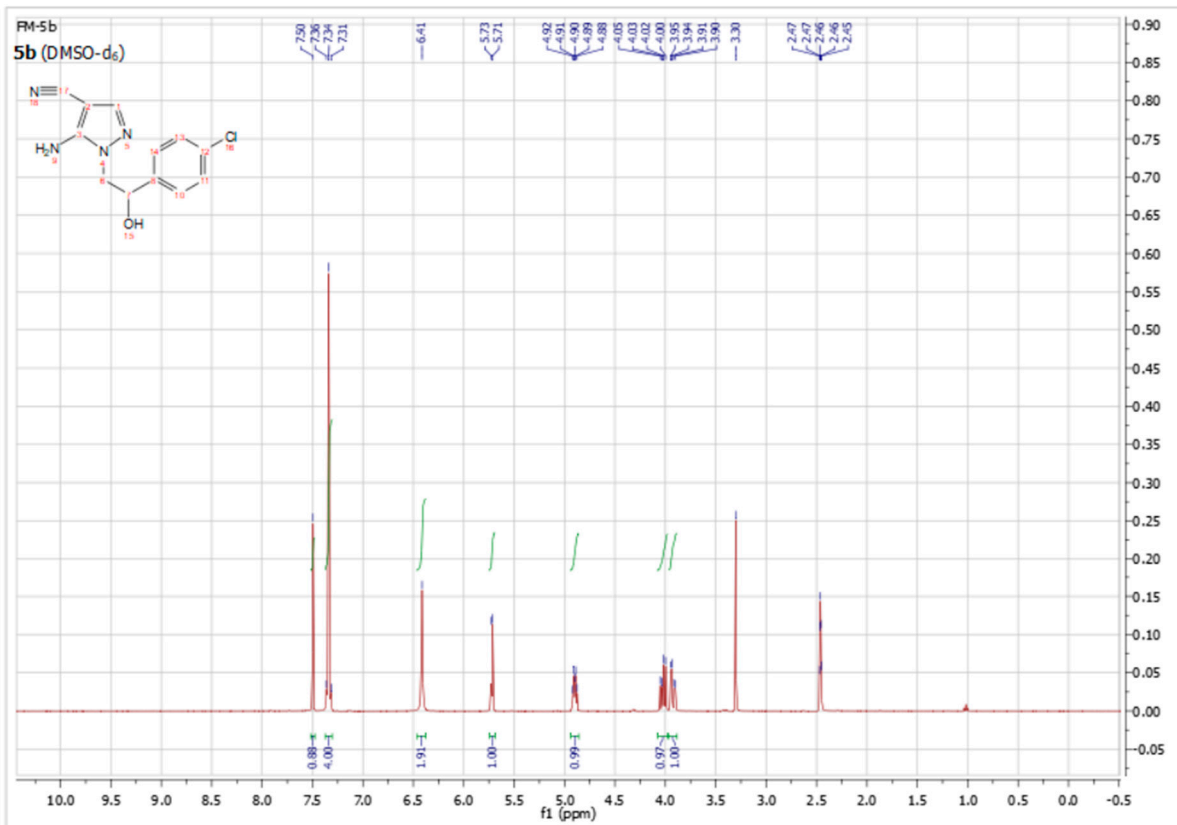


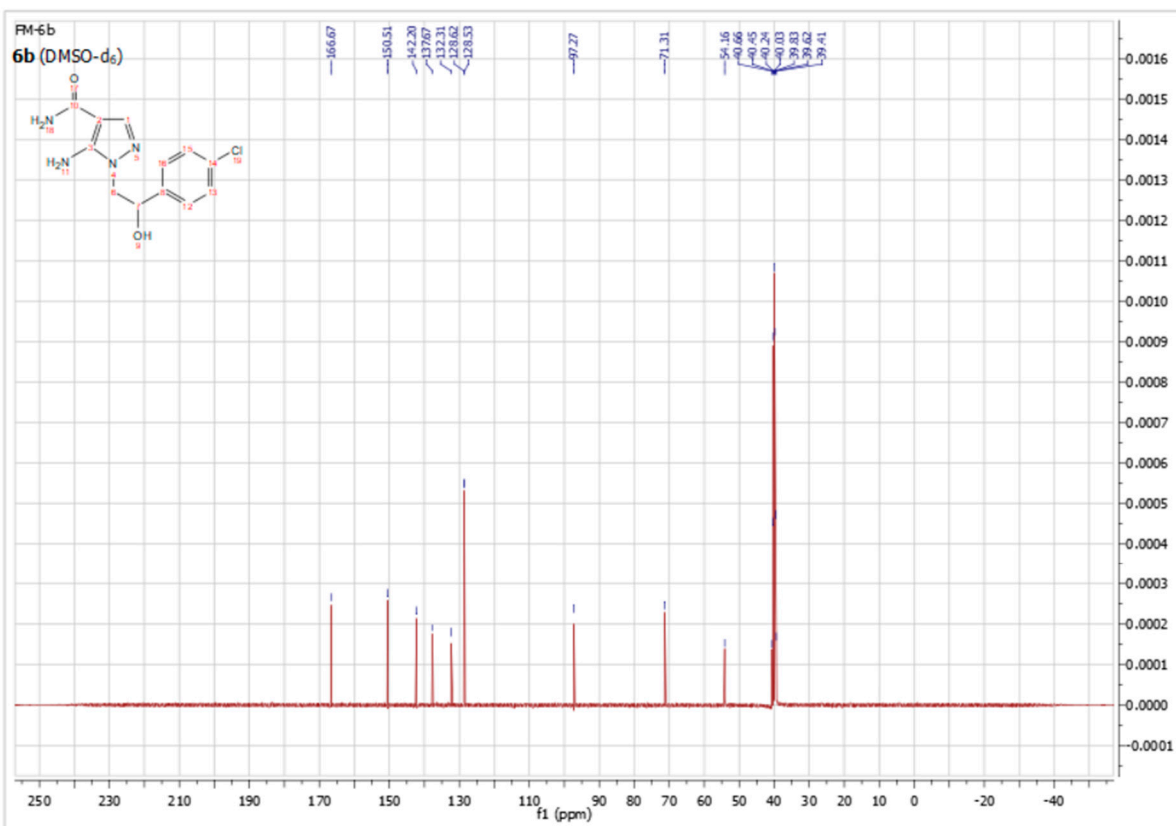
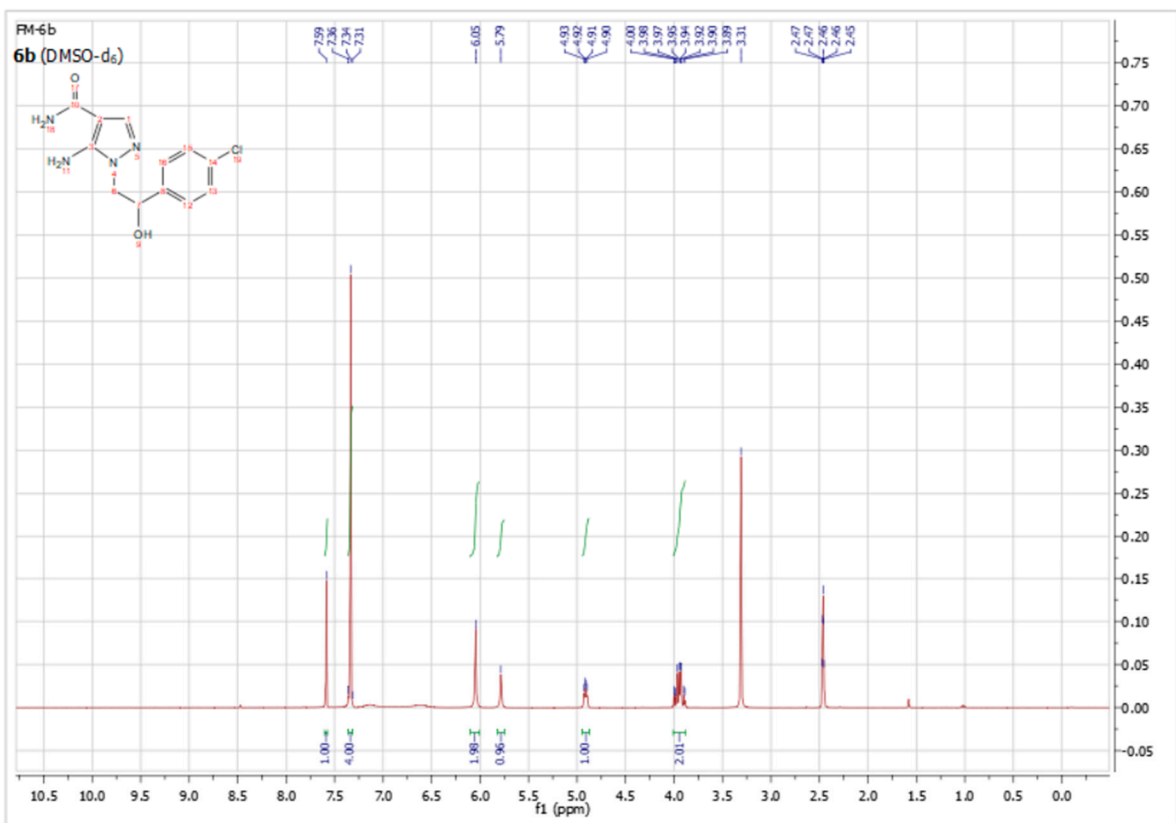


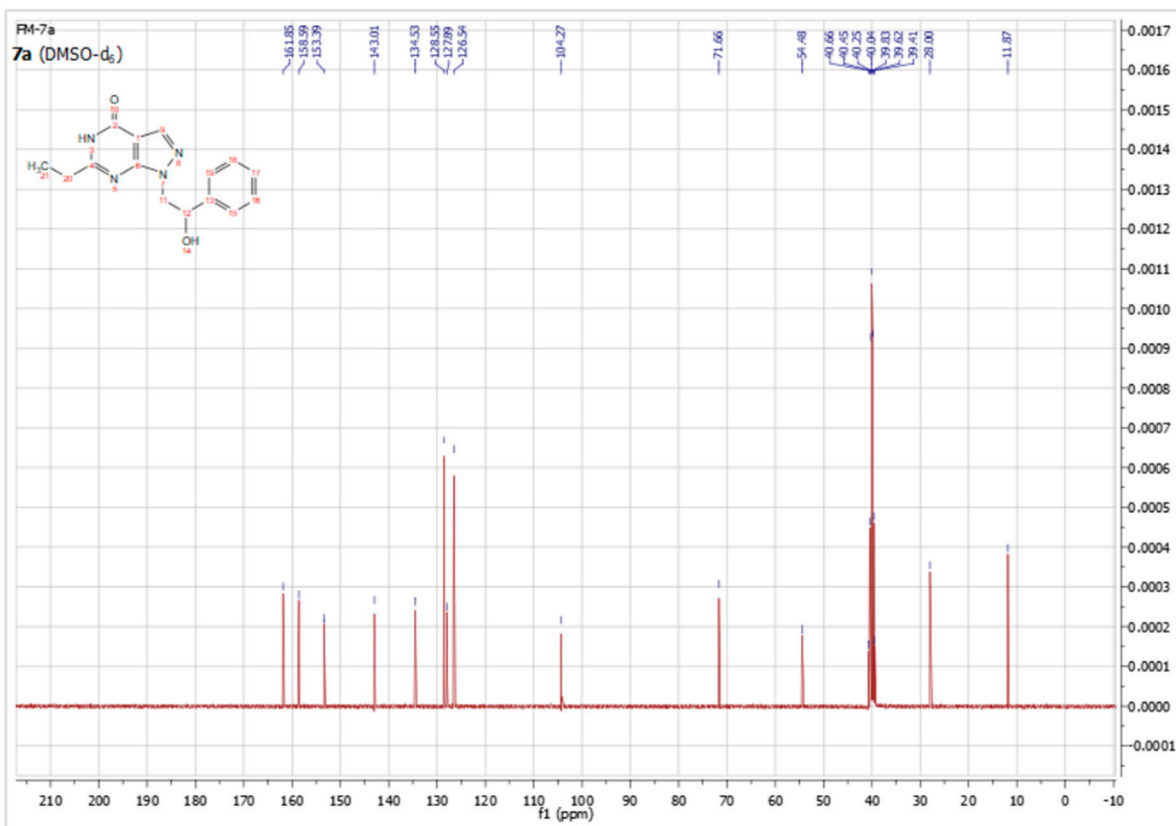
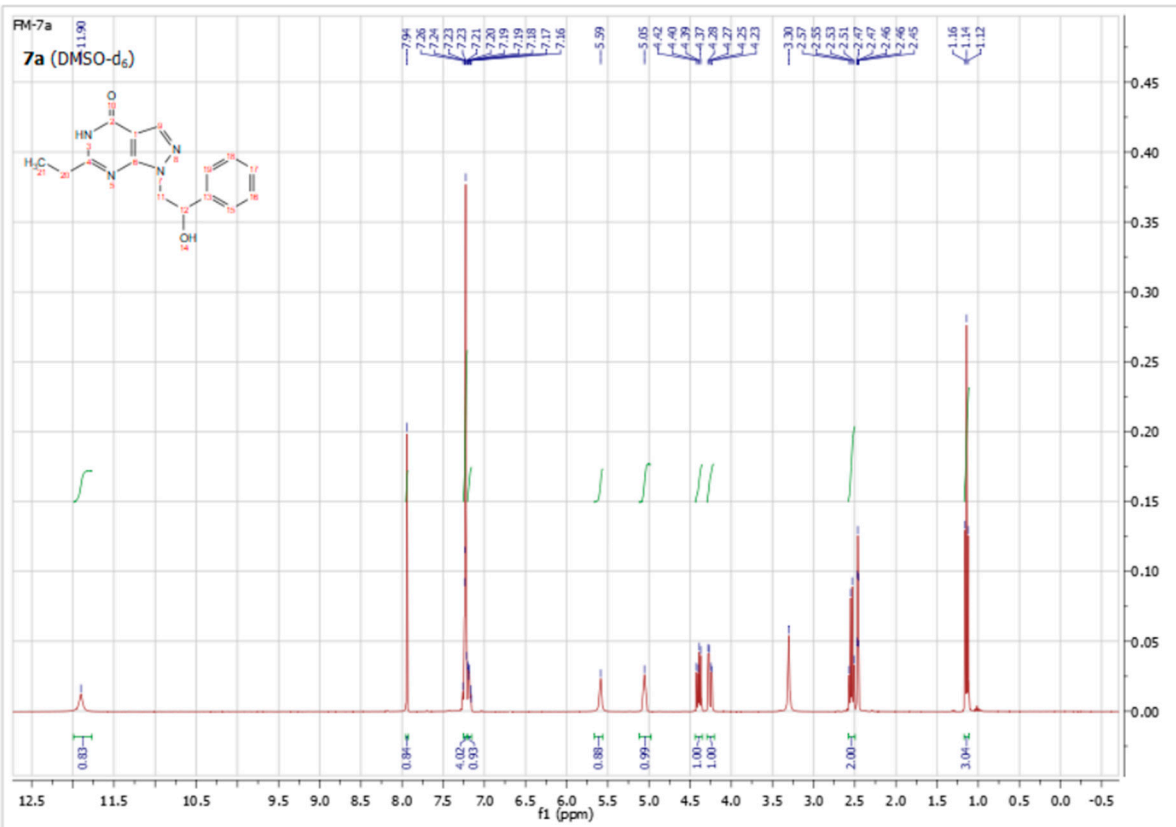


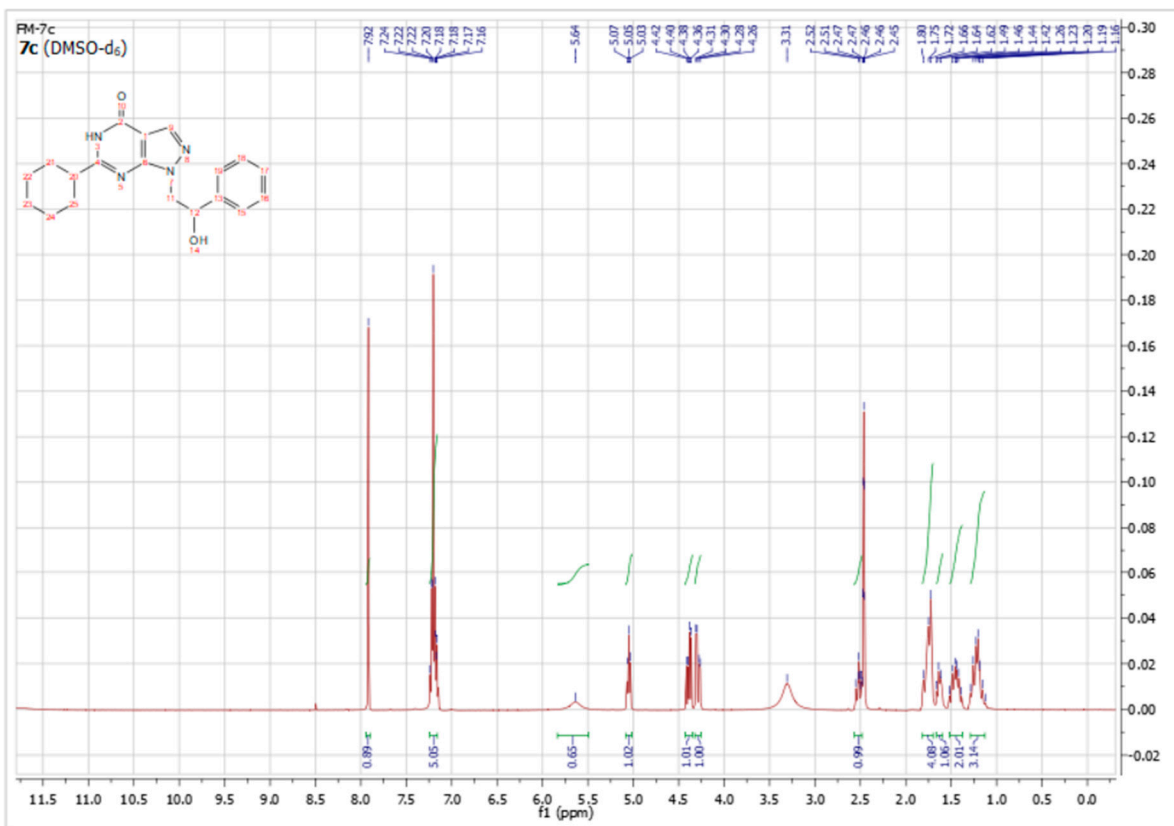
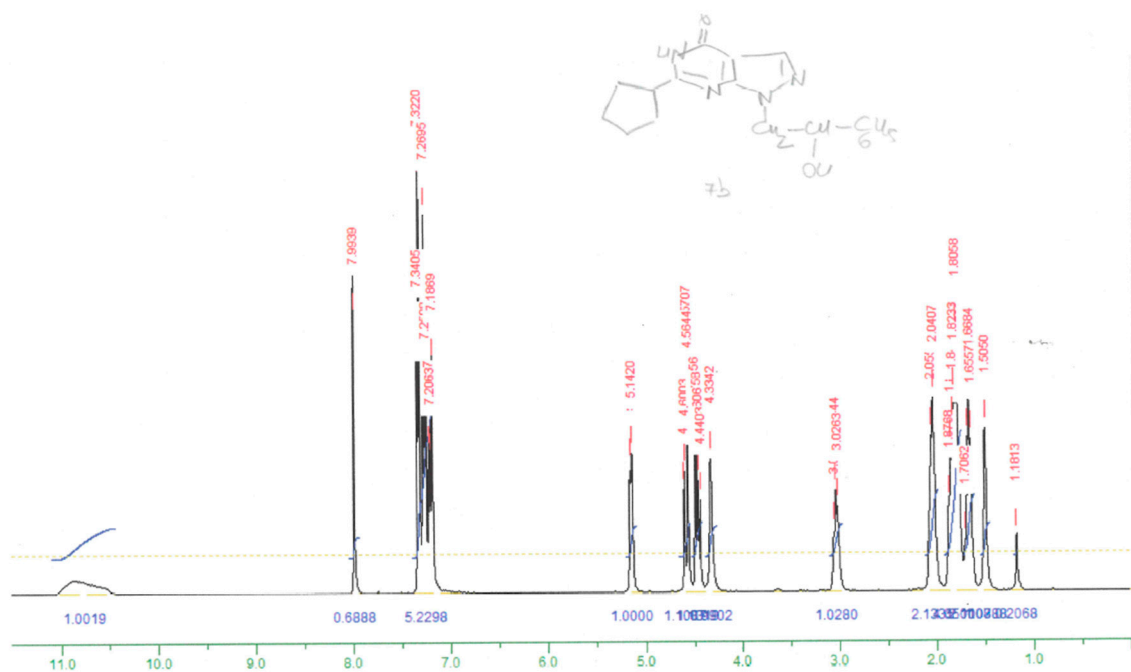


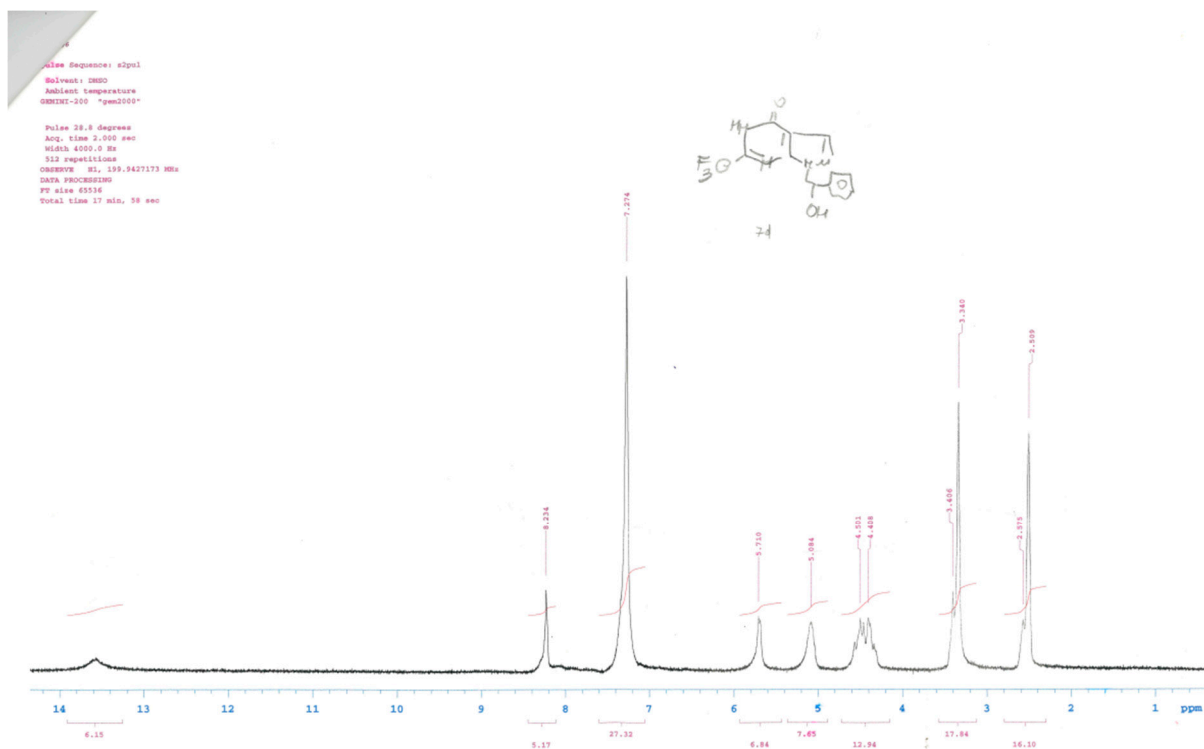
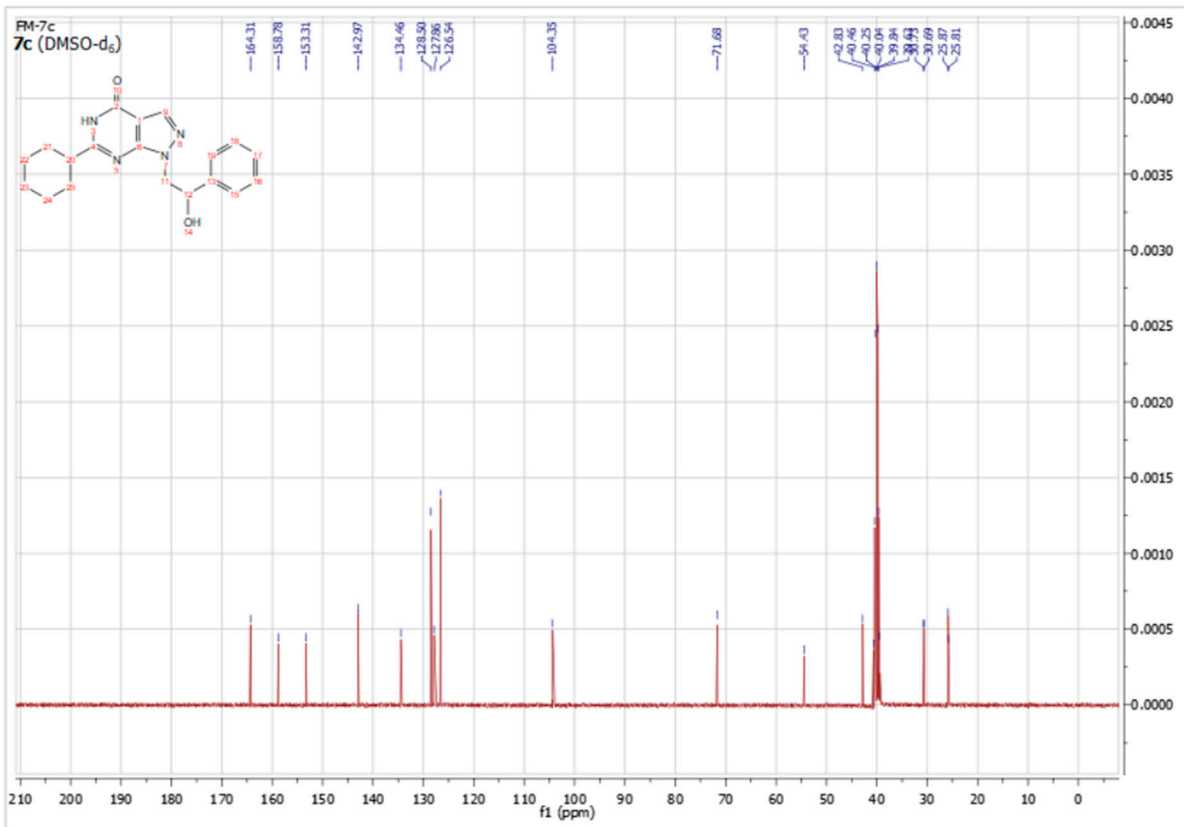












ciclo-6Ar

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

GEMINI-200 "gem2000"

Pulse 28.8 degrees

Acq. time 2.000 sec

Width 4000.0 Hz

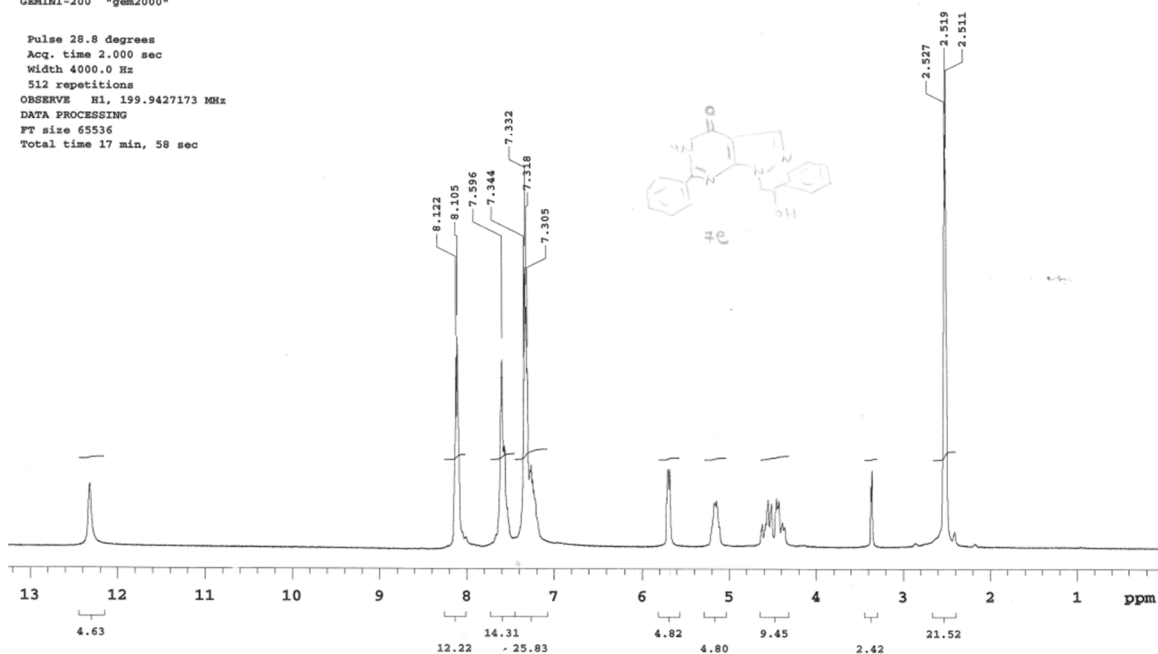
512 repetitions

OBSERVE H1, 199.9427173 MHz

DATA PROCESSING

FT size 65536

Total time 17 min, 58 sec



pCl6Meciclo

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

GEMINI-200 "gem2000"

Pulse 28.8 degrees

Acq. time 2.000 sec

Width 4000.0 Hz

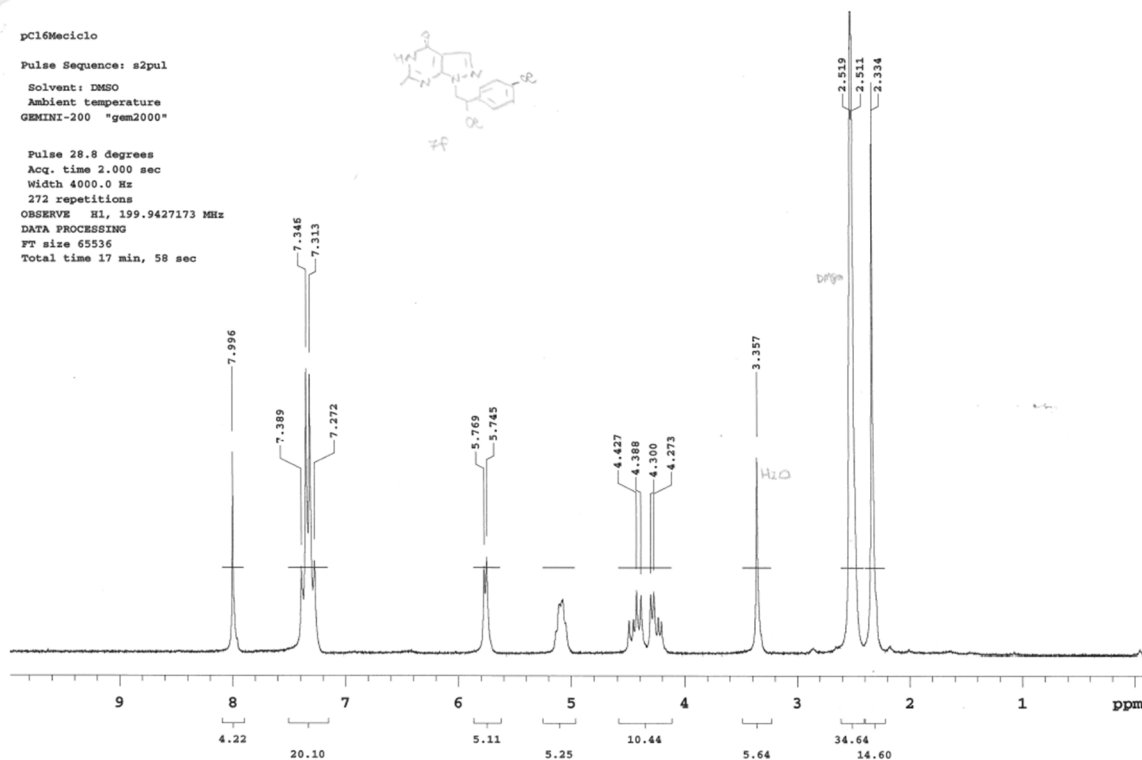
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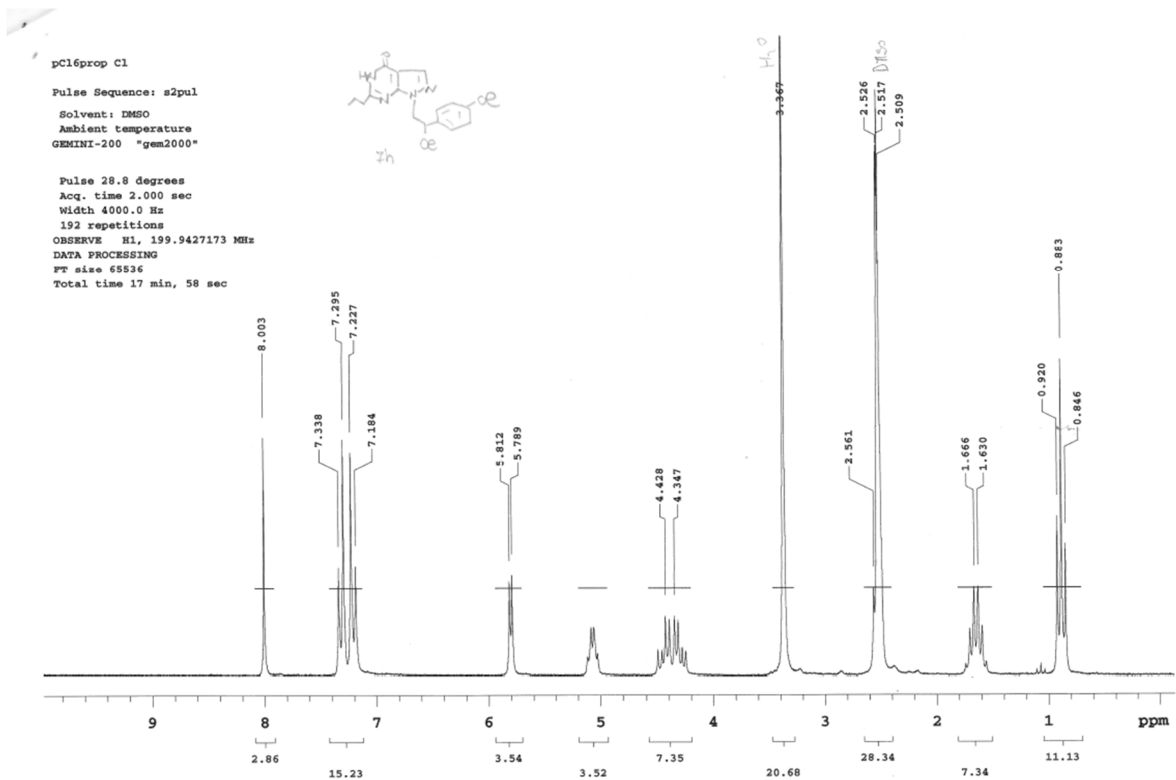
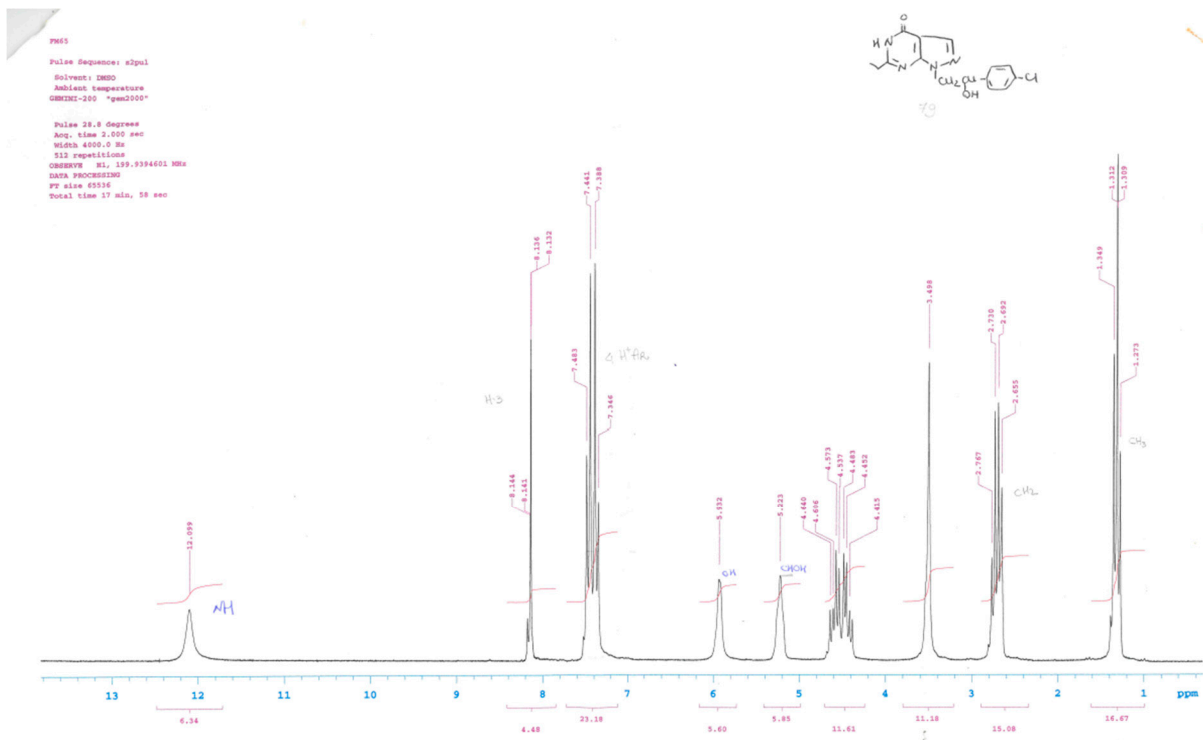
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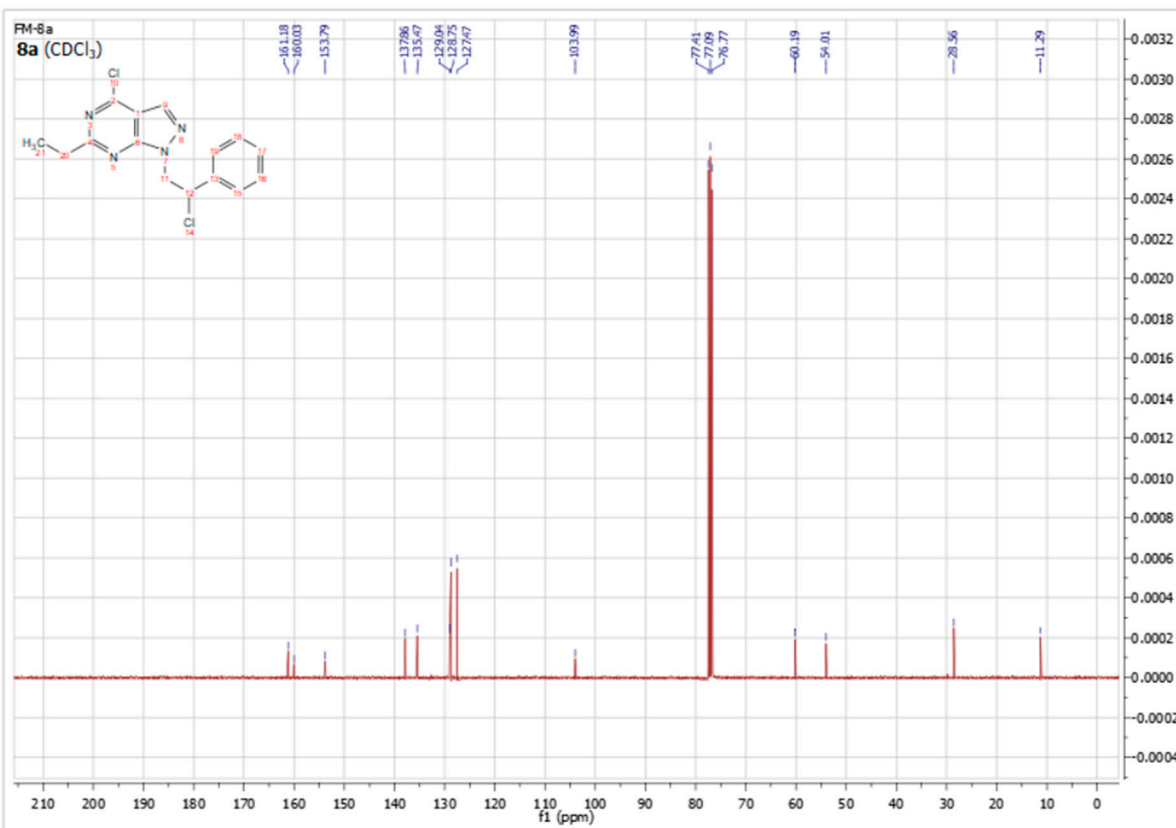
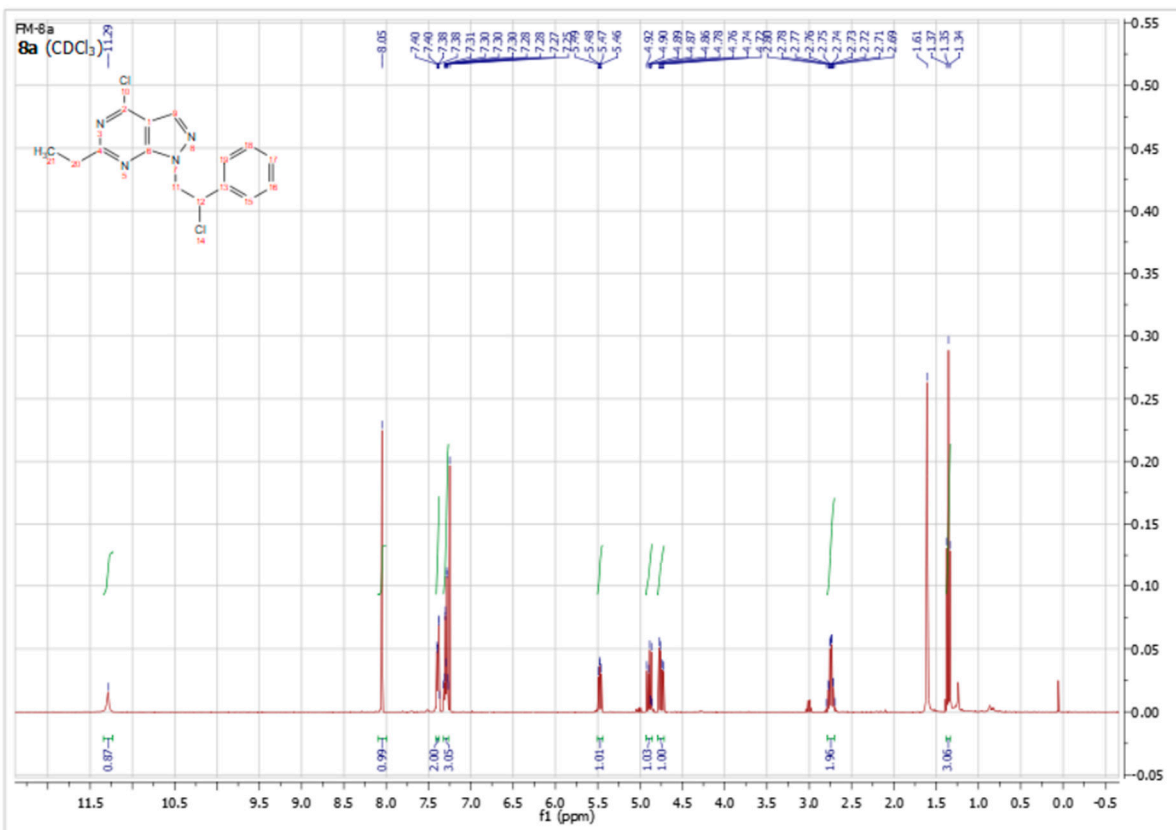
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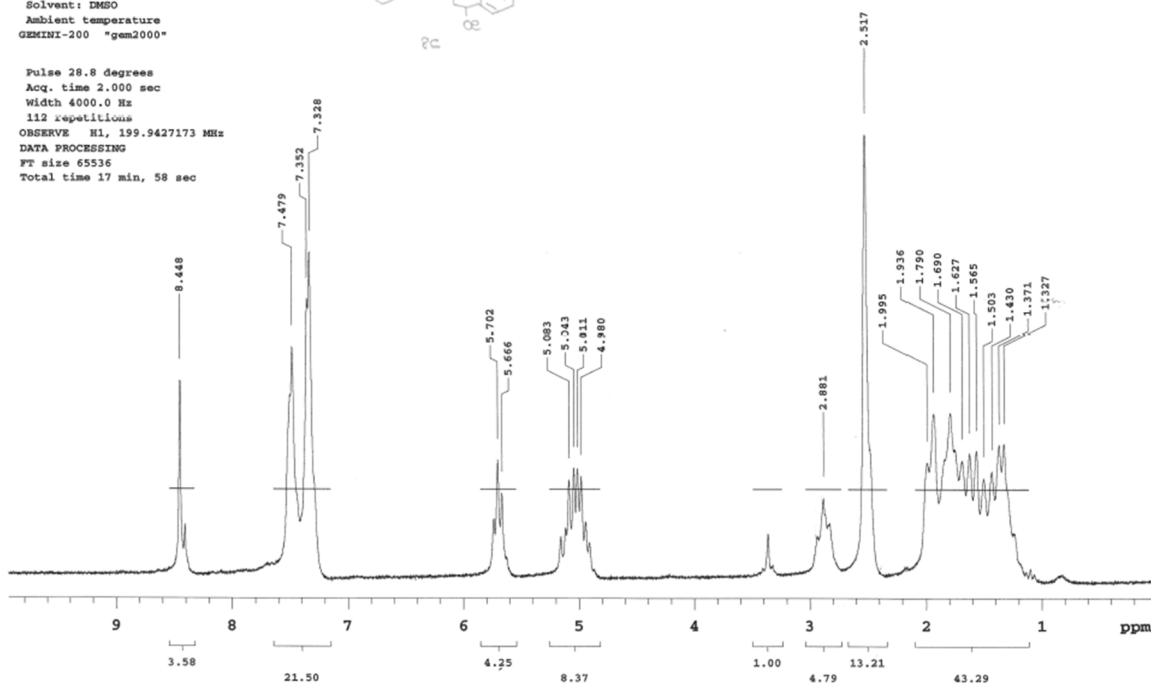
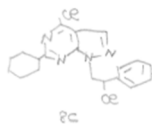




CG66

Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
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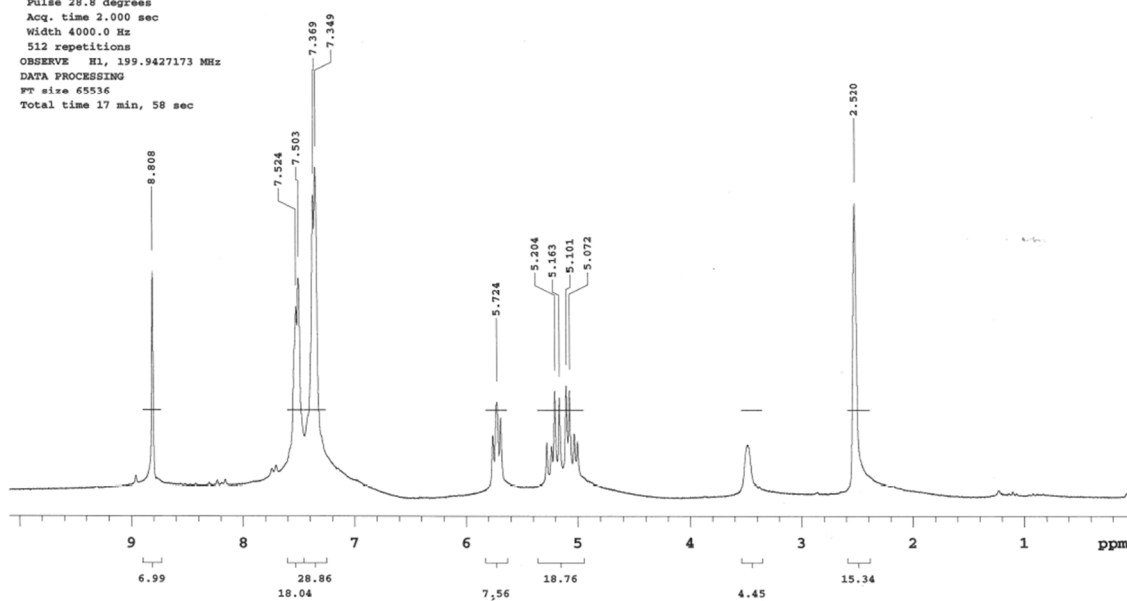
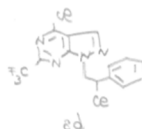
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Width 4000.0 Hz
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OBSERVE H1, 199.9427173 MHz
DATA PROCESSING
FT size 65536
Total time 17 min, 58 sec



CF3,POCl3/DMF

Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
GEMINI-200 "gem2000"

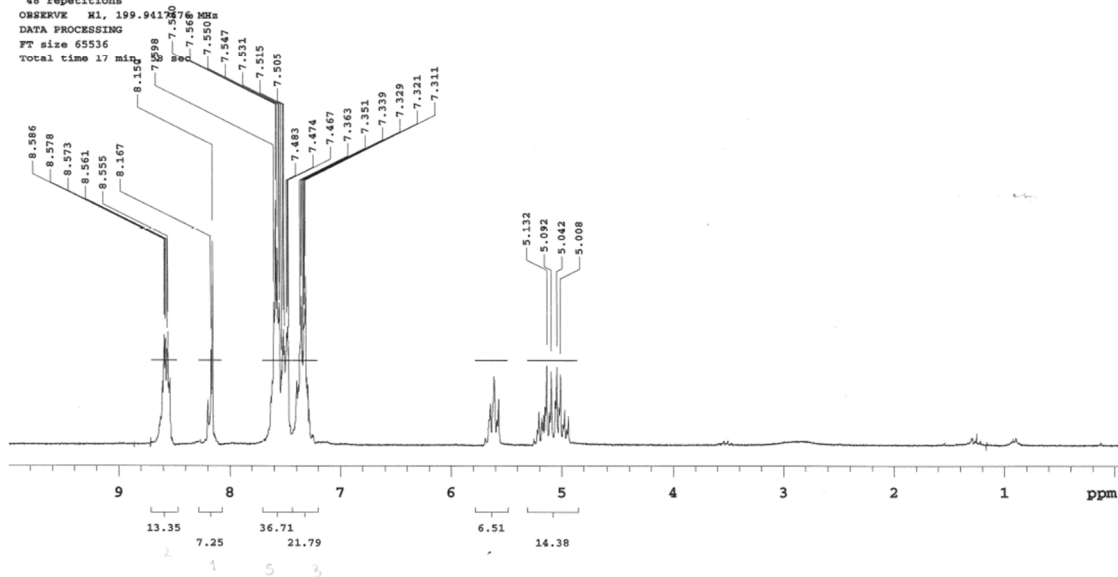
Pulse 28.8 degrees
Acq. time 2.000 sec
Width 4000.0 Hz
512 repetitions
OBSERVE H1, 199.9427173 MHz
DATA PROCESSING
FT size 65536
Total time 17 min, 58 sec



6Ar C1

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-200 "gem2000"

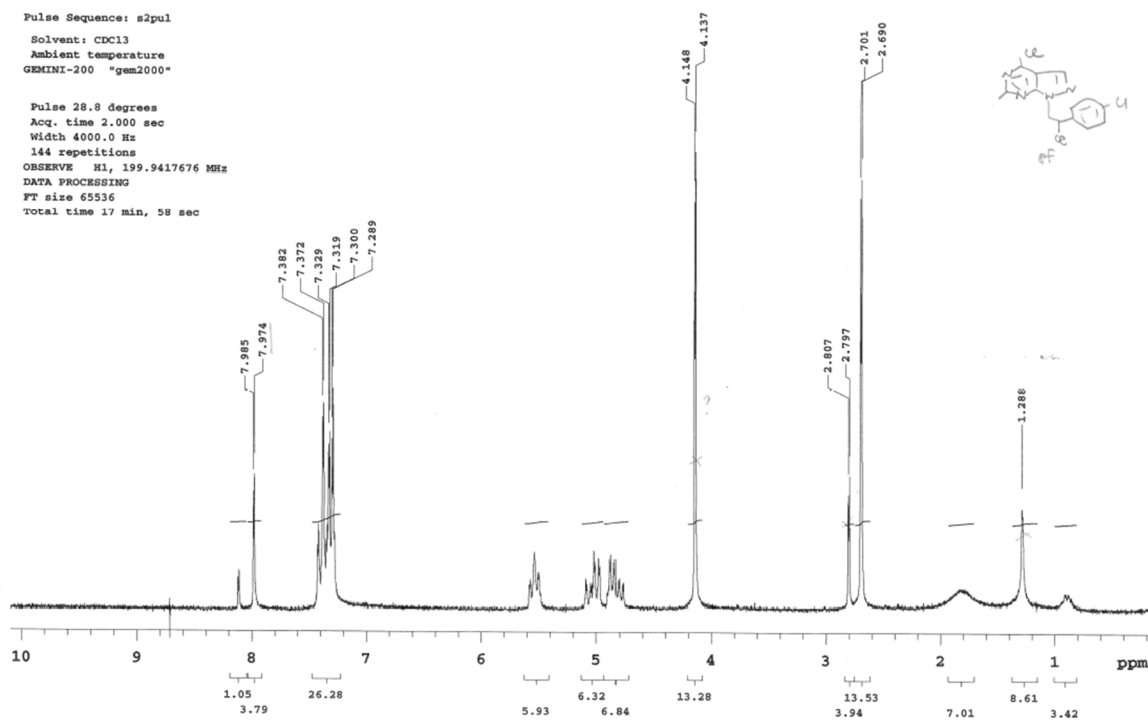
Pulse 28.8 degrees
Acq. time 2.000 sec
Width 4000.0 Hz
48 repetitions
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DATA PROCESSING
FT size 65536
Total time 17 min



CG63

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-200 "gem2000"

Pulse 28.8 degrees
Acq. time 2.000 sec
Width 4000.0 Hz
144 repetitions
OBSERVE H1, 199.9417676 MHz
DATA PROCESSING
FT size 65536
Total time 17 min, 58 sec



CG62

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

GEMINI-200 "gem2000"

Pulse 28.8 degrees

Acq. time 2.000 sec

Width 4000.0 Hz

64 repetitions

OBSERVE H1, 199.9427173 MHz

DATA PROCESSING

FT size 65536

Total time 17 min, 58 sec

