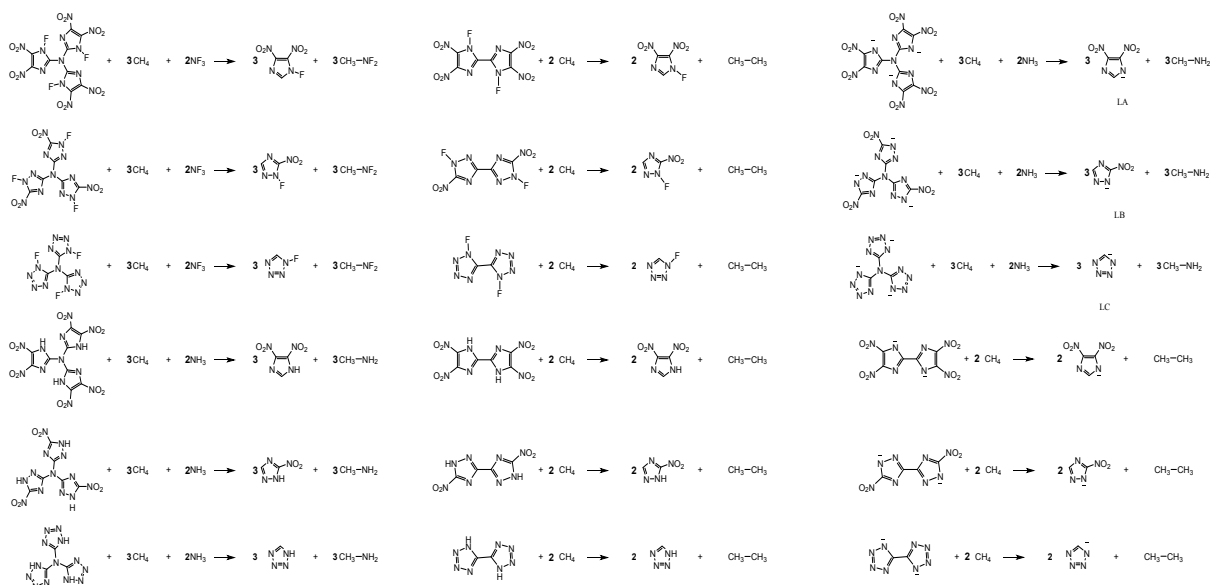


Supplementary materials

N-Fluoro functionalization of heterocyclic azoles: a new strategy towards insensitive high energy density materials

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Scheme S1 The isodesmic reactions used to calculate heats of formation.

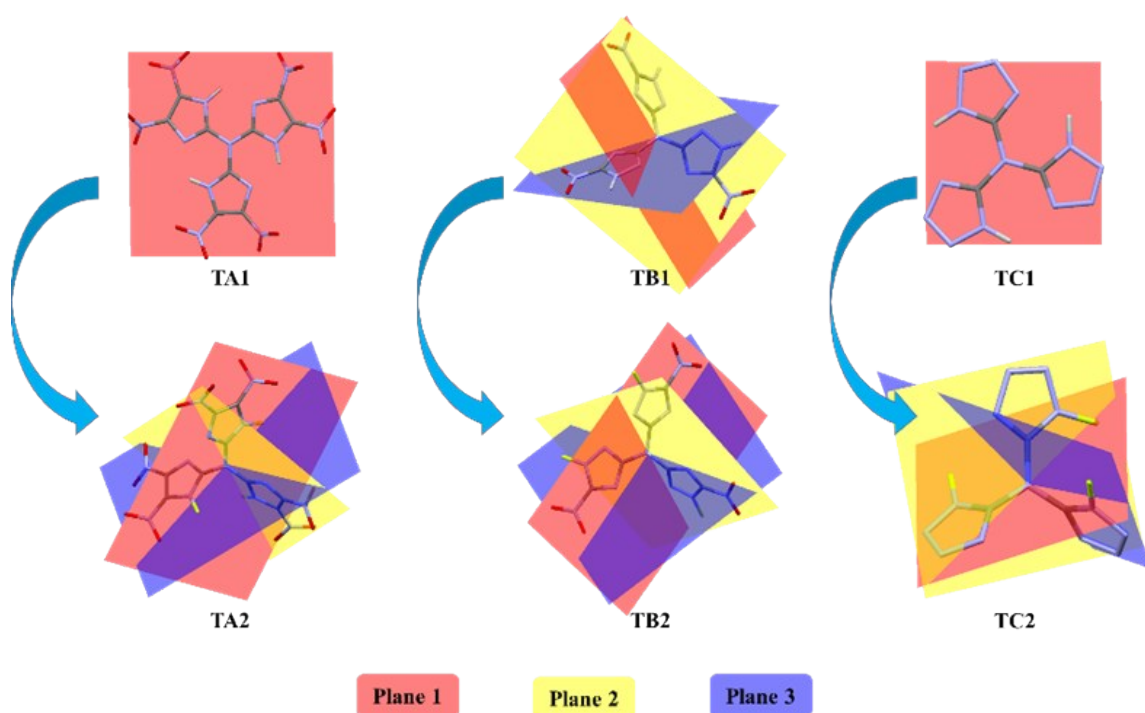


Fig. S1 The angle changes after N-fluorination for *tri*-substituted series.

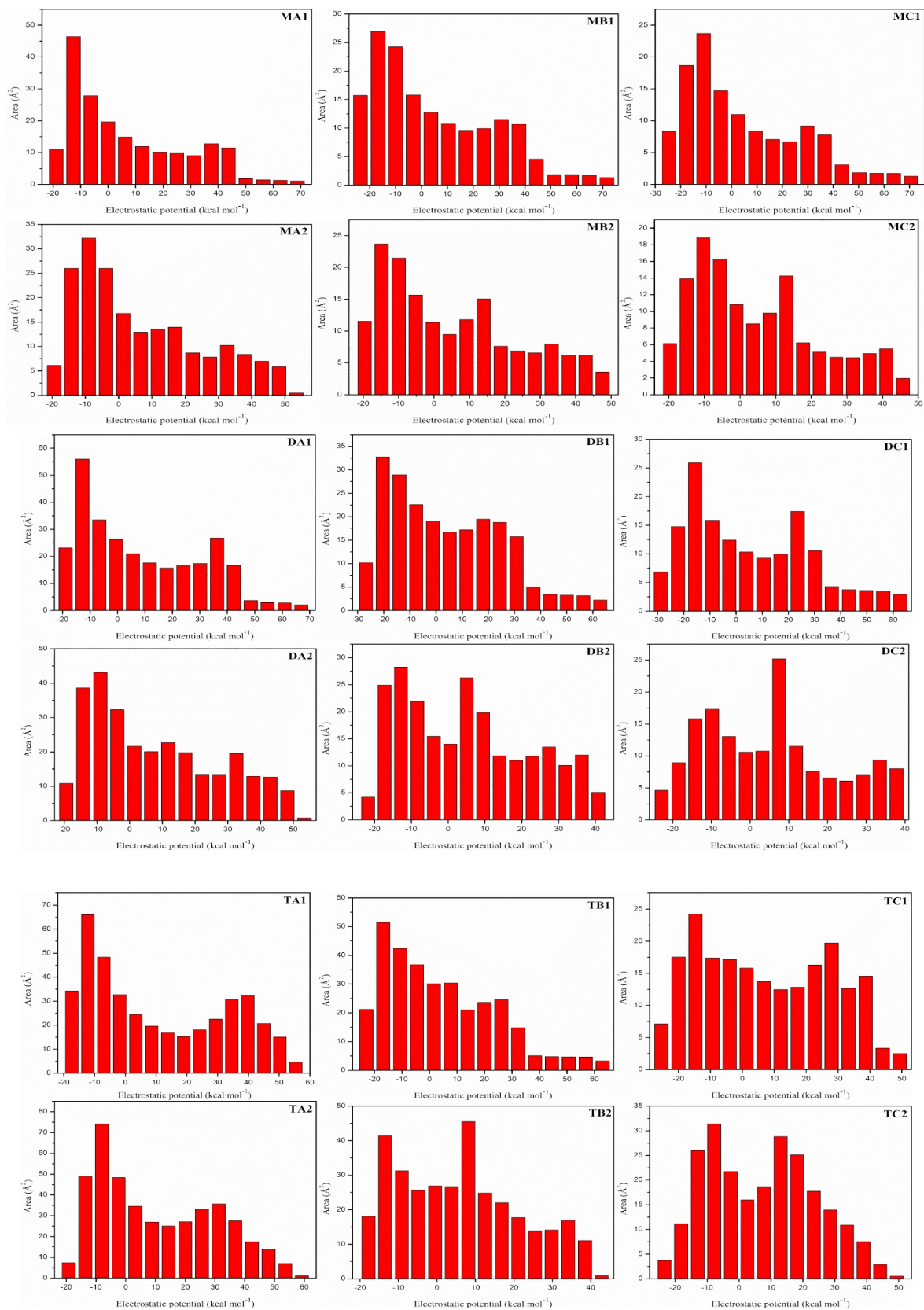


Fig. S2 Area percent in each ESP range of MA1-TC2.

Summary of surface analysis of compound MA1 to DC2.

Compound MA1

Volume: 1248.09002 Bohr³ (184.94790 Angstrom³)
Minimal value: -21.02125 kcal/mol Maximal value: 71.43181 kcal/mol
Overall surface area: 682.76183 Bohr² (191.19281 Angstrom²)
Positive surface area: 339.66786 Bohr² (95.11670 Angstrom²)
Negative surface area: 343.09397 Bohr² (96.07611 Angstrom²)
Overall average value: 0.01092624 a.u. (6.85632 kcal/mol)
Positive average value: 0.03839842 a.u. (24.09539 kcal/mol)
Negative average value: -0.01627161 a.u. (-10.21060 kcal/mol)
Overall variance (σ^2_{tot}): 0.00074441 a.u.² (293.12463 (kcal/mol)²)
Positive variance: 0.00068313 a.u.² (268.99504 (kcal/mol)²)
Negative variance: 0.00006128 a.u.² (24.12959 (kcal/mol)²)
Balance of charges (μ): 0.07554219
Product of σ^2_{tot} and μ : 0.00005623 a.u.² (22.14328 (kcal/mol)²)
Internal charge separation (Π): 0.02843921 a.u. (17.84589 kcal/mol)

Compound MA2

Volume: 1287.21429 Bohr³ (190.74552 Angstrom³)
Minimal value: -20.01859 kcal/mol Maximal value: 55.00452 kcal/mol
Overall surface area: 700.51635 Bohr² (196.16458 Angstrom²)
Positive surface area: 361.42477 Bohr² (101.20926 Angstrom²)
Negative surface area: 339.09157 Bohr² (94.95533 Angstrom²)
Overall average value: 0.01054753 a.u. (6.61868 kcal/mol)
Positive average value: 0.03416923 a.u. (21.44154 kcal/mol)
Negative average value: -0.01462995 a.u. (-9.18044 kcal/mol)
Overall variance (σ^2_{tot}): 0.00058004 a.u.² (228.40274 (kcal/mol)²)
Positive variance: 0.00051815 a.u.² (204.03004 (kcal/mol)²)
Negative variance: 0.00006190 a.u.² (24.37270 (kcal/mol)²)
Balance of charges (μ): 0.09532243
Product of σ^2_{tot} and μ : 0.00005529 a.u.² (21.77190 (kcal/mol)²)
Internal charge separation (Π): 0.02545499 a.u. (15.97326 kcal/mol)

Compound MB1

Volume: 1001.78733 Bohr³ (148.44960 Angstrom³)
Minimal value: -25.38164 kcal/mol Maximal value: 73.48092 kcal/mol
Overall surface area: 569.14787 Bohr² (159.37766 Angstrom²)
Positive surface area: 275.30605 Bohr² (77.09356 Angstrom²)
Negative surface area: 293.84182 Bohr² (82.28410 Angstrom²)
Overall average value: 0.00808600 a.u. (5.07405 kcal/mol)

Positive average value: 0.03973621 a.u. (24.93487 kcal/mol)
Negative average value: -0.02156768 a.u. (-13.53394 kcal/mol)
Overall variance (σ^2_{tot}): 0.00083220 a.u.² (327.69290 (kcal/mol)²)
Positive variance: 0.00072037 a.u.² (283.66104 (kcal/mol)²)
Negative variance: 0.00011182 a.u.² (44.03186 (kcal/mol)²)
Balance of charges (μ): 0.11631417
Product of σ^2_{tot} and μ : 0.00009680 a.u.² (38.11533 (kcal/mol)²)
Internal charge separation (Π): 0.03114414 a.u. (19.54326 kcal/mol)

Compound MB2

Volume: 1041.20573 Bohr³ (154.29080 Angstrom³)
Minimal value: -21.61178 kcal/mol Maximal value: 49.34081 kcal/mol
Overall surface area: 590.09004 Bohr² (165.24206 Angstrom²)
Positive surface area: 306.40903 Bohr² (85.80328 Angstrom²)
Negative surface area: 283.68100 Bohr² (79.43878 Angstrom²)
Overall average value: 0.00878095 a.u. (5.51013 kcal/mol)
Positive average value: 0.03329176 a.u. (20.89091 kcal/mol)
Negative average value: -0.01769363 a.u. (-11.10293 kcal/mol)
Overall variance (σ^2_{tot}): 0.00054176 a.u.² (213.32948 (kcal/mol)²)
Positive variance: 0.00046506 a.u.² (183.12594 (kcal/mol)²)
Negative variance: 0.00007670 a.u.² (30.20354 (kcal/mol)²)
Balance of charges (μ): 0.12153628
Product of σ^2_{tot} and μ : 0.00006584 a.u.² (25.92727 (kcal/mol)²)
Internal charge separation (Π): 0.02608210 a.u. (16.36678 kcal/mol)

Compound MC1

Volume: 758.45848 Bohr³ (112.39197 Angstrom³)
Minimal value: -27.61371 kcal/mol Maximal value: 72.51762 kcal/mol
Overall surface area: 448.21875 Bohr² (125.51405 Angstrom²)
Positive surface area: 209.24989 Bohr² (58.59595 Angstrom²)
Negative surface area: 238.96887 Bohr² (66.91811 Angstrom²)
Overall average value: 0.00767180 a.u. (4.81413 kcal/mol)
Positive average value: 0.03980689 a.u. (24.97922 kcal/mol)
Negative average value: -0.02046687 a.u. (-12.84316 kcal/mol)
Overall variance (σ^2_{tot}): 0.00089459 a.u.² (352.26172 (kcal/mol)²)
Positive variance: 0.00078180 a.u.² (307.84656 (kcal/mol)²)
Negative variance: 0.00011280 a.u.² (44.41516 (kcal/mol)²)
Balance of charges (μ): 0.11018809
Product of σ^2_{tot} and μ : 0.00009857 a.u.² (38.81505 (kcal/mol)²)
Internal charge separation (Π): 0.03050418 a.u. (19.14168 kcal/mol)

Compound MC2

Volume: 797.72501 Bohr³ (118.21068 Angstrom³)
Minimal value: -21.85160 kcal/mol Maximal value: 46.63270 kcal/mol
Overall surface area: 469.03403 Bohr² (131.34292 Angstrom²)
Positive surface area: 243.12079 Bohr² (68.08077 Angstrom²)
Negative surface area: 225.91324 Bohr² (63.26216 Angstrom²)
Overall average value: 0.00786216 a.u. (4.93358 kcal/mol)
Positive average value: 0.02987856 a.u. (18.74909 kcal/mol)
Negative average value: -0.01583121 a.u. (-9.93424 kcal/mol)
Overall variance (sigma²_tot): 0.00049170 a.u.² (193.61698 (kcal/mol)²)
Positive variance: 0.00041880 a.u.² (164.90843 (kcal/mol)²)
Negative variance: 0.00007291 a.u.² (28.70854 (kcal/mol)²)
Balance of charges (miu): 0.12628948
Product of sigma²_tot and miu: 0.00006210 a.u.² (24.45179 (kcal/mol)²)
Internal charge separation (Pi): 0.02341033 a.u. (14.69022 kcal/mol)

Compound DA1

Volume: 1945.22064 Bohr³ (288.25202 Angstrom³)
Minimal value: -20.78085 kcal/mol Maximal value: 68.85508 kcal/mol
Overall surface area: 1008.47192 Bohr² (282.40094 Angstrom²)
Positive surface area: 547.53082 Bohr² (153.32427 Angstrom²)
Negative surface area: 460.94110 Bohr² (129.07667 Angstrom²)
Overall average value: 0.01392378 a.u. (8.73731 kcal/mol)
Positive average value: 0.04010491 a.u. (25.16623 kcal/mol)
Negative average value: -0.01717558 a.u. (-10.77785 kcal/mol)
Overall variance (sigma²_tot): 0.00070289 a.u.² (276.77618 (kcal/mol)²)
Positive variance: 0.00063388 a.u.² (249.60106 (kcal/mol)²)
Negative variance: 0.00006901 a.u.² (27.17513 (kcal/mol)²)
Balance of charges (miu): 0.08854429
Product of sigma²_tot and miu: 0.00006224 a.u.² (24.50695 (kcal/mol)²)
Internal charge separation (Pi): 0.03003798 a.u. (18.84913 kcal/mol)

Compound DA2

Volume: 2019.33820 Bohr³ (299.23511 Angstrom³)
Minimal value: -20.53350 kcal/mol Maximal value: 54.21938 kcal/mol
Overall surface area: 1039.18310 Bohr² (291.00095 Angstrom²)
Positive surface area: 572.55376 Bohr² (160.33141 Angstrom²)
Negative surface area: 466.62933 Bohr² (130.66954 Angstrom²)
Overall average value: 0.01257360 a.u. (7.89006 kcal/mol)
Positive average value: 0.03531438 a.u. (22.16013 kcal/mol)
Negative average value: -0.01532932 a.u. (-9.61930 kcal/mol)
Overall variance (sigma²_tot): 0.00057049 a.u.² (224.64109 (kcal/mol)²)
Positive variance: 0.00050799 a.u.² (200.03080 (kcal/mol)²)

Negative variance: 0.00006250 a.u.² (24.61029 (kcal/mol)²)
Balance of charges (miu): 0.09755179
Product of sigma²_tot and miu: 0.00005565 a.u.² (21.91414 (kcal/mol)²)
Internal charge separation (Pi): 0.02641388 a.u. (16.57498 kcal/mol)

Compound DB1

Volume: 1452.88345 Bohr³ (215.29516 Angstrom³)
Minimal value: -29.39084 kcal/mol Maximal value: 64.24724 kcal/mol
Overall surface area: 782.04128 Bohr² (218.99389 Angstrom²)
Positive surface area: 395.91315 Bohr² (110.86699 Angstrom²)
Negative surface area: 386.12812 Bohr² (108.12690 Angstrom²)
Overall average value: 0.00632659 a.u. (3.97000 kcal/mol)
Positive average value: 0.03449806 a.u. (21.64788 kcal/mol)
Negative average value: -0.02255878 a.u. (-14.15586 kcal/mol)
Overall variance (sigma²_tot): 0.00067474 a.u.² (265.68976 (kcal/mol)²)
Positive variance: 0.00054138 a.u.² (213.17926 (kcal/mol)²)
Negative variance: 0.00013335 a.u.² (52.51050 (kcal/mol)²)
Balance of charges (miu): 0.15857746
Product of sigma²_tot and miu: 0.00010700 a.u.² (42.13241 (kcal/mol)²)
Internal charge separation (Pi): 0.02883975 a.u. (18.09723 kcal/mol)

Compound DB2

Volume: 1530.92883 Bohr³ (26.86030 Angstrom³)
Minimal value: -22.25468 kcal/mol Maximal value: 41.55718 kcal/mol
Overall surface area: 823.81511 Bohr²(230.69176 Angstrom²)
Positive surface area: 466.23938 Bohr²(130.56034 Angstrom²)
Negative surface area: 357.57572 Bohr² (100.13141 Angstrom²)
Overall average value: 0.00808927 a.u. (5.07610 kcal/mol)
Positive average value: 0.02816180 a.u. (17.67181 kcal/mol)
Negative average value: -0.01808310 a.u. (-11.34732 kcal/mol)
Overall variance (sigma²_tot): 0.00043271 a.u.² (170.38782 (kcal/mol)²)
Positive variance: 0.00035671 a.u.² (140.45988 (kcal/mol)²)
Negative variance: 0.00007600 a.u.² (29.92794 (kcal/mol)²)
Balance of charges (miu): 0.14479449
Product of sigma²_tot and miu: 0.00006265 a.u.² (24.67122 (kcal/mol)²)
Internal charge separation (Pi): 0.02330229 a.u. (14.62242 kcal/mol)

Compound DC1

Volume: 966.80286 Bohr³ (143.26543 Angstrom³)
Minimal value: -30.14282 kcal/mol Maximal value: 65.23525 kcal/mol
Overall surface area: 541.66315 Bohr² (151.68115 Angstrom²)

Positive surface area: 274.46728 Bohr² (76.85868 Angstrom²)
Negative surface area: 267.19588 Bohr² (74.82248 Angstrom²)
Overall average value: 0.00849216 a.u. (5.32892 kcal/mol)
Positive average value: 0.03966251 a.u. (24.88862 kcal/mol)
Negative average value: -0.02352645 a.u. (-14.76308 kcal/mol)
Overall variance (σ^2_{tot}): 0.00079617 a.u.² (313.50795 (kcal/mol)²)
Positive variance: 0.00065554 a.u.² (258.13082 (kcal/mol)²)
Negative variance: 0.00014063 a.u.² (55.37713 (kcal/mol)²)
Balance of charges (μ): 0.14543642
Product of σ^2_{tot} and μ : 0.00011579 a.u.² (45.59547 (kcal/mol)²)
Internal charge separation (Π): 0.03208041 a.u. (20.13078 kcal/mol)

Compound DC2

Volume: 1043.98025 Bohr³ (154.70195 Angstrom³)
Minimal value: -24.05070 kcal/mol Maximal value: 39.13179 kcal/mol
Overall surface area: 581.15956 Bohr² (162.74127 Angstrom²)
Positive surface area: 338.03430 Bohr² (94.65926 Angstrom²)
Negative surface area: 243.12526 Bohr² (68.08202 Angstrom²)
Overall average value: 0.00825081 a.u. (5.17746 kcal/mol)
Positive average value: 0.02670583 a.u. (16.75818 kcal/mol)
Negative average value: -0.01740852 a.u. (-10.92402 kcal/mol)
Overall variance (σ^2_{tot}): 0.00043328 a.u.² (170.61123 (kcal/mol)²)
Positive variance: 0.00034334 a.u.² (135.19570 (kcal/mol)²)
Negative variance: 0.00008994 a.u.² (35.41553 (kcal/mol)²)
Balance of charges (μ): 0.16449072
Product of σ^2_{tot} and μ : 0.00007127 a.u.² (28.06396 (kcal/mol)²)
Internal charge separation (Π): 0.02209189 a.u. (13.86288 kcal/mol)

Compound TA1

Volume: 2906.83684 Bohr³ (430.74887 Angstrom³)
Minimal value: -18.83521 kcal/mol Maximal value: 56.01930 kcal/mol
Overall surface area: 1435.19191 Bohr² (401.89472 Angstrom²)
Positive surface area: 803.17731 Bohr² (224.91259 Angstrom²)
Negative surface area: 632.01460 Bohr² (176.98214 Angstrom²)
Overall average value: 0.01733211 a.u. (10.87607 kcal/mol)
Positive average value: 0.04369001 a.u. (27.41592 kcal/mol)
Negative average value: -0.01616405 a.u. (-10.14311 kcal/mol)
Overall variance (σ^2_{tot}): 0.00066315 a.u.² (261.12724 (kcal/mol)²)
Positive variance: 0.00060282 a.u.² (237.37115 (kcal/mol)²)
Negative variance: 0.00006033 a.u.² (23.75609 (kcal/mol)²)
Balance of charges (μ): 0.08269867
Product of σ^2_{tot} and μ : 0.00005484 a.u.² (21.59487 (kcal/mol)²)

Internal charge separation (Pi): 0.03170842 a.u. (19.89735 kcal/mol)

Compound TA2 :

Volume: 3074.05051 Bohr³ (455.52739 Angstrom³)

Minimal value: -19.68635 kcal/mol Maximal value: 58.42148 kcal/mol

Overall surface area: 1532.00390 Bohr² (429.00485 Angstrom²)

Positive surface area: 903.12636 Bohr² (252.90118 Angstrom²)

Negative surface area: 628.87753 Bohr² (176.10367 Angstrom²)

Overall average value: 0.01694446 a.u. (10.63282 kcal/mol)

Positive average value: 0.03823968 a.u. (23.99578 kcal/mol)

Negative average value: -0.01363745 a.u. (-8.55764 kcal/mol)

Overall variance (sigma²_tot): 0.00059216 a.u.² (233.17479 (kcal/mol)²)

Positive variance: 0.00054073 a.u.² (212.92135 (kcal/mol)²)

Negative variance: 0.00005143 a.u.² (20.25344 (kcal/mol)²)

Balance of charges (miu): 0.07931491

Product of sigma²_tot and miu: 0.00004697 a.u.² (18.49424 (kcal/mol)²)

Internal charge separation (Pi): 0.02768148 a.u. (17.37041 kcal/mol)

Compound TB1

Volume: 2217.58109 Bohr³ (328.61168 Angstrom³)

Minimal value: -24.85803 kcal/mol Maximal value: 65.42844 kcal/mol

Overall surface area: 1140.66622 Bohr² (319.41912 Angstrom²)

Positive surface area: 571.17585 Bohr² (159.94555 Angstrom²)

Negative surface area: 569.49036 Bohr² (159.47357 Angstrom²)

Overall average value: 0.00653819 a.u. (4.10278 kcal/mol)

Positive average value: 0.03262490 a.u. (20.47245 kcal/mol)

Negative average value: -0.01962573 a.u. (-12.31534 kcal/mol)

Overall variance (sigma²_tot): 0.00069425 a.u.² ((kcal/mol)²)

Positive variance: 0.00058895 a.u.² (231.90887 (kcal/mol)²)

Negative variance: 0.00010530 a.u.² (41.46336 (kcal/mol)²)

Balance of charges (miu): 0.12866874

Product of sigma²_tot and miu: 0.00008933 a.u.² (35.17446 (kcal/mol)²)

Internal charge separation (Pi): 0.02653995 a.u. (16.65408 kcal/mol)

Compound TB2

Volume: 2334.97192 Bohr³ (346.00722 Angstrom³)

Minimal value: -19.49760 kcal/mol Maximal value: 43.06441 kcal/mol

Overall surface area: 1204.42582 Bohr² (337.27363 Angstrom²)

Positive surface area: 728.11938 Bohr² (203.89422 Angstrom²)

Negative surface area: 476.30644 Bohr² (133.37941 Angstrom²)

Overall average value: 0.00966833 a.u. (6.06697 kcal/mol)

Positive average value: 0.02618258 a.u. (16.42983 kcal/mol)
Negative average value: -0.01557664 a.u. (-9.77450 kcal/mol)
Overall variance (σ^2_{tot}): 0.00038827 a.u.² (152.88983 (kcal/mol)²)
Positive variance: 0.00032027 a.u.² (126.11267 (kcal/mol)²)
Negative variance: 0.00006800 a.u.² (26.77716 (kcal/mol)²)
Balance of charges (μ): 0.14446614
Product of σ^2_{tot} and μ : 0.00005609 a.u.² (22.08740 (kcal/mol)²)
Internal charge separation (Π): 0.02101354 a.u. (13.18621 kcal/mol)

Compound TC1

Volume: 1447.70039 Bohr³ (214.52711 Angstrom³)
Minimal value: -26.09009 kcal/mol Maximal value: 50.93846 kcal/mol
Overall surface area: 741.36041 Bohr² (207.60209 Angstrom²)
Positive surface area: 427.96867 Bohr² (119.84345 Angstrom²)
Negative surface area: 313.39173 Bohr² (87.75864 Angstrom²)
Overall average value: 0.01190513 a.u. (7.47059 kcal/mol)
Positive average value: 0.03539949 a.u. (22.21353 kcal/mol)
Negative average value: -0.02017884 a.u. (-12.66242 kcal/mol)
Overall variance (σ^2_{tot}): 0.00052833 a.u.² (208.03858 (kcal/mol)²)
Positive variance: 0.00040739 a.u.² (160.41787 (kcal/mol)²)
Negative variance: 0.00012094 a.u.² (47.62070 (kcal/mol)²)
Balance of charges (μ): 0.17650654
Product of σ^2_{tot} and μ : 0.00009325 a.u.² (36.72017 (kcal/mol)²)
Internal charge separation (Π): 0.02834593 a.u. (17.78736 kcal/mol)

Compound TC2

Volume: 1612.07542 Bohr³ (238.88498 Angstrom³)
Estimated density according to mass and volume: 1.9124 g/cm³
Minimal value: -24.43607 kcal/mol Maximal value: 51.76366 kcal/mol
Overall surface area: 844.59867 Bohr² (236.51175 Angstrom²)
Positive surface area: 508.60445 Bohr² (142.42377 Angstrom²)
Negative surface area: 335.99422 Bohr² (94.08798 Angstrom²)
Overall average value: 0.01162547 a.u. (7.29510 kcal/mol)
Positive average value: 0.02964808 a.u. (18.60446 kcal/mol)
Negative average value: -0.01565590 a.u. (-9.82423 kcal/mol)
Overall variance (σ^2_{tot}): 0.00038439 a.u.² (151.36069 (kcal/mol)²)
Positive variance: 0.00030457 a.u.² (119.92904 (kcal/mol)²)
Negative variance: 0.00007982 a.u.² (31.43166 (kcal/mol)²)
Balance of charges (μ): 0.16453769
Product of σ^2_{tot} and μ : 0.00006325 a.u.² (24.90454 (kcal/mol)²)
Internal charge separation (Π): 0.02282237 a.u. (14.32127 kcal/mol)

MA3 anion:

Volume: 1279.74657 Bohr³ (189.63892 Angstrom³)

Estimated density according to mass and volume: 1.7693 g/cm³
Minimal value: -107.91492 kcal/mol Maximal value: -55.87074 kcal/mol
Overall surface area: 690.50574 Bohr² (193.36133 Angstrom²)
Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)
Negative surface area: 690.50574 Bohr² (193.36133 Angstrom²)
Overall average value: -0.13171476 a.u. (-82.65233 kcal/mol)
Positive average value: NaN a.u. (NaN kcal/mol)
Negative average value: -0.13171476 a.u. (-82.65233 kcal/mol)
Overall variance (sigma²_tot): 0.00029689 a.u.² (116.90794 (kcal/mol)²)
Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Negative variance: 0.00029689 a.u.² (116.90794 (kcal/mol)²)
Balance of charges (miu): 0.00000000
Product of sigma²_tot and miu: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Internal charge separation (Pi): 0.01359900 a.u. (8.53351 kcal/mol)

MB3 anion:

Volume: 1038.23191 Bohr³ (153.85013 Angstrom³)
Estimated density according to mass and volume: 1.7059 g/cm³
Minimal value: -113.96418 kcal/mol Maximal value: -61.04470 kcal/mol
Overall surface area: 580.13742 Bohr² (162.45505 Angstrom²)
Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)
Negative surface area: 580.13742 Bohr² (162.45505 Angstrom²)
Overall average value: -0.14366820 a.u. (-90.15323 kcal/mol)
Positive average value: NaN a.u. (NaN kcal/mol)
Negative average value: -0.14366820 a.u. (-90.15323 kcal/mol)
Overall variance (sigma²_tot): 0.00035966 a.u.² (141.62191 (kcal/mol)²)
Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Negative variance: 0.00035966 a.u.² (141.62191 (kcal/mol)²)
Balance of charges (miu): 0.00000000
Product of sigma²_tot and miu: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Internal charge separation (Pi): 0.01457687 a.u. (9.14713 kcal/mol)

MC3 anion:

Volume: 797.79341 Bohr³ (118.22081 Angstrom³)
Estimated density according to mass and volume: 1.6019 g/cm³
Minimal value: -120.40369 kcal/mol Maximal value: -69.57497 kcal/mol
Overall surface area: 461.88430 Bohr² (129.34080 Angstrom²)
Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)
Negative surface area: 461.88430 Bohr² (129.34080 Angstrom²)
Overall average value: -0.16126228 a.u. (-101.19369 kcal/mol)
Positive average value: NaN a.u. (NaN kcal/mol)
Negative average value: -0.16126228 a.u. (-101.19369 kcal/mol)
Overall variance (sigma²_tot): 0.00029397 a.u.² (115.75683 (kcal/mol)²)
Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)

Negative variance: 0.00029397 a.u.² (115.75683 (kcal/mol)²)
Balance of charges (miu): 0.00000000
Product of sigma²_tot and miu: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Internal charge separation (Pi): 0.01417122 a.u. (8.89258 kcal/mol)

DA3 anion:

Volume: 2013.84699 Bohr³ (298.42140 Angstrom³)
Estimated density according to mass and volume: 1.7367 g/cm³
Minimal value: -178.44394 kcal/mol Maximal value: -116.53200 kcal/mol
Overall surface area: 1023.36120 Bohr² (286.57036 Angstrom²)
Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)
Negative surface area: 1023.36120 Bohr² (286.57036 Angstrom²)
Overall average value: -0.22228810 a.u. (-139.48801 kcal/mol)
Positive average value: NaN a.u. (NaN kcal/mol)
Negative average value: -0.22228810 a.u. (-139.48801 kcal/mol)
Overall variance (sigma²_tot): 0.00036477 a.u.² (143.63345 (kcal/mol)²)
Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Negative variance: 0.00036477 a.u.² (143.63345 (kcal/mol)²)
Balance of charges (miu): 0.00000000
Product of sigma²_tot and miu: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Internal charge separation (Pi): 0.01413093 a.u. (8.86730 kcal/mol)

DB3 anion:

Volume: 1535.23553 Bohr³ (227.49848 Angstrom³)
Estimated density according to mass and volume: 1.6357 g/cm³
Minimal value: -191.20334 kcal/mol Maximal value: -126.92306 kcal/mol
Overall surface area: 806.20684 Bohr² (225.76094 Angstrom²)
Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)
Negative surface area: 806.20684 Bohr² (225.76094 Angstrom²)
Overall average value: -0.24787202 a.u. (-155.54217 kcal/mol)
Positive average value: NaN a.u. (NaN kcal/mol)
Negative average value: -0.24787202 a.u. (-155.54217 kcal/mol)
Overall variance (sigma²_tot): 0.00047538 a.u.² (187.18912 (kcal/mol)²)
Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Negative variance: 0.00047538 a.u.² (187.18912 (kcal/mol)²)
Balance of charges (miu): 0.00000000
Product of sigma²_tot and miu: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Internal charge separation (Pi): 0.01847348 a.u. (11.59230 kcal/mol)

DC3 anion:

Volume: 1063.42398 Bohr³ (157.58321 Angstrom³)
Estimated density according to mass and volume: 1.4339 g/cm³
Minimal value: -210.79858 kcal/mol Maximal value: -176.03586 kcal/mol
Overall surface area: 574.79324 Bohr² (160.95852 Angstrom²)

Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)
Negative surface area: 574.79324 Bohr² (160.95852 Angstrom²)
Overall average value: -0.29375109 a.u. (-184.33175 kcal/mol)
Positive average value: NaN a.u. (NaN kcal/mol)
Negative average value: -0.29375109 a.u. (-184.33175 kcal/mol)
Overall variance (σ^2_{tot}): 0.00013655 a.u.² (53.76893 (kcal/mol)²)
Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Negative variance: 0.00013655 a.u.² (53.76893 (kcal/mol)²)
Balance of charges (μ): 0.00000000
Product of σ^2_{tot} and μ : 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Internal charge separation (Π): 0.00928352 a.u. (5.82550 kcal/mol)

TA3 anion:

Volume: 3063.85059 Bohr³ (454.01591 Angstrom³)
Estimated density according to mass and volume: 1.7635 g/cm³
Minimal value: -209.62527 kcal/mol Maximal value: -157.42359 kcal/mol
Overall surface area: 1507.80556 Bohr² (422.22862 Angstrom²)
Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)
Negative surface area: 1507.80556 Bohr² (422.22862 Angstrom²)
Overall average value: -0.28635540 a.u. (-179.69088 kcal/mol)
Positive average value: NaN a.u. (NaN kcal/mol)
Negative average value: -0.28635540 a.u. (-179.69088 kcal/mol)
Overall variance (σ^2_{tot}): 0.00039787 a.u.² (156.66935 (kcal/mol)²)
Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Negative variance: 0.00039787 a.u.² (156.66935 (kcal/mol)²)
Balance of charges (μ): 0.00000000
Product of σ^2_{tot} and μ : 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Internal charge separation (Π): 0.01646817 a.u. (10.33394 kcal/mol)

TB3 anion:

Volume: 2349.66249 Bohr³ (348.18413 Angstrom³)
Estimated density according to mass and volume: 1.6699 g/cm³
Minimal value: -225.79030 kcal/mol Maximal value: -170.53853 kcal/mol
Overall surface area: 1184.79051 Bohr² (331.77518 Angstrom²)
Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)
Negative surface area: 1184.79051 Bohr² (331.77518 Angstrom²)
Overall average value: -0.31699270 a.u. (-198.91609 kcal/mol)
Positive average value: NaN a.u. (NaN kcal/mol)
Negative average value: -0.31699270 a.u. (-198.91609 kcal/mol)
Overall variance (σ^2_{tot}): 0.00054246 a.u.² (213.60311 (kcal/mol)²)
Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)
Negative variance: 0.00054246 a.u.² (213.60311 (kcal/mol)²)
Balance of charges (μ): 0.00000000
Product of σ^2_{tot} and μ : 0.00000000 a.u.² (0.00000 (kcal/mol)²)

Internal charge separation (Pi): 0.02084066 a.u. (13.07772 kcal/mol)

TC3 anion:

Volume: 1649.66108 Bohr³ (244.45460 Angstrom³)

Estimated density according to mass and volume: 1.4816 g/cm³

Minimal value: -255.54724 kcal/mol Maximal value: -220.87100 kcal/mol

Overall surface area: 843.19264 Bohr² (236.11802 Angstrom²)

Positive surface area: 0.00000 Bohr² (0.00000 Angstrom²)

Negative surface area: 843.19264 Bohr² (236.11802 Angstrom²)

Overall average value: -0.37621358 a.u. (-236.07778 kcal/mol)

Positive average value: NaN a.u. (NaN kcal/mol)

Negative average value: -0.37621358 a.u. (-236.07778 kcal/mol)

Overall variance (sigma²_tot): 0.00026540 a.u.² (104.50459 (kcal/mol)²)

Positive variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)

Negative variance: 0.00026540 a.u.² (104.50459 (kcal/mol)²)

Balance of charges (miu): 0.00000000

Product of sigma²_tot and miu: 0.00000000 a.u.² (0.00000 (kcal/mol)²)

Internal charge separation (Pi): 0.01388374 a.u. (8.71219 kcal/mol)

Hydroxylammonium cation:

Volume: 291.52729 Bohr³ (43.19990 Angstrom³)

Estimated density according to mass and volume: 1.3084 g/cm³

Minimal value: 83.33440 kcal/mol Maximal value: 187.12046 kcal/mol

Overall surface area: 223.16346 Bohr² (62.49214 Angstrom²)

Positive surface area: 223.16346 Bohr² (62.49214 Angstrom²)

Negative surface area: 0.00000 Bohr² (0.00000 Angstrom²)

Overall average value: 0.24160362 a.u. (151.60869 kcal/mol)

Positive average value: 0.24160362 a.u. (151.60869 kcal/mol)

Negative average value: NaN a.u. (NaN kcal/mol)

Overall variance (sigma²_tot): 0.00250511 a.u.² (986.43403 (kcal/mol)²)

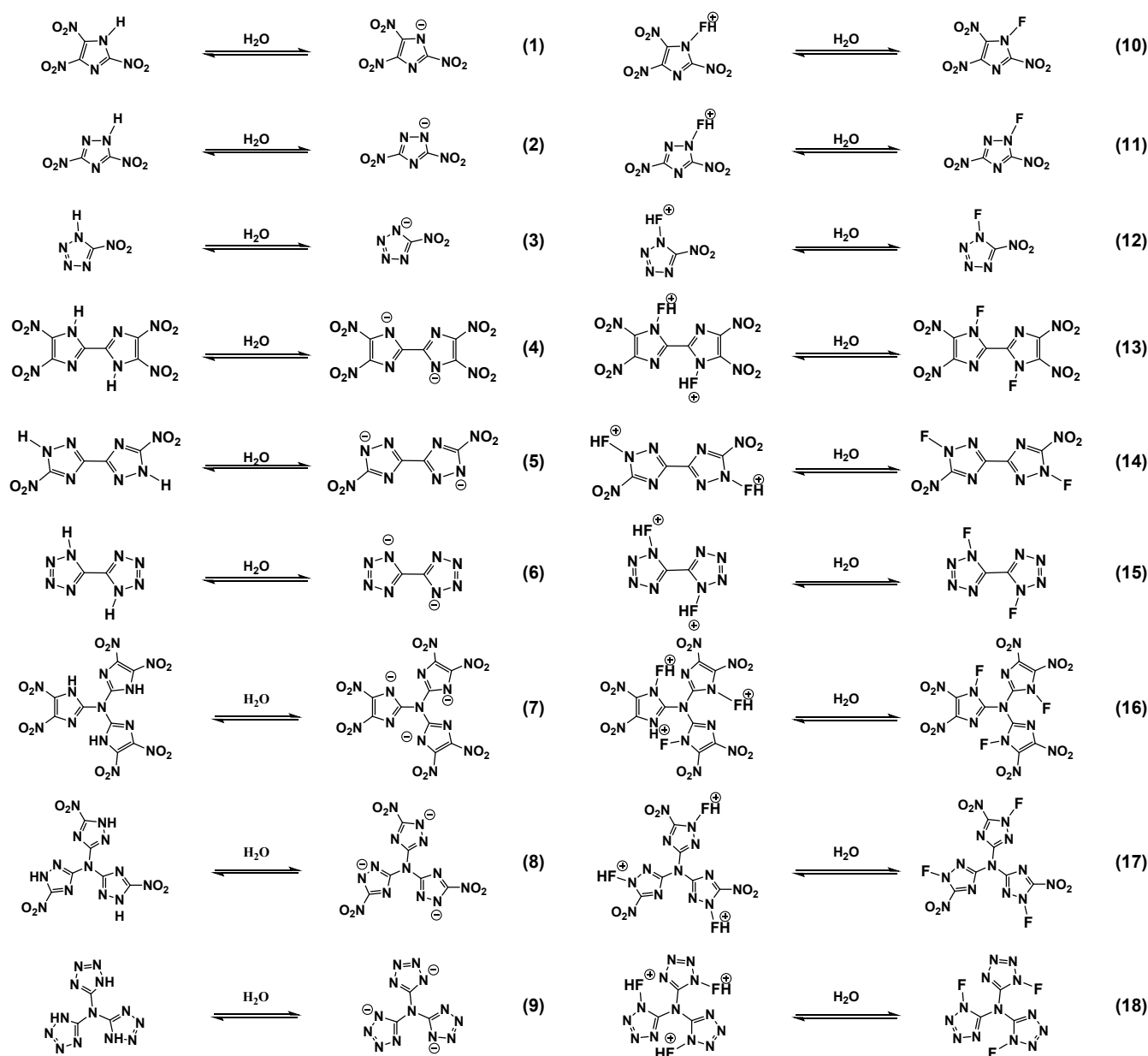
Positive variance: 0.00250511 a.u.² (986.43403 (kcal/mol)²)

Negative variance: 0.00000000 a.u.² (0.00000 (kcal/mol)²)

Balance of charges (miu): 0.00000000

Product of sigma²_tot and miu: 0.00000000 a.u.² (0.00000 (kcal/mol)²)

Internal charge separation (Pi): 0.04316710 a.u. (27.08779 kcal/mol)



Scheme S2 The deprotonation reaction of parent compounds and N-fluorination compounds.