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Supplementary materials

2 **Manuscript title:**

3 Fragmentation of typical sulfonamide drugs via heterolytic bond cleavage and
4 stepwise rearrangement

5

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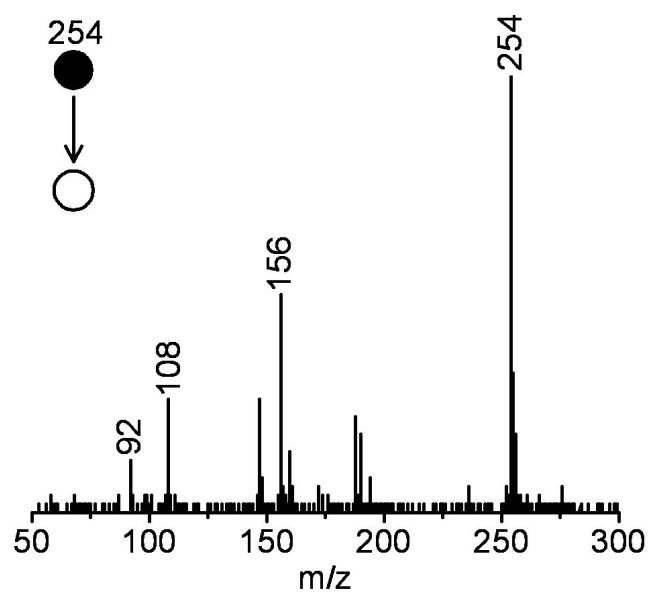
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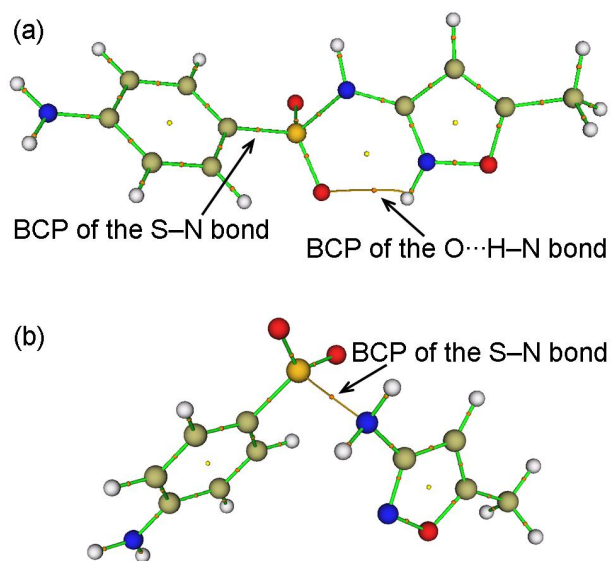
14 E-mail address: hjliu@rcees.ac.cn (H. Liu)

16 Fig. S1 The positive ESI-MS/MS spectrum of sulfamethoxazole (a representative
17 substrate for sulfonamide drugs studied in this work) recorded over a mass scan range
18 of m/z 50–300 with a collision energy of 10 eV (the capillary voltage = 3500 V, and
19 the drying gas = 10 L min^{-1} at 200 °C).



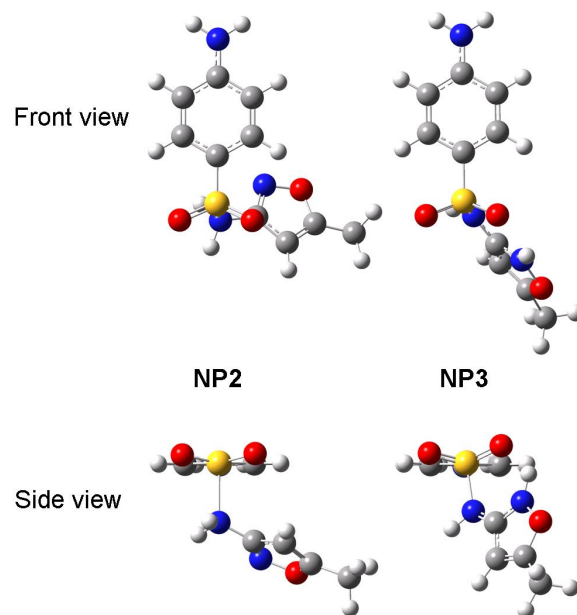
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22 Fig. S2 The topology graphs of (a) **NP3** and (b) **NP2** with the bond critical points
23 (BCP indicated by small orange points), the ring critical points (RCB indicated by
24 small yellow points), and the bond paths (covalent interaction indicated by green lines,
25 closed-shell interaction indicated by brown lines).



26

28 Fig. S3 The front and side views of the molecular structures of **NP2** and **NP3**.



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| | | | | |
|----|-------------|-------------------|-------------|-------------|
| 31 | NP1: | -1175.856091 a.u. | | |
| 32 | S | 0.08771800 | 1.70985400 | 0.34119100 |
| 33 | O | -2.81943700 | -1.68895200 | 0.28367000 |
| 34 | O | 0.53086100 | 2.98239400 | -0.22778500 |
| 35 | O | -0.37157800 | 1.56220800 | 1.71575800 |
| 36 | N | -1.08638200 | 1.16469500 | -0.75185000 |
| 37 | N | -1.64649600 | -0.94564000 | 0.13334500 |
| 38 | N | 4.70839100 | -2.13235200 | -0.26593200 |
| 39 | C | 1.44963000 | 0.53041700 | 0.12579800 |
| 40 | C | 2.51256800 | 0.88383400 | -0.70365000 |
| 41 | C | 1.42844900 | -0.67499200 | 0.83144100 |
| 42 | C | -2.02989700 | 0.17197500 | -0.44584500 |
| 43 | C | 3.55012300 | -1.19231600 | -0.13938200 |
| 44 | C | 3.59039700 | 0.00489900 | -0.84343200 |
| 45 | C | 2.49884400 | -1.55844700 | 0.69614100 |
| 46 | C | -3.42666900 | 0.19658000 | -0.71681400 |
| 47 | C | -3.86474000 | -1.00471600 | -0.23588200 |
| 48 | C | -5.19882400 | -1.65828400 | -0.16332300 |
| 49 | H | -1.38638700 | 1.92102100 | -1.35897600 |
| 50 | H | 2.50373000 | 1.83695700 | -1.22114600 |
| 51 | H | 0.58184600 | -0.92388900 | 1.46033000 |
| 52 | H | 4.42894500 | 0.26809000 | -1.48285100 |
| 53 | H | 2.49623900 | -2.50213400 | 1.23519200 |
| 54 | H | -4.00903900 | 0.98289300 | -1.17227700 |
| 55 | H | -5.95932800 | -1.01034800 | -0.60258100 |
| 56 | H | -5.19378800 | -2.61059500 | -0.70350100 |
| 57 | H | -5.47102800 | -1.86406200 | 0.87687600 |
| 58 | H | 5.33219100 | -1.84733100 | -1.02925700 |
| 59 | H | 4.39607600 | -3.08995600 | -0.46758400 |
| 60 | H | | 5.27041000 | -2.16414500 |
| | | | | 0.59433200 |

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|----|-------------|-------------------|-------------|-------------|-------------|
| 61 | NP2: | -1175.877859 a.u. | | | |
| 62 | S | 0.32167400 | 1.81823300 | 0.40575500 | |
| 63 | O | -2.67719200 | -1.79574800 | -0.64610200 | |
| 64 | O | 0.711173900 | 3.07818100 | -0.21254800 | |
| 65 | O | -0.54464700 | 1.68617800 | 1.56604400 | |
| 66 | N | -1.15792000 | 1.30413000 | -1.10064900 | |
| 67 | N | -1.68085000 | -0.97796100 | -1.14943800 | |
| 68 | N | 4.32772300 | -2.41652800 | -0.10090600 | |
| 69 | C | 1.50259600 | 0.58659600 | 0.27508700 | |
| 70 | C | 2.57551200 | 0.74996000 | -0.63603900 | |
| 71 | C | 1.36351800 | -0.59911800 | 1.03777500 | |
| 72 | C | -2.02683500 | 0.23093000 | -0.76390200 | |
| 73 | C | 3.40361700 | -1.44246200 | 0.01659300 | |
| 74 | C | 3.51375600 | -0.24775000 | -0.75314100 | |
| 75 | C | 2.30744200 | -1.59075400 | 0.91344400 | |
| 76 | C | -3.22390800 | 0.26006600 | -0.00606600 | |
| 77 | C | -3.59447500 | -1.05754300 | 0.02921500 | |
| 78 | C | -4.74290400 | -1.79018300 | 0.62225800 | |
| 79 | H | -1.65134400 | 2.19105100 | -1.22192800 | |
| 80 | H | 2.67292100 | 1.66454400 | -1.21096100 | |
| 81 | H | 0.53483700 | -0.71249900 | 1.72733800 | |
| 82 | H | 4.35334000 | -0.12150000 | -1.42946300 | |
| 83 | H | 2.22009700 | -2.49475400 | 1.50768900 | |
| 84 | H | -3.72535700 | 1.10459200 | 0.44107600 | |
| 85 | H | -5.39406800 | -1.09733300 | 1.15775100 | |
| 86 | H | -5.32547800 | -2.28853600 | -0.15927400 | |
| 87 | H | -4.39351200 | -2.55742200 | 1.32037400 | |
| 88 | H | 5.11510100 | -2.32348700 | -0.72540200 | |
| 89 | H | 4.26952200 | -3.26587300 | 0.44114600 | |
| 90 | H | | -0.63462300 | 1.09466200 | -1.95397200 |

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| 91 | NP3: | -1175.896185 a.u. | | | |
| 92 | S | 0.23666300 | 1.19592600 | 0.23815700 | |
| 93 | O | -3.97710100 | -0.34408900 | 0.90161700 | |
| 94 | O | 0.26983300 | 2.47443300 | -0.45643300 | |
| 95 | O | -0.33969200 | 1.04521600 | 1.58205100 | |
| 96 | N | -0.89077600 | 0.18318400 | -0.72897200 | |
| 97 | N | -2.65770000 | 0.04519200 | 0.85716500 | |
| 98 | N | 5.43525400 | -1.54770800 | -0.22271400 | |
| 99 | C | 1.76309500 | 0.37140500 | 0.09922000 | |
| 100 | C | 2.70822300 | 0.83308100 | -0.83634200 | |
| 101 | C | 2.04872700 | -0.72687600 | 0.93251200 | |
| 102 | C | -2.16018700 | -0.10404000 | -0.37671800 | |
| 103 | C | 4.23694100 | -0.91831900 | -0.11617000 | |
| 104 | C | 3.92849900 | 0.19305900 | -0.94131800 | |
| 105 | C | 3.26943400 | -1.36279700 | 0.82307600 | |
| 106 | C | -3.20775100 | -0.64797600 | -1.17658200 | |
| 107 | C | -4.28811200 | -0.77137700 | -0.34995900 | |
| 108 | C | -5.67505400 | -1.25827800 | -0.54454200 | |
| 109 | H | -0.68085800 | 0.14706900 | -1.72168700 | |
| 110 | H | 2.48926800 | 1.69772600 | -1.45346000 | |
| 111 | H | 1.32655100 | -1.06070900 | 1.66962200 | |
| 112 | H | 4.66443300 | 0.55441800 | -1.65295900 | |
| 113 | H | 3.49830900 | -2.20259100 | 1.47197500 | |
| 114 | H | -3.15296100 | -0.90419100 | -2.22326800 | |
| 115 | H | -5.81778600 | -1.57113400 | -1.57964900 | |
| 116 | H | -5.87842000 | -2.10717900 | 0.11618000 | |
| 117 | H | -6.39373900 | -0.46681000 | -0.30875100 | |
| 118 | H | 6.14995700 | -1.20798800 | -0.84709600 | |
| 119 | H | 5.68712200 | -2.30211000 | 0.39638100 | |
| 120 | H | | -2.25314500 | 0.47223700 | 1.68691100 |

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| 121 | OPI: | -1175.862938 a.u. | | |
| 122 | S | 0.27894900 | 1.77356600 | 0.11568900 |
| 123 | O | -2.74807000 | -1.44131100 | 0.69013800 |
| 124 | O | 0.74002100 | 3.00285400 | -0.50567100 |
| 125 | O | -0.15890900 | 1.92515600 | 1.65919500 |
| 126 | N | -1.17483200 | 1.41441400 | -0.57485300 |
| 127 | N | -1.72712400 | -0.49430600 | 0.71648700 |
| 128 | N | 4.30835500 | -2.48406000 | -0.22932000 |
| 129 | C | 1.42949600 | 0.48597800 | 0.05456800 |
| 130 | C | 2.42079000 | 0.57244800 | -0.95107400 |
| 131 | C | 1.39433500 | -0.60097500 | 0.95683400 |
| 132 | C | -2.01885100 | 0.32860000 | -0.26246400 |
| 133 | C | 3.36761800 | -1.51744800 | -0.13986700 |
| 134 | C | 3.37424700 | -0.41745100 | -1.04076000 |
| 135 | C | 2.35736000 | -1.58185400 | 0.85787300 |
| 136 | C | -3.21426000 | -0.01466100 | -0.94755500 |
| 137 | C | -3.63013000 | -1.14077500 | -0.29133400 |
| 138 | C | -4.79862100 | -2.04612100 | -0.44657700 |
| 139 | H | -1.58628100 | 2.23878400 | -1.00732500 |
| 140 | H | 2.44604400 | 1.41652300 | -1.63143800 |
| 141 | H | 0.60960500 | -0.67844700 | 1.69941700 |
| 142 | H | 4.14508600 | -0.35045700 | -1.80201000 |
| 143 | H | 2.33855400 | -2.41830800 | 1.54938800 |
| 144 | H | -3.68223200 | 0.48014200 | -1.78465800 |
| 145 | H | -5.42601300 | -1.71285800 | -1.27489100 |
| 146 | H | -4.46850200 | -3.07095500 | -0.64376200 |
| 147 | H | -5.39984600 | -2.05756400 | 0.46822300 |
| 148 | H | 5.03309000 | -2.44949900 | -0.92992300 |
| 149 | H | 4.31875800 | -3.26797100 | 0.40514600 |
| 150 | H | | 0.60754000 | 2.14117700 |
| | | | | 2.22744400 |

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| 151 | OP2: | -1175.863820 a.u. | | | |
| 152 | S | 0.22470400 | 1.79855500 | 0.14686600 | |
| 153 | O | -2.59903100 | -1.36530500 | 0.94584700 | |
| 154 | O | 0.59918500 | 2.95266400 | -0.93994700 | |
| 155 | O | 0.11427500 | 2.34847600 | 1.48690000 | |
| 156 | N | -1.15188700 | 1.37618400 | -0.67677700 | |
| 157 | N | -1.63875400 | -0.36356600 | 0.85517600 | |
| 158 | N | 4.10346000 | -2.58482200 | -0.19535600 | |
| 159 | C | 1.35294600 | 0.50447800 | 0.02070300 | |
| 160 | C | 1.66205700 | -0.05913200 | -1.23665100 | |
| 161 | C | 1.95594300 | 0.03309700 | 1.20612300 | |
| 162 | C | -1.95507500 | 0.29391000 | -0.23396600 | |
| 163 | C | 3.20517400 | -1.57704100 | -0.12336100 | |
| 164 | C | 2.57861100 | -1.08458400 | -1.30291100 | |
| 165 | C | 2.87100000 | -0.99421100 | 1.12825200 | |
| 166 | C | -3.11073200 | -0.21184200 | -0.88341600 | |
| 167 | C | -3.47528400 | -1.25910500 | -0.08040300 | |
| 168 | C | -4.58582700 | -2.24610800 | -0.12255400 | |
| 169 | H | -1.64297800 | 2.18684000 | -1.05116700 | |
| 170 | H | 1.19124400 | 0.30695200 | -2.14284400 | |
| 171 | H | 1.69167700 | 0.46446300 | 2.16488800 | |
| 172 | H | 2.82708500 | -1.52166700 | -2.26489000 | |
| 173 | H | 3.33510000 | -1.36700200 | 2.03577200 | |
| 174 | H | -3.58745100 | 0.13167300 | -1.78853000 | |
| 175 | H | -5.21069200 | -2.07191900 | -1.00006300 | |
| 176 | H | -4.19346100 | -3.26707000 | -0.16454200 | |
| 177 | H | -5.20741700 | -2.16270200 | 0.77473700 | |
| 178 | H | 4.34954600 | -3.00943500 | -1.07638800 | |
| 179 | H | 4.55409300 | -2.94649200 | 0.63139200 | |
| 180 | H | | 1.19993000 | 3.60144200 | -0.52281000 |

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|-----|--------------|-------------------|-------------|-------------|------------|
| 181 | TSP1: | -1175.864801 a.u. | | | |
| 182 | S | 0.30390300 | 1.80422600 | 0.06453400 | |
| 183 | O | -3.00926500 | -1.06922200 | 0.92117600 | |
| 184 | O | 0.77881900 | 2.99987300 | -0.60474300 | |
| 185 | O | -0.05443900 | 1.92088400 | 1.61056400 | |
| 186 | N | -1.20868400 | 1.50072200 | -0.60419400 | |
| 187 | N | -2.10331300 | -0.01532000 | 0.95528800 | |
| 188 | N | 4.20221100 | -2.58033900 | -0.11739600 | |
| 189 | C | 1.44262700 | 0.50887200 | 0.06749500 | |
| 190 | C | 2.46533900 | 0.54807500 | -0.90770300 | |
| 191 | C | 1.33302500 | -0.57287200 | 0.97051900 | |
| 192 | C | -2.02807100 | 0.39653800 | -0.29192200 | |
| 193 | C | 3.29832800 | -1.57618500 | -0.06213200 | |
| 194 | C | 3.37973100 | -0.48071000 | -0.96450600 | |
| 195 | C | 2.25340900 | -1.59641700 | 0.90148700 | |
| 196 | C | -2.86752300 | -0.33483100 | -1.17090700 | |
| 197 | C | -3.46883300 | -1.24232800 | -0.33931700 | |
| 198 | C | -4.46874400 | -2.32151100 | -0.54900800 | |
| 199 | H | -1.26574800 | 1.88447400 | -1.54392600 | |
| 200 | H | 2.54992900 | 1.39031200 | -1.58574300 | |
| 201 | H | 0.54724300 | -0.59514600 | 1.71610700 | |
| 202 | H | 4.18027700 | -0.44563700 | -1.69665800 | |
| 203 | H | 2.18656900 | -2.42241100 | 1.60261900 | |
| 204 | H | -3.00972600 | -0.21108900 | -2.23360400 | |
| 205 | H | -5.37575600 | -2.12086200 | 0.03040300 | |
| 206 | H | -4.73473100 | -2.38876600 | -1.60512900 | |
| 207 | H | -4.06925000 | -3.28653100 | -0.22179800 | |
| 208 | H | 4.96659300 | -2.56350500 | -0.77519400 | |
| 209 | H | 4.17429800 | -3.34870300 | 0.53530600 | |
| 210 | H | | -1.00029200 | 2.12073700 | 1.76918400 |

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| 211 | TSP2: | -1175.810474 a.u. | | |
| 212 | S | 0.27733500 | 1.80151300 | -0.07849600 |
| 213 | O | -2.63455700 | -1.19981100 | 1.11533100 |
| 214 | O | 0.63064700 | 3.09561800 | -0.85130200 |
| 215 | O | 0.28492100 | 2.53743600 | 1.27486500 |
| 216 | N | -1.14287100 | 1.34124300 | -0.76435000 |
| 217 | N | -1.69046600 | -0.19730600 | 0.94536200 |
| 218 | N | 4.03197100 | -2.68215600 | -0.08468600 |
| 219 | C | 1.32057600 | 0.44794000 | -0.07064700 |
| 220 | C | 1.37636600 | -0.41682800 | -1.18902500 |
| 221 | C | 2.17726600 | 0.26762100 | 1.04056100 |
| 222 | C | -1.95034100 | 0.29582300 | -0.24137500 |
| 223 | C | 3.14922000 | -1.66148700 | -0.07972000 |
| 224 | C | 2.27863700 | -1.45480400 | -1.18786600 |
| 225 | C | 3.07206100 | -0.77770200 | 1.03164600 |
| 226 | C | -3.05309700 | -0.32261900 | -0.88312100 |
| 227 | C | -3.45030200 | -1.25795900 | 0.03552500 |
| 228 | C | -4.54211700 | -2.26550300 | 0.07090900 |
| 229 | H | -1.61517700 | 2.12612600 | -1.21244100 |
| 230 | H | 0.72308900 | -0.26894900 | -2.04185900 |
| 231 | H | 2.11440500 | 0.93129400 | 1.89495400 |
| 232 | H | 2.33093800 | -2.12178900 | -2.04251300 |
| 233 | H | 3.72255000 | -0.93194700 | 1.88659400 |
| 234 | H | -3.48018900 | -0.11572400 | -1.85228900 |
| 235 | H | -5.10147800 | -2.24820600 | -0.86591900 |
| 236 | H | -4.13548200 | -3.27021900 | 0.22267300 |
| 237 | H | -5.23063700 | -2.05482500 | 0.89567800 |
| 238 | H | 4.10403000 | -3.31326200 | -0.86845800 |
| 239 | H | 4.65807800 | -2.83933400 | 0.69077300 |
| 240 | H | | 0.56438400 | 3.45730900 |
| | | | | 0.40199600 |

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|-----|---------------------|-------------|-------------|-------------|
| 241 | A: -835.201132 a.u. | | | |
| 242 | S | 2.04480300 | -0.00000200 | -0.00000100 |
| 243 | O | 2.69641700 | -1.29691700 | 0.00001600 |
| 244 | O | 2.69639200 | 1.29692600 | -0.00001200 |
| 245 | N | -3.76147400 | -0.00000100 | -0.00000800 |
| 246 | C | 0.36112300 | 0.00000100 | 0.00000700 |
| 247 | C | -0.33674600 | -1.24654100 | -0.00001100 |
| 248 | C | -0.33674400 | 1.24654400 | 0.00000200 |
| 249 | C | -2.42579000 | -0.00000300 | 0.00000300 |
| 250 | C | -1.70344300 | -1.23807200 | -0.00000400 |
| 251 | C | -1.70344100 | 1.23806700 | 0.00000800 |
| 252 | H | 0.21172700 | -2.18212000 | -0.00002400 |
| 253 | H | 0.21173000 | 2.18212100 | -0.00000300 |
| 254 | H | -2.24927400 | -2.17617300 | -0.00001100 |
| 255 | H | -2.24927300 | 2.17616800 | 0.00001000 |
| 256 | H | -4.29183300 | -0.86143200 | 0.00001900 |
| 257 | H | | -4.29183100 | 0.86143200 |
| | | | | 0.00002900 |

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| 258 | API(T): | -835.342544 a.u. | | | |
| 259 | S | 2.11608600 | -0.07480100 | -0.31673000 | |
| 260 | O | 2.60795900 | -1.33448300 | 0.28667900 | |
| 261 | O | 2.48672600 | 1.29045800 | 0.43229200 | |
| 262 | N | -3.79509300 | 0.01616600 | 0.13834300 | |
| 263 | C | 0.27853300 | -0.01123100 | -0.15336300 | |
| 264 | C | -0.37739500 | -1.25334700 | -0.06001700 | |
| 265 | C | -0.36609100 | 1.23880500 | -0.16845800 | |
| 266 | C | -2.46592000 | 0.00614100 | 0.03994000 | |
| 267 | C | -1.75560600 | -1.24645200 | 0.03987600 | |
| 268 | C | -1.74558300 | 1.24923300 | -0.06648700 | |
| 269 | H | 0.16588400 | -2.19335300 | -0.05423200 | |
| 270 | H | 0.18123200 | 2.17191900 | -0.24888700 | |
| 271 | H | -2.29969100 | -2.18390600 | 0.11839800 | |
| 272 | H | -2.28353100 | 2.19345300 | -0.07746400 | |
| 273 | H | -4.33796000 | -0.84437500 | 0.21708600 | |
| 274 | H | -4.33125000 | 0.88437700 | 0.14239700 | |
| 275 | H | | 3.44849200 | 1.50885700 | 0.46126800 |

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| 276 | TSD: | -1175.807820 a.u. | | | |
| 277 | S | 0.15863400 | -0.12392600 | 0.46031900 | |
| 278 | O | -4.23693300 | -0.90441600 | -0.74779100 | |
| 279 | O | 0.80969800 | -0.23134700 | 1.81975100 | |
| 280 | O | -0.34832100 | -1.36820300 | -0.17385100 | |
| 281 | N | -1.62544000 | 0.61003500 | 1.04607400 | |
| 282 | N | -3.00761800 | -0.88262700 | -0.12430000 | |
| 283 | N | 6.11533700 | 0.26092000 | -0.90703700 | |
| 284 | C | 2.14822400 | 0.04765600 | 0.09618400 | |
| 285 | C | 2.68923500 | 1.31536600 | -0.09007700 | |
| 286 | C | 2.89449600 | -1.12638300 | 0.19444200 | |
| 287 | C | -2.77756200 | 0.32837000 | 0.43259000 | |
| 288 | C | 4.81436400 | 0.19120800 | -0.52766900 | |
| 289 | C | 4.02379600 | 1.37317600 | -0.45896500 | |
| 290 | C | 4.22235700 | -1.05421100 | -0.19687100 | |
| 291 | C | -3.98224600 | 1.08121900 | 0.25368400 | |
| 292 | C | -4.82765100 | 0.28761800 | -0.46563900 | |
| 293 | C | -6.20965100 | 0.46127300 | -0.97638400 | |
| 294 | H | -1.56928500 | 1.54703800 | 1.43713400 | |
| 295 | H | 2.09073100 | 2.21684100 | -0.03526100 | |
| 296 | H | 2.44541100 | -2.06665600 | 0.48730700 | |
| 297 | H | 4.45919200 | 2.33038300 | -0.73014800 | |
| 298 | H | 4.81239800 | -1.96477200 | -0.24007500 | |
| 299 | H | -4.17516700 | 2.07950800 | 0.61496900 | |
| 300 | H | -6.56729400 | 1.46614600 | -0.74793200 | |
| 301 | H | -6.24152600 | 0.30769200 | -2.05958200 | |
| 302 | H | -6.88165400 | -0.26817000 | -0.51222200 | |
| 303 | H | 6.56315800 | 1.14638900 | -1.08735000 | |
| 304 | H | 6.70109000 | -0.56018500 | -0.91861600 | |
| 305 | H | | -2.31887800 | -1.56970700 | -0.42913800 |

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| 306 | TSD(T): | -1175.800778 a.u. | | | |
| 307 | S | -0.10765600 | 0.65526700 | -0.07662100 | |
| 308 | O | -4.25343800 | -1.27567000 | 0.36496400 | |
| 309 | O | 0.47276500 | 1.37518500 | 1.09364100 | |
| 310 | O | -0.41675500 | -0.79958300 | 0.15612900 | |
| 311 | N | -1.96360400 | 1.35308400 | -0.03621000 | |
| 312 | N | -3.03196100 | -0.64522300 | 0.57559500 | |
| 313 | N | 6.50231900 | -0.76933400 | -0.01996800 | |
| 314 | C | 2.55821900 | 0.20788800 | -0.25811100 | |
| 315 | C | 3.47879000 | 1.26184400 | -0.25944000 | |
| 316 | C | 2.87427500 | -1.15225600 | -0.16943100 | |
| 317 | C | -3.04563400 | 0.58846500 | 0.00583000 | |
| 318 | C | 5.20203400 | -0.44638600 | -0.09890000 | |
| 319 | C | 4.81583100 | 0.93428800 | -0.18354600 | |
| 320 | C | 4.21026500 | -1.48586800 | -0.09215300 | |
| 321 | C | -4.39314700 | 0.81447400 | -0.43108200 | |
| 322 | C | -5.06860000 | -0.34453600 | -0.19497700 | |
| 323 | C | -6.47465900 | -0.76746800 | -0.41452600 | |
| 324 | H | -2.08097300 | 2.27246200 | -0.44917500 | |
| 325 | H | 3.15004800 | 2.29496200 | -0.30041000 | |
| 326 | H | 2.09098100 | -1.90374000 | -0.15384100 | |
| 327 | H | 5.58224200 | 1.70447000 | -0.17549900 | |
| 328 | H | 4.52566400 | -2.52330000 | -0.02001600 | |
| 329 | H | -4.78160200 | 1.71704200 | -0.87660000 | |
| 330 | H | -7.02297700 | 0.01551100 | -0.94024200 | |
| 331 | H | -6.51154100 | -1.68820900 | -1.00493500 | |
| 332 | H | -6.96741600 | -0.96208700 | 0.54387800 | |
| 333 | H | 7.22484600 | -0.05993700 | -0.01661400 | |
| 334 | H | 6.80539000 | -1.73317600 | 0.04658600 | |
| 335 | H | | -2.20425700 | -1.25008800 | 0.59702400 |

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| 336 | ReNP3: -1175.900944 a.u. | | | |
| 337 | S | 0.05602800 | 0.19226100 | 1.17104200 |
| 338 | O | 4.09523500 | -1.14531500 | -0.37517800 |
| 339 | O | -0.65834400 | 0.41716900 | -0.32144100 |
| 340 | O | 0.51376400 | -1.21221600 | 1.29099500 |
| 341 | N | 1.54567300 | 1.04391700 | 0.69681400 |
| 342 | N | 2.82046200 | -0.85909600 | 0.05911400 |
| 343 | N | -6.20742500 | -0.29475400 | -0.45077300 |
| 344 | C | -2.07252400 | 0.22261800 | -0.29439900 |
| 345 | C | -2.90276500 | 1.34241000 | -0.28179200 |
| 346 | C | -2.59798200 | -1.06832400 | -0.34537500 |
| 347 | C | 2.66778800 | 0.46119300 | 0.22539500 |
| 348 | C | -4.84558900 | -0.12566900 | -0.36975900 |
| 349 | C | -4.28118500 | 1.16883600 | -0.32101300 |
| 350 | C | -3.97764600 | -1.23934300 | -0.37998700 |
| 351 | C | 3.88843500 | 1.07328300 | -0.17754400 |
| 352 | C | 4.72169500 | 0.04894200 | -0.53102800 |
| 353 | C | 6.11485800 | -0.00770900 | -1.03480000 |
| 354 | H | 1.50045000 | 2.05751000 | 0.68109300 |
| 355 | H | -2.47516700 | 2.33972500 | -0.25794600 |
| 356 | H | -1.93767700 | -1.92873300 | -0.37083000 |
| 357 | H | -4.93083000 | 2.03906400 | -0.32279600 |
| 358 | H | -4.39064400 | -2.24253100 | -0.42765200 |
| 359 | H | 4.10755000 | 2.12969000 | -0.19323000 |
| 360 | H | 6.53288200 | 0.99829900 | -1.08800500 |
| 361 | H | 6.73587200 | -0.61877500 | -0.37207500 |
| 362 | H | 6.14098300 | -0.45790500 | -2.03259700 |
| 363 | H | -6.81744300 | 0.48350200 | -0.25458900 |
| 364 | H | -6.60449700 | -1.20844900 | -0.29638400 |
| 365 | H | | 2.23533200 | -1.63257000 |
| | | | | 0.36906100 |

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| 366 | C ₄ H ₆ O ₂ N ₂ S: -814.019104 a.u. | | | | |
| 367 | S | -2.53678800 | 0.25796100 | -0.41084000 | |
| 368 | O | 1.61616900 | -1.09517900 | -0.26363400 | |
| 369 | O | -2.75803400 | -0.97202400 | 0.73178900 | |
| 370 | N | -1.12883500 | 1.05842000 | 0.06787800 | |
| 371 | N | 0.23224500 | -0.84702300 | -0.25728200 | |
| 372 | C | 0.12005200 | 0.43641400 | 0.01797200 | |
| 373 | C | 1.38951100 | 1.05589800 | 0.23283200 | |
| 374 | C | 2.28061200 | 0.04266900 | 0.03695300 | |
| 375 | C | 3.76686300 | -0.04000300 | 0.07373000 | |
| 376 | H | -1.22955300 | 1.76038600 | 0.79318400 | |
| 377 | H | 1.59706600 | 2.09002000 | 0.46221300 | |
| 378 | H | 4.19182600 | 0.93171100 | 0.33346900 | |
| 379 | H | 4.09613800 | -0.77627400 | 0.81445300 | |
| 380 | H | 4.16270700 | -0.34664200 | -0.90021000 | |
| 381 | H | | -2.16075200 | -1.69859900 | 0.48199500 |

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| 382 | TS1: | -835.146075 a.u. | | | |
| 383 | S | -2.21577200 | 0.31350900 | -0.00201600 | |
| 384 | O | -2.06232400 | -0.41726500 | 1.30899200 | |
| 385 | O | -2.94267800 | -0.28821300 | -1.12533200 | |
| 386 | N | 3.74174400 | -0.16329400 | -0.11172900 | |
| 387 | C | -0.33625800 | 0.17309500 | -0.07194200 | |
| 388 | C | 0.22879800 | -1.12762800 | 0.01155600 | |
| 389 | C | 0.42813600 | 1.35055500 | 0.07345500 | |
| 390 | C | 2.41202100 | -0.06521700 | -0.04931700 | |
| 391 | C | 1.59392700 | -1.24028700 | -0.05764200 | |
| 392 | C | 1.79517100 | 1.23519600 | 0.02133000 | |
| 393 | H | -0.40491400 | -2.00641700 | 0.03055600 | |
| 394 | H | -0.04439800 | 2.32522400 | 0.12766000 | |
| 395 | H | 2.05774700 | -2.21970700 | -0.12325200 | |
| 396 | H | 2.41747000 | 2.12493700 | -0.00014500 | |
| 397 | H | 4.20549800 | -1.06307300 | -0.15511200 | |
| 398 | H | 4.33798200 | 0.65550300 | -0.09926200 | |
| 399 | | | | | |
| 400 | P1: | -835.219879 a.u. | | | |
| 401 | O | -3.94632100 | 0.39097000 | -0.00000200 | |
| 402 | N | 3.99523300 | -0.23549500 | -0.00000100 | |
| 403 | C | -0.11371900 | 0.22687000 | 0.00000200 | |
| 404 | C | 0.71511500 | 1.37423100 | 0.00000100 | |
| 405 | C | 0.43617400 | -1.07549400 | 0.00000200 | |
| 406 | C | 2.66058300 | -0.07712400 | -0.00000100 | |
| 407 | C | 2.08051700 | 1.22567900 | 0.00000000 | |
| 408 | C | 1.80182400 | -1.22396700 | 0.00000000 | |
| 409 | H | 0.25380700 | 2.35584100 | 0.00000000 | |
| 410 | H | -0.19883700 | -1.95562100 | 0.00000300 | |
| 411 | H | 2.72266500 | 2.10057700 | -0.00000100 | |
| 412 | H | 2.23829300 | -2.21776000 | 0.00000000 | |
| 413 | H | 4.62078300 | 0.55877400 | -0.00000200 | |
| 414 | H | 4.42083800 | -1.15232500 | -0.00000200 | |
| 415 | O | -1.44255000 | 0.48766900 | 0.00000200 | |
| 416 | S | | -2.77476100 | -0.48570600 | -0.00000100 |

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| 417 | TS11(T): | -835.150250 a.u. | | | |
| 418 | S | -2.72020400 | -0.03359700 | -0.29551100 | |
| 419 | O | -2.78479800 | 1.31965600 | 0.26818800 | |
| 420 | O | -2.91858100 | -1.18948000 | 0.58386400 | |
| 421 | N | 4.00757200 | 0.06154400 | 0.19485800 | |
| 422 | C | -0.01613100 | -0.07061000 | -0.24112200 | |
| 423 | C | 0.55652100 | 1.19860700 | -0.12764700 | |
| 424 | C | 0.64882800 | -1.29879800 | -0.22185800 | |
| 425 | C | 2.68032000 | 0.01825000 | 0.04784000 | |
| 426 | C | 1.92743700 | 1.24627700 | 0.01972600 | |
| 427 | C | 2.02008400 | -1.25656300 | -0.07502800 | |
| 428 | H | -0.04824700 | 2.10038300 | -0.14133400 | |
| 429 | H | 0.11673800 | -2.24134300 | -0.30627500 | |
| 430 | H | 2.44576700 | 2.19604900 | 0.11961000 | |
| 431 | H | 2.60731700 | -2.17032100 | -0.04662200 | |
| 432 | H | 4.50481000 | 0.94134600 | 0.28829400 | |
| 433 | H | 4.56854800 | -0.78374900 | 0.22261200 | |
| 434 | | | | | |
| 435 | P11(T): | -835.160701 a.u. | | | |
| 436 | S | 3.48990700 | -0.00002300 | -0.00003900 | |
| 437 | O | 2.72327300 | 1.25179700 | -0.00001800 | |
| 438 | O | 2.72321600 | -1.25180800 | -0.00001800 | |
| 439 | N | -4.23190000 | -0.00008900 | -0.00008800 | |
| 440 | C | -0.17822700 | 0.00009200 | 0.00010800 | |
| 441 | C | -0.80544500 | 1.24975600 | 0.00007900 | |
| 442 | C | -0.80533300 | -1.24962800 | 0.00007800 | |
| 443 | C | -2.89460800 | -0.00003000 | -0.00002300 | |
| 444 | C | -2.18427200 | 1.25330700 | 0.00001100 | |
| 445 | C | -2.18415900 | -1.25330200 | 0.00001200 | |
| 446 | H | -0.22989800 | 2.16999800 | 0.00010500 | |
| 447 | H | -0.22970100 | -2.16981700 | 0.00010300 | |
| 448 | H | -2.74400800 | 2.18472100 | -0.00001800 | |
| 449 | H | -2.74381100 | -2.18476600 | -0.00001600 | |
| 450 | H | -4.76375200 | 0.86344200 | -0.00011500 | |
| 451 | H | | -4.76367500 | -0.86366800 | -0.00011400 |

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|-----|----------------------------------|-------------|-------------|-------------|
| 452 | TS12(T): -835.150925 a.u. | | | |
| 453 | N | 4.01871200 | -0.42289200 | 0.15534200 |
| 454 | C | 0.03982100 | 0.33837700 | -0.22561700 |
| 455 | C | 0.89834500 | 1.44138900 | -0.14326700 |
| 456 | C | 0.43481400 | -1.00590900 | -0.19967300 |
| 457 | C | 2.71090300 | -0.17228900 | 0.02692600 |
| 458 | C | 2.24619300 | 1.18946500 | -0.01370900 |
| 459 | C | 1.78159100 | -1.26704300 | -0.06932100 |
| 460 | H | 0.51187900 | 2.45533400 | -0.16915700 |
| 461 | H | -0.28905100 | -1.81234600 | -0.26450000 |
| 462 | H | 2.96369000 | 2.00185400 | 0.06390500 |
| 463 | H | 2.15192300 | -2.28794800 | -0.03039000 |
| 464 | H | 4.69918700 | 0.32580400 | 0.22439300 |
| 465 | H | 4.37799700 | -1.37071100 | 0.18597000 |
| 466 | O | -1.83357900 | 0.82597300 | 0.38720600 |
| 467 | O | -3.30423800 | -1.20955500 | 0.17341800 |
| 468 | S | -3.13212900 | 0.22331100 | -0.11466500 |
| 469 | | | | |
| 470 | P12(T): -835.228536 a.u. | | | |
| 471 | O | -2.90500300 | -1.06651100 | 0.71978200 |
| 472 | N | 3.79075000 | -0.61010600 | 0.02614100 |
| 473 | C | -0.19183800 | 0.52741900 | -0.05052500 |
| 474 | C | 0.82662100 | 1.51098200 | 0.12996400 |
| 475 | C | 0.15137100 | -0.84602500 | -0.20007100 |
| 476 | C | 2.50235500 | -0.23850900 | 0.00093000 |
| 477 | C | 2.14342300 | 1.14074000 | 0.15470000 |
| 478 | C | 1.47226900 | -1.21751600 | -0.17801900 |
| 479 | H | 0.52694200 | 2.54678200 | 0.24512000 |
| 480 | H | -0.61718300 | -1.59957100 | -0.31646200 |
| 481 | H | 2.92085400 | 1.88618700 | 0.29163400 |
| 482 | H | 1.74346400 | -2.26282700 | -0.29087700 |
| 483 | H | 4.53491500 | 0.06511900 | 0.15348500 |
| 484 | H | 4.06646100 | -1.57908400 | -0.07834300 |
| 485 | O | -1.43951800 | 1.00868000 | -0.06101800 |
| 486 | S | | -2.89873300 | 0.02589000 |
| | | | | -0.28747100 |

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| 487 | TS2(T): | -835.295913 | a.u. | | | |
| 488 | O | 3.08701100 | | 1.00483600 | | -0.35683000 |
| 489 | N | -3.82410600 | | 0.29563400 | | -0.12896500 |
| 490 | C | 0.17383000 | | -0.20390800 | | 0.07876400 |
| 491 | C | -0.26110300 | | 1.10286900 | | 0.20613100 |
| 492 | C | -0.55629200 | | -1.36897800 | | -0.10149000 |
| 493 | C | -2.49335800 | | 0.12809000 | | -0.06472400 |
| 494 | C | -1.64250600 | | 1.26942200 | | 0.12798300 |
| 495 | C | -1.93238300 | | -1.18842900 | | -0.17994400 |
| 496 | H | 0.40278200 | | 1.94500500 | | 0.37568800 |
| 497 | H | -0.11392300 | | -2.35850700 | | -0.15626600 |
| 498 | H | -2.06679400 | | 2.26457900 | | 0.23558600 |
| 499 | H | -2.57678800 | | -2.05508000 | | -0.30453500 |
| 500 | H | -4.25796400 | | 1.21537600 | | -0.04926800 |
| 501 | H | -4.46176200 | | -0.48983700 | | -0.25986500 |
| 502 | O | 1.78845700 | | -0.46248900 | | 1.16041700 |
| 503 | S | 2.33206700 | | -0.40204900 | | -0.29564400 |
| 504 | H | 3.79724400 | | 1.06865100 | | -1.03728500 |
| 505 | | | | | | |
| 506 | P2(T): | -835.382437 | a.u. | | | |
| 507 | S | 2.11608600 | | -0.07480100 | | -0.31673000 |
| 508 | O | 2.60795900 | | -1.33448300 | | 0.28667900 |
| 509 | O | 2.48672600 | | 1.29045800 | | 0.43229200 |
| 510 | N | -3.79509300 | | 0.01616600 | | 0.13834300 |
| 511 | C | 0.27853300 | | -0.01123100 | | -0.15336300 |
| 512 | C | -0.37739500 | | -1.25334700 | | -0.06001700 |
| 513 | C | -0.36609100 | | 1.23880500 | | -0.16845800 |
| 514 | C | -2.46592000 | | 0.00614100 | | 0.03994000 |
| 515 | C | -1.75560600 | | -1.24645200 | | 0.03987600 |
| 516 | C | -1.74558300 | | 1.24923300 | | -0.06648700 |
| 517 | H | 0.16588400 | | -2.19335300 | | -0.05423200 |
| 518 | H | 0.18123200 | | 2.17191900 | | -0.24888700 |
| 519 | H | -2.29969100 | | -2.18390600 | | 0.11839800 |
| 520 | H | -2.28353100 | | 2.19345300 | | -0.07746400 |
| 521 | H | -4.33796000 | | -0.84437500 | | 0.21708600 |
| 522 | H | -4.33125000 | | 0.88437700 | | 0.14239700 |
| 523 | H | | | 3.44849200 | | 1.50885700 |
| | | | | | | 0.46126800 |

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| 524 | B: | -361.851062 a.u. | | |
| 525 | N | -2.63793400 | 0.00000000 | -0.00000400 |
| 526 | C | 1.51285700 | 0.00000100 | 0.00000000 |
| 527 | C | 0.73892700 | 1.27496000 | 0.00000100 |
| 528 | C | 0.73892700 | -1.27496000 | 0.00000100 |
| 529 | C | -1.32273400 | 0.00000000 | 0.00000100 |
| 530 | C | -0.60929300 | 1.26811500 | 0.00000000 |
| 531 | C | -0.60929300 | -1.26811500 | 0.00000000 |
| 532 | H | 1.31558600 | 2.19495300 | 0.00000000 |
| 533 | H | 1.31558600 | -2.19495200 | 0.00000100 |
| 534 | H | -1.18439900 | 2.19000500 | 0.00000000 |
| 535 | H | -1.18439900 | -2.19000500 | -0.00000100 |
| 536 | H | -3.17226900 | 0.86363800 | 0.00000900 |
| 537 | H | -3.17226900 | -0.86363800 | 0.00000800 |
| 538 | O | 2.73141900 | -0.00000100 | -0.00000100 |
| 539 | | | | |
| 540 | SO(T): | -473.358017 a.u. | | |
| 541 | S | 0.00000000 | 0.00000000 | 0.50522000 |
| 542 | O | 0.00000000 | 0.00000000 | -1.01043900 |
| 543 | | | | |
| 544 | SOH⁺(T): | -473.595541 a.u. | | |
| 545 | S | 0.03319800 | -0.58300600 | 0.00000000 |
| 546 | O | 0.03319800 | 0.97670600 | 0.00000000 |
| 547 | H | | -0.79674200 | 1.51445200 |
| | | | | 0.00000000 |

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|-----|---|-------------|-------------|-------------|
| 548 | C(T): -286.560706 a.u. | | | |
| 549 | N | -2.20264500 | 0.00000000 | -0.00000100 |
| 550 | C | 1.84940800 | 0.00000000 | 0.00000000 |
| 551 | C | 1.22434800 | -1.24974600 | 0.00000000 |
| 552 | C | 1.22434800 | 1.24974600 | 0.00000000 |
| 553 | C | -0.86609500 | 0.00000000 | 0.00000100 |
| 554 | C | -0.15516200 | -1.25305700 | 0.00000000 |
| 555 | C | -0.15516200 | 1.25305700 | 0.00000000 |
| 556 | H | 1.79244100 | -2.17477600 | 0.00000000 |
| 557 | H | 1.79244100 | 2.17477600 | 0.00000000 |
| 558 | H | -0.71300500 | -2.18550100 | 0.00000000 |
| 559 | H | -0.71300400 | 2.18550100 | 0.00000000 |
| 560 | H | -2.73523800 | -0.86359200 | 0.00000200 |
| 561 | H | -2.73523800 | 0.86359200 | 0.00000300 |
| 562 | | | | |
| 563 | SO₂: -548.592655 a.u. | | | |
| 564 | S | 0.00000000 | 0.00000000 | 0.37373000 |
| 565 | O | 0.00000000 | 1.26065000 | -0.37373000 |
| 566 | O | 0.00000000 | -1.26065000 | -0.37373000 |