Synthesis, Crystal Structure and Herbicidal Activity of a Series of [1,2,4]Triazolo[1,5-*a*]pyrimidine-2-sulfonamide Compounds

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Table S1. Crystal data and structure refinements for compounds **8a**, **8d** and **8e**.

	8a	**8d**	**8e**
empirical formula	$C_{16}H_{14}F_4N_6O_4S$	$C_{16}H_{14}F_5N_5O_3S$	$C_{21}H_{23}F_3N_6O_6S$
Fw	462.40	451.38	544.51
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1/c$	$C2/c$	$P\bar{1}$
a (Å)	14.688(1)	30.283(1)	8.145(1)
b (Å)	15.498(1)	7.940(1)	12.848 (1)
c (Å)	17.339(1)	19.142(1)	13.091(1)
α (deg)	90	90	111.506(8)
β (deg)	91.367(3)	127.441(10)	100.055(5)
γ (deg)	90	90	95.066(7)
V (Å^3)	3945.7(2)	3654.3(3)	1237.42(17)
Z	8	8	2
D_{calc} (mg m^{-3})	1.557	1.641	1.461
μ(mm^{-1})	0.239	0.258	0.203
F(000)	1888	1840	564
Reflections collected/unique	17702 / 6943	7344 / 3215	8415 / 4363
R(int)	0.0242	0.0153	0.0200
GOF on F^2	1.022	1.046	1.017
R_1[a][$I > 2\sigma(I)$]	0.0493	0.0349	0.0642
wR_2[b][$I > 2\sigma(I)$]	0.1285	0.0913	0.1743
R_1[a] (all)	0.0740	0.0419	0.0788
wR_2[b] (all)	0.1475	0.0979	0.1881

[a] $R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo|$. [b] $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]\}^{1/2}$.

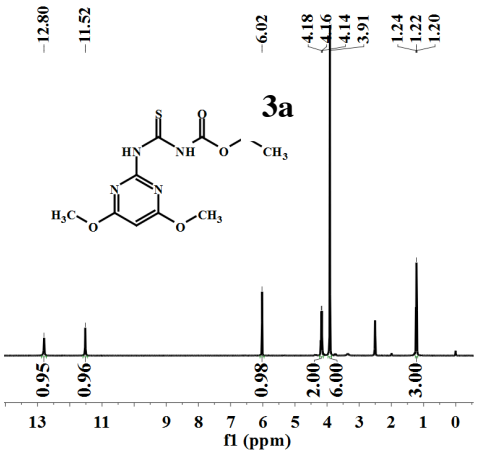
Table S2. Selected bond distances (Å) and angles (°) for **8a**, **8d** and **8e**.

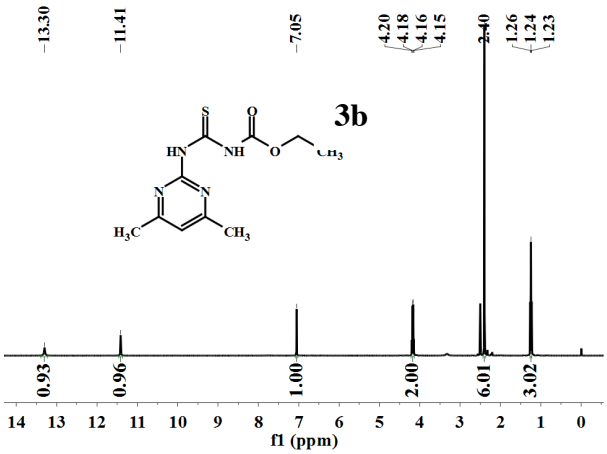
		8a	
N(2)-N(3)	1.374(3)	N(5)-S(1)	1.618(2)
N(5)-H(51)	0.892(10)	N(7)-N(8)	1.377(3)
N(10)-S(2)	1.615(2)	N(10)-H(101)	0.892(10)
O(3)-S(1)	1.419(1)	O(4)-S(1)	1.416 (1)
O(7)-S(2)	1.417(2)	O(8)-S(2)	1.416(2)
C(5)-N(5)-S(1)	123.74(18)	C(5)-N(5)-H(51)	117(2)
S(1)-N(5)-H(51)	118(2)	C(19)-N(10)-S(2)	122.73(19)
C(19)-N(10)-H(101)	118(2)	S(2)-N(10)-H(101)	119(2)
O(4)-S(1)-O(3)	120.80(13)	O(4)-S(1)-N(5)	107.45(12)
O(3)-S(1)-N(5)	105.36(12)	O(4)-S(1)-C(8)	106.74(12)
O(3)-S(1)-C(8)	108.36(12)	N(5)-S(1)-C(8)	107.52(13)
O(8)-S(2)-O(7)	121.35(14)	O(8)-S(2)-N(10)	105.07(12)
O(7)-S(2)-N(10)	107.32(13)	O(8)-S(2)-C(22)	108.04(13)
O(7)-S(2)-C(22)	106.45(13)	N(10)-S(2)-C(22)	108.06(14)
		8d	
N(1)-N(2)	1.364(2)	N(5)-S(1)	1.635 (1)

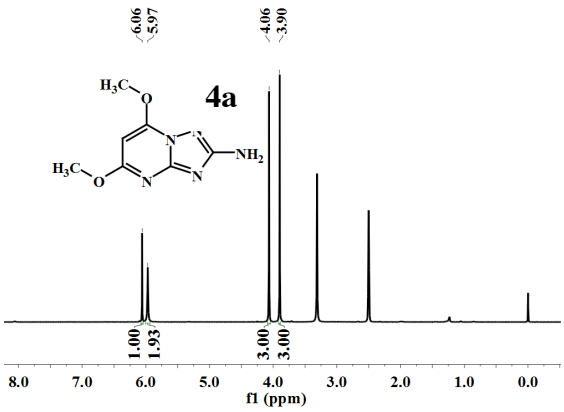
N(5)-H(51)	0.882(10)	O(1)-S(1)	1.419(1)
O(2)-S(1)	1.416(1)		
C(7)-N(5)-S(1)	123.49(12)	S(1)-N(5)-H(51)	118.7(16)
O(2)-S(1)-O(1)	119.59(10)	O(2)-S(1)-N(5)	105.00(9)
O(1)-S(1)-N(5)	107.71(9)	O(2)-S(1)-C(8)	110.31(9)
O(1)-S(1)-C(8)	107.82(9)	N(5)-S(1)-C(8)	105.50(9)
		8e	
N(2)-N(3)	1.409(4)	N(5)-S(1)	1.634(3)
N(5)-H(51)	0.895(10)	O(3)-S(1)	1.409(3)
O(4)-S(1)	1.426(2)		
C(5)-N(5)-S(1)	122.1(2)	S(1)-N(5)-H(51)	113(3)
O(3)-S(1)-O(4)	119.14(16)	O(3)-S(1)-N(5)	107.95(15)
O(4)-S(1)-N(5)	105.28(14)	O(3)-S(1)-C(8)	109.78(15)
O(4)-S(1)-C(8)	108.85(14)	N(5)-S(1)-C(8)	104.83(14)

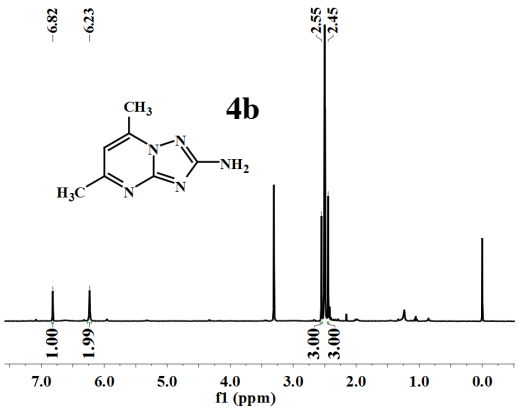
Table S3. H-bond distances (Å) and angles (°) in **8a**, **8d** and **8e**.

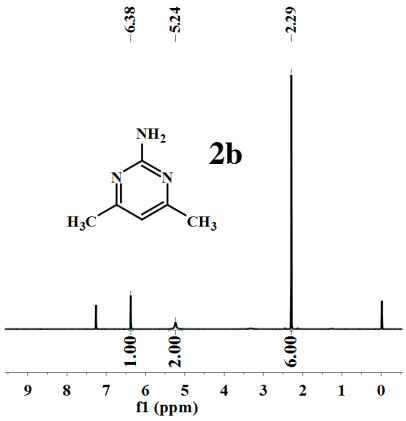
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
		8a		
N(5)-H(51) ···N(8)^{I}	0.892(10)	2.139(16)	2.989(3)	159(3)
N(10)-H(101) ···N(3)^{II}	0.892(10)	2.114(16)	2.968(3)	160(3)
Symmetric codes. I: x+1,y,z II: x-1,y,z				
		8d		
N(5)-H(51)···N(3)^{I}	0.882(10)	2.155(12)	3.009(2)	163(2)
Symmetric codes. I: -x,y,-z+1/2				
		8e		
N(5)-H(51)...O(6)	0.895(10)	2.037(13)	2.925(4)	171(4)
N(5)-H(51)...O(5)	0.895(10)	2.31(4)	2.781(3)	113(3)

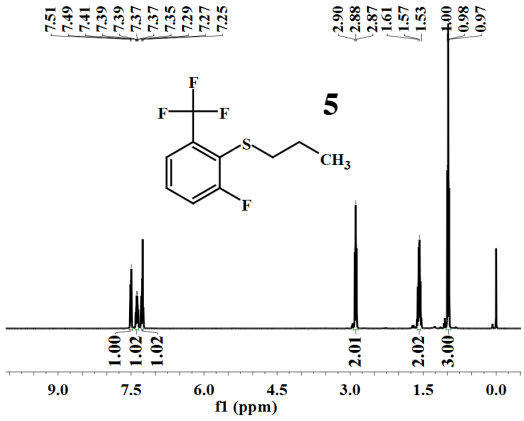

12.80
11.52
6.02
4.18
4.16
4.14
3.91
1.24
1.22
1.20
3a
0.95
0.96
0.98
2.00
6.00
3.00
f1 (ppm)


13.30
11.41
7.05
4.20
4.18
4.16
4.15
2.40
1.26
1.24
1.23
3b
0.93
0.96
1.00
2.00
6.01
3.02
f1 (ppm)


6.06
5.97
4.06
3.90
4a
1.00
1.93
3.00
3.00
f1 (ppm)


6.82
6.23
2.55
2.45
4b
1.00
1.99
3.00
3.00
f1 (ppm)


6.38
5.24
2.29
2b
NH2
N
N
H3C
CH3
1.00
2.00
6.00
9 8 7 6 5 4 3 2 1 0
f1 (ppm)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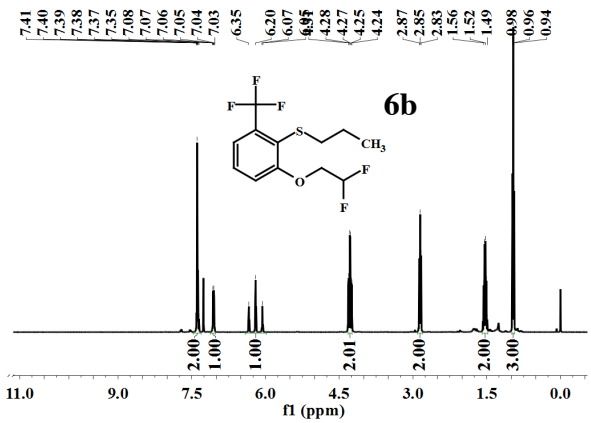
7.49
7.41
7.39
7.39
7.37
7.37
7.35
7.29
7.27
7.25
2.90
2.88
2.87
1.61
1.57
1.53
1.00
0.98
0.97
5
F
F
F
S
CH3
F
1.00
1.02
1.02
2.01
2.02
3.00
9.0 7.5 6.0 4.5 3.0 1.5 0.0
f1 (ppm)


7.41
7.40
7.39
7.38
7.37
7.35
7.08
7.07
7.06
7.05
7.04
7.03
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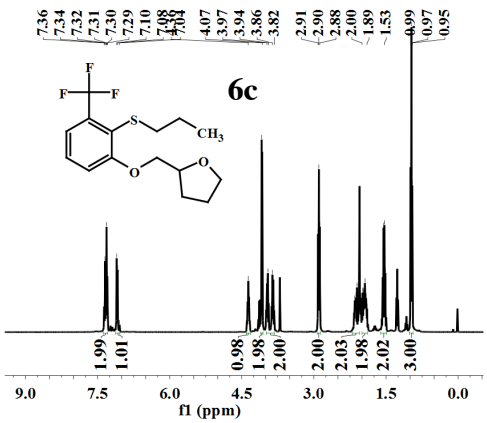
6.20
6.07
4.28
4.27
4.25
4.24
2.87
2.85
2.83
1.56
1.52
1.49
0.98
0.96
0.94
6b
F
F
F
S
CH3
O
F
F
2.00
1.00
1.00
2.01
2.00
2.00
3.00
11.0 9.0 7.5 6.0 4.5 3.0 1.5 0.0
f1 (ppm)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7.34
7.32
7.31
7.30
7.29
7.10
4.07
3.97
3.94
3.86
3.82
2.91
2.90
2.88
2.00
1.89
1.53
0.99
0.97
0.95
6c
F
F
F
S
CH3
O
O
1.99
1.01
0.98
1.98
2.00
2.00
2.03
1.98
2.02
3.00
9.0 7.5 6.0 4.5 3.0 1.5 0.0
f1 (ppm)

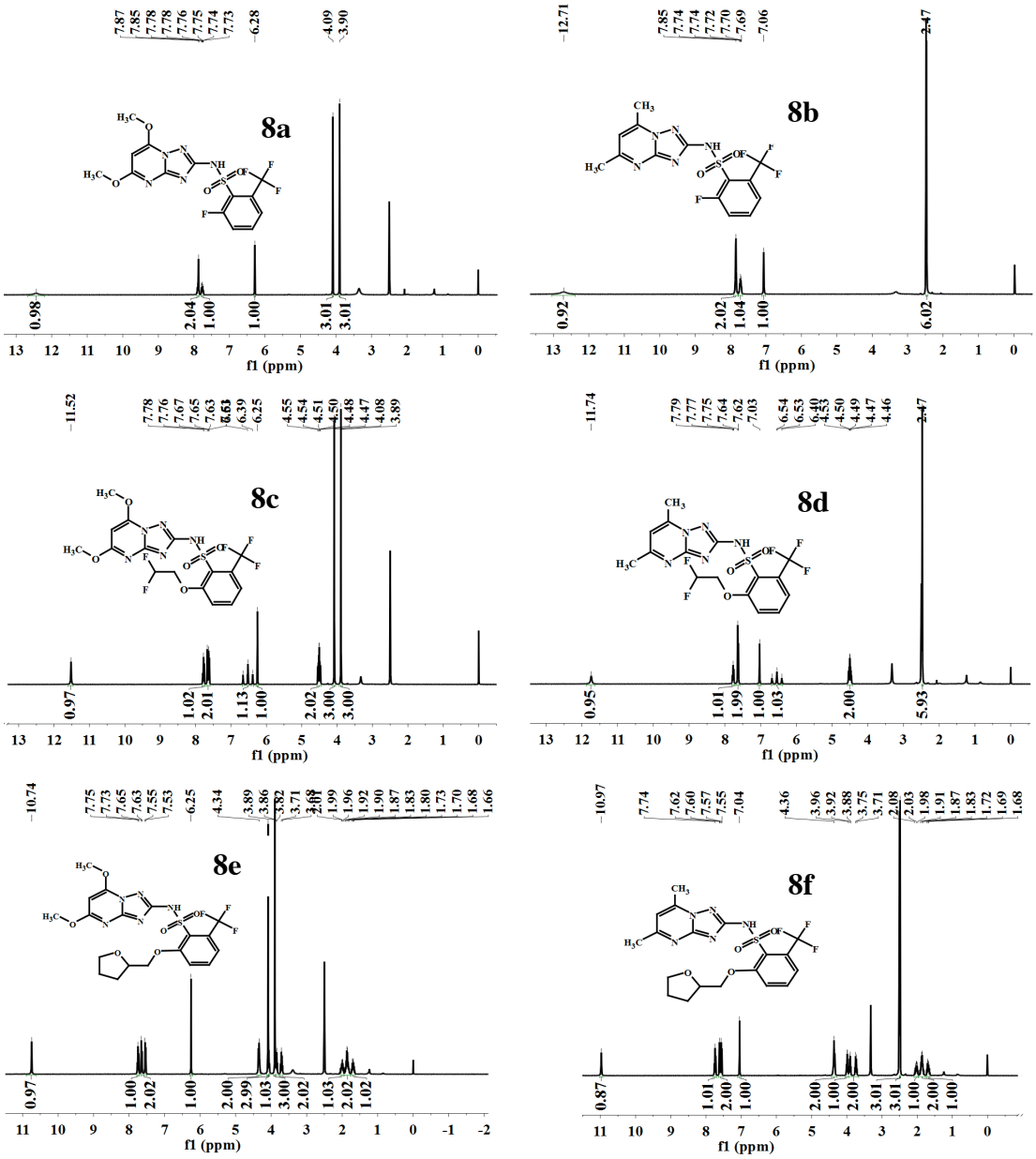


Figure. S1 ^{1}H-NMR of compounds **2b**, **3a**, **3b**, **4a**, **4b**, **5**, **6b**, **6c**, and **8a-8f**.

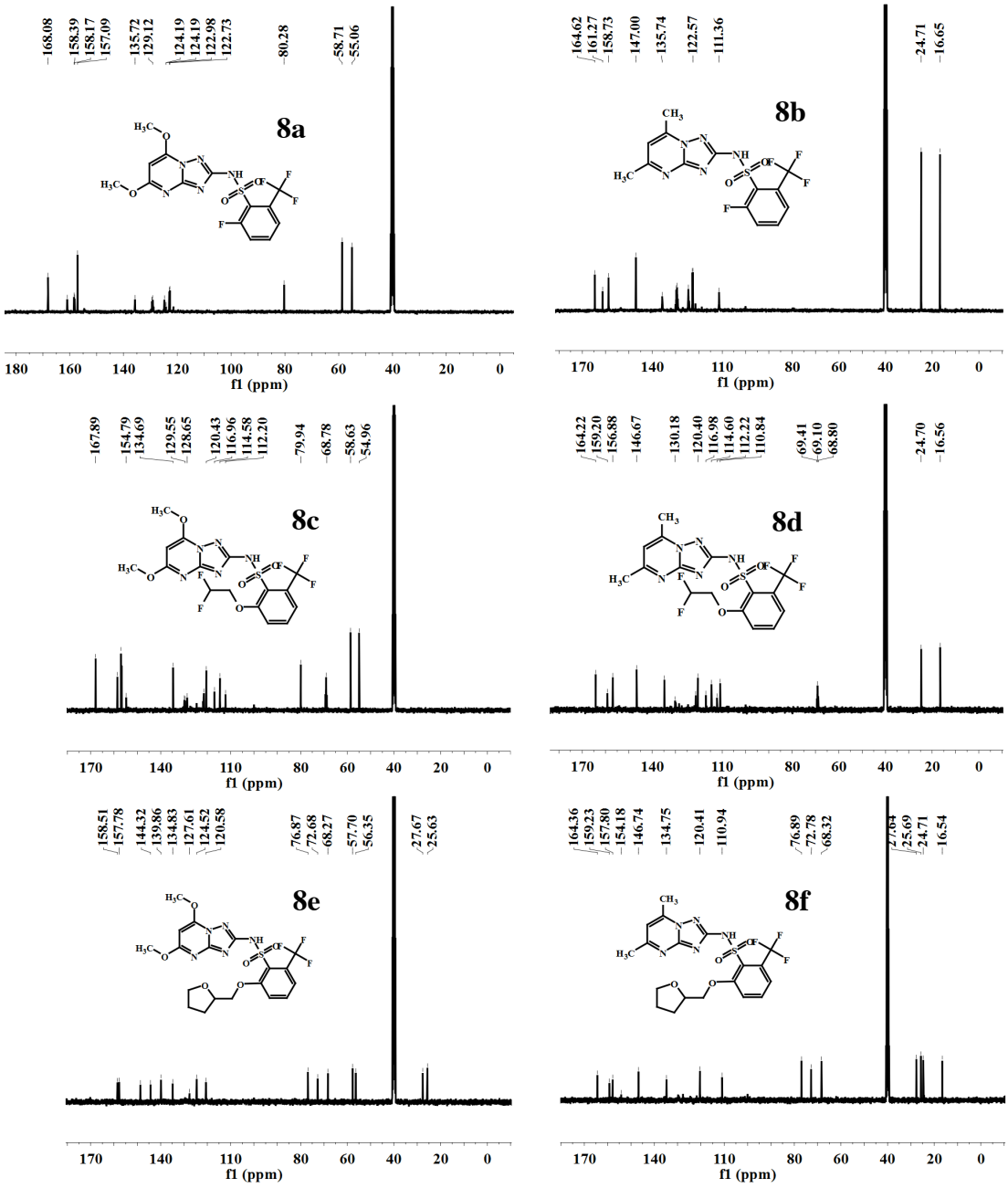


Figure. S2 ^{13}C-NMR of compounds **8a-8f**.

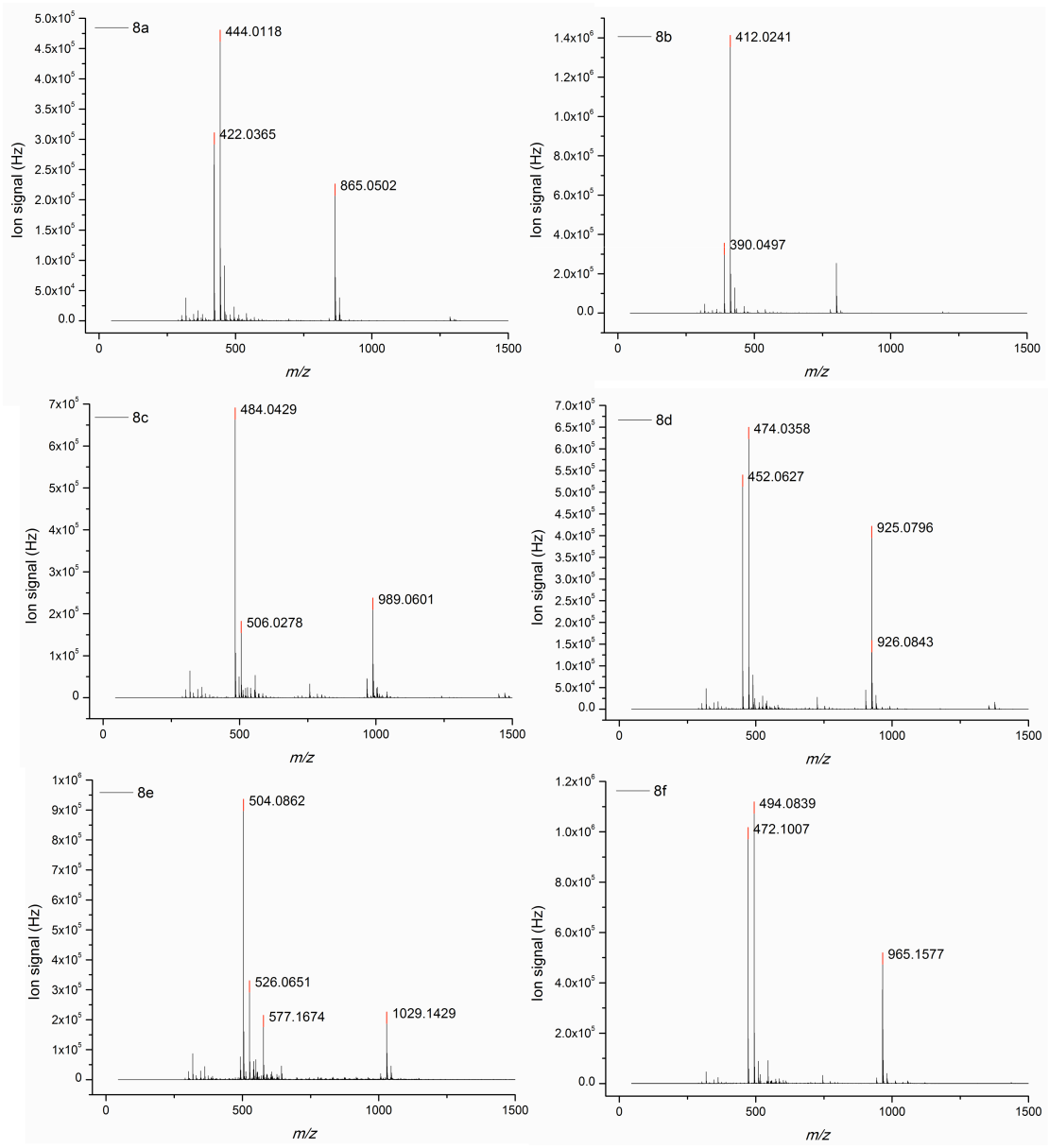


Figure. S3 HRMS of compounds **8a-8f**.

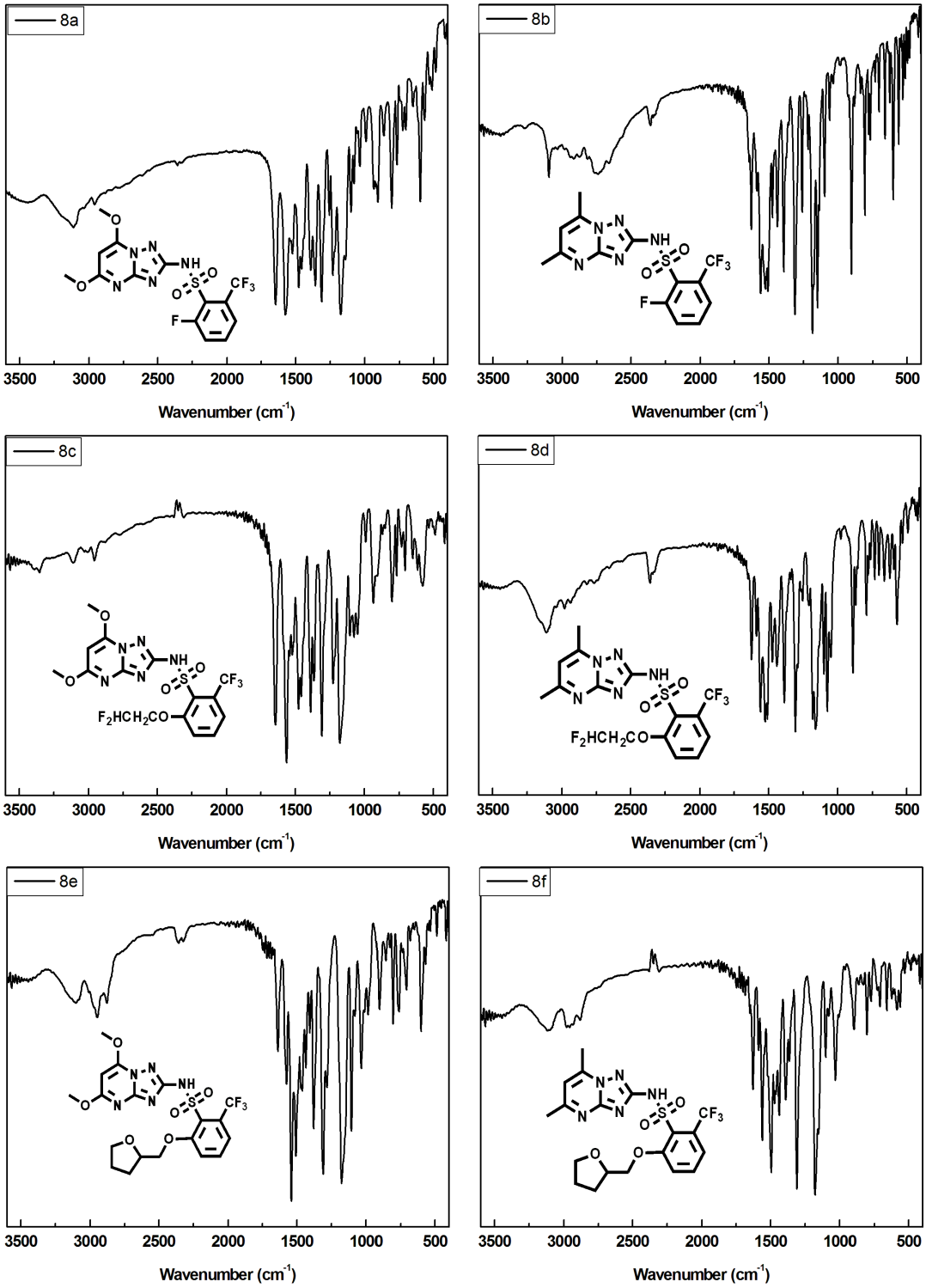
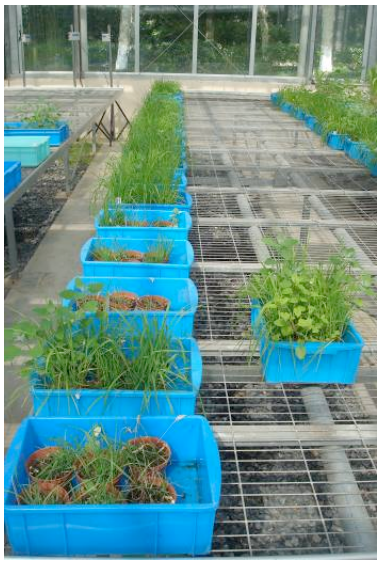


Figure. S4 IR of compounds **8a-8f**.

Blank control groups and the screening of compounds **8a-8f**. **Penoxsulam**

Picture S1. Inhibitory Effect of Compounds **8a-8f** on the Growth of Seed Roots and Shoots.

2015-4-1 chemical spray; 2015-4-30 the last survey:



Blank control groups and the screening of compounds **8a**, **8c** and **8e**.

Picture S2. Screening in Greenhouse Conditions of Compounds **8a-8f**.

Typical phytotoxicity symptoms toward soybean of compounds **8a**, **8c** and **8e** (the right pictures are blank control groups)

Typical phytotoxicity symptoms toward cotton of compounds **8a**, **8c** and **8e** (the right pictures are blank control groups)

Picture S3. Crop selectivity of Compounds **8a**, **8c** and **8e**.

Table S4. The raw data of compounds **8a-8f** crop selectivity.

compounds	dosage gai/ha	maize				rice				cotton			
		Fresh weitht /g	Plants	Fresh weitht /g	Plants	Fresh weitht /g	Plants	Fresh weitht /g	Plants	Fresh weitht /g	Plants	Fresh weitht /g	Plants
Penoxsulam	150	27.39	2	31.75	2	16.33	24	16.75	25	17.78	2	17.4	2
8a	150	22.38	3	18.31	2	10.83	23	13.61	26	21.03	2	21.76	2
8c	150	23.2	2	29.93	3	14.51	20	14.62	21	8.11	2	6.65	2
8e	150	24.17	2	32.5	3	15.37	21	13.84	17	14.51	2	5.14	2
compounds	dosage gai/ha	soybean				rape				wheat			
		Fresh weitht /g	Plants	Fresh weitht /g	Plants	Fresh weitht /g	Plants	Fresh weitht /g	Plants	Fresh weitht /g	Plants	Fresh weitht /g	Plants
Penoxsulam	150	0	3	0	3	1.98	5	1.78	5	8.4	25	5.43	16
8a	150	27.26	3	26.61	3	2.02	6	1.6	5	6.87	21	6.52	24
8c	150	17.75	3	14.35	3	0.73	5	0.77	5	7.32	13	10.12	31
8e	150	26.08	3	20.79	3	2.37	5	2.14	5	7.16	21	7.28	15