

**S1P**

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      ["H4", 1, -0.0545, ["HCMM"]],
      ["H5", 1, -0.0545, ["HCMM"]],
      ["C6", 6, 0.0531, ["C1R"]],
      ["H7", 1, 0.1190, ["HCMM"]],
      ["C8", 6, 0.2244, ["C1R"]],
      ["H9", 1, 0.0807, ["HCMM"]],
      ["O10", 8, -0.6595, ["OR"]],
      ["H11", 1, 0.4233, ["H1OR"]],
      ["C12", 6, -0.2333, ["CXC"]],
      ["H13", 1, 0.1068, ["HCMM"]],
      ["C14", 6, -0.1794, ["CXC"]],
      ["H15", 1, 0.1065, ["HCMM"]],
      ["C16", 6, 0.1127, ["C1R"]],
      ["H17", 1, 0.0008, ["HCMM"]],
      ["H18", 1, 0.0008, ["HCMM"]],
      ["C19", 6, 0.0868, ["C1R"]],
      ["H20", 1, -0.0141, ["HCMM"]],
      ["H21", 1, -0.0141, ["HCMM"]],
      ["C22", 6, -0.1354, ["C1R"]],
      ["H23", 1, 0.0224, ["HCMM"]],
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["H59", 1, 0.4082, ["HNRP"]],
["O60", 8, -0.7225, ["O2CM"]],
["O61", 8, -0.7225, ["O2CM"]],
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["H63", 1, 0.4112, ["H1OCO"]],
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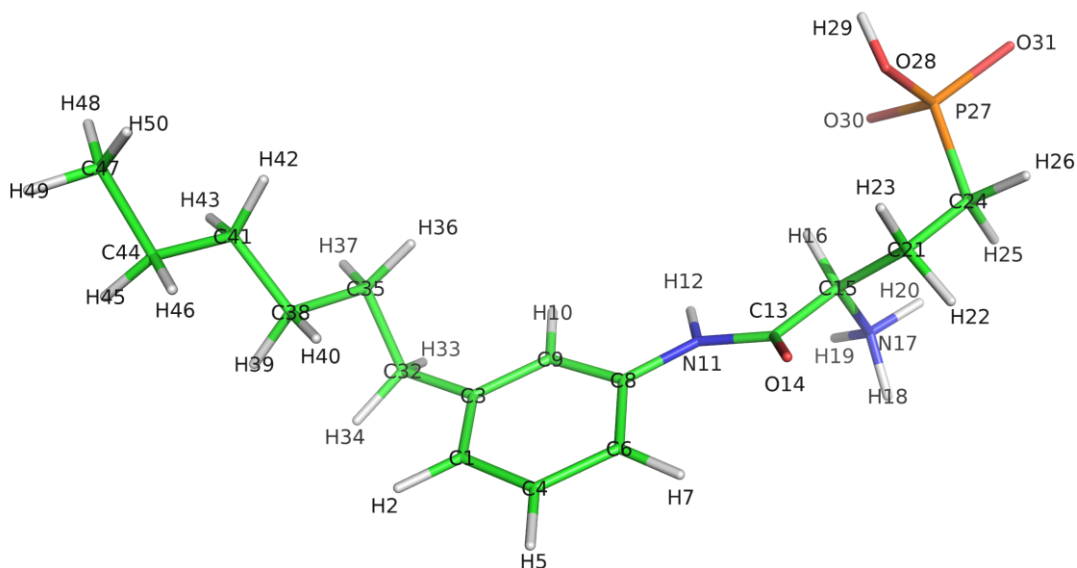
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"Improvers"[
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**ML056**

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      ["H5", 1, 0.1290, ["HCMM"]],
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      ["H12", 1, 0.2785, ["HNCO"]],
      ["C13", 6, 0.8301, ["CXO"]],
      ["O14", 8, -0.5981, ["OXC"]],
      ["C15", 6, 0.2770, ["C1R"]],
      ["H16", 1, -0.0724, ["HCMM"]],
      ["N17", 7, -1.2479, ["NRP"]],
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      ["H22", 1, -0.0862, ["HCMM"]],
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  }
}
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"Proper\_Trig" [

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["C*O", "C1R", "NRP", "HNRP", 0.0, 0.125, 0.0, 0.0, 0.125, 0.0, 0.0, 0.0, ""],
["C*O", "C1R", "C1R", "HCMM", 0.0, -0.099, -0.128, -0.029, 0.0, 0.0, 0.0, 0.0, ""],
["C*O", "C1R", "C1R", "C1R", 0.0, 0.026, 0.033, 0.078, 0.071, 0.0, 0.0, 0.0, ""],
["O*C", "C*O", "C1R", "HCMM", 0.0, -0.220, 0.330, 0.704, 0.154, 0.0, 0.0, 0.0, ""],
["O*C", "C*O", "C1R", "NRP", 0.0, 0.400, 0.0, -0.200, 0.200, 0.0, 0.0, 0.0, ""],

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["O*C", "C*O", "C1R", "C1R", 0.0, 0.645, 0.412, -0.070, 0.163, 0.0, 0.0, 0.0, ""],
["C1R", "C1R", "C1R", "HCMM", 0.0, 0.137, 0.320, 0.315, 0.132, 0.0, 0.0, 0.0, ""],
["C1R", "C1R", "C1R", "P4O", 0.0, 0.150, 0.0, 0.0, 0.150, 0.0, 0.0, 0.0, ""],
["HCMM", "C1R", "NRP", "HNRP", 0.0, 0.130, 0.0, 0.0, 0.130, 0.0, 0.0, 0.0, ""],
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["NRP", "C1R", "C1R", "HCMM", 0.0, 0.220, 0.346, 0.265, 0.139, 0.0, 0.0, 0.0, ""],
["NRP", "C1R", "C1R", "C1R", 0.0, 0.246, -0.324, -0.275, 0.295, 0.0, 0.0, 0.0, ""],
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["C1R", "C1R", "P4O", "OR", 0.0, 0.150, 0.0, 0.0, 0.150, 0.0, 0.0, 0.0, ""],
["C1R", "C1R", "P4O", "O2CM", 0.0, 0.253, 0.0, -0.144, 0.109, 0.0, 0.0, 0.0, ""],
["HCMM", "C1R", "C1R", "P4O", 0.0, 0.147, 0.0, 0.0, 0.147, 0.0, 0.0, 0.0, ""],
["C1R", "P4O", "OR", "H1OCO", 0.0, 0.325, 0.0, 0.0, 0.325, 0.0, 0.0, 0.0, ""],
["HCMM", "C1R", "P4O", "OR", 0.0, 0.247, 0.0, 0.0, 0.247, 0.0, 0.0, 0.0, ""],
["HCMM", "C1R", "P4O", "O2CM", 0.0, 0.042, 0.0, 0.065, 0.107, 0.0, 0.0, 0.0, ""],
["H1OCO", "OR", "P4O", "O2CM", 0.0, -4.467, -2.946, 1.666, 0.145, 0.0, 0.0, 0.0, ""],
["C1R", "C1R", "C1R", "C1R", 0.0, 0.558, 0.051, -0.341, 0.166, 0.0, 0.0, 0.0, ""]
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["CB", "CB", "CB", "NC*O", 0.0, 2.519, ""],
["NC*O", "C*O", "CB", "HNCO", 0.0, -1.439, ""],
["C*O", "C1R", "NC*O", "O*C", 0.0, 9.284, ""],
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["P4O", "OR", "C1R", "O2CM", 0.0, 0.0, ""],
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]
}
}

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