

1. H-NMR



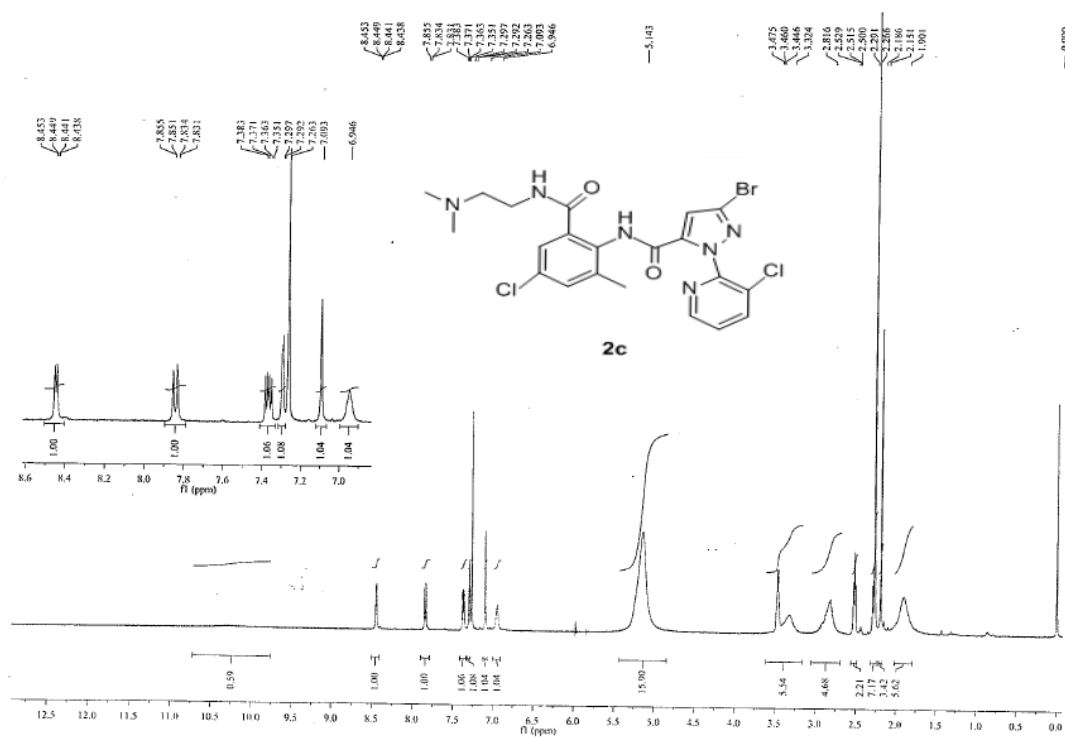


Figure S3. ^1H -NMR spectrum of compound **2c**.

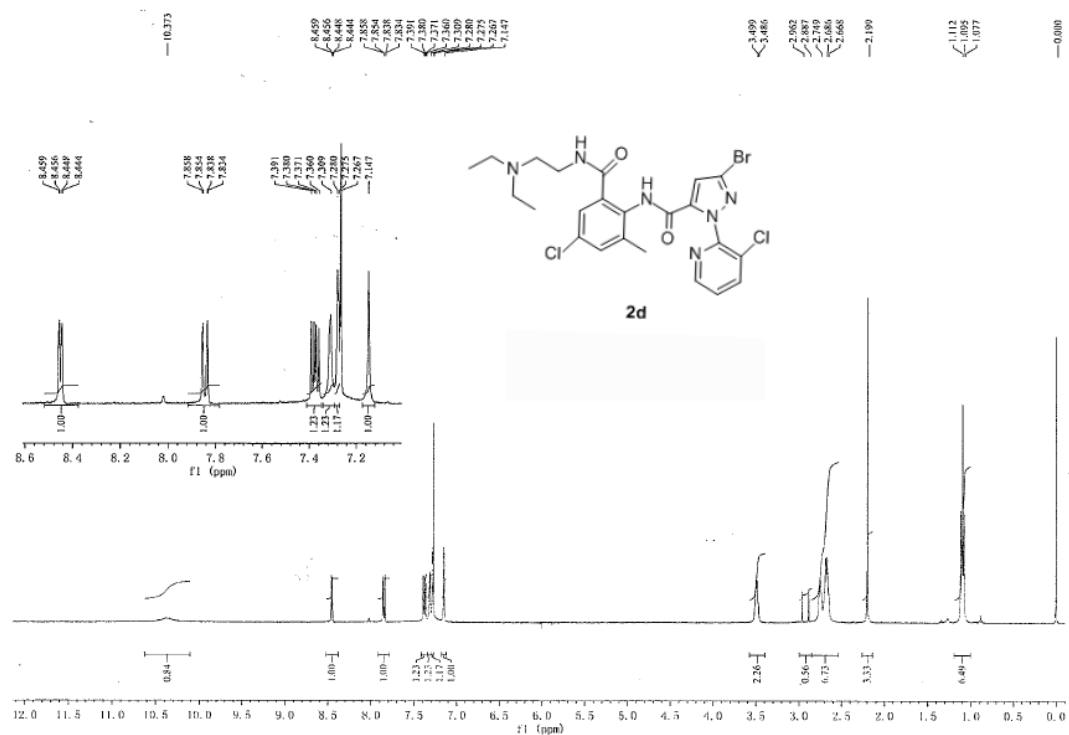


Figure S4. ^1H -NMR spectrum of compound **2d**.

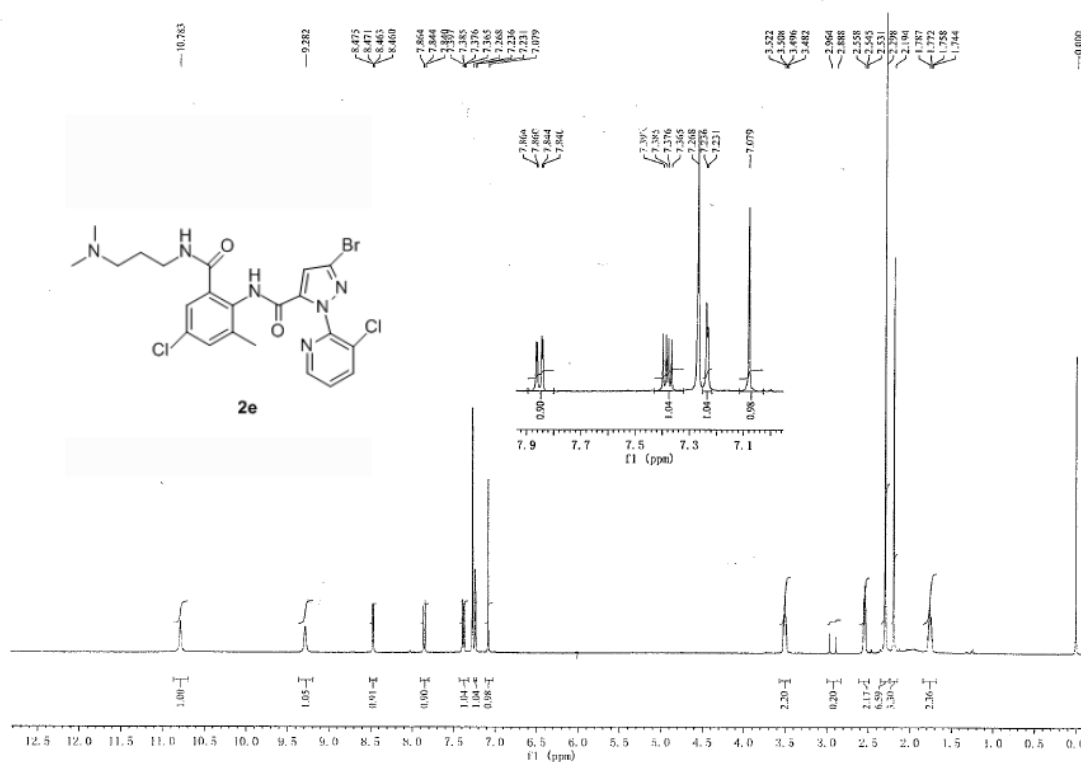
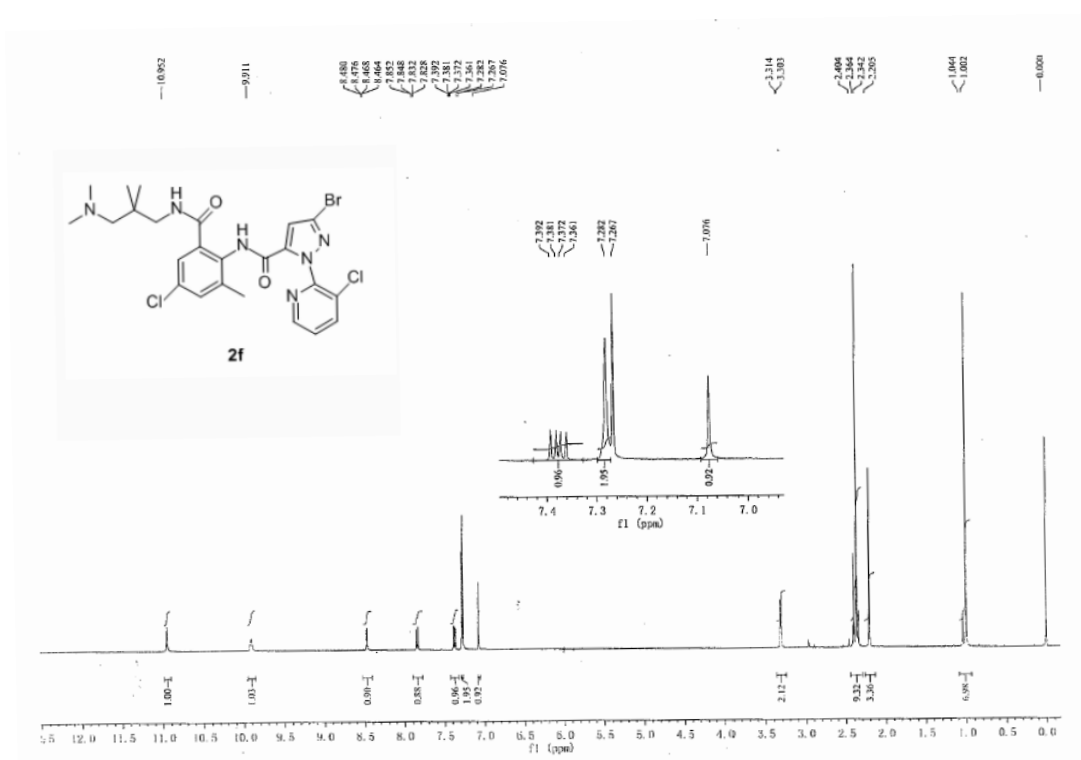


Figure S5. ^1H -NMR spectrum of compound **2e**.



Chemical structure of 2h: CCN(CC)CCNC(=O)c1cc(Cl)c(C(=O)Nc2nc3ccccc3n2)c(C(=O)Nc4nc5ccccc5n4)c1

¹H NMR spectrum (CDCl₃):

- Chemical shift (ppm):** 8.461, 8.457, 8.449, 8.445, 7.857, 7.841, 7.837, 7.831, 7.397, 7.385, 7.377, 7.369, 7.365, 7.285, 7.270, 7.265, 7.211, 7.136, 4.817, 3.394, 3.379, 3.365, 2.485, 2.480, 2.465, 2.452, 2.437, 2.422, 2.407, 2.392, 2.377, 2.356, 2.341, 2.326, 2.311, 2.296, 2.281, 2.266, 2.251, 2.236, 2.221, 2.206, 2.191, 2.176, 2.161, 2.146, 2.131, 2.116, 2.101, 2.086, 2.071, 2.056, 2.041, 2.026, 2.011, 2.000.
- Integration values:** 1.00, 0.96, 1.95, 0.96, 0.94, 0.21, 2.18, 4.30, 2.29, 3.36, 0.40, 4.46, 6.50.

Inset spectrum (7.1-7.9 ppm):

- Chemical shift (ppm):** 7.881, 7.867, 7.857, 7.397, 7.385, 7.377, 7.369, 7.365, 7.285, 7.270, 7.265, 7.211, 7.136.
- Integration values:** 0.96, 1.95, 0.96, 0.94, 0.21.

Figure S8. ^1H -NMR spectrum of compound **2h**.

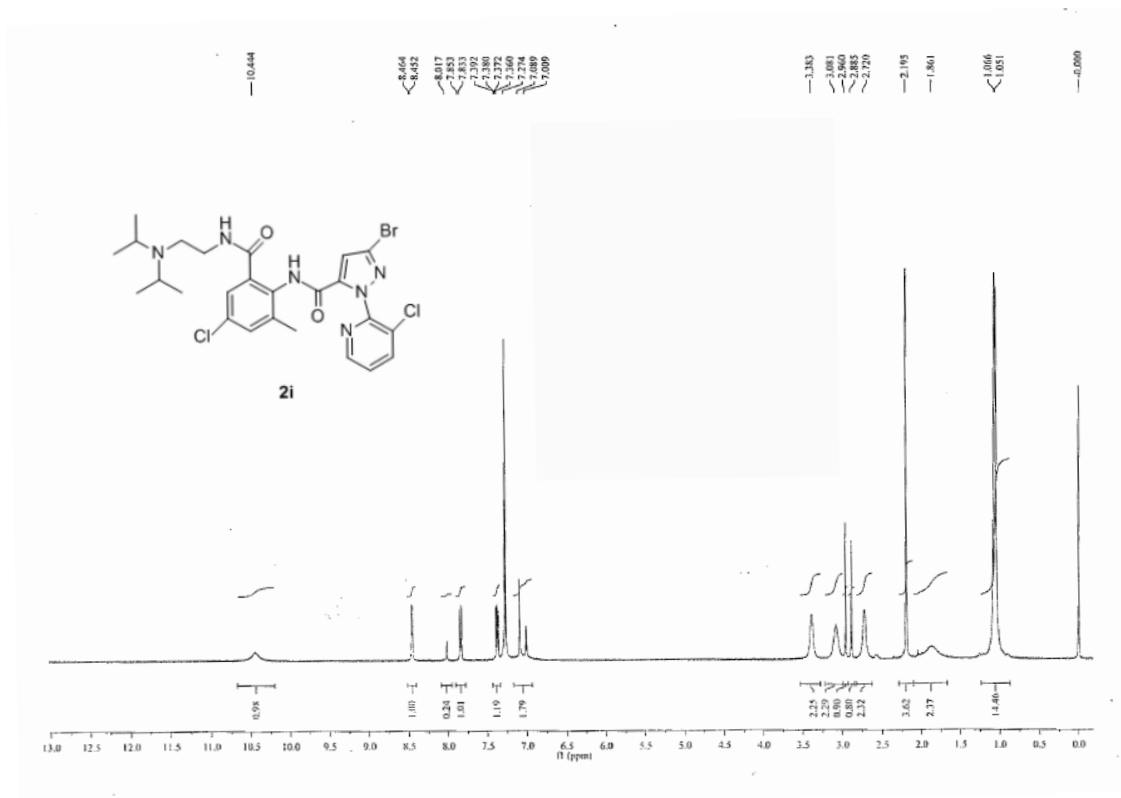


Figure S9. ¹H-NMR spectrum of compound 2i.

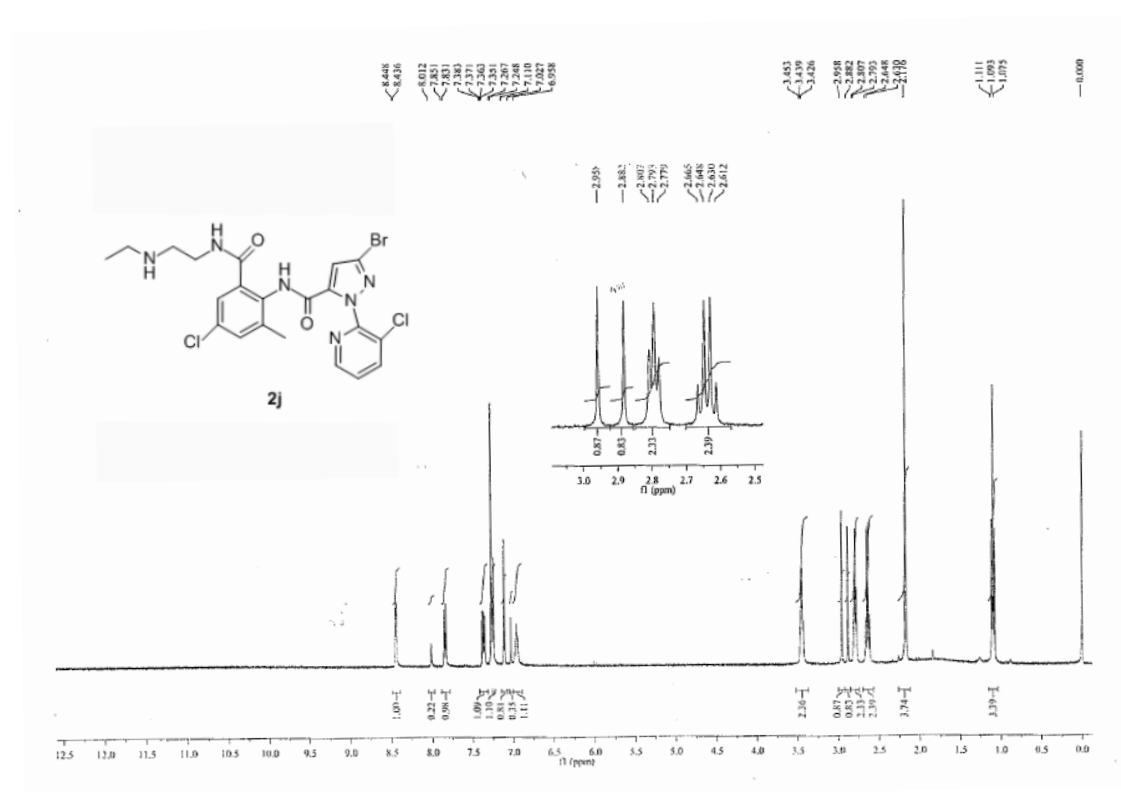


Figure S10. ¹H-NMR spectrum of compound 2j.

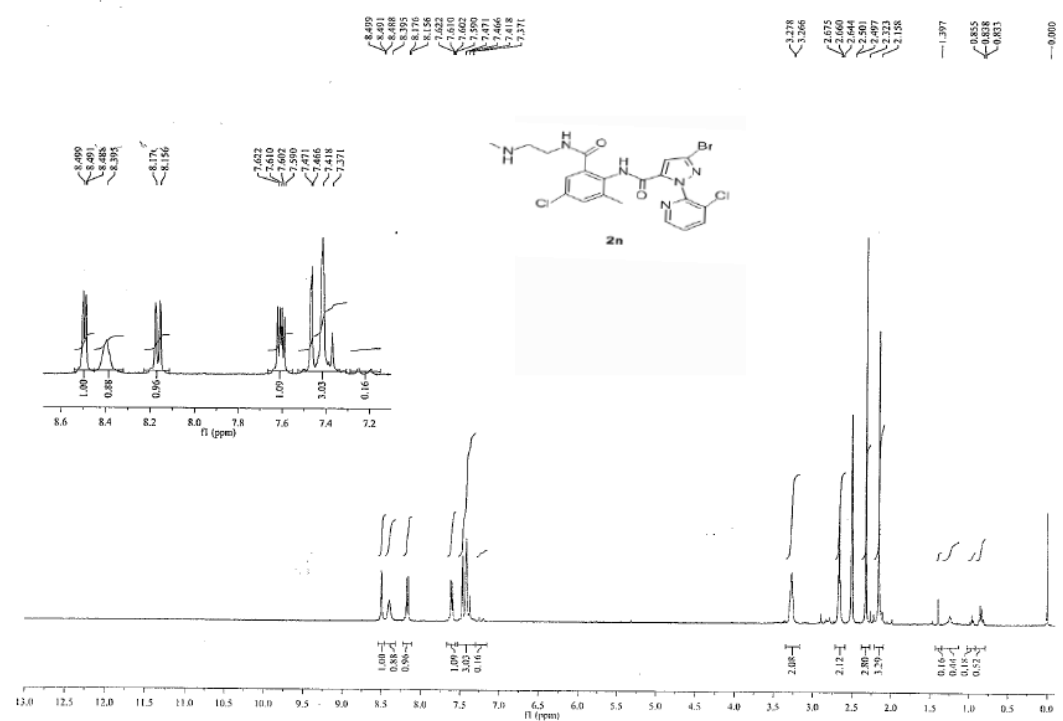
Chemical structure of compound **21** is shown as an inset. The structure is a 4-chloro-2-(2-isopropylaminoethyl)benzamide derivative with a 4-bromo-2-chloro-1H-benzotriazin-3-yl group attached via an amide linkage.

¹H NMR spectrum (CDCl₃) of compound **21** is shown. The spectrum displays peaks in the aromatic region (7.3–8.2 ppm) and aliphatic region (1.2–3.6 ppm). The chemical shifts (ppm) are listed above the peaks, and the integration values are shown below the peaks.

Chemical shifts (ppm): 8.081, 8.082, 8.048, 8.044, 8.044, 8.024, 7.575, 7.568, 7.544, 7.536, 7.538, 7.538, 7.439, 7.433, 7.372, 7.363, 3.562, 3.558, 3.554, 3.540, 3.527, 3.504, 3.384, 3.364, 3.036, 3.036, 3.008, 2.556, 2.552, 2.547, 2.223, 1.314, 1.297, 1.234, 1.218, 0.000.

Integration values: 1.00, 2.24, 1.84, 2.38, 3.41, 1.64, 0.97, 13.60, 5.07, 5.29, 10.40, 6.95.

Figure S12. ^1H -NMR spectrum of compound **2l**.



Chemical structure of **2p** is shown in the center of the figure.

¹H NMR spectrum (CDCl₃) of compound **2p** is displayed below the structure. The spectrum shows peaks in the aromatic region (7.0–8.5 ppm), a singlet at ~3.5 ppm, a multiplet at ~2.5 ppm, and a triplet at ~1.0 ppm. Integration values are provided below the baseline.

Key peak data (ppm, integration):

- ~10.0 (broad, 0.04)
- ~8.4 (1.00)
- ~7.8 (1.01)
- ~7.6 (2.18)
- ~7.4 (1.10)
- ~7.2 (0.91)
- ~7.1 (0.14)
- ~3.5 (2.31)
- ~2.5 (5.04)
- ~2.3 (2.31)
- ~2.1 (5.04)
- ~1.9 (3.54)
- ~1.5 (2.97)
- ~1.0 (7.19)

Inset 1 (7.3–7.7 ppm):

- 7.566
- 7.593
- 7.382
- 7.394
- 7.402
- 7.414

Inset 2 (2.5–2.8 ppm):

- 2.565
- 2.583
- 2.601
- 2.619
- 2.665
- 2.679
- 2.692

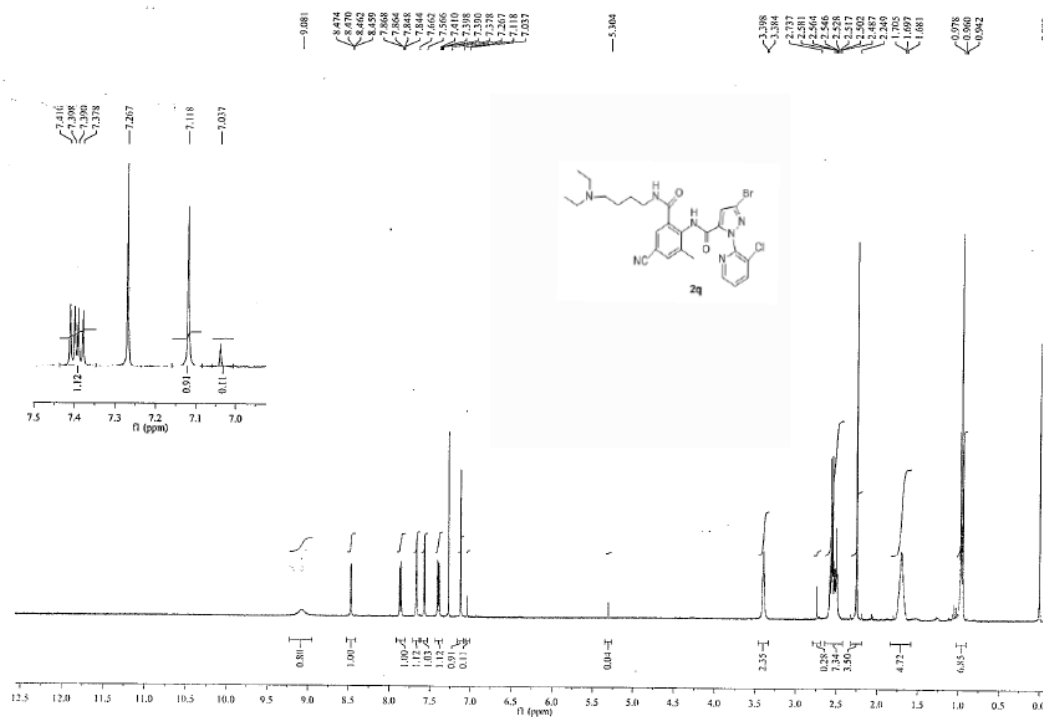


Figure S17. ^1H -NMR spectrum of compound **2q**.

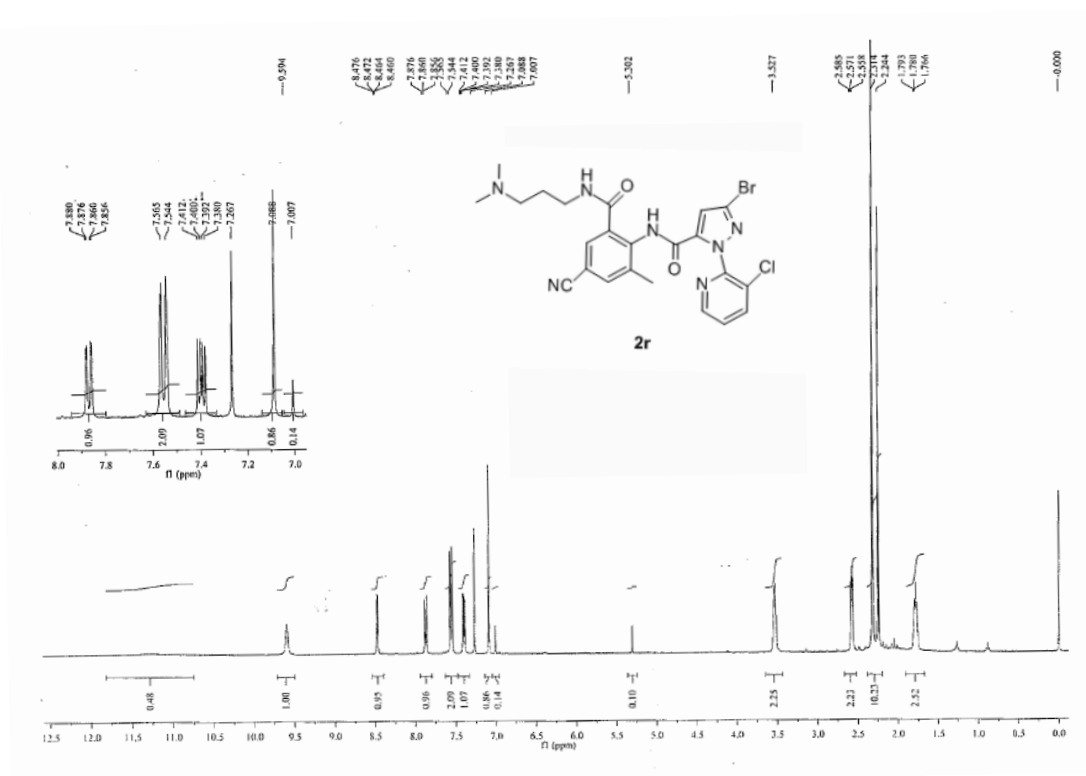


Figure S18. ^1H -NMR spectrum of compound **2r**.

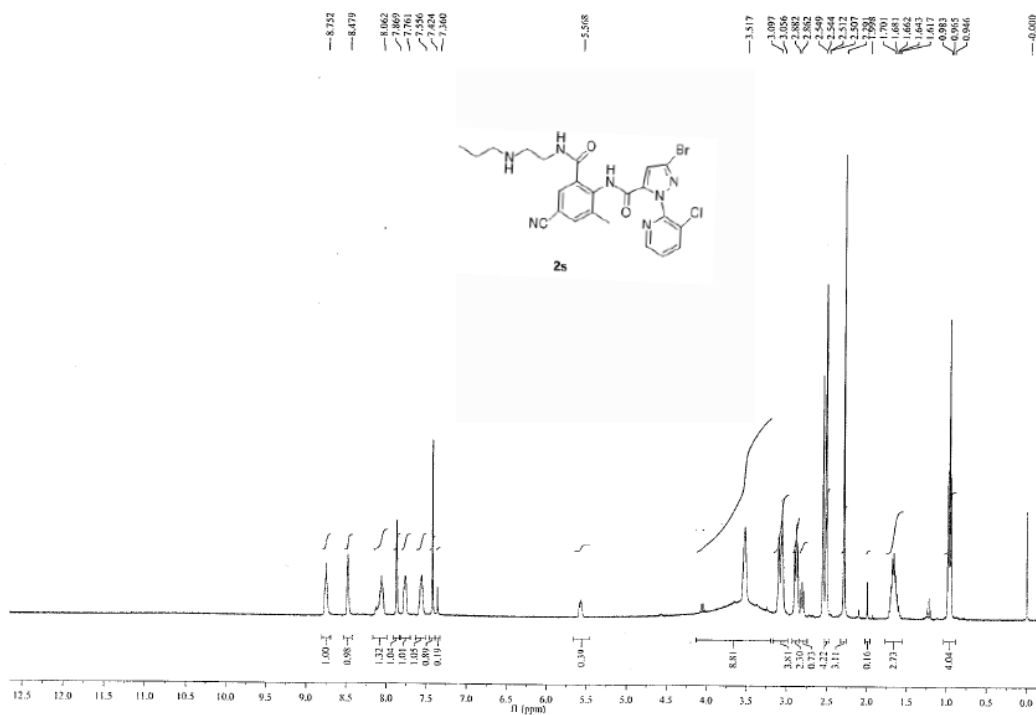
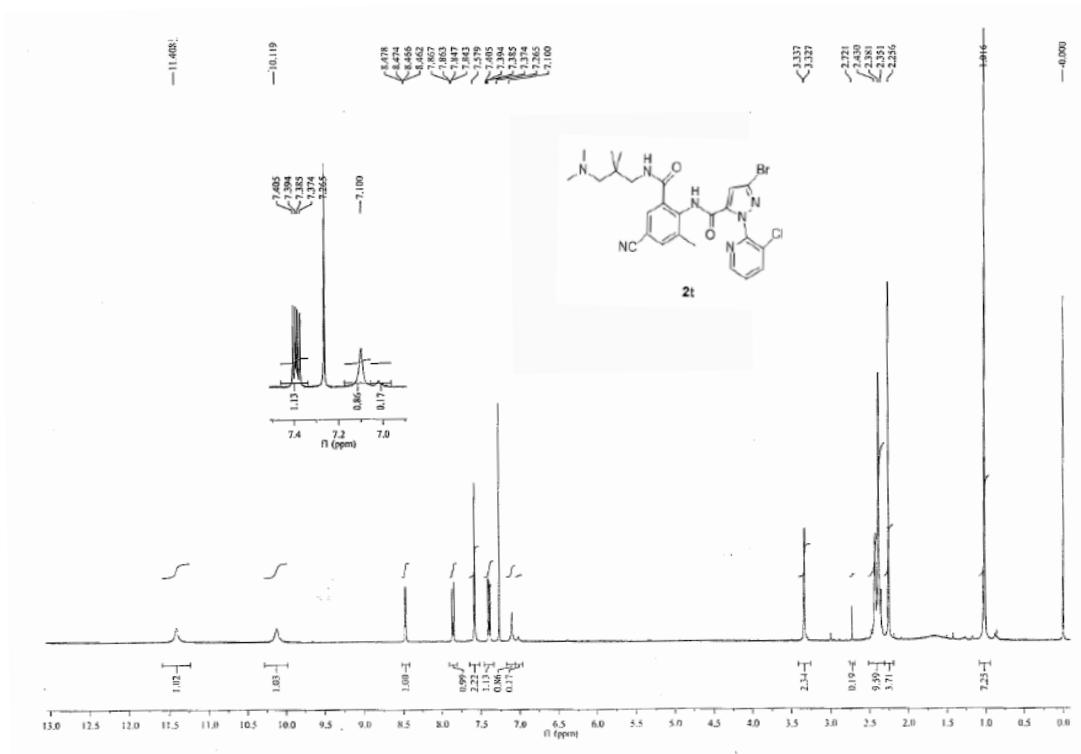


Figure S19. ^1H -NMR spectrum of compound **2s**.



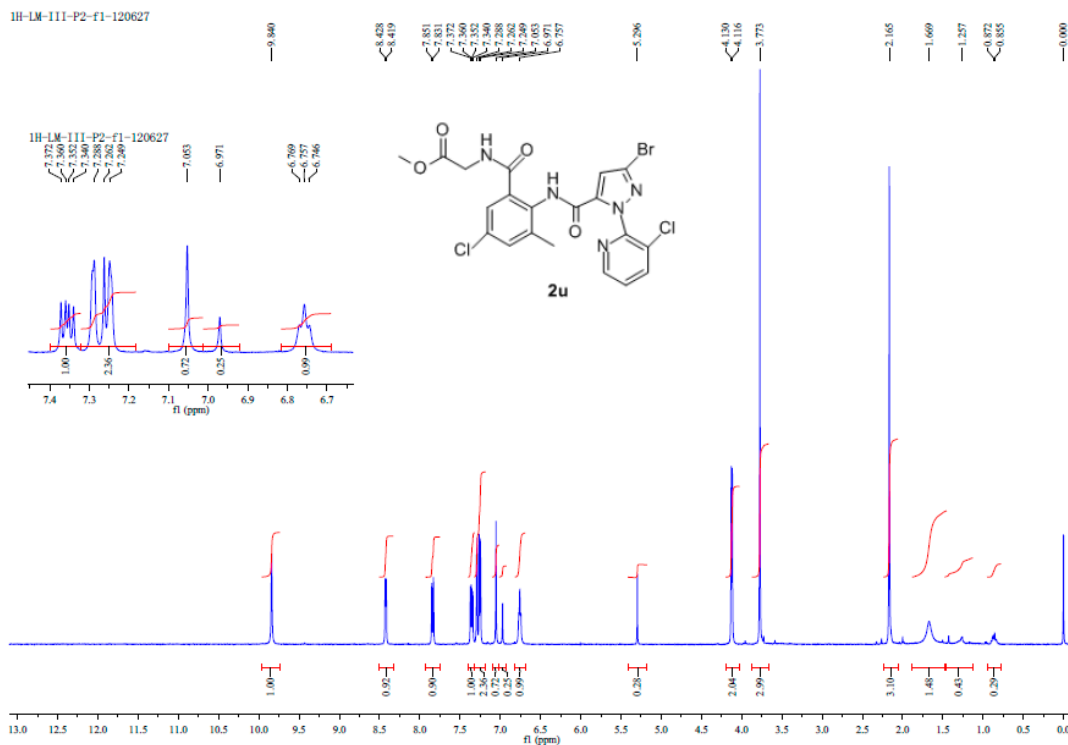


Figure S21. ^1H -NMR spectrum of compound **2u**.

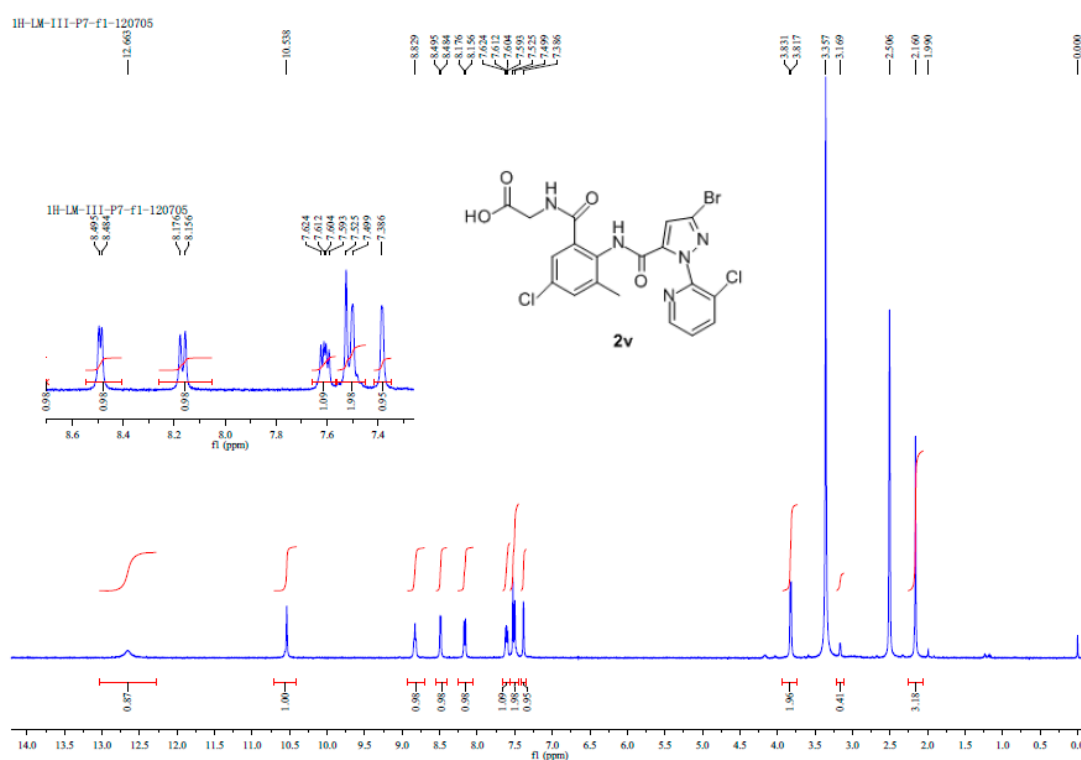
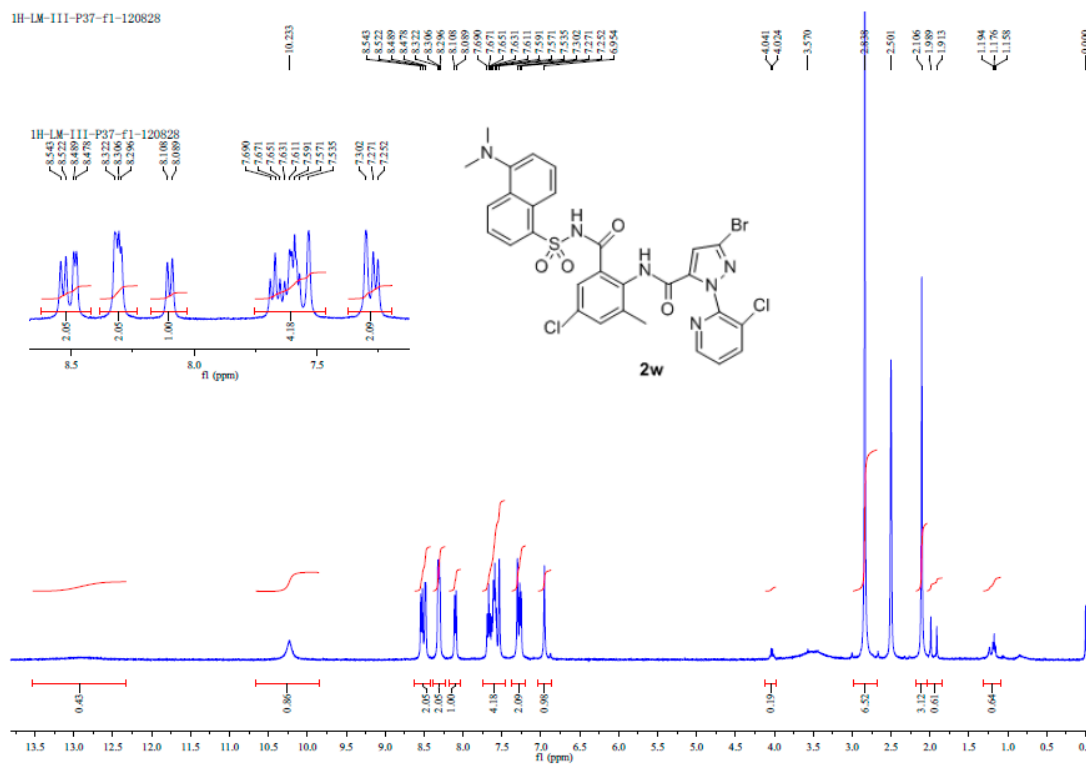
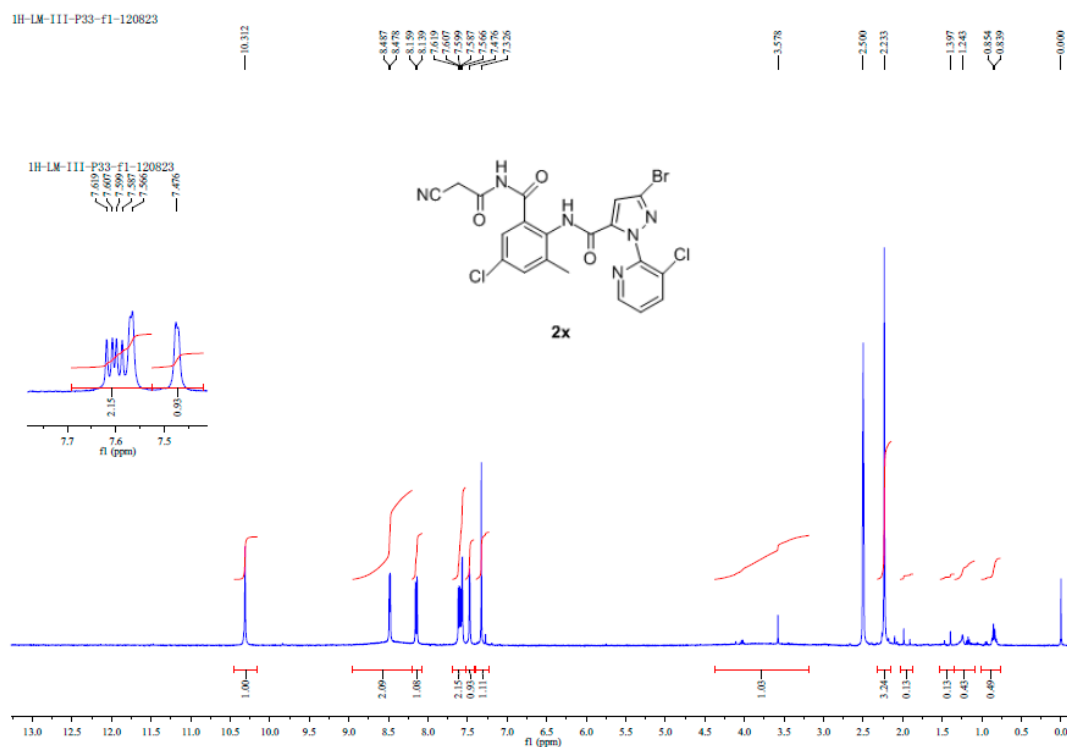


Figure S22. ^1H -NMR spectrum of compound **2v**.

Figure S23. ¹H-NMR spectrum of compound **2w**.Figure S24. ¹H-NMR spectrum of compound **2x**.

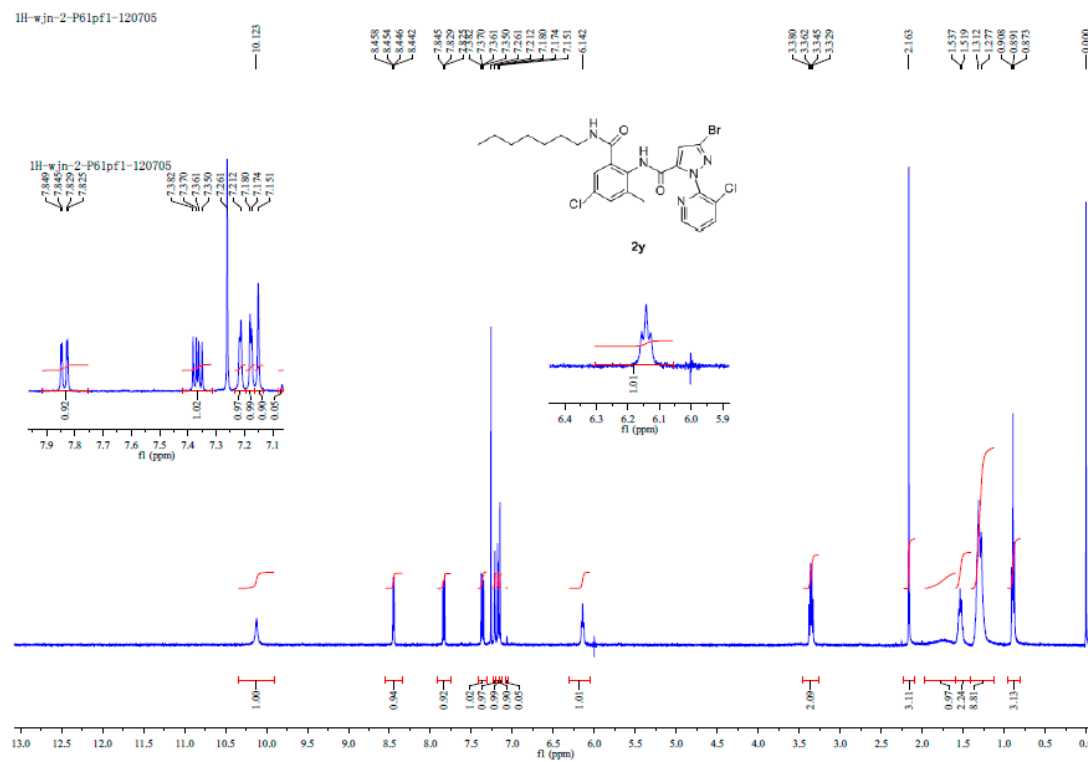


Figure S25. ^1H -NMR spectrum of compound **2y**.

2. C-NMR

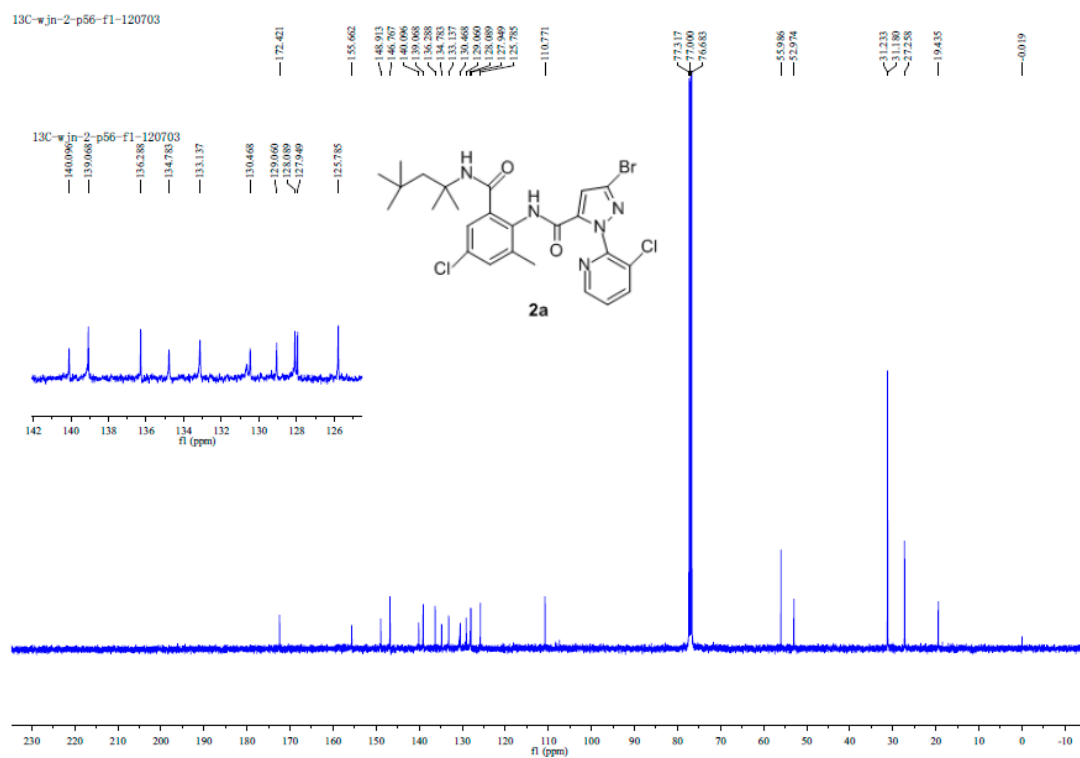


Figure S26. ^{13}C -NMR spectrum of compound **2a**.

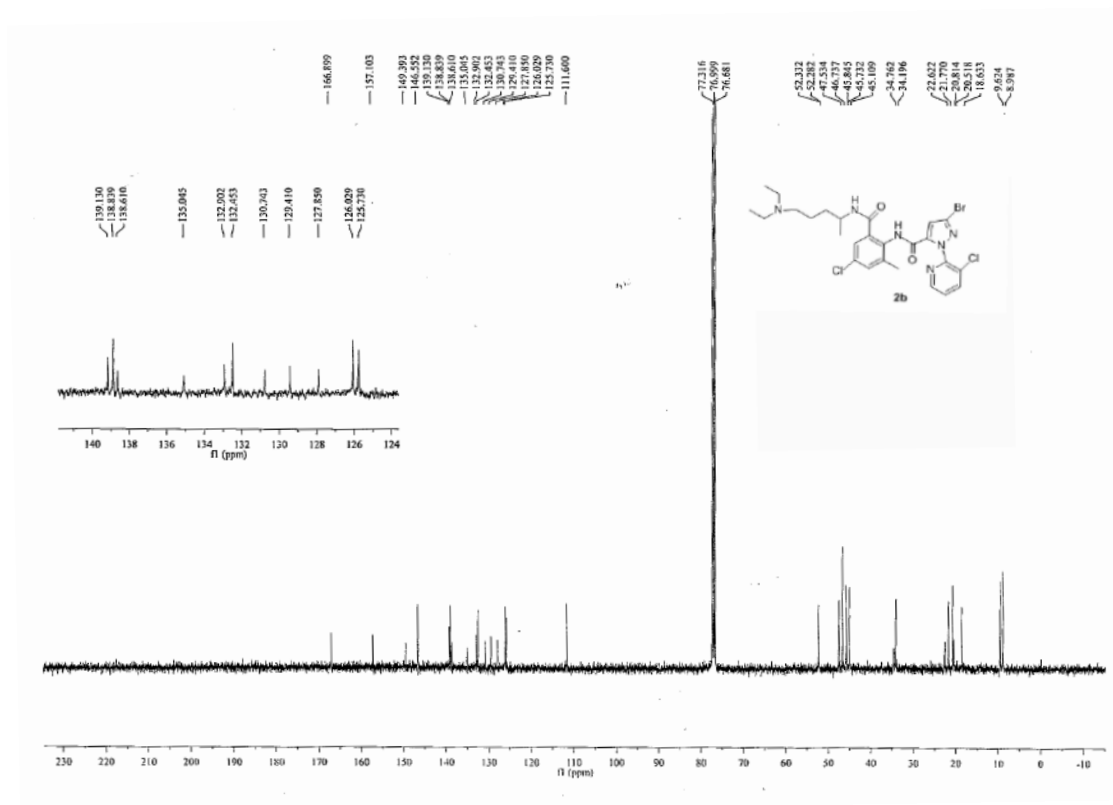


Figure S27. ^{13}C -NMR spectrum of compound **2b**.

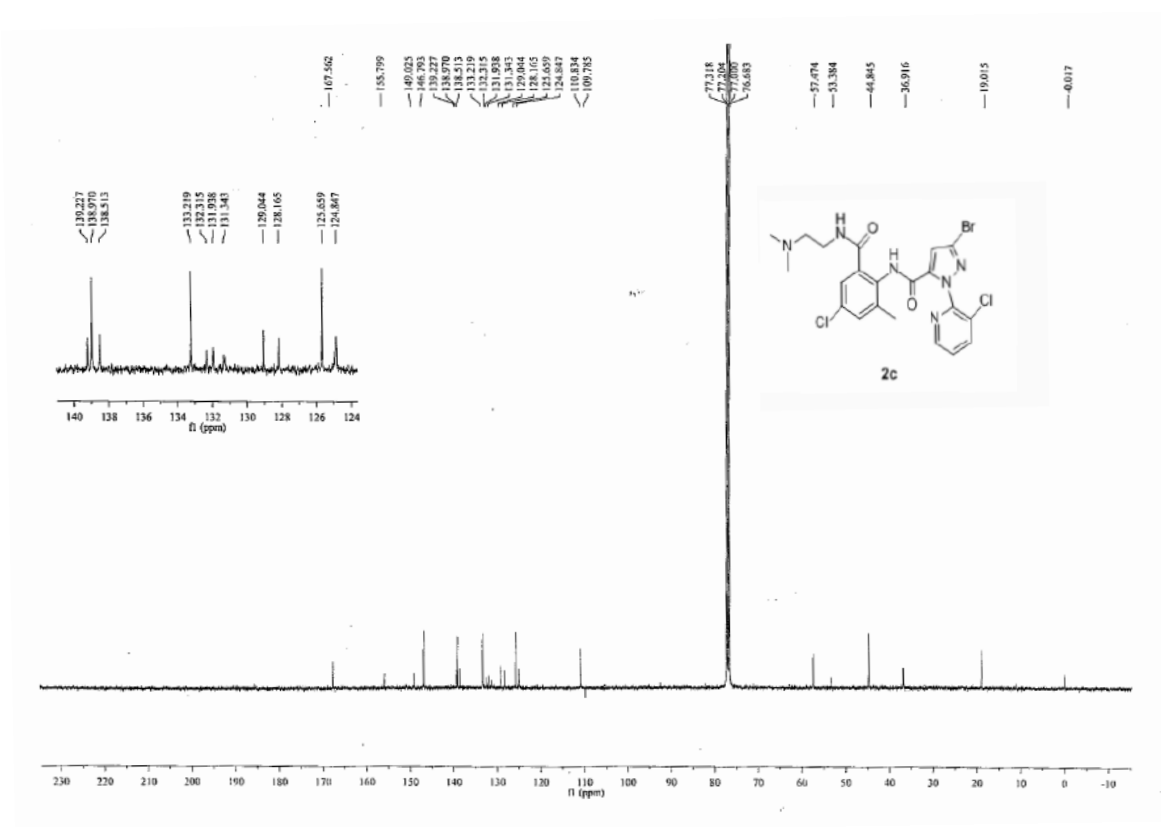


Figure S28. ^{13}C -NMR spectrum of compound **2c**.

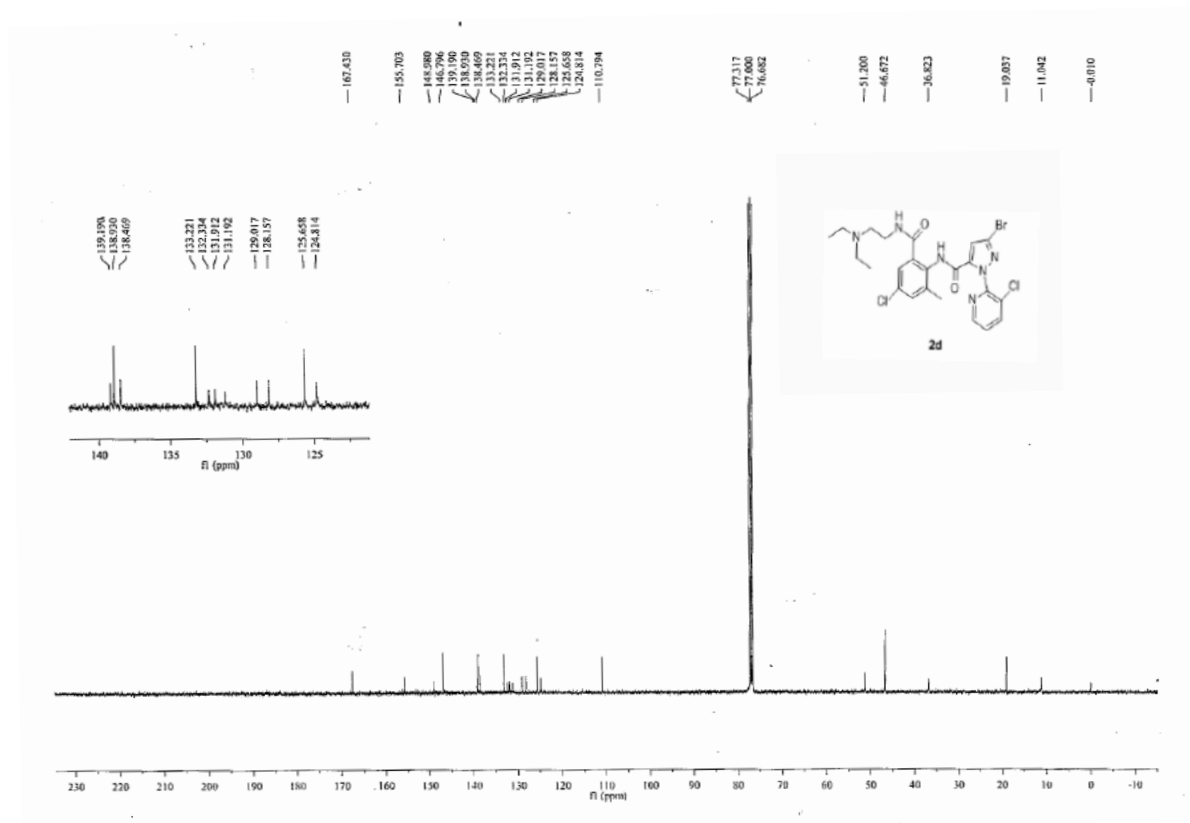


Figure S29. ^{13}C -NMR spectrum of compound **2d**.

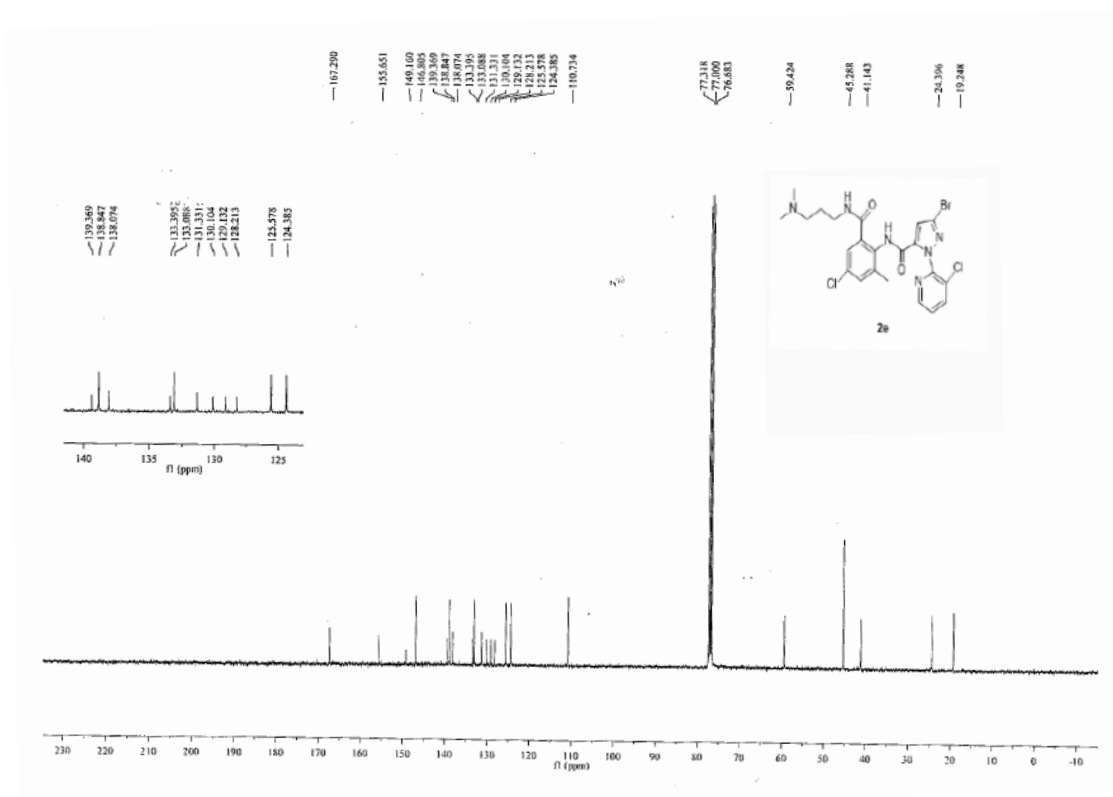


Figure S30. ^{13}C -NMR spectrum of compound **2e**.

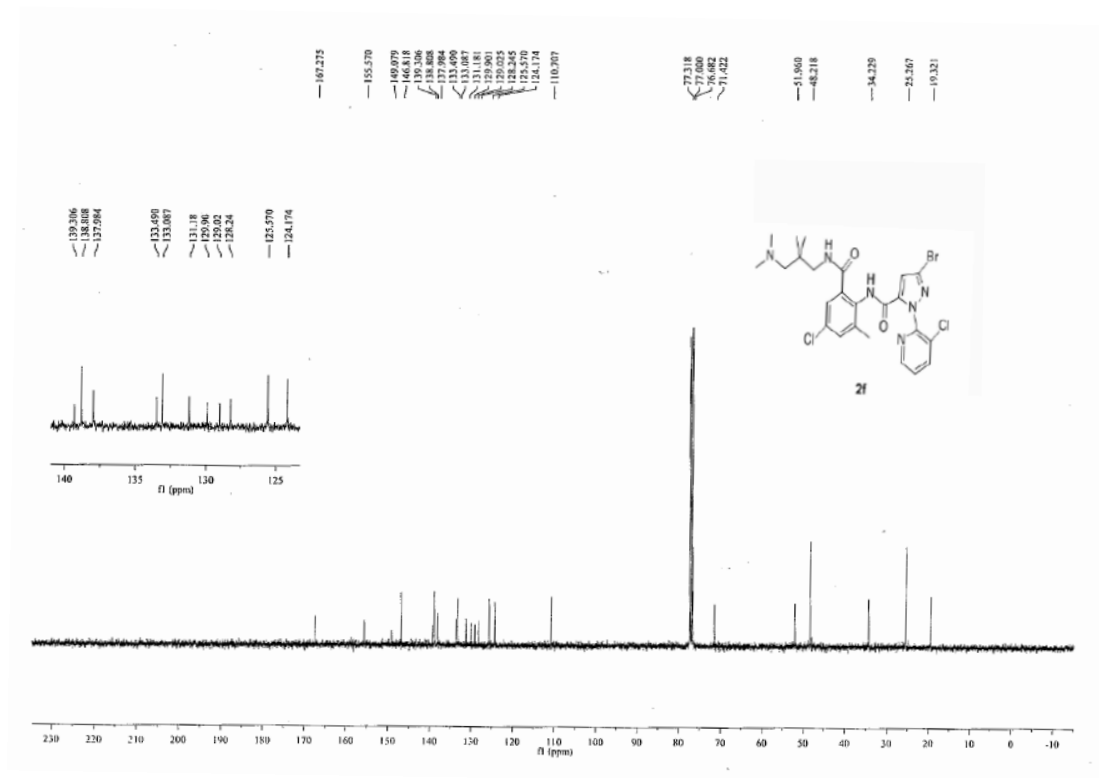


Figure S31. ¹³C-NMR spectrum of compound 2f.

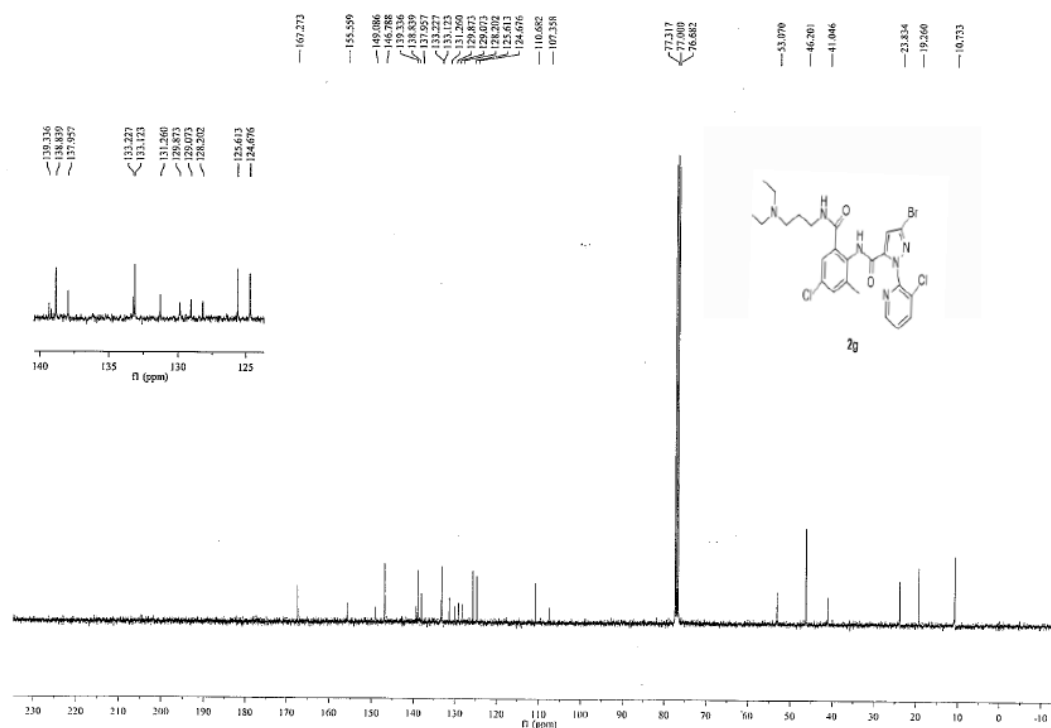


Figure S32. ¹³C-NMR spectrum of compound 2g.

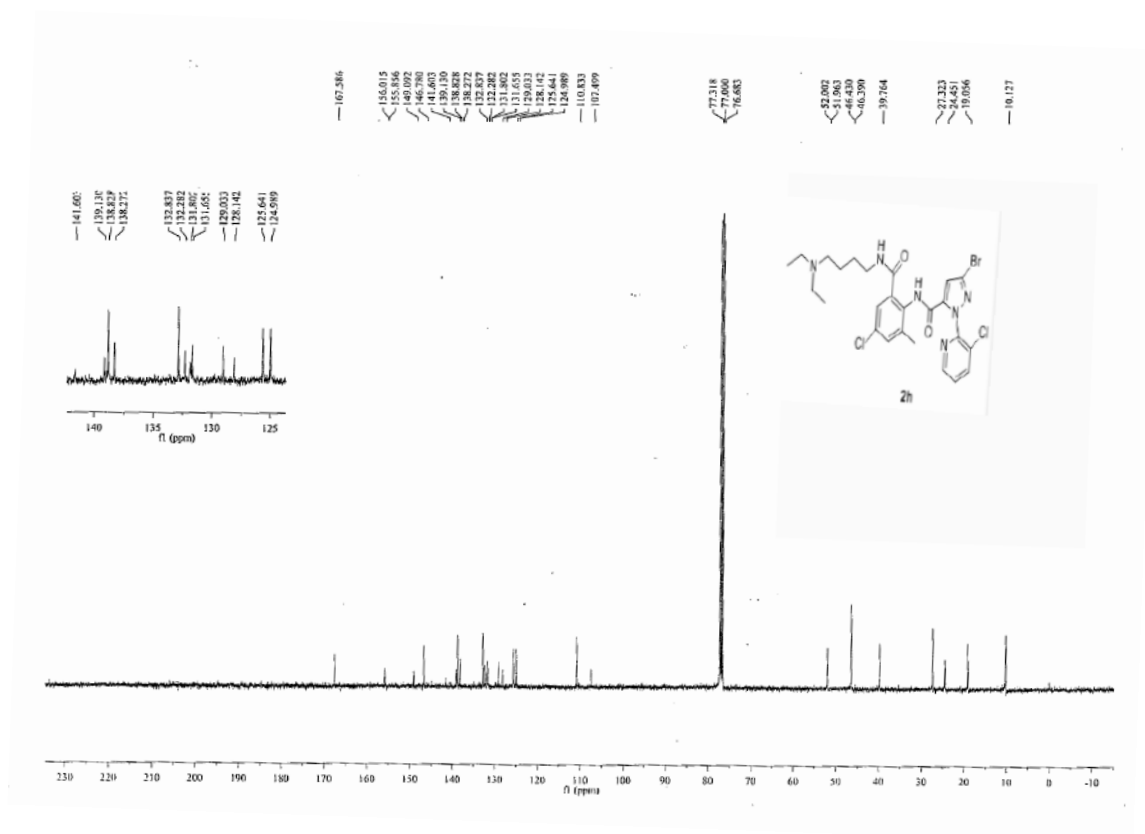


Figure S33. ^{13}C -NMR spectrum of compound **2h**.

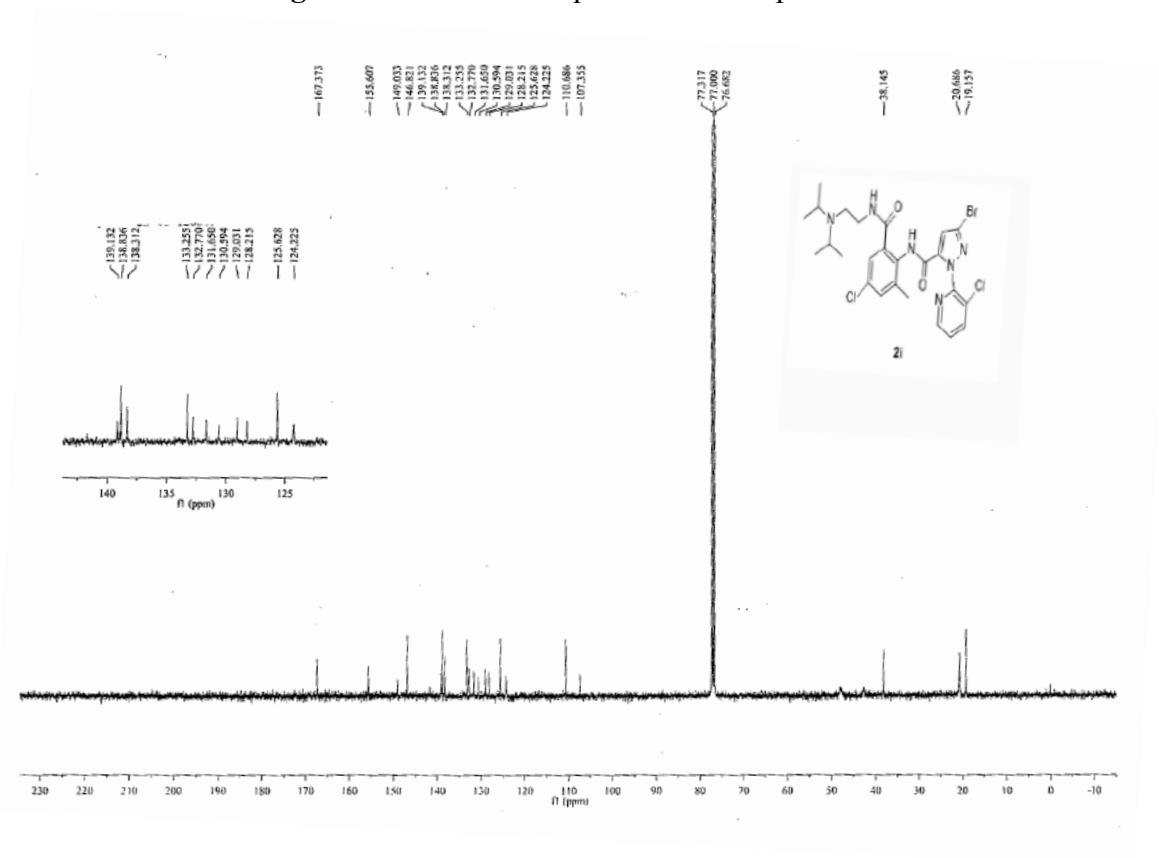


Figure S34. ^{13}C -NMR spectrum of compound **2i**.

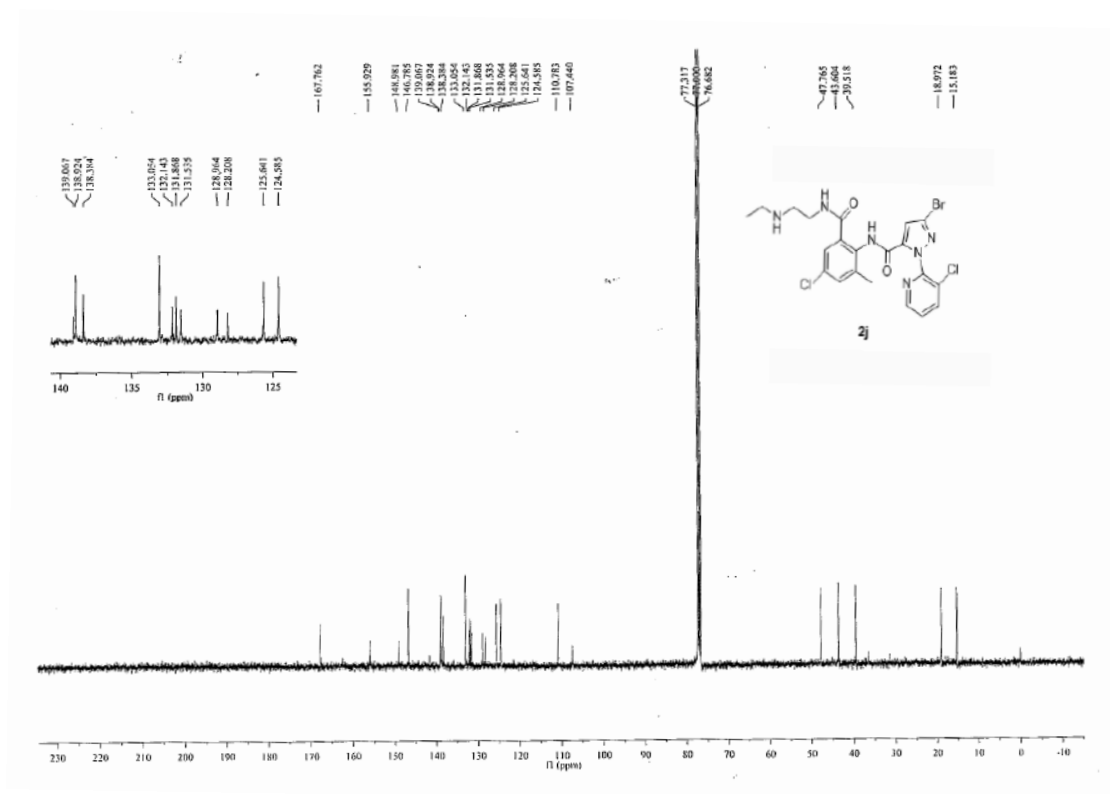


Figure S35. ^{13}C -NMR spectrum of compound 2j.

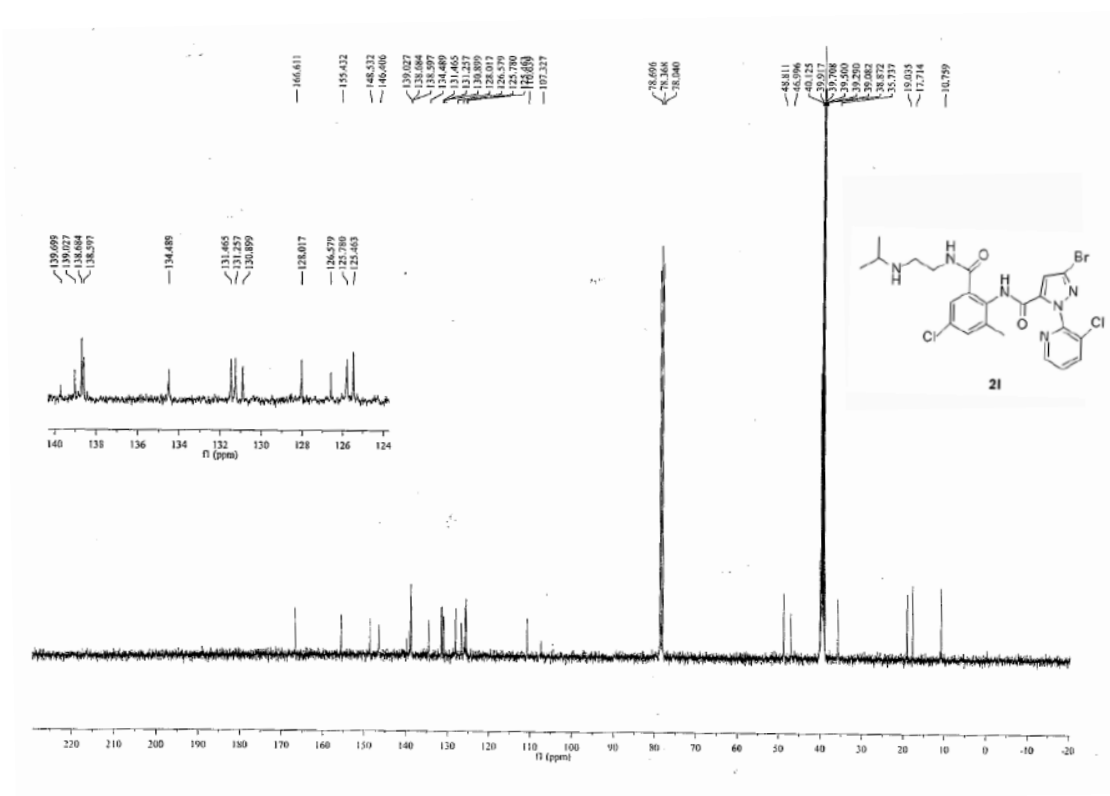


Figure S36. ^{13}C -NMR spectrum of compound 2k.

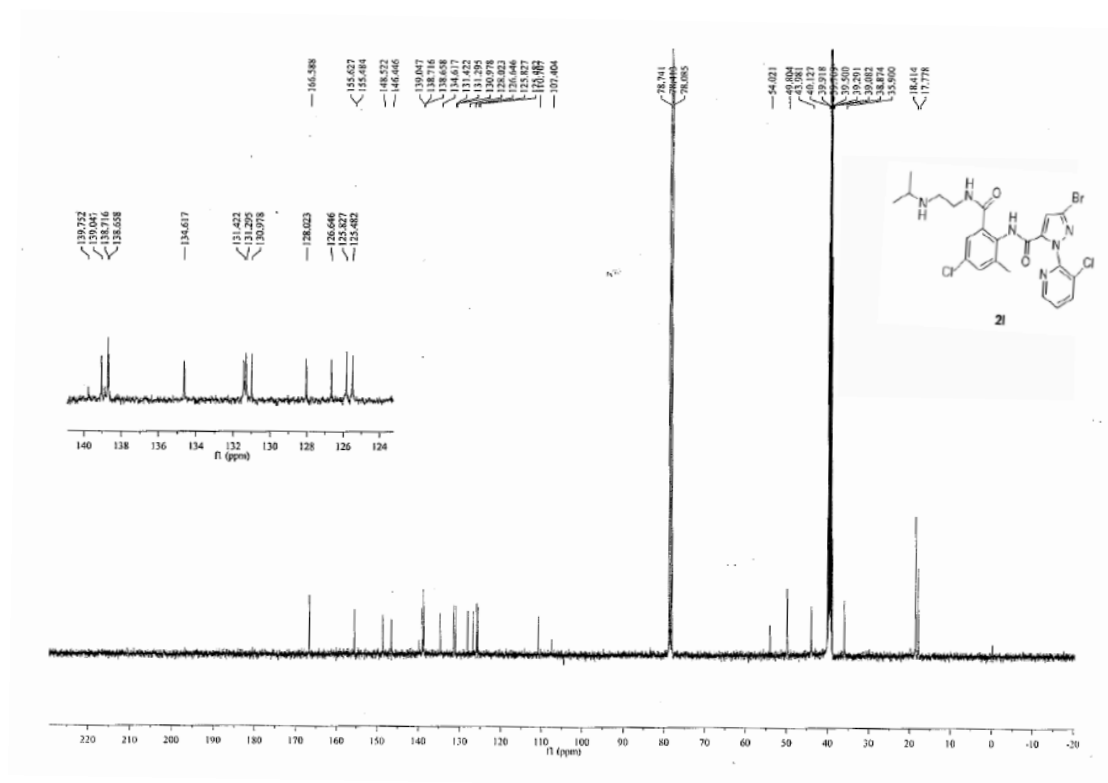


Figure S37. ^{13}C -NMR spectrum of compound **2l**.

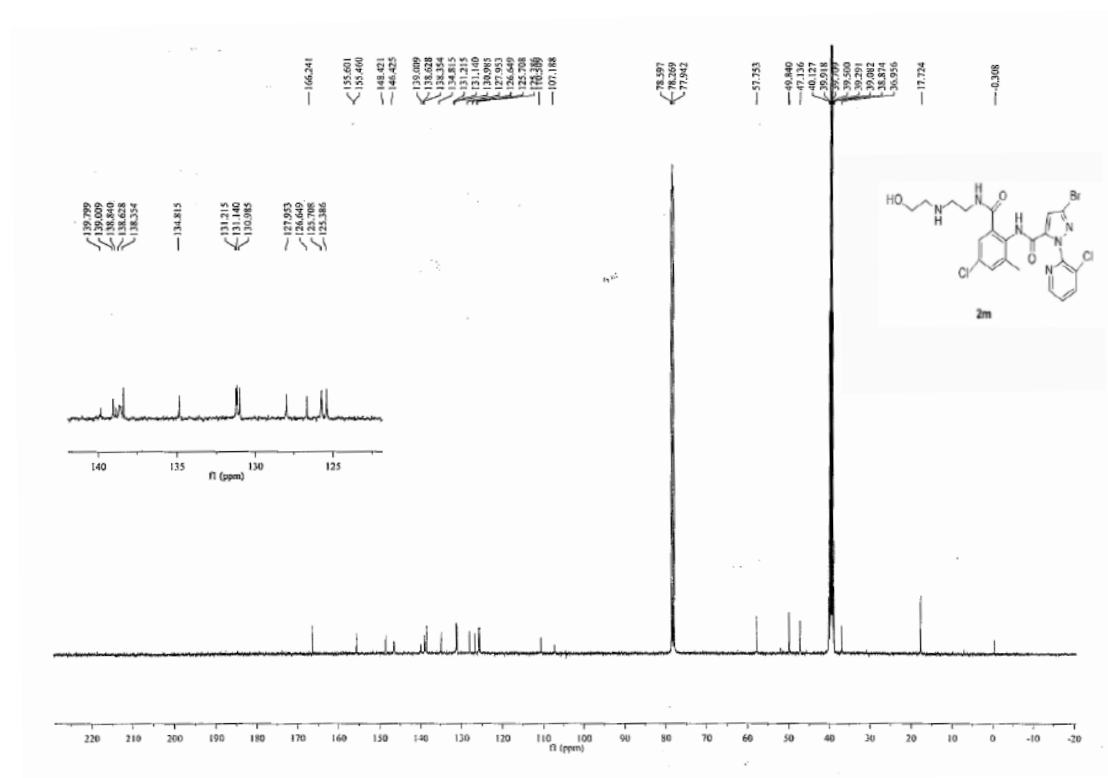


Figure S38. ^{13}C -NMR spectrum of compound **2m**.

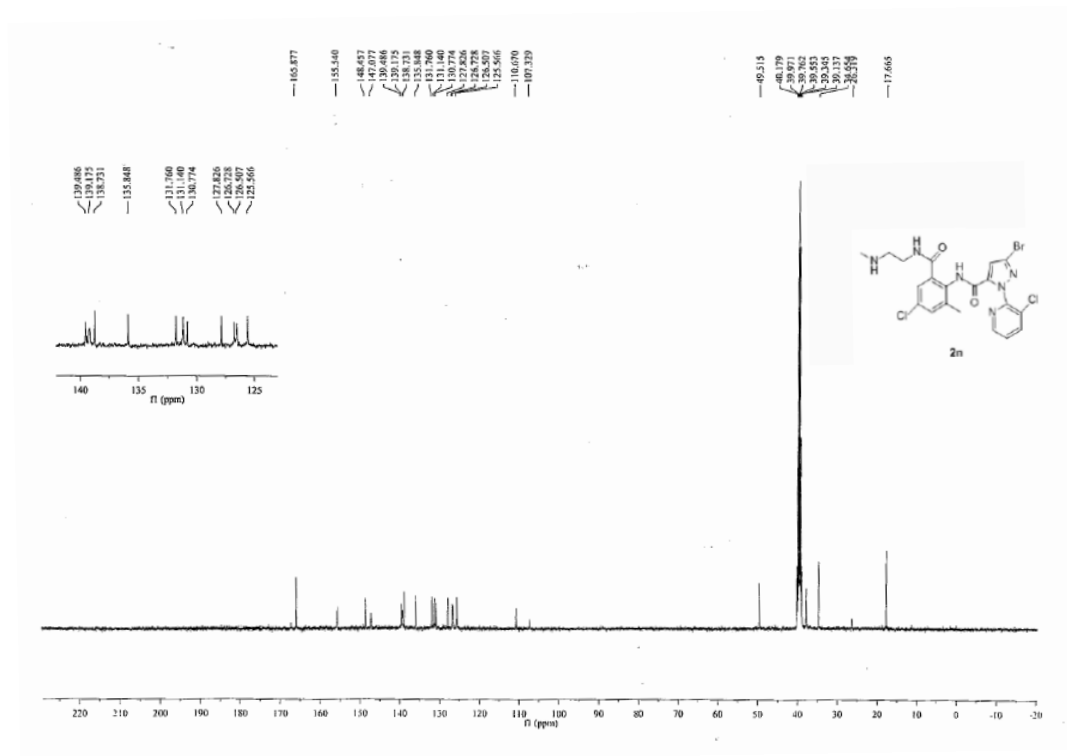


Figure S39. ^{13}C -NMR spectrum of compound **2n**.

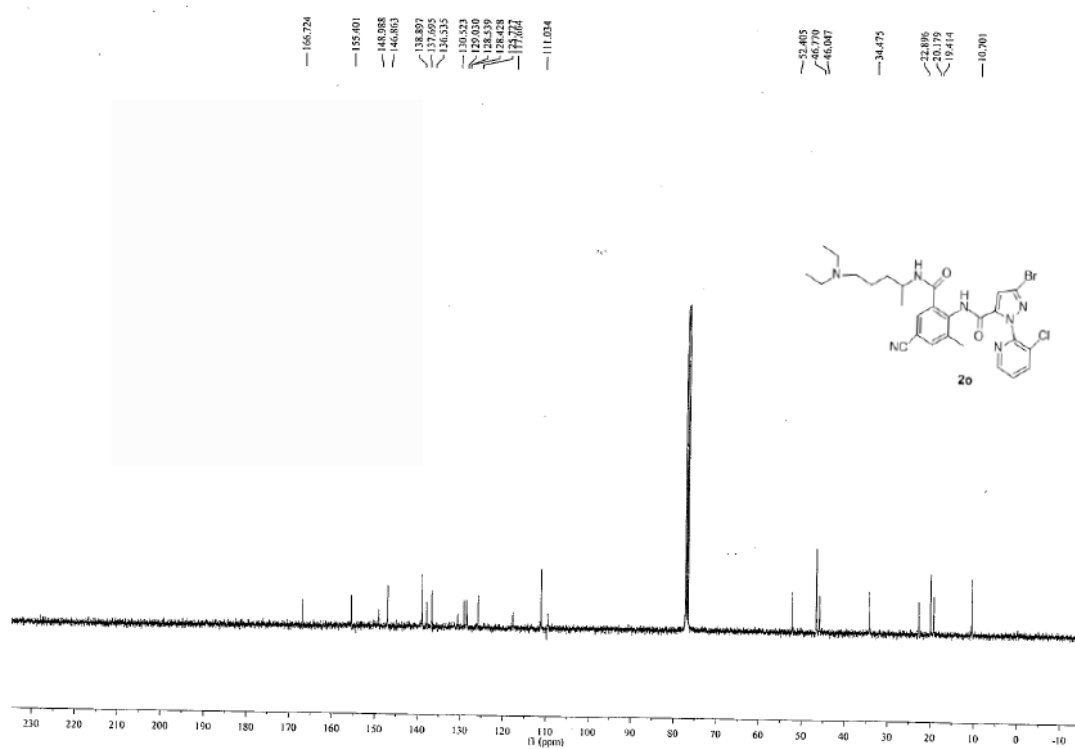


Figure S40. ^{13}C -NMR spectrum of compound **2o**.

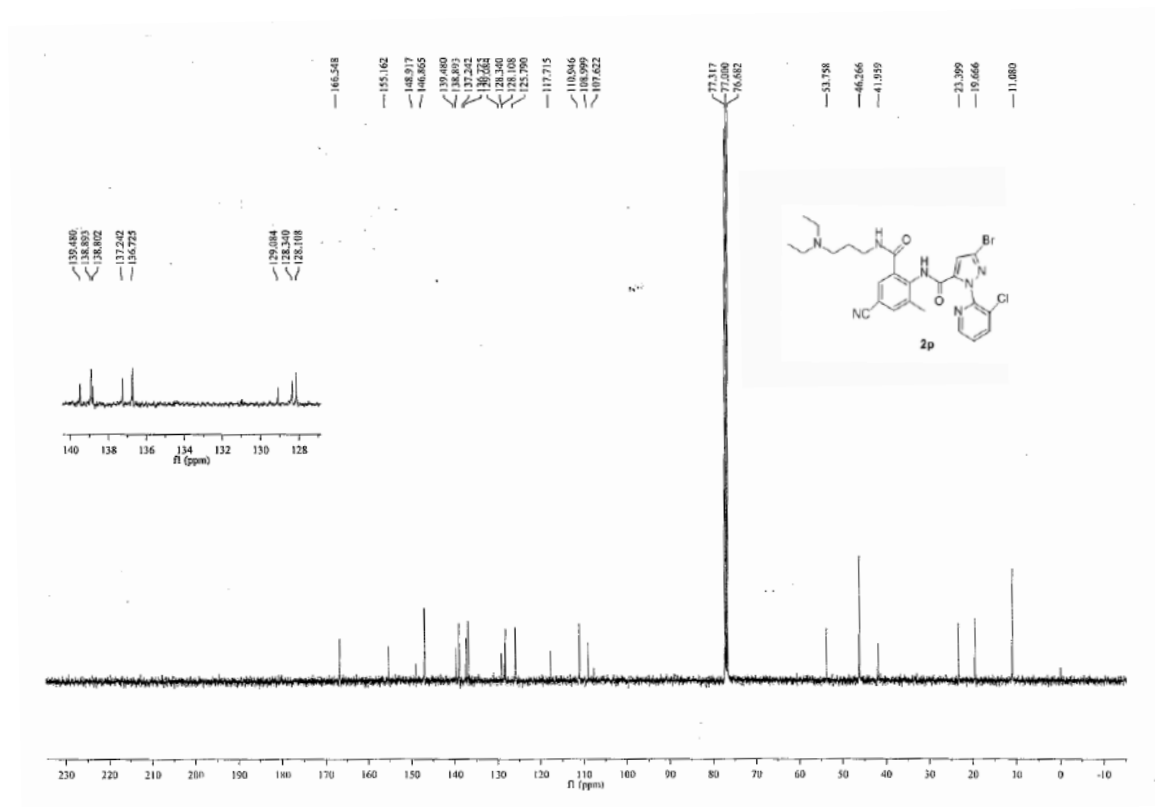


Figure S41. ^{13}C -NMR spectrum of compound **2p**.

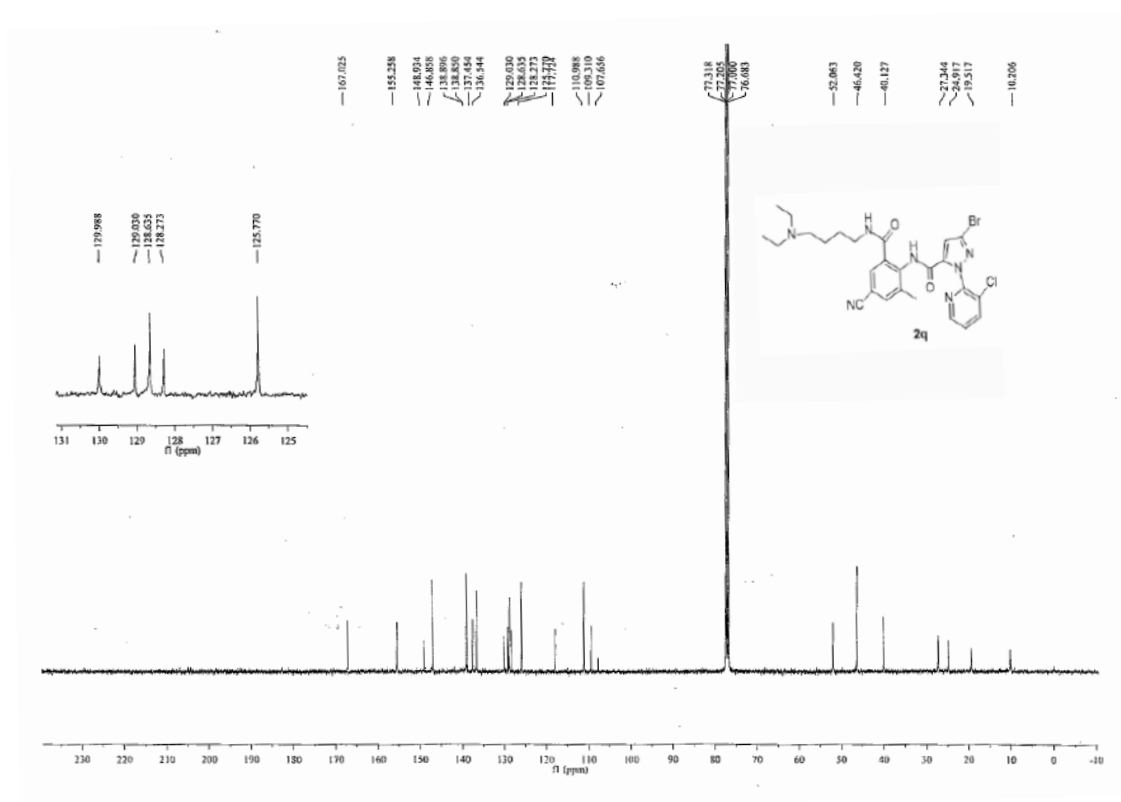


Figure S42. ^{13}C -NMR spectrum of compound **2q**.

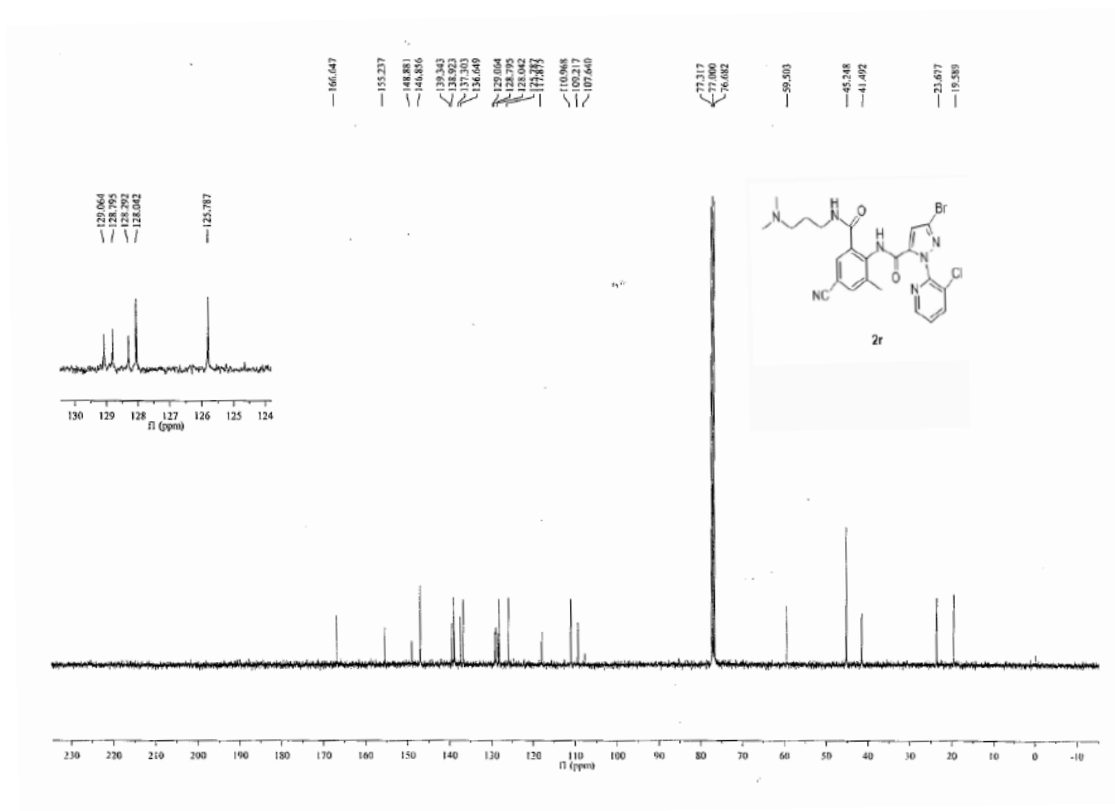


Figure S43. ^{13}C -NMR spectrum of compound 2r.

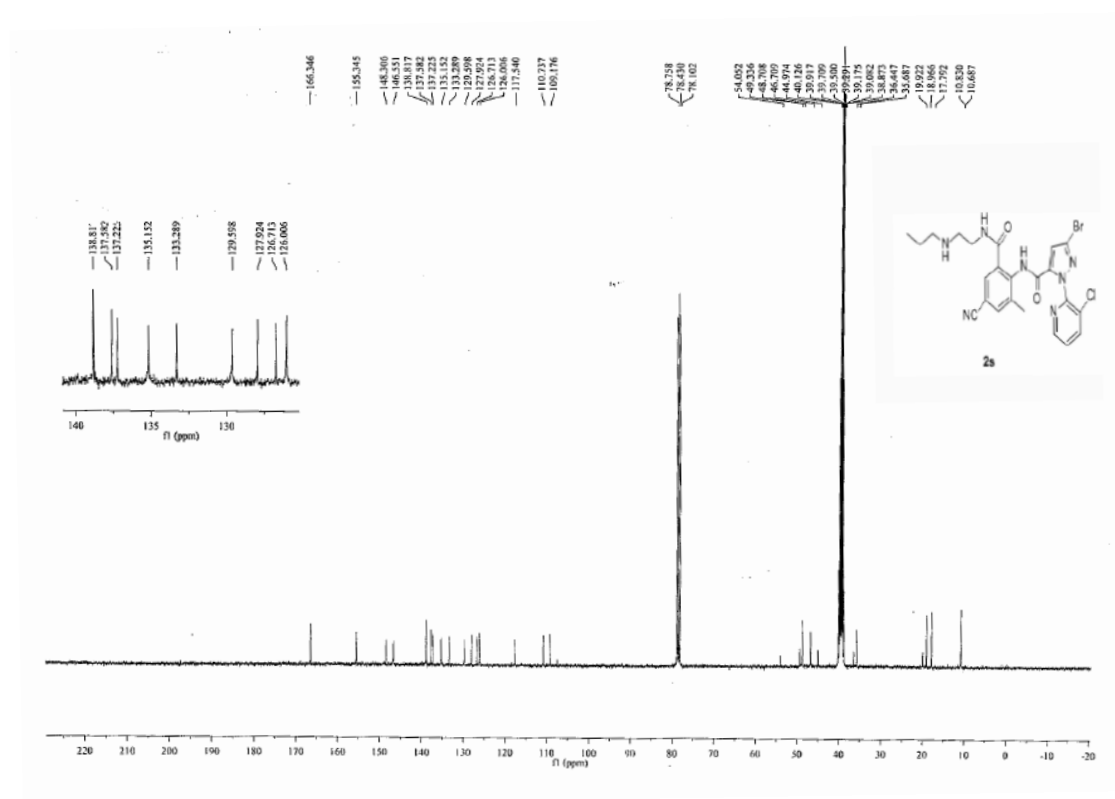


Figure S44. ^{13}C -NMR spectrum of compound 2s.

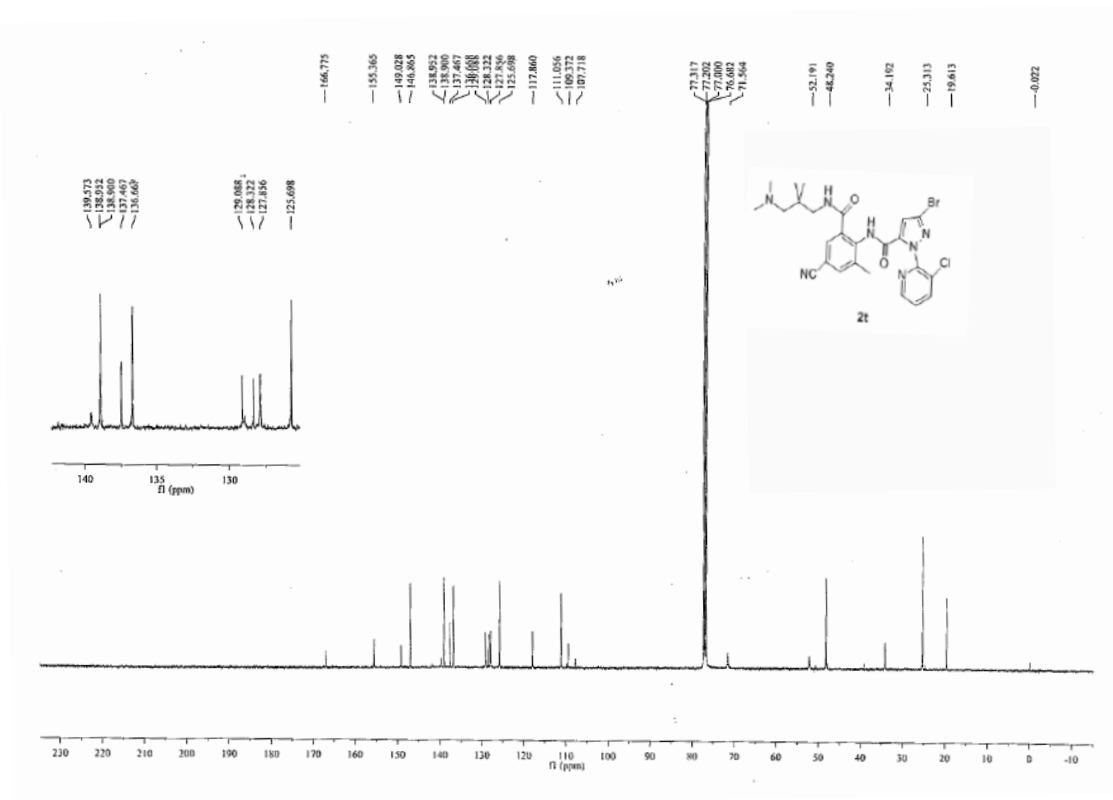


Figure S45. ^{13}C -NMR spectrum of compound **2t**.

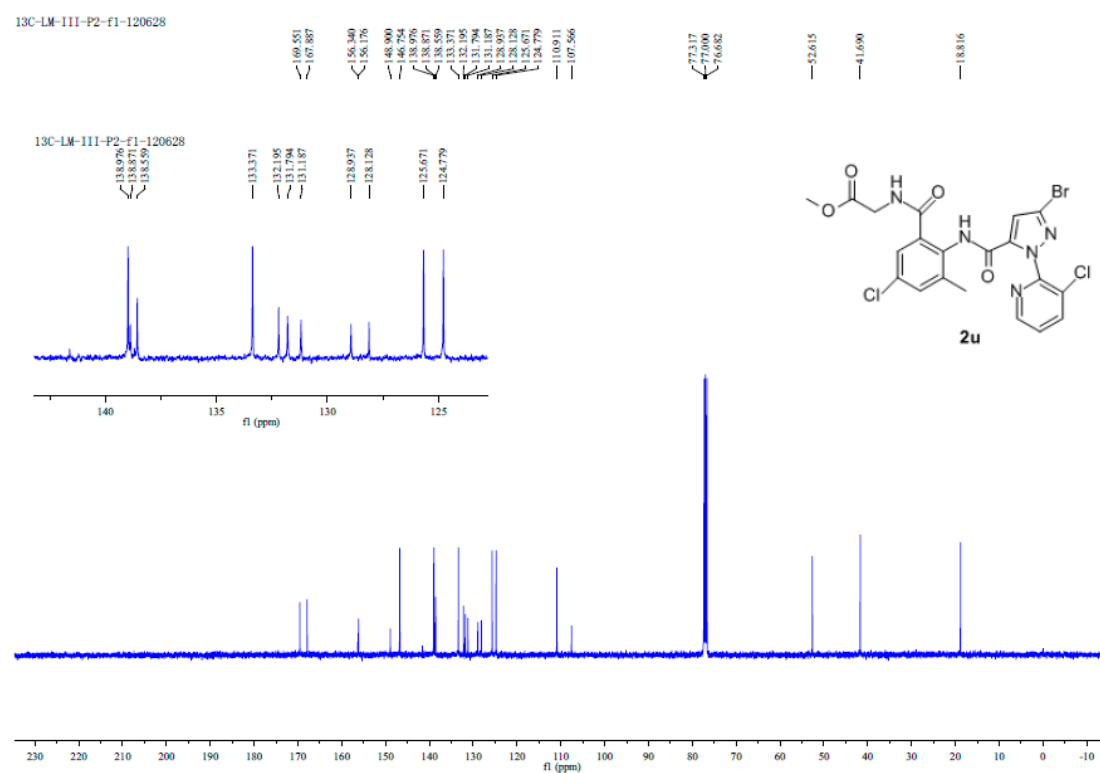


Figure S46. ^{13}C -NMR spectrum of compound **2u**.

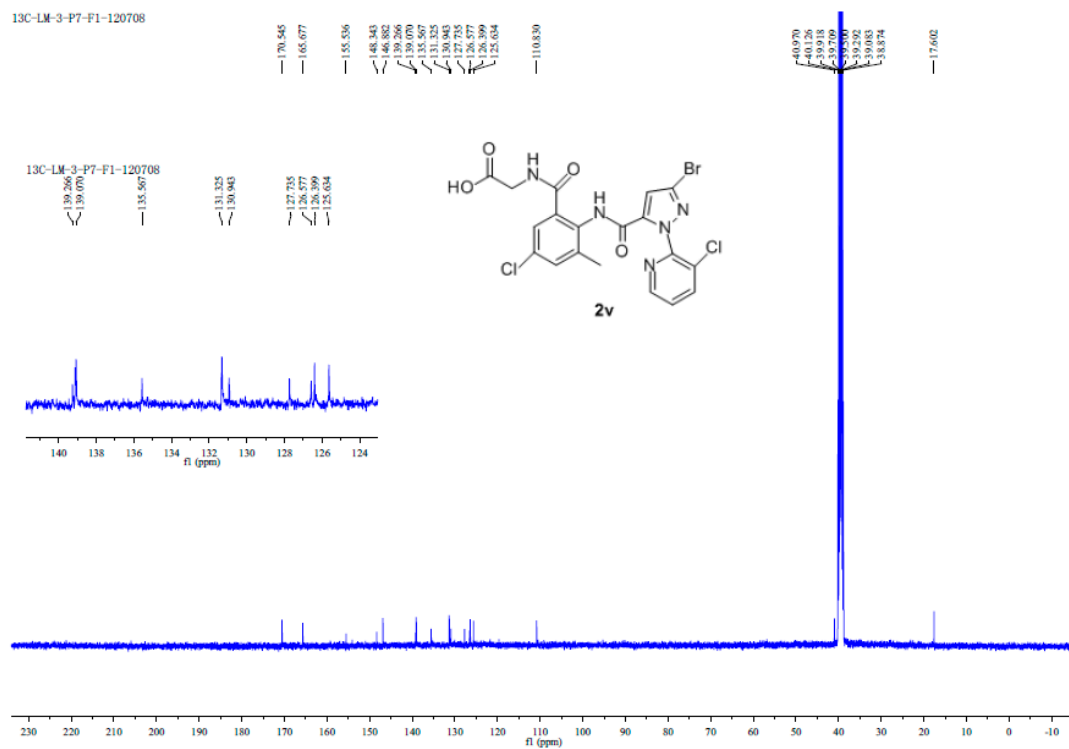


Figure S47. ^{13}C -NMR spectrum of compound **2v**.

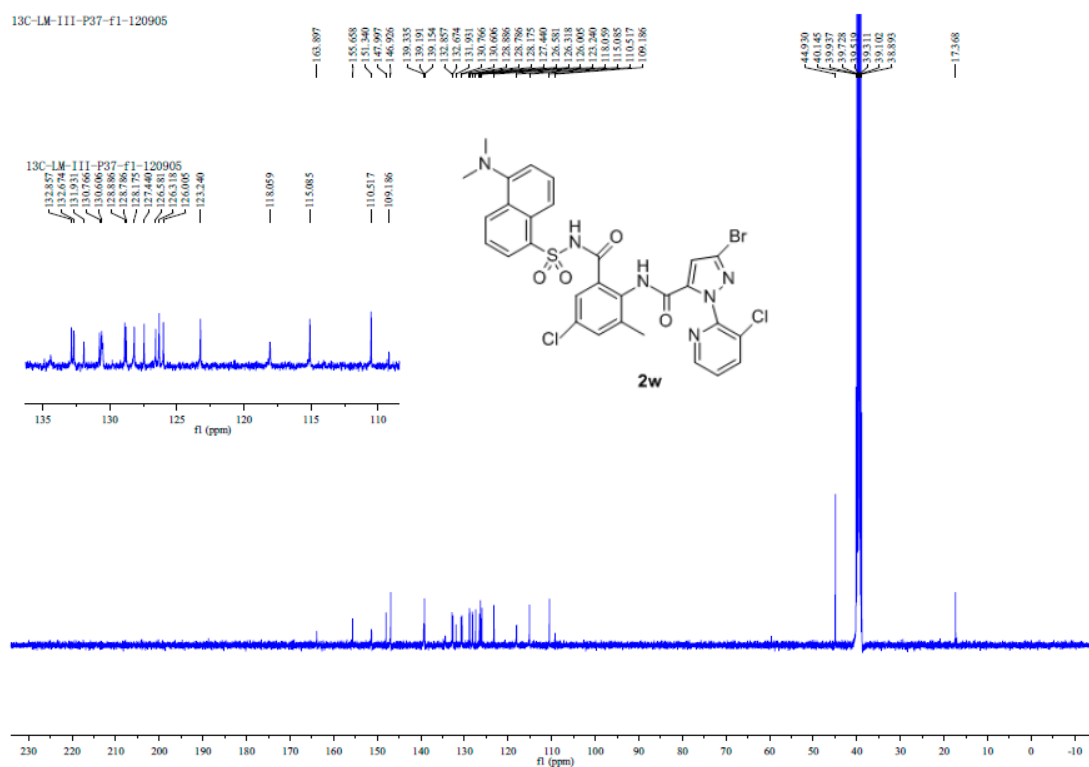


Figure S48. ^{13}C -NMR spectrum of compound **2w**.

¹³C NMR (CDCl₃) of **2y** (120708):

Chemical structure of **2y** is shown above the spectrum.

13C NMR peaks (ppm):

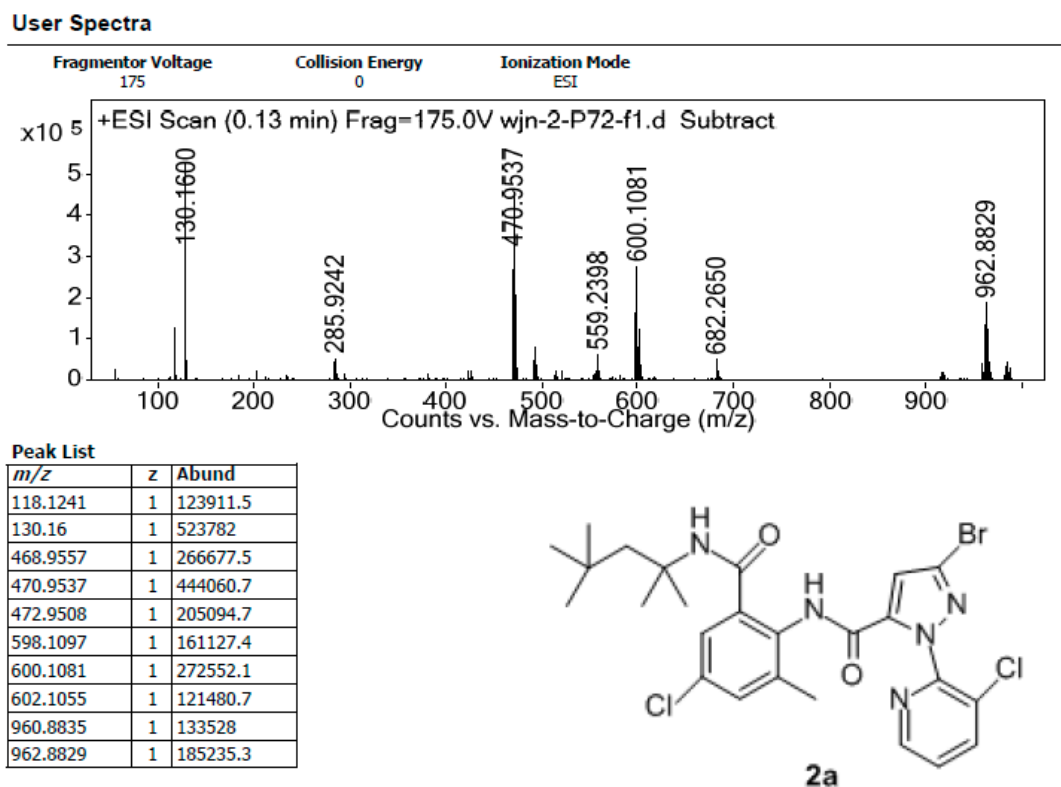
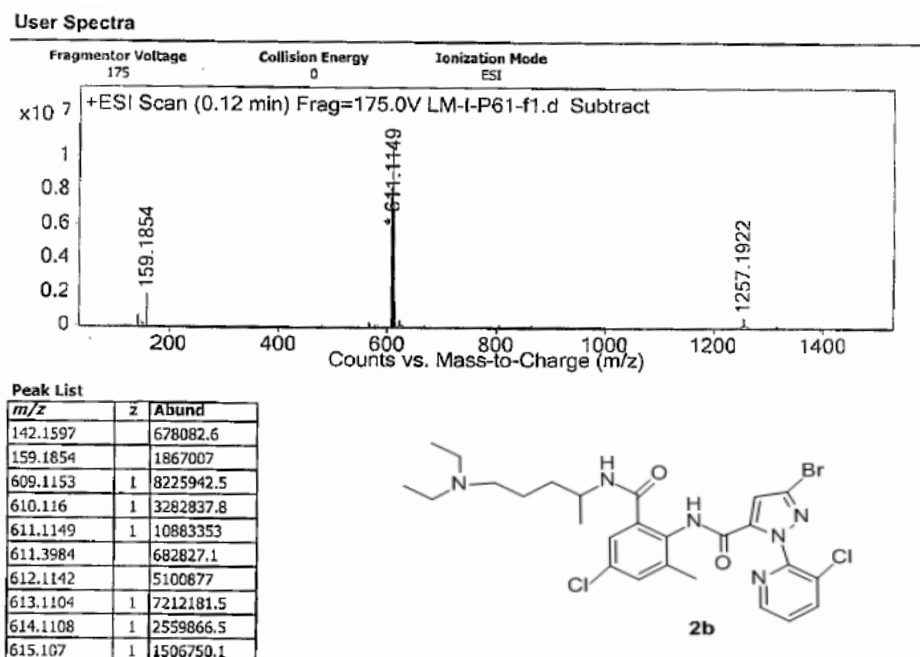
- 167.942
- 156.563
- 146.092
- 146.789
- 138.813
- 138.725
- 133.221
- 133.221
- 132.645
- 132.256
- 131.968
- 129.000
- 128.211
- 128.211
- 125.634
- 124.346
- 111.029
- 77.317
- 77.000
- 76.682
- 40.342
- 31.683
- 29.372
- 28.911
- 28.609
- 22.598
- 18.700
- 14.064
- 0.021

13C NMR spectrum (ppm):

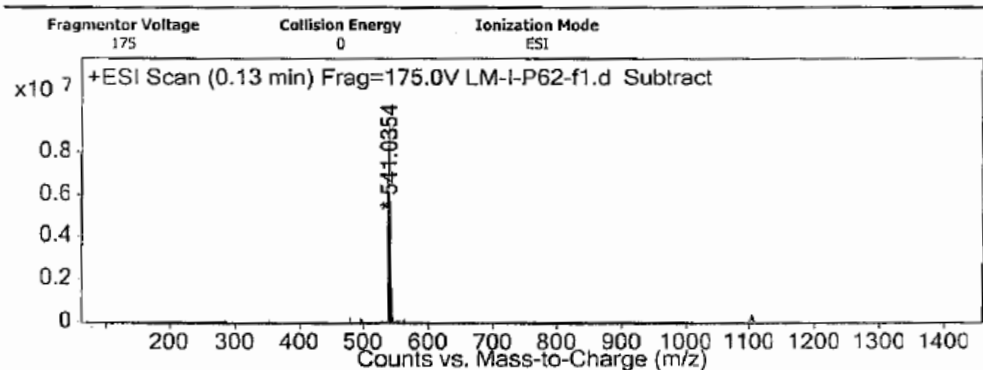
The spectrum shows peaks corresponding to the chemical structure of **2y**. Key peaks are labeled with their chemical shifts in ppm: 138.813, 138.725, 133.221, 132.645, 132.256, 131.968, 129.000, 128.211, 125.634, 124.346, 111.029, 77.317, 77.000, 76.682, 40.342, 31.683, 29.372, 28.911, 28.609, 22.598, 18.700, 14.064, and -0.021.

Figure S50. ^{13}C -NMR spectrum of compound **2y**.

3. HR-MS

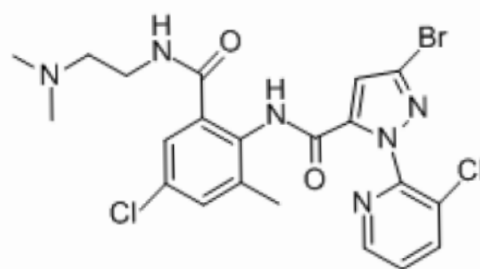
Figure S51. HR-MS spectrum of compound **2a**.Figure S52. HR-MS spectrum of compound **2b**.

User Spectra

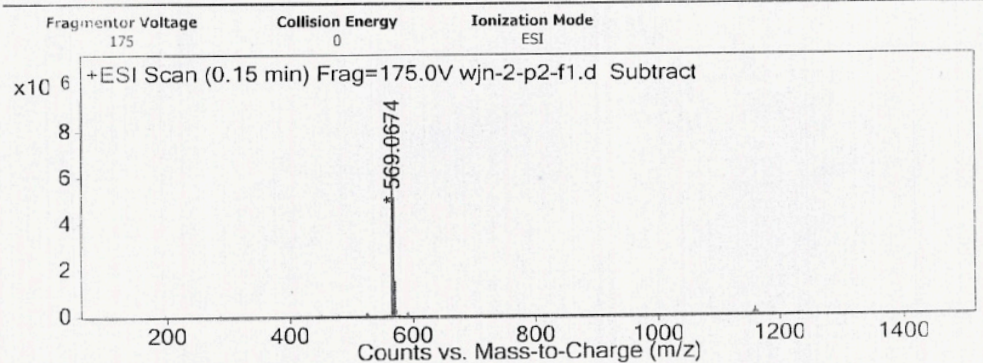


Peak List

m/z	z	Abund
539.0364	1	6839567.5
540.0376	1	2056720.6
541.0354	1	9539774
541.2309		842799.8
541.318		510480.3
542.0355	1	3298000
543.0314	1	5662681
543.2331		491559.4
544.0327	1	1541619
545.0291	1	1010198.8

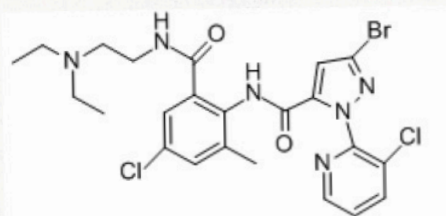
**2c****Figure S53.** HR-MS spectrum of compound **2c**.

User Spectra

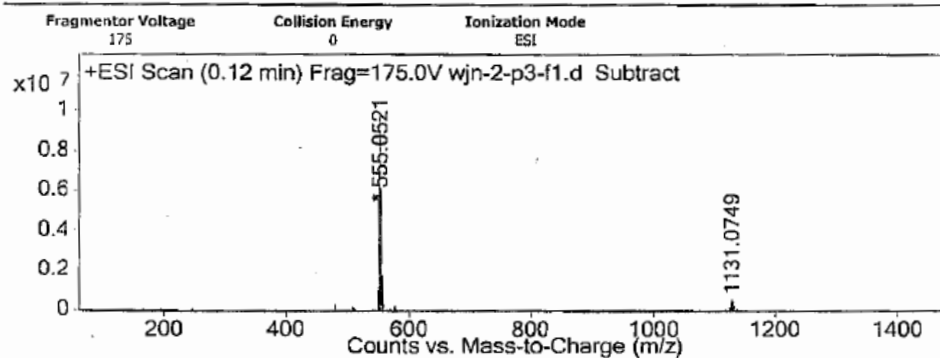


Peak List

m/z	z	Abund
567.0684	1	6086118
567.2721		485601.6
568.0699	1	1932571.3
569.0674	1	8710474
569.2649		751107.5
570.0678	1	3081166
571.0637	1	5068411
571.2718		450103.3
572.0649	1	1456247.1
573.0618	1	887745.3

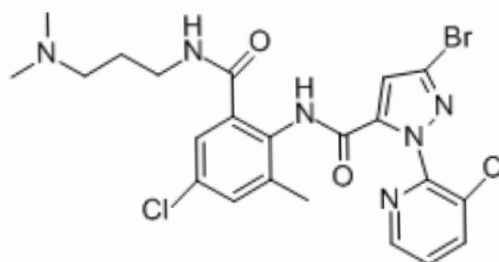
**2d****Figure S54.** HR-MS spectrum of compound **2d**.

User Spectra



Peak List

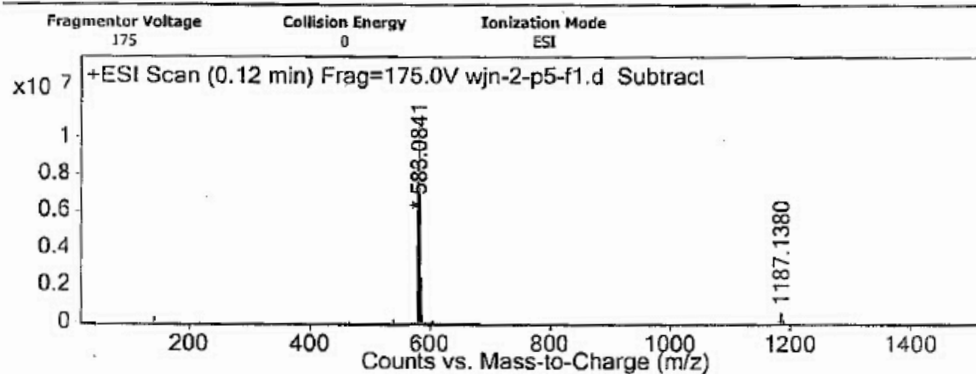
m/z	z	Abund
553.053	1	7179975.5
553.2544		508242.2
554.0542	1	2293498
555.0521	1	9874690
555.2473		907458.8
556.0521	1	3656231.8
557.048	1	6022600.5
558.0491	1	1734178
559.0455	1	1089732.3
1131.0749		530363.4



2e

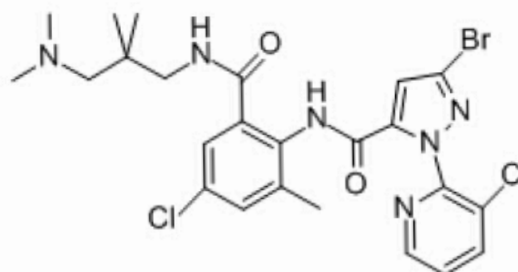
Figure S55. HR-MS spectrum of compound 2e.

User Spectra



Peak List

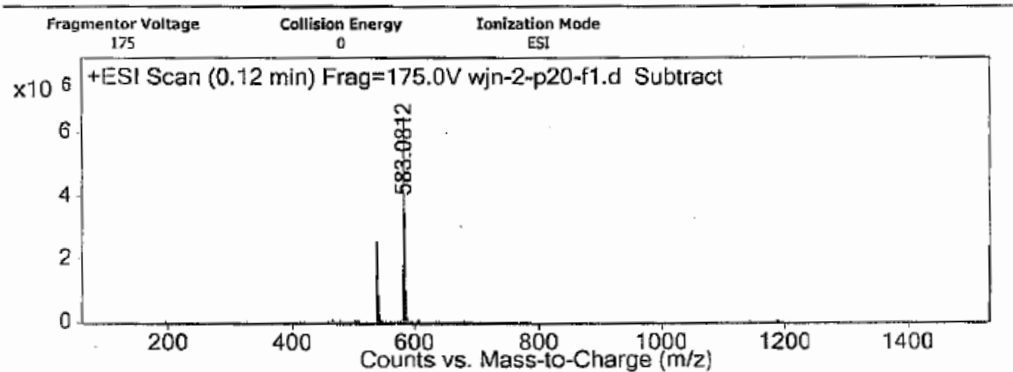
m/z	z	Abund
581.0845	1	8488467
581.2841		680058.8
582.0851	1	3105136.8
583.0841	1	11037943
583.362		676582.5
584.0834	1	4881015
585.0796	1	7297667.5
586.08	1	2419787.5
587.0761	1	1465293
1187.138		654161.3



2f

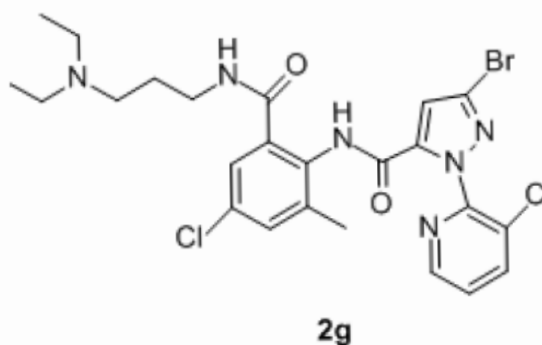
Figure S56. HR-MS spectrum of compound 2f.

User Spectra

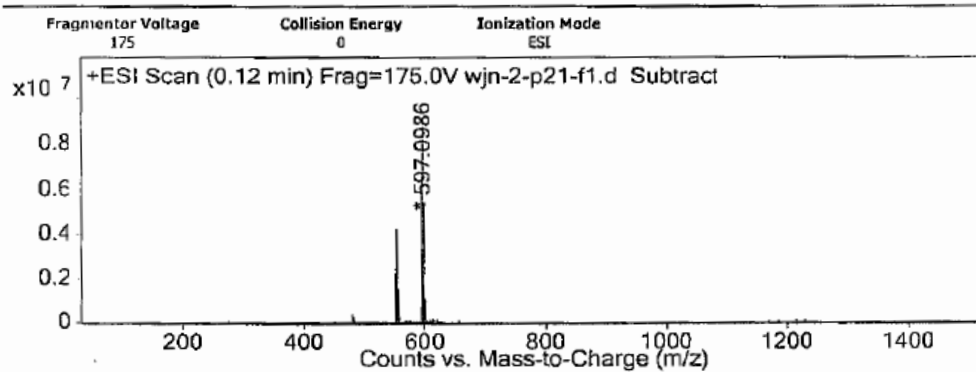


Peak List

m/z	z	Abund
537.1326	1	2552710.5
538.1362	1	720627.1
539.1301	1	2541021.5
541.1289	1	862659.5
581.0826	1	4242290.5
582.0848	1	1267022
583.0812	1	6434385
584.0824	1	2121076.8
585.078	1	3442944.8
586.0807	1	962253.3

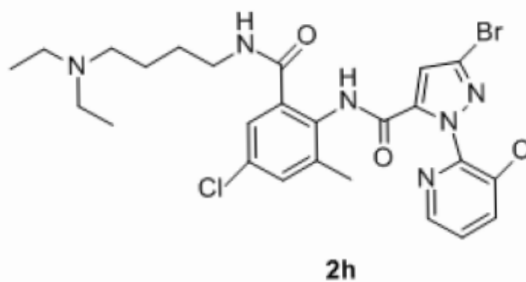
Figure S57. HR-MS spectrum of compound **2g**.

User Spectra

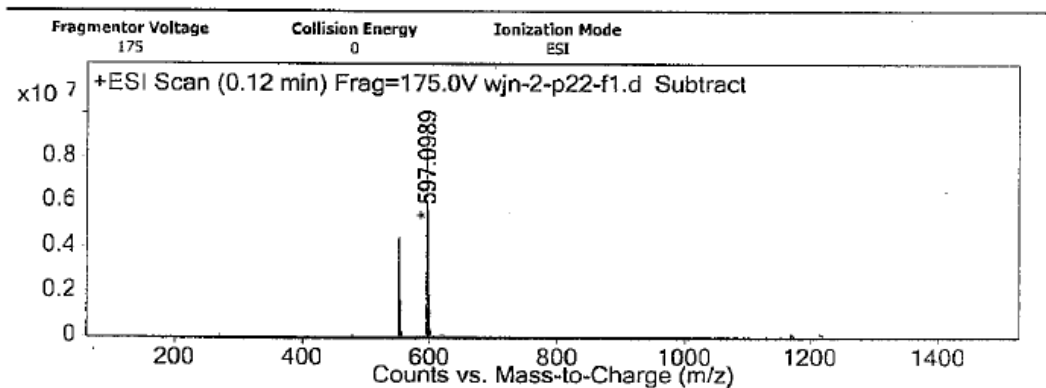


Peak List

m/z	z	Abund
551.1492	1	4181802.8
552.1514	1	1304508.4
553.1466	1	4186059.5
555.1439	1	1518909
595.0996	1	6517437
596.101	1	2253578.3
597.0986	1	9178428
598.0989	1	3565117.5
599.0949	1	5430470.5
600.0959	1	1722469.9

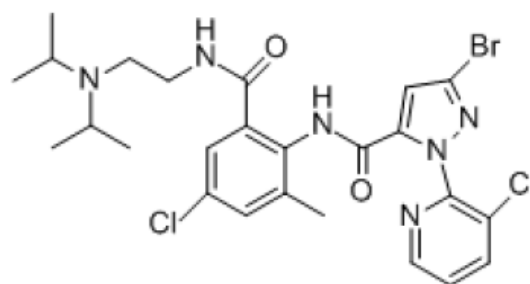
Figure S58. HR-MS spectrum of compound **2h**.

User Spectra



Peak List

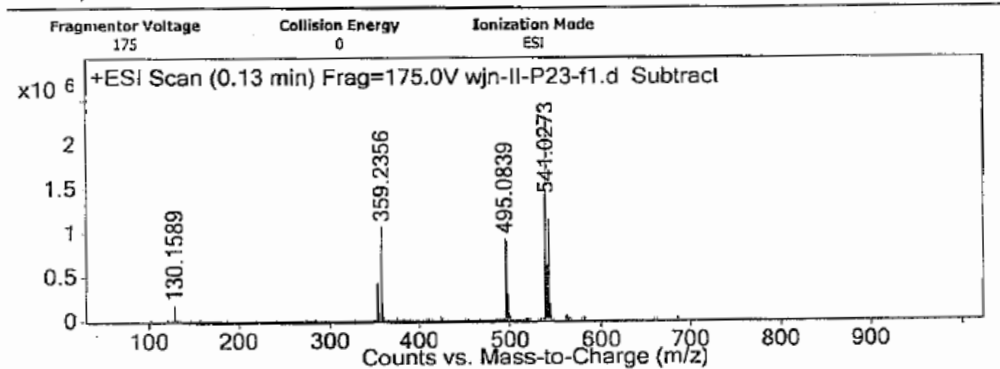
m/z	z	Abund
551.1496	1	4350049
552.1518	1	1389648.5
553.147	1	4416446
555.144	1	1634510.1
595.0999	1	6730949.5
596.1012	1	2348590.8
597.0989	1	9423324
598.0991	1	3727104.8
599.0951	1	5624904
600.0963	1	1790023.4



2i

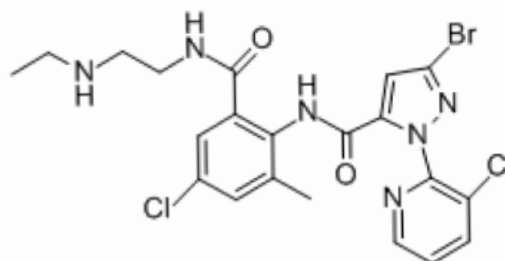
Figure S59. HR-MS spectrum of compound 2i.

User Spectra



Peak List

m/z	z	Abund
354.2851	1	411753.6
359.2356	1	1065501.4
495.0839	1	923978.9
497.0793	1	890554.1
499.0815	1	294453.5
539.0295	1	1436330.8
540.0394	1	369547
541.0273	1	2306543
542.0368	1	628012.1
543.0255	1	1138796.8



2j

Figure S60. HR-MS spectrum of compound 2j.

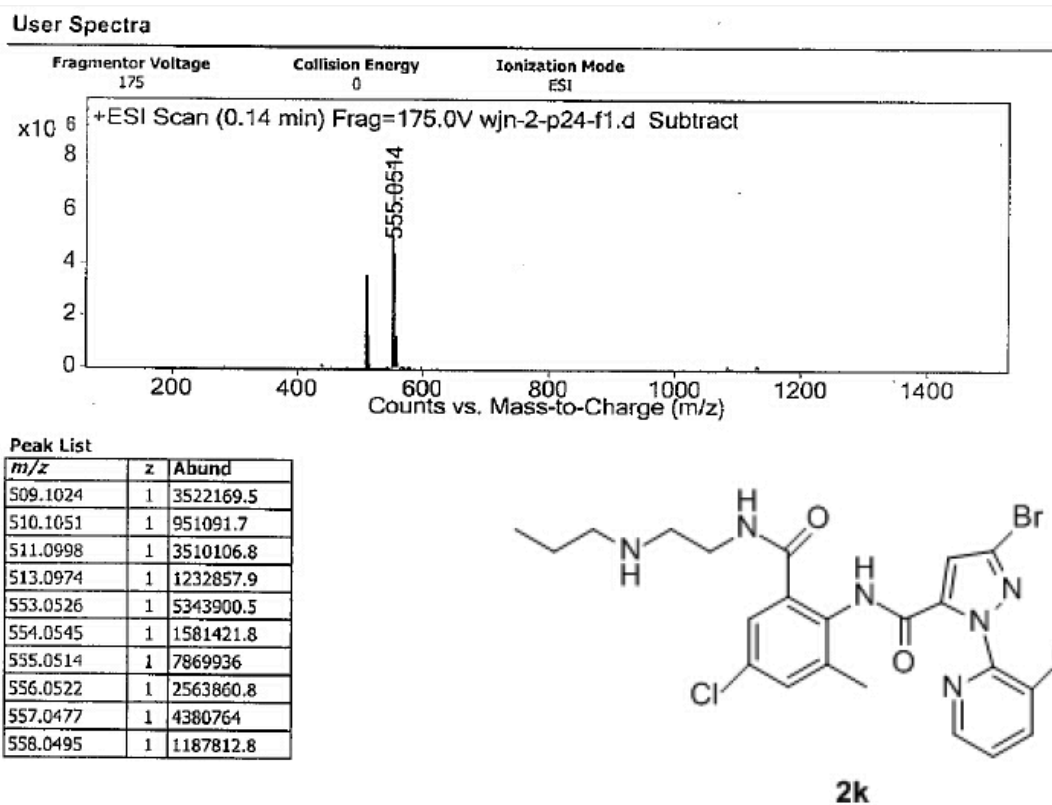


Figure S61. HR-MS spectrum of compound 2k.

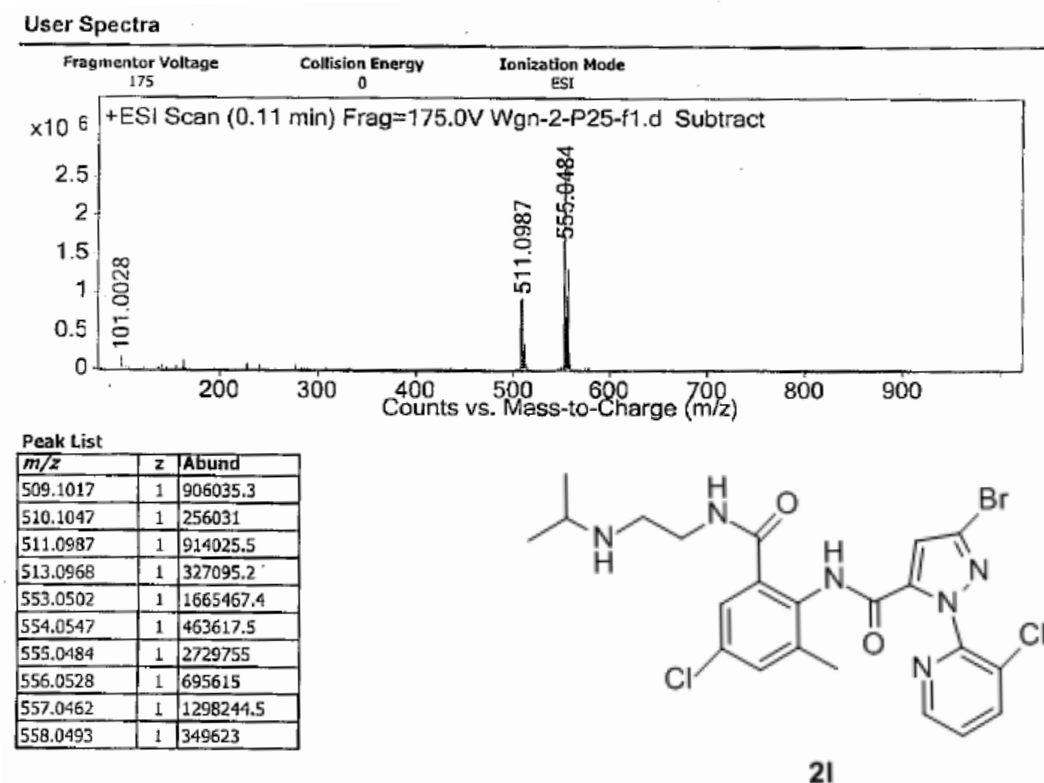
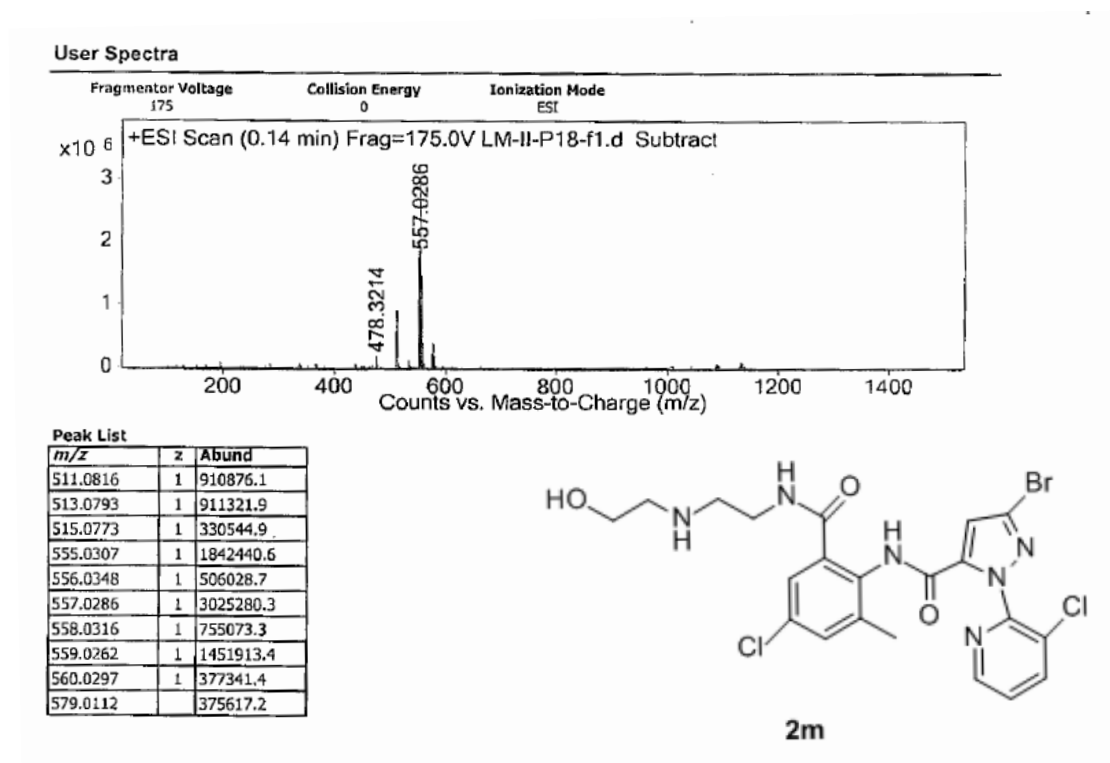
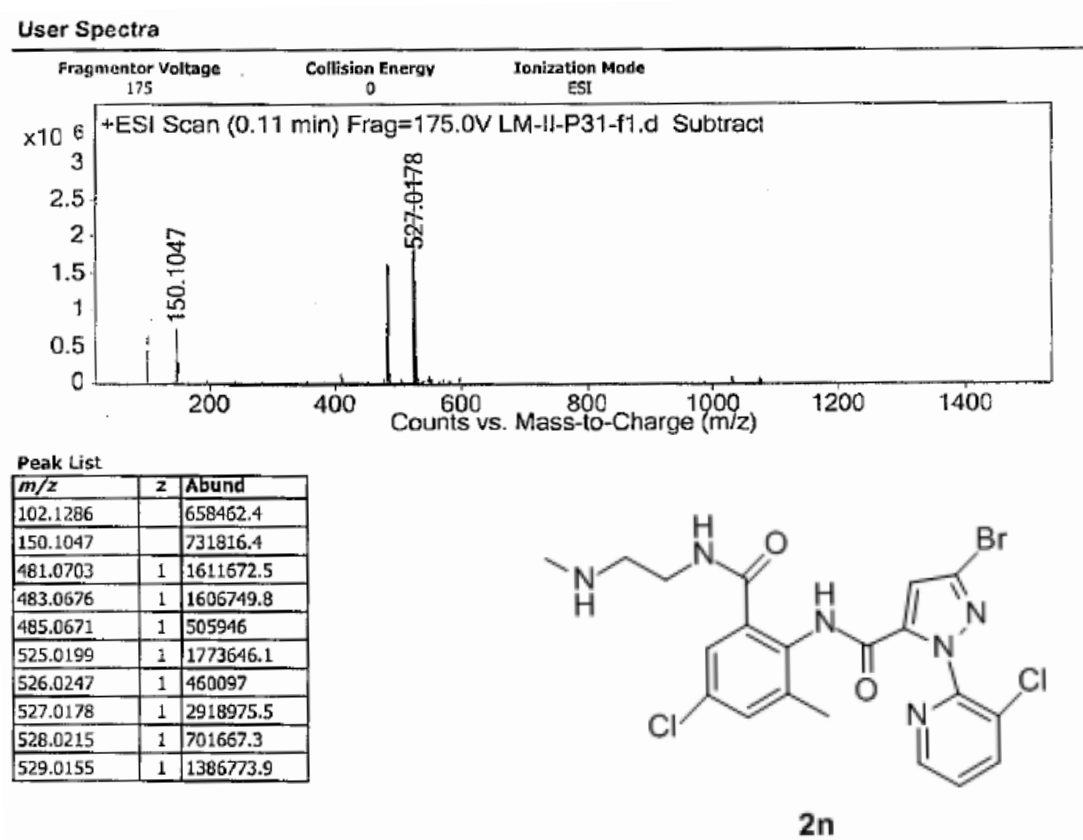
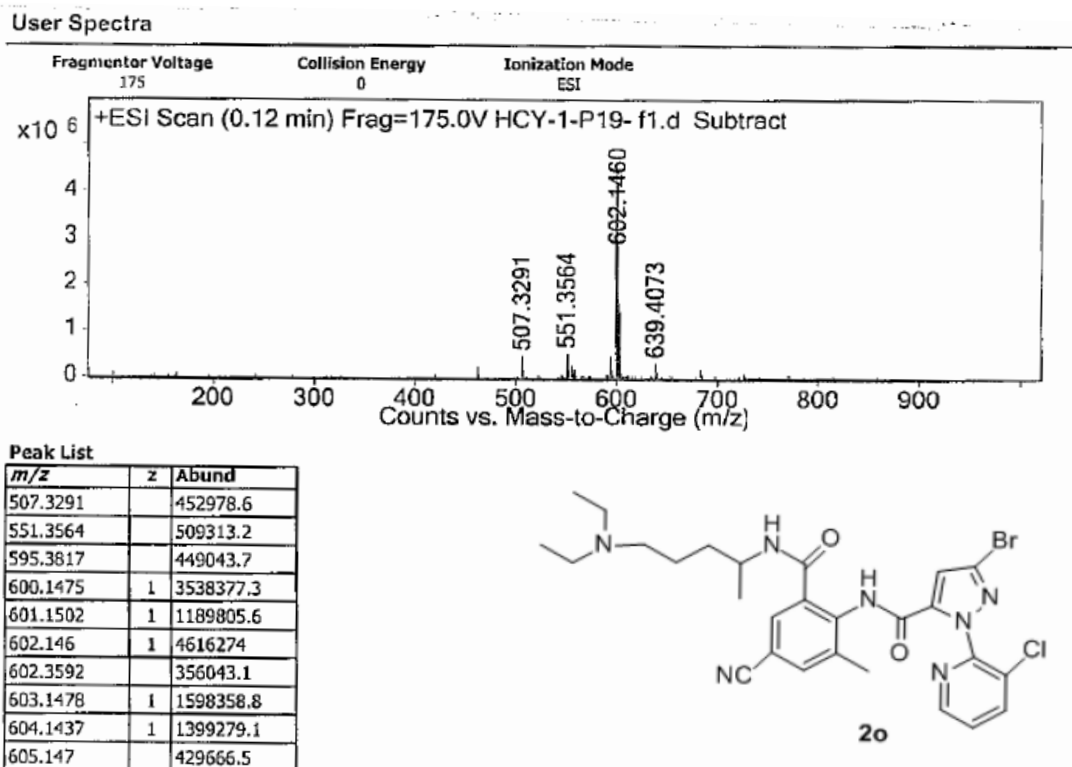
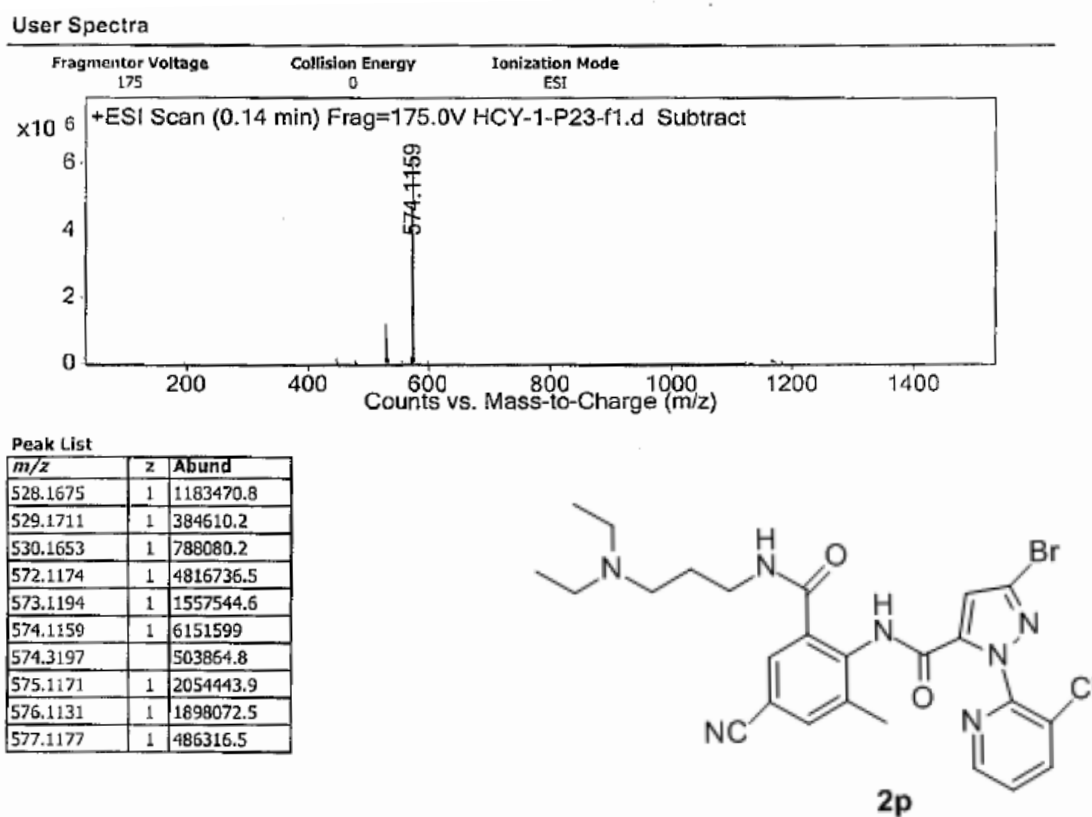
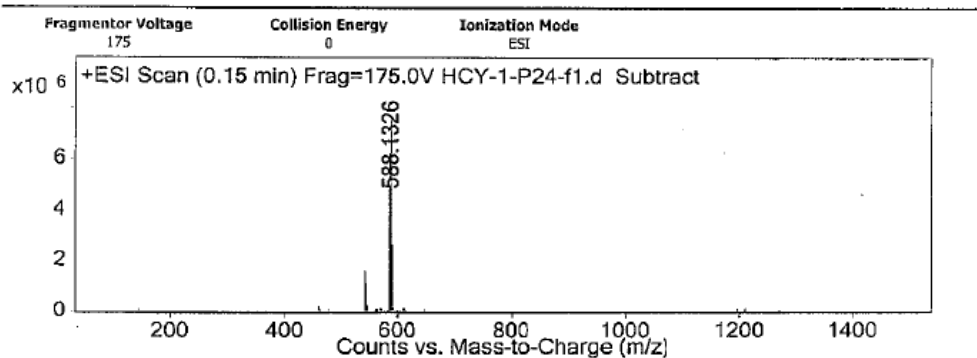


Figure S62. HR-MS spectrum of compound 2l.

Figure S63. HR-MS spectrum of compound **2m**.Figure S64. HR-MS spectrum of compound **2n**.

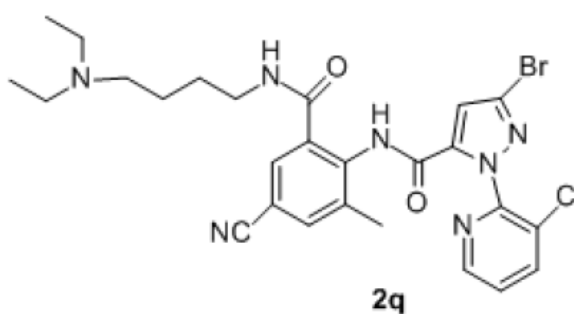
Figure S65. HR-MS spectrum of compound **2o**.Figure S66. HR-MS spectrum of compound **2p**.

User Spectra

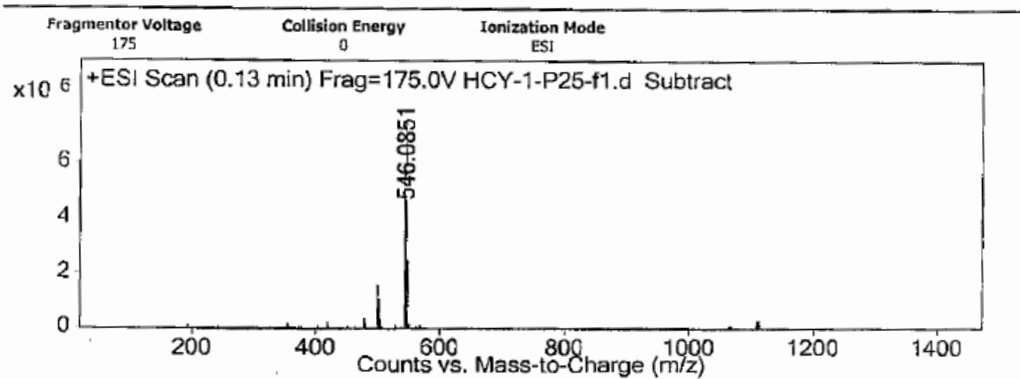


Peak List

m/z	z	Abund
542.183	1	1592069.8
543.188	1	493103.1
544.181	1	1082175.3
586.1339	1	6209576.5
587.1354	1	2182361.3
588.1326	1	7716560.5
588.3347		616641.9
589.1333	1	2874137
590.1291	1	2619945
591.1317	1	734669.8

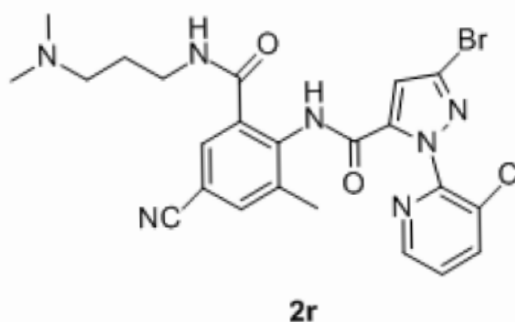
Figure S67. HR-MS spectrum of compound **2q**.

User Spectra



Peak List

m/z	z	Abund
500.1358	1	1529888.5
501.1398	1	457509.8
502.1341	1	1050037.1
544.0866	1	6038569
545.088	1	1890519.5
546.0851	1	7505626.5
546.2849		561615.4
547.086	1	2484396.8
548.0817	1	2462508
549.0856	1	611834.1

Figure S68. HR-MS spectrum of compound **2r**.

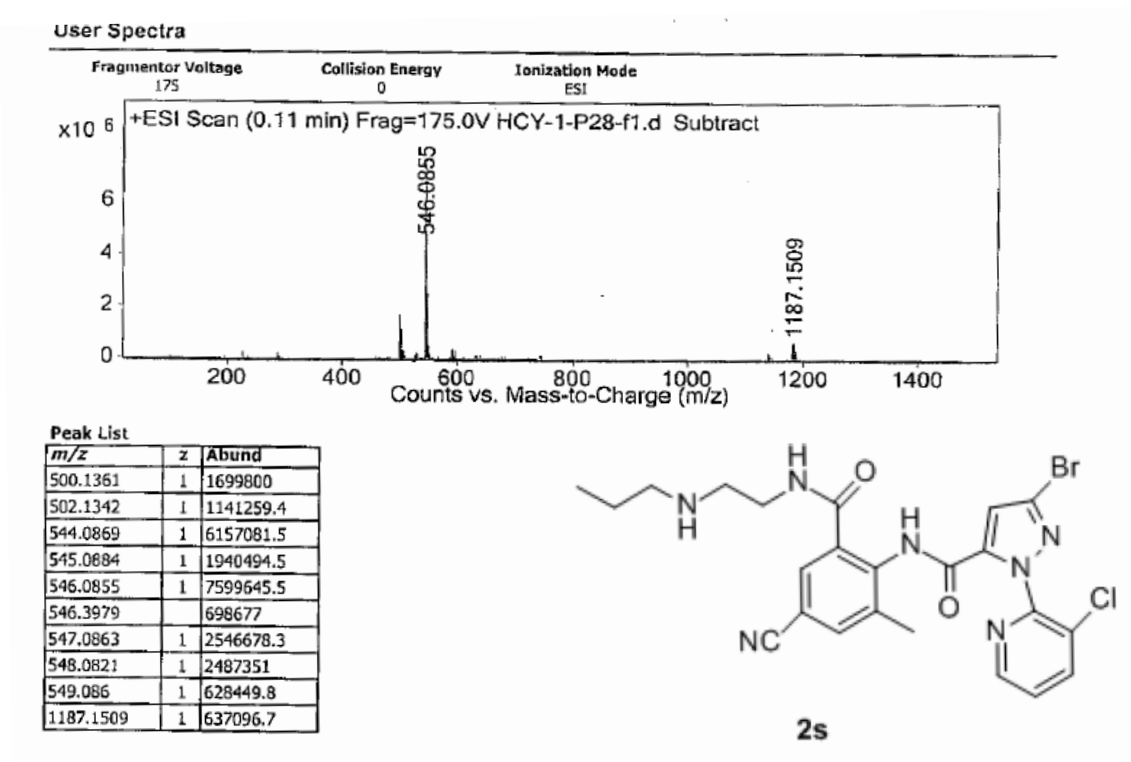


Figure S69. HR-MS spectrum of compound 2s.

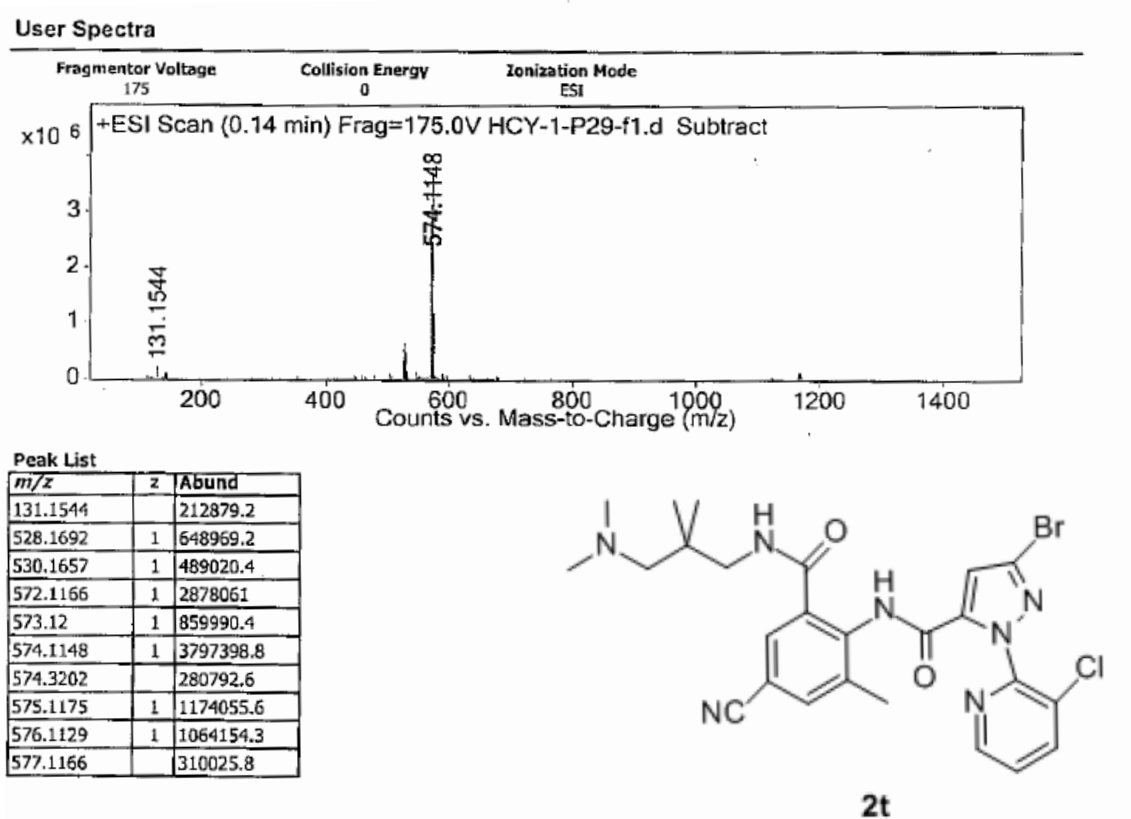
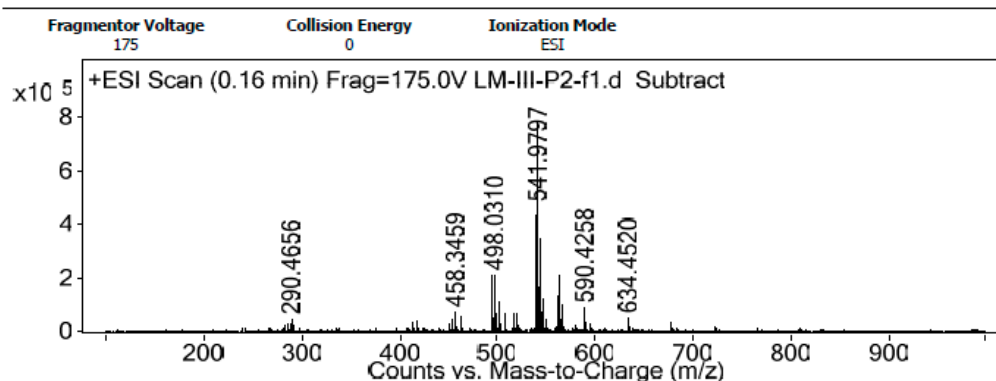


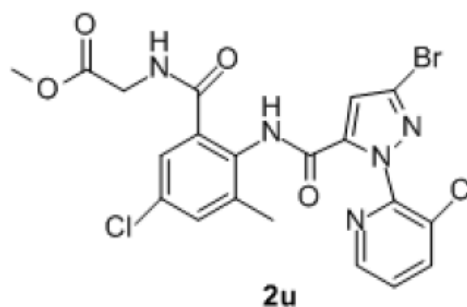
Figure S70. HR-MS spectrum of compound 2t.

User Spectra

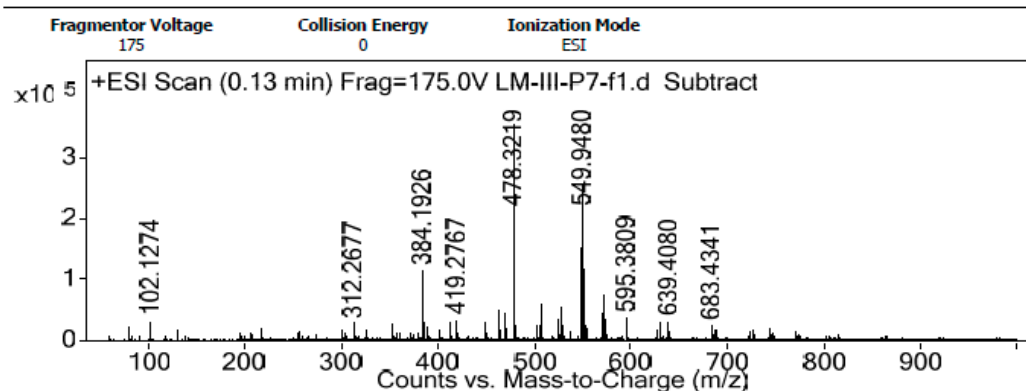


Peak List

m/z	z	Abund
496.0333	1	207511.7
498.031	1	208656.1
502.3725	1	109257.6
539.9837	1	433868.7
541.9797	1	782432.2
542.9837	1	165118.3
543.9792	1	342599.4
546.3989	1	121343.5
561.9643	1	132692.8
563.9633	1	211319.5

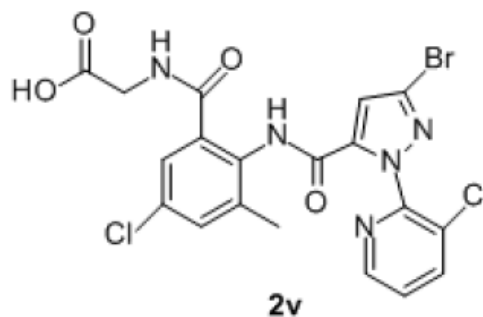
Figure S71. HR-MS spectrum of compound **2u**.

User Spectra

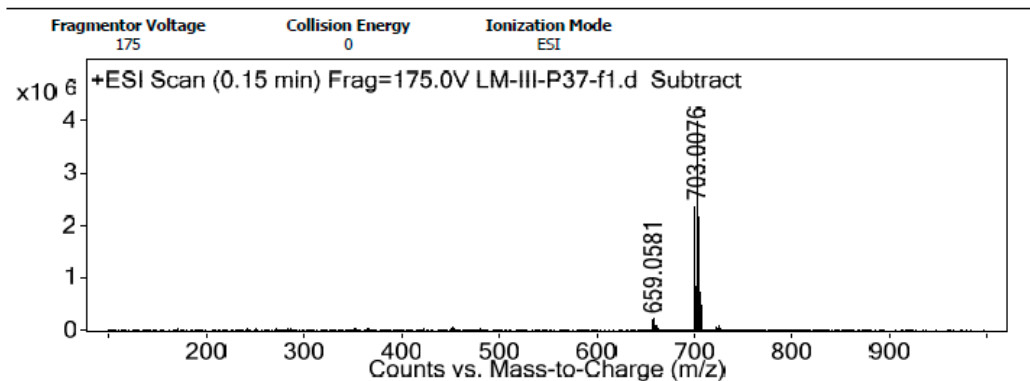


Peak List

m/z	z	Abund
384.1926	1	113644.4
478.3219	1	353356.2
479.3249	1	124734.4
507.3297		57486.6
527.9668		52194.4
547.9505	1	150210.7
549.948	1	256024.5
550.9512	1	54022.7
551.9459	1	117012
571.9301	1	75525.9

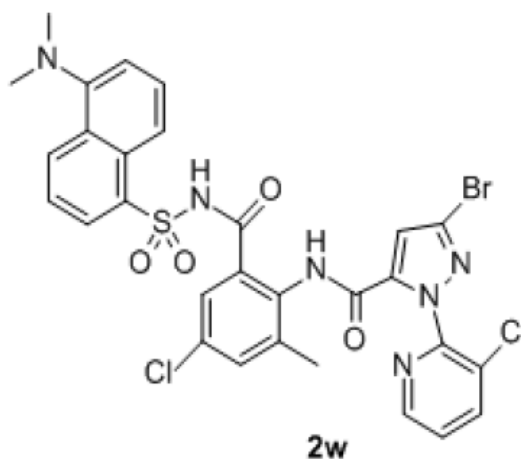
Figure S72. HR-MS spectrum of compound **2v**.

User Spectra

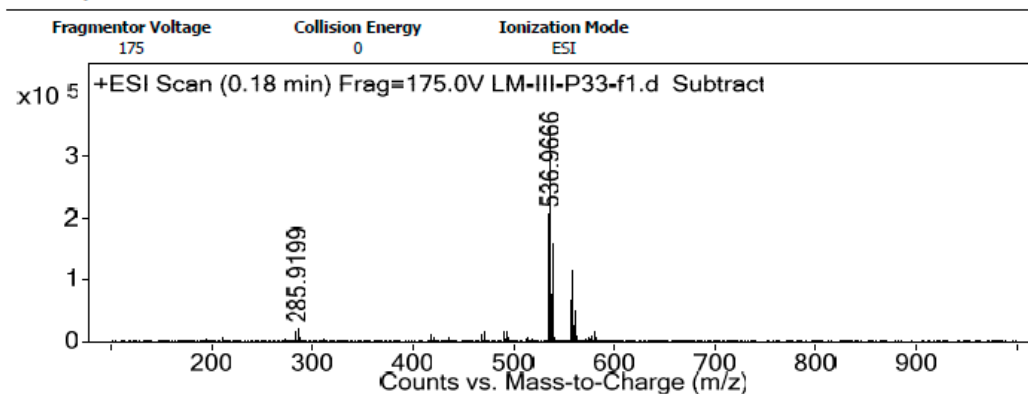


Peak List

m/z	z	Abund
659.0581		211451.5
701.0092	1	2351131.5
702.0128	1	838430.5
703.0076	1	3974236
703.2376		305006.4
704.0095	1	1447541.1
705.0049	1	2159214.5
706.0087	1	707274.3
707.005	1	472477.3

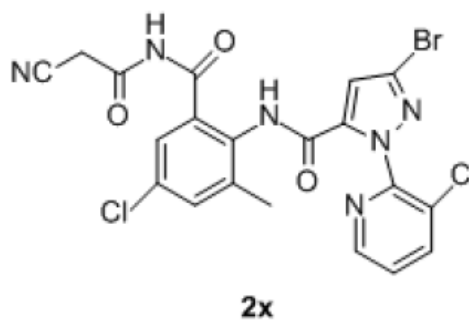
Figure S73. HR-MS spectrum of compound **2w**.

User Spectra

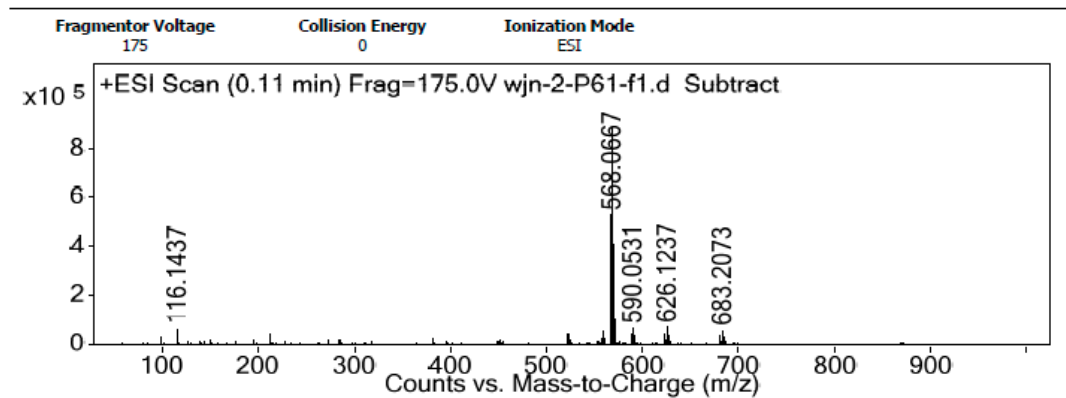


Peak List

m/z	z	Abund
534.9688	1	205748.3
535.9707	1	44536.5
536.9666	1	347538.7
537.9685	1	76448.3
538.9644	1	157774
539.9654	1	34401.2
556.95		66123.5
558.948	1	114424.5
559.9497	1	24350.9
560.9457	1	47238.7

Figure S74. HR-MS spectrum of compound **2x**.

User Spectra



Peak List

m/z	z	Abund
116.1437	1	60162.7
566.074	1	528298.6
567.0763	1	136970
568.0667	1	883447.9
569.0744	1	235335.3
570.07	1	403314.6
571.0719	1	103076.4
572.0684	1	58898
590.0531	1	63897.5
626.1237	1	69808.2

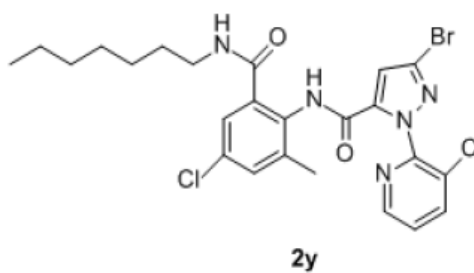


Figure S75. HR-MS spectrum of compound **2y**.