**Synthesis and spectroscopic studies of methoxy-substituted phenylthienylnicotinamidines**

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**Supplementary Material**

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**3. Experimental**

**3.1. Chemistry**

Melting points were measured in degree centigrade on Gallenkamp apparatus and are uncorrected. The infrared spectra (KBr) were explored on Thermo Scientific Nicolet iS10 FTIR spectrometer. 1H-NMR spectra were measured in DMSO-*d*6 as a solvent using 500 MHz and 13C-NMR on 125 MHz JEOL’s spectrometer. Perkin-Elmer 2400 analyzer has been used to determine the elemental analyses. A Schimadzu Qp-2010 Plus (GC-MS) spectrometer was used for recording Mass spectra.

**3.1.1. *General methodology for preparation of thienylnicotinonitrile derivatives (3a-e)****.*

To a stirred solution of 6-(5-bromothiophen-2-yl)nicotinonitrile (1.052 g, 3.98 mmol), and Pd(PPh3)4 (160 mg, 0.14 mmol) in toluene (16 mL), followed by phenylboronic acid derivatives (4.80 mmol) in methanol (4 mL). The stirred reaction mixture was heated at 80 oC for 12 hours, where after the reaction mixture was partitioned between an aqueous solution containing concentrated ammonia (5 ml) and ethyl acetate (300 mL, 3x). The organic layer was dried (anhydrous sodium sulphate), and then evaporated to dryness under reduced pressure. the solid was filtered off and recrystallized from the proper solvent to furnish the desired thienylnicotinonitrile derivatives **3a-e**.

**3.1.1.1. 6-(5-Phenylthiophen-2-yl)nicotinonitrile (3a)**.

Compound **3a** was obtained in 72% yield as yellow solid, mp 160-162 oC (EtOH). Rf = 0.5, petroleum ether-EtOAc (8:2). IR (KBr) ν’ 3060 (CH, stretch), 2226 (CN, stretch), 1586, 1547, 1503 (C=N, C=C, stretch) cm-1.1H-NMR (DMSO-*d*6); δ 7.36-7.47 (m. 3H), 7.65 (d, *J* = 4.0 Hz, 1H), 7.74-7.76 (m, 2H), 8.03 (d, *J* = 4.0 Hz, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 8.32 (dd, *J* = 8.5, 2.5 Hz, 1H), 8.95 (d, *J* = 2.5 Hz, 1H). 13C-NMR (DMSO-*d*6); δ 106.42, 117.31, 118.37, 125.45, 125,55, 128.53, 129.23, 129.57, 133.13, 140.53, 141.73, 147.85, 152.64, 154.50. MS (EI) m/e (rel. int.); 262 (M+, 100). Anal. Calcd. for: C16H10N2S: C, 73.26; H, 3.84; N, 10.68 Found: C, 73.48; H, 3.92; N, 10.49%.

**3.1.1.2. 6-[5-(4-Methoxyphenyl)thiophen-2-yl]nicotinonitrile (3b)**.

Compound **3b** was obtained in 74% yield as a golden-yellow solid, mp 194-195 oC (EtOH). Rf = 0.40, petroleum ether-EtOAc (8:2). IR (KBr) ν’ 3047, 2927 (CH, stretch), 2222 (CN, stretch), 1585, 1545, 1512 (C=C, stretch) cm-1. 1H-NMR (DMSO-*d6*); δ 3.78 (s, 3H), 7.00 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 4.0 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 2H), 7.97 (d, *J* = 4.0 Hz, 1H), 8.10 (d, *J* = 9.0 Hz, 1H), 8.28 (dd, *J* = 9.0, 2.5 Hz, 1H). 8.92 (d, *J* = 2.5 Hz, 1H). MS (EI) m/e (rel. int.); 292 (M+, 100). Anal. Calcd. for: C17H12N2OS: C, 69.84; H, 4.14; N, 9.58 Found: C, 69.71; H, 4.25; N, 9.43%.

**3.1.1.3. 5-[5-(3,4-Dimethoxyphenyl)thiophen-2-yl]nicotinonitrile (3c)**.

Compound **3c** was obtained in 80% yield as a yellow solid, mp 172-173 oC (EtOH/EtOAc). Rf = 0.56, petroleum ether-EtOAc (8:2). IR (KBr) ν’ 3050, 2964 (CH, stretch), 2225 (CN, stretch), 1589, 1544, 1515(C=C, stretch) cm-1.1H-NMR (DMSO-*d*6); δ 3.78 (s, 3H), 3.83 (s, 3H), 7.01 (d, *J* = 9.0 Hz, 1H), 7.27-7.29 (m, 2H), 7.56 (d, *J* = 3.5 Hz, 1H), 7.99 (d, *J* = 3.5 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 8.29 (dd, *J* = 8.5, 2.0 Hz, 1H), 8.92 (s, 1H). MS (EI) m/e (rel. int.); 322 (M+, 100), 307 (M+-CH3, 33). Anal. Calcd. for: C18H14N2O2S: C, 67.06; H, 4.38; N, 8.69 Found: C, 66.83; H, 4.47; N, 8.73%.

**3.1.1.4. 6-[5-(3,5-Dimethoxyphenyl)thiophen-2-yl]nicotinonitrile (3d)**.

Compound **3d** was obtained in 82% yield as a yellow solid, mp 174-175 oC (EtOH/EtOAc). Rf = 0.42, petroleum ether (60-80 oC)-EtOAc (7:3). IR (KBr) ν’ 3058, 2966 (CH, stretch), 2216 (CN, stretch), 1586, 1542 (C=C, stretch) cm-1.1H-NMR (DMSO-*d*6); δ 3.80 (s, 6H), 6.51 (s, 1H), 6.87 (s, 2H), 7.68 (d, *J* = 4.0 Hz, 1H), 8.02 (d, *J* = 4.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.30 (dd, *J* = 8.0, 2.5 Hz, 1H), 8.94 (d, *J* = 2.5 Hz, 1H). 13C-NMR (DMSO-*d*6); δ 55.41, 100.47, 103.73, 106.48, 117.35, 118.42, 126.05, 129.42, 134.97, 140.60, 141.81, 147.71, 152.67, 154.48, 160.98. MS (EI) m/e (rel. int.); 322 (M+, 100). Anal. Calcd. for: C18H14N2O2S: C, 67.06; H, 4.38; N, 8.69 Found: C, 67.12; H, 4.41; N, 8.58%.

**3.1.1.5 6-[5-(3,4,5-Trimethoxyphenyl)thiophen-2-yl]nicotinonitrile (3e)**.

Compound **3e** was obtained in 85% yield as a yellow solid, mp 201-203 oC (EtOH/DMF). Rf = 0.22, petroleum ether (60-80 oC)-EtOAc (7:3). IR (KBr) ν’ 3043, 2937 (CH, stretch), 2220 (CN, stretch), 1585, 1542 (C=C, stretch) cm-1.1H-NMR (DMSO-*d*6); δ 3.68 (s, 3H), 3.86 (s, 6H), 7.00 (s, 2H), 7.65 (d, *J* = 4.0 Hz, 1H), 8.02 (d, *J* = 4.0 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 8.31 (dd, *J* = 8.5, 2.5 Hz, 1H), 8.93 (d, *J* = 2.5 Hz, 1H). 13C-NMR (DMSO-*d*6); δ 56.06, 60.16, 103.18, 106.33, 117.37, 118.28, 125.57, 128.90, 129.47, 137.94, 140.55, 141.43, 148.18, 152.65, 153.35, 154.56.

MS (EI) m/e (rel. int.); 352 (M+, 100), 337 (M+-CH3, 88). Anal. Calcd. for: C19H16N2O3S: C, 64.76; H, 4.58; N, 7.95 Found: C, 64.42; H, 4.52; N, 8.23%.

***3.1.2. General methodology for preparation of thienylnicotinamidine derivatives (4a-e)***.

Treatment of the proper thienylnicotinonitrile derivative **3a-e** (1.5 mmol) with LiN(TMS)2 (1M solution in THF, 6 mL, 6 mmol) and the reaction was permitted to stir for overnight. The reaction mixture was then cooled, after which hydrogen chloride ethanolic solution (12 mL, 1.25 M) was added, whereupon a precipitate started forming. The mixture was left to stir for 6 hours, where after it was diluted with ether and the resultant solid was collected through filtration. The resultant thienylnicotinamidine derivative was purified by neutralization with 1N NaOH followed by filtration of the subsequent solid and washing with water to afford the free bases **4a-e**. At the end, the thienylnicotinamidine free base was stirred with hydrogen chloride ethanolic solution for overnight, diluted with ether, and the solid formed was filtered off and dried to furnish the hydrochloride salt of the target thienylnicotinamidine derivative **5a-e**.

**3.1.2.1 6-(5-Phenylthiophen-2-yl)nicotinamidine hydrochloride salt (5a)**.

Compound **5a** was obtained in 68% yield as an orange solid, mp 286-287 oC. IR (KBr) ν’ 3356, 3230 (NH, stretch), 3062 (CH, stretch), 1676, 1629, 1593 (C=N & C=C, stretch) cm-1. 1H-NMR (DMSO-*d*6); δ 7.35-7.38 (m, 1H). 7.44-7.47 (m, 2H), 7.66 (d, *J* = 4.0 Hz, 1H), 7.75-7.77 (m, 2H), 8.05 (d, *J* = 4.0 Hz, 1H), 8.20 (d, *J* = 8.0 Hz, 1H), 8.29 (dd, *J* = 8.0, 2.0 Hz, 1H), 8.94 (d, *J* = 2.0 Hz, 1H). 9.27 (s, 2H, exchangeable with D2O), 9.56 (s, 2H, exchangeable with D2O). 13C-NMR (DMSO-*d*6); δ 117.96, 122.08, 125.48, 125.58, 128.54, 129.27, 129.30, 133.23, 137.13, 141.96, 147.52, 149.08, 155.58, 163.51. MS of **4a (**free base of 5a) (EI) m/e (rel. int.); 279 (M+, 100), 262 (M+-NH3, 30). Anal. Calcd. for:C16H13N3S-1.0HCl: C, 60.85; H, 4.47; N, 13.31 Found: C, 60.93; H, 4.59; N, 13.04%.

**3.1.2.2. 6-[5-(4-Methoxyphenyl)thiophen-2-yl]nicotinamidine hydrochloride salt (5b)**.

Compound **5b** was obtained in 69% yield as a brick-red solid, mp 282-283 oC. IR (KBr) ν’ 3383, 3240 (NH, stretch), 3080, 2960 (CH, stretch), 1677, 1630, 1598 (C=N & C=C, stretch) cm-1. 1H-NMR (DMSO-*d*6); δ 3.78 (s, 3H), 7.00 (d, *J* = 9.0 Hz, 2H), 7.51 (d, *J* = 4.0 Hz, 1H), 7.68 (d, *J* = 9.0 Hz, 2H), 7.99 (d, *J* = 4.0 Hz, 1H), 8.15 (d, *J* = 9.0 Hz, 1H), 8.27 (dd, *J* = 9.0, 2.0 Hz, 1H). 8.95 (d, *J* = 2.0 Hz, 1H), 9.38 (s, 2H, exchangeable with D2O), 9.65 (s, 2H, exchangeable with D2O). 13C-NMR (DMSO-*d*6); δ 55.37, 114.70, 117.81, 121.72, 124.25, 125.96, 127.06, 129.38, 137.05, 140.77, 147.80, 149.10, 155.75, 159.60, 163.57. MS of **4b (**free base of 5b) (EI) m/e (rel. int.); 309 (M+, 100), 294 (M+-CH3, 34). 292 (M+-NH3, 21). 277 (17). Anal. Calcd. for: C17H15N3OS-1.0HCl: C, 59.04; H, 4.66; N, 12.15 Found: C, 58.87; H, 4.85; N, 12.09%.

**3.1.2.3. 5-[5-(3,4-Dimethoxyphenyl)thiophen-2-yl]nicotinamidine hydrochloride salt (5c)**.

Compound **5c** was obtained in 74% yield as an orange solid, mp 284-285 oC. IR (KBr) ν’ 3383, 3283 (NH, stretch), 3040, 2970 (CH, stretch), 1682, 1628, 1593 (C=N & C=C, stretch) cm-1.1H-NMR (DMSO-*d*6); δ 3.78 (s, 3H), 3.84 (s, 3H), 7.02 (d, *J* = 9.0 Hz, 1H), 7.27-7.30 (m, 2H), 7.57 (d, *J* = 3.5 Hz, 1H), 8.01 (d, *J* = 3.5 Hz, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 8.27 (dd, *J* = 8.5, 2.0 Hz, 1H), 8.94 (d, *J* = 2.0 Hz, 1H), 9.34 (s, 2H, exchangeable with D2O), 9.61 (s, 2H, exchangeable with D2O).13C-NMR (DMSO-*d*6); δ 55.62, 55.66, 109.15, 112.18, 117.74, 118.28, 121.71, 124.52, 126.13, 129.25, 137.00, 140.79, 148.04, 149.04, 149.10, 149.30, 155.72, 163.50. MS of **4c (**free base of 5c) (EI) m/e (rel. int.); 339 (M+, 100), 324 (M+-CH3, 28), 322 (M+ -NH3, 33), 307 (M+ -CH3/NH3, 12). Anal. Calcd. for: C18H17N3O2S-1.0HCl: C, 57.52; H, 4.83; N, 11.18 Found: C, 57.58; H, 4.97; N, 10.85%.

**3.1.2.4. 6-[5-(3,5-Dimethoxyphenyl)thiophen-2-yl]nicotinamidine hydrochloride salt (5d)**.

Compound **5d** was obtained in 77% yield as a yellow solid, mp 294-295.5 oC. IR (KBr) ν’ 3445, 3225 (NH, stretch), 3062, 2999, 2964 (CH, stretch), 1696, 1667, 1628, 1592 (C=N & C=C, stretch) cm-1.1H-NMR (DMSO-*d*6); δ 3.80 (s, 6H), 6.51 (s, 1H), 6.88 (s, 2H), 7.69 (d, *J* = 4.0 Hz, 1H), 8.04 (d, *J* = 4.0 Hz, 1H), 8.21 (d, *J* = 8.0 Hz, 1H), 8.26 (dd, *J* = 8.0, 2.0 Hz, 1H), 8.94 (d, *J* = 2.0 Hz, 1H), 9.28 (s, 2H, exchangeable with D2O), 9.56 (s, 2H, exchangeable with D2O). 13C-NMR (DMSO-*d*6); δ 55.44, 100.44, 103.72, 117.97, 122.00, 126.03, 129.08, 135.08, 137.15, 142.03, 147.34, 149.08, 155.53, 160.99, 163.53. MS of **4d (**free base of 5d) (EI) m/e (rel. int.); 339 (M+, 100), 322 (M+-NH3, 65). Anal. Calcd. for: C18H17N3O2S-1.0HCl: C, 57.52; H, 4.83; N, 11.18 Found: C, 57.67; H, 4.75; N, 11.02%.

**3.1.2.5. 6-[5-(3,4,5-Trimethoxyphenyl)thiophen-2-yl]nicotinamidine hydrochloride salt (5e)**.

Compound **5e** was obtained in 82% yield as a golden-yellow solid, mp 290-291 oC. IR (KBr) ν’ 3420, 3251 (NH, stretch), 3059, 3000 (CH, stretch), 1696, 1667, 1627, 1586 (C=N & C=C, stretch) cm-1.1H-NMR (DMSO-*d*6); δ 3.68 (s, 3H), 3.86 (s, 6H), 7.00 (s, 2H), 7.66 (d, *J* = 4.0 Hz, 1H), 8.04 (d, *J* = 4.0 Hz, 1H), 8.19 (d, *J* = 8.5 Hz, 1H), 8.29 (dd, *J* = 8.5, 2.5 Hz, 1H), 8.96 (d, *J* = 2.5 Hz, 1H), 9.37 (s, 2H, exchangeable with D2O), 9.64 (s, 2H, exchangeable with D2O).13C-NMR (DMSO-*d*6); δ 56.07, 60.16, 103.17, 117.82, 121.89, 125.55, 128.99, 129.12, 137.09, 137.88, 141.62, 147.79, 149.04, 153.35, 155.61, 163.48. MS of **4e (**free base of 5e) (EI) m/e (rel. int.); 369 (M+, 82), 354 (M+-CH3, 68), 352 (M+-NH3, 91), 337 (65), 57 (100). Anal. Calcd. for: C19H19N3O3S-1.0HCl: C, 56.22; H, 4.97; N, 10.35 Found: C, 56.26; H, 4.89; N, 10.60%.

***3.2. Computational studies***

Quantum chemical calculations were achieved using Gaussian 09W program [34] to optimize the geometry at DFT/B3LYP level [35] with standard 6-311++G(d,p) basis set. In DMSO, 1H and 13C NMR chemical shifts were calculated by the gauge-invariant atomic orbital (GIAO) method [36]. The NMR spectral data were assigned visually by Gauss View program [37]. Fukui indices have been calculated using DMol3 module of Materials Studio package from Accelrys Inc [38]. The gradient-corrected functional method (GGA) with a double numeric plus polarization (DNP) basis set (version 3.5) and B3LYP functional have been used [39].

**B) Figures for NMR Spectra of target cationic nicotinamidines 5a-e**

* **Figure S1: Compound 5a** 1H-NMR/JEOL 500 MHz
* **Figure S2: Compound 5a** 13C-NMR/JEOL 125 MHz
* **Figure S3: Compound 5b** 1H-NMR/ JEOL 500 MHz
* **Figure S4: Compound 5b** 13C-NMR/JEOL 125 MHz
* **Figure S5: Compound 5c** 1H-NMR/JEOL 500 MHz
* **Figure S6: Compound 5c** 13C-NMR/JEOL 125 MHz
* **Figure S7: Compound 5d** 1H-NMR/JEOL 500 MHz
* **Figure S8: Compound 5d** 13C-NMR/JEOL 125 MHz
* **Figure S9: Compound 5e** 1H-NMR/ JEOL 500 MHz
* **Figure S10: Compound 5e** 13C-NMR/JEOL 125 MHz

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| **Figure S1: Cationic compound 5a** 1H-NMR (DMSO-*d*6)/JEOL 500 MHz |

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| **Figure S2: Cationic compound 5a** 13C-NMR (DMSO-*d*6)/JEOL 125 MHz |

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| **Figure S3: Cationic compound 5b** 1H-NMR (DMSO-*d*6)/JEOL 500 MHz |

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| **Figure S4: Cationic compound 5b** 13C-NMR (DMSO-*d*6)/JEOL 125 MHz |

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| **Figure S5: Cationic compound 5c** 1H-NMR (DMSO-*d*6)/JEOL 500 MHz |

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| **Figure S6: Cationic compound 5c** 13C-NMR (DMSO-*d*6)/JEOL 125 MHz |

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| **Figure S7: Cationic compound 5d** 1H-NMR (DMSO-*d*6)/JEOL 500 MHz |

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| **Figure S8: Cationic compound 5d** 13C-NMR (DMSO-*d*6)/JEOL 125 MHz |

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| **Figure S9: Cationic compound 5e** 1H-NMR (DMSO-*d*6)/JEOL 500 MHz |

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| **Figure S10: Cationic compound 5e** 13C-NMR (DMSO-*d*6)/JEOL 125 MHz |

**Table S1**. The dihedral angle data for cationic compounds **5a-e**.

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| **5a** | **5b** | **5c** |
| **Dihedral angle** | **°** | **Dihedral angle** | **°** | **Dihedral angle** | **°** |
| C(10)-C(18)-N(20)-H(33) | -171.64 | C(9)-C(12)-N(20)-H(34) | 171.02 | C(15)-C(18)-N(20)-H(35) | 170.91 |
| C(10)-C(18)-N(20)-H(34) | 13.34 | C(9)-C(12)-N(20)-H(35) | -13.83 | C(15)-C(18)-N(20)-H(36) | -13.71 |
| C(9)-C(10)-C(18)-N(20) | 27.41 | C(8)-C(9)-C(12)-N(20) | -26.01 | C(14)-C(15)-C(18)-N(20) | -25.97 |
| C(11)-C(10)-C(18)-N(20) | -151.30 | C(10)-C(9)-C(12)-N(20) | 152.63 | C(16)-C(15)-C(18)-N(20) | 152.76 |
| C(10)-C(18)-N(19)-H(31) | -170.07 | C(9)-C(12)-N(19)-H(32) | 169.33 | C(15)-C(18)-N(19)-H(33) | 169.31 |
| C(10)-C(18)-N(19)-H(32) | 12.98 | C(9)-C(12)-N(19)-H(33) | -13.31 | C(15)-C(18)-N(19)-H(34) | -13.32 |
| C(11)-C(10)-C(18)-N(19) | 28.73 | C(10)-C(9)-C(12)-N(19) | -27.46 | C(16)-C(15)-C(18)-N(19) | -27.34 |
| C(9)-C(10)-C(18)-N(19) | -152.56 | C(8)-C(9)-C(12)-N(19) | 153.90 | C(14)-C(15)-C(18)-N(19) | 153.93 |
| N(19)-C(18)-N(20)-H(33) | 8.33 | N(19)-C(12)-N(20)-H(34) | -8.90 | N(19)-C(18)-N(20)-H(35) | -8.99 |
| N(19)-C(18)-N(20)-H(34) | -166.69 | N(19)-C(12)-N(20)-H(35) | 166.25 | N(19)-C(18)-N(20)-H(36) | 166.39 |
| N(20)-C(18)-N(19)-H(31) | 9.96 | N(20)-C(12)-N(19)-H(32) | -10.76 | N(20)-C(18)-N(19)-H(33) | -10.79 |
| N(20)-C(18)-N(19)-H(32) | -166.99 | N(20)-C(12)-N(19)-H(33) | 166.61 | N(20)-C(18)-N(19)-H(34) | 166.58 |
| C(18)-C(10)-C(11)-N(12) | 179.83 | C(12)-C(9)-C(10)-N(11) | -179.73 | C(18)-C(15)-C(16)-N(17) | -179.40 |
| C(8)-C(9)-C(10)-C(18) | -179.77 | C(7)-C(8)-C(9)-C(12) | 179.70 | C(13)-C(14)-C(15)-C(18) | 179.56 |
| S(3)-C(2)-C(7)-C(8) | 1.86 | S(3)-C(2)-C(6)-C(7) | -1.67 | S(4)-C(3)-C(7)-C(13) | 0.96 |
| S(3)-C(2)-C(7)-N(12) | -177.92 | S(3)-C(2)-C(6)-N(11) | 178.18 | S(4)-C(3)-C(7)-N(17) | -179.01 |
| C(1)-C(2)-C(7)-C(8) | -178.68 | C(1)-C(2)-C(6)-C(7) | 178.55 | C(2)-C(3)-C(7)-C(13) | -179.32 |
| C(1)-C(2)-C(7)-N(12) | 1.55 | C(1)-C(2)-C(6)-N(11) | -1.60 | C(2)-C(3)-C(7)-N(17) | 0.71 |
| C(2)-C(7)-N(12)-C(11) | 178.46 | C(2)-C(6)-N(11)-C(10) | -178.59 | C(3)-C(7)-N(17)-C(16) | -179.11 |
| C(2)-C(7)-C(8)-C(9) | -178.45 | C(2)-C(6)-C(7)-C(8) | 178.61 | C(3)-C(7)-C(13)-C(14) | 179.31 |
| C(7)-C(2)-S(3)-C(4) | -179.89 | C(6)-C(2)-S(3)-C(4) | 179.55 | C(7)-C(3)-S(4)-C(5) | -179.39 |
| C(5)-C(1)-C(2)-C(7) | -179.92 | C(5)-C(1)-C(2)-C(6) | -179.71 | C(1)-C(2)-C(3)-C(7) | 179.66 |
| S(3)-C(4)-C(6)-C(13) | -25.66 | S(3)-C(4)-C(13)-C(14) | 17.69 | S(4)-C(5)-C(6)-C(8) | -20.50 |
| S(3)-C(4)-C(6)-C(17) | 154.51 | S(3)-C(4)-C(13)-C(18) | -162.32 | S(4)-C(5)-C(6)-C(12) | 159.45 |
| C(5)-C(4)-C(6)-C(13) | 154.84 | C(5)-C(4)-C(13)-C(14) | -162.79 | C(1)-C(5)-C(6)-C(8) | 159.92 |
| C(5)-C(4)-C(6)-C(17) | -25.00 | C(5)-C(4)-C(13)-C(18) | 17.19 | C(1)-C(5)-C(6)-C(12) | -20.13 |
| C(4)-C(6)-C(17)-C(16) | 179.72 | C(4)-C(13)-C(18)-C(17) | -179.88 | C(5)-C(6)-C(12)-C(11) | 179.94 |
| C(4)-C(6)-C(13)-C(14) | -179.76 | C(4)-C(13)-C(14)-C(15) | 179.89 | C(5)-C(6)-C(8)-C(9) | -178.98 |
| C(6)-C(4)-C(5)-C(1) | -179.96 | C(13)-C(4)-C(5)-C(1) | 179.97 | C(2)-C(1)-C(5)-C(6) | -179.65 |
| C(2)-S(3)-C(4)-C(6) | 179.82 | C(2)-S(3)-C(4)-C(13) | -179.78 | C(3)-S(4)-C(5)-C(6) | 179.46 |
| C(10)-C(11)-N(12)-C(7) | 0.12 | C(9)-C(10)-N(11)-C(6) | -0.13 | C(15)-C(16)-N(17)-C(7) | -0.24 |
| C(9)-C(10)-C(11)-N(12) | 1.05 | C(8)-C(9)-C(10)-N(11) | -1.01 | C(14)-C(15)-C(16)-N(17) | -0.60 |
| C(8)-C(9)-C(10)-C(11) | -1.01 | C(7)-C(8)-C(9)-C(10) | 1.00 | C(13)-C(14)-C(15)-C(16) | 0.77 |
| C(7)-C(8)-C(9)-C(10) | -0.11 | C(6)-C(7)-C(8)-C(9) | 0.06 | C(7)-C(13)-C(14)-C(15) | -0.15 |
| C(8)-C(7)-N(12)-C(11) | -1.32 | C(7)-C(6)-N(11)-C(10) | 1.27 | C(13)-C(7)-N(17)-C(16) | 0.91 |
| N(12)-C(7)-C(8)-C(9) | 1.32 | N(11)-C(6)-C(7)-C(8) | -1.24 | N(17)-C(7)-C(13)-C(14) | -0.72 |
| S(3)-C(4)-C(5)-C(1) | 0.48 | S(3)-C(4)-C(5)-C(1) | -0.47 | C(2)-C(1)-C(5)-S(4) | 0.73 |
| C(2)-S(3)-C(4)-C(5) | -0.60 | C(2)-S(3)-C(4)-C(5) | 0.63 | C(3)-S(4)-C(5)-C(1) | -0.90 |
| C(1)-C(2)-S(3)-C(4) | 0.57 | C(1)-C(2)-S(3)-C(4) | -0.64 | C(2)-C(3)-S(4)-C(5) | 0.85 |
| C(2)-C(1)-C(5)-C(4) | -0.05 | C(2)-C(1)-C(5)-C(4) | -0.01 | C(5)-C(1)-C(2)-C(3) | -0.09 |
| C(5)-C(1)-C(2)-S(3) | -0.40 | C(5)-C(1)-C(2)-S(3) | 0.49 | C(1)-C(2)-C(3)-S(4) | -0.59 |
| C(17)-C(6)-C(13)-C(14) | 0.08 | C(18)-C(13)-C(14)-C(15) | -0.09 | C(12)-C(6)-C(8)-C(9) | 1.07 |
| C(13)-C(6)-C(17)-C(16) | -0.13 | C(14)-C(13)-C(18)-C(17) | 0.11 | C(8)-C(6)-C(12)-C(11) | -0.10 |
| C(15)-C(16)-C(17)-C(6) | 0.08 | C(16)-C(17)-C(18)-C(13) | -0.02 | C(10)-C(11)-C(12)-C(6) | -1.60 |
| C(14)-C(15)-C(16)-C(17) | 0.02 | C(15)-C(16)-C(17)-C(18) | -0.08 | C(9)-C(10)-C(11)-C(12) | 2.33 |
| C(13)-C(14)-C(15)-C(16) | -0.06 | C(14)-C(15)-C(16)-C(17) | 0.10 | C(8)-C(9)-C(10)-C(11) | -1.40 |
| C(6)-C(13)-C(14)-C(15) | 0.01 | C(13)-C(14)-C(15)-C(16) | -0.01 | C(6)-C(8)-C(9)-C(10) | -0.31 |
|  |  | C(17)-C(16)-O(21)-C(22) | -0.63 | C(12)-C(11)-O(21)-C(22) | 0.81 |
|  |  | C(15)-C(16)-O(21)-C(22) | 179.39 | C(10)-C(11)-O(21)-C(22) | 178.79 |
|  |  | C(14)-C(15)-C(16)-O(21) | -179.91 | C(9)-C(10)-C(11)-O(21) | -175.75 |
|  |  | O(21)-C(16)-C(17)-C(18) | 179.93 | O(21)-C(11)-C(12)-C(6) | 176.33 |
|  |  |  |  | C(11)-C(10)-O(23)-C(24) | 40.48 |
|  |  |  |  | C(9)-C(10)-O(23)-C(24) | -143.32 |
|  |  |  |  | C(8)-C(9)-C(10)-O(23) | -177.86 |
|  |  |  |  | O(23)-C(10)-C(11)-C(12) | 178.45 |
|  |  |  |  | O(23)-C(10)-C(11)-O(21) | 0.37 |
| **5d** | **5e** |  |  |
| **Dihedral angle** | **°** | **Dihedral angle** | **°** |  |  |
| C(15)-C(18)-N(20)-H(35) | 180.00 | C(15)-C(18)-N(20)-H(36) | 180.00 |  |  |
| C(15)-C(18)-N(20)-H(36) | 0.01 | C(15)-C(18)-N(20)-H(37) | 0.01 |  |  |
| C(14)-C(15)-C(18)-N(20) | 0.00 | C(14)-C(15)-C(18)-N(20) | 0.00 |  |  |
| C(16)-C(15)-C(18)-N(20) | 180.00 | C(16)-C(15)-C(18)-N(20) | 180.00 |  |  |
| C(15)-C(18)-N(19)-H(33) | 179.99 | C(15)-C(18)-N(19)-H(34) | 179.99 |  |  |
| C(15)-C(18)-N(19)-H(34) | 0.01 | C(15)-C(18)-N(19)-H(35) | 0.01 |  |  |
| C(16)-C(15)-C(18)-N(19) | 0.00 | C(16)-C(15)-C(18)-N(19) | 0.00 |  |  |
| C(14)-C(15)-C(18)-N(19) | 180.00 | C(14)-C(15)-C(18)-N(19) | 180.00 |  |  |
| N(19)-C(18)-N(20)-H(35) | 0.00 | N(19)-C(18)-N(20)-H(36) | 0.00 |  |  |
| N(19)-C(18)-N(20)-H(36) | -179.99 | N(19)-C(18)-N(20)-H(37) | -179.99 |  |  |
| N(20)-C(18)-N(19)-H(33) | -0.01 | N(20)-C(18)-N(19)-H(34) | -0.01 |  |  |
| N(20)-C(18)-N(19)-H(34) | -179.99 | N(20)-C(18)-N(19)-H(35) | -179.99 |  |  |
| C(18)-C(15)-C(16)-N(17) | 180.00 | C(18)-C(15)-C(16)-N(17) | 180.00 |  |  |
| C(13)-C(14)-C(15)-C(18) | 180.00 | C(13)-C(14)-C(15)-C(18) | 180.00 |  |  |
| S(3)-C(2)-C(7)-C(13) | 0.00 | S(3)-C(2)-C(7)-C(13) | 0.00 |  |  |
| S(3)-C(2)-C(7)-N(17) | 180.00 | S(3)-C(2)-C(7)-N(17) | 180.00 |  |  |
| C(1)-C(2)-C(7)-C(13) | 180.00 | C(1)-C(2)-C(7)-C(13) | -180.00 |  |  |
| C(1)-C(2)-C(7)-N(17) | 0.00 | C(1)-C(2)-C(7)-N(17) | 0.01 |  |  |
| C(2)-C(7)-N(17)-C(16) | 180.00 | C(2)-C(7)-N(17)-C(16) | 180.00 |  |  |
| C(2)-C(7)-C(13)-C(14) | 180.00 | C(2)-C(7)-C(13)-C(14) | 180.00 |  |  |
| C(7)-C(2)-S(3)-C(4) | 180.00 | C(7)-C(2)-S(3)-C(4) | 180.00 |  |  |
| C(5)-C(1)-C(2)-C(7) | 180.00 | C(5)-C(1)-C(2)-C(7) | 180.00 |  |  |
| S(3)-C(4)-C(6)-C(8) | 0.00 | S(3)-C(4)-C(6)-C(8) | 0.00 |  |  |
| S(3)-C(4)-C(6)-C(12) | 180.00 | S(3)-C(4)-C(6)-C(12) | 180.00 |  |  |
| C(5)-C(4)-C(6)-C(8) | 180.00 | C(5)-C(4)-C(6)-C(8) | 180.00 |  |  |
| C(5)-C(4)-C(6)-C(12) | 0.00 | C(5)-C(4)-C(6)-C(12) | -0.01 |  |  |
| C(4)-C(6)-C(12)-C(11) | 180.00 | C(4)-C(6)-C(12)-C(11) | 180.00 |  |  |
| C(4)-C(6)-C(8)-C(9) | 180.00 | C(4)-C(6)-C(8)-C(9) | 180.00 |  |  |
| C(6)-C(4)-C(5)-C(1) | 180.00 | C(6)-C(4)-C(5)-C(1) | -180.00 |  |  |
| C(2)-S(3)-C(4)-C(6) | 180.00 | C(2)-S(3)-C(4)-C(6) | 180.00 |  |  |
| C(15)-C(16)-N(17)-C(7) | 0.00 | C(15)-C(16)-N(17)-C(7) | 0.00 |  |  |
| C(14)-C(15)-C(16)-N(17) | 0.00 | C(14)-C(15)-C(16)-N(17) | 0.00 |  |  |
| C(13)-C(14)-C(15)-C(16) | 0.00 | C(13)-C(14)-C(15)-C(16) | 0.00 |  |  |
| C(7)-C(13)-C(14)-C(15) | 0.00 | C(7)-C(13)-C(14)-C(15) | 0.00 |  |  |
| C(13)-C(7)-N(17)-C(16) | 0.00 | C(13)-C(7)-N(17)-C(16) | 0.00 |  |  |
| N(17)-C(7)-C(13)-C(14) | 0.00 | N(17)-C(7)-C(13)-C(14) | 0.00 |  |  |
| S(3)-C(4)-C(5)-C(1) | 0.00 | S(3)-C(4)-C(5)-C(1) | 0.00 |  |  |
| C(2)-S(3)-C(4)-C(5) | 0.00 | C(2)-S(3)-C(4)-C(5) | 0.00 |  |  |
| C(1)-C(2)-S(3)-C(4) | 0.00 | C(1)-C(2)-S(3)-C(4) | 0.00 |  |  |
| C(2)-C(1)-C(5)-C(4) | 0.00 | C(2)-C(1)-C(5)-C(4) | 0.00 |  |  |
| C(5)-C(1)-C(2)-S(3) | 0.00 | C(5)-C(1)-C(2)-S(3) | 0.00 |  |  |
| C(12)-C(6)-C(8)-C(9) | 0.00 | C(12)-C(6)-C(8)-C(9) | 0.00 |  |  |
| C(8)-C(6)-C(12)-C(11) | 0.00 | C(8)-C(6)-C(12)-C(11) | 0.00 |  |  |
| C(10)-C(11)-C(12)-C(6) | 0.00 | C(10)-C(11)-C(12)-C(6) | 0.00 |  |  |
| C(9)-C(10)-C(11)-C(12) | 0.00 | C(9)-C(10)-C(11)-C(12) | 0.00 |  |  |
| C(8)-C(9)-C(10)-C(11) | 0.00 | C(8)-C(9)-C(10)-C(11) | 0.00 |  |  |
| C(6)-C(8)-C(9)-C(10) | 0.00 | C(6)-C(8)-C(9)-C(10) | 0.00 |  |  |
| C(12)-C(11)-O(21)-C(22) | 0.00 | C(10)-C(11)-O(23)-C(24) | -180.00 |  |  |
| C(10)-C(11)-O(21)-C(22) | 180.00 | C(12)-C(11)-O(23)-C(24) | 0.01 |  |  |
| C(9)-C(10)-C(11)-O(21) | 180.00 | C(9)-C(10)-C(11)-O(23) | -180.00 |  |  |
| O(21)-C(11)-C(12)-C(6) | 180.00 | O(23)-C(11)-C(12)-C(6) | 180.00 |  |  |
| C(10)-C(9)-O(23)-C(24) | 0.00 | C(11)-C(10)-O(21)-C(22) | 0.02 |  |  |
| C(8)-C(9)-O(23)-C(24) | 180.00 | C(9)-C(10)-O(21)-C(22) | -179.99 |  |  |
| C(6)-C(8)-C(9)-O(23) | 180.00 | C(8)-C(9)-C(10)-O(21) | -180.00 |  |  |
| O(23)-C(9)-C(10)-C(11) | 180.00 | O(21)-C(10)-C(11)-C(12) | 180.00 |  |  |
|  |  | C(10)-C(9)-O(25)-C(26) | 0.02 |  |  |
|  |  | C(8)-C(9)-O(25)-C(26) | -179.99 |  |  |
|  |  | C(6)-C(8)-C(9)-O(25) | -180.00 |  |  |
|  |  | O(25)-C(9)-C(10)-C(11) | 180.00 |  |  |
|  |  | O(21)-C(10)-C(11)-O(23) | 0.00 |  |  |
|  |  | O(25)-C(9)-C(10)-O(21) | 0.00 |  |  |

**Table S2**. The bond angle data for cationic compounds **5a-e**.

|  |  |  |  |
| --- | --- | --- | --- |
| **5a** | **5b** | **5c** | **X-ray value\*** |
| **Angle** | **°** | **Angle** | **°** | **Angle** | **°** | **°** |
| H(34)-N(20)-H(33) | 117.23 | H(35)-N(20)-H(34) | 117.28 | H(36)-N(20)-H(35) | 117.30 | 120.7 |
| H(34)-N(20)-C(18) | 120.30 | H(35)-N(20)-C(12) | 120.33 | H(36)-N(20)-C(18) | 120.31 | 119.1-120.2 |
| H(33)-N(20)-C(18) | 122.30 | H(34)-N(20)-C(12) | 122.23 | H(35)-N(20)-C(18) | 122.24 | 119.1-120.2 |
| H(32)-N(19)-H(31) | 117.26 | H(33)-N(19)-H(32) | 117.29 | H(34)-N(19)-H(33) | 117.31 | 116.6 |
| H(32)-N(19)-C(18) | 120.39 | H(33)-N(19)-C(12) | 120.45 | H(34)-N(19)-C(18) | 120.44 | 119.5-122.4 |
| H(31)-N(19)-C(18) | 122.28 | H(32)-N(19)-C(12) | 122.21 | H(33)-N(19)-C(18) | 122.20 | 119.5-122.4 |
| N(20)-C(18)-N(19) | 118.70 | N(20)-C(12)-N(19) | 118.40 | N(20)-C(18)-N(19) | 118.39 | 118.8 |
| N(20)-C(18)-C(10) | 120.62 | N(20)-C(12)-C(9) | 120.75 | N(20)-C(18)-C(15) | 120.71 | 120.2 |
| N(19)-C(18)-C(10) | 120.68 | N(19)-C(12)-C(9) | 120.86 | N(19)-C(18)-C(15) | 120.90 | 120.2 |
| C(18)-C(10)-C(11) | 121.01 | C(12)-C(9)-C(10) | 121.09 | C(18)-C(15)-C(16) | 121.14 |  |
| C(18)-C(10)-C(9) | 122.23 | C(12)-C(9)-C(8) | 122.31 | C(18)-C(15)-C(14) | 122.27 |  |
| N(12)-C(7)-C(2) | 116.53 | N(11)-C(6)-C(2) | 116.57 | N(17)-C(7)-C(3) | 116.66 | 117.8 |
| C(8)-C(7)-C(2) | 122.86 | C(7)-C(6)-C(2) | 122.93 | C(13)-C(7)-C(3) | 122.83 | 123.2 |
| C(7)-C(2)-S(3) | 123.08 | C(6)-C(2)-S(3) | 123.17 | C(7)-C(3)-S(4) | 123.10 | 118.5-121.8 |
| C(7)-C(2)-C(1) | 126.71 | C(6)-C(2)-C(1) | 126.79 | C(7)-C(3)-C(2) | 126.83 | 125.4-127.8 |
| C(17)-C(6)-C(4) | 119.91 | C(18)-C(13)-C(4) | 120.50 | C(12)-C(6)-C(5) | 119.88 | 121.1 |
| C(13)-C(6)-C(4) | 121.48 | C(14)-C(13)-C(4) | 121.92 | C(8)-C(6)-C(5) | 121.74 | 121.1 |
| C(6)-C(4)-S(3) | 121.37 | C(13)-C(4)-S(3) | 121.49 | C(6)-C(5)-S(4) | 121.35 | 118.5-121.7 |
| C(6)-C(4)-C(5) | 128.202 | C(13)-C(4)-C(5) | 128.38 | C(6)-C(5)-C(1) | 128.49 | 129.5-131.2 |
| C(11)-N(12)-C(7) | 119.21 | C(10)-N(11)-C(6) | 119.21 | C(16)-N(17)-C(7) | 119.19 | 118.5 |
| N(12)-C(11)-C(10) | 124.21 | N(11)-C(10)-C(9) | 124.34 | N(17)-C(16)-C(15) | 124.35 | 122.2 |
| C(11)-C(10)-C(9) | 116.75 | C(10)-C(9)-C(8) | 116.58 | C(16)-C(15)-C(14) | 116.58 | 118.3-122.1 |
| C(10)-C(9)-C(8) | 119.47 | C(9)-C(8)-C(7) | 119.56 | C(15)-C(14)-C(13) | 119.55 | 118.3-122.1 |
| C(9)-C(8)-C(7) | 119.74 | C(8)-C(7)-C(6) | 119.79 | C(14)-C(13)-C(7) | 119.80 | 118.3-122.1 |
| N(12)-C(7)-C(8) | 120.61 | N(11)-C(6)-C(7) | 120.50 | N(17)-C(7)-C(13) | 120.51 | 122.2 |
| S(3)-C(2)-C(1) | 110.21 | S(3)-C(2)-C(1) | 110.04 | S(4)-C(3)-C(2) | 110.07 | 110.2-110.9 |
| C(5)-C(4)-S(3) | 110.43 | C(5)-C(4)-S(3) | 110.13 | S(4)-C(5)-C(1) | 110.16 | 110.2-110.9 |
| C(4)-S(3)-C(2) | 92.01 | C(4)-S(3)-C(2) | 92.14 | C(5)-S(4)-C(3) | 92.12 | 92.8 |
| C(5)-C(1)-C(2) | 113.53 | C(5)-C(1)-C(2) | 113.70 | C(3)-C(2)-C(1) | 113.66 | 112.6-113.4 |
| C(4)-C(5)-C(1) | 113.82 | C(4)-C(5)-C(1) | 113.99 | C(5)-C(1)-C(2) | 113.99 | 112.6-113.4 |
| C(16)-C(17)-C(6) | 120.54 | C(17)-C(18)-C(13) | 121.66 | C(11)-C(12)-C(6) | 121.53 | 120.0-119.9 |
| C(17)-C(16)-C(15) | 120.25 | C(18)-C(17)-C(16) | 119.78 | C(12)-C(11)-C(10) | 119.43 | 120.0-119.9 |
| C(16)-C(15)-C(14) | 119.78 | C(17)-C(16)-C(15) | 119.37 | C(11)-C(10)-C(9) | 118.70 | 120.0-119.9 |
| C(15)-C(14)-C(13) | 120.18 | C(16)-C(15)-C(14) | 120.27 | C(10)-C(9)-C(8) | 121.56 | 120.0-119.9 |
| C(14)-C(13)-C(6) | 120.63 | C(15)-C(14)-C(13) | 121.35 | C(9)-C(8)-C(6) | 120.37 | 120.0-119.9 |
| C(17)-C(6)-C(13) | 118.61 | C(18)-C(13)-C(14) | 117.58 | C(12)-C(6)-C(8) | 118.38 | 120.0-119.9 |
|  |  | O(21)-C(16)-C(17) | 124.79 | O(21)-C(11)-C(12) | 124.09 | 125.2 |
|  |  | O(21)-C(16)-C(15) | 115.83 | O(21)-C(11)-C(10) | 116.45 | 115.4 |
|  |  | C(22)-O(21)-C(16) | 119.42 | C(22)-O(21)-C(11) | 119.13 | 117.7 |
|  |  |  |  | O(23)-C(10)-C(11) | 124.88 | 125.2 |
|  |  |  |  | O(23)-C(10)-C(9) | 116.31 | 115.4 |
|  |  |  |  | C(24)-O(23)-C(10) | 121.56 | 117.7 |
| **5d** | **5e** |  |  | **X-ray value\*** |
| **Angle** | **°** | **Angle** | **°** |  |  | **°** |
| H(36)-N(20)-H(35) | 116.72 | H(37)-N(20)-H(36) | 116.78 |  |  | 120.7 |
| H(36)-N(20)-C(18) | 121.27 | H(37)-N(20)-C(18) | 121.23 |  |  | 119.1-120.2 |
| H(35)-N(20)-C(18) | 122.01 | H(36)-N(20)-C(18) | 121.99 |  |  | 119.1-120.2 |
| H(34)-N(19)-H(33) | 116.71 | H(35)-N(19)-H(34) | 116.77 |  |  | 116.6 |
| H(34)-N(19)-C(18) | 121.40 | H(35)-N(19)-C(18) | 121.37 |  |  | 119.5-122.4 |
| H(33)-N(19)-C(18) | 121.90 | H(34)-N(19)-C(18) | 121.86 |  |  | 119.5-122.4 |
| N(20)-C(18)-N(19) | 117.32 | N(20)-C(18)-N(19) | 117.08 |  |  | 118.8 |
| N(20)-C(18)-C(15) | 121.10 | N(20)-C(18)-C(15) | 121.20 |  |  | 120.2 |
| N(19)-C(18)-C(15) | 121.58 | N(19)-C(18)-C(15) | 121.72 |  |  | 120.2 |
| C(18)-C(15)-C(16) | 121.69 | C(18)-C(15)-C(16) | 121.76 |  |  |  |
| C(18)-C(15)-C(14) | 122.52 | C(18)-C(15)-C(14) | 122.59 |  |  |  |
| N(17)-C(7)-C(2) | 116.68 | N(17)-C(7)-C(2) | 116.76 |  |  | 117.8 |
| C(13)-C(7)-C(2) | 122.99 | C(13)-C(7)-C(2) | 123.02 |  |  | 123.2 |
| C(7)-C(2)-S(3) | 123.04 | C(7)-C(2)-S(3) | 123.09 |  |  | 118.5-121.8 |
| C(7)-C(2)-C(1) | 126.77 | C(7)-C(2)-C(1) | 126.86 |  |  | 125.4-127.8 |
| C(12)-C(6)-C(4) | 119.46 | C(12)-C(6)-C(4) | 120.25 |  |  | 121.1 |
| C(8)-C(6)-C(4) | 120.73 | C(8)-C(6)-C(4) | 121.48 |  |  | 121.1 |
| C(6)-C(4)-S(3) | 121.44 | C(6)-C(4)-S(3) | 121.49 |  |  | 118.5-121.7 |
| C(6)-C(4)-C(5) | 128.46 | C(6)-C(4)-C(5) | 128.54 |  |  | 129.5-131.2 |
| C(16)-N(17)-C(7) | 119.21 | C(16)-N(17)-C(7) | 119.20 |  |  | 118.5 |
| N(17)-C(16)-C(15) | 124.85 | N(17)-C(16)-C(15) | 124.97 |  |  | 122.2 |
| C(16)-C(15)-C(14) | 115.79 | C(16)-C(15)-C(14) | 115.66 |  |  | 118.3-122.1 |
| C(15)-C(14)-C(13) | 120.08 | C(15)-C(14)-C(13) | 120.12 |  |  | 118.3-122.1 |
| C(14)-C(13)-C(7) | 119.75 | C(14)-C(13)-C(7) | 119.83 |  |  | 118.3-122.1 |
| N(17)-C(7)-C(13) | 120.33 | N(17)-C(7)-C(13) | 120.22 |  |  | 122.2 |
| S(3)-C(2)-C(1) | 110.20 | S(3)-C(2)-C(1) | 110.05 |  |  | 110.2-110.9 |
| C(5)-C(4)-S(3) | 110.10 | C(5)-C(4)-S(3) | 109.97 |  |  | 110.2-110.9 |
| C(4)-S(3)-C(2) | 92.15 | C(4)-S(3)-C(2) | 92.19 |  |  | 92.8 |
| C(5)-C(1)-C(2) | 113.49 | C(5)-C(1)-C(2) | 113.67 |  |  | 112.6-113.4 |
| C(4)-C(5)-C(1) | 114.06 | C(4)-C(5)-C(1) | 114.13 |  |  | 112.6-113.4 |
| C(11)-C(12)-C(6) | 119.35 | C(11)-C(12)-C(6) | 120.79 |  |  | 120.0-119.9 |
| C(12)-C(11)-C(10) | 120.83 | C(12)-C(11)-C(10) | 120.95 |  |  | 120.0-119.9 |
| C(11)-C(10)-C(9) | 119.58 | C(11)-C(10)-C(9) | 118.09 |  |  | 120.0-119.9 |
| C(10)-C(9)-C(8) | 120.15 | C(10)-C(9)-C(8) | 119.87 |  |  | 120.0-119.9 |
| C(9)-C(8)-C(6) | 120.28 | C(9)-C(8)-C(6) | 122.03 |  |  | 120.0-119.9 |
| C(12)-C(6)-C(8) | 119.82 | C(12)-C(6)-C(8) | 118.28 |  |  | 120.0-119.9 |
| O(21)-C(11)-C(12) | 124.49 | O(23)-C(11)-C(12) | 123.01 |  |  | 125.2 |
| O(21)-C(11)-C(10) | 114.69 | O(23)-C(11)-C(10) | 116.04 |  |  | 115.4 |
| C(22)-O(21)-C(11) | 119.14 | C(24)-O(23)-C(11) | 119.25 |  |  | 117.7 |
| O(23)-C(9)-C(10) | 124.41 | O(21)-C(10)-C(11) | 126.22 |  |  | 125.2 |
| O(23)-C(9)-C(8) | 115.44 | O(21)-C(10)-C(9) | 115.70 |  |  | 115.4 |
| C(24)-O(23)-C(9) | 118.87 | C(22)-O(21)-C(10) | 126.26 |  |  | 117.7 |
|  |  | O(25)-C(9)-C(10) | 126.78 |  |  | 125.2 |
|  |  | O(25)-C(9)-C(8) | 113.35 |  |  | 115.4 |
|  |  | C(26)-O(25)-C(9) | 126.11 |  |  | 117.7 |