

## Supplementary Material

# New Heterocyclic Compounds from Oxazol-5(4*H*)-one and 1,2,4-Triazin-6(5*H*)-one Classes: Synthesis, Characterization and Toxicity Evaluation

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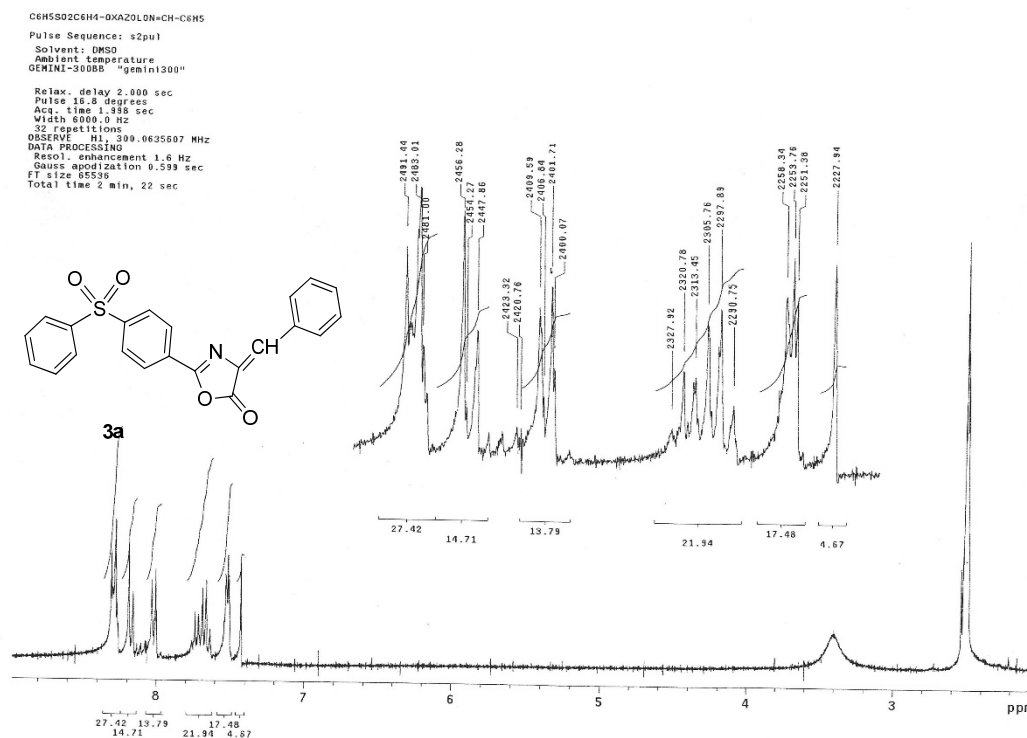


Figure S1. The  $^1\text{H}$ -NMR spectrum of oxazolone **3a**.

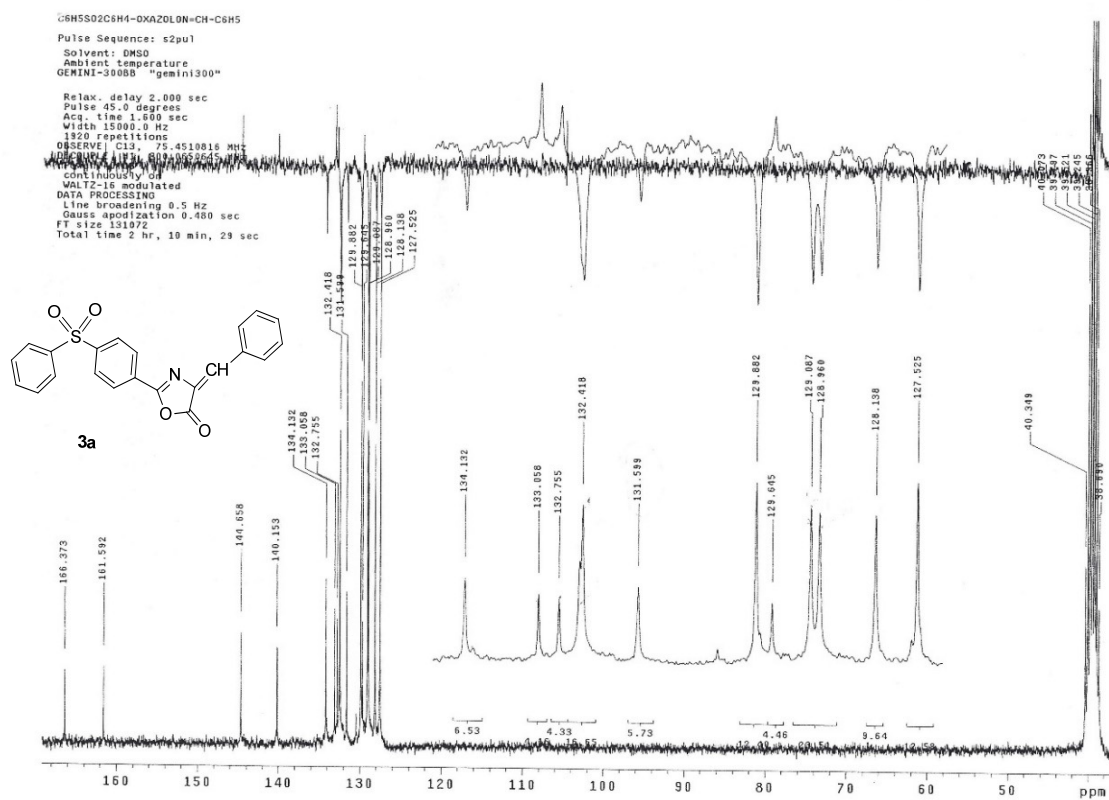


Figure S2. The  $^{13}\text{C}$ -NMR spectrum of oxazolone **3a**.

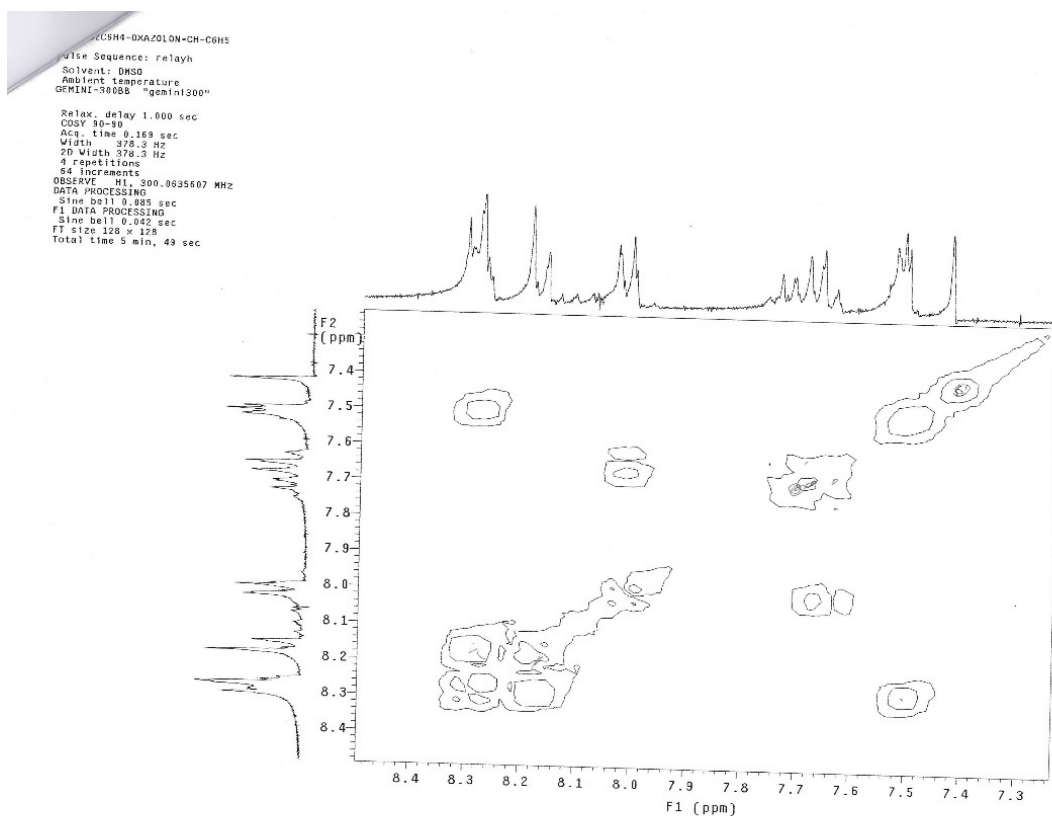


Figure S3. The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of oxazolone 3a.

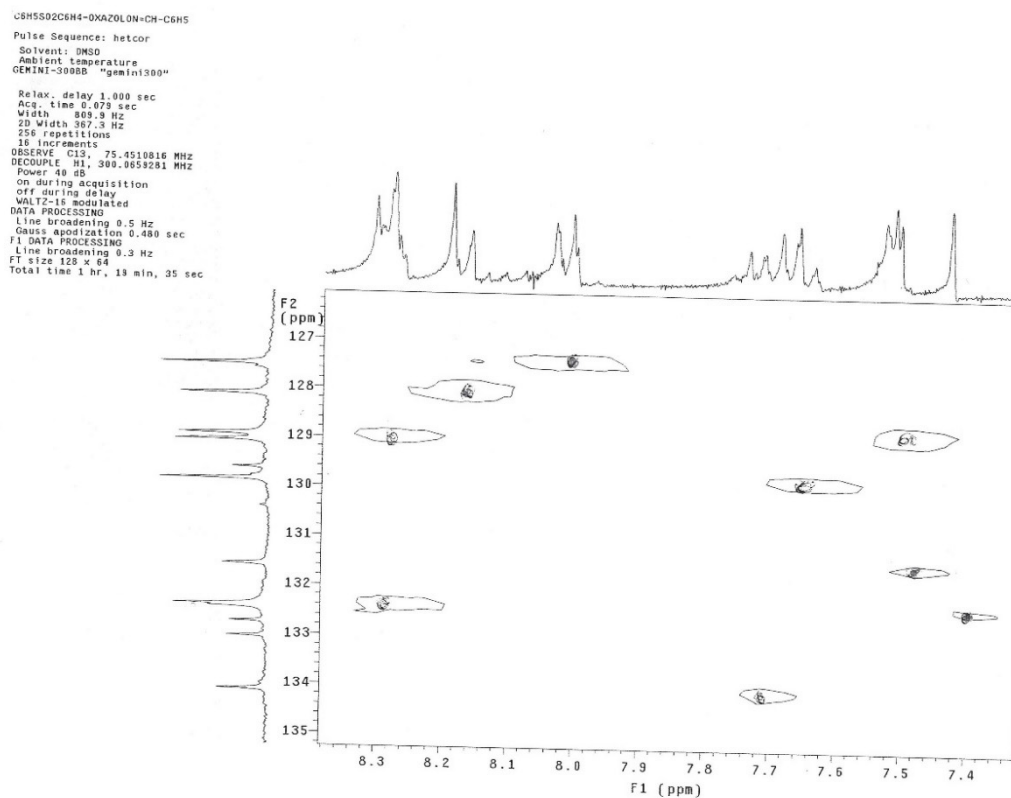
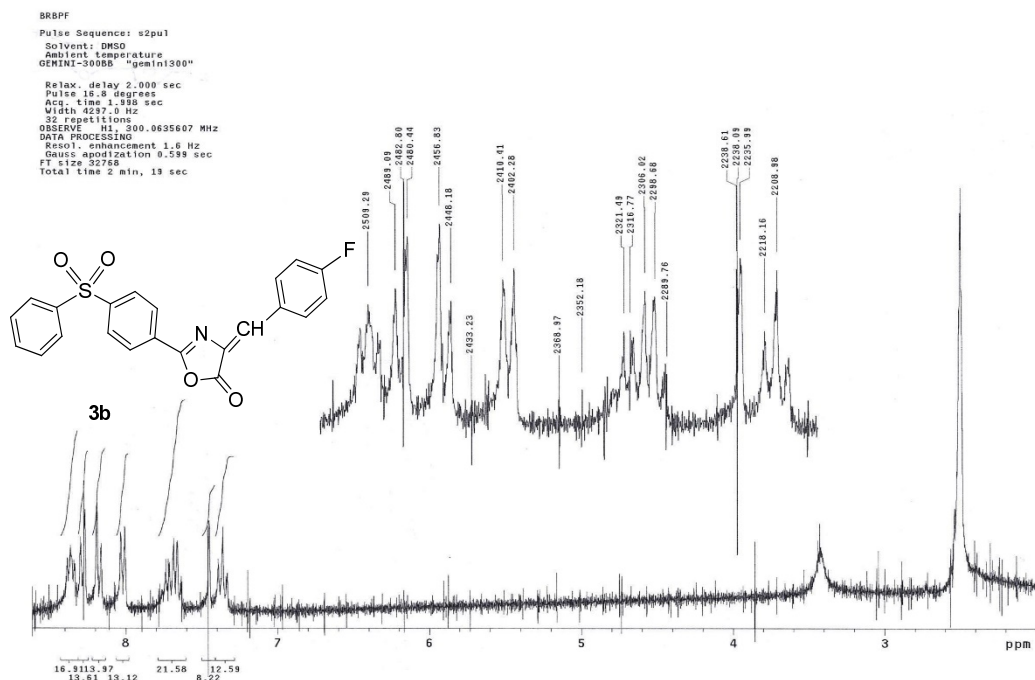
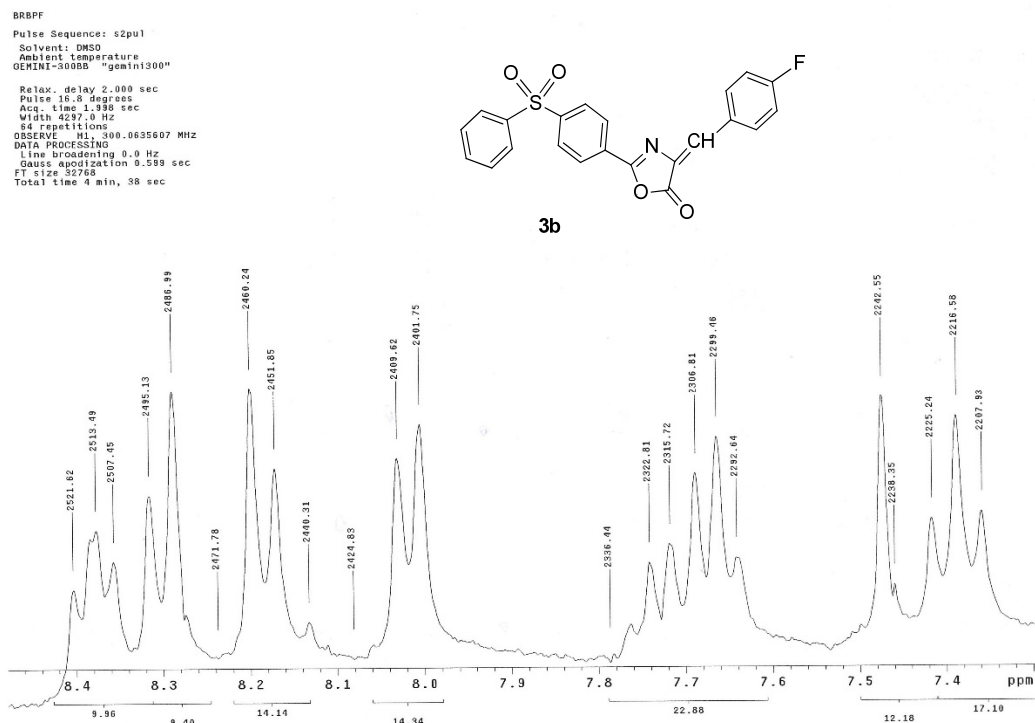


Figure S4. The  $^1\text{H}$ - $^{13}\text{C}$  COSY spectrum of oxazolone 3a.



**Figure S5.** The  $^1\text{H}$ -NMR spectrum of oxazolone **3b**.



**Figure S6.** The  $^1\text{H}$ -NMR spectrum (detailed) of oxazolone **3b**.

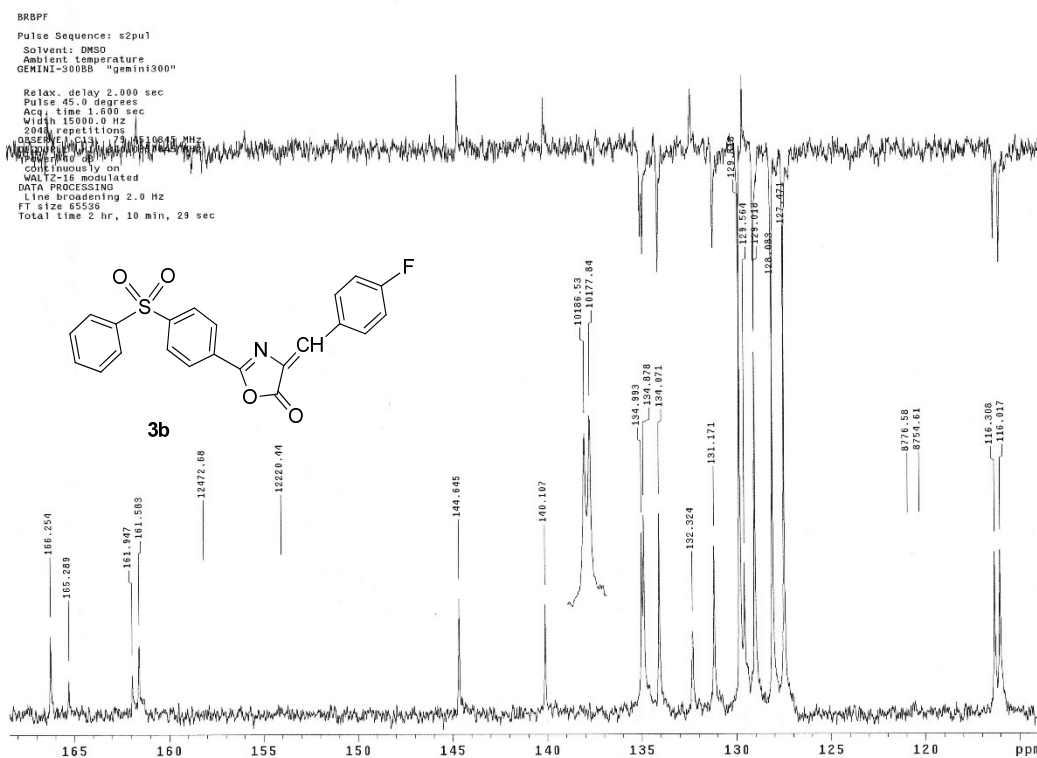


Figure S7. The  $^{13}\text{C}$ -NMR spectrum of oxazolone **3b**.

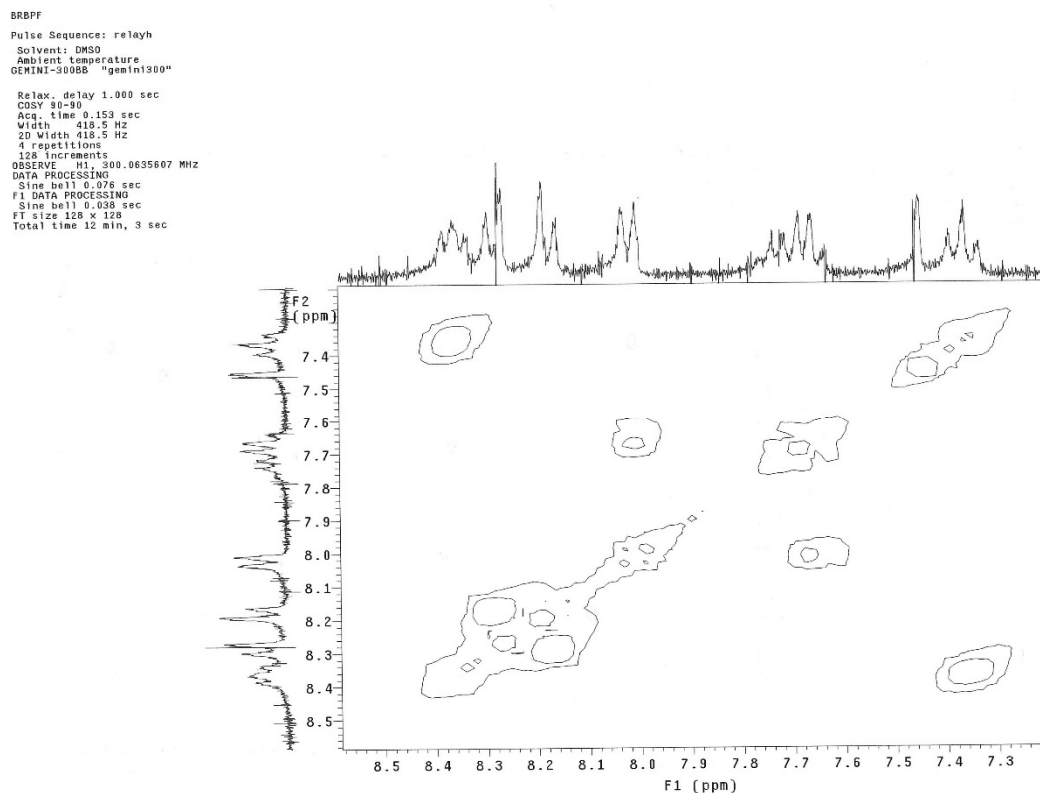


Figure S8. The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of oxazolone **3b**.

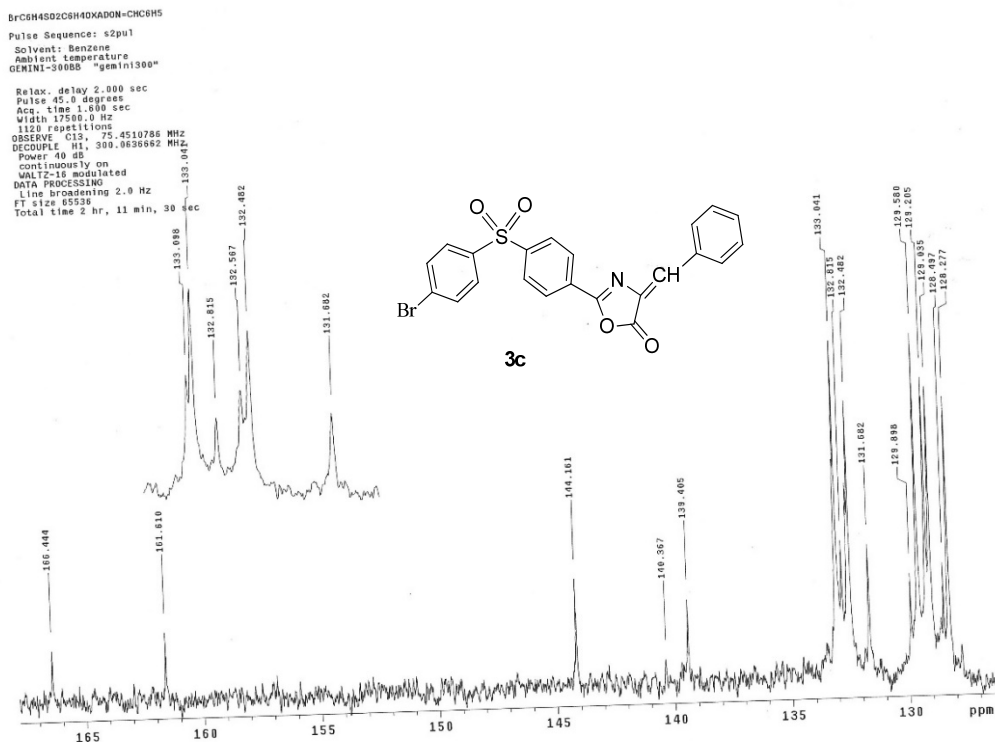


Figure S9. The  $^{13}\text{C}$ -NMR spectrum of oxazolone **3c**.

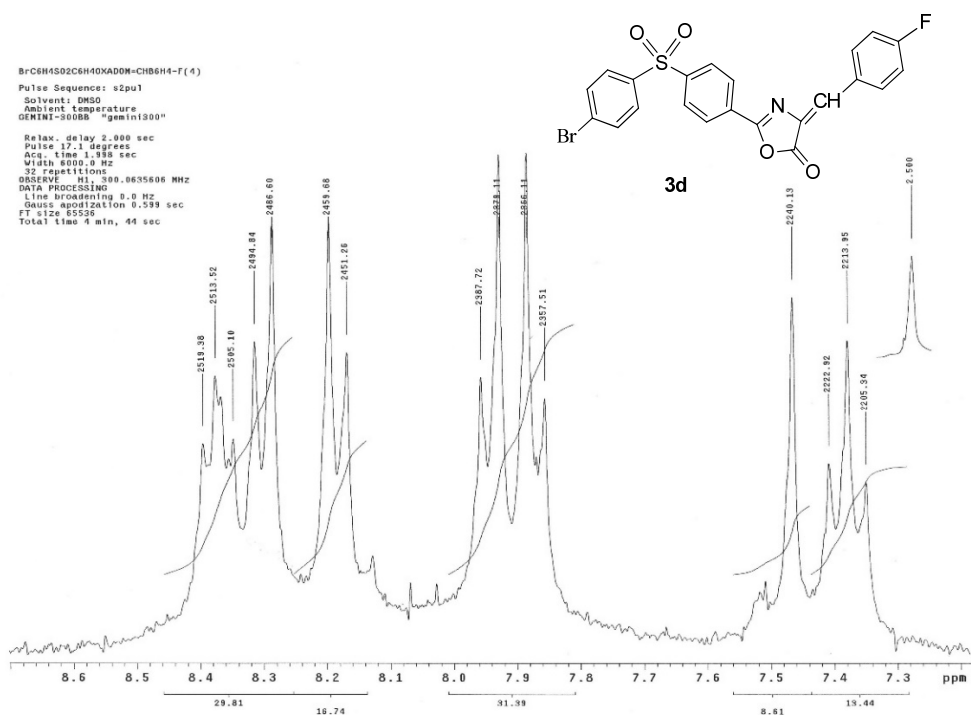


Figure S10. The  $^1\text{H}$ -NMR spectrum of oxazolone **3d**.





C6H5SO2C6H4-TRIAZINON-N(PH)=CHC6H4-F (4)  
Pulse Sequence: s2pu1  
Solvent: DMSO  
Ambient temperature  
GEMINI-300BS "gemin300"  
Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 1.998 sec  
Width 4500.3 Hz  
22 repetitions  
OBSERVE H1, 300.0722576 MHz  
DATA PROCESSING  
Resol. enhancement 1.6 Hz  
Gauss apodization 0.599 sec  
FT size 32768  
Total time 2 min, 19 sec

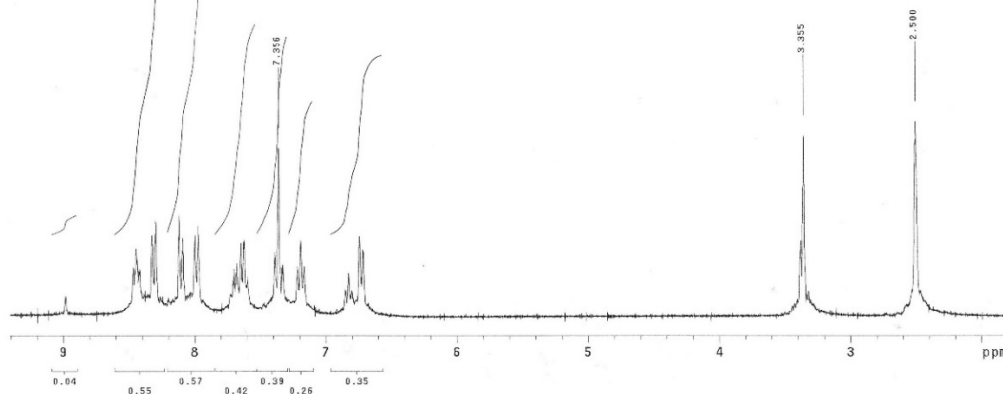
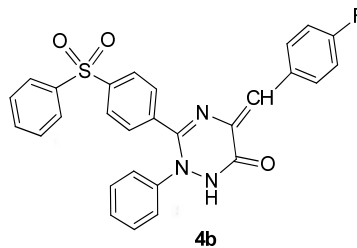


Figure S15. The  $^1\text{H}$ -NMR spectrum of triazinone **4b**.

C6H5SO2C6H4-TRIAZINON-N(PH)=CHC6H4-F (4)  
Pulse Sequence: s2pu1  
Solvent: DMSO  
Ambient temperature  
GEMINI-300BS "gemin300"  
Relax. delay 2.000 sec  
Pulse 40.0 degrees  
Acq. time 1.500 sec  
Width 17500.0 Hz  
2896 repetitions  
OBSERVE G13, 125.7603407 MHz  
DATA PROCESSING  
Power 47 dB  
continuously on  
WALTZ-16 modulated  
Line broadening 2.0 Hz  
FT size 131072  
Total time 6 hr, 25 min, 17 sec

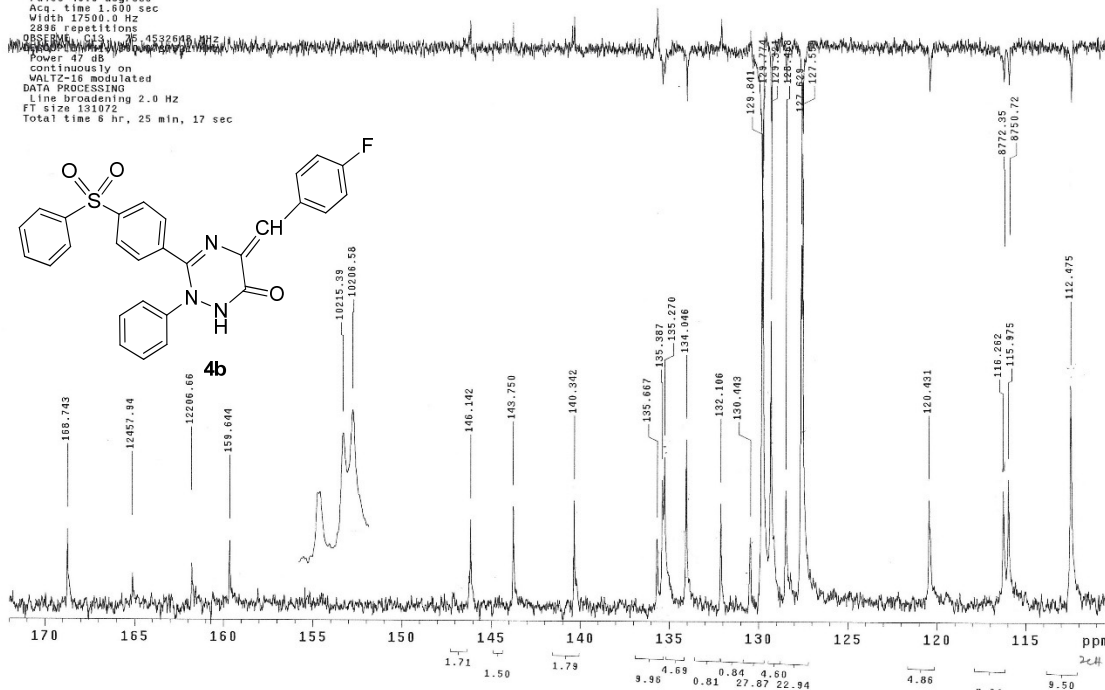
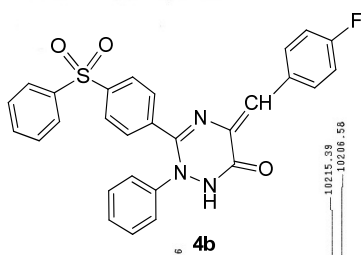


Figure S16. The  $^{13}\text{C}$ -NMR spectrum of triazinone **4b**.

UH5020RH4-TRIAZINON-N(PH)=CHC6H4-F(4)  
 Pulse Sequence: relayh  
 Solvent: DMSO  
 Ambient temperature  
 GEMINI-300SB "geminis300"  
 Relax. delay 1.000 sec  
 COSY 90-90  
 Acq. time 0.178 sec  
 Width 750.2 Hz  
 ZD Width 750.2 Hz  
 4 repetitions  
 64 increments  
 OBSERVE H1, 300.0722576 MHz  
 DATA PROCESSING  
 Sine bell 0.009 sec  
 F1 DATA PROCESSING  
 Sine bell 0.004 sec  
 FT size 256 x 256  
 Total time 9 min, 41 sec

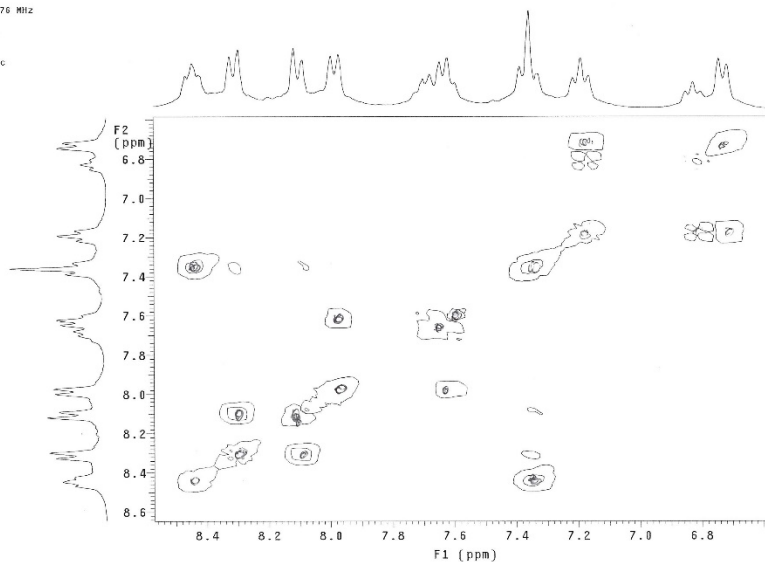


Figure S17. The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of triazinone **4b**.

BRB-114  
 Pulse Sequence: s2pu1  
 Solvent: DMSO  
 Ambient temperature  
 GEMINI-300SB "geminis300"  
 Relax. delay 2.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.998 sec  
 Width 4500.9 Hz  
 32 repetitions  
 OBSERVE H1, 300.0722576 MHz  
 DATA PROCESSING  
 Line broadening 0.599 sec  
 Gauss apodization 0.599 sec  
 FT size 32768  
 Total time 2 min, 19 sec

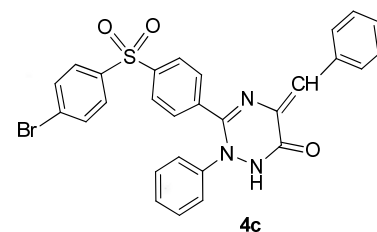
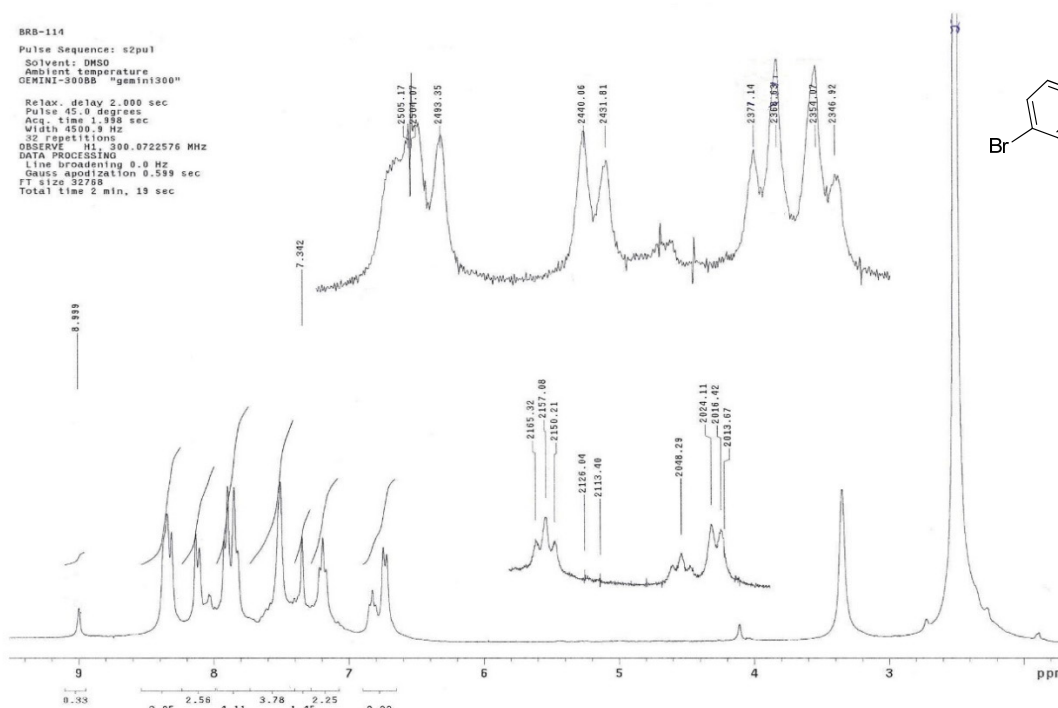


Figure S18. The  $^1\text{H}$ -NMR spectrum of triazinone **4c**.

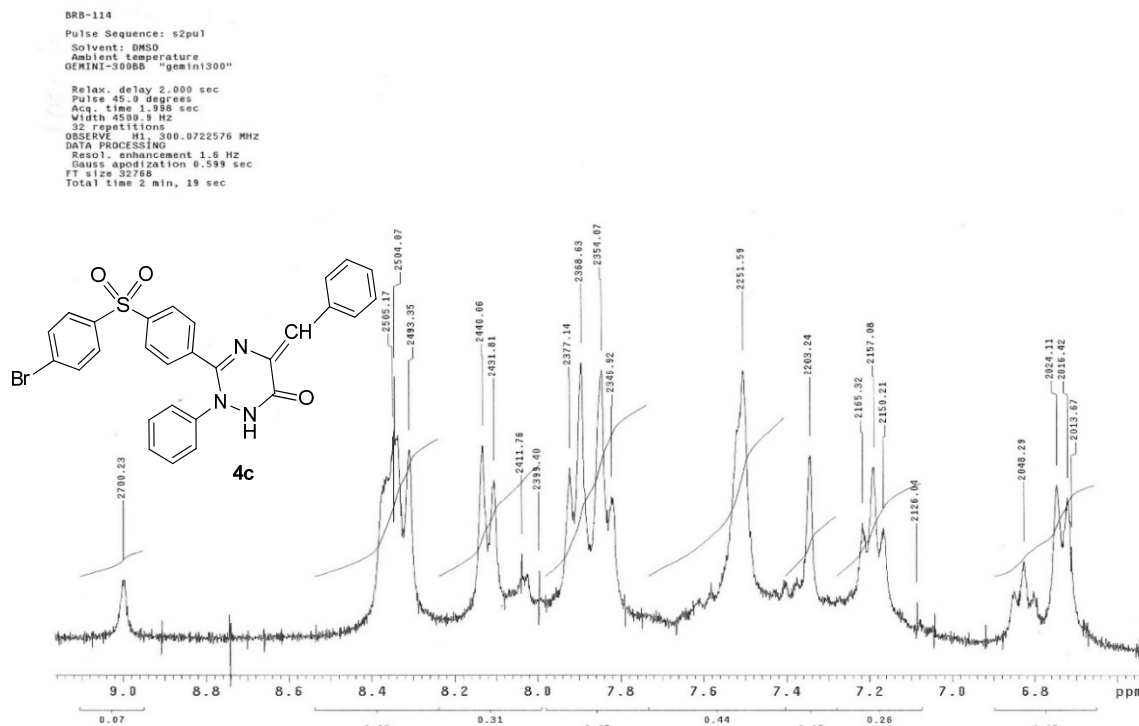


Figure S19. The  $^1\text{H}$ -NMR spectrum (detailed) of triazinone **4c**.

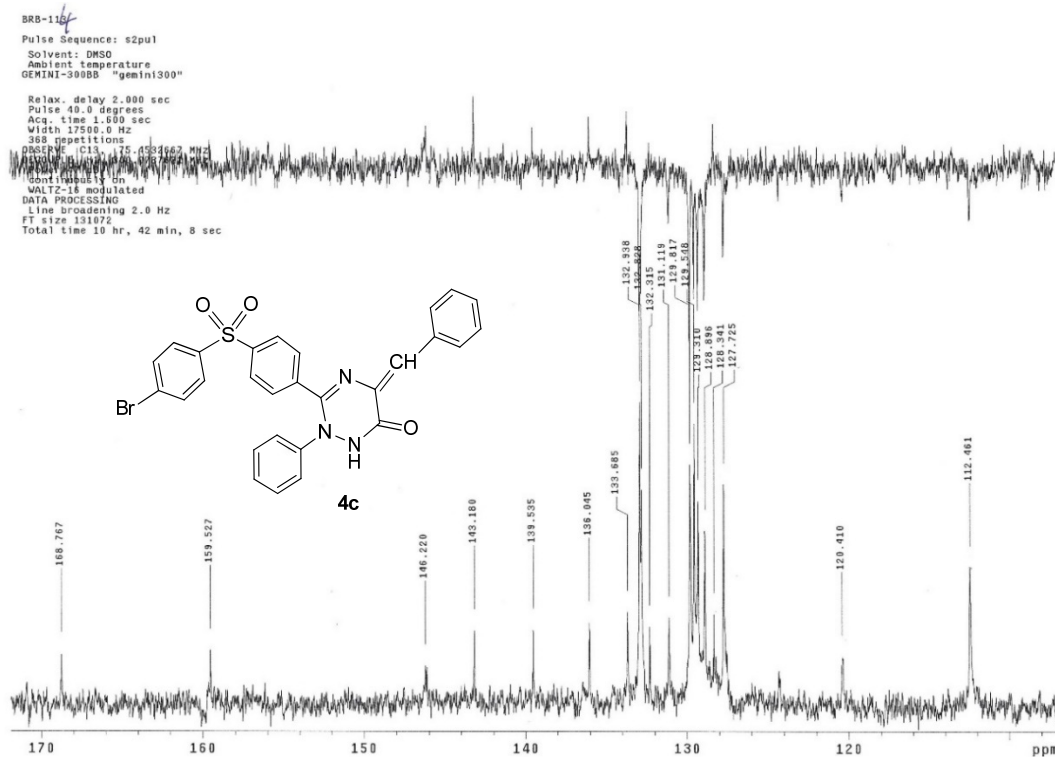


Figure S20. The  $^{13}\text{C}$ -NMR spectrum of triazinone **4c**.

BrBRB-TRIAZIN

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

GERINI-300SB "gemini300"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.998 sec

Width 4500.3 Hz

32 repetitions

OBSERVE nl 300.0635584 MHz

DATA PROCESSING

Resol. enhancement 1.6 Hz

Gauss apodization 0.599 sec

FT size 32768

Total time 2 min, 19 sec

BrC1=CC=C(S(=O)(=O)C2=CC=C(C=C2)N3C(=O)C(=NN3C4=CC=CC=C4)C=C5C(=CC=C(C=C5)F)C=C6C=CC=CC=C6)C=C1

**4d**

9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 ppm

0.05 0.15 0.14 0.15 0.29 0.22 0.15 0.08 0.11

Peak list (ppm): 2899.38, 2624.65, 2542.51, 2536.74, 2533.39, 2528.22, 2500.20, 2495.53, 2491.41, 2476.85, 2465.31, 2430.42, 2430.94, 2414.46, 2412.72, 2399.32, 2378.77, 2369.12, 2365.08, 2368.43, 2289.98, 2285.14, 2263.11, 2219.15, 2210.63, 2201.57, 2185.58, 2157.54, 2149.32, 2078.76, 2055.69, 2048.27, 2046.85, 2022.17, 2014.46

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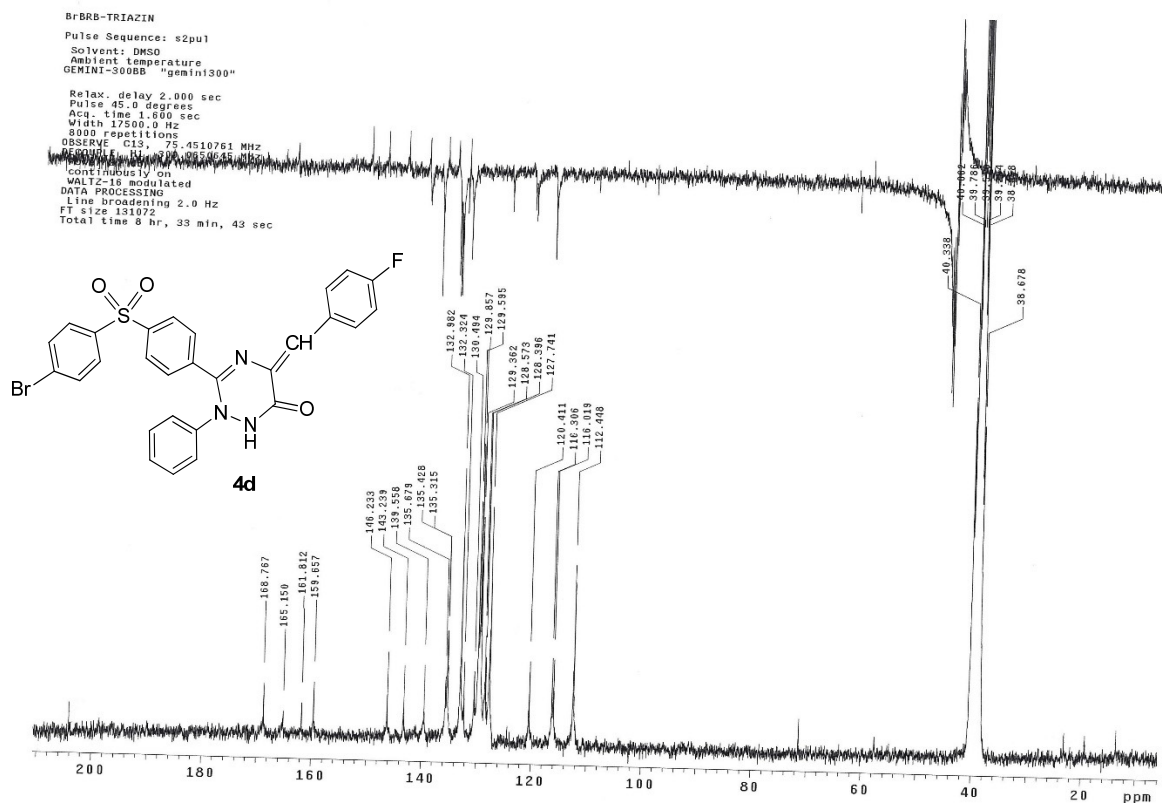


Figure S23. The  $^{13}\text{C}$ -NMR spectrum of triazinone **4d**.

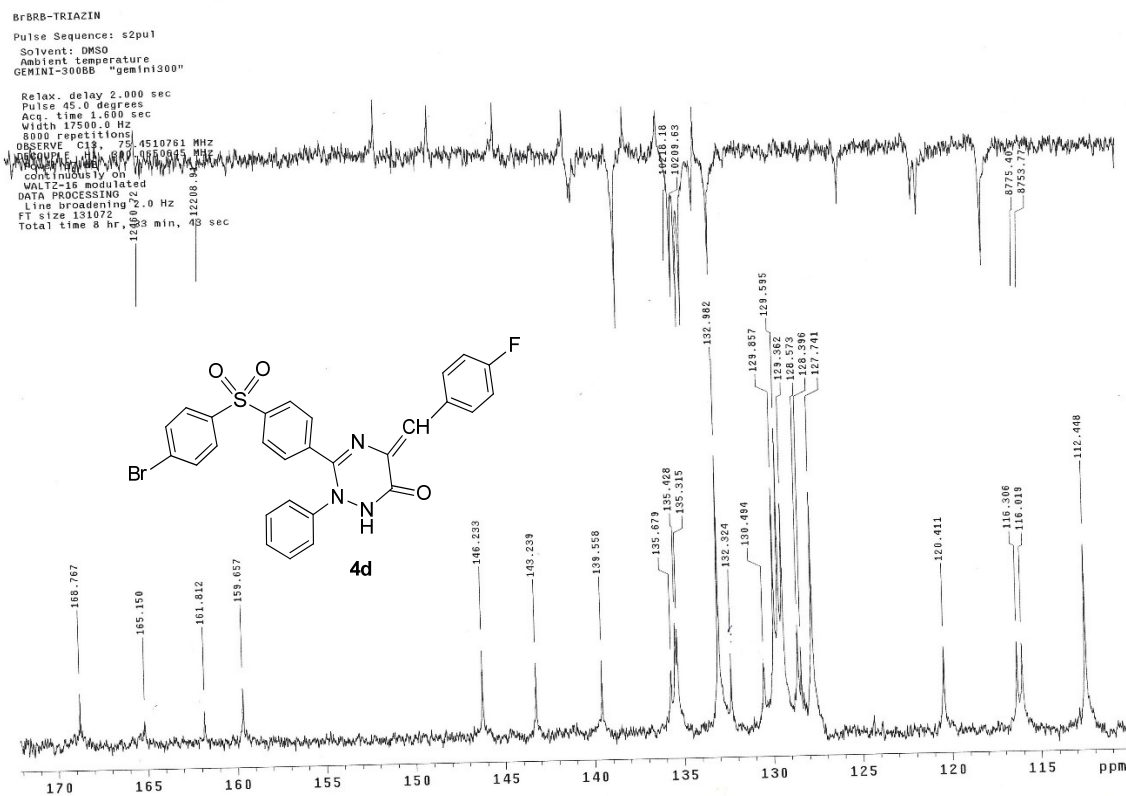
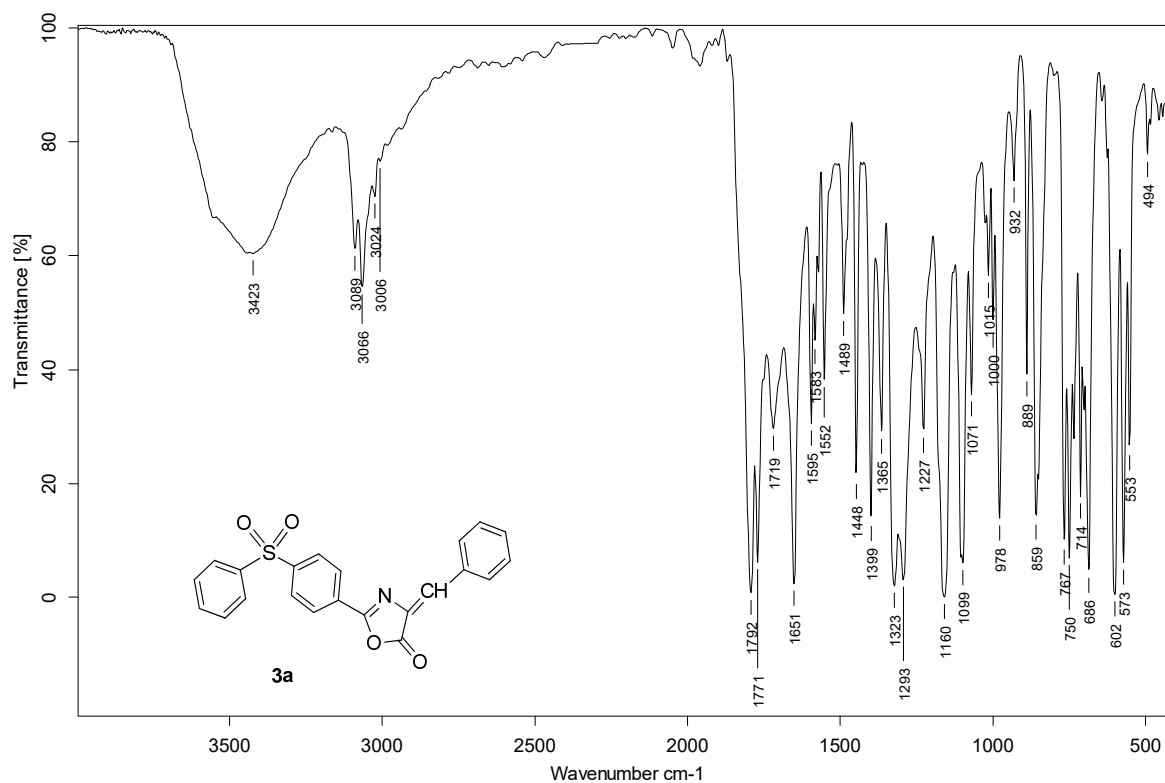
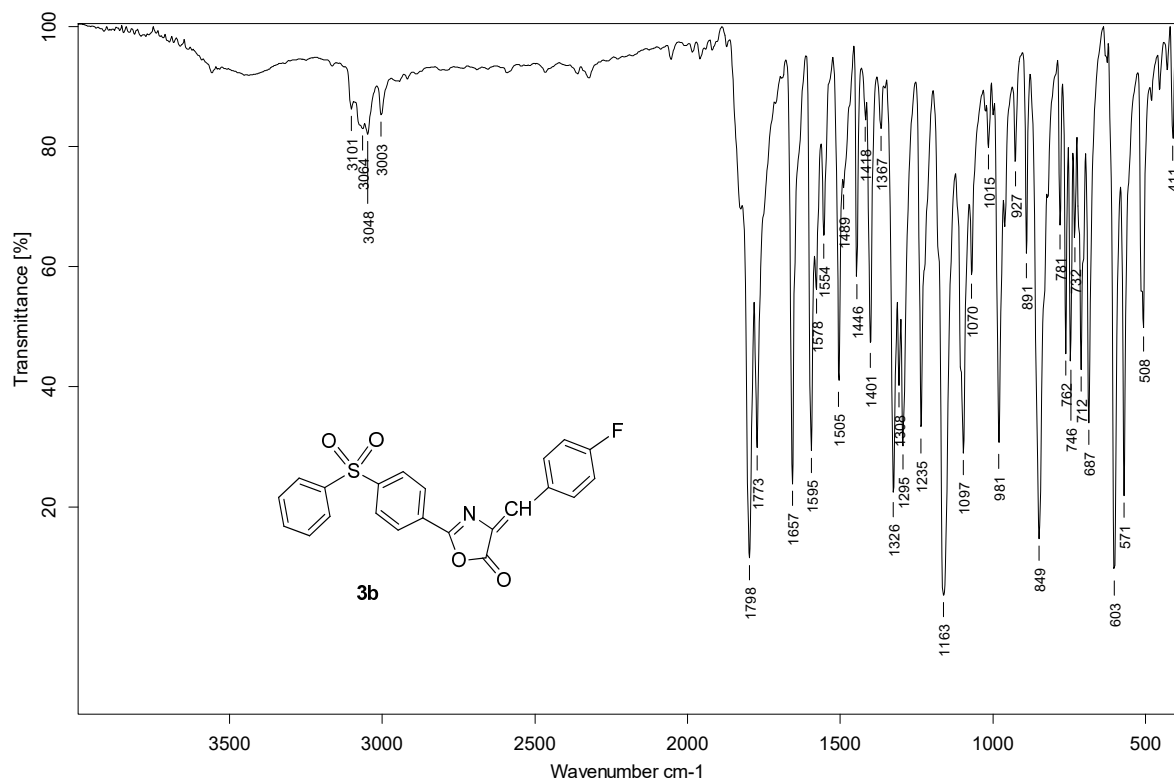


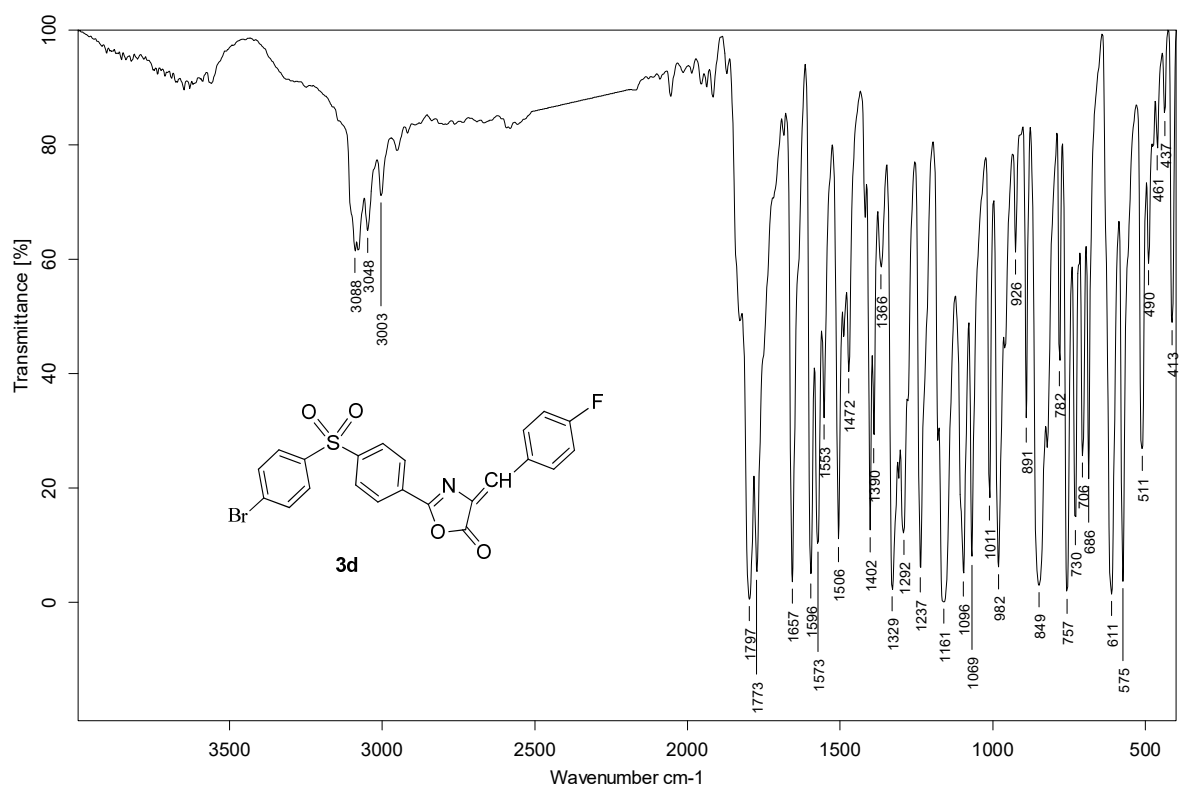
Figure S24. The  $^{13}\text{C}$ -NMR spectrum (detailed) of triazinone **4d**.



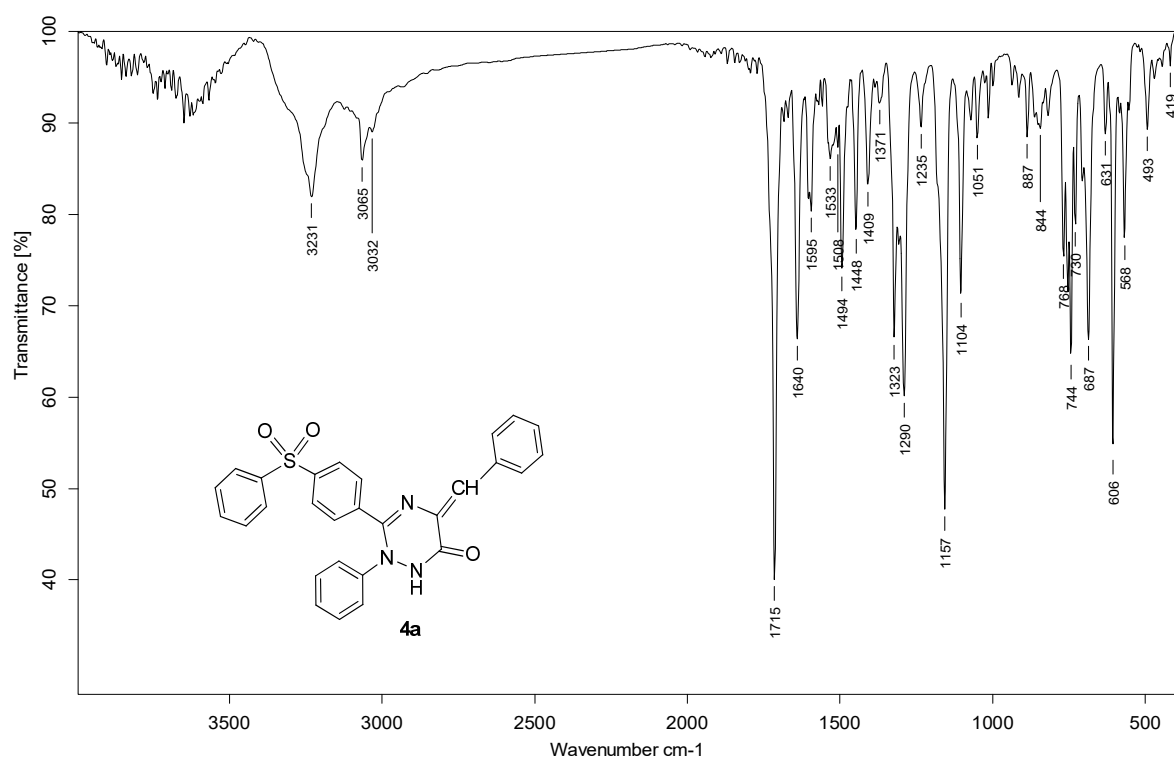
**Figure S25.** The IR spectrum of oxazol-5(4H)-one **3a**.



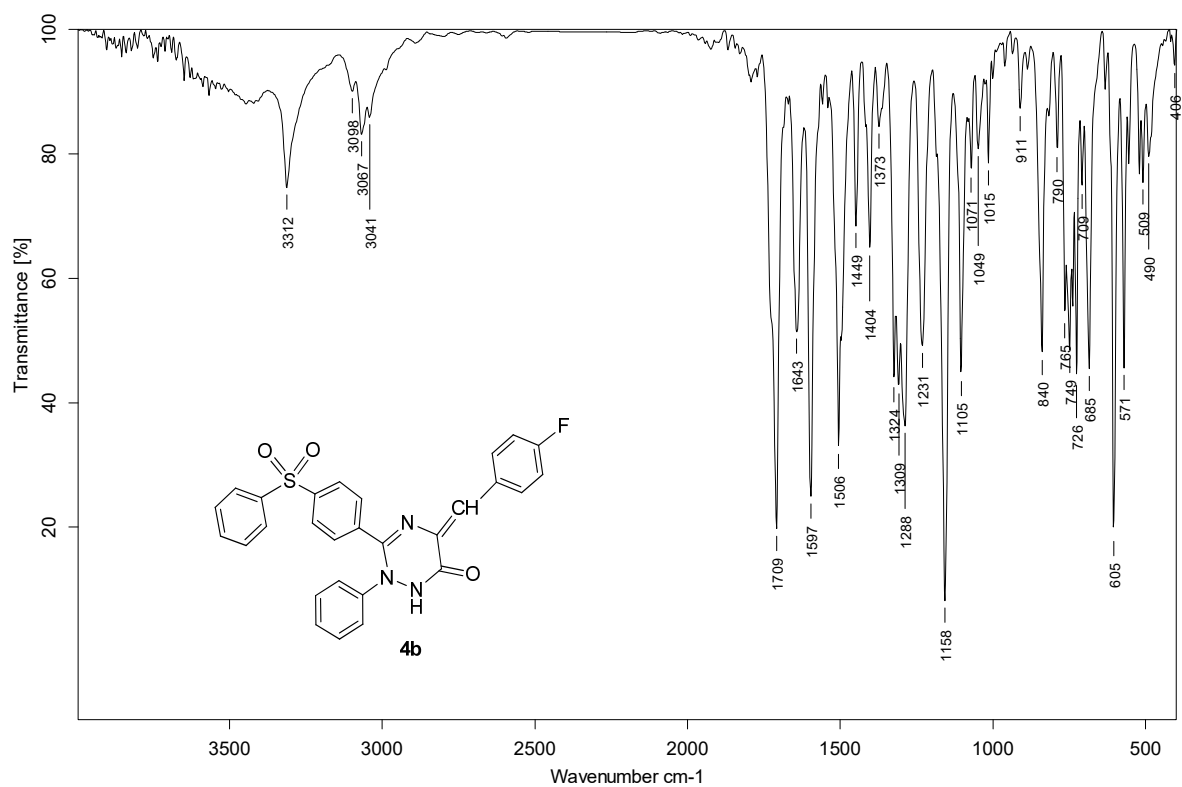
**Figure S26.** The IR spectrum of oxazol-5(4H)-one **3b**.



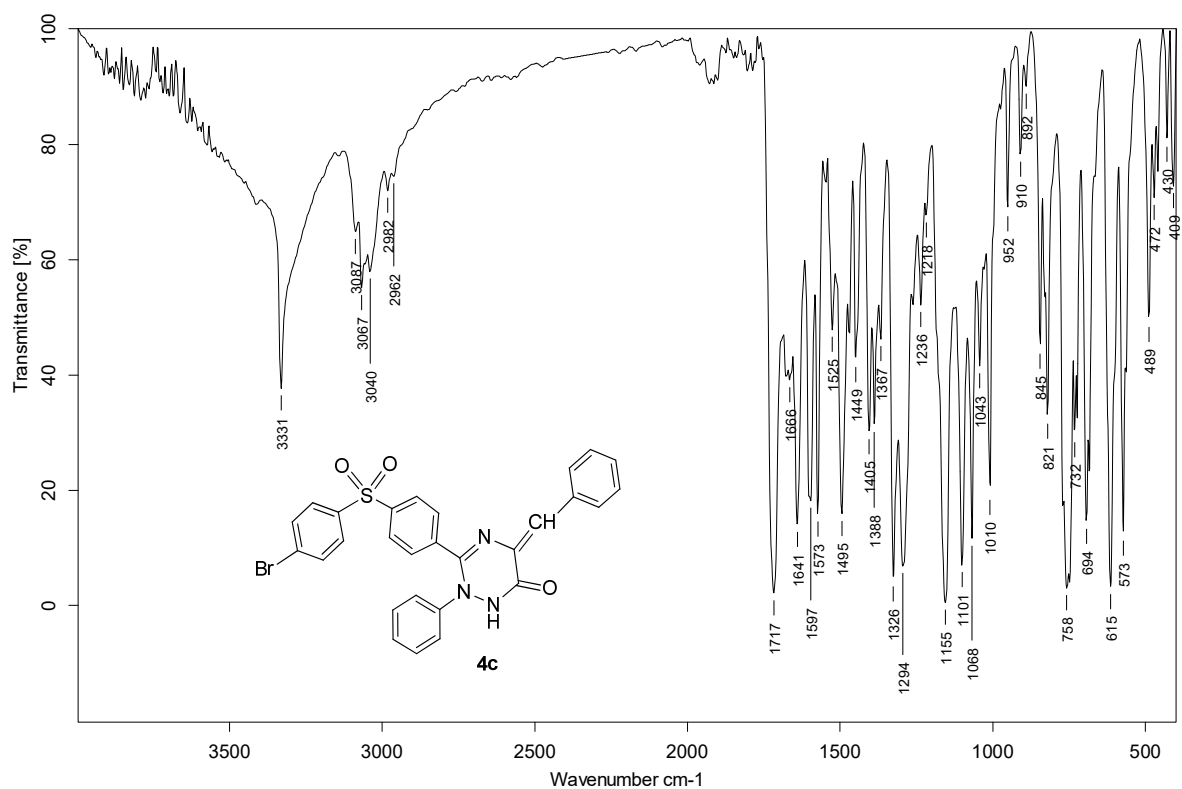
**Figure S27.** The IR spectrum of oxazol-5(4*H*)-one **3d**.



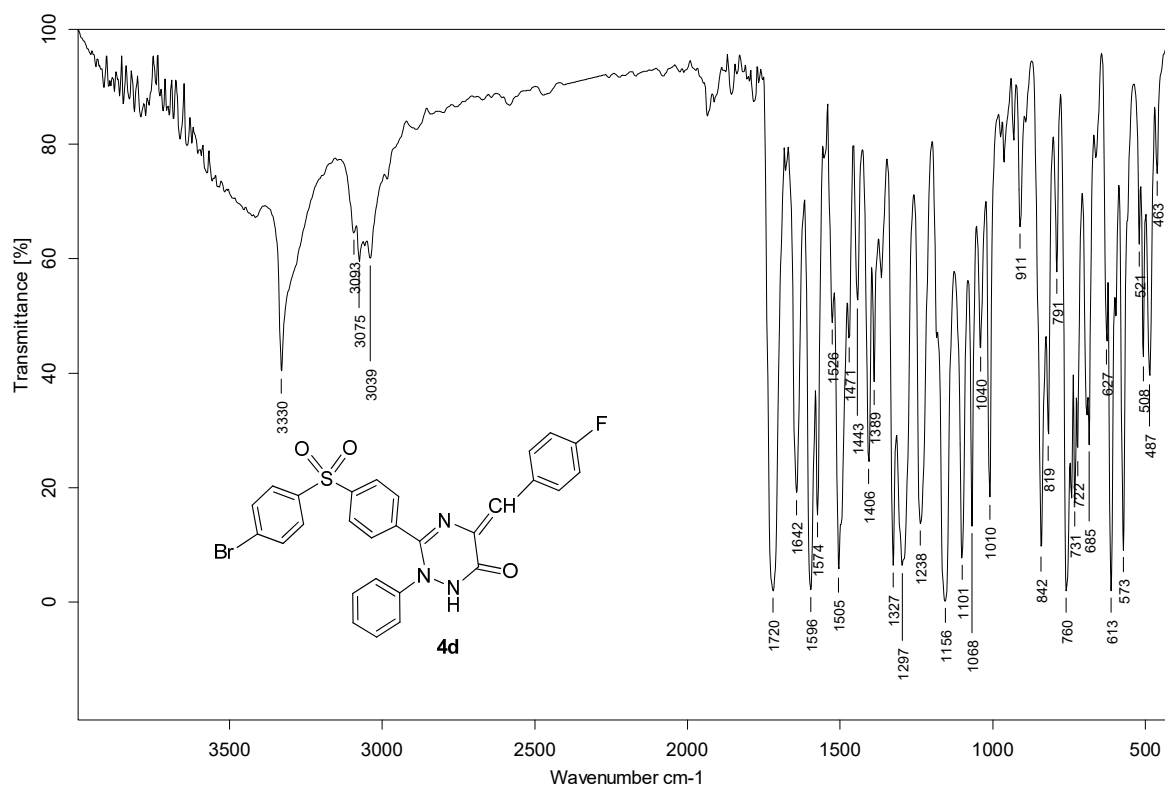
**Figure S28.** The IR spectrum of triazinone **4a**.



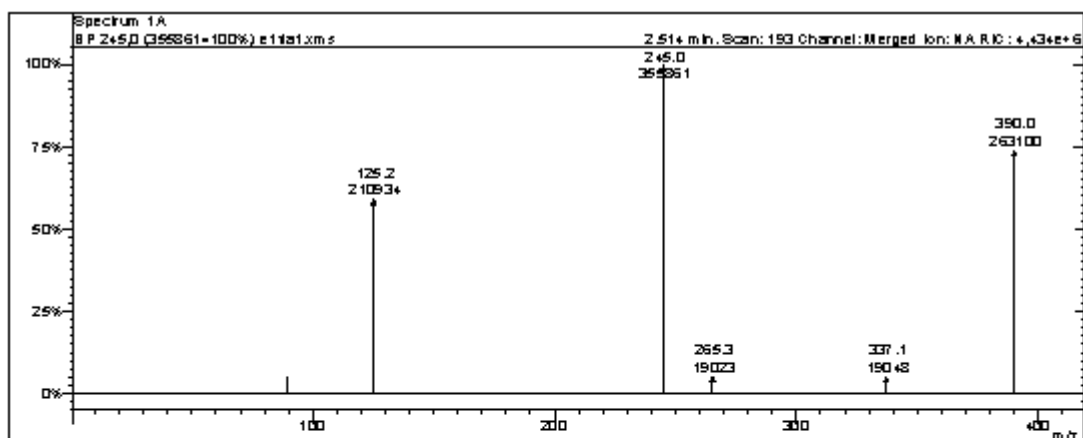
**Figure S29.** The IR spectrum of triazinone **4b**.



**Figure S30.** The IR spectrum of triazinone **4c**.



**Figure S31.** The IR spectrum of triazinone **4d**.

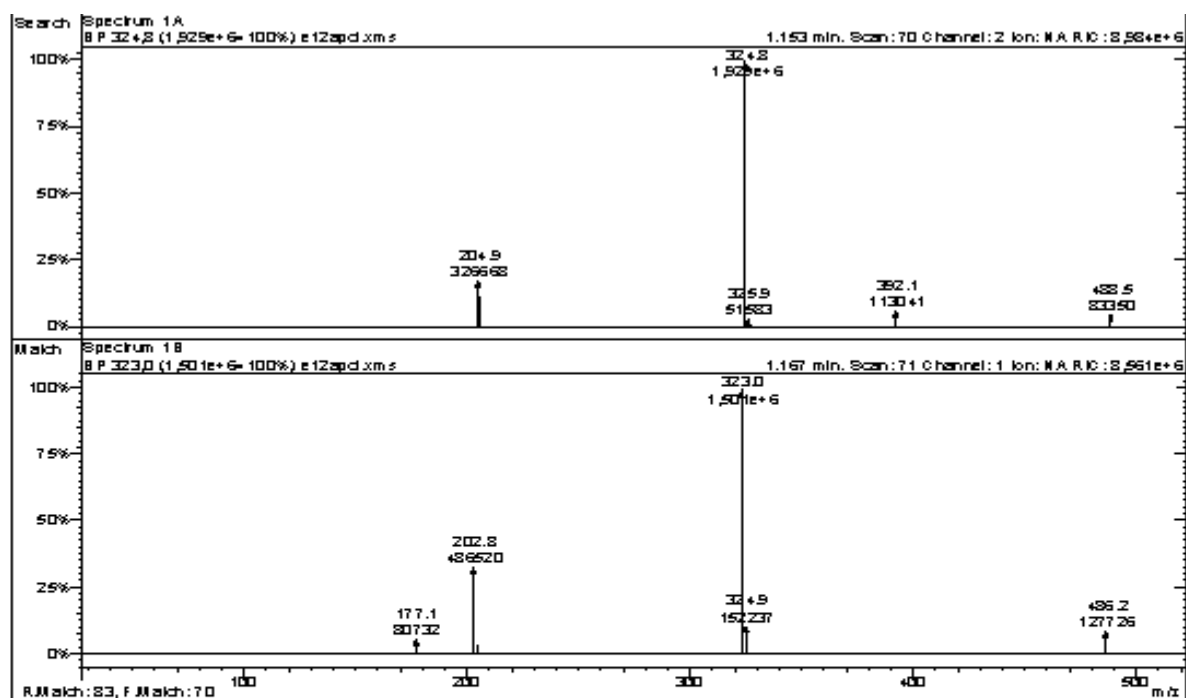


Spectrum from ...\\slcrceetartfstat\\ale\\16-10-2018\\e11a1.xms  
Scan No: 193, Time: 2.514 minutes  
No averaging. Not background corrected.  
Comment: 2.514 min. Scan: 193 Channel: Merged Ion: NA RIC: 4.434e+6  
Pair Count: 6 MW: 0 Formula: None  
CAS No: None Acquired Range: 20.0 - 400.0 m/z

Method Description: ESI  
Scan 1 Channel Description: 390.0 > 20.0 - 400.0 (-10.0 eV)  
Scan Information: cp = 0.9 PSI  
Precursor Mass Range: 390.0 - 390.0 m/z  
Product Mass Range: 20.0 - 400.0 m/z

Ion	Int	%BP	Ion	Int	%BP	Ion	Int	%BP
29.6	18338	5.2	245.0	355861	100.0	337.1	19048	5.4
125.2	210934	59.3	265.3	19023	5.3	390.0	263100	73.9

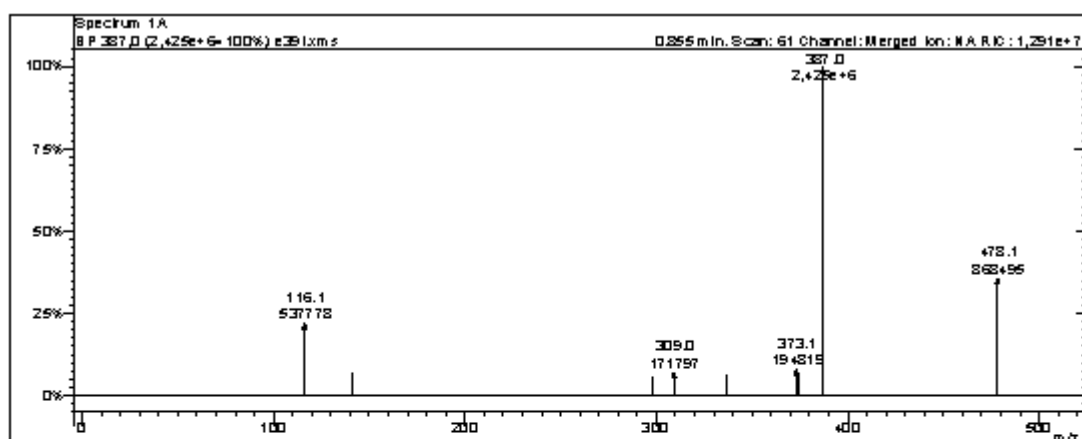
Figure S32. The +ESI-MS spectra of oxazol-5(4*H*)-one 3a.



1st Spectrum from ...s\cercetar\test\data\12-11-2018\12apcl.xms  
 Scan No: 70, Time: 1.153 minutes  
 No averaging. Not background corrected.  
 Comment: 1.153 min, Scan: 70 Channel: 2 Ion: NA RIC: 8.984e+6  
 Pair Count: 6 MW: 0 Formula: None  
 CAS No: None Acquired Range: 50.0 - 500.0 m/z

Method Description: APCI  
 Scan 1 Channel Description: 486.0 > 50.0 - 500.0 (-20.0 eV)  
 Scan 2 Channel Description: 488.0 > 50.0 - 500.0 (-20.0 eV)  
 Scan Information: op = 1.6 PSI  
 Precursor Mass Range: 488.0 - 488.0 m/z  
 Product Mass Range: 50.0 - 500.0 m/z

**Figure S33.** The +APCI-MS spectrum of oxazol-5(4*H*)-one **3d**.

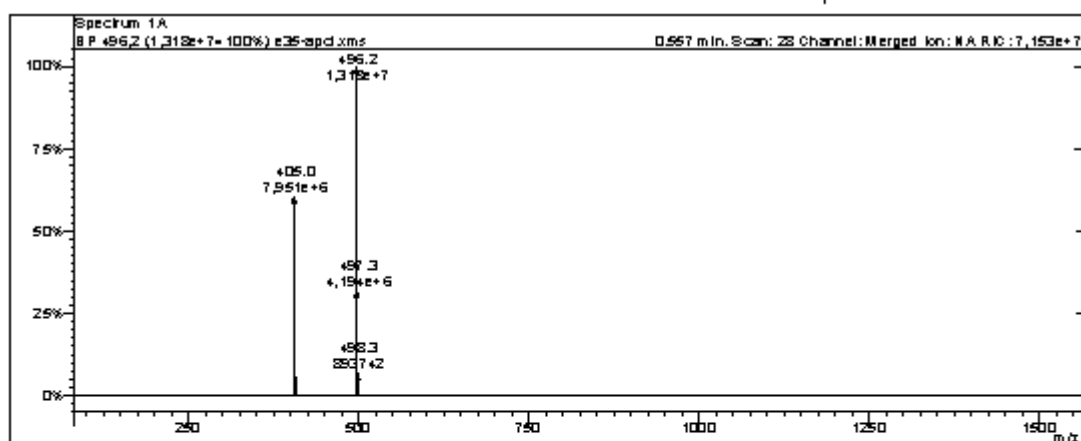


Spectrum from ...dissiliceo tarfistefalave M1-07-2019\39t.xms  
 Scan No: 61, Time: 0.855 minutes  
 No averaging. Not background corrected.  
 Comment: 0.855 min. Scan: 61 Channel: Merged Ion: NA RIC: 1.291e+7  
 Pair Count: 9 MW: 0 Formula: None  
 CAS No: None Acquired Range: 20.0 - 500.0 m/z

Method Description: APCI  
 Scan 1 Channel Description: 478.0 > 20.0 - 500.0 (30.0 eV)  
 Scan Information: cp = 1.4 PSI  
 Precursor Mass Range: 478.0 - 478.0 m/z  
 Product Mass Range: 20.0 - 500.0 m/z

Ion	Int	%BP	Ion	Int	%BP	Ion	Int	%BP
116.1	537778	22.2	309.0	171797	7.1	374.2	162592	6.7
140.8	173651	7.2	337.1	161242	6.7	387.0	2,425e+6	100.0
298.0	148674	6.1	373.1	194819	8.0	478.1	868495	35.8

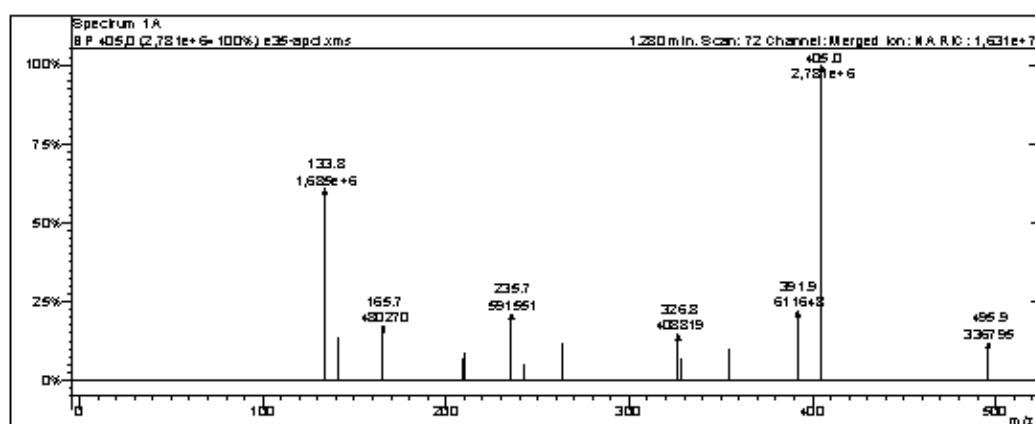
Figure S34. The -APCI-MS spectrum of triazinone 4a.



Spectrum from ...slices for triazinone 25-06-2019\35-apci.xms  
Scan No: 28, Time: 0.557 minutes  
No averaging. Not background corrected.  
Comment: 0.557 min, Scan: 28 Channel: Merged Ion: NA RIC: 7.153e+7  
Pair Count: 6 MW: 0 Formula: None  
CAS No: None Acquired Range: 150.0 - 1500.0 m/z

Method Description: APCI  
Scan 1 Channel Description: 150.0 - 1500.0 >  
Scan Information: cp = 0.0 PSI  
Precursor Mass Range: 150.0 - 1500.0 m/z

Ion	Int	%BP	Ion	Int	%BP	Ion	Int	%BP
405.0	7,951e+6	60.3	407.2	740672	5.6	497.3	4,194e+6	31.8
406.0	2,649e+6	20.1	496.2	1,318e+7	100.0	498.3	893742	6.8

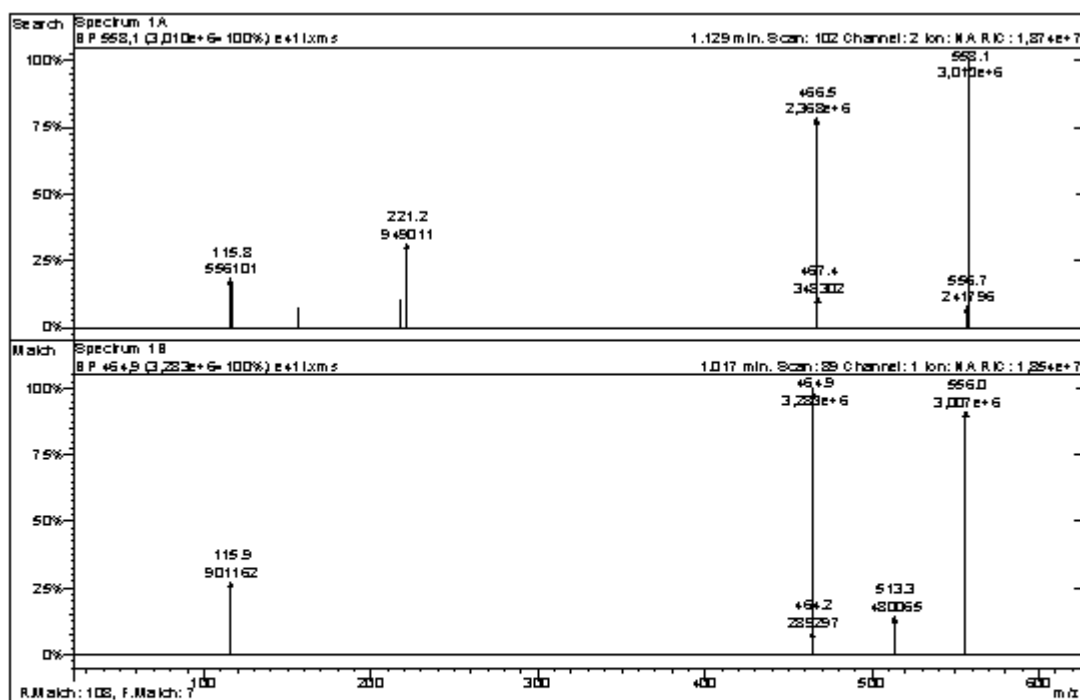


Spectrum from ...slices for triazinone 25-06-2019\35-apci.xms  
Scan No: 72, Time: 1.280 minutes  
No averaging. Not background corrected.  
Comment: 1.280 min, Scan: 72 Channel: Merged Ion: NA RIC: 1.631e+7  
Pair Count: 14 MW: 0 Formula: None  
CAS No: None Acquired Range: 20.0 - 500.0 m/z

Method Description: APCI  
Scan 1 Channel Description: 496.0 > 20.0 - 500.0 (40.0 eV)  
Scan Information: cp = 1.5 PSI  
Precursor Mass Range: 496.0 - 496.0 m/z  
Product Mass Range: 20.0 - 500.0 m/z

Ion	Int	%BP	Ion	Int	%BP	Ion	Int	%BP
133.8	1,685e+6	60.6	235.7	591551	21.3	354.9	278525	10.0
140.9	384469	13.8	242.4	151607	5.5	391.9	611648	22.0
165.7	480270	17.3	263.9	338391	12.2	405.0	2,781e+6	100.0
209.3	197649	7.1	326.8	408819	14.7	495.9	336795	12.1
210.2	252328	9.1	327.9	205470	7.4			

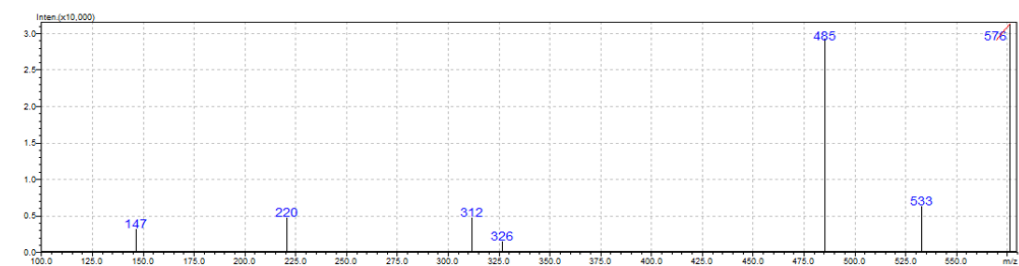
Figure S35. The -APCI-MS spectrum of triazinone **4b**.



1st Spectrum from ...d\\s\\lcnceta\\data\\11-07-2019\\411xms  
 Scan No: 102, Time: 1.129 minutes  
 No averaging. Not background corrected.  
 Comment: 1.129 min, Scan: 102 Channel: 2 Ion: NA RIC: 1.874e+7  
 Pair Count: 9 MW: 0 Formula: None  
 CAS No: None Acquired Range: 50.0 - 600.0 m/z

Method Description: APC I  
 Scan 1 Channel Description: 556.0 > 50.0 - 600.0 (30.0 eV)  
 Scan 2 Channel Description: 556.0 > 50.0 - 600.0 (30.0 eV)

Figure S36. The -APCI-MS spectrum of triazinone 4c.

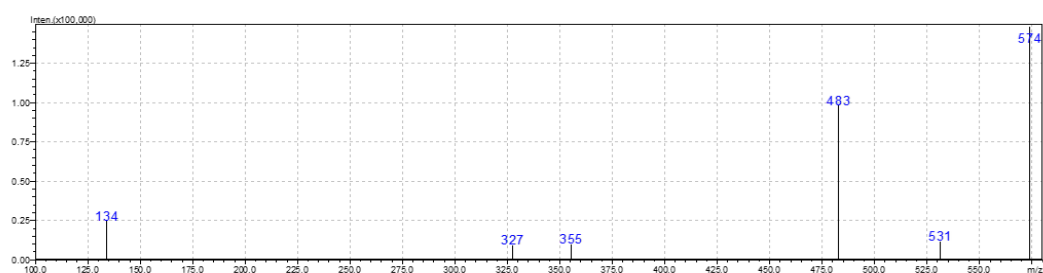


[MS Spectrum]

# of Peaks 7  
 Raw Spectrum [0.705]<sub>4</sub>(scan:[283])  
 Background No Background Spectrum  
 Precursor 576.00  
 Base Peak m/z 576.15 (Inten.: 31,271)  

m/z	Absolute Intensity	Relative Intensity
146.70	3221	10.30
220.50	4827	15.44
311.60	4827	15.44
326.40	1609	5.15
485.05	29336	93.81
532.70	6452	20.63
576.15	31271	100.00

 Event 1



[MS Spectrum]

# of Peaks 6  
 Raw Spectrum [0.592]<sub>4</sub>(scan:[238])  
 Background No Background Spectrum  
 Precursor 574.00  
 Base Peak m/z 574.05 (Inten.: 148,372)  

m/z	Absolute Intensity	Relative Intensity
134.15	24757	16.69
327.50	9662	6.51
355.35	10286	6.93
482.90	98195	66.18
531.25	12009	8.09
574.05	148372	100.00

 Event 4

**Figure S37.** The –ESI-MS spectrum of triazinone **4d**.