

Design, synthesis and SAR of novel 1,3-disubstituted imidazolidine or hexahydropyrimidine derivatives as herbicide safeners

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1 Screening of maize varieties

The sensitivity of different maize varieties to nicosulfuron was shown in **Table 1**. Kennian No. 1 exhibited the most sensitivity to nicosulfuron after 7 days treatment. The root length, plant height, root fresh weight and plant fresh weight inhibition rate were 41.00%, 32.73%, 48.81% and 35.16%, respectively. It showed that plant growth was significantly inhibited and yellowing on the surface of the leaves, which was classified as sensitive. The plant height inhibition rate of Xiawang 903, Jinguan 218 and Mige 903 was 19.54-28.05%, the sensitivity was slightly lower, and they were classified as moderate tolerant. The plant height inhibition rate of Huazhen 219 and Astragalus 268 was 1.59% and 4.29%, respectively. So they were classified as tolerant species. The inhibition rate of chlorophyll content different maize varieties was similar to the change law of growth index. Therefore, Kennian 1 was selected as the test crop for the further study the effect of the synthesized compound.

2 Table S1. Seedling growth index and chlorophyll content inhibition rate^{i, ii}

Variety	Root length inhibition rate (%)	Plant height inhibition rate (%)	Root fresh weight inhibition rate (%)	Plant fresh weight inhibition rate (%)	Chlorophyll content inhibition rate (%)
Xiawang 903	5.65 ^{cd}	22.16 ^{ab}	19.64 ^b	39.74 ^a	8.27
Jinguan 218	23.14 ^b	19.54 ^b	36.78 ^{ab}	21.29 ^b	13.17
Mige 903	13.49 ^{bc}	28.05 ^{ab}	21.47 ^b	30.62 ^{ab}	11.85
Huazhen 219	-4.24 ^d	1.59 ^c	4.81 ^c	12.89 ^c	12.59
Huangnuo 268	18.04 ^{bc}	4.29 ^c	26.95 ^{ab}	15.05 ^c	14.04
Kennian 1	41.00 ^a	32.73 ^a	48.81 ^a	35.16 ^{ab}	13.79

ⁱData are means of three repetitions.

ⁱⁱDifferent lowercase letters in the figure indicate significant difference ($P < 0.05$)

3 Table S2 The injury recovery rate (%) of root length of maize with different concentrations of compounds.

Compound	Group	Concentration (mg/kg)				
		10	15	20	25	50
Isoxadifen-ethyl	1	28.69	46.01	52.37	32.67	28.09
	2	28.79	46.23	52.54	33.65	27.72
	3	28.54	45.87	52.29	32.64	27.58
I-1	1	1.86	13.18	21.76	47.91	35.17
	2	4.93	12.67	22.43	48.30	37.86
	3	3.25	14.33	19.87	47.51	38.42
I-2	1	27.02	46.10	51.65	30.13	19.02
	2	27.79	45.83	52.37	39.75	26.84
	3	26.99	46.47	51.89	32.46	20.53
I-3	1	40.46	52.35	86.58	70.32	49.03
	2	40.35	52.16	85.35	69.54	56.37
	3	39.87	52.66	84.38	67.84	53.21
I-4	1	10.31	25.37	36.02	64.58	50.93
	2	9.96	24.88	35.91	63.69	57.73
	3	10.15	25.53	36.20	65.44	55.49
I-5	1	9.35	24.33	32.51	56.14	79.70
	2	8.63	25.12	32.37	55.98	78.61
	3	8.99	24.67	31.94	56.38	79.52
I-6	1	20.81	58.17	34.96	10.20	15.54
	2	23.96	58.34	43.97	37.52	25.96
	3	22.95	60.42	44.63	38.40	19.67
I-7	1	6.79	11.82	30.50	18.07	-2.48
	2	6.96	11.75	29.99	17.36	1.29
	3	7.02	11.45	31.08	16.73	5.41
I-8	1	-9.36	14.70	21.24	23.86	11.80
	2	-7.59	6.53	25.76	18.33	9.47
	3	-8.25	11.39	22.68	19.04	8.47
I-9	1	18.55	15.46	27.44	42.12	16.55
	2	18.80	16.01	27.58	41.93	26.56
	3	18.05	19.64	27.79	41.57	18.88
I-10	1	19.44	11.85	35.39	56.15	5.01
	2	19.35	12.06	35.87	55.73	14.33
	3	19.25	11.76	35.01	56.34	10.06
I-11	1	3.57	8.24	13.59	18.17	12.67
	2	3.42	8.05	13.67	18.03	16.56
	3	3.63	8.16	13.44	18.25	15.33
I-12	1	25.90	31.02	43.58	17.64	0.11
	2	26.03	31.65	44.00	18.13	4.32
	3	25.56	32.94	43.05	16.97	2.21
I-13	1	16.84	32.41	41.22	62.59	30.82

	2	17.04	32.13	41.34	61.98	31.45
	3	16.88	32.54	41.20	62.04	30.97
I-14	1	22.71	45.16	93.84	50.39	18.10
	2	22.68	45.30	93.67	51.01	18.47
	3	22.82	45.10	94.05	50.66	17.87
I-15	1	9.38	23.67	54.21	62.78	23.95
	2	9.42	23.53	54.47	62.59	24.09
	3	9.47	23.40	53.39	62.93	23.20
I-16	1	15.46	43.35	67.58	53.72	21.03
	2	15.61	43.57	66.98	53.24	22.19
	3	15.37	43.16	67.83	52.68	21.78
I-17	1	-3.42	10.13	15.61	17.80	-5.14
	2	-1.09	8.72	15.09	18.33	-3.27
	3	-2.45	9.39	14.06	16.59	3.20
I-18	1	12.37	24.55	52.20	69.43	42.11
	2	12.61	24.38	51.97	69.35	43.09
	3	12.18	24.63	52.39	69.17	42.47
I-19	1	3.67	24.10	37.42	58.59	15.86
	2	3.80	23.95	37.26	58.83	15.37
	3	3.42	24.23	37.67	58.21	16.02
I-20	1	20.92	41.03	52.85	75.16	42.30
	2	20.73	40.96	52.67	74.99	43.05
	3	21.14	41.26	53.03	75.44	42.55
I-21	1	14.80	19.72	26.08	38.41	57.32
	2	14.87	19.66	26.29	38.27	57.08
	3	14.80	19.72	26.08	38.41	57.32
II-1	1	2.10	15.73	48.58	11.23	14.96
	2	2.24	16.57	48.39	11.59	14.36
	3	2.01	15.45	48.66	12.00	14.55
II-2	1	30.03	47.37	54.12	78.99	46.10
	2	29.93	47.25	54.33	79.19	45.96
	3	30.14	47.62	53.97	78.82	46.22
II-3	1	27.26	31.94	52.31	40.76	18.15
	2	27.15	31.82	52.19	41.04	17.98
	3	27.33	32.09	51.57	40.55	18.32
II-4	1	5.59	6.61	25.33	46.50	28.79
	2	5.73	6.85	25.20	46.71	29.01
	3	5.44	6.79	25.48	46.29	28.93
II-5	1	9.94	13.80	20.38	45.41	50.70
	2	9.86	13.91	20.24	45.67	50.79
	3	10.08	13.75	20.44	45.30	50.58
II-6	1	0.91	17.45	36.68	23.38	15.97
	2	1.05	17.39	36.81	24.03	16.22
	3	0.99	17.29	36.55	23.57	15.88

II-7	1	12.73	35.40	68.08	63.95	24.21
	2	12.87	35.62	68.20	64.27	24.36
	3	12.50	35.57	67.87	63.88	23.79
II-8	1	15.20	21.68	29.66	39.74	1.34
	2	15.37	21.55	29.82	39.91	2.66
	3	15.08	21.73	29.54	40.02	1.59
II-9	1	19.56	21.68	25.34	27.98	38.17
	2	19.70	21.56	25.22	28.03	38.29
	3	19.33	21.74	24.98	27.66	38.54

4 Table S3 The injury recovery rate (%) of plant height of maize with different concentrations of compounds.

Compound	Group	Concentration (mg/kg)				
		10	15	20	25	50
Isoxadifen-ethyl	1	20.01	36.35	47.28	51.54	59.61
	2	19.87	36.23	48.05	50.93	59.09
	3	20.31	36.54	47.29	51.32	59.45
I-1	1	11.89	32.35	31.63	55.72	19.26
	2	12.00	32.14	31.81	55.67	19.45
	3	12.08	32.47	31.50	55.57	18.79
I-2	1	-2.83	9.90	21.94	34.53	39.06
	2	-2.67	10.03	21.82	34.76	39.20
	3	-2.95	9.77	21.76	34.58	38.99
I-3	1	34.14	72.28	99.83	88.04	35.09
	2	33.87	72.45	99.76	87.63	36.58
	3	34.45	72.43	99.71	86.98	35.47
I-4	1	18.5	26.17	58.51	72.34	41.73
	2	18.63	26.45	58.67	72.16	40.99
	3	18.87	26.45	58.23	72.46	42.47
I-5	1	21.29	56.28	98.53	74.86	32.11
	2	20.88	56.65	98.16	75.82	34.56
	3	21.73	56.94	99.32	75.33	34.28
I-6	1	15.03	24.72	30.10	47.27	18.63
	2	16.32	25.08	30.75	46.93	19.33
	3	15.32	24.55	29.87	47.54	17.53
I-7	1	34.78	49.16	58.94	11.98	15.71
	2	34.08	48.57	59.69	12.51	16.38
	3	35.20	50.09	59.33	11.37	14.88
I-8	1	19.67	36.07	47.24	50.77	59.17
	2	19.95	36.47	47.83	51.01	59.23
	3	19.58	35.94	47.11	50.58	59.4
I-9	1	6.06	11.7	39.69	15.41	8.97
	2	6.23	11.82	39.94	16.23	9.31
	3	6.31	11.76	39.52	15.76	9.44
I-10	1	14.01	39.07	41.41	40.68	23.51
	2	13.79	38.63	41.92	39.12	24.5
	3	14.33	39.26	41.59	40.05	23.73
I-11	1	17.24	23.18	29.91	40.53	24.15
	2	17.72	23.45	30.05	40.68	24.76
	3	16.99	23.65	30.73	40.92	25.08
I-12	1	12.71	28.77	29.91	37.81	4.57
	2	12.99	28.73	29.87	37.94	5.63
	3	12.67	27.56	29.72	37.63	4.99
I-13	1	29.18	34.80	47.63	59.15	20.20

	2	29.33	34.87	47.75	59.32	21.01
	3	29.09	34.67	47.47	59.19	20.58
I-14	1	10.77	27.2	40.54	40.71	9.28
	2	10.89	27.34	40.65	40.84	9.97
	3	10.63	27.41	40.35	40.82	10.08
I-15	1	34.16	59.59	87.18	76.64	54.77
	2	34.42	59.67	87.23	76.33	54.49
	3	33.92	59.35	87.54	76.78	55.12
I-16	1	1.00	28.00	67.72	88.70	68.10
	2	1.31	28.19	67.93	88.45	67.98
	3	1.25	27.87	67.37	88.56	67.61
I-17	1	7	44.51	65.6	36.69	14.89
	2	7.21	44.48	65.69	37.44	14.52
	3	7.32	44.28	65.17	36.82	14.96
I-18	1	20.00	53.73	98.53	74.81	49.47
	2	20.31	53.88	98.43	73.25	49.78
	3	19.94	53.57	98.38	74.47	48.92
I-19	1	12.32	20.77	21.47	46.88	3.13
	2	12.65	21.03	21.58	46.65	3.32
	3	12.03	20.25	21.69	46.35	3.58
I-20	1	5.50	3.30	6.98	35.12	17.07
	2	5.69	3.47	7.21	35.36	17.75
	3	5.44	3.61	7.32	34.98	17.49
I-21	1	2.17	17.11	19.2	37.54	6.57
	2	2.41	17.54	19.87	37.66	6.34
	3	2.09	17.23	19.31	37.38	6.14
II-1	1	13.33	25.08	27.43	65.49	73.84
	2	13.46	25.37	27.56	65.33	73.68
	3	13.12	25.44	27.38	63.27	73.74
II-2	1	23.58	49.86	54.01	58.65	41.95
	2	23.71	49.68	53.84	58.62	42.09
	3	23.09	49.67	54.26	58.83	41.33
II-3	1	22.49	61.71	96.15	100.83	34.94
	2	22.68	61.53	95.02	99.89	35.21
	3	22.33	61.96	97.35	100.24	34.58
II-4	1	8.00	26.03	34.20	1.50	0.98
	2	7.56	26.17	34.39	1.65	0.57
	3	8.65	26.47	33.92	1.77	0.39
II-5	1	11.85	23.99	30.15	40.84	9.63
	2	12.09	24.32	30.33	40.57	9.45
	3	11.74	24.86	29.68	41.05	9.91
II-6	1	27.79	48.53	62.17	27.03	2.69
	2	28.21	49.05	63.21	26.44	3.09
	3	27.67	48.61	61.77	27.31	3.38

II-7	1	1.83	20.06	64.61	70.21	86.16
	2	2.05	20.47	65.32	70.76	87.02
	3	2.31	20.14	64.38	70.13	86.49
II-8	1	15.3	26.49	38.14	29.51	6.62
	2	15.87	26.53	38.36	28.09	6.77
	3	14.96	26.35	38.62	28.67	6.91
II-9	1	9.16	14.64	19.96	20.88	39.19
	2	8.96	14.78	20.07	21.05	39.47
	3	9.03	14.82	19.77	20.91	39.25

5 Table S4 The injury recovery rate (%) of root fresh weight of maize with different concentrations of compounds.

Compound	Group	Concentration (mg/kg)				
		10	15	20	25	50
Isoxadifen-ethyl	1	45.37	64.26	77.35	103.44	76.49
	2	46.14	64.47	78.42	102.98	74.36
	3	46.61	64.25	77.06	104.38	77.29
I-1	1	13.87	18.92	20.89	28.61	34.18
	2	13.98	19.07	20.66	28.83	34.55
	3	13.65	18.84	21.05	28.72	34.32
I-2	1	19.05	23.61	44.74	18.44	9.24
	2	19.21	23.76	44.58	18.36	8.76
	3	18.93	23.47	44.82	18.02	9.47
I-3	1	31.51	57.00	81.89	89.32	34.31
	2	31.62	56.88	81.69	90.05	35.02
	3	31.43	56.89	82.45	90.33	34.17
I-4	1	23.02	35.13	53.53	21.89	20.76
	2	23.24	35.31	53.69	21.66	20.33
	3	22.91	35.67	53.37	21.03	20.25
I-5	1	16.78	19.82	27.36	39.56	51.70
	2	16.91	19.67	27.48	39.61	51.34
	3	16.52	20.01	27.49	39.73	51.66
I-6	1	14.18	18.02	34.37	48.85	29.86
	2	14.36	18.64	34.37	48.92	30.09
	3	13.99	18.64	34.52	48.67	29.55
I-7	1	15.56	19.57	21.63	22.21	14.50
	2	15.48	18.97	21.20	22.67	14.95
	3	15.84	19.96	21.05	22.64	14.68
I-8	1	10.43	28.49	39.68	15.97	14.26
	2	10.67	28.53	39.97	16.43	14.79
	3	10.28	28.77	39.43	15.86	13.91
I-9	1	11.23	16.09	22.01	56.16	21.17
	2	11.47	16.28	22.09	56.41	21.58
	3	11.09	16.28	22.45	55.89	20.75
I-10	1	6.55	15.97	21.16	26.07	38.9
	2	6.83	15.79	21.31	26.25	38.79
	3	6.37	14.64	21.02	26.47	38.87
I-11	1	1.75	6.33	13.35	41.21	10.48
	2	1.86	6.45	13.51	41.54	11.03
	3	1.59	6.21	13.18	41.44	10.86
I-12	1	15.98	19.12	37.08	21.24	9.86
	2	16.11	19.34	37.2	21.54	9.37
	3	15.78	18.93	37.19	21.69	10.46
I-13	1	5.18	21.43	30.69	29.86	18.89

	2	5.43	21.27	30.81	29.57	18.92
	3	5.65	21.6	30.39	29.38	17.99
I-14	1	35.30	46.25	94.56	31.46	1.88
	2	35.13	46.66	94.82	32.44	2.05
	3	35.42	45.99	93.97	31.79	1.73
I-15	1	8.73	19.14	21.71	54.13	33.72
	2	8.96	19.35	21.23	53.97	33.01
	3	8.21	19.45	22.03	54.69	33.58
I-16	1	15.15	27.54	34.37	71.04	20.89
	2	15.38	27.29	34.83	69.96	21.35
	3	14.97	27.83	34.62	71.32	20.75
I-17	1	16.62	35.89	51.44	29.22	13.15
	2	17.03	35.46	51.82	29.87	13.98
	3	16.43	35.47	52.08	29.65	12.79
I-18	1	1.18	10.72	24.76	31.21	39.69
	2	2.03	10.59	24.37	31.40	39.58
	3	1.99	10.34	24.56	30.98	39.82
I-19	1	11.46	14.52	36.71	16.39	25.74
	2	12.04	14.76	36.58	17.08	24.3
	3	11.29	15.00	36.87	16.23	26.34
I-20	1	22.04	31.75	43.75	27.39	19.47
	2	22.74	31.51	43.88	27.09	20.02
	3	22.43	31.39	42.57	26.78	21.32
I-21	1	17.65	23.73	28.73	25.64	17.59
	2	17.95	23.63	28.92	25.38	18.04
	3	17.36	24.05	28.66	26.32	17.84
II-1	1	19.66	25.61	31.47	59.05	14.42
	2	19.93	25.87	31.69	59.32	14.97
	3	19.35	25.71	31.28	58.47	15.08
II-2	1	45.82	64.83	77.86	109.55	63.59
	2	45.59	65.11	77.63	102.34	62.98
	3	46.08	65.23	78.04	103.43	63.47
II-3	1	19.62	27.85	41.59	36.72	20.49
	2	19.38	27.49	41.92	36.21	20.56
	3	20.17	27.52	41.86	36.55	20.25
II-4	1	18.39	23.25	31.34	76.78	10.21
	2	18.62	23.41	31.65	76.94	10.68
	3	18.07	23.38	31.21	77.18	11.32
II-5	1	19.42	37.44	48.13	25.15	8.70
	2	19.27	37.74	48.51	24.58	8.34
	3	19.85	37.79	47.62	24.17	8.91
II-6	1	11.05	14.61	21.70	33.44	20.24
	2	11.58	14.31	21.93	33.67	21.13
	3	10.56	14.86	21.99	33.01	20.86

II-7	1	19.51	25.02	30.89	31.32	45.31
	2	20.04	25.31	30.67	31.59	45.47
	3	19.68	24.83	30.99	31.46	45.25
II-8	1	7.02	29.13	51.53	84.89	20.76
	2	7.33	29.37	51.42	84.76	21.05
	3	6.89	28.81	51.65	85.12	20.43
II-9	1	-0.78	11.82	21.36	23.56	51.70
	2	-0.63	11.72	21.49	23.87	51.45
	3	-0.83	11.34	21.11	23.63	51.98

6 Table S5 The injury recovery rate (%) of plant fresh weight of maize with different concentrations of compounds.

Compound	Group	Concentration (mg/kg)				
		10	15	20	25	50
Isoxadifen-ethyl	1	34.22	53.98	91.36	37.39	26.18
	2	33.83	53.46	92.05	38.15	27.25
	3	33.27	54.12	92.99	38.11	27.82
I-1	1	16.28	23.46	26.95	41.11	31.98
	2	16.45	23.6	26.77	41.38	31.67
	3	16.65	23.27	26.61	41.35	32.28
I-2	1	15.28	27.96	65.39	20.12	3.23
	2	15.47	27.66	65.71	21.33	3.45
	3	15.42	28.19	65.21	20.67	3.96
I-3	1	31.34	46.83	59.98	23.02	18.66
	2	30.99	46.75	60.13	22.67	18.23
	3	31.75	46.62	60.31	23.67	18.02
I-4	1	11.92	25.60	38.94	41.43	23.20
	2	12.05	25.78	38.69	41.87	23.58
	3	12.19	25.47	39.16	41.22	22.57
I-5	1	24.65	46.61	52.79	21.21	12.33
	2	24.87	46.38	52.79	22.3	12.79
	3	24.38	46.75	53.01	21.57	13.09
I-6	1	12.31	26.13	31.86	54.67	33.68
	2	12.47	26.32	31.28	55.04	34.02
	3	12.09	26.47	32.05	54.36	34.61
I-7	1	-3.72	7.52	17.77	35.65	13.55
	2	-3.53	8.09	17.65	35.47	14.08
	3	-3.99	8.21	17.83	35.90	14.64
I-8	1	11.51	29.05	56.68	24.34	17.63
	2	11.69	29.3	56.38	25.09	17.34
	3	11.79	28.87	56.93	24.13	17.86
I-9	1	10.51	21.26	39.82	19.39	18.59
	2	10.87	21.09	39.57	19.23	18.38
	3	10.28	21.47	40.13	20.34	18.85
I-10	1	-5.60	18.31	25.38	61.18	24.73
	2	-5.23	18.64	25.49	62.45	23.62
	3	-5.98	18.79	25.87	63.21	24.76
I-11	1	1.34	12.37	19.32	15.98	-2.23
	2	-0.13	11.45	16.57	14.33	1.75
	3	1.23	12.87	19.55	14.49	-1.09
I-12	1	15.92	38.05	79.75	15.42	3.93
	2	16.23	37.79	78.43	14.33	4.32
	3	16.21	38.45	79.12	15.85	4.35
I-13	1	2.73	7.09	17.62	35.79	13.57

	2	3.45	7.28	17.36	35.58	14.34
	3	3.88	6.94	17.87	35.99	13.97
I-14	1	32.32	50.82	64.62	26.55	7.73
	2	31.97	50.68	65.03	26.22	7.81
	3	32.45	50.94	63.88	25.38	7.19
I-15	1	24.57	33.06	35.33	16.13	5.42
	2	24.31	33.56	35.67	15.78	5.93
	3	24.38	33.50	35.82	15.17	5.82
I-16	1	30.51	34.89	45.14	25.98	37.62
	2	30.23	34.65	44.71	25.18	37.24
	3	30.71	35.35	45.18	26.14	37.93
I-17	1	1.90	21.53	25.61	39.12	21.91
	2	2.54	21.67	25.39	38.66	21.58
	3	2.47	21.33	25.98	39.47	20.42
I-18	1	31.48	59.56	76.51	38.53	10.46
	2	31.32	58.79	75.37	37.39	10.38
	3	31.18	59.24	75.82	38.28	10.91
I-19	1	13.37	34.11	52.43	26.29	1.51
	2	13.76	34.27	52.85	26.72	1.28
	3	12.99	34.56	53.02	25.82	2.84
I-20	1	33.37	54.11	92.43	42.62	1.44
	2	33.58	55.09	91.25	41.35	1.74
	3	33.12	53.78	93.16	42.82	1.92
I-21	1	9.01	13.46	28.24	36.08	31.17
	2	9.45	13.66	28.12	36.35	30.17
	3	8.78	13.60	28.39	35.57	31.83
II-1	1	19.58	21.36	23.58	28.82	11.46
	2	18.35	22.12	23.13	27.82	11.21
	3	18.93	21.97	23.05	27.69	11.62
II-2	1	21.23	40.89	58.22	20.94	11.26
	2	21.54	41.07	59.31	21.01	11.47
	3	20.97	40.13	58.41	21.54	10.85
II-3	1	31.05	41.16	71.46	28.26	1.17
	2	30.65	41.38	72.82	28.18	1.09
	3	30.65	41.38	71.58	27.27	1.49
II-4	1	2.43	15.88	30.52	39.92	26.88
	2	3.02	15.36	30.22	40.08	25.48
	3	4.11	15.48	30.94	41.32	26.21
II-5	1	12.26	23.49	24.03	32.23	-1.11
	2	12.76	23.57	24.18	31.99	1.08
	3	12.03	23.31	24.14	32.09	-0.69
II-6	1	3.23	5.28	17.96	15.39	2.12
	2	4.21	5.17	16.99	15.41	2.87
	3	3.79	5.61	17.20	15.63	2.17

II-7	1	24.02	31.34	40.46	15.08	13.29
	2	24.35	31.68	40.59	15.64	13.26
	3	23.93	31.6	41.02	14.78	12.94
II-8	1	29.92	32.6	70.94	31.43	23.2
	2	30.03	32.87	71.38	30.11	24.58
	3	29.81	32.99	71.32	31.36	25.34
II-9	1	-2.33	10.21	24.65	35.3	5.58
	2	-1.97	11.3	24.13	35.24	6.01
	3	-2.46	10.61	24.39	35.42	5.86

7 **Table S6** The injury recovery rate (%) of chlorophyll content of maize with different concentrations of compounds.

Compound	Group	Concentration (mg/kg)				
		10	15	20	25	50
Isoxadifen-ethyl	1	18.59	25.34	41.60	68.77	42.56
	2	18.45	25.62	41.53	68.58	42.92
	3	18.96	25.62	41.85	67.93	41.88
I-1	1	22.54	26.73	31.94	34.52	41.07
	2	22.48	26.96	31.68	34.27	41.23
	3	22.67	26.98	31.69	34.19	41.32
I-2	1	11.33	34.69	36.68	25.79	25.82
	2	11.46	34.8	36.88	26.23	25.49
	3	11.16	34.59	36.49	26.05	25.19
I-3	1	26.69	35.67	59.11	30.39	1.91
	2	26.90	35.42	59.33	30.99	2.56
	3	26.44	35.98	58.89	30.13	1.66
I-4	1	34.81	37.16	49.72	15.65	7.98
	2	35.02	37.22	49.66	15.43	7.06
	3	35.13	36.97	49.49	16.12	7.62
I-5	1	16.12	24.94	35.53	40.18	29.64
	2	16.35	24.98	35.34	40.36	29.03
	3	15.96	24.78	35.99	40.21	28.95
I-6	1	13.96	36.93	47.81	24.24	10.10
	2	13.65	36.78	47.95	25.03	10.62
	3	13.62	36.81	47.93	24.65	9.63
I-7	1	-1.98	9.27	18.72	23.97	23.99
	2	-1.72	9.45	18.62	23.86	24.06
	3	-2.06	9.34	18.66	23.85	24.03
I-8	1	9.18	17.42	27.94	39.76	18.24
	2	9.33	17.58	27.79	40.00	18.79
	3	9.03	17.26	28.06	39.88	17.96
I-9	1	11.28	19.34	21.22	28.91	37.41
	2	11.43	19.66	21.02	28.76	37.65
	3	11.16	19.26	21.46	28.99	37.23
I-10	1	23.91	38.27	41.73	9.23	10.34
	2	24.03	38.16	41.65	9.69	11.23
	3	23.72	38.42	41.56	10.30	11.06
I-11	1	9.36	16.35	27.37	34.81	17.34
	2	9.65	16.42	27.16	34.72	17.12
	3	9.21	16.16	27.42	34.97	16.52
I-12	1	14.23	29.45	38.21	53.83	19.21
	2	14.46	29.19	38.41	53.67	19.89
	3	14.35	29.5	38.14	53.71	18.62
I-13	1	15.21	21.93	22.32	37.91	15.21

	2	15.47	21.67	22.42	38.03	14.68
	3	15.02	21.99	22.12	37.82	16.02
I-14	1	29.25	34.48	40.62	24.83	16.86
	2	29.61	34.23	40.79	24.26	16.98
	3	29.42	34.37	40.49	25.03	15.97
I-15	1	18.72	25.43	41.95	67.93	19.31
	2	18.95	25.62	41.75	67.82	19.01
	3	18.63	25.24	41.99	68.02	18.62
I-16	1	9.34	19.41	26.52	38.65	30.31
	2	9.23	19.23	26.35	38.37	30.01
	3	9.46	19.55	26.67	38.75	29.65
I-17	1	16.14	38.63	44.63	29.51	23.52
	2	16.38	38.57	45.01	28.34	23.66
	3	15.94	38.80	44.21	29.12	24.05
I-18	1	6.52	19.48	24.52	50.41	39.41
	2	7.12	19.71	24.36	51.88	39.81
	3	6.38	19.59	24.46	50.11	38.24
I-19	1	20.32	29.63	35.74	39.67	17.52
	2	20.54	29.71	35.38	39.25	16.37
	3	21.00	29.67	35.87	40.01	15.88
I-20	1	36.62	36.51	59.84	19.62	6.41
	2	36.47	36.82	60.02	18.55	6.28
	3	36.73	36.88	59.62	19.41	6.97
I-21	1	3.62	13.56	17.48	24.45	36.73
	2	3.45	13.66	17.43	25.36	36.28
	3	3.79	13.44	17.56	24.61	36.91
II-1	1	18.57	25.62	60.63	30.62	19.53
	2	18.65	25.38	61.22	31.02	19.16
	3	18.44	25.97	62.01	30.18	18.58
II-2	1	27.77	38.63	51.84	31.95	28.52
	2	27.65	38.31	50.83	32.37	28.22
	3	27.98	38.21	51.02	31.18	29.03
II-3	1	6.93	19.52	26.93	10.52	4.36
	2	5.47	18.35	24.29	10.12	5.31
	3	6.78	19.04	26.52	11.48	4.79
II-4	1	19.31	28.95	61.63	37.42	20.54
	2	19.57	28.62	60.33	37.69	21.52
	3	19.18	29.04	61.97	38.03	20.88
II-5	1	17.38	25.93	34.95	29.43	19.64
	2	17.49	25.36	34.78	28.94	19.41
	3	17.16	25.81	34.69	29.12	20.73
II-6	1	-1.27	9.42	17.86	26.95	30.47
	2	-1.09	9.37	17.32	26.38	30.65
	3	-1.12	9.49	17.76	26.84	30.78

II-7	1	36.67	40.48	47.82	56.91	24.83
	2	36.55	40.31	47.69	57.04	23.44
	3	36.48	40.57	48.01	56.79	24.38
II-8	1	26.91	37.75	49.73	57.87	60.21
	2	26.77	37.69	49.58	58.13	60.92
	3	27.05	37.93	49.22	57.61	59.67
II-9	1	11.85	24.85	30.72	28.47	17.46
	2	12.09	24.71	30.63	27.24	17.94
	3	11.69	25.01	30.58	28.13	17.92

8 Table S7 Effects of compound I-3 and isoxadifen-ethyl on in vivo GST activity in maize.^{i, ii, iii}

Compound	Concentration (mg/kg)	Group	Specific activity of GST ($\mu\text{mol min}^{-1} \text{mg}^{-1} \text{protein}$)	GST activity increase (%)
CK	-	1	7.72	-
		2	7.68	-
		3	7.58	-
Nicosulfuron	-	1	5.07	-
		2	5.08	-
		3	5.06	-
Isoxadifen-ethyl	10	1	6.38	27.68
		2	6.46	27.71
		3	6.50	27.77
	15	1	8.88	78.43
		2	8.90	78.68
		3	8.95	78.71
	20	1	6.98	40.30
		2	7.03	40.23
		3	7.09	40.24
	25	1	6.13	22.16
		2	6.06	22.08
		3	6.07	22.19
50	1	3.02	-40.10	

		2	2.93	-40.88
		3	2.88	-40.83
Compound I-3	10	1	6.89	36.14
		2	6.65	36.19
		3	6.83	36.11
	15	1	8.42	67.52
		2	8.28	67.52
		3	8.41	67.50
	20	1	8.51	69.06
		2	8.42	69.07
		3	8.50	69.03
	25	1	5.68	13.83
		2	5.72	13.96
		3	5.73	13.79
	50	1	3.24	-35.33
		2	3.21	-35.35
		3	3.19	-35.29

9 The spectroscopic data of compounds I-1~21 and II-1~9.

Data for 1,3-dis (5-methylisoxazole-3-formyl) imidazolidine (I-1). Yield 57%; white solid; mp 152.8–153.9 °C. IR (KBr, cm^{-1}) ν : 3052–2850 (C–H), 1641 (C=O), 1576 (C=C), 1223 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 8.75 (t, $J = 6.0$ Hz, 2H, Ar–H), 6.52 (s, 2H, N–CH₂–N), 3.39 (m, 4H, N–CH₂–CH₂–N), 2.50–2.45 (s, 6H, 2CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 171.57, 171.57, 159.38, 159.38, 159.38, 159.38, 101.77, 101.77, 38.92, 12.31, 12.31, 12.31, 12.31; HRMS (ESI) calcd. For $\text{C}_{13}\text{H}_{14}\text{N}_4\text{O}_4$ $[\text{M}+\text{H}]^+$ 291.1093; found 291.1088. ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{13}\text{H}_{14}\text{N}_4\text{O}_4]$: 291.1093, found 291.1088.

Data for 1,3-dis (3,5-dimethylisoxazole-4-formyl) imidazolidine (I-2). Yield 54%; white solid; mp 166.4–166.9 °C. IR (KBr, cm^{-1}) ν : 3041–2846 (C–H), 1642 (C=O), 1588 (C=C), 1229 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 8.02 (s, 2H, N–CH₂–N), 3.38–3.33 (m, 4H, N–CH₂–CH₂–N), 2.49 (s, 6H, 2CH₃), 2.28 (s, 6H, 2CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 169.92, 169.92, 162.14, 162.14, 158.69, 158.69, 113.27, 113.27, 64.32, 40.69, 40.69, 12.57, 12.57, 11.03, 11.03; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{15}\text{H}_{18}\text{N}_4\text{O}_4]$: 319.1406, found 319.1402.

Data for 1,3-dis (5-methyl-3-phenylisoxazole-4-formyl) imidazolidine (I-3). Yield 61%; white solid; mp 164.8–165.2 °C. IR (KBr, cm^{-1}) ν : 3041–2864 (C–H), 1627 (C=O), 1597–1563 (C=C), 1223 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 7.29–7.67 (m, 10H, Ph–H), 5.20–4.54 (s, 2H, N–CH₂–N), 3.59–3.78 (d, $J = 76.0$ Hz, 2H, N–CH₂), 3.05 (d, $J = 88.4$ Hz, 2H, N–CH₂), 2.83–2.05 (m, 6H, 2CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 171.01, 171.01, 161.32, 161.32, 159.61, 159.61, 130.45, 130.45, 130.45, 130.45, 129.18, 129.18, 129.18, 129.18, 128.24, 128.24, 127.31, 127.31, 110.88, 110.88, 60.72, 45.98, 45.98, 12.01, 12.01; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{25}\text{H}_{22}\text{N}_4\text{O}_4]$: 443.1719, found 443.1718.

Data for 1,3-dis (3- (2-chlorophenyl) -5-methylisoxazole-4-formyl) imidazolidine (I-4). Yield

80%; white solid; mp 170.4–171.6 °C. IR (KBr, cm^{-1}) ν : 3060–2832 (C–H), 1649 (C=O), 1590 (C=C), 1243 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 7.57–7.39 (m, 8H, Ph–H), 4.85 (s, 2H, N–CH₂–N), 3.72–3.26 (s, 4H, N–CH₂–CH₂–N), 2.59 (s, 6H, 2CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 162.80, 162.80, 159.17, 159.17, 157.93, 157.93, 132.80, 132.80, 132.80, 132.80, 129.53, 129.53, 129.53, 129.53, 127.50, 127.50, 125.14, 125.14, 107.26, 107.26, 77.24, 50.38, 50.38, 12.46, 12.46; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{25}\text{H}_{20}\text{Cl}_2\text{N}_4\text{O}_4]$: 511.0940, found 511.0936.

Data for 1,3-dis (3- (2,6-dichlorophenyl) -5-methylisoxazole-4-formyl) imidazolidine (I-5).

Yield 68%; white solid; mp 234.1–235.2 °C. IR (KBr, cm^{-1}) ν : 3009–2871 (C–H), 1622 (C=O), 1587–1566 (C=C), 1208 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 7.29 (m, 6H, Ph–H), 4.91 (s, 2H, N–CH₂–N), 3.52 (s, 4H, N–CH₂–CH₂–N), 2.61 (s, 6H, 2CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 165.16, 165.16, 160.91, 160.91, 158.73, 158.73, 135.45, 135.45, 135.45, 135.45, 131.66, 131.66, 128.44, 128.44, 128.44, 128.44, 127.84, 127.84, 113.01, 113.01, 61.15, 53.50, 53.50, 12.66, 12.66; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{25}\text{H}_{18}\text{Cl}_4\text{N}_4\text{O}_4]$: 579.0160, found 579.0152.

Data for 1,3-dis (3- (2-chloro-6-fluorophenyl) -5-methylisoxazole-4-formyl) imidazolidine (I-6). Yield 72%; white solid; mp 228.5–229.3 °C. IR (KBr, cm^{-1}) ν : 3057–2852 (C–H), 1650 (C=O), 1572 (C=C), 1250 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 7.46–7.12 (m, 6H, Ph–H), 4.92 (s, 2H, N–CH₂–N), 3.53 (s, 4H, N–CH₂–CH₂–N), 2.60 (s, 6H, 2CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 161.95, 161.95, 160.99, 160.99, 159.43, 159.43, 137.71, 137.71, 134.68, 134.68, 134.68, 134.68, 132.12, 132.12, 125.92, 125.92, 116.64, 116.64, 114.85, 114.85, 77.26, 30.98, 30.98, 12.51, 12.51; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{25}\text{H}_{18}\text{Cl}_2\text{F}_2\text{N}_4\text{O}_4]$: 547.0751, found 547.0742.

Data for 1,3-dis (5-fluoronicotinoyl) imidazolidine (I-7). Yield 50%; pink solid; mp 150.3–150.5 °C. IR (KBr, cm^{-1}) ν : 3055–2893 (C–H), 1639 (C=O), 1574 (C=C), 1260 (C–N); ^1H

NMR (400 MHz, CDCl₃) δ : 8.62–7.64 (m, 6H, Ar–H), 5.20 (s, 2H, N–CH₂–N), 3.88 (d, J = 60.0 Hz, 4H, N–CH₂–CH₂–N); ¹³C NMR (100 MHz, CDCl₃) δ : 165.54, 165.54, 154.05, 154.05, 148.44, 148.44, 138.07, 138.07, 129.52, 129.52, 124.60, 124.60, 62.37, 46.50, 46.50; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₁₅H₁₂F₂N₄O₂]: 319.1007, found 319.1002.

Data for 1,3-dis (5-bromonicotinoyl) imidazolidine (I-8). Yield 45%; clear crystal; mp 165.2–166.1 °C. IR (KBr, cm⁻¹) ν : 3051–2891 (C–H), 1640 (C=O), 1580 (C=C), 1260 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 8.83–8.07 (m, 6H, Ar–H), 5.18 (s, 2H, N–CH₂–N), 4.02–3.87 (d, J = 68.0 Hz, 4H, N–CH₂–CH₂–N); ¹³C NMR (100 MHz, CDCl₃) δ : 164.91, 164.91, 153.16, 153.16, 146.02, 146.02, 137.88, 137.88, 131.94, 131.94, 121.01, 121.01, 62.34, 46.54, 46.54; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₁₅H₁₂Br₂N₄O₂]: 438.9405, found 438.9397.

Data for 1,3-dis (6-chloronicotinoyl) imidazolidine (I-9). Yield 58%; clear crystal; mp 155.6–155.8 °C. IR (KBr, cm⁻¹) ν : 3056–2850 (C–H), 1638 (C=O), 1467 (C=C), 1260 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 8.58–7.49 (m, 6H, Ar–H), 5.16 (s, 2H, N–CH₂–N), 3.86 (m, 4H, N–CH₂–CH₂–N); ¹³C NMR (100 MHz, CDCl₃) δ : 165.45, 165.45, 153.94, 153.94, 148.38, 148.38, 138.04, 138.04, 129.53, 129.53, 124.55, 124.55, 62.34, 46.44, 46.44; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₁₅H₁₂Cl₂N₄O₂]: 351.0416, found 351.0414.

Data for 1,3-dis (6- (trifluoromethyl) nicotinyl) imidazolidine (I-10). Yield 60%; clear crystal; mp 145.7–147.3 °C. IR (KBr, cm⁻¹) ν : 3060–2850 (C–H), 1644 (C=O), 1420 (C=C), 1258 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 8.91–7.83 (m, 6H, Ar–H), 5.18 (s, 2H, N–CH₂–N), 3.87–4.09 (d, J = 83.9 Hz, 4H, N–CH₂–CH₂–N); ¹³C NMR (100 MHz, CDCl₃) δ : 165.16, 165.16, 149.90, 149.90, 148.34, 148.34, 136.89, 136.89, 133.33, 133.33, 125.08, 125.08, 120.57, 120.57, 62.20, 46.55, 46.55; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₁₇H₁₂F₆N₄O₂]: 419.0943, found 419.0935.

Data for 1,3-dis (6-bromonicotinoyl) imidazolidine (I-11). Yield 42%; clear crystal; mp 163.5–163.8 °C. IR (KBr, cm⁻¹) ν : 3054–2851 (C–H), 1634 (C=O), 1585 (C=C), 1262 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 8.61 (s, 2H, Ar–H), 7.89–7.45 (d, 4H, Ar–H), 5.18 (s, 2H, N–CH₂–N), 3.88 (d, J = 48.0 Hz, 4H, N–CH₂–CH₂–N); ¹³C NMR (100 MHz, CDCl₃) δ : 165.54, 165.54, 154.05, 154.05, 148.44, 148.44, 138.07, 138.07, 129.52, 129.52, 124.60, 124.60, 62.37, 46.50, 46.50; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₁₅H₁₂Br₂N₄O₂]: 438.9405, found 438.9395.

Data for 1,3-dis (4,6-dichloronicotinoyl) imidazolidine (I-12). Yield 56%; clear crystal; mp 174.8–175.2 °C. IR (KBr, cm⁻¹) ν : 3078–2891 (C–H), 1647 (C=O), 1569–1540 (C=C), 1260 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 8.43–7.50 (m, 4H, Ar–H), 5.38–4.95 (s, 2H, N–CH₂–N), 4.06 (t, J = 6.7 Hz, 2H, N–CH₂), 3.61 (d, 2H, N–CH₂); ¹³C NMR (100 MHz, CDCl₃) δ : 162.43, 162.43, 153.57, 153.57, 148.09, 148.09, 142.31, 142.31, 130.35, 130.35, 125.06, 125.06, 61.05, 44.08, 44.08; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₁₅H₁₀Cl₄N₄O₂]: 418.9636, found 418.9631.

Data for 1,3-dis (5,6-dichloronicotinoyl) imidazolidine (I-13). Yield 61%; clear crystal; mp 173.2–174.0 °C. IR (KBr, cm⁻¹) ν : 3060–2851 (C–H), 1637 (C=O), 1576 (C=C), 1262 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 8.49–8.00 (m, 4H, Ar–H), 5.19 (s, 2H, N–CH₂–N), 3.91 (s, 4H, N–CH₂–CH₂–N); ¹³C NMR (100 MHz, CDCl₃) δ : 151.87, 151.87, 145.45, 145.45, 138.00, 138.00, 138.00, 138.00, 131.29, 131.29, 77.28, 77.28, 58.50, 18.48, 18.48; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₁₅H₁₀Cl₄N₄O₂]: 418.9636, found 418.9634.

Data for 1,3-dis (3- (2-chlorophenyl) -5-methylisoxazole-4-formyl) -2-methylimidazolidine (I-14). Yield 53%; white solid; mp 178.9–179.7 °C. IR (KBr, cm⁻¹) ν : 2929–2828 (C–H), 1636 (C=O), 1587 (C=C), 1244 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 7.54–7.36 (m, 8H, Ph–H), 6.04 (s, 1H, N–CH–N), 3.30 (d, J = 111.9 Hz, 4H, N–CH₂–CH₂–N), 2.56 (s, 6H, 2CH₃), 1.35 (s, 3H, CH₃); ¹³C

NMR (100 MHz, CDCl₃) δ : 170.08, 170.08, 158.92, 158.92, 132.99, 132.99, 131.42, 131.42, 131.42, 131.42, 130.13, 130.13, 127.34, 127.34, 127.34, 127.34, 113.02, 113.02, 113.02, 113.02, 67.56, 34.69, 34.69, 26.94, 12.31, 12.31; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₂₆H₂₂Cl₂N₄O₄]: 525.1096, found 525.1093.

Data for 1,3-dis (3- (2,6-dichlorophenyl) -5-methylisoxazole-4-formyl) -2-methylimidazolidine (I-15). Yield 34%; white solid; mp 210.4–210.7 °C. IR (KBr, cm⁻¹) ν : 2953–2829 (C–H), 1634 (C=O), 1588–1548 (C=C), 1244 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 7.48–7.29 (m, 6H, Ph–H), 5.95 (s, 1H, N–CH–N), 3.27–3.54 (d, J = 108.0 Hz, 4H, N–CH₂–CH₂–N), 2.59 (s, 6H, 2CH₃), 1.33 (s, 3H, CH₃); ¹³C NMR (100 MHz, CDCl₃) δ : 169.84, 169.84, 159.96, 159.96, 156.97, 156.97, 135.35, 135.35, 135.35, 135.35, 131.59, 131.59, 131.59, 131.59, 128.57, 128.57, 127.11, 121.11, 113.33, 113.33, 67.39, 34.68, 34.68, 26.92, 12.58, 12.58; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₂₆H₂₀Cl₄N₄O₄]: 593.0317, found 593.0312.

Data for 1,3-bis (3- (2-chloro-6-fluorophenyl) -5-methylisoxazole-4-formyl) -2-methylimidazolidine (I-16). Yield 48%; white solid; mp 193.5–193.8 °C. IR (KBr, cm⁻¹) ν : 3064–2851 (C–H), 1636 (C=O), 1594–1559 (C=C), 1239 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 7.45–7.10 (m, 6H, Ph–H), 5.96 (s, 1H, N–CH–N), 3.21–3.48 (d, J = 112.0 Hz, 4H, N–CH₂–CH₂–N), 2.58 (s, 6H, 2CH₃), 1.31 (d, J = 4.0 Hz, 3H, CH₃); ¹³C NMR (100 MHz, CDCl₃) δ : 169.85, 169.85, 161.95, 161.95, 160.07, 160.07, 153.81, 153.81, 134.91, 134.91, 134.91, 134.91, 132.12, 132.12, 125.89, 125.89, 116.75, 116.57, 114.49, 114.49, 67.36, 44.74, 44.74, 18.30, 12.41, 12.41; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₂₆H₂₀Cl₂F₂N₄O₄]: 561.0908, found 561.0905.

Data for 1,3-dis (5-methylisoxazole-3-formyl) -4-methylimidazolidine (I-17). Yield 42%; white solid; mp 171.2–172.2 °C. IR (KBr, cm⁻¹) ν : 3141–2897 (C–H), 1642 (C=O), 1454 (C=C), 1205

(C-N); ^1H NMR (400 MHz, CDCl_3) δ : 6.59 (m, 2H, Ar-H), 5.59–5.22 (m, 2H, N-CH₂-N), 4.47 (m, H, N-CH-C), 4.00–3.79 (m, 2H, C-CH₂-N), 2.50–2.47 (s, 6H, 2CH₃), 1.28 (q, 3H, CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 175.96, 175.96, 163.88, 163.88, 162.55, 162.55, 107.90, 107.90, 66.41, 58.75, 56.56, 23.13, 16.95, 16.95; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{14}\text{H}_{16}\text{N}_4\text{O}_4]$: 305.1250, found 305.1248.

Data for 1,3-dis (3- (2-chlorophenyl) -5-methylisoxazole-4-formyl) -4-methylimidazolidine (I-18). Yield 66%; white solid; mp 211.8–212.4 °C. IR (KBr, cm^{-1}) ν : 3047–2857 (C-H), 1643 (C=O), 1588 (C=C), 1250 (C-N); ^1H NMR (400 MHz, CDCl_3) δ : 7.51–7.43 (m, 8H, Ph-H), 5.81–5.45 (d, $J = 140.0$ Hz, 2H, N-CH₂-N), 3.93–3.86 (m, 1H, N-CH-C), 3.28–3.08 (s, 2H, C-CH₂-N), 2.75 (d, $J = 4.0$ Hz, 6H, 2CH₃), 0.86 (d, $J = 8.0$ Hz, 3H, CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 173.53, 173.53, 161.94, 161.94, 158.52, 158.52, 134.00, 134.00, 134.00, 134.00, 131.89, 131.89, 130.15, 130.15, 127.46, 127.46, 111.95, 111.95, 77.25, 77.25, 45.90, 45.07, 45.07, 17.68, 13.01, 13.01; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{26}\text{H}_{22}\text{Cl}_2\text{N}_4\text{O}_4]$: 525.1096, found 525.1092.

Data for 1,3-dis (3- (2,6-dichlorophenyl) -5-methylisoxazole-4-formyl) -4-methylimidazolidine (I-19). Yield 57%; white solid; mp 241.0–241.2 °C. IR (KBr, cm^{-1}) ν : 3048–2861 (C-H), 1638 (C=O), 1594–1549 (C=C), 1264 (C-N); ^1H NMR (400 MHz, CDCl_3) δ : 7.49–7.37 (m, 6H, Ph-H), 4.99–4.78 (d, $J = 149.0$ Hz, 3H, N-CH-CH₂-N), 3.19–3.18 (m, 2H, N-CH₂-N), 2.60 (s, 6H, 2CH₃), 1.11 (d, $J = 6.4$ Hz, 3H, CH₃); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.26, 170.26, 160.88, 160.88, 160.46, 160.46, 157.00, 157.00, 135.49, 135.49, 131.66, 131.66, 128.47, 128.47, 128.38, 128.38, 126.98, 126.98, 113.30, 113.30, 60.36, 60.28, 60.28, 51.09, 18.09, 18.09; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{26}\text{H}_{20}\text{Cl}_4\text{N}_4\text{O}_4]$: 593.0317, found 593.0314.

Data for 1,3-dis (3- (2-chloro-6-fluorophenyl) -5-methylisoxazole-4-formyl) -4-

methylimidazolidine (I-20). Yield 64%; white solid; mp 226.7–227.5 °C. IR (KBr, cm^{-1}) ν : 3061–2857 (C–H), 1638 (C=O), 1594–1560 (C=C), 1241 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 7.46–7.12 (m, 6H, Ph–H), 4.96–4.74 (d, $J = 169.0$ Hz, 3H, N–CH– CH_2 –N), 3.40–3.17 (m, 2H, N– CH_2 –N), 2.59 (d, $J = 8.0$ Hz, 6H, 2 CH_3), 1.09 (d, $J = 4.4$ Hz, 3H, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.21, 170.21, 161.92, 161.92, 159.41, 159.41, 153.87, 153.87, 134.80, 134.80, 134.80, 134.80, 132.17, 132.17, 125.91, 125.91, 116.60, 116.60, 114.76, 114.76, 60.09, 51.02, 51.02, 18.05, 12.46, 12.46; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{26}\text{H}_{20}\text{Cl}_2\text{F}_2\text{N}_4\text{O}_4]$: 561.0908, found 561.0905.

Data for 1,3-dis (5,6-dichloronicotinoyl) -4-methylimidazolidine (I-21). Yield 48%; white solid; mp 164.9–166.8 °C. IR (KBr, cm^{-1}) ν : 3051–2851 (C–H), 1640 (C=O), 1243 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 8.61–8.34 (m, 4H, Ar–H), 5.24–4.96 (m, 2H, N– CH_2 –N), 4.62 (m, 1H, N–CH–C), 4.96–3.47 (m, 2H, C– CH_2 –N), 1.23 (s, 3H, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ : 163.19, 163.19, 149.11, 149.11, 146.38, 146.38, 138.29, 138.29, 132.12, 132.12, 129.34, 129.34, 60.89, 51.75, 51.75, 17.99; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{16}\text{H}_{12}\text{Cl}_4\text{N}_4\text{O}_2]$: 432.9793, found 432.9787.

Data for 1,3-dis (5-methylisoxazole-3-formyl) hexahydropyrimidine (II-1). Yield 60%; white solid; mp 133.5–134.2 °C. IR (KBr, cm^{-1}) ν : 3050–2851 (C–H), 1637 (C=O), 1260 (C–N); ^1H NMR (400 MHz, CDCl_3) δ : 8.69 (t, $J = 6.0$ Hz, 2H, Ar–H), 6.51 (s, 2H, N– CH_2 –N), 3.32–3.25 (d, $J = 8.0$ Hz, 4H, 2N– CH_2 –C), 2.50–2.46 (s, 6H, 2 CH_3), 1.72 (m, 2H, C– CH_2 –C); ^{13}C NMR (100 MHz, CDCl_3) δ : 171.59, 171.59, 159.44, 159.44, 159.17, 159.17, 101.74, 101.74, 40.66, 40.66, 36.90, 29.21, 12.31, 12.31; ESI-HRMS: m/z $[\text{M}+\text{H}]^+$ calcd. For $[\text{C}_{14}\text{H}_{16}\text{N}_4\text{O}_4]$: 305.1250, found 305.1248.

Data for 1,3-dis (5-methyl-3-phenylisoxazole-4-formyl) hexahydropyrimidine (II-2). Yield 63%; white solid; IR (KBr, cm^{-1}) ν : 3058–2874 (C–H), 1650 (C=O), 1491 (C=C), 1281 (C–N); ^1H

NMR (400 MHz, CDCl₃) δ : 7.70–7.46 (m, 10H, Ph–H), 4.27–4.25 (m, 2H, N–CH₂–N), 3.17–3.02 (m, 4H, 2N–CH₂–C), 2.56–2.38 (d, J = 73.6 Hz, 6H, 2CH₃), 1.28 (s, 2H, C–CH₂–C); ¹³C NMR (100 MHz, CDCl₃) δ : 170.52, 170.52, 162.53, 162.53, 159.94, 159.94, 130.43, 130.43, 130.43, 130.43, 130.43, 130.43, 129.00, 129.00, 129.00, 129.00, 127.82, 127.82, 110.32, 110.32, 68.88, 46.57, 46.57, 25.26, 11.75, 11.75; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₂₆H₂₄N₄O₄]: 457.1876, found 457.1869.

Data for 1,3-dis (3- (2,6-dichlorophenyl) -5-methylisoxazole-4-formyl) hexahydropyrimidine (II-3). Yield 79%; white solid; IR (KBr, cm⁻¹) ν : 3036–2847 (C–H), 1631 (C=O), 1420 (C=C), 1280 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 7.44–7.35 (m, 6H, Ph–H), 4.93 (s, 2H, N–CH₂–N), 3.51 (s, 4H, 2N–CH₂–C), 2.49 (s, 6H, 2CH₃), 1.44 (s, 2H, C–CH₂–C); ¹³C NMR (100 MHz, CDCl₃) δ : 164.35, 164.35, 161.24, 161.24, 157.43, 157.43, 135.80, 135.80, 135.80, 135.80, 131.99, 131.99, 128.53, 128.53, 128.53, 128.53, 127.24, 127.24, 111.95, 111.95, 53.72, 35.52, 35.52, 29.19, 13.13, 13.13; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₂₆H₂₀Cl₄N₄O₄]: 593.0317, found 593.0316.

Data for 1,3-dis (3- (2-chloro-6-fluorophenyl) -5-methylisoxazole-4-formyl) hexahydropyrimidine (II-4). Yield 82%; white solid; IR (KBr, cm⁻¹) ν : 3062–2852 (C–H), 1664 (C=O), 1450–1428 (C=C), 1243 (C–N); ¹H NMR (400 MHz, CDCl₃) δ : 7.67–7.41 (m, 6H, Ph–H), 4.96–4.92 (s, 2H, N–CH₂–N), 3.54 (s, 4H, 2N–CH₂–C), 2.34–2.26 (s, 6H, 2CH₃), 1.45 (s, 2H, C–CH₂–C); ¹³C NMR (100 MHz, CDCl₃) δ : 167.08, 167.08, 161.76, 161.76, 160.74, 160.74, 159.27, 159.27, 159.27, 159.27, 133.59, 133.59, 133.59, 133.59, 126.36, 126.36, 115.57, 115.57, 97.00, 97.00, 74.51, 64.55, 64.55, 40.61, 25.49, 25.49; ESI-HRMS: m/z [M+H]⁺ calcd. For [C₂₆H₂₀Cl₂F₂N₄O₄]: 561.0908, found 561.0894.

Data for 1,3-dis (4,6-dichloronicotinoyl) hexahydropyrimidine (II-5). Yield 71%; white solid; mp 150.4–150.8 °C. IR (KBr, cm⁻¹) ν : 3057–2825 (C–H), 1630 (C=O), 1567–1437 (C=C), 1277

(C–N); ¹H NMR (400 MHz, CDCl₃) δ: 8.63–7.44 (m, 4H, Ar–H), 3.61–3.60 (q, 2H, N–CH₂–N), 1.91 (m, 4H, 2N–CH₂–C), 1.26 (s, 2H, C–CH₂–C); ¹³C NMR (100 MHz, CDCl₃) δ: 165.29, 165.29, 155.73, 155.73, 149.36, 149.36, 148.05, 148.05, 128.84, 128.84, 122.10, 122.10, 65.47 43.18, 43.18, 20.83; ESI-HRMS: *m/z* [M+H]⁺ calcd. For [C₁₆H₁₂Cl₄N₄O₂]: 432.9793, found 432.9784.

Data for 1,3-dis (5,6-dichloronicotinoyl) hexahydropyrimidine (II-6). Yield 65%; white solid; mp 144.8–145.1 °C. IR (KBr, cm⁻¹) ν: 3050–2849 (C–H), 1639 (C=O), 1446 (C=C), 1258 (C–N); ¹H NMR (400 MHz, CDCl₃) δ: 8.78–8.07 (m, 4H, Ar–H), 5.00–4.94 (d, *J* = 147.9 Hz, 2H, N–CH₂–C), 3.80–3.55 (d, *J* = 103.7 Hz, 4H, 2N–CH₂–C), 1.72 (s, 2H, C–CH₂–C); ¹³C NMR (100 MHz, CDCl₃) δ: 164.80, 164.80, 146.40, 146.40, 138.57, 138.57, 132.40, 132.40, 129.76, 129.76, 129.66, 129.66, 78.24, 42.09, 42.09, 25.32; ESI-HRMS: *m/z* [M+H]⁺ calcd. For [C₁₆H₁₂Cl₄N₄O₂]: 432.9793, found 432.9786.

Data for 1,3-dis (3- (2,6-dichlorophenyl) -5-methylisoxazole-4-formyl) -5,5-dimethylhexahydropyrimidine (II-7). Yield 76%; white solid; IR (KBr, cm⁻¹) ν: 3053–2843 (C–H), 1624 (C=O), 1549–1420 (C=C), 1287 (C–N); ¹H NMR (400 MHz, CDCl₃) δ: 7.41–7.32 (m, 6H, Ph–H), 4.82–4.79 (s, 2H, N–CH₂–N), 3.25–2.89 (m, 4H, 2N–CH₂–C), 2.56 (s, 6H, 2CH₃), 0.81 (s, 6H, 2CH₃); ¹³C NMR (100 MHz, CDCl₃) δ: 162.26, 162.26, 162.20, 162.20, 162.15, 162.15, 135.73, 135.73, 135.73, 135.73, 131.54, 131.54, 131.54, 131.54, 128.29, 128.29, 127.19, 127.19, 112.51, 112.51, 77.30, 53.49, 53.49, 34.24, 23.12, 23.12, 12.34, 12.34; ESI-HRMS: *m/z* [M+H]⁺ calcd. For [C₂₈H₂₄Cl₄N₄O₄]: 621.0630, found 621.0628.

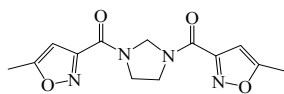
Data for 1,3-dis (3- (2-chloro-6-fluorophenyl) -5-methylisoxazole-4-formyl) -5,5-dimethylhexahydropyrimidine (II-8). Yield 80%; white solid; IR (KBr, cm⁻¹) ν: 3041–2846 (C–H), 1642 (C=O), 1426 (C=C), 1229 (C–N); ¹H NMR (400 MHz, CDCl₃) δ: 7.46–7.10 (m, 6H, Ph–H),

4.78–4.74 (s, 2H, N–CH₂–N), 3.30–2.88 (s, 4H, 2N–CH₂–C), 2.54 (s, 6H, 2CH₃), 0.82 (s, 6H, 2CH₃);
¹³C NMR (100 MHz, CDCl₃) δ: 162.00, 162.00, 159.49, 159.49, 153.92, 153.92, 135.25, 135.25,
132.00, 132.00, 132.00, 132.00, 125.76, 125.76, 116.82, 116.82, 116.64, 116.64, 114.48, 114.48,
114.26, 77.26, 77.26, 32.28, 23.08, 23.08, 12.16, 12.16; ESI-HRMS: *m/z* [M+H]⁺ calcd. For
[C₂₈H₂₄Cl₂F₂N₄O₄]: 589.1221, found 589.1218.

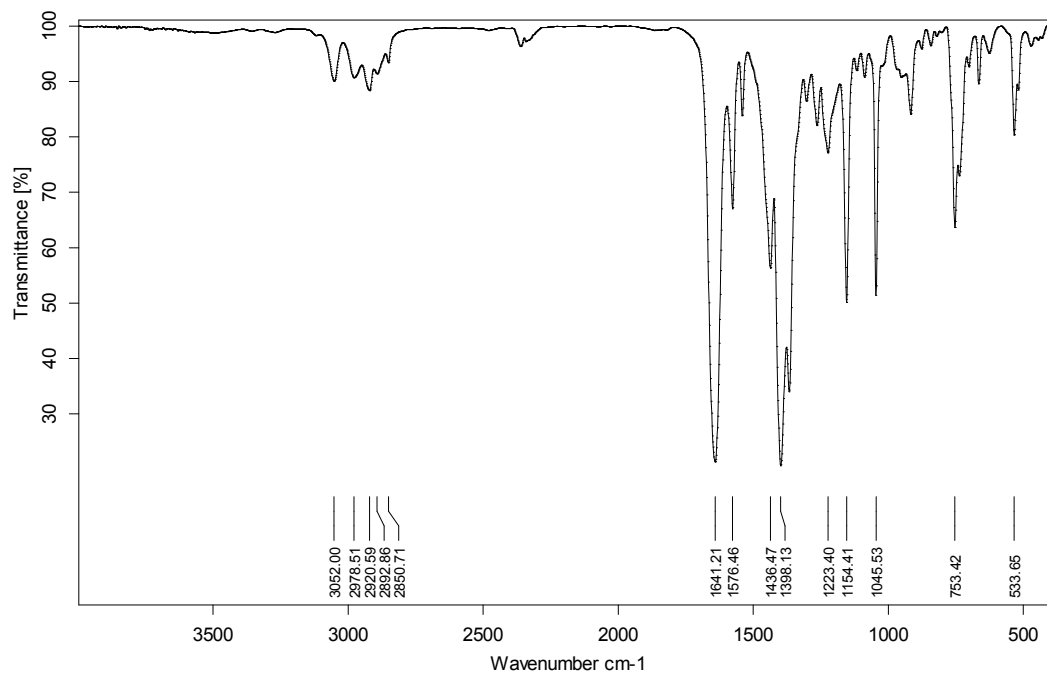
Data for 1,3-dis (6-chloronicotinoyl) -5,5-dimethylhexahydropyrimidine (II-9). Yield 64%;
white solid; mp 169.1–172.4 °C. IR (KBr, cm⁻¹) *v*: 3052–2857 (C–H), 1644 (C=O), 1427 (C=C),
1287 (C–N); ¹H NMR (400 MHz, CDCl₃) δ: 8.45–7.44 (m, 6H, Ar–H), 5.11 (s, 2H, N–CH₂–N),
3.33–3.62 (d, *J* = 119.6 Hz, 4H, 2N–CH₂–C), 0.94 (s, 6H, 2CH₃); ¹³C NMR (100 MHz, CDCl₃) δ:
167.26, 167.26, 154.83, 154.83, 150.44, 150.44, 141.52, 141.52, 125.46, 125.46, 119.30, 119.30,
68.90, 53.04, 53.04, 29.71, 17.63, 17.63; ESI-HRMS: *m/z* [M+H]⁺ calcd. For [C₁₈H₁₈Cl₂N₄O₂]:
393.0885, found 393.0877.

10 The spectrogram of compounds I-1~21 and II-1~9.

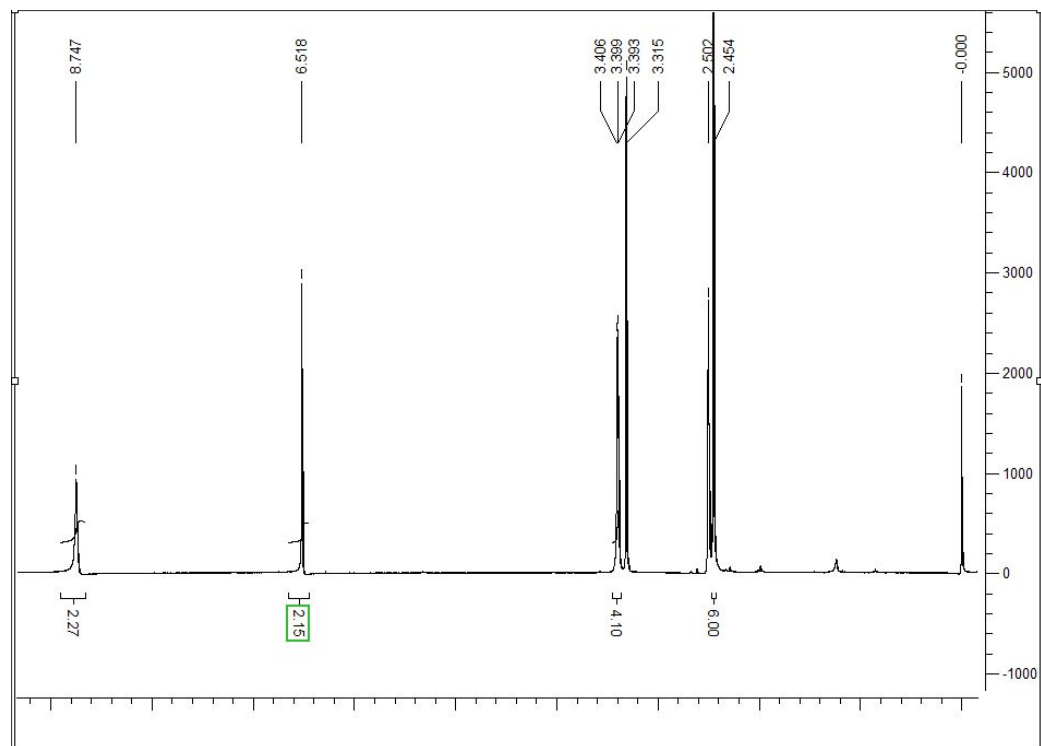
I-1



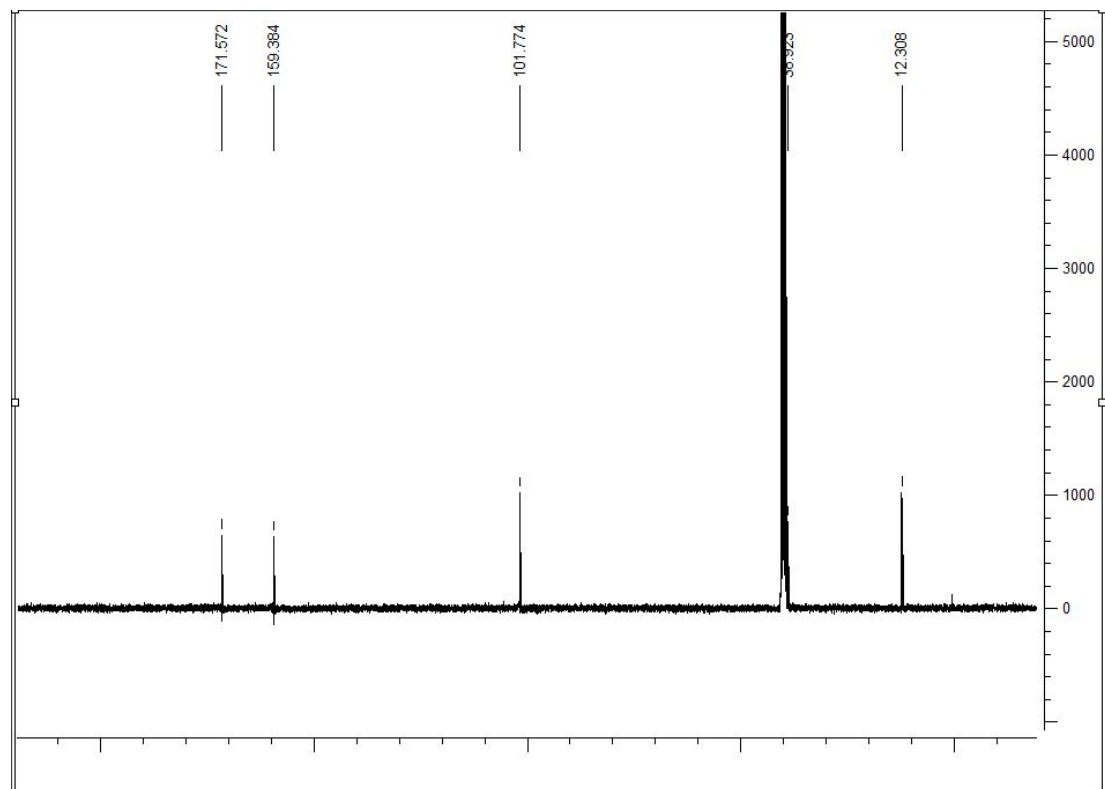
IR



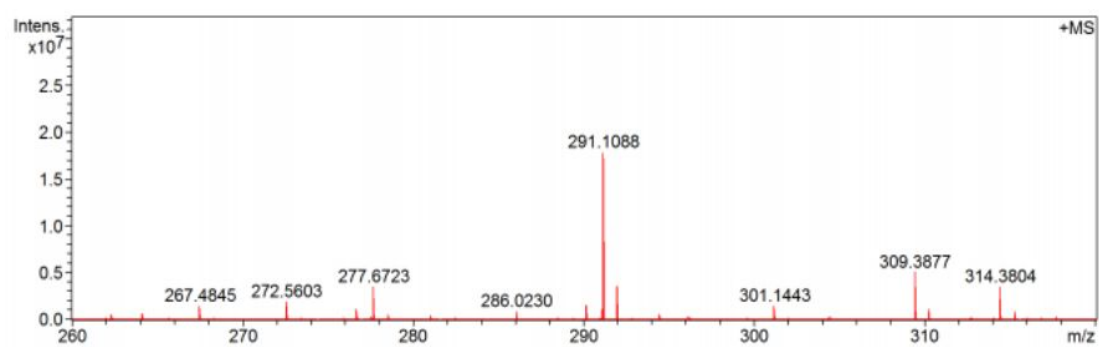
¹H NMR



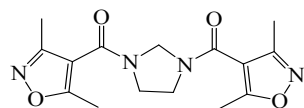
¹³C NHR



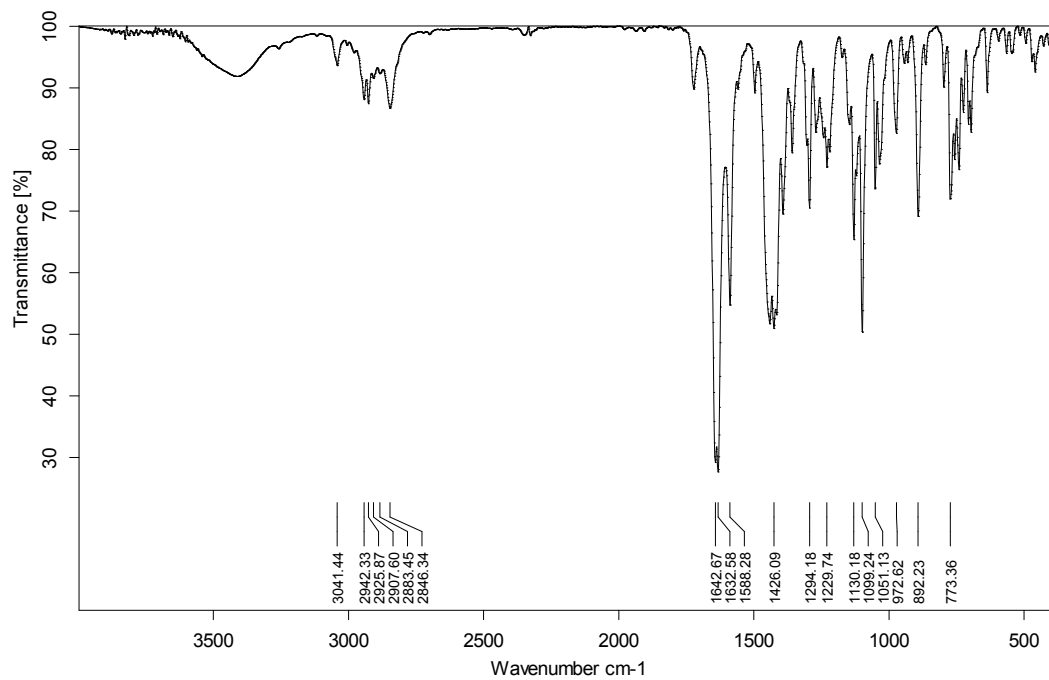
HRMS



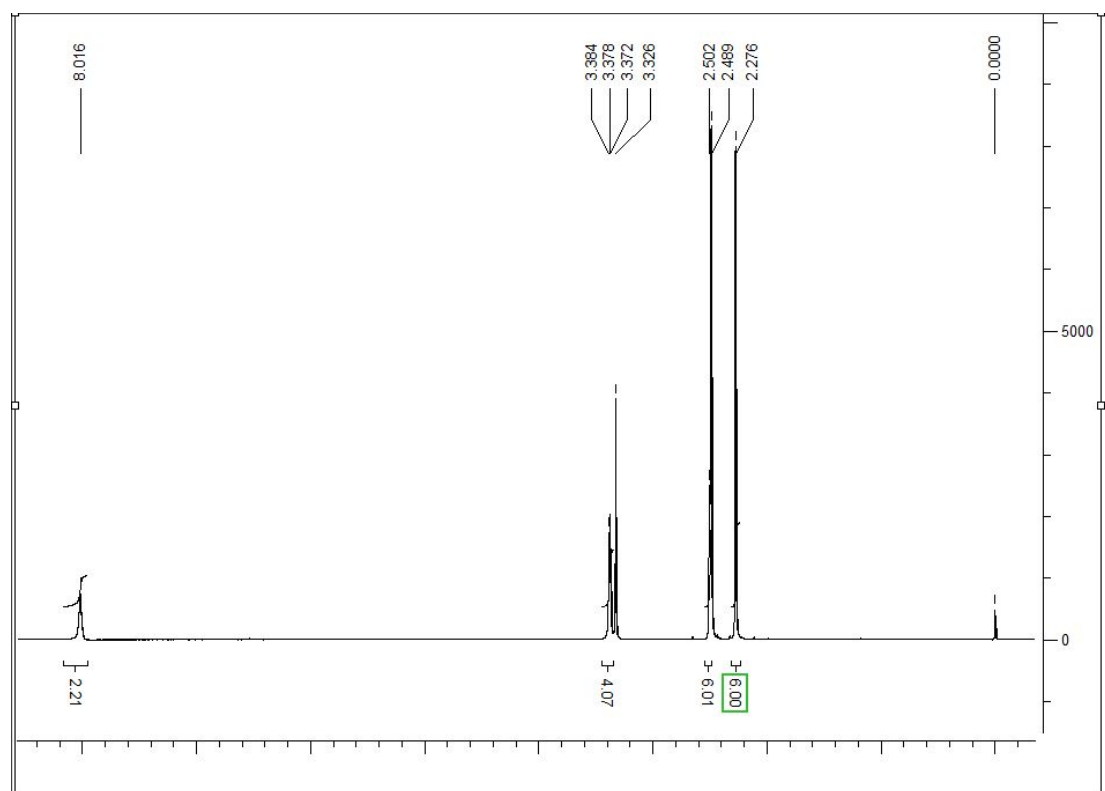
I-2



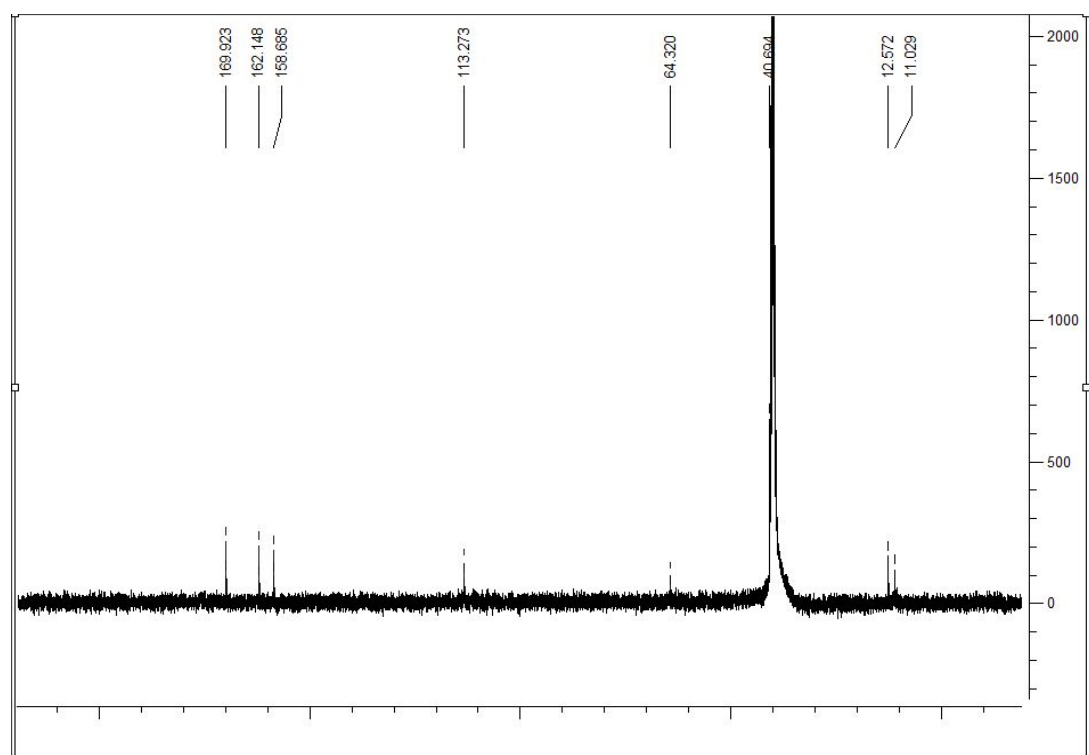
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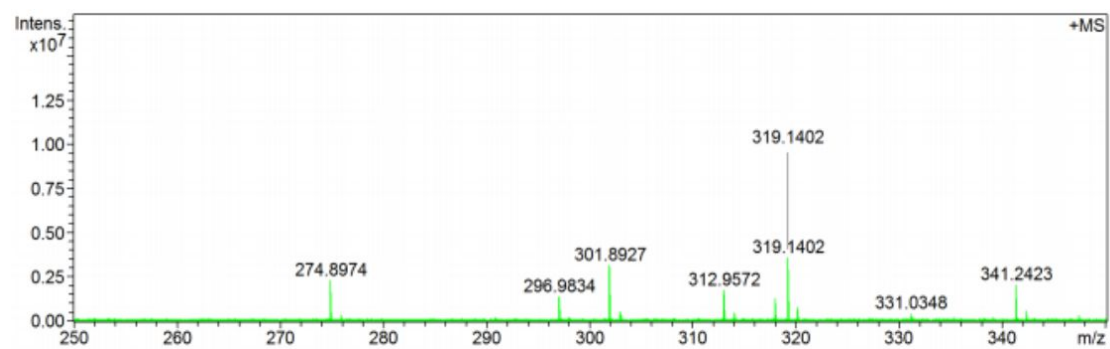
¹H NMR



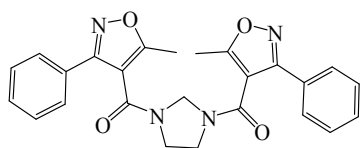
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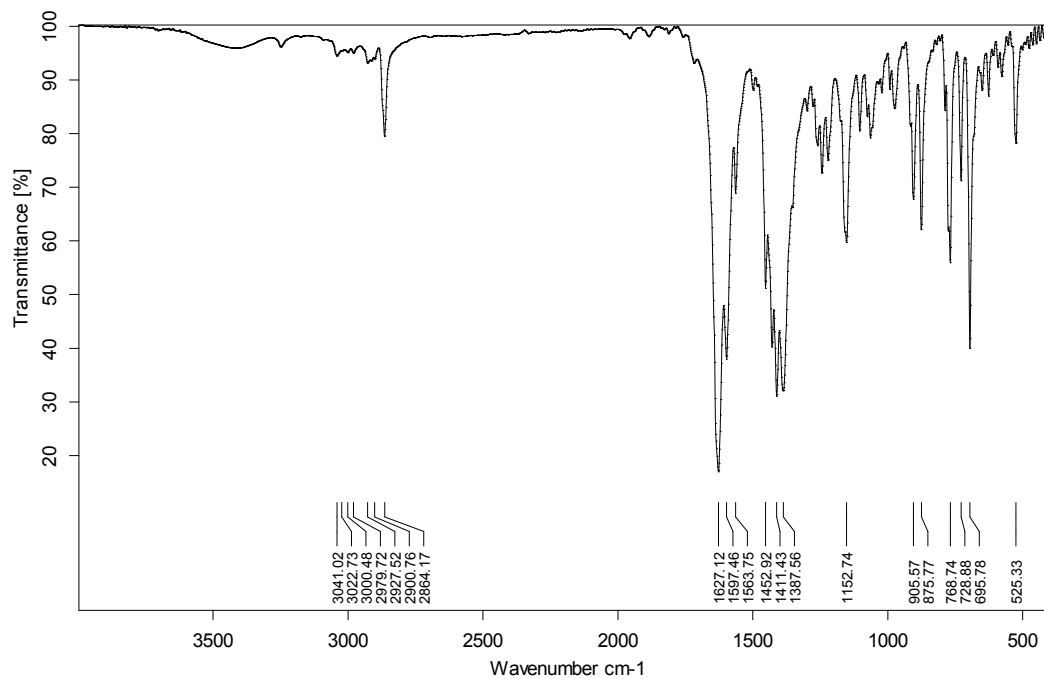
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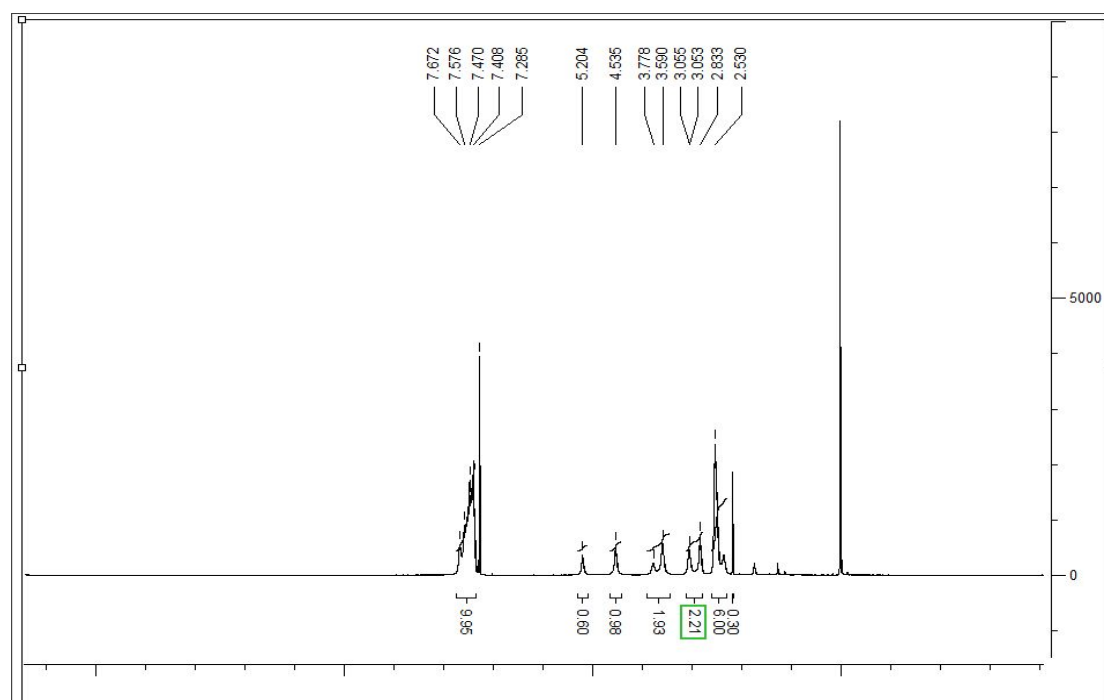
I-3



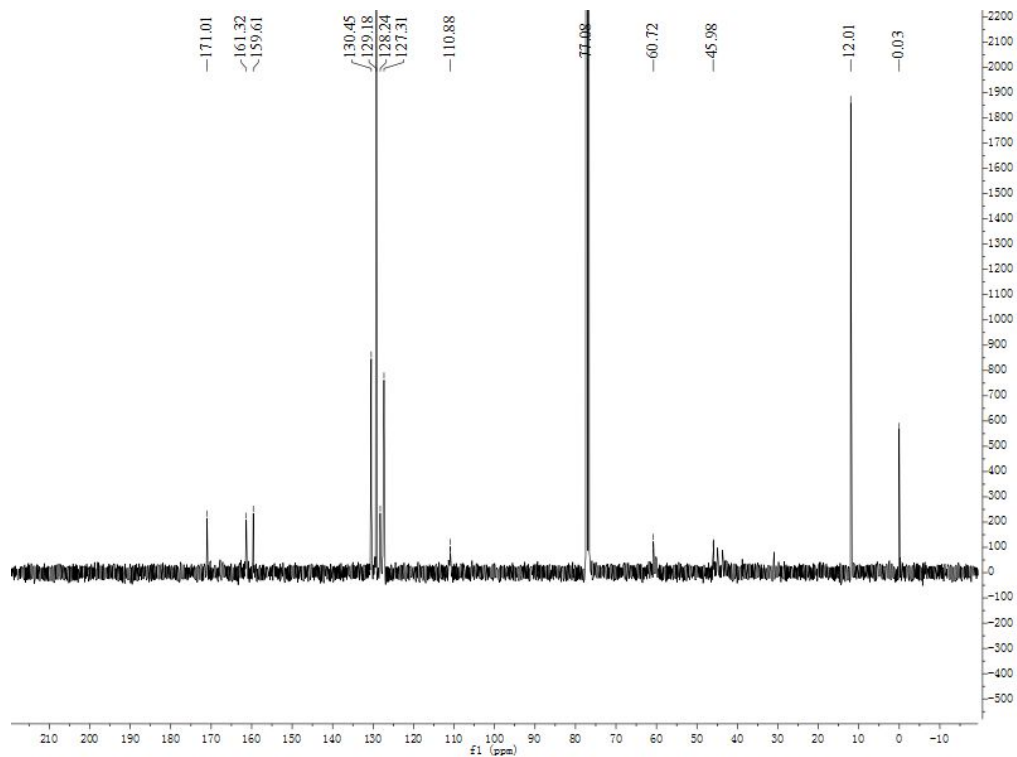
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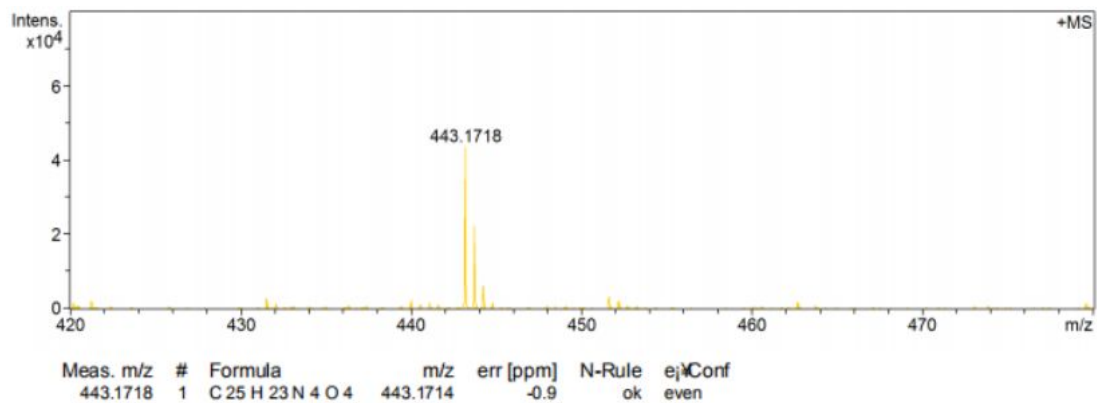
¹H NMR



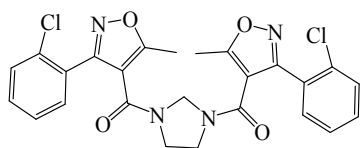
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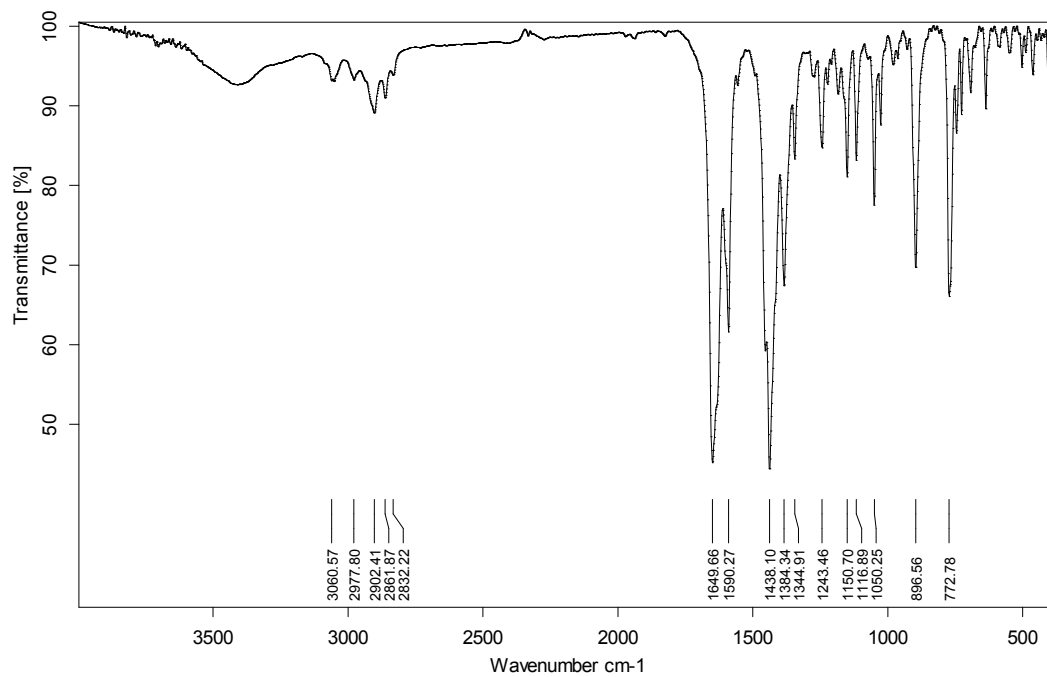
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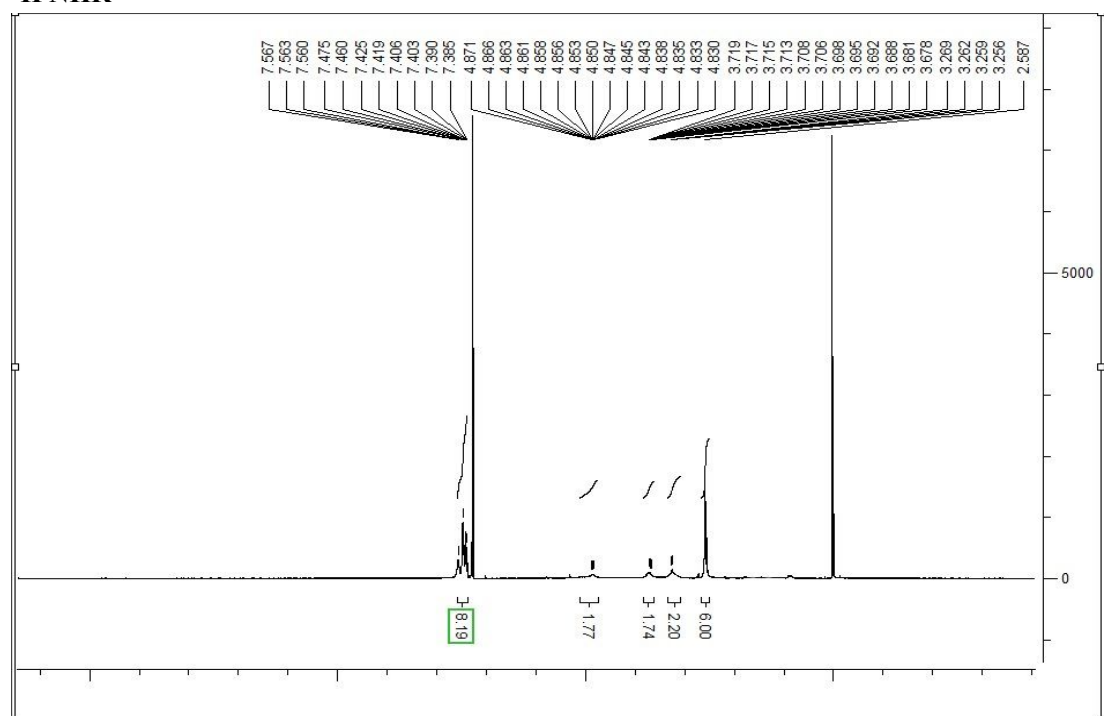
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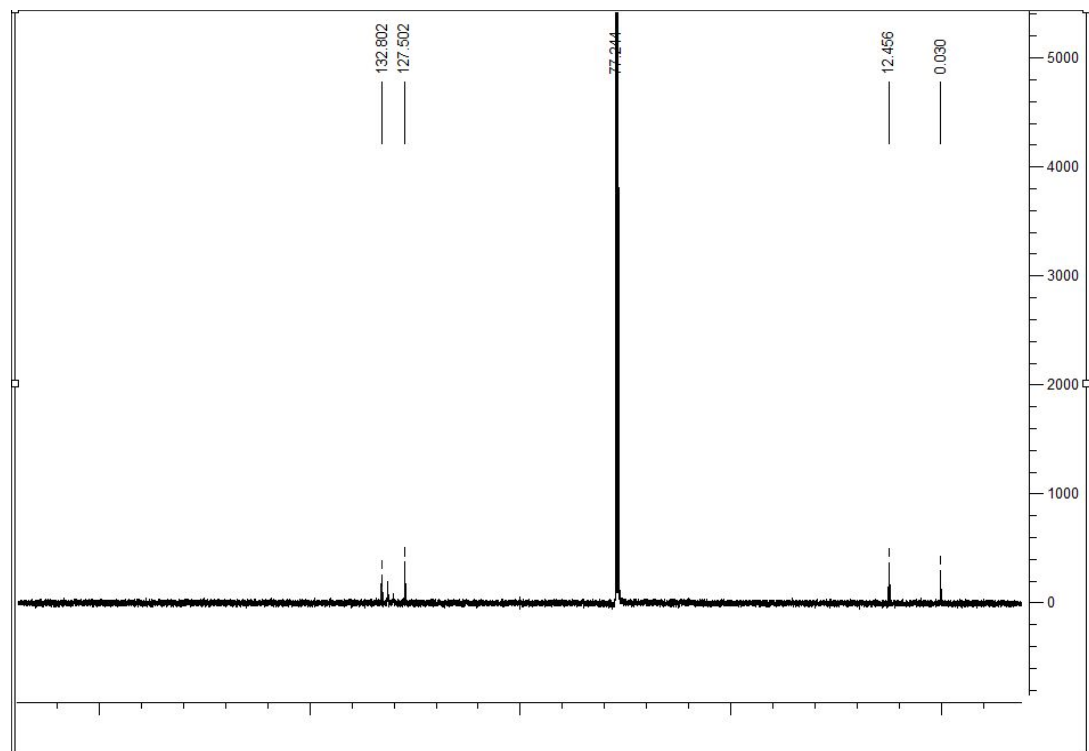
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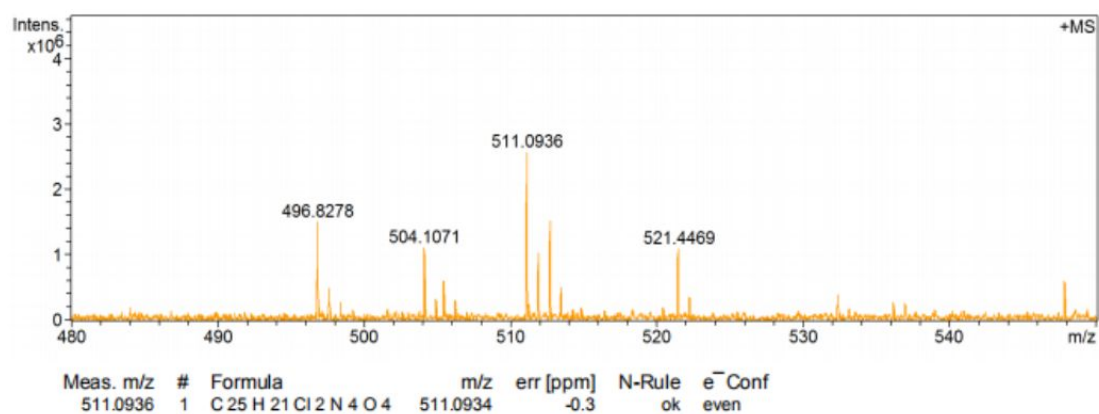
¹H NMR



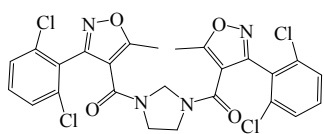
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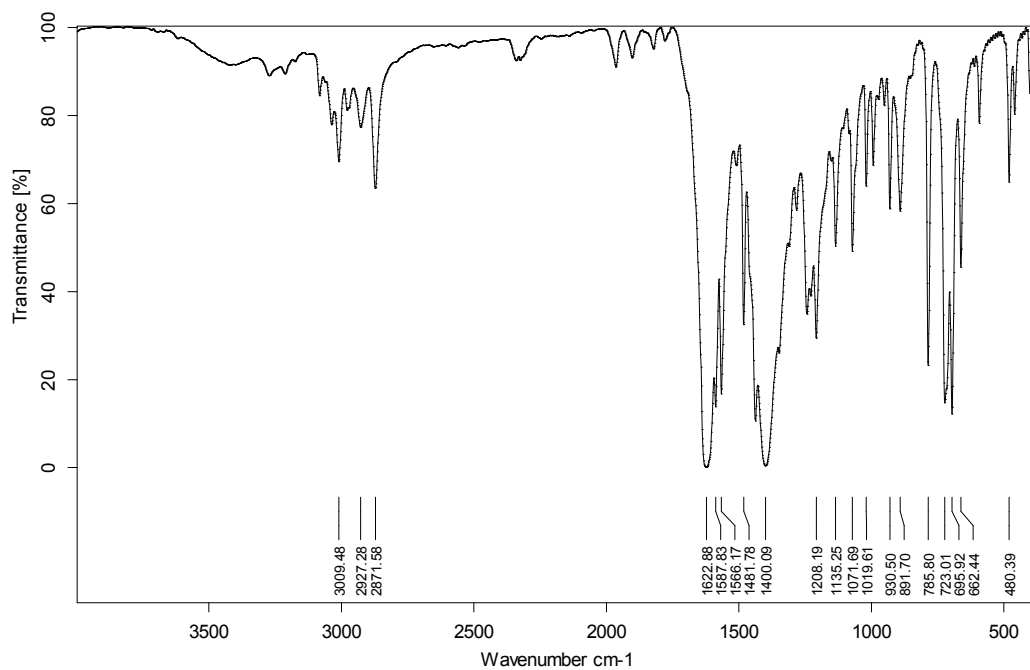
HRMS



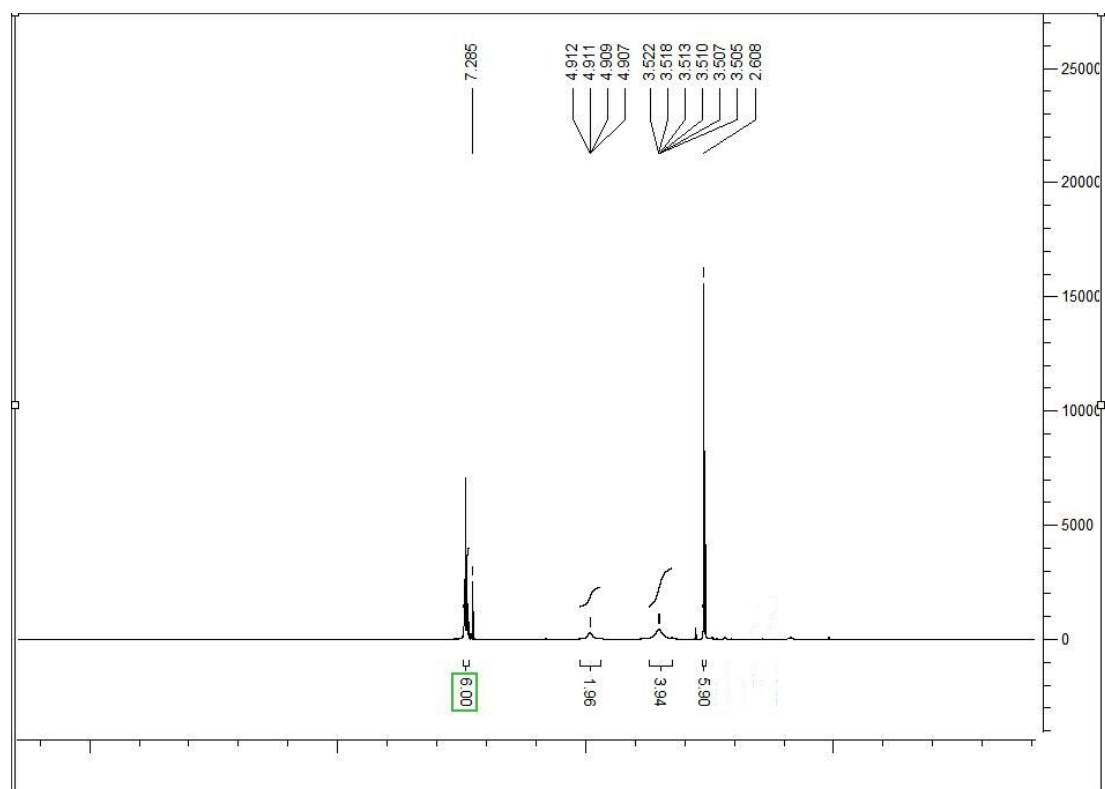
I-5



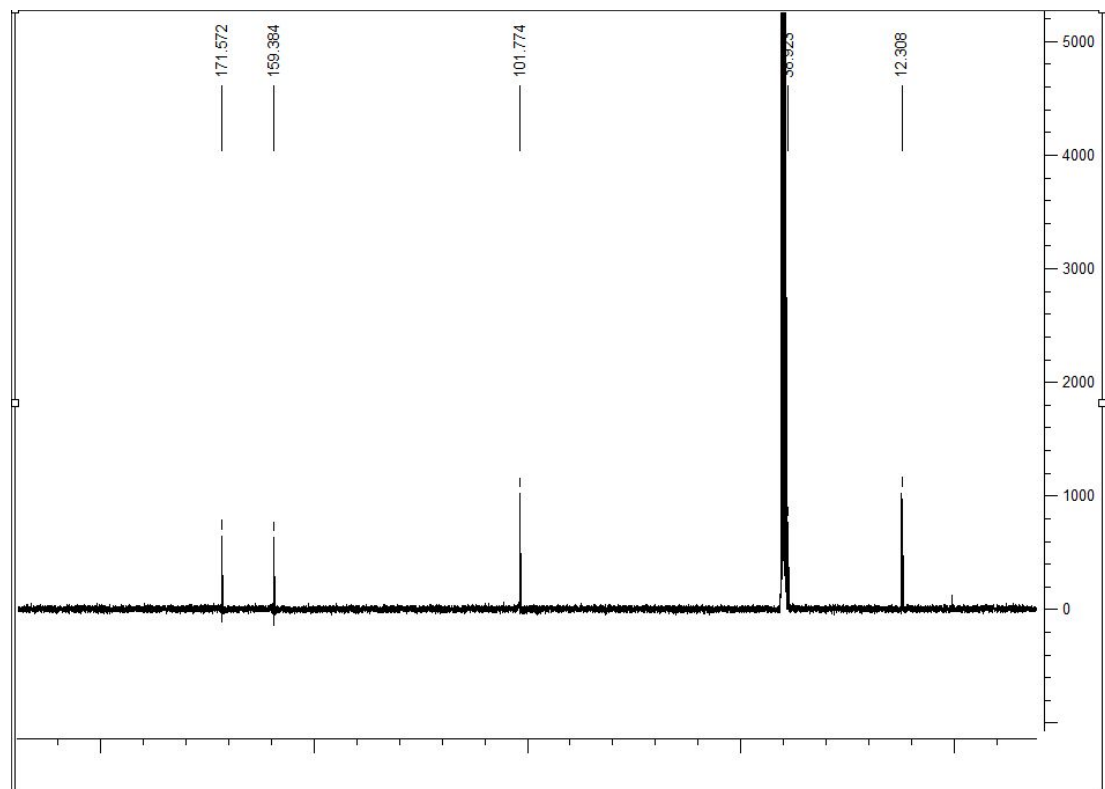
IR



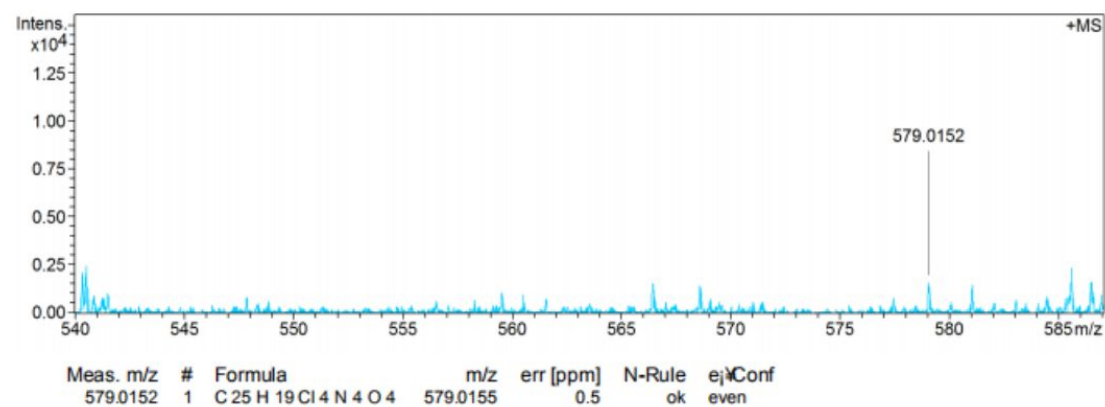
¹H NMR



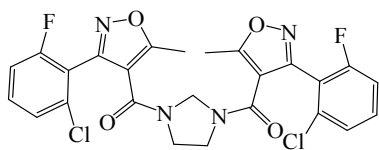
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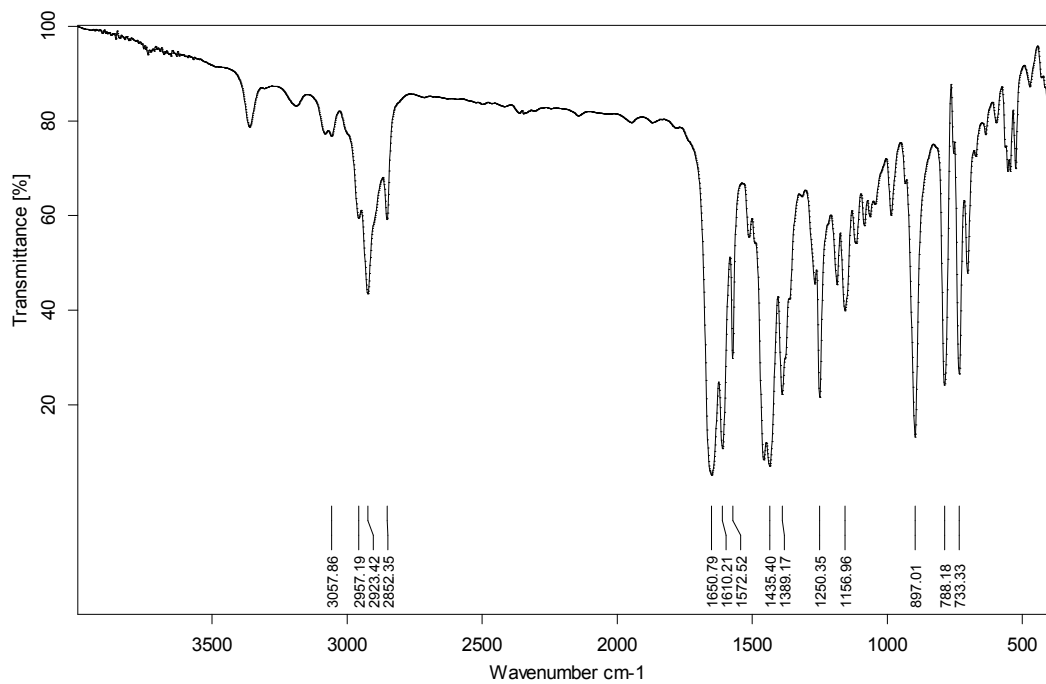
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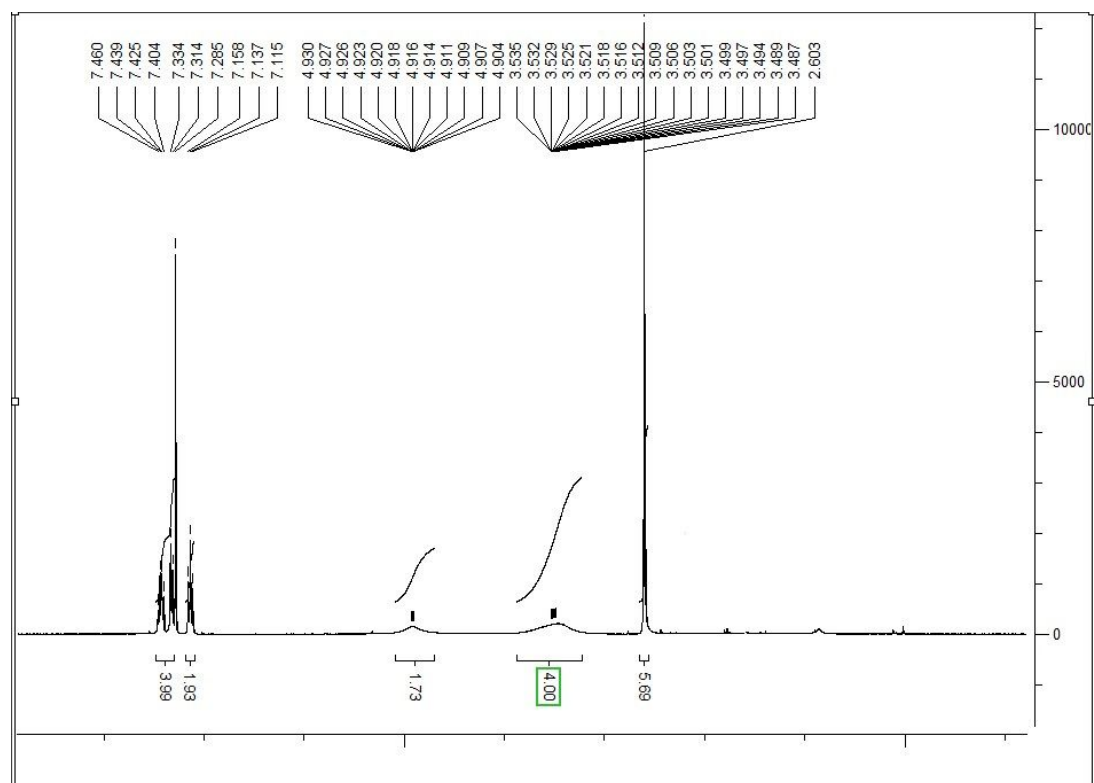
I-6



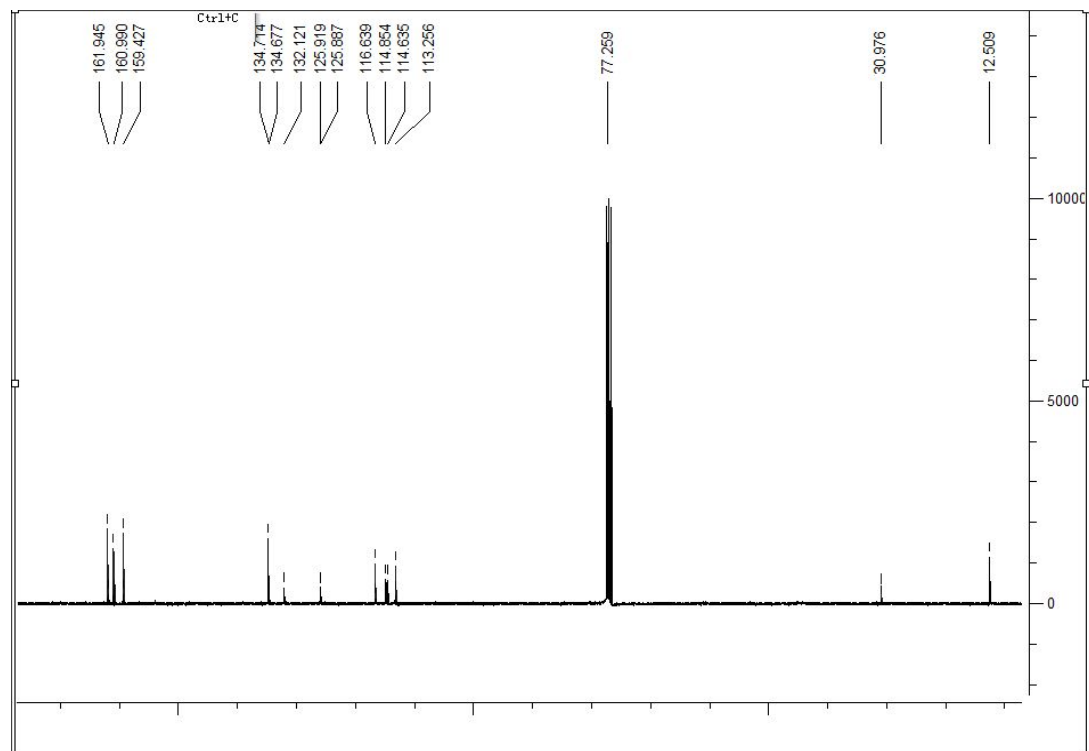
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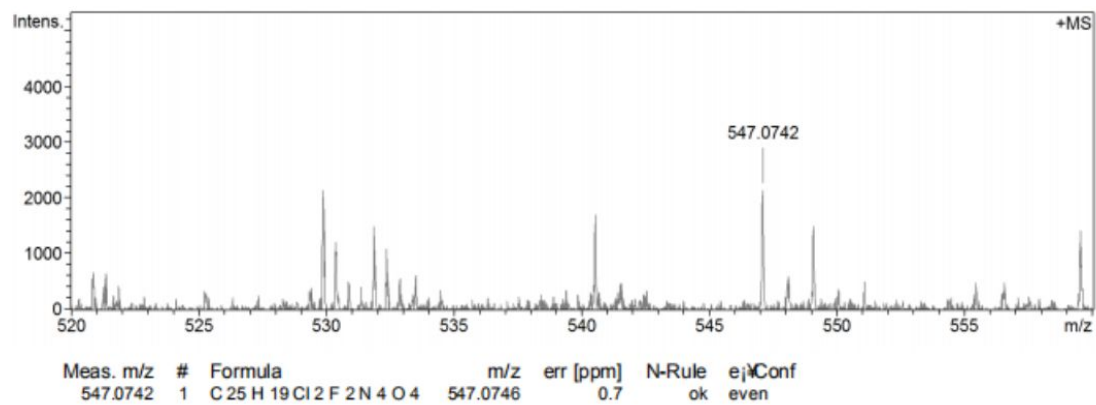
¹H NMR



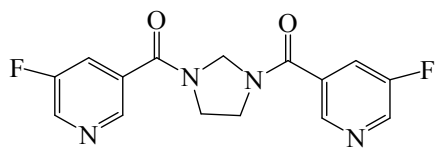
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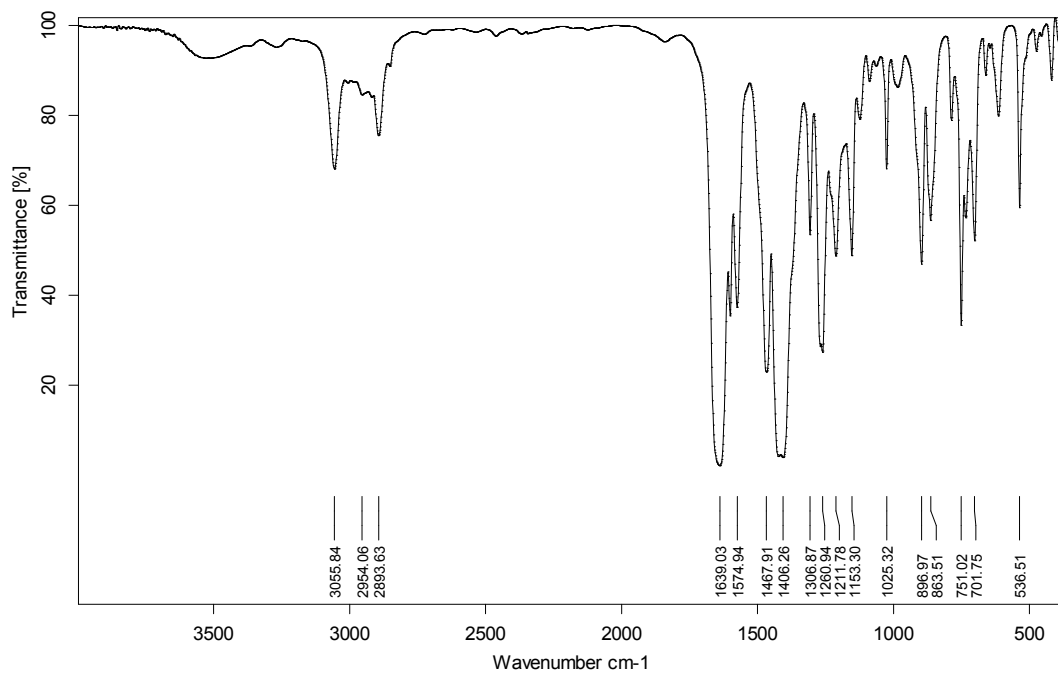
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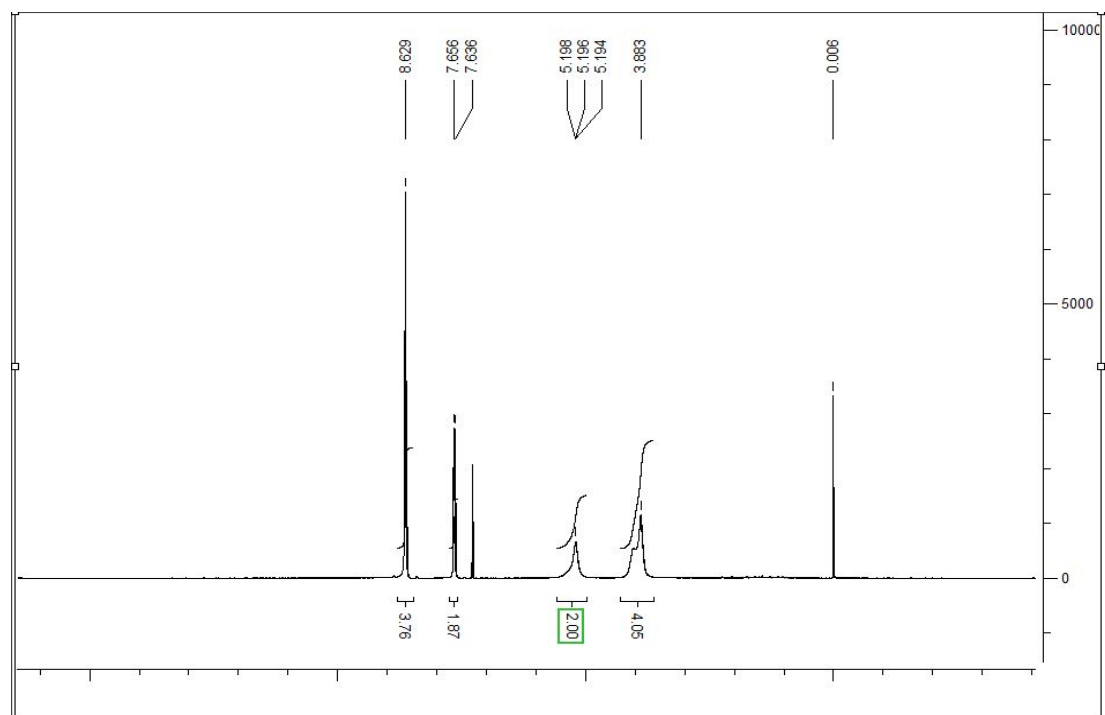
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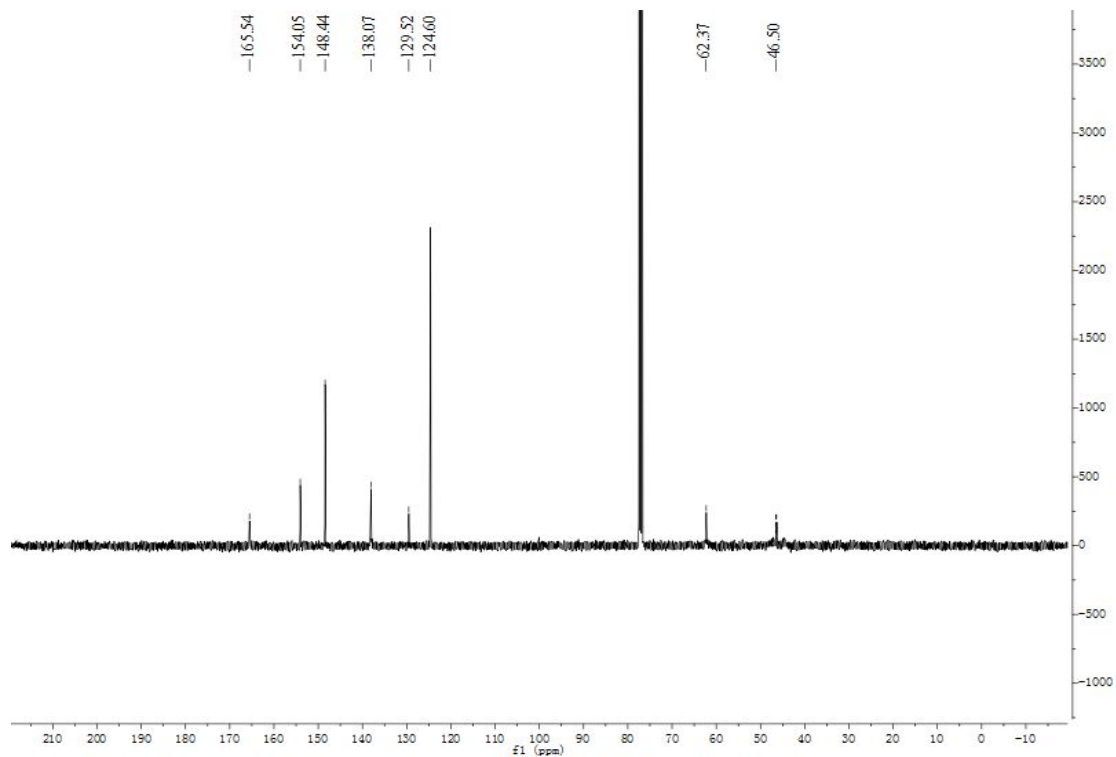
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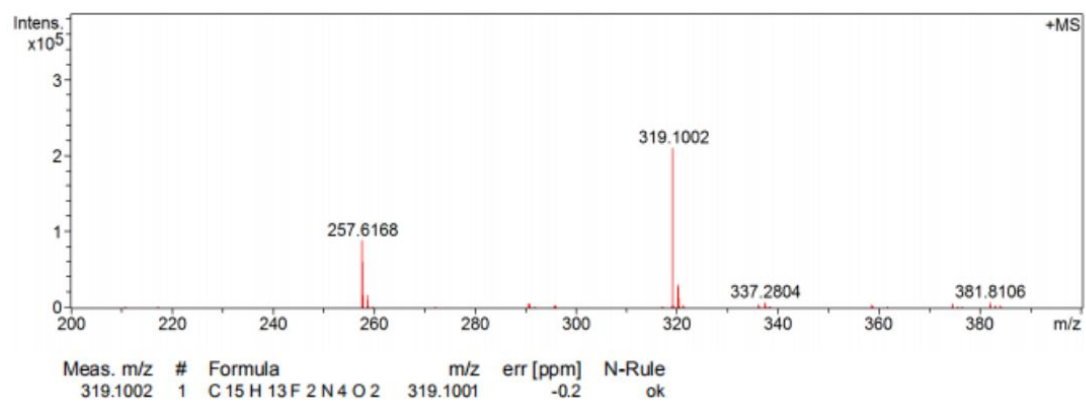
$^1\text{H NMR}$



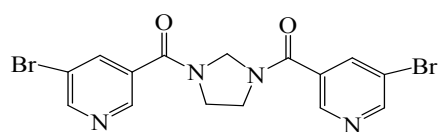
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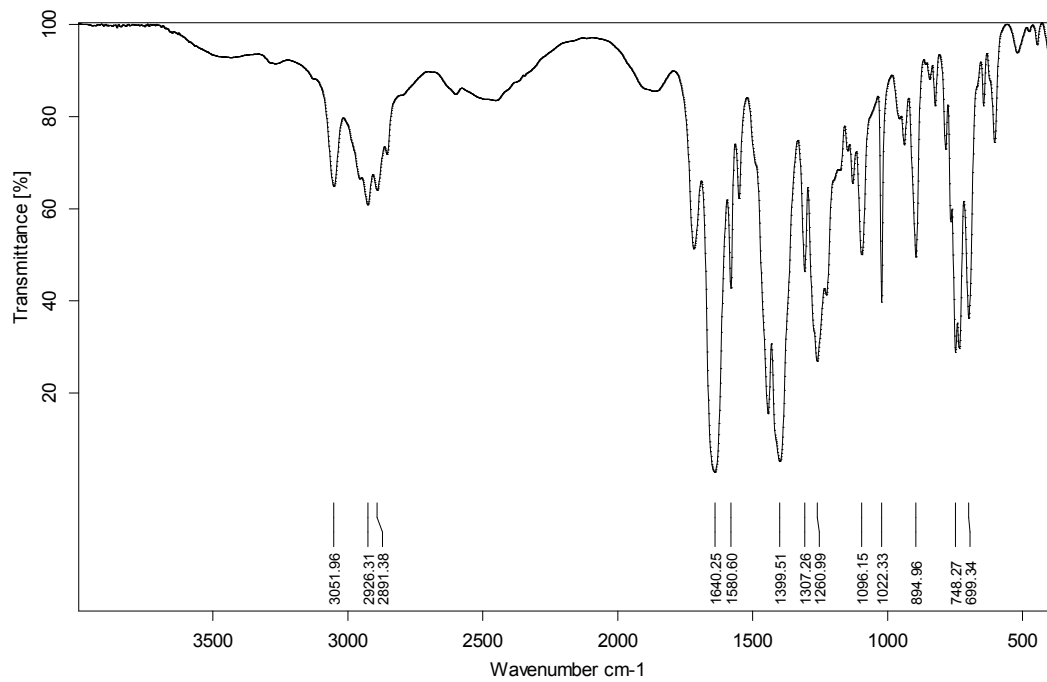
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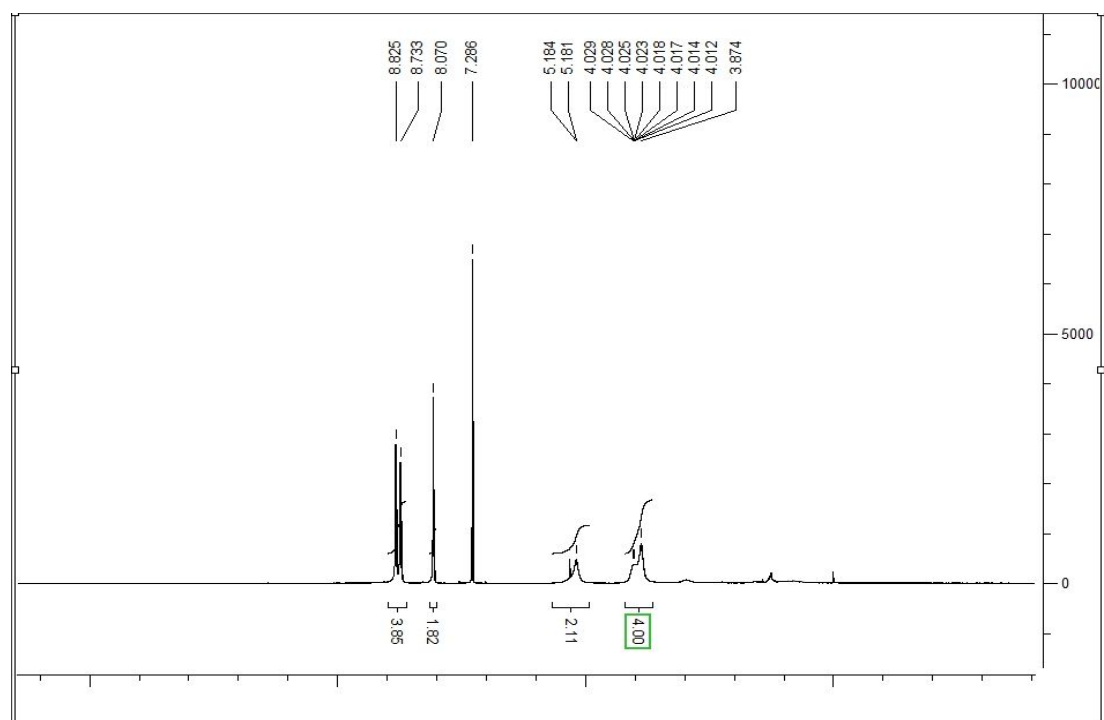
I-8



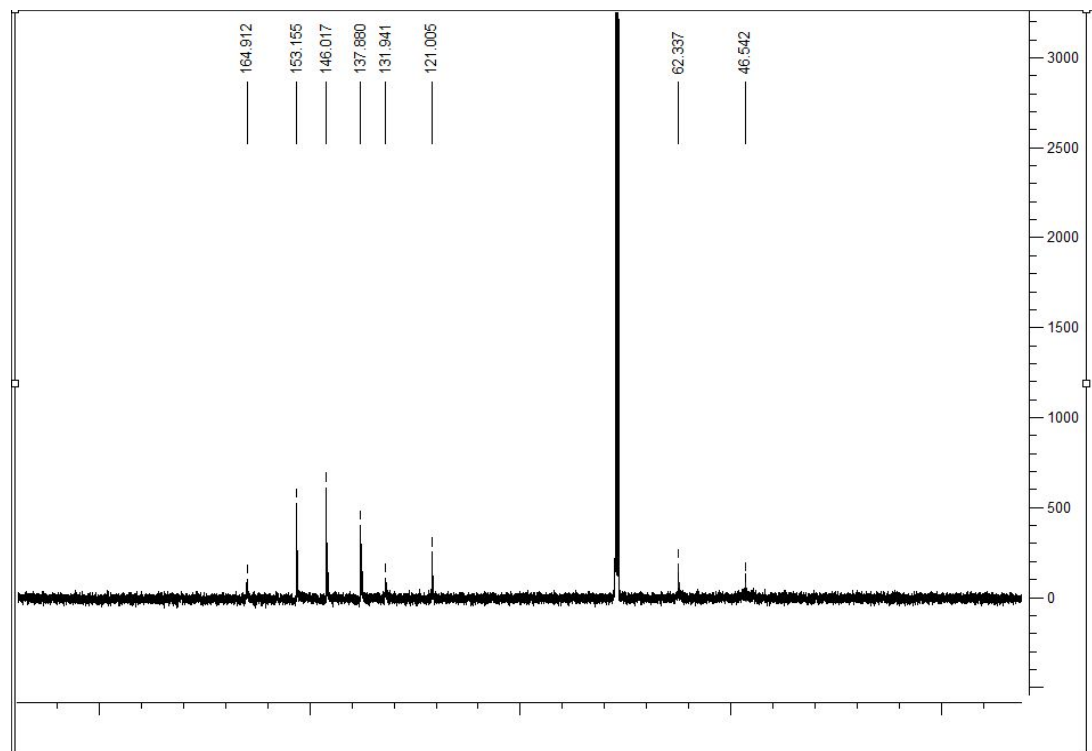
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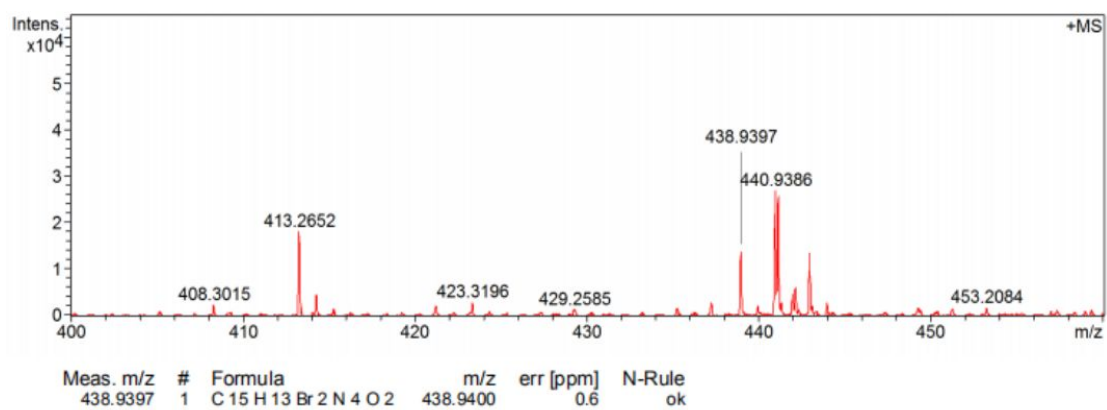
¹H NMR



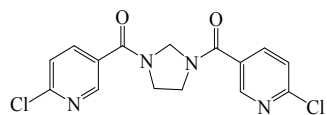
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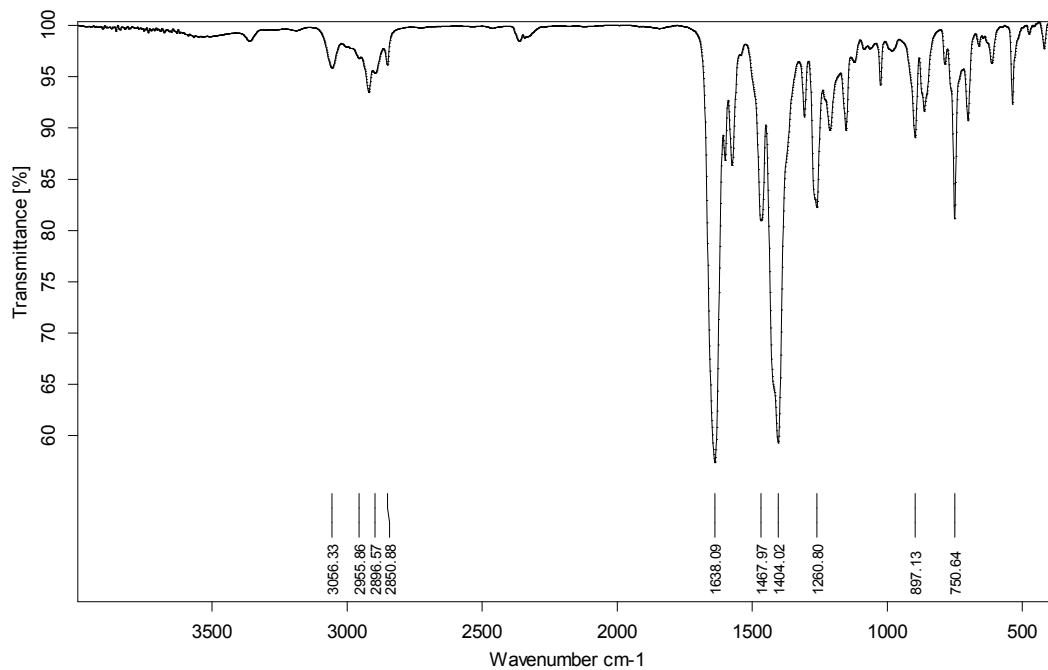
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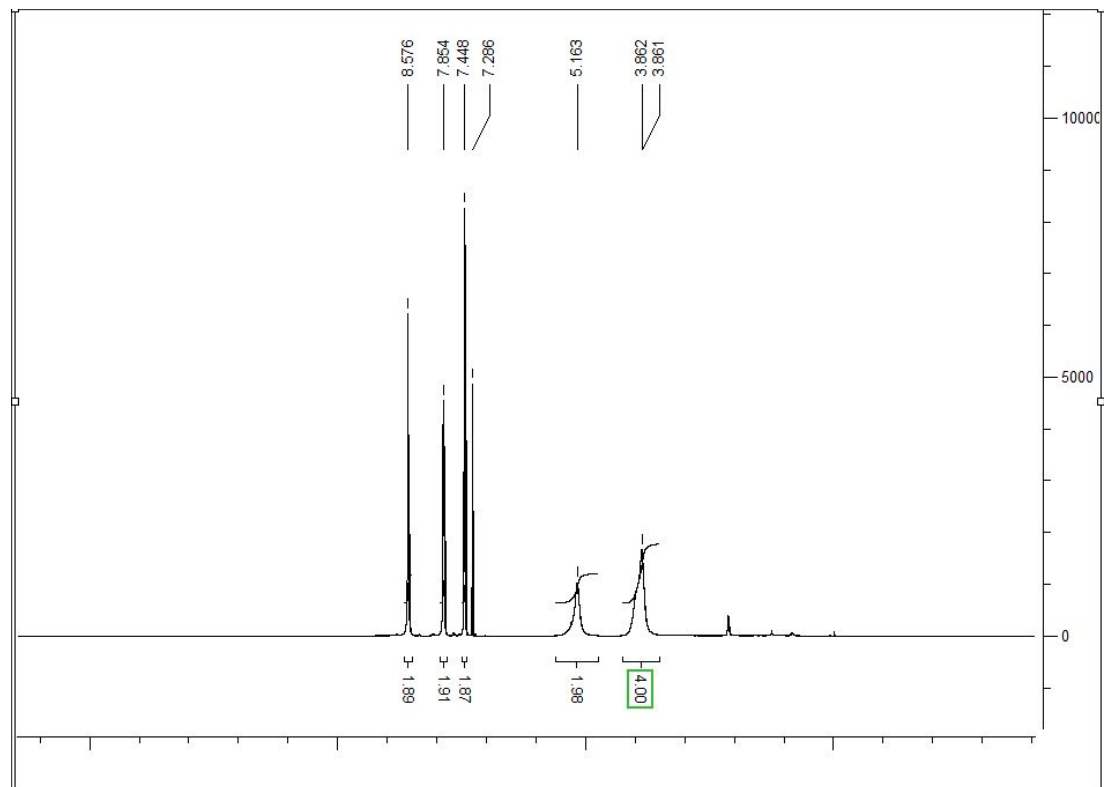
I-9



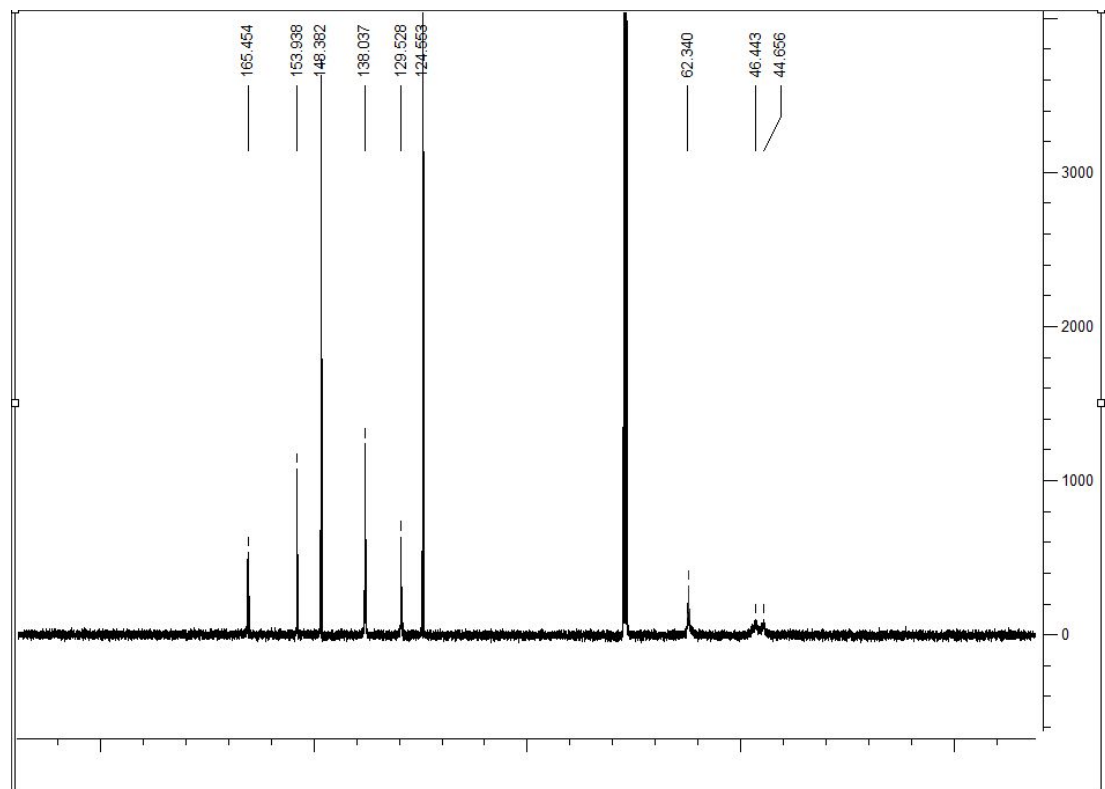
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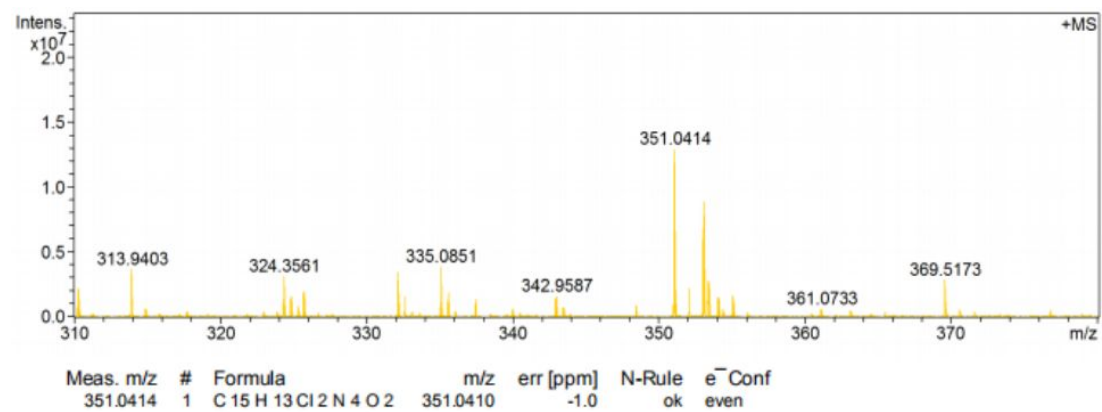
¹H NMR



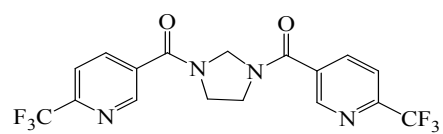
¹³C NHR



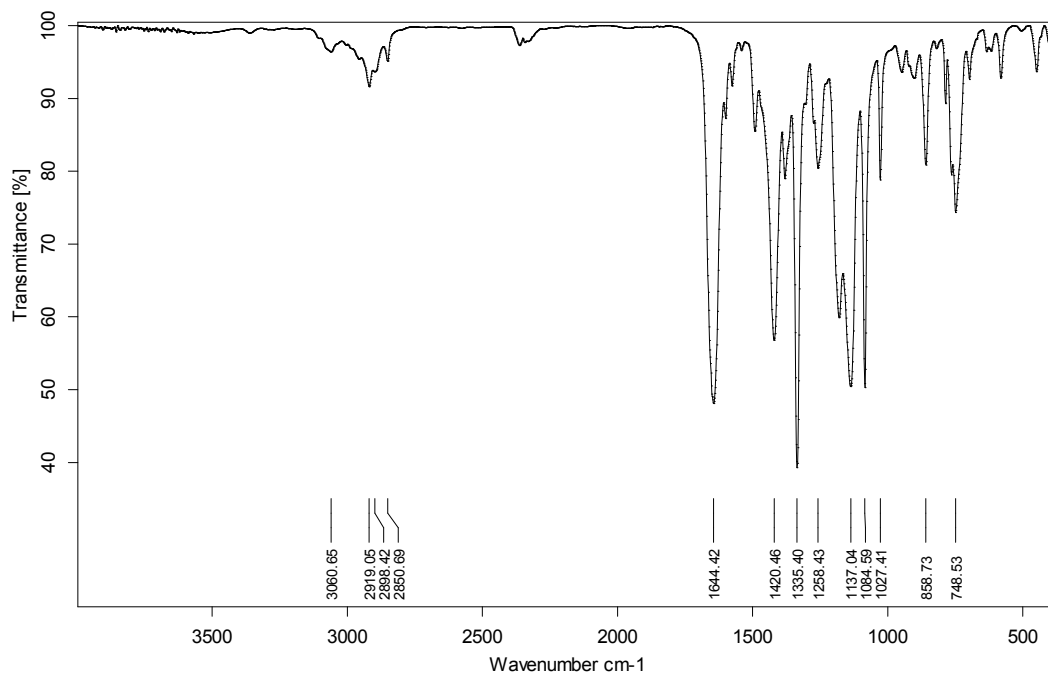
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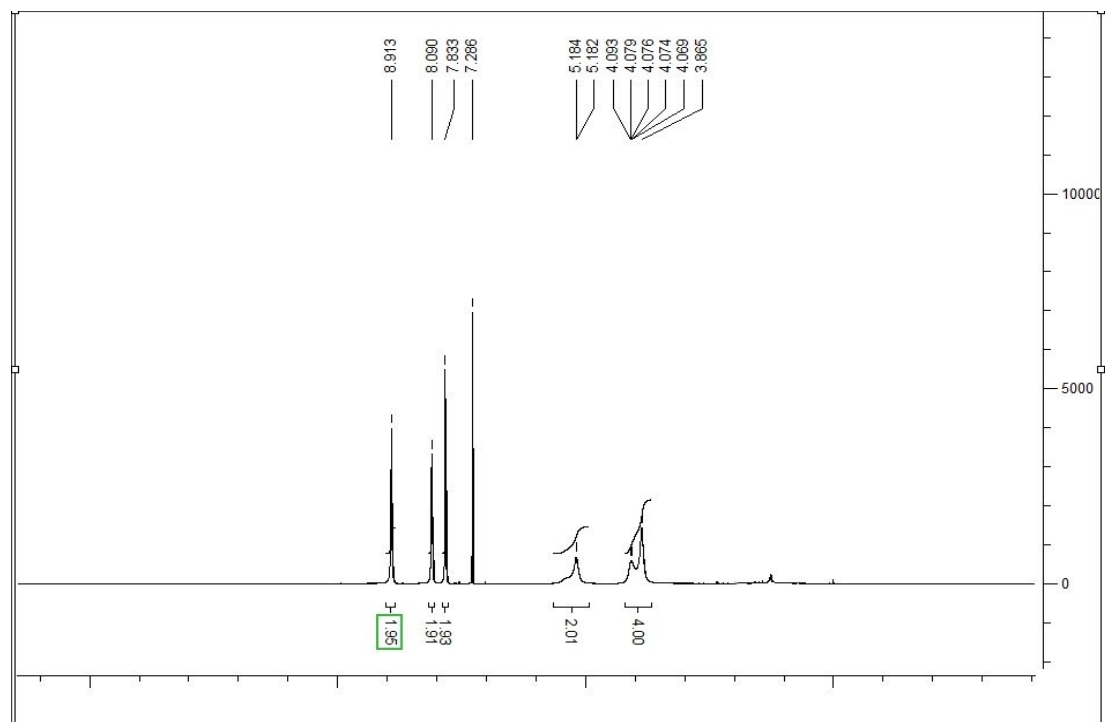
I-10



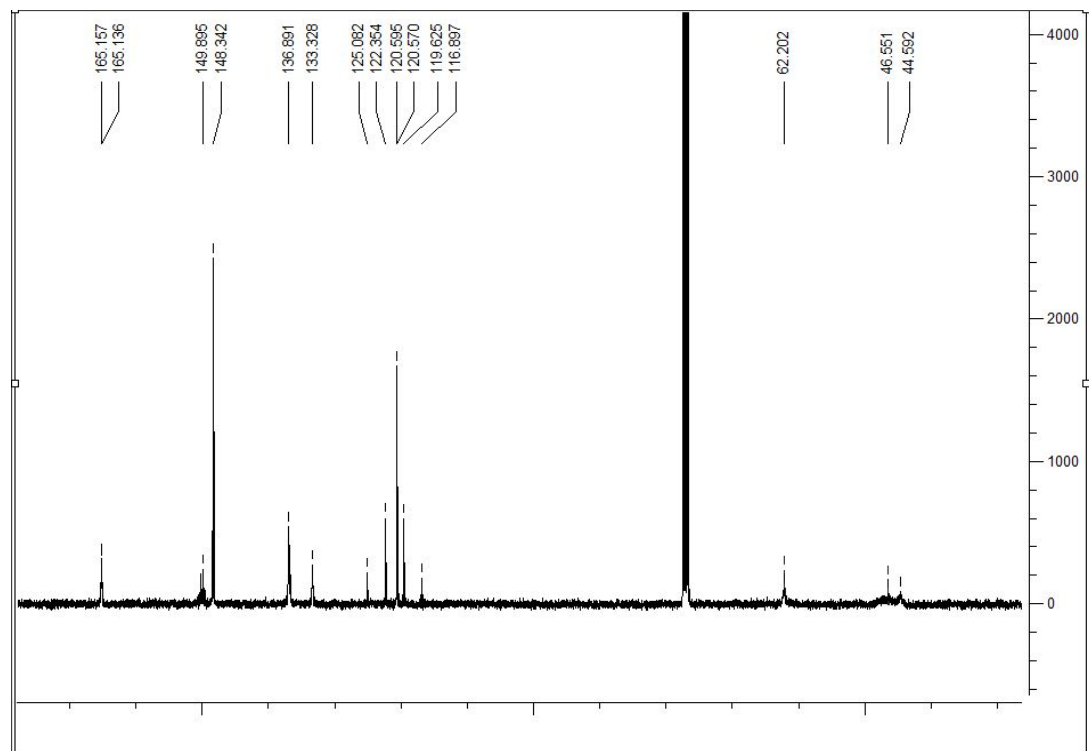
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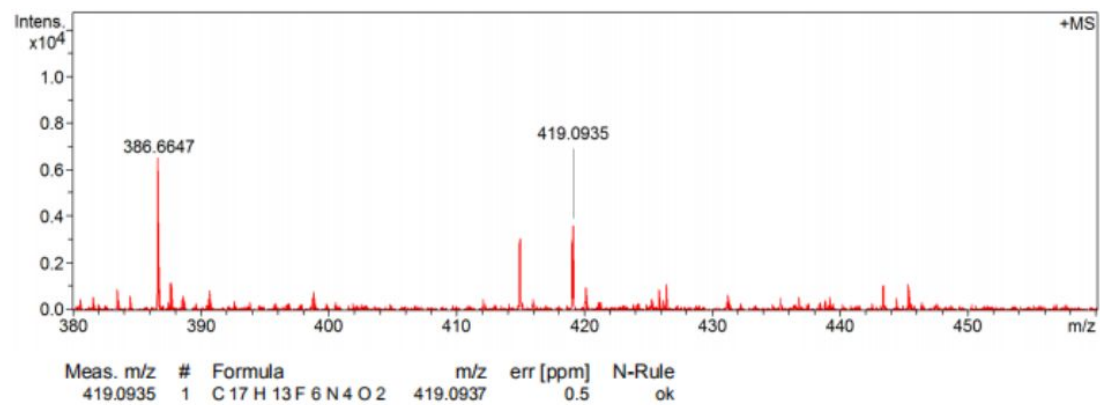
$^1\text{H NMR}$



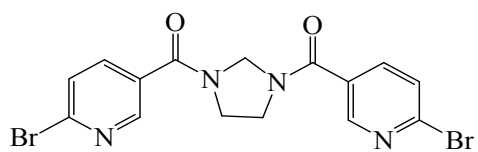
¹³C NHR



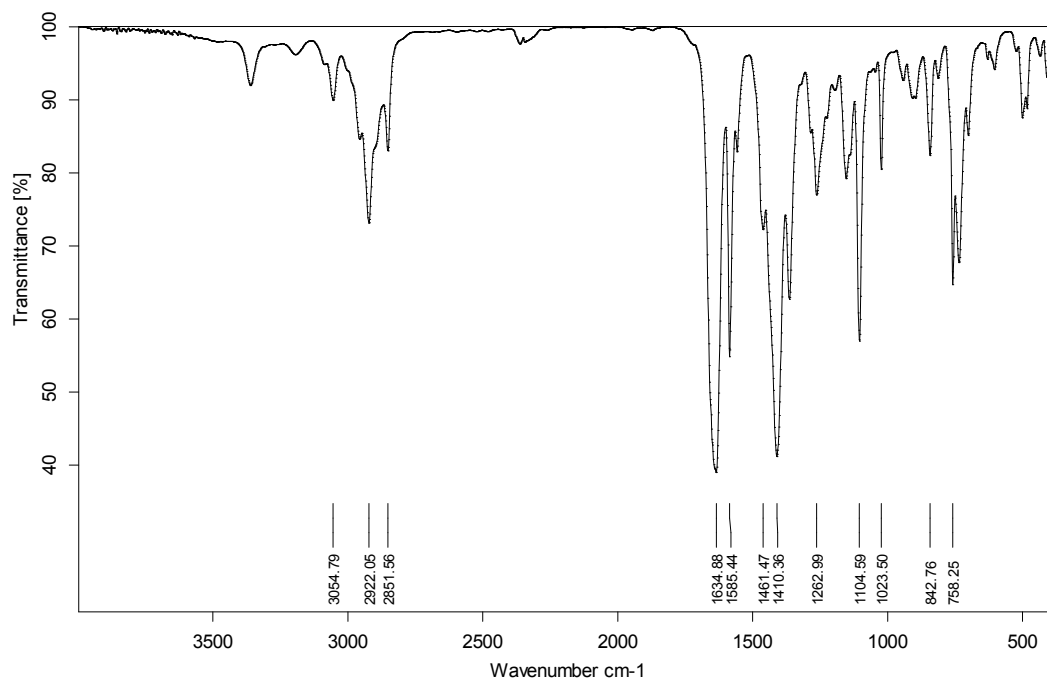
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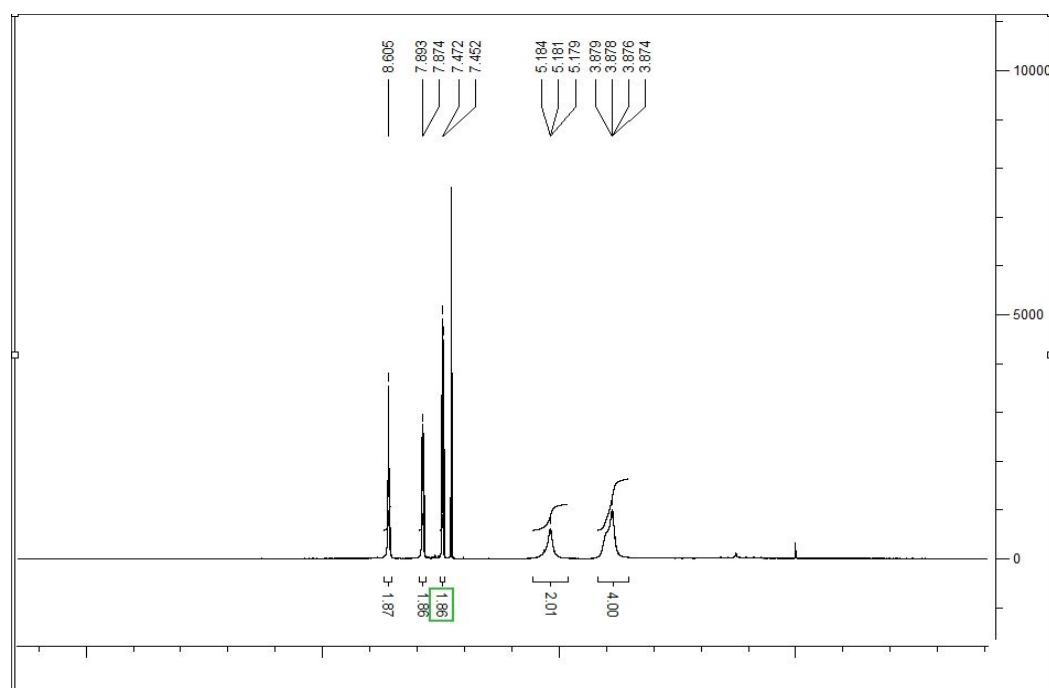
I-11



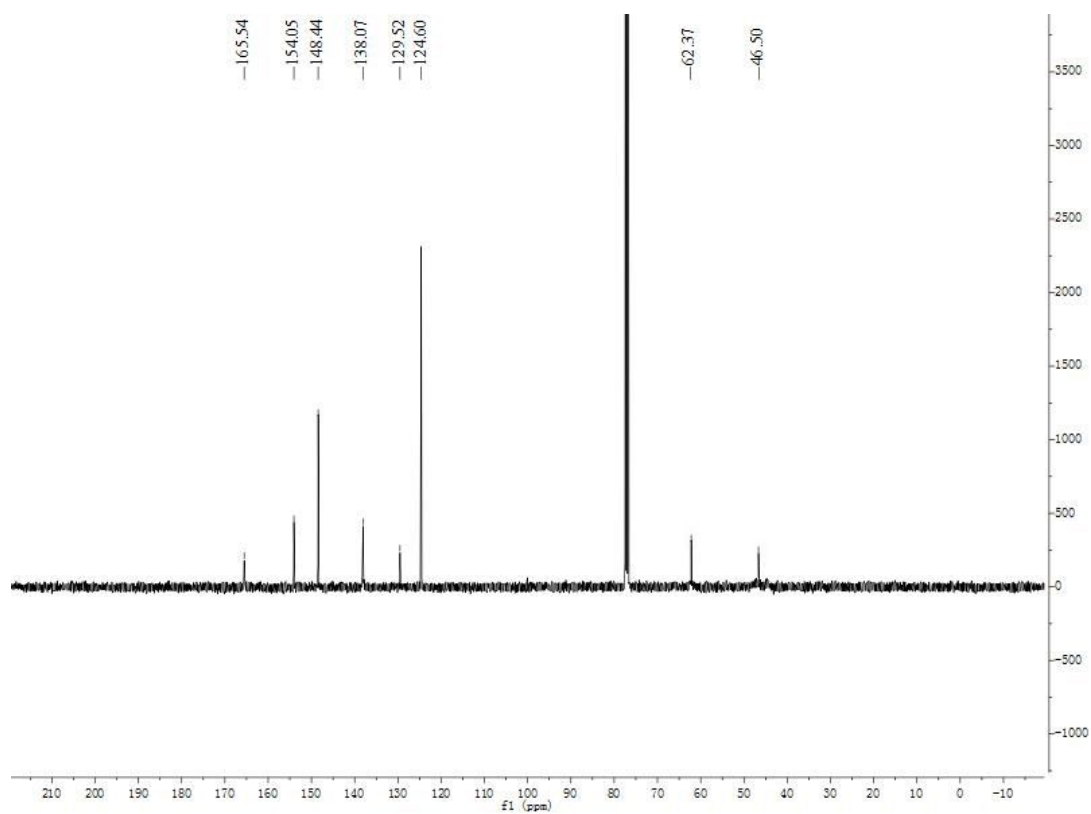
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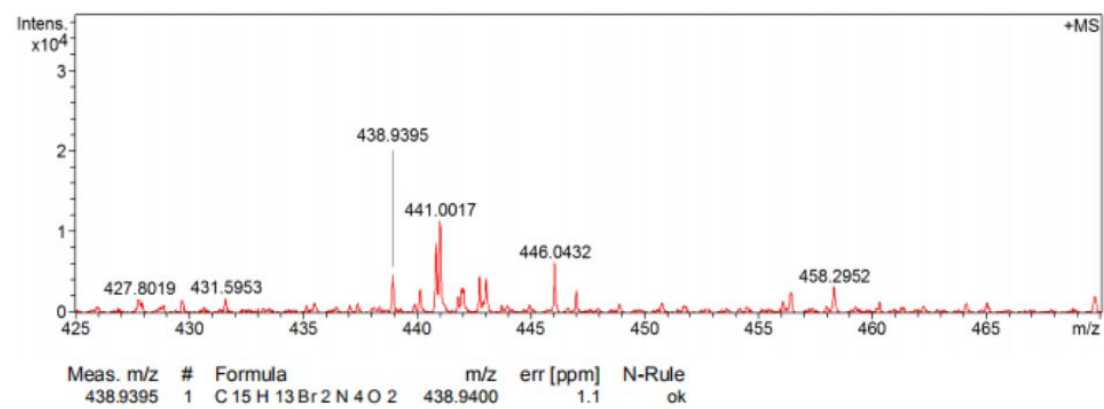
¹H NMR



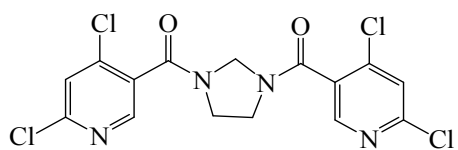
¹³C NHR



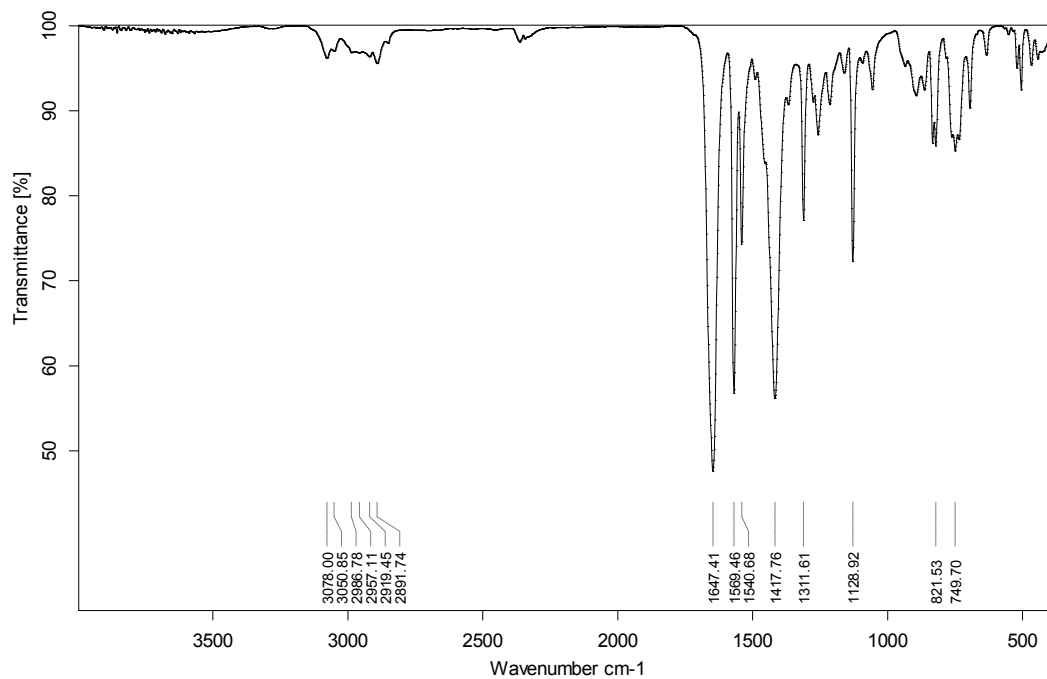
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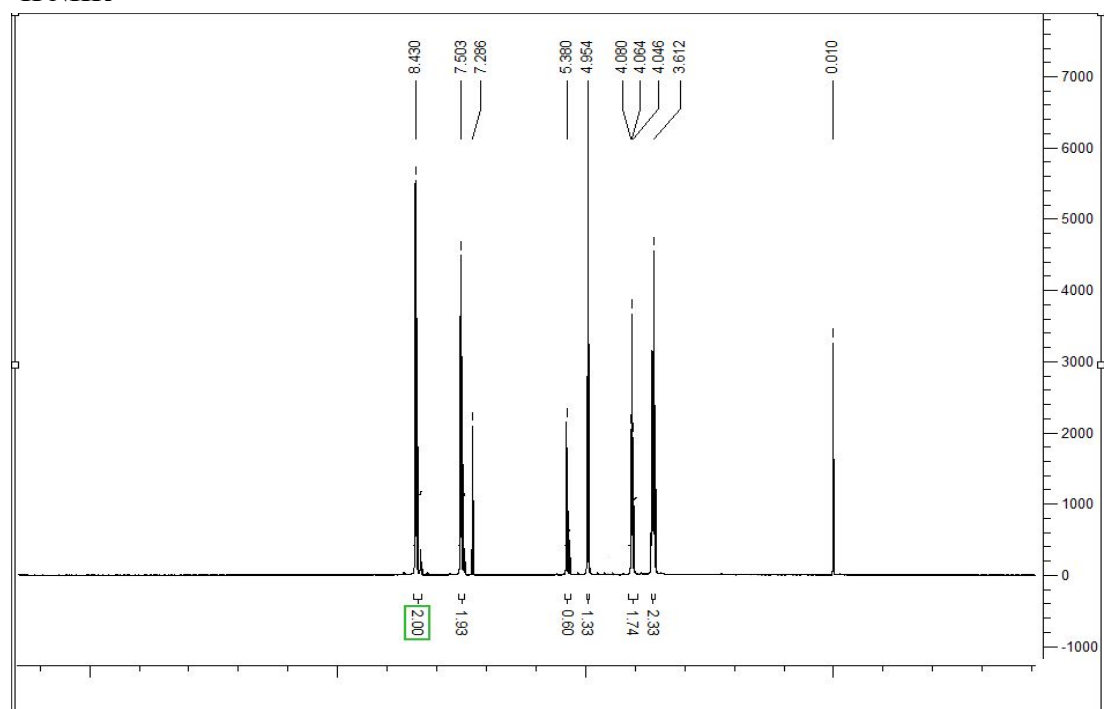
I-12



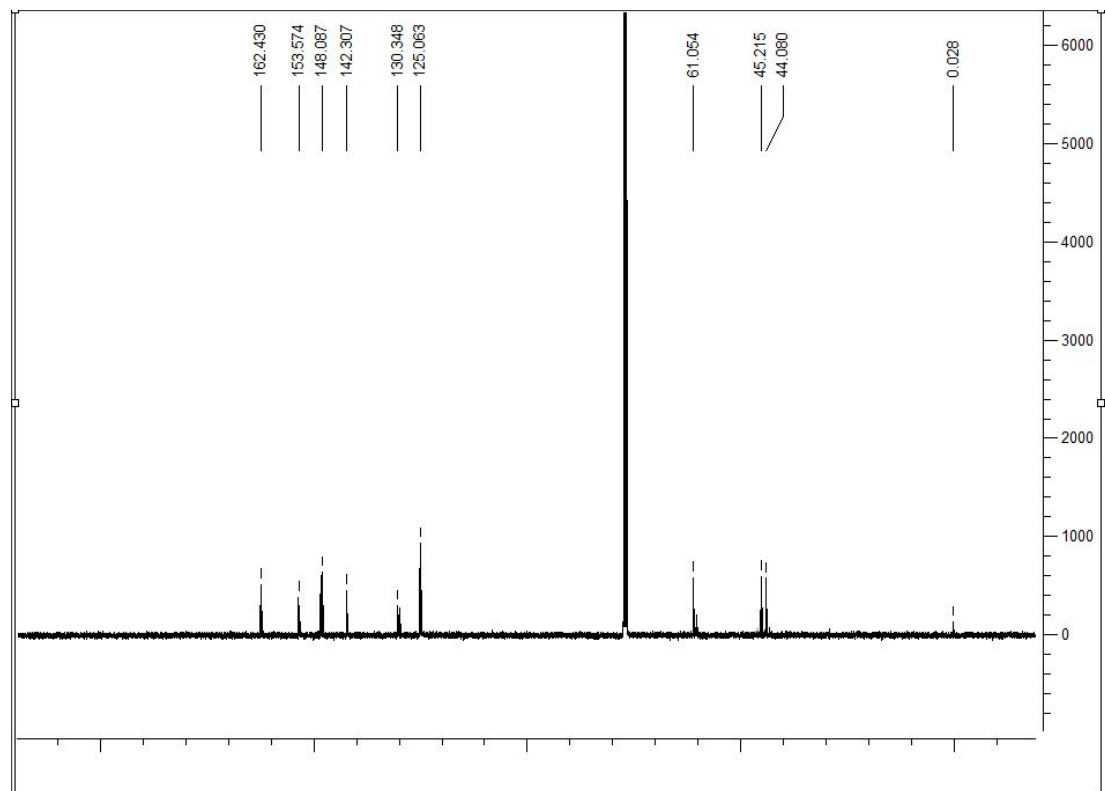
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¹H NMR

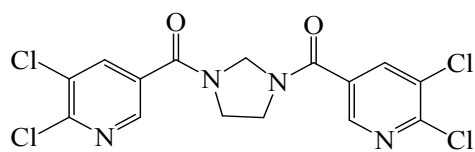


¹³C NHR

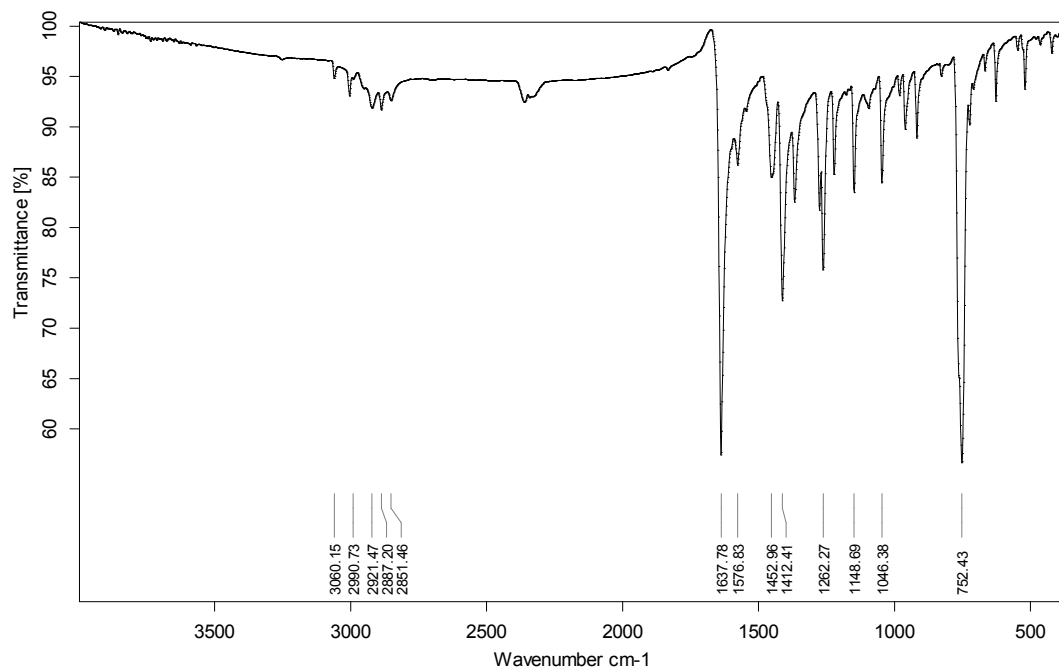


HRMS

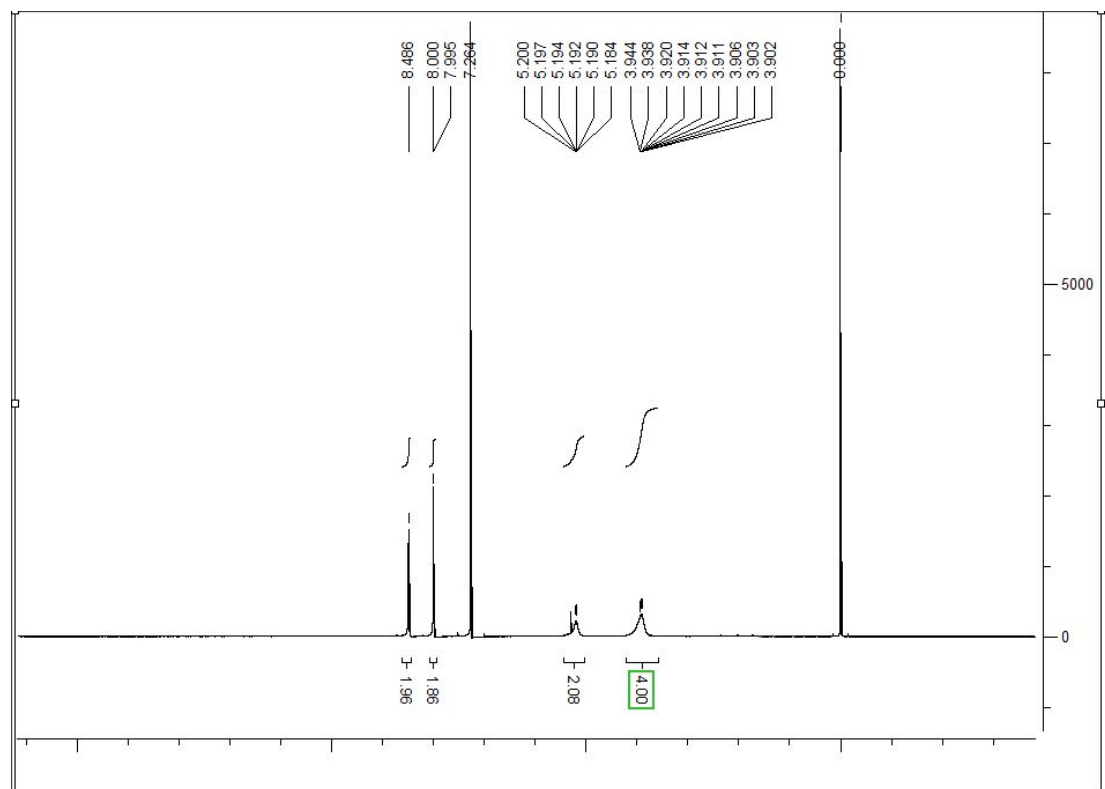
I-13



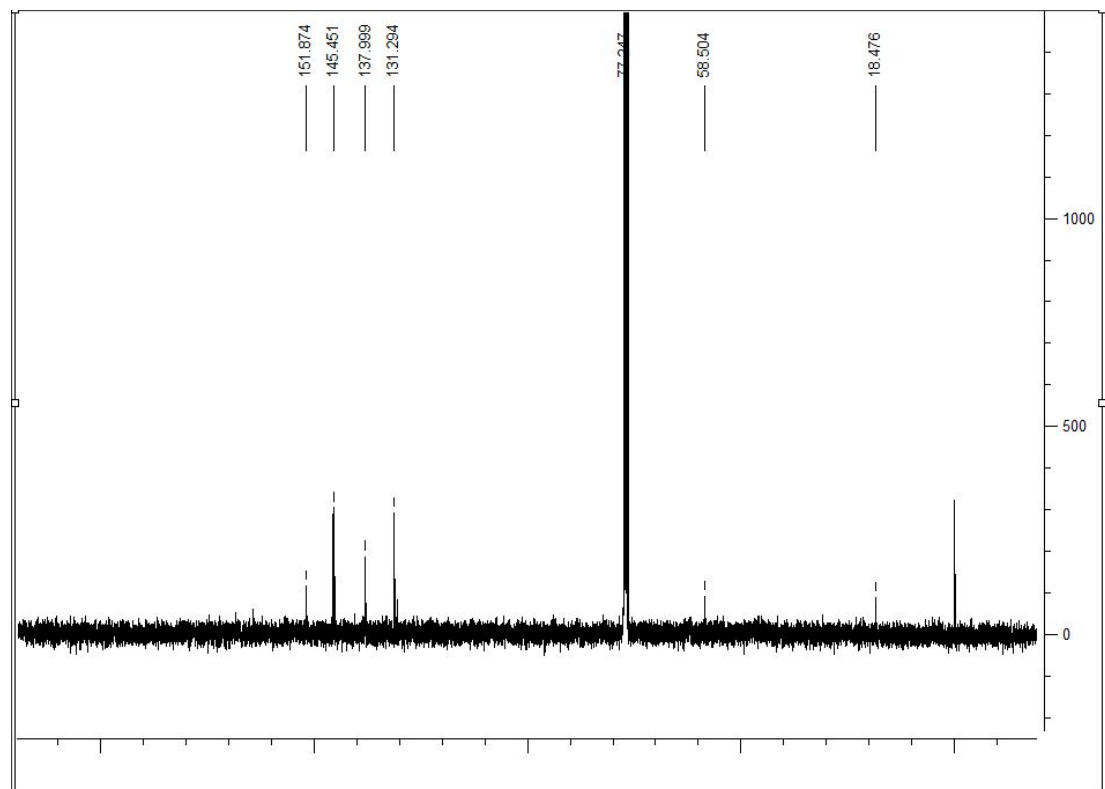
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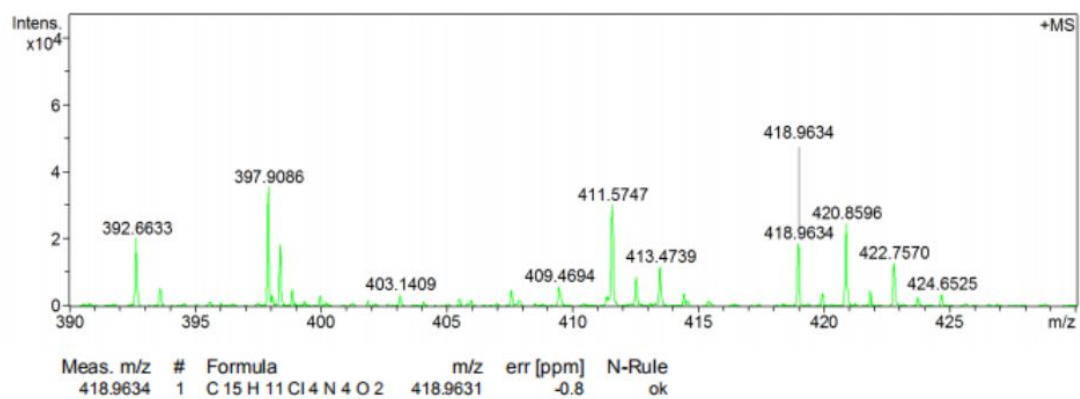
¹H NMR



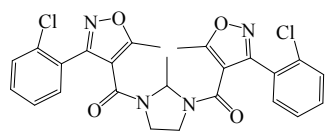
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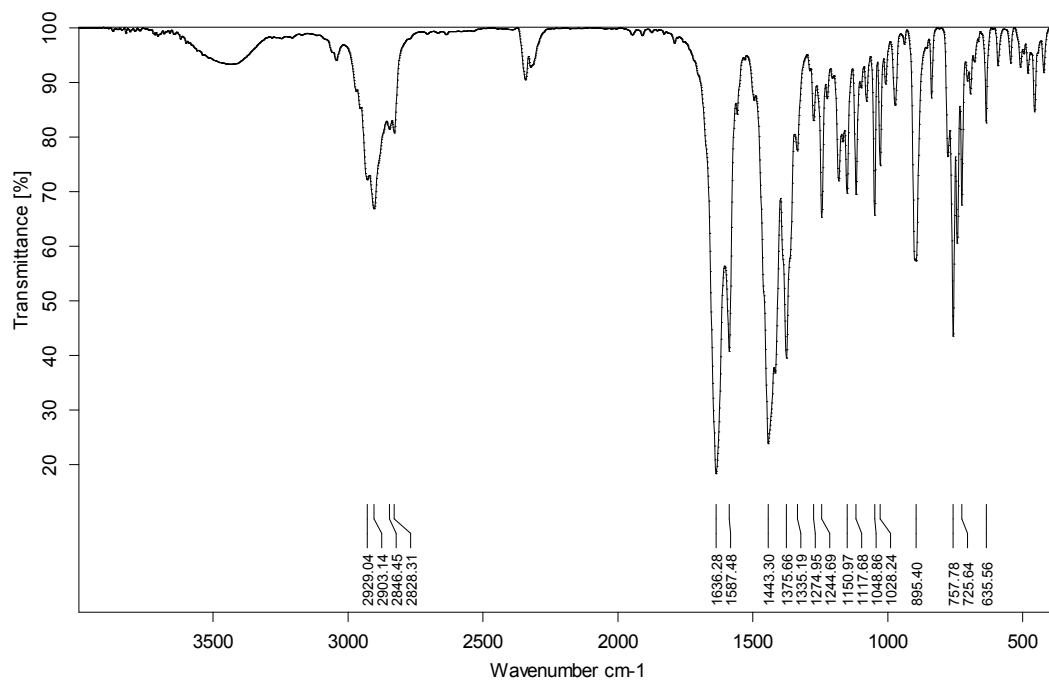
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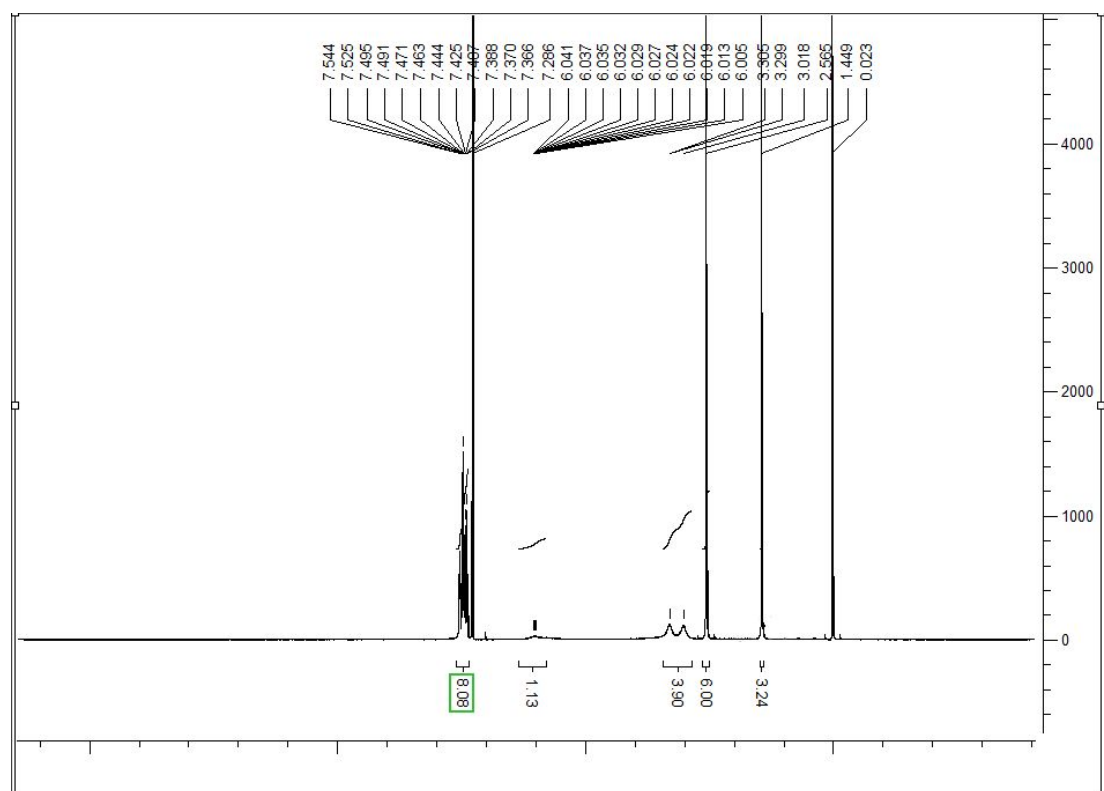
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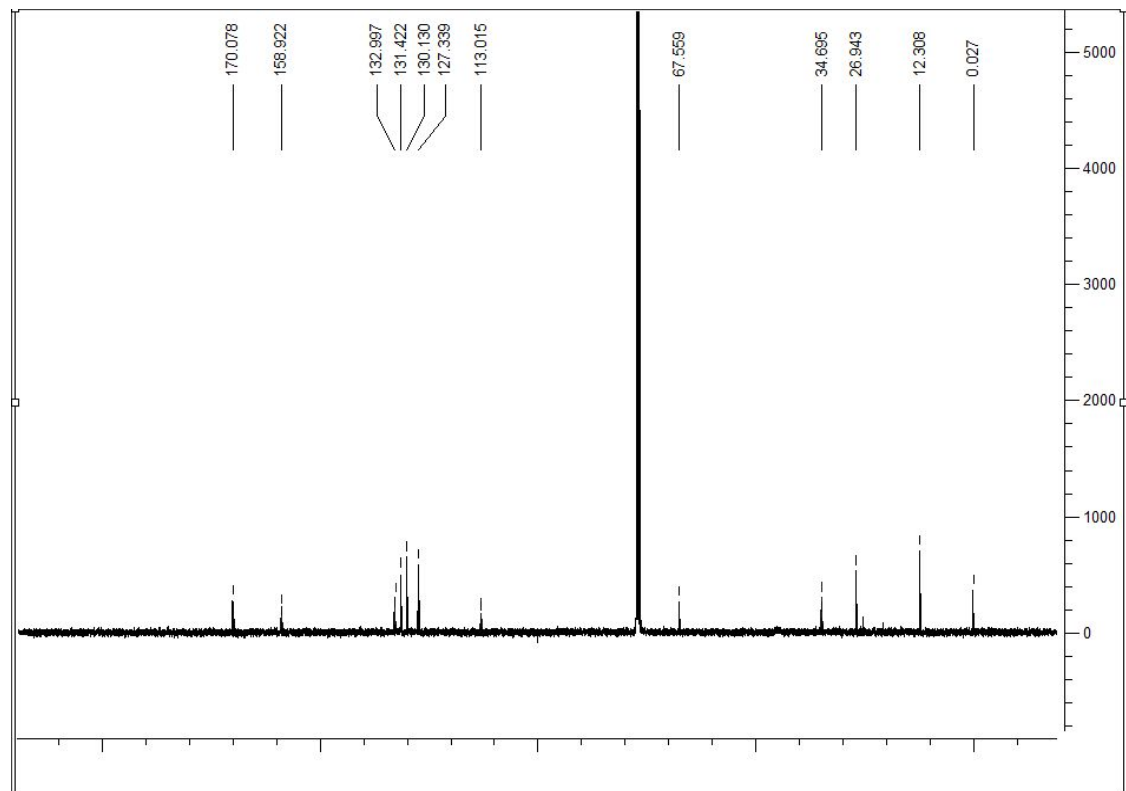
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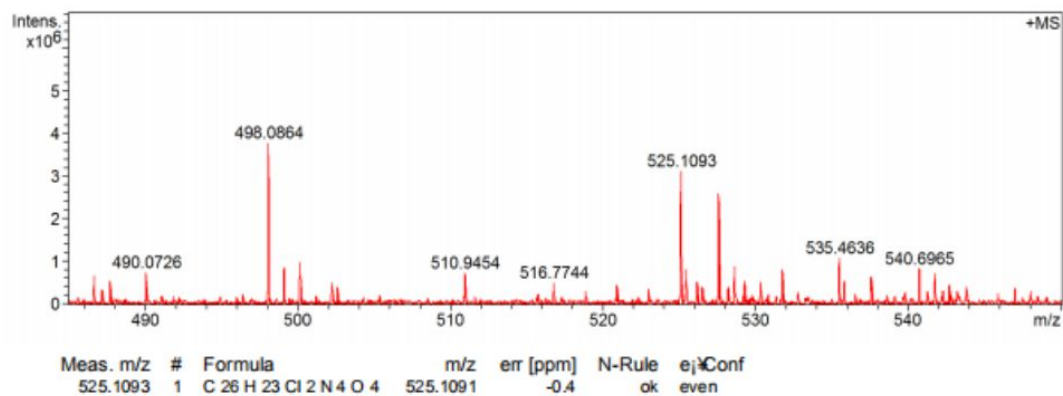
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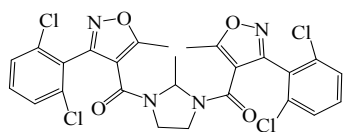
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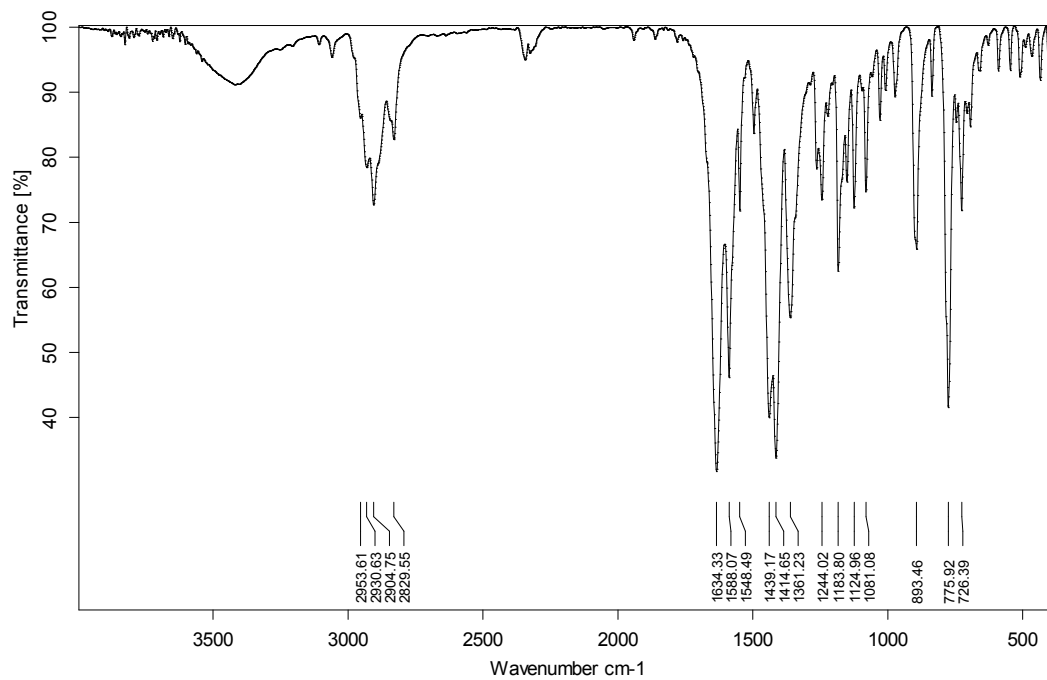
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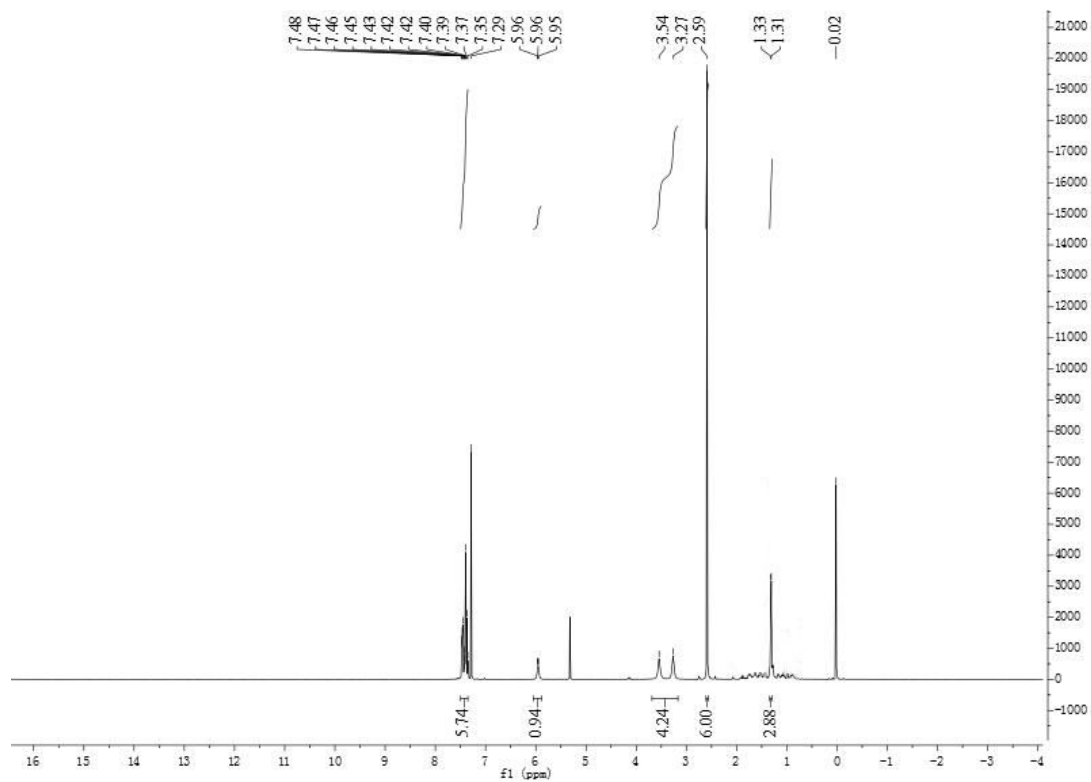
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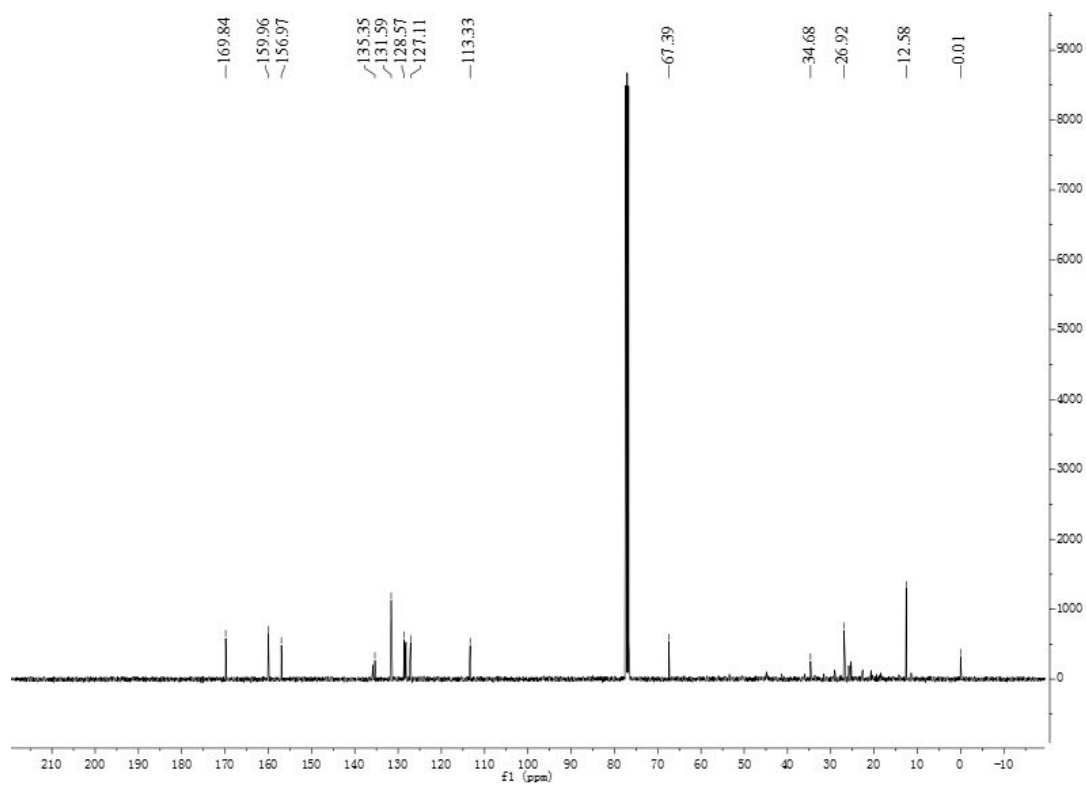
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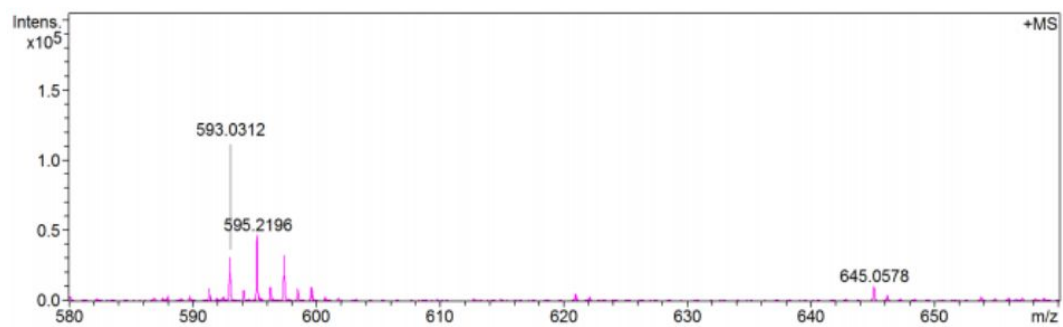
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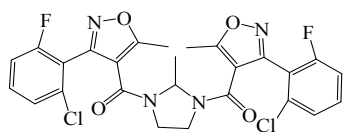
¹³C NMR



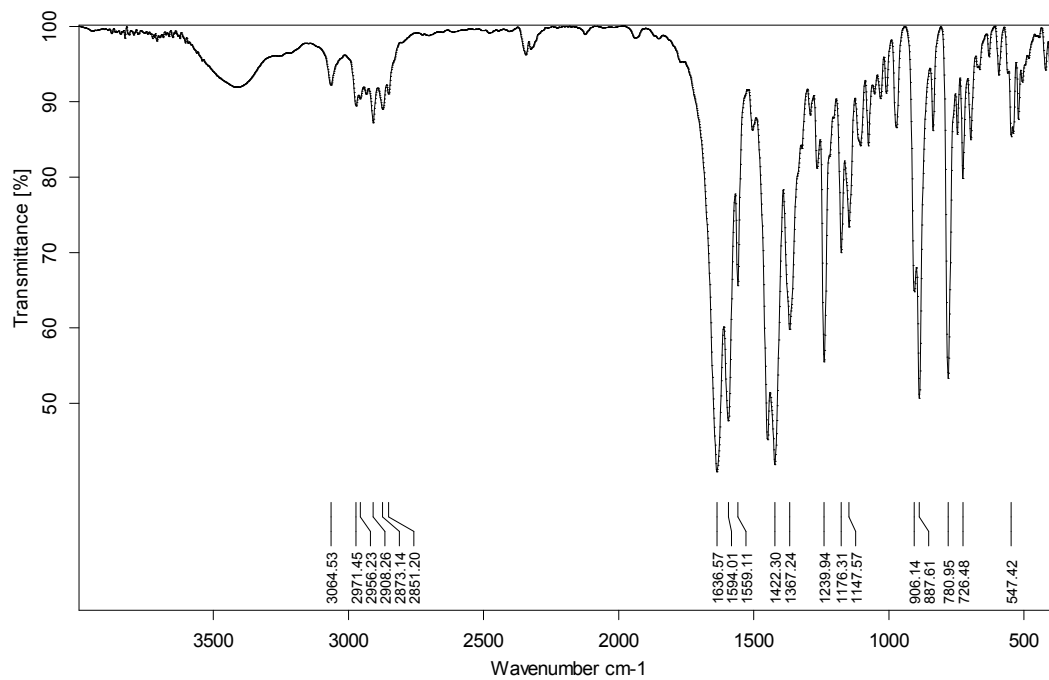
HRMS



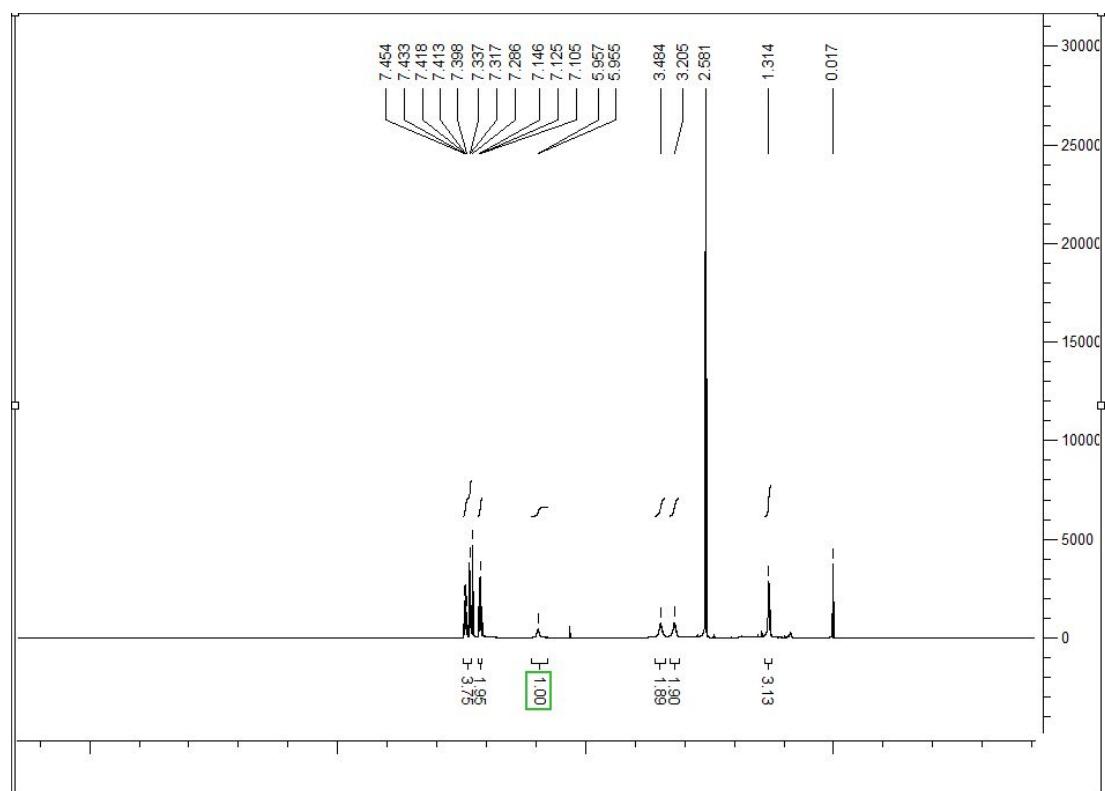
I-16



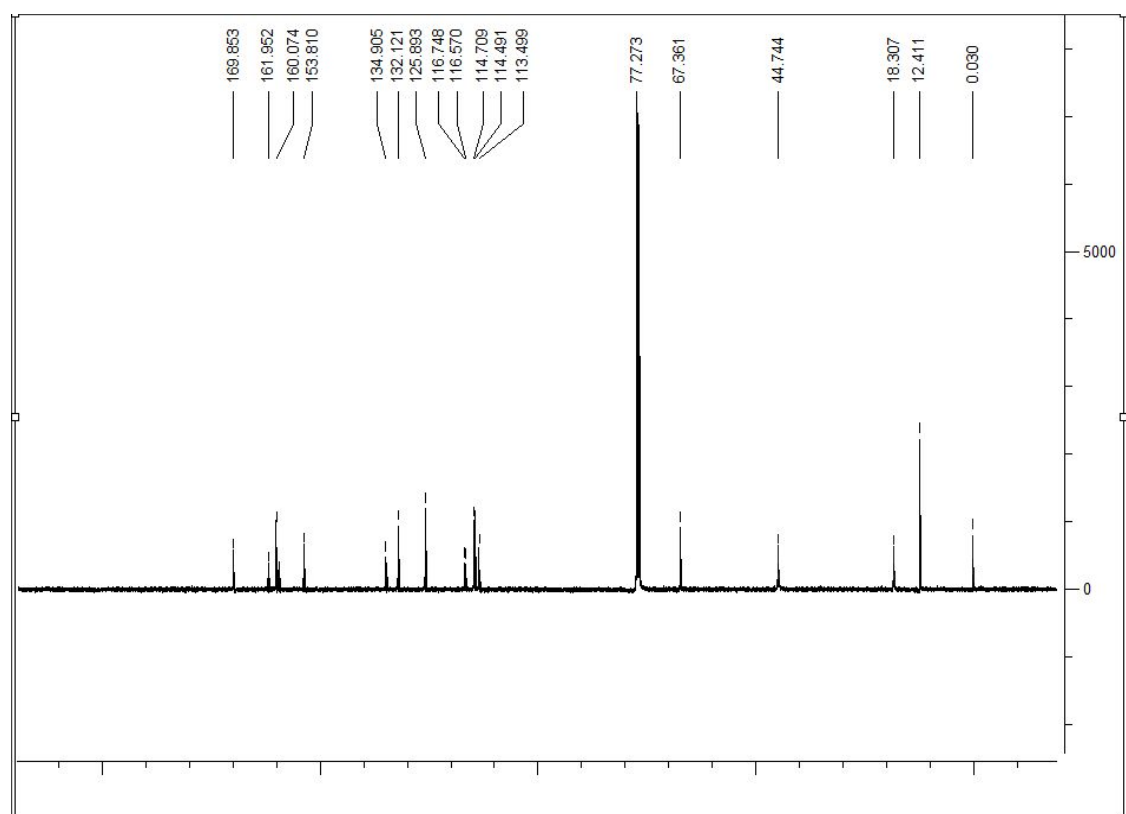
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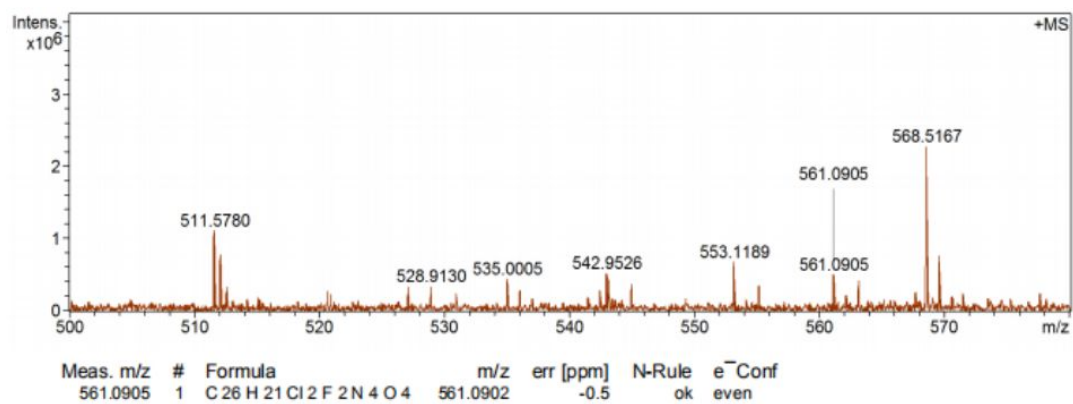
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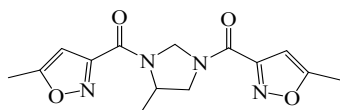
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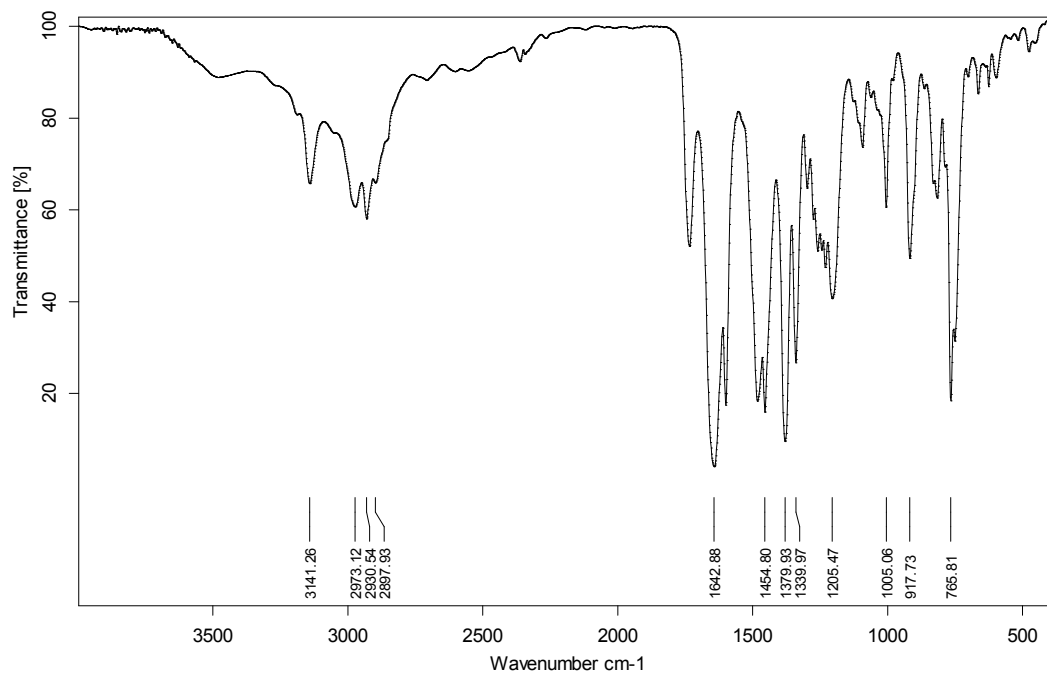
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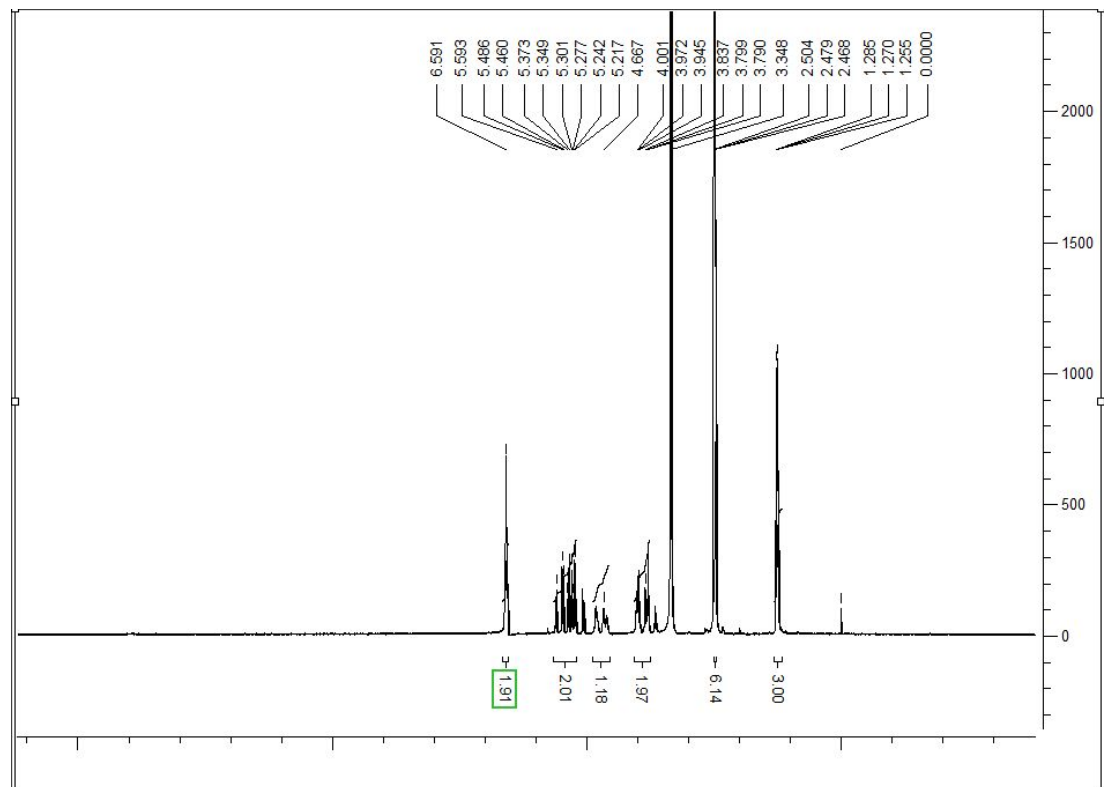
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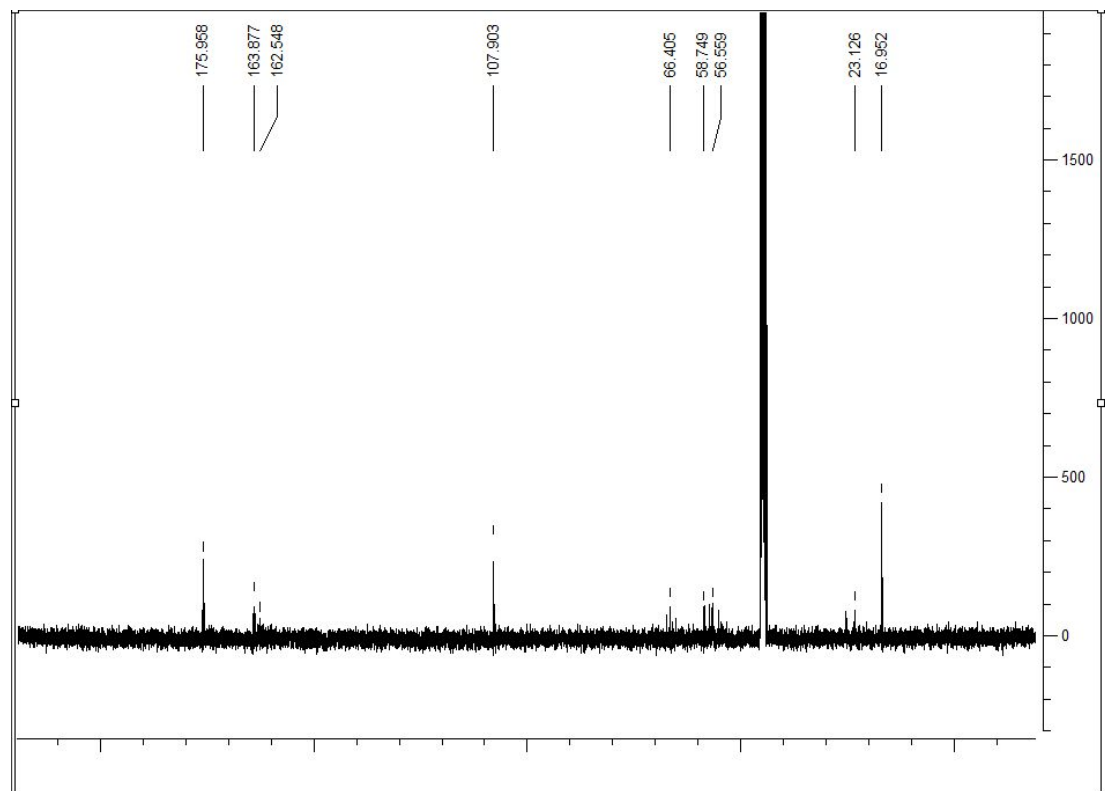
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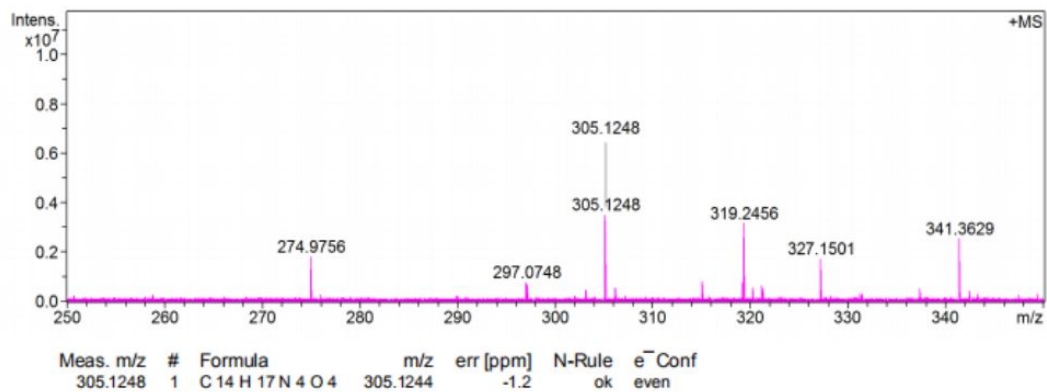
¹H NMR



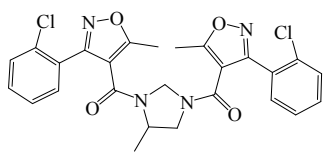
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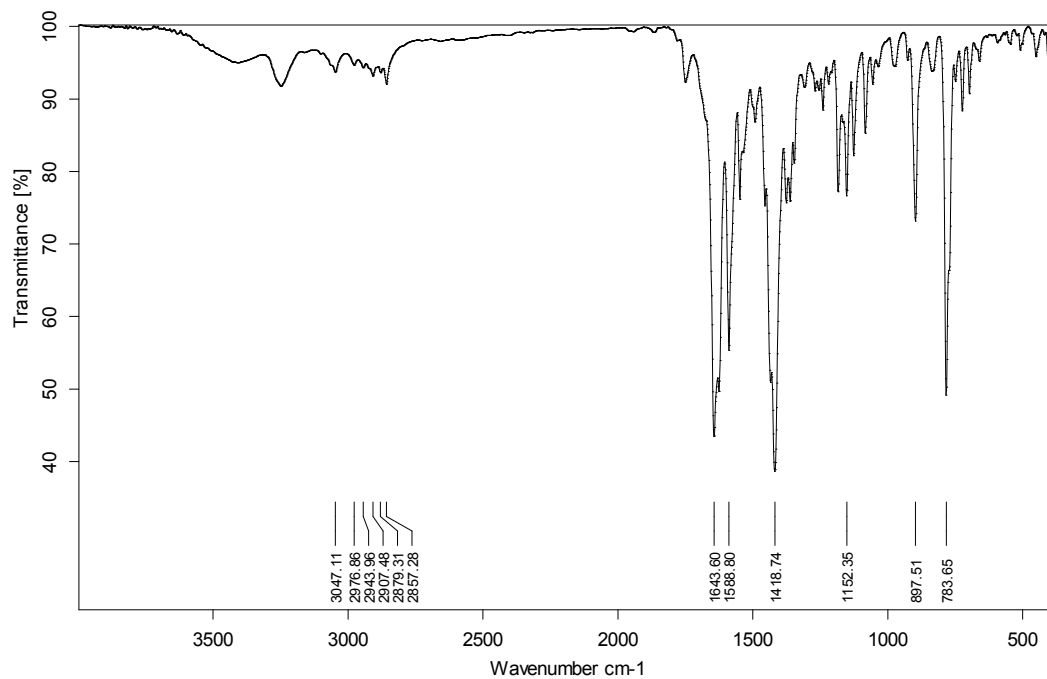
HRMS



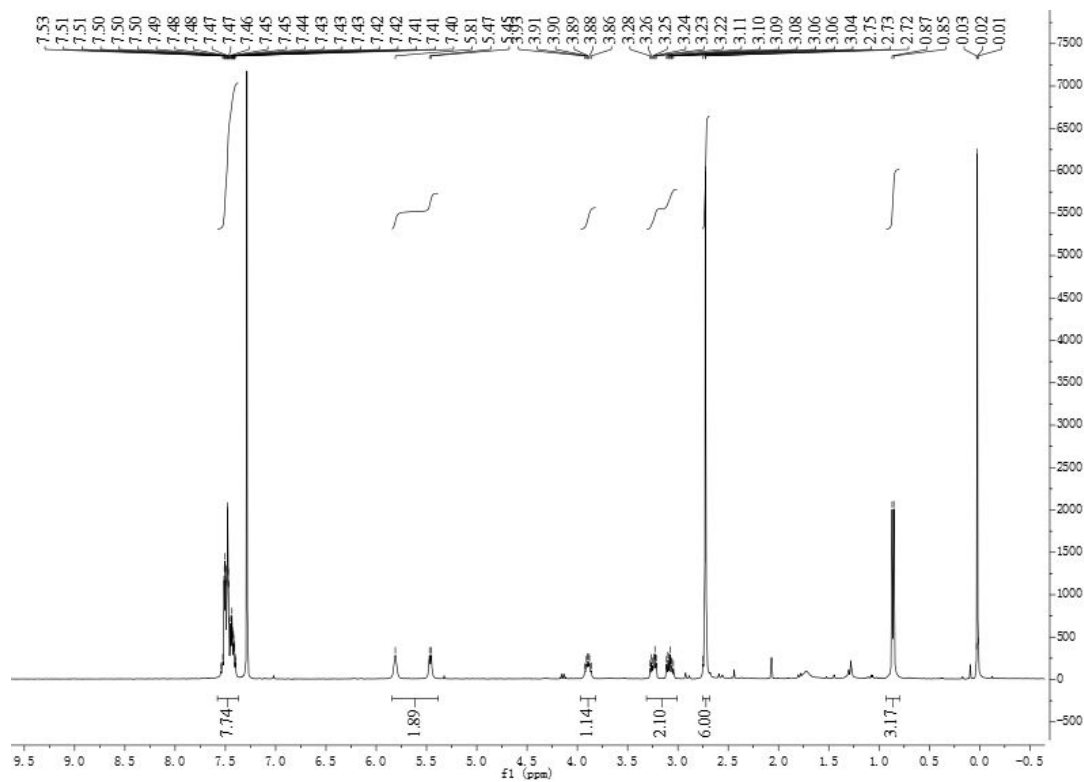
I-18



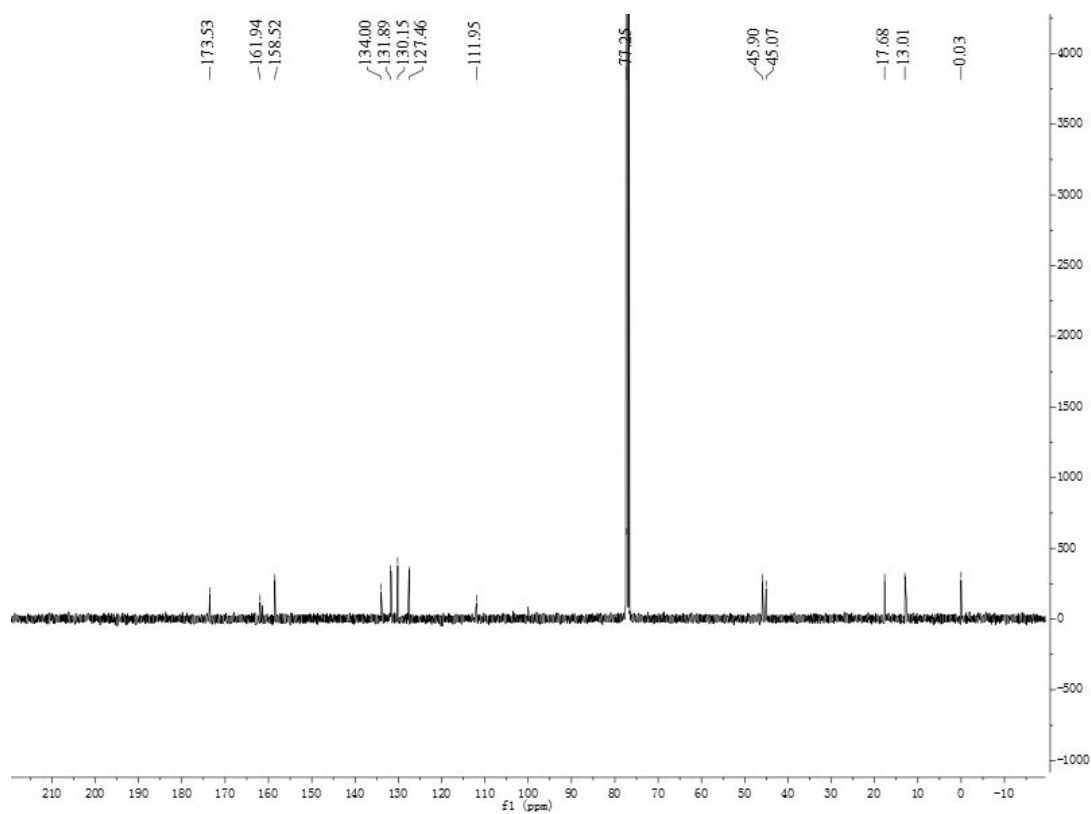
IR



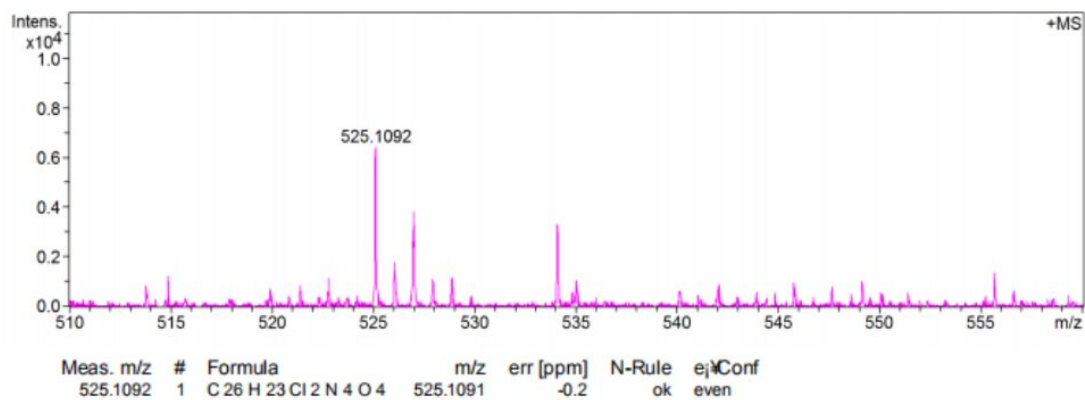
¹H NMR



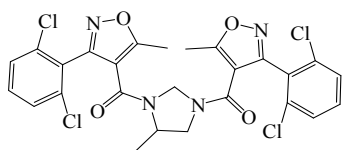
¹³C NHR



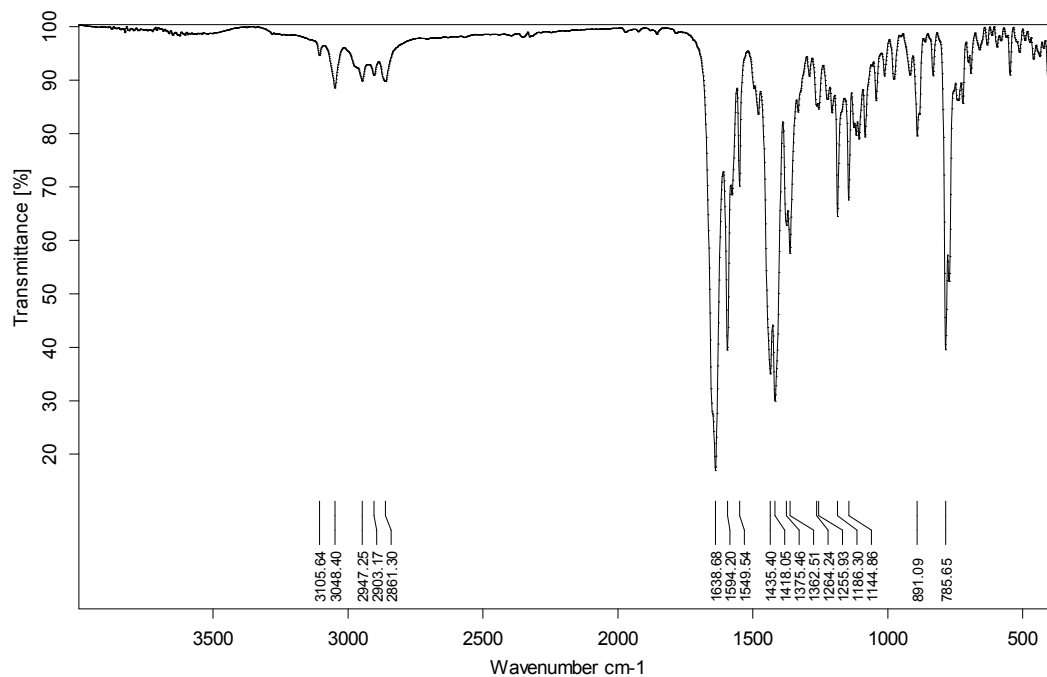
HRMS



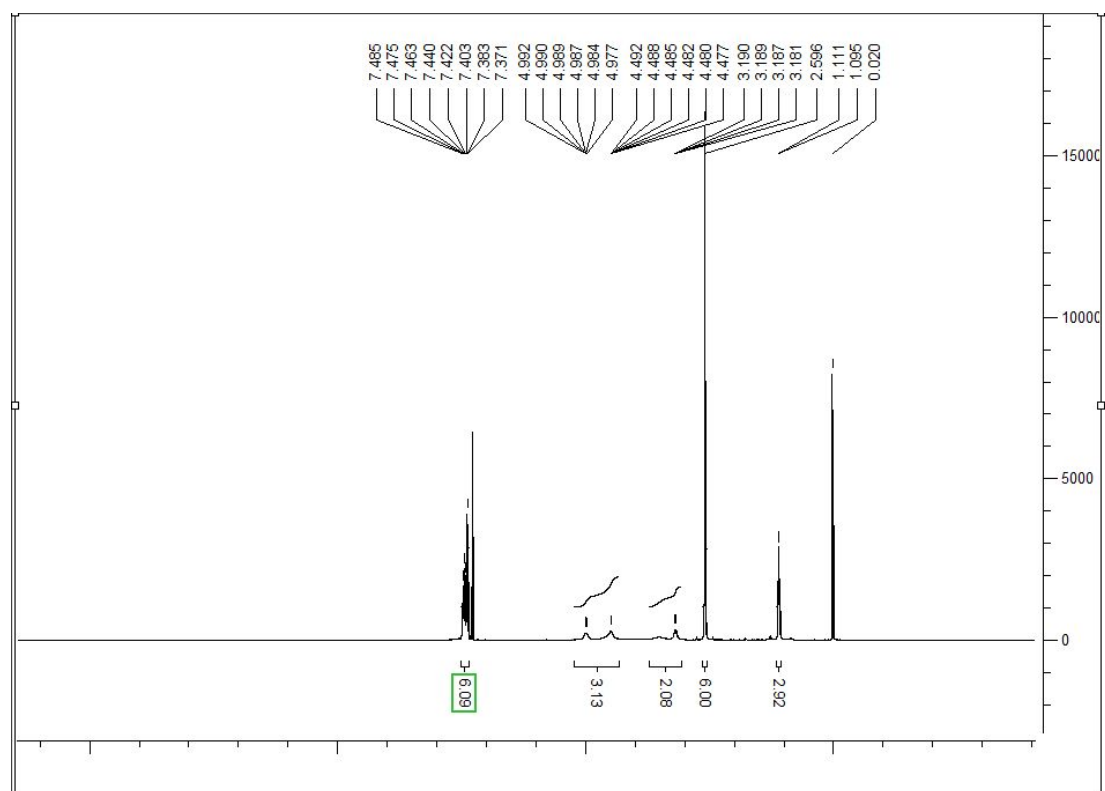
I-19



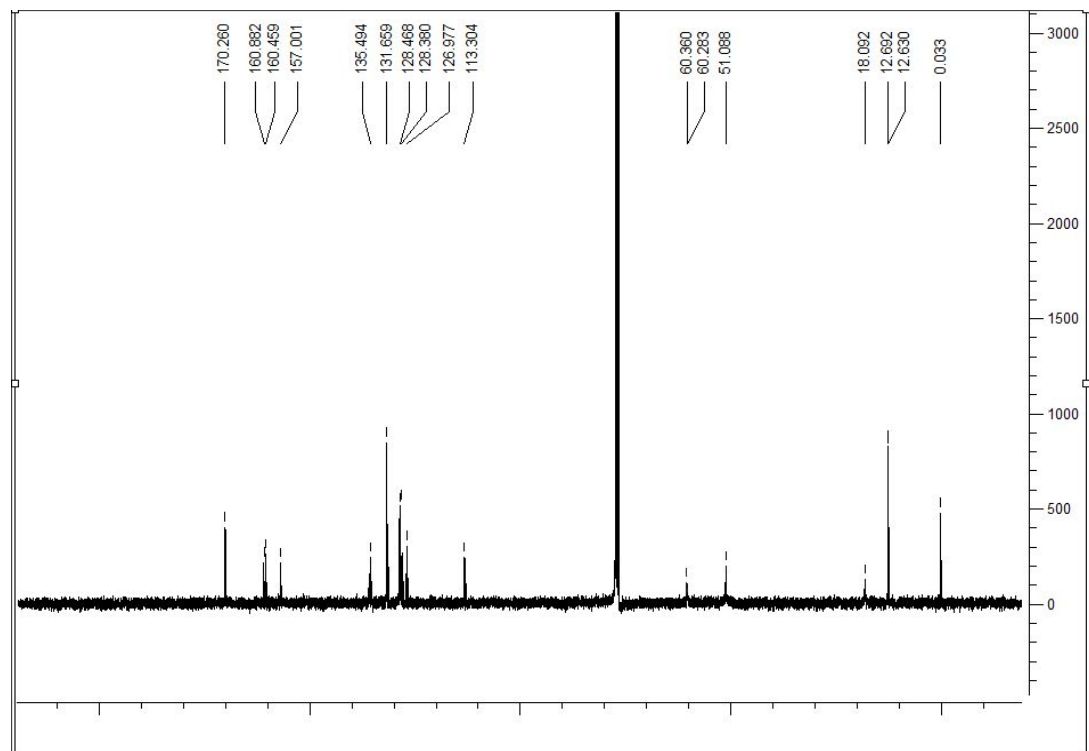
IR



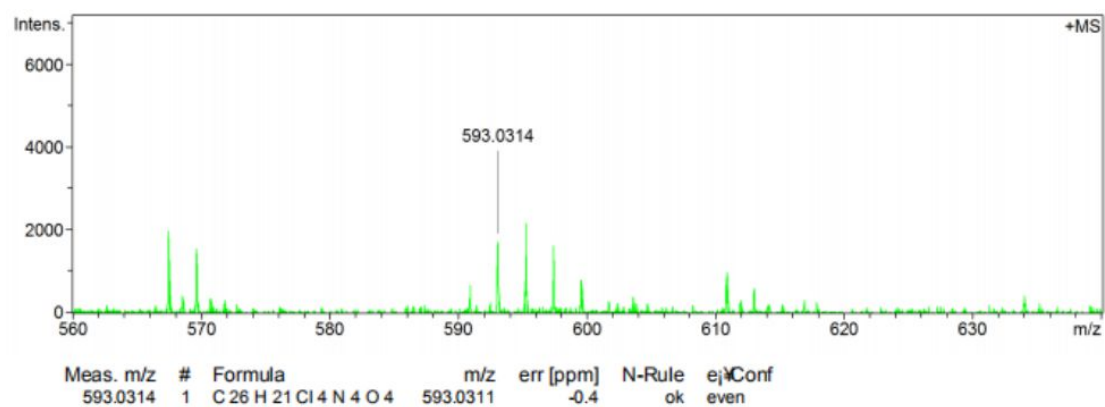
¹H NMR



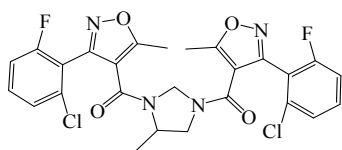
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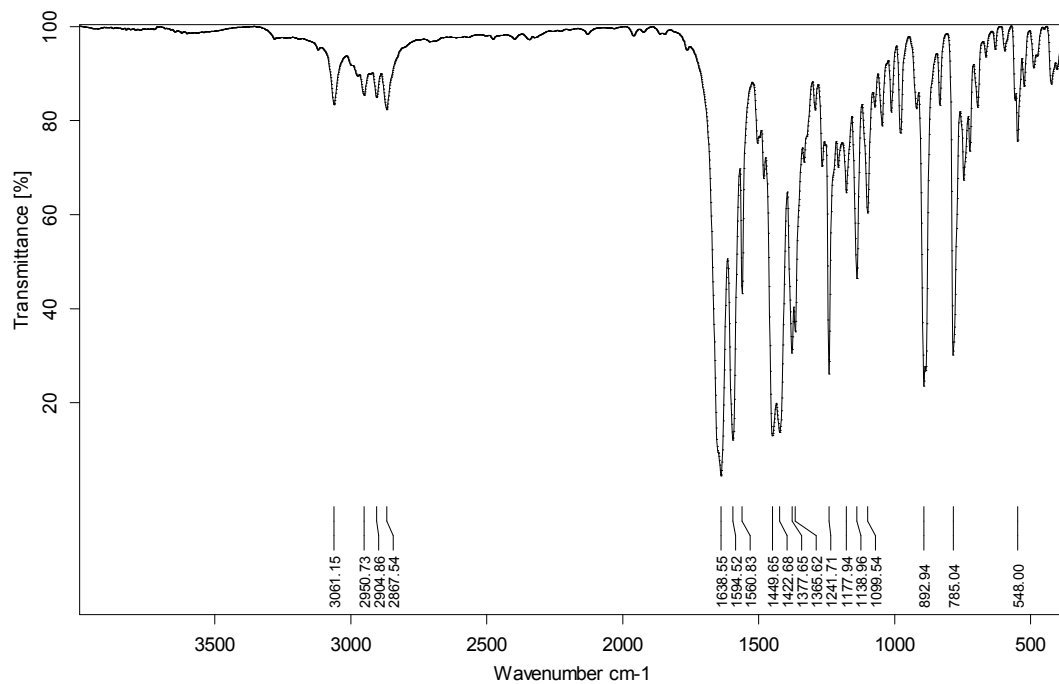
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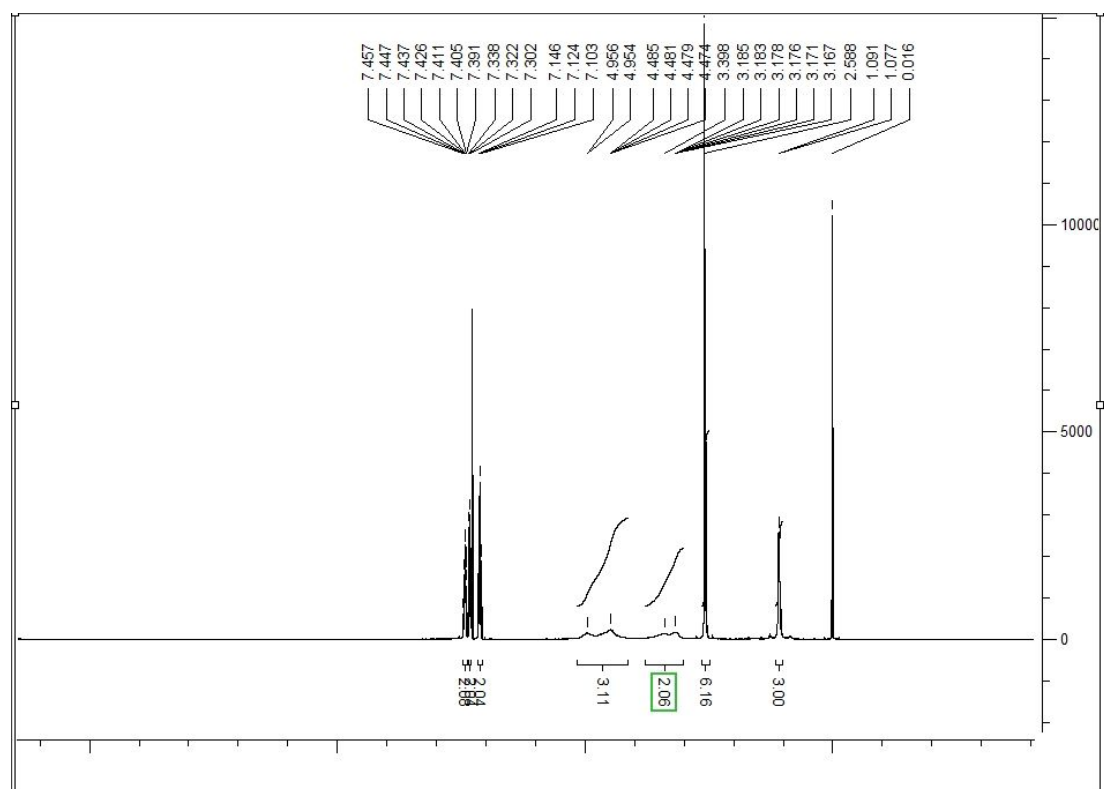
I-20



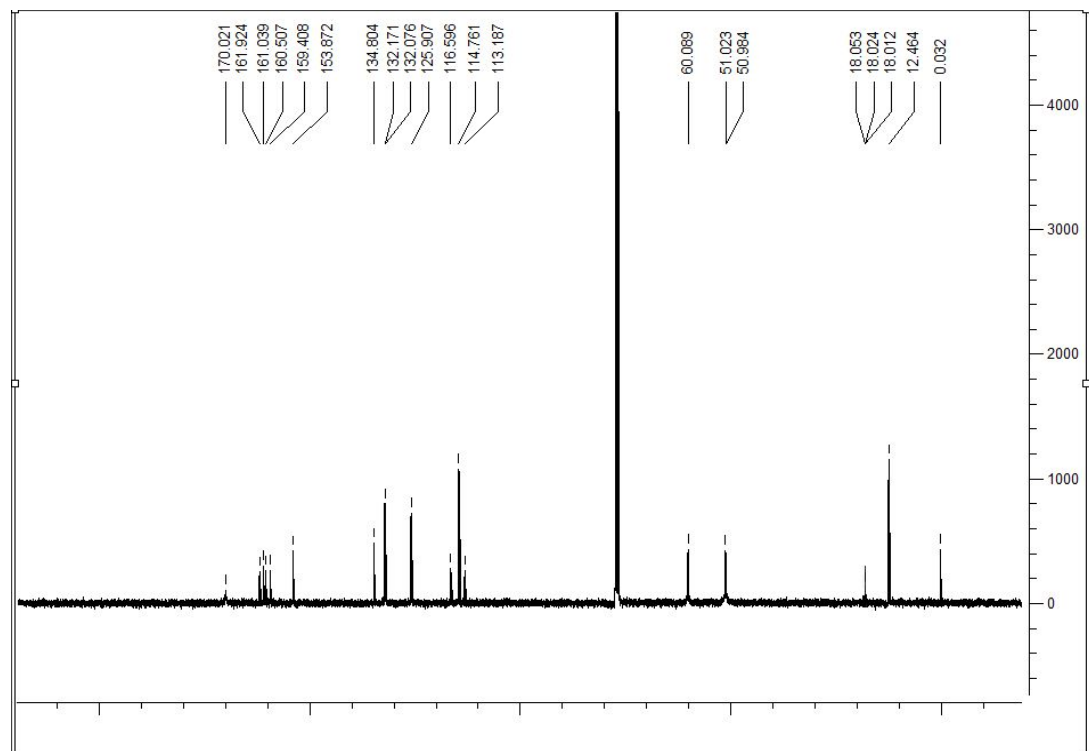
IR



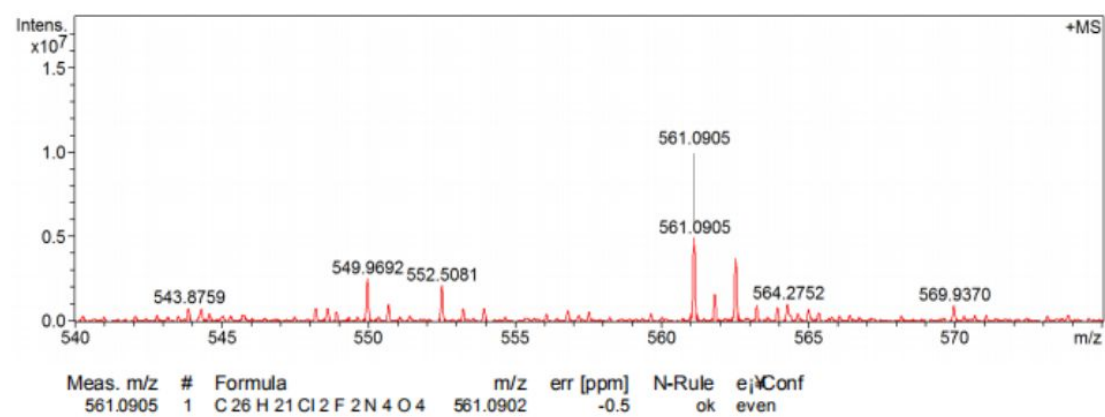
¹H NMR



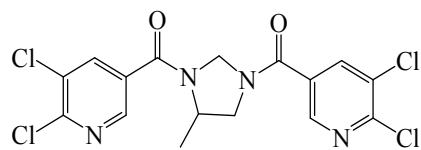
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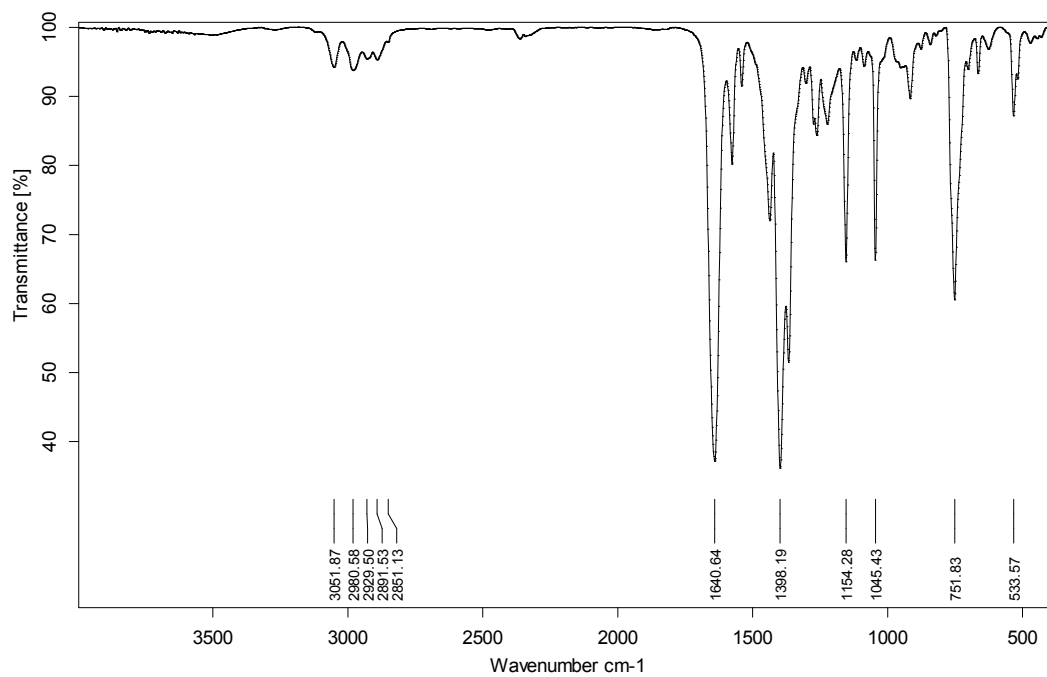
HRMS



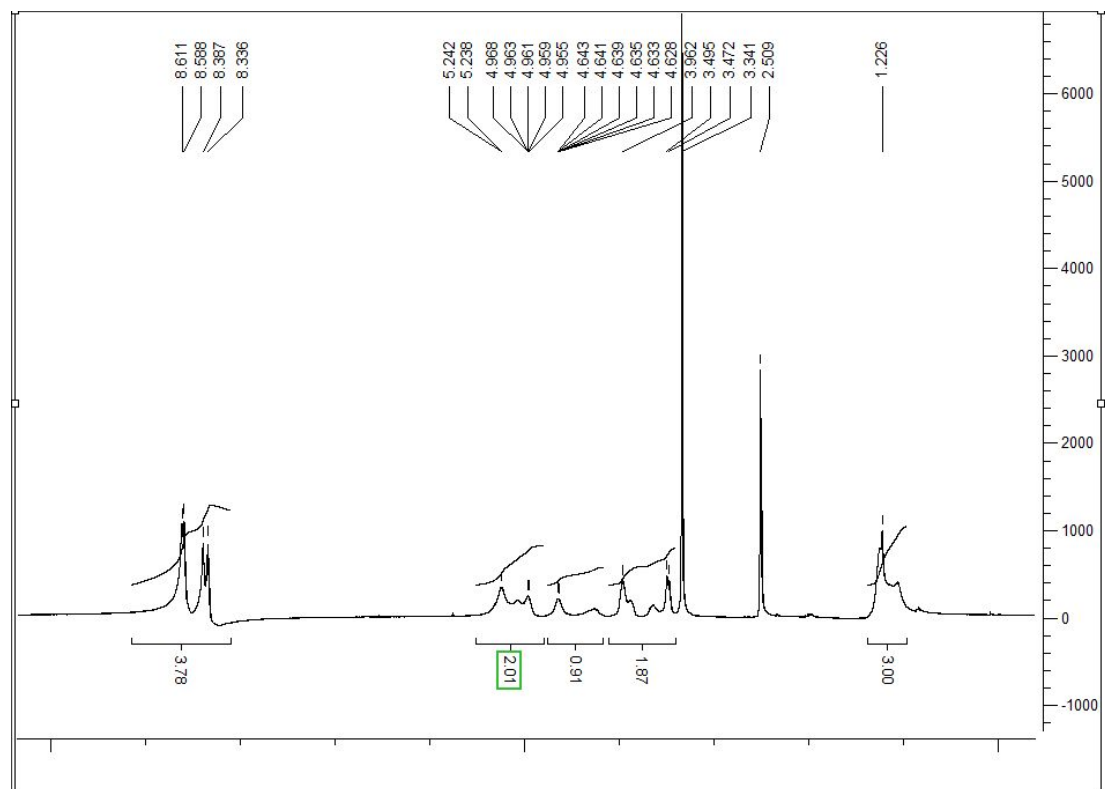
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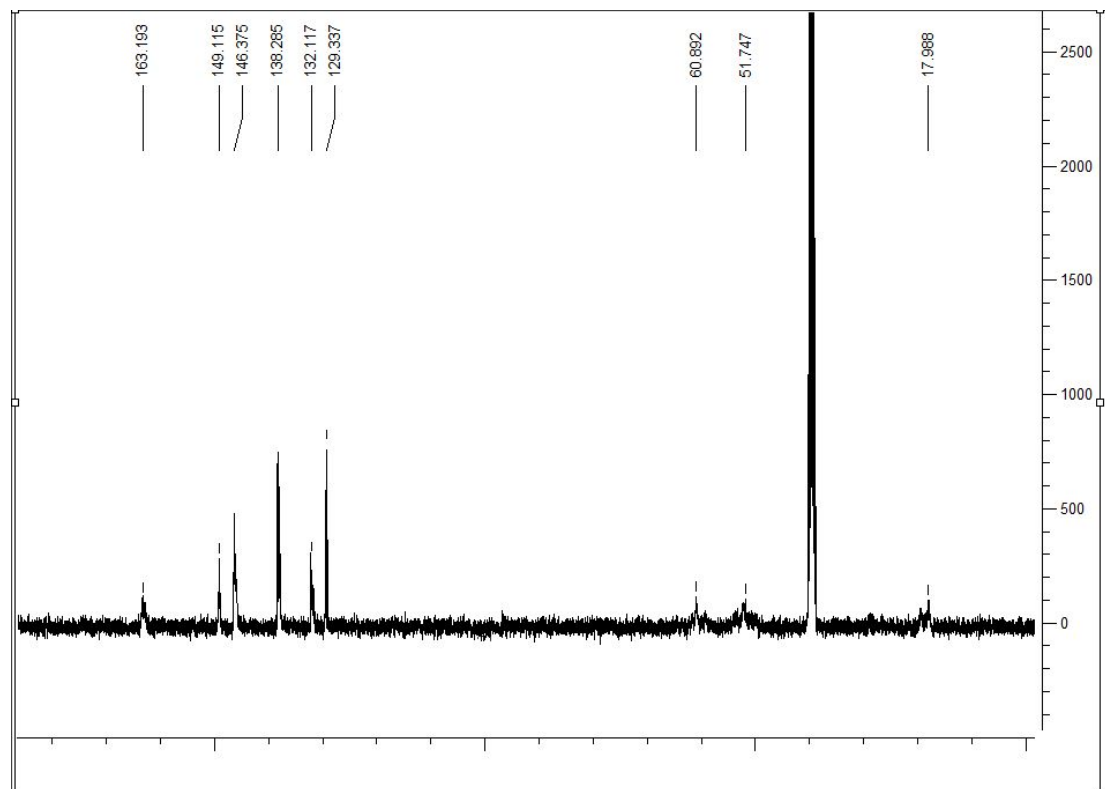
IR



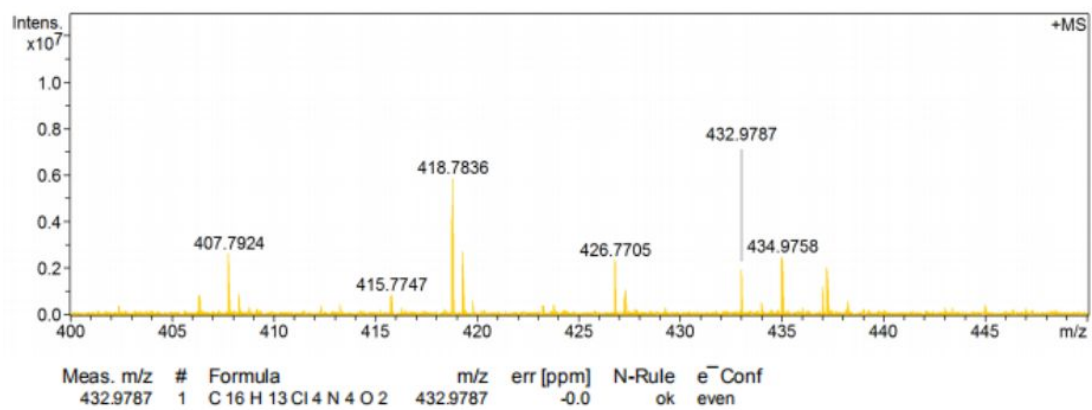
¹H NMR



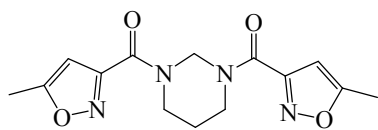
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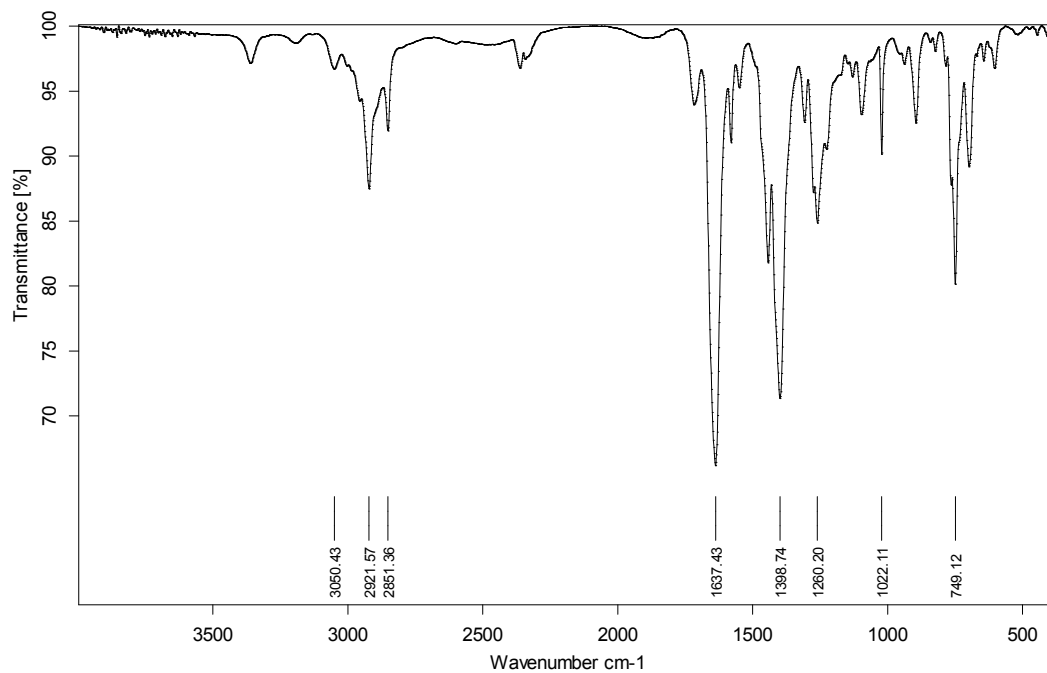
HRMS



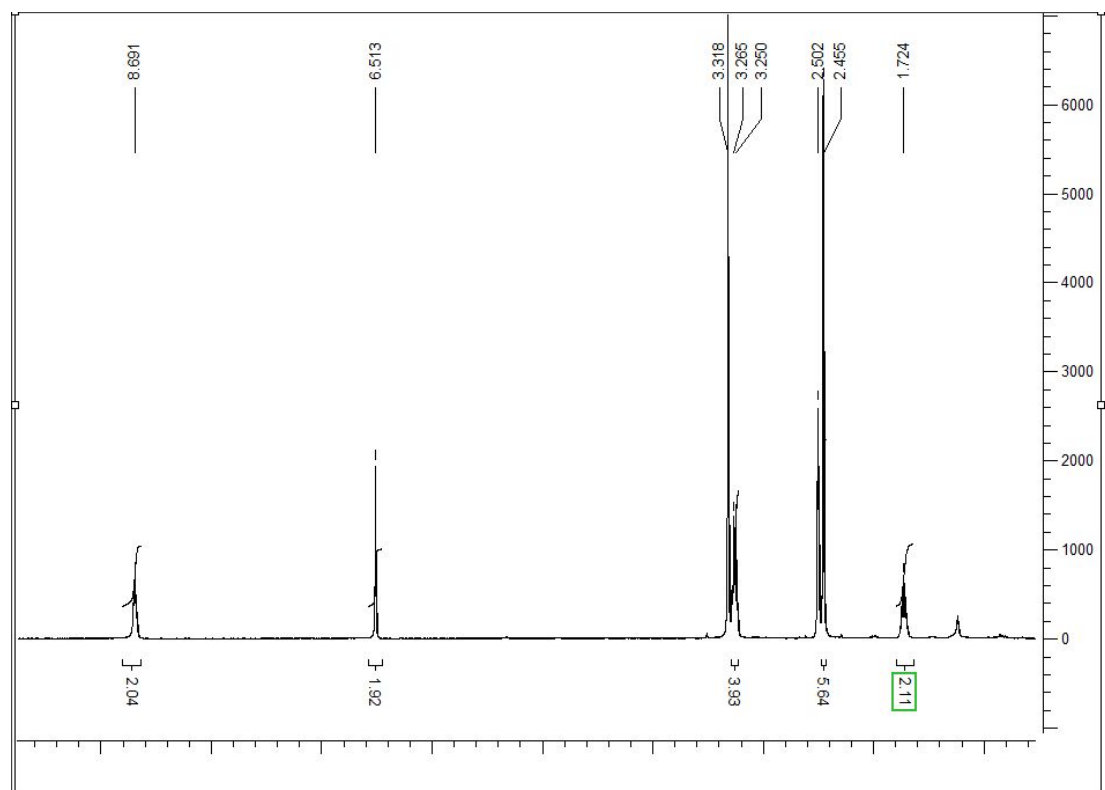
II-1



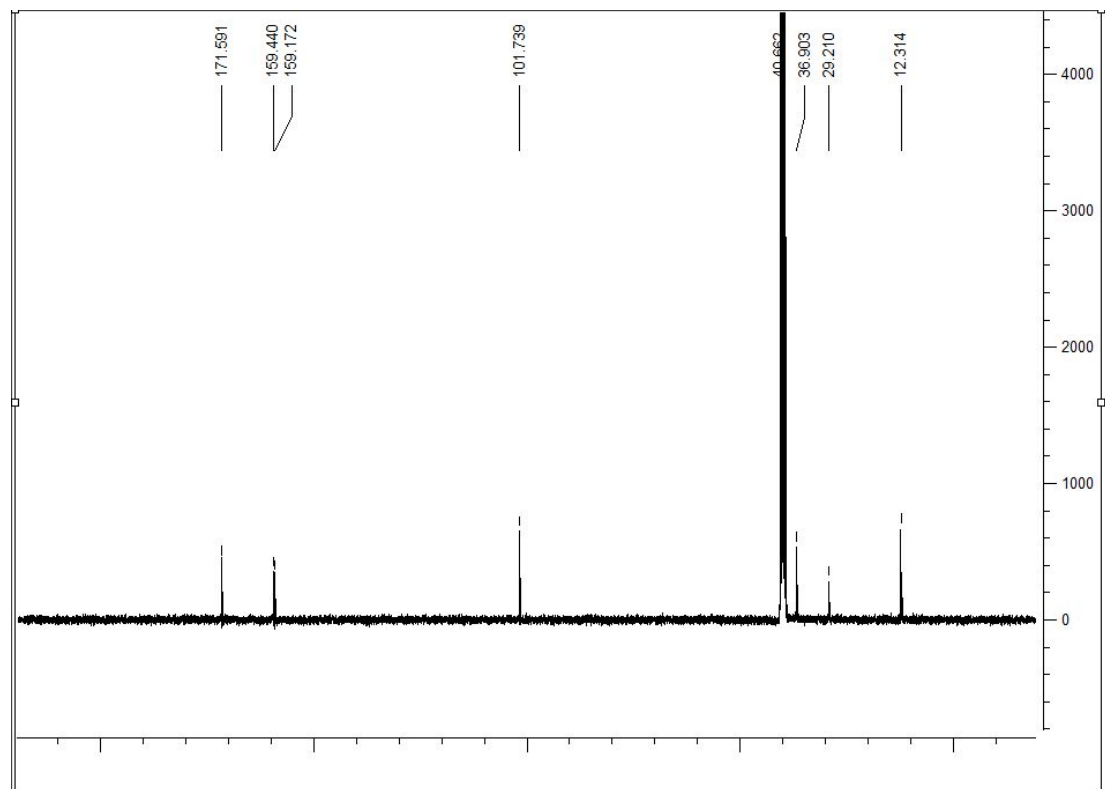
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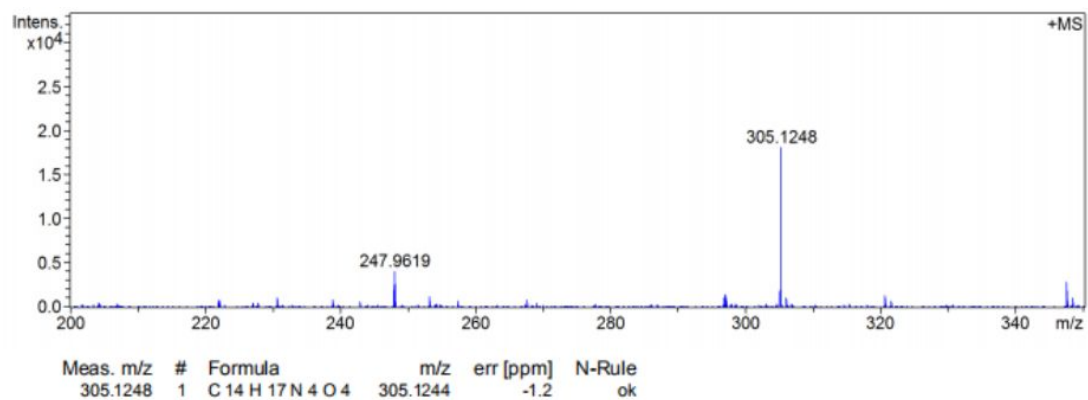
¹H NMR



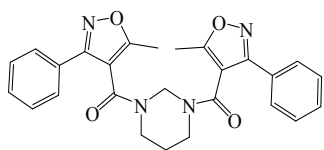
¹³C NHR



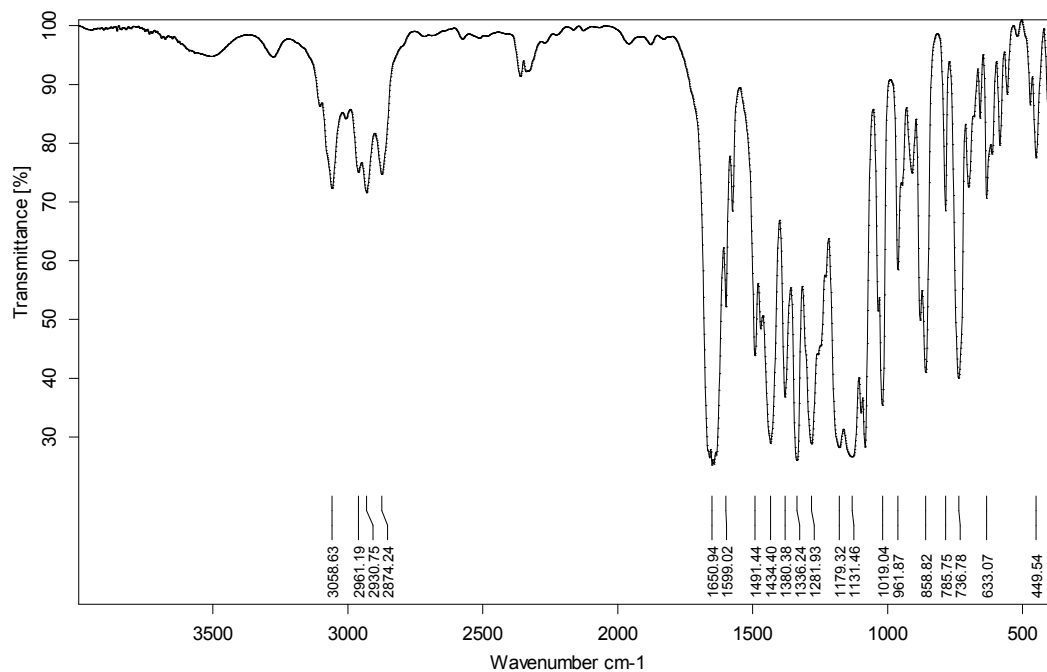
HRMS



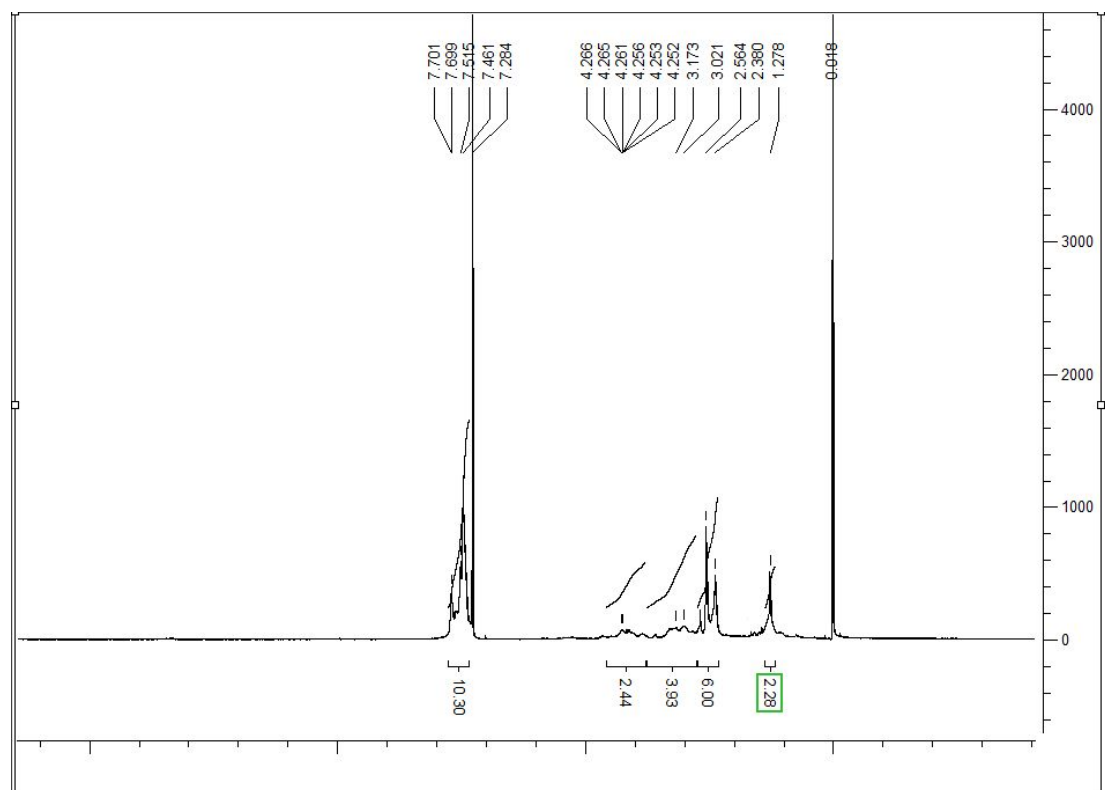
II-2



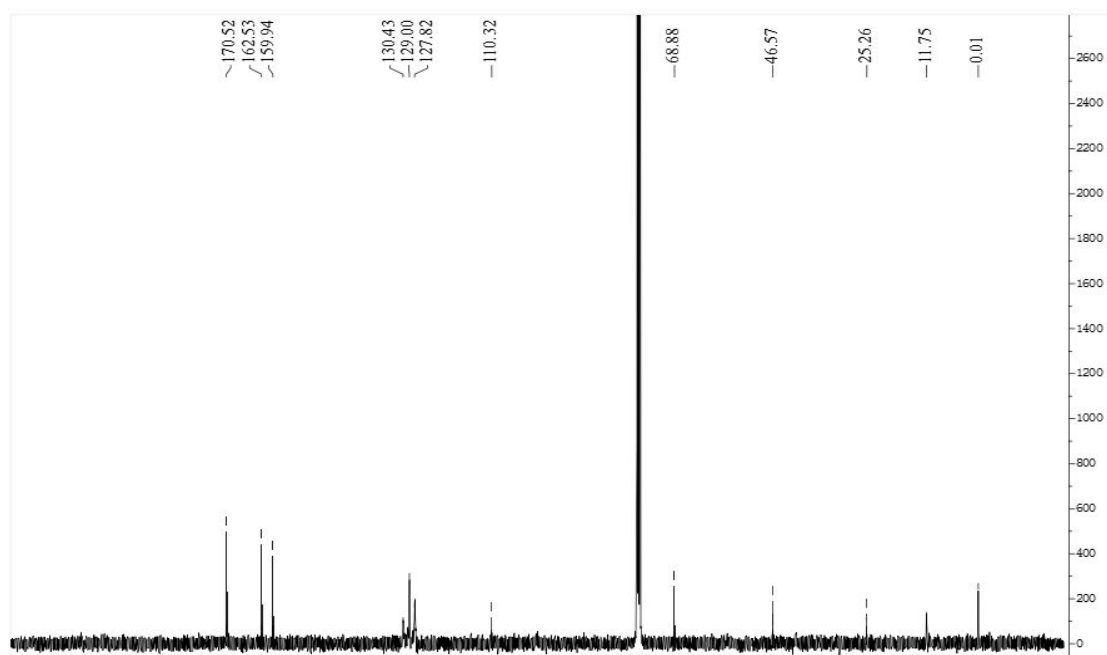
IR



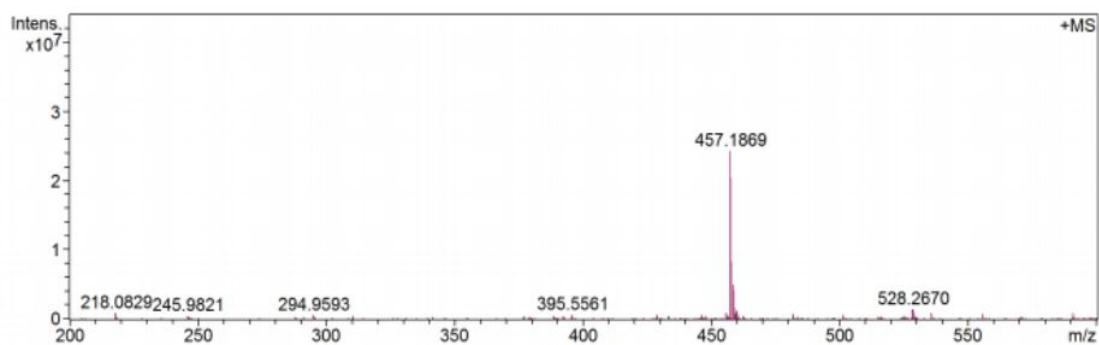
$^1\text{H NMR}$



¹³C NMR

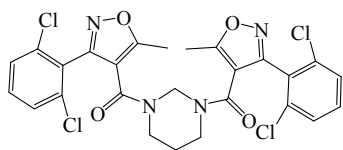


HRMS

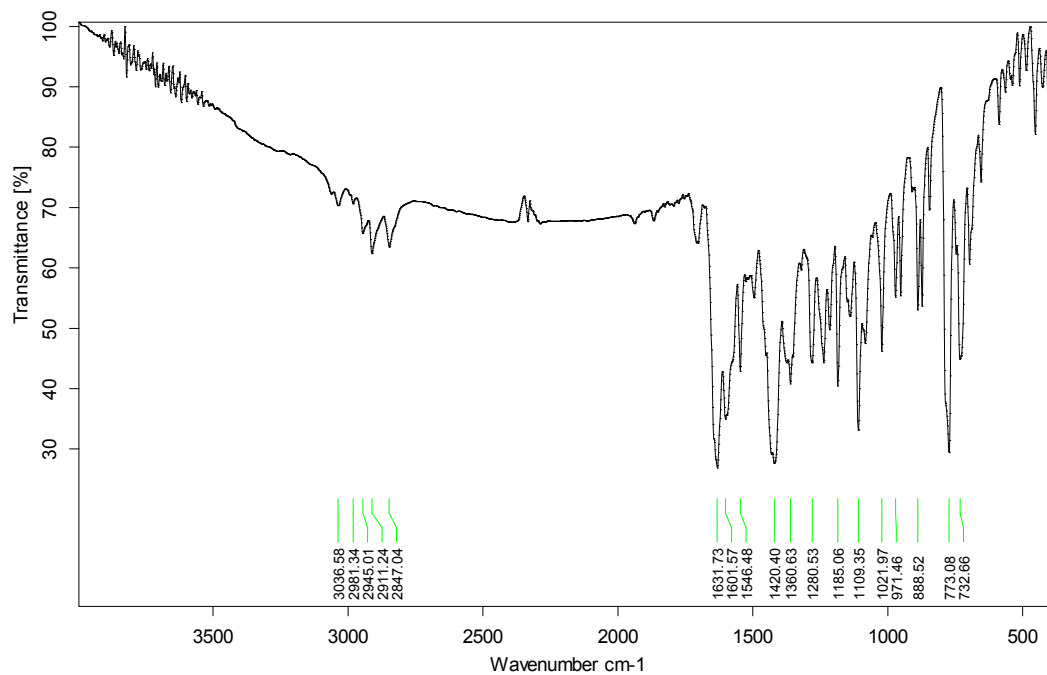


Meas. m/z	#	Formula	m/z	err [ppm]	N-Rule	e ⁻ Conf
457.1869	1	C ₂₆ H ₂₅ N ₄ O ₄	457.1870	0.3	ok	even

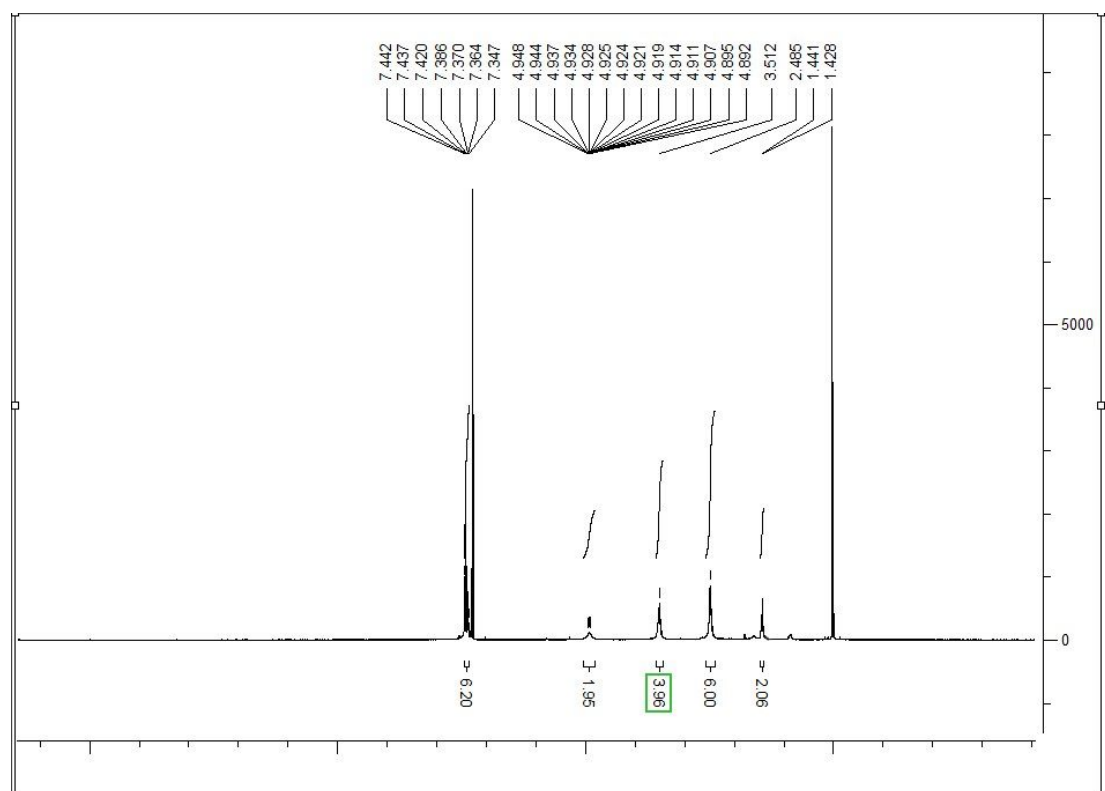
II-3



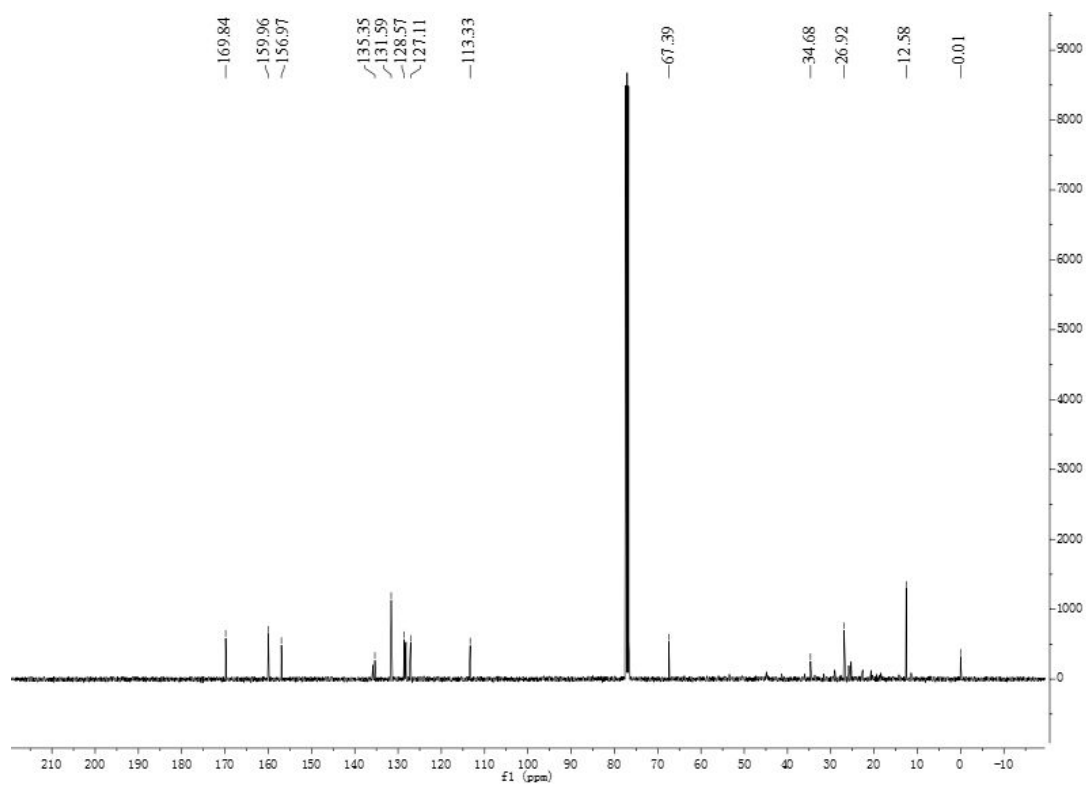
IR



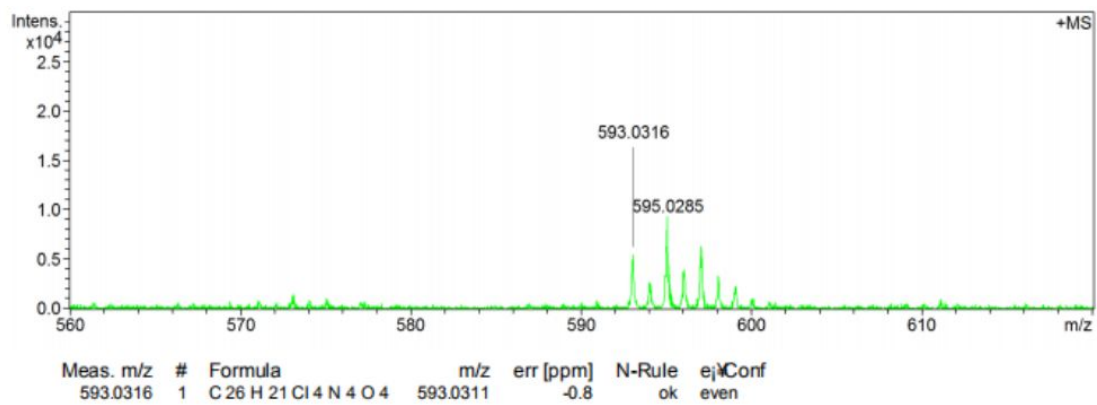
¹H NMR



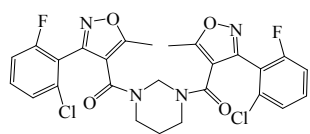
¹³C NMR



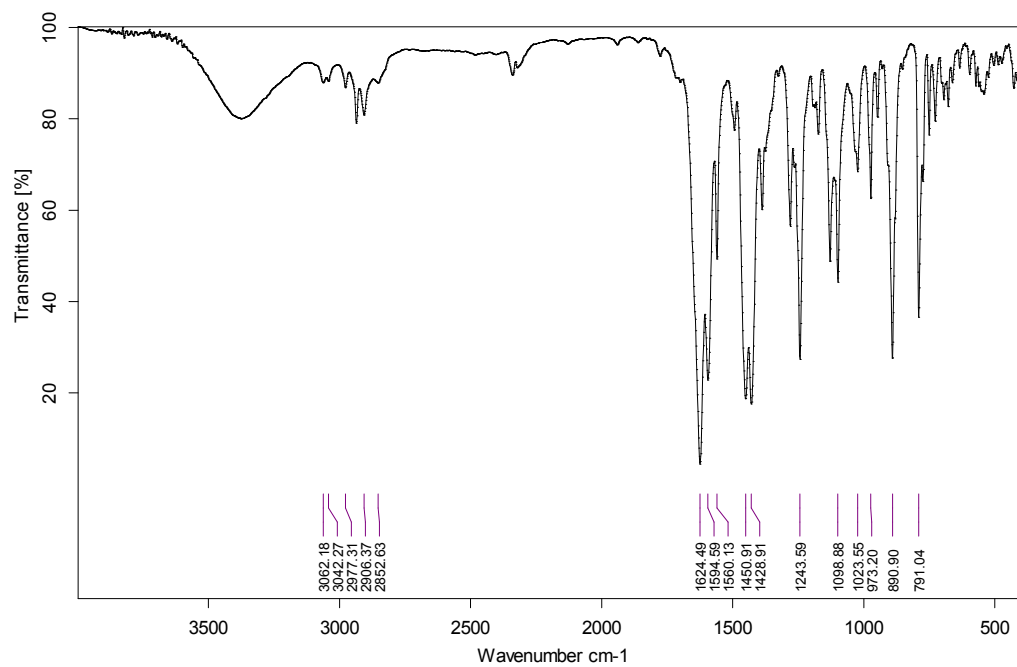
HRMS



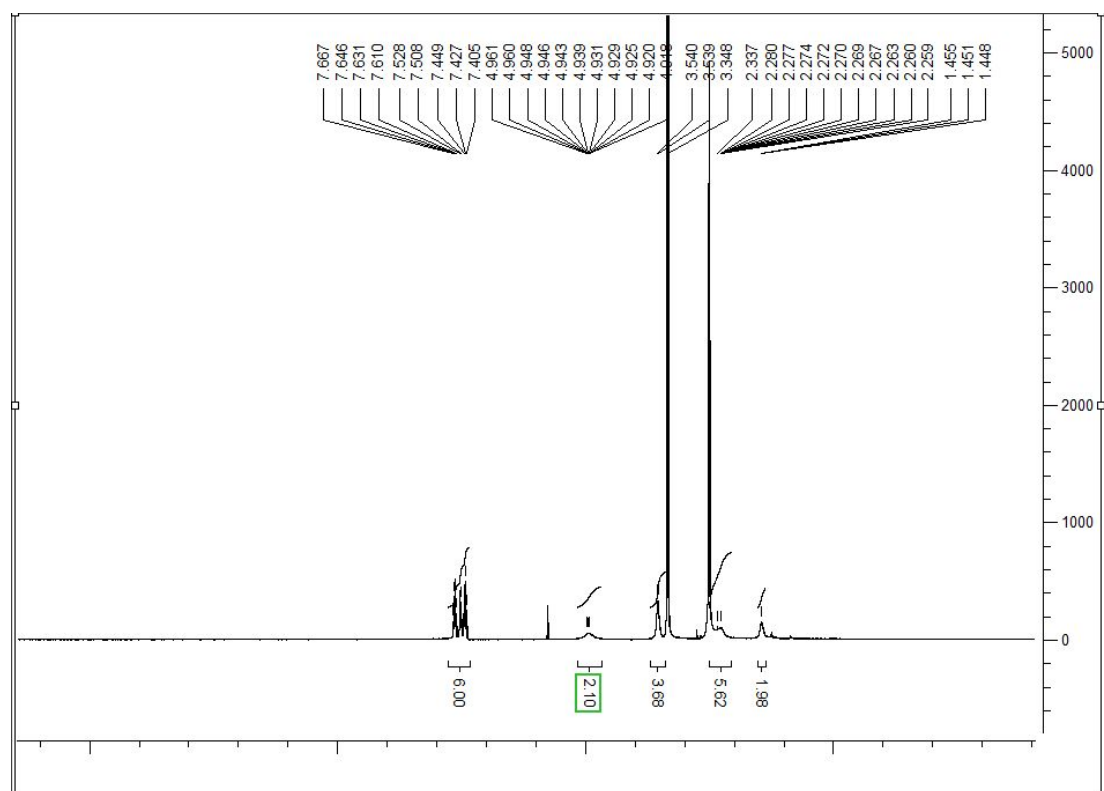
II-4



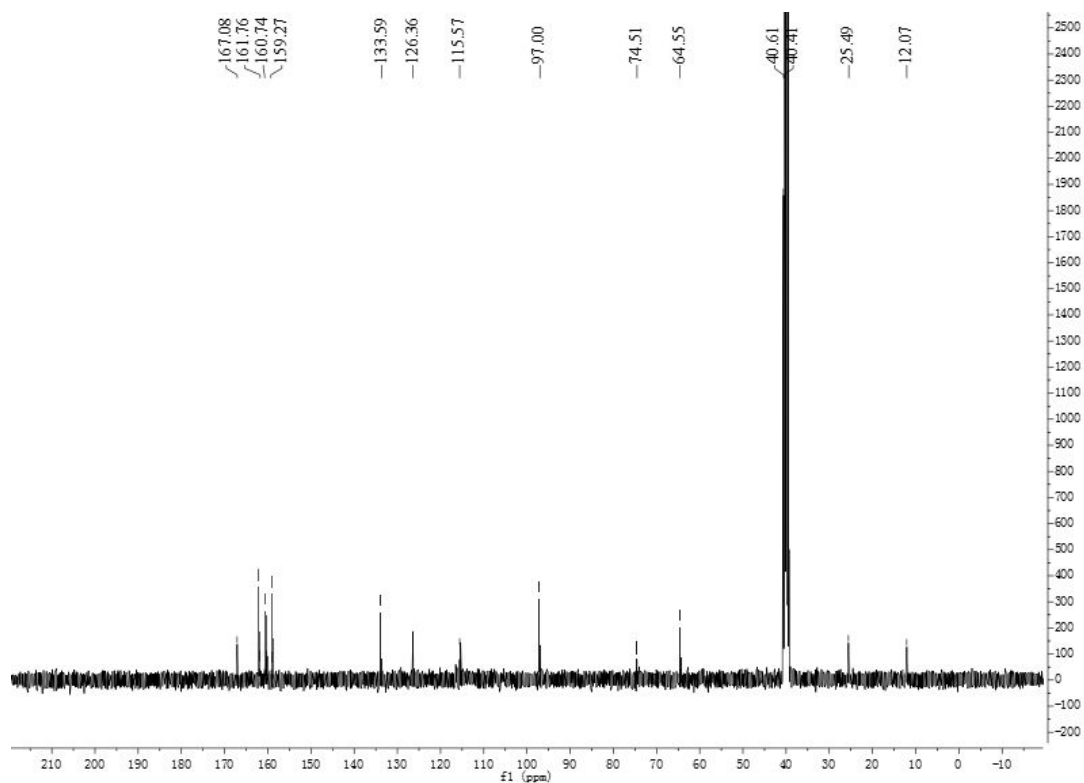
IR



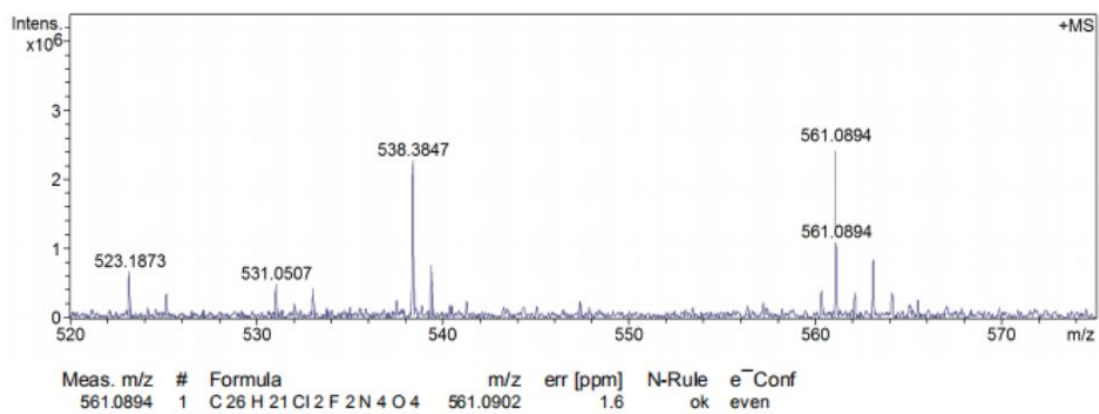
¹H NMR



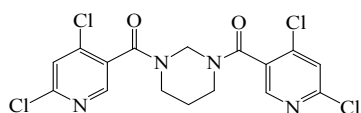
¹³C NHR



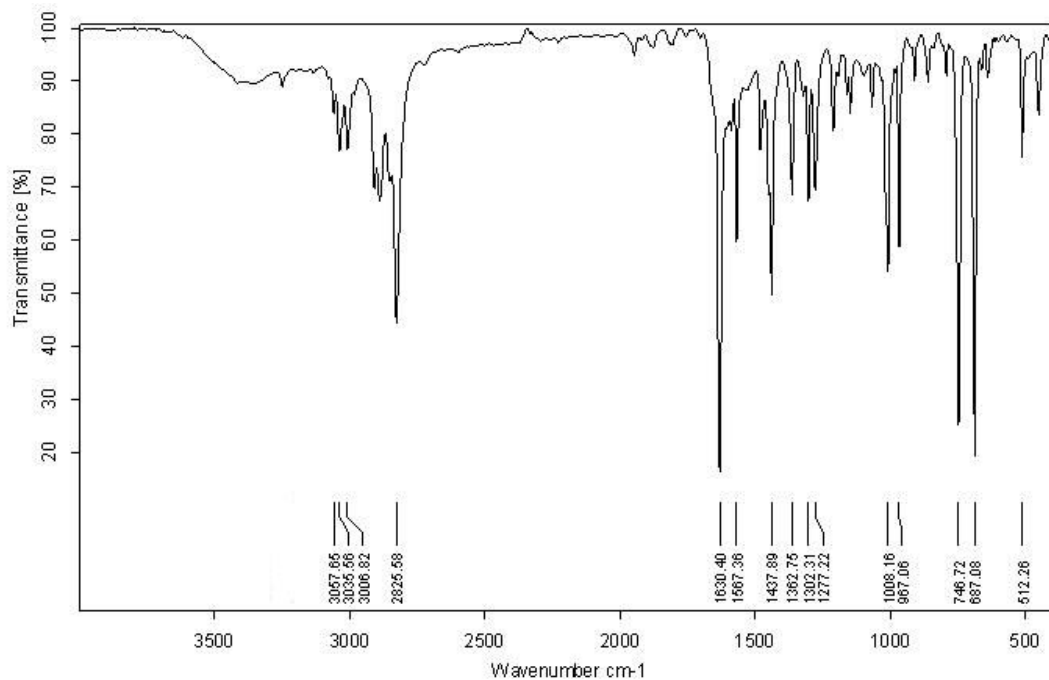
HRMS



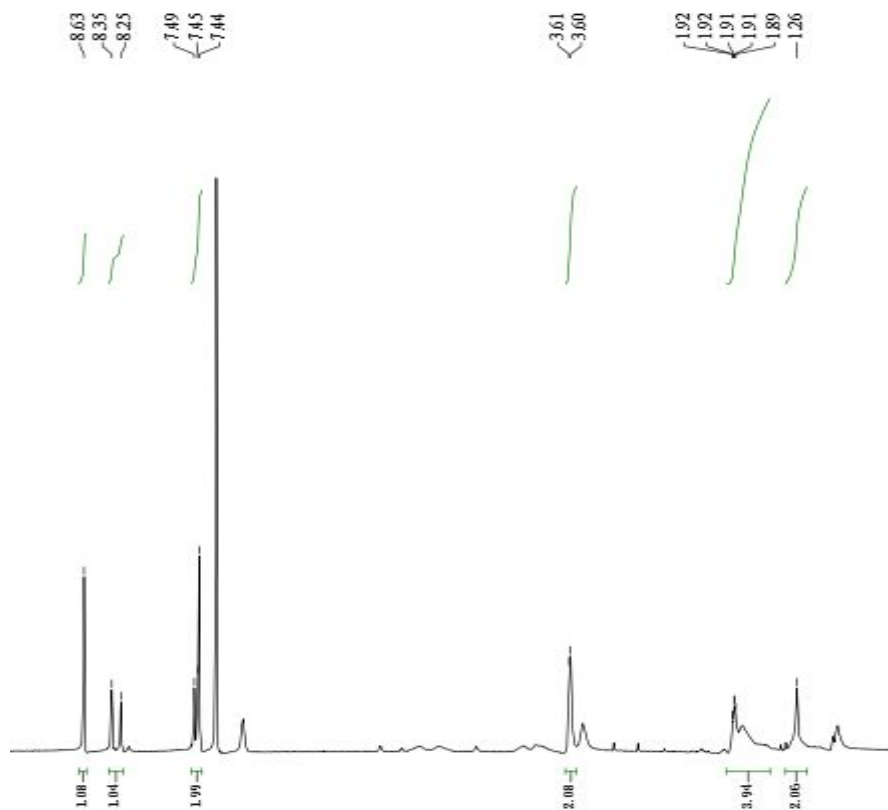
II-5



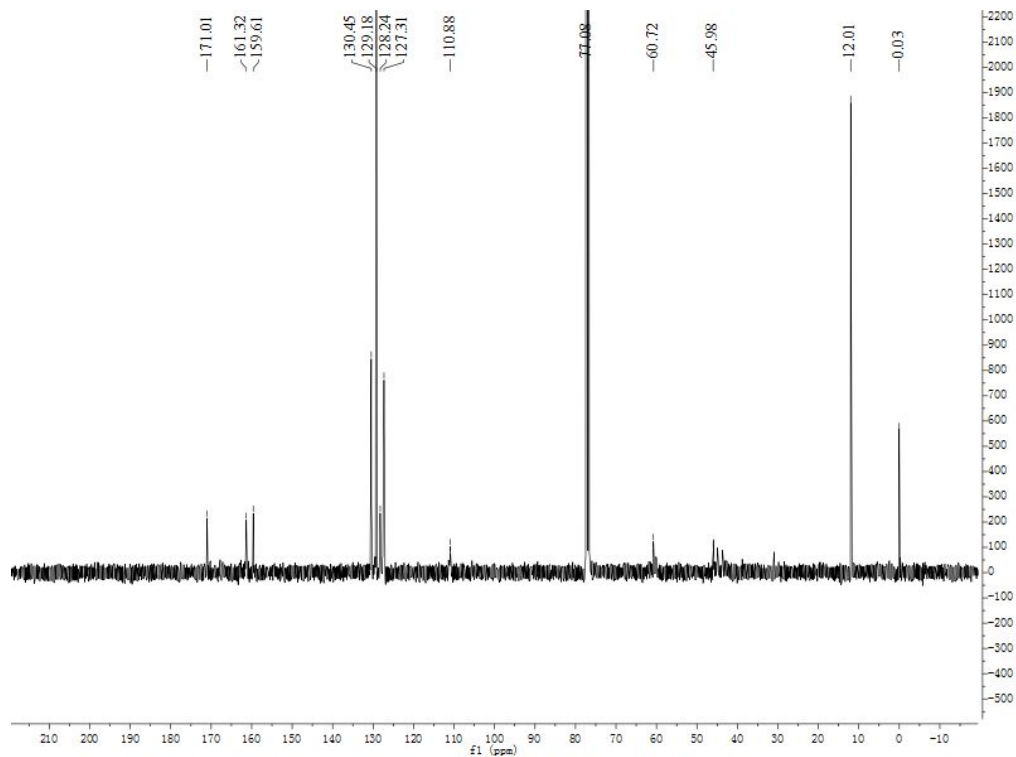
IR



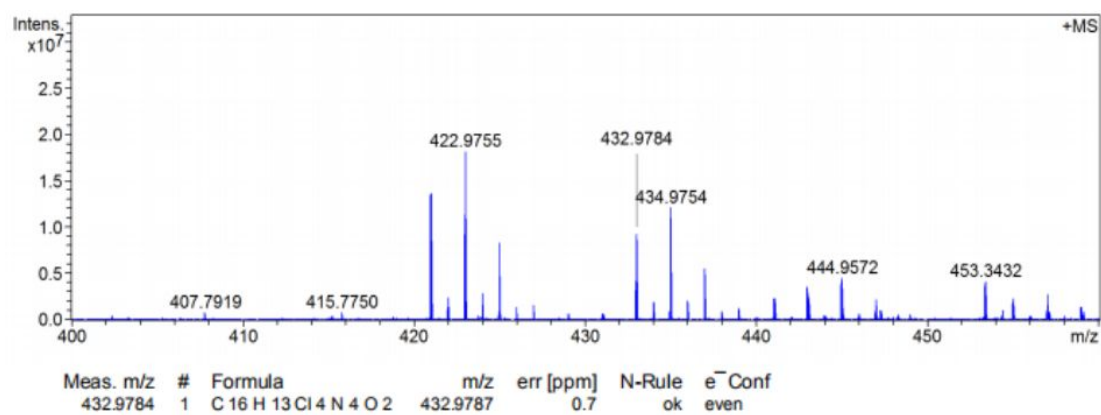
¹H NMR



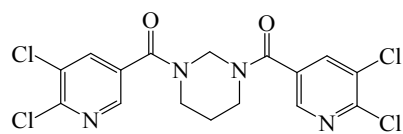
¹³C NHR



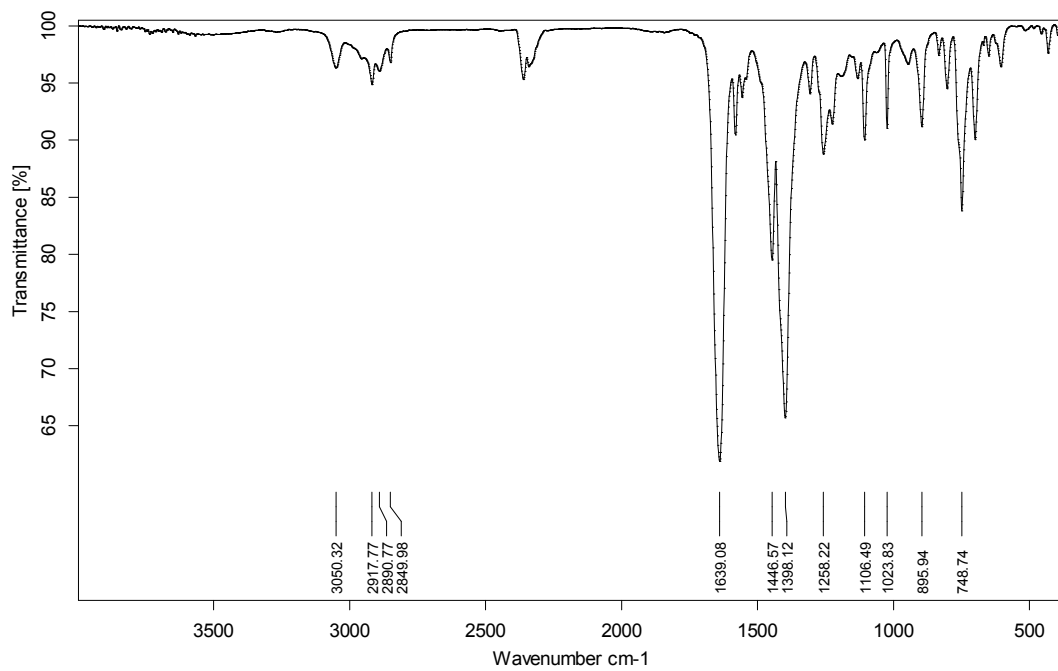
HRMS



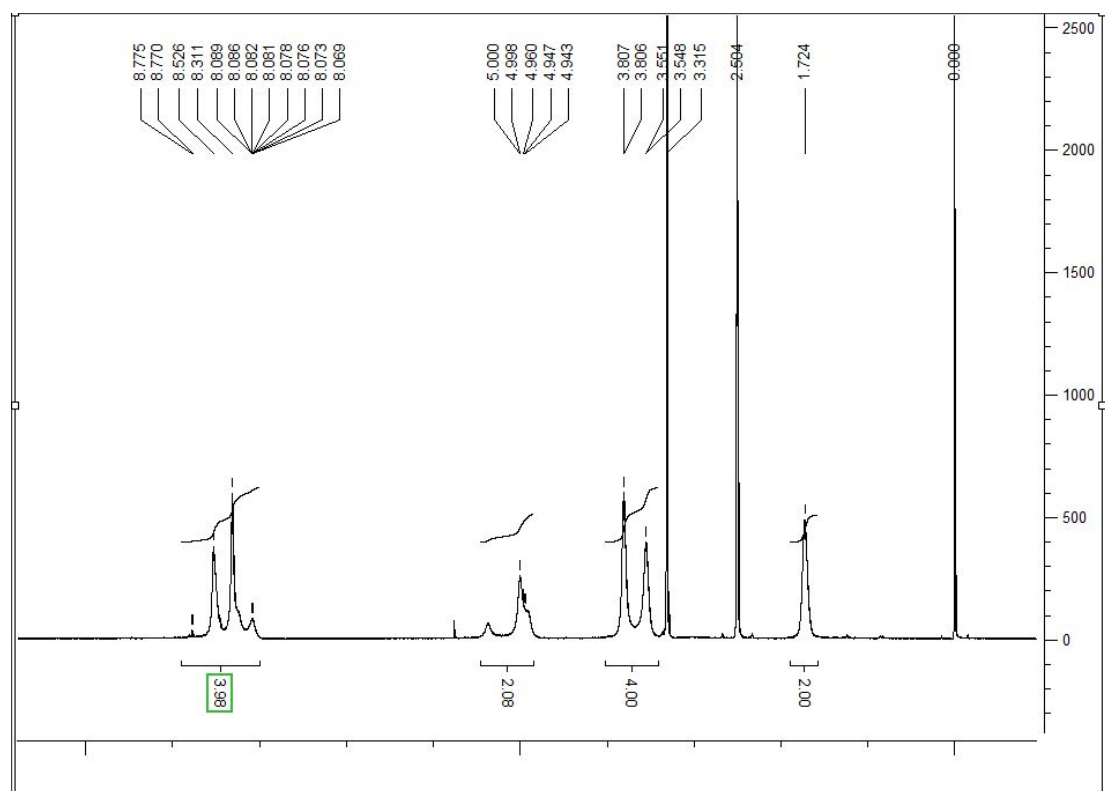
II-6



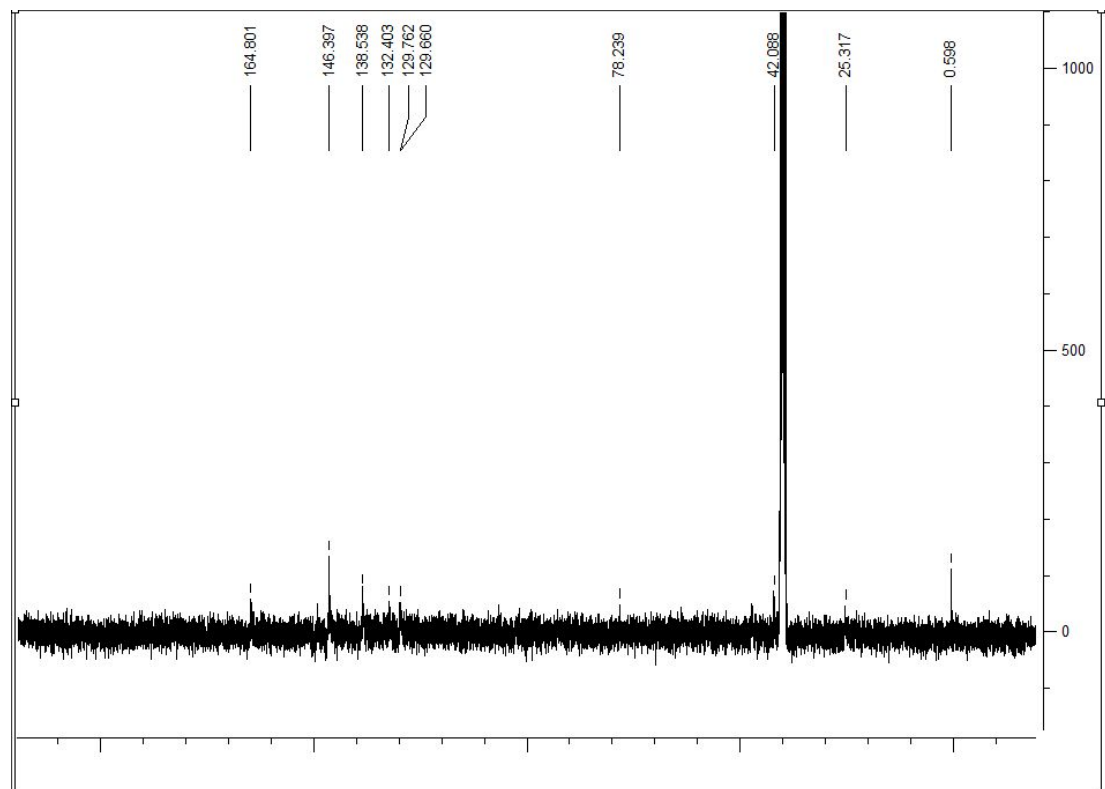
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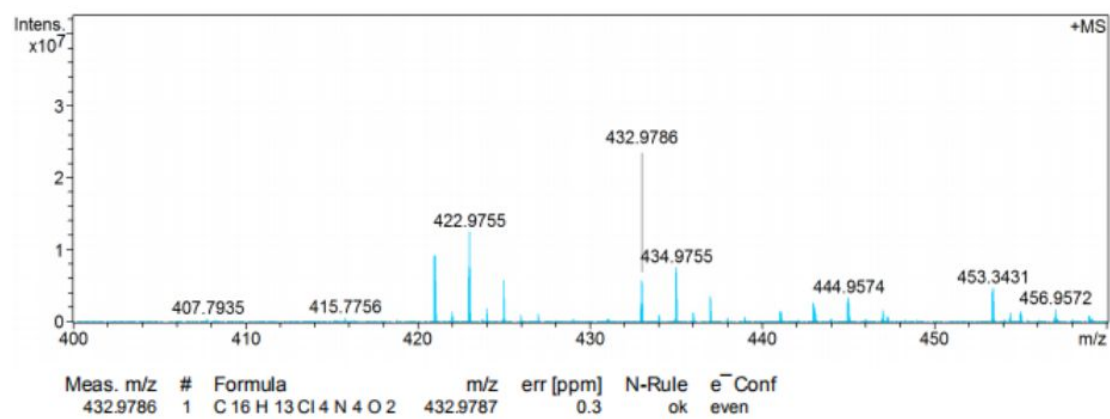
¹H NMR



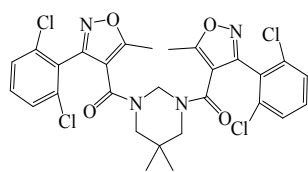
¹³C NHR



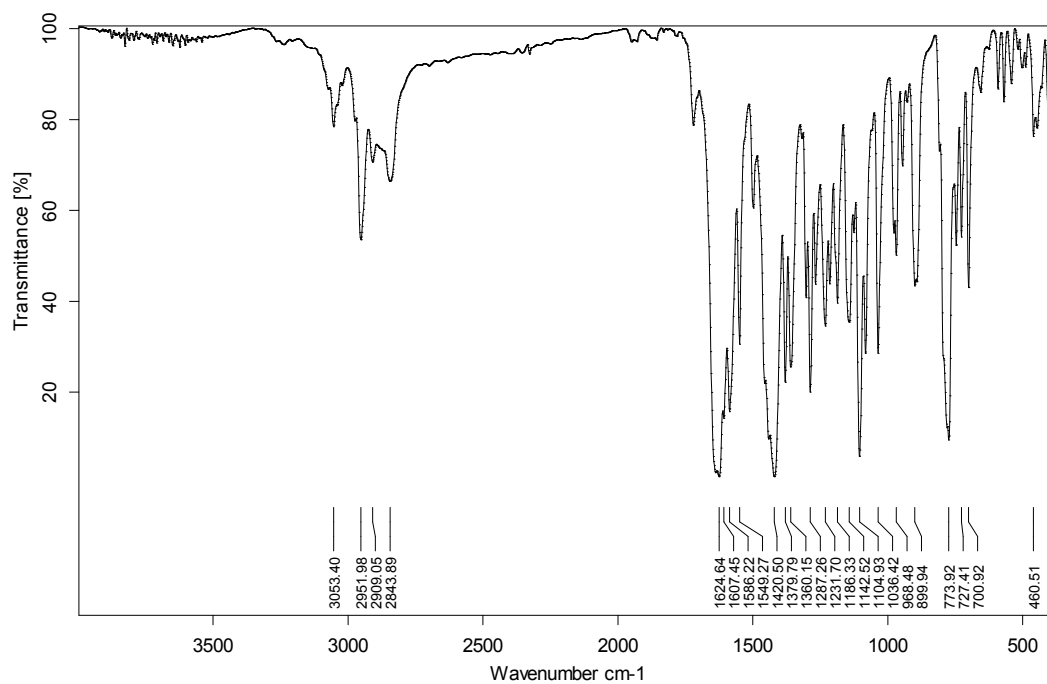
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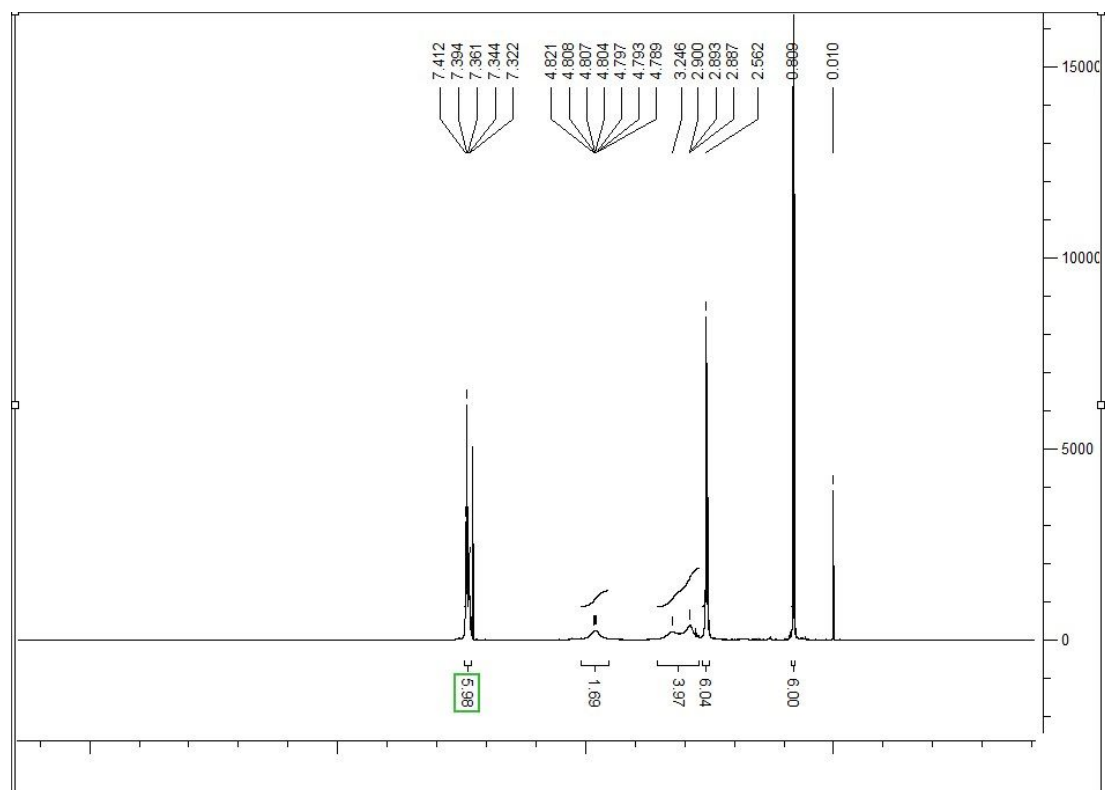
II-7



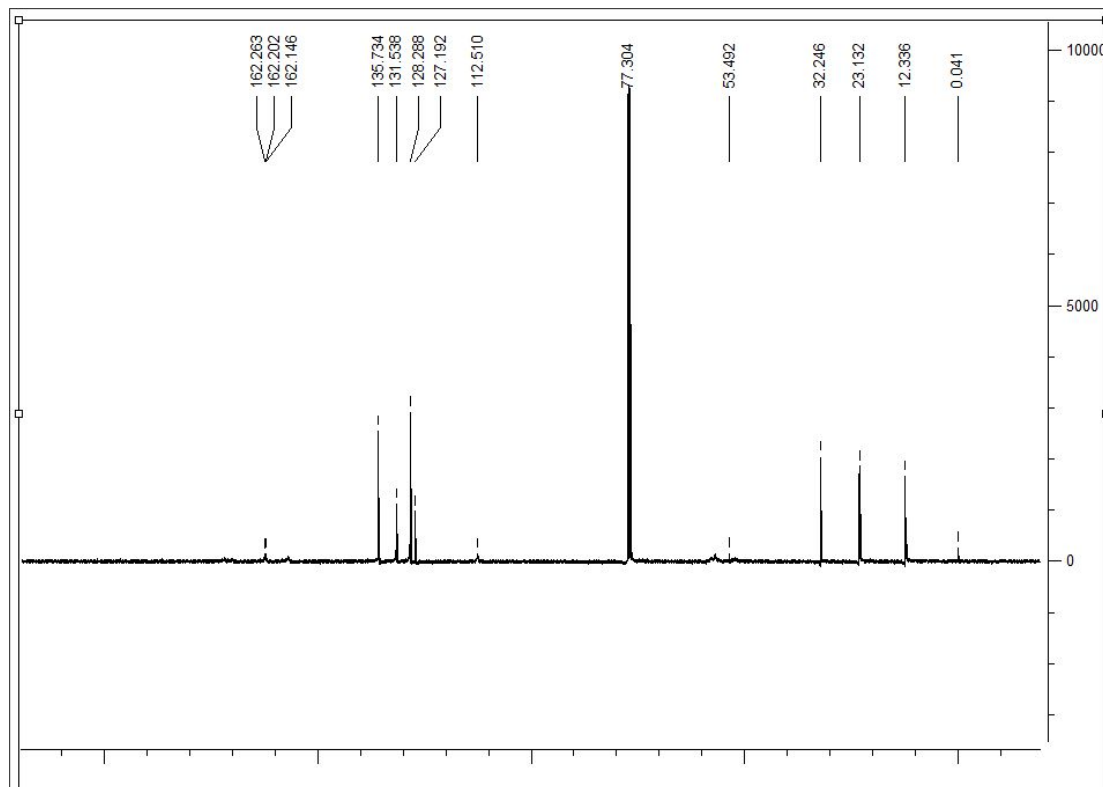
IR



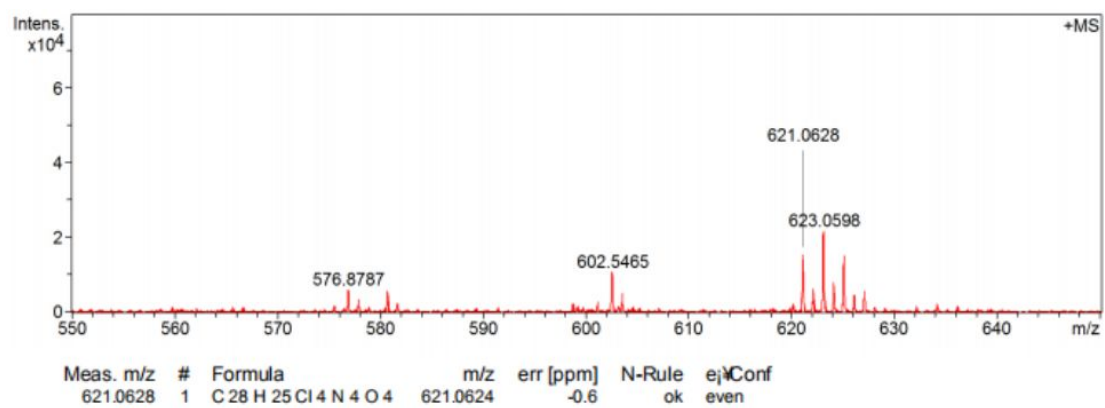
¹H NMR



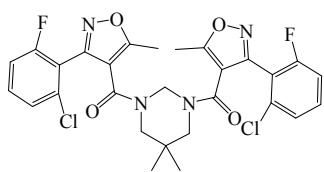
¹³C NHR



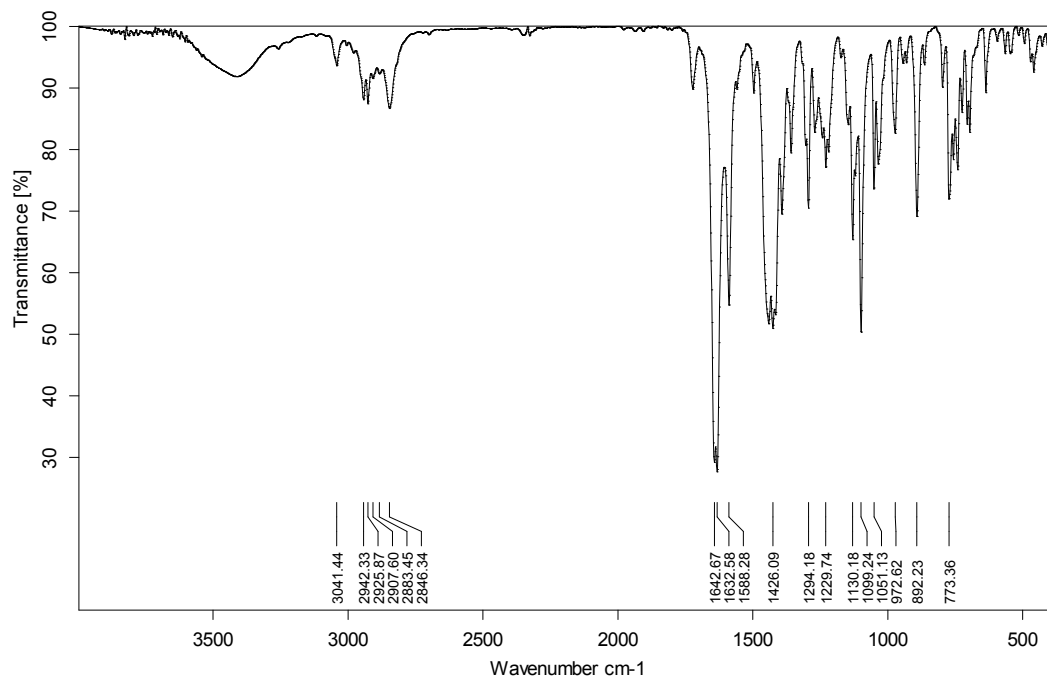
HRMS



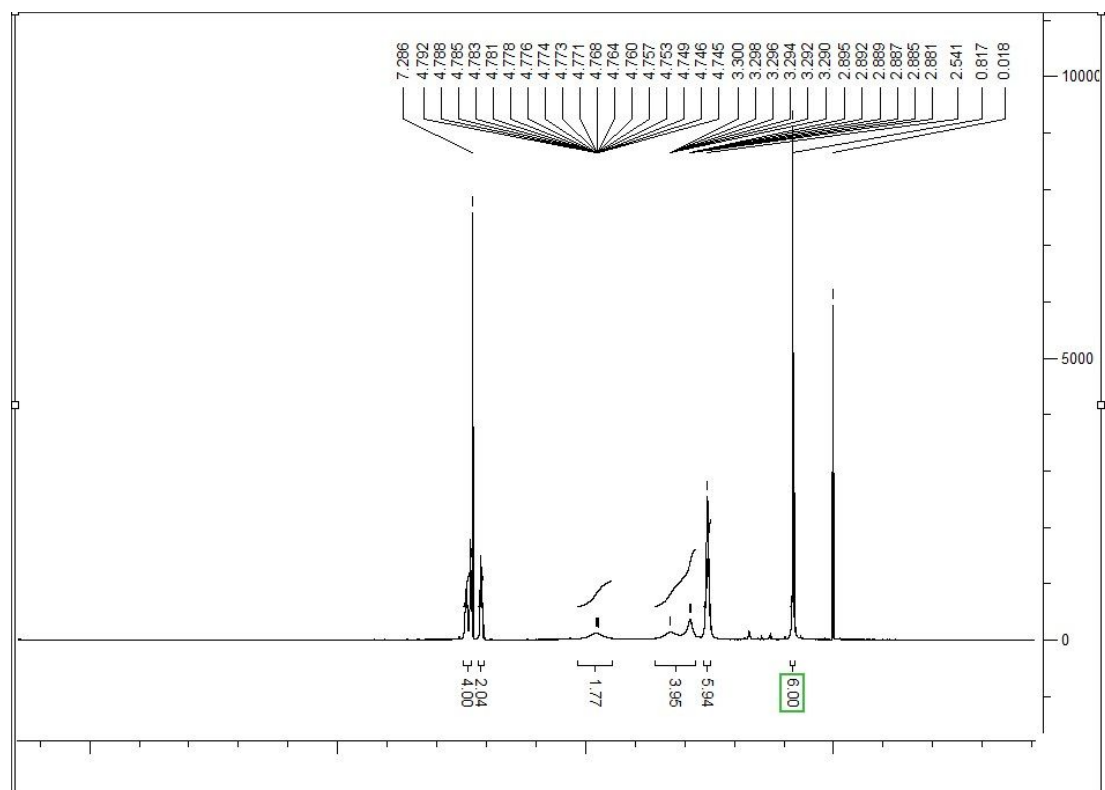
II-8



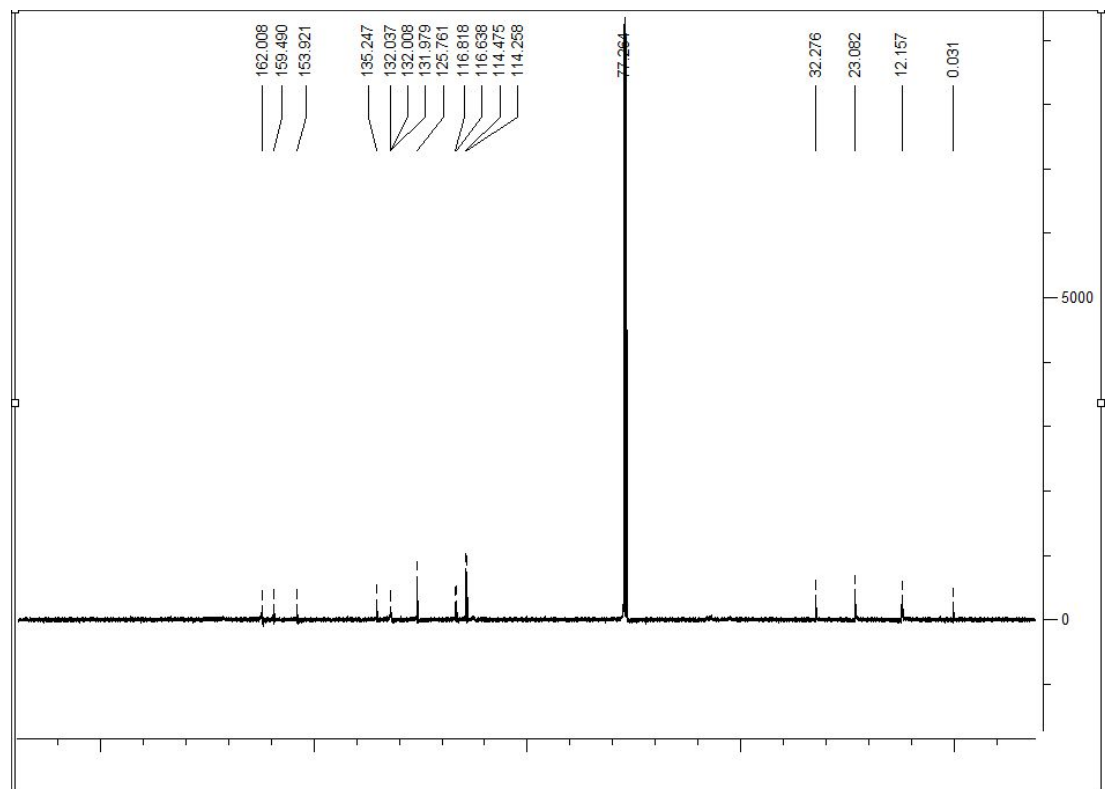
IR



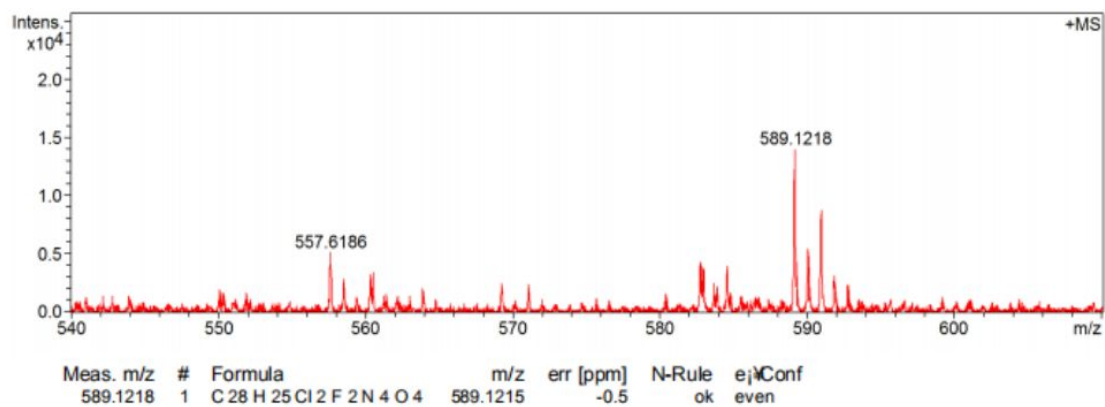
¹H NMR



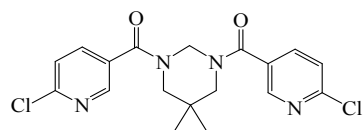
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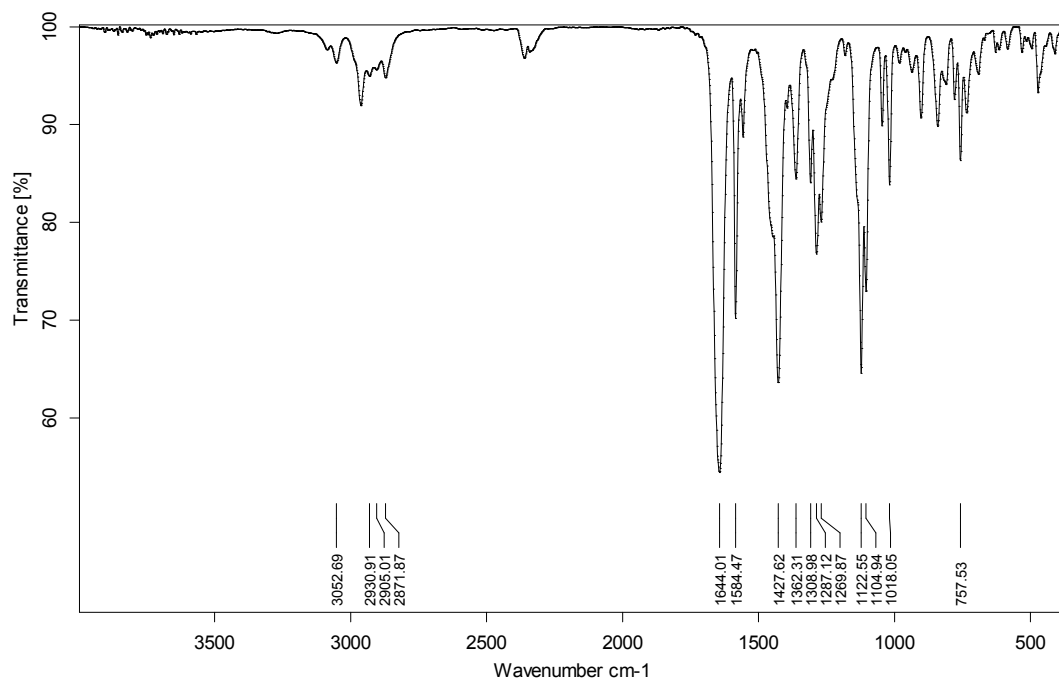
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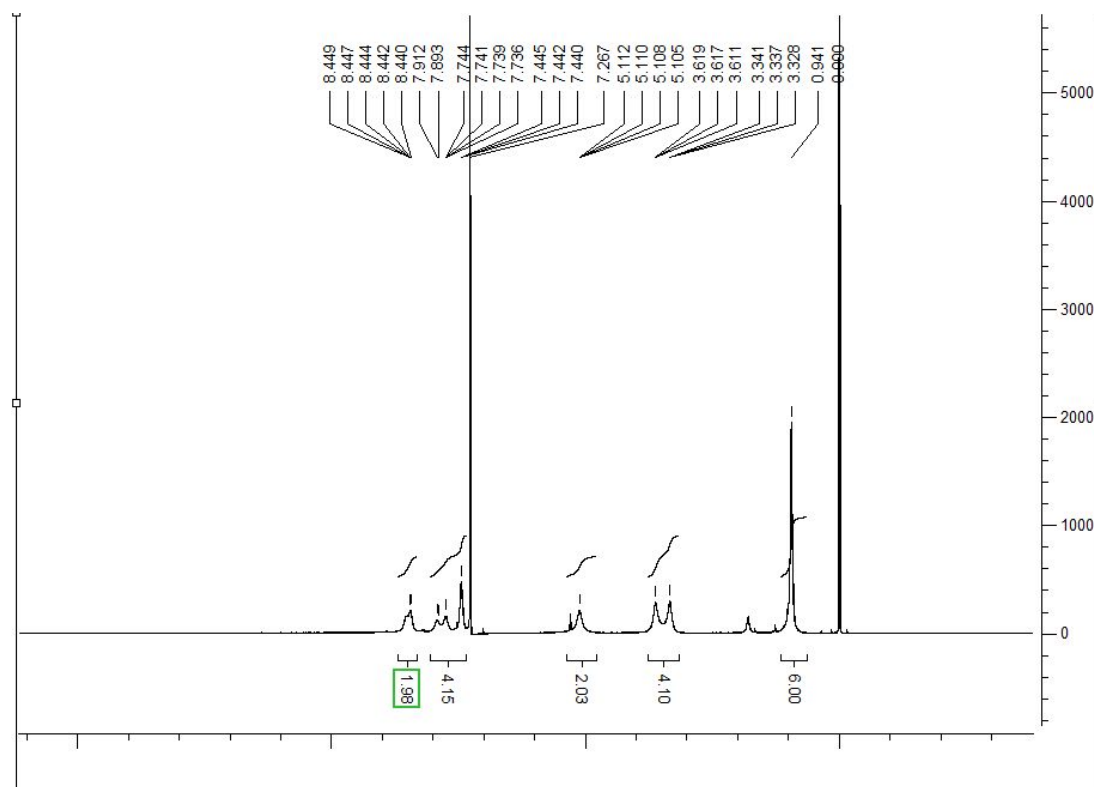
II-9



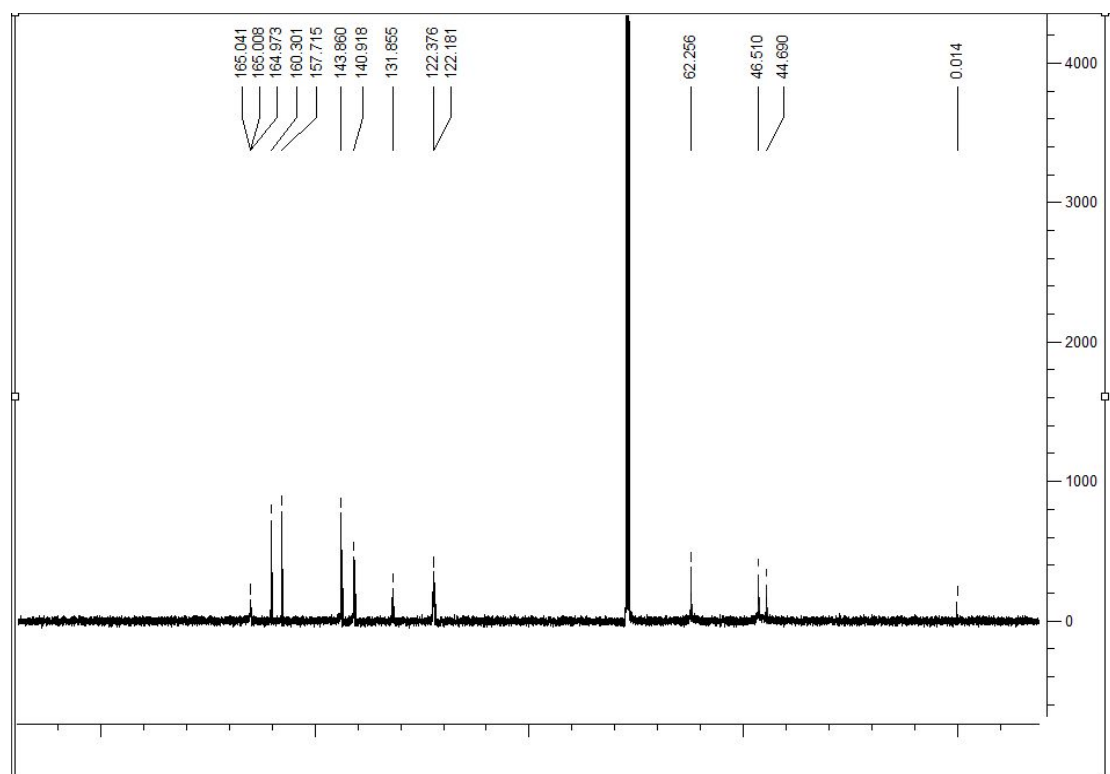
IR



¹H NMR



¹³C NHR



HRMS

