

Supporting Information

Exploration of the DNA Photocleavage Activity of O-Halo-Phenyl Carbamoyl Amidoximes: Studies of the UVA-Induced Effects on a Major Crop Pest, the Whitefly *Bemisia tabaci*

Anastasios Panagopoulos ¹, Konstantina Alipranti ², Kyriaki Mylona ², Polinikis Paisidis ³,
Stergios Rizos ³, Alexandros E. Koumbis ³, Emmanouil Roditakis ^{2,4} and Konstantina C. Fylaktakidou ^{1,3,4,*}

¹ Laboratory of Organic, Bioorganic and Natural Product Chemistry, Molecular Biology and Genetics Department, Democritus University of Thrace, 68100 Alexandroupolis, Greece

² Department of Agriculture, School of Agricultural Sciences, Hellenic Mediterranean University, Gianni Kornarou, Estavromenos 1, 714 10 Heraklion, Greece

³ Laboratory of Organic Chemistry, Chemistry Department, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

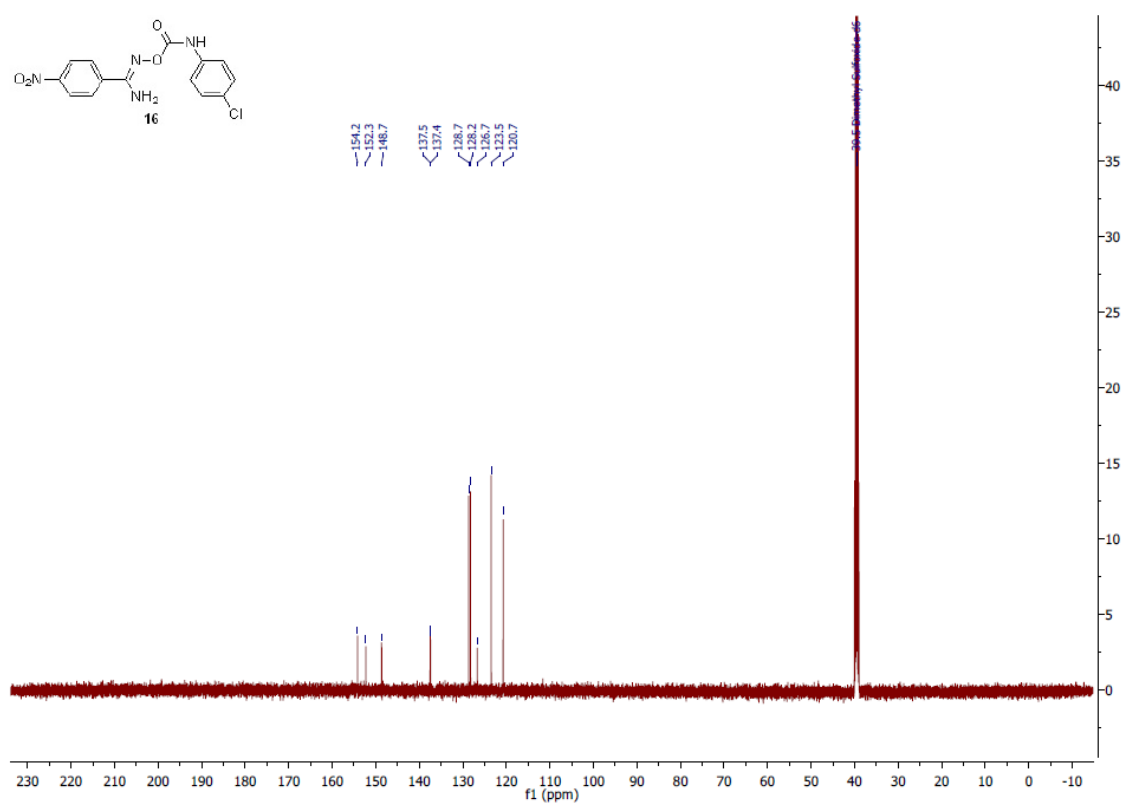
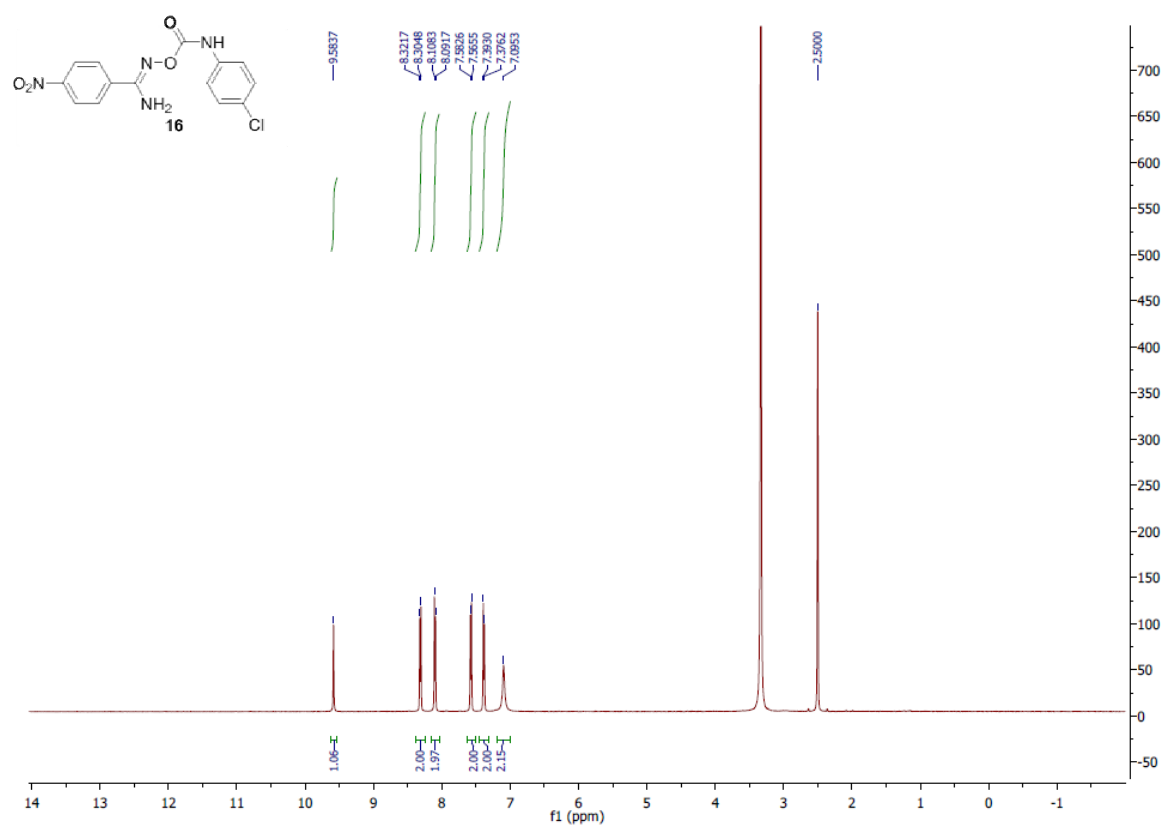
⁴ Institute of Agri-Food and Life Sciences Agro-Health, Hellenic Mediterranean University Research Center, 71410 Heraclion, Greece

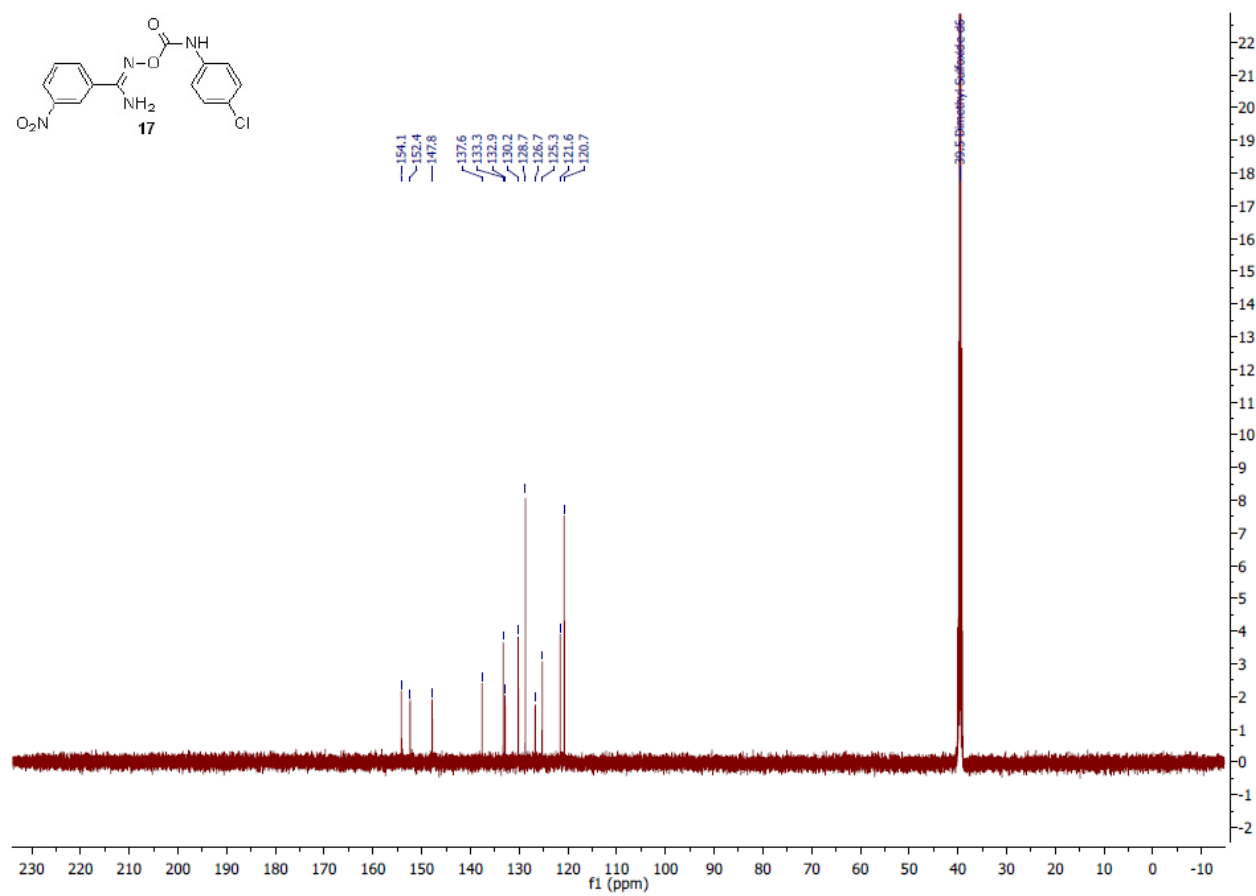
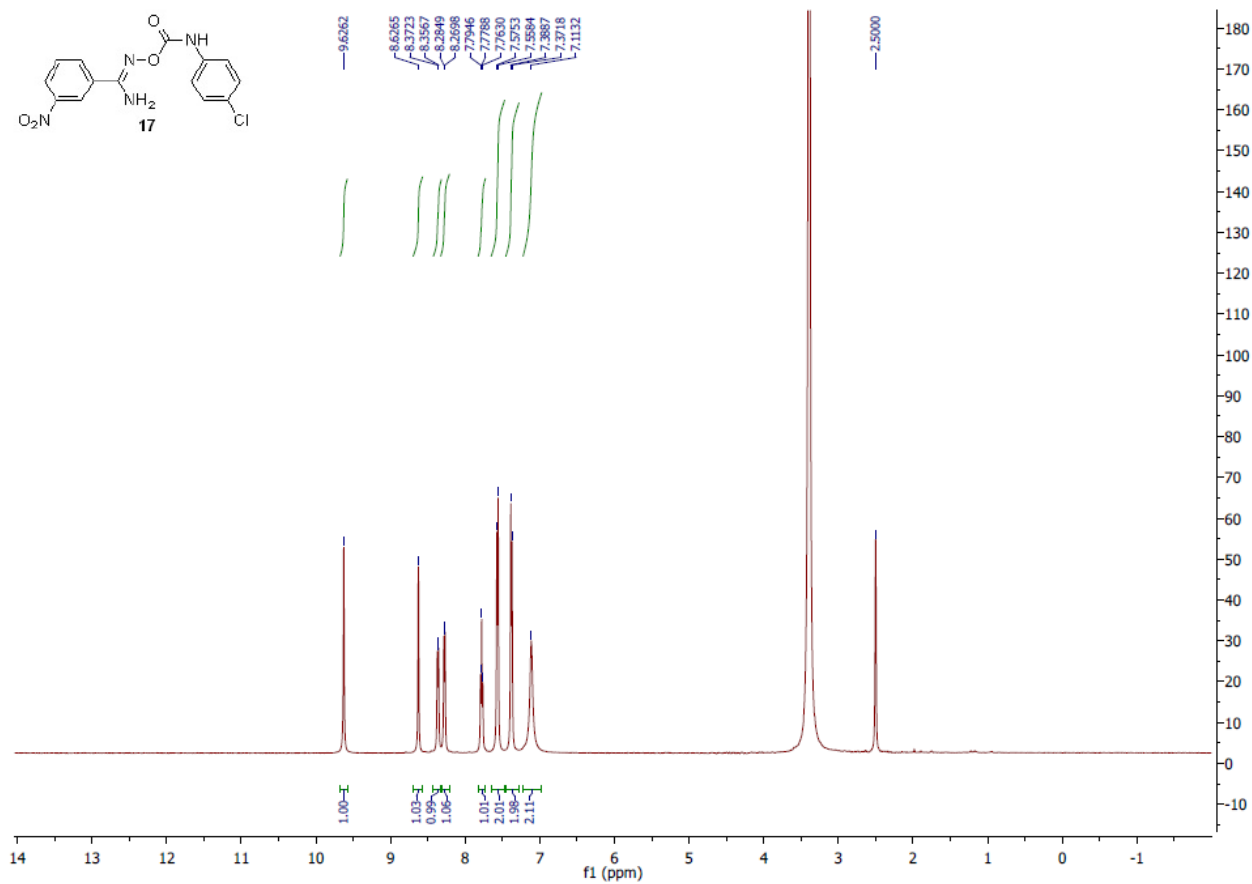
* Correspondence: kfylakta@chem.auth.gr

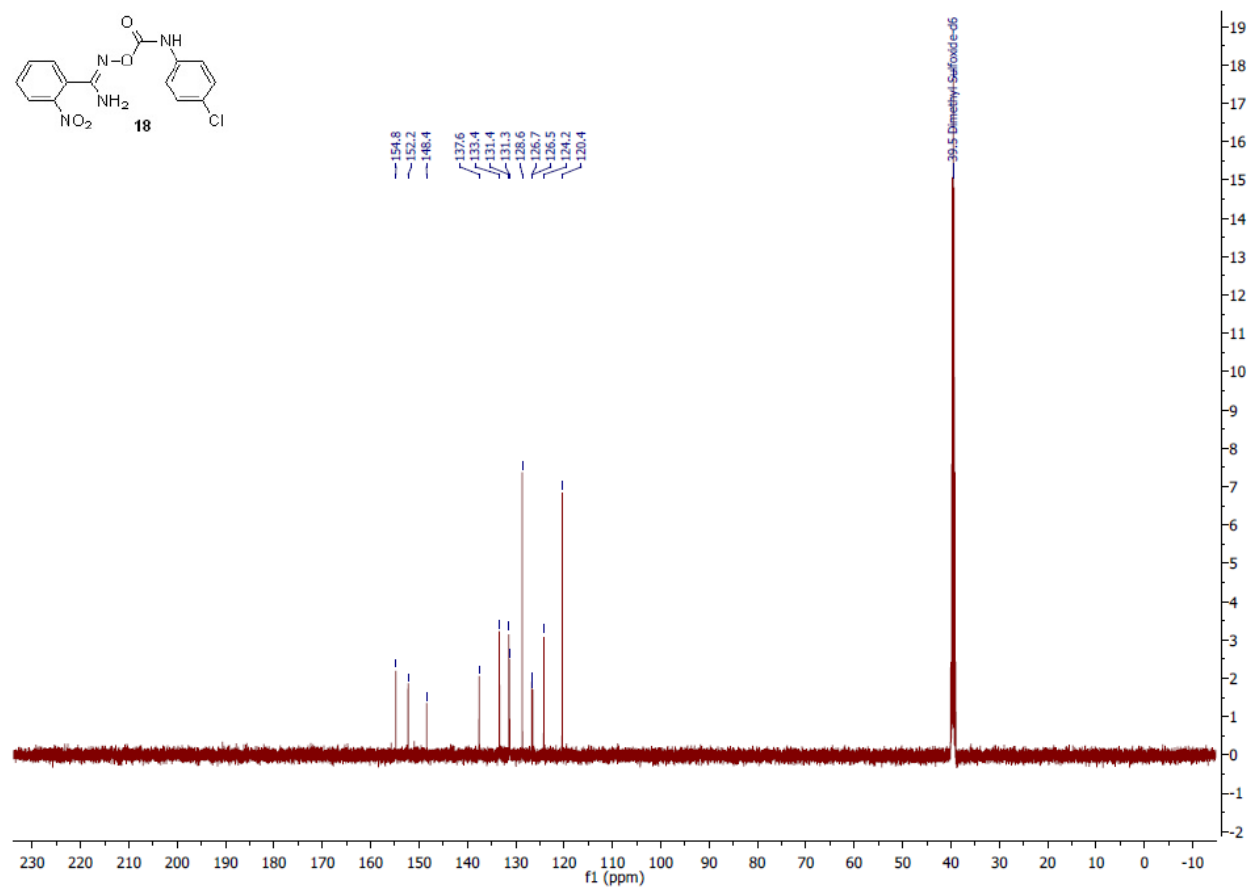
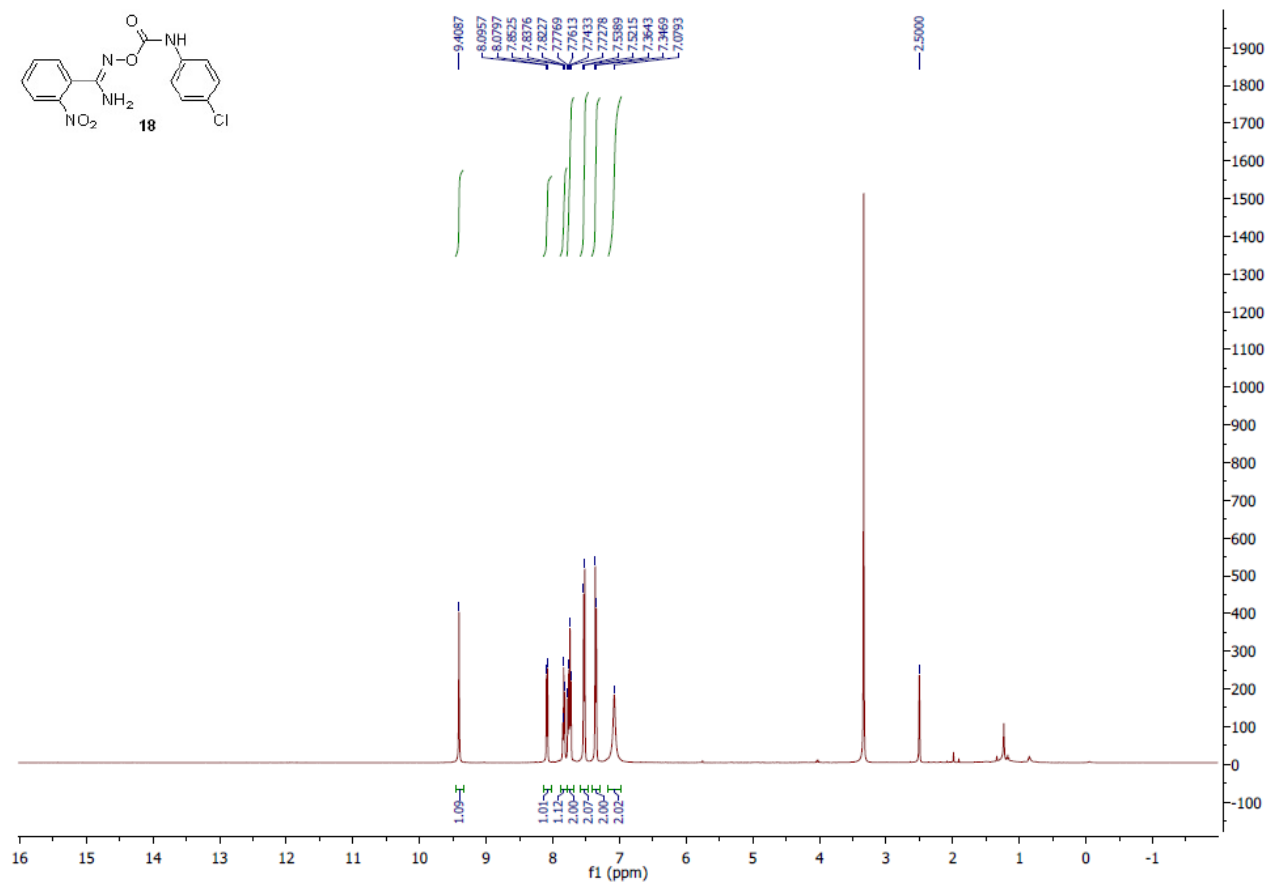
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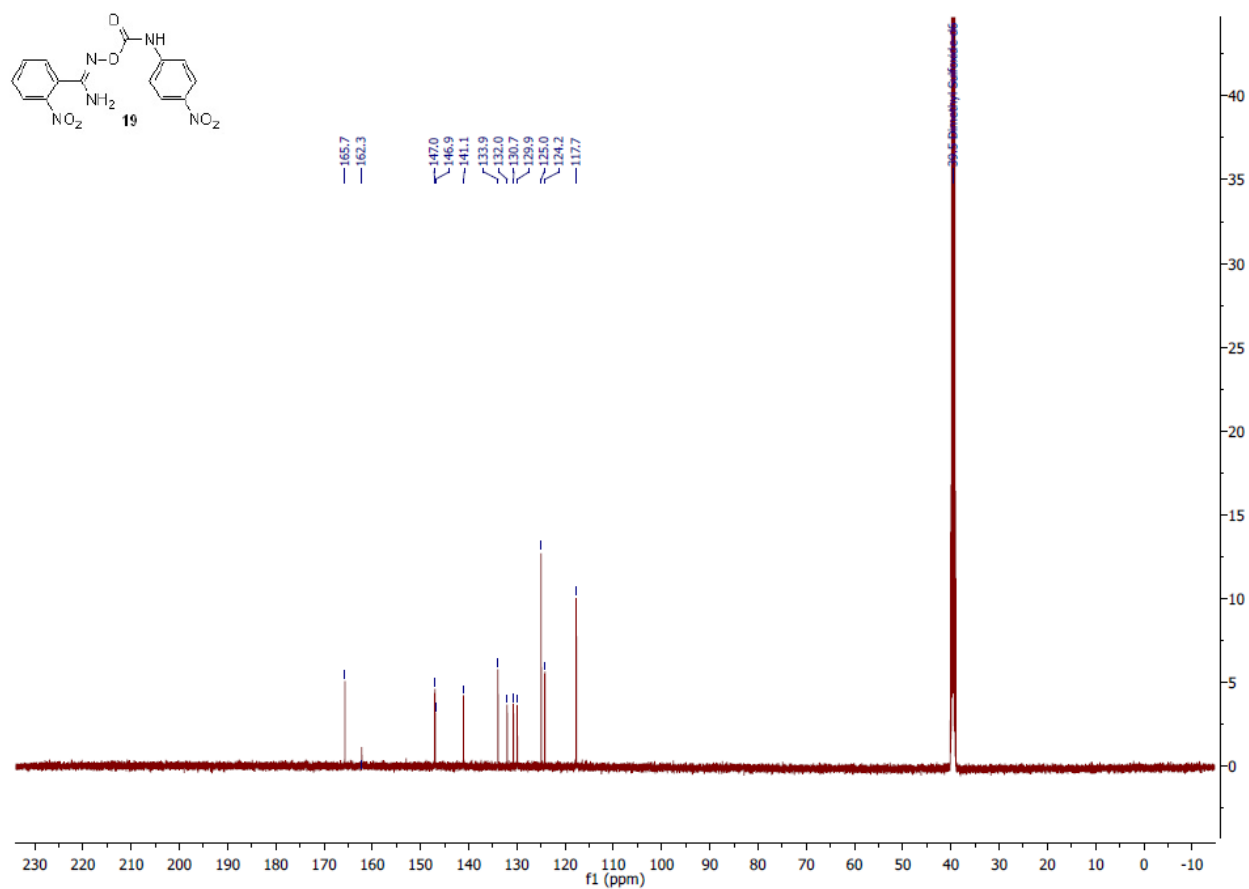
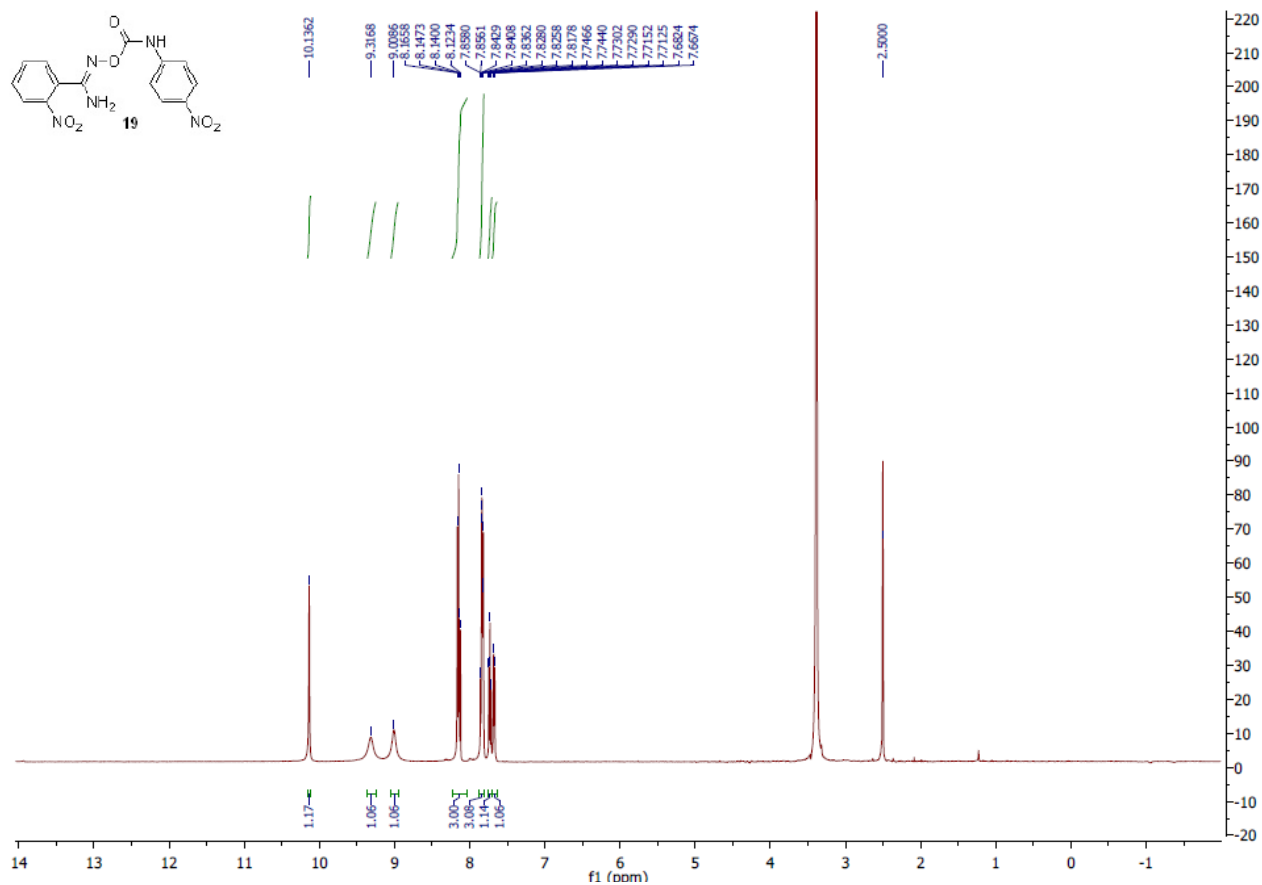
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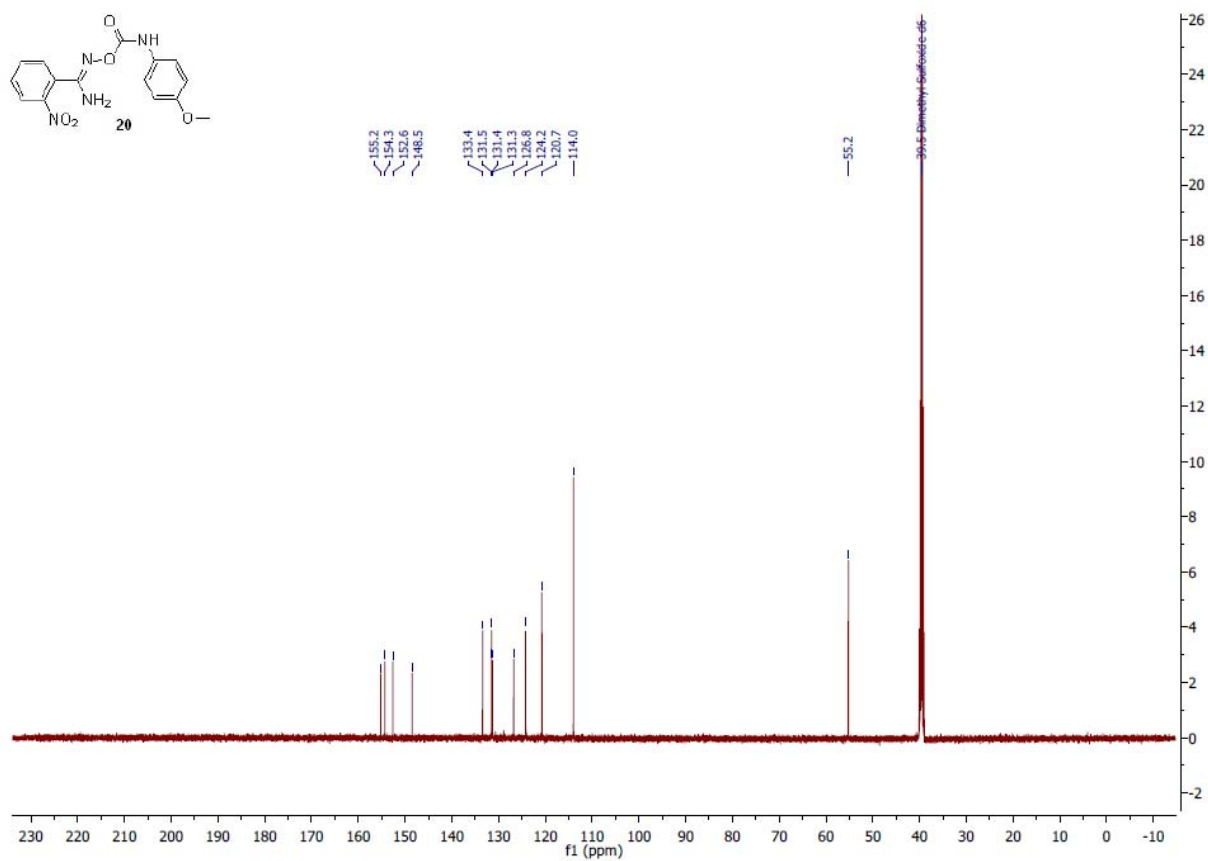
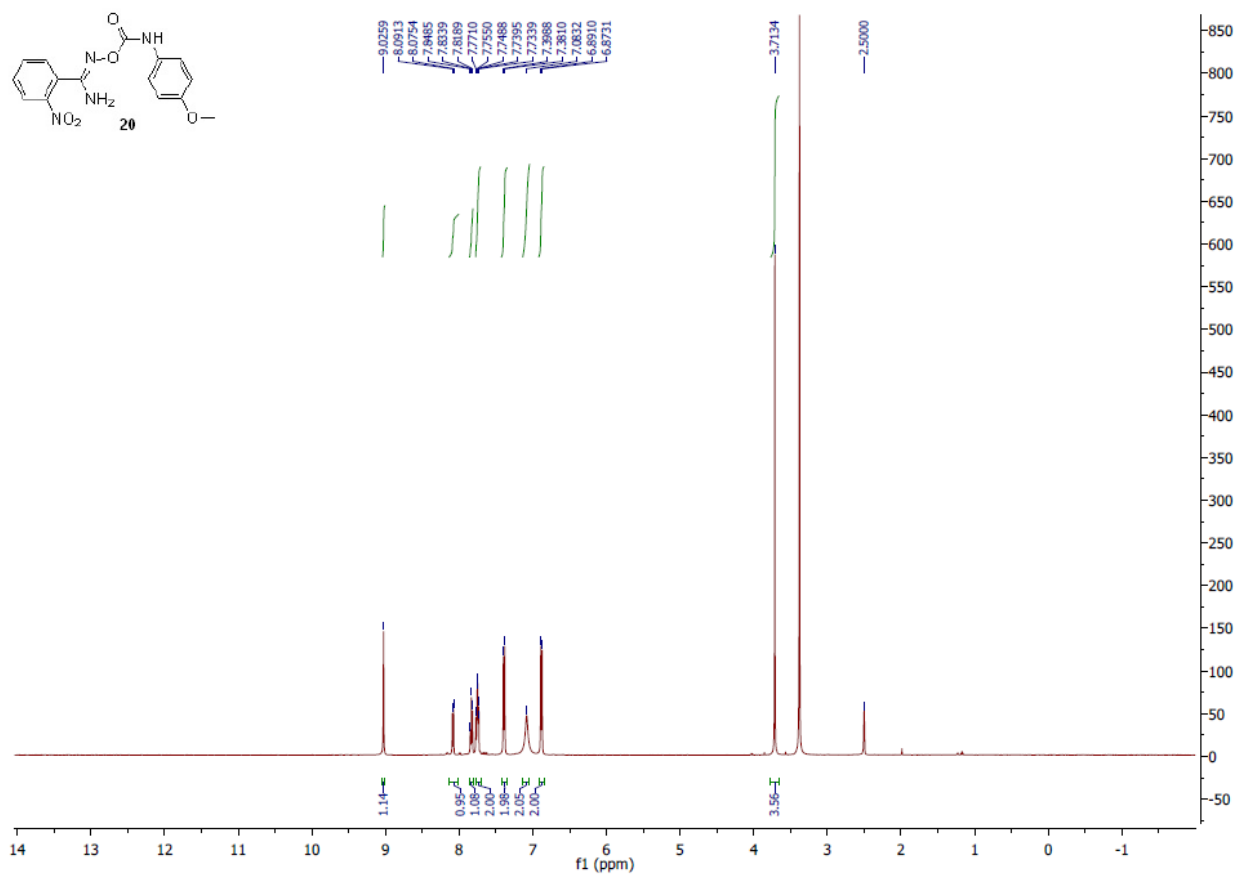
S1A Copies of NMR spectra of compounds 16-29 and 32

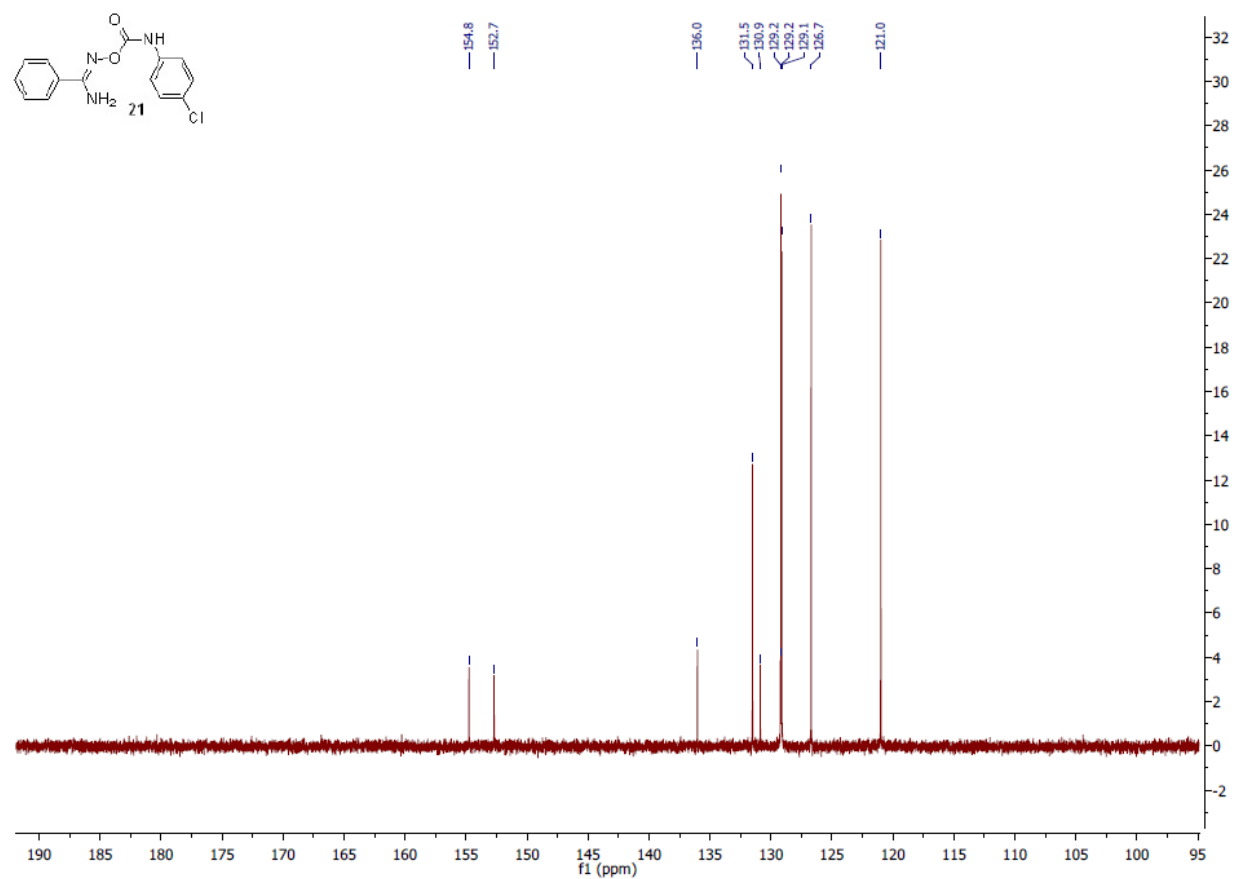
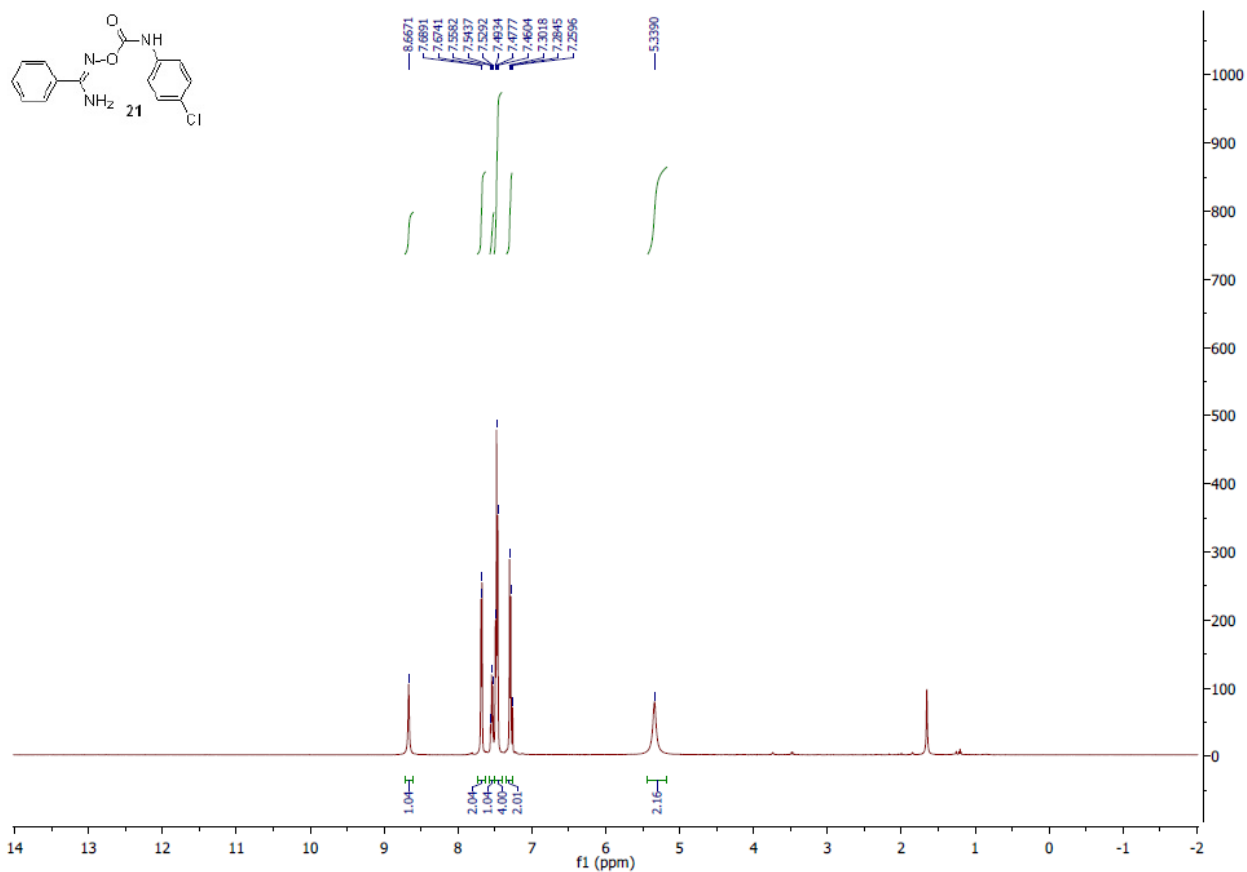


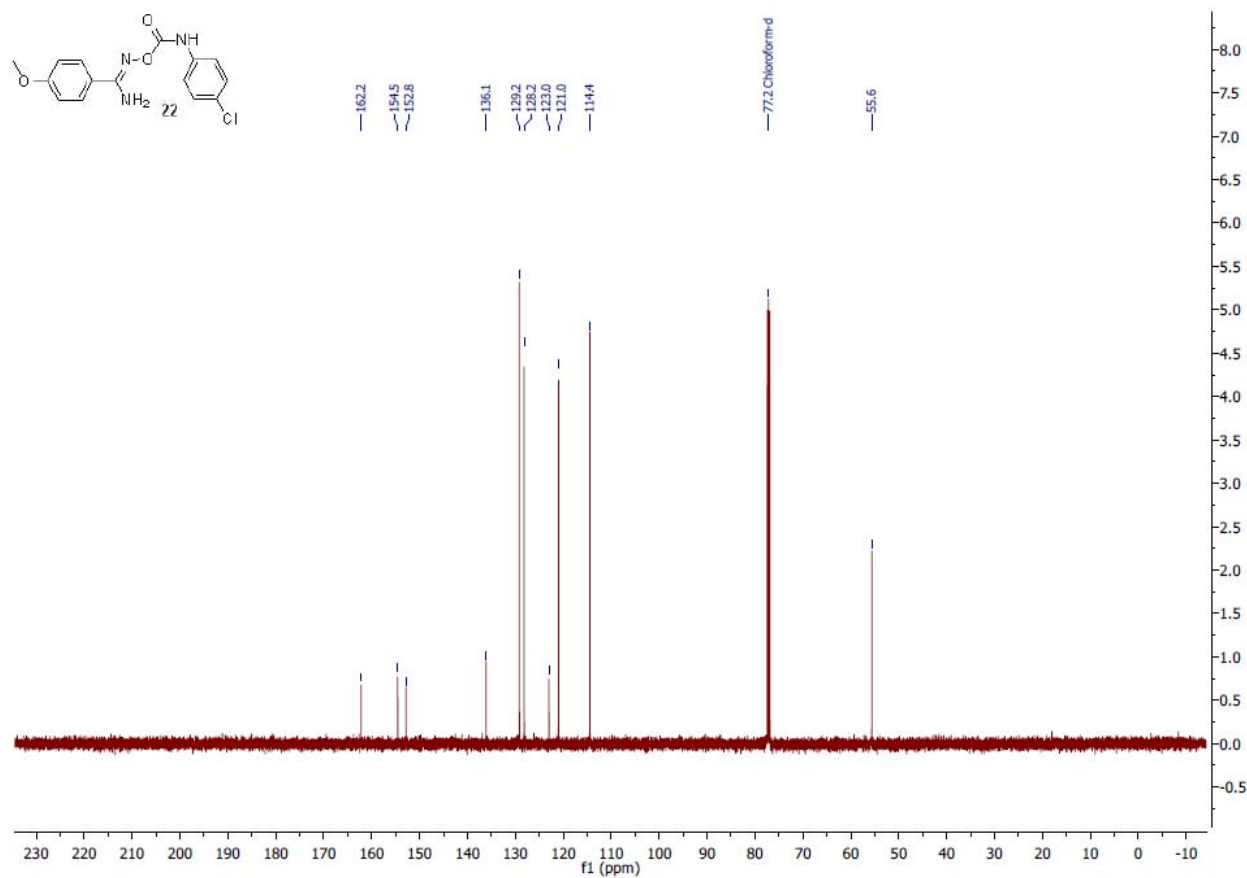
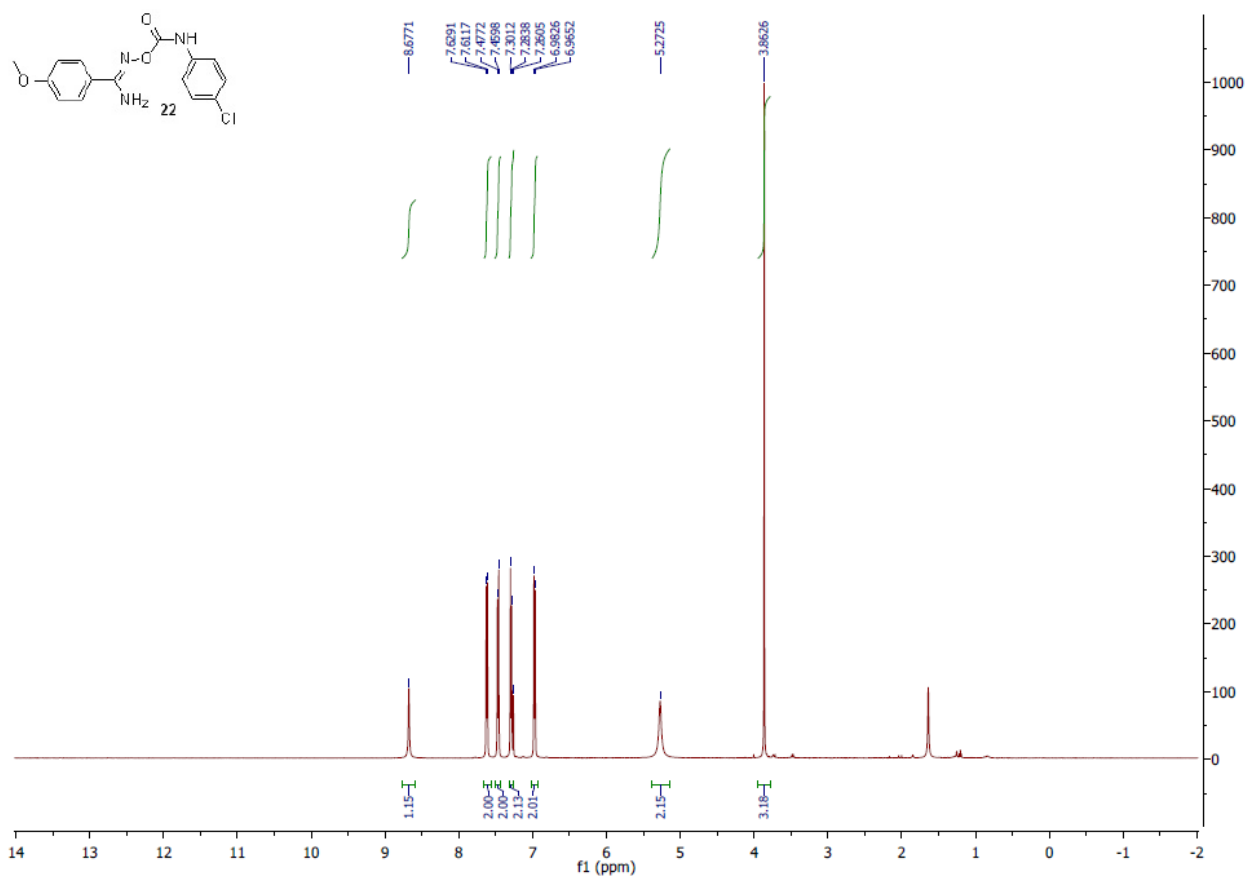


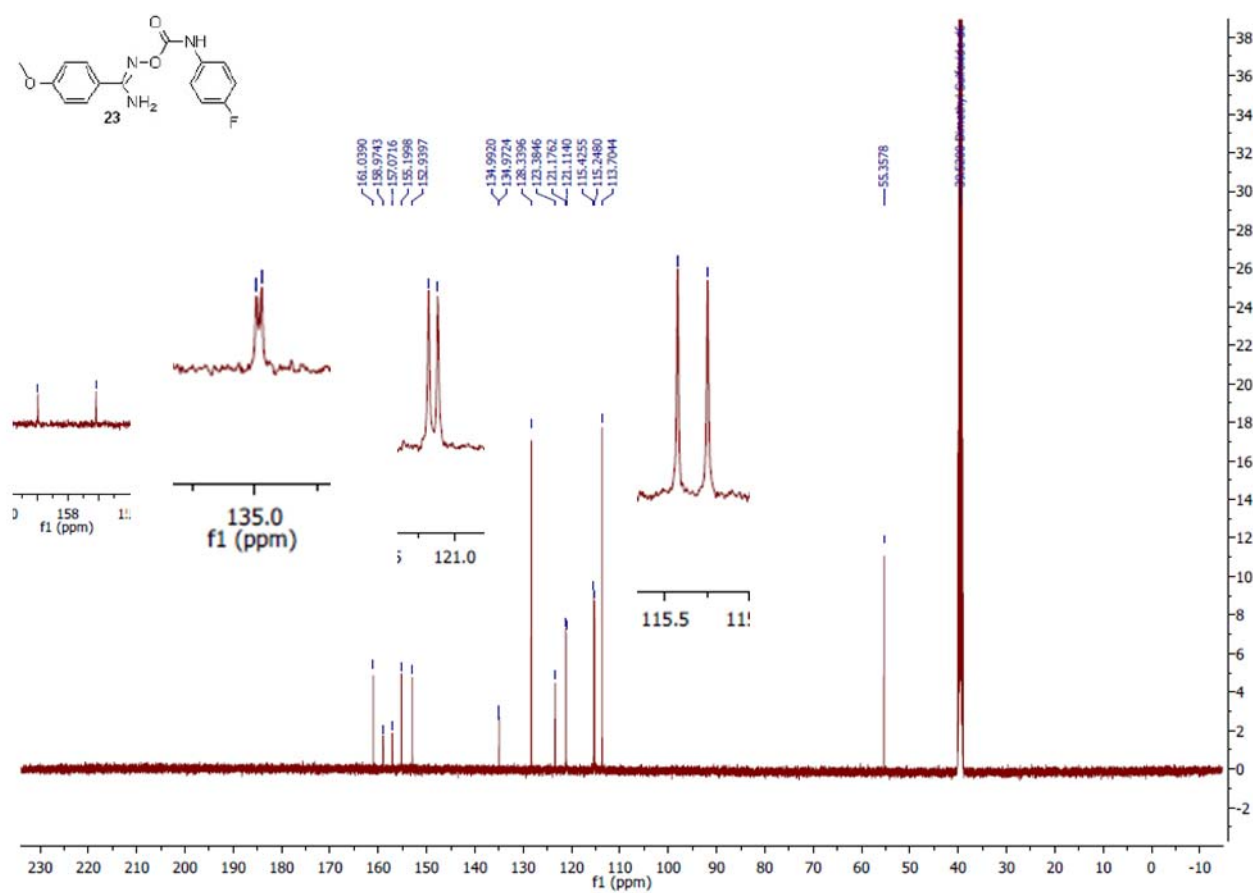
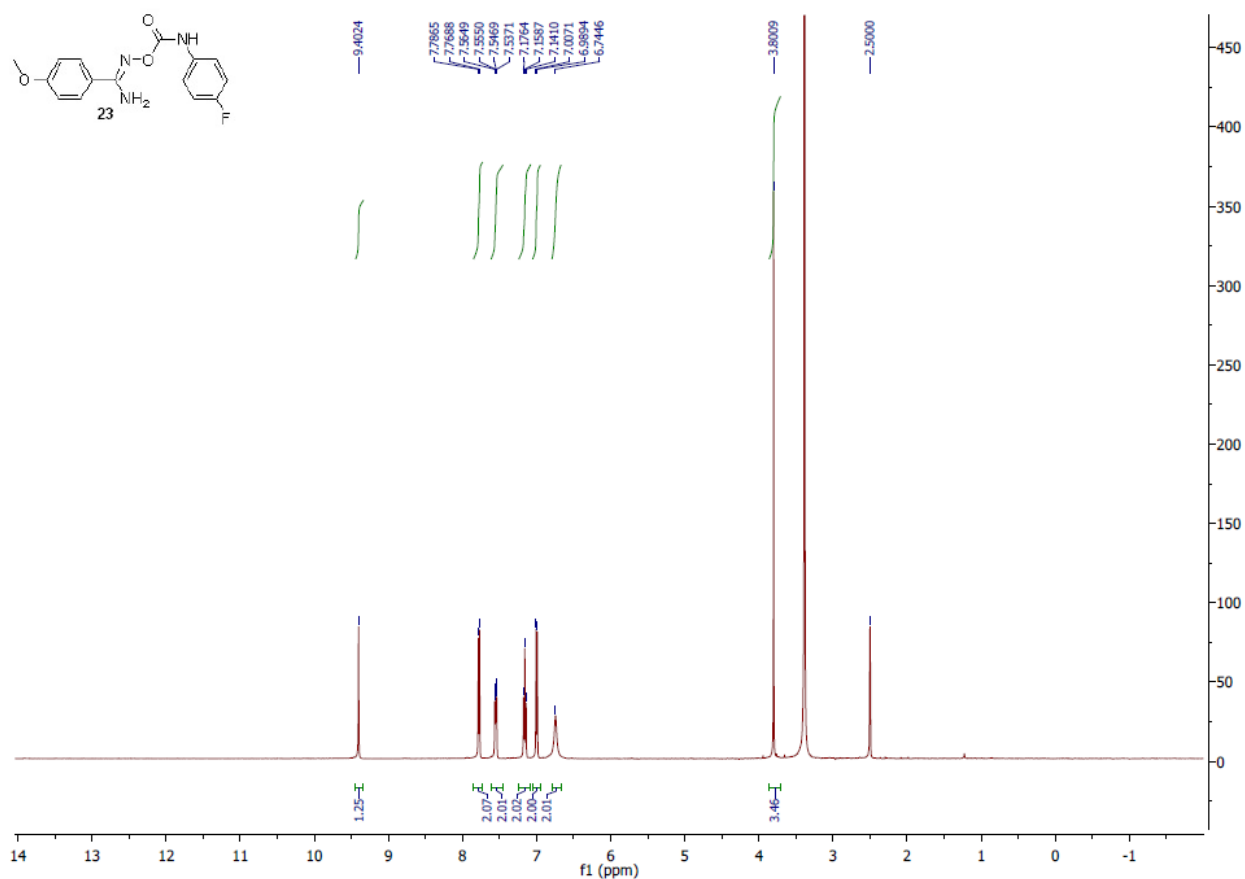


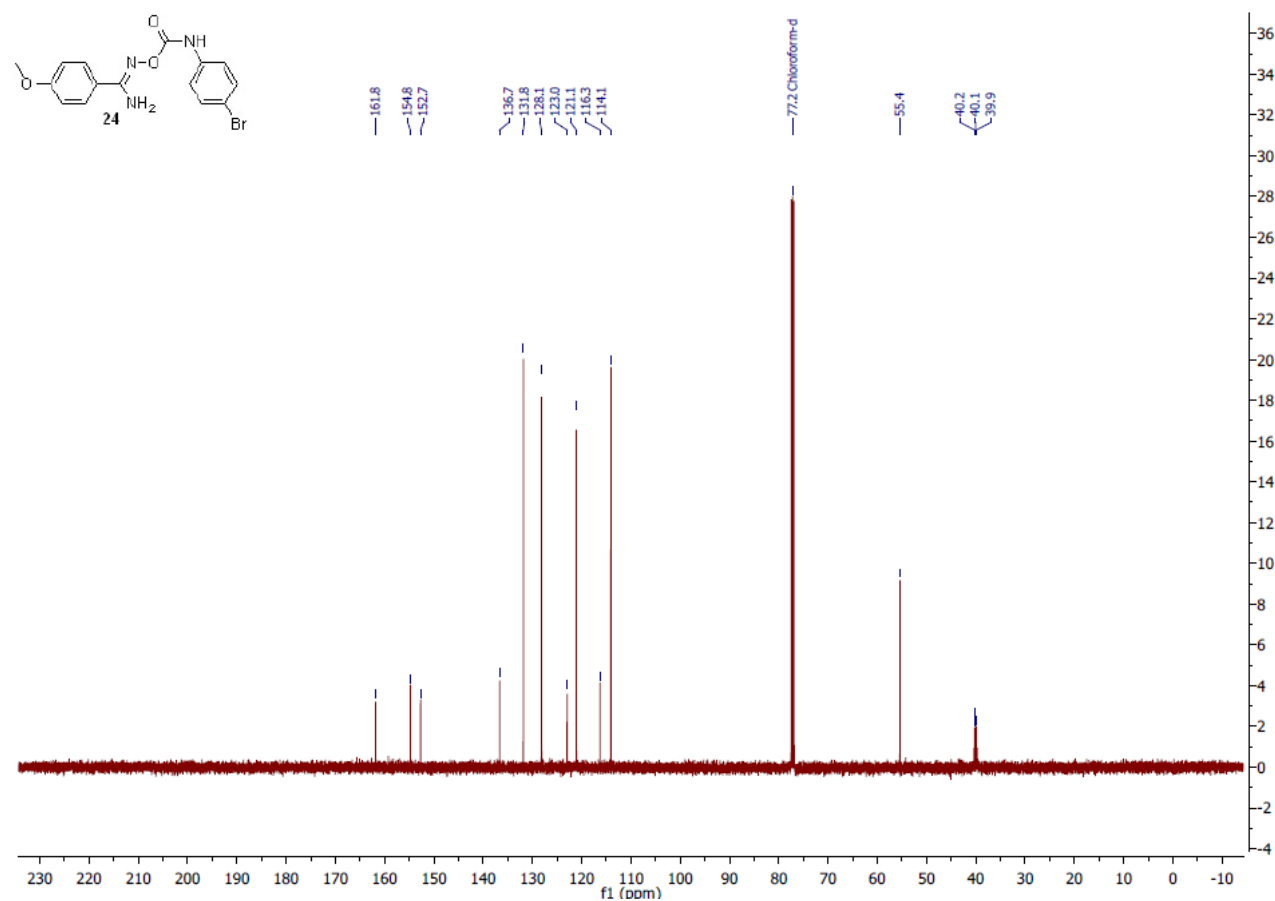
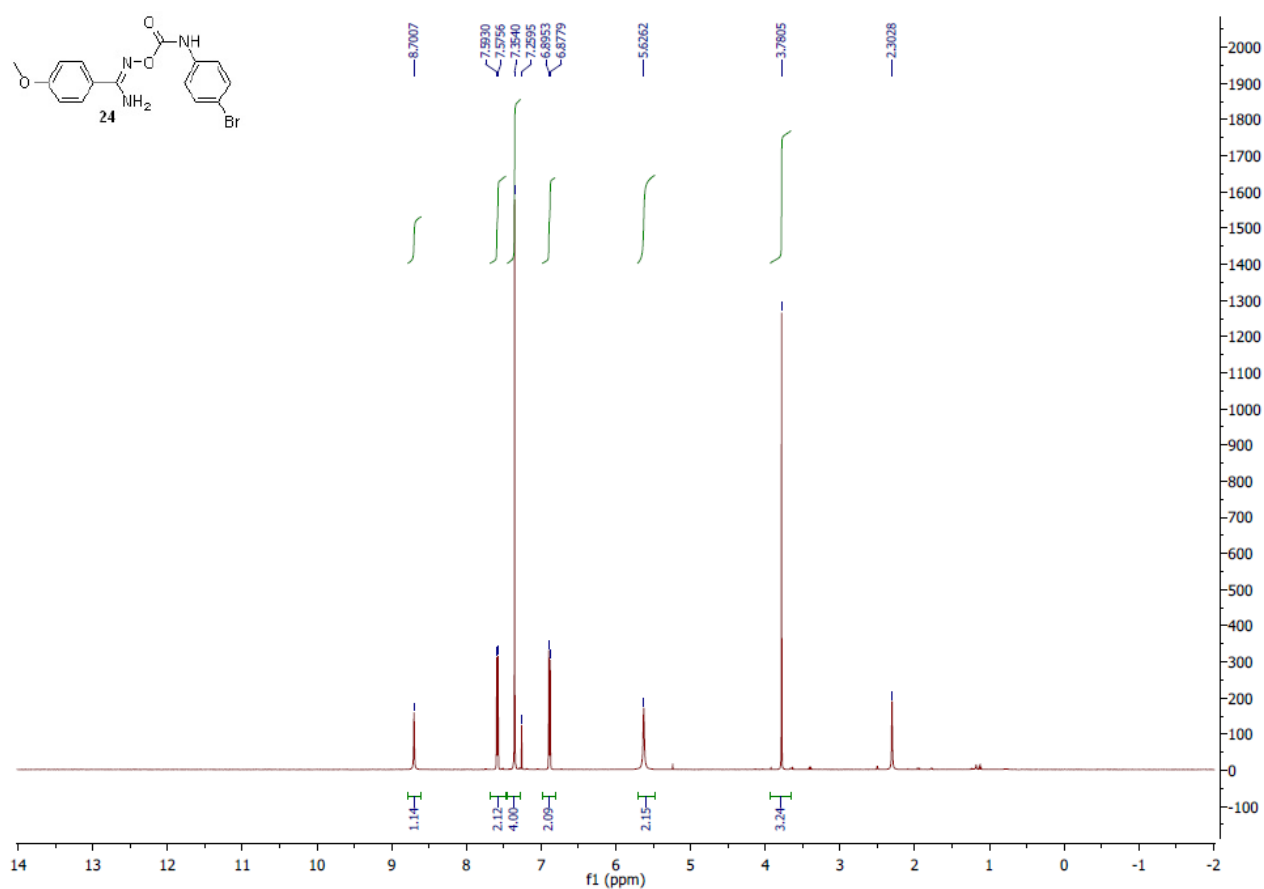


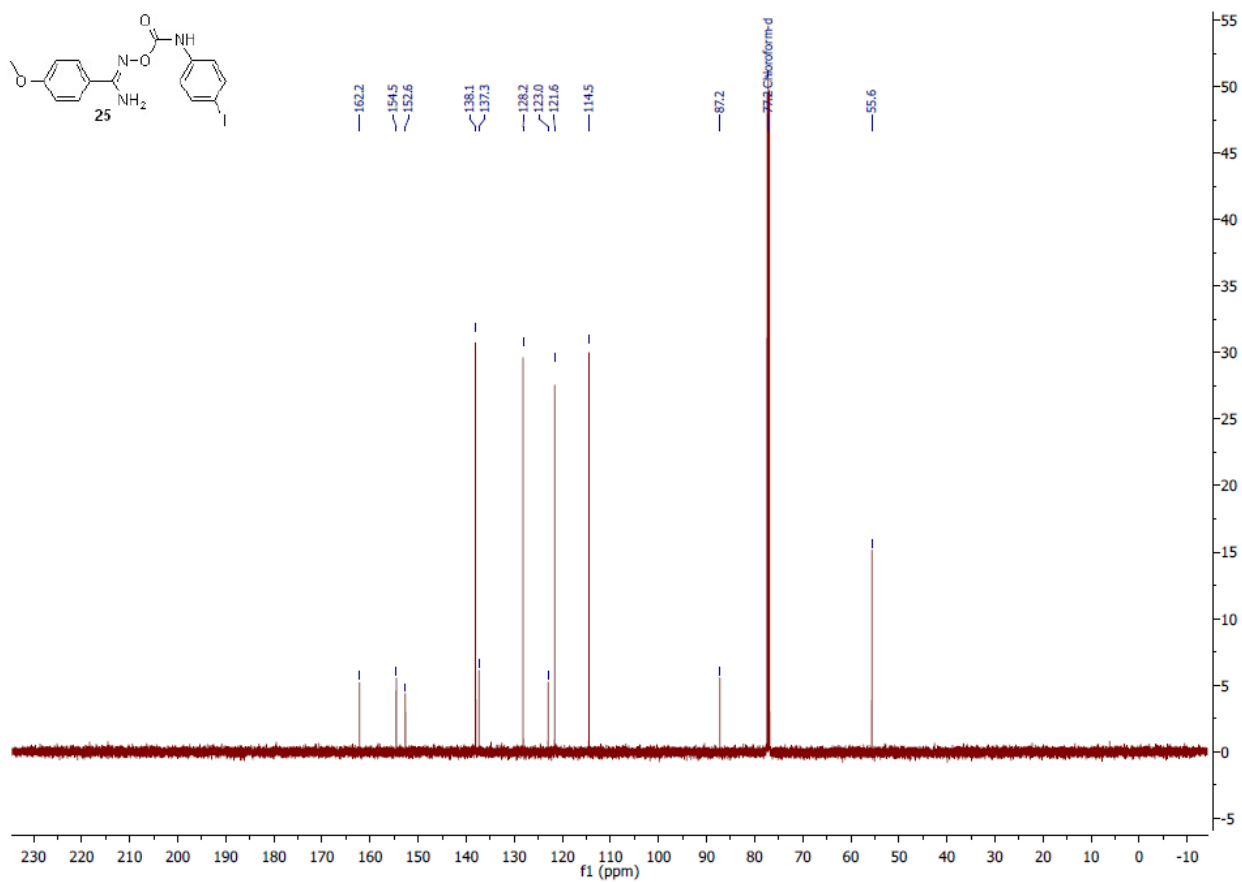
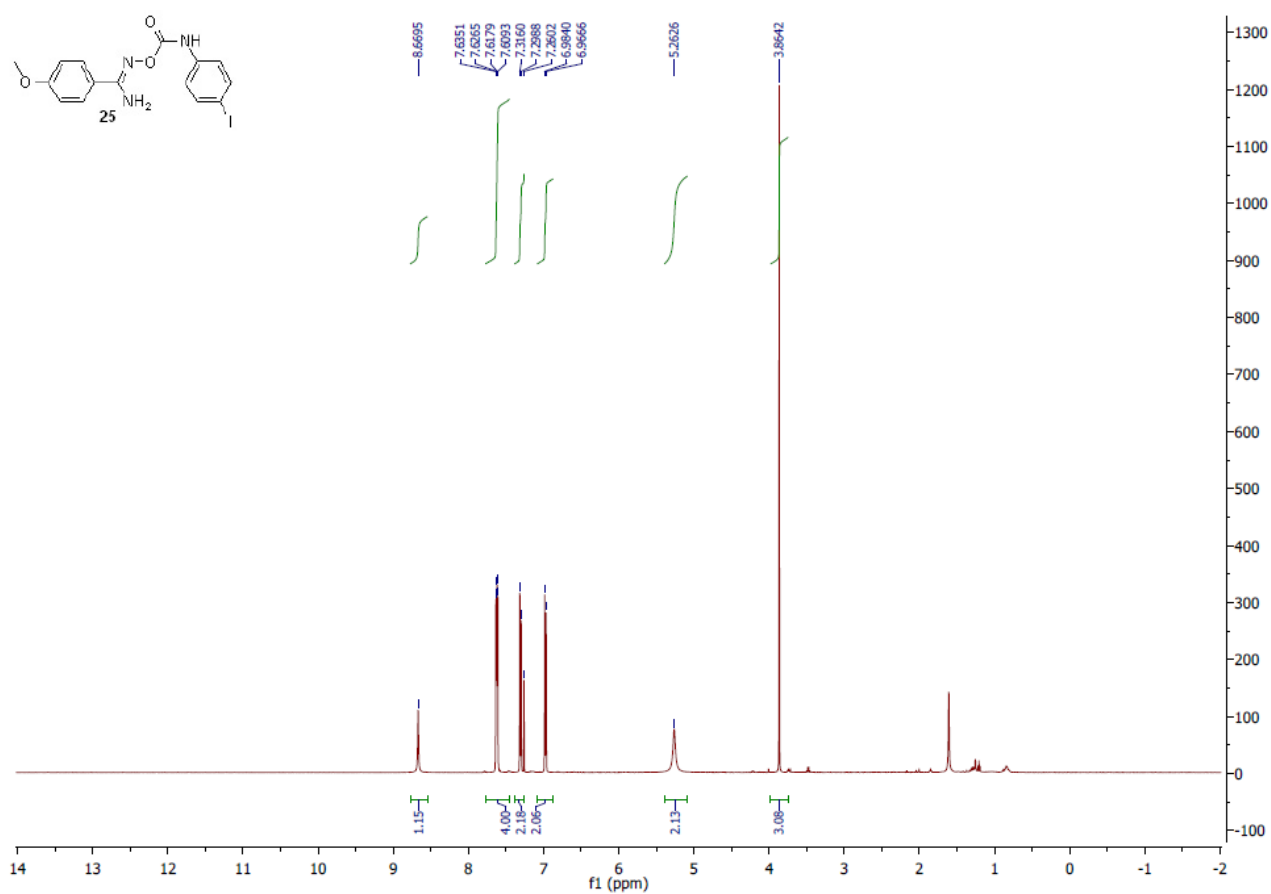


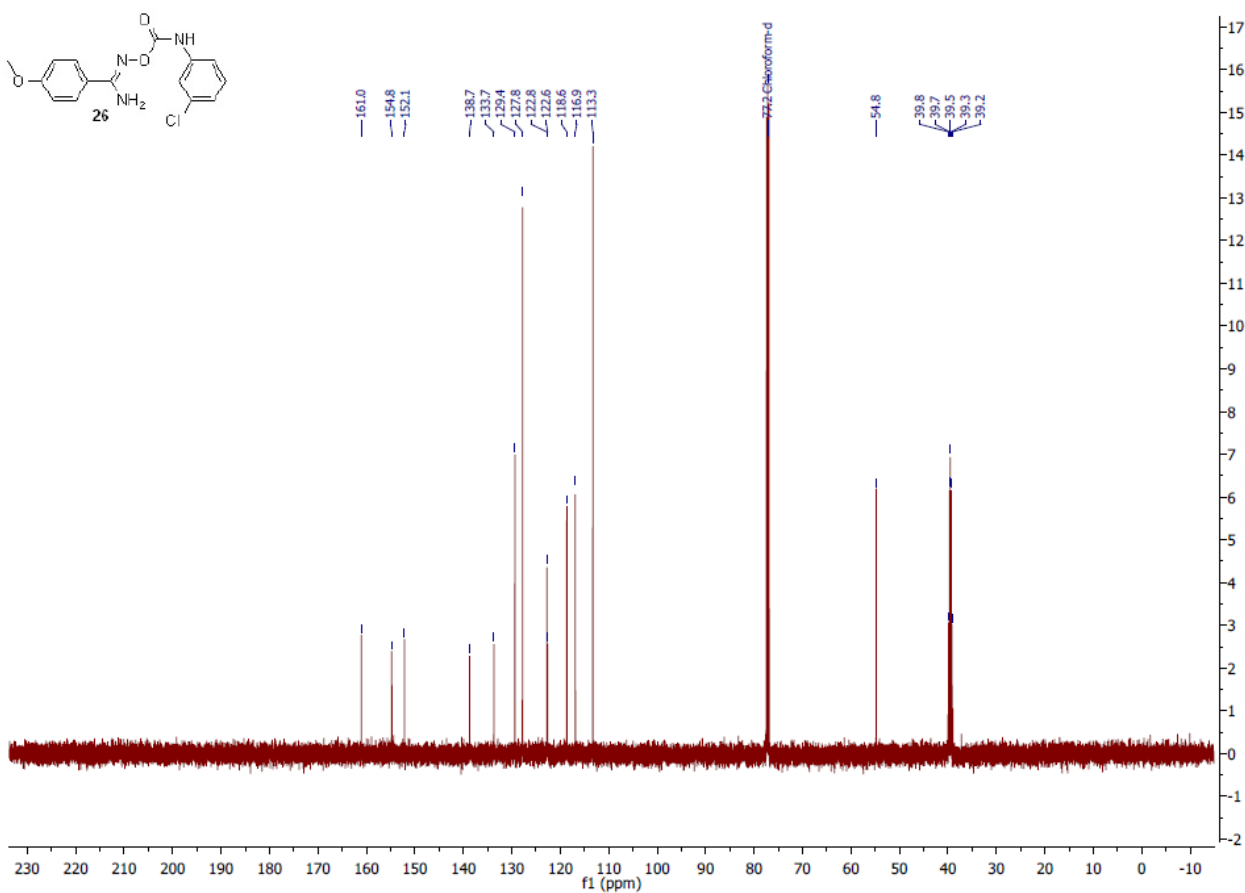
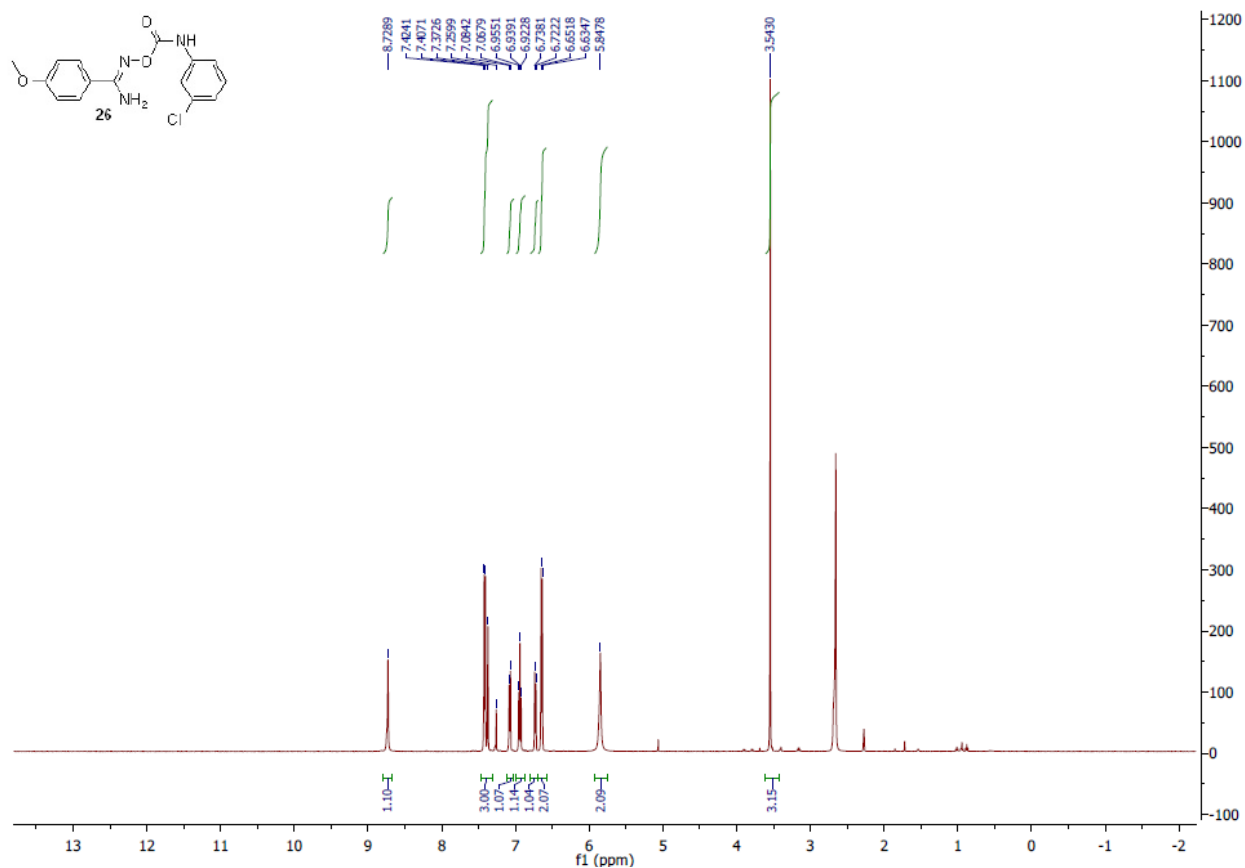


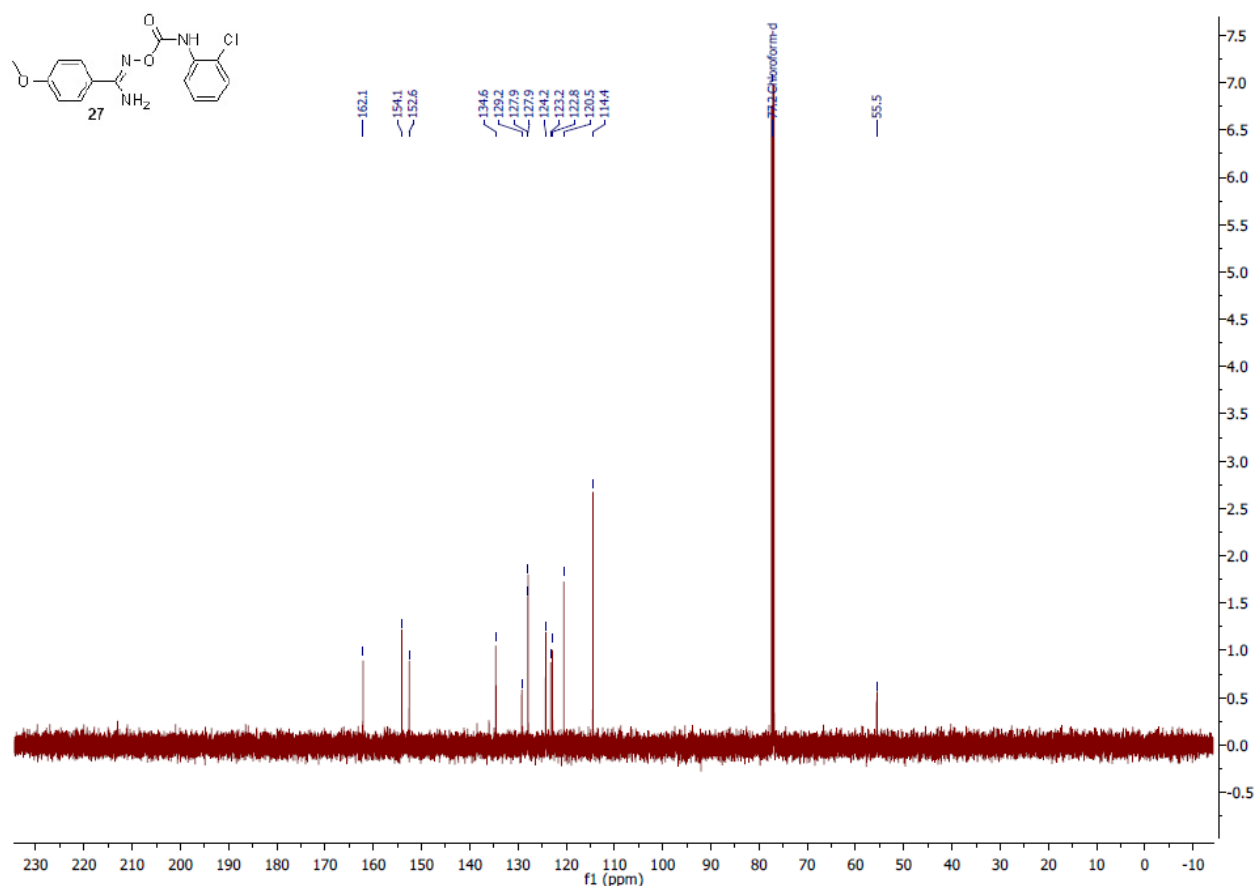
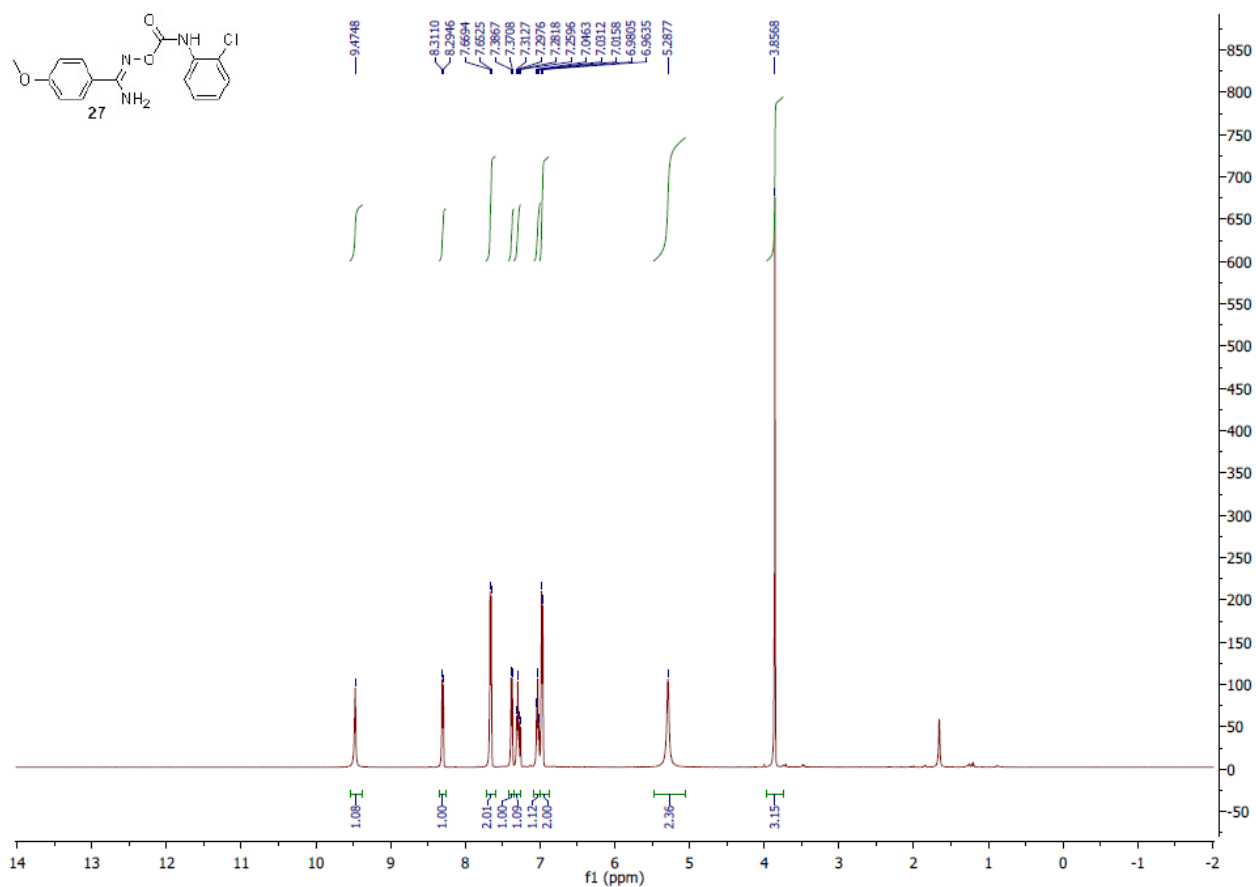


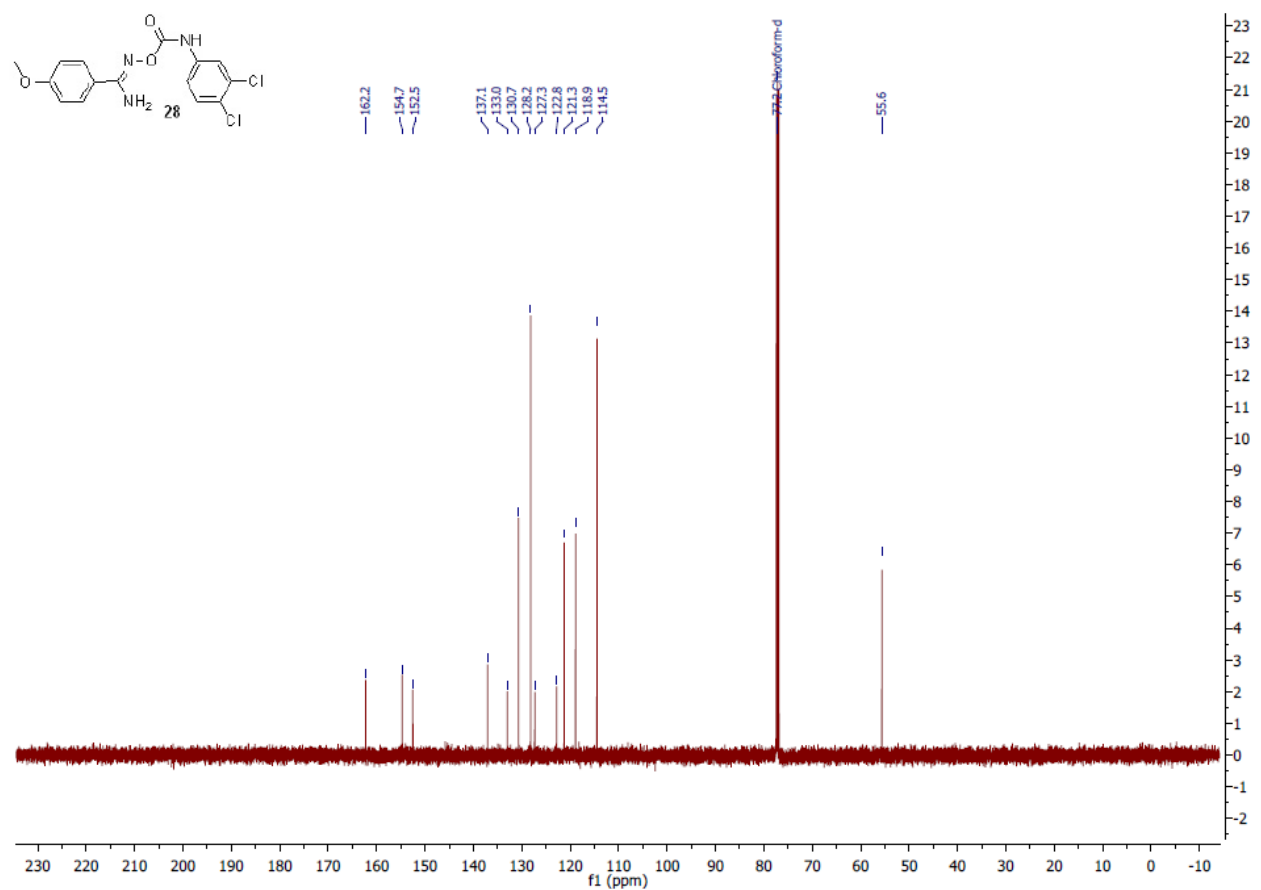
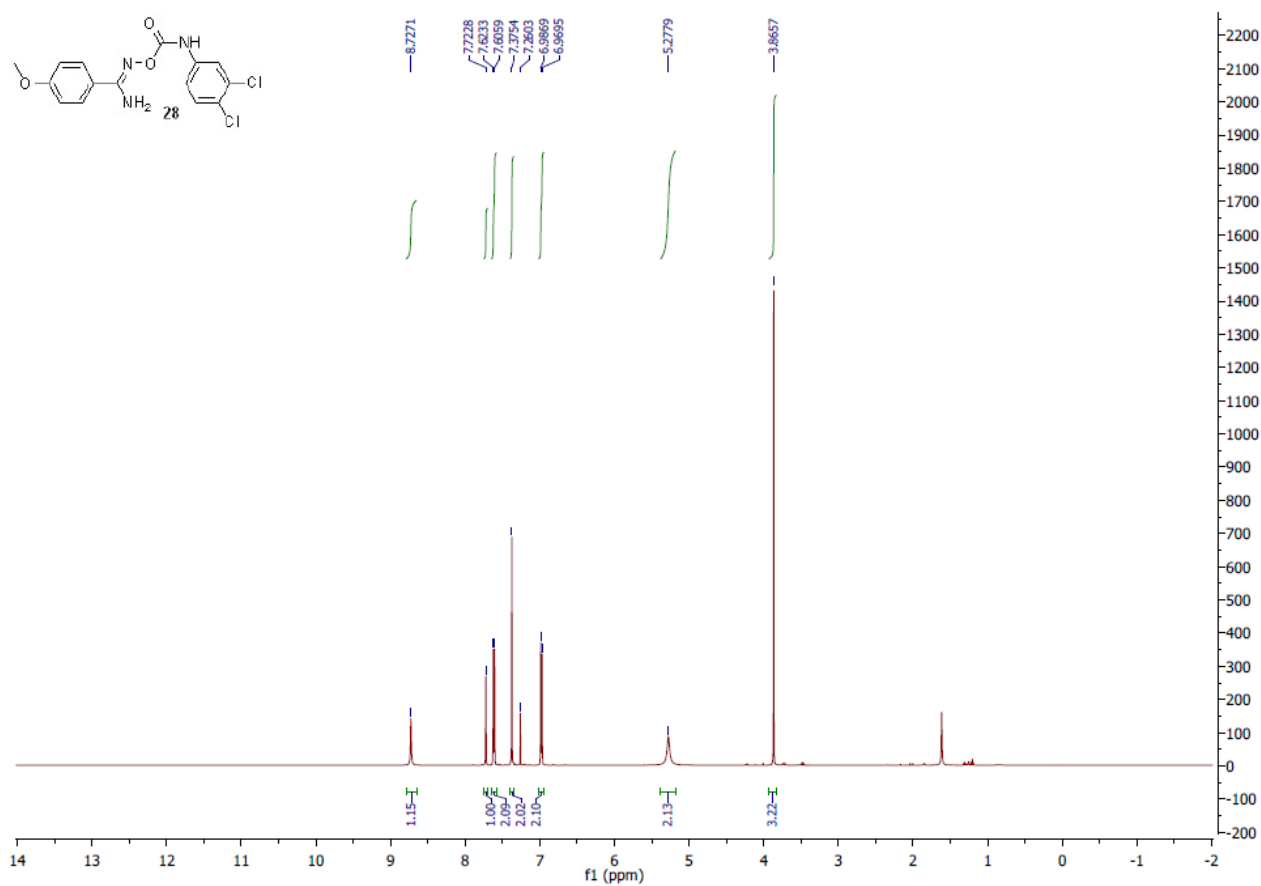


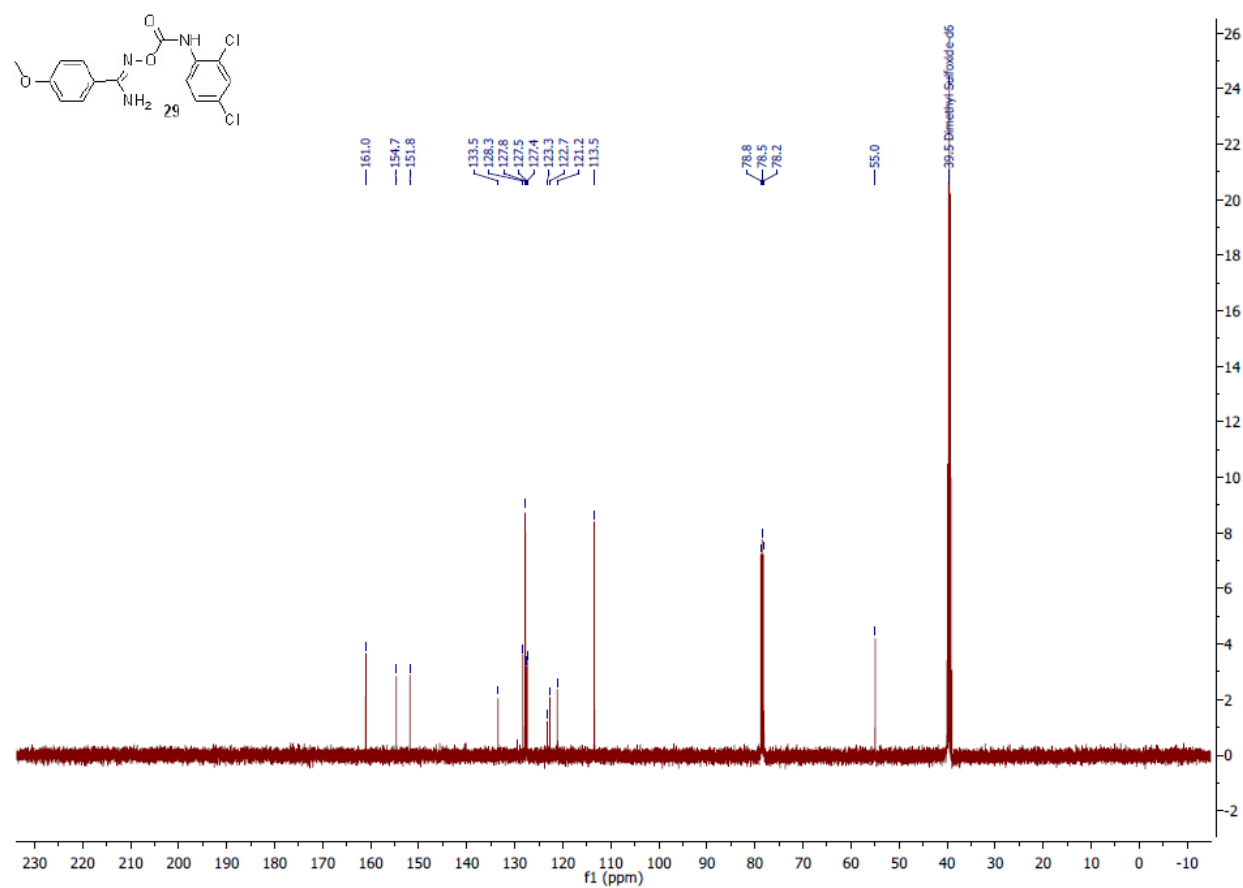
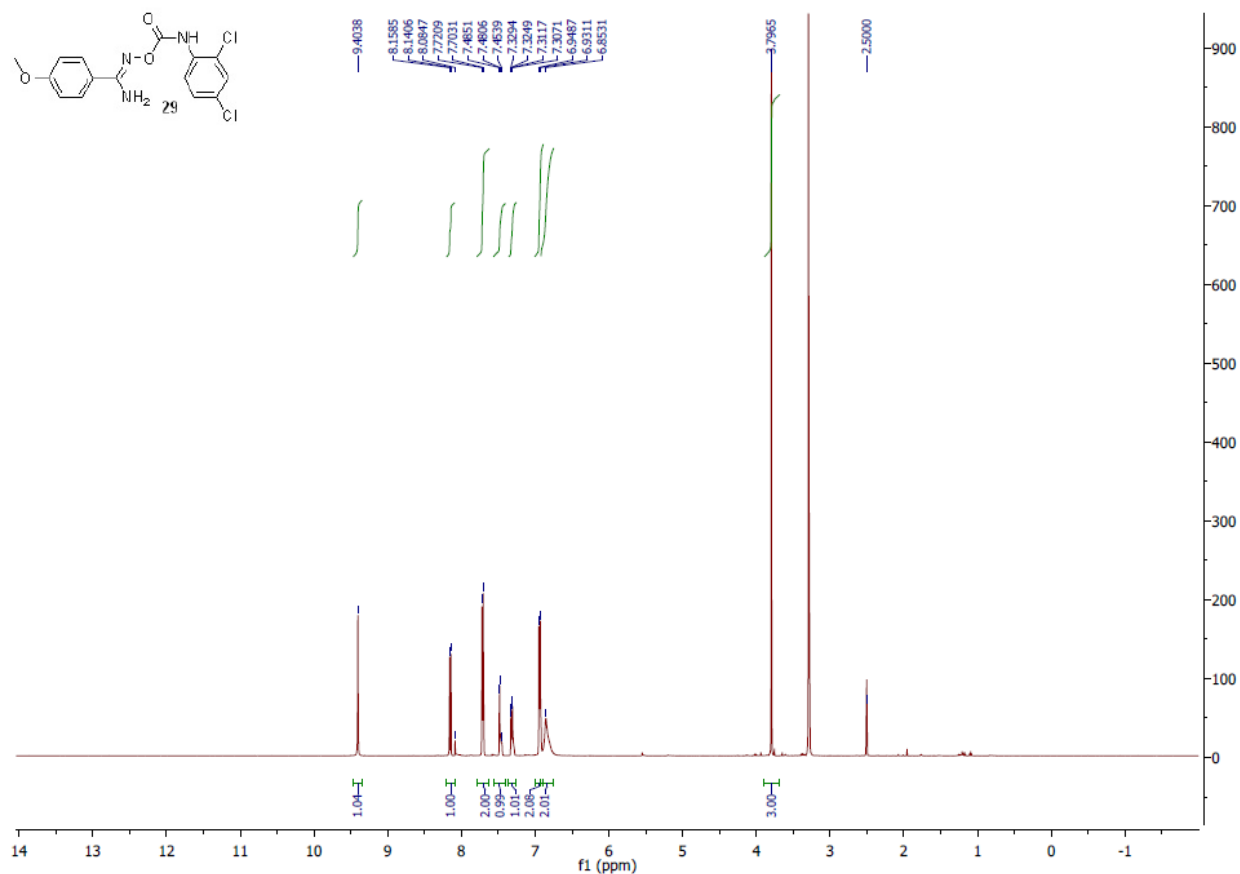


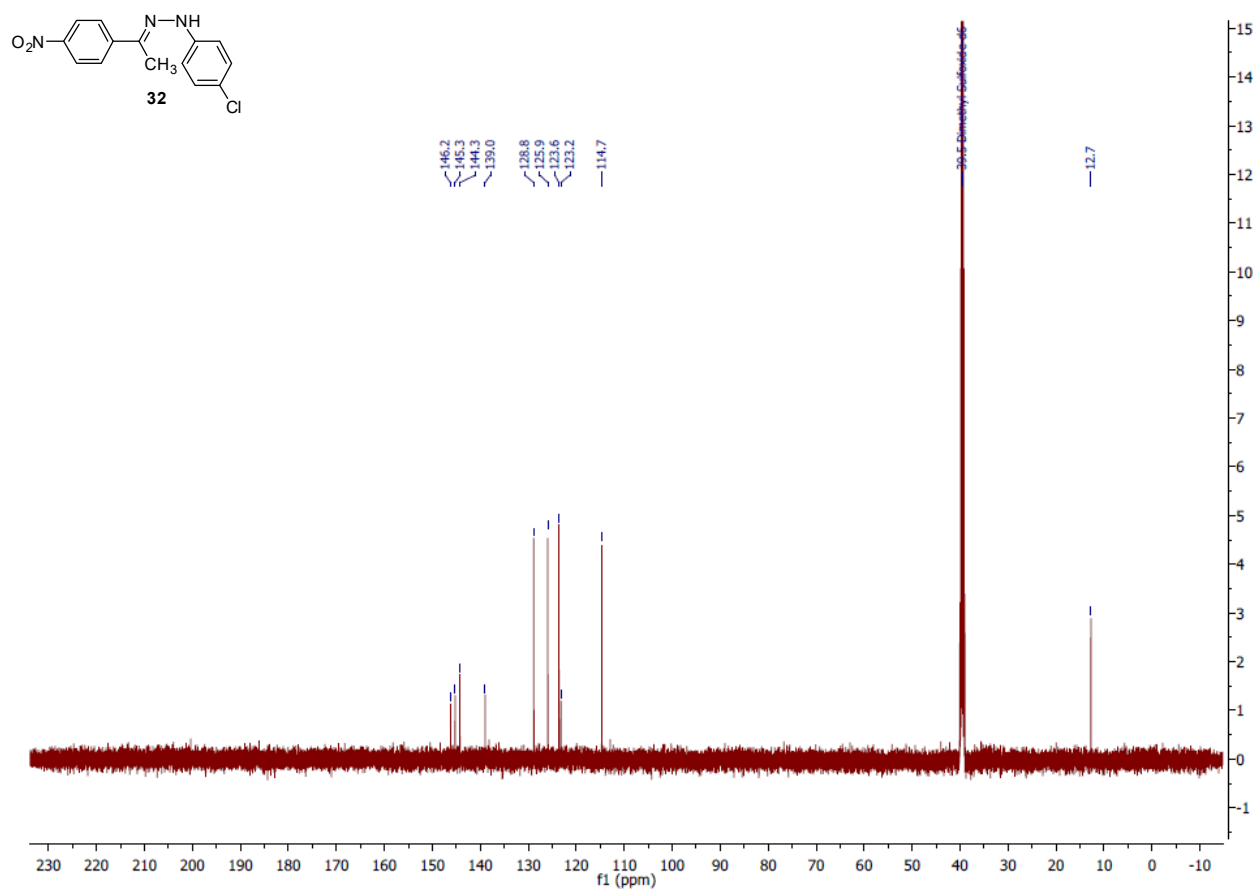
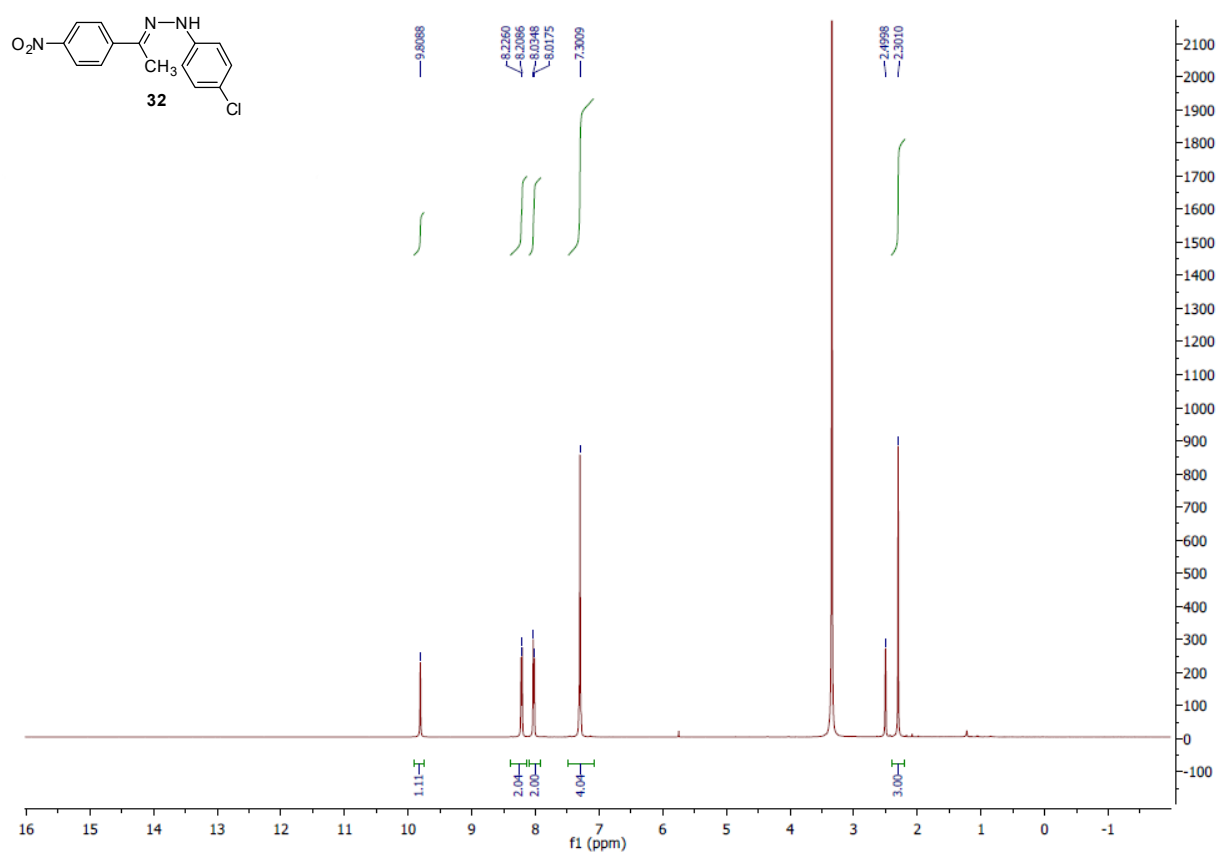






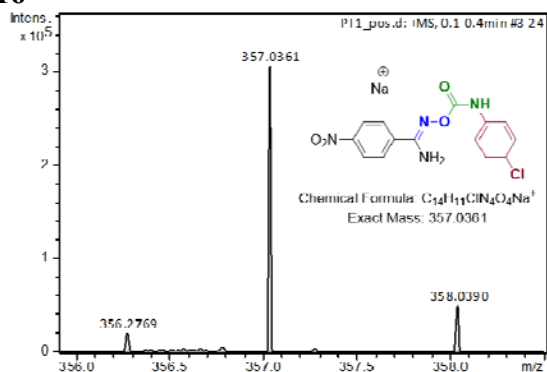






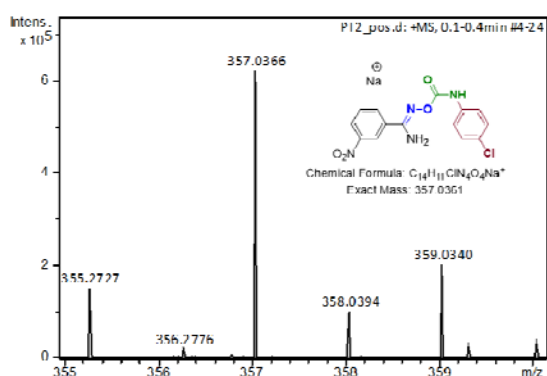
S1B. Copies of HRMS measurements.

16



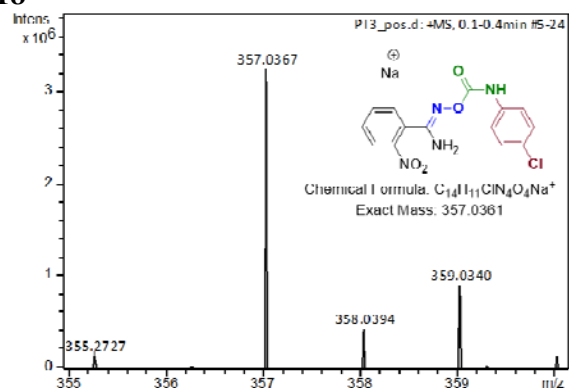
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$[M+Na]^+$ 357.0361	357.0361	0.00

17



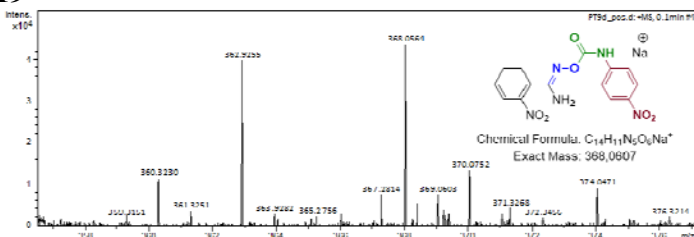
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 357.0361	357.0366	1.40

18

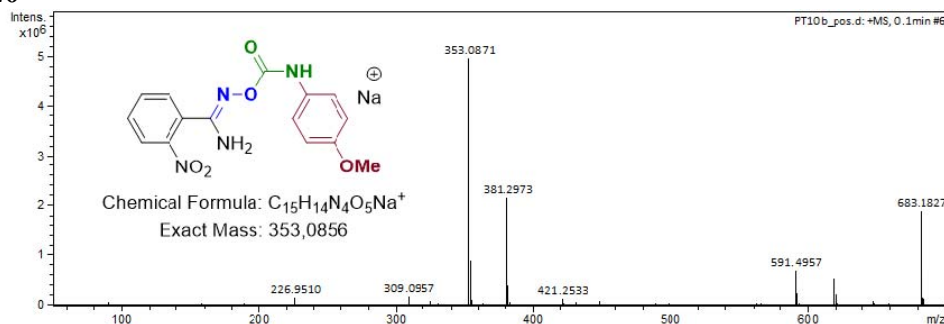


Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 357.0361	357.0367	1.68

19

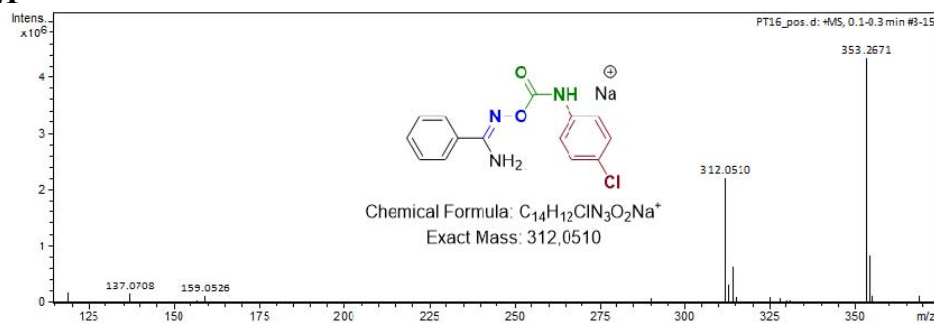


20



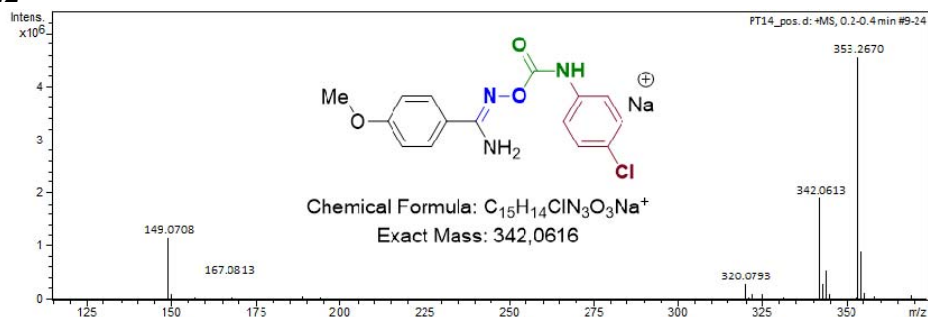
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 353.0856	353.0871	4.25

21



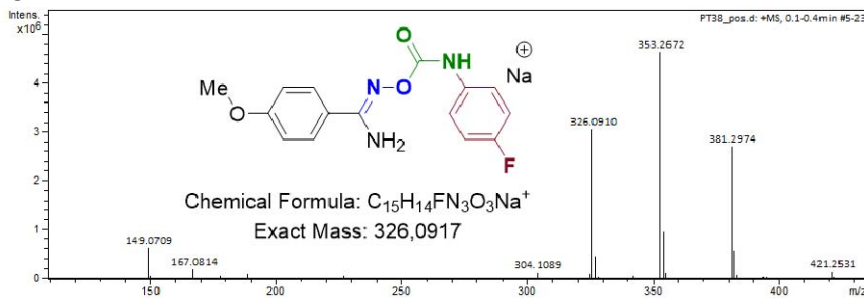
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 312.0510	312.0510	0.00

22



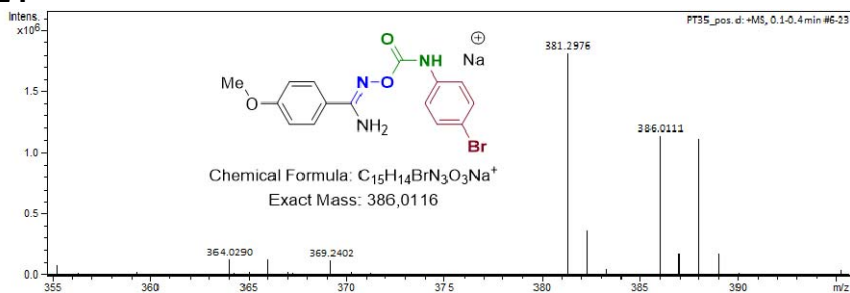
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 342.0616	342.0613	0.88

23



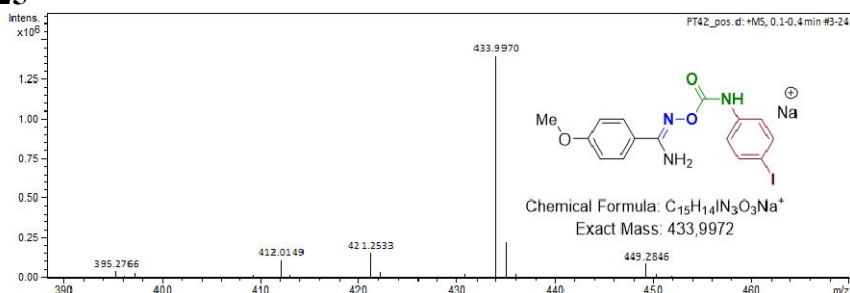
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 326.0917	326.0910	2.15
$[M+H]^+$ 304.1092	304.1089	0.99

24



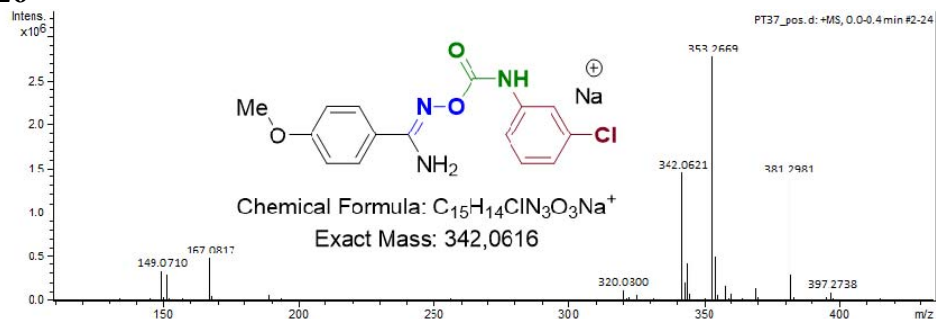
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 386.0116	386.0111	1.31
$[M+H]^+$ 364.0291	364.0290	0.27

25



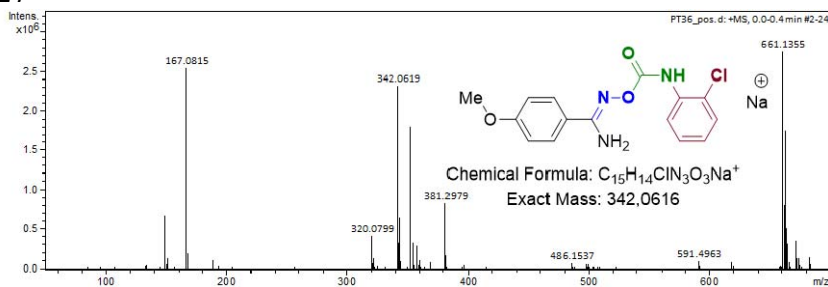
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 433.9972	433.9970	0.46
$[M+H]^+$ 412.0152	412.0149	0.73

26



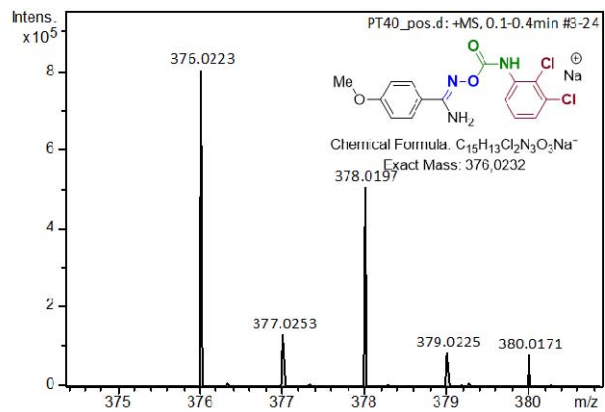
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 342.0616	342.0621	1.46
$[M+H]^+$ 320.0796	320.0800	1.25

27



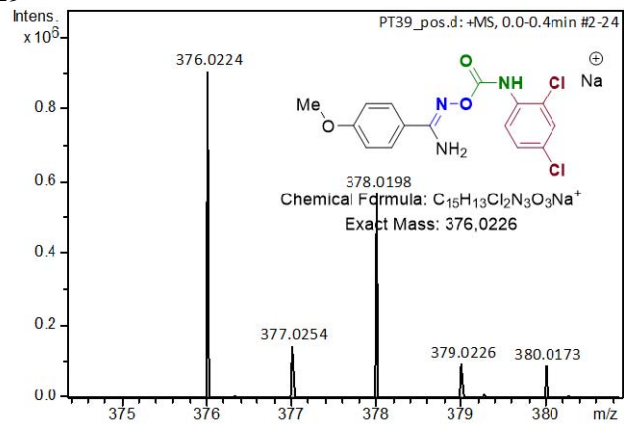
Ion m/z theoretical	ion m/z observed	mass error (ppm)
$[M+Na]^+$ 342.0616	342.0619	0.88
$[M+H]^+$ 320.0796	320.0799	0.94

28



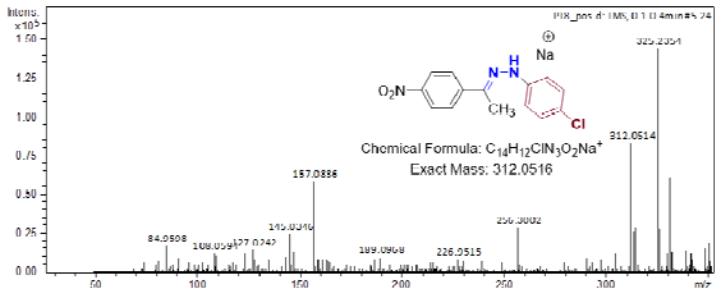
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[M+Na] ⁺ 376.0226	376.0223	2.39

29



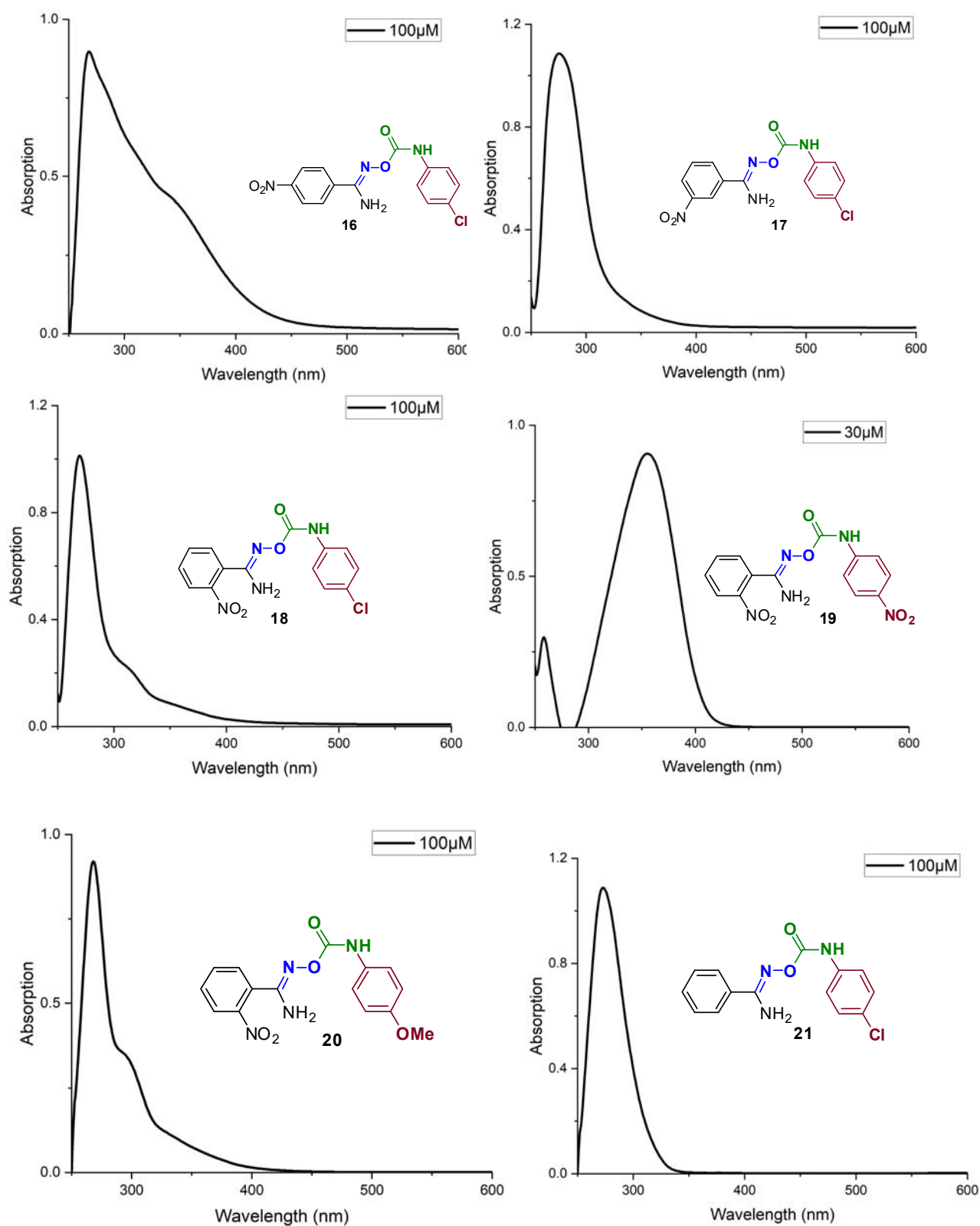
Ion m/z theoretical	ion m/z observed	mass error (ppm)
[M+Na] ⁺ 376.0226	376.0224	0.53

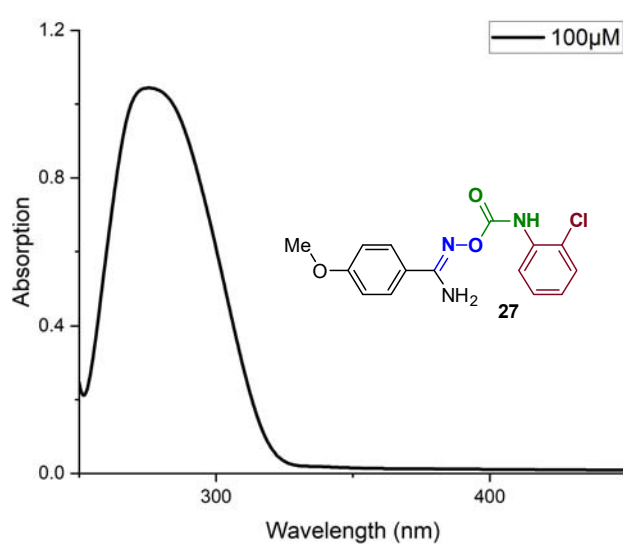
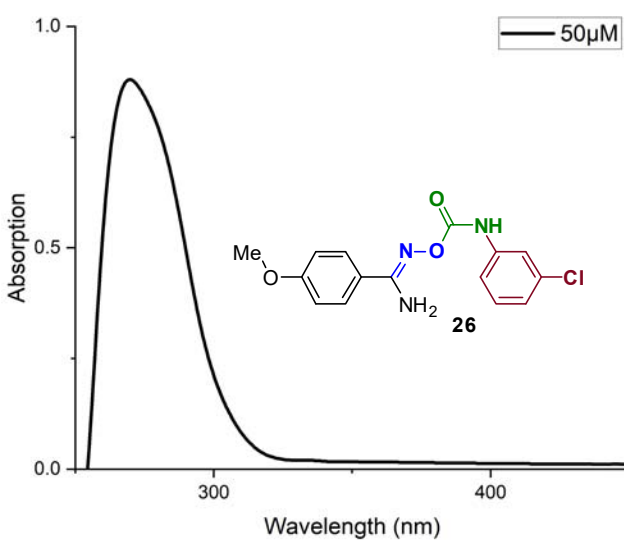
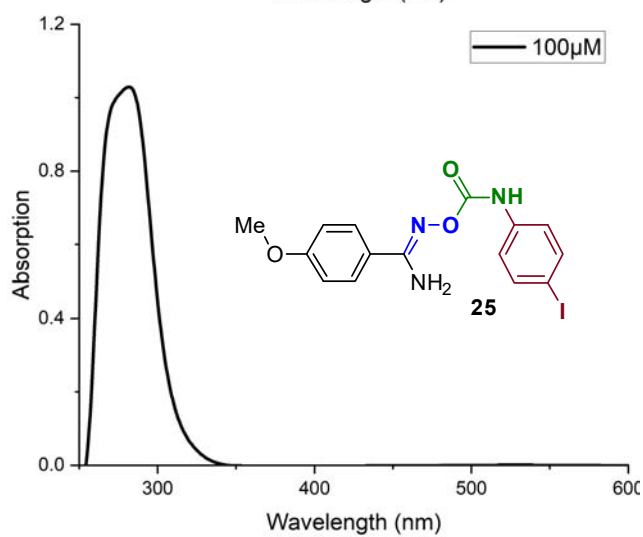
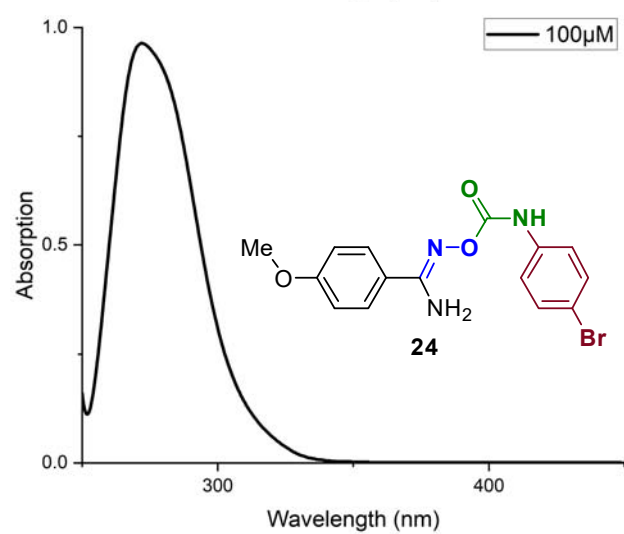
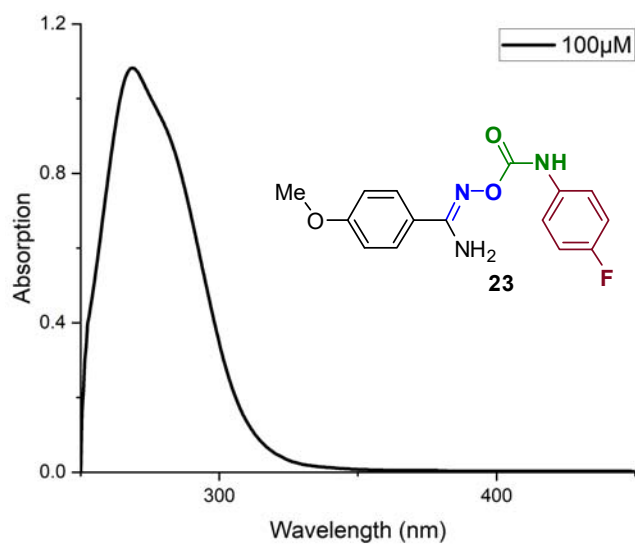
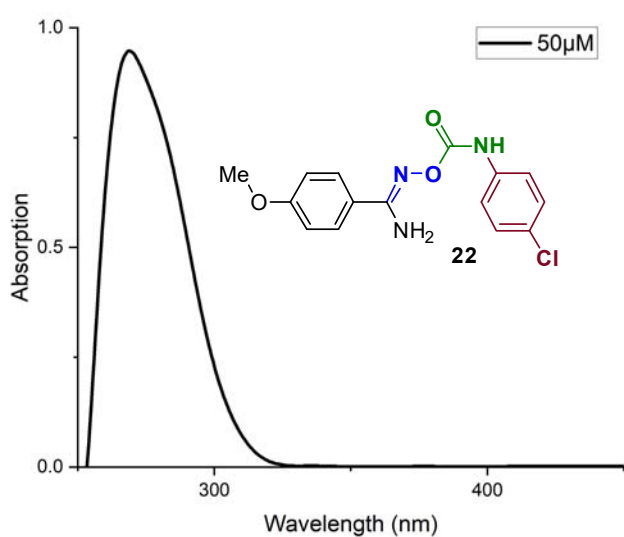
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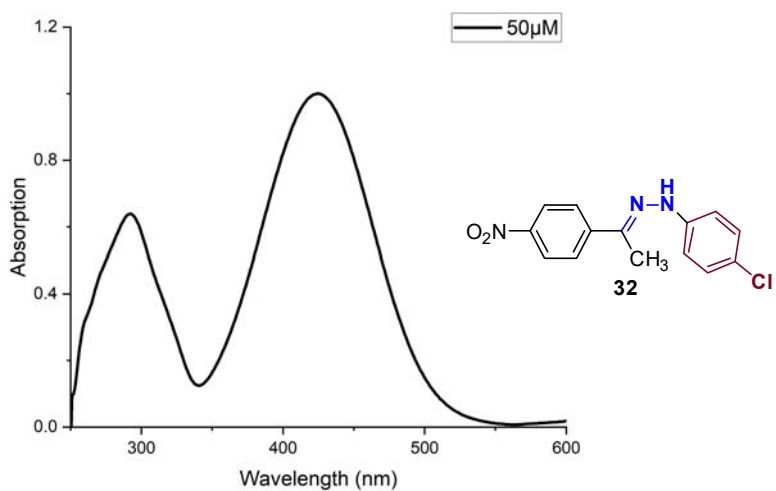
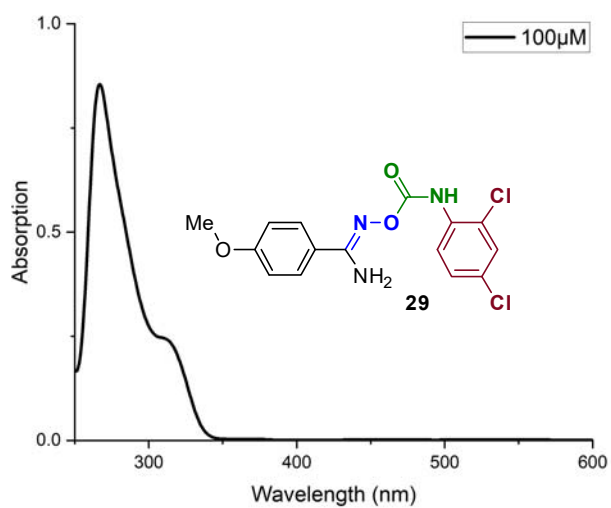
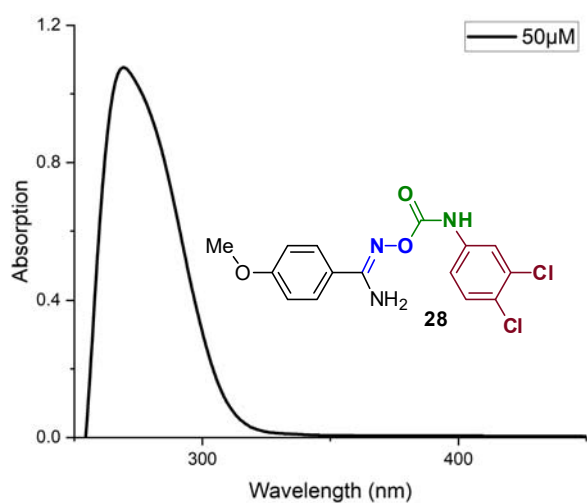


Ion m/z theoretical	ion m/z observed	mass error (ppm)
[M+Na] ⁺ 312.0516	312.0514	0.64

S2A. UV-vis spectra, in DMSO.







S2B. Copies of UV-Vis spectra of compounds 17, 22, 26 and 28 upon increasing amounts of CT-DNA

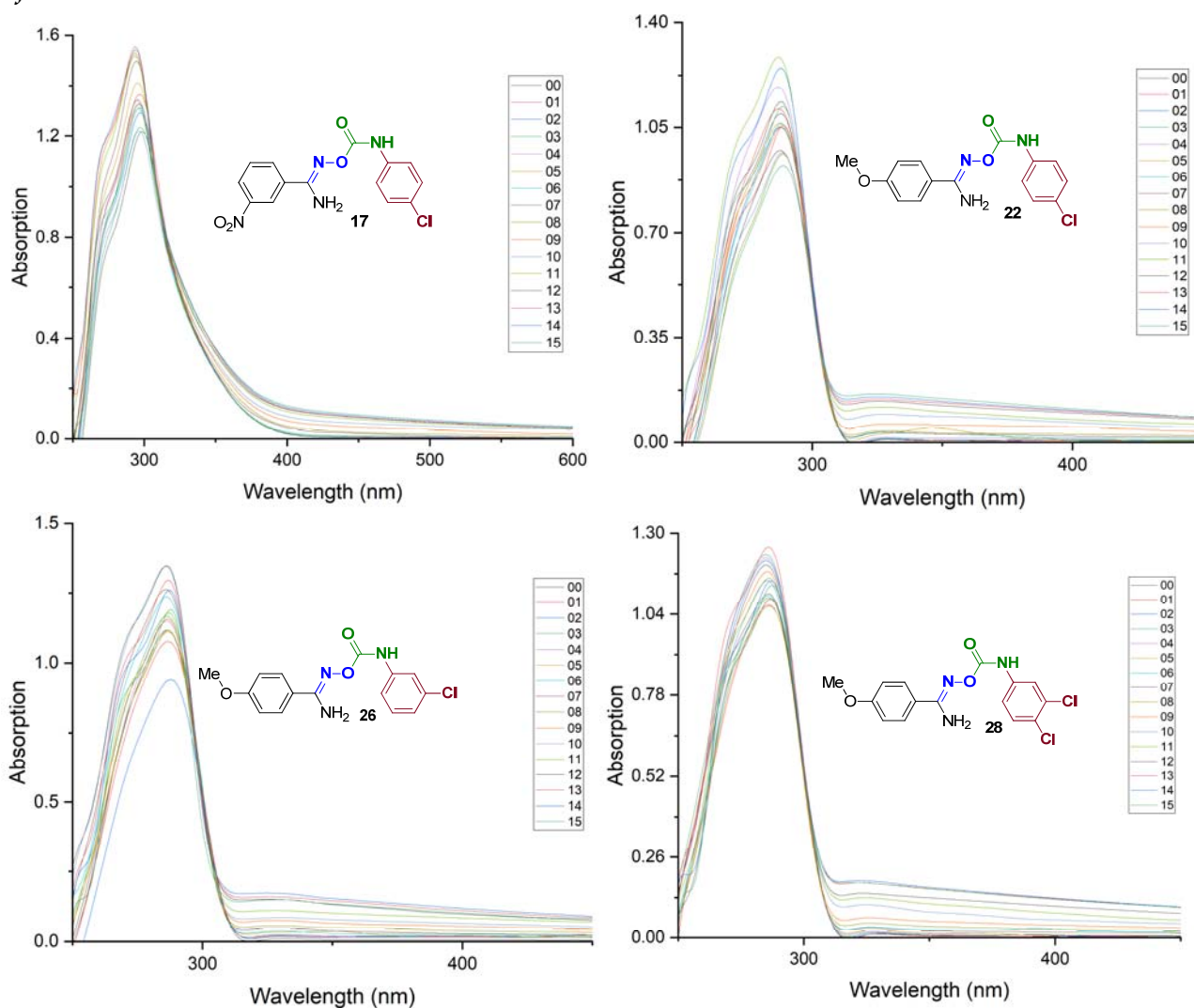


Table. UV-vis spectral features of the interaction of the compounds **17**, **22**, **26** and **28** (500 μ M) with CT DNA. UV-band (λ in nm) (percentage of the observed hyper-/hypochromism ($\Delta A/A_0$, in %), blue-/red-shift of the λ_{\max} ($\Delta\lambda$, in nm)) and DNA-binding constants (K_b , in M^{-1}).

Compound	λ (nm) ($\Delta A/A_0$ (%), ^a $\Delta\lambda$ (nm) ^b)	K_b (M^{-1})
17	298 (+25, ^a -5 ^b)	$4.66(\pm 0.15) \times 10^6$
22	287 (+22, 0)	$9.11(\pm 0.09) \times 10^5$
26	286 (+21, 0)	$4.24(\pm 0.13) \times 10^5$
28	285 (-11, ^a +2 ^b)	$7.24(\pm 0.08) \times 10^5$

^a "+" denotes hyperchromism, "-" denotes hypochromism.

^b "+" denotes red-shift, "-" denotes blue-shift.

S3. Gel electrophoresis pictures and plots

S3A.

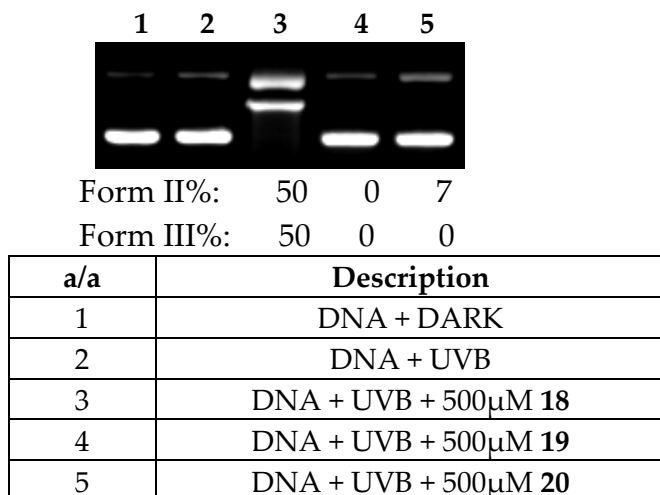


Figure S3A. Gel electrophoresis picture of the UVB irradiation of compounds **18-20** upon incubation with plasmid DNA.

S3B.

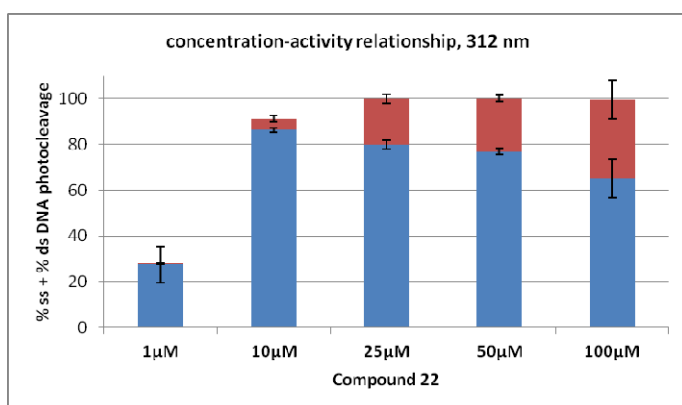


Figure S3B. Plots that depict all values derived from all experiments for compound **22** at various concentrations.

S3C.

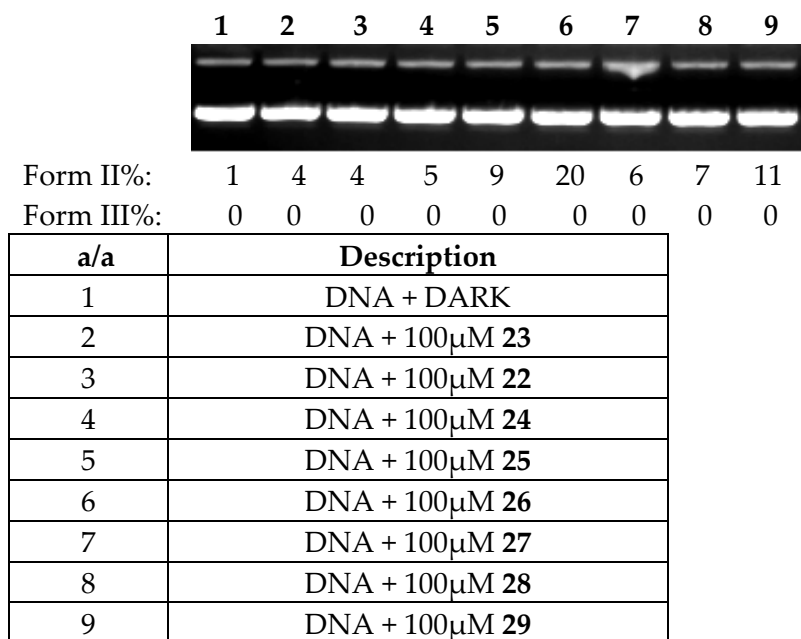
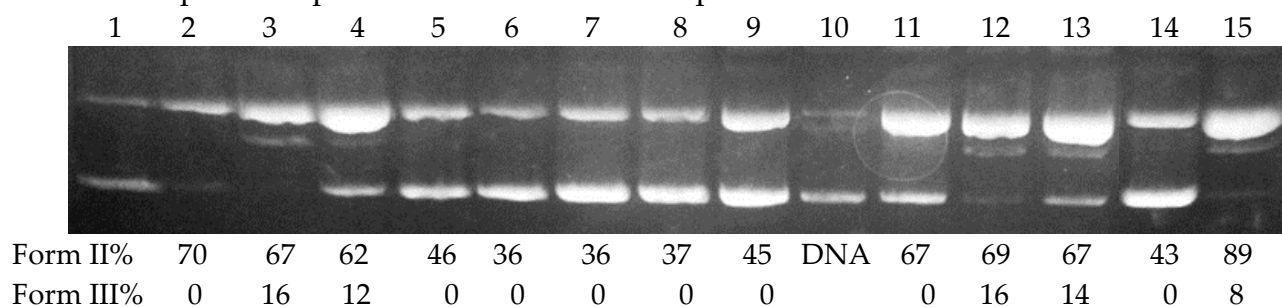


Figure S3C. Gel electrophoresis picture of compounds **22-29** upon incubation with plasmid DNA for 30 min in dark.

S3D.

Figure S3D. Gel electrophoresis picture of compounds **16-29** and **32** under UVA irradiation. pBluescript SK II was used in this experiment.



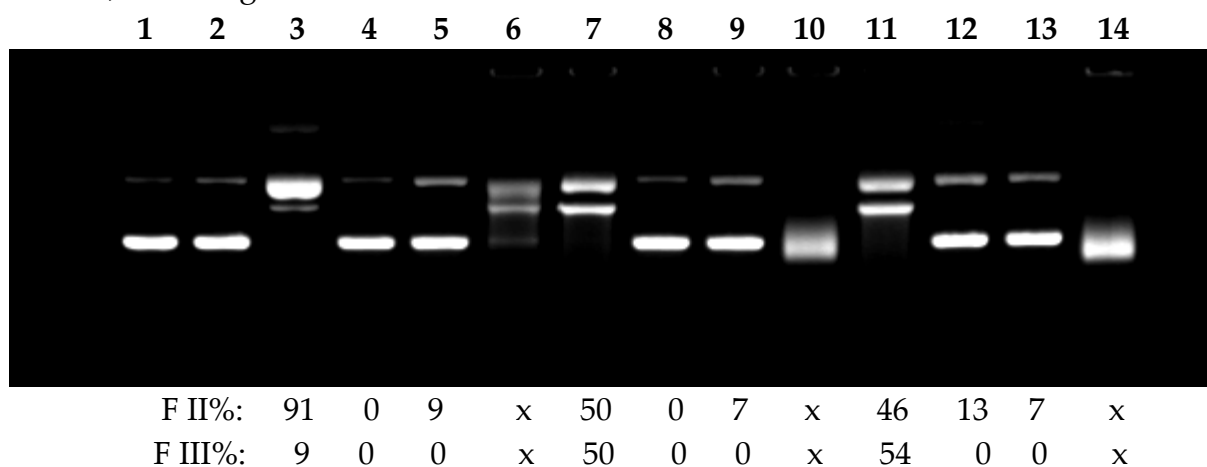
1	DNA + UVA	10	DNA + UVA
2	DNA + UVA + 100μM 23	11	DNA + UVA + 100μM 16
3	DNA + UVA + 100μM 22	12	DNA + UVA + 100μM 17
4	DNA + UVA + 100μM 24	13	DNA + UVA + 100μM 18
5	DNA + UVA + 100μM 25	14	DNA + UVA + 100μM 31
6	DNA + UVA + 100μM 26	15	DNA + UVA + 100μM 21
7	DNA + UVA + 100μM 27		
8	DNA + UVA + 100μM 28		
9	DNA + UVA + 100μM 29		

S.4. Uncropped gels

312 nm

1. 312nm, 15cm, 30min, tris pH=6.8, C= 500 μ M

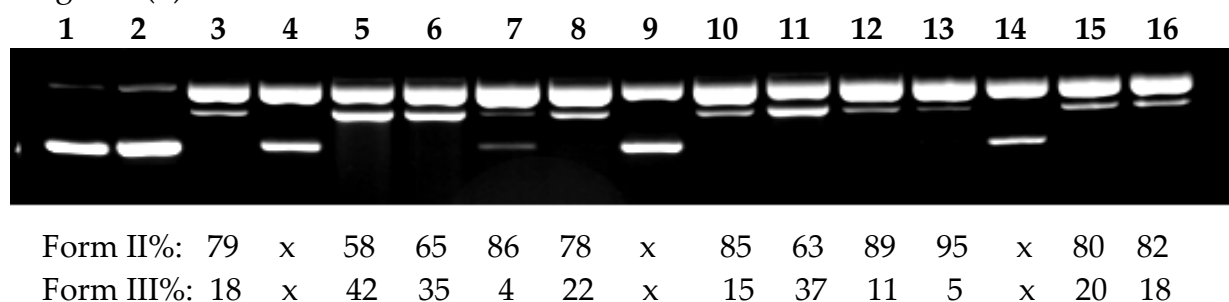
Lines 1, 7-9 in Figure S.3.A.



a/a	description	a/a	description
1	DNA + DARK	8	DNA + UVB + 19
2	DNA + UVB	9	DNA + UVB + 20
3	DNA + UVB + 18	10	Irrelevant (x)
4	DNA + UVB + 19	11	DNA + UVB + 18
5	DNA + UVB + 20	12	DNA + UVB + 19
6	Irrelevant (x)	13	DNA + UVB + 20
7	DNA + UVB + 18	14	Irrelevant (x)

2. 312nm, 15cm, 30min, tris pH=6.8, C= 100 μ M

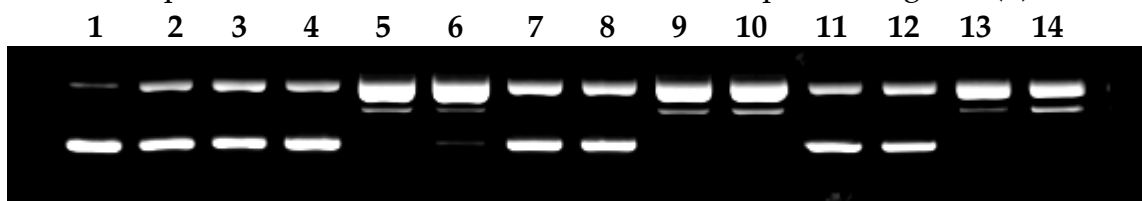
Lines 1,2,5,6,7,8 of present gel in Figure 2(a) for controls and compounds 22, 21, 18 and 16, respectively. The values of the rest are incorporated in the statistics of 22, 21, 18 and 16 in plots of Figure 2(b).



a/a	description	a/a	description
1	DNA+ dark	9	Irrelevant (x)
2	DNA+ UVB	10	DNA + UVB + 22
3	DNA + UVB + 16	11	DNA + UVB + 21
4	Irrelevant (x)	12	DNA + UVB + 18
5	DNA + UVB + 22	13	DNA + UVB + 16
6	DNA + UVB + 21	14	Irrelevant (x)
7	DNA + UVB + 18	15	DNA + UVB + 22
8	DNA + UVB + 16	16	DNA + UVB + 21

3. 312nm, 15cm, 30min, tris pH=6.8

Lines 12,13,4,5,8,9 of present gel in Figure 2(a) for compounds **21**, **18** and **16**. The values of the rest are incorporated in the statistics of **21**, **18** and **16** in plots of Figure 2(b).



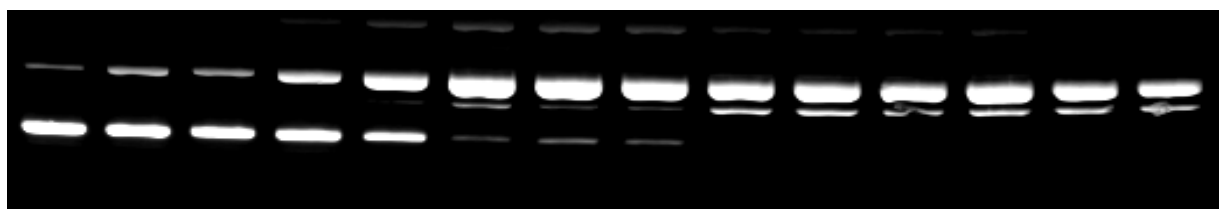
Form II%: 35 30 91 94 42 40 90 87 35 41 95 81
Form III%: 0 0 9 4 0 0 10 13 0 0 5 19

a/a	description	a/a	description
1	DNA + dark	9	DNA + UVB + 16 , 50μM
2	DNA + UVB	10	DNA + UVB + 16 , 50μM
3	DNA + UVB + 18 , 1μM	11	DNA + UVB + 21 , 1μM
4	DNA + UVB + 18 , 1μM	12	DNA + UVB + 21 , 1μM
5	DNA + UVB + 18 , 50μM	13	DNA + UVB + 21 , 50μM
6	DNA + UVB + 18 , 50μM	14	DNA + UVB + 21 , 50μM
7	DNA + UVB + 16 , 1μM		
8	DNA + UVB + 16 , 1μM		

4. 312nm, 15cm, 30min, tris pH=6.8

Lines 4,9 of present gel in Figure 2(a) for compound **22**. The values of the rest are incorporated in the statistics of **22** in plots of Figure 2(b) and SI, S.3.B.

1 2 3 4 5 6 7 8 9 10 11 12 13 14

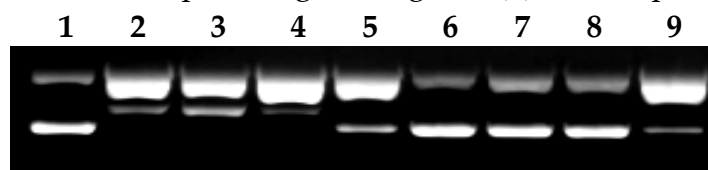


Form II%: 0 20 42 83 84 88 76 74 83 76 75 72
Form III%: 0 0 1 10 3 3 24 26 17 24 25 28

a/a	description	a/a	description
1	DNA+ dark	9	DNA + UVB + 22 , 25μM
2	DNA + UVB	10	DNA + UVB + 22 , 25μM
3	DNA + UVB + 22 , 1μM	11	DNA + UVB + 22 , 25μM
4	DNA + UVB + 22 , 1μM	12	DNA + UVB + 22 , 50μM
5	DNA + UVB + 22 , 1μM	13	DNA + UVB + 22 , 50μM
6	DNA + UVB + 22 , 10μM	14	DNA + UVB + 22 , 50μM
7	DNA + UVB + 22 , 10μM		
8	DNA + UVB + 22 , 10μM		

5. 312nm, 15cm, 30min, tris pH=6.8, 100 μ M

Lines 1-9 of present gel in Figure 3(a) for compounds **22-29**.

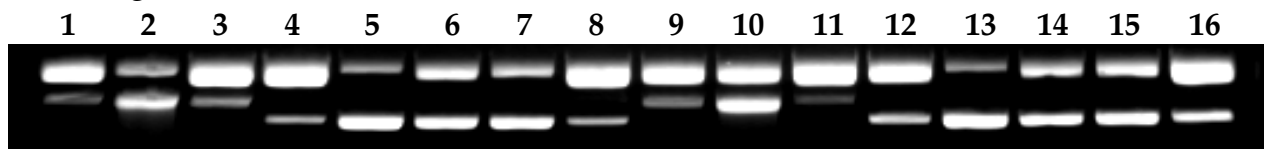


F II%: 87 74 95 74 3 18 15 87
F III%: 13 26 5 0 0 0 0 0

a/a	description
1	DNA+ UVB
2	DNA + UVB + 23
3	DNA + UVB + 22
4	DNA + UVB + 24
5	DNA + UVB + 25
6	DNA + UVB + 26
7	DNA + UVB + 27
8	DNA + UVB + 28
9	DNA + UVB + 29

6. 312nm, 15cm, 30min, tris pH=6.8, 100 μ M

The values of the present and the former gels are incorporated in the statistics of **22-29** in plots of Figure 3(b).

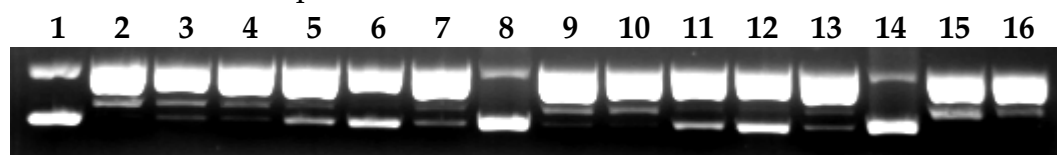


FI %: 82 19 79 73 1 30 20 72 76 42 90 58 0 26 27 54
FIII%: 18 81 21 0 0 0 0 0 24 58 10 0 0 0 0 0

a/a	description	a/a	description
1	DNA + UVB + 23	9	DNA + UVB + 23
2	DNA + UVB + 22	10	DNA + UVB + 22
3	DNA + UVB + 24	11	DNA + UVB + 24
4	DNA + UVB + 25	12	DNA + UVB + 25
5	DNA + UVB + 26	13	DNA + UVB + 26
6	DNA + UVB + 27	14	DNA + UVB + 27
7	DNA + UVB + 28	15	DNA + UVB + 28
8	DNA + UVB + 29	16	DNA + UVB + 29

7. 312nm, 15cm, 30min, tris pH=6.8, 100 μ M, mechanistic study of the DNA photocleavage of compound 22

The values of the present gel lanes 1-8 are incorporated in Figure 4(b). The rest is the second run of the experiment.

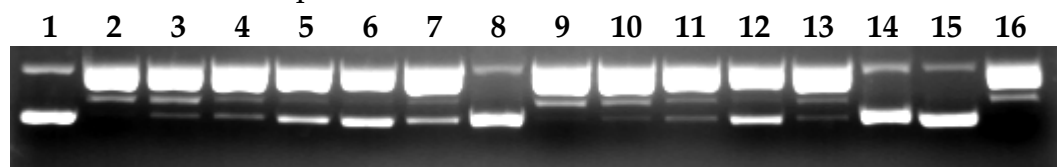


FII%: 80 76 86 73 52 80 0 83 84 70 46 87 0 72 87
FIII%: 20 17 11 6 0 7 0 14 14 5 6 6 0 28 13

a/a	description	a/a	description
1	DNA + UVB	9	DNA + UVB + 22
2	DNA + UVB + 22	10	DNA + UVB + 22 + 1500 μ M cyst
3	DNA + UVB + 22 + argon	11	DNA + UVB + 22 + 250 μ M KI
4	DNA + UVB + 22 + 1500 μ M cyst	12	DNA + UVB + 22 + 20 mM NaN ₃
5	DNA + UVB + 22 + 250 μ M KI	13	DNA + UVB + 22 + D ₂ O
6	DNA + UVB + 22 + 20 mM NaN ₃	14	DNA + UVB + 22 + 20% DMSO
7	DNA + UVB + 22 + D ₂ O	15	DNA + UVB + 22 + 750 μ M Mannitol
8	DNA + UVB + 22 + 20% DMSO	16	DNA + UVB + 22 + 250 μ M hist

8. 312nm, 15cm, 30min, tris pH=6.8, 100 μ M, mechanistic study of the DNA photocleavage of compound 21

The values of the present gel, lanes 1-8 are incorporated in Figure 4(a). The rest is the second run of the experiment.



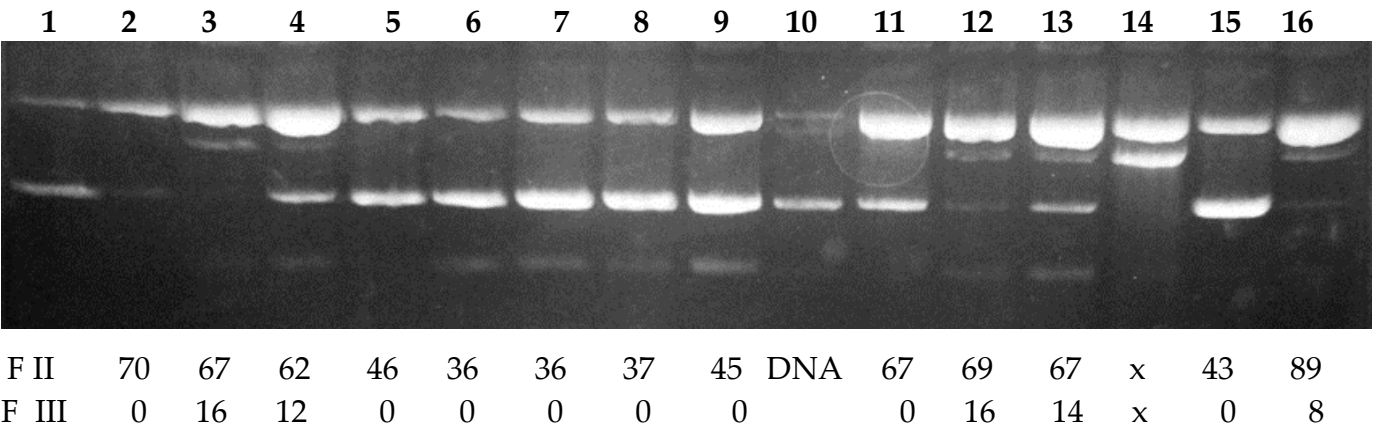
FII%: 83 71 75 56 45 61 0 77 70 63 52 74 1 0 78
FIII%: 17 21 12 10 8 10 0 23 20 19 7 14 0 0 22

a/a	description	a/a	description
1	DNA + UVB	9	DNA + UVB + 21
2	DNA + UVB + 21	10	DNA + UVB + 21 + 1500 μ M cyst
3	DNA + UVB + 21 + argon	11	DNA + UVB + 21 + 250 μ M KI
4	DNA + UVB + 21 + 1500 μ M cyst	12	DNA + UVB + 21 + 20 mM NaN ₃
5	DNA + UVB + 21 + 250 μ M KI	13	DNA + UVB + 21 + D ₂ O
6	DNA + UVB + 21 + 20 mM NaN ₃	14	DNA + UVB + 21 + 20% DMSO
7	DNA + UVB + 21 + D ₂ O	15	Mannitol 750 μ M control
8	DNA + UVB + 21 + 20% DMSO	16	DNA + UVB + 21 + 750 μ M Mannitol

365 nm

1. 365nm, 10cm, 120 min, tris pH=6.8, C= 100 µM

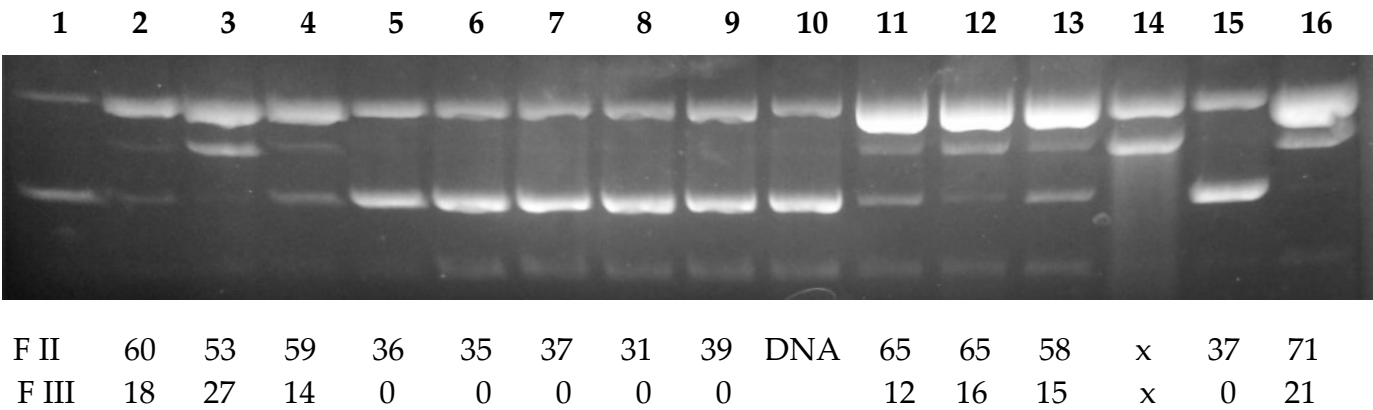
The values of the present gel are incorporated in plots of Figure 5. The whole gel except lane 14 is found in SI, S.3.D.



a/a	description	a/a	description
1	DNA + UVA	10	DNA + UVA
2	DNA + UVA + 23	11	DNA + UVA + 16
3	DNA + UVA + 22	12	DNA + UVA + 17
4	DNA + UVA + 24	13	DNA + UVA + 18
5	DNA + UVA + 25	14	Irrelevant (x)
6	DNA + UVA + 26	15	DNA + UVA + 32
7	DNA + UVA + 27	16	DNA + UVA + 21
8	DNA + UVA + 28		
9	DNA + UVA + 29		

2. 365nm, 10cm, 120 min, tris pH=6.8, C= 100 µM

The values of the present gel are incorporated in plots of Figure 5. pBluescript SK II was used in this experiment.

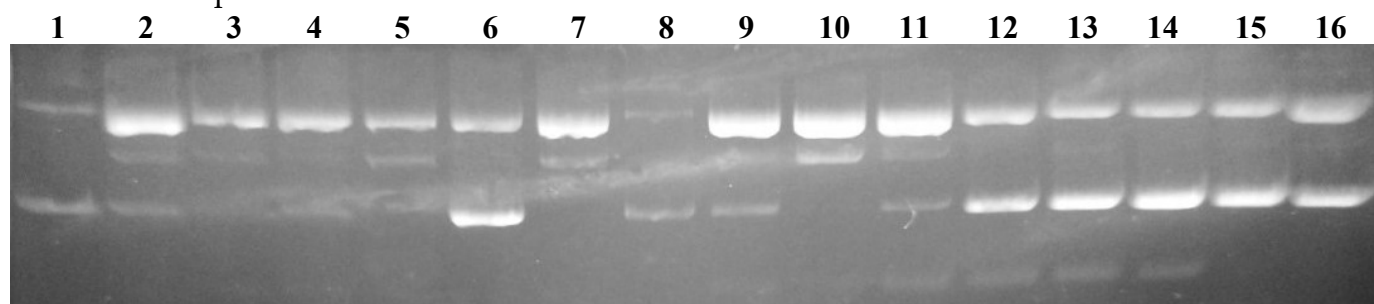


a/a	description	a/a	description
1	DNA + UVA	10	DNA + UVA
2	DNA + UVA + 23	11	DNA + UVA + 16
3	DNA + UVA + 22	12	DNA + UVA + 17
4	DNA + UVA + 24	13	DNA + UVA + 18
5	DNA + UVA + 25	14	Irrelevant (x)

6	DNA + UVA + 26	15	DNA + UVA + 32
7	DNA + UVA + 27	16	DNA + UVA + 21
8	DNA + UVA + 28		
9	DNA + UVA + 29		

3. 365nm, 10cm, 120 min, tris pH=6.8, C= 100 µM

The values of the present gel are incorporated in plots of Figure 5. pBluescript SK II was used in this experiment.



F II	60	49	41	x	37	48	DNA	44	46	55	47	39	34	33	47
F III	14	3	1	x	0	16		2	15	5	0	0	0	0	0

a/a	description	a/a	description
1	DNA + UVA	8	DNA + UVA
2	DNA + UVA + 16	9	DNA + UVA + 23
3	DNA + UVA + 17	10	DNA + UVA + 22
4	DNA + UVA + 18	11	DNA + UVA + 24
5	Irrelevant (x)	12	DNA + UVA + 25
6	DNA + UVA + 32	13	DNA + UVA + 26
7	DNA + UVA + 21	14	DNA + UVA + 27
		15	DNA + UVA + 28
		16	DNA + UVA + 29