Supplementary Information

Stereoselective assembly of 3,4-epoxypyrrolines via nucleophilic addition induced domino cyclization of 6-halo-1-oxa-4azahexatrienes

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Table of Contents

1. General experimental details	S2
2. Synthesis of aminal 4a	S2
3. Synthesis of epoxypyrrolines 5a – zb	S 3
4. Gram-scale synthesis of epoxypyrroline 5j	S18
5. Synthesis of halohydrins 6a-d	S 19
6. Synthesis of epoxypyrrolines 5zd , 5ze	S21
7. Synthesis of pyrrole 11	S22
8. Synthesis of oxazatrienes 12a –c	S23
9. Synthesis of compound 13	S24
10. ¹ H and ¹³ C NMR spectra	S26
11. X-ray data of compounds 5c,6b,13	S66
12. Calculation details	S 70
13. References	S76

1. General experimental details

All solvents were distilled and dried prior to use. 1,2-Dichloroethane (DCE) and dichloromethane were washed with concentrated H₂SO₄, water, then distilled from P₂O₅ and stored over anhydrous K₂CO₃. Melting points were determined on a hot stage microscope and are uncorrected. ¹H (400 MHz) and ¹³C (100 MHz) NMR spectra were recorded on a Bruker AVANCE 400 spectrometer in solvent indicated below. Chemical shifts (δ) are reported in ppm downfield from tetramethylsilane. IR spectra were recorded on a Shimadzu IR Affinity-1 spectrophotometer in KBr. Crystallographic data for the structures **5c** (CCDC 1936159), **6b** (CCDC 1936158), **13** (CCDC 1936916) have been deposited with the Cambridge Crystallographic Data Centre. Photochemical experiments were carried out with a mercury lamp Tungsram HGOK 400 (main radiation bands 310, 360, 365 nm). Column chromatography was performed on silica gel 60 M (0.04–0.063 mm). Thin-layer chromatography (TLC) was conducted on aluminum sheets precoated with SiO₂ ALUGRAM SIL G/UV254. 2*H*-Azirines **1a–d,f**, ¹**1e**, ²**1g**, ³**1h**, ⁴**1i**⁵ diazo compounds **2a**, ⁶**2b**, **c**, **e**, **f**, ⁷**2d**, ⁸**2g**, ⁹**2h**¹⁰ and oxazatrienes **3a–e,zb,zc** ⁴ were prepared by the reported procedures.

2. Synthesis of aminal 4a

Methyl (*E*)-2-bromo-3-{[1-methoxy-1,3-dioxo-2-(phenethylamino)-3-phenylpropan-2-yl]amino}-3-phenylacrylate (4a)



To a solution of oxazatriene **3a** (129 mg, 0.3 mmol) in anhydrous CH_2Cl_2 (2 mL) a solution of 2phenylethan-1-amine (40 mg, 0.33 mmol) in CH_2Cl_2 (1 mL) was added dropwise under stirring. The mixture was stirred at room temperature for 30 min, the solvent was removed under reduced pressure, and the residue was purified by column chromatography (hexane/EtOAc, 5:1) to give **4a** (147 mg, 89%) as a colorless solid. M.p. 88–89 °C (Et₂O–hexane). ¹H NMR (300 MHz, C_6D_6) δ 2.50–2.66 (m, 2H), 2.89–3.07 (m, 5H), 3.63 (s, 3H), 6.61 (d, 2H, *J* 7.3 Hz), 6.84–6.96 (br. s, 1H), 6.99–7.24 (m, 12H), 8.33–8.36 (m, 2H), 11.68 (s, 1H). ¹³C NMR (75 MHz, C₆D₆) δ 36.4, 43.1, 52.0, 52.6, 80.4, 85.0, 126.5, 128.5, 128.8, 129.1, 129.4, 129.9, 130.1, 133.4, 134.0, 135.8, 139.9 (signal of one carbon is overlapped), 160.6, 167.8, 169.4, 189.2. HRMS–ESI: [M + H]⁺ calcd for C₂₈H₂₈⁷⁹BrN₂O₅⁺ [M+H]⁺: 551.1176; found 551.1178.

3. Synthesis of epoxypyrrolines 5

3.1. Synthesis of dimethyl 2,5-diphenyl-4-(2-phenylethyl)-6-oxa-3-azabicyclo[3.1.0]hex-2ene-1,4-dicarboxylate (5a)



To a solution of oxazatriene **3a** (129 mg, 0.3 mmol) in anhydrous CH₂Cl₂ (2 mL) a solution of 2phenylethan-1-amine (40 mg, 0.33 mmol) in CH₂Cl₂ (1 mL) was added dropwise under stirring. The mixture was stirred at room temperature for 30 min and the solvent was removed under reduced pressure. The residue was dissolved in anhydrous acetonitrile (5 mL) and dry K₂CO₃ (124 mg, 0.9 mmol) was added. The resulting mixture was refluxed for 1 h under stirring. The reaction mixture was washed with water (10 mL) and the aqueous layer was extracted with CH₂Cl₂ (2×5 mL). The combined organic layers were dried over Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography (hexane/EtOAc, from 10:1 to 4:1) to give 5a (89 mg, 63%) as a colorless oil (unseparated mixture of diastereomers 5:1). ¹H NMR (400 MHz, CDCl₃) δ 2.18 (br. s, 1H), 2.52 (br. s, 1H), 2.70–2.98 (m, 2H), 3.05– 3.35 (m, 2H), 3.57 (s, 3H), 3.67 and 3.69 (2 s, 6H), 3.80 (s, 3H), 7.10-7.64 (m, 13H), 7.82 (d, 2H, J 7.1 Hz). ¹³C NMR (100 MHz, CDCl₃) δ 36.7, 37.1, 45.1, 45.5, 52.6, 52.7, 52.82, 52.83, 67.8, 69.8, 75.2, 78.7, 91.4, 92.9, 126.0, 126.1, 127.9, 128.0, 128.1, 128.16, 128.23, 128.3, 128.5, 128.67, 128.7, 128.8, 128.9, 129.2, 129.4, 129.5, 131.6, 131.75, 131.8, 139.2, 139.7 (signals of three carbons are overlapped), 164.3, 164.9, 168.0, 169.7, 172.3, 172,4. HRMS-ESI: $[M + H]^+$ calcd for $C_{28}H_{27}N_2O_5^+$ $[M+H]^+$: 471.1914; found 471.1905.

3.2. General procedures for the preparation of epoxypyrrolines 5b–5zb

Procedure A (from oxazatrienes 3)

To a solution of oxazatrienes **3a–e** (0.3 mmol) in anhydrous CH_2Cl_2 (2 mL) a solution of nucleophile (quantities are indicated below) in CH_2Cl_2 (1 mL) was added dropwise under stirring. The mixture was stirred at room temperature for 24 h, the solvent was removed under reduced pressure and the residue was purified by column chromatography to give pure epoxypyrroline **5b–g,j–z**. In the case of compounds **5h,i,5za** the reaction mixture was washed with water (2×1 mL), the organic layer was dried over Na₂SO₄, the solvent was removed under reduced pressure and the residue was crystallized from hexane/Et₂O/CH₂Cl₂ mixture to give pure **5h,i,5za**.

Procedure B (from azirines 1)

To a solution of diazo compound **2a–h** (quantities are indicated below) and azirine **1a–i** (0.5 mmol) in anhydrous 1,2-dichloroethane (1.5 mL) at reflux under argon Rh₂(OAc)₄ (2 mol %) was added. The stirred mixture was heated under reflux until nitrogen evolution stopped. The resulting mixture was evaporated under reduced pressure, and the residue was filtered through a pad of silica gel using toluene/EtOAc 30:1 mixture as eluent. The filtrate was concentrated under reduced pressure, and the residue was dissolved in anhydrous CH₂Cl₂ (5 mL). A solution of nucleophile (quantities are indicated below) in CH₂Cl₂ (1.5 mL) was added dropwise to the resulting mixture under stirring. The mixture was stirred at room temperature for 24 h, the solvent was removed under reduced pressure and the residue was purified by column chromatography to give epoxypyrroline **5b–5za**.

Procedure C (from halohydrins 6)

To a solution of halohydrin **6a–d** (0.3 mmol) in anhydrous CH_2Cl_2 (3 mL) under stirring 1,8diazabicyclo[5.4.0]undec-7-ene (DBU) (91 mg, 0.6 mmol) was added. The reaction mixture was stirred at room temperature for 12 h, then washed with water (2×1 mL), the organic layer was dried over Na₂SO₄. The solvent was removed under reduced pressure and the residue was crystallized from Et₂O/hexane mixture to give epoxypyrroline **5b,d,z,zb**.

Dimethyl *rac-(1R,4R,5S)*-5-methyl-2-phenyl-4-(piperidin-1-yl)-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5b)



Compound **5b** (124 mg, 95%) was obtained as a colorless solid according to procedure A from oxazatriene **3a** (129 mg, 0.3 mmol) and piperidine (77 mg, 0.9 mmol) using hexane/EtOAc mixture (from 5:1 to 2:1) as eluent for chromatography. Compound **5b** (174 mg, 80%) was also obtained according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and piperidine (128 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. Compound **5b** (126 mg, 95%) was also obtained according to the procedure C from chlorohydrin **6a** (141 mg, 0.3 mmol). M.p. 141–142 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 1.42–1.52 (m, 2H), 1.58–1.71 (m, 4H), 2.70–2.84 (m, 2H), 3.02–3.15 (m, 2H), 3.59 (s, 3H), 3.69 (s, 3H), 7.33–7.43 (m, 5H), 7.44–7.57 (m, 3H), 7.79–7.86 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 24.4, 26.3, 50.2, 52.6, 52.7, 68.1, 73.4, 98.1, 128.1 (2C),

128.4, 128.7, 129.2, 130.8, 131.6, 132.0, 164.7, 169.0, 171.8. HRMS-ESI: $[M+H]^+$ calcd for $C_{25}H_{27}N_2O_5^+[M+H]^+$ 435.1914; found 435.1921. $v_{max/cm^{-1}}$ 1756 (C=O), 1613 (C=N).

4-Ethyl 1-methyl *rac*-(1*R*,4*R*,5*S*)-5-methyl-2-phenyl-4-(piperidin-1-yl)-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5c)



Compound **5c** (118 mg, 88%) was obtained as a colorless solid according to procedure A from oxazatriene **3b** (133 mg, 0.3 mmol) or **3zc** (120 mg, 0.3 mmol) and piperidine (77 mg, 0.9 mmol) using hexane/EtOAc mixture (from 5:1 to 2:1) as eluent for chromatography. Compound **5c** (173 mg, 77%) was also obtained according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2b** (1.31 g, 6 mmol) and piperidine (128 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 141–142 °C (Et₂O/hexane). ¹H NMR (300 MHz, CDCl₃) δ 1.17 (t, 3H, *J* 7.3 Hz), 1.40–1.53 (m, 2H), 1.56–1.70 (m, 4H), 2.69–2.86 (m, 2H), 2.98–3.16 (m, 2H), 3.59 (s, 3H), 4.02–4.24 (m, 2H), 7.30–7.59 (m, 8H), 7.75–7.87 (m, 2H). ¹³C NMR (75 MHz, CDCl₃) δ 13.8, 24.5, 26.3, 50.2, 52.7, 61.9, 68.2, 73.2, 98.0, 128.0, 128.1, 128.3, 128.7, 129.2, 130.8, 131.5, 132.1, 164.8, 168.3, 171.9. HRMS–ESI: [M+H]⁺ calcd for C₂₆H₂₉N₂O₅⁺ [M+H]⁺ 449.2071; found 449.2064. vmax/cm⁻¹ 1757 (C=O), 1749 (C=O), 1613 (C=N).

4-Ethyl 1-methyl *rac*-(1*R*,4*R*,5*S*)-5-methyl-2-phenyl-4-(piperidin-1-yl)-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5d)



Compound **5d** (44 mg, 38%) was obtained as a colorless solid according to procedure A from oxazatriene **3c** (115 mg, 0.3 mmol) using hexane/EtOAc mixture (from 5:1 to 2:1) as eluent for chromatography. Compound **5d** (66 mg, 34%) was also obtained according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2c** (234 mg, 1.5 mmol) and piperidine (128 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. Compound **5d** (112 mg, 97%) was also obtained according to procedure C from chlorohydrin **6b** (127 mg, 0.3 mmol). M.p. 135–136 °C (Et₂O–hexane). ¹H NMR (300 MHz, CDCl₃) δ 1.28 (t,

3H, *J* 7.1 Hz), 1.41–1.55 (m, 2H), 1.59–1.72 (m, 7H), 2.67–2.86 (m, 2H), 2.87–3.05 (m, 2H), 3.78 (m, 3H), 4.27 (q, 2H, *J* 7.1 Hz), 7.38–7.57 (m, 3H), 7.68–7.80 (m, 2H). ¹³C NMR (75 MHz, CDCl₃) δ 13.5, 14.0, 24.5, 26.4, 49.7, 52.8, 62.0, 67.5, 70.0, 96.4, 128.0, 128.6, 131.5, 132.2, 165.5, 168.7, 172.3. HRMS–ESI: [M+Na]⁺ calcd for C₂₁H₂₆N₂NaO₅⁺ [M+Na]⁺ 409.1734; found 409.1733. v_{max/cm⁻¹} 1750 (C=O), 1599 (C=N).

Dimethyl *rac*-(1*R*,4*R*,5*S*)-5-(4-cyanophenyl)-2-phenyl-4-(piperidin-1-yl)-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5e)



Compound **5e** (111 mg, 80%) was obtained as a colorless solid according to procedure A from oxazatriene **3d** (137 mg, 0.3 mmol) and piperidine (77 mg, 0.9 mmol) using hexane/EtOAc mixture (from 5:1 to 2:1) as eluent for chromatography. Compound **5e** (138 mg, 60%) was also obtained according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2d** (229 mg, 1.0 mmol) and piperidine (128 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 174–175 °C (Et₂O/hexane). ¹H NMR (300 MHz, CDCl₃) δ 1.39–1.53 (m, 2H), 1.54–1.76 (m, 4H), 2.61–2.81 (m, 2H), 2.89–3.10 (m, 2H), 3.60 (s, 3H), 3.73 (s, 3H), 7.42–7.62 (m, 5H), 7.66–7.70 (m, 2H), 7.75–7.81 (m, 2H). ¹³C NMR (75 MHz, CDCl₃) δ 24.3, 26.3, 50.3, 52.9, 53.0, 68.4, 72.6, 98.1, 113.3, 118.0, 128.1, 128.8, 129.1, 131.6, 131.9, 132.1, 136.1, 164.1, 168.9, 171.6. HRMS–ESI: [M+Na]⁺ calcd for C₂₆H₂₅N₃NaO₅⁺ [M+Na]⁺ 482.1686; found 482.1668. vmax/cm⁻¹ 2229 (C=N), 1757 (C=O), 1741 (C=O), 1604 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-2-(4-methoxyphenyl)-5-phenyl-4-(piperidin-1-yl)-6-oxa-3azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5f)



Compound **5f** (113 mg, 81%) was obtained as a colorless solid according to procedure A from oxazatriene **3e** (138 mg, 0.3 mmol) and piperidine (77 mg, 0.9 mmol) using hexane/EtOAc mixture (from 5:1 to 2:1) as eluent for chromatography. Compound **5f** (144 mg, 62%) was also

obtained according to procedure B from azirine **1b** (142 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and piperidine (128 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 160–162 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 1.40–1.52 (m, 2H), 1.57–1.68 (m, 4H), 2.67–2.84 (m, 2H), 2.98–3.13 (m, 2H), 3.60 (s, 3H), 3.68 (s, 3H), 3.88 (s, 3H), 6.91–7.03 (m, 2H), 7.31–7.45 (m, 5H), 7.71–7.83 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 24.4, 26.3, 50.2, 52.6, 52.7, 55.4, 68.0, 73.5, 97.9, 114.1, 124.7, 128.1, 128.3, 129.1, 129.9, 130.9, 162.4, 164.9, 169.3, 170.8. HRMS–ESI: [M+H]⁺ calcd for C₂₆H₂₉N₂O₆⁺ [M+H]⁺ 465.2020; found 465.2029.

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-2,5-diphenyl-6-oxa-3azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5g)



Compound **5g** (179 mg, 74%) was obtained as a colorless oil according procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and 1,2,3,4-tetrahydroisoquinoline (200 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. ¹H NMR (400 MHz, CDCl₃) δ 2.85–3.08 (m, 2H), 3.17–3.36 (m, 2H), 3.65 (s, 3H), 3.70 (s, 3H), 4.02 and 4.40 (AB-q, 2H, *J* 15 Hz), 7.00–7.07 (m, 1H), 7.07–7.17 (m, 3H), 7.33–7.46 (m, 5H), 7.47–7.61 (m, 3H), 7.81–7.90 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 29.8, 47.5, 51.3, 52.8, 52.9, 68.2, 73.6, 97.5, 125.4, 125.8, 126.6, 128.0, 128.1, 128.5, 128.6, 128.7, 129.4, 130.3, 131.8, 131.9, 134.5, 135.0, 164.7, 168.7, 172.5. HRMS–ESI: [M+H]⁺ calcd for C₂₉H₂₇N₂O₅⁺ [M+H]⁺ 483.1914; found 483.1919. vmax/cm⁻¹ 1756 (C=O), 1740 (C=O), 1609 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(4-carbamoylpiperidin-1-yl)-2,5-diphenyl-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5h)



Compound **5h** (125 mg, 87%) was obtained as a colorless solid according to procedure A from oxazatriene **3a** (129 mg, 0.3 mmol) and piperidine-4-carboxamide (115 mg, 0.9 mmol). Compound **5h** (177 mg, 74%) was also obtained according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and piperidine-4-carboxamide (192 mg, 1.5 mmol) using EtOAc as eluent for chromatography. M.p. 115–117 °C (hexane/Et₂O/CH₂Cl₂). ¹H NMR (400 MHz, CDCl₃) δ 1.71–2.00 (m, 4H), 2.09–2.23 (m, 1H), 2.43 (td, 1H, *J* 11.4 Hz, *J* 2.6 Hz), 2.79 (td, 1H, *J* 11.4 Hz, *J* 2.6 Hz), 3.23 (d, 1H, *J* 11.5 Hz), 3.49 (d, 1H, *J* 11.5 Hz), 3.59 (s, 3H), 3.65 (s, 3H), 5.72 (br. d, 2H, *J* 57.8 Hz), 7.30–7.42 (m, 5H), 7.43–7.60 (m, 3H), 7.75–7.81 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 29.2 (2C), 42.8, 48.3, 49.4, 52.7, 52.8, 68.0, 73.2, 97.6, 127.9, 128.0, 128.5, 128.7, 129.4, 130.2, 131.8, (signal of one carbon is overlapped), 164.6, 168.7, 172.3, 177.5. HRMS–ESI: [M+H]⁺ calcd for C₂₆H₂₈N₃O₆⁺ [M+H]⁺ 478.1973; found 478.1969. v_{max/cm⁻¹} 1745 (C=O), 1687 (C=O), 1609 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(4-benzhydrylpiperazin-1-yl)-2,5-diphenyl-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5i)



Compound **5i** (157 mg, 87%) was obtained as a colorless solid according to procedure A from oxazatriene **3a** (129 mg, 0.3 mmol) and 1-benzhydrylpiperazine (227 mg, 0.9 mmol). Compound **5i** (225 mg, 75%) was also obtained according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and 1-benzhydrylpiperazine (378 mg, 1.5 mmol) using EtOAc as eluent for chromatography. M.p. 222–226 °C (dec., hexane/Et₂O/CH₂Cl₂). ¹H NMR (400 MHz, CDCl₃) δ 2.51 (br. s, 4H), 2.80–2.95 (m, 2H), 3.14–3.27 (m, 2H), 3.61 (s, 3H), 3.66 (s, 3H), 4.25 (s, 1H), 7.14–7.20 (m, 2H), 7.24–7.28 (m, 2H), 7.31–7.46 (m, 9H), 7.46–7.60 (m, 3H), 7.78–7.88 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.2, 52.1, 52.6, 52.8, 68.0, 73.4, 76.1, 97.3, 126.8, 126.81, 127.91, 127.93, 127.95, 128.1, 128.36, 128.37, 128.5, 128.7, 129.4, 130.3, 131.7, 131.9, 142.8 (signal of one carbon is overlapped), 164.7, 168.5, 172.2. HRMS–ESI: [M+H]⁺ calcd for C₃₇H₃₆N₃O₅⁺ [M+H]⁺ 602.2649; found 602.2641. v_{max/cm⁻¹}1762 (C=O), 1743 (C=O), 1609 (C=N).

Dimethyl *rac*-(1*R*,4*R*,5*S*)-4-(morpholin-4-yl)-2,5-phenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5j)



Compound **5j** (174 mg, 80%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 154–155 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.79–2.94 (m, 2H), 3.09–3.23 (m, 2H), 3.60 (s, 3H), 3.69 (s, 3H), 3.75–3.80 (m, 4H), 7.32–7.43 (m, 5H), 7.44–7.60 (m, 3H), 7.76–7.89 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.4, 52.7, 52.8, 67.1, 68.0, 73.2, 97.0, 127.8, 128.0, 128.5, 128.7, 129.4, 130.2, 131.7, 131.8, 164.5, 168.2, 172.4. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₅N₂O₆⁺ [M+H]⁺ 437.1707; found 437.1701.

Dimethyl *rac*-(1*R*,4*R*,5*S*)-5-(4-chlorophenyl)-4-(morpholin-4-yl)-2-phenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5k)



Compound **5k** (188 mg, 80%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2e** (835 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 184–186 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.84 (dt, 2H, *J* 10 Hz, *J* 4.6 Hz), 3.11 (dt, 2H, *J* 10 Hz, *J* 4.6 Hz), 3.63 (s, 3H), 3.72 (s, 3H), 3.76 (t, 4H, *J* 4.6 Hz), 7.30–7.40 (m, 4H), 7.45–7.52 (m, 2H), 7.52–7.60 (m, 1H), 7.77–7.84 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.5, 52.9, 53.0, 67.1, 68.2, 72.6, 96.9, 128.0, 128.75, 128.81, 128.9, 129.3, 131.6, 132.0, 135.7, 164.3, 168.2, 172.4. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₄³⁵ClN₂O₆⁺ [M+H]⁺ 471.1317; found 471.1321. vmax/cm⁻¹1743 (C=O), 1610 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-5-(4-bromophenyl)-4-(morpholin-4-yl)-2-phenyl-6-oxa-3azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5l)



Compound **51** (201 mg, 78%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2f** (991 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 198–199 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.83 (dt, 2H, *J* 9.8 Hz, *J* 4.6 Hz), 3.11 (dt, 2H, *J* 9.8 Hz, *J* 4.6 Hz), 3.64 (s, 3H), 3.72 (s, 3H), 3.77 (t, 4H, *J* 4.6 Hz), 7.24–7.30 (m, 2H), 7.45–7.60 (m, 5H), 7.77–7.84 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.5, 52.9, 53.0, 67.1, 68.2, 72.6, 96.9, 124.0, 128.1, 128.8, 129.3, 129.6, 131.6, 131.8, 132.0, 164.3, 168.2, 172.4. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₄⁷⁹BrN₂O₆⁺ [M+H]⁺ 515.0812; found 515.0808. vmax/cm⁻¹ 1741 (C=O), 1608 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-5-(3-bromophenyl)-4-(morpholin-4-yl)-2-phenyl-6-oxa-3azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5m)



Compound **5m** (193 mg, 75%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2g** (991 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 128–129 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.77–2.90 (m, 2H), 3.06–3.18 (m, 2H), 3.64 (s, 3H), 3.74 (s, 3H), 3.77 (t, 4H, *J* 4.7 Hz), 7.23–7.31 (m, 1H), 7.31–7.38 (m, 1H), 7.45–7.61 (m, 5H), 7.76–7.86 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.5, 52.9, 53.0, 67.1, 68.1, 72.4, 97.0, 122.5, 126.7, 128.1, 128.8, 130.1, 131.0, 131.6, 132.0, 132.5, 132.7, 164.2, 168.1, 172.3. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₄⁷⁹BrN₂O₆⁺ [M+H]⁺ 515.0812; found 515.0805. vmax/cm⁻¹ 1756 (C=O), 1735 (C=O), 1606 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(morpholin-4-yl)-5-(4-nitrophenyl)-2-phenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5n)



Compound **5n** (180 mg, 75%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2h** (299 mg, 1.2 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 205–207 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.76–2.88 (m, 2H), 3.04–3.16 (m, 2H), 3.63 (s, 3H), 3.70–3.81 (m, 7H), 7.47–7.52 (m, 2H), 7.54–7.66 (m, 3H), 7.78–7.83 (m, 2H), 8.23–8.28 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.5, 53.1, 53.2, 67.1, 68.5, 72.3, 97.0, 123.7, 128.1, 128.8, 129.2, 131.3, 132.2, 137.4, 148.4, 163.9, 168.1, 172.2. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₄N₃O₈⁺ [M+H]⁺ 482.1558; found 482.1550.

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(morpholin-4-yl)-5-phenyl-2-(4-methylphenyl)-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (50)



Compound **50** (153 mg, 68%) was obtained as a colorless solid according to procedure B from azirine **1c** (134 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 73–75 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.44 (s, 3H), 2.80–2.92 (m, 2H), 3.10–3.21 (m, 2H), 3.61 (s, 3H), 3.69 (s, 3H), 3.77 (t, 4H, *J* 4.7 Hz), 7.28–7.30 (m, 2H), 7.31–7.42 (m, 5H), 7.68–7.73 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 21.6, 49.5, 52.7, 52.8, 67.2, 68.1, 73.2, 96.9, 127.9, 128.1, 128.5, 129.0, 129.41, 129.43, 130.3, 142.5, 164.6, 168.3, 172.2. HRMS–ESI: [M+H]⁺ calcd for C₂₅H₂₇N₂O₆⁺ [M+H]⁺ 451.1864; found 451.1857. vmax/cm⁻¹ 1750 (C=O), 1735 (C=O), 1605 (C=N).

Dimethyl *rac*-(1*R*,4*R*,5*S*)-2-(4-chlorophenyl)-4-(morpholin-4-yl)-5-phenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5p)



Compound **5p** (195 mg, 83%) was obtained as a colorless solid according to procedure B from azirine **1d** (144 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 126–127 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.77–2.91 (m, 2H), 3.07–3.21 (m, 2H), 3.61 (s, 3H), 3.69 (s, 3H), 3.77 (t, 4H, *J* 4.6 Hz), 7.31–7.43 (m, 5H), 7.44–7.49 (m, 2H), 7.72–7.76 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.4, 52.8, 52.9, 67.1, 67.8, 73.4, 97.1, 127.9, 128.6, 129.1, 129.4, 129.6, 130.0, 130.2, 138.2, 164.4, 168.1, 171.5. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₄³⁵ClN₂O₆⁺ [M+H]⁺ 471.1317; found 471.1317. vmax/cm⁻¹ 1741 (C=O), 1621 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-2-(4-bromophenyl)-4-(morpholin-4-yl)-5-phenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5q)



Compound **5q** (207 mg, 80%) was obtained as a colorless solid according to procedure B from azirine **1e** (167 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 138–140 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.78–2.90 (m, 2H), 3.09–3.19 (m, 2H), 3.62 (s, 3H), 3.69 (s, 3H), 3.78 (t, 4H, *J* 4.7 Hz), 7.31–7.44 (m, 5H), 7.59–7.73 (m, 4H). ¹³C NMR (100 MHz, CDCl₃) δ 49.5, 52.8, 53.0, 67.2, 67.8, 73.5, 97.1, 126.7, 127.9, 128.6, 129.56, 129.58, 130.0, 130.6, 132.1, 164.4, 168.1, 171.6. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₄⁷⁹BrN₂O₆⁺ [M+H]⁺ 515.0812; found 515.0819.

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(morpholin-4-yl)-2-(4-nitrophenyl)-5-phenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5r)



Compound **5r** (195 mg, 81%) was obtained as a colorless solid according to procedure B from azirine **1f** (150 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 165–167 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.78–2.91 (m, 2H), 3.08–3.21 (m, 2H), 3.61 (s, 3H), 3.69 (s, 3H), 3.77 (t, 4H, *J* 4.7 Hz), 7.29–7.46 (m, 5H), 7.92–8.04 (m, 2H), 8.30–8.40 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.4, 52.9, 53.0, 67.1, 67.6, 73.7, 97.4, 123.9, 127.8, 128.6, 129.1, 129.6, 129.7, 137.2, 149.6, 164.1, 167.7, 171.1. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₄N₃O₈⁺ [M+H]⁺ 482.1558; found 482.1560. vmax/cm⁻¹ 1740 (C=O), 1603 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(morpholin-4-yl)-2-(naphthalen-2-yl)-5-phenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5s)



Compound **5s** (187 mg, 77%) was obtained as a colorless solid according to procedure B from azirine **1g** (152 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 167–169 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.84–2.97 (m, 2H), 3.15–3.27 (m, 2H), 3.63 (s, 3H), 3.72 (s, 3H), 3.80 (t, 4H, *J* 4.7 Hz), 7.36–7.47 (m, 5H), 7.52–7.65 (m, 2H), 7.86–8.01 (m, 4H), 8.26 (br. s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 49.5, 52.8, 52.9, 67.2, 68.2, 73.4, 97.1, 124.4, 126.8, 127.8, 127.9, 128.55, 128.61, 128.9, 129.0, 129.2, 129.5, 130.2, 132.8, 134.9, 164.6, 168.3, 172.5. HRMS–ESI: [M+H]⁺ calcd for C₂₈H₂₇N₂O₆⁺ [M+H]⁺ 487.1864; found 487.1856. vmax/cm⁻¹ 1756 (C=O), 1604 (C=N).

Dimethyl *rac*-(1*R*,4*R*,5*S*)-2-(furan-2-yl)-4-(morpholin-4-yl)-5-phenyl-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5t)



Compound **5t** (149 mg, 77%) was obtained as a colorless solid according to procedure B from azirine **1h** (122 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 153–155 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.79–2.92 (m, 2H), 3.07–3.20 (m, 2H), 3.66 (s, 3H), 3.70 (s, 3H), 3.77 (t, 4H, *J* 4.6 Hz), 6.60 (dd, 1H, *J* 3.5 Hz, 1.7 Hz), 7.08 (d, 1H, *J* 3.5 Hz), 7.31–7.44 (m, 5H), 7.65 (d, 1H, *J* 1.7 Hz). ¹³C NMR (100 MHz, CDCl₃) δ 49.4, 52.8, 52.9, 67.1, 67.7, 73.1, 96.9, 112.5, 115.9, 127.8, 128.5, 129.5, 129.8, 146.2, 147.1, 162.3, 163.9, 168.0. HRMS–ESI: [M+H]⁺ calcd for C₂₂H₂₃N₂O₇⁺ [M+H]⁺ 427.1500; found 427.1504. vmax/cm⁻¹ 1758 (C=O), 1616 (C=N).

1-Benzyl 4-methyl 4-(morpholin-4-yl)-2,5-diphenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5u)



Compound **5u** (197 mg, 77%) (unseparated mixture of diastereomers, 10:1) was obtained as a colorless oil according to procedure B from azirine **1i** (165 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and morpholine (131 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. ¹H NMR (400 MHz, CDCl₃) δ 2.79–2.94 (m, 2H), 3.07–3.23 (m, 2H), 3.64 and 3.72 (2s, 3H), 3.77 (t, 4H, *J* 4.6 Hz), 5.00 and 5.13 (AB-q, 2H, *J* 12 Hz), 6.99–7.03 (m, 2H), 7.18–7.60 (m, 11H), 7.76–7.85 (2m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 49.4, 52.60, 52.64, 67.2, 67.6, 68.1, 73.3, 97.0, 127.9, 128.0, 128.10, 128.14, 128.39, 128.42, 128.47, 128.5, 128.6, 129.4, 130.1, 131.67, 131.69, 134.3, 163.8, 163.9, 168.0, 168.2, 172.7 (other signals are overlapped). HRMS–ESI: [M+H]⁺ calcd for C₃₀H₂₉N₂O₆⁺ [M+H]⁺ 513.2020; found 513.2027.

Dimethyl *rac-*(1*R*,4*R*,5*S*)-2,5-diphenyl-4-(pyrrolidin-1-yl)-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5v)



Compound **5v** (158 mg, 75%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and pyrrolidine (107 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 169–170 °C (Et₂O/hexane).¹H NMR (400 MHz, CDCl₃) δ 1.71–1.92 (m, 4H), 2.88–3.05 (m, 2H), 3.10–3.29 (m, 2H), 3.62 (s, 3H), 3.66 (s, 3H), 7.31–7.43 (m, 5H), 7.44–7.66 (m, 3H), 7.79–7.85 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 24.2, 49.4, 52.7, 52.8, 67.5, 73.9, 96.1, 127.8, 128.0, 128.6, 128.7, 129.4, 129.9, 131.6, 132.0, 164.8, 168.4, 172.2. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₅N₂O₅⁺ [M+H]⁺ 421.1758; found 421.1757. v_{max/cm⁻¹}1755 (C=O), 1609 (C=N).

Dimethyl 4-(1*H*-imidazol-1-yl)-2,5-diphenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5w)



Compound **5w** (101 mg, 81%) (unseparated mixture of diastereomers, 7:1) was obtained as a colorless solid according to procedure A from oxazatriene **3a** (129 mg, 0.3 mmol) and imidazole (61 mg, 0.9 mmol) using EtOAc as eluent for chromatography. Compound **5w** (156 mg, 75%) was also obtained according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and imidazole (102 mg, 1.5 mmol) using EtOAc as eluent for chromatography. M.p. 152–158 °C (dec., hexane/Et₂O/CH₂Cl₂). ¹H NMR (400 MHz, CDCl₃) δ 3.53 and 3.63 (2s, 3H), 3.83 and 3.89 (2s, 3H), 6.99–7.12 (m, 2H), 7.22–7.72 (m, 9H), 7.81–7.97 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 53.1 (2C), 53.7, 53.9, 70.0, 70.3, 74.2, 80.2, 89.7, 90.6, 117.2, 118.4, 127.1, 127.8, 127.9, 128.3, 128.4, 128.5, 128.55, 128.6, 128.9, 129.0, 129.1, 129.5, 130.0, 130.3, 130.5, 130.8, 133.0, 133.1, 135.1, 136.5, 163.2, 163.3, 165.55, 165.6, 175.8, 176.2. HRMS–ESI: [M+H]⁺ calcd for C₂₃H₂₀N₃O₅⁺ [M+H]⁺ 418.1397; found 418.1391. vmax/cm⁻¹ 1764 (C=O), 1735 (C=O), 1599 (C=N).

Dimethyl *rac*-(1*R*,4*R*,5*S*)-4-(dimethylamino)-2,5-diphenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5x)



Compound **5x** (144 mg, 73%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and 2M solution of dimethylamine in CH₂Cl₂ (1 ml, 2.0 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 128–130 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.63 (s, 6H), 3.61 (s, 3H), 3.67 (s, 3H), 7.26–7.45 (m, 5H), 7.44–7.61 (m, 3H), 7.76–7.91 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 41.9, 52.7, 52.8, 67.9, 73.4, 97.6, 127.7, 128.0, 128.6, 128.7, 129.4, 130.1, 131.7, 131.9, 164.6, 168.7, 172.5. HRMS–ESI: [M+H]⁺ calcd for C₂₂H₂₃N₂O₅⁺ [M+H]⁺ 395.1601; found 395.1595. vmax/cm⁻¹ 1745 (C=O), 1726 (C=O), 1611 (C=N).

Dimethyl *rac*-(1*R*,4*R*,5*S*)-4-(diethylamino)-2,5-diphenyl-6-oxa-3-azabicyclo[3.1.0]hex-2ene-1,4-dicarboxylate (5y)



Compound **5y** (165 mg, 78%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and diethylamine (110 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. M.p. 101–103 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 1.09 (t, 6H, *J* 7.1 Hz), 2.92–3.10 (m, 4H), 3.56 (s, 3H), 3.70 (s, 3H), 7.32–7.57 (m, 8H), 7.77–7.87 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 14.5, 44.9, 52.4, 52.7, 68.8, 74.0, 98.8, 127.9, 128.0, 128.3, 128.6, 129.2, 131.1, 131.5, 132.2, 164.6, 169.9, 170.5. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₇N₂O₅⁺ [M+H]⁺ 423.1914; found 423.1917. vmax/cm⁻¹ 1755 (C=O), 1740 (C=O), 1608 (C=N).

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-[benzyl(methyl)amino]-2,5-diphenyl-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5z)



Compound **5z** (183 mg, 78%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and *N*-benzyl-*N*-methylamine (182 mg, 1.5 mmol) using hexane/EtOAc mixture (from 10:1 to 2:1) as eluent for chromatography. Compound **5z** (140 mg, 99%) was also obtained according to procedure C from chlorohydrin **6c** (152 mg, 0.3 mmol). M.p. 76–78 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.49 (s, 3H), 3.63 (s, 3H), 3.72 (s, 3H), 3.98 and 4.12 (AB-q, 2H, *J* 14 Hz), 7.22–7.62 (m, 13H), 7.85–7.94 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 37.4, 52.5, 52.8, 58.0, 68.6, 73.9, 97.8, 126.7, 127.9, 128.0, 128.1, 128.4, 128.5, 128.7, 129.3, 130.7, 131.7, 131.9, 139.8, 164.6, 169.1, 172.1. HRMS–ESI: [M+H]⁺ calcd for C₂₈H₂₇N₂O₅⁺ [M+H]⁺ 471.1914; found 471.1920.

Dimethyl *rac-*(1*R*,4*S*,5*R*)-4-[2-(diethylamino)ethylsulfanyl]-2,5-diphenyl-6-oxa-3-azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5za)



Compound **5za** (171 mg, 71%) was obtained as a colorless solid according to procedure B from azirine **1a** (127 mg, 0.5 mmol), diazo compound **2a** (714 mg, 3.5 mmol) and 2-(*N*,*N*-diethylamino)ethanethiol (200 mg, 1.5 mmol). M.p. 77–79 °C (hexane/Et₂O/CH₂Cl₂). ¹H NMR (400 MHz, CDCl₃) δ 0.97 (t, 6H, *J* 7.2 Hz), 2.42–2.57 (m, 4H), 2.63–2.84 (m, 3H), 2.88–2.99 (m, 1H), 3.60 (s, 3H, CH₃), 3.65 (s, 3H), 7.34–7.61 (m, 8H), 7.80–7.90 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 11.8, 28.0, 46.8, 52.4, 52.9, 53.2, 69.2, 79.0, 86.9, 128.0, 128.3, 128.5, 128.7, 128.9, 129.8, 131.5, 132.0, 164.4, 166.8, 171.7. HRMS–ESI: [M+Na]⁺ calcd for C₂₆H₃₀N₂NaO₅S⁺ [M+Na]⁺ 505.1768; found 505.1779. vmax/cm⁻¹ 1754 (C=O), 1735 (C=O), 1599 (C=N).

Dimethyl *rac*-(1*R*,4*R*,5*S*)-5-cyclopropyl-4-(morpholin-4-yl)-2-phenyl-6-oxa-3-azabicyclo-[3.1.0]hex-2-ene-1,4-dicarboxylate (5zb)



Compound **5zb** (113 mg, 94%) was obtained as a colorless solid according to procedure C from bromohydrin **6d** (144 mg, 0.3 mmol). M.p. 135–136 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 0.46–0.57 (m, 1H), 0.60–0.87 (m, 3H), 1.30–1.41 (m, 1H), 2.74–3.04 (m, 4H), 3.68–3.82 (m, 7H), 3.84 (s, 3H), 7.34–7.60 (m, 3H), 7.64–7.84 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 2.0, 3.3, 7.0, 49.2, 52.8, 53.1, 67.3, 68.2, 72.3, 96.2, 127.8, 128.7, 131.77, 131.8, 165.1, 168.7, 173.1. HRMS–ESI: [M+H]⁺ calcd for C₂₁H₂₅N₂O₆⁺ [M+H]⁺ 401.1707; found 401.1711. v_{max/em⁻¹}1748 (C=O), 1602 (C=N).

4. Gram-scale synthesis of epoxypyrroline 5j



To a solution of diazo compound **2a** (5.712 g, 28.0 mmol) and azirine **1a** (1.016 g, 4.0 mmol) in anhydrous 1,2-dichloroethane (10 mL) at reflux under inert atmosphere $Rh_2(OAc)_4$ (35 mg, 2 mol %) was added. The stirred mixture was heated under reflux until nitrogen evolution stopped (1.5 min). The resulting mixture was evaporated under reduced pressure, and the residue was filtered through a pad of silica gel using toluene/EtOAc 30:1 mixture as eluent. The filtrate was concentrated under reduced pressure, and the residue was dissolved in anhydrous CH_2Cl_2 (30 mL). A solution of morpholine (1.044 g, 12 mmol) in CH_2Cl_2 (10 mL) was added dropwise to the resulting mixture under stirring. The mixture was stirred at room temperature for 24 h, the solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel (hexane/EtOAc, from 10:1 to 2:1) to afford epoxypyrroline **5j** (1.33 g, 76%).

5. Synthesis of halohydrins 6a-d

General procedure for preparation of halohydrins 6a-c

To a solution of oxazatriene 3zb-zd (0.3 mmol) in anhydrous CH₂Cl₂ (2 mL) a solution of the amine (quantities are indicated below) in CH₂Cl₂ (1 mL) was added dropwise under stirring. The mixture was stirred at room temperature for 6 h, the solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel.

Dimethyl *rac-(2R,3S,4S)-4-*chloro-3-hydroxy-3,5-diphenyl-2-(piperidin-1-yl)-3,4-dihydro-2*H*-pyrrole-2,4-dicarboxylate (6a)



Compound **6a** (116 mg, 82%) was obtained as a colorless solid according to the general procedure from oxazatriene **3zb** (116 mg, 0.3 mmol) and piperidine (28 mg, 0.33 mmol) using hexane/EtOAc mixture (5:1) as eluent for column chromatography. M.p. 137–139 °C (Et₂O/hexane). ¹H NMR (300 MHz, CDCl₃) δ 1.35–1.80 (m, 6H), 2.60–2.90 (m, 2H), 2.88–3.65 (m, 2H), 3.75 (s, 6H), 6.79 (br. s, 1H), 7.30–7.70 (m, 8H), 7.96–8.19 (m, 2H). ¹³C NMR (75 MHz, CDCl₃) δ 24.7, 26.7, 49.2, 51.9, 52.9, 77.1, 86.2, 97.5, 127.1, 128.0 (2C), 128.1, 129.6, 131.1, 132.3, 137.0, 167.0, 168.7, 169.8. HRMS–ESI: [M+H]⁺ calcd for C₂₅H₂₈³⁵ClN₂O₅⁺ [M+H]⁺: 471.1681; found 471.1689. vmax/cm⁻¹ 1750 (C=O), 1741 (C=O), 1626 (C=N).

2-Ethyl 4-methyl *rac-(2R,3S,4S)-*4-chloro-3-hydroxy-3-methyl-5-phenyl-2-(piperidin-1-yl)-3,4-dihydro-2*H*-pyrrole-2,4-dicarboxylate (6b)



Compound **6b** (46 mg, 36%) was obtained as a colorless solid according to the general procedure from oxazatriene **3zc** (101 mg, 0.3 mmol) and piperidine (28 mg, 0.33 mmol) using hexane/EtOAc mixture (from 10:1 to 5:1) as eluent for chromatography. M.p. 124–126 °C (Et₂O/hexane). ¹H NMR (300 MHz, CDCl₃) δ 1.26 (t, 3H, *J* 7.3 Hz), 1.48–1.73 (m, 6H), 1.83 (s, 3H), 2.73–3.07 (m, 2H), 3.20–3.63 (m, 2H), 3.78 (s, 3H), 4.11–4.34 (m, 2H), 5.67 (br. s, 1H), 7.35–7.52 (m, 3H), 7.90–8.00 (m, 2H). ¹³C NMR (75 MHz, CDCl₃) δ 14.2, 22.0, 24.7, 26.8,

49.4, 53.0, 61.3, 78.2, 83.4, 96.3, 128.0, 129.2, 131.0, 131.9, 166.6, 167.8, 168.4. HRMS-ESI: $[M+H]^+$ calcd for $C_{21}H_{28}{}^{35}CIN_2O_5^+[M+H]^+$: 423.1681; found 423.1704.

Dimethyl *rac-*(2*R*,3*S*,4*S*)-2-(benzyl(methyl)amino)-4-chloro-3-hydroxy-3,5-diphenyl-3,4-dihydro-2*H*-pyrrole-2,4-dicarboxylate (6c)



Compound **6c** (136 mg, 89%) was obtained as a colorless solid according to the general procedure from oxazatriene **3zb** (116 mg, 0.3 mmol) and *N*-benzyl-*N*-methylamine (40 mg, 0.33 mmol) using hexane/EtOAc mixture (5:1) as eluent for column chromatography. M.p. 118–120 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.54 (br. s, 3H), 3.72 (s, 3H), 3.79–3.91 (m, 4H), 4.38 (br. s, 1H), 6.67 (br. s, 1H), 7.26–7.57 (m, 11H), 7.62–7.72 (m, 2H), 8.06–8.16 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 37.1, 52.2, 52.8, 56.5, 77.7, 85.6, 99.0, 127.16, 127.2, 128.0, 128.1, 128.3, 128.4, 128.7, 129.6, 131.2, 132.3, 136.4, 138.6, 166.4, 169.1, 170.0. HRMS–ESI: [M+H]⁺ calcd for C₂₈H₂₈³⁵ClN₂O₅⁺ [M+H]⁺: 507.1681; found 507.1691. vmax/cm⁻¹ 1748 (C=O), 1616 (C=N).

Dimethyl *rac-(2R,3S,4S)-*4-bromo-3-cyclopropyl-3-hydroxy-2-(morpholin-4-yl)-5-phenyl-3,4-dihydro-2*H*-pyrrole-2,4-dicarboxylate (6d)



To a solution of diazo compound **2i** (101 mg, 0.6 mmol) and azirine **1a** (76 mg, 0.3 mmol) in anhydrous 1,2-dichloroethane (1 mL) at reflux under argon $Rh_2(OAc)_4$ (2 mol %) was added. The stirred mixture was heated under reflux until nitrogen evolution stopped. The resulting mixture was evaporated under reduced pressure, and the residue was filtered through a pad of silica gel using toluene/EtOAc 30:1 mixture as eluent. The filtrate was concentrated under reduced pressure, and the residue was dissolved in anhydrous CH_2Cl_2 (3 mL). A solution of morpholine (29 mg, 0.33 mmol) in CH_2Cl_2 (1 mL) was added dropwise to the resulting mixture under stirring. The mixture was stirred at room temperature for 6 h, the solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel using hexane/EtOAc mixture (5:1). Compound **6d** (122 mg, 85%) was obtained as a colorless solid. M.p. 155–157 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 0.39–0.50 (m, 1H), 0.51–0.61 (m, 1H), 0.62–0.81 (m, 2H), 1.87–1.99 (m, 1H), 3.06–3.20 (m, 2H), 3.20–3.41 (m, 2H), 3.63–3.88 (m, 10H), 5.35 (s, 1H), 7.36–7.53 (m, 3H), 7.92–8.00 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 3.1, 3.6, 14.7, 49.0, 52.1, 53.2, 67.6, 71.4, 84.1, 95.9, 128.1, 129.2, 131.2, 131.7, 166.5, 167.4, 170.3. HRMS–ESI: [M+H]⁺ calcd for C₂₁H₂₆⁷⁹BrN₂O₆⁺ [M+H]⁺ 481.0969; found 481.0961.

6. Synthesis of epoxypyrrolines 5zd,5ze

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(morpholin-4-yl)-2-phenyl-5-(3-(pyridin-2-yl)phenyl)-6-oxa-3azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5zd)



The mixture of epoxypyrroline **51** (103 mg, 0.2 mmol), 2-(tributylstannyl)pyridine (220 mg, 0.6 mmol), CuI (11 mg, 30 mol %) and Pd(PPh₃)₄ (23 mg, 10 mol %) in anhydrous 1,4-dioxane (2 mL) was placed in a screw-capped tube, degassed with argon and then heated at 100 °C for 2 h under stirring. The resulting mixture was cooled, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography (hexane/EtOAc, from 2:1 to 1:2) to give compound **5zd** (71 mg, 69%) as a colorless solid. M.p. 114–116 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.83–2.97 (m, 2H), 3.12–3.26 (m, 2H), 3.62 (s, 3H), 3.74 (s, 3H), 3.79 (t, 4H, *J* 4.7 Hz), 7.22–7.28 (m, 1H), 7.43–7.61 (m, 5H), 7.69–7.81 (m, 2H), 7.81–7.89 (m, 2H), 8.01–8.12 (m, 2H), 8.67–8.70 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 49.5, 52.9 (2C), 67.2, 68.4, 73.3, 97.0, 120.2, 122.5, 126.4, 127.7, 128.1, 128.4, 128.7, 129.0, 130.8, 131.8, 131.9, 136.8, 139.5, 149.8, 156.1, 164.5, 168.3, 172.5. HRMS–ESI: [M+H]⁺ calcd for C₂₉H₂₈N₃O₆⁺ [M+H]⁺ 514.1973; found 514.1969.

Dimethyl *rac-*(1*R*,4*R*,5*S*)-4-(morpholin-4-yl)-5-phenyl-2-(4-(pyridin-2-yl)phenyl)-6-oxa-3azabicyclo[3.1.0]hex-2-ene-1,4-dicarboxylate (5ze)



The mixture of epoxypyrroline **5q** (103 mg, 0.2 mmol), 2-(tributylstannyl)pyridine (110 mg, 0.3 mmol), CuI (11 mg, 30 mol %) and Pd(PPh₃)₄ (23 mg, 10 mol %) in anhydrous 1,4-dioxane (2 mL) was placed in a screw-capped tube, degassed with argon and then heated at 100 °C for 2 h under stirring. The resulting mixture was cooled, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography (hexane/EtOAc, from 2:1 to 1:2) to give compound **5ze** (90 mg, 88%) as a colorless solid. M.p. 175–177 °C (Et₂O/hexane). ¹H NMR (400 MHz, CDCl₃) δ 2.81–2.95 (m, 2H), 3.11–3.24 (m, 2H), 3.62 (s, 3H), 3.70 (s, 3H), 3.78 (t, 4H, *J* 4.7 Hz), 7.25–7.34 (m, 1H), 7.37–7.45 (m, 5H), 7.76–7.85 (m, 2H), 7.90–7.94 (m, 2H), 8.12–8.15 (m, 2H), 8.73–8.76 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 49.5, 52.7, 52.9, 67.2, 68.1, 73.3, 97.1, 120.8, 122.8, 127.1, 127.9, 128.5, 129.5, 130.2, 132.0, 136.9, 142.5, 149.9, 156.1, 164.5, 168.2, 172.1. HRMS–ESI: [M+H]⁺ calcd for C₂₉H₂₈N₃O₆⁺ [M+H]⁺ 514.1973; found 514.1965.

7. Synthesis of pyrrole 11

Dimethyl 3,5-diphenyl-1*H*-pyrrole-2,4-dicarboxylate (11)



To a solution of epoxypyrroline **5j** (218 mg, 0.5 mmol) in CH₂Cl₂/MeOH mixture (3/3 mL) Pd/C (80 mg, 10 wt %) was added, and the resulting suspension was stirred overnight under an atmosphere of hydrogen. After the completion of the reaction (control by TLC) the reaction mixture was filtered and evaporated to give after recrystallization from hexane/EtOAc mixture (1:1) compound **11** (152 mg, 91%) as a colorless solid. M.p: 123–124 °C (EtOAc–hexane) (lit.,¹¹ 124–125 °C). ¹H NMR (400 MHz, CDCl₃) δ 3.51 (s, 3H), 3.64 (s, 3H), 7.32–7.52 (m, 8H), 7.56–7.67 (m, 2H), 9.55 (br. s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 51.0, 51.5, 114.6, 119.3, 127.16, 127.19, 128.4, 128.8, 129.0, 129.9, 131.1, 133.5, 134.0, 139.0, 161.4, 165.0. HRMS–ESI: [M+H]⁺ calcd for C₂₀H₁₈NO₄⁺ [M+H]⁺: 336.1230; found 336.1231.

8. Synthesis of oxazatrienes 12a-c

General procedure

The solution of epoxypyrroline 5j,k,n (0.4 mmol) in anhydrous toluene (10 mL) was stirred and irradiated by UV lamp for 4 h. The resulting mixture was evaporated under reduced pressure and the residue was purified by column chromatography (hexane/EtOAc, 1:1) to give oxazatriene **12a–c**.

Methyl 2-benzoyl-3-[(2-methoxy-1-morpholino-2-oxoethylidene)amino]-3-phenylacrylate (12a)



Compound **12a** (unseparated mixture of C=C isomers 1:1) (164 mg, 94%) was obtained as a yellow oil according to the general procedure from epoxypyrroline **5j** (174 mg, 0.4 mmol). ¹H NMR (400 MHz, CDCl₃) δ 3.00–3.12 (m, 2H), 3.31–3.40 (m, 2H), 3.48–3.65 and 3.77–3.85 (2m, 10H), 7.09–7.21 and 7.26–7.54 (2m, 8H), 7.78–7.86 (m, 1H), 7.91–7.99 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 45.6, 46.2, 51.3, 51.6, 52.5, 52.7, 65.8, 66.4, 115.0, 117.6, 127.75, 127.8, 128.0, 128.1, 128.5, 128.8, 128.9, 129.0, 129.3, 129.6, 131.9, 132.4, 137.2, 137.8, 138.2, 138.6, 149.3, 150.3, 161.2, 161.27, 161.28, 162.3, 165.7, 167.3, 194.3, 194.5. HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₅N₂O₆⁺ [M+H]⁺ 437.1707; found 437.1719.

Methyl 2-(4-chlorobenzoyl)-3-[(2-methoxy-1-morpholino-2-oxoethylidene)amino]-3-phenylacrylate (12b)



Compound **12b** (unseparated mixture of C=C isomers 1:0.9) (181 mg, 96%) was obtained as a yellow oil according to the general procedure from epoxypyrroline **5k** (188 mg, 0.4 mmol). ¹H NMR (400 MHz, CDCl₃) δ 3.07–3.19 (m, 2H), 3.38–3.49 (m, 2H), 3.50–3.69 and 3.76–3.87 (2m, 10H), 7.11–7.49 (m, 7H), 7.74–7.78 (m, 1H), 7.88–7.92 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 45.7, 46.3, 51.5, 51.7, 52.7, 52.8, 66.0, 66.5, 114.6, 117.3, 127.9, 128.0, 128.4, 128.5,

128.53, 128.9, 129.6, 129.8, 130.4, 130.6, 136.7, 137.1, 137.14, 137.7, 138.3, 138.8, 149.3, 150.6, 161.25, 161.29, 161.7, 162.8, 165.6, 167.1, 193.2, 193.4. HRMS–ESI: $[M+H]^+$ calcd for $C_{24}H_{24}^{35}ClN_2O_6^+[M+H]^+ 471.1317$; found 471.1321.

Methyl 3-[(2-methoxy-1-morpholino-2-oxoethylidene)amino]-2-(4-nitrobenzoyl)-3-phenylacrylate (12c)



Compound **12c** (unseparated mixture of isomers 1:1) (179 mg, 93%) was obtained as a yellow oil according to the general procedure from epoxypyrroline **5n** (192 mg, 0.4 mmol). ¹H NMR (400 MHz, CDCl₃) δ 2.80–4.10 (m, 14H), 6.90–7.63 (m, 5H), 7.74–8.50 (m, 4H). ¹³C NMR (100 MHz, CDCl₃) δ 45.8, 46.4, 51.6, 52.8, 66.1, 66.4, 114.1, 117.0, 123.3, 128.1, 128.8, 129.7, 130.0, 137.0, 137.5, 143.3, 149.5, 150.9, 161.1, 163.3, 164.2, 165.5, 167.0, 193.1 (other signals are overlapped). HRMS–ESI: [M+H]⁺ calcd for C₂₄H₂₄N₃O₈⁺ [M+H]⁺ 482.1558; found 482.1563.

9. Synthesis of compound 13

Methyl (Z)-3-(2-methoxy-2-oxoacetamido)-2-(4-nitrobenzoyl)-3-phenylacrylate (13)



To a solution of oxazatriene **12c** (192 mg, 0.4 mmol) in CH₂Cl₂ (3 mL) a saturated solution of HCl in Et₂O (1 mL) was added, and the resulting emulsion was stirred overnight. The reaction mixture was washed with 10% solution of Na₂CO₃ (10 mL) and the aqueous layer was extracted with CH₂Cl₂ (2×5 mL). The combined organic layers were dried over Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography (hexane/EtOAc, from 8:1 to 2:1) to give **13** (67 mg, 41%) as a colorless solid. M.p. 177–178 °C (EtOAc–hexane). ¹H NMR (400 MHz, CDCl₃) δ 3.80 (s, 3H), 3.98 (s, 3H), 7.11–7.28 (m, 5H), 7.80–7.87 (m, 2H), 8.12–8.20 (m, 2H), 12.55 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 52.8, 54.2, 113.9, 123.6, 128.2,

 $128.3, 129.7, 130.2, 131.6, 141.8, 150.1, 152.3, 153.8, 160.2, 166.3, 190.7. \ HRMS-ESI: \ [M+H]^+ \ calcd \ for \ C_{20}H_{17}N_2O_8^+ \ [M+H]^+: 413.0979; \ found \ 413.0971.$

10. ¹H and ¹³C NMR spectra

¹H and ¹³C NMR spectra of compound **4a**



¹H and ¹³C NMR spectra of compound **5a**





1 H and 13 C NMR spectra of compound **5b**



1 H and 13 C NMR spectra of compound **5**c

100 90

80

70

60 50 40 30 20

10

0

130 120 110 f1 (мд)

230 220 210 200

190 180

170 160

150 140

¹H and ¹³C NMR spectra of compound **5d**



¹H and ¹³C NMR spectra of compound **5e**







¹H and ¹³C NMR spectra of compound **5g**



¹H and ¹³C NMR spectra of compound **5h**





¹H and ¹³C NMR spectra of compound **5**i

3.783 3.771 3.771 3.356 3.359 0 Ρh MeO₂C ,∖CO₂Me Ph 'N N Ó 2.00[.] 3.14_. 5.004 2.02 2.01 4.094 3.014 3.007 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 f1 (мд) 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 131.77 131.67 131.67 130.15 129.41 128.47 127.99 127.82 ~ 172.43 -- 168.16 -- 164.46 -77.32 -77.00 76.68 -73.18 -68.02 -68.02 - 96.98 -52.77 -52.66 -49.40 1 1 0 110 100 f1 (мд) 210 70 50 40 30 20 10 200 190 180 170 160 . 150 140 130 . 120 90 80 60

¹H and ¹³C NMR spectra of compound **5**j


1 H and 13 C NMR spectra of compound **5**k



¹H and ¹³C NMR spectra of compound **5**l



¹H and ¹³C NMR spectra of compound **5m**



 1 H and 13 C NMR spectra of compound **5n**

¹H and ¹³C NMR spectra of compound **50**



¹H and ¹³C NMR spectra of compound **5p**





1 H and 13 C NMR spectra of compound **5**q









1 H and 13 C NMR spectra of compound **5**s





¹H and ¹³C NMR spectra of compound **5**t

150 140

110 100 f1 (мд)







 1 H and 13 C NMR spectra of compound **5v**





¹H and ¹³C NMR spectra of compound 5x





1 H and 13 C NMR spectra of compound **5**y

¹H and ¹³C NMR spectra of compound **5**z





¹H and ¹³C NMR spectra of compound **5za**

¹H and ¹³C NMR spectra of compound **5zb**



¹H and ¹³C NMR spectra of compound **5zd**





¹H and ¹³C NMR spectra of compound **5ze**

¹H and ¹³C NMR spectra of compound **6a**



¹H and ¹³C NMR spectra of compound **6b**



¹H and ¹³C NMR spectra of compound **6c**









¹H and ¹³C NMR spectra of compound **11**

110 100 f1 (мд) 170 160



¹H and ¹³C NMR spectra of compound **12a**

60 50

30

20 10 0 -10

40

170 160 150 140 130 120 110 100 90 80 70 f1 (мд)

210 200 190 180



¹H and ¹³C NMR spectra of compound **12b**

 ^1H and ^{13}C NMR spectra of compound 12c





¹H and ¹³C NMR spectra of compound **13**



11. X-ray data of compounds 5c,6b,13

Single crystals of compounds **5c**, **6b** and **13** were grown by slow evaporation of their solutions in CH₂Cl₂–hexane mixture at room temperature. For single crystal X-ray diffraction experiment suitable crystals were fixed on a micro mount and placed on a diffractometer and measured at a temperature of 100K using monochromated MoKα radiation. The structures have been solved by the direct methods by means of the SHELX program¹² incorporated in the OLEX2 program package.¹³ Empirical absorption correction was applied in CrysAlisPro program complex¹⁴ using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The crystallographic data and some parameters of refinement are placed in Tables S1–S3.

Figure S1. X-ray crystal ctructure of compound 5c with 50% ellipsoid probability (CCDC 1936159)



Т	able	e S1	. (Crystal	data	and	structure	refinement	for	compound	. 5	c
				~						1		

90.00
121.849(3)
90.00
4565.24(17)
8
1.305
0.091
1904.0
$0.59 \times 0.39 \times 0.23$
Mo K α ($\lambda = 0.7107$)
5.28 to 61
$-46 \le h \le 46, -11 \le k \le 11, -27 \le l \le 27$
60028
6943 [$R_{int} = 0.0497$, $R_{sigma} = 0.0251$]
6943/0/410
1.043
$R_1 = 0.0409, wR_2 = 0.1000$
$R_1 = 0.0520, wR_2 = 0.1080$
0.48/-0.21

Figure S2. X-ray crystal ctructure of compound **6b** with 50% ellipsoid probability (CCDC 1936158)



Table S2. Crystal data and structure refinement for compound 6b

Identification code	dax43
Empirical formula	$C_{21}H_{27}ClN_2O_5$
Formula weight	422.90
Temperature/K	120

Crystal system	monoclinic			
Space group	$P2_1/c$			
a/Å	8.9966(3)			
b/Å	10.4109(3)			
c/Å	22.3370(7)			
α/°	90.00			
β/°	92.301(10)			
γ/°	90.00			
Volume/Å ³	2090.46(11)			
Z	4			
$\rho_{calc}g/cm^3$	1.344			
μ/mm^{-1}	0.218			
F(000)	896.0			
Crystal size/mm ³	0.44 imes 0.4 imes 0.08			
Radiation	MoKa ($\lambda = 0.71073$)			
2Θ range for data collection/°	3.64 to 60			
Index ranges	$-12 \le h \le 12, -14 \le k \le 14, -31 \le l \le 31$			
Reflections collected	36120			
Independent reflections	$6112 [R_{int} = 0.0314, R_{sigma} = 0.0210]$			
Data/restraints/parameters	6112/0/370			
Goodness-of-fit on F ²	0.997			
Final R indexes $[I \ge 2\sigma(I)]$	$R_1 = 0.0340, wR_2 = 0.0878$			
Final R indexes [all data]	$R_1 = 0.0465, wR_2 = 0.0960$			
Largest diff. peak/hole / e Å ⁻³	0.40/-0.21			

Figure S3. X-ray crystal ctructure of compound **13** with 50% ellipsoid probability (CCDC 1936916)



Table 55. Crystal data and structur	te termement for compound 15				
Identification code	smi12				
Empirical formula	$C_{20}H_{16}N_2O_8$				
Formula weight	412.35				
Temperature/K	100(2)				
Crystal system	monoclinic				
Space group	P2 ₁ /n				
a/Å	11.9680(4)				
b/Å	11.1729(4)				
c/Å	13.8802(4)				
α/°	90				
β/°	92.759(3)				
$\gamma/^{\circ}$	90				
Volume/Å ³	1853.86(10)				
Z	4				
$\rho_{calc}g/cm^3$	1.477				
μ/mm^{-1}	0.116				
F(000)	856.0				
Crystal size/mm ³	0.30 imes 0.22 imes 0.12				
Radiation	MoKa ($\lambda = 0.71073$)				
2 Θ range for data collection/°	6.818 to 54.988				
Index ranges	$\text{-15} \le h \le 14, \text{-12} \le k \le 14, \text{-18} \le l \le 18$				
Reflections collected	12802				
Independent reflections	4254 [$R_{int} = 0.0379$, $R_{sigma} = 0.0396$]				
Data/restraints/parameters	4254/0/273				
Goodness-of-fit on F^2	1.041				
Final R indexes $[I \ge 2\sigma(I)]$	$R_1 = 0.0393, wR_2 = 0.0844$				
Final R indexes [all data]	$R_1 = 0.0550, wR_2 = 0.0952$				
Largest diff. peak/hole / e Å ⁻³	0.31/-0.25				

 Table S3. Crystal data and structure refinement for compound 13

12. Calculation details

All calculations were performed by using the Gaussian 09 suite of quantum chemical programs.¹⁵ Geometry optimizations of dimethylamine, compounds 3zb,6e,7a,8a and transition states TS1–TS3 were performed at the DFT B3LYP/6-31+G(d,p) level using PCM model for CH₂Cl₂. Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate. Single point calculations of energies for stationary points were carried out at the DFT wB97XD/cc-pVTZ level using PCM solvation model for toluene. Thermal corrections to Gibbs free energies obtained in the optimization calculations were used.

Table S4. Energies (au) and cartesian coordinates of stationary points for dimethylamine, compounds **3zb,6e,7a,8a** and transition states TS1–TS3 calculated at wB97XD/cc-pVTZ level (PCM, CH₂Cl₂).

Me ₂ NH	Oxazatriene 3zb				
Zero-point correction = 0.092285					
Thermal correction to Energy $= 0.096680$	CO ₂ Me O				
Thermal correction to Enthalpy $= 0.097624$	CI—(\Ph				
Thermal correction to Gibbs Free Energy $= 0.066822$	Ph CO ₂ Me				
$E_0 = -135.0810186, E = -135.0766236,$	-				
H = -135.0756796, G = -135.1064816.	Zero-point correction $= 0.320660$				
Imaginary frequency $= 0$.	Thermal correction to Energy $= 0.346556$				
	Thermal correction to Enthalpy = 0.347500				
	Thermal correction to Gibbs Free Energy = 0.259104 E ₀ = -1662.8389561 , E = -1662.5182961 , H = -1662.5182961 , G = -1662.5798521 .				
	Imaginary frequency $= 0$.				
N -0.00008700 0.56771200 -0.15253900					
C 1.21785300 -0.22417600 0.02025700					
C -1.21781600 -0.22418700 0.02026800					
H -0.00000700 1.32945100 0.52109400	<u>ه</u>				
H 1.26304000 -0.76106100 0.98495600					
H $1.28342100 -0.97097600 -0.77921200$	C -1.62065859 -1.51927360 -1.17317372				
H = 2.09500200 = 0.42564600 = 0.05389700	C 1.56017641 0.09979440 -0.27976772				
H = -1.20301400 - 0.70120000 - 0.98489900	C 0.35331941 0.10810340 0.35256728				
$H = \frac{-2.09307200}{0.42342000} + \frac{0.03401000}{0.77020500}$	N -0.23167159 -1.06381260 0.84497628				
-1.20270000 -0.7/103000 -0.7/920300	C -1.11942759 -1.75773260 0.25925028				

С	2 29730041	-1 14937760	-0 58349772
Cl	2 36558841	1 61671040	-0.66510072
0	-0.85103959	-1 76578560	-2 09262372
C C	2 08055250	0.08847060	1 36744072
C	-2.98933239	-0.98847900	-1.30744072
C	-0.40052139	1.55588040	0.75457528
C	-1.00040259	-2.99920300	0.92773228
C	-0.79662359	2.27338240	-0.2330/3/2
С	-1.54942159	3.38843440	0.13863128
С	-1.91418859	3.57958540	1.47514628
С	-1.53109159	2.64429640	2.44121328
С	-0.78988259	1.51965040	2.07382528
С	-3.50906859	-0.91523260	-2.67289272
С	-4.79304159	-0.42211260	-2.88569672
С	-5.56785259	0.00706940	-1.79964772
С	-5.05617559	-0.05740060	-0.50001672
С	-3.77150059	-0.55574460	-0.28254772
0	-2.32529759	-3.80887560	0.29724528
0	-1.34680159	-3.09911260	2.21315028
Ċ	-1 80864859	-4 29023860	2 89922428
0	1 93179741	-2 25445060	-0.21065772
Õ	3 41646241	-0.94242760	-1 29650072
Č	A 19168541	-2 11908060	-1 61550772
ч	0.52004759	2 12876040	1 27177072
П Ц	1 85136150	2.12870040 4 10650440	0.61768672
	-1.85150159	4.10030440	1 76120028
п	-2.49520159	4.43119940	2 49097429
п	-1.809/3039	2.78710340	3.46067426
H	-0.49448/59	0.79310340	2.82370928
H	-2.89/45159	-1.25298660	-3.50267472
H	-5.19421059	-0.37209860	-3.89312972
Н	-6.56955859	0.39099240	-1.96798572
Н	-5.65463359	0.27949040	0.34031928
Н	-3.38035259	-0.59173260	0.72997928
Н	-1.45700459	-4.18188260	3.92317528
Н	-1.37770459	-5.17749860	2.43221728
Н	-2.89838459	-4.34154760	2.86488528
Н	5.03740441	-1.75413260	-2.19596072
Н	4.53417941	-2.60559360	-0.69987872
Н	3.59283141	-2.81796160	-2.20284972

Chlorobydrin 60	Dataina 7a			
Chioronyarin de	Betaine /a			
MeO ₂ C - (""Ph	MeO,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			
Ph NMe ₂				
ČO ₂ Me				
Zero-point correction $= 0.418346$	Ph [′]			
Thermal correction to Energy $= 0.447078$	Zero-point correction = 0.417567			
Thermal correction to Enthalpy $= 0.448022$	Thermal correction to Energy $= 0.447190$			
Thermal correction to Enthalpy $= 0.446022$	Thermal correction to Enthalpy = 0.448134			
Thermal correction to Gibbs Free Energy = 0.358145	Thermal correction to Enthalpy = 0.448154 Thermal correction to Cibbs Free Energy = 0.256142			
$E_0 = -1797.6268591, E = -1797.5981271,$	The that contends to Orbos Free Energy = 0.550145			
H = -1797.5971831, G = -1797.6870601.	$E_0 = -1797.6046046, E = -1797.5749816,$			
Imaginary frequency $= 0$	H = -1797.5740376, G = -1797.6660286.			
inaginary nequency of	Imaginary frequency $= 0$.			
C 1 29559625 1 10545968 0 70210801				
C = 0.24033075 + 1.36734068 + 0.26108001	C -1.48801404 0.91555469 0.52815023			
C = -0.24055975 - 1.50754000 - 0.20190001	C 1.39914196 1.40083369 0.20792323			
C = -0.83390475 - 0.04228832 - 0.24474701	C 1.23374496 0.04183169 -0.24906777			
N -0.08300475 -0.94882432 0.75175801	N 0.16413096 -0.55433331 -0.73286077			
C 1.18743625 -0.43940932 1.22892101	C -1.15764404 -0.01656631 -0.70603177			
C -0.91640475 2.22759068 1.35009701	C = 1.01702696 - 2.57664569 - 0.47884377			
Cl -0.44146975 2.16816168 -1.36254999	$C_1 = 2.43705396 + 1.61031060 + 1.65320023$			
O 1.61147225 1.93415768 1.78712401	CI = 2.45703590 1.01051009 1.03529923			
C 2.28597725 1.32634068 -0.43262699	0 -1.88846904 2.05503369 0.33879523			
C -2.17229175 -0.38872332 -0.28780599	C -1.34874004 0.35588469 1.90501923			
$C \qquad 2 34171025 -1 34957232 -0.22174701$	C 2.43170196 -0.86744831 -0.20560577			
N 1 10156325 0 40506332 2 72512201	C -2.22495404 -1.15518731 -0.70129677			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N -1.41104104 0.79234269 -2.01684277			
C 2.48314423 -0.38720332 3.41419001	C -2.81628804 1.24261769 -2.29110277			
C 0.14108225 -1.19194/32 3.3955/901	C -0.86612204 0.10212369 -3.23360477			
C -2.43664275 -1.72845632 -0.63076699	C 2.29627096 -2.21345731 0.16752223			
C -3.69176475 -2.10587432 -1.10372999	$C \qquad 3 39748296 -3 07223131 - 0 14930223$			
C -4.70833975 -1.15285632 -1.23572999	$C = \frac{3.57740270}{5.07223131} = 0.14750225$			
C -4.45751775 0.17936668 -0.89617499	C = 4.04737270 - 2.00047231 - 0.20440977			
C -3.19775975 0.56162768 -0.43147199	C 4.79029796 -1.20344331 -0.05201177			
C 3 25974425 2 32607968 -0 32719099	C 3.69272396 -0.40182531 -0.61363577			
$C \qquad \qquad 4.17071325 2.52607768 1.35007100$	C -1.63211704 1.21788269 2.98089723			
$C = \frac{4.17971525}{4.12950025} \frac{2.55002700}{1.74977776} -1.559971799$	C -1.54896804 0.76278569 4.29447223			
C 4.13859025 1.74877708 -2.51275599	C -1.18471104 -0.56367431 4.55441223			
C 3.105//425 0./498/668 -2.62/39799	C -0.90348604 -1.42926031 3.49339723			
C 2.24644825 0.54498368 -1.59846999	C -0.98379804 -0.97442231 2.17674923			
O 3.51885325 -1.06756632 0.83524901	0 -3 35077104 -0 95979331 -0 27866377			
O 1.90437925 -2.50235032 0.20348901	$\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $			
C 2.92526225 -3.42850432 -0.24307299	$\begin{array}{c} 0 & -1.79240304 & -2.30197531 & -1.21303777 \\ 0 & 2.75019104 & 2.20050021 & 1.247720777 \\ \end{array}$			
O -1.40653475 1.71715368 2.34088001	$\begin{array}{c} C & -2.75918104 & -3.39059931 & -1.24/63077 \\ 0.00000000000000000000000000000000$			
0 -0.87832875 3 53162868 1 10871501	0 0.38836996 2.62475069 -1.57136777			
C = -1.42864275 = 4.39250368 = 2.13758701	O 1.42046796 3.73872769 0.09787523			
$ \begin{array}{c} \bullet & \bullet \\ \bullet & \bullet $	C 1.09301896 4.95313669 -0.60128977			
п 1.34230123 1.38990608 2.3/1/0301	Н -0.77941804 1.63974069 -1.86096177			
Н 2.34354025 -0.28157432 4.45418301	Н -2.75977004 2.00819569 -3.06592877			
--	---			
Н 2.83280425 -1.63039632 3.40474201	Н -3.40471904 0.40001269 -2.65393377			
Н 3.25443625 0.03954068 2.96690001	Н -3.25695204 1.66028769 -1.39318377			
Н 0.18388825 -0.94830132 4.46012701	Н -0.99453404 0.78401169 -4.07451577			
Н -0.84383075 -0.92151632 3.02216901	Н 0.18667496 -0.11696631 -3.08449577			
Н 0.28640325 -2.27561632 3.28013001	Н -1.41791204 -0.82034531 -3.41478077			
Н -1.64622775 -2.46310232 -0.52464799	Н 1.32339096 -2.58179431 0.47326323			
H $-3.87720475 -3.14181132 -1.37103699$	H $3.27936596 -4.10808531 -0.45412223$			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H = 5.50357706 - 3.26883131 - 0.28608577			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H $5.55552770^{\circ} -5.20005151^{\circ} -0.20000577$ H $5.75566196^{\circ} -0.89222231^{\circ} -0.98367877$			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$			
H = -5.05015575 - 1.00177808 - 0.17891499	H = 5.80007890 = 0.05558209 = 0.91200077			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H = -1.91353104 - 2.24314809 - 2.70998323			
H = 4.92900825 - 5.51584808 - 1.25828299	H = -1.70773804 + 1.43890009 + 5.11518723			
H 4.8540/525 1.91012968 -3.313/4999	H -1.12088/04 -0.92018531 5.5/814123			
H 3.1193/525 0.13118168 -3.518/9699	H -0.62015504 -2.458/3931 3.68890/23			
H 1.493/8825 -0.22901932 -1./1945299	H $-0.74811804 -1.66100131 1.37215823$			
H 2.37982625 -4.28709932 -0.63057899	H -2.22140/04 -4.22834231 -1.68663277			
Н 3.56105325 -3.72025132 0.59480801	Н -3.61671904 -3.11310831 -1.86268877			
Н 3.53146025 -2.96894532 -1.02588599	Н -3.08649404 -3.62619331 -0.23367377			
Н -1.30524875 5.40404068 1.75606501	H 1.49532696 5.75429869 0.01854423			
Н -2.48397075 4.16200268 2.29231501	Н 1.55807096 4.97086269 -1.58984877			
Н -0.87495975 4.25753168 3.06829401	Н 0.01116696 5.06153369 -0.70554977			
Zwitterion 8a	TS1			
CI_O	H, / Me			
MeO ₂ C -7 - (Ph	MeO 6 ⁺ NO			
Ph NHMe ₂	CI 8 Ph			
N ≂ ČO₂Me	Ph CO ₂ Me			
Zero-point correction $= 0.419218$	Zero-point correction = 0.415736			
Thermal correction to Energy $= 0.448002$	Thermal correction to Energy = 0.445695			
	The section to Each 1 = 0.446620			
Thermal correction to Enthalpy $= 0.448946$	I hermal correction to Enthalny – $II / I/I = 10$			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024	Thermal correction to Enthalpy = 0.446639 Thermal correction to Cibbs Erect Energy = 0.252807			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$,	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$,			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, H = -1797.5741833, $G = -1797.6631053$.	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, H = -1797.5593799, $G = -1797.6532119$.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, H = -1797.5741833 , G = -1797.6631053 . Imaginary frequency = 0 .	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, H = -1797.5593799, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, H = -1797.5741833 , G = -1797.6631053 . Imaginary frequency = 0 .	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, H = -1797.5593799, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, H = -1797.5741833, $G = -1797.6631053$. Imaginary frequency = 0 .	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, H = -1797.5593799, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, $H = -1797.5741833$, $G = -1797.6631053$. Imaginary frequency = 0 .	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, H = -1797.5593799, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, $H = -1797.5741833$, $G = -1797.6631053$. Imaginary frequency = 0 .	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, $H = -1797.5593799$, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, $H = -1797.5741833$, $G = -1797.6631053$. Imaginary frequency = 0 .	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, $H = -1797.5593799$, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, H = -1797.5741833, $G = -1797.6631053$. Imaginary frequency = 0 .	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, $H = -1797.5593799$, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113, E = -1797.5751273,$ H = -1797.5741833, G = -1797.6631053. Imaginary frequency = $0.$	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.663239$, $H = -1797.5593799$, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113, E = -1797.5751273,$ H = -1797.5741833, G = -1797.6631053. Imaginary frequency = $0.$	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 E ₀ = -1797.5902829, E = -1797.6503239, H = -1797.5593799, G = -1797.6532119. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, H = -1797.5741833, $G = -1797.6631053$. Imaginary frequency = 0 . C 1.18993494 0.60307697 0.15225807 C -0.43388706 0.50059297 -0.25275593 C -0.87936806 -0.82102103 0.35582507	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, $H = -1797.5593799$, $G = -1797.6532119$. Imaginary frequency = 1.			
Thermal correction to Enthalpy = 0.448946 Thermal correction to Gibbs Free Energy = 0.360024 $E_0 = -1797.6039113$, $E = -1797.5751273$, H = -1797.5741833, $G = -1797.6631053$. Imaginary frequency = 0 . C 1.18993494 0.60307697 0.15225807 C -0.43388706 0.50059297 -0.25275593 C -0.87936806 -0.82102103 0.35582507 N -0.06084506 -1.33608503 1.20669807	Thermal correction to Enthalpy = 0.446639 Thermal correction to Gibbs Free Energy = 0.352807 $E_0 = -1797.5902829$, $E = -1797.5603239$, $H = -1797.5593799$, $G = -1797.6532119$. Imaginary frequency = 1.			
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H -2.65604012 -3.94602924 0.34776631 H -0.17554212 5.99129376 -0.92039569 H -0.29919212 5.09473076 -2.46806069 H -1.54619712 4.87253776 -1.20943469			н	-3.75685812 -3.44287024 -0.96561069
H -0.17554212 5.99129376 -0.92039569 H -0.29919212 5.09473076 -2.46806069 H -1.54619712 4.87253776 -1.20943469			Н	-2 65604012 -3 94602924 0 34776631
Н -0.29919212 5.09473076 -2.46806069 Н -1.54619712 4.87253776 -1.20943469			н	-0 17554212 5 99129376 -0 92039569
Н -1.54619712 4.87253776 -1.20943469			н	-0.29919212 5.09473076 -2.46806069
			н	-1 54619712 4 87253776 -1 20943469

TS2	TS3		
MeO、 O	0 8-2H		
H×NMe ₂	MeO		
CI	CI / Me		
Ph´ ^N CO ₂ Me	Ph Ph CO.Mo		
Zero-point correction $= 0.418406$			
Thermal correction to Energy $= 0.446018$	Zero-point correction $= 0.419212$		
Thermal contection to Energy $= 0.4470718$	Thermal correction to Energy $= 0.447174$		
Thermal correction to Enthalpy = 0.447862	Thermal correction to Enthalpy = 0.448118		
Thermal correction to Gibbs Free Energy $= 0.359460$	Thermal correction to Gibbs Free Energy $= 0.361469$		
$E_0 = -1797.5967545, E = -1797.5682425,$	E = 1707.6027076 $E = 1707.5757656$		
H = -17975672985G = -17976557005	$E_0 = -1797.6037276, E = -1797.5757656,$		
II = 1171.5012905, G = 1171.0551005.	H = -1797.5748216, G = -1797.6614706.		
Imaginary inequency = 1.	Imaginary frequency $= 1$.		
C 1 18242686 0 72645067 0 00002480			
C 1.18342686 -0.72645067 0.00002480	C 1.20201565 0.82726179 0.39590971		
C -0.83102814 -0.78065267 0.41928880	C -0.40399735 0.82115779 -0.07558629		
C -1.15824314 0.55551633 -0.15857920	C -0.90636735 -0.55795621 0.32635671		
N -0.29981614 1.12886633 -0.93781220	N -0.12669235 -1.22169821 1.10648371		
C 0.93014386 0.40729033 -1.13673220	C 1.10175565 -0.51863621 1.39784871		
C -1.23261014 -1.95155367 -0.36782620	C = -1.06693035 + 1.89477879 + 0.79263871		
Cl -1.19039314 -0.90768667 2.17528380	C1 = -0.66417235 + 1.4989079 + 1.84271529		
Q 1.57647586 -1.85486667 -0.40281120	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		
C 1 77738986 -0 18495667 1 29783080	$C = \frac{1.47570005}{2.12002765} = 0.51220070 = 0.70000020$		
C = -2.42500414 + 1.27648233 + 0.13242480	C 2.12992703 0.31330979 -0.79990029		
C = 2.42300414 + 1.27040233 + 0.13242400 $C = 2.14120696 + 1.26407922 + 1.22052720$	C -2.20162835 -1.140/9221 -0.090/0/29		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C 2.31223065 -1.45960521 1.32790871		
N 0.80104080 -0.32311/07 -2.30731020	N 0.98359965 0.06478179 2.82865871		
C 2.02913486 -0.98902067 -3.07647220	C 2.25140365 0.55212379 3.48454771		
C 0.18009286 0.54167733 -3.56782320	C 0.22344265 -0.81199421 3.78058971		
C -2.46158914 2.68112633 0.07021480	C -2.35934935 -2.53942021 -0.07454029		
C -3.65322314 3.36857833 0.29684980	C -3.57757735 -3.11831221 -0.42478329		
C -4.82851314 2.66212633 0.57741480	C = -4.66122335 -2.30936521 -0.78589129		
C -4.80315614 1.26532733 0.63627880	$C = \frac{4516122555}{451615025} = \frac{2.50750521}{0.1010021} = 0.70505127$		
C = -3.60800314 + 0.57655233 + 0.42382080	C -4.31013933 -0.91919921 -0.80003029		
C = -3.00000314 + 0.37035253 + 0.42302000	C -3.29294935 -0.33748521 -0.46390729		
C = 2.04293280 -1.03383007 -2.00124280	C 3.14790965 1.43055079 -1.08302129		
C 5.24903186 -0.6224006/ 3.18914980	C 4.03949665 1.21348179 -2.13800729		
C 3.00151386 0.65723233 3.69561280	C 3.92578065 0.06712479 -2.92941229		
C 2.13912286 1.51344433 3.00475980	C 2.90996265 -0.85545221 -2.65774629		
C 1.52908286 1.09519133 1.81942080	C 2.01900265 -0.63133821 -1.60502429		
O 3.27566886 0.96613333 -1.41794220	O 3.44491965 -1.12697421 1.62540671		
O 1.81894786 2.64664933 -1.05015420	$0 \qquad 1.99439165 -2.67160621 0.85964071$		
C 2.92208786 3.58601133 -1.03857920	C = 3.09802465 -3.58682521 - 0.65204271		
0 -1.23386014 -1.95482867 -1.60850020	$\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $		
0 -1 50620614 -3 04978167 0 33933380			
-1.J0020014 -J.047/010/ 0.JJ7JJJ00	O -1.31532735 3.03928579 0.17885771		

С	-1.78338114 -4.25447667 -0.41123320	С	-1.85302335 4.10960379 0.99556871
Н	0.11003186 -1.07219767 -2.28319920	Н	0.43417465 0.92362879 2.65170471
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Н	-0.92878114 -4.51322267 -1.03835420	Η	-1.14853435 4.35602779 1.79140771

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