Supporting Information

for

Synthesis of novel 5-alkyl/aryl/heteroaryl substituted diethyl 2H-pyrrole-4,4(3H)-dicarboxylates by aziridine ring expansion of 2-[(aziridin-1-yl)-1-alkyl/aryl/heteroaryl-methylene]malonic acid diethyl esters

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General information, experimental procedures, spectral data of compounds 18f–18j, 19b,19c, 19f–19g, 19i, 20a–20j, 21a–21j, 23, 24, 28, 29, 31, 32, spectra of 20a, 20c, 20d, 20f, 20g, and 20h (¹H NMR, ¹³C NMR, IR, MS).
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1. General information

All the required acid chlorides were freshly distilled prior to use. Aziridine was synthesized from ethanolamine and purified by fractional distillation. Laboratory grade (LR grade) solvents and reagents were used in the reactions. Reactions were monitored by TLC, using Merck aluminium-backed plates precoated with silica (0.25 mm, 60, F254). The plates were visualized under UV light and developed using a solution of basic KMnO₄. Chromatographic purification of products was carried out by gravity column chromatography on silica gel (60–120 mesh), purchased from SRL. Infrared spectra were recorded on a Perkin–Elmer 1650 Fourier transform spectrometer. NMR spectra were measured in CDCl₃, (all with TMS as internal standard) on Varian Gemini 200 MHz FT and 400 MHz FT magnetic resonance spectrometers. Chemical shifts (δ) are reported in ppm, and coupling constants (J) in Hz. The following abbreviations were used for multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. MS spectra were recorded on an HP-5989A quadrupole mass spectrometer.

The synthesis of diethyl acyl malonates 18 was carried by the method of Rathke and Cowan [1] and the physical and spectral data were compared with the literature values [1,2]. Compound 18h [3] and 18j [4] have been previously reported, however, since no spectral characterization was given, the spectral data were recorded and results reported below. Compound 18f, 18g, and 18i were novel and were characterized by MS and NMR and IR spectroscopy.

The chlorination of diethyl 2-acylmalonates 18 was carried out by the method of Hormi [5] and the physical and spectral data of 2-(1-alkyl/aryl/heteroaryl-1-chloromethylene)malonates 19 were compared with the literature reports [6-8]. Compounds 19f, 19g, and 19i were novel and were characterized by MS, NMR and IR spectroscopy. Compound 19b and 19c have been previously reported [9], however, since no spectral characterization was given, the spectral data were recorded and results reported below.

The synthesis of N-vinylaziridines 20 was carried out on a maximum of 24 mmol and minimum of 15 mmol scale whereas their rearrangement to pyrroline derivatives 21 was carried out on a maximum of 21 mmol and a minimum of 10 mmol scale. Compound 23 was reported as perchlorate salt [10], but we isolated 23 in the form of a free base. Compound 24, although reported in literature [11], was not completely characterized. We have carried out characterization of 24 by NMR and MS and HRMS and the spectral results of 24 were found to be similar to its methyl ester analogue [12].
The synthesis of ethyl 3-chloro-2-cyano-3-phenylacrylate (27) was carried out by a known procedure via the acylation of ethyl cyanoacetate with benzoyl chloride and subsequent chlorination of ethyl 2-benzoylcynoacetate with phosphorus oxychloride [13]. The synthesis of 2-butylaziridine 30 was carried by the general procedure reported in a patent [14] from (±) norleucinol instead of (S)-(+)leucinol.

2. General procedures

2.1. General procedure for preparation of \(N\)-vinylaziridines 20a–20j
The chloro alkenyl malonate derivative (16.1 mmol) and THF (40.0 mL) were placed in a round bottom flask and cooled to 0–10 °C. Aziridine (48.2 mmol) was added slowly over 15 minutes through a syringe to the above mixture. The reaction mixture was then raised to room temperature and stirred for 8–13 h. After disappearance of the starting chloro compound (TLC), the reaction was quenched with water (80 mL). The reaction mixture was extracted twice with 80 mL dichloromethane. The combined extracts were washed twice with 80 mL 10% sodium chloride solution. The organic layer was dried over \(\text{Na}_2\text{SO}_4\) and concentrated under vacuum to afford the \(N\)-vinylaziridines. The products were sufficiently pure for the subsequent reactions; however, the crude products were purified by chromatography on silica gel (60–120 mesh) using a mixture of hexanes and ethyl acetate (90:10) as eluent, and the spectral data recorded for the column purified products, which were used for the next step (for yields see Table 1).

2.2. General procedure for the ring expansion of \(N\)-vinylaziridines to synthesize pyrrolines 21a–21j
Anhydrous sodium iodide (4.5 g, 30 mmol) was added to a solution of the \(N\)-vinylaziridine derivative (15 mmol) in acetone (40.0 mL) under a nitrogen atmosphere and the reaction mixture stirred for 12–24 h at room temperature. After disappearance of the \(N\)-vinylaziridine (TLC), the reaction mixture was diluted with water (80 mL) and extracted three times with 80 mL DCM. The combined DCM layers were washed twice with 80 mL of 10% sodium chloride solution, dried over \(\text{Na}_2\text{SO}_4\) and concentrated under vacuum to afford the crude pyrroline derivatives which were purified by column chromatography on silica gel (60–120 mesh) with a mixture of hexanes and ethyl acetate (95:5) as eluent to afford the pure pyrrolines 21.
3. Spectral data of novel diethyl acyl malonates

3.1. Diethyl 2-(3-chlorobenzoyl)malonate (18f)
M.F.: C_{14}H_{15}ClO_{5}, Mol. Wt: 298.72
IR (neat, cm\(^{-1}\)): 3651, 3070, 2984, 1754, 1734, 1698, 1571, 1424, 1369, 1301, 1249, 1151, 1095, 1031, 797, 744, 682, 616; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 13.4 and 5.21 (s, 1H), 7.88 (s, 1H), 7.769–7.762 (m, 1H), 7.57–7.55 (m, 1H), 4.29–4.0 (m, 4H), 1.25 and 1.05 (t, \(J = 7.2\) Hz, 6H); \(^13\)C NMR (CDCl\(_3\), 50 MHz) \(\delta\): 187 and 173, 164.39, 136.9, 134.3, 133.3, 130.11, 128.49, 126.48, 125.7 and 61.39, 62.52 and 61.84, 14.06 and 13.88; MS (ESI): \(m/z = 299.1\) [M + H]^+.

3.2. Diethyl 2-(4-fluorobenzoyl)malonate (18g)
M.F.: C_{14}H_{15}FO_{5}, Mol. Wt: 282.26
IR (neat, cm\(^{-1}\)): 3070, 2990, 2876, 1751, 1733, 1691, 1594, 1508, 1478, 1447, 1413, 1371, 1296, 1230, 1185, 1160, 1034, 1006, 907, 852, 817, 635, 580; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 7.96–7.92 (m, 2H), 7.16 (t, \(J = 8.6\) Hz, 2H), 13.4 & 5.22 (s, 1H), 4.28 (q, \(J = 7.0\) Hz, 4H), 1.25 (t, \(J = 7.4\) Hz, 6H); \(^13\)C NMR (CDCl\(_3\), 50 MHz) \(\delta\): 187.3, 168.7, 164.6 & 163.5, 131.7, 131.3 & 131.1, 116.3 & 115.8, 62.48 & 61.88, 61.7 & 61.3, 13.9, MS (ESI): \(m/z = 283.1\) [M + H]^+.

3.3. Diethyl 2-(3-methoxybenzoyl)malonate (18i)
M.F.: C_{15}H_{16}O_{6}, Mol. Wt: 294.30
IR (neat, cm\(^{-1}\)): 3077, 2983, 2839, 1754, 1736, 1693, 1598, 1583, 1487, 1450, 1431, 1369, 1293, 1234, 1178, 1095, 1037, 868, 789, 686; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 13.4 and 5.26 (s, 1H), 7.47–7.0 (m, 4H), 4.27 (q, \(J = 7.0\) Hz, 4H), 3.85 (s, 3H), 1.25 (t, 6H, 7.2 Hz); \(^13\)C NMR (CDCl\(_3\), 100 MHz) \(\delta\): 171.6, 166.6, 159.5, 130.6, 129.4, 122.5, 120.3, 114.4, 61.4, 55.3, 41.6, 13.9 MS (ESI): \(m/z = 295.2\) [M + H]^+.
4. Spectral data of known diethyl 2-acylmalonates for which no spectral characterization was reported before in literature

4.1. Diethyl 2-(4-nitrobenzoyl)malonate (18h)
M.F.: C_{14}H_{15}NO_2, Mol. Wt: 309.27
IR (neat, cm\(^{-1}\)): 3112, 2985, 2874, 1754, 1732, 1701, 1649, 1605, 1588, 1529, 1466, 1370, 1348, 1297, 1252, 1147, 1084, 1036, 855, 767, 687; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 13.4 and 5.5 (s, s, 1H), 8.34 and 8.27 (d, \(J = 8.8\) Hz, and d, \(J = 8.8\) Hz, 2H), 8.08 and 7.75 (d, \(J = 7.2\) Hz, and d, \(J = 8.8\) Hz, 2H), 4.39–4.07 (m, 4H), 1.08–1.38 (m, 6H);
\(^{13}\)C NMR (CDCl\(_3\), 50 MHz) \(\delta\): 187.6 and 164.1, 172.2 and 170.5, 166.5 and 165.2, 150.6 and 149.0, 139.8 and 139.8, 129.5 and 128.7, 124.0 and 123.4, 101.9 and 41.6, 62.7 and 62.1, 61.5 and 61.4, 14.0 and 13.9; MS (ESI): \(m/z = 310.1\) [M + H]\(^+\).

4.2. Diethyl 2-(thiophene-2-carbonyl)malonate (18j)
M.F.: C\(_{12}\)H\(_{14}\)O\(_5\)S, Mol. Wt: 270.30
IR (neat, cm\(^{-1}\)): 3460, 3106, 2985, 1735, 1670, 1519, 1446, 1413, 1305, 1245, 1179, 1035, 854, 736, 616; \(^1\)HNMR (CDCl\(_3\), 400 MHz) \(\delta\): 13.26 and 5.14 (s, s, 1H), 7.69–7.73 (m, 2H), 7.14 (dd, \(J = 3.8\) Hz, \(J = 5.0\) Hz, 1H), 4.18–4.32 (m, 4H), 1.24–1.32 (m, 6H); \(^{13}\)C NMR (CDCl\(_3\), 50 MHz) \(\delta\): 181.1, 164.2, 142.2, 135.3, 133.1, 128.3, 62.46 and 62.40, 13.8; MS (ESI): \(m/z = 271.1\) [M + H]\(^+\).

5. Spectral data of novel diethyl 2-chloromethylene malonates

5.1. Diethyl 2-(chloro(3-chlorophenyl)methylene)malonate (19f)
M.F.: C\(_{14}\)H\(_{14}\)Cl\(_2\)O\(_4\), Mol Wt: 316.03
IR (neat): 3454; 3067, 2983, 1732, 1621, 1567, 1472, 1446, 1390, 1367, 1249, 1208, 1079, 1019, 935, 864, 788, 717, 690; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 7.42–7.29 (m, 4H ArH), 4.35 (q, \(J = 7.2\) Hz, 2H), 4.09 (q, \(J = 6.9\) Hz, 2H), 1.36 (t, \(J = 7.6\), 3H), 1.07 (t, \(J = 8.0\) Hz, 3H); \(^{13}\)C NMR (50 MHz, CDCl\(_3\)) \(\delta\): 163.0, 162.3, 145.3, 138.3, 134.1, 130.2, 129.4, 128.1, 127.8, 126.2, 62.1, 14.0; MS (ESI): \(m/z = 339.0\) [M + Na]\(^+\).
5.2. Diethyl 2-(chloro(4-fluorophenyl)methylene)malonate (19g)
M.F.: C_{14}H_{14}ClFO_4, Mol. Wt: 300.71.
IR (neat): 3452; 3109, 2985, 1732, 1601, 1507, 1368, 1301, 1253, 1227, 1160, 1079, 1015, 908, 841. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta:\) 7.45–7.40 (m, 2H), 7.10–7.05 (m, 2H), 4.35 (q, \(J = 7.0\) Hz, 2H), 4.06 (q, \(J = 7.3\) Hz, 2H), 1.36 (t, \(J = 7.0\) Hz, 3H), 1.08 (t, \(J = 7.2\) Hz, 3H); \(^{13}\)C NMR (50 MHz, CDCl\(_3\)) \(\delta\): 166.1, 163.1, 162.5 & 161.1, 146.1, 132.8 & 130.4, 127.2, 115.5, & 115.11, 61.9 & 61.7, 13.9 & 13.6; MS (ESI): \(m/z = 301.0\) [M + H].

5.3. Diethyl 2-(chloro(3-methoxyphenyl)methylene)malonate (19i)
M.F.: C_{15}H_{17}ClO_5, Mol. Wt: 312.75
IR (neat): 3453, 3071, 2983, 1732, 1597, 1485, 1465, 1390, 1368, 1290, 1228, 1174, 1164, 1078, 1039, 1023, 949, 921, 865, 788, 761, 695; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 7.30–7.27(d, \(J = 3.2\) Hz, 1H), 7.01–6.93 (m, 2H), 4.35 (q, \(J = 7.3\) Hz, 2H), 4.07 (q, \(J = 7.2\) Hz, 2H), 3.8 (s, 3H), 1.36 (t, \(J = 7.0\) Hz, 3H), 1.05 (t, \(J = 6.8\) Hz, 3H); \(^{13}\)C NMR (50 MHz, CDCl\(_3\)) \(\delta\): 163.2, 162.8, 159.2, 146.9, 138.0, 129.2, 127.1, 120.3, 116.2, 113.3, 61.9, 61.7, 55.3, 14.0, 13.6; MS (ESI): \(m/z = 335.1\) [M + Na].

6. Spectral data of known 2-chloromethylenemalonic acid diethyl ester derivatives for which no spectral characterization was reported in literature

6.1. Diethyl 2-(1-chloropropylidene)malonate (19b)
M.F.: C_{10}H_{15}ClO_4, Mol. Wt: 234.68
IR (neat): 2982, 2940, 1727, 1626, 1461, 1389, 1367, 1286, 1258, 1230, 1044, 1062, 905, 866, 755, 667; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 4.32 (q, \(J = 6.8\) Hz, 2H), 4.24 (q, \(J = 6.4\) Hz, 2H), 2.92 (q, \(J = 7.2\) Hz, 2H), 1.33 (t, \(J = 7.4\) Hz, 3H) 1.29 (t, \(J = 7.2\) Hz, 3H), 1.23 (t, \(J = 7.4\) Hz, 3H); \(^{13}\)C NMR (50 MHz, CDCl\(_3\)) \(\delta\): 164.1, 162.0, 155.7, 125.8, 61.6 and 61.5, 30.4, 13.9, 12.0; MS (ESI): \(m/z = 235.1\) [M + H].

6.2. Diethyl 2-(1-chlorobutylidene)malonate (19c)
M.F.: C_{11}H_{17}ClO_4, Mol. Wt: 248.70
IR (neat): 3441, 2967, 2875, 1735, 1625, 1465, 1388, 1367, 1274, 1245, 1223, 1141, 1086, 1055, 1022, 921, 865, 759, 665; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 4.30 (q, \(J = 7.0\) Hz,
Spectral data of 2-(aziridin-1-yl-1-alkyl/aryl/heteroaryl methylene)malonates (20a–20j)

7.1. 2-(1-Aziridin-1-yl-ethylidene)malonic acid diethyl ester (20a)
M.F.: C₁₁H₁₇NO₄, Mol. Wt: 227.26
IR (neat): 2981, 1704, 1591, 1446, 1381, 1225, 1182, 1142, 1061, 973, 868, 773; ¹H NMR (CDCl₃, 400 MHz) δ: 4.27 (q, J = 7.2 Hz, 2H), 4.19 (q, J = 7.06 Hz, 2H), 2.24 (s, 3H), 2.17 (s, 4H), 1.26 (t, J = 7.2 Hz, 3H), 1.22 (t, J = 7.2 Hz, 3H); ¹³C NMR (CDCl₃, 50 MHz) δ: 165.9, 165.3, 109.9, 60.6, 60.3, 28.8, 20.0, 14.1; MS (ESI): m/z = 228.1 [M + H]⁺.

7.2. 2-(1-Aziridin-1-yl-propylidene)malonic acid diethyl ester (20b)
M.F.: C₁₂H₁₉NO₄, Mol. Wt: 241.28
IR (neat, cm⁻¹): 3405, 2981, 2939, 1707, 1587, 1464, 1383, 1367, 1260, 1221, 1179, 1142, 1095, 1065, 1034, 941, 814, 676; ¹H NMR (CDCl₃, 400 MHz) δ: 4.26 (q, J = 7.2 Hz, 2H), 4.20 (q, J = 7.0 Hz, 2H), 2.56 (dd, J = 6.0, 7.8 Hz, 2H), 2.18 (s, 4H), 1.2–1.4 (m, 9H); ¹³C NMR (CDCl₃, 50 MHz) δ: 169.7, 165.9, 109.9, 60.6, 60.4, 28.3, 26.8, 14.2, 14.1, 12.9; MS (ESI): m/z = 242.2 [M + H]⁺.

7.3. 2-(1-Aziridin-1-yl-butylidene)malonic acid diethyl ester (20c)
M.F.: C₁₃H₂₁NO₄, Mol. Wt: 255.31
IR (neat, cm⁻¹): 3070, 2978, 2874, 1705, 1586, 1464, 1378, 1241, 1218, 1178, 1141, 1096, 1063, 1039, 985, 868, 811, 756, 667; ¹H NMR (CDCl₃, 400 MHz) δ: 4.28 (q, J = 7.0 Hz, 2H), 4.20 (q, J = 7.0 Hz, 2H), 2.58–2.54 (m, 2H), 2.18 (s, 4H), 1.69–1.65 (m, 2H), 1.30 (t, J = 7.6 Hz, 3H), 1.27 (t, J = 7.2 Hz, 3H), 0.989 (t, J = 7.4 Hz, 3H); ¹³C NMR (CDCl₃, 50 MHz) δ: 168.4, 166.0, 165.8, 109.6, 60.5, 60.4, 35.2, 28.5, 21.9, 14.17, 14.11, 14.0; MS (ESI): m/z = 256.2 [M + H]⁺, 278.2 [M + Na]⁺.
7.4. 2-(1-Aziridin-1-yl-2,2-dimethylpropylidene)malonic acid diethyl ester (20d)
M.F.: C_{14}H_{23}NO_4, Mol. Wt: 269.34
IR (neat, cm^{-1}): 3069, 2979, 2874, 1712, 1557, 1471, 1399, 1365, 1260, 1224, 1198, 1145, 1095, 1059, 957, 869, 818, 772, 692; ^1H NMR (CDCl_3, 400 MHz) δ: 4.21 (q, J = 7.0 Hz, 4H), 2.18 (s, 4H), 1.34 (s, 9H), 1.27 (t, J = 7.2 Hz, 6H); ^13C NMR (CDCl_3, 50 MHz) δ: 173.8, 166.6, 111.1, 60.6, 38.5, 30.6, 29.7, 13.9; MS (ESI): m/z = 270 [M + H]^+, 292.2 [M + Na]^+.

7.5. 2-(Aziridin-1-yl-phenylmethylene)malonic acid diethyl ester (20e)
M.F.: C_{16}H_{19}NO_4, Mol. Wt: 289.34
IR (neat, cm^{-1}): 3061, 2981, 2902, 1708, 1570, 1489, 1469, 1444, 1369, 1280, 1240, 1205, 1143, 1089, 1053, 939, 920, 860, 759, 700, 624; ^1H NMR (CDCl_3, 400 MHz) δ: 7.41–7.32 (m, 5H), 4.32–4.26 (m, 2H), 3.95–3.90 (m, 2H), 2.21 (s, 4H), 1.33 (t, J = 7.2 Hz, 3H), 0.94 (t, J = 7.2 Hz, 3H); ^13C NMR (CDCl_3, 100 MHz) δ: 165.9, 165.7, 164.13, 137.3, 128.8, 127.9, 127.2, 110.7, 60.6 and 60.58, 31.1, 14.1, 13.5; MS (ESI): m/z = 290.2 [M + H]^+, 312.2 [M + Na]^+.

7.6. 2-[Aziridin-1-yl-(3-chlorophenyl)methylene]malonic acid diethyl ester (20f)
M.F.: C_{16}H_{18}ClNO_4, Mol. Wt: 323.77
IR (neat, cm^{-1}): 3423, 3067, 2981, 2915, 1715, 1602, 1581, 1473, 1413, 1370, 1284, 1240, 1207, 1145, 1091, 1055, 891, 864, 804, 784; ^1H NMR (CDCl_3, 400 MHz) δ: 7.36–7.21 (m, 4H, ArH), 4.29 (q, J = 7.2 Hz, 2H), 3.98 (q, J = 7.0 Hz, 2H), 2.21 (s, 4H), 1.33 (t, J = 3.8 Hz, 3H), 1.01 (t, J = 7.0 Hz, 3H); ^13C NMR (CDCl_3, 50 MHz) δ: 165.5, 164.1, 163.5, 138.9, 134.0, 129.4, 129.0, 127.5, 126.5, 116.1, 111.3, 60.8, 31.0, 30.1, 14.2, 13.68; MS (ESI): m/z = 346.1 [M + Na]^+.

7.7. 2-[Aziridin-1-yl-(4-fluorophenyl)methylene]malonic acid diethyl ester (20g)
M.F.: C_{16}H_{18}FNO_4, Mol. Wt: 307.32
IR (neat, cm^{-1}): 3073, 2938, 2874, 1715, 1605, 1579, 1507, 1474, 1370, 1277, 1207, 1145, 1089, 1054, 934, 864, 841, 789; ^1H NMR (CDCl_3, 400 MHz) δ: 7.36–7.32 (m, 2H), 7.06–7.03 (m, 2H), 4.30 (q, J = 7.2 Hz, 2H), 3.97 (q, J = 7.0 Hz, 2H), 2.20 (s, 4H), 1.33 (t, J = 7.4 Hz, 3H), 1.01 (t, J = 7.2 Hz, 3H); ^13C NMR (CDCl_3, 50 MHz) δ: 165.8, 165.4 & 164.3, 160.4, 133.3, 129.5 & 129.4, 115.4 & 114.9, 111.1, 60.8, 31.1, 14.2, 13.7; MS (ESI): m/z = 308.2 [M + H]^+.
7.8. 2-[Aziridin-1-yl-(4-nitrophenyl)methylene]malonic acid diethyl ester (20h)
M.F.: C_{16}H_{18}N_{2}O_{6}, Mol. Wt: 334.32
IR (neat, cm\(^{-1}\)): 3077, 2983, 2873, 1714, 1604, 1581, 1523, 1347, 1279, 1241, 1208, 1145, 1090, 1055, 857, 745, 700; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 8.26 (dt, \(J = 2.0\) Hz, \(J = 8.8\) Hz, 2H), 7.52 (dt, \(J = 2.0\) Hz, \(J = 8.8\) Hz, 2H), 4.34 (q, \(J = 7.0\) Hz, 2H), 3.99 (q, \(J = 7.0\) Hz, 2H), 2.20 (s, 3H), 1.36 (t, \(J = 7.0\) Hz, 3H), 1.03 (t, \(J = 7.0\) Hz, 3H); \(^{13}\)C NMR (CDCl\(_3\), 50 MHz) \(\delta\): 164.8, 164.4, 162.4, 147.9, 143.5, 128.7, 123.4, 111.8, 61.2, 61.0, 30.6, 29.7, 14.2, 13.8; MS (ESI): \(m/z = 335.1\) [M + 1], 357.1 [M + Na]*.

7.9. 2-[Aziridin-1-yl-(3-methoxyphenyl)methylene]malonic acid diethyl ester (20i)
M.F.: C_{17}H_{21}NO_{5}, Mol. Wt: 319.35
IR (neat, cm\(^{-1}\)): 3072, 2981, 2938, 2837, 1714, 1574, 1465, 1370, 1290, 1177, 1143, 1093, 1053, 869, 787, 692; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 7.28–7.24 (m, 1H), 6.92–6.89 (m, 3H), 4.30 (q, \(J = 7.2\) Hz, 2H), 3.96 (q, \(J = 7.2\) Hz, 2H), 3.79 (s, 3H), 2.22 (s, 3H), 1.33 (t, \(J = 7.2\) Hz, 3H), 0.98 (t, \(J = 7.4\) Hz, 3H); \(^{13}\)C NMR (CDCl\(_3\), 100 MHz) \(\delta\): 166.0, 165.4, 164.0, 159.2, 138.6, 129.1, 119.6, 114.88, 112.5, 110.8, 60.7, 60.6, 60.1, 55.2, 31.3, 14.1, 13.6; MS (ESI): \(m/z = 320.2\) [M + H]*.

7.10. 2-[(Aziridin-1-yl)-(thiophen-2-yl)methylene]malonic acid diethyl ester (20j)
M.F.: C_{14}H_{17}NO_{4}S, Mol. Wt: 295.35
IR (neat, cm\(^{-1}\)): 3637, 3103, 2981, 2610, 1710, 1574, 1370, 1278, 1221, 1144, 1052, 859, 713; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 7.42 (dd, \(J = 1.2\), \(J = 5.2\) Hz, 1H), 7.20 (dd, \(J = 1.0\), \(J = 3.6\) Hz, 1H), 6.98 (dd, \(J = 3.6\), 5.2 Hz, 1H), 4.28 (q, \(J = 7.2\) Hz 2H), 4.07 (q, \(J = 7.0\) Hz, 2H), 2.29 (s, 4H), 1.31 (t, \(J = 7.0\) Hz, 3H), 1.10 (t, \(J = 7.0\) Hz, 3H); \(^{13}\)C NMR (CDCl\(_3\), 50 MHz) \(\delta\): 166.3, 163.4, 158.3, 137.8, 128.3, 127.9, 126.4, 111.3, 61.1, 60.6, 32.4, 14.1, 13.7; MS (ESI): \(m/z = 296.1\) [M + H]*, 318.1 [M + Na]*.
8. Spectral data of diethyl 5-alkyl/aryl/heteroaryl substituted 3,4-dihydro-2H-pyrrole-4,4-dicarboxylates (21a–21j)

8.1. Diethyl 3,4-dihydro-5-methyl-2H-pyrrole-4,4-dicarboxylate (21a)
M.F.: C_{11}H_{17}NO_{4}, Mol. Wt: 227.26
IR (neat): 2982, 2936, 2874, 1731, 1651, 1595, 1446, 1367, 1263, 1178, 1093, 1060, 1023, 973, 927, 861, 796; ¹H NMR (CDCl₃, 400 MHz) δ: 4.25 (q, J = 7.0 Hz, 4H), 3.87–3.83 (m, 2H), 2.56 (t, J = 6.8 Hz, 2H), 2.20 (s, 3H); ¹³C NMR (CDCl₃, 50 MHz) δ: 168.4, 168.0, 71.3, 61.9, 58.8, 33.7, 18.0, 13.9; MS (ESI): m/z = 228 [M + H]⁺, 246 [M + Na]⁺; HRMS calculated for [C_{11}H_{17}NO_{4} + H]⁺: 228.36, found 228.1231.

8.2. Diethyl 3,4-dihydro-5-ethyl-2H-pyrrole-4,4-dicarboxylate (21b)
M.F.: C_{12}H_{19}NO_{4}, Mol. Wt: 241.28
IR (neat, cm⁻¹): 3407, 2981, 2940, 1731, 1646, 1678, 1463, 1447, 1367, 1267, 1179, 1098, 991, 861, 666; ¹H NMR (CDCl₃, 400 MHz) δ: 4.22 (q, J = 7.2 Hz, 4H), 3.88 (t, J = 2.2 Hz, 2H), 2.57–2.48 (m, 4H), 1.28 (t, J = 6.8 Hz, 6H), 1.20 (t, J = 7.2 Hz, 3H); ¹³C NMR (CDCl₃, 50 MHz) δ: 172.3, 168.6, 71.4, 61.9, 58.8, 33.9, 24.7, 13.9, 10.7; MS (ESI): m/z = 242 [M + H]⁺; HRMS calculated for [C_{12}H_{19}NO_{4} + H]⁺: 242.1392, found 242.1388.

8.3. Diethyl 3,4-dihydro-5-propyl-2H-pyrrole-4,4-dicarboxylate (21c)
M.F.: C_{13}H_{21}NO_{4}, Mol. Wt: 255.31
IR (neat, cm⁻¹): 3393, 3303, 3079, 2966, 2875, 1731, 1648, 1545, 1445, 1370, 1218, 1179, 1157, 1096, 1026, 861, 756, 666; ¹H NMR (CDCl₃, 400 MHz) δ: 4.24 (q, J = 7.2 Hz, 4H), 3.91–3.86 (m, 2H), 2.54 (t, J = 7.2 Hz, 2H), 2.48–2.43 (m, 2H), 1.71 (q, J = 7.4 Hz, 2H), 1.29 (t, J = 7.2 Hz, 6H), 0.96 (t, J = 7.4 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ: 171.1, 168.6, 71.5, 61.7, 58.9, 35.1, 33.6, 33.3, 28.4, 19.6, 13.9, 13.8, 13.7, MS (ESI): m/z = 256 [M + H]⁺; HRMS calculated for [C_{13}H_{21}NO_{4} + H]⁺: 256.1549, found 256.1551.

8.4. Diethyl 3,4-dihydro-5-tert-butyl-2H-pyrrole-4,4-dicarboxylate (21d)
M.F.: C_{14}H_{23}NO_{4}, Mol. Wt: 269.34
IR (neat, cm⁻¹): 3445.84, 2981.42, 2871.32, 1731.88, 1622.02, 1481.34, 1463.83, 1393.26, 1365.44, 1304.88, 1260.48, 1177.68, 1084.71, 1025.92, 999.27, 963.15, 864.89 and 772.29; ¹H NMR (CDCl₃, 400 MHz) δ: 4.24 (q, J = 7.2 Hz, 4H), 3.85 (t, J = 6.6 Hz, 2H), 2.50 (t, J = 6.8 Hz, 2H), 2.22 (s, 3H); MS (ESI): m/z = 268 [M + H]⁺; HRMS calculated for [C_{14}H_{23}NO_{4} + H]⁺: 268.1705, found 268.1700.

8.5. Spectral data of diethyl 5-alkyl/aryl/heteroaryl substituted 3,4-dihydro-2H-pyrrole-4,4-dicarboxylates (21j)
8.5. Diethyl 3,4-dihydro-5-phenyl-2H-pyrrole-4,4-dicarboxylate (21e)
M.F.: C_{16}H_{19}NO_{4}, Mol. Wt: 289.33
IR (neat, cm\(^{-1}\)): 3419, 2981, 1732, 1464, 1451, 1473, 1369, 1265, 1178, 1024, 858, 806, 752, 682; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 7.87–7.85 (m, 2H), 7.39–7.32 (m, 3H), 4.23–4.15 (m, 4H), 4.10 (t, \(J = 6.8\) Hz, 2H), 2.77 (t, \(J = 6.8\) Hz, 2H), 1.16 (t, \(J = 7.0\) Hz, 6H); \(^{13}\)C NMR (CDCl\(_3\), 50 MHz) \(\delta\): 169.0, 167.9, 133.1, 130.1, 128.6, 127.8, 70.0, 62.0, 59.1, 37.0, 13.7; MS (ESI): \(m/z = 290\) [M + H]\(^{+}\); HRMS calculated for [C\(_{16}\)H\(_{19}\)NO\(_4\) + H]\(^{+}\): 290.1392, found 290.1396.

8.6. Diethyl 5-(3-chlorophenyl)-3,4-dihydro-2H-pyrrole-4,4-dicarboxylate (21f)
Mol. Wt: C\(_{16}\)H\(_{18}\)ClNO\(_4\), Mol. Wt: 323.77
IR (neat, cm\(^{-1}\)): 3325, 3066, 2983, 2869, 1732, 1602, 1591, 1510, 1446, 1390, 1367, 1365, 1261, 1179, 1085, 1014, 864, 813, 758, 590; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 7.90 (m, 2H), 7.07–7.01 (m, 2H), 4.24–4.17 (m, 4H), 4.09 (t, \(J = 6.8\) Hz, 2H), 2.77 (t, \(J = 6.8\) Hz, 2H), 1.18 (t, \(J = 7.2\) Hz, 6H); \(^{13}\)C NMR (CDCl\(_3\), 50 MHz) \(\delta\): 168.7, 166.8, 146.3, 134.9, 133.9, 130.1, 129.0, 128.8, 126.8, 166.1, 70.1, 62.2, 59.1, 36.9, 30.1, 21.4, 13.8; MS (ESI): \(m/z = 324/326\) [M + H]\(^{+}\); HRMS calculated for [C\(_{16}\)H\(_{18}\)ClNO\(_4\) + H]\(^{+}\): 324.1003, found 324.0992.

8.7. Diethyl 3,4-dihydro-5-(4-fluorophenyl)-2H-pyrrole-4,4-dicarboxylate (21g)
M.F.: C\(_{16}\)H\(_{18}\)FNO\(_4\), Mol. Wt: 307.32
IR (neat, cm\(^{-1}\)): 3450, 3073, 2983, 2869, 1732, 1602, 1590, 1510, 1446, 1390, 1367, 1261, 1179, 1085, 1014, 846, 813, 758, 590; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\): 7.90 (m, 2H), 7.07–7.01 (m, Hz, 2H), 4.24–4.17 (m, 4H), 4.09 (t, \(J = 6.8\) Hz, 2H), 2.77 (t, \(J = 6.8\) Hz, 2H), 1.18 (t, \(J = 7.2\) Hz, 6H); \(^{13}\)C NMR (CDCl\(_3\), 100 MHz) \(\delta\): 169.3, 167.1 & 166.3, 162.1, 130.3 & 130.2, 129.2 & 129.1, 115.6 & 115.2, 61.7, 50.0, 38.0, 28.0, 13.9; MS (ESI): \(m/z = 308\) [M + H]\(^{+}\); HRMS calculated for [C\(_{15}\)H\(_{18}\)FNO\(_4\) + H]\(^{+}\): 308.1298, found 308.1305.
8.8. Diethyl 3,4-dihydro-5-(4-nitrophenyl)-2H-pyrrole-4,4-dicarboxylate (21h)
M.F.: C₁₆H₁₈N₂O₆, Mol. Wt: 334.32
IR (neat, cm⁻¹): 3437, 3075, 2983, 2866, 1753, 1597, 1517, 1342, 1318, 1262, 1176, 1081, 1024, 854, 742, 690; ¹H NMR (CDCl₃, 400 MHz) δ: 8.22 (d, J = 8.8 Hz, 2H), 8.07 (d, J = 8.8 Hz, 2H), 4.25–4.21 (m, 6H), 2.80 (t, J = 6.8 Hz, 2H), 1.20 (t, J = 7.0 Hz, 6H); ¹³C NMR (CDCl₃, 50 MHz) δ: 168.6, 166.3, 148.62, 139.1, 129.7, 123.0, 70.2, 62.4, 59.6, 36.8, 13.9; MS (ESI): m/z = 335 [M + H]⁺; HRMS calculated for [C₁₆H₁₈N₂O₆ + H]⁺ 335.1243, found 335.1251.

8.9. Diethyl 3,4-dihydro-5-(3-methoxyphenyl)-2H-pyrrole-4,4-dicarboxylate (21i)
M.F.: C₁₇H₂₁NO₅, Mol. Wt: 319.35
IR (neat, cm⁻¹): 3448, 3076, 2981, 2939, 2837, 1729, 1600, 1579, 1488, 1464, 1366, 1320, 1262, 1178, 1085, 1020, 863, 789, 693; ¹H NMR (CDCl₃, 400 MHz) δ: 7.48 (s, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.25 (d, J = 8.4 Hz, 1H), 6.96 (dd, J = 2.2 Hz, J = 8.0 Hz, 1H), 4.29–4.23 (m, 4H), 4.10 (t, J = 6.8 Hz, 2H), 3.82 (s, 3H), 2.77 (t, J = 6.4 Hz, 2H), 1.18 (t, J = 7.2 Hz, 6H); ¹³C NMR (CDCl₃, 100 MHz) δ: 169.3, 167.2, 159.6, 135.6, 129.4, 118.5, 117.7, 112.0, 61.6, 55.3, 50.0, 38.0, 28.1, 13.9; MS (ESI): m/z = 320 [M + H]⁺; HRMS calculated for [C₁₇H₂₁NO₅ + H]⁺ 320.1498, found 320.1491.

8.10. Diethyl 3,4-dihydro-5-(thiophen-2-yl)-2H-pyrrole-4,4-dicarboxylate (21j)
M.F.: C₁₄H₁₇NO₄S, Mol. Wt: 295.35
IR (neat, cm⁻¹): 3453, 3105, 2982, 1731, 1601, 1429, 1316, 1262, 1180, 1085, 1005, 848, 754; ¹H NMR (400 MHz, CDCl₃) δ: 7.45 (dd, J = 1.0 Hz, J = 4.2 Hz, 1H), 7.38 (dd, J = 1.0 Hz, J = 3.8 Hz 1H), 7.01 (dd, J = 3.6 Hz, 5.2 Hz, 1H), 4.28–4.16 (m, 4H), 4.19 (t, J = 3.4 Hz, 2H), 2.77 (t, J = 6.4 Hz, 2H), 1.21 (t, J = 7.0 Hz, 6H); ¹³C NMR (50 MHz, CDCl₃) δ: 168.6, 162.2, 137.4, 130.2, 129.1, 127.2, 70.4, 62.1, 59.2, 36.5, 13.8; MS (ESI): m/z = 296 [M + H]⁺; HRMS calculated for [C₁₄H₁₇NO₄S + H]⁺ 296.0957, found 296.0963.
9. Spectral data of 23, 24, 28, 29, 31 and 32

9.1. 5-phenyl-3,4-dihydro-2H-pyrrole (23)
M.F.: C\textsubscript{10}H\textsubscript{11}N, Mol. Wt: 145.09
IR (neat, cm\textsuperscript{-1}): 3390, 3057, 2960, 2860, 1616, 1573, 1494, 1446, 1340, 1311, 1178, 1076, 1047, 1026, 988, 966, 921; \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 400 MHz) \( \delta \): 7.85–7.82 (m, 2H), 7.42–7.36 (m, 3H), 4.07–4.03 (m, 2H), 2.96–2.91 (m, 2H), 2.06–1.98 (m, 2H); \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 100 MHz) \( \delta \): 173.1, 134.5, 130.1, 128.2, 127.4, 61.3, 34.8, 22.5; MS (ESI): \( m/z = 146.1 \) [M + H]\textsuperscript{+}; HRMS calculated for [C\textsubscript{10}H\textsubscript{11}N + H]\textsuperscript{+}: 146.0970, found 146.0972.

9.2. Ethyl 5-phenyl-3,4-dihydro-2H-pyrrole-4-carboxylate (24)
M.F.: C\textsubscript{13}H\textsubscript{15}NO\textsubscript{2}, Mol. Wt: 217.26
IR (CHCl\textsubscript{3}, cm\textsuperscript{-1}): 2980, 1730, 1617, 1446, 1368, 1327, 1254, 1219, 1157, 1044; \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 400 MHz) \( \delta \): 7.87–7.85 (dd, \( J =1.8 \) Hz, \( J = 2H \)), 7.42–7.38 (m, 3H), 4.20–4.06 (m, 5H), 2.38–2.32 (m, 2H), 1.14 (t, \( J = 7.0 \)); \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 100 MHz) \( \delta \): 171.9, 169.1, 133.1, 130.3, 128.2, 127.6, 60.85, 60.81, 53.3, 29.47, 29.42, 29.1, 29.05, 13.8, 13.7; MS (ESI): \( m/z = 218.2 \) [M + H]\textsuperscript{+}; HRMS calculated for [C\textsubscript{13}H\textsubscript{15}NO\textsubscript{2} + H]\textsuperscript{+}: 218.1181, found 218.1180.

9.3. Ethyl 3-(aziridin-1-yl)-2-cyano-3-phenylacrylate (28)
M.F.: C\textsubscript{14}H\textsubscript{14}N\textsubscript{2}O\textsubscript{2}, Mol. Wt: 242.27
IR (neat, cm\textsuperscript{-1}): 3019, 2401, 2215, 1712, 1581, 1538, 1488, 1473, 1403, 1283, 1249, 1216, 1174, 1135, 1108, 1062, 1038, 1018, 850; \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 400 MHz) \( \delta \): 7.56–7.2 (m, 5H), 4.29 and 4.09 (q, \( J = 7.0 \) Hz and q, \( J = 7.2 \) Hz, 2H), 2.48 and 2.44 (s, s, 4H), 1.37 and 1.17 (t, \( J = 7.0 \) Hz and t, \( J = 7.2 \) Hz, 3H); \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 100 MHz) \( \delta \): 176.8 and 176.0, 162.68, 136.1 and 135.8, 130.67 and 130.0, 128.6 and 128.1, 127.4 and 127.1, 117.88 and 117.24, 87.8, 87.6, 61.0 and 60.9, 32.7 and 30.0, 14.2 and 13.9; MS (ESI): \( m/z = 243.1 \) [M + H]\textsuperscript{+}.

9.4. Ethyl 4-cyano-5-phenyl-3,4-dihydro-2H-pyrrole-4-carboxylate (29)
M.F.: C\textsubscript{14}H\textsubscript{14}N\textsubscript{2}O\textsubscript{2}, Mol. Wt: 242.27
IR (neat, cm\textsuperscript{-1}): 3019, 2401, 2215, 1712, 1581, 1538, 1488, 1473, 1403, 1283, 1249, 1216, 1174, 1135, 1108, 1062, 1038, 1018, 850; \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 400 MHz) \( \delta \): 7.93 (d, \( J = 7.6 \) Hz, 2H), 7.52–7.42 (m, 3H), 4.35–4.22 (m, 4H), 2.82–2.78 (m, 2H), 1.25–1.21
(m, 3H); $^{13}$C NMR (CDCl$_3$, 100 MHz) δ: 166.6, 163.4, 131.3, 129.0, 128.6, 127.8, 116.9, 63.4, 60.4, 56.3, 37.9, 13.6; MS (ESI): $m/z = 243.2$ [M + H]$^+$; HRMS calculated for [C$_{14}$H$_{14}$N$_2$O$_2$ + H]$^+$: 243.1134, found 243.1133.

9.5. 2-Butylaziridine (30)
IR (neat, cm$^{-1}$): 2922, 2851, 1595, 1464, 1219, 772; $^1$H NMR (CDCl$_3$, 400 MHz) δ: 1.94–1.91 (m, 1H), 1.75 (d, J = 5.6 Hz), 1.48–1.32 (m, 7H), 0.91 (t, J = 7.0 Hz, 3H); $^{13}$C NMR (CDCl$_3$, 100 MHz) δ: 34.0, 30.3, 29.6, 25.0, 22.4, 13.9; MS (ESI): $m/z = 100.1$ [M + H]$^+$, 199.1 [2M + H]$^+$.

9.6. Diethyl 2-[(2-buty laziridin-1-yl)phenylmethylen]malonate (31)
M.F.: C$_{20}$H$_{27}$NO$_4$, Mol. Wt: 345.43
IR (neat, cm$^{-1}$): 3020, 2961, 2933, 2400, 1709, 1605, 1584, 1570, 1491, 1445, 1412, 1369, 1337, 1276, 1215, 1155, 1080, 1026, 928, 851; $^1$H NMR (CDCl$_3$, 400 MHz) δ: 7.36–7.29 (m, 5H), 4.33–4.24 (m, 2H), 3.88–3.94 (m, 2H), 2.28–2.27 (d, J = 3.2 Hz, 1H), 2.20–2.15 (m, 2H), 1.62–1.57 (m, 2H), 1.33 (t, J = 7.2 Hz, 3H), 1.19–1.08 (m, 4H), 0.93 (t, J = 7.0 Hz, 3H), 0.79 (t, J = 3.2 Hz, 3H); $^{13}$C NMR (CDCl$_3$, 100 MHz) δ: 166.0, 164.5, 137.5, 128.7, 127.9, 127.5, 110.2, 60.6 and 60.5, 41.6, 37.8, 32.0, 28.3, 22.2, 14.2, 13.8, 13.6; MS (ESI): $m/z = 346.2$ [M + H]$^+$.

9.7. Diethyl 2-butyl-3,4-dihydro-5-phenyl-2H-pyrrole-4,4-dicarboxylate (32)
M.F.: C$_{20}$H$_{27}$NO$_4$, Mol. Wt: 345.43
IR (CHCl$_3$, cm$^{-1}$): 2932, 1730, 1606.3, 1446, 1367, 1258, 1219, 1184, 1126, 1096, 1061; $^1$H NMR (CDCl$_3$, 400 MHz) δ: 7.87–7.84 (m, 2H), 7.39–7.31 (m, 3H), 4.24–4.13 (m, 5H), 2.96–2.91 (dd, J = 6.8 Hz, J = 13.6 Hz, 1H); 2.32–2.26 (dd, J = 7.8 Hz, J = 13.0 Hz, 1H), 1.89–1.84 (m, 1H), 1.56–1.37 (m, 5H), 1.19 (t, J = 7.2 Hz, 3H), 1.13 (t, J = 7.2 Hz, 3H), 0.94 (t, J = 7.2 Hz, 3H); $^{13}$C NMR (CDCl$_3$, 100 MHz) δ: 169.7, 168.8, 166.3, 133.3, 130.0, 128.7, 127.8, 70.9, 70.6, 62.0, 61.9, 42.4, 35.6, 28.9, 22.7, 14.0, 13.8, 13.7; MS (ESI): $m/z = 346.2$ [M + H]$^+$; HRMS calculated for [C$_{20}$H$_{27}$NO$_4$ + H]$^+$: 346.2018, found 346.2006.
10. References

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12. Spectra of 2-[(aziridin-1-yl)-1-alkyl/aryl/heteroaryl-methylene]malonic acid diethyl esters (N-vinyl aziridines) - 20a, 20c, 20d, 20f–20h

$^1$H NMR spectrum of 20a

$^{13}$C NMR spectrum of 20a
Mass spectrum of 20a

![Mass spectrum of 20a](image)

IR spectrum of 20a

![IR spectrum of 20a](image)
$^{1}H$ NMR spectrum of 20c

$^{13}C$ NMR spectrum of 20c
Mass spectrum of 20c

IR spectrum of 20c
$^{1}{\text{H}}$ NMR spectrum of 20d

$^{13}{\text{C}}$ NMR spectrum of 20d
Mass spectrum of 20d

![Mass spectrum graph]

IR spectrum of 20d

![IR spectrum graph]
$^1$H NMR spectrum of 20f

$^{13}$C NMR spectrum of 20f
Mass spectrum of 20f

IR spectrum of 20f
$^1$H NMR spectrum of 20g

$^{13}$C NMR spectrum of 20g
Mass spectrum of 20g

IR spectrum of 20g
$^1$H NMR spectrum of 20h

$^{13}$C NMR spectrum of 20h
Mass spectrum of 20h

**Mass Analysis Report**

- **Data Filename**: 090218004.d
- **Sample Name**: TKM-054
- **Sample Position**: Vial 4
- **Instrument Name**: Instrument 1
- **Acq Method**: DA.m
- **DA Method**: DA.m

**User Spectra**

- **Fragmentor Voltage**: 70
- **Collision Energy**: 0
- **Ionization Mode**: ESI

*Scan (0.122 min) 090218004.d: Subtract (1)*

```
289.10
335.10
```

- **Formula**: 2-(Azirin-1-yl-(4-nitro-phenyl)-methylene)-malonic acid diethyl ester

--- End Of Report ---

IR spectrum of 20h

**DR. REDDY'S LABORATORIES LIMITED**

**Date**: 3/3/09
**Time**: 5:27:31 PM

**TDC/CCS-ANALYTICAL RESEARCH**

```
4000.0   3000.0   2000.0   1500.0   1000.0   450.0

15.0
30.0
45.0
60.0
75.0
90.0

2983.50
3188.26
3277.79
3363.98
2940.12
3075.53
1955.73
1204.05
2191.94
1337.10
```

**Formula**: 2-(Azirin-1-yl-(44,44-dimethylphenyl)-methylene)-malonic acid diethyl ester

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**S29**