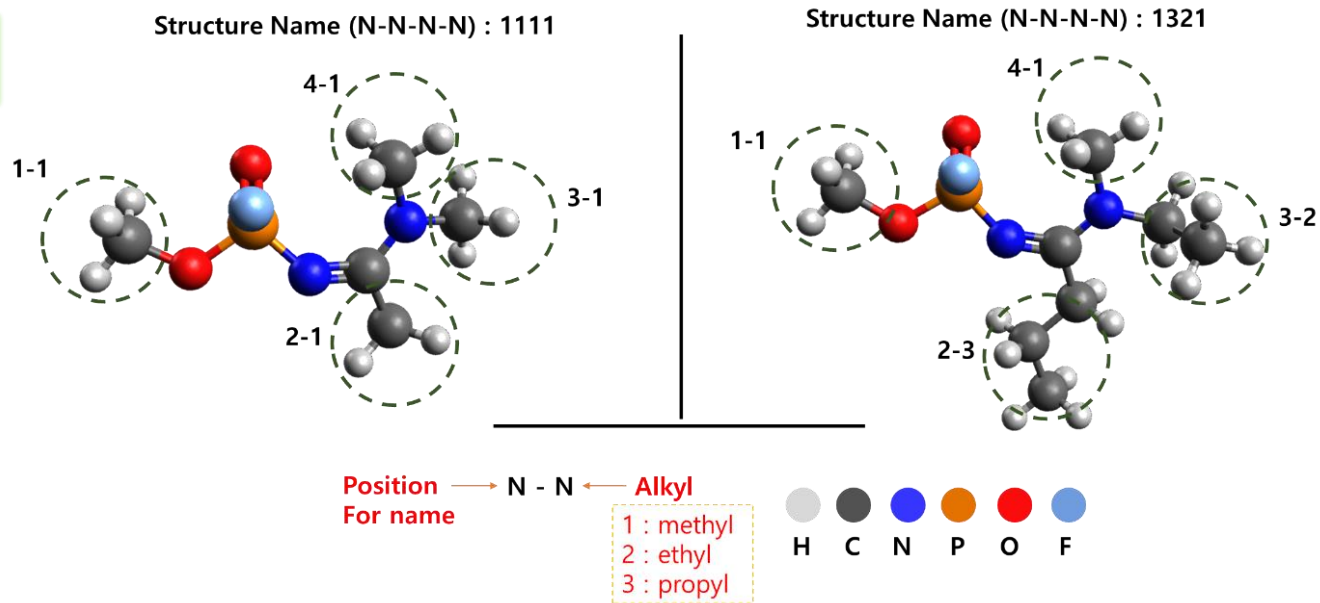


SI2. Each Novichok candidate structure and averaged ^1H and ^{13}C NMR chemical shift.

Structure index rule



1111 C

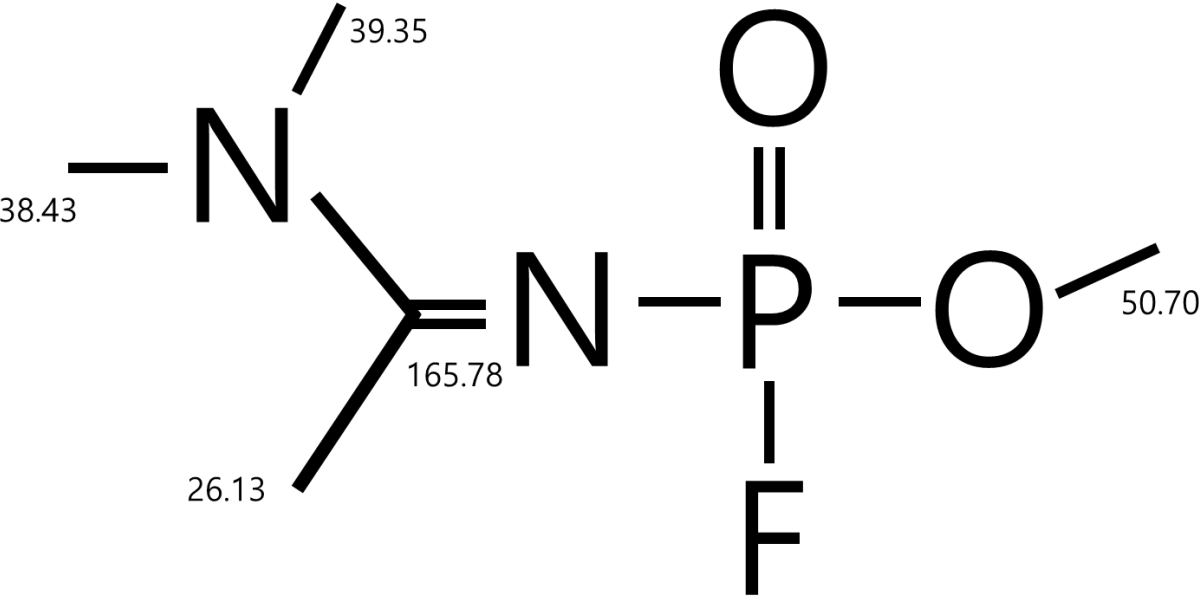


Figure S1. Structural index rule (upper figure) structure 1111 and its ^{13}C chemical shift (lower figure)

1112 C

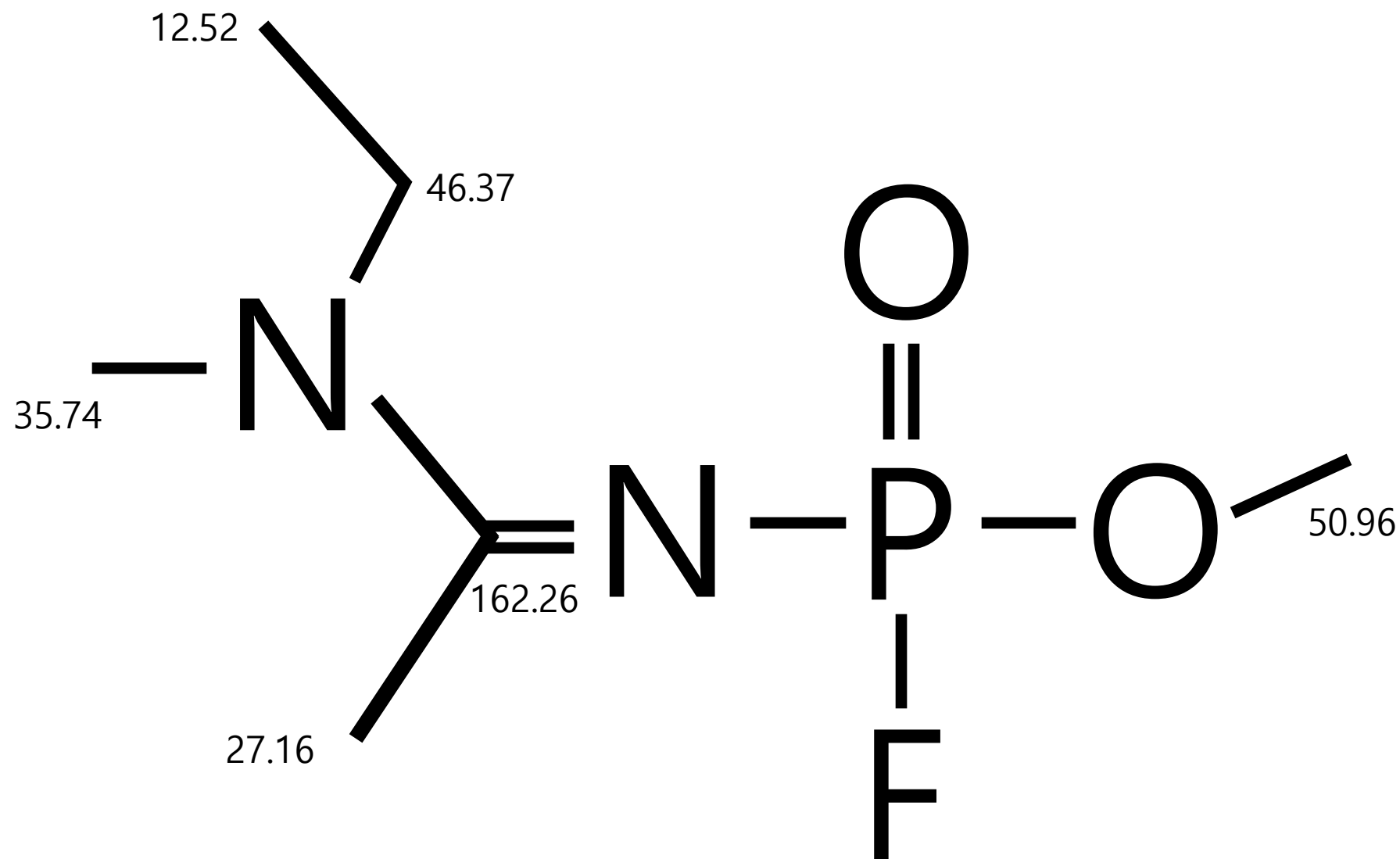


Figure S2. Structure 1112 and its ¹³C chemical shift

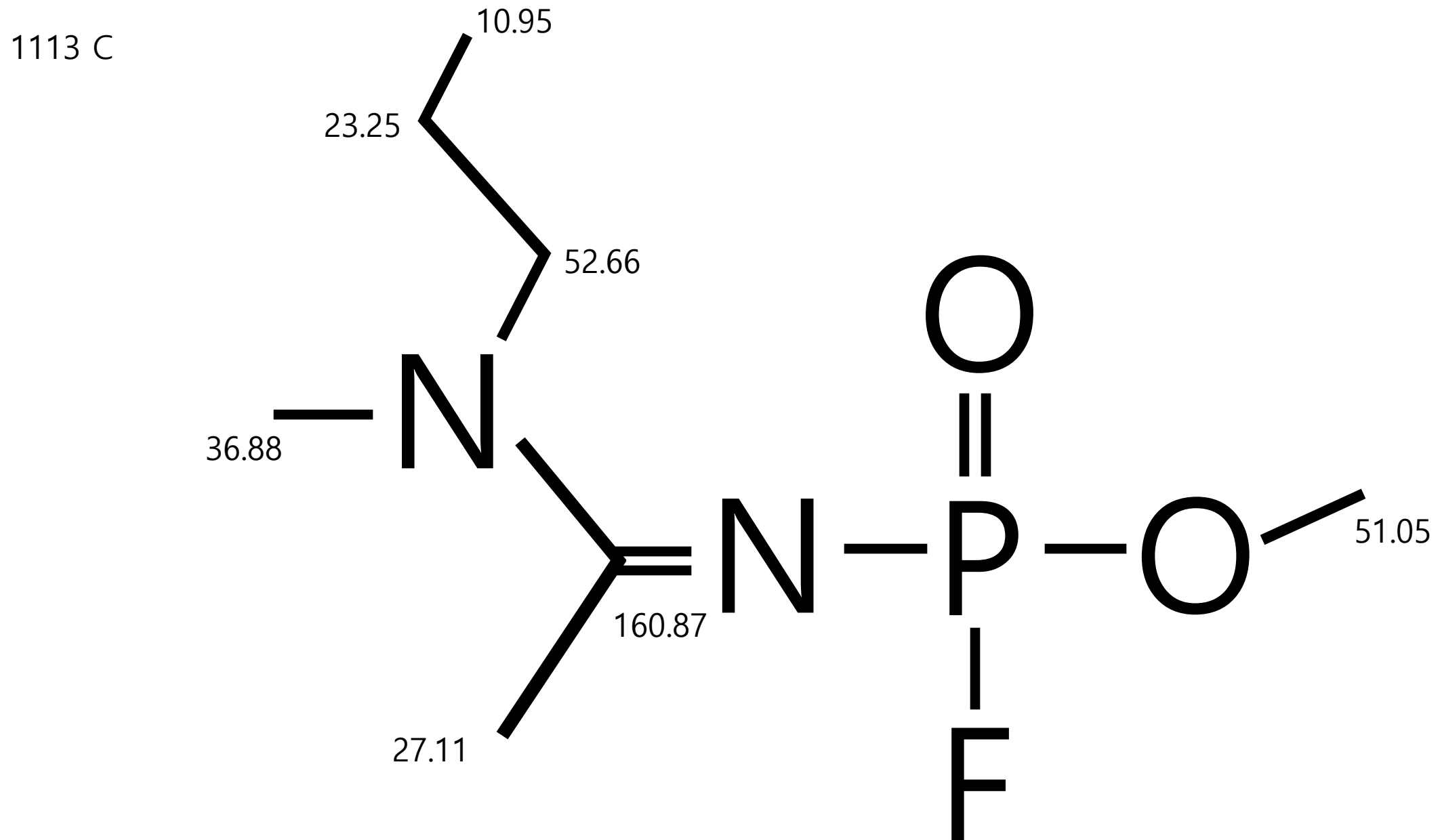


Figure S3. Structure 1113 and its ¹³C chemical shift

1121 C

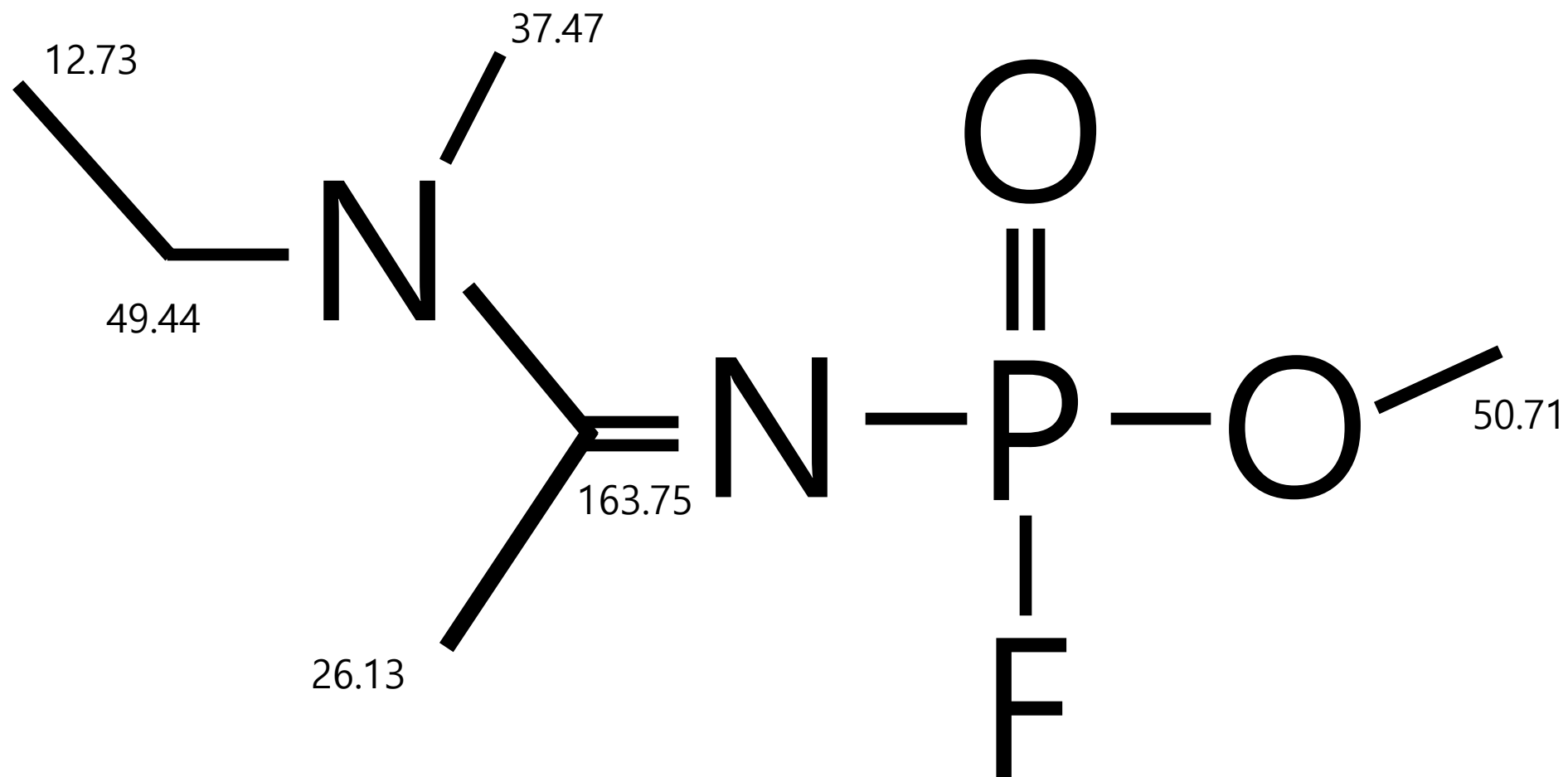


Figure S4. Structure 1121 and its ¹³C chemical shift

1122 C

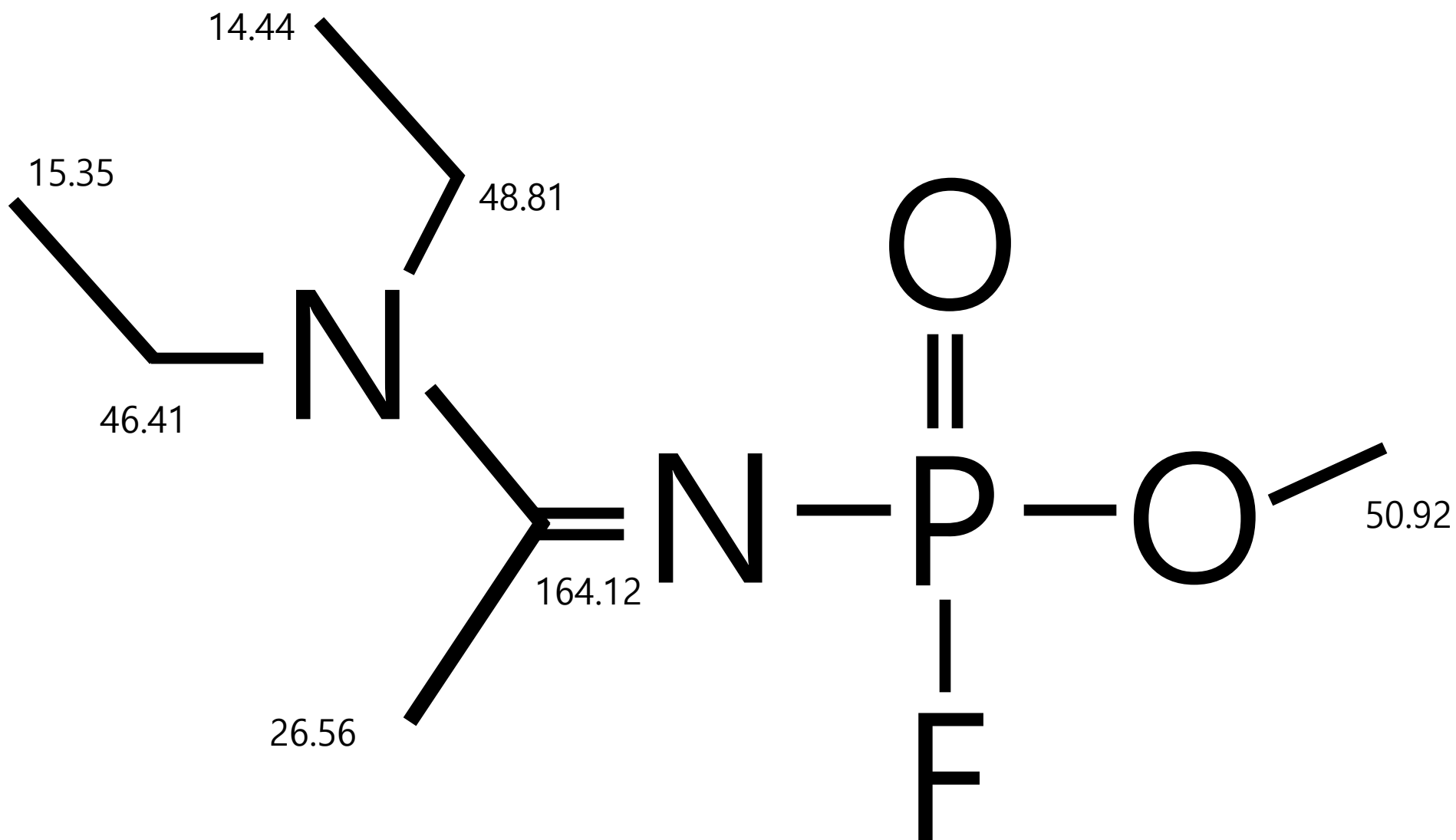


Figure S5. Structure 1122 and its ¹³C chemical shift

1131 C

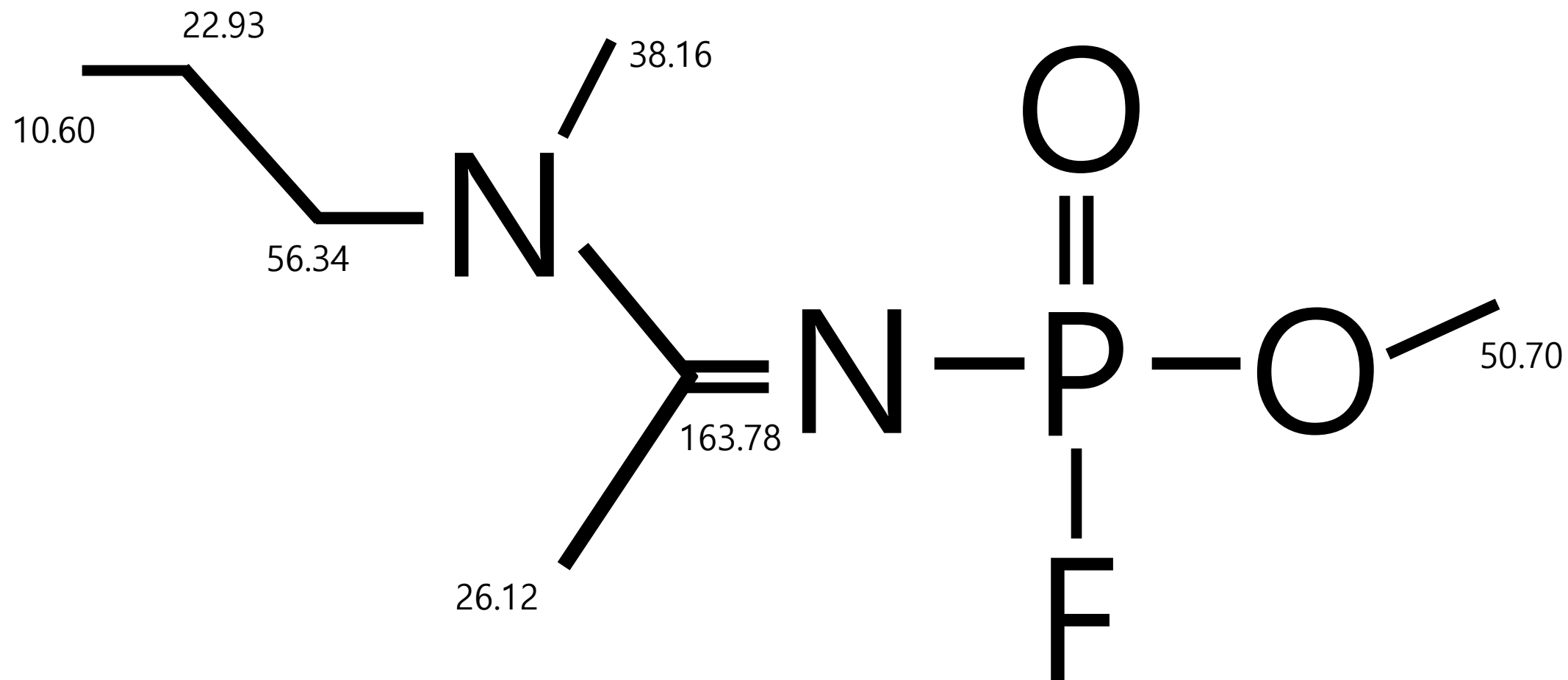


Figure S7. Structure 1131 and its ¹³C chemical shift

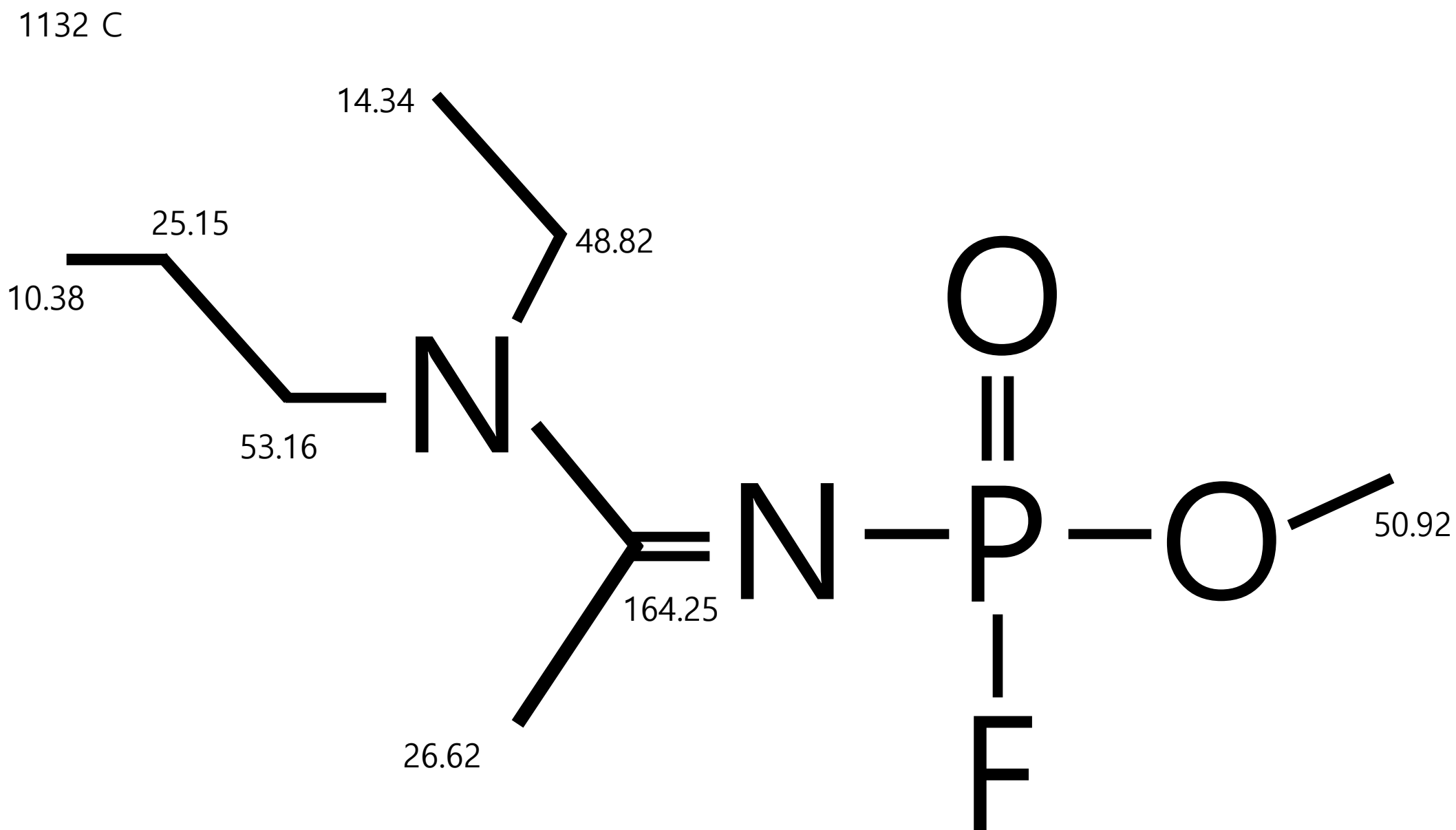


Figure 8. Structure 1132 and its ¹³C chemical shift

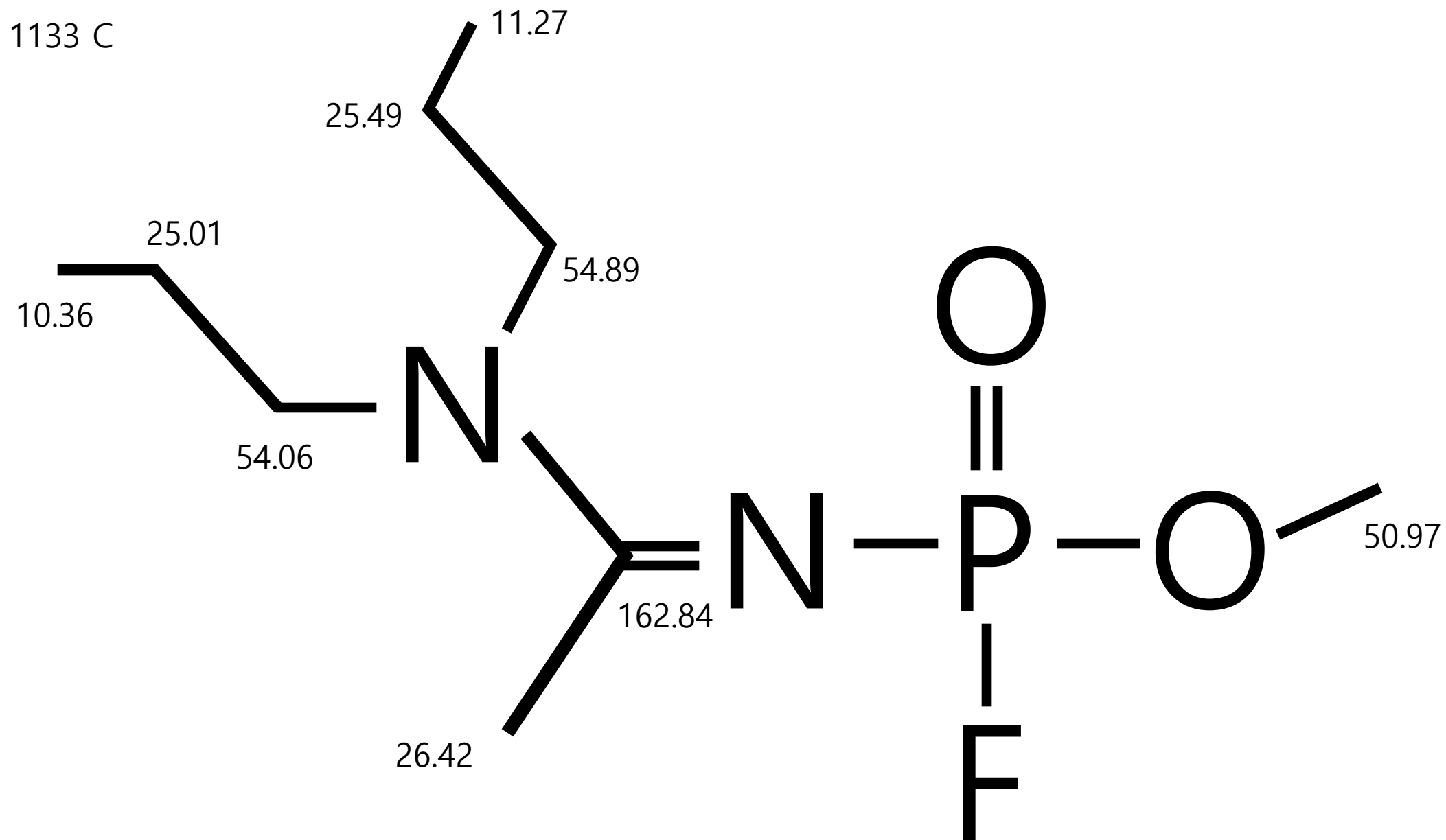


Figure S9. Structure 1133 and its ¹³C chemical shift

1211 C

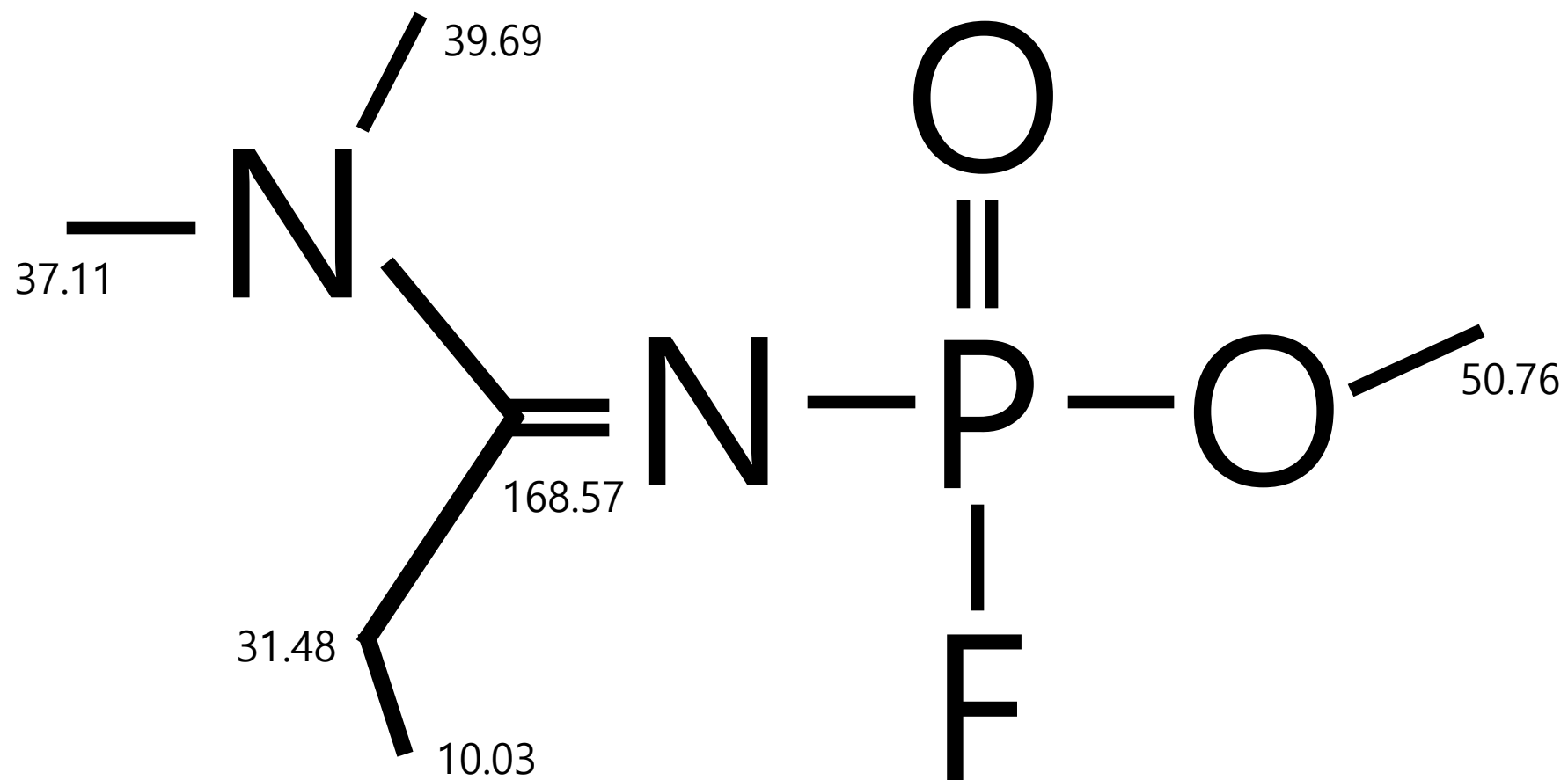


Figure S10. Structure 1211 and its ^{13}C chemical shift

1212 C

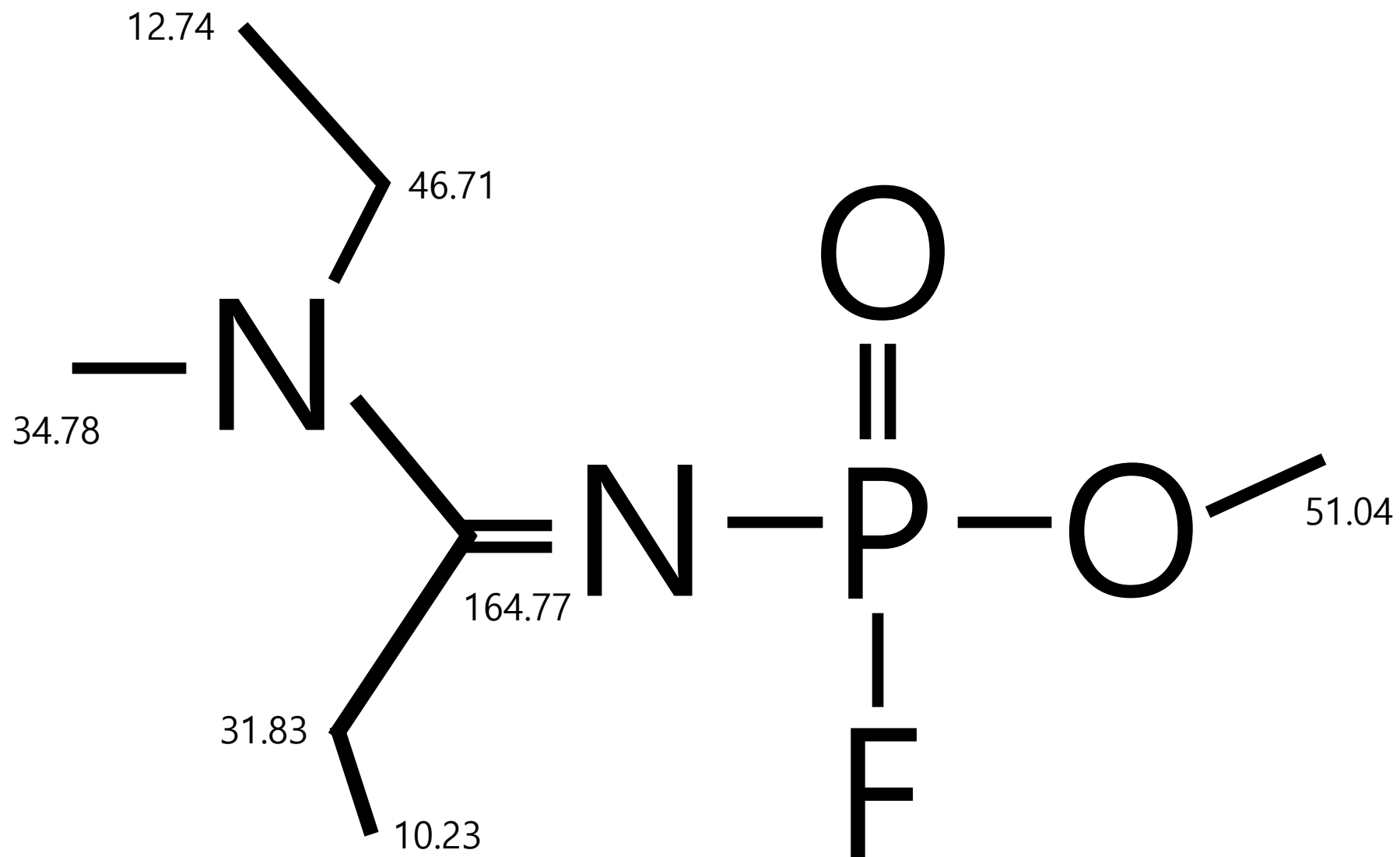


Figure S11. Structure 1212 and its ^{13}C chemical shift

1213 C

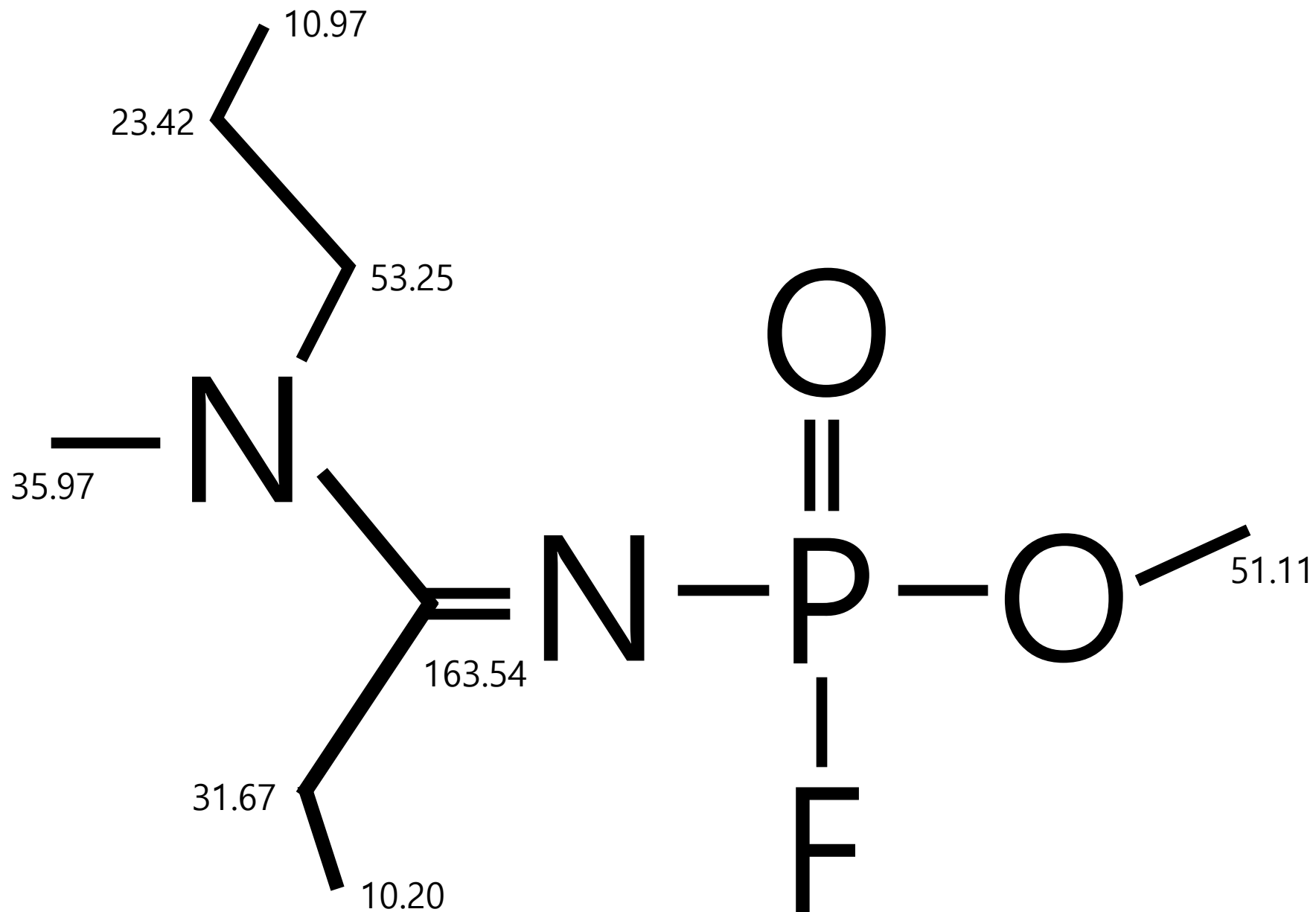


Figure S12. Structure 1213 and its ^{13}C chemical shift

1221 C

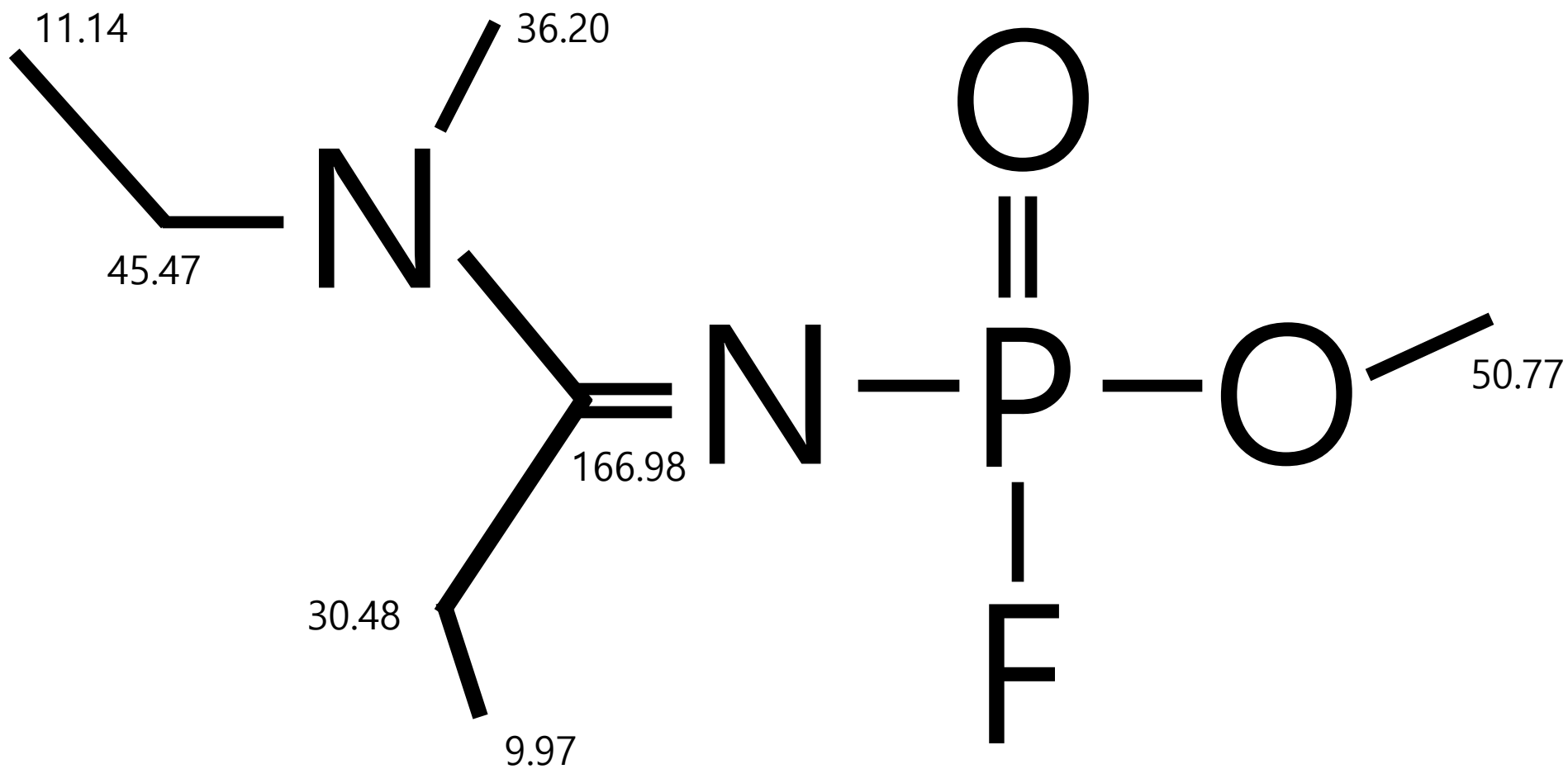


Figure S13. Structure 1221 and its ¹³C chemical shift

1222 C

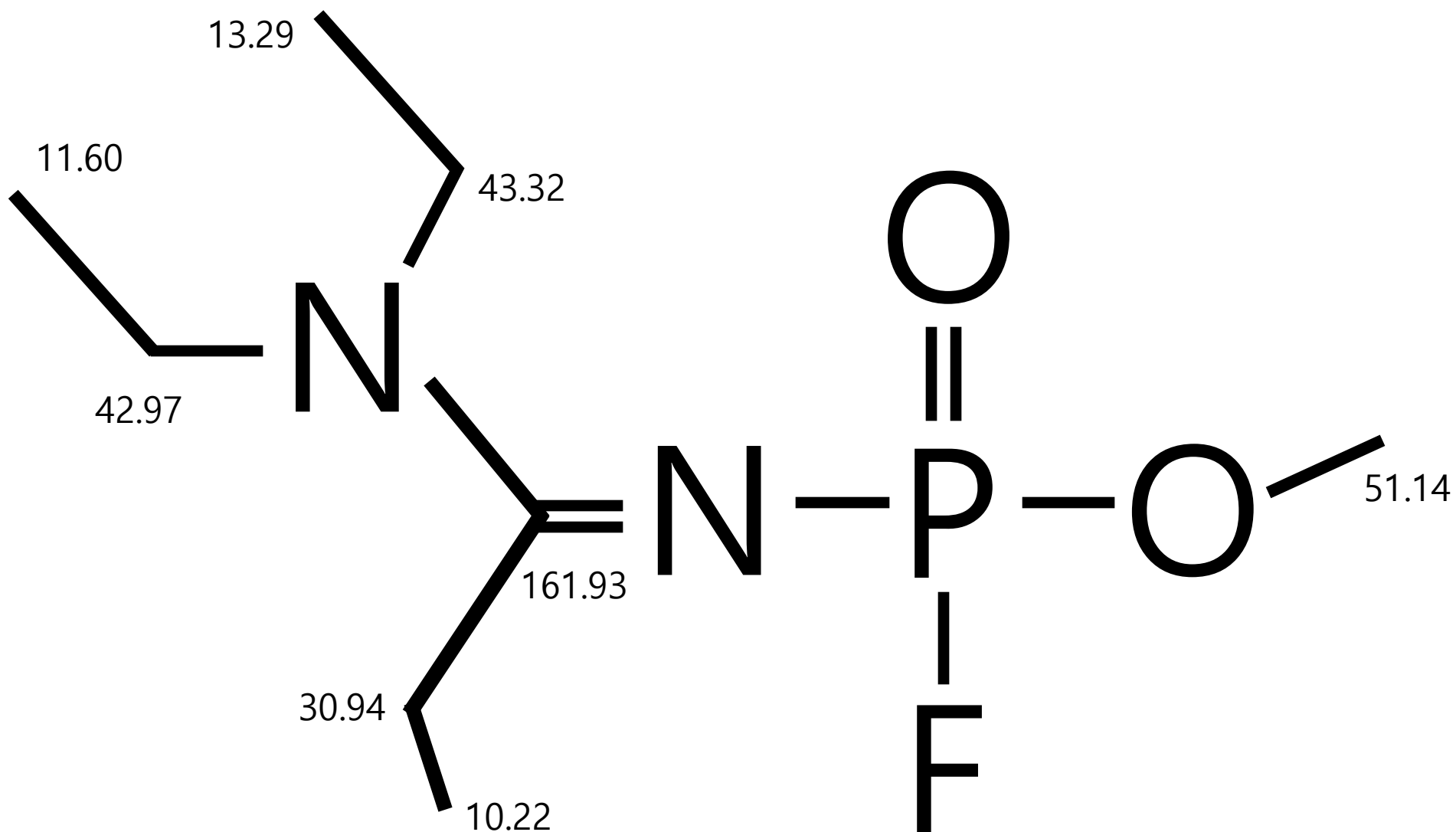


Figure S14. Structure 1222 and its ^{13}C chemical shift

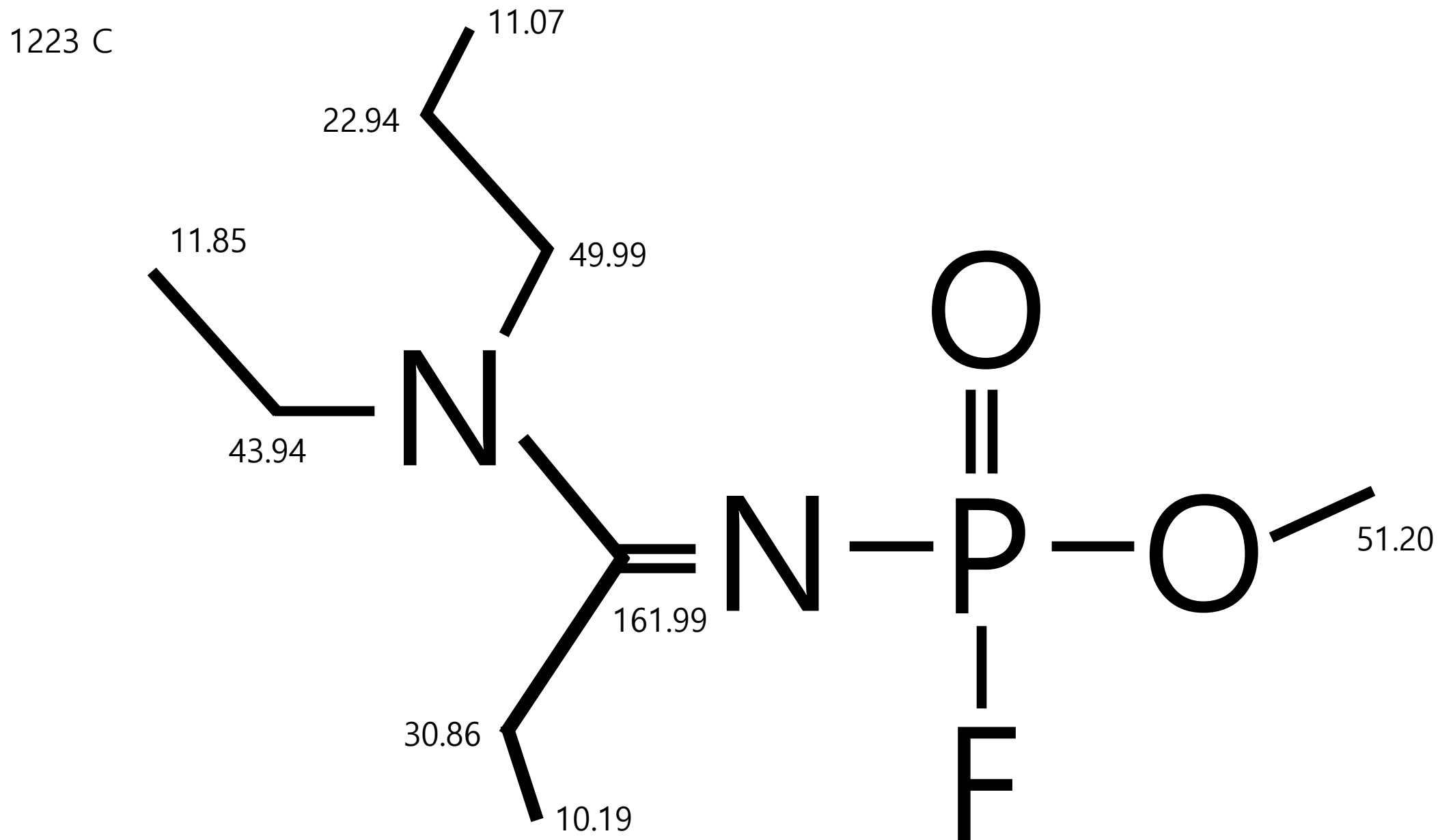


Figure S15. Structure 1223 and its ¹³C chemical shift

1231 C

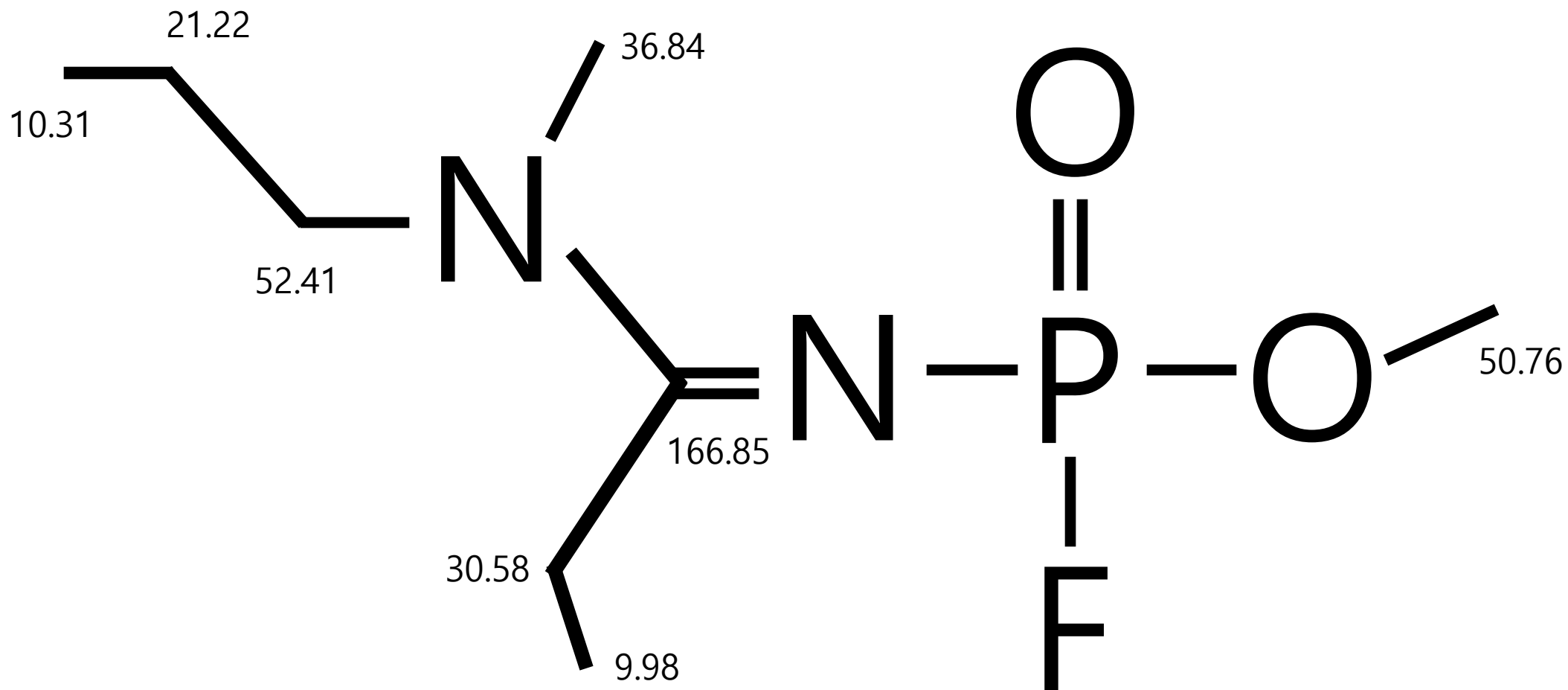


Figure S16. Structure 1231 and its ¹³C chemical shift

The chemical structure is 1,1,1-trifluoro-2-methyl-2-(2-methyl-2-oxoethyl)hydrazine-5-phosphate. The ¹³C NMR chemical shifts (in ppm) are labeled on the structure as follows:

- 10.44: Methyl carbon of the 2-methyl-2-oxoethyl group.
- 21.77: Methyl carbon of the 2-methyl-2-oxoethyl group.
- 49.95: Carbonyl carbon of the 2-methyl-2-oxoethyl group.
- 13.34: Methyl carbon of the 2-methyl-2-oxoethyl group.
- 43.98: Methyl carbon of the 2-methyl-2-oxoethyl group.
- 161.98: Carbonyl carbon of the 2-methyl-2-oxoethyl group.
- 31.07: Methyl carbon of the 2-methyl-2-oxoethyl group.
- 10.21: Methyl carbon of the 2-methyl-2-oxoethyl group.
- 51.14: Methyl carbon of the phosphate group.

Figure S17. Structure 1232 and its ^{13}C chemical shift

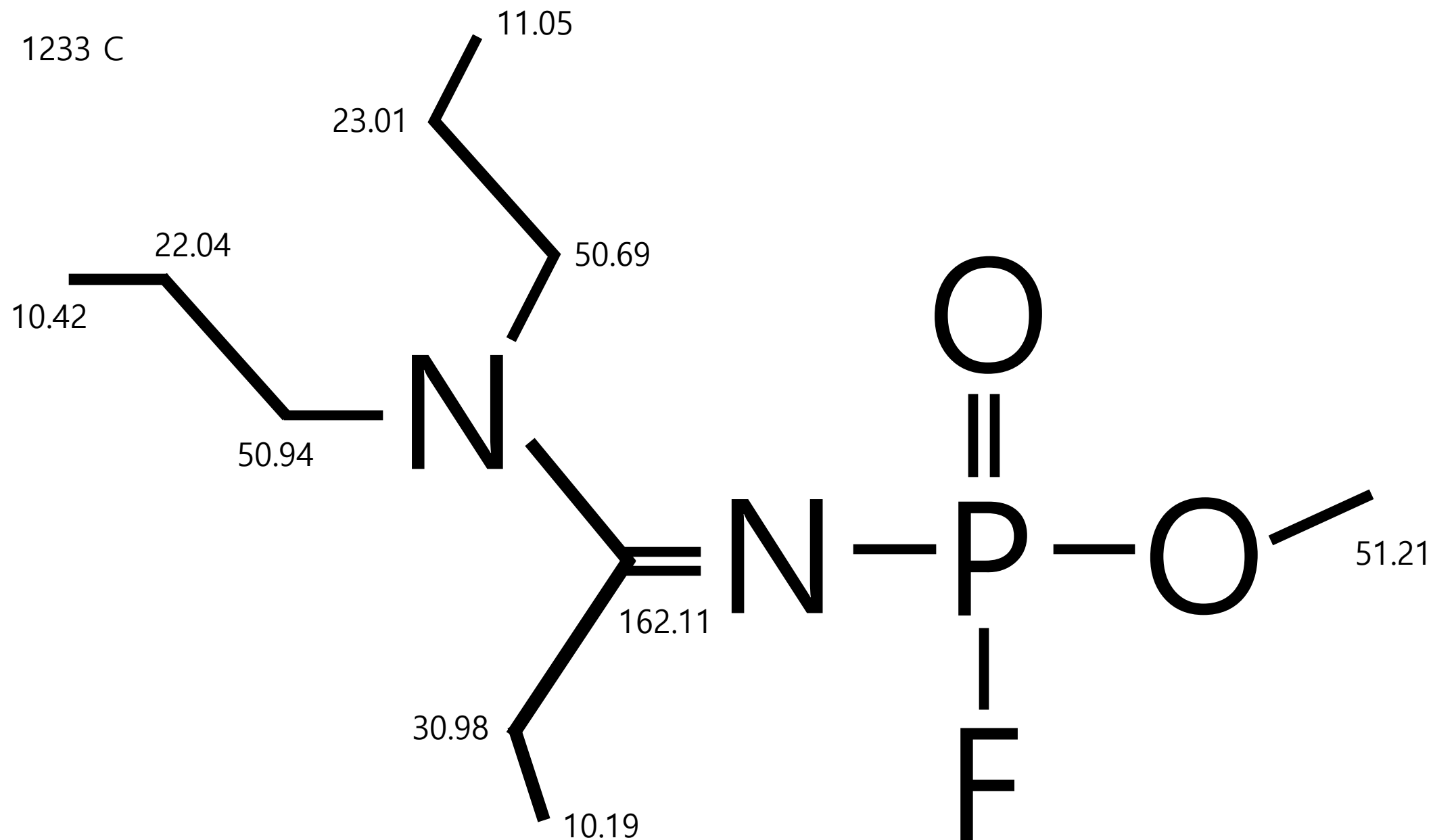


Figure S18. Structure 1233 and its ¹³C chemical shift

1311 C

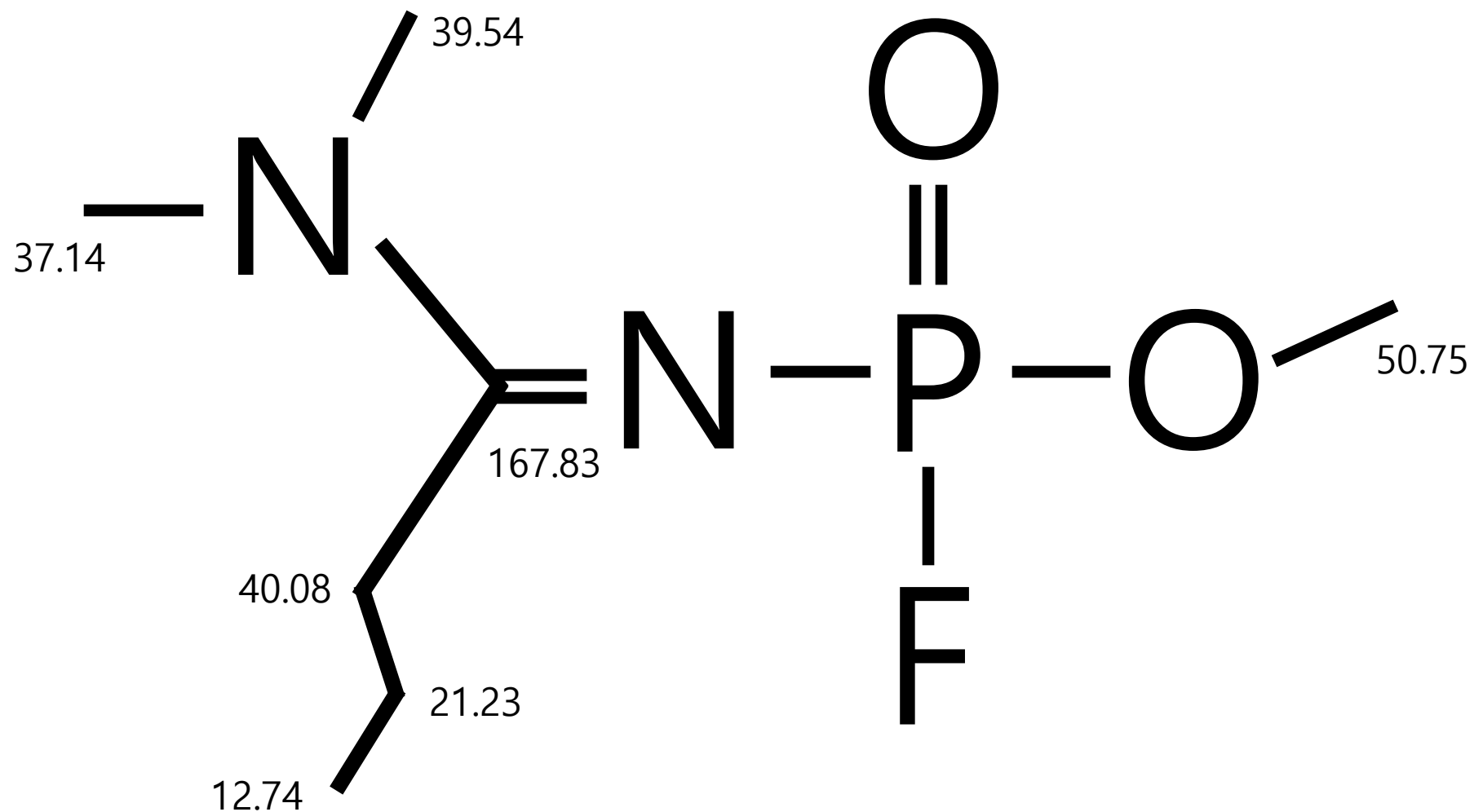


Figure S19. Structure 1311 and its ¹³C chemical shift

1312 C

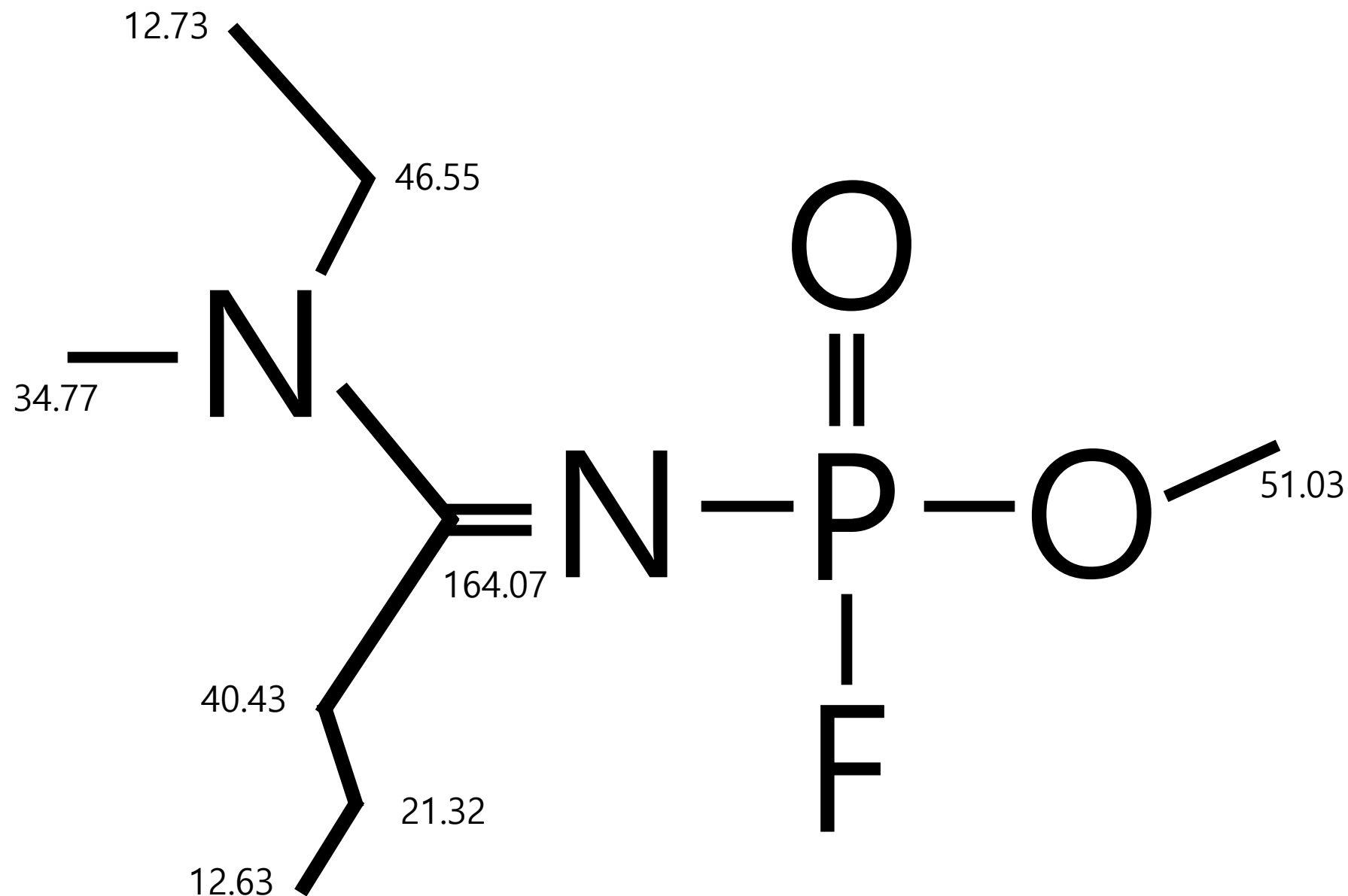


Figure S20. Structure 1312 and its ¹³C chemical shift

1313 C

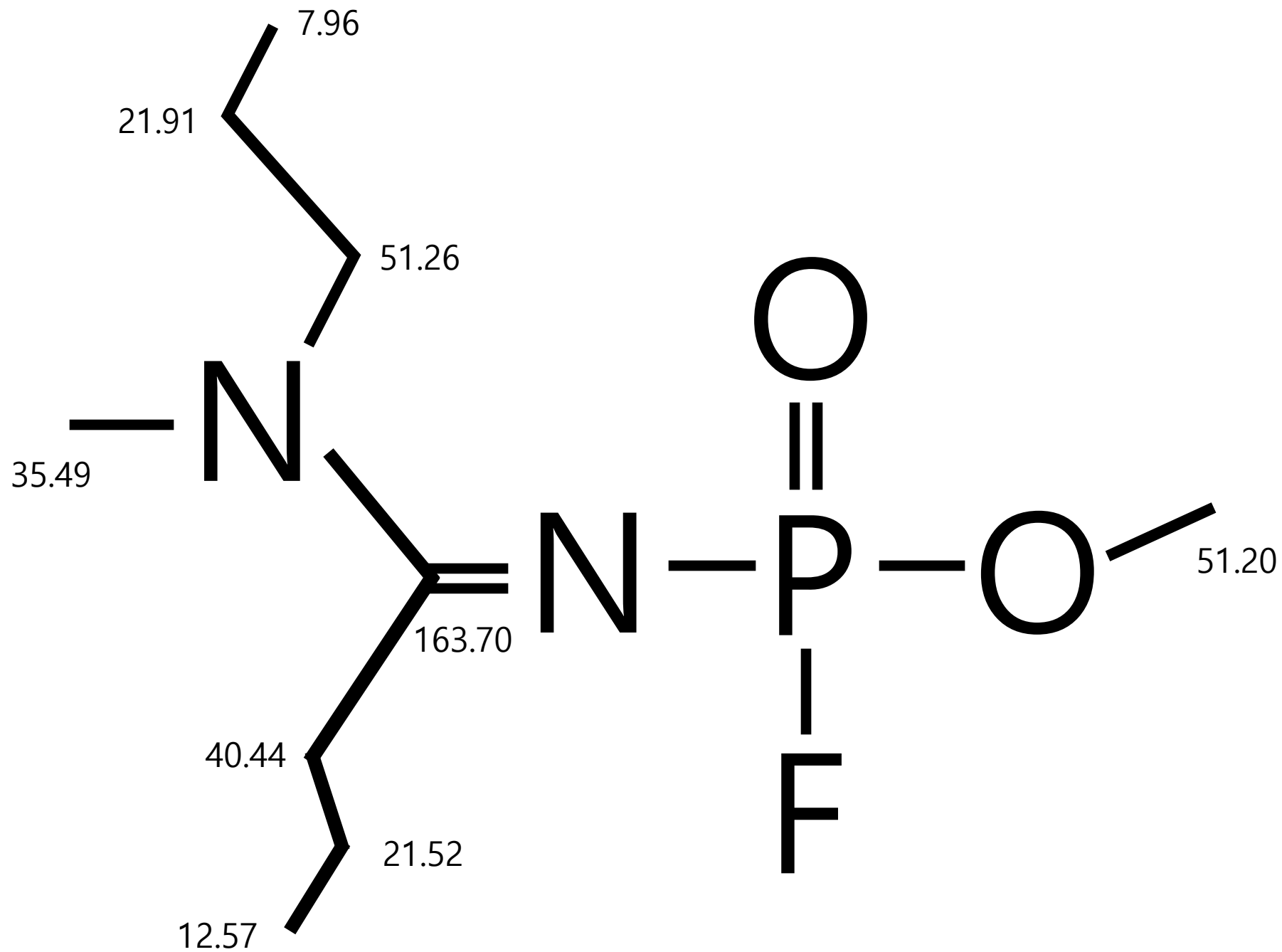


Figure S21. Structure 1313 and its ¹³C chemical shift

1321 C

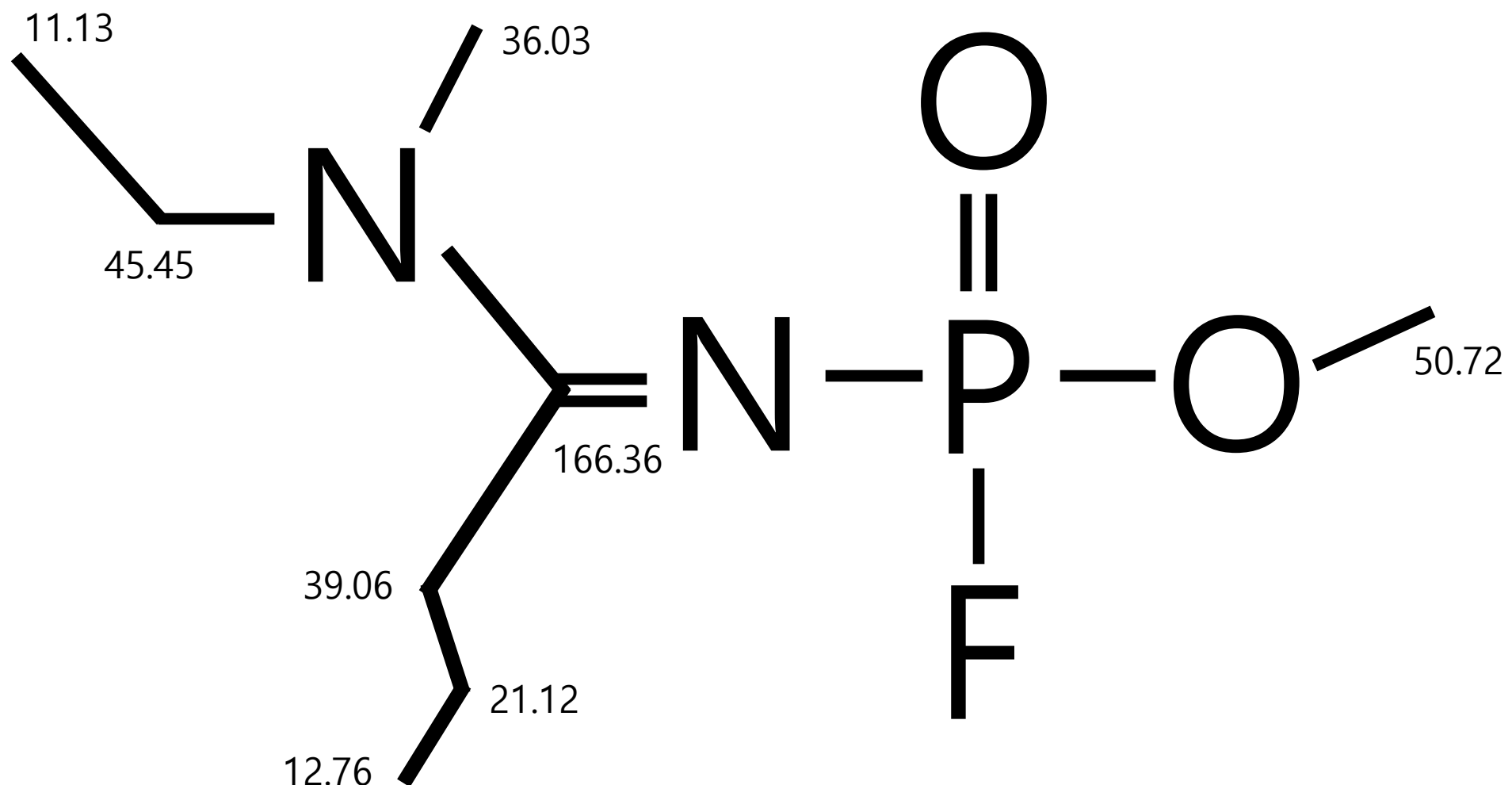


Figure S22. Structure 1321 and its ^{13}C chemical shift

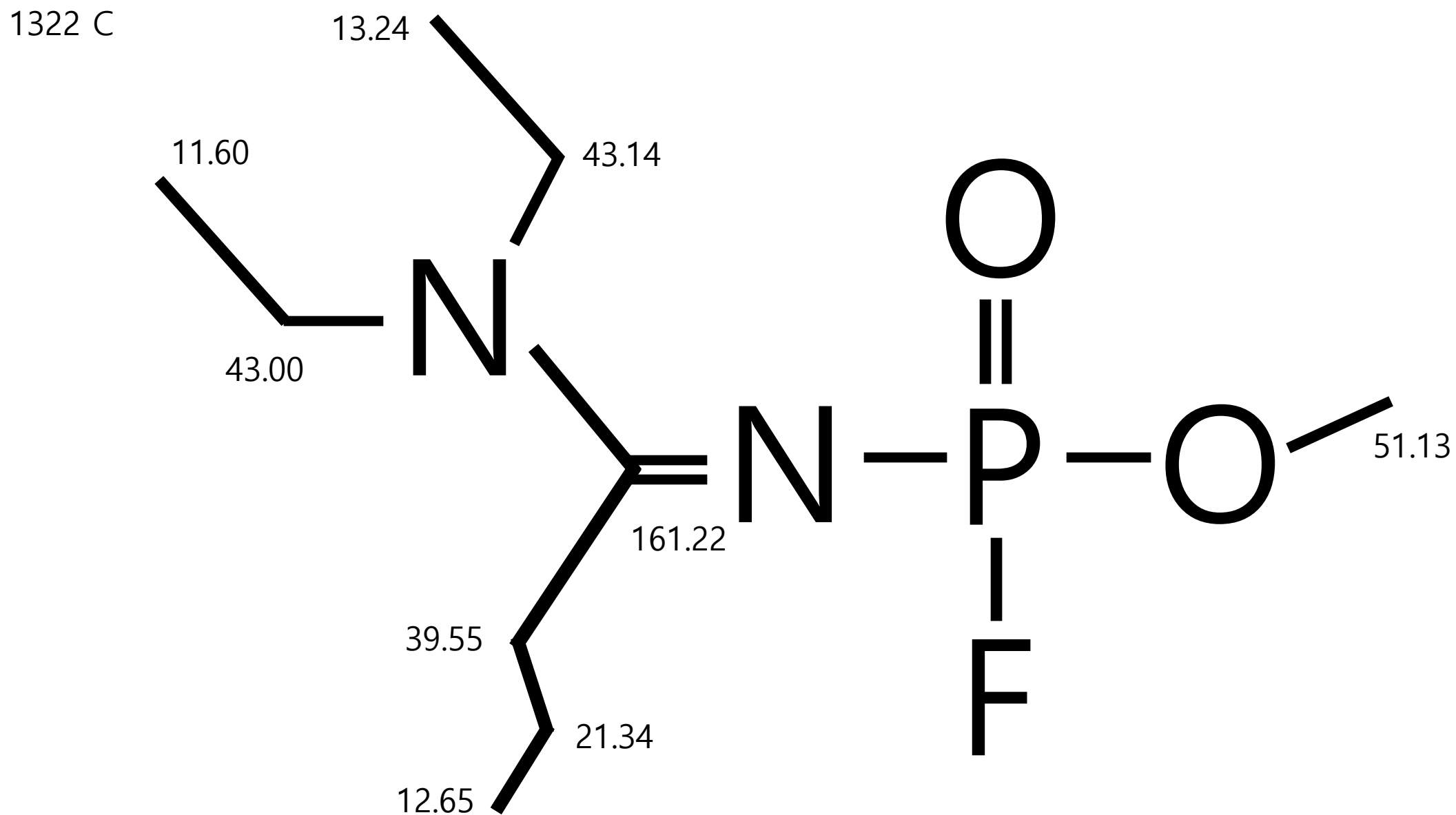


Figure S23. Structure 1322 and its ¹³C chemical shift

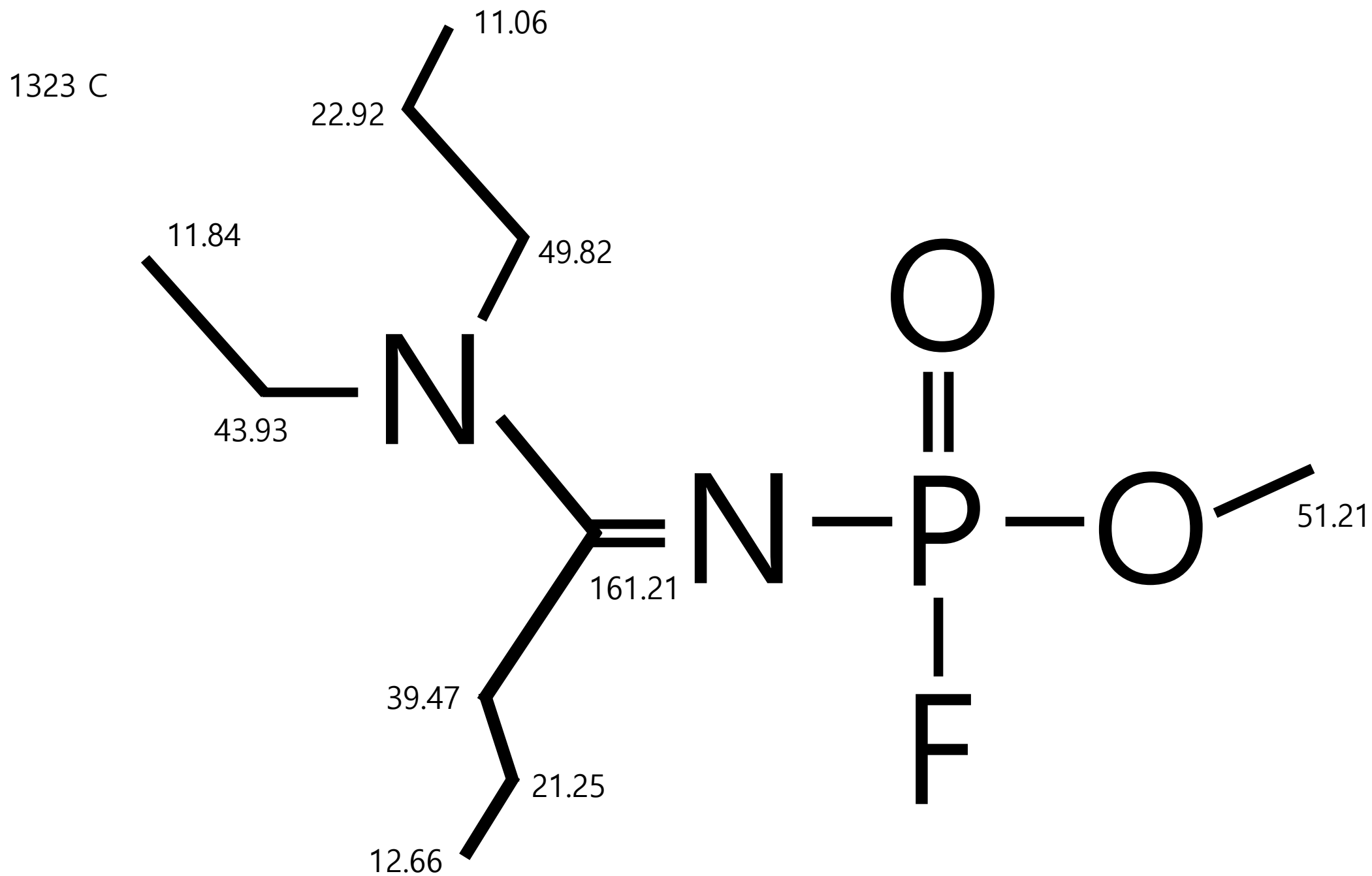


Figure S24. Structure 1323 and its ¹³C chemical shift

1331 C

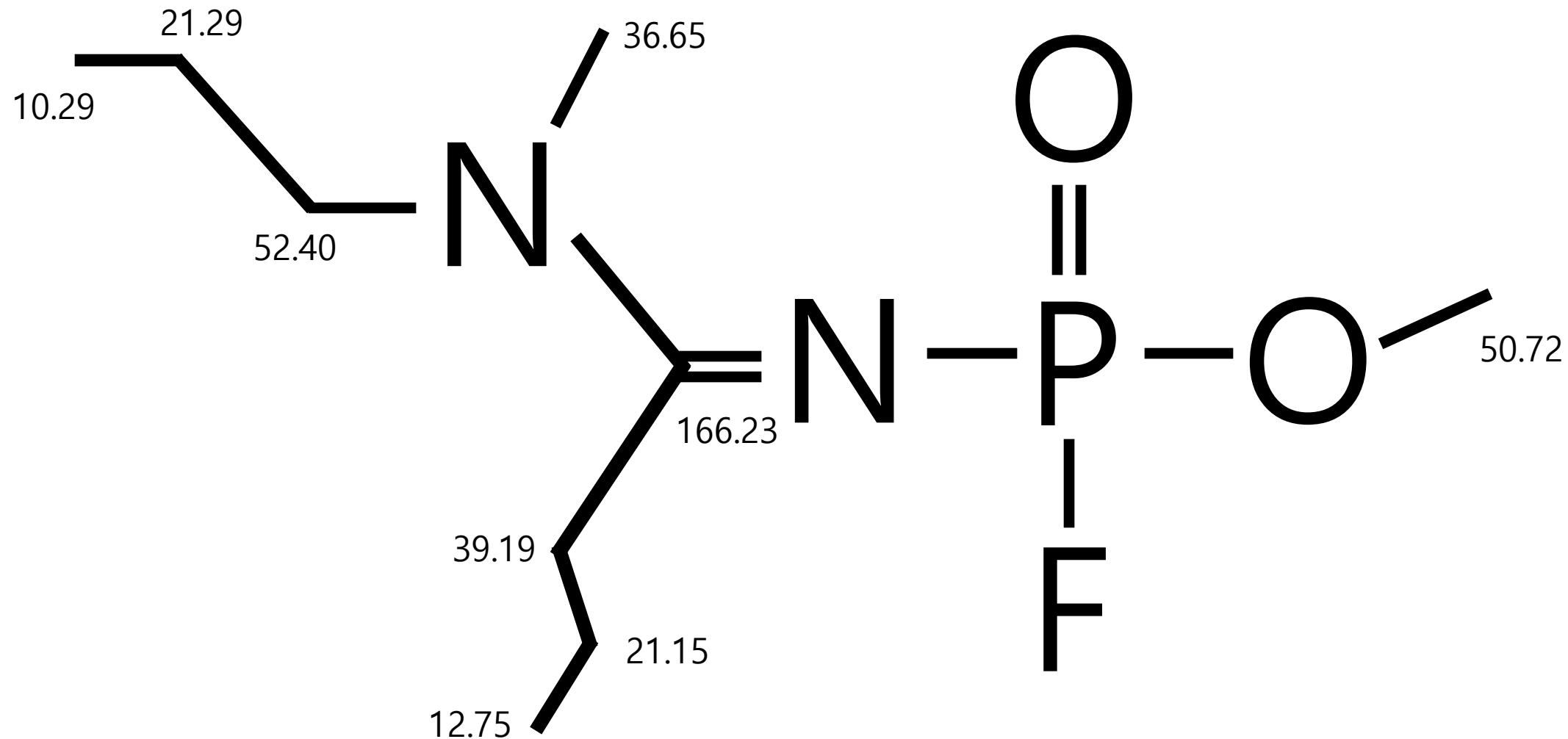


Figure S25. Structure 1331 and its ¹³C chemical shift

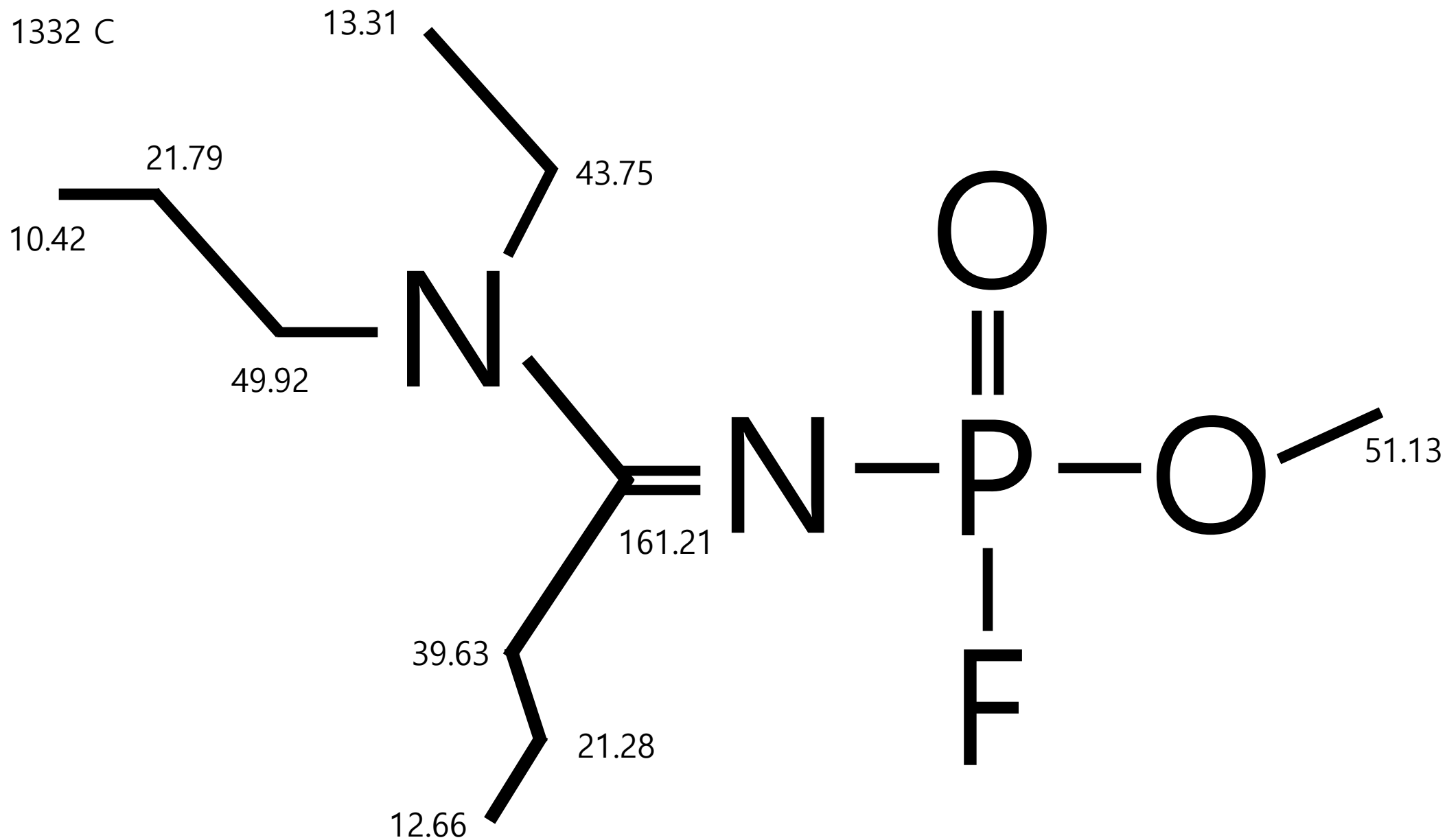


Figure S26. Structure 1332 and its ¹³C chemical shift

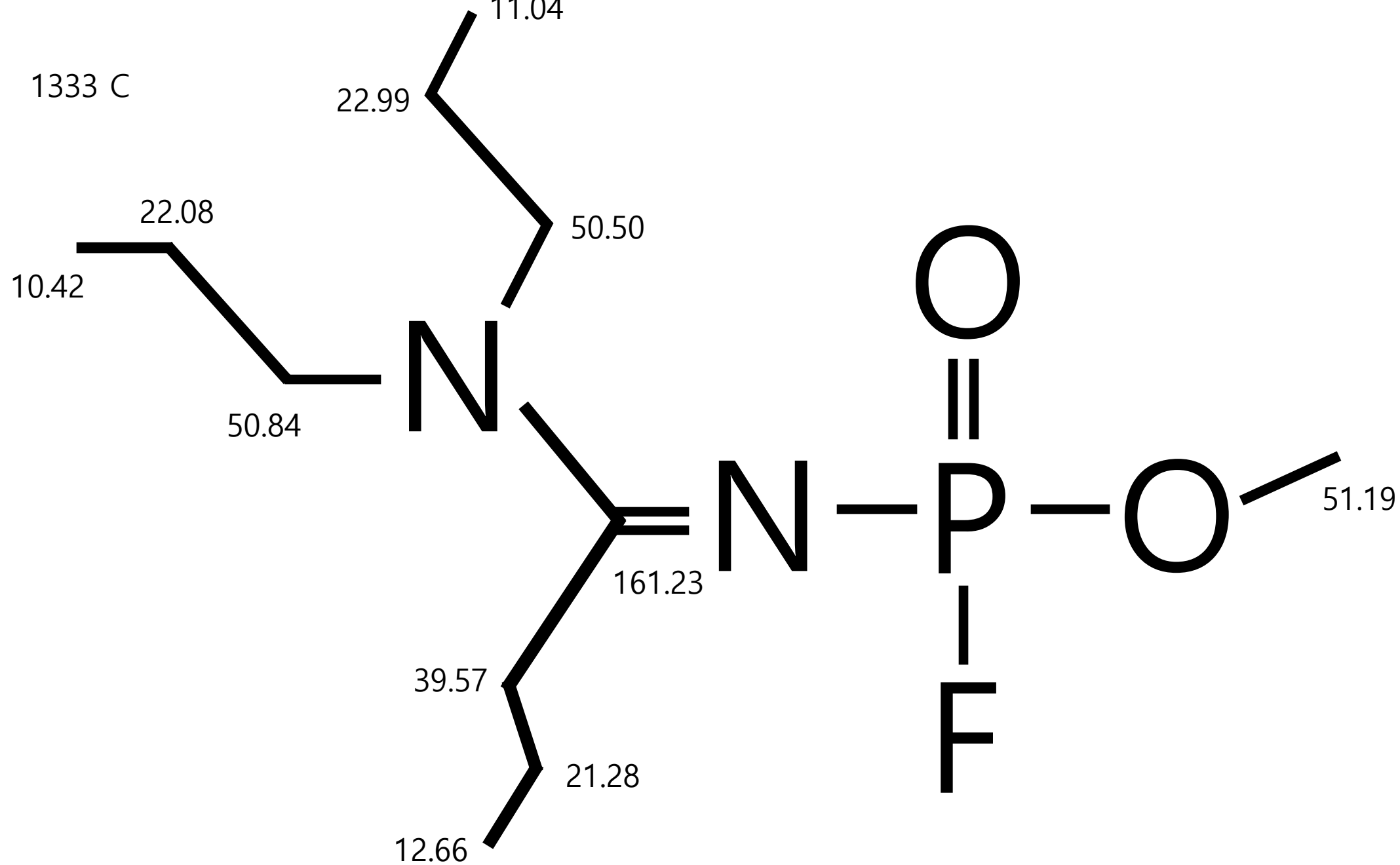


Figure S27. Structure 1333 and its ¹³C chemical shift

2111 C

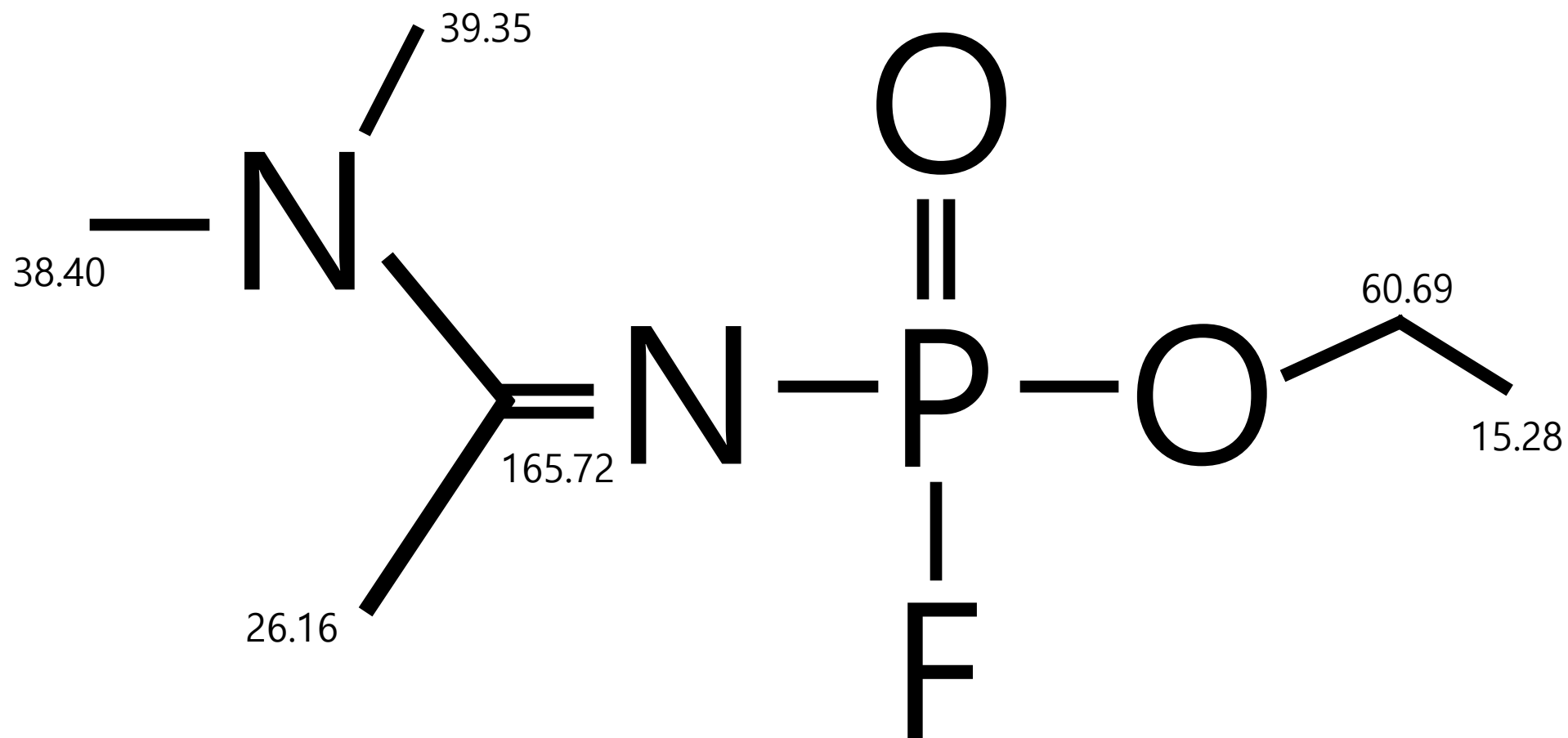


Figure S28. Structure 2111 and its ^{13}C chemical shift

2112 C

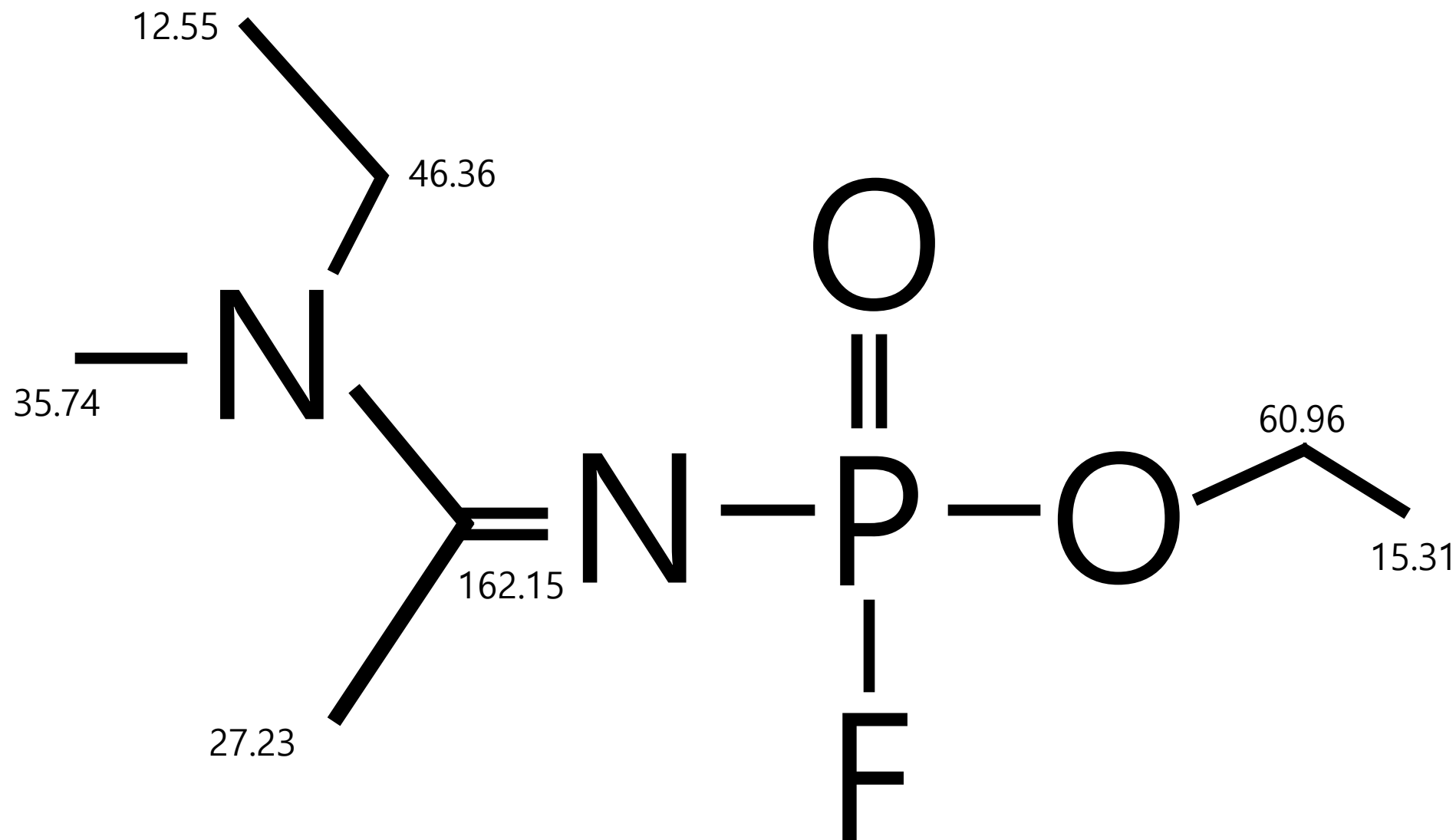


Figure S29. Structure 2112 and its ¹³C chemical shift

2113 C

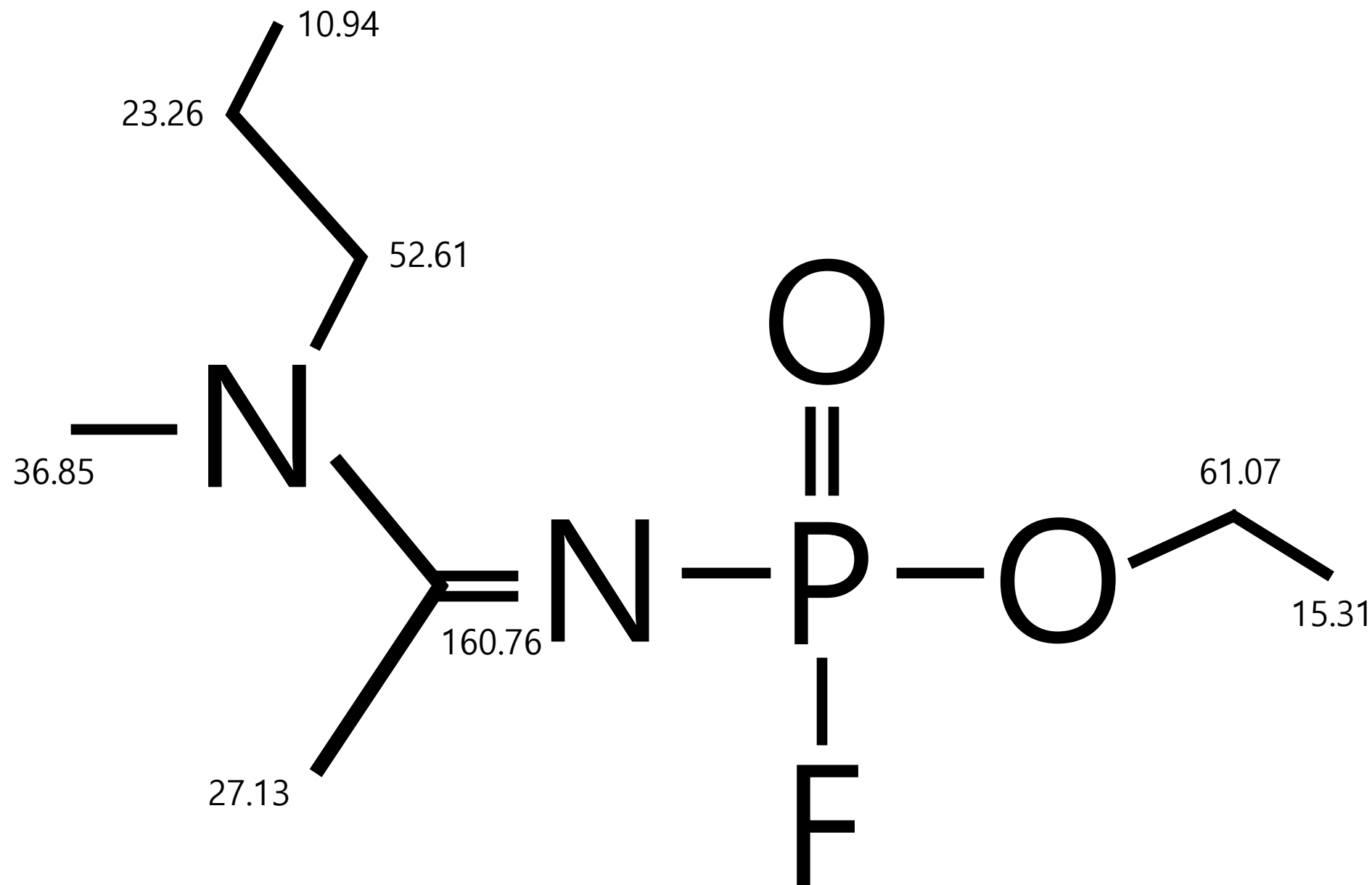


Figure S30. Structure 2113 and its ¹³C chemical shift

2121 C

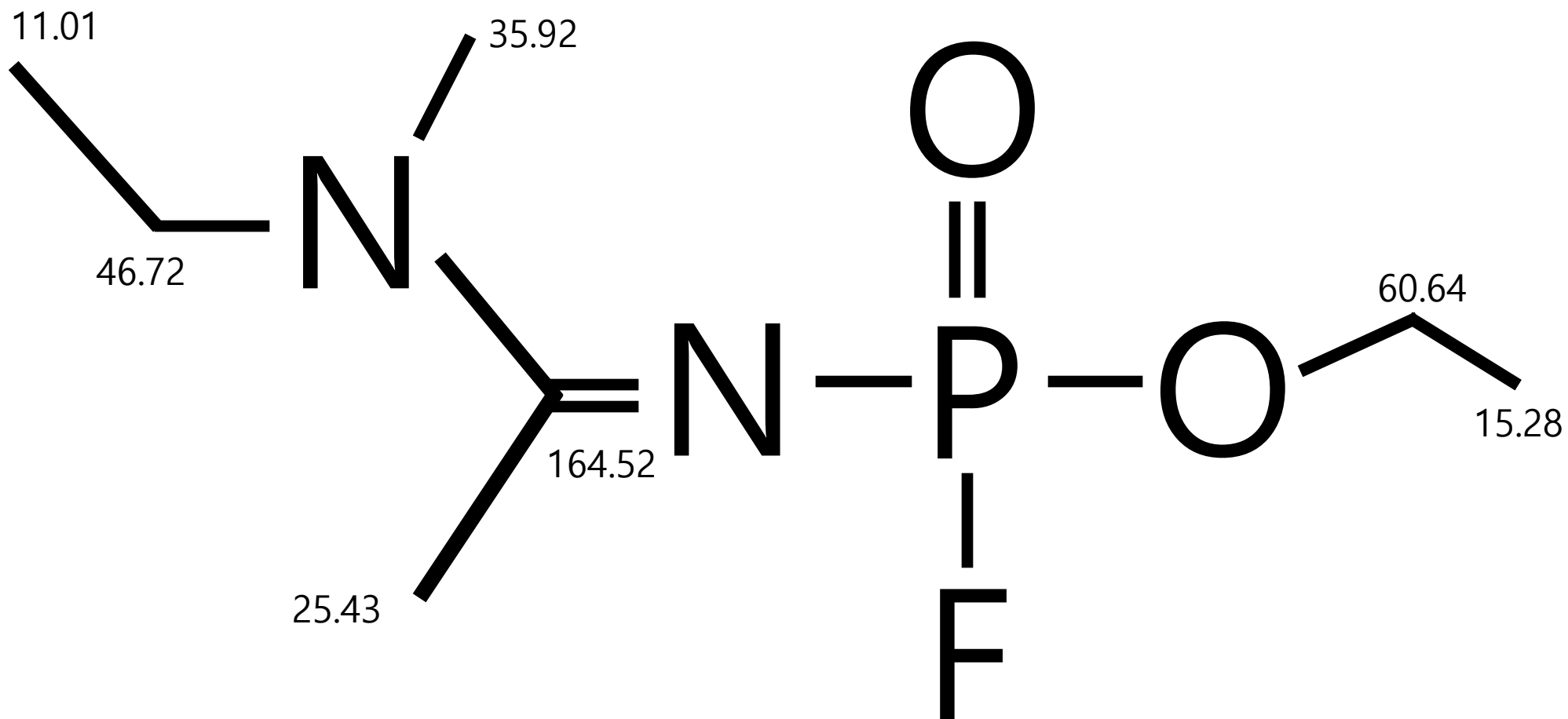


Figure S31. Structure 2121 and its ^{13}C chemical shift

2122 C

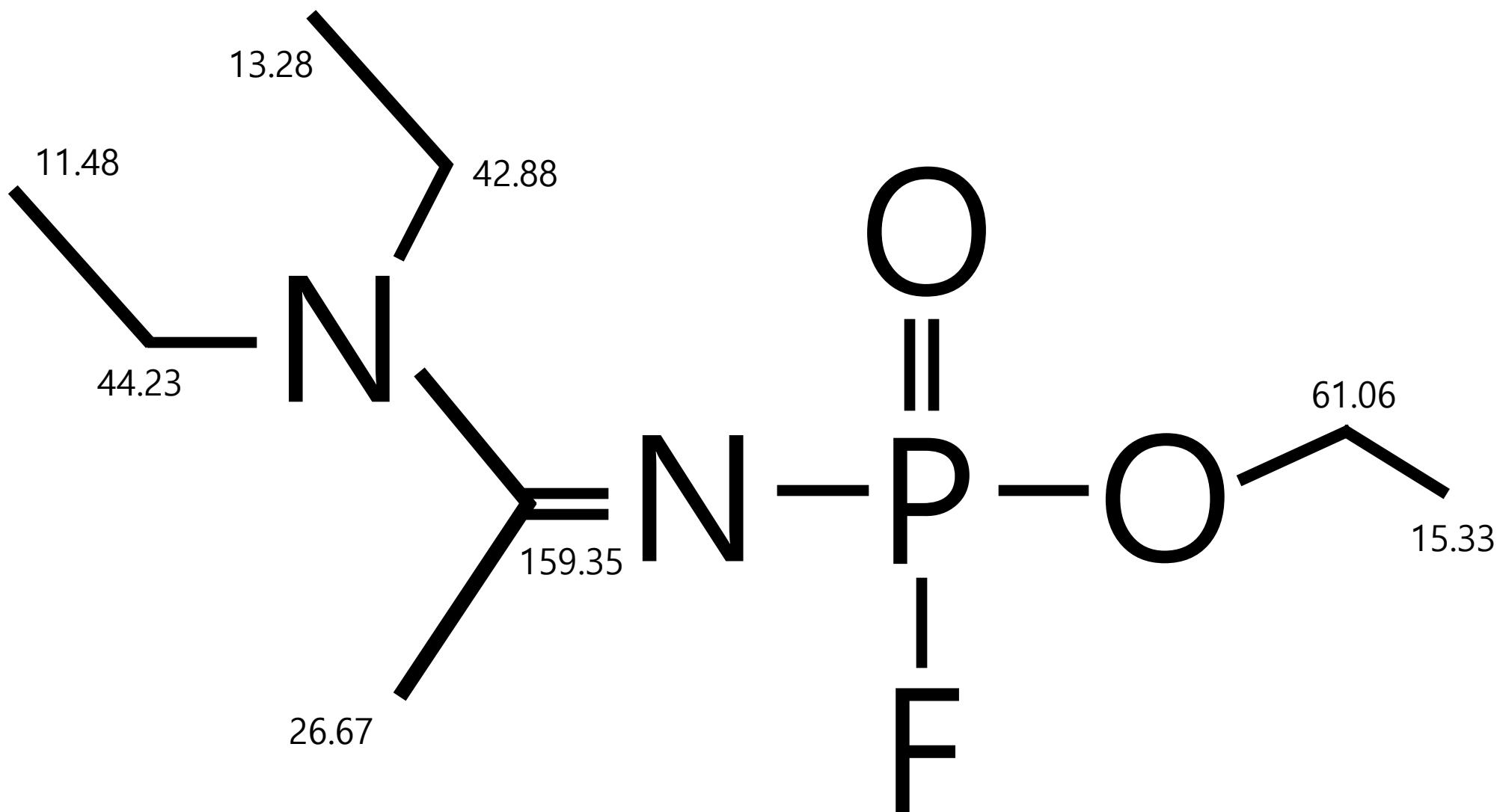


Figure S32. Structure 2122 and its ^{13}C chemical shift

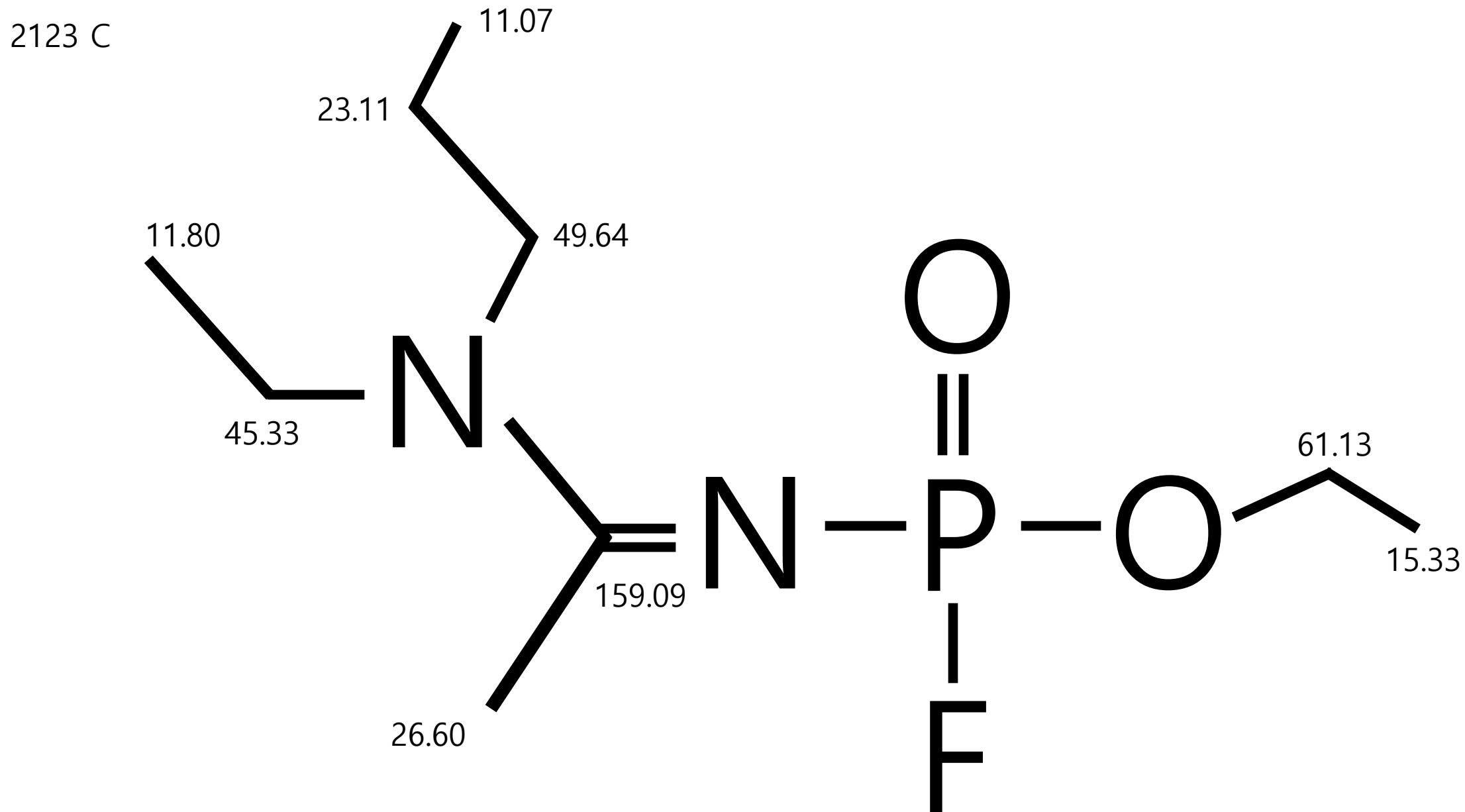


Figure S33. Structure 2123 and its ^{13}C chemical shift

2131 C

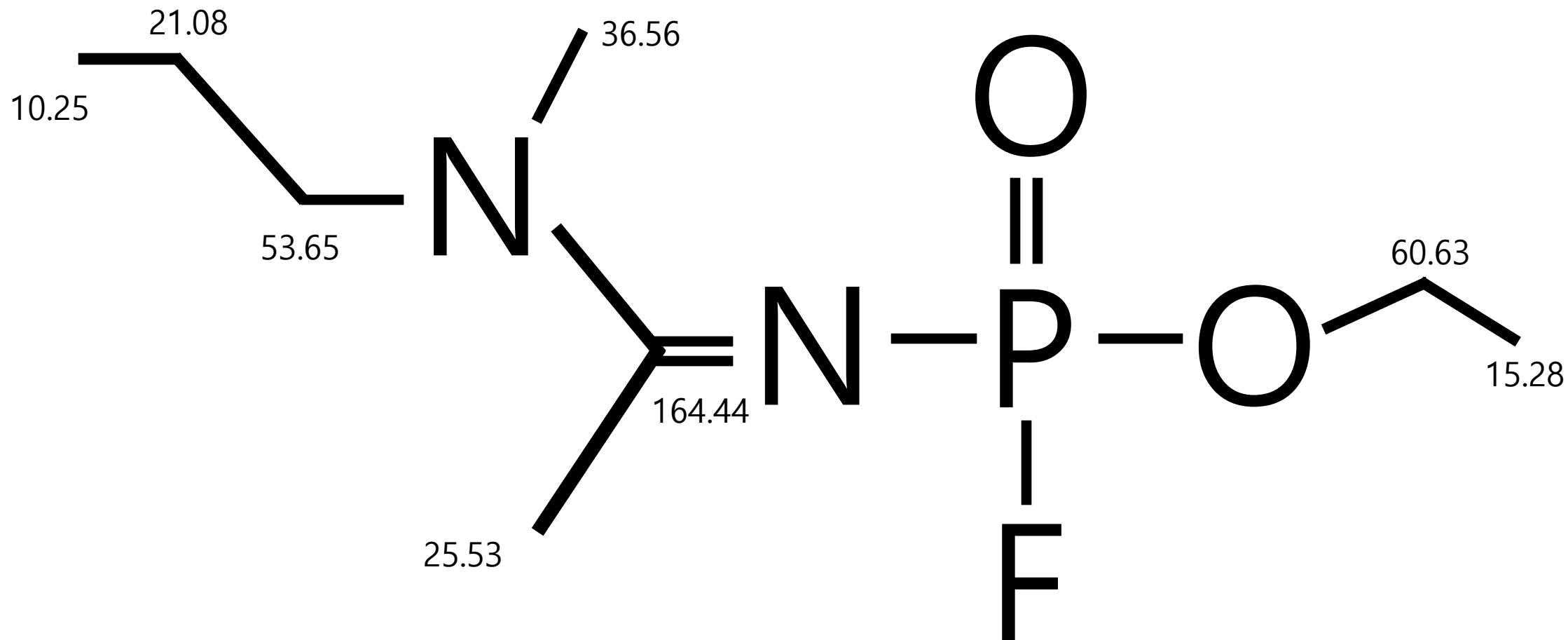


Figure S34. Structure 2131 and its ^{13}C chemical shift

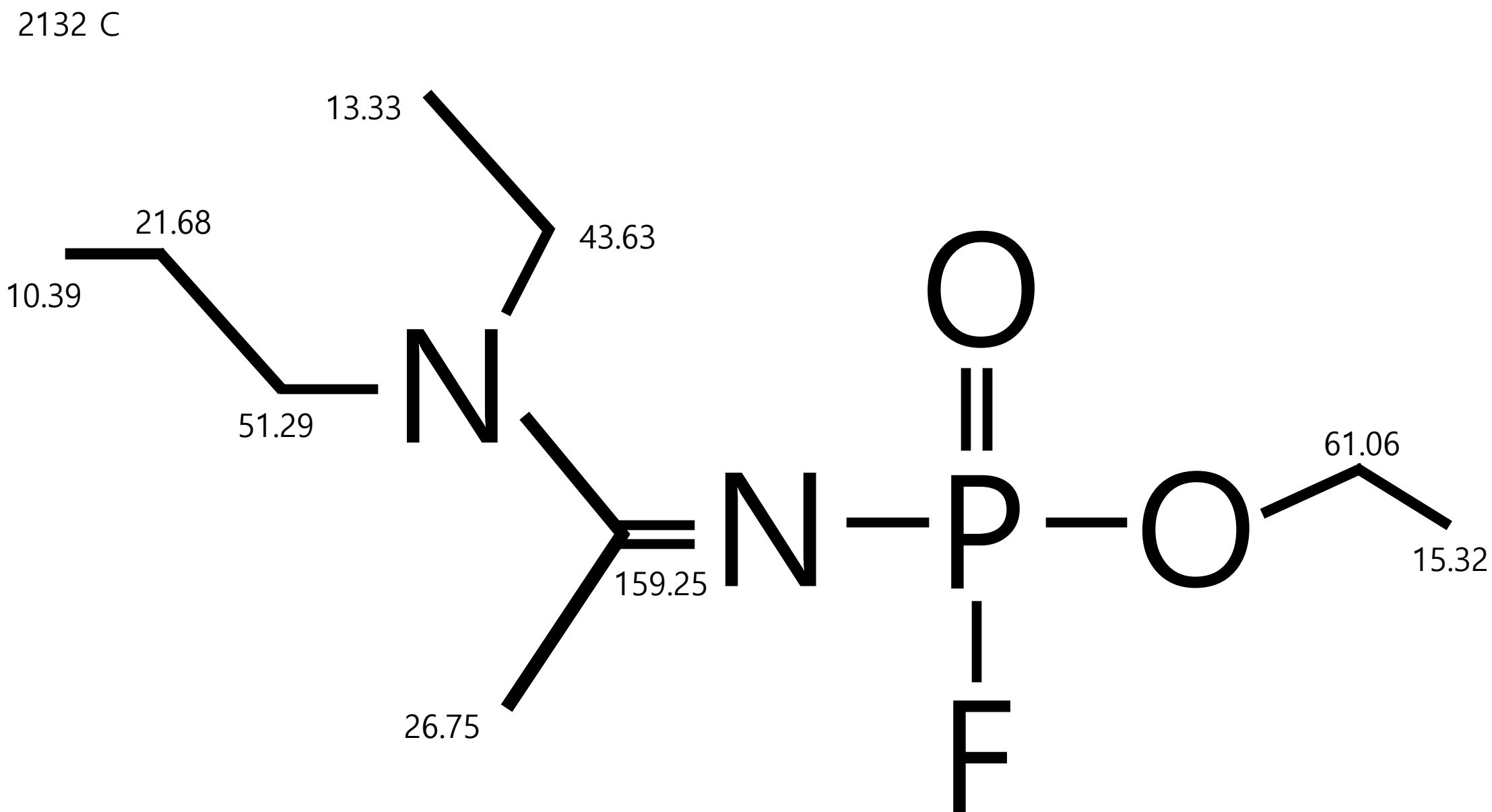


Figure S35. Structure 2132 and its ¹³C chemical shift

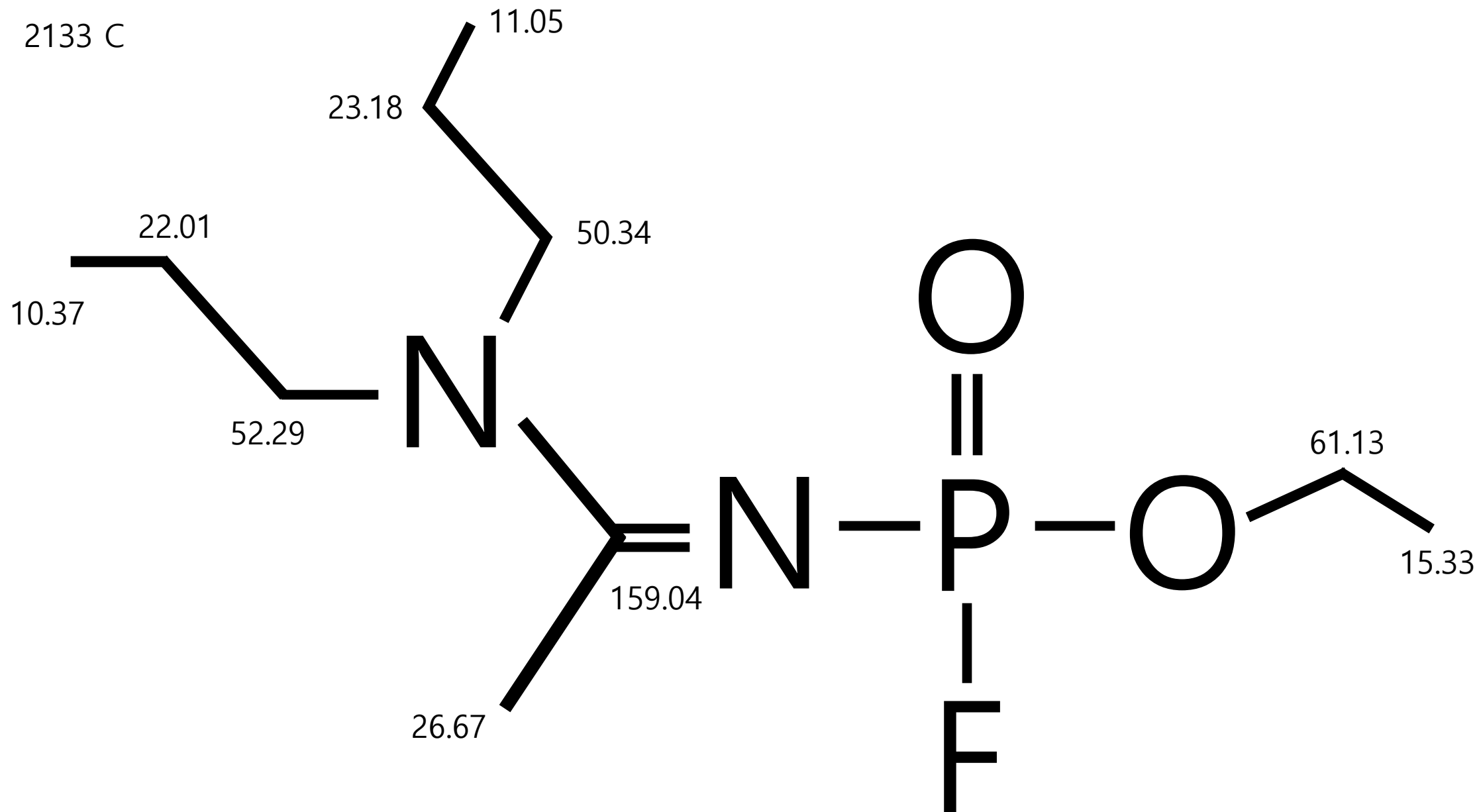


Figure S36. Structure 2133 and its ¹³C chemical shift

2211 C

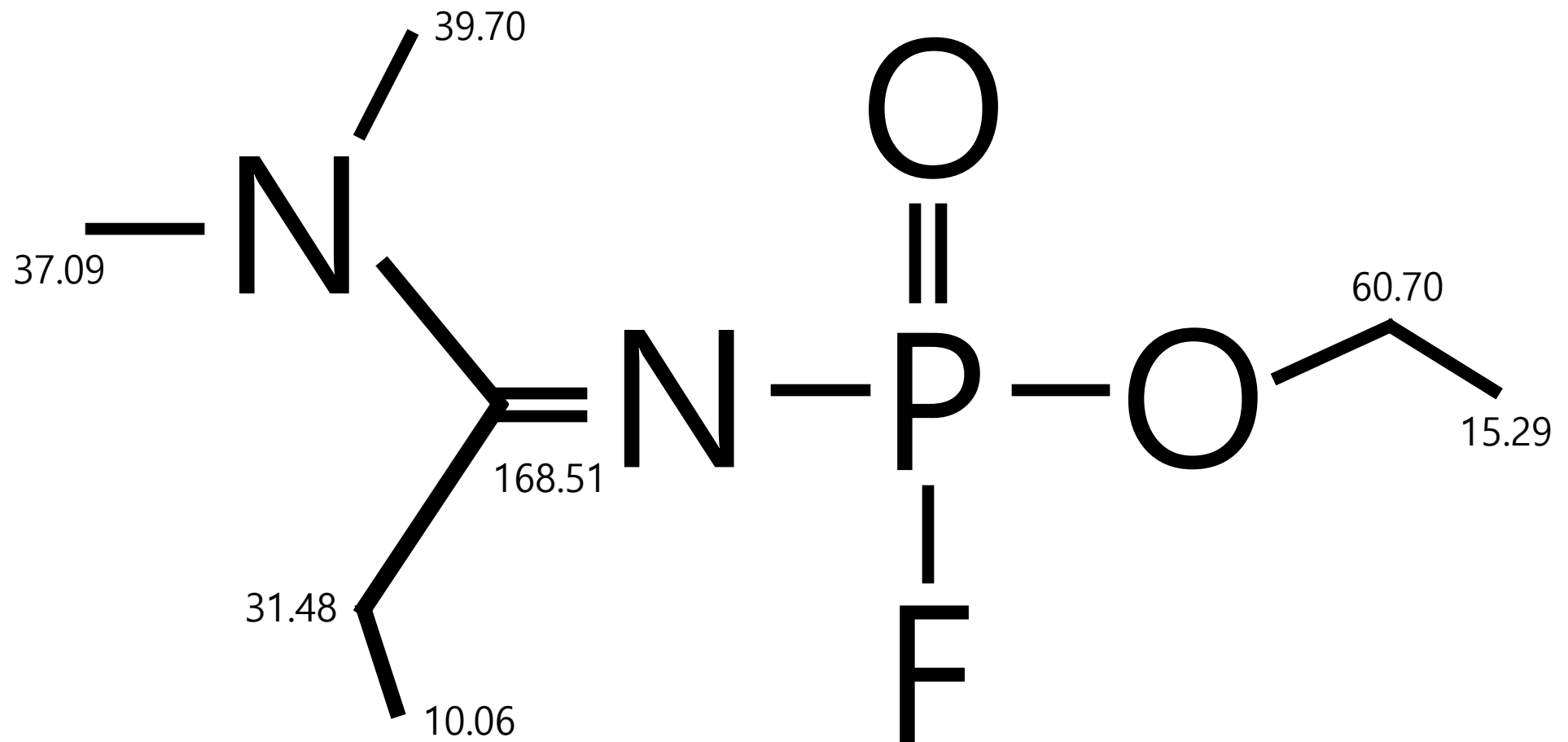


Figure S37. Structure 2211 and its ^{13}C chemical shift

2212 C

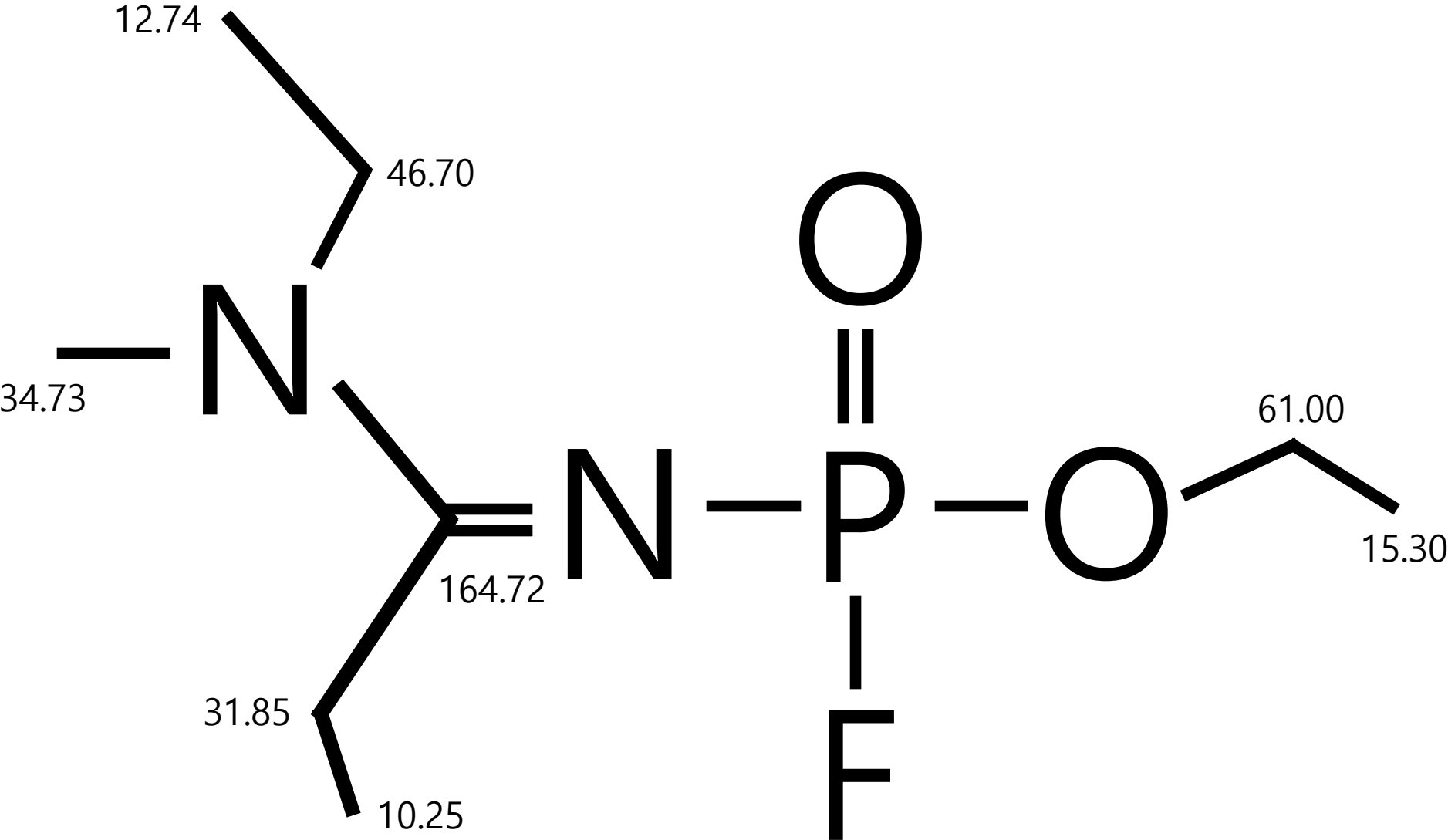


Figure S38. Structure 2212 and its ¹³C chemical shift

2213 C

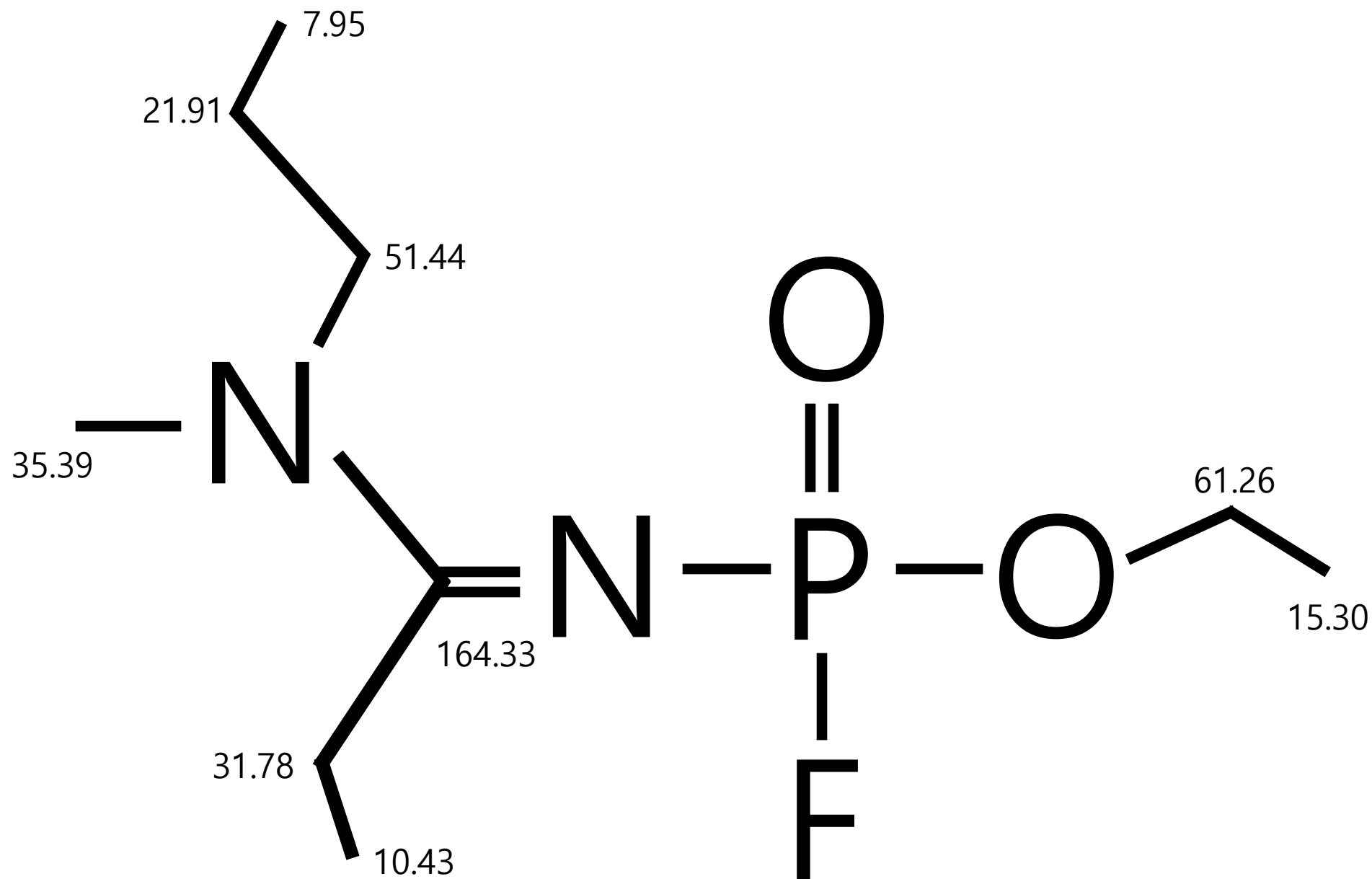


Figure S39. Structure 2213 and its ^{13}C chemical shift

2221 C

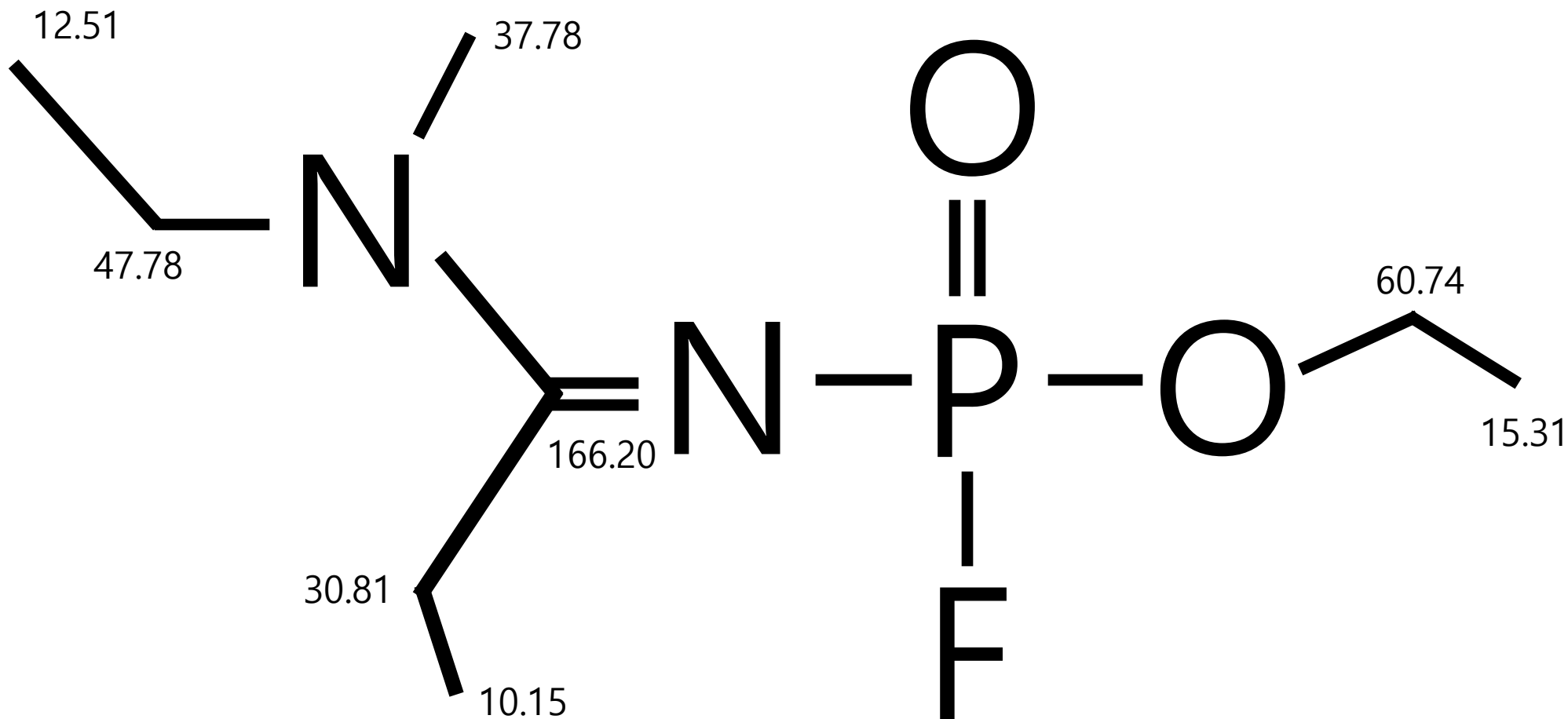


Figure S40. Structure 2221 and its ¹³C chemical shift

2222 C

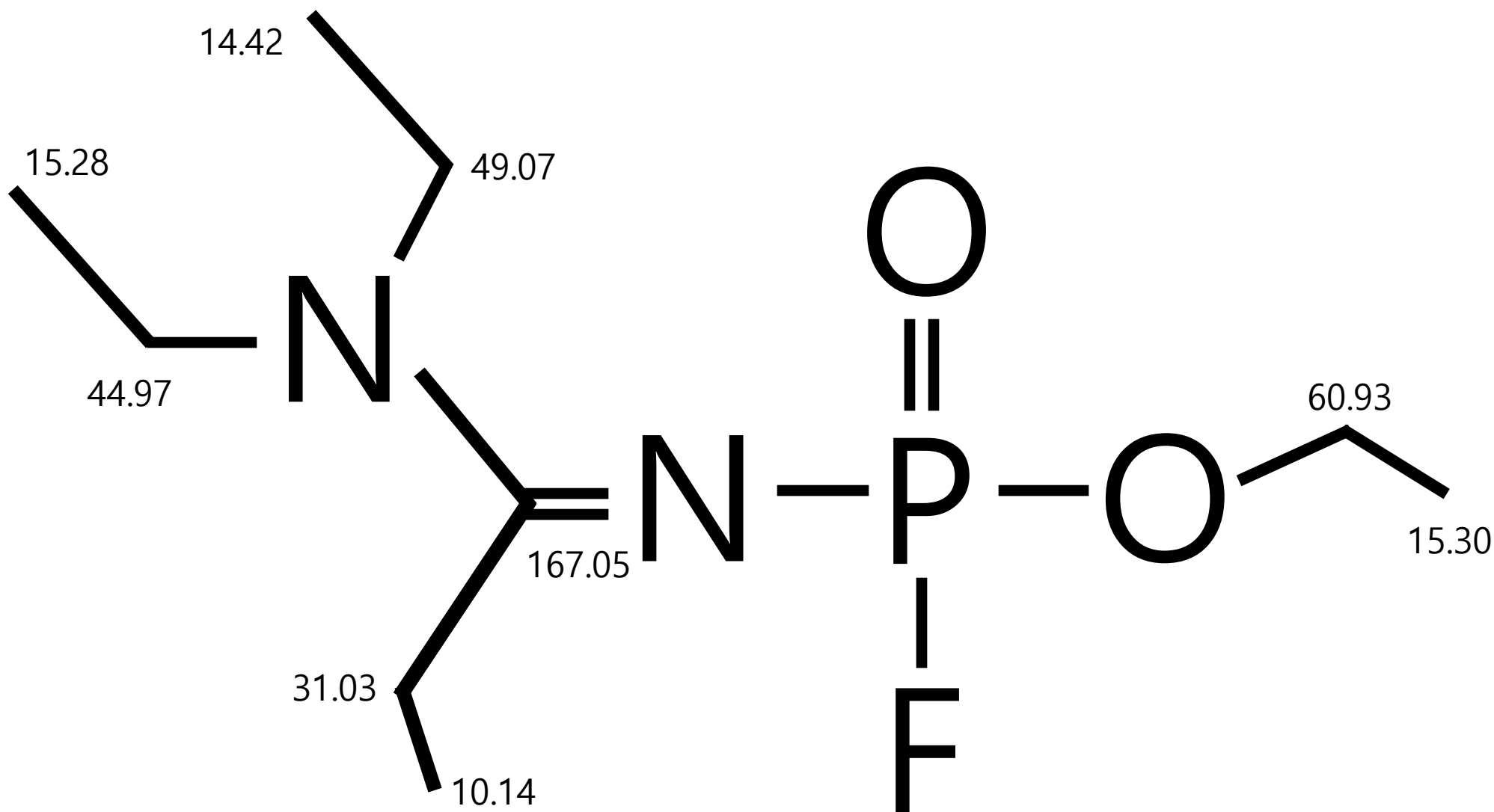


Figure S41. Structure 2222 and its ^{13}C chemical shift

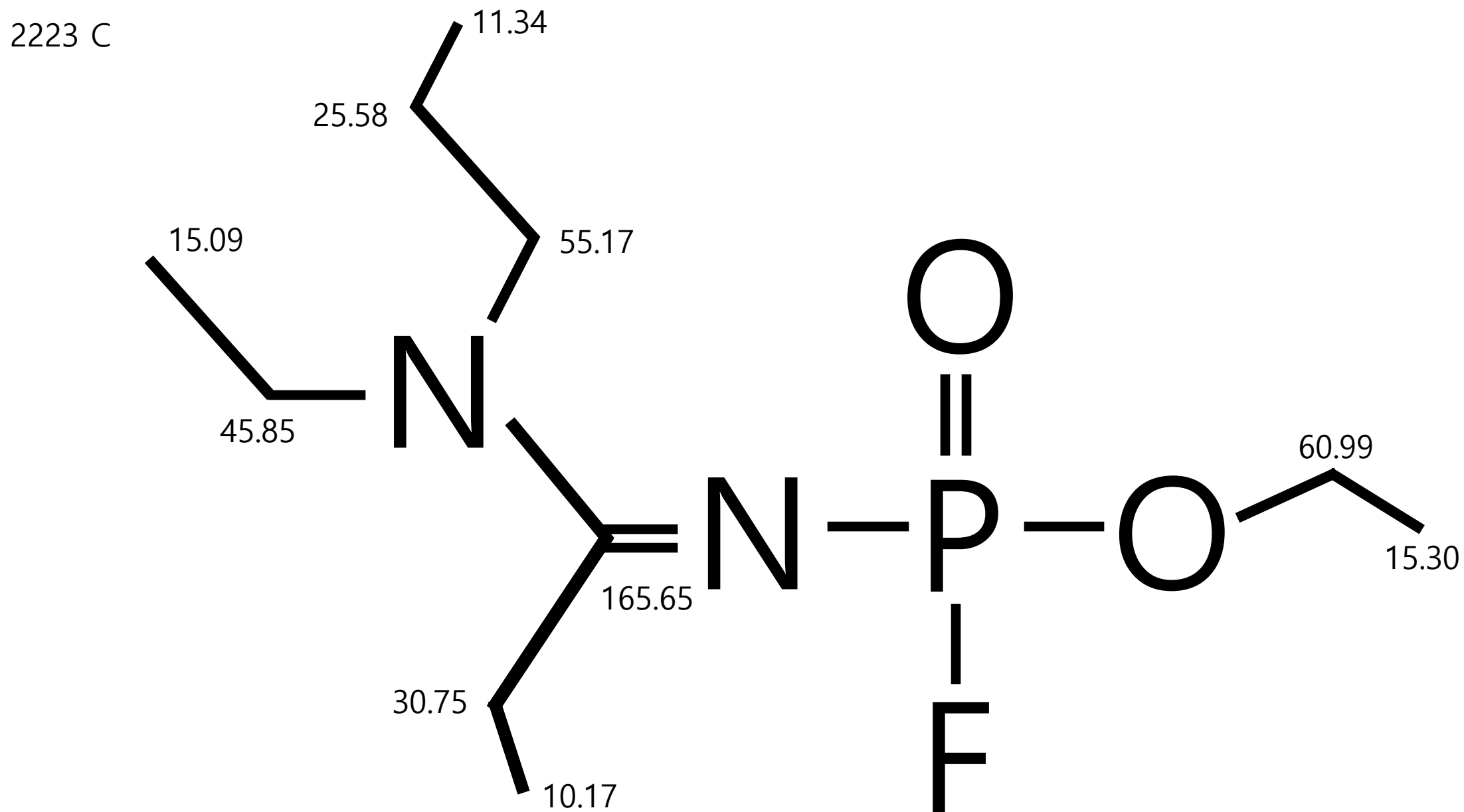


Figure S42. Structure 2223 and its ¹³C chemical shift

2231 C

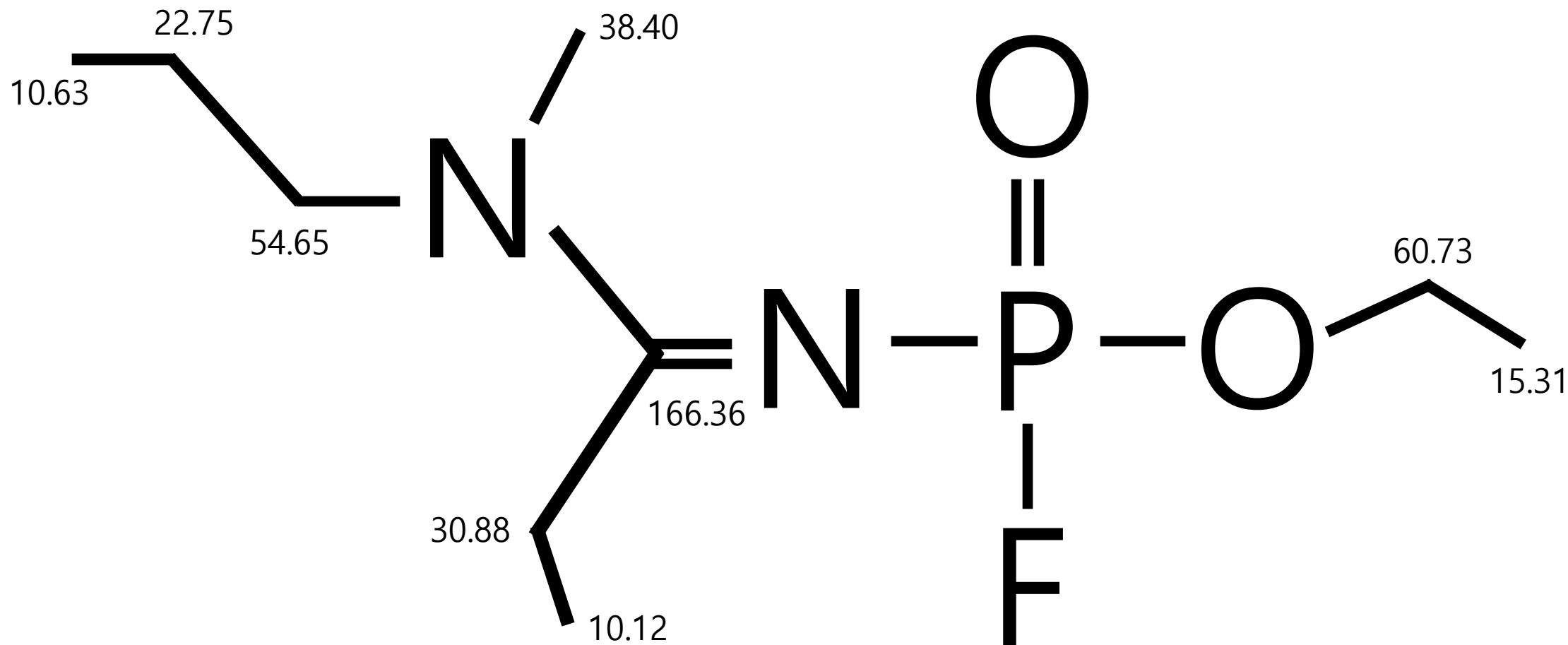


Figure S43. Structure 2231 and its ¹³C chemical shift

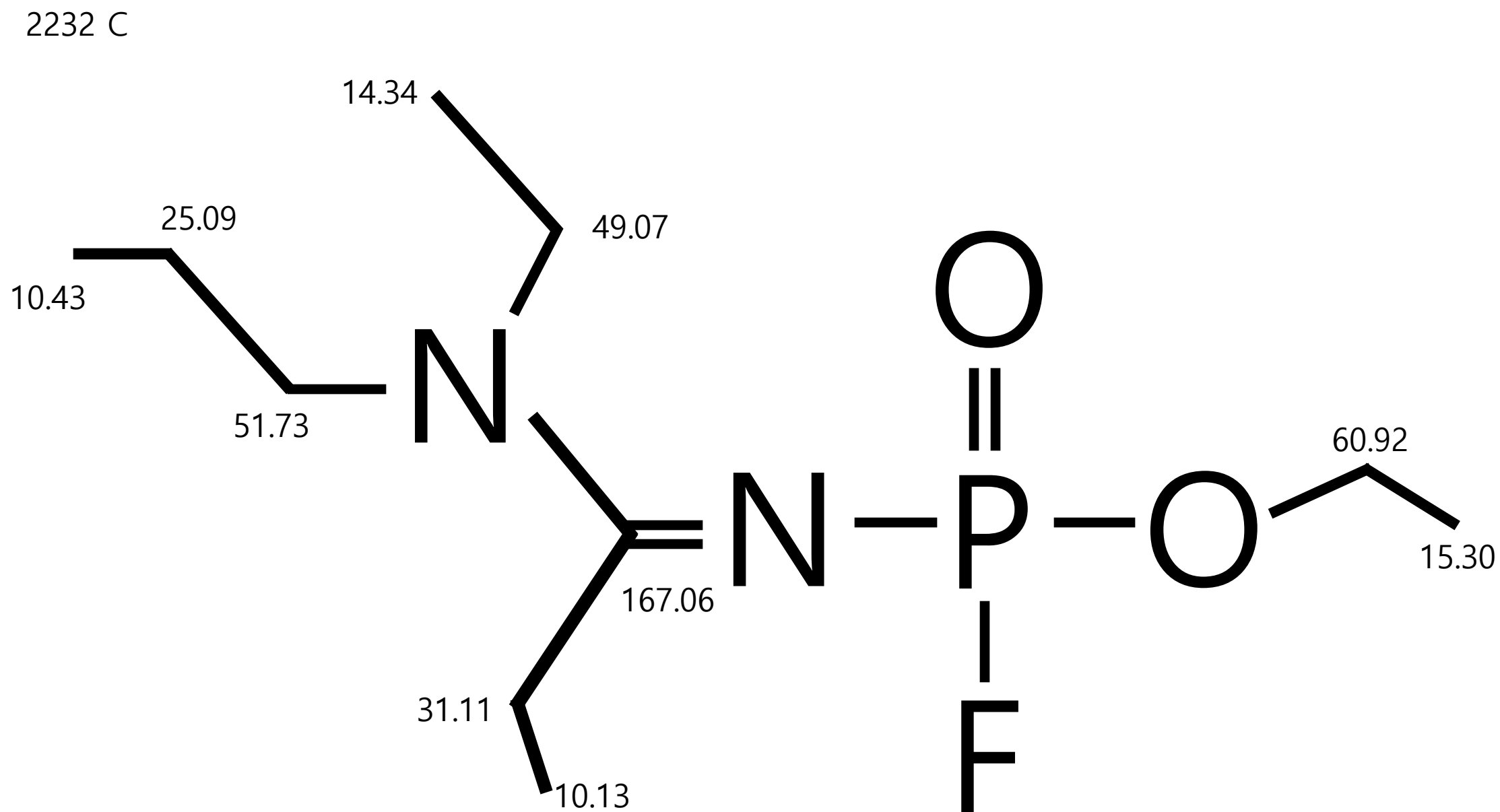


Figure S44. Structure 2232 and its ¹³C chemical shift

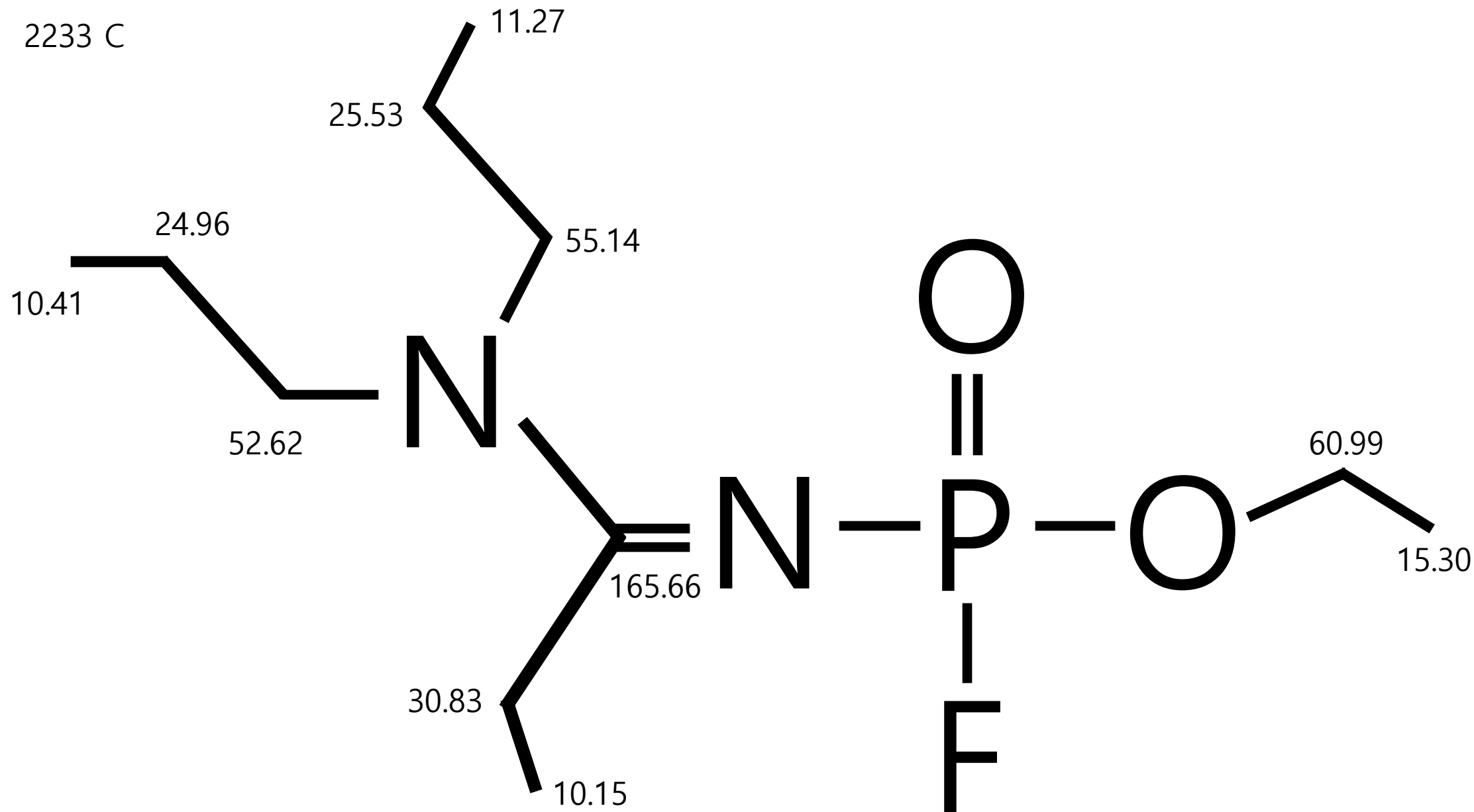


Figure S45. Structure 2233 and its ¹³C chemical shift

2311 C

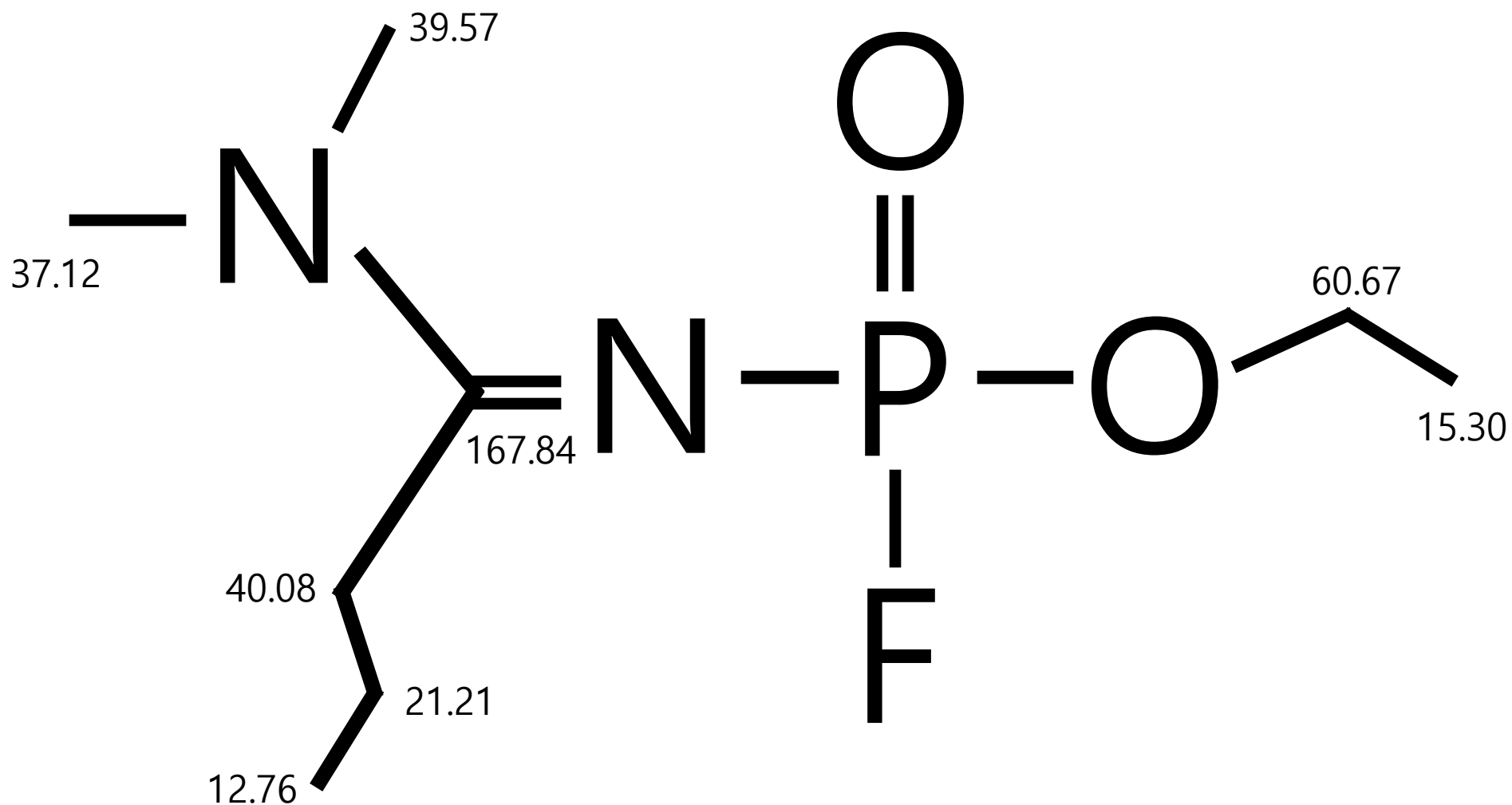


Figure S46. Structure 2311 and its ¹³C chemical shift

2312 C

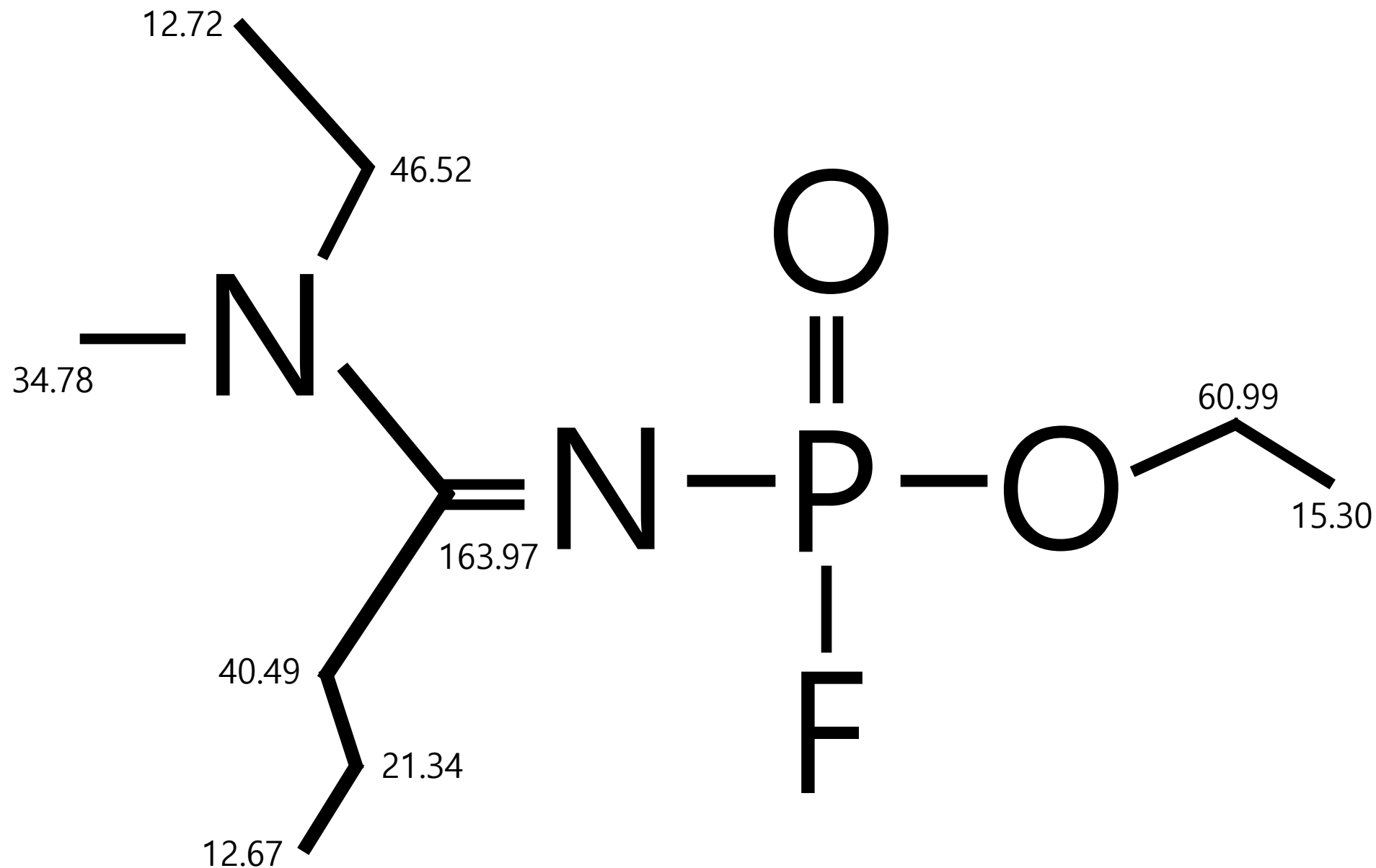


Figure S47. Structure 2312 and its ^{13}C chemical shift

2313 C

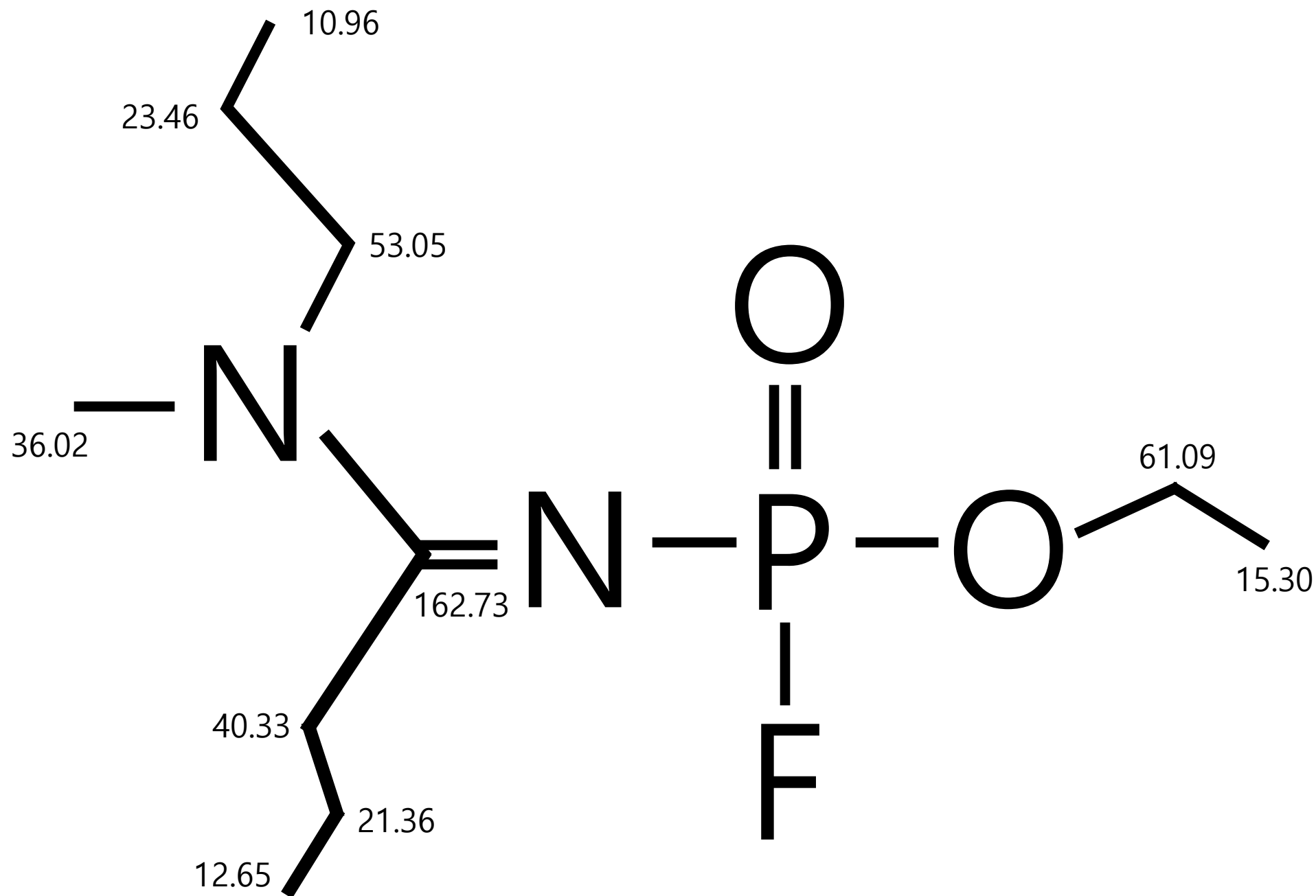


Figure S48. Structure 2313 and its ¹³C chemical shift

2321 C

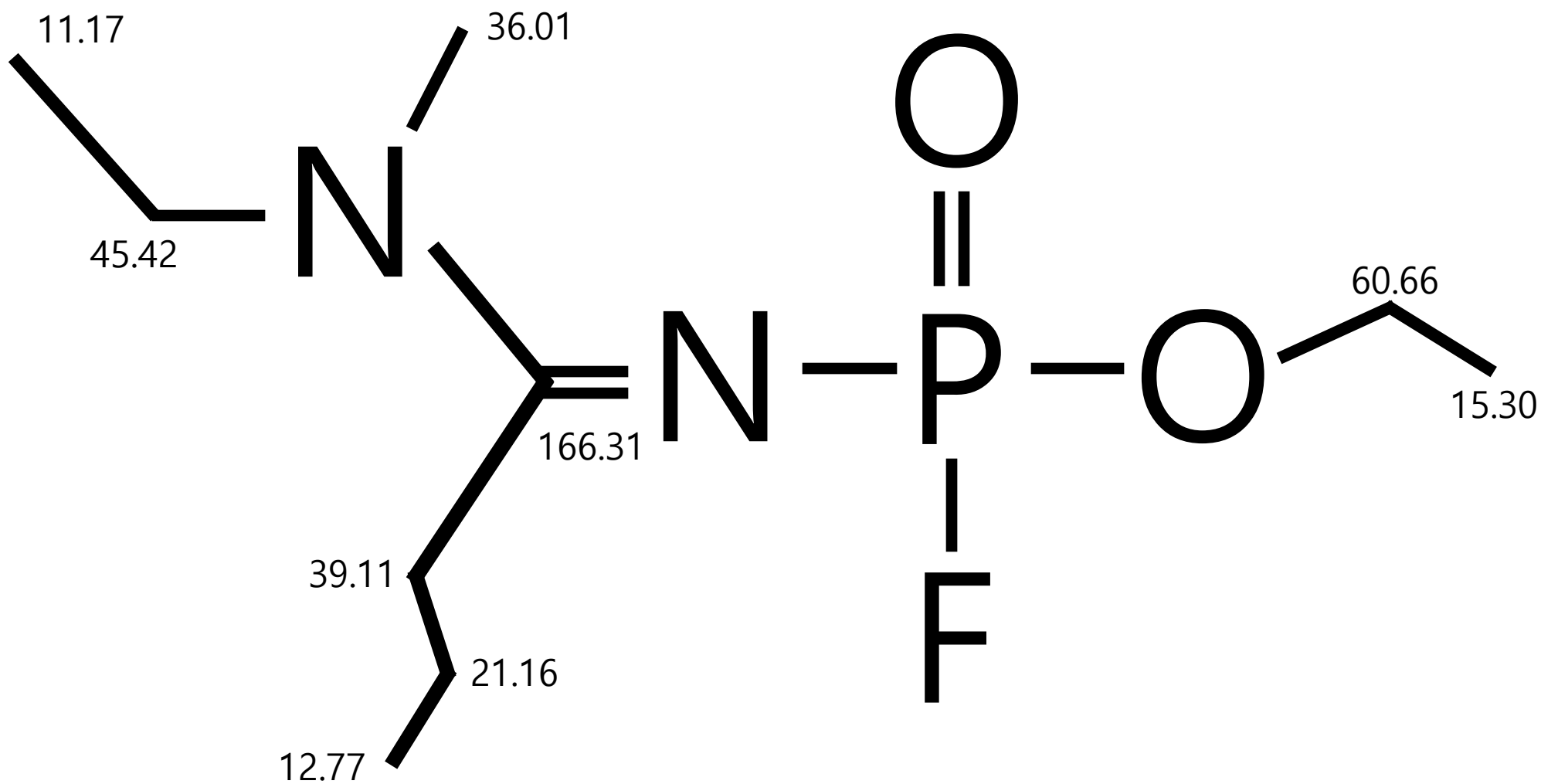


Figure S49. Structure 2321 and its ¹³C chemical shift

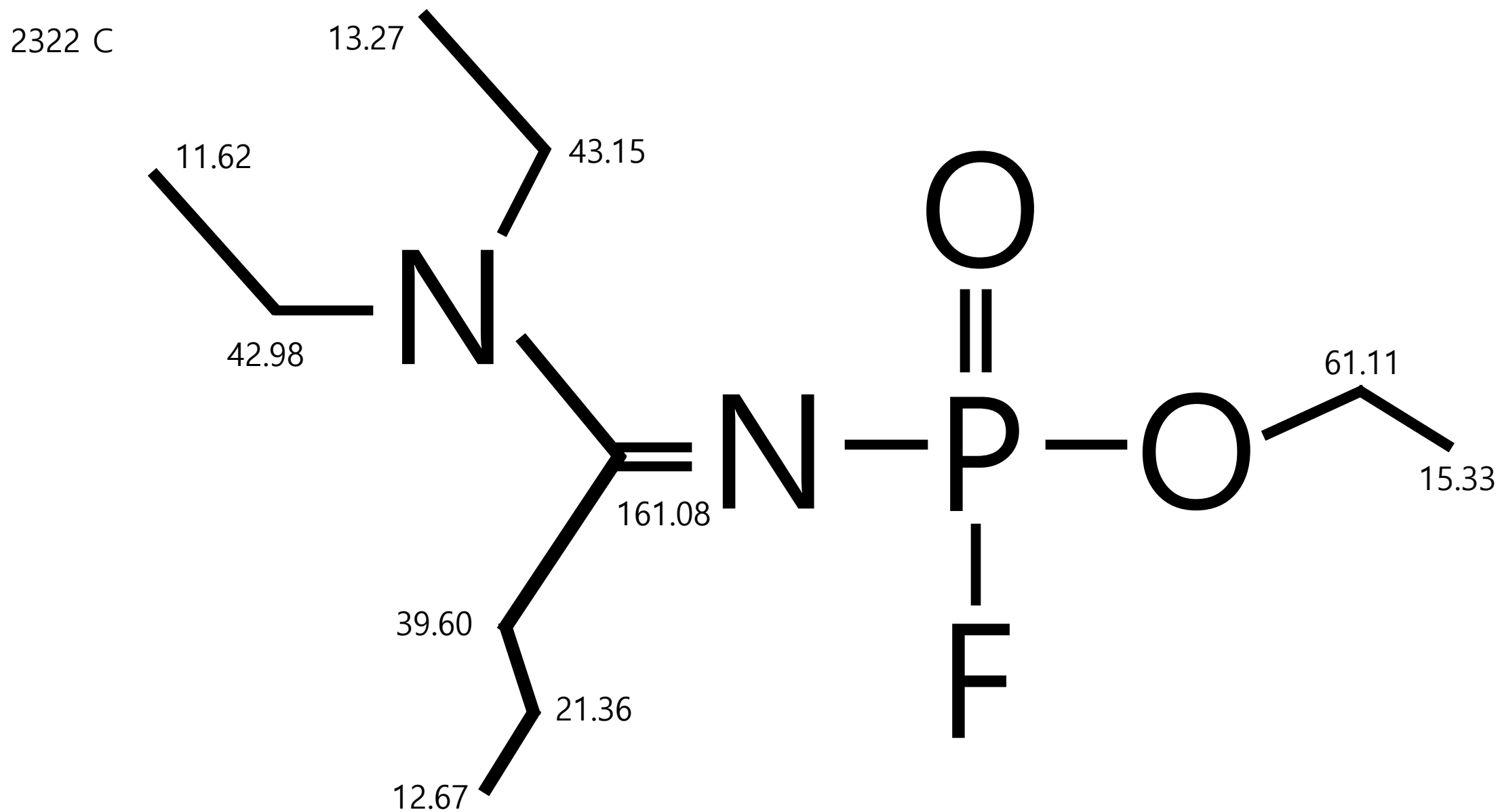


Figure S50. Structure 2322 and its ^{13}C chemical shift

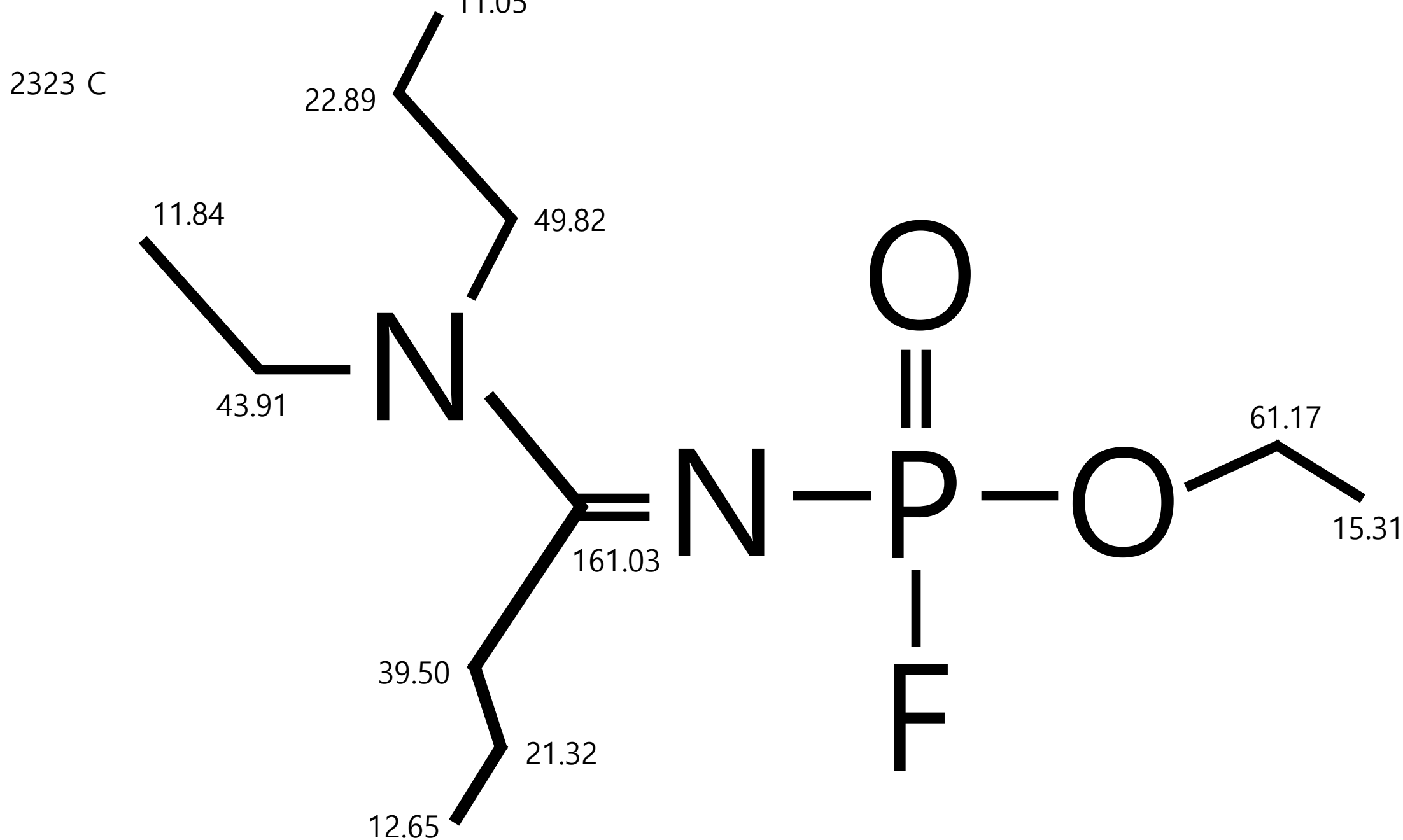


Figure S51. Structure 2323 and its ^{13}C chemical shift

2331 C

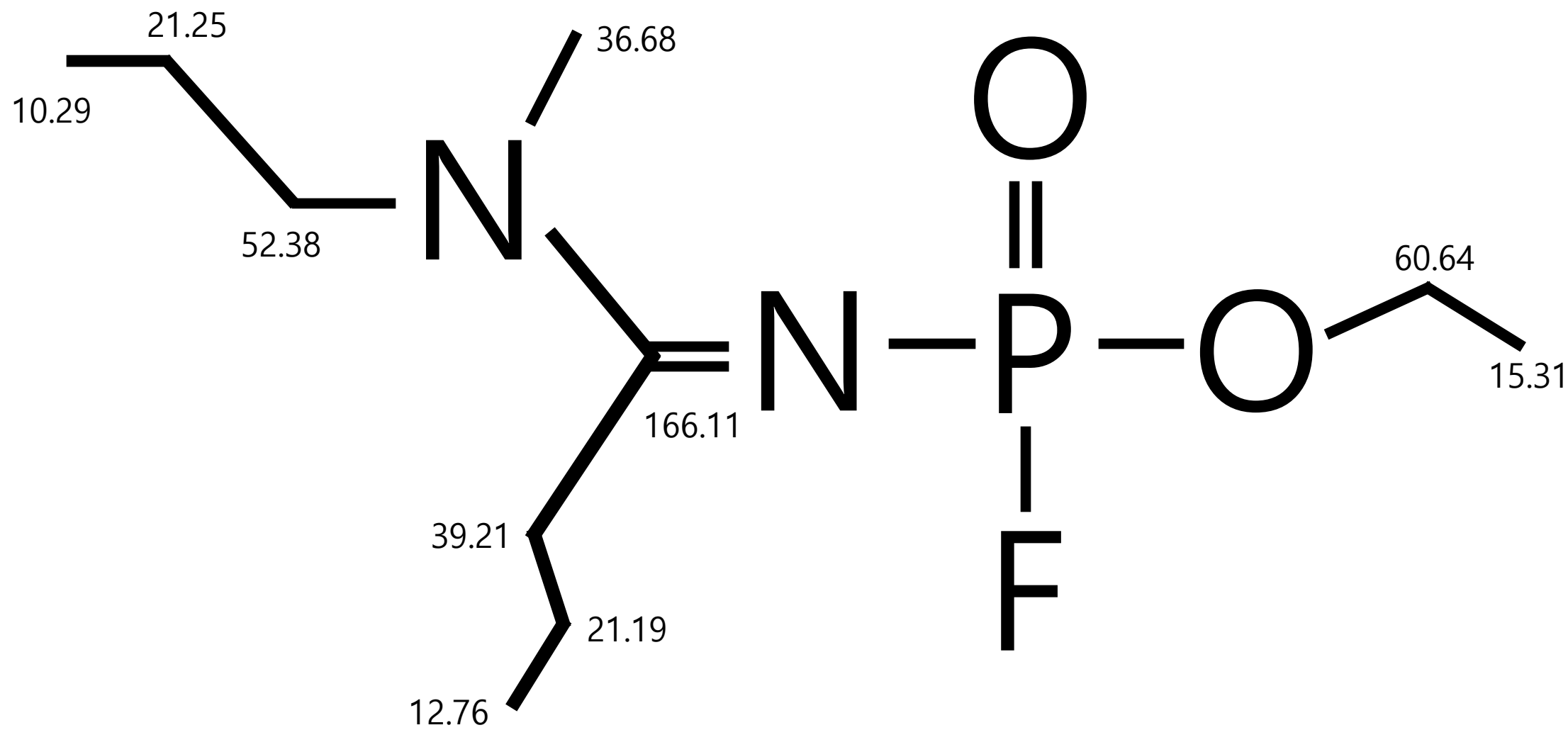


Figure S52. Structure 2331 and its ¹³C chemical shift

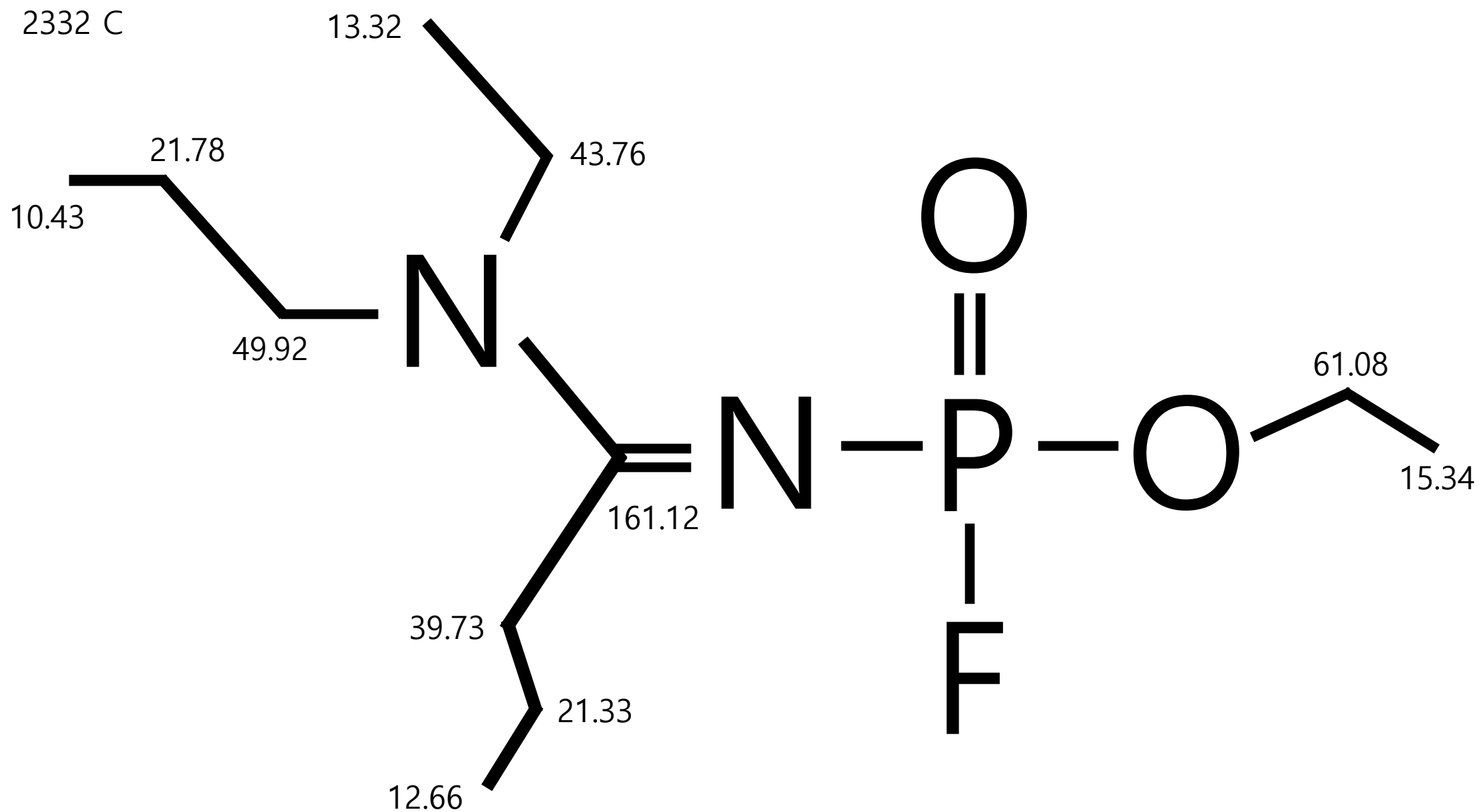


Figure S53. Structure 2332 and its ¹³C chemical shift

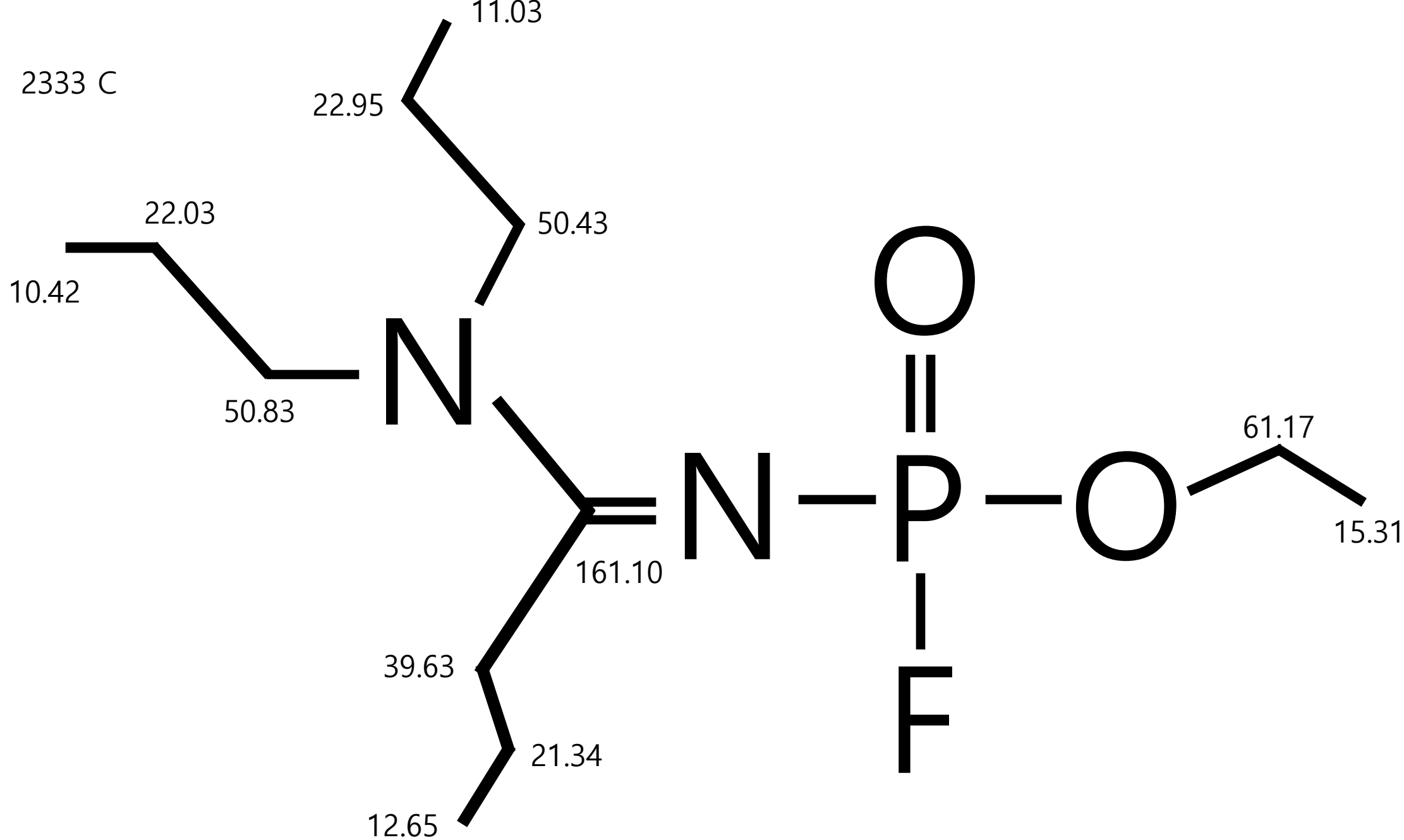


Figure S54. Structure 2333 and its ¹³C chemical shift

3111 C

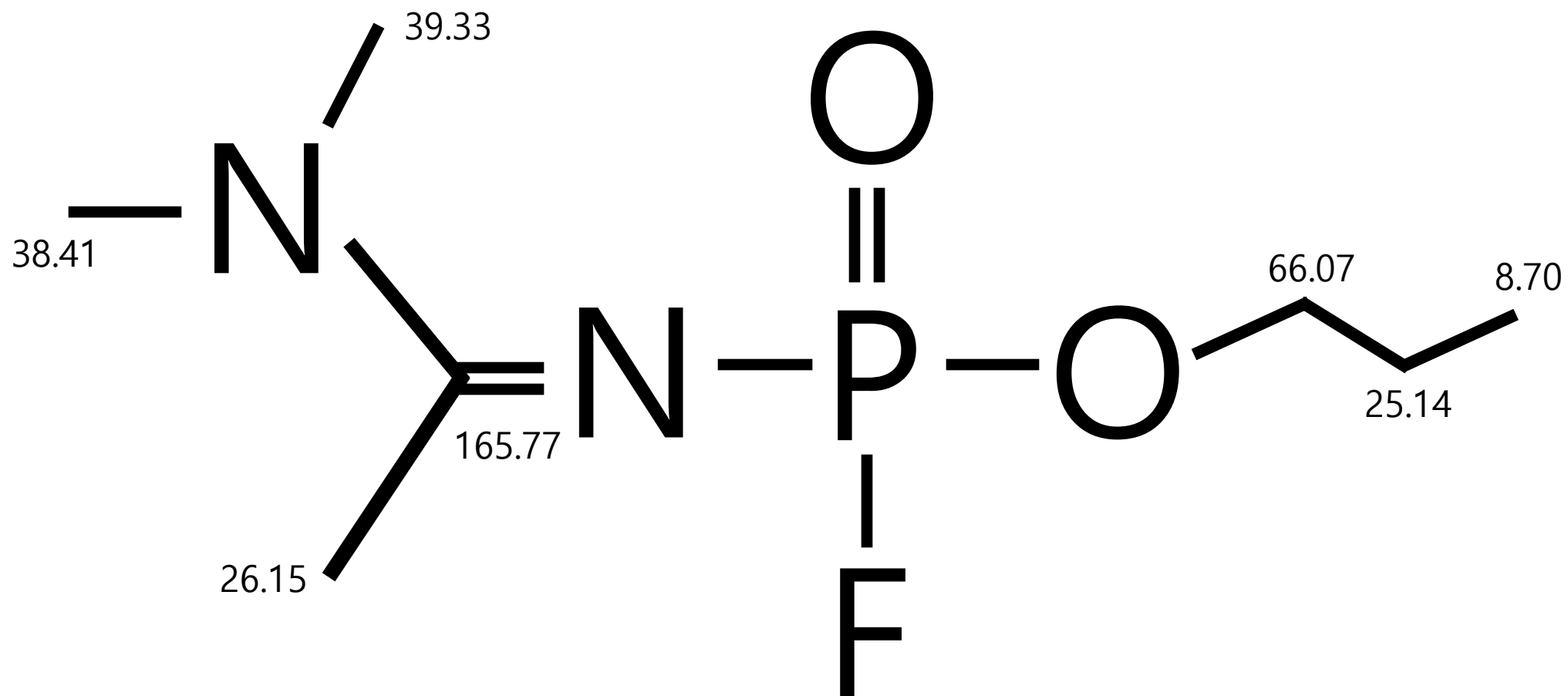


Figure S55. Structure 3111 and its ^{13}C chemical shift

3112 C

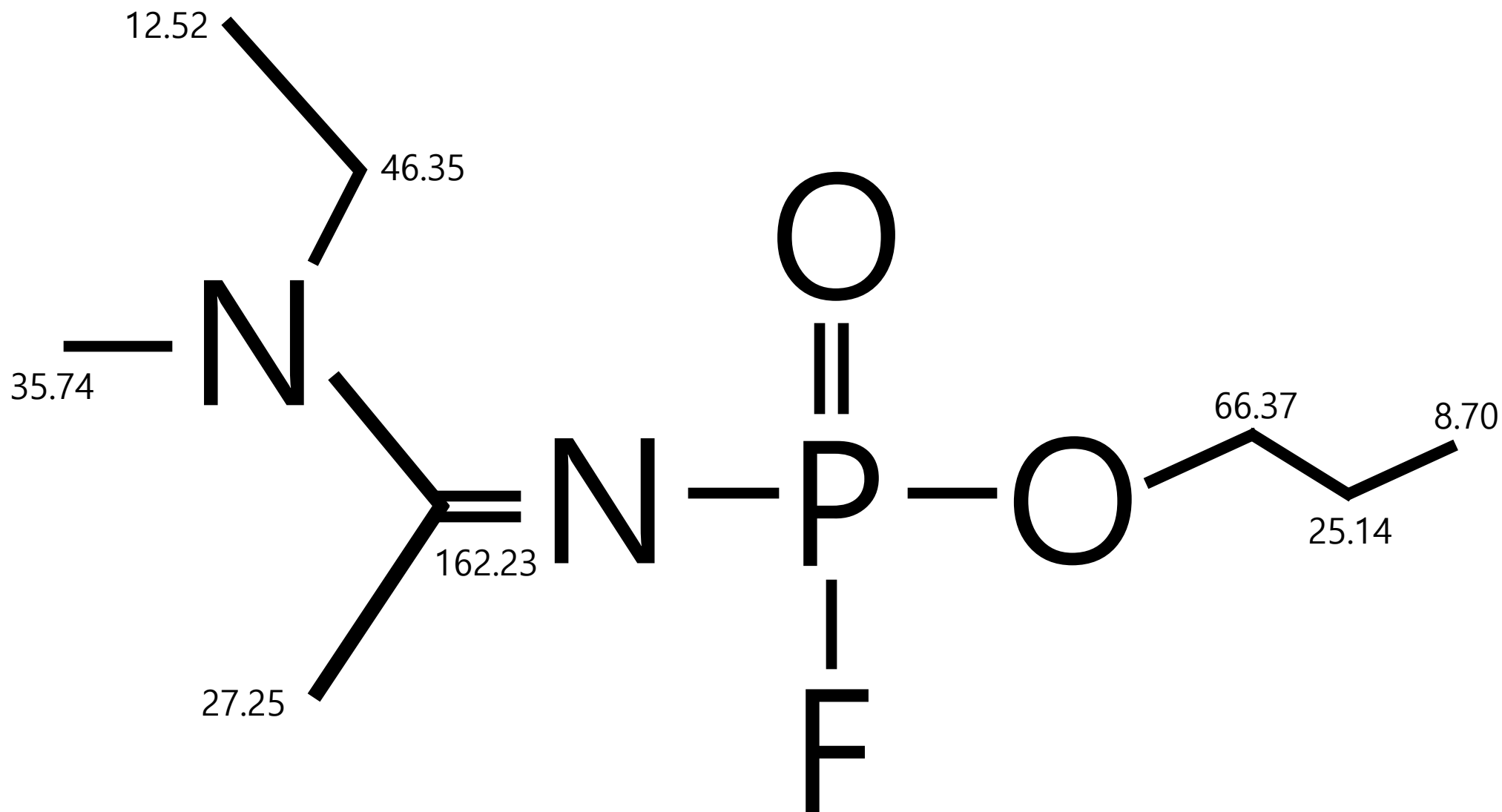


Figure S56. Structure 3112 and its ¹³C chemical shift

3113 C

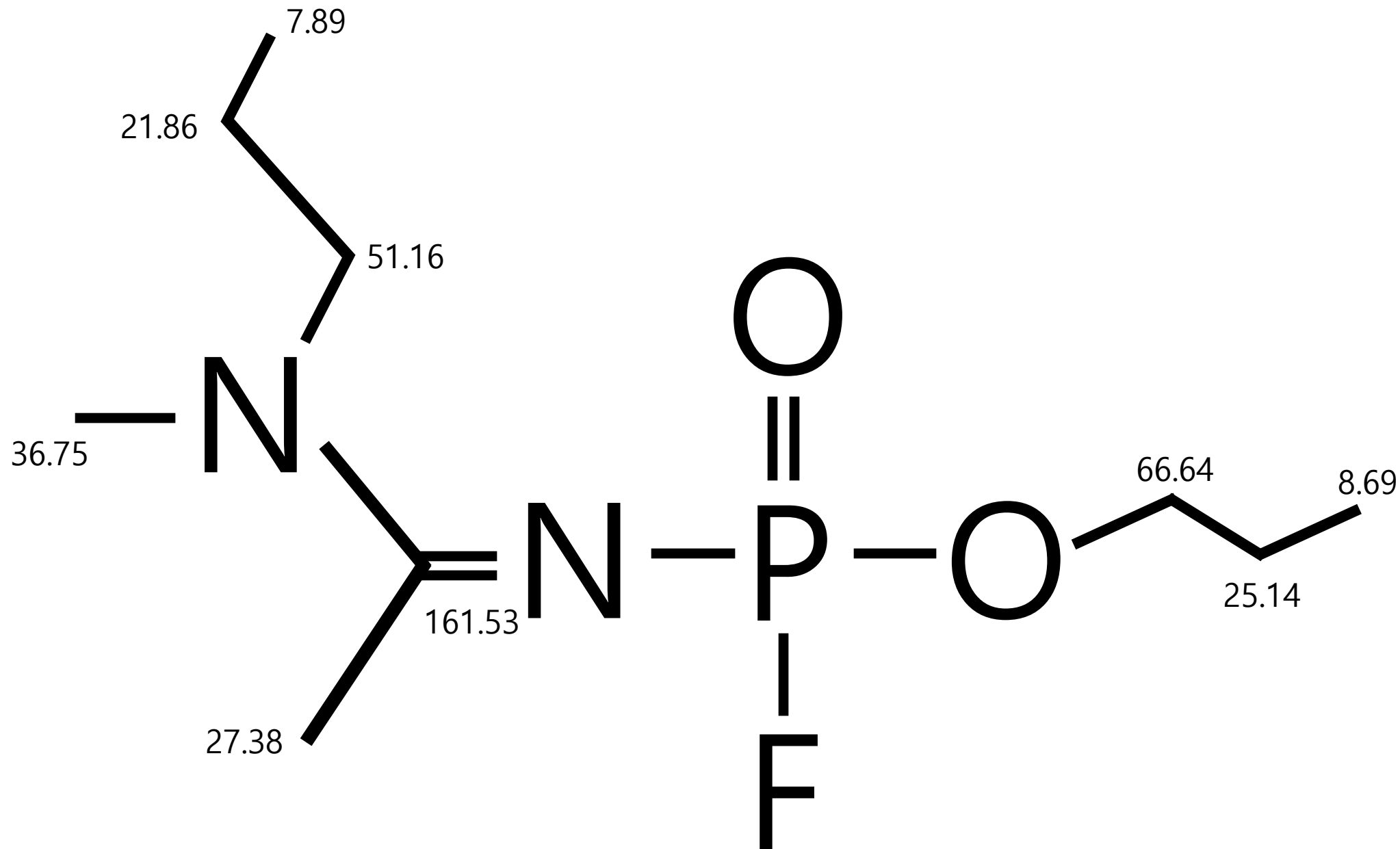


Figure S57. Structure 3113 and its ¹³C chemical shift

3121 C

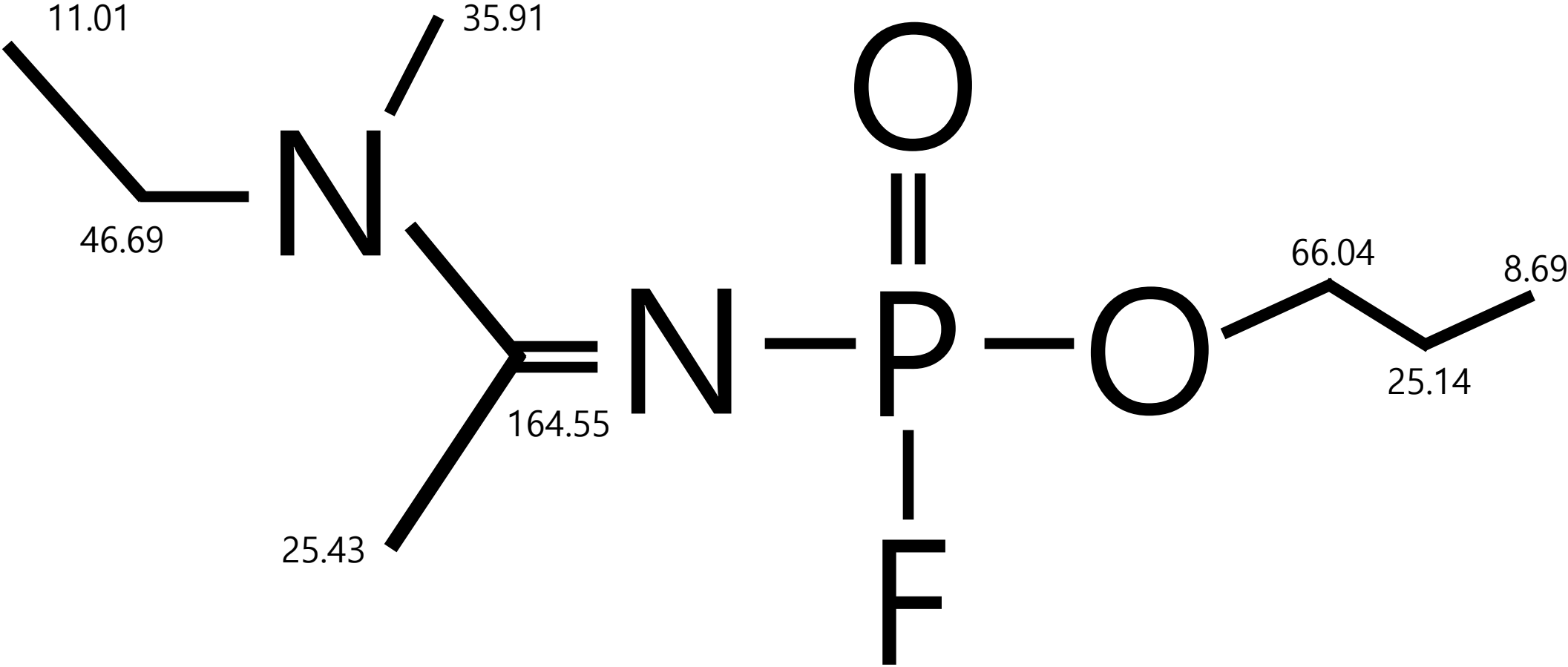


Figure S58. Structure 3121 and its ¹³C chemical shift

3122 C

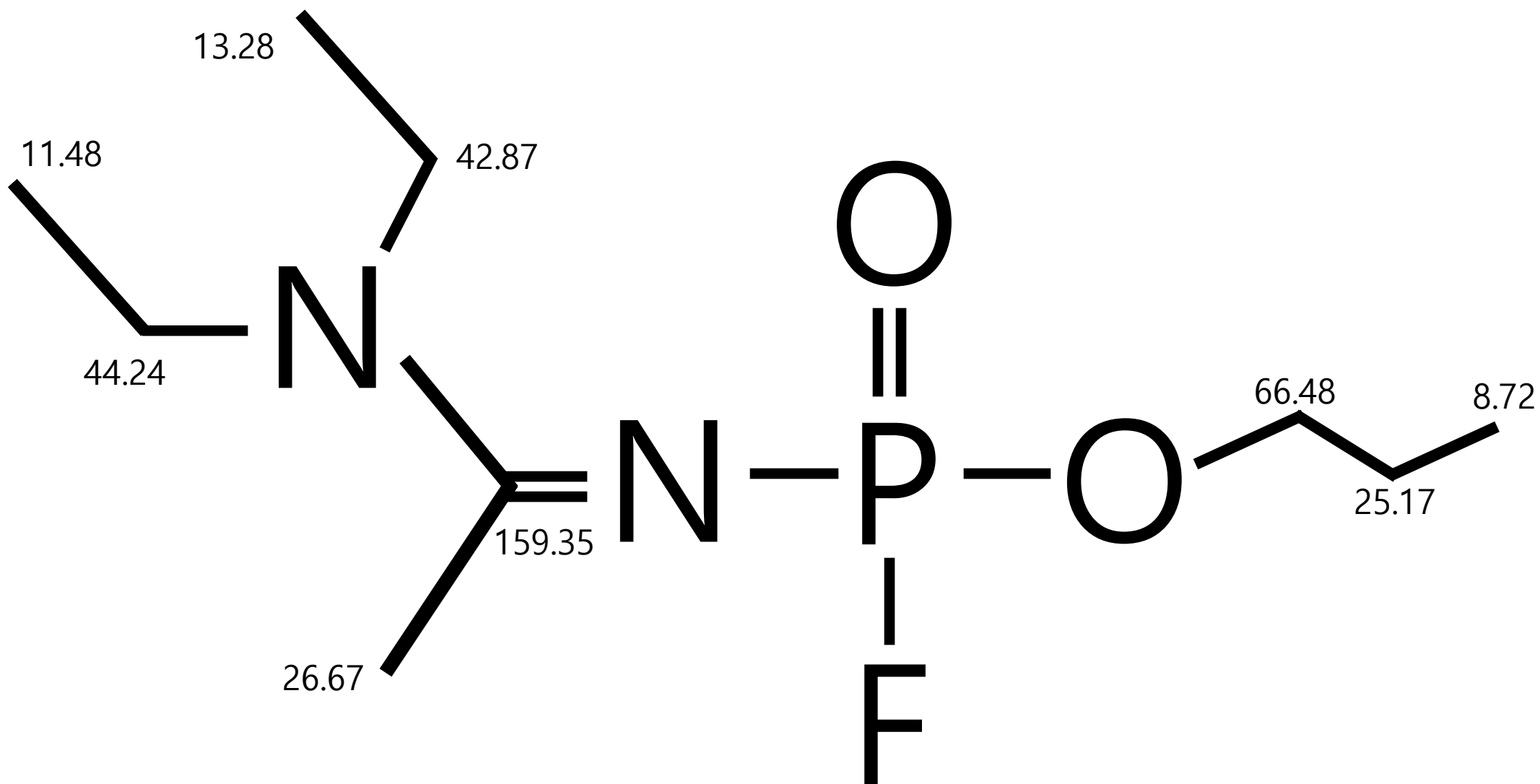


Figure S59. Structure 3122 and its ¹³C chemical shift

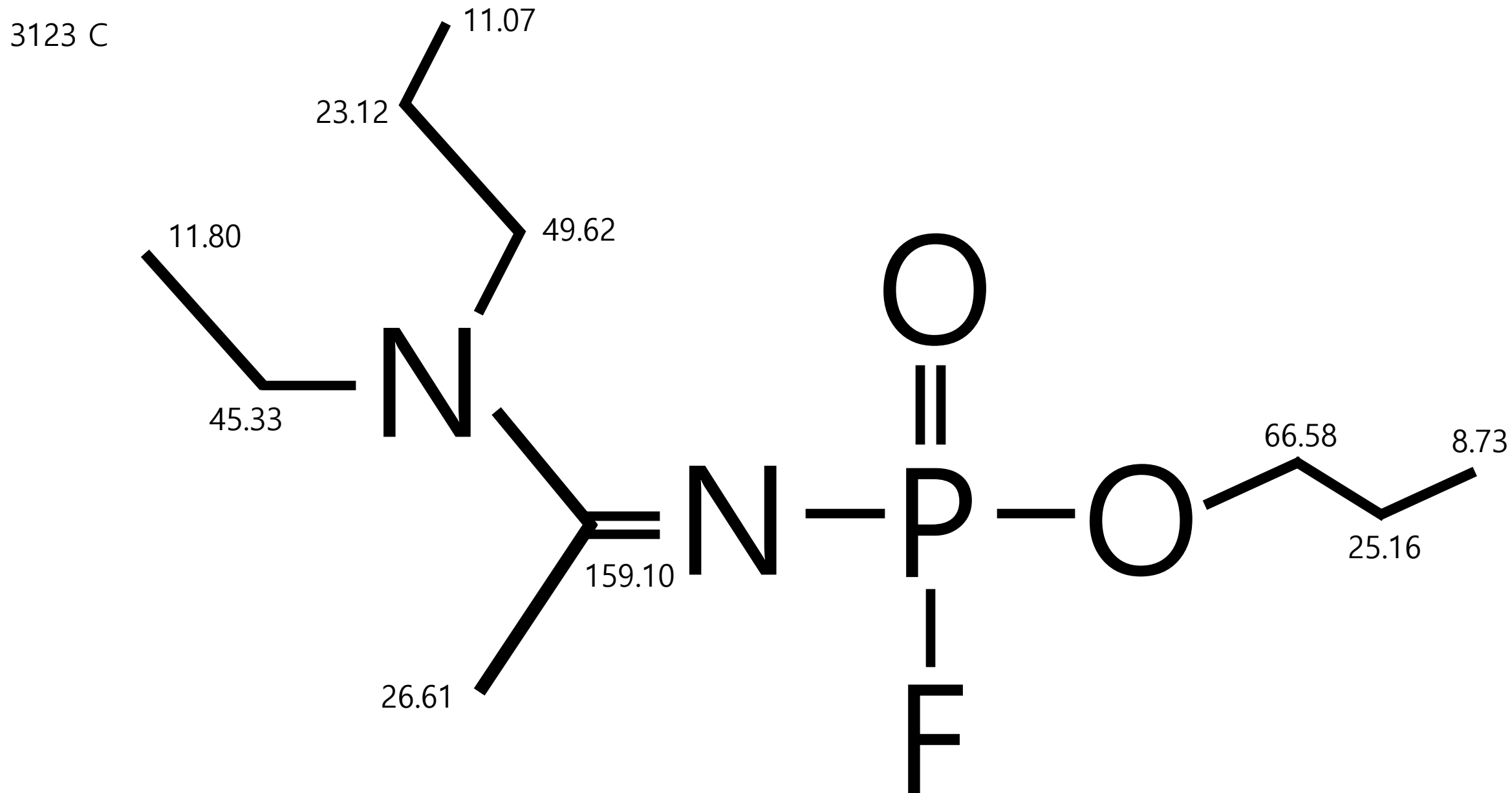


Figure S60. Structure 3123 and its ¹³C chemical shift

3131 C

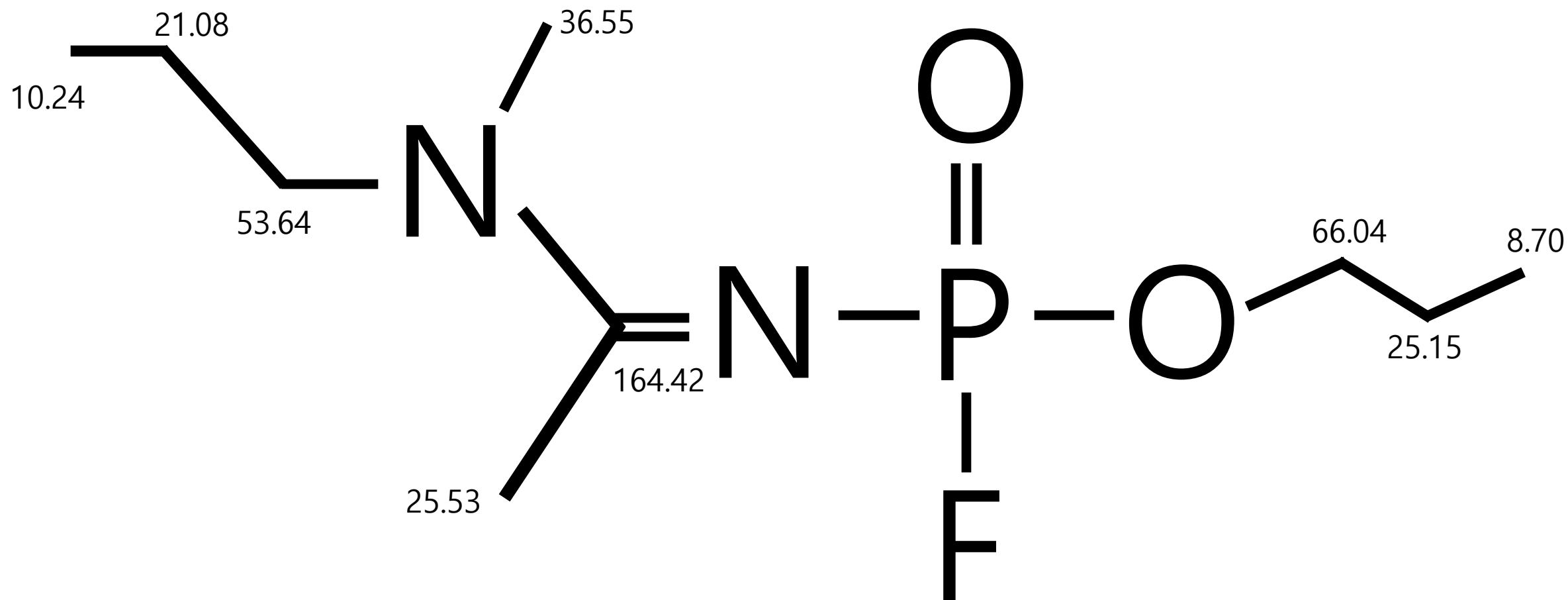


Figure S61. Structure 3131 and its ^{13}C chemical shift

3132 C

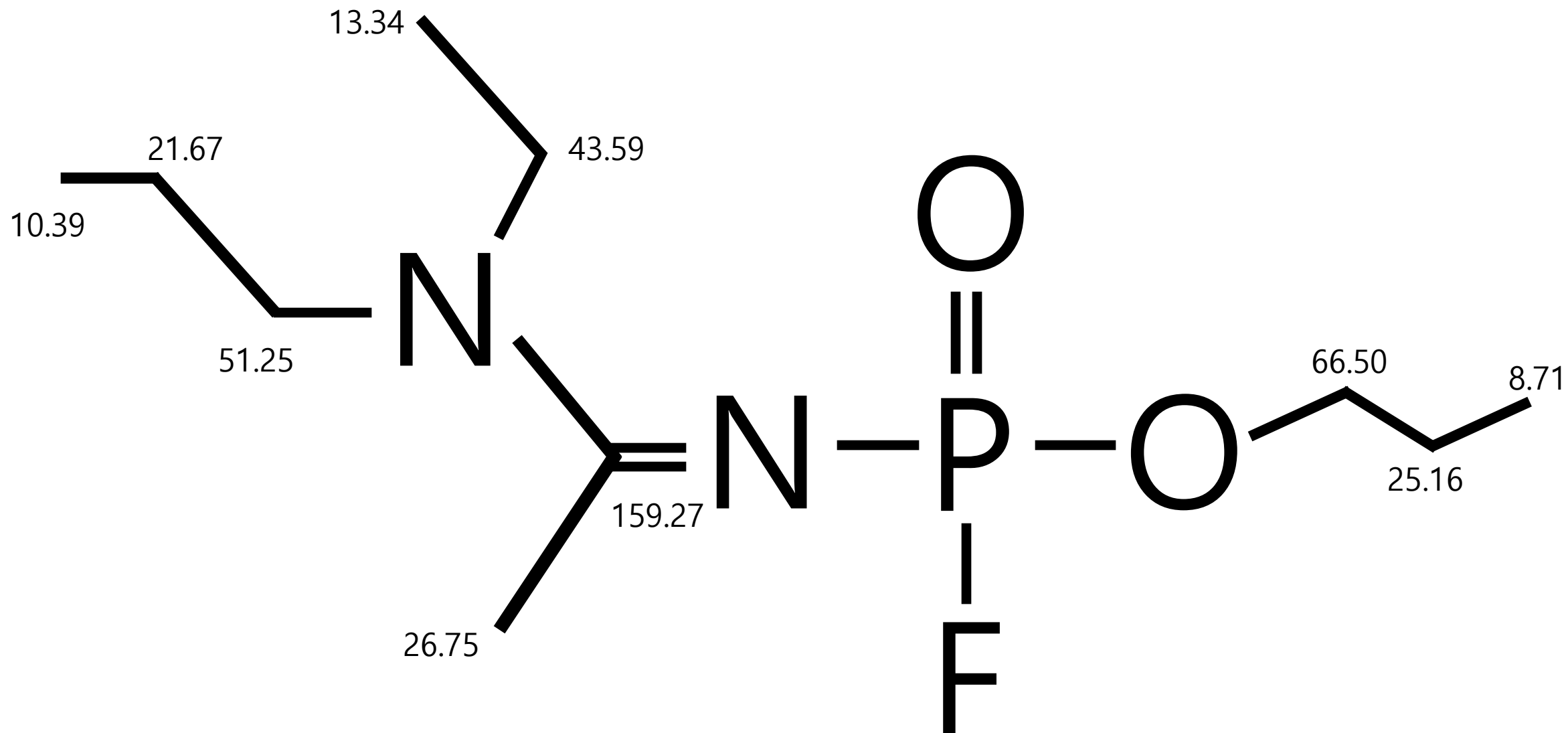


Figure S62. Structure 3132 and its ^{13}C chemical shift

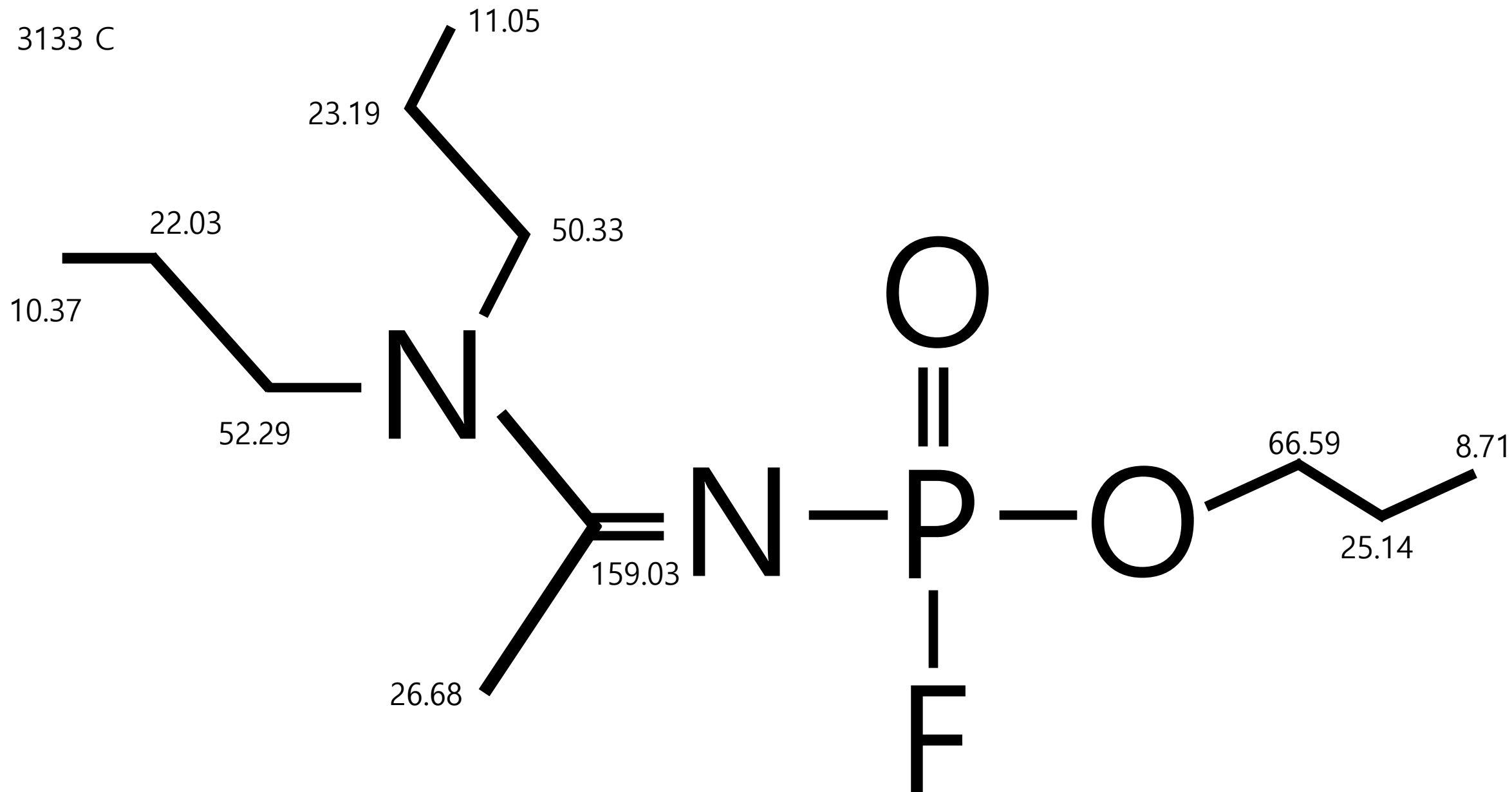


Figure S63. Structure 3133 and its ^{13}C chemical shift

3211 C

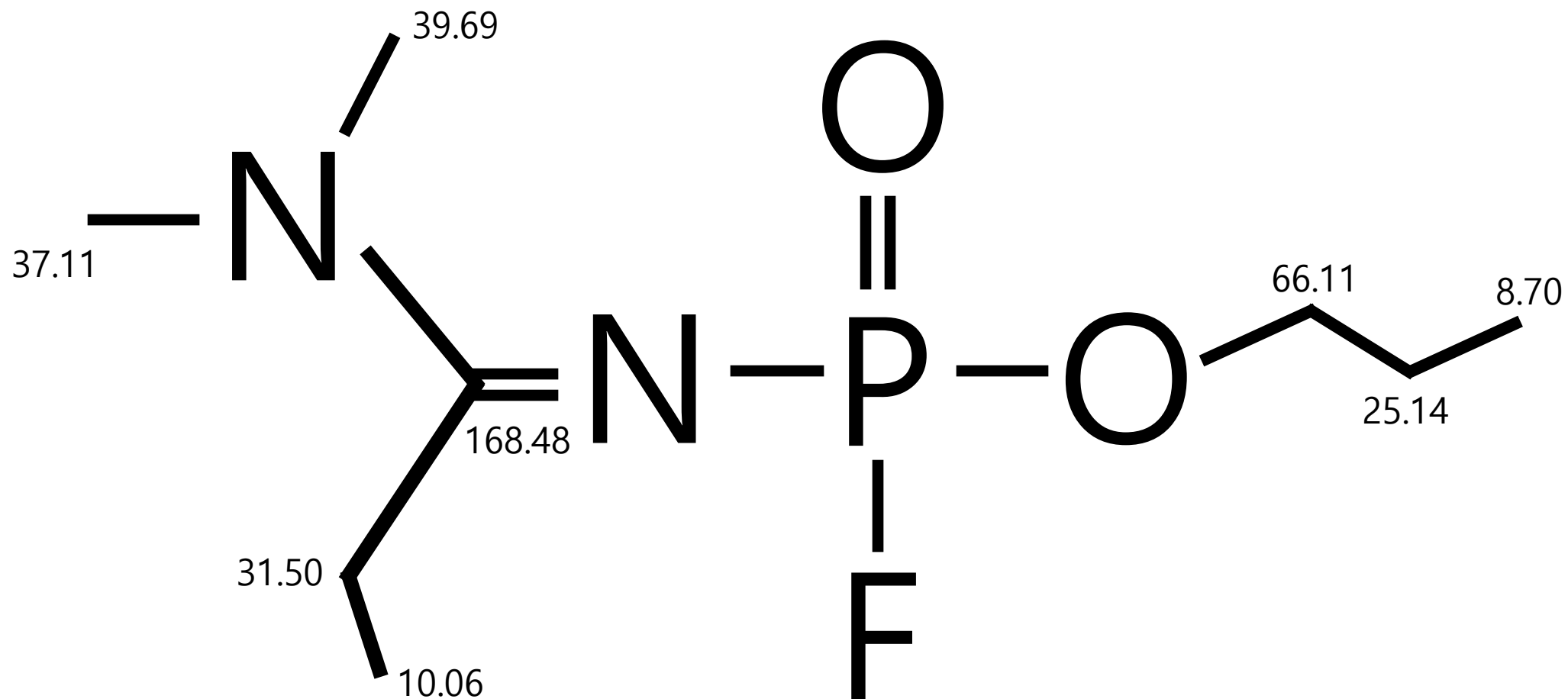


Figure S64. Structure 3211 and its ^{13}C chemical shift

3212 C

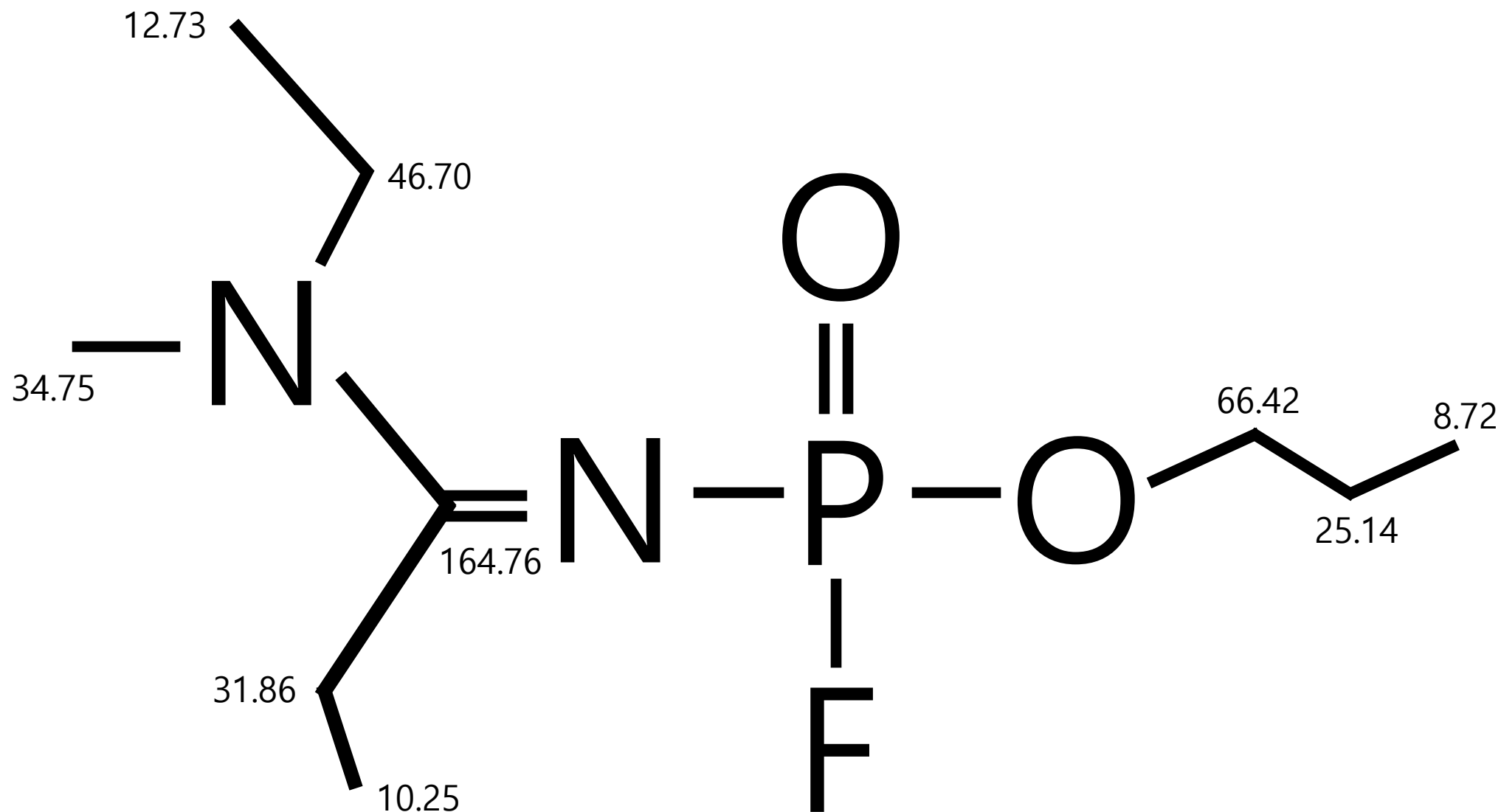


Figure S65. Structure 3212 and its ¹³C chemical shift

3213 C

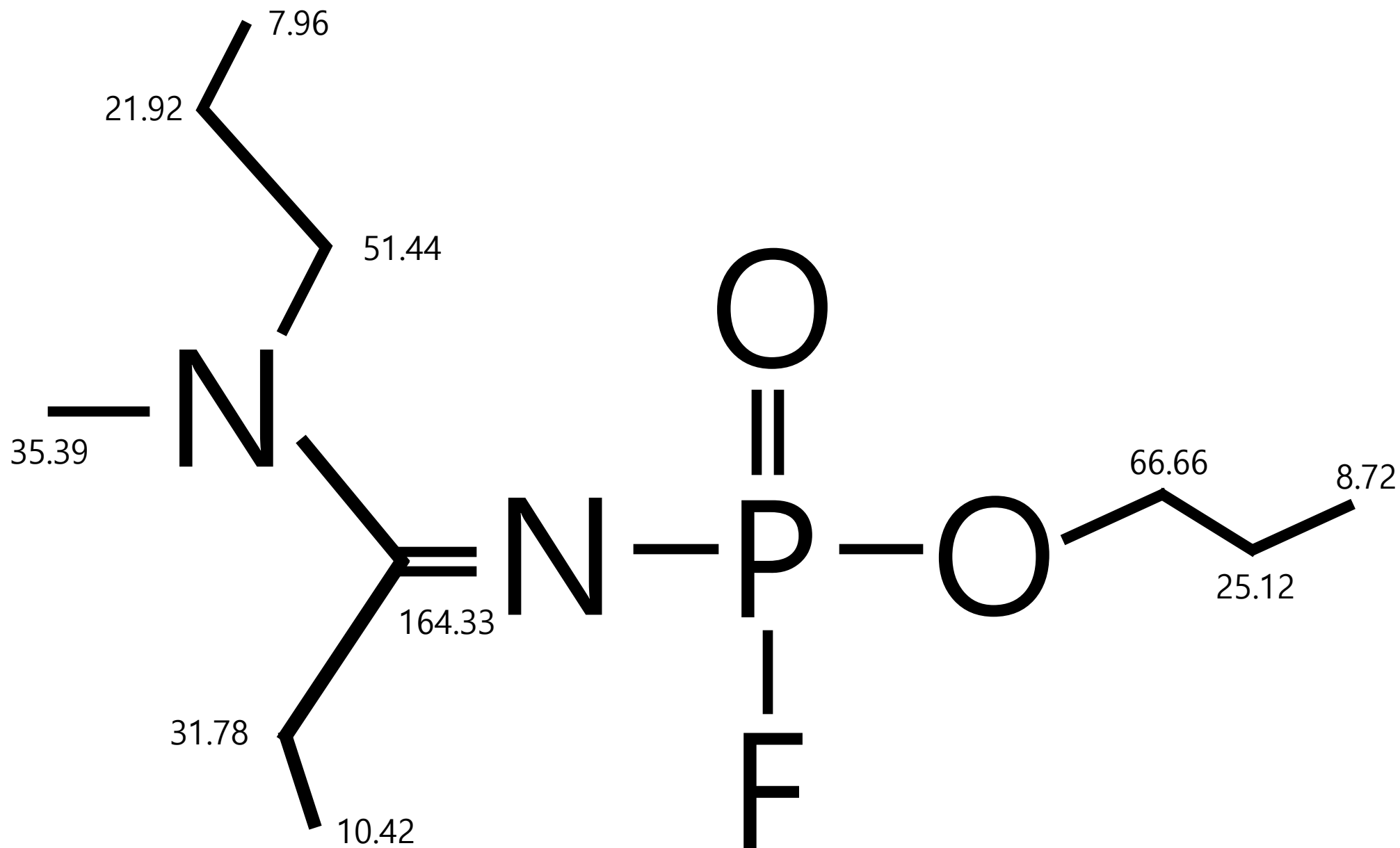


Figure S66. Structure 3213 and its ¹³C chemical shift

3221 C

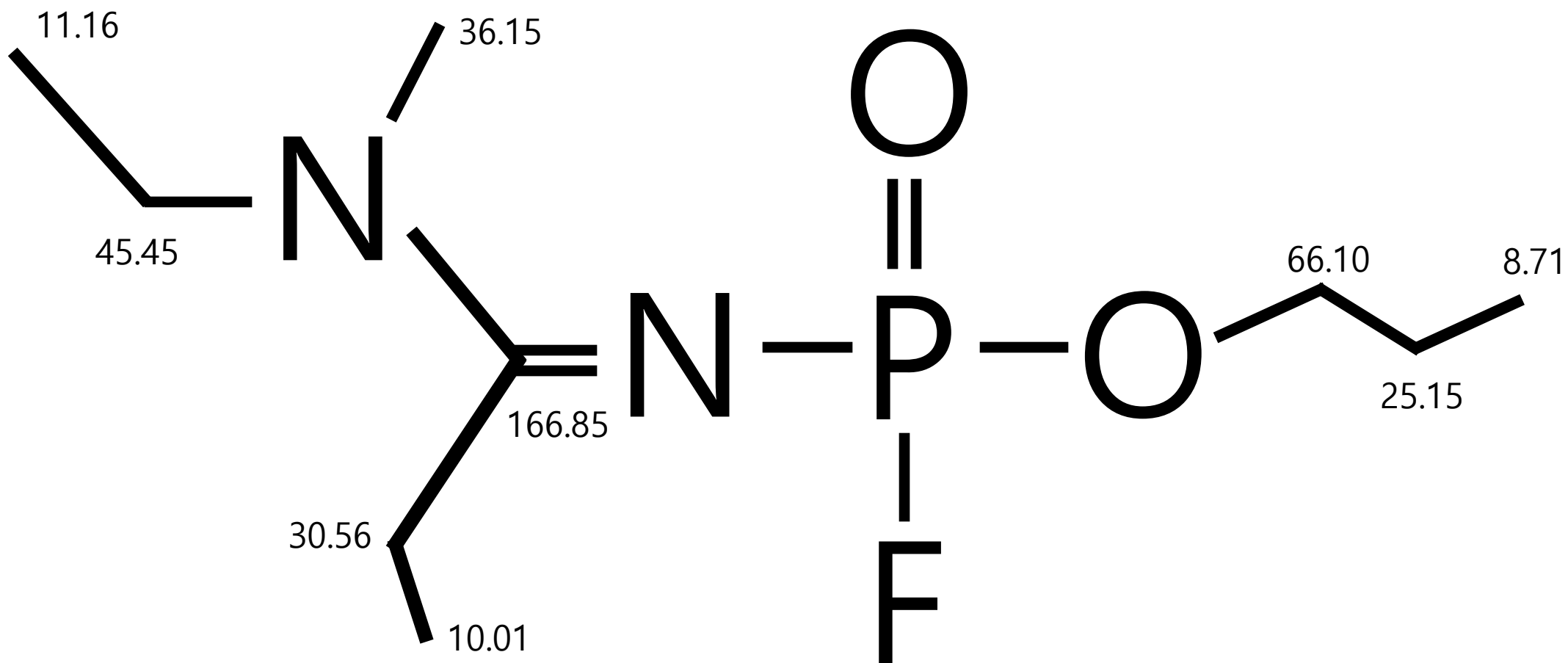


Figure S67. Structure 3221 and its ^{13}C chemical shift

3222 C

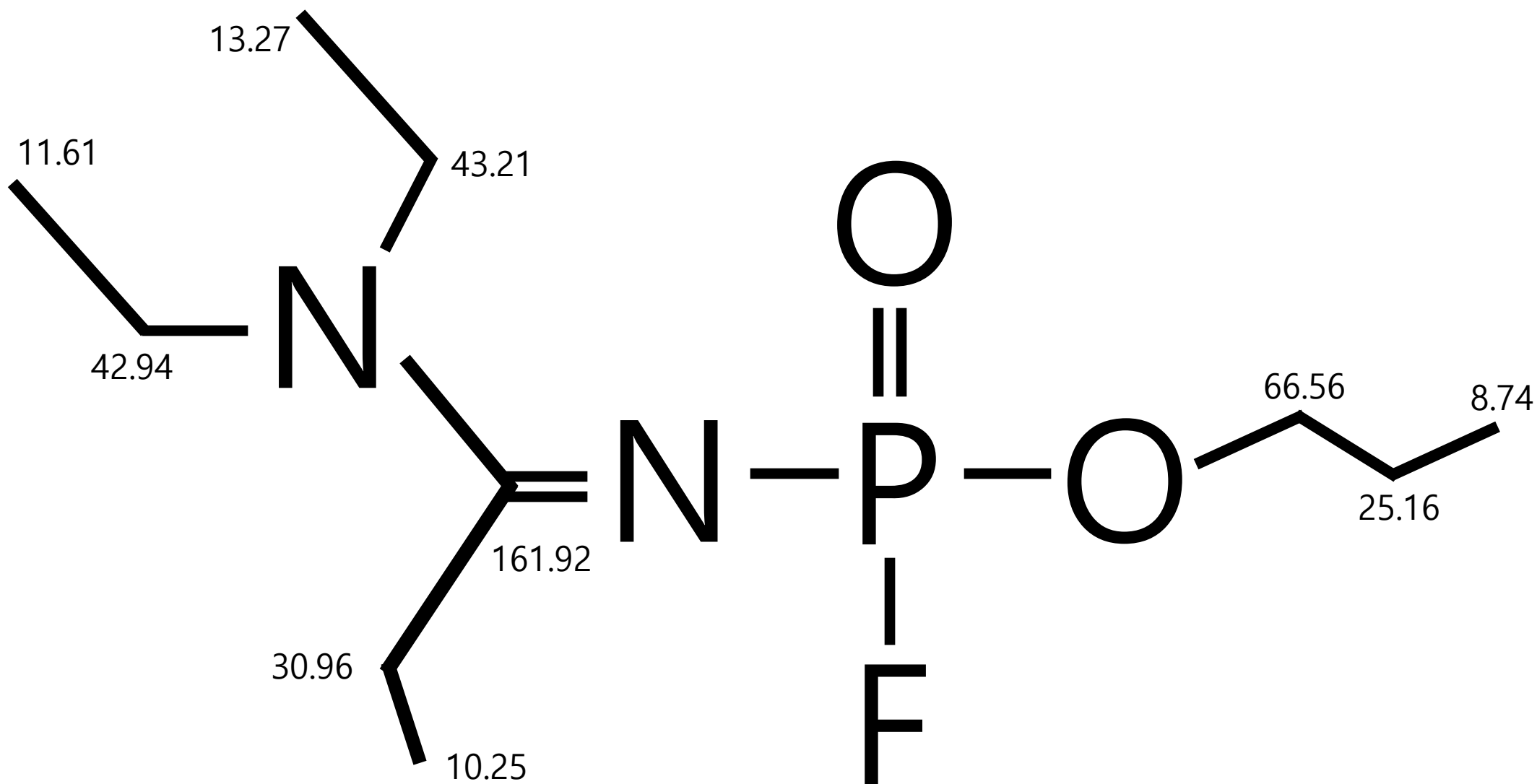


Figure S68. Structure 3222 and its ^{13}C chemical shift

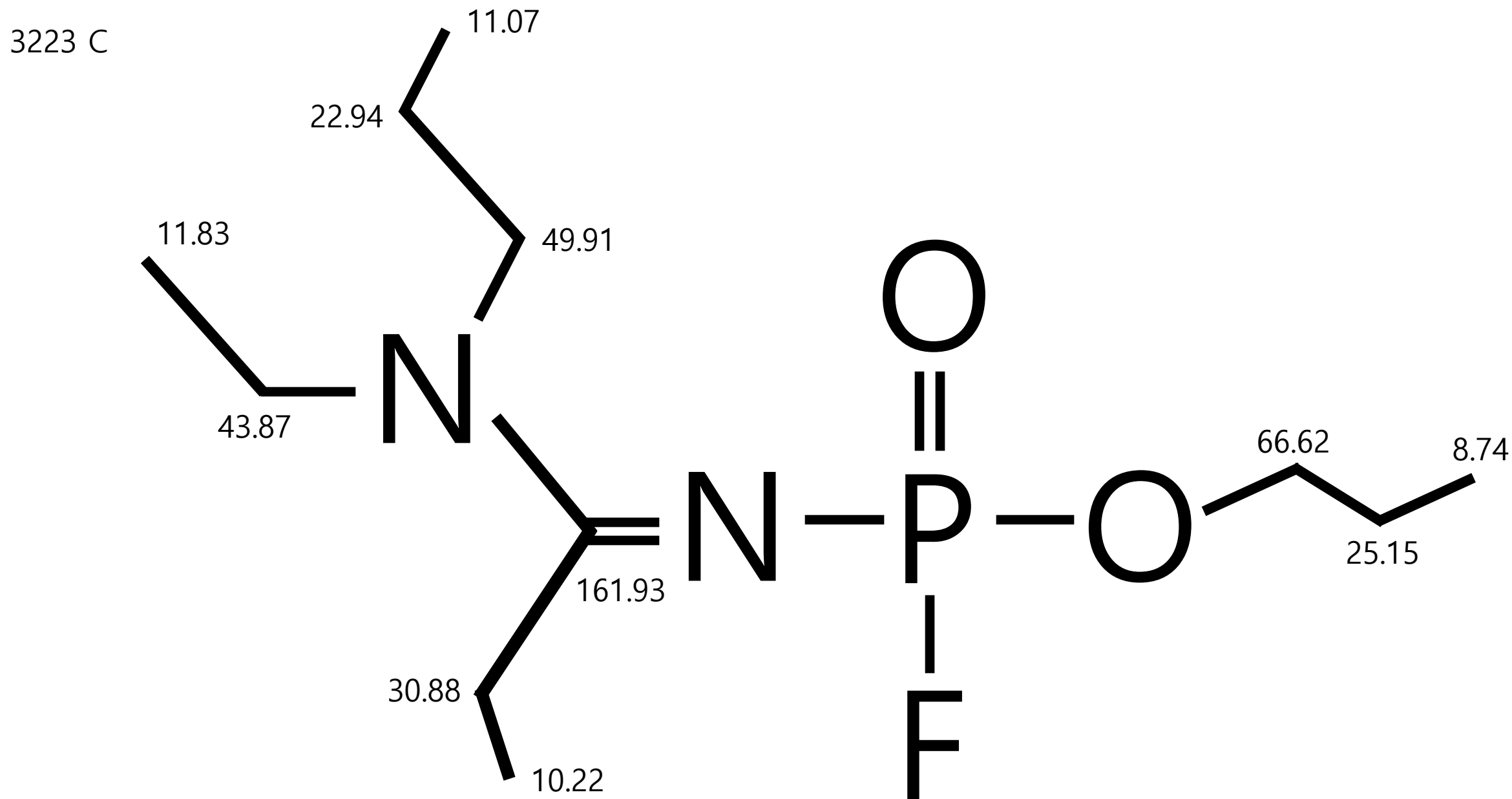


Figure S69. Structure 3223 and its ^{13}C chemical shift

3231 C

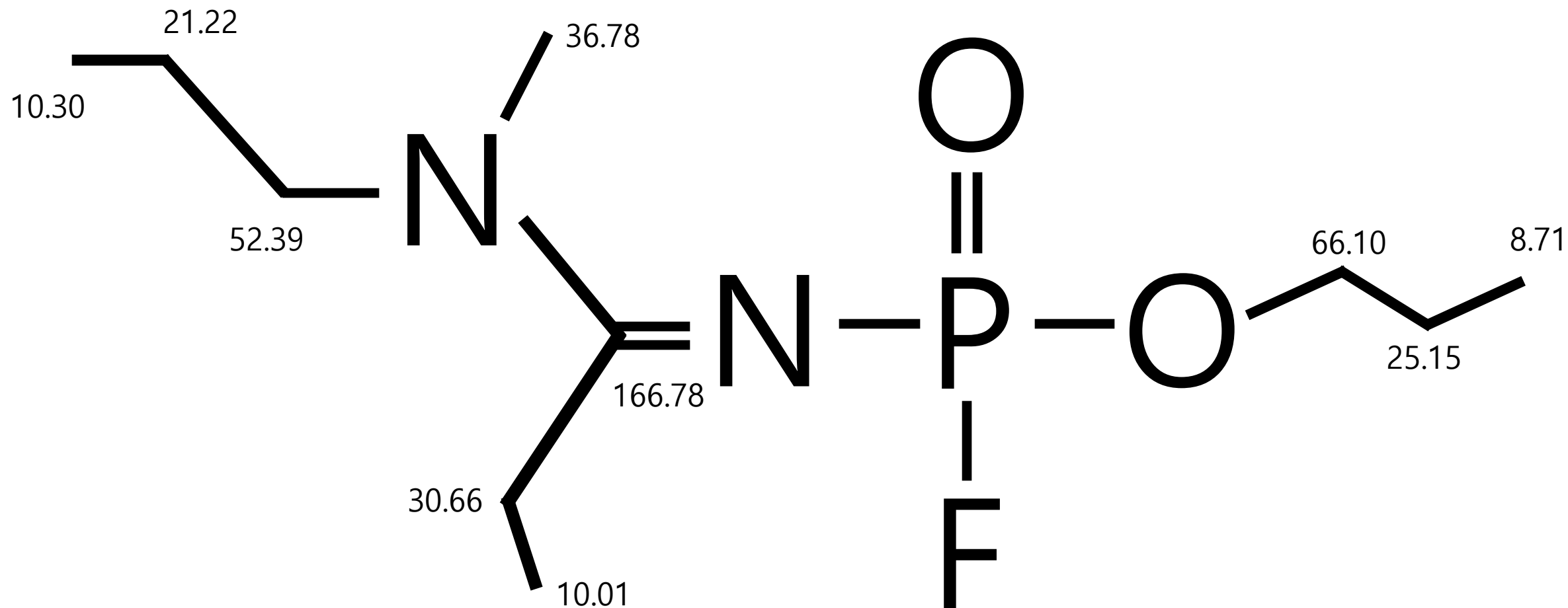


Figure S70. Structure 3231 and its ¹³C chemical shift

The chemical structure is 1-(diethylamino)-3-(3-ethoxypropyl)urea. The ¹³C NMR chemical shifts (in ppm) are labeled for each carbon atom in the structure:

- 10.43: Methyl carbon of the ethyl group on the left nitrogen.
- 21.76: Methyl carbon of the ethyl group on the left nitrogen.
- 49.90: Methyl carbon of the ethyl group on the left nitrogen.
- 13.33: Methyl carbon of the ethyl group on the right nitrogen.
- 43.84: Methyl carbon of the ethyl group on the right nitrogen.
- 161.96: Carbonyl carbon of the urea group.
- 31.05: Methyl carbon of the ethyl group on the right nitrogen.
- 10.24: Methyl carbon of the ethyl group on the right nitrogen.
- 66.56: Methyl carbon of the ethoxy group.
- 25.16: Methyl carbon of the ethoxy group.
- 8.73: Methyl carbon of the ethoxy group.

Figure S71. Structure 3232 and its ^{13}C chemical shift

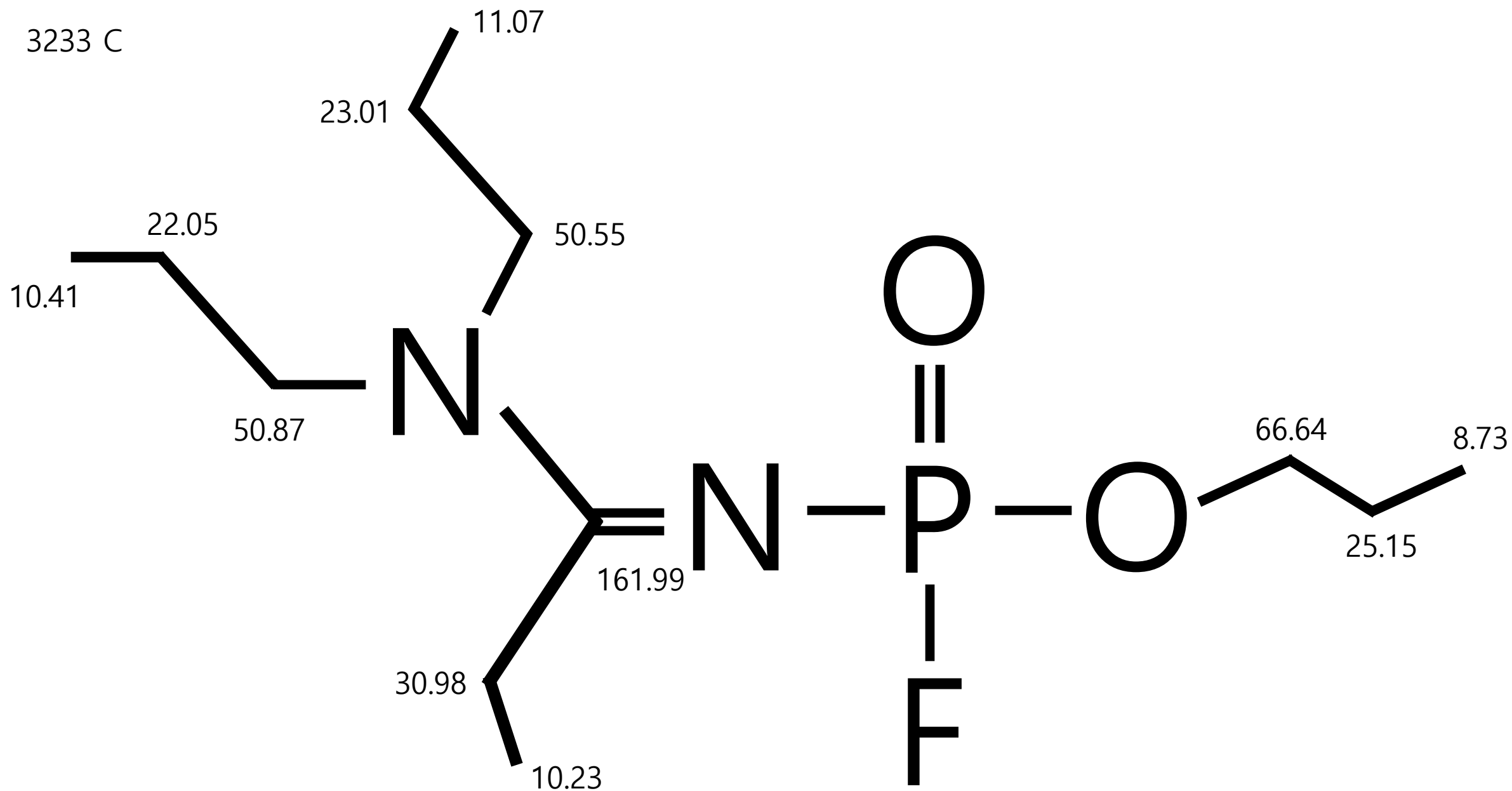


Figure S72. Structure 3233 and its ¹³C chemical shift

3311 C

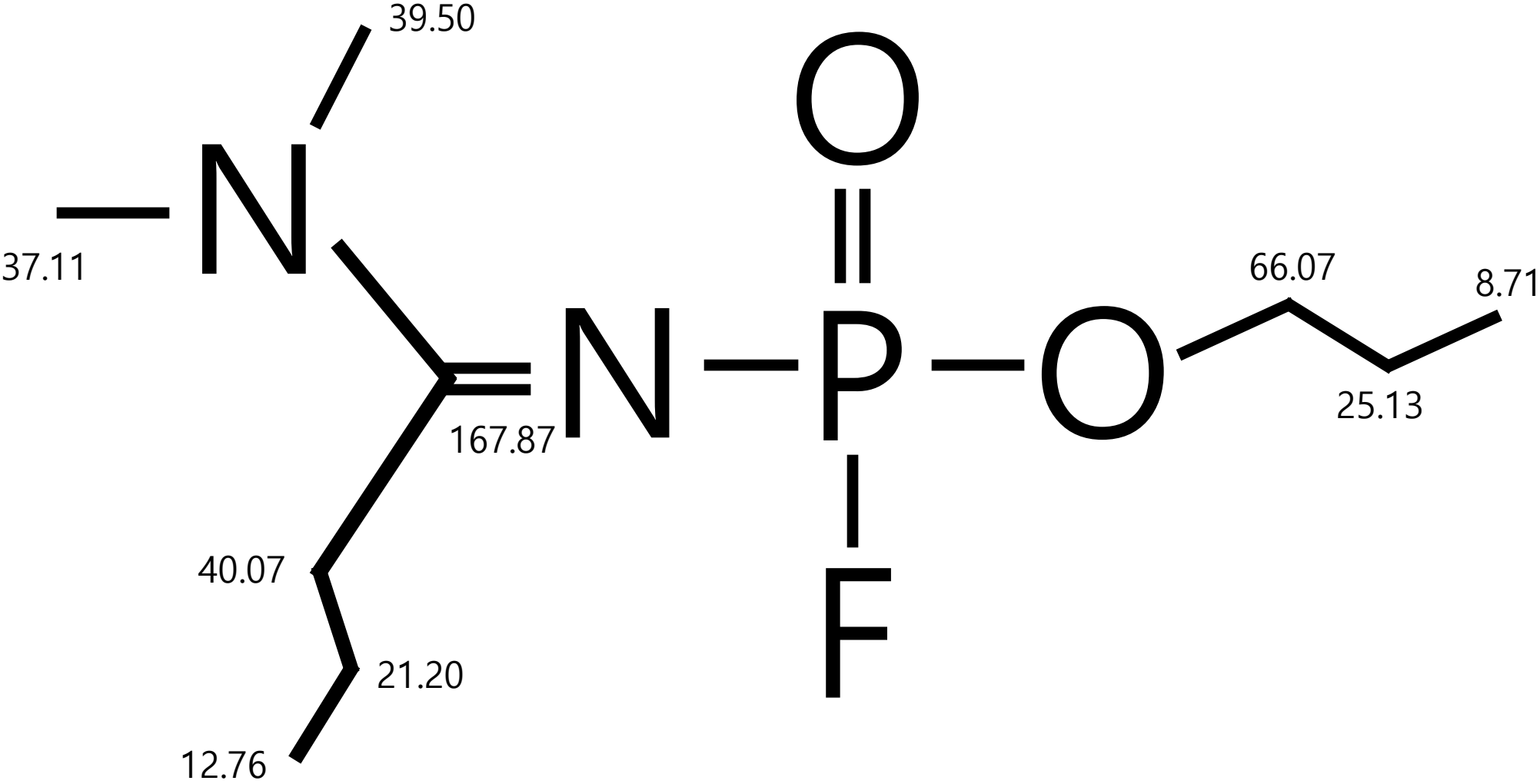


Figure S73. Structure 3311 and its ¹³C chemical shift

3312 C

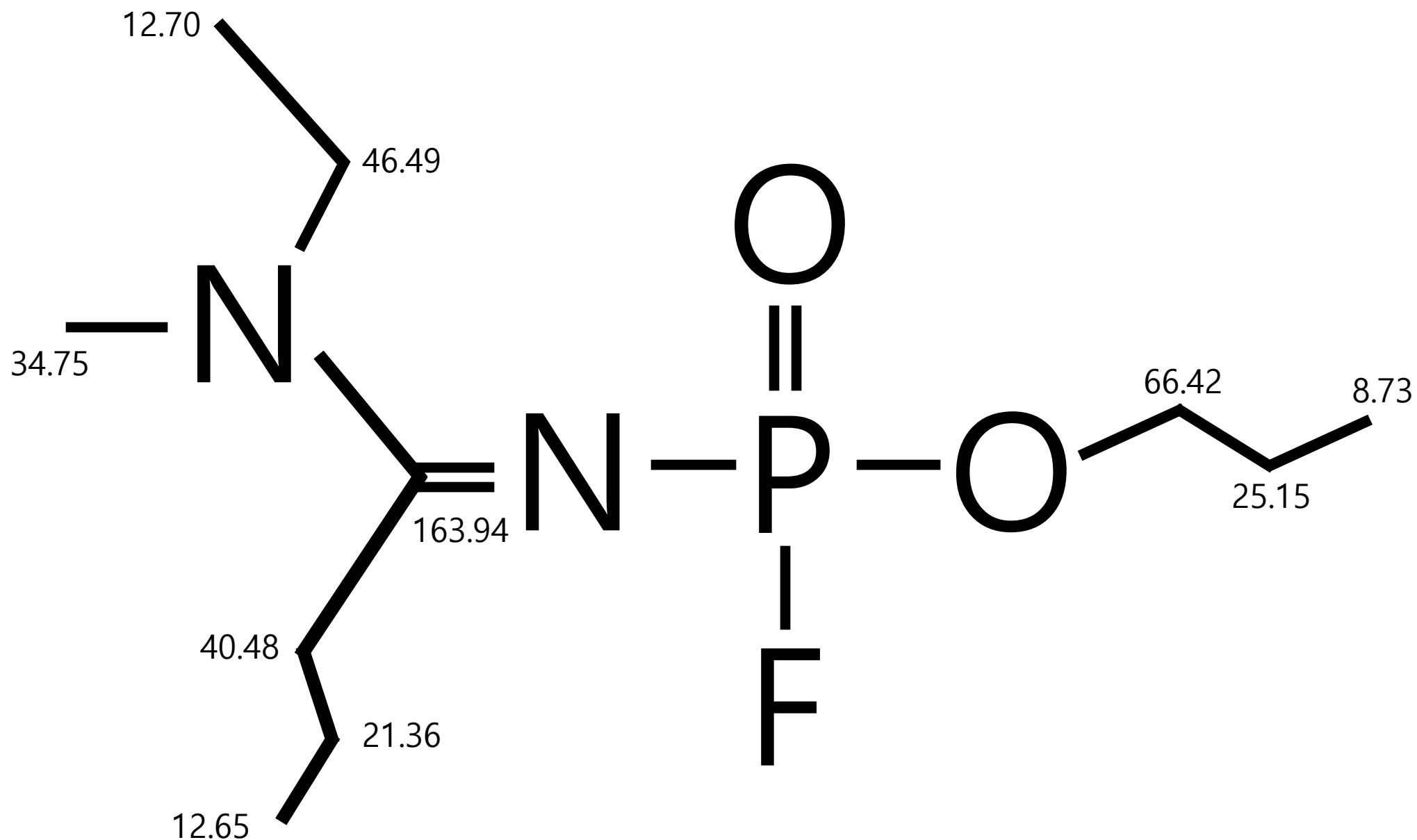


Figure S74. Structure 3312 and its ¹³C chemical shift

3313 C

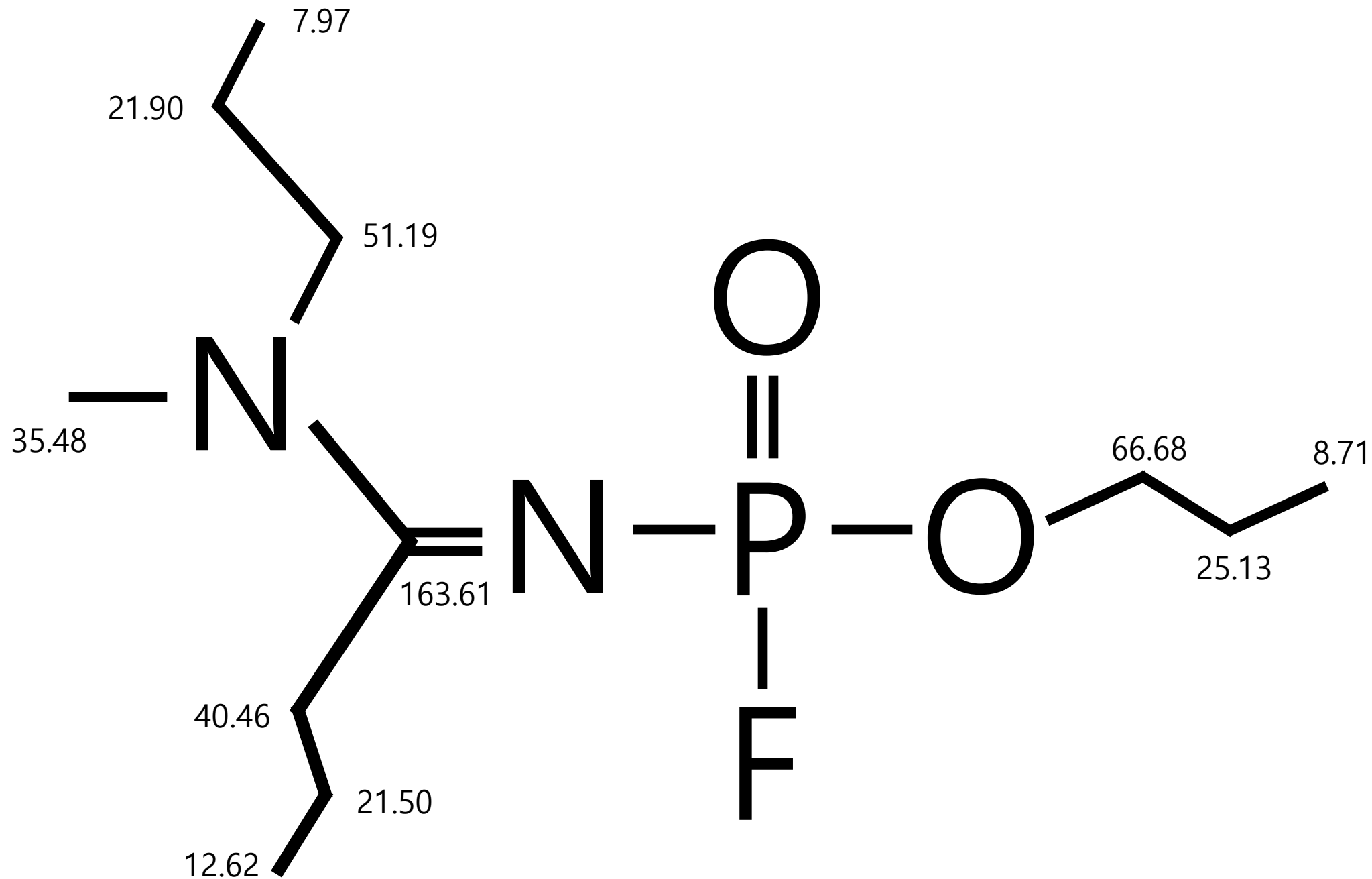


Figure S75. Structure 3313 and its ¹³C chemical shift

3321 C

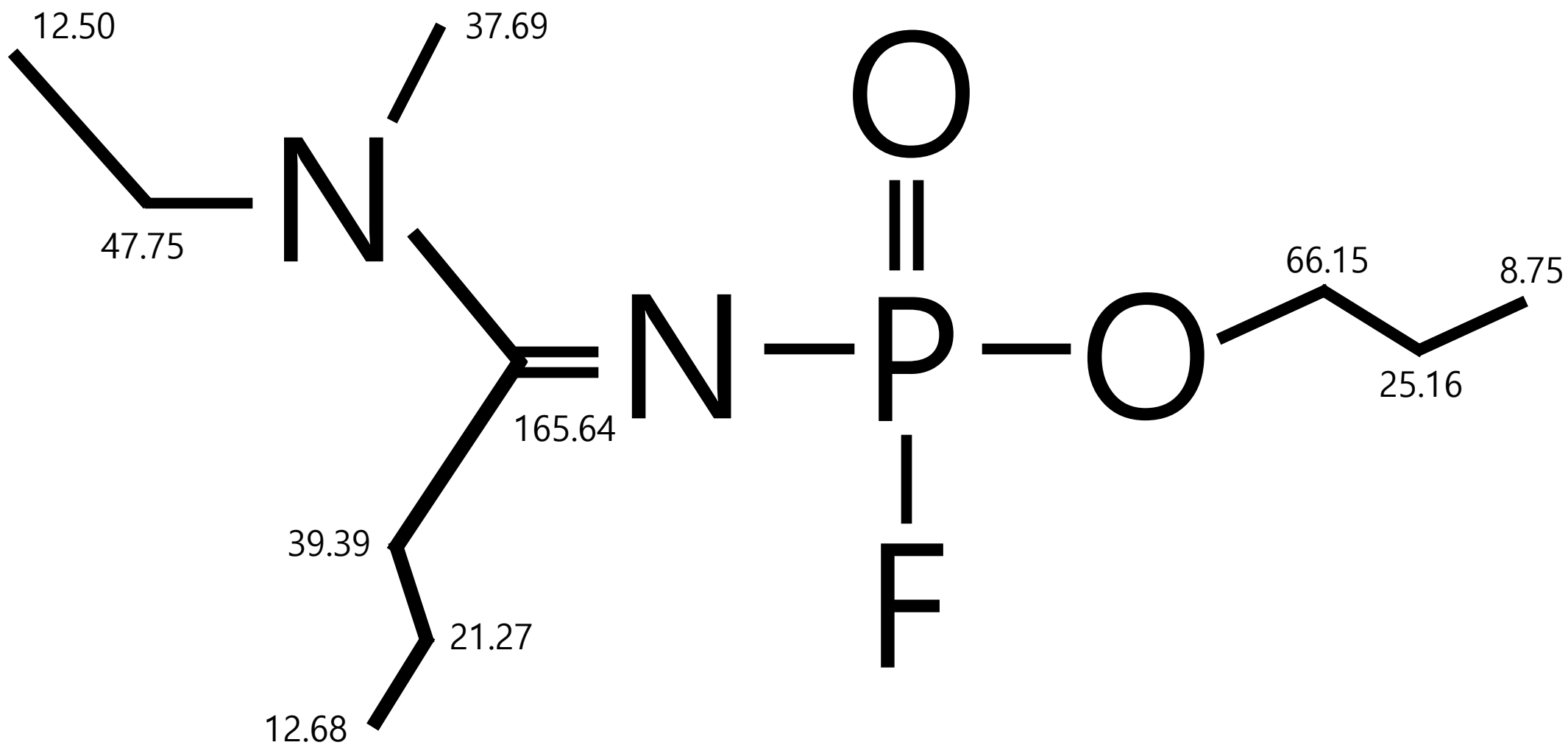


Figure S76. Structure 3321 and its ^{13}C chemical shift

3322 C

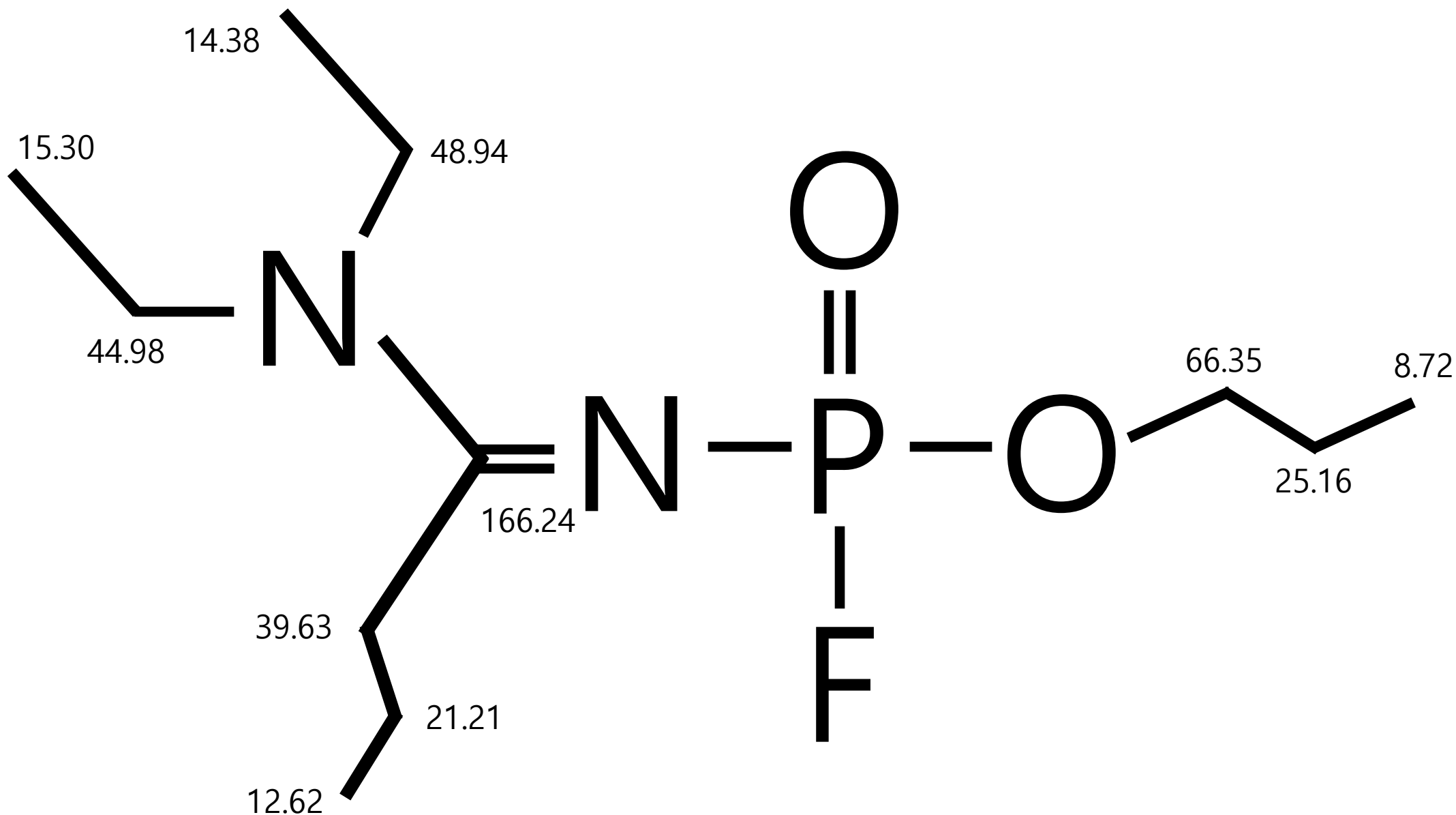


Figure S77. Structure 3322 and its ¹³C chemical shift

3323 C

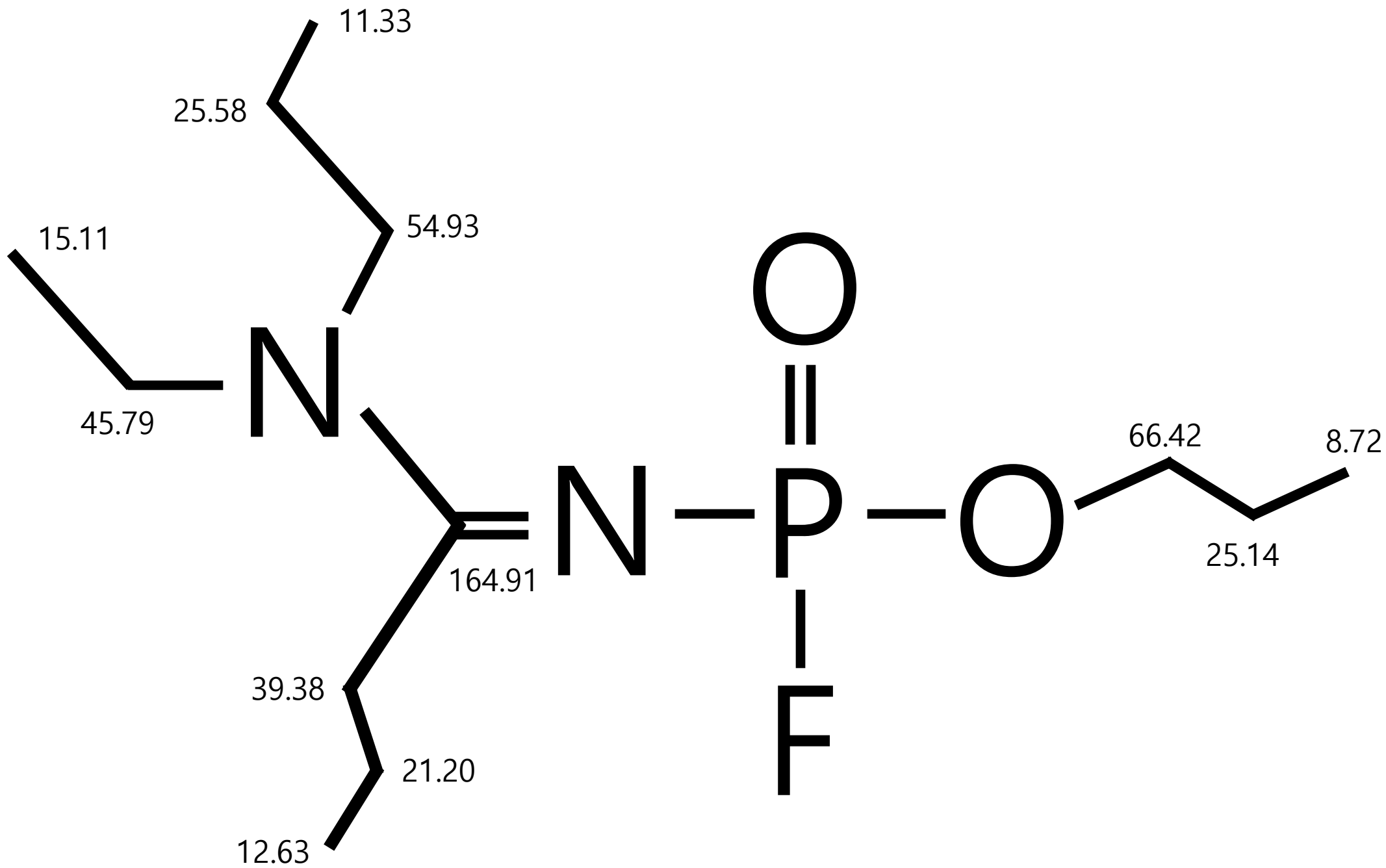


Figure S78. Structure 3323 and its ^{13}C chemical shift

3331 C

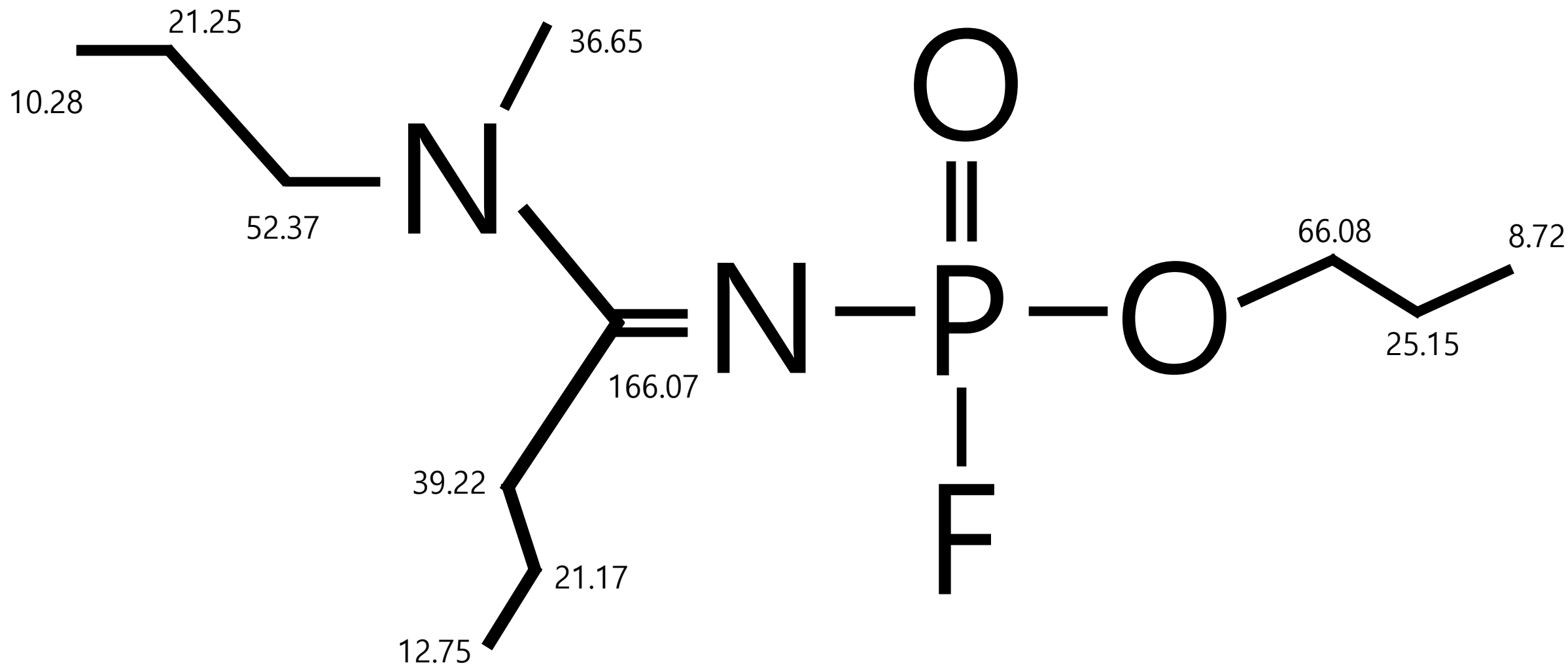


Figure S79. Structure 3331 and its ^{13}C chemical shift

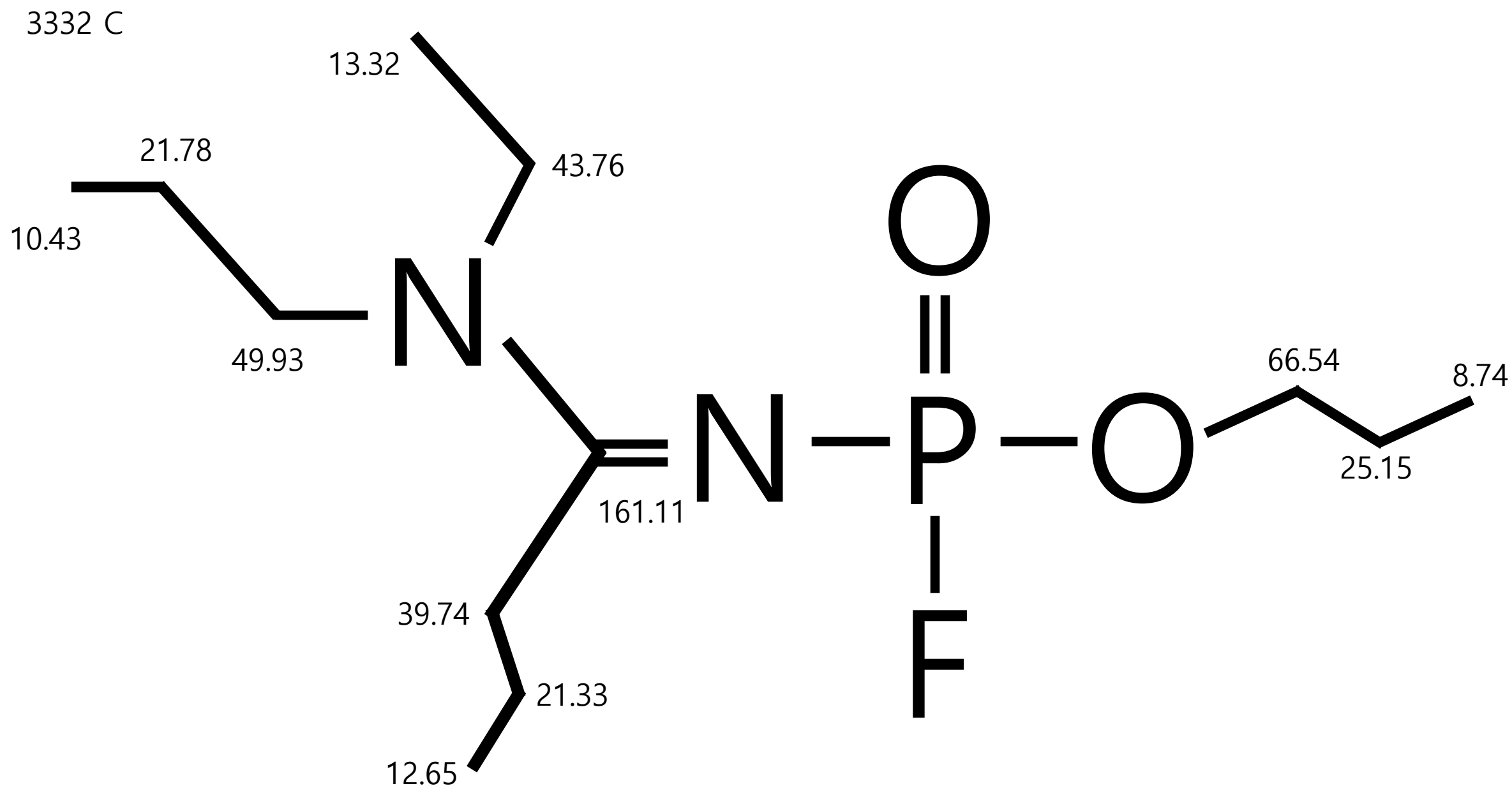


Figure S80. Structure 3332 and its ¹³C chemical shift

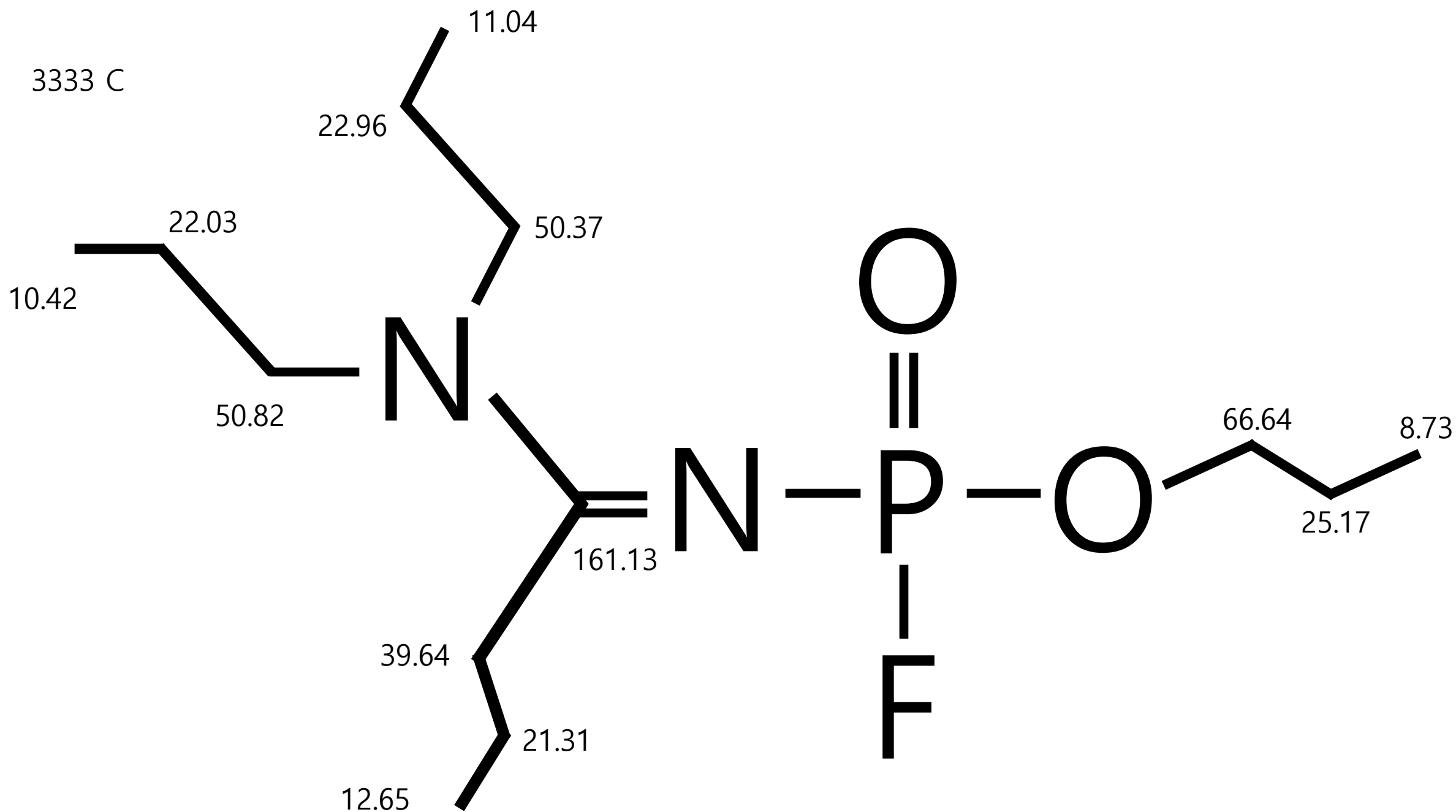


Figure S81. Structure 3333 and its ^{13}C chemical shift

A242 C

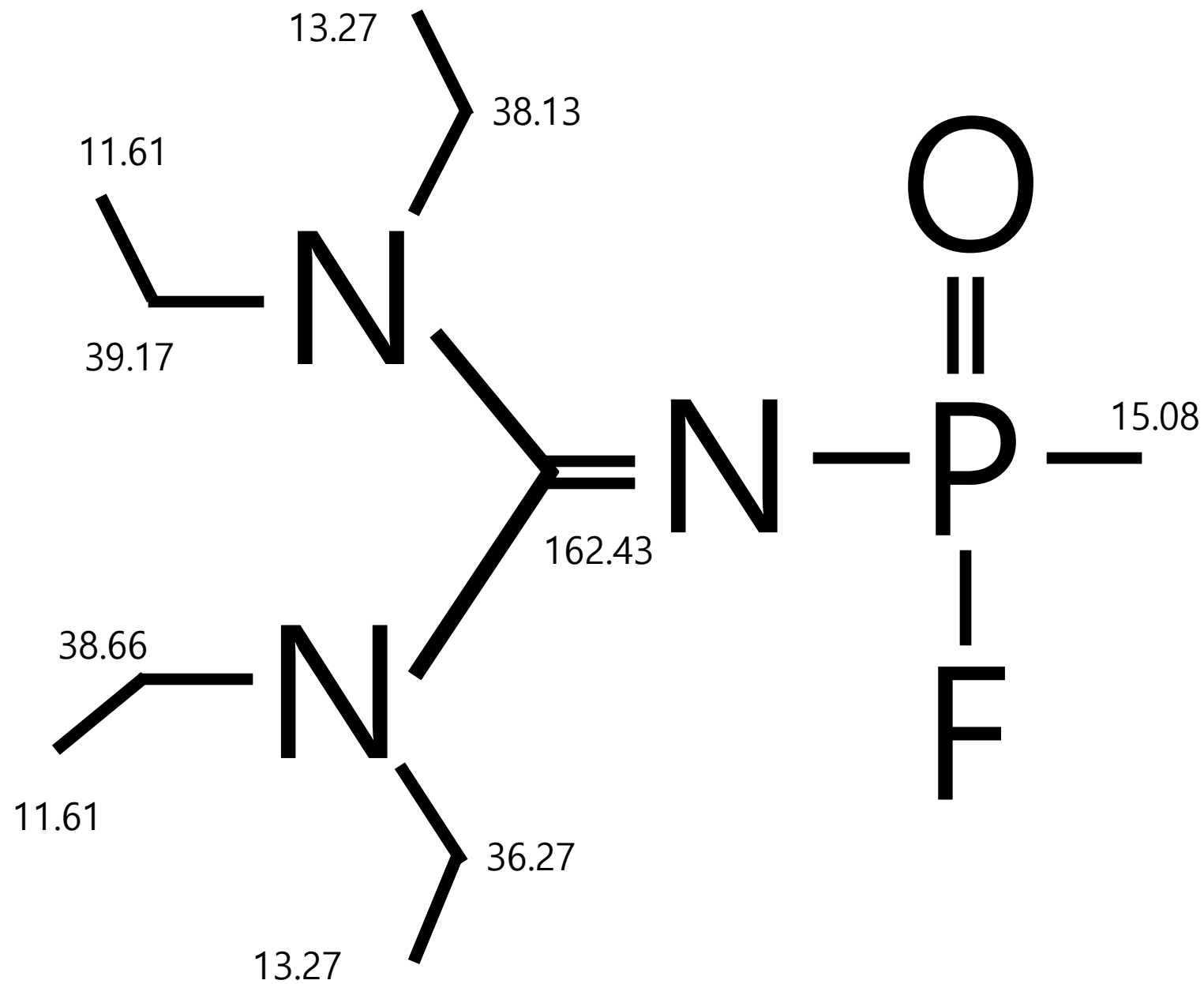


Figure S82. Structure A242 and its ¹³C chemical shift

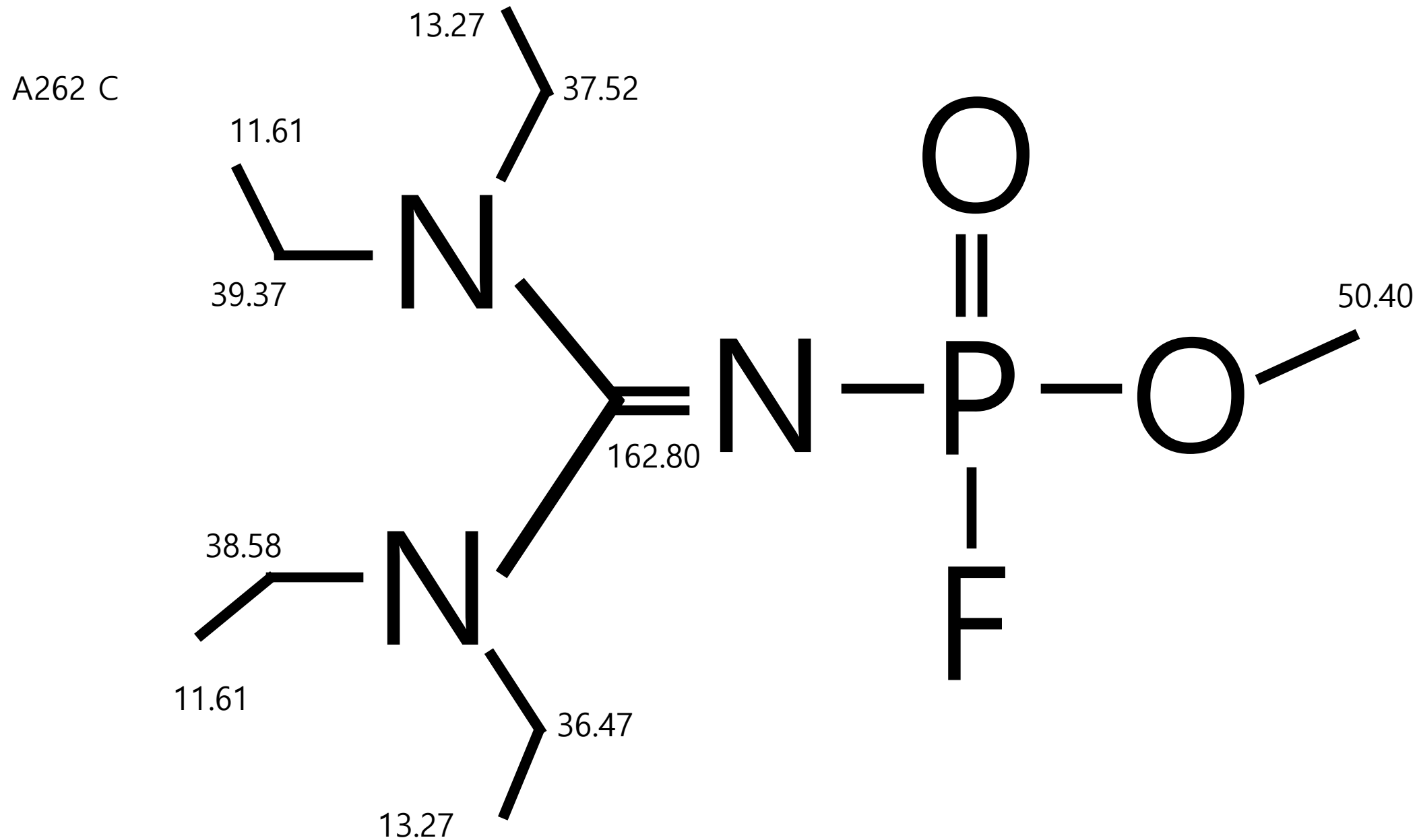


Figure S83. Structure A262 and its ¹³C chemical shift

1111 H

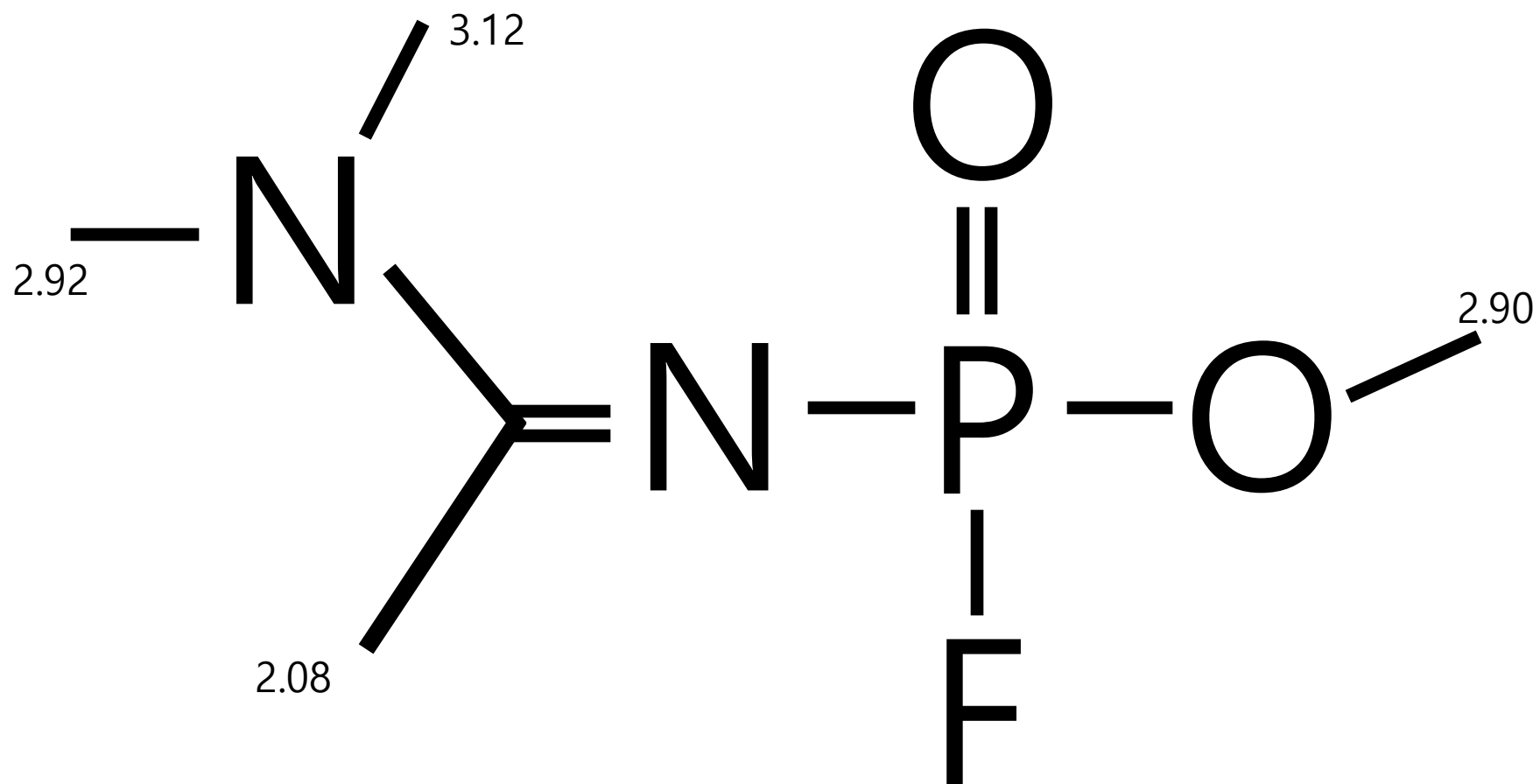


Figure S84. Structure 1111 and its ^1H chemical shift

1112 H

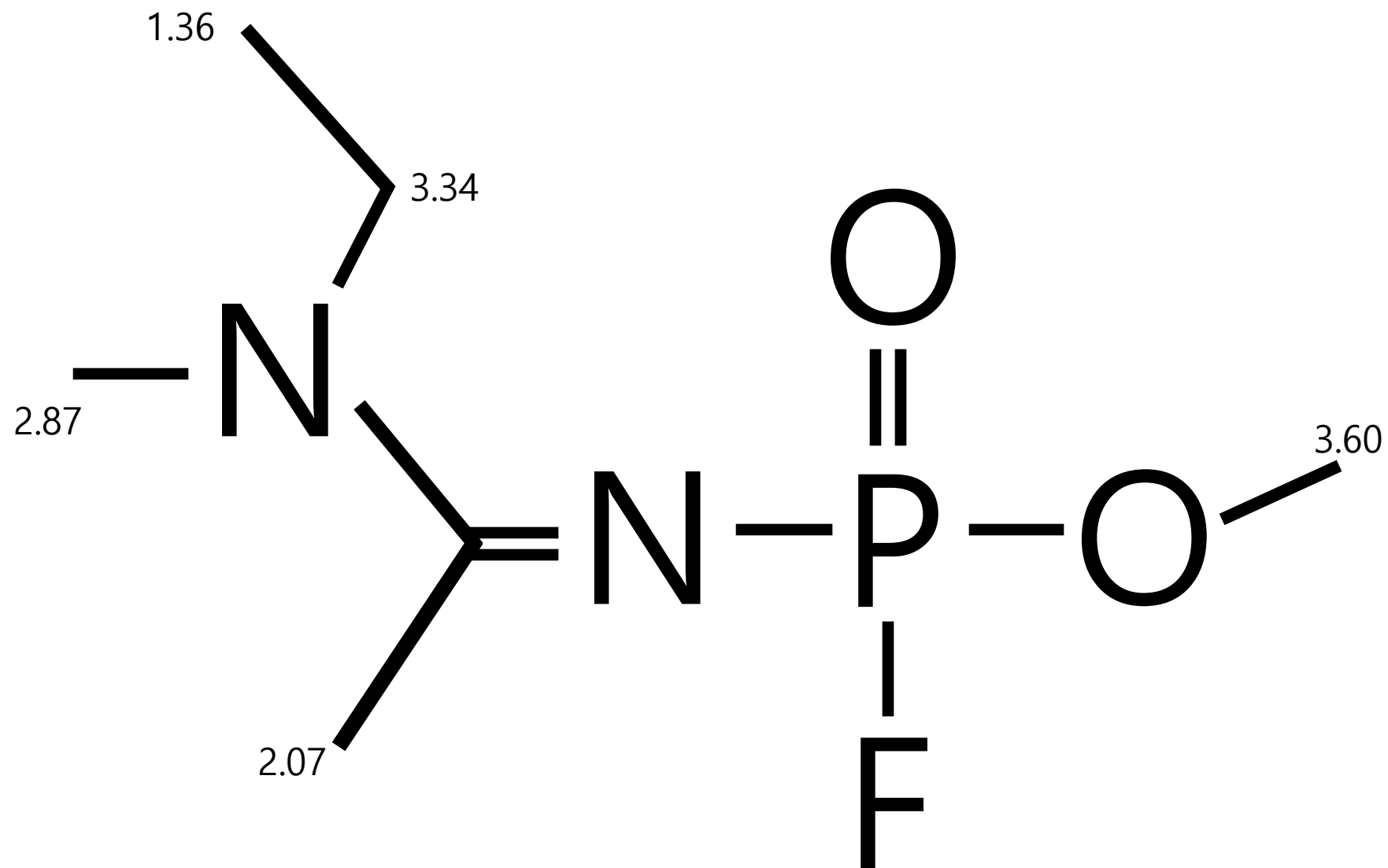


Figure S85. Structure 1112 and its ¹H chemical shift

1113 H

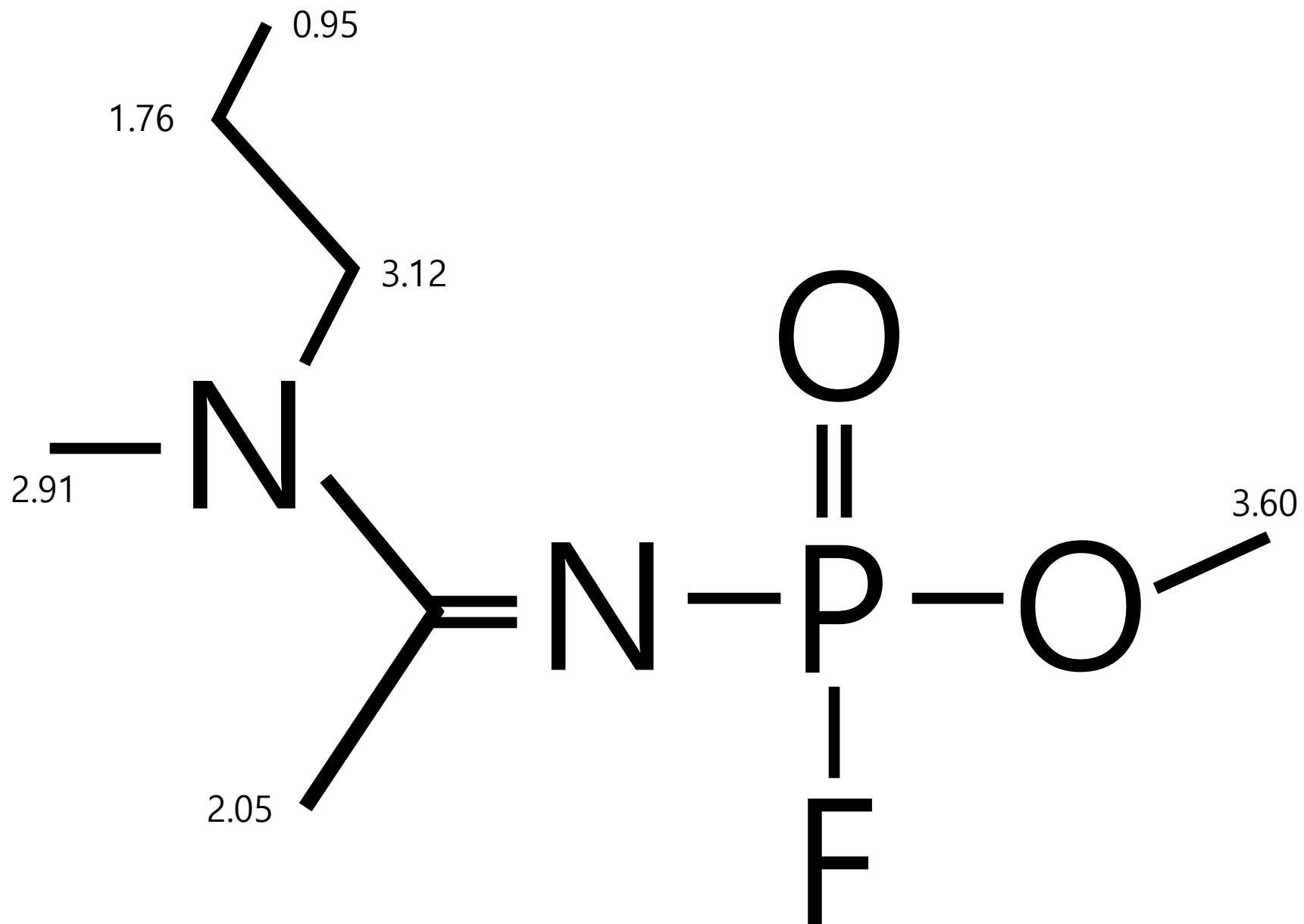


Figure S86. Structure 1113 and its ¹H chemical shift

1121 H

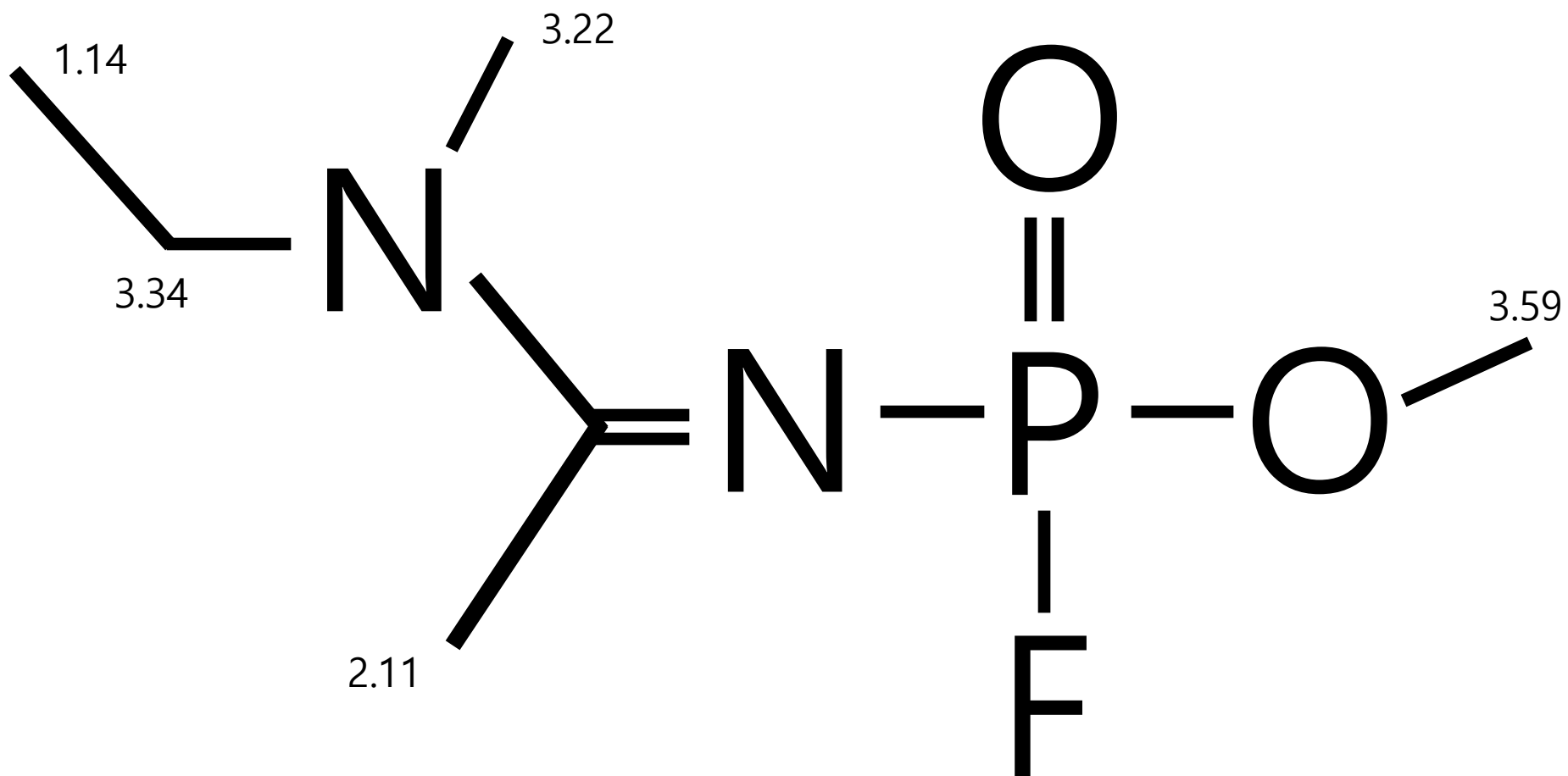


Figure S87. Structure 1121 and its ^1H chemical shift

1122 H

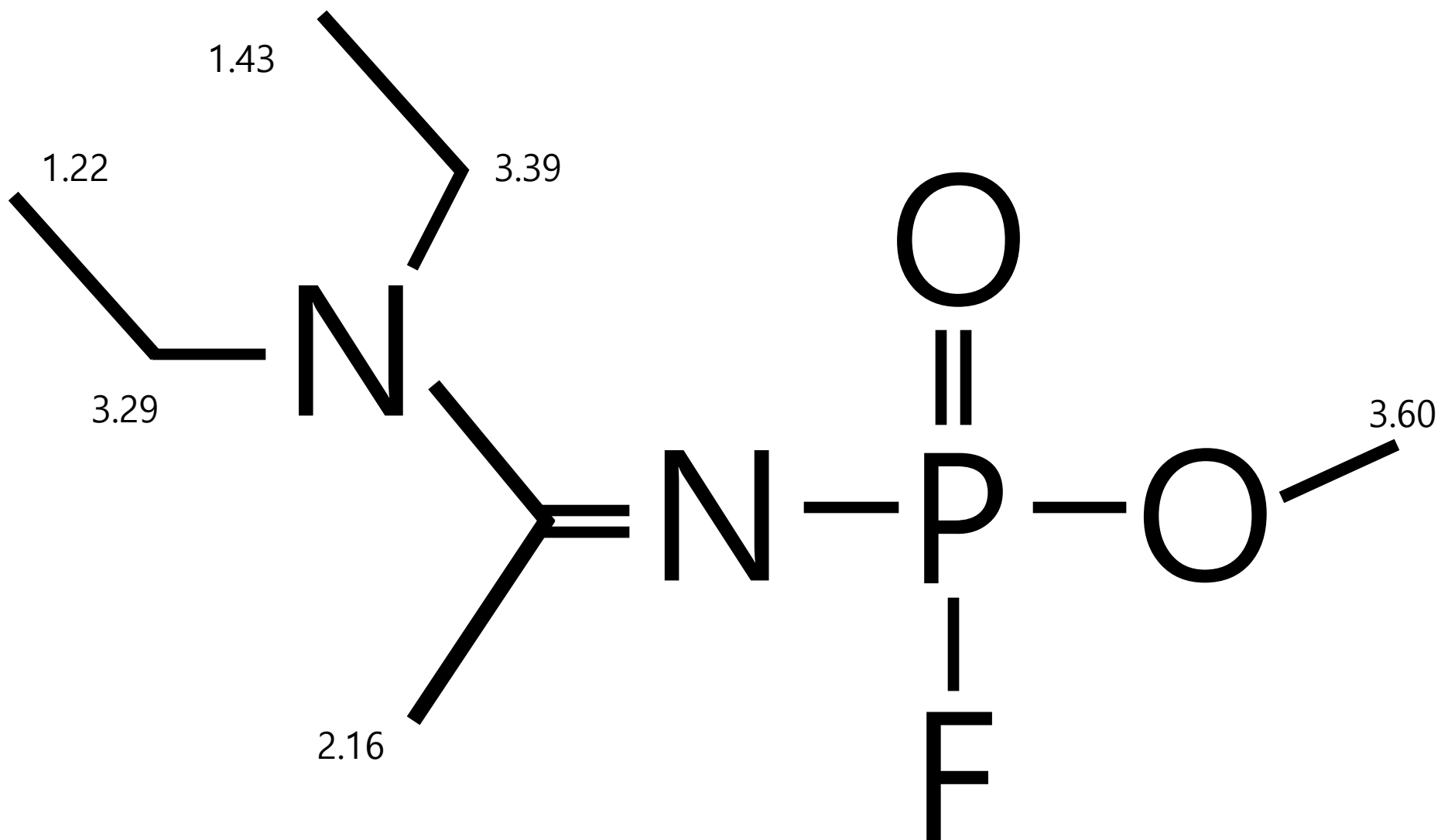


Figure S88. Structure 1122 and its ^1H chemical shift

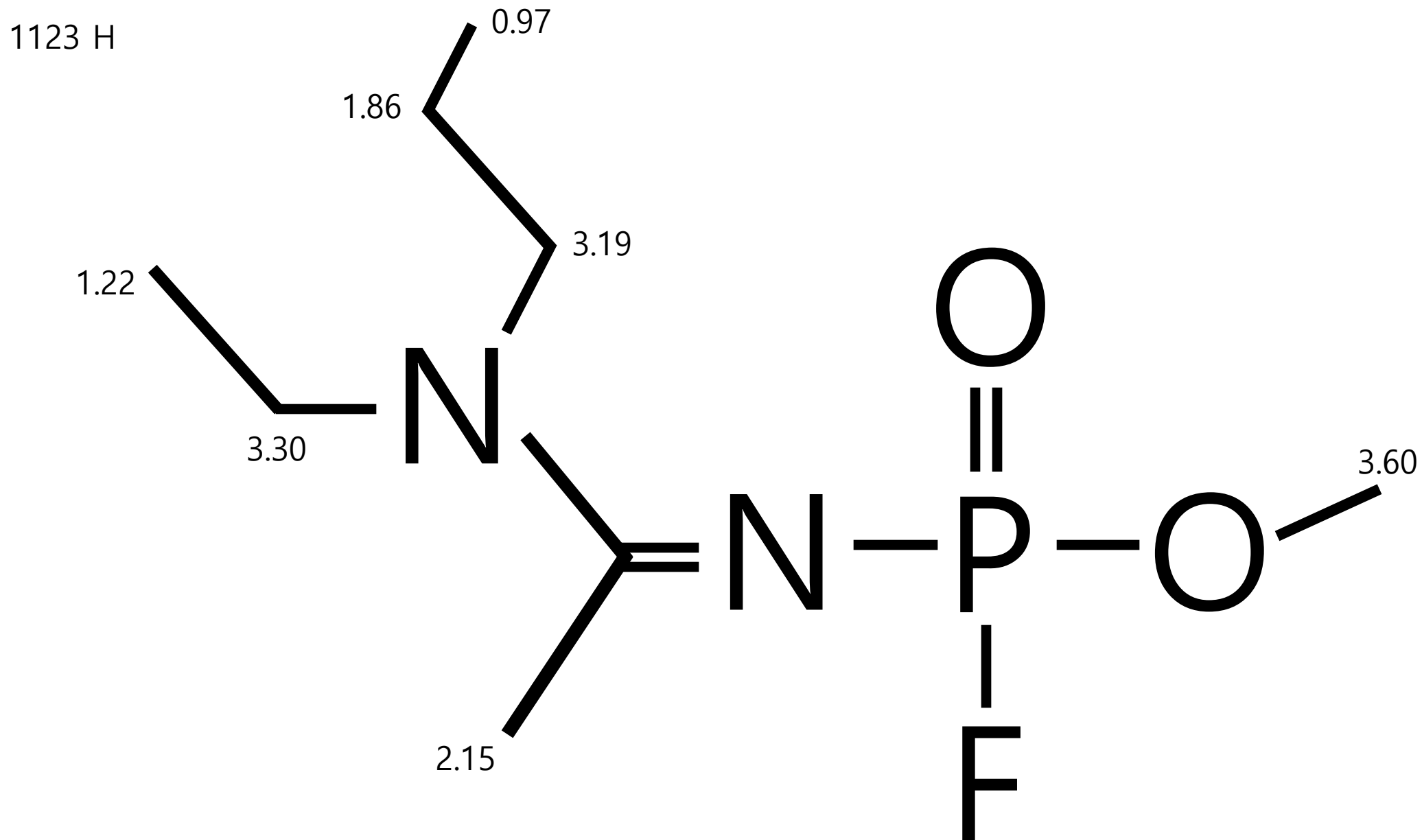


Figure S89. Structure 1123 and its ^1H chemical shift

1131 H

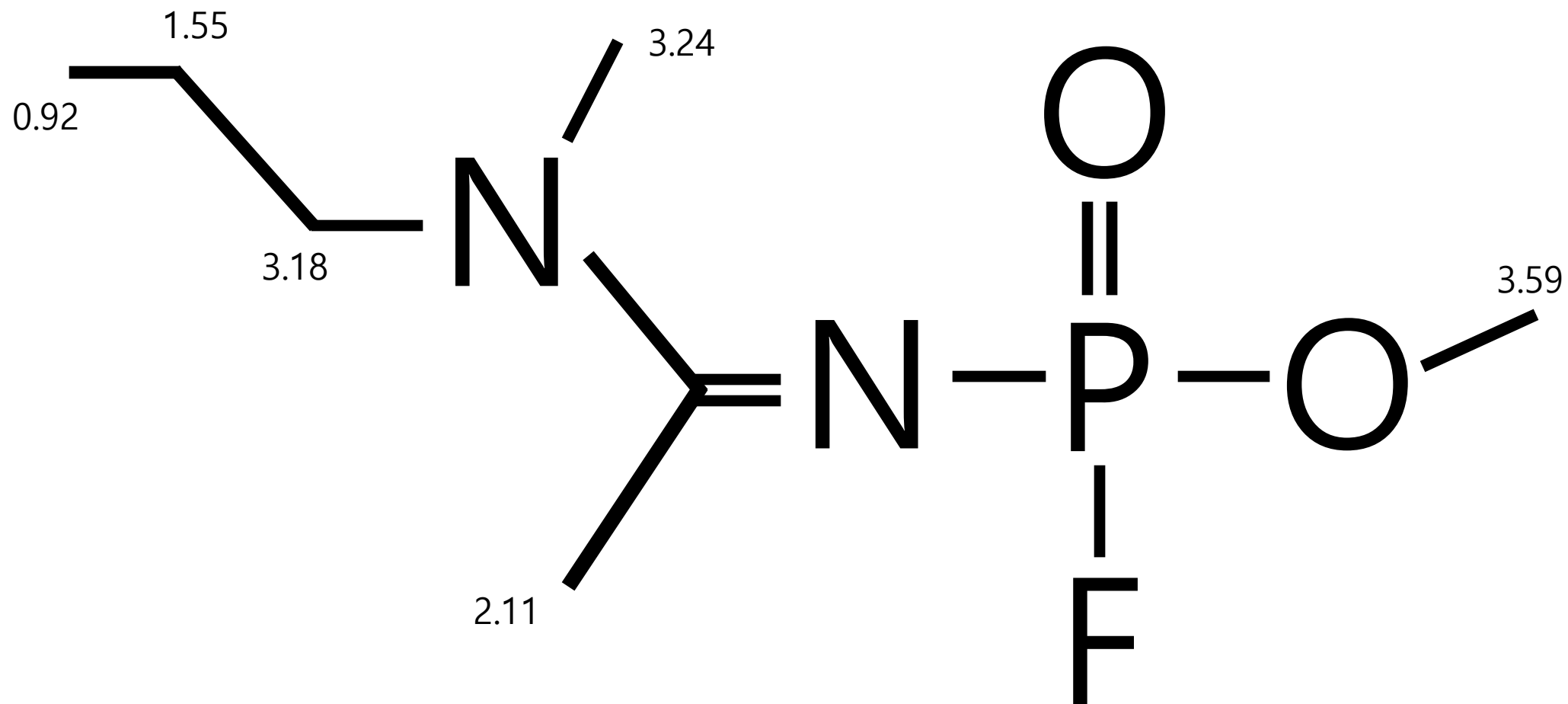


Figure S90. Structure 1131 and its ^1H chemical shift

1132 H

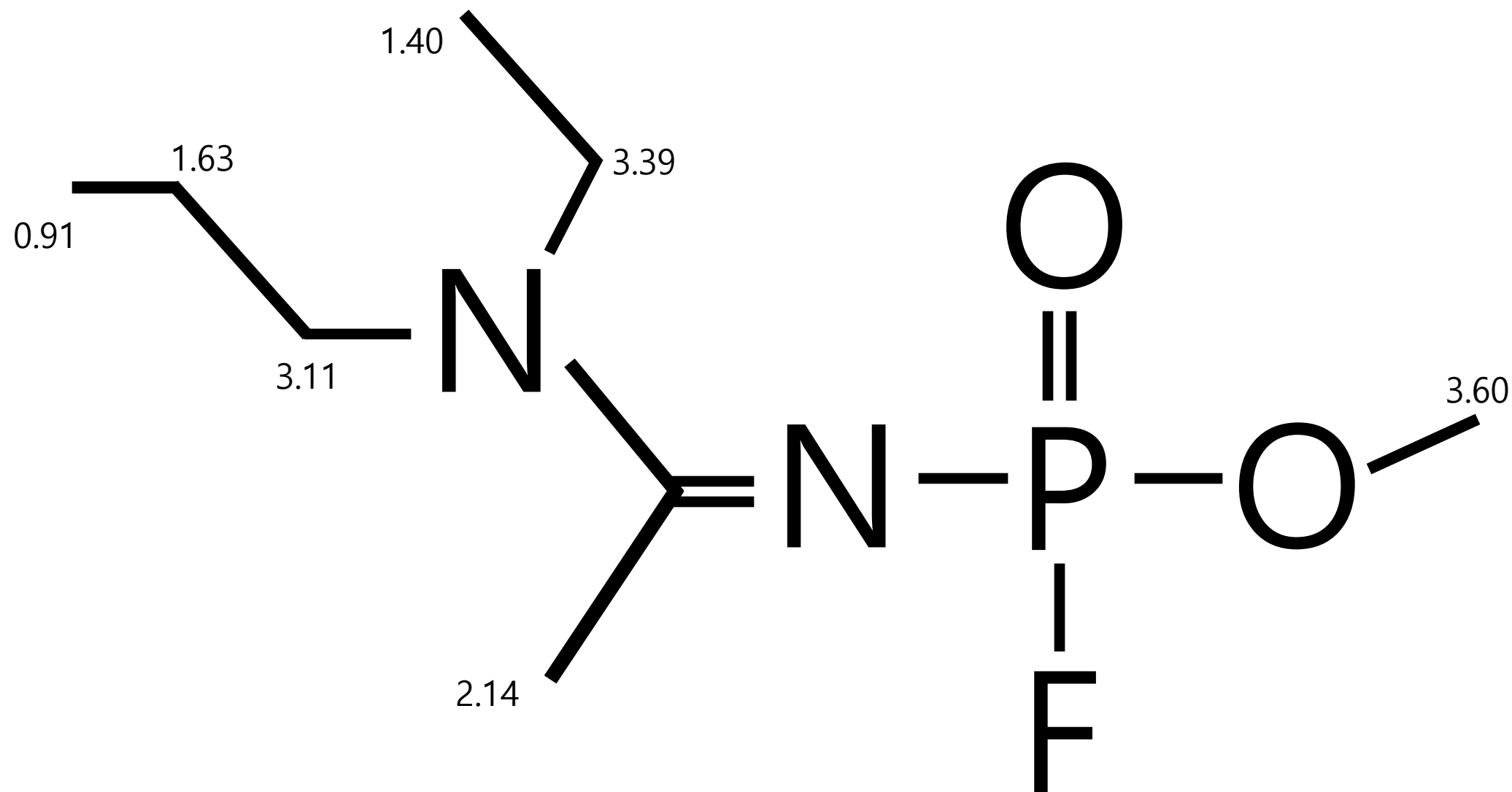


Figure S91. Structure 1132 and its ^1H chemical shift

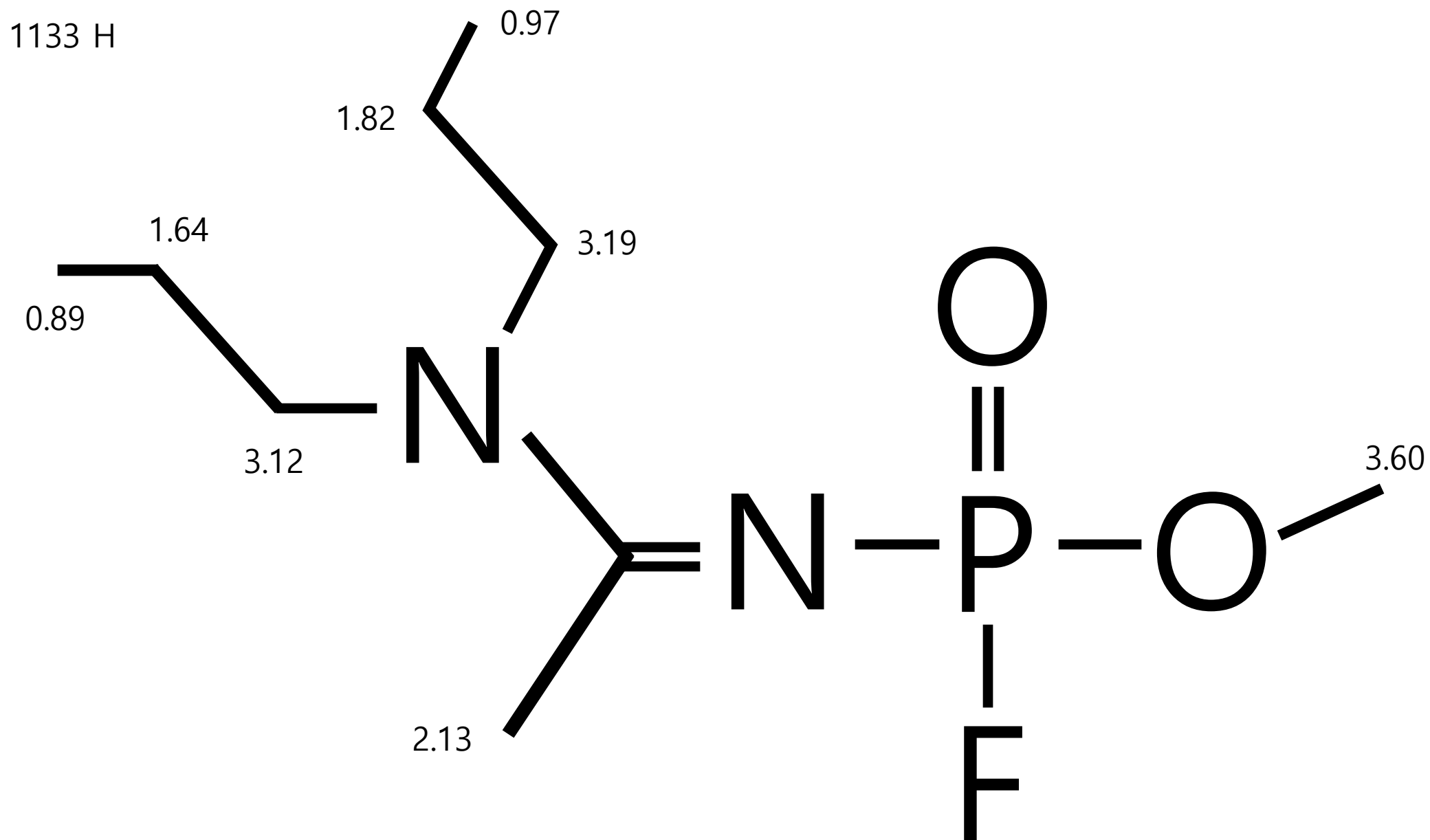


Figure S92. Structure 1133 and its ¹H chemical shift

1211 H

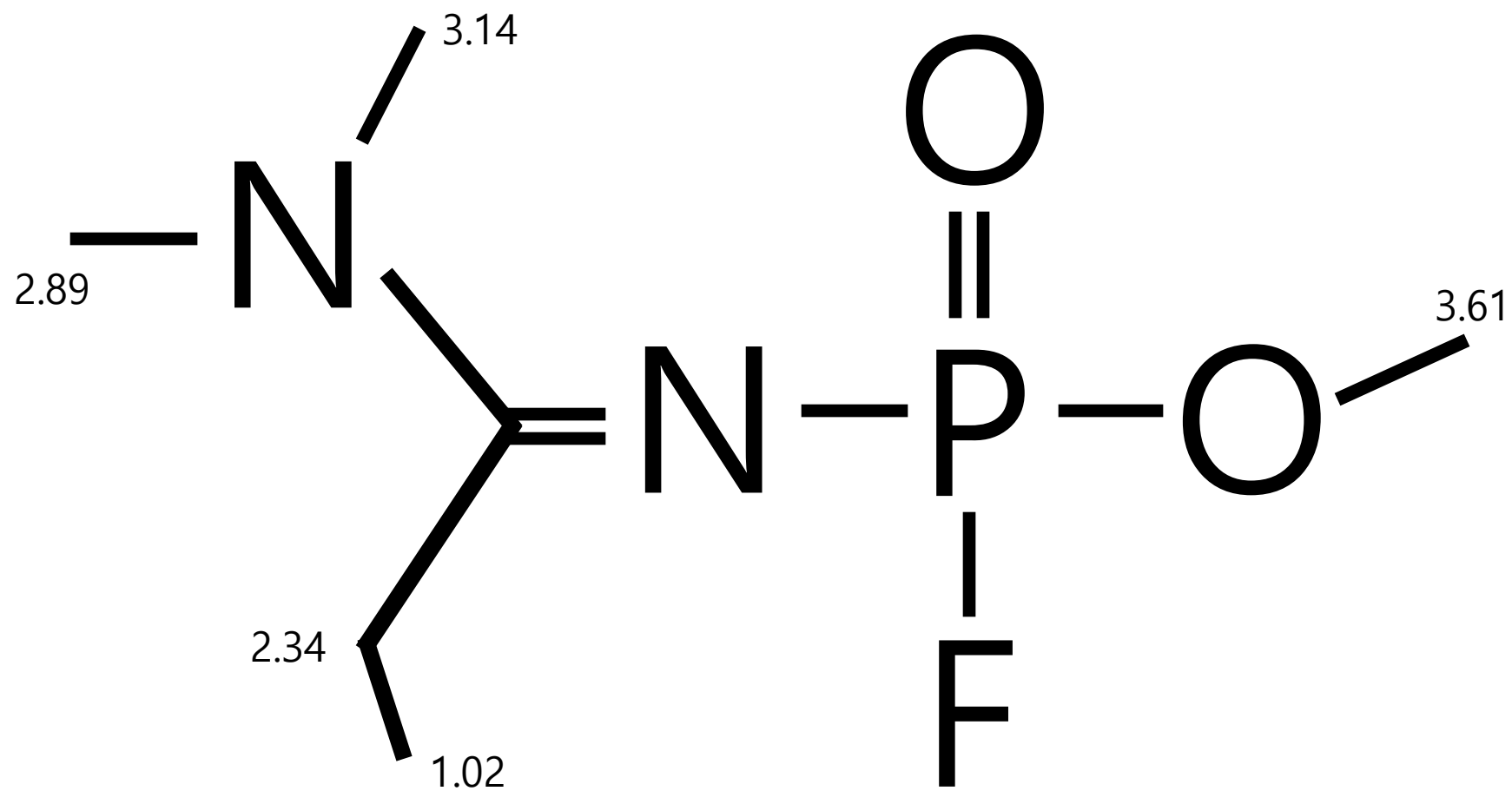


Figure S93. Structure 1211 and its ¹H chemical shift

1212 H

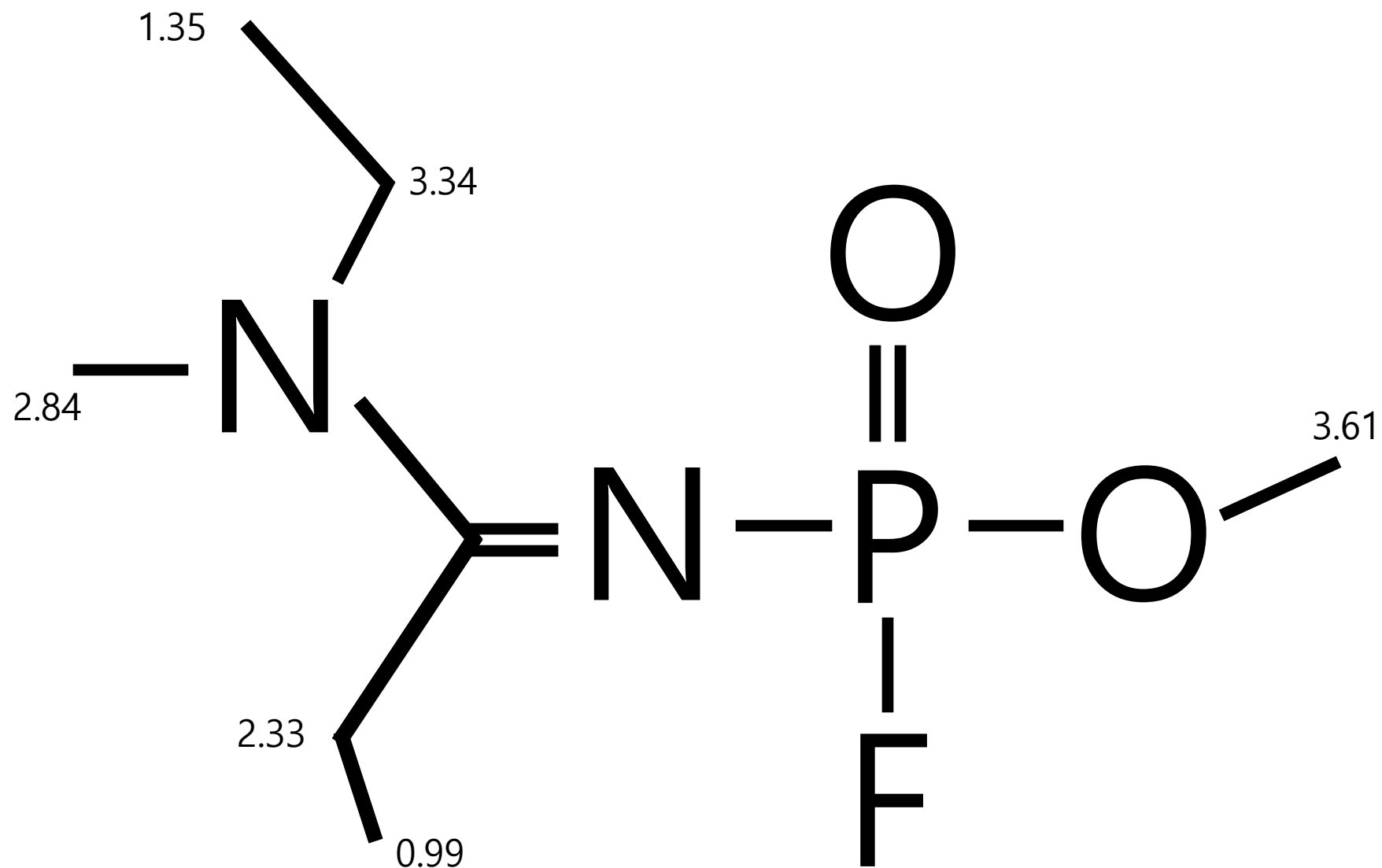


Figure S94. Structure 1212 and its ¹H chemical shift

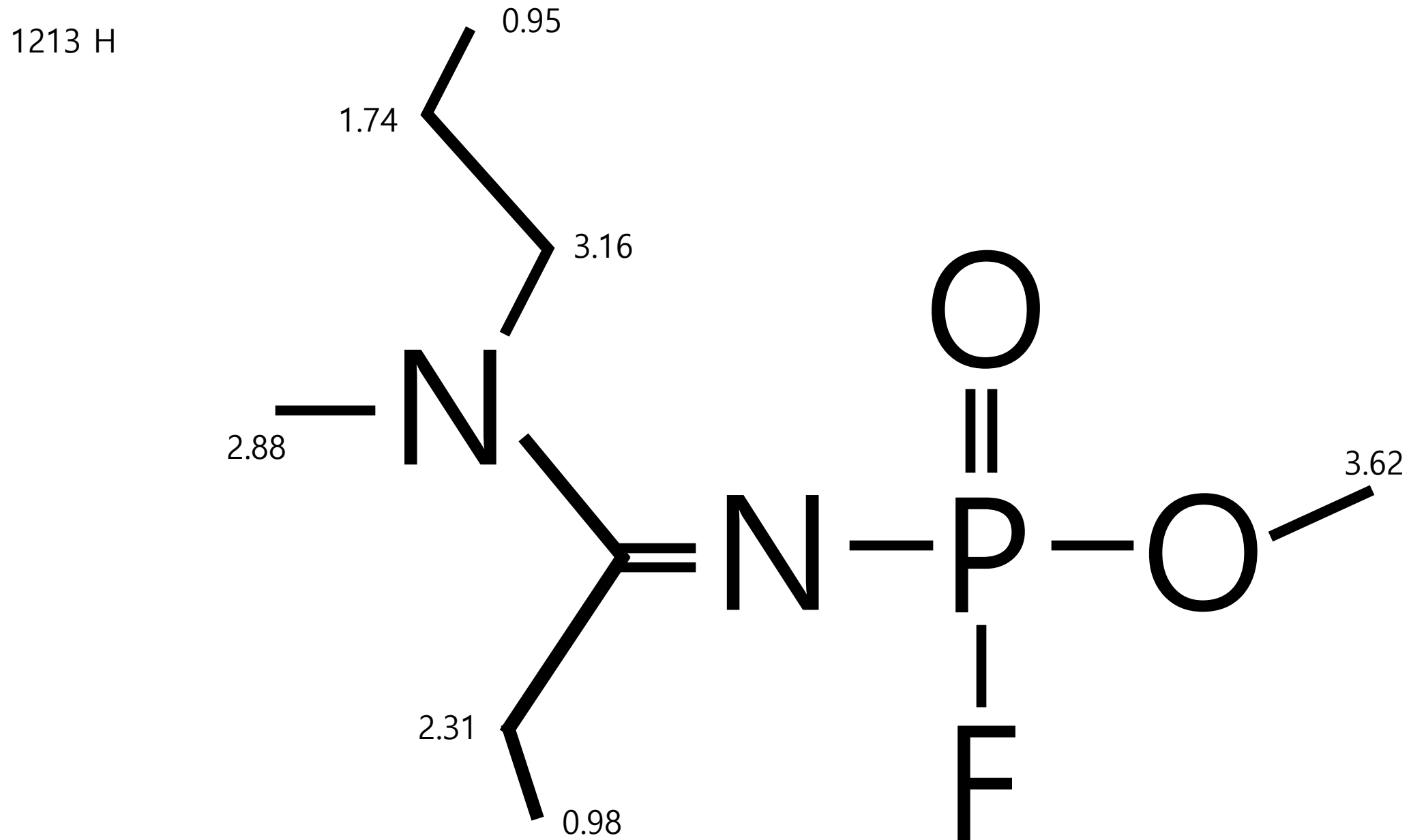


Figure S95. Structure 1213 and its ¹H chemical shift

1221 H

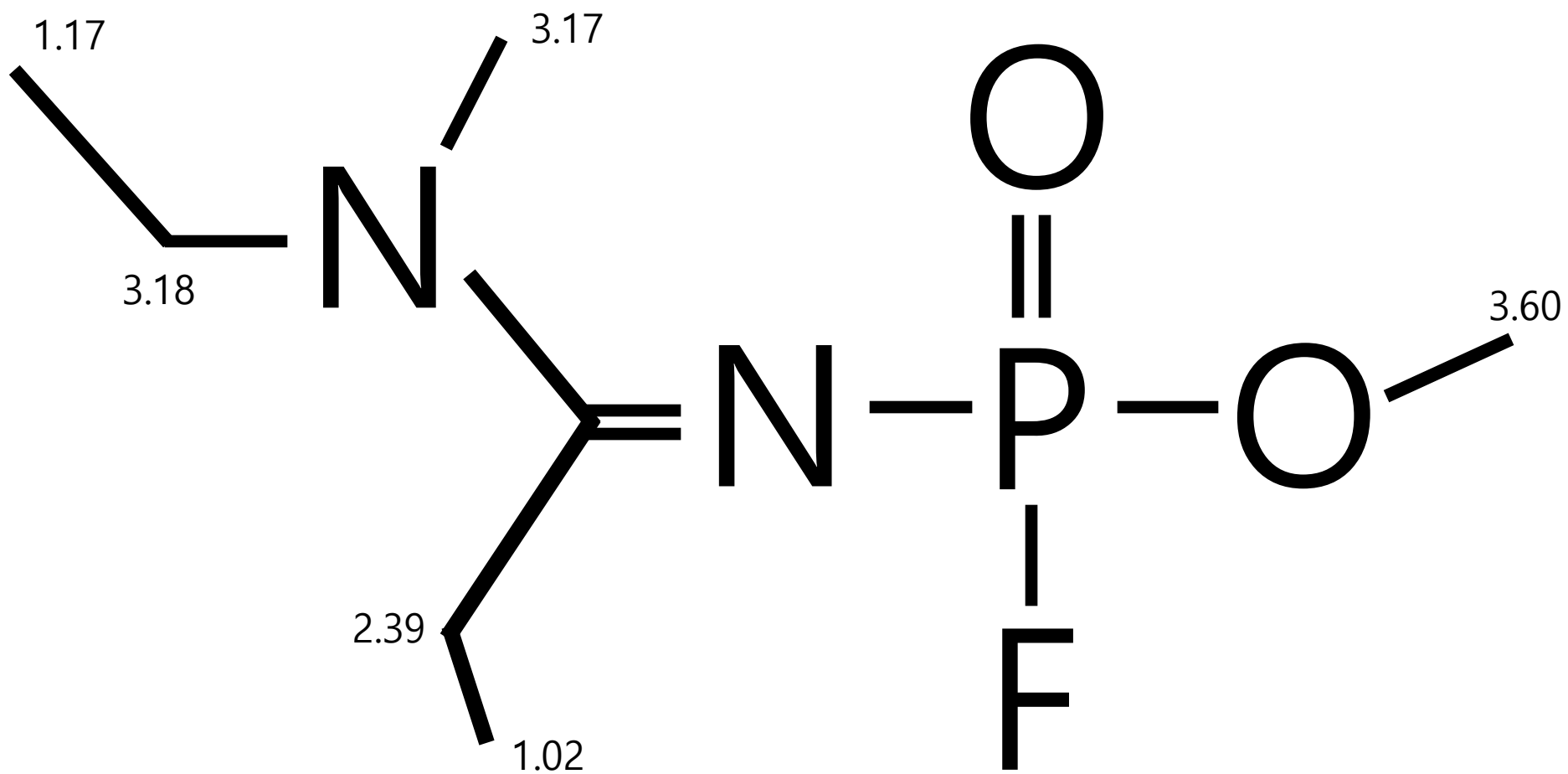


Figure S96. Structure 1221 and its ^1H chemical shift

1222 H

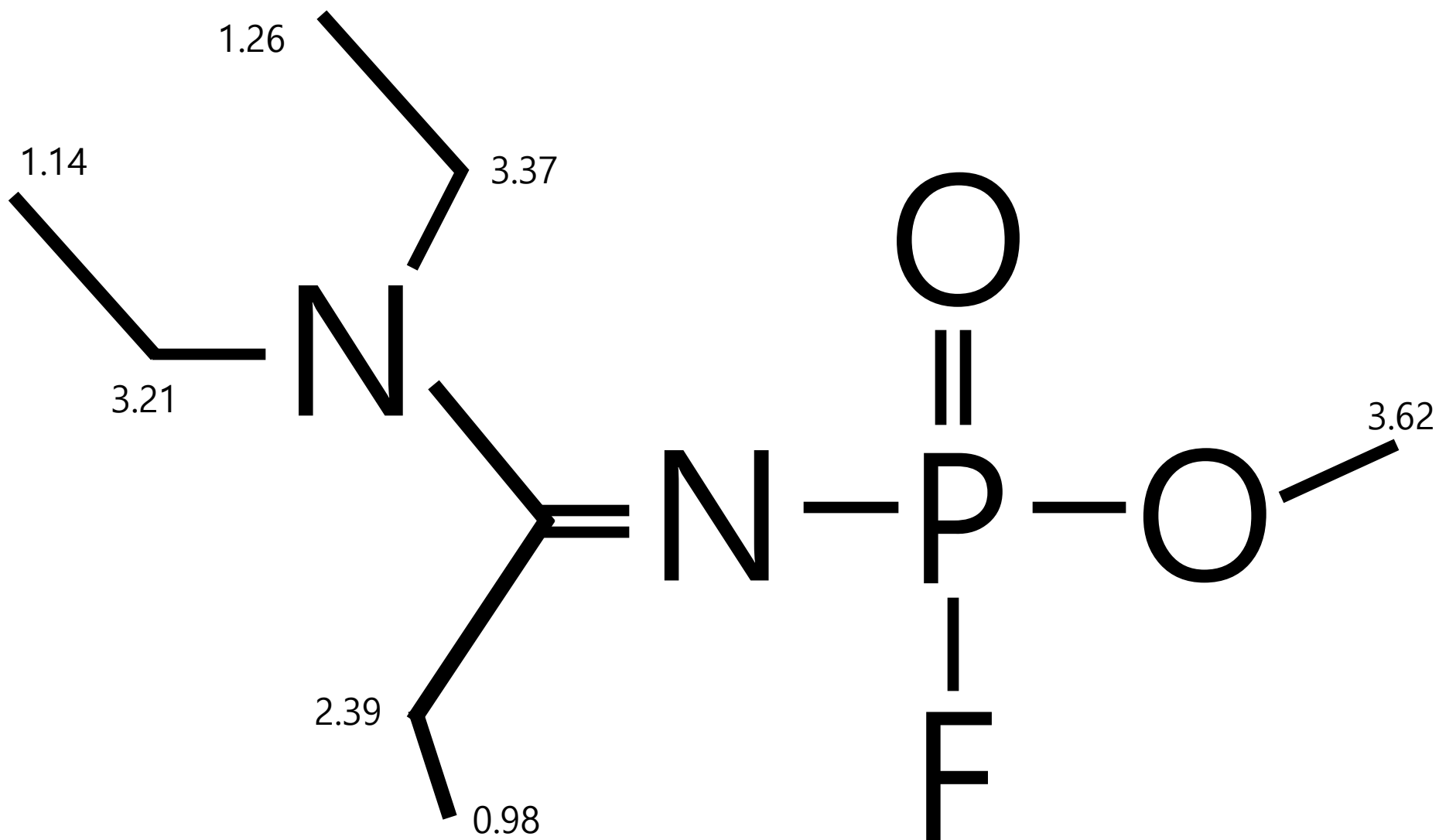


Figure S97. Structure 1222 and its ^1H chemical shift

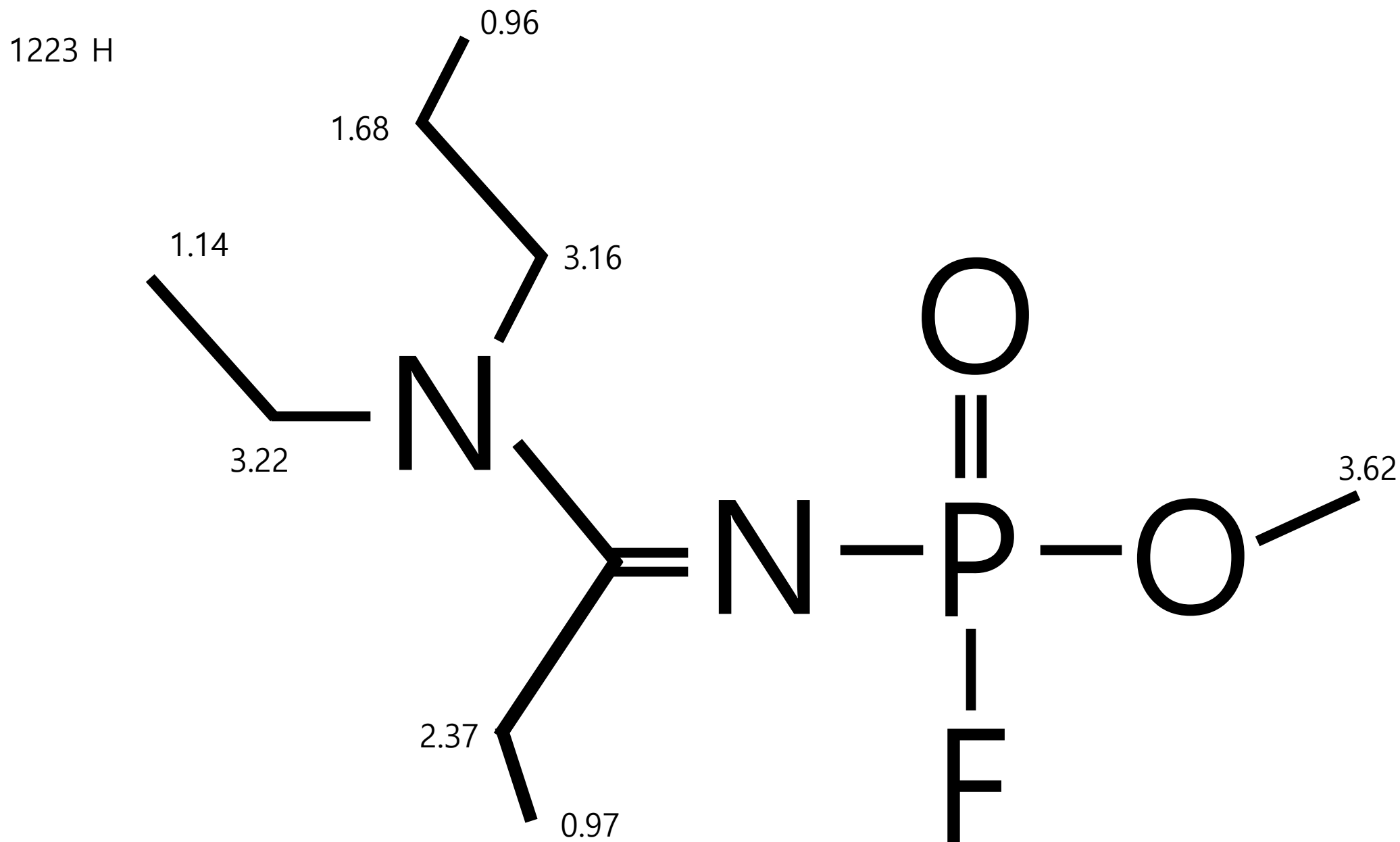


Figure S98. Structure 1223 and its ^1H chemical shift

1231 H

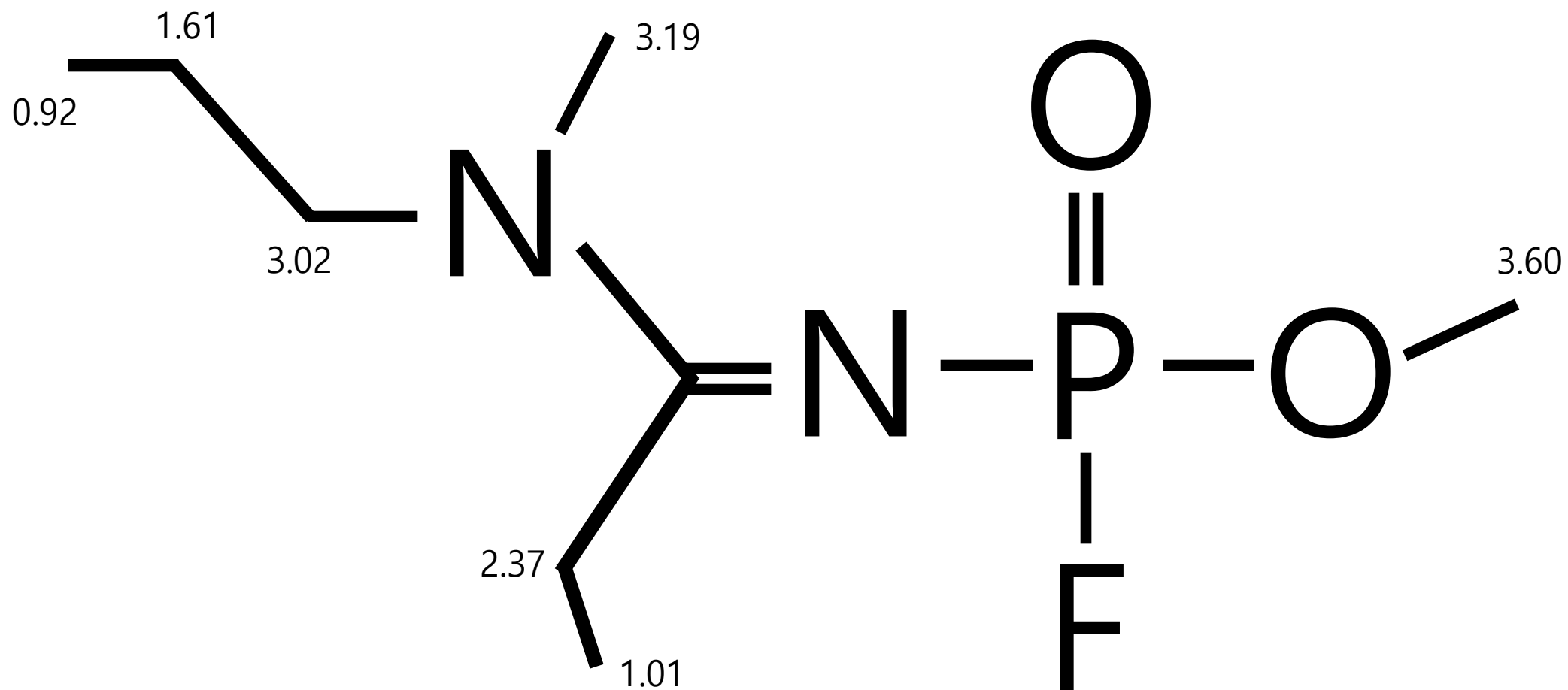


Figure S99. Structure 1231 and its ¹H chemical shift

1232 H

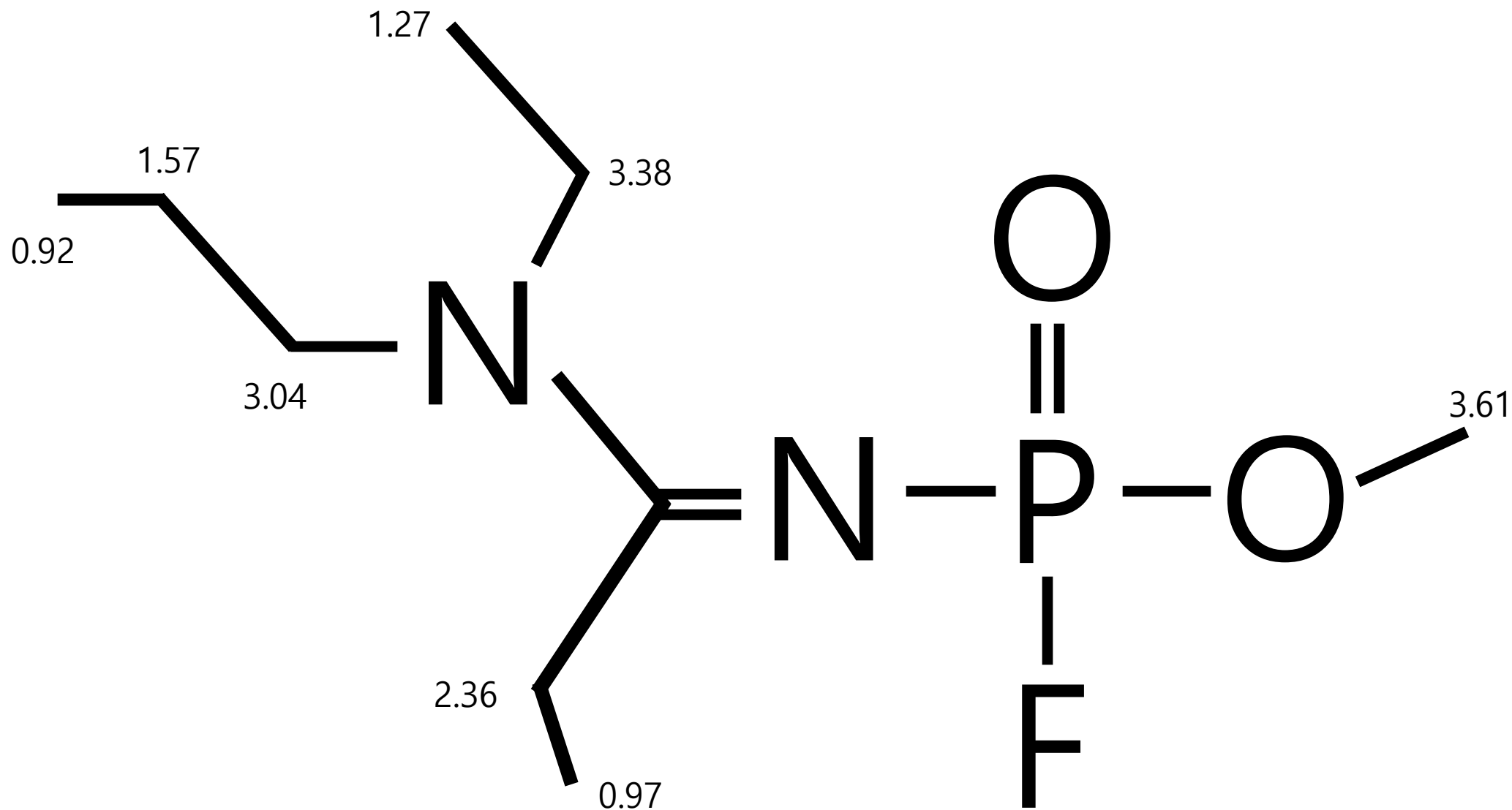


Figure S100. Structure 1232 and its ^1H chemical shift

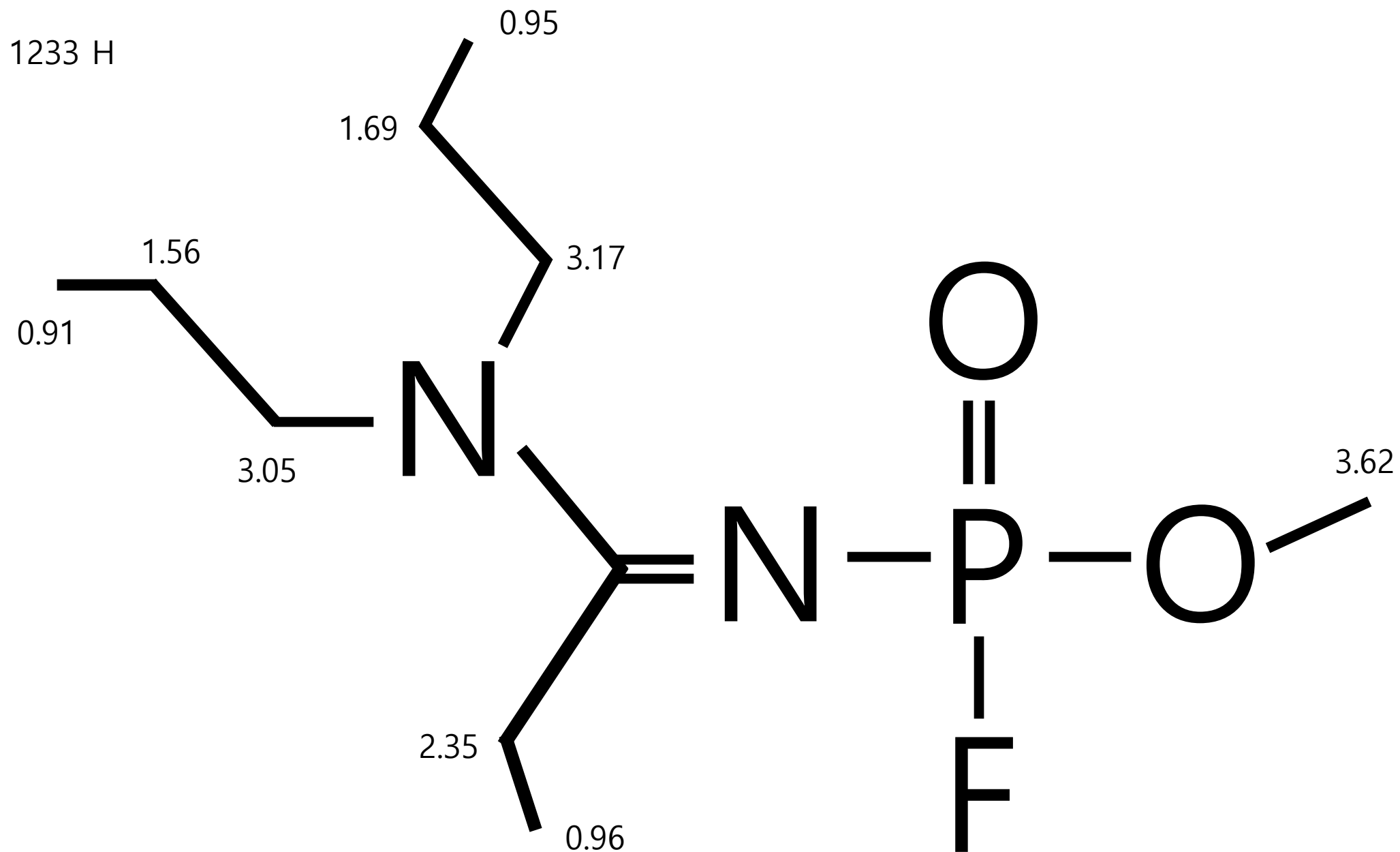


Figure S101. Structure 1233 and its ¹H chemical shift

1311 H

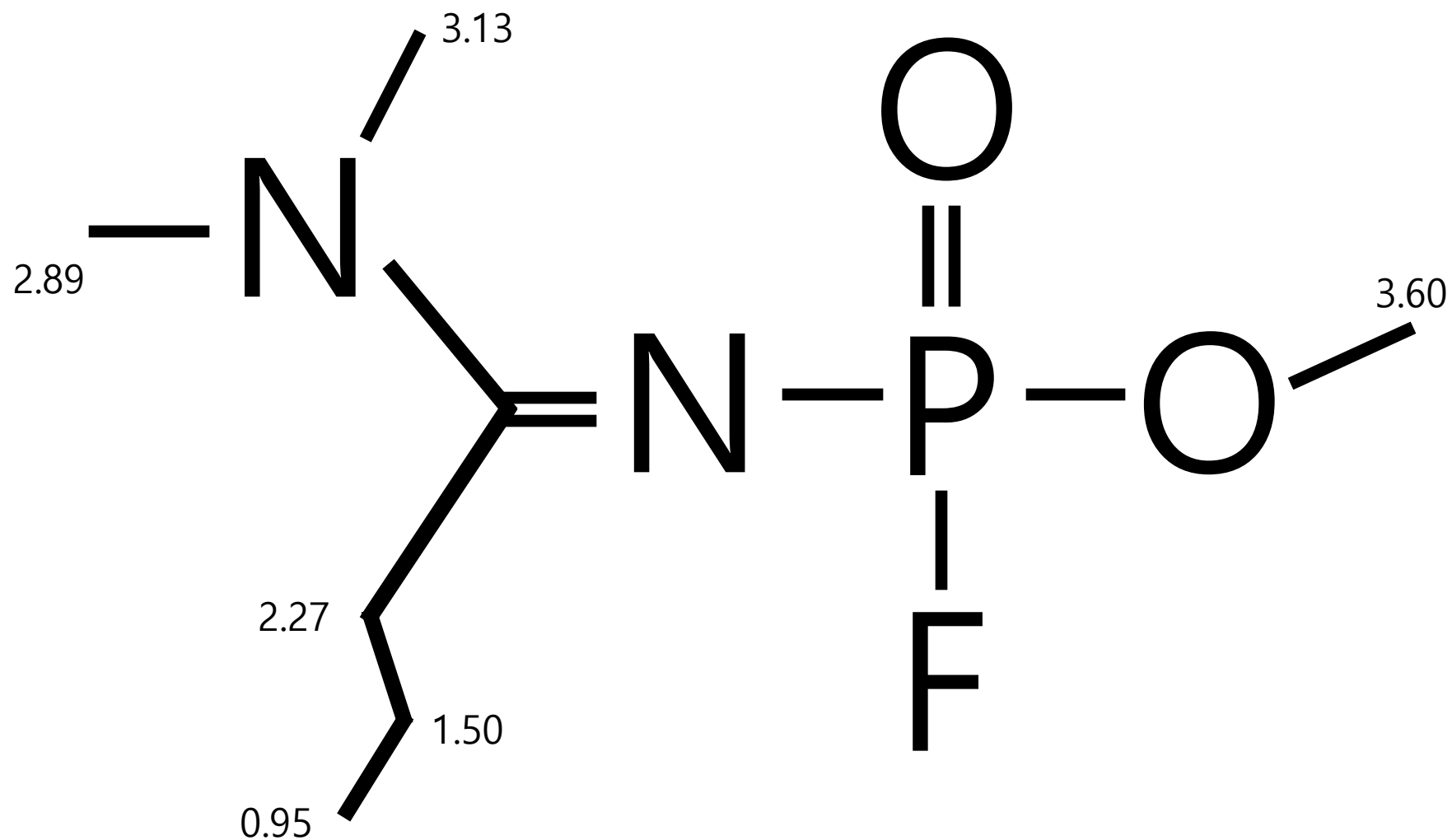


Figure S102. Structure 1311 and its ¹H chemical shift

1312 H

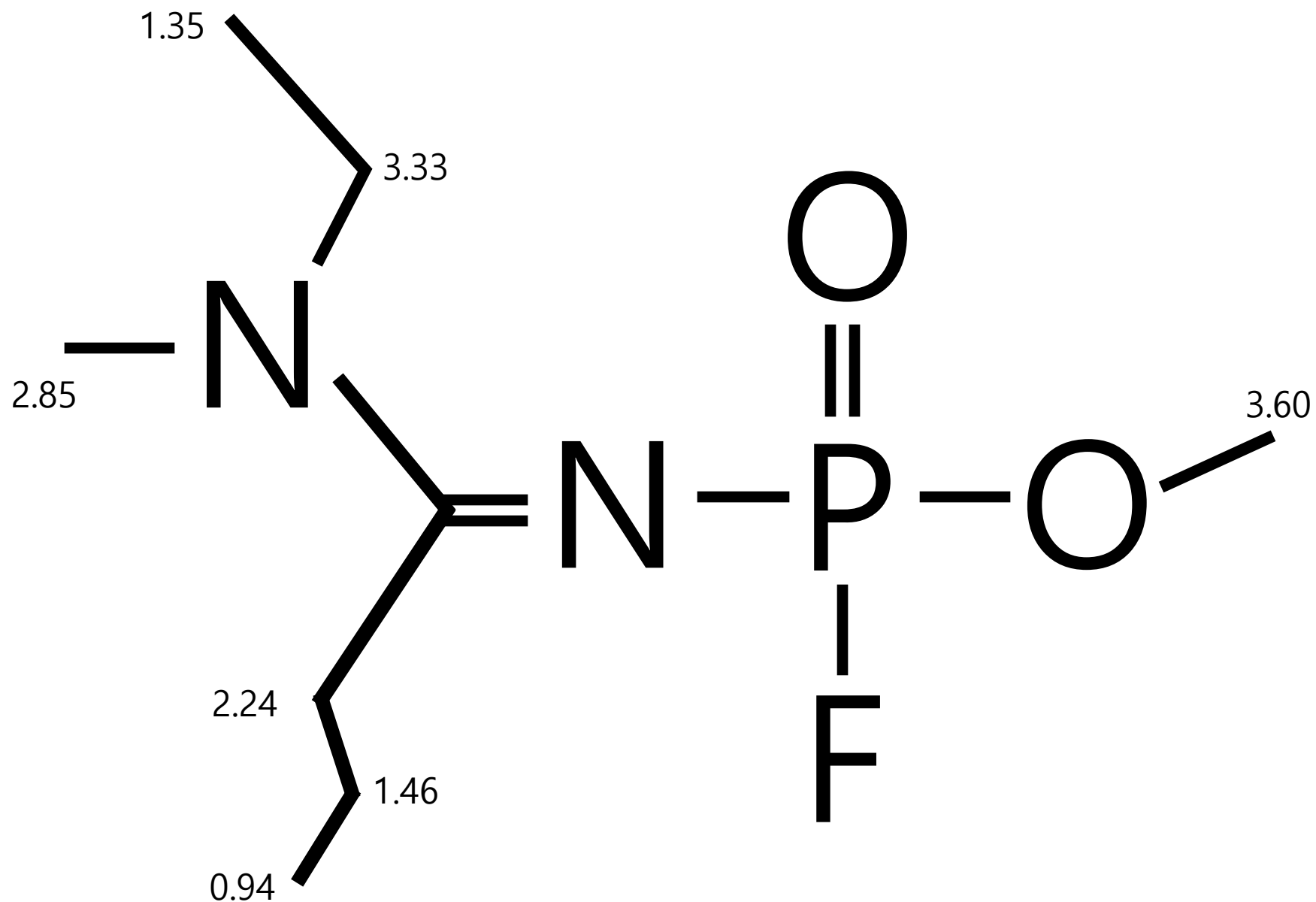


Figure S104. Structure 1312 and its ¹H chemical shift

1313 H

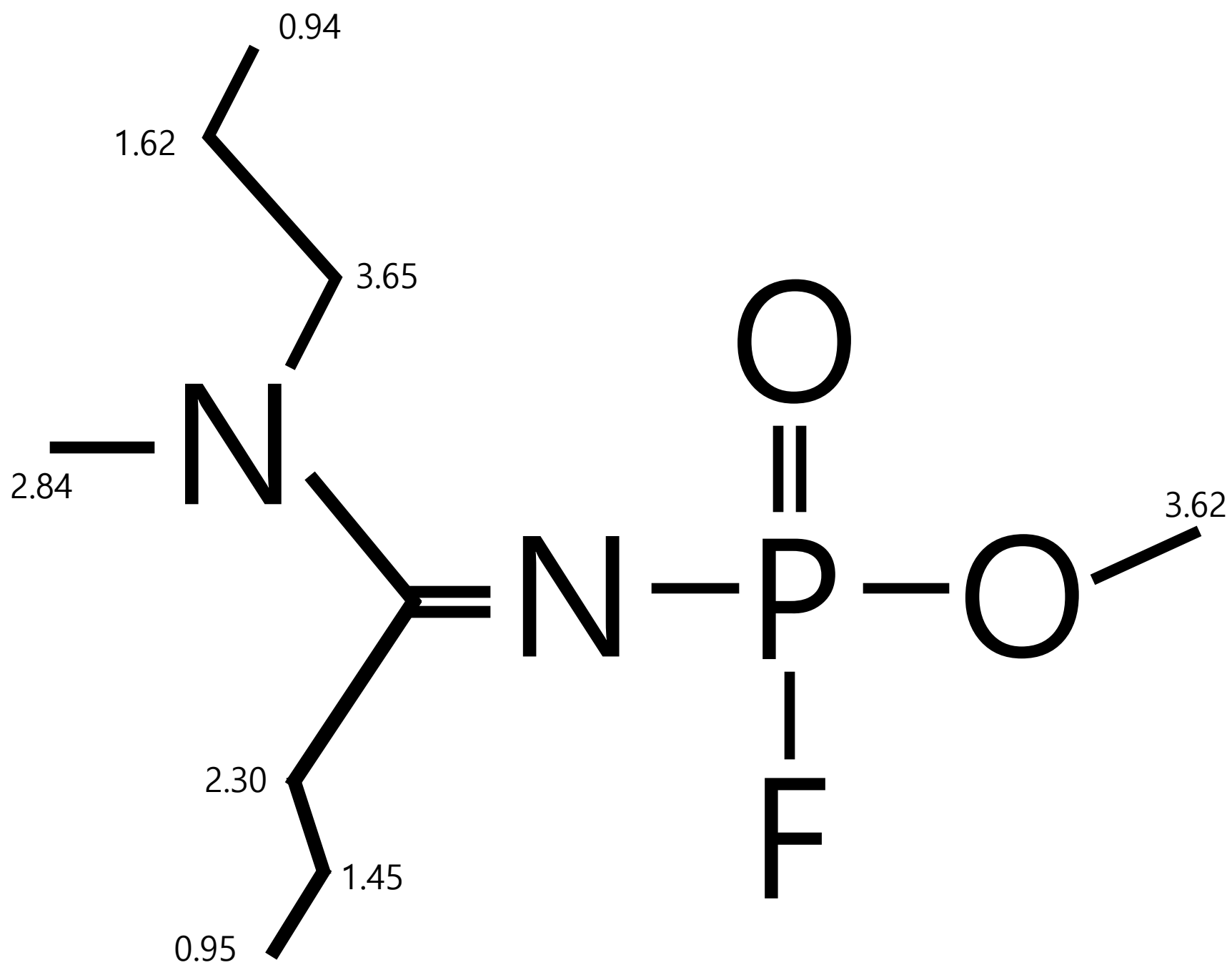


Figure S104. Structure 1313 and its ¹H chemical shift

1321 H

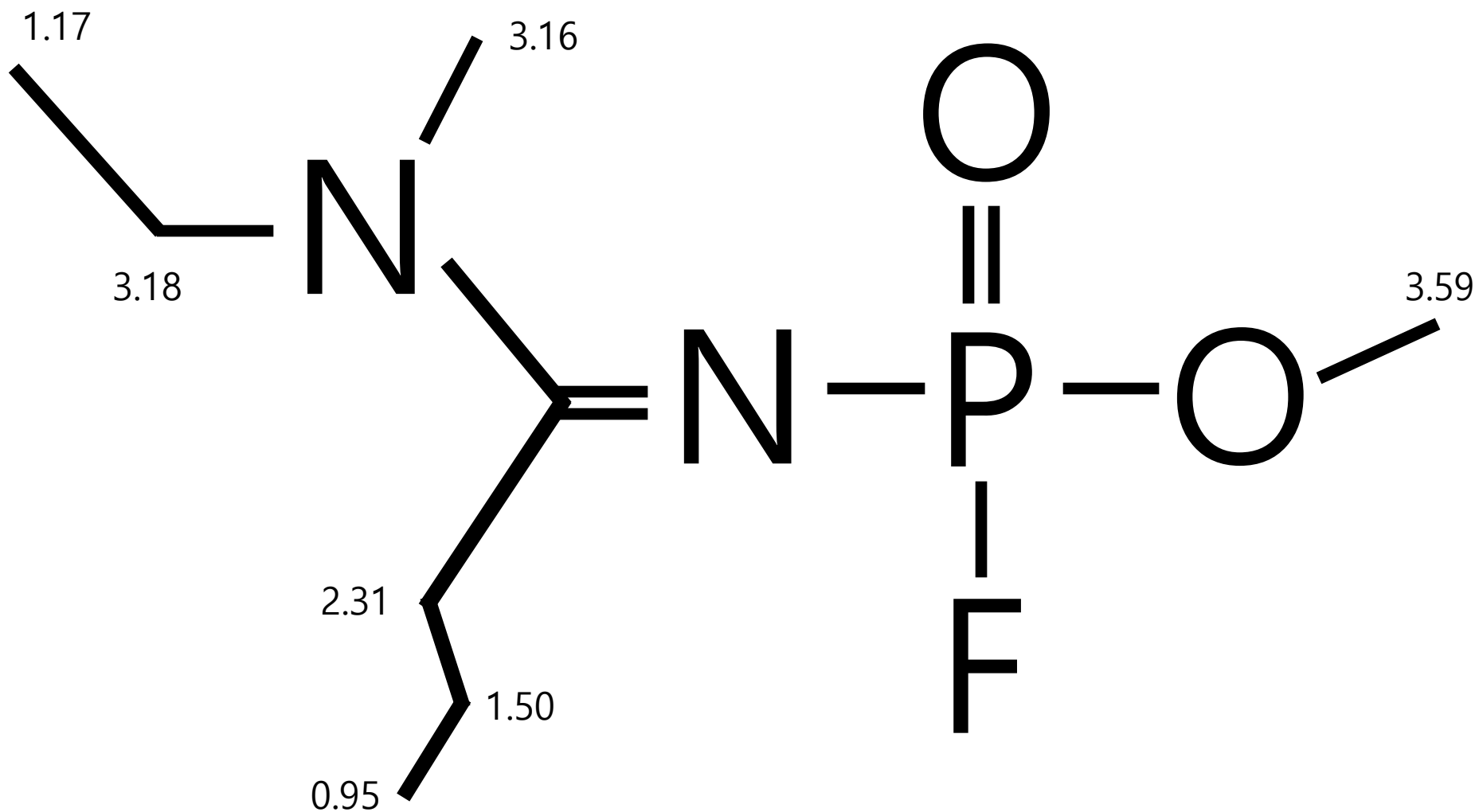


Figure S105. Structure 1321 and its ^1H chemical shift

1322 H

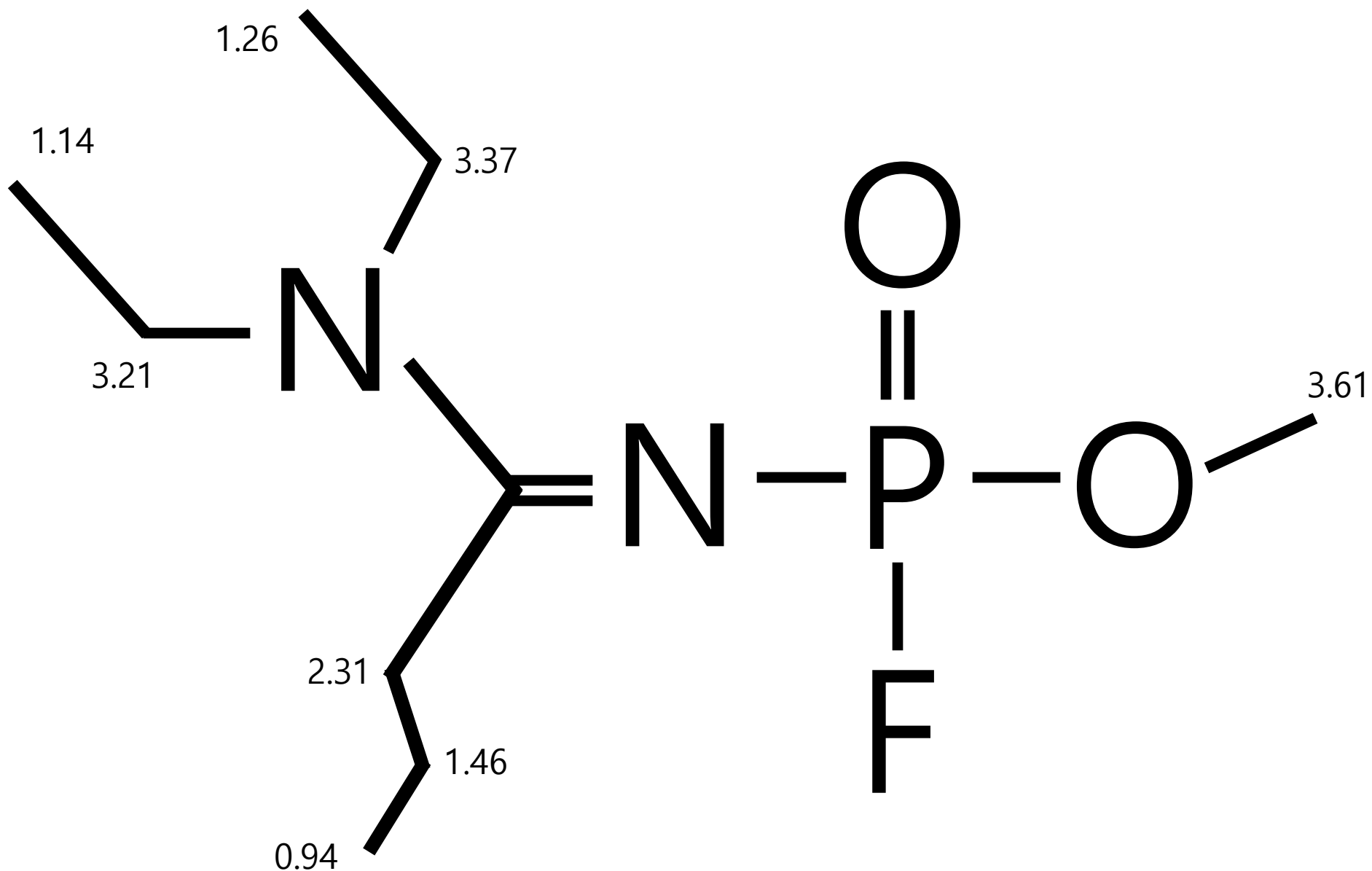


Figure S106. Structure 1322 and its ¹H chemical shift

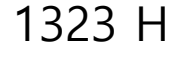


Figure S107. Structure 1323 and its ^1H chemical shift

1331 H

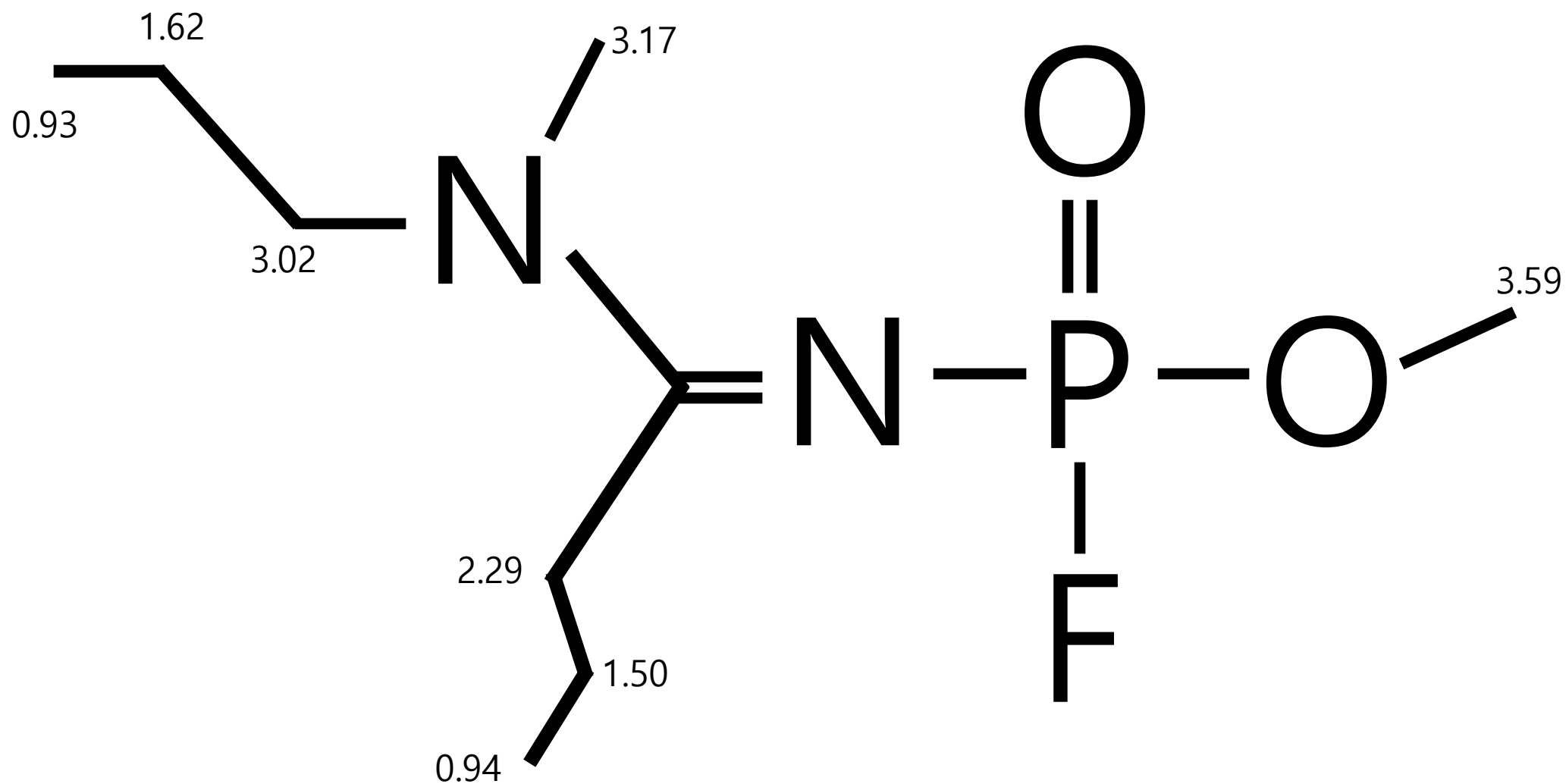


Figure S108. Structure 1331 and its ¹H chemical shift

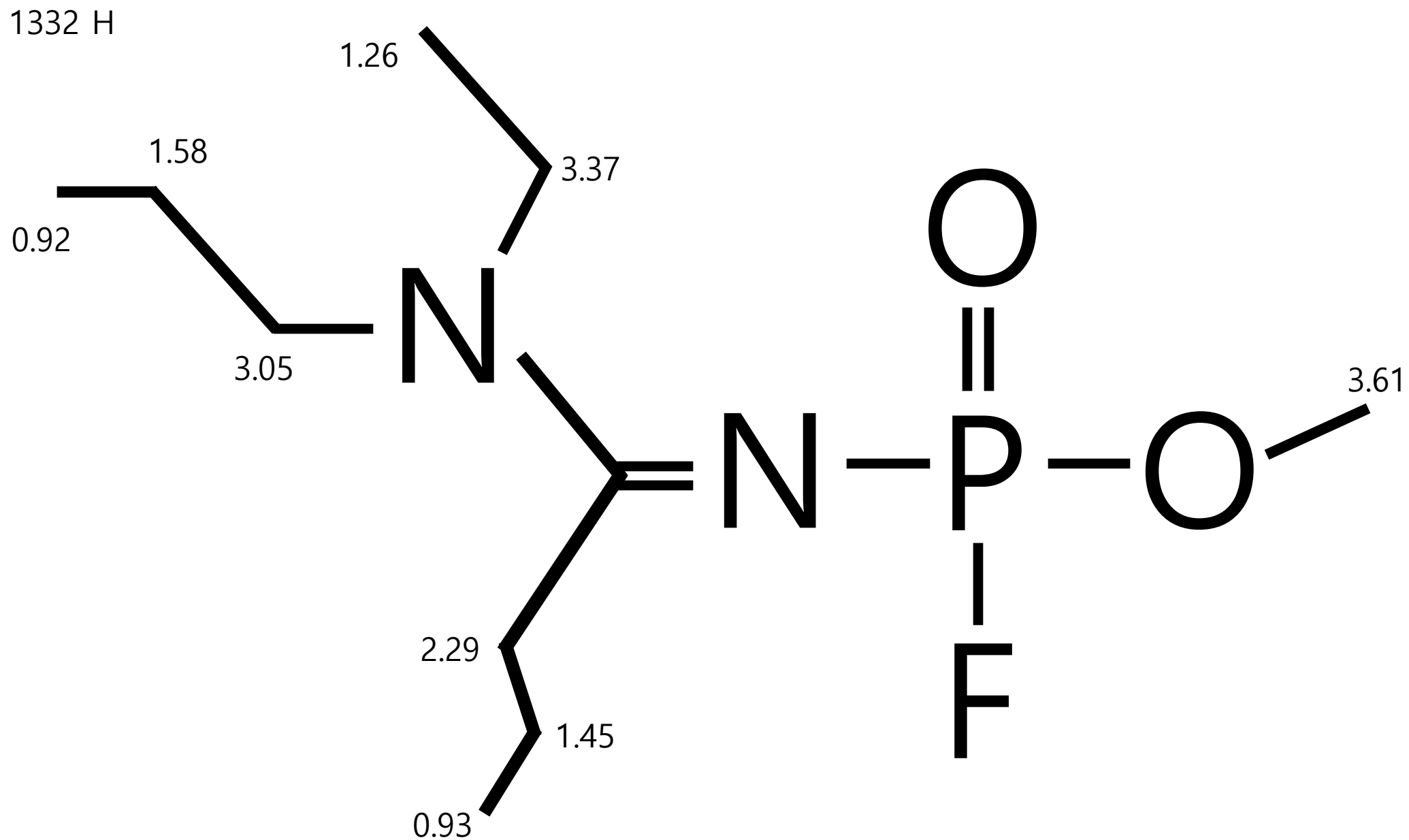


Figure S109. Structure 1332 and its ¹H chemical shift

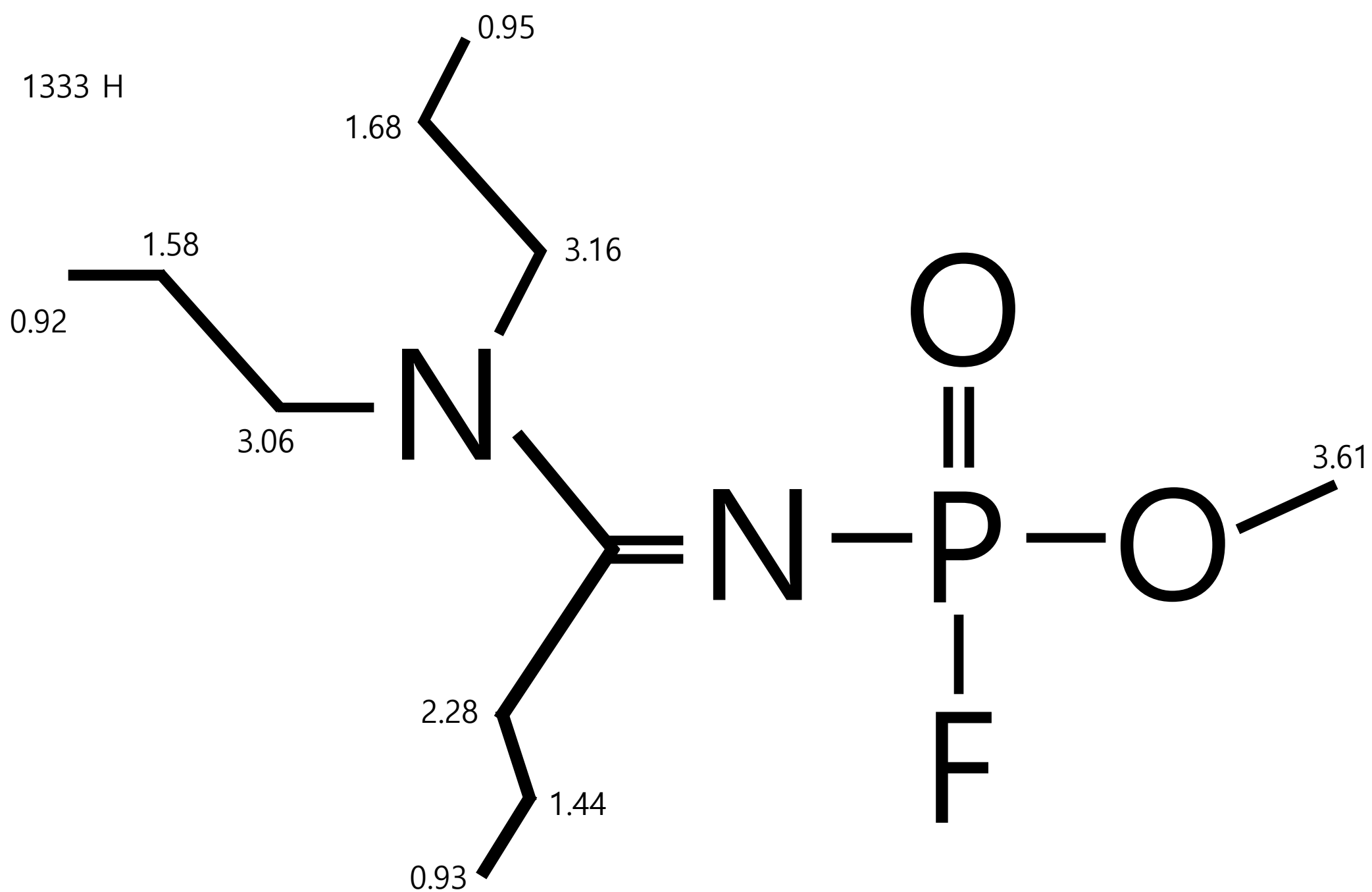


Figure S110. Structure 1333 and its ^1H chemical shift

2111 H

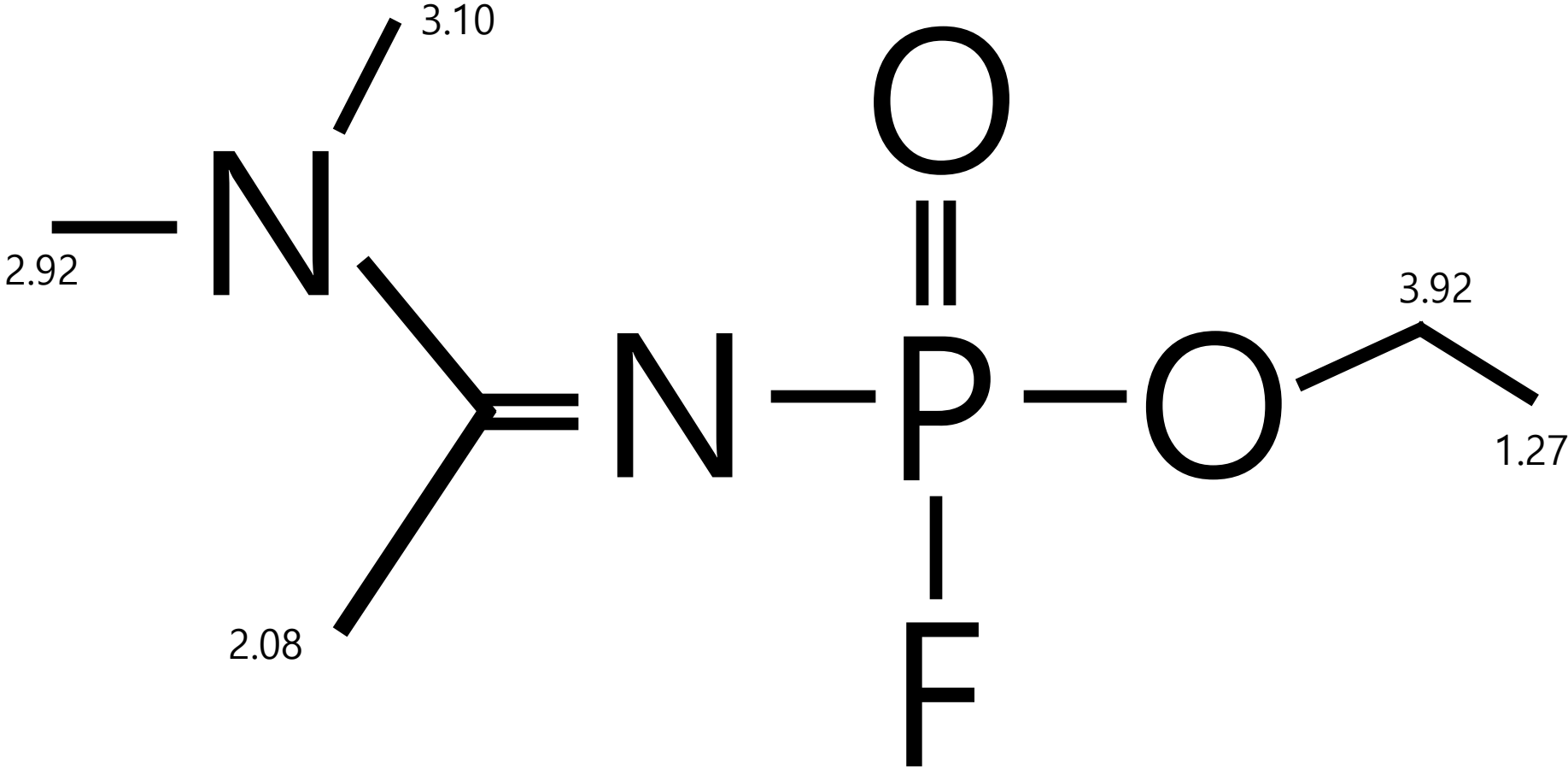


Figure S111. Structure 2111 and its ¹H chemical shift

2112 H

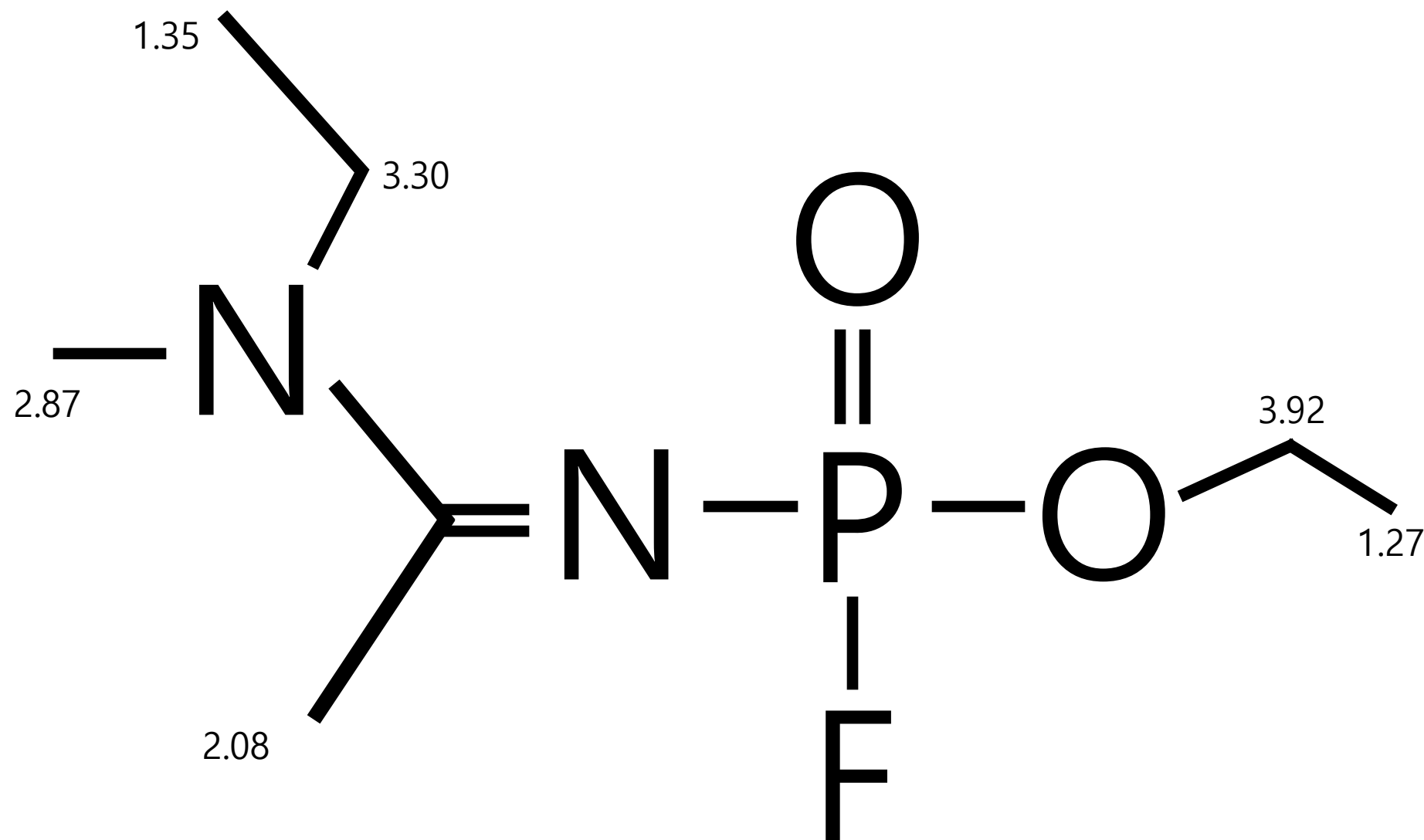


Figure S112. Structure 2112 and its ¹H chemical shift

2113 H

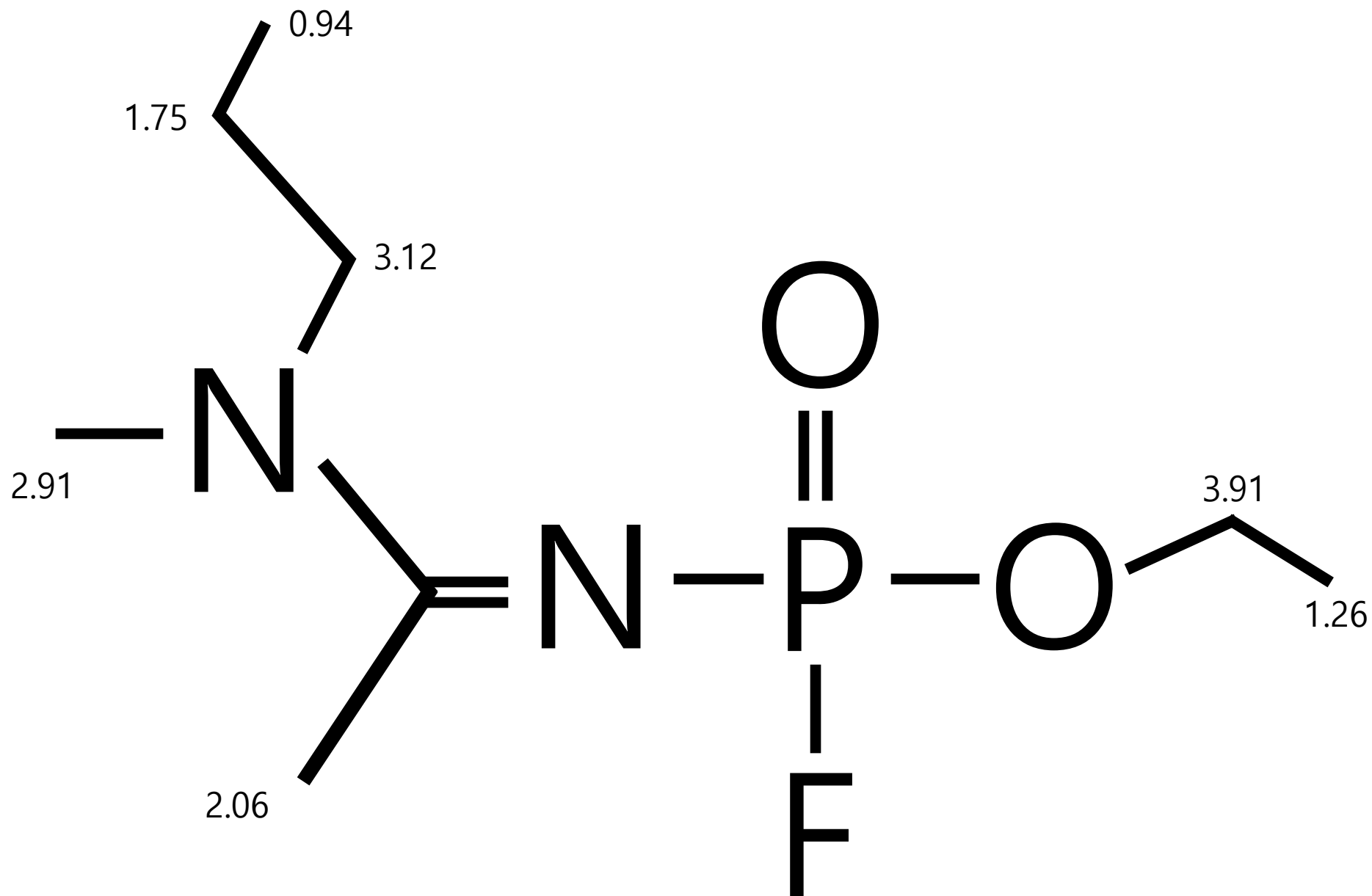


Figure S113. Structure 2113 and its ¹H chemical shift

2121 H

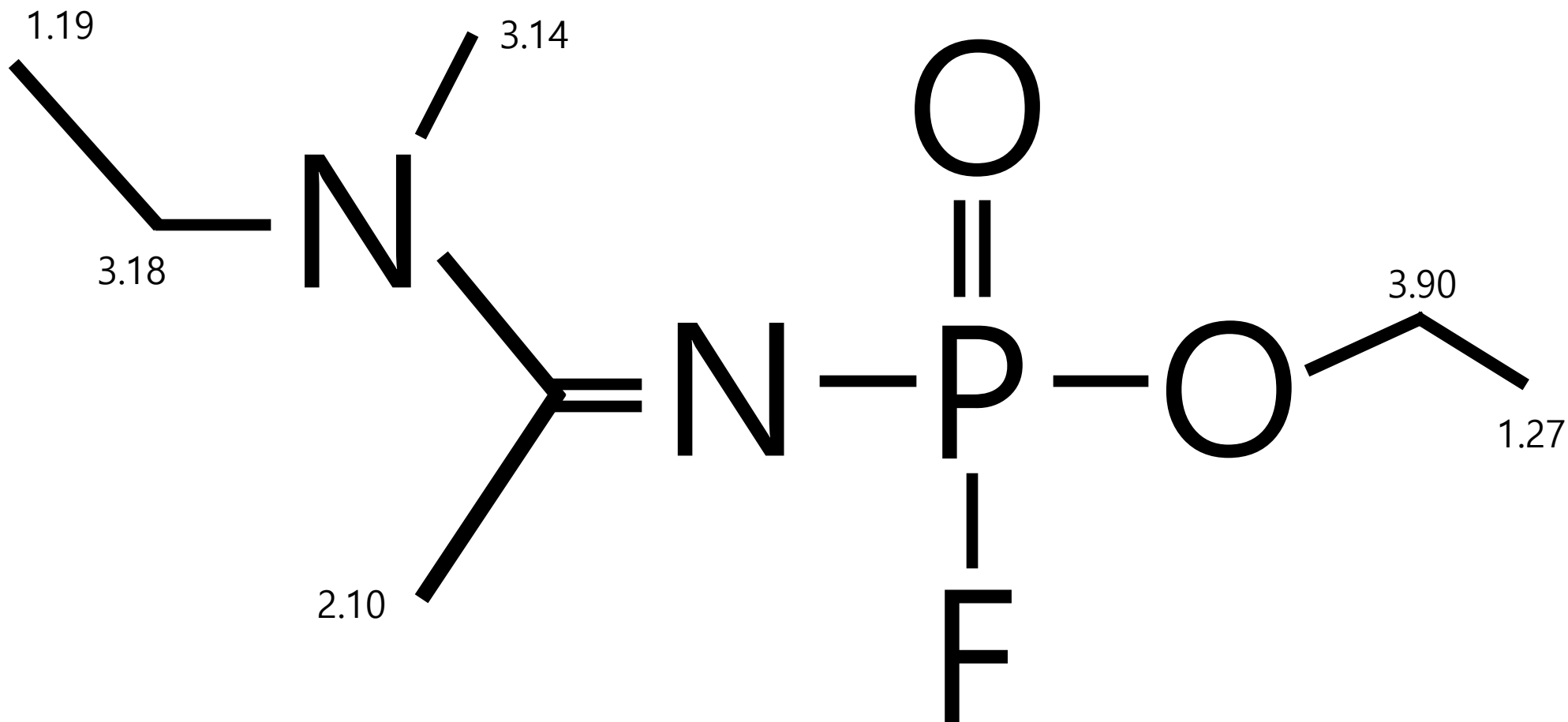


Figure S114. Structure 2121 and its ¹H chemical shift

2122 H

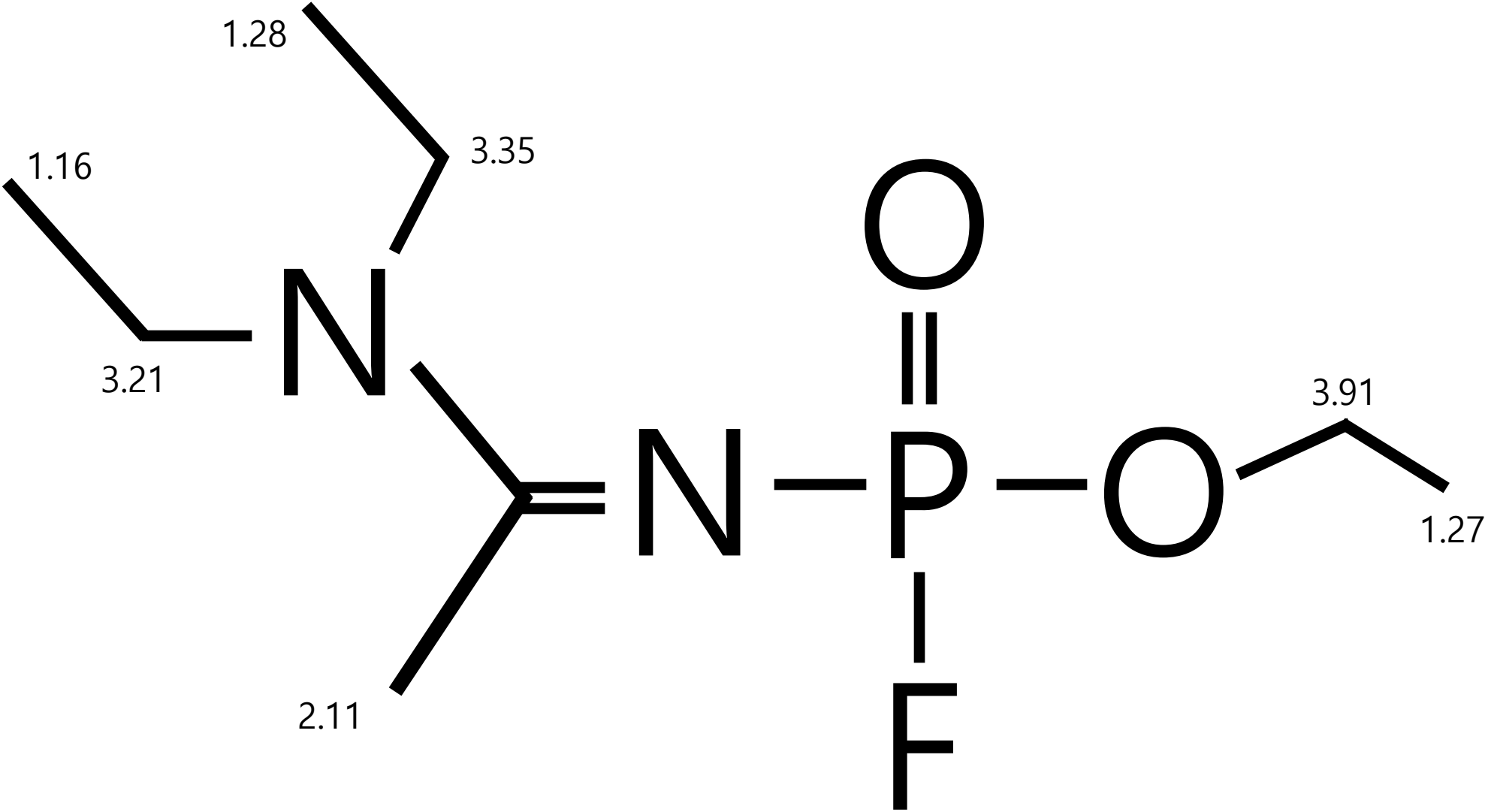


Figure S115. Structure 2122 and its ¹H chemical shift

2123 H

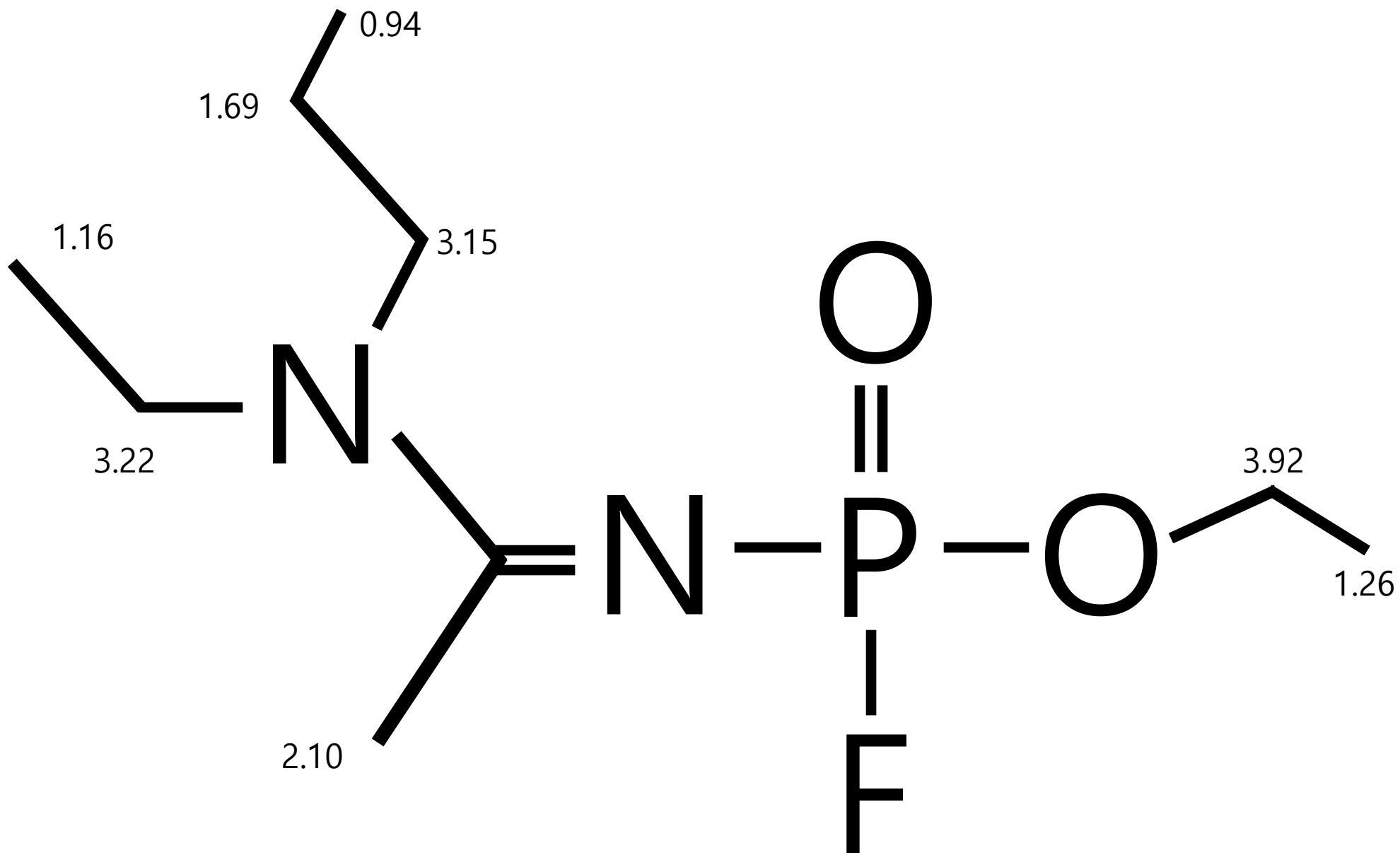


Figure S116. Structure 2123 and its ^1H chemical shift

2131 H

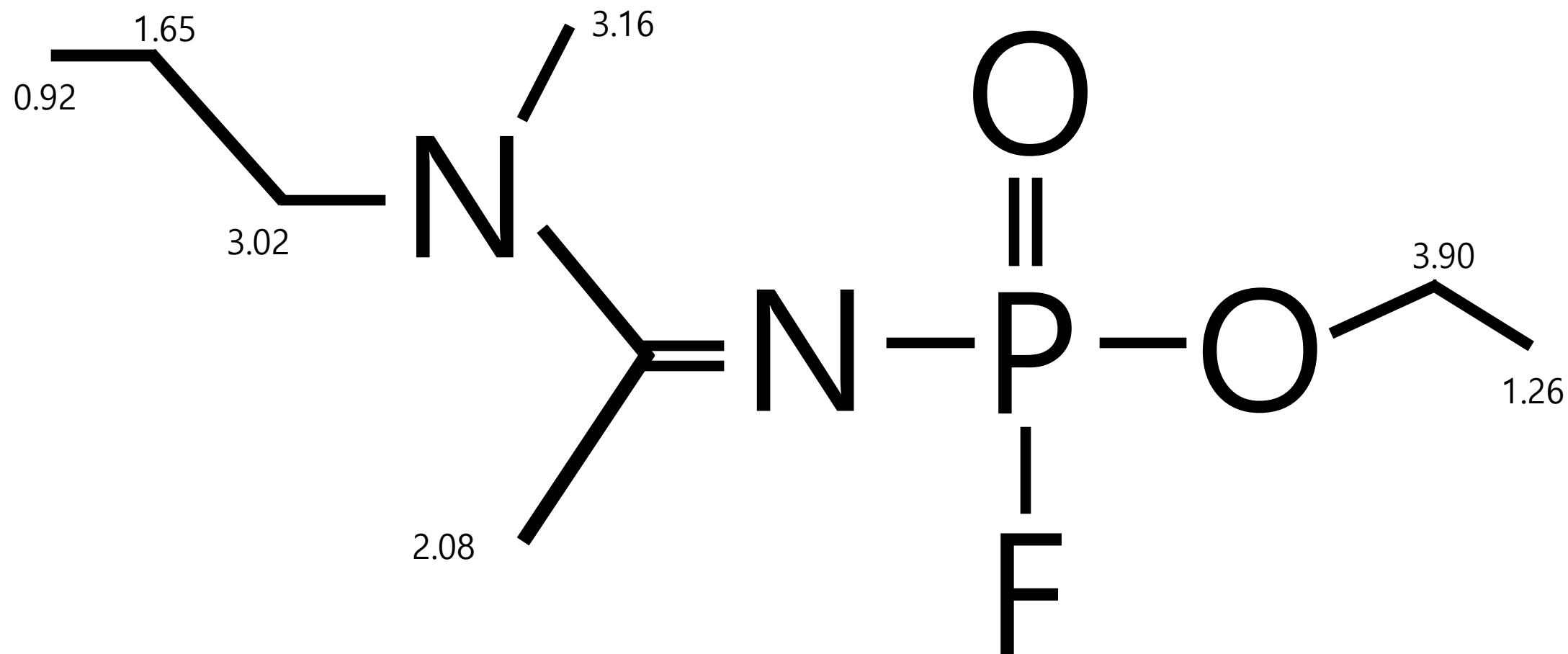


Figure S117. Structure 2131 and its ¹H chemical shift

2132 H

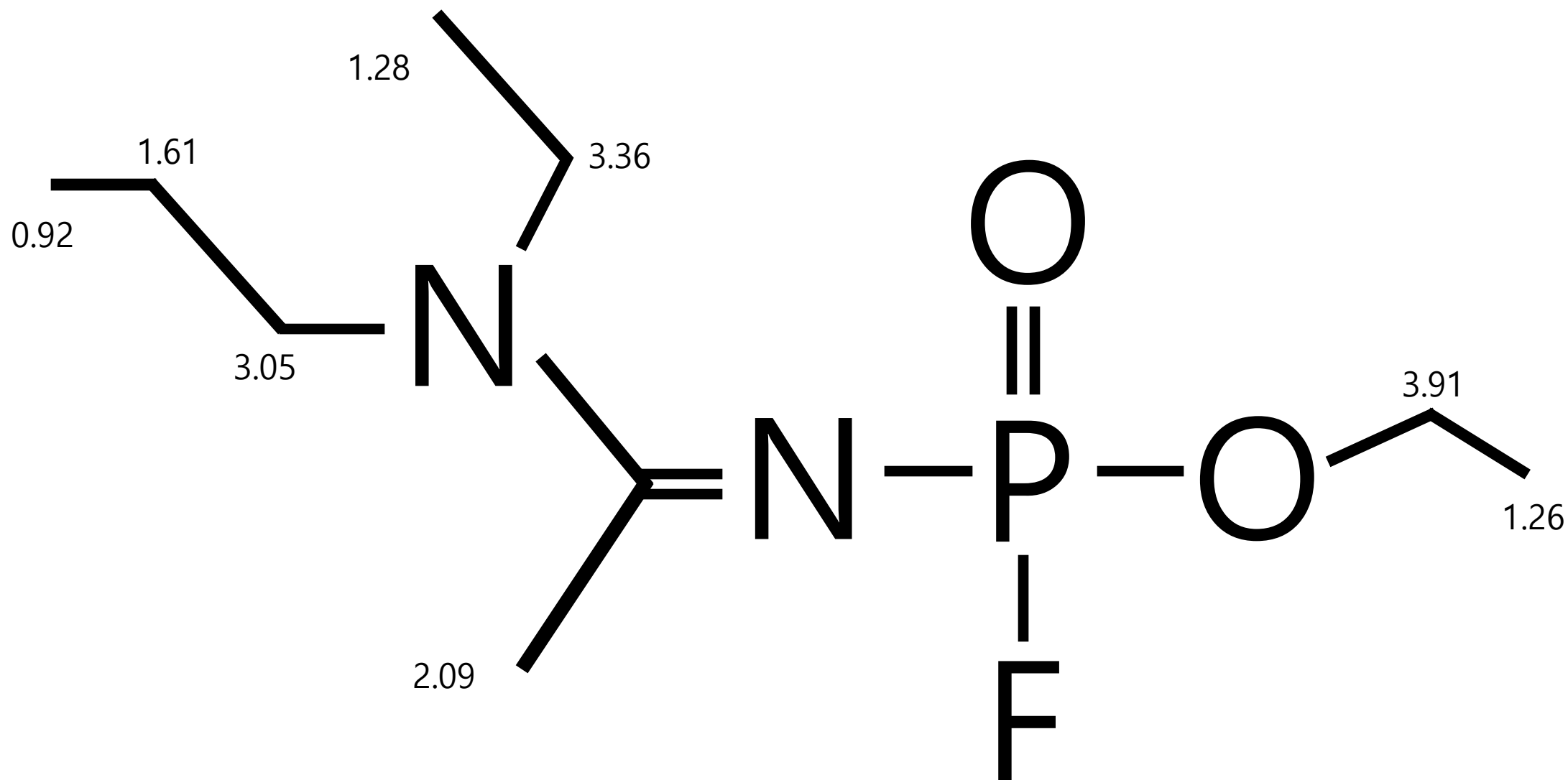


Figure S118. Structure 2132 and its ^1H chemical shift

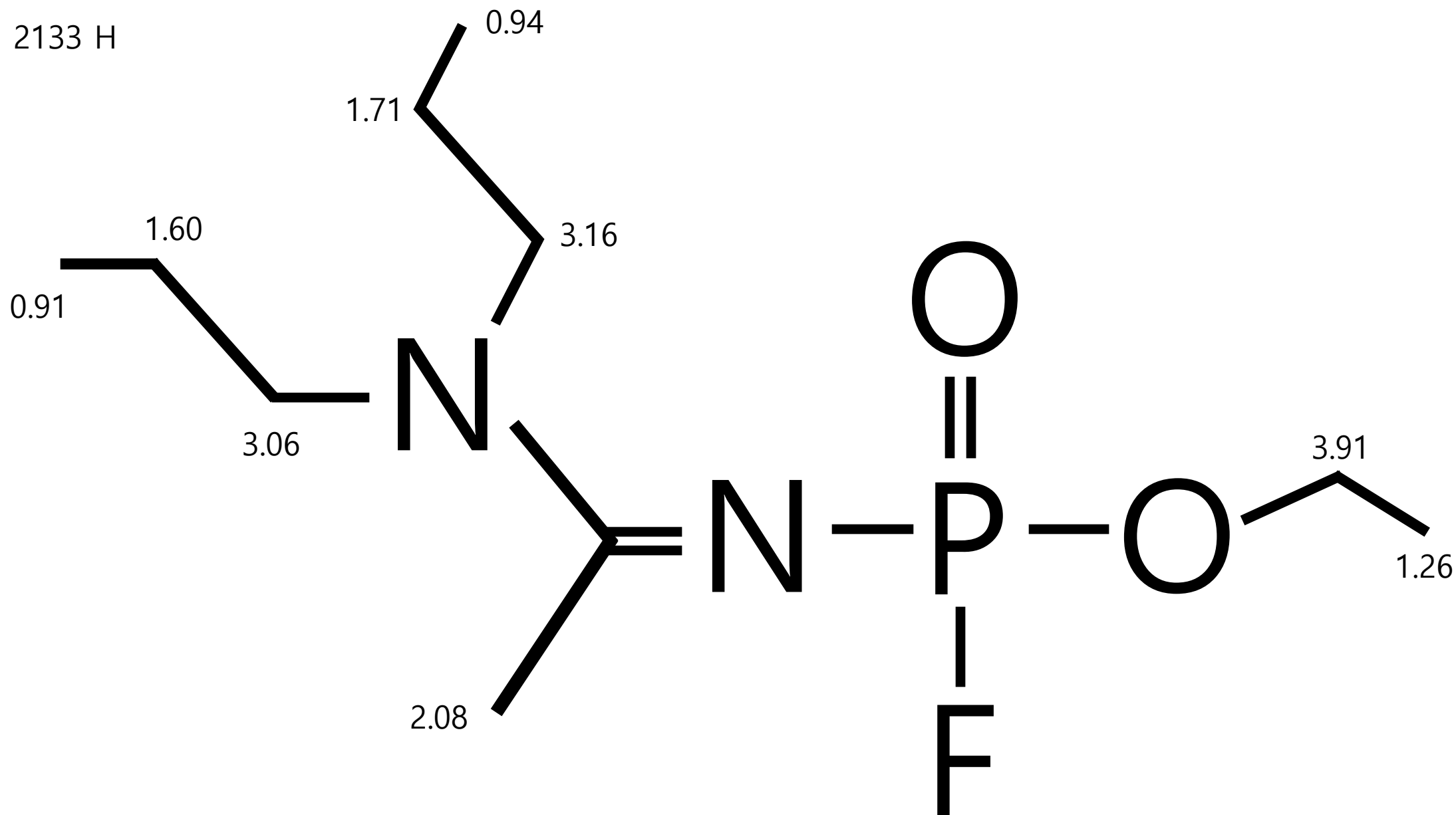


Figure S119. Structure 2133 and its ¹H chemical shift

2211 H

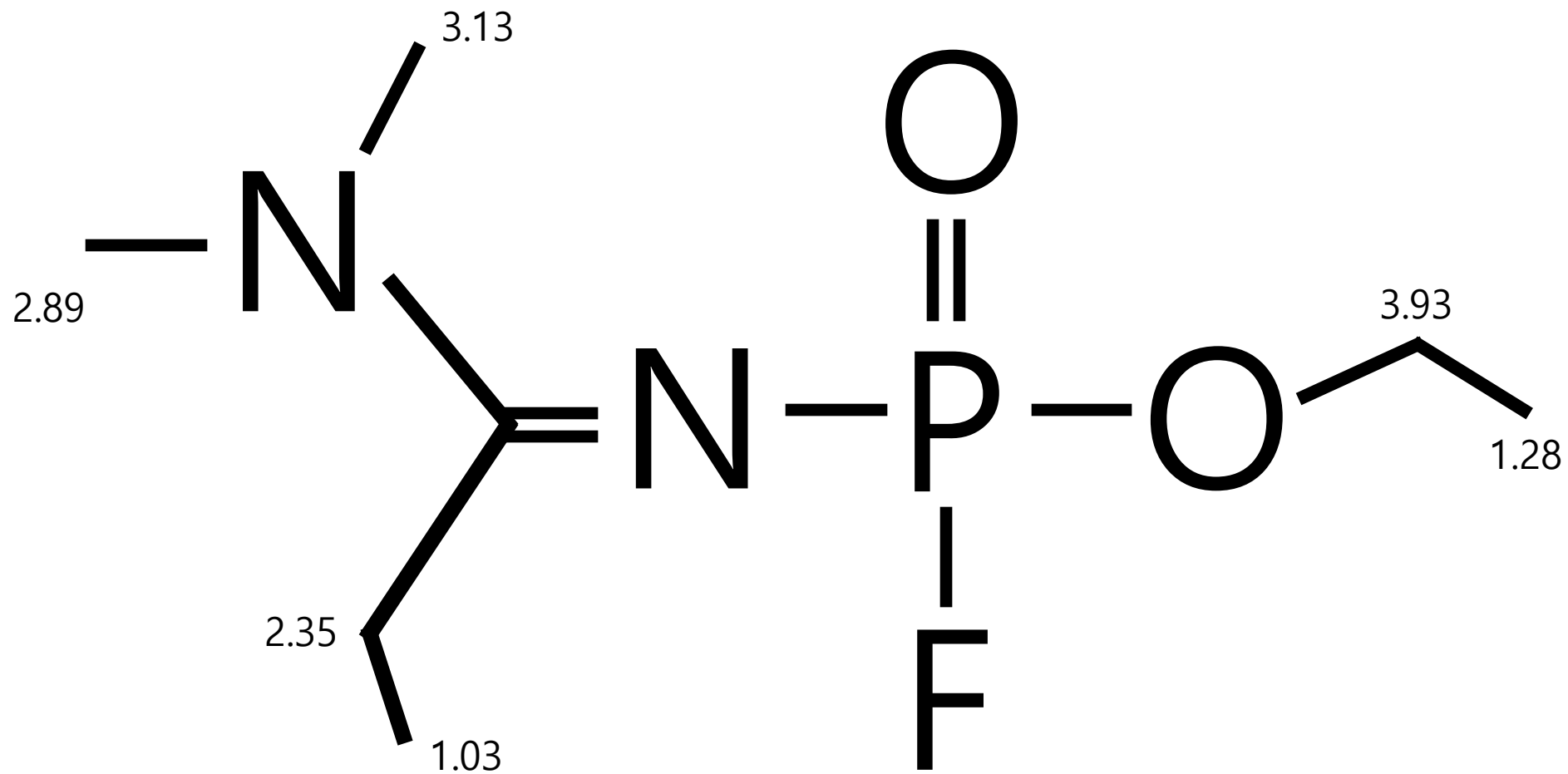


Figure S120. Structure 2211 and its ¹H chemical shift

2212 H

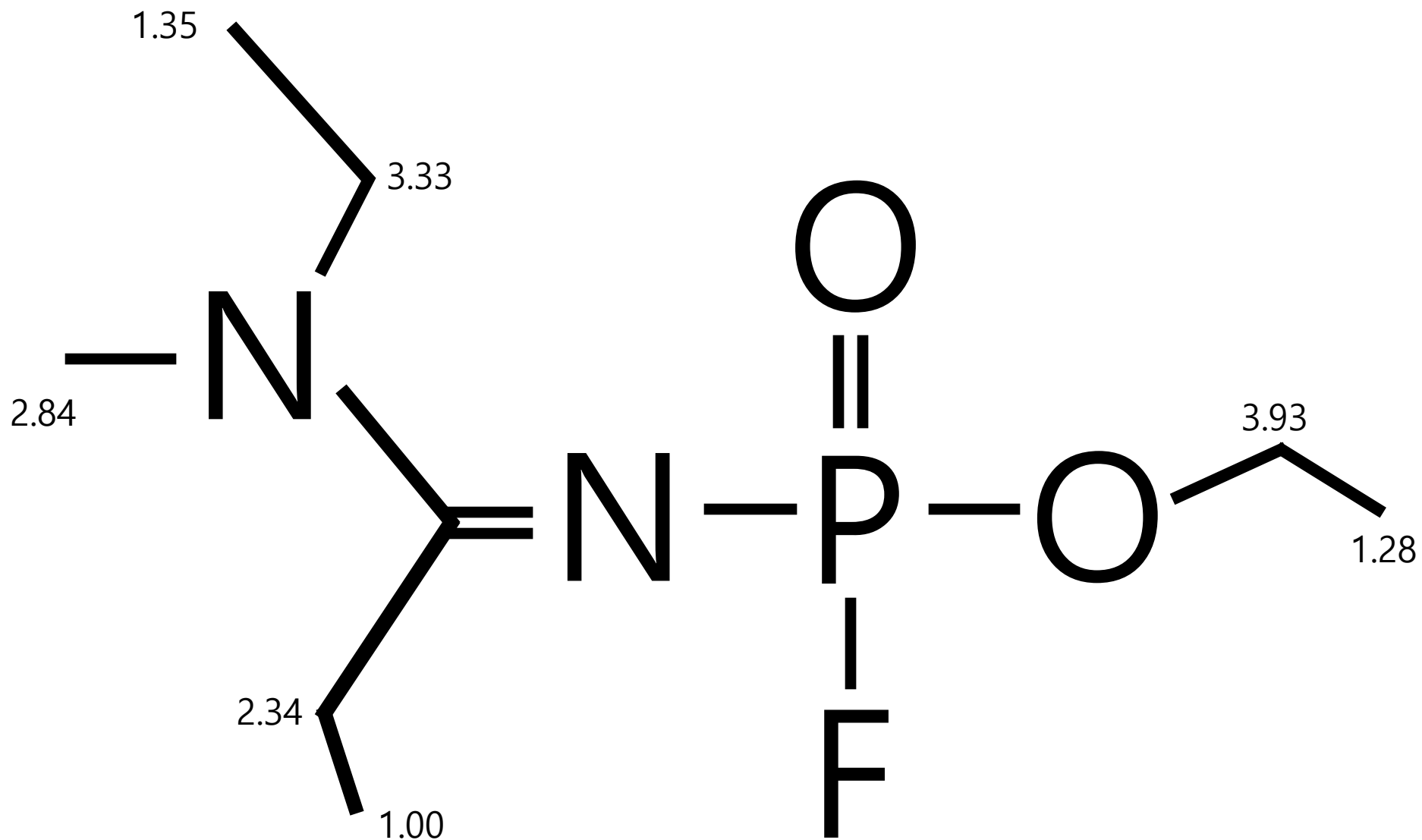


Figure S121. Structure 2212 and its ^1H chemical shift

2213 H

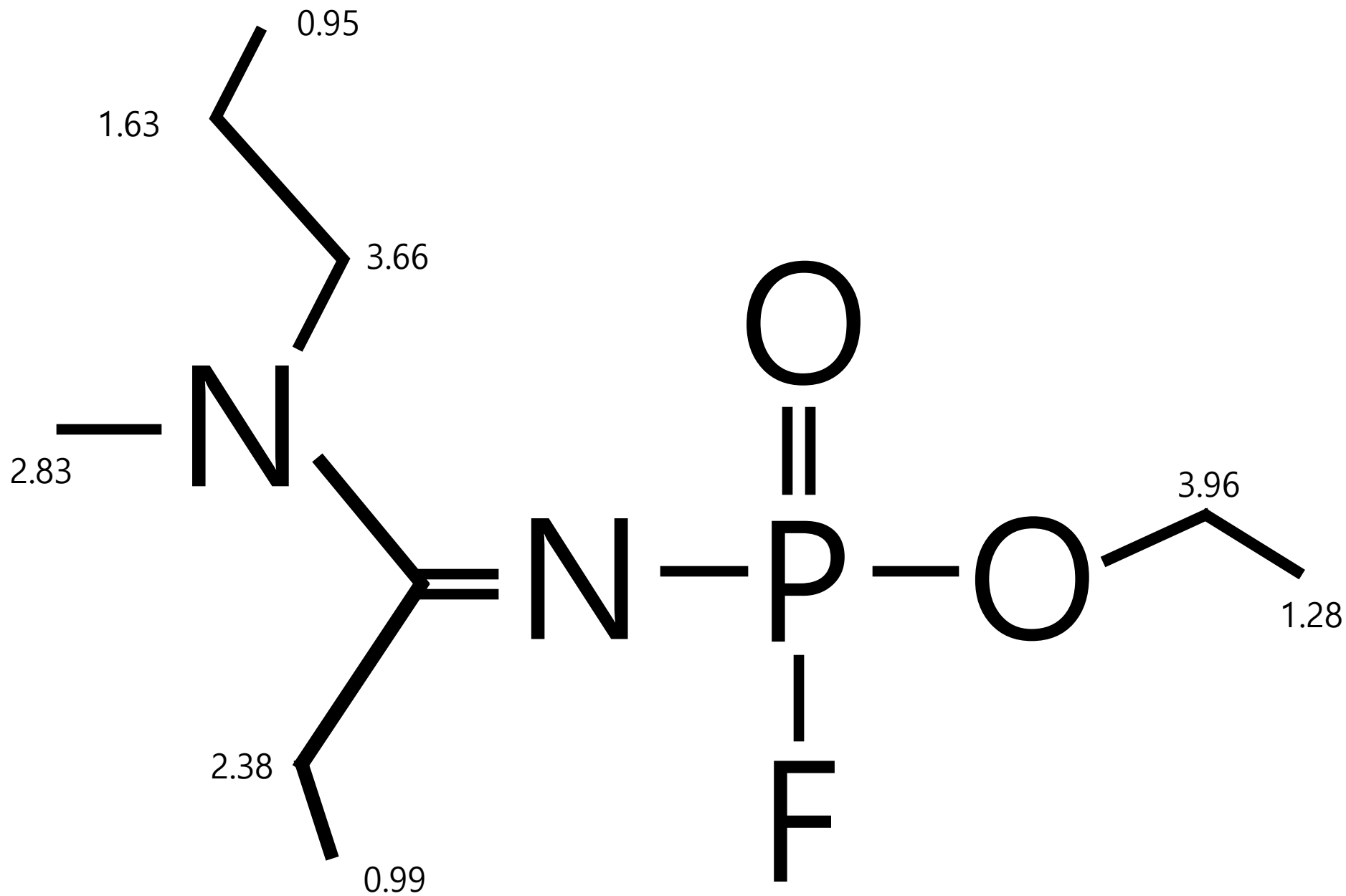


Figure S122. Structure 2213 and its ^1H chemical shift

2221 H

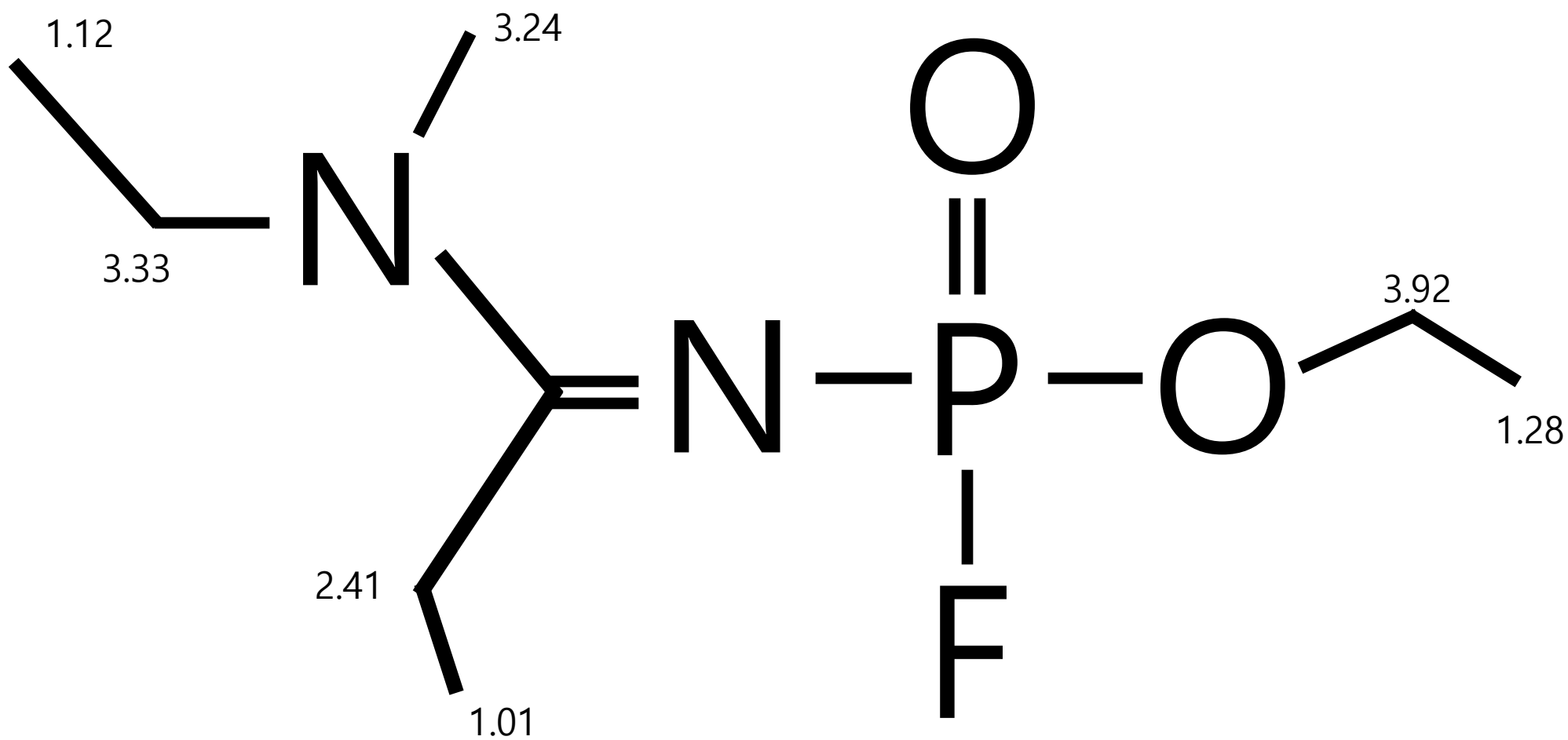


Figure S123. Structure 2221 and its ¹H chemical shift

2222 H

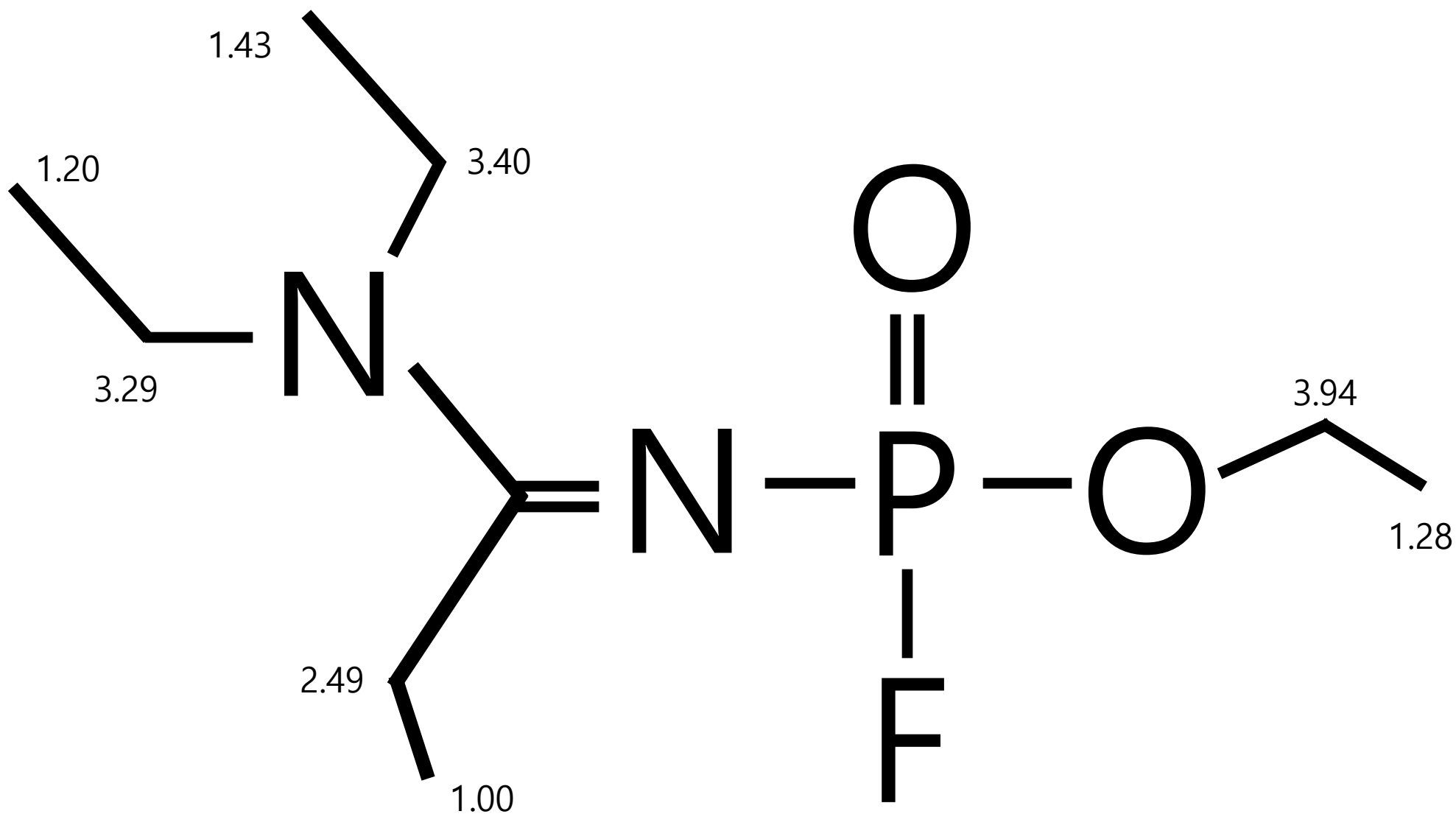


Figure S124. Structure 2222 and its ^1H chemical shift

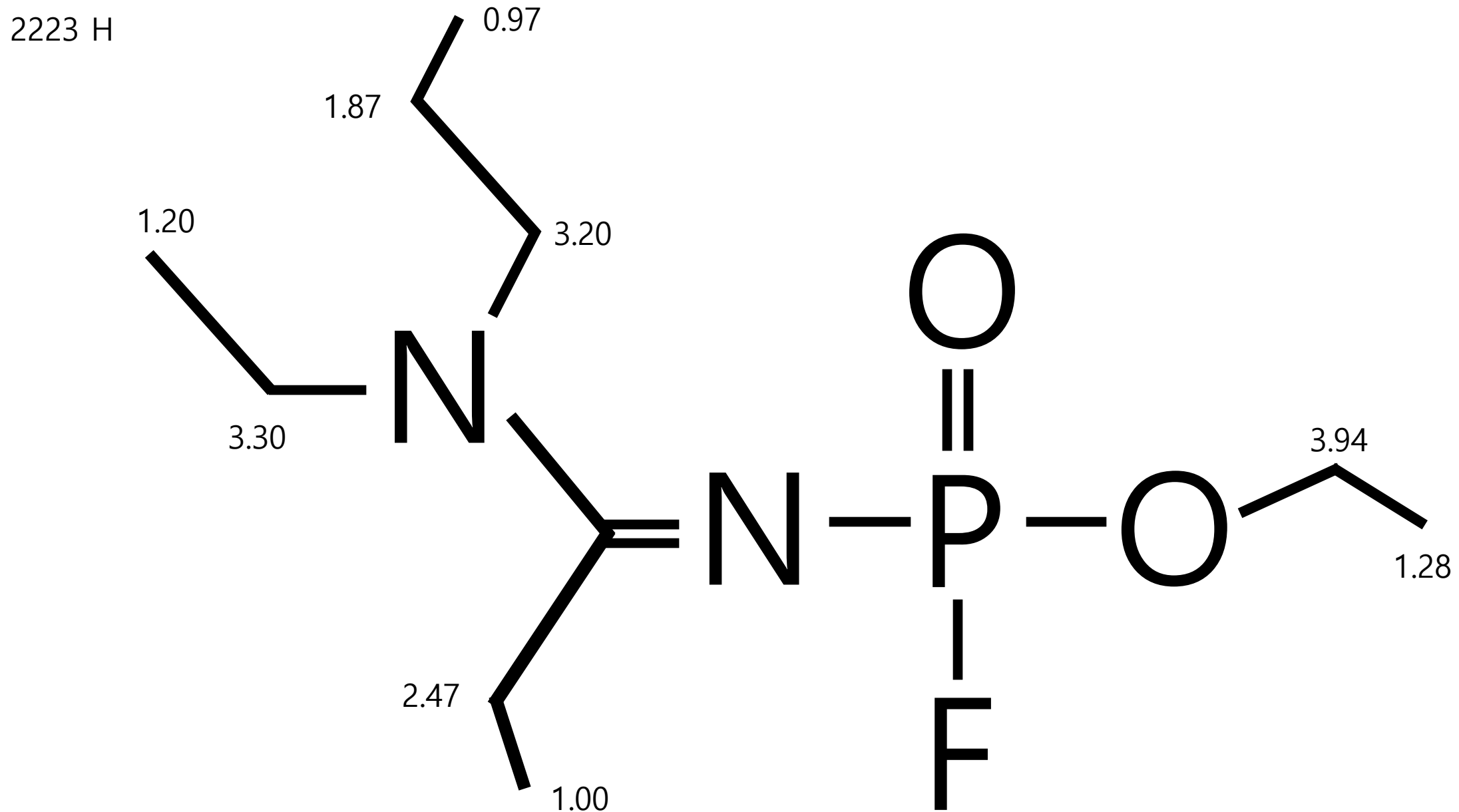


Figure S125. Structure 2223 and its ^1H chemical shift

2231 H

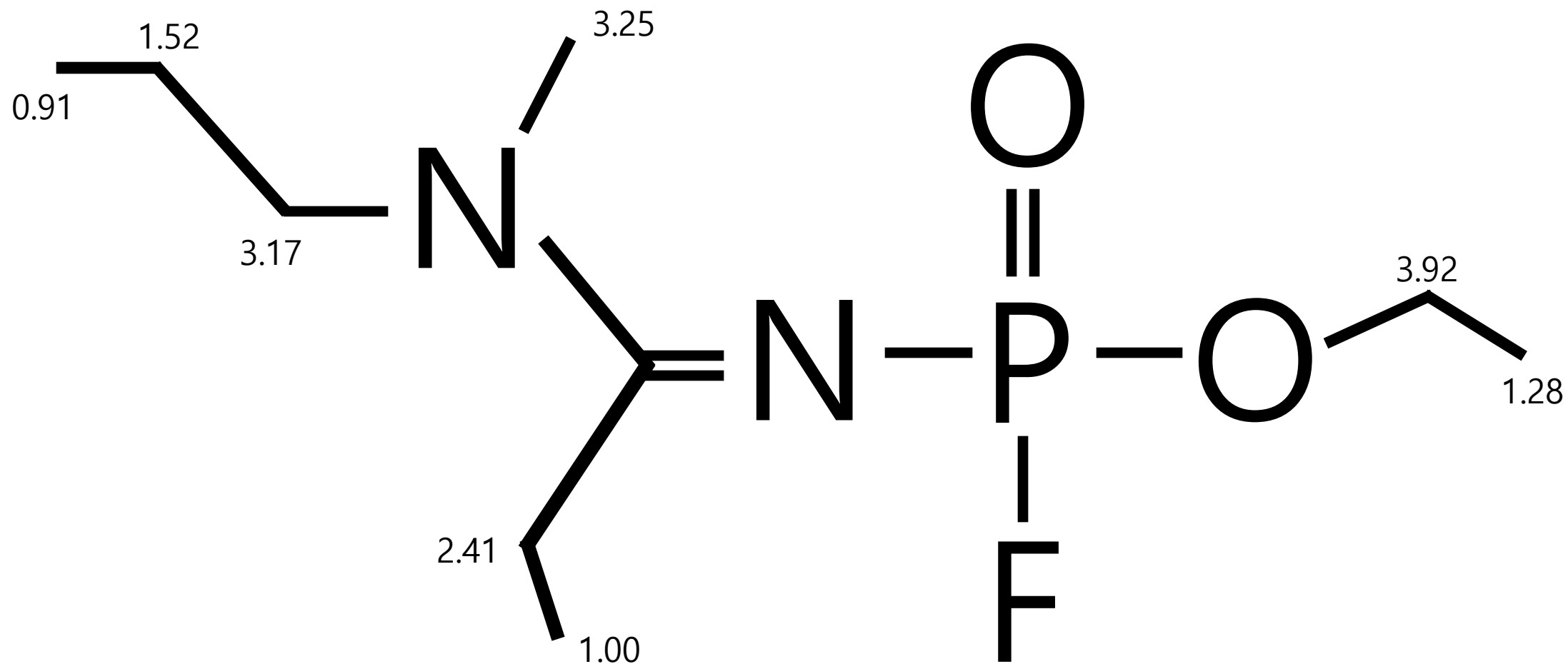


Figure S126. Structure 2231 and its ^1H chemical shift

2232 H

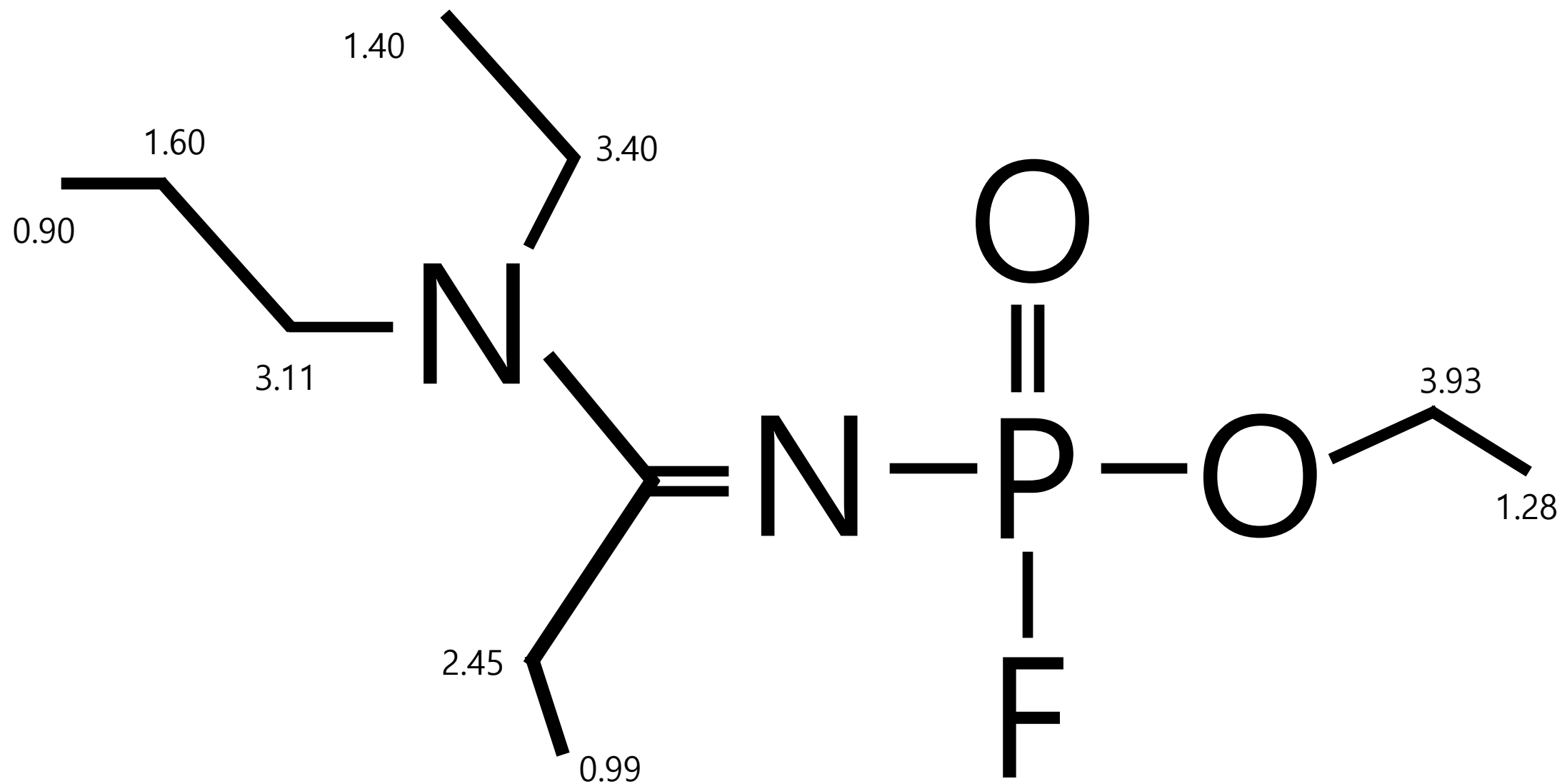


Figure S127. Structure 2232 and its ¹H chemical shift

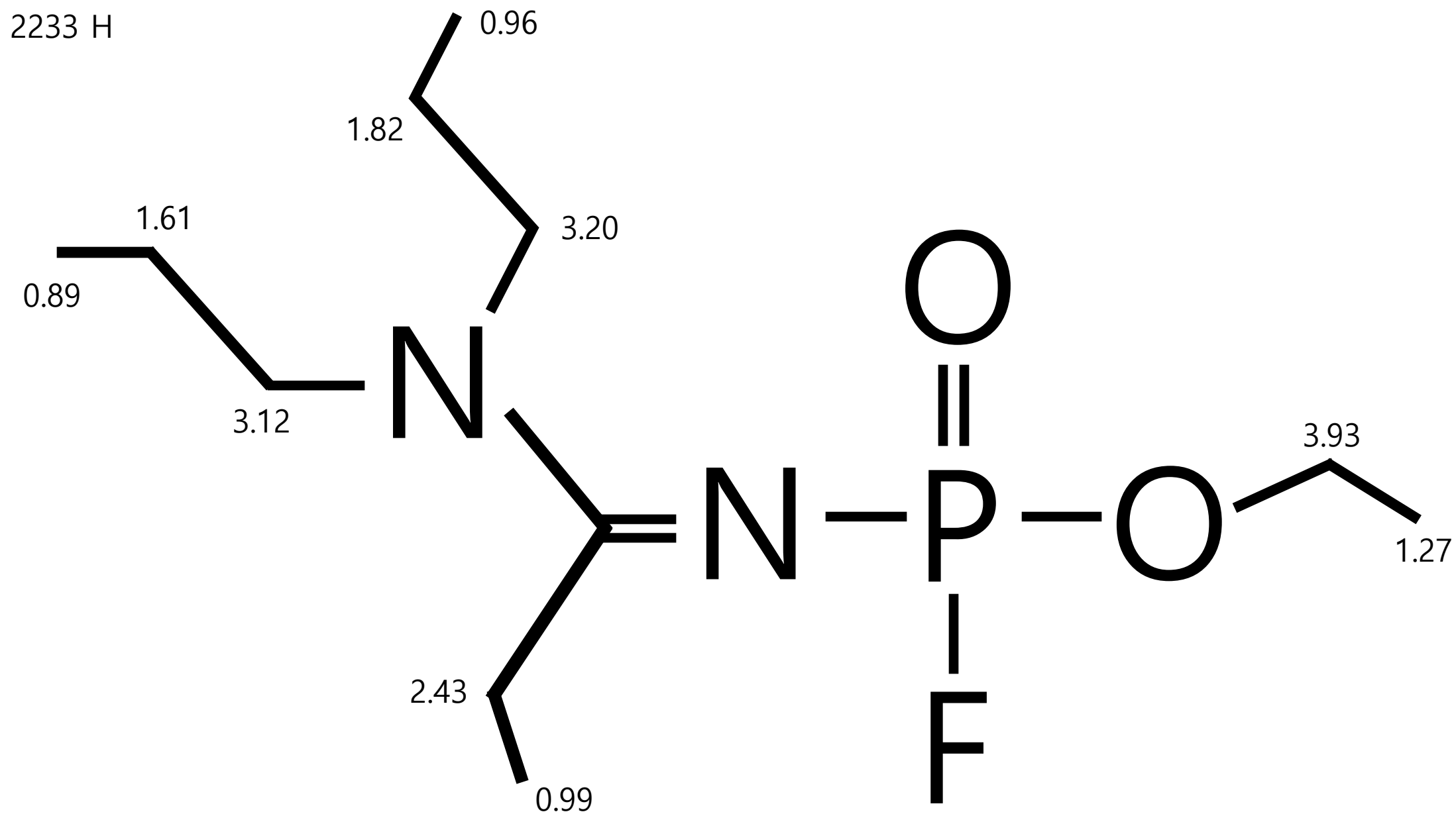


Figure S128. Structure 2233 and its ^1H chemical shift

2311 H

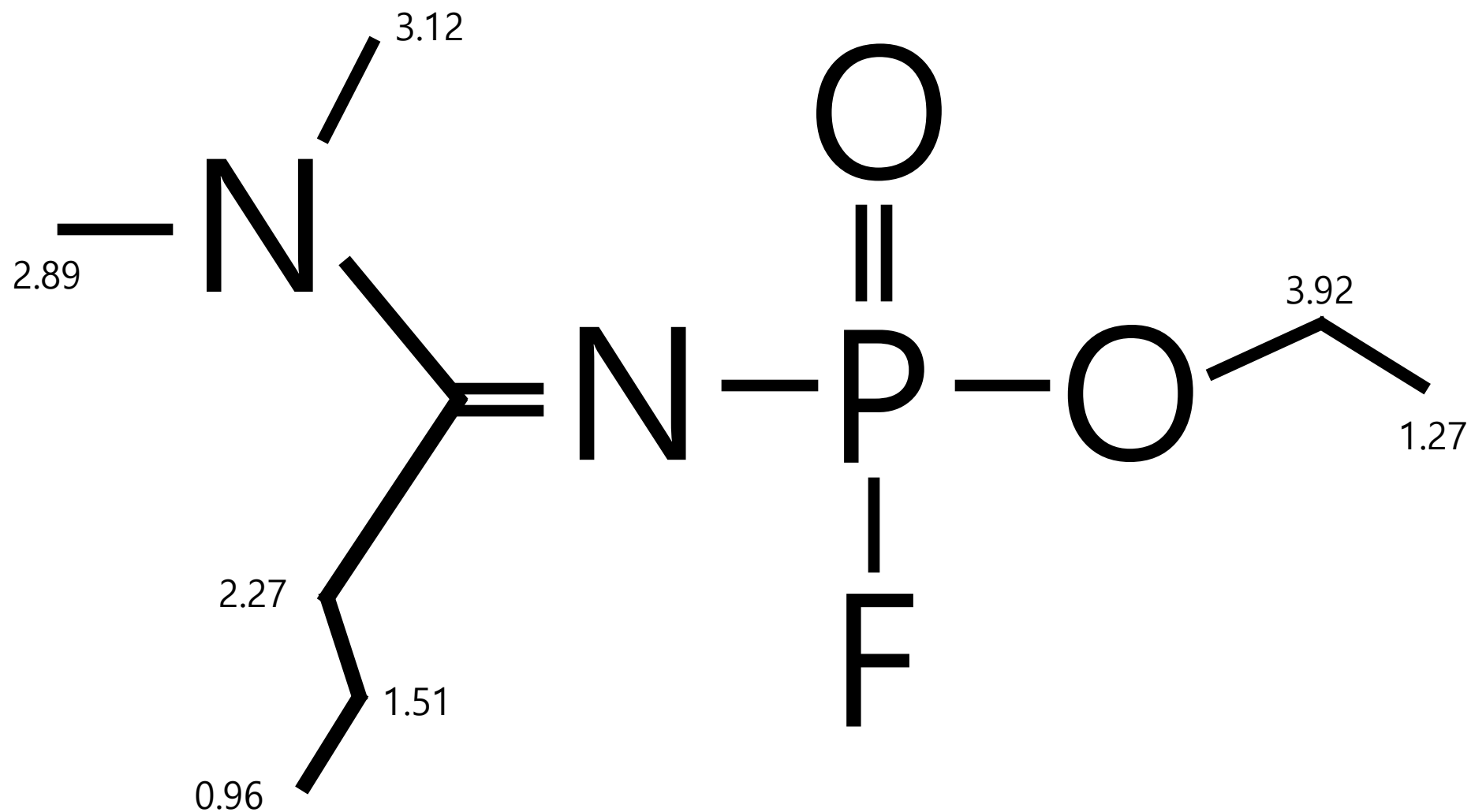


Figure S129. Structure 2311 and its ¹H chemical shift

2312 H

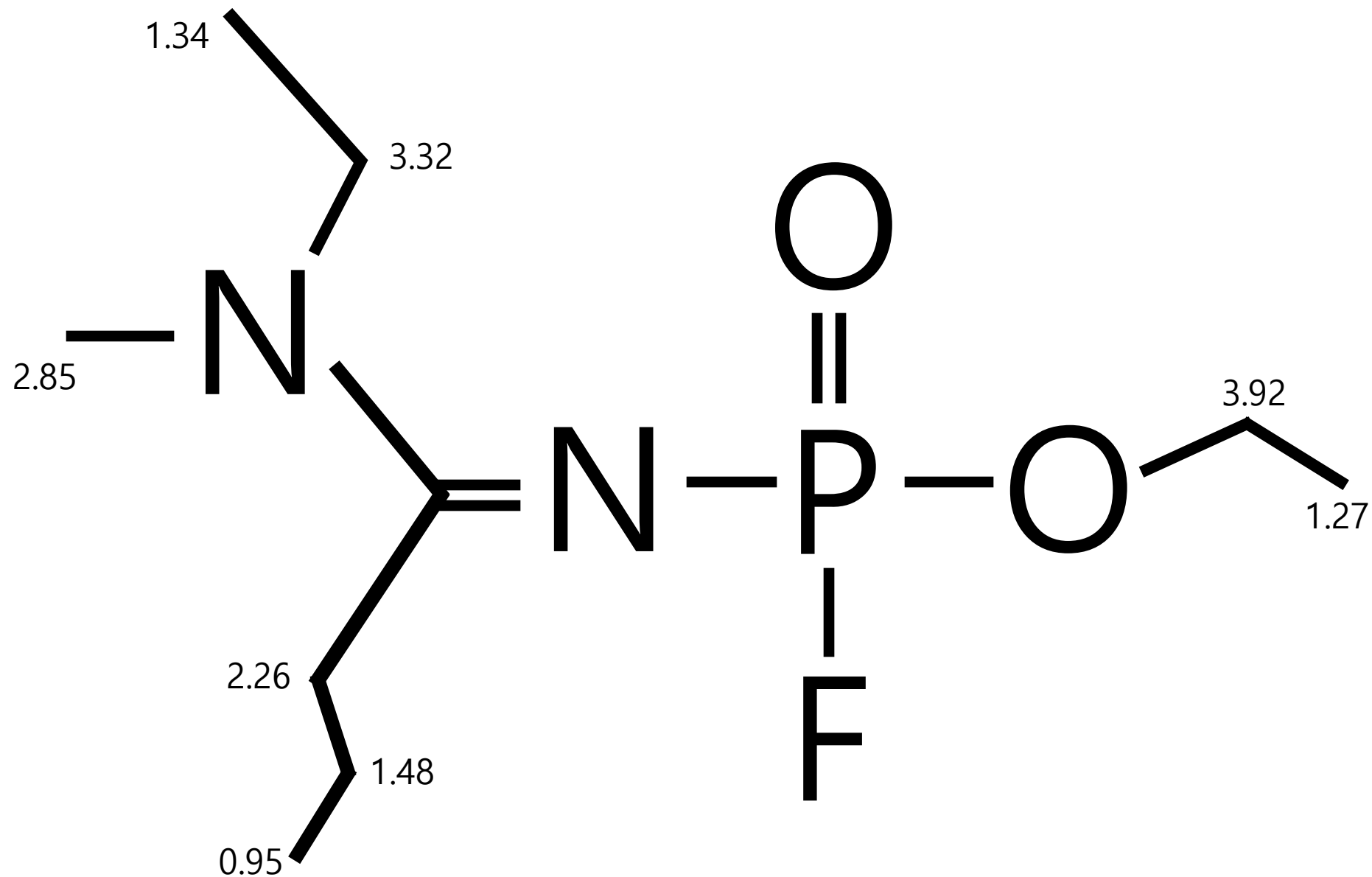


Figure S130. Structure 2312 and its ¹H chemical shift

2313 H

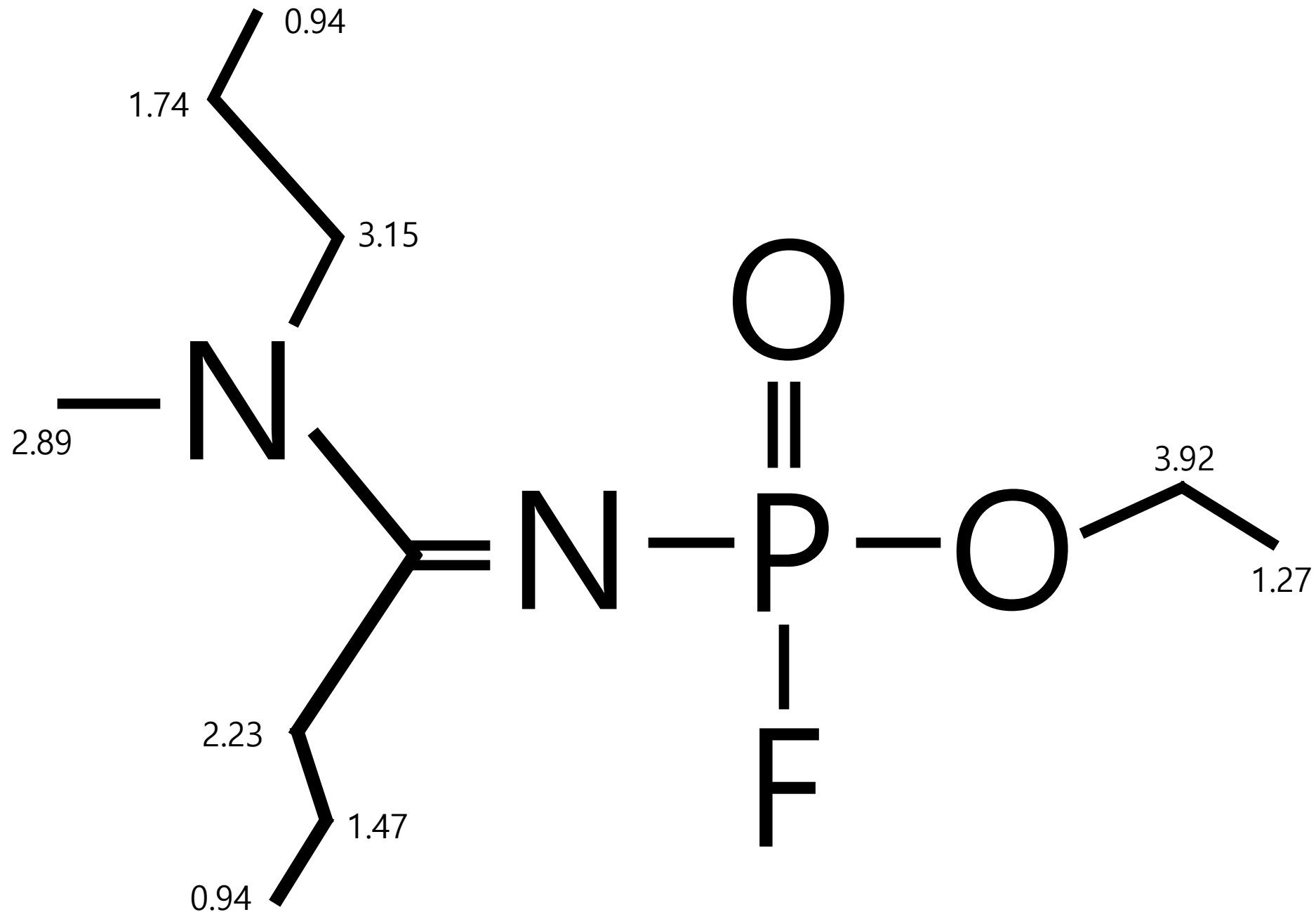


Figure S131. Structure 2313 and its ¹H chemical shift

2321 H

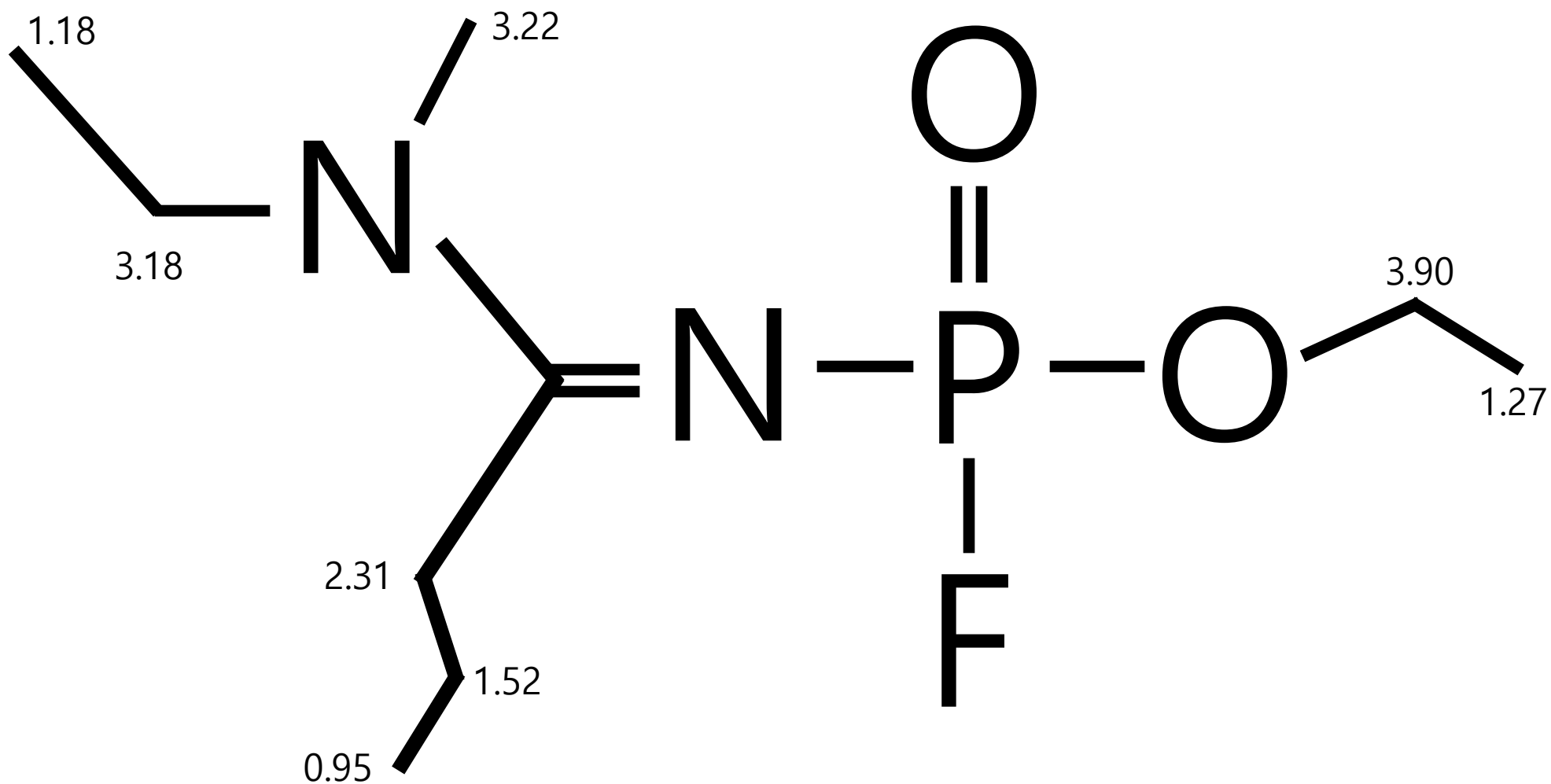


Figure S132. Structure 2321 and its ¹H chemical shift

2322 H

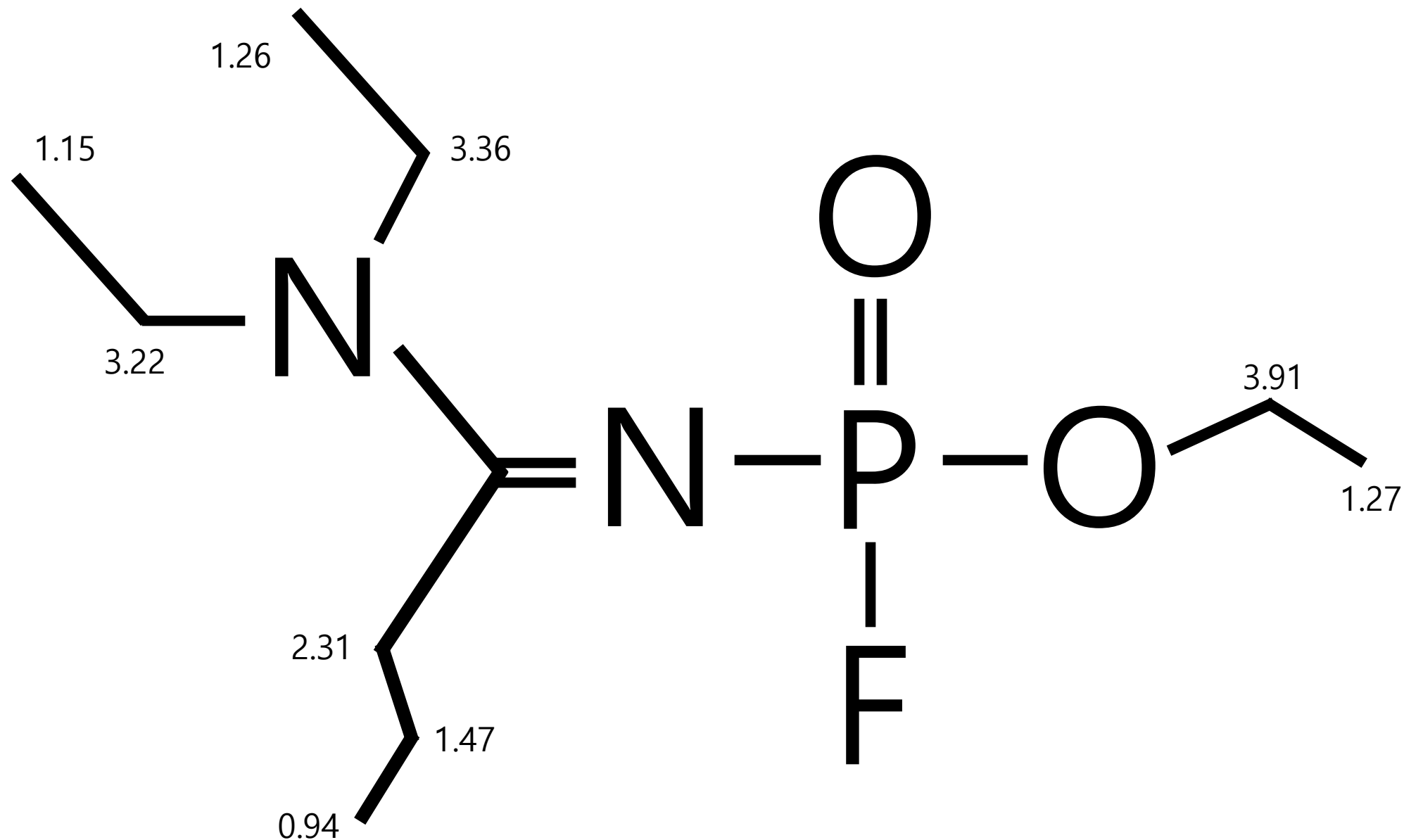


Figure S133. Structure 2322 and its ¹H chemical shift

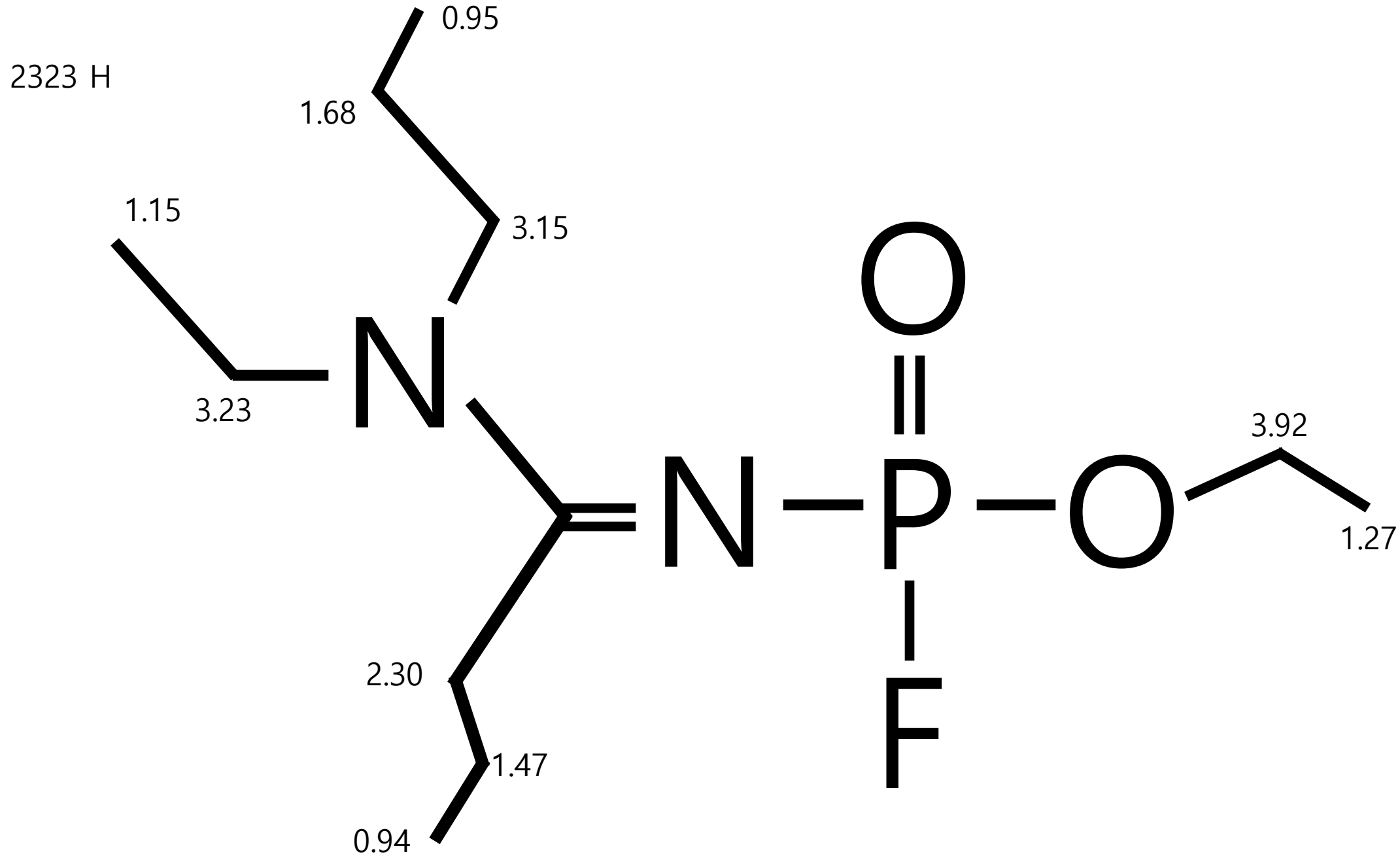


Figure S134. Structure 2323 and its ^1H chemical shift

2331 H

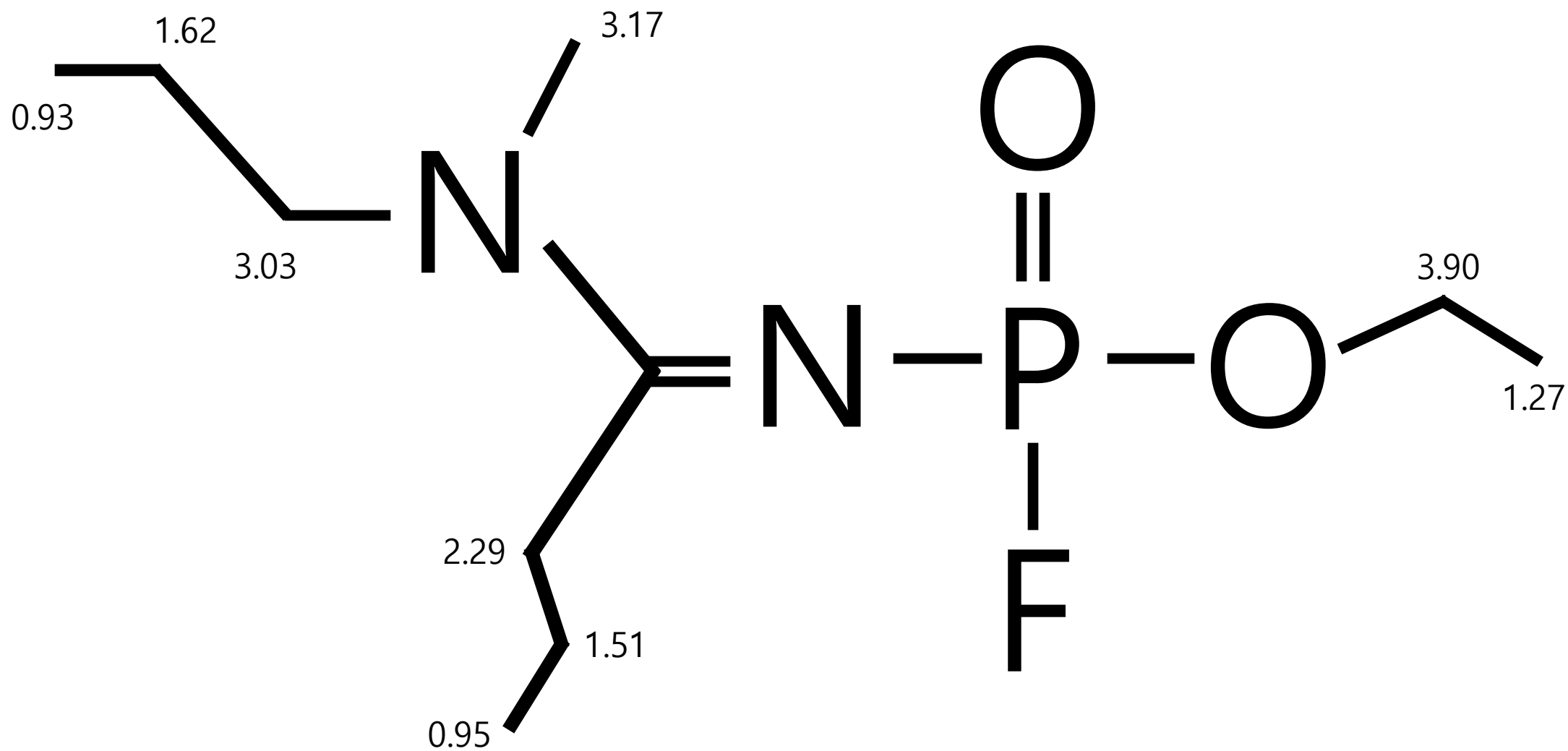


Figure S135. Structure 2331 and its ^1H chemical shift

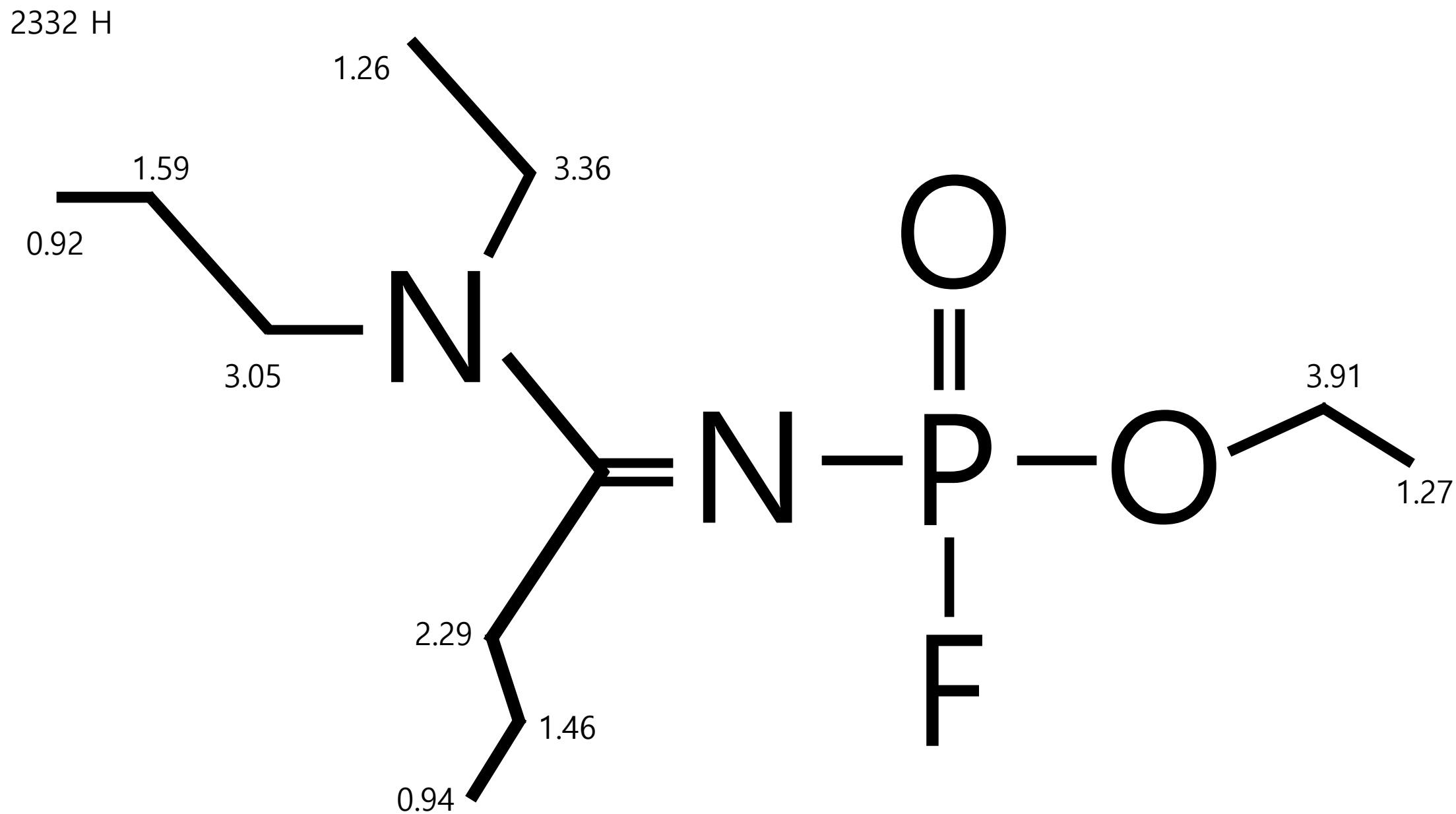


Figure S136. Structure 2332 and its ^1H chemical shift

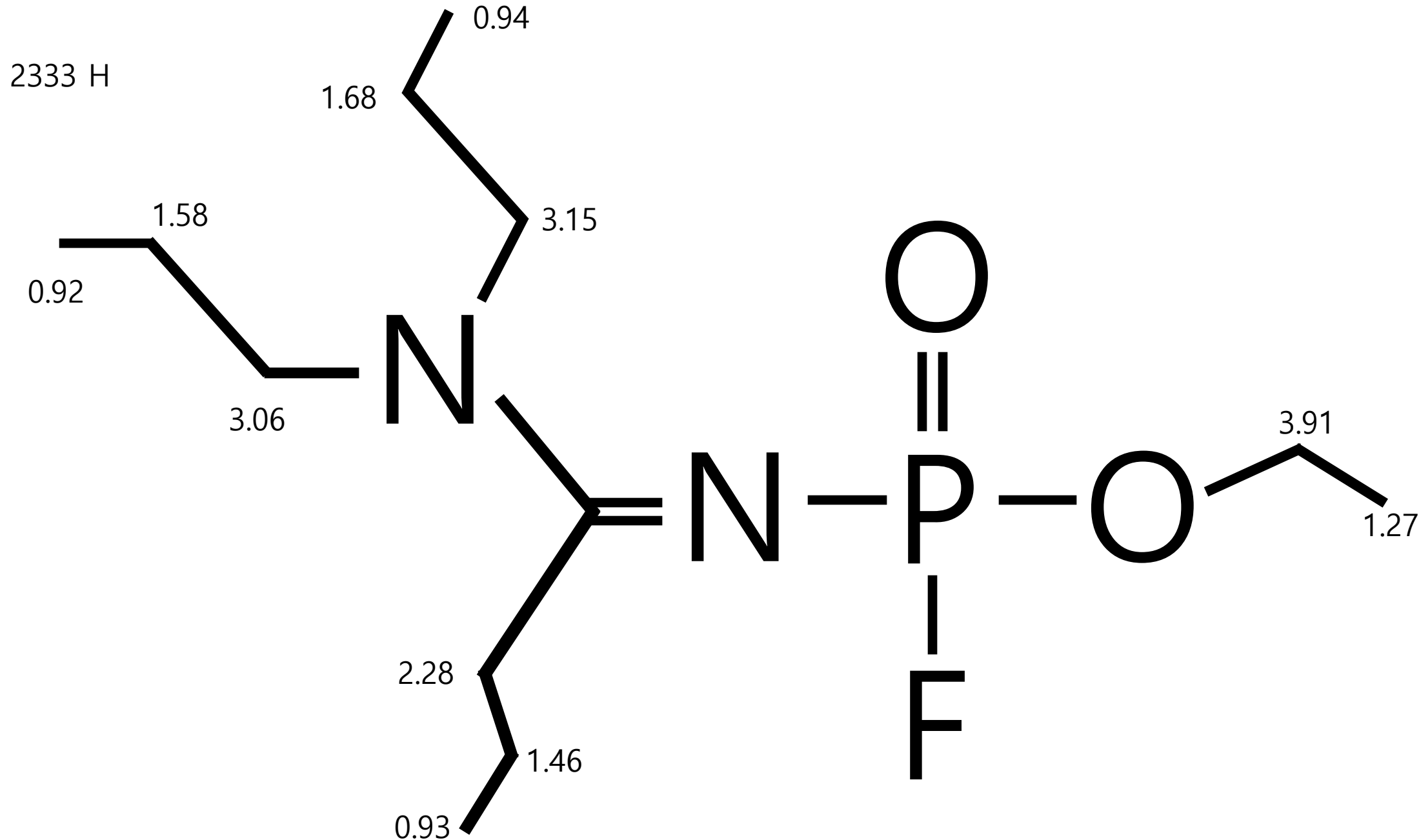


Figure S137. Structure 2333 and its ^1H chemical shift

3111 H

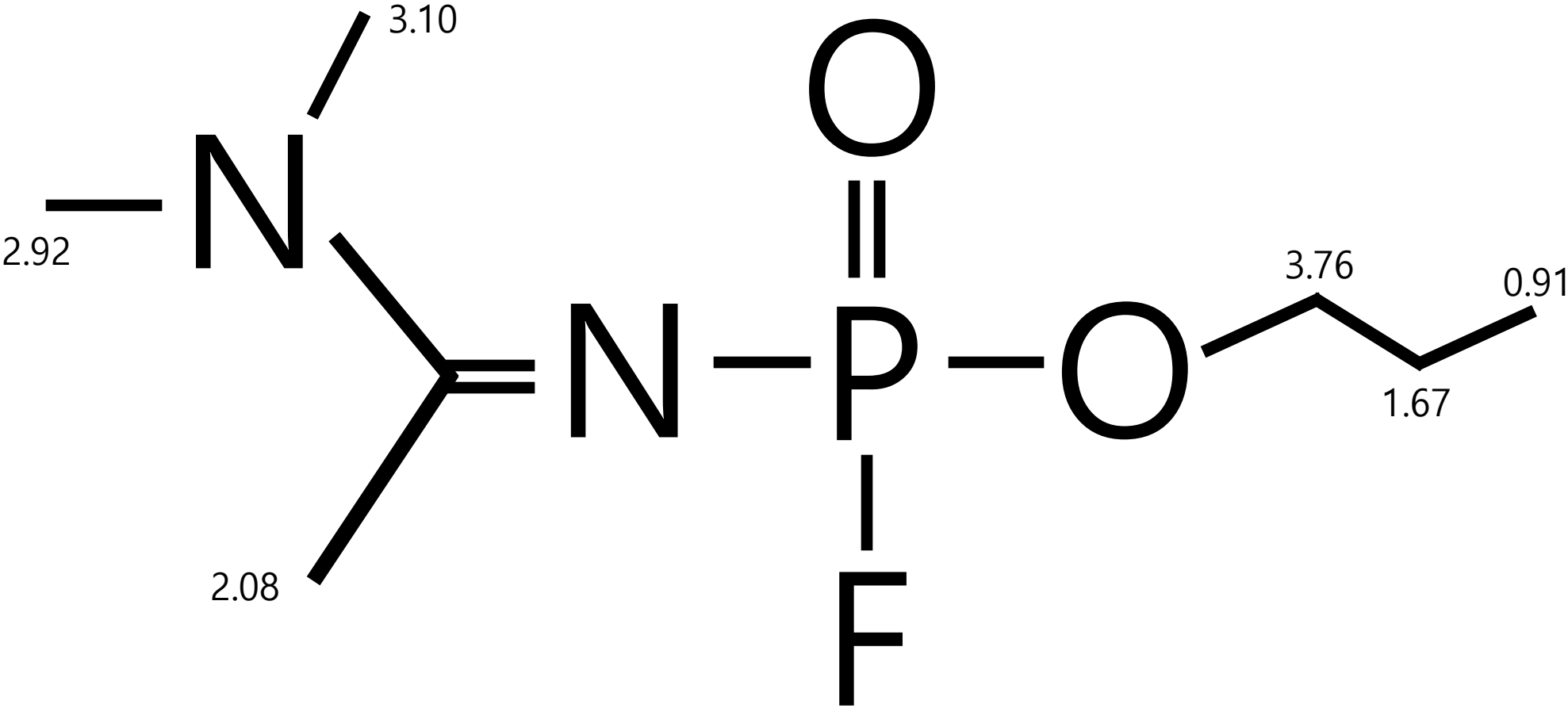


Figure S138. Structure 3111 and its ¹H chemical shift

3112 H

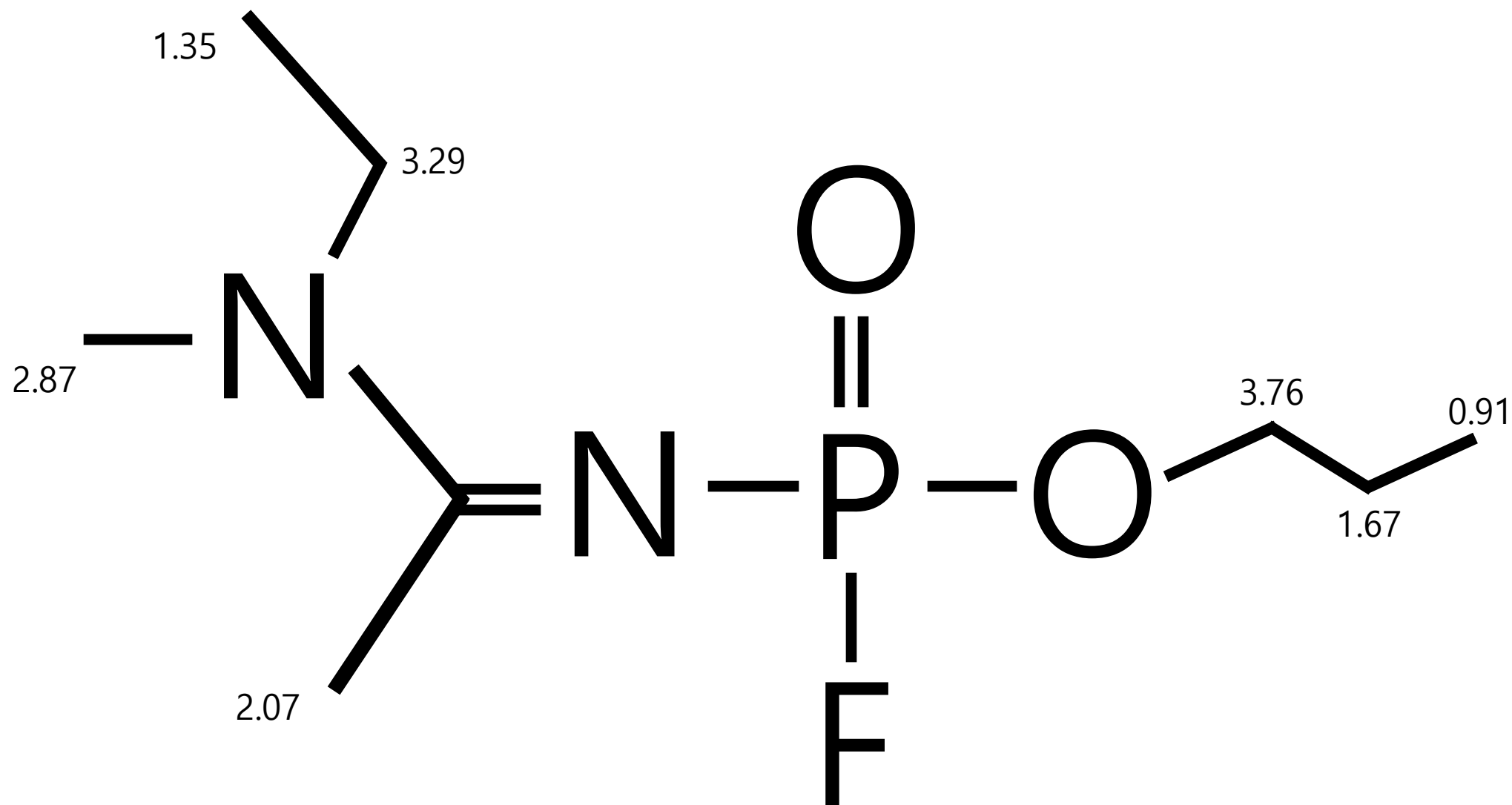


Figure S139. Structure 3112 and its ¹H chemical shift

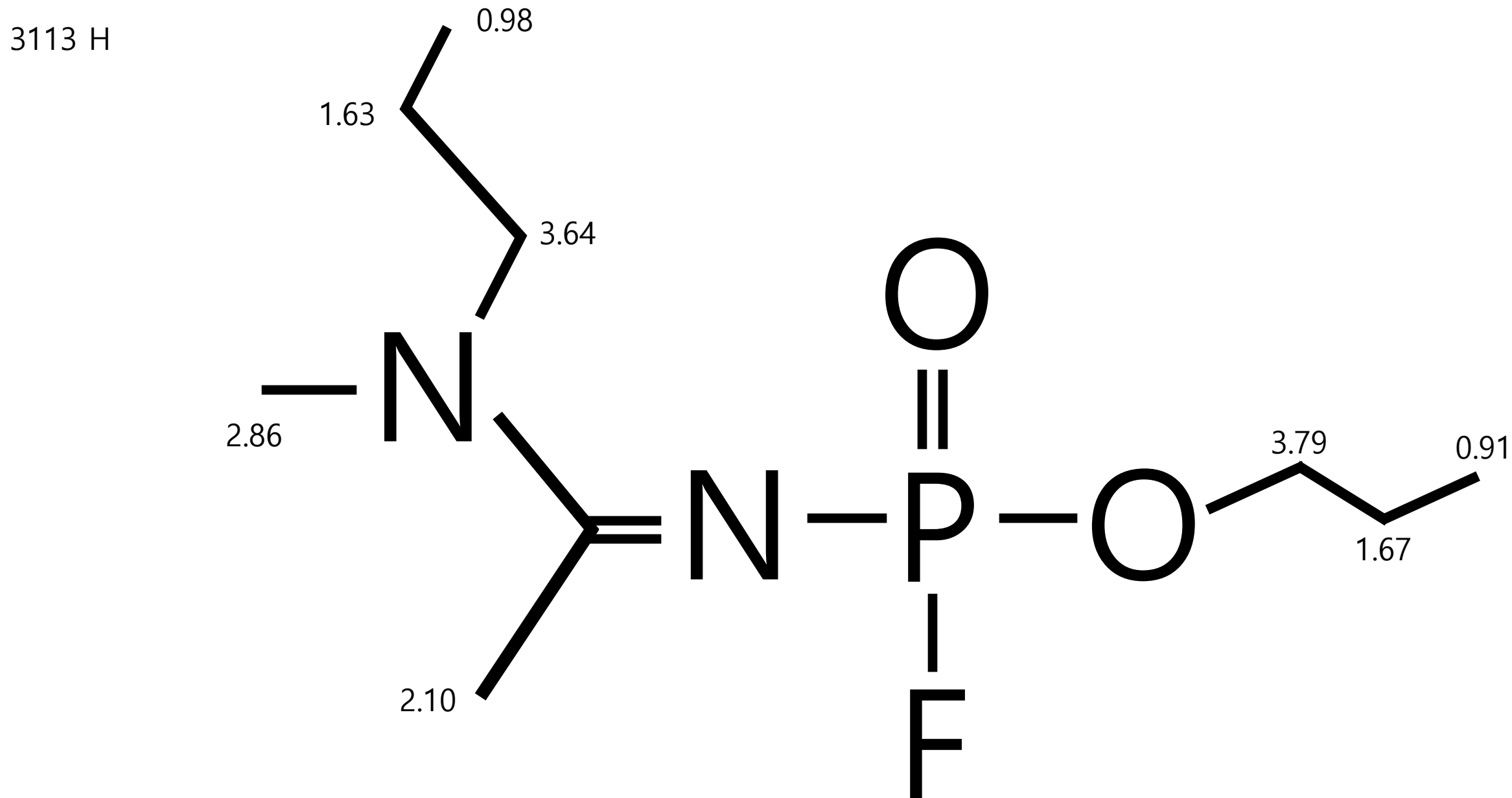


Figure S140. Structure 3113 and its ¹H chemical shift

3121 H

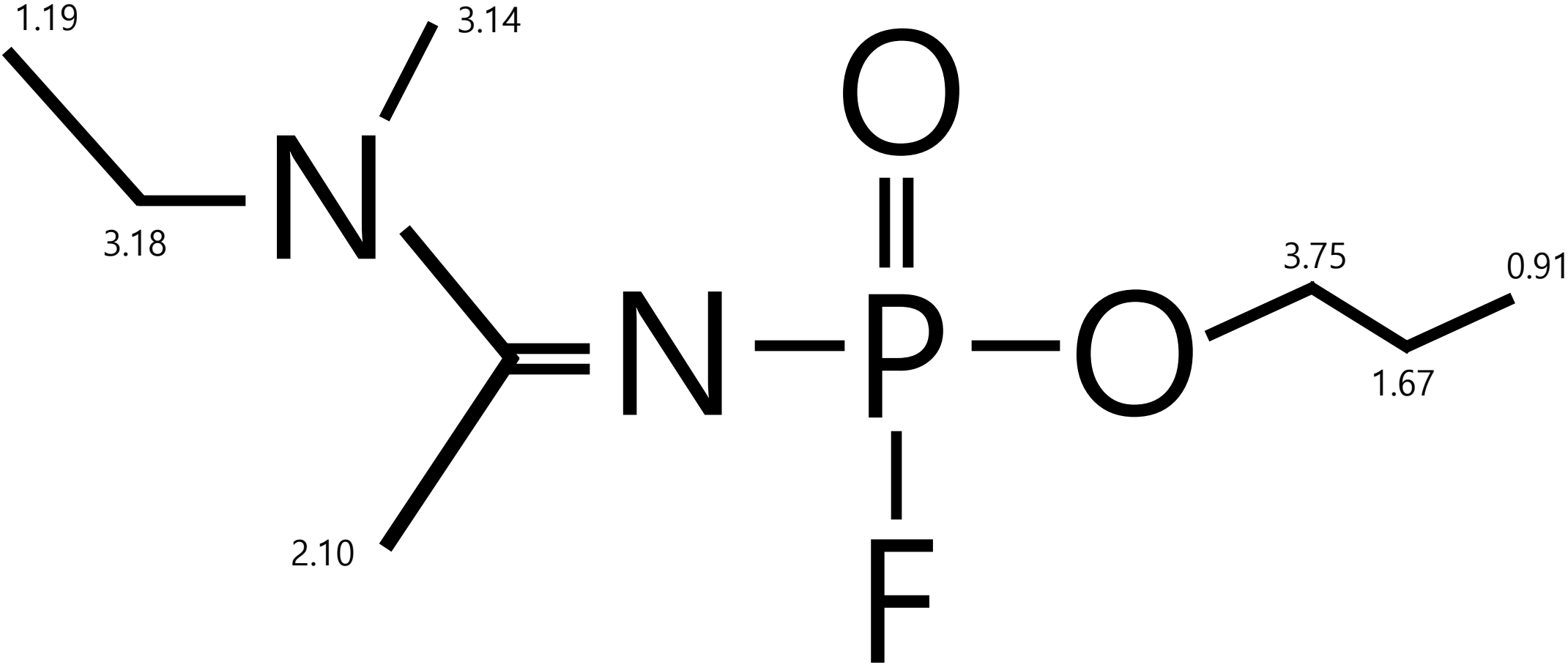


Figure S141. Structure 3121 and its ¹H chemical shift

3122 H

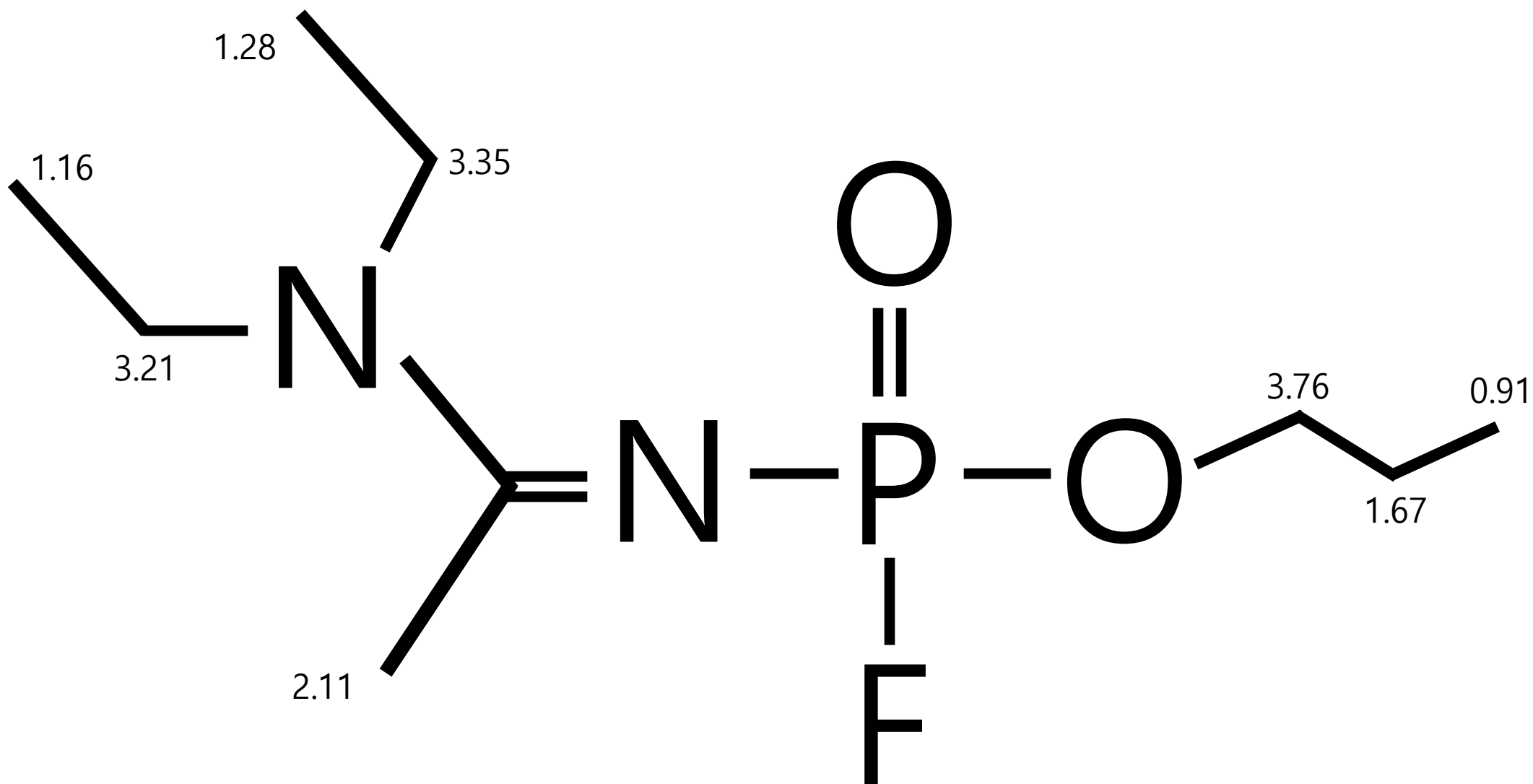


Figure S142. Structure 3122 and its ^1H chemical shift

3123 H

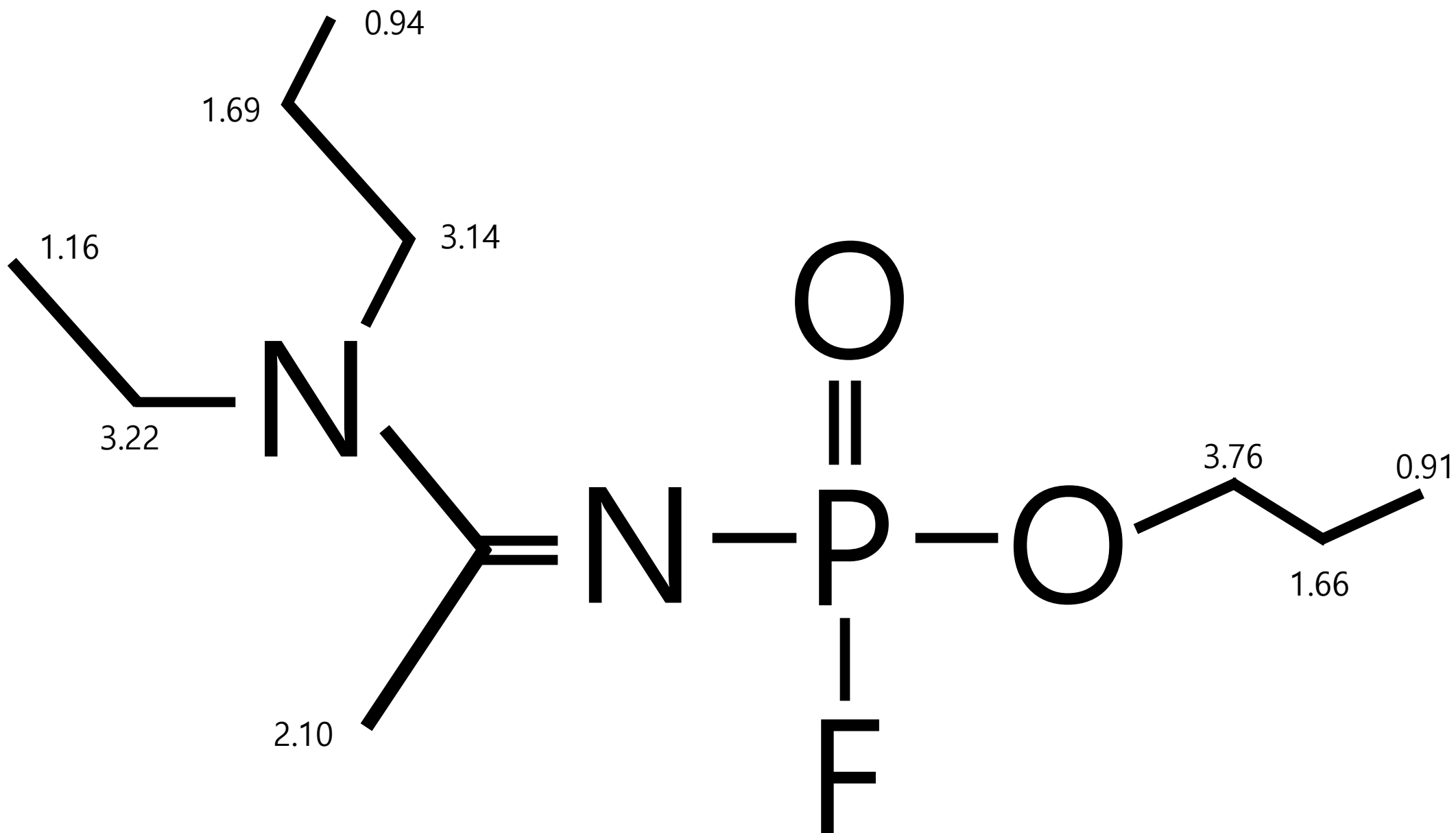


Figure S143. Structure 3123 and its ^1H chemical shift

3131 H

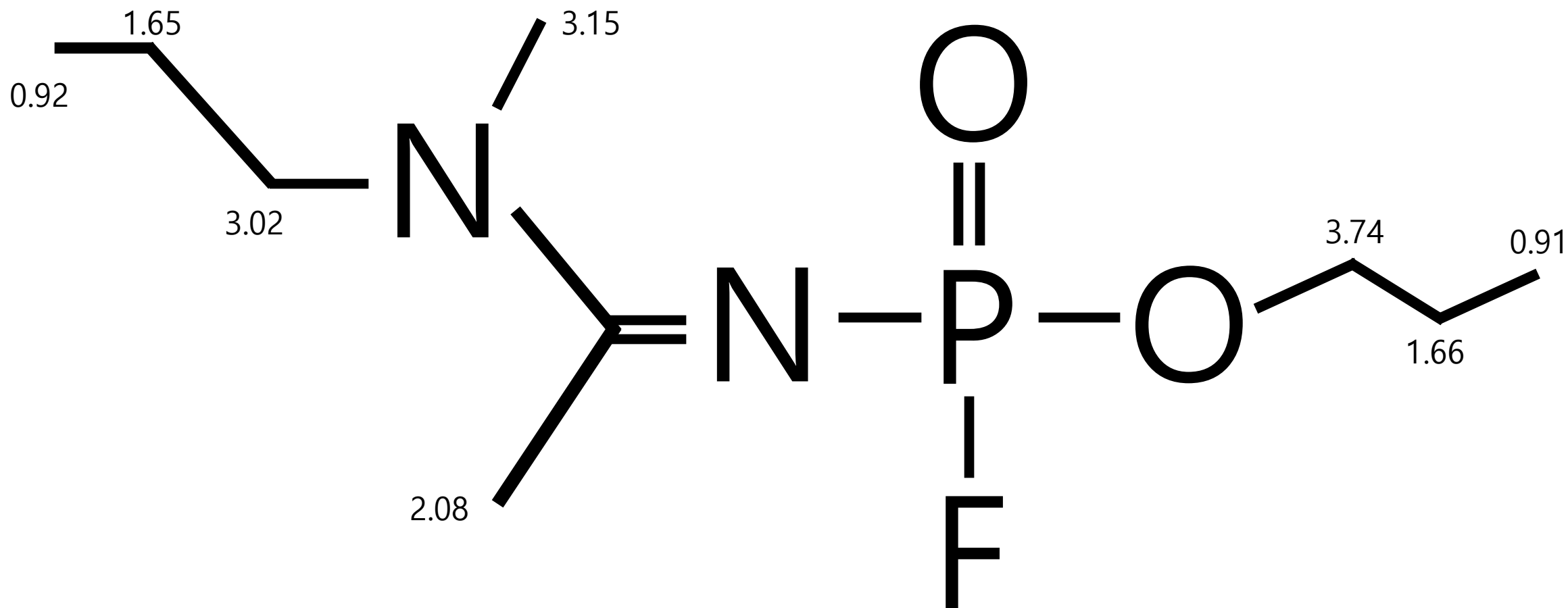


Figure S144. Structure 3131 and its ¹H chemical shift

3132 H

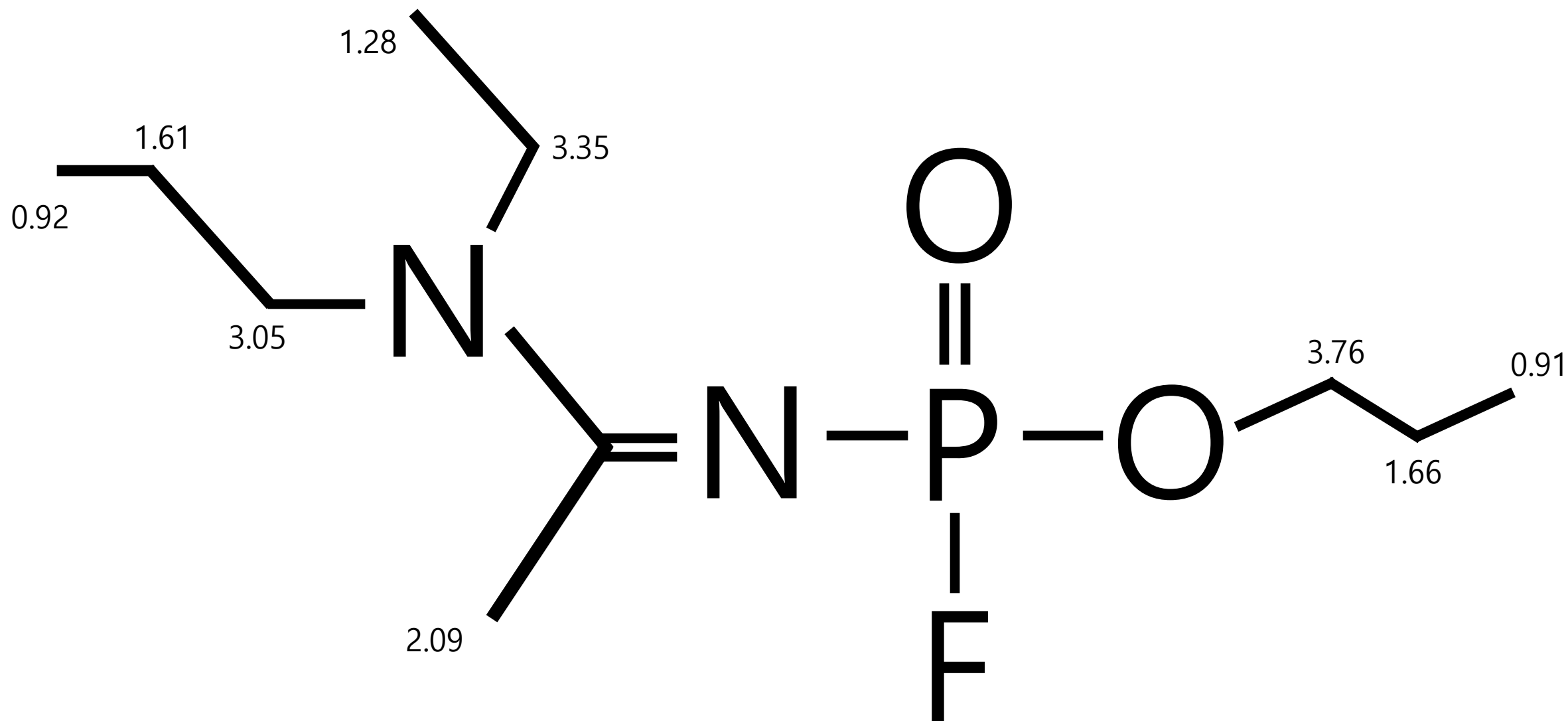


Figure S145. Structure 3132 and its ¹H chemical shift

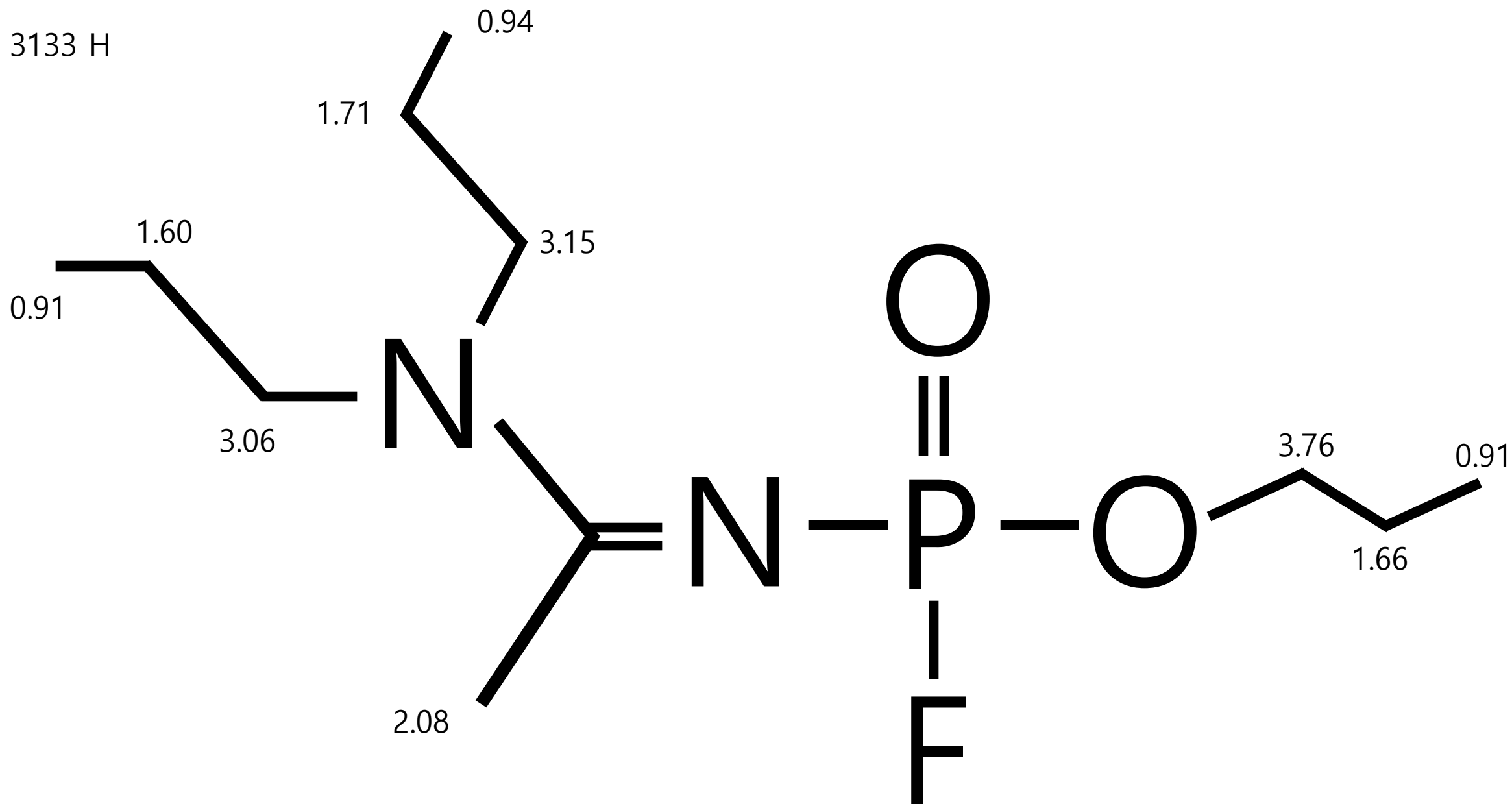


Figure S146. Structure 3133 and its ¹H chemical shift

3211 H

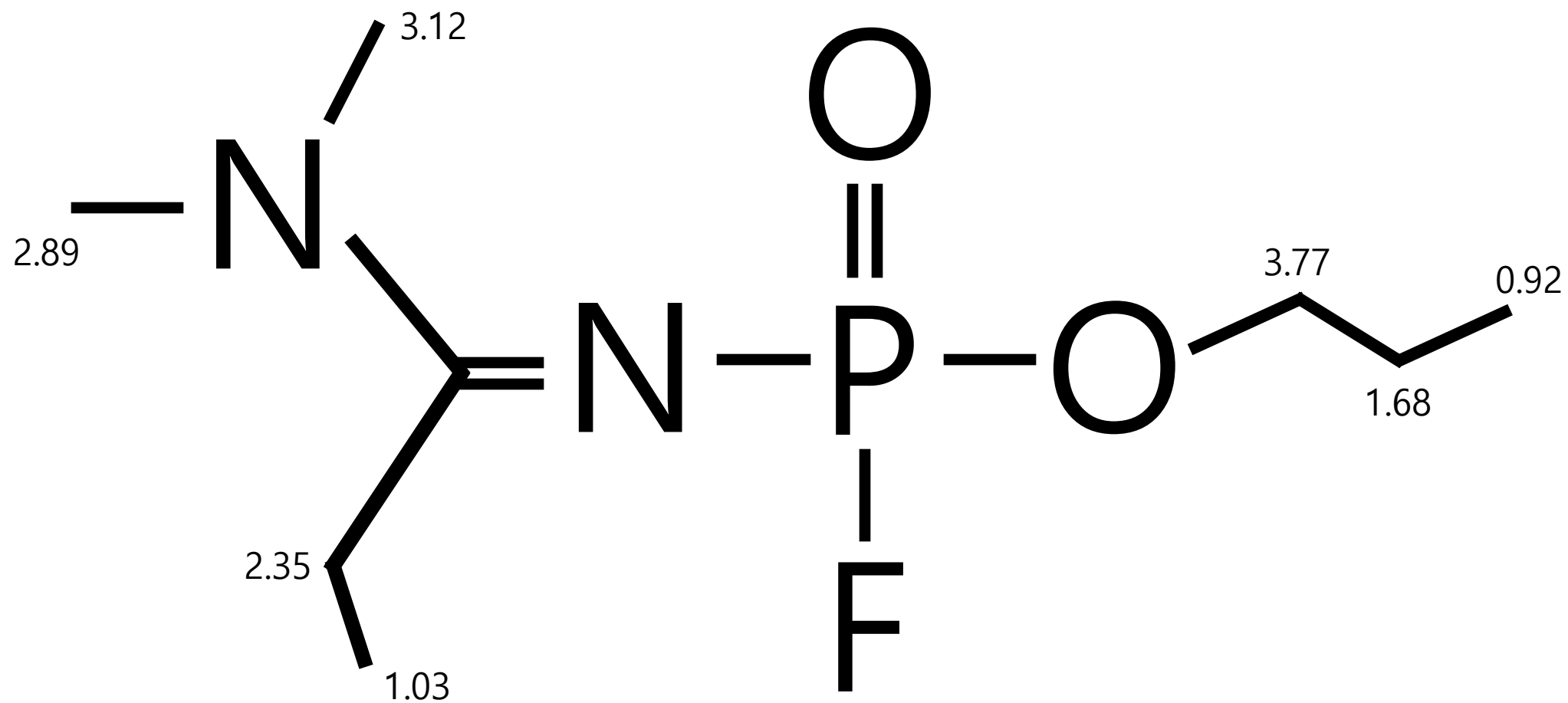


Figure S147. Structure 3211 and its ¹H chemical shift

3212 H

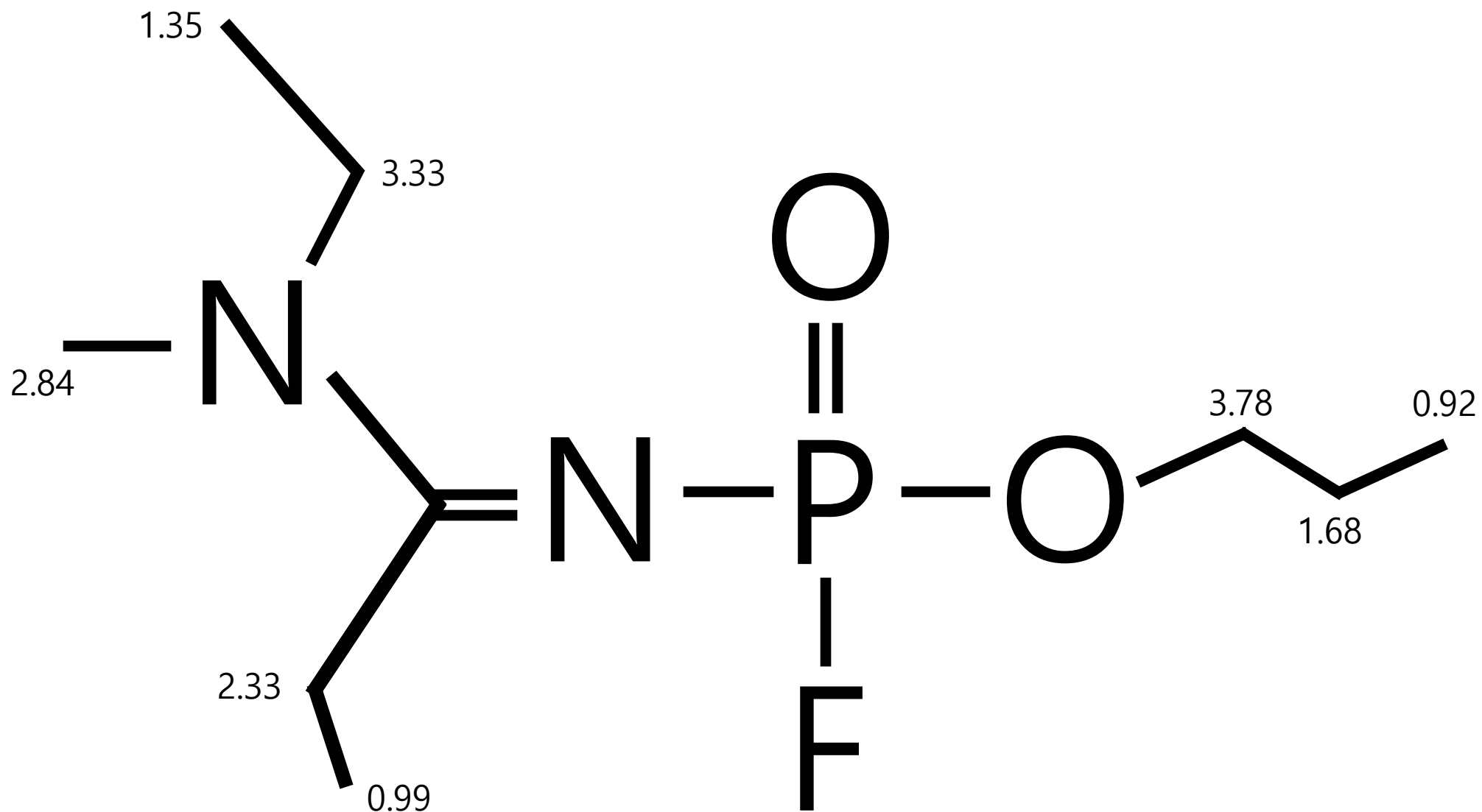


Figure S148. Structure 3212 and its ¹H chemical shift

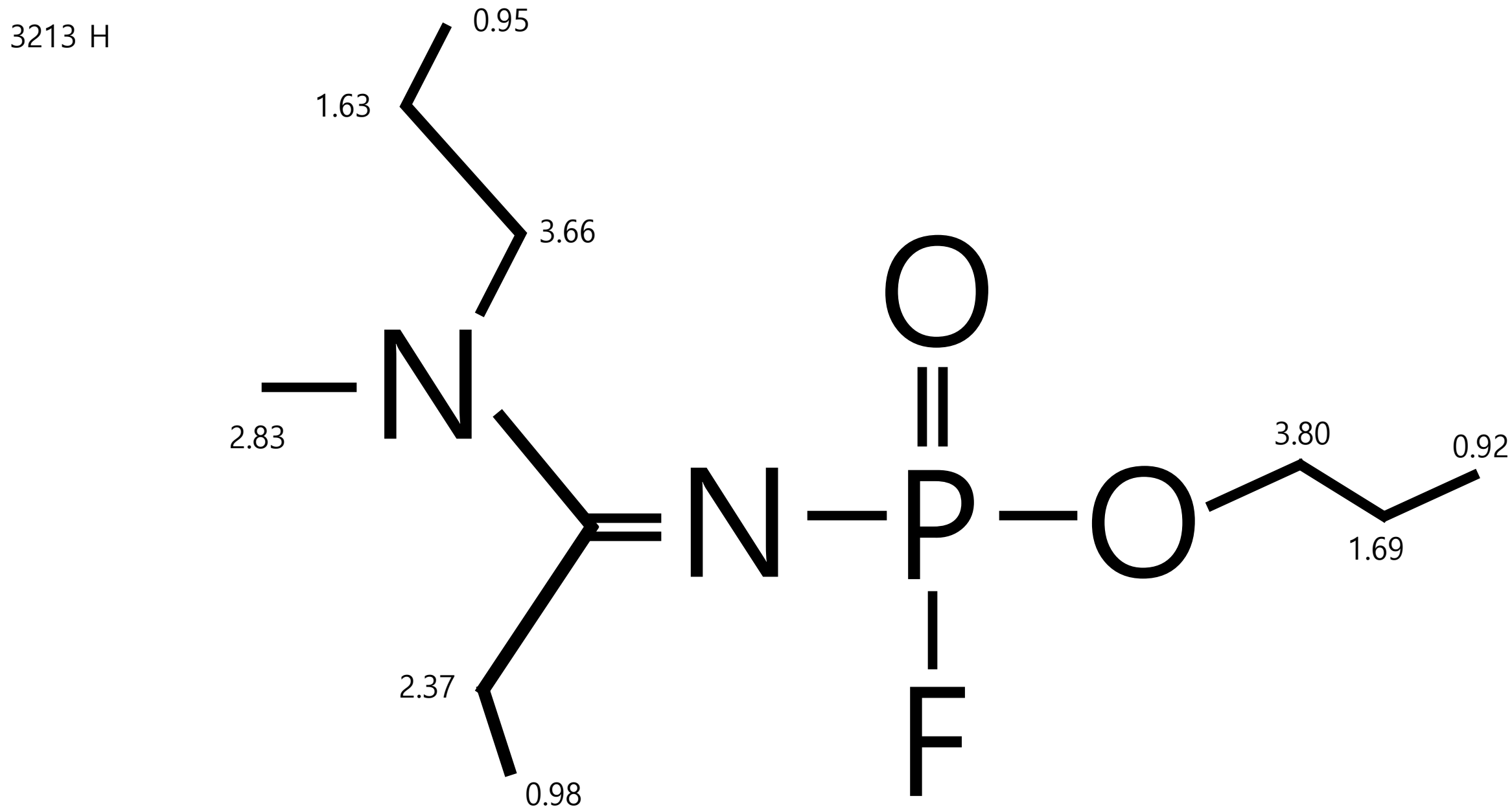


Figure S149. Structure 3213 and its ¹H chemical shift

3221 H

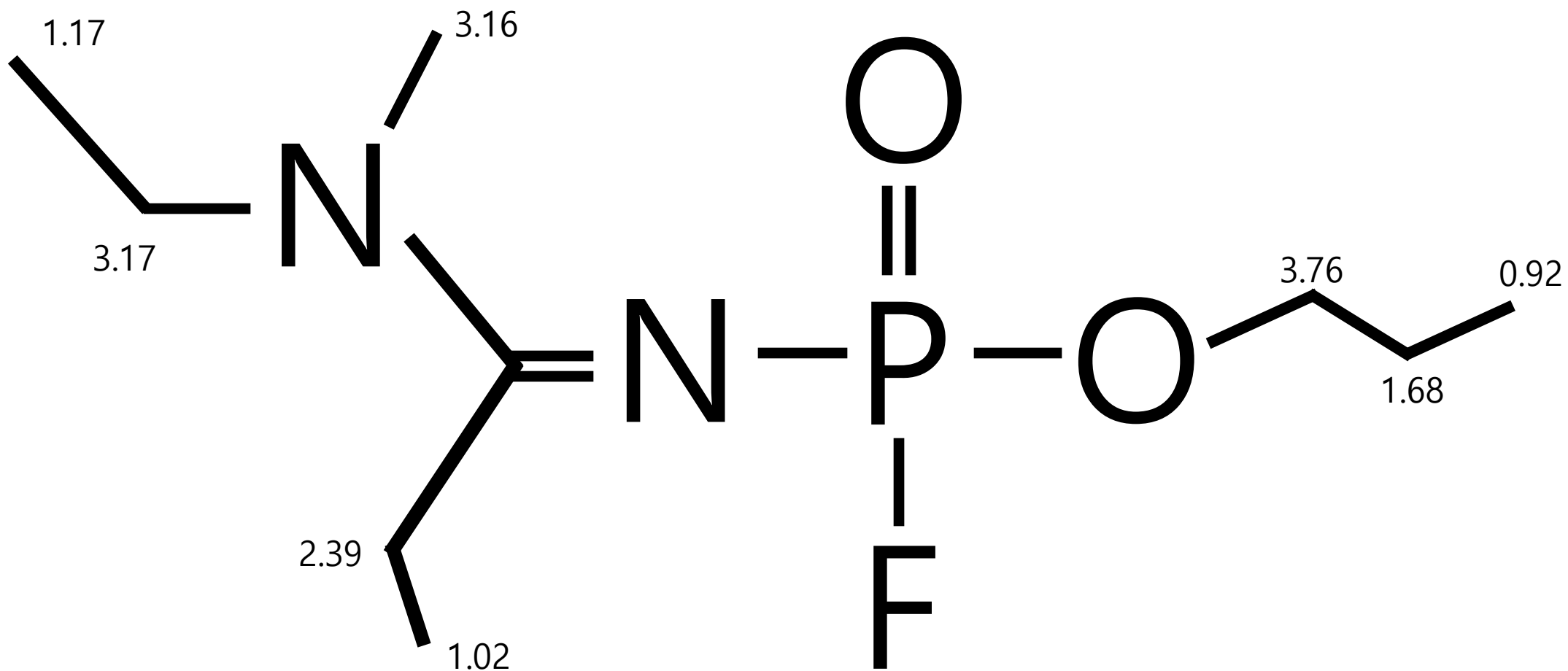


Figure S150. Structure 3221 and its ^1H chemical shift

3222 H

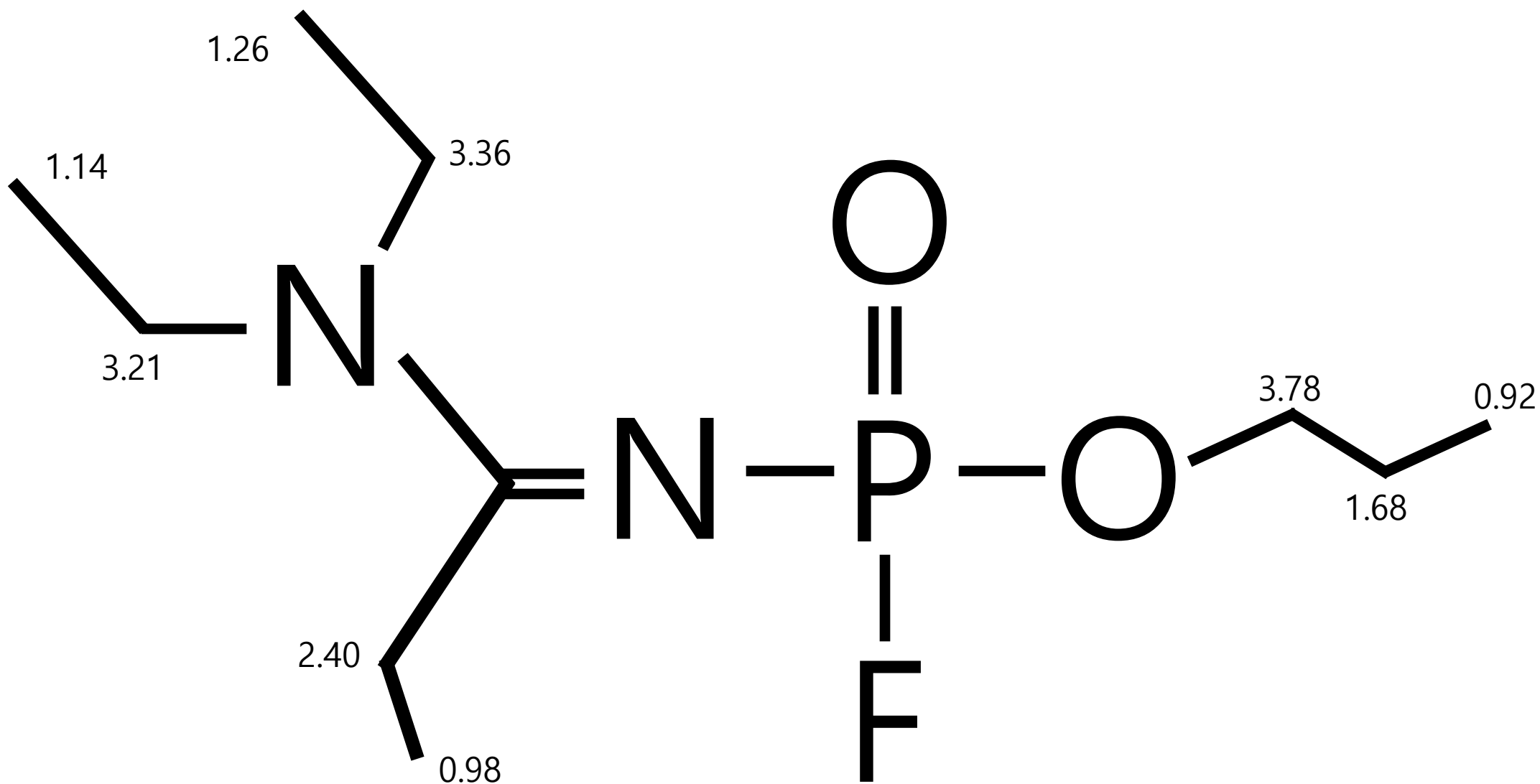


Figure S151. Structure 3222 and its ¹H chemical shift

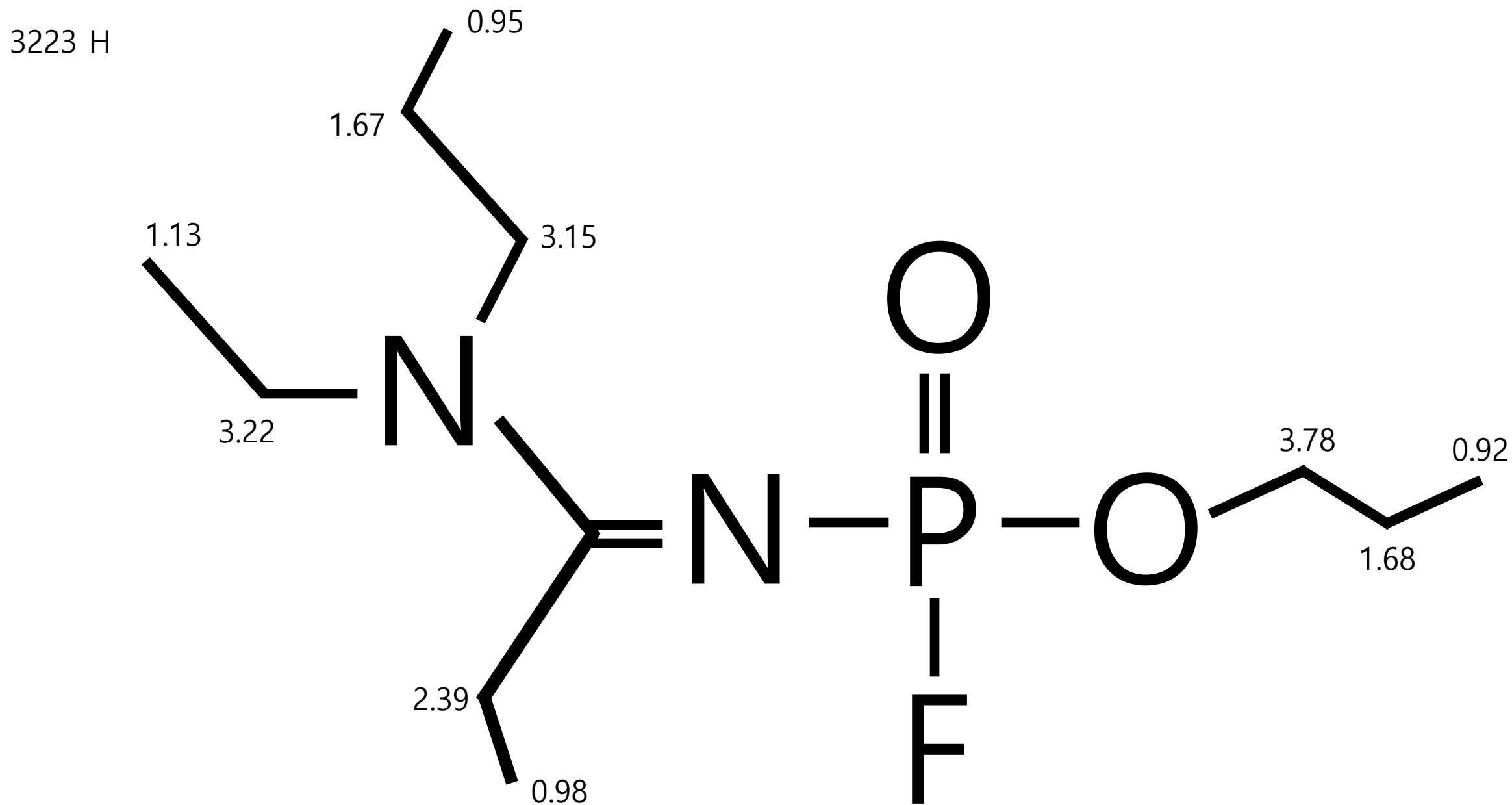


Figure S152. Structure 3223 and its ^1H chemical shift

3231 H

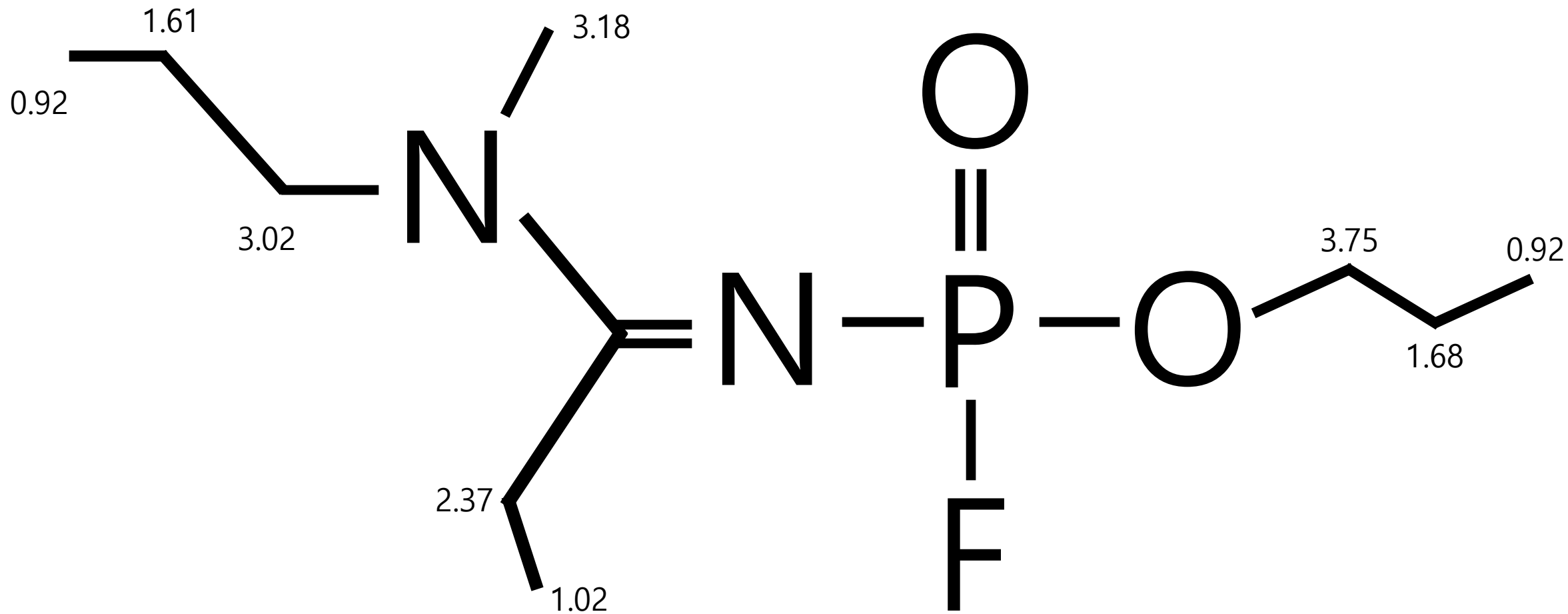


Figure S153. Structure 3231 and its ^1H chemical shift

3232 H

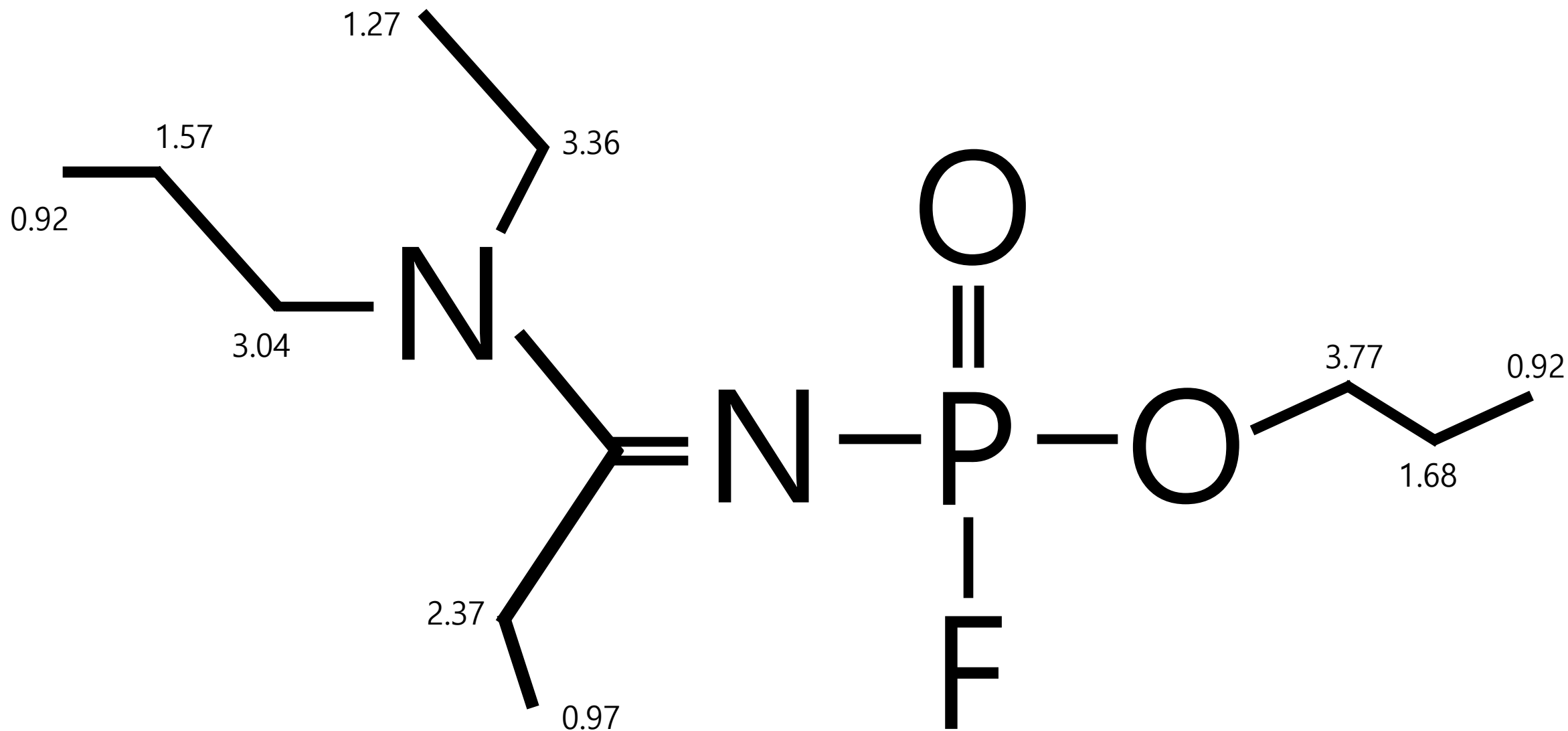


Figure S154. Structure 3232 and its ^1H chemical shift

3311 H

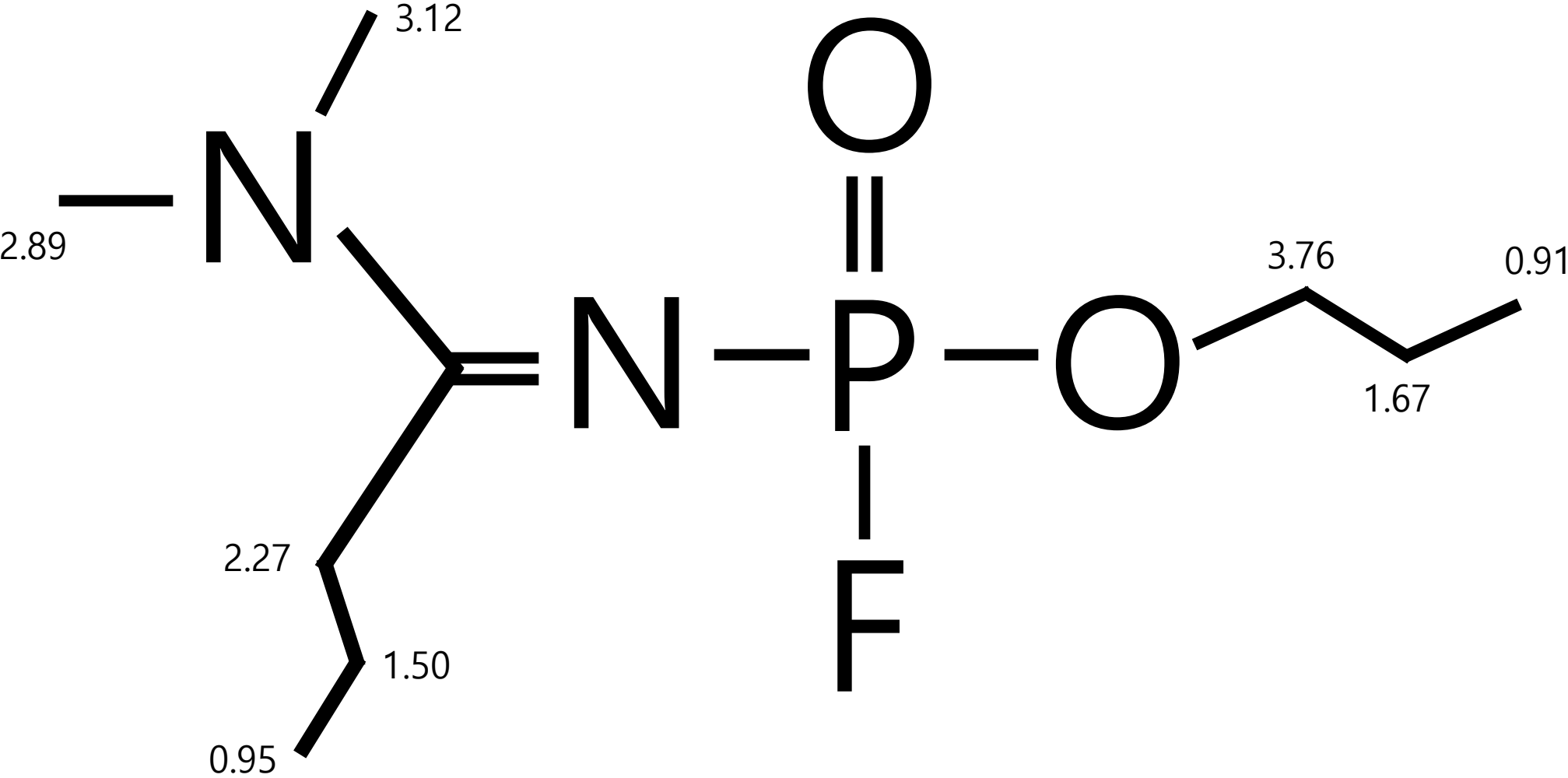


Figure S156. Structure 3311 and its ¹H chemical shift

3312 H

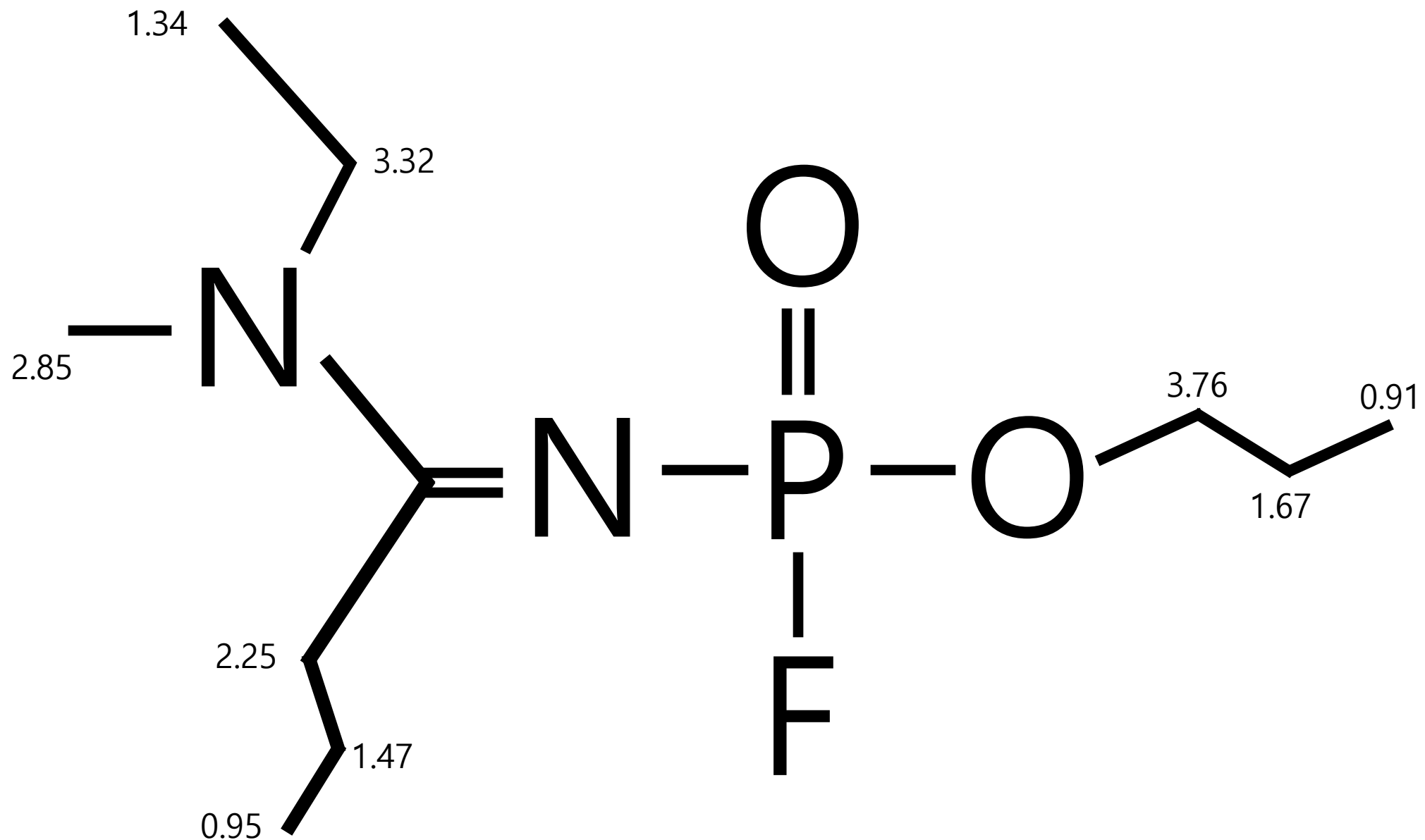


Figure S157. Structure 3312 and its ¹H chemical shift

3313 H

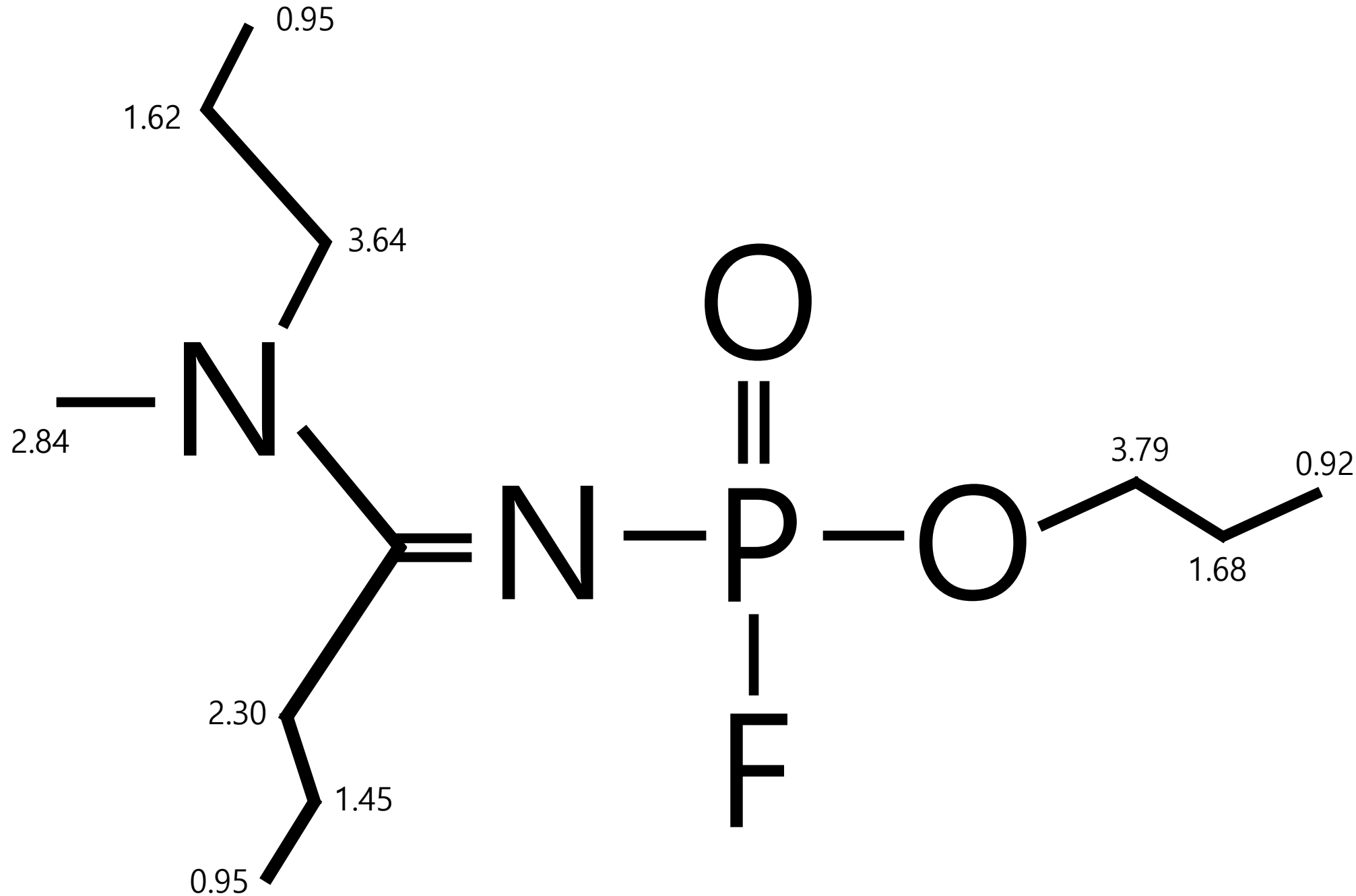


Figure S158. Structure 3313 and its ¹H chemical shift

3321 H

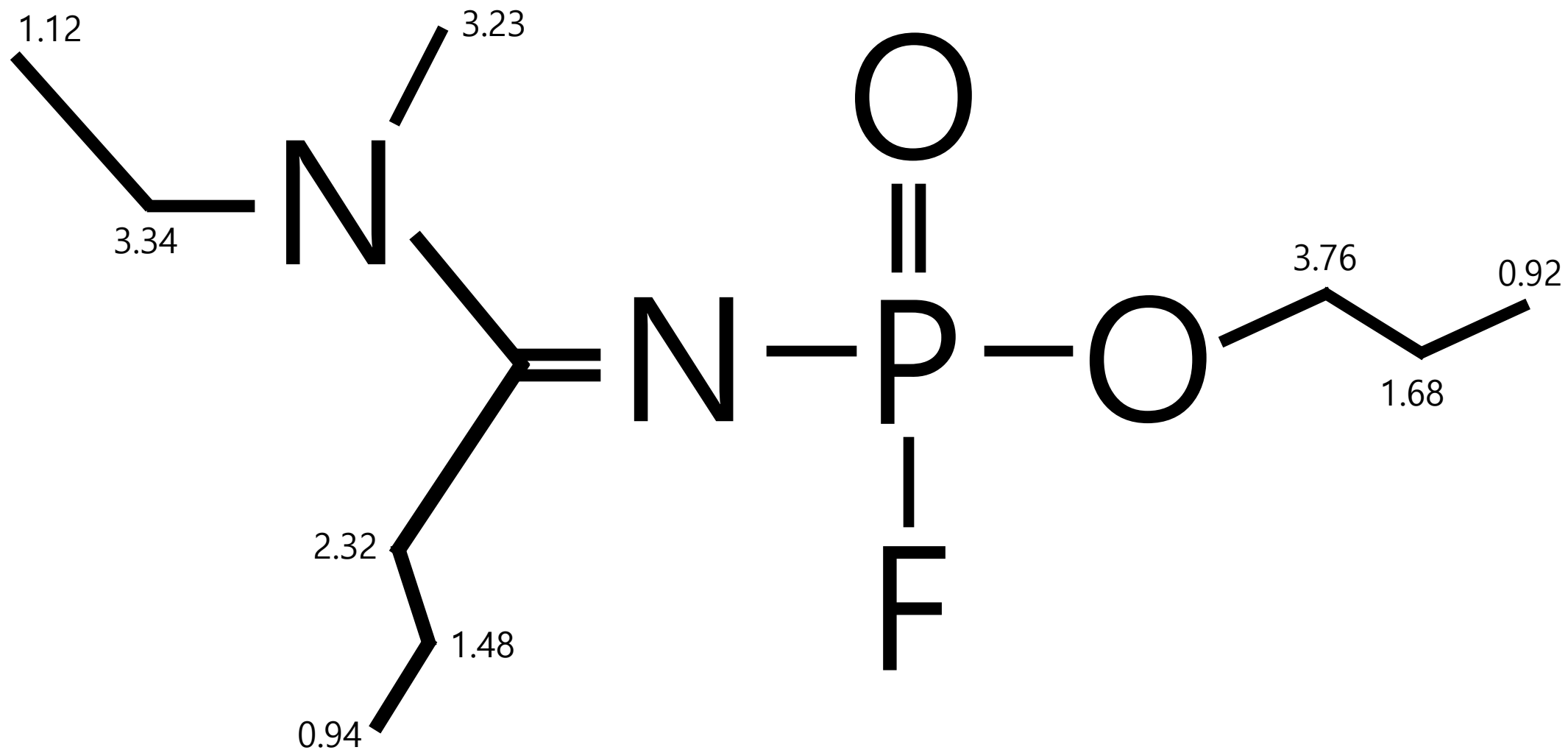


Figure S159. Structure 3321 and its ^1H chemical shift

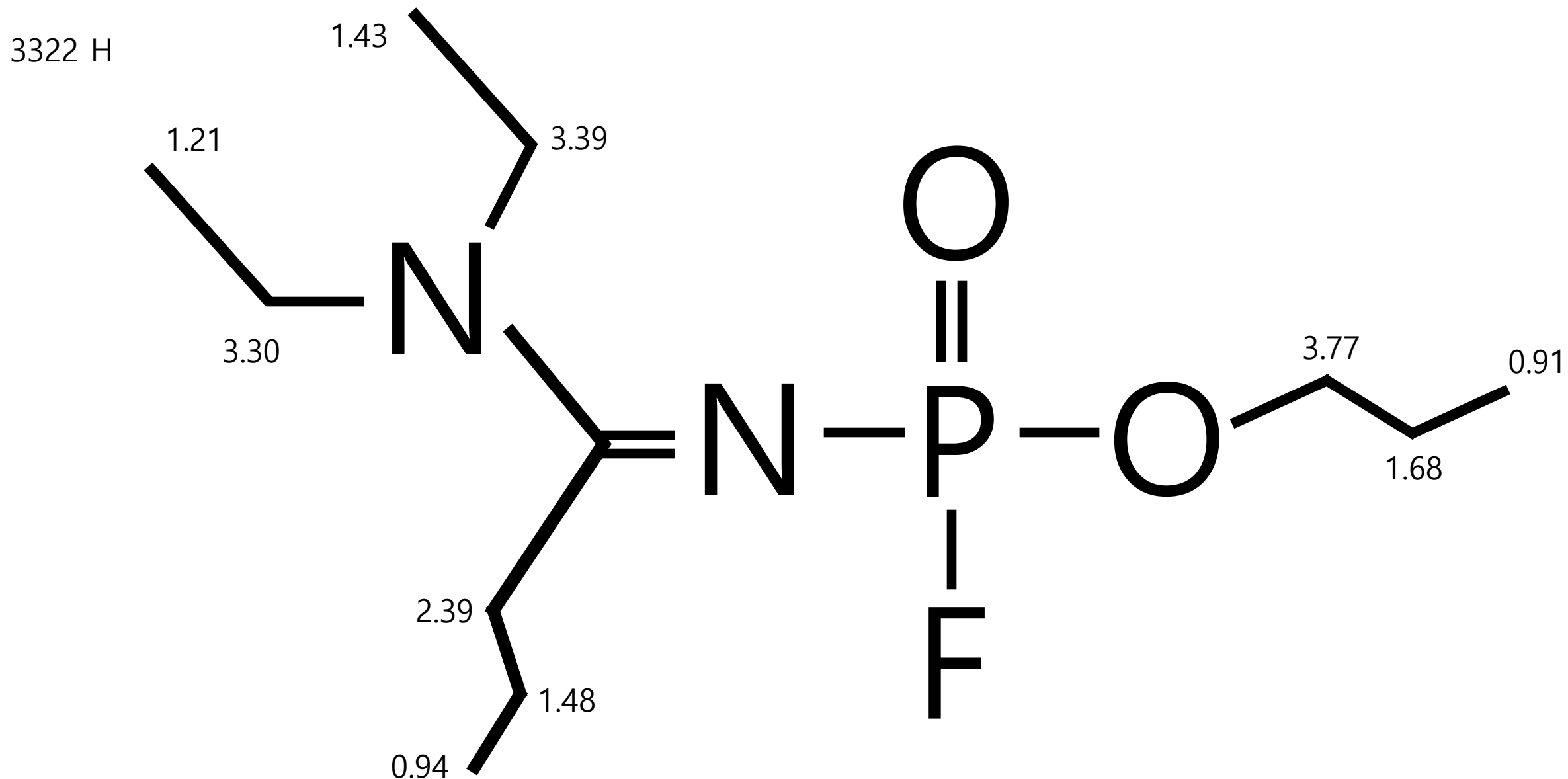


Figure S160. Structure 3322 and its ¹H chemical shift

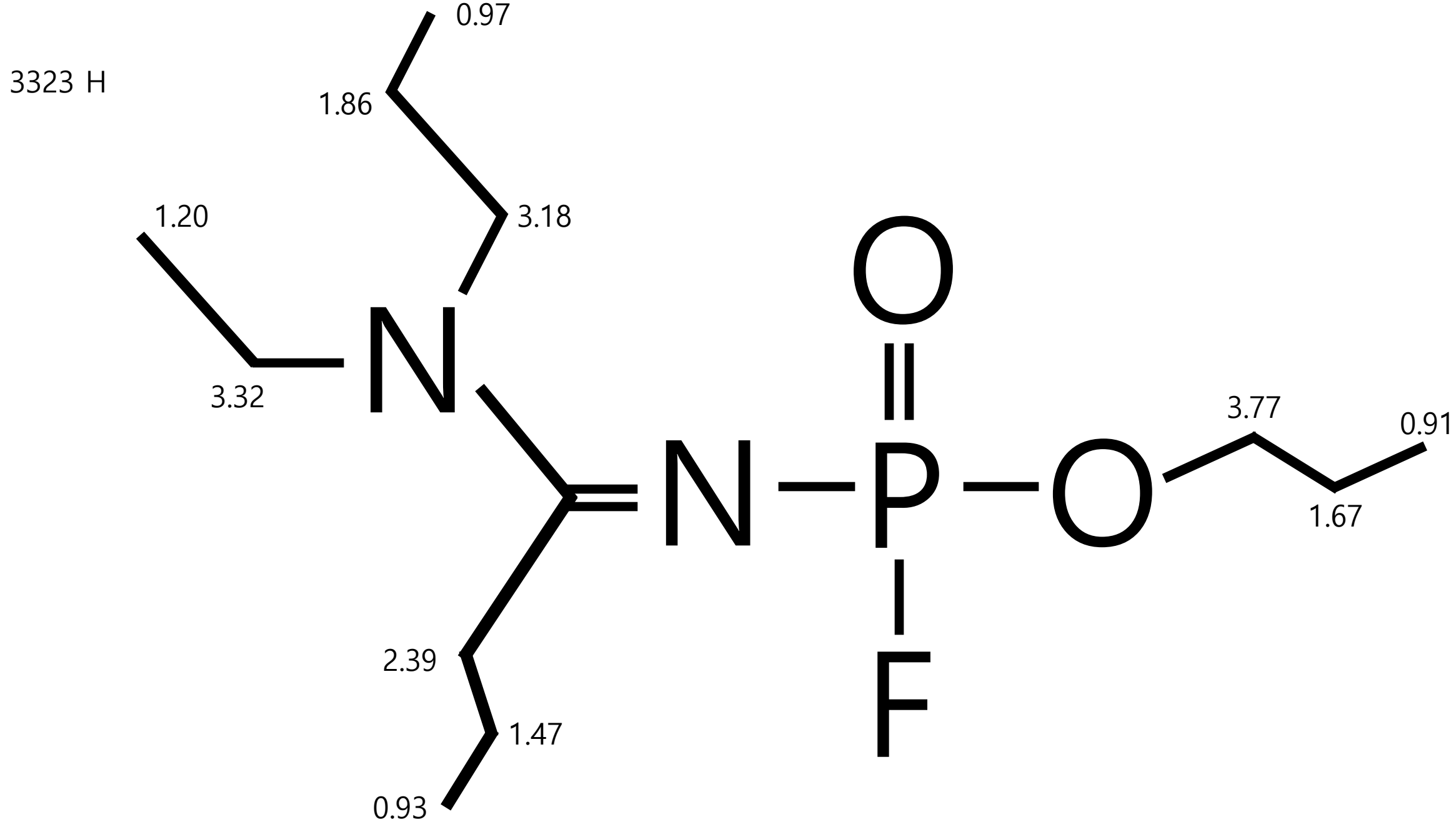


Figure S161. Structure 3323 and its ^1H chemical shift

3331 H

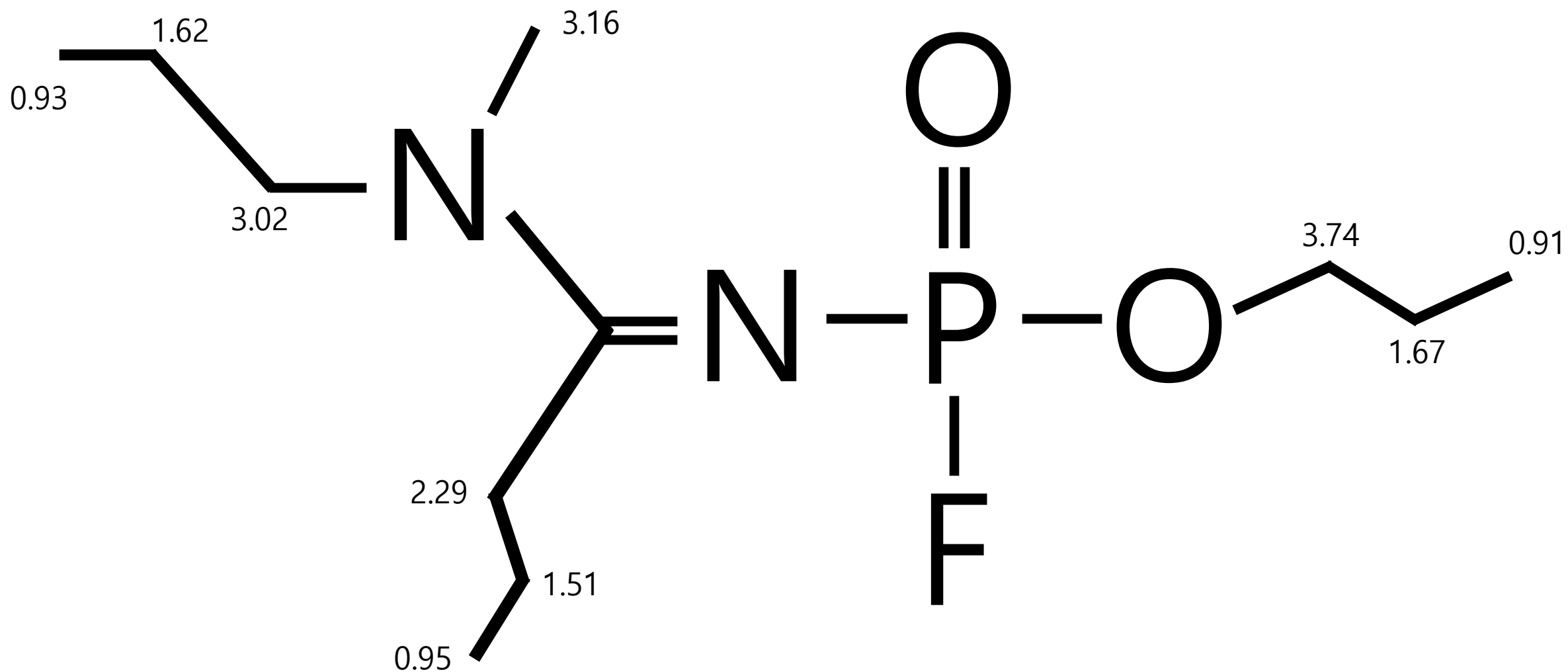


Figure S162. Structure 3331 and its ¹H chemical shift

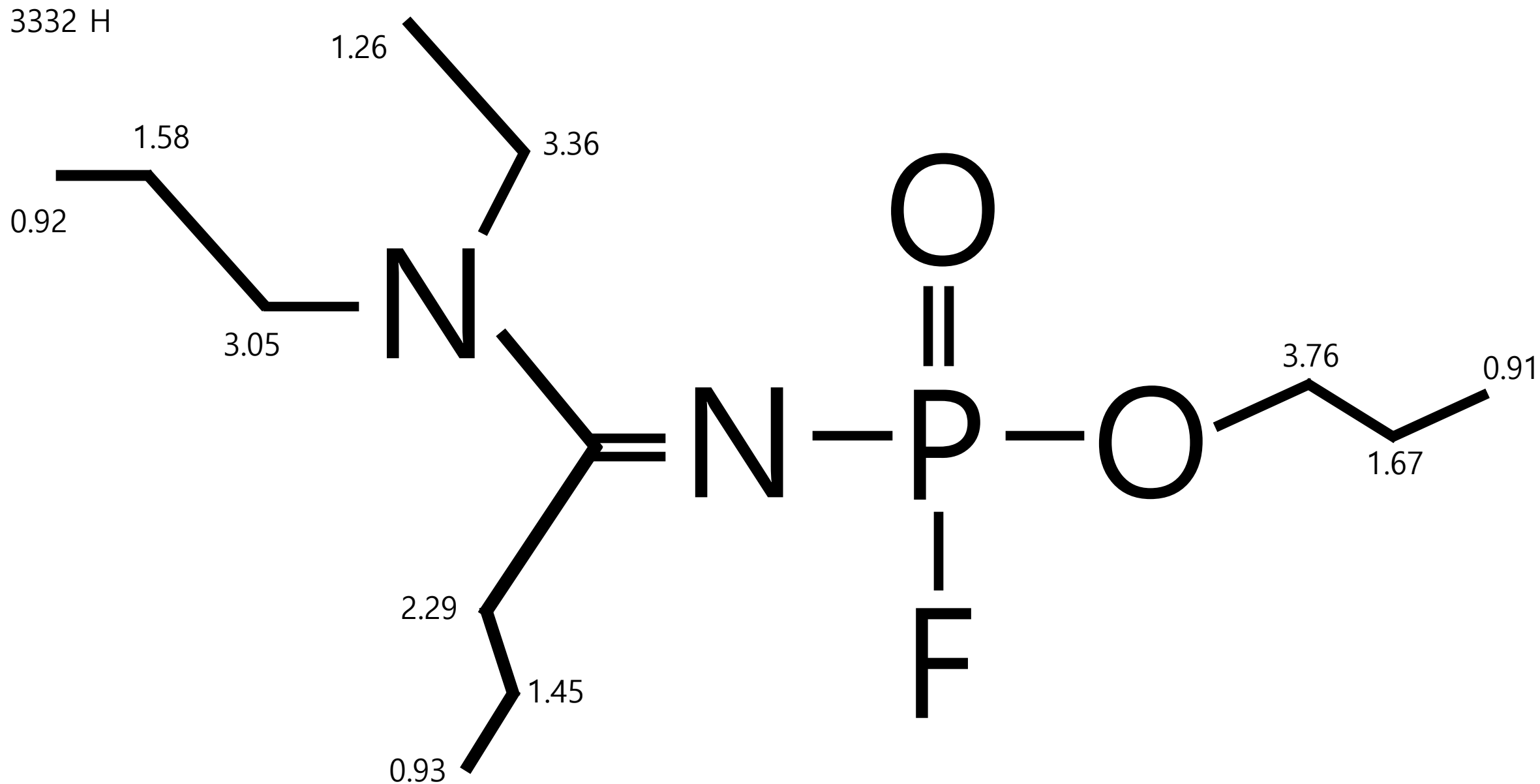


Figure S163. Structure 3332 and its ^1H chemical shift

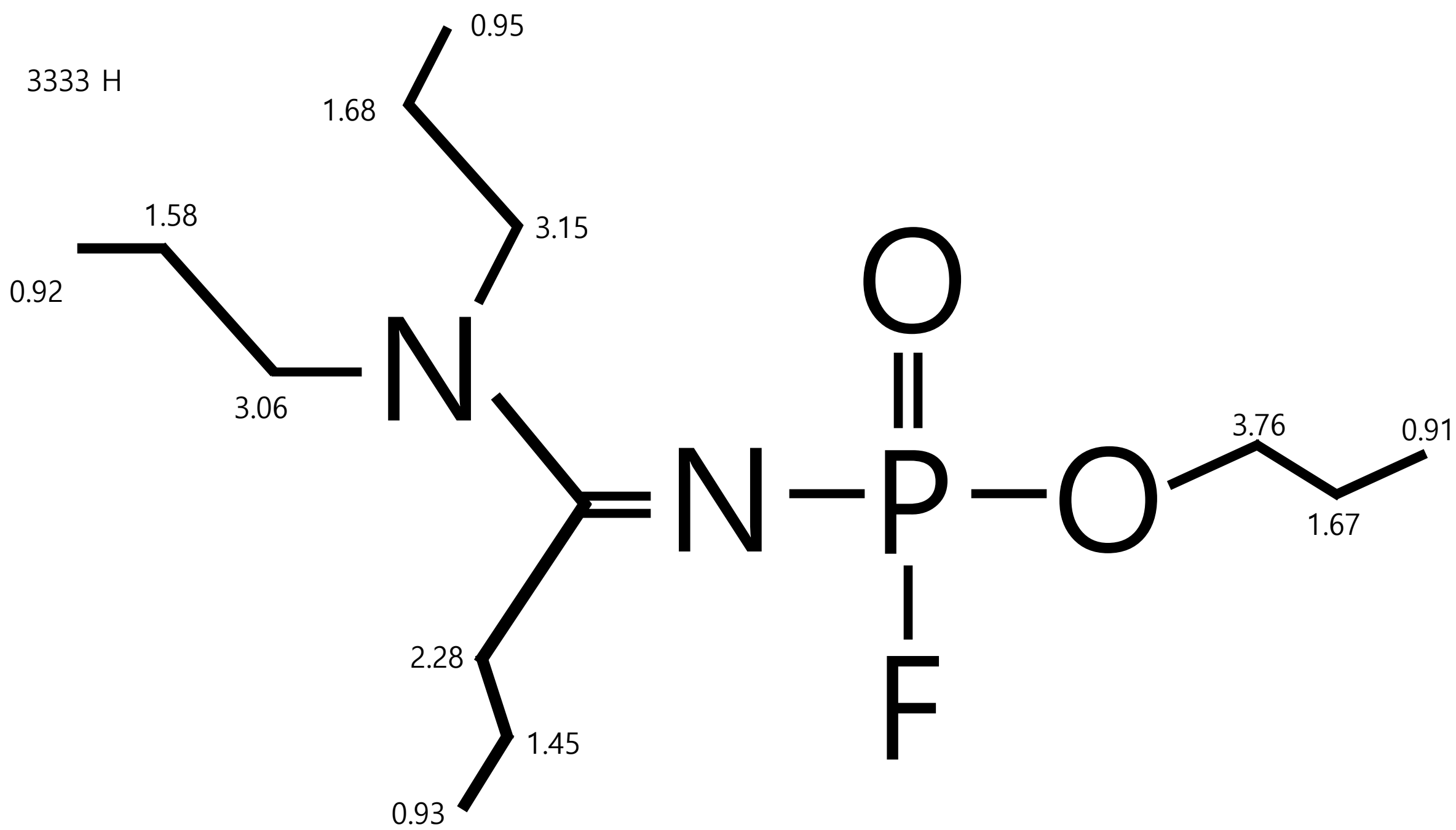


Figure S164. Structure 3333 and its ¹H chemical shift

A242 H

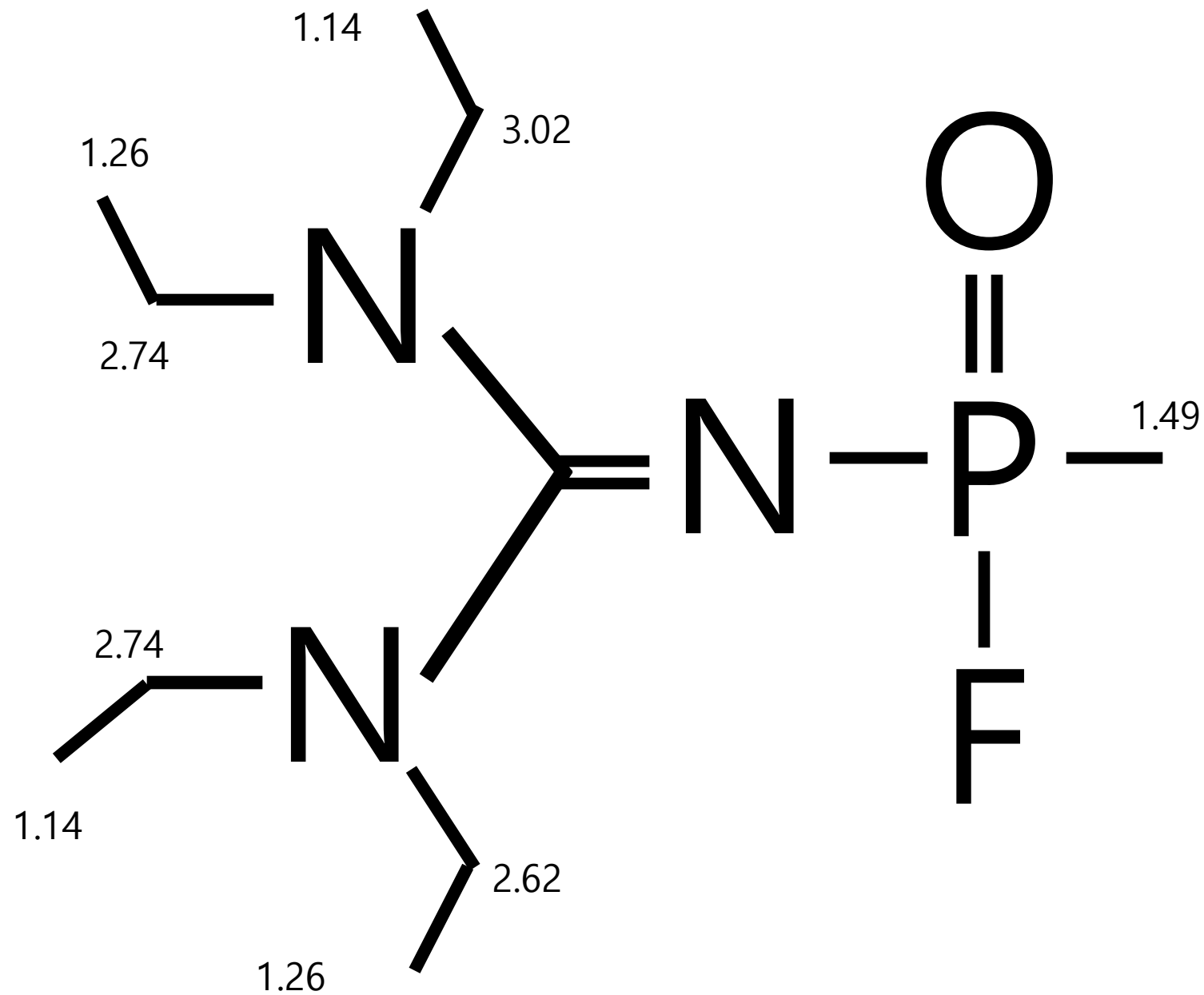


Figure S165. Structure A242 and its ^1H chemical shift

A262 H

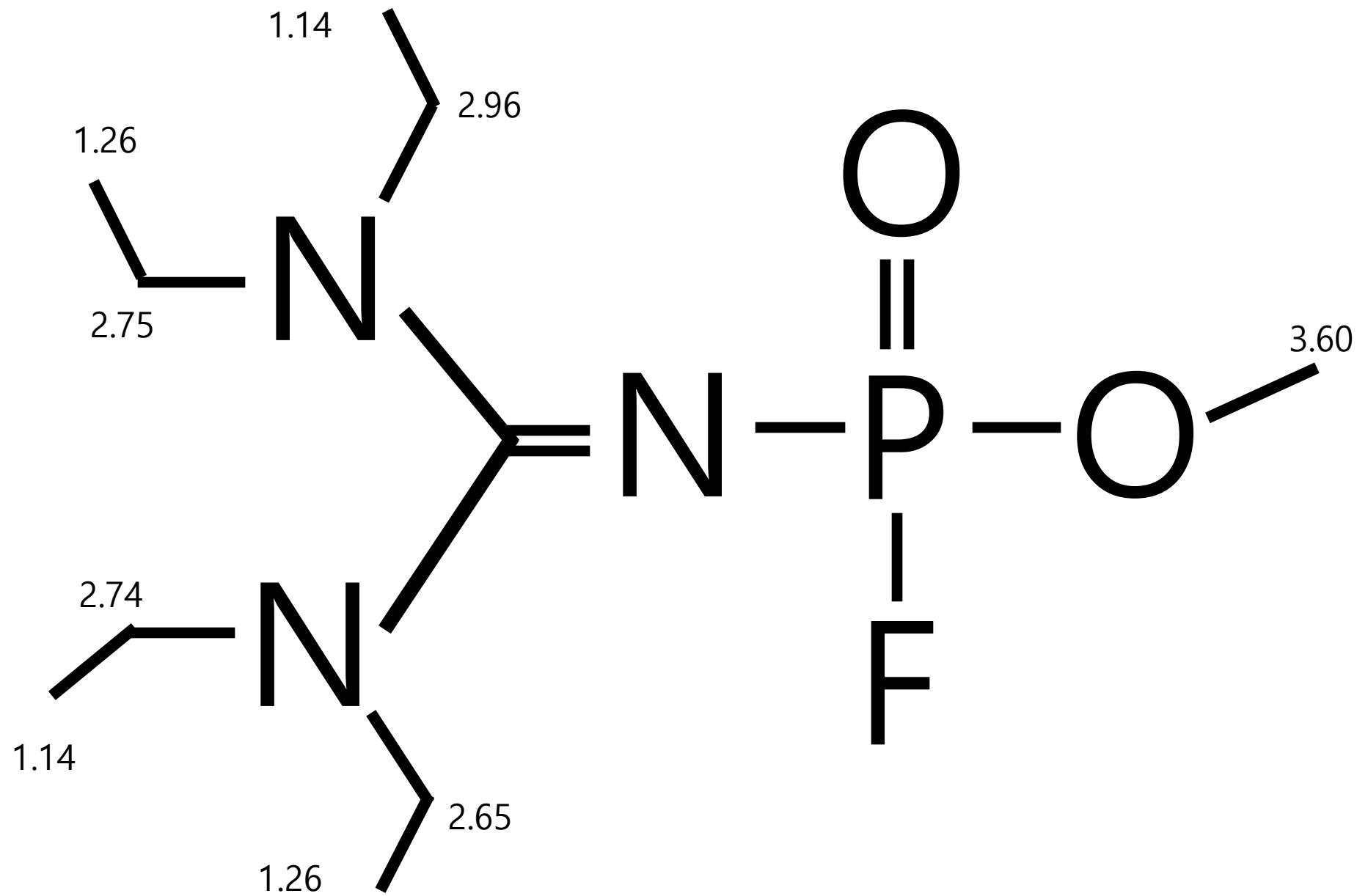


Figure S166. Structure A262 and its ^1H chemical shift