Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPLEMENTARY INFORMATION

Synthesis of triazolidine-3-one derivatives through the nanocellulose/hydroxyapatite-catalyzed reaction of aldehydes and semicarbazide

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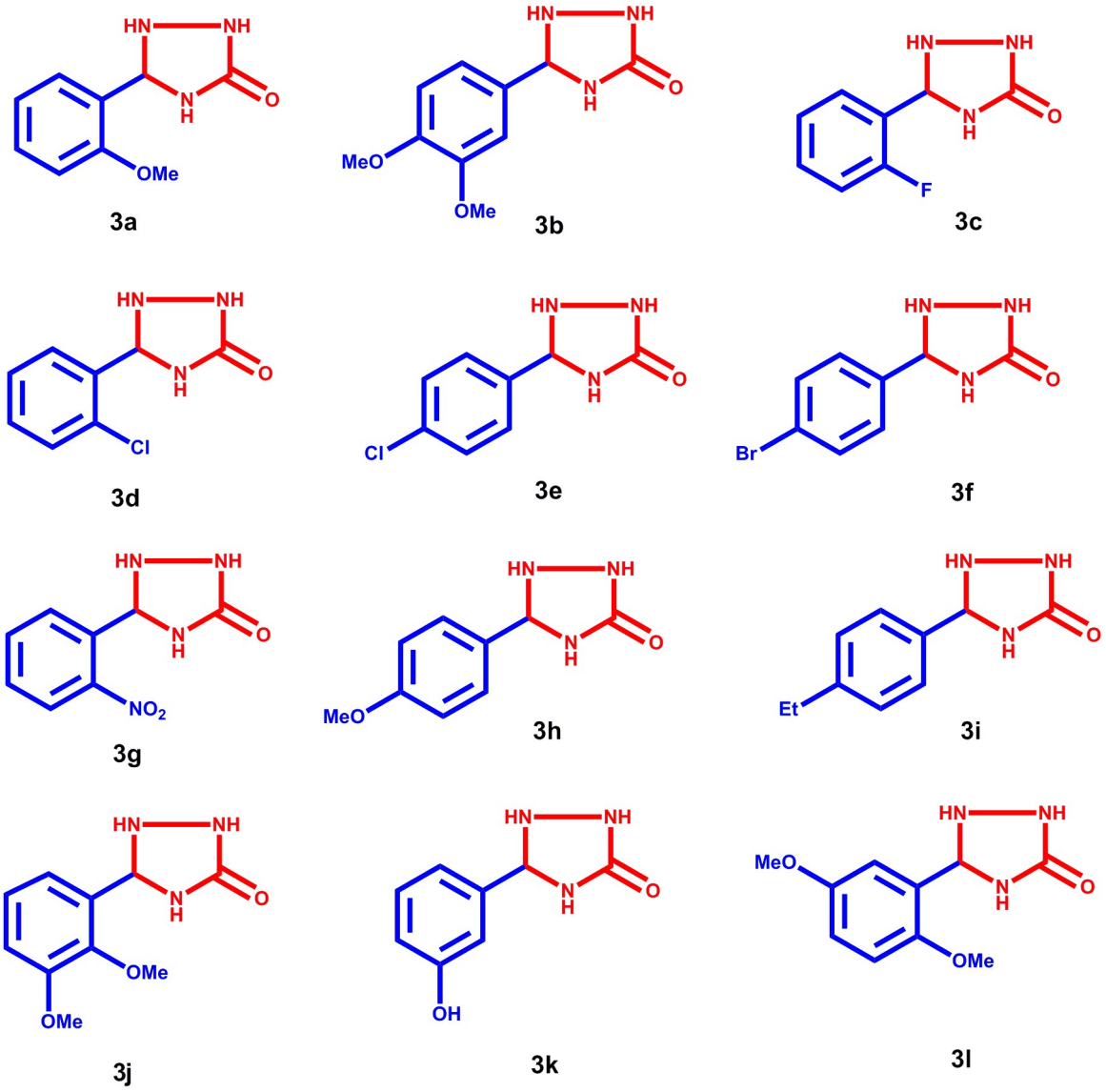


Chart S1 A summary of all compounds prepared.

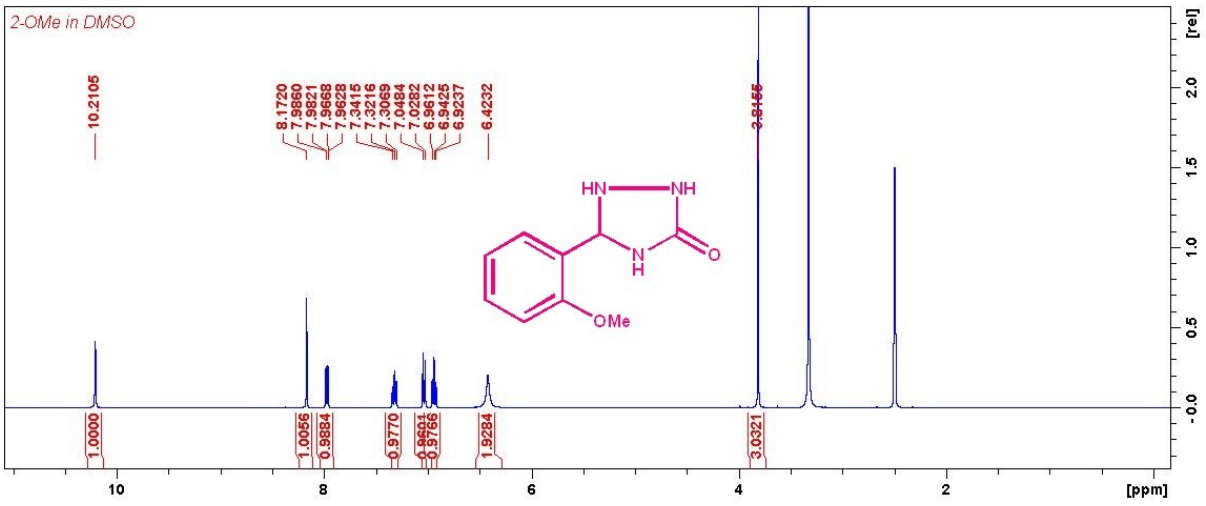


Fig. S1 5-(2-methoxyphenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

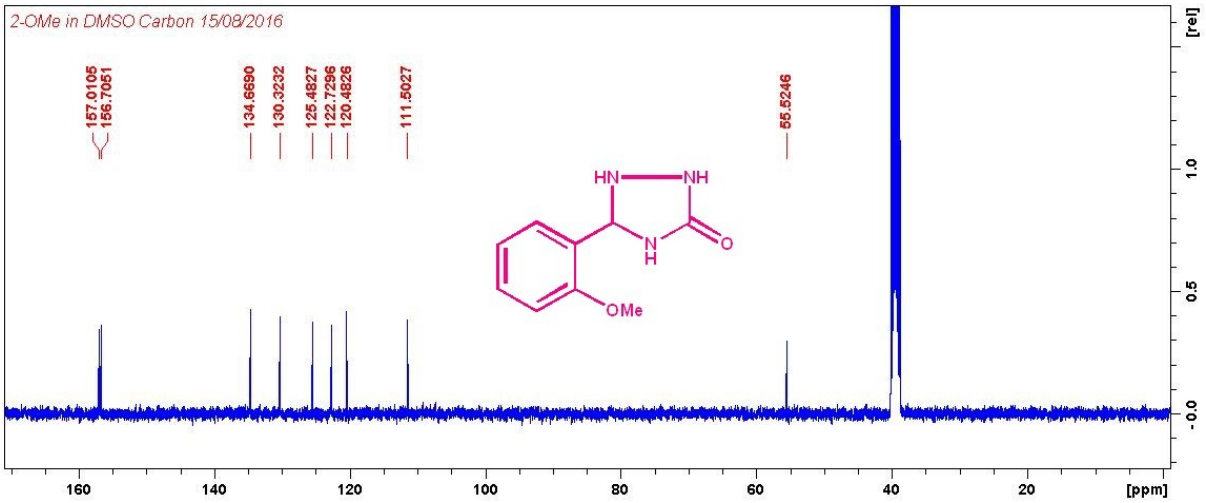


Fig. S2 5-(2-methoxyphenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

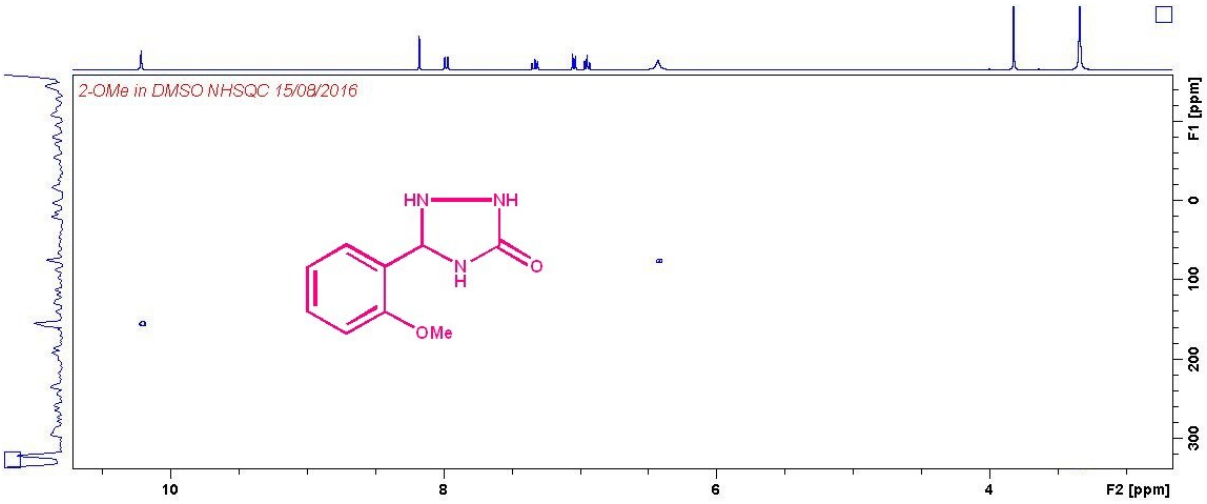
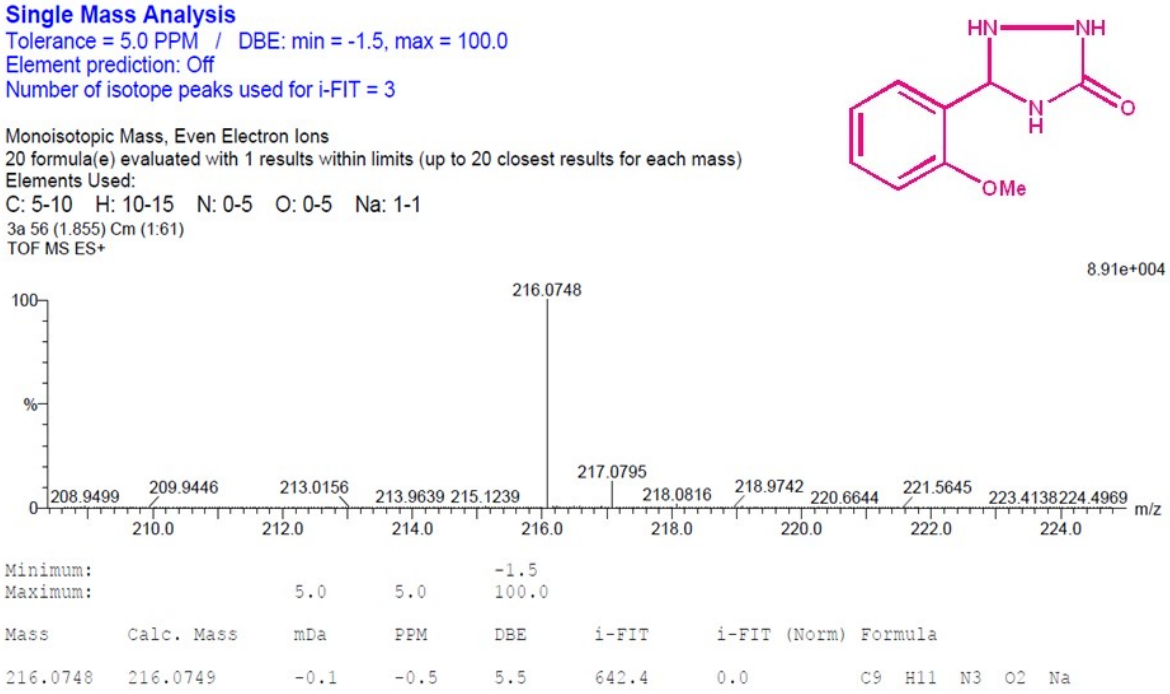


Fig. S3 5-(2-methoxyphenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
216.0748	216.0749	-0.1	-0.5	5.5	642.4	0.0	C9 H11 N3 O2 Na

Fig. S4 5-(2-methoxyphenyl)-1,2,4-triazolidin-3-one HRMS spectrum

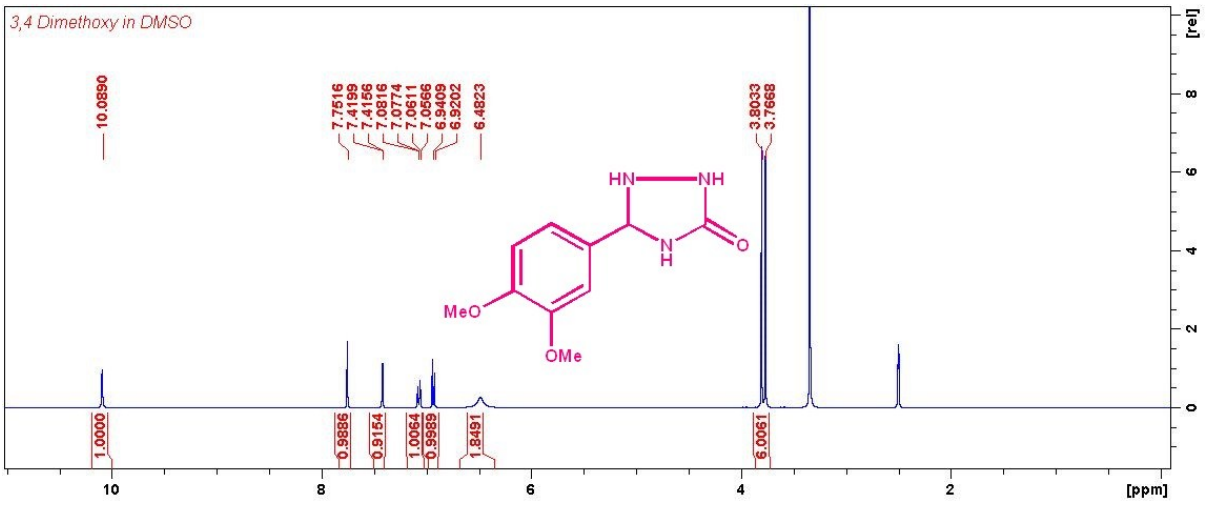


Fig. S5 5-(3,4-methoxyphenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

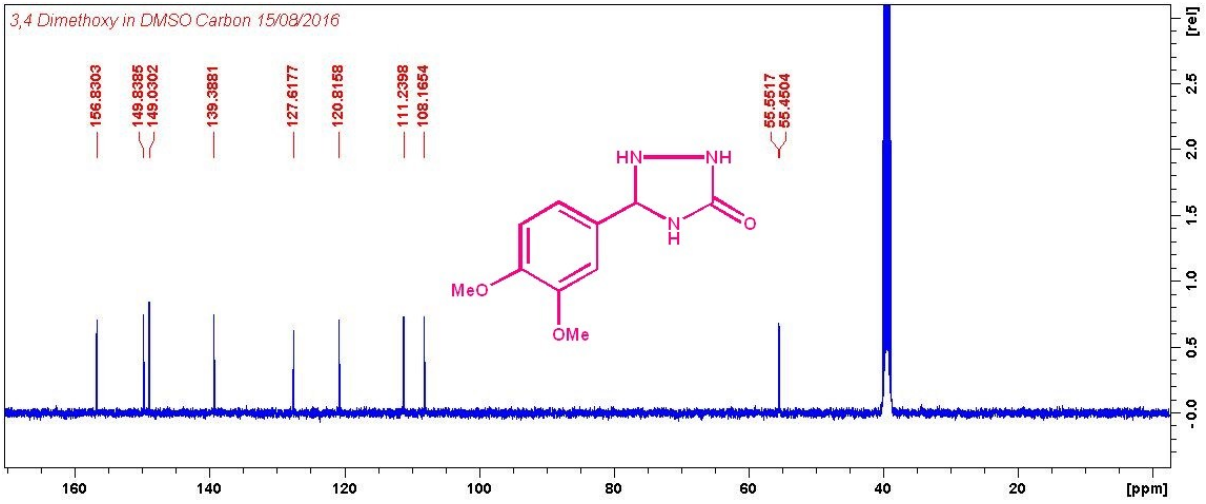


Fig. S6 5-(3,4-methoxyphenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

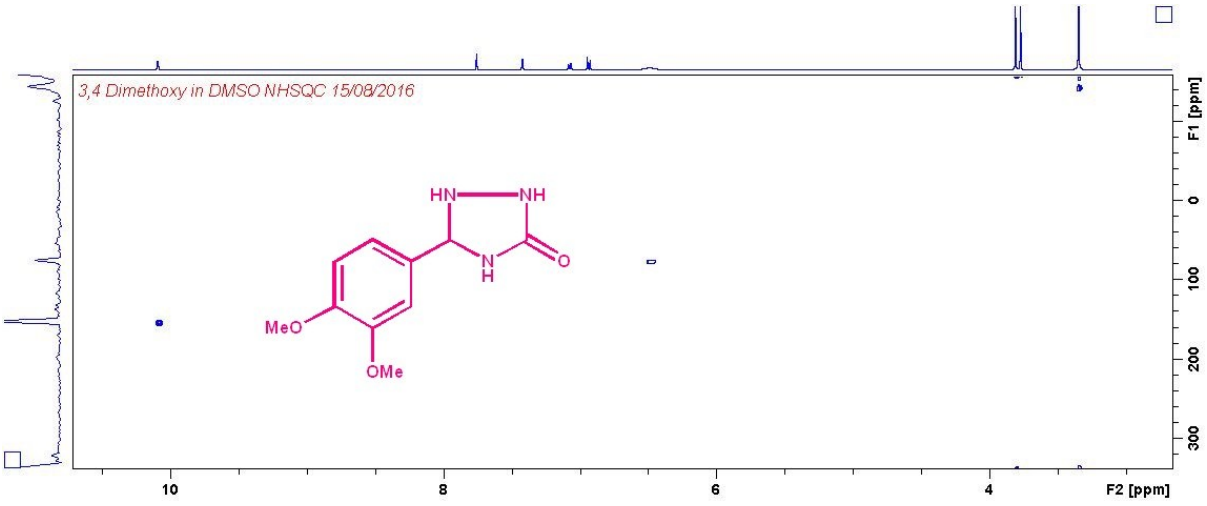


Fig. S7 5-(3,4-methoxyphenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

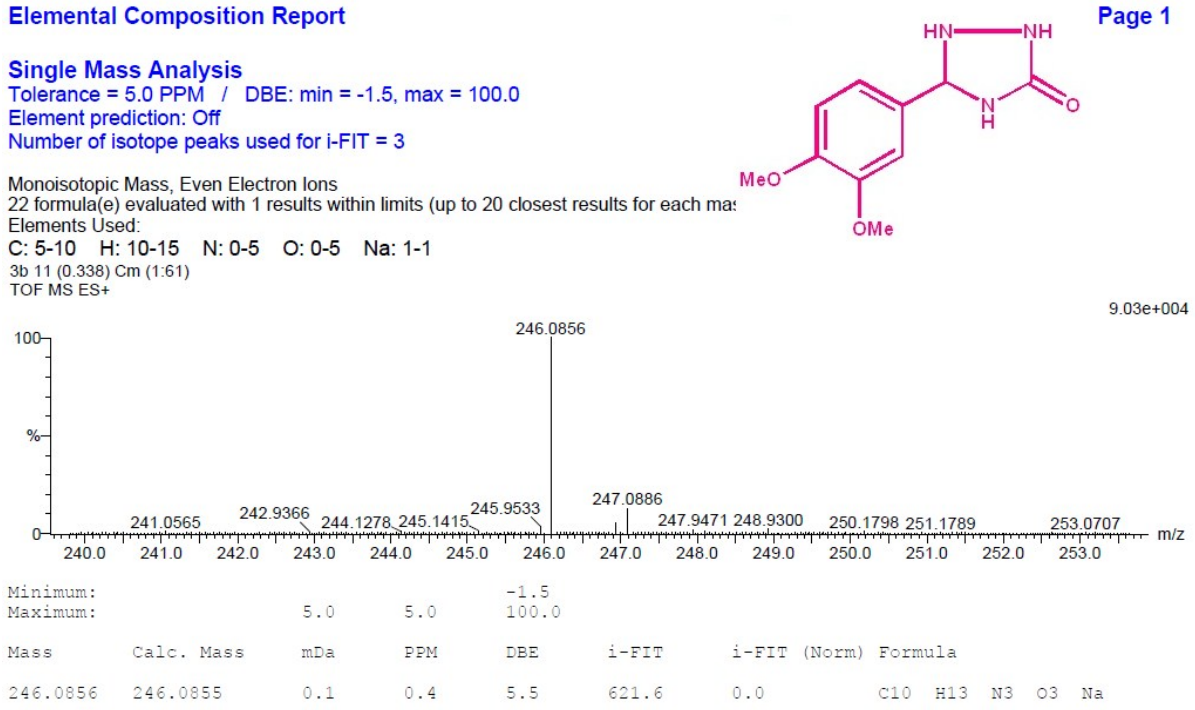


Fig. S8 5-(3,4-methoxyphenyl)-1,2,4-triazolidin-3-one HRMS spectrum

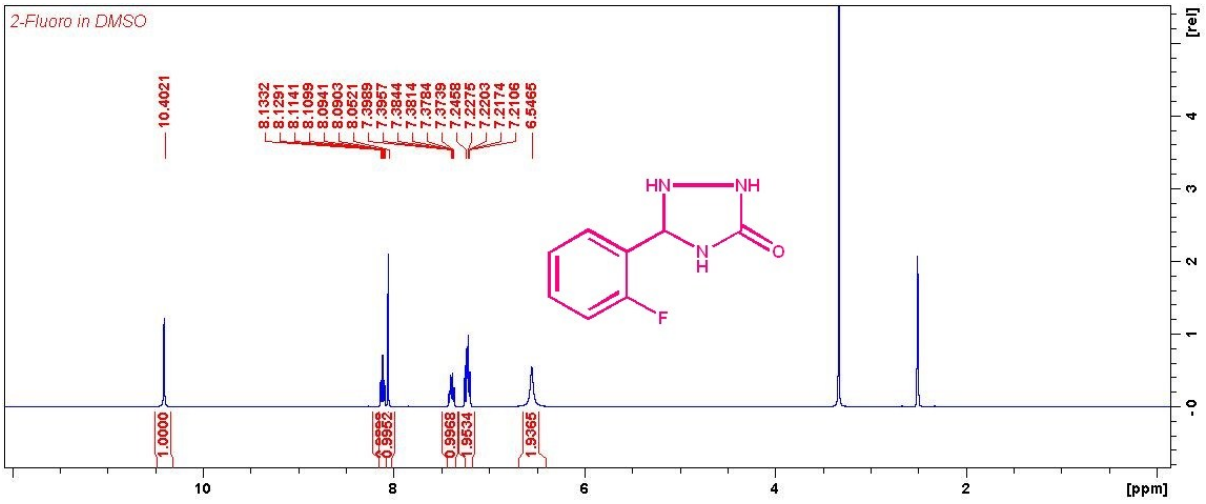


Fig. S9 5-(2-fluorophenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

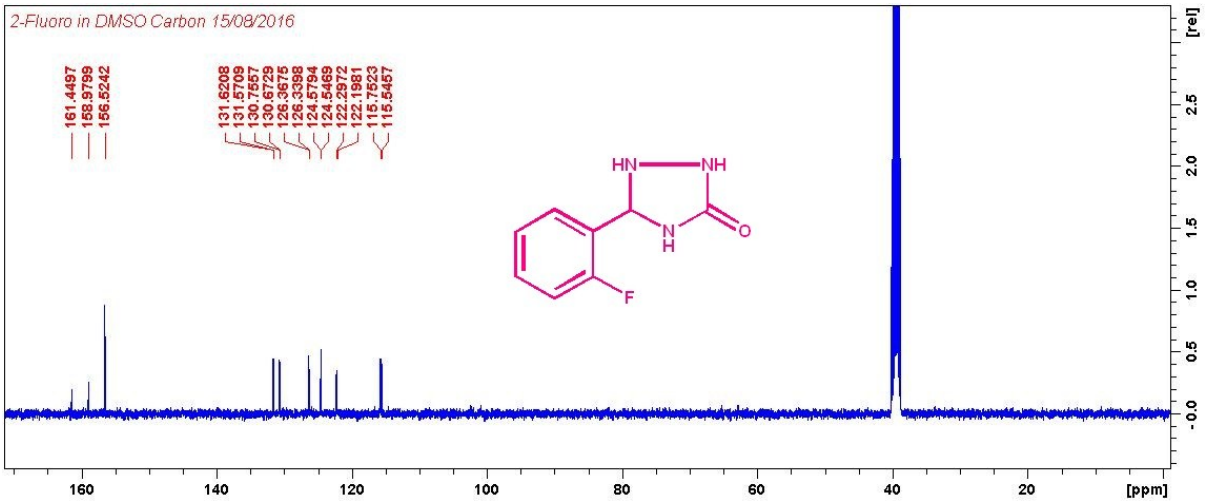


Fig. S10 5-(2-fluorophenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

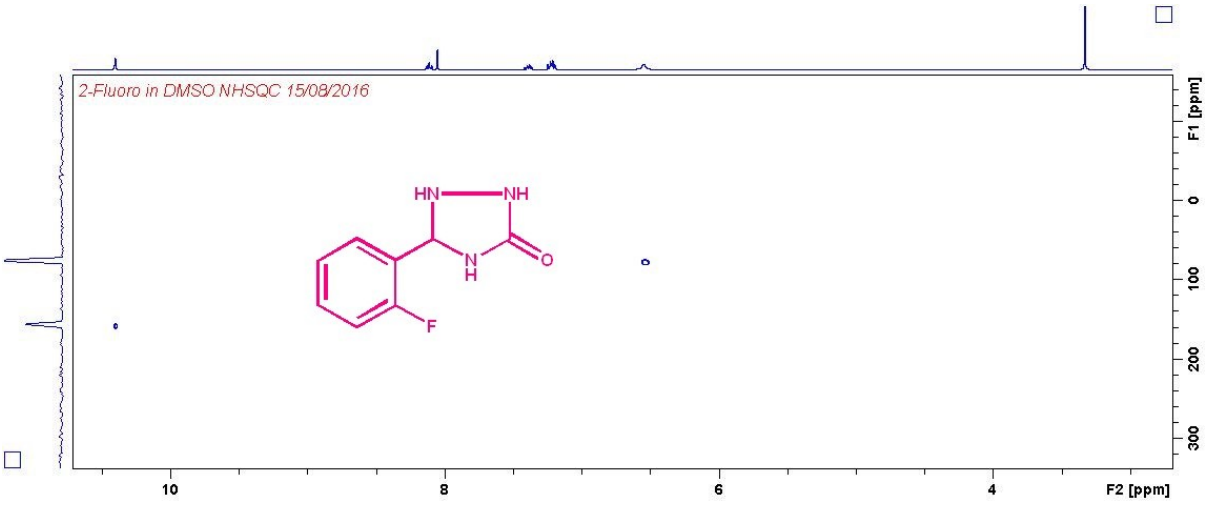


Fig. S11 5-(2-fluorophenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

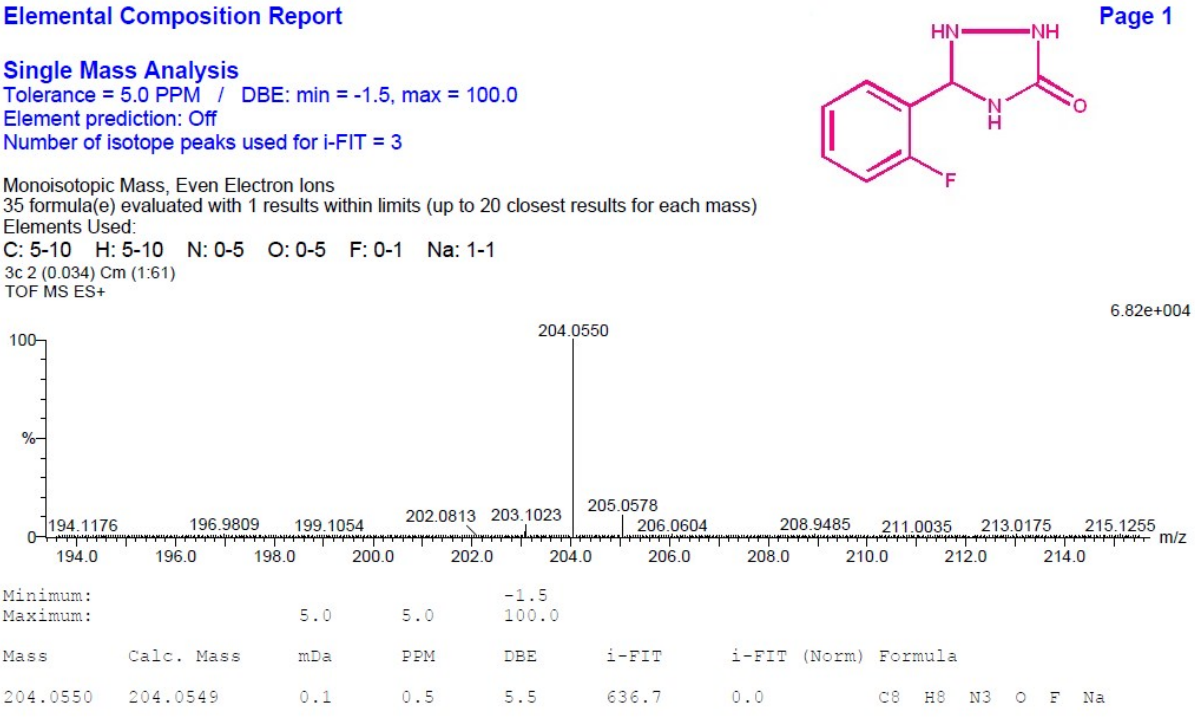


Fig. S12 5-(2-fluorophenyl)-1,2,4-triazolidin-3-one HRMS spectrum

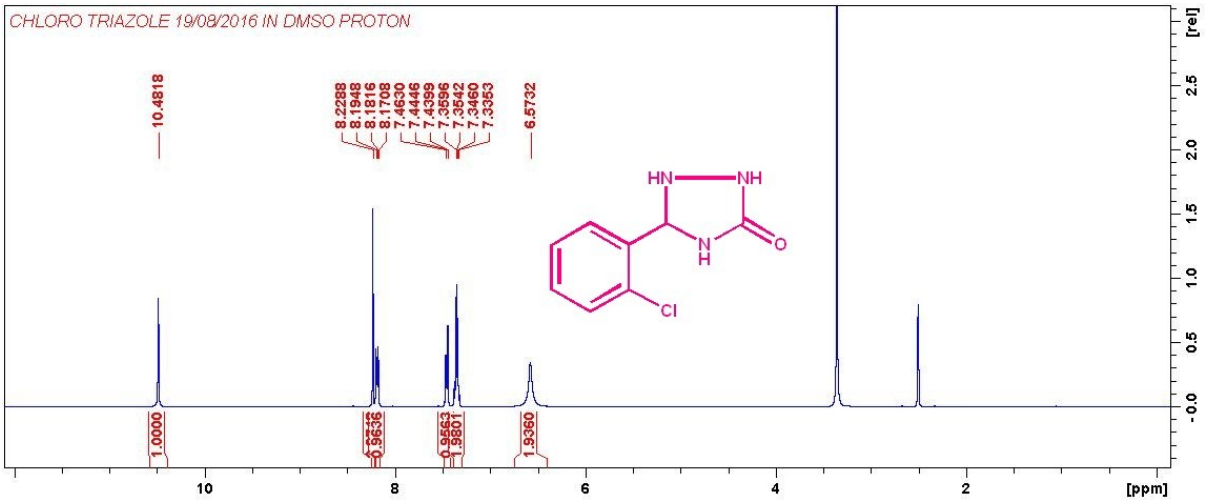


Fig. S13 5-(2-chlorophenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

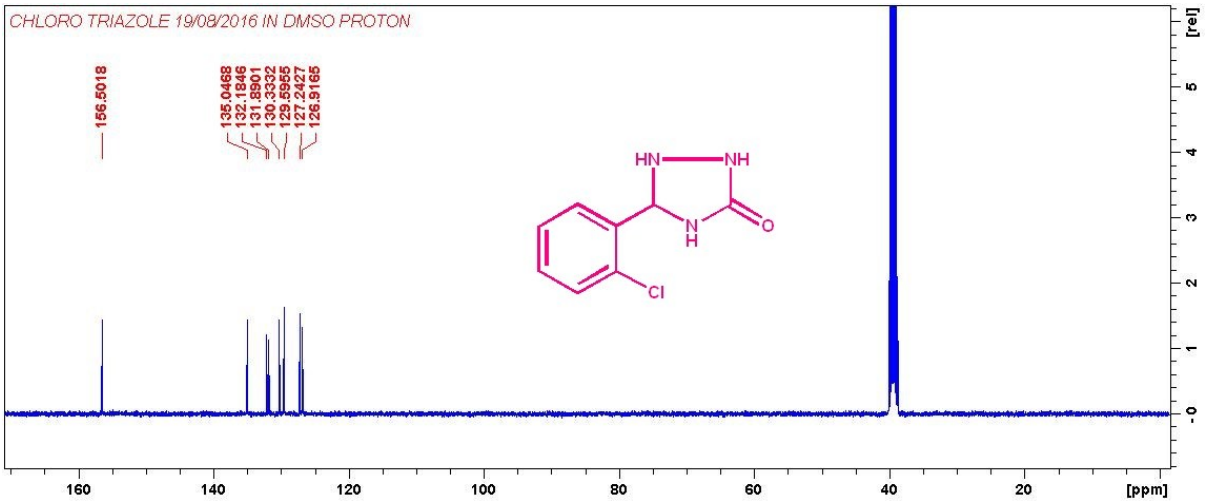


Fig. S14 5-(2-chlorophenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

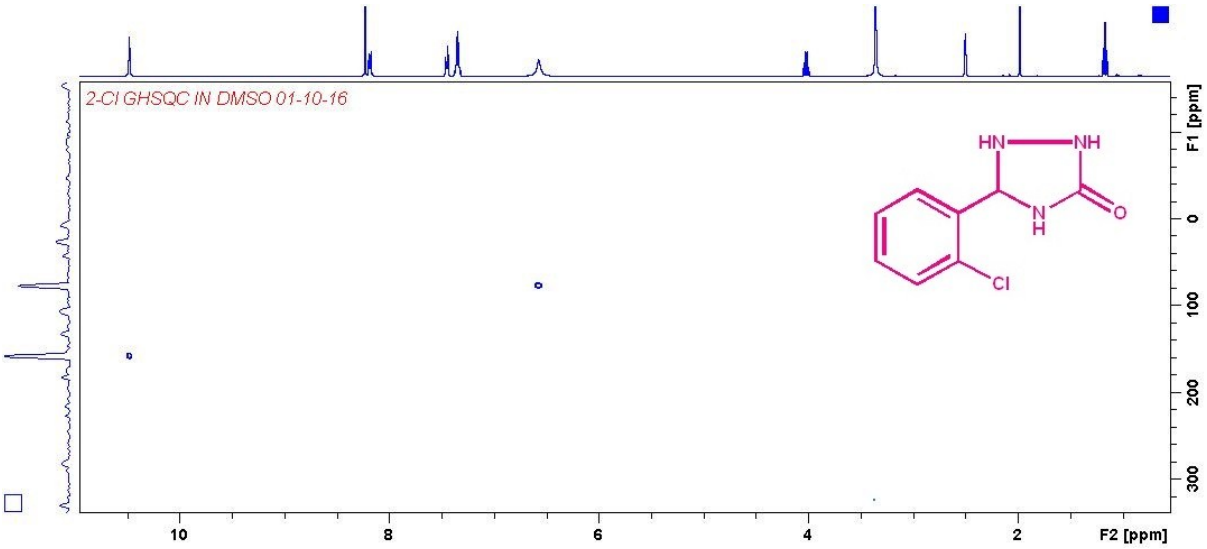
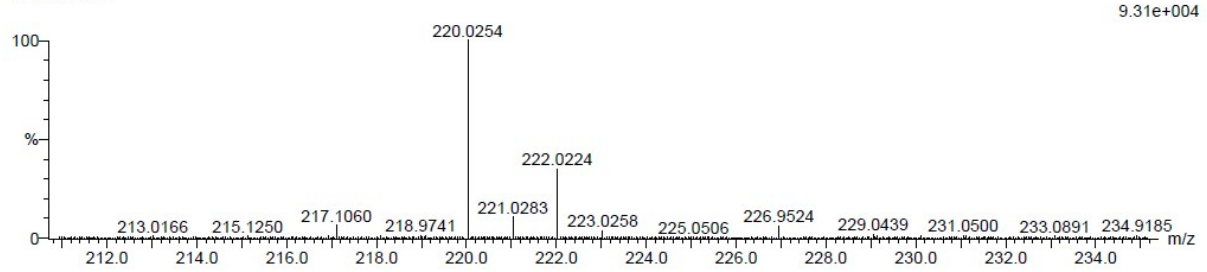


Fig. S15 5-(2-chlorophenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 5-10 H: 5-10 N: 0-5 O: 0-5 Na: 1-1 Cl: 0-1
3d 48 (1.586) Cm (1:61)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
220.0254	220.0254	0.0	0.0	5.5	656.5	0.0	C8 H8 N3 O Na Cl

Fig. S16 5-(2-chlorophenyl)-1,2,4-triazolidin-3-one HRMS NMR spectrum

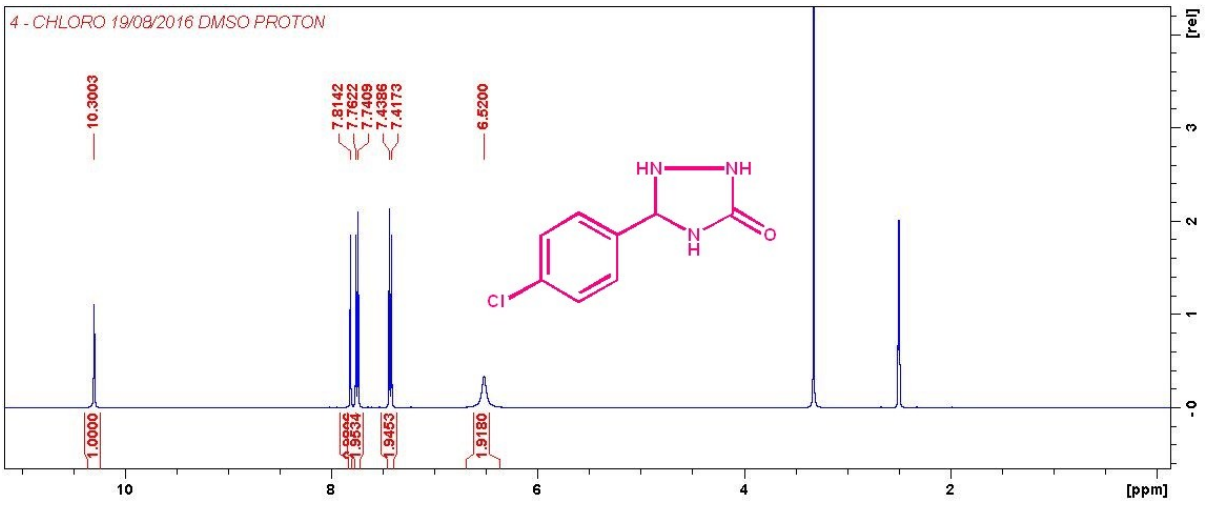


Fig. S17 5-(4-chlorophenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

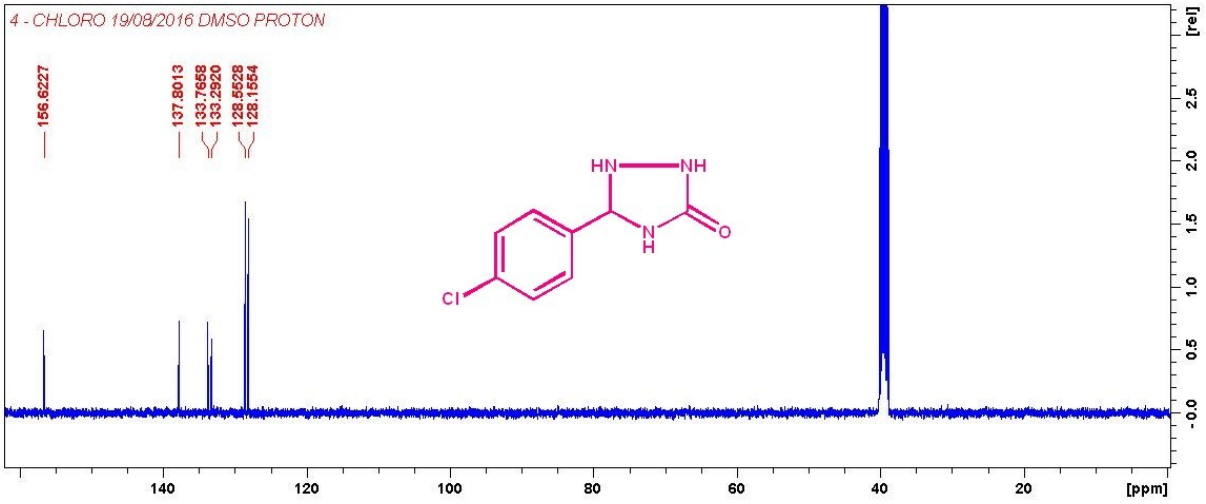


Fig. S18 5-(4-chlorophenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

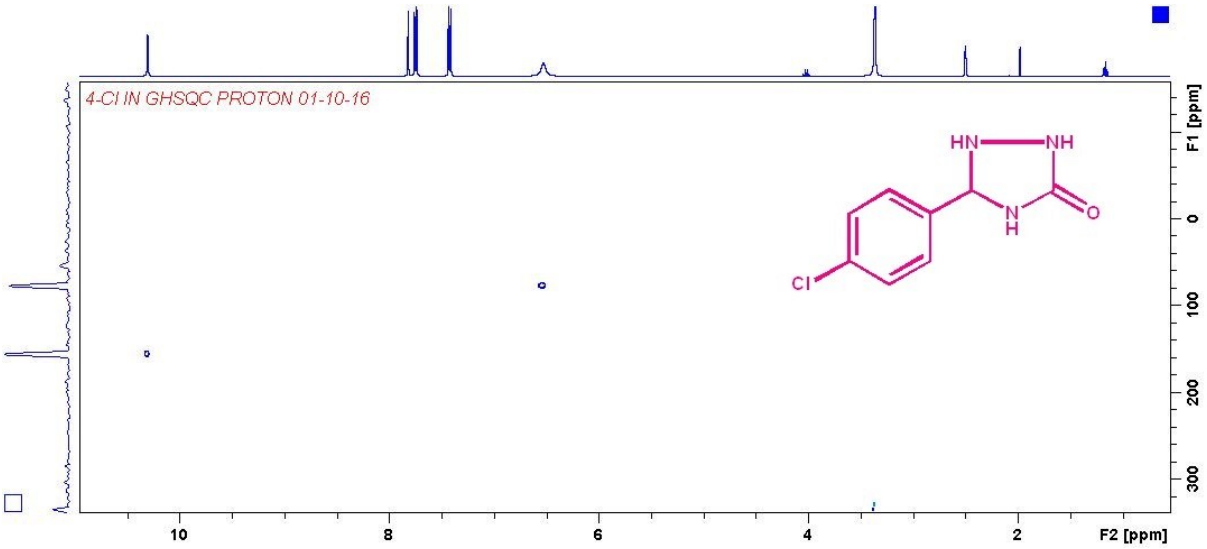


Fig. S18 5-(4-chlorophenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

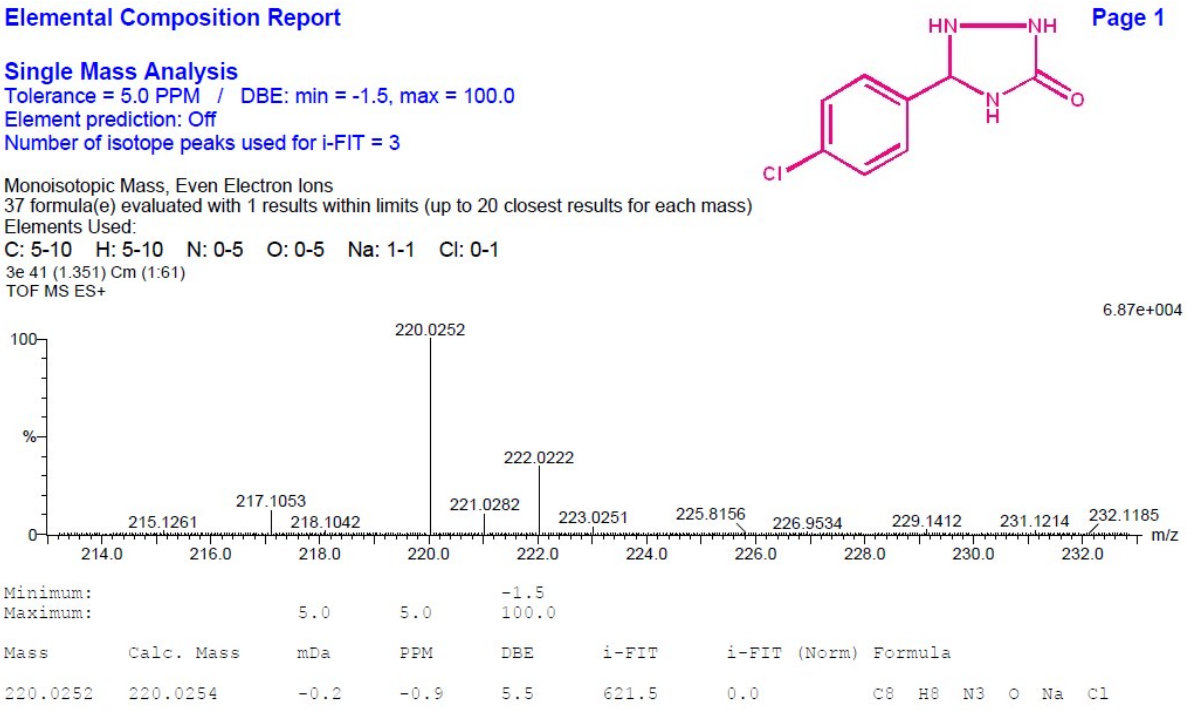


Fig. S19 5-(4-chlorophenyl)-1,2,4-triazolidin-3-one HRMS spectrum

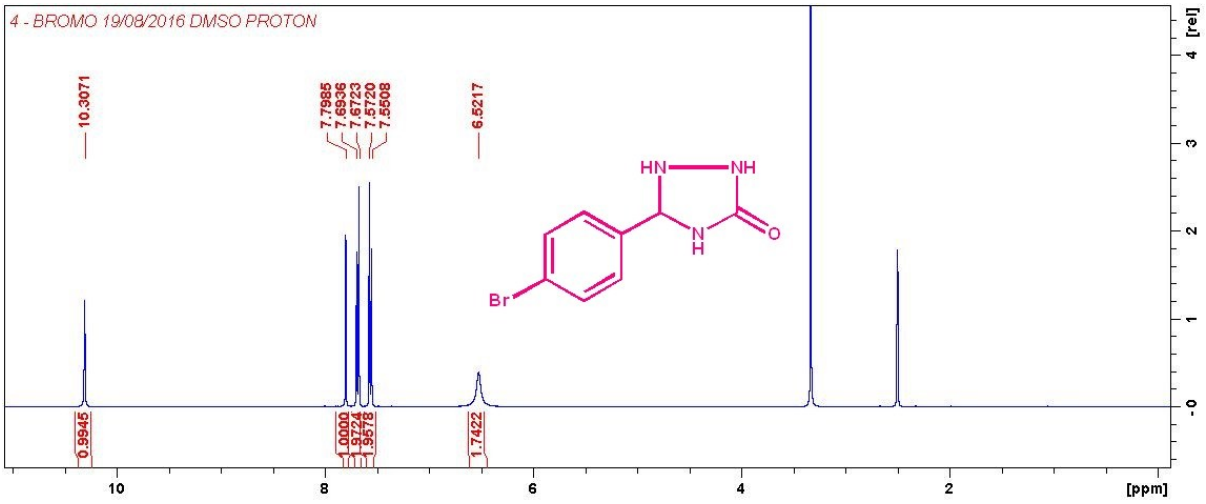


Fig. S20 5-(4-bromophenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

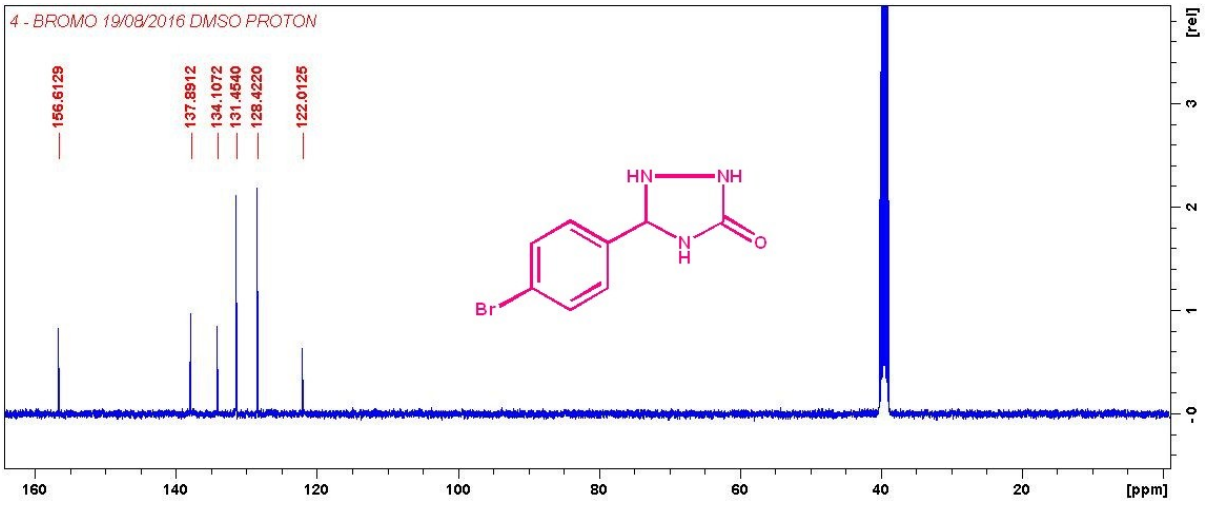


Fig. S21 5-(4-bromophenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

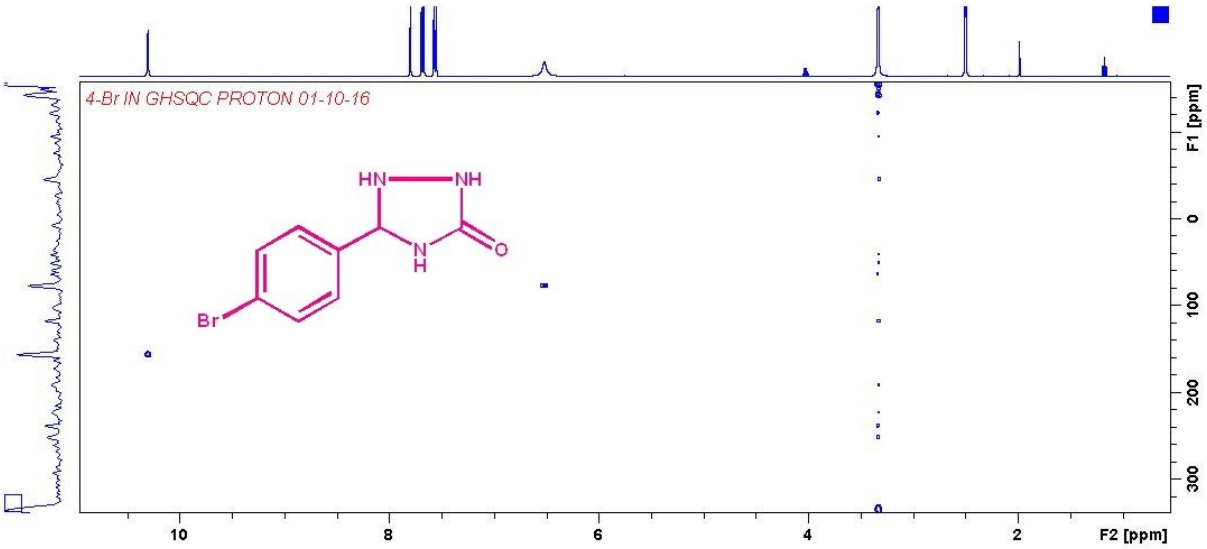
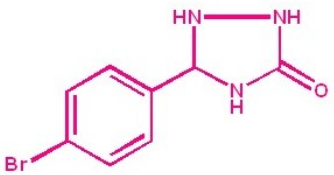


Fig. S22 5-(4-bromophenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

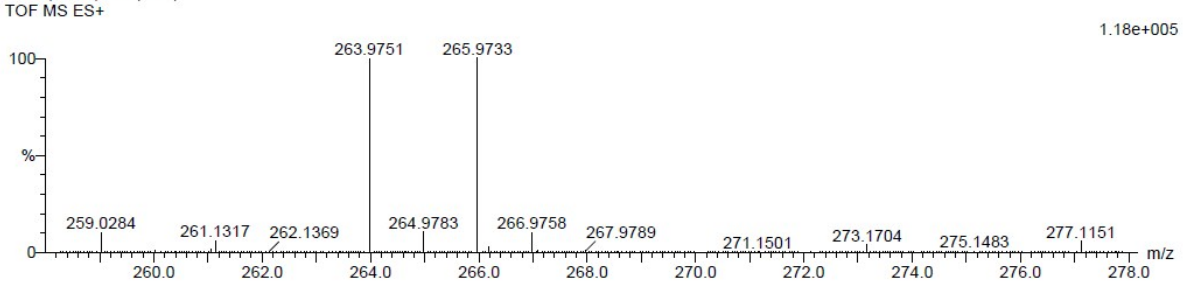
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
42 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass,
Elements Used:
C: 5-10 H: 5-10 N: 0-5 O: 0-5 Na: 1-1 Br: 0-1



3f 56 (1.856) Cm (1:61)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
263.9751	263.9748	0.3	1.1	5.5	589.1	0.0	C8 H8 N3 O Na Br

Fig. S23 5-(4-bromophenyl)-1,2,4-triazolidin-3-one HRMS spectrum

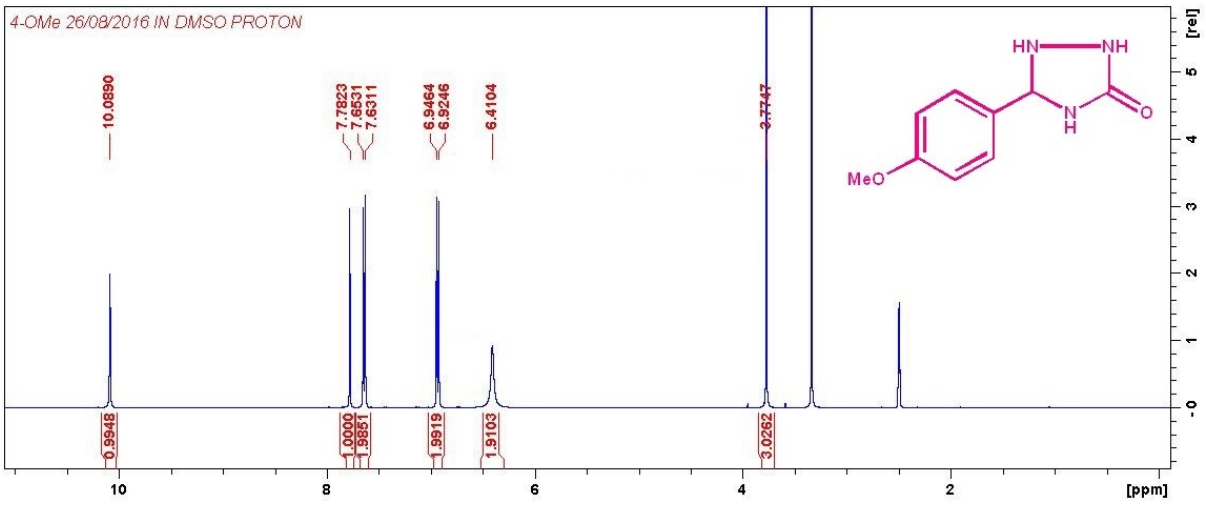


Fig. S24 5-(4-methoxyphenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

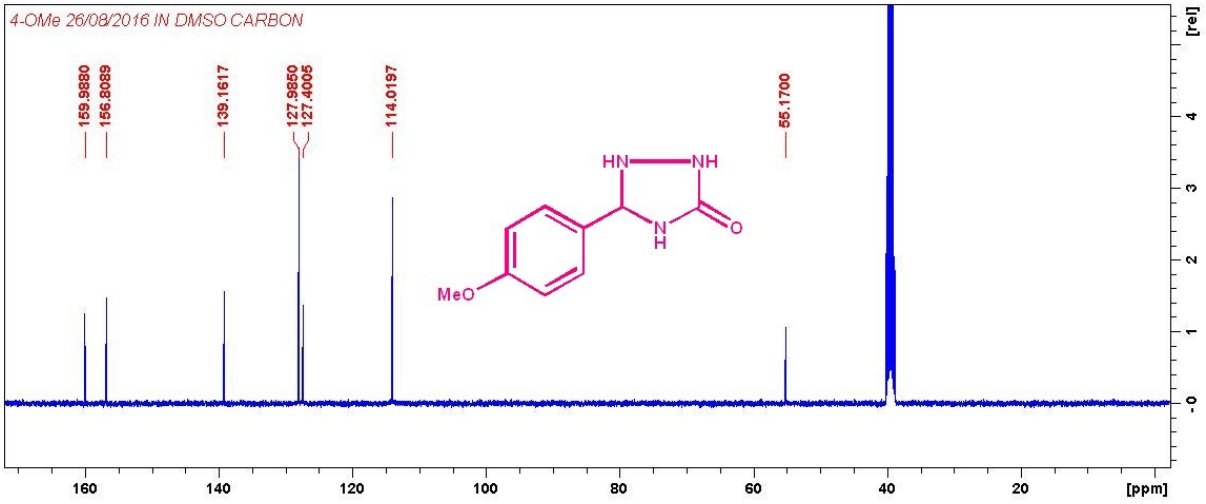


Fig. S25 5-(4-methoxyphenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

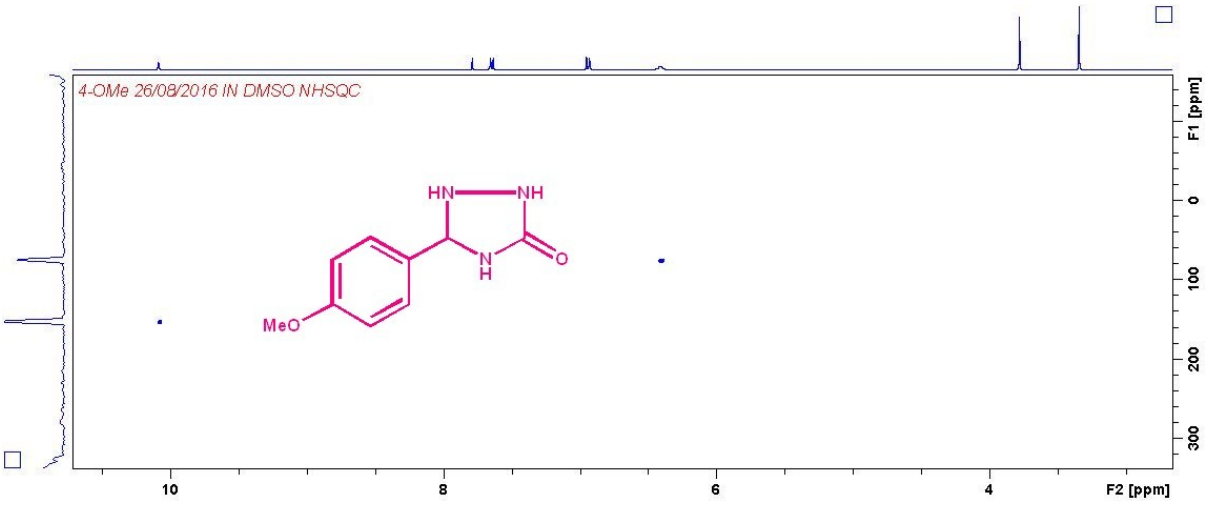
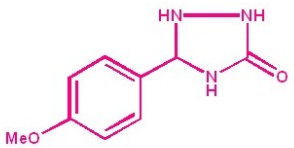


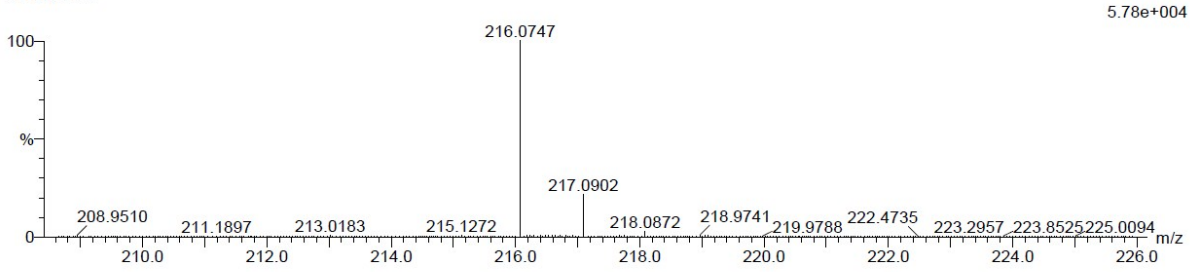
Fig. S26 5-(4-methoxyphenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

Elemental Composition Report **Page 1**



Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 5-10 H: 10-15 N: 0-5 O: 0-5 Na: 1-1
3h 51 (1.687) Cm (1:61)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
216.0747	216.0749	-0.2	-0.9	5.5	645.3	0.0	C9 H11 N3 O2 Na

Fig. S27 5-(4-methoxyphenyl)-1,2,4-triazolidin-3-one HRMS spectrum

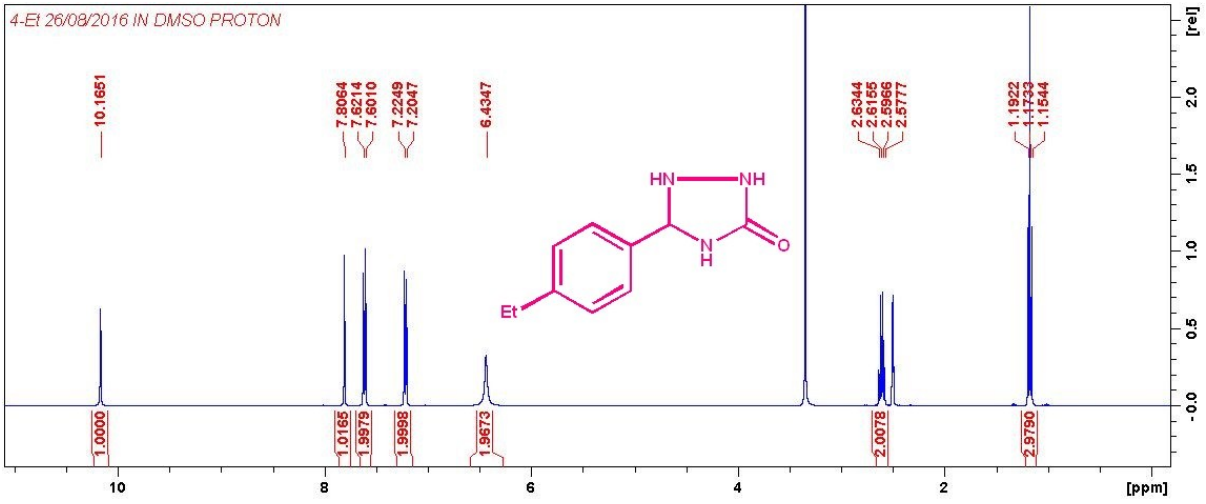


Fig. S28 5-(4-ethylphenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

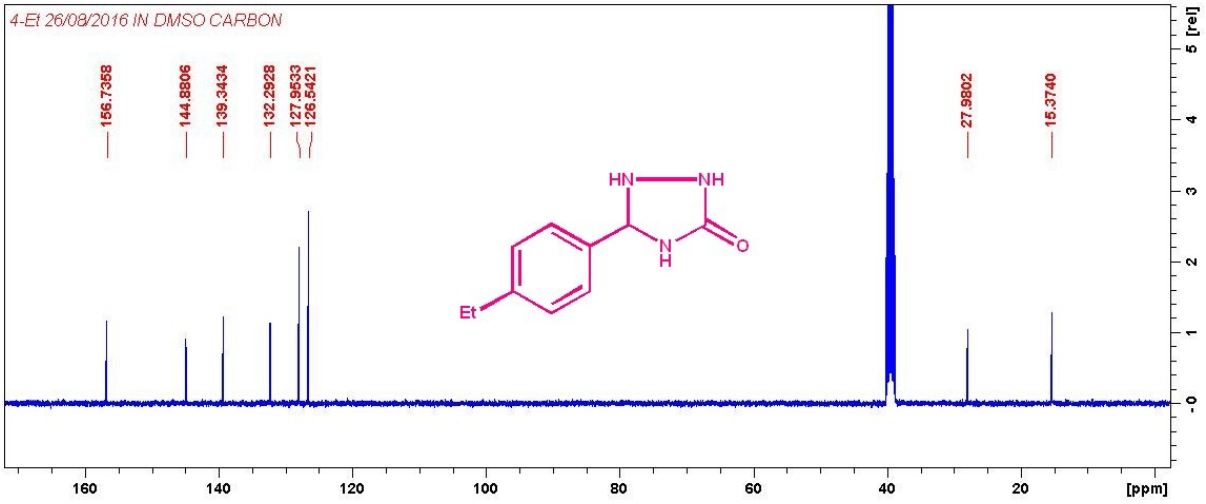


Fig. S29 5-(4-ethylphenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

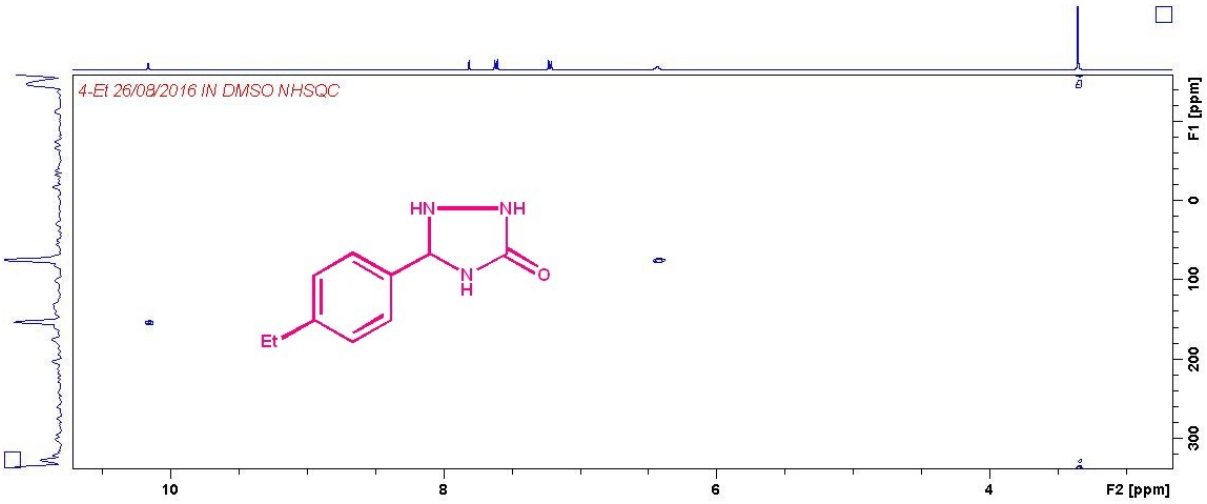


Fig. S30 5-(4-ethylphenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

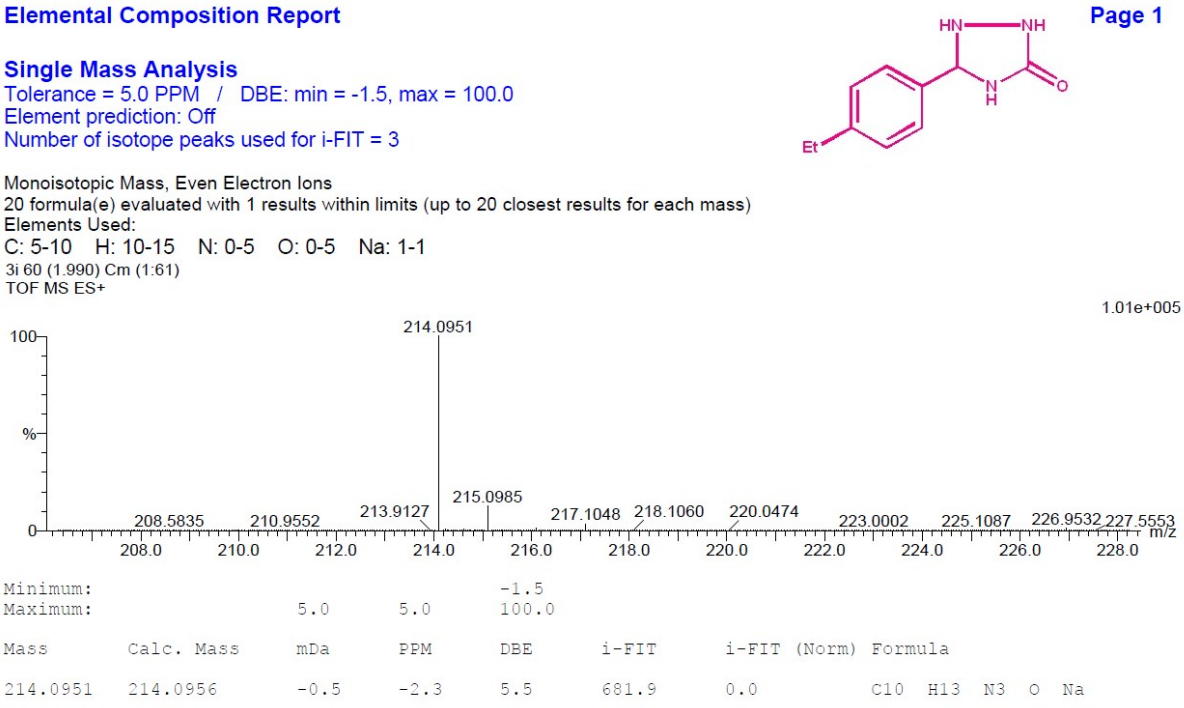


Fig. S31 5-(4-ethylphenyl)-1,2,4-triazolidin-3-one HRMS spectrum

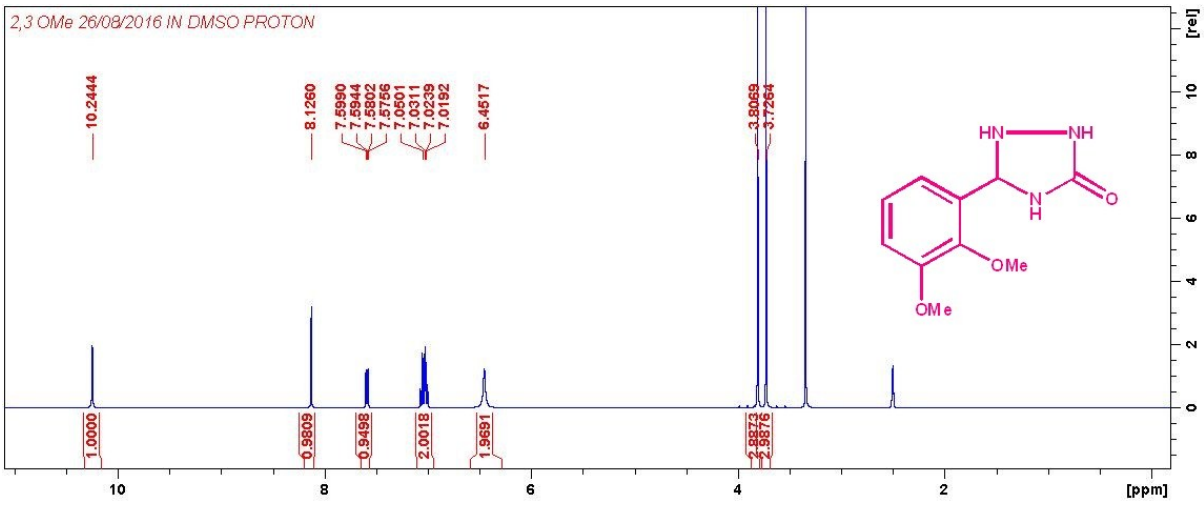


Fig. S32 5-(2,3-methoxyphenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

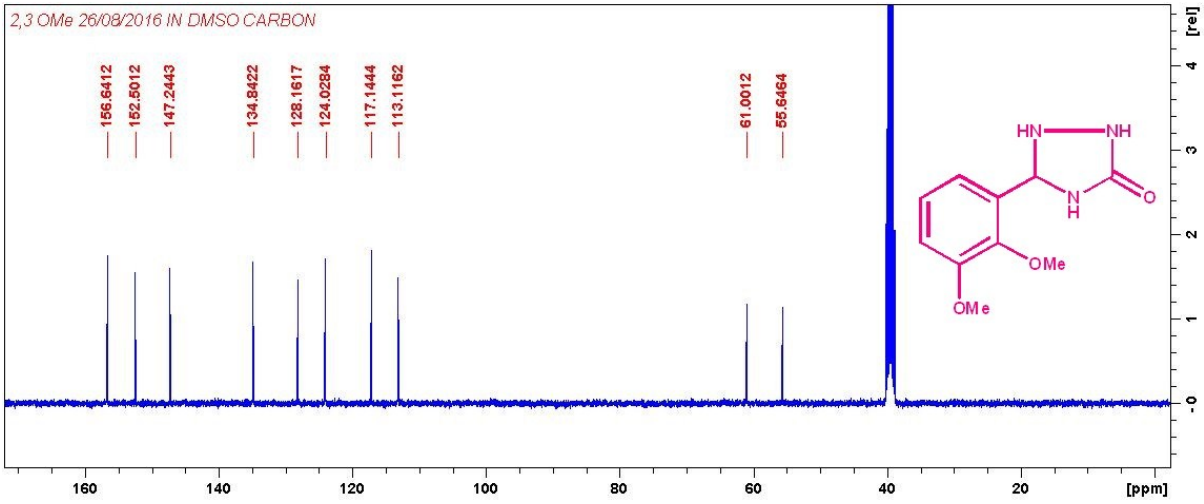


Fig. S33 5-(2,3-methoxyphenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

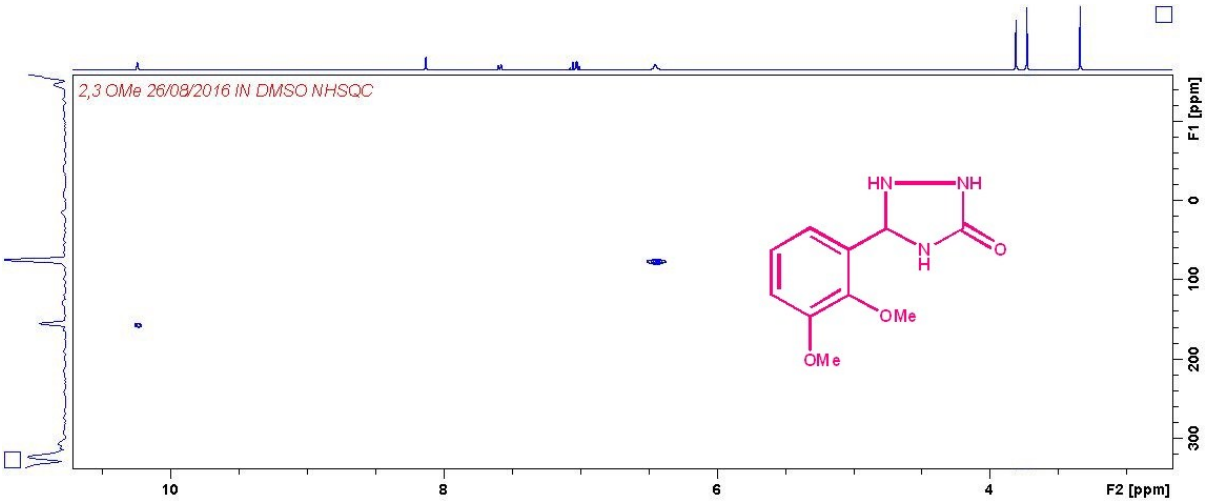


Fig. S34 5-(2,3-methoxyphenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

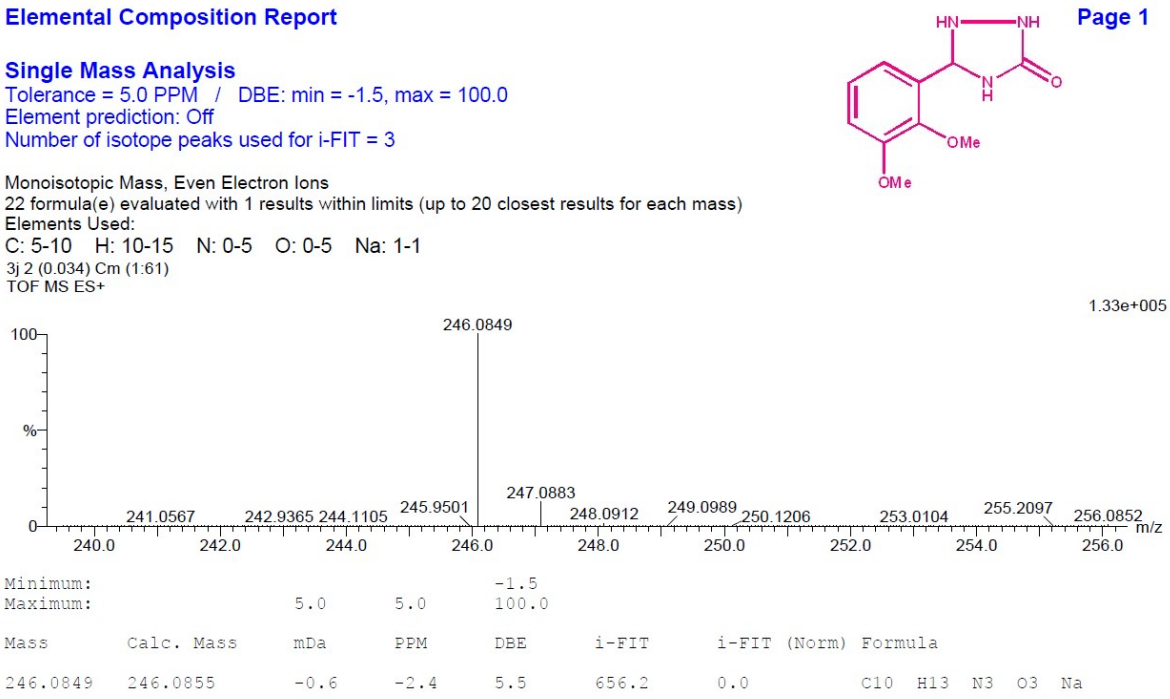


Fig. S35 5-(2,3-methoxyphenyl)-1,2,4-triazolidin-3-one HRMS spectrum

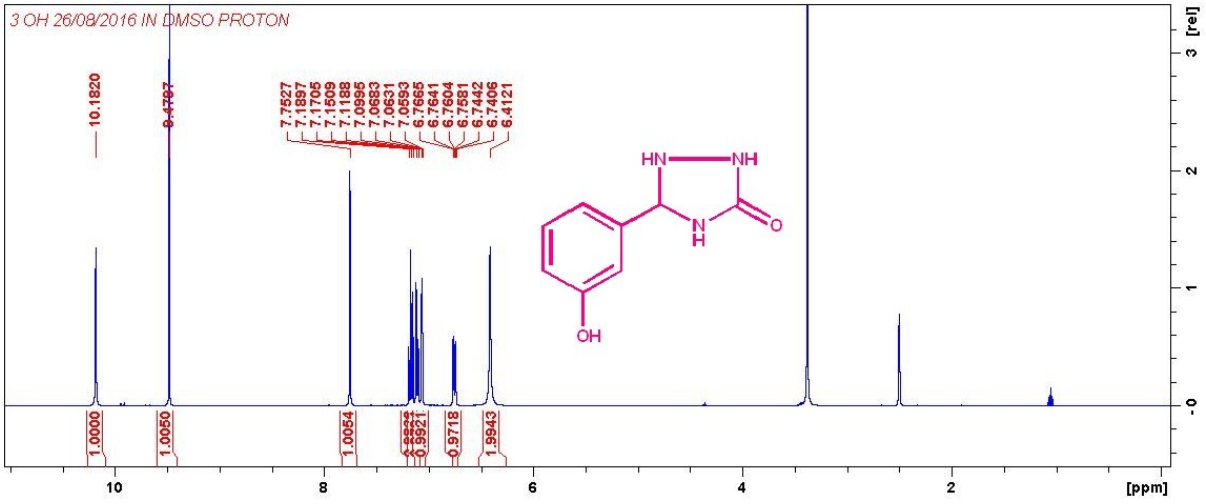


Fig. S36 5-(3-hydroxyphenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

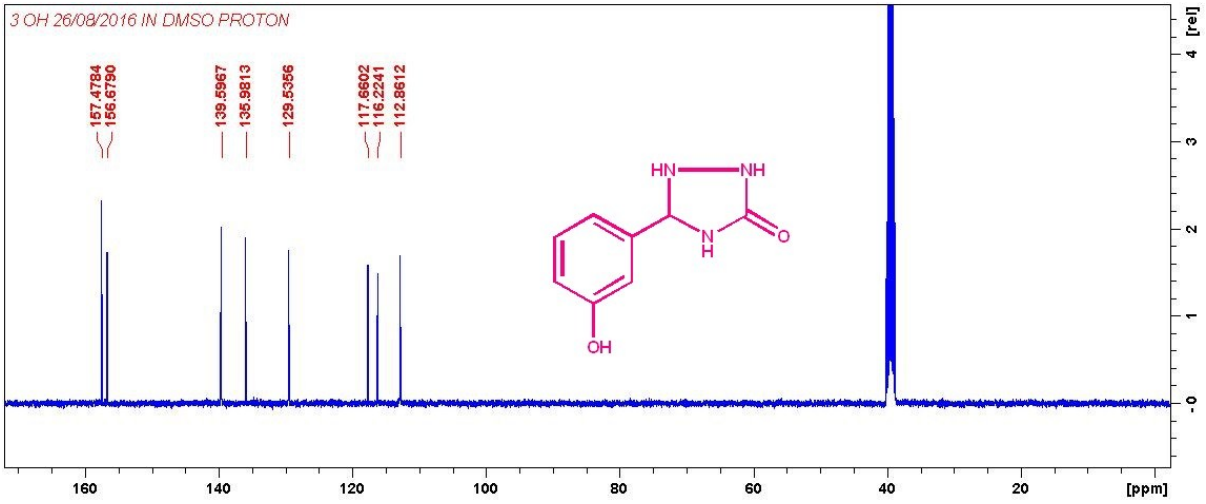


Fig. S37 5-(3-hydroxyphenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

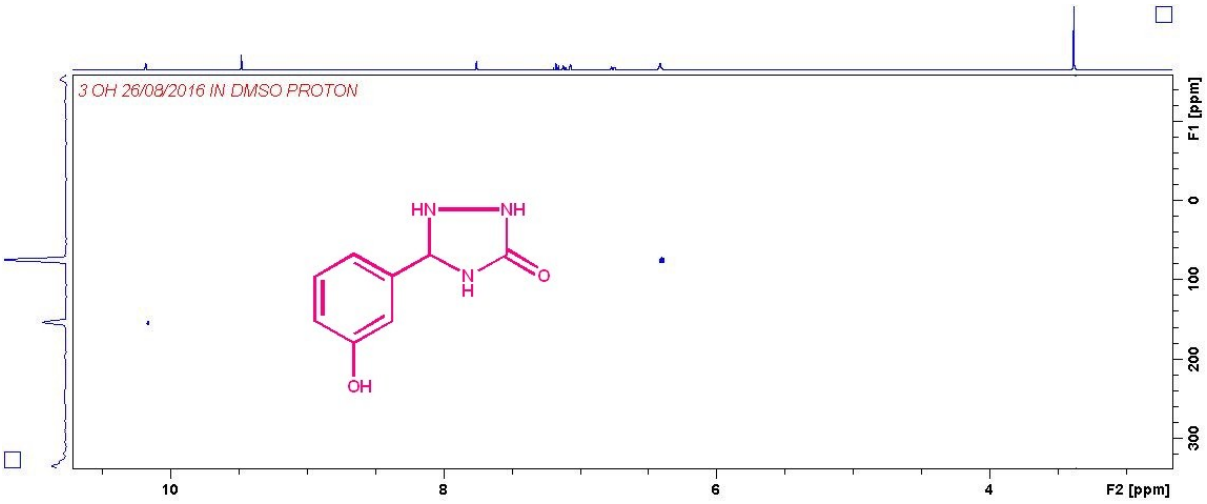


Fig. S38 5-(3-hydroxyphenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

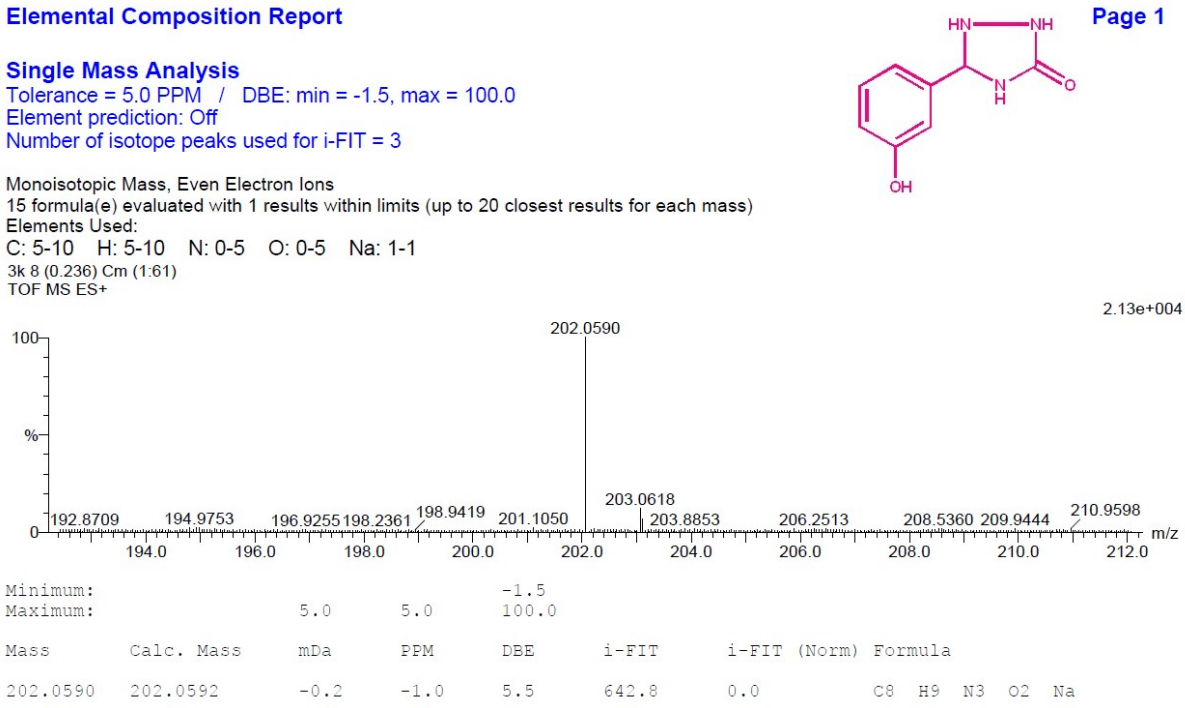


Fig. S39 5-(3-hydroxyphenyl)-1,2,4-triazolidin-3-one HRMS NMR spectrum

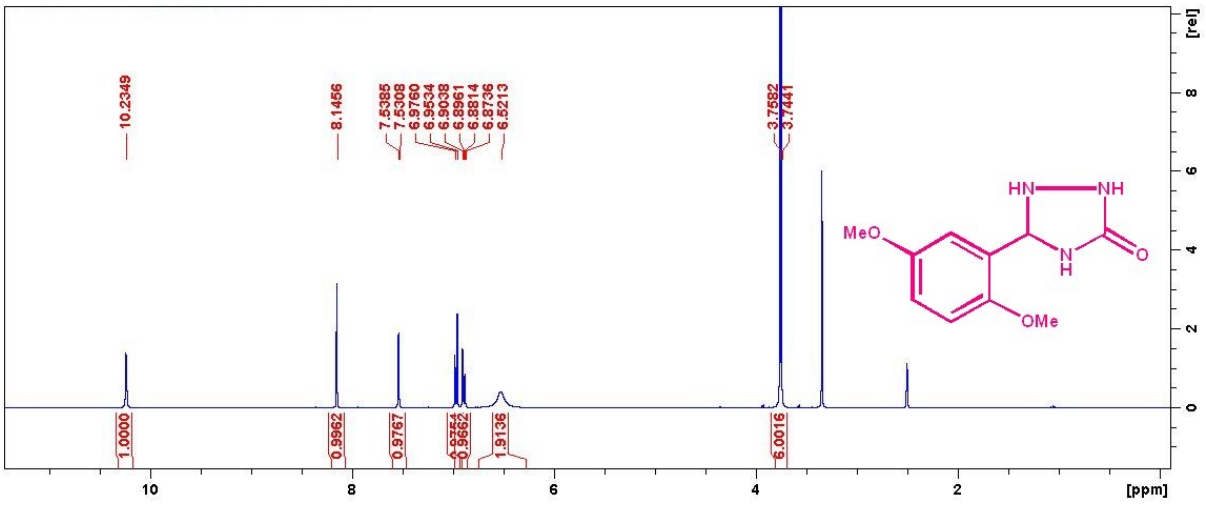


Fig. S40 5-(2,5-methoxyphenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

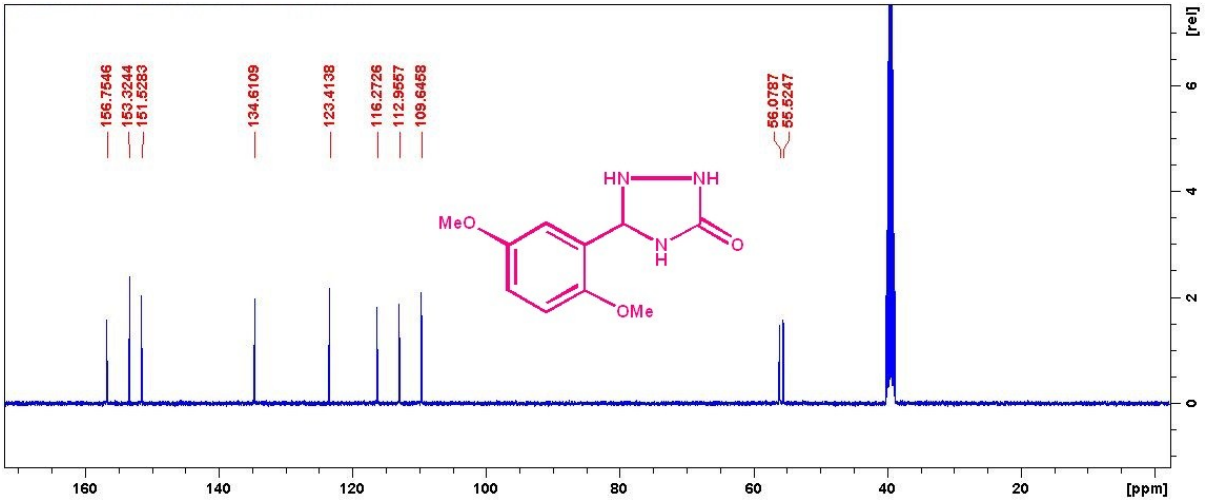


Fig. S41 5-(2,5-methoxyphenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

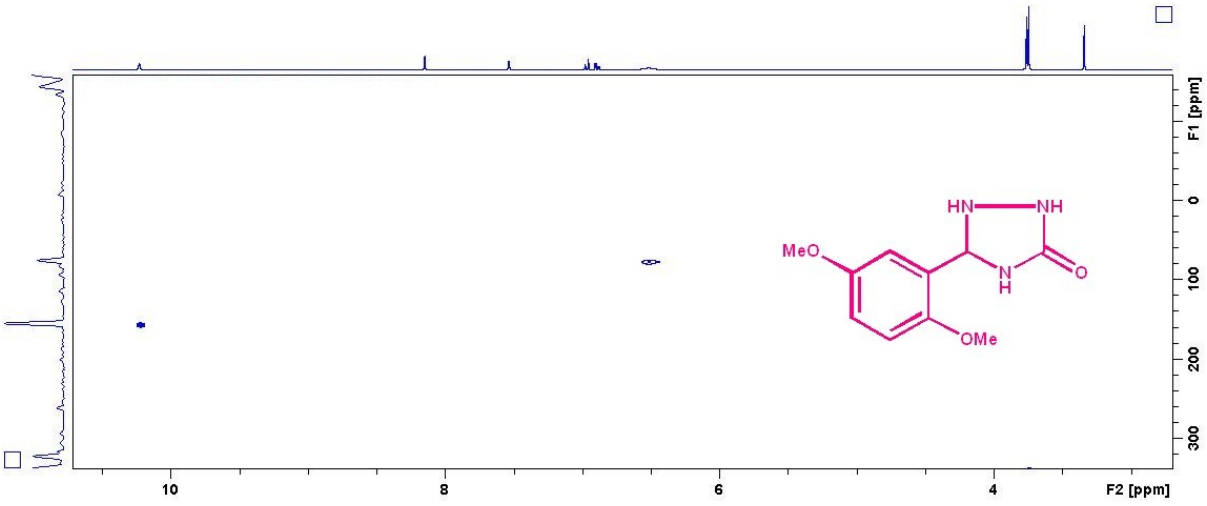


Fig. S42 5-(2,5-methoxyphenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

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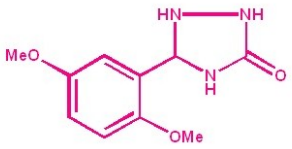
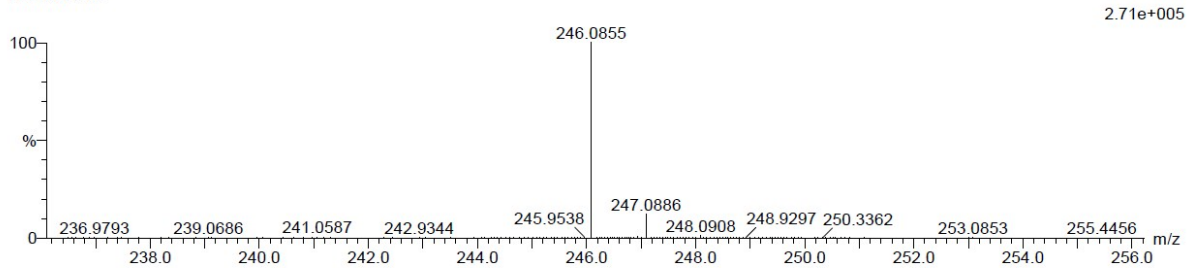


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 5-10 H: 10-15 N: 0-5 O: 0-5 Na: 1-1
3l 51 (1.687) Cm (1:61)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
246.0855	246.0855	0.0	0.0	5.5	685.5	0.0	C10 H13 N3 O3 Na

Fig. S43 5-(2,5-methoxyphenyl)-1,2,4-triazolidin-3-one HRMS spectrum

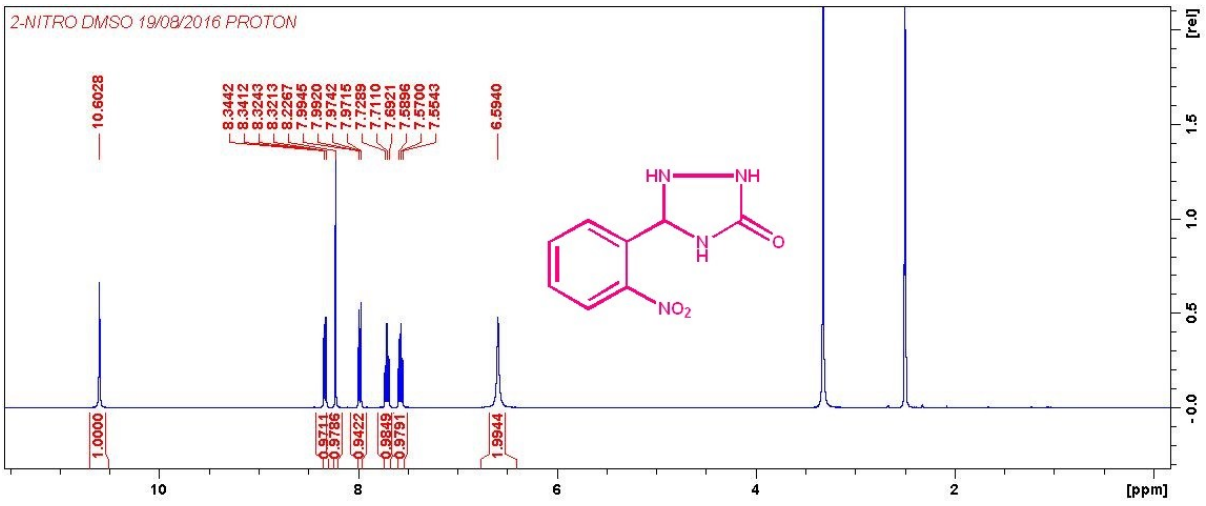


Fig. S44 5-(2-nitrophenyl)-1,2,4-triazolidin-3-one ^{1}H NMR spectrum

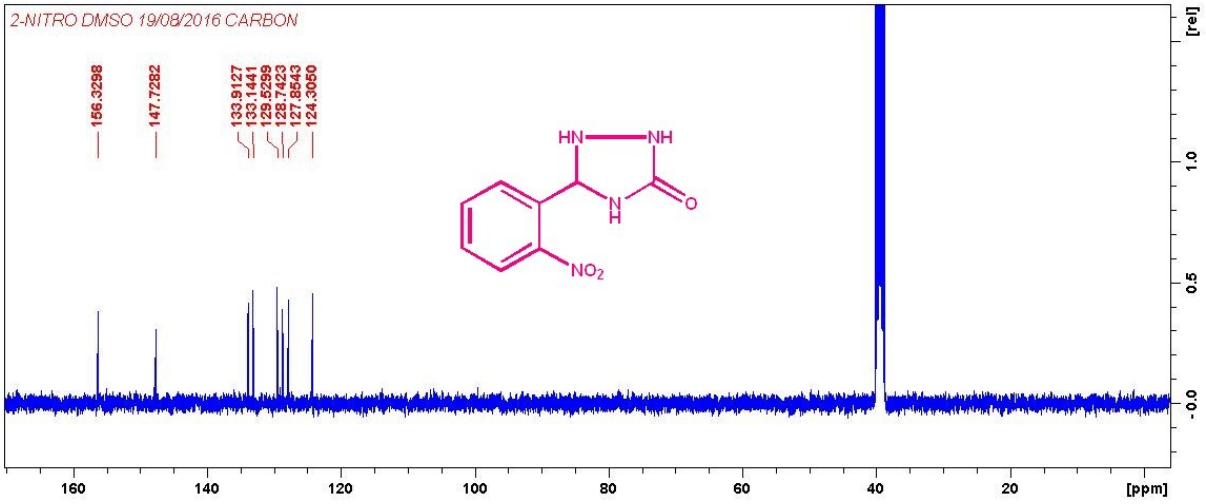


Fig. S45 5-(2-nitrophenyl)-1,2,4-triazolidin-3-one ^{13}C NMR spectrum

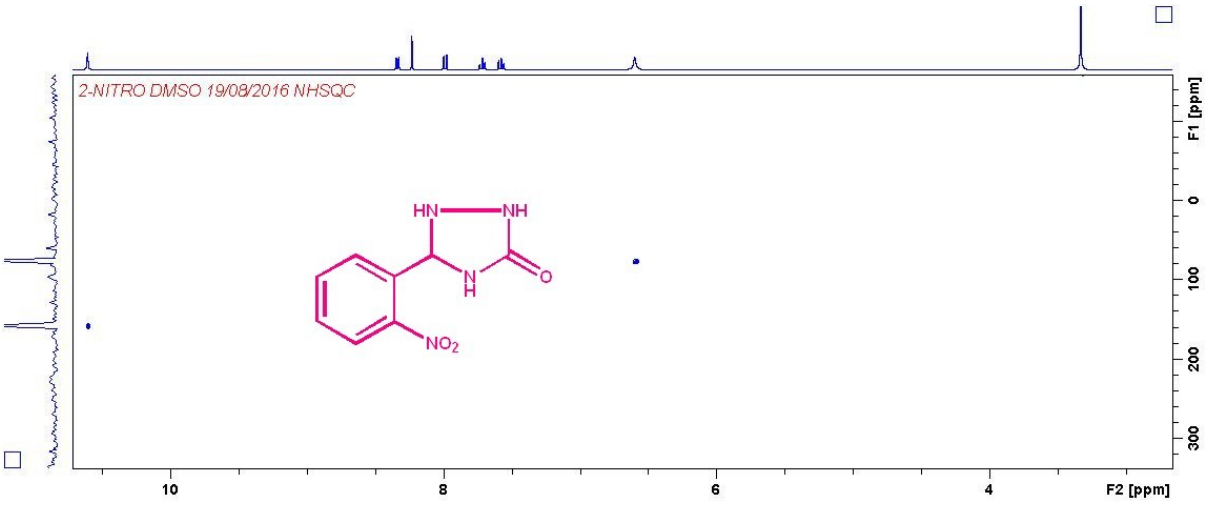


Fig. S46 5-(2-nitrophenyl)-1,2,4-triazolidin-3-one ^{15}N-HSQC NMR spectrum

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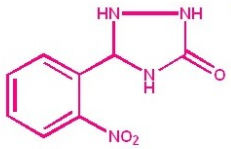
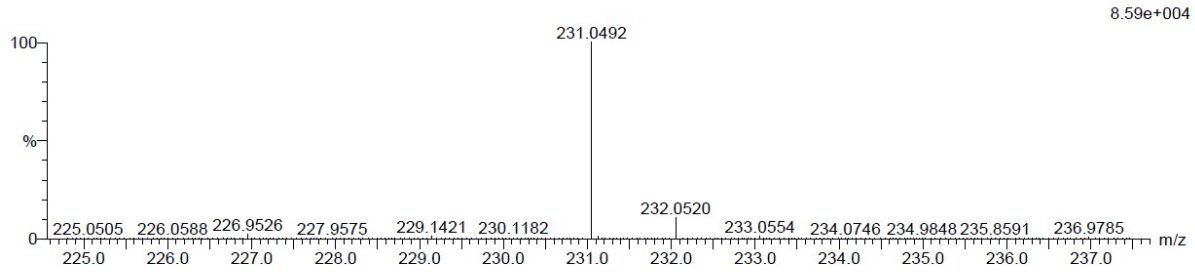


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 5-10 H: 5-10 N: 0-5 O: 0-5 Na: 1-1
3g 10 (0.304) Cm (1:61)
TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
231.0492	231.0494	-0.2	-0.9	6.5	672.0	0.0	C8 H8 N4 O3 Na

Fig. S46 5-(2-nitrophenyl)-1,2,4-triazolidin-3-one HRMS spectrum