Supporting Information

Efficient Synthesis of Cyclic Amidines-Based Fluorophores via 6π-Electrocyclic Ring Closure

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### Index:

| Topic                                                                 | Page(s)  |
|----------------------------------------------------------------------|----------|
| General methods                                                     | S3       |
| General procedure and spectral data for the synthesis of 3          | S4-S16   |
| General procedure and appraised data for the synthesis of 4         | S17-S18  |
| Confocal imaging experiments                                        | S19      |
| Cytotoxicity assays                                                 | S19      |
| Photophysical properties of 3                                        | S20-S23  |
| X-ray Structure of 3aw                                               | S24-S26  |
| Copies of $^1$H and $^{13}$C NMR of 3                               | S27-S84  |
| Computational Details                                               | S85-S94  |
| References                                                          | S95      |
General methods:

Unless stated otherwise, all solvents were purified and dried according to standard methods prior to use. The solvents were distilled from indicated drying reagents: dichlormethane (CaH₂), tetrahydrofuran (Na), diethyl ether (Na), ethyl acetate (CaCl₂), 1,4-Dioxane (Na), toluene (Na). N-sulfonly triazoles 1[1] were prepared according to literature and phenylamine 2 were purchased from Energy chemical and Macklin (China). The reaction products were purified by chromatograph, using 200-300 mesh silica gel (Qingdao, China). ¹H and ¹³C NMR spectra were recorded on a Varian instrument (400 MHz and 100 MHz, respectively) and internally referenced to tetramethylsilane signal or residual protio solvent signals. Data for ¹H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet or unresolved, coupling constant (s) in Hz, integration). Data for ¹³C NMR are reported in terms of chemical shift (δ, ppm). High resolution mass spectra (HRMS) were obtained by the ESI ionization sources. IR spectra were recorded on a FT-IR spectrometer and only major peaks were reported in cm⁻¹. Absorption spectra were obtained on a SHIMADZU UV-2600 spectrophotometer. Fluorescence spectra and absolute fluorescence quantum yield were obtained on a HORIBA Fluoromax-4 spectrofluorometer with a calibrated integrating sphere. The photostability was tested on an EDINBURGH FLS920 spectrometer. WT 22RV1 cells or NK-1 receptors-overexpressed 22RV1 cells were supplied by the Mou laboratory of Lanzhou University. Hela cells were supplied by the Li laboratory of Sun Yat-Sen University. The confocal imaging experiments were performed on a ZEISS LSM T-PMT confocal fluorescent microscope. NK1R inhibitor aprepitant was purchased from Sigma-Aldrich.
General procedure and spectral data for the synthesis of 3

A solution of N-sulfonly triazoles 1 (0.10 mmol, 1.0 equiv) and phenylamine 2 (0.12 mmol, 1.2 equiv) in dry CHCl₃ (2 mL) was stirred at 120 °C for 4h in a well-sealed tube. After completion of the reaction as indicated by TLC, the reaction was cooled to room temperature, and the mixture was purified by silica gel column flash chromatography (DCM: MeOH = 20:1 to 10:1) to afford product 3 as yellow solid.

1 mmol scale for the synthesis of 3au

A solution of N-sulfonly triazoles 1a (1.0 mmol, 1.0 equiv) and 3-(4-aminophenyl)propanoic acid (1.2 mmol, 1.2 equiv) in dry CHCl₃ (20 mL) was stirred at 120 °C for 4h in a well-sealed tube. After completion of the reaction as indicated by TLC, the reaction was cooled to room temperature, and the mixture was purified by silica gel column flash chromatography (DCM: MeOH = 20:1 to 10:1) to afford product 3au in 92.4% yield as yellow solid.

Spectral data for the cyclic amidines 3

4-methyl-N-(2-phenylisoquinolin-3(2H)-ylidene)benzenesulfonamide (3aa)

Yellow solid (34.0 mg, 91% yield);

\(^{1}\text{H NMR (400 MHz, CDCl}_3\):} \(\delta 8.44 \text{ (s, 1H), 7.93 \text{ (s, 1H), 7.67 \text{ (d, } J = 8.2 \text{ Hz, 2H), 7.58 \text{ (d, } J = 8.5 \text{ Hz, 1H), 7.51 \text{ (d, } J = 5.1 \text{ Hz, 2H), 7.49 - 7.42 \text{ (m, 3H), 7.35 - 7.28 \text{ (m, 2H), 7.22 - 7.15 \text{ (m, 1H), 7.12 \text{ (d, } J = 8.0 \text{ Hz, 2H), 2.33 \text{ (s, 3H);}}}

\(^{13}\text{C NMR (100 MHz, CDCl}_3\):} \(\delta 152.5, 142.7, 141.8, 141.6, 141.3, 141.1, 134.2, 129.6, 129.4, 128.9, 127.9, 126.6, 126.2, 125.7, 125.4, 120.0, 111.4, 21.4;

IR: 2923, 1640, 1601, 1494, 1471, 1367, 1274, 1262, 1131, 1080, 951, 763 cm\(^{-1}\);}
HRMS (ESI): C_{22}H_{18}N_{2}O_{2}S+H, Calc: 375.1162, Found: 375.1148.

4-methyl-N-(2-(o-tolyl)isoquinolin-3(2H)-yldene)benzenesulfonamide (3ab)

Yellow solid (27.9 mg, 72% yield);

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.34 (s, 1H), 8.02 (s, 1H), 7.67 (d, $J = 8.2$ Hz, 2H), 7.63 – 7.48 (m, 3H), 7.44 (dd, $J = 10.8$, 4.1 Hz, 1H), 7.41 – 7.32 (m, 2H), 7.25 – 7.08 (m, 4H), 2.34 (s, 3H), 2.02 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 152.6, 142.0, 142.0, 141.5, 141.2, 141.0, 134.3, 134.0, 131.2, 129.9, 128.8, 127.7, 127.2, 126.4, 126.2, 125.9, 125.3, 120.0, 111.5, 21.3, 17.6;

IR: 2922, 1640, 1600, 1468, 1367, 1269, 1131, 1081, 950, 763 cm$^{-1}$;

HRMS (ESI): C_{23}H_{20}N_{2}O_{2}S+H, Calc: 389.1318, Found: 389.1318.

N-(2-(3-(benzyloxy)phenyl)isoquinolin-3(2H)-yldene)-4-methylbenzenesulfonamide (3ac)

Yellow solid (41.3 mg, 86% yield);

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.45 (s, 1H), 7.95 (s, 1H), 7.74 (d, $J = 8.2$ Hz, 2H), 7.59 (d, $J = 8.6$ Hz, 1H), 7.52 (d, $J = 3.4$ Hz, 2H), 7.38 (dt, $J = 11.8$, 4.1 Hz, 6H), 7.25 – 7.18 (m, 1H), 7.11 (ddd, $J = 9.8$, 8.4, 4.9 Hz, 3H), 7.00 (t, $J = 2.2$ Hz, 1H), 6.92 (dd, $J = 7.8$, 1.2 Hz, 1H), 4.97 (s, 2H), 2.36 – 2.26 (m, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 159.3, 152.4, 142.6, 141.8, 141.5, 141.1, 136.3, 134.1, 130.2, 128.9 128.7, 128.2, 127.9, 127.6, 126.2, 125.8, 125.3, 119.9 119.0, 116.4, 113.4, 111.4, 70.4, 21.3;

IR: 2922, 1640, 1601, 1469, 1367, 1131, 1080, 953 cm$^{-1}$;

HRMS (ESI): C_{29}H_{26}N_{2}O_{3}S+H, Calc: 481.1580, Found: 481.1580.

4-methyl-N-(2-(3-(methylthio)phenyl)isoquinolin-3(2H)-yldene)benzenesulfonamide (3ad)
N-(2-(3-chlorophenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3ae)

Yellow solid (28.6 mg, 70% yield);

**1H NMR (400 MHz, CDCl3):** δ 8.40 (s, 1H), 8.01 (s, 1H), 7.73 (d, J = 8.2 Hz, 2H), 7.56 (dd, J = 14.3, 7.0 Hz, 3H), 7.52 – 7.41 (m, 2H), 7.36 (t, J = 1.8 Hz, 1H), 7.32 – 7.25 (m, 2H), 7.25 – 7.11 (m, 3H), 2.37 (s, 3H);

**13C NMR (100 MHz, CDCl3):** δ 152.5, 142.4, 142.0, 142.0, 141.3, 141.2, 135.0, 134.3, 130.5, 130.0, 129.0, 127.8, 127.1, 126.1, 125.9, 125.6, 125.0, 120.0, 111.7, 21.4;

**IR:** 2922, 1641, 1601, 1469, 1368, 1268, 1132, 1081, 952 cm⁻¹;

**HRMS (ESI):** C_{22}H_{17}N_{2}O_{2}SCl+H, Calc: 409.0772, Found: 409.0772.

N-(2-(3-bromophenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3af)

Yellow solid (33.4 mg, 74% yield);

**1H NMR (400 MHz, CDCl3):** δ 8.42 (d, J = 2.2 Hz, 1H), 8.01 (d, J = 5.7 Hz, 1H), 7.79 – 7.70 (m, 2H), 7.63 – 7.48 (m, 3H), 7.46 – 7.32 (m, 2H), 7.25 – 7.13 (m, 4H), 7.13 – 7.06 (m, 1H), 2.46 (s, 3H), 2.36 (s, 3H);

**13C NMR (100 MHz, CDCl3):** δ 152.5, 142.2, 142.2, 141.9, 141.4, 141.1, 140.8, 134.2, 129.6, 128.9, 127.7, 127.3, 126.2, 125.9, 125.4, 124.0, 122.9, 119.9, 111.6, 21.4, 15.5.

**IR:** 3056, 1639, 1600, 1467, 1366, 1265, 1130, 1080, 951 cm⁻¹;

**HRMS (ESI):** C_{23}H_{20}N_{2}O_{2}S_{2}+H, Calc: 421.1039, Found: 421.1039.
1H NMR (400 MHz, CDCl3): δ 8.39 (s, 1H), 7.98 (s, 1H), 7.71 (d, J = 8.2 Hz, 2H), 7.63 (d, J = 8.0 Hz, 1H), 7.60 – 7.46 (m, 4H), 7.37 (t, J = 8.0 Hz, 1H), 7.31 (d, J = 8.6 Hz, 1H), 7.24 – 7.12 (m, 3H), 2.35 (s, 3H);

13C NMR (100 MHz, CDCl3): δ 152.4, 142.4, 142.0, 141.3, 141.2, 141.1, 134.4, 132.9, 130.8, 129.9, 129.0, 127.8, 126.1, 125.9, 125.6, 125.5, 122.6, 120.0, 111.7, 21.5;

IR: 3026, 1643, 1601, 1474, 1369, 1269, 1130, 1136, 1084, 766, 743 cm⁻¹;

HRMS (ESI): C22H17N2O2SBr+H, Calc: 453.0267, Found: 453.0264.

4-methyl-N-(2-(p-tolyl)isoquinolin-3(2H)-ylidene)benzenesulfonamide (3ag)

Yellow solid (36.1 mg, 93% yield);

1H NMR (400 MHz, CDCl3): δ 8.35 (s, 1H), 7.84 (s, 1H), 7.63 (d, J = 8.2 Hz, 2H), 7.49 (d, J = 8.5 Hz, 1H), 7.46 – 7.37 (m, 2H), 7.25 – 7.15 (m, 2H), 7.15 – 7.01 (m, 5H), 2.33 (s, 3H), 2.25 (s, 3H);

13C NMR (100 MHz, CDCl3): δ 152.7, 142.9, 141.7, 141.3, 141.1, 134.1, 129.9, 128.9, 127.9, 126.3, 125.7, 125.3, 119.9, 111.2, 21.4, 21.3;

IR: 1640, 1600, 1468, 1366, 1130, 1080, 950, 750 cm⁻¹;

HRMS (ESI): C23H20N2O2S+H, Calc: 389.1318, Found: 389.1318.

N-(2-(4-ethylphenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3ah)

Yellow solid (33.8 mg, 84% yield);

1H NMR (400 MHz, CDCl3): δ 8.44 (s, 1H), 7.91 (s, 1H), 7.70 (d, J = 8.2 Hz, 2H), 7.57 (d, J = 8.5 Hz, 1H), 7.49 (d, J = 4.6 Hz, 2H), 7.25 (dd, J = 23.5, 8.3 Hz, 4H), 7.19 – 7.14 (m, 1H), 7.12 (d, J = 8.0 Hz, 2H), 2.71 (q, J = 7.6 Hz, 2H), 2.33 (s, 3H), 1.27 (t, J = 7.6 Hz, 3H);

13C NMR (100 MHz, CDCl3): δ 152.7, 146.0 142.7, 141.8, 141.4, 141.0, 139.4, 134.0, 128.8, 127.8, 126.4, 126.3, 125.8, 125.3, 119.9, 111.4, 28.6, 21.4, 15.4;

IR: 2965, 1640, 1600, 1468, 1366, 1130, 1080, 949 cm⁻¹;
HRMS (ESI): C_{24}H_{22}N_{2}O_{2}S+H, Calc: 403.1475, Found: 403.1475.

N-(2-(4-methoxyphenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3ai)

Yellow solid (34.7 mg, 86% yield);

^1H NMR (400 MHz, CDCl$_3$): δ 8.44 (s, 1H), 7.95 (s, 1H), 7.74 (d, $J = 8.2$ Hz, 2H), 7.62 – 7.47 (m, 3H), 7.29 (dd, $J = 6.2$, 2.7 Hz, 2H), 7.24 – 7.12 (m, 3H), 7.04 – 6.96 (m, 2H), 3.88 (s, 3H), 2.36 (s, 3H);

^13C NMR (100 MHz, CDCl$_3$): δ 160.2, 152.8, 142.9, 141.7, 141.4, 141.1 134.5, 134.0, 128.9, 127.8, 127.7, 126.3, 125.8, 125.3, 119.9, 114.5, 111.4, 55.7, 21.4;

IR: 3057, 2925, 1640, 1600, 1509, 1469, 1367, 1249, 1131, 1081, 951 cm$^{-1}$;

HRMS (ESI): C_{23}H_{20}N_{2}O_{3}S+H, Calc: 405.1267, Found: 405.1267.

N-(2-(4-fluorophenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3aj)

Yellow solid (33.8 mg, 86% yield);

^1H NMR (400 MHz, CDCl$_3$): δ 8.45 (s, 1H), 7.88 (s, 1H), 7.68 (d, $J = 8.2$ Hz, 2H), 7.59 (d, $J = 8.6$ Hz, 1H), 7.53 – 7.44 (m, 2H), 7.37 – 7.28 (m, 2H), 7.21 – 7.07 (m, 5H), 2.33 (s, 3H);

^13C NMR (100 MHz, CDCl$_3$): δ 164.0, 161.5, 152.6, 142.6, 141.9, 141.3, 141.2, 137.5, 134.3, 129.2, 128.9, 128.6, 128.6, 127.9, 126.1, 125.8, 125.5, 120.0, 116.5, 116.3, 111.4, 21.4;

IR: 1641, 1600, 1505, 1469, 1367, 1131, 1080, 950, 839, 749 cm$^{-1}$;

HRMS (ESI): C_{22}H_{17}N_{2}O_{2}S+H, Calc: 393.1068, Found: 393.1068.

N-(2-(4-chlorophenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3ak)

Yellow solid (26.9 mg, 66% yield);

HRMS (ESI): C_{23}H_{22}N_{2}O_{2}S+H, Calc: 403.1475, Found: 403.1475.
$^1$H NMR (400 MHz, CDCl$_3$): δ 8.42 (s, 1H), 7.92 (s, 1H), 7.69 (d, $J$ = 8.2 Hz, 2H), 7.58 (d, $J$ = 8.5 Hz, 1H), 7.51 (d, $J$ = 3.6 Hz, 2H), 7.44 (d, $J$ = 8.6 Hz, 2H), 7.29 (d, $J$ = 8.6 Hz, 2H), 7.23 – 7.10 (m, 3H), 2.35 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): δ 152.4, 142.4, 141.9, 141.4, 141.1, 139.9, 135.7, 134.4, 129.6, 129.0, 128.0, 127.9, 126.2, 125.8, 125.6, 120.1, 111.6, 21.4;

IR: 3066, 1644, 1602, 1471, 1368, 1233, 1075, 948 cm$^{-1}$;

HRMS (ESI): C$_{22}$H$_{17}$N$_2$O$_2$SCl$^+$H, Calc: 409.0772, Found: 409.0772.

N-(2-(4-bromophenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3al)

Yellow solid (31.6 mg, 70% yield);

$^1$H NMR (400 MHz, CDCl$_3$): δ 8.38 (s, 1H), 7.93 (s, 1H), 7.69 (d, $J$ = 8.2 Hz, 2H), 7.65 – 7.59 (m, 2H), 7.57 (d, $J$ = 8.6 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.25 – 7.11 (m, 5H), 2.35 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): δ 152.5, 142.1, 142.0, 141.3, 141.1, 140.5, 134.3, 132.6, 129.0 128.3, 127.8, 126.2, 125.9, 125.6, 123.8, 120.0, 111.6, 21.4;

IR: 3063, 1641, 1600, 1470, 1366, 1075, 945, 682 cm$^{-1}$;

HRMS (ESI): C$_{22}$H$_{17}$N$_2$O$_2$SBr$^+$H, Calc: 453.0267, Found: 453.0268.

N-(2-(4-iodophenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3am)

Yellow solid (37.5 mg, 75% yield);

$^1$H NMR (400 MHz, CDCl$_3$): δ 8.41 (s, 1H), 7.90 (s, 1H), 7.78 (d, $J$ = 8.5 Hz, 2H), 7.68 (d, $J$ = 8.1 Hz, 2H), 7.58 (d, $J$ = 8.6 Hz, 1H), 7.49 (d, $J$ = 2.9 Hz, 2H), 7.22 – 7.11 (m, 3H), 7.07 (dd, $J$ = 9.0, 2.2 Hz, 2H), 2.35 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): δ 152.4, 142.2, 141.9, 141.3, 141.2, 141.1, 138.5, 134.3, 129.0, 128.4, 127.9, 126.2, 125.8, 125.5, 120.0, 111.4, 95.4, 21.4;

IR: 3056, 2924, 1641, 1602, 1469, 1367, 1264, 1132, 1082, 950, 731 cm$^{-1}$;
HRMS (ESI): $C_{22}H_{17}N_2O_2S^+$, Calc: 501.0128, Found: 501.0128.

N-(2-(3,4-dimethylphenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3an)

Yellow solid (33.4 mg, 83% yield);

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.44 (s, 1H), 7.91 (s, 1H), 7.71 (d, $J = 8.2$ Hz, 2H), 7.57 (d, $J = 8.4$ Hz, 1H), 7.49 (d, $J = 3.8$ Hz, 2H), 7.23 – 7.08 (m, 4H), 7.07 – 6.97 (m, 2H), 2.33 (s, 3H), 2.28 (s, 3H), 2.24 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 152.6, 142.9, 141.6, 141.4, 141.0, 139.4, 138.3, 137.9, 134.0, 130.3, 128.8, 127.9, 127.3, 126.3, 125.7, 125.2, 123.6, 119.9, 111.3, 21.4, 19.8, 19.6;

IR: 2918, 1639, 1599, 1493, 1470, 1365, 1269, 1130, 1083, 951, 736, 662 cm$^{-1}$;

HRMS (ESI): $C_{24}H_{22}N_2O_2S^+$, Calc: 403.1475, Found: 403.1475.

N-(2-(3,4-dimethoxyphenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3ao)

Yellow solid (39.5 mg, 91% yield);

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.46 (s, 1H), 7.96 (s, 1H), 7.74 (d, $J = 8.2$ Hz, 2H), 7.59 (d, $J = 8.5$ Hz, 1H), 7.56 – 7.45 (m, 2H), 7.24 – 7.18 (m, 1H), 7.16 (d, $J = 8.0$ Hz, 2H), 6.89 (ddd, $J = 12.2$, 10.9, 5.5 Hz, 3H), 3.95 (s, 3H), 3.77 (s, 3H), 2.35 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 152.6, 149.9, 149.0, 143.0, 141.7, 141.5, 141.1, 134.6, 134.0, 128.9, 127.8, 126.2, 125.7, 125.3, 119.9, 118.6, 111.3, 110.9, 110.3, 56.2, 56.1, 21.4;

IR: 2926, 1640, 1599, 1469, 1367, 1266, 1130, 1081, 954, 750 cm$^{-1}$;

HRMS (ESI): $C_{24}H_{22}N_2O_4S^+$, Calc: 435.1373, Found: 435.1373.

4-methyl-N-(2-(o-tolyl)isoquinolin-3(2H)-ylidene)benzenesulfonamide (3ap)
Yellow solid (35.8 mg, 89% yield);

\( ^1H \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 8.30 (s, 1H), 7.97 (s, 1H), 7.68 (d, \( J = 8.2 \) Hz, 2H), 7.60 – 7.48 (m, 3H), 7.23 – 7.17 (m, 1H), 7.17 – 7.08 (m, 4H), 7.03 (d, \( J = 7.7 \) Hz, 1H), 2.41 (s, 3H), 2.33 (s, 3H), 1.96 (s, 3H);

\( ^{13}C \) NMR (100 MHz, CDCl\(_3\)): \( \delta \) 152.8, 142.3, 141.9, 141.5, 141.0, 139.9, 138.8, 133.9, 133.8, 131.8, 128.8, 127.8, 127.6, 126.3, 126.1, 125.9, 125.2, 120.0, 111.4, 21.4, 21.2, 17.5;

IR: 2860, 1640, 1600, 1494, 1468, 1366, 1268, 1131, 1081, 952 cm\(^{-1}\);

HRMS (ESI): \( \text{C}_{24}\text{H}_{22}\text{N}_{2}\text{O}_{2}\text{S}+\text{H}, \text{Calc: 403.1475, Found: 403.1475.} \)

N-(2-(4-chloro-2-methylphenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3aq)

Yellow solid (36.3 mg, 86% yield);

\( ^1H \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 8.32 (s, 1H), 7.98 (s, 1H), 7.67 (d, \( J = 8.2 \) Hz, 2H), 7.63 – 7.49 (m, 3H), 7.39 – 7.29 (m, 2H), 7.25 – 7.19 (m, 1H), 7.13 (dd, \( J = 17.1, 8.2 \) Hz, 3H), 2.35 (s, 3H), 1.98 (s, 3H);

\( ^{13}C \) NMR (100 MHz, CDCl\(_3\)): \( \delta \) 152.6, 142.1, 142.0, 141.3, 141.1, 139.6, 136.3, 135.6, 134.3, 131.1, 128.9, 127.7, 127.4, 126.2, 125.9, 125.5, 120.0, 111.5, 21.4, 17.6;

IR: 3056, 1639, 1600, 1490, 1467, 1366, 1267, 1131, 1080, 950 cm\(^{-1}\);

HRMS (ESI): \( \text{C}_{23}\text{H}_{19}\text{N}_{2}\text{O}_{2}\text{SCl}+\text{H}, \text{Calc: 423.0929, Found: 423.0929.} \)

N-(2-(3,5-dimethoxyphenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3ar)

Yellow solid (36.9 mg, 85% yield);

\( ^1H \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 8.46 (s, 1H), 7.92 (s, 1H), 7.75 (d, \( J = 8.2 \) Hz, 2H), 7.60 (d, \( J = 8.5 \) Hz, 1H), 7.55 – 7.46 (m, 2H), 7.24 – 7.09 (m, 3H), 6.55 (d, \( J = 2.1 \) Hz, 1H), 6.48 (d, \( J = 2.2 \) Hz, 2H), 3.75 (s, 6H), 2.35 (s, 3H).
\[ \text{C NMR (100 MHz, CDCl}_3\text{): } \delta 161.1, 152.4, 143.1, 142.6, 141.8, 141.6, 141.1, 134.1, 128.8, 128.0, 126.2, 125.8, 125.3, 119.8, 111.3, 105.2, 101.7, 55.7, 21.4. \]

IR: 2981, 1600, 1464, 1366, 1270, 1190, 1155, 1132, 1083, 957 cm\(^{-1}\);

HRMS (ESI): C\(_{24}\)H\(_{22}\)N\(_2\)O\(_4\)S+H, Calc: 435.1373, Found: 435.1373.

N-(2-(4-(2-azidoethyl)phenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3as)

Yellow solid (24.8 mg, 56% yield);

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta 8.41 (s, 1H), 7.95 (s, 1H), 7.71 (d, J = 8.2 Hz, 2H), 7.59 – 7.47 (m, 3H), 7.36 (d, J = 8.4 Hz, 2H), 7.33 – 7.28 (m, 2H), 7.22 – 7.17 (m, 1H), 7.15 (d, J = 8.0 Hz, 2H), 3.59 (t, J = 7.0 Hz, 2H), 2.98 (t, J = 7.0 Hz, 2H), 2.34 (s, 3H); \]

\[ \text{C NMR (100 MHz, CDCl}_3\text{): } \delta 152.7, 142.5, 141.9, 141.2, 140.3, 140.0, 134.2, 129.8, 128.9, 127.8, 126.8, 126.3, 125.8, 125.4, 119.9, 111.5, 52.1, 35.0, 21.4; \]

IR: 2094, 1640, 1600, 1469, 1367, 1261, 1130, 1080, 949, 749 cm\(^{-1}\);

HRMS (ESI): C\(_{24}\)H\(_{21}\)N\(_5\)O\(_2\)S+H, Calc: 444.1489, Found: 444.1489.

N-(2-(4-(2-hydroxyethyl)phenyl)isoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3at)

Yellow solid (38.0 mg, 91% yield);

\[ \text{H NMR (400 MHz, CDCl}_3\text{): } \delta 8.48 (s, 1H), 7.88 (s, 1H), 7.74 (d, J = 8.2 Hz, 2H), 7.59 – 7.47 (m, 1H), 7.55 – 7.48 (m, 2H), 7.35 (d, J = 8.3 Hz, 2H), 7.24 – 7.14 (m, 5H), 3.87 (t, J = 6.2 Hz, 2H), 2.90 (t, J = 6.2 Hz, 2H), 2.34 (s, 3H); \]

\[ \text{C NMR (100 MHz, CDCl}_3\text{): } \delta 152.7, 143.1, 141.8, 141.4, 141.3, 140.8, 139.7, 134.2, 130.3, 129.0, 128.0, 126.4, 126.4, 125.7, 125.5, 120.0, 111.1, 63.0, 38.9, 21.4; \]

IR: 3420, 1639, 1600, 1493, 1468, 1366, 1129, 1080, 951, 749 cm\(^{-1}\);

HRMS (ESI): C\(_{24}\)H\(_{22}\)N\(_2\)O\(_3\)S+H, Calc: 419.1424, Found: 419.1424.

3-(4-(3-(tosylimino)isoquinolin-2(3H)-yl)phenyl)propanoic acid (3au)
Yellow solid (41.0 mg, 92% yield);

\[^1\text{H} \text{NMR (400 MHz, CDCl}_{3}\text{)}\]: \( \delta 8.48 (s, 1 \text{H}), 7.85 (s, 1 \text{H}), 7.69 (d, J = 8.1 \text{ Hz}, 2 \text{H}), 7.60 (d, J = 8.5 \text{ Hz}, 1 \text{H}), 7.48 (s, 2 \text{H}), 7.34 – 7.25 (m, 2 \text{H}), 7.23 – 7.07 (m, 5 \text{H}), 2.97 (t, J = 7.2 \text{ Hz}, 2 \text{H}), 2.67 (t, J = 7.2 \text{ Hz}, 2 \text{H}), 2.33 (s, 3 \text{H});

\[^{13}\text{C} \text{ NMR (100 MHz, CDCl}_{3}\text{)}\]: \( \delta 177.0, 152.2, 143.4, 142.2, 141.7, 141.4, 140.9, 139.7, 134.3, 129.3, 129.0, 128.2, 126.6, 126.3, 125.6, 125.5, 120.1, 111.1, 35.2, 30.2, 21.4; \)

\text{IR}: 3008, 1723, 1640, 1600, 1469, 1367, 1128, 1079, 750 \text{ cm}^{-1};

\text{HRMS (ESI)}: \text{C}_{26}\text{H}_{19}\text{N}_{2}\text{O}_{3}\text{S}+\text{H}, \text{Calc}: 447.1373, \text{Found}: 447.1373.

4-methyl-N-(2-(naphthalen-1-yl)isoquinolin-3(2H)-ylidene)benzenesulfonamide (3av)

Yellow solid (41.0 mg, 60% yield);

\[^1\text{H} \text{NMR (400 MHz, CDCl}_{3}\text{)}\]: \( \delta 8.43 (s, 1 \text{H}), 8.11 (s, 1 \text{H}), 8.05 (d, J = 8.3 \text{ Hz}, 1 \text{H}), 7.99 (d, J = 8.3 \text{ Hz}, 1 \text{H}), 7.61 (ddd, J = 15.9, 13.3, 8.1 \text{ Hz}, 5 \text{H}), 7.49 – 7.35 (m, 4 \text{H}), 7.27 – 7.20 (m, 1 \text{H}), 7.03 (d, J = 14.6, 8.3 \text{ Hz}, 3 \text{H}), 2.31 (s, 3 \text{H});

\[^{13}\text{C} \text{ NMR (100 MHz, CDCl}_{3}\text{)}\]: \( \delta 153.4, 143.1, 142.2, 141.0, 138.5, 134.2, 134.0, 130.3, 128.6, 128.5, 128.5, 127.8, 127.0, 126.3, 126.0, 125.4, 124.5, 122.0, 120.0, 111.5, 21.3; \)

\text{IR}: 1640, 1600, 1472, 1368, 1275, 1132, 1081, 765, 750 \text{ cm}^{-1};

\text{HRMS (ESI)}: \text{C}_{26}\text{H}_{19}\text{N}_{2}\text{O}_{3}\text{S}+\text{H}, \text{Calc}: 425.1318, \text{Found}: 425.1318.

4-methyl-N-(2-(pyridin-2-yl)isoquinolin-3(2H)-ylidene)benzenesulfonamide (3aw)

Yellow solid (22.9 mg, 61% yield);
$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.69 (s, 1H), 8.59 (d, $J = 5.3$ Hz, 1H), 7.87 (dd, $J = 18.1$, 6.4 Hz, 3H), 7.81 – 7.72 (m, 2H), 7.58 (d, $J = 8.5$ Hz, 1H), 7.49 (d, $J = 3.8$ Hz, 2H), 7.44 (dd, $J = 4.8$, 2.0 Hz, 1H), 7.17 (t, $J = 6.4$ Hz, 3H), 2.33 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 152.4, 152.0, 149.3, 142.2, 142.0, 141.3, 141.0, 137.9, 134.5, 129.0, 128.3, 126.3, 125.7, 125.4, 124.9, 123.2, 120.1, 111.2, 21.4;

IR: 1641, 1602, 1473, 1368, 1264, 1132, 1081, 952, 748 cm$^{-1}$;

HRMS (ESI): C$_{21}$H$_{17}$N$_3$O$_2$S+$\text{H}$, Calc: 376.1114, Found: 376.1114.

4-methyl-N-(2-(phenylamino)isoquinolin-3(2H)-ylidene)benzenesulfonamide (3ax)

![Structural diagram of 4-methyl-N-(2-(phenylamino)isoquinolin-3(2H)-ylidene)benzenesulfonamide (3ax)]

Yellow solid (29.2 mg, 75% yield);

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.91 (s, 1H), 8.66 (s, 1H), 7.95 (s, 1H), 7.66 – 7.58 (m, 3H), 7.57 – 7.50 (m, 2H), 7.29 – 7.26 (m, 1H), 7.26 – 7.21 (m, 2H), 7.12 (t, $J = 7.4$ Hz, 1H), 7.06 (d, $J = 8.0$ Hz, 2H), 6.76 – 6.62 (m, 2H), 2.31 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 150.5, 145.8, 141.5, 141.3, 140.5, 140.2, 134.0, 129.6, 129.0, 127.5, 126.5, 125.9, 125.7, 124.8, 119.8, 117.7, 110.7, 21.4;

IR: 3020, 1639, 1602, 1471, 1367, 1264, 1132, 1080, 958, 750 cm$^{-1}$;

HRMS (ESI): C$_{22}$H$_{19}$N$_3$O$_2$S+$\text{H}$, Calc: 390.1271, Found: 390.1270.

N-(8-fluoro-2-phenylisoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3ba)

![Structural diagram of N-(8-fluoro-2-phenylisoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3ba)]

Yellow solid (22.3 mg, 57% yield);

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.60 (s, 1H), 8.03 (s, 1H), 7.68 (d, $J = 8.2$ Hz, 2H), 7.59 – 7.49 (m, 3H), 7.48 – 7.41 (m, 1H), 7.36 (ddd, $J = 15.0$, 9.5, 6.2 Hz, 3H), 7.14 (d, $J = 8.0$ Hz, 2H), 6.79 (dd, $J = 10.3$, 7.4 Hz, 1H), 2.34 (s, 3H).
\textbf{13C NMR (100 MHz, CDCl\textsubscript{3})}: \(\delta\) 153.2, 143.4, 142.4, 141.6, 141.3, 141.0, 139.3, 137.9, 134.5, 134.4, 129.9, 129.7, 129.5, 128.9, 126.6, 126.5, 126.2, 121.9, 111.5, 107.5, 107.3, 21.5, 21.4.

\textbf{IR}: 2923, 1654, 1607, 1495, 1473, 1376, 1275, 1134, 1077, 913, 763 cm\textsuperscript{-1}; 1

\textbf{HRMS (ESI)}: \(C_{22}H_{17}N_2O_2\)F\textsubscript{S}+H, Calc: 393.1068, Found: 393.1068.

\textbf{N-(7-fluoro-2-phenylisoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3bb)}

\textsf{\[\begin{array}{c}
\text{F} \\
\text{N} & \text{T}s \\
\hline
\text{N} & \text{Ts} \\
\text{Cl} & \text{N} & \text{T}s
\end{array}\]}

Yellow solid (35.3 mg, 90% yield);

\textbf{1H NMR (400 MHz, CDCl\textsubscript{3})}: \(\delta\) 8.36 (s, 1H), 8.02 (s, 1H), 7.66 (d, \(J = 8.2\) Hz, 2H), 7.56 (dd, \(J = 9.4, 5.1\) Hz, 1H), 7.52 – 7.45 (m, 3H), 7.39 – 7.28 (m, 3H), 7.20 – 7.09 (m, 3H), 2.33 (s, 3H);

\textbf{13C NMR (100 MHz, CDCl\textsubscript{3})}: \(\delta\) 160.4, 157.9, 152.5, 141.5, 141.2, 141.1, 139.4, 129.7, 129.4, 129.0, 128.9, 126.5, 126.2, 126.1, 119.6, 119.5, 112.4, 109.2, 109.0, 21.4;

\textbf{IR}: 3066, 2921, 2851, 1649, 1604, 1494, 1432, 1350, 1131, 1080, 758 cm\textsuperscript{-1}; 1

\textbf{HRMS (ESI)}: \(C_{22}H_{17}N_2O_2\)F\textsubscript{S}+H, Calc: 393.1068, Found: 393.1068.

\textbf{N-(7-chloro-2-phenylisoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3bc)}

\textsf{\[\begin{array}{c}
\text{Cl} \\
\text{N} & \text{T}s \\
\hline
\text{N} & \text{T}s \\
\text{Cl} & \text{N} & \text{T}s
\end{array}\]}

Yellow solid (37.5 mg, 92% yield);

\textbf{1H NMR (400 MHz, CDCl\textsubscript{3})}: \(\delta\) 8.35 (s, 1H), 7.97 (s, 1H), 7.72 – 7.60 (m, 2H), 7.59 – 7.45 (m, 5H), 7.39 (dd, \(J = 9.2, 2.0\) Hz, 1H), 7.36 – 7.28 (m, 2H), 7.13 (d, \(J = 8.0\) Hz, 2H), 2.34 (s, 3H);

\textbf{13C NMR (100 MHz, CDCl\textsubscript{3})}: \(\delta\) 152.9, 141.4, 141.3, 141.1, 140.0, 135.2, 130.8, 129.8, 129.5, 128.9, 127.7, 126.5, 126.1, 125.5, 119.9, 112.1, 21.4;

\textbf{IR}: 1641, 1593, 1470, 1493, 1348, 1275, 1132, 1081, 950, 764, 751 cm\textsuperscript{-1}; 1

\textbf{HRMS (ESI)}: \(C_{22}H_{17}N_2O_2\)Cl\textsubscript{S}+H, Calc: 409.0772, Found: 409.0772.

\textbf{4-methyl-N-(6-methyl-2-phenylisoquinolin-3(2H)-ylidene)benzenesulfonamide (3bd)}
Yellow solid (33.8 mg, 87% yield);

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.35 (s, 1H), 7.82 (s, 1H), 7.68 (d, $J = 7.3$ Hz, 2H), 7.48 (d, $J = 8.4$ Hz, 4H), 7.37 – 7.27 (m, 3H), 7.12 (d, $J = 7.7$ Hz, 2H), 7.02 (d, $J = 8.7$ Hz, 1H), 2.44 (s, 3H), 2.33 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 152.5, 145.4, 142.2, 142.1, 141.7, 141.5, 141.0, 129.5, 129.3, 128.8, 128.3, 127.6, 126.7, 126.2, 123.9, 118.7, 110.3, 22.6, 21.4;

IR: 1645, 1609, 1503, 1413, 1238, 1207, 1076, 925, 759 cm$^{-1}$;

HRMS (ESI): C$_{23}$H$_{20}$N$_2$O$_2$S+H, Calc: 389.1318, Found: 389.1317.

N-(6-fluoro-2-phenylisoquinolin-3(2H)-ylidene)-4-methylbenzenesulfonamide (3be)

Yellow solid (20.0 mg, 51% yield);

$^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.41 (s, 1H), 7.88 (s, 1H), 7.67 (d, $J = 8.2$ Hz, 2H), 7.61 (dd, $J = 9.2$, 5.5 Hz, 1H), 7.55 – 7.47 (m, 3H), 7.38 – 7.30 (m, 2H), 7.12 (dd, $J = 14.2$, 5.0 Hz, 3H), 2.34 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 152.6, 142.6, 141.5, 141.2, 141.2, 131.6, 129.7, 129.5, 128.9, 126.6, 126.2, 117.9, 117.4, 110.5, 110.5, 109.1, 108.1, 108.1, 107.9, 21.4;

IR: 3008, 1643, 1496, 1450, 1275, 1134, 1082, 938, 764 cm$^{-1}$;

HRMS (ESI): C$_{22}$H$_{17}$N$_2$O$_2$S+H, Calc: 393.1068, Found: 393.1068.
synthesis of 4 (3au-N-hemokinin-1)

The fluorescent probe 4 (3au-N-hemokinin-1) was synthesized by conjugating cyclic amidine 3au with the N-terminal of the hemokinin-1 (HK-1) peptide (TGKASQFFGLM-NH$_2$) using Fmoc solid-phase method as described before. The method of linking cyclic amidine 3au was the same as the method of linking the amino acids, and the condensation method used HATU and DIEA in DMF solvent. The characteristics of the peptide were confirmed by ESI-TOF mass spectrometry. The purity of peptide was quantified to be >95% using reversed-phase HPLC by a C18 column as the solid phase and a H$_2$O : acetonitrile gradient as the liquid phase.
| Entry | Retention time (min) | Area (AU*sec) | Height (AU) | % Area |
|-------|---------------------|---------------|-------------|--------|
| 1     | 1.794               | 812           | 369         | 0.23   |
| 2     | 2.262               | 1852          | 283         | 0.51   |
| 3     | 2.527               | 9429          | 1670        | 2.61   |
| 4     | 8.405               | 348752        | 24224       | 96.65  |
Confocal imaging experiments

WT 22RV1 cells or NK-1 receptors-overexpressed 22RV1 cells with good growth states were digested with trypsin, centrifuged at 800 r/min, resuspended in medium, counted, and inoculated with \( 4 \times 10^4 \) cells per dish. The culture dish was placed in a 5% carbon dioxide incubator at 37 °C and cultured overnight. The culture dish was then taken out and the medium was discarded. The fluorescent probe \( 4 (\text{3au-N-hemokinin-1}) (1 \mu M) \) was added, and the culture dish was placed in a 37 °C incubator and incubated for 30 minutes. It was then washed three times with pre-cooled PBS and then photographed with laser confocal. In the antagonist group, the medium of NK-1 receptors-overexpressed 22RV1 cells was discarded and the NK1R inhibitor aprepitant (1 \( \mu \)M) was added and incubated at 37 °C for 30 minutes. Subsequently, The cells were washed 3 times with pre-cooled PBS, the fluorescent probe \( 4 (\text{3au-N-hemokinin-1}) (1 \mu M) \) was added, and the culture dish was placed in a 37 °C incubator for 30 min. This was followed by washing 3 times with pre-cooled PBS and then taking a photo with laser confocal. Sigma-Aldrich.

Cytotoxicity assays

WT Hela cells were seeded at \( 7 \times 10^3 \) cells/well in 96-well plates and incubated overnight before being treated in the presence of 6.25-200 \( \mu \)M of \( \text{3aa} \) for 24h. Cell viability (%) was measured by adding 10% CCK-8) for an additional 1 hour. Absorbance was measured at a wavelength of 450 nm. Cell viability was calculated from 3 independent experiments and normalized to the absorbance of wells containing medium only (100%) and that of wells containing untreated cells (0%).
Photophysical properties of 3
Hydrolytic stability of 3aa

Figure S1. Emission spectra of 3aa (λex = 433 nm) at different storage time in H₂O at 20 μM.
X-ray Structure of 3aw

Bond precision: C-C = 0.0025 Å  Wavelength=1.54184

Cell: 
\[ a = 17.4822(3) \quad b = 9.78677(16) \quad c = 20.9912(4) \]
\[ \alpha = 90 \quad \beta = 103.5756(17) \quad \gamma = 90 \]

Temperature: 100 K

| Calculated | Reported |
|------------|----------|
| Volume     | 3491.13(11) | 3491.14(11) |
| Space group| C 2/c     | C 1 2/c 1   |
| Hall group | -C 2yc    | -C 2yc     |
| Moiety formula | C21 H17 N3 O2 S | C21 H17 N3 O2 S |
| Sum formula | C21 H17 N3 O2 S | C21 H18 N2 O2 S |
| Mr         | 375.44    | 362.43     |
| Dx, g cm\(^{-3}\) | 1.429 | 1.379 |
| Z          | 8         | 8          |
| Mu (mm-1)  | 1.832     | 1.793      |
| F000       | 1568.0    | 1520.0     |
| F000'      | 1574.97   |            |
| h,k,lmax   | 20,11,25  | 20,11,25   |
| Nref       | 3113      | 3089       |
| Tmin, Tmax | 0.683,0.836 | 0.357,1.000 |
| Tmin'      | 0.556     |            |
Correction method= # Reported T Limits: Tmin=0.357 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.992  Theta(max)= 67.079

R(reflections)= 0.0369( 2793)  \(wR^2\)(reflections)= 0.0982( 3089)

\(S = 1.035\)  \(Npar= 245\)

The following ALERTS were generated. Each ALERT has the format

```
test-name_ALERT_alert-type_alert-level
```

Click on the hyperlinks for more details of the test.

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### Alert level B

**PLAT043_ALERT_1_B** Calculated and Reported Mol. Weight Differ by ..  Check

### Alert level C

**PLAT041_ALERT_1_C** Calc. and Reported SumFormula Strings Differ Please Check

**PLAT051_ALERT_1_C** Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.19 %

**PLAT068_ALERT_1_C** Reported F000 Differs from Calcd (or Missing) Please Check

**PLAT911_ALERT_3_C** Missing FCF Refl Between Thmin & STh/L= 0.597 25 Report

**PLAT913_ALERT_3_C** Missing # of Very Strong Reflections in FCF .... 7 Note

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### Alert level G

**FORMU01_ALERT_1_G** There is a discrepancy between the atom counts in the _chemical_formula_sum and _chemical_formula_moiety. This is usually due to the moiety formula being in the wrong format.

- Atom count from _chemical_formula_sum: C21 H18 N2 O2 S1
- Atom count from _chemical_formula_moiety: C21 H17 N3 O2 S1

**FORMU01_ALERT_2_G** There is a discrepancy between the atom counts in the _chemical_formula_sum and the formula from the _atom_site* data.

- Atom count from _chemical_formula_sum: C21 H18 N2 O2 S1
- Atom count from the _atom_site data: C21 H17 N3 O2 S1

**CELLZ01_ALERT_1_G** Difference between formula and atom_site contents detected.

**CELLZ01_ALERT_1_G** ALERT: Large difference may be due to a symmetry error - see SYMMG tests

- From the CIF: _cell_formula_units_Z 8
- From the CIF: _chemical_formula_sum C21 H18 N2 O2 S

**TEST: Compare cell contents of formula and atom_site data**

| atom | Z*formula | cif sites diff |
|------|-----------|----------------|
| C    | 168.00    | 168.00         | 0.00          |
| H    | 144.00    | 136.00         | 8.00          |
| N    | 16.00     | 24.00          | -8.00         |
| O    | 16.00     | 16.00          | 0.00          |
| S    | 8.00      | 8.00           | 0.00          |

**PLAT432_ALERT_2_G** Short Inter X...Y Contact  C8 ..C8  3.13 Ang.

\(1-x,y,1/2-z = 2_655\)  Check
PLAT909_ALERT_3_G Percentage of I > 2σ(I) Data at θ_{max} Still 83% Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) L_{max} Differ by . 1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 8 Info

0 ALERT level A = Most likely a serious problem - resolve or explain
1 ALERT level B = A potentially serious problem, consider carefully
5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
8 ALERT level G = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
Computational Details

DFT calculations were carried out at the B3LYP level of theory. All structures/species studied in this paper were fully optimized in dichloromethane solvent. Frequency calculations were performed to ensure that a transition state has only one imaginary frequency and a local minimum has no imaginary frequencies. Intrinsic reaction coordinate (IRC) calculations were run to ensure that transition states connect relevant minima. The 6-31G** basis set was used to describe C, H, N and O, while the SDD plus polarization basis set was employed to describe S. All DFT calculations were performed using the Gaussian 09 D.01.

Cartesian coordinates for all of the calculated structures

A, E = -1507.20640620 , G = -1506.918217

|  |  |  |
|---|---|---|
| 6 | 3.829104 | -4.050669 | -0.117305 |
| 6 | 2.532607 | -3.747341 | -0.515773 |
| 6 | 2.038510 | -2.427654 | -0.483510 |
| 6 | 2.910457 | -1.38790 | -0.056711 |
| 6 | 4.215711 | -1.720507 | 0.350381 |
| 6 | 4.676911 | -3.030435 | 0.327361 |
| 1 | 4.176752 | -5.078654 | -0.152322 |
| 1 | 4.176752 | -5.078654 | -0.152322 |
| 1 | 1.874033 | -4.544221 | -0.848619 |
| 1 | 4.861537 | -0.910466 | 0.670842 |
| 1 | 5.691077 | -3.256557 | 0.641688 |
| 6 | 2.511057 | 0.025832 | -0.067865 |
| 7 | 3.223985 | 0.938562 | 0.486763 |
| 6 | 2.790315 | 2.277622 | 0.465451 |
| 6 | 3.772392 | 3.275137 | 0.332961 |
|   | 1.444551 | 2.659051 | 0.624278 |
|---|----------|----------|----------|
| 6 | 3.413766 | 4.620968 | 0.308184 |
| 1 | 4.810235 | 2.971586 | 0.235325 |
| 6 | 1.097080 | 4.010223 | 0.617018 |
| 1 | 0.678117 | 1.908569 | 0.792027 |
| 6 | 2.073684 | 4.995359 | 0.449717 |
| 1 | 4.181870 | 5.379843 | 0.188975 |
| 1 | 0.056639 | 4.292336 | 0.751685 |
| 1 | 1.796151 | 6.045249 | 0.446217 |
| 6 | 0.634872 | -2.266616 | -0.888080 |
| 6 | -0.204676 | -1.262667 | -0.711902 |
| 7 | -1.021071 | -0.343332 | -0.641708 |
| 6 | -2.001484 | -0.258320 | 0.879588 |
| 8 | -1.732505 | 1.102000 | 1.398052 |
| 8 | -1.739495 | -1.453497 | 1.713989 |
| 6 | -6.50815 | -0.33836 | 0.204451 |
| 6 | -4.242634 | 0.837402 | -0.273137 |
| 6 | -4.311273 | -1.562942 | 0.165611 |
| 6 | -5.526638 | 0.765524 | -0.806466 |
| 1 | -3.711906 | 1.781432 | -0.222350 |
| 6 | -5.595744 | -1.611281 | -0.370713 |
| 1 | -3.831756 | -2.455186 | 0.552082 |
| 6 | -6.222023 | -0.455347 | -0.863043 |
| 1 | -5.997882 | 1.666978 | -1.182474 |
| 1 | -6.120800 | -2.561401 | -0.405945 |
| 6 | -7.624223 | -0.515159 | -1.415504 |
| 1 | -8.358368 | -0.317451 | -0.624886 |
| 1 | -7.773272 | 0.234099 | -2.196952 |
| 1 | -7.848253 | -1.501389 | -1.830557 |
| 1 | 0.177113 | -3.129911 | -1.369981 |
| 1 | 1.593822 | 0.281474 | -0.606906 |

TSA-B, E = -1507.19491798, G = -1506.906707

|   | 3.925472 | -4.176418 | -0.166612 |
|---|----------|----------|----------|
| 6 | 2.591267 | -3.863971 | -0.407785 |
| 6 | 2.149185 | -2.528219 | -0.472777 |
| 6 | 3.098863 | -1.494072 | -0.303257 |
| 6 | 4.439504 | -1.823496 | -0.070347 |
| 6 | 4.857749 | -3.152257 | 0.007237 |
| 1 | 4.235299 | 5.215868 | -0.117578 |
| 1 | 1.867531 | 4.662579 | -0.543672 |
| 1 | 5.162565 | 1.021960 | 0.051037 |
| 1 | 5.901829 | -3.382552 | 0.195027 |
| 6 | 2.753293 | -0.046007 | -0.416187 |
|   | X    | Y    | Z    |
|---|------|------|------|
| 1 | 2.775451 | 2.400568 | 1.432077 |
| 1 | 1.151451 | 1.894683 | -1.534493 |
| 6 | 1.524941 | 4.752754 | 0.279517 |
| 1 | 2.351999 | 4.851615 | 2.270783 |
| 1 | 0.722482 | 4.327629 | -1.676732 |
| 1 | 1.323936 | 5.818306 | 0.220274 |
| 6 | 0.721711 | -2.314576 | -0.739096 |
| 6 | -0.016756 | -1.224585 | -0.632836 |
| 7 | -0.783569 | -0.261047 | -0.626176 |
| 6 | -1.671196 | 0.034700 | 0.927937 |
| 8 | -1.355911 | 1.433026 | 1.286688 |
| 8 | -1.405421 | -1.073263 | 1.875016 |
| 6 | -3.353583 | -0.069523 | 0.335233 |
| 6 | -3.941439 | 1.060769 | -0.236112 |
| 6 | -4.044219 | -1.276037 | 0.456444 |
| 6 | -5.250846 | 0.967953 | -0.700630 |
| 1 | -3.387063 | 1.989723 | -0.308462 |
| 6 | -5.353977 | -1.344702 | -0.013267 |
| 1 | -3.567481 | -2.135983 | 0.913338 |
| 6 | -5.976393 | -0.229941 | -0.596471 |
| 1 | -5.718491 | 1.840110 | -1.148456 |
| 1 | -5.902031 | -2.278190 | 0.076415 |
| 6 | -7.404746 | -0.307487 | -1.075493 |
| 1 | -8.094993 | 0.006766 | -0.283061 |
| 1 | -7.573912 | 0.349086 | -1.933426 |
| 1 | -7.675899 | -1.327623 | -1.359992 |
| 1 | 0.155300 | -3.189045 | -1.058001 |
| 1 | 2.947401 | 0.426278 | -1.391128 |

45

B, E = -1507.25484508, G = -1506.960864
|   | 1     | 2.447822 | -1.706306 | -1.564442 |
|---|--------|-----------|-----------|-----------|
|   | 1     | 4.193293 | -4.182328 | -1.430506 |
|   | 6     | 2.431919 | -0.061370 | -0.417538 |
|   | 7     | 1.471154 | 0.669252  | 0.184157  |
|   | 6     | 1.559927 | 2.117063  | 0.070186  |
|   | 6     | 2.122010 | 2.853512  | 1.112566  |
|   | 6     | 1.127748 | 2.731765  | -1.103778 |
|   | 6     | 2.250623 | 4.235298  | 0.972176  |
|   | 1     | 2.449063 | 2.350479  | 2.016224  |
|   | 6     | 1.261668 | 4.115765  | -1.234176 |
|   | 1     | 0.690763 | 2.135766  | -1.898440 |
|   | 6     | 1.821305 | 4.866626  | -0.198614 |
|   | 1     | 2.687851 | 4.817082  | 1.777463  |
|   | 1     | 0.928484 | 4.603025  | -2.145094 |
|   | 1     | 1.923960 | 5.942338  | -0.302983 |
|   | 6     | 0.402074 | -1.319788 | 0.967360  |
|   | 6     | 0.397241 | 0.088969  | 0.900652  |
|   | 7     | -0.459105 | 0.985635 | 1.398908  |
|   | 6     | -1.832478 | 0.522886 | 2.184603  |
|   | 8     | -2.393645 | 1.769555 | 2.767890  |
|   | 8     | -1.646101 | -0.641407 | 3.107517  |
|   | 6     | -2.968053 | -0.011859 | 0.881958  |
|   | 6     | -3.356345 | 0.094447  | -0.101559 |
|   | 6     | -3.465711 | -1.312293 | 0.881513  |
|   | 6     | -4.241711 | 0.499841  | -1.095251 |
|   | 1     | -2.968793 | 1.917826  | -0.086052 |
|   | 6     | -4.356106 | -1.702335 | -0.122814 |
|   | 1     | -3.166525 | -2.002843 | 1.662205  |
|   | 6     | -4.756133 | -0.808947 | -1.123432 |
|   | 1     | -4.544111 | 1.209468  | -1.861160 |
|   | 1     | -4.745929 | -2.717627 | -0.123937 |
|   | 6     | -5.721501 | -1.227527 | -2.206195 |
|   | 1     | -6.644492 | -0.638292 | -2.160439 |
|   | 1     | -5.291790 | -1.071461 | -3.201904 |
|   | 1     | -5.991310 | -2.282685 | -2.115257 |
|   | 1     | -0.377169 | -1.796863 | 1.545773  |
|   | 1     | 3.199514 | 0.505896  | -0.930527 |

TSA-C, E = -1507.15828152, G = -1506.873618

|   | 45    | 4.201393 | -3.859864 | -0.589197 |
|---|-------|-----------|-----------|-----------|
|   | 6     | 2.851883 | -3.628891 | -0.382409 |
|   | 6     | 2.347793 | -2.311947 | -0.280143 |
|   | 6     | 3.286116 | -1.238035 | -0.357575 |
|   | 6     | 4.653010 | -1.486747 | -0.621503 |

S88
|   | 6    | 5.109754 | -2.788669 | -0.715677 |
|---|------|----------|-----------|-----------|
| 1  | 4.564059 | -4.880628 | -0.664418 |           |
| 1  | 2.159825 | -4.462010 | -0.306902 |           |
| 1  | 5.332549 | -0.645061 | -0.705353 |           |
| 1  | 6.166015 | -2.984750 | -0.867860 |           |
| 6  | 2.799744 | 0.097160 | -0.260190 |           |
| 7  | 3.208310 | 1.218501 | 0.044432  |           |
| 6  | 2.710106 | 2.522751 | -0.006509 |           |
| 6  | 3.651498 | 3.562785 | 0.048997  |           |
| 6  | 1.334231 | 2.814752 | -0.076778 |           |
| 6  | 3.225857 | 4.888298 | 0.004965  |           |
| 1  | 4.705028 | 3.313710 | 0.118868  |           |
| 6  | 0.924965 | 4.146089 | -0.102865 |           |
| 1  | 0.597467 | 2.017229 | -0.087449 |           |
| 6  | 1.862311 | 5.183596 | -0.069443 |           |
| 1  | 3.958005 | 5.689090 | 0.037749  |           |
| 1  | -0.135554 | 4.373964 | -0.149913 |           |
| 1  | 1.529643 | 6.216710 | -0.094570 |           |
| 6  | 0.942813 | -2.046880 | -0.162651 |           |
| 6  | 0.456329 | -0.771926 | -0.236057 |           |
| 7  | -0.596999 | -0.048184 | -0.035000 |           |
| 6  | -1.640389 | -0.456371 | 1.260484  |           |
| 8  | -1.617094 | 0.677018 | 2.221367  |           |
| 8  | -1.389282 | -1.833353 | 1.770467  |           |
| 6  | -3.227122 | -0.442546 | 0.418332  |           |
| 6  | -3.901730 | 0.768052 | 0.251633  |           |
| 6  | -3.762754 | -1.642234 | -0.049707 |           |
| 6  | -5.129021 | 0.769392 | -0.407464 |           |
| 1  | -3.474744 | 1.687174 | 0.637307  |           |
| 6  | -4.993402 | -1.620692 | -0.704494 |           |
| 1  | -3.228313 | -2.573261 | 0.103533  |           |
| 6  | -5.694331 | -0.420275 | -0.893792 |           |
| 1  | -5.659070 | 1.708161 | -0.543250 |           |
| 1  | -5.416958 | -2.551433 | -1.071704 |           |
| 6  | -7.039765 | -0.409333 | -1.577497 |           |
| 1  | -7.186383 | 0.508368 | -2.154327 |           |
| 1  | -7.152962 | -1.262907 | -2.251226 |           |
| 1  | -7.850526 | -0.462965 | -0.840561 |           |
| 1  | 0.242630 | -2.875246 | -0.138435 |           |
| 1  | 1.426589 | -0.058902 | -0.625553 |           |
45
C, E = -1507.18331074 , G = -1506.893060
6  5.030192    -3.238176    0.079491
6  3.679769    -3.151917    0.337958
|   |   |   |   |
|---|---|---|---|
| 6 | 2.925251 | -1.989896 | 0.004991 |
| 6 | 3.703354 | -0.861688 | -0.455464 |
| 6 | 5.094953 | -0.974622 | -0.755065 |
| 6 | 5.744735 | -2.158119 | -0.502640 |
| 1 | 5.558093 | -4.159271 | 0.308738 |
| 1 | 3.147665 | -4.003774 | -0.422146 |
| 7 | 2.693484 | 1.475340 | -0.267767 |
| 6 | 2.054251 | 2.687466 | -0.097749 |
| 6 | 2.677408 | 3.863041 | -0.540560 |
| 6 | 0.796346 | 2.704065 | 0.527484 |
| 6 | 2.020463 | 5.076646 | -0.354593 |
| 1 | 3.650076 | 3.814504 | -1.017067 |
| 6 | 0.163605 | 3.923290 | 0.700929 |
| 1 | 0.334794 | 1.779401 | 0.861838 |
| 6 | 0.767628 | 5.115480 | 0.264059 |
| 1 | 2.491161 | 5.993627 | -0.693919 |
| 1 | -0.808344 | 3.962384 | 1.182862 |
| 1 | 0.263461 | 6.065920 | 0.406475 |
| 6 | 1.512882 | -1.951614 | 0.137618 |
| 6 | 0.703151 | -1.152230 | -0.674862 |
| 7 | -0.598160 | -0.861255 | -0.640799 |
| 6 | -1.441848 | -1.174774 | 0.763634 |
| 8 | -1.137784 | -0.113419 | 1.778432 |
| 8 | -1.358773 | -2.594204 | 1.235247 |
| 6 | -3.126742 | -0.902514 | 0.186674 |
| 6 | -3.608064 | 0.402225 | 0.054931 |
| 6 | -3.938323 | -1.998419 | -0.094643 |
| 6 | -4.915057 | 0.601765 | -0.380748 |
| 1 | -2.969345 | 1.244035 | 0.299296 |
| 6 | -5.247946 | -1.781043 | -0.528100 |
| 1 | -3.550355 | -3.002971 | 0.032718 |
| 6 | -5.755125 | -0.484254 | -0.681011 |
| 1 | -5.293814 | 1.615368 | -0.484318 |
| 1 | -5.884863 | -2.633895 | -0.746578 |
| 6 | -7.169136 | -0.249005 | -1.155383 |
| 1 | -7.725988 | 0.373893 | -0.446854 |
| 1 | -7.179470 | 0.274228 | -2.118461 |
| 1 | -7.711399 | -1.189836 | -1.278611 |
| 1 | 1.043718 | -2.642080 | 0.830159 |
| 1 | 1.189735 | -0.717839 | -1.555613 |
TSC-D, $E = -1507.15794479$, $G = -1506.870012$

|   | 5.406347 | 0.835507 | 0.778773 |
|---|---|---|---|
| 6 | 4.466128 | 1.453791 | 0.021393 |
| 6 | 3.273599 | 0.772522 | -0.468112 |
| 6 | 3.225139 | -0.681864 | -0.180553 |
| 6 | 4.246269 | -1.287739 | 0.666215 |
| 6 | 5.292588 | -0.561086 | 1.128855 |
| 1 | 6.261761 | 1.400144 | 1.138787 |
| 1 | 4.562589 | 2.509300 | -0.216868 |
| 1 | 4.151121 | -2.343916 | 0.896977 |
| 1 | 6.052307 | -1.024607 | 1.749471 |
| 6 | 2.309360 | -1.508427 | -0.718878 |
| 7 | 1.650343 | -2.332722 | -1.317195 |
| 6 | 0.418107 | -2.978362 | -1.064104 |
| 6 | -0.318041 | -2.752767 | 0.109085 |
| 6 | -0.034399 | -3.885787 | -2.028154 |
| 6 | -1.507832 | -3.450492 | 0.307330 |
| 1 | 0.035841 | -2.093747 | 0.836314 |
| 6 | -1.230152 | -4.573242 | -1.820636 |
| 1 | 0.557108 | -4.042272 | -2.924136 |
| 6 | -1.966384 | -4.359149 | -0.653338 |
| 1 | 2.078832 | -3.286969 | 1.216607 |
| 1 | -1.582906 | -5.277250 | -2.567783 |
| 1 | -2.894370 | -4.898511 | -0.489788 |
| 6 | 2.337299 | 1.493437 | -1.152496 |
| 6 | 1.047282 | 1.023251 | -1.689494 |
| 7 | -0.100983 | 0.930635 | -1.112968 |
| 6 | -0.223694 | 1.425569 | 0.557062 |
| 8 | 0.367100 | 2.769903 | 0.782863 |
| 8 | 0.205267 | 0.282565 | 1.407808 |
| 6 | -2.009648 | 1.587529 | 0.664297 |
| 6 | -2.564564 | 2.860946 | 0.765327 |
| 6 | -2.810101 | 0.441964 | 0.676572 |
| 6 | -3.950586 | 2.986358 | 0.874924 |
| 1 | -1.921694 | 3.733747 | 0.761094 |
| 6 | -4.189528 | 0.588171 | 0.782051 |
| 1 | -2.364106 | -0.543449 | 0.598691 |
| 6 | -4.781971 | 1.859037 | 0.885046 |
| 1 | -4.389588 | 3.976804 | 0.954254 |
| 1 | -4.819329 | -0.297341 | 0.787219 |
| 6 | -6.279222 | 1.994424 | 1.016872 |
| 1 | -6.596693 | 3.036208 | 0.927687 |
| 1 | -6.798144 | 1.410736 | 0.249465 |
| 1 | -6.620908 | 1.621610 | 1.989574 |
|   |       |       |          | D, E = -1507.23993076, G = -1506.943096 |
|---|-------|-------|----------|----------------------------------------|
| 6 | -3.251727 | 1.727026 | 2.686334 |
| 6 | -2.215144 | 1.969027 | 1.792068 |
| 6 | -1.846742 | 0.994180 | 0.852163 |
| 6 | -2.542358 | -0.238808 | 0.807472 |
| 6 | -3.602060 | -0.458175 | 1.706793 |
| 6 | -3.950569 | 0.511635 | 2.639162 |
| 6 | -3.525465 | 2.483982 | 3.414884 |
| 6 | -1.677719 | 2.910590 | 1.800815 |
| 6 | -0.787433 | 1.267443 | -0.143340 |
| 6 | -2.138704 | -1.235583 | -0.165359 |
| 6 | -4.142902 | -1.399469 | 1.666312 |
| 6 | -4.766760 | 0.327592 | 3.331434 |
| 6 | -1.099238 | -1.071854 | -0.877760 |
| 6 | -2.738732 | -2.128043 | -0.305343 |
| 6 | -0.632389 | -1.806462 | -1.579835 |

|   |       |       |          |
| 6 | -0.233437 | 0.099489 | -0.773916 |
| 6 | 1.510176  | -0.220792 | -0.706437 |
| 8 | 2.162284  | 1.039183  | -0.306853 |
| 8 | 1.819876  | -0.892582 | -1.985526 |
| 6 | 1.694753  | -1.409679 | 0.624461 |
| 6 | 1.760937  | -0.944020 | 1.941120 |
| 6 | 1.799678  | -2.766680 | 0.322026 |
| 6 | 1.921625  | -1.868146 | 2.968120 |
| 6 | 1.701595  | 0.117596  | 2.153870 |
| 6 | 1.962112  | -3.674916 | 1.368164 |
| 6 | 1.771795  | -3.102202 | -0.708376 |
| 6 | 2.020869  | -3.244871 | 2.700910 |
| 2.049891  | -4.733532 | 1.142095 |
| 6 | 2.185830  | -4.230259 | 3.831052 |
| 6 | 3.027812  | -3.954157 | 4.474391 |
| 6 | 1.291310  | -4.250230 | 4.464076 |
| 6 | 2.357413  | -5.242672 | 3.458131 |
| 6 | -0.462449 | 2.476063  | -0.414324 |
| 6 | 0.324574  | 2.937966  | -1.477971 |
| 6 | 0.205181  | 2.447117  | -2.792761 |
| 6 | 1.158946  | 4.044549  | -1.242893 |
| 6 | 0.919308  | 3.043054  | -3.831292 |
| 6 | -0.455792 | 1.612064  | -2.997534 |
| 6 | 1.887845  | 4.618330  | -2.282327 |
|   |        |        |        |
|---|--------|--------|--------|
| 1 | 1.229274 | 4.435504 | -0.232577 |
| 6 | 1.771601 | 4.122905 | -3.584153 |
| 1 | 0.808433 | 2.658519 | -4.841547 |
| 1 | 2.538443 | 5.464027 | -2.077284 |
| 1 | 2.330038 | 4.577677 | -4.396868 |

45

$E, E=-1506.7104405 \ G=-1506.410929$

|   |        |        |        |
|---|--------|--------|--------|
| C | -1.75065500 | 4.38152100 | -0.65602900 |
| C | -1.04293800 | 3.76120200 | 0.38167900 |
| C | -1.60410300 | 2.59183400 | 0.86341000 |
| C | -2.78396800 | 2.05759600 | 0.35347700 |
| C | -3.49255800 | 2.66031200 | -0.67182800 |
| C | -2.93984800 | 3.84829700 | -1.16737600 |
| H | -1.37031900 | 5.30633900 | -1.07782800 |
| H | -0.12645000 | 4.18819900 | 0.77372900 |
| H | -4.42140400 | 2.26530300 | -1.07068200 |
| H | -3.44684800 | 4.37585300 | -1.96876400 |
| C | -2.73988500 | 0.85858500 | 1.29404000 |
| H | -3.59954700 | 0.57155400 | 1.89781300 |
| N | -1.92230200 | -0.27948800 | 0.81833900 |
| C | -2.38210900 | -1.41231300 | 0.11189500 |
| C | -3.44341900 | -1.24667600 | -0.7746500 |
| C | -1.85694900 | -2.67978500 | 0.36492700 |
| C | -3.97020100 | -2.35596600 | -1.43233000 |
| H | -3.84290100 | -0.25403500 | -0.96045600 |
| C | -2.38272000 | -3.77767500 | -0.30634200 |
| H | -1.04126200 | -2.80068900 | 1.06938900 |
| C | -3.43931600 | -3.62274500 | -1.20286200 |
| H | -4.79416400 | -2.22571600 | -2.12586300 |
| H | -1.97000700 | -4.76294300 | -0.11681300 |
| H | -3.84886000 | -4.48601600 | -1.71620200 |
| C | -0.74313200 | 0.24607100 | 1.25636500 |
| C | -1.41883600 | 1.46446700 | 1.86882800 |
| N | 0.52215400 | 0.00142700 | 1.20850100 |
| S | 1.15538500 | -1.21446500 | 0.26169000 |
| O | 0.44833300 | -1.29375100 | -1.03174600 |
| O | 1.30672000 | -2.44134400 | 1.07163800 |
| C | 2.78406300 | -0.56434200 | -0.03715400 |
| C | 3.00299200 | 0.20901000 | -1.17514900 |
| C | 3.80527400 | -0.84681900 | 0.86513100 |
| C | 4.28025800 | 0.70357000 | -1.40618100 |
| H | 2.18963800 | 0.38645500 | -1.86840400 |
| C | 5.07248700 | -0.33530600 | 0.61766600 |
| H | 3.60539900 | -1.46526200 | 1.73350700 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 5.32670000| 0.44671200| -0.51646500|
| H       | 4.46820200| 1.29943600| -2.29419900|
| H       | 5.88189500| -0.54963800| 1.30968400|
| H       | -1.26213000| 1.65784800| 2.92763600|
| C       | 6.70644700| 0.99862300| -0.76074300|
| H       | 6.95917300| 1.75108400| -0.00765700|
| H       | 7.45936500| 0.20854200| -0.69745000|
| H       | 6.77834300| 1.46584800| -1.74446400|
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