# Supplementary Data 6 - Modeling Results for the Agilent 6545 Q-TOF LC/MS [MS:1002791] platform for:

## LipidCreator workbench to probe the lipidomic landscape

Bing Peng[1,2,#], Dominik Kopczynski[1,#], Brian S Pratt[3], Christer S Ejsing[4,5], Bo Burla[6], Martin Hermansson[4,7], Peter Imre Benke[8], Sock Hwee Tan[9,10], Mark Y Chan[9,10,11], Federico Torta[8], Dominik Schwudke[12,13,14], Sven Meckelmann[15], Cristina Coman[1,17], Oliver J Schmitz[15], Brendan MacLean[3], Mailin-Christin Manke[16], Oliver Borst[16], Markus R Wenk[6,8], Nils Hoffmann[1], Robert Ahrends[1,17,*]

[1] Leibniz-Institut für Analytische Wissenschaften – ISAS - e.V., 44139 Dortmund, Germany

[2] Division of Rheumatology, Department of Medicine Solna, Karolinska Institutet, Karolinska University Hospital, SE-171 76 Stockholm, Sweden

[3] University of Washington, Department of Genome Sciences, WA 98195 Seattle, USA

[4] Department of Biochemistry and Molecular Biology, University of Southern Denmark, DK-5230 Odense, Denmark

[5] Cell Biology and Biophysics Unit, European Molecular Biology Laboratory, 69117 Heidelberg, Germany

[6] Singapore Lipidomics Incubator (SLING), Life Science Institute, National University of Singapore, 117456 Singapore, Singapore

[7] Wihuri Research Institute, 00290 Helsinki, Finland

[8] Singapore Lipidomics Incubator (SLING), Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore, 117596 Singapore, Singapore

[9] Department of Medicine, Yong Loo Lin School of Medicine, National University Hospital, 119228 Singapore, Singapore

[10] Cardiovascular Research Institute, National University of Singapore, 117599 Singapore, Singapore

[11] National University Heart Centre, National University Health System, 117599 Singapore, Singapore

[12] Research Center Borstel, Leibniz Lung Center, Borstel, Germany

[13] German Center for Infection Research (DZIF), 38124 Braunschweig, Germany

[14] Airway Research Center North Member of the German Center for Lung Research (DZL), 22927 Großhansdorf, Germany

[15] Institute of Applied Analytical Chemistry, University of Duisburg-Essen, 45141 Essen, Germany

[16] Department of Cardiology and Cardiovascular Medicine, University of Tübingen, 72076 Tübingen, Germany

[17] Department of Analytical Chemistry, University of Vienna, Währinger Strasse 38, 1090 Vienna, Austria

[#] Two authors contributed equally to this work

[*] Corresponding author

# Table of Contents

# 1. Agilent 6545 Q-TOF LC/MS [MS:1002791]

## 1.1. 10-HDoHE [M-H]1- 1min0239

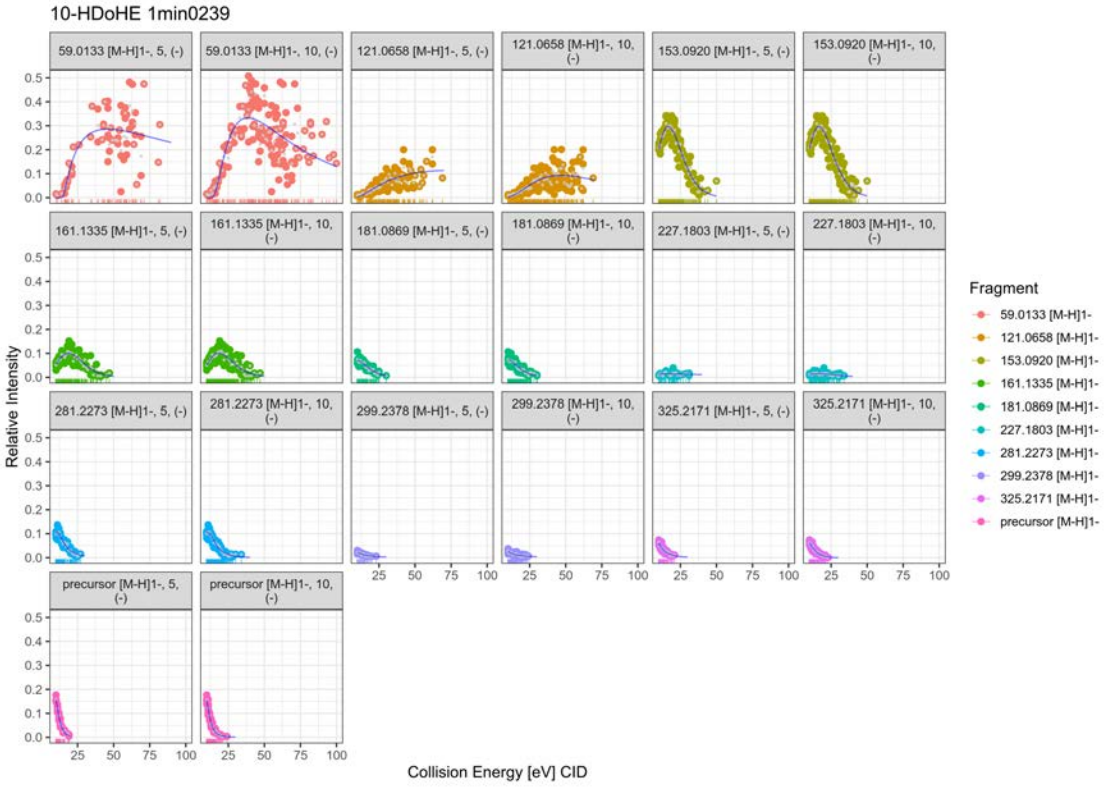


*Figure 1. Nonlinear fit*

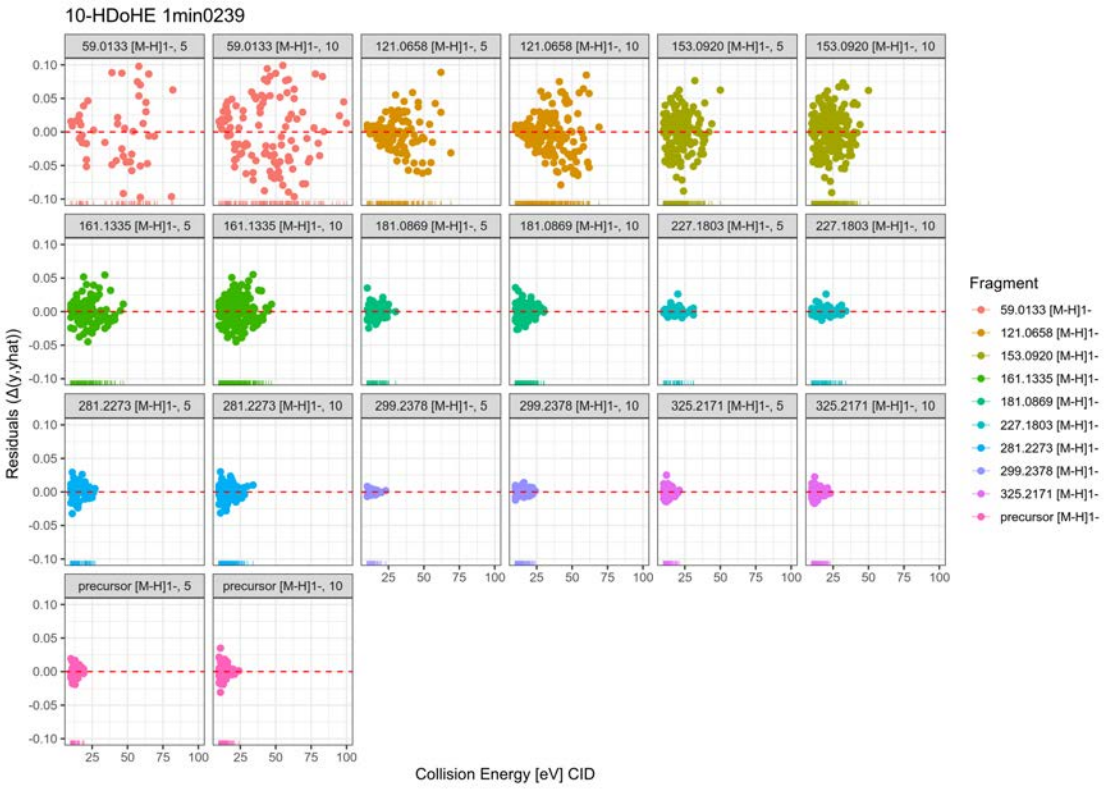


*Figure 2. Residuals of nonlinear fit*

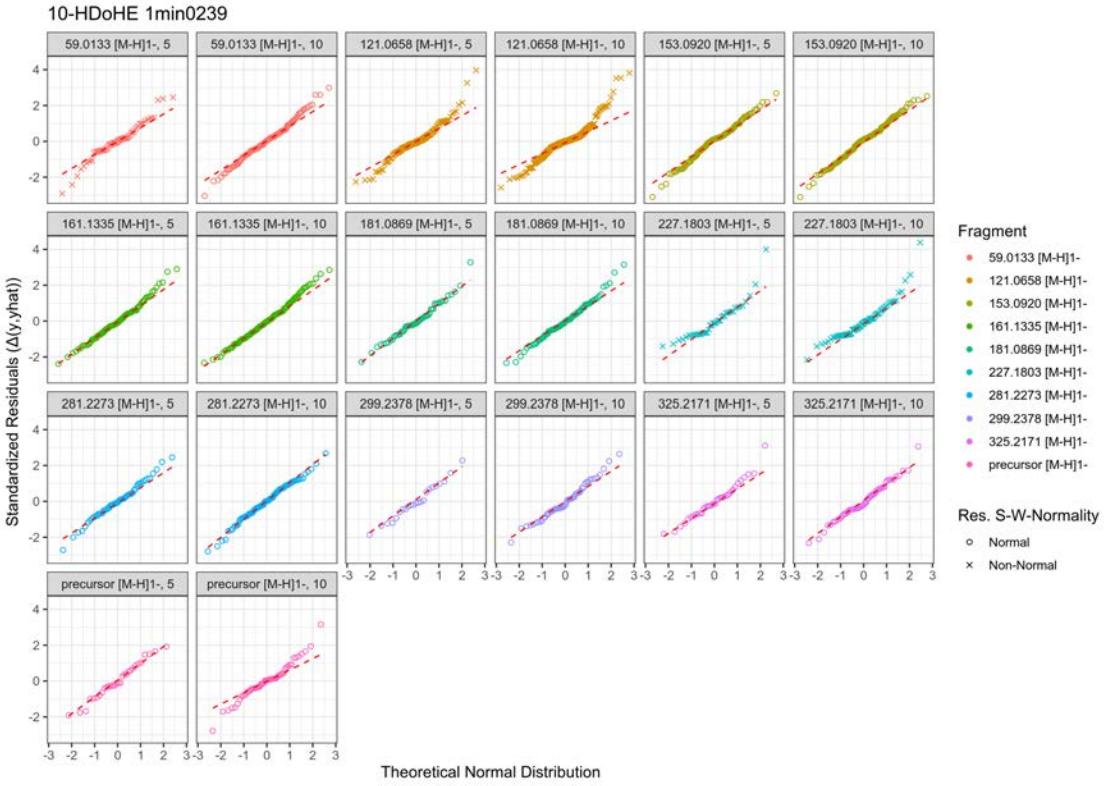


*Figure 3. Quantile-quantile plot of residuals*

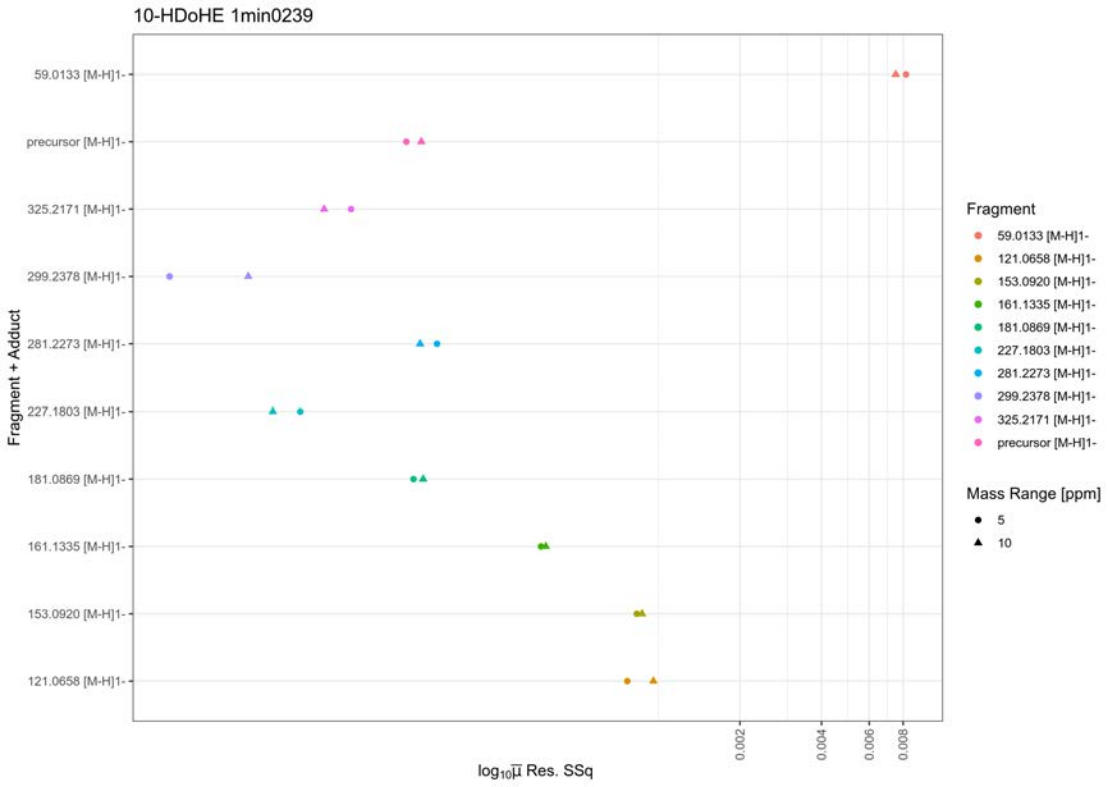


*Figure 4. Normalized sum-of-squares of the residuals*

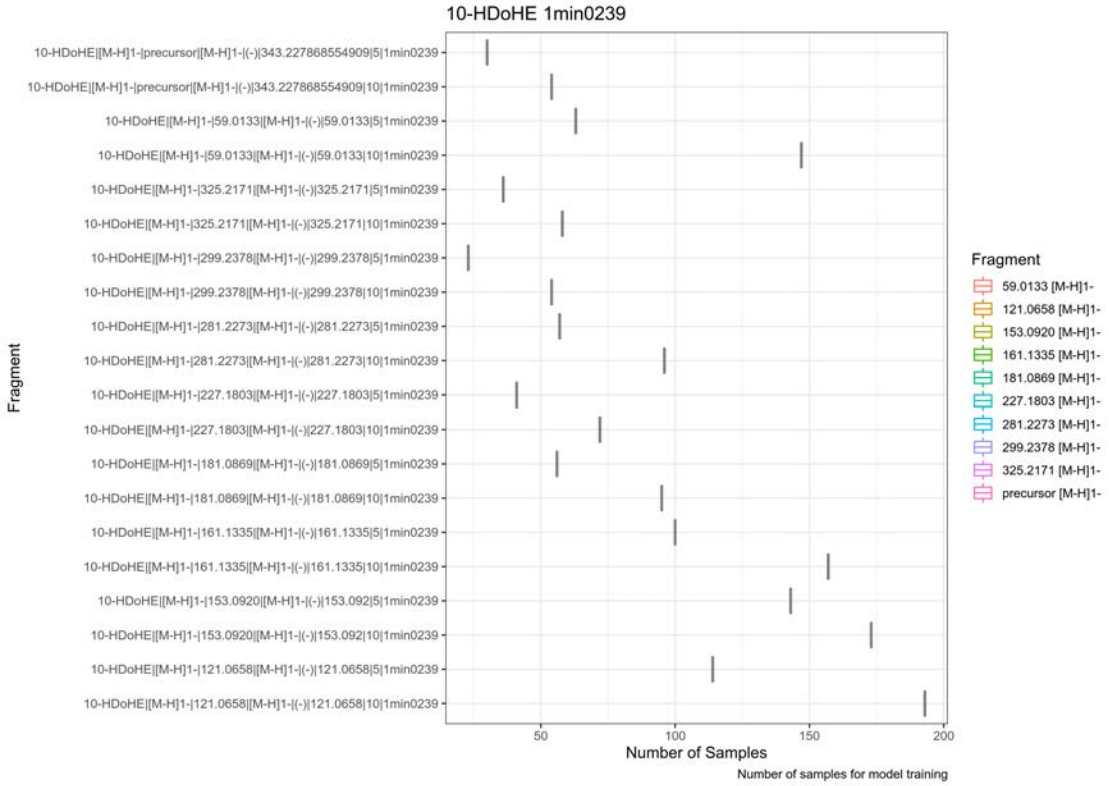


*Figure 5. Number of samples used for training per combination Id*

# 1.2. 11(12)-EET{d11} [M-H]1- 1min0077

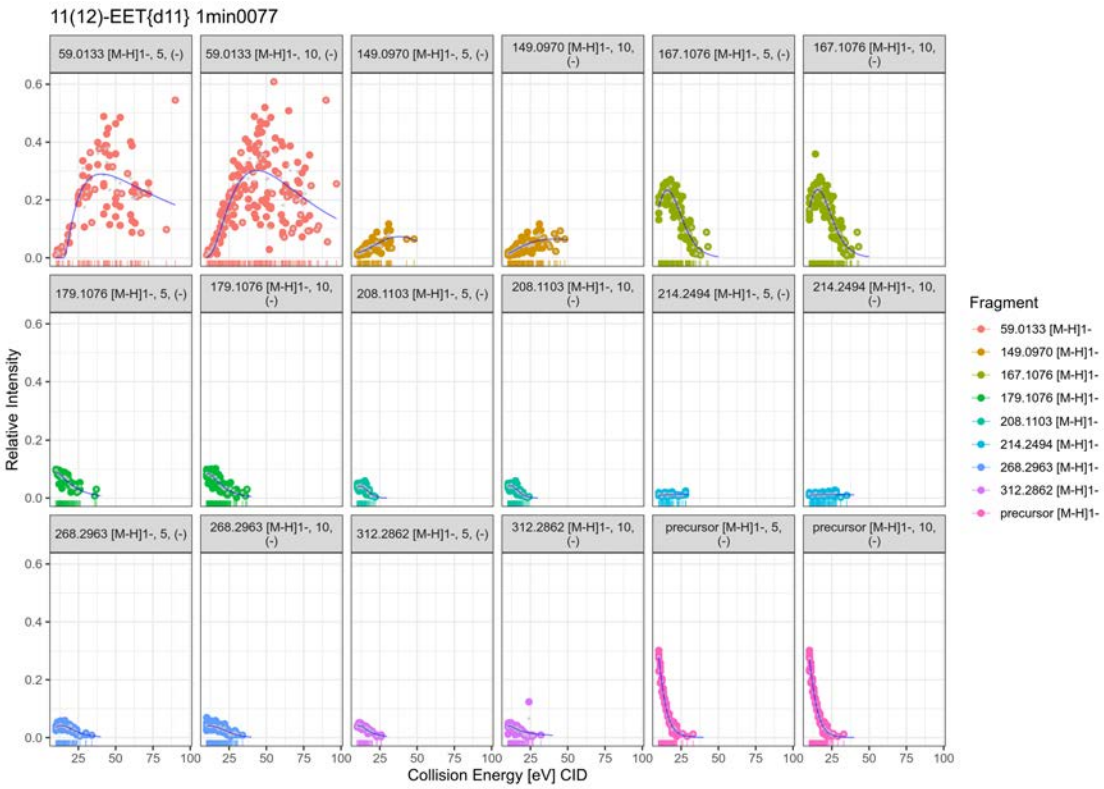


*Figure 6. Nonlinear fit*

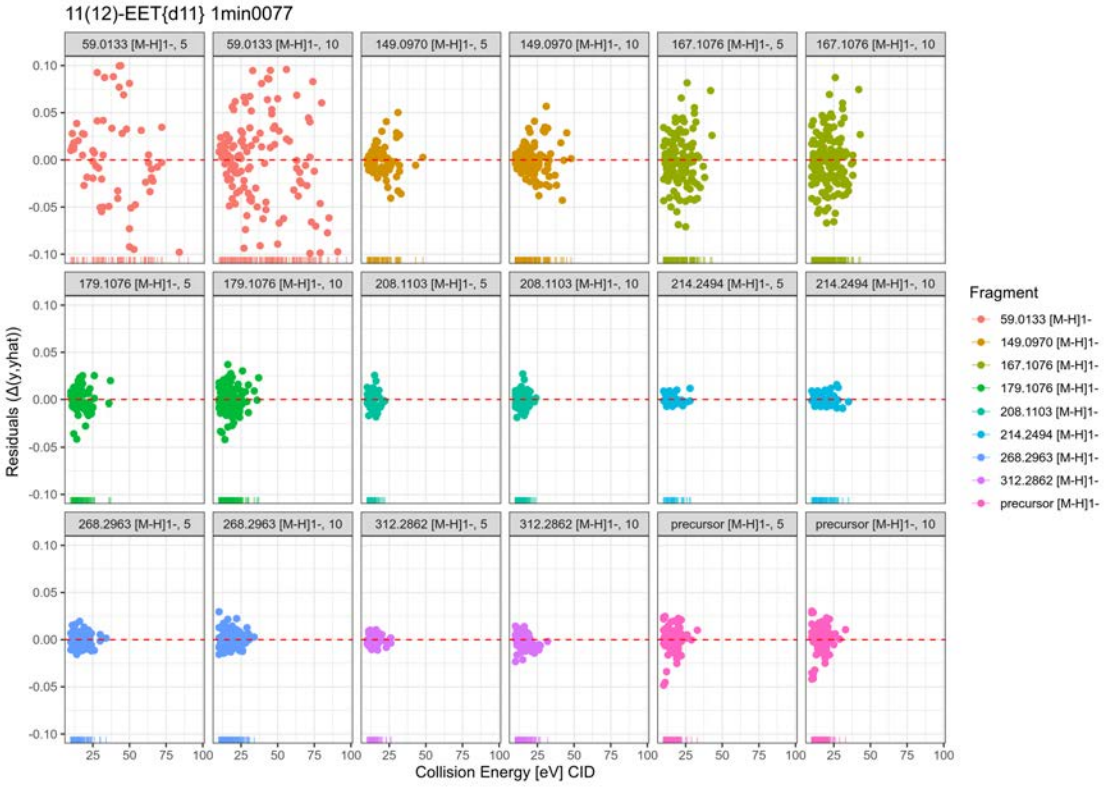


*Figure 7. Residuals of nonlinear fit*

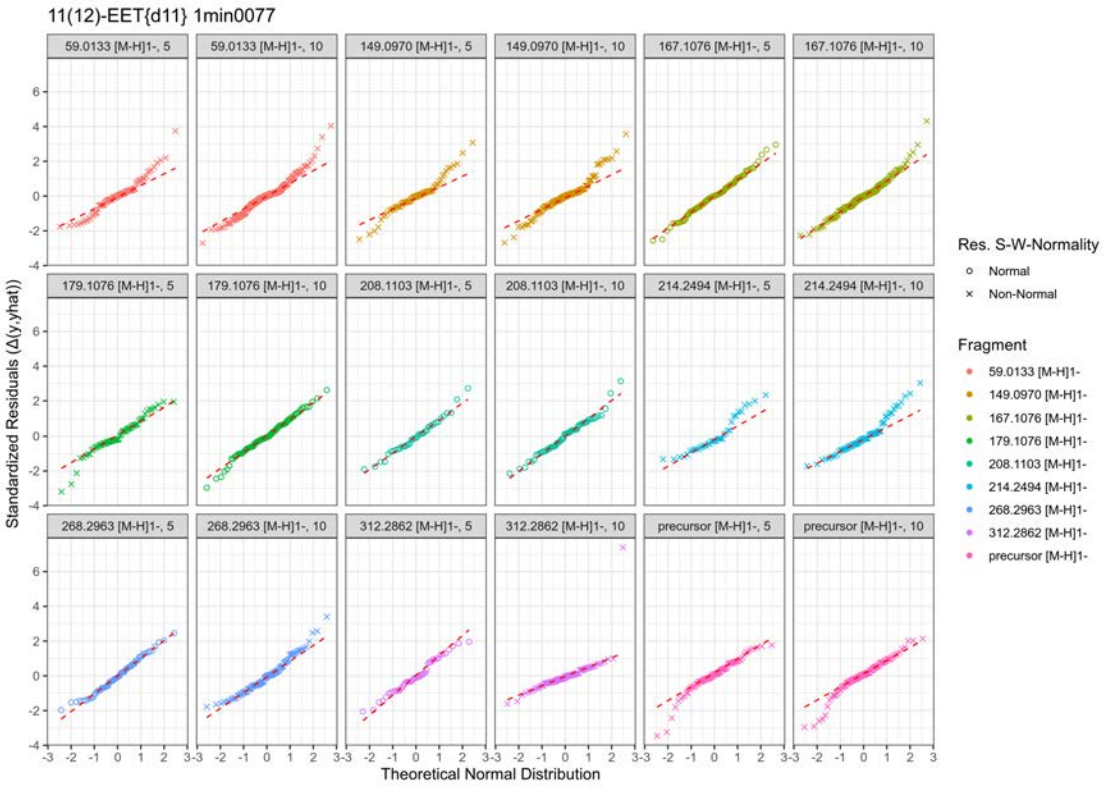


*Figure 8. Quantile-quantile plot of residuals*

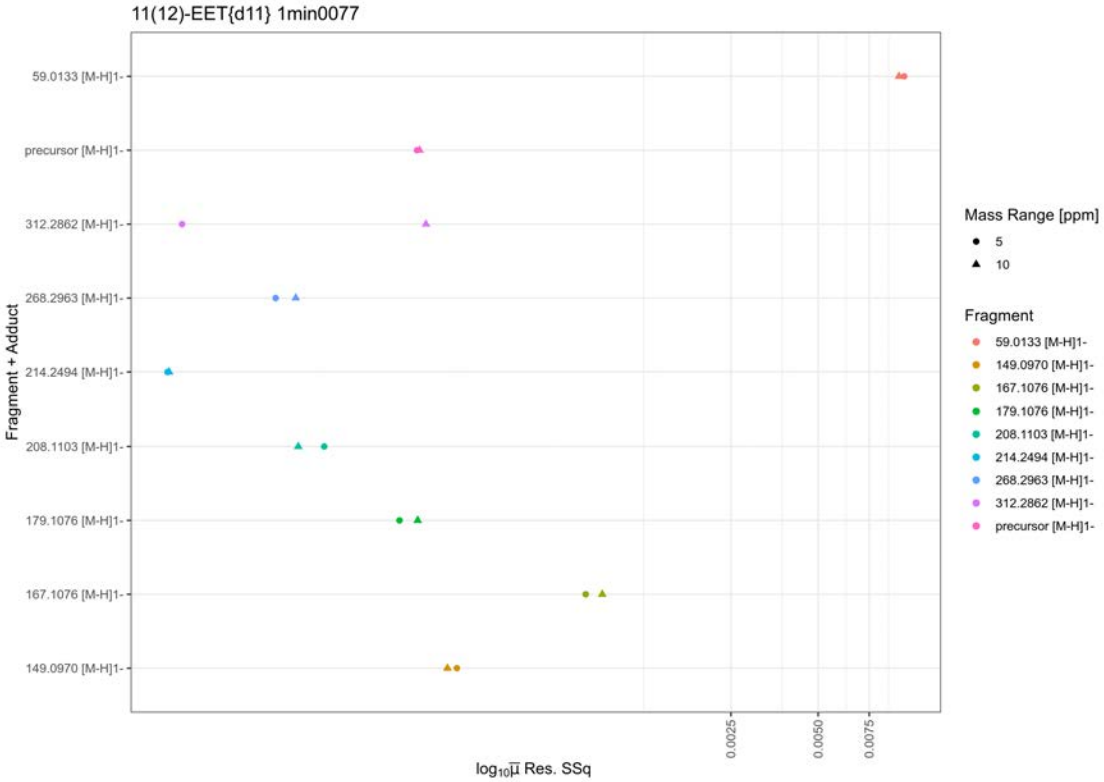


*Figure 9. Normalized sum-of-squares of the residuals*

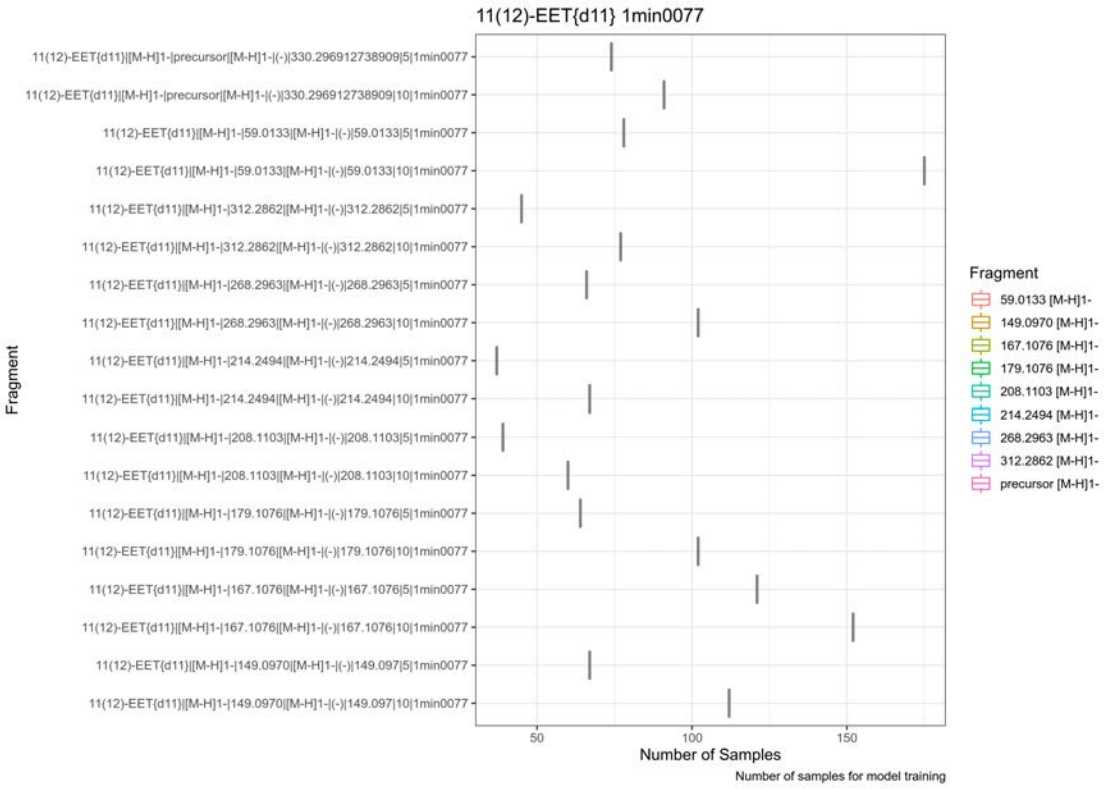


*Figure 10. Number of samples used for training per combination Id*

# 1.3. 11,12-DHET{d11} [M-H]1- 1min0230

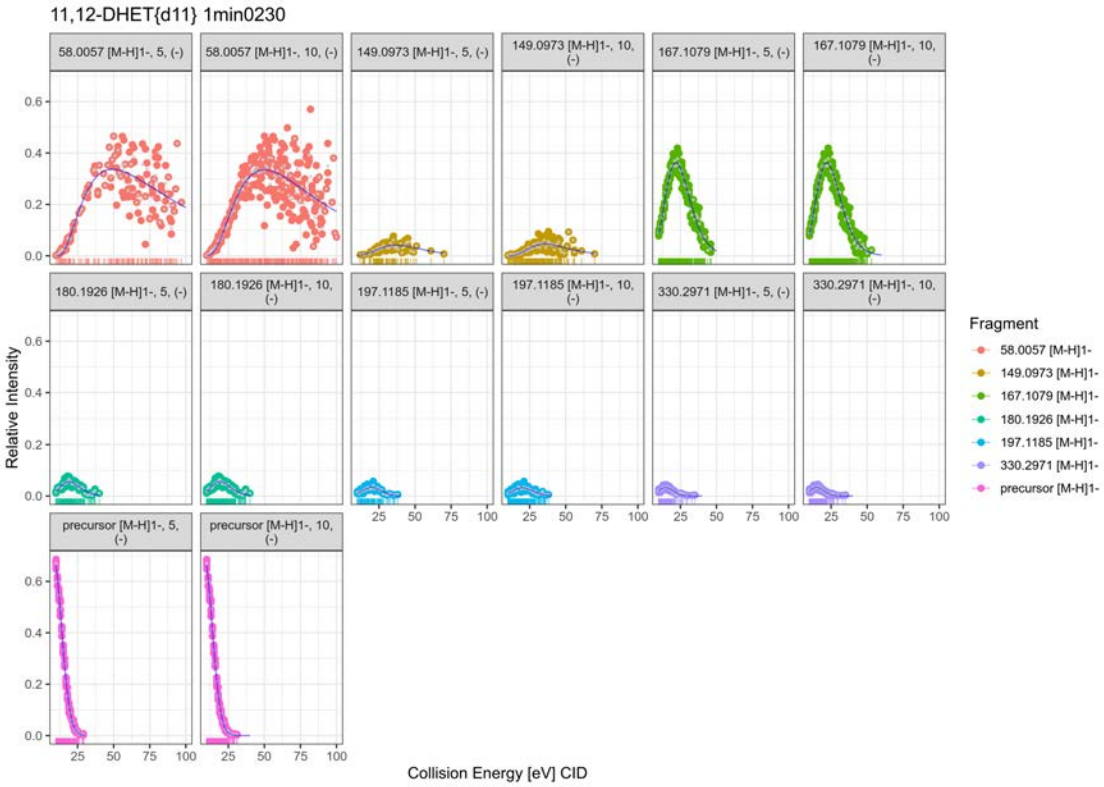


*Figure 11. Nonlinear fit*

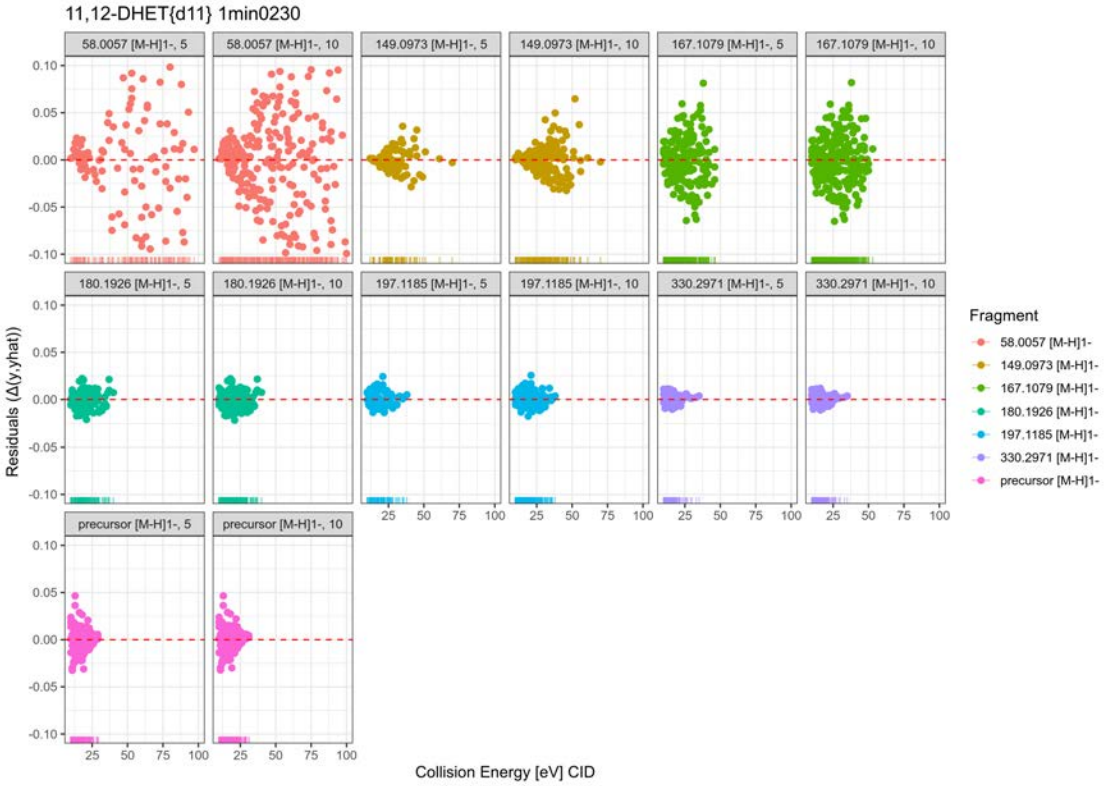


*Figure 12. Residuals of nonlinear fit*

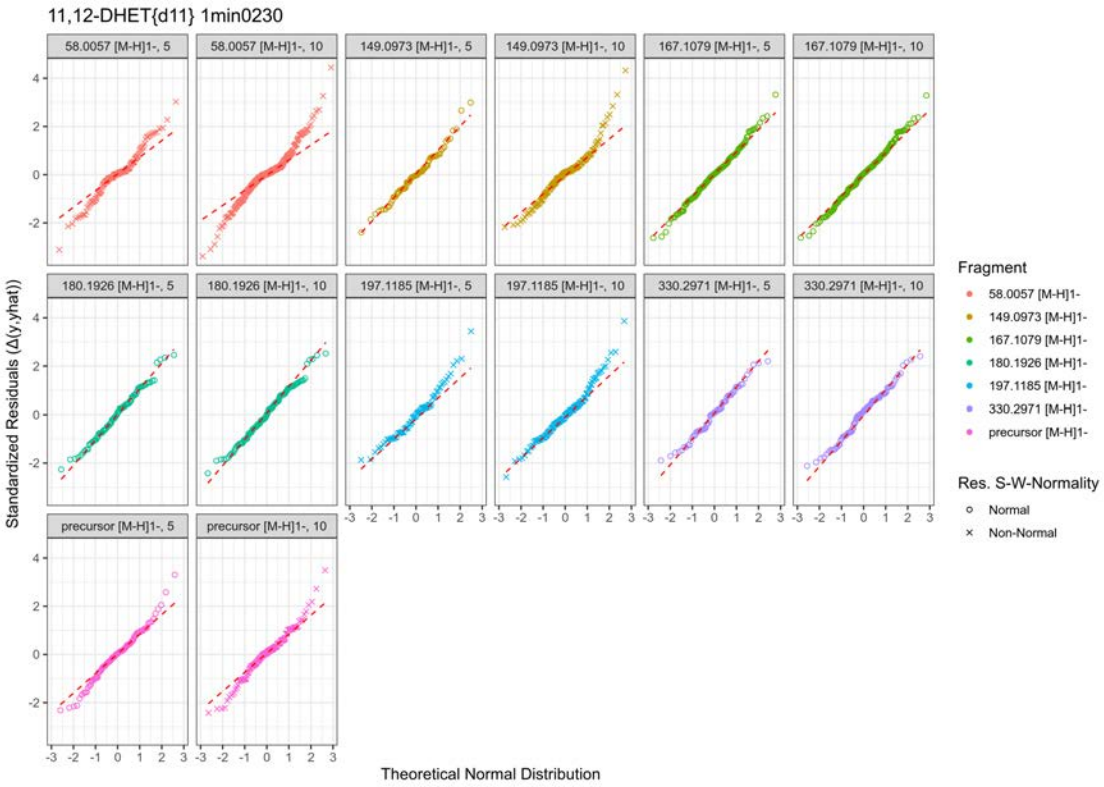


*Figure 13. Quantile-quantile plot of residuals*

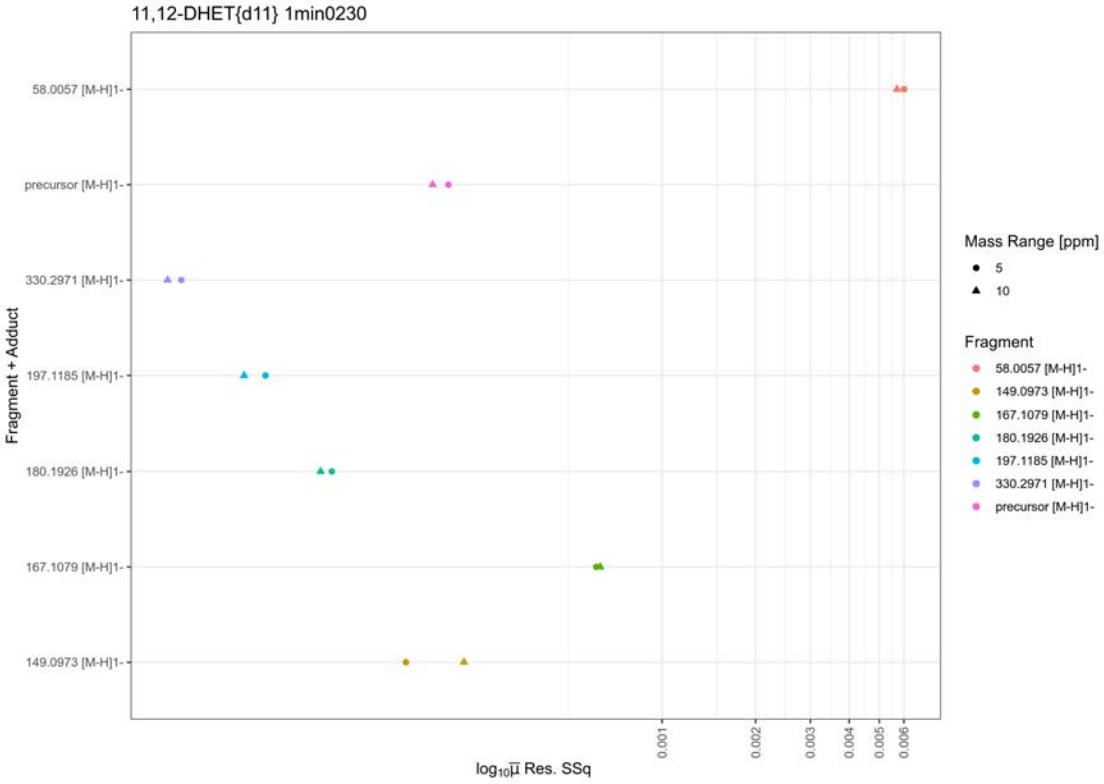


*Figure 14. Normalized sum-of-squares of the residuals*

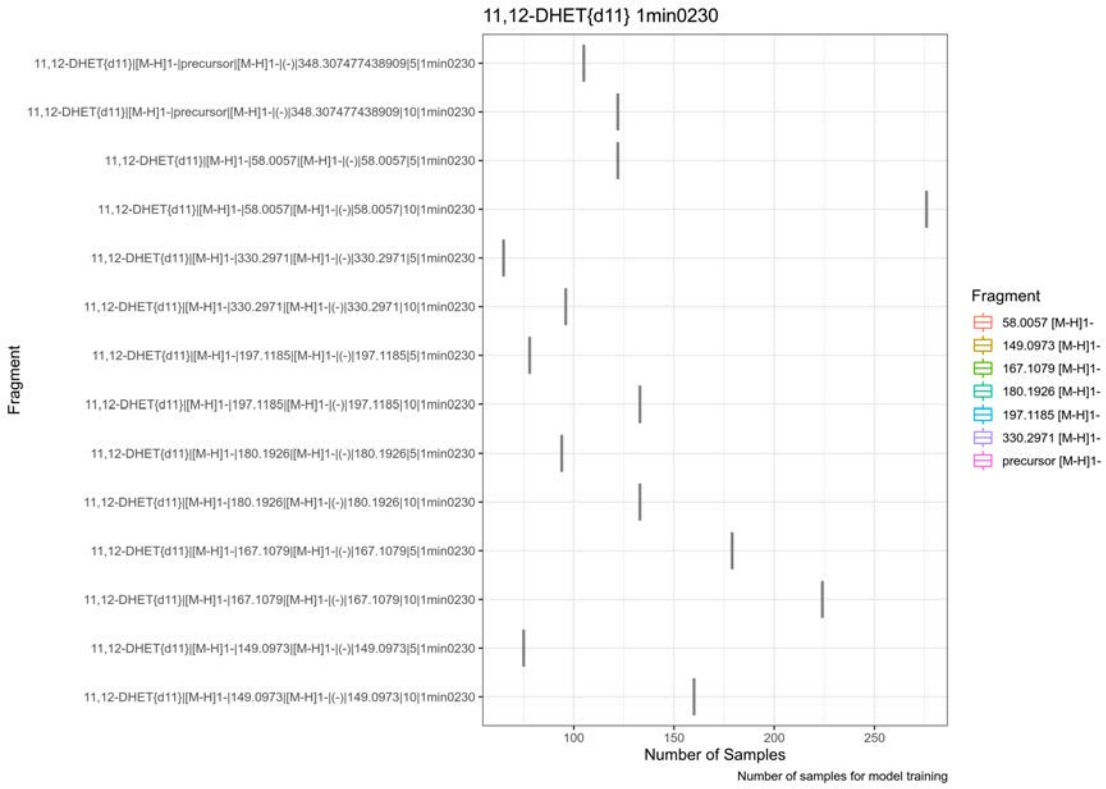


*Figure 15. Number of samples used for training per combination Id*

# 1.4. 11-HDoHE [M-H]1- 1min0079

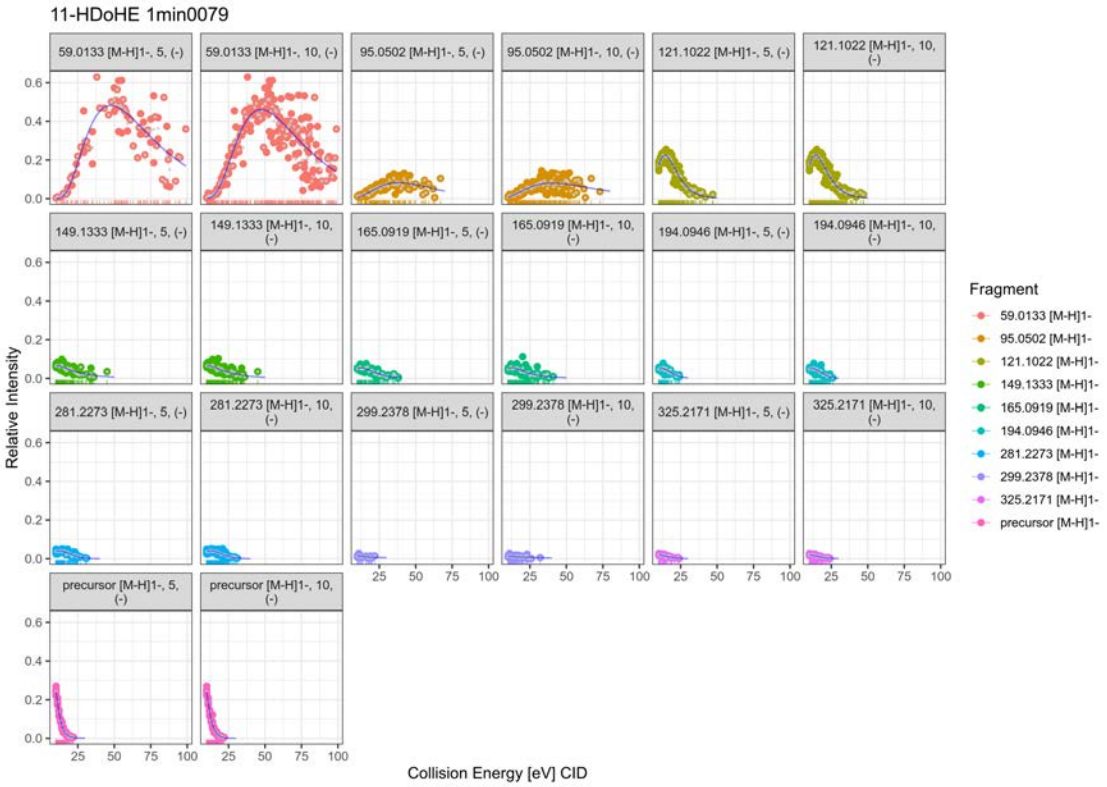


*Figure 16. Nonlinear fit*

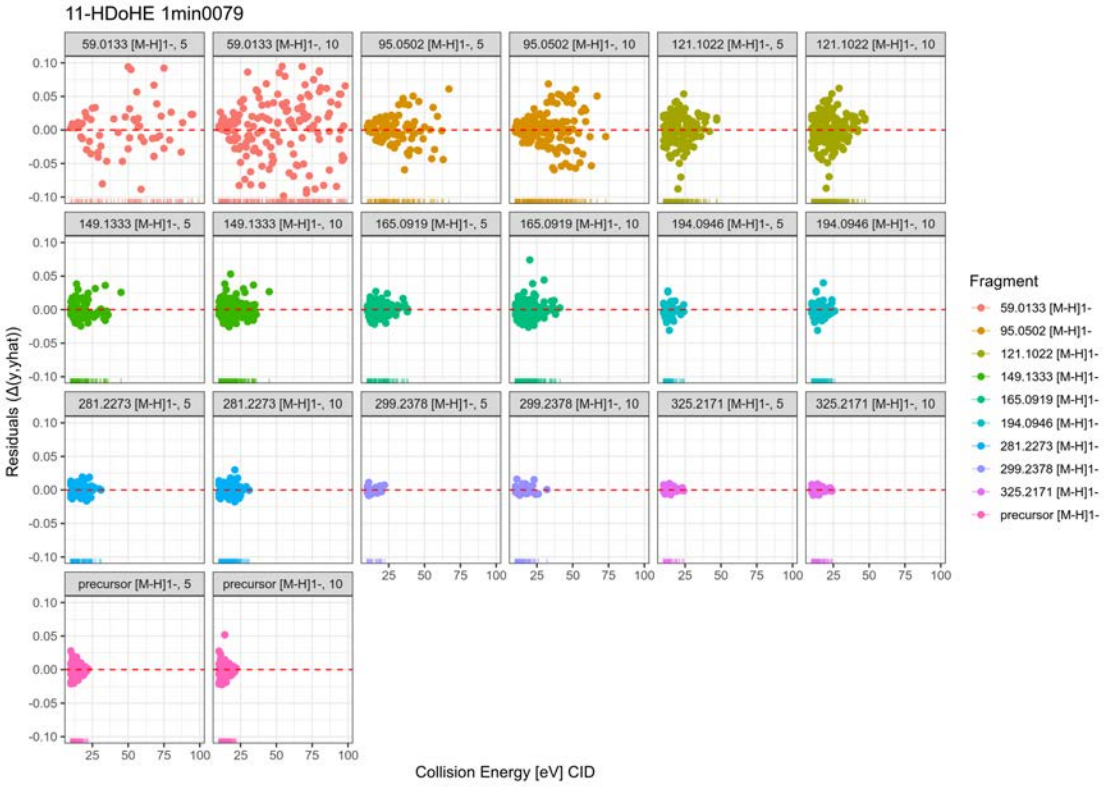


*Figure 17. Residuals of nonlinear fit*

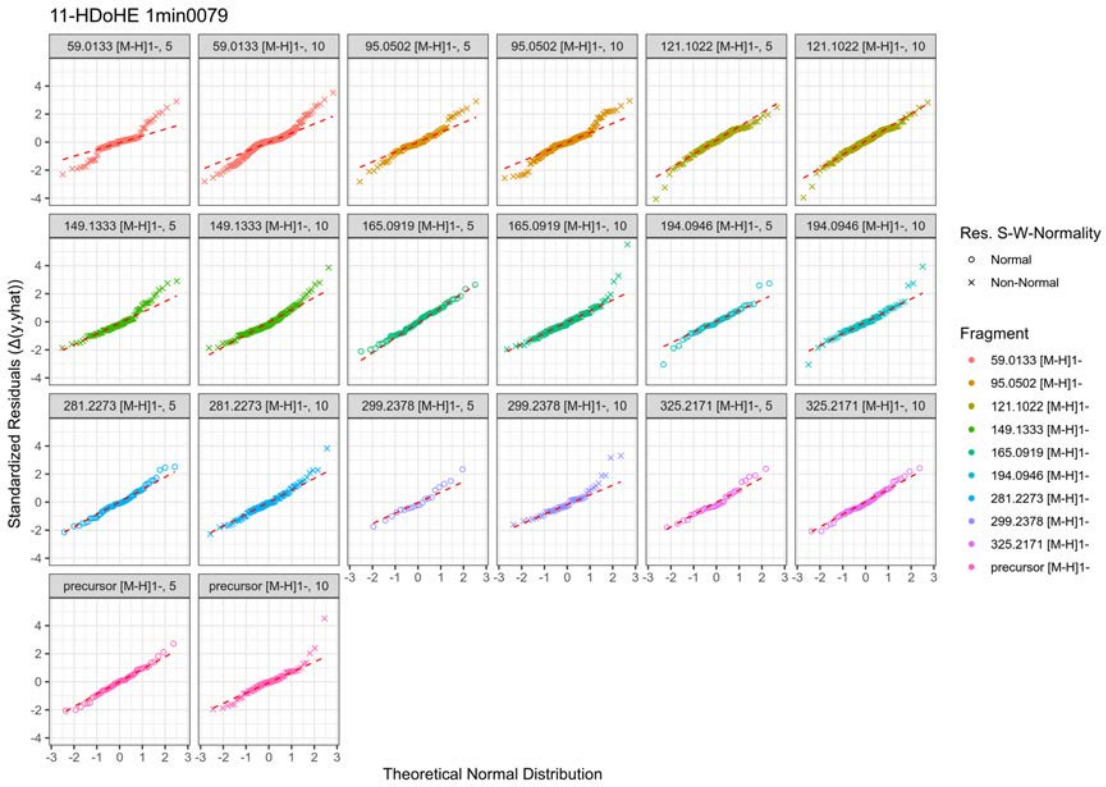


*Figure 18. Quantile-quantile plot of residuals*

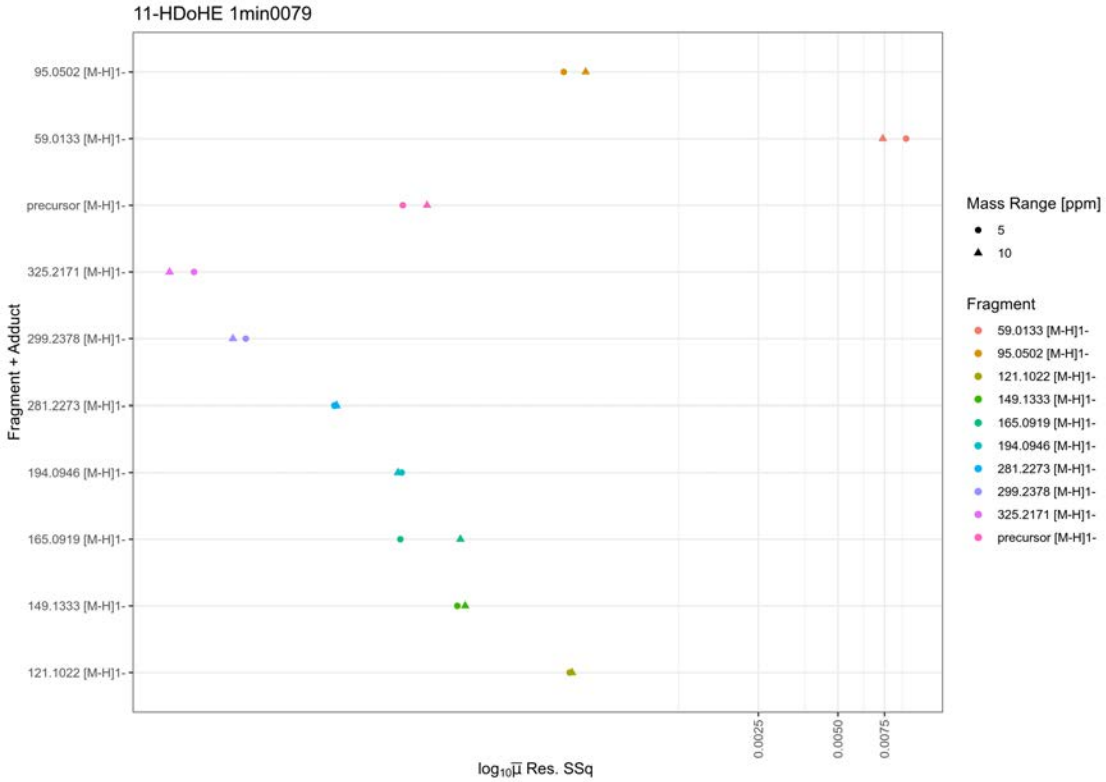


*Figure 19. Normalized sum-of-squares of the residuals*

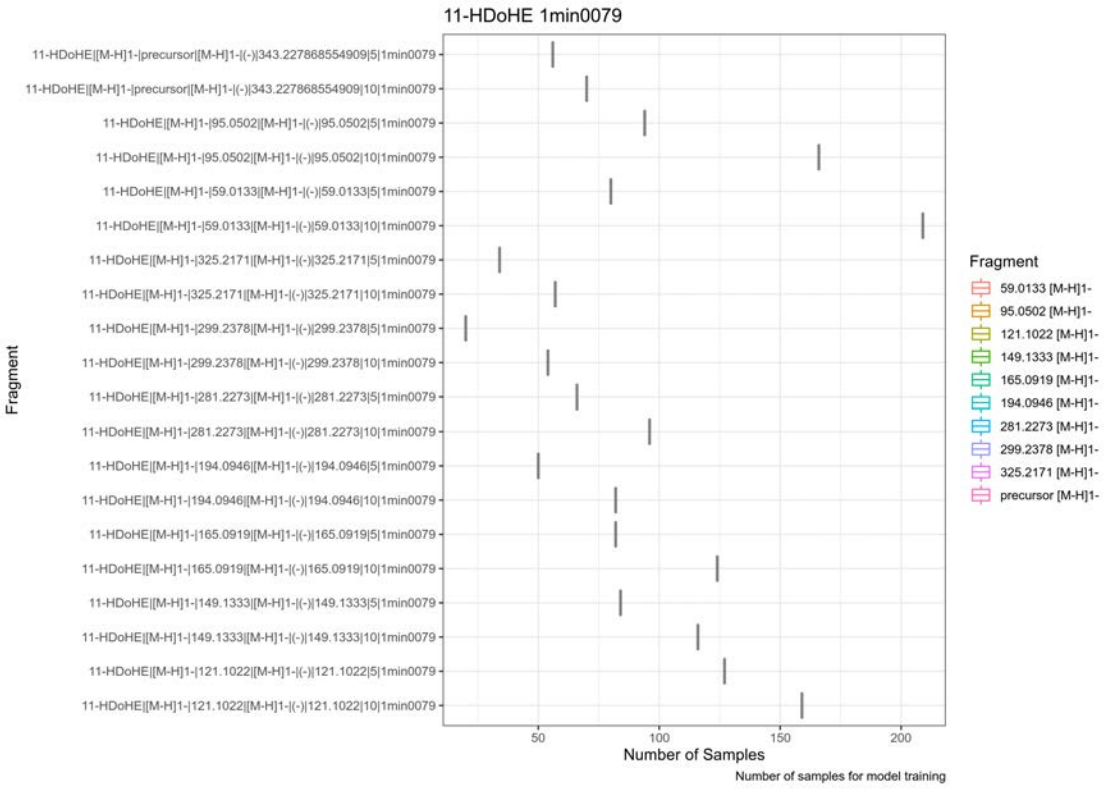


*Figure 20. Number of samples used for training per combination Id*

# 1.5. 11-HETE [M-H]1- 1min0081

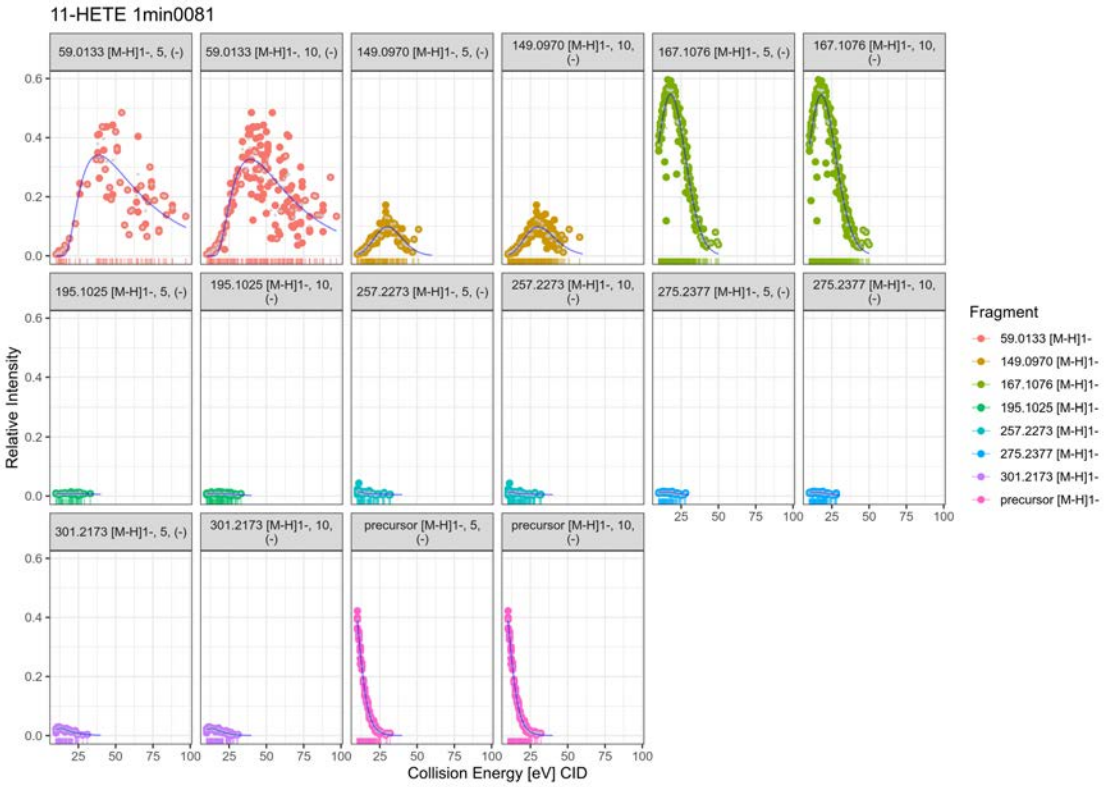


*Figure 21. Nonlinear fit*

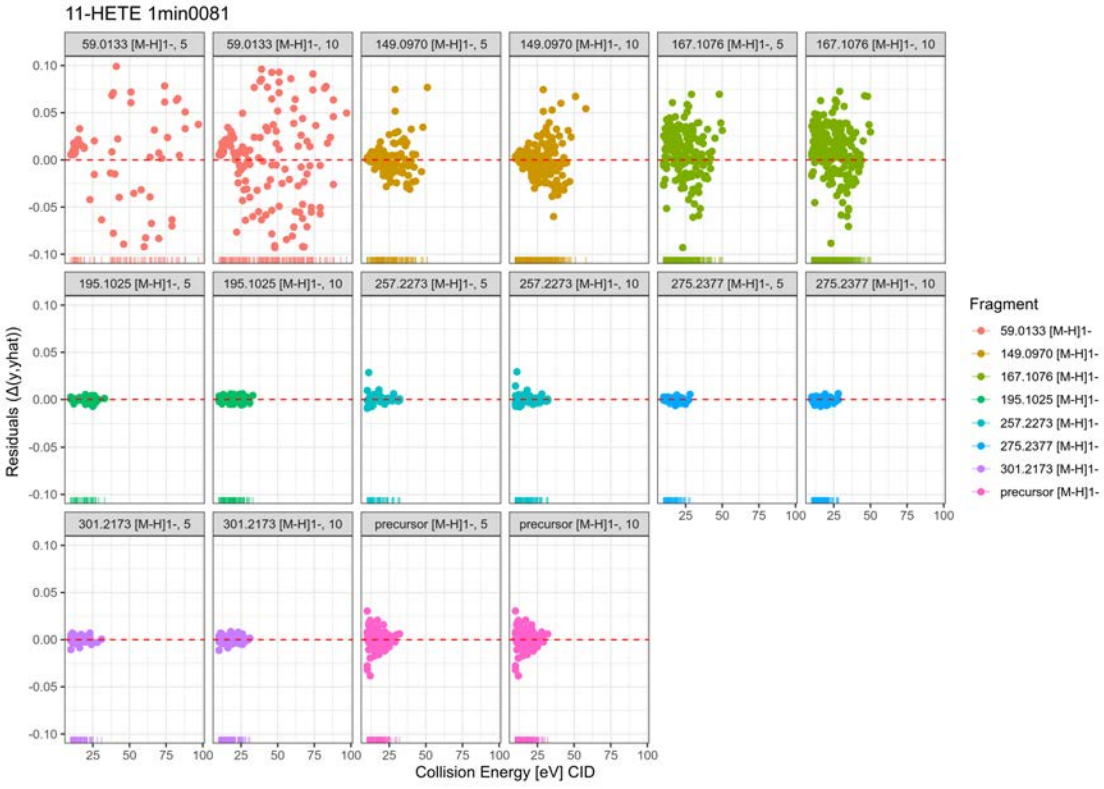


*Figure 22. Residuals of nonlinear fit*

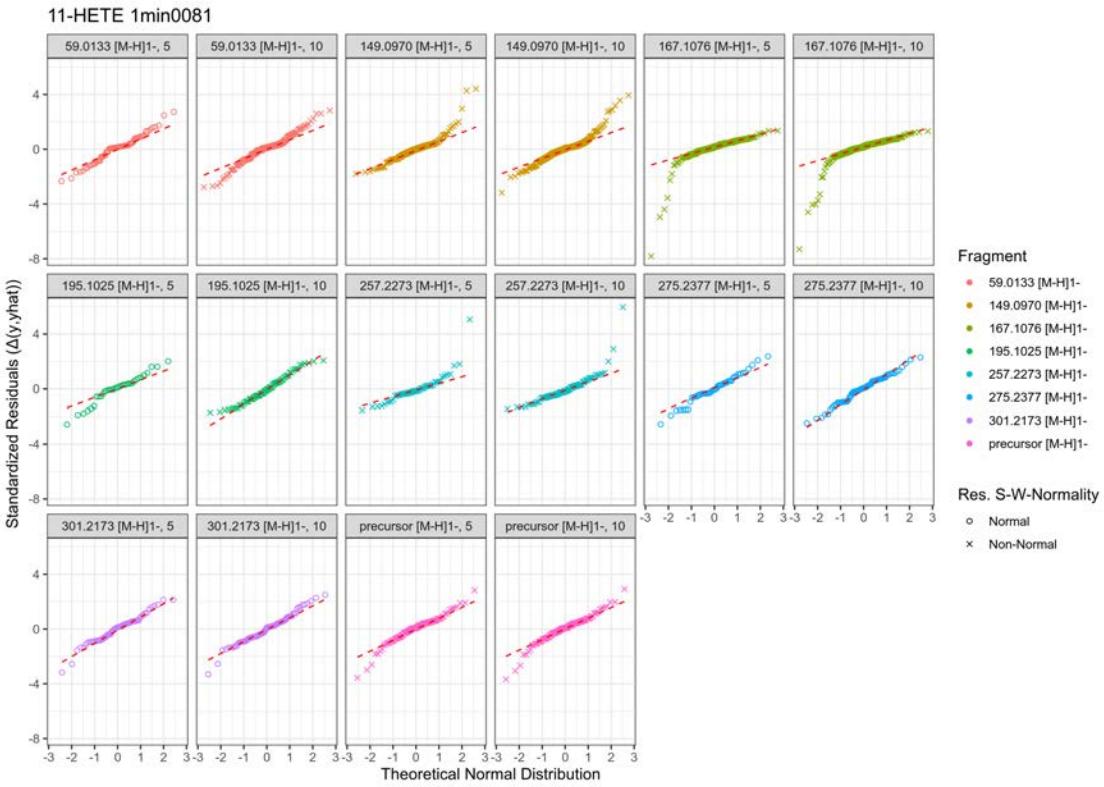


*Figure 23. Quantile-quantile plot of residuals*

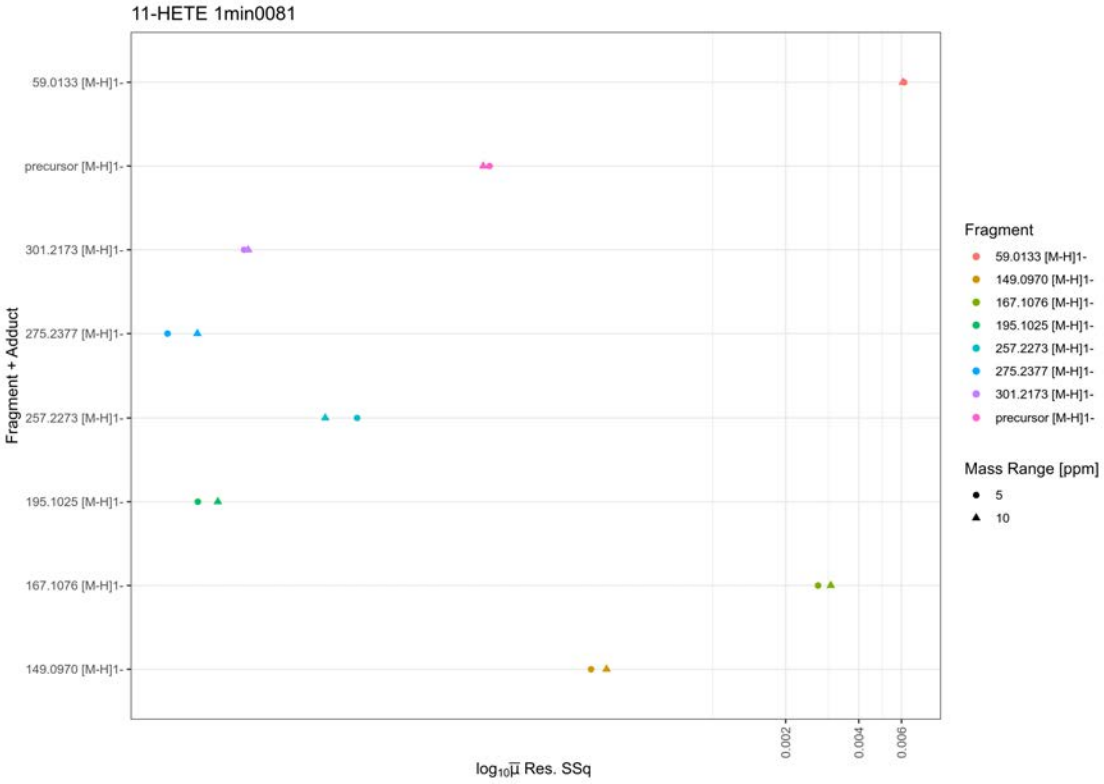


*Figure 24. Normalized sum-of-squares of the residuals*

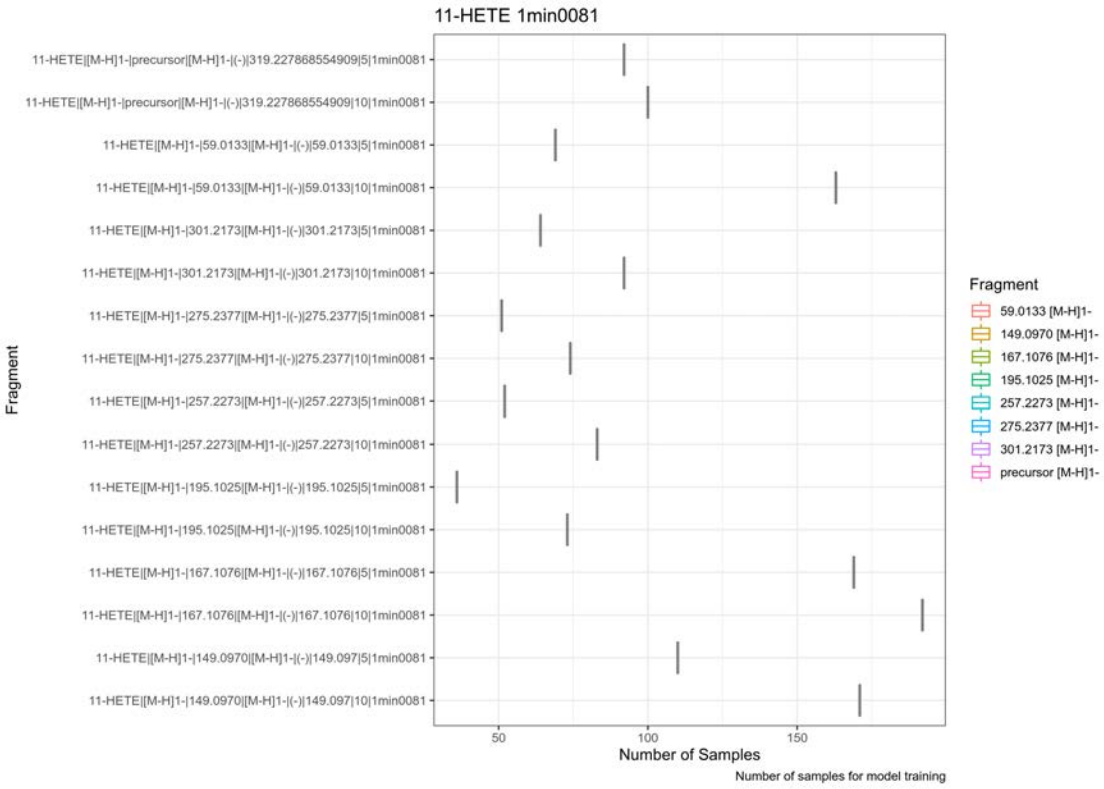


*Figure 25. Number of samples used for training per combination Id*

# 1.6. 12(13)-EpOME{d4} [M-H]1- 1min0082

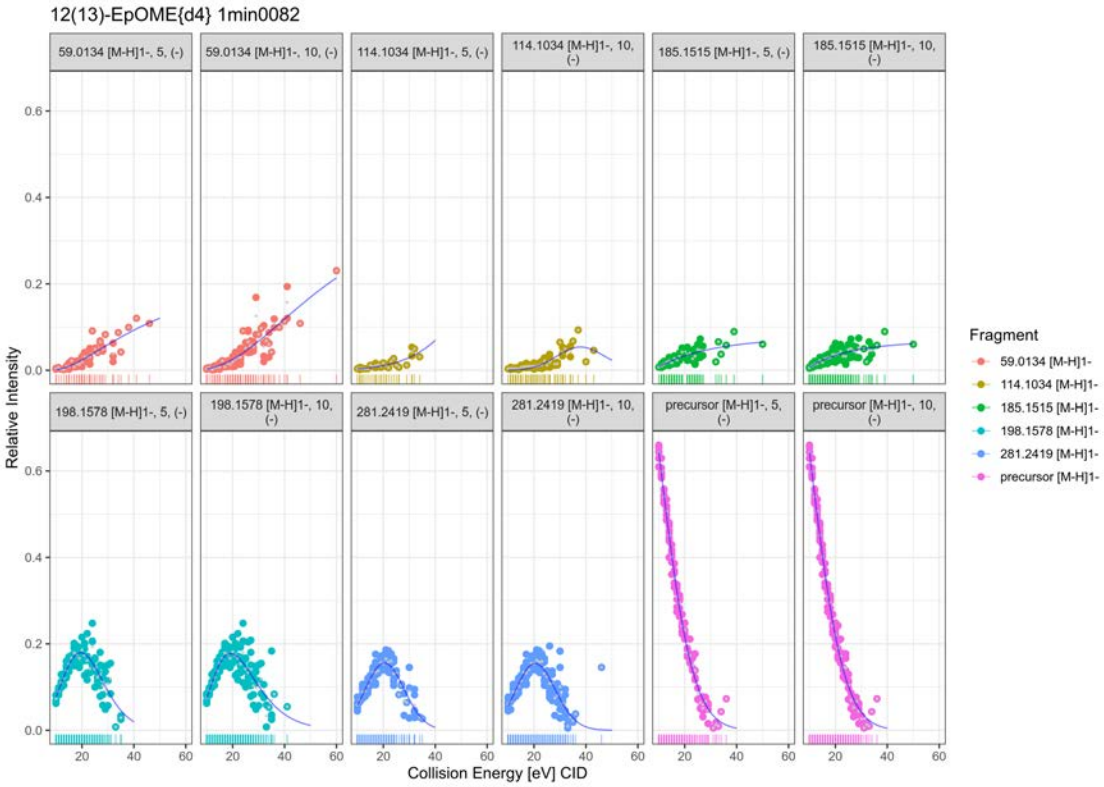


*Figure 26. Nonlinear fit*

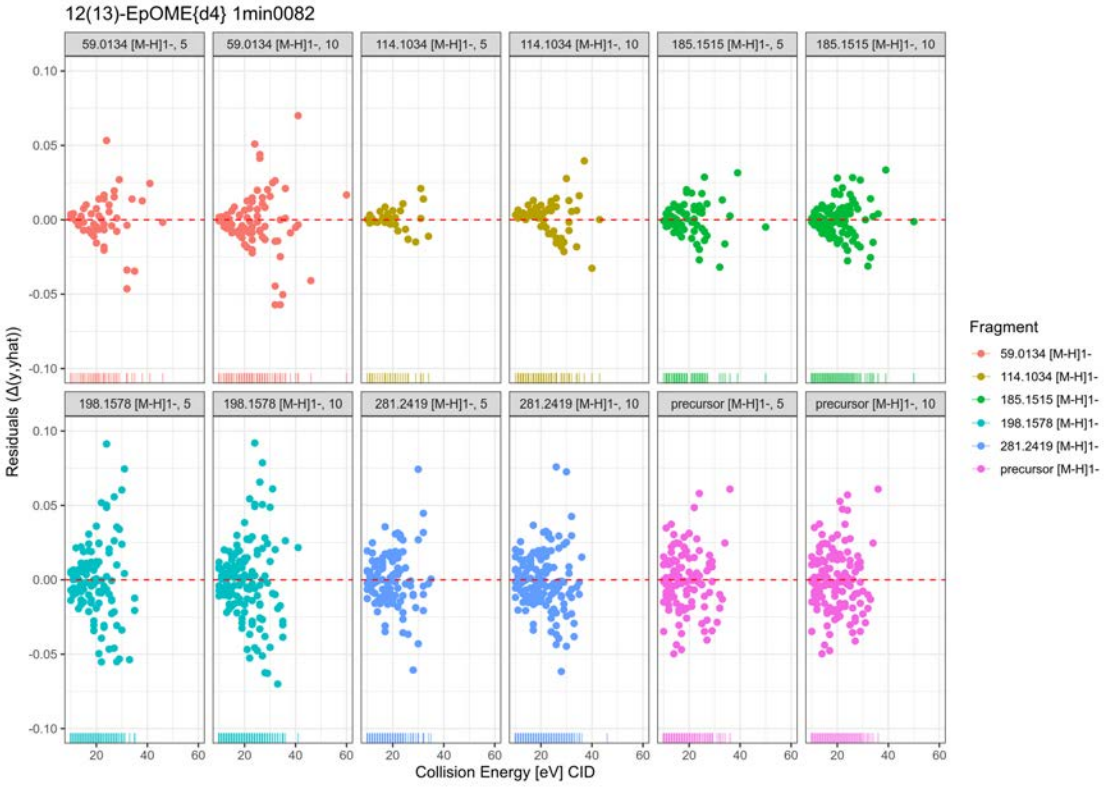


*Figure 27. Residuals of nonlinear fit*

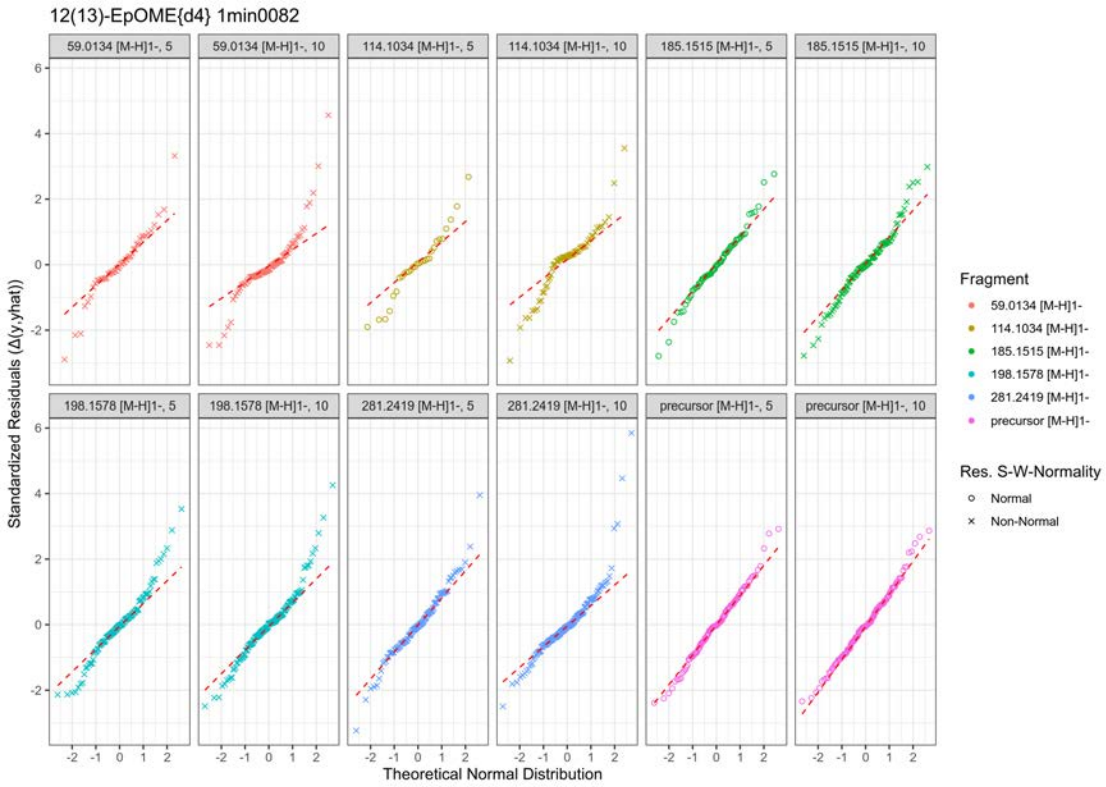


*Figure 28. Quantile-quantile plot of residuals*

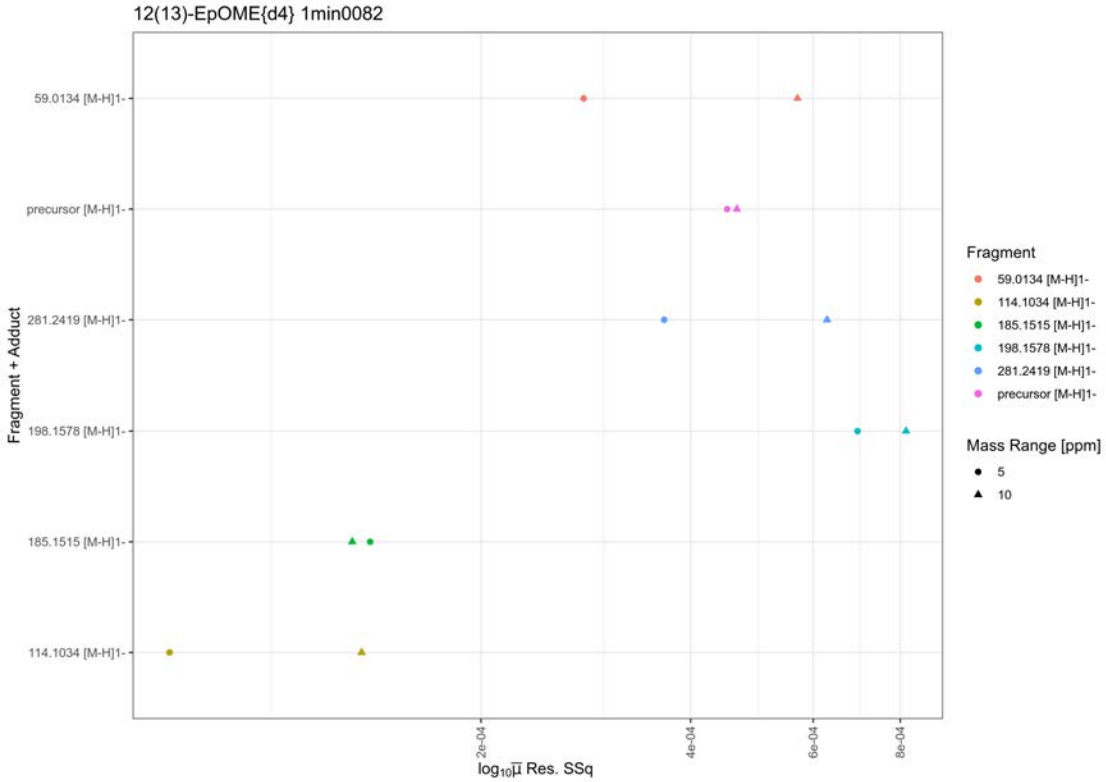


*Figure 29. Normalized sum-of-squares of the residuals*

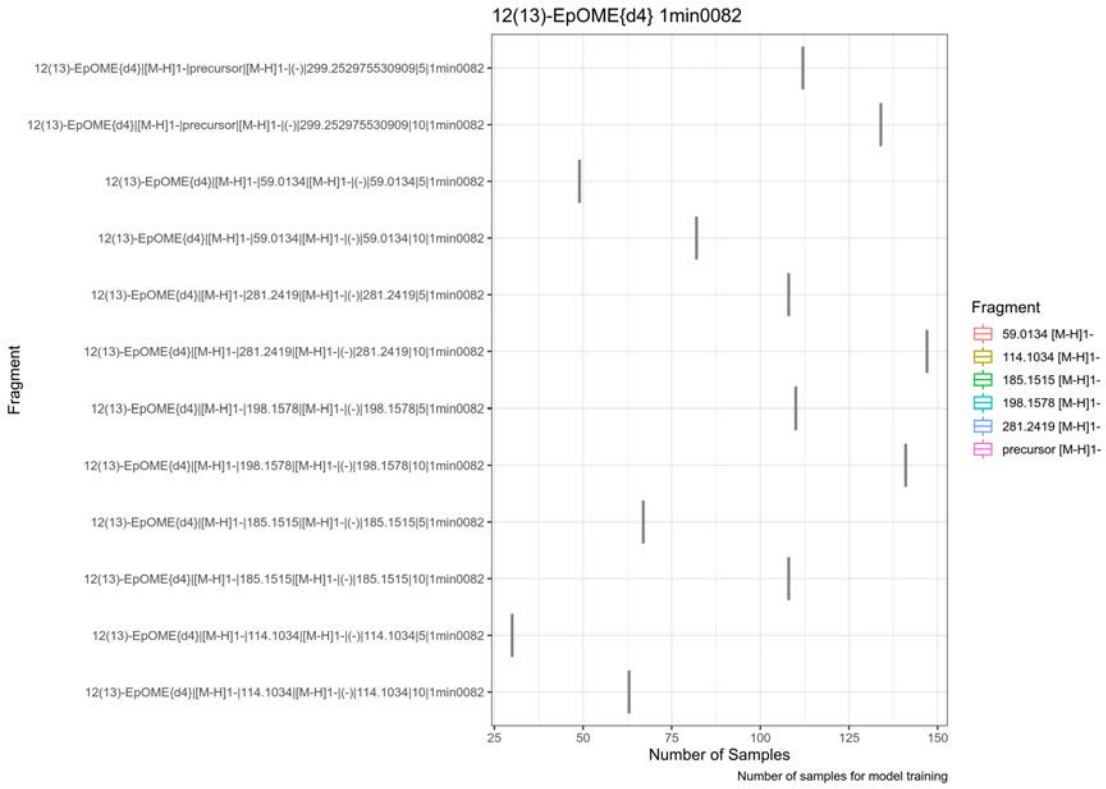


*Figure 30. Number of samples used for training per combination Id*

# 1.7. 12-HEPE [M-H]1- 1min0085

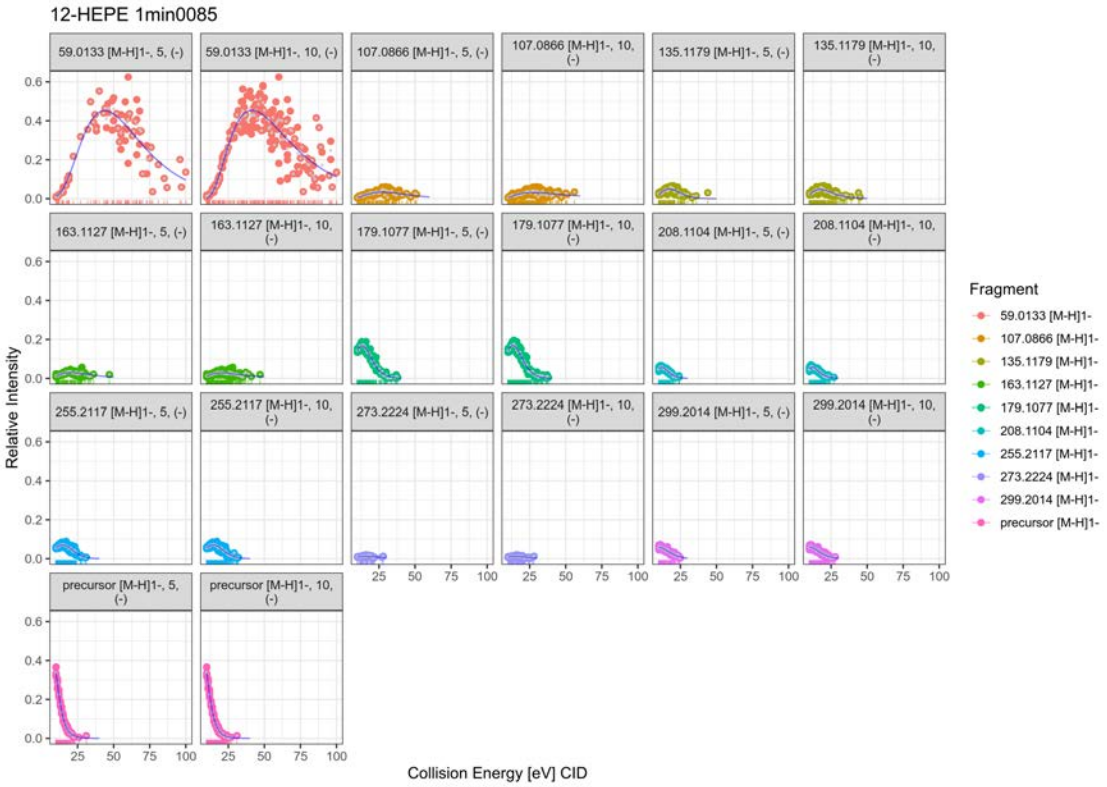


*Figure 31. Nonlinear fit*

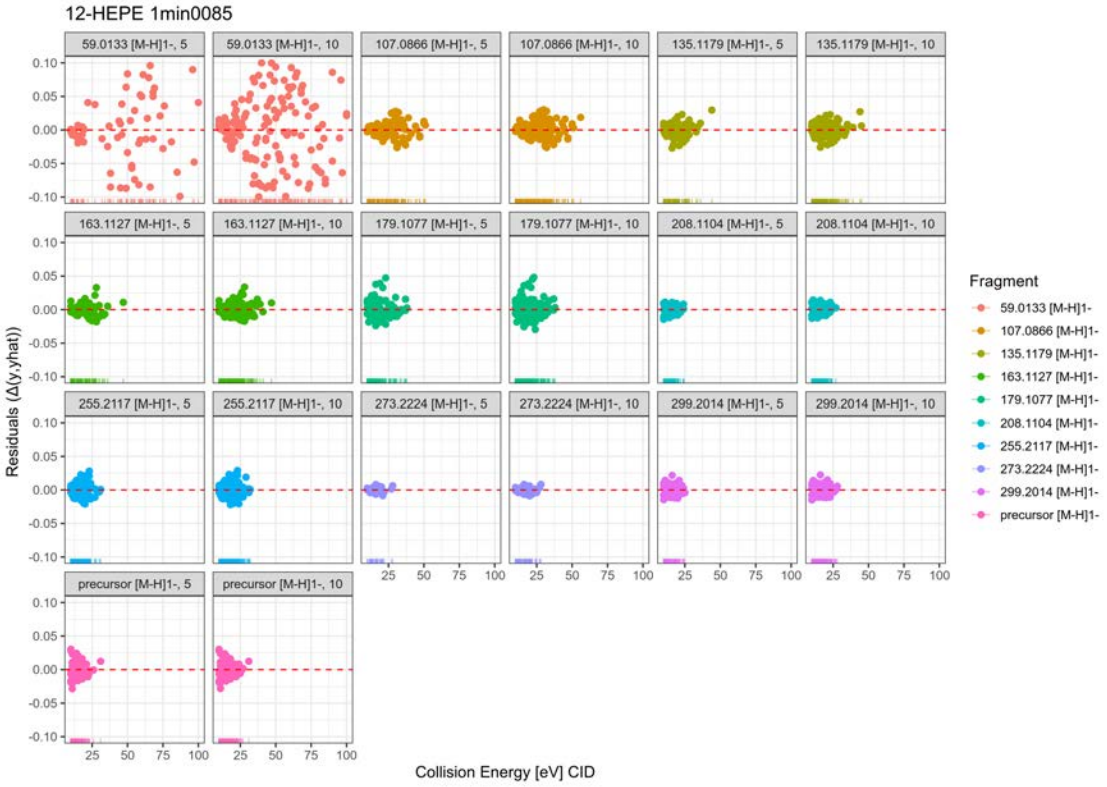


*Figure 32. Residuals of nonlinear fit*

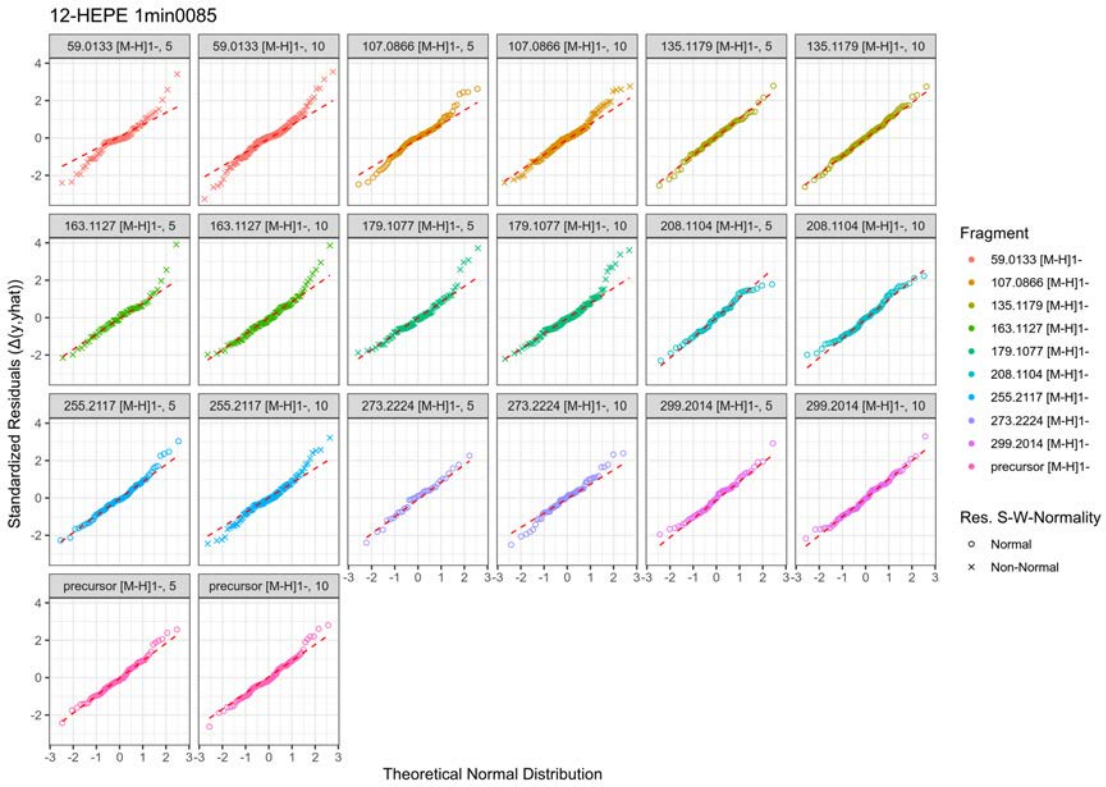


*Figure 33. Quantile-quantile plot of residuals*

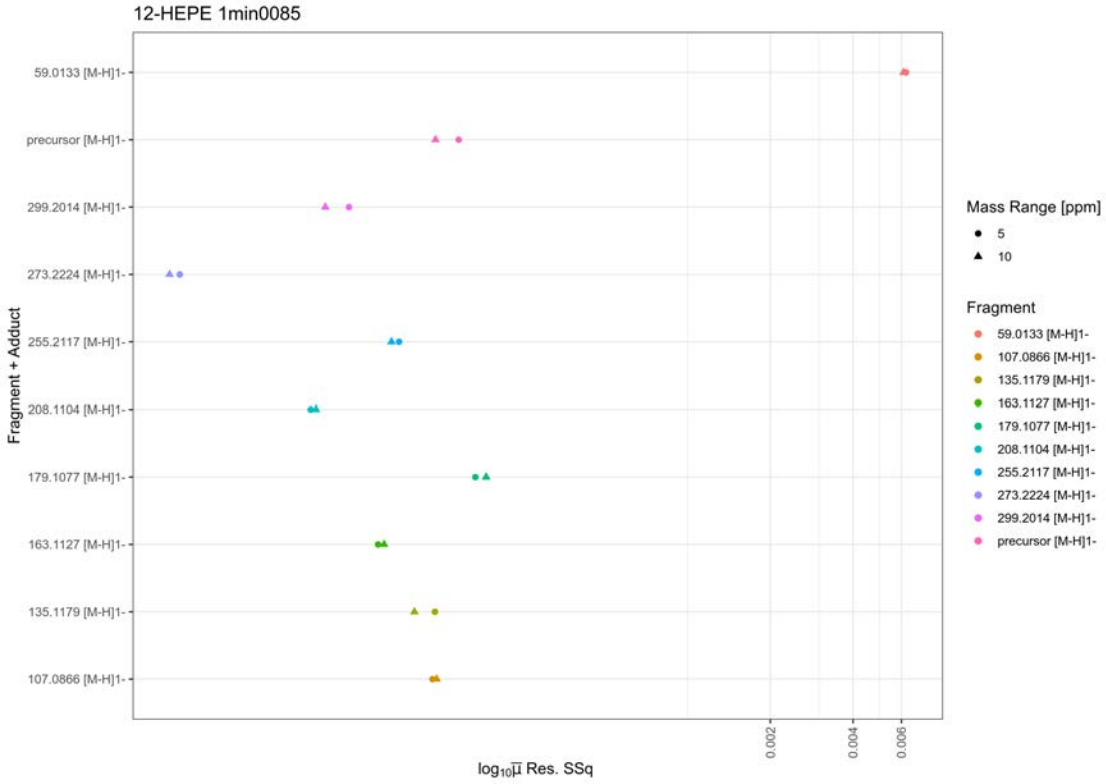


*Figure 34. Normalized sum-of-squares of the residuals*

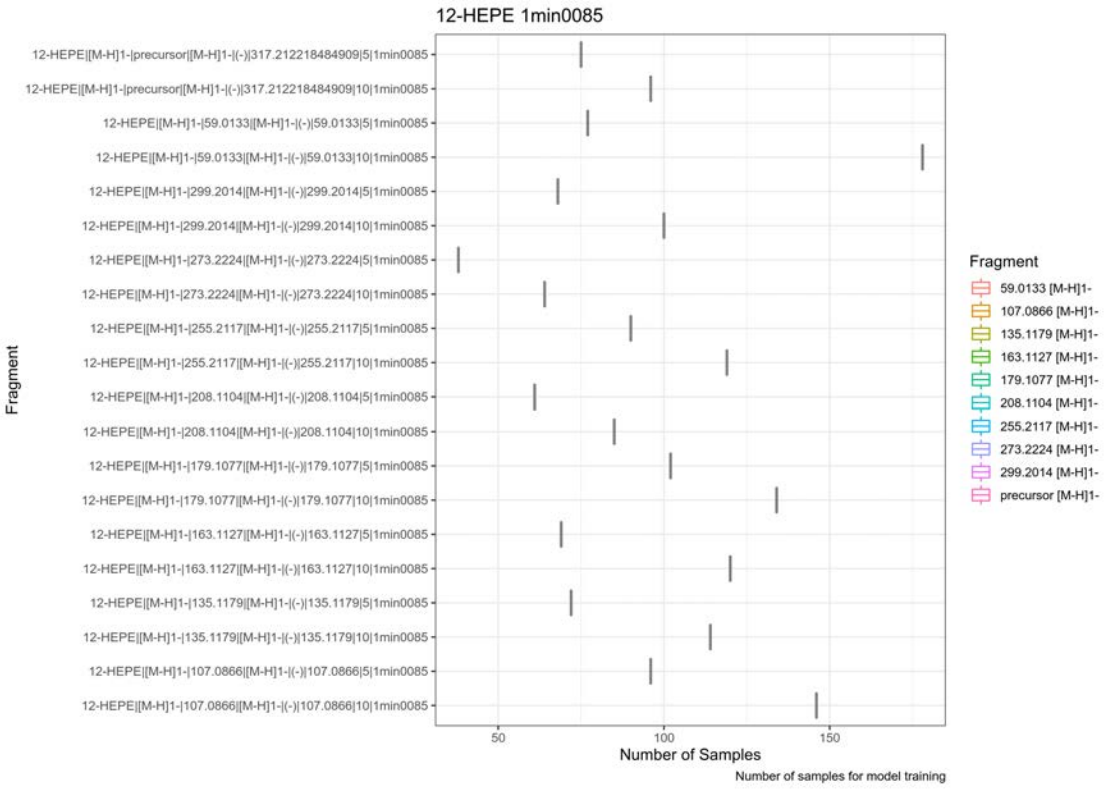


*Figure 35. Number of samples used for training per combination Id*

# 1.8. 12-HETE{d8} [M-H]1- 1min0088

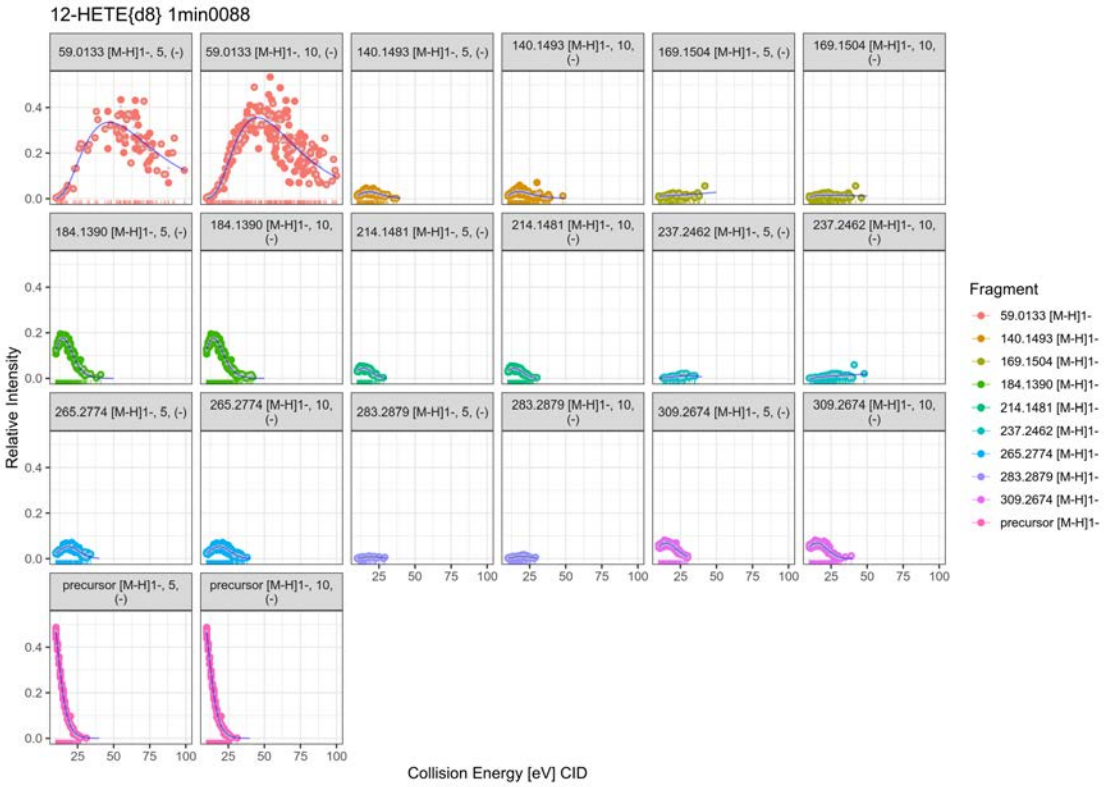


*Figure 36. Nonlinear fit*

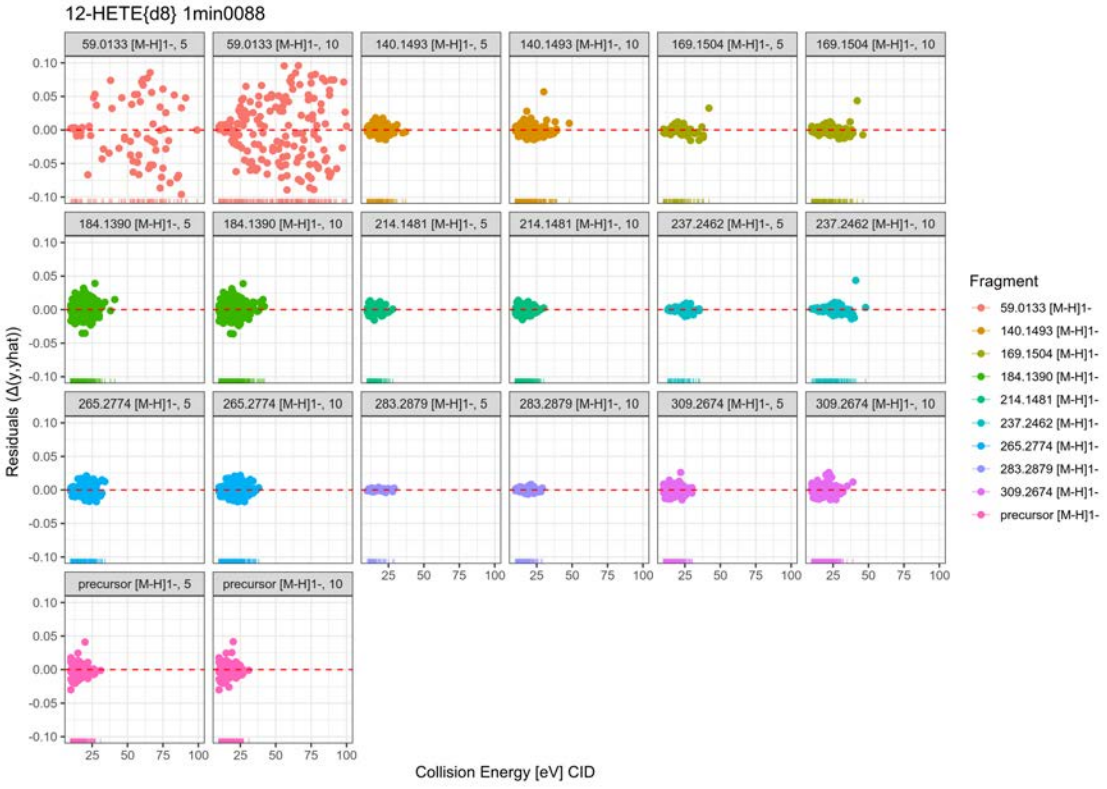


*Figure 37. Residuals of nonlinear fit*

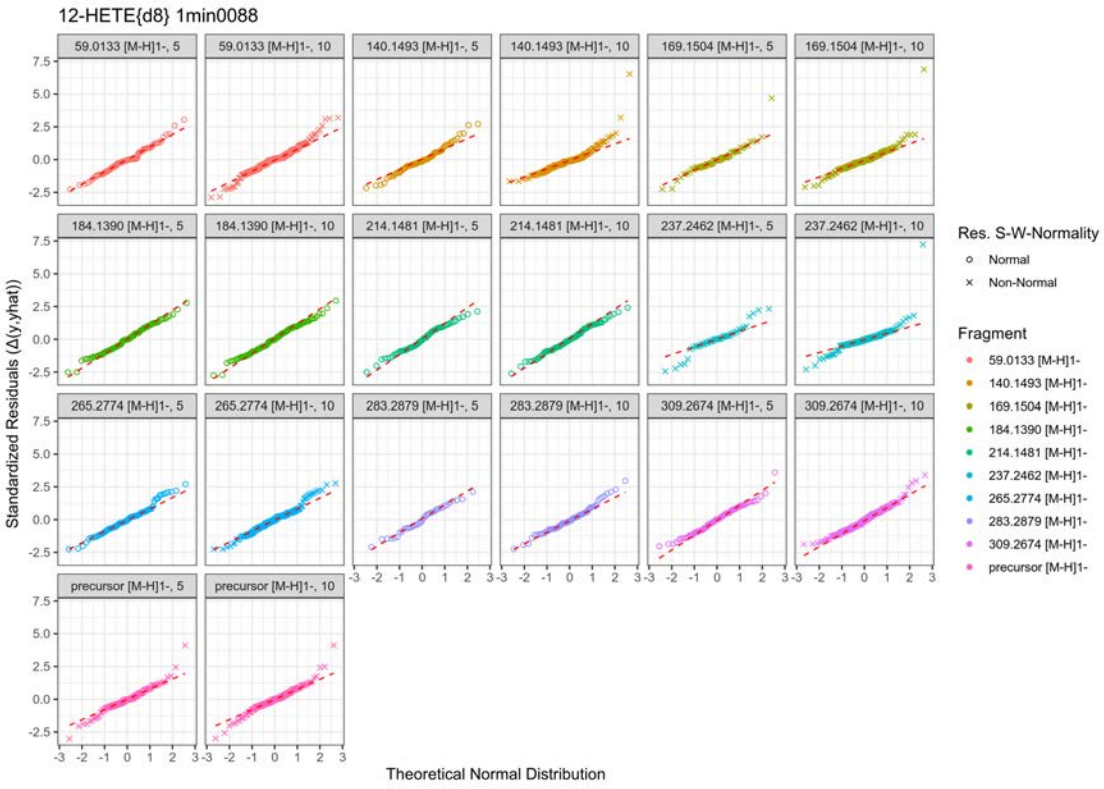


*Figure 38. Quantile-quantile plot of residuals*

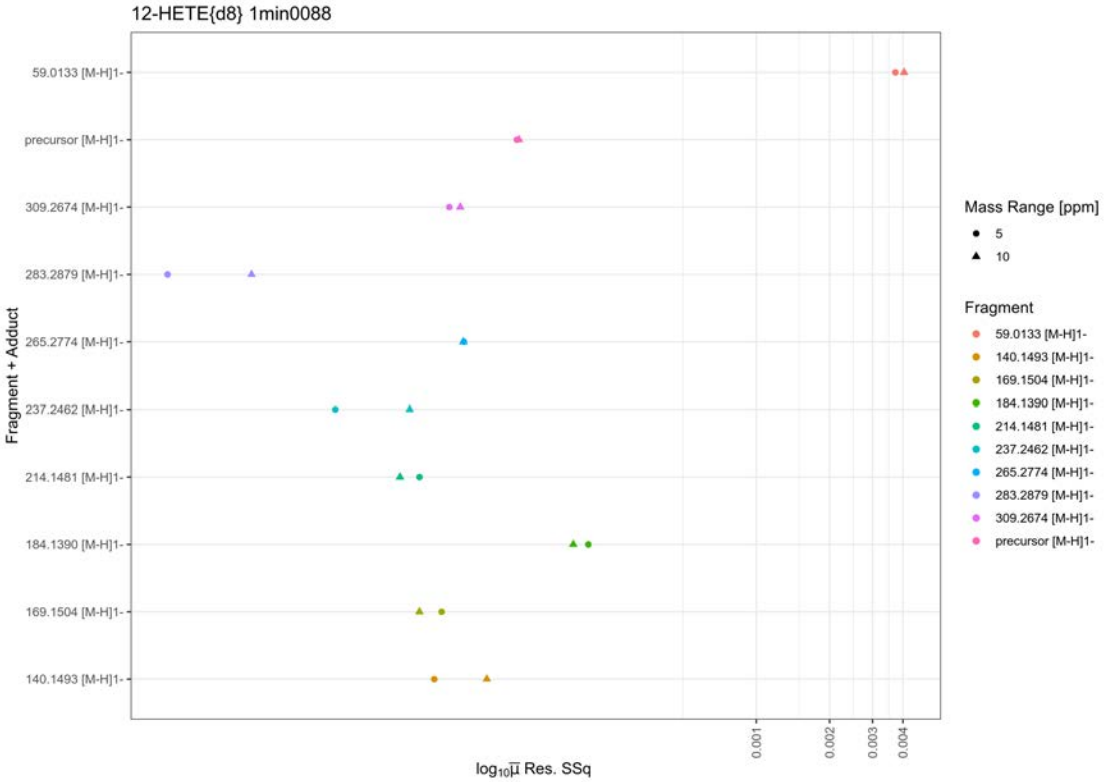


*Figure 39. Normalized sum-of-squares of the residuals*

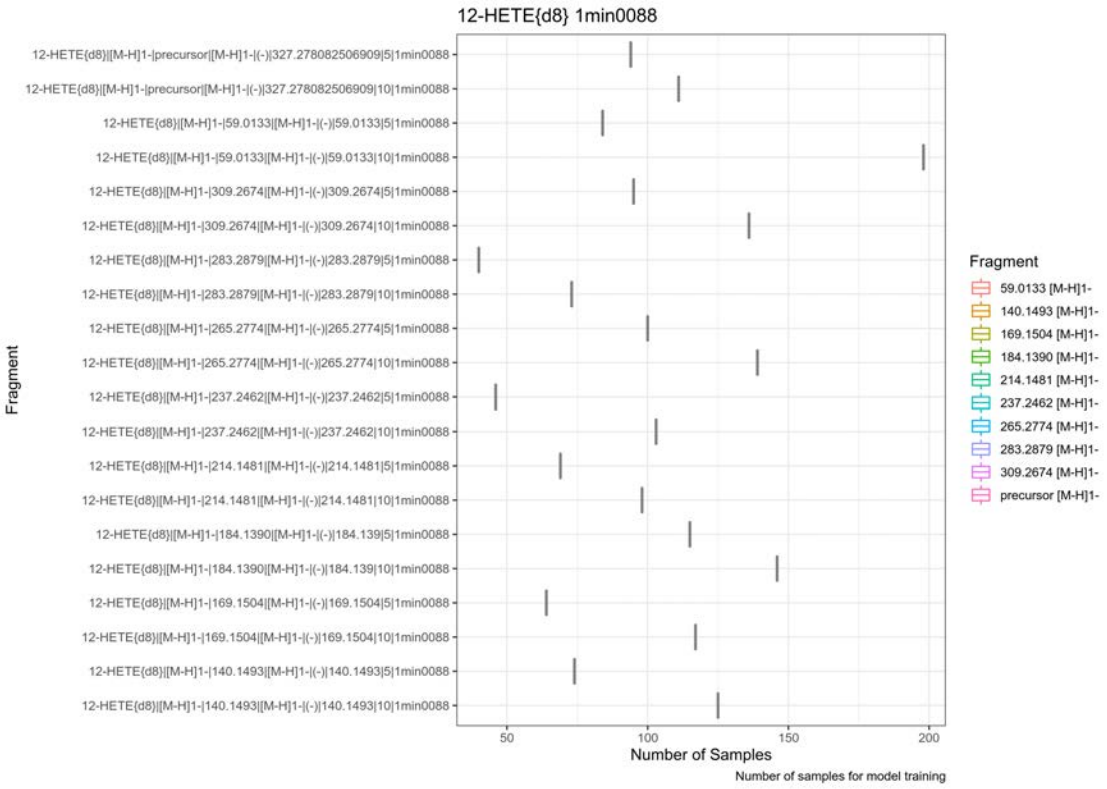


*Figure 40. Number of samples used for training per combination Id*

# 1.9. 12-HHTrE [M-H]1- 1min0089

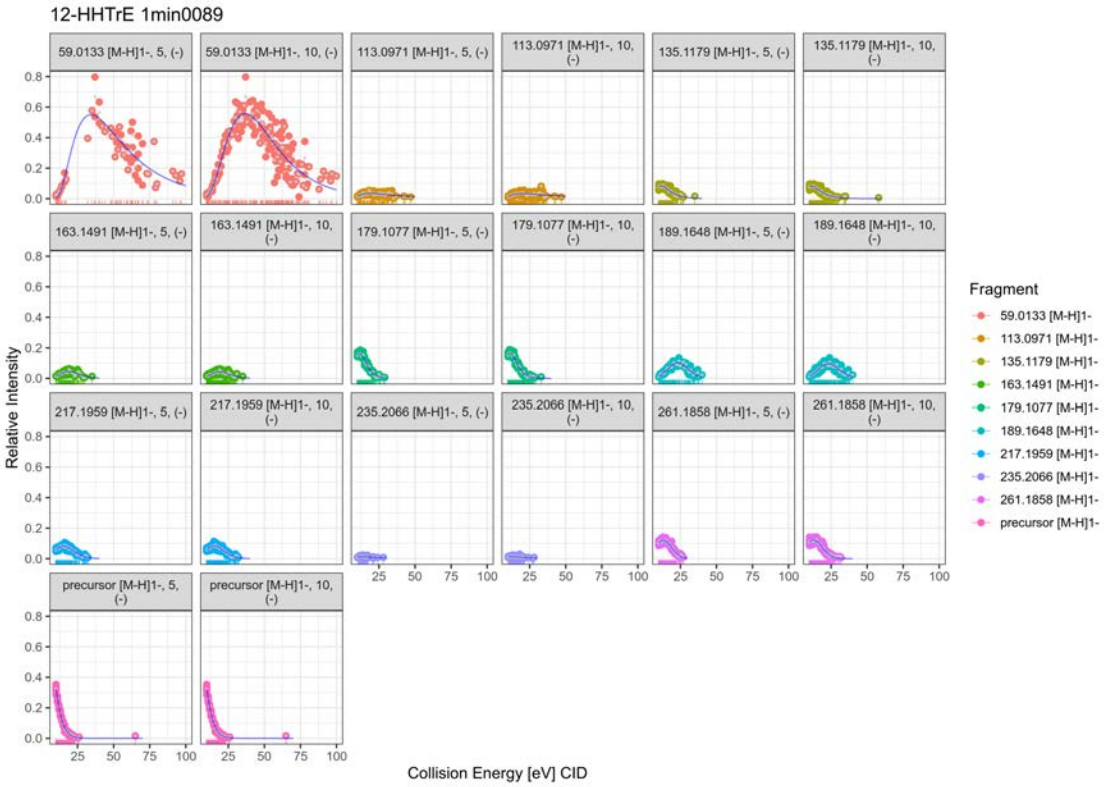


*Figure 41. Nonlinear fit*

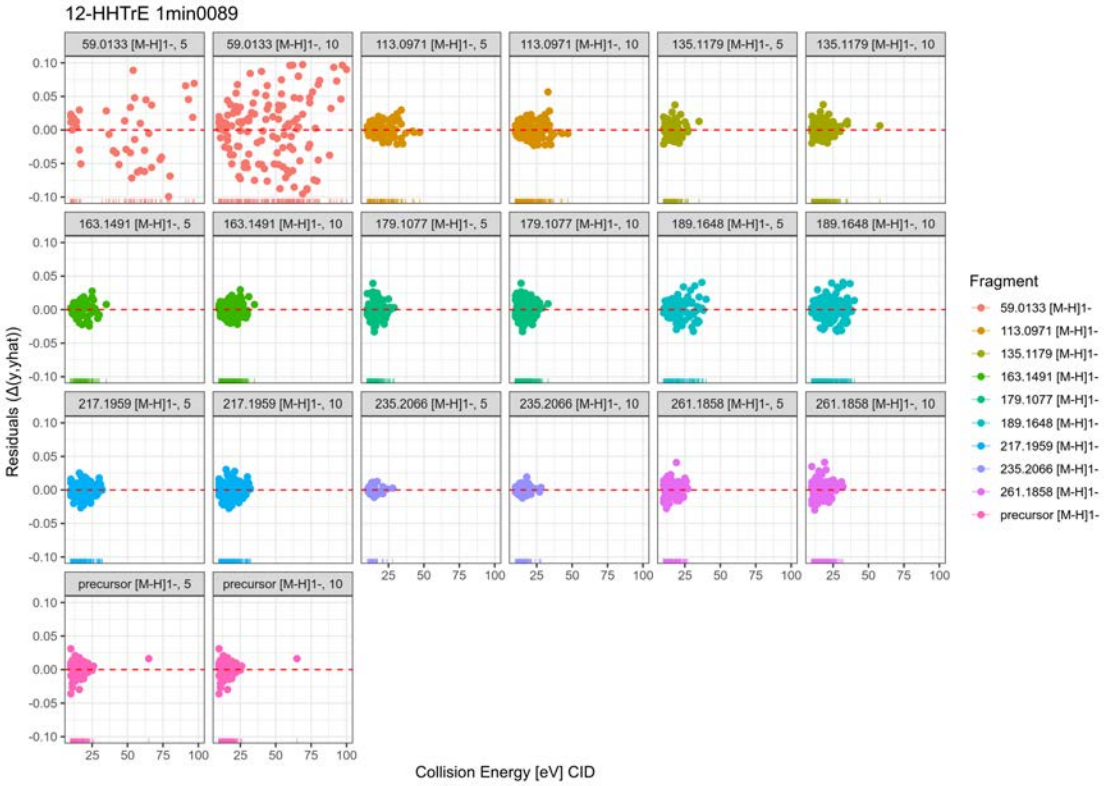


*Figure 42. Residuals of nonlinear fit*

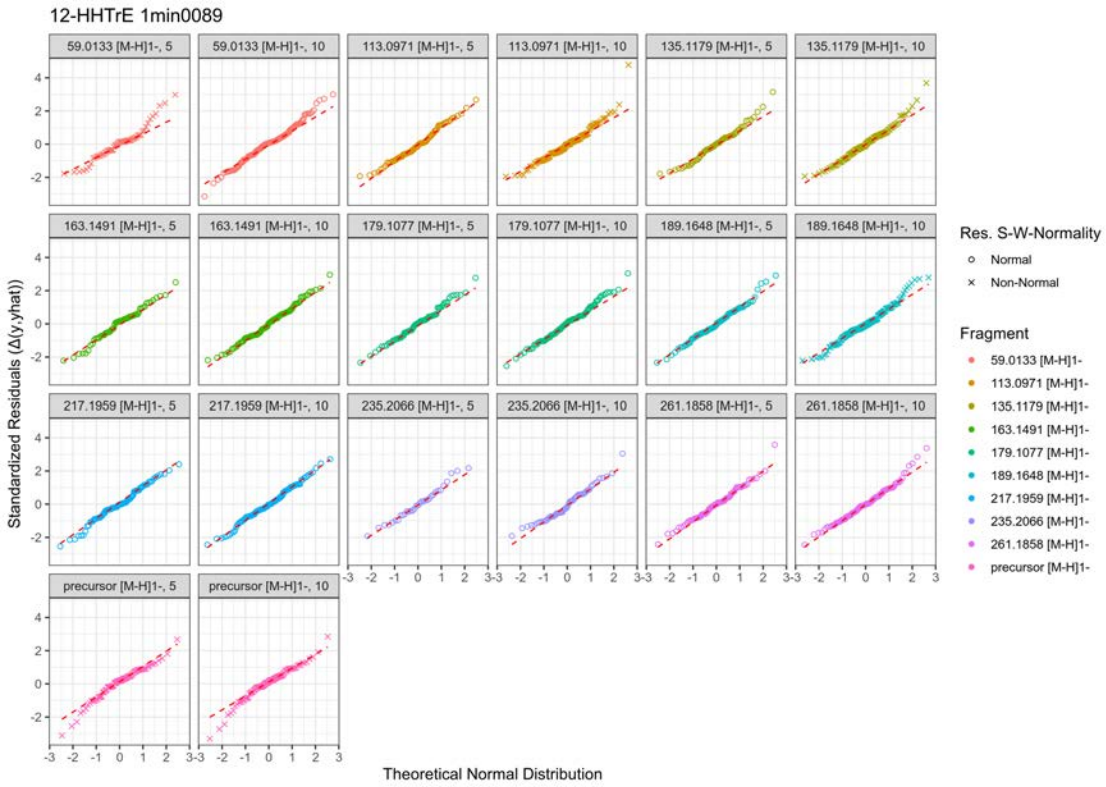


*Figure 43. Quantile-quantile plot of residuals*

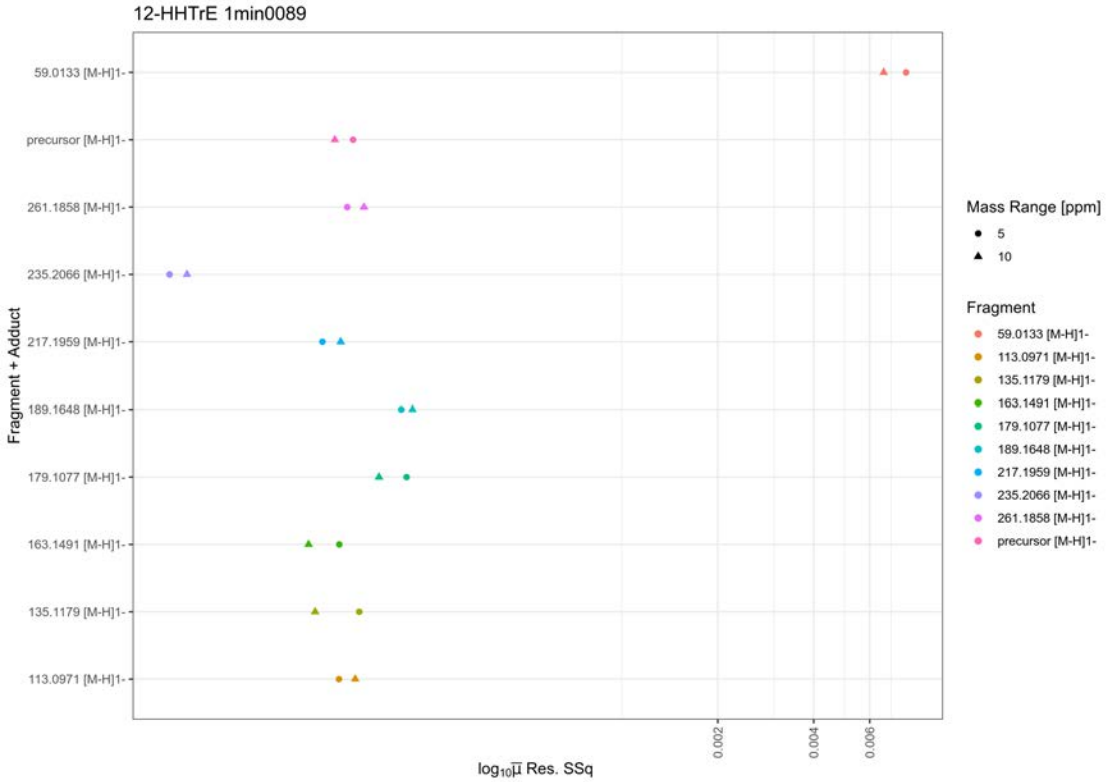


*Figure 44. Normalized sum-of-squares of the residuals*

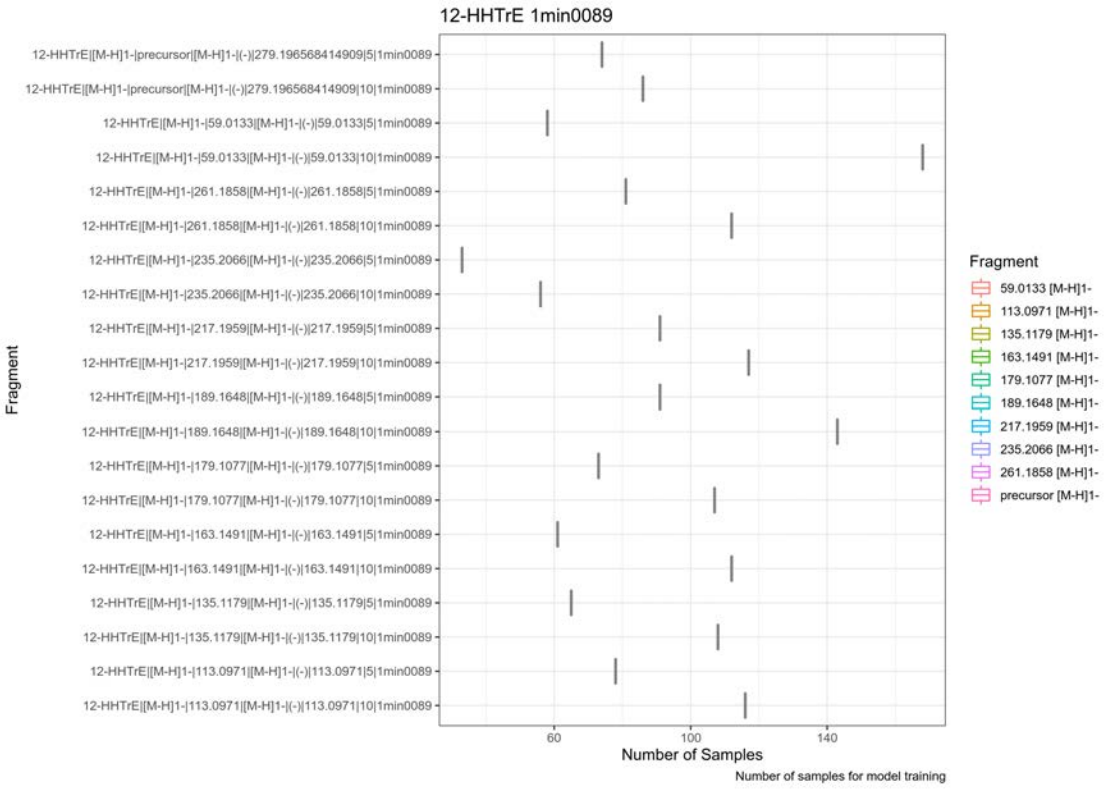


*Figure 45. Number of samples used for training per combination Id*

# 1.10. 12-OxoETE [M-H]1- 1min0165

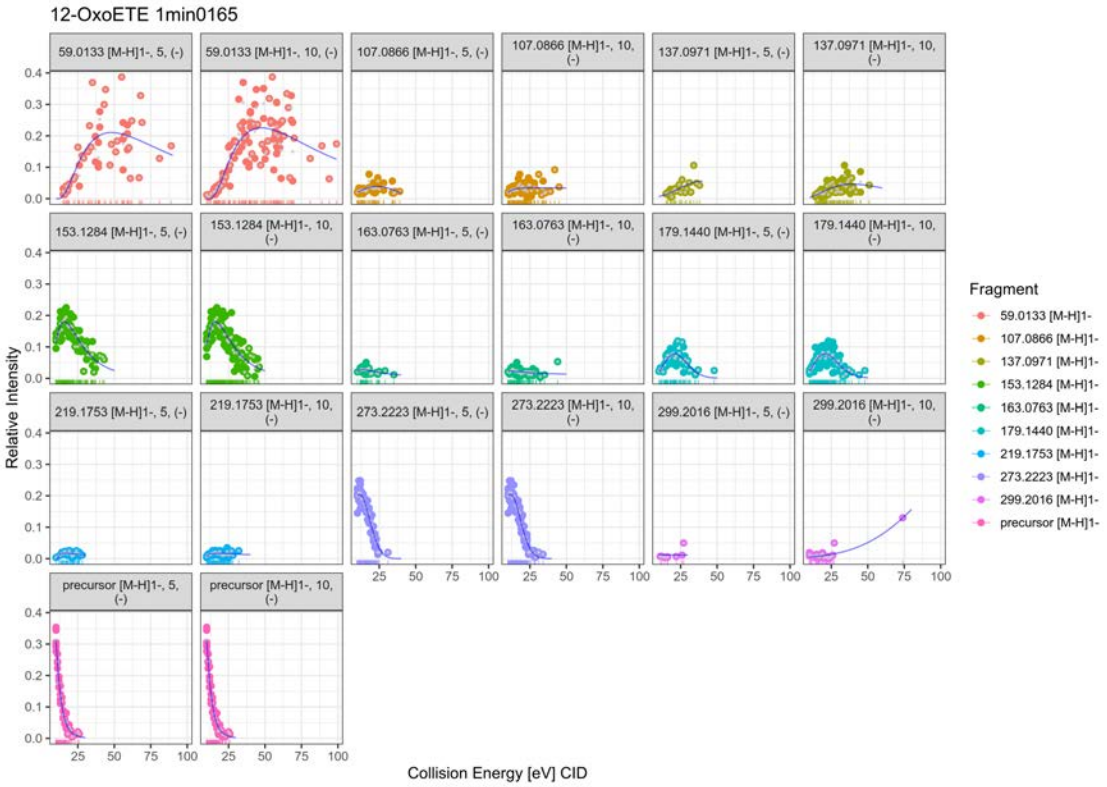


*Figure 46. Nonlinear fit*

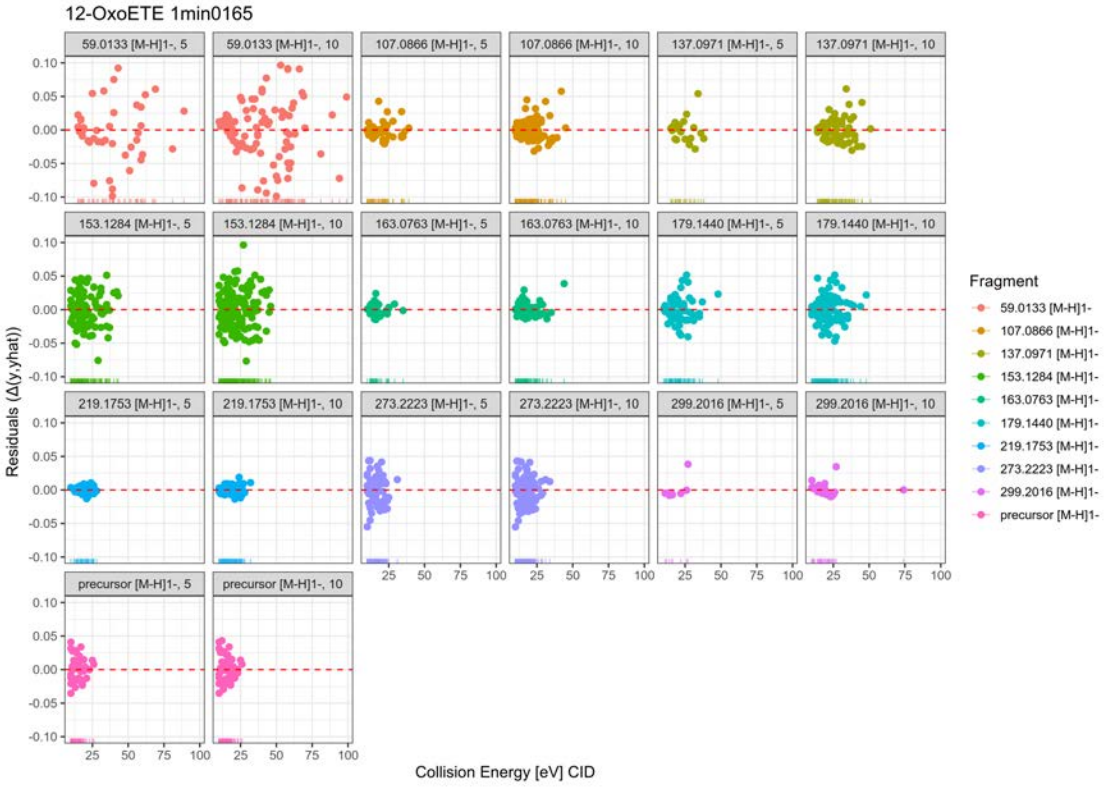


*Figure 47. Residuals of nonlinear fit*

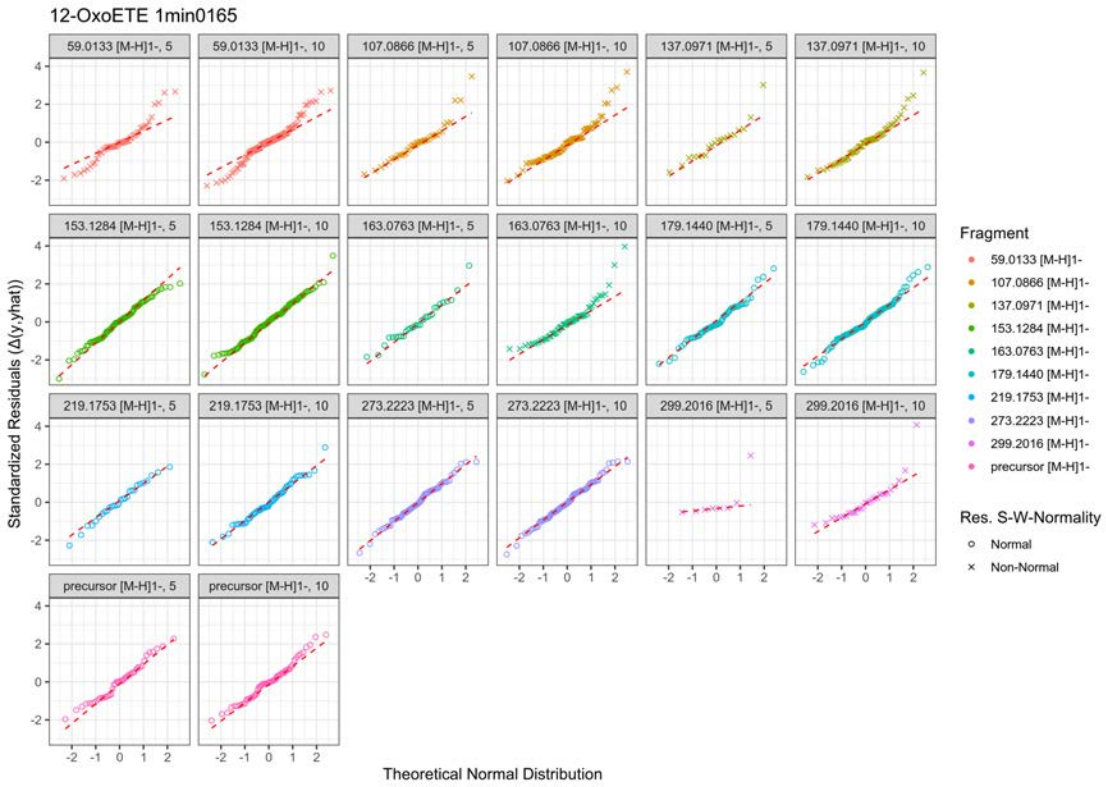


*Figure 48. Quantile-quantile plot of residuals*

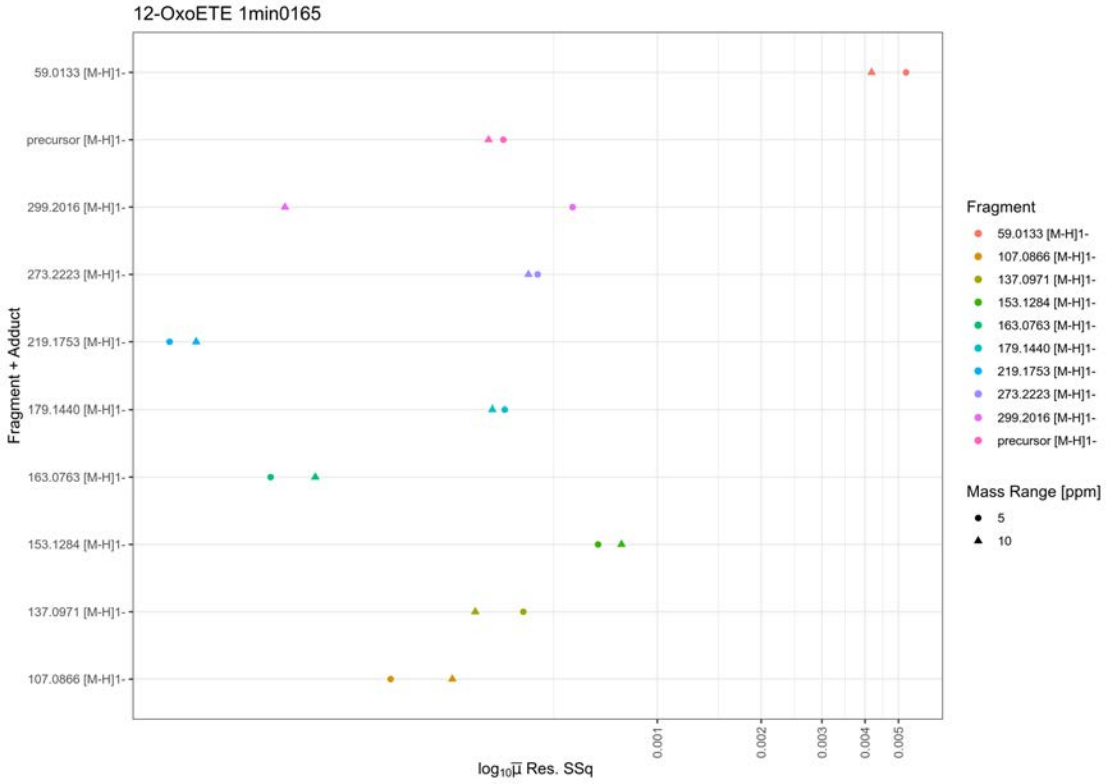


*Figure 49. Normalized sum-of-squares of the residuals*

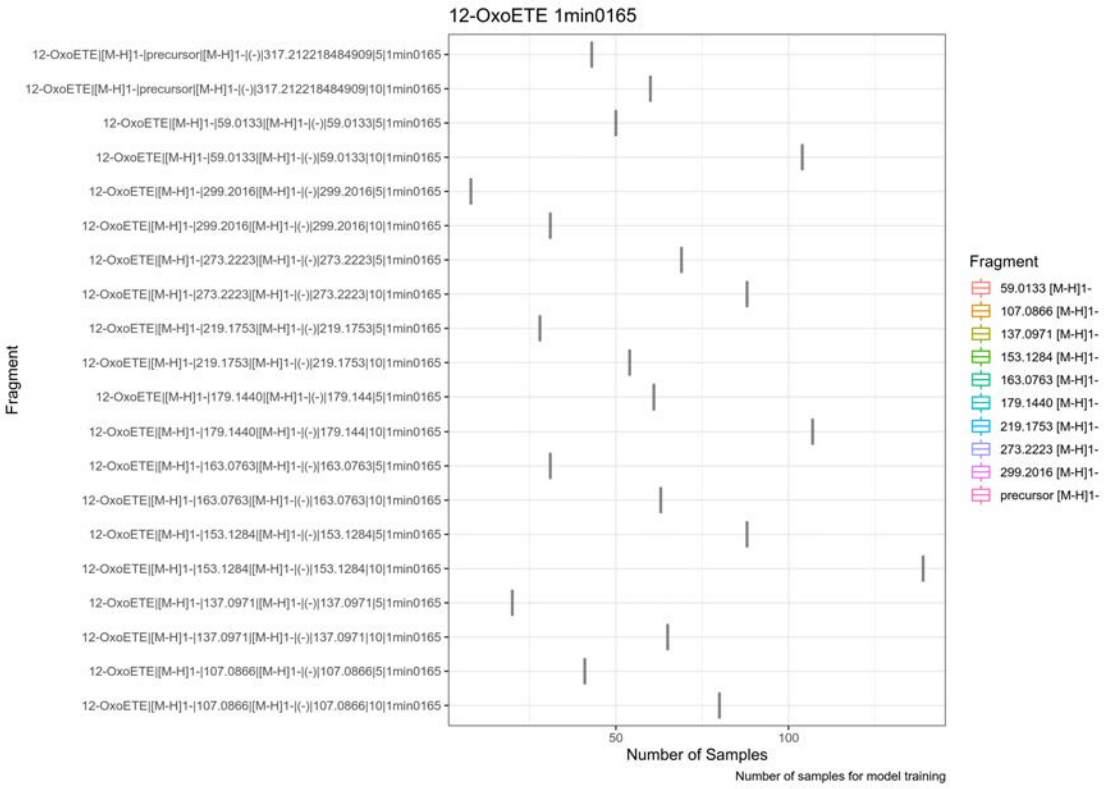


*Figure 50. Number of samples used for training per combination Id*

# 1.11. 13-HODE{d4} [M-H]1- 1min0095

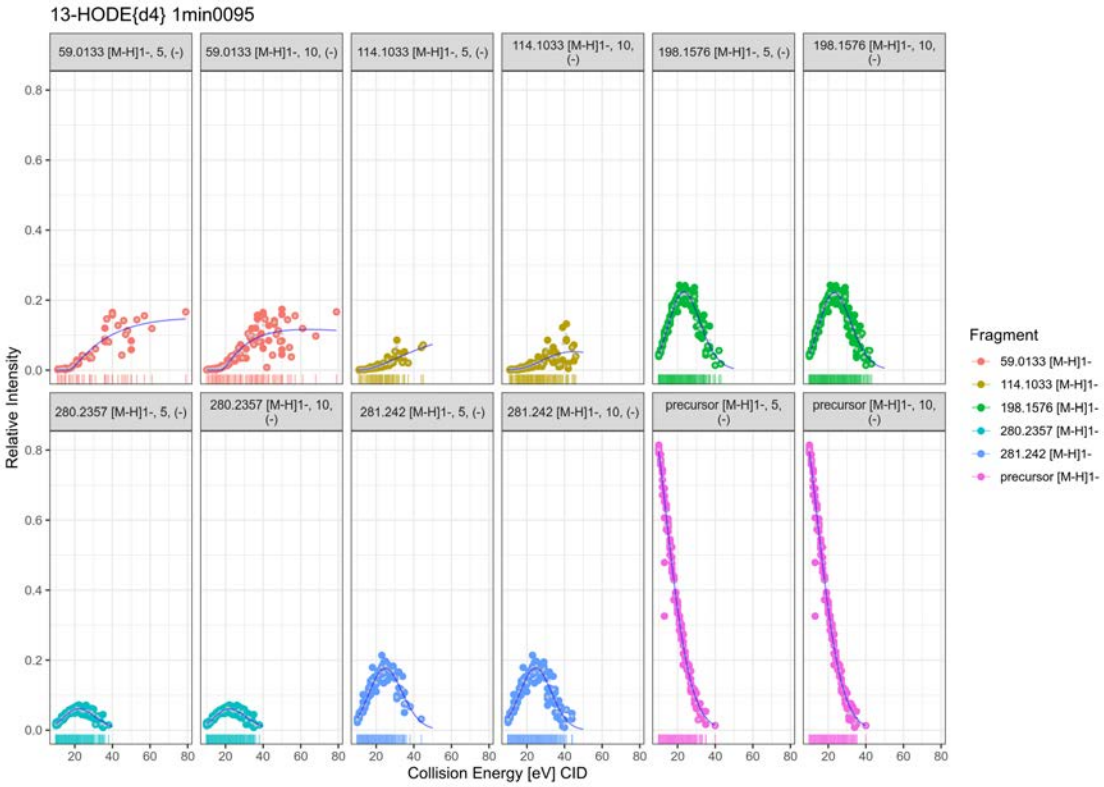


*Figure 51. Nonlinear fit*

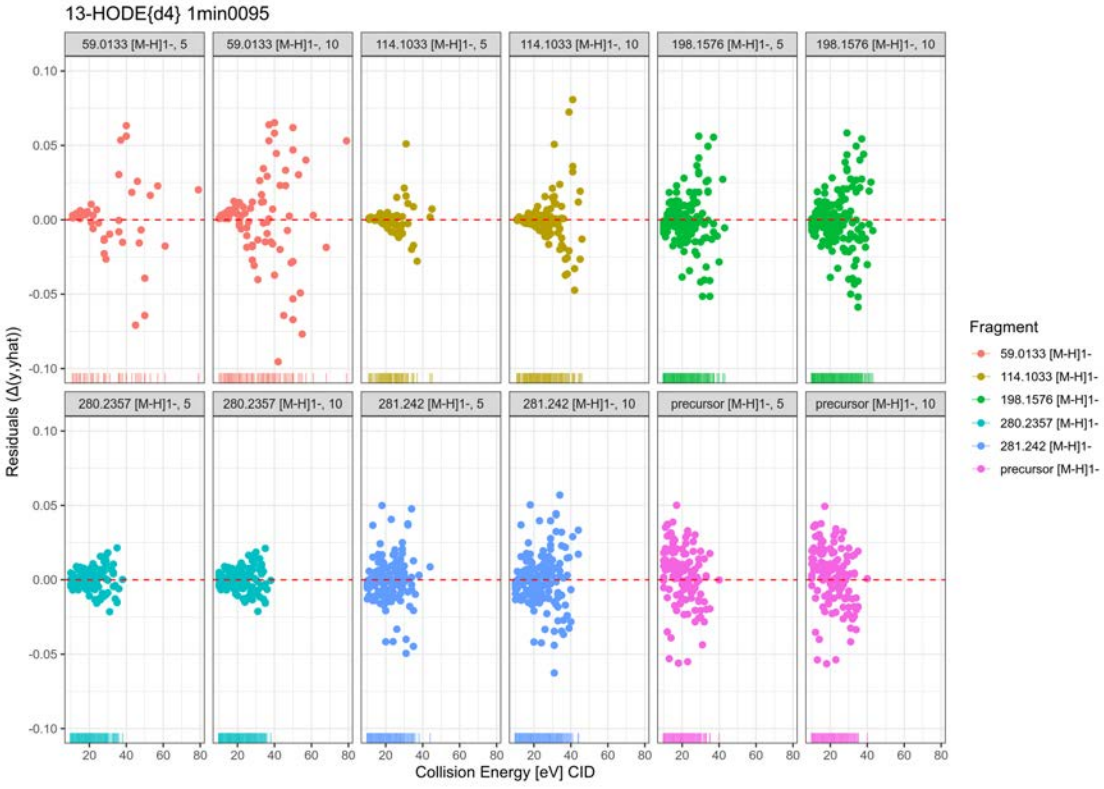


*Figure 52. Residuals of nonlinear fit*

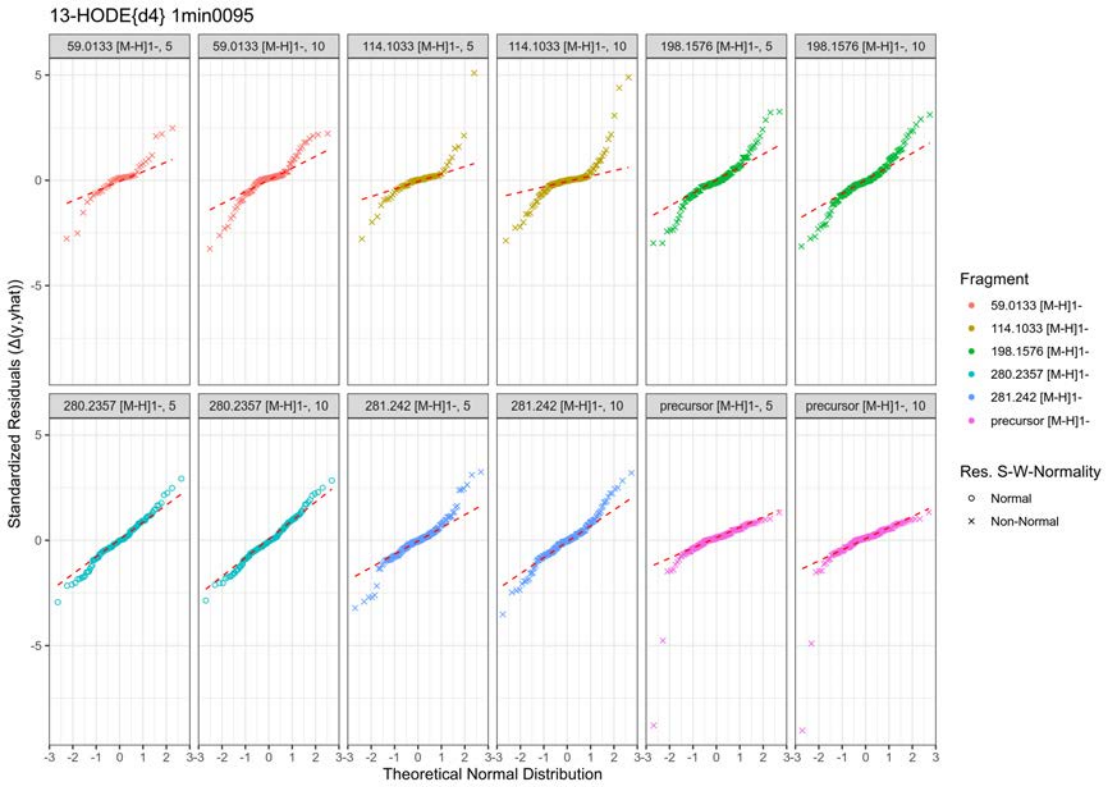


*Figure 53. Quantile-quantile plot of residuals*

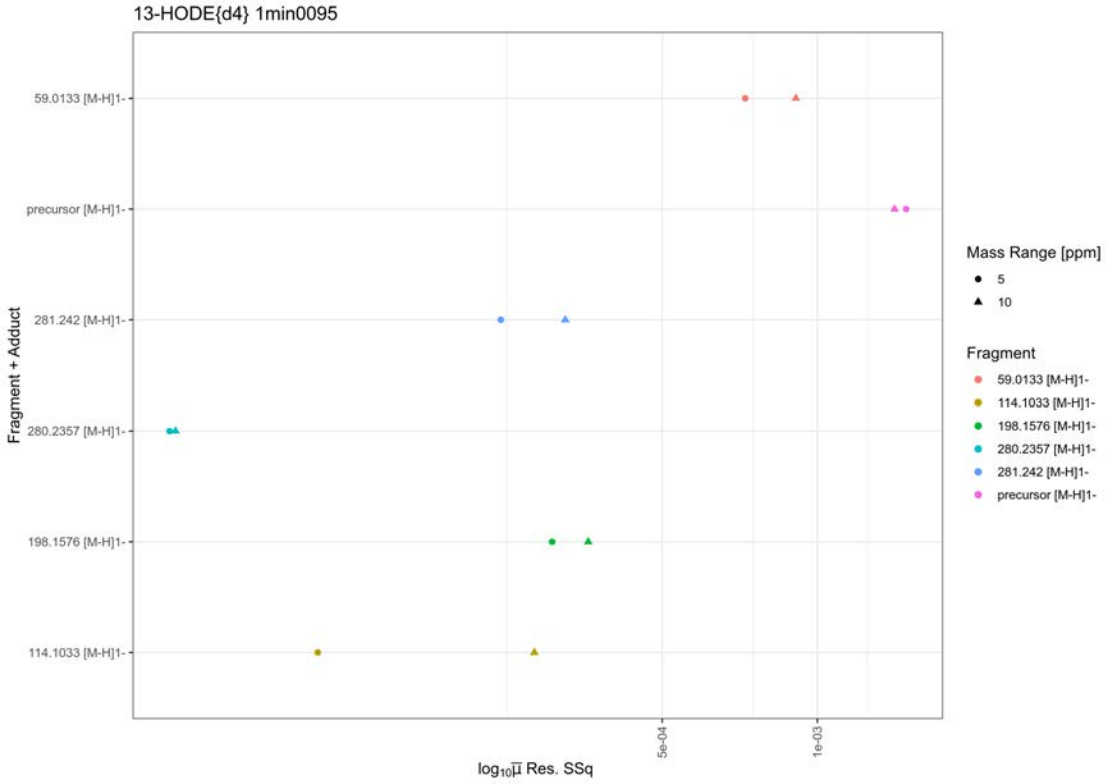


*Figure 54. Normalized sum-of-squares of the residuals*

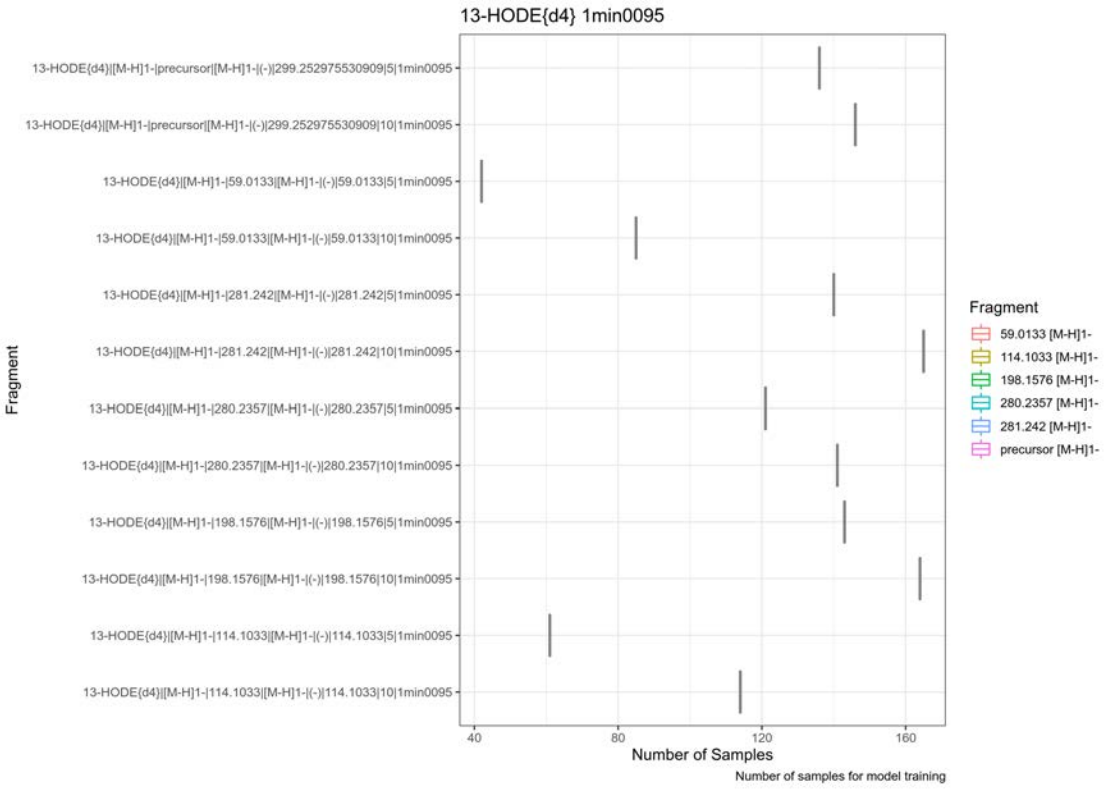


*Figure 55. Number of samples used for training per combination Id*

# 1.12. 13-HOTrE [M-H]1- 1min0099

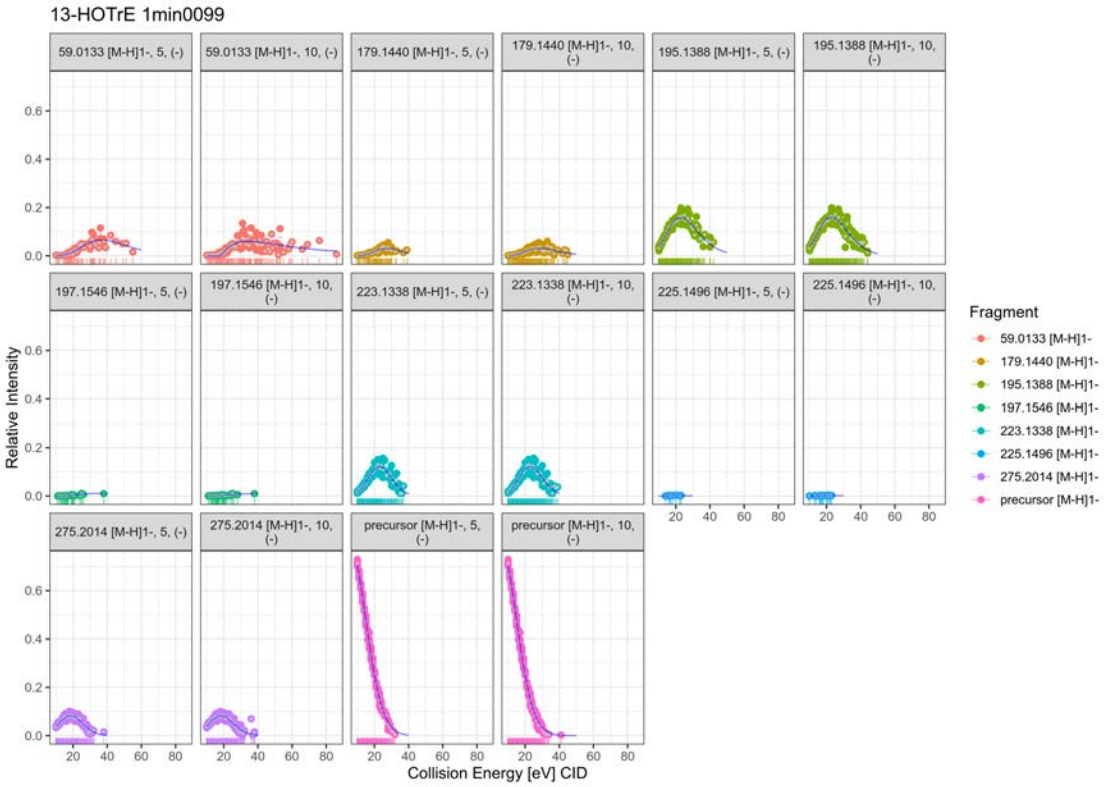


*Figure 56. Nonlinear fit*

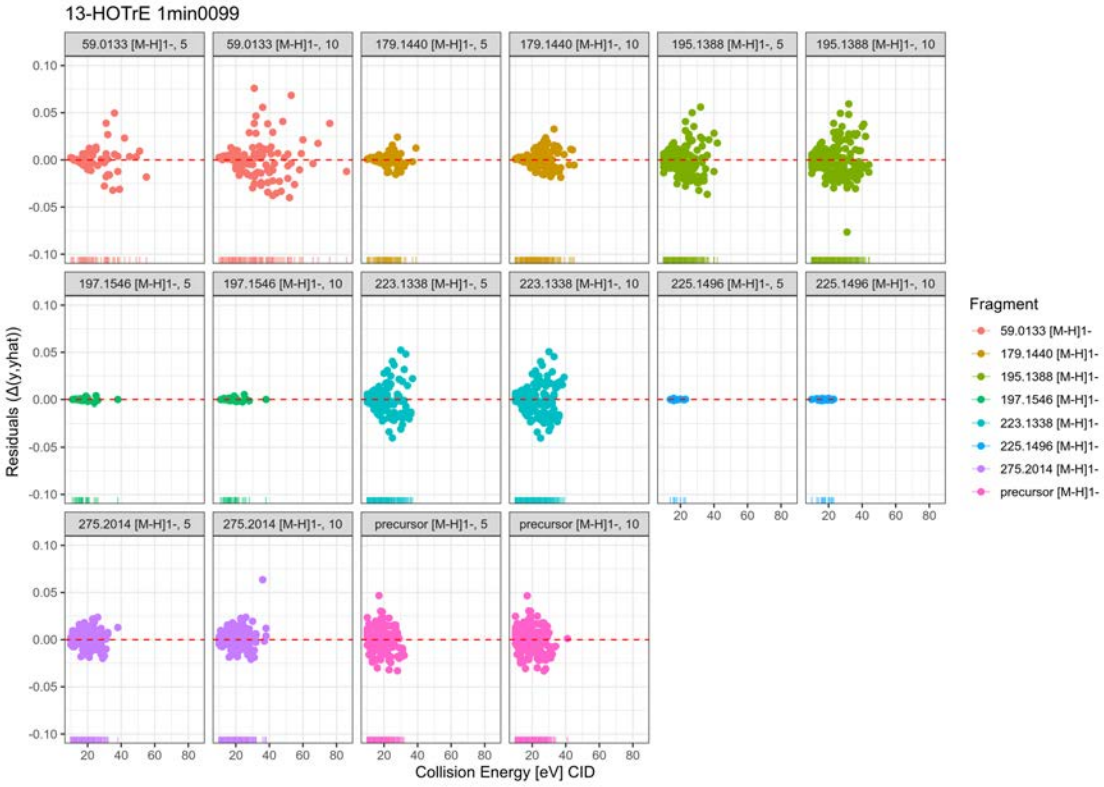


*Figure 57. Residuals of nonlinear fit*

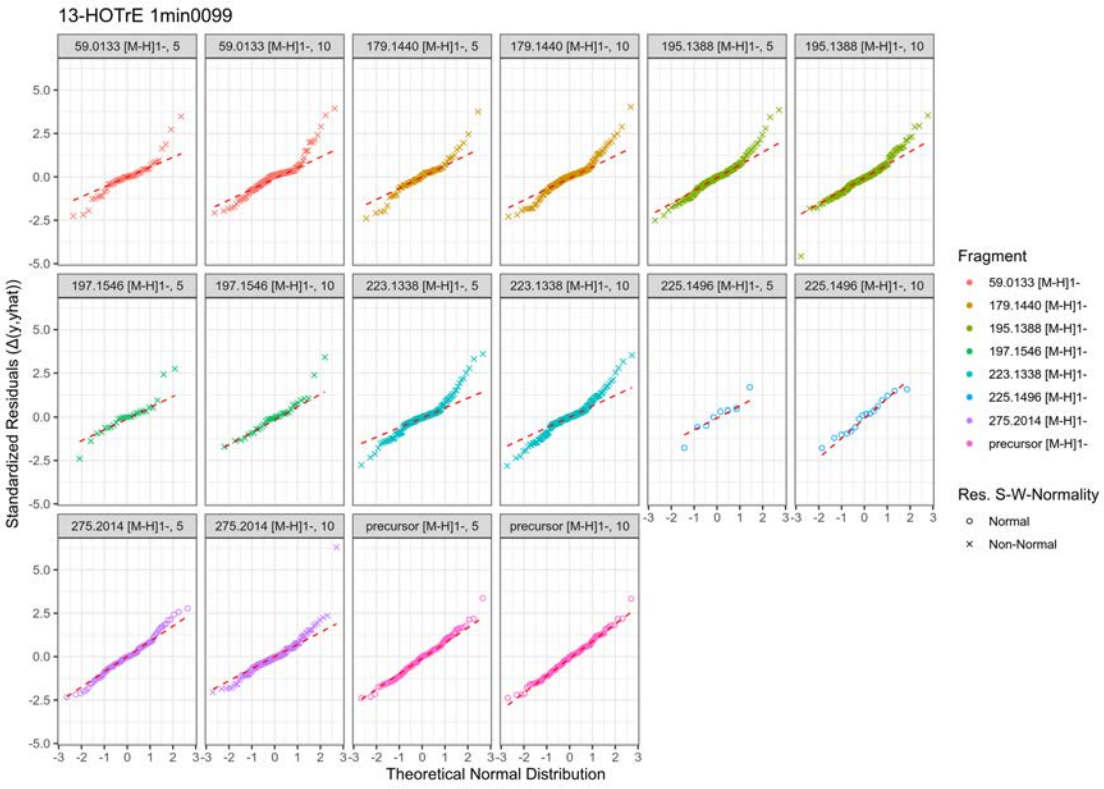


*Figure 58. Quantile-quantile plot of residuals*

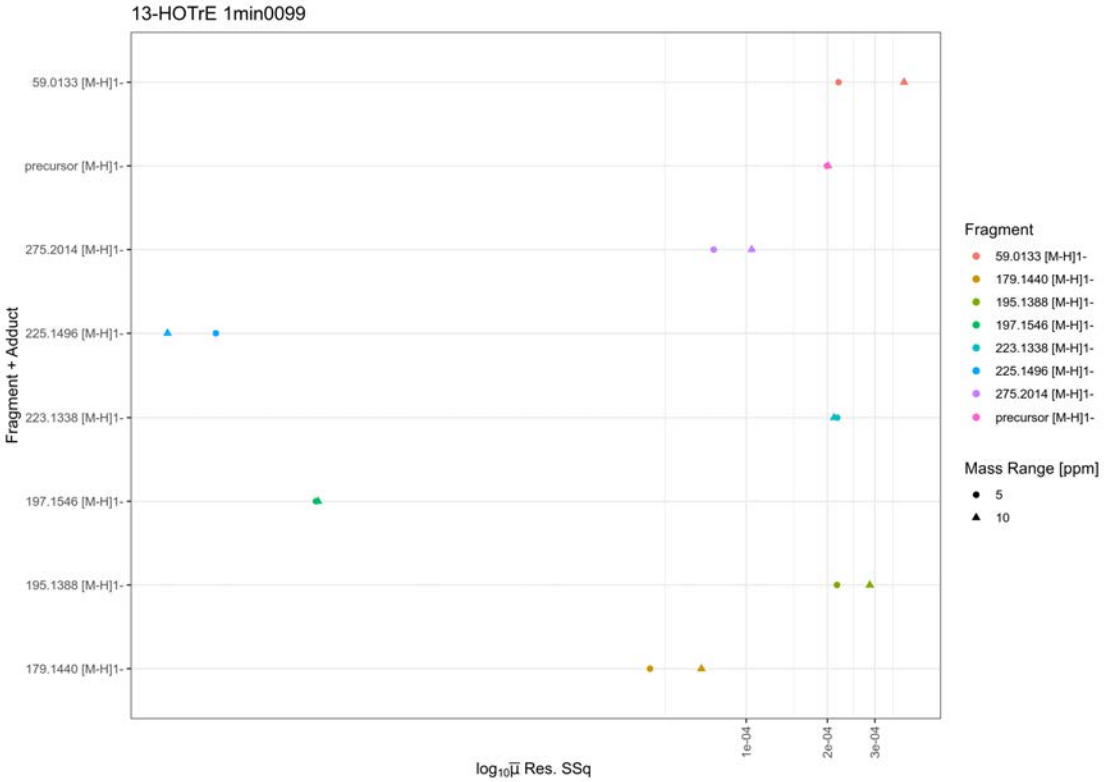


*Figure 59. Normalized sum-of-squares of the residuals*

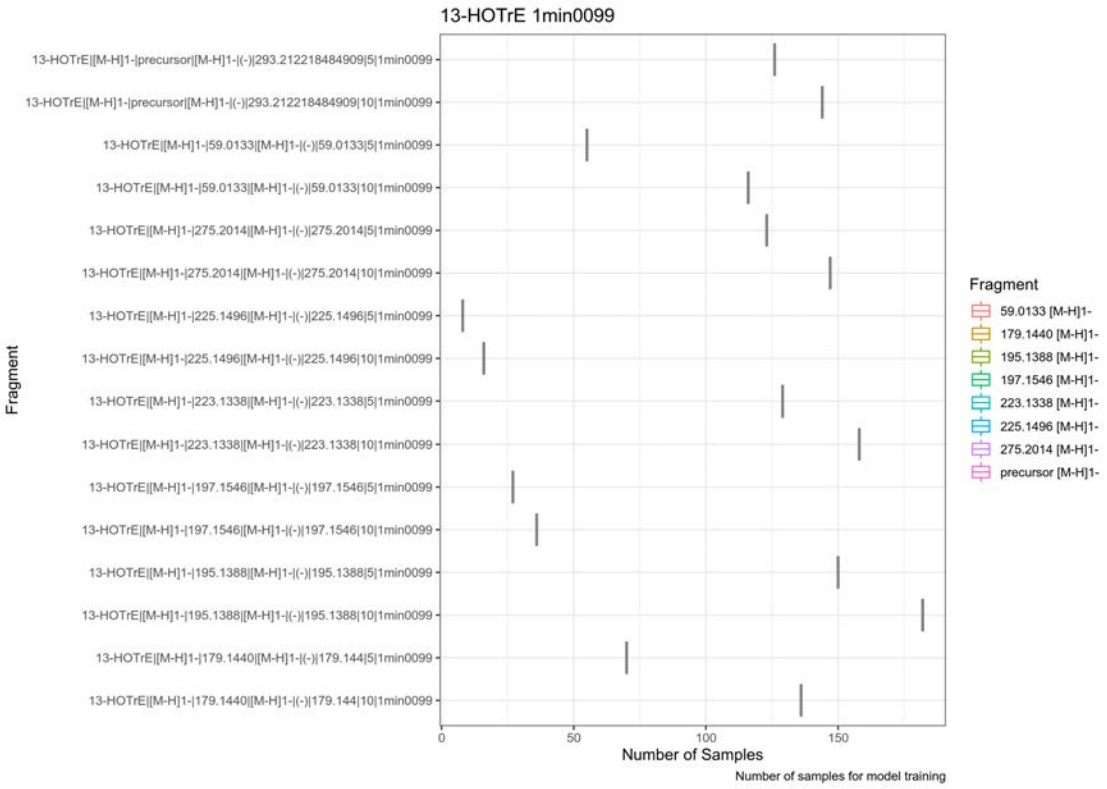


*Figure 60. Number of samples used for training per combination Id*

# 1.13. 14(15)-EET{d11} [M-H]1- 1min0101

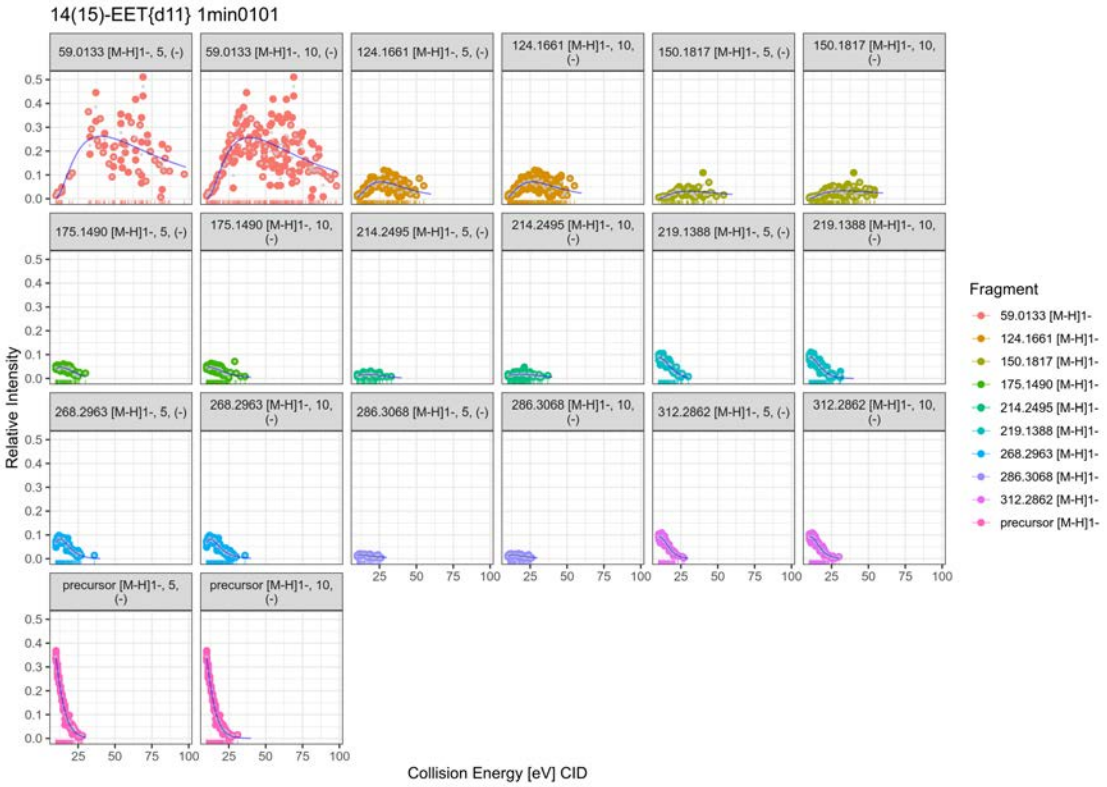


*Figure 61. Nonlinear fit*

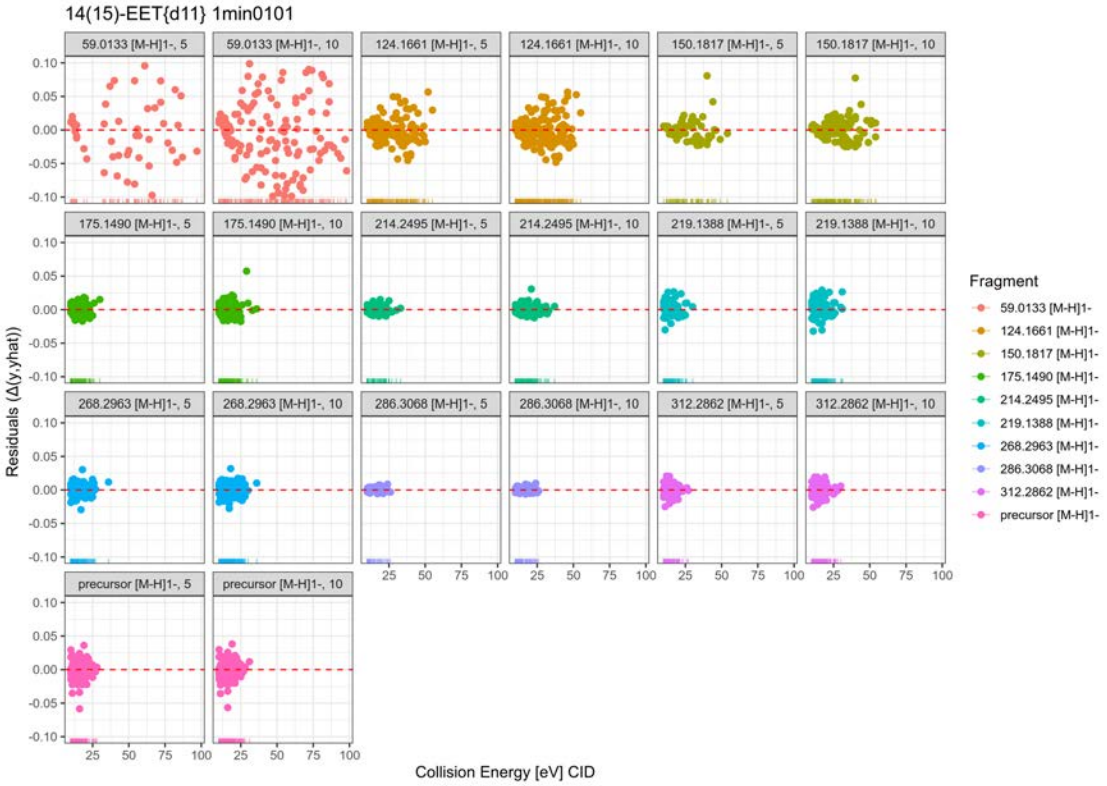


*Figure 62. Residuals of nonlinear fit*

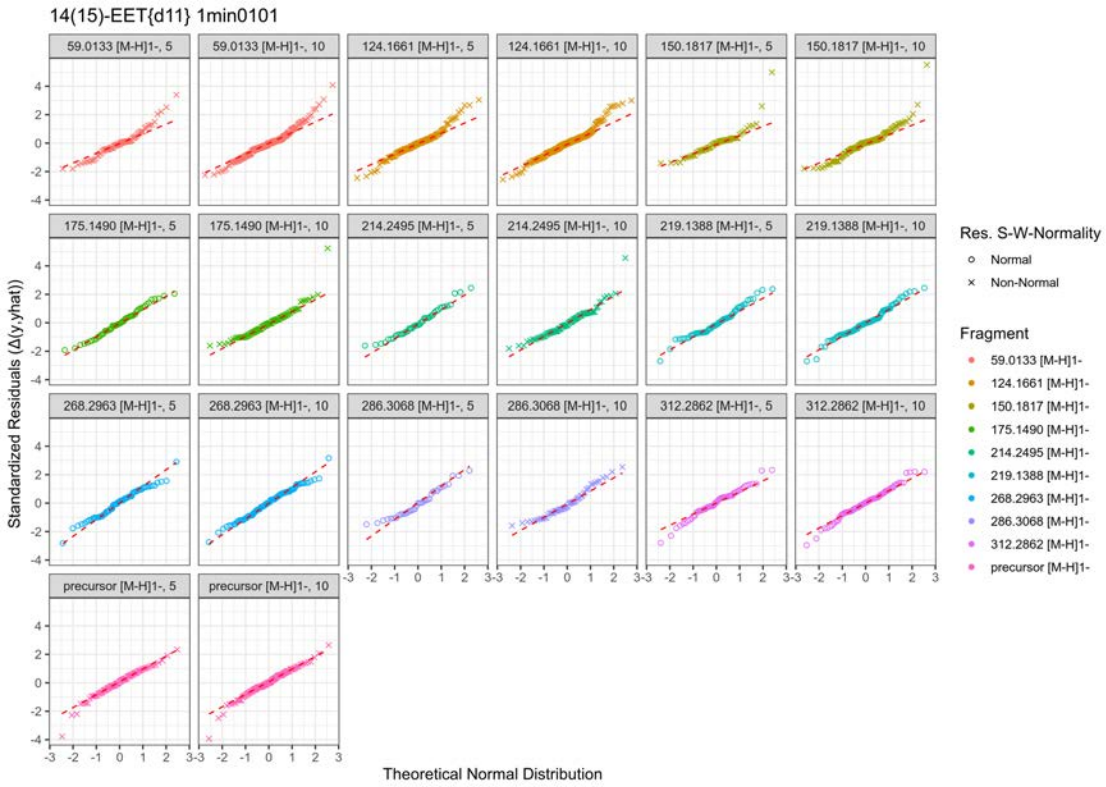


*Figure 63. Quantile-quantile plot of residuals*

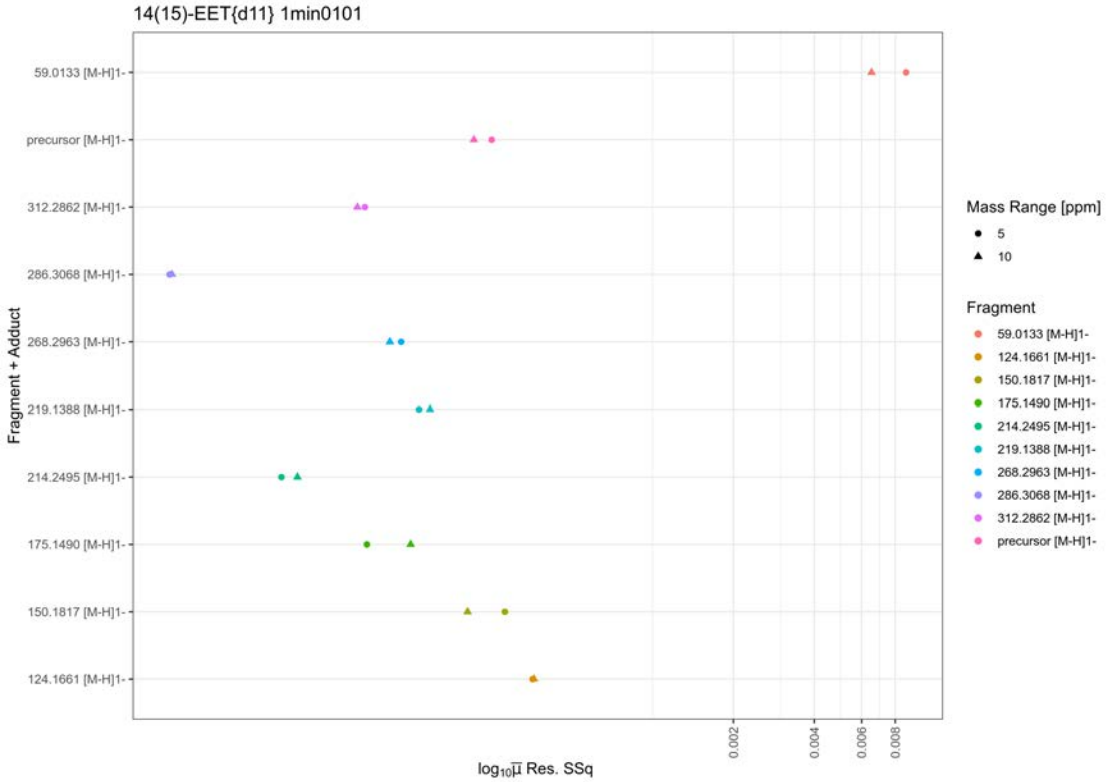


*Figure 64. Normalized sum-of-squares of the residuals*

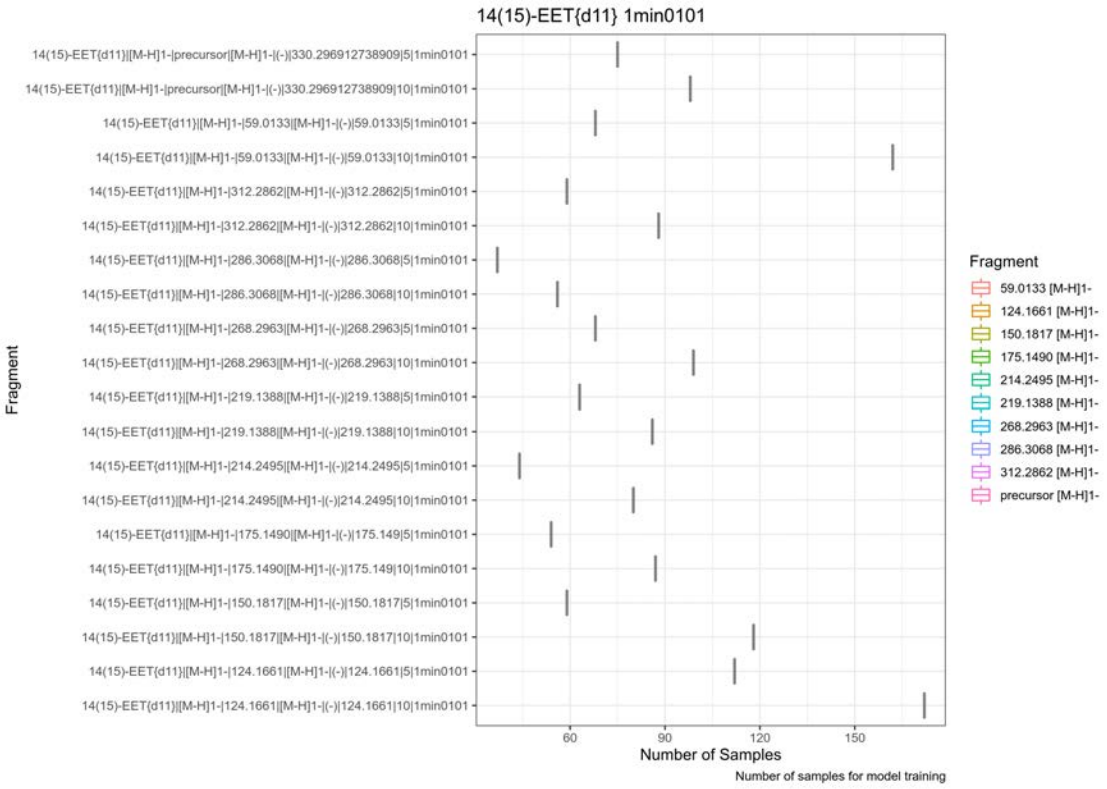


*Figure 65. Number of samples used for training per combination Id*

# 1.14. 14(15)-EpETE [M-H]1- 1min0104

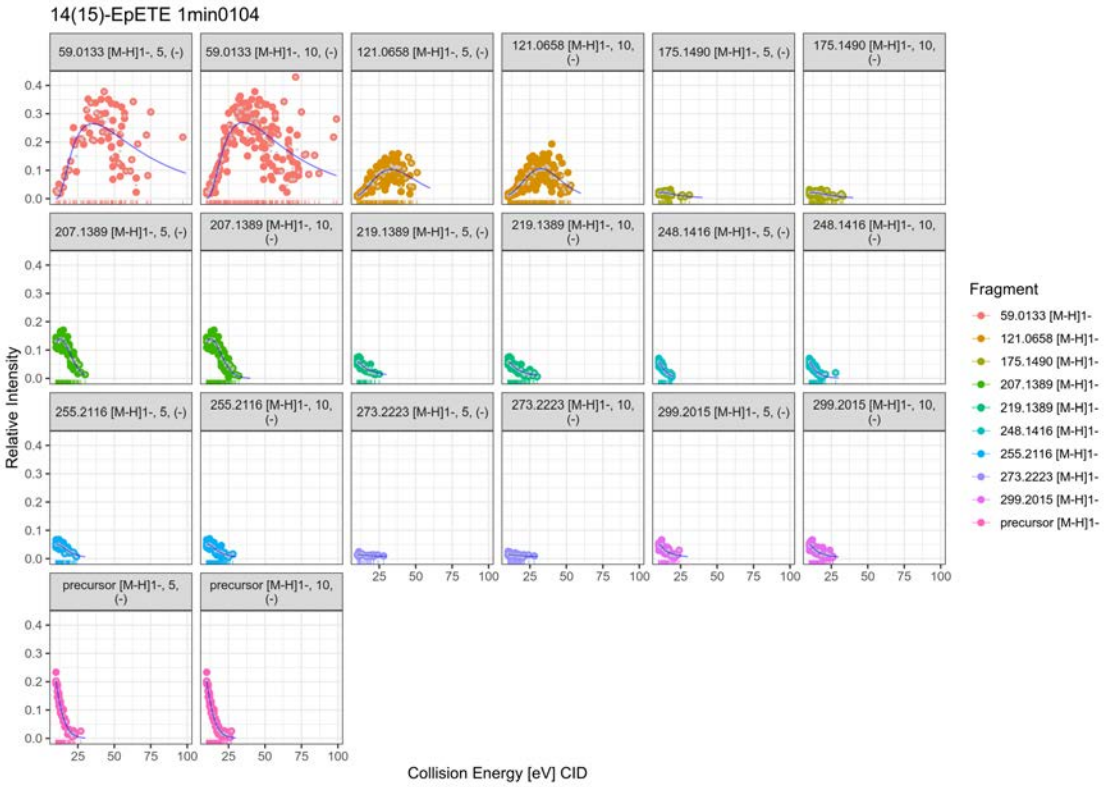


*Figure 66. Nonlinear fit*

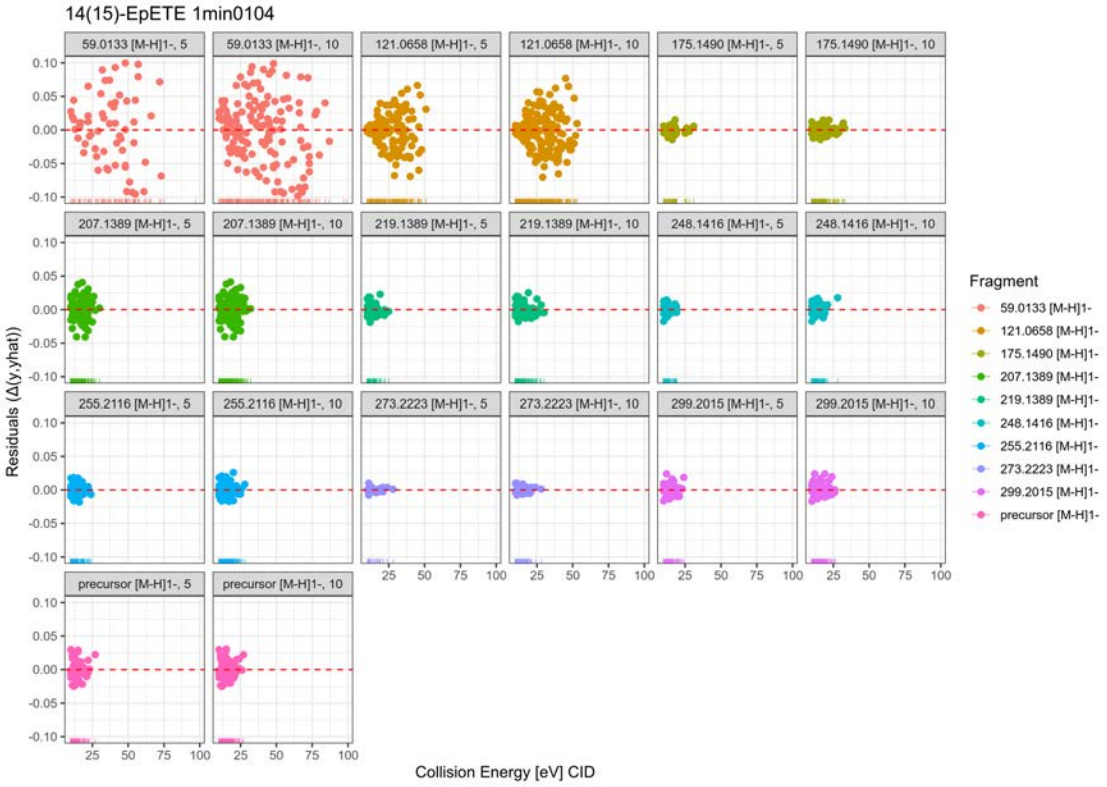


*Figure 67. Residuals of nonlinear fit*

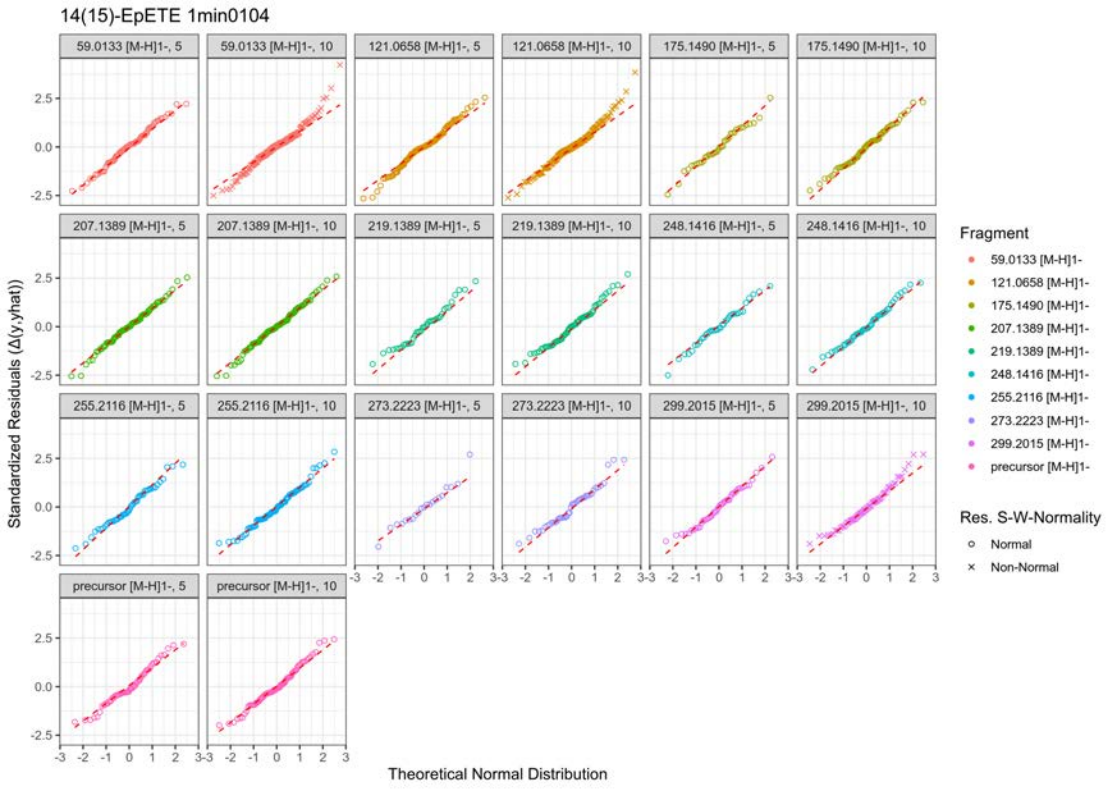


*Figure 68. Quantile-quantile plot of residuals*

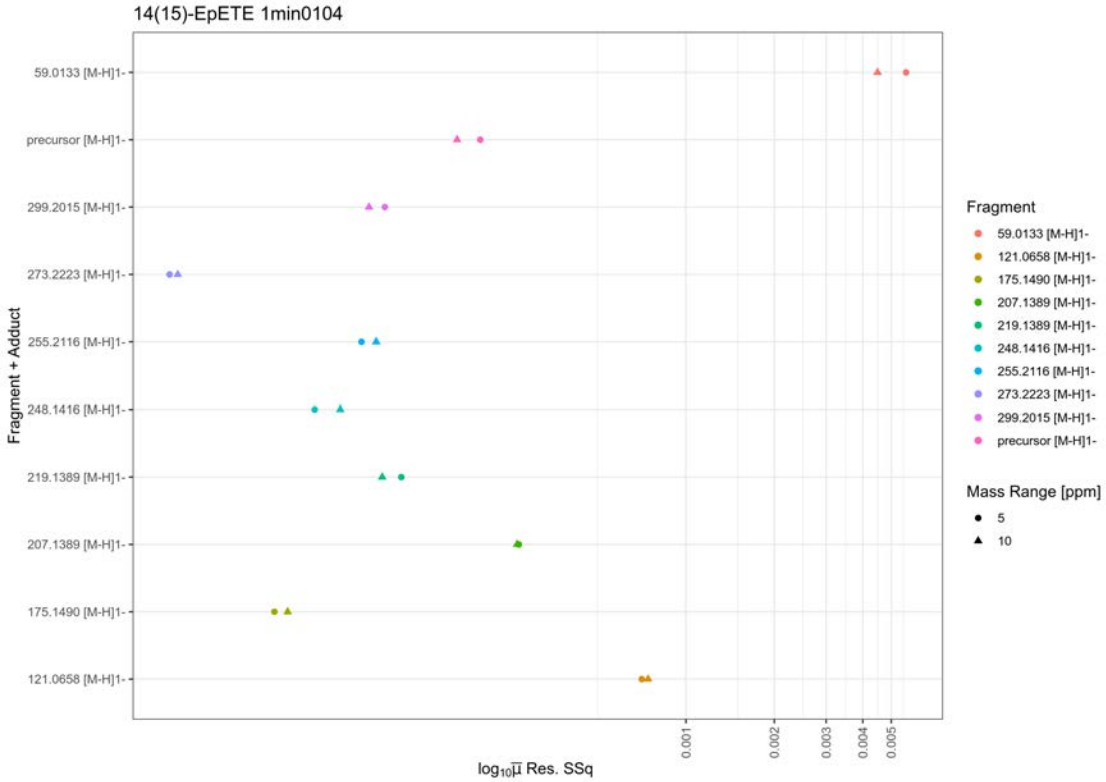


*Figure 69. Normalized sum-of-squares of the residuals*

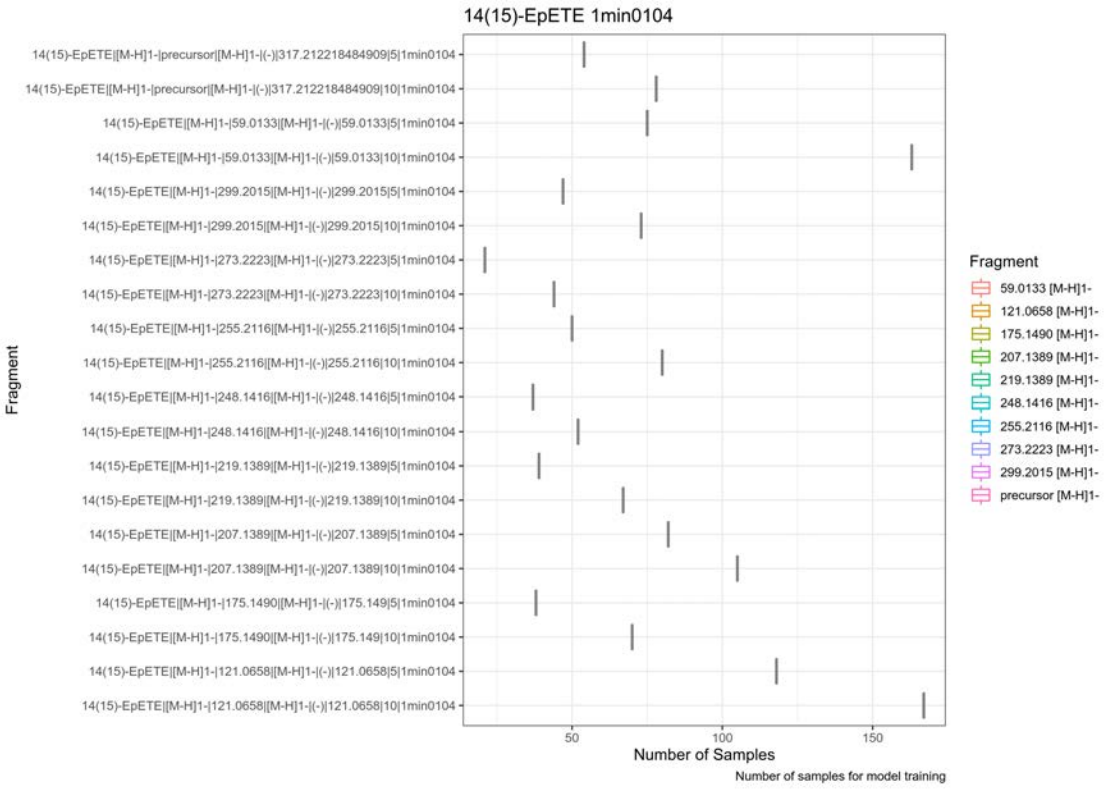


*Figure 70. Number of samples used for training per combination Id*

# 1.15. 14,15-DHET{d11} [M-H]1- 1min0224

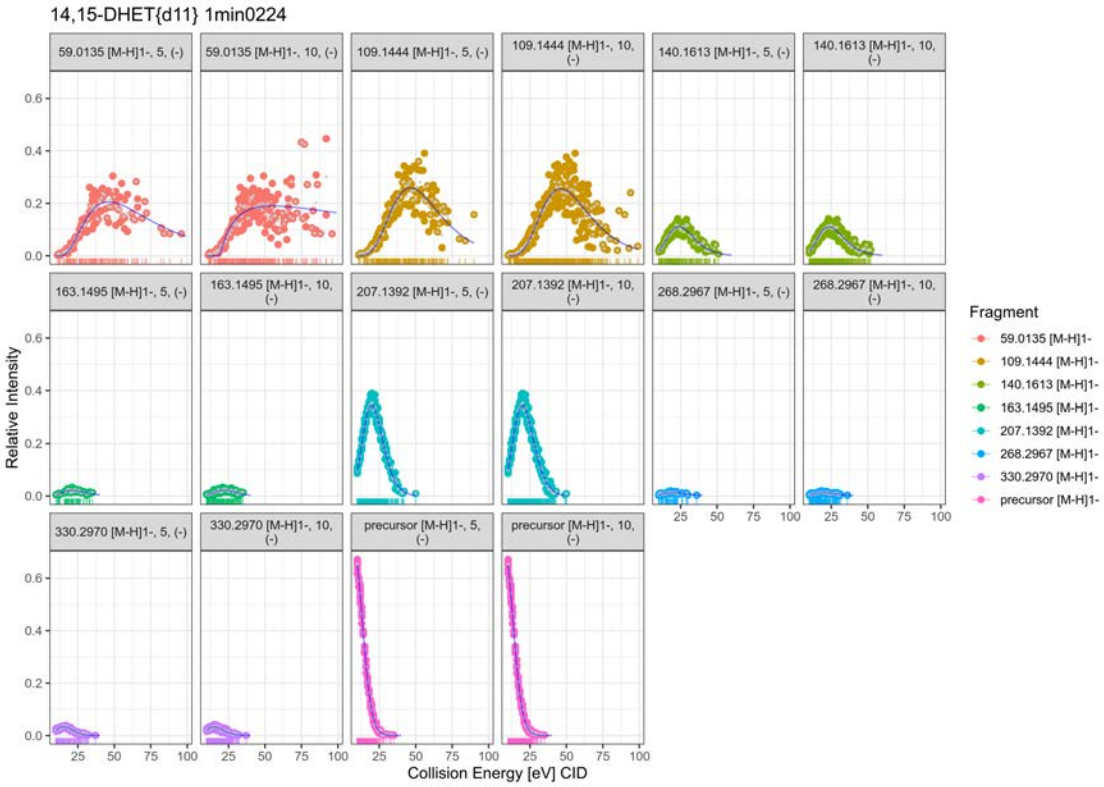


*Figure 71. Nonlinear fit*

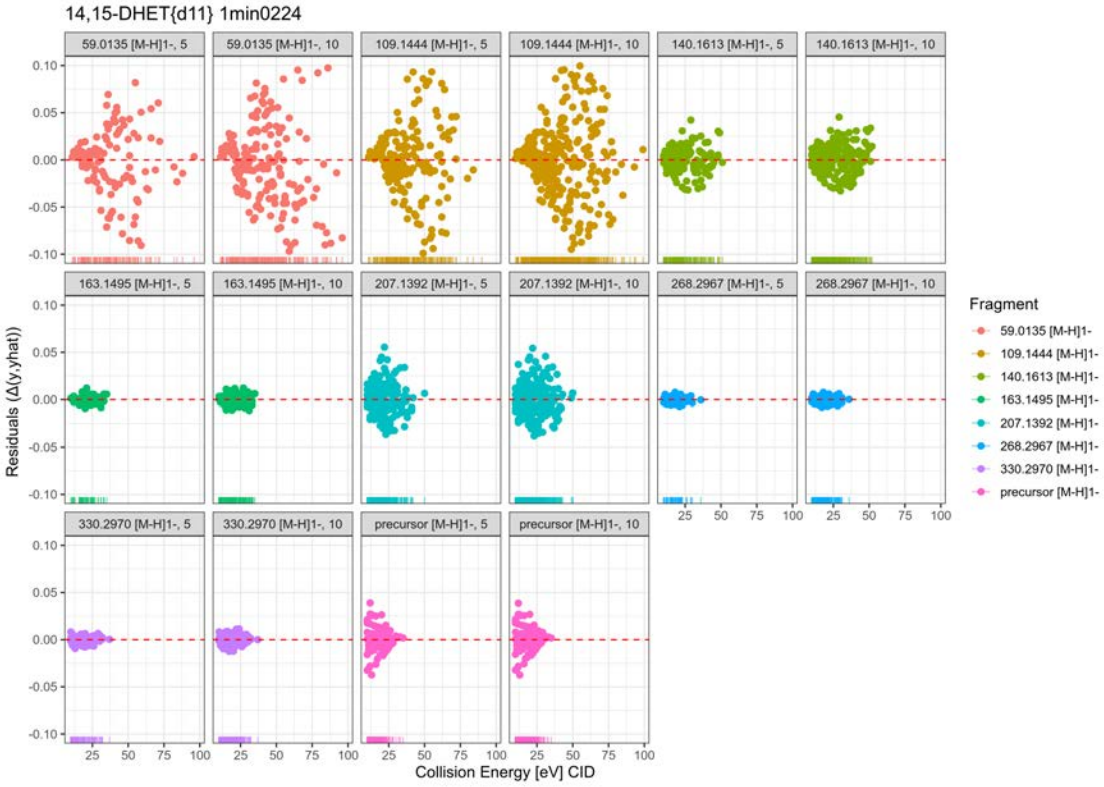


*Figure 72. Residuals of nonlinear fit*

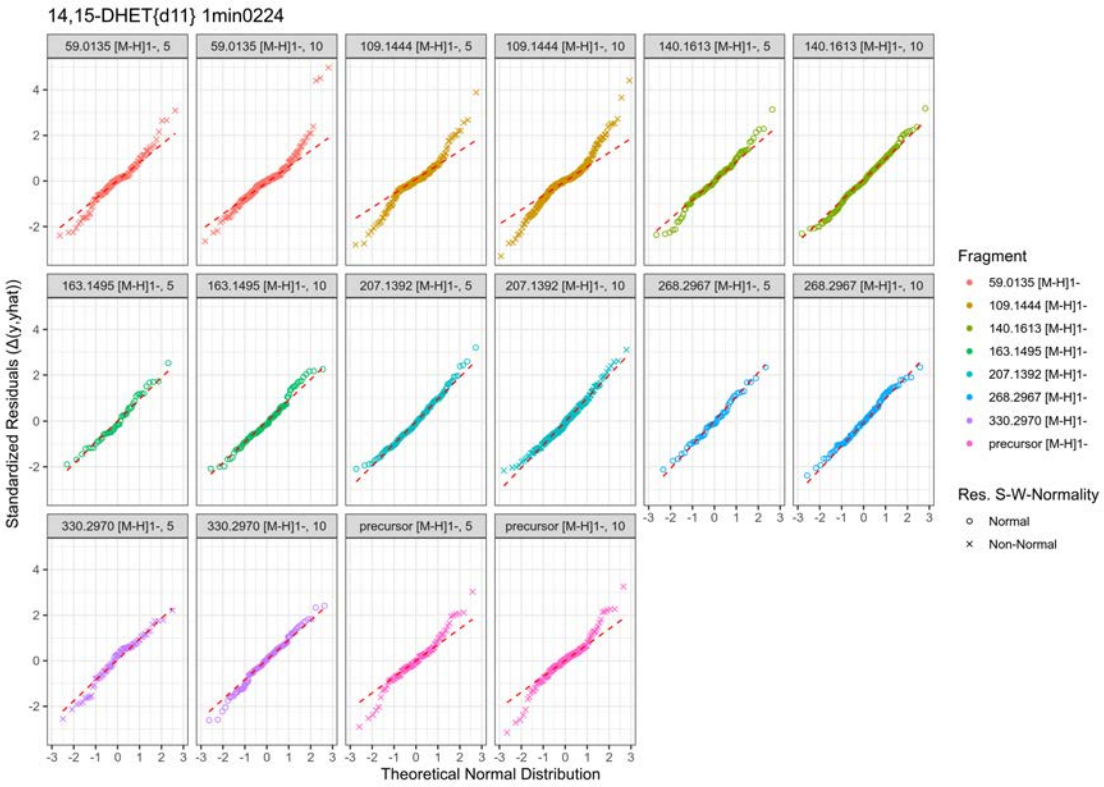


*Figure 73. Quantile-quantile plot of residuals*

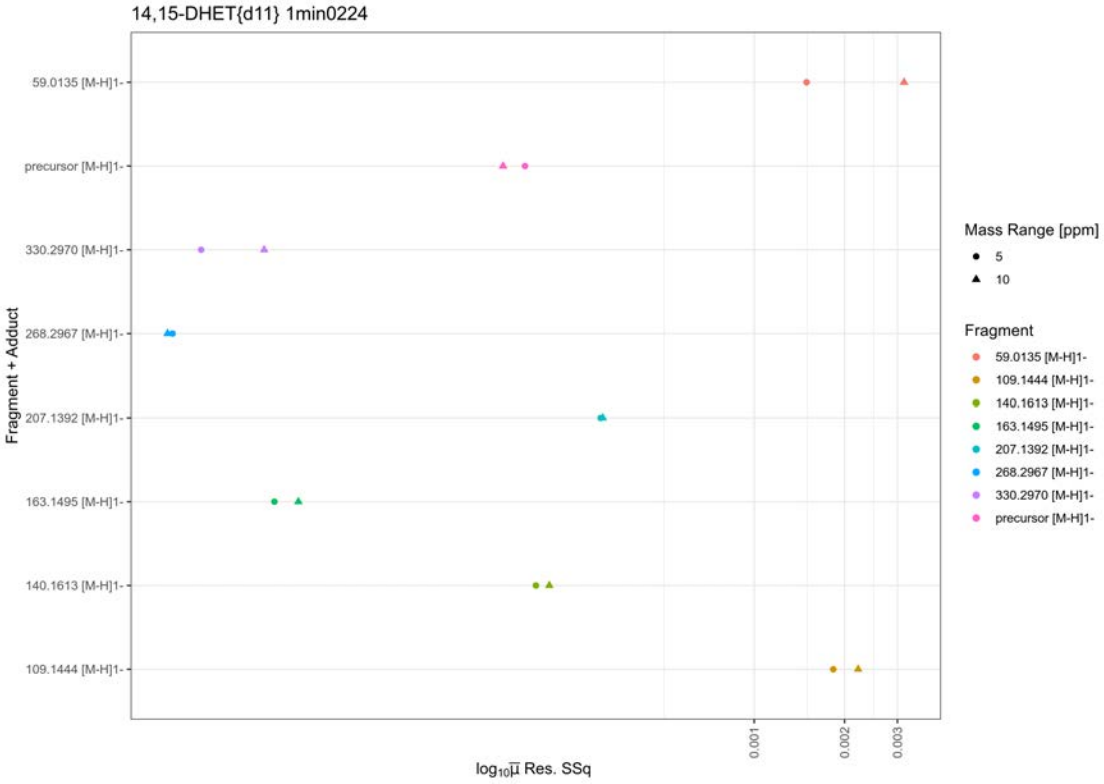


*Figure 74. Normalized sum-of-squares of the residuals*

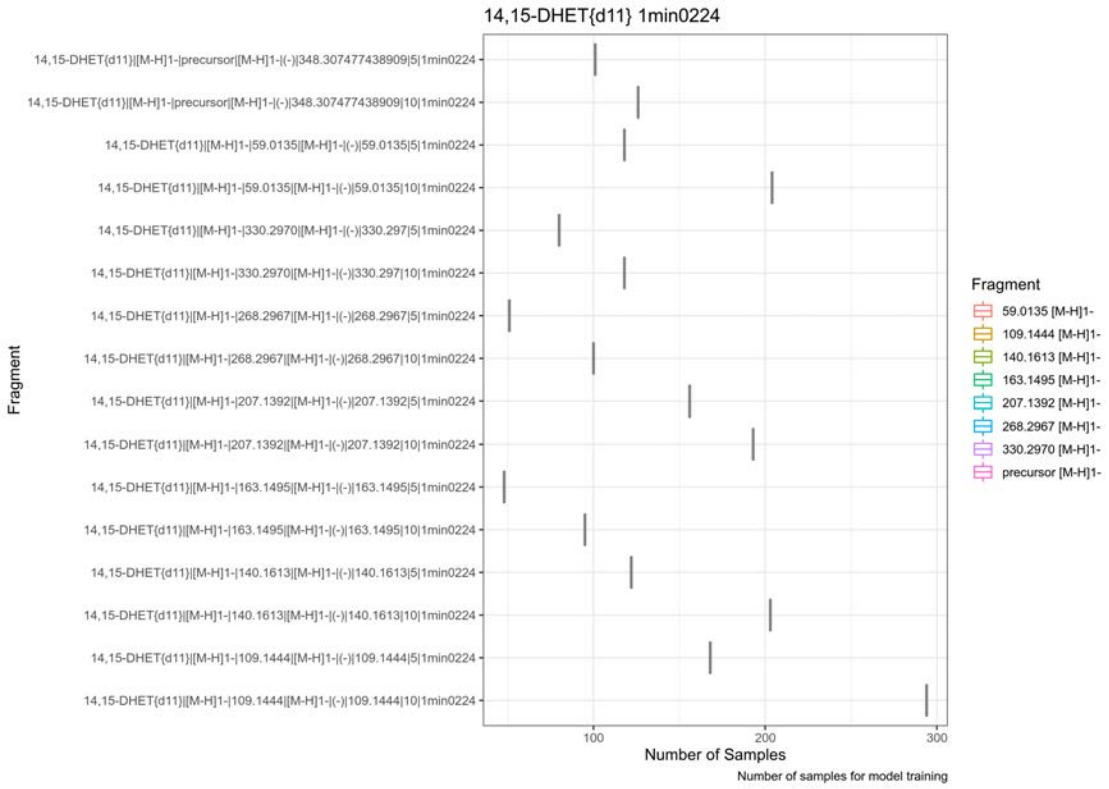


*Figure 75. Number of samples used for training per combination Id*

# 1.16. 15-HEPE [M-H]1- 1min0208

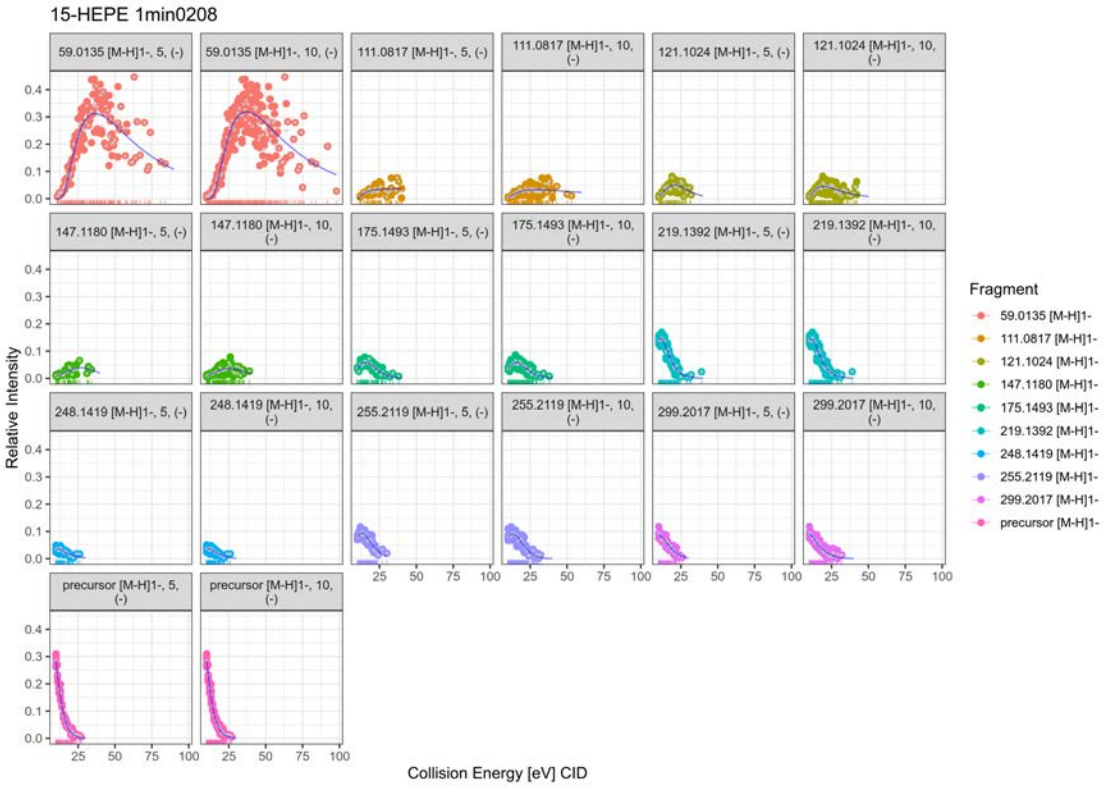


*Figure 76. Nonlinear fit*

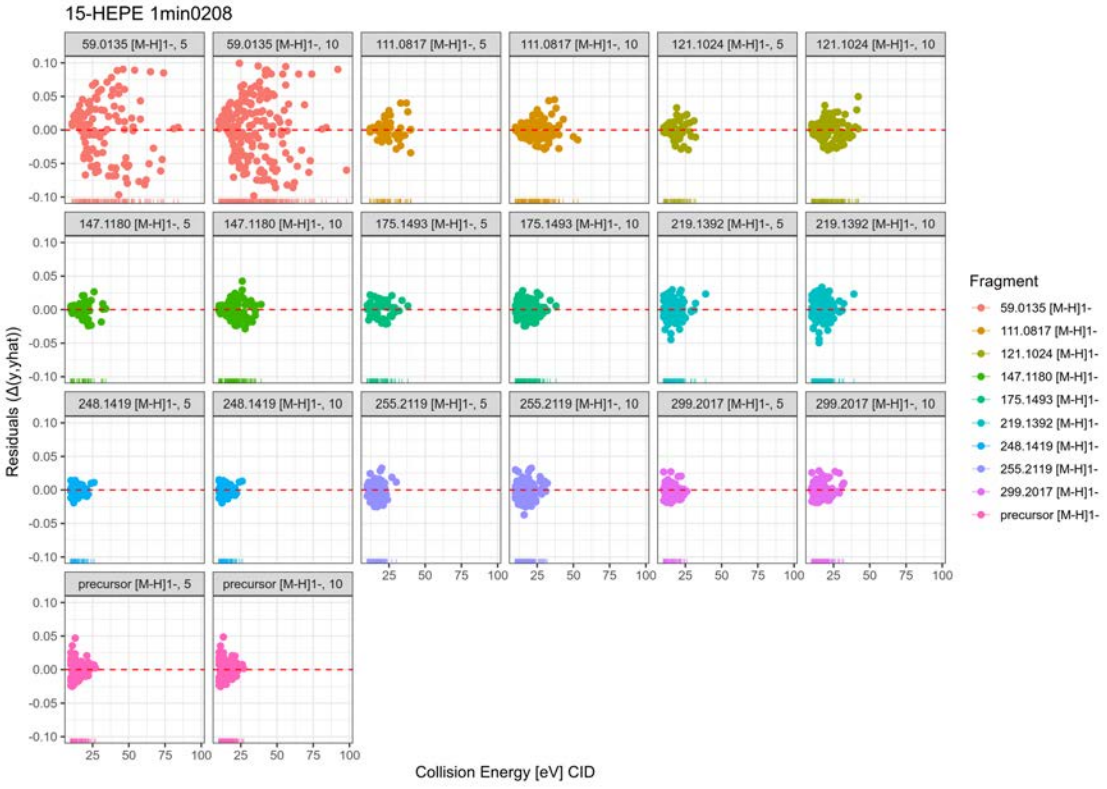


*Figure 77. Residuals of nonlinear fit*

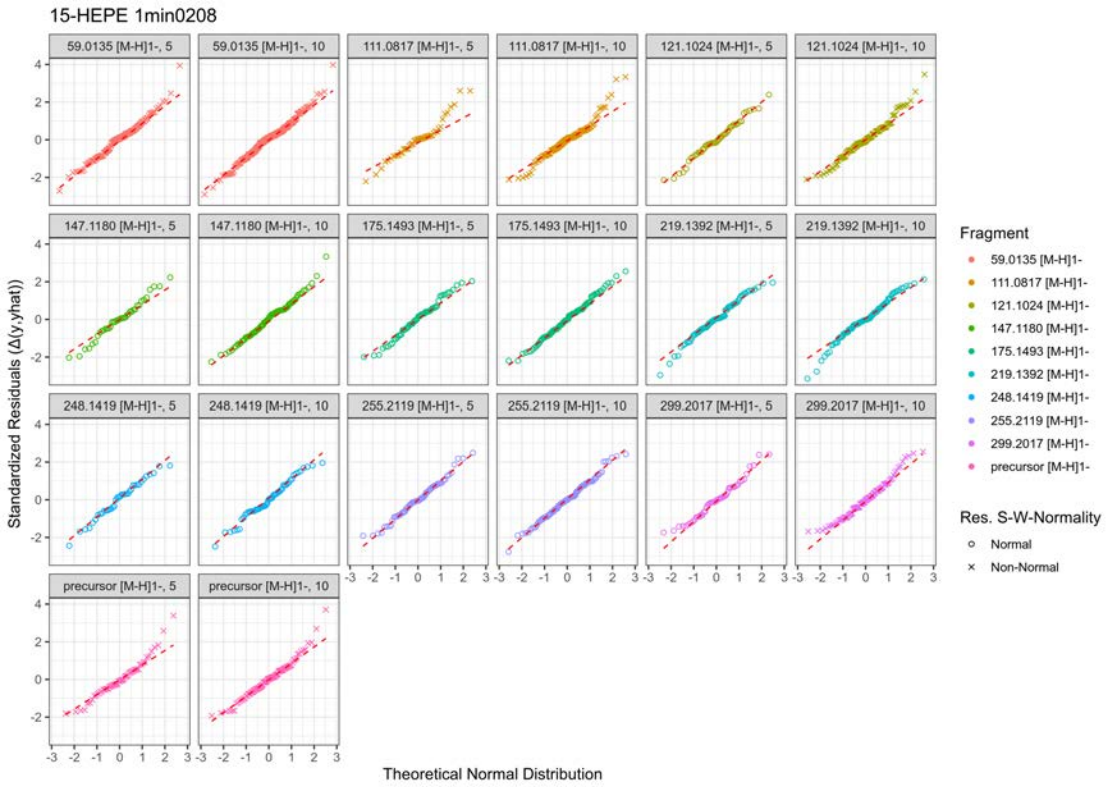


*Figure 78. Quantile-quantile plot of residuals*

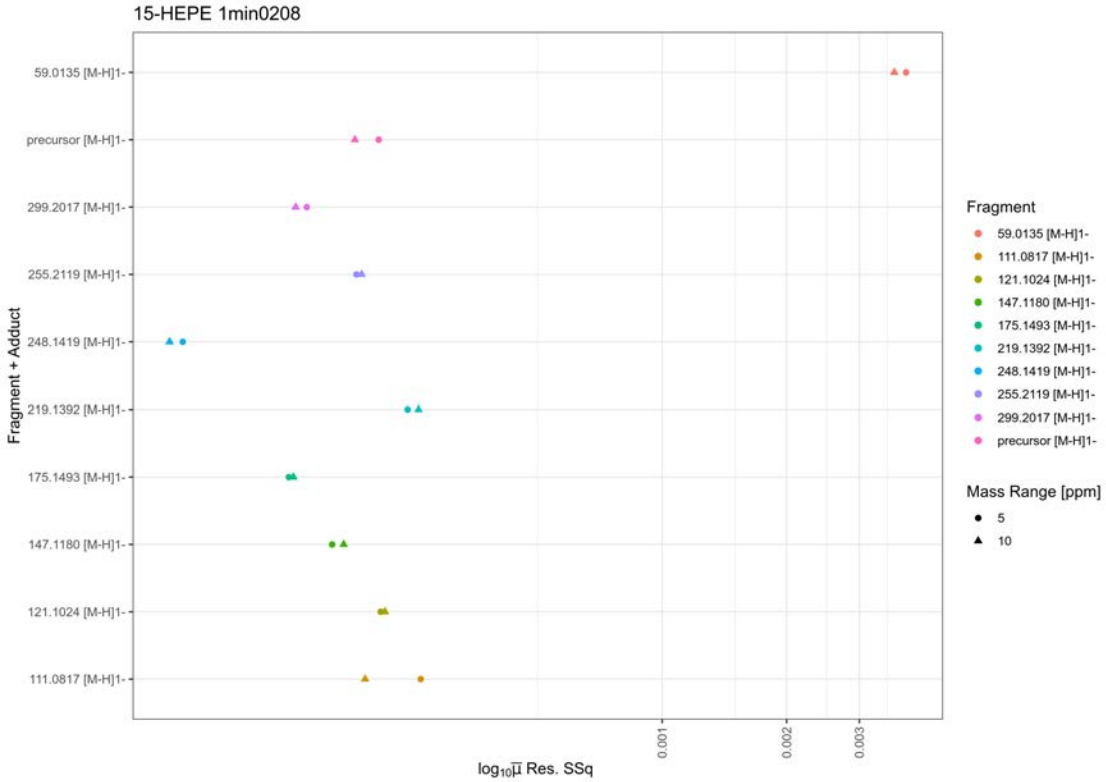


*Figure 79. Normalized sum-of-squares of the residuals*

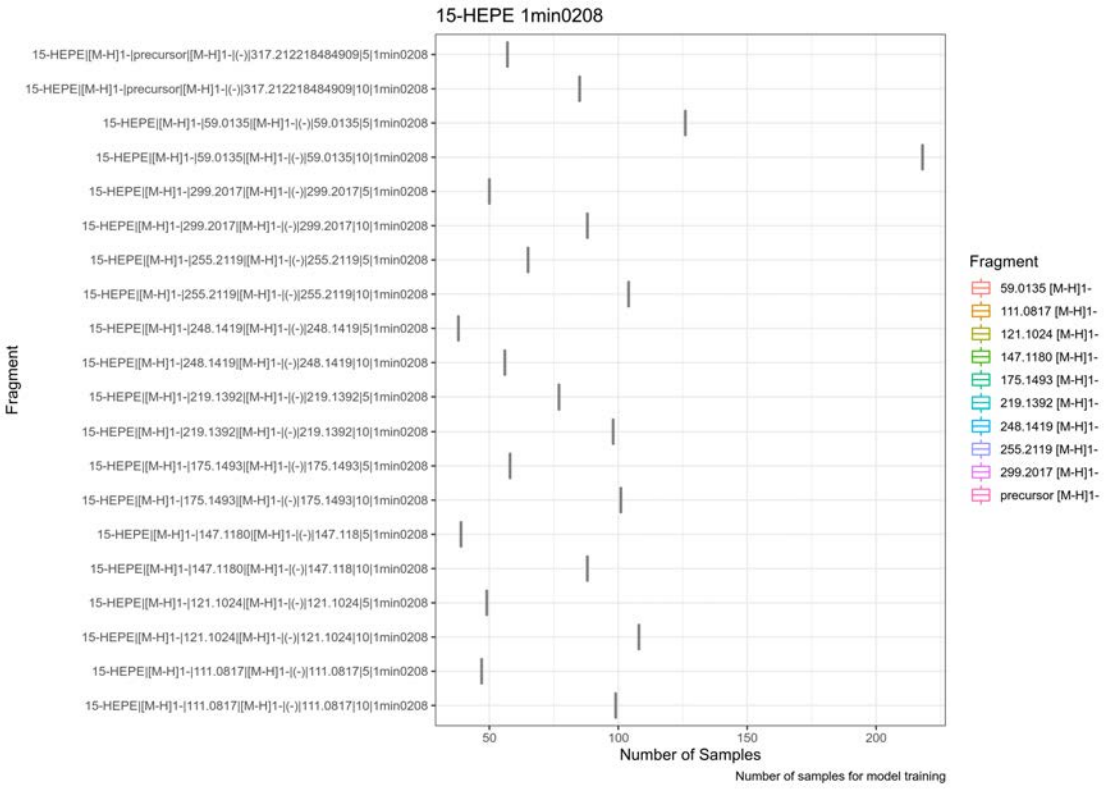


*Figure 80. Number of samples used for training per combination Id*

# 1.17. 15-HETE{d8} [M-H]1- 1min0108

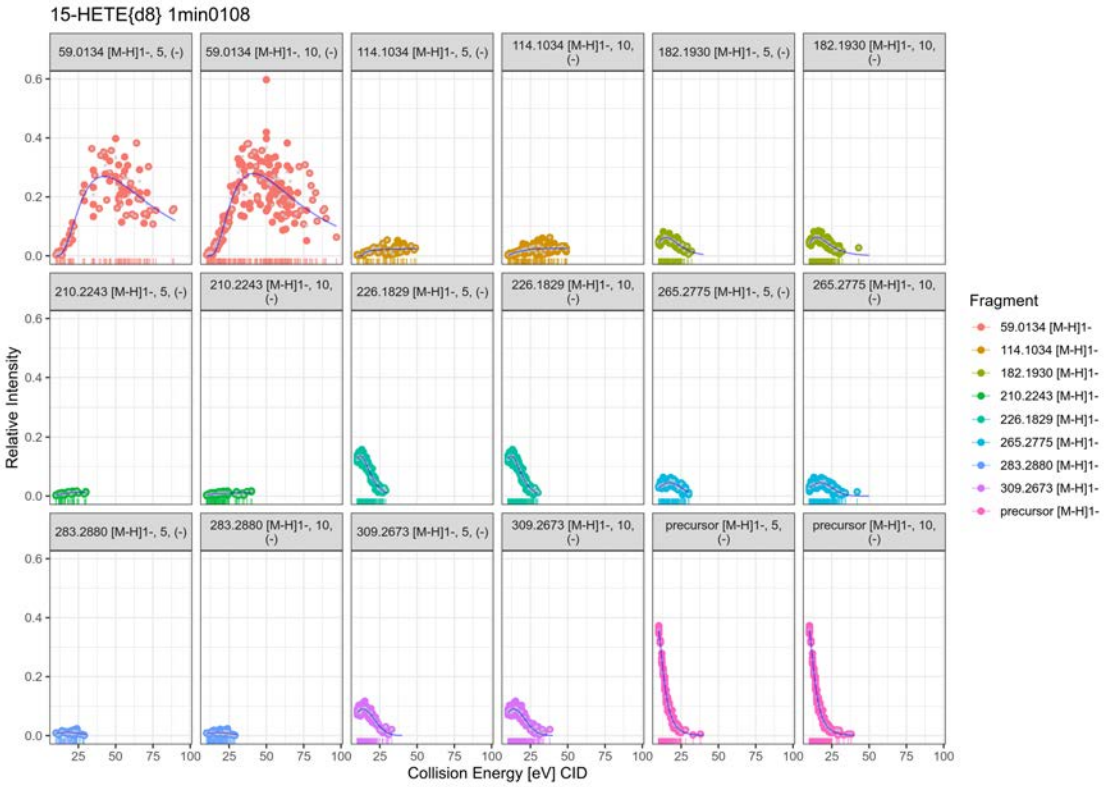


*Figure 81. Nonlinear fit*

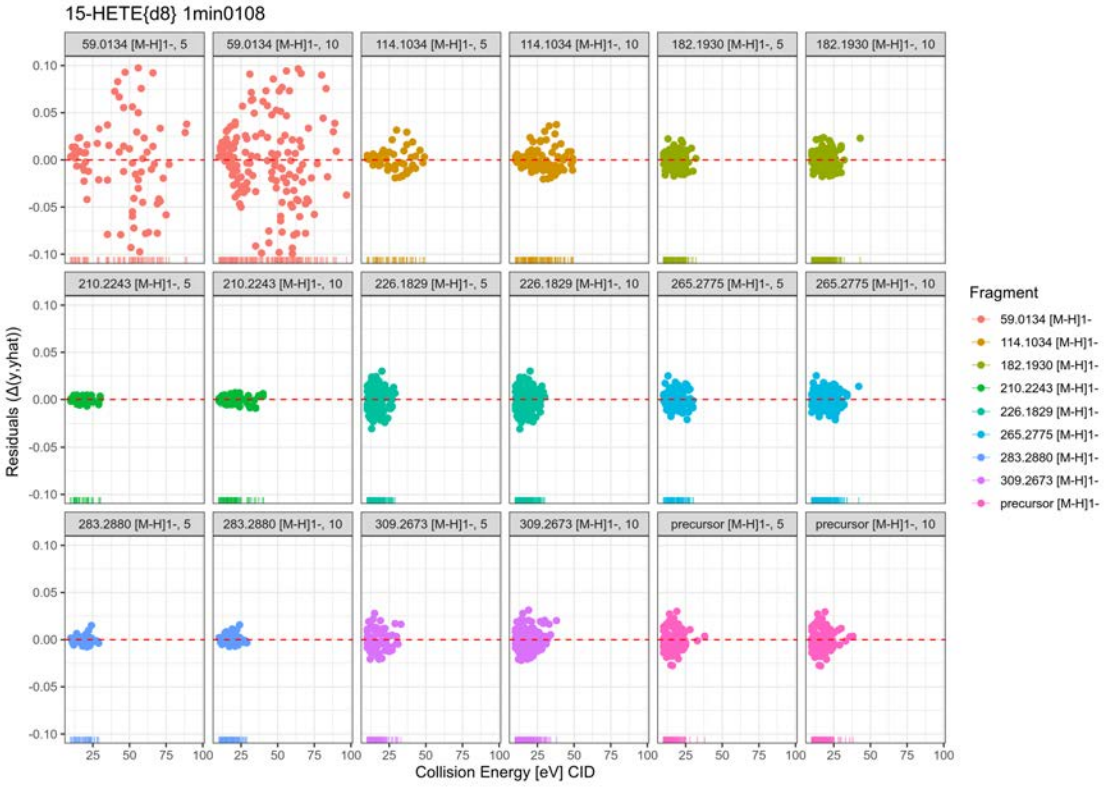


*Figure 82. Residuals of nonlinear fit*

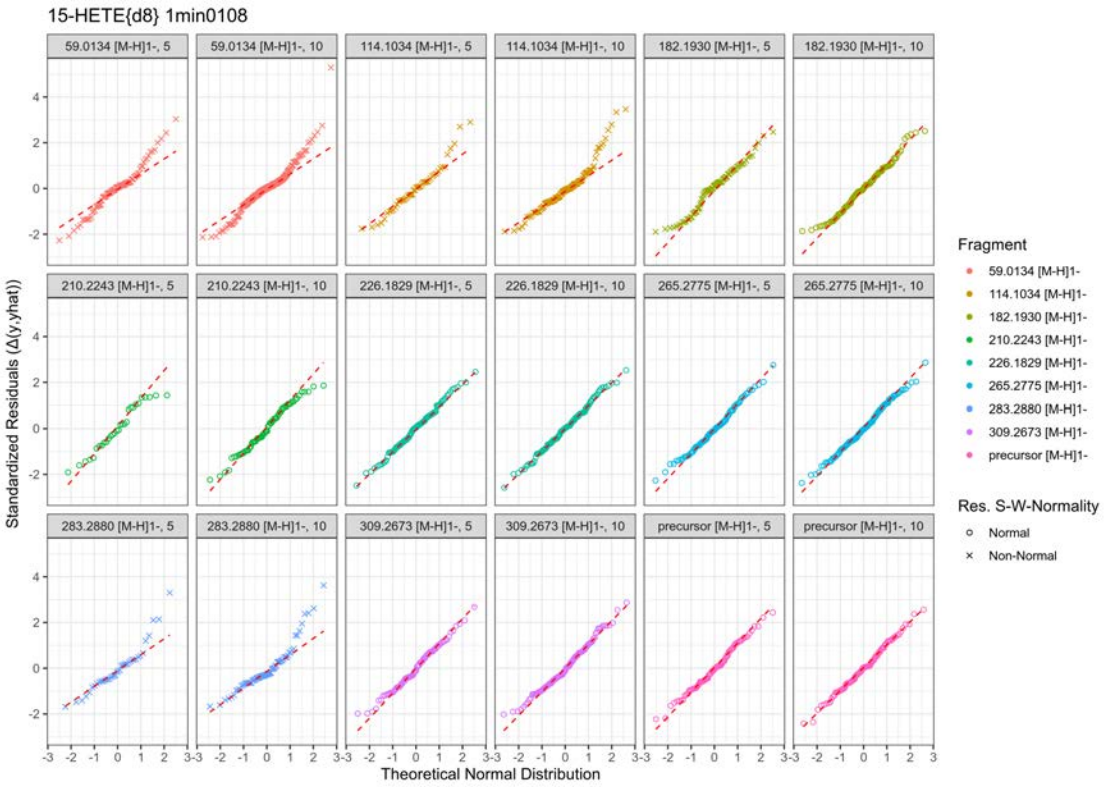


*Figure 83. Quantile-quantile plot of residuals*

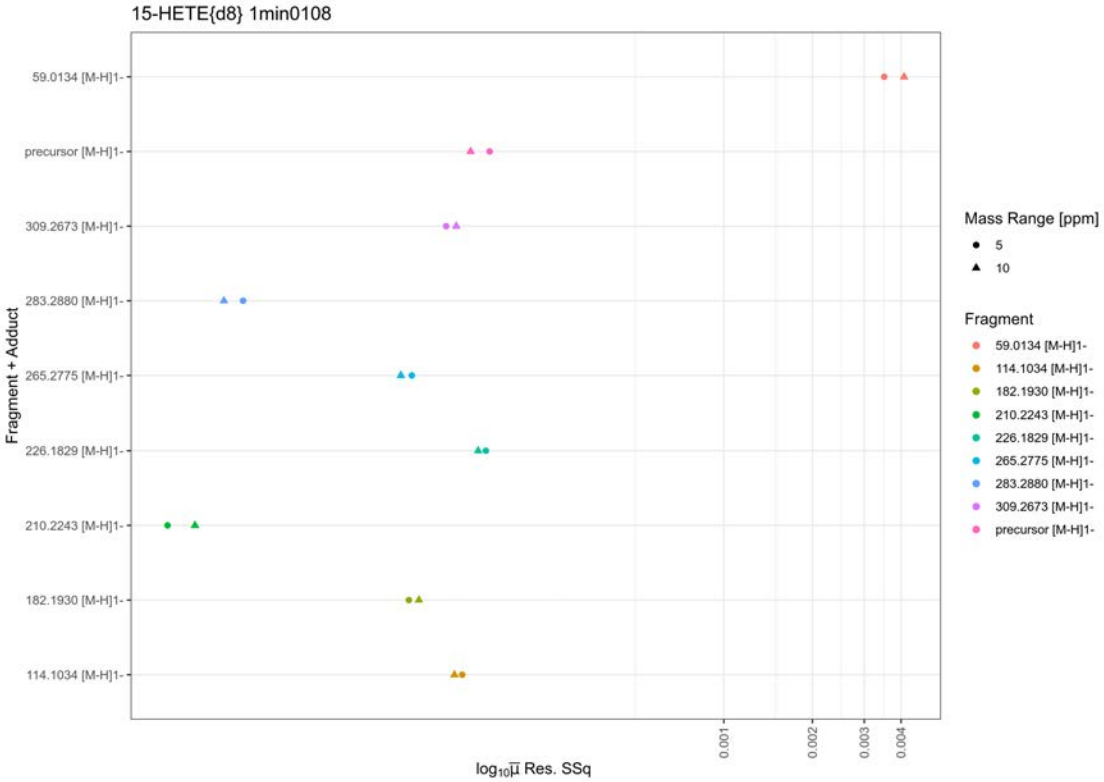


*Figure 84. Normalized sum-of-squares of the residuals*

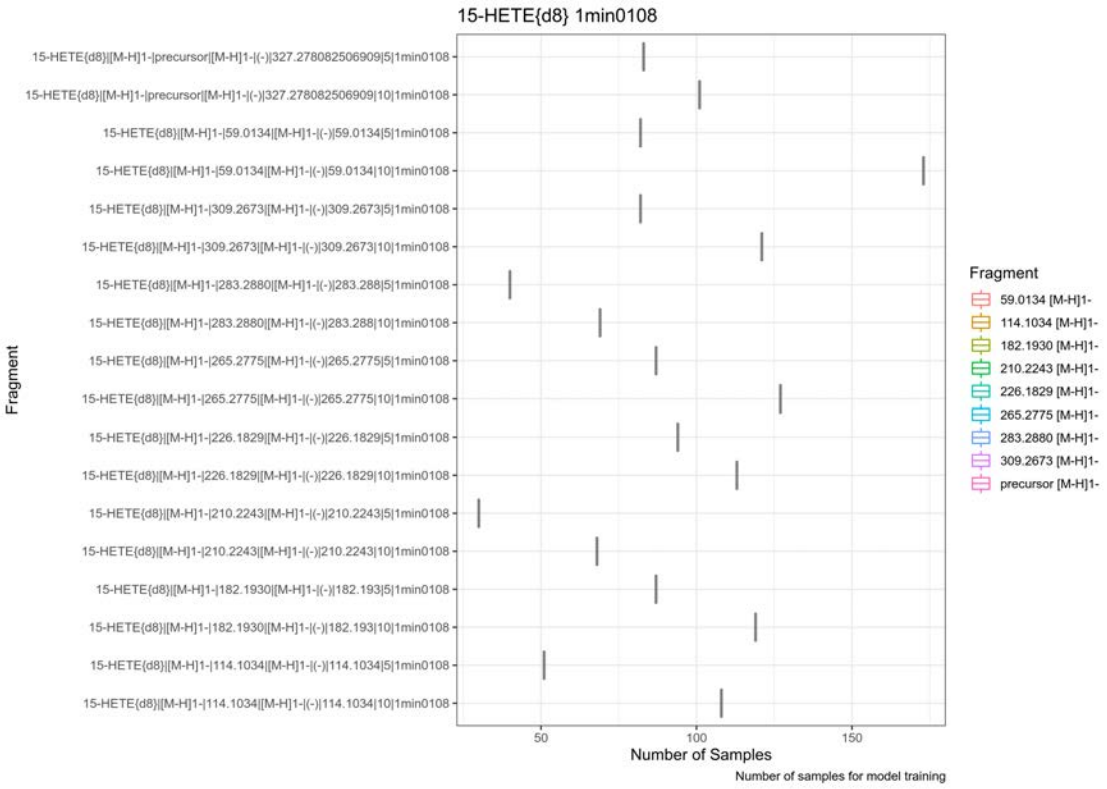


*Figure 85. Number of samples used for training per combination Id*

# 1.18. 15d-PGJ2{d4} [M-H]1- 1min0219

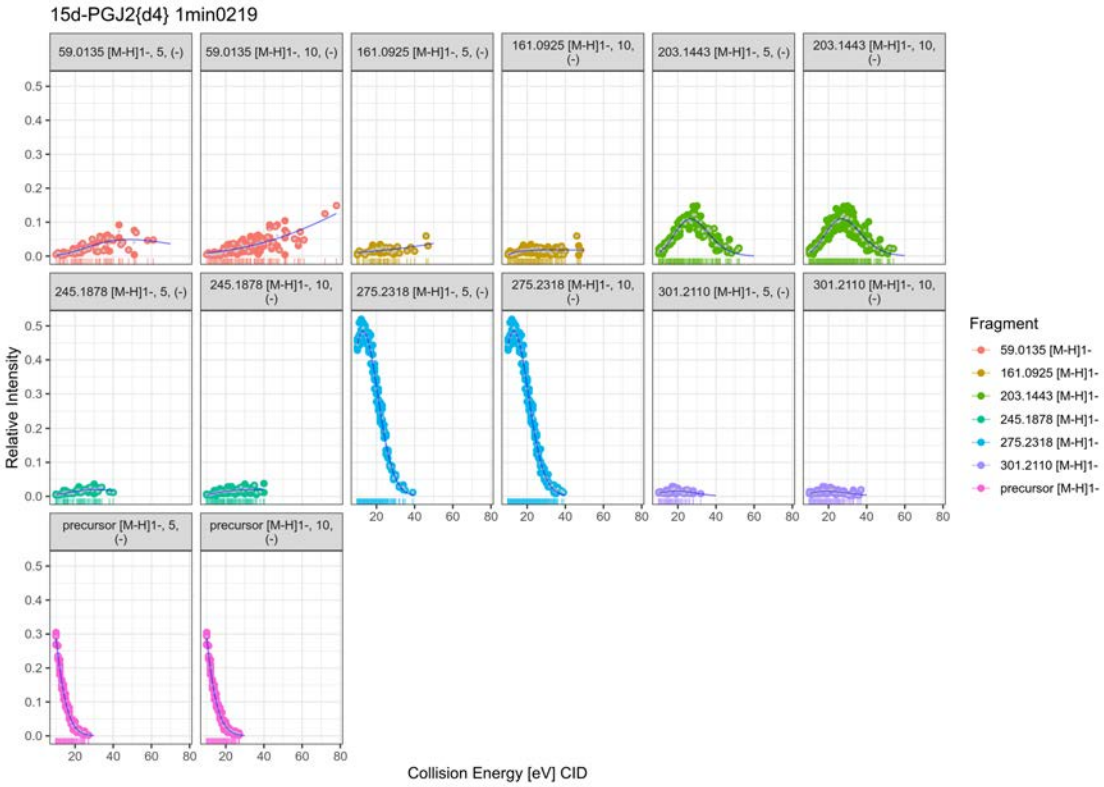


*Figure 86. Nonlinear fit*

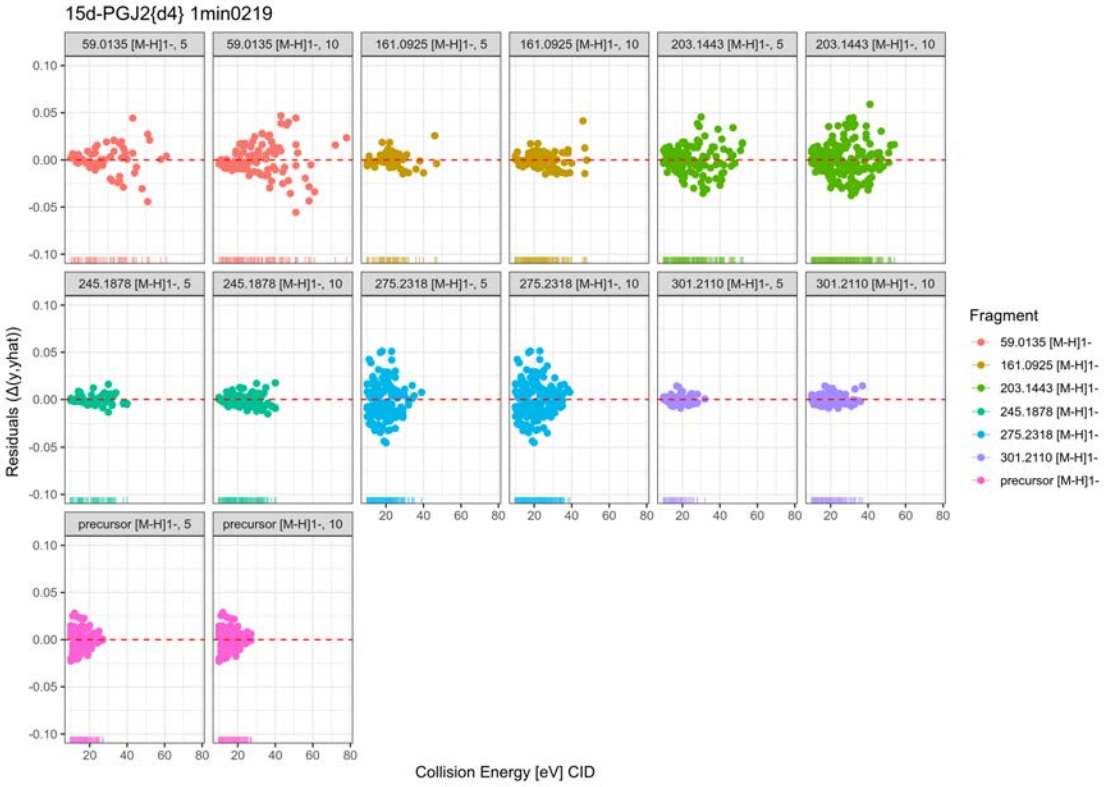


*Figure 87. Residuals of nonlinear fit*

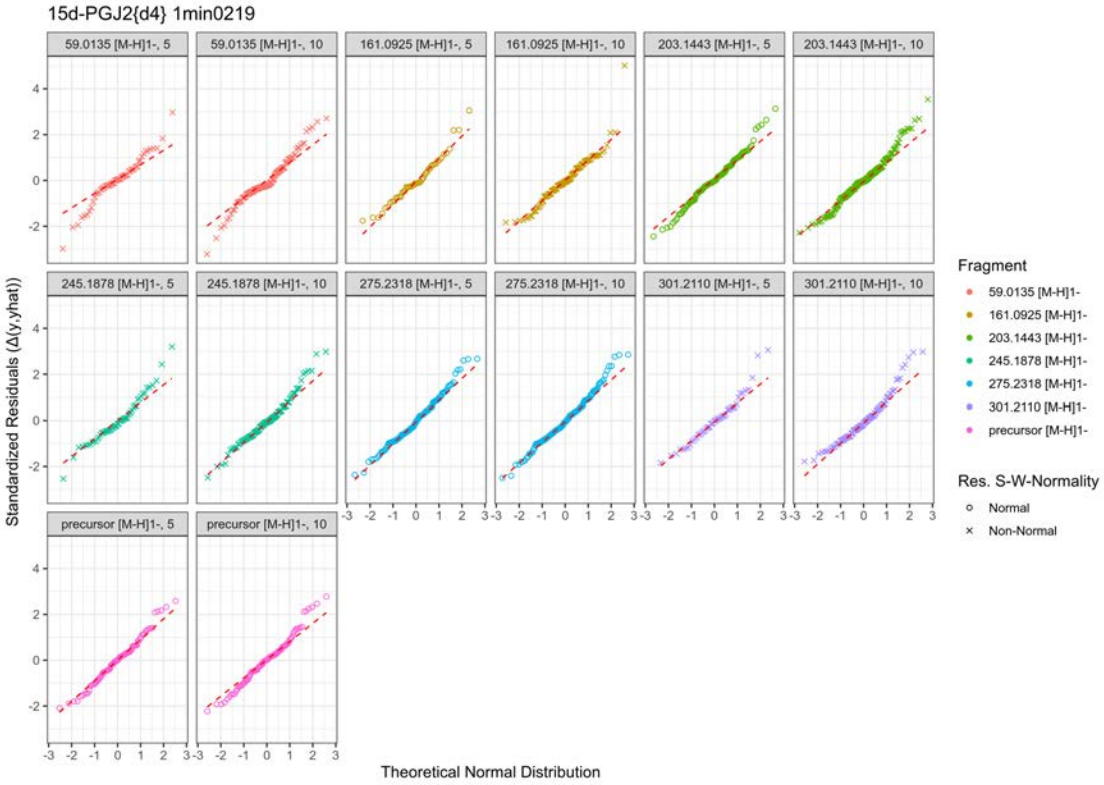


*Figure 88. Quantile-quantile plot of residuals*

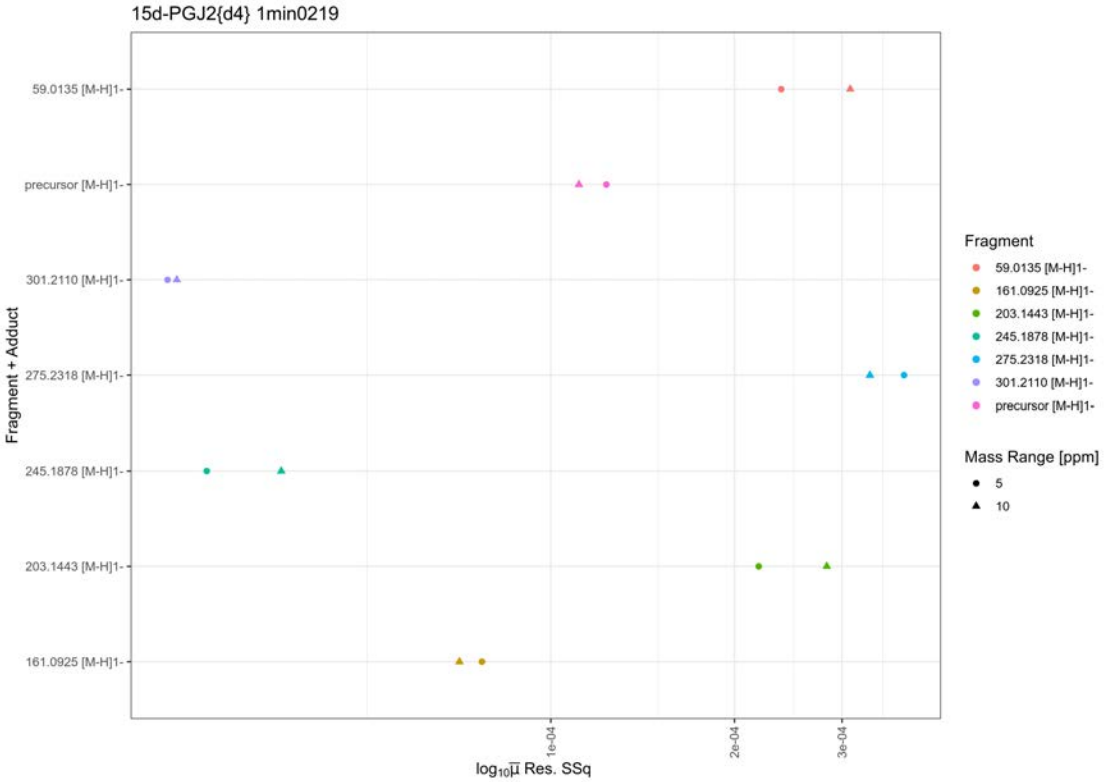


*Figure 89. Normalized sum-of-squares of the residuals*

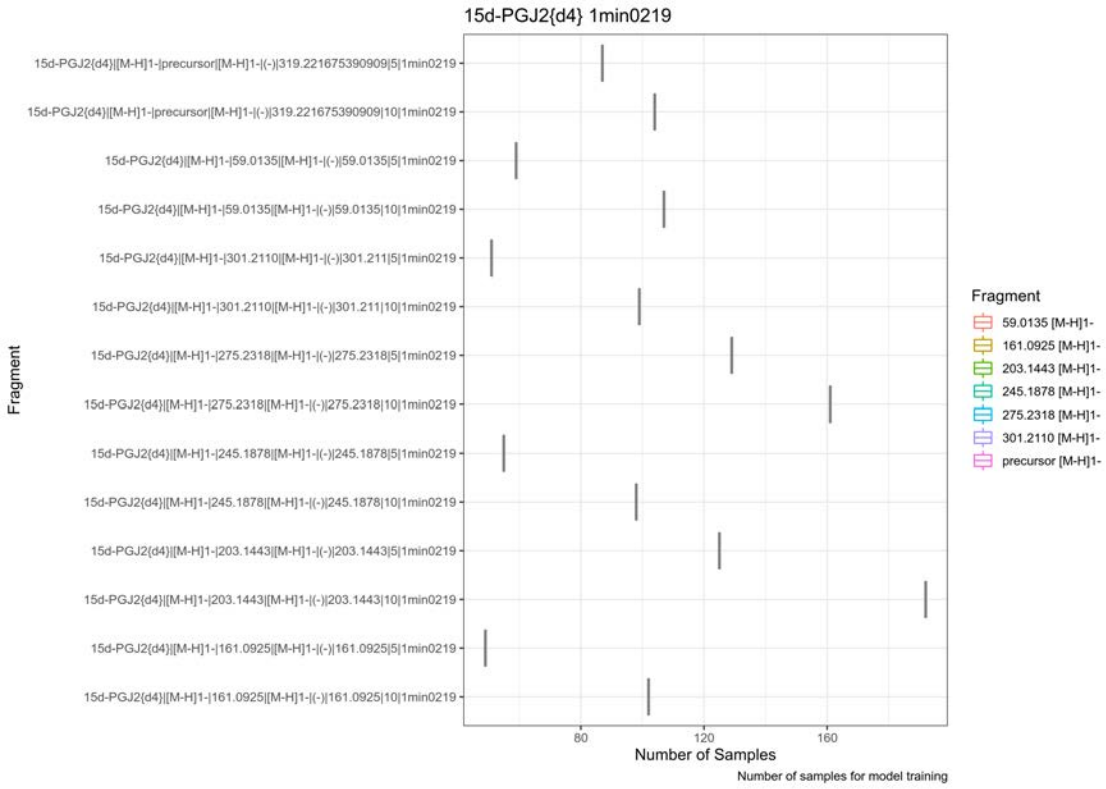


*Figure 90. Number of samples used for training per combination Id*

# 1.19. 16-HDoHE [M-H]1- 1min0112

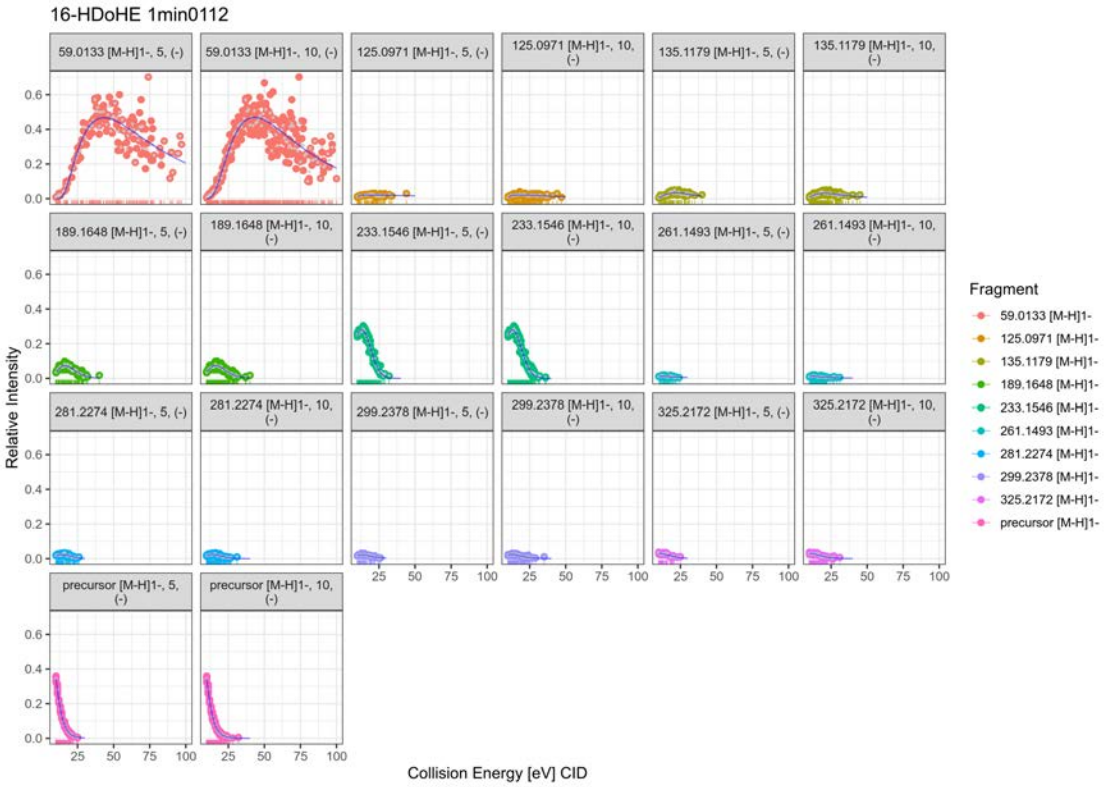


*Figure 91. Nonlinear fit*

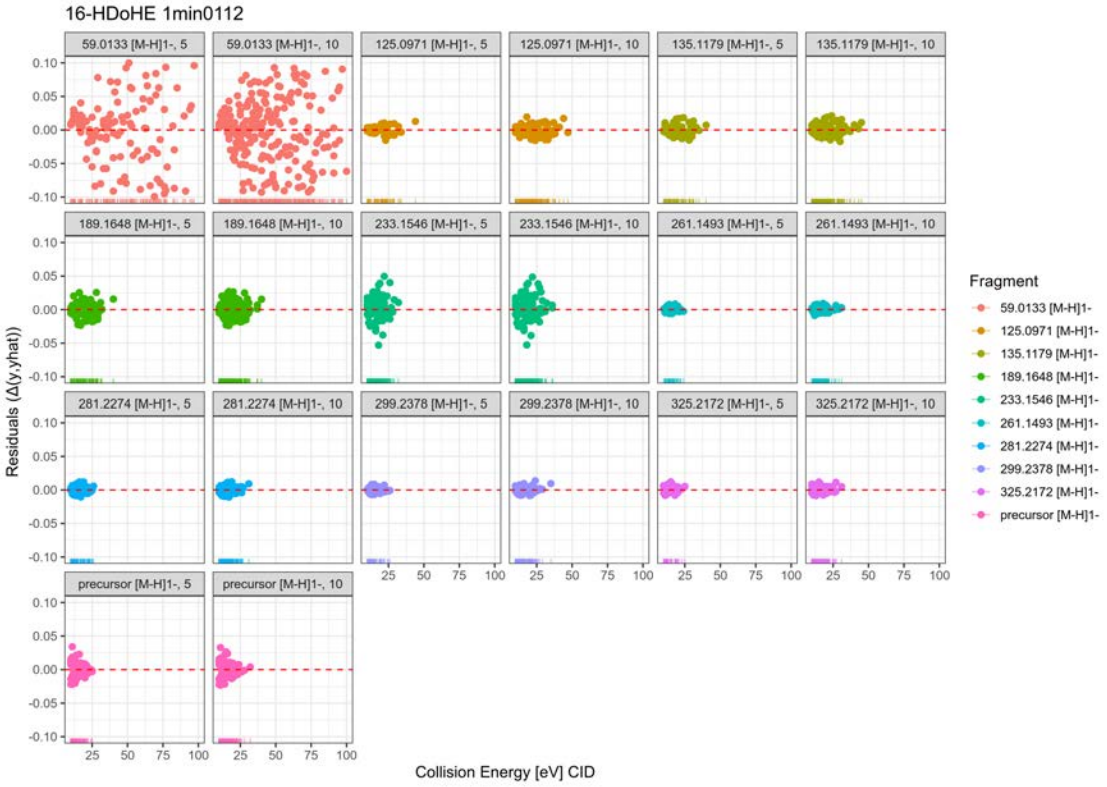


*Figure 92. Residuals of nonlinear fit*

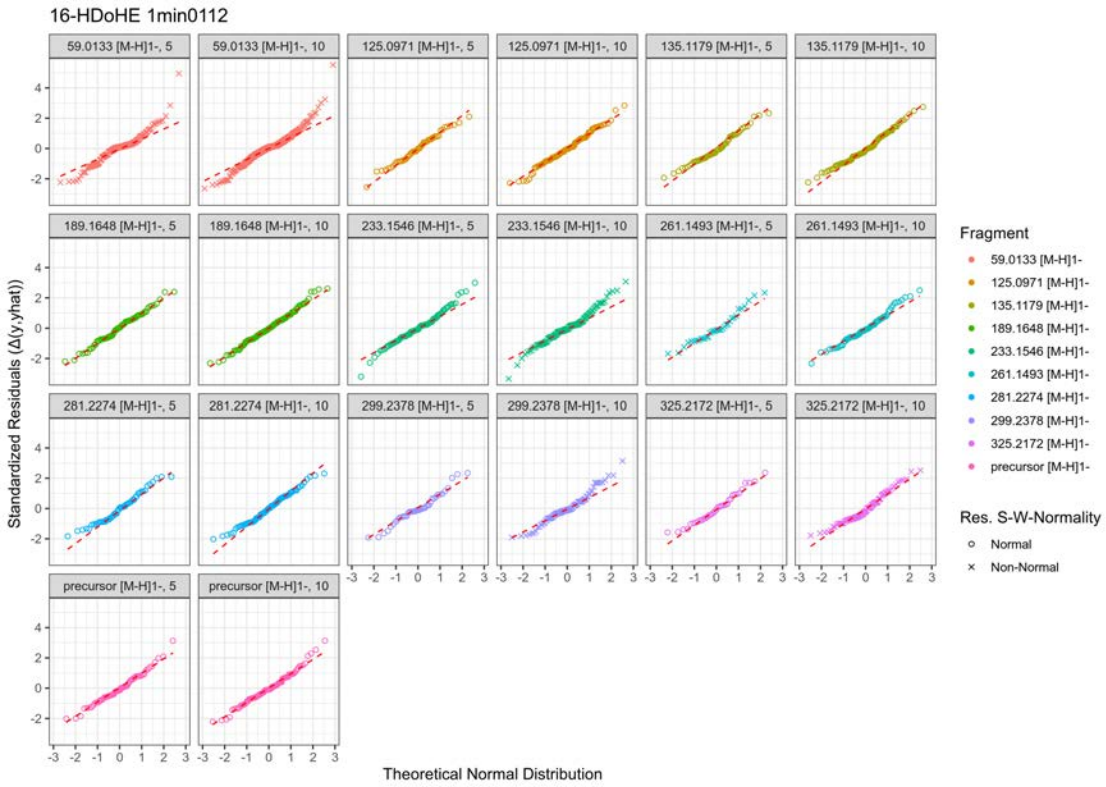


*Figure 93. Quantile-quantile plot of residuals*

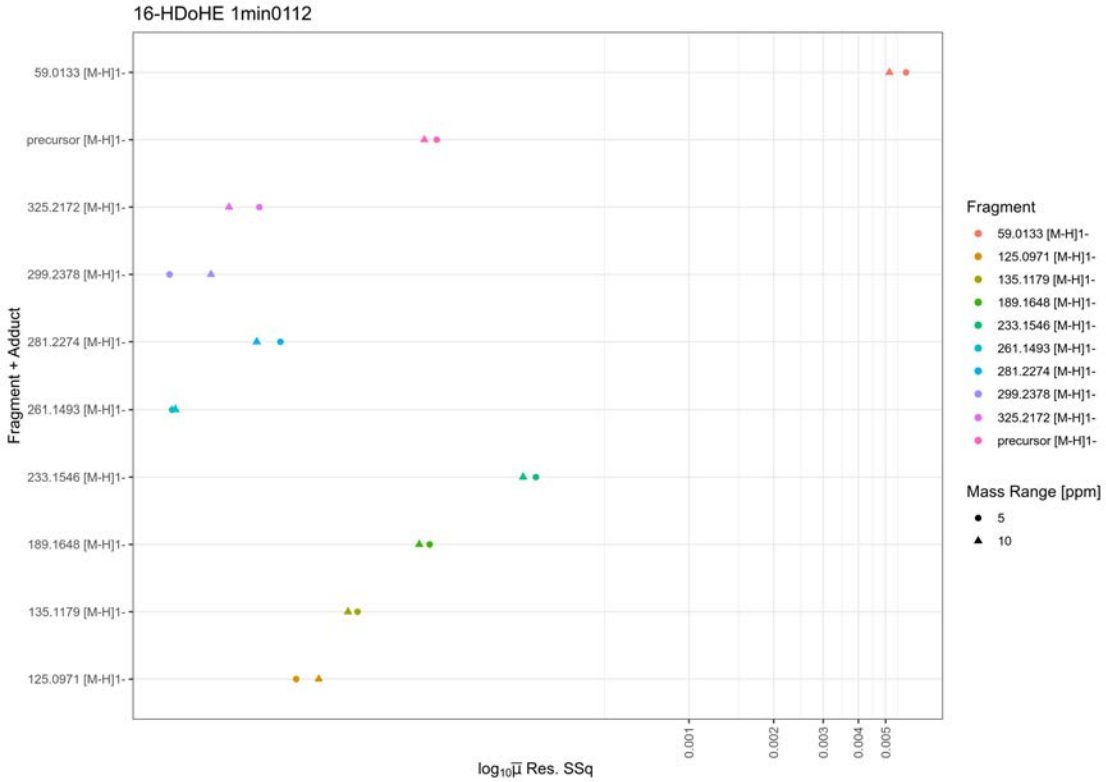


*Figure 94. Normalized sum-of-squares of the residuals*

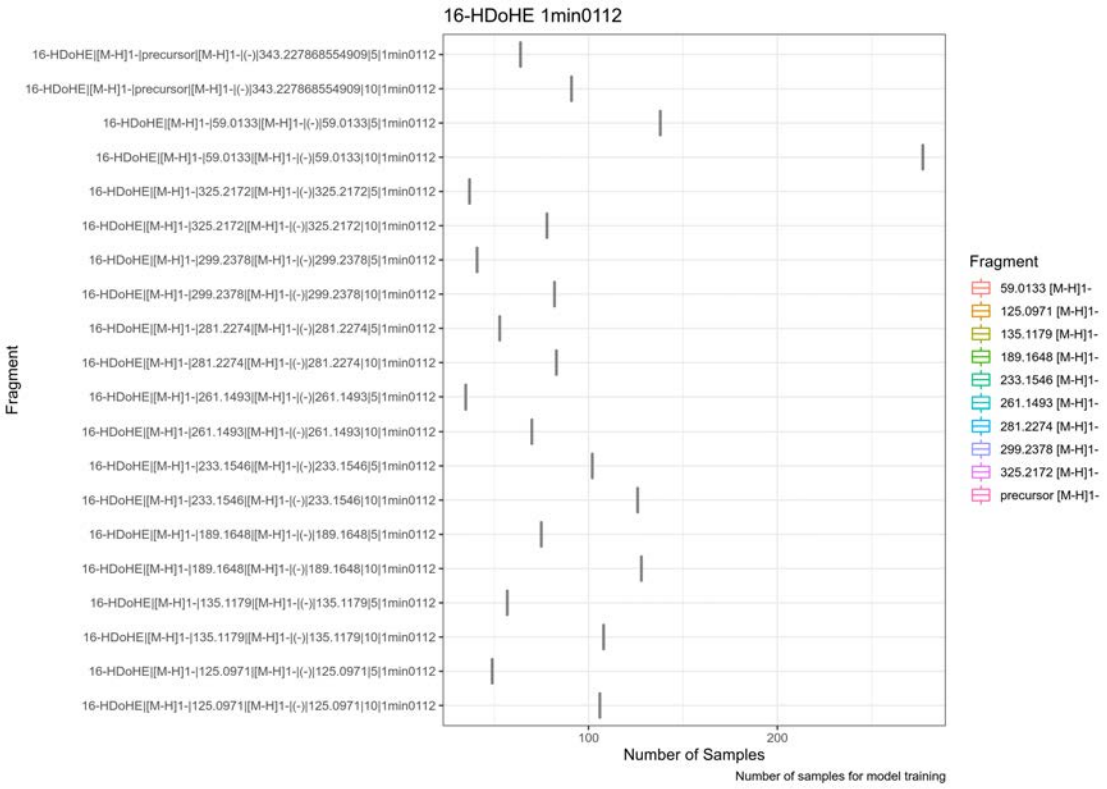


*Figure 95. Number of samples used for training per combination Id*

# 1.20. 18-HEPE [M-H]1- 1min0199

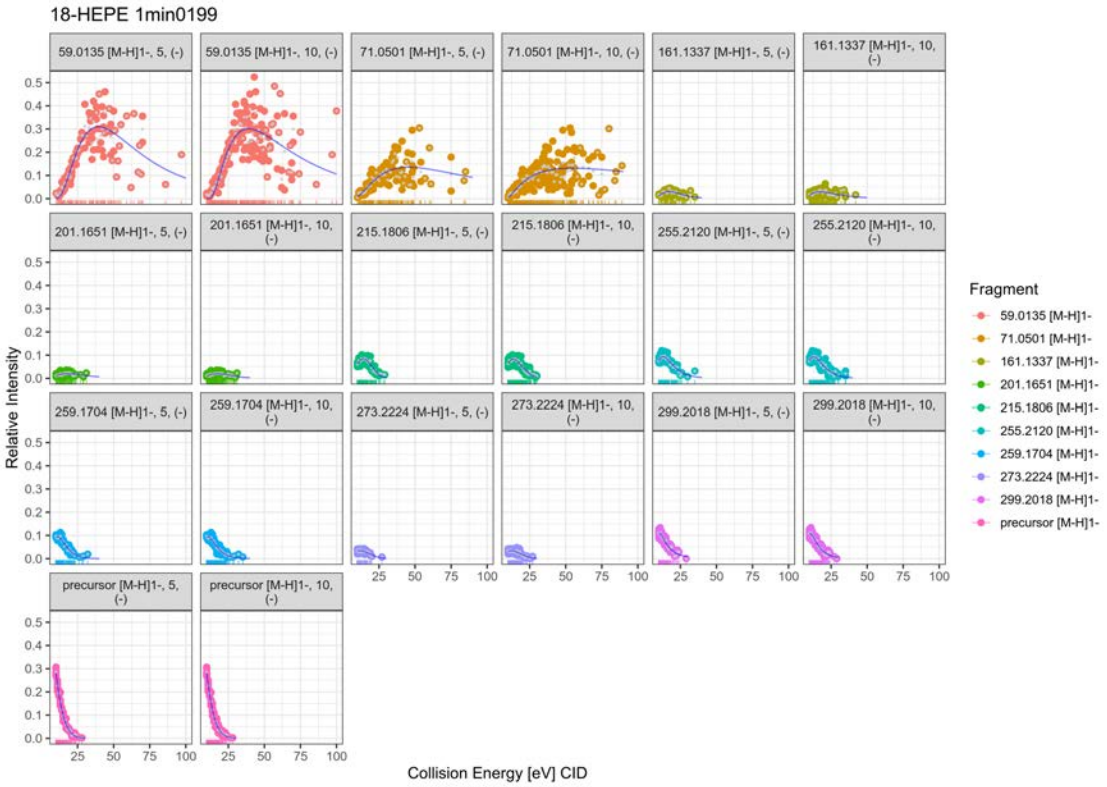


*Figure 96. Nonlinear fit*

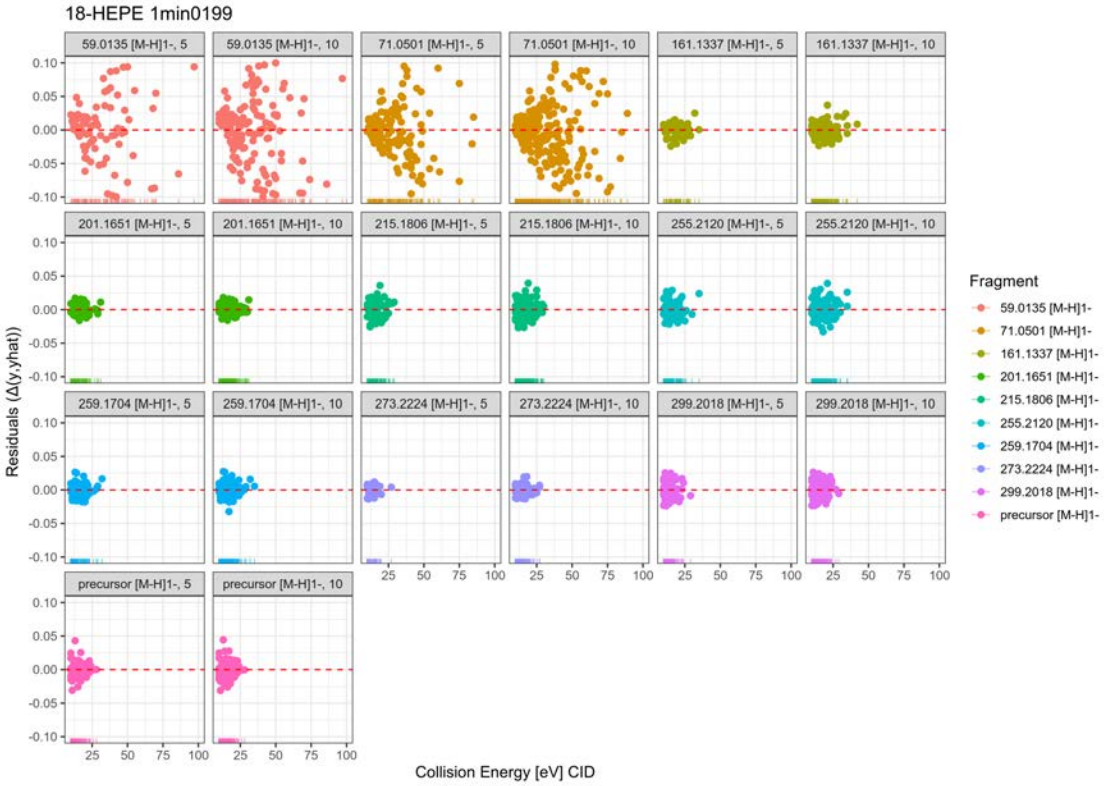


*Figure 97. Residuals of nonlinear fit*

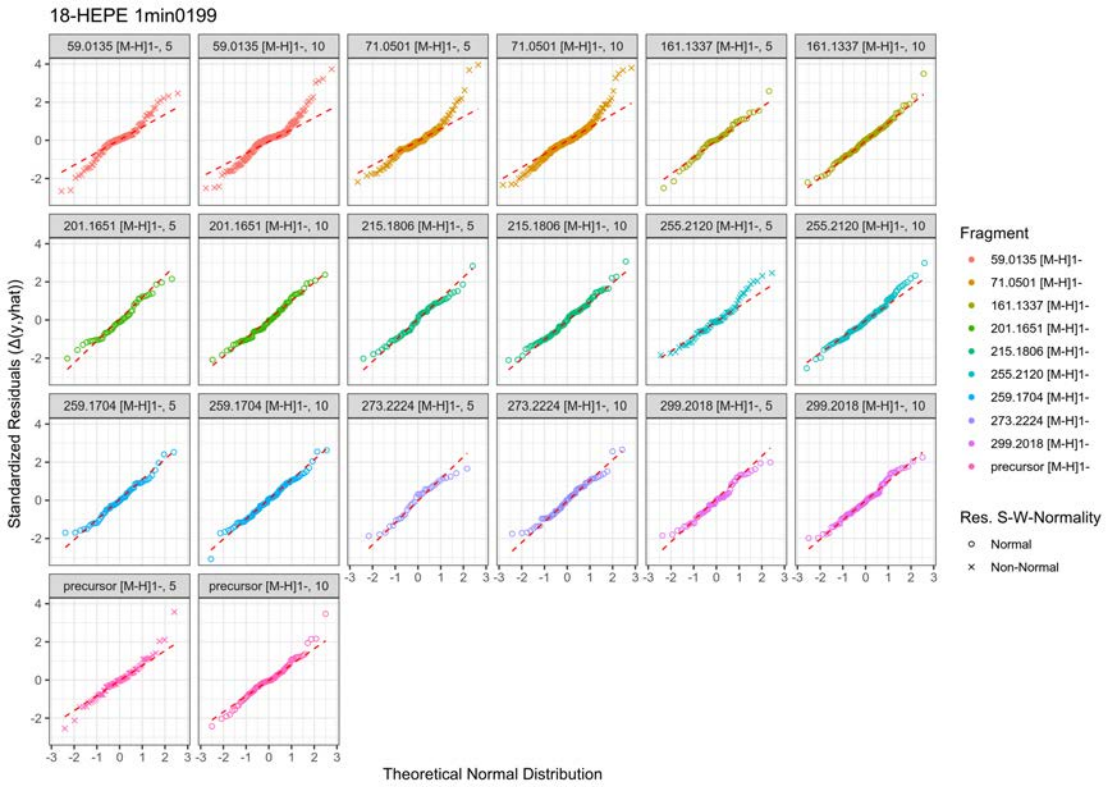


*Figure 98. Quantile-quantile plot of residuals*

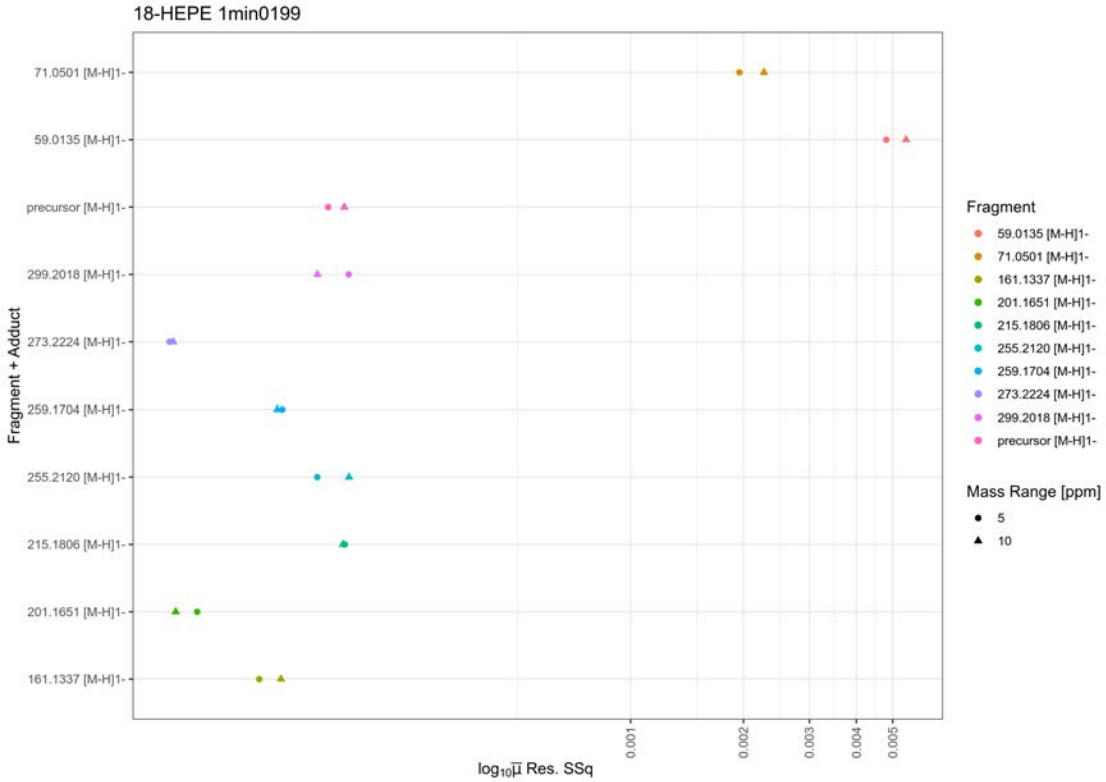


*Figure 99. Normalized sum-of-squares of the residuals*

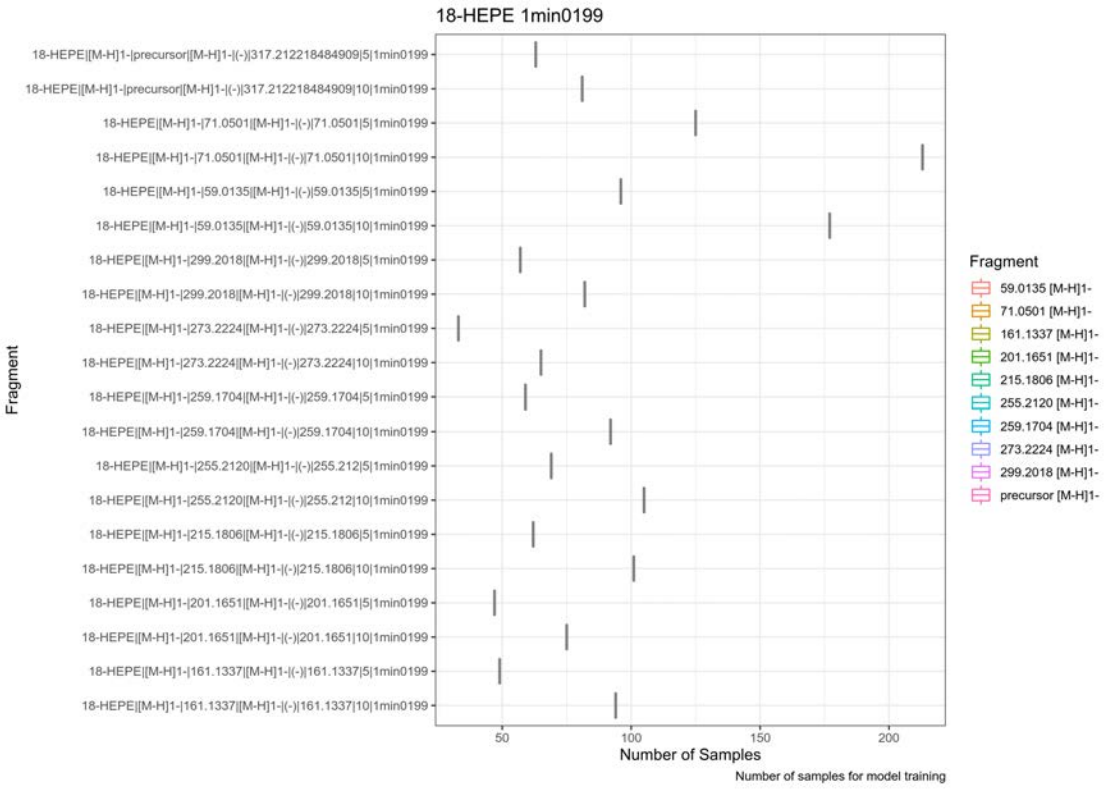


*Figure 100. Number of samples used for training per combination Id*

# 1.21. 5(6)-EET{d11} [M-H]1- 1min0227

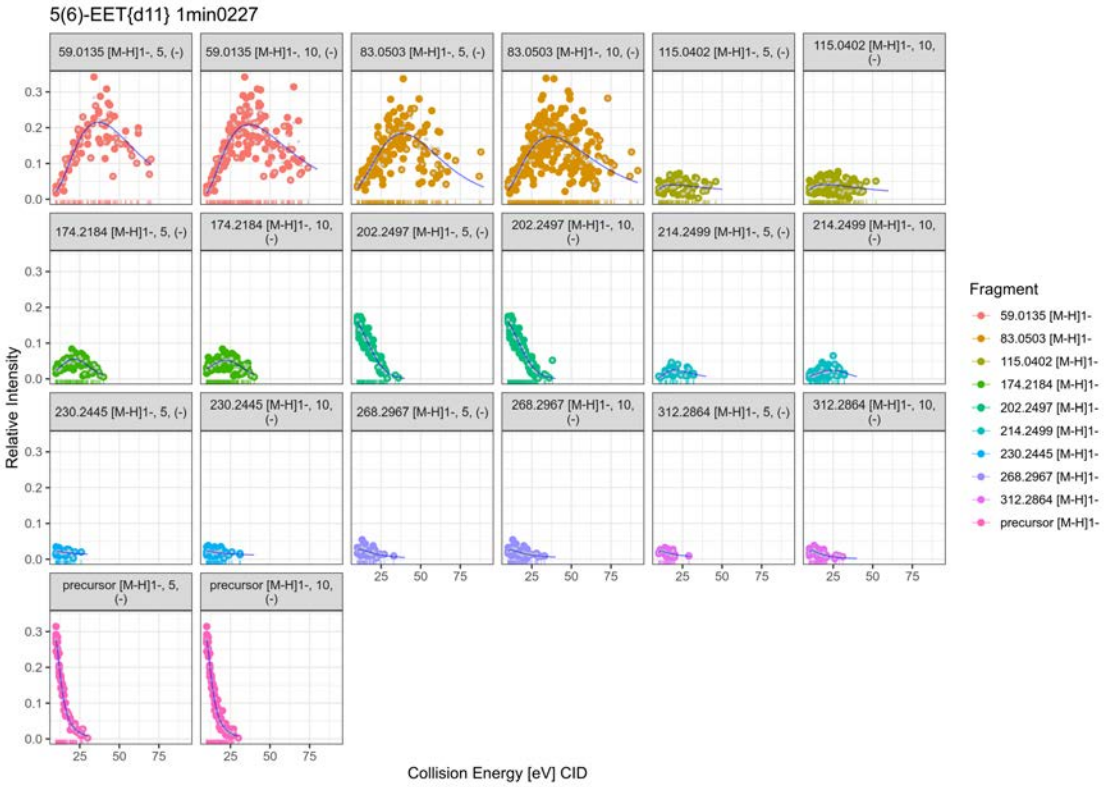


*Figure 101. Nonlinear fit*

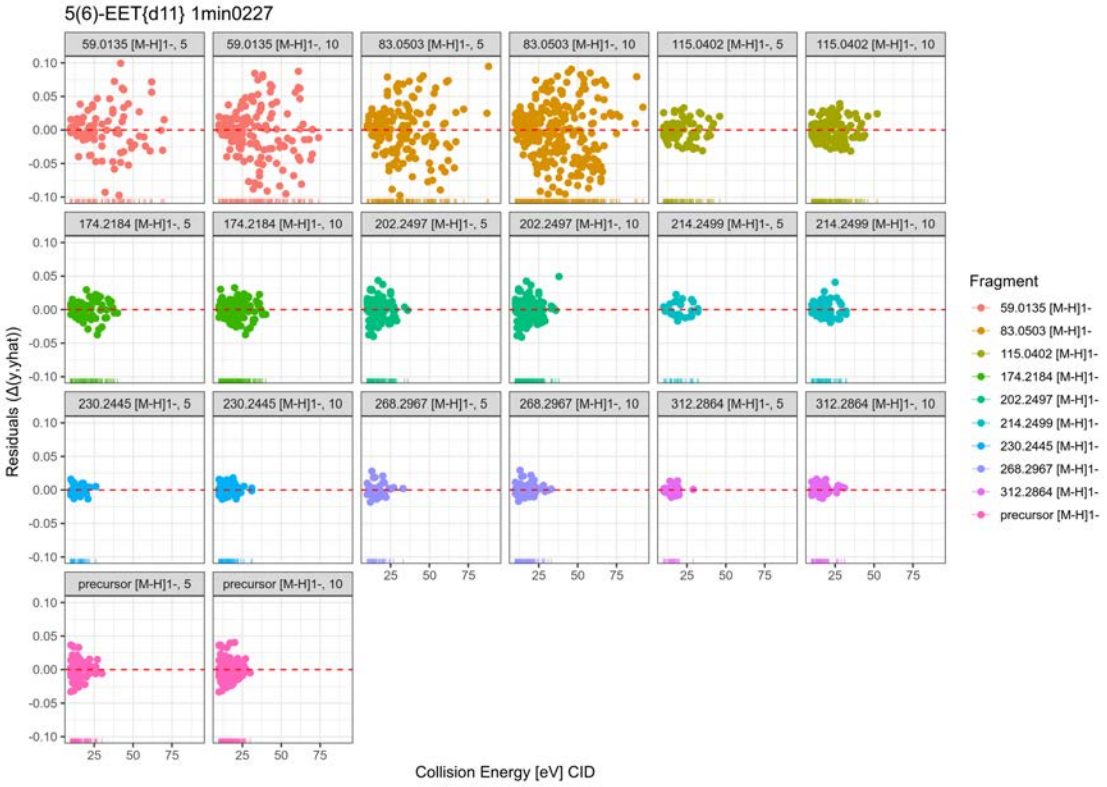


*Figure 102. Residuals of nonlinear fit*

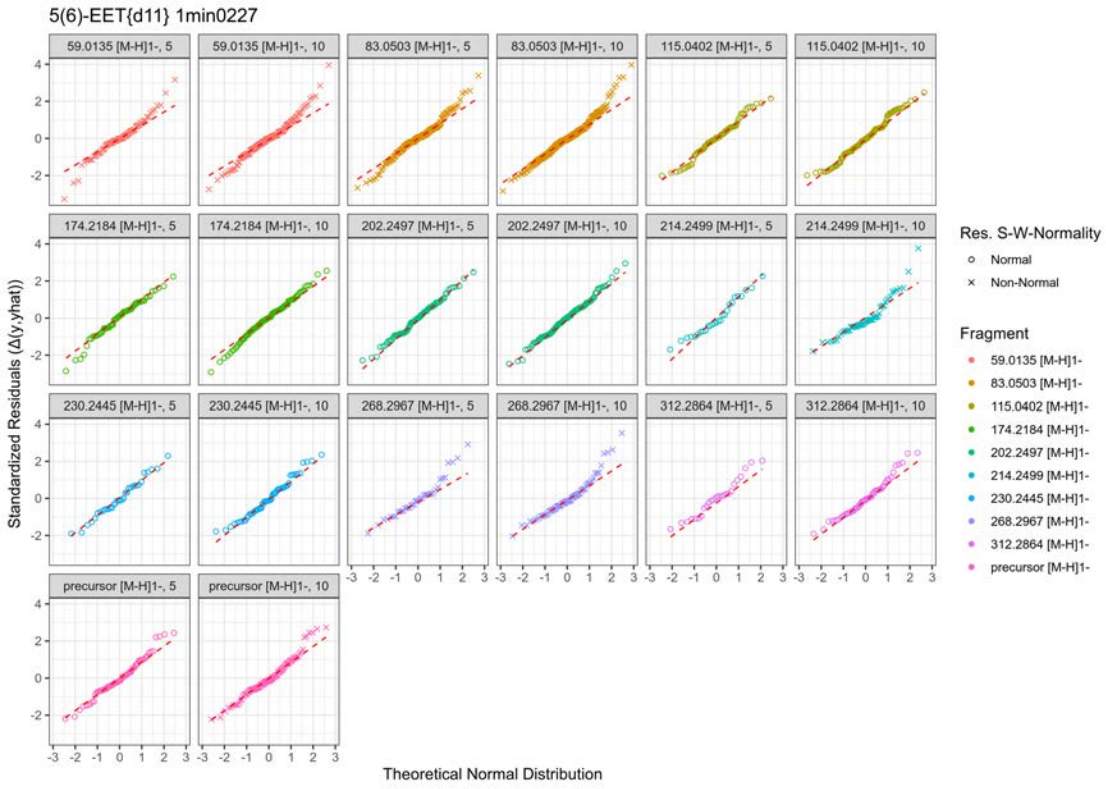


*Figure 103. Quantile-quantile plot of residuals*

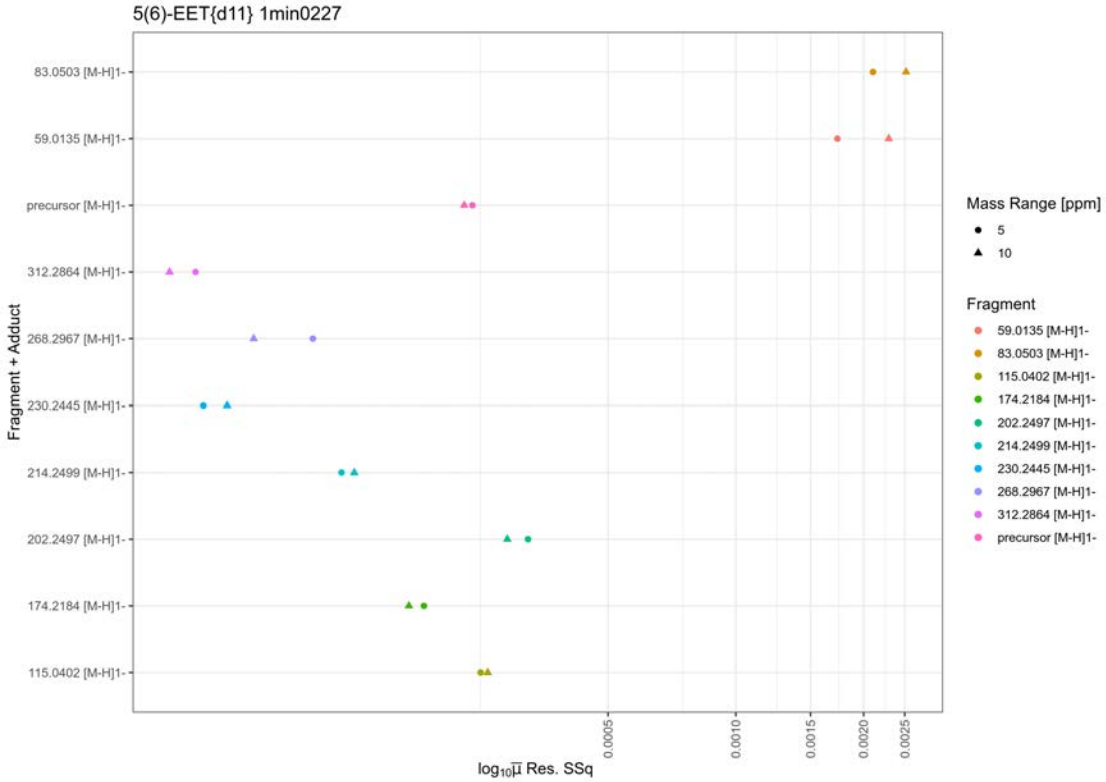


*Figure 104. Normalized sum-of-squares of the residuals*

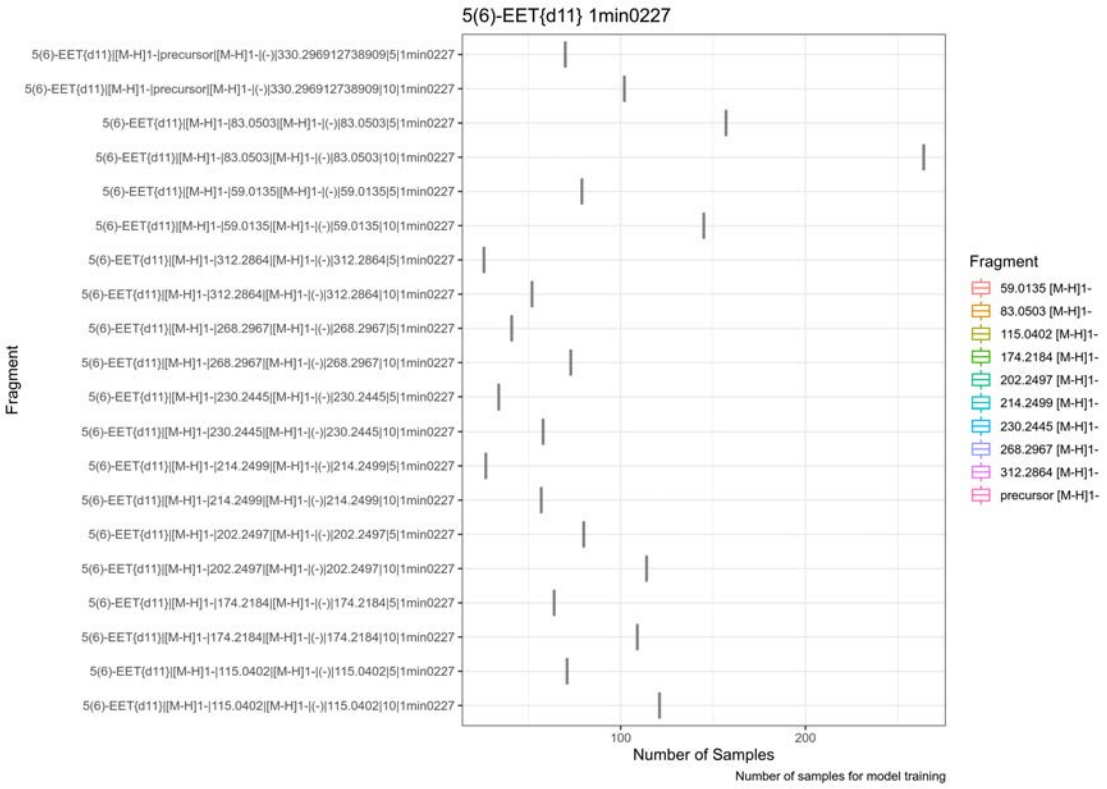


*Figure 105. Number of samples used for training per combination Id*

# 1.22. 5,6-DiHETE [M-H]1- 1min0116

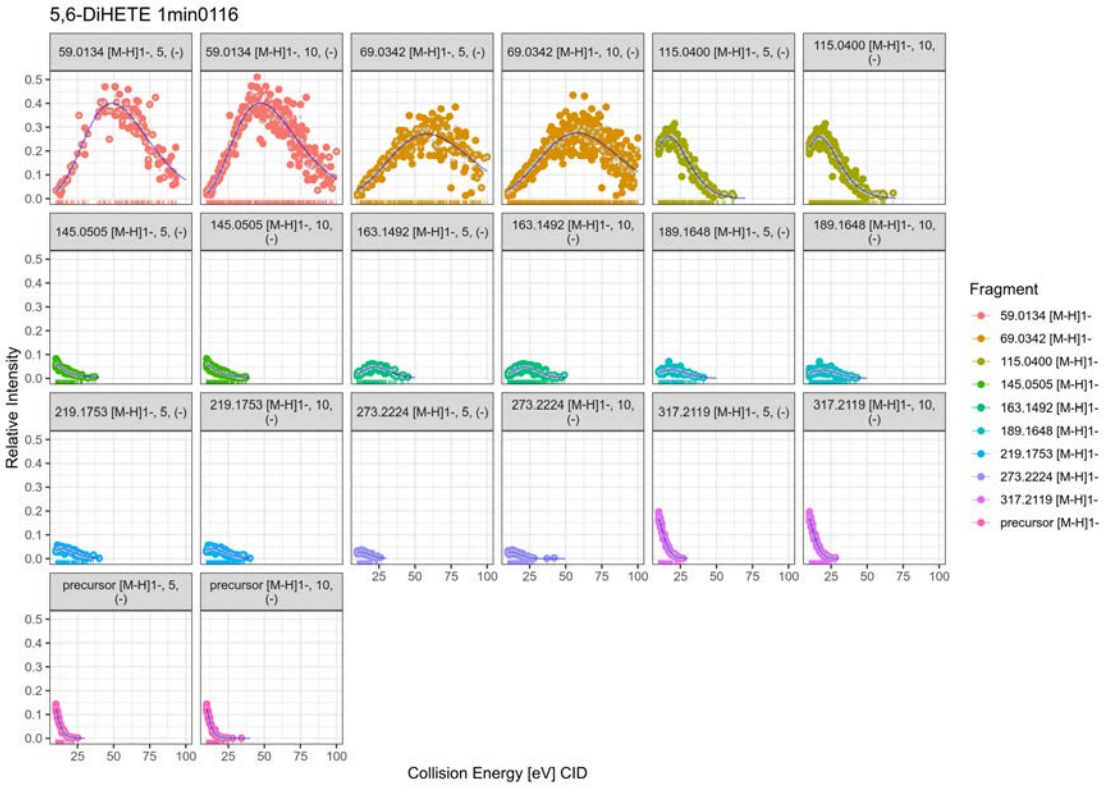


*Figure 106. Nonlinear fit*

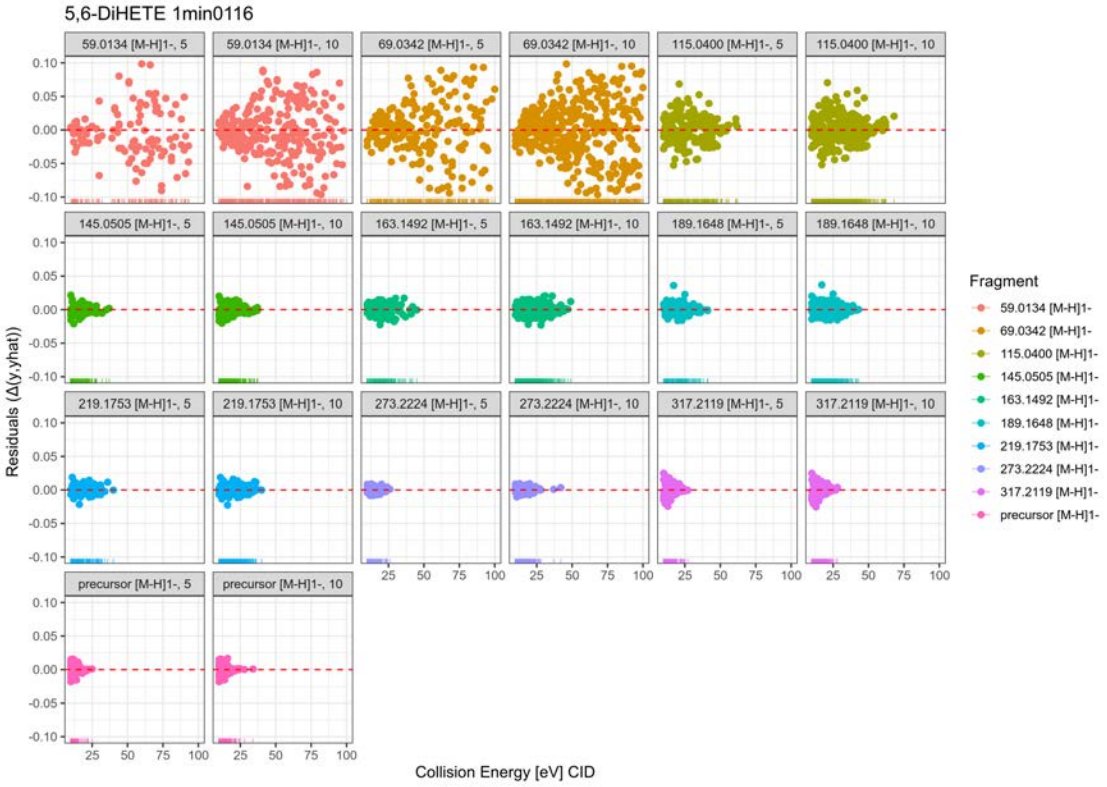


*Figure 107. Residuals of nonlinear fit*

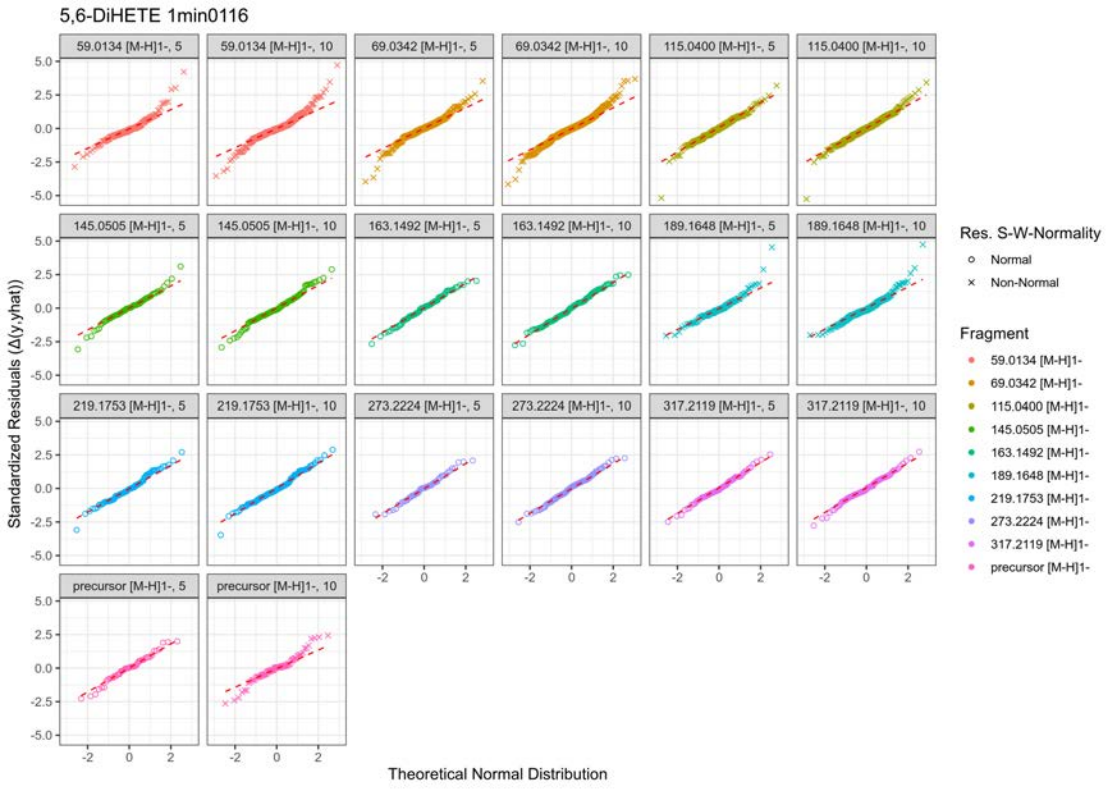


*Figure 108. Quantile-quantile plot of residuals*

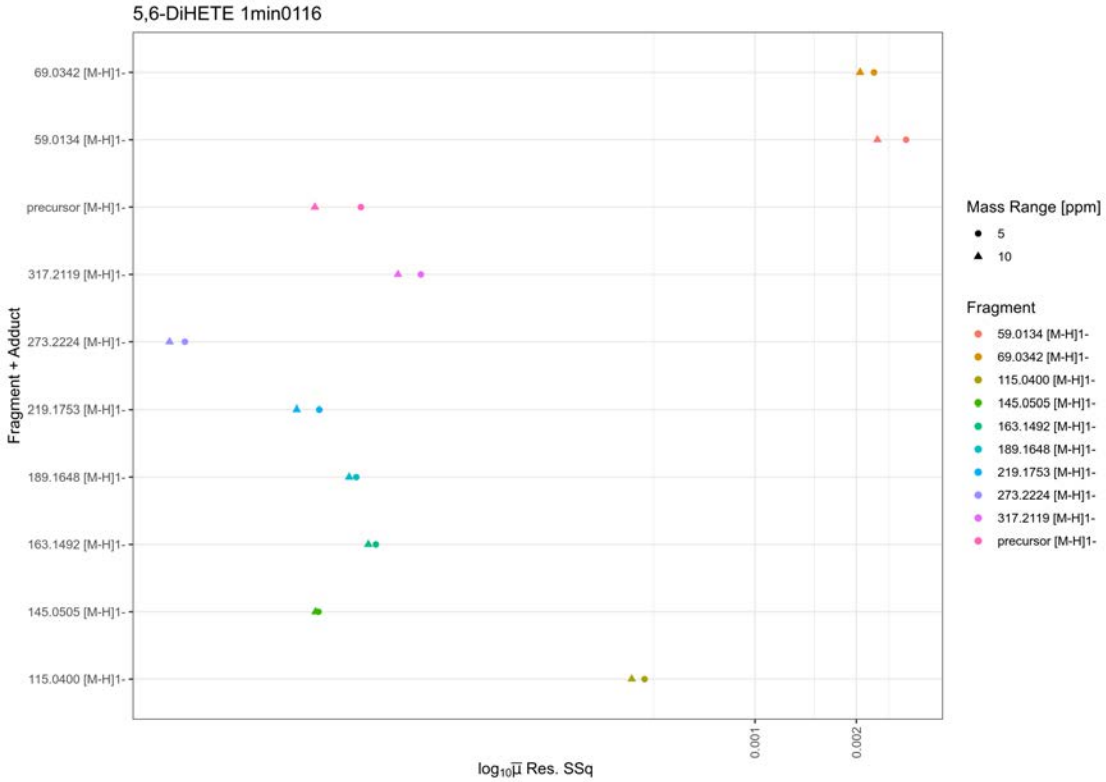


*Figure 109. Normalized sum-of-squares of the residuals*

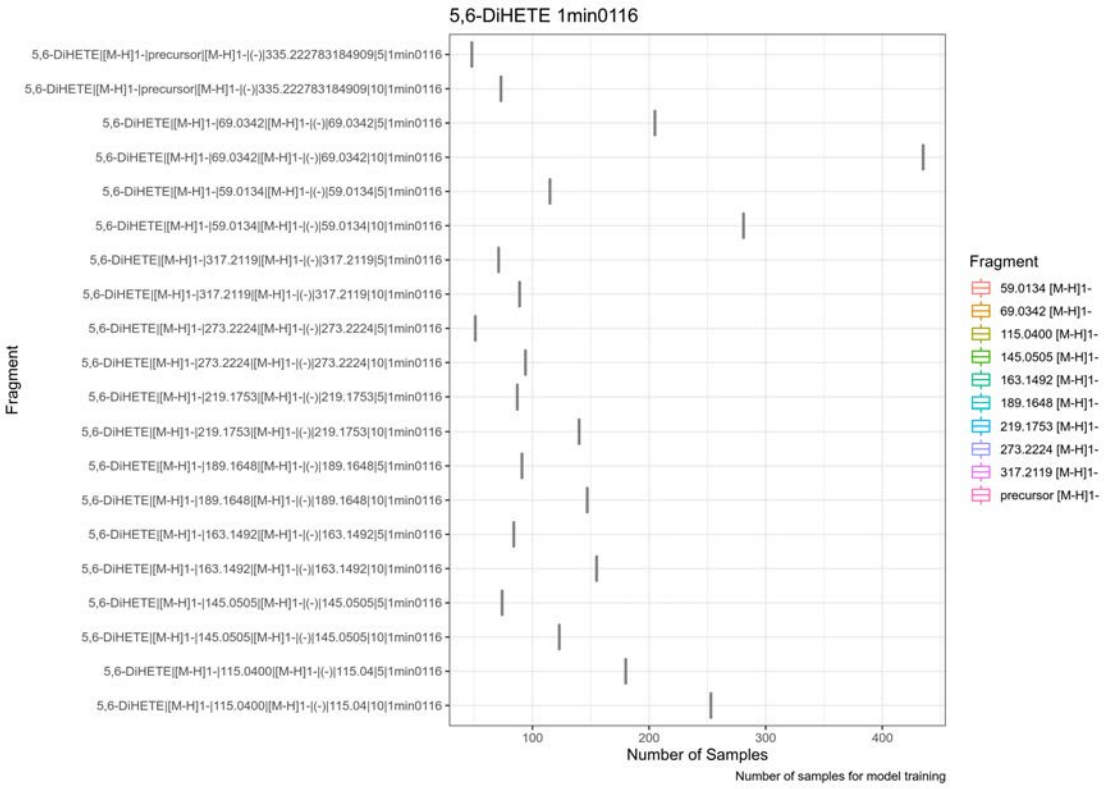


*Figure 110. Number of samples used for training per combination Id*

# 1.23. 5-HEPE [M-H]1- 1min0203

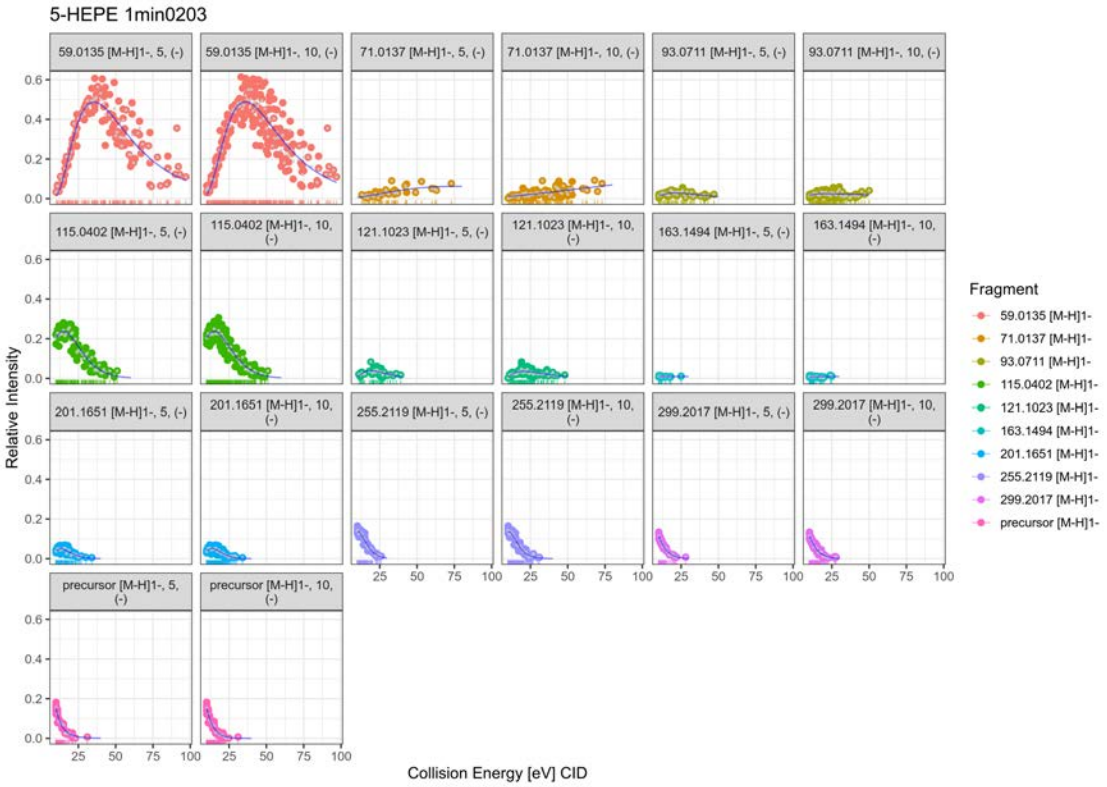


*Figure 111. Nonlinear fit*

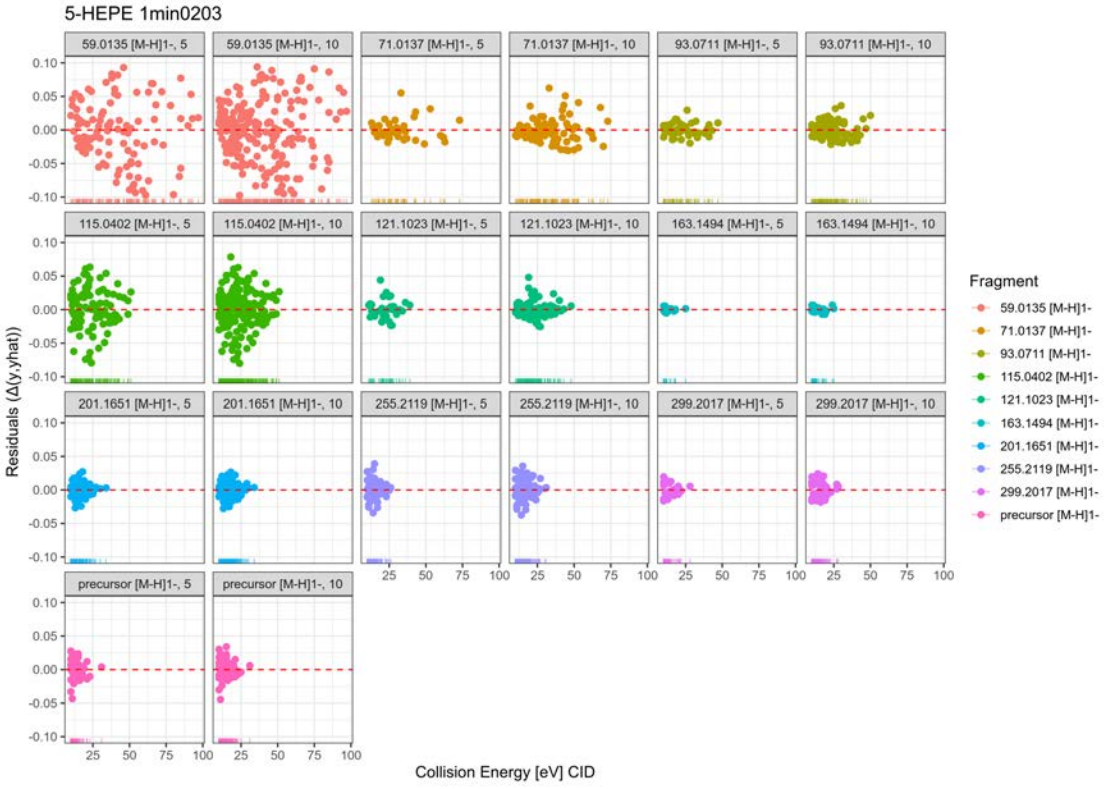


*Figure 112. Residuals of nonlinear fit*

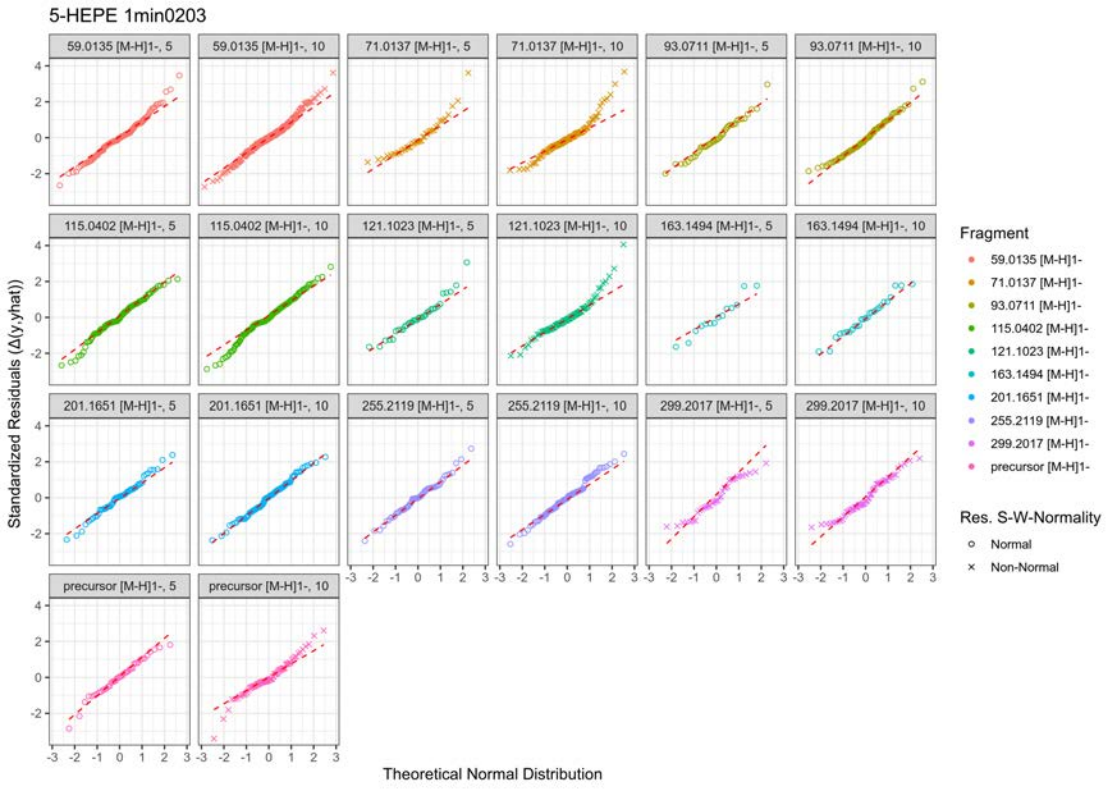


*Figure 113. Quantile-quantile plot of residuals*

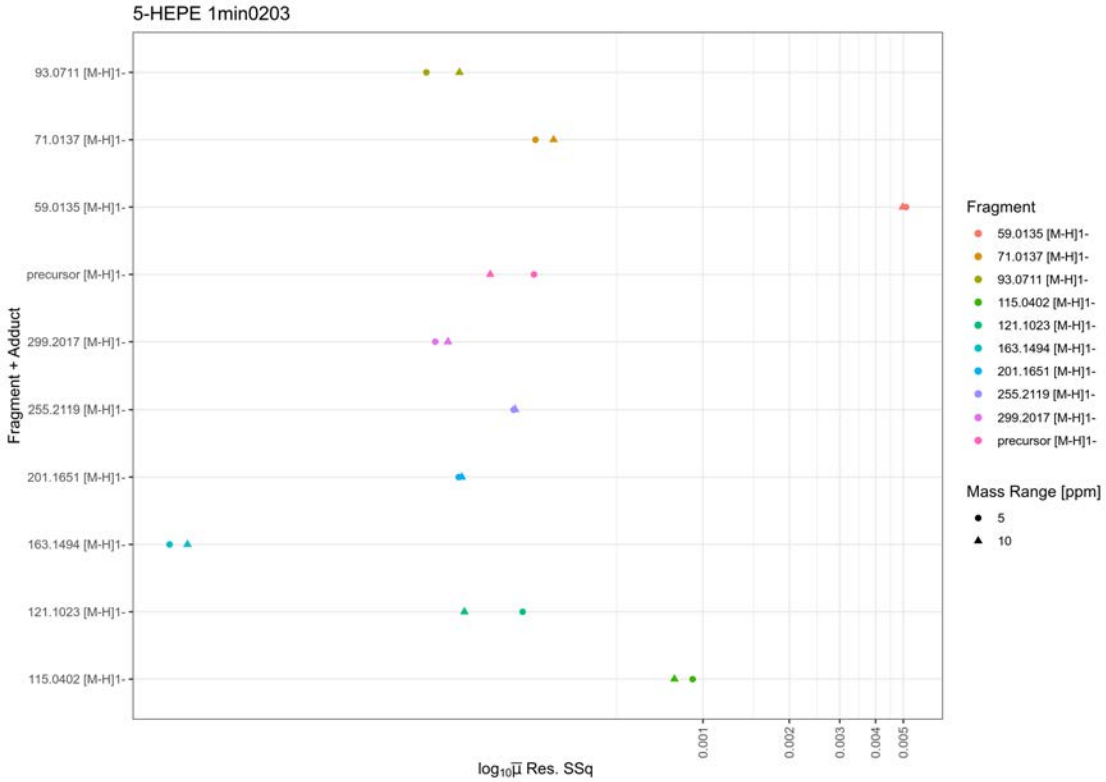


*Figure 114. Normalized sum-of-squares of the residuals*

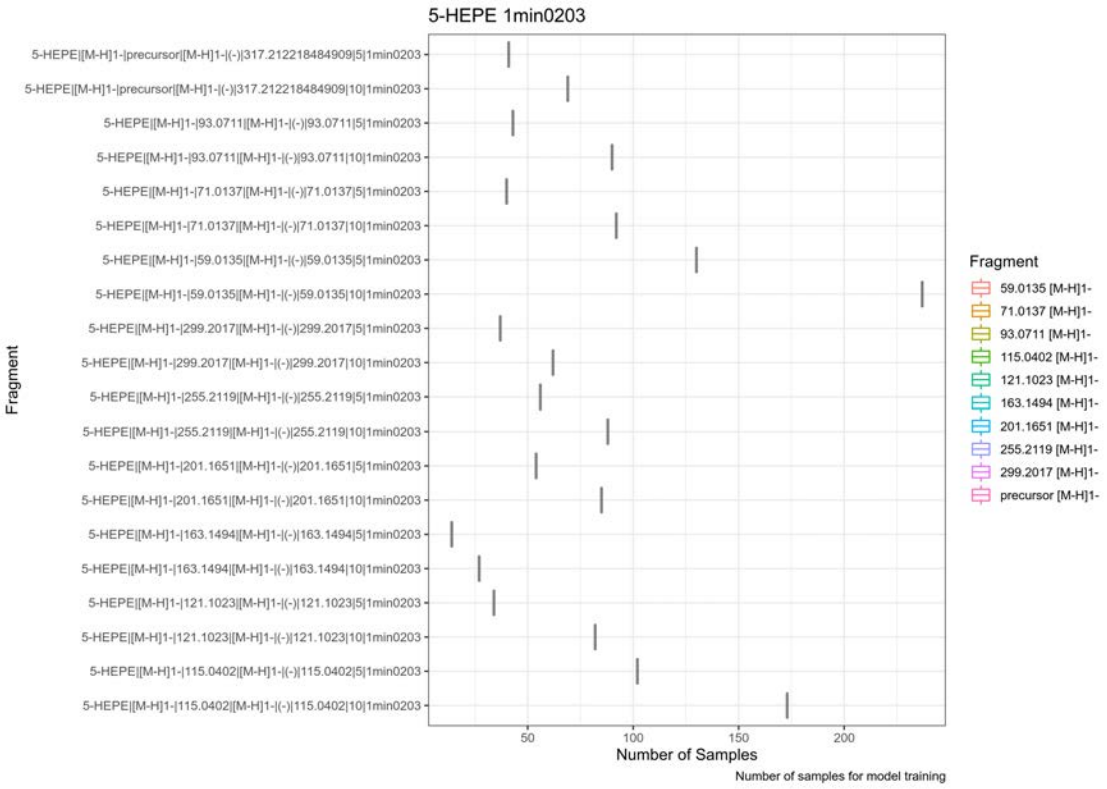


*Figure 115. Number of samples used for training per combination Id*

# 1.24. 5-HETE{d8} [M-H]1- 1min0215

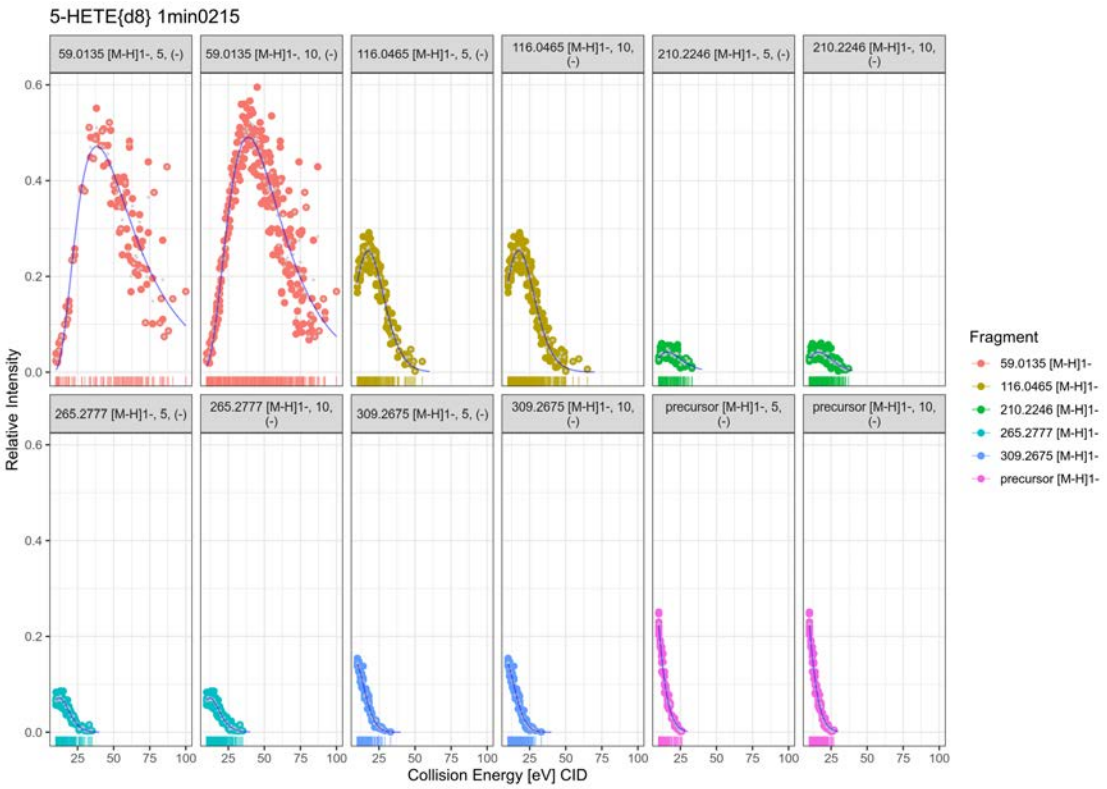


*Figure 116. Nonlinear fit*

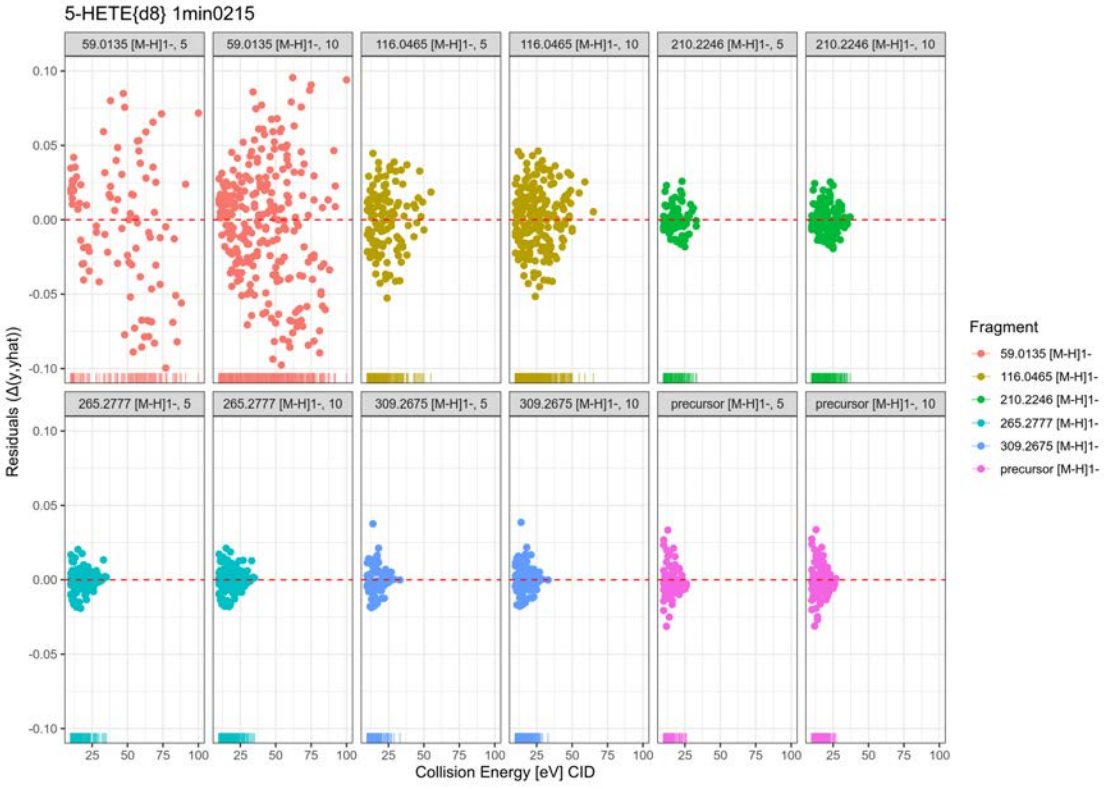


*Figure 117. Residuals of nonlinear fit*

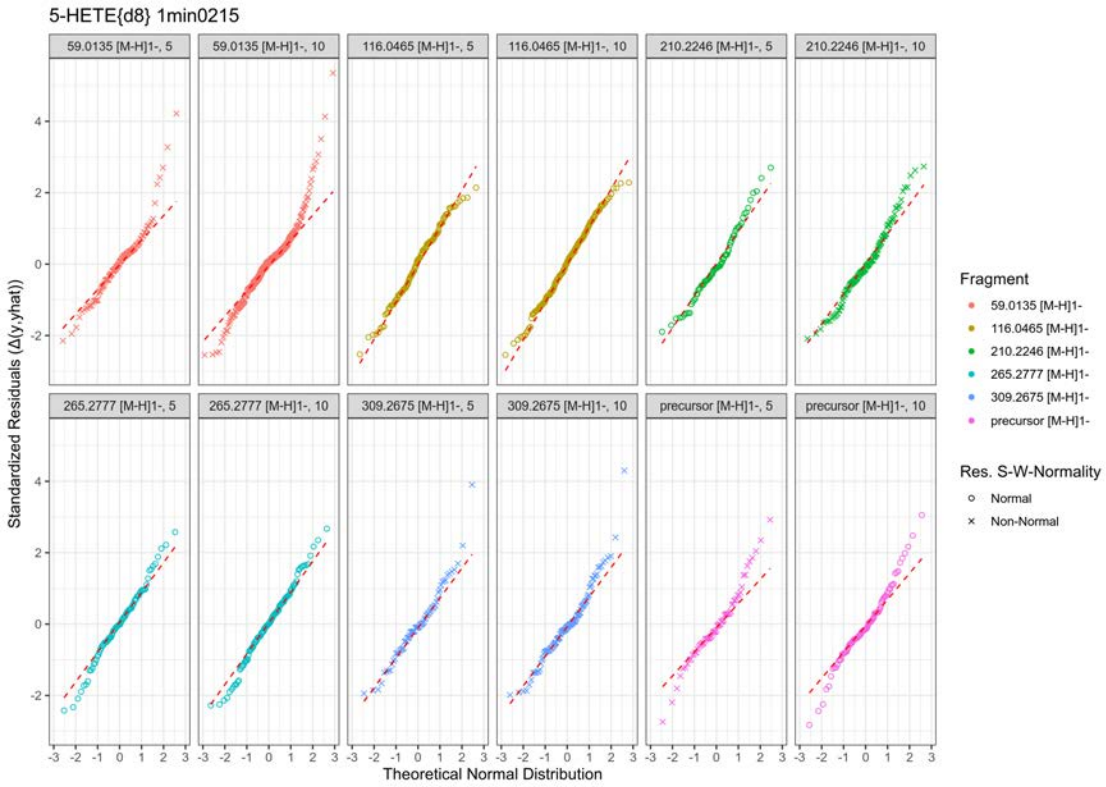


*Figure 118. Quantile-quantile plot of residuals*

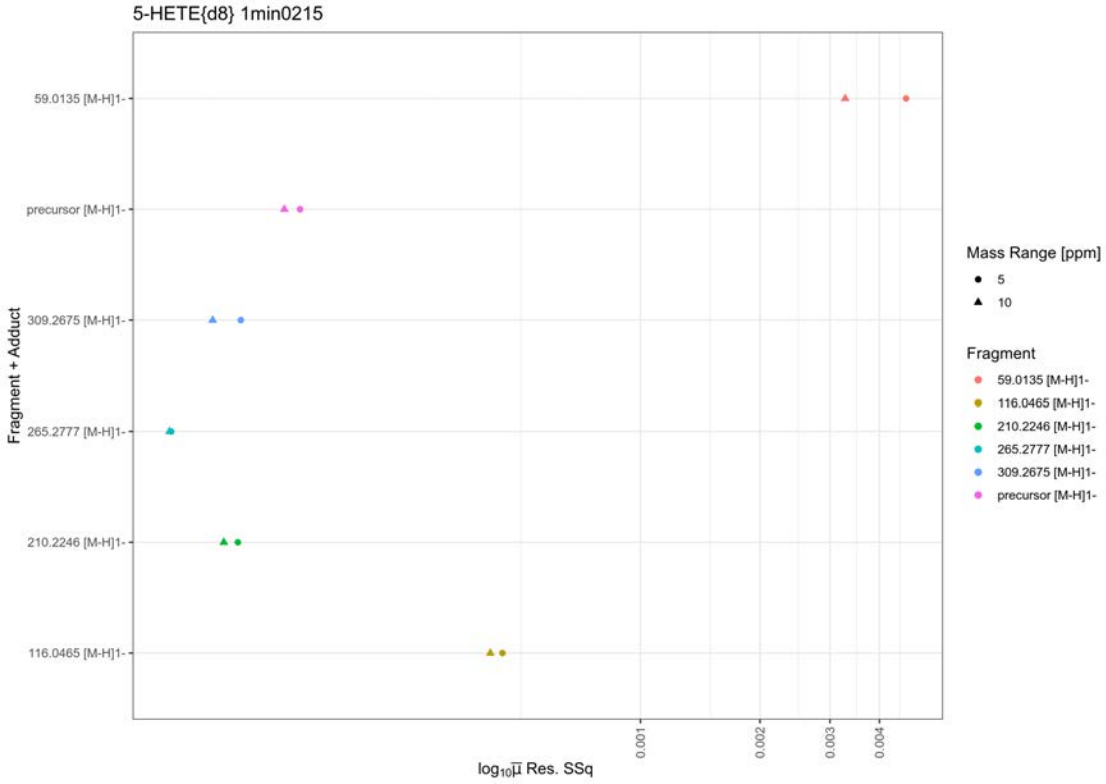


*Figure 119. Normalized sum-of-squares of the residuals*

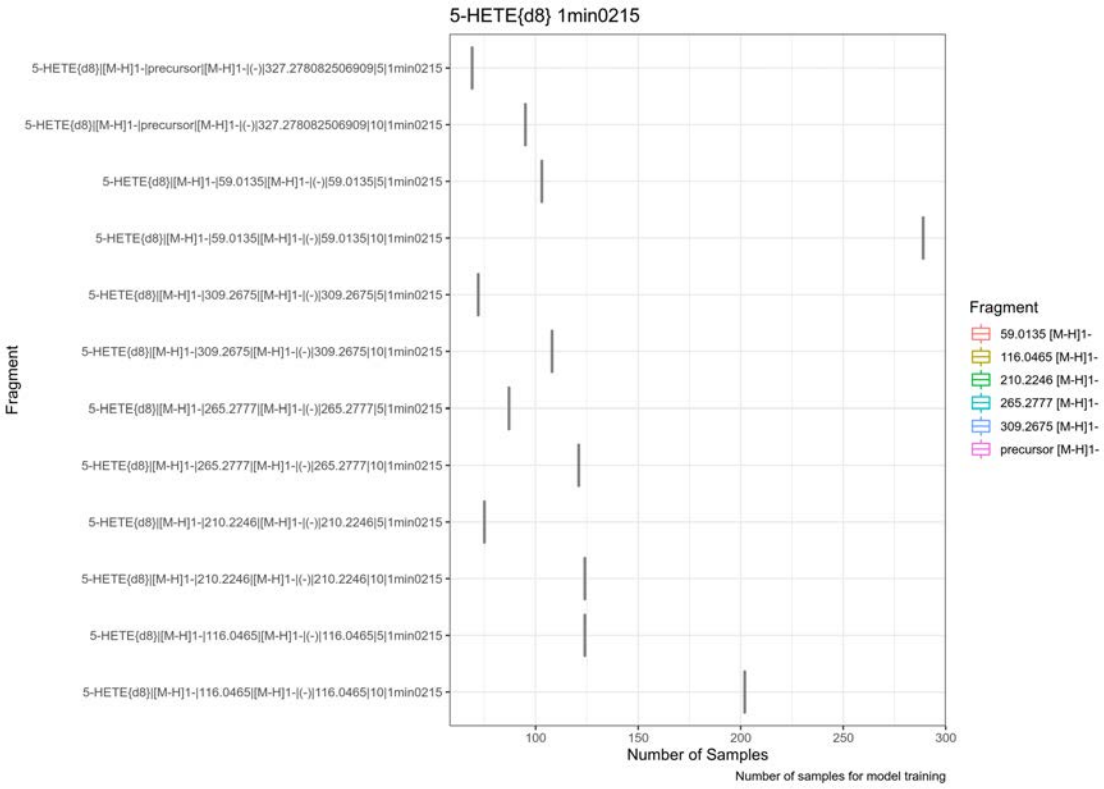


*Figure 120. Number of samples used for training per combination Id*

# 1.25. 5-OxoETE{d7} [M-H]1- 1min0217

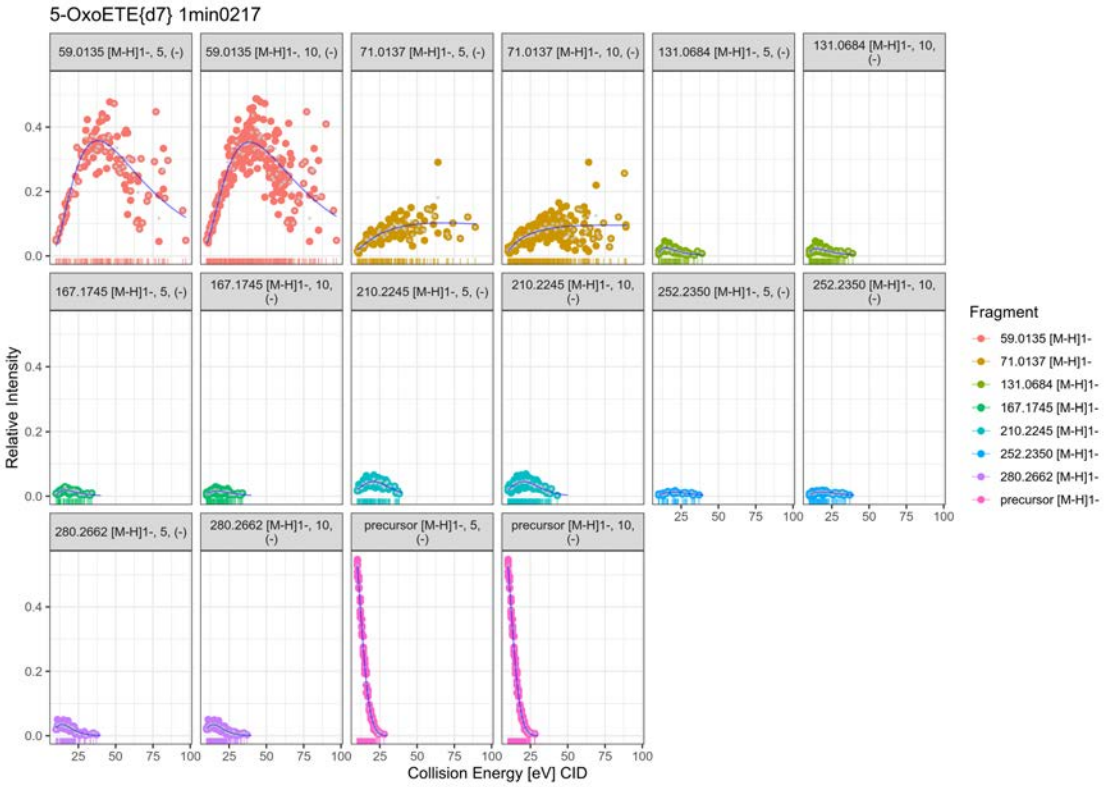


*Figure 121. Nonlinear fit*

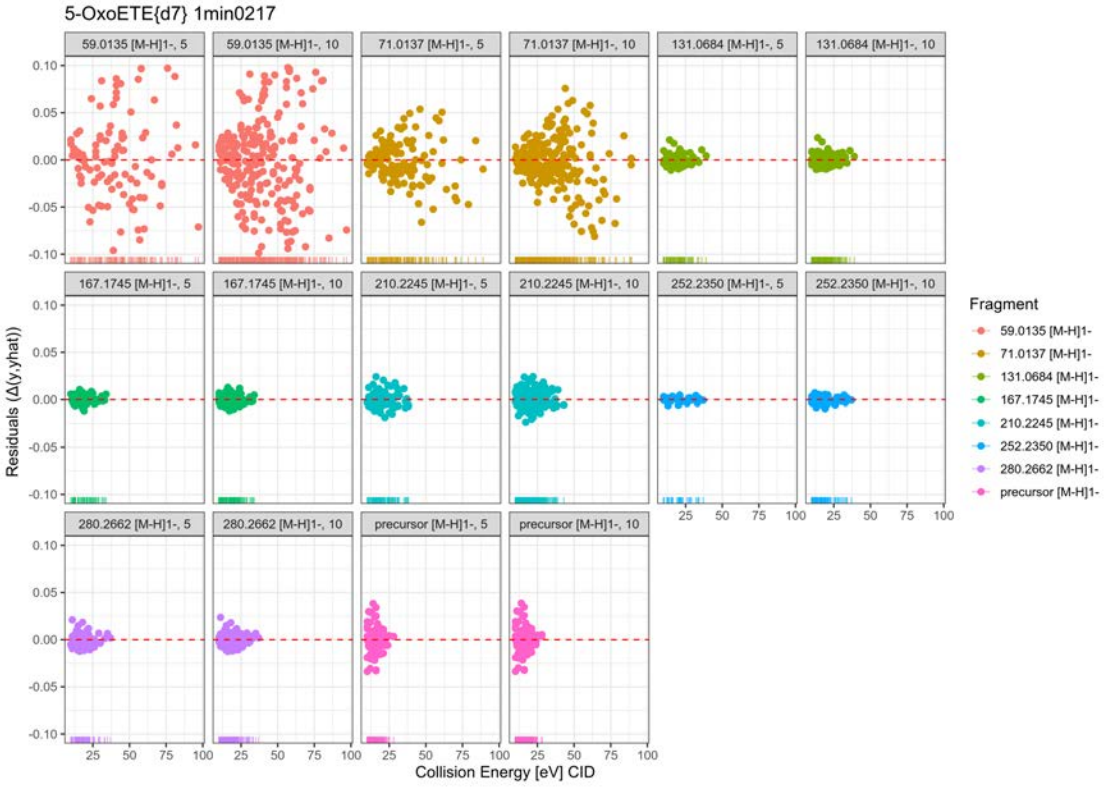


*Figure 122. Residuals of nonlinear fit*

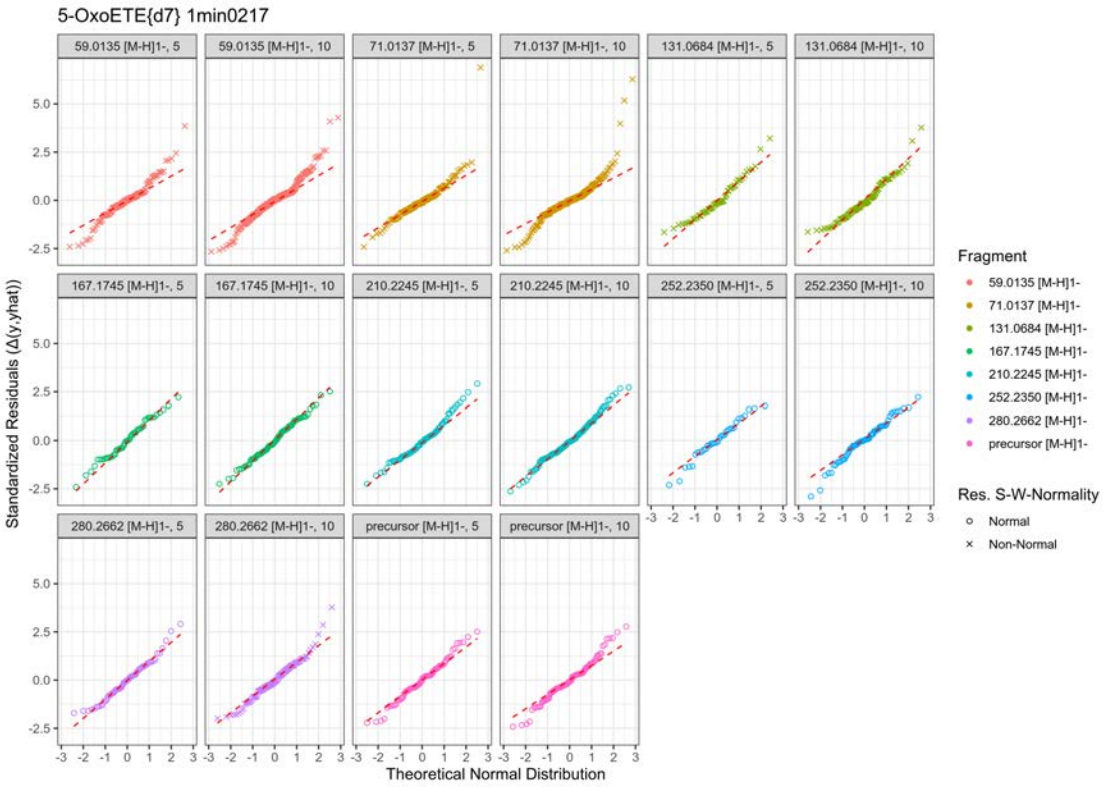


*Figure 123. Quantile-quantile plot of residuals*

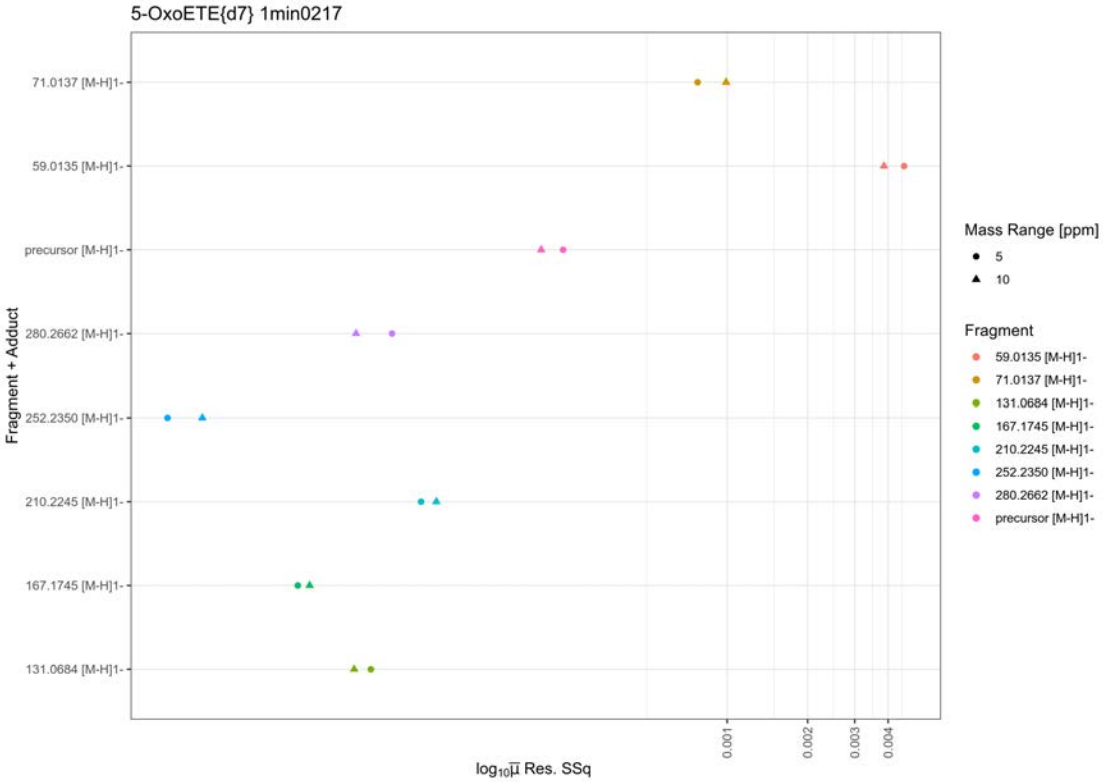


*Figure 124. Normalized sum-of-squares of the residuals*

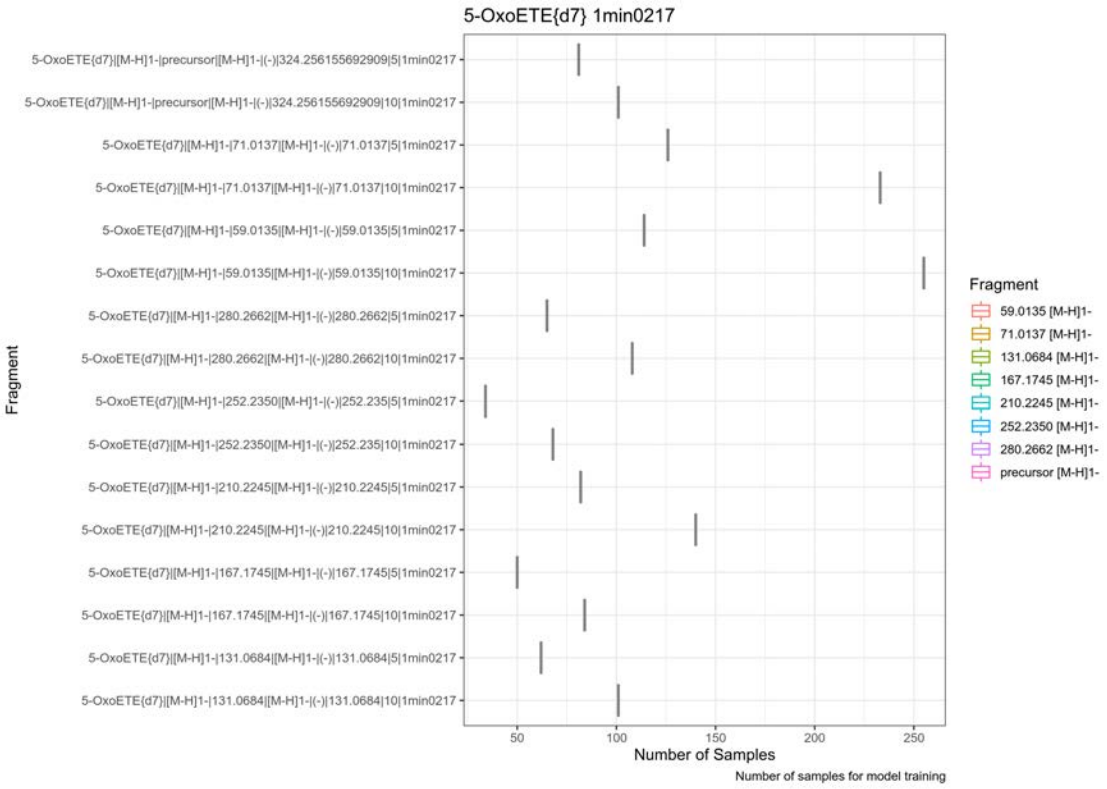


*Figure 125. Number of samples used for training per combination Id*

# 1.26. 8(9)-EET{d11} [M-H]1- 1min0118

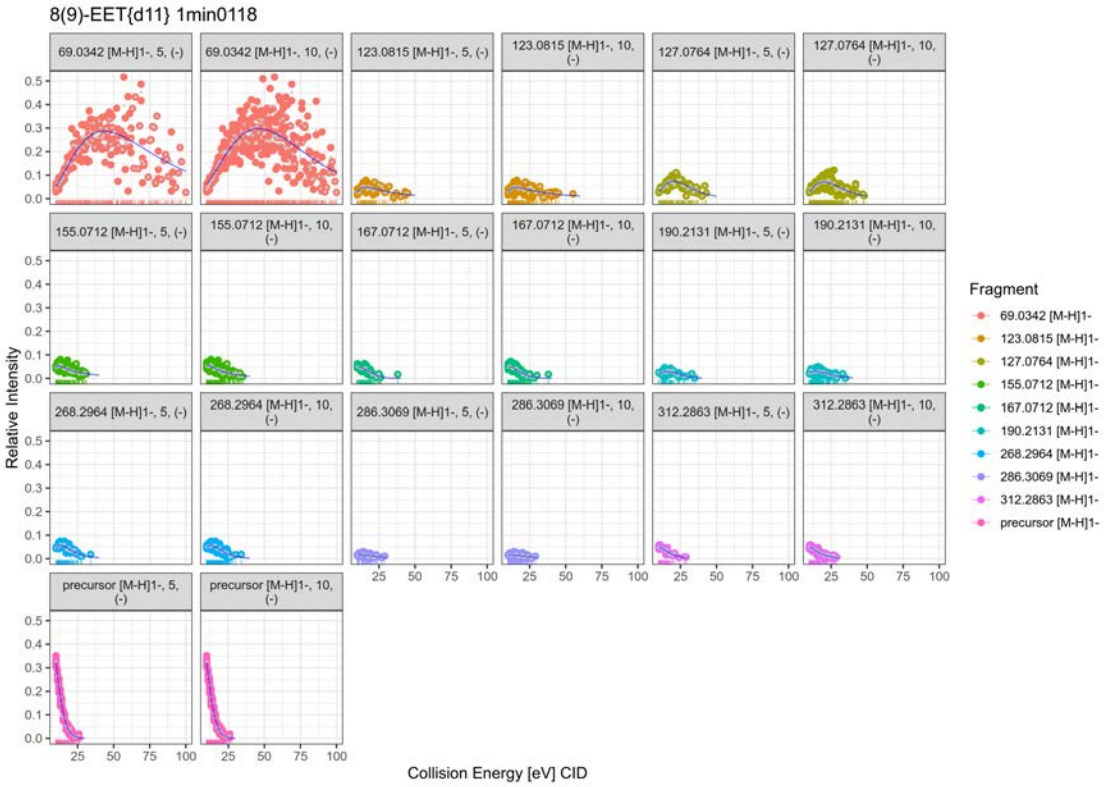


*Figure 126. Nonlinear fit*

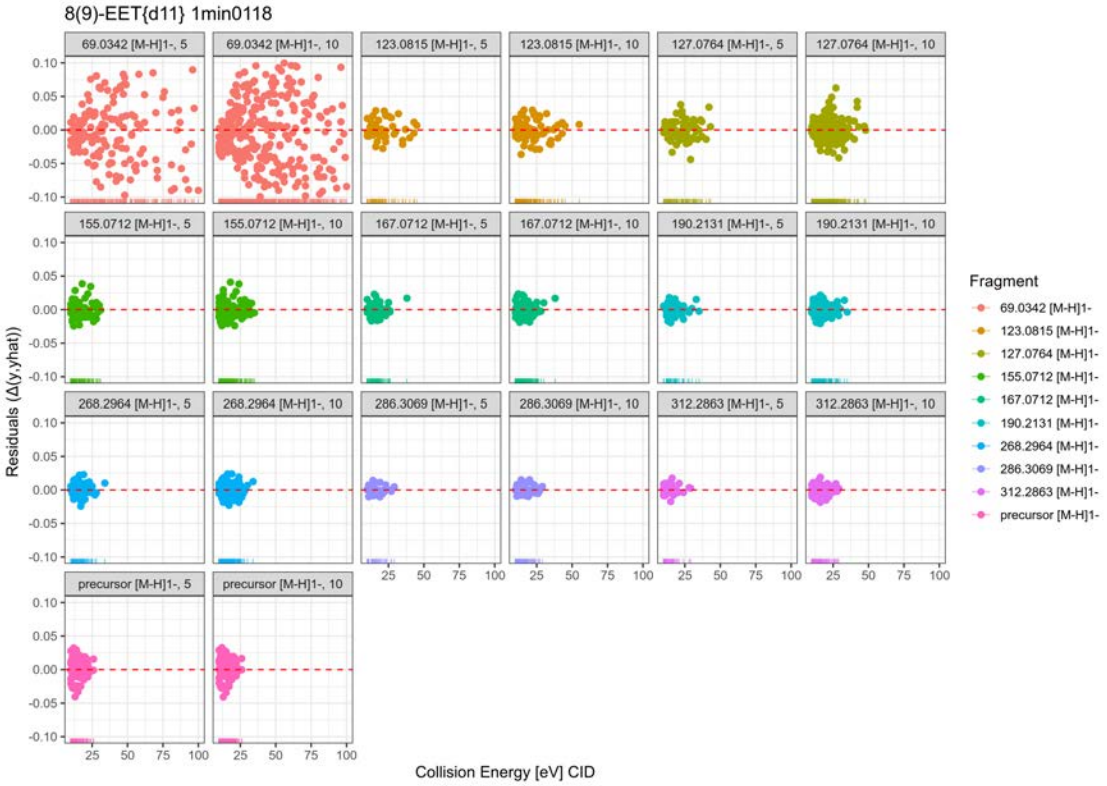


*Figure 127. Residuals of nonlinear fit*

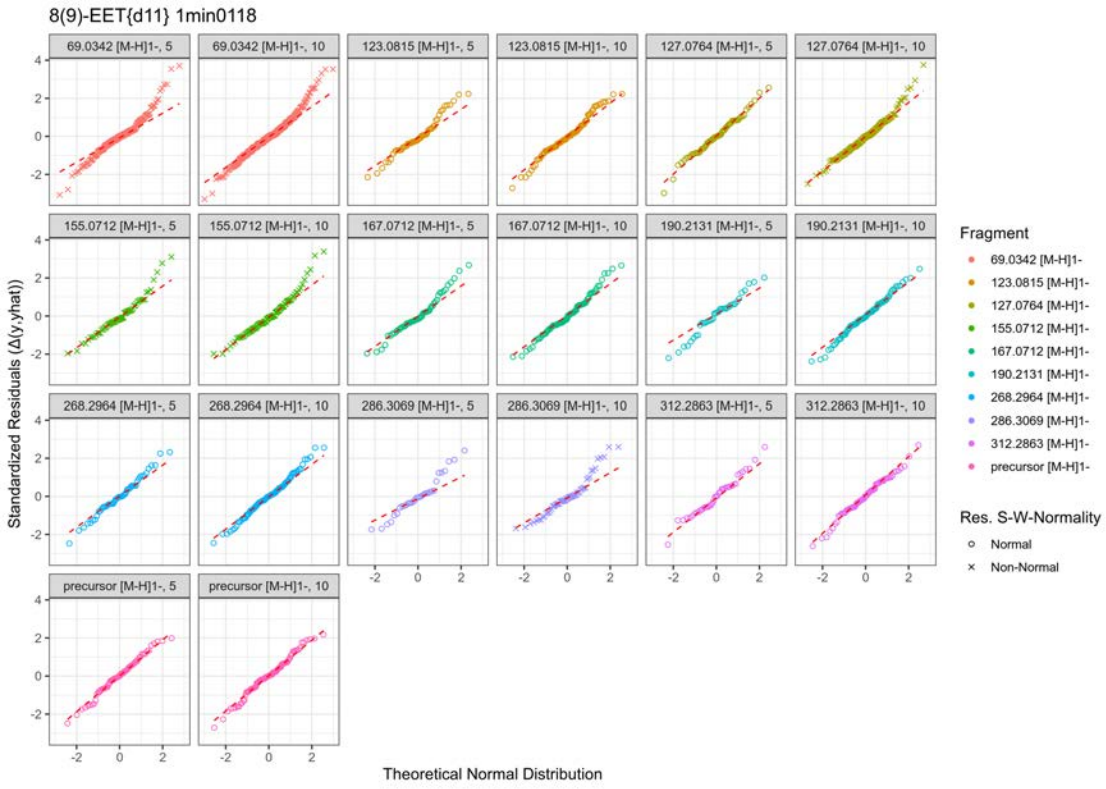


*Figure 128. Quantile-quantile plot of residuals*

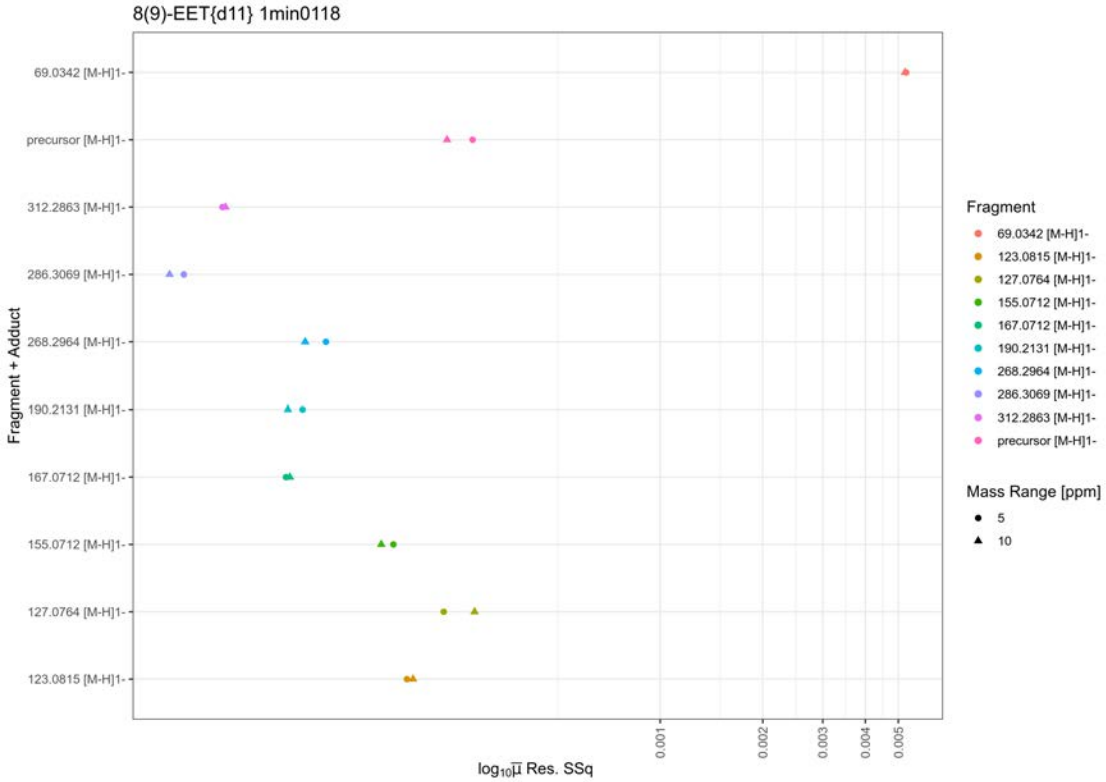


*Figure 129. Normalized sum-of-squares of the residuals*

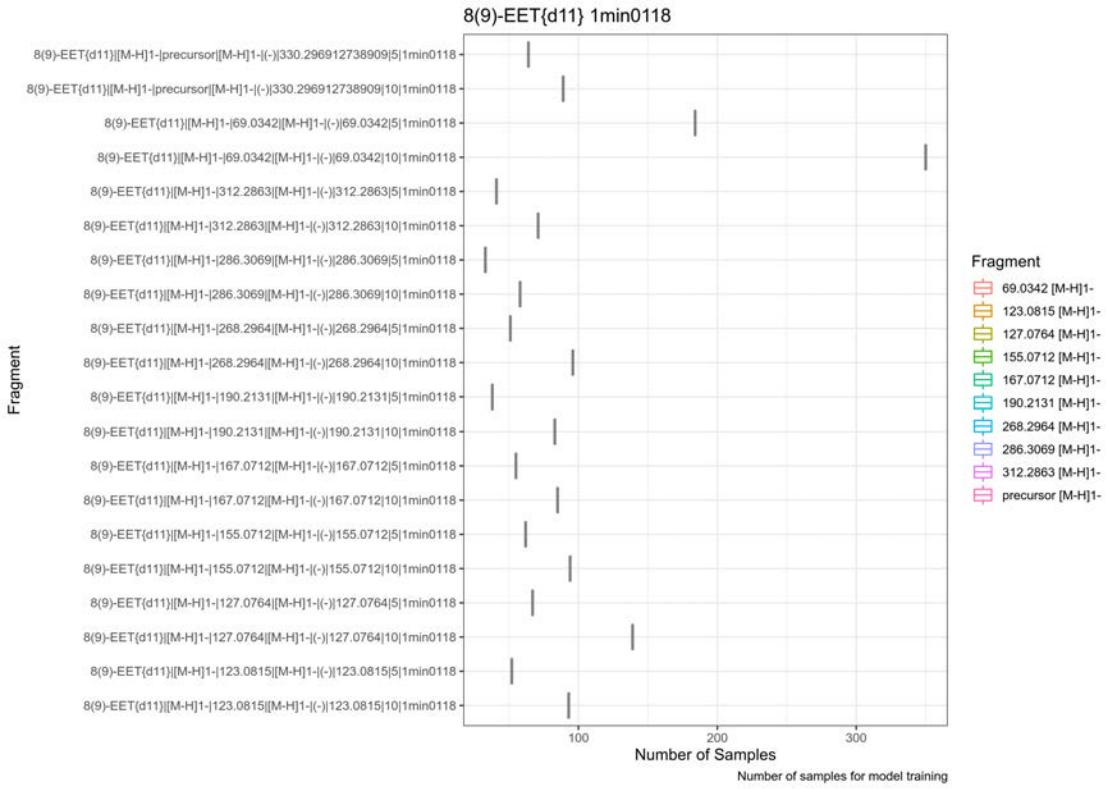


*Figure 130. Number of samples used for training per combination Id*

# 1.27. 8,9-DHET{d11} [M-H]1- 1min0235

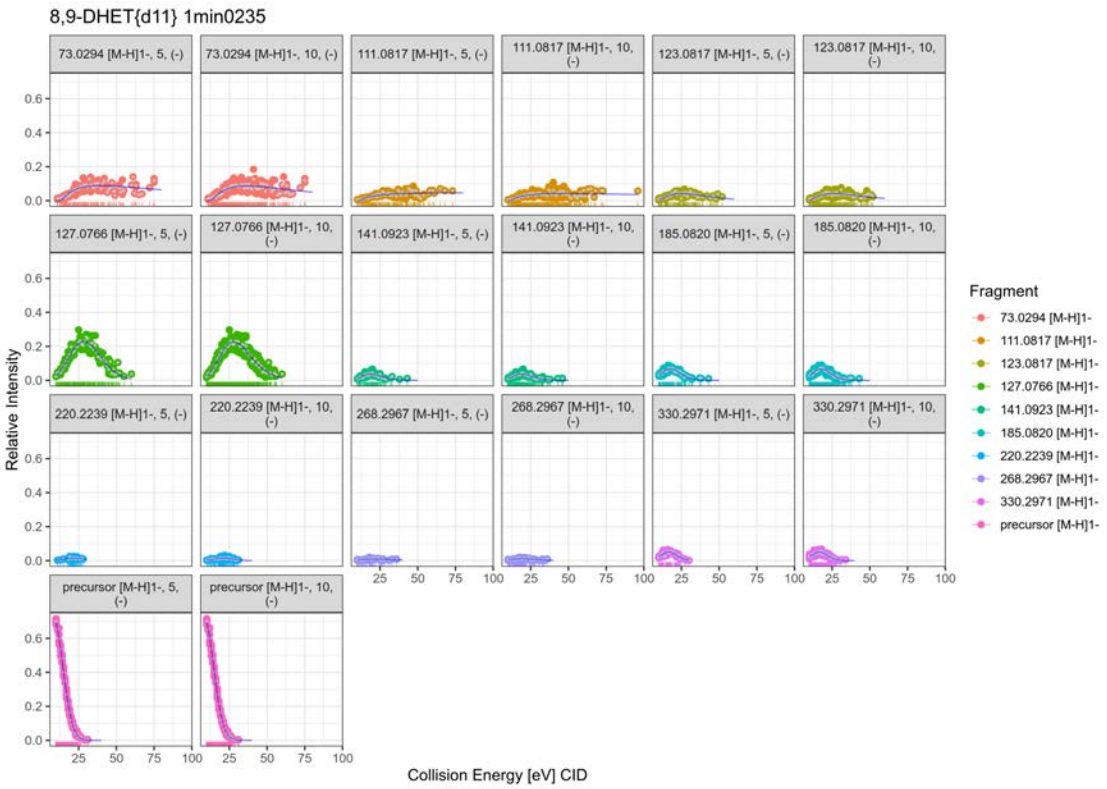


*Figure 131. Nonlinear fit*

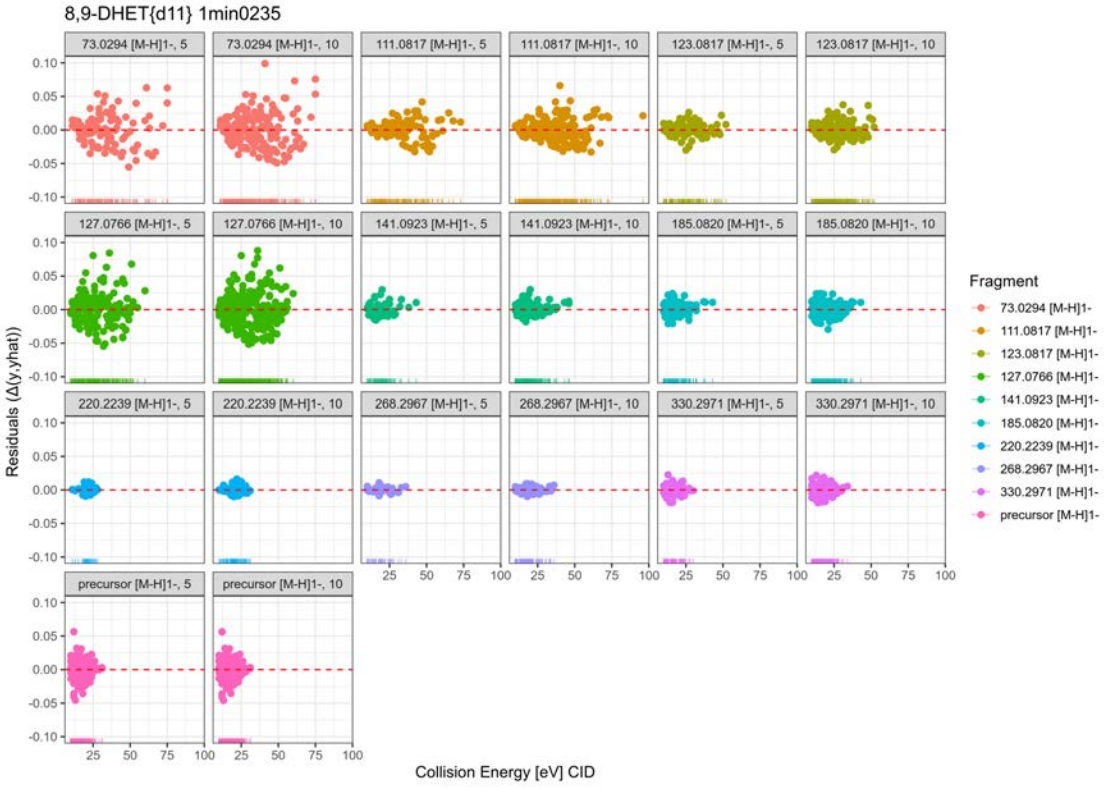


*Figure 132. Residuals of nonlinear fit*

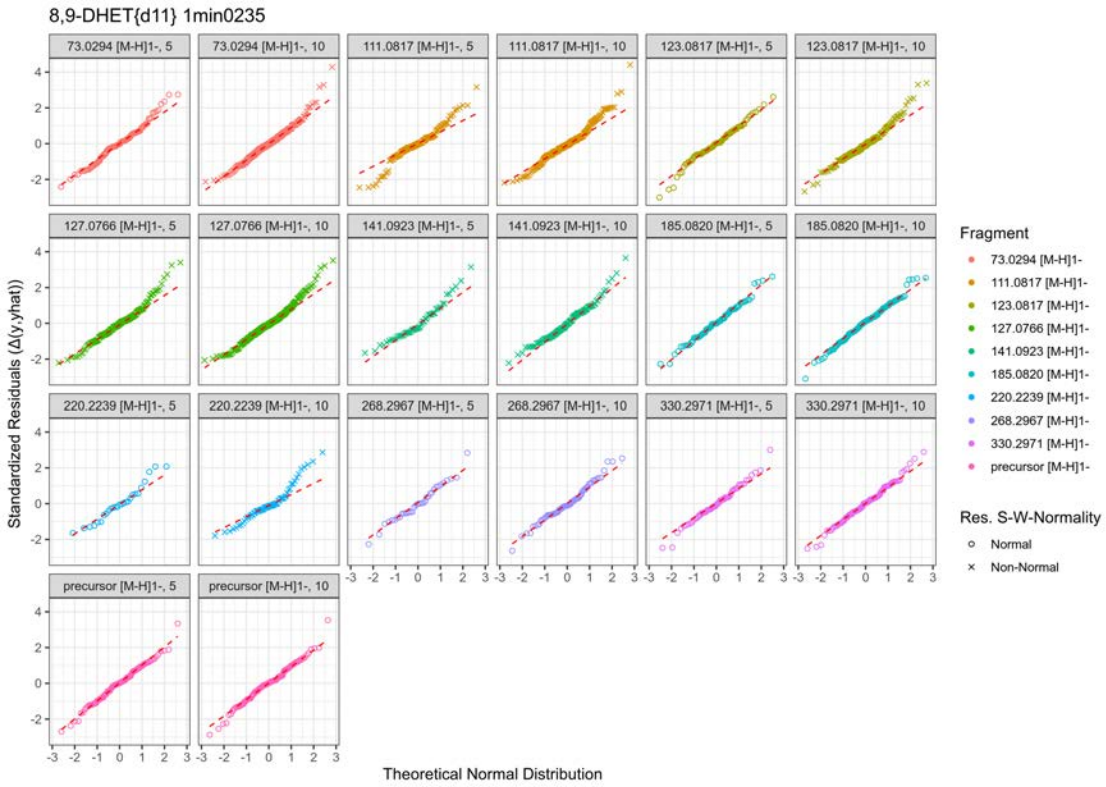


*Figure 133. Quantile-quantile plot of residuals*

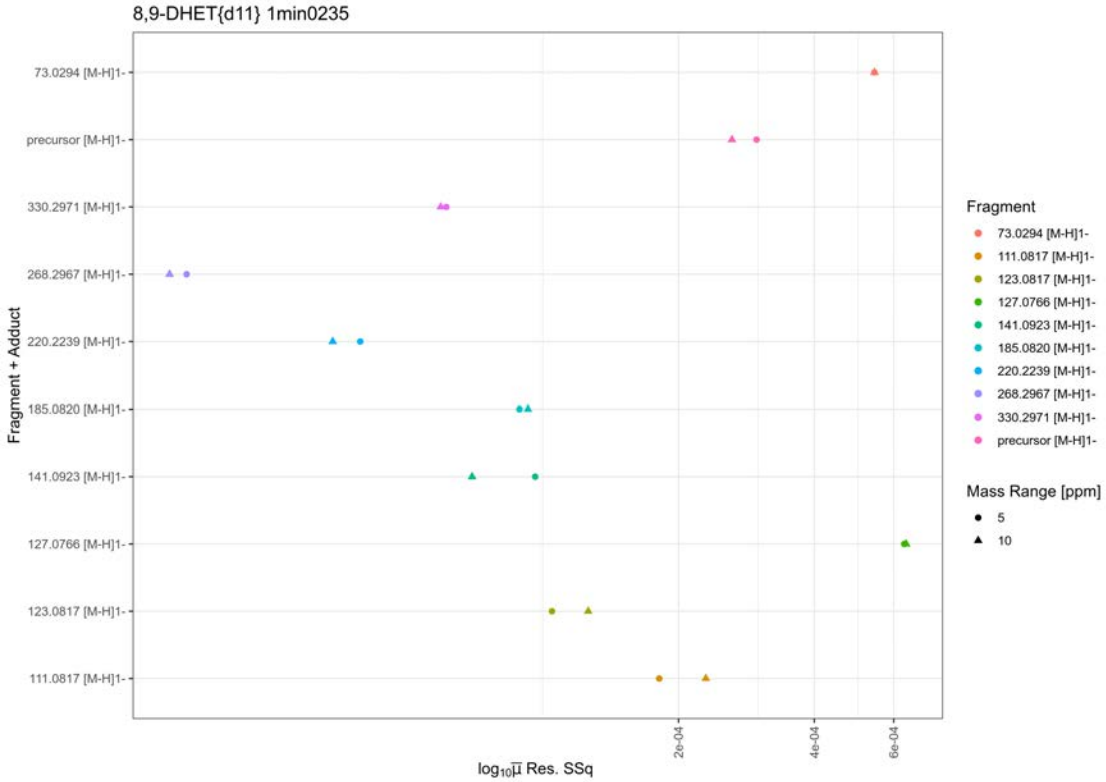


*Figure 134. Normalized sum-of-squares of the residuals*

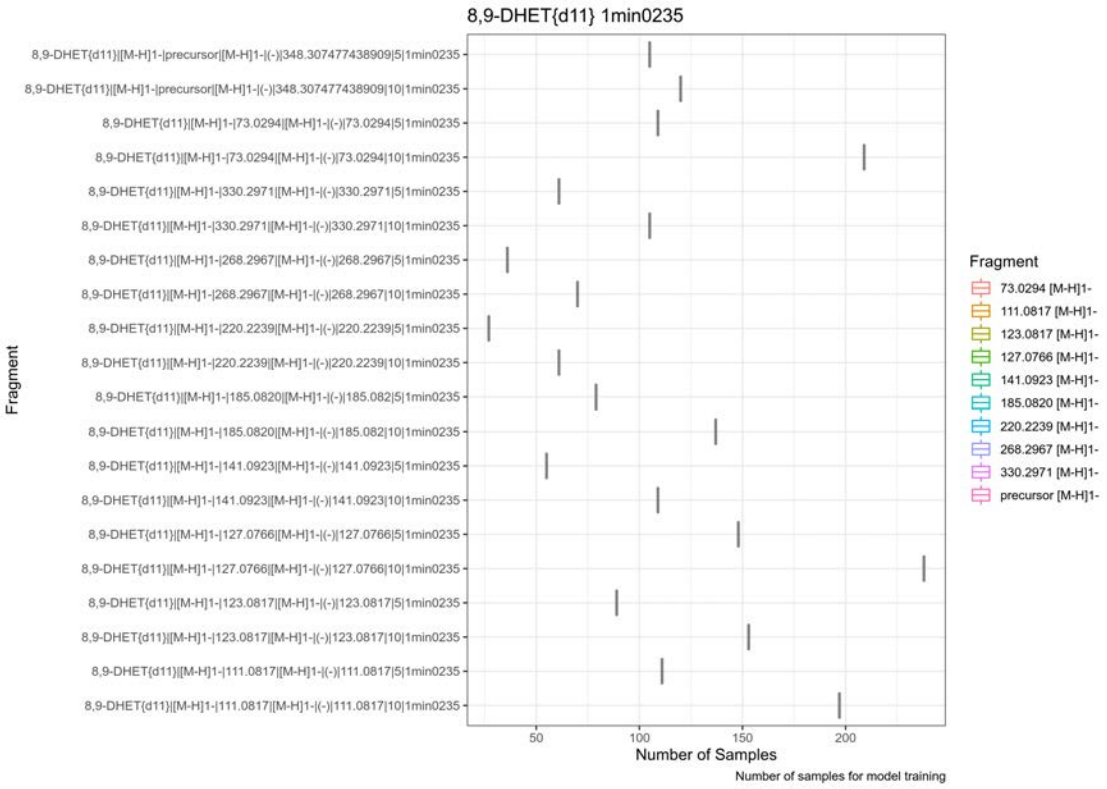


*Figure 135. Number of samples used for training per combination Id*

# 1.28. 8-HDoHE [M-H]1- 1min0120

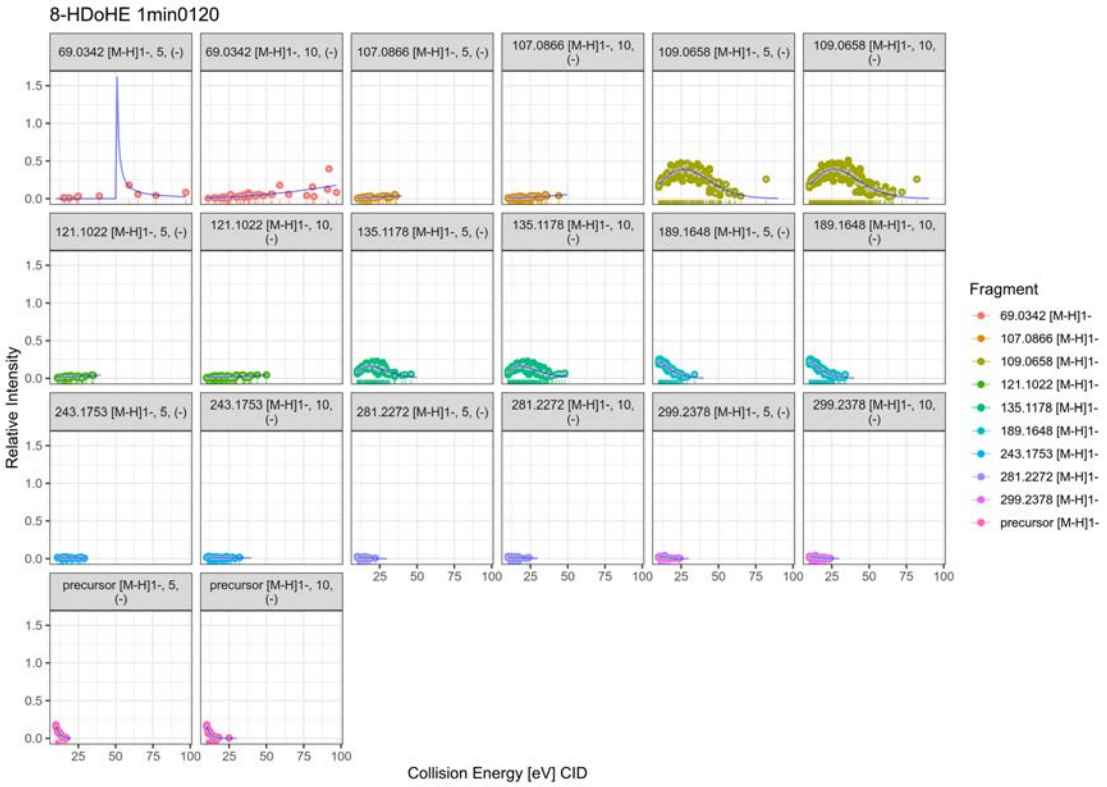


*Figure 136. Nonlinear fit*

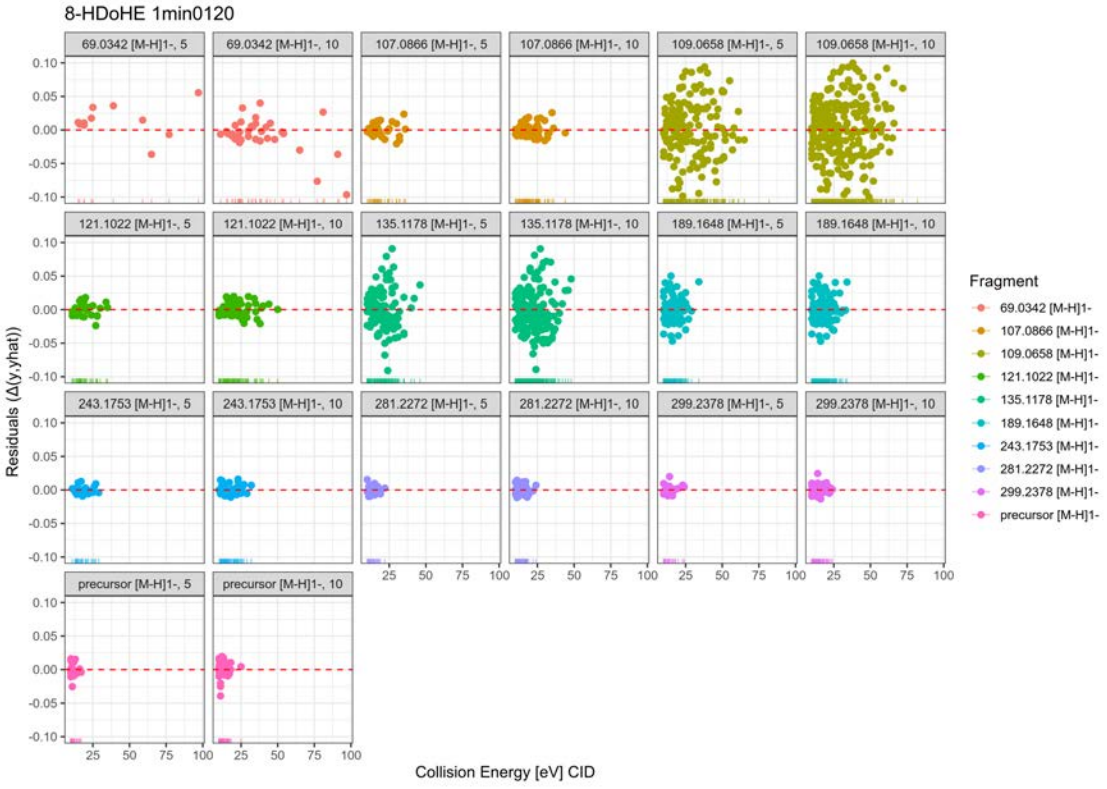


*Figure 137. Residuals of nonlinear fit*

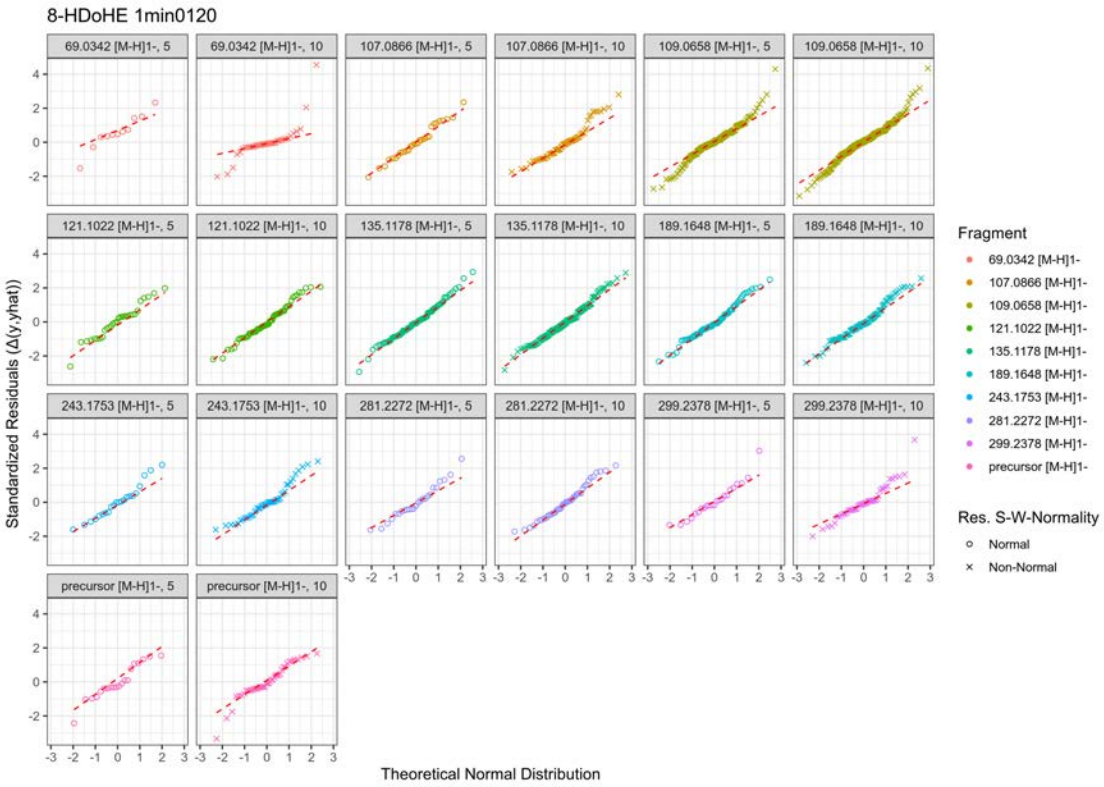


*Figure 138. Quantile-quantile plot of residuals*

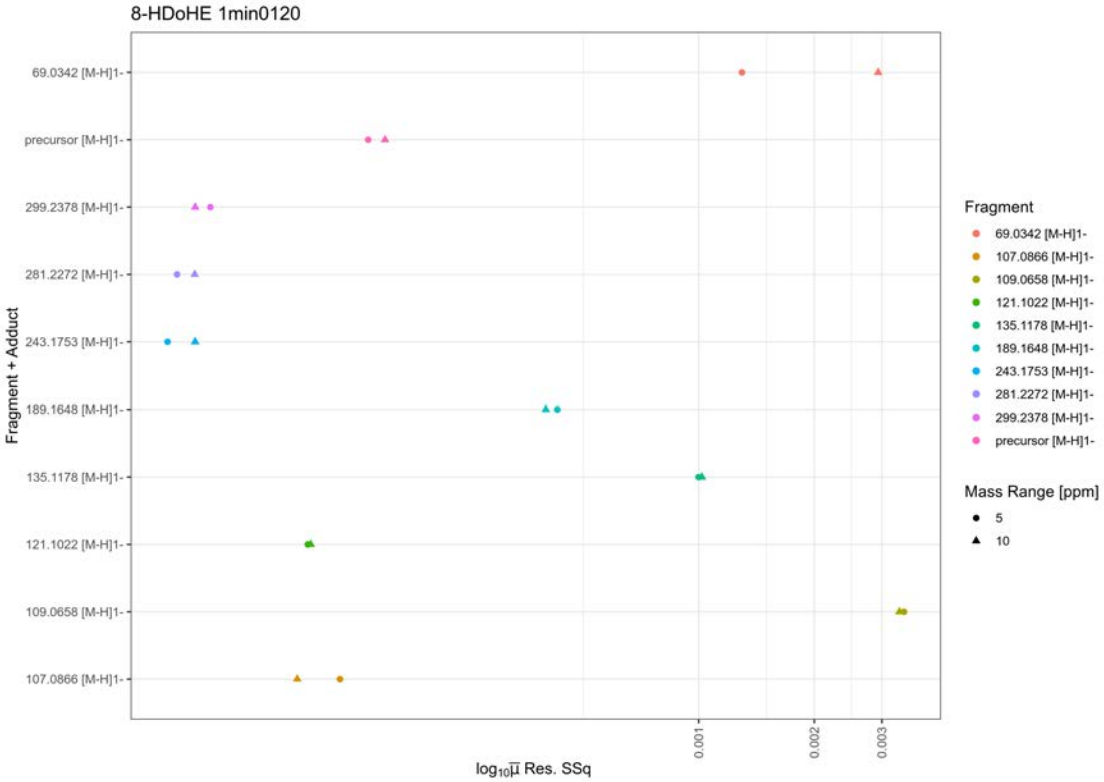


*Figure 139. Normalized sum-of-squares of the residuals*

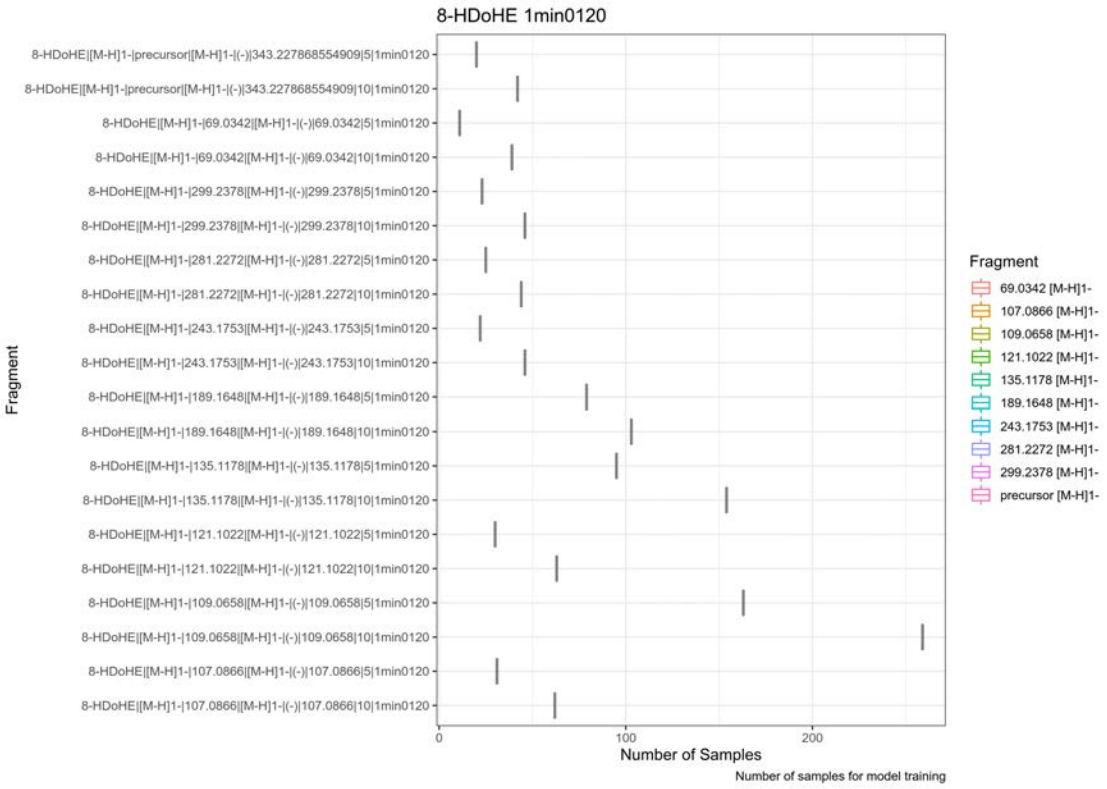


*Figure 140. Number of samples used for training per combination Id*

# 1.29. 8-HETE [M-H]1- 1min0122

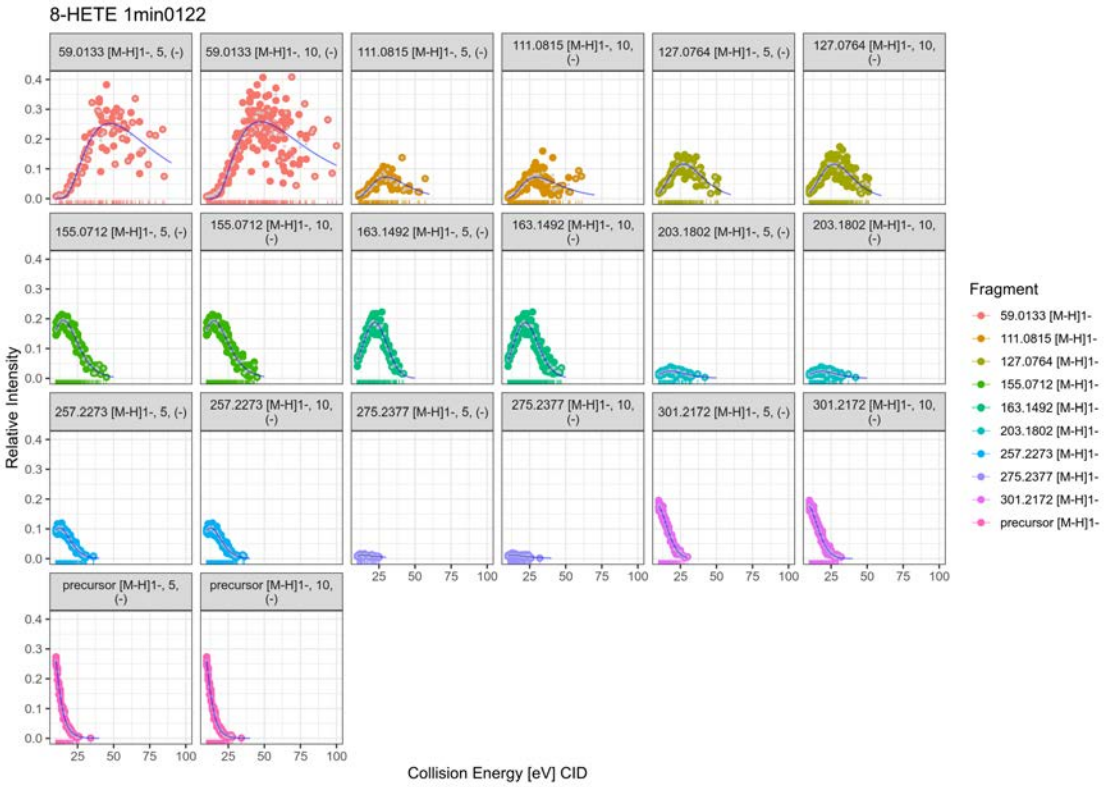


*Figure 141. Nonlinear fit*

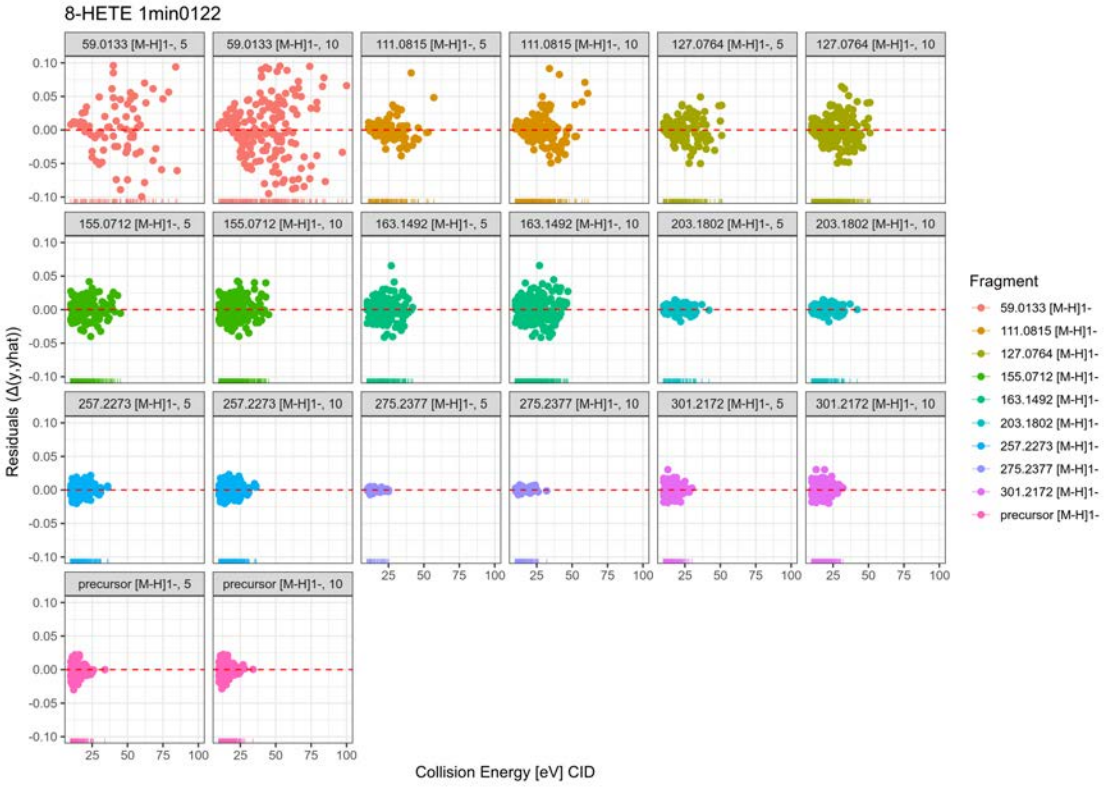


*Figure 142. Residuals of nonlinear fit*

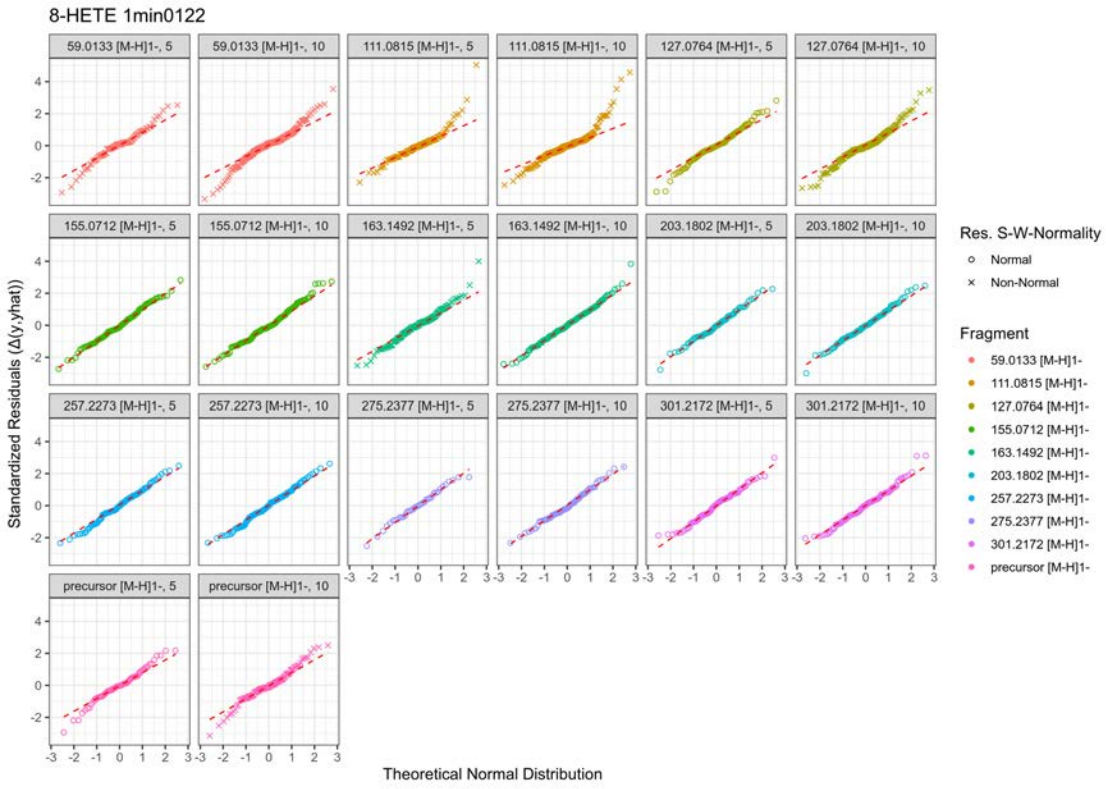


*Figure 143. Quantile-quantile plot of residuals*

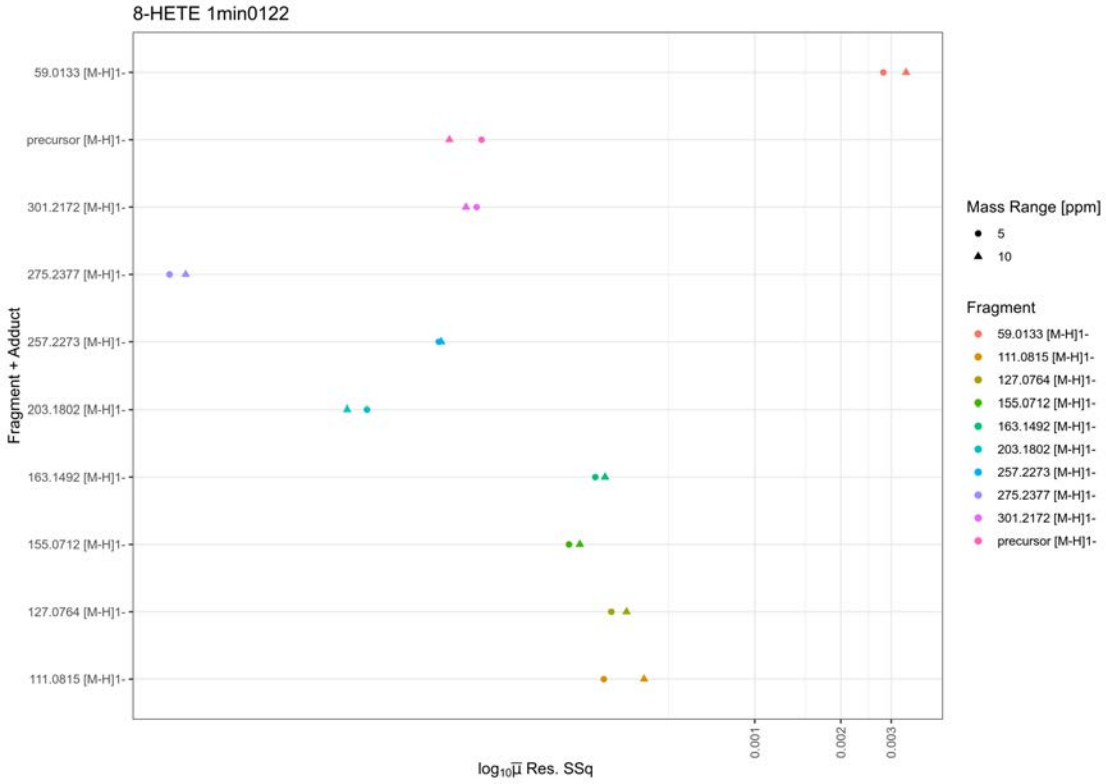


*Figure 144. Normalized sum-of-squares of the residuals*

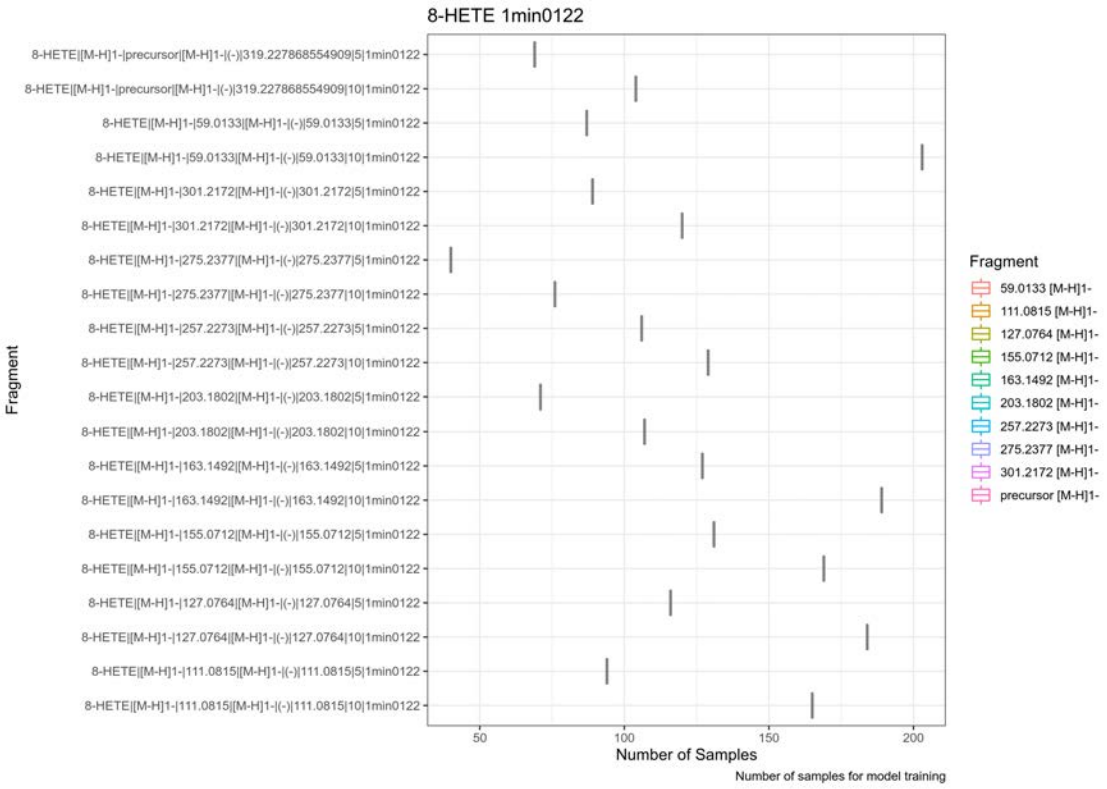


*Figure 145. Number of samples used for training per combination Id*

# 1.30. 9(10)-EpOME{d4} [M-H]1- 1min0124

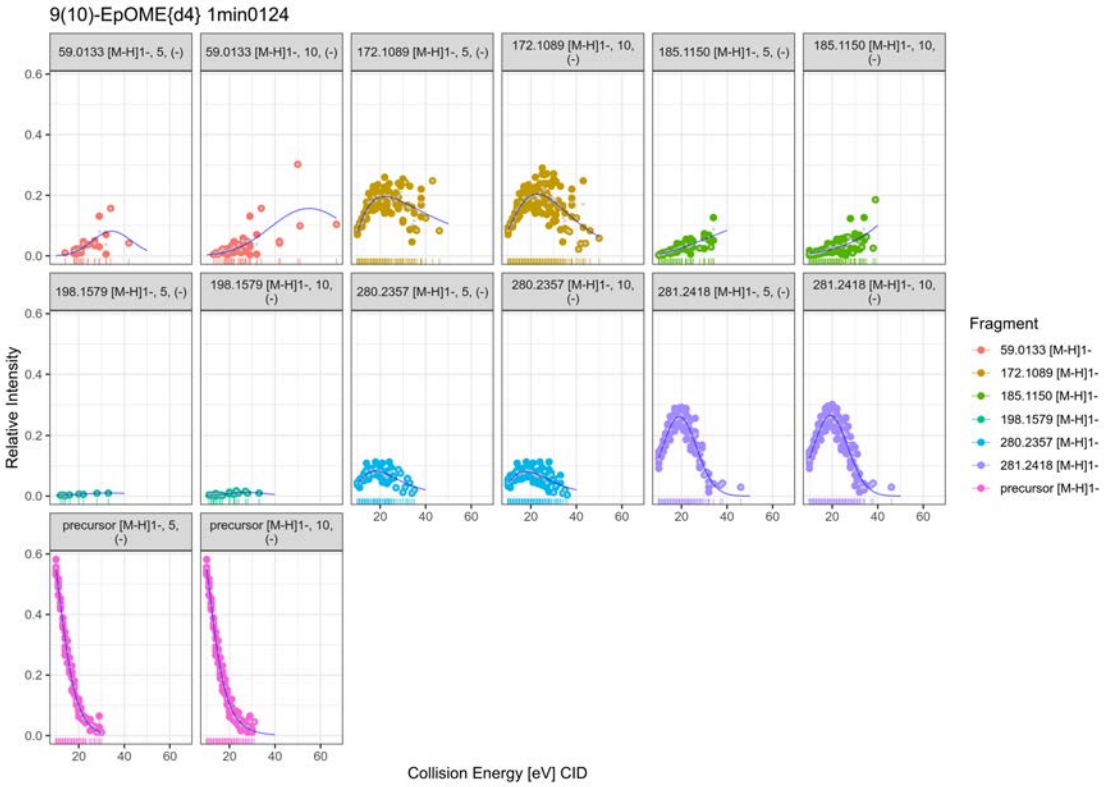


*Figure 146. Nonlinear fit*

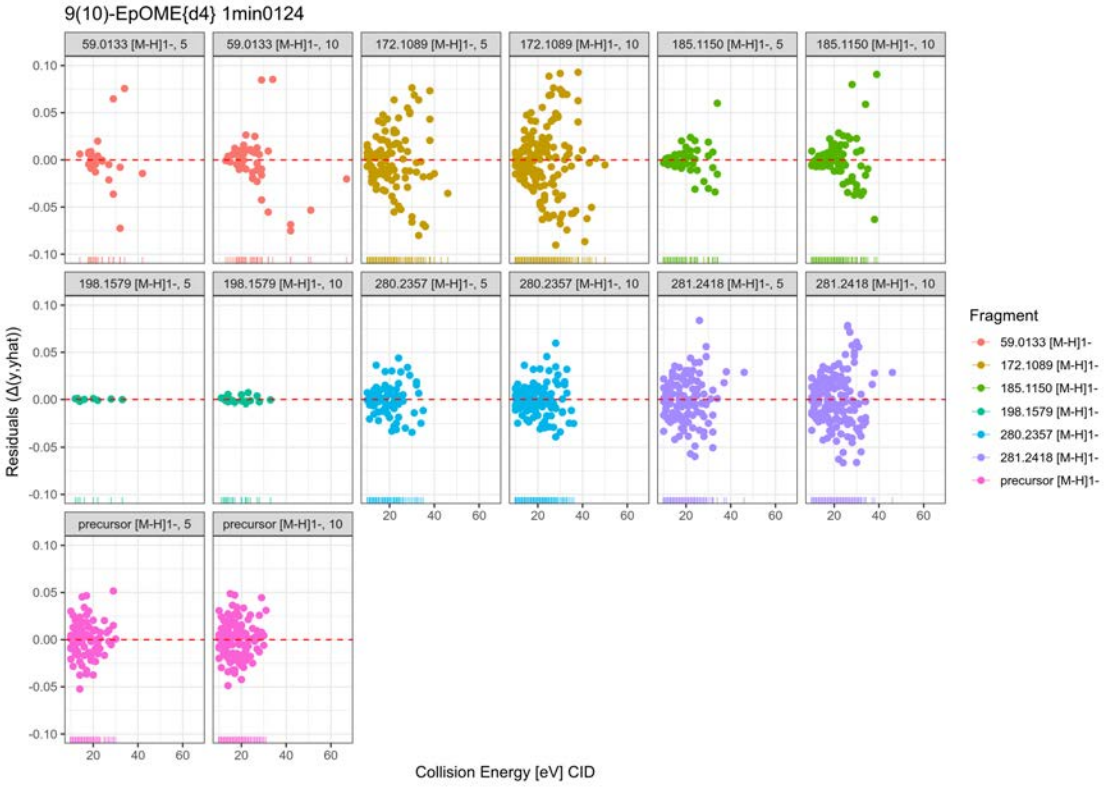


*Figure 147. Residuals of nonlinear fit*

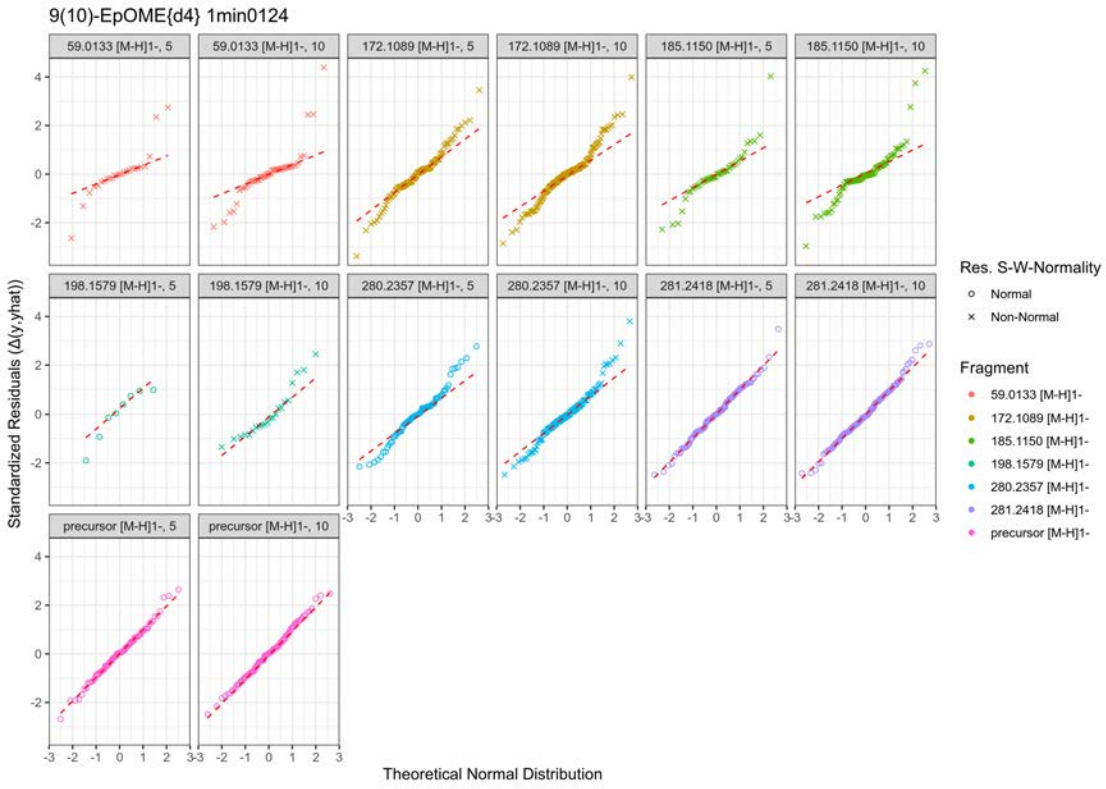


*Figure 148. Quantile-quantile plot of residuals*

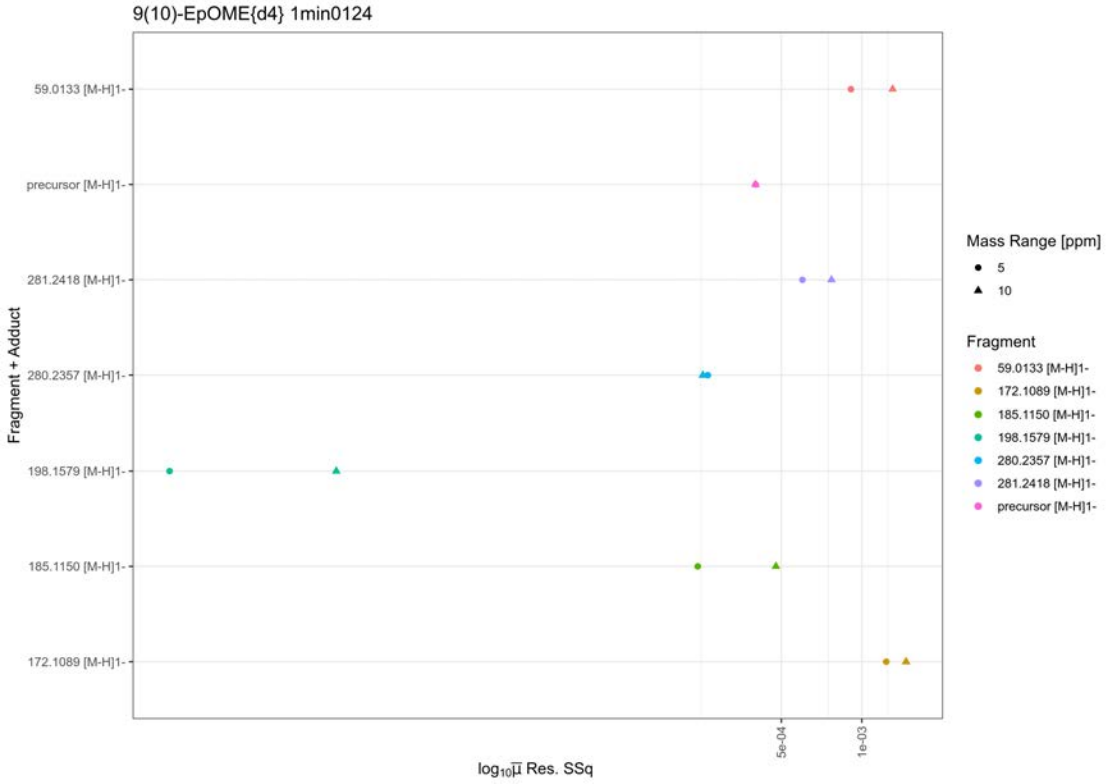


*Figure 149. Normalized sum-of-squares of the residuals*

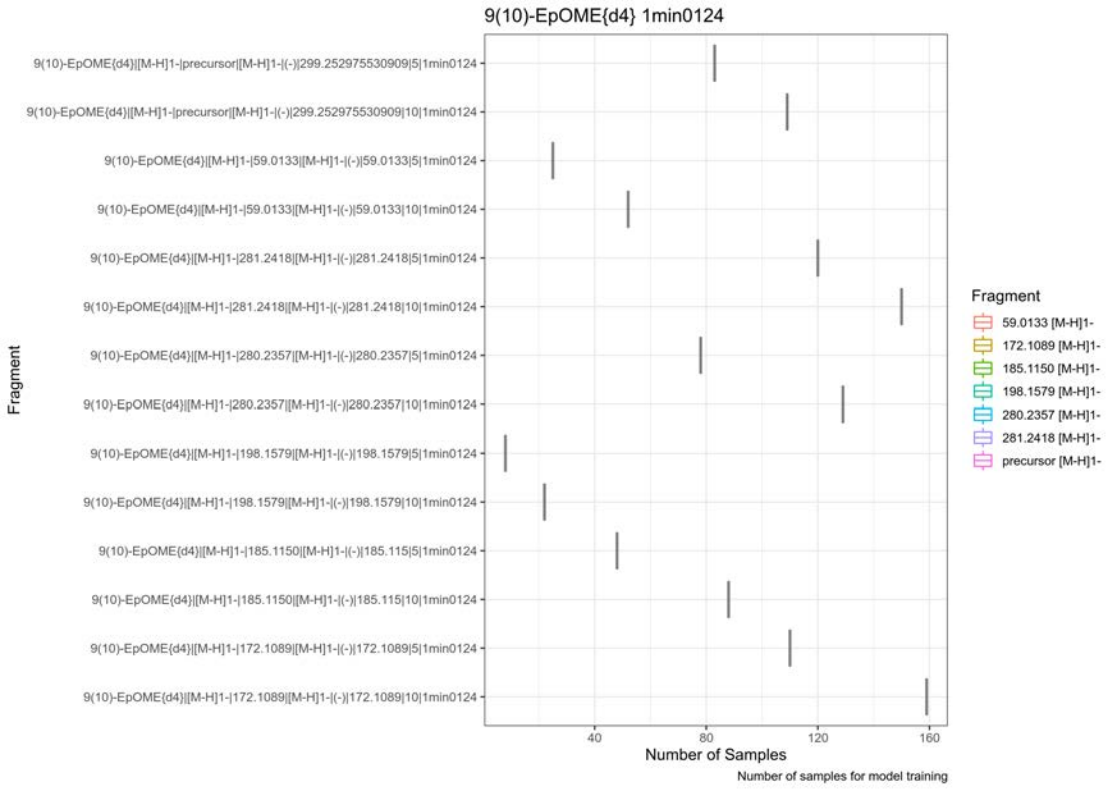


*Figure 150. Number of samples used for training per combination Id*

# 1.31. 9-HEPE [M-H]1- 1min0128

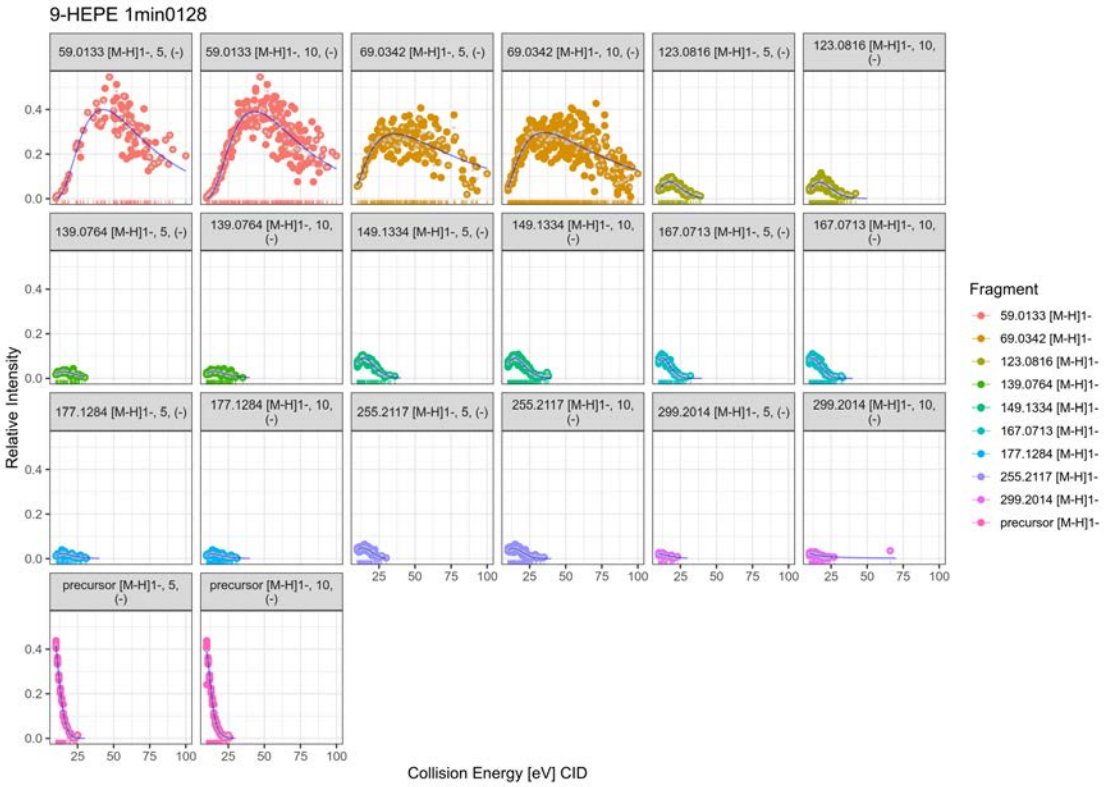


*Figure 151. Nonlinear fit*

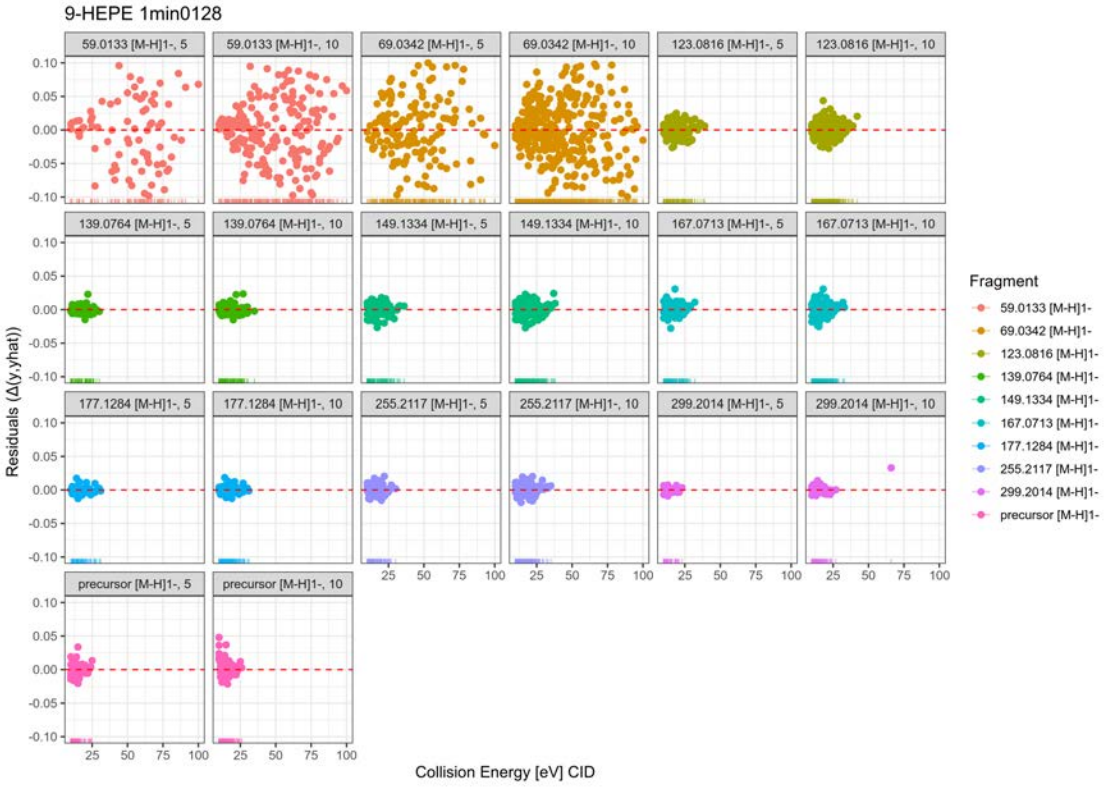


*Figure 152. Residuals of nonlinear fit*

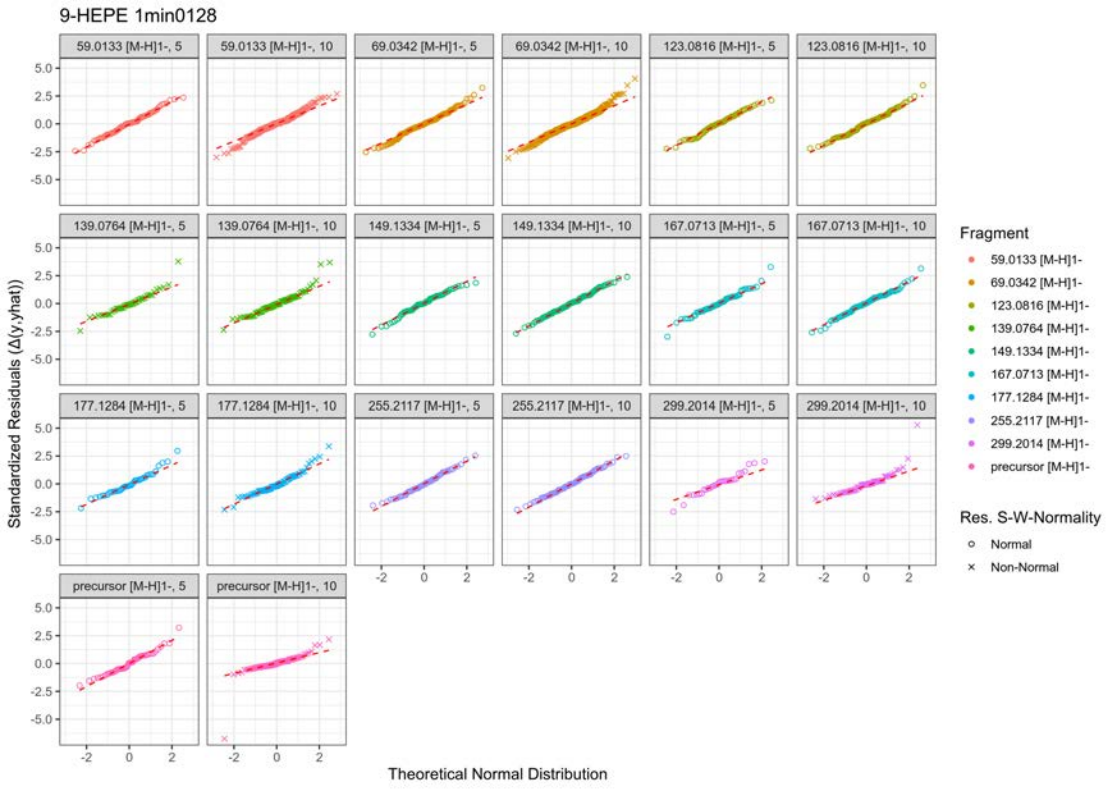


*Figure 153. Quantile-quantile plot of residuals*

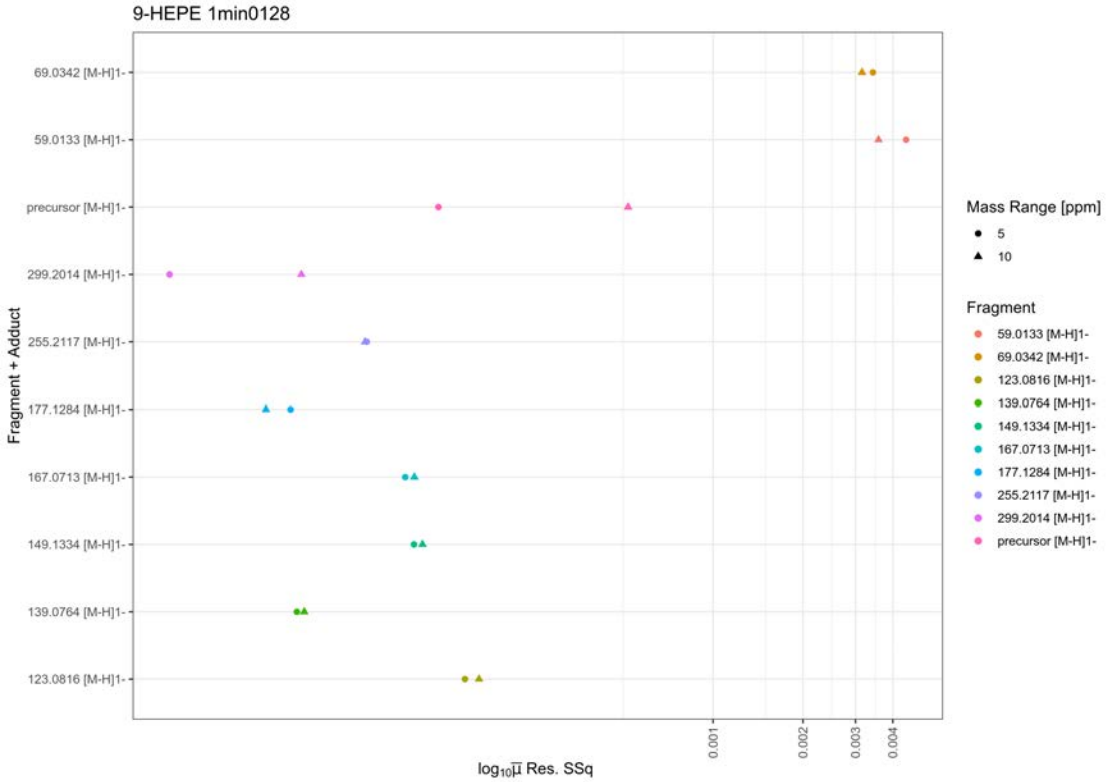


*Figure 154. Normalized sum-of-squares of the residuals*

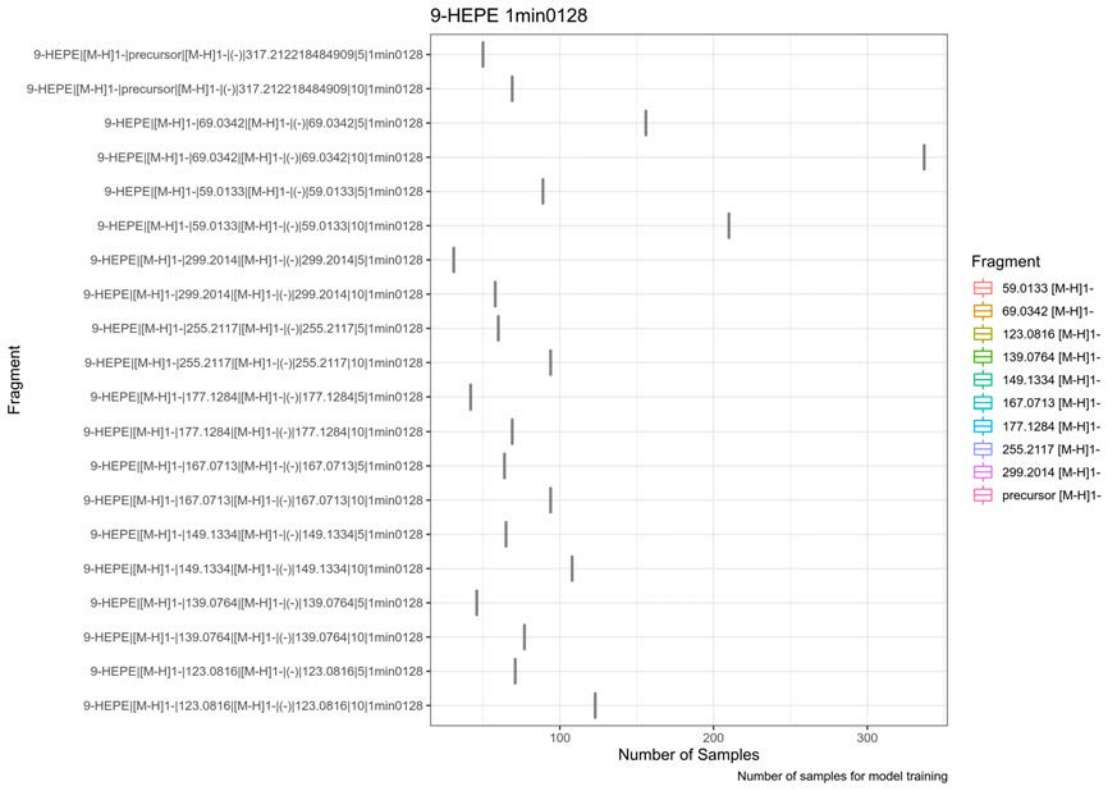


*Figure 155. Number of samples used for training per combination Id*

# 1.32. 9-HETE [M-H]1- 1min0130

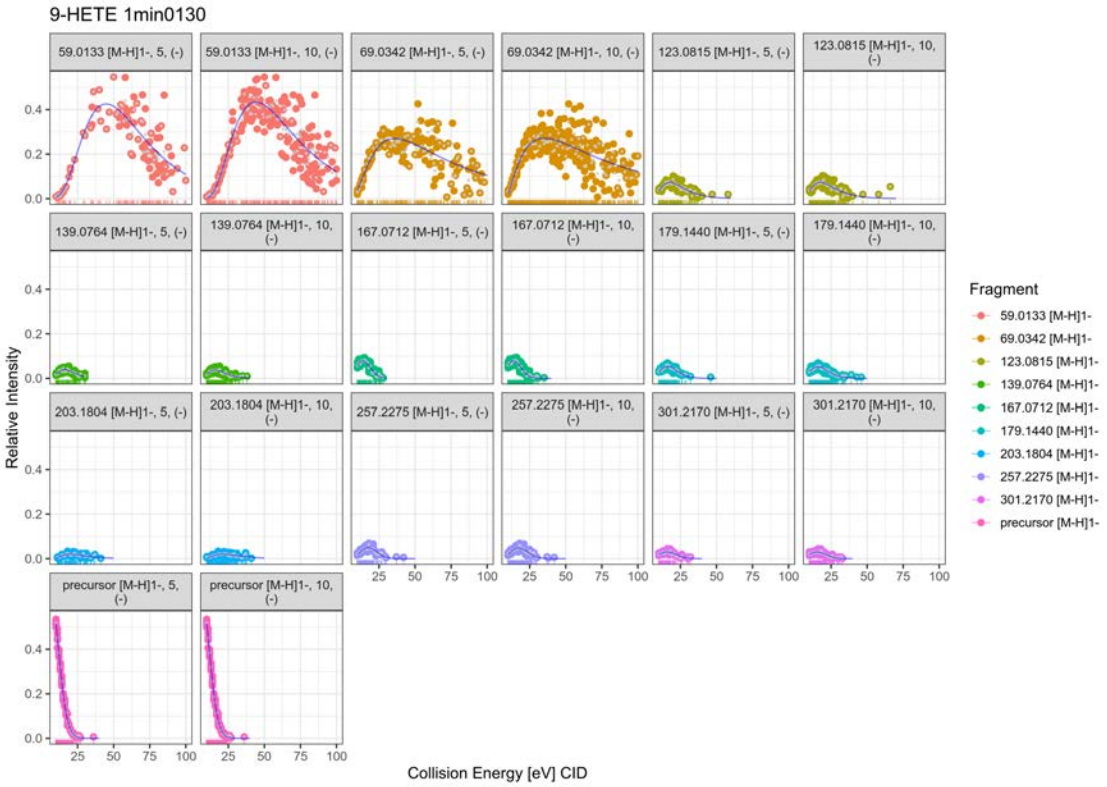


*Figure 156. Nonlinear fit*

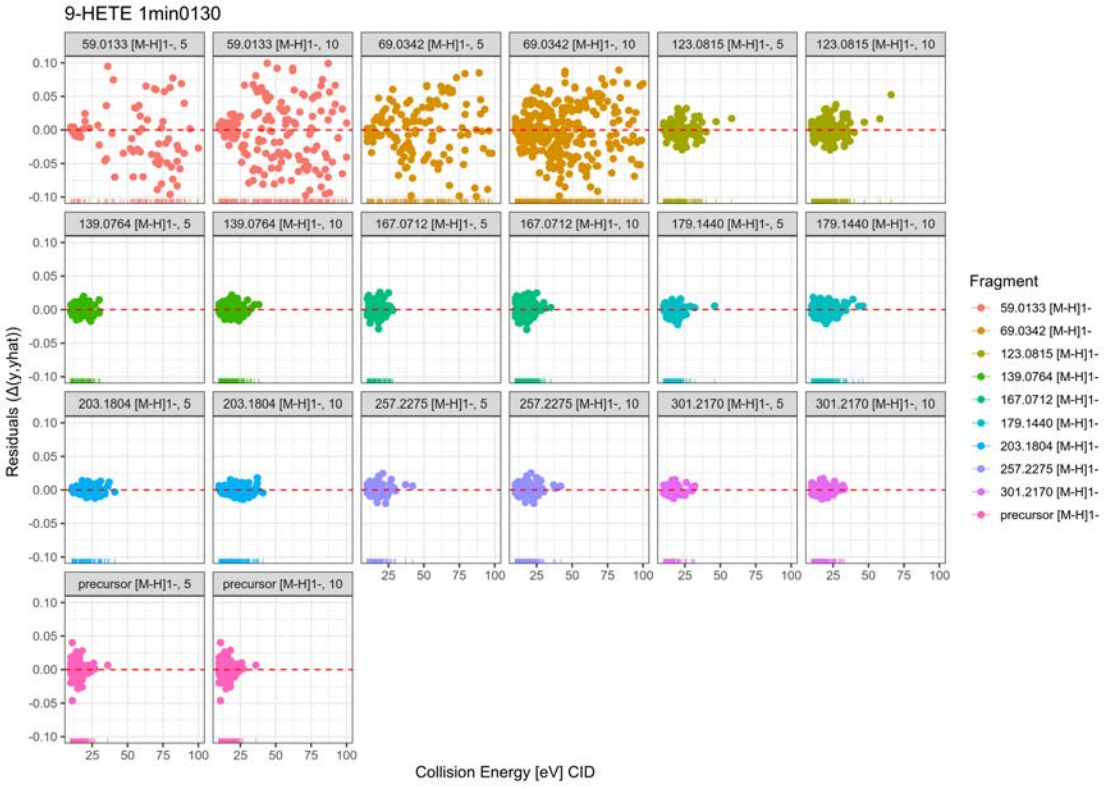


*Figure 157. Residuals of nonlinear fit*

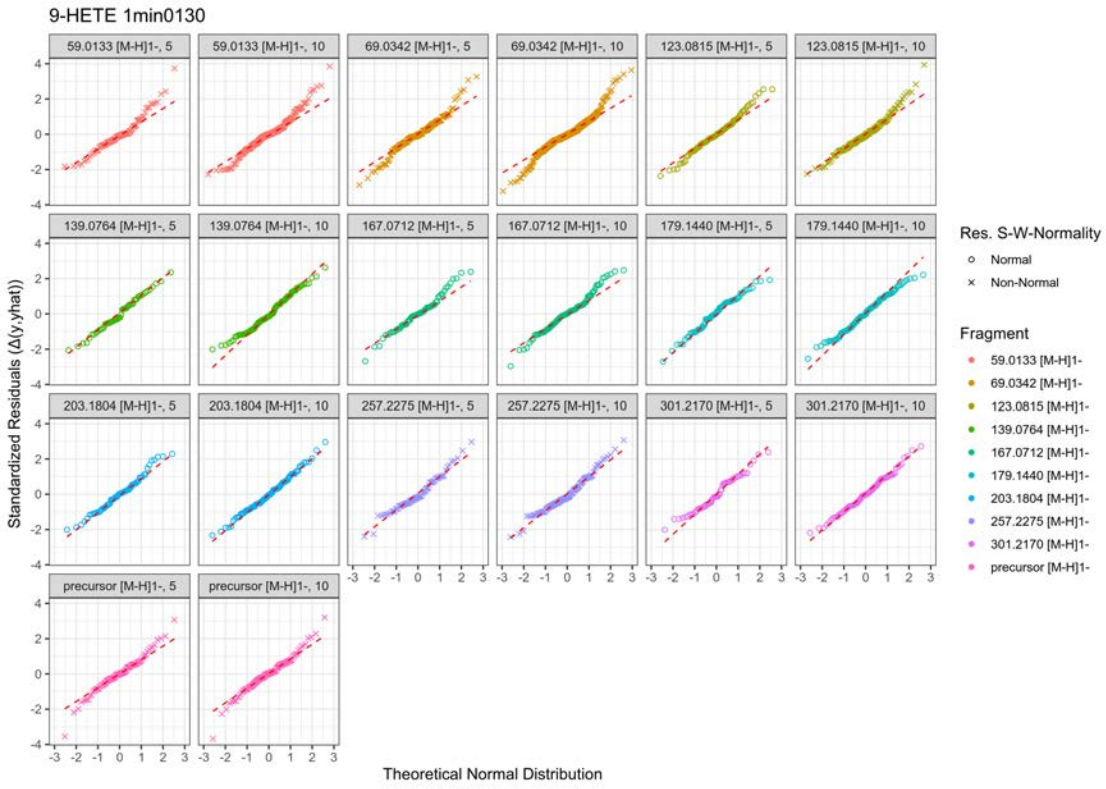


*Figure 158. Quantile-quantile plot of residuals*

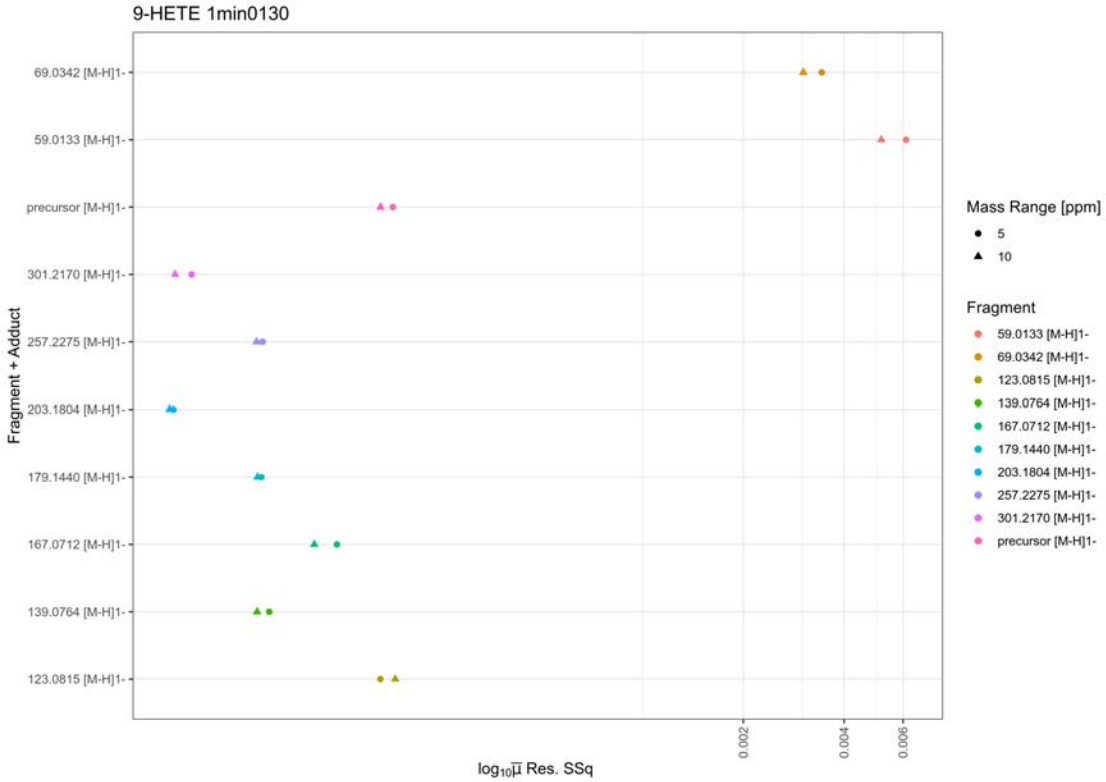


*Figure 159. Normalized sum-of-squares of the residuals*

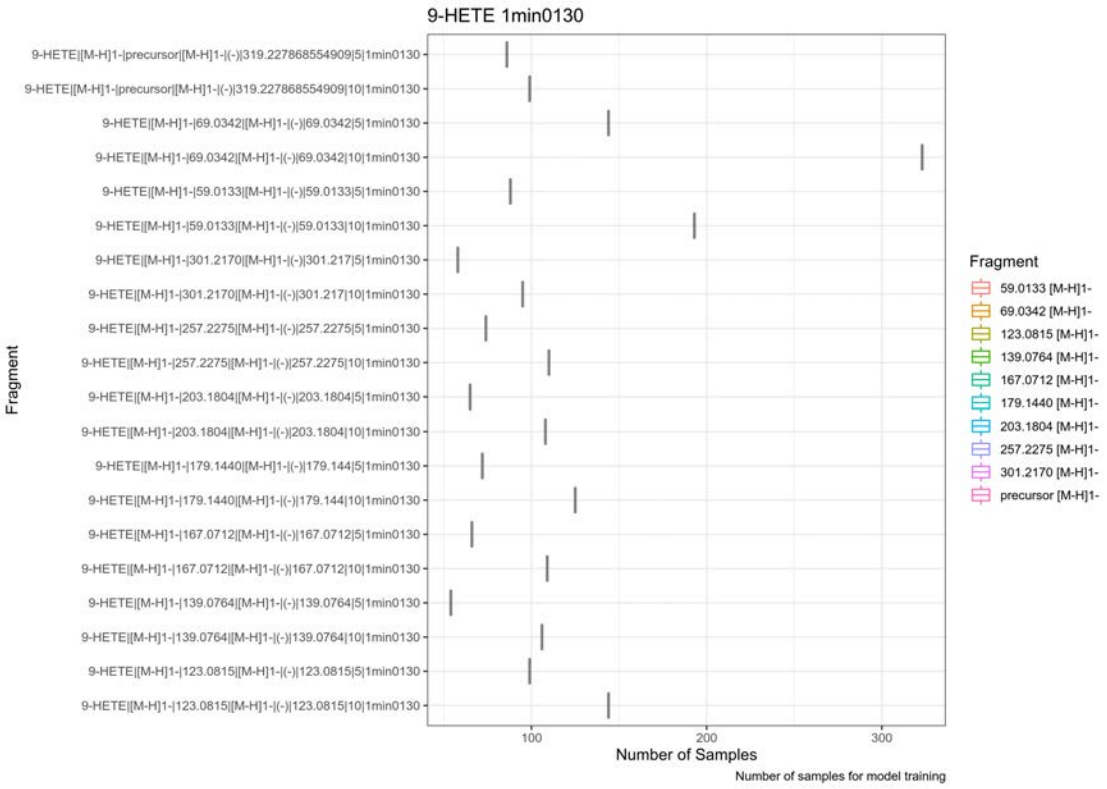


*Figure 160. Number of samples used for training per combination Id*

# 1.33. 9-HODE [M-H]1- 1min0132

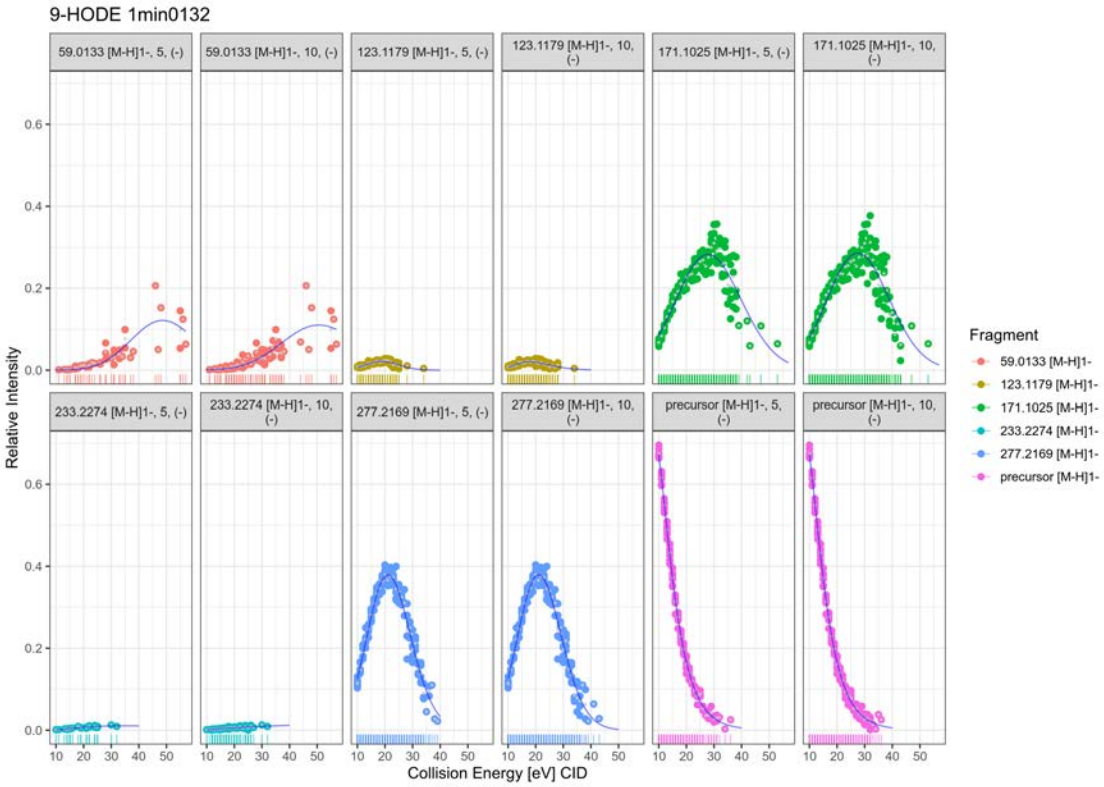


*Figure 161. Nonlinear fit*

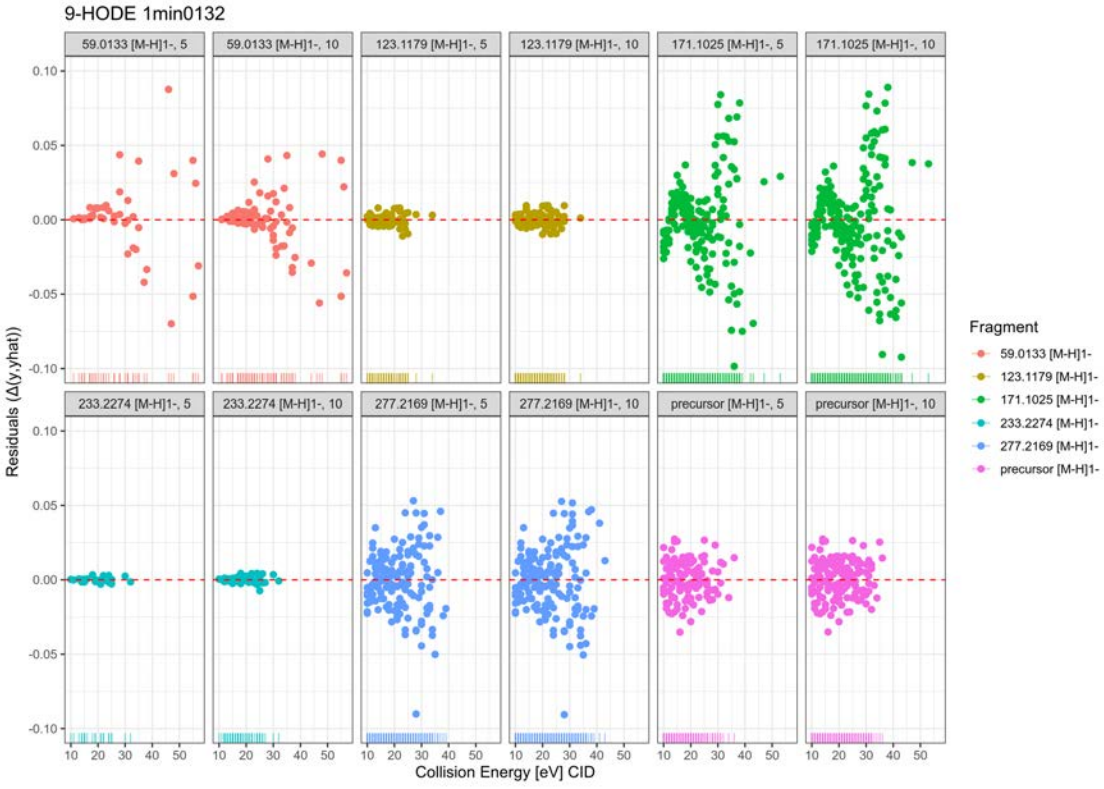


*Figure 162. Residuals of nonlinear fit*

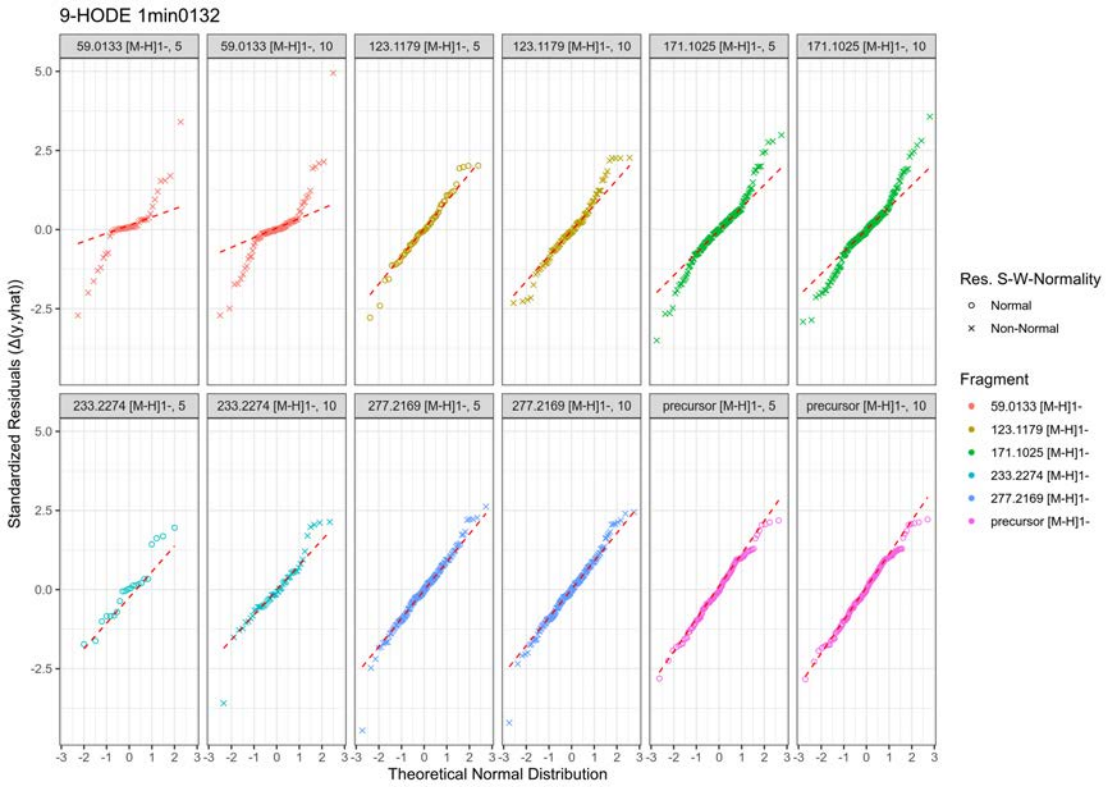


*Figure 163. Quantile-quantile plot of residuals*

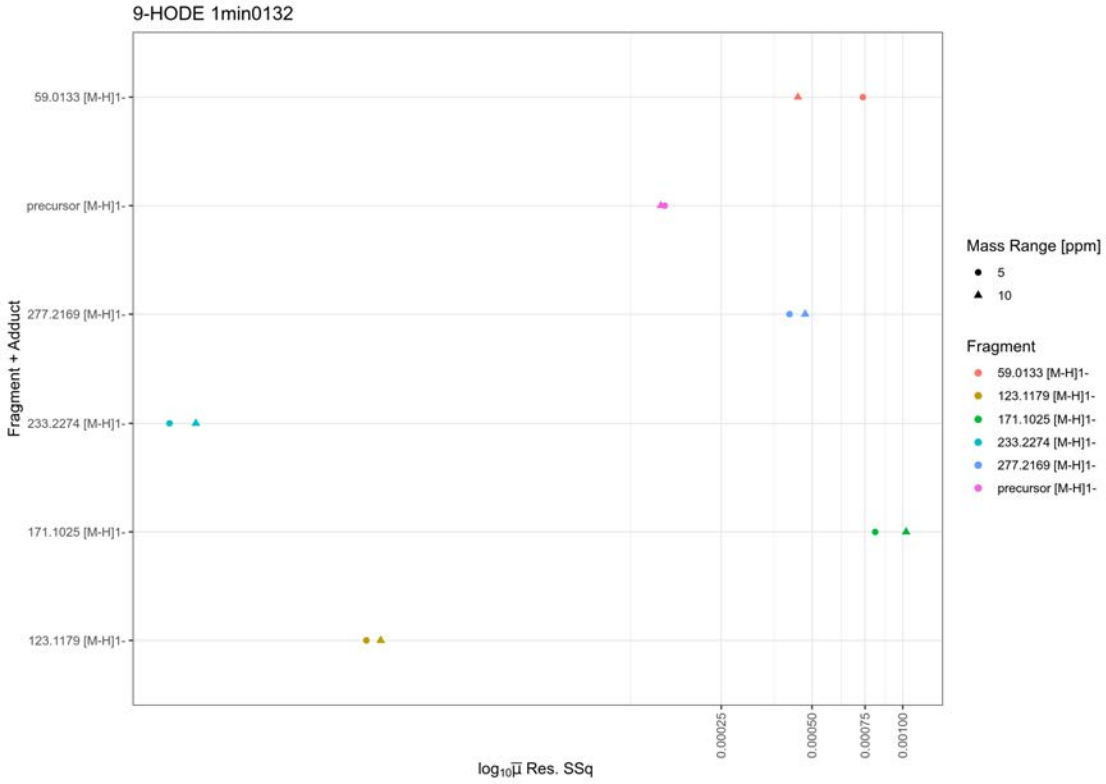


*Figure 164. Normalized sum-of-squares of the residuals*

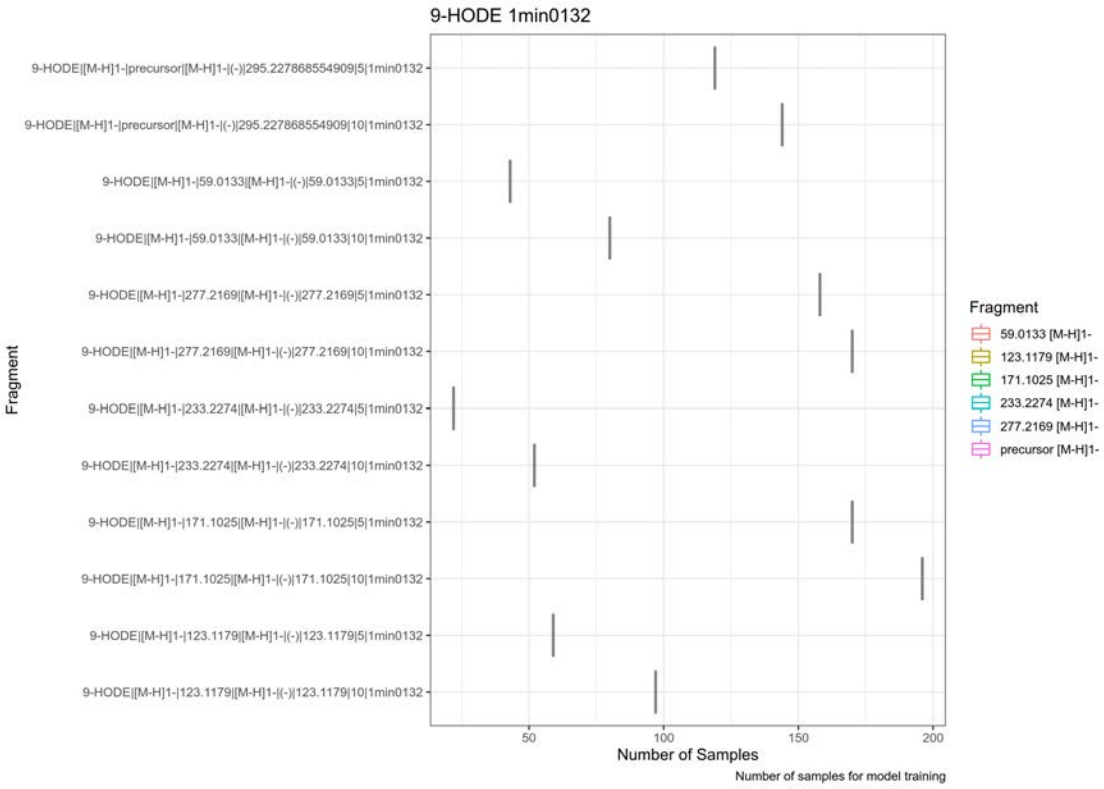


*Figure 165. Number of samples used for training per combination Id*

# 1.34. 9-HOTrE [M-H]1- 1min0205

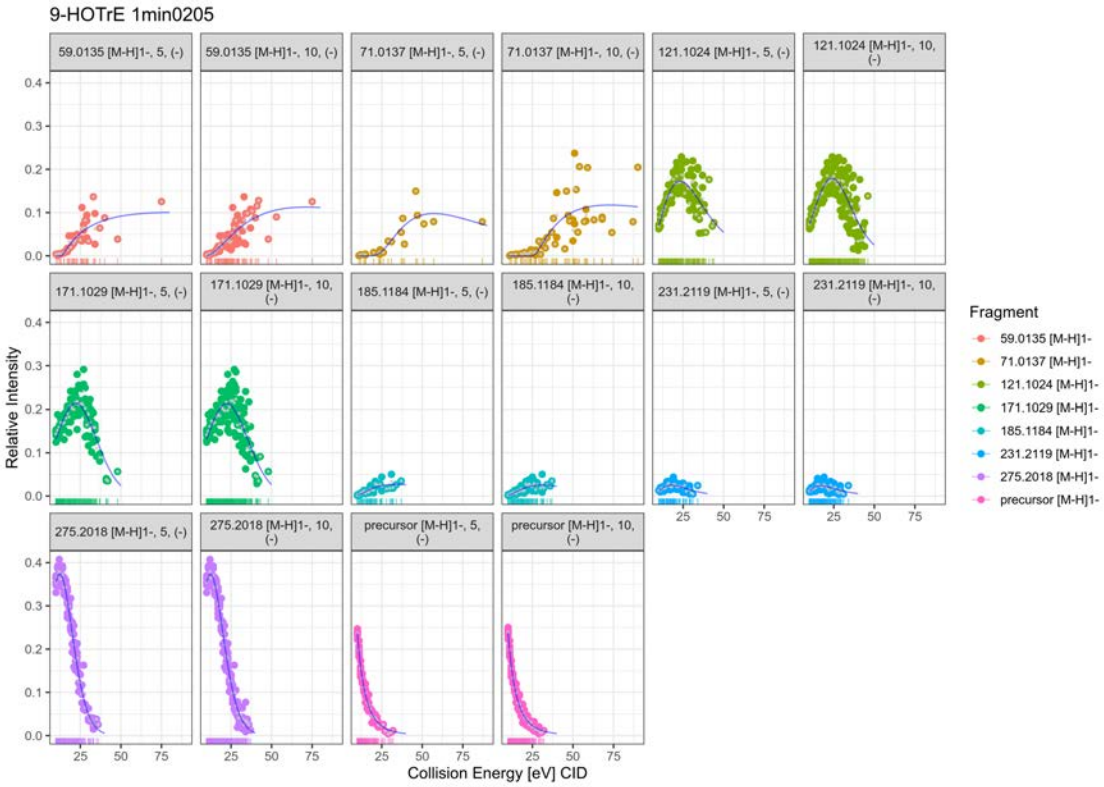


*Figure 166. Nonlinear fit*


*Figure 167. Residuals of nonlinear fit*

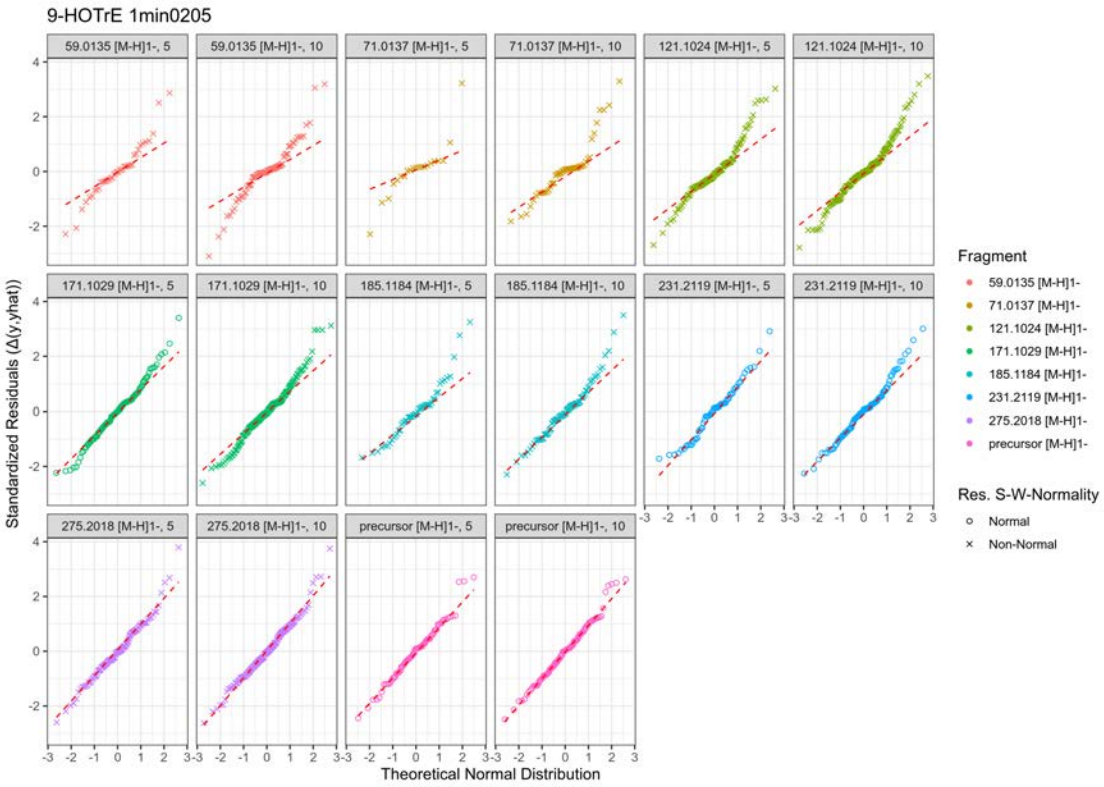


*Figure 168. Quantile-quantile plot of residuals*

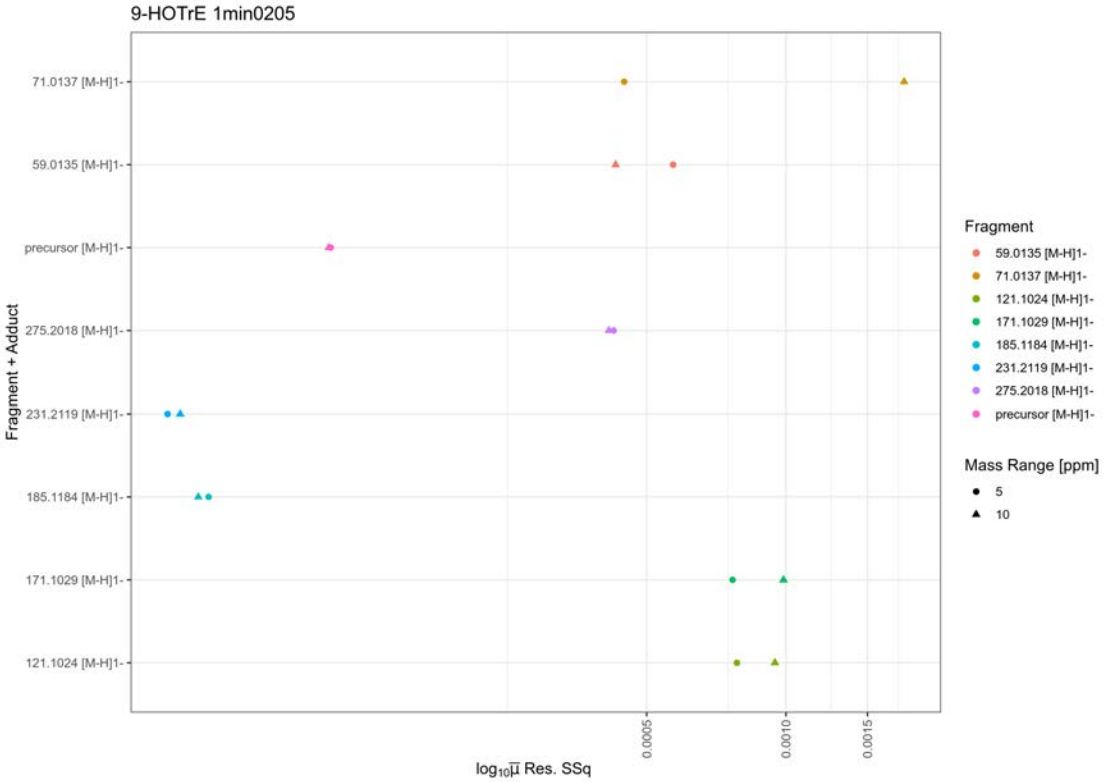


*Figure 169. Normalized sum-of-squares of the residuals*

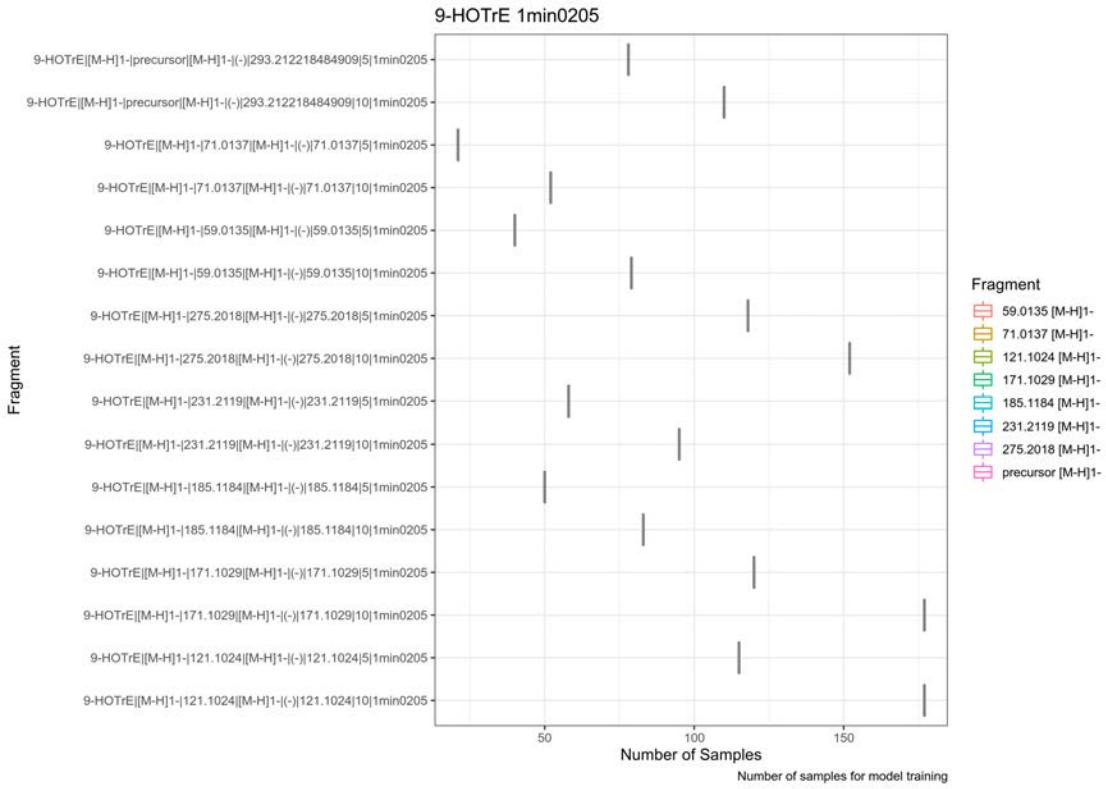


*Figure 170. Number of samples used for training per combination Id*

# 1.35. AA{d8} [M-H]1- 1min0134

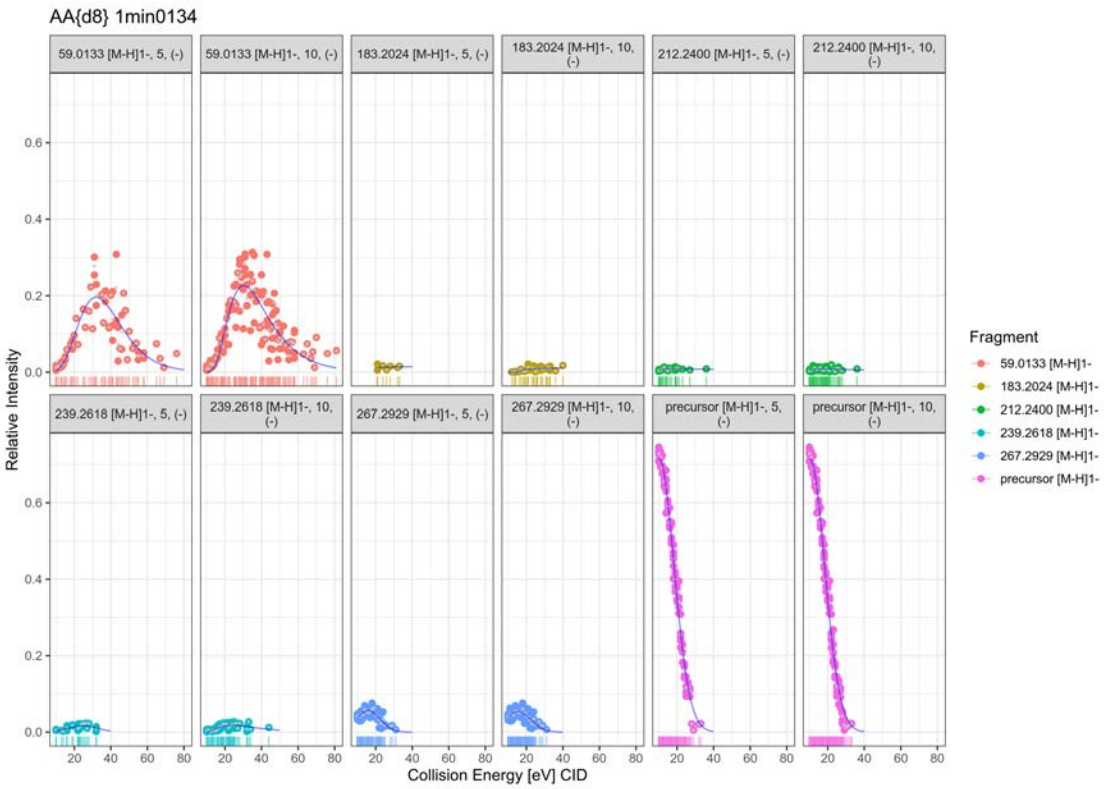


*Figure 171. Nonlinear fit*

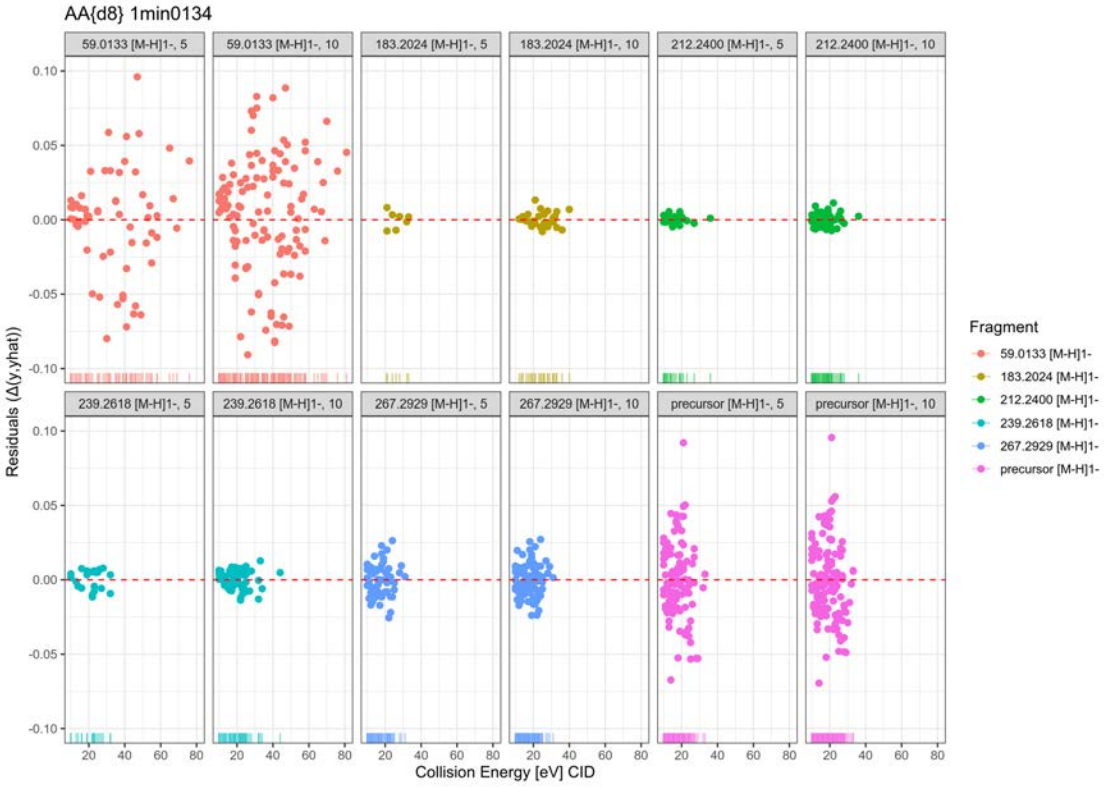


*Figure 172. Residuals of nonlinear fit*

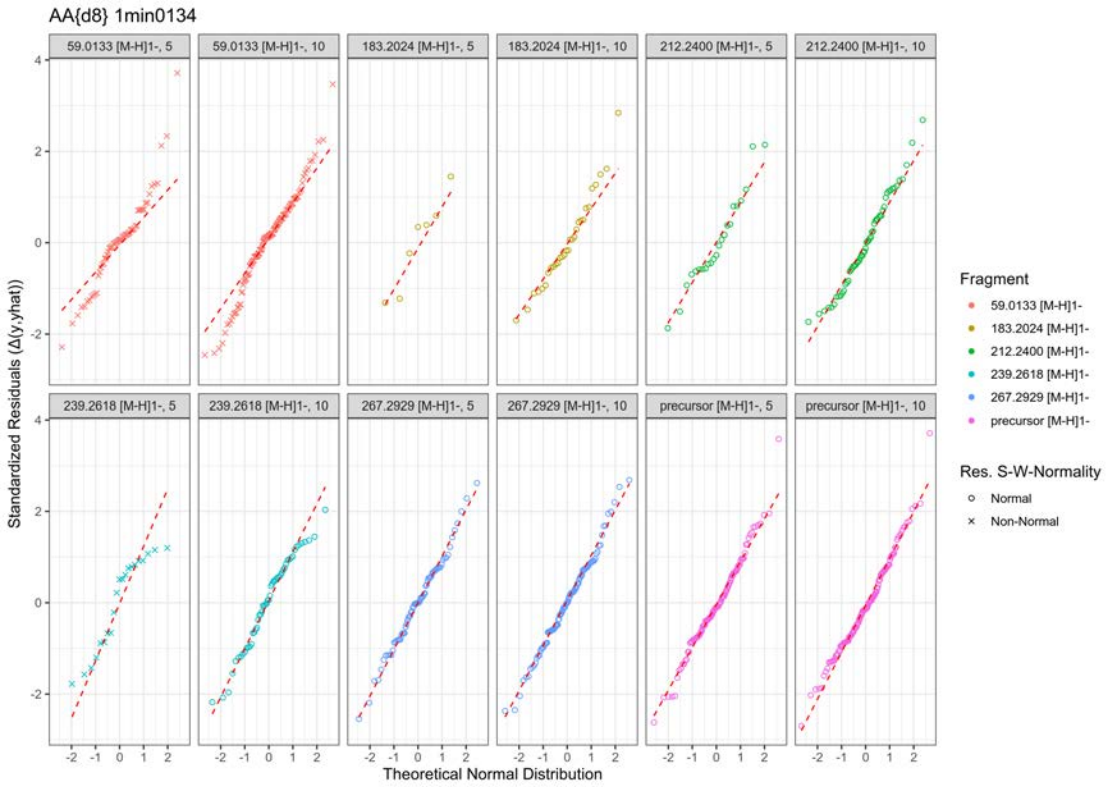


*Figure 173. Quantile-quantile plot of residuals*

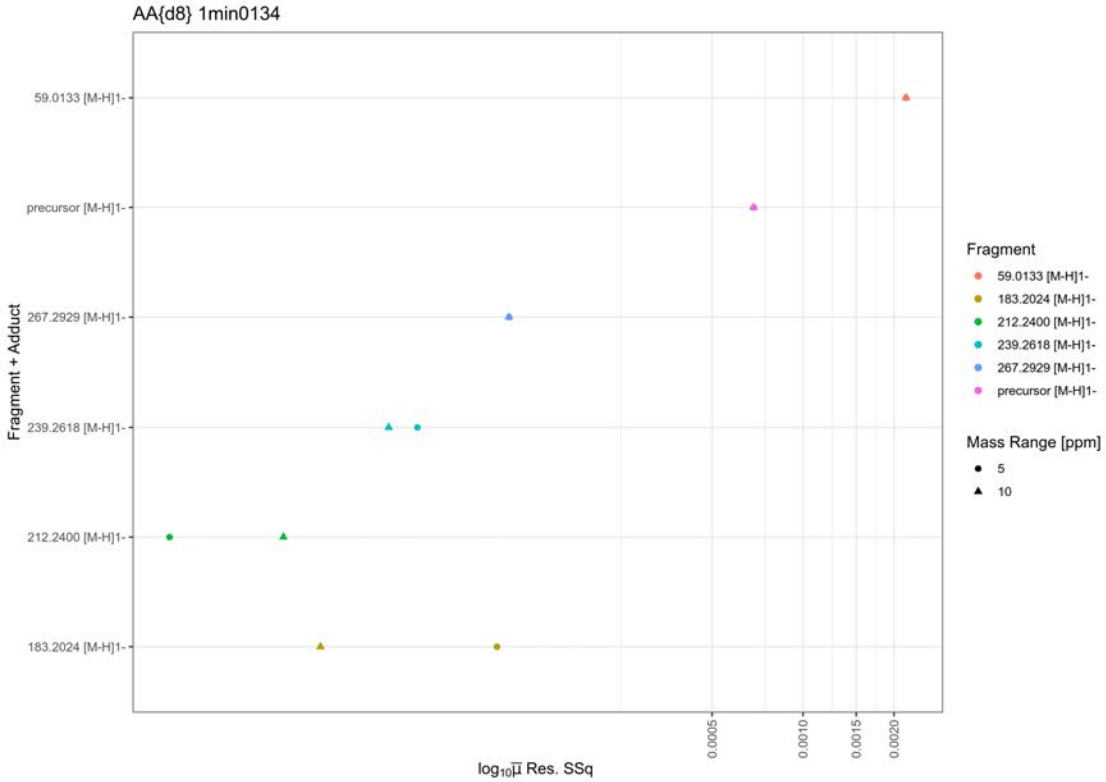


*Figure 174. Normalized sum-of-squares of the residuals*

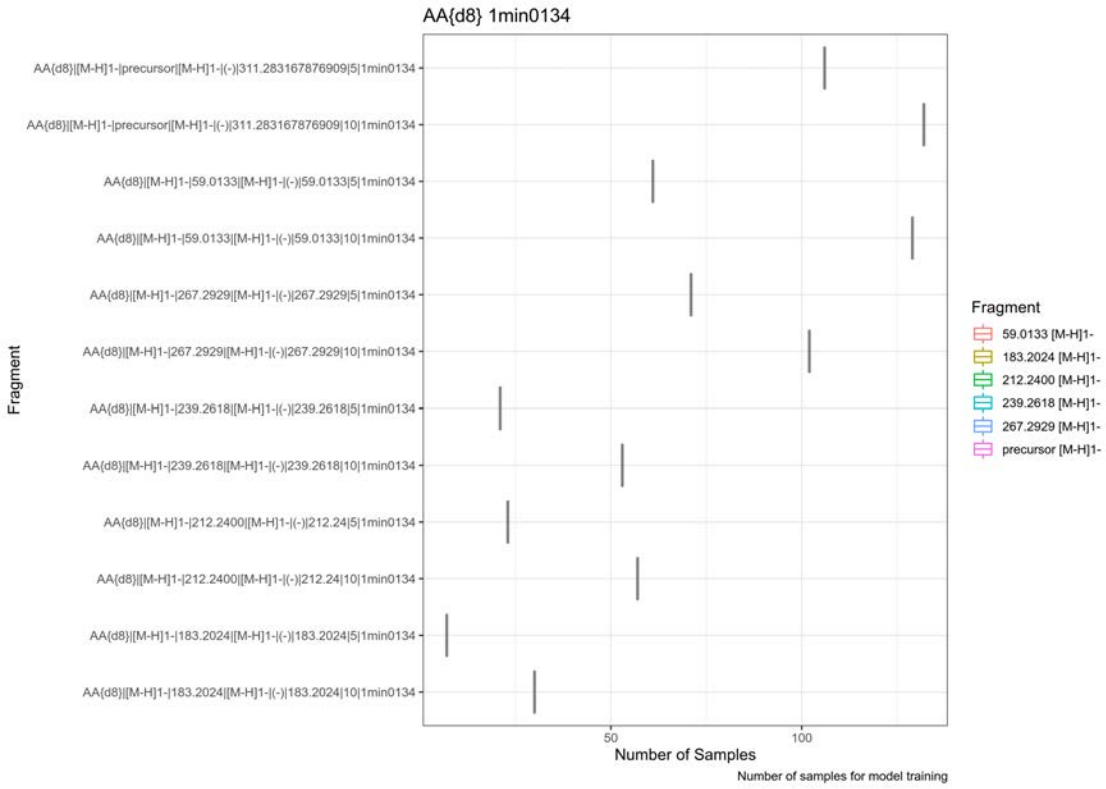


*Figure 175. Number of samples used for training per combination Id*

# 1.36. DHA{d5} [M-H]1- 1min0137

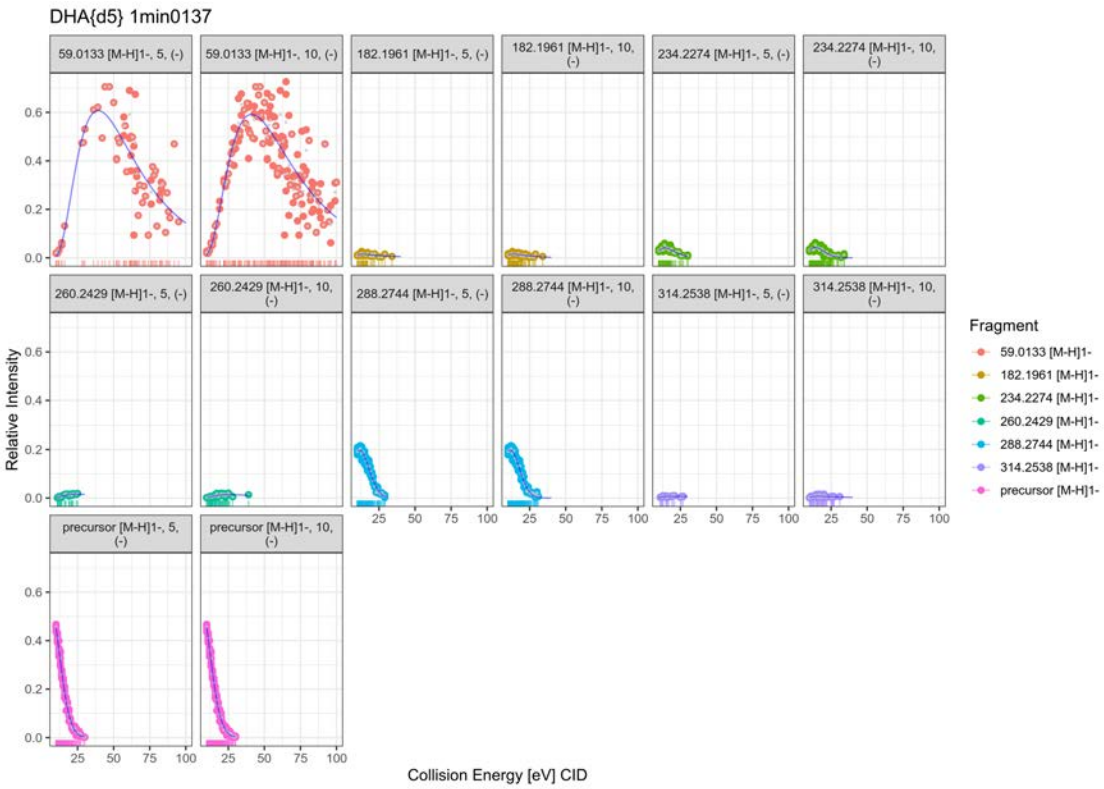


*Figure 176. Nonlinear fit*

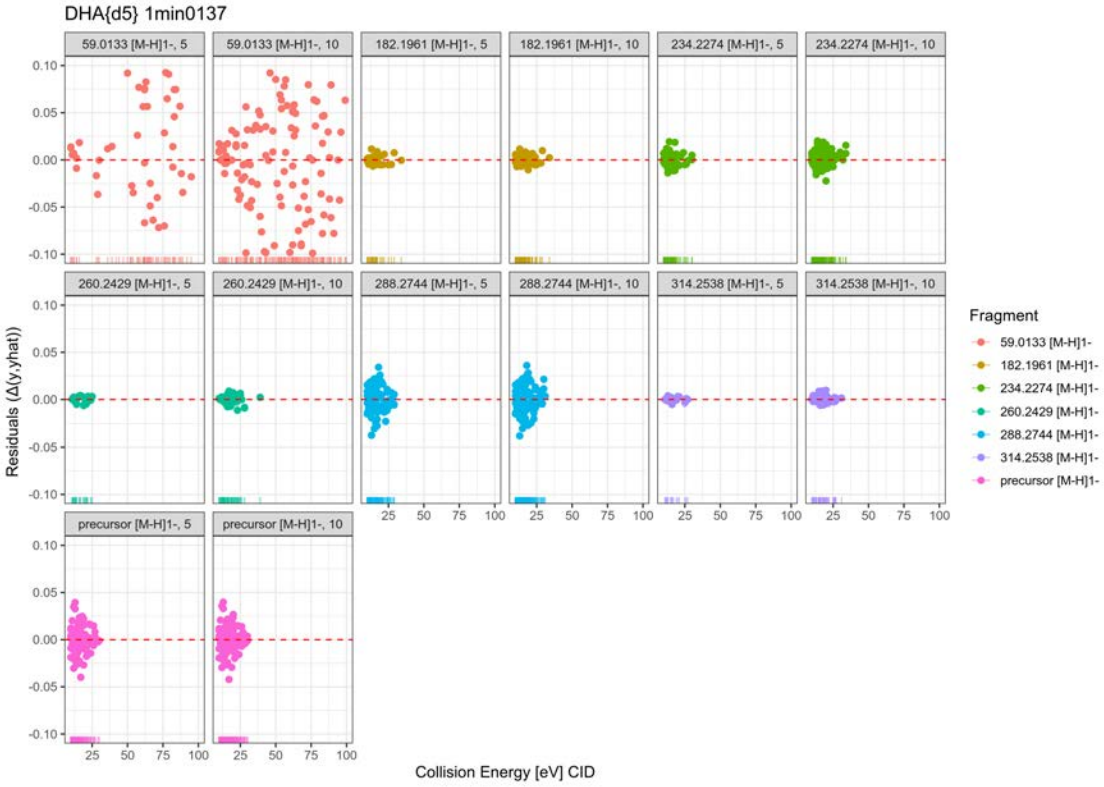


*Figure 177. Residuals of nonlinear fit*

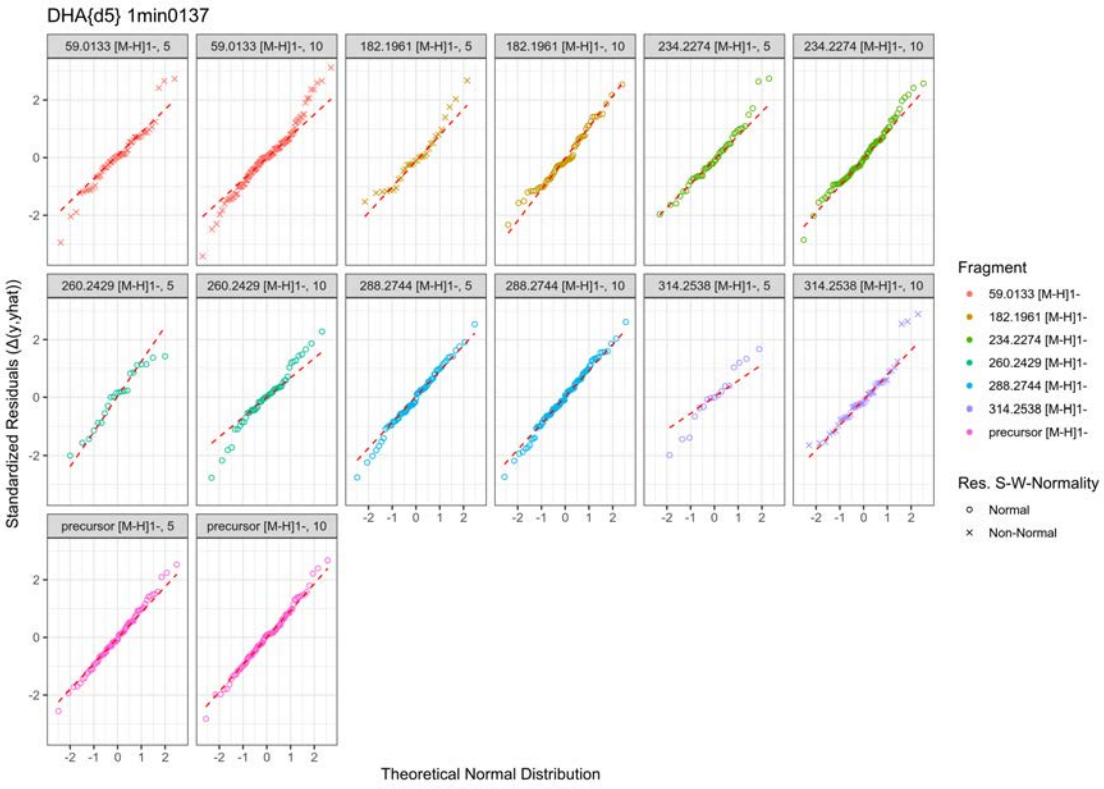


*Figure 178. Quantile-quantile plot of residuals*

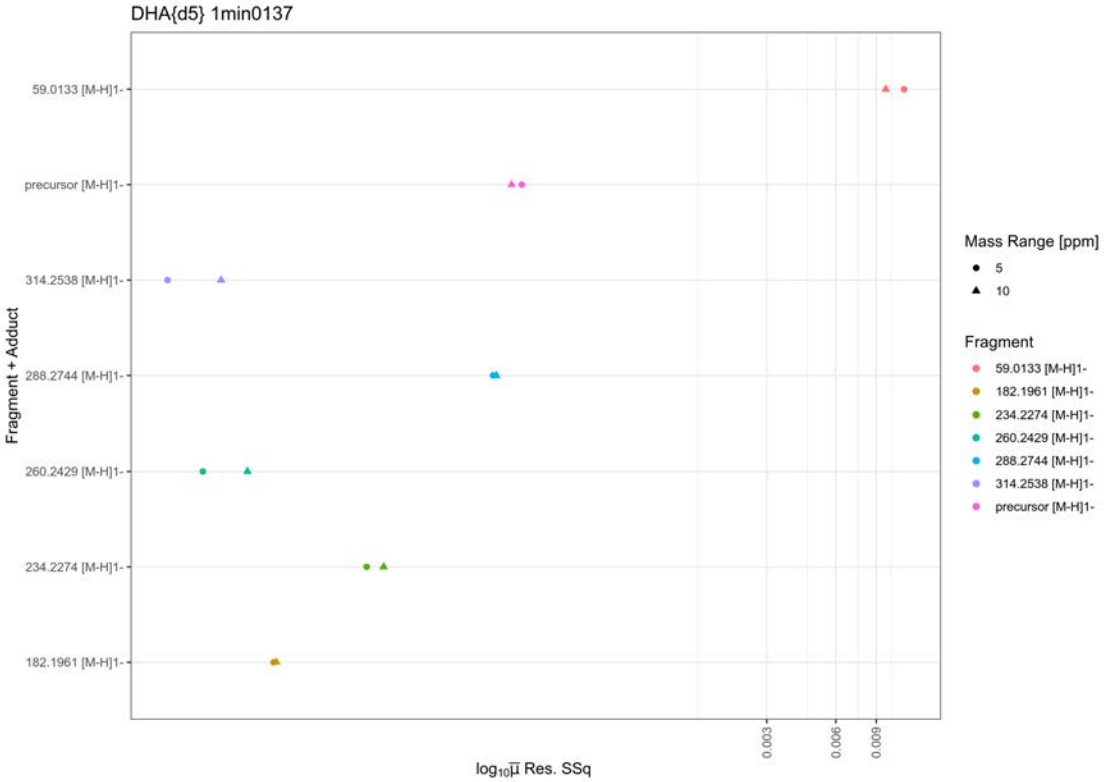


*Figure 179. Normalized sum-of-squares of the residuals*

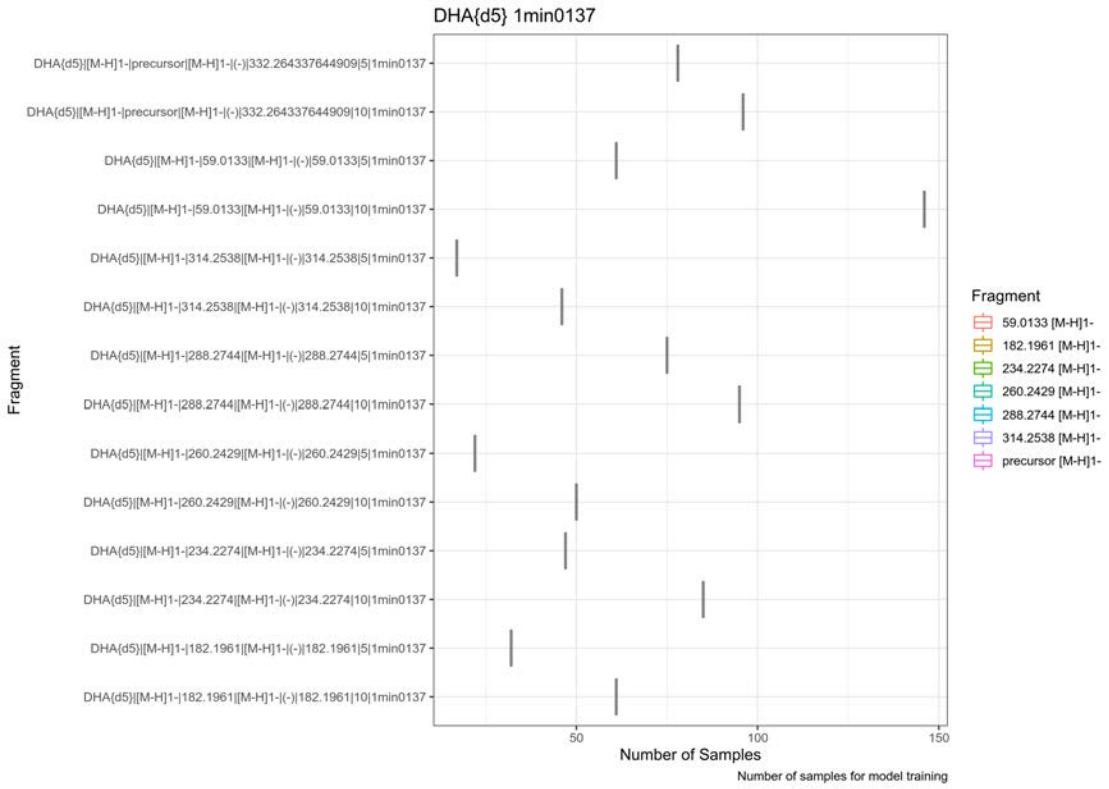


*Figure 180. Number of samples used for training per combination Id*

# 1.37. EPA{d5} [M-H]1- 1min0139

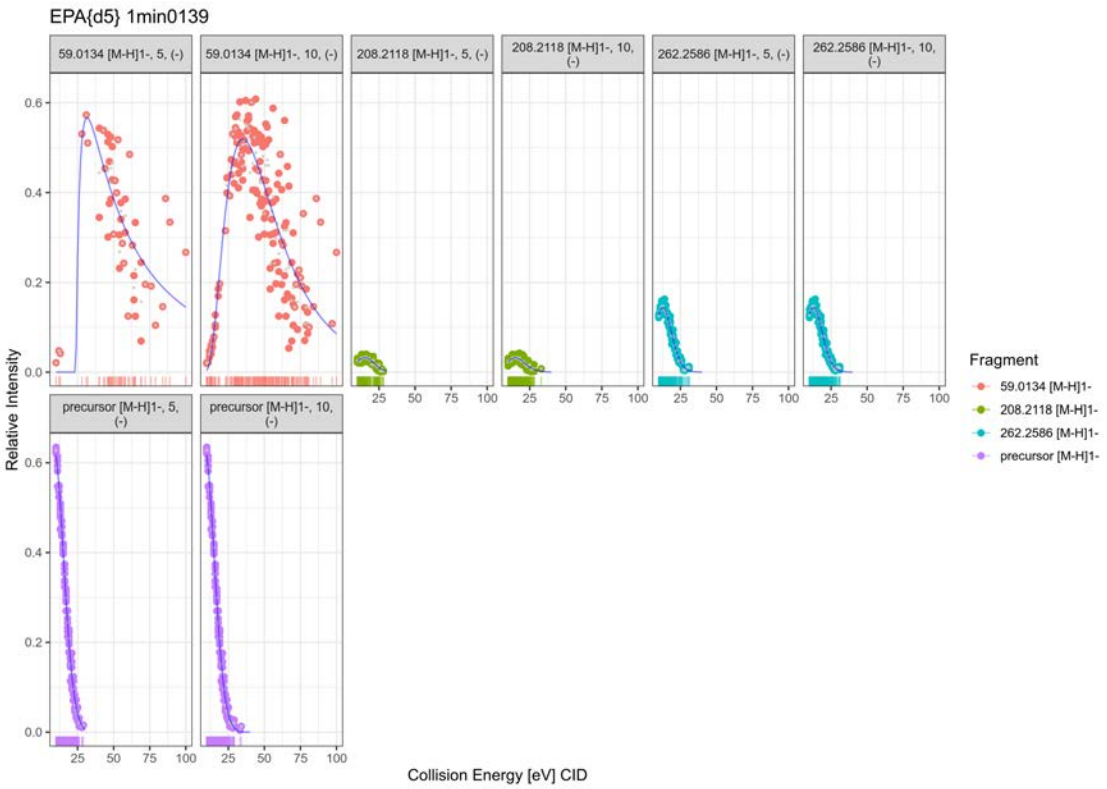


*Figure 181. Nonlinear fit*

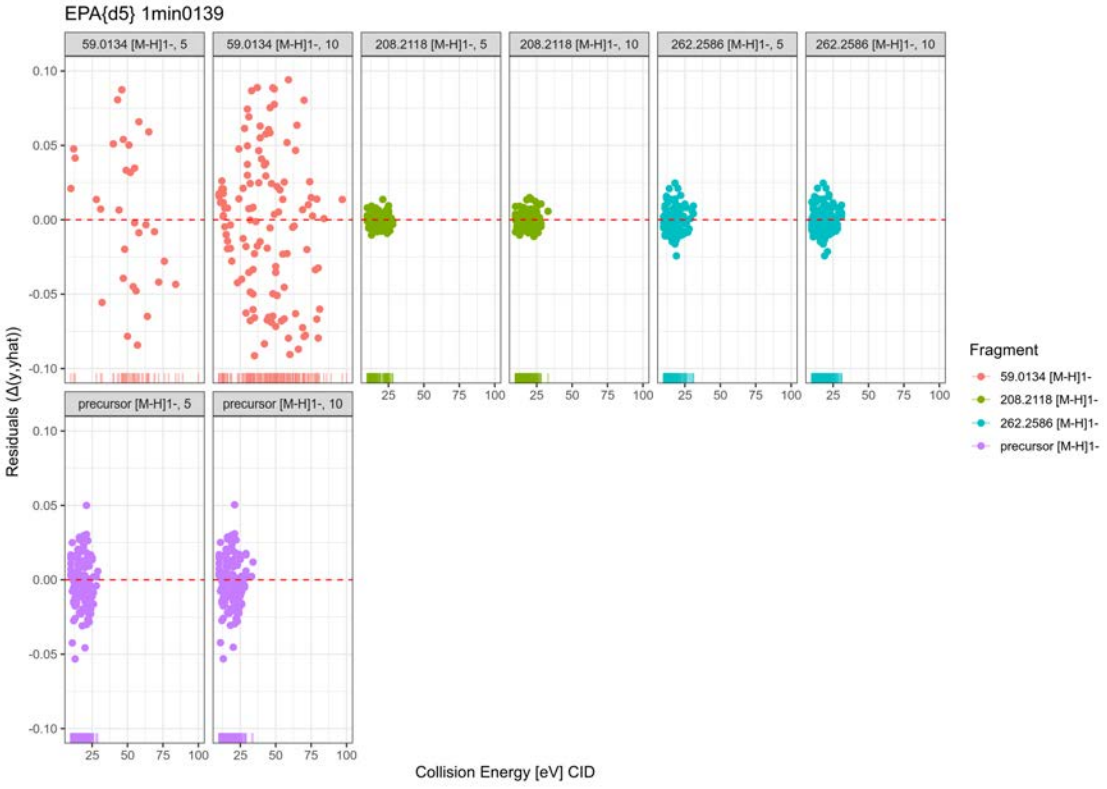


*Figure 182. Residuals of nonlinear fit*

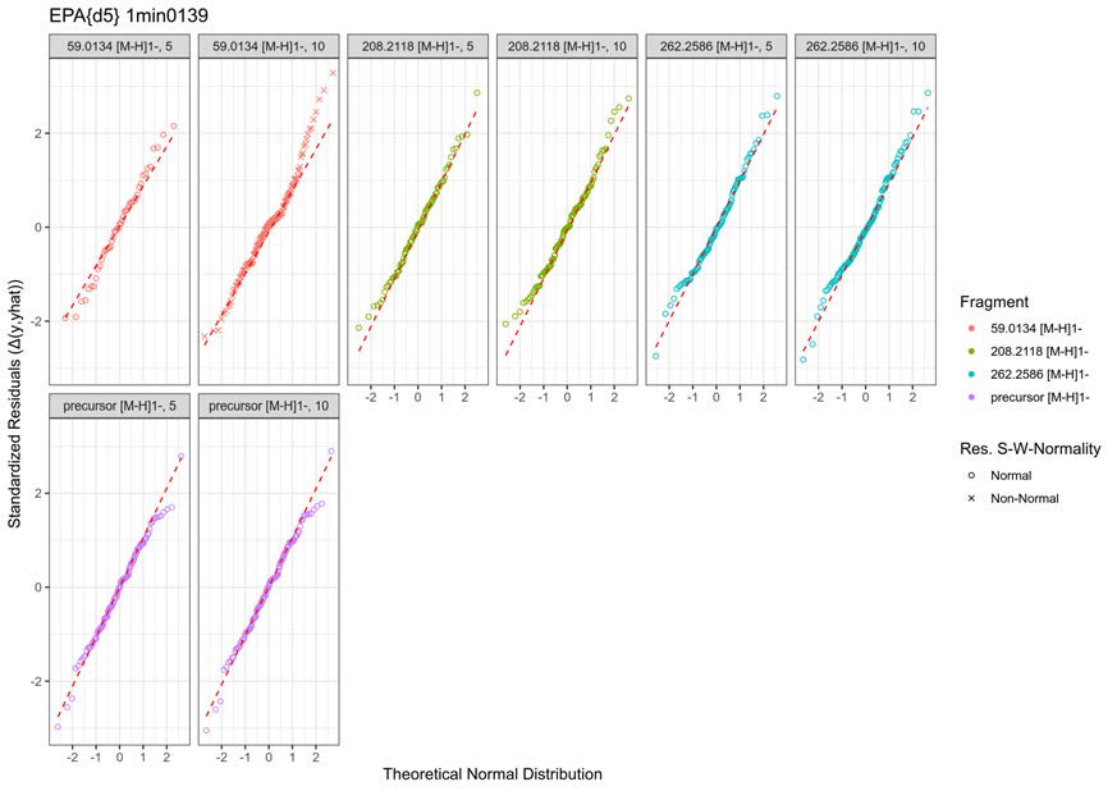


*Figure 183. Quantile-quantile plot of residuals*

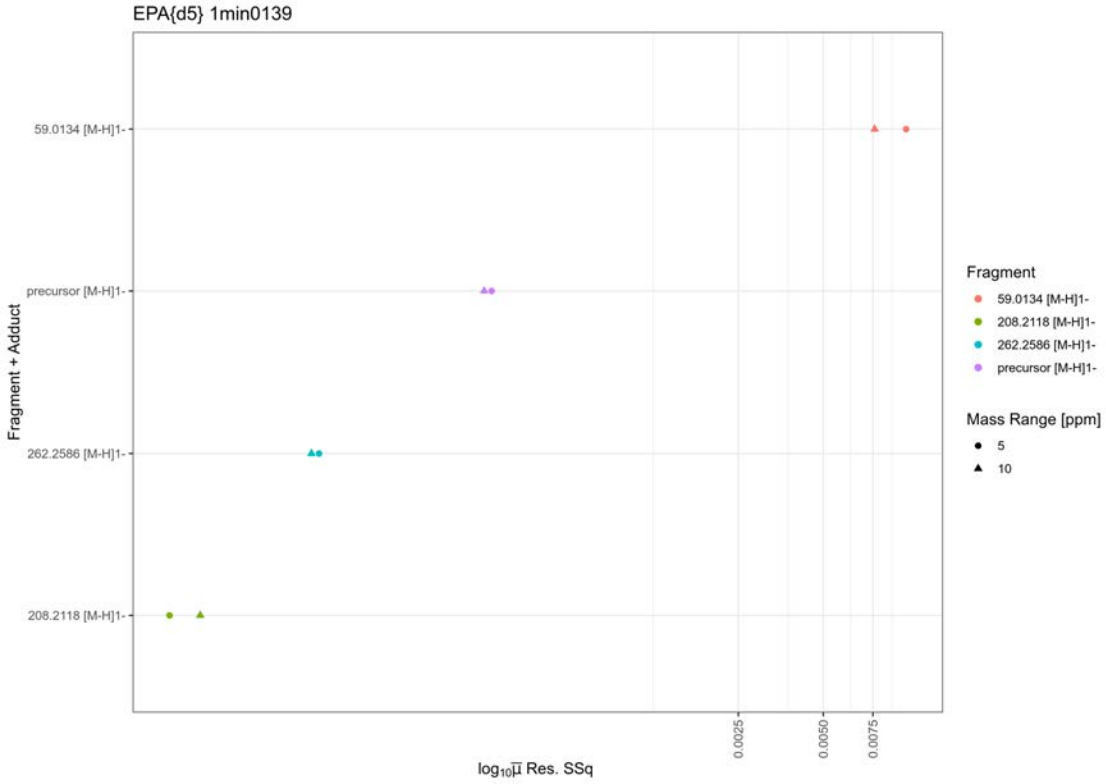


*Figure 184. Normalized sum-of-squares of the residuals*

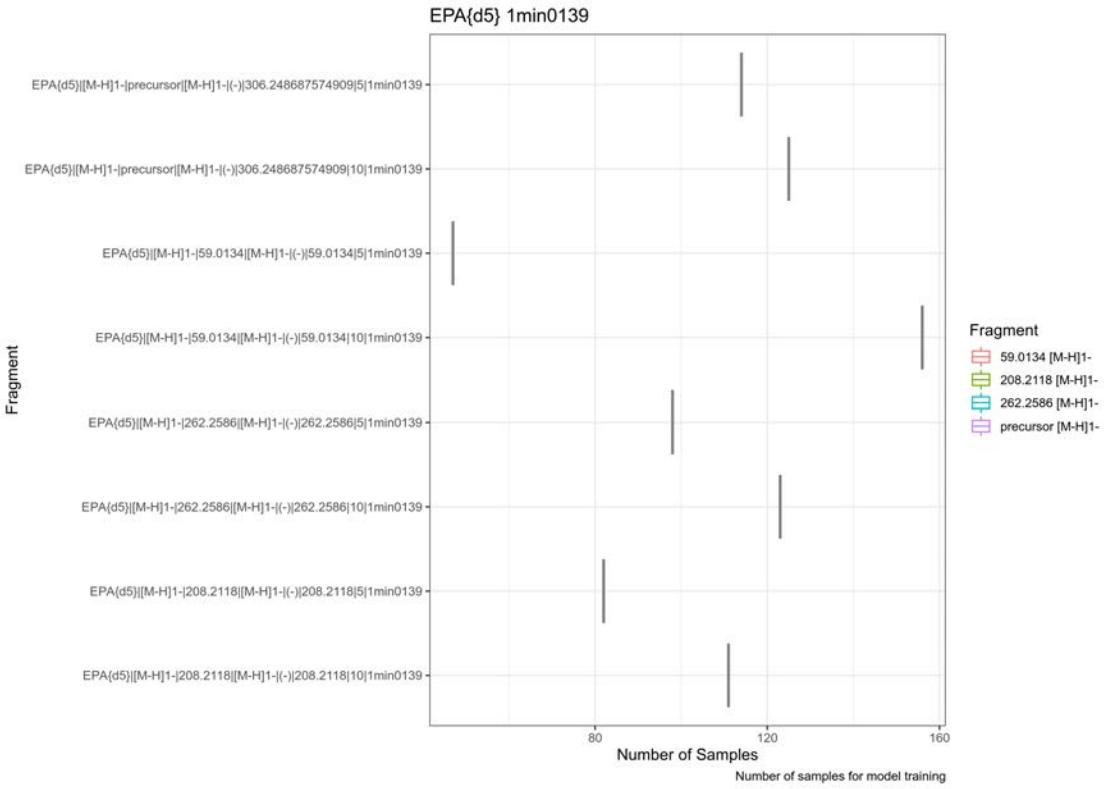


*Figure 185. Number of samples used for training per combination Id*

# 1.38. LTB4{d4} [M-H]1- 1min0145

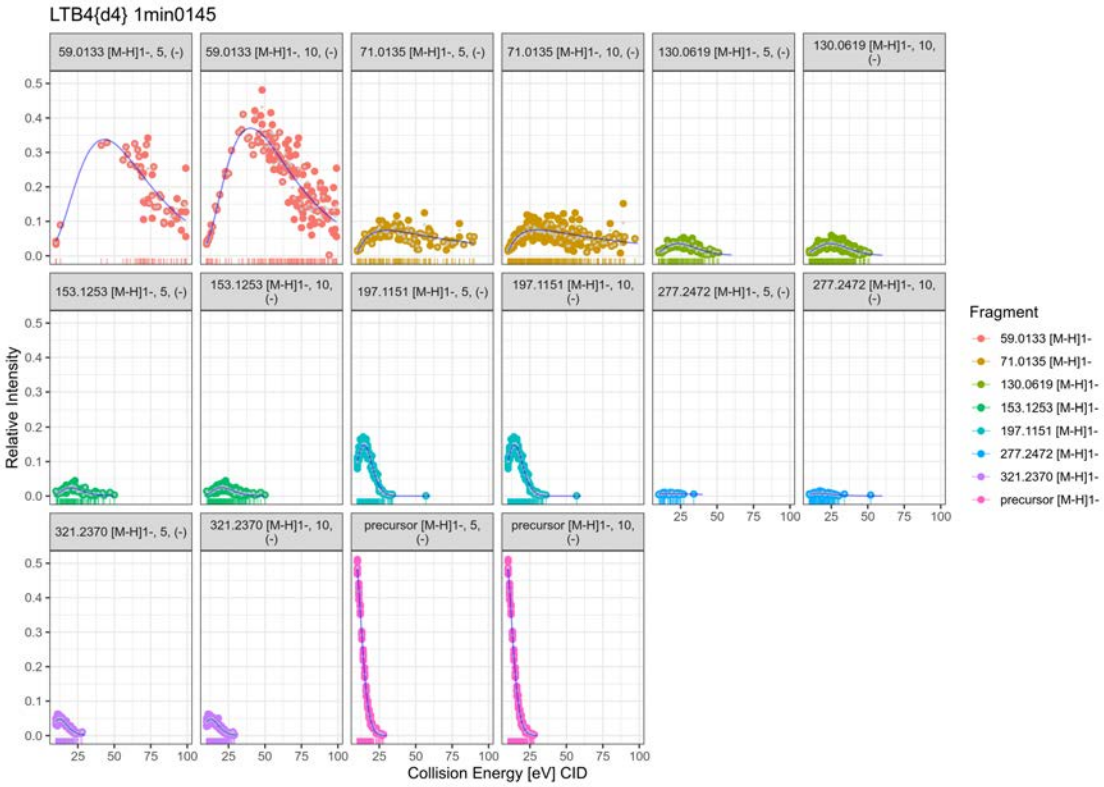


*Figure 186. Nonlinear fit*

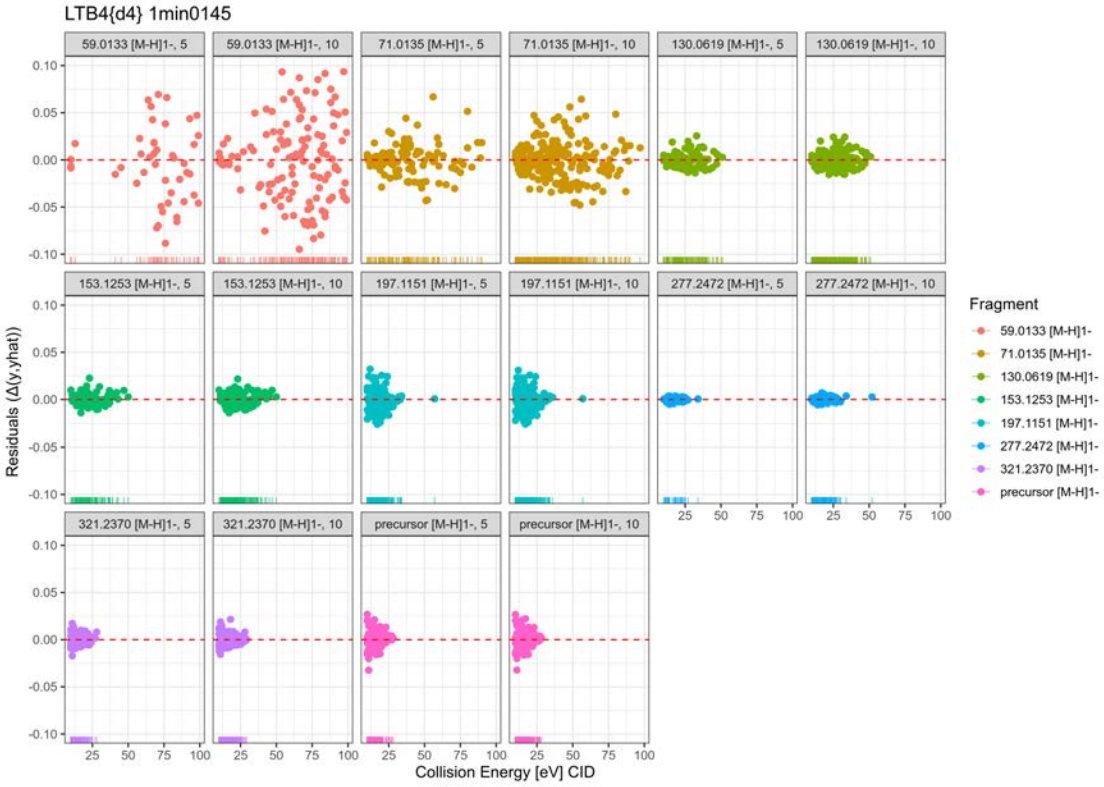


*Figure 187. Residuals of nonlinear fit*

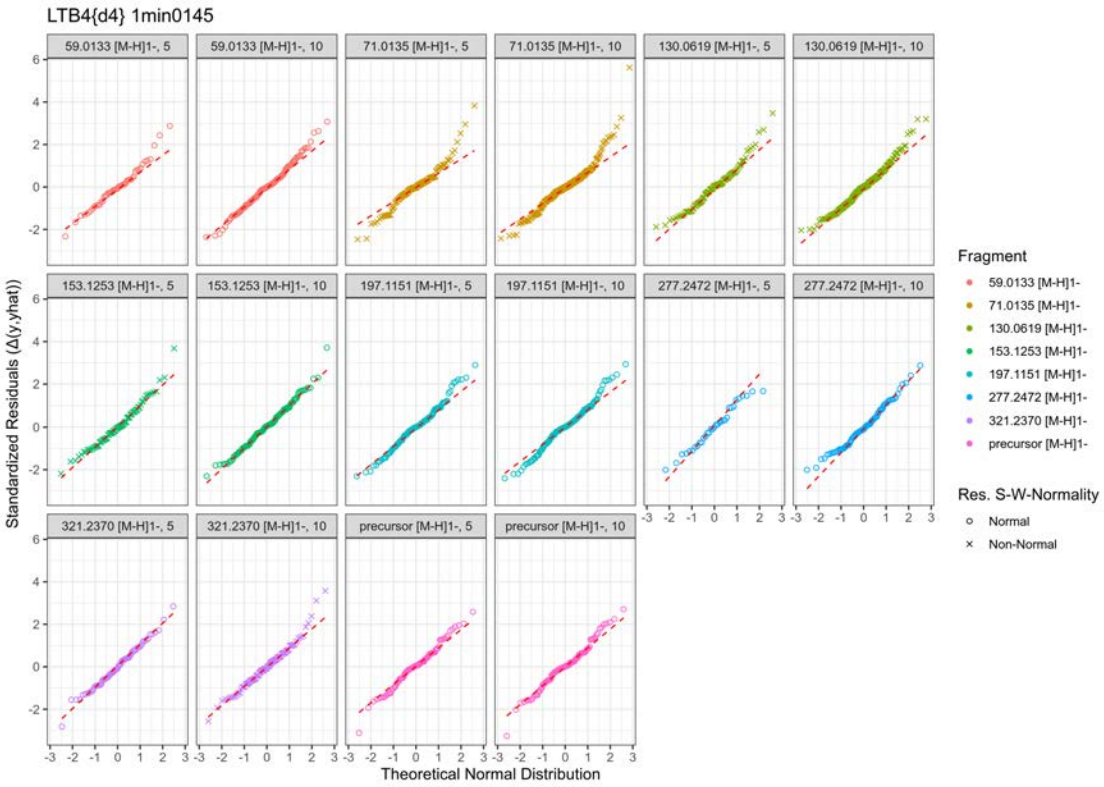


*Figure 188. Quantile-quantile plot of residuals*

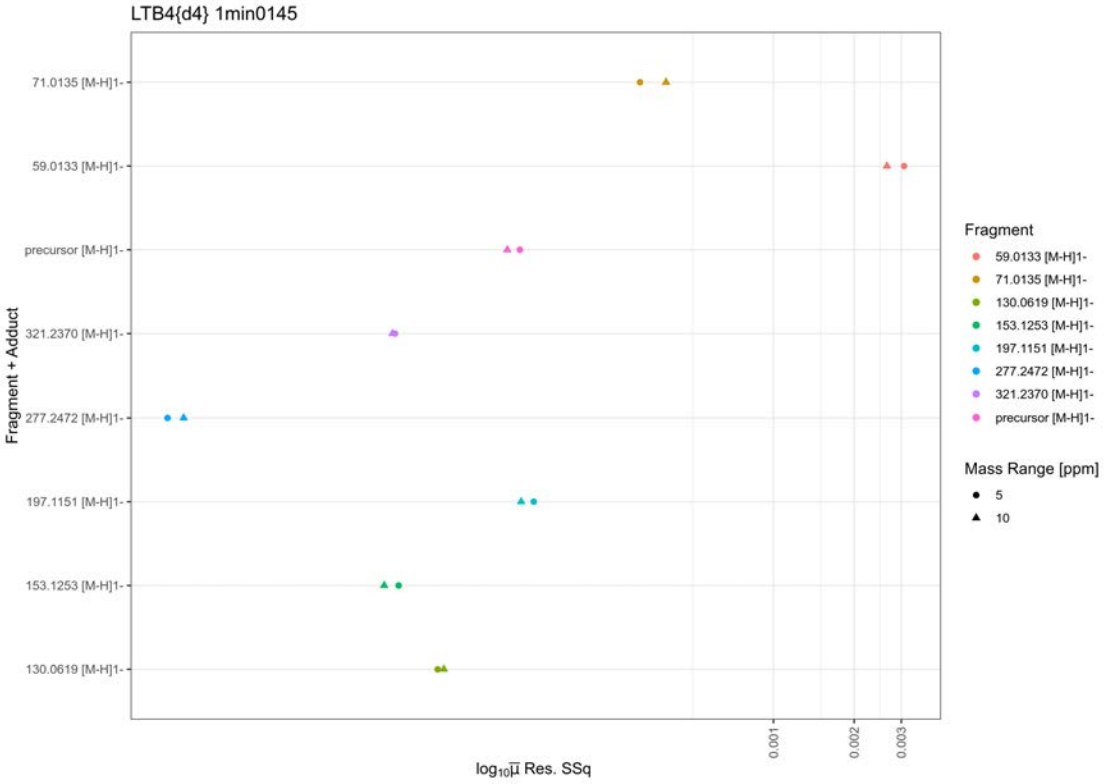


*Figure 189. Normalized sum-of-squares of the residuals*

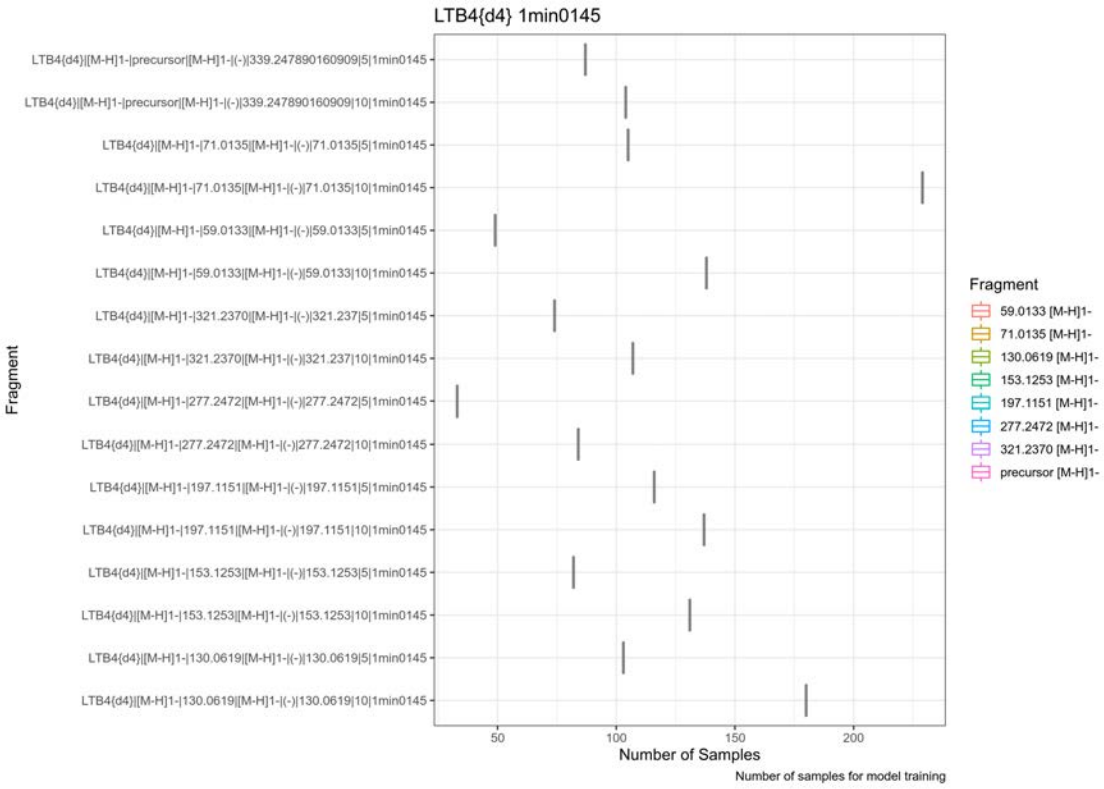


*Figure 190. Number of samples used for training per combination Id*

# 1.39. LTC4{d5} [M-H]1- 1min0232

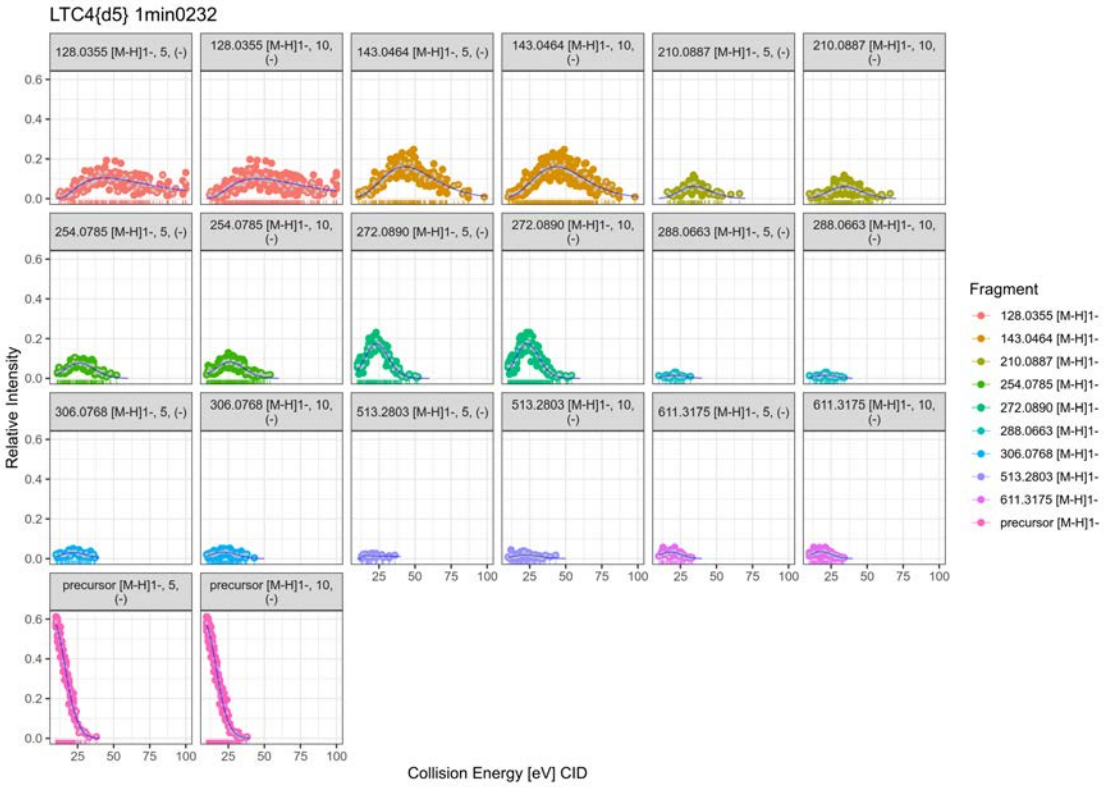


*Figure 191. Nonlinear fit*

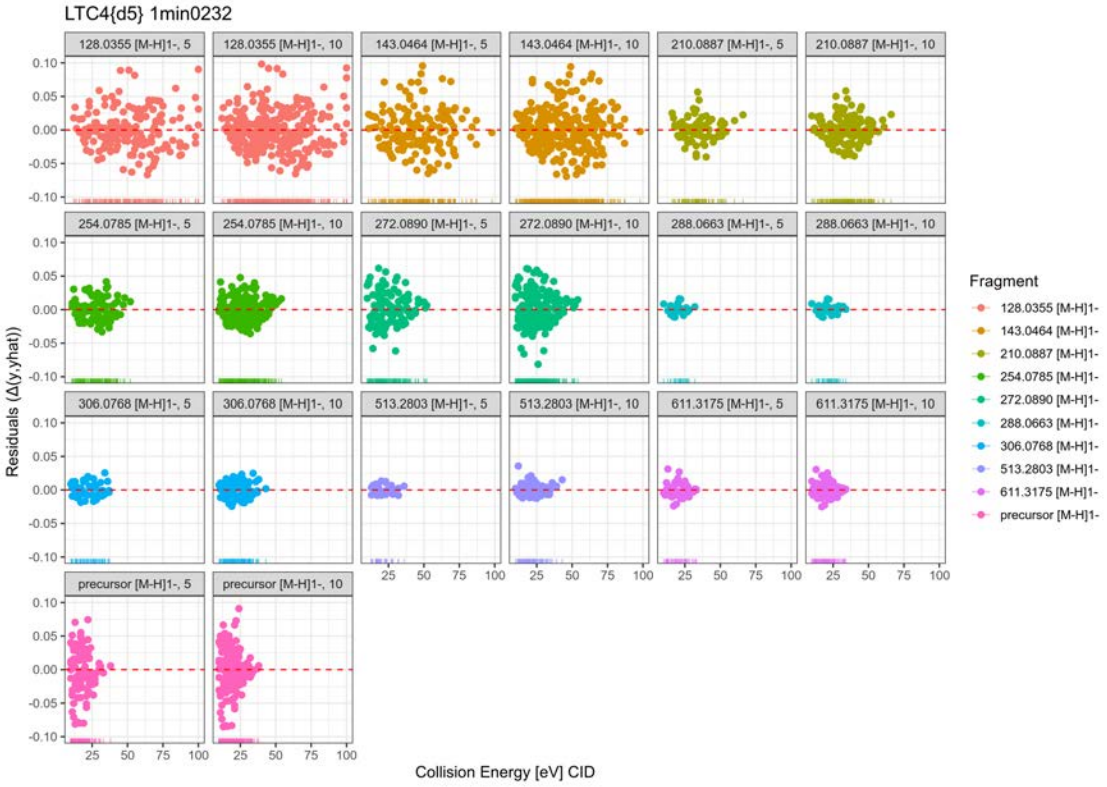


*Figure 192. Residuals of nonlinear fit*

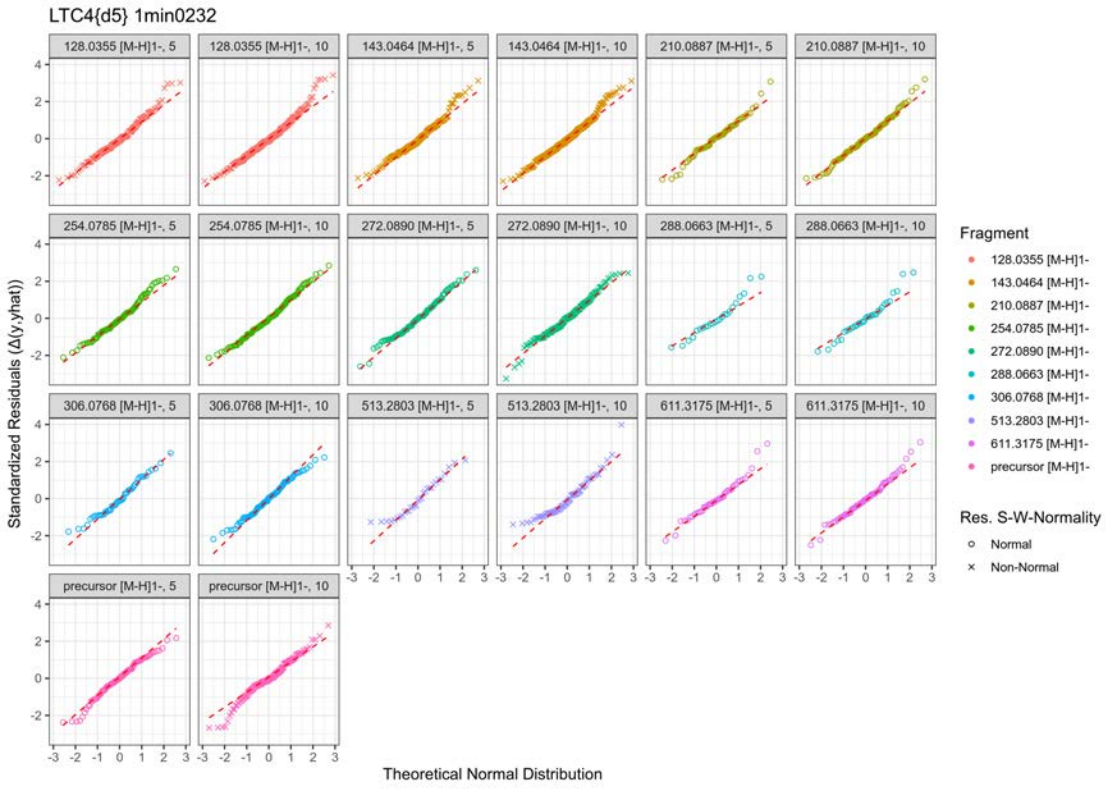


*Figure 193. Quantile-quantile plot of residuals*

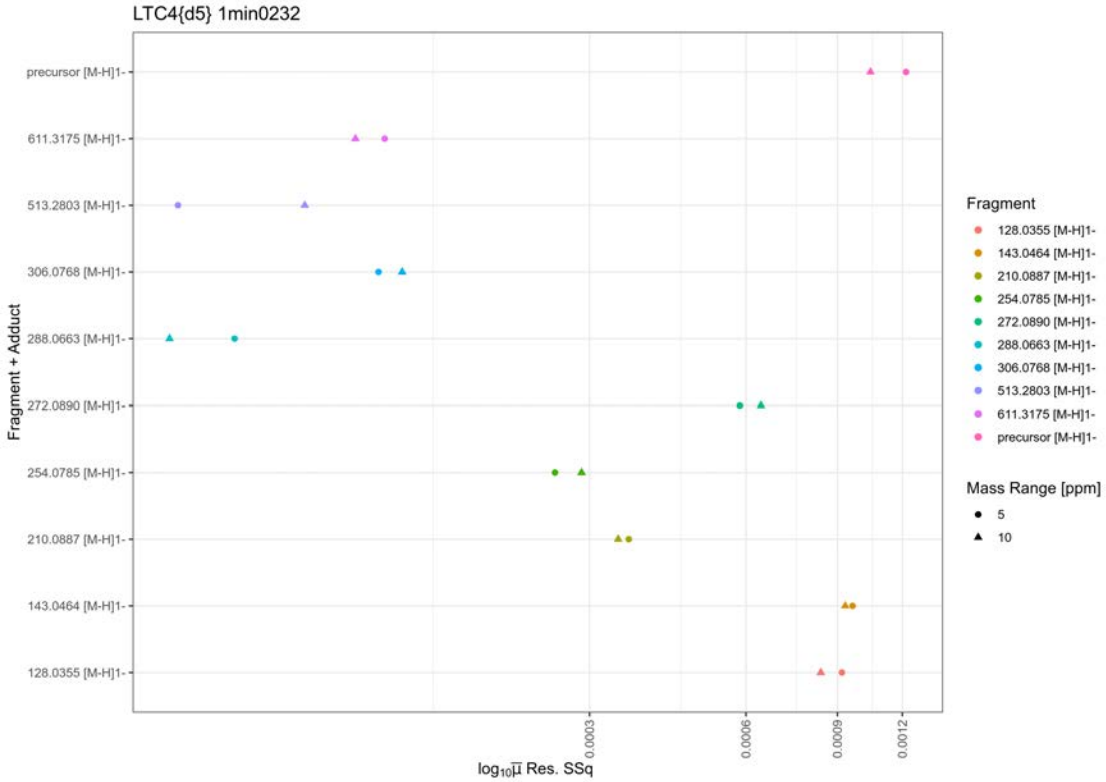


*Figure 194. Normalized sum-of-squares of the residuals*

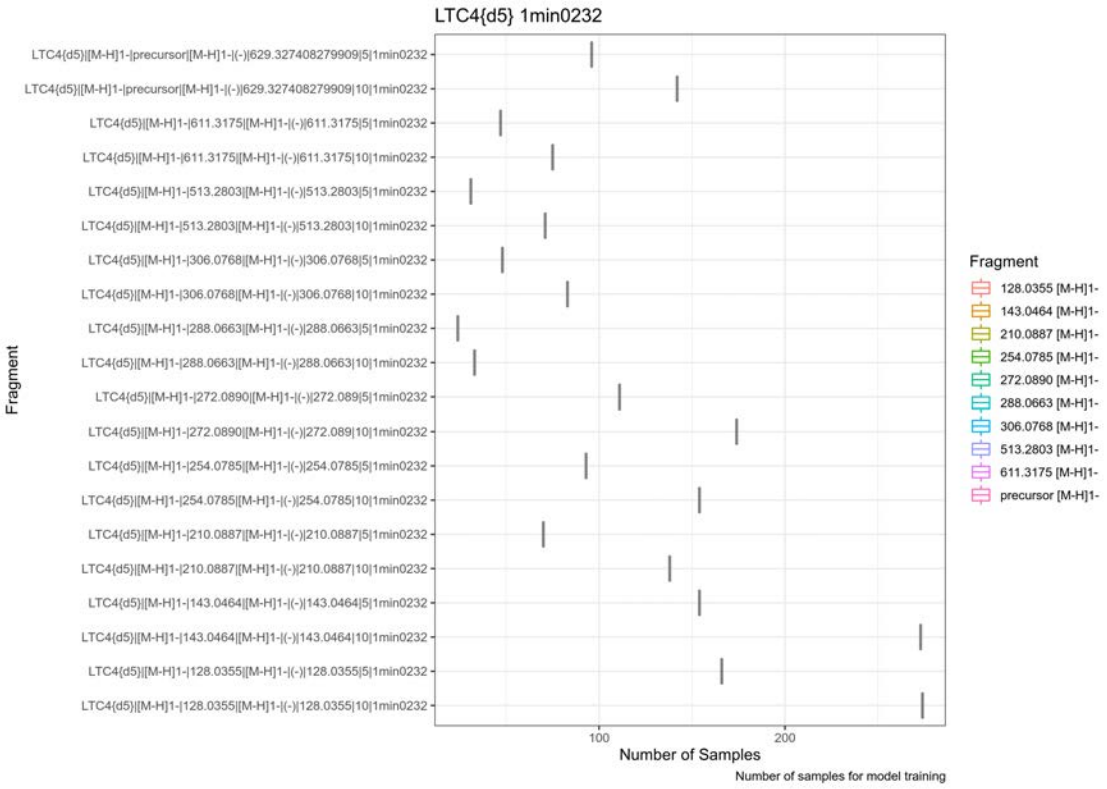


*Figure 195. Number of samples used for training per combination Id*

# 1.40. LTD4{d5} [M-H]1- 1min0222

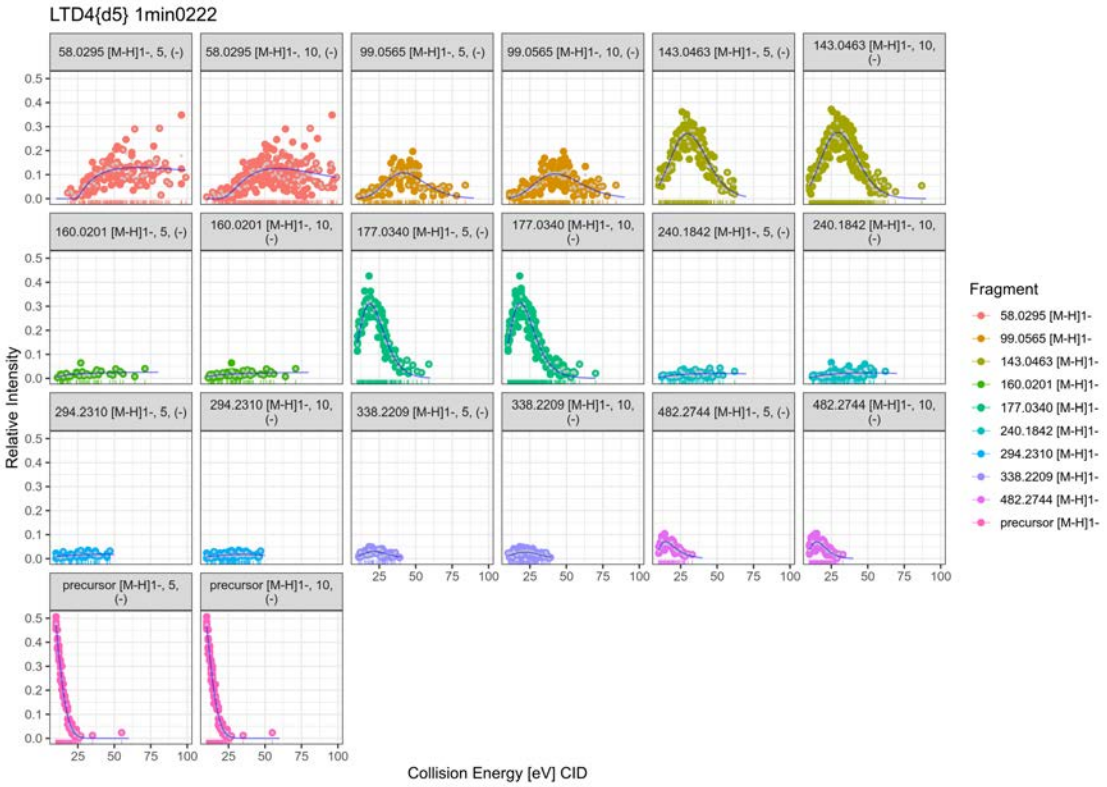


*Figure 196. Nonlinear fit*

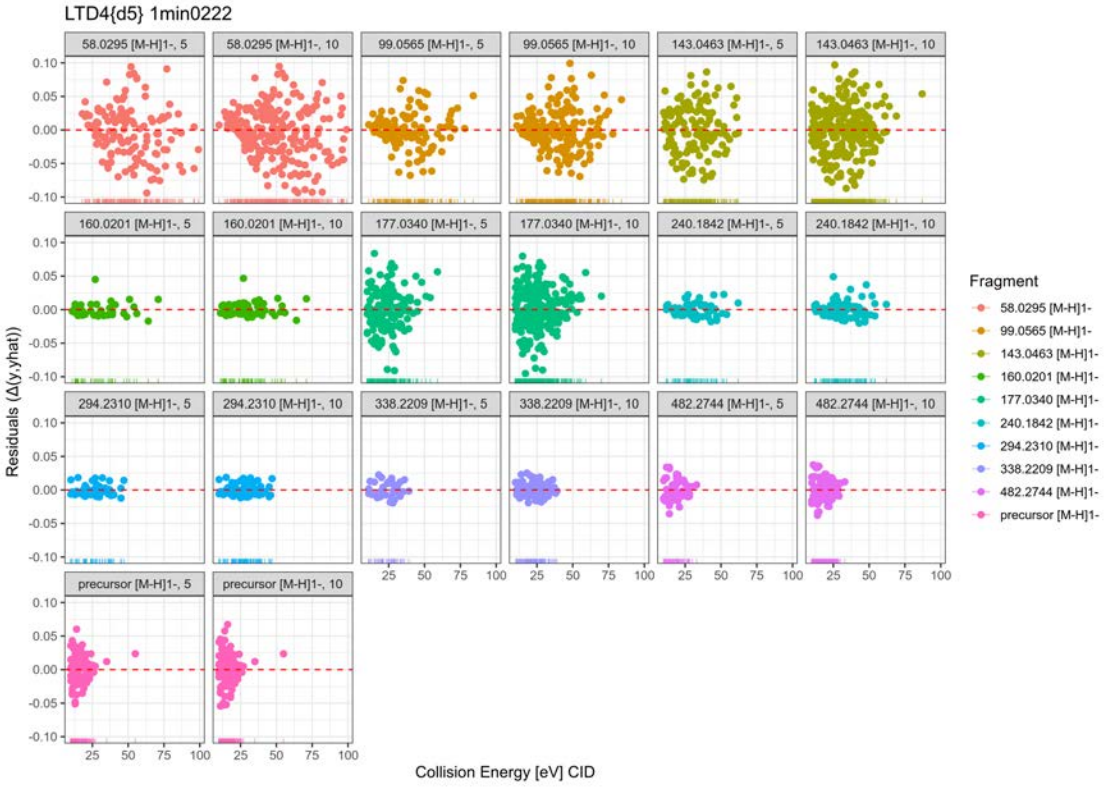


*Figure 197. Residuals of nonlinear fit*

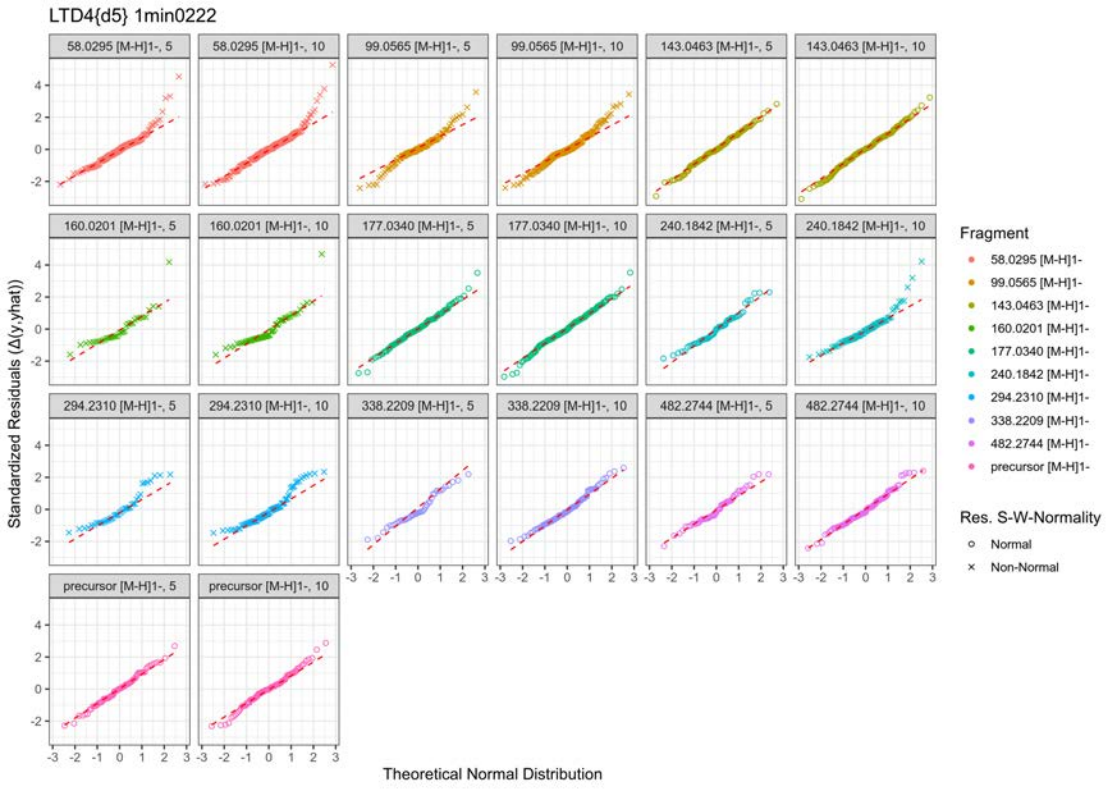


*Figure 198. Quantile-quantile plot of residuals*

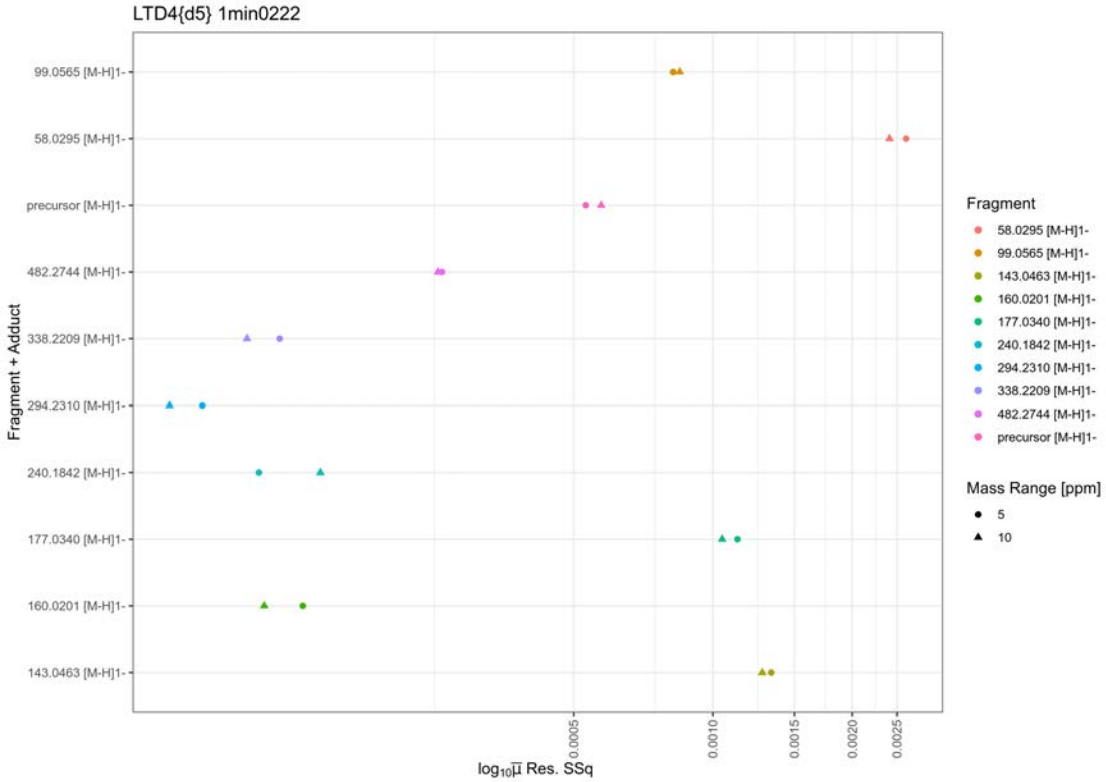


*Figure 199. Normalized sum-of-squares of the residuals*

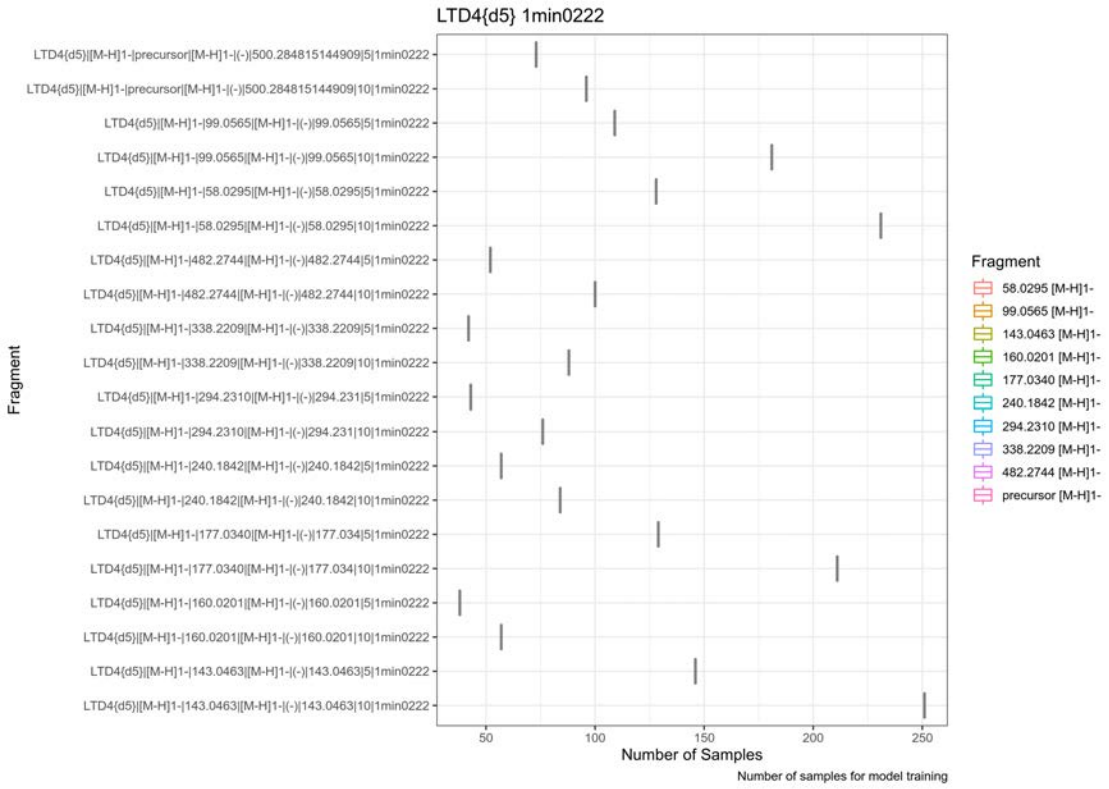


*Figure 200. Number of samples used for training per combination Id*

# 1.41. PGB2{d4} [M-H]1- 1min0220

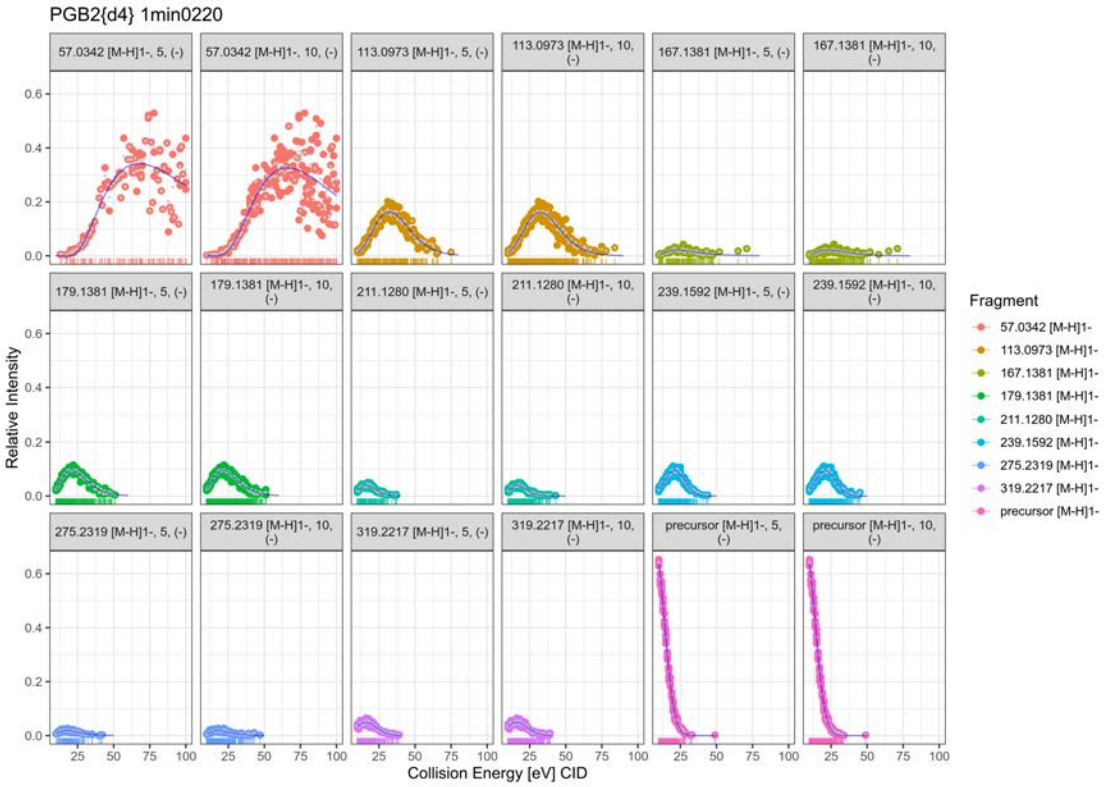


*Figure 201. Nonlinear fit*


*Figure 202. Residuals of nonlinear fit*

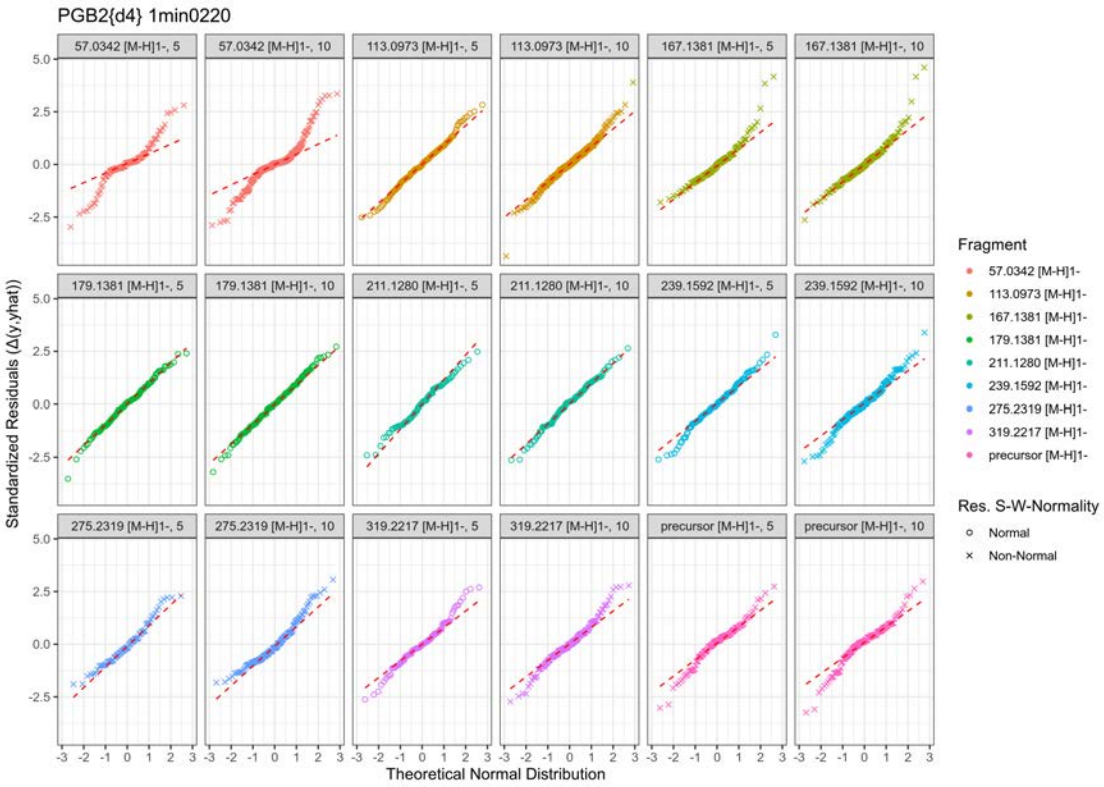


*Figure 203. Quantile-quantile plot of residuals*

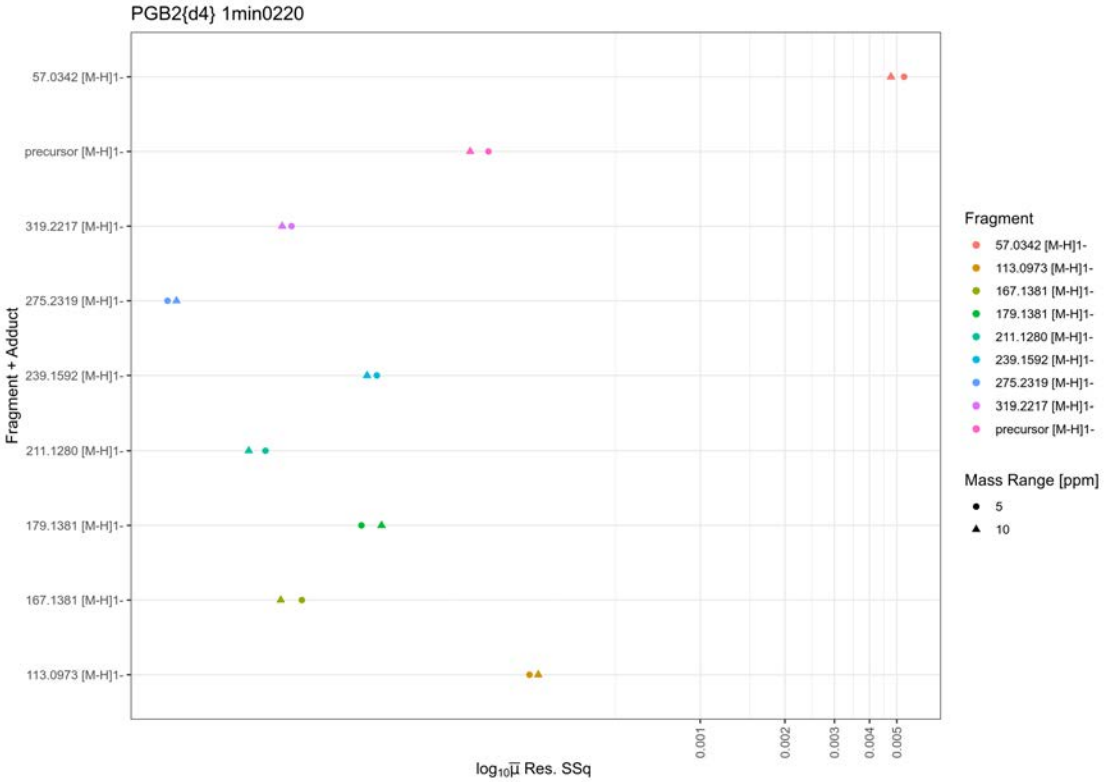


*Figure 204. Normalized sum-of-squares of the residuals*

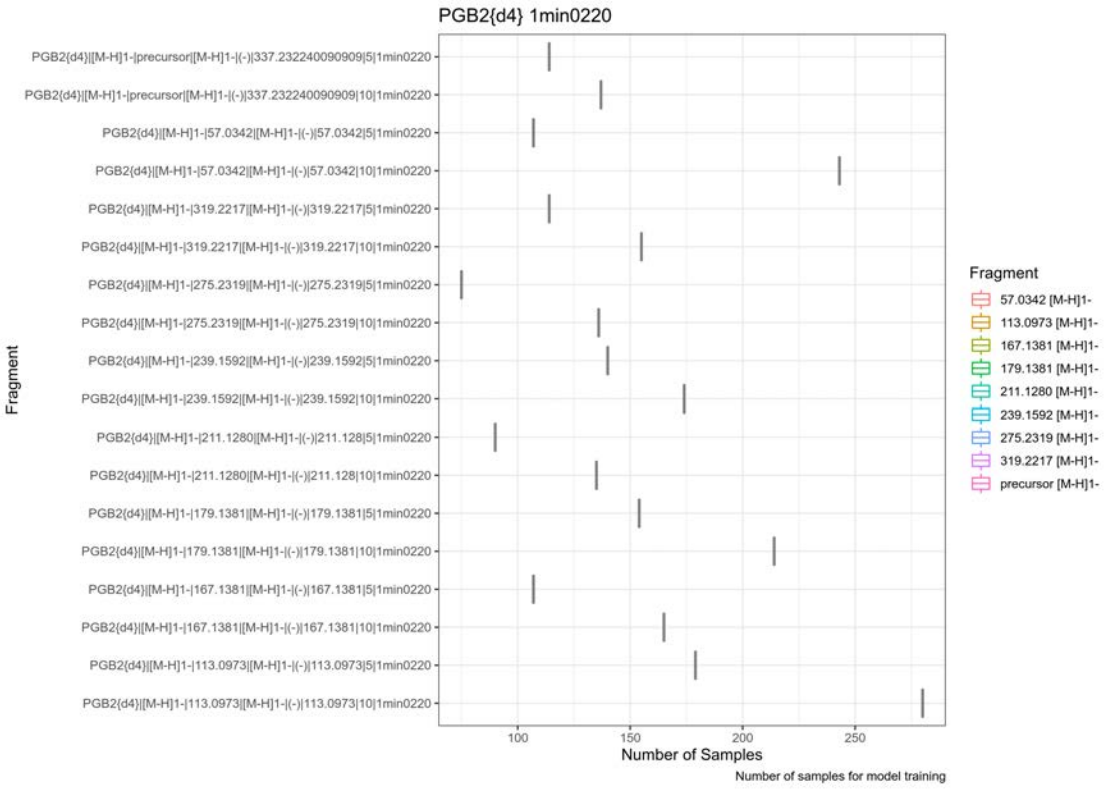


*Figure 205. Number of samples used for training per combination Id*

# 1.42. PGD2{d4} [M-H]1- 1min0151

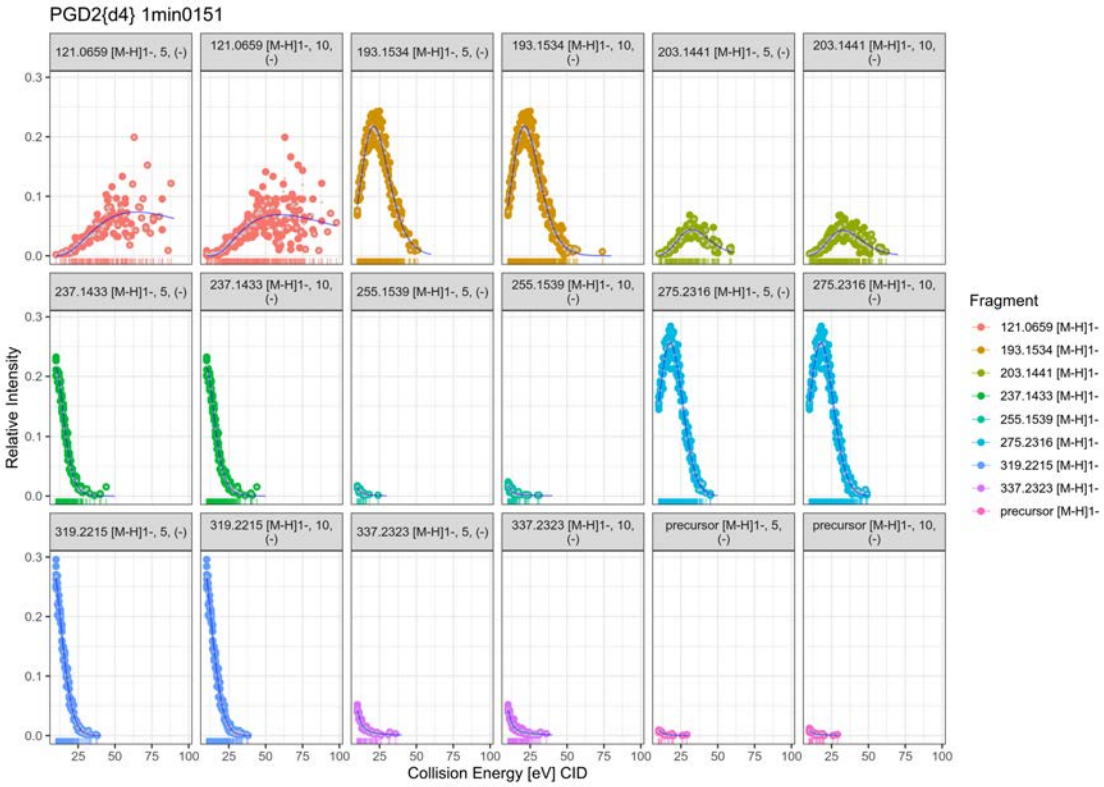


*Figure 206. Nonlinear fit*

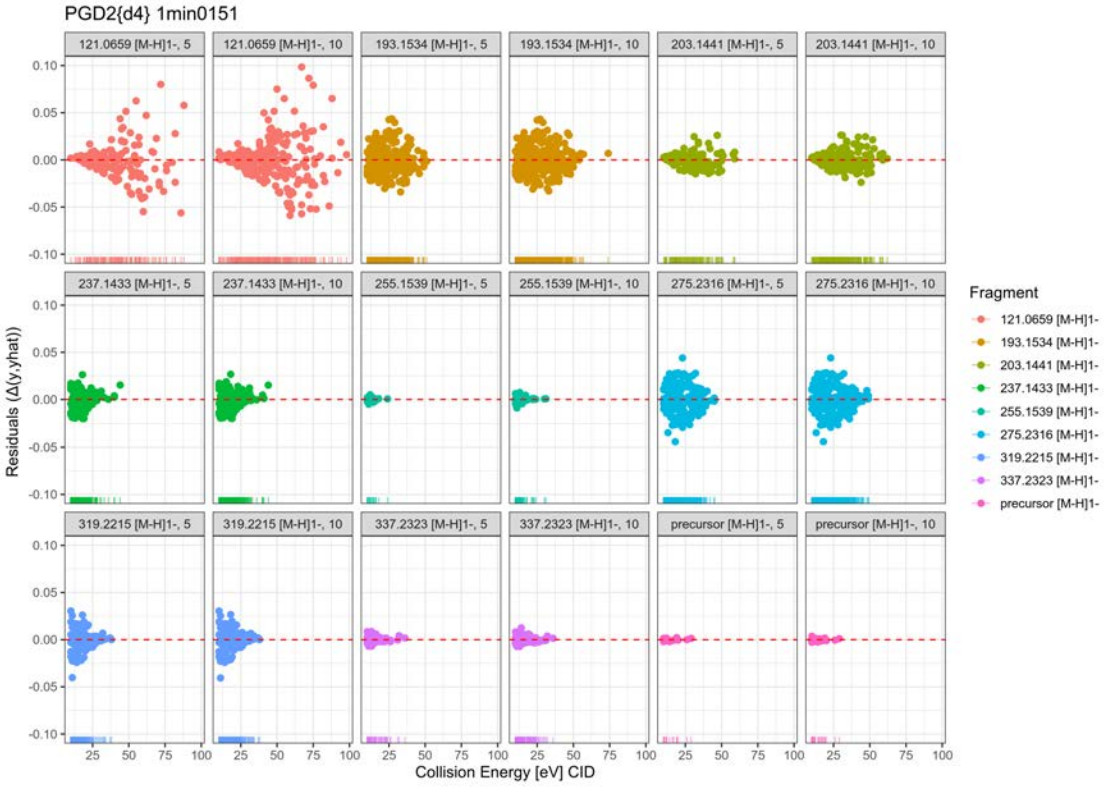


*Figure 207. Residuals of nonlinear fit*

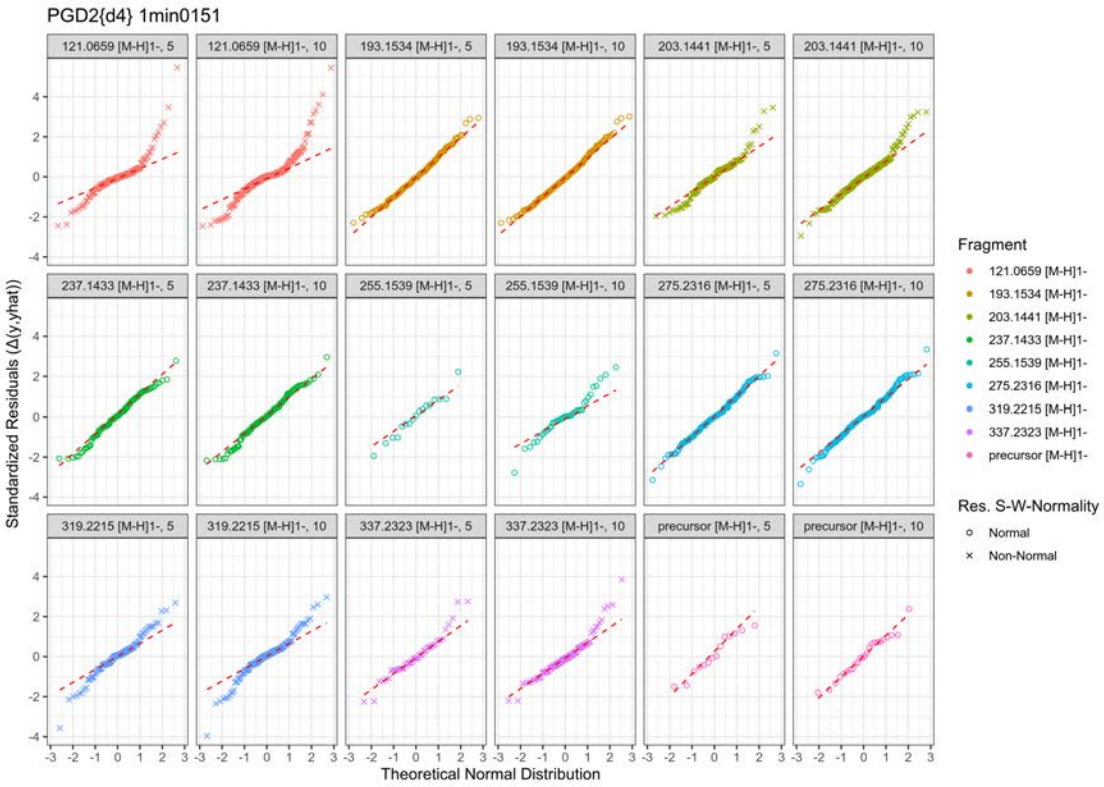


*Figure 208. Quantile-quantile plot of residuals*

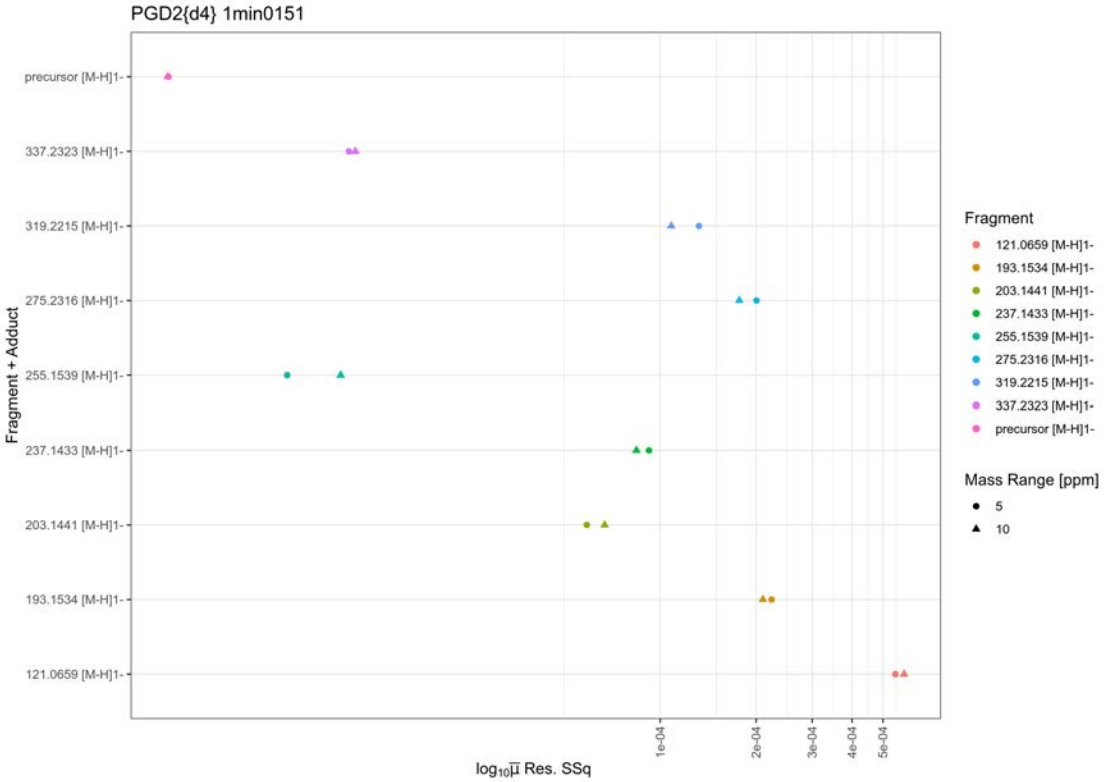


*Figure 209. Normalized sum-of-squares of the residuals*

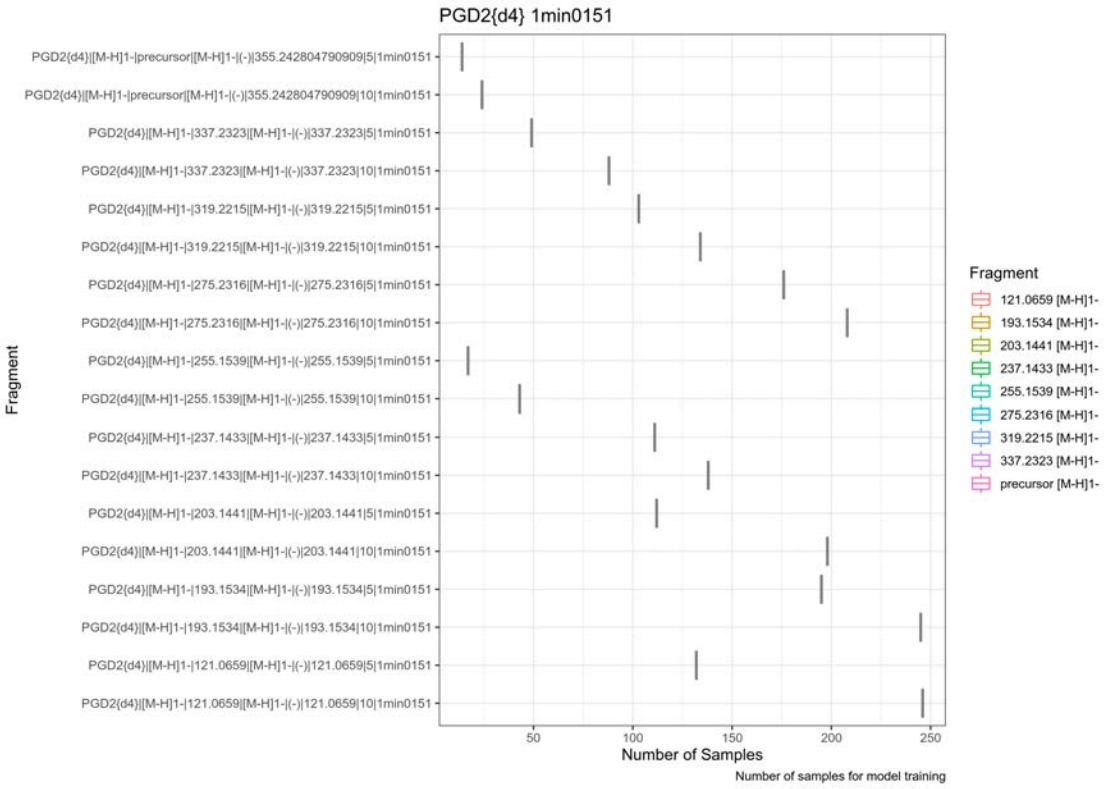


*Figure 210. Number of samples used for training per combination Id*

# 1.43. PGE2{d4} [M-H]1- 1min0241

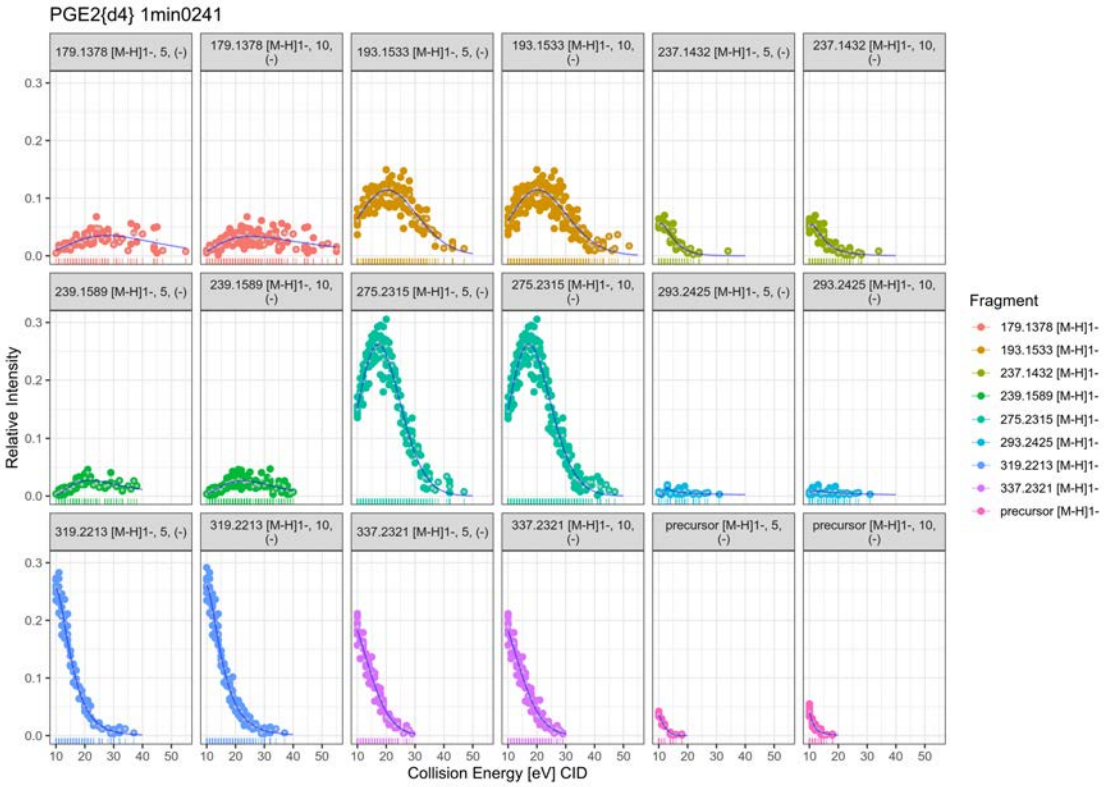


*Figure 211. Nonlinear fit*

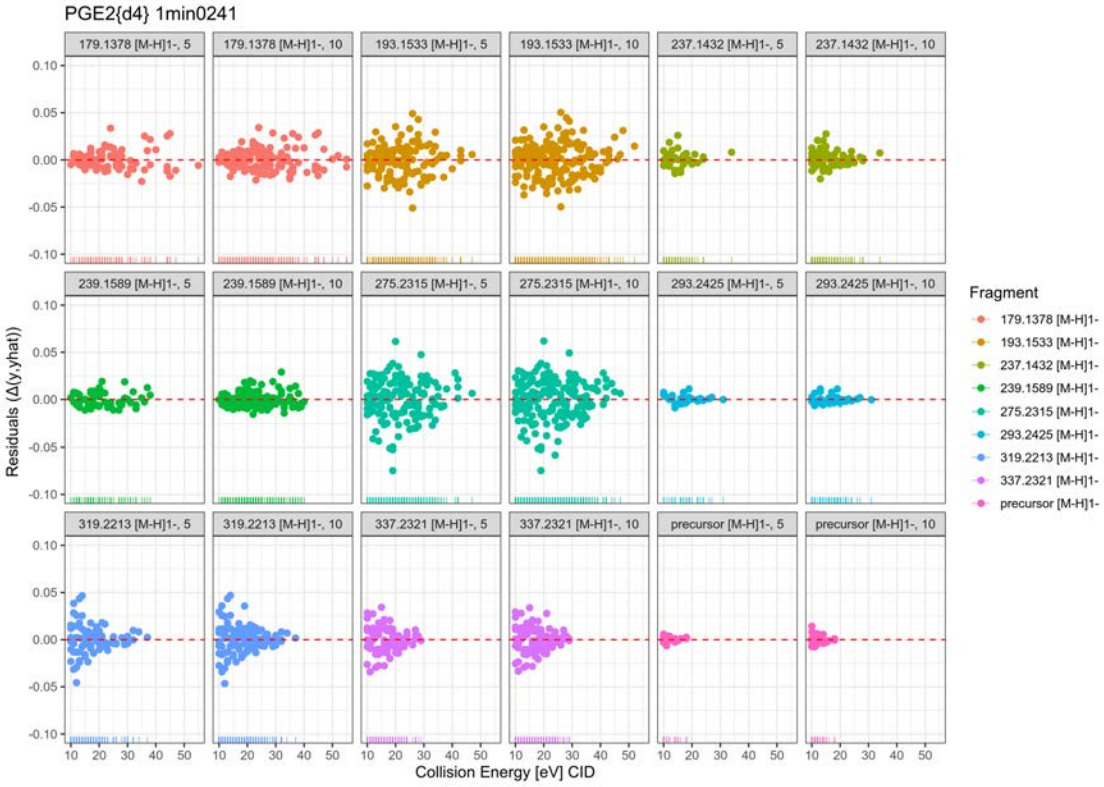


*Figure 212. Residuals of nonlinear fit*

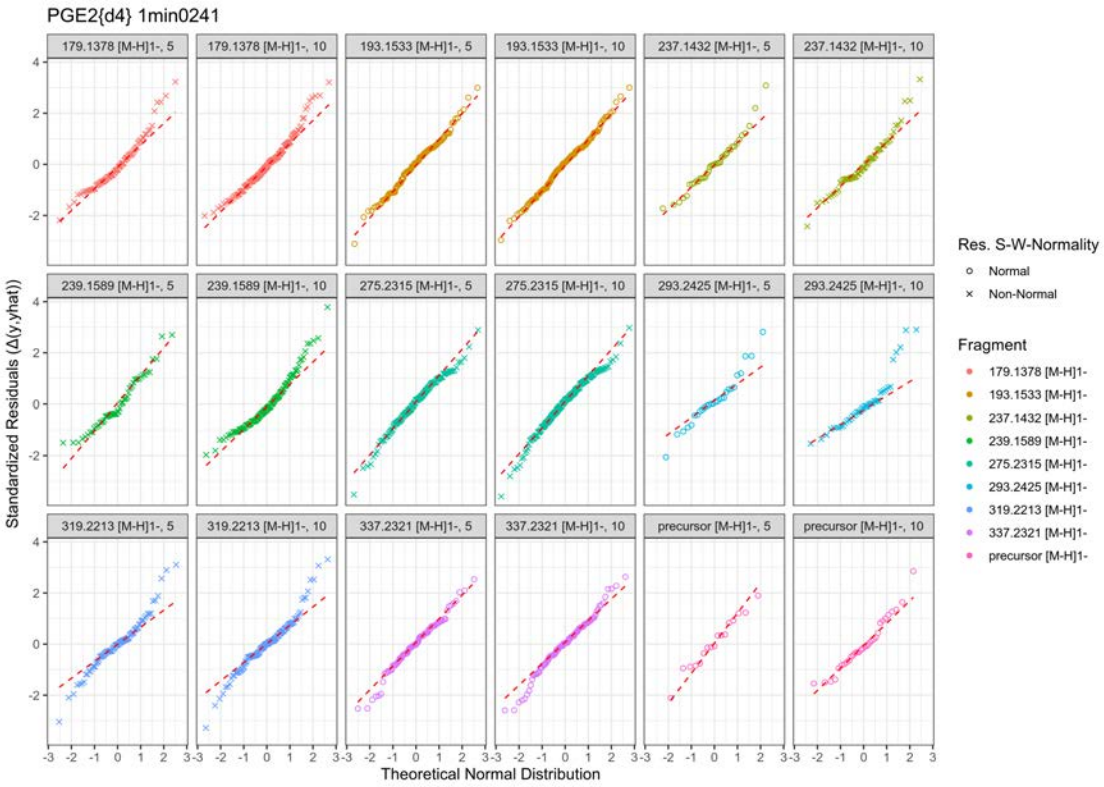


*Figure 213. Quantile-quantile plot of residuals*

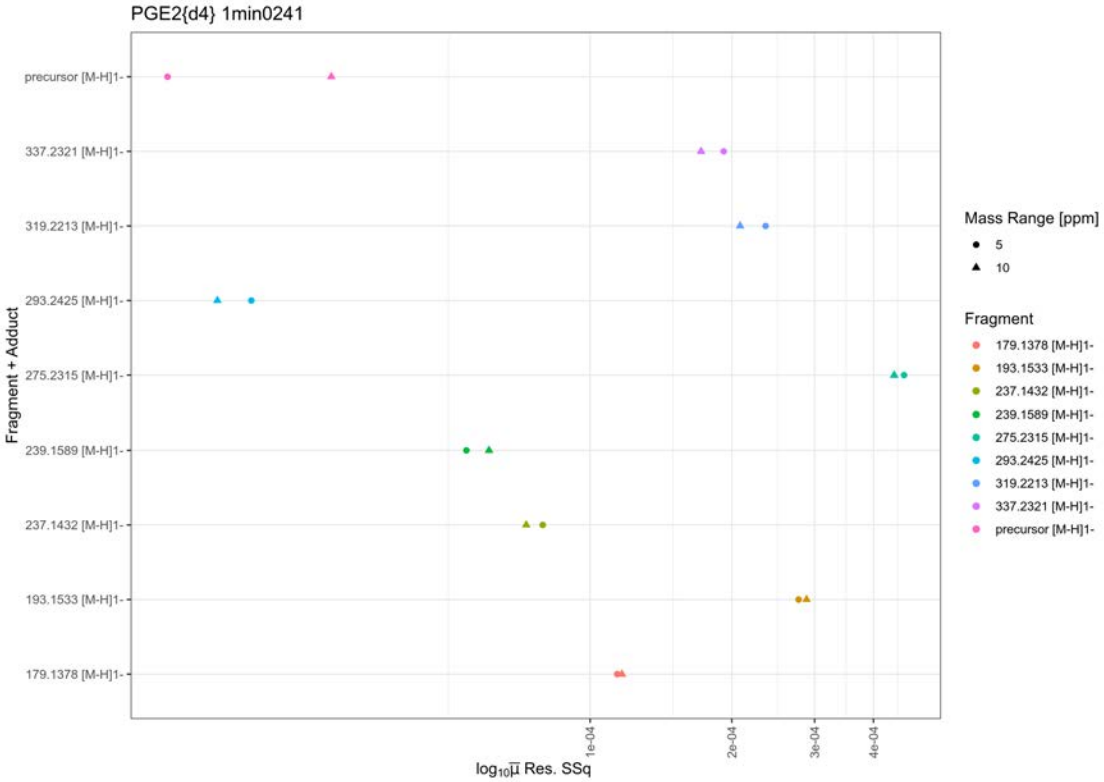


*Figure 214. Normalized sum-of-squares of the residuals*

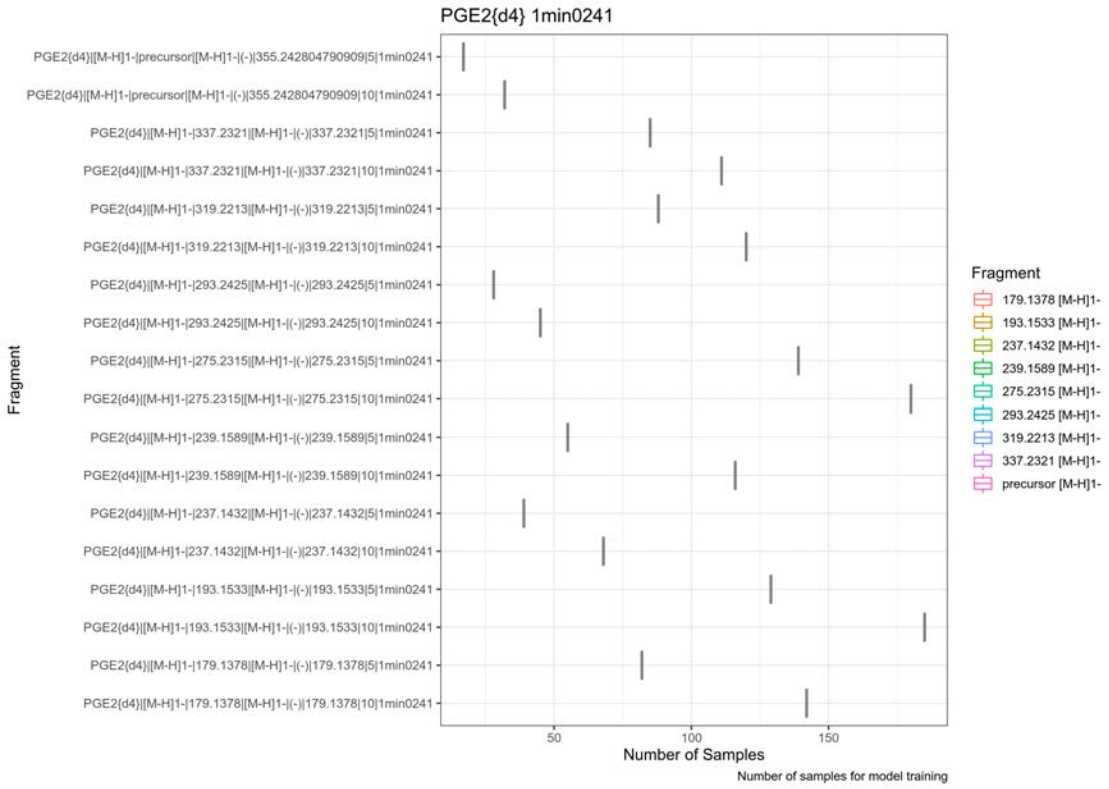


*Figure 215. Number of samples used for training per combination Id*

# 1.44. PGE2{d9} [M-H]1- 1min0164

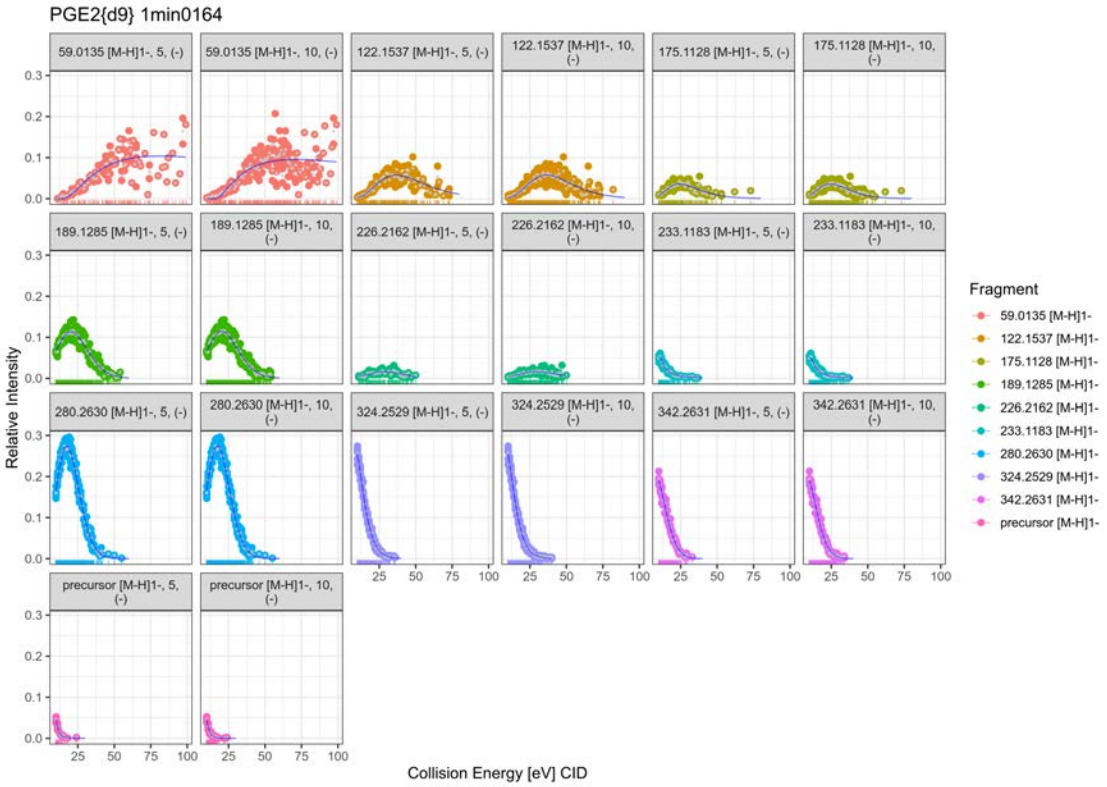


*Figure 216. Nonlinear fit*

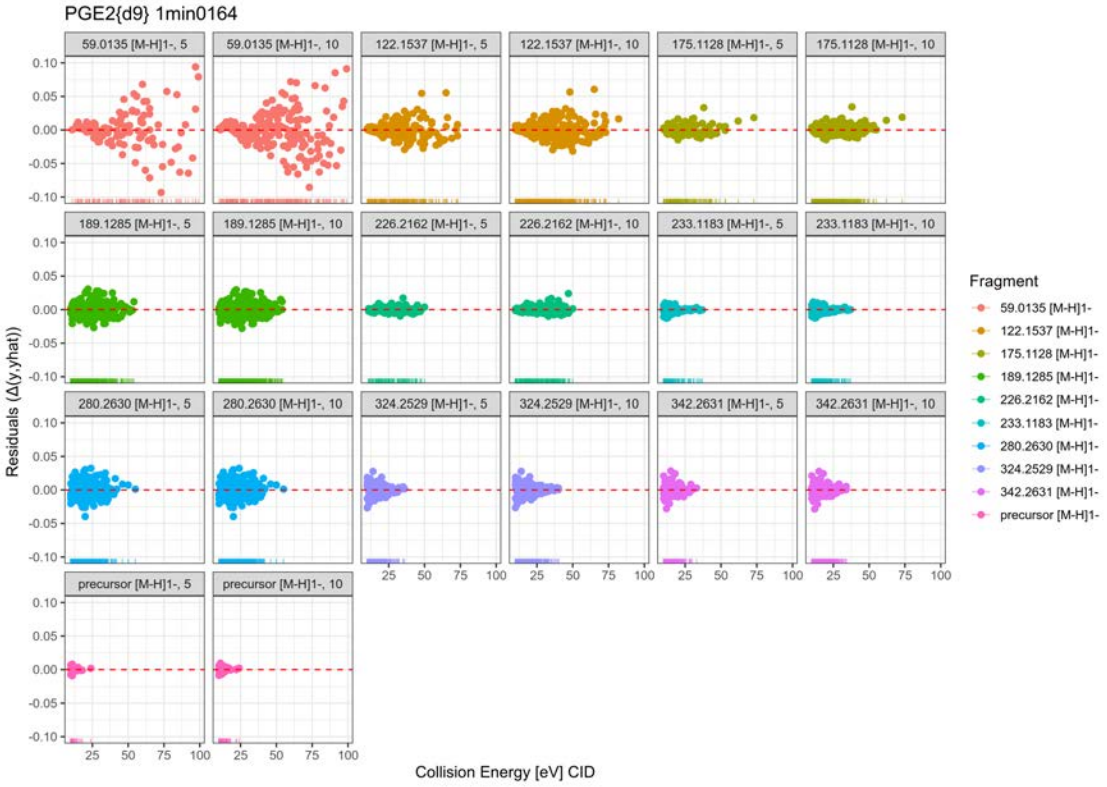


*Figure 217. Residuals of nonlinear fit*

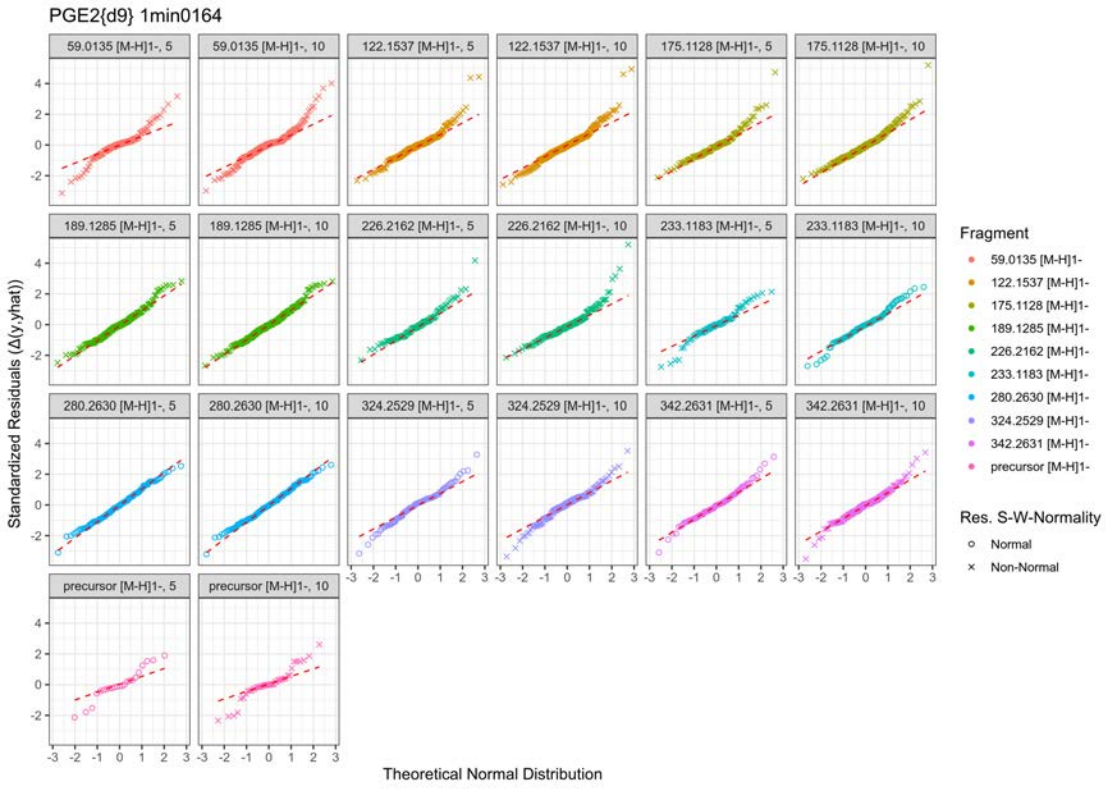


*Figure 218. Quantile-quantile plot of residuals*

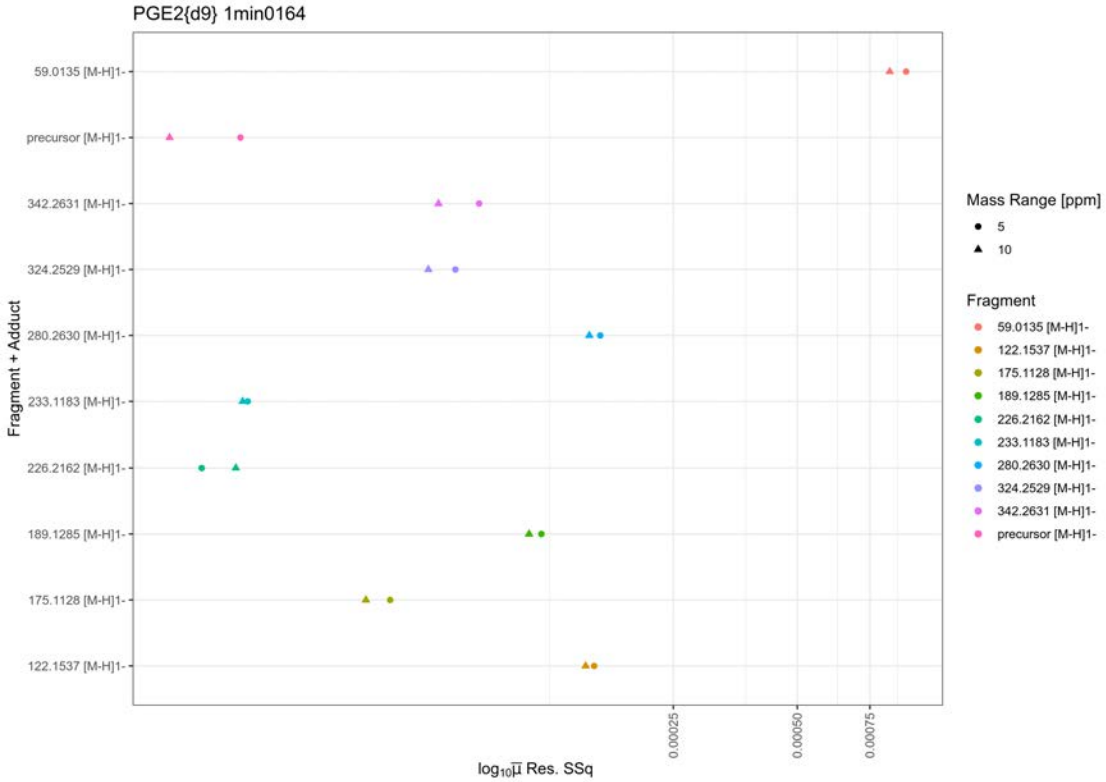


*Figure 219. Normalized sum-of-squares of the residuals*

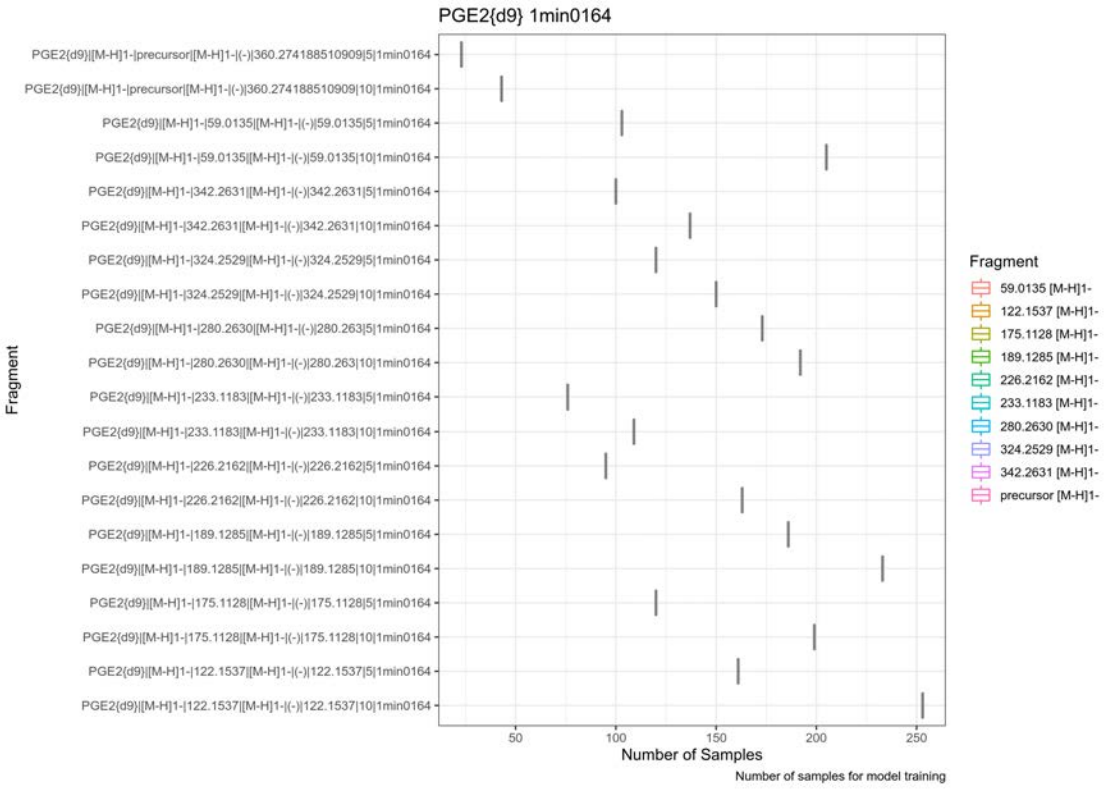


*Figure 220. Number of samples used for training per combination Id*

# 1.45. PGF2alpha{d4} [M-H]1- 1min0194

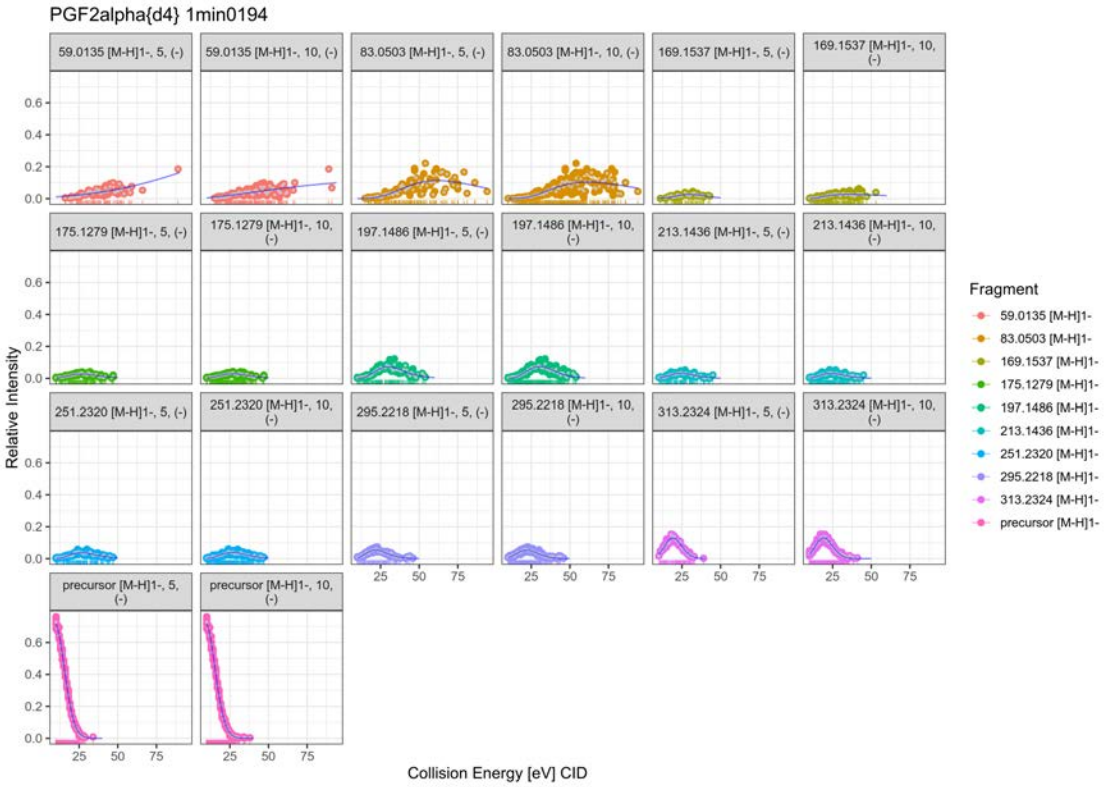


*Figure 221. Nonlinear fit*

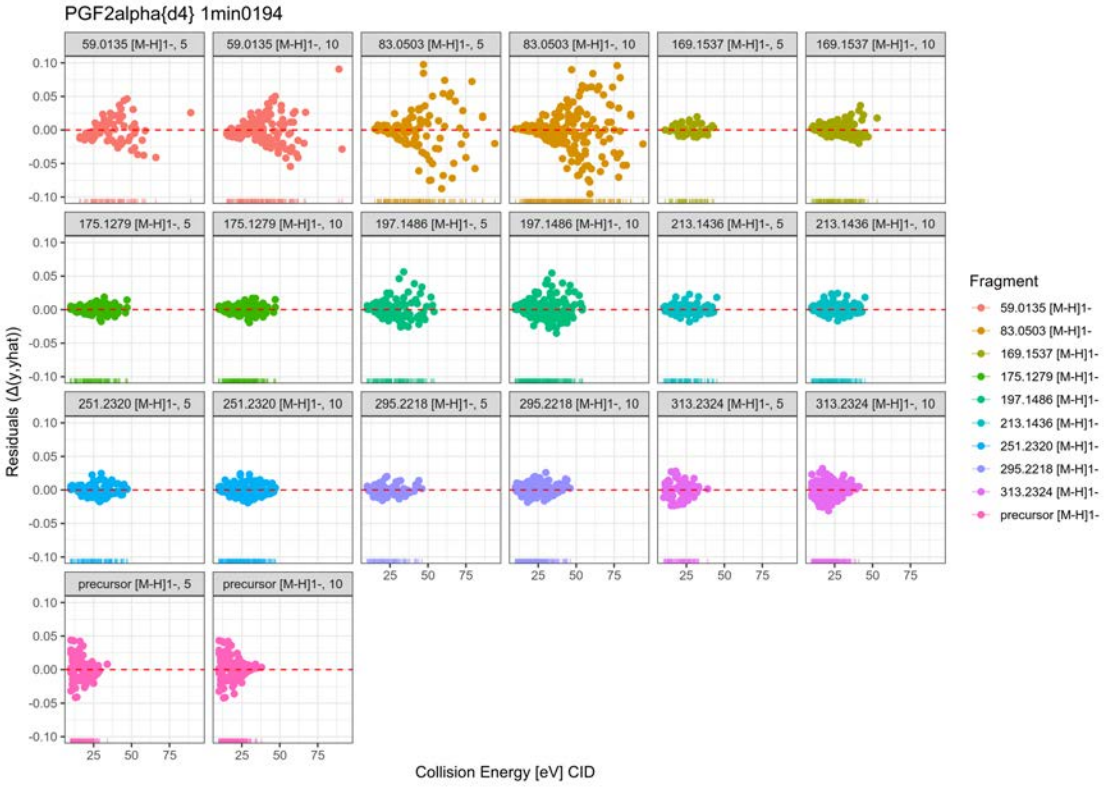


*Figure 222. Residuals of nonlinear fit*

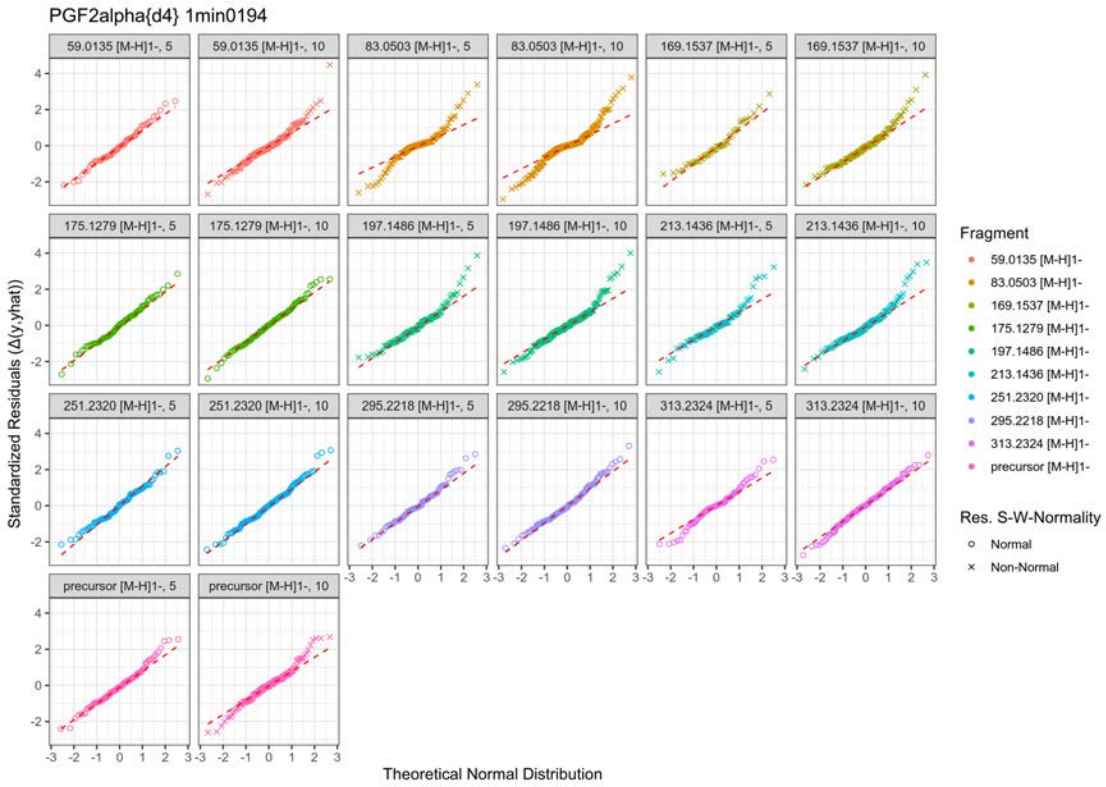


*Figure 223. Quantile-quantile plot of residuals*

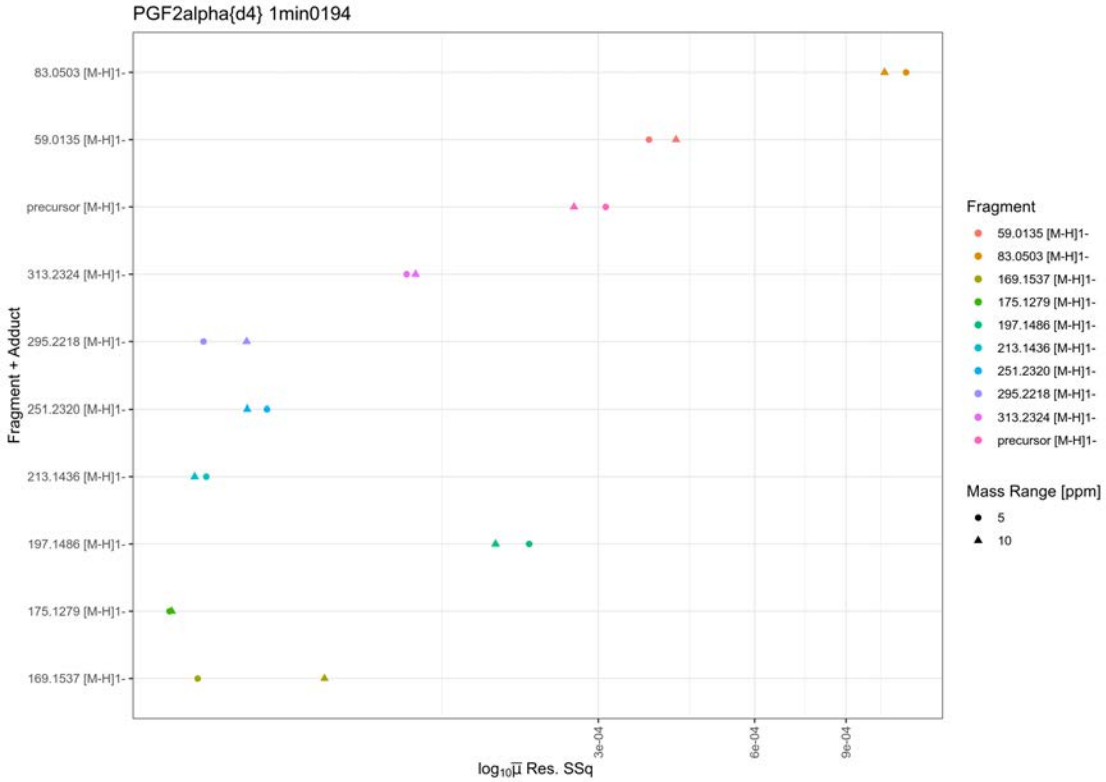


*Figure 224. Normalized sum-of-squares of the residuals*

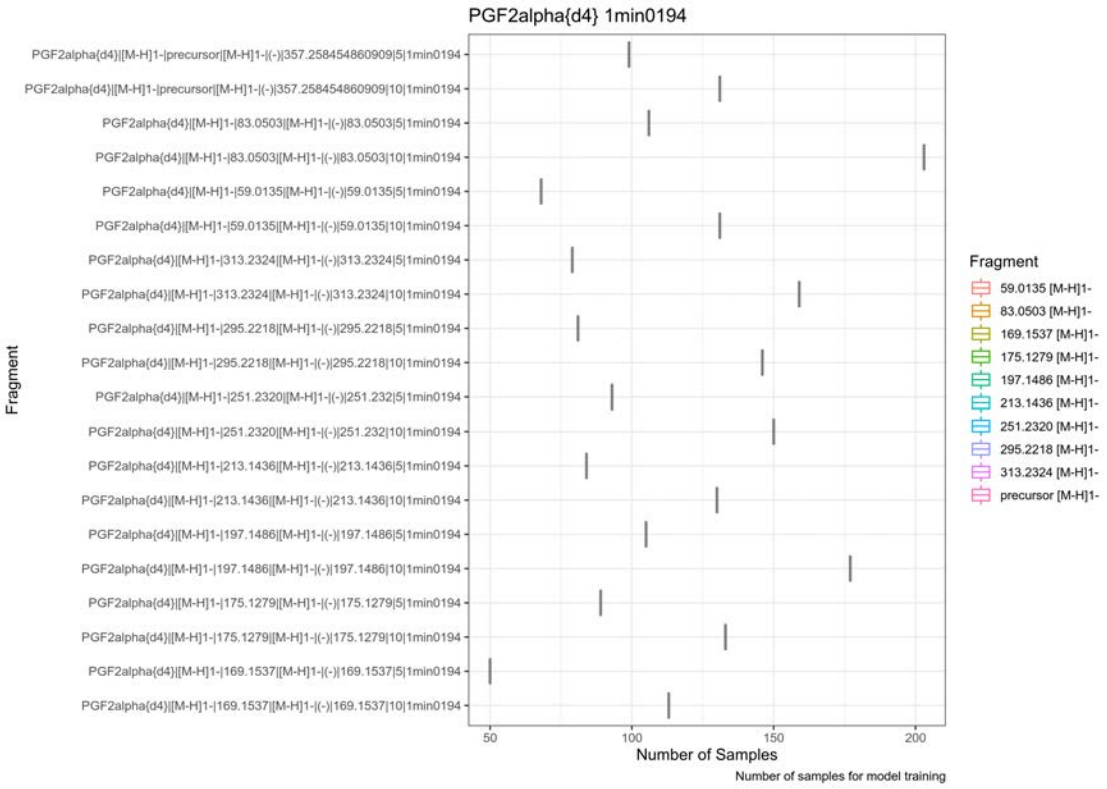


*Figure 225. Number of samples used for training per combination Id*

# 1.46. PGI2 [M-H]1- 1min0196

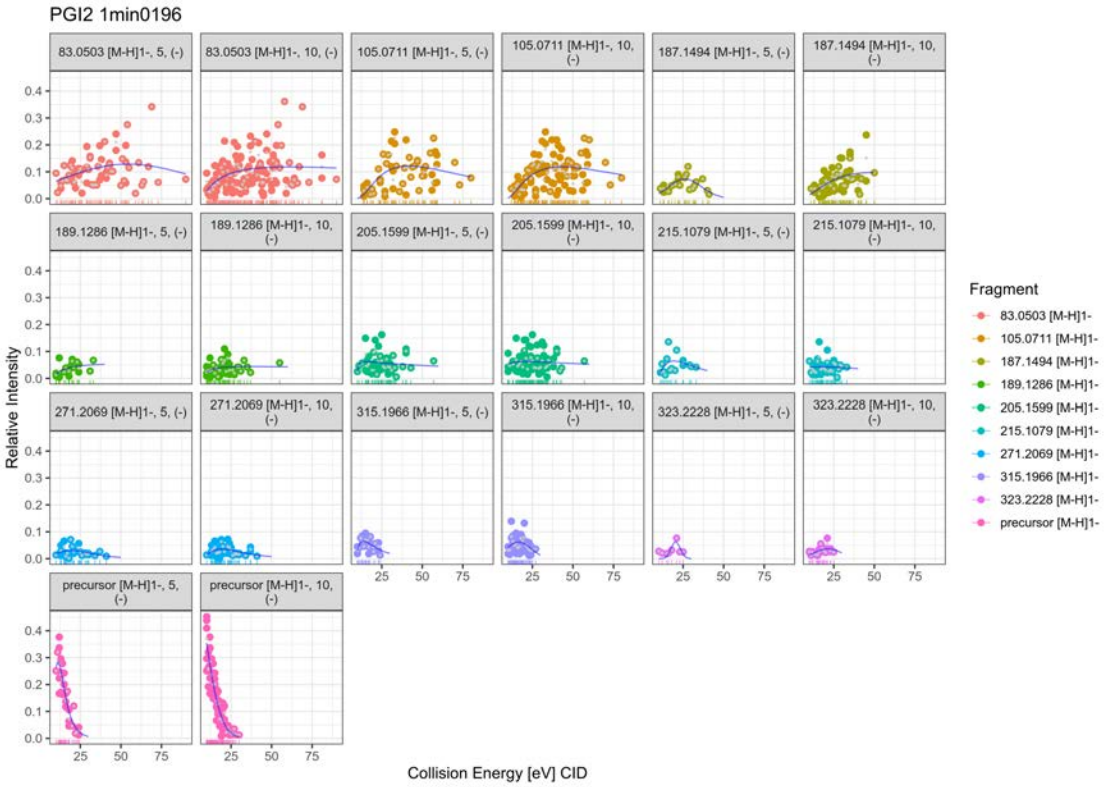


*Figure 226. Nonlinear fit*

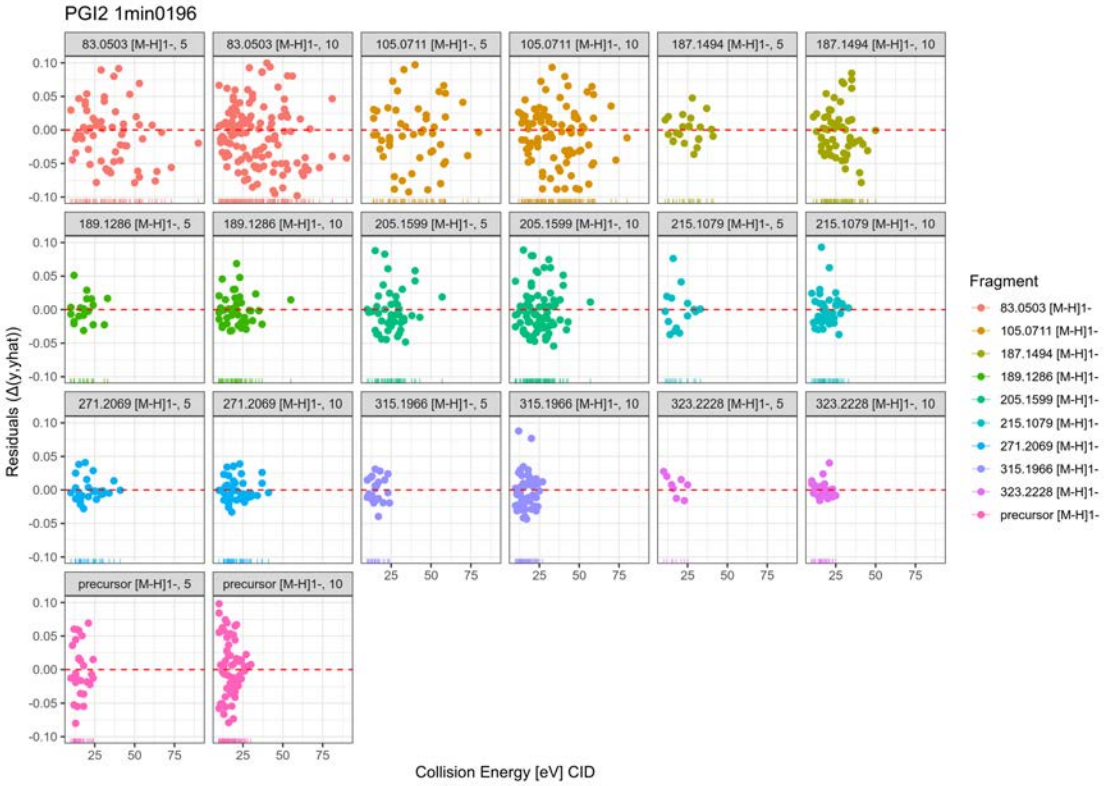


*Figure 227. Residuals of nonlinear fit*

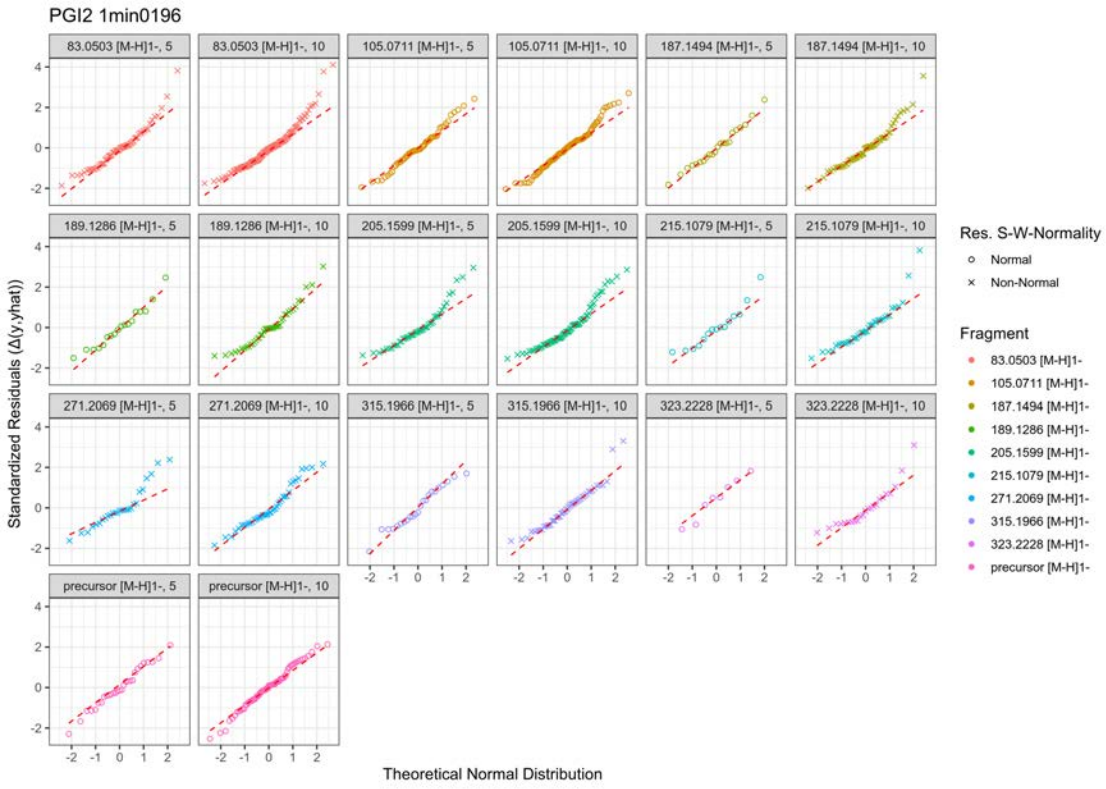


*Figure 228. Quantile-quantile plot of residuals*

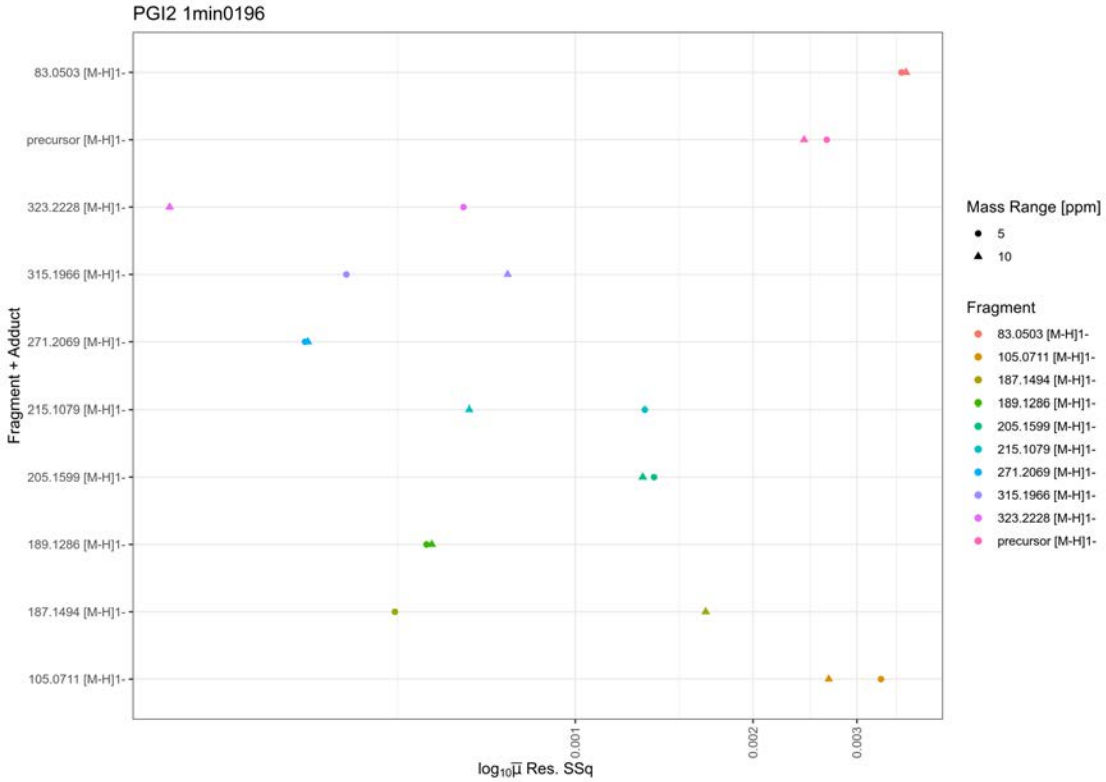


*Figure 229. Normalized sum-of-squares of the residuals*

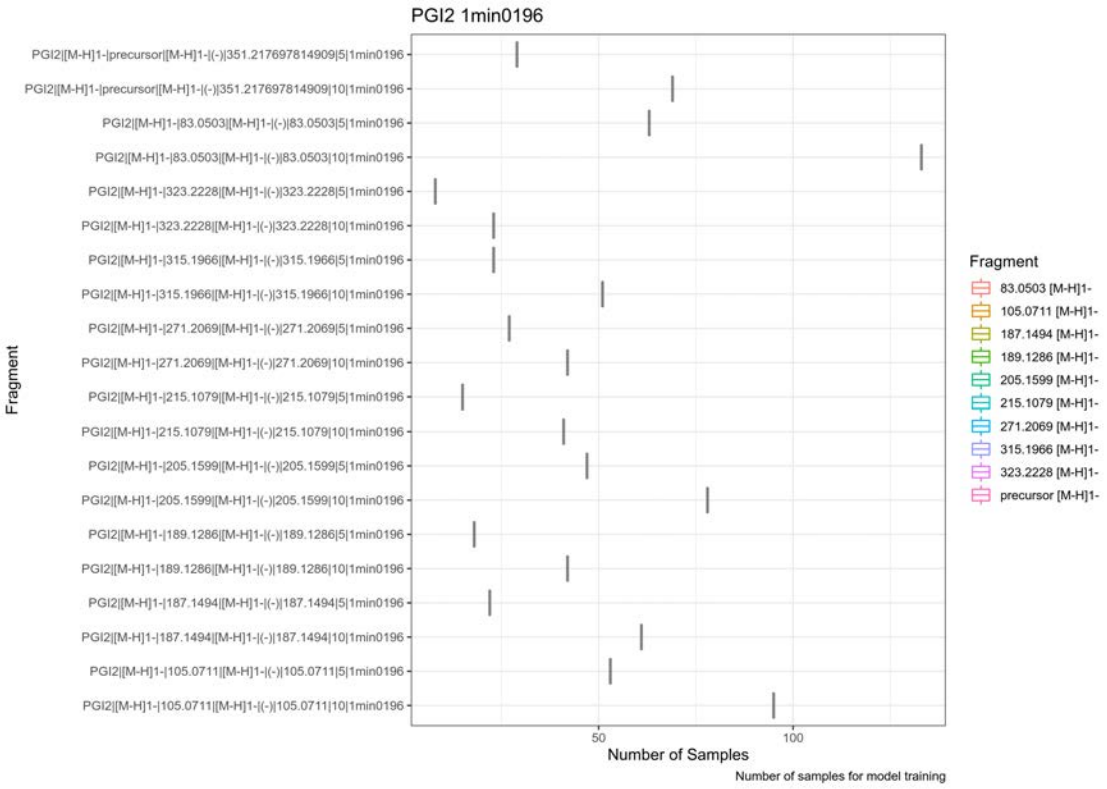


*Figure 230. Number of samples used for training per combination Id*

# 1.47. Resolvin D1{d5} [M-H]1- 1min0152

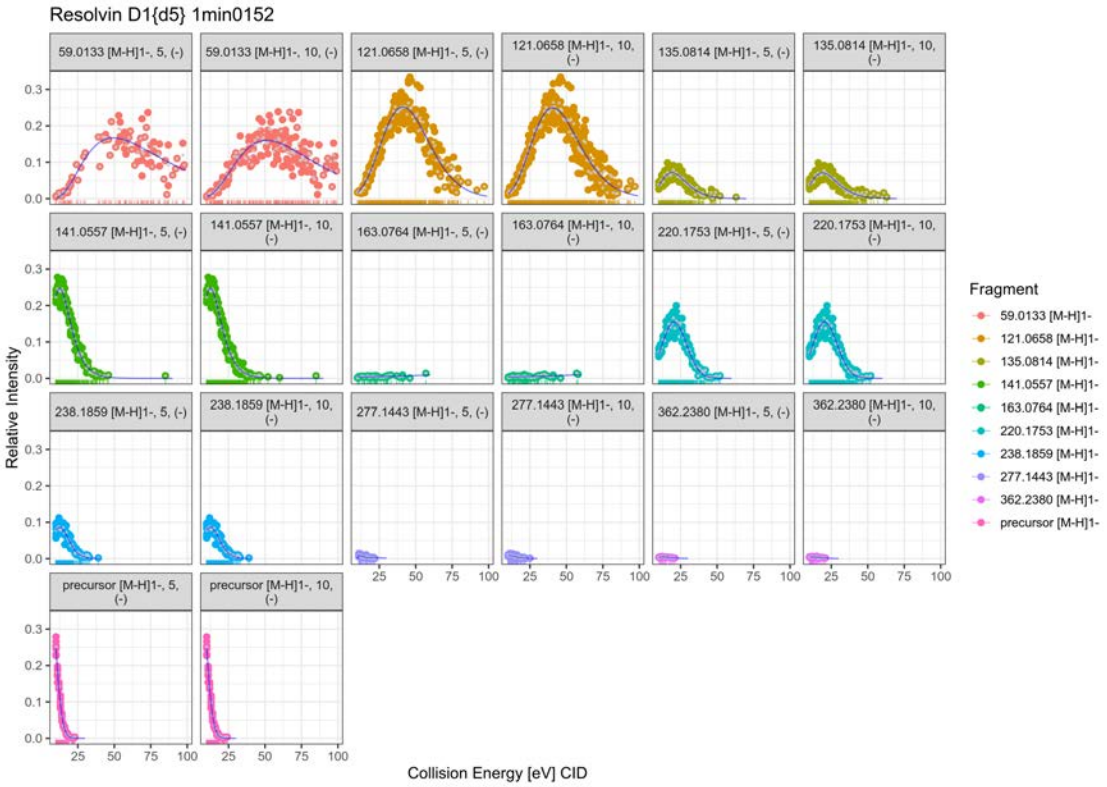


*Figure 231. Nonlinear fit*

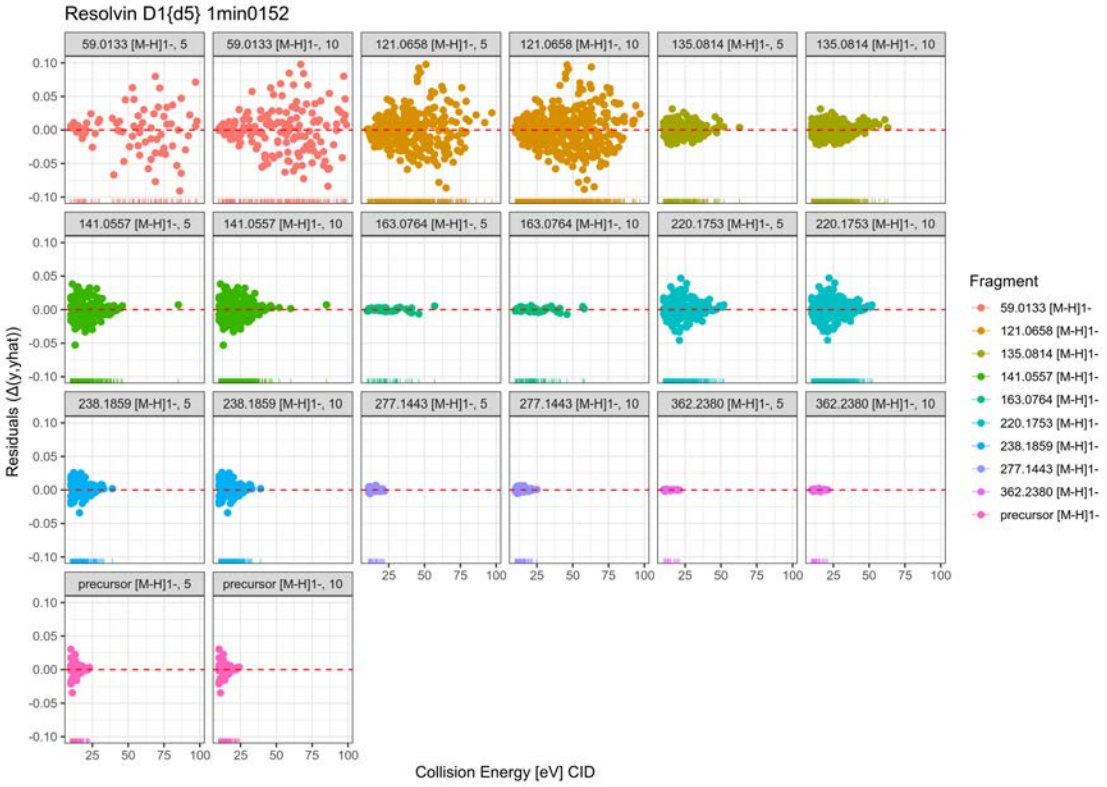


*Figure 232. Residuals of nonlinear fit*

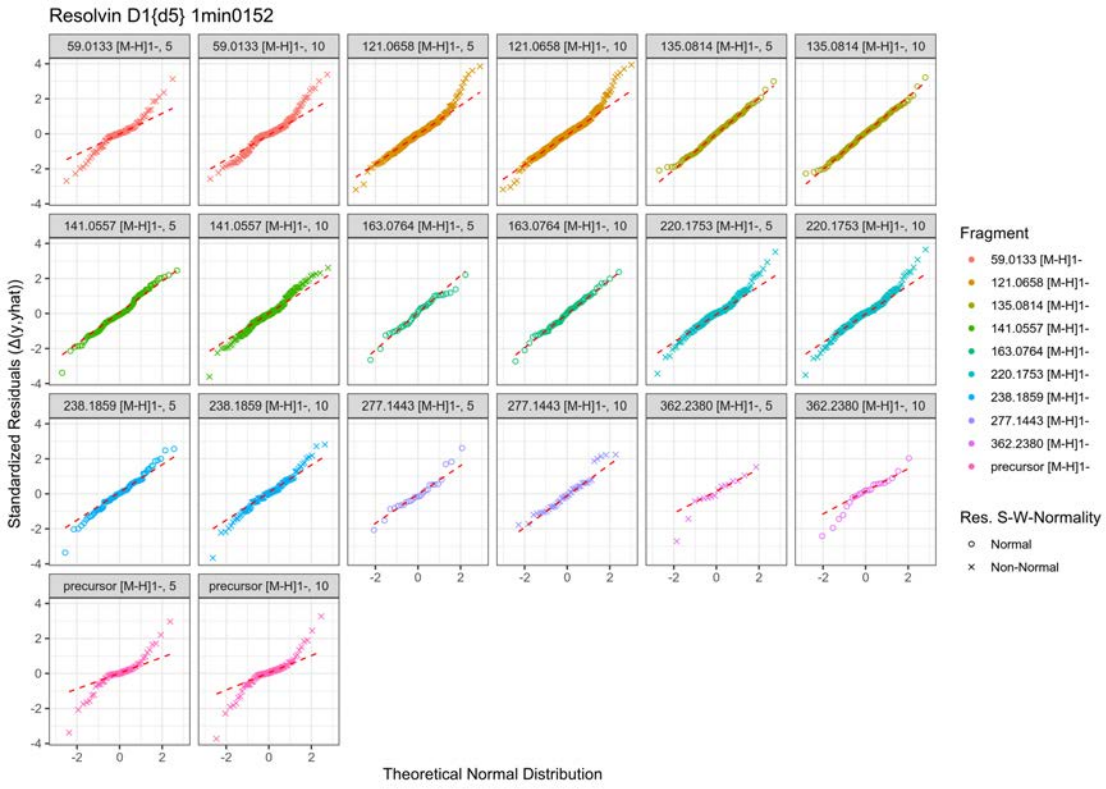


*Figure 233. Quantile-quantile plot of residuals*

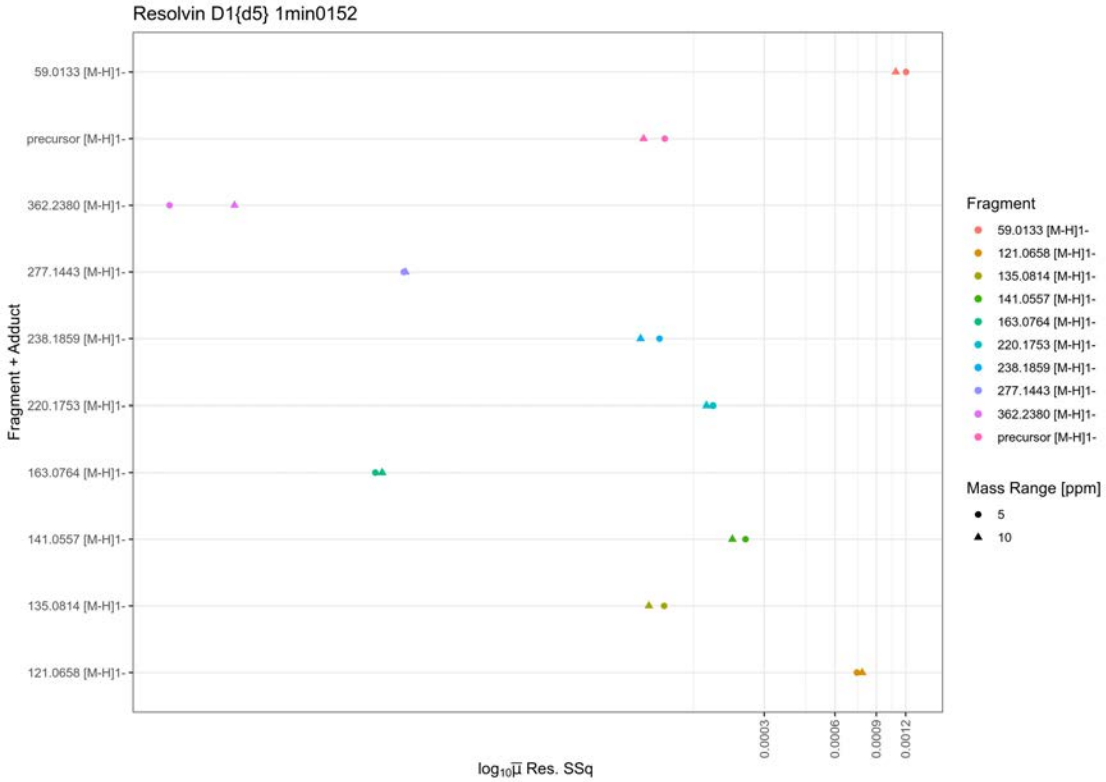


*Figure 234. Normalized sum-of-squares of the residuals*

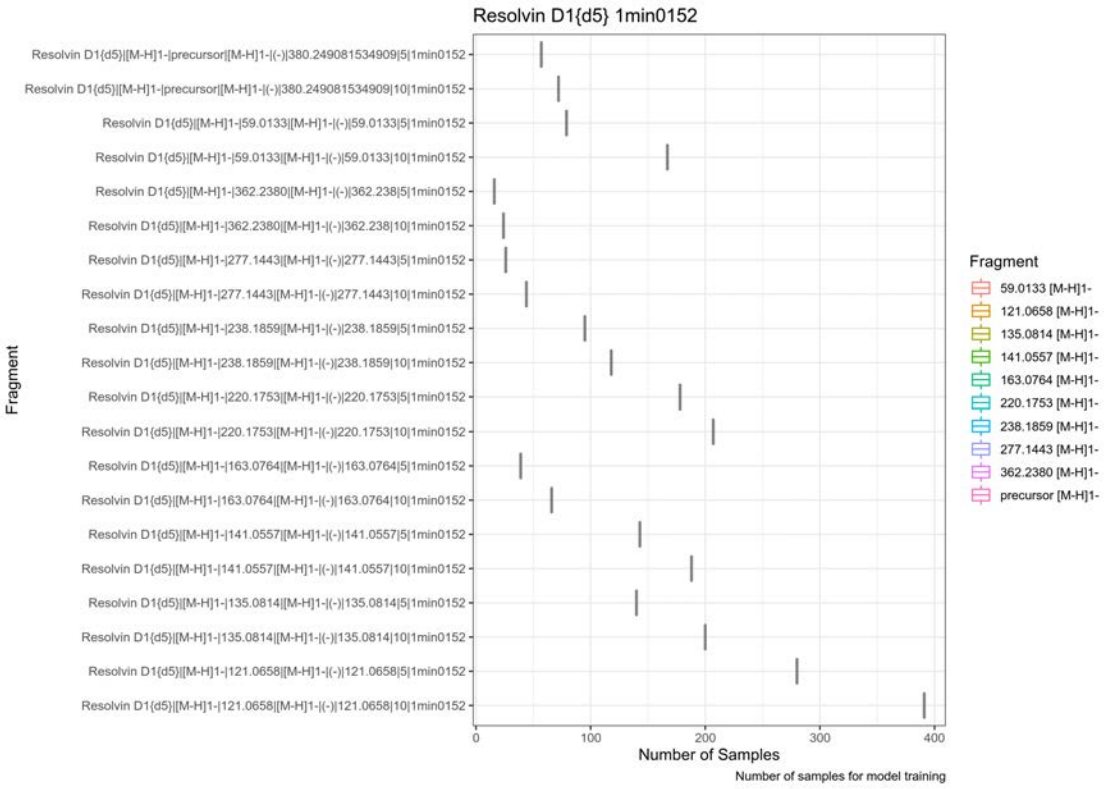


*Figure 235. Number of samples used for training per combination Id*

# 1.48. Resolvin D2{d5} [M-H]1- 1min0197

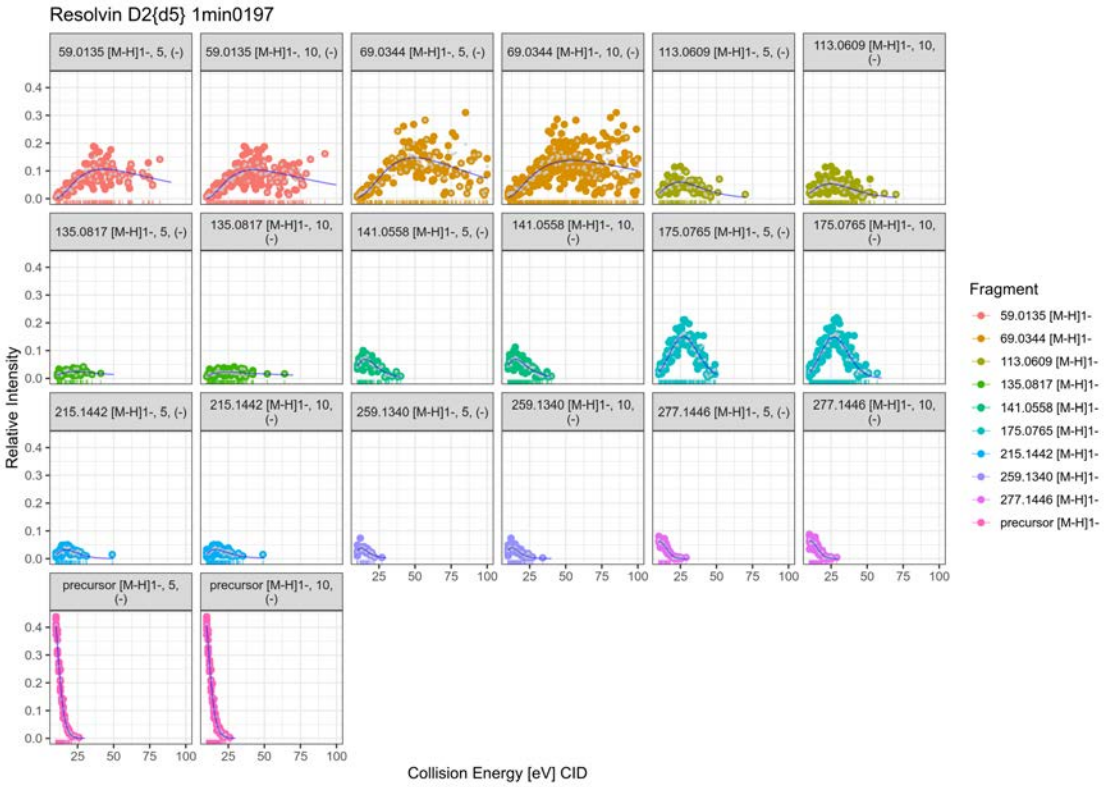


*Figure 236. Nonlinear fit*

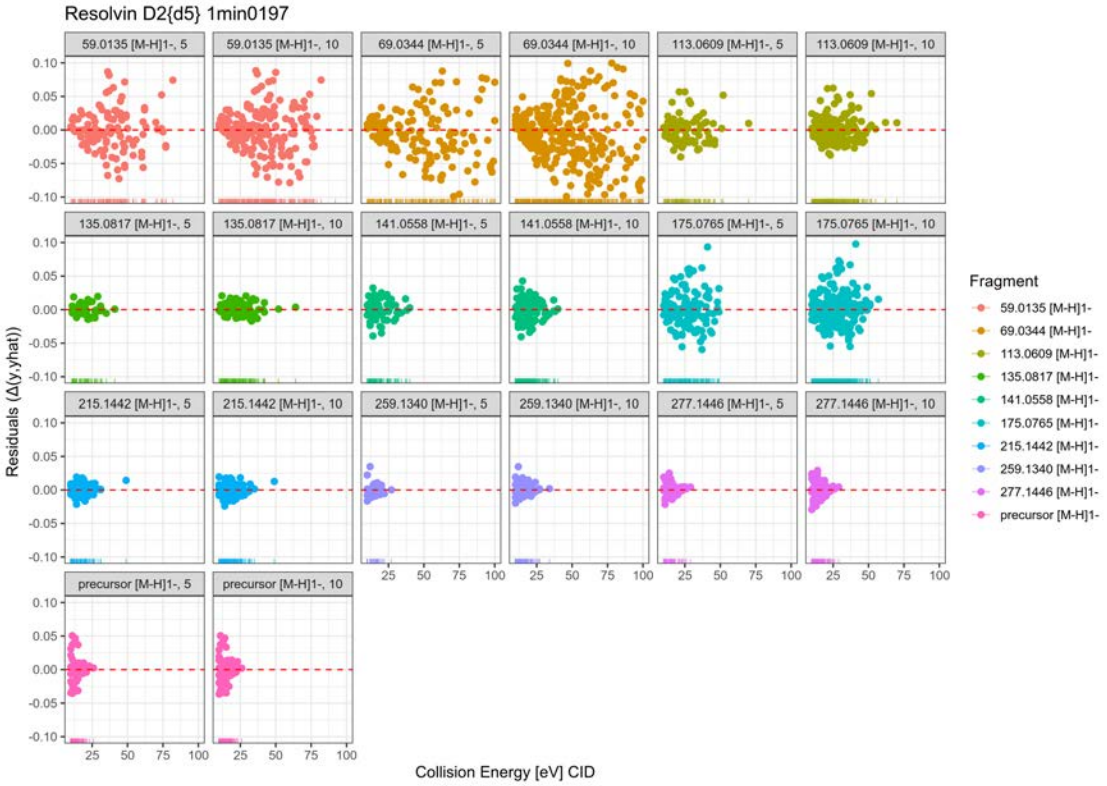


*Figure 237. Residuals of nonlinear fit*

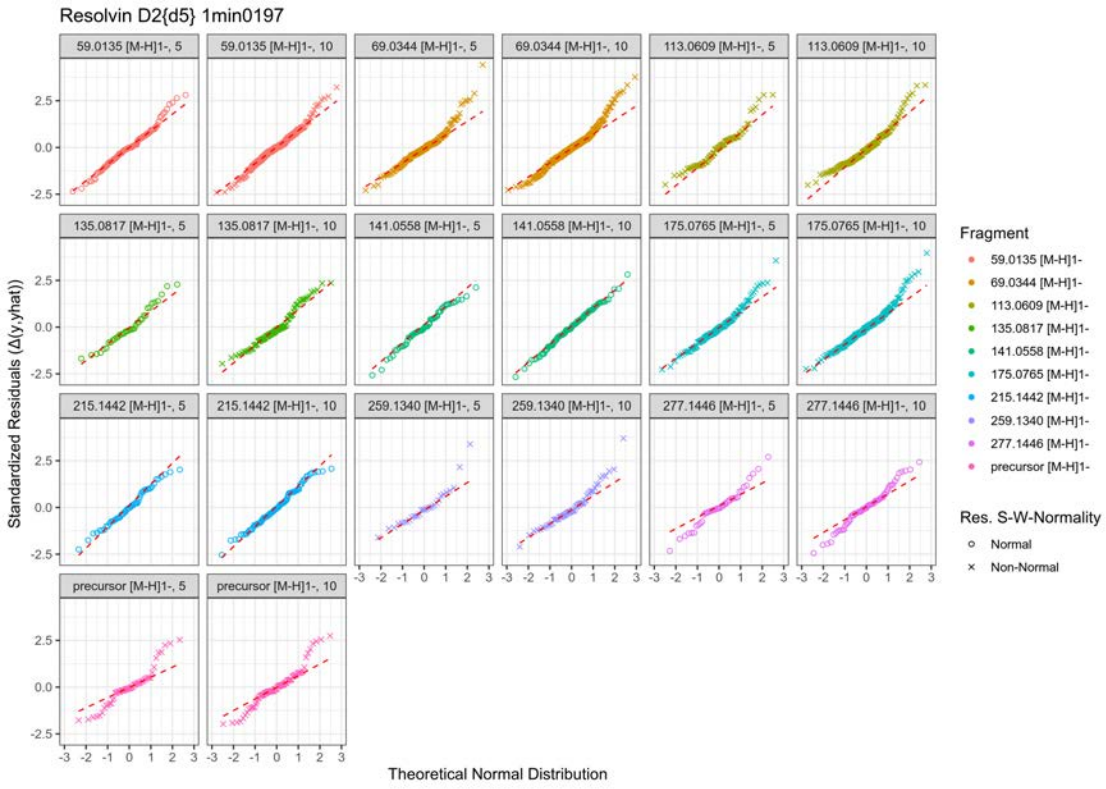


*Figure 238. Quantile-quantile plot of residuals*

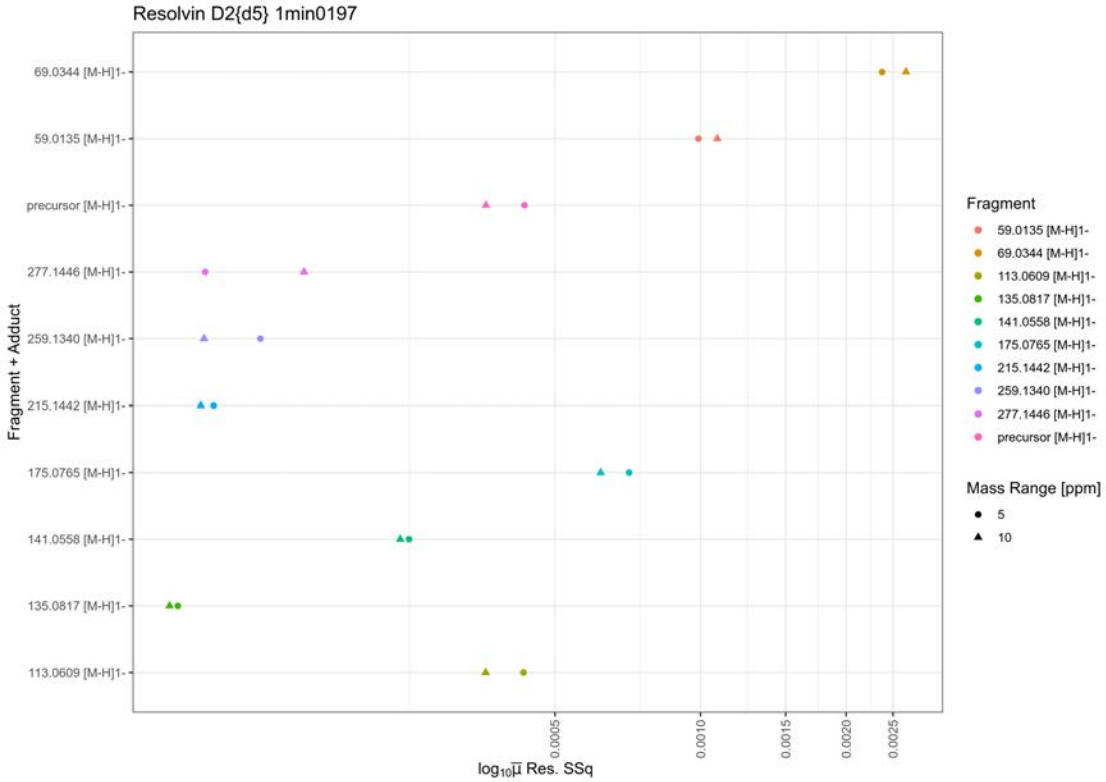


*Figure 239. Normalized sum-of-squares of the residuals*

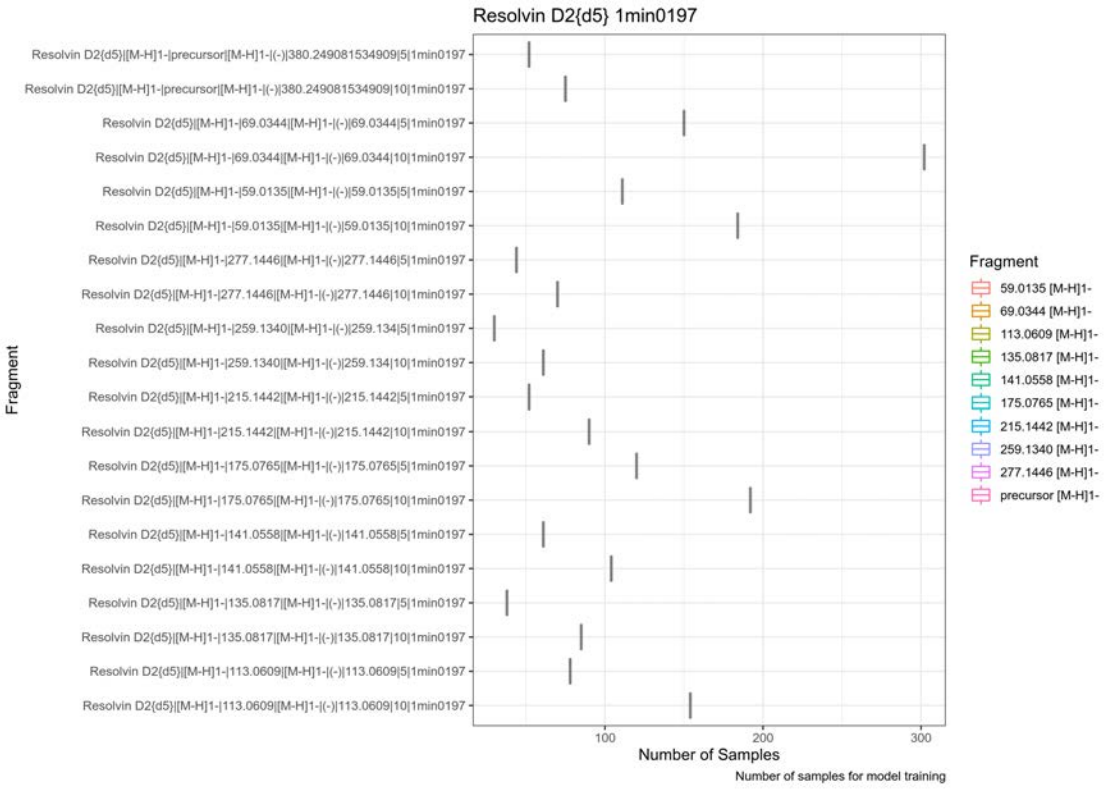


*Figure 240. Number of samples used for training per combination Id*

# 1.49. Resolvin D3 [M-H]1- 1min0210

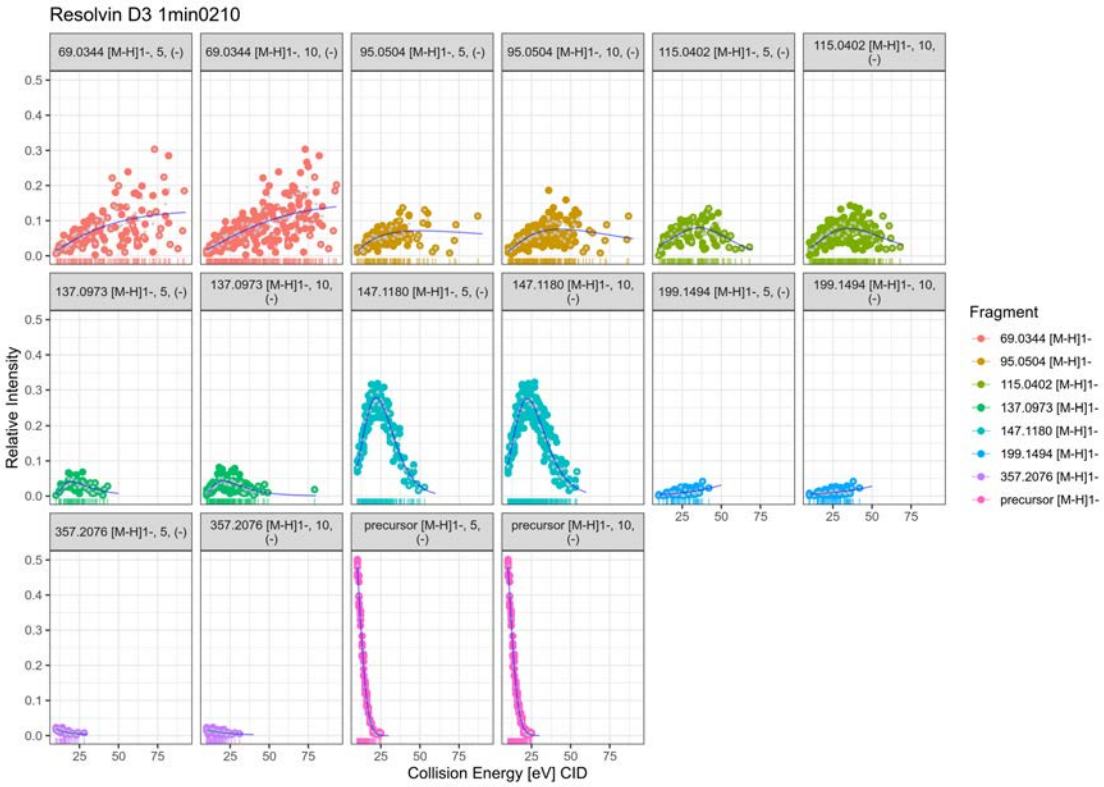


*Figure 241. Nonlinear fit*

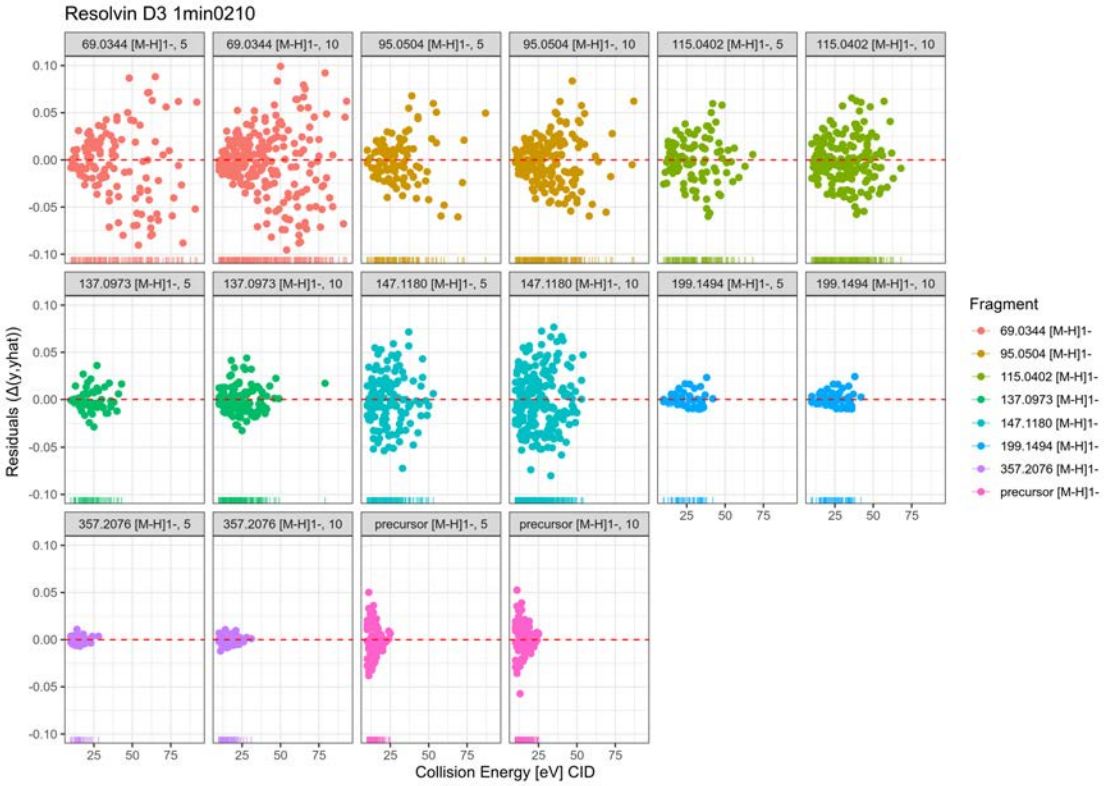


*Figure 242. Residuals of nonlinear fit*

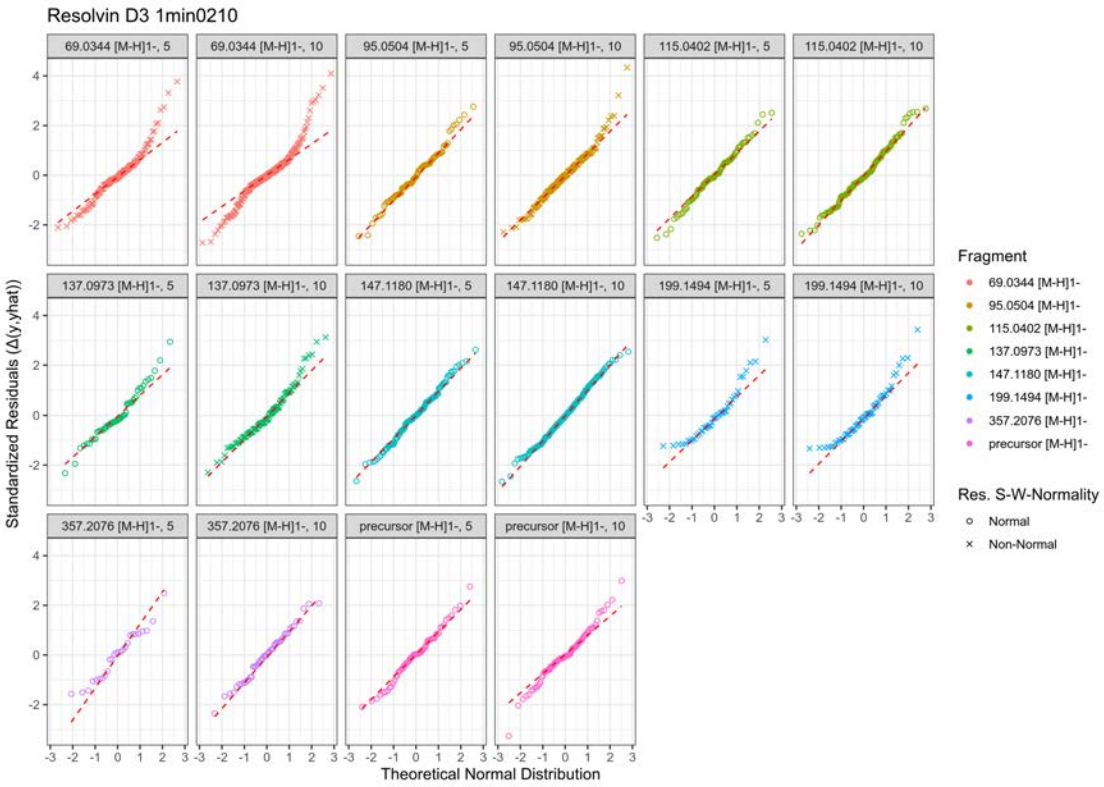


*Figure 243. Quantile-quantile plot of residuals*

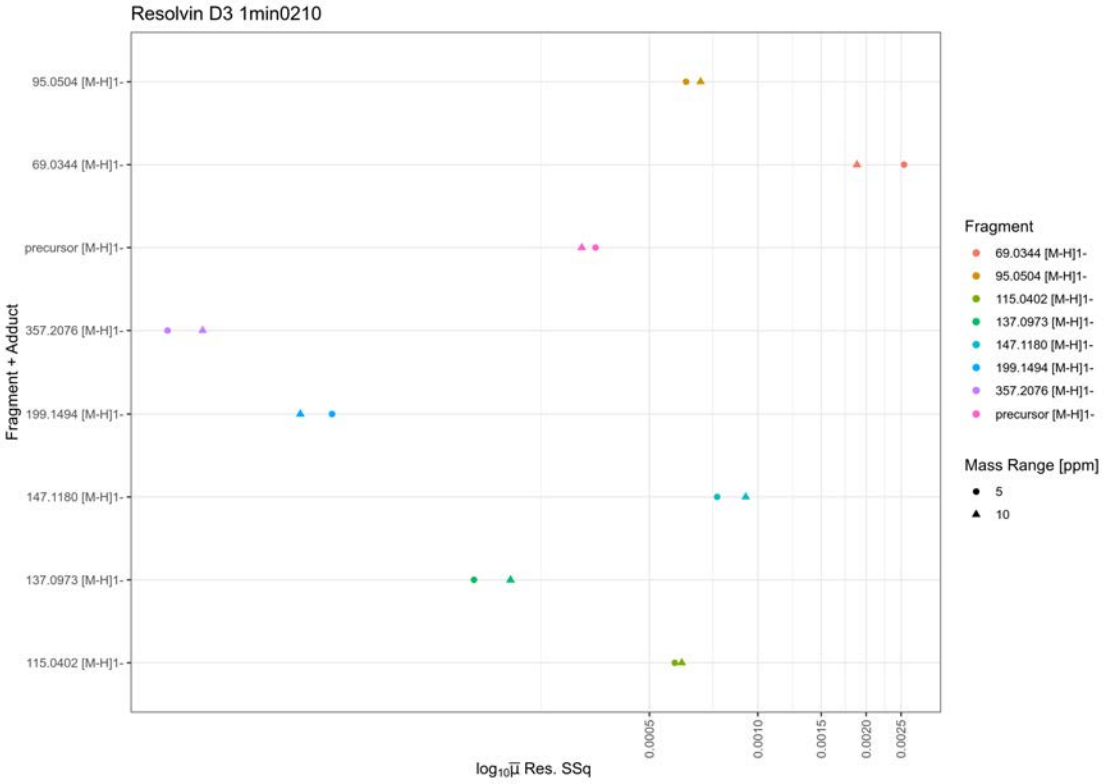


*Figure 244. Normalized sum-of-squares of the residuals*

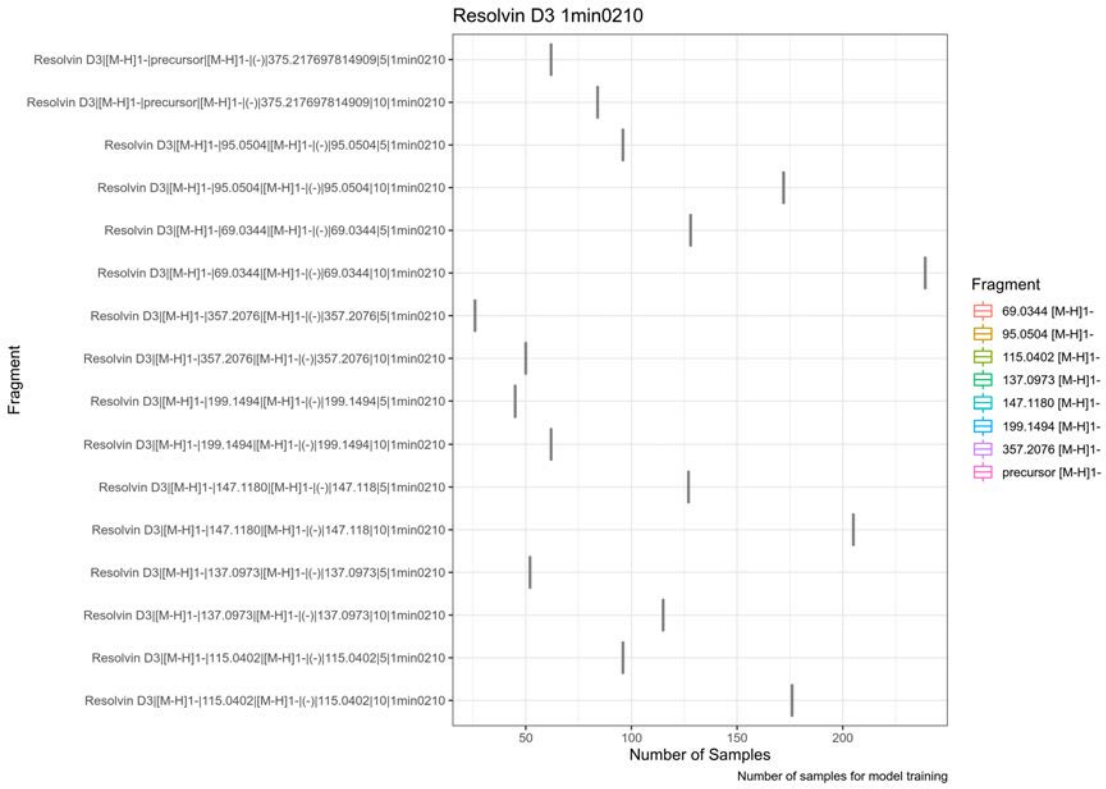


*Figure 245. Number of samples used for training per combination Id*

# 1.50. Resolvin D5 [M-H]1- 1min0212

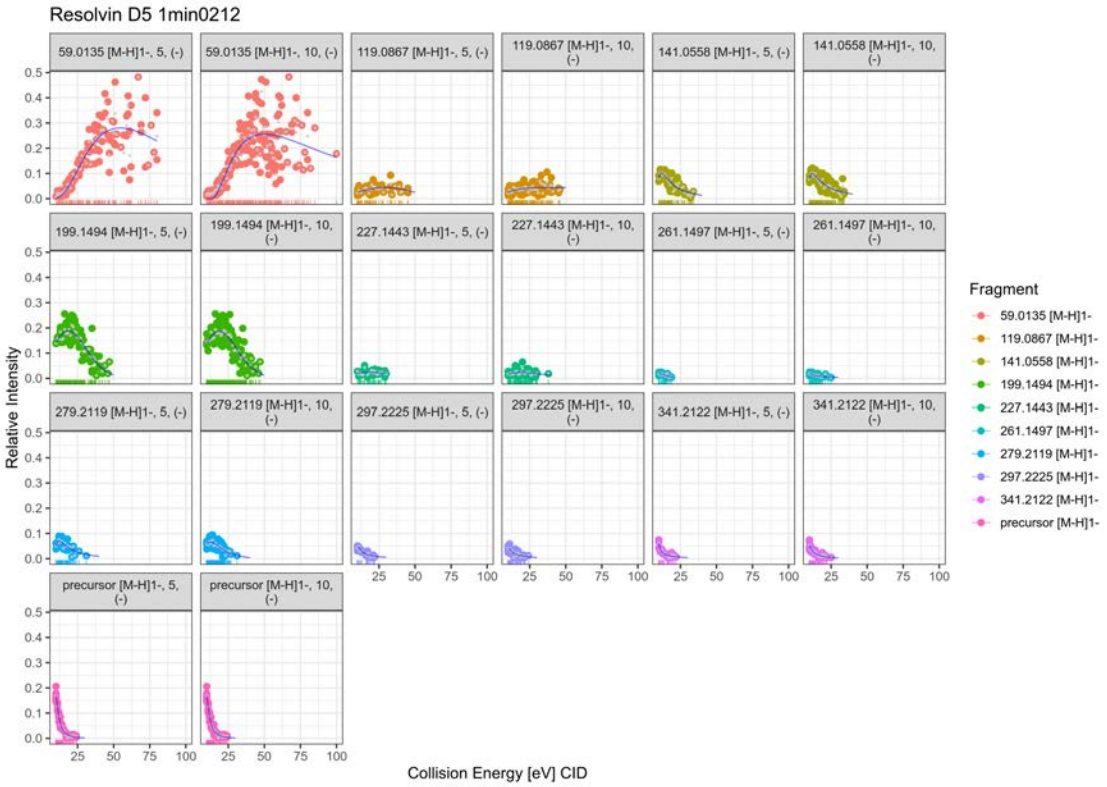


*Figure 246. Nonlinear fit*

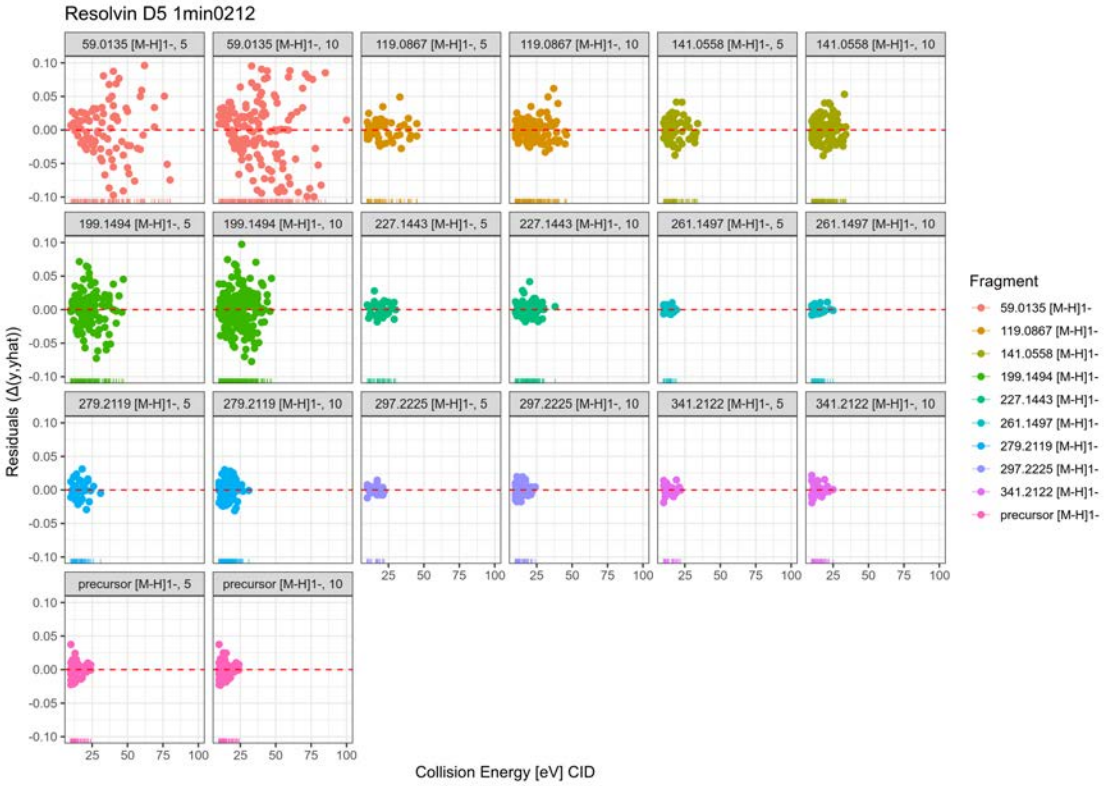


*Figure 247. Residuals of nonlinear fit*

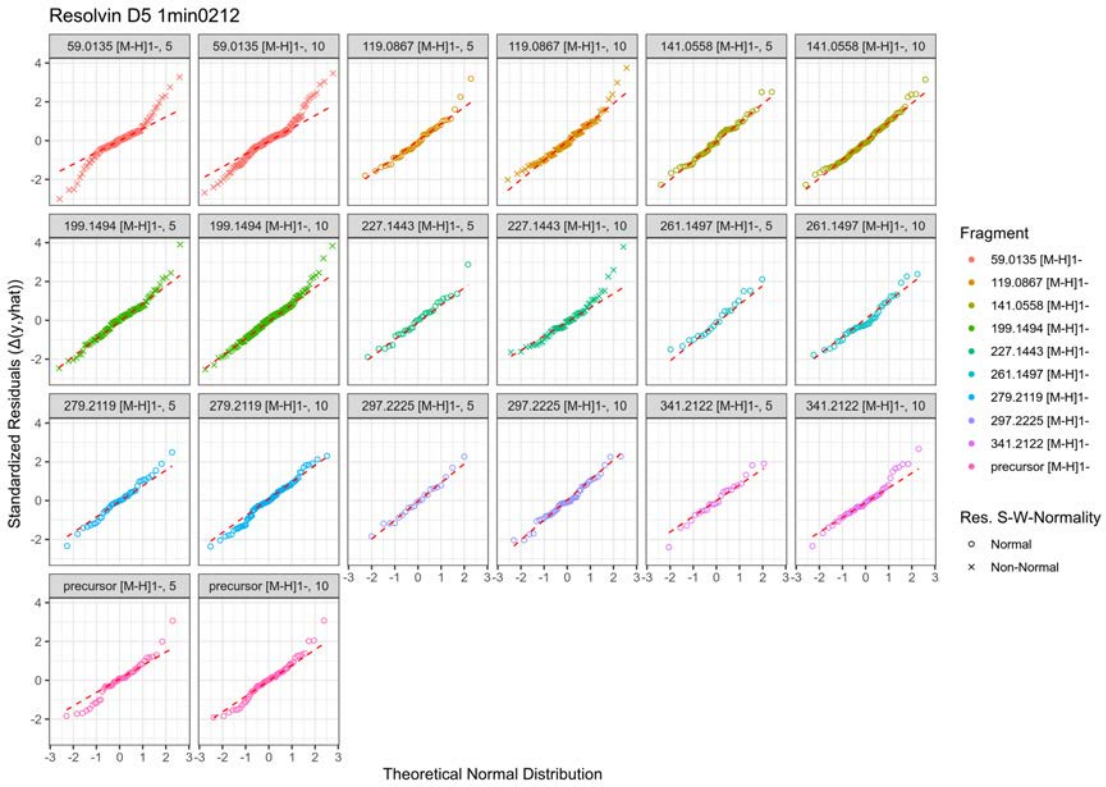


*Figure 248. Quantile-quantile plot of residuals*

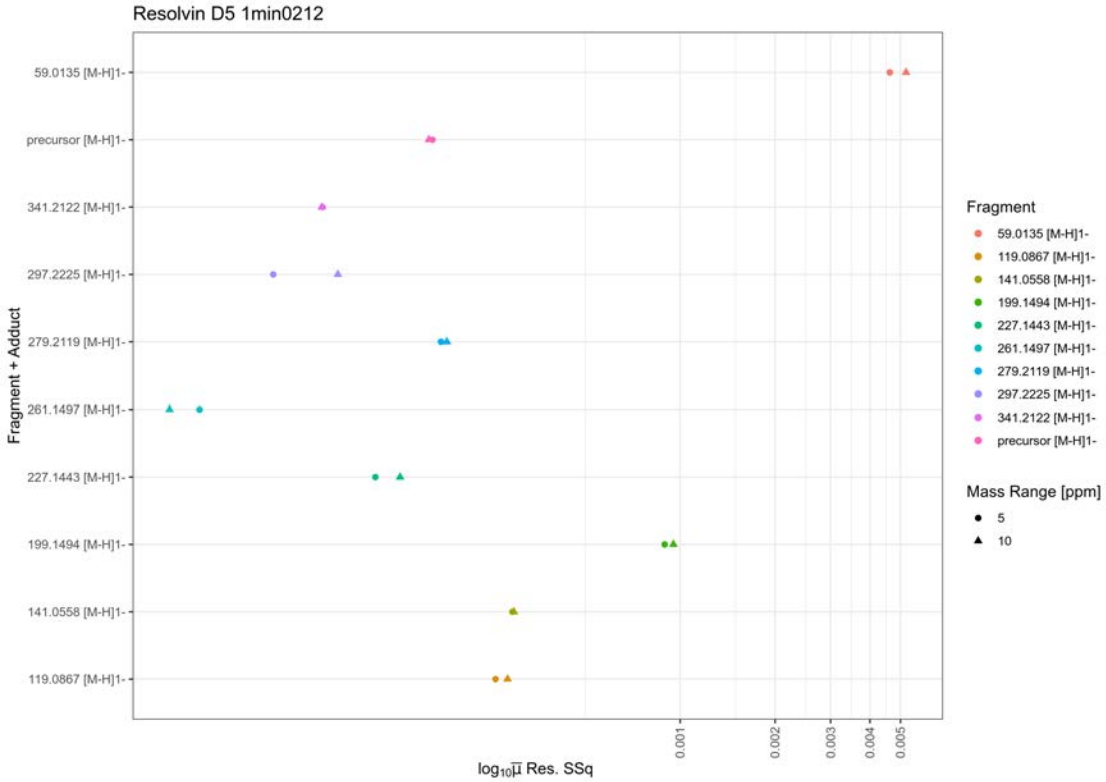


*Figure 249. Normalized sum-of-squares of the residuals*

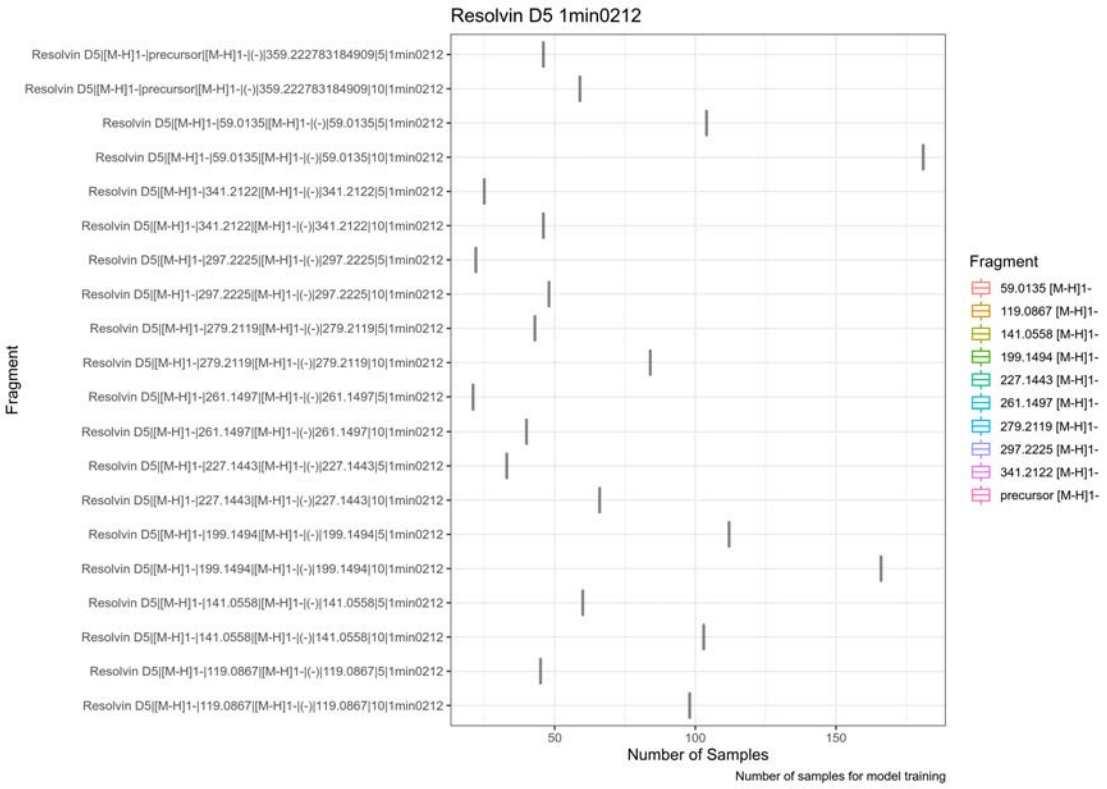


*Figure 250. Number of samples used for training per combination Id*

# 1.51. TXB1 [M-H]1- 1min0155

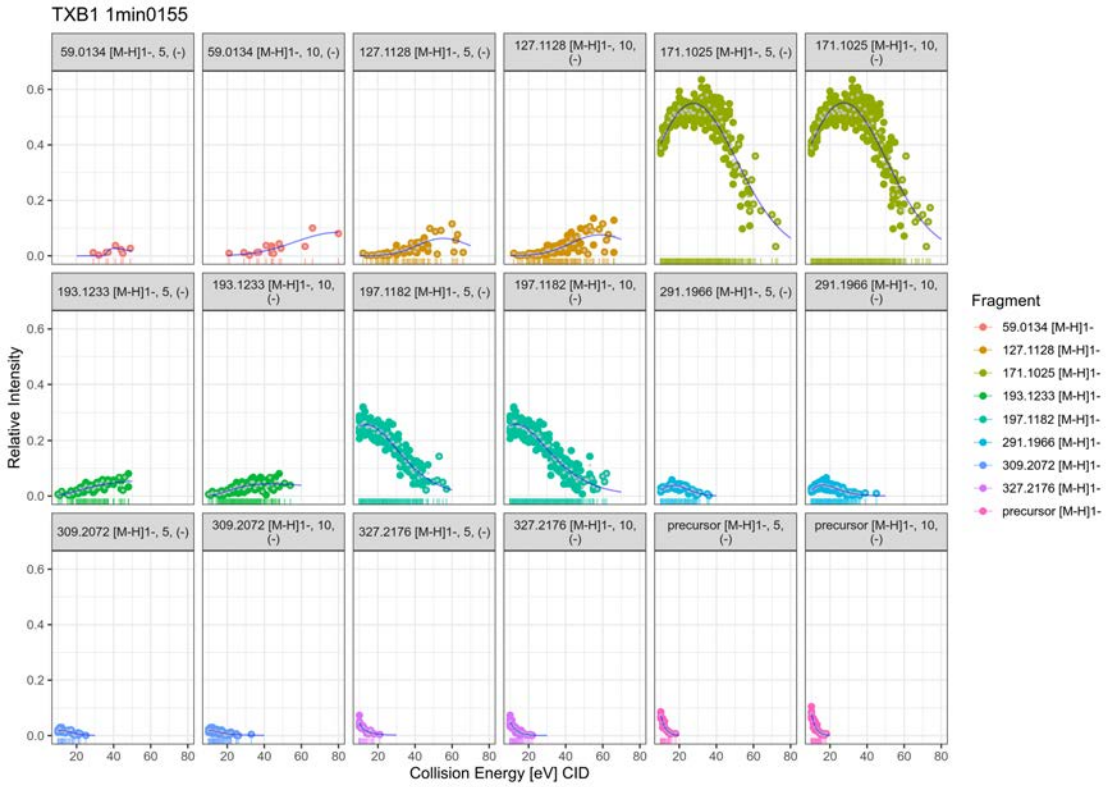


*Figure 251. Nonlinear fit*

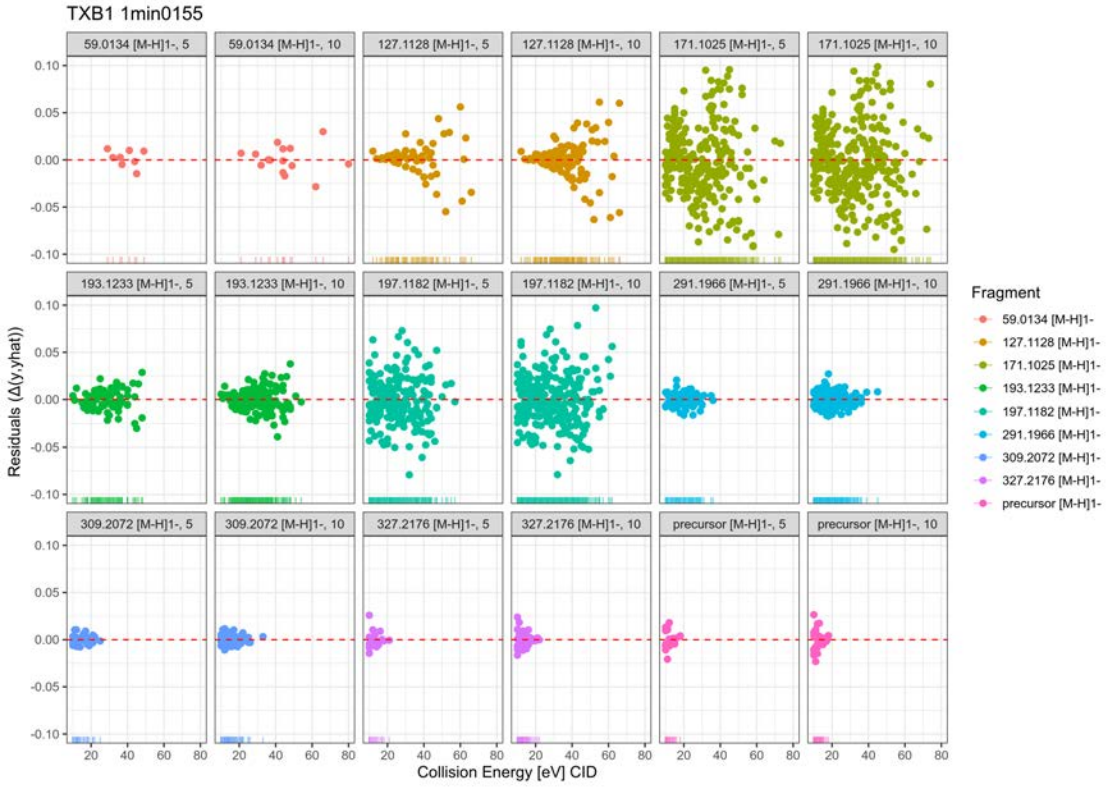


*Figure 252. Residuals of nonlinear fit*

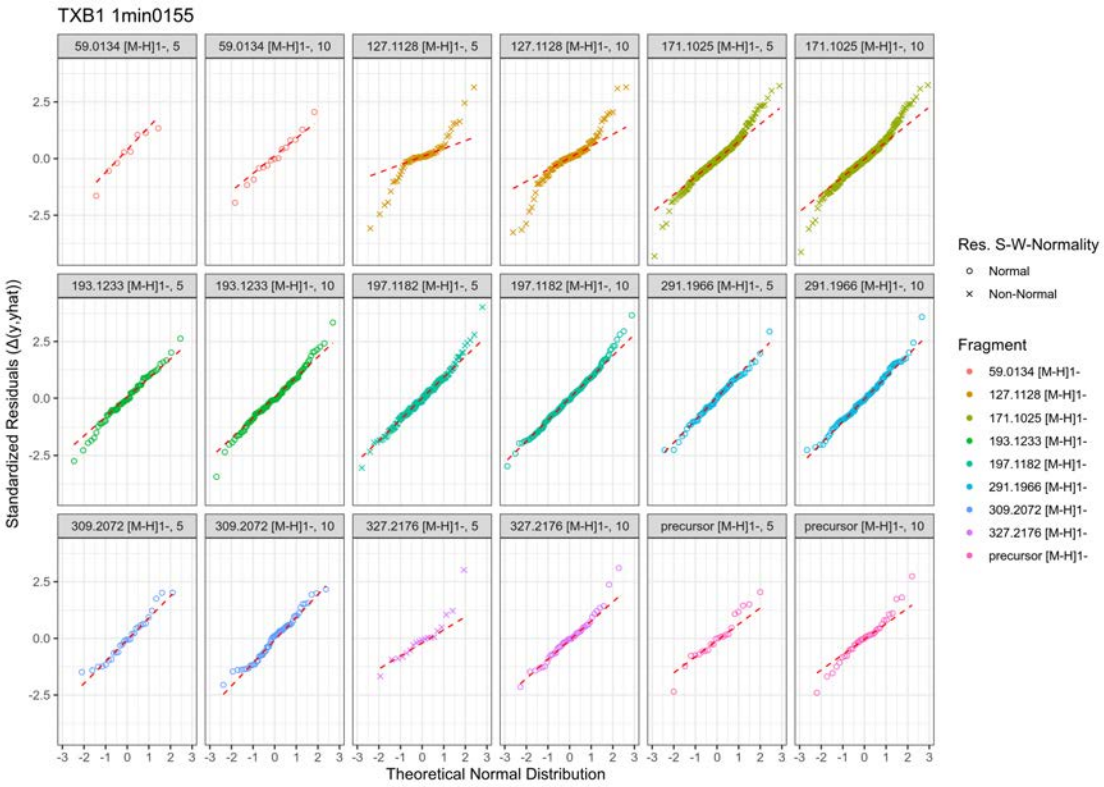


*Figure 253. Quantile-quantile plot of residuals*

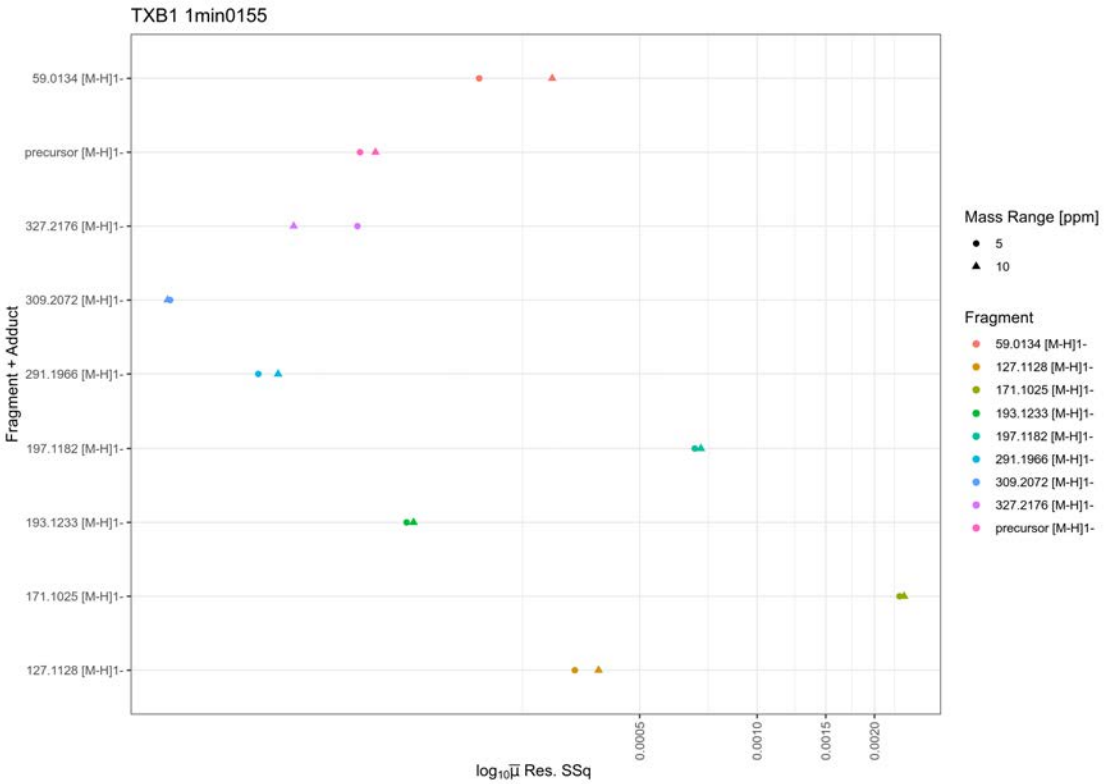


*Figure 254. Normalized sum-of-squares of the residuals*

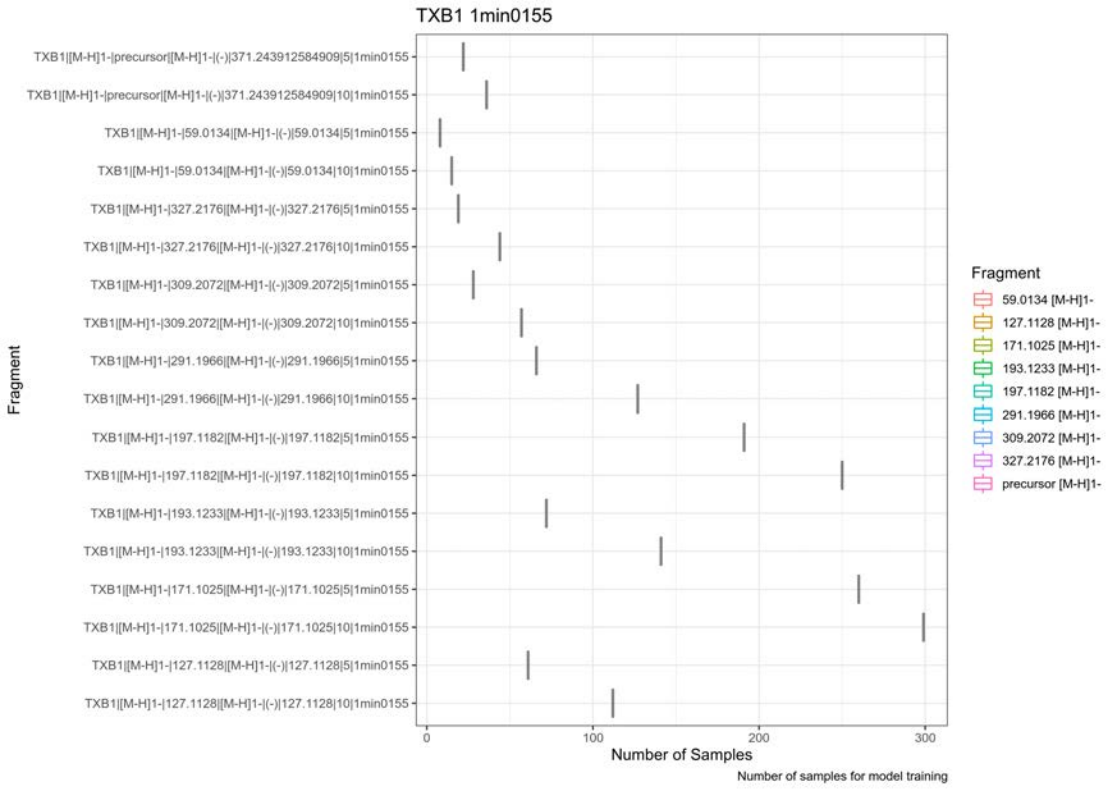


*Figure 255. Number of samples used for training per combination Id*

# 1.52. TXB2{d4} [M-H]1- 1min0071

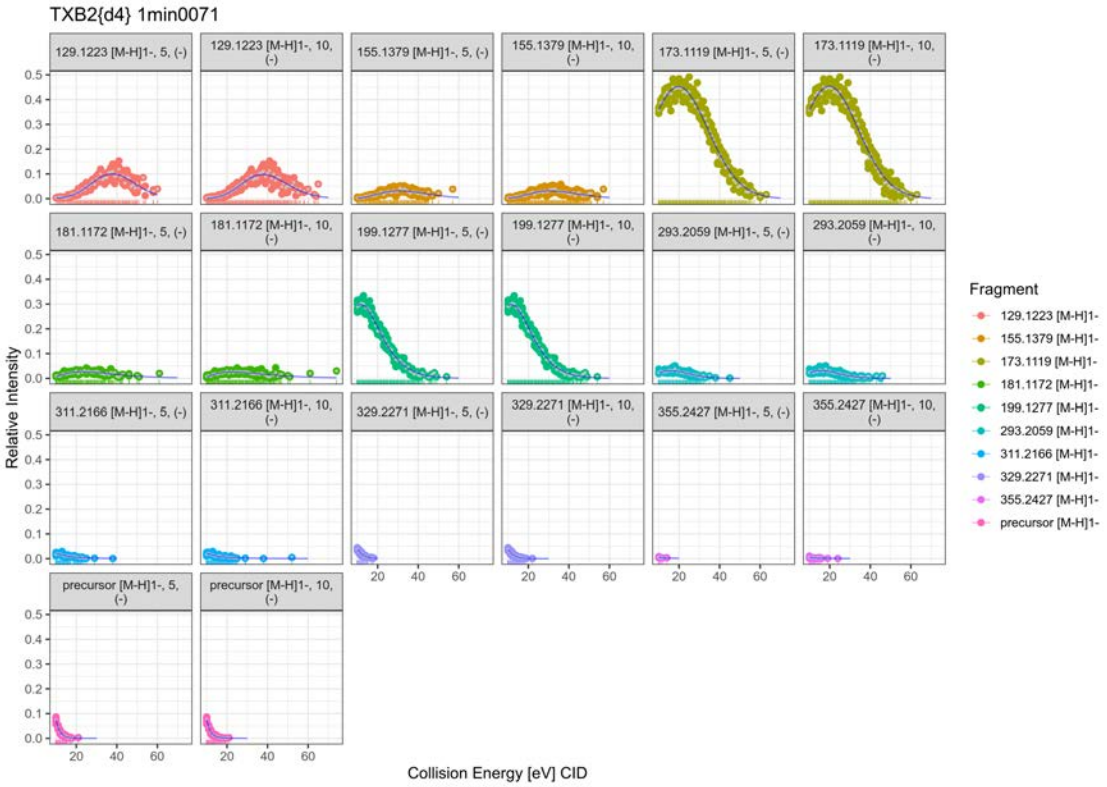


*Figure 256. Nonlinear fit*

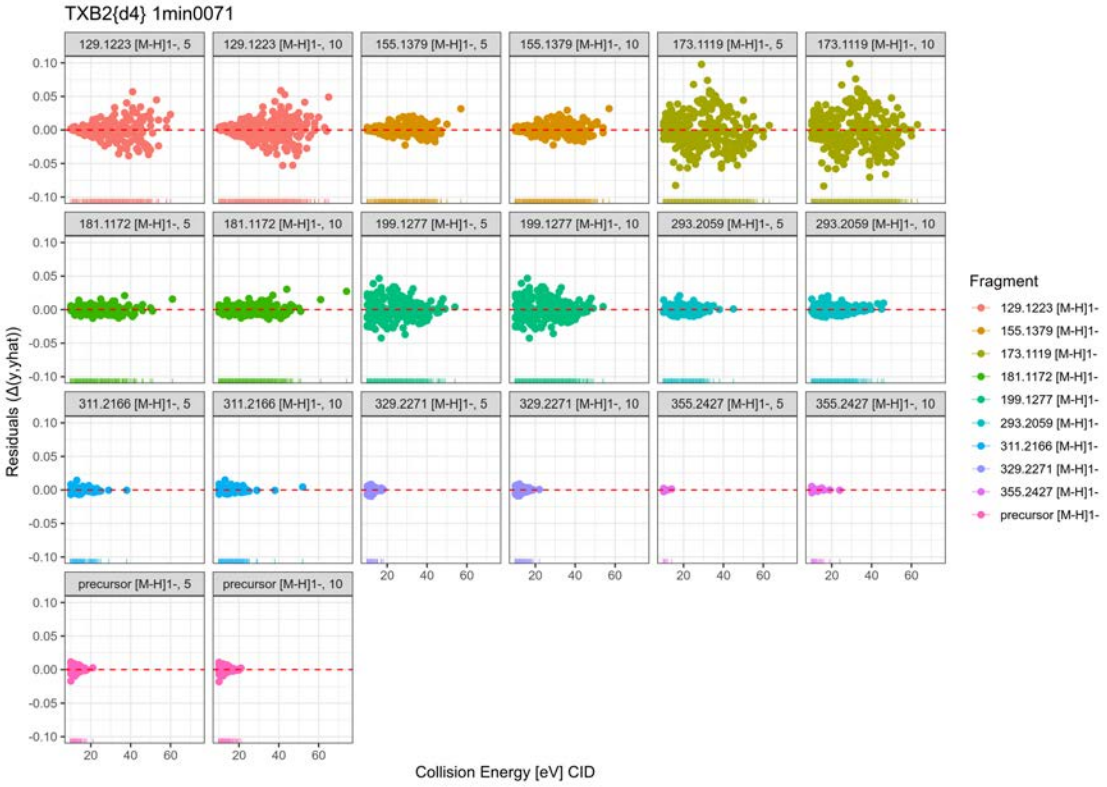


*Figure 257. Residuals of nonlinear fit*

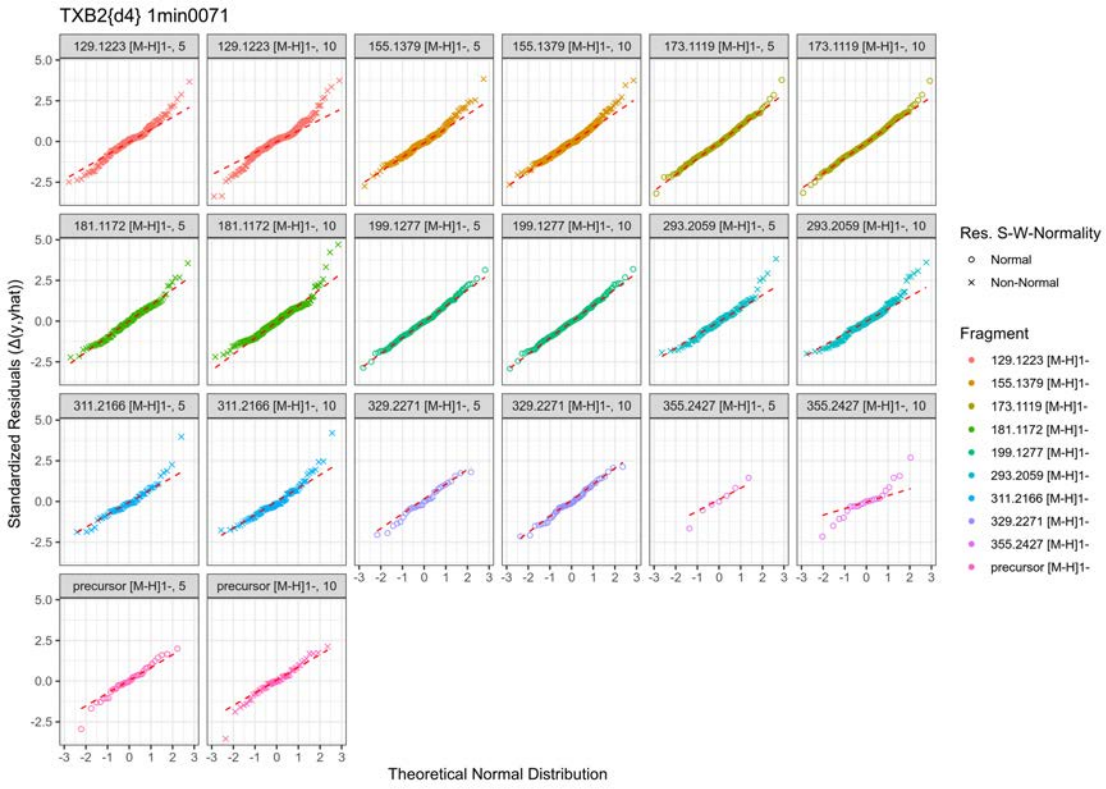


*Figure 258. Quantile-quantile plot of residuals*

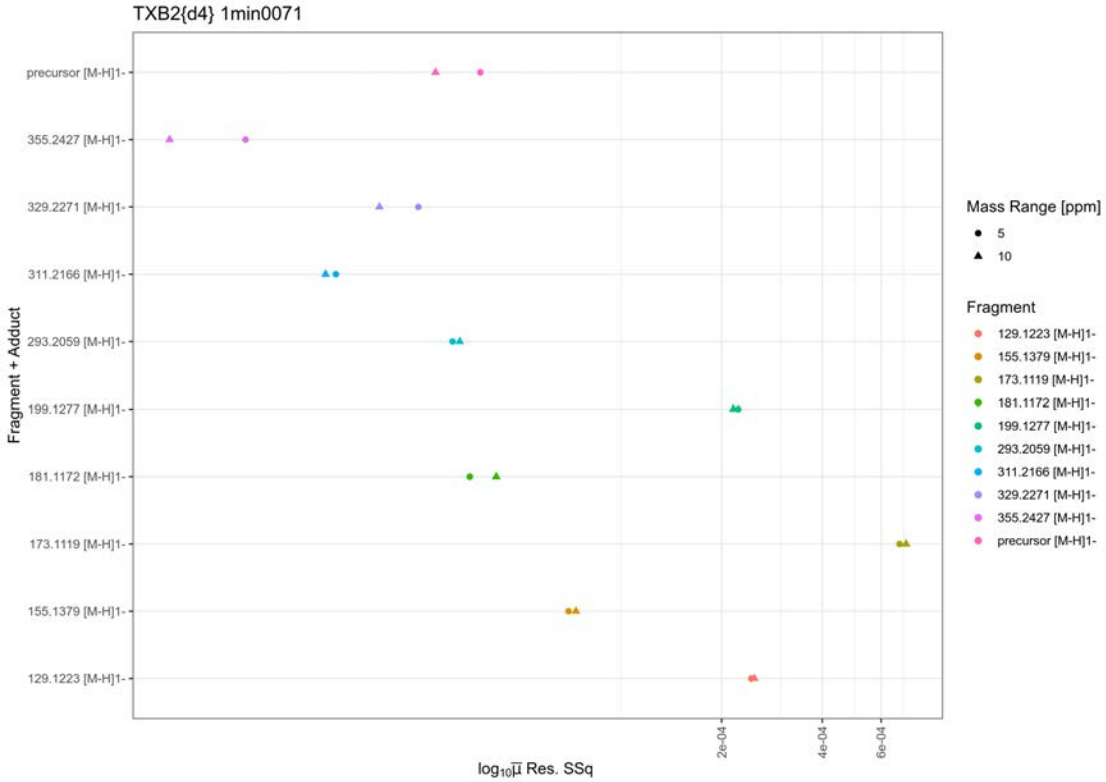


*Figure 259. Normalized sum-of-squares of the residuals*

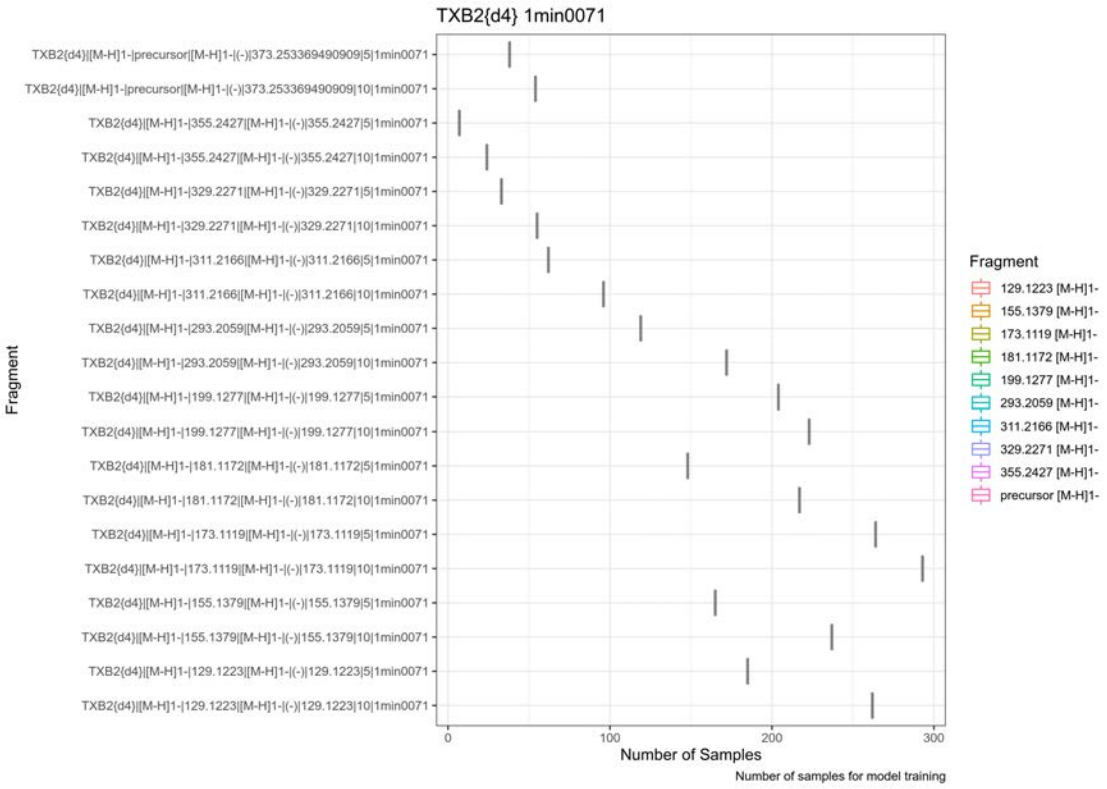


*Figure 260. Number of samples used for training per combination Id*

# 1.53. TXB3 [M-H]1- 1min0072

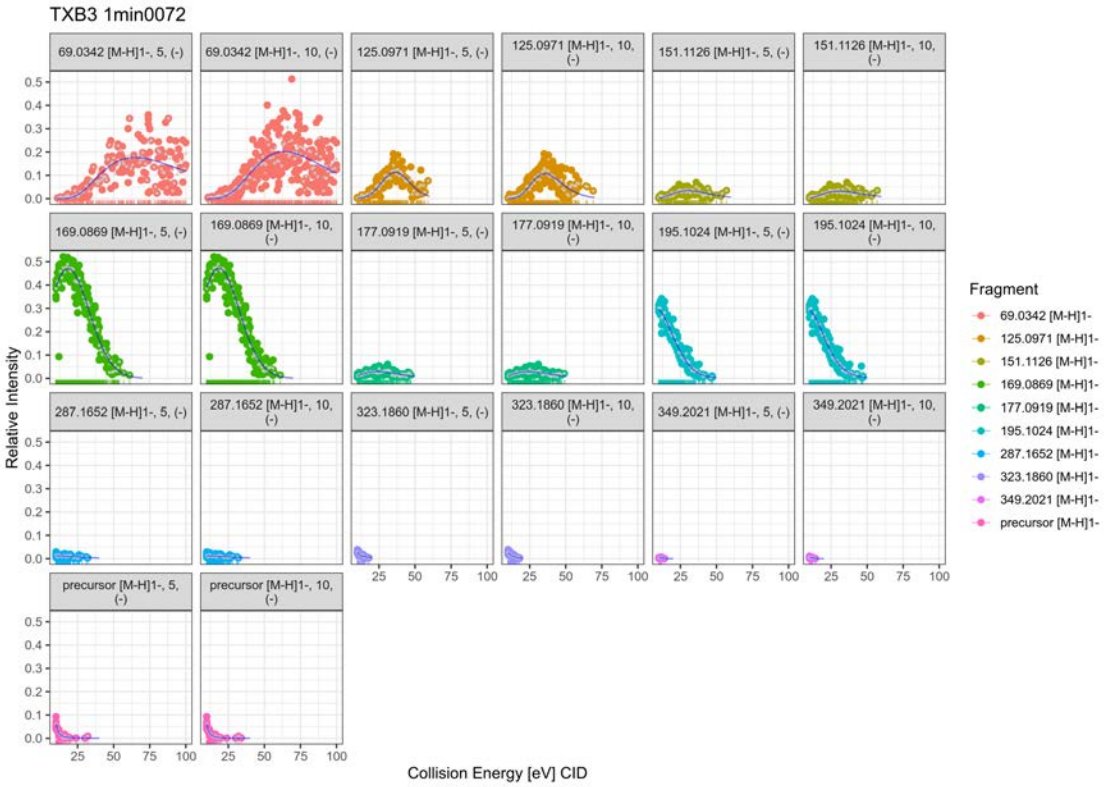


*Figure 261. Nonlinear fit*

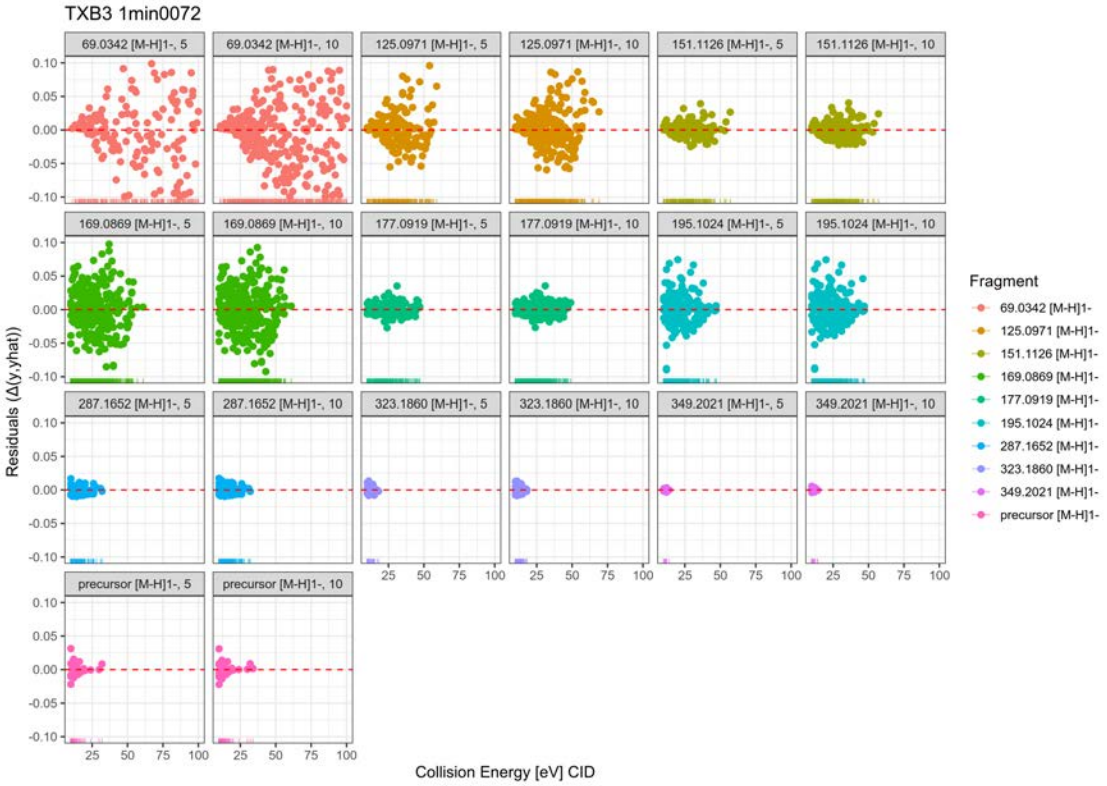


*Figure 262. Residuals of nonlinear fit*

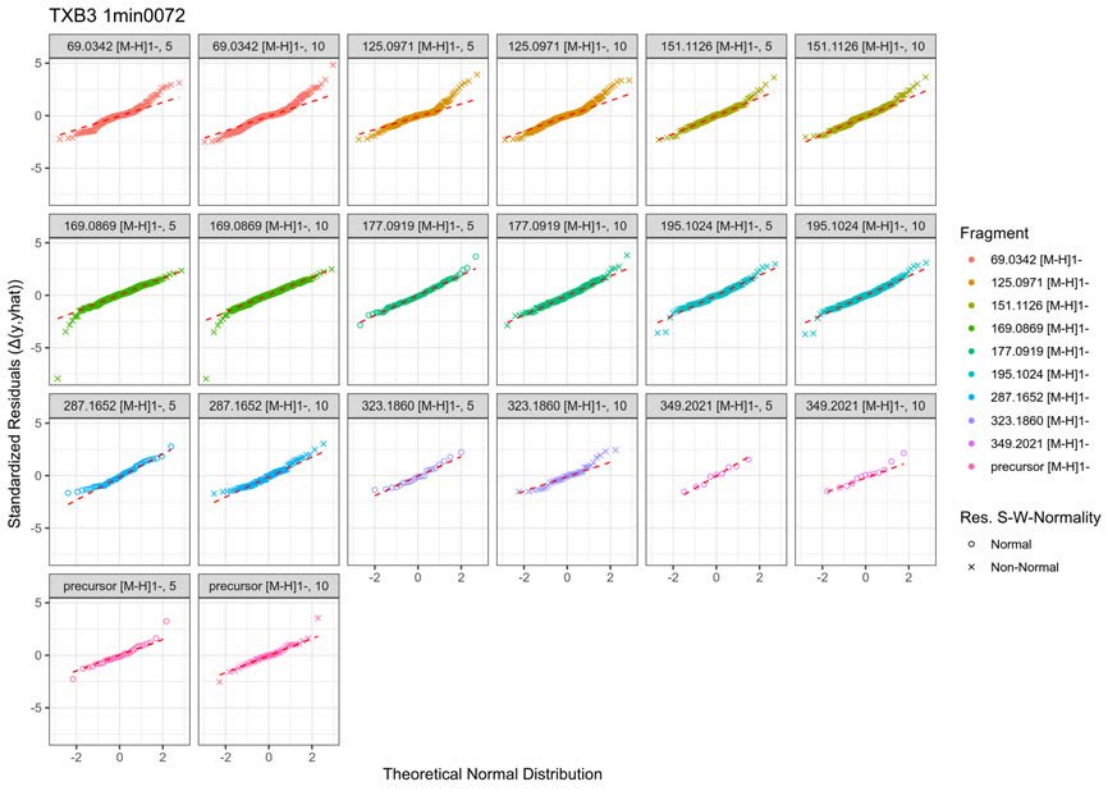


*Figure 263. Quantile-quantile plot of residuals*

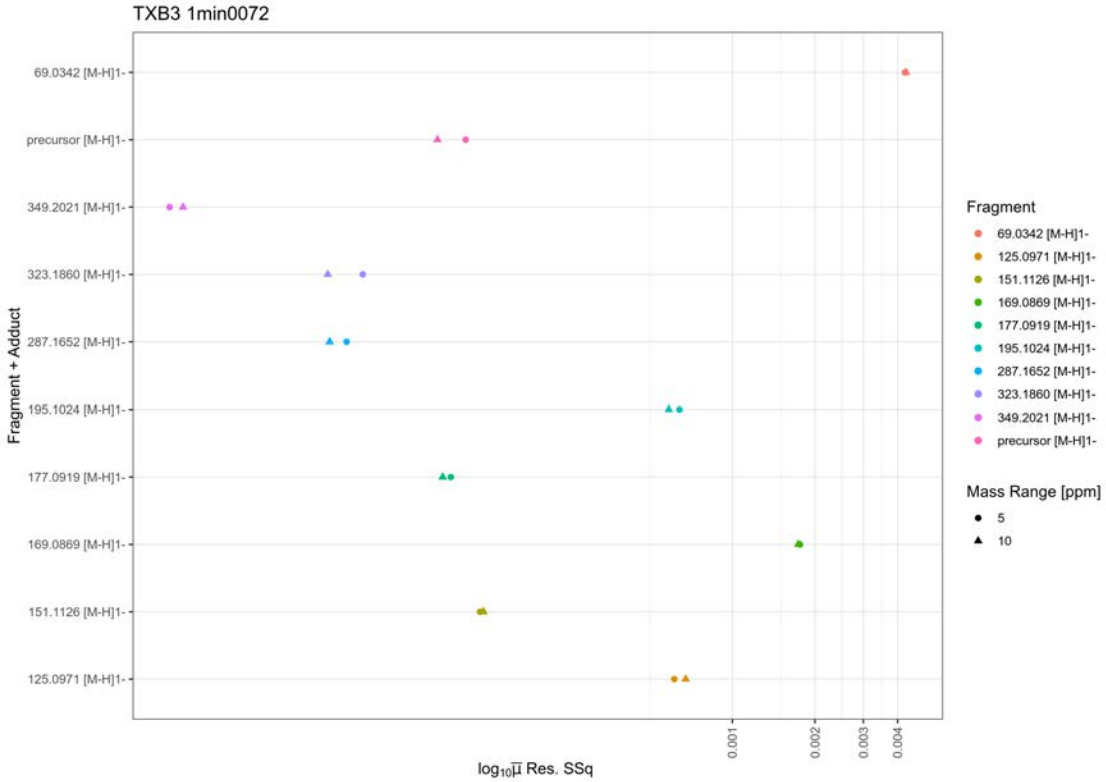


*Figure 264. Normalized sum-of-squares of the residuals*

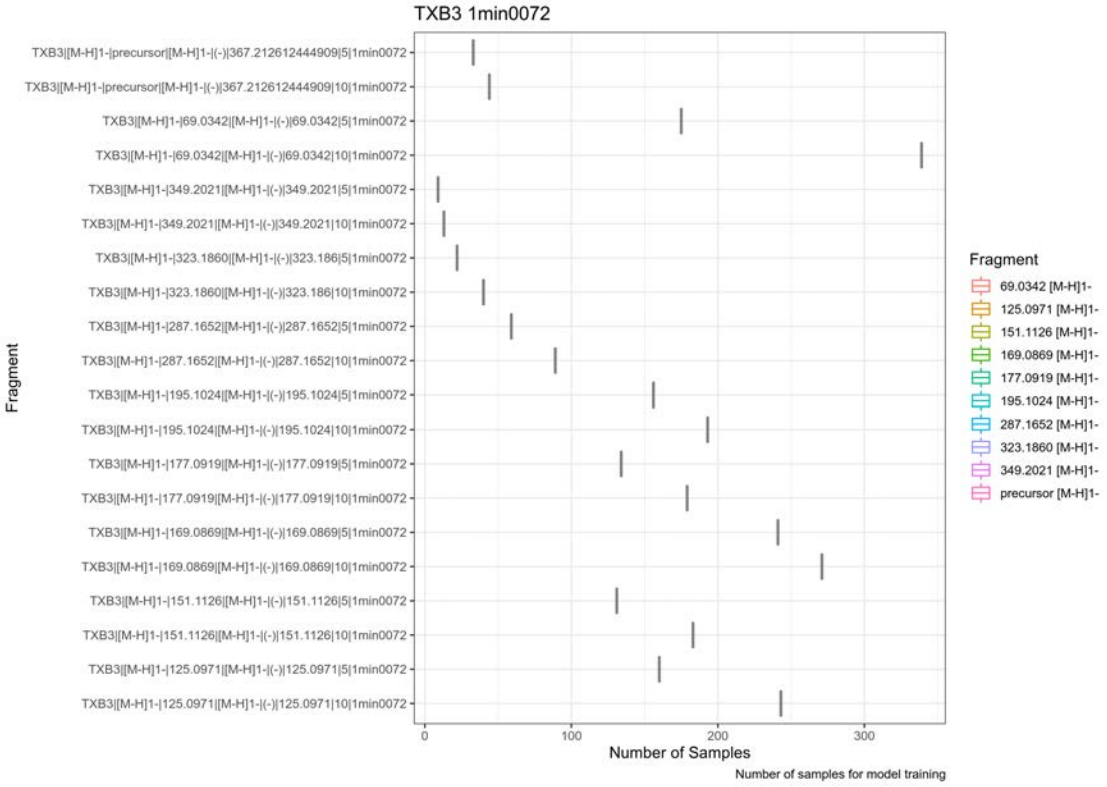


*Figure 265. Number of samples used for training per combination Id*

# 1.54. alpha-LA{d14} [M-H]1- 1min0201

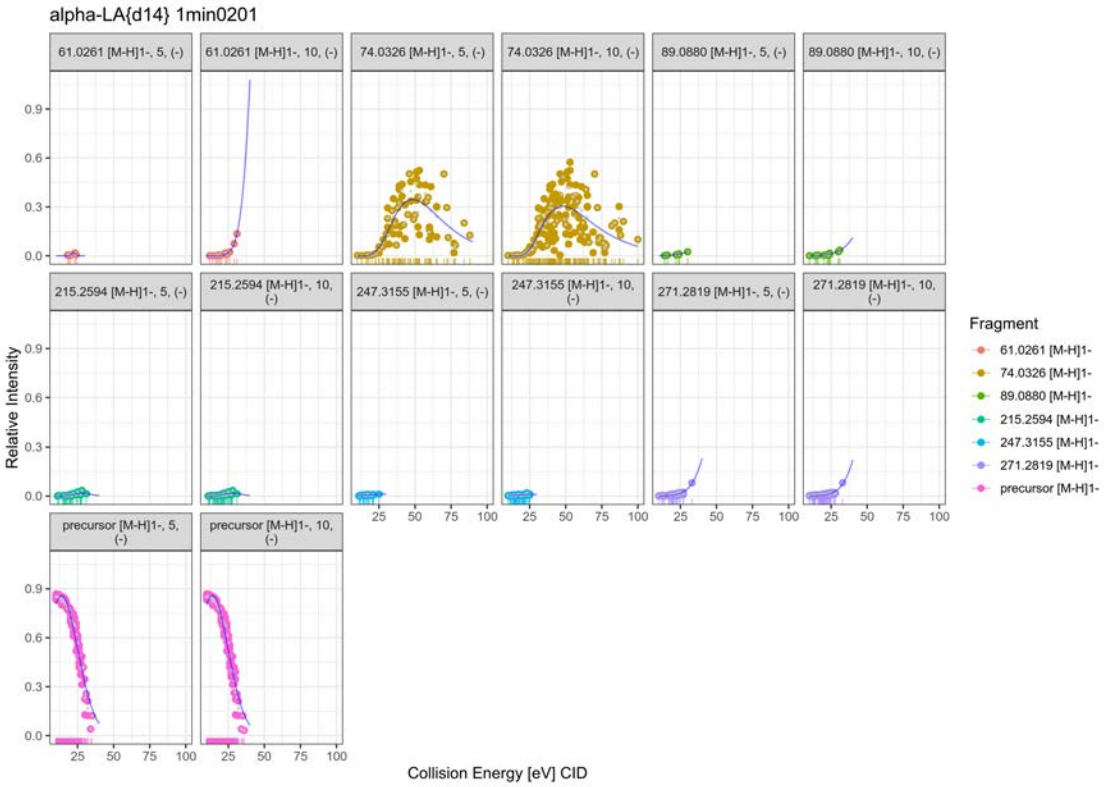


*Figure 266. Nonlinear fit*

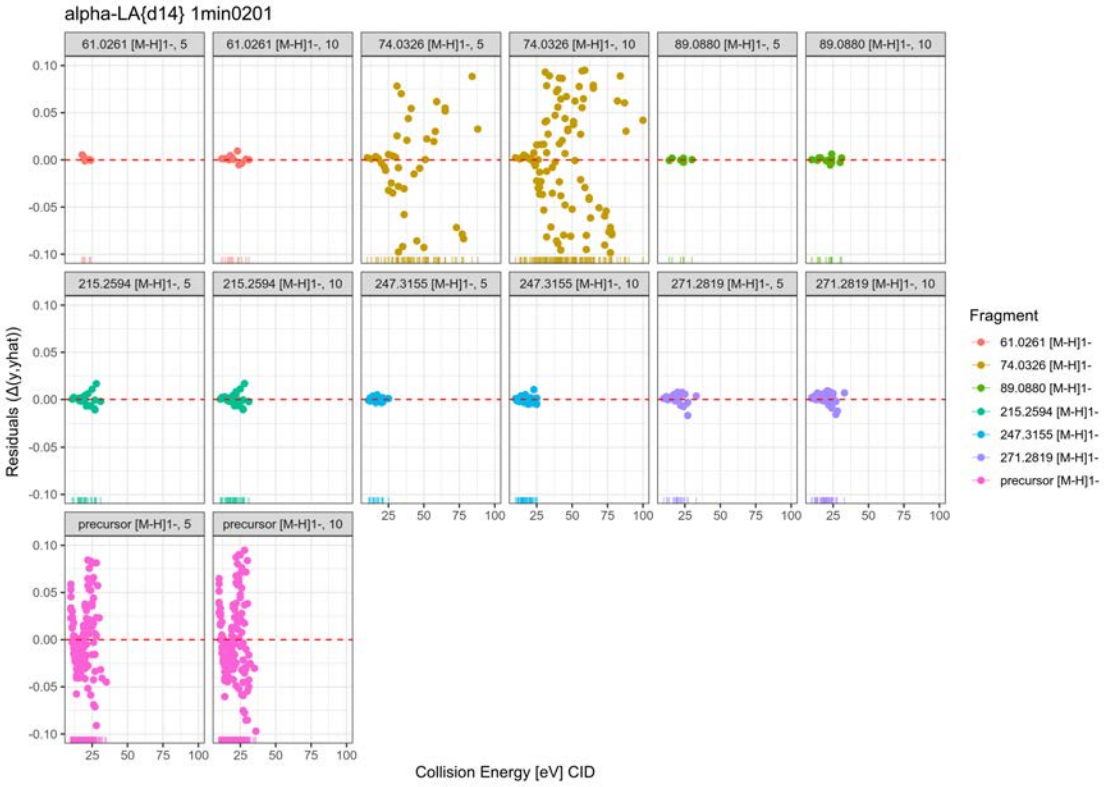


*Figure 267. Residuals of nonlinear fit*

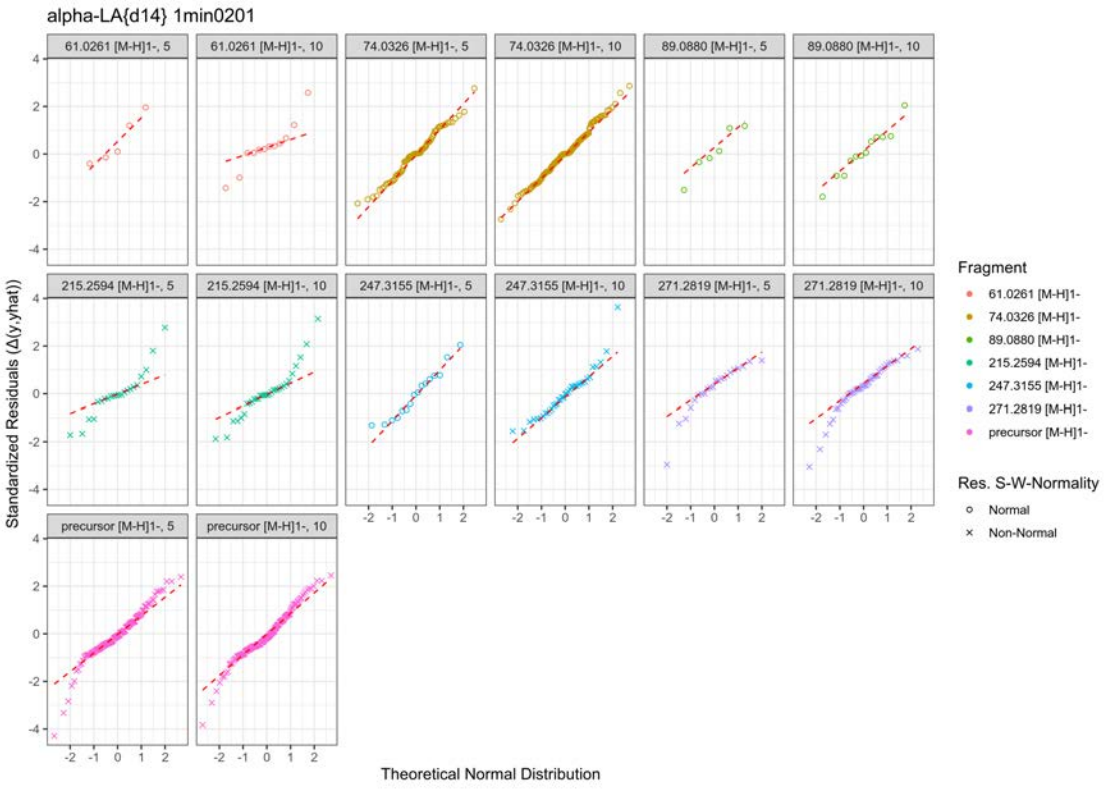


*Figure 268. Quantile-quantile plot of residuals*

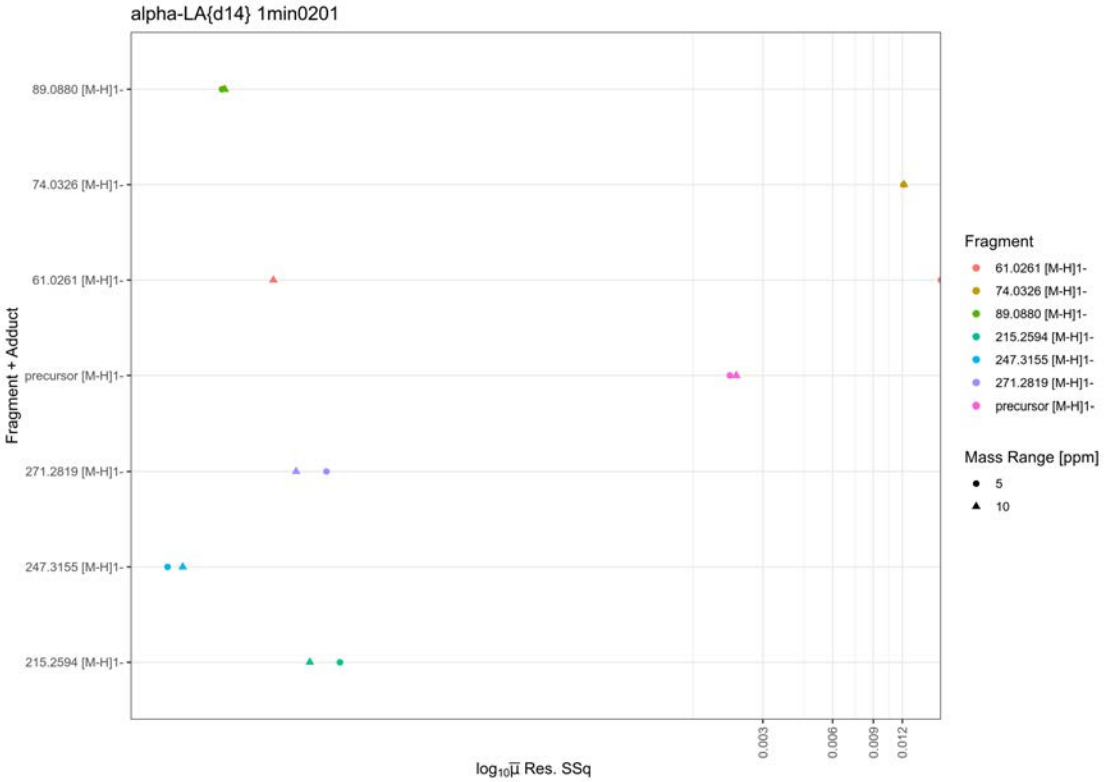


*Figure 269. Normalized sum-of-squares of the residuals*

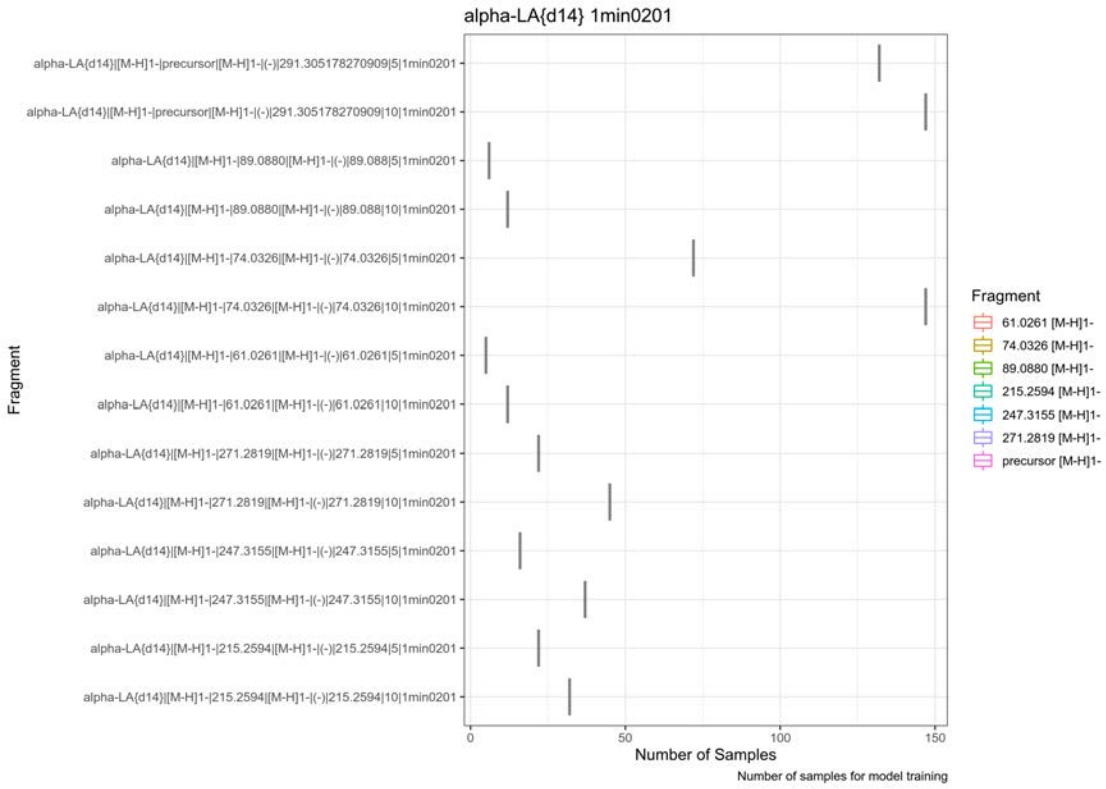


*Figure 270. Number of samples used for training per combination Id*

# 1.55. tetranor-12-HETE [M-H]1- 1min0069

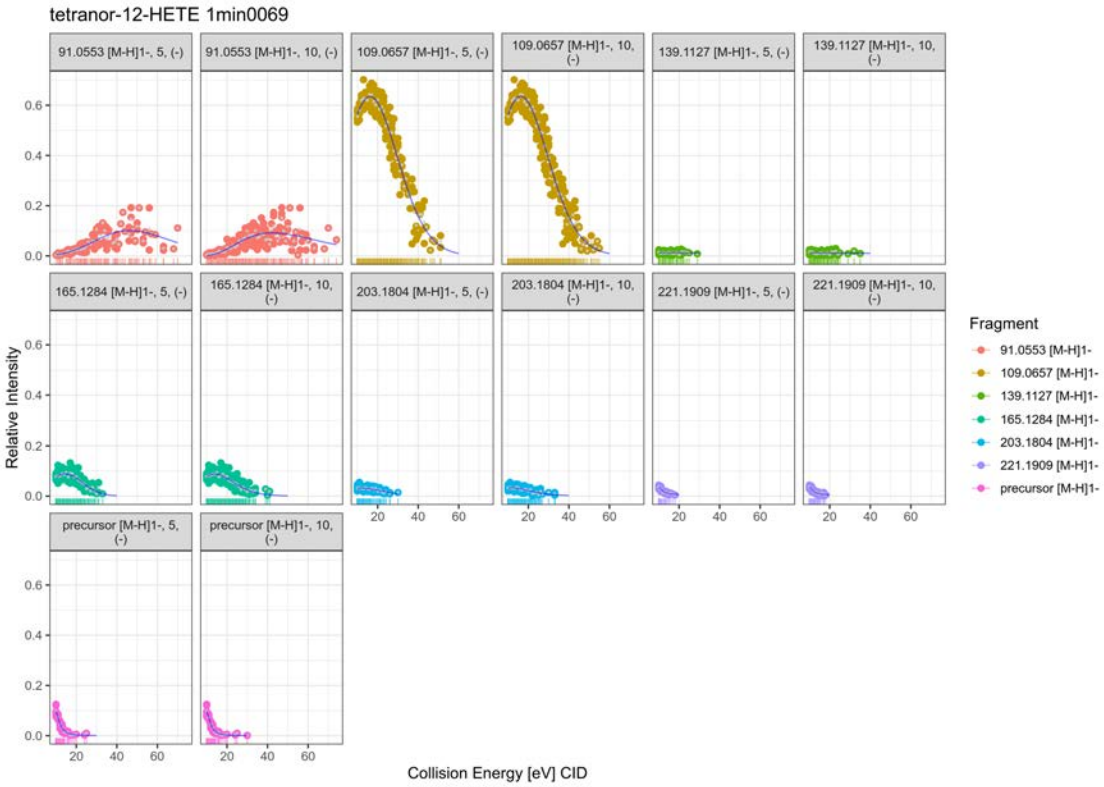


*Figure 271. Nonlinear fit*

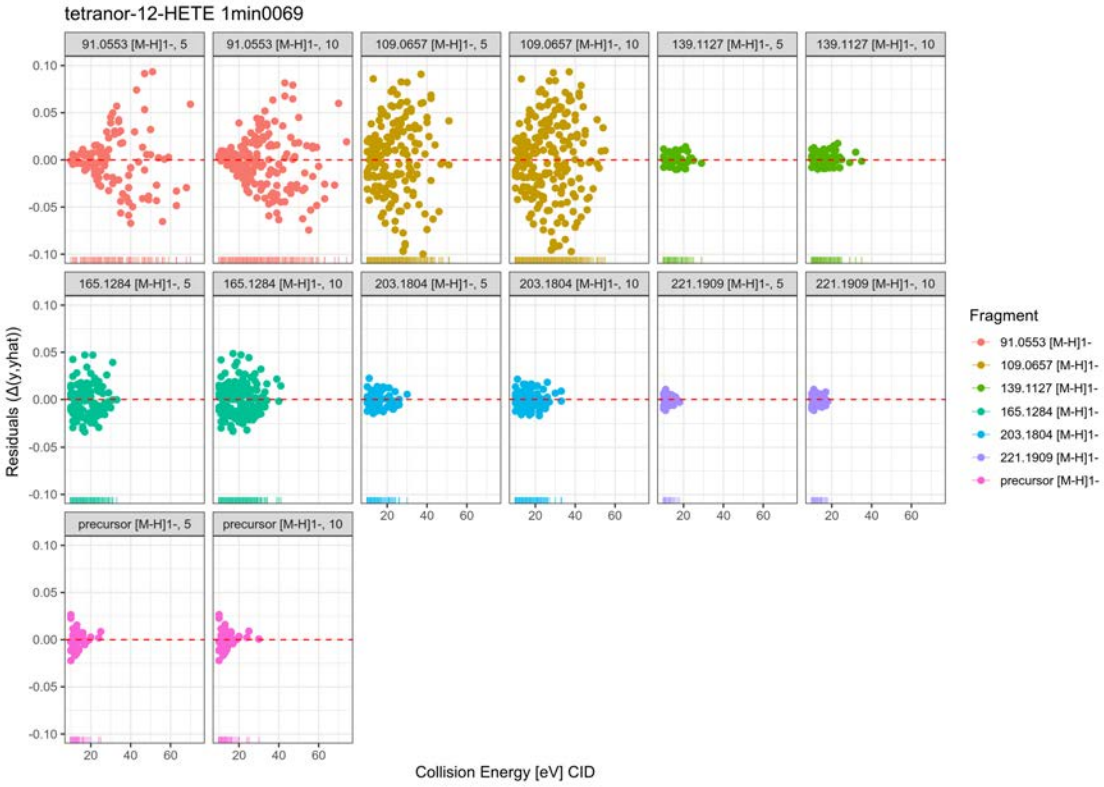


*Figure 272. Residuals of nonlinear fit*

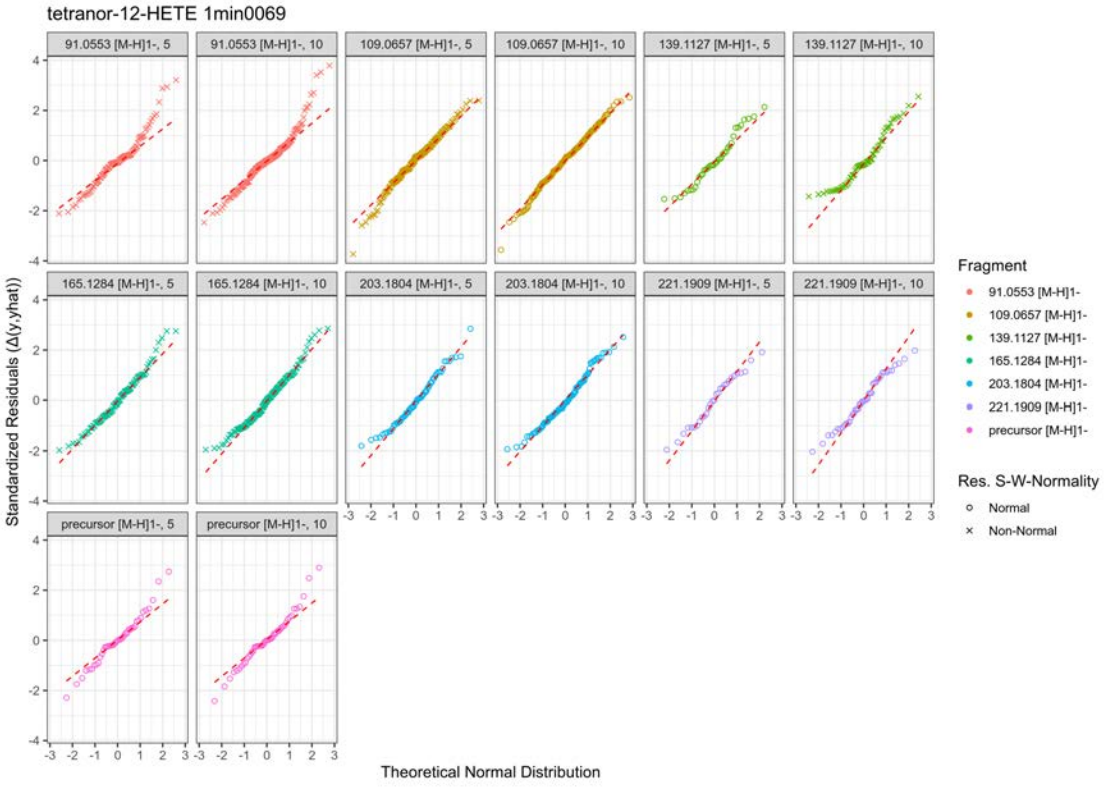


*Figure 273. Quantile-quantile plot of residuals*

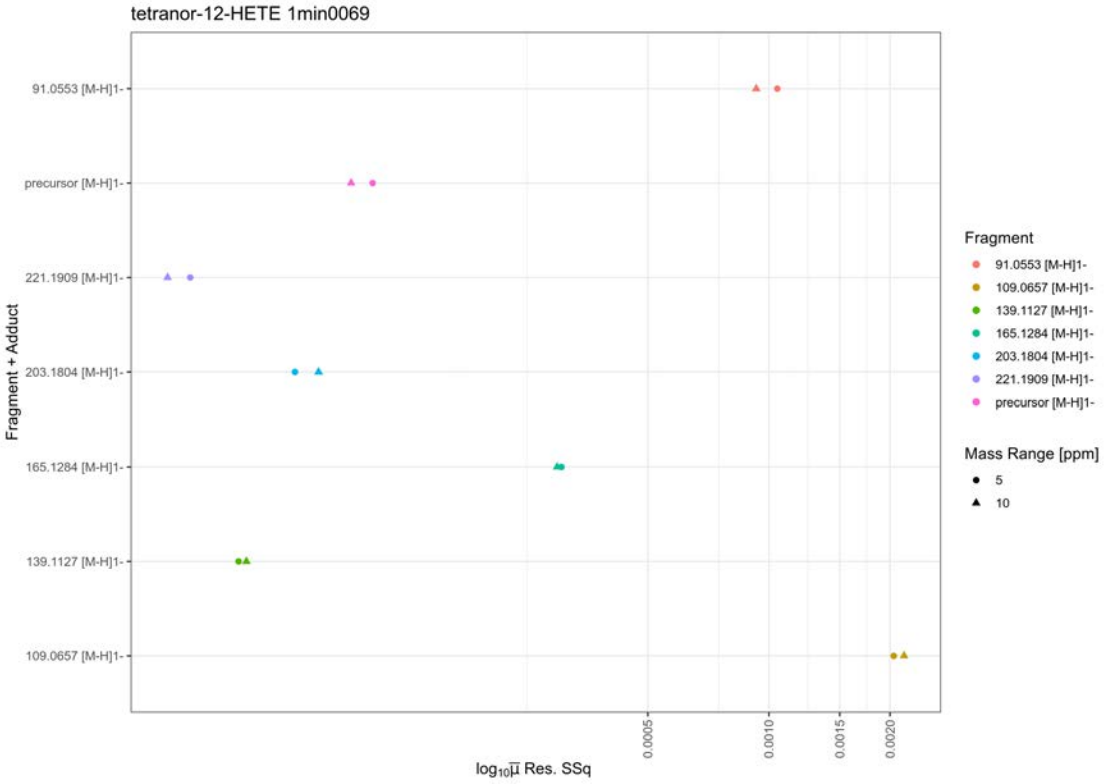


*Figure 274. Normalized sum-of-squares of the residuals*

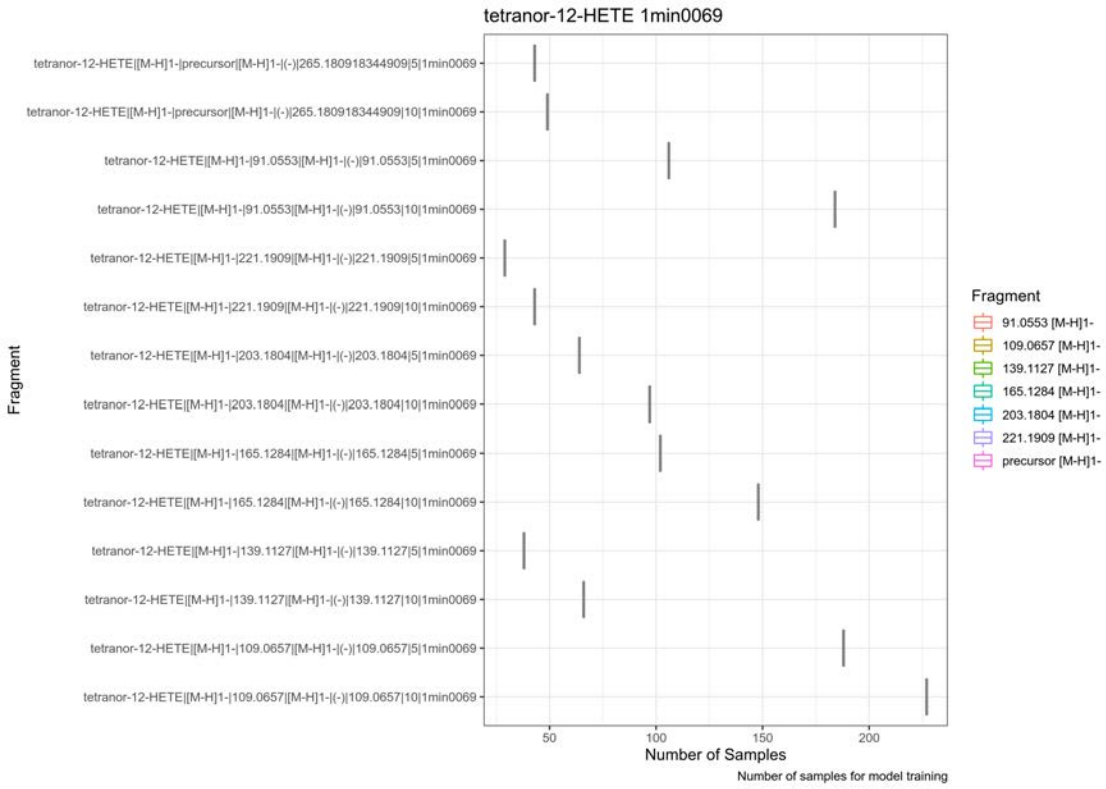


*Figure 275. Number of samples used for training per combination Id*