|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Residue (met group) | $$p\_{a}$$$$(\%)$$ | $$p\_{b}$$ | $$p\_{c}$$ | $$k\_{ex,ab}$$$$(s^{-1})$$ | $$k\_{ex,ac}$$ | $$∆ω\_{C,ab}$$$$(ppm)$$ | $$∆ω\_{H,ab}$$ | $$∆ω\_{C,ac}$$ | $$∆ω\_{H,ac}$$ |
| L41 (met 2) | $$99.86\pm 0.03$$ |  | $$0.14\pm 0.03$$ |  | $$1000\pm 200$$ |  |  | $$1.5\pm 0.3$$ | - |
| V58 (met 1) | $$85\pm 9$$ | $$13\pm 9$$ | $$1.1\pm 0.2$$ | $$4\pm 2$$ | $$800\pm 100$$ | $$-0.70\pm 0.02$$ | - | $$0.61\pm 0.05$$ | - |
| L73 (met 2) | $$99.88\pm 0.02$$ |  | $$0.12\pm 0.02$$ |  | $$2400\pm 300$$ |  |  | $$1.9\pm 0.3$$ | - |
| L73 (met 1) | $$99.88\pm 0.02$$ |  | $$0.12\pm 0.02$$ |  | $$2400\pm 300$$ |  |  | $$2.9\pm 0.5$$ | - |
| L74 (met 2) | $$98.66\pm 0.01$$ | $$1.34\pm $$0.01 |  | $$241\pm 7$$ |  | $$-0.75\pm 0.01$$ | - |  |  |
| V79 (met 1) | $$98.52\pm 0.02$$ | $$1.34\pm $$0.01 | $$0.14\pm 0.02$$ | $$241\pm 7$$ | $$2900\pm 500$$ | $$0.2\pm 0.1$$ | - | $$3.1\pm 0.3$$ | - |
| L101 (met 2) | $$98\pm 1$$ | $$1.34\pm $$0.03 | $$0\pm 1$$(0.1,0.2,2.2) | $$241\pm 7$$ | $$7000\pm 3000$$ | $$0.66\pm 0.02$$ | $$0.23\pm 0.02$$ | $$2\pm 1$$ | - |
| L101 (met 1) | $$100\pm 1$$ |  | $$0\pm 1$$(0.1,0.2,2.2) |  | $$7000\pm 3000$$ |  |  | $$3\pm 1$$ | - |
| L118 (met 1) | $$80\pm 10$$ |  | $$20\pm 10$$ |  | $$31000\pm 9000$$ |  |  | $$1.0\pm 0.4$$ | - |
| L121 (met 1) | $$95\pm 2$$ | $$1.29\pm $$0.03 | $$4\pm 2$$ | $$241\pm 7$$ | $$19000\pm 7000$$ | $$0.39\pm 0.02$$ | - | $$0.9\pm 0.7$$ | - |
| L131 (met 1) | $$99\pm 2$$ | $$1.34\pm $$0.04 | $$0\pm 2$$(0.1,0.1,1.0) | $$241\pm 7$$ | $$4000\pm 2000$$ | $$0.68\pm 0.03$$ | $$0.2\pm 0.1$$ | $$1.9\pm 0.8$$ | - |
| L131 (met 2) | $$100\pm 2$$ |  | $$0\pm 2$$(0.1,0.1,1.0) |  | $$4000\pm 2000$$ |  |  | $$4\pm 1$$ | - |
| L187 (met 1) | $$98.66\pm 0.01$$ | $$1.34\pm $$0.01 |  | $$241\pm 7$$ |  | $$0.417\pm 0.005$$ | $$0.084\pm 0.004$$ |  |  |
| L192 (met 1) | $$98.51\pm 0.04$$ | $$1.34\pm $$0.01 | $$0.16\pm 0.04$$ | $$241\pm 7$$ | $$2000\pm 500$$ | $$-0.943\pm 0.005$$ | $$0.224\pm 0.006$$ | $$2.1\pm 0.5$$ | $$0.28\pm 0.04$$ |
| L198 (met 2) | $$98.42\pm 0.04$$ | $$1.34\pm $$0.01 | $$0.24\pm 0.04$$ | $$241\pm 7$$ | $$3300\pm 700$$ | $$1.406\pm 0.009$$ | $$0.23\pm 0.01$$ | $$2.6\pm 0.3$$ | - |
| L212 (met 1) | $$60\pm 20$$ |  | $$40\pm 20$$ |  | $$7000\pm 1200$$ |  |  | $$0\pm 1$$(0.2,0.2,3.8) | - |
| L221 (met 1) | $$98.6\pm 0.2$$ | $$1.34\pm $$0.02 | $$0\pm 0.2$$(0.03,0.04,0.16) | $$241\pm 7$$ | $$2000\pm 2000$$ | $$0.863\pm 0.005$$ | $$0.342\pm 0.009$$ | $$3.1\pm 0.7$$ | - |
| I237 | $$94.4\pm 0.8$$ | $$1.28\pm $$0.02 | $$4.3\pm 0.9$$ | $$241\pm 7$$ | $$12000\pm 1000$$ | $$1.23\pm 0.01$$ | - | $$3.3\pm 0.7$$ | - |
| L252 (met 2) | $$99.86\pm 0.05$$ |  | $$0.14\pm 0.05$$ |  | $$1100\pm 200$$ |  |  | $$1.4\pm 0.5$$ | - |
| L259 (met 1) | $$74\pm 5$$ | $$26\pm 5$$ | $$0.11\pm 0.01$$ | $$320\pm 60$$ | $$860\pm 70$$ | $$-0.06\pm 0.01$$ | - | $$2.7\pm 0.2$$ | - |
| L269\* (met 2) | $$100\pm 2$$ |  | $$1\pm 2$$(0.2,0.3,4.6) |  | $$700\pm 200$$ |  |  | $$0.6\pm 0.2$$ | - |
| L279 (met 2) | $$100\pm 6$$ |  | $$0\pm 6$$(0.1,0.1,0.3) |  | $$1600\pm 800$$ |  |  | $$3.2\pm 0.7$$ | - |
| V285 (met 2) | $$100\pm 20$$ |  | $$0\pm 20$$(2,40,40) |  | $$13000\pm 7000$$ |  |  | $$3\pm 2$$ | - |