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C₃H₇NO₂	α-Alanine (2-aminopropanoic acid) Equilibrium structure by ED and QC <i>E. P. Altova, A. N. Rykov, L. V. Khristenko, E. Yu. L'vova, and I. F. Shishkov</i> Manuscript in preparation
C₄H₉NO₃	Threonine (2-amino-3-hydroxybutanoic acid) Equilibrium structure by ED and QC <i>D. S. Tikhonov, L. S. Khaikin, O. E. Grikina, and A. N. Rykov</i> Work in progress
C₅H₄N₂O₄	Orotic acid (1,2,3,6-tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid) Molecular structure and conformations by ED and QC <i>N. Vogt, E. P. Altova, A. N. Rykov, J. Vogt, and I. F. Shishkov</i> Manuscript in preparation
C₅H₅N₃O	Pyrazinamide Semi-experimental equilibrium structure from ED <i>D. S. Tikhonov, Yu. V. Vishnevskiy, A. N. Rykov, O. E. Grikina, and L. S. Khaikin</i> J. Mol. Struct., 1132 (2017) 20
C₅H₉N₃	Histamine Equilibrium structure by ED and QC <i>D. S. Tikhonov, A. N. Rykov, O. E. Grikina, and L. S. Khaikin</i> Phys. Chem. Chem. Phys., 18 (2016) 6092
C₆H₅NO₂	Pyridine-2-carboxylic acid (picolinic acid) Molecular structure and conformations by ED and coupled cluster calculations <i>I. I. Marochkin, N. Vogt, A. N. Rykov, and J. Vogt</i> Manuscript in preparation
C₆N₂H₁₂	N,N'-Dimethyl-3-cyclopropyldiaziridine Synthesis and structure <i>V. V. Kuznetsov, I. I. Marochkin, E. P. Altova, N. N. Makhova, and I. F. Shishkov</i> Manuscript in preparation
C₇H₇NS	Thiobenzamide Equilibrium molecular structure by ED and QC <i>I. N. Kolesnikova, A. N. Rykov, and I. F. Shishkov</i> Work in progress

C₈H₅NO₂	1H-indole-2,3-dione, isatin Molecular structure by ED and QC <i>A. V. Belyakov, K. O. Nikolaenko, P. B. Davidovich, A. D. Ivanov, A. V. Garabadzhiu, A. N. Rykov, and I. F. Shishkov</i> J. Mol. Struct., 1132 (2017) 44
C₉H₆N₂O₃	Nitroxoline Equilibrium structure by ED and QC <i>D. S. Tikhonov, D. I. Sharapa, A. N. Rykov, O. E. Grikina, and L. S. Khaikin</i> Manuscript complete.
C₉H₉Cl₂N₃	N-(2,6-dichlorophenyl)-4,5-dihydro-1H-imidazol-2-amine, clonidine Molecular structure by ED, XD and QC <i>I. N. Kolesnikova, A. N. Rykov, I. F. Shishkov, V. A. Tafeenko, and L. A. Aslanov</i> Phys. Chem. Chem. Phys., 19 (2017) 4618
C₉H₁₂ClN₅O	Moxonidine Molecular structure ED and QC <i>I. N. Kolesnikova, A. N. Rykov, and I. F. Shishkov</i> Work in progress
C₉H₁₃NO₃	Adrenaline Structure by ED <i>E. P. Altova, I. I. Marochkin, A. N. Rykov, and I. F. Shishkov</i> Work in progress
C₁₀H₁₂N₂	Tryptamine Molecular structure by ED <i>I. I. Marochkin, E. P. Altova, A. N. Rykov, and I. F. Shishkov</i> J. Mol. Struct., (2017) Manuscript in preparation
	Methyl pseudohalides CH₃NCX (X=O, S, Se) Structures and anharmonic vibrational frequencies by QC, interpretation of experimental vibrational spectra <i>L. S. Khaikin and O. E. Grikina</i> It will be prepared as abstract to ESGED17
	1,2-Bis(2-acetamidoethyl)diaziridine, 3,3-diethyldiaziridine Comparable study by XD and QC <i>V. V. Kuznetsov, I. I. Marochkin, A. S. Goloveshkin, N. N. Makhova, and I. F. Shishkov</i> Struct. Chem., (2017) in press