Supporting information

(S)-5-benzyl- and 5-benzylidene-imidazo-4-one derivatives synthetized and studied towards an understanding of their thermal reactivity.

A. J. Pepino,[a] W. J. Peláez,[a,]* M. S. Faillace,[a] N. M. Ceballos,[a] E. L. Moyano,[b] and G. A. Argüello[a]

Table of Contents

Rate constants obtained by FVP

Table S1. Rate constants for thermal reaction of **7**

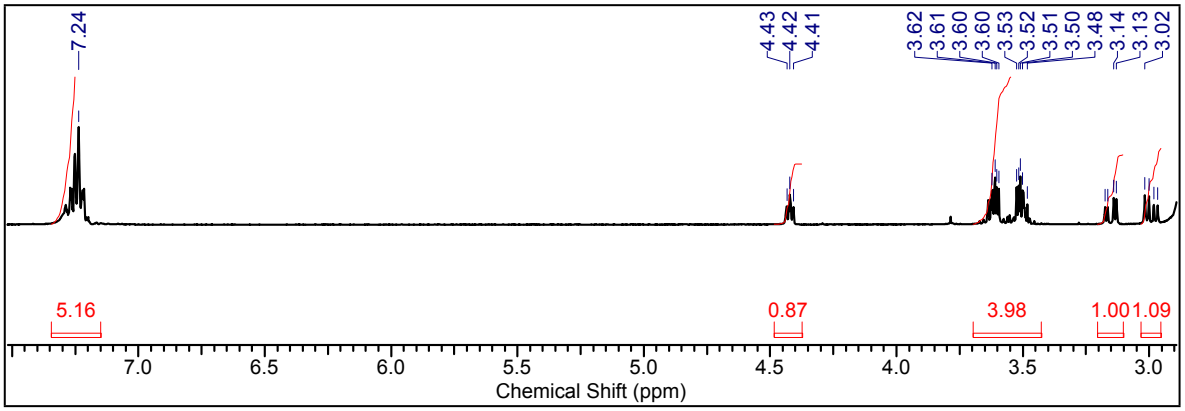
T [ºC]	C/C_0	Contact time $[10^{-2}s]$	k $[10^{-2}s^{-1}]$
500	0.96±0.02	1,60±0.07	0.02±0.01
550	0.73±0.02	1,51±0.07	0.11±0.02
575	0.67±0.02	1,48±0.06	0.21±0.02
600	0.55±0.02	1,41±0.06	0.29±0.03
625	0.11±0.02	1,39±0.05	1.59±0.03
650	0.04±0.02	1,01±0.05	3.18±0.04

Table S2. Rate constants for the thermal reaction of **8**

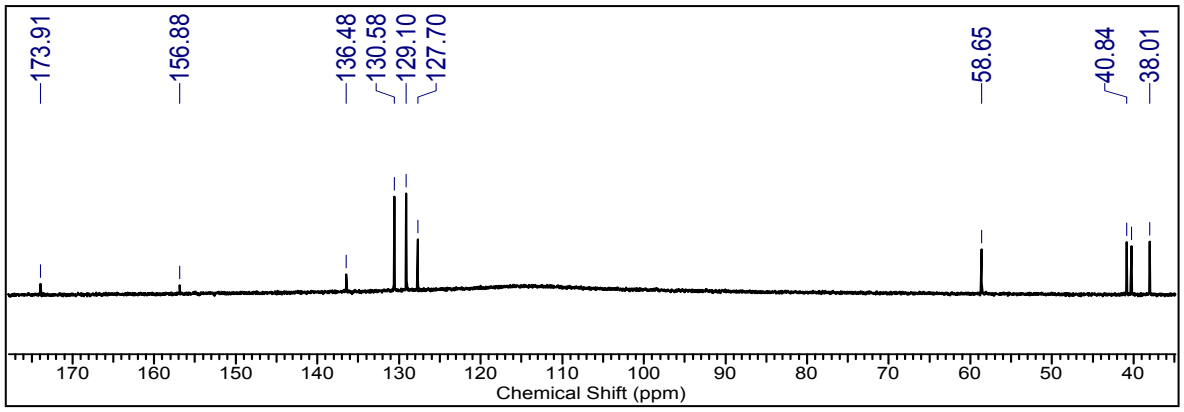
T [ºC]	C/C_0	Contact time $[10^{-2}s]$	k $[10^{-2}s^{-1}]$
525	0.94±0.02	1.57±0.07	0.04±0.02
550	0.74±0.02	1.52±0.07	0.19±0.02
575	0.53±0.02	1.48±0.07	0.42±0.02
600	0.46±0.02	1.43±0.06	0.54±0.02
650	0.33±0.02	1.35±0.06	0.82±0.02
675	0.26±0.02	1.32±0.05	1.05±0.02
700	0.20±0.02	1.29±0.05	1.29±0.02
750	0.17±0.02	1.23±0.05	1.49±0.02

Characterization for compounds

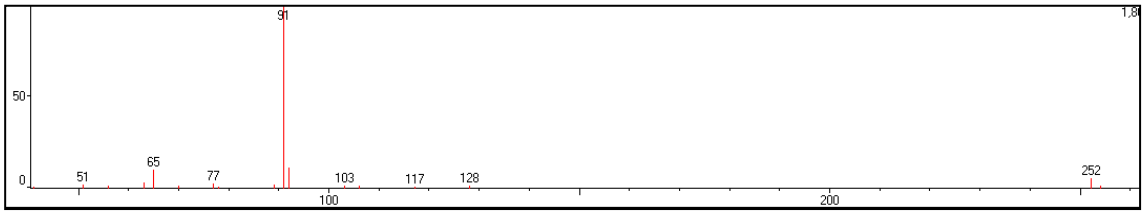
5-benzyl-3-(2-chloroethyl)imidazolidine-2,4-dione (7): ^{1}H NMR (400.16 MHz, acetone-d_6, 22ºC) δ = 2.99 (dd, J_1 = 14.1 Hz, J_2 = 6.1 Hz, 1H); δ = 3.15 (dd, J_1 = 14.1 Hz, J_2 = 4.5 Hz, 1H); 3.55 (m, 4H); 4.42 (m, 1H); 7.24 (m, 5H) ppm.



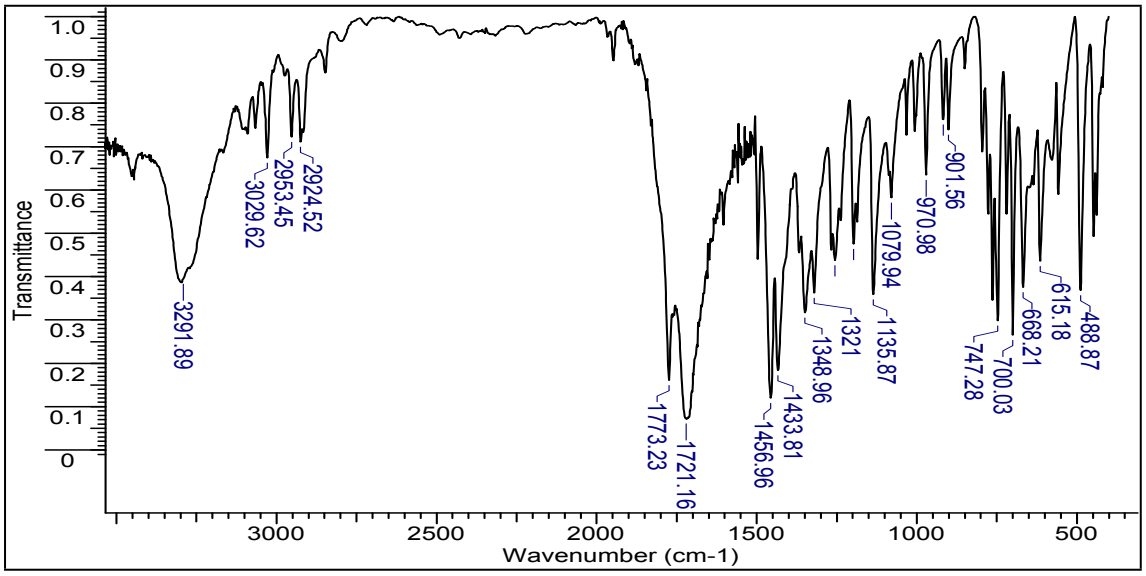
^{13}C RMN (100.56 MHz, acetone-d_6) δ = 38.0, 40.3, 40.8, 58.7, 127.7, 129.1 (x2), 130.6 (x2), 136.5, 156.9, 173.9ppm.



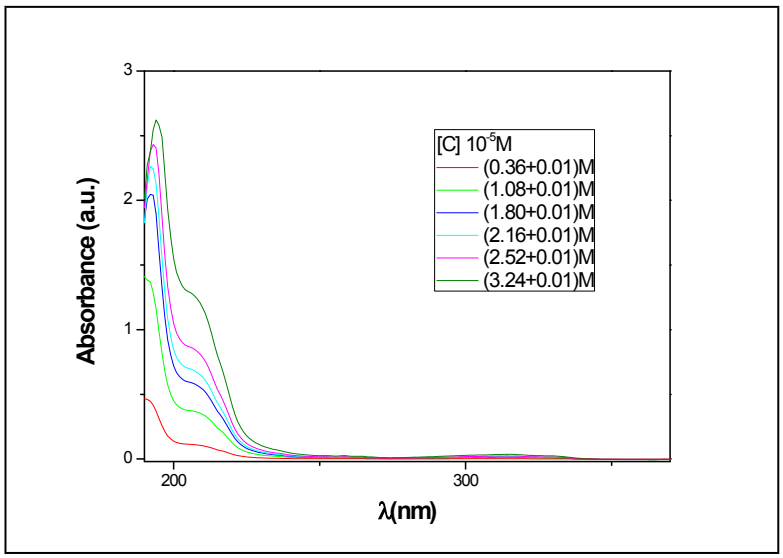
GC-MS *t* (min): 7.82. MS (EI): *m*/*z* (%) = 65(10), 91(100), 92(11), 252(5)[M$^+$], 254(2) [M+2].



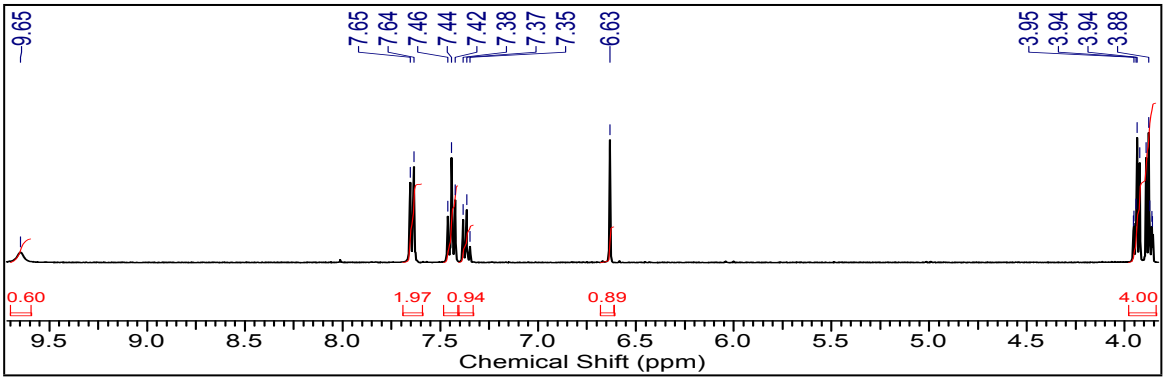
IR (KBr): 3292 (NH st), 2924 (C-H sp^3 st), 1773 (C=O st), 1721 (C=O st) cm^{-1}.



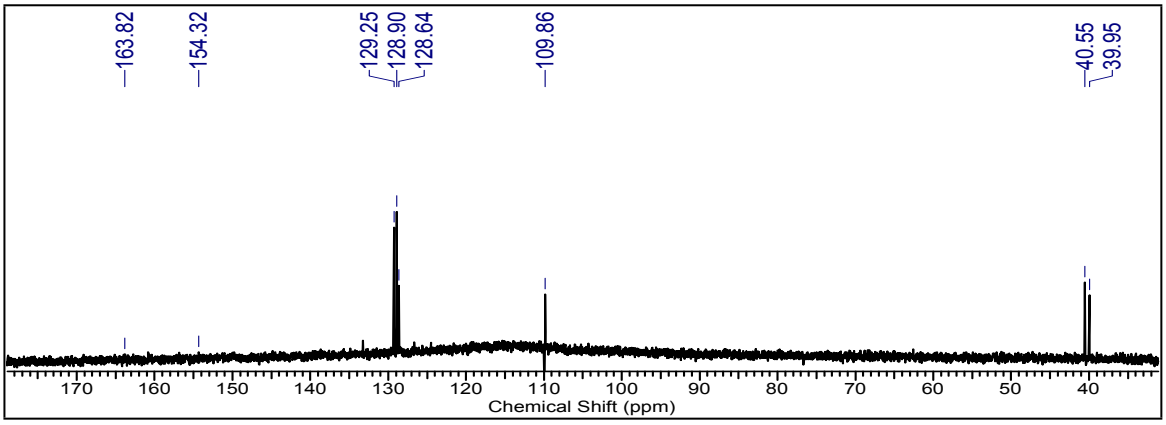
Uv-V(CH_3CN): ε_{191}= (1.102±0.006)10^6 M^{-1} cm^{-1}, ε_{191}= (3.781±0.006)10^5 M^{-1} cm^{-1}. ε_{314}= (1.149±0.006)10^3 M^{-1} cm^{-1}.



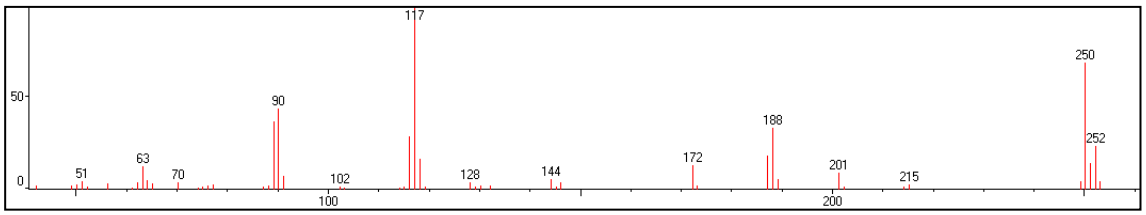
(Z)-5-benzylidene-3-(2-chloroethyl)imidazolidine-2,4-dione (8): ^{1}H NMR (400.16MHz, acetone-d_6, 22ºC) δ = 3.90 (m, 4H); 6.63 (s, 1H); 7.36 (t, J = 7.4 Hz, 1H); 7.43 (t, J = 7.4 Hz, 2H); 7.63 (d, J= 7.2, 2H); 9.65 (br. s. 1H) ppm.



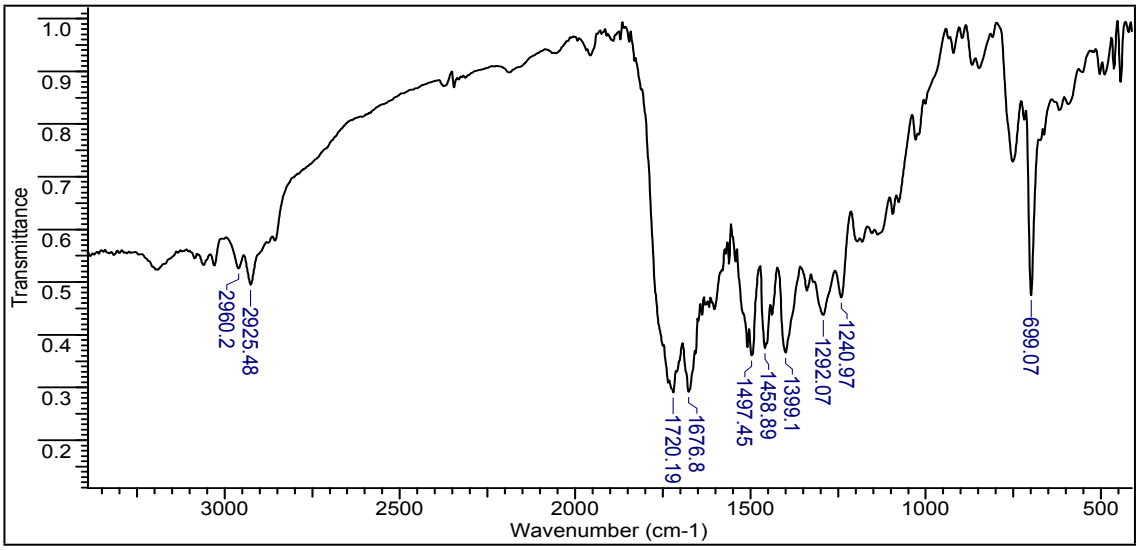
^{13}C RMN (100.56 MHz, DMSO-d_6) δ = 39.9, 40.6, 109.9, 128.6, 128.6, 128.9 (x2), 129.3 (x2), 154.3, 163.8 ppm.



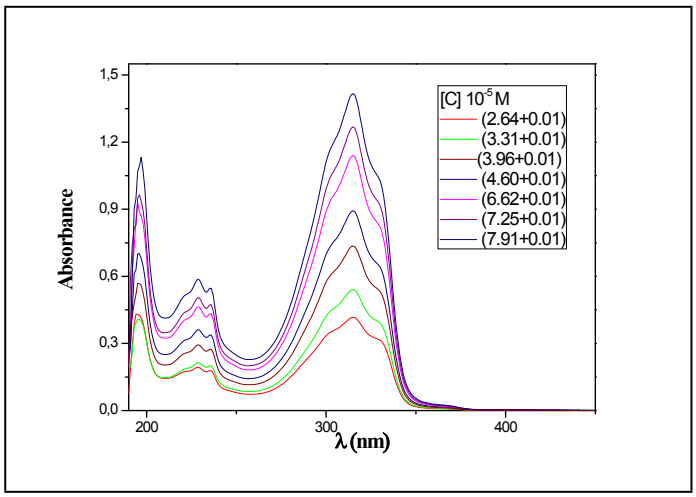
GC-MS: *t* (min): 9.10. MS (EI): *m/z* (%) = 63(13), 64(5), 89(37), 90(44), 91(7), 116(28), 117(100), 118(16), 144(5), 172(13), 187(18), 188(33), 250(68)[M^{+}]. 251(14), 252(23)



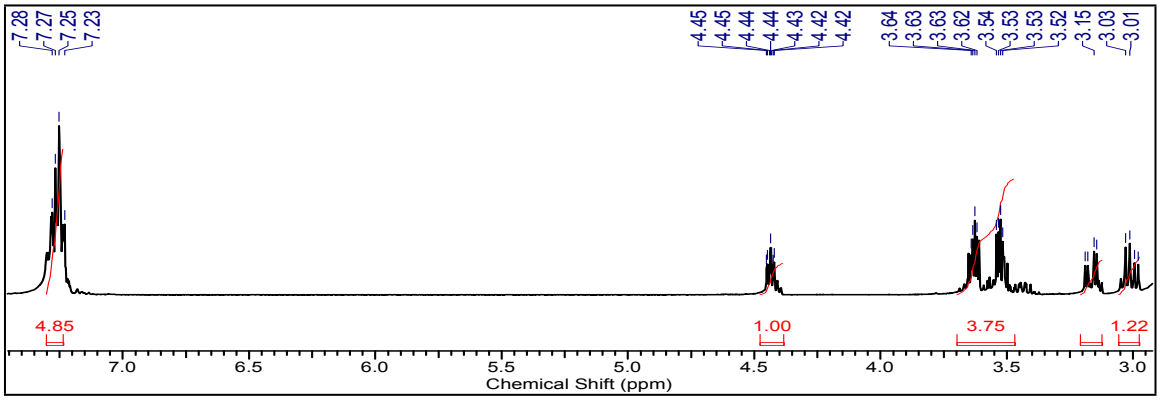
IR (KBr): 2925 (C-H sp^3 st), 1720 (C=O st) cm^{-1}.



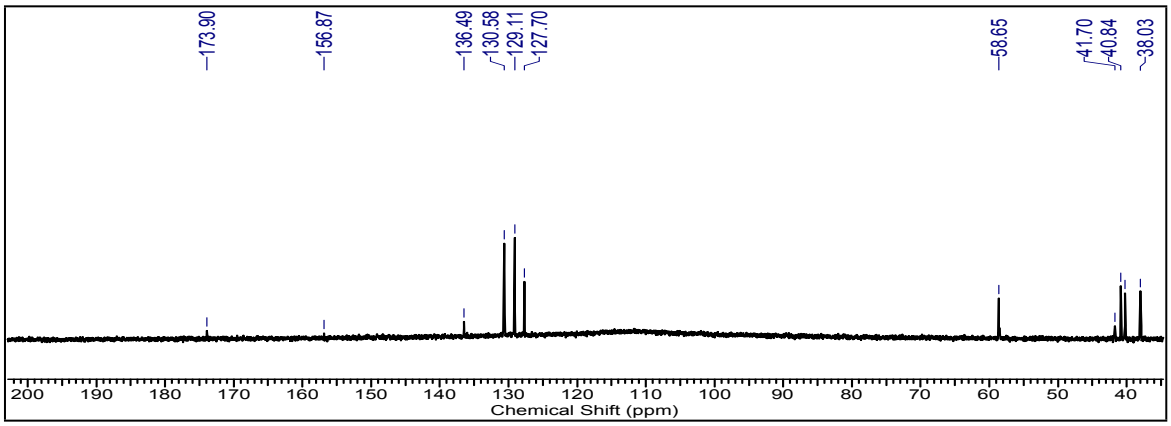
Uv-V(CH_3CN): ε_{315} = (1.81±0.01)10^4 M^{-1} cm^{-1} and ε_{228}= (7.24±0.01)10^3 M^{-1} cm^{-1}.



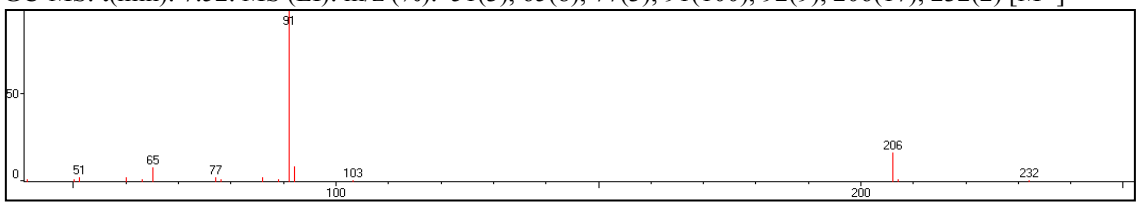
6-benzyl-2,3-dihydroimidazo[2,1-b]thiazol-5(6H)-one (11): ^{1}H NMR (400.16MHz, acetone-d_6, 22ºC) δ = 3.01 (dd, J_1 = 15.2 Hz, J_2 = 6.3 Hz, 1H); δ = 3.16 (dd, J_1 = 15.1 Hz, J_2 = 5.4 Hz, 1H); 3.58 (m, 4H); 4.43 (m, 1H); 7.52 (m, 5H) ppm.



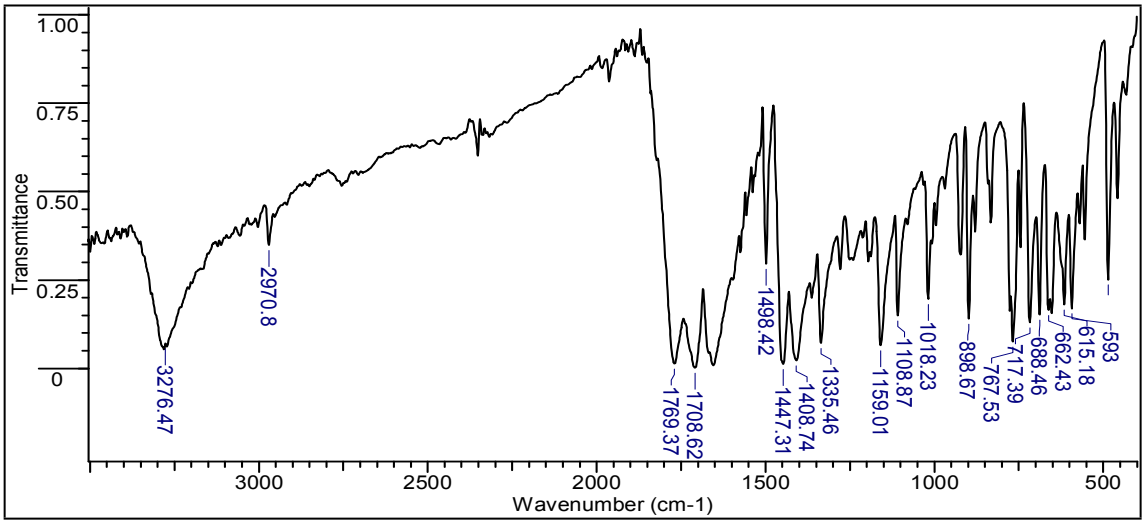
^{13}C RMN (100.56 MHz, acetone-d_6) δ = 38.0, 40.3, 40.8, 58.7, 127.7, 129.1 (x2), 130.6 (x2), 136.5, 156.9, 173.9 ppm.



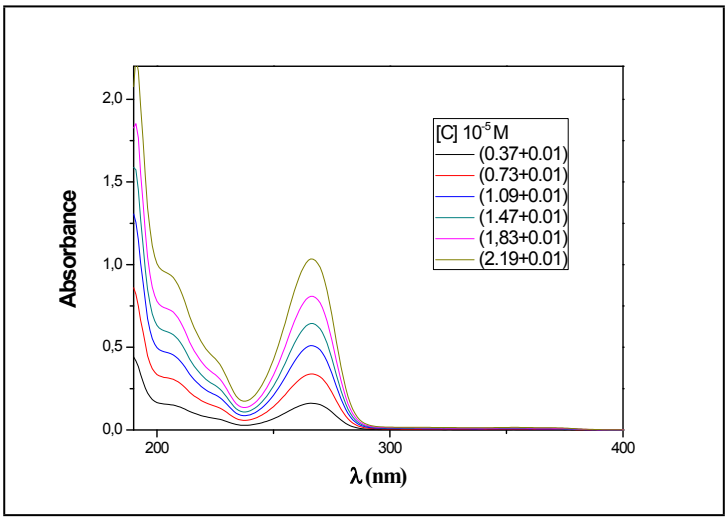
GC-MS: t(min): 7.52. MS (EI): m/z (%). 51(3), 65(8), 77(3), 91(100), 92(9), 206(17), 232(2) [M+]



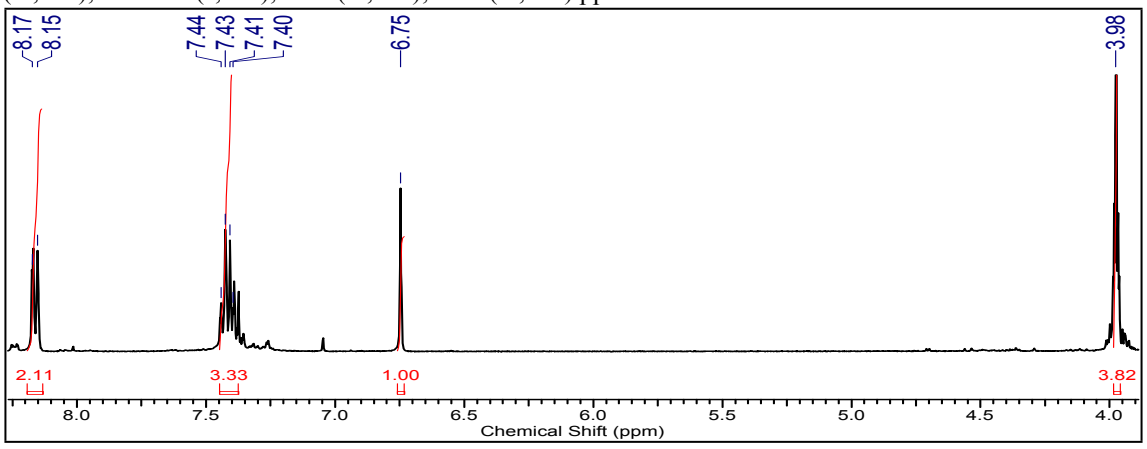
IR (KBr): 3276 (N-H st), 2925 (C-H sp^3 st), 1769 (C=O st), 1708 (C=O st) cm^{-1}.



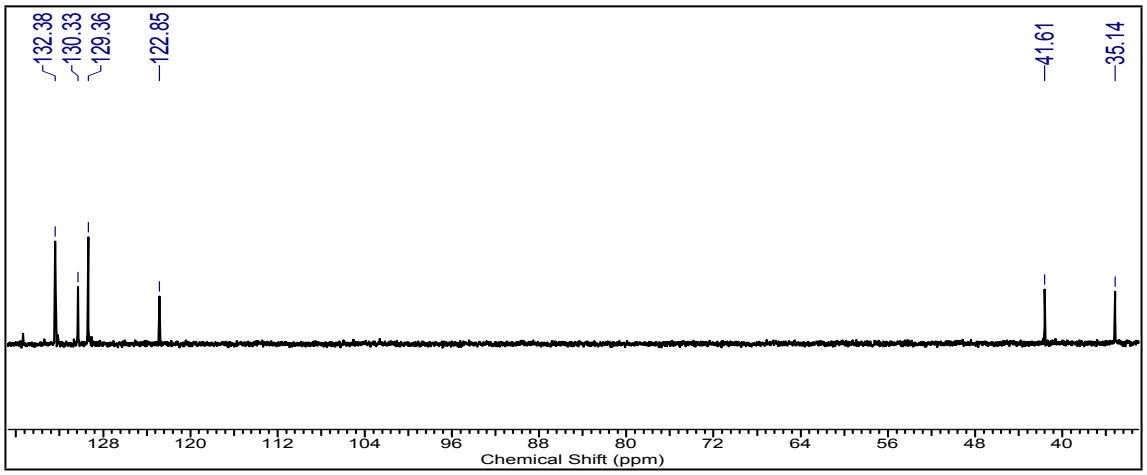
Uv-V(CH_3CN): $\varepsilon_{267} = (4.61 \pm 0.01)10^4\ M^{-1}\ cm^{-1}$



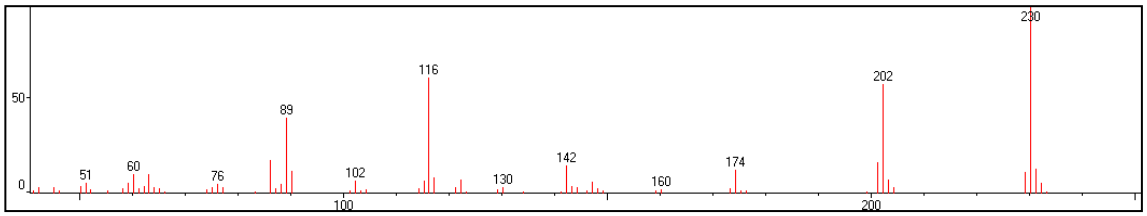
(Z)-6-benzylidene-2,3-dihydroimidazo[2,1-b]thiazol-5(6H)-one (12): ^{1}H NMR (400.16MHz, acetone-d_6, 22ºC) δ = 3.98 (m, 1H); δ = 6.73 (s, 1H); 7.42 (m, 3H); 8.16 (m, 2H) ppm.



^{13}C RMN (100.56 MHz, DMSO-d_6) δ = 35.1, 41.6, 122.9, 129.4(x2), 130.3, 132.4 (x2) ppm.

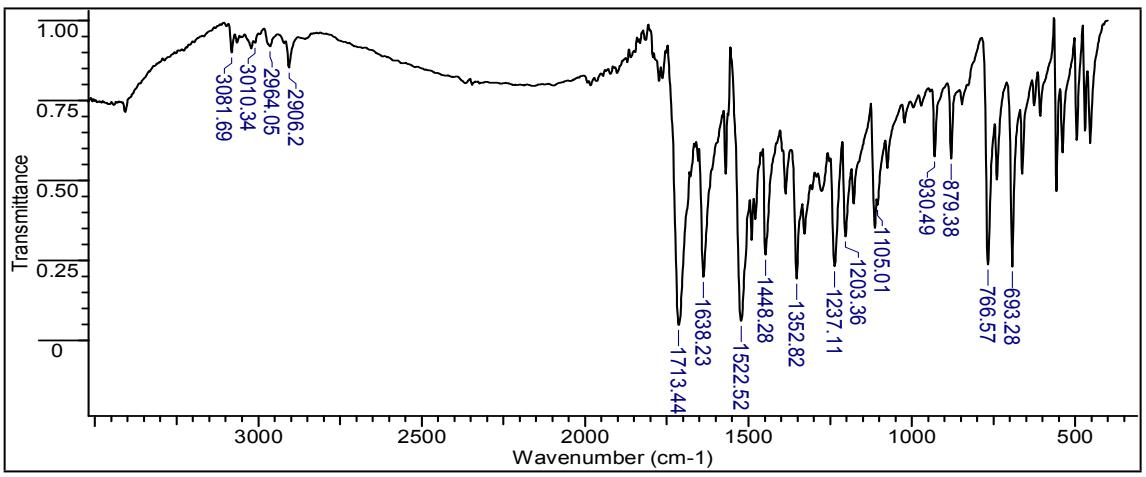


GC-MS: t(min): 11.82. MS (EI): m/z (%). 51(5), 59(6), 60(10), 63(10), 76(5), 86(18), 89(40), 90(11), 102(7), 115(7), 116(60), 117(8), 122(7), 142(14), 147(6), 174(12), 201(16), 202(57), 203(7), 229(11), 230(100)[M+]

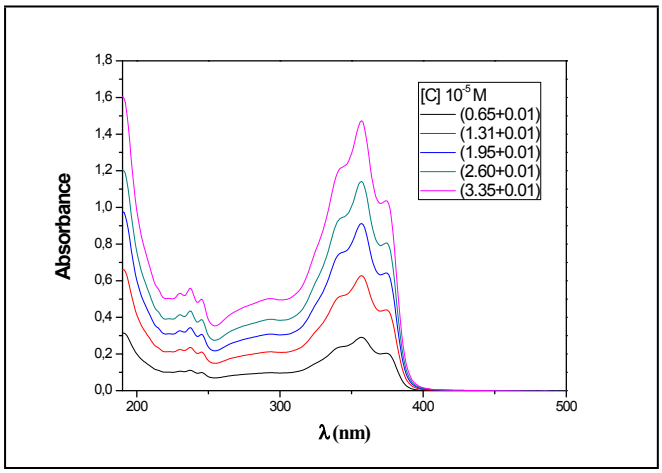


IR (KBr): 2906 (C-H sp^3 st), 1713 (C=O st) cm^{-1}

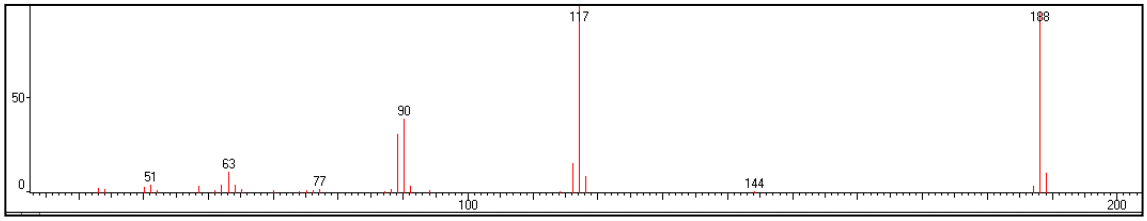
.



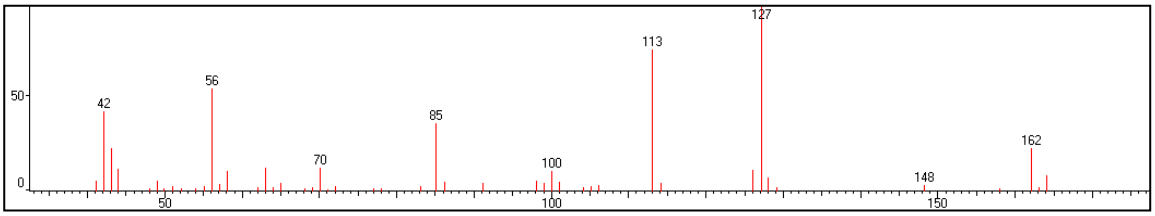
Uv-V(CH_3CN): $\varepsilon_{366} = (4.67\pm0.01)10^4\ M^{-1}\ cm^{-1}$



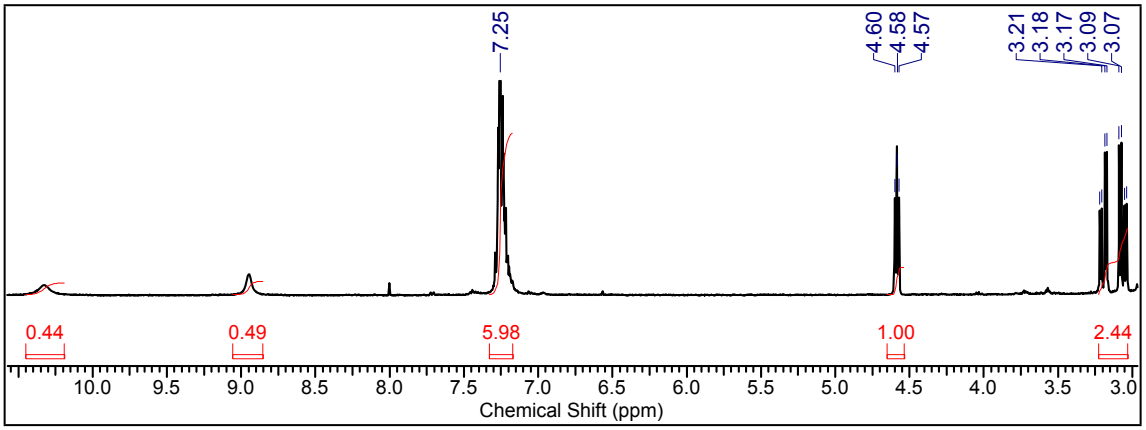
(Z)-5-benzylideneimidazolidine-2,4-dione (15): GC-MS *t* (min): 5.62. MS (EI): *m/z* (%) = 51(4), 62(4), 63(10), 64(4), 89(31), 90(39), 116(15), 117(100), 118(9), 188(95) [M+]



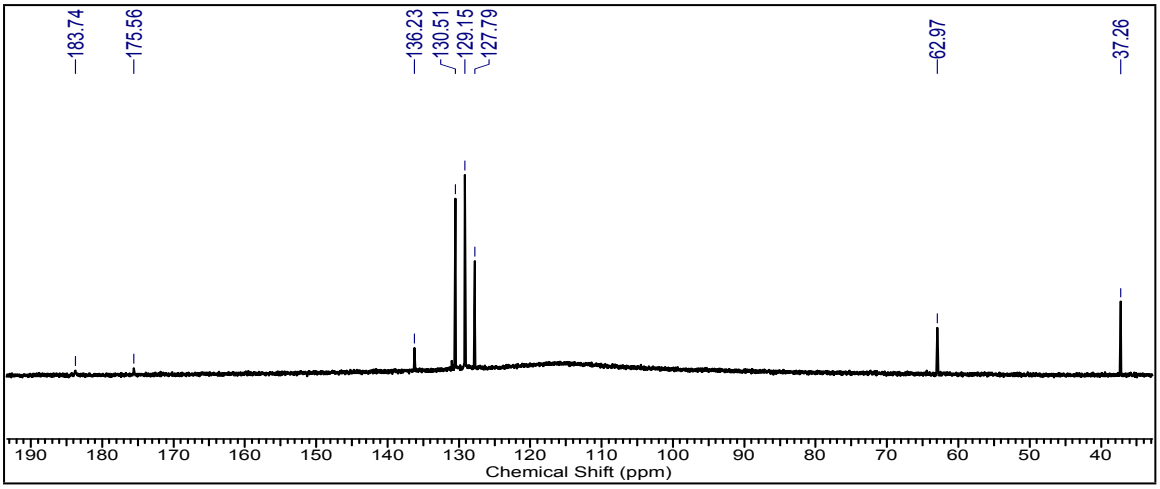
3-(2-chloroethyl)imidazolidine-2,4-dione (17): GC-MS *t* (min): 3.61. MS (EI): *m/z* (%) = 41(5),42(42), 43(22), 44(12), 49(5), 56(54), 58(11), 63(12), 70(12), 85(35), 98(5), 100(11), 113(74), 126(11), 127(100), 128(7), 162(22), 164(8)[M+2]



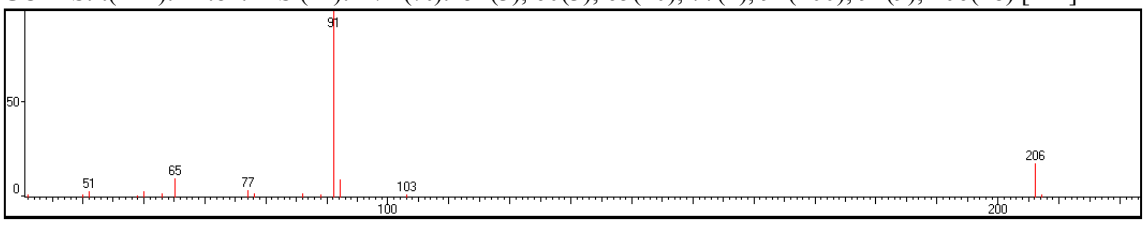
5-benzyl-2-thioxoimidazolidin-4-one (20): ^{1}H NMR (400.16MHz, acetone-d_6, 22ºC) δ = 3.12 (dt, 2H); 4.58 (t, 1H); 7.25 (m, 5H); 8.9 (br.s. 1H); 10.61 (br.s. 1H) ppm.



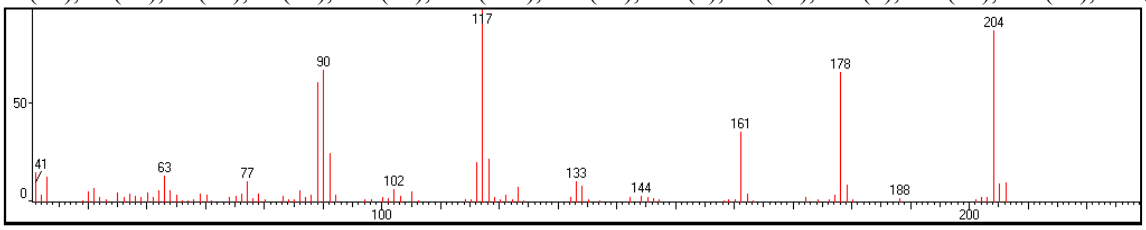
^{13}C RMN (100.56 MHz, DMSO-d_6) δ = 37.26, 62.9, 127.8, 129.2(x2), 130.5 (x2), 136.23, 175.6, 183.7 ppm.



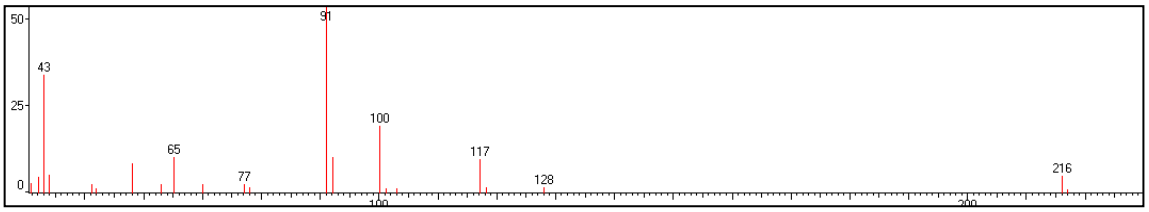
GC-MS: t(min): 11.82. MS (EI): m/z (%). 51(3), 60(3), 65(10), 77(4), 91(100), 92(9), 206(18) [M+]



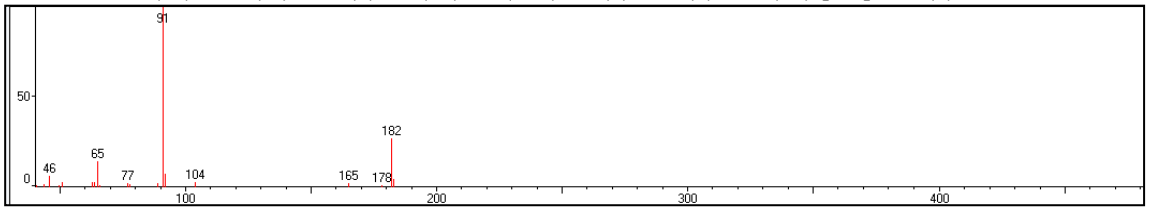
(Z)-5-benzylidene-2-thioxoimidazolidin-4-one (22): GC-MS: t(min): 9.03. MS (EI): m/z (%). 41(15), 43(13), 51(7), 63(13), 77(11), 89(61), 90(67), 116(20), 117(100), 118(22), 123(8),133(11), 134(8), 161(36), 178(66), 179(9), 204(87)[M+]



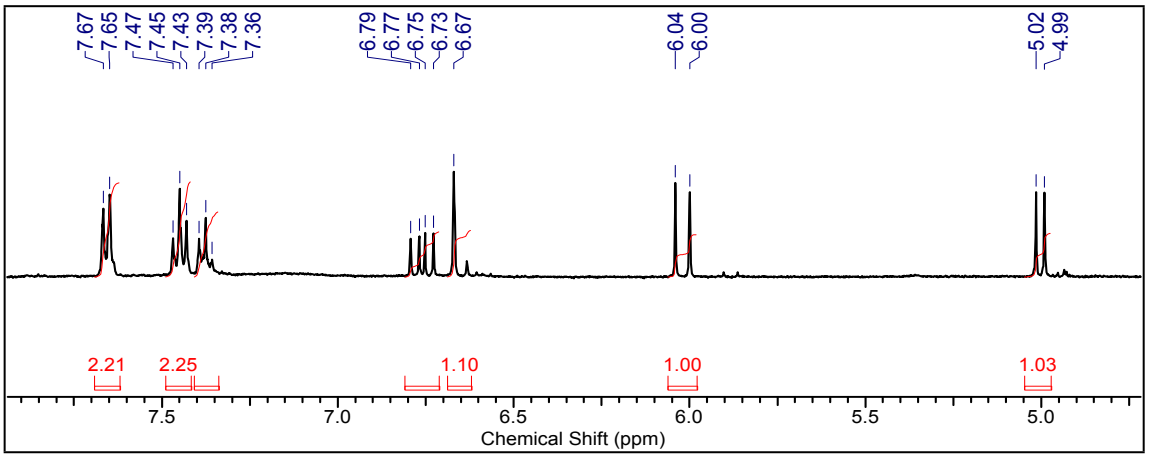
5-benzyl-3-vinylimidazolidine-2,4-dione (25): GC-MS: t (min): 6.20. MS (EI): m/z (%). 42(6), 43(30), 44(6), 58(8), 65(11), 83(9), 91(100), 92(14), 100(24), 117(13), 149(7), 216(8)[M+]



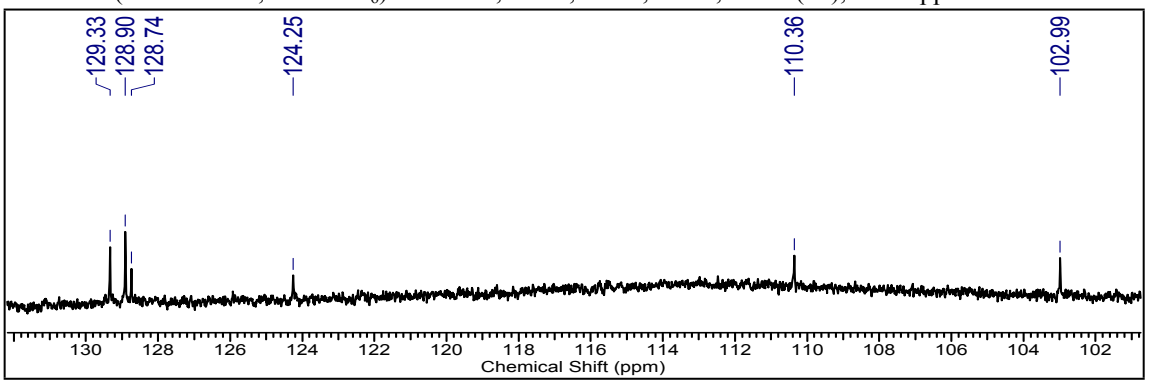
1-2-Diphenylethane (26): This compound was characterized by comparison with authentic sample. GC-MS: *t* (min): 5.94min. MS (EI): *m/z* (%) = 46(6), 65(14), 91(100), 92(7), 165(2), 182(27) [M^+], 183(4).



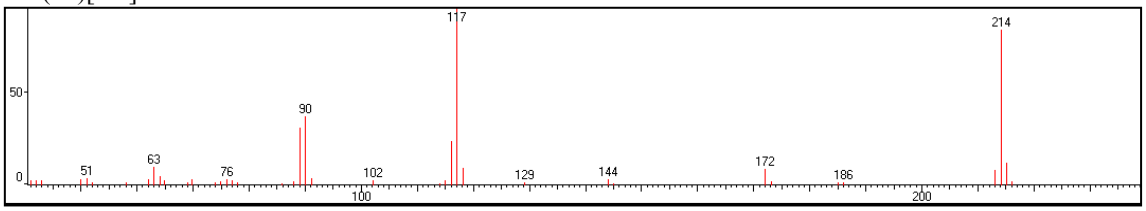
(Z)-5-benzylidene-3-vinylimidazolidine-2,4-dione (27): ^{1}H NMR (400.16MHz, acetone-d_6, 22ºC) δ = 5.50 (dd, J_1 = 410.1 Hz, J_2 = 16.3 Hz, 2H); 6.67 (s, 1H); 6.76 (c, J_1 = 16.3 Hz, J_2 = 9.8 Hz, 1H); 7.38 (t, J = 7.3 Hz, 1H); 7.45 (t, J= 7.2, 2H) ; 7.66 (d, J= 7.3, 2H) ppm



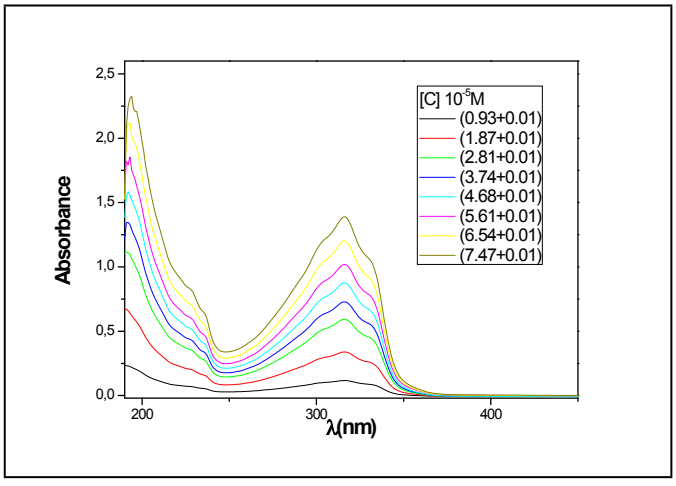
^{13}C RMN (100.56 MHz, DMSO-d_6) δ = 102.9, 110.4, 124.3, 128.8, 128.9 (x2), 129.3 ppm.



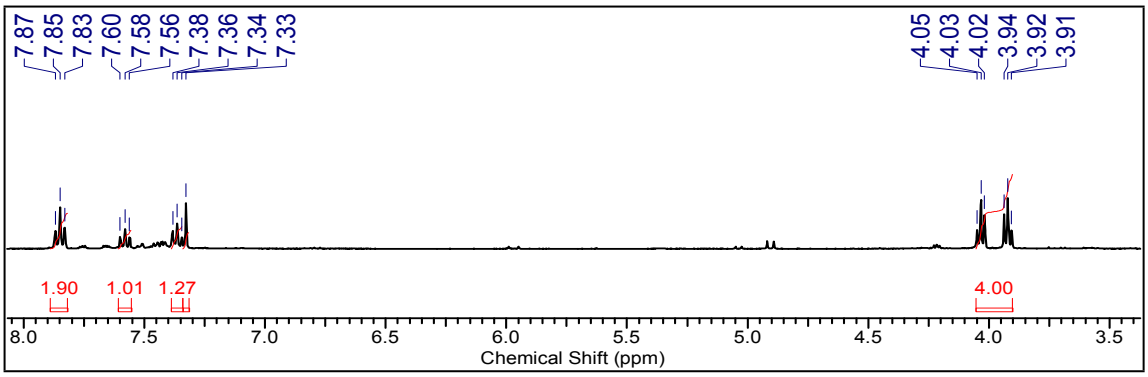
GC-MS: *t* (min): 7.10. MS (EI): *m/z* (%). 63(10), 64(5), 89(31), 90(37), 116(24), 117(100), 118(9), 172(9), 213(8), 214(84)[M^+]



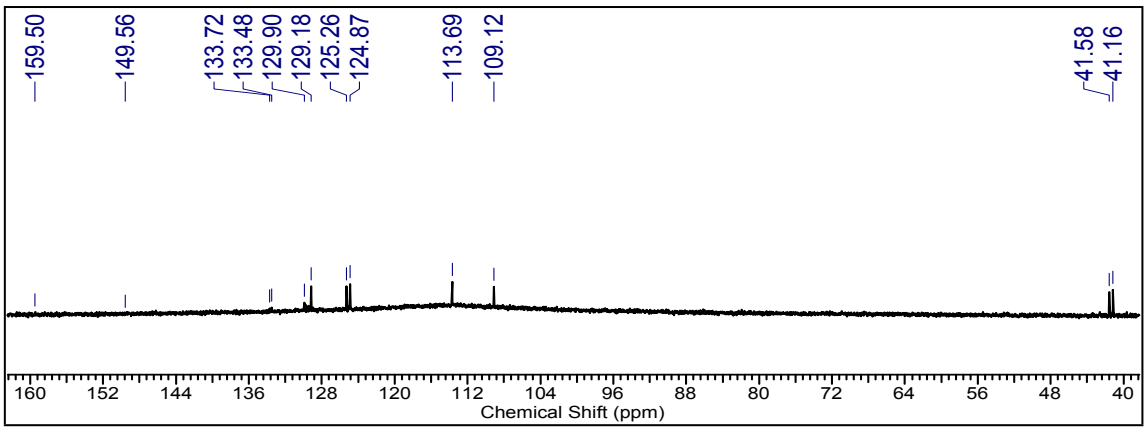
Uv-V(CH_3CN): ε_{316} = (1.87±0.01)10^4 M^{-1} cm^{-1}



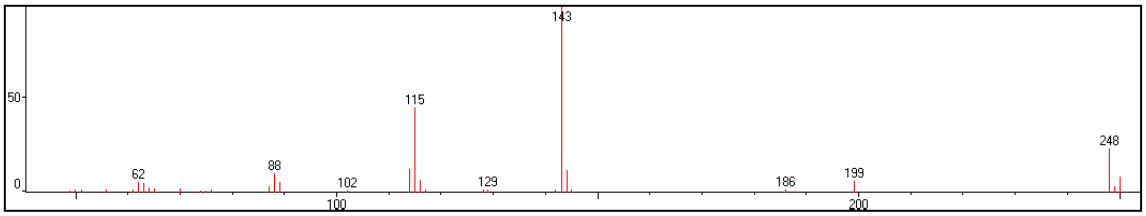
2-(2-chloroethyl)-1H-imidazo[1,5-a]indole-1,3(2H)-dione (28): mp.: ^{1}H NMR (400.16MHz, acetone-d_6, 22ºC) δ = 4.00 (m, 4H); 7.33 (s, 1H); 7.37 (t, *J*= 7.8, 1H); 7.58 (t, *J* = 7.7 Hz, 1H); 7.85 (t, *J*= 7.6, 2H) ppm.



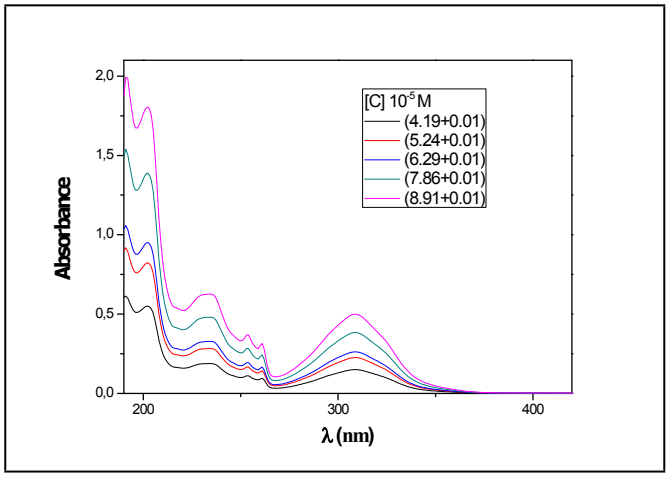
^{13}C RMN (100.56 MHz, DMSO-d_6) δ = 41.2, 41.6, 109.1, 124.9, 129.2, 113.7, 125.3, 133.5, 133.7, 149.5, 159.54, ppm.



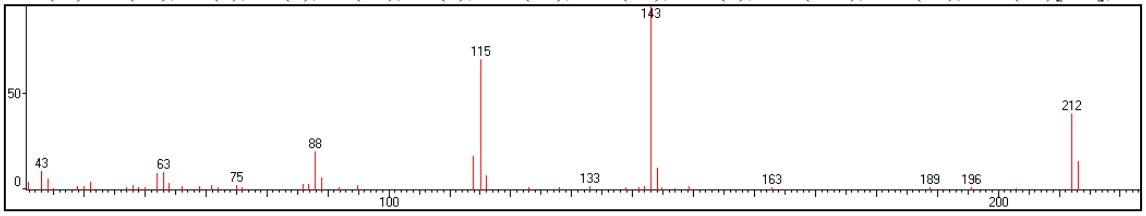
GC-MS: *t* (min): 6.06. MS MS (EI): *m/z* (%). 62(5), 63(5), 88(10), 89(6), 114(13), 115(45), 116(6), 143(100), 144(12), 199(6), 248(23)[M^+], 250(8)



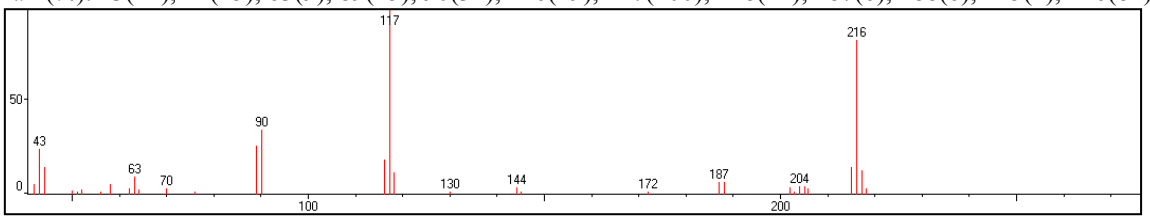
Uv-V(CH_3CN): ε_{202} = (2.54±0.01)10^5 M^{-1} cm^{-1} , ε_{235} = (4.26±0.01)10^4 M^{-1} cm^{-1} , ε_{319} = (7.12±0.01)10^4 M^{-1} cm^{-1}



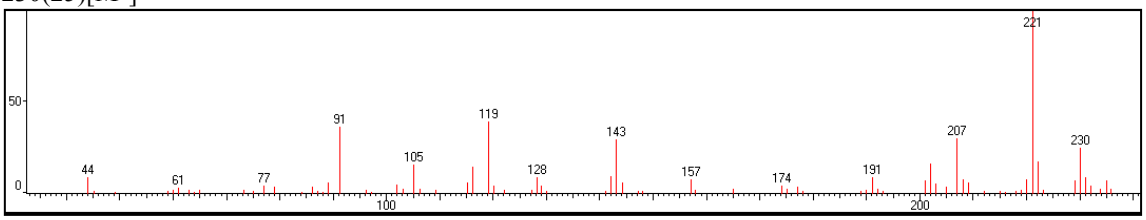
2-vinyl-1H-imidazo[1,5-a]indole-1,3(2H)-dione (29): This compound was characterized by GC-MS t(min)=5.91 MS (EI): *m/z* (%). 43(10), 44(6), 62(9), 88(20), 89(6), 114(18), 115(68), 116(8), 143(100), 144(11), 212(40)[M^+], 213(15)



(Z)-5-benzylidene-3-ethylimidazolidine-2,4-dione (30): This compound was characterized by GC-MS t(min)=6.89 MS (EI): *m/z* (%). 43(24), 44(15), 63(9), 89(25), 90(34), 116(19), 117(100), 118(11), 187(6), 188(6), 215(1), 216(81)[M^+], 217(13)



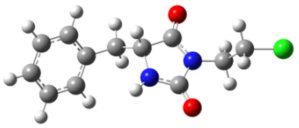
6-benzylimidazo[2,1-b]thiazol-5(6H)-one (33): GC-MS t(min)=6.89 MS (EI): *m/z* (%). 44(9), 91(36), 105(15), 116(14), 119(39), 128(9), 142(9), 143(29), 157(8), 191(9), 201(7), 202(16), 107(30), 208(8), 220(8), 221(100), 222(17), 229(7), 230(25)[M^+]



Computational calculations

All calculations were performed with the GAUSSIAN09 program system, using a B3LYP/6-31+G(d,p) approach. Transition state theory was used to evaluate the energy of the different channels. The transition states were characterized by the presence of one negative frequency and the internal reaction's coordinate (IRC) method was applied to verify that the correct states were connected. Though we knew that more precise methods were available, we had to make a compromise between the size of the molecules under study and the computational cost.

7
Energy (a.u.)= -1185.118111



N	-0.31376900	0.93023500	-0.34119200
C	-0.54008600	-0.50271700	-0.22884400
C	0.85251900	-1.00308900	0.17948300
N	1.68010800	0.10239000	0.21119600
C	0.98666100	1.29319200	-0.12810800
C	-1.62745000	-0.90047700	0.79218700
C	-3.00850400	-0.43922800	0.37637000
C	-3.77401300	-1.19593700	-0.52472700
C	-5.03416900	-0.75798200	-0.93746100
C	-5.55143500	0.44752000	-0.45353900
C	-4.80209400	1.20727600	0.44771100
C	-3.54083800	0.76558700	0.85890800
O	1.16606000	-2.15098300	0.43524300
H	-3.38478300	-2.14064600	-0.89792600
H	-5.61438900	-1.36053500	-1.63040600
H	-6.53299900	0.78707200	-0.77067300
H	-5.19936100	2.14052900	0.83645900
H	-2.96909800	1.35635500	1.57034700
H	-1.36186700	-0.47630600	1.76653600
H	-1.59508300	-1.99084800	0.88780600
H	-0.78539400	-0.94176100	-1.20568700
H	-0.98377800	1.59214500	-0.70262700
C	3.08892000	0.08039500	0.58548200
H	3.31491600	1.01390500	1.10478400

H	3.23808400	-0.76193600	1.26428400
C	3.97832600	-0.06594900	-0.64976000
H	3.85748600	0.78155800	-1.32519300
H	3.77600000	-0.99972700	-1.17598600
Cl	5.72111800	-0.10517200	-0.15490500
O	1.49017300	2.39950700	-0.19581500

7TS
Energy (a.u.): -1184.995566

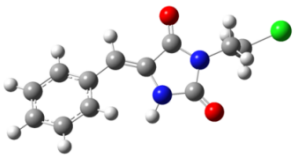
N	-0.22257600	1.00949100	-0.29753500
C	-0.48609600	-0.34517500	0.14886500
C	0.82095100	-0.76181800	0.55533200
N	1.71347800	0.24269300	0.53729600
C	1.05966100	1.40183100	-0.05130200
C	-1.66733100	-0.48108900	1.11507400
C	-3.00944300	-0.28255900	0.43042900
C	-3.47057600	-1.19358700	-0.53235300
C	-4.70719000	-1.01228400	-1.15263400
C	-5.50444400	0.09016300	-0.82480000
C	-5.05512800	1.00530000	0.12830100
C	-3.81565700	0.81748800	0.75036400
O	0.98364400	-2.04341000	0.61856100
H	-2.85343200	-2.04789700	-0.79831700
H	-5.05009500	-1.73075700	-1.89182100
H	-6.46664300	0.23136300	-1.30831800
H	-5.66596900	1.86410900	0.39166400
H	-3.47595000	1.52999800	1.49847700
H	-1.57153900	0.25283900	1.92905100
H	-1.62583400	-1.47761000	1.56924600
H	-0.08463100	-1.83335100	-0.11645500
H	-0.89981900	1.64740500	-0.68864900
C	3.16861600	0.15088300	0.65981600
H	3.52559200	1.12235600	1.00679600
H	3.39816600	-0.60428200	1.41325100
C	3.81642200	-0.20540700	-0.67929800
H	3.62722800	0.56698800	-1.42515100
H	3.47370500	-1.17477300	-1.04309200
Cl	5.61150600	-0.31969500	-0.47351100
O	1.63367900	2.44599200	-0.30007200

7OH
Energy (a.u.): -1185.079652

N	0.31288100	-1.30746300	-0.73897600
C	0.51942700	-0.85828400	0.58798000
C	-0.71281000	-0.52892700	1.04656300
N	-1.65572900	-0.73674100	0.04220900
C	-1.00995300	-1.19981700	-1.11180700
C	1.86142200	-0.87827000	1.24657400
C	2.94114600	-0.08862800	0.51209600
C	2.72831300	1.24675000	0.13906400
C	3.72702600	1.97233500	-0.51195600
C	4.95569500	1.37107200	-0.80551800
C	5.17624800	0.04125500	-0.44280100
C	4.17329500	-0.68210500	0.21144600
H	1.77088500	1.71512000	0.35339900
H	3.54610300	3.00575700	-0.79358600
H	5.73141000	1.93479200	-1.31532200
H	6.12503700	-0.43643300	-0.66976900
H	4.35241900	-1.71762300	0.49173100
H	2.20869400	-1.91340500	1.37253400
H	1.75433700	-0.47560300	2.26378000
H	1.04048700	-1.46952500	-1.41832200
C	-3.08936200	-0.50996200	0.11897200

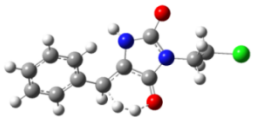
H	-3.56736800	-1.21471600	-0.56499200
H	-3.42610200	-0.71489300	1.13737900
C	-3.43877400	0.92490100	-0.28117500
H	-3.15960500	1.12035400	-1.31685400
H	-2.96349100	1.65089600	0.37973500
Cl	-5.22944200	1.19122300	-0.15235500
O	-1.53190600	-1.44675900	-2.19593200
O	-1.17252800	-0.07545100	2.24441900
H	-0.46691600	-0.11032200	2.90317800

8
Energy (a.u.): -1183.922090



C	-3.44607600	0.85654800	-0.31529400
C	-4.76843700	1.24082900	-0.09498700
C	-5.70157700	0.31864900	0.38822800
C	-5.30578800	-1.00025300	0.63170800
C	-3.98691900	-1.38811500	0.40471000
C	-3.02509700	-0.46477600	-0.05518100
H	-2.75589200	1.57526600	-0.74515000
H	-5.07374400	2.26018700	-0.31241800
H	-6.72975200	0.62194500	0.56087400
H	-6.02615800	-1.72738400	0.99458500
H	-3.68564400	-2.41523400	0.59181200
C	-1.65531400	-0.93124400	-0.26027600
H	-1.51401000	-2.00159200	-0.38894400
C	-0.50559300	-0.22513200	-0.27692000
C	0.83560400	-0.83899300	-0.51626500
C	1.10079500	1.42162700	-0.09595800
O	1.11200900	-1.99948300	-0.76530500
N	1.74544700	0.21270900	-0.40329200
N	-0.25628800	1.13744900	-0.07823500
H	-0.90771000	1.80575300	0.30529700
O	1.63340800	2.49624800	0.10605300
C	3.18485900	0.09099000	-0.59468000
H	3.35540400	-0.71264000	-1.31419700
H	3.55187600	1.03311800	-1.00667400
C	3.88785800	-0.22119700	0.72719500
H	3.54388800	-1.16851800	1.14399200
H	3.74537800	0.58254000	1.45041200
Cl	5.67194300	-0.37836900	0.45361400

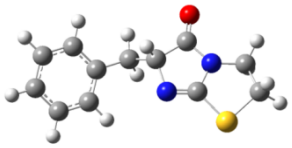
8TS
Energy (a.u.)= -1184.992862



H	-4.71878200	2.31212600	0.92317900
C	-4.54595400	1.31339400	0.53269300
C	-5.62994700	0.51201300	0.16029400
H	-6.64479000	0.88565700	0.26189200
C	-5.40250900	-0.77304300	-0.34141500
H	-6.23852600	-1.40233700	-0.63211200
C	-4.09829800	-1.24869700	-0.46678100
H	-3.92448900	-2.25067300	-0.85129800
C	-2.99828900	-0.44983000	-0.10222400
C	-3.24021700	0.84004800	0.40597500
H	-2.40229800	1.46848300	0.68229300
C	-1.64058500	-1.01117300	-0.24577800
H	-1.26718400	-1.83554700	1.05243100
H	-1.62277900	-1.97007100	-0.75787000
C	-0.44482600	-0.25056900	-0.37936400
C	0.74829300	-0.87729000	0.03458100
O	0.82836300	-2.05913000	0.53165700
H	-0.35892600	-2.16493800	1.06728700
N	1.67483700	0.15514400	0.21690100
C	1.00205300	1.30296600	-0.13105200
O	1.69048700	2.45940000	-0.18415000
C	3.06066100	0.01218600	0.64198900
H	3.33967700	0.89158200	1.22609800

H	3.11544800	-0.86852400	1.28617400
C	3.99298700	-0.14678800	-0.56053300
H	3.75084400	-1.04277100	-1.13350200
H	3.95883700	0.72891400	-1.20966000
Cl	5.70654300	-0.32203700	0.00349300
N	-0.25261400	1.13564700	-0.43966900
H	-0.67744798	1.58099024	-1.22782221

11
Energy (a.u.): -1047.247980



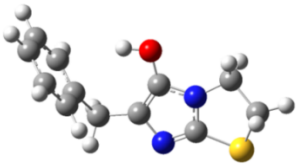
N	-0.50008700	-0.74158600	-0.32857200
C	0.00511500	0.64835600	-0.32164900
C	-1.22883400	1.55194800	-0.09157300
N	-2.28714500	0.65933500	-0.08493500
C	-1.76359800	-0.63753100	-0.18238200
C	1.10540100	0.89706800	0.73288300
C	2.44096300	0.27803500	0.37857500
C	3.45659600	1.06331600	-0.18605900
C	4.68986700	0.50334400	-0.53121900
C	4.92603600	-0.85603700	-0.31294600
C	3.92162600	-1.64825600	0.25142800
C	2.69010500	-1.08577600	0.59372600
O	-1.29232000	2.75909200	0.05706700
S	-3.04238900	-1.85098400	-0.04766700
H	3.28276500	2.12416600	-0.35186000
H	5.46475800	1.12968500	-0.96442100
H	5.88440500	-1.29392800	-0.57711100
H	4.09657100	-2.70643700	0.42481200
H	1.90863200	-1.70861600	1.01827500
H	0.74848900	0.51381400	1.69595600
H	1.21121200	1.98251600	0.83372500
H	0.41353200	0.87739000	-1.31533600
C	-4.33584900	-0.52658200	-0.21533600
H	-5.19858700	-0.80057200	0.39317900
H	-4.63844400	-0.46903900	-1.26345100
C	-3.69243000	0.79271100	0.25511300
H	-3.80980900	0.92876100	1.33731200
H	-4.12609800	1.65746000	-0.25374700

11TS
Energy (a.u.): -1047.136034

N	-0.83266400	-0.89038300	1.00341500
C	-0.08931200	0.25241700	0.96990600
C	-0.73127300	1.27029300	0.18451800
N	-1.96387600	0.65047000	-0.17185800
C	-1.94560000	-0.59630200	0.34276200
C	1.27396100	0.35751300	1.58177000
C	2.40724400	-0.00106700	0.62735100
C	3.20497600	1.00074500	0.05863600
C	4.23425000	0.67432900	-0.83047600
C	4.47815800	-0.66050800	-1.16104100
C	3.68695000	-1.66680500	-0.59703500
C	2.65955900	-1.33933400	0.28995500
O	-0.50456700	2.61963300	0.04456700
S	-3.41460800	-1.50900600	0.02347200
H	3.02073900	2.04134900	0.31376900
H	4.84540000	1.46349700	-1.25950500
H	5.27912200	-0.91609400	-1.84879800
H	3.87159000	-2.70809600	-0.84632400
H	2.04356500	-2.12396300	0.72115300
H	1.29376700	-0.31158800	2.44837500
H	1.41344000	1.38287600	1.94099400
H	0.02146100	1.54065100	-0.68725900
C	-3.96753200	-0.16109400	-1.13969100
H	-5.04825800	-0.04344200	-1.05411300

H	-3.71749400	-0.47052900	-2.15715100
C	-3.21049400	1.12611100	-0.74547600
H	-3.76284200	1.71024900	0.00074600
H	-3.01977100	1.76372900	-1.61195200

11OH
Energy (a.u.): -1047.227967

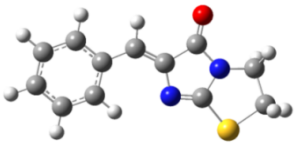


N	1.33608400	-1.59622000	-0.07637300
C	0.15927800	-0.88885200	-0.34319500
C	0.43743000	0.46177900	-0.39303400
N	1.78454800	0.59230300	-0.13201400
C	2.26426500	-0.68451400	0.02349700
C	-1.15099600	-1.60630500	-0.53580200
C	-2.36740800	-0.78244900	-0.14945400
C	-3.20601700	-0.22396600	-1.12652400
C	-4.31819800	0.54809600	-0.76739600
C	-4.60966100	0.77015100	0.57960100
C	-3.78264500	0.21714100	1.56419900
C	-2.67301400	-0.54799200	1.20218900
S	4.02348200	-0.72032500	0.22941000
H	-2.99224600	-0.40396900	-2.17760800
H	-4.95517800	0.96784400	-1.54082100
H	-5.47322900	1.36511500	0.86195800
H	-4.00437400	0.38125300	2.61497600
H	-2.03222900	-0.97116400	1.97160400
H	-1.11439700	-2.51879400	0.06996600
H	-1.25626900	-1.93638200	-1.57845000
C	3.99132800	1.11359400	0.52646800
H	4.91947700	1.54933400	0.15429900
H	3.91339900	1.29107600	1.60217500
C	2.75526600	1.67046000	-0.21034100
H	2.98346500	1.89936800	-1.25931400
H	2.37504900	2.57430400	0.27274800
O	-0.29334800	1.58962900	-0.60237300
H	-1.23458100	1.35474800	-0.60566000

12TS
Energy (a.u.): -1047.155921

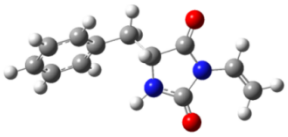
N	0.53471700	-0.71013100	-0.49494000
C	0.09418000	0.61658300	-0.43250900
C	1.16201900	1.47723000	-0.06692700
N	2.25009300	0.63425600	0.10415600
C	1.81037000	-0.63168000	-0.23709800
C	-1.22375700	1.13701400	-0.29431800
C	-2.44228600	0.33110200	-0.09517700
C	-2.41576400	-0.97281100	0.43443500
C	-3.60261900	-1.68294800	0.61362000
C	-4.83161100	-1.10841200	0.27390300
C	-4.87095300	0.18760500	-0.24969200
C	-3.68643900	0.89990400	-0.42817300
S	3.13788100	-1.78678500	-0.36520800
H	-1.46430500	-1.42735900	0.68282500
H	-3.56803100	-2.69039700	1.01806900
H	-5.75253600	-1.66652600	0.41659400
H	-5.82106300	0.64118400	-0.51627400
H	-3.71938300	1.91000100	-0.82913000
H	-1.40152100	2.06805300	-0.82673800
H	-0.97970500	2.07298900	0.97735200
C	4.23730000	-0.57919100	0.52148100
H	5.26006200	-0.70454200	0.16409100
H	4.19790500	-0.79481300	1.59205800
C	3.68661200	0.82900700	0.21973500
H	4.09093700	1.22221400	-0.72134000
H	3.91799600	1.53049100	1.02538600
O	1.02439900	2.67154700	0.38657300
H	-0.15761200	2.56559200	0.94766700

12
Energy (a.u): -1046.059090



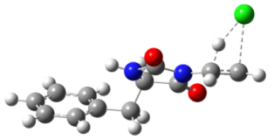
N	0.51126600	-0.71809900	-0.01743300
C	0.05536800	0.61761300	-0.00191600
C	1.23068800	1.55528200	-0.00181100
N	2.31202300	0.66798700	0.03728200
C	1.80067400	-0.62100900	-0.01346000
C	-1.22280000	1.07370500	0.01087000
C	-2.48011600	0.34134200	0.01074800
C	-3.68011000	1.08546700	0.01863800
C	-4.92040800	0.45094500	0.01725700
C	-4.98865200	-0.94554100	0.00778600
C	-3.80801800	-1.69789500	0.00020900
C	-2.56497900	-1.06926500	0.00179900
O	1.29736300	2.77456300	-0.02943500
S	3.07230700	-1.83057300	-0.09167300
H	-3.62920200	2.17124700	0.02558500
H	-5.83110700	1.04275700	0.02334500
H	-5.95355700	-1.44442100	0.00655700
H	-3.85804800	-2.78305100	-0.00690000
H	-1.65210700	-1.65224300	-0.00382000
H	-1.30419700	2.15932200	0.02020400
C	4.34335300	-0.52509000	0.28574200
H	5.25886000	-0.76102900	-0.25796100
H	4.54507300	-0.54502500	1.35911100
C	3.74174300	0.82785100	-0.14772700
H	3.96749300	1.04593900	-1.19897700
H	4.11749300	1.64951100	0.46734100

25
Energy (a.u.): -724.303185



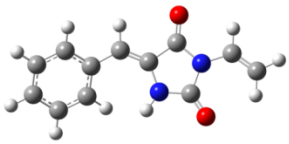
C	2.98841100	1.08406700	-0.47954600
C	4.24645300	0.57145400	-0.80264200
C	4.67754000	-0.63529900	-0.24307800
C	3.84357400	-1.32130700	0.64280700
C	2.58418100	-0.80525800	0.96354500
C	2.13854500	0.40202700	0.40552100
H	2.66675900	2.02950000	-0.91072500
H	4.89227300	1.11687100	-1.48483300
H	5.65737100	-1.03286500	-0.49052700
H	4.17267800	-2.25513800	1.08953800
H	1.94569300	-1.33957800	1.66278300
C	-1.65907600	1.17803800	-0.04870700
C	-1.92043000	-1.11213800	-0.34991500
O	-1.91391000	2.34577300	0.17431500
N	-2.57042200	0.12553000	-0.06572200
N	-0.58592100	-0.82651600	-0.45286200
H	0.05740900	-1.52965900	-0.78395600
O	-2.46038500	-2.19525100	-0.46465800
C	-3.94599100	0.32760000	0.18093600
H	-4.15255400	1.37472300	0.37460200
C	-4.89943800	-0.60840200	0.18543700
H	-4.69873000	-1.65307400	-0.00983800
H	-5.91789700	-0.30042600	0.39341700
C	-0.28032400	0.58956500	-0.35517100
H	0.05108700	0.99158400	-1.32283200
C	0.76256600	0.94689300	0.72535000
H	0.41260900	0.55820500	1.68762700
H	0.78600300	2.03914400	0.80034900

25TS
Energy (a.u.)= -1185.032017



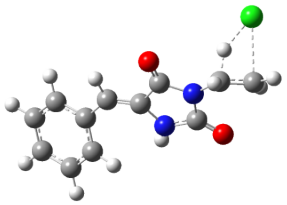
C	3.56352100	-1.25621700	0.62812300
C	4.80422300	-0.88130500	1.14768000
C	5.41862600	0.29832200	0.71639900
C	4.78602400	1.09631200	-0.23956100
C	3.54333500	0.71826700	-0.75728700
C	2.91479600	-0.46005000	-0.32881000
H	3.09911100	-2.18166100	0.96136500
H	5.29371400	-1.51272500	1.88350300
H	6.38512400	0.58848600	1.11751100
H	5.25948500	2.00984700	-0.58744400
H	3.06258400	1.33823500	-1.51013300
C	-0.96810800	-0.85297000	-0.44169000
C	-1.02127100	1.44196000	-0.04247000
O	-1.29886400	-1.97218200	-0.79034100
N	-1.75575900	0.28539500	-0.45157900
N	0.24298900	1.00740100	0.22473300
H	0.92479600	1.62448600	0.64025000
O	-1.47979900	2.56467900	0.01009600
C	-3.11864900	0.39879800	-0.86136300
H	-3.84620400	0.56463600	0.15261000
H	-3.31918700	1.26358400	-1.49207200
C	-3.93576800	-0.73902300	-0.96533900
H	-3.63609500	-1.70642000	-0.58680300
H	-4.89241600	-0.65152200	-1.46480600
Cl	-5.09505600	-0.16321700	1.29552400
C	0.40823900	-0.43085100	0.08351100
H	0.55306600	-0.90822300	1.06262000
C	1.55275400	-0.85193700	-0.86231700
H	1.38196800	-0.39416600	-1.84272000
H	1.48235100	-1.93724700	-0.98916500

27
Energy(a.u.): -723.107582



H	3.95489700	-2.45570000	0.72626100
C	3.76647800	-1.43607200	0.40309100
C	4.82051000	-0.64193100	-0.05855500
H	5.82718500	-1.04575100	-0.10839800
C	4.57210000	0.68013700	-0.44040400
H	5.38613100	1.30901400	-0.78862100
C	3.28033400	1.19766800	-0.37091000
H	3.09360600	2.22680400	-0.66543000
C	2.19997400	0.40321300	0.06622300
C	2.47136300	-0.92259900	0.46563600
H	1.68153000	-1.54078300	0.88026300
C	0.86745700	1.00168200	0.10639300
H	0.81557100	2.08709500	0.13931300
C	-0.33967400	0.39931500	0.06885000
C	-1.62998800	1.14066200	0.13404300
O	-1.81628900	2.33581700	0.27122700
N	-2.63362000	0.16343800	0.00825800
C	-2.06807700	-1.11950800	-0.15065000
O	-2.65269200	-2.16823800	-0.33491000
C	-4.00482400	0.49527900	0.03525300
H	-4.13898100	1.56283800	0.17212700
C	-5.02904000	-0.35388000	-0.08625900
H	-6.03545700	0.04655800	-0.04322900
H	-4.89706300	-1.41840200	-0.22587500
N	-0.69466000	-0.94662000	-0.04880400
H	-0.07728700	-1.69383400	-0.32939000

27TS
Energy (a.u.)= -1183.836012

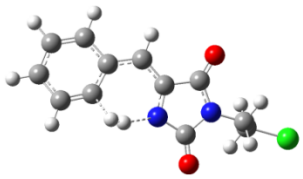


C	3.36135800	0.87965500	0.14170600
C	4.66984900	1.20643000	-0.21238900
C	5.56587800	0.20725900	-0.60449200
C	5.14875700	-1.12727800	-0.62058300
C	3.84439200	-1.45706300	-0.25867500
C	2.91854900	-0.45962700	0.11114100
H	2.70267800	1.66554000	0.49756900
H	4.99401600	2.24210200	-0.17119200
H	6.58322300	0.46520900	-0.88255500
H	5.84140100	-1.91137000	-0.91142000
H	3.52607200	-2.49583200	-0.27011200
C	1.56078700	-0.86902500	0.46295000
H	1.42208700	-1.90265700	0.77057300
C	0.41623200	-0.15594500	0.42300100
C	-0.91017700	-0.70559900	0.82097300
C	-1.17997600	1.46945300	0.04719600
O	-1.18463200	-1.78616700	1.30404300
N	-1.82810500	0.32098200	0.54416600
N	0.16542100	1.16140100	0.01554500
H	0.80640000	1.75186300	-0.49346700
O	-1.70850100	2.51689600	-0.27926900
C	-3.21879400	0.22952600	0.85215300
H	-3.74714100	-0.69146000	0.16307400
H	-3.43841900	-0.03229100	1.88717000
C	-4.14487600	1.00042300	0.13257800
H	-3.88287800	1.51284400	-0.78277000
H	-5.15445400	1.10668900	0.50936300
Cl	-4.88594200	-1.13190600	-1.18857300

28
Energy (a.u.): -1182.734200

C	2.20316800	-0.43127300	-0.02726300
C	2.86820200	-1.65694200	-0.04385300
C	4.25137500	-1.62239400	0.12860800
C	4.94462000	-0.40764700	0.31022200
C	4.27225900	0.81027300	0.32508800
C	2.87713900	0.81337000	0.15515700
H	2.32967800	-2.58694300	-0.18479600
H	4.80774100	-2.55467800	0.12228800
H	6.02220800	-0.42705600	0.44008000
H	4.81253100	1.74171000	0.46509400
C	1.88909400	1.86960300	0.11955500
H	2.06250700	2.93082200	0.22753800
C	0.68172900	1.25967400	-0.07779700
C	-0.75992600	1.51750300	-0.22888700
C	-0.35504400	-0.78961800	-0.36599700
O	-1.38557300	2.56001800	-0.22506700
N	-1.32303500	0.22882000	-0.39432000
N	0.85646300	-0.12092600	-0.16789300
O	-0.53815200	-1.98196500	-0.48827200
C	-2.74027600	-0.02122300	-0.62487000
H	-3.15442200	0.86410800	-1.11191300
H	-2.83141900	-0.87865000	-1.29509700
C	-3.47091000	-0.29450400	0.69088100
H	-3.41138300	0.56291700	1.36236800
H	-3.07957200	-1.18508800	1.18398300
Cl	-5.22768500	-0.59575100	0.36868200

28TS
Energy (a.u.)= -1183.743637

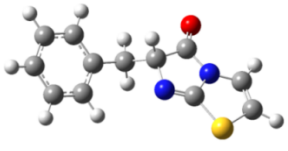


C	-3.19596400	0.77830200	0.09078400
C	-4.39258600	1.42132500	0.23186100
C	-5.43095600	0.58047300	0.66805100
C	-5.25610300	-0.81753700	0.67288000
C	-4.04656200	-1.39095100	0.32613900
C	-2.90512000	-0.58231500	-0.00246600
H	-2.66511100	1.89450800	-1.58225700
H	-4.50328600	2.49911500	0.18612800
H	-6.34697500	1.02702100	1.04448400
H	-6.09599400	-1.45573500	0.92926700
H	-3.94768700	-2.46827800	0.21662900
C	-1.64886300	-1.14170900	-0.35719200
H	-1.55888400	-2.21938500	-0.43952100
C	-0.50071100	-0.37893200	-0.50400800
C	0.87861700	-1.00241700	-0.60241800
C	0.94833900	1.27919500	-0.39153500
O	1.18500000	-2.17531700	-0.72990100
N	1.71978400	0.08675900	-0.51518000
N	-0.41622900	0.95303500	-0.44270100
H	-1.99529100	1.78451400	-1.21733800
O	1.43532900	2.38639500	-0.28317100
C	3.17277900	0.04270900	-0.56714100
H	3.46143600	-0.82067100	-1.17140000
H	3.52184500	0.95753200	-1.05079600
C	3.76498300	-0.07013300	0.83860400
H	3.43916900	-0.98572500	1.33372300
H	3.50714700	0.79797800	1.44611100
Cl	5.57464800	-0.13447800	0.74666900

29
Energy(a.u): -721.920075

C	-1.39993700	-0.37872300	0.00168100
C	-2.13687000	-1.56321200	0.00181500
C	-3.52518700	-1.43796400	-0.00051200
C	-4.15501300	-0.17570700	-0.00257700
C	-3.41186600	1.00020600	-0.00246600
C	-2.00913200	0.91237100	-0.00039100
H	-1.64679100	-2.52982800	0.00346700
H	-4.13629500	-2.33536400	-0.00069500
H	-5.23939300	-0.12489700	-0.00424100
H	-3.90348300	1.96838500	-0.00401400
C	-0.95763900	1.90501800	-0.00004600
H	-1.07217900	2.97958600	-0.00175100
C	0.22189800	1.21344100	0.00275800
C	1.67979100	1.37815000	0.00096100
C	1.14616200	-0.91331000	0.00108400
O	2.36431100	2.38124100	-0.00014700
N	2.18566700	0.04230100	0.00033000
N	-0.02988100	-0.15591900	0.00423200
O	1.23746400	-2.12094400	-0.00000700
C	3.57197200	-0.21642200	-0.00186200
H	4.13420000	0.71115700	-0.00251400
C	4.16047300	-1.41628200	-0.00289200
H	5.24366600	-1.45555900	-0.00435200
H	3.60765000	-2.34592800	-0.00190800

33
Energy (a.u.): -1046.043895



N	-0.55945800	-0.73274600	-0.36249500
C	-0.06494600	0.65939500	-0.32796500
C	-1.29622500	1.56431500	-0.09531400
N	-2.35717400	0.65562700	-0.05978700
C	-1.82512200	-0.63691200	-0.21361900
C	1.02812300	0.89444500	0.73876100
C	2.36426800	0.27466800	0.38784100
C	3.38378500	1.06114100	-0.16785000
C	4.61803900	0.50064100	-0.50843700
C	4.85082700	-0.85996700	-0.29426600
C	3.84235500	-1.65310600	0.26140800
C	2.60979200	-1.09023700	0.59909900
O	-1.37147600	2.76969300	0.03230100
S	-3.14071800	-1.82122000	-0.14337000
H	3.21270500	2.12301900	-0.32992700
H	5.39632700	1.12749300	-0.93462800
H	5.81000900	-1.29817200	-0.55480800
H	4.01497300	-2.71212100	0.43174200
H	1.82522700	-1.71349500	1.01728200
H	0.66154900	0.50164800	1.69416000
H	1.13695900	1.97844900	0.85164800
H	0.34767200	0.90881300	-1.31502000
C	-4.30757300	-0.49601300	0.10577500
H	-5.35726000	-0.72338400	0.22126100
C	-3.73620100	0.72246400	0.12363300
H	-4.21117800	1.68456300	0.25537800

33TS

Energy (a.u.): -1047.040576

N	-0.48516800	-0.74726700	-0.25711900
C	0.00381000	0.65900000	-0.28089200
C	-1.24369400	1.54504400	-0.02604700
N	-2.30972300	0.64665000	-0.09438100
C	-1.74046700	-0.64821000	-0.16861600
C	1.12293900	0.92166700	0.74698600
C	2.44919200	0.29499000	0.37323300
C	3.42364100	1.04908700	-0.29699300
C	4.64614600	0.47907200	-0.66195500
C	4.91300100	-0.85823400	-0.35796200
C	3.95047100	-1.61850300	0.31247500
C	2.72917900	-1.04590400	0.67457300
O	-1.30223200	2.73675300	0.19000100
S	-3.11284400	-1.86432100	-0.07452200
H	3.22732200	2.09356100	-0.52872100
H	5.38985000	1.08076500	-1.17679100
H	5.86381500	-1.30294100	-0.63718900
H	4.15021700	-2.65850900	0.55473300
H	1.98198500	-1.64464100	1.18706400
H	0.78615500	0.55708500	1.72408200
H	1.22692000	2.00896700	0.82621900
H	0.38403500	0.87266600	-1.28823100
C	-4.23817200	-0.58872800	-0.26003000
H	-4.95524000	-0.51491100	-1.08077700
H	-4.49416000	1.38519300	-1.34109800
C	-3.65589400	0.59882900	0.41671300
H	-3.62141800	0.55139300	1.51723600
H	-4.31277300	1.48215000	-0.45260200