Supplementary Material for PCCP


# Supplementary information: Quantitative prediction of the absorption maxima of azobenzene dyes from bond lengths and critical points in the electron density

Bård Buttingsrud, Bjørn K. Alsberg and Per-Olof Åstrand*

Department of Chemistry, Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway
* Corresponding author. E-mail: per-olof.aastrand@chem.ntnu.no

Table 1: Specification of compound number A1-A191. measured and predicted absorption wavelengths and their difference is also shown. See figure 2 for specification of the substituents. The column named *Set* indicates whether each molecule was included into the calibration set (c), test set (t) or detected as an outlier (o). The predicted values ($\lambda_{max}^{pred}$) for the outliers are estimated using the bond length model **a**. All other $\lambda_{max}^{pred}$ –values are for model **h** using AIM descriptors since this is the model with highest accuracy. The error for each molecule is also given ($\Delta\lambda$). X1 is shorthand notation for $N(CH_2CH(OH)CH_2(OH))C_2H_5$.

| | $R_{16}$ | $R_{20}$ | $R_{24}$ | $R_{21}$ | $R_{17}$ | $R_{18}$ | $R_{23}$ | $R_{25}$ | $R_{22}$ | $R_{19}$ | Set | $\lambda_{max}^{exp}$ | $\lambda_{max}^{pred}$ | $\Delta\lambda$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A1 | | | | | | | | | | | c | 318 | 313 | 5 |
| A2 | | | $N(C_2H_5)_2$ | | | | | | | | t | 415 | 416 | -1 |
| A3 | | | $N(CH_3)C_2H_5$ | | | | | | | | c | 411 | 410 | 1 |
| A4 | | | $N(CH_3)_2$ | | | | | | | | c | 407 | 410 | -3 |
| A5 | | | $N(C_2H_4OH)_2$ | | | | | | | | c | 407 | 409 | -2 |
| A6 | | | $N(C_2H_4OH)C_2H_4CN$ | | | | | | | | c | 397 | 399 | -2 |
| A7 | | | $N(C_2H_4Cl)_2$ | | | | | | | | c | 397 | 394 | 3 |
| A8 | | | $N(C_2H_5)C_2H_4CN$ | | | | | | | | c | 399 | 399 | 0 |
| A9 | | | $N(C_2H_4CN)_2$ | | | | | | | | t | 382 | 385 | -3 |
| A10 | | | $NHC_2H_5$ | | | | | | | | c | 405 | 407 | -2 |
| A11 | | | $NHCH_3$ | | | | | | | | c | 402 | 410 | -8 |
| A12 | | | $NHC_2H_4CN$ | | | | | | | | c | 390 | 387 | 3 |
| A13 | | | $NH_2$ | | | | | | | | t | 389 | 405 | -16 |
| A14 | | | $NHCOCH_3$ | | | | | | | | c | 348 | 353 | -5 |
| A15 | | | $OCH_3$ | | | | | | | | c | 345 | 347 | -2 |
| A16 | | | OH | | | | | | | | c | 348 | 346 | 2 |
| A17 | | | $CH_3$ | | | | | | | | c | 333 | 322 | 11 |
| A18 | | | $N(CH_3)_2$ | | | | | $N(CH_3)_2$ | | | c | 457 | 458 | -1 |
| A19 | | | $N(CH_3)_2$ | | | | | $NHCOCH_3$ | | | c | 431 | 431 | 0 |
| A20 | | | $N(CH_3)_2$ | | | | | OH | | | c | 435 | 413 | 22 |
| A21 | | | $N(CH_3)_2$ | | | | | $OCH_3$ | | | c | 407 | 412 | -5 |
| A22 | | | $N(CH_3)_2$ | | | | | $CH_3$ | | | t | 407 | 413 | -6 |
| A23 | | | $N(CH_3)_2$ | | | | | F | | | t | 407 | 414 | -7 |
| A24 | | | $N(CH_3)_2$ | | | | | Br | | | t | 419 | 425 | -6 |
| A25 | | | $N(CH_3)_2$ | | | | | $CF_3$ | | | t | 427 | 431 | -4 |
| A26 | | | $N(CH_3)_2$ | | | | | CN | | | t | 451 | 452 | -1 |
| A27 | | | $N(CH_3)_2$ | | | | | $COCH_3$ | | | t | 447 | 453 | -6 |
| A28 | | | $N(CH_3)C_2H_5$ | | | | | $COCH_3$ | | | t | 454 | 454 | 0 |
| A29 | | | $N(C_2H_5)_2$ | | | | | $COCH_3$ | | | c | 462 | 459 | 3 |
| A30 | | | $N(C_2H_5)_2$ | | | | | CN | | | c | 466 | 462 | 4 |

*continued on next page*

*continued from previous page*

| | $R_{16}$ | $R_{20}$ | $R_{24}$ | $R_{21}$ | $R_{17}$ | $R_{18}$ | $R_{23}$ | $R_{25}$ | $R_{22}$ | $R_{19}$ | Set | $\lambda_{max}^{exp}$ | $\lambda_{max}^{pred}$ | $\Delta\lambda$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A31 | | | $N(C_2H_4Cl)_2$ | | | | | $CH_3$ | | | c | 407 | 398 | 9 |
| A32 | | | $N(C_2H_4Cl)_2$ | | | | | Cl | | | t | 405 | 406 | -1 |
| A33 | | | $N(C_2H_4Cl)_2$ | | | | | Br | | | c | 405 | 410 | -5 |
| A34 | | | $N(C_2H_4Cl)_2$ | | | | | $COCH_3$ | | | c | 435 | 432 | 3 |
| A35 | | | $N(C_2H_5)C_2H_4CN$ | | | | | Cl | | | c | 409 | 411 | -2 |
| A36 | | | $N(C_2H_5)C_2H_4CN$ | | | | | $CF_3$ | | | c | 416 | 419 | -3 |
| A37 | | | $N(C_2H_5)C_2H_4CN$ | | | | | CN | | | c | 433 | 440 | -7 |
| A38 | | | OH | | | | | $OCH_3$ | | | c | 357 | 354 | 3 |
| A39 | | | OH | | | | | $CH_3$ | | | c | 353 | 352 | 1 |
| A40 | | | OH | | | | | $NHCOCH_3$ | | | c | 368 | 372 | -4 |
| A41 | | | OH | | | | | $NH_2$ | | | c | 385 | 389 | -4 |
| A42 | | | OH | | | | | Cl | | | t | 356 | 356 | 0 |
| A43 | | | $OCH_3$ | | | | | $OCH_3$ | | | c | 354 | 355 | -1 |
| A44 | | | $N(CH_3)_2$ | | | | | Cl | | | c | 417 | 423 | -6 |
| A45 | $NHCOCH_3$ | | | | | | | | | | t | 326 | 340 | -14 |
| A46 | | $CH_3$ | | | | | | | | | t | 322 | 327 | -5 |
| A47 | | | $N(CH_3)_2$ | | | | $OCH_3$ | | | | c | 412 | 414 | -2 |
| A48 | | | $N(CH_3)_2$ | | | $OCH_3$ | | | | | c | 413 | 415 | -2 |
| A49 | | | $N(CH_3)_2$ | | | | $CH_3$ | | | | c | 407 | 414 | -7 |
| A50 | | | $N(CH_3)_2$ | | | $CH_3$ | | | | | c | 407 | 410 | -3 |
| A51 | | | $N(CH_3)_2$ | | | | F | | | | t | 418 | 418 | 0 |
| A52 | | | $N(CH_3)_2$ | | | F | | | | | c | 418 | 414 | 4 |
| A53 | | | $N(CH_3)_2$ | | | | Cl | | | | c | 420 | 421 | -1 |
| A54 | | | $N(CH_3)_2$ | | | Cl | | | | | t | 424 | 422 | 2 |
| A55 | | | $N(CH_3)_2$ | | | | Br | | | | c | 421 | 422 | -1 |
| A56 | | | $N(CH_3)_2$ | | | Br | | | | | c | 425 | 419 | 6 |
| A57 | | | $N(CH_3)_2$ | | | | $CF_3$ | | | | t | 423 | 425 | -2 |
| A58 | | | $N(CH_3)_2$ | | | $CF_3$ | | | | | t | 429 | 426 | 3 |
| A59 | | | $N(CH_3)_2$ | | | | CN | | | | c | 435 | 435 | 0 |
| A60 | | | $N(CH_3)_2$ | | | CN | | | | | t | 449 | 451 | -2 |
| A61 | | | $N(CH_3)_2$ | | | | $COCH_3$ | | | | c | 420 | 423 | -3 |
| A62 | | | $N(CH_3)_2$ | | | $CF_3$ | | Cl | | | c | 442 | 439 | 3 |
| A63 | | | $N(CH_3)_2$ | | | $CF_3$ | | | $CF_3$ | | c | 450 | 450 | 0 |
| A64 | | | $N(CH_3)C_2H_5$ | | | | $CF_3$ | | | | c | 426 | 427 | -1 |
| A65 | | | $N(C_2H_5)_2$ | | | | CN | | | | c | 446 | 442 | 4 |

*continued on next page*

*continued from previous page*

| | $R_{16}$ | $R_{20}$ | $R_{24}$ | $R_{21}$ | $R_{17}$ | $R_{18}$ | $R_{23}$ | $R_{25}$ | $R_{22}$ | $R_{19}$ | Set | $\lambda_{max}^{exp}$ | $\lambda_{max}^{pred}$ | $\Delta\lambda$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A66 | | | $N(C_2H_5)_2$ | | | CN | | | | | c | 462 | 459 | 3 |
| A67 | | | $N(C_2H_5)_2$ | | | | CN | CN | | | c | 500 | 492 | 8 |
| A68 | | | $N(C_2H_5)_2$ | | | CN | | CN | | | t | 514 | 516 | -2 |
| A69 | | | $N(C_2H_5)_2$ | | | CN | CN | | | | t | 490 | 495 | -5 |
| A70 | | | $N(C_2H_5)_2$ | | | CN | | | CN | | t | 495 | 501 | -6 |
| A71 | | | $N(C_2H_5)_2$ | | | | CN | | CN | | c | 478 | 479 | -1 |
| A72 | | | $N(C_2H_5)_2$ | | | CN | | | | CN | o | 503 | 509 | -6 |
| A73 | | | $N(C_2H_5)_2$ | | | CN | | CN | | CN | o | 562 | 600 | -38 |
| A74 | | | $N(C_2H_4Cl)_2$ | | | $OCH_3$ | | | | | c | 405 | 401 | 4 |
| A75 | | | $N(C_2H_4Cl)_2$ | | | | $CH_3$ | | | | c | 395 | 399 | -4 |
| A76 | | | $N(C_2H_4Cl)_2$ | | | $CH_3$ | | | | | c | 395 | 395 | 0 |
| A77 | | | $N(C_2H_4Cl)_2$ | | | | Cl | | | | c | 406 | 404 | 2 |
| A78 | | | $N(C_2H_5)C_2H_4CN$ | | | Cl | | | | | c | 412 | 410 | 2 |
| A79 | | | $N(C_2H_5)C_2H_4CN$ | | | $CF_3$ | | | | | c | 416 | 412 | 4 |
| A80 | | | $N(C_2H_5)C_2H_4CN$ | | | CN | | | | | c | 434 | 439 | -5 |
| A81 | | | $N(C_2H_5)C_2H_4CN$ | | | Cl | | | | Cl | o | 396 | 357 | 39 |
| A82 | | | OH | | | | $OCH_3$ | | | | c | 349 | 351 | -2 |
| A83 | | | OH | | | $OCH_3$ | | | | | c | 351 | 358 | -7 |
| A84 | | | OH | | | | $CH_3$ | | | | c | 349 | 351 | -2 |
| A85 | | | OH | | | $CH_3$ | | | | | c | 350 | 346 | 4 |
| A86 | | | OH | | | | Cl | | | | t | 357 | 353 | 4 |
| A87 | | | OH | | | Cl | | | | | t | 360 | 355 | 5 |
| A88 | | | OH | | | Cl | | Cl | | | c | 366 | 363 | 3 |
| A89 | | | OH | | | Cl | | | Cl | | c | 370 | 368 | 2 |
| A90 | | | OH | | | Cl | | Br | | | c | 368 | 365 | 3 |
| A91 | | | OH | | | Cl | | | Br | | c | 370 | 373 | -3 |
| A92 | | | OH | | | Cl | | CN | | | c | 378 | 389 | -11 |
| A93 | | | OH | | | Cl | | | CN | | c | 372 | 377 | -5 |
| A94 | $CH_3$ | | OH | | | | | | | | c | 354 | 349 | 5 |
| A95 | | $CH_3$ | OH | | | | | | | | c | 354 | 353 | 1 |
| A96 | $OCH_3$ | | OH | | | | | | | | c | 372 | 370 | 2 |
| A97 | OH | | OH | | | | | | | | t | 380 | 375 | 5 |
| A98 | OH | | OH | | | | | $OCH_3$ | | | c | 388 | 378 | 10 |
| A99 | OH | | OH | | | | | $CH_3$ | | | c | 386 | 378 | 8 |
| A100 | OH | | OH | | | | | Cl | | | c | 387 | 385 | 2 |

*continued on next page*

*continued from previous page*

| | $R_{16}$ | $R_{20}$ | $R_{24}$ | $R_{21}$ | $R_{17}$ | $R_{18}$ | $R_{23}$ | $R_{25}$ | $R_{22}$ | $R_{19}$ | Set | $\lambda_{max}^{exp}$ | $\lambda_{max}^{pred}$ | $\Delta\lambda$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A101 | OH | | OH | | | | | Br | | | t | 390 | 388 | 2 |
| A102 | OH | | $OCH_3$ | | | | | | | | t | 375 | 375 | 0 |
| A103 | $OCH_3$ | | $OCH_3$ | | | | | | | | c | 362 | 375 | -13 |
| A104 | $OCH_3$ | | $OCH_3$ | | | $OCH_3$ | | $OCH_3$ | | | t | 381 | 379 | 2 |
| A105 | | $OCH_3$ | $OCH_3$ | | | | $OCH_3$ | $OCH_3$ | | | t | 370 | 377 | -7 |
| A106 | $CH_3$ | | $N(CH_3)_2$ | | | | | | | | t | 409 | 415 | -6 |
| A107 | $CH_3$ | | $N(CH_3)_2$ | | | | | $NH_2$ | | | c | 460 | 442 | 18 |
| A108 | $CH_3$ | | $N(CH_3)_2$ | | | | | $COCH_3$ | | | t | 452 | 460 | -8 |
| A109 | $CH_3$ | | $N(CH_3)_2$ | | | | $COCH_3$ | | | | c | 424 | 431 | -7 |
| A110 | $CH_3$ | | X1 | | | | | | | | c | 420 | 423 | -3 |
| A111 | $CH_3$ | | X1 | | | | | $COCH_3$ | | | t | 457 | 471 | -14 |
| A112 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | | | | | | c | 415 | 413 | 2 |
| A113 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | | | $OCH_3$ | | | t | 414 | 412 | 2 |
| A114 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | $OCH_3$ | | | | | c | 424 | 415 | 9 |
| A115 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | | | $CH_3$ | | | c | 416 | 414 | 2 |
| A116 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | $CH_3$ | | | | | c | 418 | 411 | 7 |
| A117 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | | | F | | | c | 417 | 417 | 0 |
| A118 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | | | Cl | | | c | 424 | 426 | -2 |
| A119 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | | | Br | | | c | 425 | 430 | -5 |
| A120 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | | | $CF_3$ | | | t | 434 | 436 | -2 |
| A121 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | $CF_3$ | | | | | c | 434 | 432 | 2 |
| A122 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | $CF_3$ | | Cl | | | t | 447 | 448 | -1 |
| A123 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | | $CF_3$ | | $CF_3$ | | c | 454 | 458 | -4 |
| A124 | $CH_3$ | | $N(C_2H_4OH)_2$ | | | Cl | | | $CF_3$ | | c | 450 | 456 | -6 |
| A125 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | | | | | c | 403 | 402 | 1 |
| A126 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | $OCH_3$ | | | | c | 407 | 406 | 1 |
| A127 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | $OCH_3$ | | | | | c | 409 | 408 | 1 |
| A128 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | | $CH_3$ | | | c | 402 | 410 | -8 |
| A129 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | $CH_3$ | | | | c | 402 | 406 | -4 |
| A130 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | $CH_3$ | | | | | c | 405 | 401 | 4 |
| A131 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | F | | | | t | 415 | 410 | 5 |
| A132 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | F | | | | | t | 417 | 412 | 5 |
| A133 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | | Cl | | | c | 413 | 414 | -1 |
| A134 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | Cl | | | | t | 410 | 414 | -4 |
| A135 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | Cl | | | | | c | 412 | 416 | -4 |

*continued on next page*

*continued from previous page*

| | $R_{16}$ | $R_{20}$ | $R_{24}$ | $R_{21}$ | $R_{17}$ | $R_{18}$ | $R_{23}$ | $R_{25}$ | $R_{22}$ | $R_{19}$ | Set | $\lambda_{max}^{exp}$ | $\lambda_{max}^{pred}$ | $\Delta\lambda$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A136 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | Br | | | | c | 414 | 415 | -1 |
| A137 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | Br | | | | | c | 417 | 412 | 5 |
| A138 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | | $CF_3$ | | | t | 421 | 423 | -2 |
| A139 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | $CF_3$ | | | | t | 418 | 418 | 0 |
| A140 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | $CF_3$ | | | | | c | 419 | 418 | 1 |
| A141 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | | | CN | | | c | 437 | 447 | -10 |
| A142 | $CH_3$ | | $N(C_2H_4OH)C_2H_4CN$ | | | CN | | | | | c | 438 | 448 | -10 |
| A143 | $CH_3$ | | $NHC_2H_4CN$ | | | | | | | | c | 396 | 391 | 5 |
| A144 | $CH_3$ | | $NHC_2H_4CN$ | | | | | $NHCOCH_3$ | | | c | 403 | 415 | -12 |
| A145 | $CH_3$ | | $NHC_2H_4CN$ | | | | | $OCH_3$ | | | c | 395 | 392 | 3 |
| A146 | $CH_3$ | | $NHC_2H_4CN$ | | | | $OCH_3$ | | | | c | 394 | 393 | 1 |
| A147 | $CH_3$ | | $NHC_2H_4CN$ | | | $OCH_3$ | | | | | c | 394 | 399 | -5 |
| A148 | $CH_3$ | | $NHC_2H_4CN$ | | | | | $CH_3$ | | | c | 395 | 395 | 0 |
| A149 | $CH_3$ | | $NHC_2H_4CN$ | | | | $CH_3$ | | | | c | 400 | 391 | 9 |
| A150 | $CH_3$ | | $NHC_2H_4CN$ | | | $CH_3$ | | | | | t | 400 | 391 | 9 |
| A151 | $CH_3$ | | $NHC_2H_4CN$ | | | | | F | | | c | 398 | 396 | 2 |
| A152 | $CH_3$ | | $NHC_2H_4CN$ | | | | F | | | | t | 406 | 398 | 8 |
| A153 | $CH_3$ | | $NHC_2H_4CN$ | | | F | | | | | t | 404 | 401 | 3 |
| A154 | $CH_3$ | | $NHC_2H_4CN$ | | | | | Cl | | | t | 404 | 403 | 1 |
| A155 | $CH_3$ | | $NHC_2H_4CN$ | | | | C | | | | c | 408 | 400 | 8 |
| A156 | $CH_3$ | | $NHC_2H_4CN$ | | | Cl | | | | | c | 408 | 402 | 6 |
| A157 | $CH_3$ | | $NHC_2H_4CN$ | | | | | $CF_3$ | | | c | 411 | 410 | 1 |
| A158 | $CH_3$ | | $NHC_2H_4CN$ | | | | | CN | | | c | 428 | 434 | -6 |
| A159 | $CH_3$ | | $NHC_2H_4CN$ | | | CN | | | | | t | 429 | 432 | -3 |
| A190 | $OCH_3$ | | | $CH_3$ | | | | | | | c | 360 | 363 | -3 |
| A191 | $OCH_3$ | | | $OCH_3$ | | $OCH_3$ | | | $OCH_3$ | | o | 411 | 405 | 6 |
| B160 | | | | | | | | | | | c | 418 | 419 | -1 |
| B161 | | | | | | | | Cl | | | c | 434 | 432 | 2 |
| C162 | | | | | | | | | | | t | 410 | 408 | 2 |
| C163 | | | | | | | | $OCH_3$ | | | c | 406 | 413 | -7 |
| C164 | | | | | | | | $CH_3$ | | | t | 410 | 412 | -2 |
| C165 | | | | | | | | Cl | | | c | 420 | 421 | -1 |
| C166 | | | | | | | | Br | | | c | 420 | 424 | -4 |
| C167 | | | | | | | | $CF_3$ | | | c | 428 | 427 | 1 |
| C168 | | | | | | | | $COCH_3$ | | | c | 448 | 449 | -1 |

*continued on next page*

*continued from previous page*

| | $R_{16}$ | $R_{20}$ | $R_{24}$ | $R_{21}$ | $R_{17}$ | $R_{18}$ | $R_{23}$ | $R_{25}$ | $R_{22}$ | $R_{19}$ | Set | $\lambda_{max}^{exp}$ | $\lambda_{max}^{pred}$ | $\Delta\lambda$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C169 | | | | | | CN | | | | | t | 448 | 449 | -1 |
| C170 | | | | | | | | CN | | | c | 450 | 449 | 1 |
| C171 | | | | | | | $CF_3$ | | $CF_3$ | | c | 450 | 440 | 10 |
| D172 | | | | | | | | | | | c | 425 | 426 | -1 |
| D173 | | | | | | | | OH | | | c | 414 | 439 | -25 |
| D174 | | | | | | | | $OCH_3$ | | | c | 417 | 427 | -10 |
| D175 | | | | | | | | $CH_3$ | | | c | 422 | 429 | -7 |
| D176 | | | | | | | | F | | | c | 426 | 432 | -6 |
| D177 | | | | | | | | Cl | | | c | 444 | 441 | 3 |
| D178 | | | | | | | | Br | | | c | 448 | 443 | 5 |
| D179 | | | | | | | | $CF_3$ | | | c | 461 | 450 | 11 |
| D180 | | | | | | | | $COCH_3$ | | | c | 482 | 471 | 11 |
| D181 | | | | | | | | CN | | | c | 487 | 476 | 11 |
| E182 | | | | | | | | | | | c | 442 | 445 | -3 |
| E183 | | | | | | | | OH | | | c | 449 | 450 | -1 |
| E184 | | | | | | | | $OCH_3$ | | | t | 452 | 450 | 2 |
| E185 | | | | | | | | $CH_3$ | | | c | 446 | 447 | -1 |
| E186 | | | | | | | | F | | | c | 450 | 447 | 3 |
| E187 | | | | | | | | Cl | | | c | 461 | 458 | 3 |
| E188 | | | | | | | | Br | | | c | 464 | 460 | 4 |
| E189 | | | | | | | | $CF_3$ | | | t | 471 | 469 | 2 |