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Decorated multi-walled carbon nanotubes with Sm doped fluorapatites: Synthesis, characterization and catalytic activity

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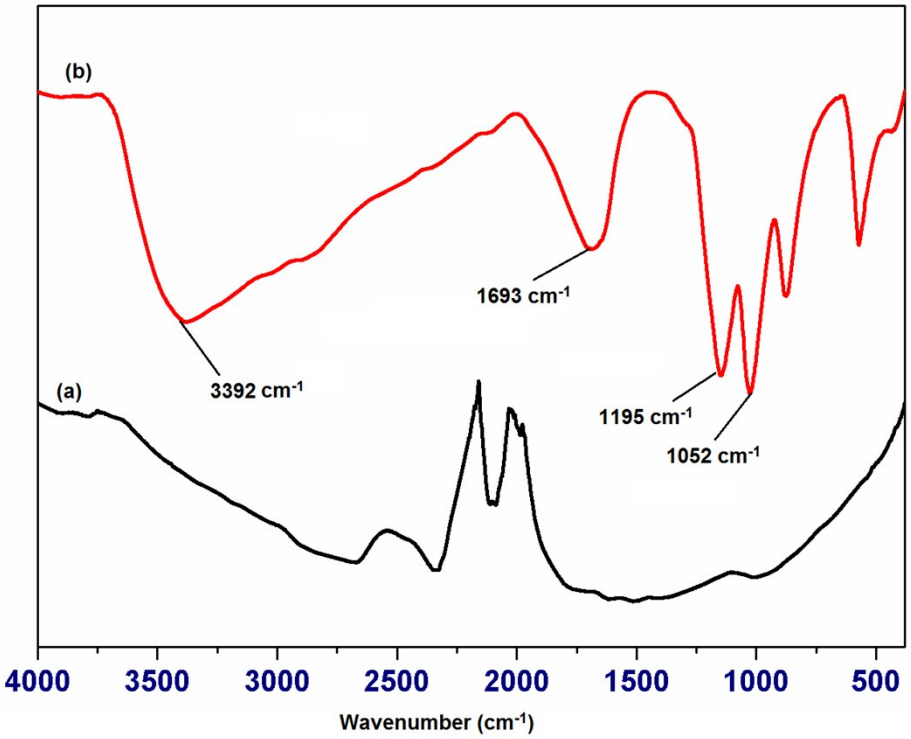


Fig. S1. FT-IR spectra of (a) Pristine MWCNT (b) Oxidized MWCNT

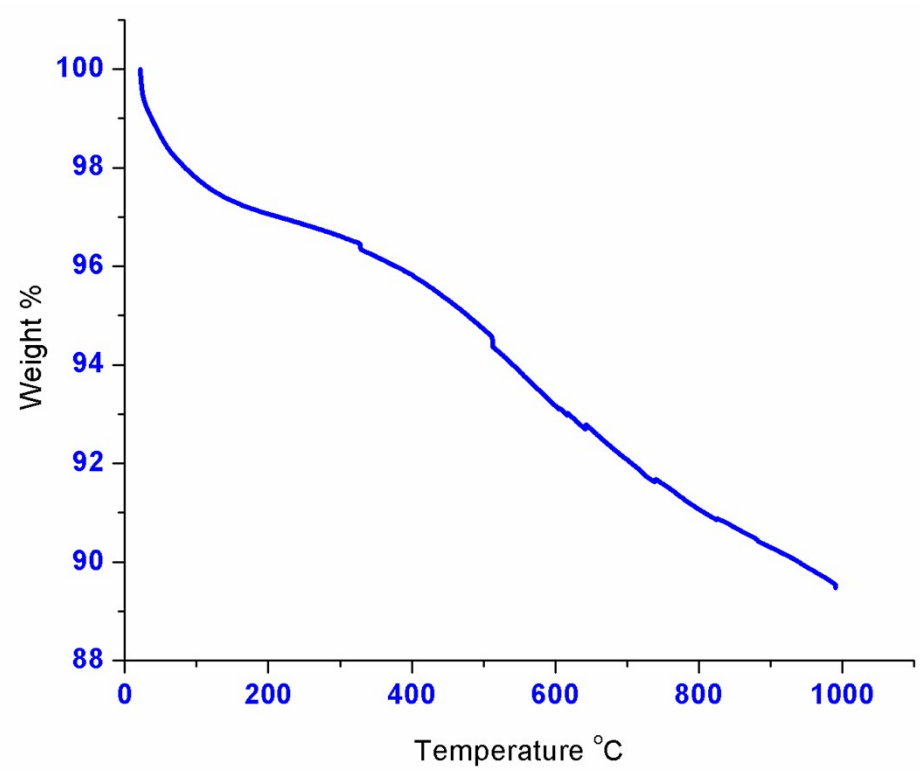


Fig. S2. TGA curve of MWCNT/5% Sm-FAp

Products characterization data:

Spectral data of 5-(2-flurophenyl)-1,2,4-triazolidine-3-thione: 1H NMR (400 MHz, DMSO-d_6) δ 7.20 – 7.26 (m, 2H, ArH), 7.40 – 7.46 (m, 1H, ArH), 8.06 (s, 1H, NH), 8.20 – 8.24 (m, 1H, ArH), 8.28 (s, 1H, NH), 8.28 (s, 1H, CH), 11.54 (s, 1H, NH): 13C NMR (100 MHz, DMSO-d_6): 115.61, 115.82, 121.69, 121.79, 124.60, 124.63, 126.77, 126.79, 131.59, 131.67, 134.64, 134.69, 159.53, 162.01, 178.14; 15N NMR (40.55 MHz, DMSO-d_6) δ 8.06 (s, 1H, NH), 8.28 (s, 1H, NH), 11.54 (s, 1H, NH); FT-IR: 1284, 1371, 1482, 1516, 3017, 3147, 3248, 3432.

Spectral data of 5-(3,4-dimethoxyphenyl)-1,2,4-triazolidine-3-thione: ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.76 (s, 3H, OCH_3), 3.79 (s, 3H, OCH_3), 6.94 (d, *J* = 8.32 Hz, 1H, ArH), 7.14 (dd, *J* = 8.28 Hz, 1.8 Hz, 1H, ArH), 7.48 (d, *J* = 1.76 Hz,1H, ArH), 7.96 (s, 1H, CH), 7.97 (s, 1H, NH), 8.06(s, 1H, NH), 11.25 (s, 1H, NH): ^{13}C NMR (100 MHz, DMSO-d_6): 55.45, 55.60, 108.35, 111.17, 122.21, 126.75, 142.75, 149.03, 150.54, 177.39; ^{15}N NMR (40.55 MHz, DMSO-d_6) δ 7.97 (s, 1H, NH), 8.06 (s, 1H, NH), 11.25 (s, 1H, NH); FT-IR: 1235, 1445, 1510, 1618, 2960, 3182, 3261, 3261, 3351.

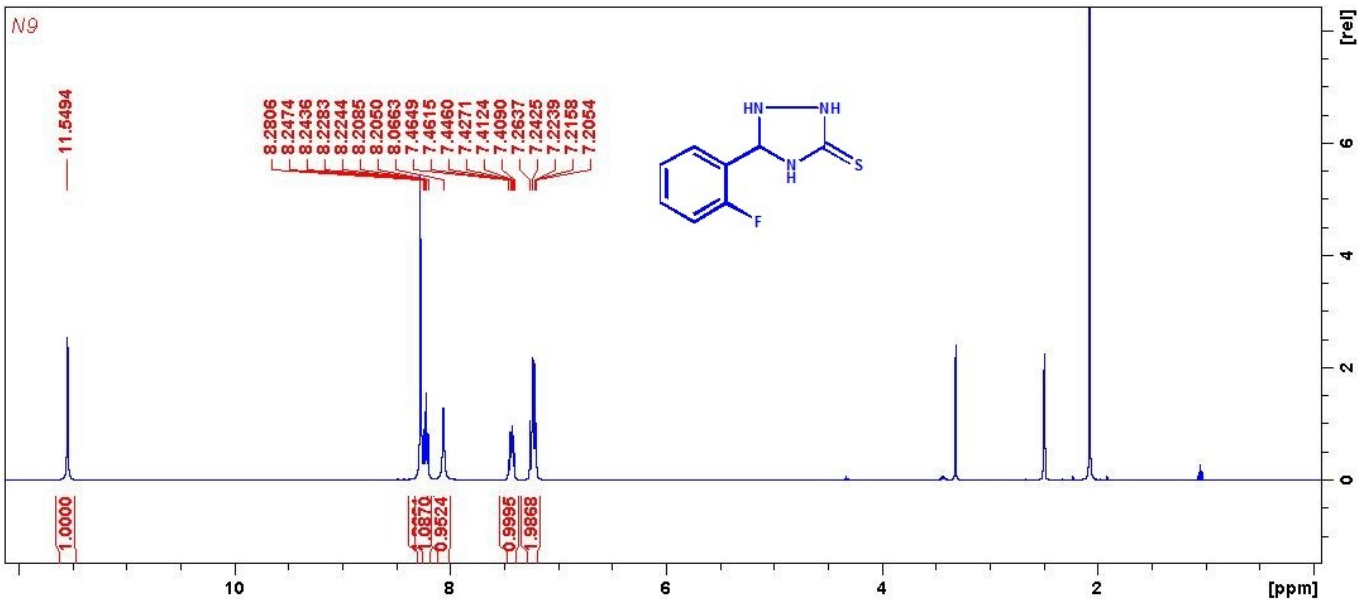
Spectral data of 5-(4-ethylphenyl)-1,2,4-triazolidine-3-thione: 1H NMR (400 MHz, DMSO-d_6) δ 1.15 (t, *J* = 7.56 Hz, 3H, CH_3), 2.56 – 2.62 (m, 2H, CH_2), 7.22 (d, *J* = 8.16 Hz, 2H, ArH), 7.67 (d, *J* = 8.16 Hz, 2H, ArH), 7.91 (s, 1H, NH), 8.01 (s, 1H, CH), 8.10(s, 1H, NH), 11.33 (s, 1H, NH): 13C NMR (100 MHz, DMSO-d_6): 15.30, 28.03, 127.31, 128.08, 131.55, 142.60, 145.97, 177.71; 15N NMR (40.55 MHz, DMSO-d_6) δ 7.91 (s, 1H, NH), 8.10 (s, 1H, NH), 11.33 (s, 1H, NH); FT-IR: 1289, 1368, 1457, 1533, 2927, 2955, 3024, 3153, 3247, 3403, 3650.

Spectral data of 5-(3,4-dihydroxyphenyl)-1,2,4-triazolidine-3-thione: 1H NMR (400 MHz, DMSO-d_6) δ 6.74 (d, *J* = 8.08 Hz, 1H, ArH), 7.00 (d, *J* = 7.64 Hz, 1H, ArH), 7.17 (s, 1H, CH), 7.70 (s, 1H, NH), 7.88 (s, 1H, ArH), 8.01(s, 1H, NH), 8.99 (s, 1H, OH), 9.46 (s, 1H, OH), 11.18 (s, 1H, NH): 13C NMR (100 MHz, DMSO-d_6): 113.74, 115.48, 120.18, 125.49, 143.29, 145.46, 147.69, 177.27; 15N NMR (40.55 MHz, DMSO-d_6) δ 7.70 (s, 1H, NH), 8.01 (s, 1H, NH), 11.18 (s, 1H, NH); FT-IR: 1276,1328, 1463, 1591, 1619, 1933, 2090, 3053, 3178, 3320, 3442

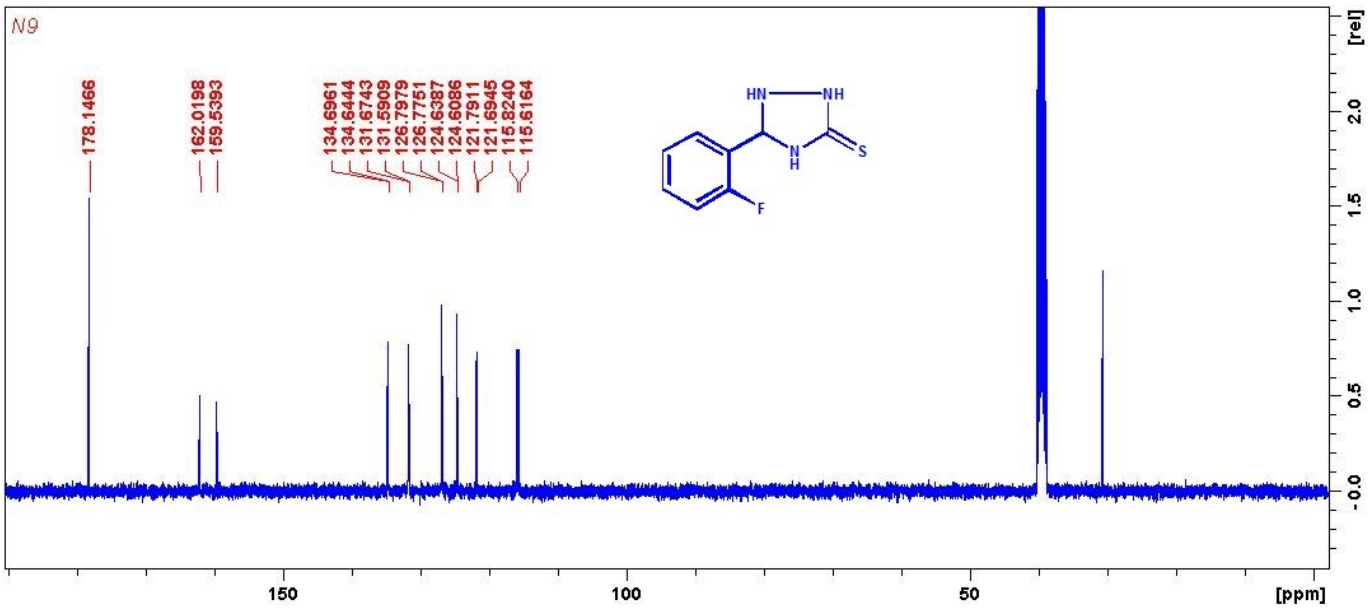
Table 1: Optimization of the amount of MWCNT/5%Sm-FAp as catalyst in the model reaction[a]

Entry	Catalyst (mg)	Time (min)	Yield (%)
1	10	35	80
2	20	25	87
3	30	10	96
4	40	15	93
5	50	15	91

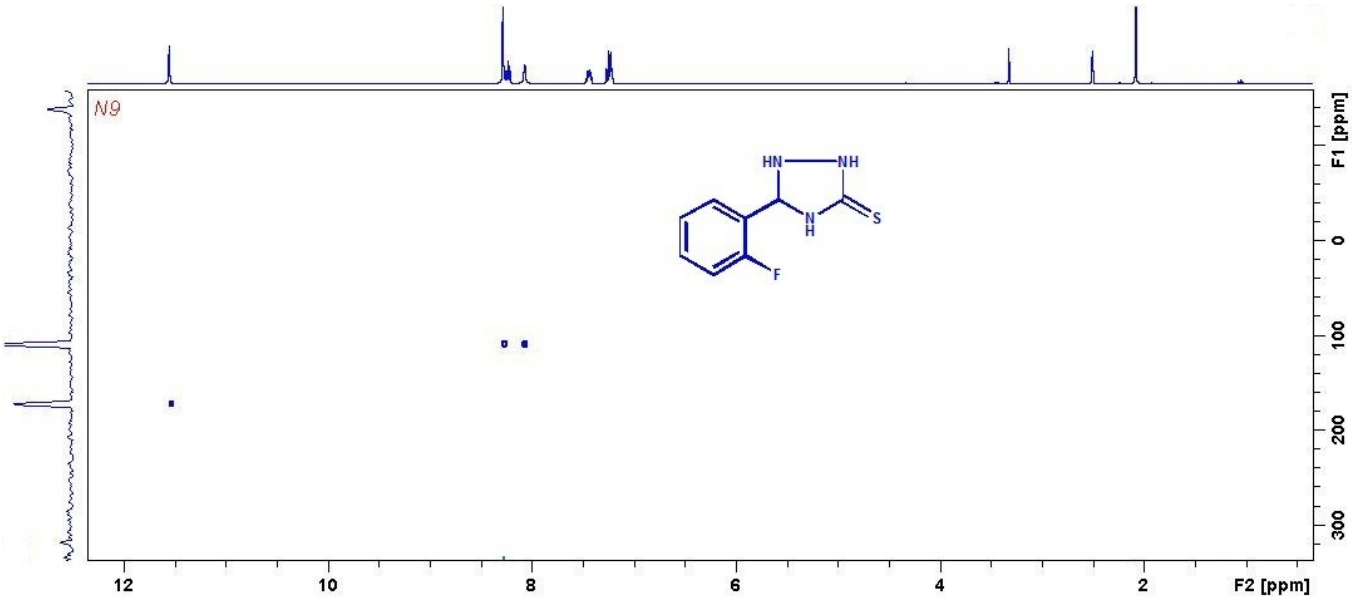
[a]Reaction conditions: 2-methoxybenzaldehyde (1.0 mmol), thiosemicarbazide (1.0 mmol), catalyst and ethanol (5.0 mL) were stirred at room temperature



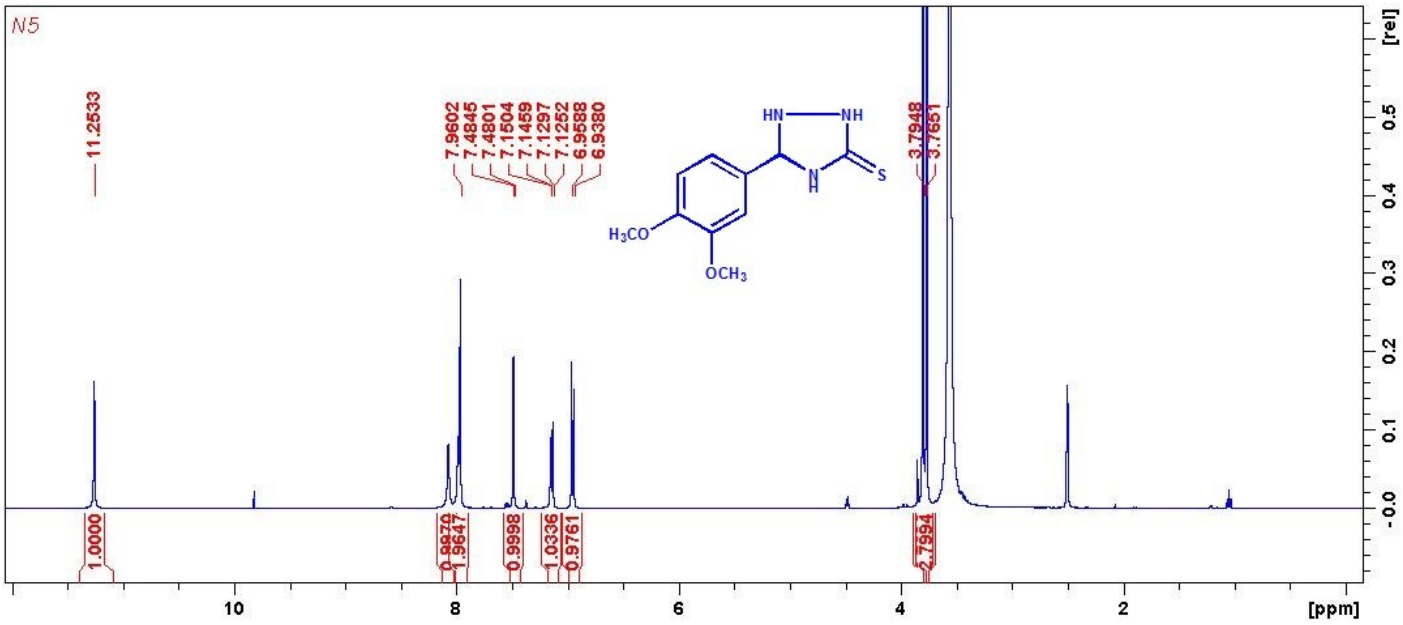
^{1}H NMR spectrum of 5-(2-flurophenyl)-1,2,4-triazolidine-3-thione



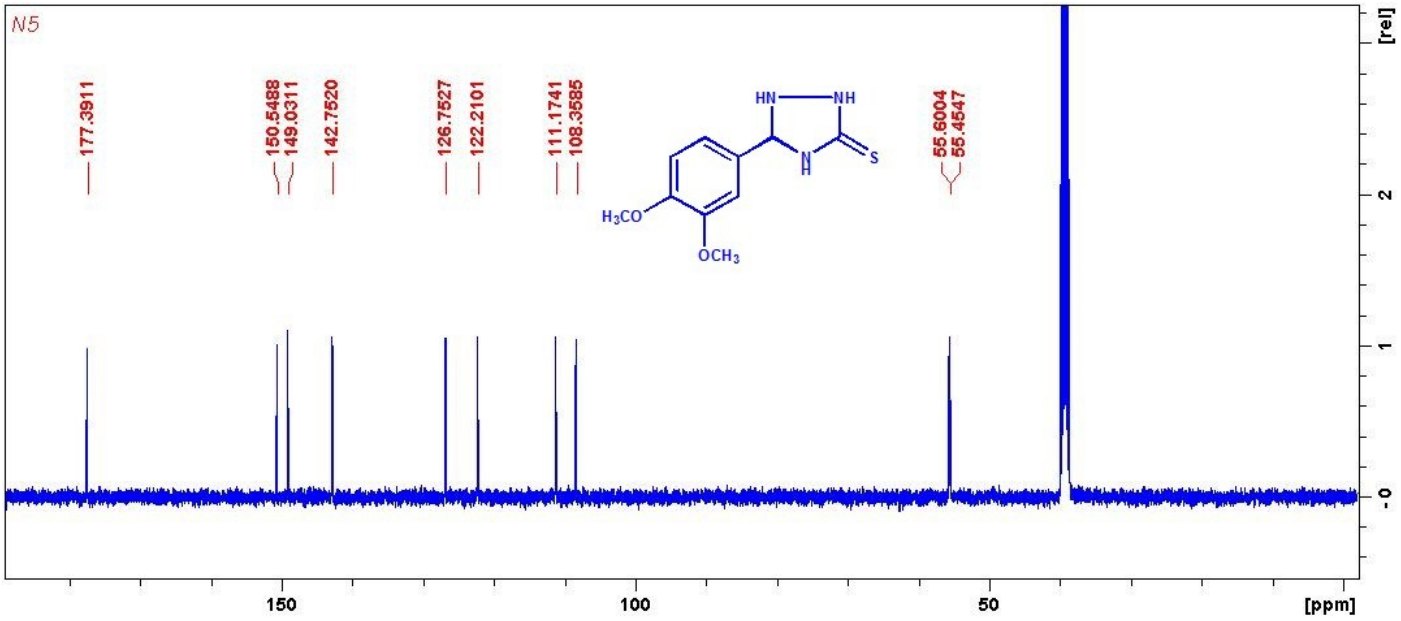
^{13}C NMR spectrum of 5-(2-flurophenyl)-1,2,4-triazolidine-3-thione



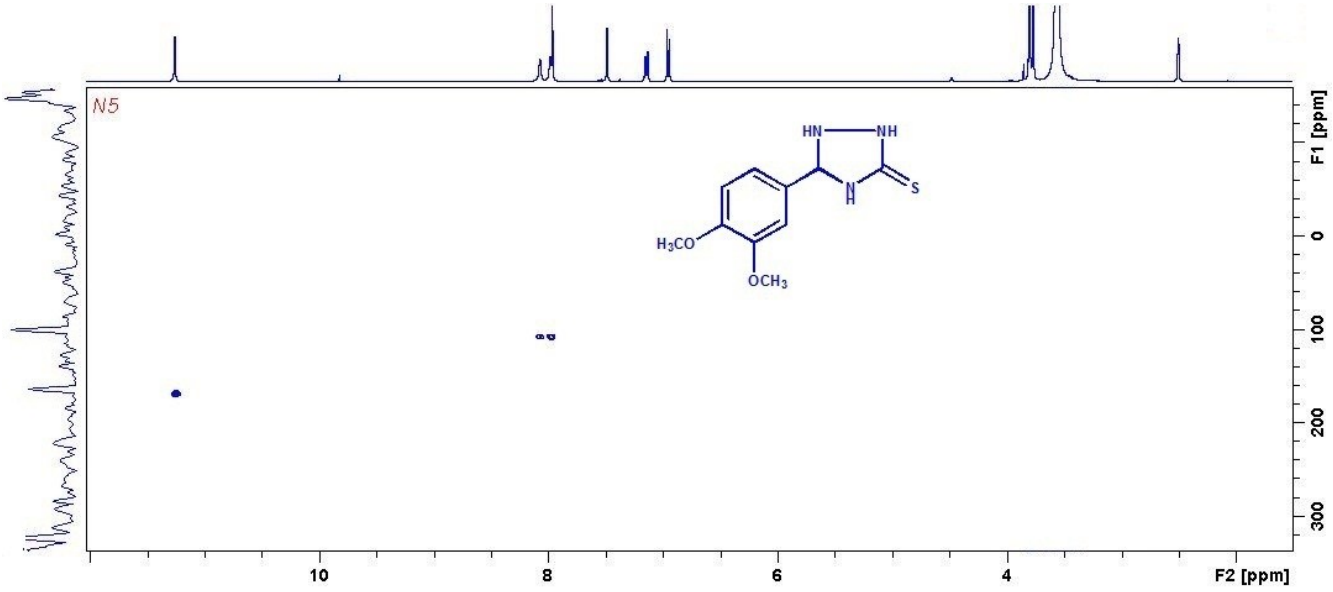
^{15}N NMR spectrum of 5-(2-flurophenyl)-1,2,4-triazolidine-3-thione



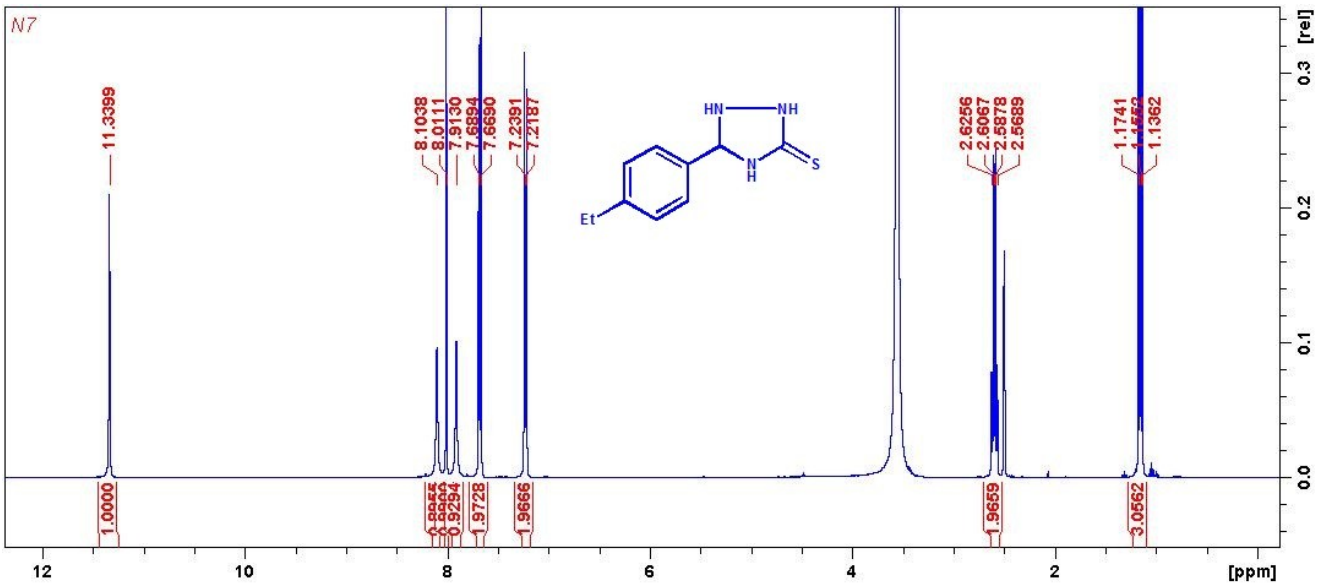
^{1}H NMR spectrum of 5-(3,4-dimethoxyphenyl)-1,2,4-triazolidine-3-thione



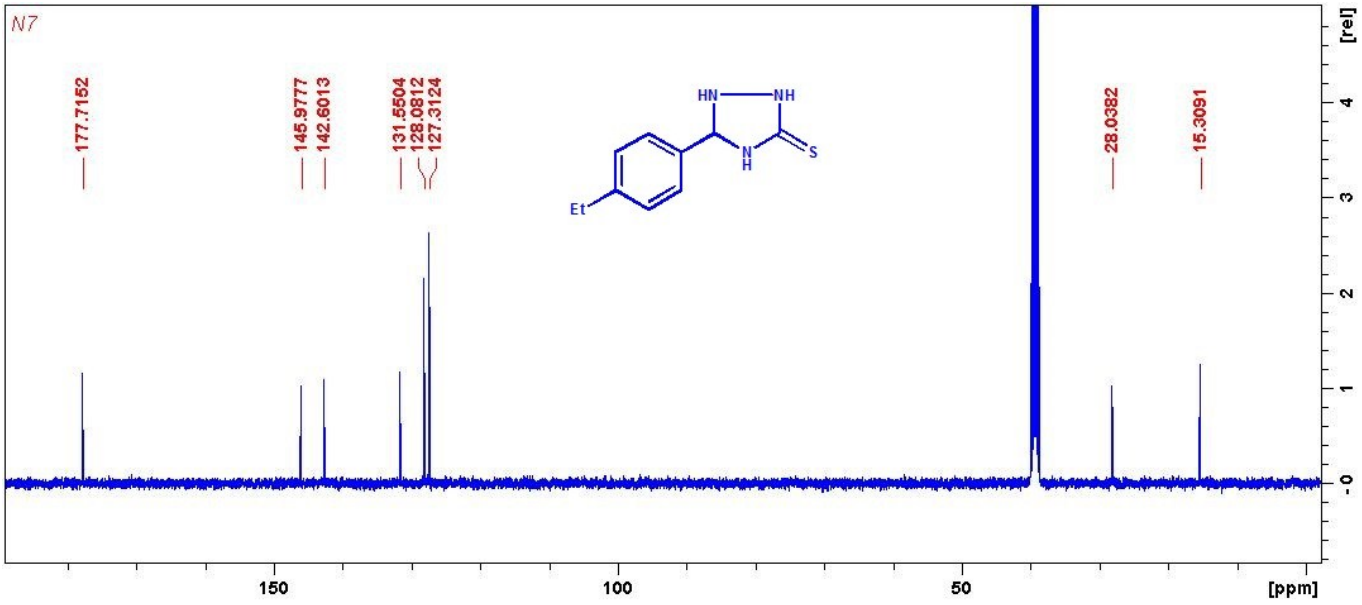
^{13}C NMR spectrum of 5-(3,4-dimethoxyphenyl)-1,2,4-triazolidine-3-thione



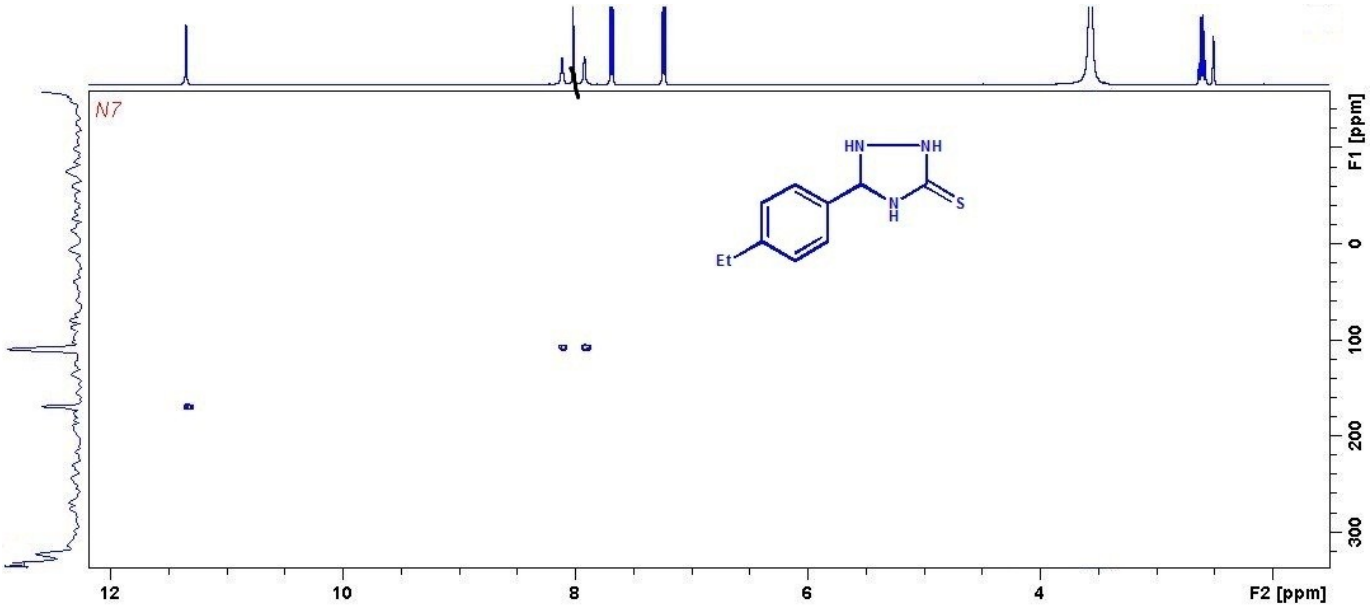
^{15}N NMR spectrum of 5-(3,4-dimethoxyphenyl)-1,2,4-triazolidine-3-thione



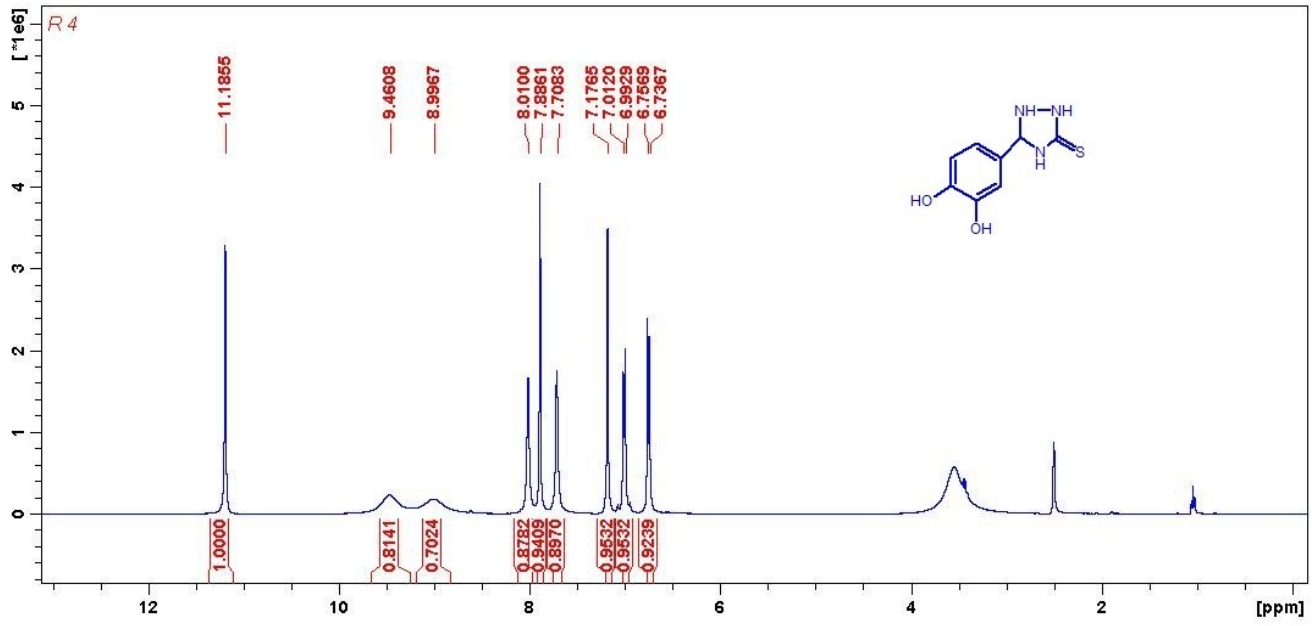
^{1}H NMR spectrum of 5-(4-ethylphenyl)-1,2,4-triazolidine-3-thione



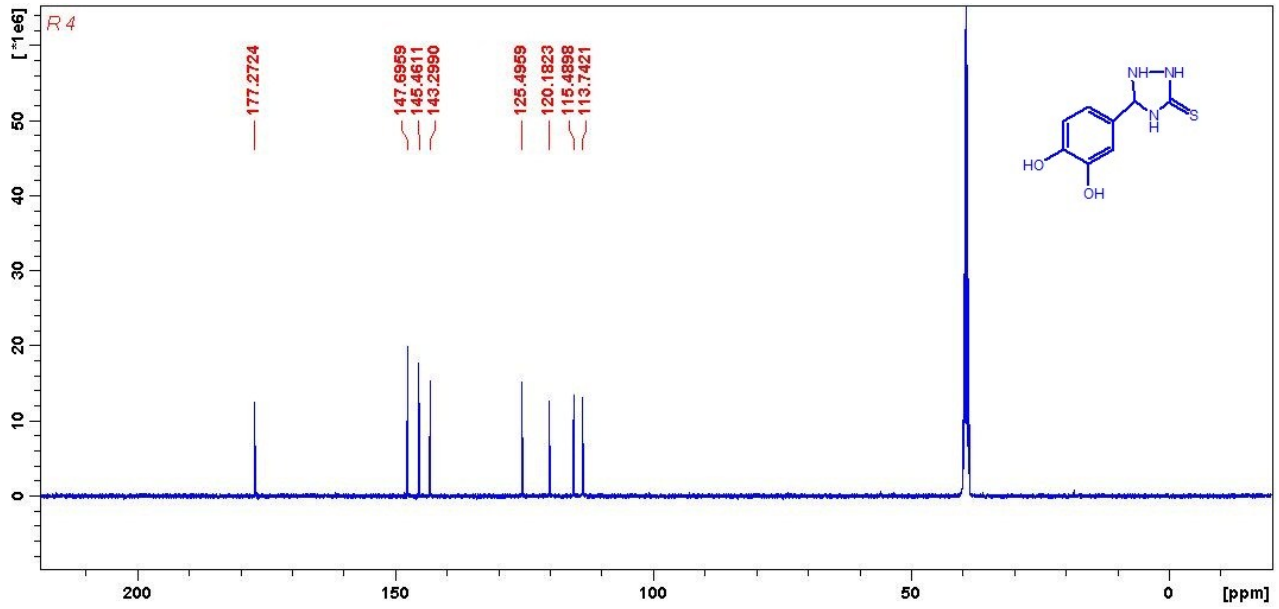
^{13}C NMR spectrum of 5-(4-ethylphenyl)-1,2,4-triazolidine-3-thione



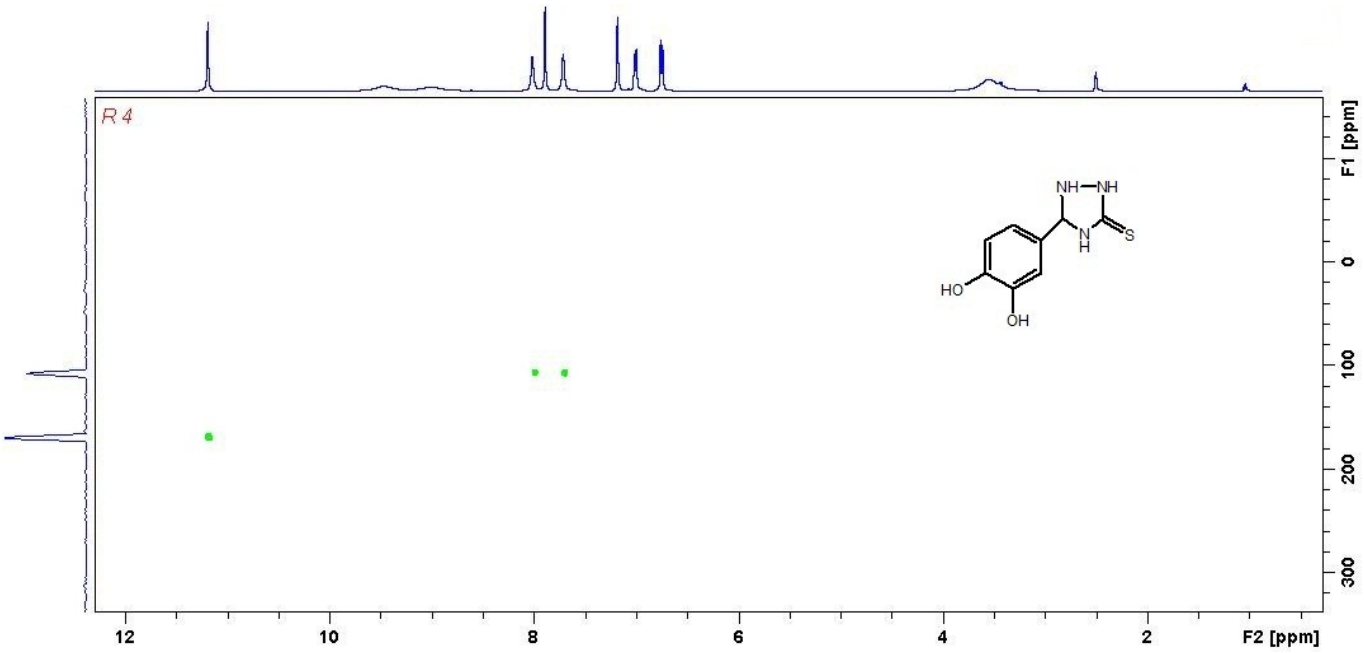
^{15}N NMR spectrum of 5-(4-ethylphenyl)-1,2,4-triazolidine-3-thione



^{1}H NMR spectrum of 5-(3,4-dihydroxy)-1,2,4-triazolidine-3-thione



^{13}C NMR spectrum of 5-(3,4-dihydroxy)-1,2,4-triazolidine-3-thione



^{15}N NMR spectrum of 5-(3,4-dihydroxy)-1,2,4-triazolidine-3-thione