Retro Diels Alder Protocol for Regioselective Synthesis of Novel [1,2,4]Triazolo[4,3-*a*]pyrimidin-7(1*H*)-ones

Awad I. Said,[a,b] Márta Palkó,[a] Matti Haukka[c] and Ferenc Fülöp*[a]

[a]Institute of Pharmaceutical Chemistry, University of Szeged, Eötvös u. 6, H-6720 Szeged, Hungary.
E-mail: fulop@pharm.u-szeged.hu
[b]Chemistry Department, Faculty of Science, Assiut University, Assiut, Egypt 71516.
E-mail: awadsaid@aun.edu.eg
[c]Department of Chemistry, University of Jyväskylä, FIN-40014, Jyväskylä, Finland

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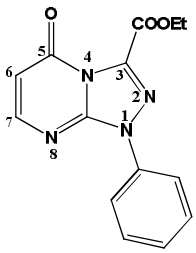
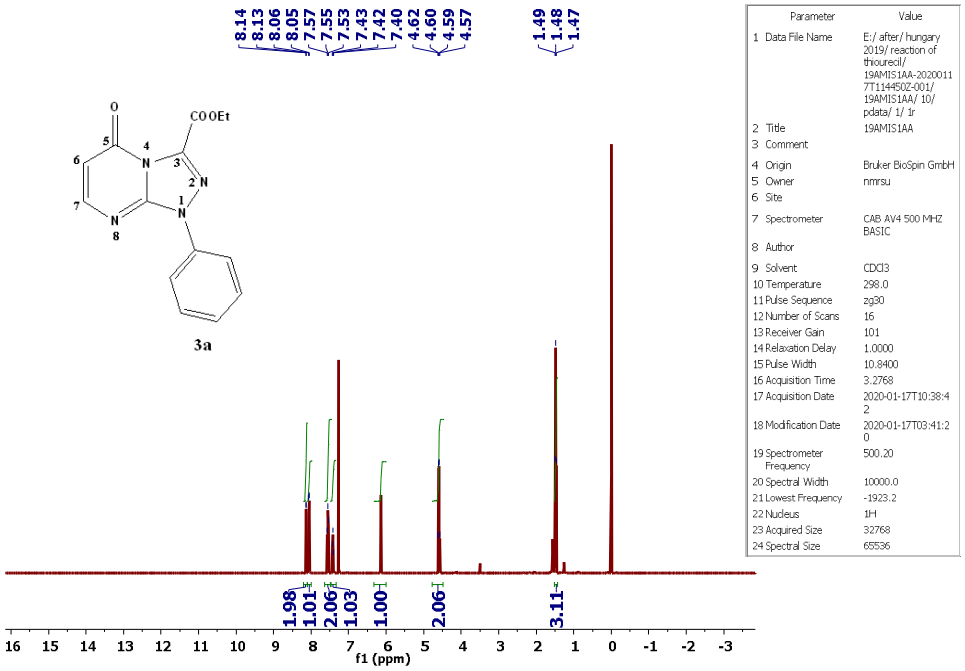
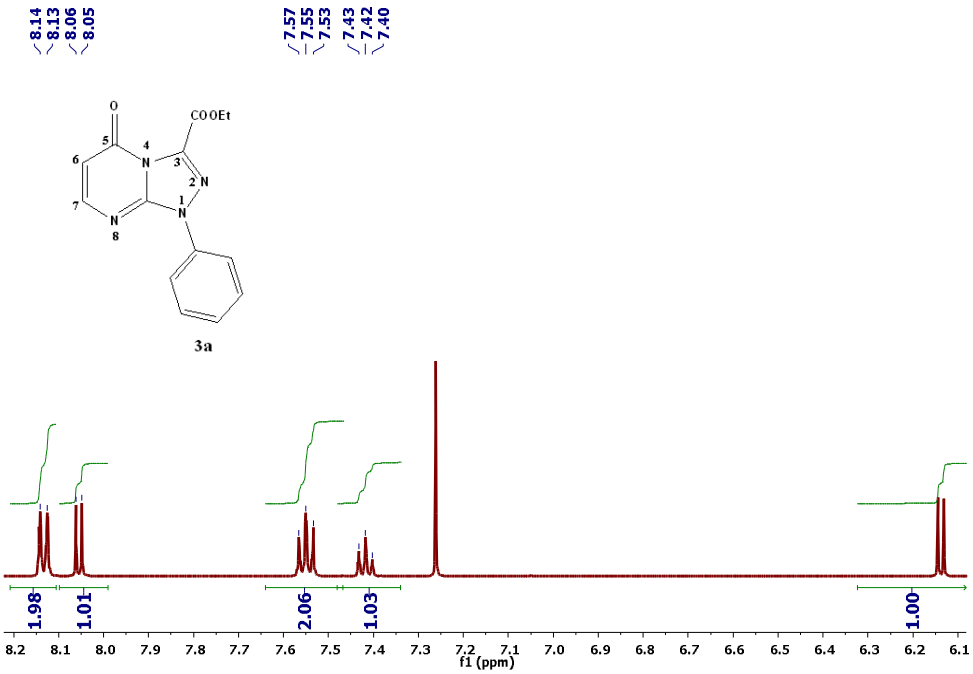
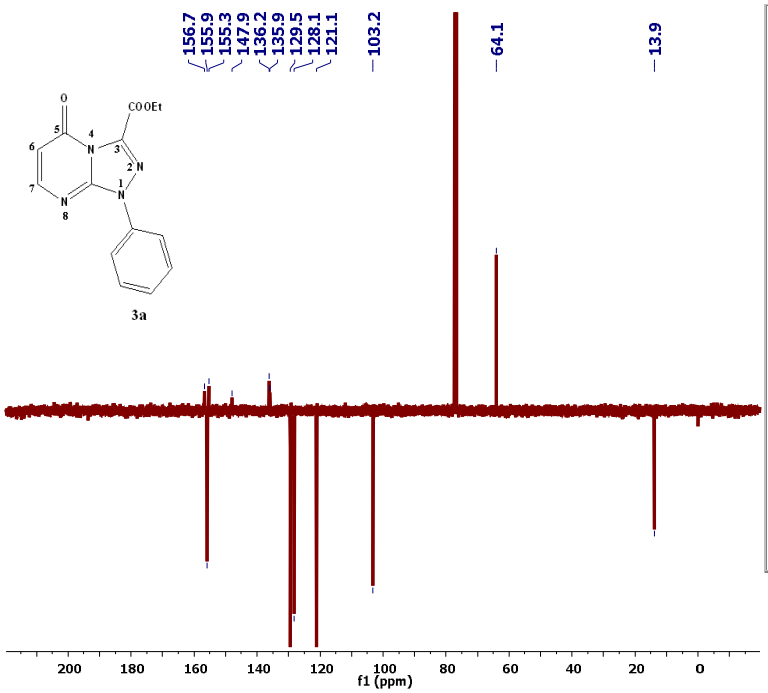


3a

Ethyl 5-oxo-1-phenyl-1,5-dihydro[1,2,4]triazolo[4,3-*a*]pyrimidine-3-carboxylate (3a)







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5	Owner	nmrsu
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9	Solvent	CDCl3
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11	Pulse Sequence	jmod
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13	Receiver Gain	101
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15	Pulse Width	10.0000
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22	Nucleus	13C
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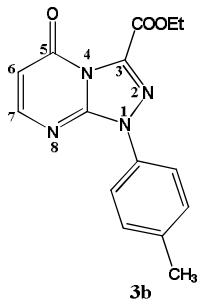
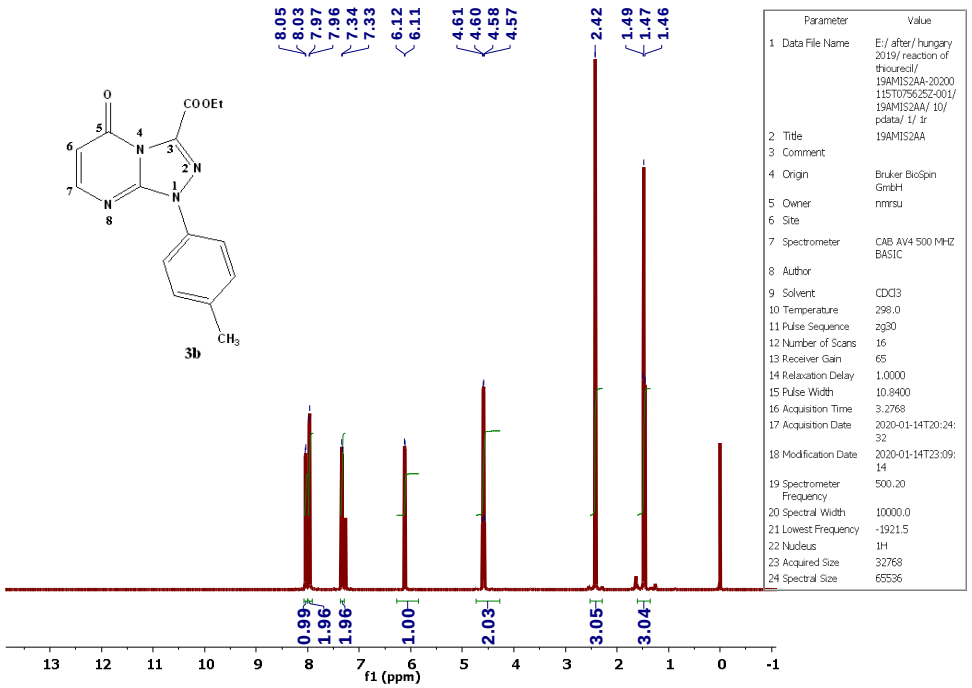
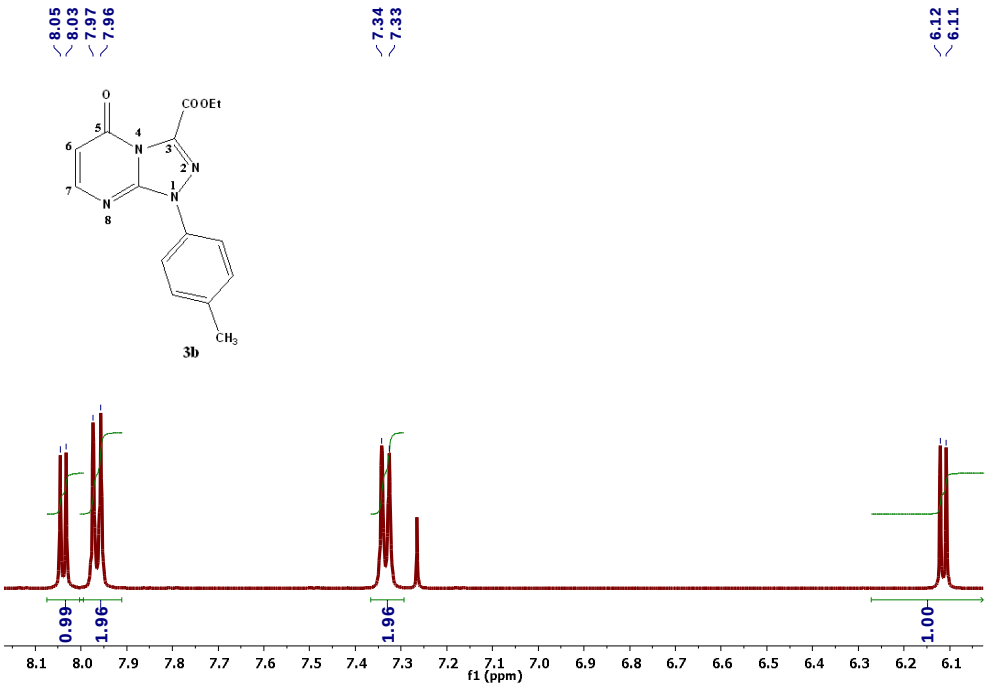
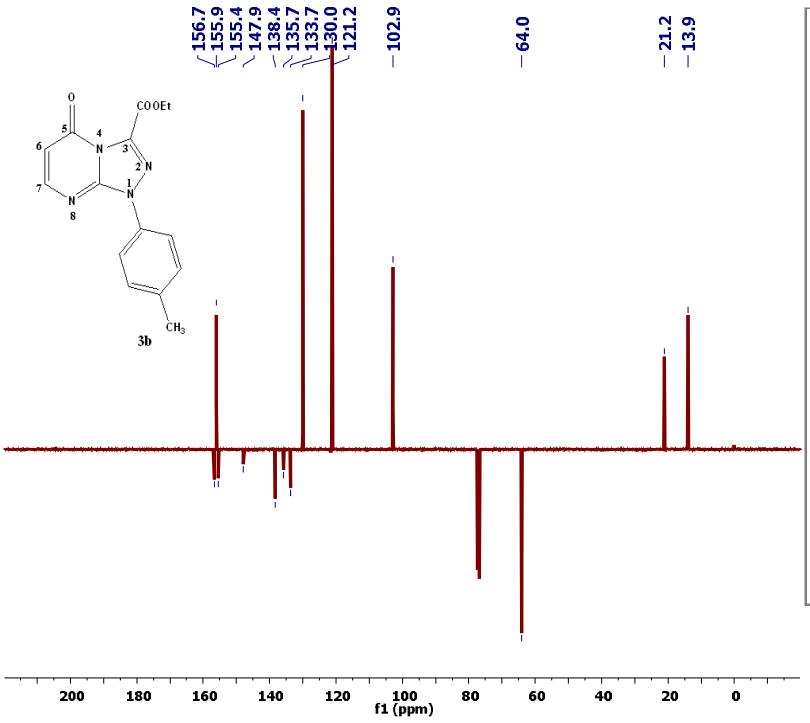


Ethyl 5-oxo-1-(*p*-tolyl)-1,5-dihydro[1,2,4]triazolo[4,3-*a*]pyrimidine-3-carboxylate (3b)







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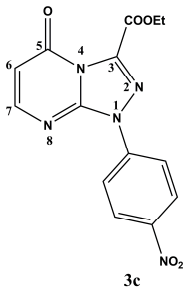
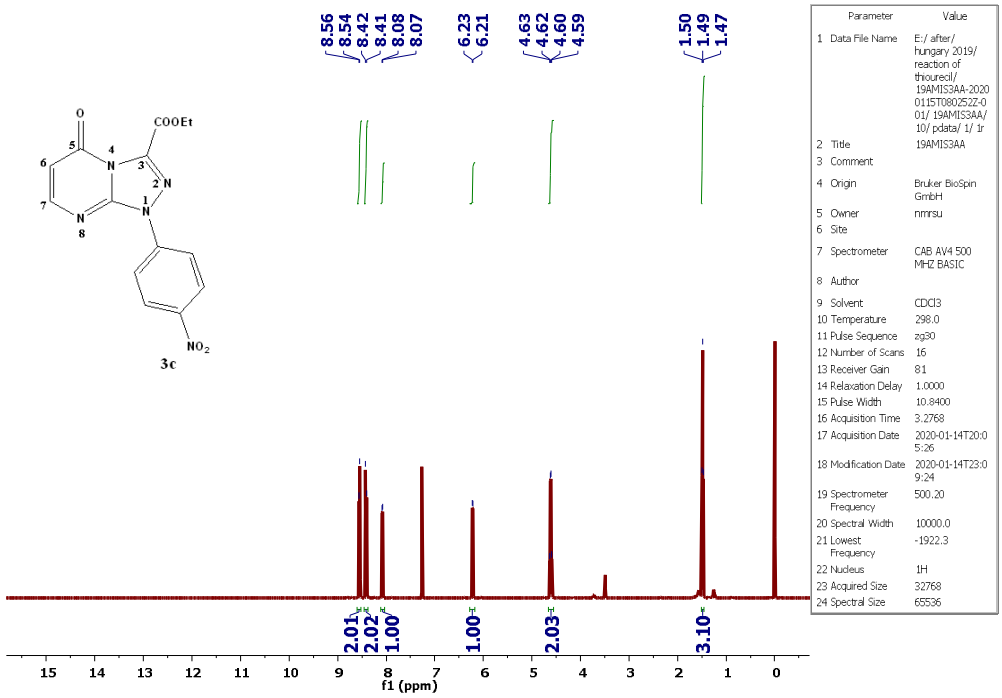
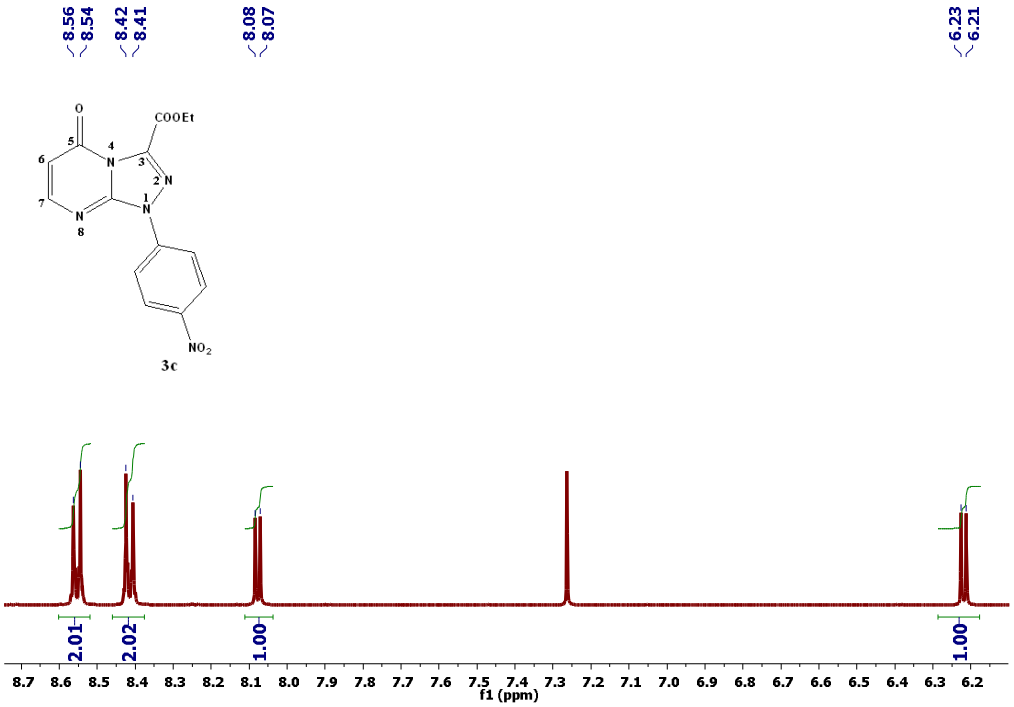
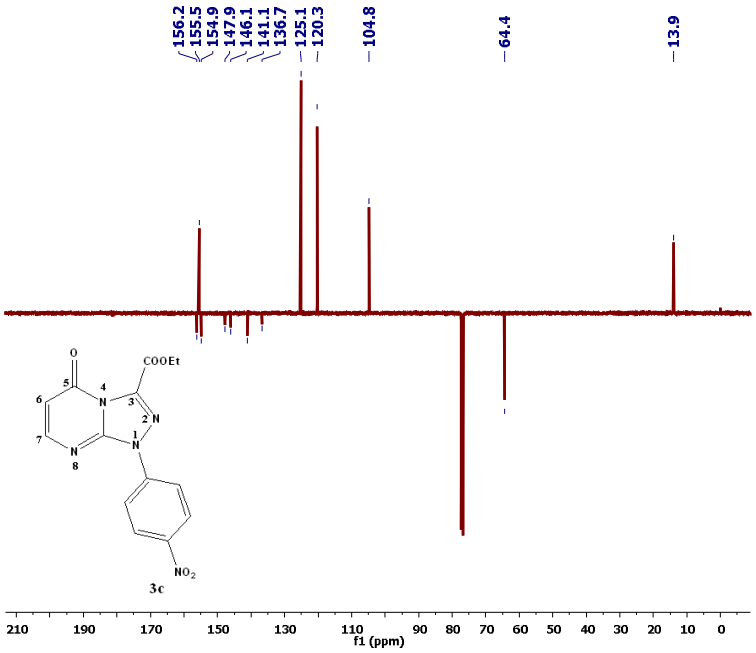


Ethyl 1-(4-nitrophenyl)-5-oxo-1,5-dihydro[1,2,4]triazolo[4,3-*a*]-pyrimidine-3-carboxylate (3c)







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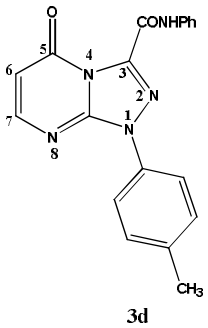
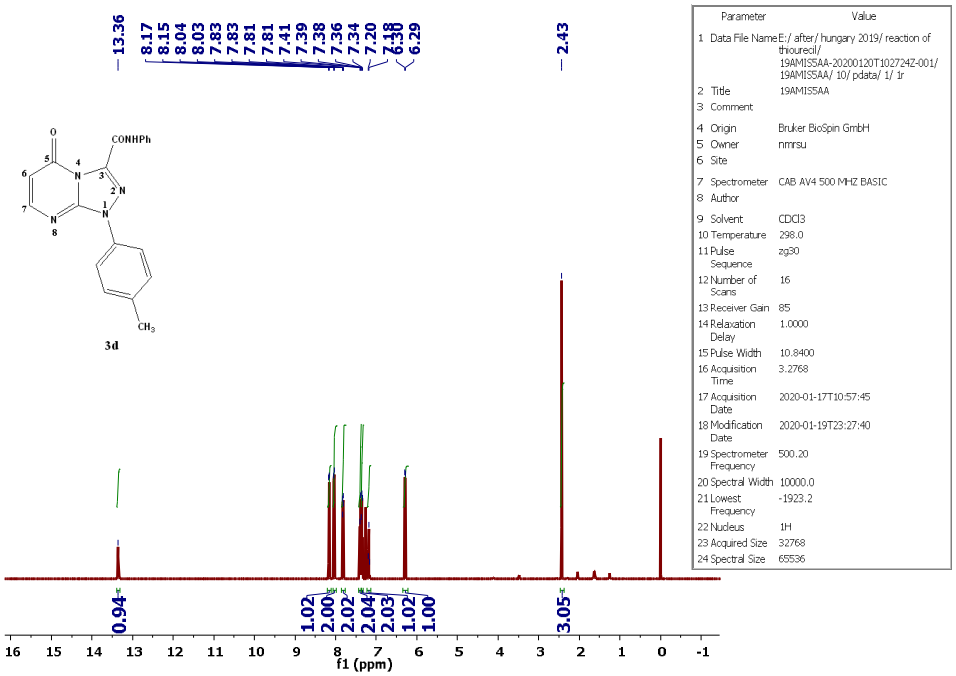
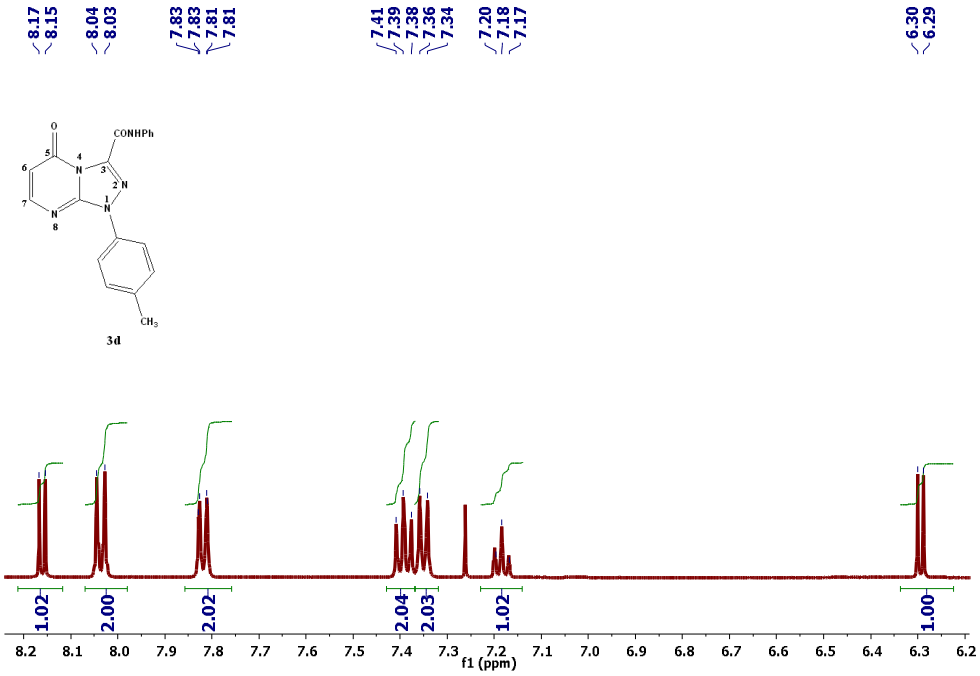
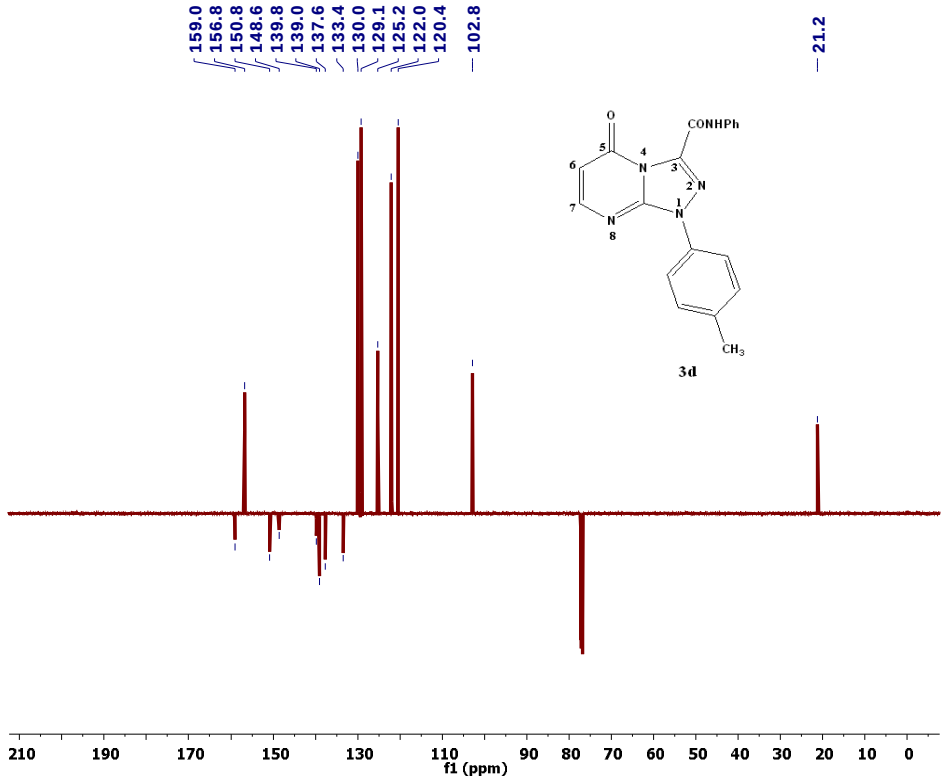


3d

5-Oxo-*N*-phenyl-1-(*p*-tolyl)-1,5-dihydro[1,2,4]triazolo[4,3-*a*]pyrimidine-3-carboxamide (3d)







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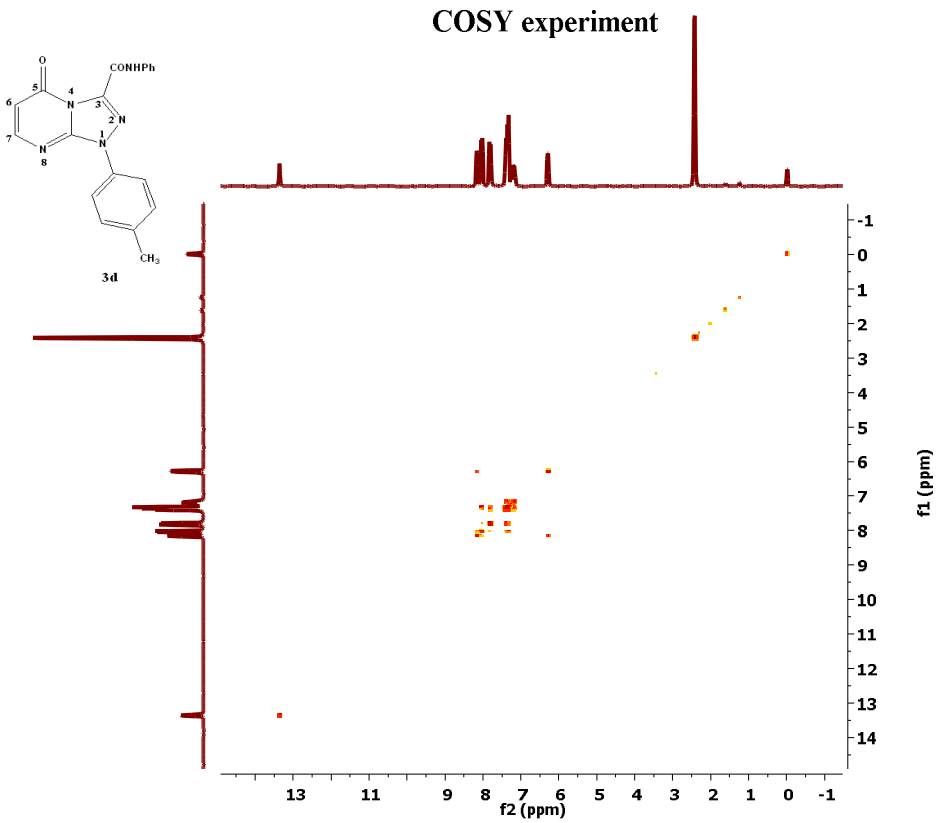

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9	Solvent	CDCl3
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11	Pulse Sequence	cosygpppqf
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13	Receiver Gain	101
14	Relaxation Delay	2.0328
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18	Modification Date	2020-01-19T23:27: 56
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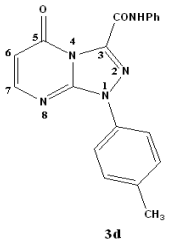
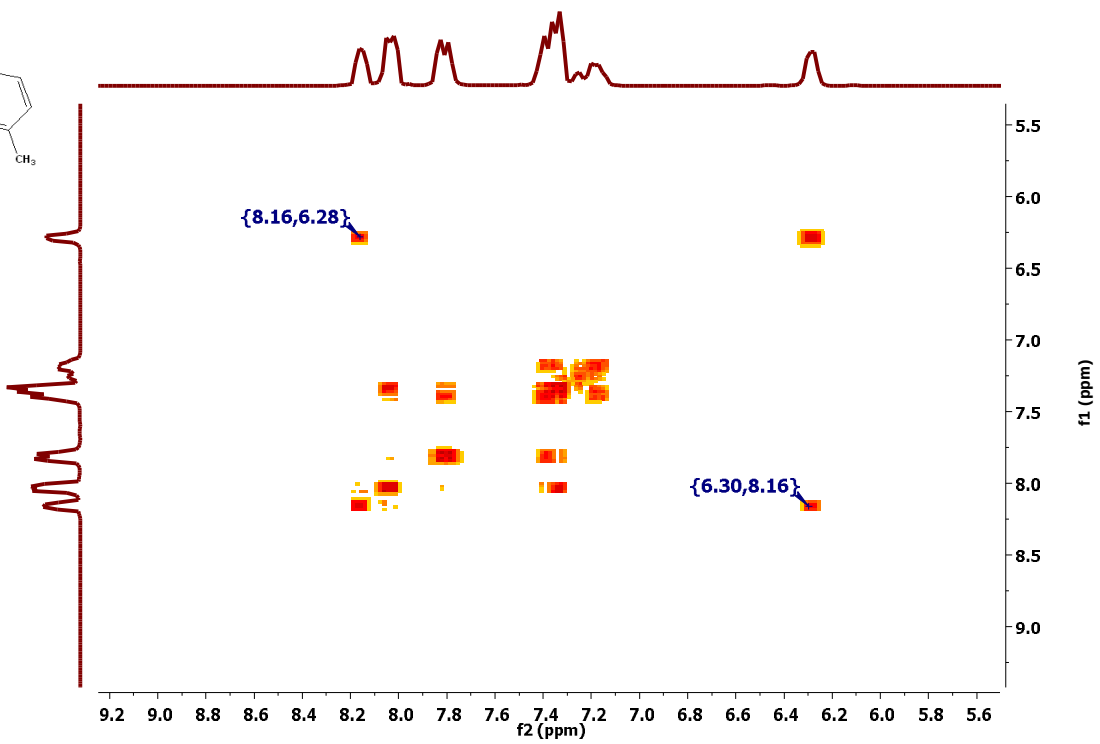
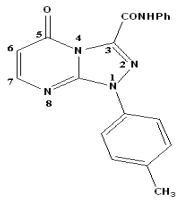
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)

COSY experiment





TOCSY experiment



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11	Pulse Sequence	mlevphpp
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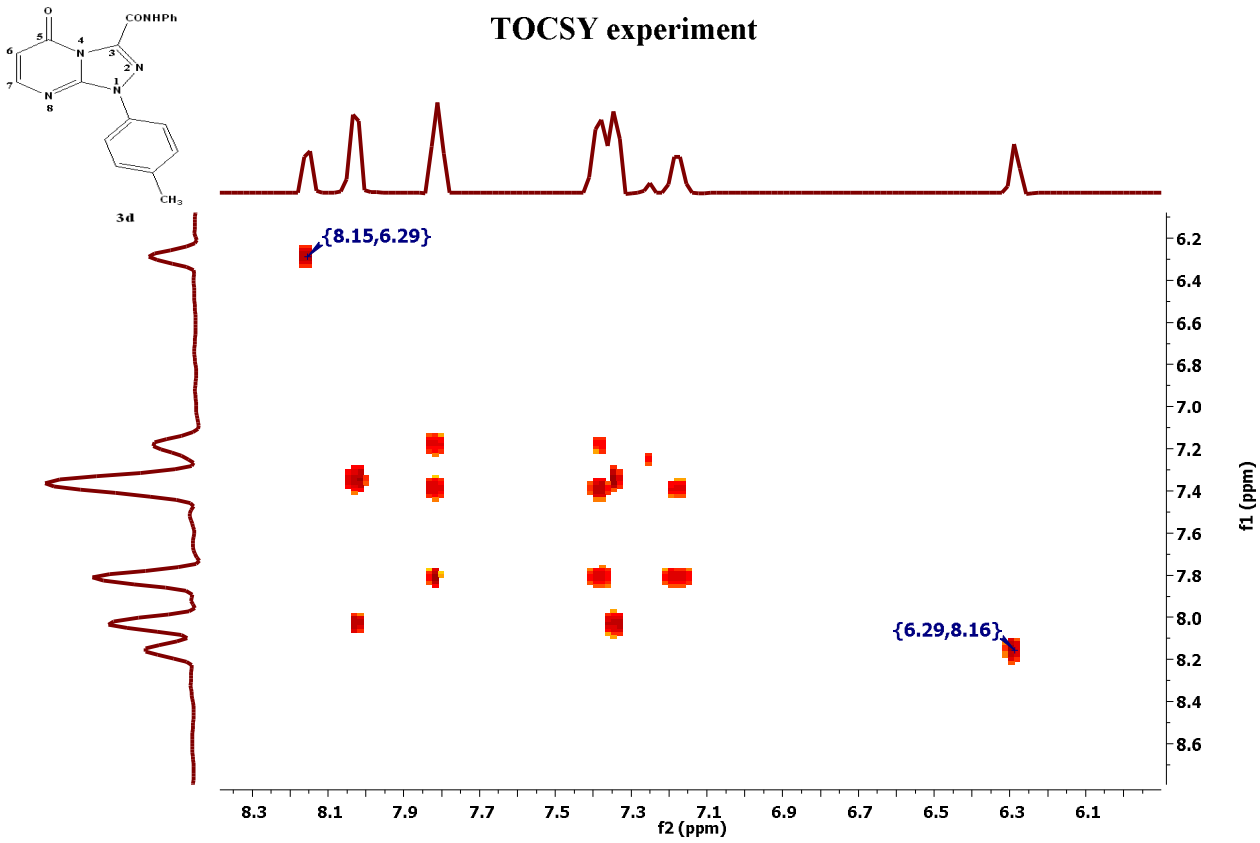

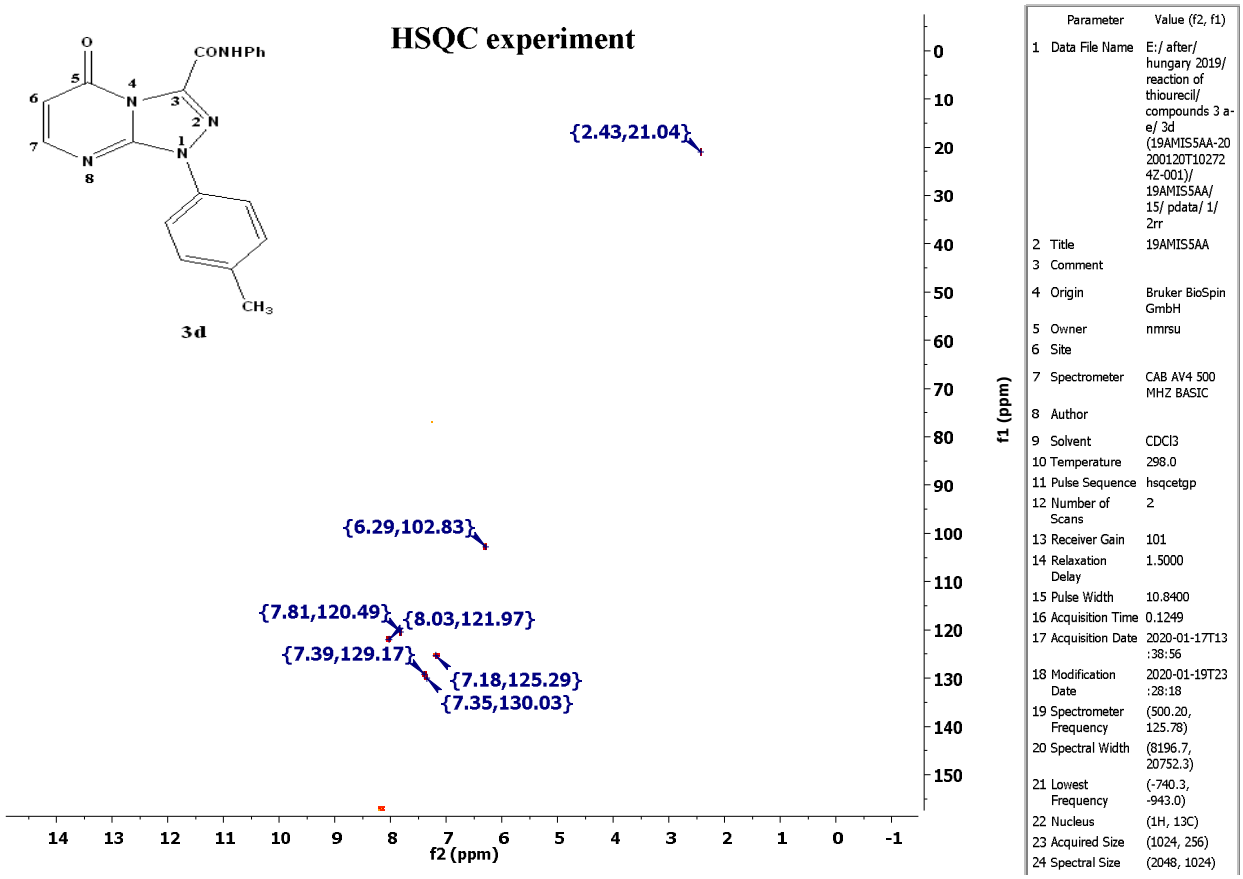

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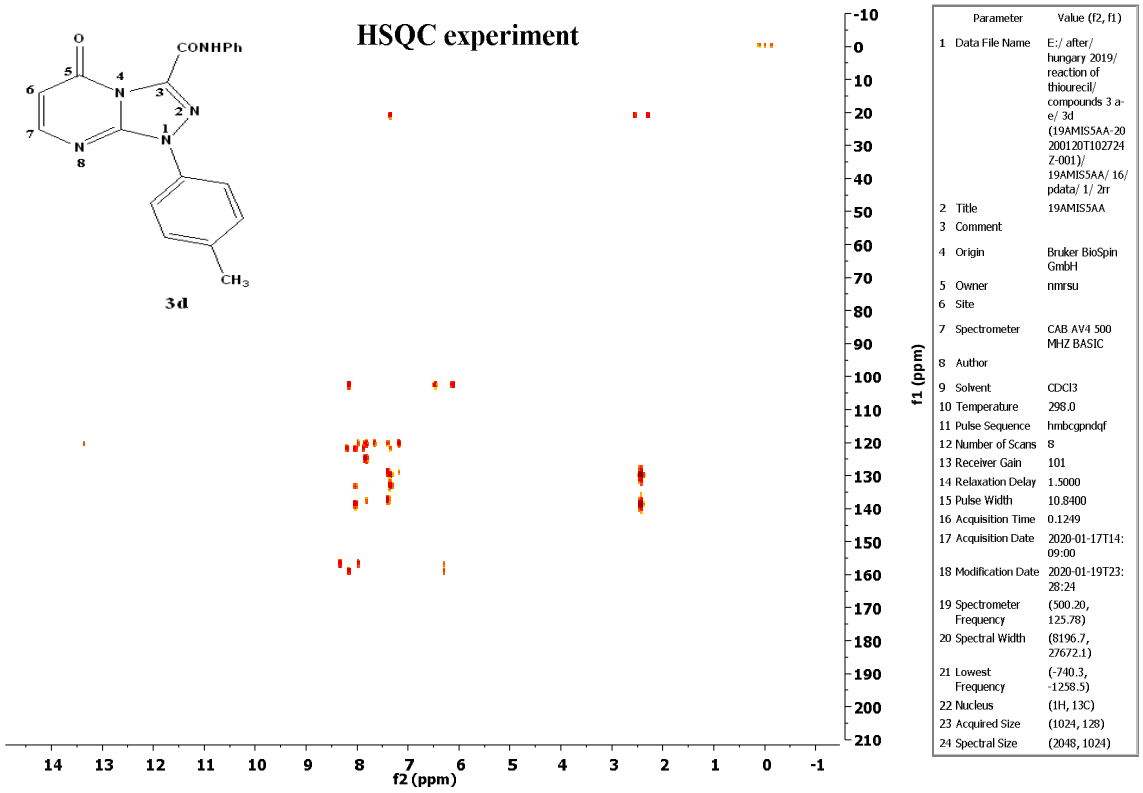

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9	Solvent	CDCl3
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13	Receiver Gain	101
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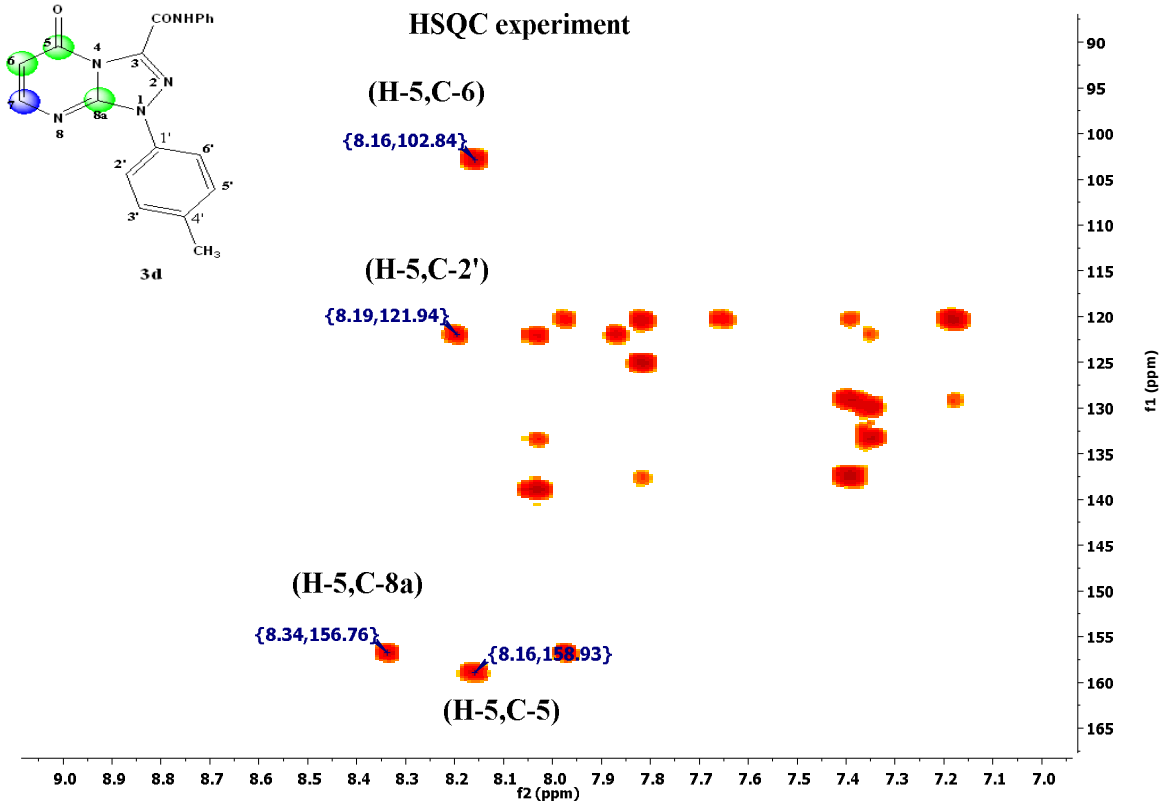
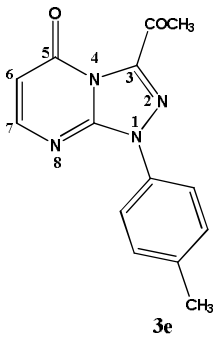
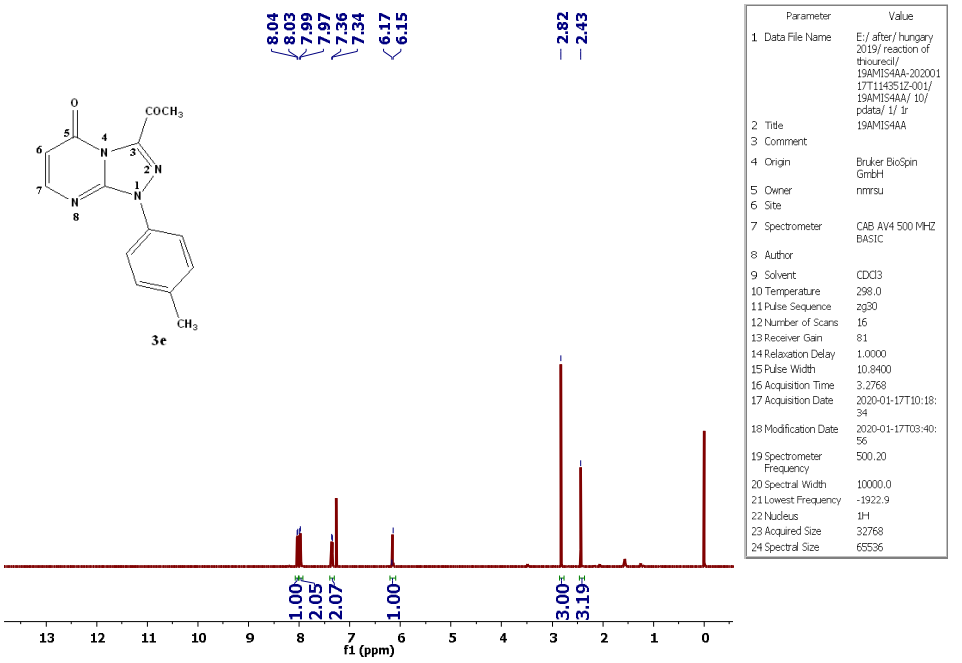




3-Acetyl-1-(*p*-tolyl)-[1,2,4]triazolo[4,3-*a*]pyrimidin-5(1H)-one (3e)



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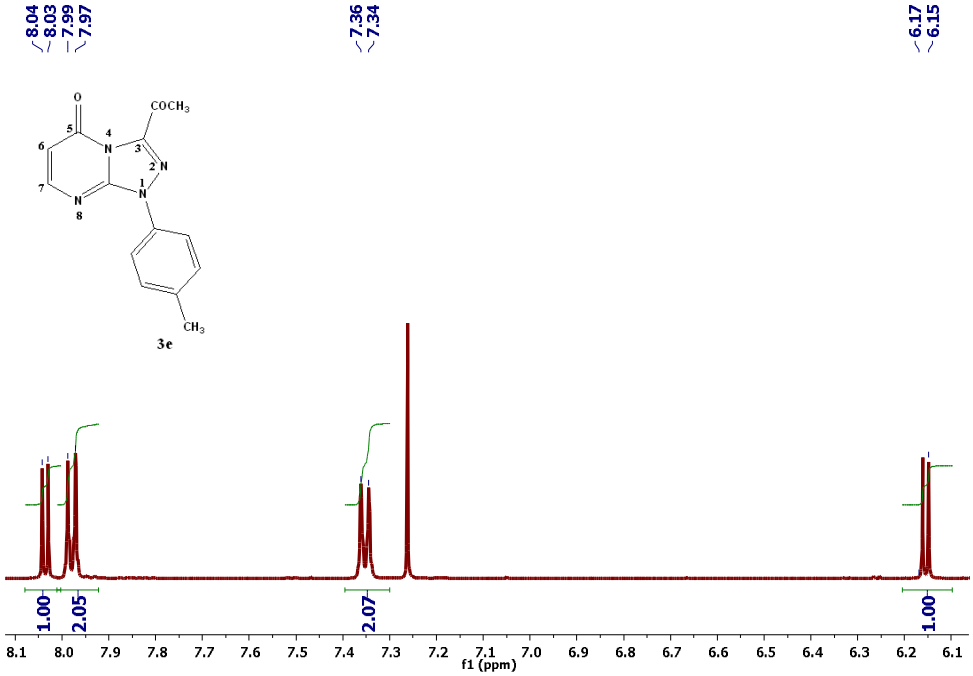

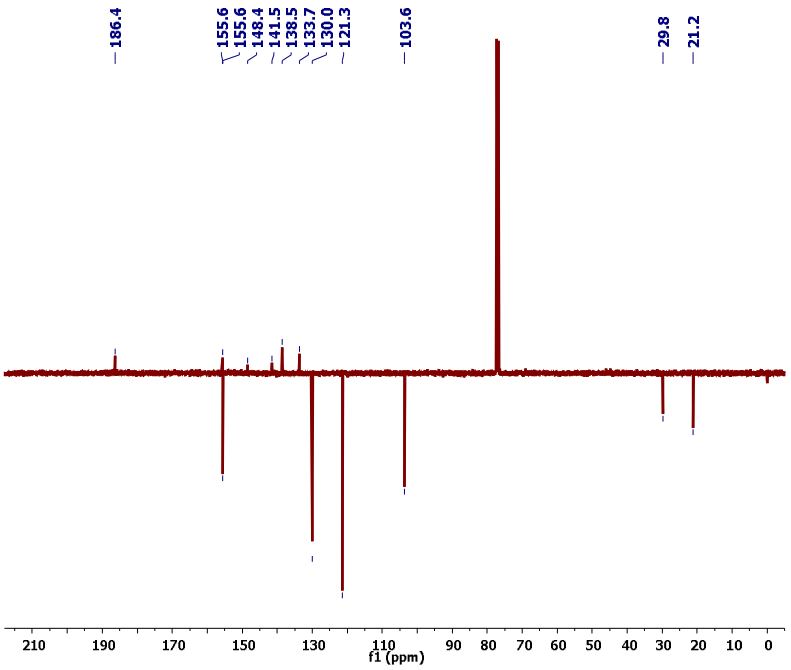

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5	Owner	nmrsu
6	Site	
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8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
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21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
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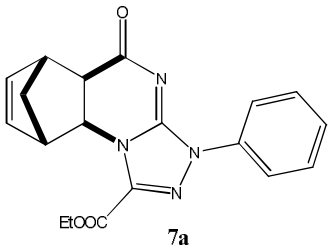
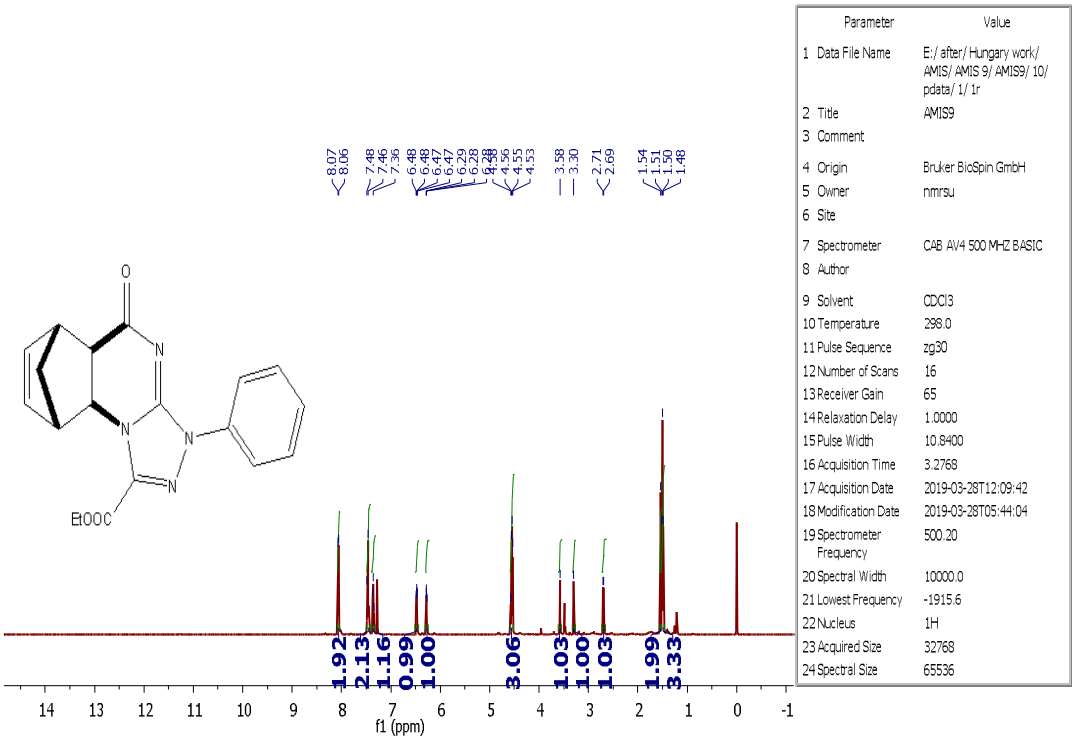


7a

Ethyl (4a*S,5*S**,8*R**,8a*R**)-1-phenyl-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline-3-carboxylate (7a)**



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8 Author	
9 Solvent	CDCl3
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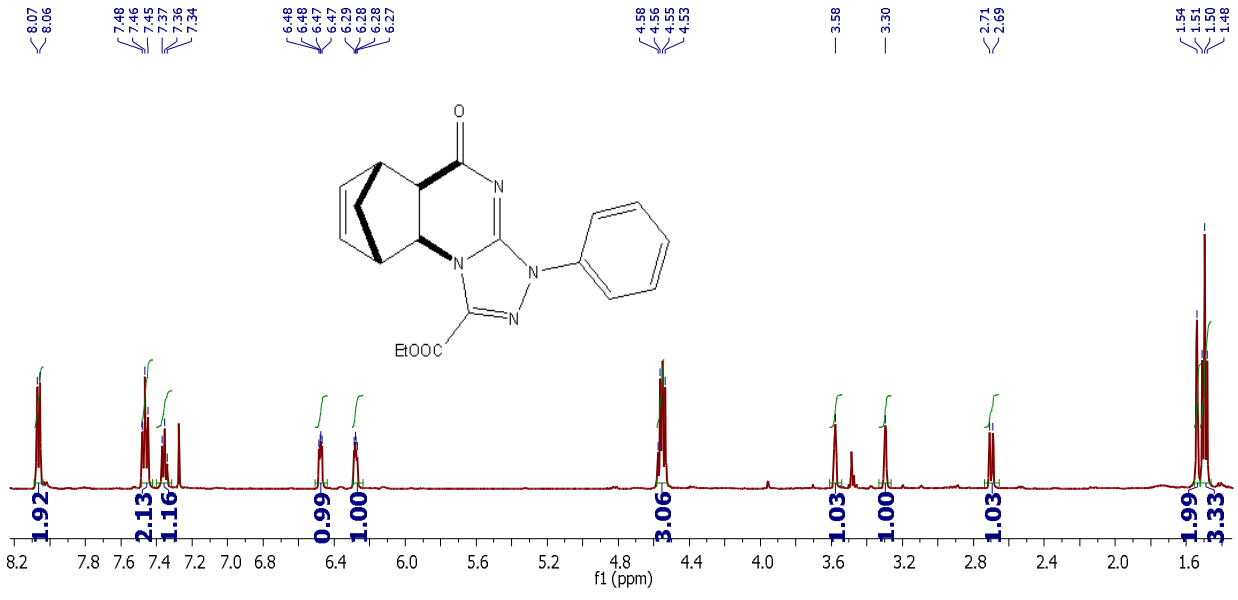
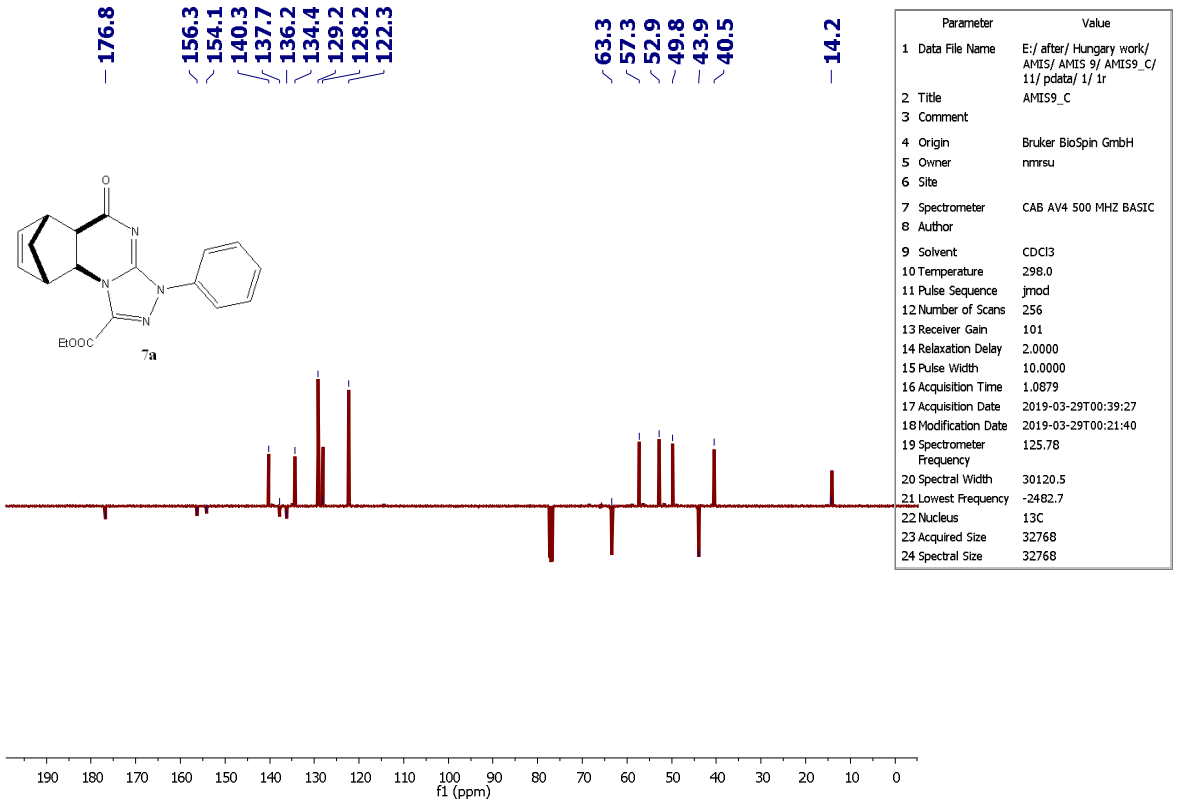
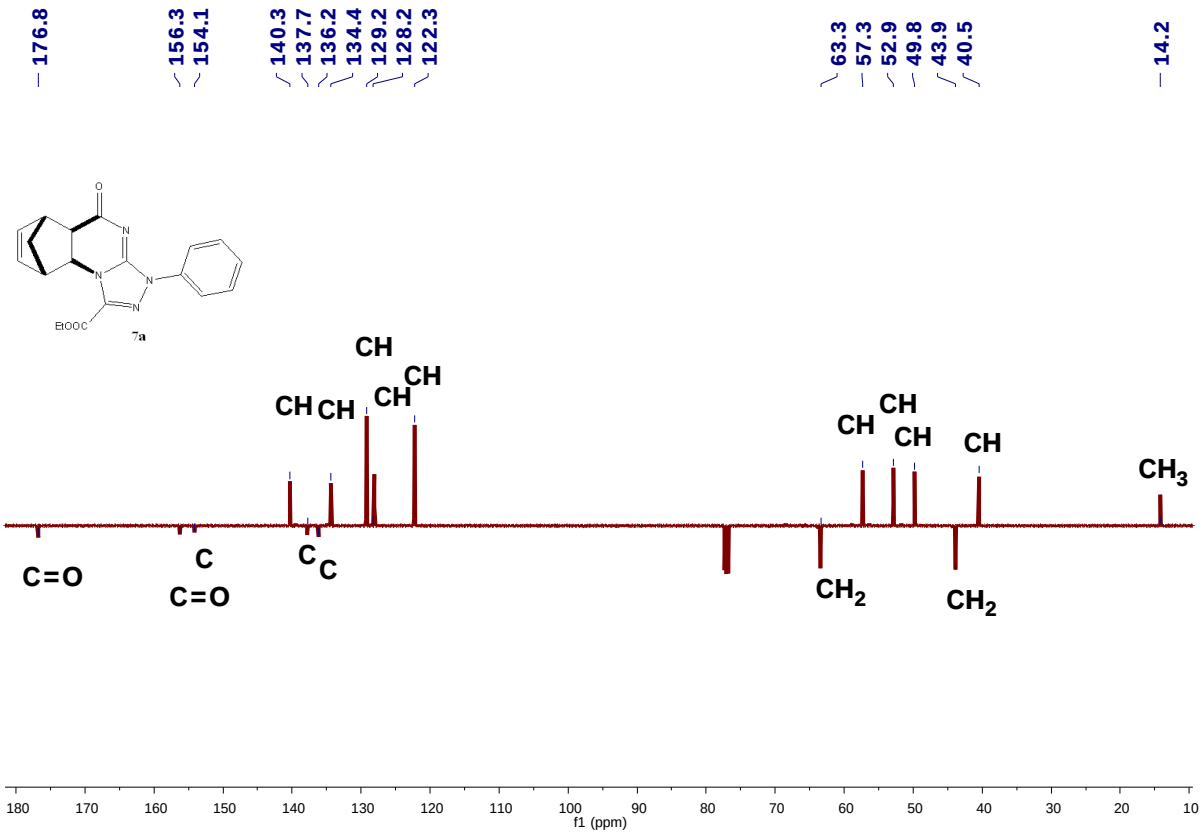
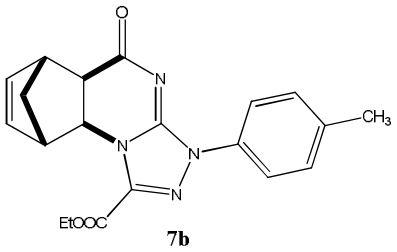
23 Acquired Size	32768
24 Spectral Size	65536





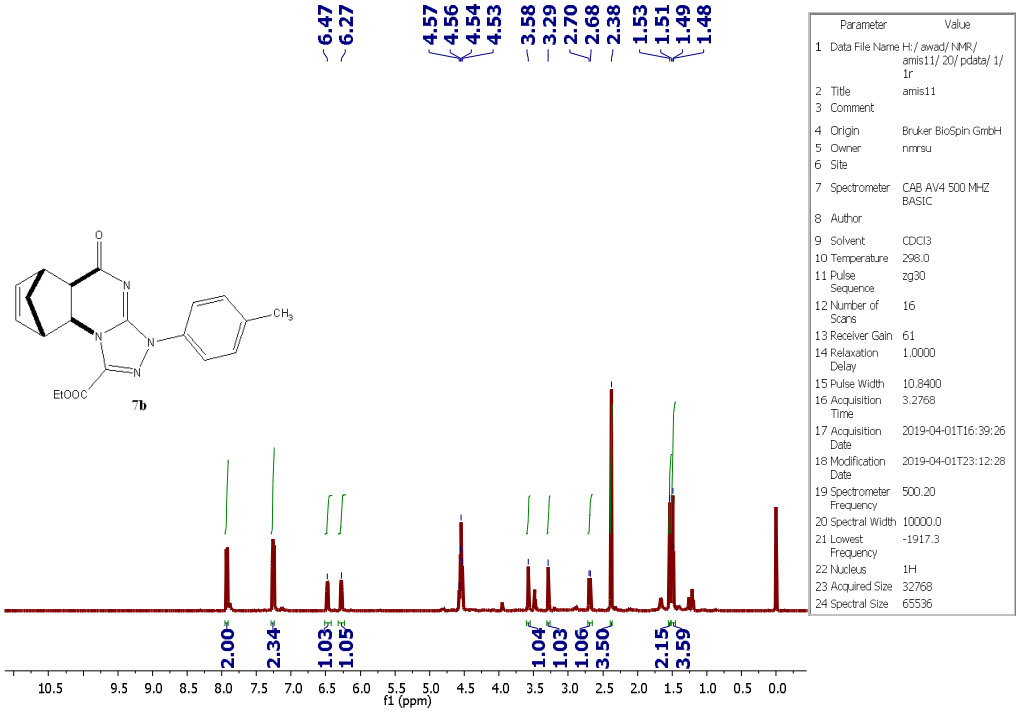
Parameter	Value
1 Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 9/ AMIS9_C/ 11/ pdata/ 1/ 1r
2 Title	AMIS9_C
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	CAB AV4 500 MHZ BASIC
8 Author	
9 Solvent	CDCl3
10 Temperature	298.0
11 Pulse Sequence	jmod
12 Number of Scans	256
13 Receiver Gain	101
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.0879
17 Acquisition Date	2019-03-29T00:39:27
18 Modification Date	2019-03-29T00:21:40
19 Spectrometer Frequency	125.78
20 Spectral Width	30120.5
21 Lowest Frequency	-2482.7
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	32768

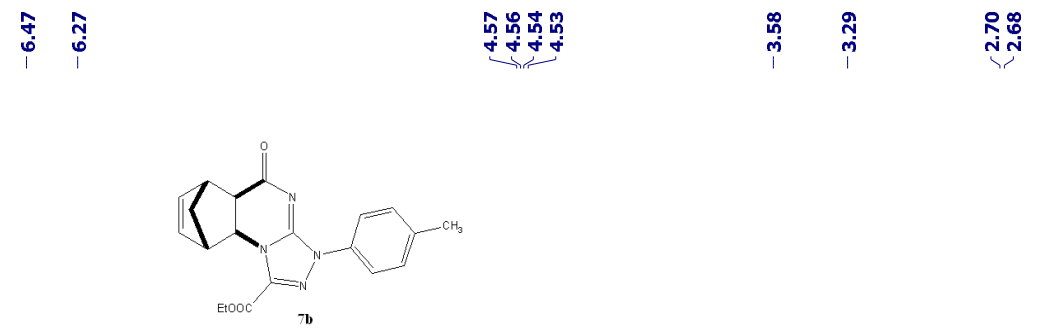


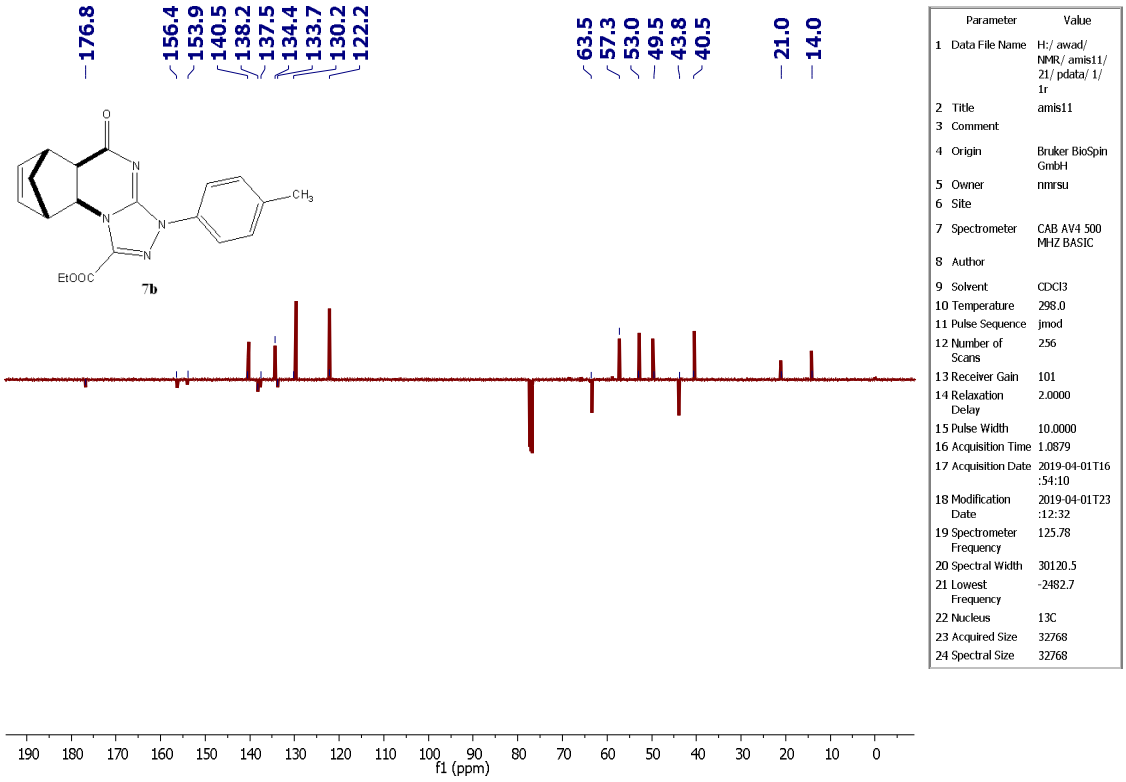


7b

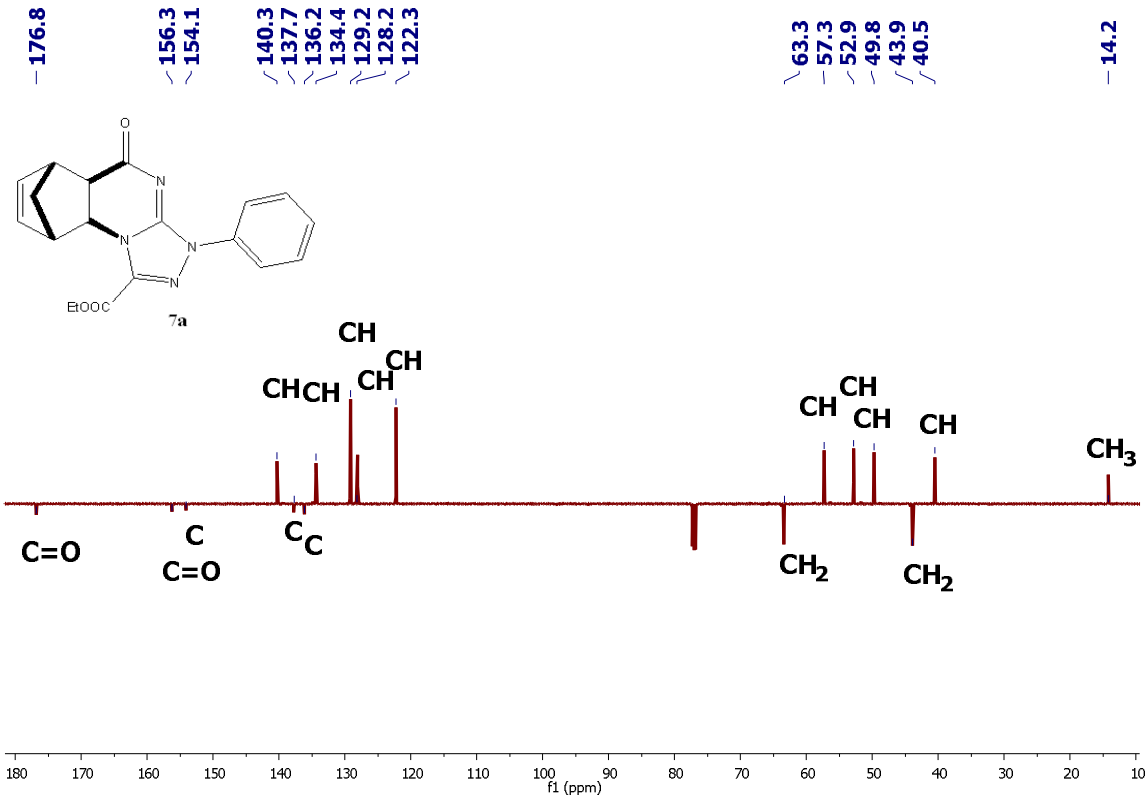
Ethyl (4a*S,5*S**,8*R**,8a*R**)-1-(*p*-tolyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline-3-carboxylate (7b)**

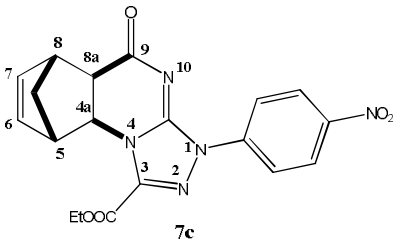






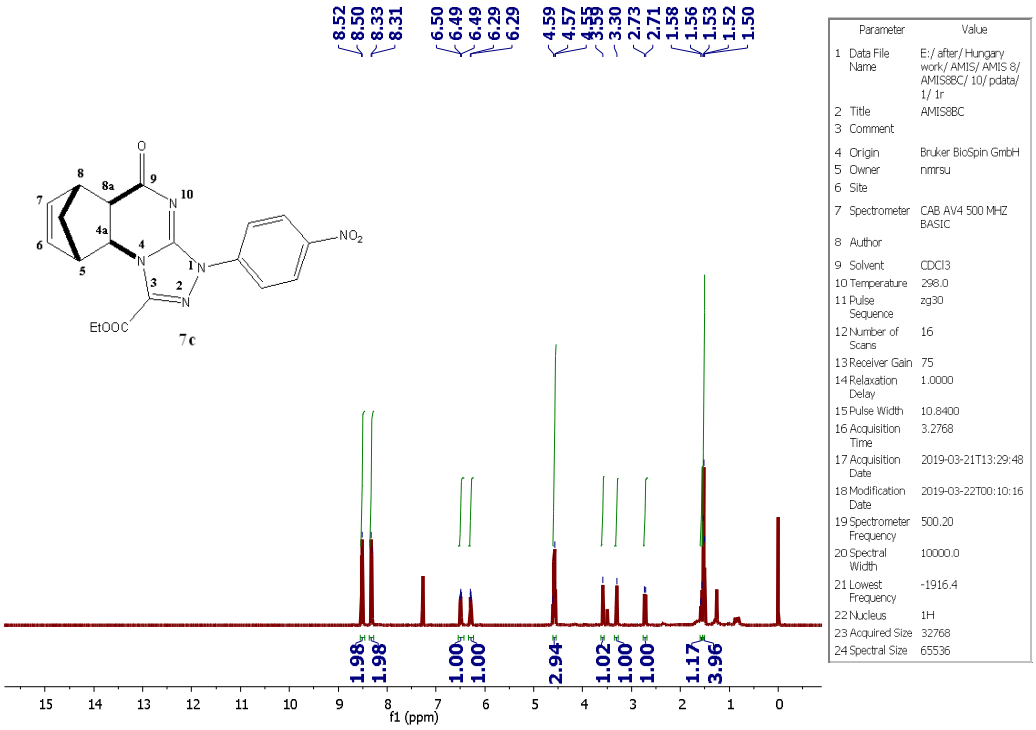
	Parameter	Value
1	Data File Name	H:/ awad/ NMR/ amis11/ 21/ pdata/ 1/ 1r
2	Title	amis11
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-01T16 :54:10
18	Modification Date	2019-04-01T23 :12:32
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768



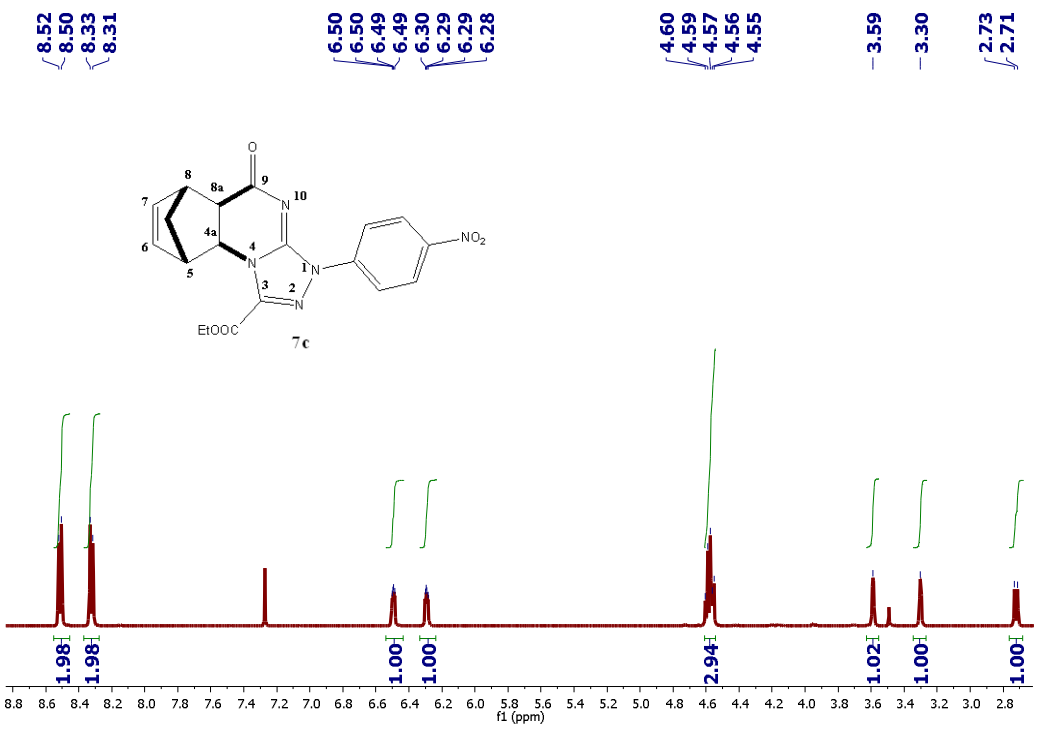


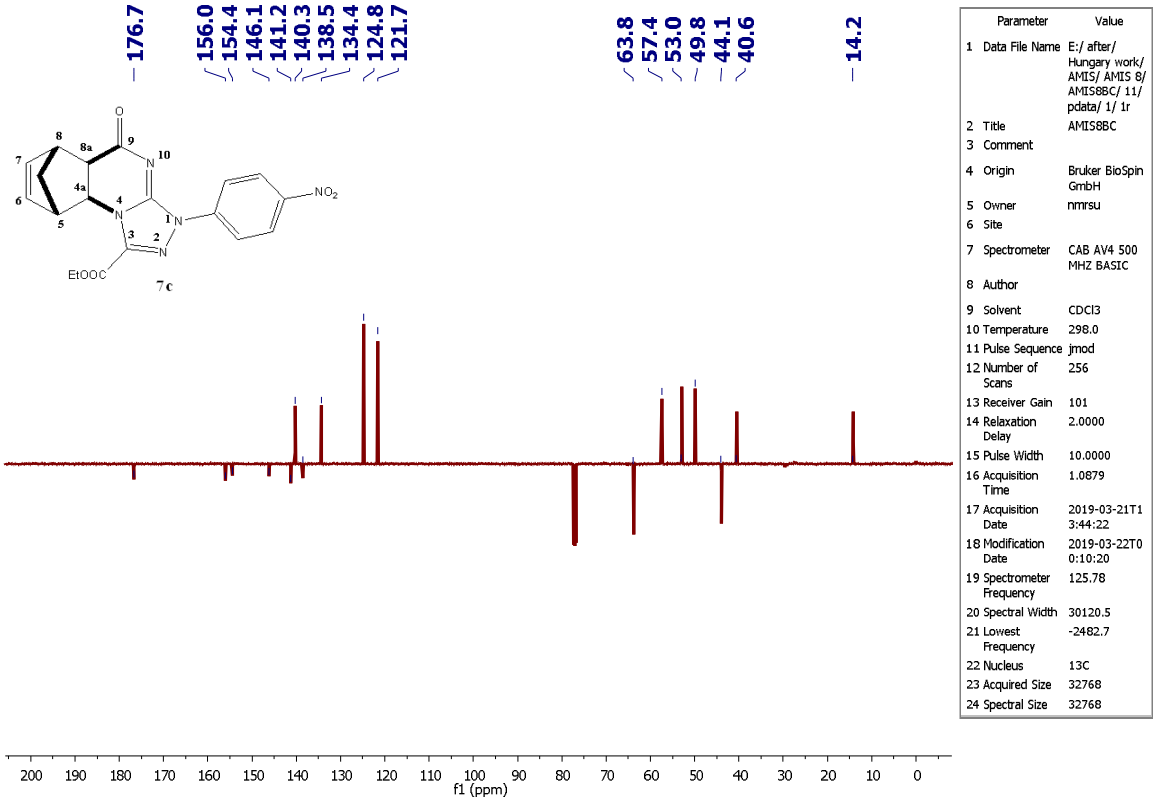
7c

Ethyl (4a*S,5*S**,8*R**,8a*R**)-1-(4-nitrophenyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline-3-carboxylate (7c)**

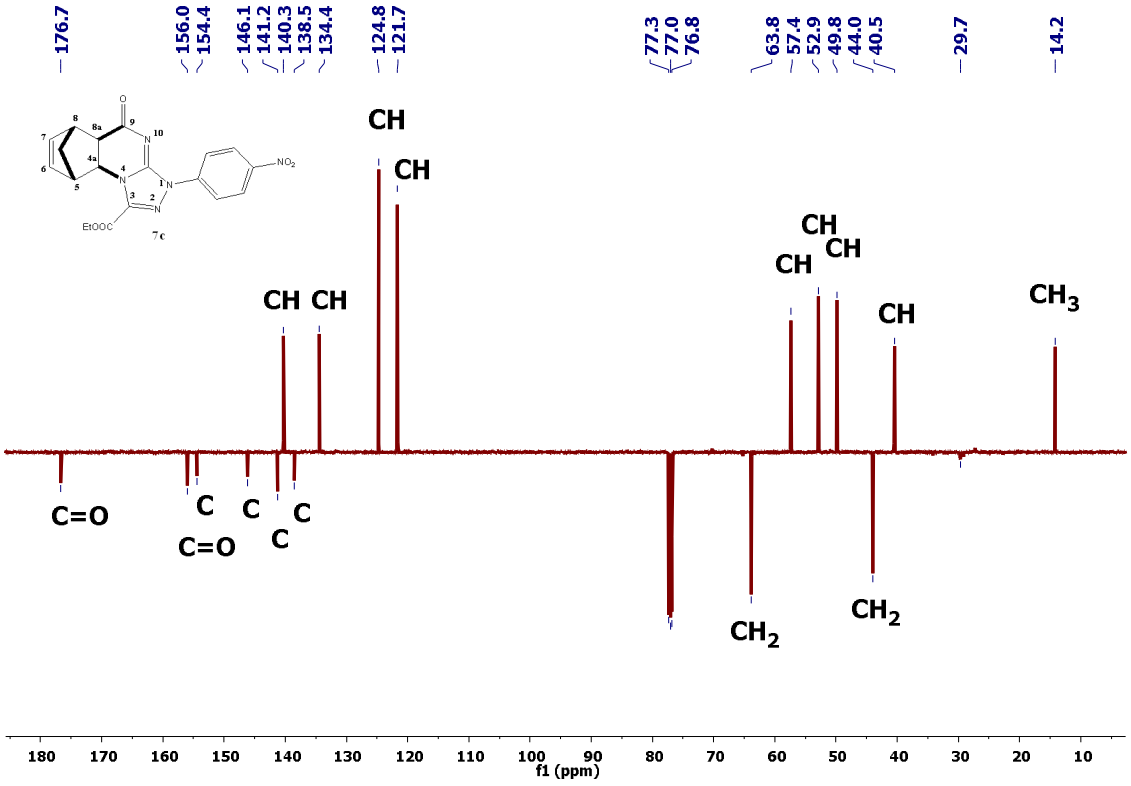


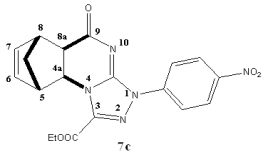
	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 8/ AMIS8BC/ 10/ pdata/ 1/ 1r
2	Title	AMIS8BC
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	75
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-03-21T13:29:48
18	Modification Date	2019-03-22T00:10:16
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1916.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536





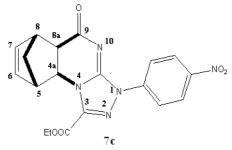
	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 8/ AMIS8BC/ 11/ pdata/ 1/ 1r
2	Title	AMIS8BC
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-03-21T13:44:22
18	Modification Date	2019-03-22T00:10:20
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768



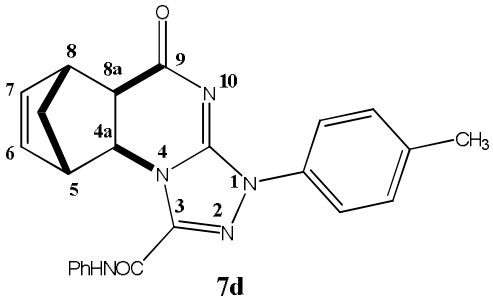


COSY Experiment

	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 8/ AMIS8BC/ 12/ pdata/ 1/ 2rr
2	Title	AMIS8BC
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	cosygpppqf
12	Number of Scans	1
13	Receiver Gain	101
14	Relaxation Delay	1.9427
15	Pulse Width	10.8400
16	Acquisition Time	0.2109
17	Acquisition Date	2019-03-21T13:50:10
18	Modification Date	2019-03-22T00:10:26
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(4854.4, 4854.4)
21	Lowest Frequency	(-103.0, -103.0)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)

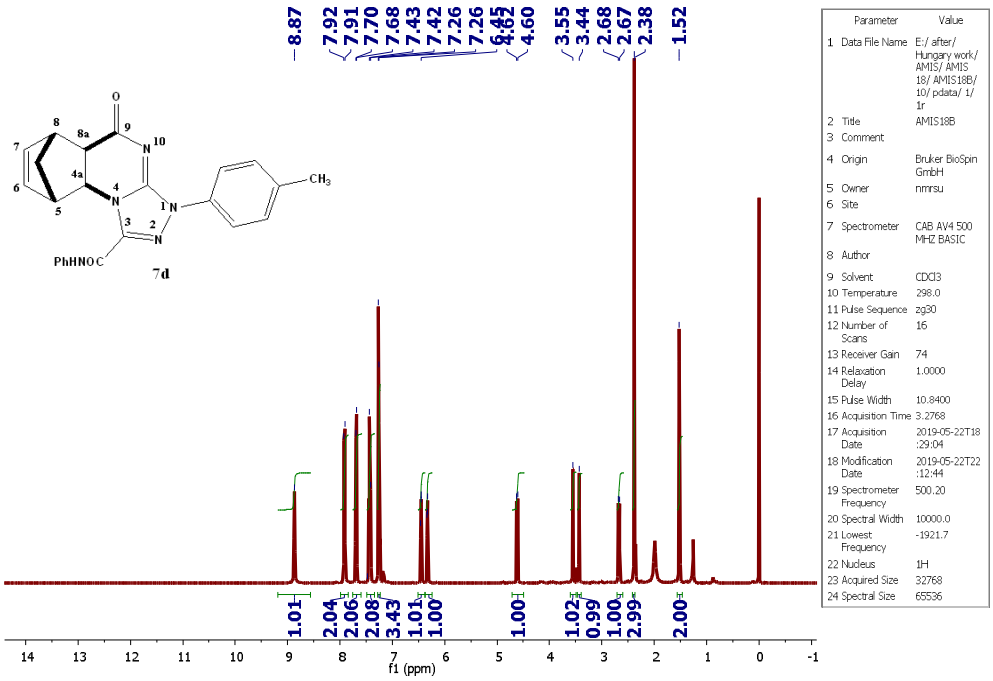


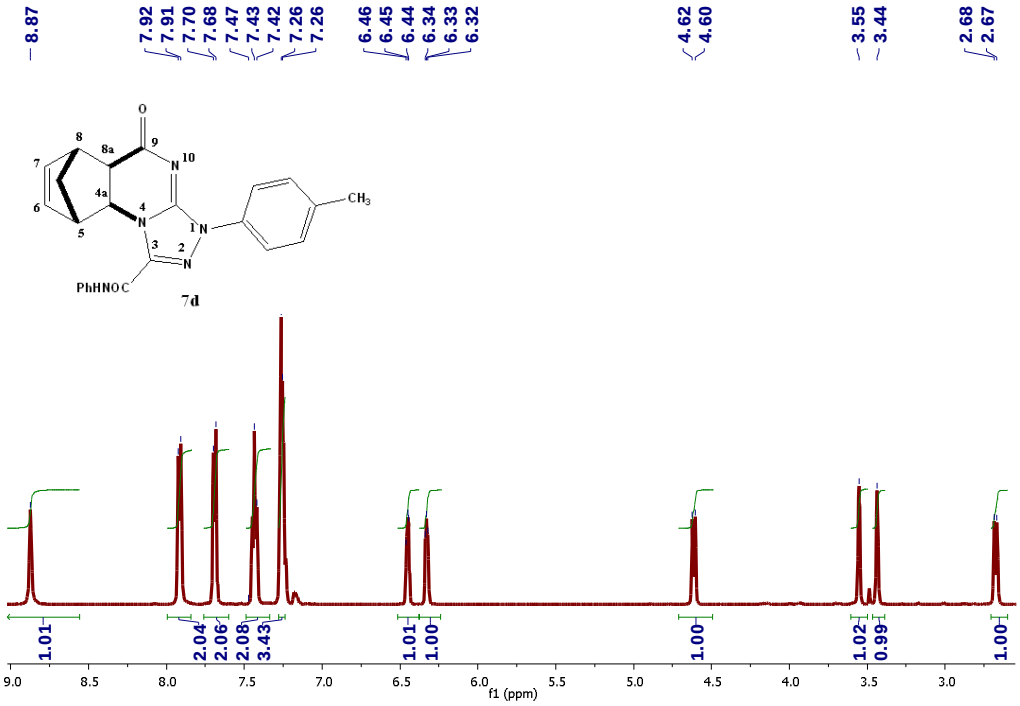
COSY experiment (expansion)

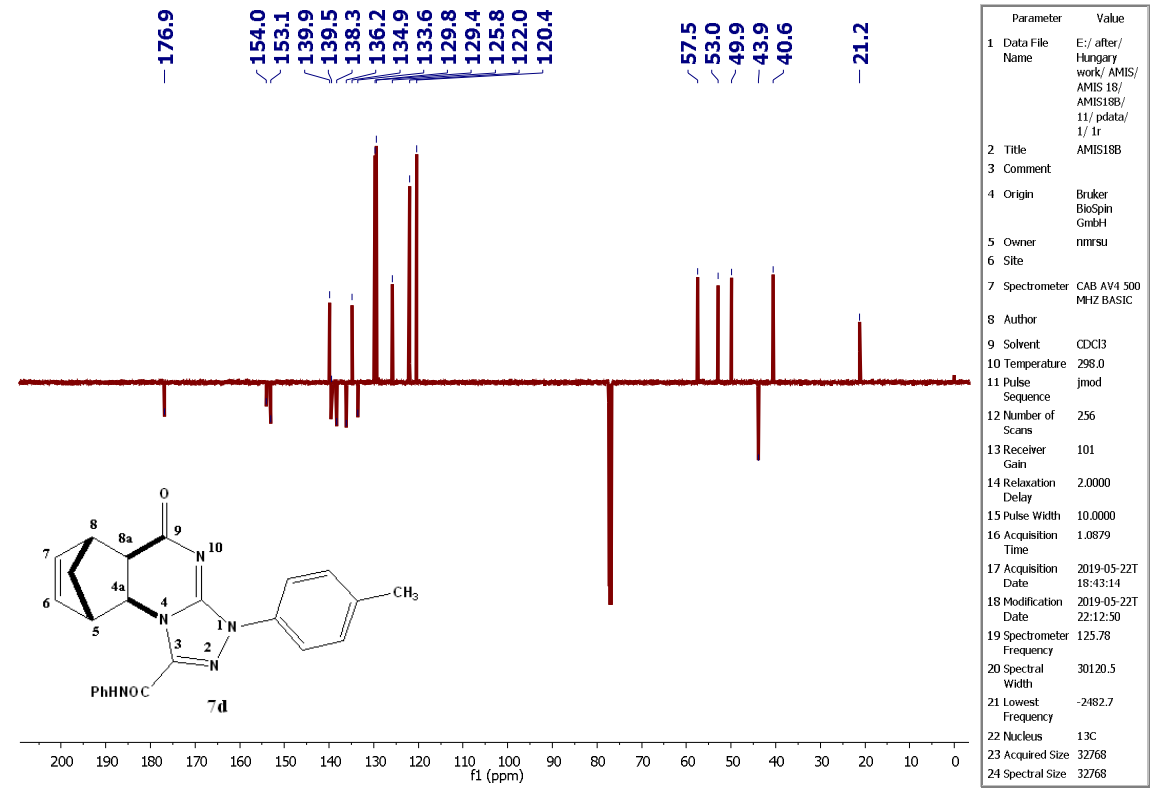


7d

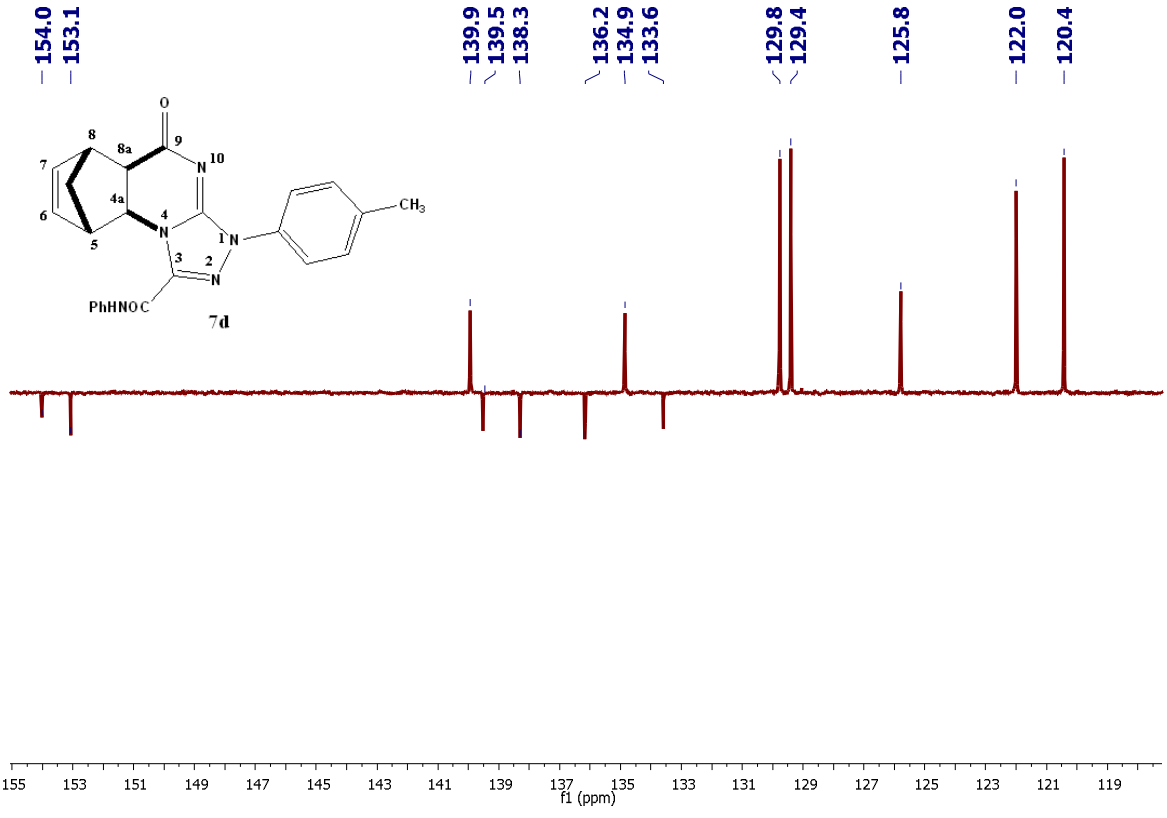
(4a*S,5*S**,8*R**,8a*R**)-*N*-Phenyl-1-(*p*-tolyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline-3-carboxamide(7d)**

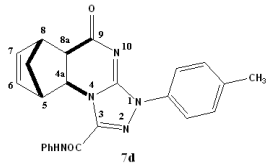




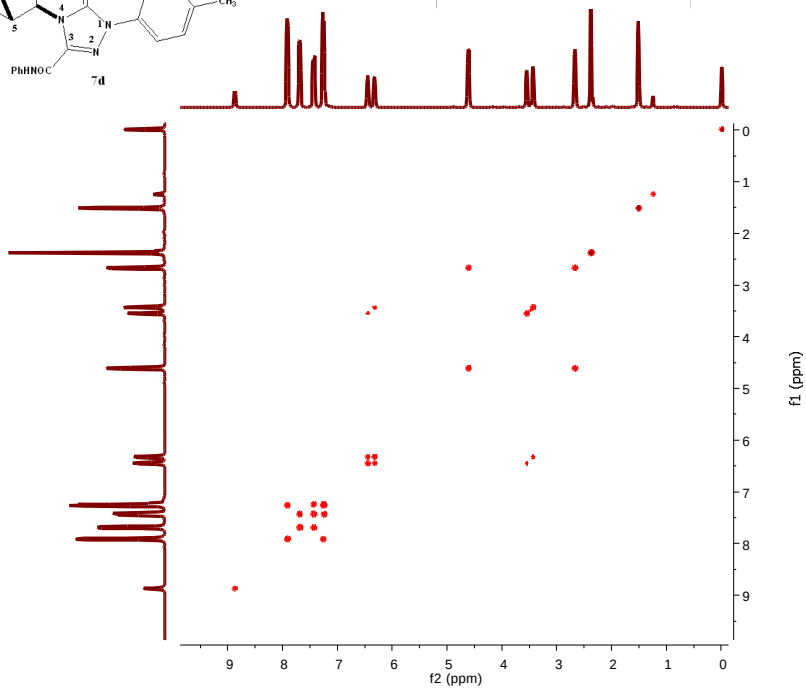


	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 18/ AMIS18B/ 11/ pdata/ 1/ 1r
2	Title	AMIS18B
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-05-22T 18:43:14
18	Modification Date	2019-05-22T 22:12:50
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

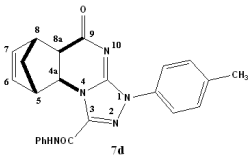




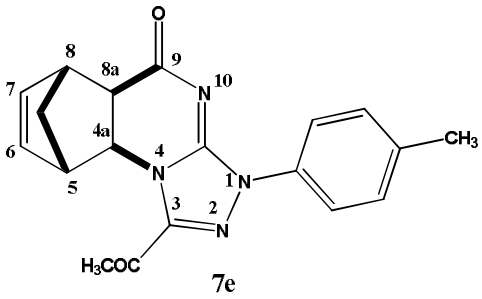
COSY Experiment



	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 18/ AMIS18B/ 12/ pdata/ 1/ 2rr
2	Title	AMIS18B
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	cosygpppqf
12	Number of Scans	1
13	Receiver Gain	101
14	Relaxation Delay	1.9529
15	Pulse Width	10.8400
16	Acquisition Time	0.2048
17	Acquisition Date	2019-05-22T18:49:01
18	Modification Date	2019-05-22T22:12:54
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(5000.0, 5000.0)
21	Lowest Frequency	(-66.1, -66.1)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)

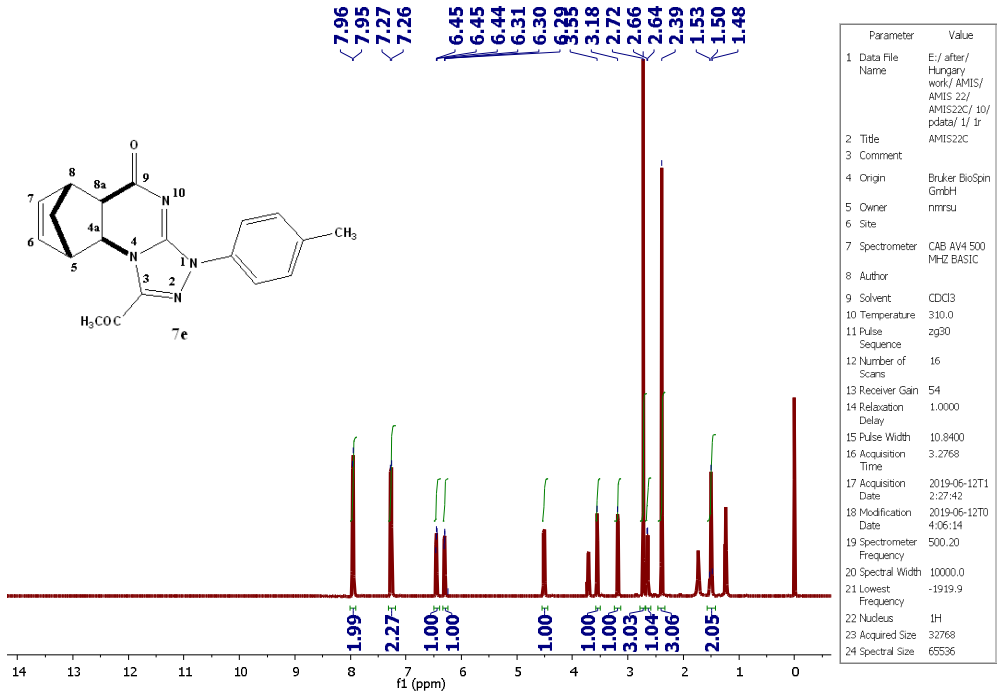


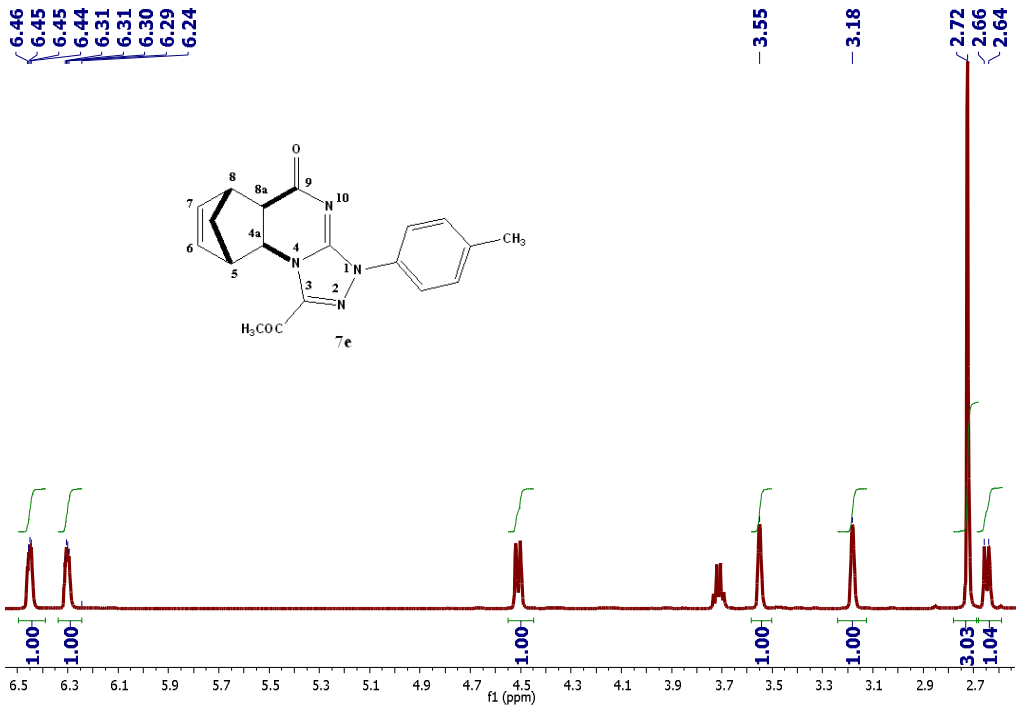
COSY Experiment

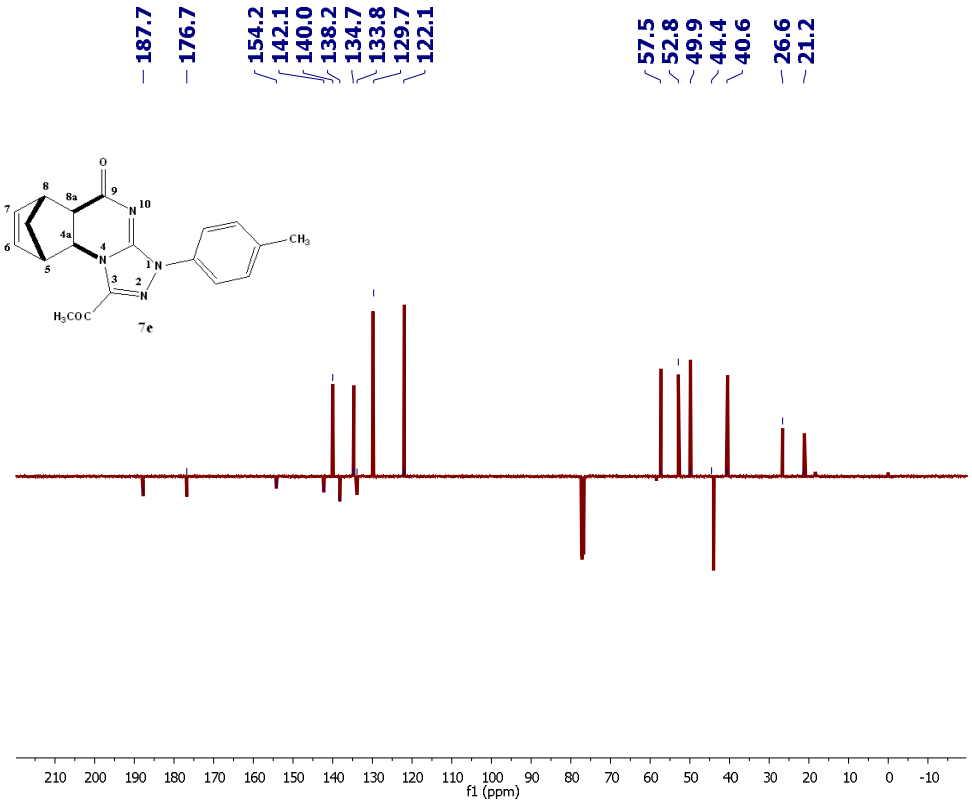


7e

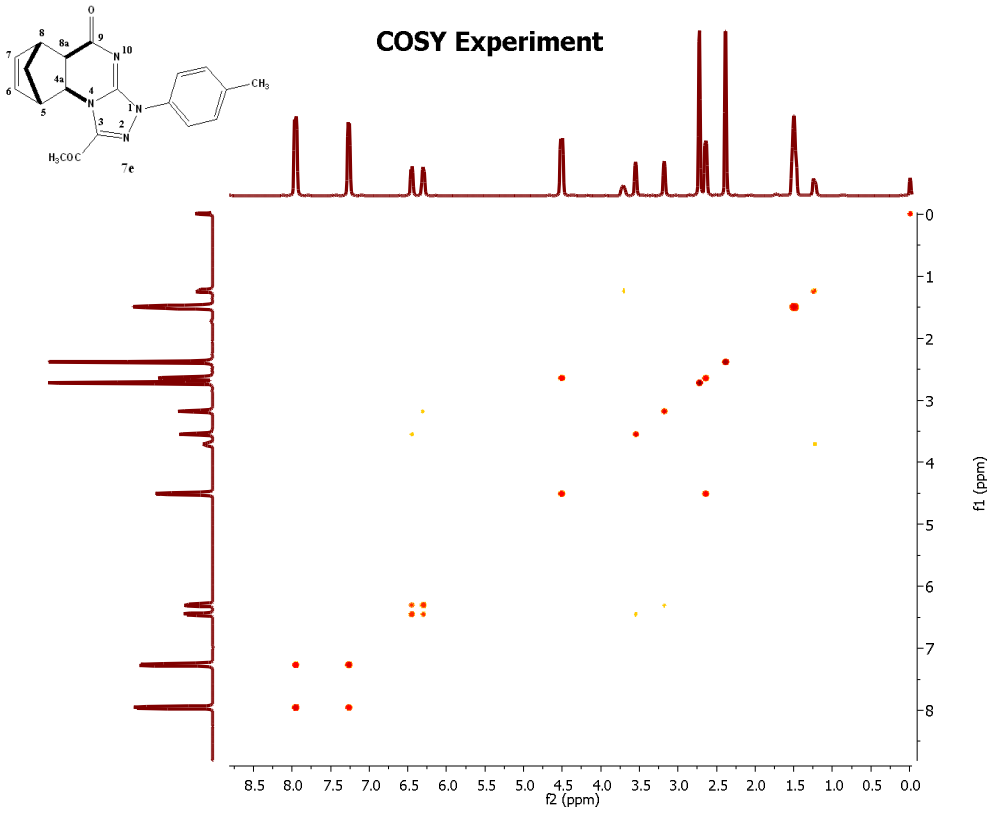
(4a*S,5*S**,8*R**,8a*R**)-3-Acetyl-1-(*p*-tolyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline (7e)**



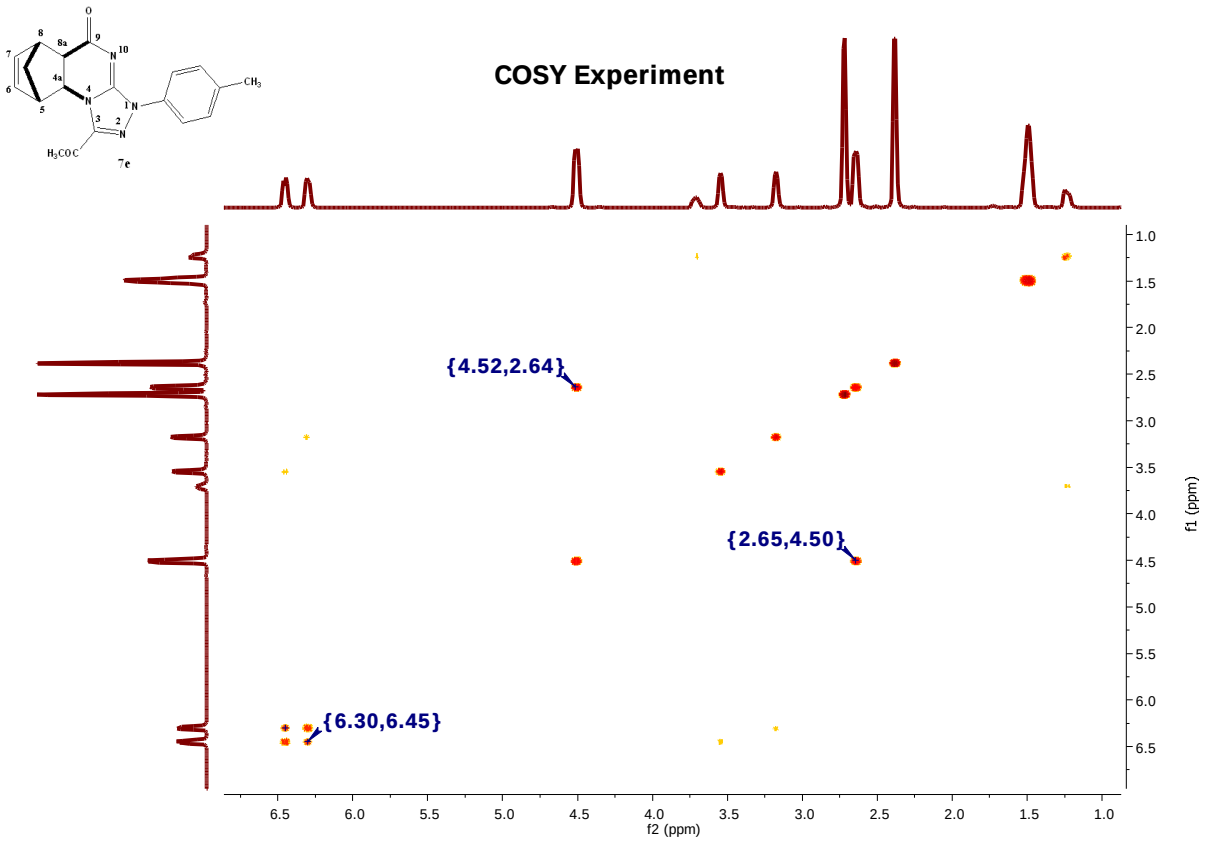


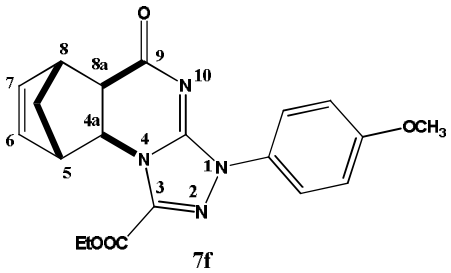


	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 22/ AMIS22C/ 11/ pdata/ 1/ 1r
2	Title	AMIS22C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-06-12T12:41:55
18	Modification Date	2019-06-12T04:06:22
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768



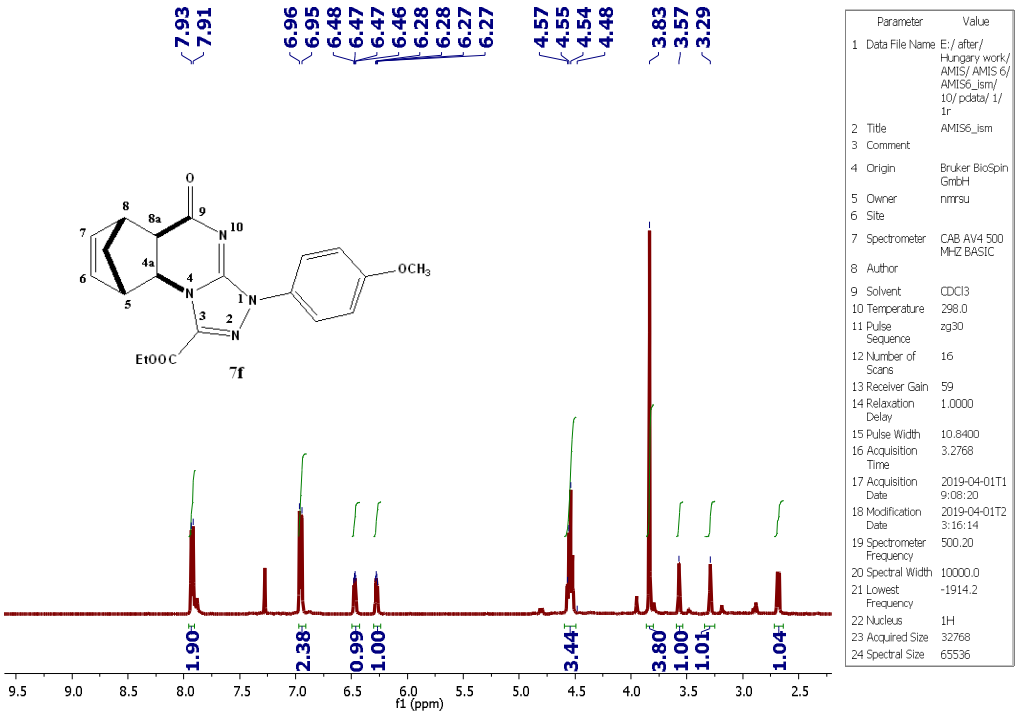
	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 22/ AMIS22C/ 12/ pdata/ 1/ 2rr
2	Title	AMIS22C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	cosygpppqf
12	Number of Scans	1
13	Receiver Gain	101
14	Relaxation Delay	1.9263
15	Pulse Width	10.8400
16	Acquisition Time	0.2314
17	Acquisition Date	2019-06-12T11:47:44
18	Modification Date	2019-06-12T03:06:30
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(4424.8, 4424.8)
21	Lowest Frequency	(-16.5, -16.5)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)


COSY Experiment
{4.52,2.64}
{2.65,4.50}
{6.30,6.45}
f2 (ppm)
f1 (ppm)
7e

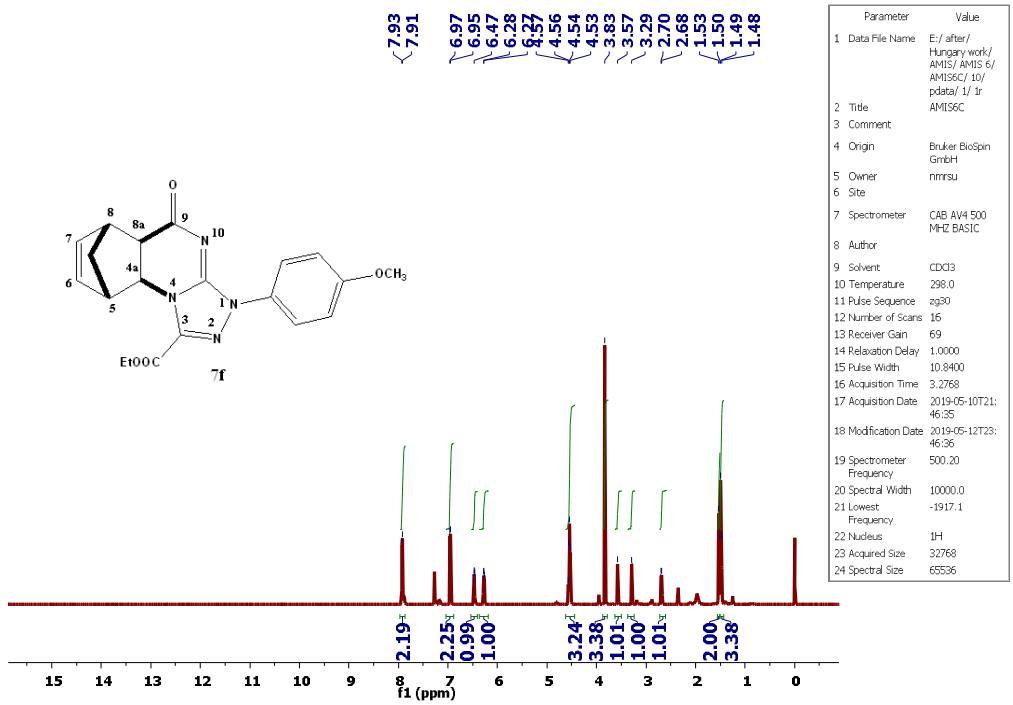


7f

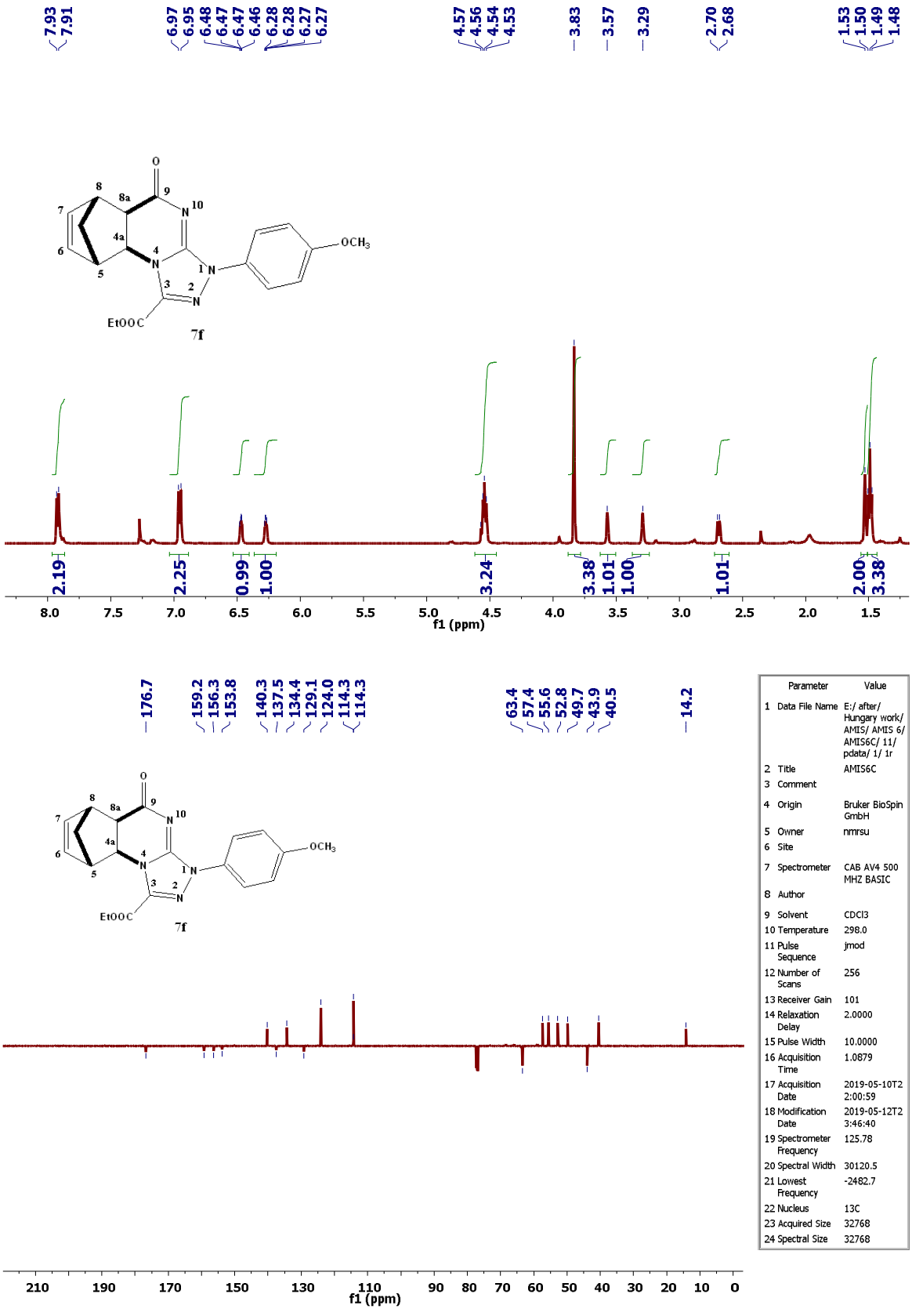
Ethyl (4a*S,5*S**,8*R**,8a*R**)-1-(4-methoxyphenyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]-quinazoline-3-carboxylate(7f)**



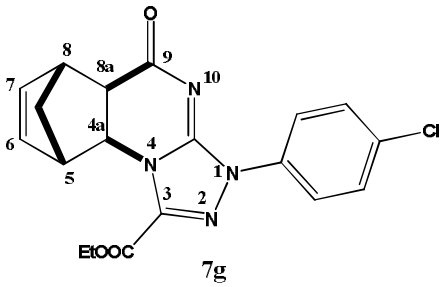
	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 6/ AMIS6_ism/ 10/ pdata/ 1/ 1r
2	Title	AMIS6_ism
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	59
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-04-01T19:08:20
18	Modification Date	2019-04-01T23:16:14
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1914.2
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 6/ AMIS6C/ 10/ pdata/ 1/ 1r
2	Title	AMIS6C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	69
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-05-10T21:46:35
18	Modification Date	2019-05-12T23:46:36
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1917.1
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

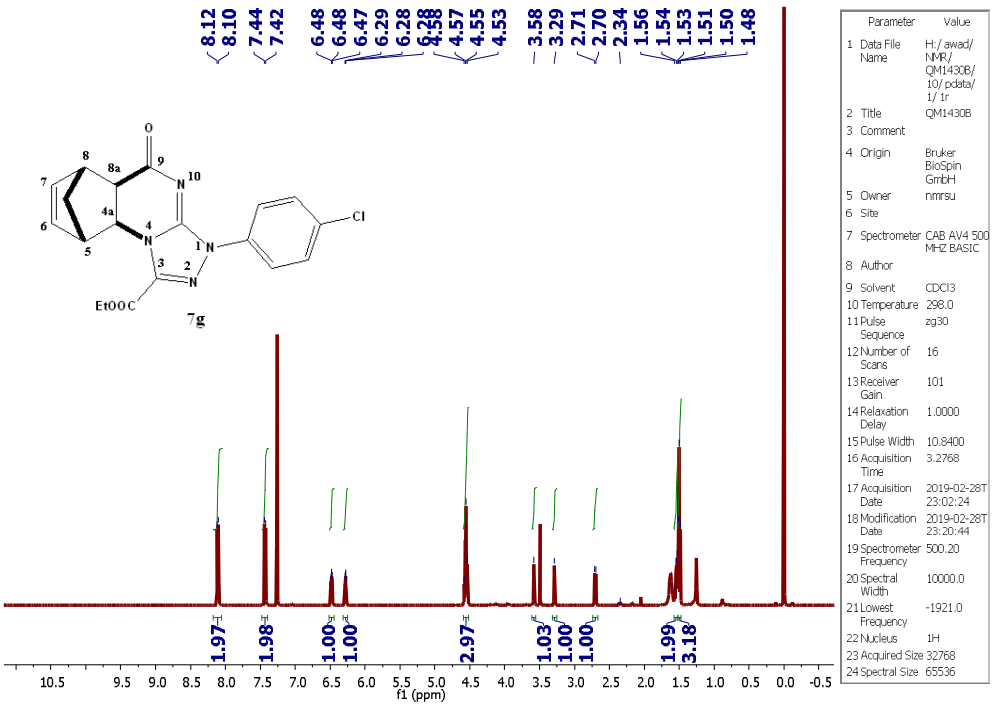


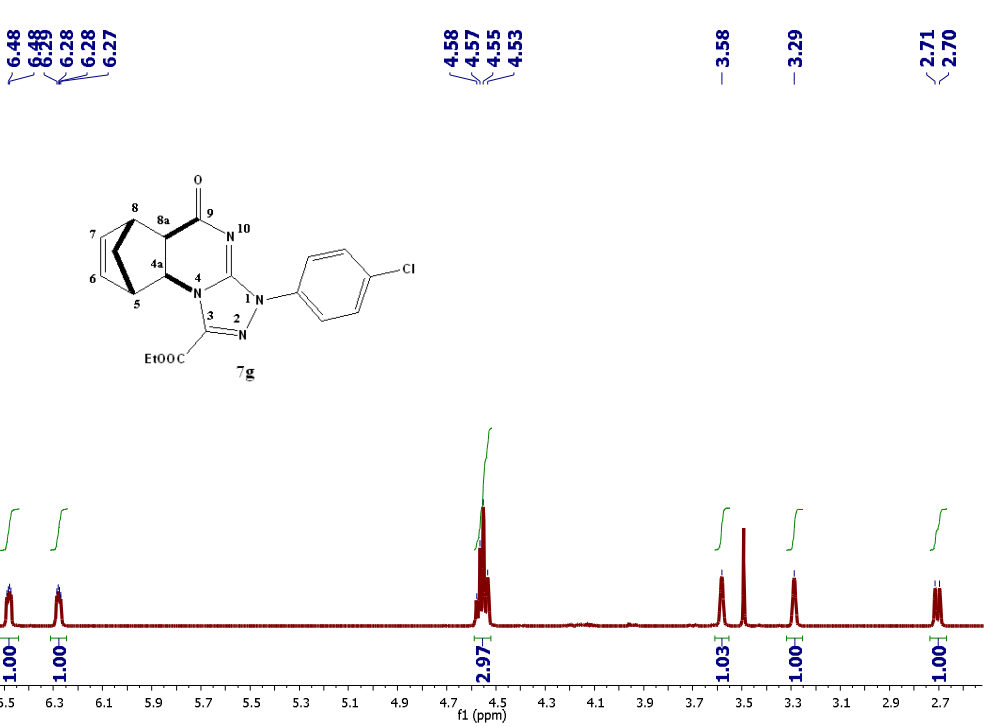
	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 6/ AMIS6C/ 11/ pdata/ 1/ 1r
2	Title	AMIS6C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-05-10T2 2:00:59
18	Modification Date	2019-05-12T2 3:46:40
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

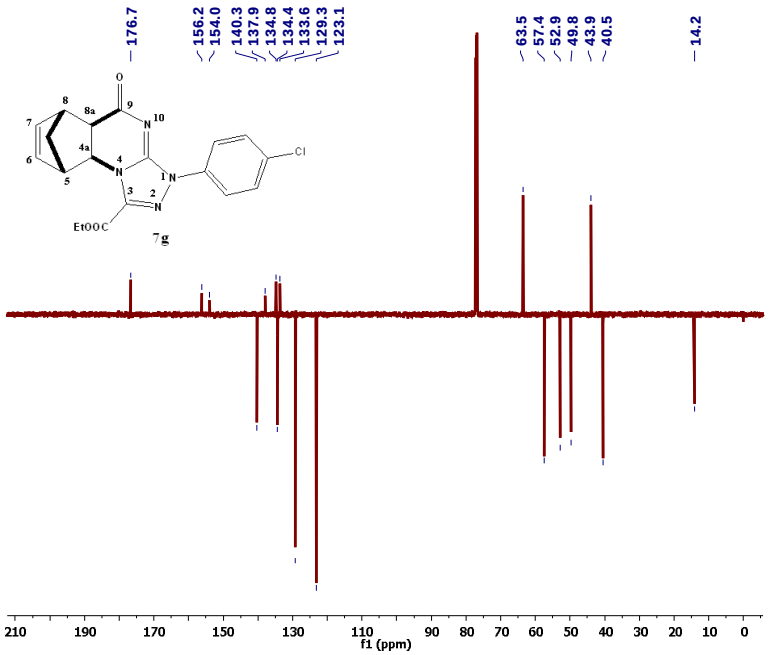


7g

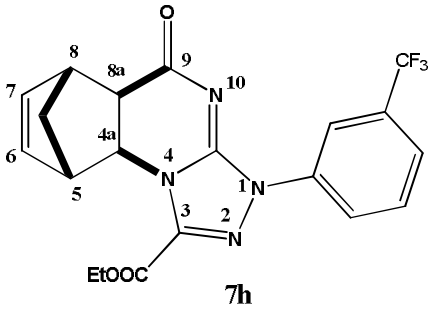
Ethyl (4a*S,5*S**,8*R**,8a*R**)-1-(4-chlorophenyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]-quinazoline-3-carboxylate (7g)**





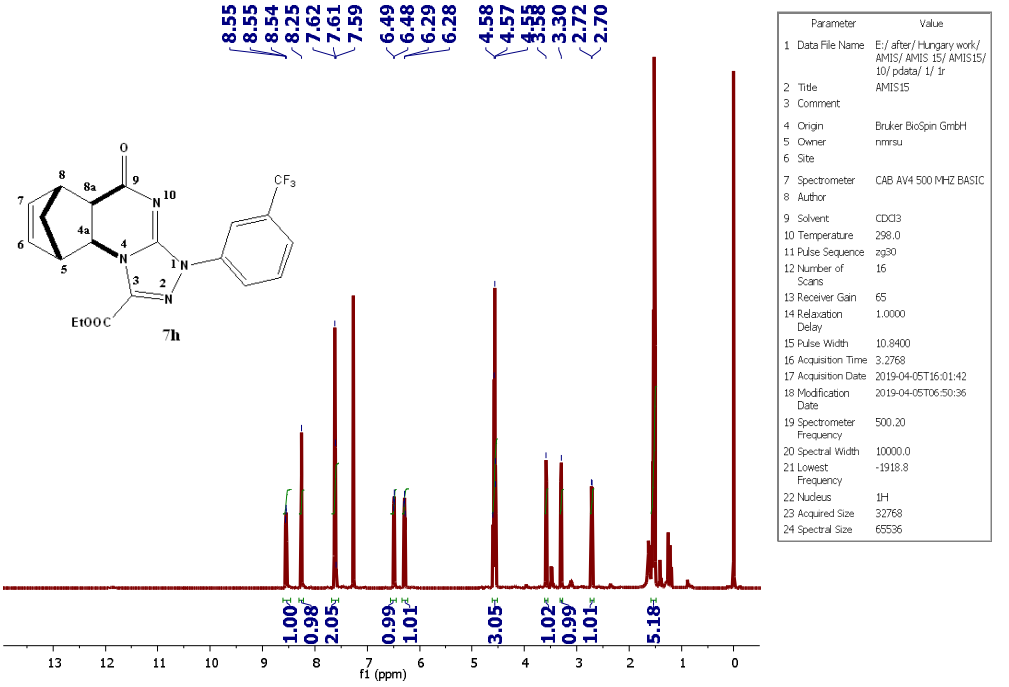


	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM_1430_C/ 11/ pdata/ 1/ 1r
2	Title	PM_1430_C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-05T13:40:33
18	Modification Date	2019-04-05T05:08:30
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

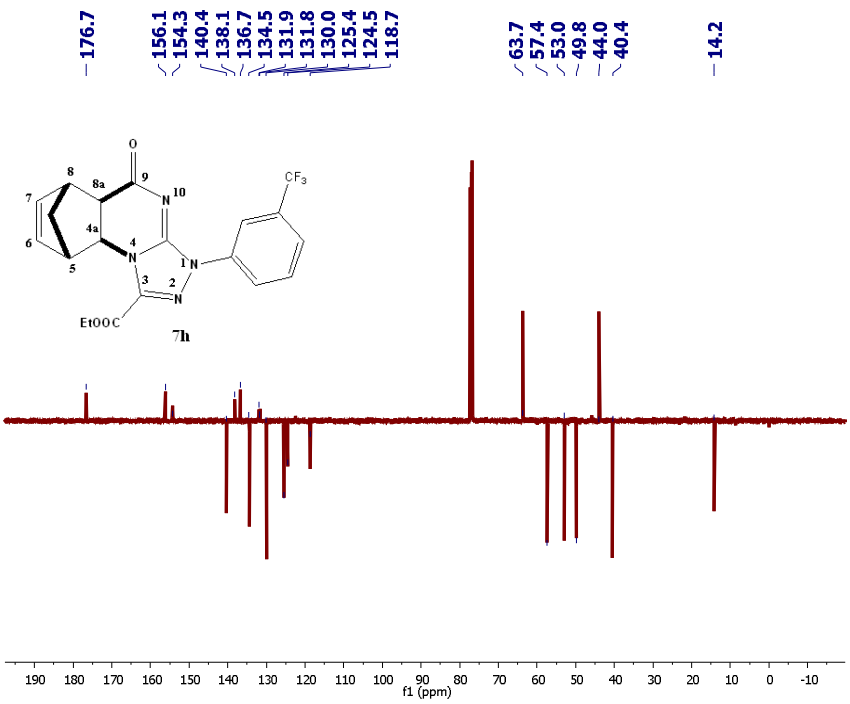


7h

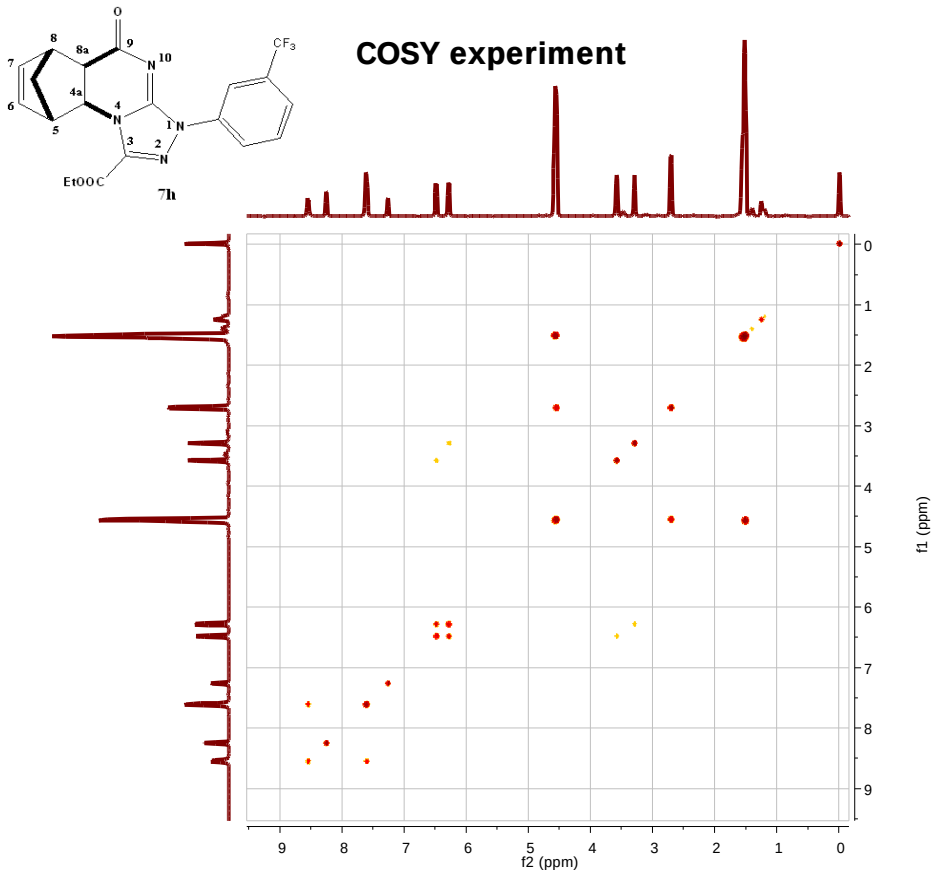
Ethyl (4a*S,5*S**,8*R**,8a*R**)-1-(3-(trifluoromethyl)phenyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]-quinazoline-3-carboxylate (7h)**



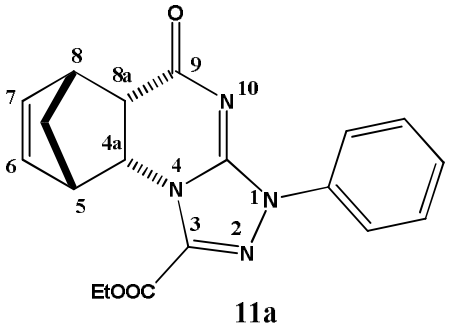
	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 15/ AMIS15/ 10/ pdata/ 1/ 1r
2	Title	AMIS15
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	65
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-04-05T16:01:42
18	Modification Date	2019-04-05T06:50:36
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1918.8
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 15/ AMIS15/ 11/ pdata/ 1/ 1r
2	Title	AMIS15
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-05T16:15:50
18	Modification Date	2019-04-05T06:50:40
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

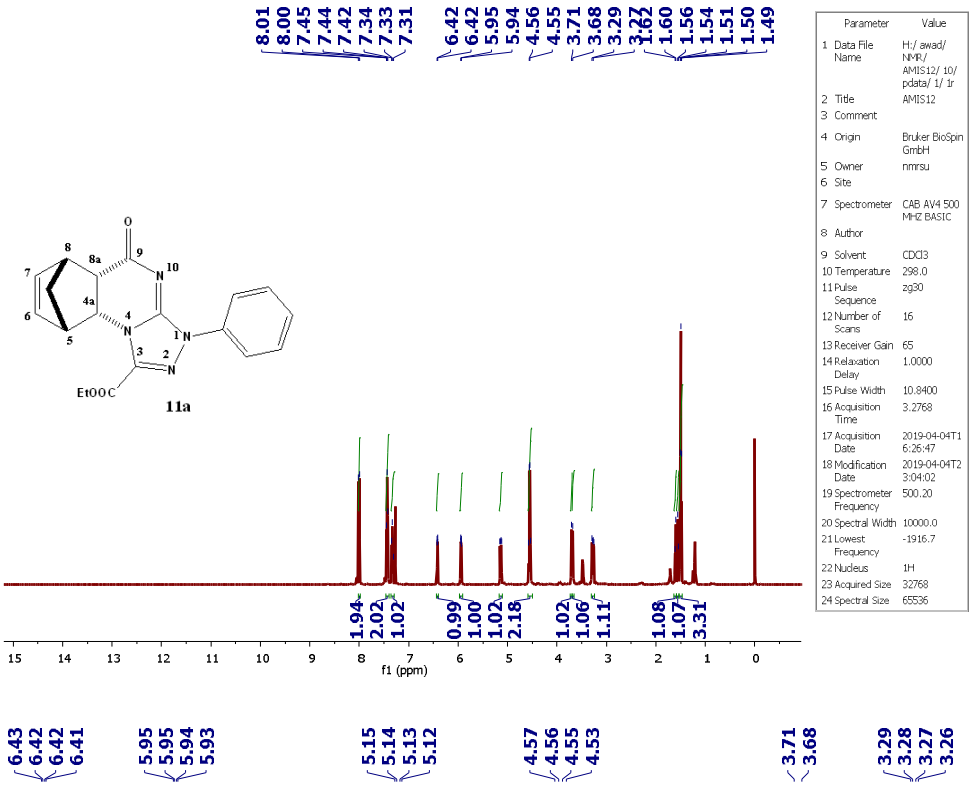


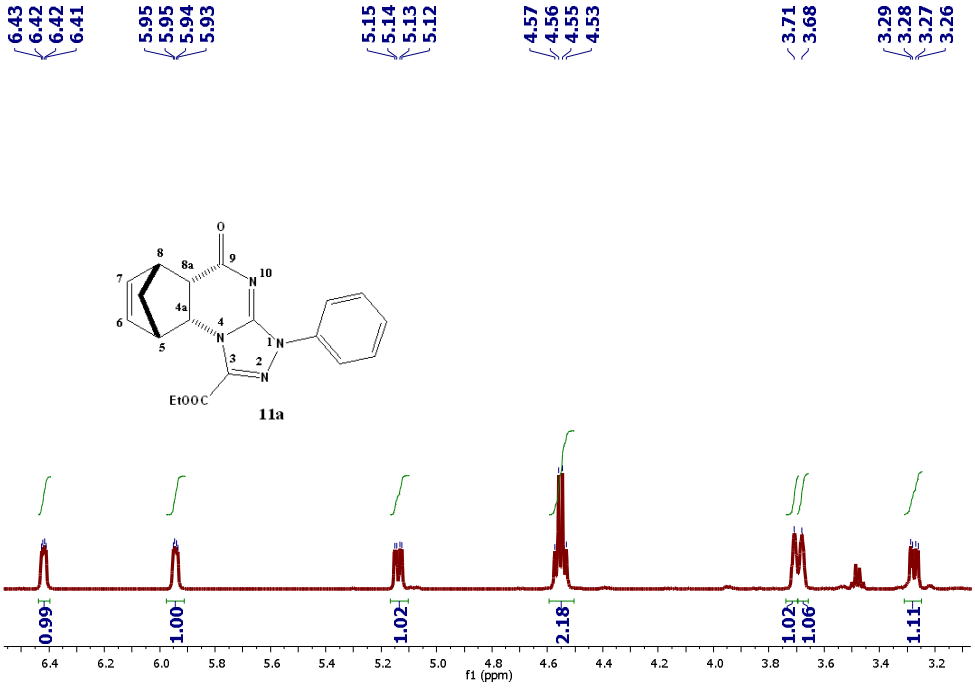
	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 15/ AMIS15/ 12/ pdata/ 1/ 2rr
2	Title	AMIS15
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	cosygpppqf
12	Number of Scans	1
13	Receiver Gain	101
14	Relaxation Delay	1.9427
15	Pulse Width	10.8400
16	Acquisition Time	0.2109
17	Acquisition Date	2019-04-05T16:21:39
18	Modification Date	2019-04-05T06:50:46
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(4854.4, 4854.4)
21	Lowest Frequency	(-84.7, -84.7)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)

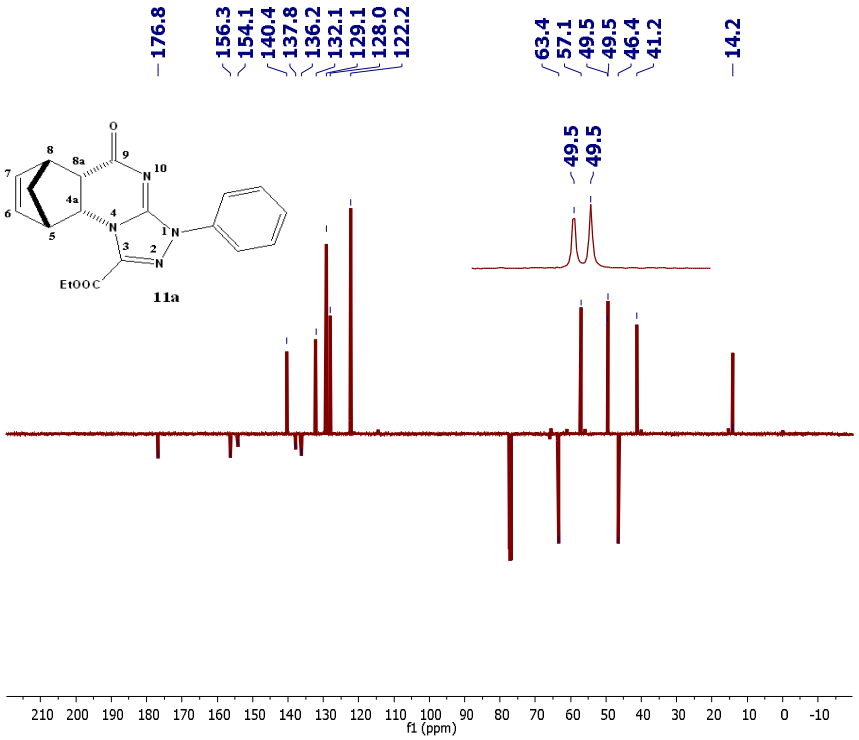


11a

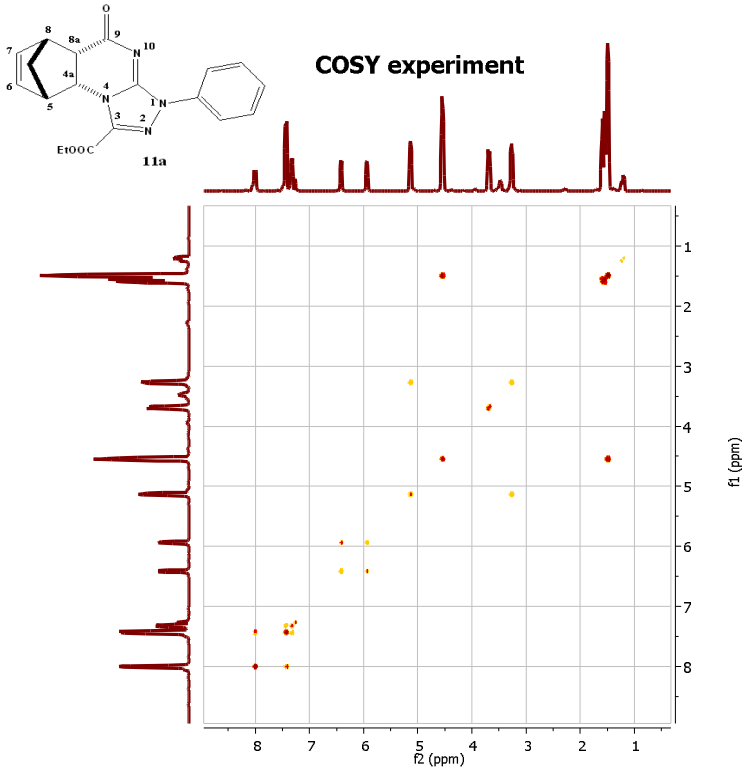
Ethyl (4a*R,5*S**,8*R**,8a*S**)-1-phenyl-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline-3-carboxylate (11a)**



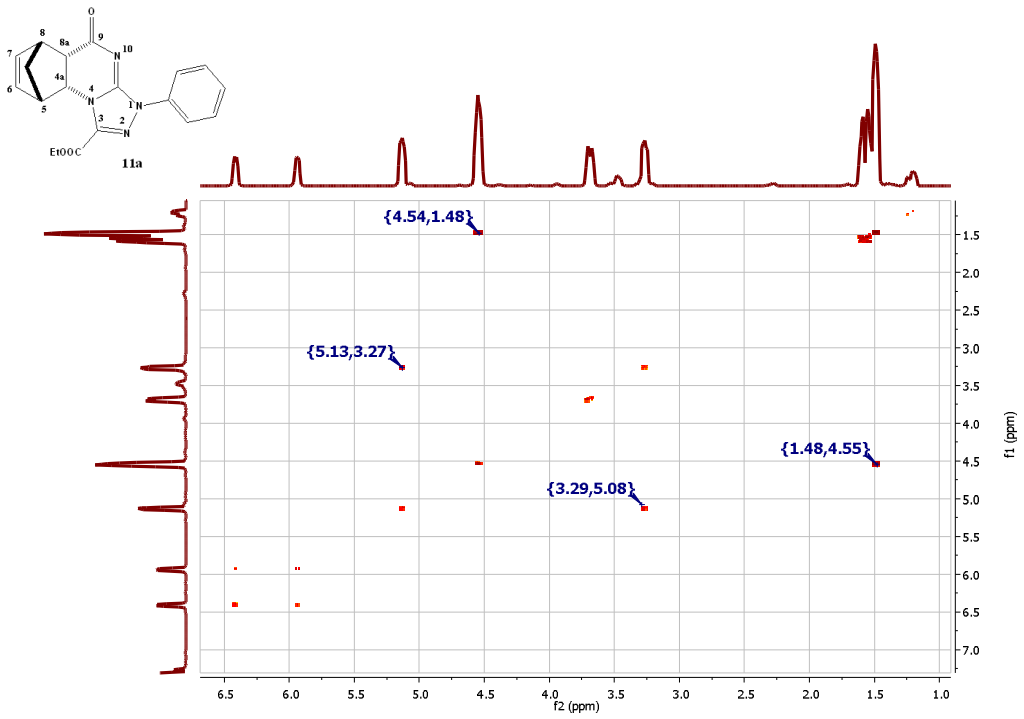




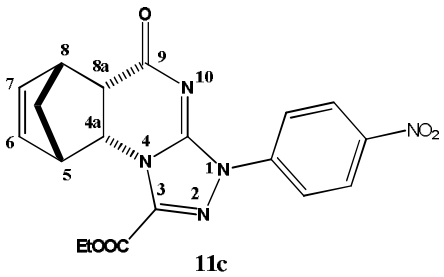
	Parameter	Value
1	Data File Name	H:/ awad/ NMR/ AMIS12/ 11/ pdata/ 1/ 1r
2	Title	AMIS12
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-04T16:40:59
18	Modification Date	2019-04-04T23:04:08
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768



	Parameter	Value (f2, f1)
1	Data File Name	H:/ awad/ NMR/ AMIS12/ 12/ pdata/ 1/ 2rr
2	Title	AMIS12
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	cosygpppqf
12	Number of Scans	1
13	Receiver Gain	101
14	Relaxation Delay	1.9181
15	Pulse Width	10.8400
16	Acquisition Time	0.2376
17	Acquisition Date	2019-04-04T16:46:48
18	Modification Date	2019-04-04T23:04:16
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(4310.3, 4310.3)
21	Lowest Frequency	(165.8, 165.8)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)

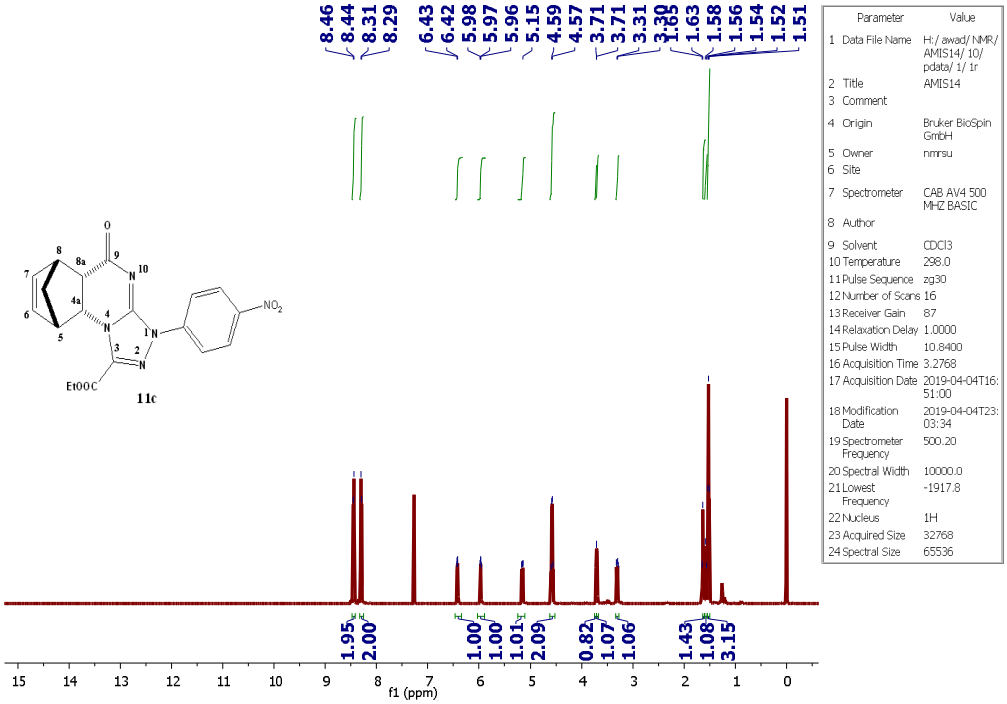


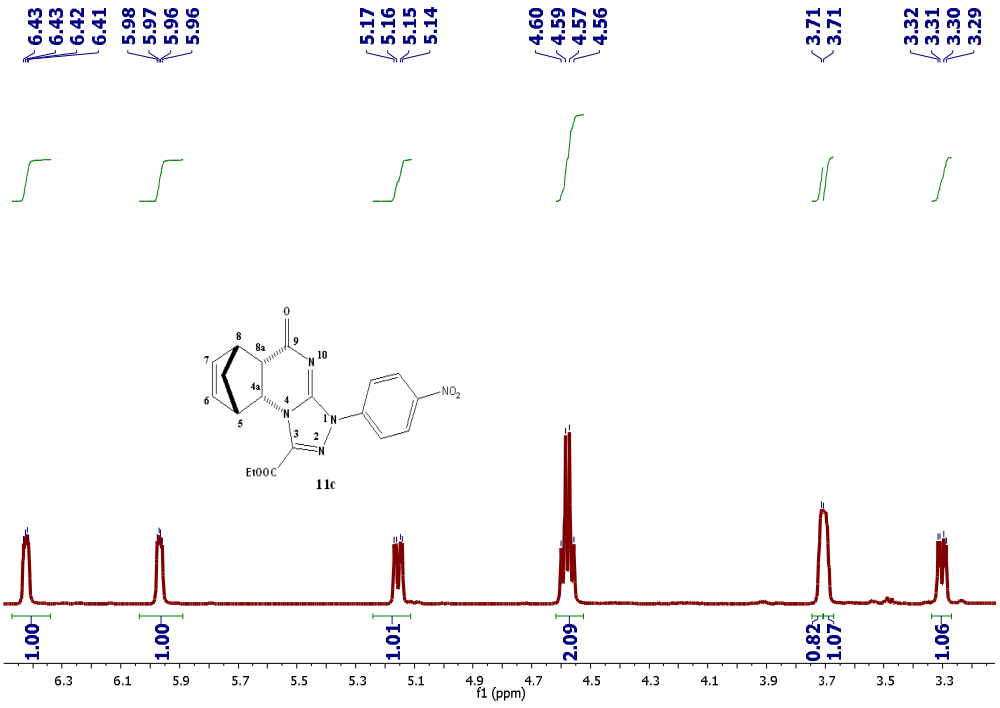
11a

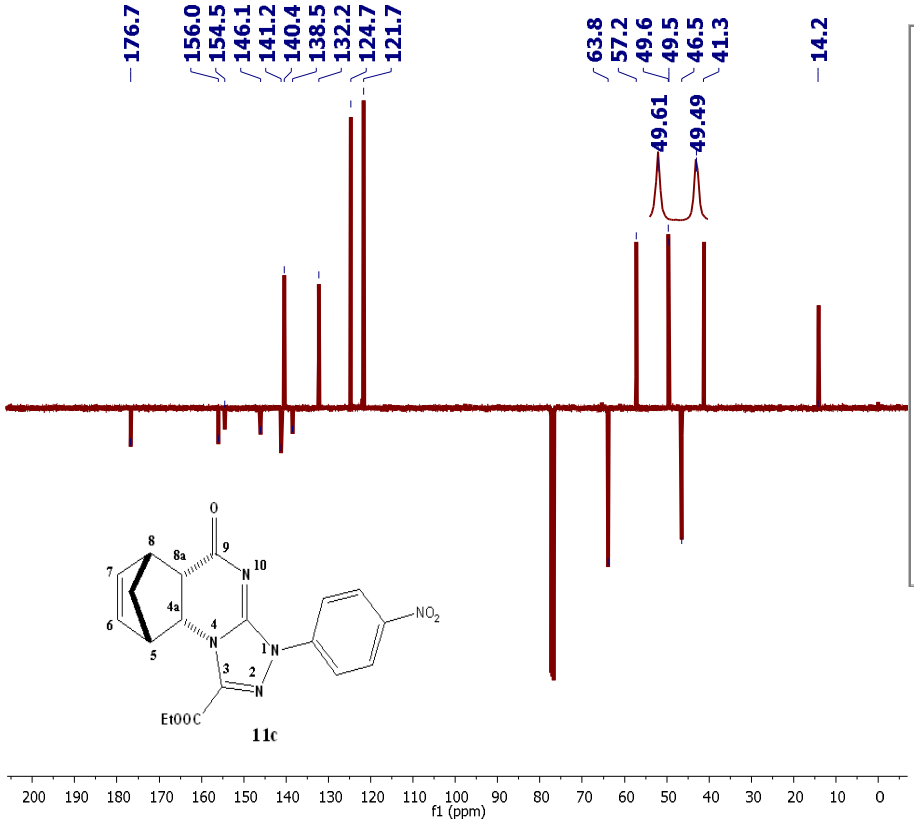


11c

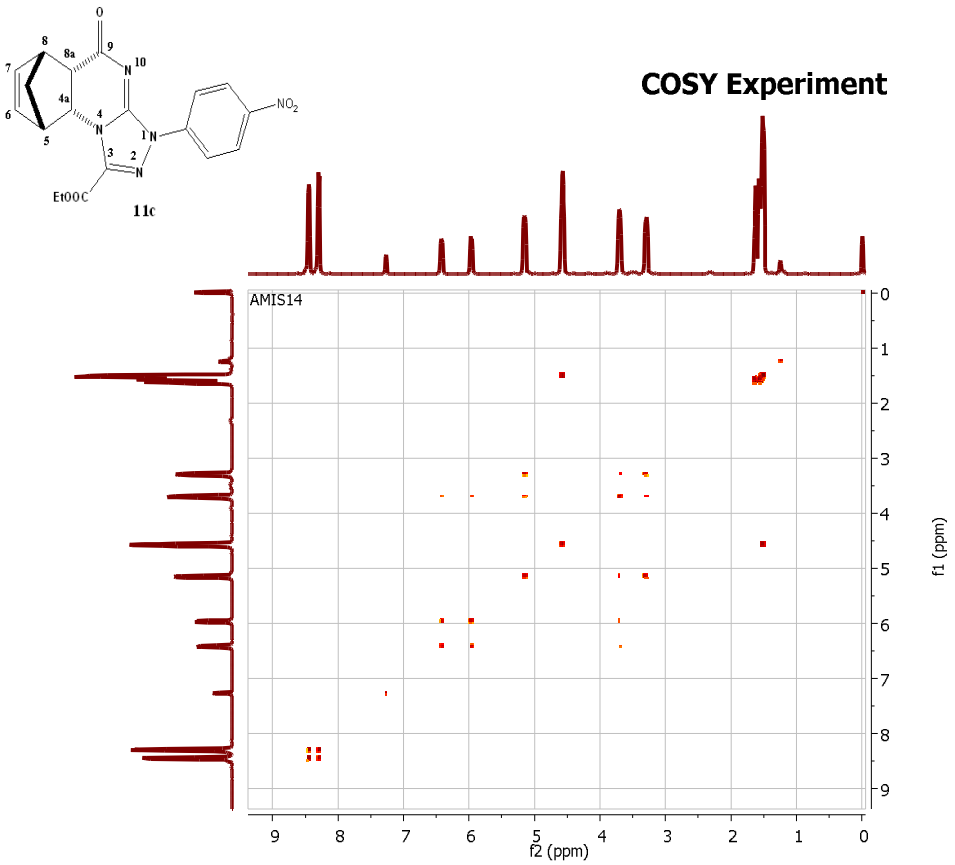
Ethyl (4a*R*,5*S***,8*R***,8a*S***)-1-(4-nitrophenyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline-3-carboxylate (11c)**



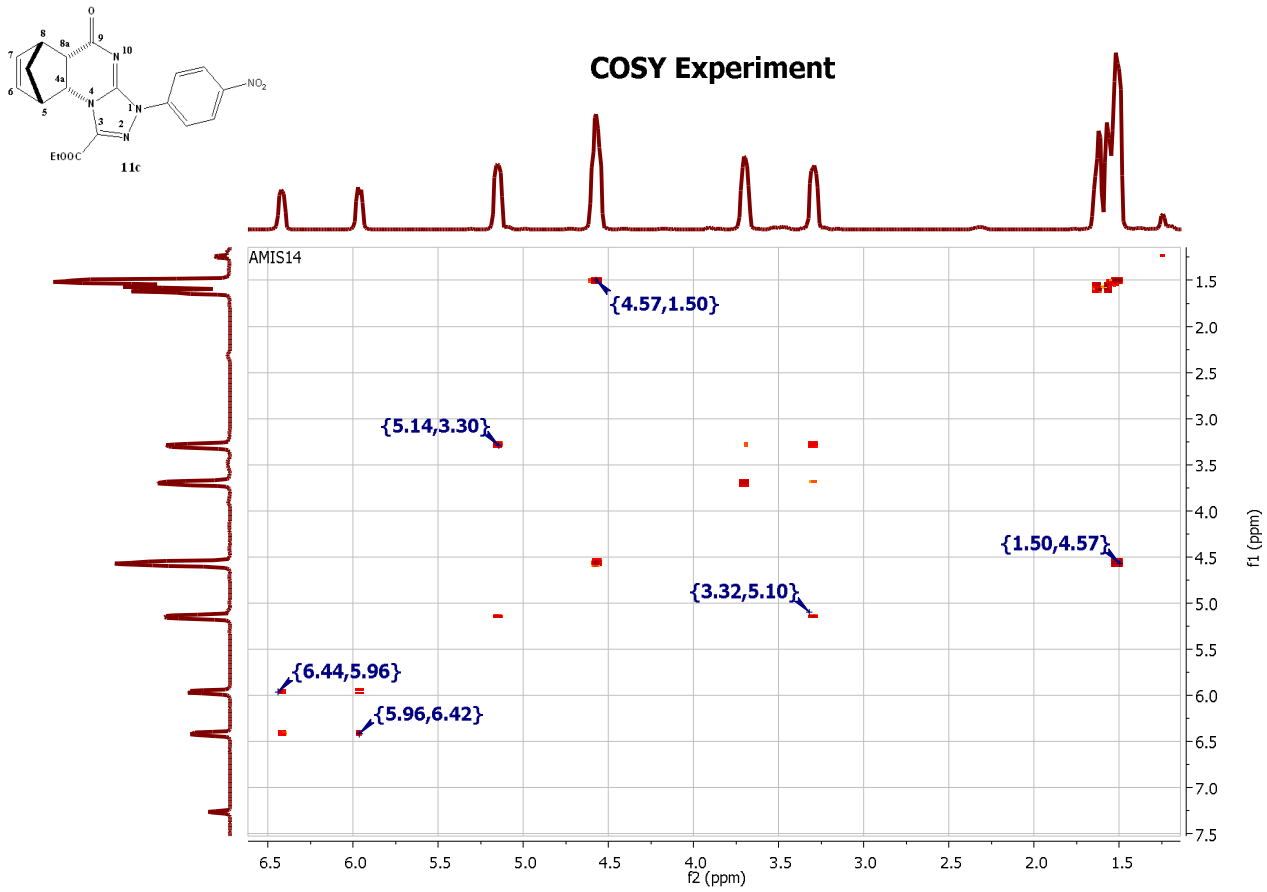


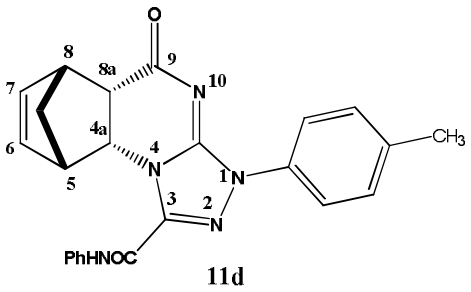


	Parameter	Value
1	Data File Name	H:/ awad/ NMR/ AMIS14/ 11/ pdata/ 1/ 1r
2	Title	AMIS14
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-04T17:05:09
18	Modification Date	2019-04-04T23:03:42
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768



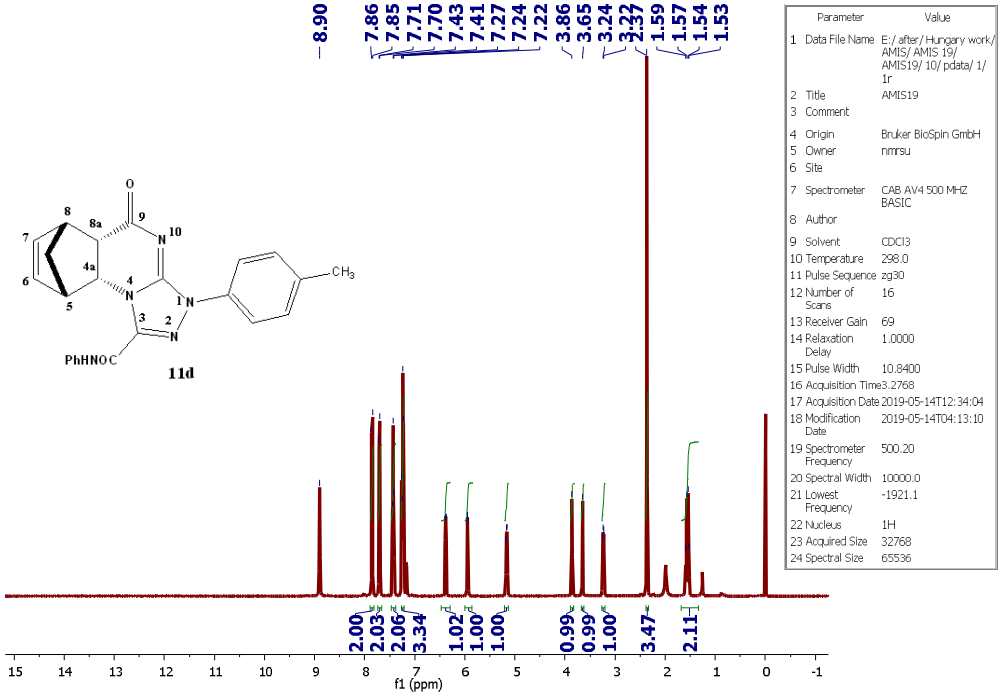
	Parameter	Value (f2, f1)
1	Data File Name	H:/ awad/ NMR/ AMIS14/ 12/ pdata/ 1/ 2rr
2	Title	AMIS14
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	cosygpppqf
12	Number of Scans	1
13	Receiver Gain	101
14	Relaxation Delay	1.9406
15	Pulse Width	10.8400
16	Acquisition Time	0.2171
17	Acquisition Date	2019-04-04T17:10:57
18	Modification Date	2019-04-04T23:03:54
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(4717.0, 4717.0)
21	Lowest Frequency	(-28.7, -28.7)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)

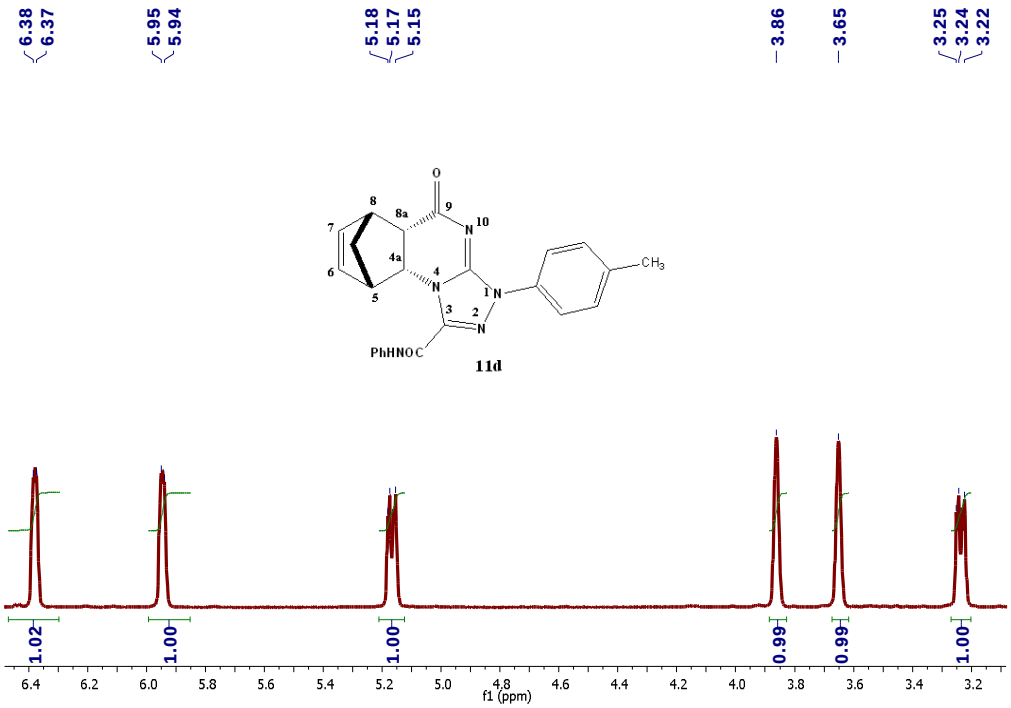

COSY Experiment
AMIS14
{4.57,1.50}
{5.14,3.30}
{1.50,4.57}
{3.32,5.10}
{6.44,5.96}
{5.96,6.42}
f2 (ppm)
f1 (ppm)
11c

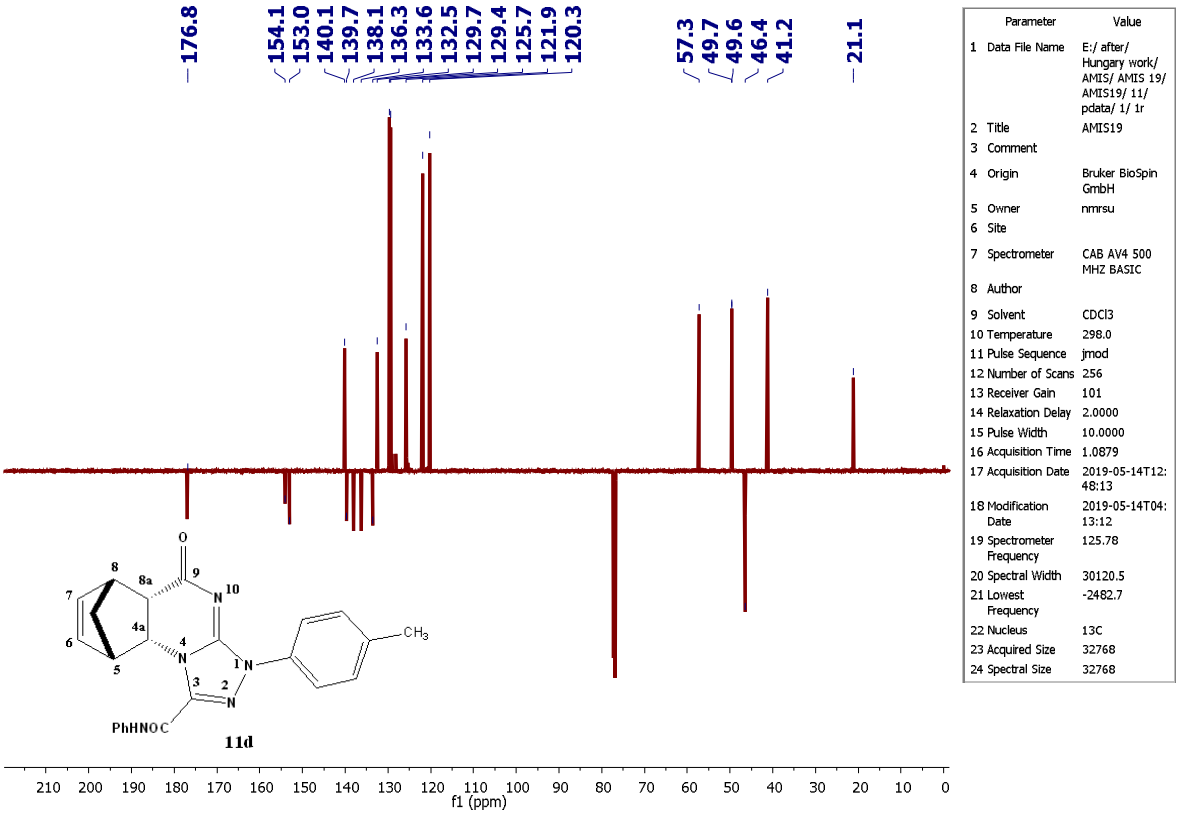


11d

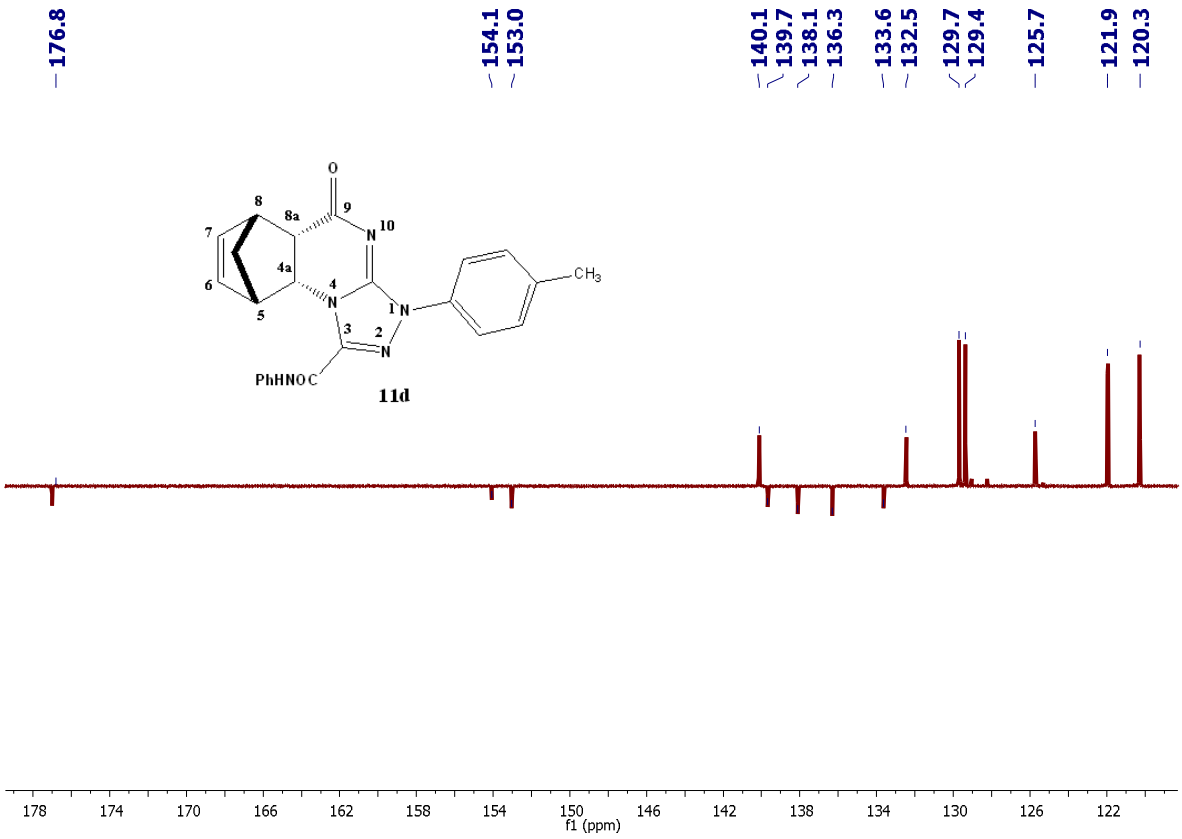
(4a*R*,5*S***,8*R***,8a*S***)-*N*-Phenyl-1-(*p*-tolyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline-3-carboxamide(11d)**

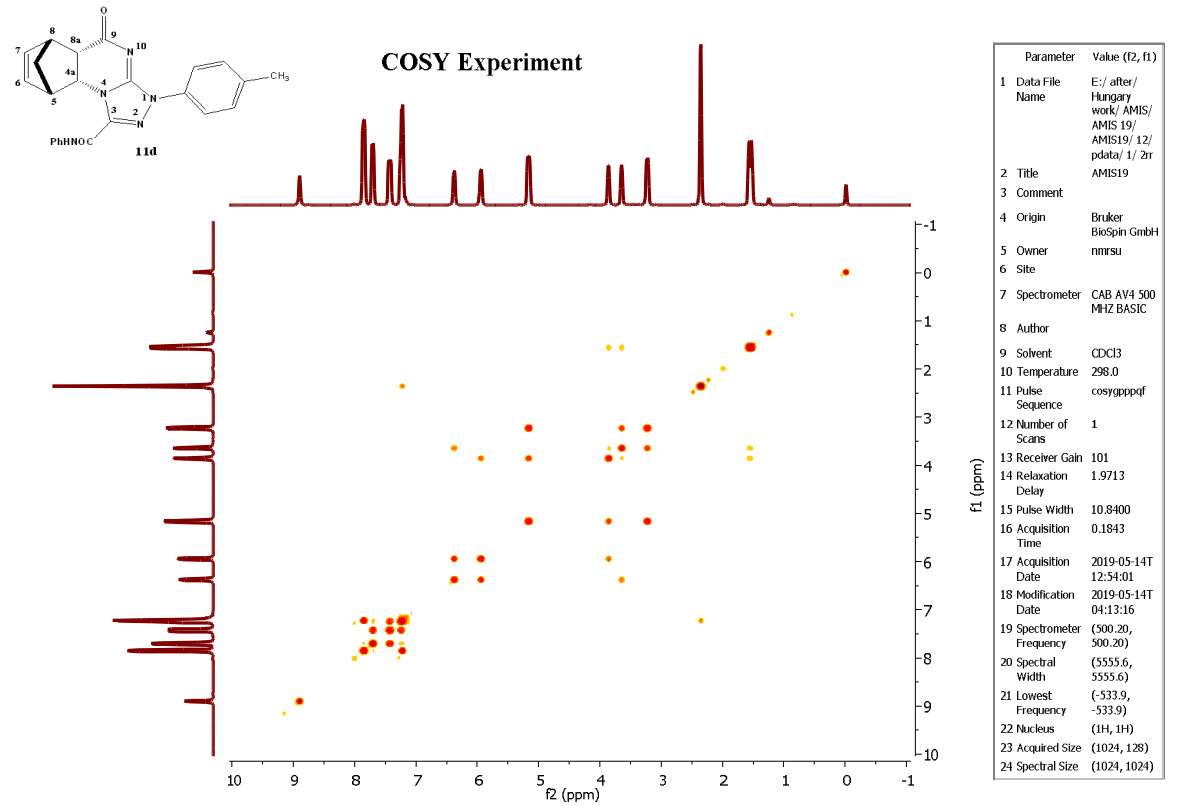


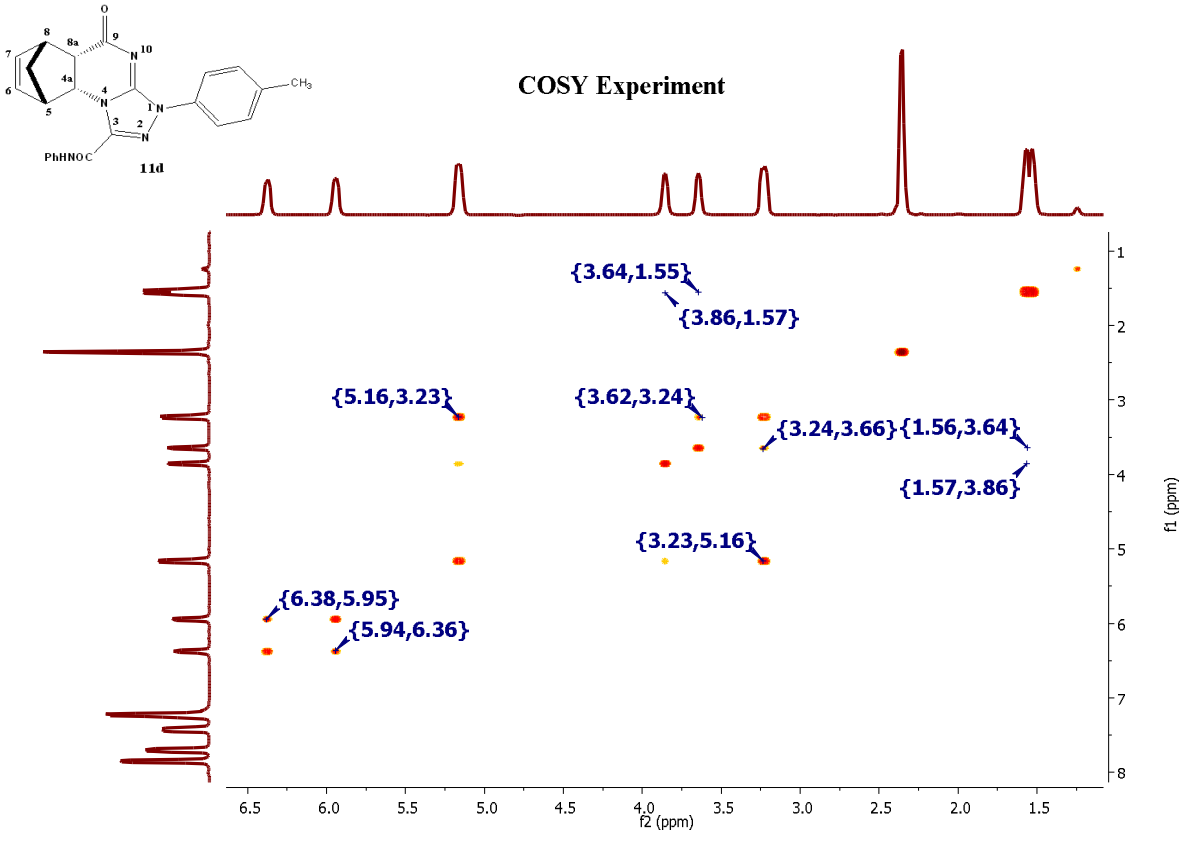


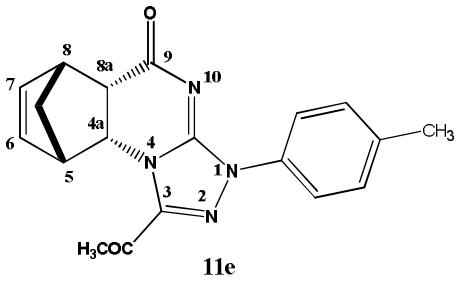


	Parameter	Value
1	Data File Name	E:/ after/ Hungary work/ AMIS/ AMIS 19/ AMIS19/ 11/ pdata/ 1/ 1r
2	Title	AMIS19
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-05-14T12:48:13
18	Modification Date	2019-05-14T04:13:12
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768



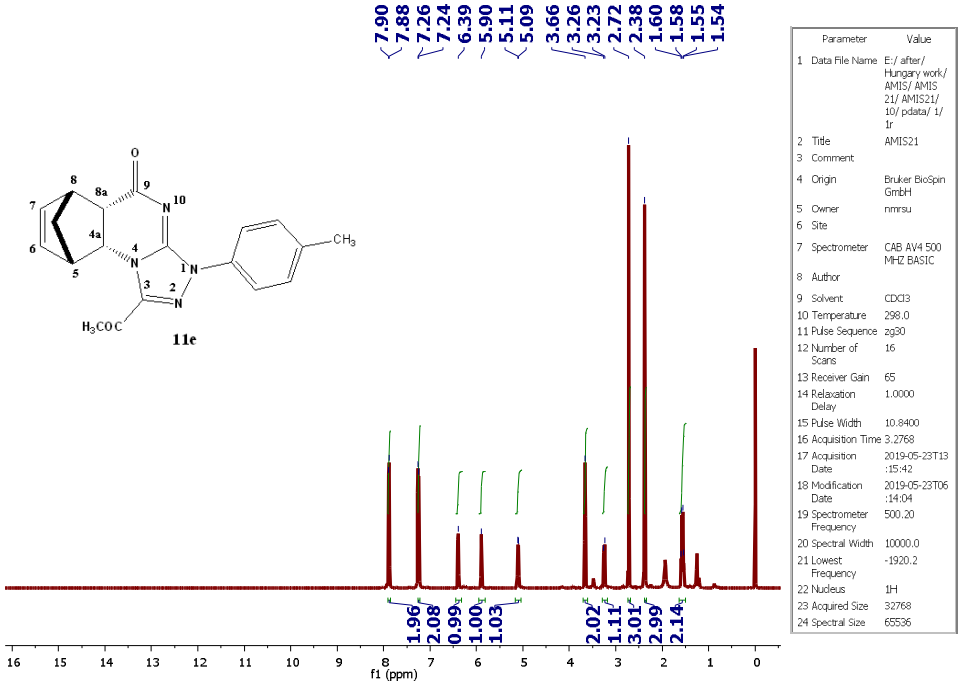

COSY Experiment
11d
PhHNOC
f2 (ppm)
f1 (ppm)
Parameter Value (f2, f1)
1 Data File Name E:/ after/ Hungary work/ AMIS/ AMIS 19/ AMIS19/ 12/ pdata/ 1/ 2rr
2 Title AMIS19
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer CAB AV4 500 MHZ BASIC
8 Author
9 Solvent CDCl3
10 Temperature 298.0
11 Pulse Sequence cosygpppqf
12 Number of Scans 1
13 Receiver Gain 101
14 Relaxation Delay 1.9713
15 Pulse Width 10.8400
16 Acquisition Time 0.1843
17 Acquisition Date 2019-05-14T 12:54:01
18 Modification Date 2019-05-14T 04:13:16
19 Spectrometer Frequency (500.20, 500.20)
20 Spectral Width (5555.6, 5555.6)
21 Lowest Frequency (-533.9, -533.9)
22 Nucleus (1H, 1H)
23 Acquired Size (1024, 128)
24 Spectral Size (1024, 1024)

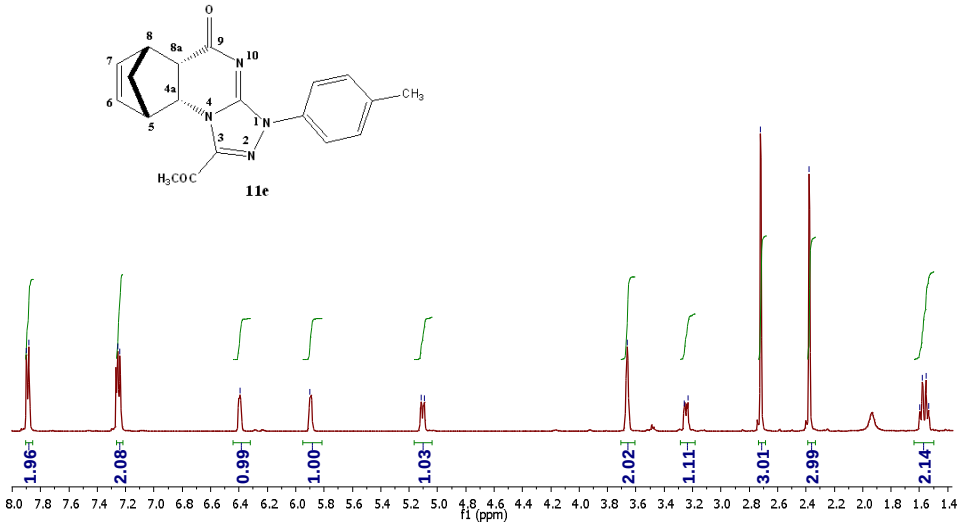

COSY Experiment
11d
PhHNOC
{3.64,1.55}
{3.86,1.57}
{5.16,3.23}
{3.62,3.24}
{3.24,3.66}
{1.56,3.64}
{1.57,3.86}
{3.23,5.16}
{6.38,5.95}
{5.94,6.36}
f2 (ppm)
f1 (ppm)

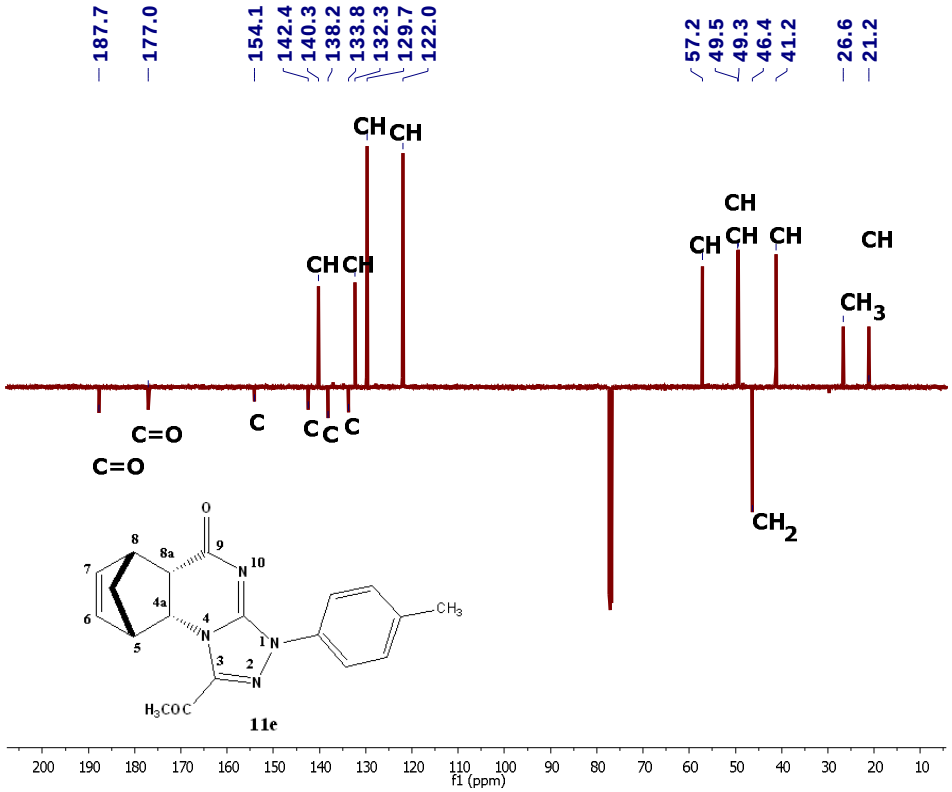


11e

(4a*R,5*S**,8*R**,8a*S**)-3-Acetyl-1-(*p*-tolyl)-9-oxo-1,4a,5,8,8a,9-hexahydro-5,8-methano[1,2,4]triazolo[4,3-*a*]quinazoline(11e)**







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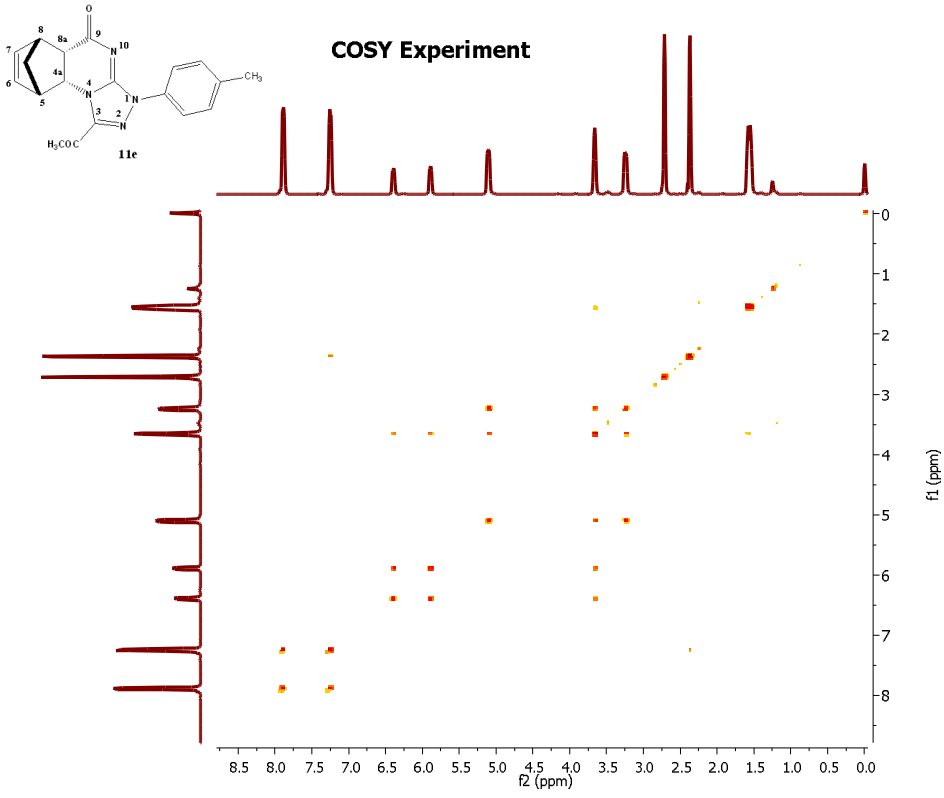
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-05-23T 13:29:52
18	Modification Date	2019-05-23T 06:14:36
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768



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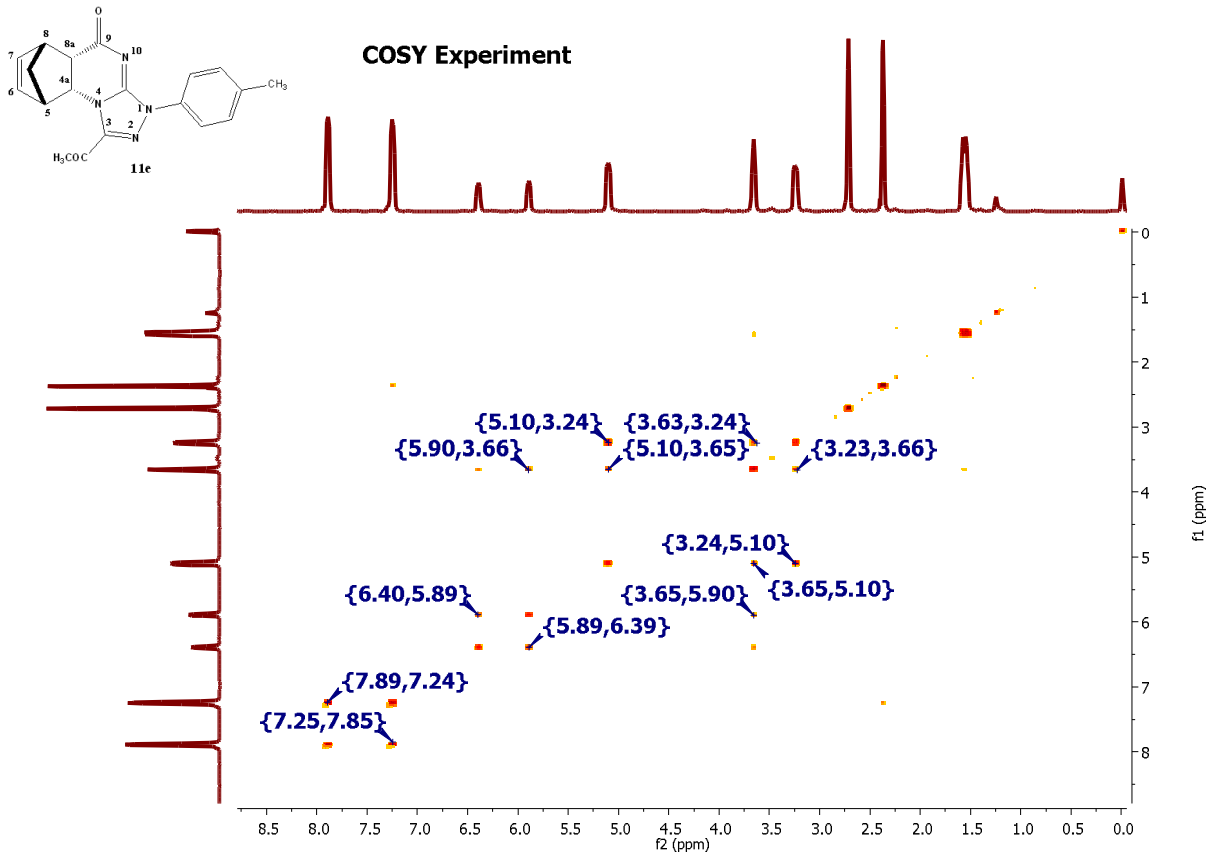
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	cosygpppqf
12	Number of Scans	1
13	Receiver Gain	101
14	Relaxation Delay	1.9242
15	Pulse Width	10.8400
16	Acquisition Time	0.2314
17	Acquisition Date	2019-05-23T1 3:35:41
18	Modification Date	2019-05-23T0 6:14:52
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(4424.8, 4424.8)
21	Lowest Frequency	(-26.7, -26.7)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)


COSY Experiment
11e
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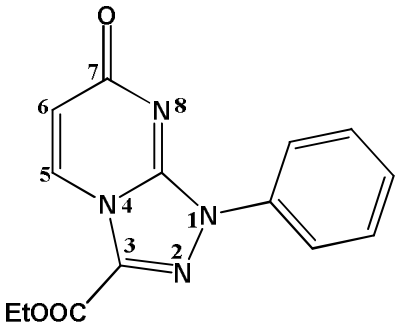
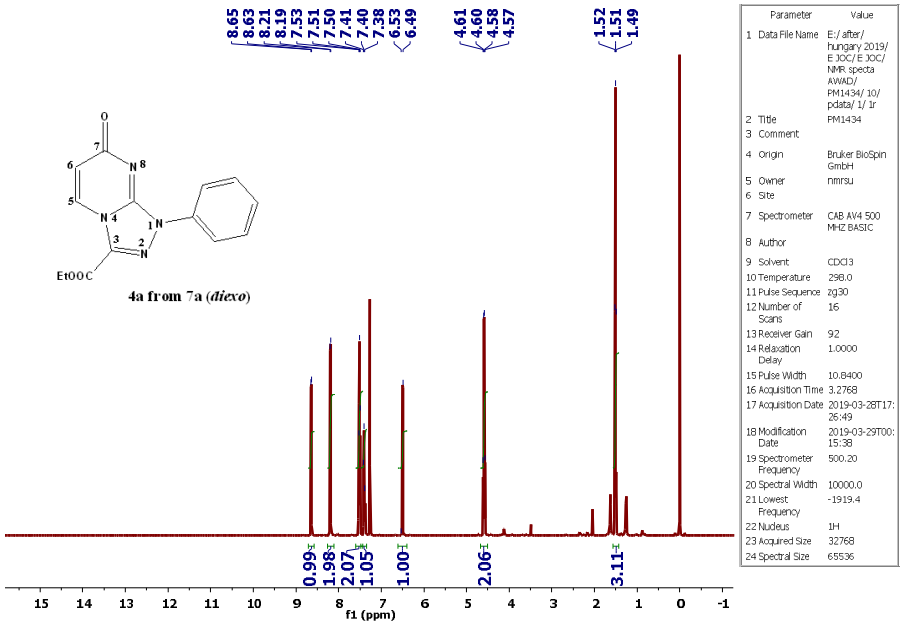
f2 (ppm)
f1 (ppm)



4a

Ethyl7-oxo-1-phenyl-1,7-dihydro[1,2,4]triazolo[4,3-*a*]-pyrimidine-3-carboxylate(4a)

From *Diexo* 7a



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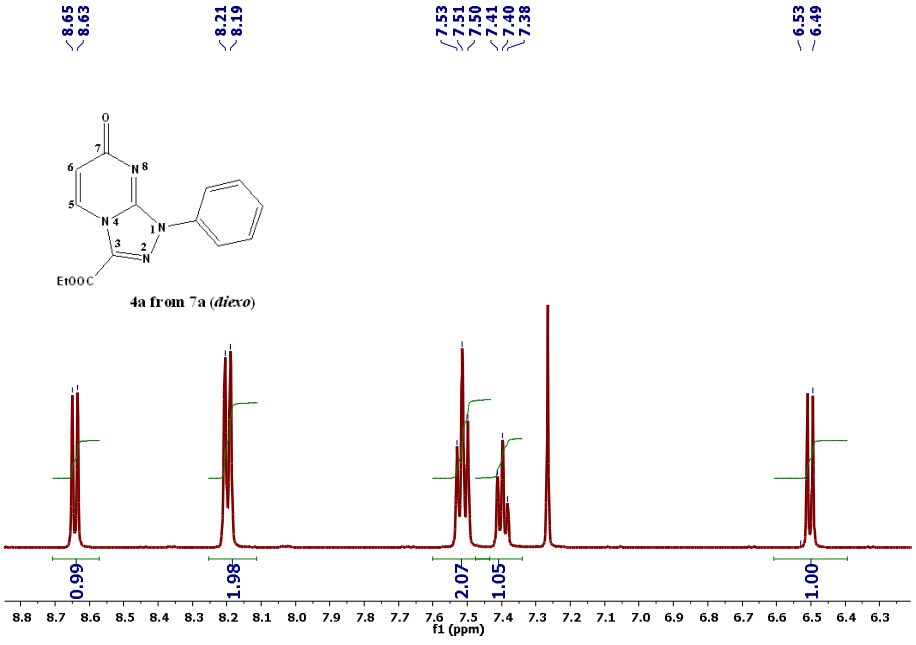
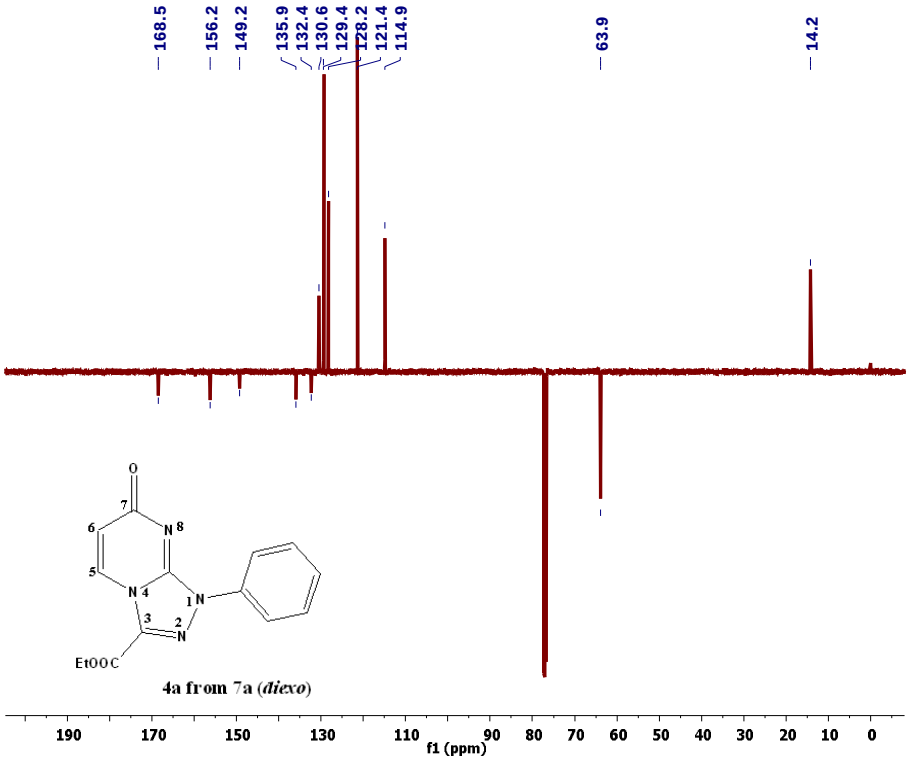
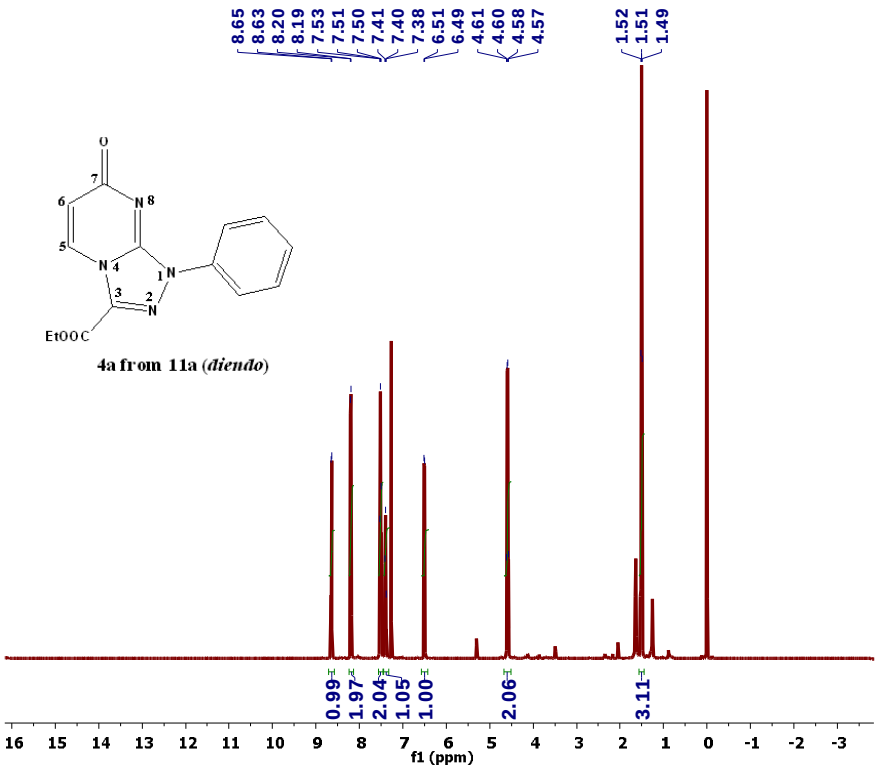
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM1434/ 10/ pdata/ 1/ 1r
2	Title	PM1434
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	92
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-03-28T17:26:49
18	Modification Date	2019-03-29T00:15:38
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1919.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536





	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM1434/ 11/ pdata/ 1/ 1r
2	Title	PM1434
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-03-28T17:40:57
18	Modification Date	2019-03-29T00:15:44
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

From *Diendo* 11a



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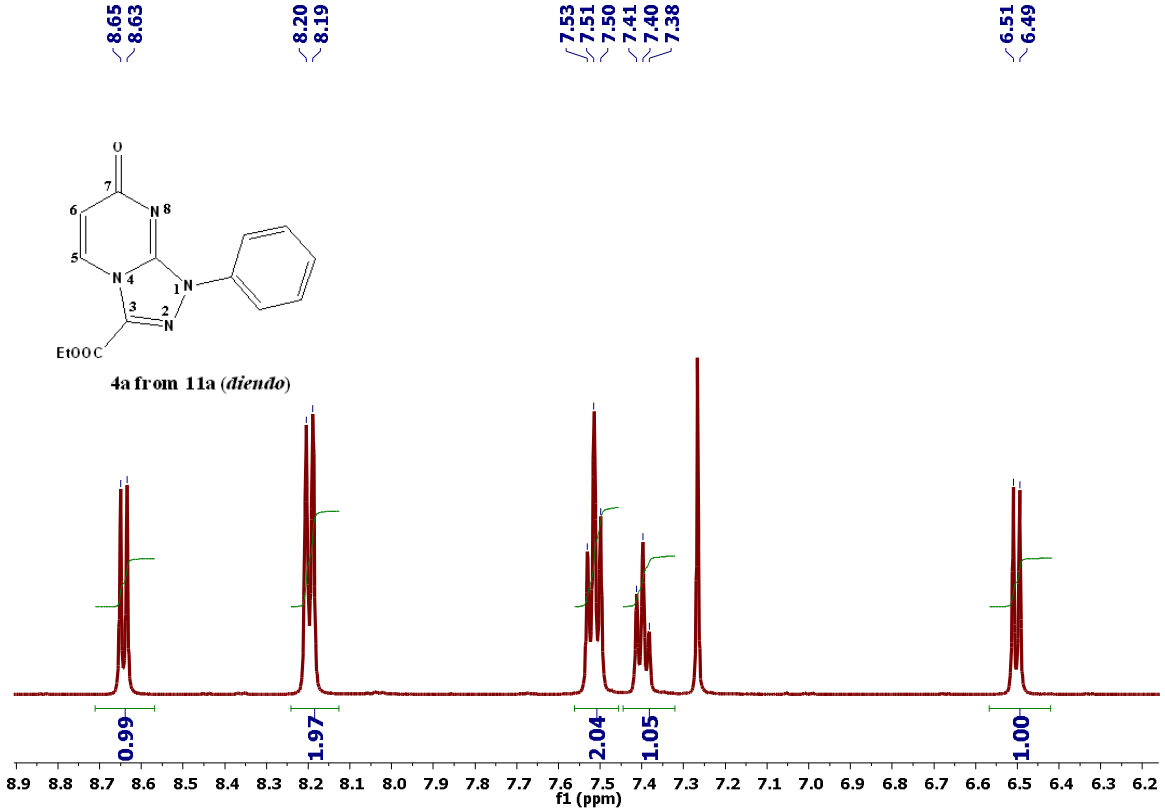
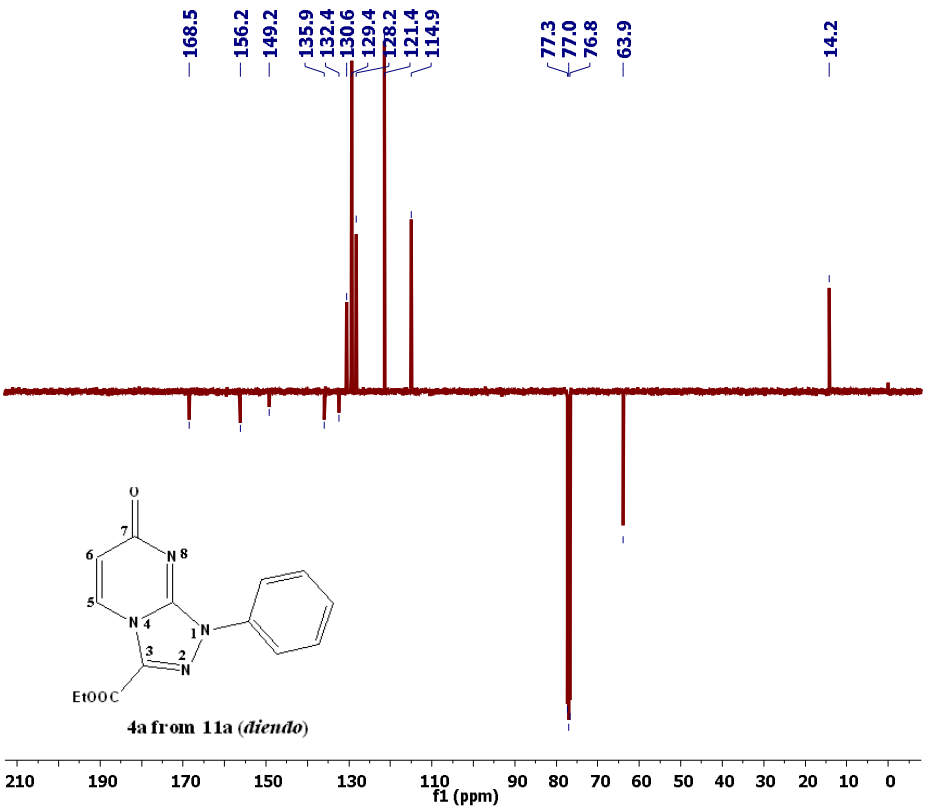
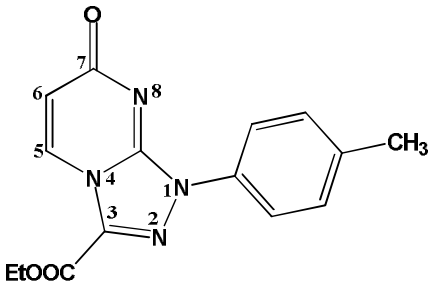
2	Title	PM_1437
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	101
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-04-05T14:03:05
18	Modification Date	2019-04-05T05:17:32
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1918.7
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



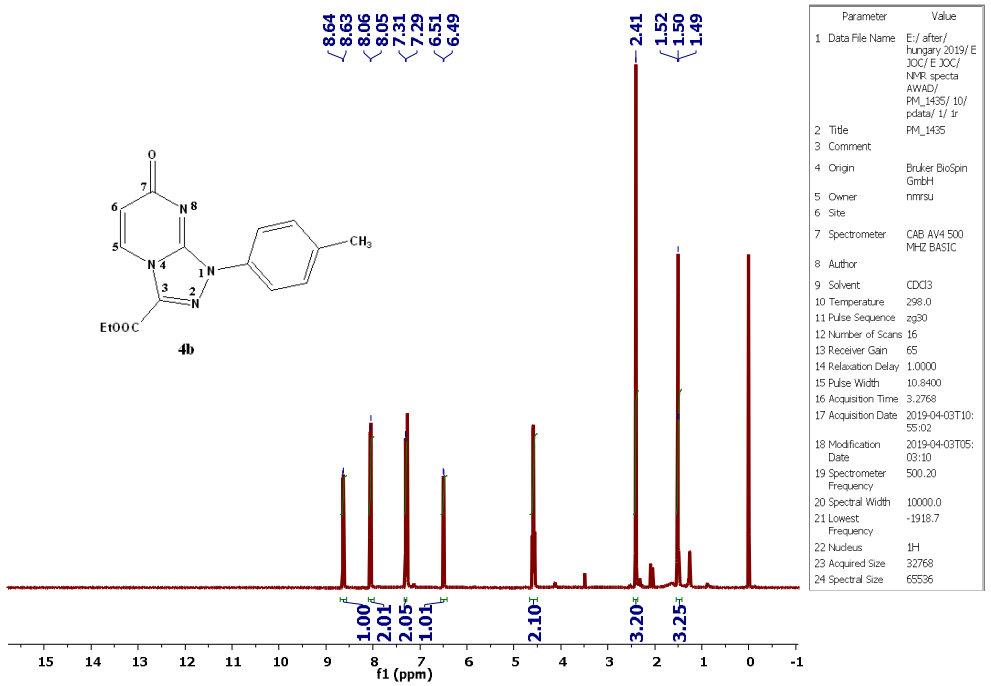


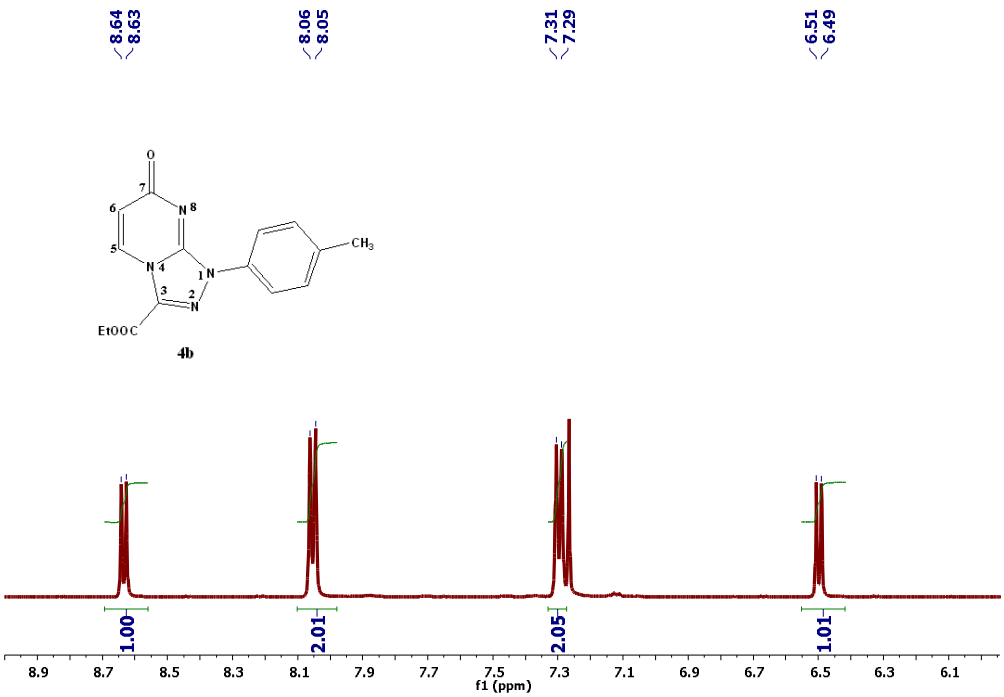
	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM_1437/ 11/ pdata/ 1/ 1r
2	Title	PM_1437
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-05T14:17:14
18	Modification Date	2019-04-05T05:17:38
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

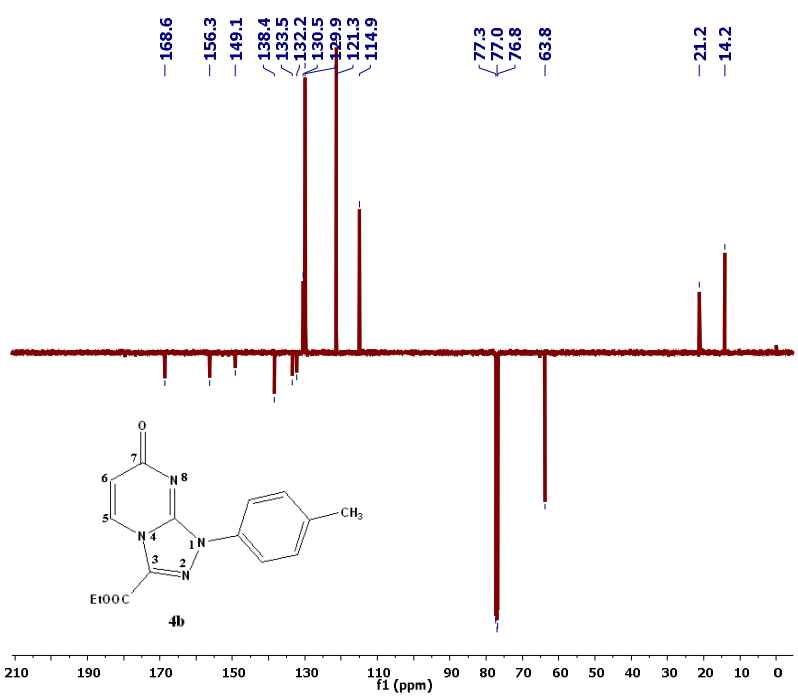


4b

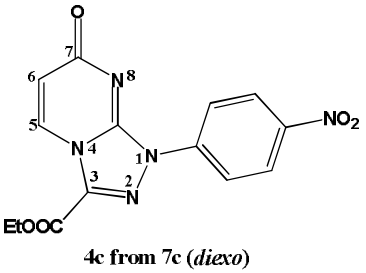
Ethyl7-oxo-1-(*p*-tolyl)-1,7-dihydro[1,2,4]triazolo[4,3-*a*]-pyrimidine-3-carboxylate (4b)







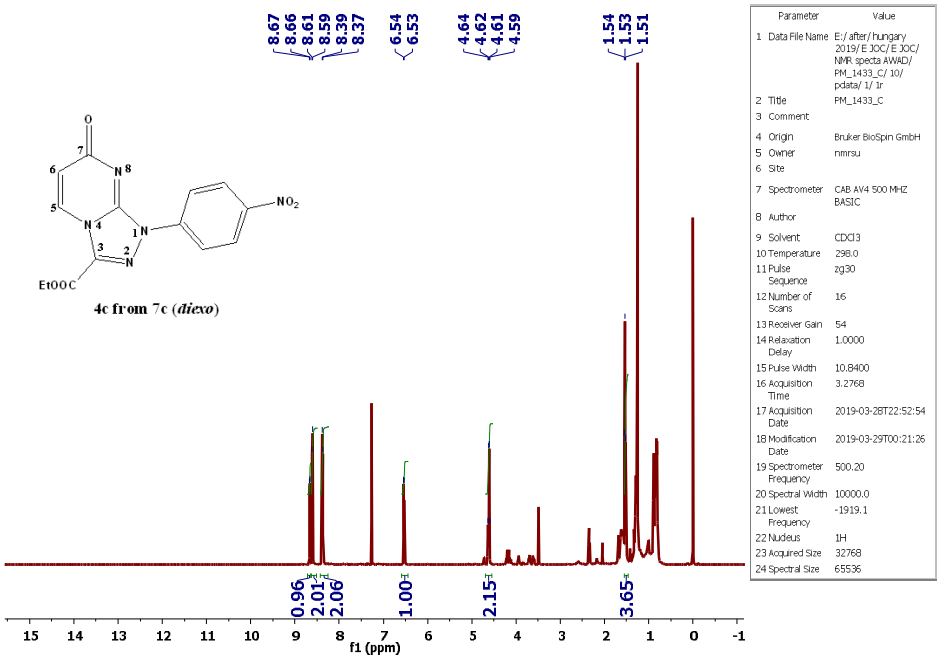
	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM_1435/ 11/ pdata/ 1/ 1r
2	Title	PM_1435
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-03T11:09:38
18	Modification Date	2019-04-03T05:03:14
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

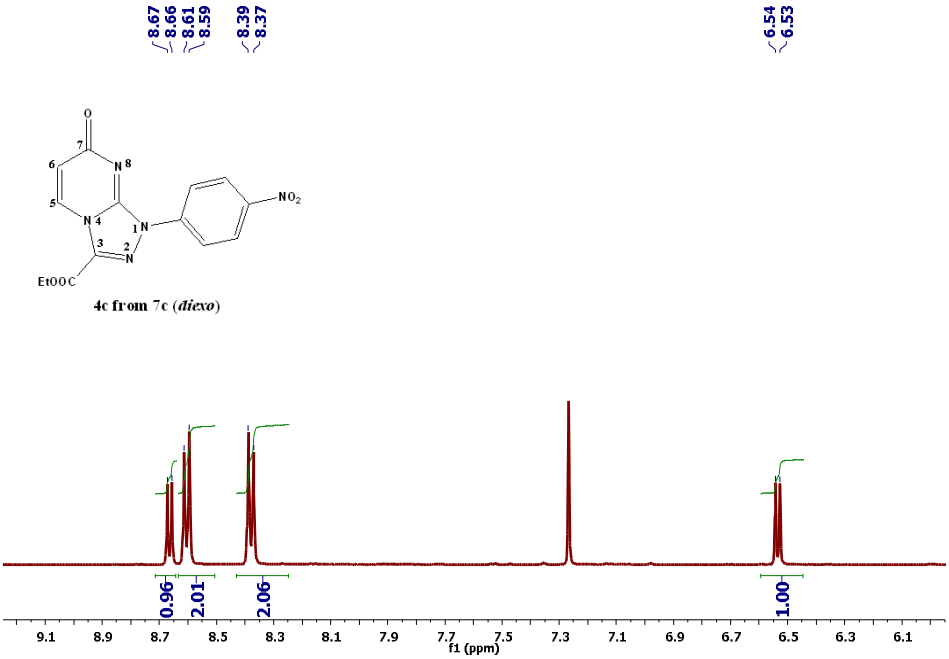


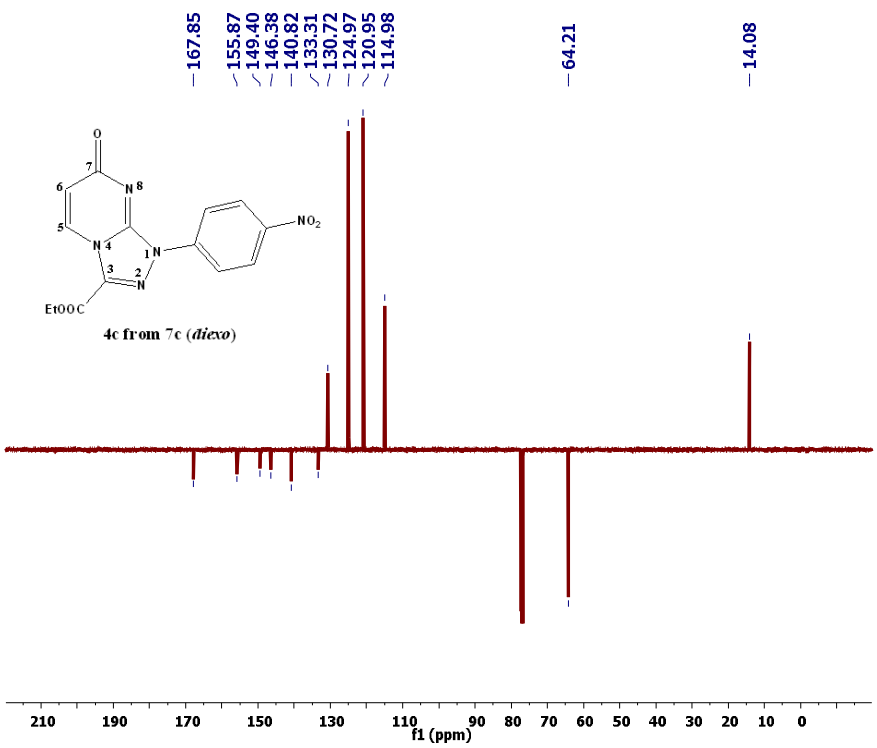
4c from 7c (*diexo*)

Ethyl 1-(4-nitrophenyl)-7-oxo-1,7-dihydro[1,2,4]triazolo[4,3-*a*]-pyrimidine-3-carboxylate (4c)

From *Diexo* 7c







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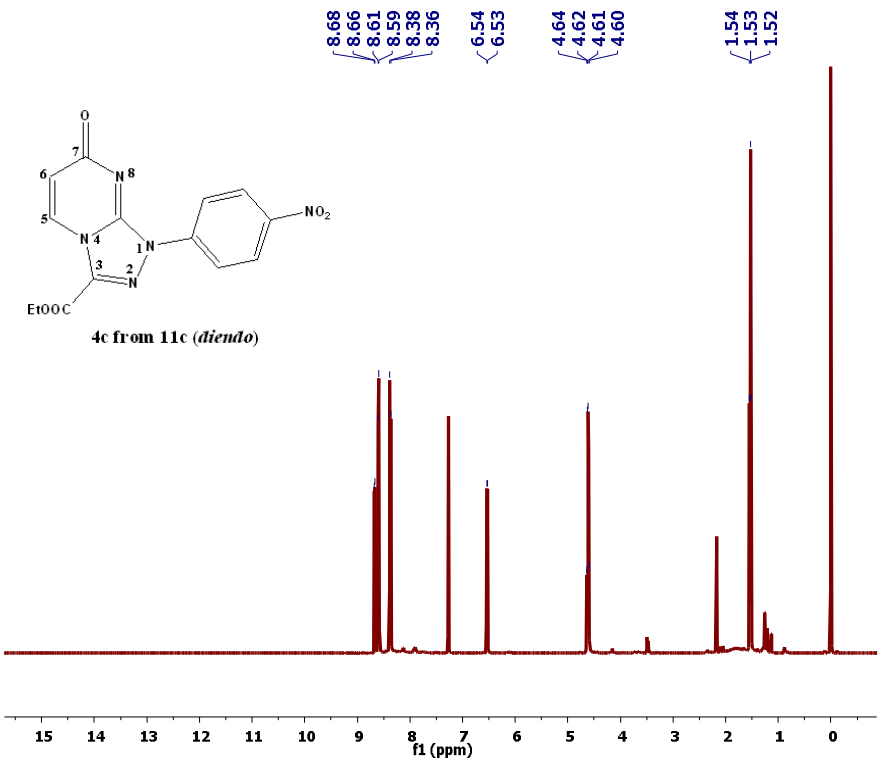
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2020-02-11T14:02:35
18	Modification Date	2020-02-11T05:57:04
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

From *Diendo*11c



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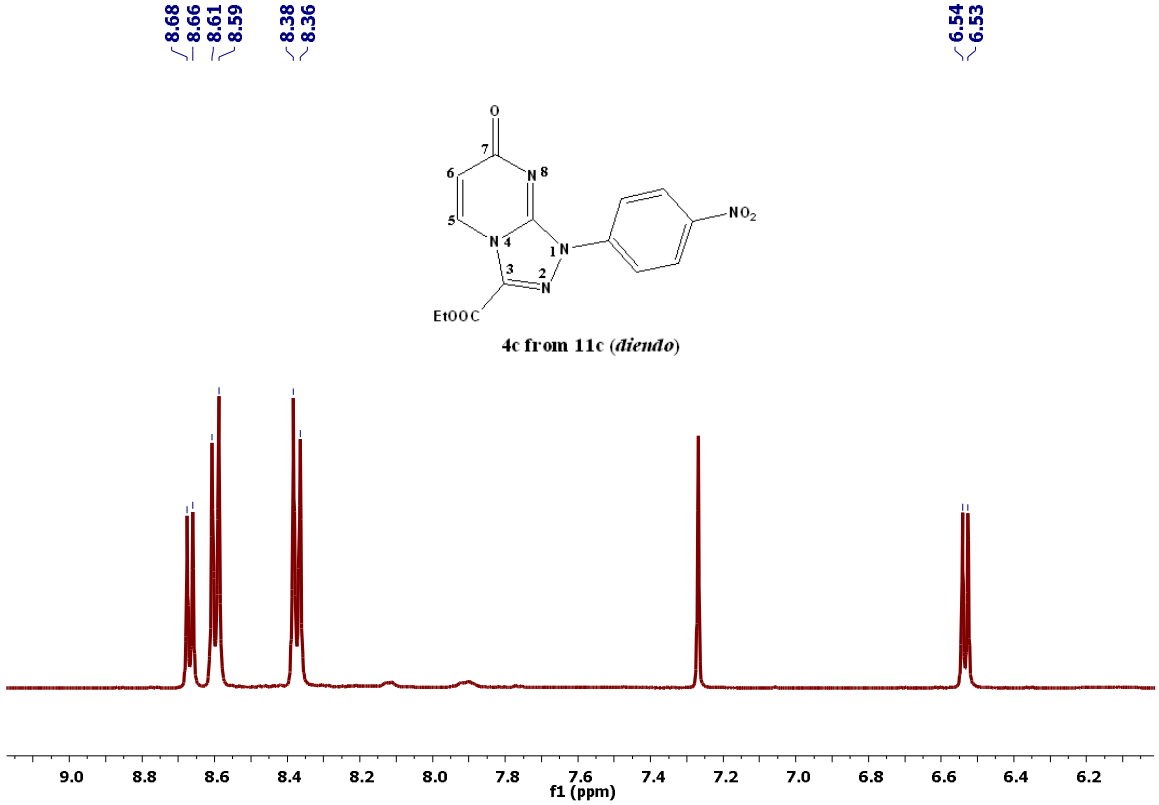
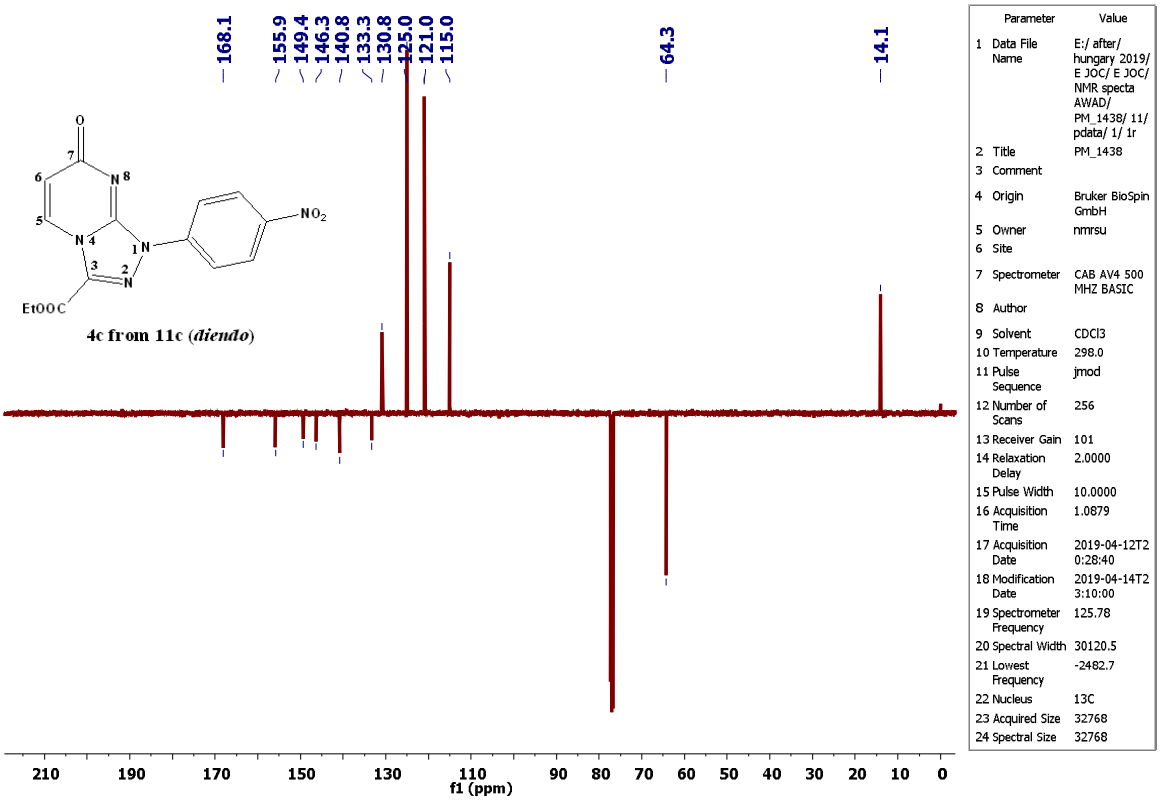
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	83
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-04-12T20:14:31
18	Modification Date	2019-04-14T23:09:56
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1919.0
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



4c from 11c (*dienđo*)



4c from 11c (*dienđo*)

	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM_1438/ 11/ pdata/ 1/ 1r
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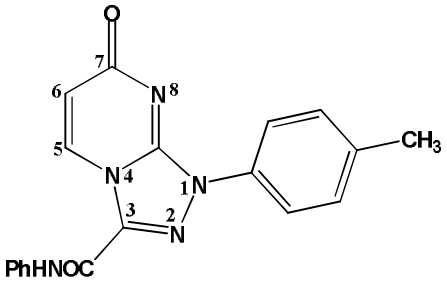
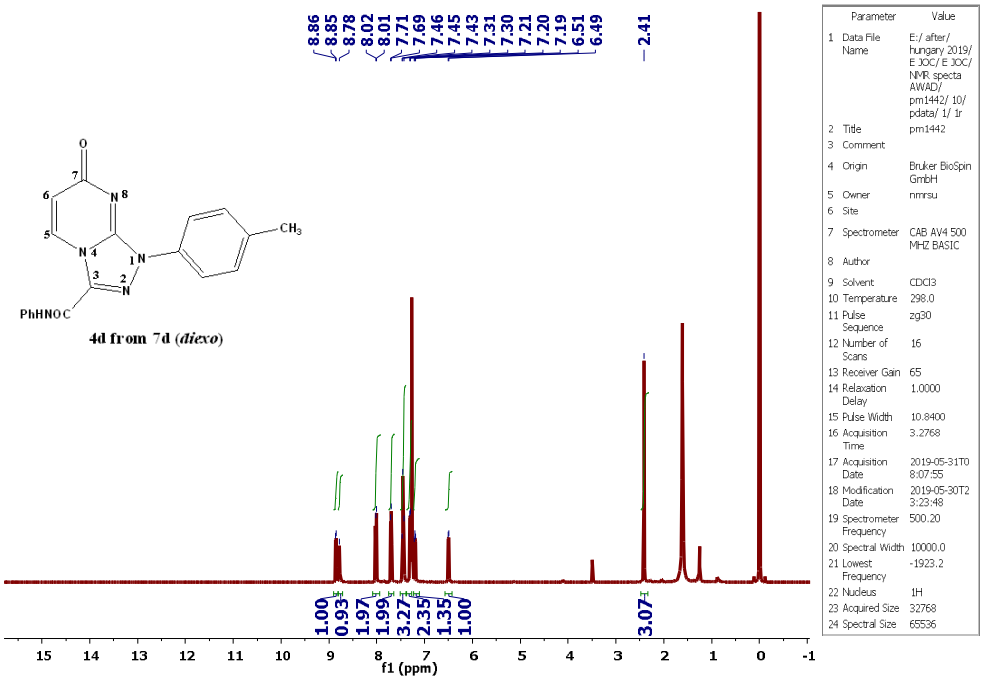
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-12T2 0:28:40
18	Modification Date	2019-04-14T2 3:10:00
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

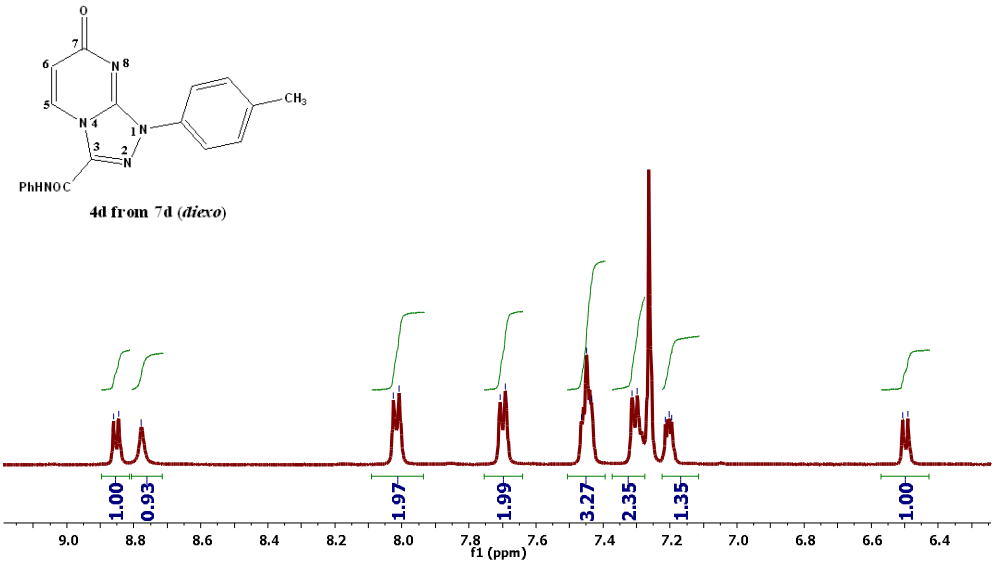


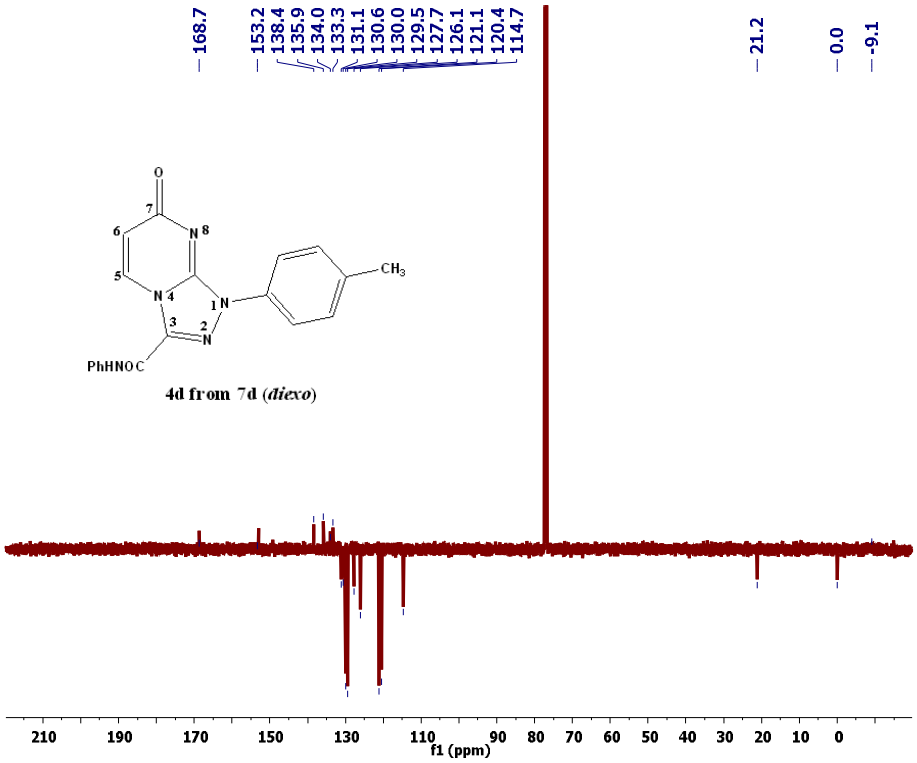
4d

7-Oxo-*N*-phenyl-1-(*p*-tolyl)-1,7-dihydro[1,2,4]triazolo-[4,3-*a*]pyrimidine-3-carboxamide (4d)

From *Diexo* 7d







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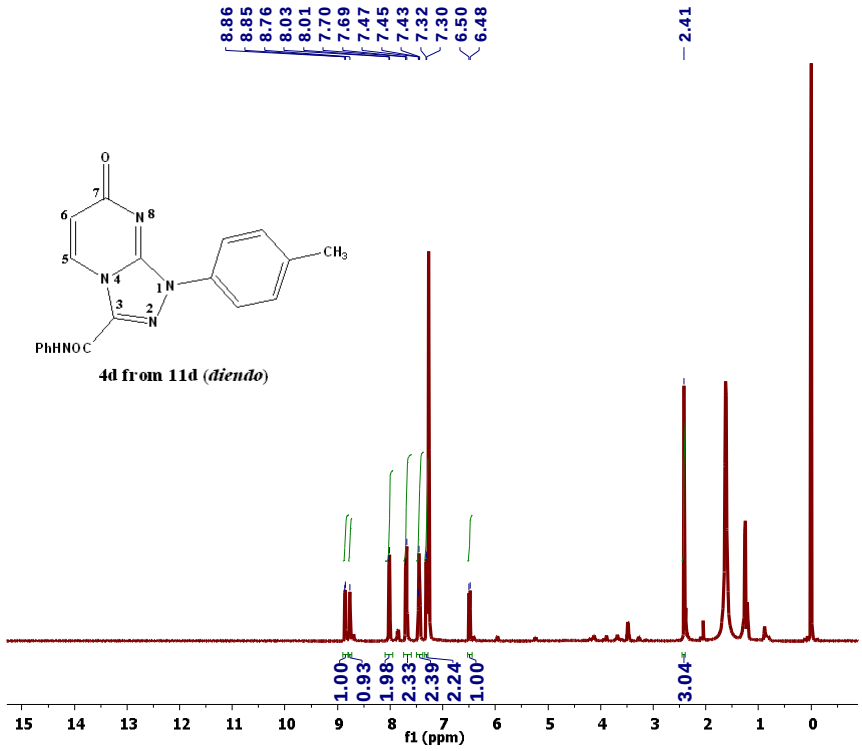
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ pm1442/ 11/ pdata/ 1/ 1r
2	Title	pm1442
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-05-31T08 :22:05
18	Modification Date	2019-05-30T23 :23:54
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

From *Diendo* 7d



	Parameter	Value
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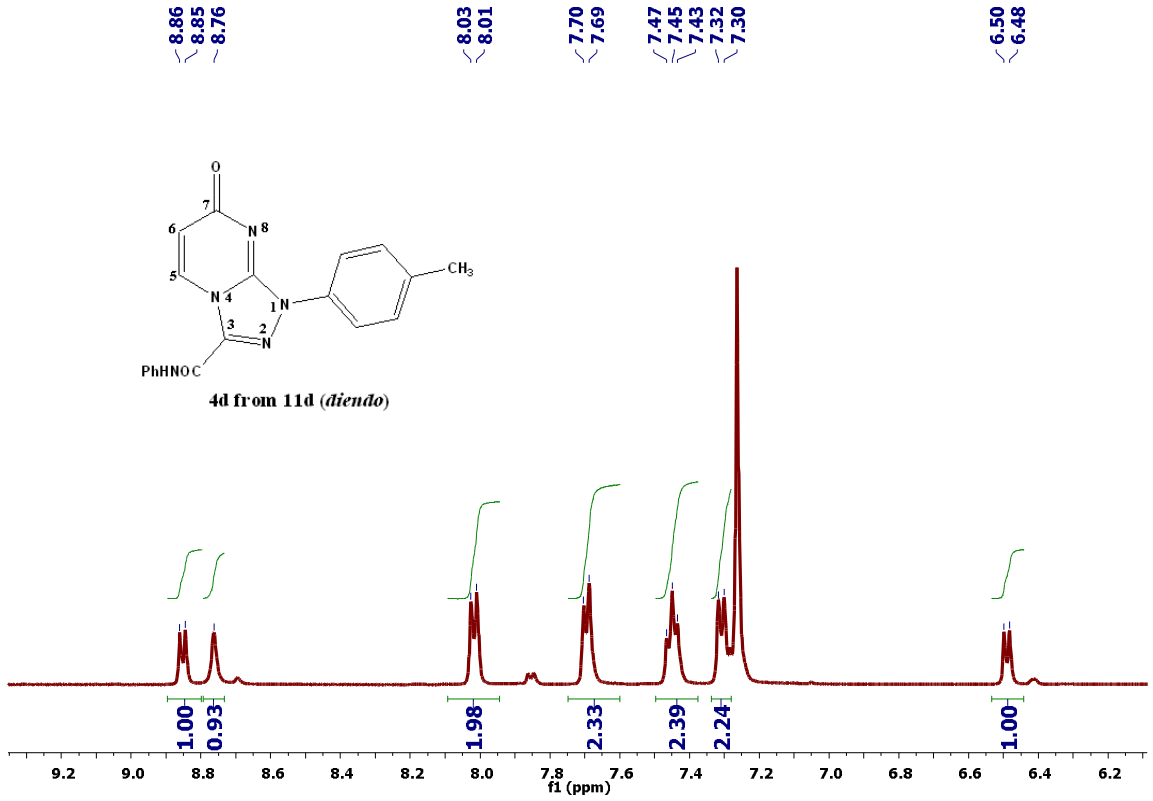
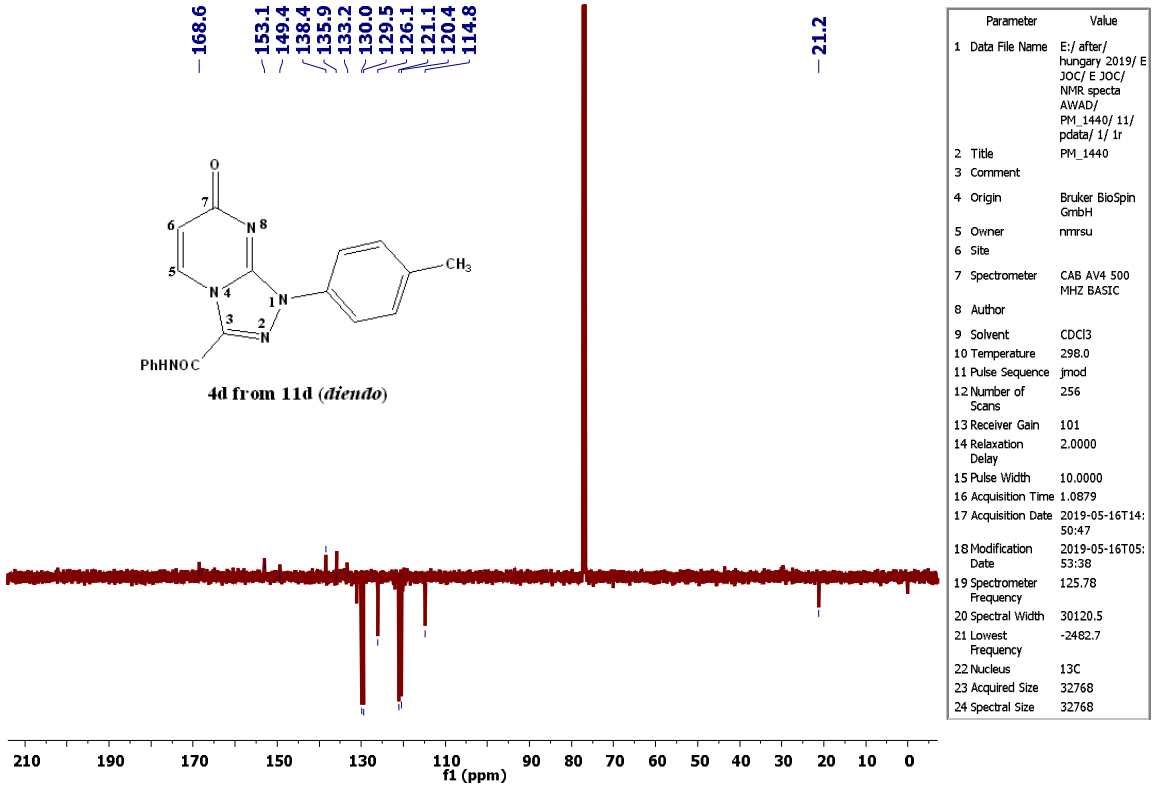
2	Title	PM_1440
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	81
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-05-16T14:36:37
18	Modification Date	2019-05-16T05:53:34
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1922.0
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536





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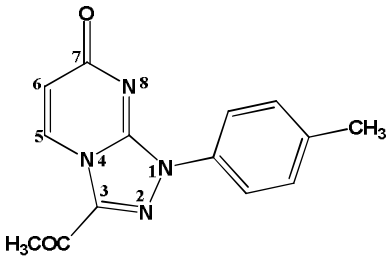
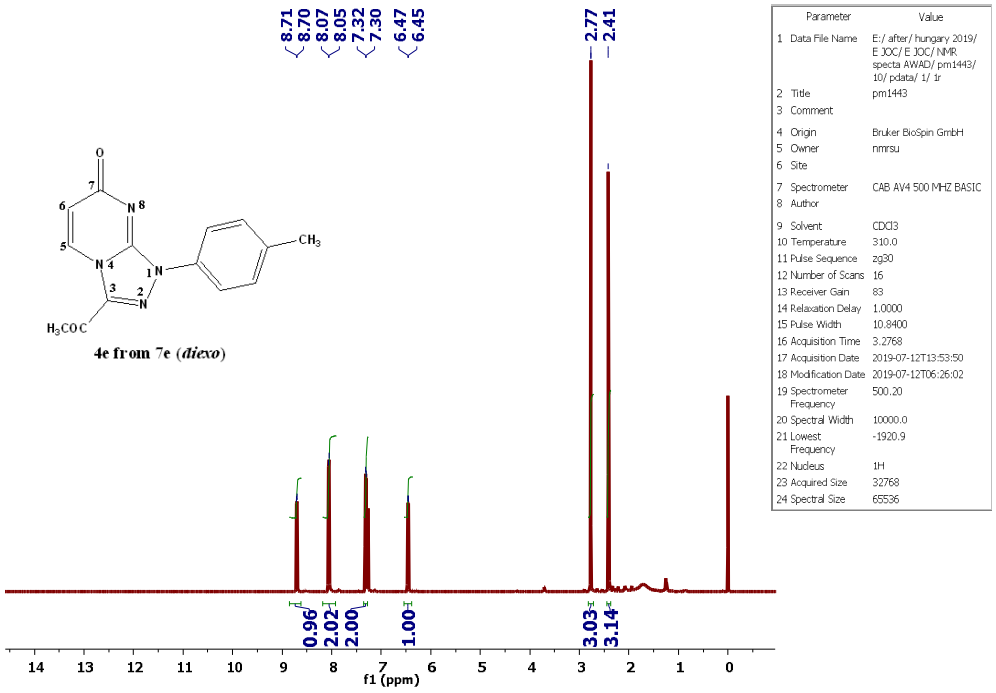
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM_1440/ 11/ pdata/ 1/ 1r
2	Title	PM_1440
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-05-16T14:50:47
18	Modification Date	2019-05-16T05:53:38
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

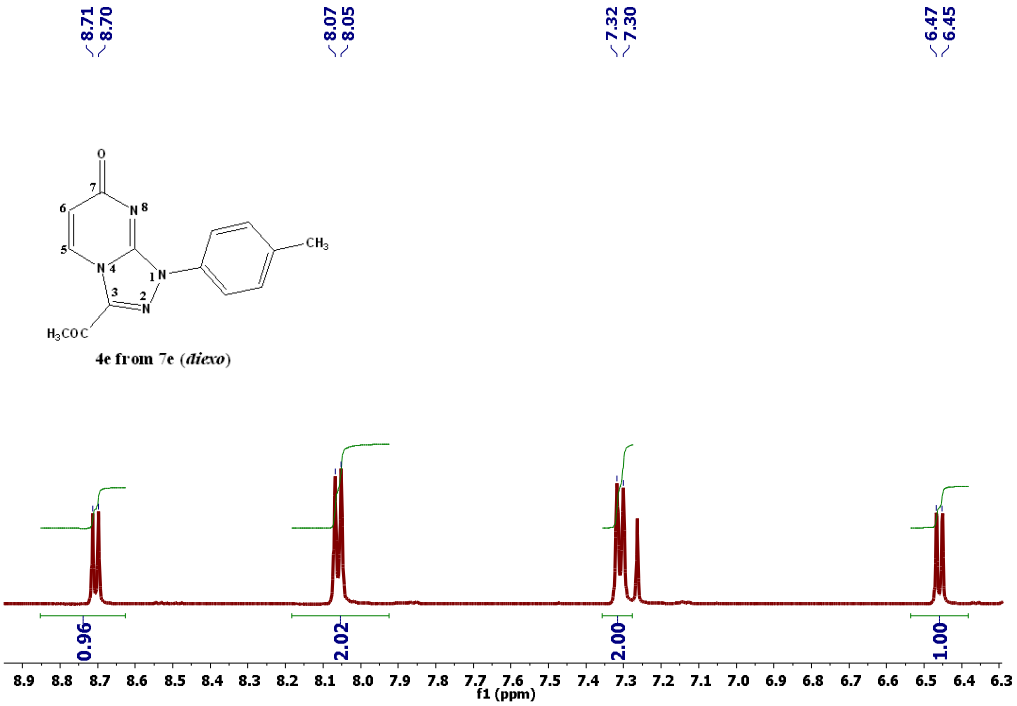


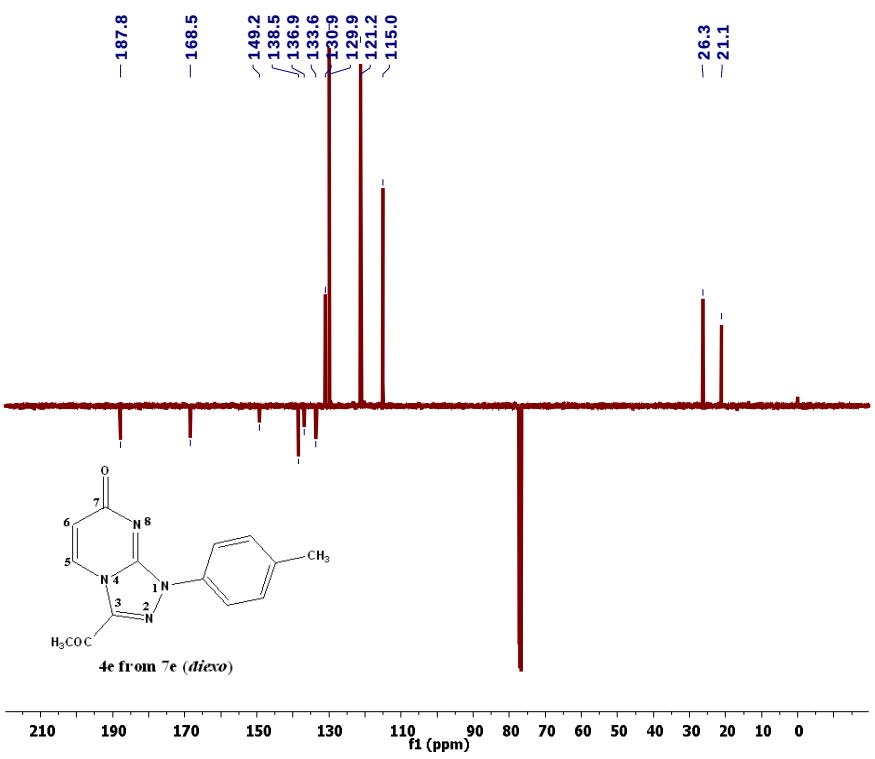
4e

3-Acetyl-1-(*p*-tolyl)-[1,2,4]triazolo[4,3-*a*]pyrimidin-7(1H)-one (4e)

From *Diexo* 7e







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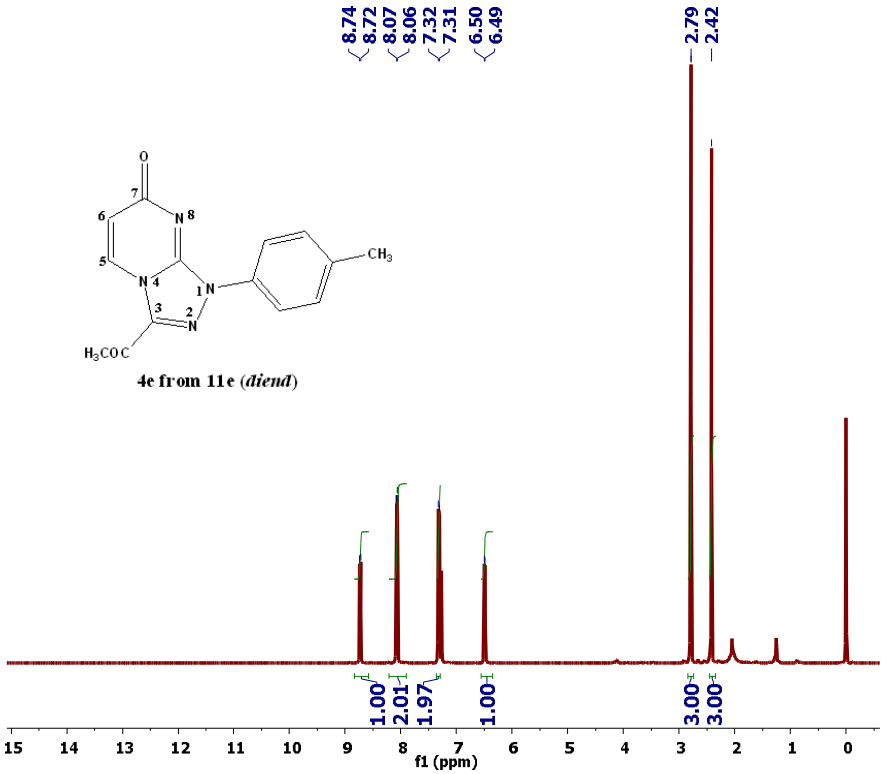
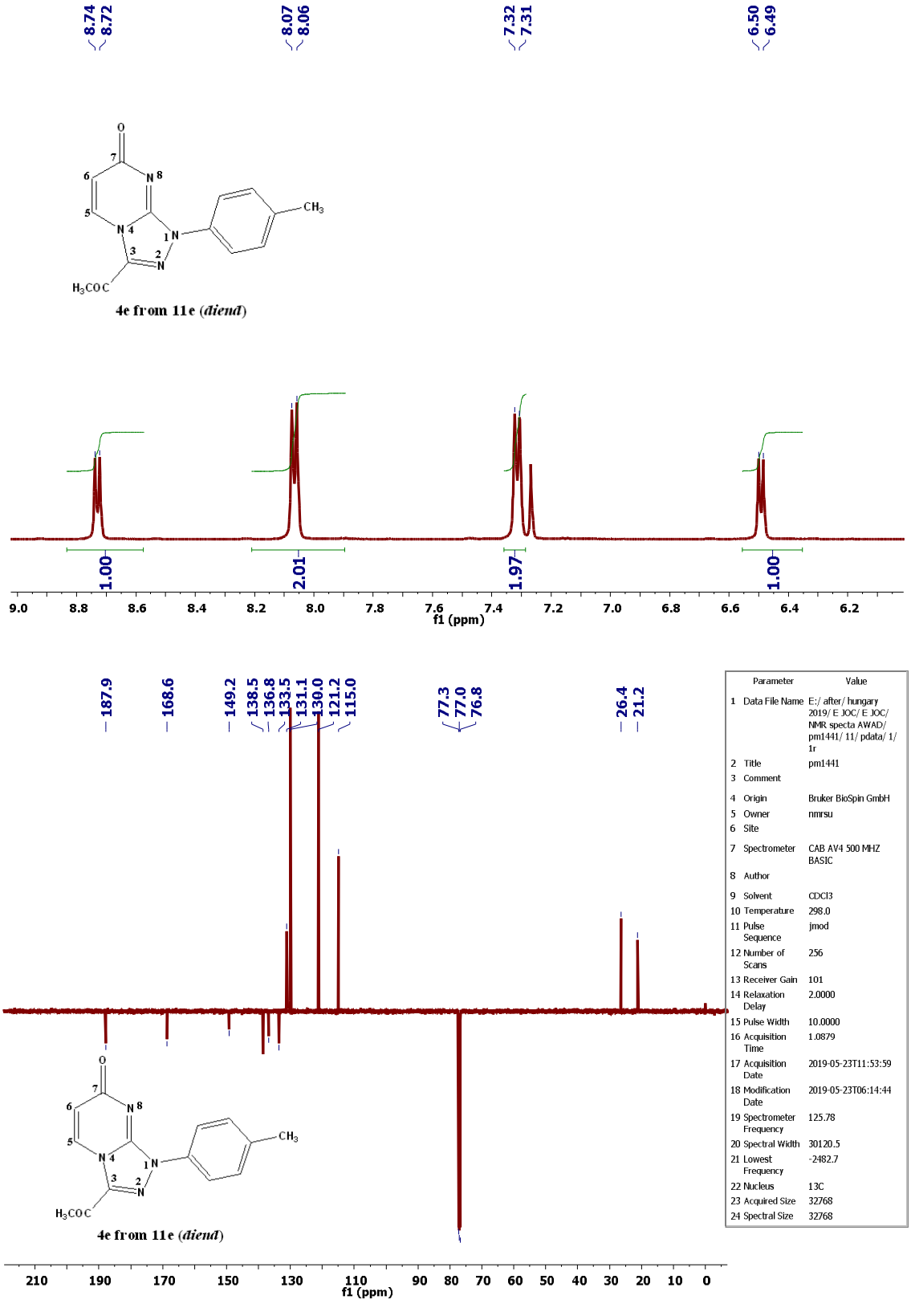
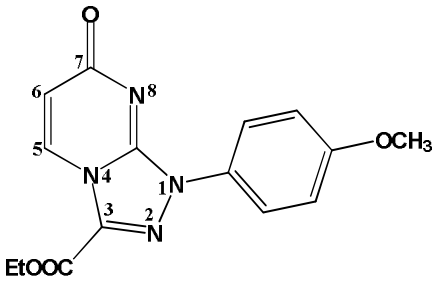
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ pm1443/ 11/ pdata/ 1/ 1r
2	Title	pm1443
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-07-12T14:07:59
18	Modification Date	2019-07-12T06:26:06
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

From *Diendo* 7e



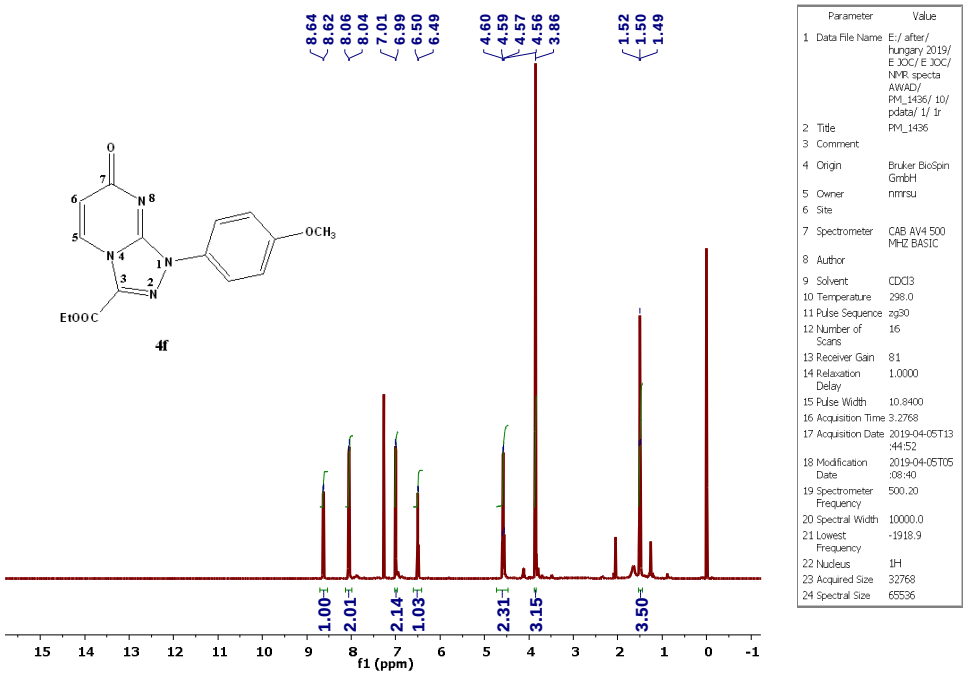
	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ pm1441/ 10/ pdata/ 1/ 1r
2	Title	pm1441
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	65
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-05-23T11:39:50
18	Modification Date	2019-05-23T06:14:42
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1919.5
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536


8.74
8.72
8.07
8.06
7.32
7.31
6.50
6.49
4e from 11e (diend)
1.00
2.01
1.97
1.00
f1 (ppm)
187.9
168.6
149.2
138.5
136.8
133.5
131.1
130.0
121.2
115.0
77.3
77.0
76.8
26.4
21.2
4e from 11e (diend)
f1 (ppm)
Parameter
Value
1 Data File Name E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ pm1441/ 11/ pdata/ 1/ 1r
2 Title pm1441
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer CAB AV4 500 MHZ BASIC
8 Author
9 Solvent CDCl3
10 Temperature 298.0
11 Pulse Sequence jmod
12 Number of Scans 256
13 Receiver Gain 101
14 Relaxation Delay 2.0000
15 Pulse Width 10.0000
16 Acquisition Time 1.0879
17 Acquisition Date 2019-05-23T11:53:59
18 Modification Date 2019-05-23T06:14:44
19 Spectrometer Frequency 125.78
20 Spectral Width 30120.5
21 Lowest Frequency -2482.7
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 32768

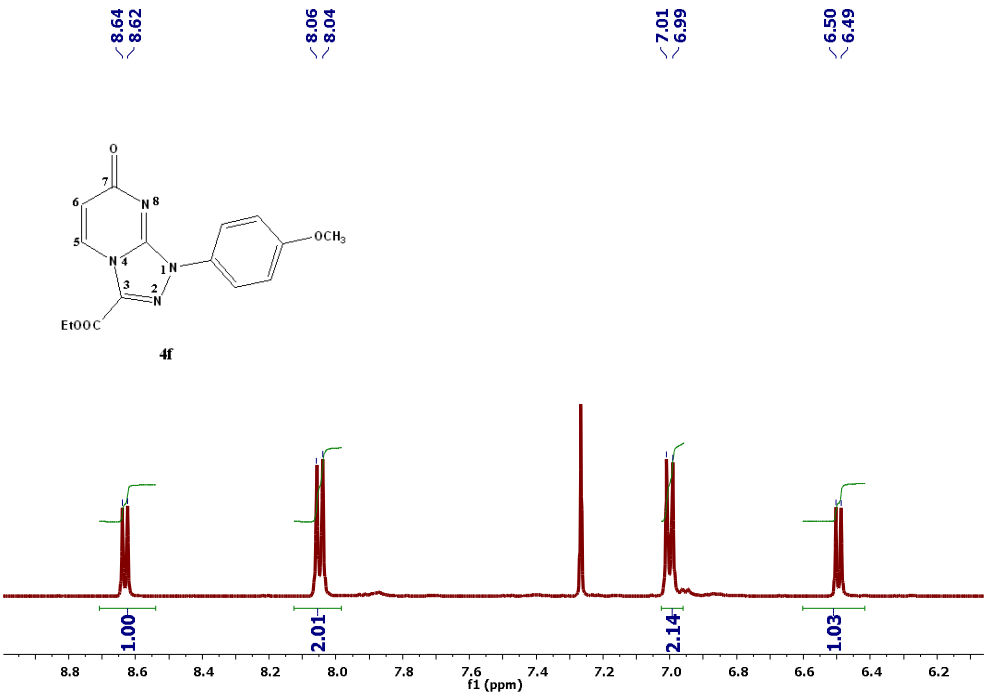


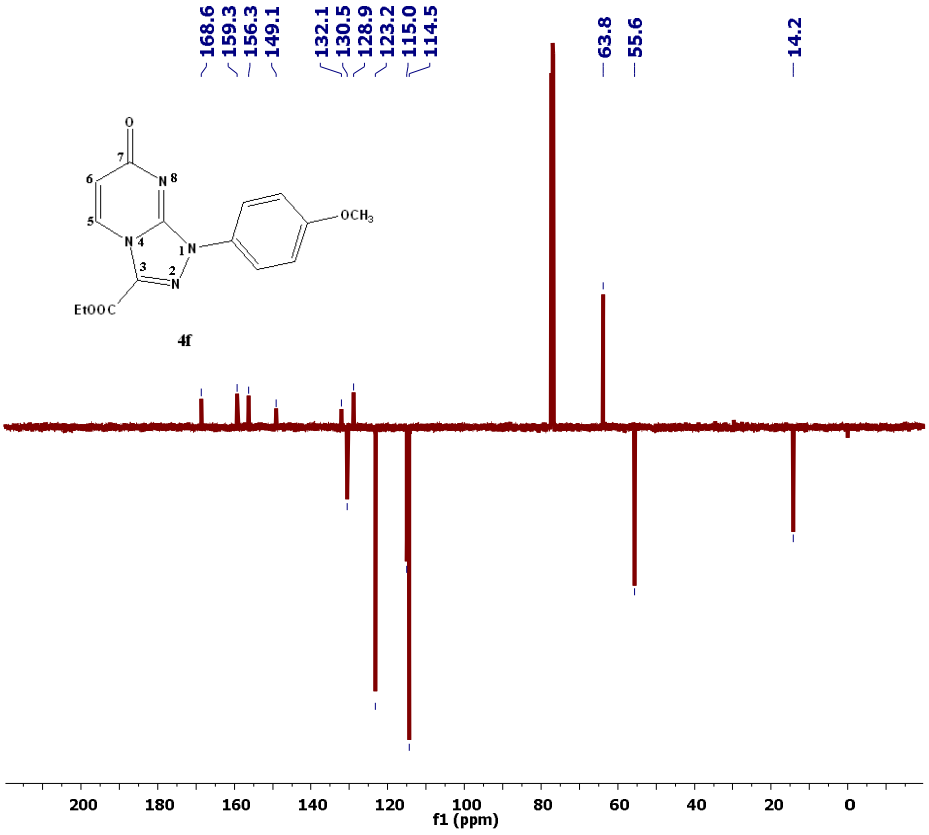
4f

Ethyl 1-(4-methoxyphenyl)-7-oxo-1,7-dihydro[1,2,4]-triazolo[4,3-*a*]pyrimidine-3-carboxylate (4f)

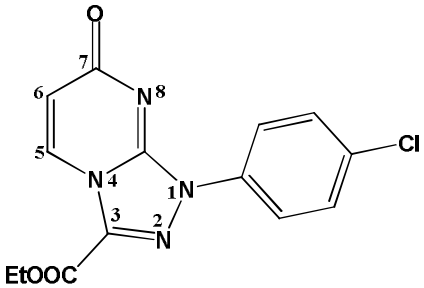


	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM_1436/ 10/ pdata/ 1/ 1r
2	Title	PM_1436
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	81
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-04-05T13 :44:52
18	Modification Date	2019-04-05T05 :08:40
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1918.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



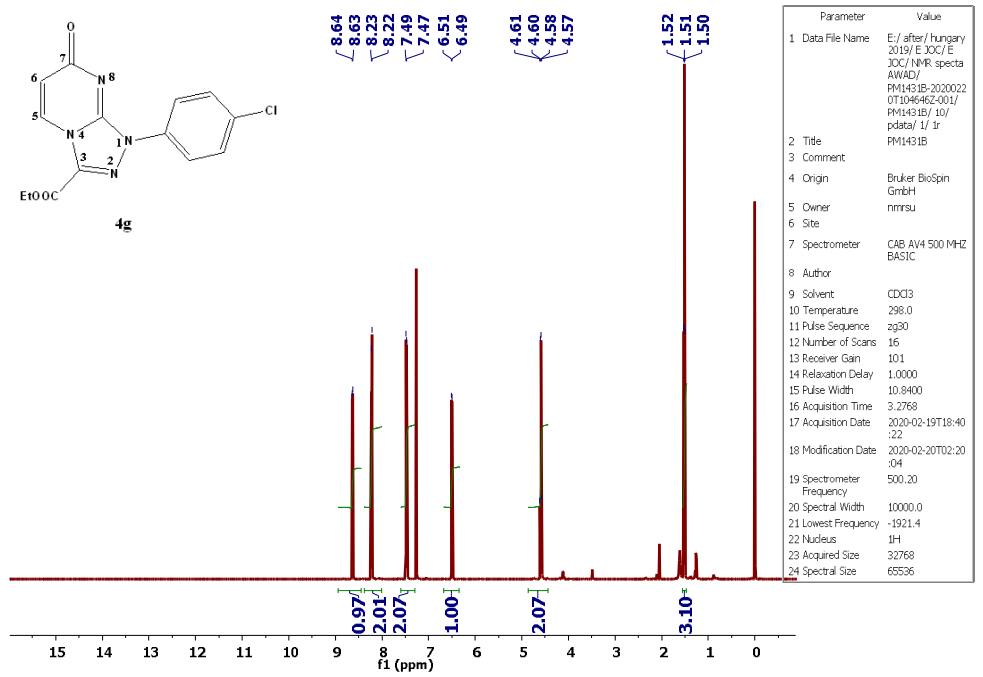


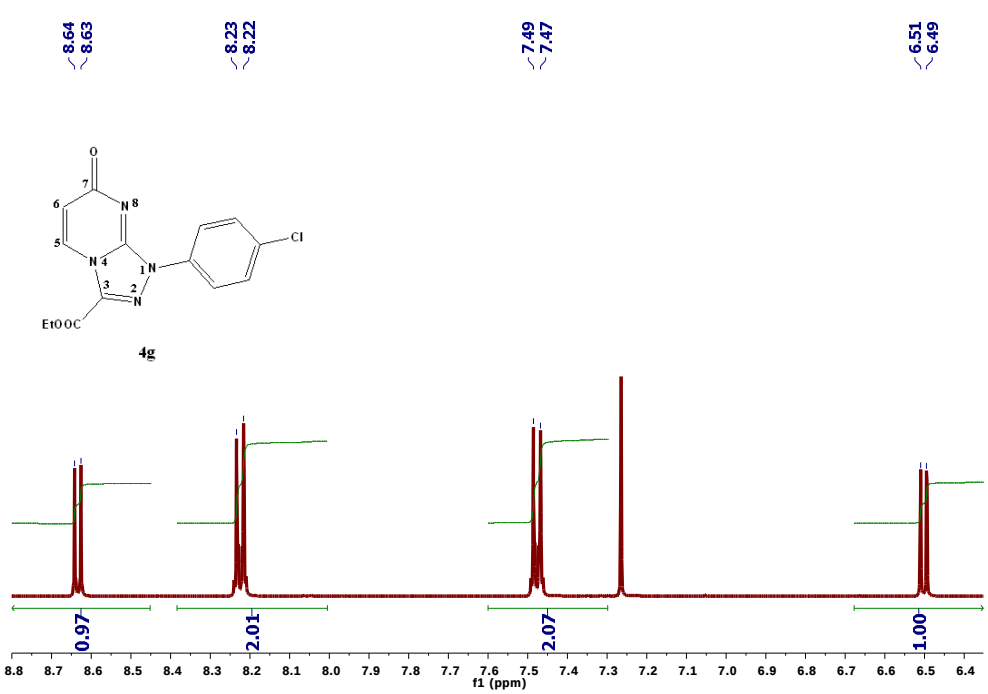
	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM_1436/ 11/ pdata/ 1/ 1r
2	Title	PM_1436
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-05T13:59:01
18	Modification Date	2019-04-05T05:08:06
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

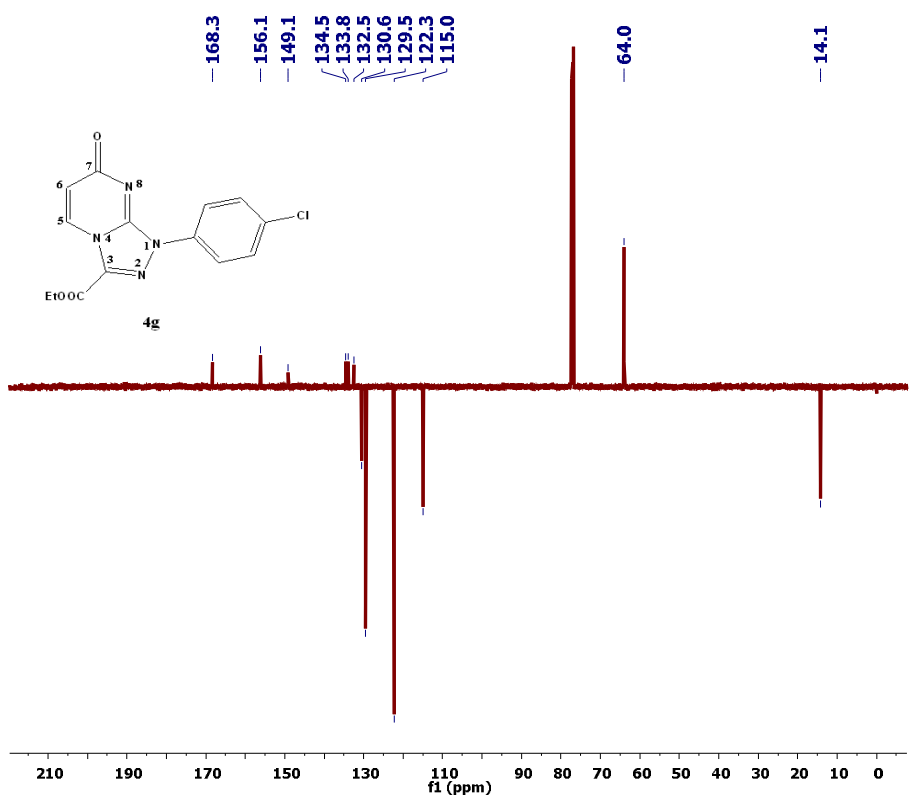


Ethyl 1-(4-chlorophenyl)-7-oxo-1,7-dihydro[1,2,4]triazolo[4,3-*a*]-pyrimidine-3-carboxylate (4g)

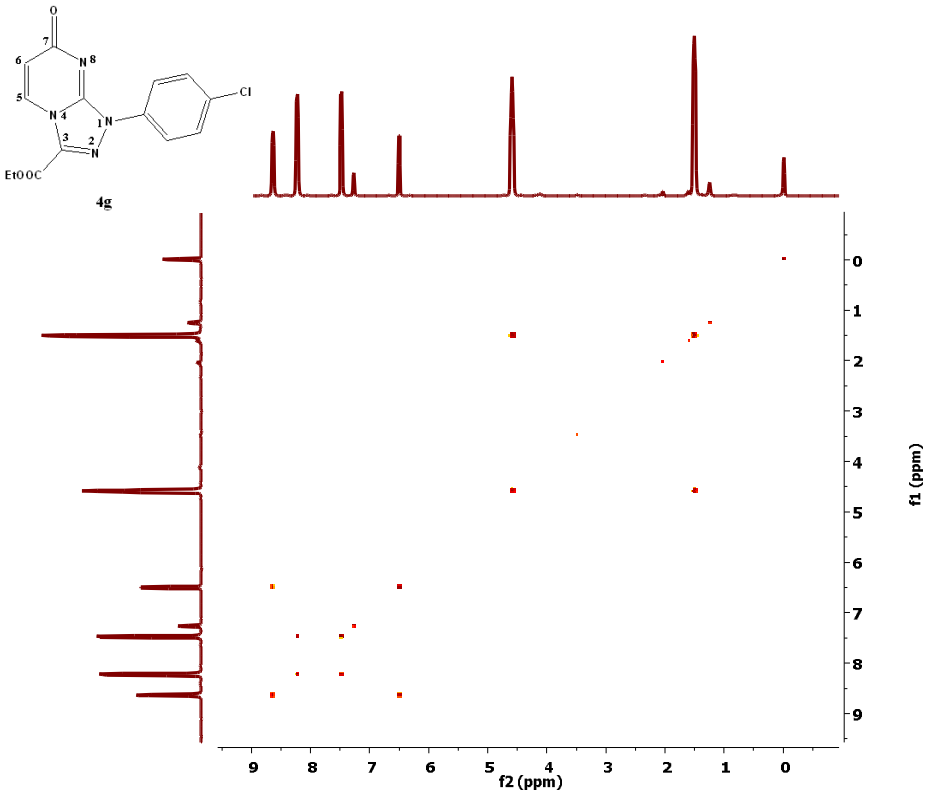
4g



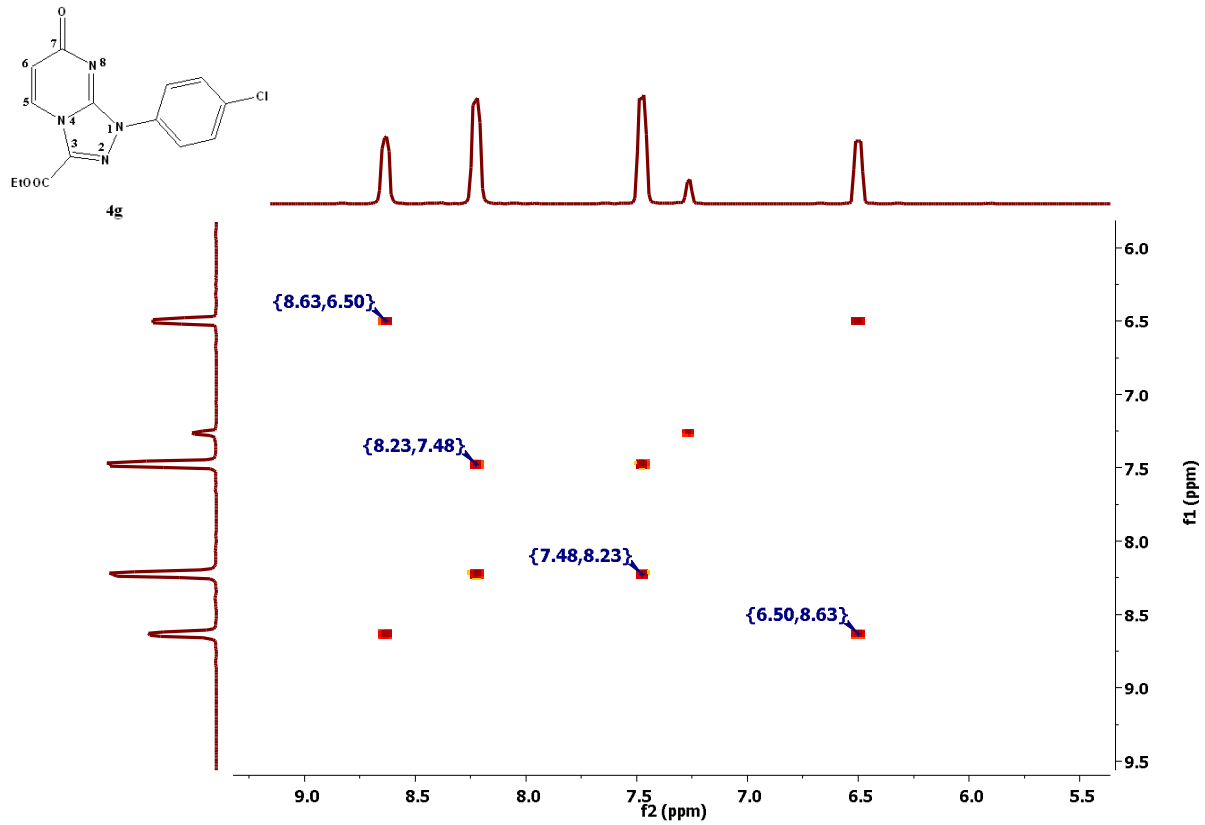


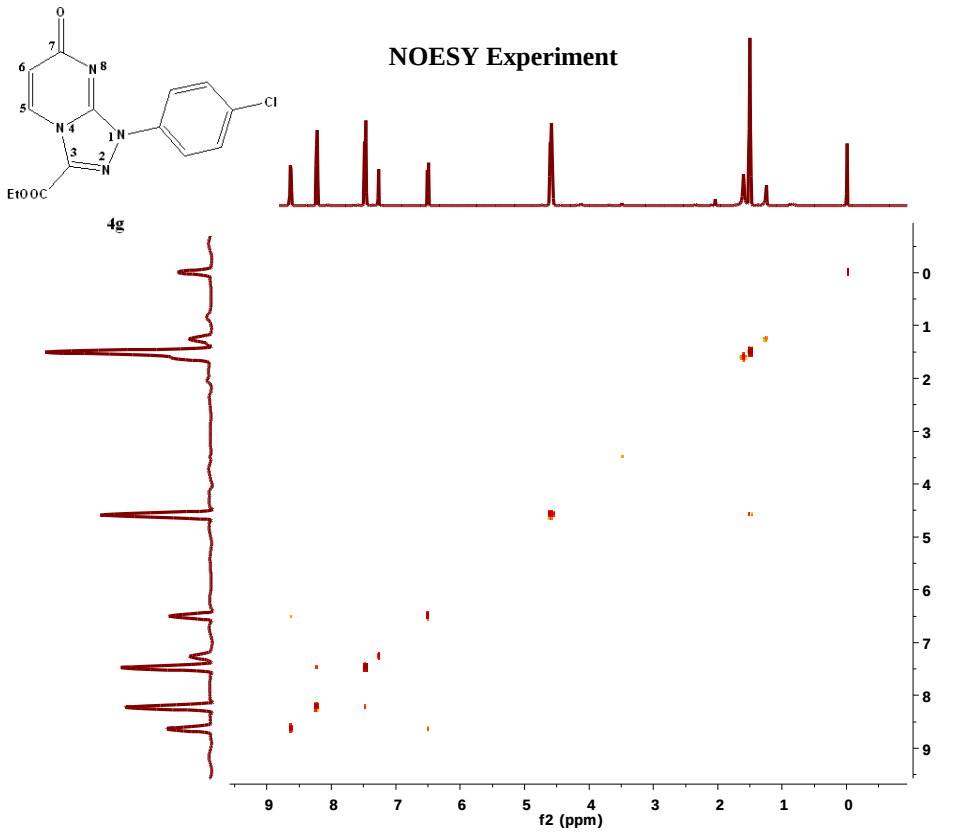


	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM1431B-20200220T104646Z-001/ PM1431B/ 11/ pdata/ 1/ 1r
2	Title	PM1431B
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2020-02-19T18:54:32
18	Modification Date	2020-02-20T02:20:08
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

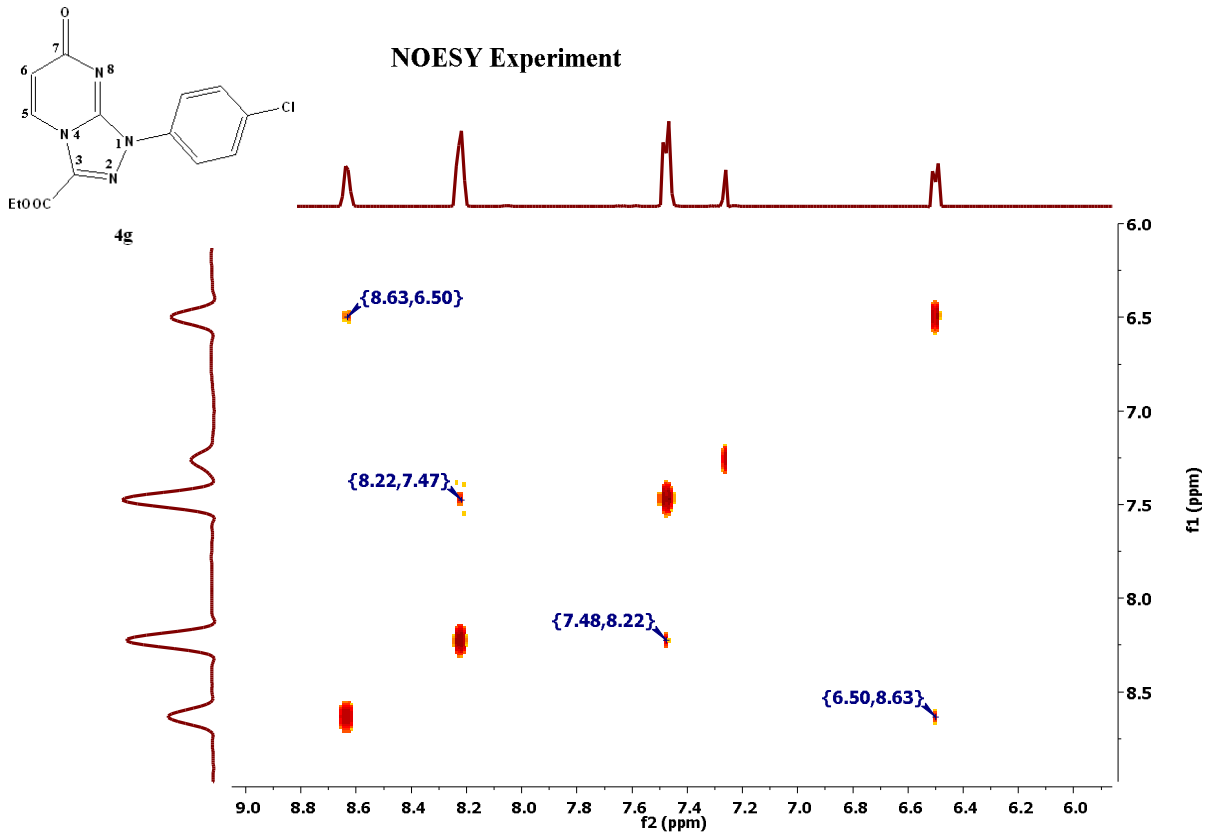


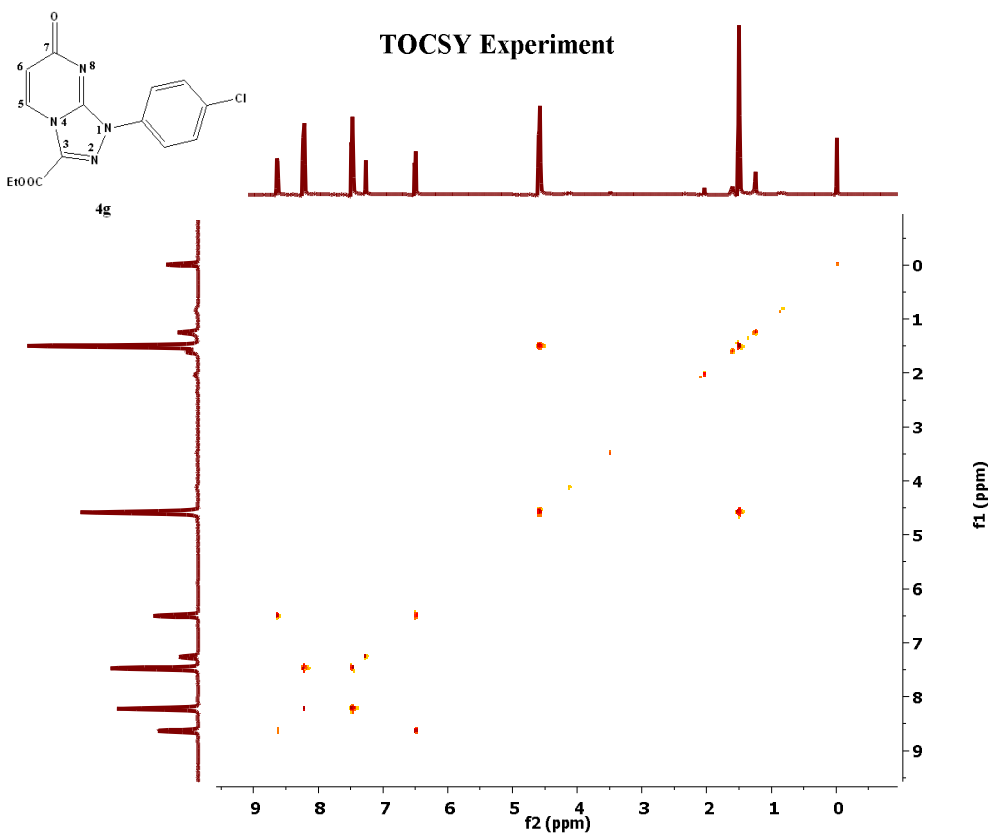
	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM1431B-20200220T104646Z-001/ PM1431B/ 12/ pdata/ 1/ 2r
2	Title	PM1431B
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	cosygpppqf
12	Number of Scans	1
13	Receiver Gain	101
14	Relaxation Delay	1.9652
15	Pulse Width	10.8400
16	Acquisition Time	0.1946
17	Acquisition Date	2020-02-19T19:00:23
18	Modification Date	2020-02-20T02:20:12
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(5263.2, 5263.2)
21	Lowest Frequency	(-473.6, -473.6)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)



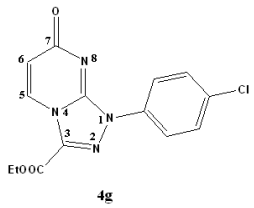


	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM1431B-20200220T104646Z-001/ PM1431B/ 13/ pdata/ 1/ 2rr
2	Title	PM1431B
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	noesygpphpp
12	Number of Scans	4
13	Receiver Gain	101
14	Relaxation Delay	2.0143
15	Pulse Width	10.8400
16	Acquisition Time	0.1946
17	Acquisition Date	2020-02-19T19:45:57
18	Modification Date	2020-02-20T02:20:18
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(5263.2, 5263.2)
21	Lowest Frequency	(-473.6, -473.6)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 256)
24	Spectral Size	(1024, 1024)



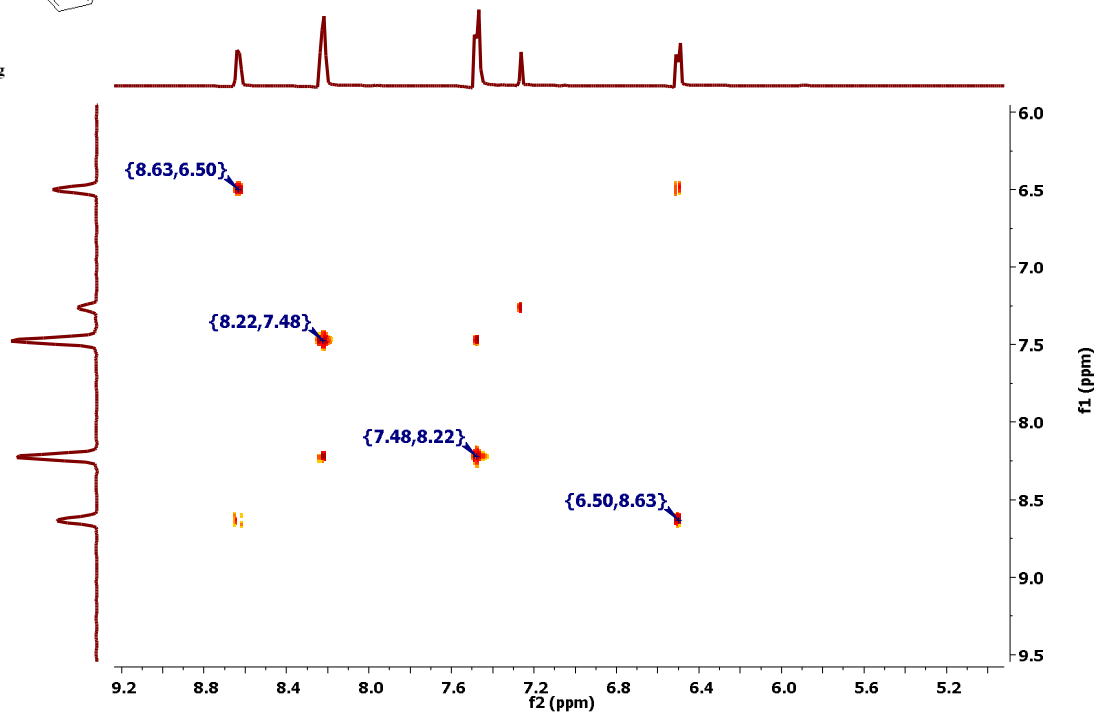


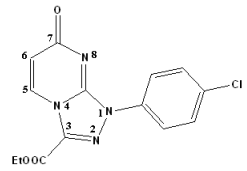
	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM1431B-20200220T104646Z-001/ PM1431B/ 14/ pdata/ 1/ 2rr
2	Title	PM1431B
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	mlevphpp
12	Number of Scans	8
13	Receiver Gain	101
14	Relaxation Delay	2.0143
15	Pulse Width	10.8400
16	Acquisition Time	0.1946
17	Acquisition Date	2020-02-19T21:06:46
18	Modification Date	2020-02-20T02:20:22
19	Spectrometer Frequency	(500.20, 500.20)
20	Spectral Width	(5263.2, 5263.2)
21	Lowest Frequency	(-473.6, -473.6)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 256)
24	Spectral Size	(1024, 1024)



4g

TOCSY Experiment

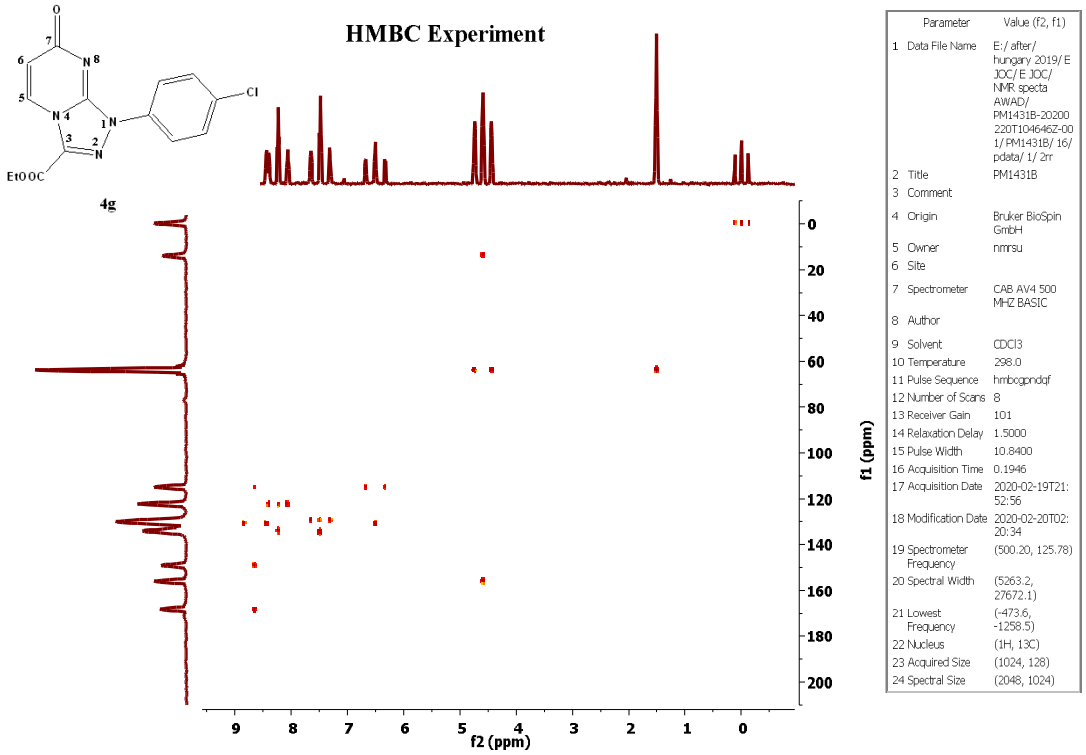




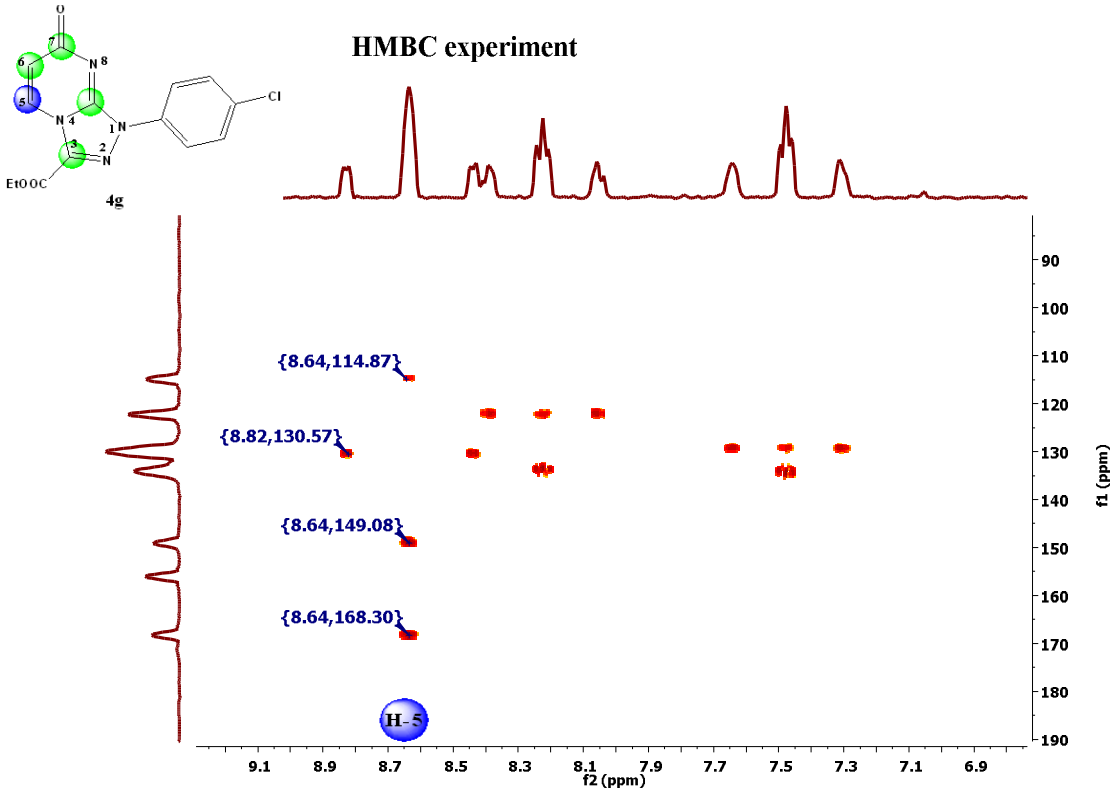
4g

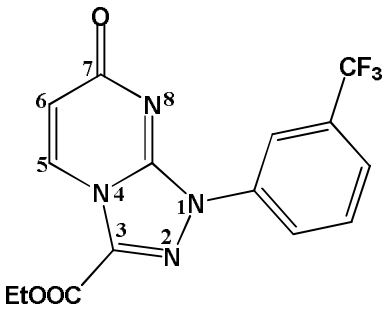
HMRC Experiment

	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM1431B-20200220T104646Z-001/ PM1431B/ 15/ pdata/ 1/ 2rr
2	Title	PM1431B
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	hsqcetgp
12	Number of Scans	2
13	Receiver Gain	101
14	Relaxation Delay	1.5000
15	Pulse Width	10.8400
16	Acquisition Time	0.0973
17	Acquisition Date	2020-02-19T21:21:39
18	Modification Date	2020-02-20T02:20:26
19	Spectrometer Frequency	(500.20, 125.78)
20	Spectral Width	(5263.2, 20752.3)
21	Lowest Frequency	(-473.6, -943.0)
22	Nucleus	(1H, 13C)
23	Acquired Size	(512, 256)
24	Spectral Size	(1024, 1024)



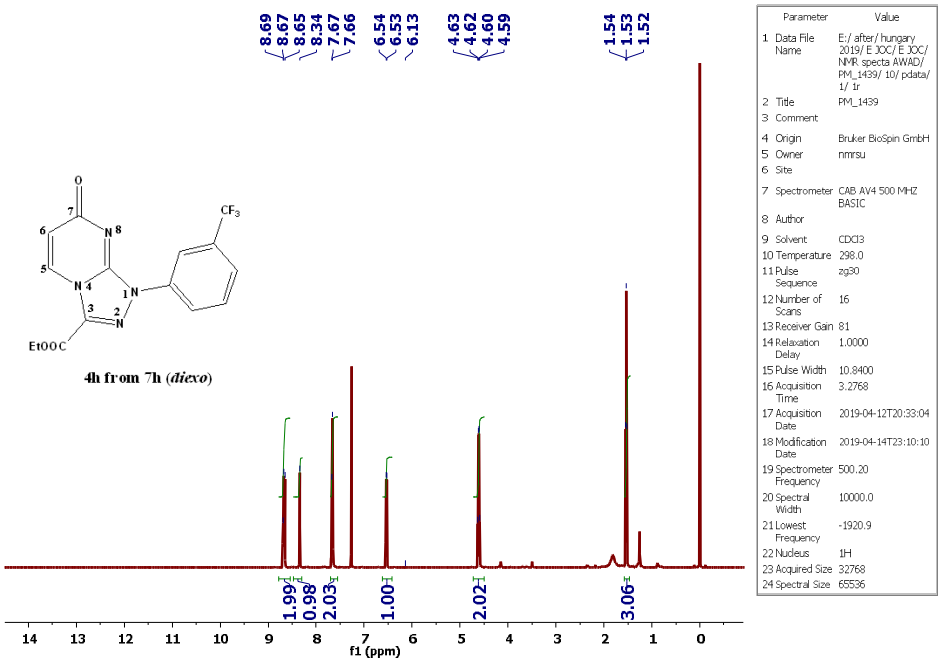
	Parameter	Value (f2, f1)
1	Data File Name	E:/ after/ hungary 2019/ E JOC/ E JOC/ NMR specta AWAD/ PM1431B-20200220T104646Z-001/ PM1431B/ 16/ pdata/ 1/ 2rr
2	Title	PM1431B
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	hmbcgpndqf
12	Number of Scans	8
13	Receiver Gain	101
14	Relaxation Delay	1.5000
15	Pulse Width	10.8400
16	Acquisition Time	0.1946
17	Acquisition Date	2020-02-19T21:52:56
18	Modification Date	2020-02-20T02:20:34
19	Spectrometer Frequency	(500.20, 125.78)
20	Spectral Width	(5263.2, 27672.1)
21	Lowest Frequency	(-473.6, -1258.5)
22	Nucleus	(1H, 13C)
23	Acquired Size	(1024, 128)
24	Spectral Size	(2048, 1024)

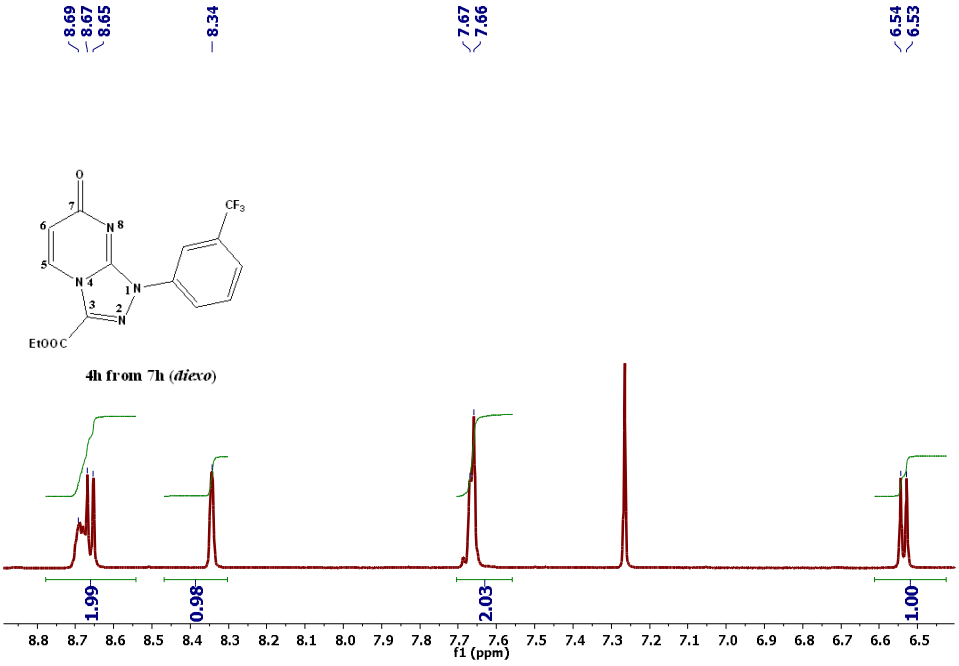


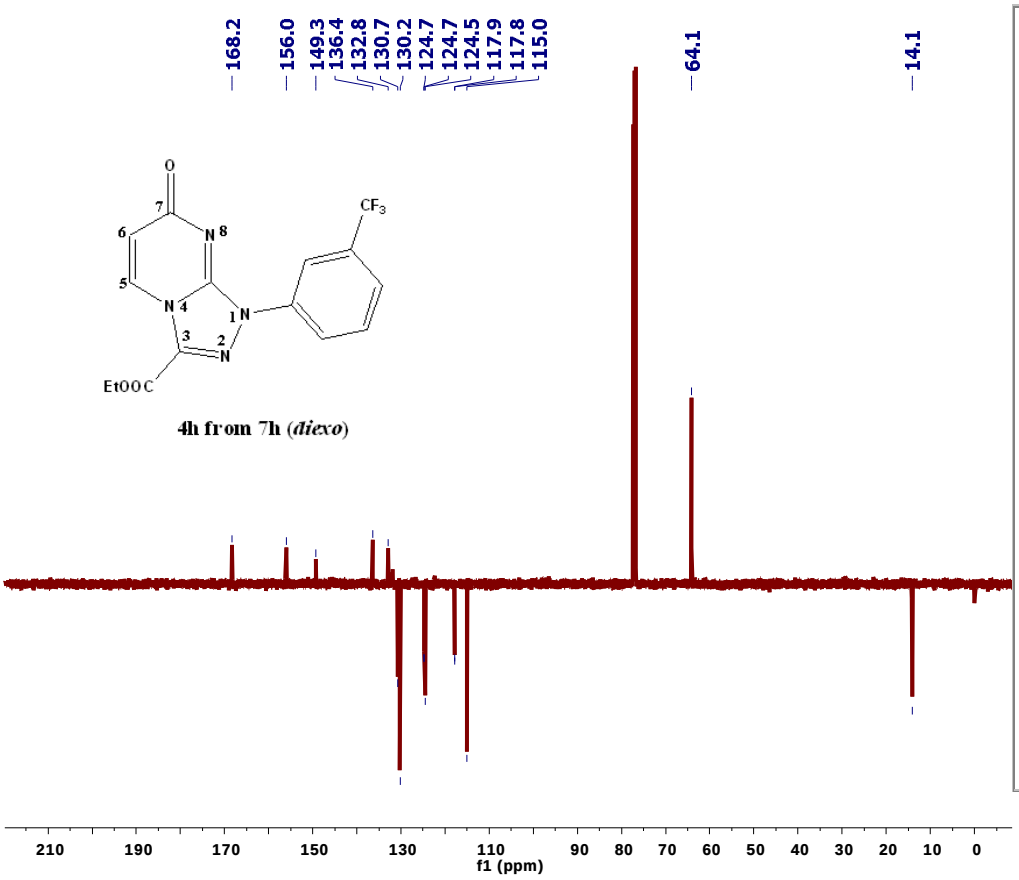


Ethyl7-oxo-1-(3-(trifluoromethyl)phenyl)-1,7-dihydro[1,2,4]triazolo[4,3-*a*]pyrimidine-3-carboxylate (4h)

4h from 7h (*diexo*)







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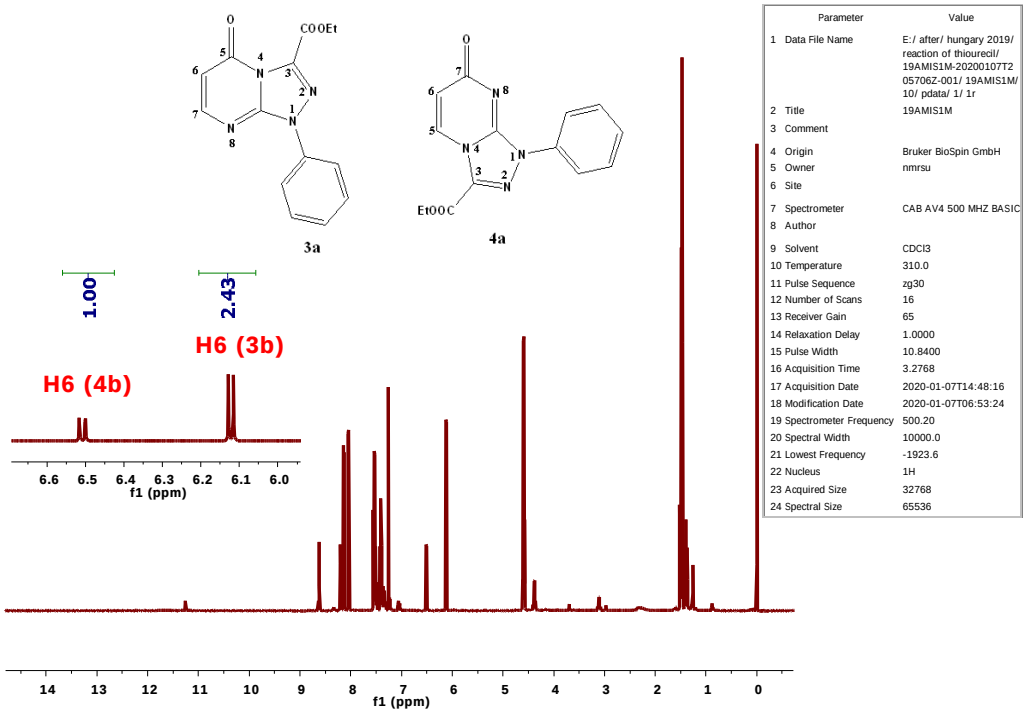
2	Title	PM_1439
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2019-04-12T20:47:12
18	Modification Date	2019-04-14T23:10:20
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

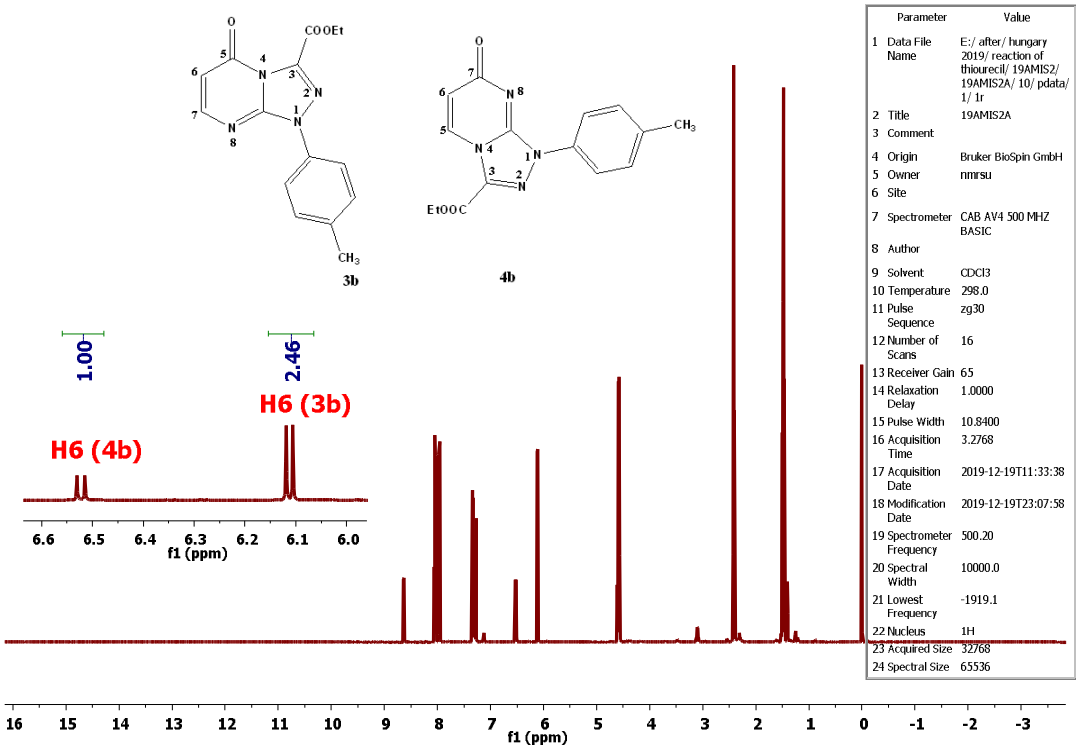
Reaction of thiouracil with hydrazonoyl chlorides 2(a-e)

Reaction of Thiouracil 1 with 2a



	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ reaction of thiouracil/ 19AMIS1M-20200107T205706Z-001/ 19AMIS1M/ 10/ pdata/ 1/ 1r
2	Title	19AMIS1M
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	65
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2020-01-07T14:48:16
18	Modification Date	2020-01-07T06:53:24
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1923.6
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Reaction of Thiouracil 1 with 2b



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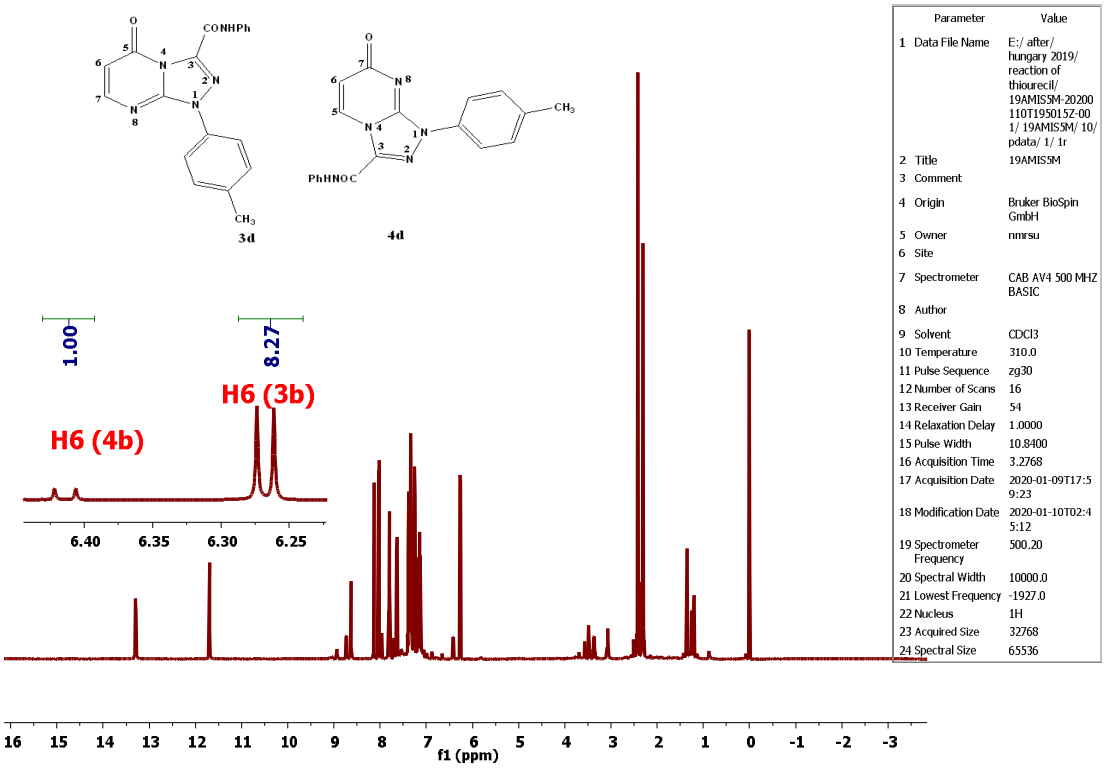
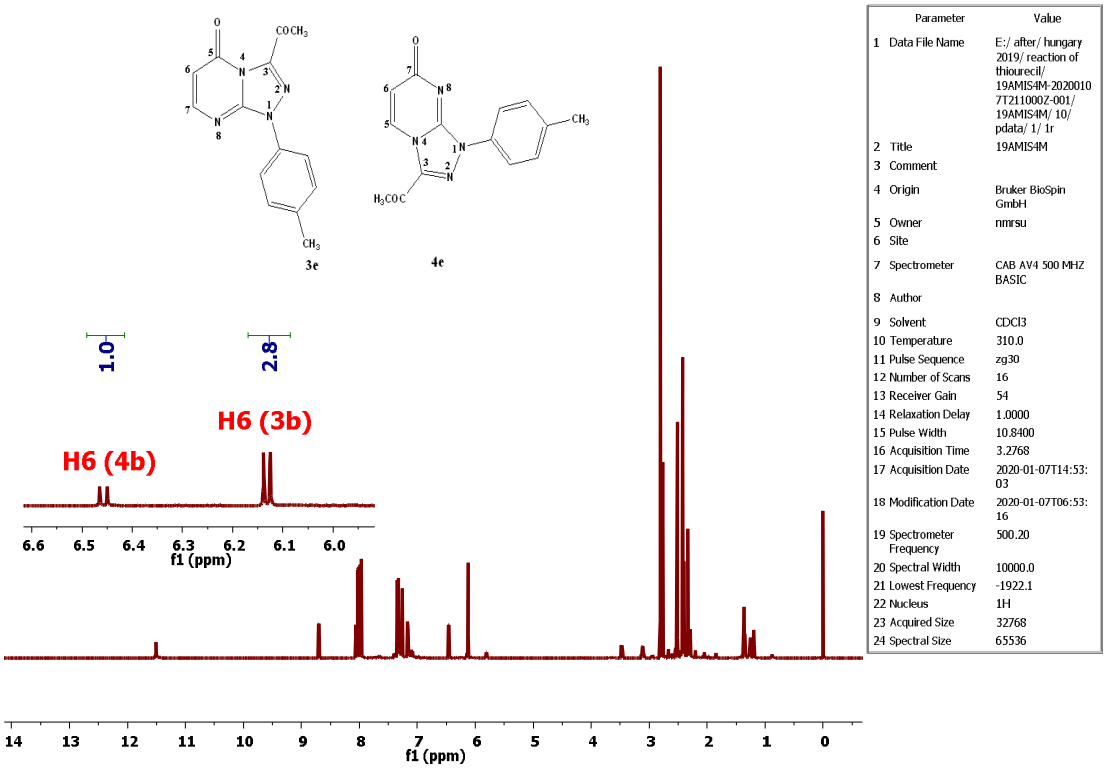
2	Title	19AMIS2A
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	65
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-12-19T11:33:38
18	Modification Date	2019-12-19T23:07:58
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1919.1
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Reaction of Thiouracil 1 with 2d



	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ reaction of thiouracil/ 19AMIS5M-20200110T195015Z-001/ 19AMIS5M/ 10/ pdata/ 1/ 1r
2	Title	19AMIS5M
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	54
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2020-01-09T17:59:23
18	Modification Date	2020-01-10T02:45:12
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1927.0
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Reaction of Thiouracil 1 with 2e

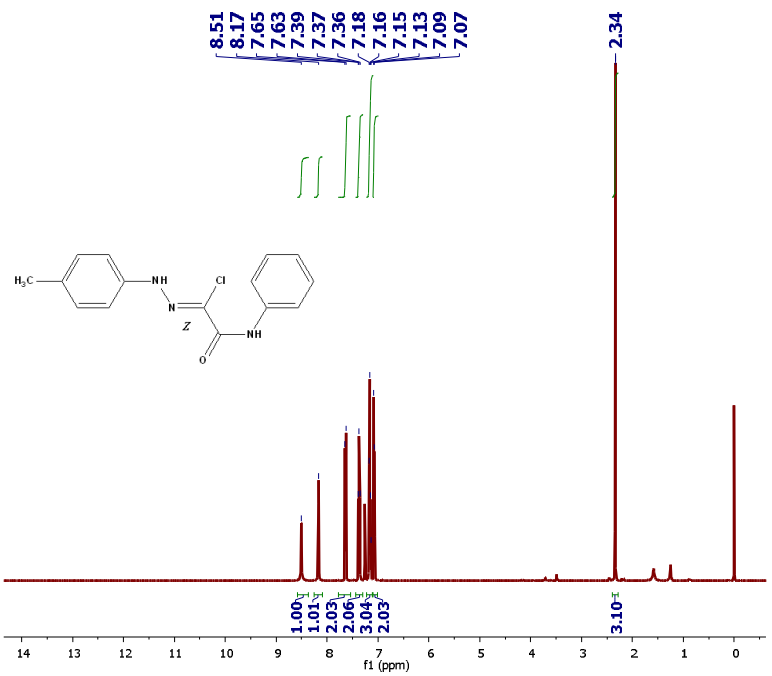


	Parameter	Value
1	Data File Name	E:/ after/ hungary 2019/ reaction of thiouracil/ 19AMIS4M-20200107T211000Z-001/ 19AMIS4M/ 10/ pdata/ 1/ 1r
2	Title	19AMIS4M
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	54
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2020-01-07T14:53:03
18	Modification Date	2020-01-07T06:53:16
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1922.1
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Side Product of the Reactions

hydrazonoyl chloride 2e

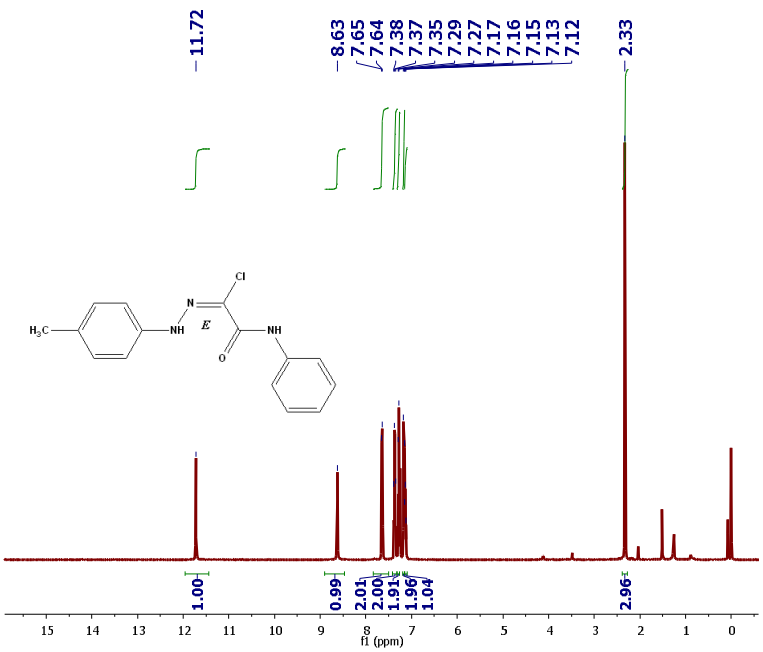
M.P. 153-154°C



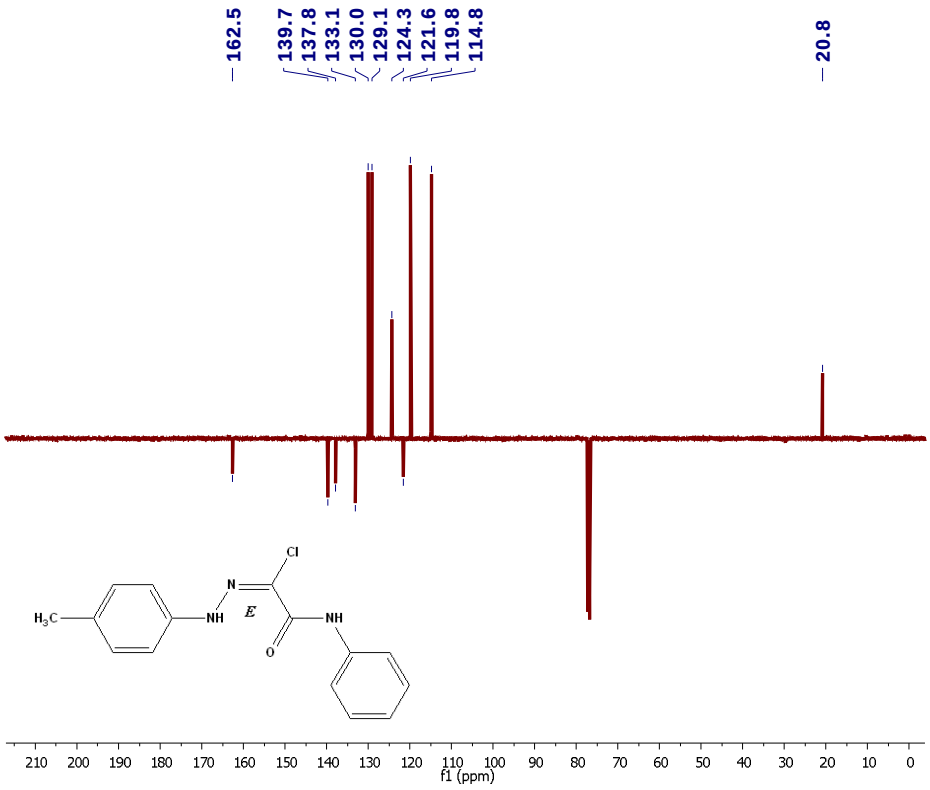
	Parameter	Value
1	Data File Name	F:/ after/ Hungary work/ awad/ NMR/ AMIS17/ 10/ pdata/ 1/ 1r
2	Title	AMIS17
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	74
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-04-18T 13:42:04
18	Modification Date	2019-04-18T 05:51:16
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1925.5
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Reaction using hydrazonoyl chloride 2d

Side product; yield 10%, m.p. 225-228°C



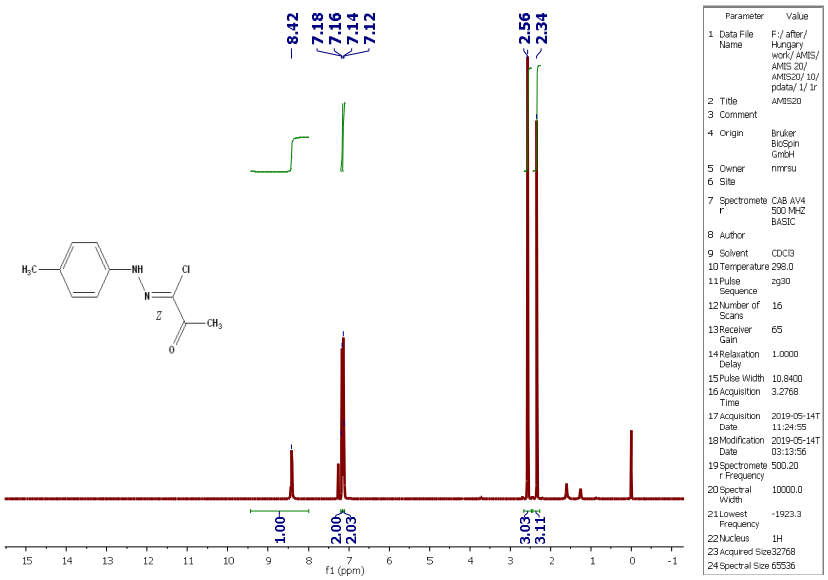
	Parameter	Value
1	Data File Name	F:/ after/ hungary 2019/ reaction of thiourea/ 19AMIS5X-20200207T202630Z-001/ 19AMIS5X/ 10/ pdata/ 1/ 1r
2	Title	19AMIS5X
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	81
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2020-02-06T14:48:30
18	Modification Date	2020-02-07T00:59:56
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1928.8
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	F:/ after/ hungary 2019/ reaction of thiourecil/ 19AMIS5X-20200207T202630Z-001/ 19AMIS5X/ 11/ pdata/ 1/ 1r
2	Title	19AMIS5X
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	310.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2020-02-06T15:03:15
18	Modification Date	2020-02-07T00:59:58
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768

hydrazonoyl chloride 2e

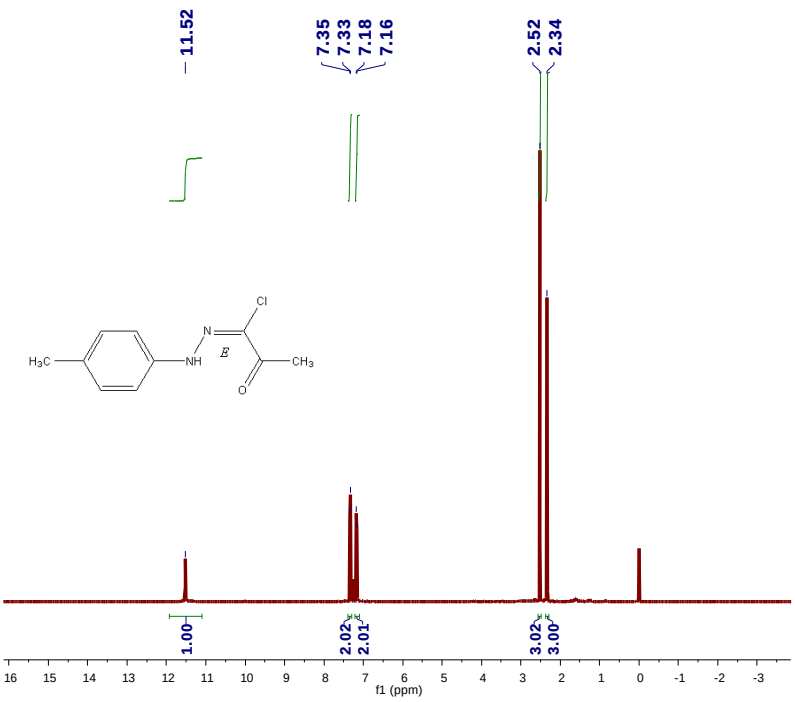
M.P. 153-154°C



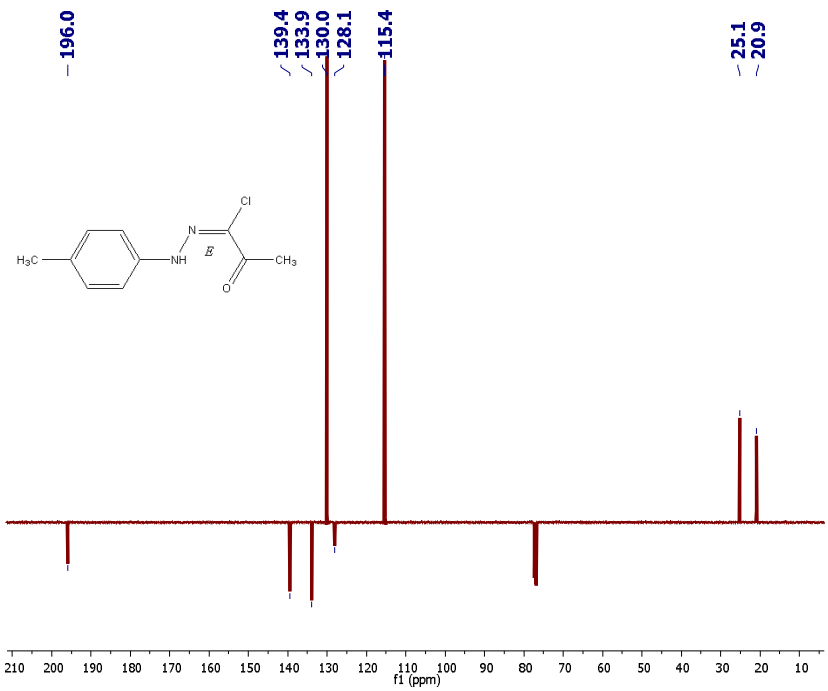
	Parameter	Value
1	Data File Name	F:/ after/ Hungary work/ AMIS/ AMIS 20/ AMIS20/ 10/ pdata/ 1/ 1r
2	Title	AMIS20
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	65
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2019-05-14T 11:24:55
18	Modification Date	2019-05-14T 03:13:56
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1923.3
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Reaction using hydrazonoyl chloride 2e

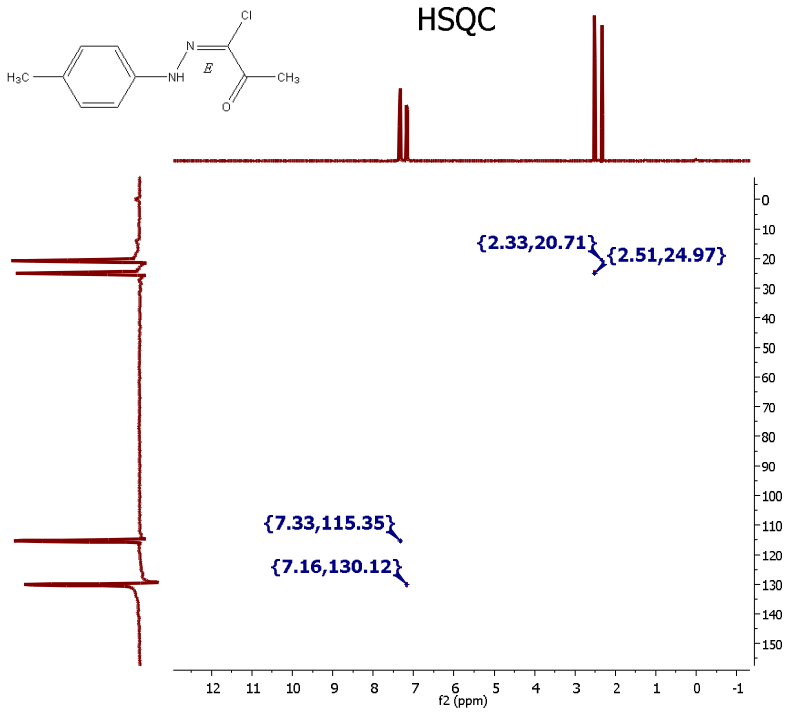
Side product; yield 13%, m.p. 218-222°C



	Parameter	Value
1	Data File Name	H:/ RSC advances manuscript/ New folder/ AMIS22X2-20200703T093140Z-001/ AMIS22X2/ 10/ pdata/ 1/ 1r
2	Title	AMIS22X2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	65
14	Relaxation Delay	1.0000
15	Pulse Width	10.8400
16	Acquisition Time	3.2768
17	Acquisition Date	2020-07-02T18:41:16
18	Modification Date	2020-07-02T09:40:18
19	Spectrometer Frequency	500.20
20	Spectral Width	10000.0
21	Lowest Frequency	-1928.1
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	H:/ RSC advances manuscript/ New folder/ AMIS22X2-20200703T093140Z-001/ AMIS22X2/ 11/ pdata/ 1/ 1r
2	Title	AMIS22X2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	jmod
12	Number of Scans	256
13	Receiver Gain	101
14	Relaxation Delay	2.0000
15	Pulse Width	10.0000
16	Acquisition Time	1.0879
17	Acquisition Date	2020-07-02T18:55:25
18	Modification Date	2020-07-02T09:54:28
19	Spectrometer Frequency	125.78
20	Spectral Width	30120.5
21	Lowest Frequency	-2482.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	32768



	Parameter	Value (f2, f1)
1	Data File Name	H:/ RSC advances manuscript/ New folder/ AMIS22X2-20200703T093140Z-001/ AMIS22X2/ 14/ pdata/ 1/ 2rr
2	Title	AMIS22X2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	CAB AV4 500 MHZ BASIC
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	hsqcetgp
12	Number of Scans	2
13	Receiver Gain	101
14	Relaxation Delay	1.5000
15	Pulse Width	10.8400
16	Acquisition Time	0.1434
17	Acquisition Date	2020-07-02T20:02:33
18	Modification Date	2020-07-02T11:01:36
19	Spectrometer Frequency	(500.20, 125.78)
20	Spectral Width	(7142.9, 20752.3)
21	Lowest Frequency	(-667.8, -943.0)
22	Nucleus	(1H, 13C)
23	Acquired Size	(1024, 256)
24	Spectral Size	(2048, 1024)

Computational Calculations

Table S1. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **1A** (Total energy: RB3LYP/6-31G(d,p): -737.86780311 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	1.127507	-1.70876	0
C	1.841058	-0.55098	0
N	1.294762	0.707088	0
C	0	0.770034	0
N	-0.80531	-0.32614	0
C	-0.31753	-1.66903	0
O	-1.10609	-2.59204	0
S	-0.70016	2.405597	0
H	1.603738	-2.67916	0
H	2.925881	-0.57204	0
H	-1.81399	-0.24886	0
H	-1.99683	2.032641	0

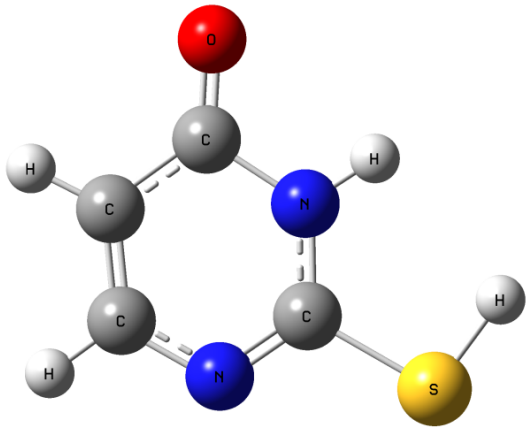


Table S2. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **1B**. (Total energy: RB3LYP/6-31G(d,p): -737.85582808 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	0.76725	-1.89043	0
C	1.708613	-0.93064	0
N	1.337008	0.399412	0
C	0	0.713109	0
N	-0.95149	-0.14318	0
C	-0.66043	-1.53491	0
O	-1.55063	-2.35795	0
S	-0.33517	2.473701	0
H	1.032503	-2.93829	0
H	2.773877	-1.12242	0
H	2.037824	1.124088	0
H	-1.66768	2.284537	0

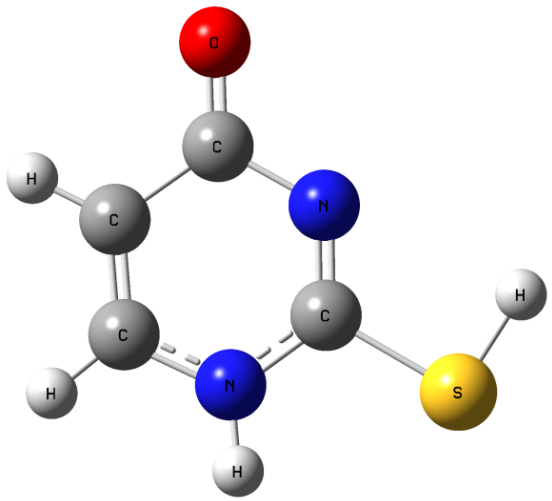


Table S3. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **6A**. (Total energy: RB3LYP/6-31G(d,p): -932.01629414 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-2.87571	-1.28608	-0.32887
C	-1.47182	-1.49801	0.212904
C	-3.1904	0.000084	-0.14663
C	-2.00006	0.673599	0.52062
C	-1.4719	-0.49265	1.386555
C	-0.4915	-0.77111	-0.78633
N	0.882108	-1.15341	-0.49398
C	1.72549	-0.28594	-0.14002
N	1.481701	1.081445	0.026004
C	-0.87913	0.740603	-0.59218
C	0.24313	1.672115	-0.18452
O	0.098871	2.867283	-0.04364
S	3.410629	-0.84383	0.136489
H	-3.45334	-2.03451	-0.85649
H	-1.16666	-2.52189	0.417708
H	-4.07382	0.519399	-0.49617
H	-2.18196	1.632981	1.000393
H	-0.48085	-0.31884	1.814525
H	-2.1668	-0.77236	2.179488
H	-0.69488	-1.09969	-1.80746
H	2.231862	1.723273	0.239127
H	-1.29211	1.176131	-1.50308
H	3.84216	0.246671	0.803995

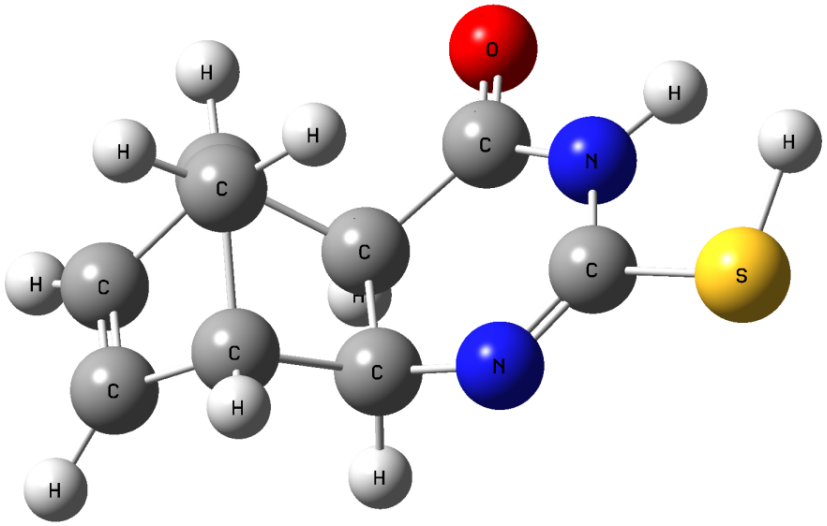


Table S4. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **6B**. (Total energy: RB3LYP/6-31G(d,p): -932.02237343 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-2.89295	-1.28151	-0.30342
C	-1.50825	-1.46641	0.299465
C	-3.18653	0.020611	-0.23069
C	-2.01151	0.725651	0.429894
C	-1.53147	-0.38015	1.397825
C	-0.51208	-0.81434	-0.73248
N	0.88485	-1.09057	-0.40795
C	1.786864	-0.13304	-0.10735
N	1.584939	1.137638	0.016661
C	-0.83939	0.708647	-0.62226
C	0.302253	1.639574	-0.17744
O	0.054363	2.813971	-0.00703
S	3.445673	-0.76304	0.153301
H	-3.46438	-2.06013	-0.79246
H	-1.23337	-2.48087	0.590524
H	-4.05003	0.523236	-0.64793
H	-2.19069	1.719782	0.830482
H	-2.25492	-0.59756	2.184506
H	-0.5533	-0.18144	1.843943
H	-0.70285	-1.19135	-1.73974
H	1.201247	-2.044	-0.49669
H	-1.18464	1.105662	-1.57742
H	3.937012	0.459823	0.42589

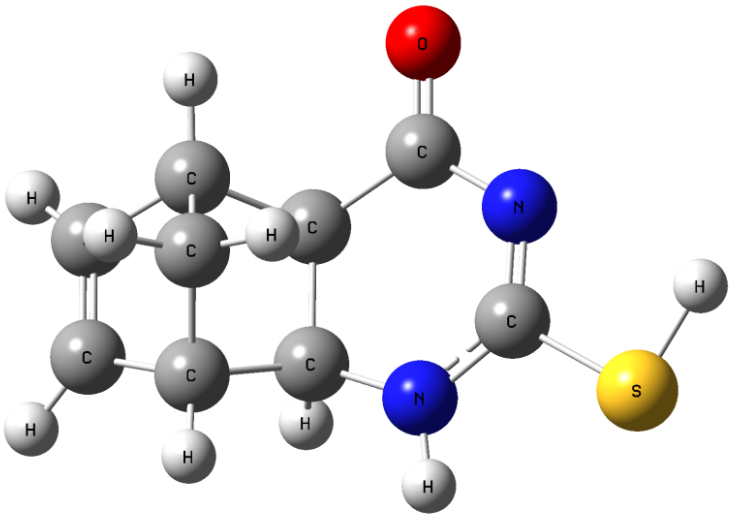


Table S5. Cartesian coordinates (in Å) of B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **10A**. (Total energy: RB3LYP/6-31G(d,p): -932.01161448 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	0.989021	0.735986	-0.7603
C	2.225855	0.525738	0.197109
C	1.68404	-0.04618	1.499266
C	1.278576	-1.29676	1.254815
C	0.506198	-0.73243	-1.03469
C	1.542652	-1.58768	-0.21379
C	2.822095	-0.75104	-0.43859
C	-0.03542	1.686039	-0.18359
N	-1.28982	1.141898	0.044665
C	-1.62093	-0.19261	-0.20478
N	-0.86488	-1.07673	-0.69344
O	0.194999	2.84852	0.070784
S	-3.31846	-0.56416	0.25379
H	1.339452	1.205428	-1.68331
H	2.859271	1.406388	0.278094
H	1.561975	0.517951	2.414875
H	0.756416	-1.96018	1.931119
H	0.632969	-0.97032	-2.09493
H	1.556945	-2.63584	-0.50735
H	3.676671	-1.13519	0.120324
H	3.091822	-0.63197	-1.49254
H	-1.9781	1.778504	0.42427
H	-3.23172	-1.83895	-0.16875

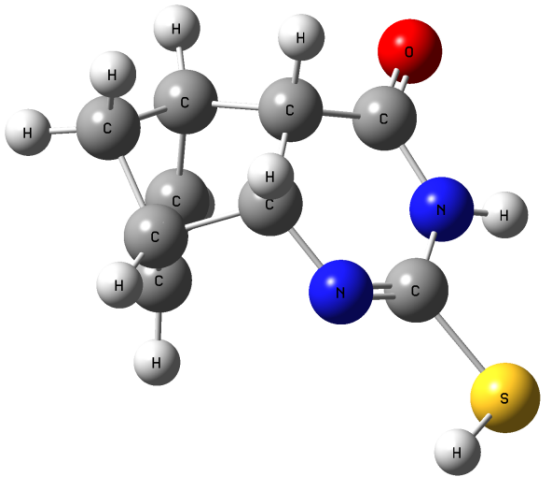


Table S6. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **10B**. (Total energy: RB3LYP/6-31G(d,p): -932.02617458 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	0.944761	0.710941	-0.78292
C	2.216457	0.572976	0.137783
C	1.725918	0.045734	1.477115
C	1.354151	-1.22636	1.301196
C	0.529519	-0.77504	-1.00328
C	1.591752	-1.57414	-0.15996
C	2.840718	-0.71039	-0.4554
C	-0.10404	1.656011	-0.18686
N	-1.38615	1.188909	0.072948
C	-1.66726	-0.05328	-0.13976
N	-0.85453	-1.02305	-0.61566
O	0.214285	2.80223	0.048181
S	-3.35735	-0.48541	0.261511
H	1.246892	1.158097	-1.73274
H	2.817571	1.478096	0.162306
H	1.603045	0.648457	2.367076
H	0.871392	-1.87247	2.022511
H	0.635189	-1.04424	-2.05862
H	1.642903	-2.63485	-0.40909
H	3.718377	-1.04993	0.096185
H	3.081367	-0.62978	-1.52006
H	-1.22103	-1.94906	-0.7613
H	-3.29943	-1.79541	-0.06447

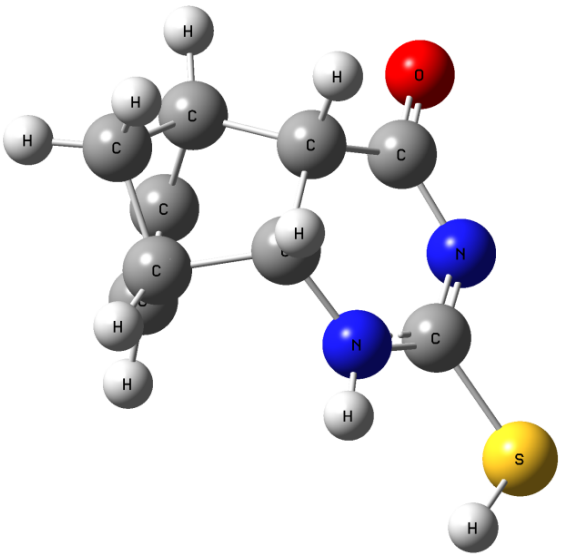


Table S7. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **7a**. (Total energy: RB3LYP/6-31G(d,p): -1179.79649107 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	3.6231814	-2.5953427	0.3307926
C	3.7988378	-1.3125293	0.6624493
C	2.4350561	-0.7521691	1.0393888
C	1.6462911	-0.6720171	-0.3221891
C	1.3866860	-2.1771167	-0.6681503
C	2.1470411	-2.9195170	0.4958798
C	1.7908820	-1.9996435	1.6854853
N	0.3821406	0.0691931	-0.2092586
C	-0.8453117	-0.5583758	-0.2687490
N	-1.1190570	-1.8072408	-0.4933659
C	-0.0728156	-2.6753408	-0.7279321
C	0.1401164	1.4131721	0.0196200
N	-1.1326675	1.6543367	0.1221472
N	-1.7592065	0.4570568	-0.0470965
O	-0.2594168	-3.8506433	-0.9730802
C	1.1112643	2.5407643	0.0951463
C	-3.1880556	0.4013303	0.0145717
C	-3.8808872	1.5796666	0.3130098
C	-5.2684763	1.5578070	0.3792327
C	-5.9715125	0.3757054	0.1527265
C	-5.2702422	-0.7892116	-0.1422386
C	-3.8790182	-0.7918124	-0.2151292
O	0.8125456	3.6434440	0.4659877
O	2.3369870	2.1750599	-0.3256660
C	3.3401351	3.2308045	-0.3293984
C	4.6092395	2.6615422	-0.9261704
H	4.3610304	-3.2760258	-0.0748358
H	4.7064682	-0.7286473	0.5812059
H	2.4318784	0.1784445	1.6032051
H	2.2424806	-0.1742716	-1.0813010
H	1.8246370	-2.4341178	-1.6325313
H	1.8740393	-3.9696020	0.5555053
H	0.7160713	-1.9087889	1.8642431
H	2.2897702	-2.2901422	2.6107298
H	-3.3296199	2.4923345	0.4870648
H	-5.8003878	2.4735394	0.6105366
H	-7.0539426	0.3648086	0.2061884
H	-5.8037785	-1.7157285	-0.3206180
H	-3.3311210	-1.6938022	-0.4415847
H	3.4815014	3.5719595	0.6983153
H	2.9507819	4.0690323	-0.9097628
H	5.3792395	3.4366936	-0.9503401
H	4.4411112	2.3156045	-1.9481616

H	4.9859765	1.8261050	-0.3328482

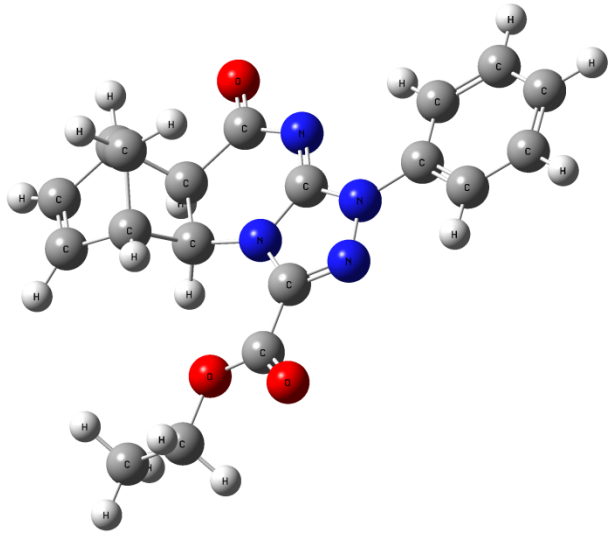


Table S8. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **8a**. (Total energy: RB3LYP/6-31G(d,p): -1179.77716107 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-5.0185299	-0.3478910	-0.0971949
C	-4.7093454	-1.6458290	-0.1780672
C	-3.2713037	-1.8059268	0.2844580
C	-2.3649469	-1.1816243	-0.8492656
C	-2.7479734	0.3504054	-0.7712963
C	-3.7924474	0.3831639	0.4268453
C	-3.1994925	-0.6967270	1.3576209
N	-0.9675474	-1.5448442	-0.6537398
C	-0.1627984	-0.6476203	-0.2629820
N	-0.4344778	0.7267972	-0.0577867
C	-1.6228869	1.3257843	-0.5189793
N	1.2035274	-0.7425142	0.0187722
N	1.7249260	0.4854400	0.3700034
C	0.7584930	1.3373973	0.3143477
O	-1.6986826	2.5188251	-0.6774574
C	2.0387371	-1.8908335	0.0311660
C	0.8346062	2.7218530	0.9045471
C	1.5797940	-3.1177058	-0.4606181
C	2.4294001	-4.2210621	-0.4350927
C	3.7226551	-4.1198531	0.0683838
C	4.1685240	-2.8924343	0.5556337
C	3.3373523	-1.7789918	0.5428213
O	0.0967601	3.0201150	1.8012798
O	1.7797597	3.5541063	0.4577123
C	2.5292519	3.2834373	-0.7590509
C	3.2689931	4.5572000	-1.1109734
H	-5.9251495	0.1383933	-0.4342622
H	-5.3175232	-2.4395285	-0.5931680
H	-2.9489608	-2.8069634	0.5630314
H	-2.6603637	-1.5894464	-1.8172178
H	-3.2307924	0.6990745	-1.6838042
H	-3.9501326	1.3816617	0.8300411
H	-2.1882665	-0.4792830	1.7092283
H	-3.8421517	-0.9012093	2.2149475
H	0.5744383	-3.1955336	-0.8455483
H	2.0676959	-5.1690966	-0.8171006
H	4.3752909	-4.9848341	0.0833478
H	5.1720305	-2.7969121	0.9546761
H	3.6793904	-0.8282489	0.9252323
H	1.8317414	2.9987469	-1.5512130
H	3.2138008	2.4540437	-0.5772880
H	3.8547967	4.4041904	-2.0211223
H	3.9489186	4.8426068	-0.3059683

H	2.5690496	5.3773627	-1.2806546

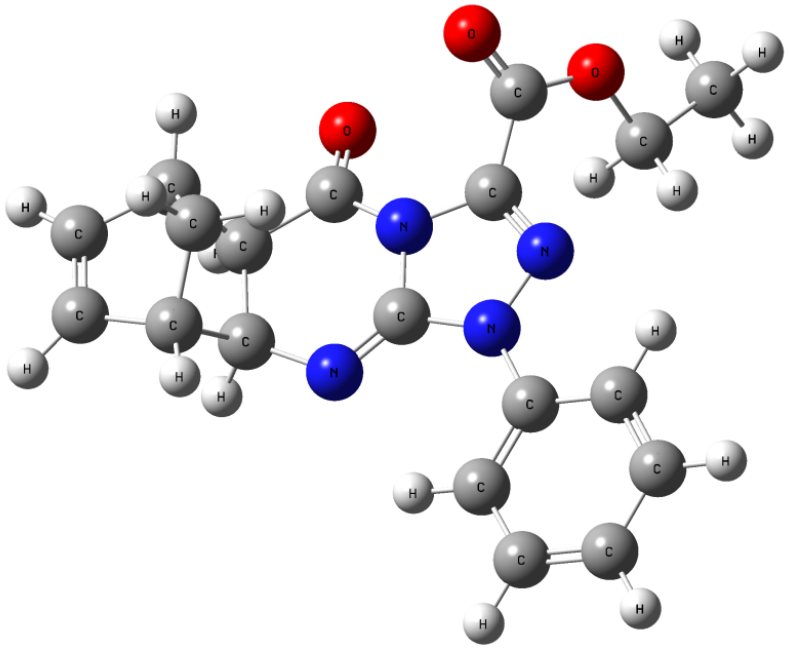


Table S9. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of 7**b**. (Total energy: RB3LYP/6-31G(d,p): -1219.12420686 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	3.9843767	-2.5471329	0.3403646
C	4.1389123	-1.2616915	0.6722806
C	2.7651694	-0.7225144	1.0440869
C	1.9801883	-0.6552678	-0.3204326
C	1.7450658	-2.1644279	-0.6664171
C	2.5128851	-2.8942980	0.5004409
C	2.1383348	-1.9796680	1.6884475
N	0.7045538	0.0665269	-0.2131141
C	-0.5128216	-0.5797215	-0.2784488
N	-0.7665227	-1.8334926	-0.5026207
C	0.2934389	-2.6853982	-0.7307510
O	0.1268800	-3.8643692	-0.9740914
C	0.4405330	1.4070339	0.0123554
N	-0.8369481	1.6279015	0.1072347
N	-1.4431833	0.4212194	-0.0637308
C	-2.8713737	0.3429161	-0.0125632
C	1.3930135	2.5494278	0.0920720
O	1.0744298	3.6490742	0.4558250
O	2.6285806	2.2014153	-0.3158573
C	3.6149812	3.2725142	-0.3134698
C	4.8990465	2.7205790	-0.8943420
C	-3.5897335	1.5063931	0.2714554
C	-4.9776315	1.4588598	0.3267001
C	-5.6795464	0.2710023	0.1056308
C	-4.9349968	-0.8784431	-0.1746477
C	-3.5459980	-0.8608457	-0.2377234
C	-7.1869290	0.2248300	0.1603687
H	4.7341425	-3.2162353	-0.0627047
H	5.0375996	-0.6637532	0.5937162
H	2.7451371	0.2082369	1.6072417
H	2.5717943	-0.1490960	-1.0775650
H	2.1901016	-2.4151622	-1.6292369
H	2.2560916	-3.9484876	0.5595544
H	1.0616393	-1.9055481	1.8634535
H	2.6385407	-2.2620796	2.6155138
H	3.7402707	3.6201571	0.7141717
H	3.2189889	4.1023026	-0.9014599
H	5.6575421	3.5071533	-0.9128838
H	4.7473745	2.3684801	-1.9168039
H	5.2816383	1.8929490	-0.2938723
H	-3.0605822	2.4323470	0.4449773
H	-5.5229406	2.3701900	0.5484269
H	-5.4476264	-1.8187767	-0.3502610

H	-2.9857605	-1.7579214	-0.4537683
H	-7.6041731	1.1887845	0.4578883
H	-7.5354169	-0.5269890	0.8747618
H	-7.6102724	-0.0354852	-0.8149880

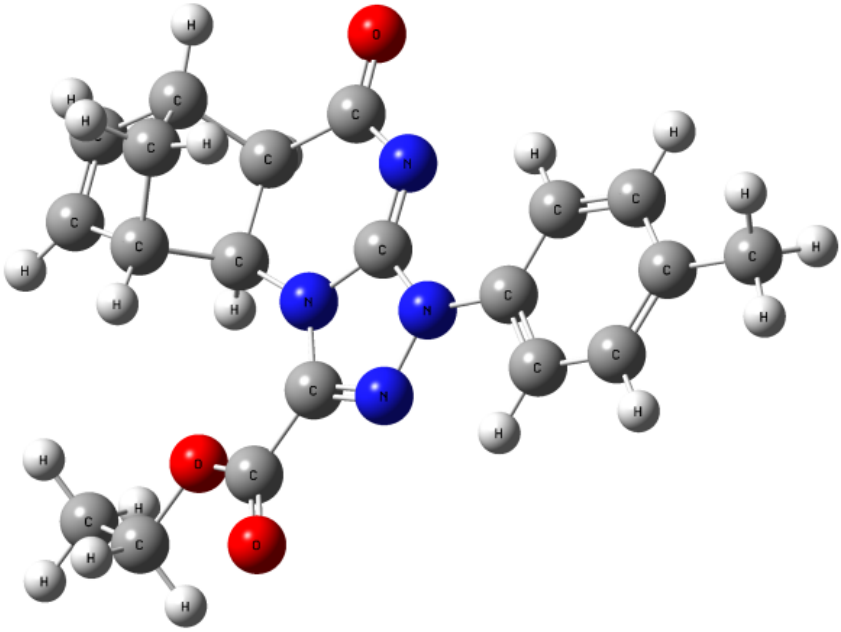


Table S10. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **8b**. (Total energy: RB3LYP/6-31G(d,p): -1219.10466090 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-4.4459821	-2.7470884	-0.0999750
C	-3.5203056	-3.7107299	-0.1420671
C	-2.2063952	-3.1070135	0.3232578
C	-1.7272686	-2.1392724	-0.8312812
C	-2.8324474	-1.0091877	-0.7927157
C	-3.7673332	-1.4821782	0.4024261
C	-2.7222183	-2.0875673	1.3636190
N	-0.3396505	-1.7413441	-0.6341170
C	-0.1044057	-0.5549289	-0.2559505
N	-1.0375993	0.4931425	-0.0686699
C	-2.3562198	0.4048112	-0.5574350
N	1.1190407	0.0597204	0.0261058
N	0.9429808	1.3837069	0.3657262
C	-0.3221521	1.6279663	0.2997529
O	-3.0186717	1.3942061	-0.7477382
C	2.4239023	-0.5018663	0.0290708
C	-0.9653729	2.8559852	0.8878208
C	2.6526464	-1.8005451	-0.4309911
C	3.9493059	-2.3105867	-0.4179051
C	5.0344844	-1.5637895	0.0403092
C	4.7774459	-0.2655195	0.4975674
C	3.4963296	0.2669325	0.4980931
O	-1.7826854	2.7331499	1.7568121
O	-0.5474626	4.0563053	0.4742421
C	6.4350932	-2.1262064	0.0491970
C	0.2693884	4.2183230	-0.7179208
C	0.2747526	5.6964063	-1.0478012
H	-5.4688049	-2.7965805	-0.4513087
H	-3.6360093	-4.7134375	-0.5337401
H	-1.4245826	-3.7984864	0.6302648
H	-1.7684048	-2.6651154	-1.7863485
H	-3.4112685	-0.9687066	-1.7149482
H	-4.4152534	-0.6920277	0.7769026
H	-1.9661444	-1.3778248	1.7068780
H	-3.1838822	-2.5680634	2.2272399
H	1.8252247	-2.3958047	-0.7861750
H	4.1116509	-3.3211197	-0.7785131
H	5.5963446	0.3447516	0.8653671
H	3.3167888	1.2694456	0.8589121
H	6.8431263	-2.1624101	1.0642881
H	7.1144424	-1.5123024	-0.5504490
H	6.4577075	-3.1400117	-0.3550957
H	-0.1664278	3.6316700	-1.5308682

H	1.2735826	3.8448717	-0.5139627
H	0.8839961	5.8738928	-1.9379013
H	0.6937444	6.2736787	-0.2213046
H	-0.7381617	6.0540431	-1.2415084

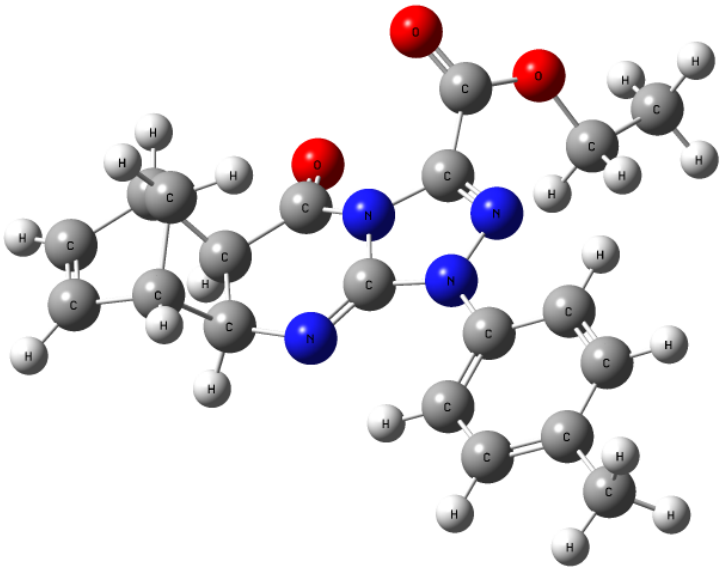


Table S11. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **7c**. (Total energy: RB3LYP/6-31G(d,p): -1384.35253168 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	4.5261290	-2.5100247	0.3766575
C	4.6630921	-1.2214879	0.7037164
C	3.2804631	-0.6968539	1.0635712
C	2.5051758	-0.6443324	-0.3067816
C	2.2912761	-2.1578777	-0.6493553
C	3.0576679	-2.8738702	0.5277669
C	2.6637178	-1.9585561	1.7088133
N	1.2183559	0.0619904	-0.2106790
C	0.0111458	-0.6008249	-0.2859898
N	-0.2273312	-1.8535663	-0.5105303
C	0.8485357	-2.6965988	-0.7274214
O	0.6920529	-3.8749526	-0.9698287
C	0.9362169	1.3985539	0.0139855
N	-0.3417037	1.6097218	0.1005753
N	-0.9352624	0.3923216	-0.0772069
C	-2.3530798	0.2987373	-0.0403418
C	1.8801870	2.5523839	0.1043246
O	1.5512887	3.6369957	0.4995737
O	3.1079801	2.2261697	-0.3343906
C	4.0877012	3.3064753	-0.3277208
C	5.3594746	2.7808688	-0.9570517
C	-3.0843425	1.4648817	0.2271966
C	-4.4676274	1.4128329	0.2713080
C	-5.1088080	0.1982900	0.0487913
C	-4.3942770	-0.9627432	-0.2166918
C	-3.0067847	-0.9198335	-0.2632424
N	-6.5827050	0.1448100	0.0966331
O	-7.1183079	-0.9372926	-0.1035960
O	-7.1799955	1.1871129	0.3339534
H	5.2866968	-3.1728367	-0.0161003
H	5.5555520	-0.6136529	0.6314297
H	3.2458868	0.2356277	1.6234030
H	3.0940450	-0.1328899	-1.0622200
H	2.7488153	-2.4063759	-1.6068242
H	2.8134528	-3.9308556	0.5900168
H	1.5850595	-1.8966555	1.8772734
H	3.1606353	-2.2311281	2.6403560
H	4.2357718	3.6248297	0.7062206
H	3.6687005	4.1480484	-0.8817098
H	6.1114571	3.5736135	-0.9719837
H	5.1838775	2.4579074	-1.9852236
H	5.7636067	1.9393832	-0.3909151
H	-2.5617690	2.3946760	0.3962554

H	-5.0552897	2.2965255	0.4756213
H	-4.9258394	-1.8886543	-0.3851308
H	-2.4294598	-1.8088934	-0.4669163

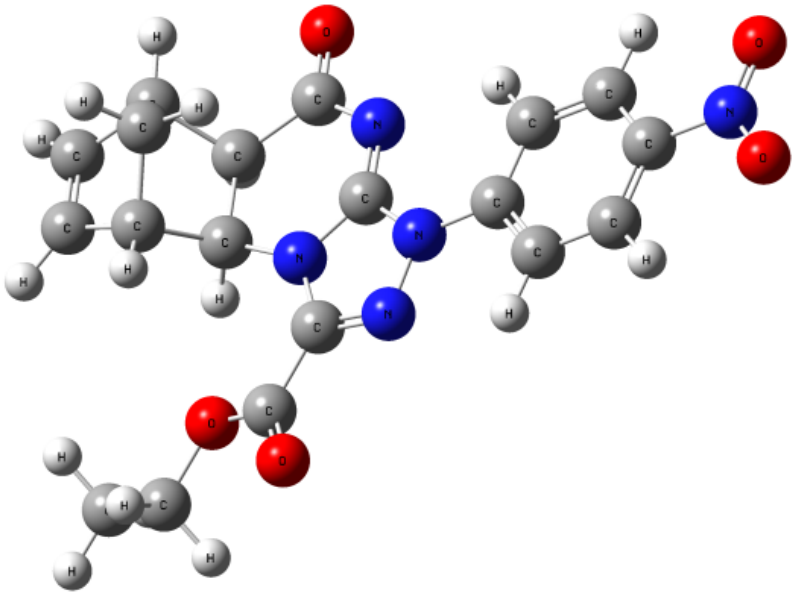


Table S12. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **8c**. (Total energy: RB3LYP/6-31G(d,p): -1384.33444747 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-4.2458640	-3.5410370	-0.1310330
C	-3.1444800	-4.2916390	-0.2301910
C	-1.9726750	-3.4576100	0.2587480
C	-1.7179830	-2.3572340	-0.8454020
C	-3.0321460	-1.4831950	-0.7509280
C	-3.8298840	-2.1897600	0.4291580
C	-2.6673860	-2.6154420	1.3519500
N	-0.4391930	-1.6905860	-0.6256780
C	-0.4480730	-0.4900240	-0.2271940
N	-1.5708150	0.3429880	-0.0160430
C	-2.8585800	-0.0108230	-0.4671960
N	0.6291510	0.3578550	0.0665250
N	0.1847160	1.6197970	0.4304210
C	-1.1016520	1.5921230	0.3707370
O	-3.7192930	0.8238980	-0.5939110
C	2.0096010	0.0823860	0.0489190
C	-1.9883150	2.6675850	0.9560790
C	2.4891370	-1.1638460	-0.3825390
C	3.8557160	-1.4032740	-0.3945360
C	4.7327650	-0.4079630	0.0196600
C	4.2687320	0.8311450	0.4520380
C	2.9067700	1.0782330	0.4682200
O	-2.6542540	2.4073880	1.9175550
O	-1.9430420	3.8891950	0.4245180
N	6.1814740	-0.6679460	0.0009240
O	6.9255140	0.2339210	0.3670670
O	6.5568700	-1.7699410	-0.3803340
C	-1.2888180	4.1408290	-0.8510000
C	-1.6793730	5.5399570	-1.2779520
H	-5.2436900	-3.7815310	-0.4749620
H	-3.0602130	-5.2773500	-0.6696510
H	-1.0630730	-3.9909840	0.5263220
H	-1.6549840	-2.8313030	-1.8258480
H	-3.6210170	-1.5307960	-1.6665190
H	-4.6183090	-1.5662850	0.8461280
H	-2.0646120	-1.7845900	1.7267780
H	-3.0081310	-3.2200850	2.1931420
H	1.7910620	-1.9228510	-0.7005280
H	4.2503270	-2.3541710	-0.7240110
H	4.9776430	1.5821790	0.7709480
H	2.5259140	2.0309250	0.8044370
H	-1.6282260	3.3968480	-1.5765730
H	-0.2099430	4.0437670	-0.7204250

H	-1.2050140	5.7792390	-2.2331370
H	-1.3550620	6.2734000	-0.5373810
H	-2.7613210	5.6206800	-1.3961320

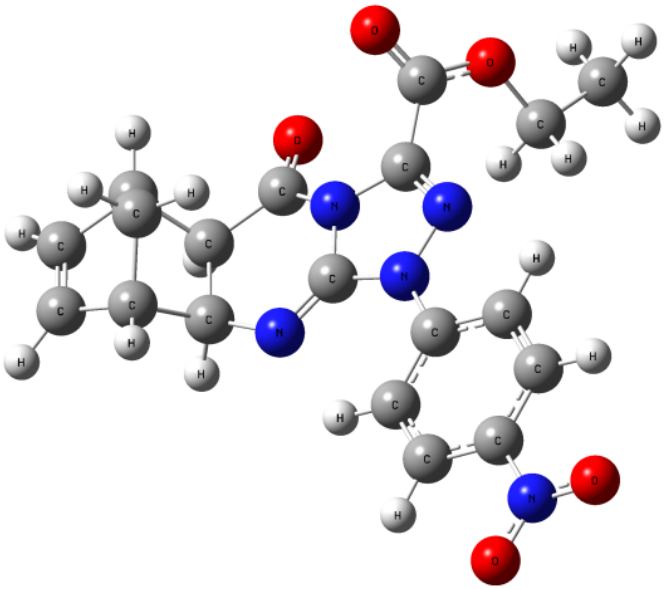


Table S13. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **7d**. (Total energy: RB3LYP/6-31G(d,p): -1351.72359928 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-0.0021560	5.2620430	0.1687660
C	-1.0914900	4.5246920	0.4055810
C	-0.6186450	3.1497360	0.8538540
C	-0.0183830	2.5021460	-0.4498040
C	1.2971710	3.3217690	-0.6800500
C	1.2154770	4.4001830	0.4657690
C	0.6670320	3.5316150	1.6199440
N	0.2791480	1.0678360	-0.3022650
C	1.5699720	0.5760940	-0.2730310
N	2.6916020	1.2166510	-0.3839470
C	2.6484720	2.5819360	-0.5955520
O	3.6643340	3.2370590	-0.7149190
C	-0.5680820	-0.0086950	-0.1900250
N	0.0896400	-1.1251720	-0.0700960
N	1.4151780	-0.7901470	-0.1112290
C	2.4109000	-1.8104540	-0.0182160
C	-2.0612980	0.0591500	-0.2418580
O	-2.6415010	1.1137210	-0.4482000
N	-2.6402310	-1.1579960	-0.0409840
C	-4.0089110	-1.4989870	-0.0305220
C	2.0002740	-3.1466110	0.0448320
C	2.9484650	-4.1545630	0.1423510
C	4.3191030	-3.8710650	0.1783240
C	4.7018560	-2.5313580	0.1122230
C	3.7716140	-1.4990030	0.0149390
C	5.3366410	-4.9807090	0.2786140
C	-4.3276930	-2.8458000	0.1919700
C	-5.6535210	-3.2578280	0.2192770
C	-6.6795620	-2.3346440	0.0255150
C	-6.3598600	-0.9976840	-0.1953970
C	-5.0358570	-0.5669990	-0.2261160
H	0.0383440	6.2586530	-0.2525470
H	-2.1242310	4.7836040	0.2126380
H	-1.3573860	2.5250090	1.3484160
H	-0.7190580	2.5959900	-1.2745820
H	1.2871390	3.8042830	-1.6575500
H	2.1629510	4.9124330	0.6099270
H	1.3081280	2.6825320	1.8742050
H	0.4562530	4.1088050	2.5210750
H	-1.9879210	-1.9177770	0.1066720
H	0.9473230	-3.3860530	0.0168960
H	2.6127540	-5.1856200	0.1903250
H	5.7556150	-2.2746180	0.1364280

H	4.0878120	-0.4685780	-0.0441200
H	5.1546110	-5.6083270	1.1562640
H	6.3504290	-4.5836820	0.3551730
H	5.2992840	-5.6333970	-0.5994740
H	-3.5318740	-3.5684220	0.3437070
H	-5.8835110	-4.3027990	0.3926310
H	-7.7144630	-2.6548140	0.0465520
H	-7.1497170	-0.2708400	-0.3477590
H	-4.7916170	0.4693940	-0.3985960

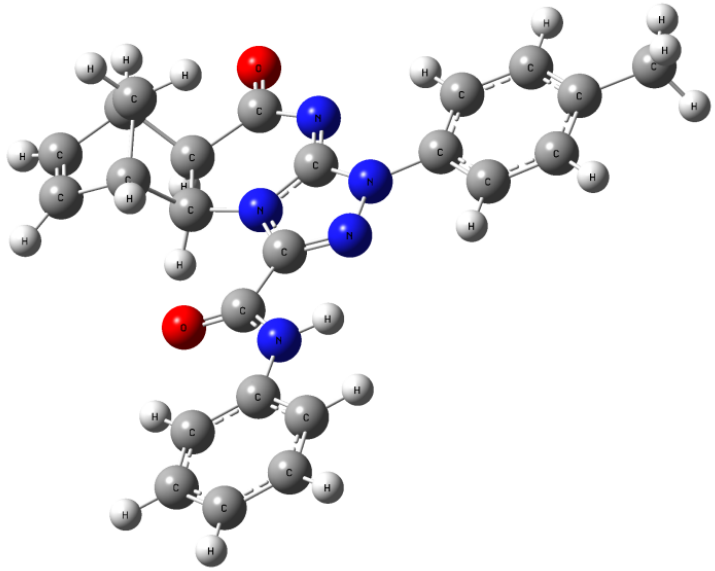


Table S14. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **8d**. (Total energy: RB3LYP/6-31G(d,p): -1351.70014180 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-5.0302124	-2.1130213	0.6044033
C	-4.3185455	-3.2233936	0.8186038
C	-2.8786442	-2.8058566	1.0737084
C	-2.3021573	-2.3070743	-0.3043511
C	-3.1533234	-0.9962275	-0.5535657
C	-4.0800325	-0.9290850	0.7168735
C	-3.1051204	-1.4587660	1.7951614
N	-0.8533213	-2.1748767	-0.2312884
C	-0.3355998	-1.0701041	-0.5762911
N	-1.0084512	0.1154810	-0.9646748
C	-2.3791552	0.2939050	-0.7408236
N	1.0077724	-0.6987603	-0.6301995
N	1.1481764	0.6145843	-1.0360352
C	-0.0370018	1.0830607	-1.2166096
O	-2.8709105	1.3972653	-0.7053058
C	2.1638956	-1.4743845	-0.3527587
C	-0.3154690	2.3774537	-1.9357090
C	2.0654780	-2.8215188	0.0042824
C	3.2266974	-3.5458704	0.2646820
C	4.4938640	-2.9687436	0.1821452
C	4.5647345	-1.6181064	-0.1792352
C	3.4249150	-0.8723669	-0.4438208
O	-0.8696656	2.3480393	-3.0148207
N	0.1795179	3.5140901	-1.3642380
C	5.7438185	-3.7584747	0.4860605
C	0.5512748	3.7168363	-0.0034596
C	-0.2971532	3.3169635	1.0319863
C	0.0794985	3.5354589	2.3547561
C	1.2799565	4.1782130	2.6490623
C	2.1110822	4.5989187	1.6121862
C	1.7543834	4.3619586	0.2881490
H	-6.0676484	-2.0418477	0.3027717
H	-4.6586437	-4.2474227	0.7292970
H	-2.2273744	-3.5354003	1.5503356
H	-2.5175037	-3.0446277	-1.0811041
H	-3.7581933	-1.0893941	-1.4590260
H	-4.5280076	0.0507678	0.8653342
H	-2.1933018	-0.8634173	1.9017320
H	-3.5807976	-1.5749724	2.7698940
H	1.0941585	-3.2866758	0.0745790
H	3.1335550	-4.5919364	0.5384873
H	5.5337629	-1.1351561	-0.2576930
H	3.4979256	0.1683913	-0.7243490

H	0.1075150	4.3275897	-1.9621470
H	6.5094847	-3.6044157	-0.2796393
H	5.5339705	-4.8286908	0.5400119
H	6.1797544	-3.4583316	1.4451006
H	-1.2528602	2.8646211	0.7935401
H	-0.5789519	3.2200860	3.1560588
H	1.5644240	4.3550050	3.6797725
H	3.0457527	5.1012326	1.8336691
H	2.4086272	4.6598806	-0.5231768

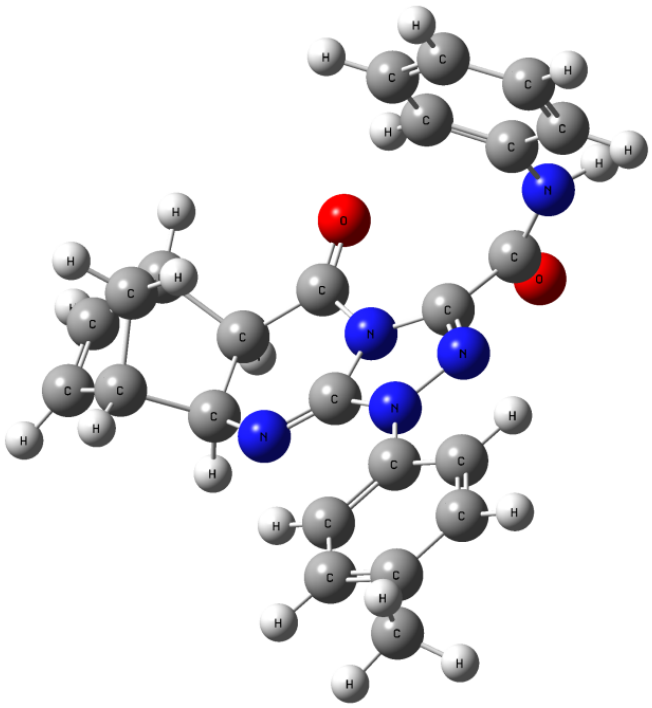


Table S15. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **7e**. (Total energy: RB3LYP/6-31G(d,p): -1104.55203654 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	4.8113018	-1.3100399	0.1349454
C	4.7071549	0.0004924	0.3756049
C	3.2815255	0.2633008	0.8377381
C	2.4093498	0.0613396	-0.4572869
C	2.4735649	-1.4869653	-0.6890078
C	3.4660404	-1.9482344	0.4447387
C	2.9898929	-1.0457499	1.6050832
N	1.0176408	0.5087386	-0.2984462
C	-0.0433870	-0.3691856	-0.2665690
N	-0.0437414	-1.6610938	-0.3762558
C	1.1645159	-2.2984215	-0.5900553
O	1.2330355	-3.5057127	-0.7034795
C	0.4993584	1.7839545	-0.1897117
N	-0.7988380	1.7573314	-0.0674864
N	-1.1566927	0.4446814	-0.1048368
C	-2.5366071	0.0835903	-0.0022142
C	1.2686389	3.0526515	-0.2565018
O	2.4675571	3.0350753	-0.4545998
C	0.4841587	4.3299145	-0.0730620
C	-3.4817651	1.1000533	0.1715027
C	-4.8274512	0.7769133	0.2731240
C	-5.2701077	-0.5492164	0.2058176
C	-4.3059267	-1.5439175	0.0369991
C	-2.9489686	-1.2490632	-0.0684209
C	-6.7391035	-0.8828045	0.2900807
H	5.6553721	-1.8341251	-0.2954703
H	5.4384630	0.7728119	0.1766453
H	3.1056213	1.2115113	1.3389746
H	2.8304691	0.6232248	-1.2865134
H	2.8864843	-1.7148541	-1.6719623
H	3.4479615	-3.0253255	0.5873145
H	1.9375720	-1.1873973	1.8679414
H	3.6044775	-1.1463337	2.5004353
H	1.1594264	5.1729129	-0.2088565
H	0.0431314	4.3629412	0.9267455
H	-0.3411532	4.3846290	-0.7859315
H	-3.1569754	2.1288676	0.2278723
H	-5.5483627	1.5764361	0.4101861
H	-4.6131907	-2.5831751	-0.0139149
H	-2.2170082	-2.0317854	-0.1982899
H	-7.2475450	-0.2606893	1.0311949
H	-6.8945615	-1.9287161	0.5620755
H	-7.2366148	-0.7151101	-0.6714644

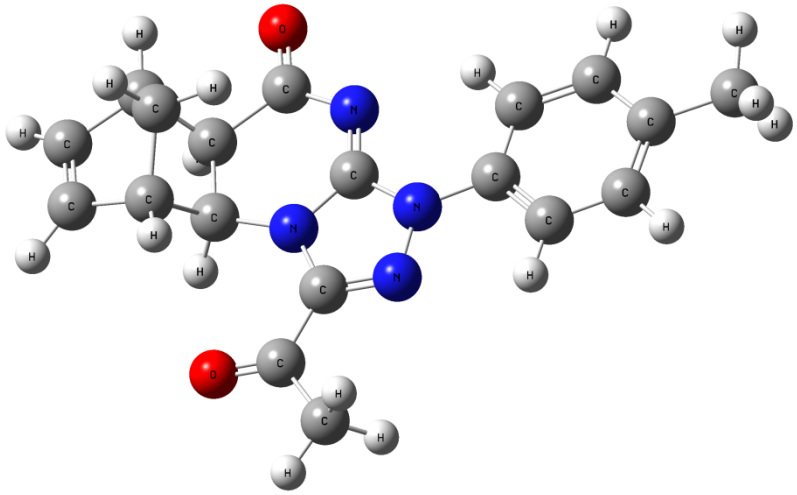

O
H
C
N
O

Table S16. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **8e**. (Total energy: RB3LYP/6-31G(d,p): -1104.53724342 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-4.3937373	-2.3644605	0.1670495
C	-3.4585828	-3.3178045	0.2272600
C	-2.1435821	-2.6501680	0.5913162
C	-1.6925734	-1.8272237	-0.6798198
C	-2.8155291	-0.7214816	-0.7760777
C	-3.7194172	-1.0404510	0.4921109
C	-2.6530593	-1.5128866	1.5042869
N	-0.3150926	-1.3751128	-0.5428237
C	-0.1051825	-0.1456200	-0.3217729
N	-1.0526762	0.9052420	-0.2552891
C	-2.3615099	0.7204588	-0.7657599
N	1.1164360	0.5162316	-0.1371659
N	0.9274539	1.8609378	0.0327585
C	-0.3449942	2.0889947	-0.0419090
O	-3.0309111	1.6444295	-1.1464977
C	2.4288744	-0.0273104	-0.0742825
C	-0.9399191	3.4057814	0.3537291
C	2.6618455	-1.3873533	-0.2897490
C	3.9647058	-1.8767578	-0.2185437
C	5.0520888	-1.0497290	0.0612183
C	4.7913595	0.3101640	0.2710147
C	3.5046877	0.8241205	0.2073606
O	-2.0135758	3.4393788	0.9068201
C	-0.1037593	4.6254876	0.0561531
C	6.4593833	-1.5894614	0.1380553
H	-5.4215230	-2.4659710	-0.1576281
H	-3.5701822	-4.3623205	-0.0348472
H	-1.3501711	-3.2913928	0.9695710
H	-1.7248404	-2.4700633	-1.5608959
H	-3.4126374	-0.8234830	-1.6813839
H	-4.3693399	-0.2147743	0.7758544
H	-1.8983089	-0.7605435	1.7434585
H	-3.0973535	-1.8849346	2.4285227
H	1.8332065	-2.0432057	-0.5084496
H	4.1296074	-2.9358658	-0.3879714
H	5.6126681	0.9849454	0.4911149
H	3.3233788	1.8760911	0.3734113
H	-0.1605728	4.8433756	-1.0155625
H	0.9462626	4.4528140	0.2973708
H	-0.4973053	5.4731275	0.6151780
H	6.9006077	-1.4100333	1.1235394
H	7.1104266	-1.1099182	-0.5996808
H	6.4825310	-2.6651984	-0.0463813

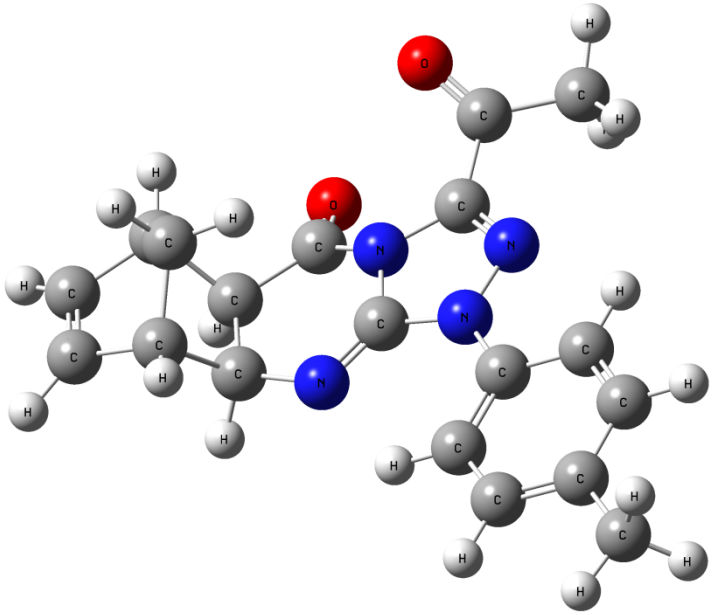

O
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Table S17. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **7f**. (Total energy: RB3LYP/6-31G(d,p): -1294.35382015 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
Symbol	X	Y	Z
C	4.8929933	-2.1485815	0.2243986
C	4.8760237	-0.8353534	0.4727818
C	3.4594802	-0.4730808	0.8934772
C	2.6155271	-0.6030318	-0.4300635
C	2.5755598	-2.1504672	-0.6726573
C	3.4962032	-2.6891917	0.4871662
C	3.0503224	-1.7621454	1.6401230
N	1.2553600	-0.0582818	-0.3085742
C	0.1344028	-0.8598307	-0.3019738
N	0.0463210	-2.1495728	-0.4228154
C	1.2089774	-2.8674719	-0.6195534
O	1.1975187	-4.0754947	-0.7511156
C	0.8210214	1.2478080	-0.1977812
N	-0.4749287	1.3139094	-0.0996303
N	-0.9185964	0.0272331	-0.1533076
C	-2.3220501	-0.2360920	-0.0645143
C	1.7122216	2.4315863	-0.2437017
O	2.9074565	2.3558528	-0.4206633
O	1.0314800	3.5656956	-0.0763700
C	1.8088333	4.7928255	-0.1282456
C	0.8415466	5.9436692	0.0480305
C	-3.1921847	0.8385450	0.1136257
C	-4.5644887	0.6244364	0.2057097
C	-5.0783498	-0.6726286	0.1209975
C	-4.1975285	-1.7444137	-0.0576945
C	-2.8305555	-1.5389939	-0.1510890
O	-6.4000136	-0.9916705	0.2001546
C	-7.3407215	0.0566385	0.3848347
H	5.7098227	-2.7293990	-0.1853166
H	5.6667880	-0.1167057	0.3018406
H	3.3368506	0.4823448	1.3969896
H	3.1015694	-0.0677754	-1.2412461
H	3.0014627	-2.4018609	-1.6441940
H	3.3955581	-3.7630070	0.6196716
H	1.9831560	-1.8292694	1.8698723
H	3.6281907	-1.9127229	2.5528510
H	2.3304649	4.8319342	-1.0868675
H	2.5614994	4.7588562	0.6625697
H	1.3868211	6.8903348	0.0161057
H	0.3251165	5.8749690	1.0074665
H	0.0942962	5.9485794	-0.7478448
H	-2.7946014	1.8411044	0.1795655

H	-5.2157540	1.4766428	0.3437152
H	-4.6069777	-2.7448528	-0.1225745
H	-2.1541684	-2.3691093	-0.2891525
H	-8.3170961	-0.4235133	0.4206729
H	-7.3185007	0.7682188	-0.4481867
H	-7.1665242	0.5917910	1.3250855

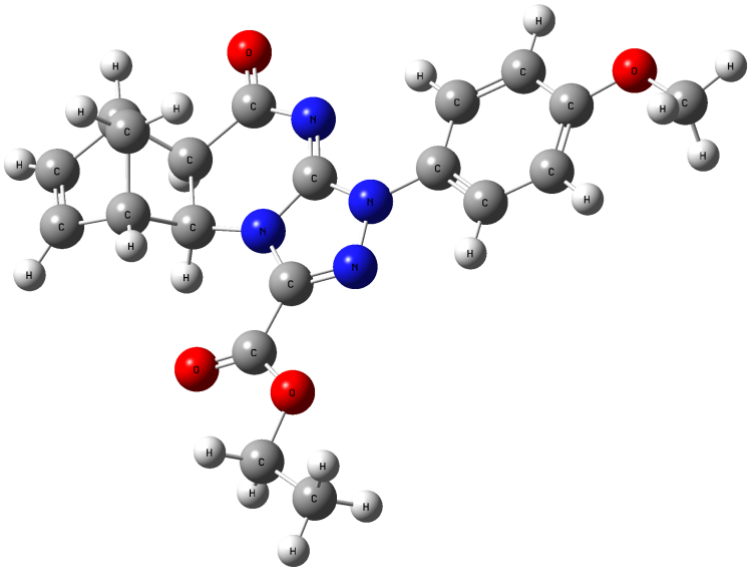


Table S18. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **8f**. (Total energy: RB3LYP/6-31G(d,p): -1294.32986623 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-3.9353200	-3.6536210	-0.0855830
C	-2.8088280	-4.3686870	-0.1666850
C	-1.6652670	-3.4803550	0.2920890
C	-1.4498830	-2.4034540	-0.8437500
C	-2.7950650	-1.5752640	-0.7717720
C	-3.5640570	-2.2725120	0.4322980
C	-2.3854050	-2.6311630	1.3629940
N	-0.1978400	-1.6853650	-0.6452850
C	-0.2530410	-0.4793610	-0.2568560
N	-1.4084850	0.3158720	-0.0637920
C	-2.6725700	-0.0887540	-0.5347190
N	0.7882260	0.4057080	0.0282760
N	0.3054820	1.6505940	0.3645790
C	-0.9821700	1.5893050	0.3006180
O	-3.5580620	0.7103270	-0.7123670
C	2.1884660	0.1597160	0.0563850
C	-1.8950630	2.6375430	0.8786560
C	2.7246150	-1.0285240	-0.4374940
C	4.1030940	-1.2436600	-0.3969590
C	4.9552220	-0.2742470	0.1316080
C	4.4082680	0.9173730	0.6240980
C	3.0427200	1.1345410	0.5916510
O	-2.6562550	2.3397660	1.7561280
O	-1.7752770	3.8962290	0.4433280
O	6.3117960	-0.3859750	0.2163940
C	6.9214840	-1.5785890	-0.2555130
C	-1.0248670	4.2267340	-0.7573250
C	-1.3894090	5.6499950	-1.1251870
H	-4.9247730	-3.9377180	-0.4207990
H	-2.6926360	-5.3627710	-0.5796570
H	-0.7363820	-3.9727780	0.5718830
H	-1.3738630	-2.9045290	-1.8101790
H	-3.3846240	-1.6720020	-1.6829180
H	-4.3721230	-1.6644500	0.8344320
H	-1.8105240	-1.7696850	1.7103800
H	-2.7035010	-3.2222870	2.2227910
H	2.0670620	-1.7832120	-0.8418890
H	4.4903670	-2.1757050	-0.7854420
H	5.0779970	1.6619880	1.0364540
H	2.6273870	2.0535290	0.9795980
H	7.9896940	-1.4537990	-0.0859850
H	6.7407220	-1.7268660	-1.3262120
H	6.5680970	-2.4566060	0.2969500

H	-1.2987890	3.5292150	-1.5531740
H	0.0408050	4.1217200	-0.5499550
H	-0.8429340	5.9506620	-2.0229510
H	-1.1294040	6.3355580	-0.3163300
H	-2.4594010	5.7372020	-1.3226150

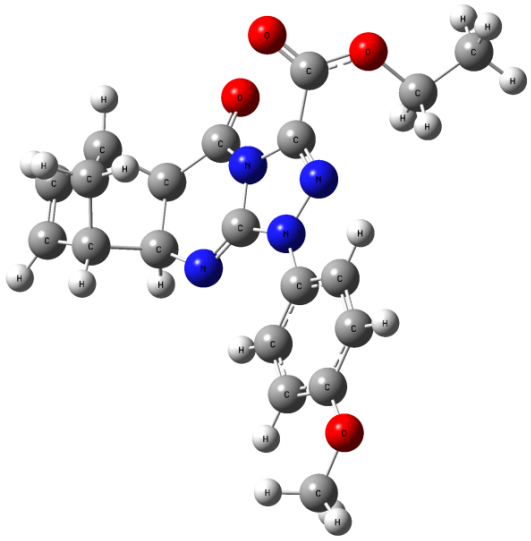


Table S19. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **7g**. (Total energy: RB3LYP/6-31G(d,p): -1639.41790070 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	4.2975038	-2.5266354	0.3542165
C	4.4423542	-1.2399205	0.6853001
C	3.0636693	-0.7091607	1.0510917
C	2.2841313	-0.6480015	-0.3166239
C	2.0606569	-2.1592202	-0.6629472
C	2.8276218	-2.8831112	0.5085898
C	2.4422327	-1.9697348	1.6940036
N	1.0023619	0.0651701	-0.2146223
C	-0.2091379	-0.5906174	-0.2863315
N	-0.4544132	-1.8444336	-0.5122934
C	0.6138510	-2.6904265	-0.7356000
O	0.4540439	-3.8691324	-0.9803453
C	0.7272896	1.4033554	0.0106341
N	-0.5514398	1.6165973	0.1002561
N	-1.1481382	0.4040622	-0.0747790
C	-2.5722750	0.3140858	-0.0312947
C	1.6726274	2.5532268	0.0961052
O	1.3441675	3.6474277	0.4662531
O	2.9087917	2.2157598	-0.3146995
C	3.8894152	3.2934465	-0.3084424
C	5.1757286	2.7518768	-0.8936580
C	-3.3002757	1.4752418	0.2485722
C	-4.6867745	1.4271799	0.2989086
C	-5.3409306	0.2206845	0.0709793
C	-4.6235997	-0.9354388	-0.2068570
C	-3.2333188	-0.8959630	-0.2601583
Cl	-7.0974114	0.1618861	0.1361593
H	5.0532520	-3.1916752	-0.0442266
H	5.3376450	-0.6364711	0.6107643
H	3.0355366	0.2218621	1.6134890
H	2.8744623	-0.1378957	-1.0720056
H	2.5127690	-2.4073574	-1.6231131
H	2.5776038	-3.9389172	0.5678035
H	1.3643978	-1.9025214	1.8651725
H	2.9404431	-2.2480374	2.6232847
H	4.0133713	3.6362349	0.7209134
H	3.4869701	4.1232367	-0.8919124
H	5.9293394	3.5431349	-0.9090639
H	5.0250058	2.4042444	-1.9177604
H	5.5641301	1.9237013	-0.2977010
H	-2.7781801	2.4048011	0.4231755
H	-5.2544704	2.3227664	0.5147530
H	-5.1421012	-1.8687420	-0.3830893

H	-2.6634174	-1.7878460	-0.4737151

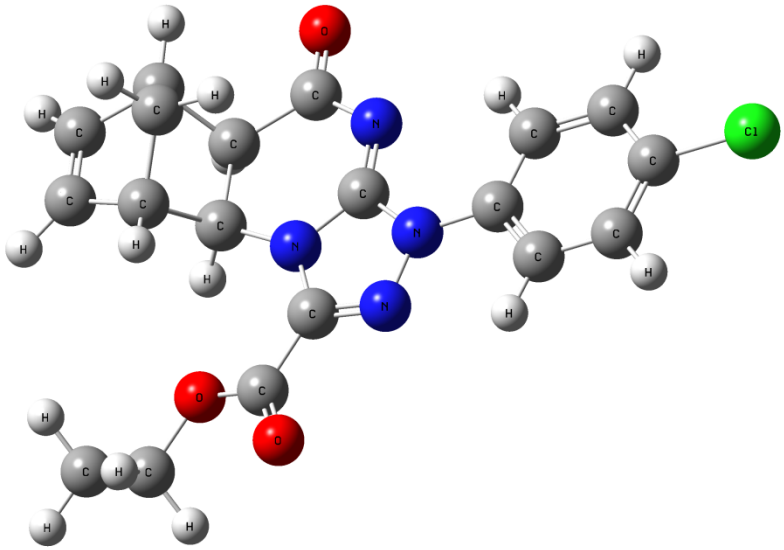


Table S20. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **8g**. (Total energy: RB3LYP/6-31G(d,p): -1639.39858952 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-4.2130670	-3.3767830	-0.1386770
C	-3.1463490	-4.1780560	-0.2204200
C	-1.9413920	-3.3920720	0.2677620
C	-1.6300430	-2.3170640	-0.8468540
C	-2.9028990	-1.3818330	-0.7686050
C	-3.7405550	-2.0398530	0.4107860
C	-2.6052840	-2.5079100	1.3470630
N	-0.3233080	-1.7077610	-0.6315700
C	-0.2792040	-0.5049980	-0.2366420
N	-1.3649810	0.3788820	-0.0310890
C	-2.6622360	0.0836900	-0.4946250
N	0.8321480	0.2927180	0.0525510
N	0.4491480	1.5715680	0.4082480
C	-0.8381660	1.6082120	0.3490910
O	-3.4830370	0.9550310	-0.6397960
C	2.2059210	-0.0515180	0.0413790
C	-1.6684420	2.7220810	0.9371920
C	2.6316890	-1.3032090	-0.4166570
C	3.9890610	-1.6101360	-0.4218910
C	4.9139520	-0.6755320	0.0244880
C	4.4981340	0.5701110	0.4828100
C	3.1454420	0.8830390	0.4932160
O	-2.3971850	2.4845060	1.8587080
O	-1.5081720	3.9573440	0.4563750
Cl	6.6293800	-1.0686890	0.0122930
C	-0.7901500	4.2089900	-0.7833960
C	-1.0914930	5.6378590	-1.1841810
H	-5.2178910	-3.5752550	-0.4892130
H	-3.1041090	-5.1711220	-0.6494540
H	-1.0582290	-3.9623670	0.5476860
H	-1.5878180	-2.8054890	-1.8215540
H	-3.4872570	-1.4084090	-1.6880120
H	-4.5031310	-1.3775530	0.8160160
H	-1.9689030	-1.7006510	1.7176070
H	-2.9791840	-3.0877440	2.1918060
H	1.9036650	-2.0226270	-0.7599040
H	4.3217530	-2.5771990	-0.7761130
H	5.2250520	1.2914440	0.8326620
H	2.8124040	1.8461760	0.8513800
H	-1.1343550	3.5035970	-1.5442410
H	0.2759260	4.0520530	-0.6131030
H	-0.5664680	5.8791170	-2.1120980
H	-0.7620820	6.3330760	-0.4096660

H	-2.1622380	5.7776360	-1.3430660

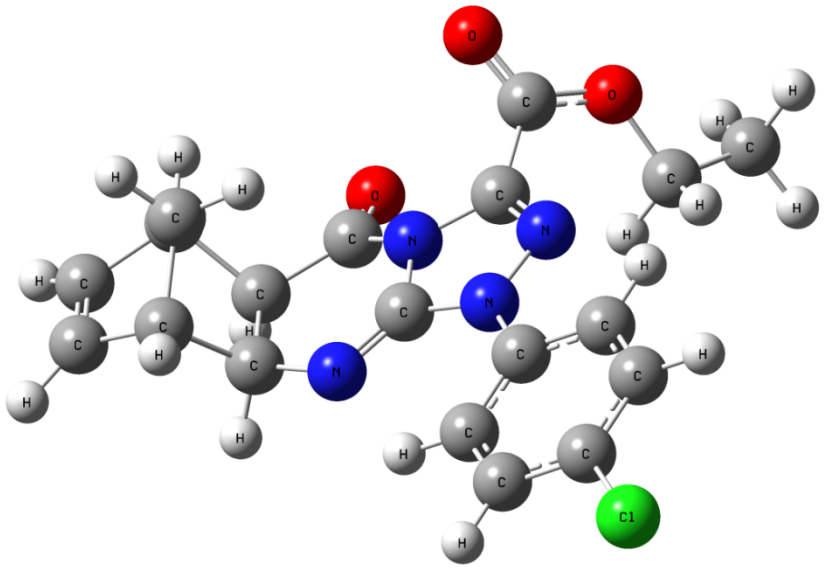


Table S21. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **7h**. (Total energy: RB3LYP/6-31G(d,p): -1516.93409180 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-3.9522560	3.1690920	0.3203260
C	-4.4165750	1.9531900	0.6241600
C	-3.2230920	1.1027390	1.0339620
C	-2.4267380	0.8632470	-0.3054810
C	-1.8322190	2.2786990	-0.6182830
C	-2.4474390	3.1583150	0.5357020
C	-2.3419500	2.1709490	1.7194020
N	-1.3589740	-0.1382920	-0.1692370
C	-0.0232900	0.2066250	-0.1904260
N	0.5261280	1.3638980	-0.3871470
C	-0.2983590	2.4464580	-0.6307710
O	0.1497490	3.5531550	-0.8472620
C	-1.4230460	-1.5042700	0.0462390
N	-0.2387320	-2.0220240	0.1760760
N	0.6396290	-0.9879670	0.0375610
C	2.0398290	-1.2453530	0.1295510
C	-2.6229520	-2.3898450	0.0827460
O	-2.5911570	-3.5234560	0.4774360
O	-3.7131710	-1.7702810	-0.4038600
C	-4.9277100	-2.5740140	-0.4516130
C	-5.9934180	-1.7569760	-1.1492620
C	2.4549370	-2.5507290	0.4219070
C	3.8101310	-2.8324860	0.5141780
C	4.7612030	-1.8323910	0.3216130
C	4.3334130	-0.5410890	0.0327800
C	2.9765250	-0.2308360	-0.0674330
C	5.3277700	0.5734990	-0.1642090
F	5.2531270	1.4897530	0.8268770
F	5.1163110	1.2351310	-1.3217640
F	6.6012190	0.1229530	-0.1894810
H	-4.5083950	3.9999490	-0.0949960
H	-5.4273950	1.5846580	0.5068360
H	-3.4435340	0.1892570	1.5828860
H	-3.0915950	0.5166870	-1.0909840
H	-2.1730710	2.6354740	-1.5901540
H	-1.9523950	4.1217630	0.6216130
H	-1.3200980	1.8438220	1.9299660
H	-2.7948160	2.5555100	2.6338960
H	-5.2058130	-2.8325360	0.5723480
H	-4.7025080	-3.5005560	-0.9822490
H	-6.9198190	-2.3343710	-1.2002110
H	-5.6907080	-1.5066180	-2.1681140
H	-6.1984000	-0.8304420	-0.6092870

H	1.7137820	-3.3227740	0.5695520
H	4.1277060	-3.8436790	0.7386770
H	5.8177540	-2.0525990	0.3913700
H	2.6450660	0.7723070	-0.2936340

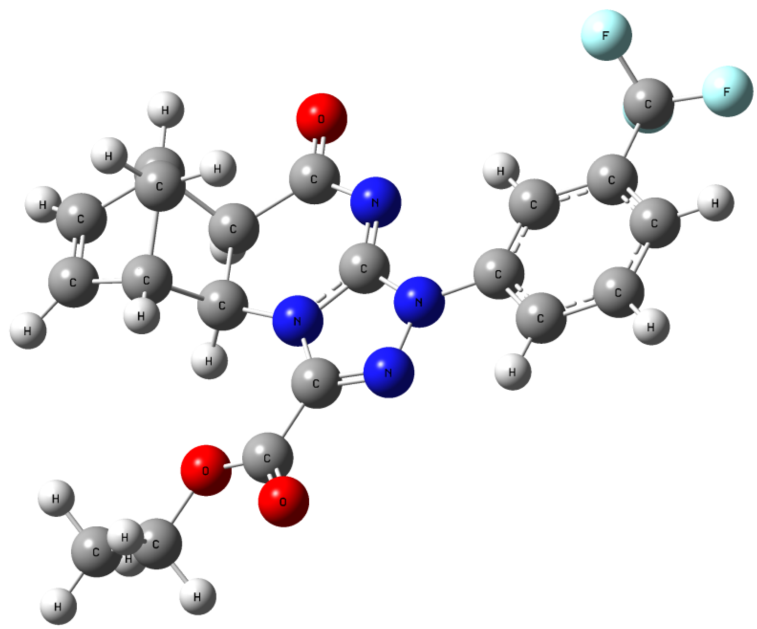


Table S22. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **8h**. (Total energy: RB3LYP/6-31G(d,p): -1516.91590448 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-5.5429812	-2.0385640	0.1662884
C	-4.8055423	-3.1412751	0.0018963
C	-3.3696700	-2.7912241	0.3524158
C	-2.8385256	-1.8659905	-0.8126881
C	-3.7265969	-0.5697140	-0.6351103
C	-4.6120040	-0.9309107	0.6346600
C	-3.6020720	-1.7485010	1.4685614
N	-1.3902832	-1.7154707	-0.7342068
C	-0.9227081	-0.5978882	-0.3652866
N	-1.6388975	0.5877103	-0.0783150
C	-2.9989284	0.7358050	-0.4183923
N	0.4093558	-0.2083669	-0.1875642
N	0.4951380	1.1198302	0.1857463
C	-0.7104357	1.5728138	0.2389099
O	-3.5008168	1.8280125	-0.5092995
C	1.5887531	-0.9819170	-0.3008060
C	-1.0817894	2.8819185	0.8913791
C	1.5457545	-2.2999404	-0.7707886
C	2.7295105	-3.0243375	-0.8756280
C	3.9513915	-2.4634461	-0.5226091
C	3.9790291	-1.1493733	-0.0566023
C	2.8107075	-0.4045911	0.0586746
O	-1.7789989	2.8682454	1.8664069
O	-0.5603265	4.0088323	0.4036496
C	0.1149100	4.0485398	-0.8847316
C	0.2743018	5.5088281	-1.2522148
C	5.2803414	-0.5382649	0.3886844
F	5.5015997	-0.7410511	1.7086627
F	6.3380790	-1.0632782	-0.2671235
F	5.3107816	0.7982162	0.1922024
H	-6.5877162	-1.8984945	-0.0803345
H	-5.1287729	-4.0912336	-0.4044831
H	-2.6950639	-3.6191390	0.5598860
H	-3.0509568	-2.3331137	-1.7754123
H	-4.3751901	-0.3973492	-1.4935302
H	-5.0756561	-0.0604236	1.0945641
H	-2.7058213	-1.1938201	1.7563895
H	-4.0573674	-2.1831252	2.3592515
H	0.5968198	-2.7359279	-1.0443515
H	2.6912748	-4.0428609	-1.2436641
H	4.8695800	-3.0284958	-0.6127695
H	2.8398203	0.6135438	0.4161906
H	-0.4937935	3.5184349	-1.6219797

H	1.0788074	3.5459089	-0.7944246
H	0.7854116	5.5928475	-2.2147588
H	0.8665297	6.0327774	-0.4996533
H	-0.6987761	5.9970425	-1.3299456

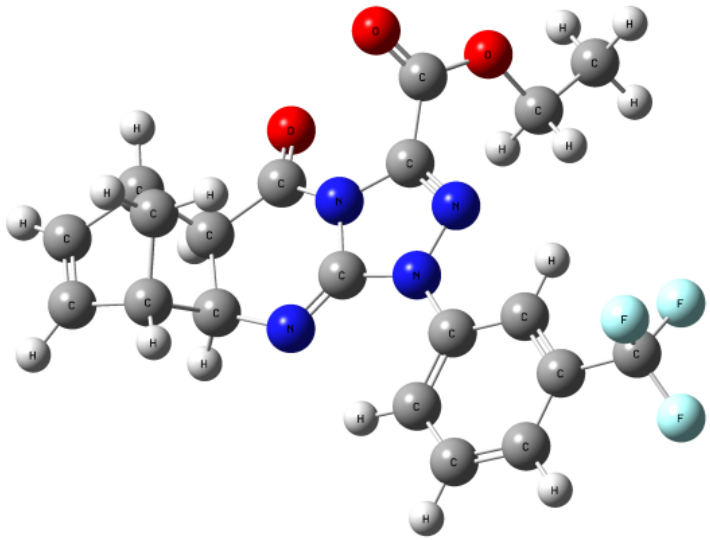


Table S23. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **11a**. (Total energy: RB3LYP/6-31G(d,p): -1179.79664465 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-3.0060620	-1.2737260	1.7474130
C	-2.6092390	0.0026850	1.7854550
C	-3.0825320	0.6699410	0.5030440
C	-2.2340990	0.0706250	-0.6772420
C	-2.6689600	-1.4308450	-0.7083740
C	-3.7497490	-1.4867350	0.4379200
N	-0.7798070	0.1950510	-0.5097220
C	0.0326230	-0.9096770	-0.3594350
N	-0.2763400	-2.1680960	-0.3582770
C	-1.6023790	-2.5199430	-0.5296760
C	-4.4031210	-0.0986870	0.2601150
C	0.0301270	1.3117030	-0.4625090
N	1.2775200	0.9845120	-0.2844750
N	1.3062270	-0.3779200	-0.2166870
O	-1.9584410	-3.6813940	-0.5322300
C	2.5567670	-1.0490650	-0.0434600
C	2.6191040	-2.4382550	0.1044230
C	3.8618000	-3.0441050	0.2741450
C	5.0315790	-2.2911810	0.2988680
C	4.9554110	-0.9077110	0.1495190
C	3.7267650	-0.2819180	-0.0218560
C	-0.4740140	2.6908080	-0.7331320
O	0.2562560	3.7572050	-0.3947780
O	-1.5400180	2.8402420	-1.2805460
C	1.4708600	3.7490110	0.4075440
C	1.7162510	5.1830900	0.8284860
H	-2.7636180	-2.0584540	2.4517840
H	-1.9851900	0.4709680	2.5358280
H	-3.1246220	1.7561750	0.4909260
H	-2.4938930	0.5825770	-1.6010110
H	-3.1588630	-1.6469950	-1.6601480
H	-4.3784690	-2.3709300	0.3745060
H	-5.1507210	0.1204620	1.0236090
H	-4.8311150	0.0631990	-0.7336440
H	1.7103300	-3.0199060	0.0762980
H	3.9053300	-4.1212480	0.3867550
H	5.8576210	-0.3069130	0.1636200
H	3.6658530	0.7897420	-0.1410810
H	1.3349160	3.0918050	1.2676510
H	2.2872430	3.3573960	-0.1986520
H	2.6308160	5.2390860	1.4248590
H	1.8330580	5.8279900	-0.0444920
H	0.8866060	5.5605780	1.4293190

H	5.9923330	-2.7748680	0.4309420

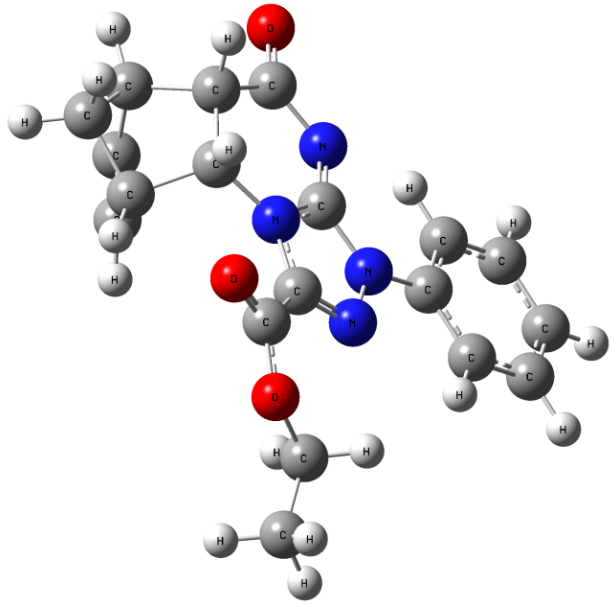


Table S24. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **12a**. (Total energy: RB3LYP/6-31G(d,p): -1179.77717111 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	3.1992365	-0.8118762	1.6456559
C	2.5028655	-1.9518261	1.7091065
C	2.7351461	-2.7082352	0.4104491
C	1.9652191	-1.9268223	-0.7144874
C	2.7774070	-0.5734331	-0.7838101
C	3.9039590	-0.7784385	0.2955362
C	4.1866734	-2.2845858	0.0941810
N	0.5348100	-1.8656238	-0.4635230
C	-0.0164571	-0.7252251	-0.4841900
N	0.6052693	0.5366642	-0.6639626
C	1.9987440	0.7047368	-0.5716914
N	-1.3605992	-0.3873882	-0.3002489
N	-1.5445132	0.9790164	-0.3655045
C	-0.3869750	1.5071272	-0.5708438
O	2.4852362	1.7837947	-0.3434885
C	-2.4823642	-1.2381073	-0.1167261
C	-0.1891022	2.9431140	-0.9841093
C	-2.3187526	-2.6170683	0.0558223
C	-3.4438745	-3.4180768	0.2363017
C	-4.7222655	-2.8687182	0.2491420
C	-4.8728340	-1.4940100	0.0753856
C	-3.7649980	-0.6757888	-0.1085579
O	0.2922481	3.1880047	-2.0542205
O	-0.6283421	3.9056193	-0.1672452
C	-1.0050657	3.6303983	1.2098393
C	-1.1099523	4.9683549	1.9118697
H	3.1977143	0.0031588	2.3575426
H	1.8142919	-2.2567153	2.4856632
H	2.5045512	-3.7721886	0.4203592
H	2.1019704	-2.4695109	-1.6550280
H	3.2360515	-0.4677951	-1.7725294
H	4.7330301	-0.0816567	0.1960202
H	4.5092066	-2.5399161	-0.9199798
H	4.9047435	-2.6731083	0.8176155
H	-1.3270393	-3.0423841	0.0389537
H	-3.3101002	-4.4859432	0.3679966
H	-5.8617223	-1.0496130	0.0784904
H	-3.8806807	0.3889661	-0.2494371
H	-0.2393154	3.0008299	1.6705638
H	-1.9542509	3.0928928	1.2172856
H	-1.3992286	4.8165640	2.9550869
H	-1.8626705	5.5970119	1.4322923
H	-0.1535417	5.4937799	1.8880268

H	-5.5905713	-3.5015199	0.3901419

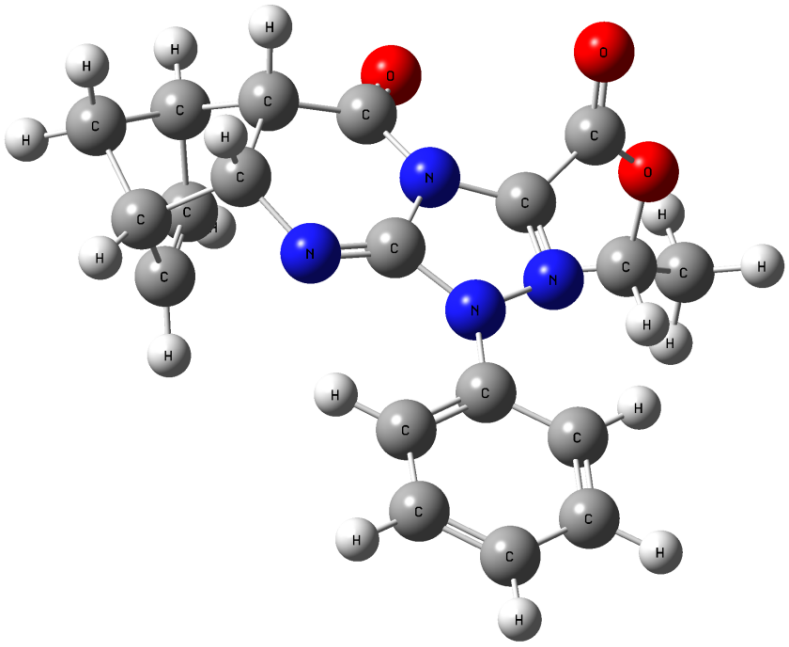


Table S25. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **11c**. (Total energy: RB3LYP/6-31G(d,p): -1384.35287581 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-2.3269029	-2.6816684	1.6659049
C	-2.5055626	-1.3978878	1.9941914
C	-3.4049871	-0.7756529	0.9369537
C	-2.5742472	-0.6829433	-0.3952934
C	-2.3236756	-2.1814052	-0.7667115
C	-3.0967635	-2.9404644	0.3800543
C	-4.2957355	-1.9876630	0.5768851
N	-1.3097734	0.0529645	-0.2754514
C	-0.0907243	-0.5876748	-0.3677485
N	0.1757329	-1.8228699	-0.6496262
C	-0.8790632	-2.6842986	-0.8933411
O	-0.6975440	-3.8471739	-1.1900662
C	-1.0533230	1.3824476	0.0067411
N	0.2198352	1.6124041	0.1130520
N	0.8361869	0.4135209	-0.1092766
C	2.2549007	0.3444556	-0.0674937
C	-2.0199713	2.5138092	0.1275279
O	-1.7254003	3.5829742	0.5866992
O	-3.2270947	2.1884771	-0.3674266
C	-4.2288447	3.2475560	-0.3366236
C	-5.4865482	2.7111944	-0.9852885
C	2.9636448	1.5131490	0.2462777
C	4.3473808	1.4847263	0.2963561
C	5.0120880	0.2909794	0.0336536
C	4.3201528	-0.8724522	-0.2775073
C	2.9324255	-0.8531664	-0.3302816
N	6.4862047	0.2626732	0.0874917
O	7.0427724	-0.8014422	-0.1492028
O	7.0633470	1.3062760	0.3658923
H	-1.6726867	-3.3973933	2.1456955
H	-2.0333882	-0.8559360	2.8032892
H	-3.9019752	0.1549877	1.2008615
H	-3.1667200	-0.1839259	-1.1594334
H	-2.8039242	-2.4068441	-1.7209455
H	-3.2940035	-3.9798225	0.1314638
H	-4.8959682	-1.8439494	-0.3268414
H	-4.9413124	-2.2831031	1.4049136
H	-3.8253384	4.1116685	-0.8672174
H	-4.3878039	3.5365312	0.7042110
H	-6.2543886	3.4887252	-0.9865345

H	-5.8775054	1.8491453	-0.4407310
H	-5.2990258	2.4162671	-2.0198250
H	2.4233709	2.4266378	0.4458010
H	4.9176831	2.3710405	0.5355706
H	4.8694135	-1.7818668	-0.4763479
H	2.3721658	-1.7441442	-0.5699627

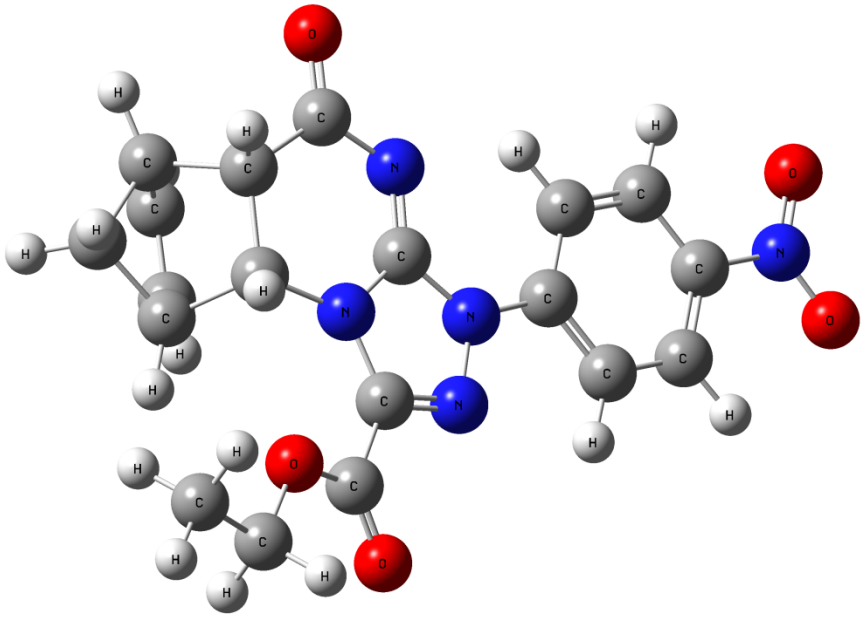


Table S26. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **12c**. (Total energy: RB3LYP/6-31G(d,p): -1384.33532821 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	3.0887073	-2.1965586	1.7125855
C	1.9306182	-2.8654478	1.7104573
C	1.8451248	-3.6367067	0.4026867
C	1.6074981	-2.5776697	-0.7336255
C	2.9716506	-1.7815814	-0.7300574
C	3.7984260	-2.5016825	0.3995235
C	3.3381449	-3.9584977	0.1680841
N	0.3710745	-1.8342791	-0.5433118
C	0.4396713	-0.5716684	-0.5446550
N	1.5950209	0.2380142	-0.6622669
C	2.8965671	-0.2859703	-0.5275865
N	-0.5882475	0.3714374	-0.4007417
N	-0.0885409	1.6630575	-0.4392021
C	1.1873161	1.5645422	-0.5868705
O	3.8308953	0.4298927	-0.2719798
C	-1.9734734	0.1639045	-0.2598484
C	2.0737529	2.7297841	-0.9601760
C	-2.5028676	-1.1328850	-0.1724327
C	-3.8720080	-1.3039626	-0.0261154
C	-4.7027199	-0.1913559	0.0322396
C	-4.1897646	1.0995909	-0.0575269
C	-2.8251228	1.2794350	-0.2042096
O	2.6221629	2.7226988	-2.0253886
O	2.1554485	3.7632749	-0.1209982
N	-6.1537187	-0.3802125	0.1910037
O	-6.8550520	0.6231286	0.2434123
O	-6.5737602	-1.5287930	0.2622999
C	1.6593181	3.6837616	1.2447329
C	2.1734706	4.9091498	1.9704421
H	3.4391172	-1.4852819	2.4491113
H	1.1400554	-2.8101340	2.4467530
H	1.1341964	-4.4603753	0.3697091
H	1.5109815	-3.1141421	-1.6822100
H	3.4801706	-1.9140942	-1.6905414
H	4.8637242	-2.2865665	0.3605313
H	3.5557813	-4.3349417	-0.8360733
H	3.7407835	-4.6449339	0.9138701
H	-1.8409550	-1.9835725	-0.2228962
H	-4.3038983	-2.2924131	0.0440829
H	-4.8640613	1.9432015	-0.0135833
H	-2.4079572	2.2722791	-0.2807224
H	2.0322621	2.7650522	1.7053203
H	0.5691230	3.6529109	1.2242396

H	1.8210861	4.8998196	3.0050817
H	1.8123526	5.8205909	1.4903844
H	3.2647069	4.9277735	1.9739230

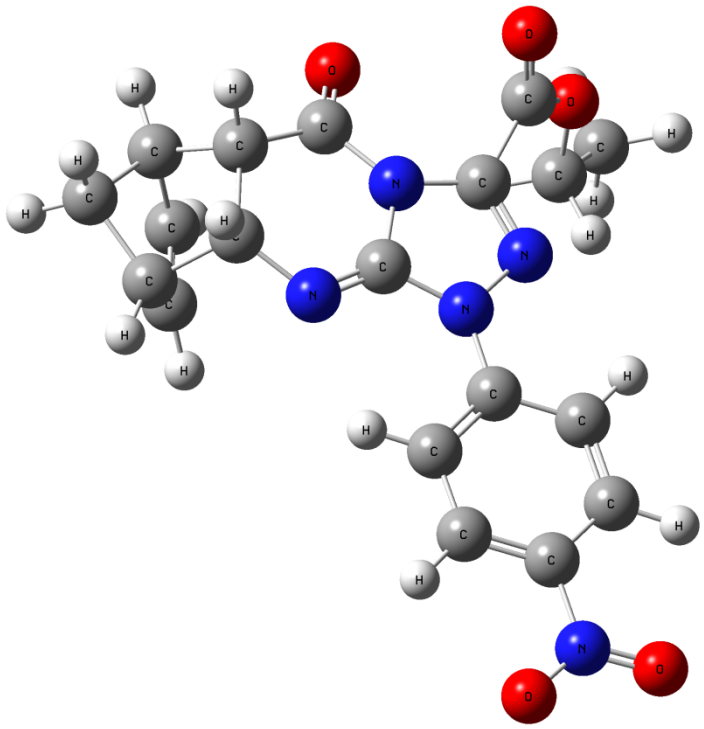


Table S27. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **11d**. (Total energy: RB3LYP/6-31G(d,p): -1351.72380140 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	1.5973100	-3.6196080	1.6623630
C	0.4474420	-2.9720970	1.8781650
C	-0.4816790	-3.2820410	0.7142750
C	0.0980000	-2.5577450	-0.5550280
C	1.4640240	-3.2813190	-0.7934240
C	1.4629520	-4.3708670	0.3467070
C	-0.0390810	-4.7266180	0.3821160
N	0.2905460	-1.1095770	-0.4015100
C	1.5489550	-0.5367890	-0.3830310
N	2.7083330	-1.0934830	-0.5449210
C	2.7585570	-2.4555260	-0.7727480
O	3.8125010	-3.0347330	-0.9475000
C	-0.6215310	-0.0940900	-0.2469990
N	-0.0351110	1.0591290	-0.1074720
N	1.3082530	0.8120990	-0.1776000
C	2.2361910	1.8913040	-0.0540020
C	-2.1073860	-0.2534940	-0.2980060
O	-2.6215450	-1.3342350	-0.5420630
N	-2.7614150	0.9171300	-0.0560110
C	-4.1487260	1.1717970	-0.0411620
C	1.7432190	3.1748360	0.2000240
C	2.6250240	4.2397350	0.3277200
C	4.0074170	4.0645080	0.2077410
C	4.4743250	2.7723660	-0.0414200
C	3.6135080	1.6868270	-0.1748600
C	4.9549440	5.2335670	0.3173990
C	-4.5515250	2.4900660	0.2138470
C	-5.9005650	2.8177010	0.2468680
C	-6.8666840	1.8375080	0.0268330
C	-6.4636580	0.5290210	-0.2258630
C	-5.1153090	0.1827280	-0.2626650
H	2.5088690	-3.5518270	2.2413250
H	0.2283470	-2.2766250	2.6781630
H	-1.5420790	-3.0955160	0.8581800
H	-0.5835850	-2.7036960	-1.3910280
H	1.4463640	-3.7865050	-1.7613660
H	2.1826150	-5.1647350	0.1644930
H	-0.4262300	-5.0995920	-0.5710820
H	-0.2912610	-5.4260690	1.1803510
H	-2.1576430	1.7127110	0.1087380
H	0.6790580	3.3315060	0.2984630
H	2.2254490	5.2285800	0.5282360
H	5.5412620	2.5980980	-0.1341960

H	3.9926520	0.6942980	-0.3656870
H	4.5733450	5.9939670	1.0029820
H	5.1001750	5.7146730	-0.6562190
H	5.9374090	4.9175320	0.6748460
H	-3.8028460	3.2571610	0.3857880
H	-6.1956510	3.8417080	0.4449960
H	-7.9195910	2.0918970	0.0521810
H	-7.2061850	-0.2417690	-0.3988890
H	-4.8067010	-0.8317580	-0.4602830

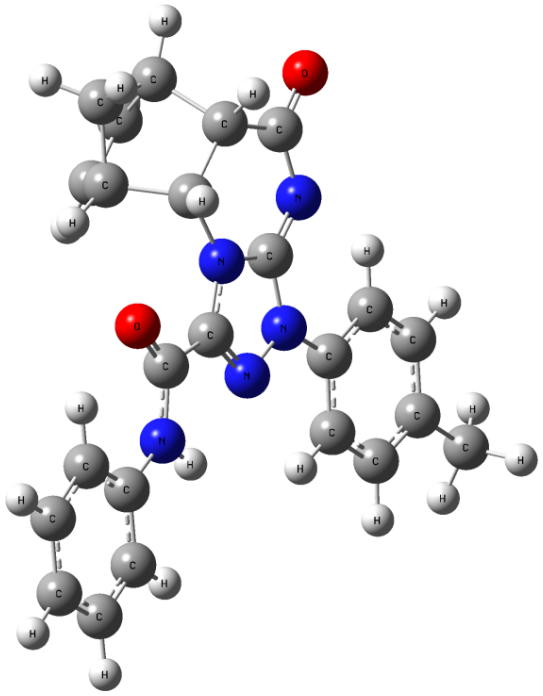


Table S28. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **12d**. (Total energy: RB3LYP/6-31G(d,p): -1351.70164871 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-3.9284407	-0.6920497	1.2474397
C	-3.9770814	0.6212264	0.9988425
C	-4.3043954	0.7998680	-0.4741882
C	-3.0219918	0.3551352	-1.2800939
C	-2.9878681	-1.2010830	-1.0177089
C	-4.2303113	-1.4166032	-0.0549838
C	-5.2170265	-0.4229970	-0.7079826
N	-1.8494999	1.1394888	-0.9295764
C	-0.9340563	0.5618794	-0.2675349
N	-0.8651711	-0.8042487	0.1044781
C	-1.7214795	-1.7717796	-0.4367470
N	0.2637164	1.0787271	0.2267476
N	0.9957217	0.1073620	0.8835728
C	0.3285788	-0.9903043	0.7945725
O	-1.4379486	-2.9474811	-0.4165044
C	0.7641839	2.4047976	0.1568788
C	0.6161370	-2.2049657	1.6384989
C	0.0575836	3.4139625	-0.5017503
C	0.5884375	4.7016913	-0.5472628
C	1.8098382	5.0207314	0.0454629
C	2.4986726	3.9906702	0.6975032
C	1.9942692	2.6998902	0.7585352
O	-0.1811958	-2.5303172	2.4946417
N	1.8256054	-2.8091864	1.4558241
C	2.3755195	6.4191985	-0.0086591
C	2.6745107	-2.7300859	0.3135161
C	2.1521811	-2.8977118	-0.9713584
C	2.9999889	-2.8269910	-2.0737773
C	4.3671167	-2.6229651	-1.8999548
C	4.8873732	-2.4825240	-0.6144400
C	4.0439227	-2.5264205	0.4914500
H	-3.6142312	-1.1779377	2.1621595
H	-3.7231158	1.4241765	1.6777047
H	-4.6733527	1.7786211	-0.7758454
H	-3.2151676	0.5287844	-2.3422411
H	-3.1703213	-1.7577789	-1.9390200
H	-4.5253497	-2.4612344	0.0235918
H	-5.4162697	-0.6320874	-1.7634788
H	-6.1582659	-0.3544084	-0.1605002
H	-0.8885761	3.1862603	-0.9686548
H	0.0277330	5.4747147	-1.0629113
H	3.4533710	4.2004735	1.1698536
H	2.5393871	1.9164460	1.2647391

H	2.0318418	-3.5145430	2.1518193
H	2.5193969	6.8298202	0.9958048
H	1.7119690	7.0947358	-0.5522033
H	3.3499758	6.4361867	-0.5071440
H	1.0955102	-3.1057157	-1.0942953
H	2.5912258	-2.9523443	-3.0699153
H	5.0246174	-2.5785348	-2.7603614
H	5.9503359	-2.3252326	-0.4717168
H	4.4358574	-2.3884352	1.4926481

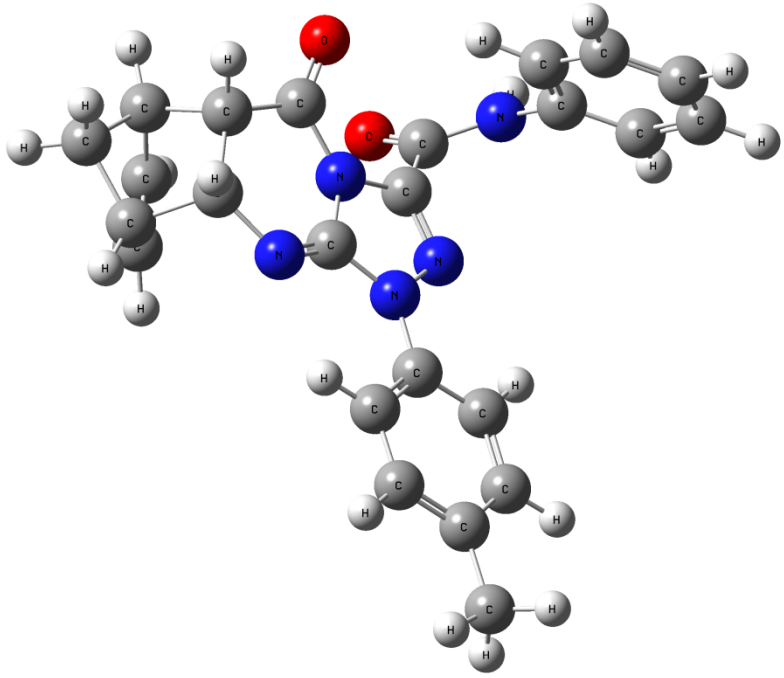


Table S29. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **11e**. (Total energy: RB3LYP/6-31G(d,p): -1104.55225821 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	-2.5671982	-1.7811457	1.7134589
C	-2.5253721	-0.4605245	1.9161584
C	-3.3210840	0.1970401	0.7989584
C	-2.4955523	0.0178002	-0.5302036
C	-2.5172002	-1.5293203	-0.7589456
C	-3.3869675	-2.0313074	0.4576025
C	-4.4077919	-0.8763695	0.5560065
N	-1.1237394	0.5276069	-0.4649776
C	-0.0390743	-0.3287895	-0.4349785
N	0.0027112	-1.6131855	-0.6249365
C	-1.1805689	-2.2823225	-0.8499833
O	-1.2151392	-3.4730409	-1.0933557
C	-0.6488212	1.8049788	-0.2127402
N	0.6395092	1.7970997	-0.0373564
N	1.0360371	0.4982553	-0.1716043
C	2.4241443	0.1755847	-0.0461358
C	-1.3980794	3.1084420	-0.2259418
O	-1.0008395	4.0222634	0.4563459
C	-2.5839863	3.2519974	-1.1581743
C	3.3115575	1.1935496	0.3176309
C	4.6644118	0.9105896	0.4431404
C	5.1692903	-0.3746512	0.2150375
C	4.2604717	-1.3725562	-0.1404614
C	2.8980743	-1.1175806	-0.2754834
C	6.6465436	-0.6607334	0.3282475
H	-2.0321699	-2.5454435	2.2611352
H	-1.9569880	0.0724850	2.6668683
H	-3.6567984	1.2173654	0.9822687
H	-3.0026653	0.5225351	-1.3528667
H	-3.0509006	-1.7553029	-1.6838956
H	-3.7596145	-3.0418385	0.3122487
H	-4.9869107	-0.7232692	-0.3599763
H	-5.0831537	-0.9755344	1.4066510
H	-2.8044893	4.3134280	-1.2623926
H	-3.4663581	2.7544062	-0.7468597
H	-2.3792055	2.8148633	-2.1389387
H	2.9351640	2.1901821	0.4980698
H	5.3409990	1.7095871	0.7286048
H	4.6168959	-2.3819296	-0.3176226
H	2.2079700	-1.9028392	-0.5442276
H	7.0955969	-0.1157142	1.1624956
H	7.1768684	-0.3576188	-0.5812511
H	6.8351794	-1.7256665	0.4787324

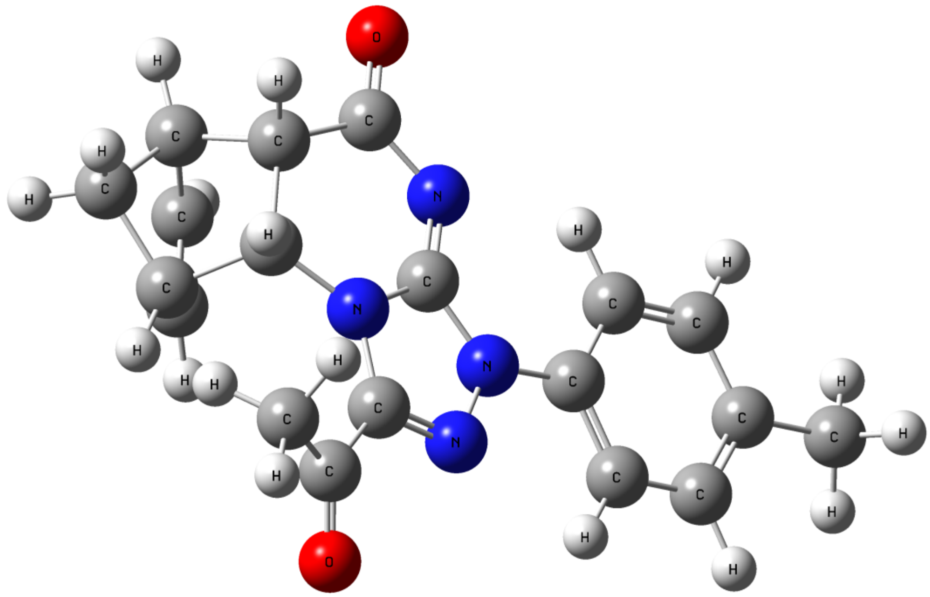
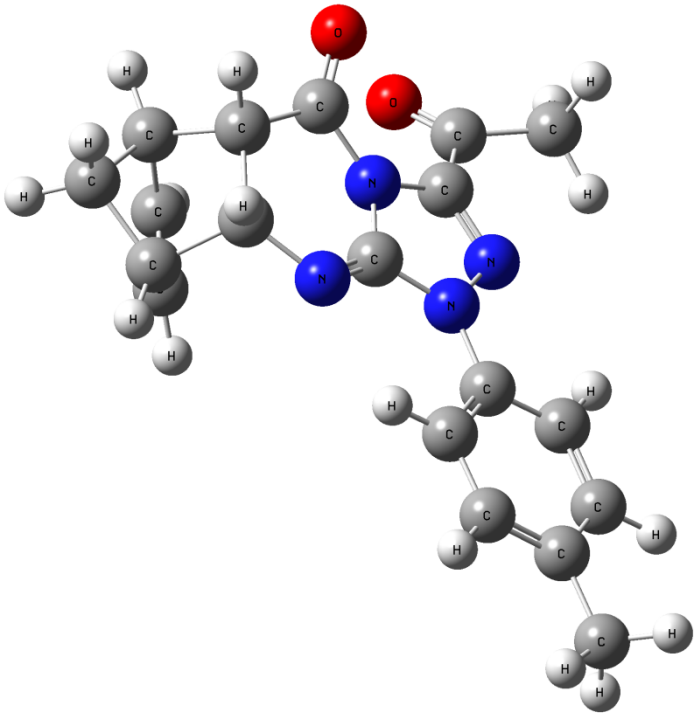


Table S30. Cartesian coordinates (in Å) of the B3LYP/6–311G (d,p) optimized structure of the electronic ground state of **12e**. (Total energy: RB3LYP/6-31G(d,p): --1104.53842370 a.u., 0 imaginary frequencies).

Symbol	X	Y	Z
C	2.9555382	-1.1571188	1.5723643
C	1.9556509	-2.0427605	1.6396031
C	2.0262929	-2.9117242	0.3950590
C	1.5910570	-2.0018540	-0.8193744
C	2.7898093	-0.9846344	-0.9240038
C	3.7189432	-1.4228379	0.2847850
C	3.5535151	-2.9551695	0.1720168
N	0.2513862	-1.4621497	-0.6578963
C	0.1440659	-0.2236392	-0.4119980
N	1.1700192	0.7519590	-0.3546257
C	2.4553962	0.4851578	-0.8835622
N	-1.0178563	0.5271327	-0.1855328
N	-0.7204699	1.8475950	0.0188005
C	0.5638743	1.9773923	-0.0838278
O	3.1865342	1.3647662	-1.2573555
C	-2.3668732	0.0864803	-0.1031387
C	1.2709148	3.2247581	0.3503677
C	-2.7111858	-1.2458850	-0.3416248
C	-4.0471360	-1.6323866	-0.2522907
C	-5.0598580	-0.7288987	0.0684082
C	-4.6879069	0.6008822	0.3019986
C	-3.3661780	1.0131049	0.2204857
O	2.3477074	3.1468558	0.8935295
C	0.5393614	4.5208485	0.1068480
C	-6.5040281	-1.1570143	0.1627531
H	3.1431402	-0.3226843	2.2356179
H	1.1655824	-2.0826827	2.3774802
H	1.4871330	-3.8568293	0.4295737
H	1.5751857	-2.6243099	-1.7180523
H	3.3471187	-1.1330827	-1.8506084
H	4.7219521	-1.0059344	0.2168383
H	3.8477641	-3.3575387	-0.8020425
H	4.0779000	-3.4884935	0.9663178
H	-1.9412606	-1.9597903	-0.5910928
H	-4.2988032	-2.6709534	-0.4409252
H	-5.4483616	1.3331757	0.5545775
H	-3.0987615	2.0433999	0.4049854
H	-0.5205334	4.4267788	0.3485619
H	0.6104528	4.7749771	-0.9560036
H	1.0044905	5.3101959	0.6955303
H	-7.1291638	-0.6073906	-0.5480444
H	-6.9096360	-0.9696820	1.1619756
H	-6.6172051	-2.2220966	-0.0485155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Crystal Data

Table S31. Crystal Data.of compounds **7e** and **11d**.

	7e	**11d**		**7e**	**11d**
CCDC	1980577	1980578	γ (deg)	103.319(3)	90
empirical formula	$C_{21}H_{24}N_4O_3$	$C_{24}H_{21}N_5O_2$	V (Å^3)	1928.87(11)	2011.59(3)
mw	380.44	411.46	Z	4	4
temp (K)	120(2)	120(2)	ρ_{calc} (Mg/m^3)	1.310	1.359
λ(Å)	0.71073	1.54184	μ(Mo Kα) (mm^{-1})	0.090	0.725
crystal syst.	Triclinic	Monoclinic	No. reflns.	34591	55685
space group	P-1	P2$_1$/n	Unique reflns.	10787	4250
a (Å)	9.5893(2)	15.91340(10)	GOOF (F^2)	1.030	1.031
b (Å)	14.2652(5)	8.38680(10)	R_{int}	0.0277	0.0291
c (Å)	15.8257(5)	16.48080(10)	R1[a] ($I \geq 2\sigma$)	0.0492	0.0373
α (deg)	104.318(3	90	wR2[b] ($I \geq 2\sigma$)	0.1219	0.0978
β(deg)	104.565(3)	113.8600(10)			

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$.

[b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.