Supplementary Materials

Table S1. Selected geometrical parameters and other properties of the global minimum structure, SKF86002**B**, compared with conformers SKF86002**A**, SKF86002**C** and SKF86002**D***

Parameters	SKF86002B	SKF86002A (Δ)	SKF86002C (Δ)	SKF86002D (Δ)
R1[a]	8.382	8.383 (-0.001)	8.412 (-0.030)	8.373 (+0.009)
R2a [a]	6.856	6.852 (+0.004)	7.007 (-0.151)	6.78 (+0.076)
R2b[a]	7.987	7.985 (+0.002)	7.959 (+0.028)	7.896 (+0.091)
R3 [a]	8.283	8.283 (0.000)	8.341 (-0.058)	8.256 (+0.027)
Bond length (Å)				
$C_{(21)}$-$F_{(2)}$	1.361	1.361 (0.000)	1.349 (+0.012)	1.34 (+0.021)
$C_{(10)}$-$C_{(12)}$	1.474	1.474 (0.000)	1.512 (-0.038)	1.43 (+0.044)
$C_{(8)}$-$N_{(4)}$	1.308	1.309 (-0.001)	1.336 (-0.028)	1.31 (-0.002)
$C_{(8)}$-$N_{(3)}$	1.366	1.362 (+0.004)	1.402 (-0.036)	1.36 (+0.006)
$C_{(8)}$-$S_{(1)}$	1.765	1.766 (-0.001)	1.730 (+0.035)	1.72 (+0.045)
$C_{(9)}$-$S_{(1)}$	1.856	1.857 (-0.001)	1.791 (+0.065)	1.84 (+0.016)
$C_{(7)}$-$C_{(11)}$	1.468	1.468 (0.000)	1.491 (-0.023)	1.44 (+0.028)
$C_{(20)}$-$N_{(5)}$	1.342	1.342 (0.000)	1.361 (-0.019)	1.35 (-0.008)
$C_{(19)}$-$N_{(5)}$	1.340	1.339 (+0.001)	1.355 (-0.015)	1.35 (-0.010)
$C_{(10)}$-$C_{(7)}$	1.395	1.397 (-0.002)	1.431 (-0.036)	1.39 (+0.005)
$N_{(3)}$-$C_{(6)}$	1.460	1.458 (+0.002)	1.491 (-0.031)	1.45 (+0.01)
Bond angle (°)				
$C_{(8)}$-$S_{(1)}$-$C_{(9)}$	88.94	88.63 (+0.31)	93.74 (-4.80)	91.72 (-2.78)
$N_{(3)}$-$C_{(6)}$-$C_{(9)}$	104.33	104.67 (-0.34)	109.66 (-5.33)	106.45 (-2.12)
$C_{(10)}$-$N_{(4)}$-$C_{(8)}$	104.86	104.92 (-0.06)	106.54 (-1.68)	103.06 (+1.80)
$C_{(7)}$-$N_{(3)}$-$C_{(6)}$	134.44	136.21 (-1.77)	141.45 (-7.01)	133.45 (+0.99)
$N_{(4)}$-$C_{(8)}$-$S_{(1)}$	132.86	133.4 (-0.54)	132.42 (+0.44)	134.40 (-1.54)
Dihedral angle (°)				
$C_{(14)}$-$C_{(11)}$-$C_{(7)}$-$C_{(10)}$	-47.90	42.63 (-90.53)	-52.78 (+4.88)	-90.15 (+42.25)
$C_{(16)}$-$C_{(12)}$-$C_{(10)}$-$N_{(4)}$	148.12	30.35 (+117.77)	164.89 (-16.77)	90.34 (+57.78)
$N_{(3)}$–$C_{(8)}$–$S_{(1)}$–$C_{(9)}$	9.99	15.1 (-5.11)	-1.70 (+11.69)	10.16 (-0.17)
$C_{(10)}$-$N_{(4)}$-$C_{(8)}$-$N_{(3)}$	1.66	0.32 (+1.34)	-0.19 (+1.85)	-0.17 (+1.83)

$C_{(8)}$-$S_{(1)}$-$C_{(9)}$-$C_{(6)}$	-25.42	-26.8 (+1.38)	2.84 (-28.26)	-18.56 (-6.86)
$N_{(3)}$-$C_{(6)}$-$C_{(9)}$-$S_{(1)}$	33.75	31.44 (+2.31)	-3.28 (+37.03)	21.85 (+11.90)
$N_{(4)}$-$C_{(8)}$-$S_{(1)}$-$C_{(9)}$	-175.55	-166.14 (-9.41)	178.43 (-353.98)	-169.42 (-6.13)
$C_{(11)}$-$C_{(7)}$-$N_{(3)}$-$C_{(6)}$	-19.65	-8.51 (-11.14)	-0.39 (-19.26)	-1.94 (-17.71)
$C_{(12)}$-$C_{(10)}$-$C_{(7)}$-$C_{(11)}$	-4.85	6.53 (-11.38)	1.95 (-6.80)	-0.19 (-4.66)
$\langle R^2 \rangle$ (a.u.)	7310.6635	7311.3428 (-0.6793)	7569.4695 (-258.8060)	6976.9344 (+333.7291)
***μ* (D)**	5.34	5.37 (-0.03)	5.92 (-0.58)	5.34 (0.00)
***E* (E_h)**	-1279.243354	-1279.2433 (-0.00008)	-1278.0769 (-1.16645)	-1278.082 (-1.16132)
ZPE (kcal·mol^{-1})	157.14303	157.09623 (+0.04680)	155.64052 (+1.50251)	157.43193 (-0.28890)
***E* + ZPE (E_h)**	-1278.993197	-1278.9929 (-0.00027)	-1278.9761 (-0.01713)	-1278.9733 (-0.01995)
HOMO-LUMO gap (eV)	0.17	0.16 (+0.01)	0.16 (+0.01)	0.18 (-0.01)
Rotational Const. A (GHz)	0.3550	0.3560 (-0.0010)	0.3451 (+0.0099)	0.3771 (-0.0221)
B (GHz)	0.2098	0.2095 (+0.0003)	0.2029 (+0.0069)	0.2091 (+0.0007)
C (GHz)	0.1374	0.1373 (+0.0001)	0.1318 (+0.0056)	0.1486 (-0.0112)

***** Using the B3LYP/6-31+G* level of theory.

[a] Perimeters [17] of the fluorophenyl (R1), imidazolyl (R2a), thiophenyl (R2b) and pyridinyl (R3) aromatic rings, respectively.