Supplementary Information file

Design and Synthesis of Amino Acid Derivatives of Substituted Benzimidazoles and Pyrazoles as Sirt1 Inhibitors

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Table S1. The top 3 molecules obtain from computational virtual screening of *in-house* virtual library (1 million e-molecules) over Sirt1 (PDB id. 4I5I).

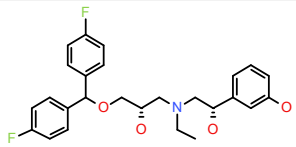
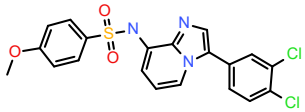
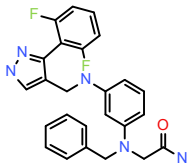
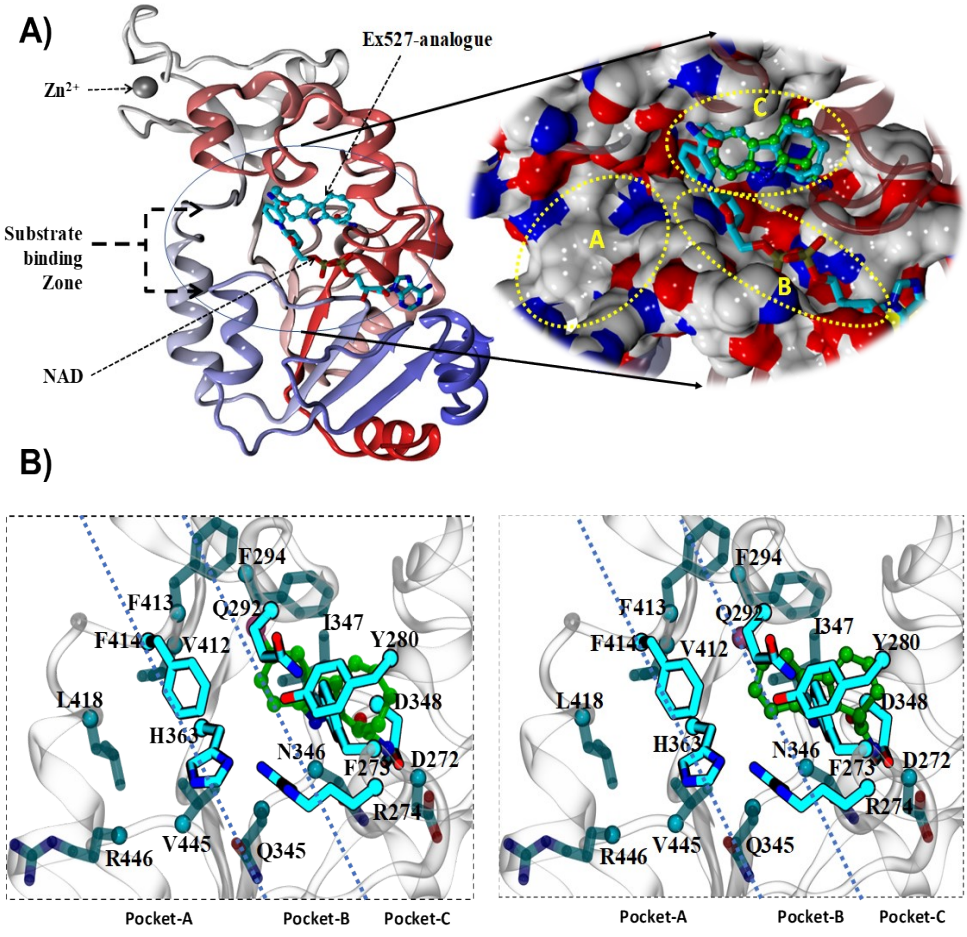
Name	Chemical structure	Molecule ID	Docking score (kcal/mol)	MMGBSA (kcal/mol)
V1		3281091	-14.07	-90.45
V2		2746690	-13.64	-92.64
V3		49334118	-13.14	-74.44

Fig. S1. Architecture of Sirt1 catalytic site: **(A)** Structure of Human Sirt1 with inhibitor Ex527-analogue (Ex527*) and co-factor NAD, "PDB id: 4I5I". In right-inset, enlarged surface view of catalytic grove (cut-off distance 6.0 Å), with Ex527*, NAD^+ and docked Ex527. NAD+ is shown in licorice representation rendered in atom wise i.e. carbon atom in cyan color, while Ex527* and Ex527 are shown in ball and sticks representation in which carbon atoms are in cyan and green color, respectively. **(B)** Comparison of interaction pattern of docked Sirt1-Ex527 complex with published crystal structure Sirt1-Ex527* (PDB id. 4I5I) in 3D space. Ex527, Ex427* are shown with "green" color and "ball-stick" representation. The key residues which cover the pocket from front face are shown in fluorescent cyan color stick representation. Other interacting residues are highlighted in transparent cyan color.



Sirt1-Ex527*
PDB id. 4I5I
Dock-score: -6.67
MMGBSA: -70.23 kcal/mol

Sirt1-Ex527
Docked-complex
Dock-score: -7.78
MMGBSA: -63.58 kcal/mol

Fig. S2: The concentration-response curve of Sirt1-inhibition. Data was shown as Mean±SEM, n=3.

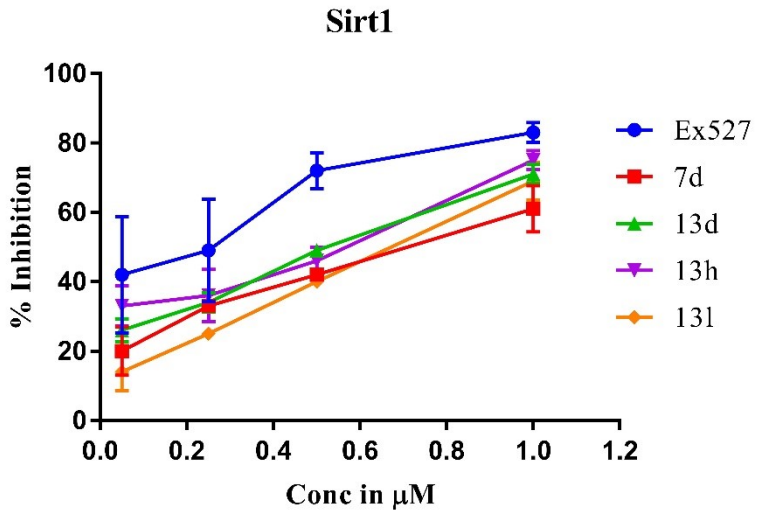


Fig. S3. Heat map of MM-GBSA and docking score of all designed compounds docked on Sirt1, Sirt2 and Sirt3. The cut-off scores are highlighted with dotted black box. All ligands are represented in the form of small square, color of square represent respective color of MM-GBSA heat-map. Ligand 7d, 13d, 13h and 13l are marked with arrows in left most panel.

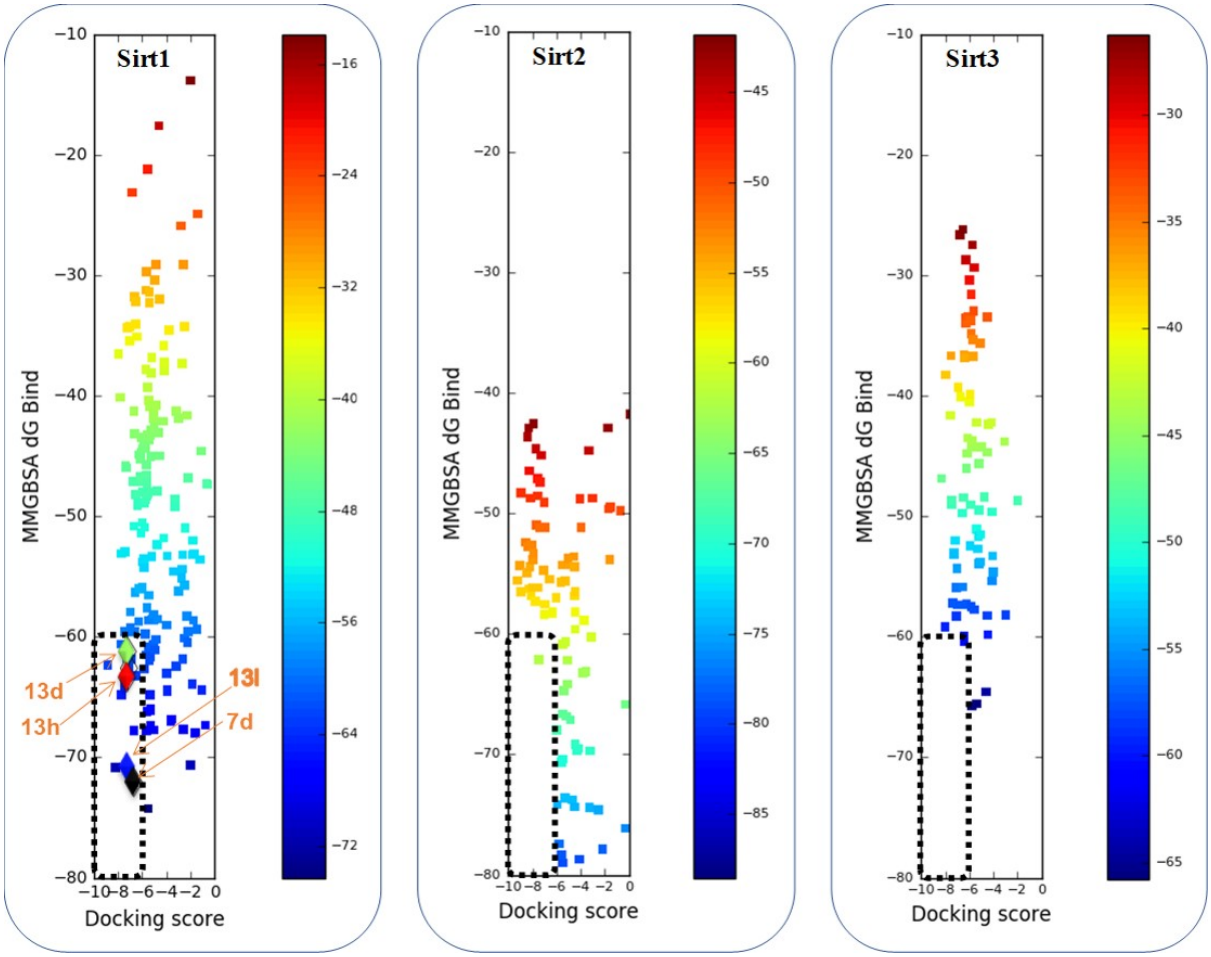


Fig. S4. The comparison of the 2d-interaction map of Sirt1 co-crystal (4I5I, Sirt1-Ex527*) with docked complex (Sirt1-Ex527).

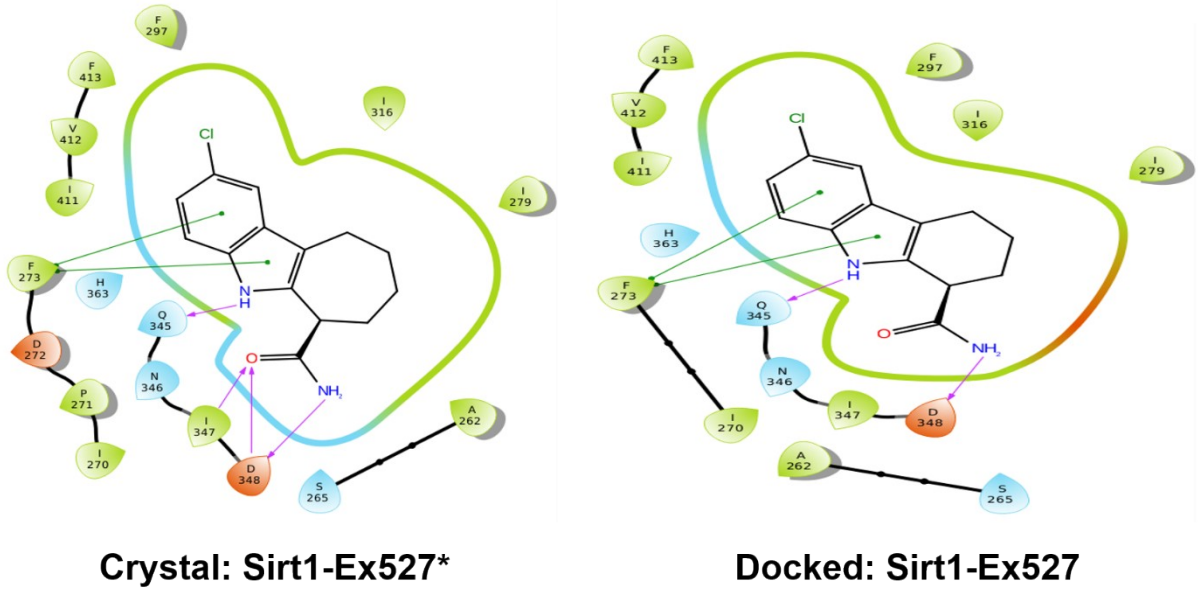


Fig. S5. The residue interaction fraction analysis of Ex527*. The region highlighted in yellow background represents *hot-spot2*. The dashed line in light-blue color represent **cut-off** value **0.5**, which indicated that the specific interaction is maintained **≥ 50%** of the total simulation time **(A)** Potential key residues within 3.5 Å cut-off from Ex527*, in the most stable pose extracted from dynamics. **(B)** Residue interaction fraction analysis.

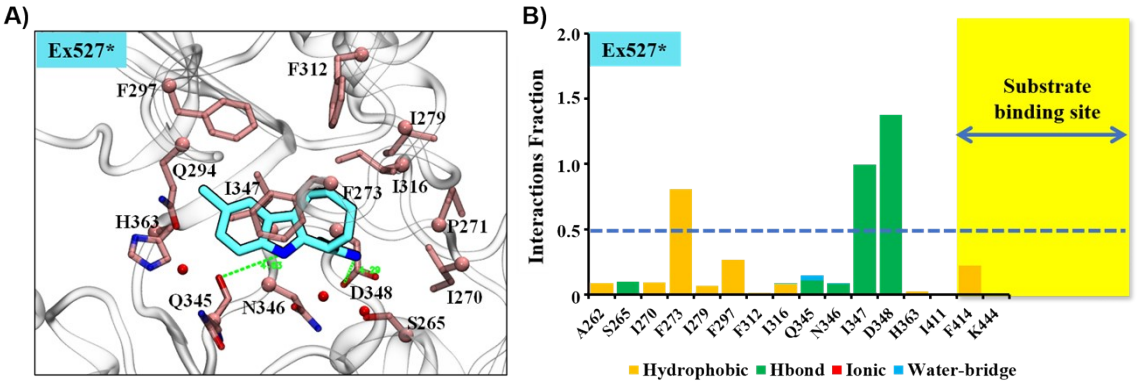


Fig. S6. Establishment of SAR of Scheme1 compounds. (A) Binding of scheme1 inhibitor (ball and stick representation), with –OMe substitution in R1 position, in catalytic pocket of Sirt1. The compound 7d is shown in color-type element with C in green. **(B)** Overlay binding of compounds 7l-7d, and 7h-7d at the catalytic pocket to speculate the difference in their binding pose. Sirt1 catalytic pocket is shown in the surface view. 7d is shown in representation "stick", while compound 7l and 7h are shown in representation "ball and stick". **(C)** MD trajectory analysis of scheme1 molecules (7l, 7h and 7d). The Root mean square deviation (RMSD) of protein (all backbone atoms) and ligand (no hydrogen atom) in coordinates as a function of the simulation time.

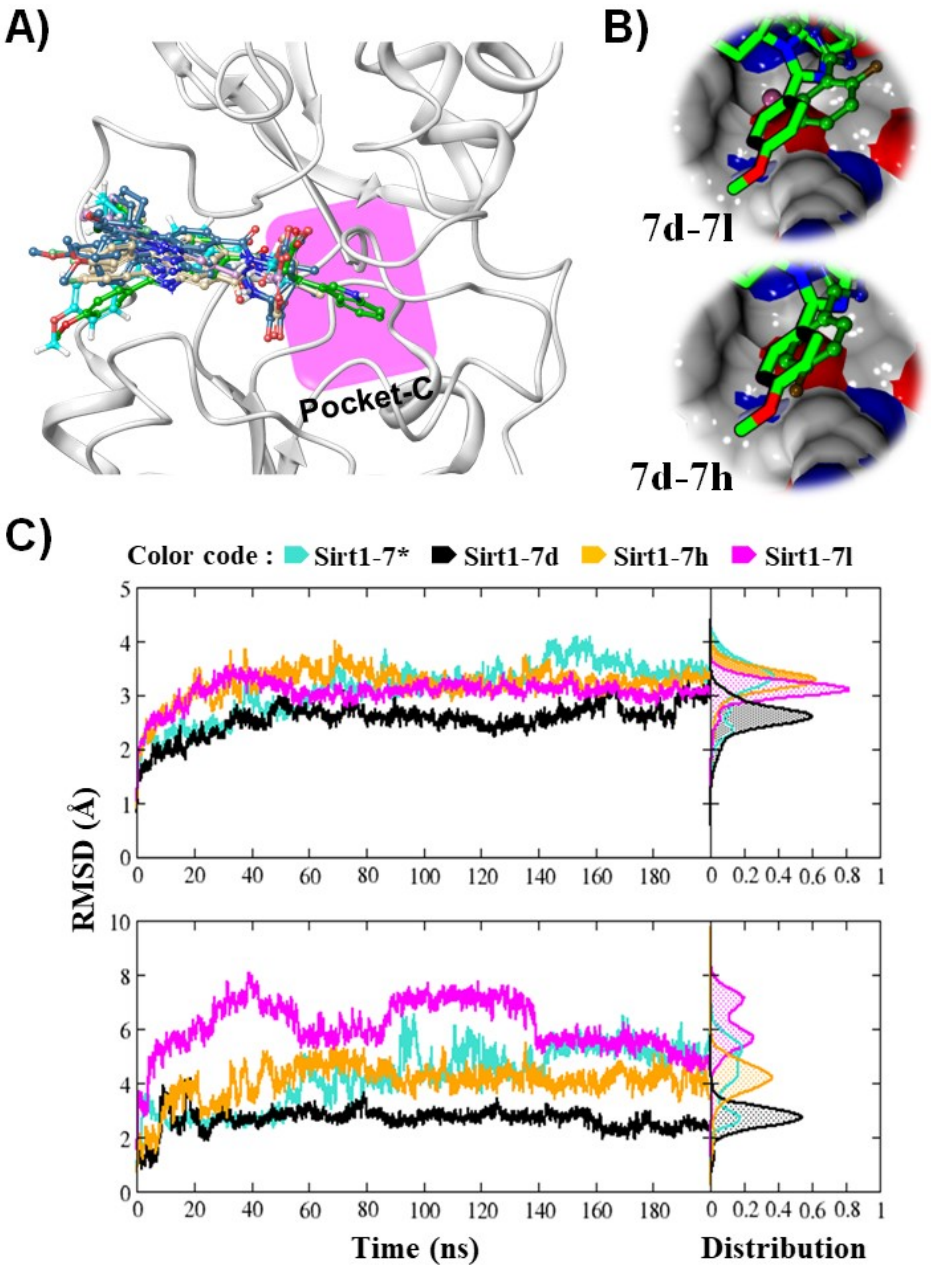
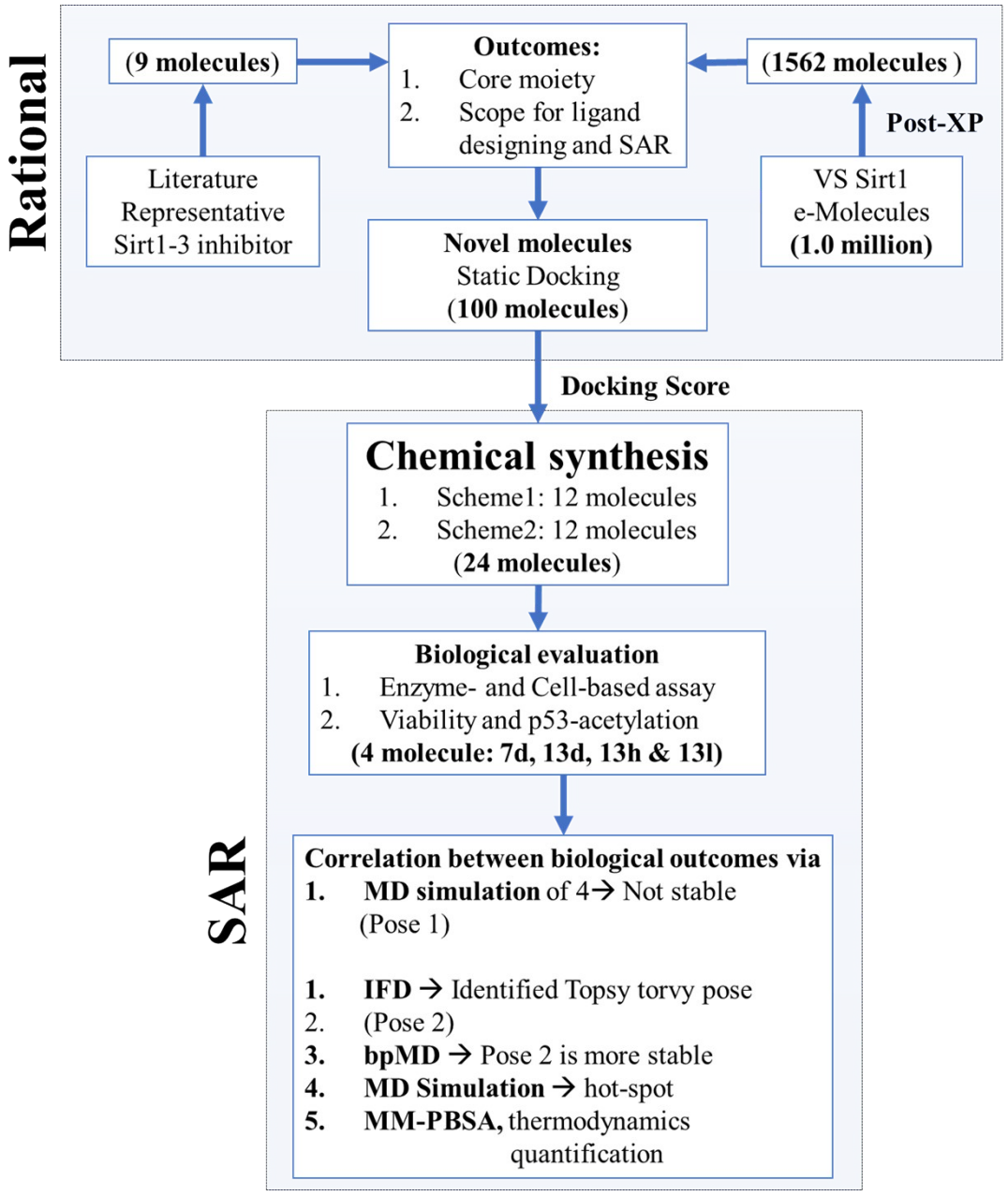


Fig. S7. The flow chart of overall computational protocol implemented in this study.



Experimental chemistry

Procedure for the synthesis of ethyl 4-(cyclohexylamino)-3-nitrobenzoate (3)

To a clear solution of ethyl 4-chloro-3-nitrobenzoate (**2,** 0.01 mol, 1.0 equiv.) in 15 mL of THF, cyclohexylamine (0.02 mol, 2.0 equiv.) and triethylamine (0.03 mol, 3.0 equiv.) were added and stirred at room temperature for 24 h. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was quenched with crushed ice and left undisturbed for two hours. The resulting yellow solid was washed with water, filtered and dried. The crude product was recrystallized from ethyl alcohol to obtain the pure product.

Procedure for the synthesis of benzimidazole esters (4a-c)

Sodium dithionite (0.03 mol, 3.0 equiv.) was added to a clear solution of ethyl 4-(cyclohexylamino)-3-nitrobenzoate **(3)** (0.01 mol; 1.0 equiv.) and substituted benzaldehyde **(**0.01 mol; 1.0 equiv.) in DMSO (15 mL). The reaction mixture was stirred at 90 °C for 3 h. After completion of the reaction (monitored by TLC hexane: ethyl acetate (8: 2, v/v)), the reaction mass was allowed to cool to room temperature and poured onto crushed ice. The solid separated was filtered, washed with water, dried and recrystallized from ethyl alcohol to obtain the pure product.

Ethyl 1-cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carboxylate (4a): Yield 92%; Mp 118-120 °C; Off white to pale yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3001 (Ar-H), 2933, 2856 (C-H), 1705 (C=O), 1610 (C=N), 1529 (C=C), 1172 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.52 (d, 1H, Ar-H, J = 1.2 Hz), 7.98 (dd, 1H, Ar-H, J = 1.6 Hz, 8.8 Hz), 7.66 (d, 1H, Ar-H, J = 8.8 Hz), 7.59 (d, 2H, Ar-H, J = 6.8 Hz), 7.07 (d, 2H, Ar-H, J = 6.8 Hz), 4.40-4.45 (q, 2H, -CH_2 of ethyl, J = 7.2 Hz), 4.33-4.39 (m, 1H, N-CH of cyclohexyl), 3.90 (s, 3H, O-CH_3), 2.27-2.36 (m, 2H, cyclohexyl), 1.95-1.99 (m, 4H, cyclohexyl), 1.77-1.79 (m, 1H, cyclohexyl), 1.43 (t, 3H, -CH_3 of ethyl, J = 7.2 Hz), 1.33-1.38 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 167.2, 160.9, 155.5, 143.4, 137.3, 130.8, 124.3, 123.4, 122.8, 122.2, 114.2, 112.0, 60.8, 57.1, 55.4, 31.4, 25.9, 25.2, 14.4; ESI-MS (*m/z*): 379.2 $[M+H]^+$; Anal. calcd. for $C_{23}H_{26}N_2O_3$: C, 72.99; H, 6.92; N, 7.40. Found: C, 72.97; H, 6.94; N, 7.37.

Ethyl 1-cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carboxylate (4b): Yield 87%; Mp 130-132 °C; Off white to pale brown solid; FT IR (ATR, υ_{max}, cm^{-1}): 3050 (Ar-H), 2927, 2850 (C-H), 1705 (C=O), 1602 (C=N), 1527 (C=C), 1300 (C-O), 1224 (C-F); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.52 (d, 1H, Ar-H, J = 1.2 Hz), 8.00 (dd, 1H, Ar-H, J = 1.6 Hz, 8.8 Hz), 7.67 (d, 1H, Ar-H, J = 8.8 Hz), 7.62-7.66 (m, 2H, Ar-H), 7.23-7.27 (m, 2H, Ar-H), 4.4-4.45 (q, 2H, -CH_2 of ethyl group, J = 7.2 Hz), 4.29-4.35 (m, 1H, cyclohexyl N-CH), 2.27-2.36

(m, 2H, cyclohexyl), 1.95-2.03 (m, 4H, cyclohexyl), 1.76-1.8 (m, 1H, cyclohexyl), 1.43 (t, 3H, -CH_3 of ethyl group, J = 7.2 Hz), 1.35-1.36 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 167.1, 163.7 (d, $^1J_{F\text{-}C}$ = 249.1 Hz), 154.4, 143.3, 137.1, 131.4 (d, $^3J_{F\text{-}C}$ = 8.6 Hz), 126.8 (d, $^4J_{F\text{-}C}$ = 3.5 Hz), 124.6, 123.7, 122.46, 116.0 (d, $^2J_{F\text{-}C}$ = 21.8 Hz), 112.1, 60.8, 57.3, 31.5, 25.9, 25.2, 14.4; ESI-MS (*m/z*): 367.3 $[M+H]^+$; Anal. calcd. for $C_{22}H_{23}N_2FO_2$: C, 72.11; H, 6.33; N, 7.64. Found: C, 72.10; H, 6.29; N, 7.62.

Ethyl 2-(2-chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carboxylate (4c): Yield 82%; Mp 104-106 °C; Pale yellow crystalline solid; FT IR (ATR, υ_{max}, cm^{-1}): 3000 (Ar-H), 2943, 2858 (C-H), 1710 (C=O), 1618 (C=N), 1570 (C=C), 1298 (C-O), 1249 (C-F), 790 (C-Cl); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.49 (d, 1H, Ar-H, J = 1.6 Hz), 7.96 (dd, 1H, Ar-H, J = 1.6 Hz, 8.8 Hz), 7.61 (d, 1H, Ar-H, J = 8.4 Hz), 7.39-7.45 (m, 1H, Ar-H), 7.31 (d, 1H, Ar-H, J = 8.0 Hz), 7.10 (t, 1H, Ar-H, J = 8.4 Hz), 4.32-4.37 (q, 2H, -CH_2 of ethyl group, J = 6.8 Hz), 3.74-3.81 (m, 1H, cyclohexyl N-CH), 2.05-2.14 (m, 2H, cyclohexyl), 1.83-1.99 (m, 4H, cyclohexyl), 1.67 (m, 1H, cyclohexyl), 1.34 (t, 3H, -CH_3 of ethyl group, J = 6.8 Hz), 1.20-1.21 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 167.0, 161.5 (d, $^1J_{F\text{-}C}$ = 250.5 Hz), 146.7, 143.6, 136.5, 136.1 (d, $^3J_{F\text{-}C}$ = 8.6 Hz), 132.3 (d, $^3J_{F\text{-}C}$ = 9.4 Hz), 125.6 (d, $^4J_{F\text{-}C}$ = 3.5 Hz), 124.5, 124.0, 122.9, 119.4 (d, $^2J_{F\text{-}C}$ = 20 Hz), 114.4 (d, $^2J_{F\text{-}C}$ = 21.6 Hz), 111.8, 60.8, 57.9, 31.4, 25.9, 25.2, 14.4; ESI-MS (*m/z*): 401.3 $[M+H]^+$, 403.3 $[M+2+H]^+$; Anal. calcd. for $C_{22}H_{22}N_2ClFO_2$: C, 65.91; H, 5.53; N, 6.99. Found: C, 65.89; H, 5.51; N, 7.02.

Procedure for the synthesis of benzimidazole carboxylic acids (5a-c)

To a clear solution of **4 a-c** (0.01 mol) in minimum amount of ethanol, catalytic amount of sodium hydroxide in 20 mL of water was added and the solution was refluxed for 3 h. After the completion of the reaction (monitored by TLC, hexane: ethyl acetate (8:2, v/v)), the cooled reaction mixture was poured onto crushed ice and acidified with dilute HCl. The solid obtained was washed with water, filtered, dried and recrystallized from ethyl alcohol to obtain pure product.

1-Cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carboxylic acid (5a): Yield 92%; Mp 244-246 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3462 (O-H), 3001 (Ar-H), 2933, 2856 (C-H), 1702 (C=O), 1610 (C=N), 1529 (C=C), 1172 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 12.81 (bs, 1H, CO_2H), 8.53 (d, 1H, Ar-H, J = 1.2 Hz), 7.98 (dd, 1H, Ar-H, J = 1.6 Hz, 8.8 Hz), 7.66 (d, 1H, Ar-H, J = 8.8 Hz), 7.59 (d, 2H, Ar-H, J = 6.8 Hz), 7.07 (d,

2H, Ar-H, J = 6.8 Hz), 4.33-4.39 (m, 1H, N-CH of cyclohexyl), 3.90 (s, 3H, O-CH_3), 2.27-2.36 (m, 2H, cyclohexyl), 1.95-1.99 (m, 4H, cyclohexyl), 1.77-1.79 (m, 1H, cyclohexyl), 1.33-1.38 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 167.3, 160.9, 155.5, 143.4, 137.3, 130.8, 124.3, 123.4, 122.8, 122.2, 114.2, 112.0, 57.1, 55.4, 31.4, 25.9, 25.2; ESI-MS (*m/z*): 351.1 $[M+H]^+$; Anal. calcd. for $C_{21}H_{22}N_2O_3$: C, 71.98; H, 6.33; N, 7.99. Found: C, 71.97; H, 6.30; N, 7.94.

1-Cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carboxylic acid (5b): Yield 94%; Mp 248-250 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3450 (O-H), 3050 (Ar-H), 2927, 2850 (C-H), 1703 (C=O), 1601 (C=N), 1527 (C=C), 1300 (C-O), 1224 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 12.80 (bs, 1H, CO_2H), 8.51 (d, 1H, Ar-H, J = 1.2 Hz), 8.00 (dd, 1H, Ar-H, J = 1.6 Hz, 8.8 Hz), 7.67 (d, 1H, Ar-H, J = 8.8 Hz), 7.62-7.66 (m, 2H, Ar-H), 7.23-7.27 (m, 2H, Ar-H), 4.29-4.35 (m, 1H, cyclohexyl N-CH), 2.27-2.36 (m, 2H, cyclohexyl), 1.95-2.03 (m, 4H, cyclohexyl), 1.76-1.8 (m, 1H, cyclohexyl), 1.35-1.36 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 167.1, 163.7 (d, $^1J_{F\text{-}C}$ = 240 Hz), 154.4, 143.3, 137.1, 131.4 (d, $^3J_{F\text{-}C}$ = 10 Hz), 126.8, 124.6, 123.7, 122.46, 116.1 (d, $^2J_{F\text{-}C}$ = 21.4 Hz), 112.1, 57.3, 31.5, 25.9, 25.2; ESI-MS (*m/z*): 339.3 $[M+H]^+$; Anal. calcd. for $C_{20}H_{19}N_2FO_2$: C, 70.99; H, 5.66; N, 8.28. Found: C, 70.97; H, 5.62; N, 8.24.

2-(2-Chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carboxylic acid (5c): Yield 96%; Mp 232-234 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3500 (O-H), 2941, 2862 (C-H), 1706 (C=O), 1620 (C=N), 1572 (C=C), 1298 (C-O), 1248 (C-F), 779 (C-Cl); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 12.82 (bs, 1H, CO_2H), 8.30 (s, 1H, Ar-H), 8.01 (d, 1H, Ar-H, J = 12.0 Hz), 7.93 (d, 1H, Ar-H, J = 8.4 Hz), 7.73-7.71 (m, 1H, Ar-H), 7.63 (d, 1H, Ar-H, J = 8.0 Hz), 7.51 (t, 1H, Ar-H, J = 8.0 Hz), 3.84-3.90 (m, 1H, cyclohexyl N-CH), 2.14-2.23 (m, 2H, cyclohexyl), 1.78-1.92 (m, 4H, cyclohexyl), 1.58 (m, 1H, cyclohexyl), 1.23-1.32 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 167.6, 160.7 (d, $^1J_{F\text{-}C}$ = 240 Hz), 146.1, 143.0, 136.5, 136.1 (d, $^3J_{F\text{-}C}$ = 8.6 Hz), 132.3 (d, $^3J_{F\text{-}C}$ = 9.4 Hz), 125.9, 124.7, 123.8, 121.5, 118.3 (d, $^2J_{F\text{-}C}$ = 20 Hz), 115.0 (d, $^2J_{F\text{-}C}$ = 20 Hz), 112.7, 57.2, 30.7, 25.2, 24.3; ESI-MS (*m/z*): 373.3 $[M+H]^+$, 375.3 $[M+2+H]^+$; Anal. calcd. for $C_{20}H_{18}N_2ClFO_2$: C, 64.43; H, 4.87; N, 7.51. Found: C, 64.41; H, 4.83; N, 7.54.

Procedure for the synthesis of benzimidazole monopeptide esters (6a-l)

To a clear solution of **5a-c** (0.01 mol) in 15 mL of DMF, NMM (0.025 mol, 2.5 equiv.) and TBTU (0.0125 mol, 1.25 equiv.) were added and stirred for an hour at room temperature. To

the clear resulting solution, amino acid methyl ester hydrochloride (0.01 mol, 1.0 equiv.) was added and stirred at room temperature for 4 h. After completion of the reaction (monitored by TLC hexane: ethyl acetate (7:3, v/v)), the reaction mass was poured onto crushed ice. The precipitated solid was washed with water, filtered, dried column purified using 5-15% of ethyl acetate in hexane to obtain the pure product.

Methyl (S)-(1-cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carbonyl)alaninate (6a): Yield 90%; Mp 134-136 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3078 (Ar-H), 2935 and 2854 (C-H), 1726 (C=O of ester), 1652 (C=O of amide), 1612 (C=N), 1577 (C=C), 1029 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.65 (d, 1H, amide N-H, J = 7.2 Hz), 8.27 (d, 1H, Ar-H, J = 1.2 Hz), 7.90 (d, 1H, Ar-H, J = 8.4Hz), 7.80 (dd, 1H, Ar-H, J = 1.6 Hz, 7.2 Hz), 7.61 (d, 1H, Ar-H, J = 8.8 Hz), 7.15 (d, 1H, Ar-H, J = 9.2 Hz), 4.42-4.49 (m, 1H, chiral CH), 4.26-4.32 (m, 1H, N-CH), 3.86 (s, 3H, OCH_3), 3.79 (s, 3H, OCH_3), 2.25-2.33 (m, 2H, cyclohexyl), 1.84-1.92 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H, cyclohexyl), 1.42-1.44 (d, 3H, CH_3, J = 7.2 Hz), 1.23-1.39 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 174.4, 166.4, 160.4, 154.7, 142.8, 135.7, 130.8, 127.5, 122.5, 121.6, 118.7, 114.2, 112.4, 56.7, 55.3, 51.9, 48.2, 30.5, 25.5, 24.4, 16.9; ESI-MS (*m/z*): 436.2 $[M+H]^+$; Anal. calcd. for $C_{25}H_{29}N_3O_4$: C, 68.95; H, 6.71; N, 9.65. Found: C, 68.96; H, 6.70; N, 9.62.

Methyl (S)-(1-cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carbonyl)valinate (6b): Yield 62%; Mp 68-70 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3409 (NH), 3100 (Ar-H), 2935 and 2850 (C-H), 1722 (C=O of ester), 1650 (C=O of amide), 1612 (C=N), 1581 (C=C), 1029 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.33 (d, 1H, amide NH, J = 8.0 Hz); 8.27 (d, 1H, Ar-H, J = 1.2 Hz), 7.89 (d, 1H, Ar-H, J = 8.8 Hz), 7.79 (dd, 1H, Ar-H, J = 1.6 Hz, 8.4 Hz), 7.61 (d, 2H, Ar-H, J = 8.8 Hz), 7.15 (d, 2H, Ar-H, J = 8.8 Hz), 4.26-4.32 (m, 2H, N-CH and chiral CH), 3.86 (s, 3H, OCH_3), 3.79 (s, 3H, OCH_3), 2.19-2.33 (m, 3H, CH and cyclohexyl), 1.84-1.90 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H, cyclohexyl), 1.23-1.41 (m, 3H, cyclohexyl), 0.97-1.01 (m, 6H, diastereotopic CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 174.3, 166.9, 160.4, 154.6, 142.7, 135.7, 130.8, 127.8, 122.5, 121.7, 118.8, 114.2, 112.4, 58.6, 56.7, 55.3, 51.8, 30.5, 29.6, 25.5, 24.4, 19.4, 18.8; ESI-MS (*m/z*): 464.4 $[M+H]^+$; Anal. calcd. for $C_{27}H_{33}N_3O_4$: C, 69.96; H, 7.18; N, 9.06. Found: C, 69.94; H, 7.15; N, 9.03.

Methyl (S)-(1-cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carbonyl)leucinate (6c): Yield 75%; Mp: 82-84 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3074 (Ar-H), 2935 and 2862 (C-H), 1726 (C=O of ester), 1650 (C=O of amide), 1612 (C=N), 1577 (C=C), 1029

(C-O); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.33 (d, 1H, amide NH, J = 6.8 Hz), 8.23 (s, 1H, Ar-H), 7.88 (d, 1H, Ar-H, J = 8.4 Hz), 7.78 (d, 1H, Ar-H, J = 8.4 Hz), 7.60 (d, 1H, Ar-H, J = 8.4 Hz), 7.14 (d, 1H, Ar-H, J = 8.8 Hz), 4.37-4.40 (m, 1H, chiral CH), 4.25-4.31 (m, 1H, C-NH), 3.86 (s, 3H, OCH_3), 3.79 (s, 3H, OCH_3), 2.24-2.33 (m, 2H, cyclohexyl), 1.83-1.90 (m, 4H, cyclohexyl), 1.62-1.76 (m, 4H, isobutyl CH, CH_2 and cyclohexyl), 1.24-1.41 (m, 3H, cyclohexyl), 0.89-0.92 (m, 6H, diastereotopic CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 174.4, 166.4, 160.4, 154.6, 142.8, 135.6, 130.8, 128.0, 122.5, 121.5, 118.6, 114.2, 112.4, 56.6, 55.3, 52.2, 30.5, 29.6, 25.5, 24.6, 23.0, 21.6, 18.9; ESI-MS (*m/z*): 478.4 $[M+H]^+$; Anal. calcd. for $C_{28}H_{35}N_3O_4$: C, 70.42; H, 7.39; N, 8.80. Found: C, 70.40; H, 7.35; N, 8.81.

Methyl (S)-(1-cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carbonyl)tryptophanate (6d): Yield 99%, Mp: 86-88 °C; Off white to pale brown solid; FT IR (ATR, υ_{max}, cm^{-1}): 3055 (Ar-H), 2933 and 2856 (C-H), 1728 (C=O of ester), 1643 (C=O of amide), 1612 (C=N), 1577 (C=C), 1178 (C-O); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 10.81 (s, 1H, indole NH), 8.62 (d, 1H, amide NH, J = 7.6 Hz), 8.20 (d, 1H, Ar-H, J = 1.6 Hz), 7.88 (d, 1H, Ar-H, J = 8.4 Hz), 7.73 (dd, 1H, Ar-H, J = 8.4 Hz, 1.6 Hz), 7.59-7.63 (m, 3H, Ar-H), 7.32 (d, 1H, Ar-H, J = 8.0 Hz), 7.23 (d, 1H, Ar-H, J = 2.0 Hz), 7.15 (d, 2H, Ar-H, J = 8.8 Hz), 7.04-7.08 (m, 1H, Ar-H), 6.97-7.01 (m, 1H, Ar-H), 4.66-4.72 (m, 1H, chiral CH), 4.25-4.31 (m, 1H, C-NH), 3.86 (s, 3H, OCH_3), 3.79 (s, 3H, OCH_3), 2.23-2.29 (m, 2H, cyclohexyl), 1.83-1.89 (m, 4H, cyclohexyl), 1.62-1.65 (m, 1H, cyclohexyl), 1.25-1.41 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 173.7, 166.6, 160.4, 154.6, 142.6, 136.1, 135.6, 130.9, 127.6, 127.1, 125.76, 123.6, 121.6, 120.9, 118.5, 118.4, 118.1, 114.2, 112.5, 111.4, 110.5, 56.7, 55.3, 53.7, 52.4, 30.5, 26.6, 25.5, 24.3; ESI-MS (*m/z*): 551.3 $[M+H]^+$; Anal. calcd. for $C_{33}H_{34}N_4O_4$: C, 71.98; H, 6.22; N, 10.17. Found: C, 71.95; H, 6.20; N, 10.13

Methyl (S)-(1-cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carbonyl)alaninate (6e): Yield 86%; Mp 128-130 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3071 (Ar-H), 2932 and 2861 (C-H), 1730 (C=O of ester), 1653 (C=O of amide), 1614 (C=N), 1578 (C=C), 1265 (C-O), 1230 (C-F); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.63 (d, 1H, amide N-H, J = 7.2 Hz), 8.29 (s, 1H, Ar-H), 7.93 (d, 1H, Ar-H, J = 8.8 Hz), 7.83 (d, 1H, Ar-H, J = 8.8 Hz), 7.71-7.75 (m, 2H, Ar-H), 7.42-7.46 (m, 2H, Ar-H), 4.41-4.48 (m, 1H, chiral CH), 4.20-4.26 (m, 1H, N-CH), 3.79 (s, 3H, OCH_3), 2.24-2.32 (m, 2H, cyclohexyl), 1.83-1.93 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H, cyclohexyl), 1.42-1.44 (d, 3H, CH_3, J = 7.2 Hz), 1.23-1.38 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 174.5, 166.3, 163.1 (d, $^1J_{F\text{-}C}$ = 246 Hz), 153.7, 142.7, 135.7, 131.8 (d, $^3J_{F\text{-}C}$ = 8.5 Hz), 127.7, 126.9, 121.9, 118.9, 115.9 (d, $^2J_{F\text{-}C}$ = 21.5 Hz), 112.6,

56.8, 52.1, 48.4, 30.5, 25.4, 24.3, 17.1; ESI-MS (*m/z*): 424.4 $[M+H]^+$; Anal. calcd. for $C_{24}H_{26}N_3FO_3$: C, 68.07; H, 6.19; N, 9.92. Found: C, 68.02; H, 6.15; N, 9.91.

Methyl (S)-(1-cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carbonyl)valinate (6f): Yield 92%; 118-120 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3407 (N-H), 3074 (Ar-H), 2935 and 2864 (C-H), 1721 (C=O of ester), 1654 (C=O of amide), 1614 (C=N), 1581 (C=C), 1265 (C-O), 1232 (C-F); ^1H NMR (400 MHz, $CDCl_3$, δ ppm): 8.52 (d, 1H, amide N-H, J = 7.6 Hz), 8.20 (d, 1H, Ar-H, J = 1.2 Hz), 7.90 (d, 1H, Ar-H, J = 8.8 Hz), 7.74-7.76 (m, 1H, Ar-H), 7.71-7.73 (m, 2H, Ar-H), 7.42-7.46 (m, 2H, Ar-H), 4.29-4.32 (m, 1H, chiral CH), 4.26-4.28 (m, 1H, N-CH), 3.79 (s, 3H, OCH_3), 2.25-2.33 (m, 2H, cyclohexyl), 2.20-2.25 (m, 1H, C-H of isopropyl), 1.84-1.90 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H, cyclohexyl), 1.24-1.41 (m, 3H, cyclohexyl), 0.97-1.01 (m, 6H, diastereotopic CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 174.4, 166.9, 162.9 (d, $^1J_{F-C}$ = 250 Hz), 154.6, 142.8, 135.7, 131.8 (d, $^3J_{F-C}$ = 9.6 Hz), 127.5, 122.5, 121.6, 118.7, 115.8 (d, $^2J_{F-C}$ = 21 Hz), 112.4, 58.6, 56.3, 52.3, 30.5, 29.6, 25.5, 24.4, 19.4, 18.8; ESI-MS (*m/z*): 452.4 $[M+H]^+$; Anal. calcd. for $C_{26}H_{30}N_3FO_3$: C, 69.16; H, 6.70; N, 9.31. Found: C, 69.13; H, 6.69; N, 9.32.

Methyl (S)-(1-cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carbonyl)leucinate (6g): Yield 96%, 102-104 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3409 (N-H), 3071 (Ar-H), 2934 and 2865 (C-H), 1717 (C=O of ester), 1654 (C=O of amide), 1614 (C=N), 1579 (C=C), 1265 (C-O), 1231 (C-F); ^1H NMR (400 MHz, $CDCl_3$, δ ppm): 8.59 (d, 1H, amide N-H, J = 7.6 Hz), 8.3 (s, 1H, Ar-H), 7.93 (d, 1H, Ar-H, J = 8.4 Hz), 7.84 (d, 2H, Ar-H, J = 8.4 Hz), 7.72-7.75 (m, 2H, Ar-H), 7.42-7.46 (m, 2H, Ar-H), 4.47-4.52 (m, 1H, chiral CH), 4.20-4.26 (m, 1H, N-CH), 3.79 (s, 3H, OCH_3), 2.24-2.32 (m, 2H, cyclohexyl), 1.59-1.92 (m, 8H, cyclohexyl, isobutyl CH and diastereotopic CH_2), 1.23-1.41 (m, 3H, cyclohexyl), 0.95 (d, 3H, diastereotopic CH_3, J = 6.4 Hz) 0.91 (d, 3H, diastereotopic CH_3, J = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 174.4, 166.7, 162.9 (d, $^1J_{F-C}$ = 250 Hz), 153.7, 142.6, 135.6, 131.7 (d, $^3J_{F-C}$ = 9.6 Hz), 127.7, 126.8, 121.9, 118.9, 115.8 (d, $^2J_{F-C}$ = 20 Hz), 112.6, 56.8, 52.1, 50.9, 30.5, 25.4, 24.6, 24.3, 22.9, 21.2; ESI-MS (*m/z*): 466.4 $[M+H]^+$; Anal. calcd. for $C_{27}H_{32}N_3FO_3$: C, 69.66; H, 6.93; N, 9.03. Found: C, 69.64; H, 6.91; N, 9.04.

Methyl (S)-(1-cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carbonyl)-tryptophanate (6h): Yield 96%; Mp 78-80 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3409 (N-H), 3056 (Ar-H), 2933 and 2858 (C-H), 1720 (C=O of ester), 1641 (C=O of amide), 1614 (C=N), 1527 (C=C), 1296 (C-O), 1230 (C-F); ^1H NMR (400 MHz, $CDCl_3$, δ ppm): 10.79

(s, 1H, indole-NH), 8.52 (d, 1H, amide-NH, J = 7.6 Hz), 8.2 (d, 1H, Ar-H, J = 1.2 Hz), 7.90 (d, 1H, Ar-H, J = 8.8 Hz), 7.71-7.76 (m, 3H, Ar-H), 7.62 (d, 1H, Ar-H, J = 8.0 Hz), 7.44 (m, 2H, Ar-H, J = 8.8 Hz), 7.32 (d, 1H, Ar-H, J = 8.0 Hz), 7.22 (d, 1H, Ar-H, J = 2.0 Hz), 7.03-7.07 (m, 1H, Ar-H); 6.95-6.99 (m, 1H, Ar-H); 4.63-4.68 (m, 1H, chiral C-H), 4.19-4.25 (m, 1H, -NC-H), 3.79 (s, 3H, OCH_3), 3.35 (dd, 1H, indole CH_2, J = 4.2 Hz, 14.6 Hz), 3.26 (dd, 1H, indole CH_2, J = 9.2 Hz, 14.4 Hz), 2.22-2.31 (m, 2H, cyclohexyl), 1.82-1.92 (m, 4H, cyclohexyl), 1.62-1.65 (m, 1H, cyclohexyl), 1.26-1.40 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 173.8, 166.3, 162.9 (d, $^1J_{F\text{-}C}$ = 250 Hz), 164.2, 161.7, 153.7, 142.6, 136.0, 135.6, 131.7 (d, $^3J_{F\text{-}C}$ = 9.6 Hz), 128.0, 127.3, 126.9, 125.9, 123.5, 121.7, 120.8, 118.7, 118.2, 115.8 (d, $^2J_{F\text{-}C}$ = 20 Hz), 112.6, 111.3, 110.7, 56.8, 54.1, 51.9, 30.5, 26.8, 25.4, 24.3; ESI-MS (*m/z*): 539.22 $[M+H]^+$; Anal. calcd. for $C_{32}H_{31}N_4FO_3$: C, 71.36; H, 5.80; N, 10.40. Found: C, 71.37; H, 5.78; N, 10.36.

Methyl (S)-(2-(2-chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carbonyl)-alaninate (6i): Yield 88%; Mp 104-106 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 2928 and 2863 (C-H), 1738 (C=O of ester), 1642 (C=O of amide), 1614 (C=N), 1532 (C=C), 1159 (C-O), 781 (C-C-Cl); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.27 (s, 1H, Ar-H), 7.86 (d, 1H, Ar-H, J = 8.0 Hz), 7.70 (d, 1H, Ar-H, J = 8.0 Hz), 7.47-7.51 (m, 1H, Ar-H), 7.37-7.39 (m, 1H, Ar-H), 7.17 (t, 1H, Ar-H, J = 8.0 Hz), 6.90 (bs, 1H, amide N-H), 4.83-4.86 (m, 1H, chiral CH), 3.83-3.87 (m, 1H, N-CH), 3.79 (s, 3H, OCH_3), 1.91-2.18 (m, 6H, cyclohexyl), 1.55 (d, 3H, CH_3, J = 8.0 Hz), 1.27-1.31 (m, 4H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 173.7, 167.2, 161.5 (d, $^1J_{F\text{-}C}$ = 250 Hz), 146.7, 143.6, 136.1, 135.7, 132.4 (d, $^3J_{F\text{-}C}$ = 10 Hz), 128.2, 125.6, 122.3, 119.4, 114.4 (d, $^2J_{F\text{-}C}$ = 21 Hz), 112.4, 58.0, 52.5, 48.6, 31.5, 25.9, 25.1, 18.6; ESI-MS (*m/z*): 458.2 $[M+H]^+$, 460.2 $[M+2+H]^+$; Anal. calcd. for $C_{24}H_{25}N_3ClFO_3$: C, 62.95; H, 5.50; N, 9.18. Found: C, 62.92; H, 5.48; N, 9.15.

Methyl (S)-(2-(2-chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carbonyl)-valinate (6j): Yield 86%; Mp 58-60 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3362 (O-H), 3073 (Ar-H), 2947 and 2861 (C-H), 1724 (C=O of ester), 1644 (C=O of amide), 1621 (C=N), 1574 (C=C), 1297 (C-O), 1246 (C-F); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.61 (d, 1H, amide N-H, J = 8.0 Hz), 8.34 (s, 1H, Ar-H), 7.97 (d, 1H, Ar-H, J = 8.4 Hz), 7.87 (d, 1H, Ar-H, J = 8.8 Hz), 7.71-7.77 (m, 1H, Ar-H), 7.62 (m, 1H, Ar-H), 7.49-7.54 (m, 1H, Ar-H), 4.29-4.32 (m, 1H, chiral CH), 4.26-4.28 (m, 1H, N-CH), 3.79 (s, 3H, OCH_3), 2.25-2.33 (m, 2H, cyclohexyl), 2.20-2.25 (m, 1H, C-H of isopropyl), 1.84-1.90 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H, cyclohexyl), 1.24-1.41 (m, 3H, cyclohexyl), 0.97-1.01 (m, 6H, diastereotopic CH_3); ^{13}C NMR

(100 MHz, $CDCl_3$, δ ppm): 174.4, 166.4, 161.4 (d, $^1J_{F\text{-}C}$ = 254 Hz), 146.8, 143.7, 136.1 (d, $^3J_{F\text{-}C}$ = 8 Hz), 135.0, 132.7, 125.6 (d, $^4J_{F\text{-}C}$ = 3 Hz), 124.5, 122.9, 119.3, 114.4 (d, $^2J_{F\text{-}C}$ = 21 Hz), 112.4, 58.7, 56.6, 52.4, 30.5, 29.6, 25.5, 24.4, 19.4, 18.9; ESI-MS (*m/z*): 486.4 $[M+H]^+$, 488.4 $[M+2+H]^+$; Anal. calcd. for $C_{26}H_{29}N_3ClFO_3$: C, 64.26; H, 6.02; N, 8.65. Found: C, 64.20; H, 5.99; N, 8.61.

Methyl (S)-(2-(2-chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carbonyl)-leucinate (6k): Yield 96%; Mp 54-56 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3355 (O-H), 3080 (Ar-H), 2948 and 2864 (C-H), 1722 (C=O of ester), 1643 (C=O of amide), 1620 (C=N), 1571 (C=C), 1299 (C-O), 1249 (C-F); ^1H NMR (400 MHz, $CDCl_3$, δ ppm): 12.51 (s, 1H, CO_2H), 8.61 (d, 1H, amide N-H, *J* = 8.0 Hz), 8.34 (s, 1H, Ar-H), 7.97 (d, 1H, Ar-H, *J* = 8.4 Hz), 7.87 (d, 1H, Ar-H, *J* = 8.8 Hz), 7.71-7.77 (m, 1H, Ar-H), 7.62 (m, 1H, Ar-H), 7.49-7.54 (m, 1H, Ar-H), 4.47-4.51 (m, 1H, chiral C-H), 3.84-3.90 (m, 1H, N-CH), 3.79 (s, 3H, OCH_3), 2.12-2.21 (m, 2H, cyclohexyl), 1.60-1.84 (m, 8H, cyclohexyl, isobutyl CH and diastereotopic CH_2), 1.24-1.29 (m, 3H, cyclohexyl), 0.94 (d, 3H, diastereotopic CH_3, *J* = 6.4 Hz), 0.90 (d, 3H, diastereotopic CH_3, *J* = 6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 174.4, 166.4, 161.6 (d, $^1J_{F\text{-}C}$ = 230 Hz), 146.8, 143.7, 136.5, 135.3, 132.3 (d, $^3J_{F\text{-}C}$ = 10 Hz), 125.5, 124.5, 124.0, 122.9, 119.4, 114.4 (d, $^2J_{F\text{-}C}$ = 20 Hz), 111.9, 56.6, 50.9, 52.1, 48.6, 30.5, 25.5, 24.6, 24.3, 23.1, 21.6; ESI-MS (*m/z*): 500.2 $[M+H]^+$, 502.2 $[M+2+H]^+$; Anal. calcd. for $C_{27}H_{31}N_3ClFO_3$: C, 64.86; H, 6.25; N, 8.40. Found: C, 64.85; H, 6.23; N, 8.42.

Methyl (S)-(2-(2-chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carbonyl)-tryptophanate (6l): Yield 97%; Mp 84-86 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3409 (N-H), 3056 (Ar-H), 2937 and 2858 (C-H), 1724 (C=O of ester), 1641 (C=O of amide), 1620 (C=N), 1573 (C=C), 1299 (C-O), 1251 (C-F); ^1H NMR (400 MHz, $CDCl_3$, δ ppm): 10.80 (s, 1H, indole-NH), 8.67 (d, 1H, amide N-H, *J* = 7.6 Hz), 8.27 (s, 1H, Ar-H), 7.95 (d, 1H, Ar-H, *J* = 8.4 Hz), 7.71-7.80 (m, 2H, Ar-H), 7.60-7.63 (m, 2H, Ar-H), 7.49-7.53 (m, 1H, Ar-H), 7.32 (d, 1H, Ar-H, *J* = 8.0 Hz), 7.23 (s, 1H, Ar-H), 7.04-7.08 (m, 1H, Ar-H), 6.98-7.01 (m, 1H, Ar-H), 4.67-4.72 (m, 1H, chiral C-H), 3.83-3.89 (m, 1H, N-CH), 3.79 (s, 3H, OCH_3), 3.22-3.28 (m, 2H, indolyl CH_2), 2.07-2.18 (m, 2H, cyclohexyl), 1.79-1.90 (m, 4H, cyclohexyl), 1.59-1.61 (m, 1H, cyclohexyl), 1.17-1.28 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 173.6, 166.6, 160.7 (d, $^1J_{F\text{-}C}$ = 240 Hz), 145.8, 142.8, 136.2, 135.1, 134.8, 133.6, 128.1, 127.2, 125.9, 123.6, 122.5, 120.9, 119.2, 118.4, 118.1, 114.9, 112.3, 111.5, 110.5, 57.2, 53.9, 52.2, 30.8, 26.6, 25.3, 24.3; ESI-MS (*m/z*): 573.3 $[M+H]^+$, 575.3 $[M+2+H]^+$; Anal. calcd. for $C_{32}H_{30}N_4ClFO_3$: C, 67.07; H, 5.28; N, 9.78. Found: C, 67.05; H, 5.27; N, 9.76.

Procedure for the synthesis of benzimidazole monopeptides (7a-l)

To a stirred clear solution of **6a-l** (0.01 mol) in 20 mL of THF:water (2:1) mixture, $LiOH.H_2O$ (0.015 mol, 1.5 equiv.) was added at 0 °C. The stirring was continued at this temperature for 4 h. After completion of the reaction (monitored by TLC, hexane: ethyl acetate (4:6, v/v)), the reaction mass was quenched to crushed ice, acidified with dilute HCl. The resulting solid was washed with water and dried. The solid was subjected to column chromatography using 10-50% of ethyl acetate in hexane to obtain pure benzimidazole monopeptides.

(S)-(1-Cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carbonyl)alanine (7a): Yield 71%; Mp 278-280 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3406 (O-H), 3078 (Ar-H), 2935 and 2854 (C-H), 1716 (C=O of acid), 1654 (C=O of amide), 1612 (C=N), 1577 (C=C), 1029 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 12.44 (s, 1H, CO_2H), 8.65 (d, 1H, amide N-H, J = 7.2 Hz), 8.27 (d, 1H, Ar-H, J = 1.2 Hz), 7.90 (d, 1H, Ar-H, J = 8.4Hz), 7.80 (dd, 1H, Ar-H, J = 1.6 Hz, 7.2 Hz), 7.61 (d, 1H, Ar-H, J = 8.8 Hz), 7.15 (d, 1H, Ar-H, J = 9.2 Hz), 4.42-4.49 (m, 1H, chiral CH), 4.26-4.32 (m, 1H, N-CH), 3.86 (s, 3H, OCH_3), 2.25-2.33 (m, 2H, cyclohexyl), 1.84-1.92 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H, cyclohexyl), 1.42-1.44 (d, 3H, CH_3, J = 7.2 Hz), 1.23-1.39 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 174.4, 166.4, 160.4, 154.7, 142.8, 135.7, 130.8, 127.5, 122.5, 121.6, 118.7, 114.2, 112.4, 56.7, 55.3, 48.2, 30.5, 25.5, 24.4, 16.9; ESI-MS (*m/z*): 422.4 $[M+H]^+$; Anal. calcd. for $C_{24}H_{27}N_3O_4$: C, 68.39; H, 6.46; N, 9.97. Found: C, 68.35; H, 6.47; N, 9.94.

(S)-(1-Cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carbonyl)valine (7b): Yield 50%; Mp 194-196 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3409 (O-H), 3379 and 3409 (NH), 3100 (Ar-H), 2935 and 2850 (C-H), 1712 (C=O of acid), 1650 (C=O of amide), 1612 (C=N), 1581 (C=C), 1029 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.33 (d, 1H, amide NH, J = 8.0 Hz); 8.27 (d, 1H, Ar-H, J = 1.2 Hz), 7.89 (d, 1H, Ar-H, J = 8.8 Hz), 7.79 (dd, 1H, Ar-H, J = 1.6 Hz, 8.4 Hz), 7.61 (d, 2H, Ar-H, J = 8.8 Hz), 7.15 (d, 2H, Ar-H, J = 8.8 Hz), 4.26-4.32 (m, 2H, N-CH and chiral CH), 3.86 (s, 3H, OCH_3), 2.19-2.33 (m, 3H, CH and cyclohexyl), 1.84-1.90 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H, cyclohexyl), 1.23-1.41 (m, 3H, cyclohexyl), 0.97-1.01 (m, 6H, diastereotopic CH_3); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 174.3, 166.9, 160.4, 154.6, 142.7, 135.7, 130.8, 127.8, 122.5, 121.7, 118.8, 114.2, 112.4, 58.6, 56.7, 55.3, 30.5, 29.6, 25.5, 24.4, 19.4, 18.8; ESI-MS (*m/z*): 450.4 $[M+H]^+$; Anal. calcd. for $C_{26}H_{31}N_3O_4$: C, 69.47; H, 6.95; N, 9.35. Found: C, 69.45; H, 6.92; N, 9.37.

(S)-(1-Cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carbonyl)leucine (7c): Yield 66%; Mp: 224-226 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3413 (O-H), 3074 (Ar-H), 2935 and 2862 (C-H), 1712 (C=O of acid), 1650 (C=O of amide), 1612 (C=N), 1577 (C=C), 1029 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.33 (d, 1H, amide NH, J = 6.8 Hz), 8.23 (s, 1H, Ar-H), 7.88 (d, 1H, Ar-H, J = 8.4 Hz), 7.78 (d, 1H, Ar-H, J = 8.4 Hz), 7.60 (d, 1H, Ar-H, J = 8.4 Hz), 7.14 (d, 1H, Ar-H, J = 8.8 Hz), 4.37-4.40 (m, 1H, chiral CH), 4.25-4.31 (m, 1H, C-NH), 3.86 (s, 3H, OCH_3), 2.24-2.33 (m, 2H, cyclohexyl), 1.83-1.90 (m, 4H, cyclohexyl), 1.62-1.76 (m, 4H, isobutyl CH, CH_2 and cyclohexyl), 1.24-1.41 (m, 3H, cyclohexyl), 0.89-0.92 (m, 6H, diastereotopic CH_3); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 174.4, 166.4, 160.4, 154.6, 142.8, 135.6, 130.8, 128.0, 122.5, 121.5, 118.6, 114.2, 112.4, 56.6, 55.3, 30.5, 29.6, 25.5, 24.6, 23.0, 21.6, 18.9; ESI-MS (*m/z*): 464.4 $[M+H]^+$; Anal. calcd. for $C_{27}H_{33}N_3O_4$: C, 69.95; H, 7.18; N, 9.06. Found: C, 69.96; H, 7.15; N, 9.04.

(S)-(1-Cyclohexyl-2-(4-methoxyphenyl)-1H-benzo[d]imidazole-5-carbonyl)tryptophan (7d): Yield 99%, Mp: 172-174 °C; Off white to pale brown solid; FT IR (ATR, υ_{max}, cm^{-1}): 3406 (O-H), 3055 (Ar-H), 2933 and 2856 (C-H), 1720 (C=O of acid), 1643 (C=O of amide), 1612 (C=N), 1577 (C=C), 1178 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.81 (s, 1H, indole NH), 8.62 (d, 1H, amide NH, J = 7.6 Hz), 8.20 (d, 1H, Ar-H, J = 1.6 Hz), 7.88 (d, 1H, Ar-H, J = 8.4 Hz), 7.73 (dd, 1H, Ar-H, J = 8.4 Hz, 1.6 Hz), 7.59-7.63 (m, 3H, Ar-H), 7.32 (d, 1H, Ar-H, J = 8.0 Hz), 7.23 (d, 1H, Ar-H, J = 2.0 Hz), 7.15 (d, 2H, Ar-H, J = 8.8 Hz), 7.04-7.08 (m, 1H, Ar-H), 6.97-7.01 (m, 1H, Ar-H), 4.66-4.72 (m, 1H, chiral CH), 4.25-4.31 (m, 1H, C-NH), 3.86 (s, 3H, OCH_3), 2.23-2.29 (m, 2H, cyclohexyl), 1.83-1.89 (m, 4H, cyclohexyl), 1.62-1.65 (m, 1H, cyclohexyl), 1.25-1.41 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 173.7, 166.6, 160.4, 154.6, 142.6, 136.1, 135.6, 130.9, 127.6, 127.1, 125.76, 123.6, 121.6, 120.9, 118.5, 118.4, 118.1, 114.2, 112.5, 111.4, 110.5, 56.7, 55.3, 53.7, 30.5, 26.6, 25.5, 24.3; ESI-MS (*m/z*): 537.5 $[M+H]^+$; Anal. calcd. for $C_{32}H_{32}N_4O_4$: C, 71.62; H, 6.01; N, 10.44. Found: C, 71.59; H, 6.02; N, 10.41.

(S)-(1-Cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carbonyl)alanine (7e): Yield 75%; Mp 272-274 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3411 (O-H), 3071 (Ar-H), 2932 and 2861 (C-H), 1706 (C=O of acid), 1653 (C=O of amide), 1614 (C=N), 1578 (C=C), 1265 (C-O), 1230 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.63 (d, 1H, amide N-H, J = 7.2 Hz), 8.29 (s, 1H, Ar-H), 7.93 (d, 1H, Ar-H, J = 8.8 Hz), 7.83 (d, 1H, Ar-H, J = 8.8 Hz), 7.71-7.75 (m, 2H, Ar-H), 7.42-7.46 (m, 2H, Ar-H), 4.41-4.48 (m, 1H, chiral CH), 4.20-4.26 (m, 1H, N-CH), 2.24-2.32 (m, 2H, cyclohexyl), 1.83-1.93 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H,

cyclohexyl), 1.42-1.44 (d, 3H, CH_3, J = 7.2 Hz), 1.23-1.38 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 174.5, 165.2 (d, $^1J_{F\text{-}C}$ = 213.8 Hz), 161.7, 153.7, 142.7, 135.7, 131.8 (d, $^3J_{F\text{-}C}$ = 8.5 Hz), 127.7, 126.9, 121.9, 118.9, 115.9 (d, $^2J_{F\text{-}C}$ = 21.5 Hz), 112.6, 56.8, 48.4, 30.5, 25.4, 24.3, 17.1; ESI-MS (*m/z*): 410.4 $[M+H]^+$; Anal. calcd. for $C_{23}H_{24}N_3FO_3$: C, 67.47; H, 5.91; N, 10.26. Found: C, 67.43; H, 5.88; N, 10.27.

(S)-(1-Cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carbonyl)valine (7f): Yield 89%; 262-264 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3407 (O-H), 3074 (Ar-H), 2935 and 2864 (C-H), 1706 (C=O of acid), 1654 (C=O of amide), 1614 (C=N), 1581 (C=C), 1265 (C-O), 1232 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.29 (d, 1H, amide N-H, J = 10.4 Hz), 8.25 (d, 1H, Ar-H, J = 1.6 Hz), 7.92 (d, 1H, Ar-H, J = 11.6 Hz), 7.78-7.82 (m, 3H, Ar-H), 7.41-7.46 (m, 2H, Ar-H), 4.22-4.27 (m, 2H, chiral CH and N-CH), 2.18-2.28 (m, 3H, cyclohexyl), 1.81-1.90 (m, 4H, cyclohexyl), 1.63-1.66 (m, 1H, cyclohexyl), 1.24-1.32 (m, 3H, cyclohexyl), 0.97-1.01 (m, 6H, diastereotopic CH_3); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 173.9, 167.4, 162.9 (d, $^1J_{F\text{-}C}$ = 250 Hz), 154.2, 142.9, 136.03, 132.3 (d, $^3J_{F\text{-}C}$ = 12 Hz), 128.6, 127.2, 122.4, 119.4, 116.4 (d, $^2J_{F\text{-}C}$ = 29 Hz), 113.2, 59.33, 57.3, 30.9, 30.3, 25.9, 24.8, 19.9, 19.3; ESI-MS (*m/z*): 438.4 $[M+H]^+$; Anal. calcd. for $C_{25}H_{28}N_3FO_3$: C, 68.63; H, 6.45; N, 9.60. Found: C, 68.65; H, 6.44; N, 9.62.

(S)-(1-Cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carbonyl)leucine (7g): Yield 90%, 244-248 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3409 (O-H), 3071 (Ar-H), 2934 and 2865 (C-H), 1707 (C=O of acid), 1654 (C=O of amide), 1614 (C=N), 1579 (C=C), 1265 (C-O), 1231 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.59 (d, 1H, amide N-H, J = 7.6 Hz), 8.3 (s, 1H, Ar-H), 7.93 (d, 1H, Ar-H, J = 8.4 Hz), 7.84 (d, 1H, Ar-H, J = 8.4 Hz), 7.72-7.75 (m, 2H, Ar-H), 7.42-7.46 (m, 2H, Ar-H), 4.47-4.52 (m, 1H, chiral CH), 4.20-4.26 (m, 1H, N-CH), 2.24-2.32 (m, 2H, cyclohexyl), 1.59-1.92 (m, 8H, cyclohexyl, isobutyl CH and diastereotopic CH_2), 1.23-1.41 (m, 3H, cyclohexyl), 0.95 (d, 3H, diastereotopic CH_3, J = 6.4 Hz) 0.91 (d, 3H, diastereotopic CH_3, J = 6.4 Hz); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 174.4, 166.7, 162.9 (d, $^1J_{F\text{-}C}$ = 246.7 Hz), 153.7, 142.6, 135.6, 131.8 (d, $^3J_{F\text{-}C}$ = 8.6 Hz), 127.7, 126.8, 121.9, 118.9, 115.8 (d, $^2J_{F\text{-}C}$ = 21.7 Hz), 112.6, 56.8, 50.9, 30.5, 25.4, 24.6, 24.3, 22.9, 21.2; ESI-MS (*m/z*): 450.4 $[M-H]^-$; Anal. calcd. for $C_{26}H_{30}N_3FO_3$: C, 69.16; H, 6.70; N, 9.31. Found: C, 69.14; H, 6.73; N, 9.34.

(S)-(1-Cyclohexyl-2-(4-fluorophenyl)-1H-benzo[d]imidazole-5-carbonyl)tryptophan (7h): Yield 91%; Mp 164-166 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3409 (O-H), 3056

(Ar-H), 2933 and 2858 (C-H), 1720 (C=O of acid), 1641 (C=O of amide), 1614 (C=N), 1527 (C=C), 1296 (C-O), 1230 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.79 (s, 1H, indole-NH), 8.66 (d, 1H, amide-NH, J = 10 Hz), 8.20 (d, 1H, Ar-H, J = 1.2 Hz), 7.90 (d, 1H, Ar-H, J = 11.6 Hz), 7.69-7.76 (m, 3H, Ar-H), 7.61 (d, 1H, Ar-H, J = 10.4 Hz), 7.43 (t, 2H, Ar-H, J = 12 Hz), 7.32 (d, 1H, Ar-H, J = 10.4 Hz), 7.23 (d, 1H, Ar-H, J = 2.4 Hz), 6.99-7.06 (m, 2H, Ar-H); 4.64-4.68 (m, 1H, chiral C-H), 4.16-4.24 (m, 1H, -NC-H), 3.25-3.32 (m, 2H, indole CH_2), 2.23-2.27 (m, 2H, cyclohexyl), 1.81-1.91 (m, 4H, cyclohexyl), 1.62-1.65 (m, 1H, cyclohexyl), 1.26-1.40 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 174.3, 167.2, 162.9 (d, $^1J_{F\text{-}C}$ = 250 Hz), 154.3, 142.9, 136.5, 136.1, 132.3 (d, $^3J_{F\text{-}C}$ = 11 Hz), 128.2, 127.6, 124.1, 123.5, 121.5, 119.3, 118.9, 118.6, 118.2, 116.4 (d, $^2J_{F\text{-}C}$ = 29 Hz), 113.2, 111.9, 110.9, 57.3, 54.3, 30.9, 27.1, 25.9, 24.8; ESI-MS (*m/z*): 524.22 $[M+H]^+$; Anal. calcd. for $C_{31}H_{29}N_4FO_3$: C, 70.98; H, 5.57; N, 10.68. Found: C, 70.95; H, 5.58; N, 10.66.

(S)-(2-(2-Chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carbonyl)alanine (7i): Yield 70%; Mp 248-250 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3372 (O-H), 3078 (Ar-H), 2948 and 2862 (C-H), 1721 (C=O of acid), 1642 (C=O of amide), 1620 (C=N), 1576 (C=C), 1296 (C-O), 1247 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.61 (d, 1H, amide N-H, J = 8.0 Hz), 8.34 (s, 1H, Ar-H), 7.97 (d, 1H, Ar-H, J = 8.4 Hz), 7.87 (d, 1H, Ar-H, J = 8.8 Hz), 7.71-7.77 (m, 1H, Ar-H), 7.62 (m, 1H, Ar-H), 7.49-7.54 (m, 1H, Ar-H), 4.63-4.68 (m, 1H, chiral CH), 4.19-4.25 (m, 1H, N-CH), 2.22-2.31 (m, 2H, cyclohexyl), 1.82-1.92 (m, 4H, cyclohexyl), 1.62-1.65 (m, 1H, cyclohexyl), 1.42-1.44 (d, 3H, CH_3, J = 7.2 Hz), 1.26-1.40 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 175.8, 166.2, 161.1 (d, $^1J_{F\text{-}C}$ = 251 Hz), 145.7, 141.7, 135.8, 134.6, 132.3 (d, $^3J_{F\text{-}C}$ = 10 Hz), 128.8, 125.3, 125.3, 123.3, 118.9 (d, $^2J_{F\text{-}C}$ = 20 Hz), 114.5 (d, $^2J_{F\text{-}C}$ = 12 Hz), 112.2, 58.0, 48.8, 31.1, 30.1, 25.6, 18.5; ESI-MS (*m/z*): 444.4 $[M+H]^+$, 446.4 $[M+2+H]^+$; Anal. calcd. for $C_{23}H_{23}N_3ClFO_3$: C, 62.23; H, 5.22; N, 9.47. Found: C, 62.25; H, 5.21; N, 9.45.

(S)-(2-(2-Chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carbonyl)valine (7j): Yield 81%; Mp 88-90 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3362 (O-H), 3073 (Ar-H), 2947 and 2861 (C-H), 1724 (C=O of acid), 1644 (C=O of amide), 1621 (C=N), 1574 (C=C), 1297 (C-O), 1246 (C-F); ^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.94 (m, 1H, amide N-H), 8.00 (d, 1H, Ar-H, J = 8.0 Hz), 7.74 (d, 1H, Ar-H, J = 8.0 Hz), 7.54-7.56 (m, 2H, Ar-H), 7.42 (d, 1H, Ar-H, J = 8.0 Hz), 7.21 (t, 1H, Ar-H, J = 8.0 Hz), 4.70-4.74 (m, 1H, chiral CH), 3.83-3.86 (m, 1H, N-CH), 2.20-2.40 (m, 1H, C-H of isopropyl), 2.17-2.21 (m, 2H, cyclohexyl), 1.91-2.16 (m, 4H, cyclohexyl), 1.20-1.30 (m, 4H, cyclohexyl), 1.0-1.03 (m, 6H, diastereotopic CH_3); ^{13}C

NMR (100 MHz, $CDCl_3$, δ ppm): 174.4, 166.4, 161.4 (d, $^1J_{F-C}$ = 254 Hz), 146.0, 142.4, 136.1, 135.0, 129.2 (d, $^3J_{F-C}$ = 8 Hz), 125.7, 123.4, 119.3, 115.1, 114.4 (d, $^2J_{F-C}$ = 21 Hz), 112.4, 60.4, 58.1, 31.6, 29.4, 25.8, 22.7, 21.0, 18.9; ESI-MS (*m/z*): 472.4 $[M+H]^+$, 474.4 $[M+2+H]^+$; Anal. calcd. for $C_{25}H_{27}N_3ClFO_3$: C, 63.62; H, 5.77; N, 8.90. Found: C, 63.60; H, 5.74; N, 8.91.

(S)-(2-(2-Chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carbonyl)leucine (7k): Yield 98%; Mp 124-126 °C; Off white solid; IR (ATR, υ_{max}, cm^{-1}): 3355 (O-H), 3080 (Ar-H), 2948 and 2864 (C-H), 1722 (C=O of acid), 1643 (C=O of amide), 1620 (C=N), 1571 (C=C), 1299 (C-O), 1249 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 12.51 (s, 1H, CO_2H), 8.43 (d, 1H, amide N-H, *J* = 10.0 Hz), 8.28 (s, 1H, Ar-H), 7.96 (d, 1H, Ar-H, *J* = 11.6 Hz), 7.85 (d, 1H, Ar-H, *J* = 11.2 Hz), 7.69-7.74 (m, 1H, Ar-H), 7.59-7.61 (m, 1H, Ar-H), 7.47-7.53 (m, 1H, Ar-H), 4.41 (m, 1H, chiral C-H), 2.10-2.19 (m, 2H, cyclohexyl), 1.64-1.89 (m, 8H, cyclohexyl, isobutyl CH and diastereotopic CH_2), 1.58-1.60 (m, 5H, cyclohexyl), 1.21-1.24 (m, 6H, diastereotopic CH_3); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 175.1, 166.8, 161.6 (d, $^1J_{F-C}$ = 230 Hz), 146.3, 143.3, 135.4, 135.2, 134.2, 128.9, 126.4, 122.8, 119.5, 119.0 (d, $^2J_{F-C}$ = 26 Hz), 115.5 (d, $^2J_{F-C}$ = 29 Hz), 112.9, 57.7, 52.3, 31.2, 25.8, 25.1, 24.7, 23.5, 21.9; ESI-MS (*m/z*): 485.4 $[M+H]^+$, 487.4 $[M+2+H]^+$; Anal. calcd. for $C_{26}H_{29}N_3ClFO_3$: C, 64.26; H, 6.01; N, 8.65. Found: C, 64.25; H, 6.03; N, 8.66.

(S)-(2-(2-Chloro-6-fluorophenyl)-1-cyclohexyl-1H-benzo[d]imidazole-5-carbonyl)tryptophan (7l): Yield 97%; Mp 182-184 °C; Off white solid; FT IR (ATR, υ_{max}, cm^{-1}): 3409 (O-H), 3056 (Ar-H), 2937 and 2858 (C-H), 1724 (C=O of acid), 1641 (C=O of amide), 1620 (C=N), 1573 (C=C), 1299 (C-O), 1251 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.80 (s, 1H, indole-NH), 8.67 (d, 1H, amide N-H, *J* = 7.6 Hz), 8.27 (s, 1H, Ar-H), 7.95 (d, 1H, Ar-H, *J* = 8.4 Hz), 7.71-7.80 (m, 2H, Ar-H), 7.60-7.63 (m, 2H, Ar-H), 7.49-7.53 (m, 1H, Ar-H), 7.32 (d, 1H, Ar-H, *J* = 8.0 Hz), 7.23 (s, 1H, Ar-H), 7.04-7.08 (m, 1H, Ar-H), 6.98-7.01 (m, 1H, Ar-H), 4.67-4.72 (m, 1H, chiral C-H), 3.83-3.89 (m, 1H, N-CH), 3.22-3.28 (m, 2H, indolyl CH_2), 2.07-2.18 (m, 2H, cyclohexyl), 1.79-1.90 (m, 4H, cyclohexyl), 1.59-1.61 (m, 1H, cyclohexyl), 1.17-1.28 (m, 3H, cyclohexyl); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 173.6, 166.6, 160.7 (d, $^1J_{F-C}$ = 240 Hz), 154.3, 145.8, 142.8, 136.2, 135.1, 134.8, 133.6, 128.1, 127.6, 127.2, 125.9, 123.6, 122.5, 120.9, 119.2, 118.2 (d, $^2J_{F-C}$ = 25 Hz), 114.9, 112.3, 111.5, 110.5, 57.2, 53.9, 30.8, 26.6, 25.3, 24.3; ESI-MS (*m/z*): 559.3 $[M+H]^+$, 561.3 $[M+2+H]^+$; Anal. calcd. for $C_{31}H_{28}N_4ClFO_3$: C, 66.60; H, 5.05; N, 10.02. Found: C, 66.57; H, 5.08; N, 10.01.

General procedure for the synthesis of 3-aryl-1*H*-pyrazole-4-carboxaldehydes (10a-c)

3-Aryl-1*H*-pyrazole-4-carboxaldehydes **(10a-c)** were prepared according to the general procedure described in the literature[11] by means of Vilsmeier-Haack reaction on 2-(1-arylethylidene)hydrazine carboxamides **(9a-c)** which in-turn were prepared by the reaction of substituted acetophenones **(8a-c)** with semicarbazide hydrochloride in acetic acid-sodium acetate buffer. In a typical experiment, to an ice-cold solution of 2-(1-arylethylidene)hydrazine carboxamides **(9a-c)** (10 mmol) in DMF (20 mL), $POCl_3$ (50 mmol) was added dropwise with stirring at 0 °C. After complete addition, the reaction mass was stirred at room temperature for about 30 min and then at 60-65 °C for 8 h. The reaction mixture was allowed to cool to room temperature and then quenched with crushed ice, followed by neutralization with 25% sodium hydroxide solution. The solid obtained was filtered, washed with water and dried. The crude product was used as such for the next step.

General procedure for the synthesis of 2-(4-oxo-2-thioxothiazolidin-3-yl)amino acids (12a-d)

2-(4-Oxo-2-thioxothiazolidin-3-yl)amino acids **(12a-d)** were prepared according to the reported procedure.[21] Appropriate amino acid **(11a-d,** 10 mmol) was dissolved in a solution of potassium hydroxide (10 mmol) in water (10 mL). Carbon disulfide (10 mmol) was added dropwise to the above clear solution and stirred at room temperature for 6-12 h. An aqueous solution of potassium chloroacetate (10 mmol) was then added and continued stirring for further 30 min. The reaction mixture was acidified with 2N HCl to pH 3.0 and stirred at 90 °C for 1-3 h. The reaction mixture was poured onto crushed ice and solid obtained was filtered, washed with water, dried and used as such for the next step. Whenever a gummy solid was obtained, it was extracted to ethyl acetate, concentrated *in vacuo* and triturated with hexane to get orange solid.

General procedure for the synthesis of pyrazole conjugated rhodanine carboxylic acids (13a-l)

β-Alanine (0.02 mol, 2.0 equiv.) was added to a clear solution of pyrazole aldehyde (**10a-c**, 0.01 mol, 1.0 equiv.) and rhodanine amino acid (**12a-d**, 0.01 mol, 1.0 equiv.) in acetic acid (10 mL). Then the reaction mixture was heated to reflux for 16-18 h. After completion of the reaction (monitored by TLC hexane: ethyl acetate (2:1, v/v)), the reaction mass was allowed to cool to room temperature and poured onto crushed ice to get yellow to orange colored solid. The solid separated was filtered, washed with water, dried and subjected to column purification using 10-60 % ethyl acetate in hexane to obtain pure product.

(S)-2-(5-((3-(4-Methoxyphenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)acetic acid (13a): Yield 60%; Mp 164-166 °C; Red solid; FT IR (ATR, υ_{max}, cm^{-1}): 3400 (O-H), 3001 (Ar-H), 2933 and 2858 (C-H), 1705 (C=O), 1610 (C=N), 1529 (C=C), 1228 (C=S), 1106 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.05 (s, 1H, pyrazole-5H), 7.53 (s, 1H, =C-H), 7.49 (d, 2H, Ar-H, J = 8.4 Hz), 7.12 (d, 2H, Ar-H, J = 8.8 Hz), 3.57 (s, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.6, 166.0, 160.1, 130.1, 125.4, 117.4, 114.6, 112.8, 55.3, 43.1; ESI-MS (*m/z*): 374.2 $[M-H]^-$; Anal. calcd. for $C_{16}H_{13}N_3O_4S_2$: C, 51.19; H, 3.49; N, 11.19. Found: C, 51.21; H, 3.46; N, 11.14.

(S)-2-(5-((3-(4-Methoxyphenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)propanoic acid (13b): Yield 65%; Mp 150-152 °C; Red solid; FT IR (ATR, υ_{max}, cm^{-1}): 3496 (O-H), 3172 (Ar-H), 2903 and 2856 (C-H), 1709 (C=O), 1608 (C=N), 1516 (C=C), 1247 (C=S), 1111 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.05 (s, 1H, pyrazole-5H), 7.53 (s, 1H, =C-H), 7.49 (d, 2H, Ar-H, J = 8.4 Hz), 7.12 (d, 2H, Ar-H, J = 8.8 Hz), 5.55-5.61 (q, 1H, J = 7.2 Hz), 3.82 (s, 3H, OCH_3), 1.51 (d, 3H, CH_3, J = 6.8 Hz); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.6, 166.0, 160.1, 130.1, 125.4, 117.4, 114.6, 112.8, 55.3, 52.8, 13.4; ESI-MS (*m/z*): 388.2 $[M-H]^-$; Anal. calcd. for $C_{17}H_{15}N_3O_4S_2$: C, 52.43; H, 3.88; N, 10.79. Found: C, 52.41; H, 3.85; N, 10.81.

(S)-2-(5-((3-(4-Methoxyphenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)-3-phenylpropanoic acid (13c): Yield 48%; Mp 122-124 °C; Red solid; FT IR (ATR, υ_{max}, cm^{-1}): 3279 (O-H), 3001 (Ar-H), 2933 and 2858 (C-H), 1702 (C=O), 1610 (C=N), 1529 (C=C), 1250 (C=S), 1172 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 7.86 (s, 1H, pyrazole-5H), 7.32-7.35 (m, 3H, Ar-H), 6.92-7.12 (m, 7H, Ar-H, =C-H, Ph), 5.67 (overlapped multiplet, 1H, chiral CH), 3.68 (s, 3H, OCH_3), 3.13-3.16 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.6, 166.0, 160.1, 136.5, 130.1, 128.9, 128.2, 126.7, 125.4, 117.4, 114.6, 112.8, 58.1, 55.3, 33.1; ESI-MS (*m/z*): 464.2 $[M-H]^-$; Anal. calcd. for $C_{23}H_{19}N_3O_4S_2$: C, 59.34; H, 4.11; N, 9.03. Found: C, 59.31; H, 4.10; N, 9.05.

(S)-3-(1H-Indol-3-yl)-2-(5-((3-(4-methoxyphenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)propanoic acid (13d): Yield 85%; Mp 160-162 °C; Red solid; FT IR (ATR, υ_{max}, cm^{-1}): 3274 (O-H), 3001 (Ar-H), 2929 and 2853 (C-H), 1705 (C=O), 1608 (C=N), 1513 (C=C), 1253 (C=S), 1177 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.77 (s, 1H, indole NH), 7.98 (s, 1H, pyrazole-5H), 7.45-7.49 (m, 4H, Ar-H, =C-H), 7.27-7.29 (m, 1H, Ar-H), 7.12-7.15 (d, 2H, Ar-H, J = 8.4 Hz), 6.99-7.05 (m, 2H, Ar-H), 6.89-6.93 (m, 1H, Ar-H),

5.86 (overlapped multiplet, 1H, chiral CH), 3.83 (s, 3H, OCH_3), 3.58 (dd, 2H, CH_2, J = 14.8 Hz, 5.2 Hz); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.1, 166.3, 160.1, 135.9, 130.1, 127.1, 125.2, 123.7, 120.9, 118.4, 117.8, 114.6, 112.7, 111.3, 108.9, 58.0, 55.3, 23.0; ESI-MS (*m/z*): 503.2 $[M-H]^-$; Anal. calcd. for $C_{25}H_{20}N_4O_4S_2$: C, 59.51; H, 4.00; N, 11.10. Found: C, 59.49; H, 4.10; N, 11.06.

(S)-2-(5-((3-(3,5-Difluorophenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)acetic acid (13e): Yield 83%; Mp 108-110 °C; Yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3325 (O-H), 3001 (Ar-H), 2929 and 2848 (C-H), 1703 (C=O), 1605 (C=N), 1512 (C=C), 1253 (C=S), 1122 (C-F), 1060 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.16 (s, 1H, pyrazole-5H), 7.51 (s, 1H, =C-H), 7.29-7.38 (m, 3H, Ar-H), 3.57 (s, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.5, 167.2, 166.0, 162.5 (d, $^1J_{F-C}$ = 245.5 Hz), 124.7, 119.4, 113.3, 111.8 (d, $^2J_{F-C}$ = 26 Hz), 104.4, 43.1; ESI-MS (*m/z*): 374.2 $[M-H]^-$; Anal. calcd. for $C_{15}H_9N_3F_2O_3S_2$: C, 47.24; H, 2.38; N, 11.02. Found: C, 47.27; H, 2.35; N, 11.04.

(S)-2-(5-((3-(3,5-Difluorophenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)propanoic acid (13f): Yield 57%; Mp 110-112 °C; Yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3246 (O-H), 3087 (Ar-H), 2922 and 2858 (C-H), 1712 (C=O), 1604 (C=N), 1534 (C=C), 1243 (C=S), 1120 (C-F), 1056 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.21 (s, 1H, pyrazole-5H), 7.55 (s, 1H, =C-H), 7.29-7.38 (m, 3H, Ar-H), 5.55-5.61 (q, 1H, chiral CH, J = 7.2 Hz), 1.52 (d, 3H, CH_3, J = 7.2 Hz); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.5, 165.9, 162.5 (d, $^1J_{F-C}$ = 246 Hz), 124.4, 118.9, 113.3, 111.8 (d, $^2J_{F-C}$ = 19 Hz), 104.3, 52.8, 13.3; ESI-MS (*m/z*): 394.2 $[M-H]^-$; Anal. calcd. for $C_{16}H_{11}N_3F_2O_3S_2$: C, 48.60; H, 2.80; N, 10.63. Found: C, 48.57; H, 2.81; N, 10.66.

(S)-2-(5-((3-(3,5-Difluorophenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)-3-phenylpropanoic acid (13g): Yield 61%; Mp 114-116 °C; Yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3253 (O-H), 3025 (Ar-H), 2924 and 2858 (C-H), 1716 (C=O), 1604 (C=N), 1535 (C=C), 1230 (C=S), 1122 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.29 (s, 1H, pyrazole-5H), 7.54 (s, 1H, =C-H), 7.32-7.41 (m, 3H, Ar-H), 7.14-7.22 (m, 5H, Ar-H), 5.85 (overlapped multiplet, 1H, chiral CH), 3.29-3.33 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.2, 168.7, 166.2, 162.5 (d, $^1J_{F-C}$ = 246 Hz), 136.5, 128.9, 128.2, 126.6, 124.6, 118.3, 113.2, 111.8 (d, $^2J_{F-C}$ = 26 Hz), 104.3, 58.2, 33.1; ESI-MS (*m/z*): 470.2 $[M-H]^-$; Anal. calcd. for $C_{22}H_{15}N_3F_2O_3S_2$: C, 56.04; H, 3.21; N, 8.91. Found: C, 56.01; H, 3.24; N, 8.89.

(S)-2-(5-((3-(3,5-Difluorophenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)-3-(1H-indol-3-yl)propanoic acid (13h): Yield 83%; Mp 120-122 °C; Yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3411 (O-H), 3081 (Ar-H), 2924 and 2858 (C-H), 1709 (C=O), 1604 (C=N), 1534 (C=C), 1223 (C=S), 1121 (C-F); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.77 (s, 1H, indole-NH), 8.16 (s, 1H, pyrazole-5H), 7.51 (s, 1H, =C-H),7.45-7.47 (m, 1H, Ar-H), 7.36-7.45 (m, 1H, Ar-H), 7.26-7.30 (m, 3H, Ar-H), 6.99-7.05 (m, 2H, Ar-H), 6.89-6.92 (m, 1H, Ar-H), 5.86 (s, 1H, chiral C-H), 3.58 (dd, 2H, CH_2, J = 14.8 Hz and 4.8 Hz); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.0, 166.2, 162.5 (d, $^1J_{F\text{-}C}$ = 245.5 Hz), 135.9, 127.0, 124.2, 123.7, 120.9, 118.6, 118.4, 117.8, 113.2, 111.7 (d, $^2J_{F\text{-}C}$ = 19 Hz), 108.9, 104.4, 58.1, 23.0; ESI-MS (*m/z*): 509.2 $[M-H]^-$; Anal. calcd. for $C_{24}H_{16}N_4F_2O_3S_2$: C, 56.46; H, 3.16; N, 10.97. Found: C, 56.42; H, 3.18; N, 10.94.

(S)-2-(5-((3-(4-Nitrophenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)acetic acid (13i): Yield 72%; Mp 136-138 °C; Yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3332 (O-H), 3116 (Ar-H), 2967 and 2856 (C-H), 1703 (C=O), 1601 (C=N), 1548 (C=C), 1332 (N=O), 1241 (C=S), 1127 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.40 (d, 2H, Ar-H, J = 8.0 Hz), 8.30 (s, 1H, pyrazole-5H), 7.87 (d, 2H, Ar-H, J = 8.4 Hz), 7.56 (s, 1H, =C-H), 3.56 (s, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.6, 165.9, 147.4, 129.8, 124.3, 124.1, 119.3, 113.6, 43.1; ESI-MS (*m/z*): 479.2 $[M-H]^-$; Anal. calcd. for $C_{15}H_{10}N_4O_5S_2$: C, 46.15; H, 2.58; N, 14.35. Found: C, 46.12; H, 2.55; N, 14.29.

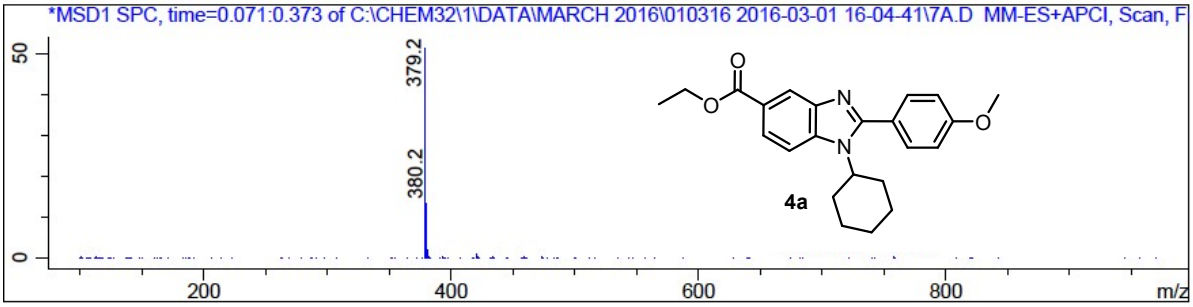
(S)-2-(5-((3-(4-Nitrophenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)propanoic acid (13j): Yield 68%; Mp 240-242 °C; Yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3223 (O-H), 3116 (Ar-H), 2967 and 2862 (C-H), 1702 (C=O), 1601 (C=N), 1548 (C=C), 1336 (N=O), 1247 (C=S), 1127 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.39 (d, 2H, Ar-H, J = 8.4 Hz), 8.30 (s, 1H, pyrazole-5H), 7.87 (d, 2H, Ar-H, J = 8.8 Hz), 7.58 (s, 1H, =C-H), 5.56-5.62 (q, 1H, chiral CH, J = 7.2 Hz), 1.52 (d, 3H, CH_3, J = 6.8 Hz); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.5, 165.9, 147.4, 129.7, 124.3, 124.1, 119.3, 113.6, 52.8, 13.3; ESI-MS (*m/z*): 403.2 $[M-H]^-$; Anal. calcd. for $C_{16}H_{12}N_4O_5S_2$: C, 47.52; H, 2.99; N, 13.85. Found: C, 47.55; H, 2.96; N, 13.82.

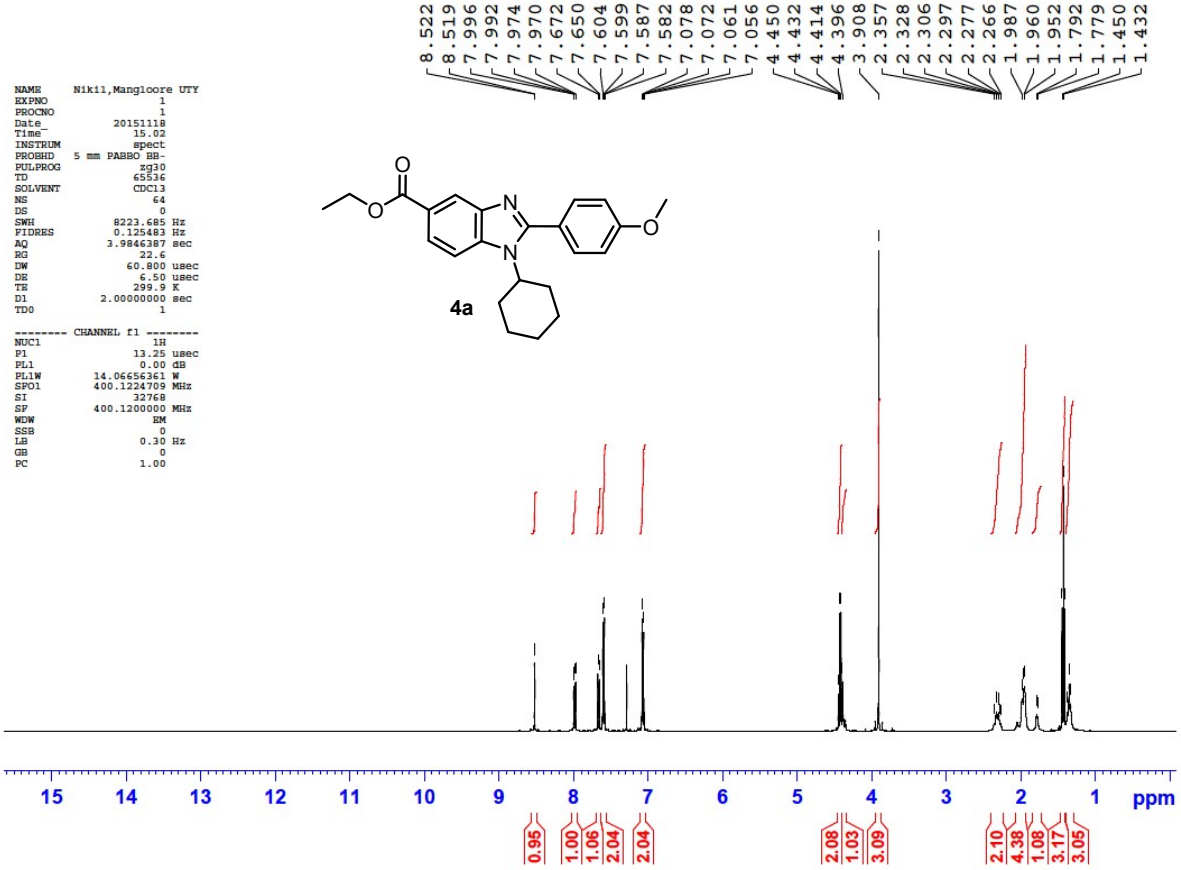
(S)-2-(5-((3-(4-Nitrophenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)-3-phenylpropanoic acid (13k): Yield 67%; Mp 90-92 °C; Yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3256 (O-H), 3025 (Ar-H), 2921 and 2851 (C-H), 1713 (C=O), 1601 (C=N), 1337 (N=O), 1230 (C=S), 1107 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 8.40 (d, 2H, Ar-H, J = 8.0

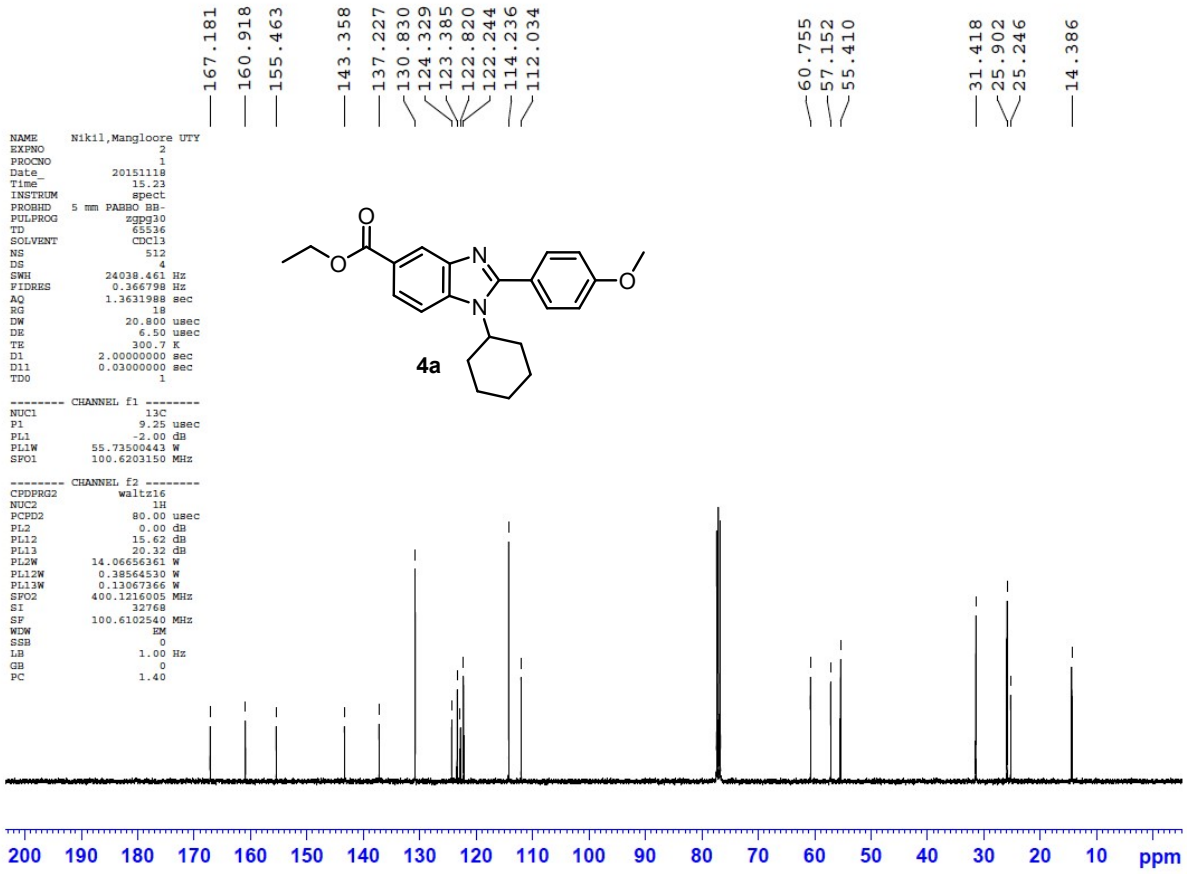
Hz), 8.30 (s, 1H, pyrazole-5H), 7.87 (d, 2H, Ar-H, *J* = 8.4 Hz), 7.56 (s, 1H, =C-H), 7.13-7.2 (m, 5H, Ar-H), 5.86 (overlapped multiplet, 1H, chiral CH), 2.09 (s, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 168.7, 166.1, 147.4, 136.5, 129.7, 128.9, 128.2, 126.7, 124.4, 124.1, 118.6, 113.5, 58.1, 33.1; ESI-MS (*m/z*): 479.2 $[M-H]^-$; Anal. calcd. for $C_{22}H_{16}N_4O_5S_2$: C, 54.99; H, 3.36; N, 11.66. Found: C, 54.96; H, 3.38; N, 11.63.

(S)-3-(1H-indol-3-yl)-2-(5-((3-(4-nitrophenyl)-1H-pyrazol-4-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)propanoic acid (13l): Yield 83%; Mp 152-154 °C; Yellow solid; FT IR (ATR, υ_{max}, cm^{-1}): 3271 (O-H), 3023 (Ar-H), 2928 and 2852 (C-H), 1713 (C=O), 1603 (C=N), 1334 (N=O), 1231 (C=S), 1108 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.84 (s, 1H, indole-NH), 8.47 (d, 2H, Ar-H, *J* = 8.3 Hz), 8.38 (s, 1H, pyrazole-5H), 7.92 (d, 2H, Ar-H, *J* = 8.5 Hz), 7.59 (s, 1H, =C-H), 7.53 (d, 1H, Ar-H, *J* = 7.6 Hz), 7.33 (d, 1H, Ar-H, *J* = 8.0 Hz), 7.11 (s, 1H, Ar-H), 7.05-7.09 (m, 1H, Ar-H), 6.95-6.99 (m, 1H, Ar-H), 5.91 (overlapped multiplet, 1H, chiral CH), 3.64 (dd, 2H, CH_2, *J* = 15.2 Hz, 5.2 Hz); ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 192.1, 169.4, 166.1, 147.6, 135.9, 129.7, 127.1, 124.3, 124.1, 123.7, 120.9, 119.3, 118.4, 117.8, 113.6, 111.3, 108.9, 55.3, 23.0; ESI-MS (*m/z*): 518.2 $[M-H]^-$; Anal. calcd. for $C_{24}H_{17}N_5O_5S_2$: C, 55.48; H, 3.30; N, 13.48. Found: C, 55.44; H, 3.28; N, 13.45.

Figure S8. Mass, ^{1}H and ^{13}C NMR spectral data of the compounds.



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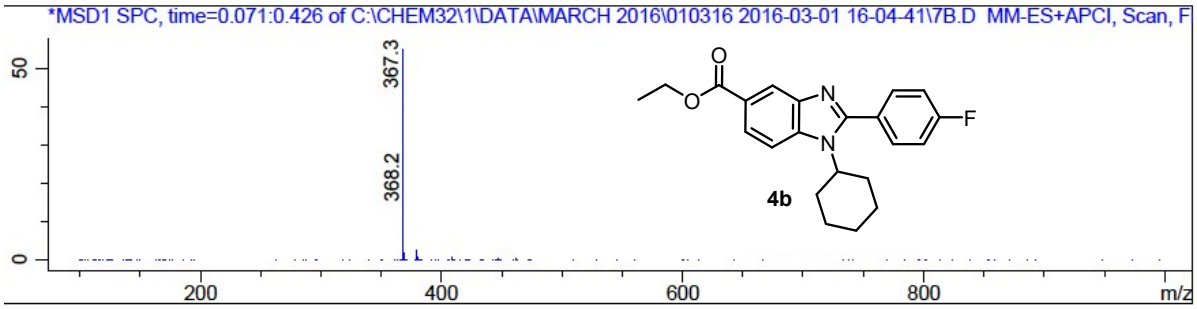
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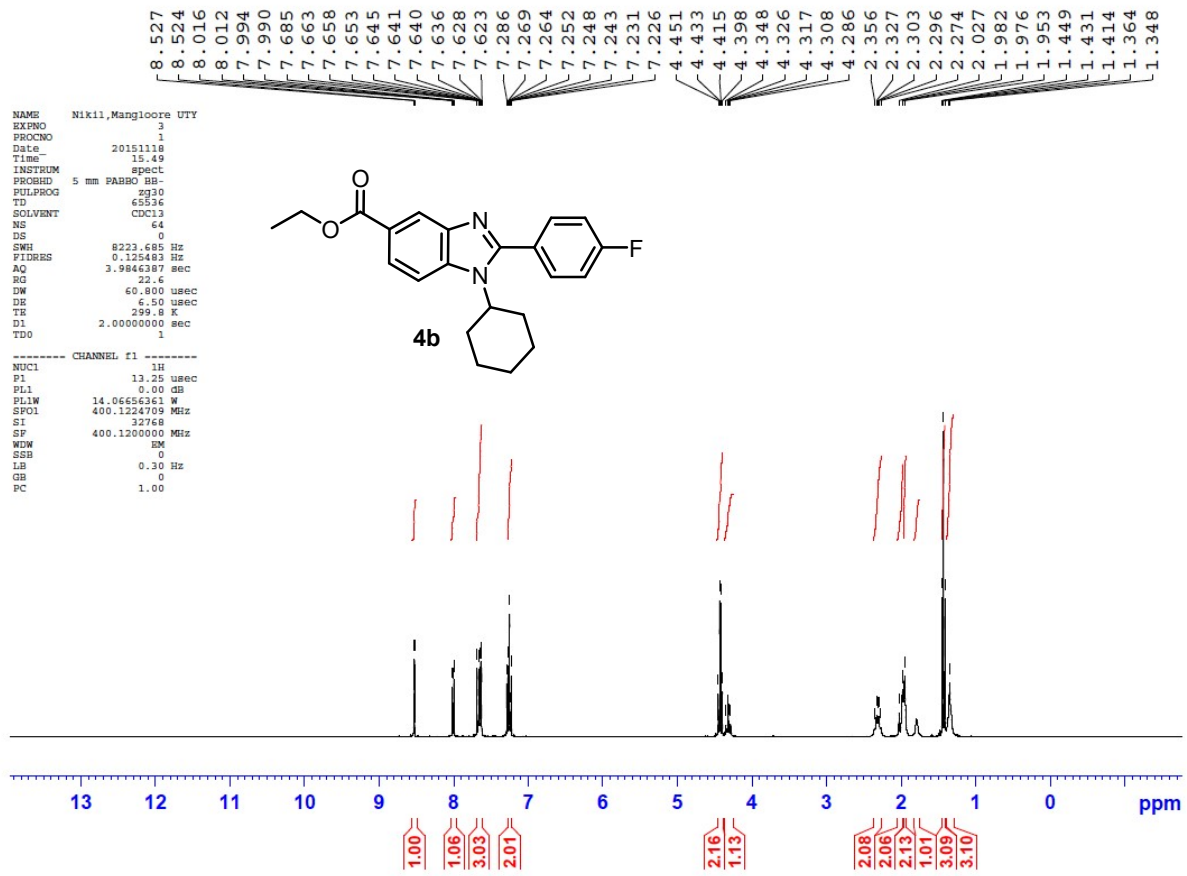
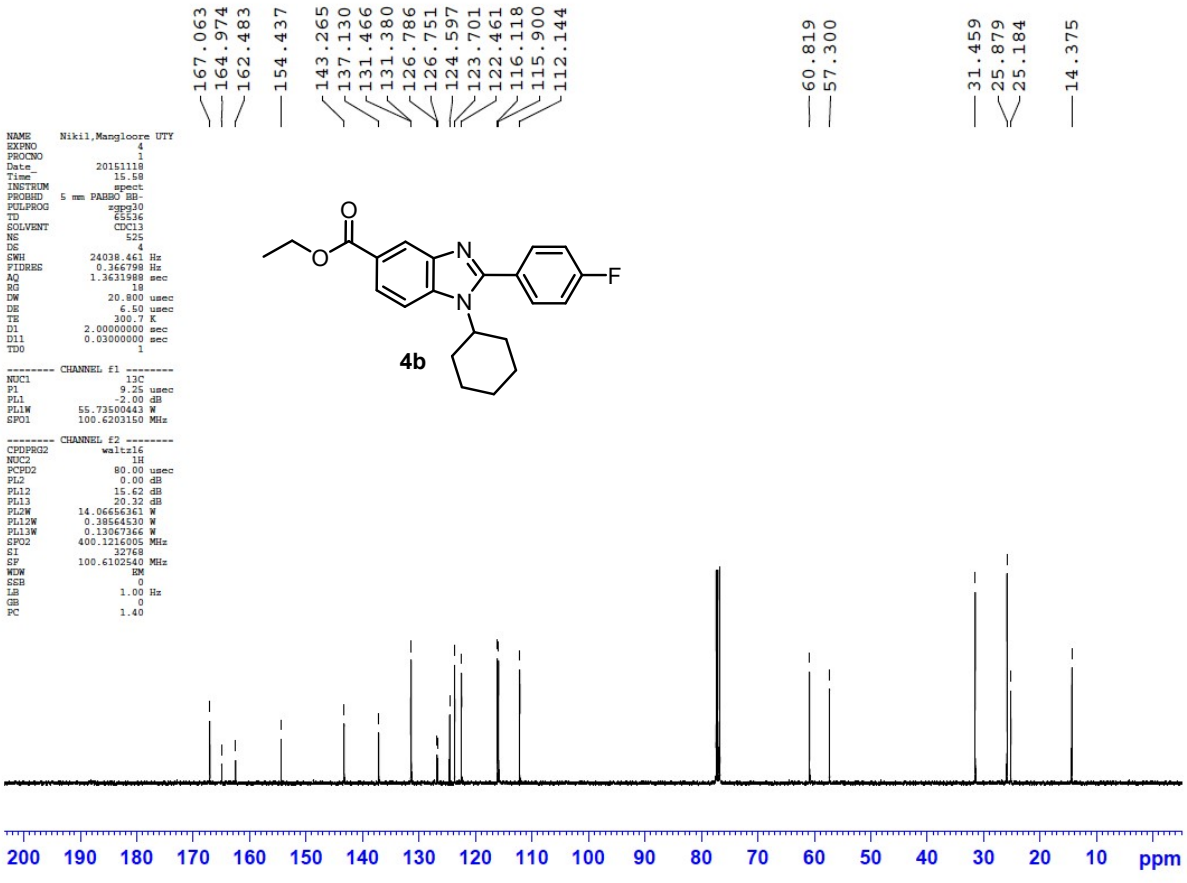
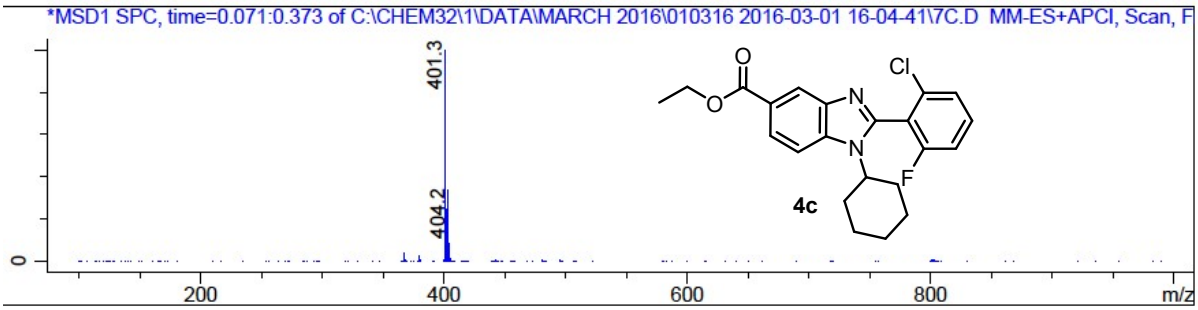
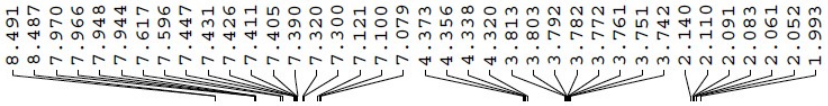
F
4b

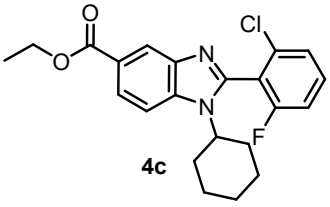

8.527
8.524
8.016
8.012
7.994
7.990
7.685
7.663
7.658
7.653
7.645
7.641
7.640
7.636
7.628
7.623
7.286
7.269
7.264
7.252
7.248
7.243
7.231
7.226
4.451
4.433
4.415
4.398
4.348
4.326
4.317
4.308
4.286
2.356
2.327
2.303
2.296
2.274
2.027
1.982
1.976
1.953
1.449
1.431
1.414
1.364
1.348
NAME Nikil,Mangloore UTY
EXPNO 3
PROCNO 1
Date_ 20151118
Time_ 15.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 22.6
DW 60.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 13.25 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 400.1224709 MHz
SI 32768
SF 400.1200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
4b
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.06 3.03 2.01 2.16 1.13 2.08 2.06 2.13 1.01 3.09 3.10

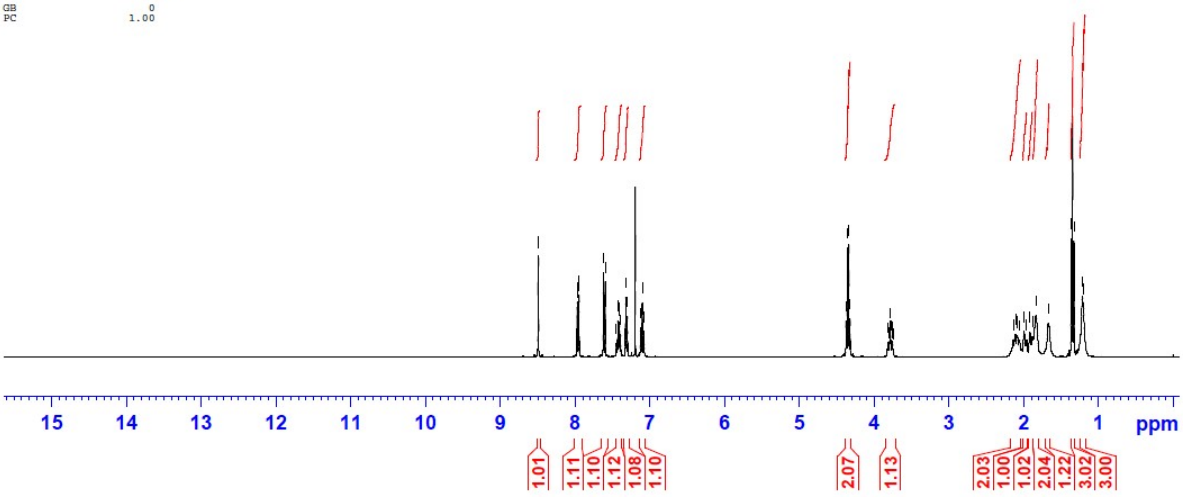

167.063
164.974
162.483
154.437
143.265
137.130
131.466
131.380
126.786
126.751
124.597
123.701
122.461
116.118
115.900
112.144
60.819
57.300
31.459
25.879
25.184
14.375
NAME Nikil,Mangloore UTY
EXPNO 4
PROCNO 1
Date_ 20151118
Time_ 15.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 525
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 18
DW 20.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.25 usec
PL1 -2.00 dB
PL1W 55.73500443 W
SFO1 100.6203150 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.62 dB
PL13 20.32 dB
PL2W 14.06656361 W
PL12W 0.38564530 W
PL13W 0.13067366 W
SFO2 400.1216005 MHz
SI 32768
SF 100.6102540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
4b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

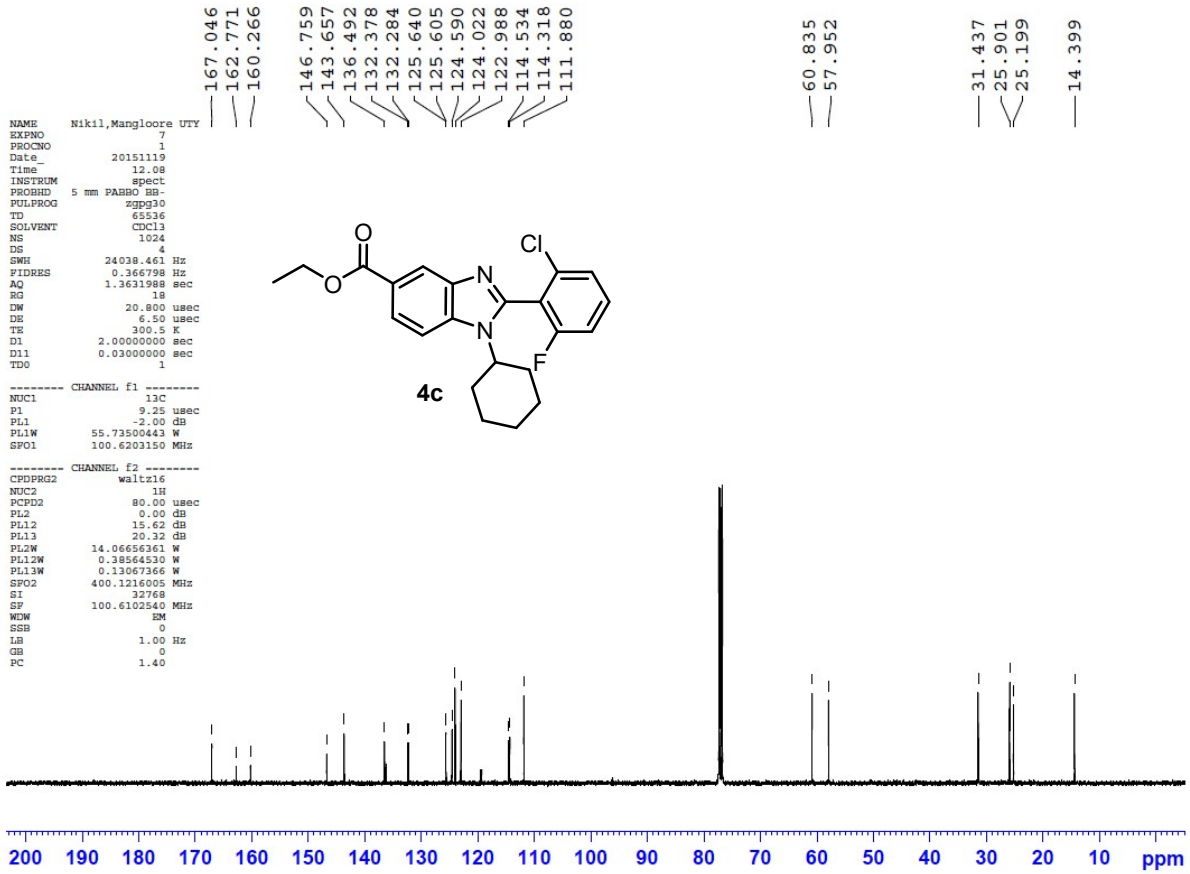


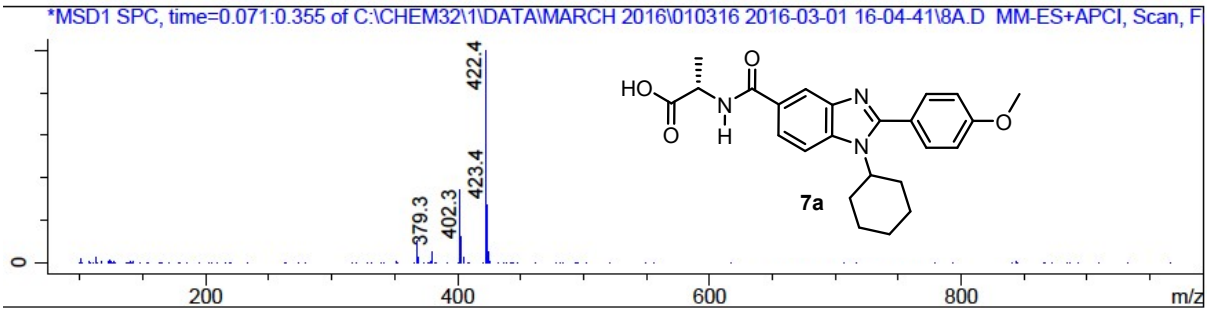

```
NAME        Nikil,Mangloore UTY
EXPNO                     6
PROCNO                    1
Date_              20151119
Time_                 11.08
INSTRUM               spect
PROBHD     5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       64
DS                        0
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                     22.6
DW                   60.800 usec
DE                    6.50 usec
TE                   299.4 K
D1                2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   13.25 usec
PL1                   0.00 dB
PL1W             14.06656361 W
SFO1            400.1224709 MHz
SI                    32768
SF              400.1200375 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

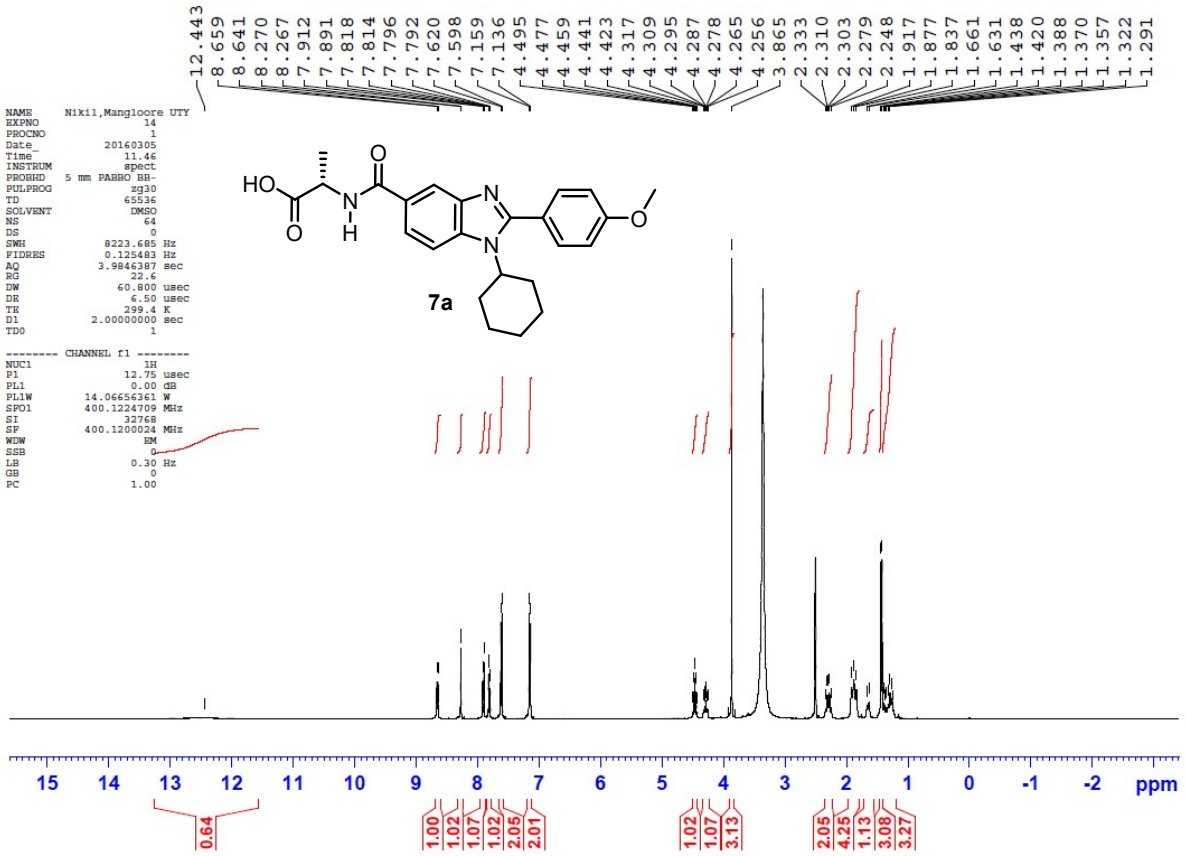


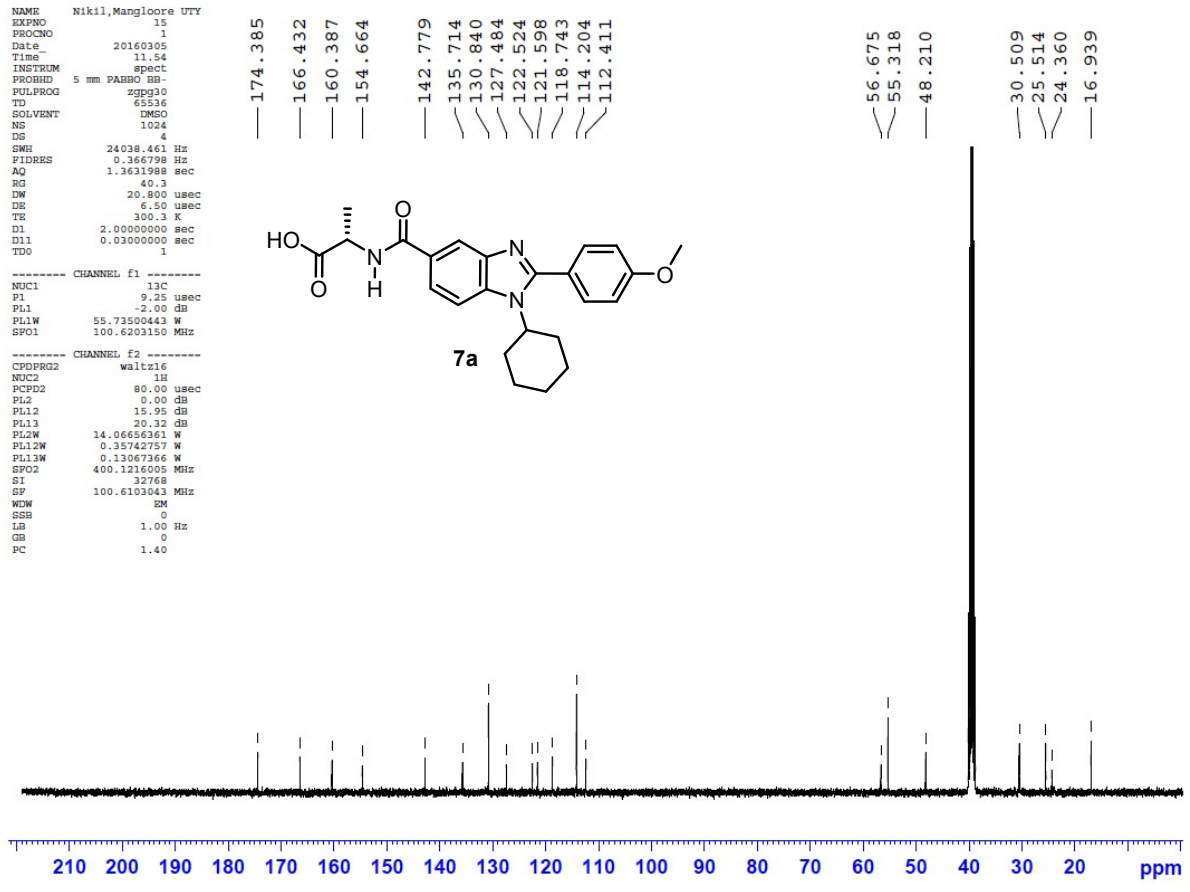


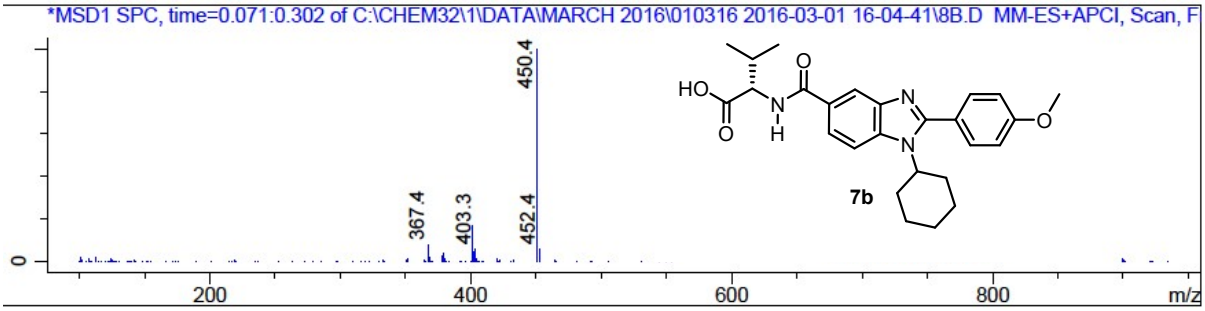


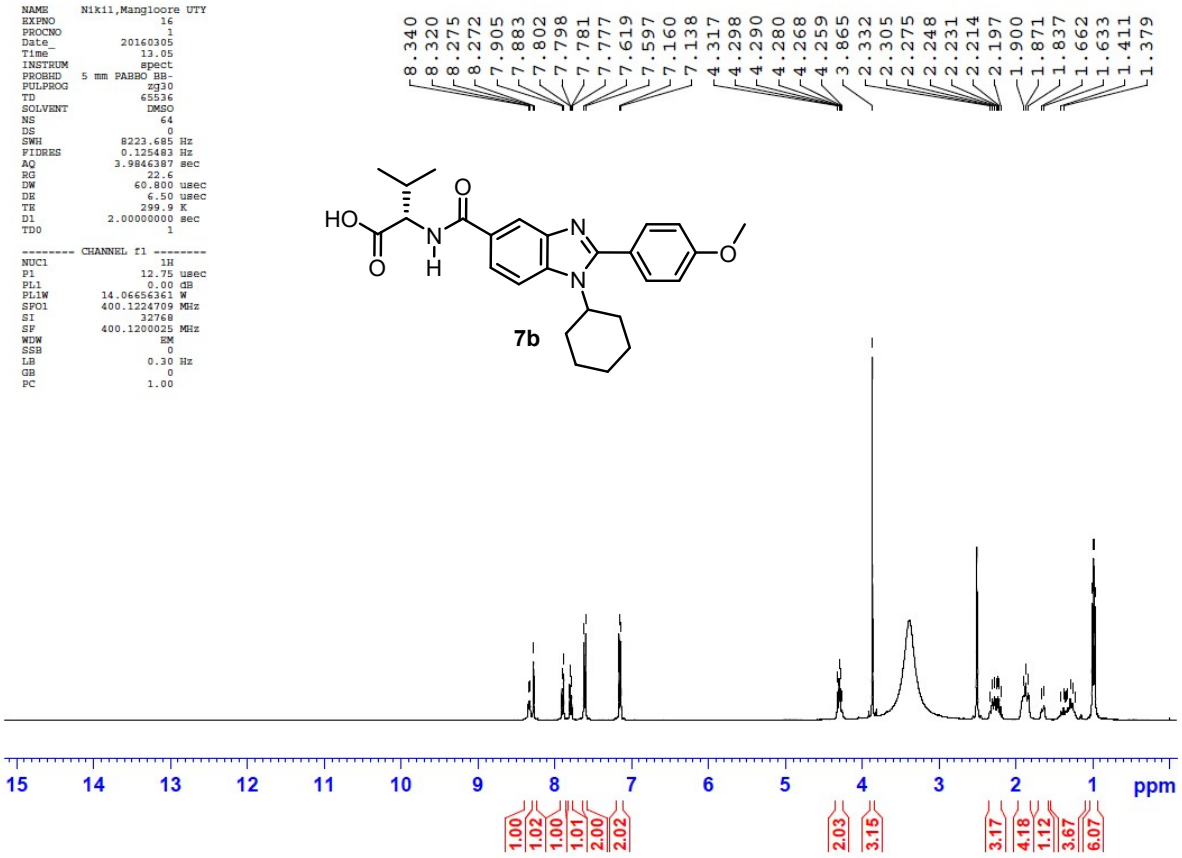

167.046
162.771
160.266
146.759
143.657
136.492
132.378
132.284
125.640
125.605
124.590
124.022
122.988
114.534
114.318
111.880
60.835
57.952
31.437
25.901
25.199
14.399
NAME Nikil,Mangloore UTY
EXPNO 7
PROCNO 1
Date_ 20151119
Time 12.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 18
DW 20.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.25 usec
PL1 -2.00 dB
PL1W 55.73500443 W
SFO1 100.6203150 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.62 dB
PL13 20.32 dB
PL2W 14.06656361 W
PL12W 0.38564530 W
PL13W 0.13067366 W
SFO2 400.1216005 MHz
SI 32768
SF 100.6102540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
N
N
Cl
F
4c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

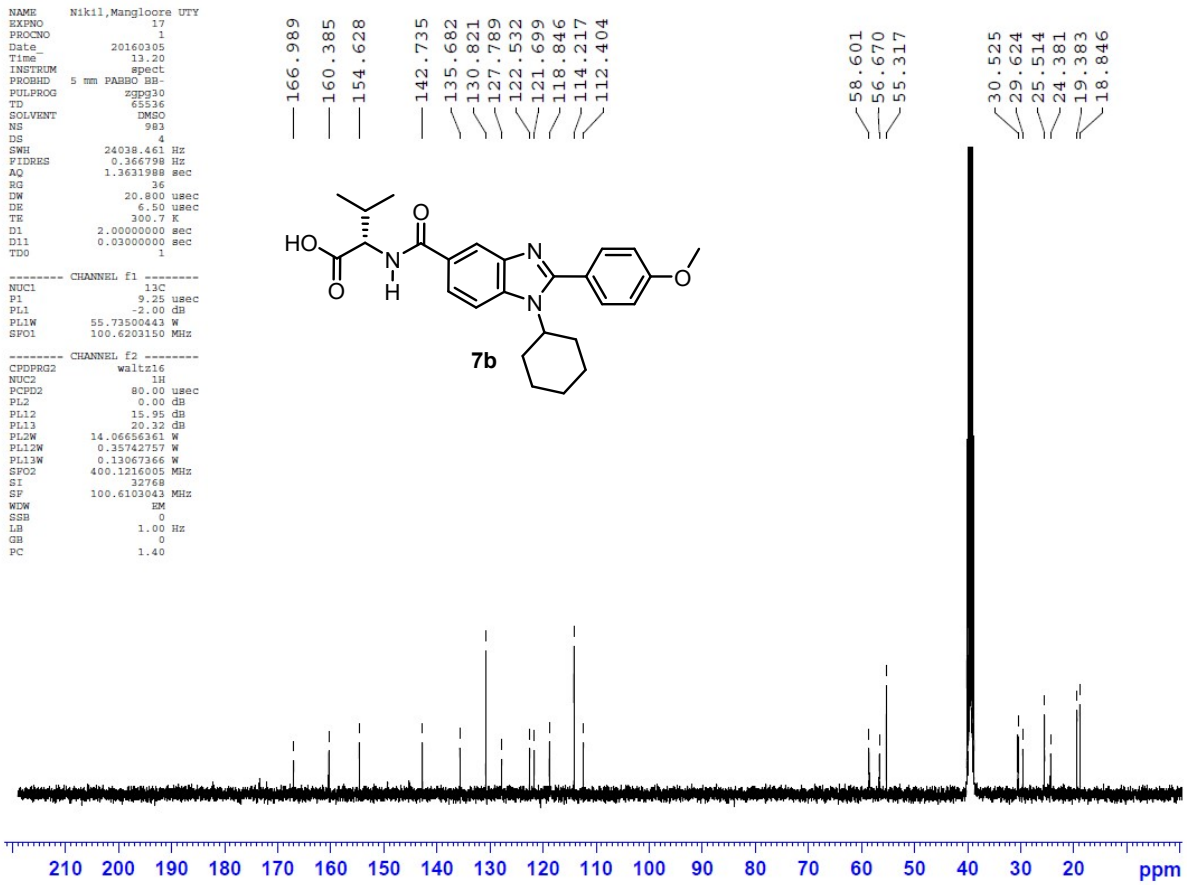

*MSD1 SPC, time=0.071:0.355 of C:\CHEM32\1\DATA\MARCH 2016\010316 2016-03-01 16-04-41\8A.D MM-ES+APCI, Scan, F
422.4
423.4
379.3
402.3
0
200
400
600
800
m/z
HO
O
N
H
O
N
N
O
7a

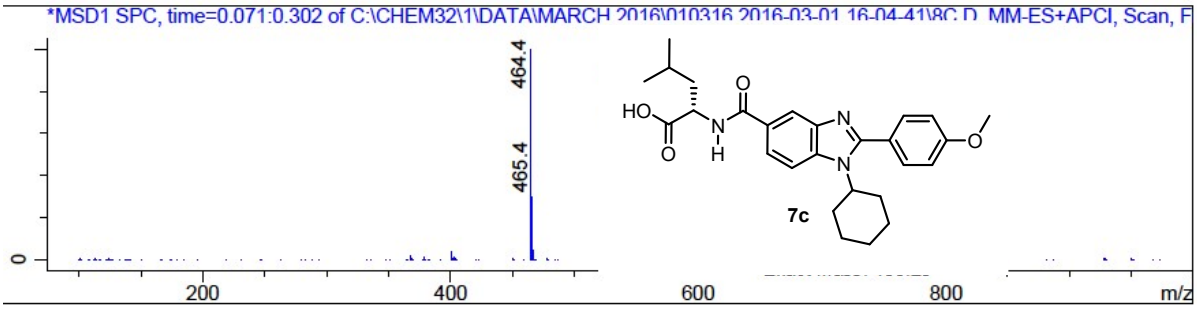

12.443
8.659
8.641
8.270
8.267
7.912
7.891
7.818
7.814
7.796
7.792
7.620
7.598
7.159
7.136
4.495
4.477
4.459
4.441
4.423
4.317
4.309
4.295
4.287
4.278
4.265
4.256
3.865
2.333
2.310
2.303
2.279
2.248
1.917
1.877
1.837
1.661
1.631
1.438
1.420
1.388
1.370
1.357
1.322
1.291
NAME Niki1,Mangloore UTY
EXPNO 14
PROCNO 1
Date_ 20160305
Time_ 11.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 22.6
DW 60.800 usec
DR 6.50 usec
TE 299.4 K
D1 2.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 12.75 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 400.1224709 MHz
SI 32768
SF 400.1200024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HO
O
N
H
O
N
N
O
7a
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.64
1.00
1.02
1.07
1.02
2.05
2.01
1.02
1.07
3.13
2.05
4.25
1.13
3.08
3.27

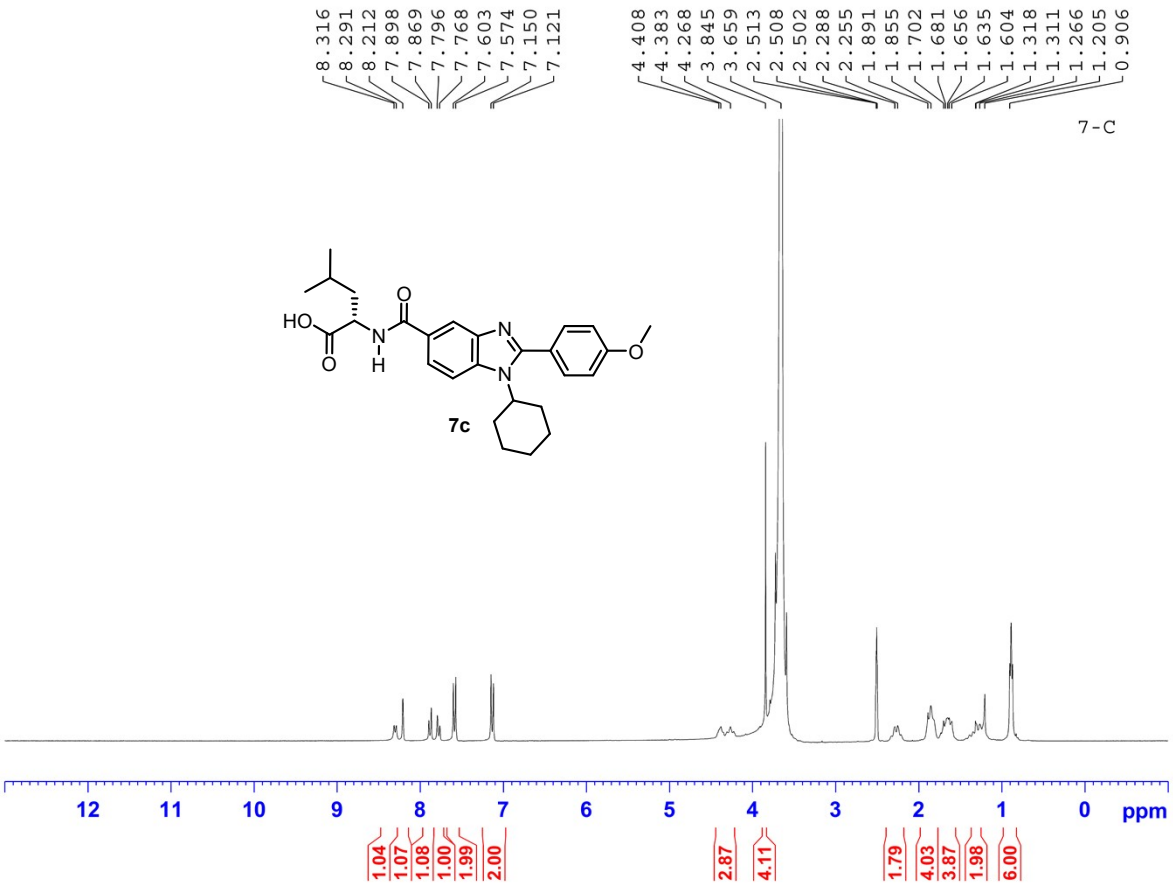

NAME Niki1,Mangloore UTY
EXPNO 15
PROCNO 1
Date_ 20160305
Time_ 11.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 40.3
DW 20.800 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.25 usec
PL1 -2.00 dB
PL1W 55.73500443 W
SFO1 100.6203150 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.95 dB
PL13 20.32 dB
PL2W 14.06656361 W
PL12W 0.35742757 W
PL13W 0.13067366 W
SFO2 400.1216005 MHz
SI 32768
SF 100.6103043 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
174.385
166.432
160.387
154.664
142.779
135.714
130.840
127.484
122.524
121.598
118.743
114.204
112.411
56.675
55.318
48.210
30.509
25.514
24.360
16.939
HO
O
N
H
O
N
N
O
7a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

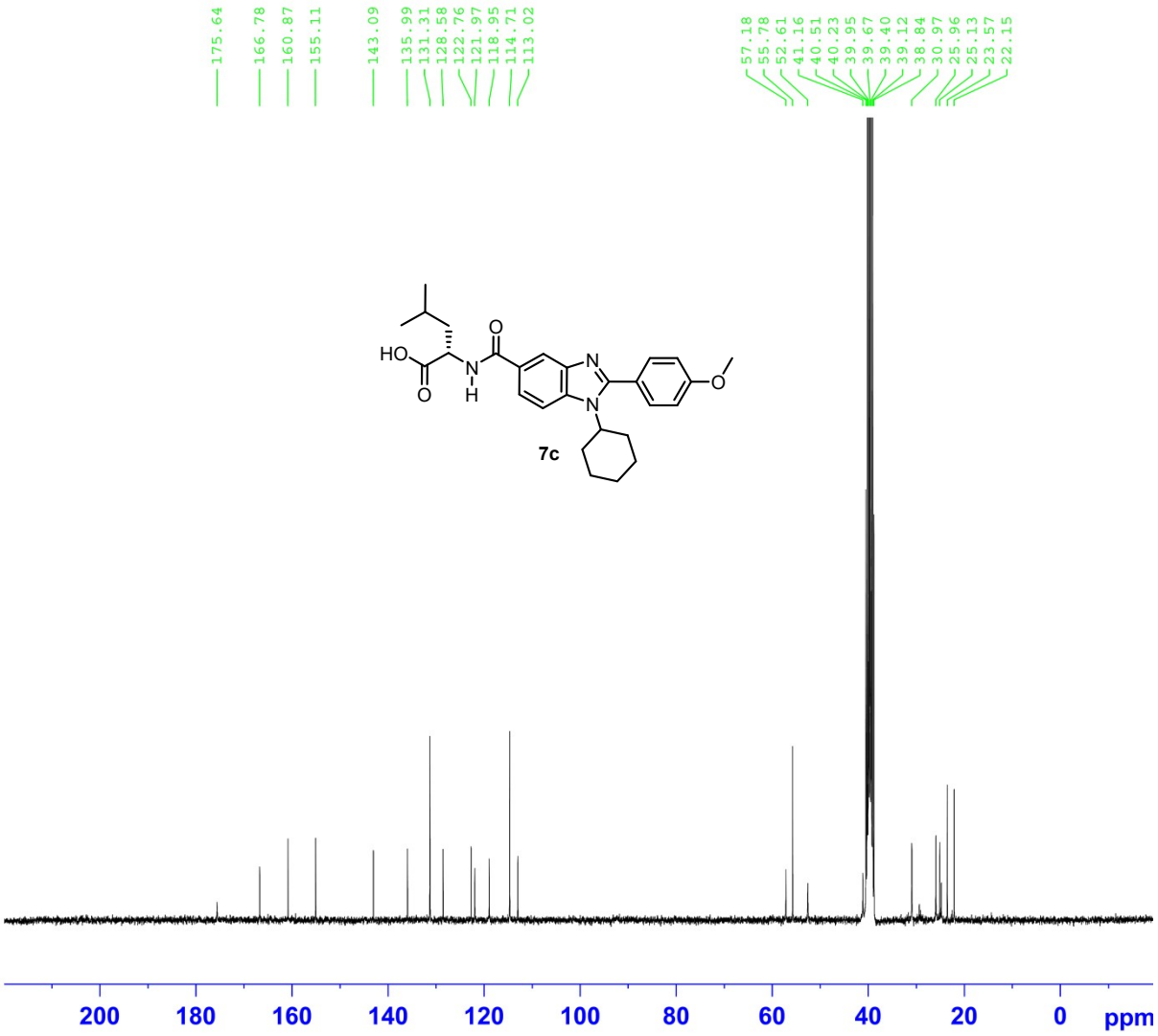

*MSD1 SPC, time=0.071:0.302 of C:\CHEM32\1\DATA\MARCH 2016\010316 2016-03-01 16-04-41\8B.D MM-ES+APCI, Scan, F
450.4
367.4
403.3
452.4
0
200
400
600
800
m/z
HO
O
N
H
O
N
N
O
7b

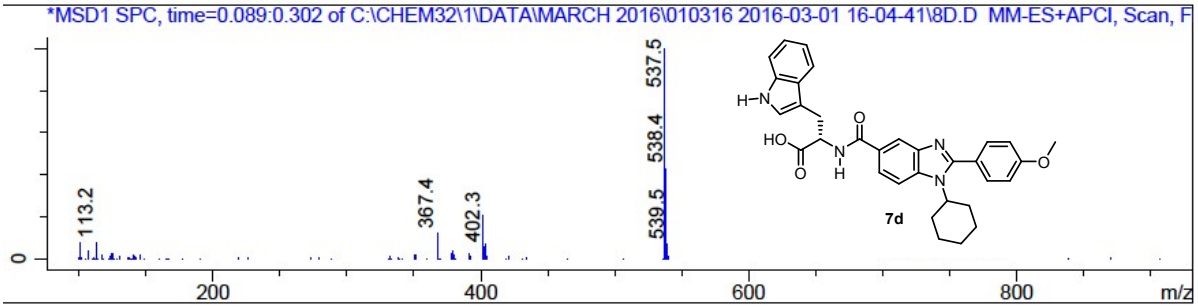

NAME Nikil,Mangloore UTY
EXPNO 16
PROCNO 1
Date_ 20160305
Time 13.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 22.6
DW 60.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 12.75 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 400.1224709 MHz
SI 32768
SF 400.1200025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.340
8.320
8.275
8.272
8.905
7.883
7.802
7.798
7.781
7.777
7.619
7.597
7.160
7.138
4.317
4.298
4.290
4.280
4.268
4.259
3.865
2.332
2.305
2.275
2.248
2.231
2.214
2.197
1.900
1.871
1.837
1.662
1.633
1.411
1.379
HO
O
N
H
O
N
N
O
7b
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
1.00
1.01
2.00
2.02
2.03
3.15
3.17
4.18
1.12
3.67
6.07

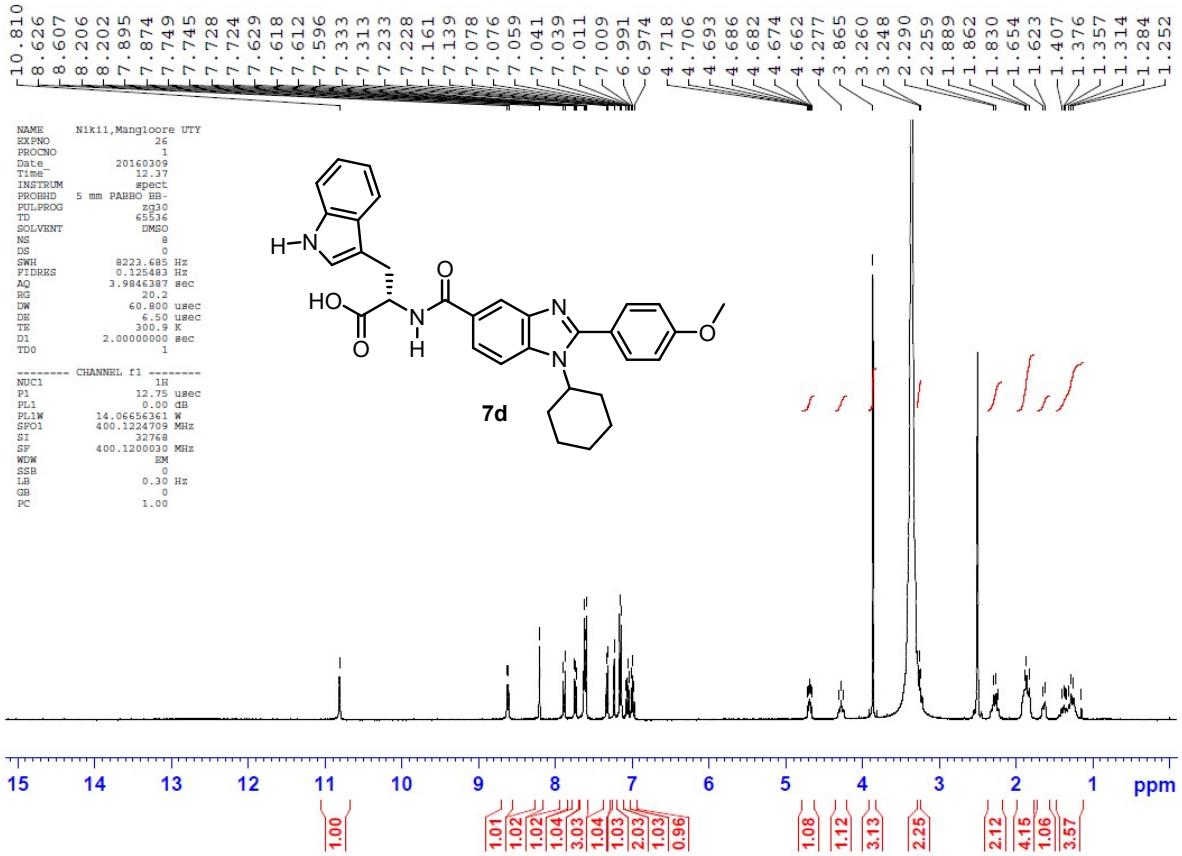

NAME Nikil,Mangloore UTY
EXPNO 17
PROCNO 1
Date_ 20160305
Time 13.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 983
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 36
DW 20.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.25 usec
PL1 -2.00 dB
PL1W 55.73500443 W
SFO1 100.6203150 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.95 dB
PL13 20.32 dB
PL2W 14.06656361 W
PL12W 0.35742757 W
PL13W 0.13067366 W
SFO2 400.1216005 MHz
SI 32768
SF 100.6103043 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
166.989
160.385
154.628
142.735
135.682
130.821
127.789
122.532
121.699
118.846
114.217
112.404
58.601
56.670
55.317
30.525
29.624
25.514
24.381
19.383
18.846
HO
O
N
H
O
N
N
O
7b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

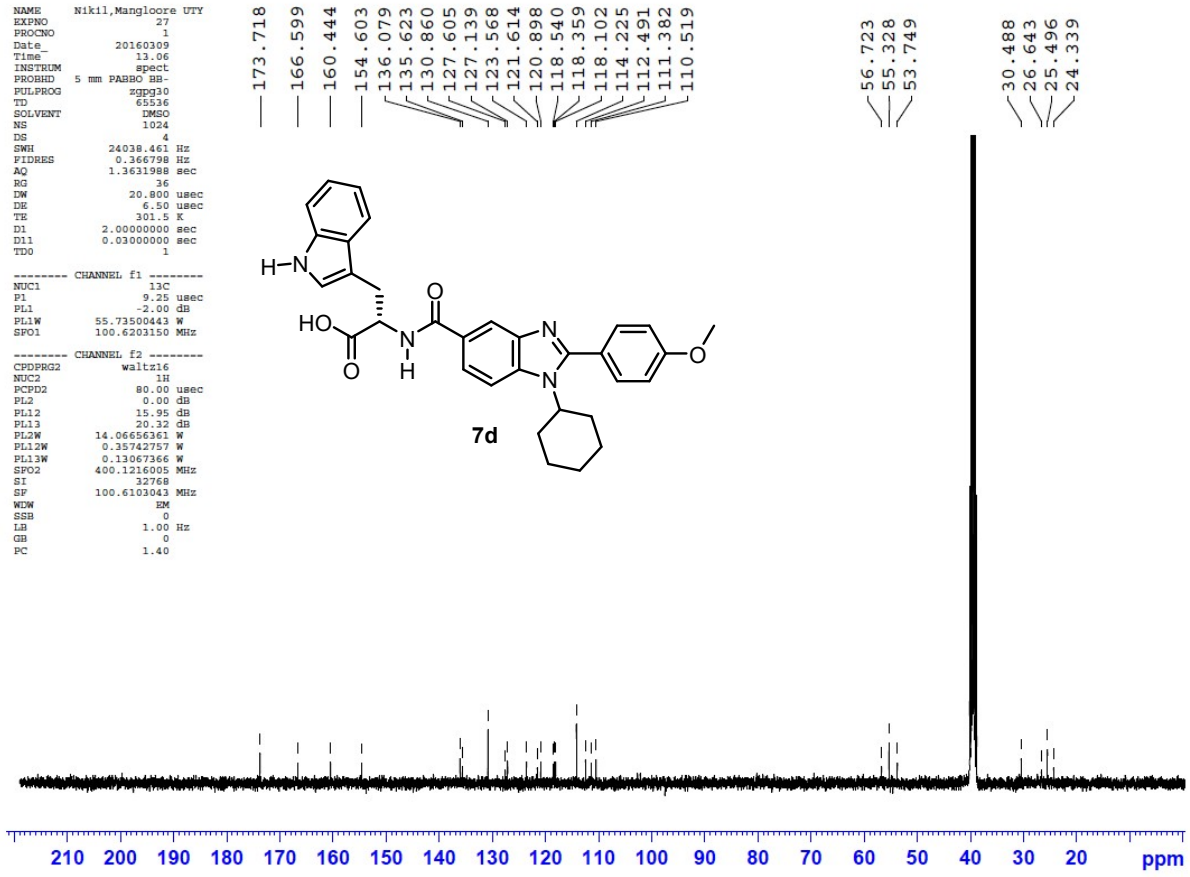

*MSD1 SPC, time=0.071:0.302 of C:\CHEM32\1\DATA\MARCH 2016\010316 2016-03-01 16-04-41\8C D MM-ES+APCI, Scan, F
464.4
465.4
0
200
400
600
800
m/z
HO
O
N
H
O
N
N
O
7c

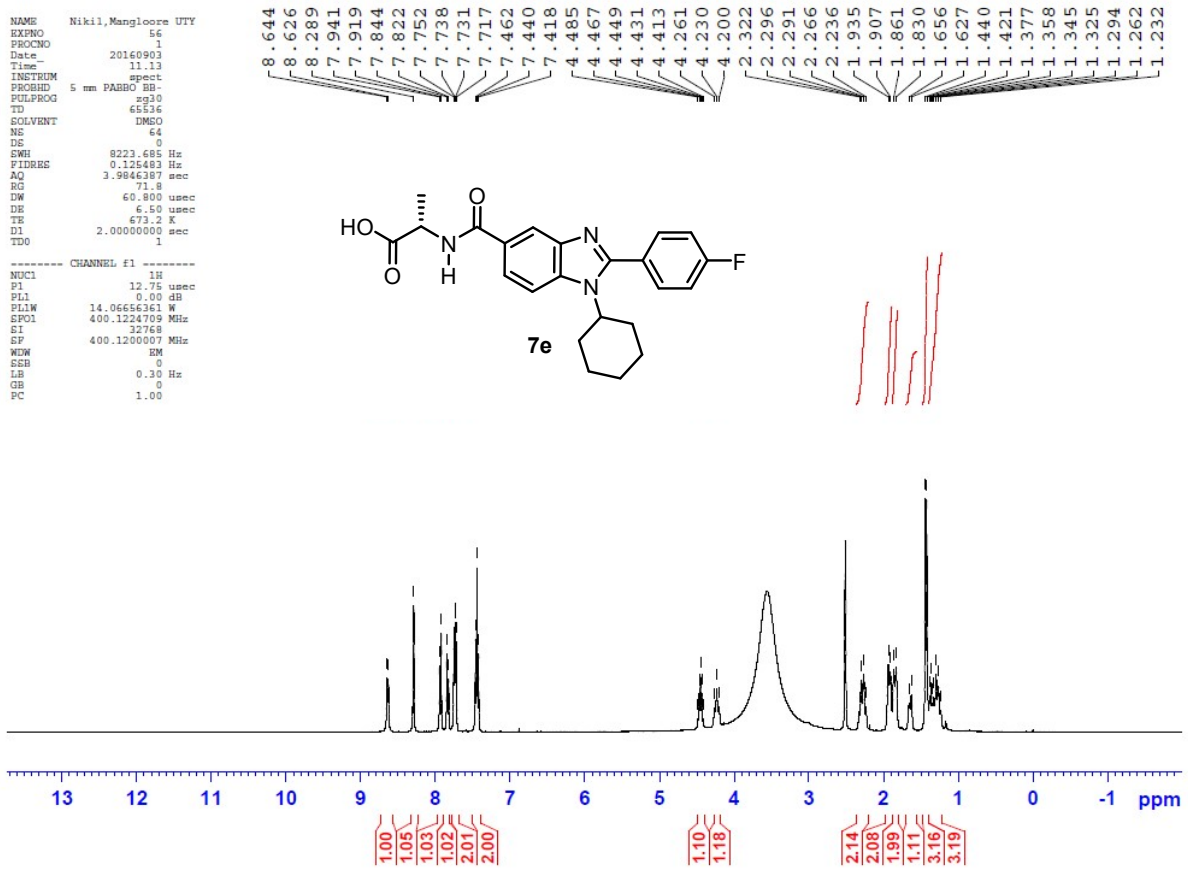

8.316
8.291
8.212
7.898
7.869
7.796
7.768
7.603
7.574
7.150
7.121
4.408
4.383
4.268
3.845
3.659
2.513
2.508
2.502
2.288
2.255
1.891
1.855
1.702
1.681
1.656
1.635
1.604
1.318
1.311
1.266
1.205
0.906
7-C
HO
O
N
H
O
N
N
O
7c
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
1.07
1.08
1.00
1.99
2.00
2.87
4.11
1.79
4.03
3.87
1.98
6.00

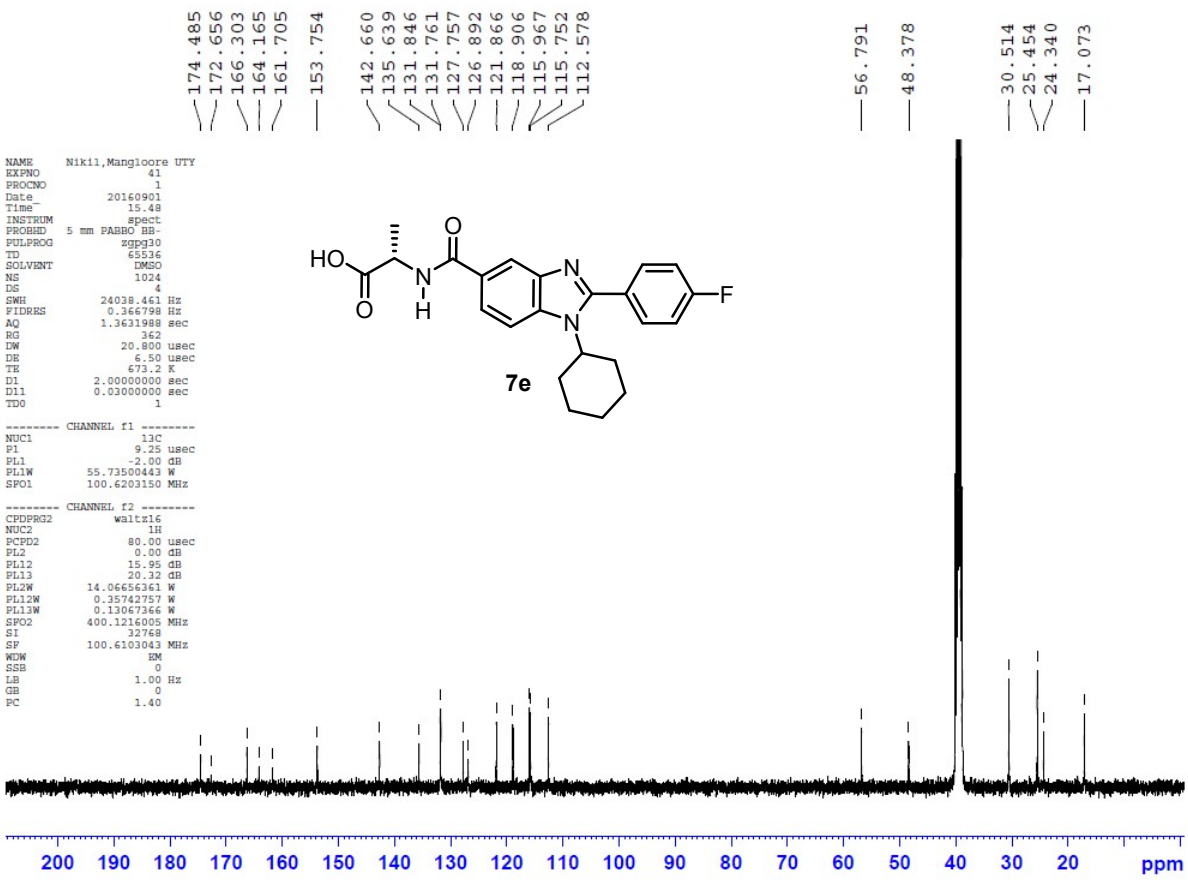

175.64
166.78
160.87
155.11
143.09
135.99
131.31
128.58
122.76
121.97
118.95
114.71
113.02
57.18
55.78
52.61
41.16
40.51
40.23
39.95
39.67
39.40
39.12
38.84
30.97
25.96
25.13
23.57
22.15
HO
O
N
H
O
N
N
O
7c
200
180
160
140
120
100
80
60
40
20
0
ppm

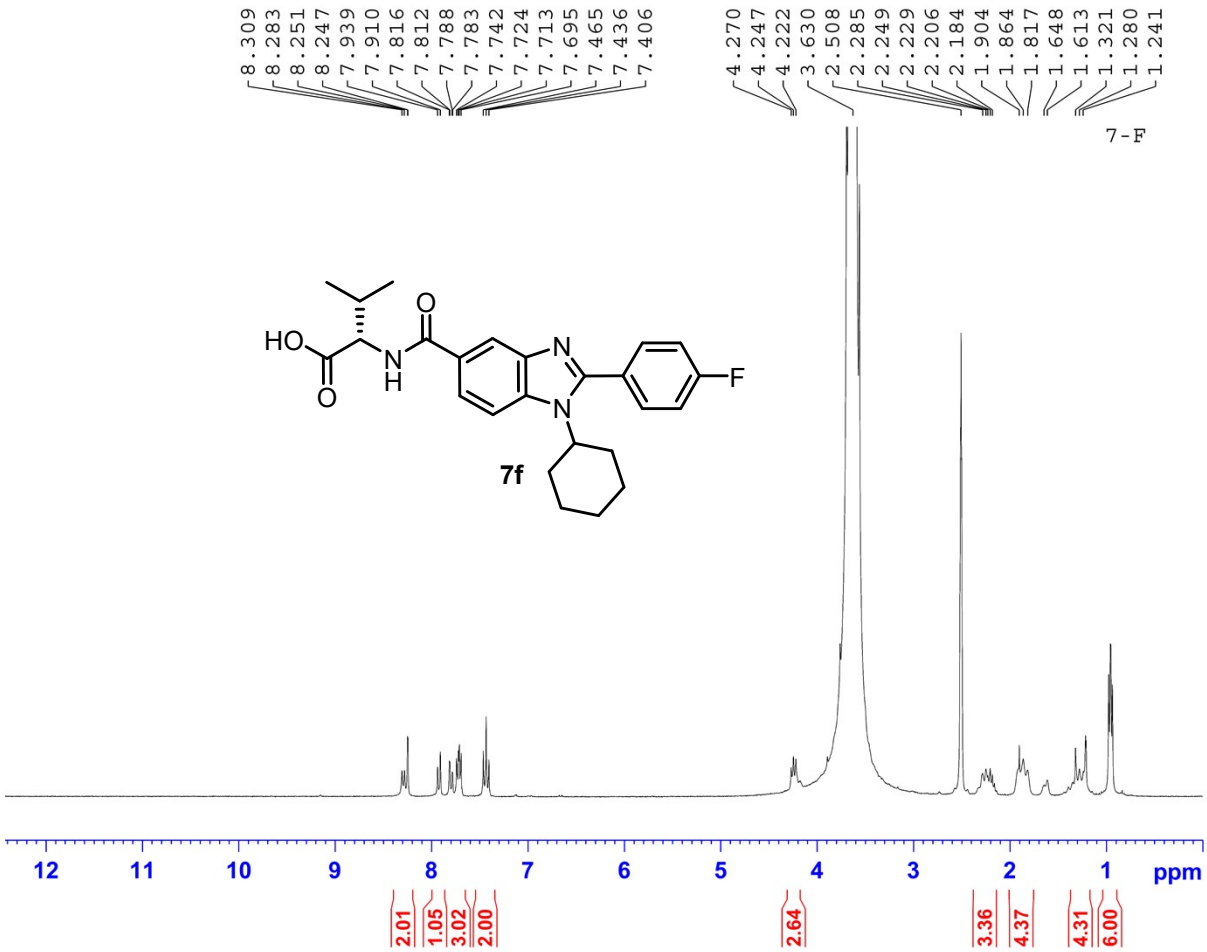

*MSD1 SPC, time=0.089:0.302 of C:\CHEM32\1\DATA\MARCH 2016\010316 2016-03-01 16-04-41\8D.D MM-ES+APCI, Scan, F
537.5
538.4
539.5
113.2
367.4
402.3
0
200
400
600
800
m/z
7d

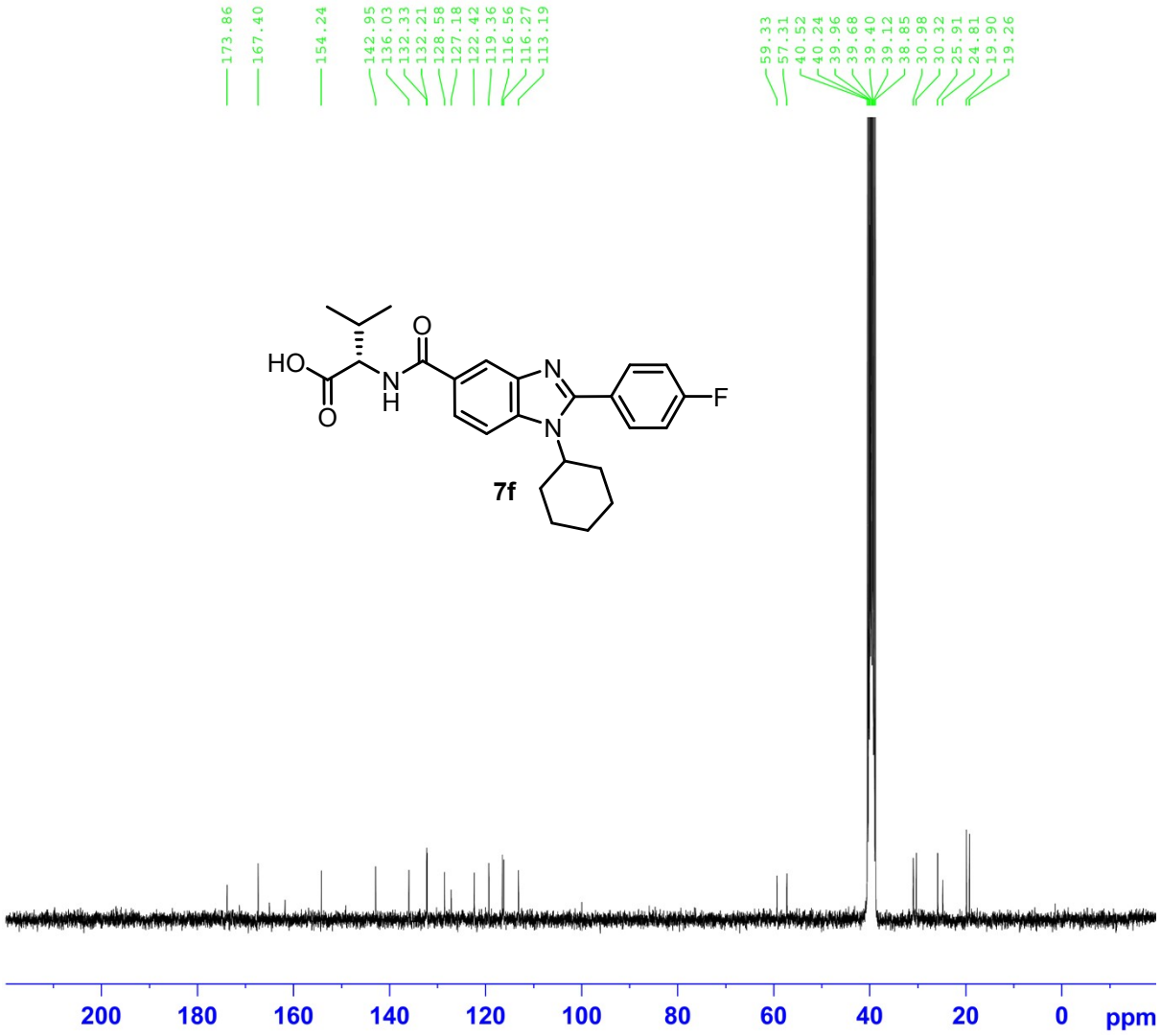

10.810
8.626
8.607
8.206
8.202
7.895
7.874
7.749
7.745
7.728
7.724
7.629
7.618
7.612
7.596
7.333
7.313
7.233
7.228
7.161
7.139
7.078
7.076
7.059
7.041
7.039
7.011
7.009
6.991
6.974
4.718
4.706
4.693
4.686
4.682
4.674
4.662
4.277
3.865
3.260
3.248
2.290
2.259
1.889
1.862
1.830
1.654
1.623
1.407
1.376
1.357
1.314
1.284
1.252
NAME Nikil,Mangloore UTY
EXPNO 26
PROCNO 1
Date_ 20160309
Time_ 12.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 20.2
DW 60.800 usec
DE 6.50 usec
TE 300.9 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 12.75 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 400.1224709 MHz
SI 32768
SF 400.1200030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7d
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.02
1.02
1.04
3.03
1.04
1.03
2.03
1.03
0.96
1.08
1.12
3.13
2.25
2.12
4.15
1.06
3.57

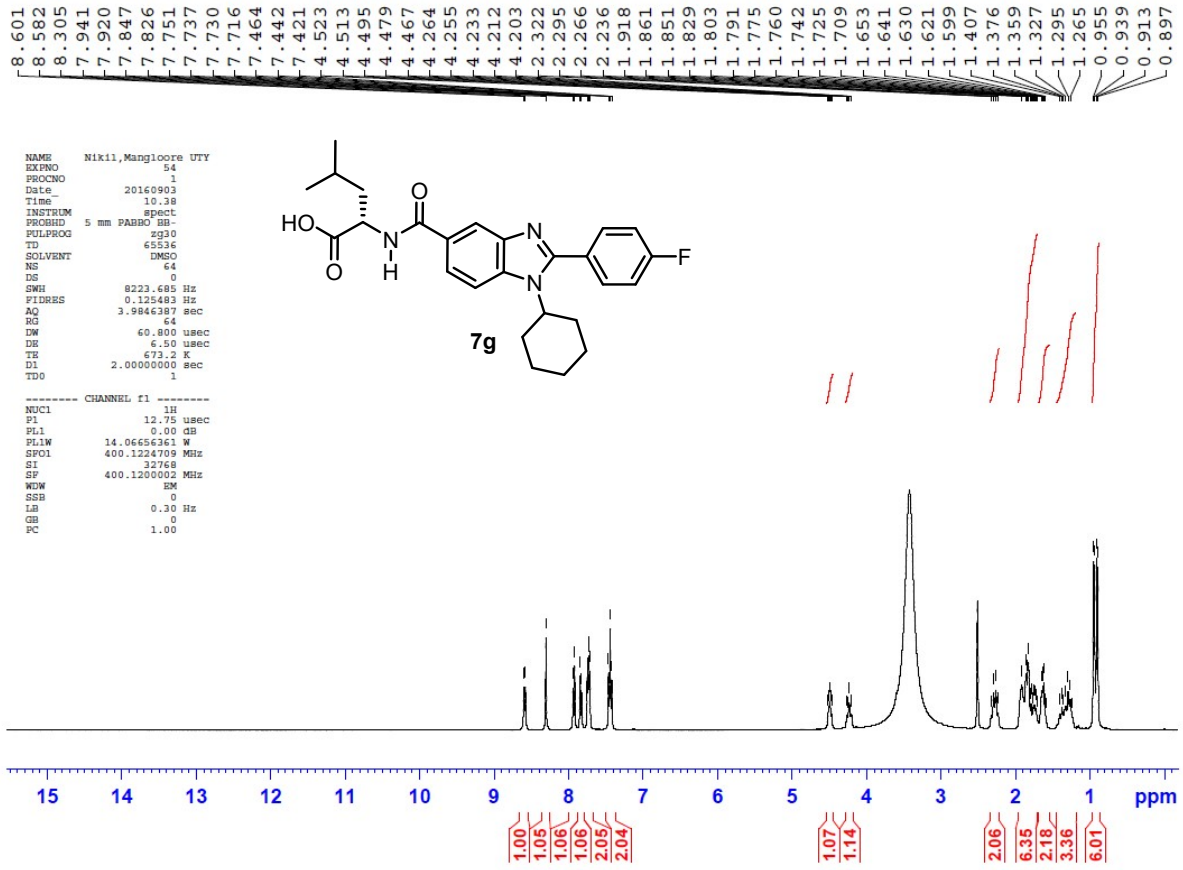

NAME Nikil,Mangloore UTY
EXPNO 27
PROCNO 1
Date_ 20160309
Time_ 13.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 36
DW 20.800 usec
DE 6.50 usec
TE 301.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.25 usec
PL1 -2.00 dB
PL1W 55.73500443 W
SFO1 100.6203150 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.95 dB
PL13 20.32 dB
PL2W 14.06656361 W
PL12W 0.35742757 W
PL13W 0.13067366 W
SFO2 400.1216005 MHz
SI 32768
SF 100.6103043 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
173.718
166.599
160.444
154.603
136.079
135.623
130.860
127.605
127.139
123.568
121.614
120.898
118.540
118.359
118.102
114.225
112.491
111.382
110.519
56.723
55.328
53.749
30.488
26.643
25.496
24.339
7d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

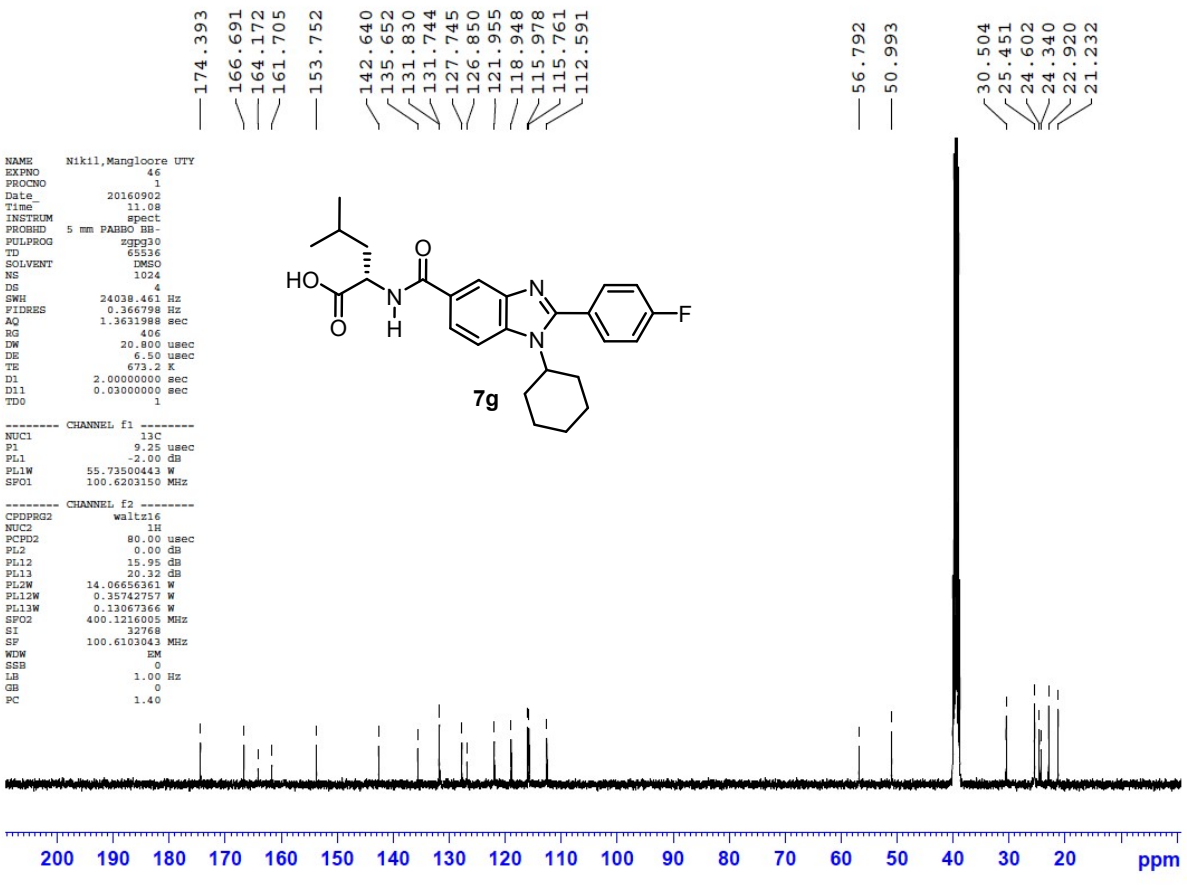

NAME Nikil,Mangloore UTY
EXPNO 56
PROCNO 1
Date_ 20160903
Time 11.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NE 64
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 71.8
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 12.75 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 400.1224709 MHz
SI 32768
SF 400.1200007 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.644
8.626
8.289
7.941
7.919
7.844
7.822
7.752
7.738
7.731
7.717
7.462
7.440
7.418
4.485
4.467
4.449
4.431
4.413
4.261
4.230
4.200
2.322
2.296
2.291
2.266
2.236
1.935
1.907
1.861
1.830
1.656
1.627
1.440
1.421
1.377
1.358
1.345
1.325
1.294
1.262
1.232
HO
O
N
H
O
N
N
F
7e
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.00
1.05
1.03
1.02
2.01
2.00
1.10
1.18
2.14
2.08
1.99
1.11
3.16
3.19

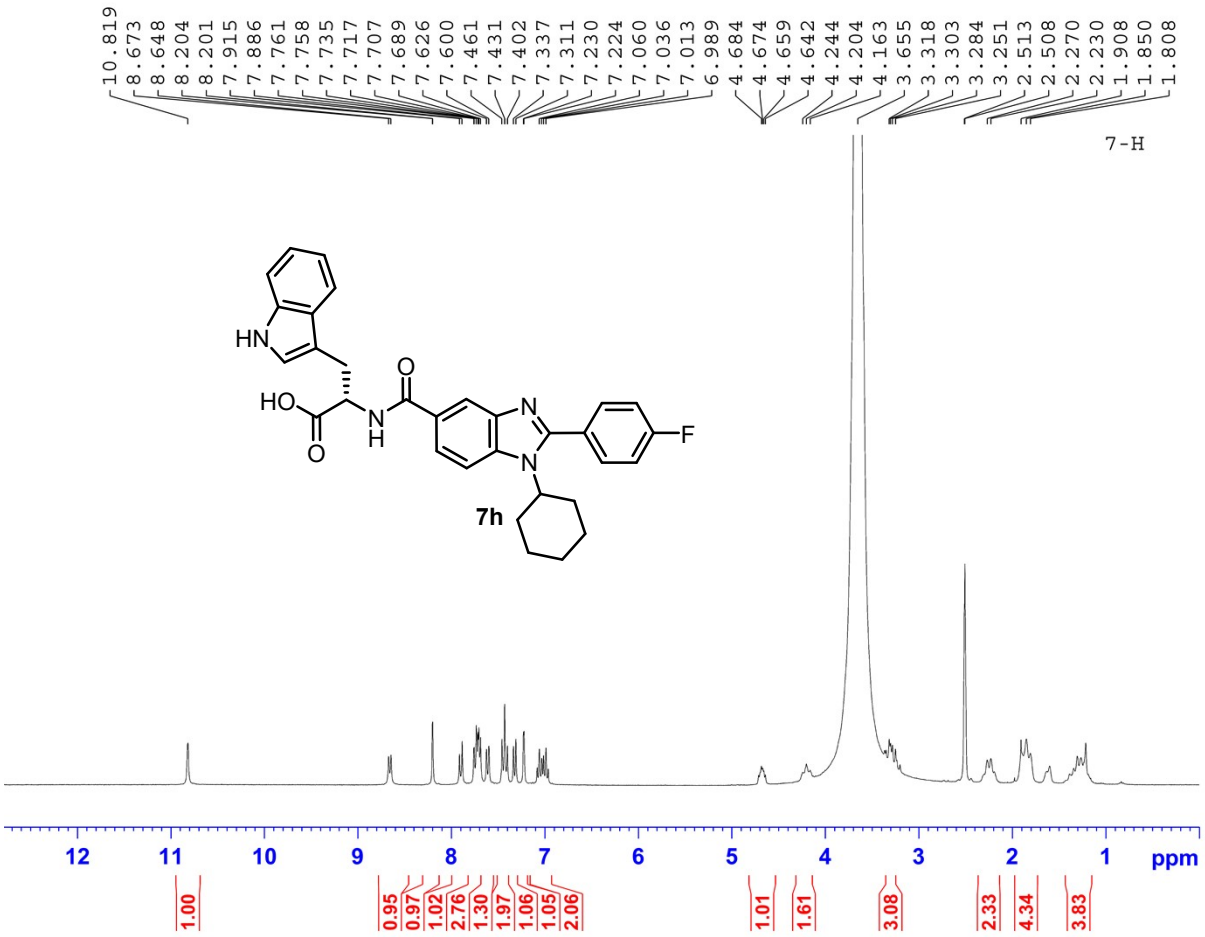

NAME Nikil,Mangloore UTY
EXPNO 41
PROCNO 1
Date_ 20160901
Time 15.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 362
DW 20.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.25 usec
PL1 -2.00 dB
PL1W 55.73500443 W
SFO1 100.6203150 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.95 dB
PL13 20.32 dB
PL2W 14.06656361 W
PL12W 0.35742757 W
PL13W 0.13067366 W
SFO2 400.1216005 MHz
SI 32768
SF 100.6103043 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
174.485
172.656
166.303
164.165
161.705
153.754
142.660
135.639
131.846
131.761
127.757
126.892
121.866
118.906
115.967
115.752
112.578
56.791
48.378
30.514
25.454
24.340
17.073
HO
O
N
H
O
N
N
F
7e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

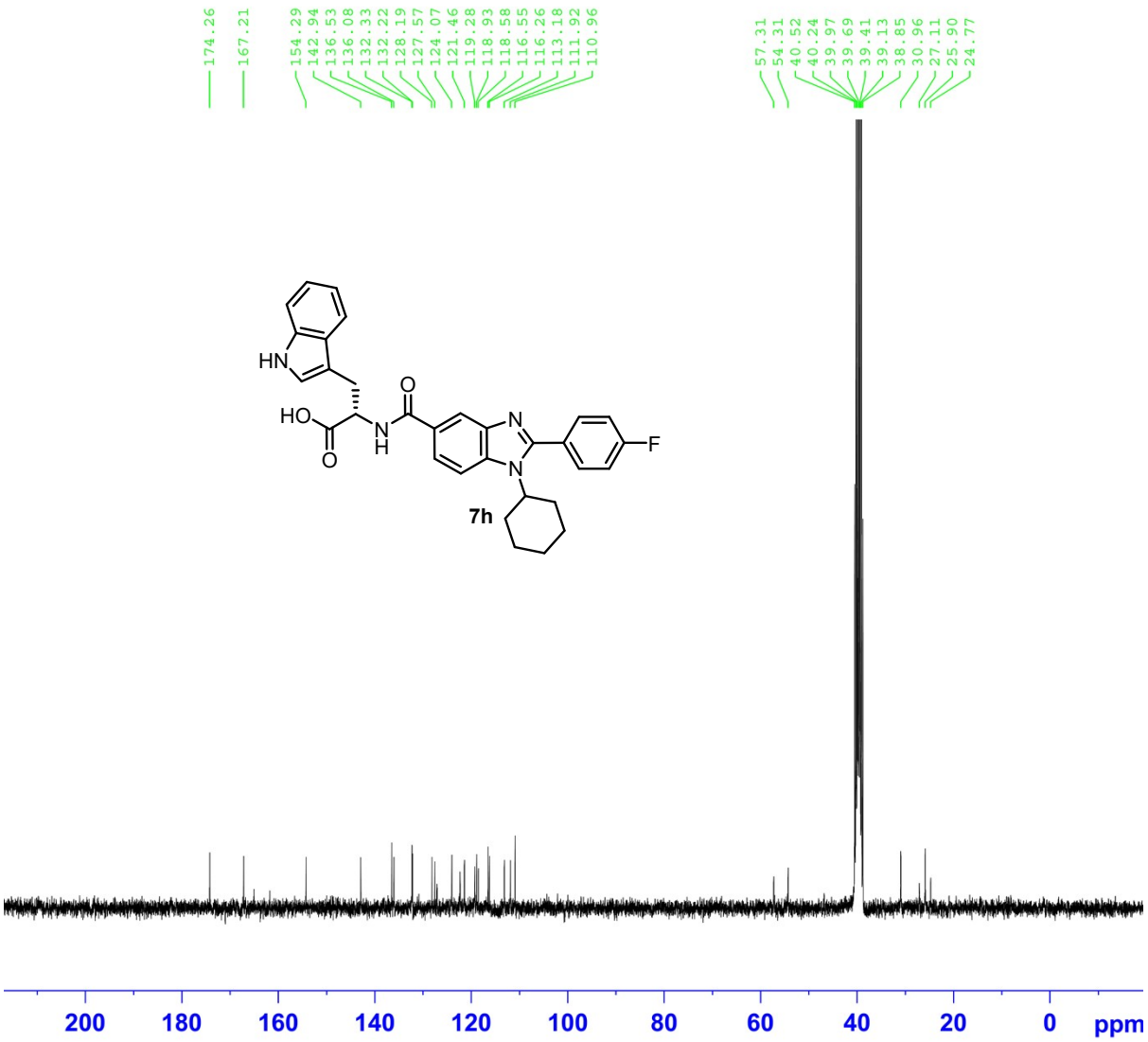

8.309
8.283
8.251
8.247
7.939
7.910
7.816
7.812
7.788
7.783
7.742
7.724
7.713
7.695
7.465
7.436
7.406
4.270
4.247
4.222
3.630
2.508
2.285
2.249
2.229
2.206
2.184
1.904
1.864
1.817
1.648
1.613
1.321
1.280
1.241
7-F
HO
O
N
H
O
N
N
F
7f
12
11
10
9
8
7
6
5
4
3
2
1
ppm
2.01
1.05
3.02
2.00
2.64
3.36
4.37
4.31
6.00

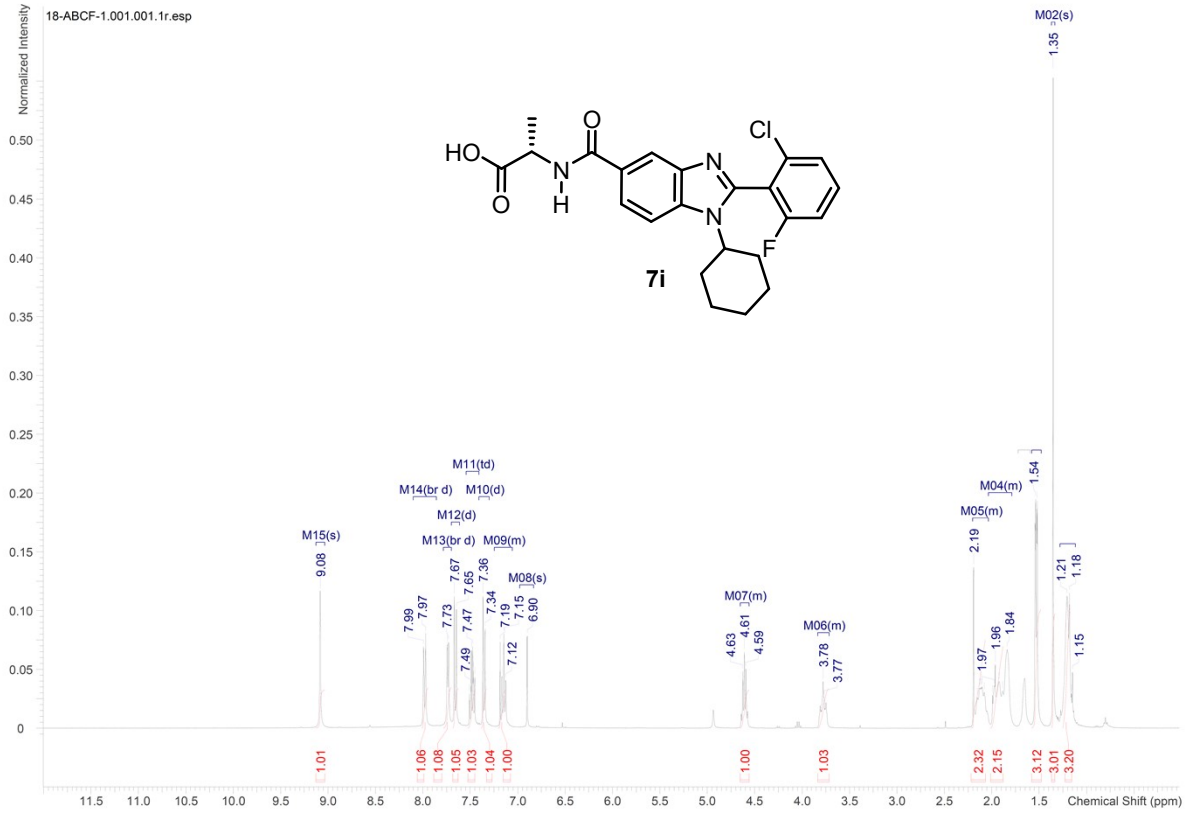

173.86
167.40
154.24
142.95
136.03
132.33
132.21
128.58
127.18
122.42
119.36
116.56
116.27
113.19
59.33
57.31
40.52
40.24
39.96
39.68
39.40
39.12
38.85
30.98
30.32
25.91
24.81
19.90
19.26
HO
O
N
H
O
N
N
F
7f
200
180
160
140
120
100
80
60
40
20
0
ppm

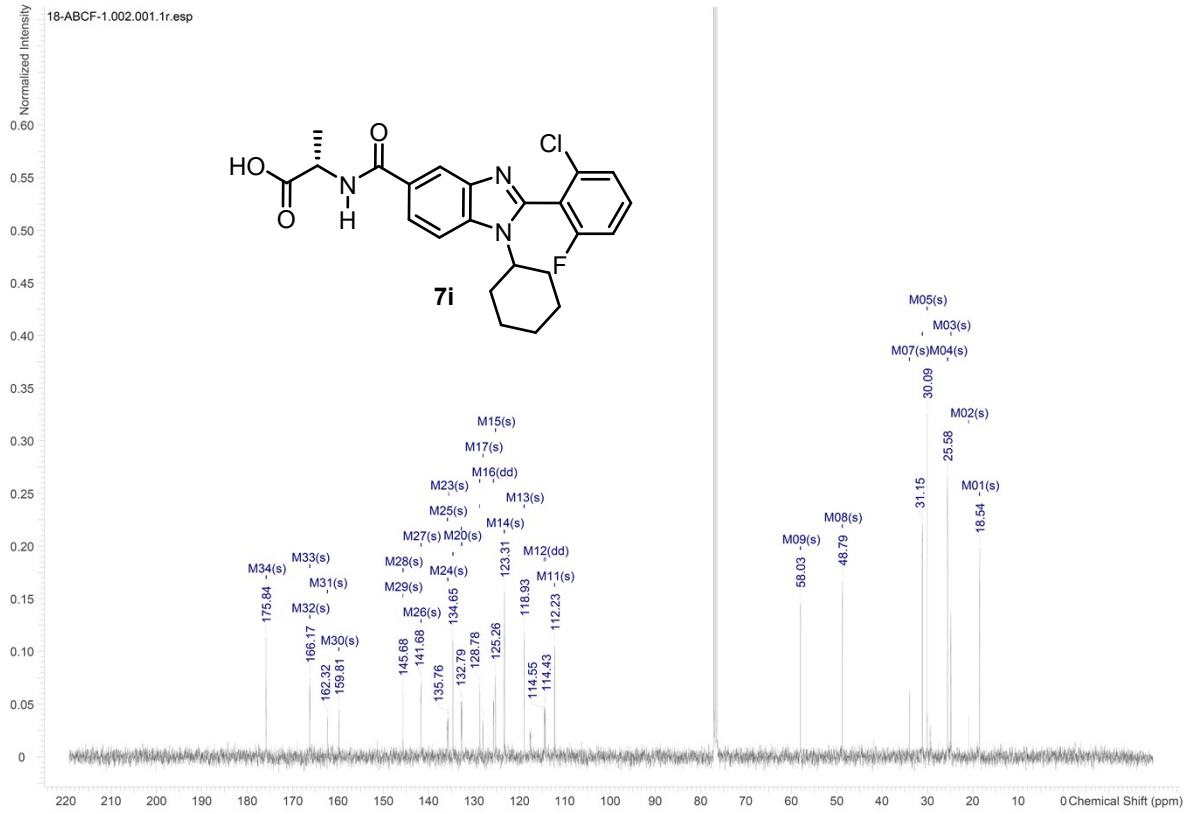

8.601
8.582
8.305
7.941
7.920
7.847
7.826
7.751
7.737
7.730
7.716
7.464
7.442
7.421
4.523
4.513
4.495
4.479
4.467
4.264
4.255
4.233
4.212
4.203
2.322
2.295
2.266
2.236
1.918
1.861
1.851
1.829
1.803
1.791
1.775
1.760
1.742
1.725
1.709
1.653
1.641
1.630
1.621
1.599
1.407
1.376
1.359
1.327
1.295
1.265
0.955
0.939
0.913
0.897
NAME Nikil,Mangloore UTY
EXPNO 54
PROCNO 1
Date_ 20160903
Time_ 10.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 12.75 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 400.1224709 MHz
SI 32768
SF 400.1200002 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HO
O
N
H
O
N
N
F
7g
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.05
1.06
1.06
2.05
2.04
1.07
1.14
2.06
6.35
2.18
3.36
6.01

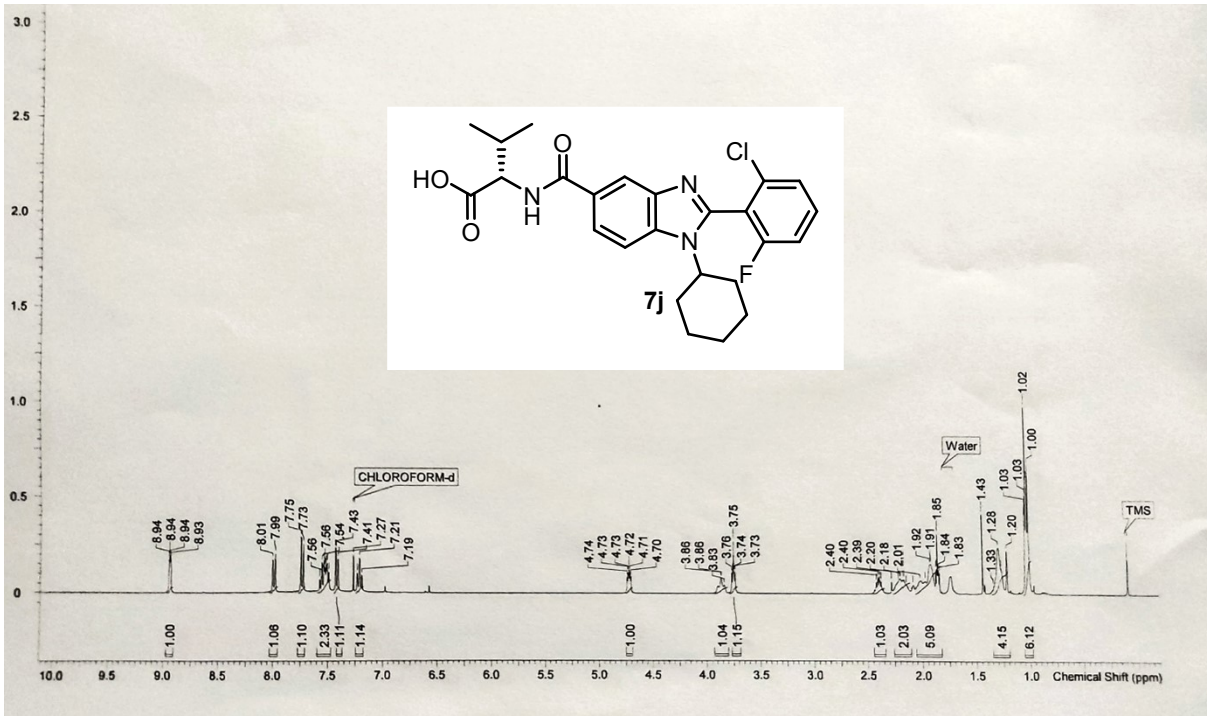

174.393
166.691
164.172
161.705
153.752
142.640
135.652
131.830
131.744
127.745
126.850
121.955
118.948
115.978
115.761
112.591
56.792
50.993
30.504
25.451
24.602
24.340
22.920
21.232
NAME Nikil,Mangloore UTY
EXPNO 46
PROCNO 1
Date_ 20160902
Time_ 11.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 406
DW 20.800 usec
DE 6.50 usec
TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.25 usec
PL1 -2.00 dB
PL1W 55.73500443 W
SFO1 100.6203150 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.95 dB
PL13 20.32 dB
PL2W 14.06656361 W
PL12W 0.35742757 W
PL13W 0.13067366 W
SFO2 400.1216005 MHz
SI 32768
SF 100.6103043 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HO
O
N
H
O
N
N
F
7g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

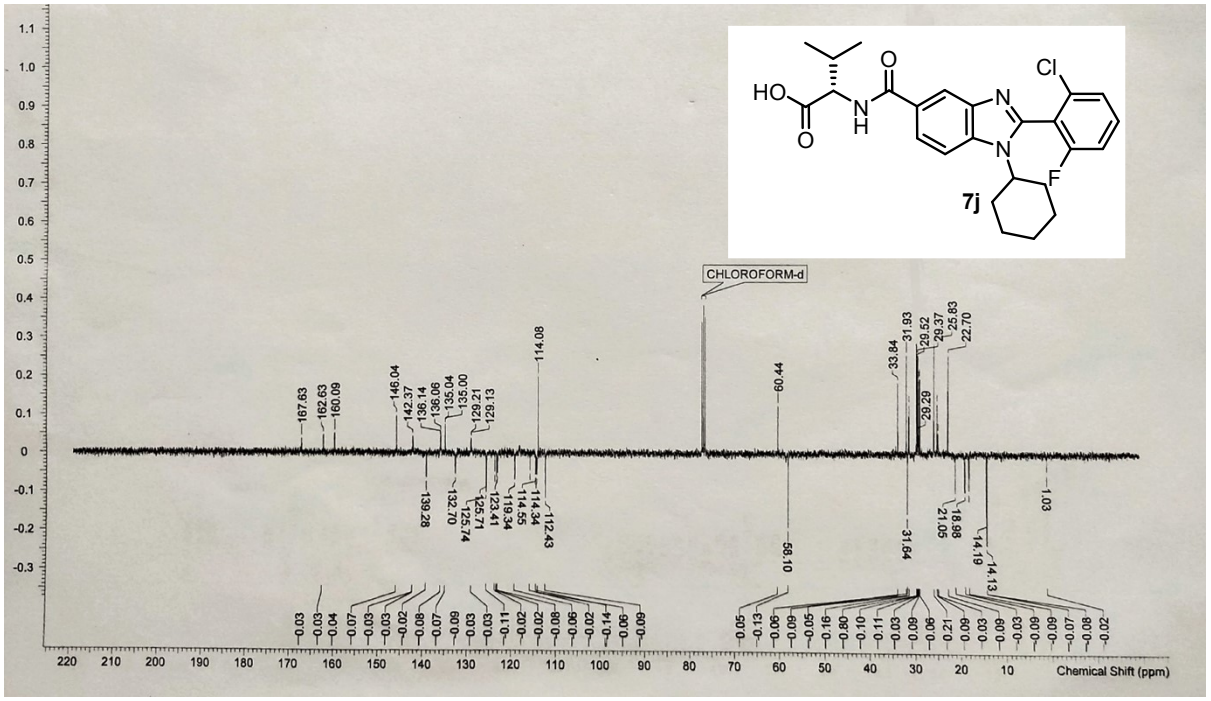

10.819
8.673
8.648
8.204
8.201
7.915
7.886
7.761
7.758
7.735
7.717
7.707
7.689
7.626
7.600
7.461
7.431
7.402
7.337
7.311
7.230
7.224
7.060
7.036
7.013
6.989
4.684
4.674
4.659
4.642
4.244
4.204
4.163
3.655
3.318
3.303
3.284
3.251
2.513
2.508
2.270
2.230
1.908
1.850
1.808
7-H
HN
HO
O
N
H
O
N
N
F
7h
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.95
0.97
1.02
2.76
1.30
1.97
1.06
1.05
2.06
1.01
1.61
3.08
2.33
4.34
3.83

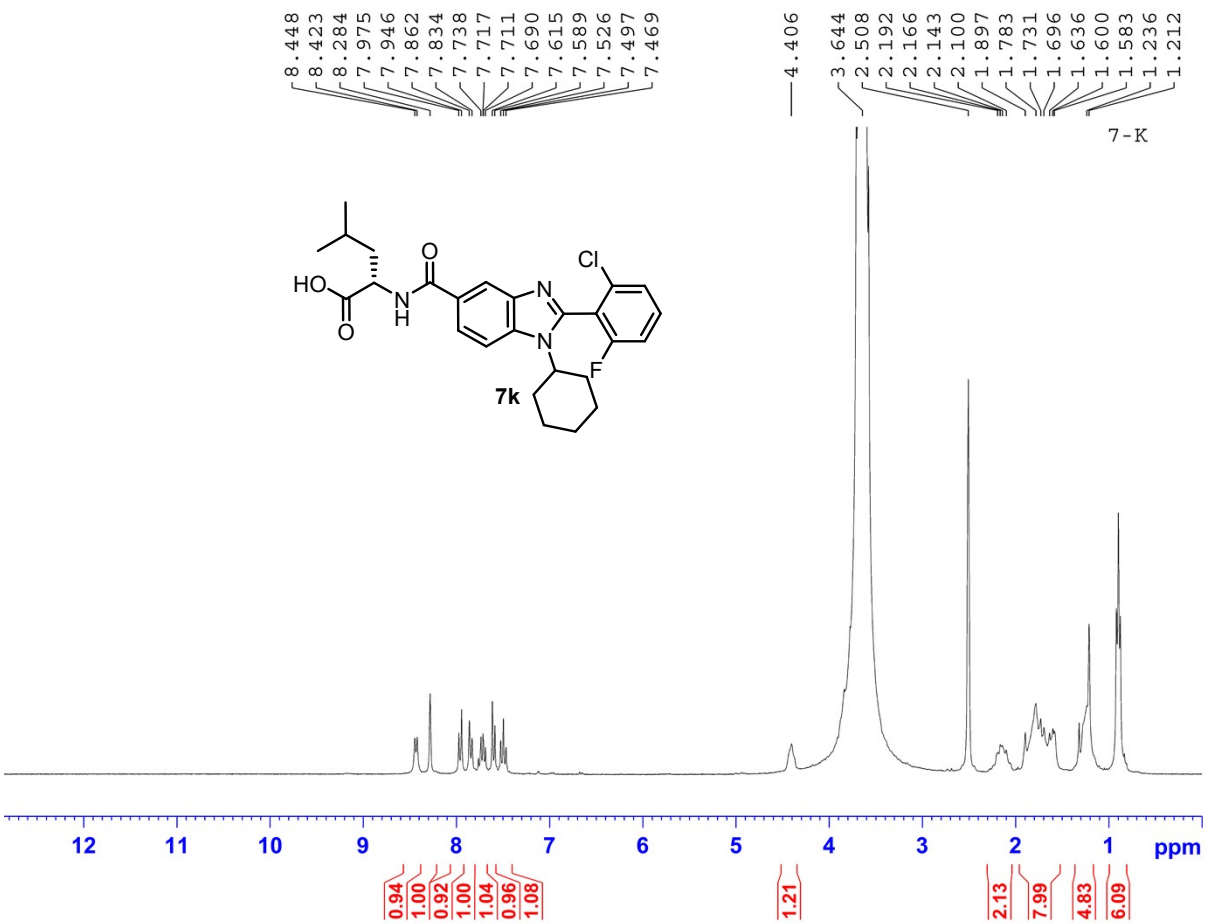

174.26
167.21
154.29
142.94
136.53
136.08
132.33
132.22
128.19
127.57
124.07
121.46
119.28
118.93
118.58
116.55
116.26
113.18
111.92
110.96
57.31
54.31
40.52
40.24
39.97
39.69
39.41
39.13
38.85
30.96
27.11
25.90
24.77
HN
HO
O
N
H
O
N
N
F
7h
200
180
160
140
120
100
80
60
40
20
0
ppm

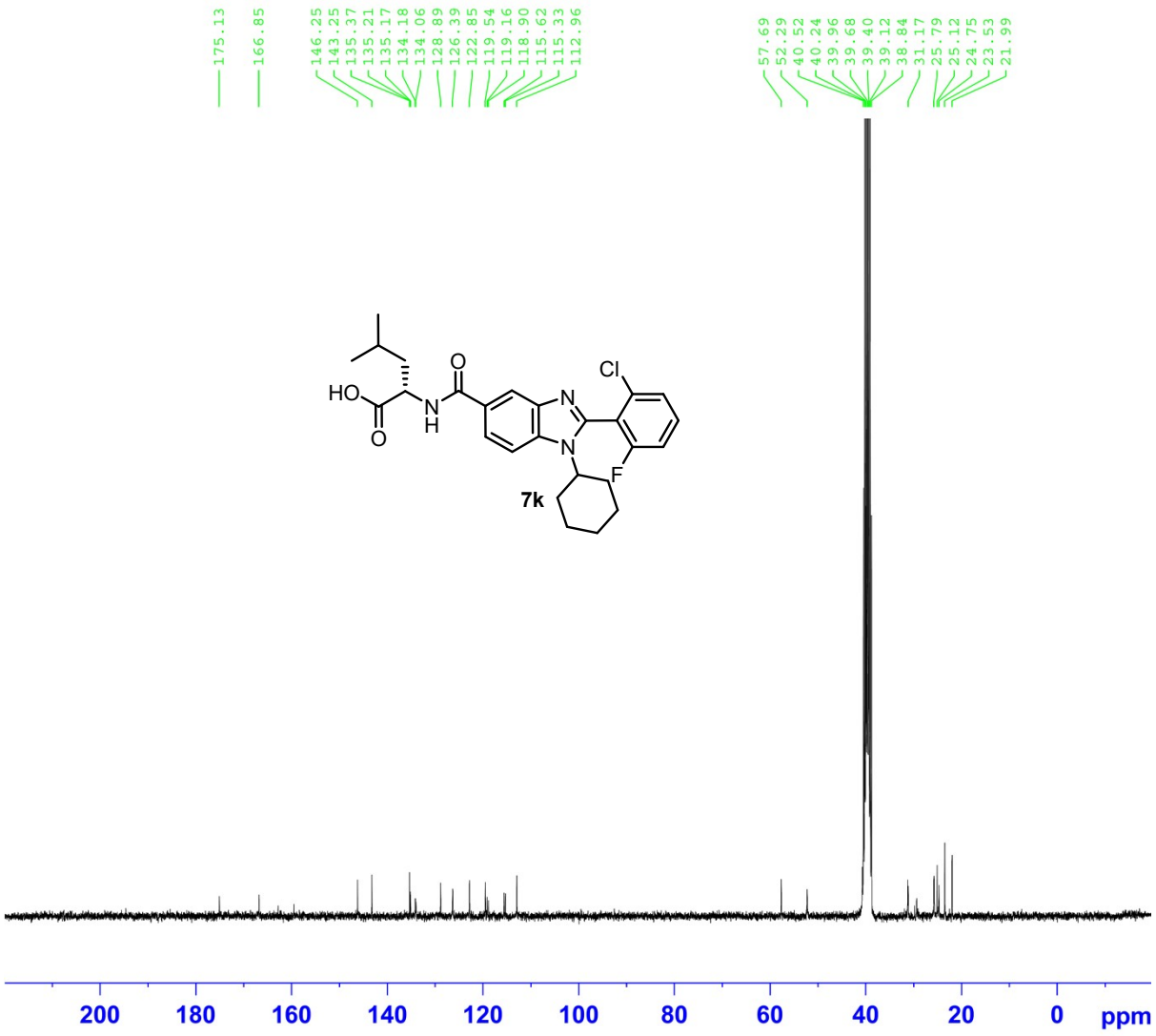

18-ABCF-1.001.001.1r.esp
Normalized Intensity
7i
Chemical Shift (ppm)

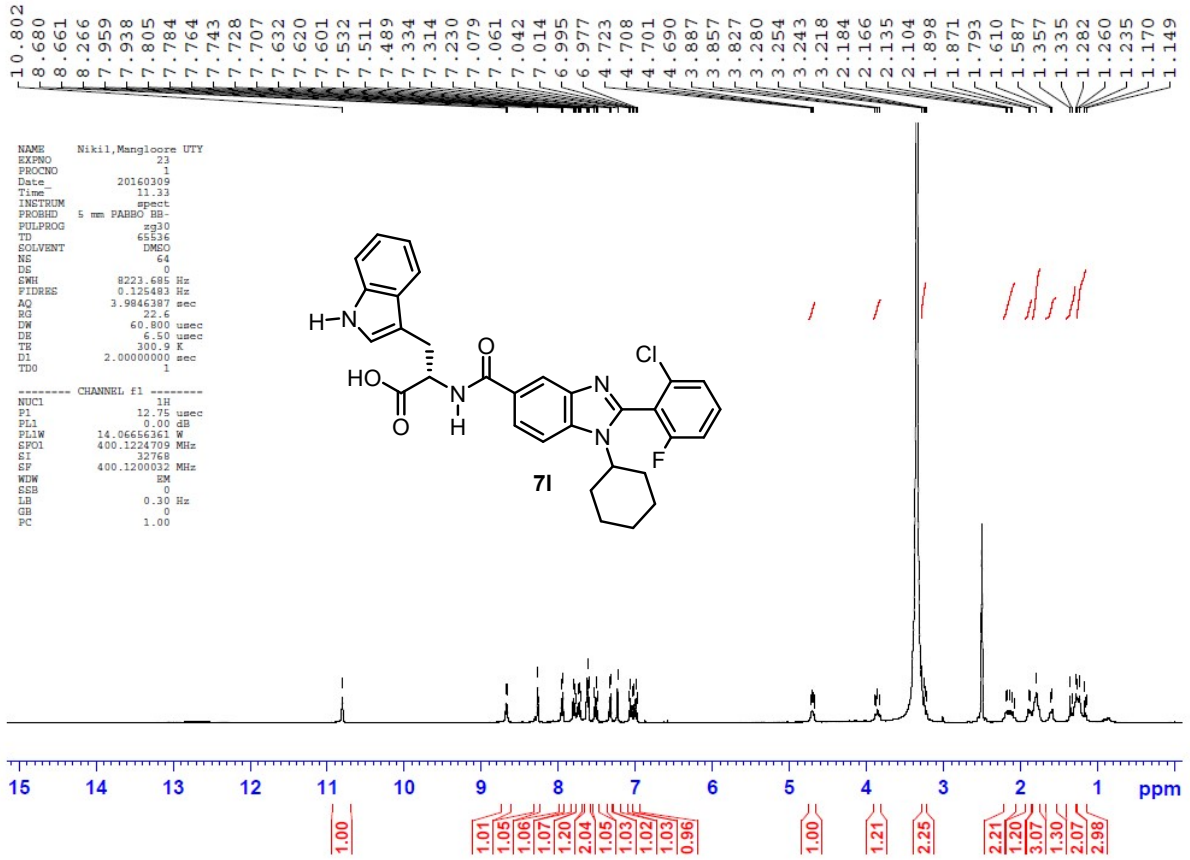

18-ABCF-1.002.001.1r.esp
Normalized Intensity
7i
Chemical Shift (ppm)

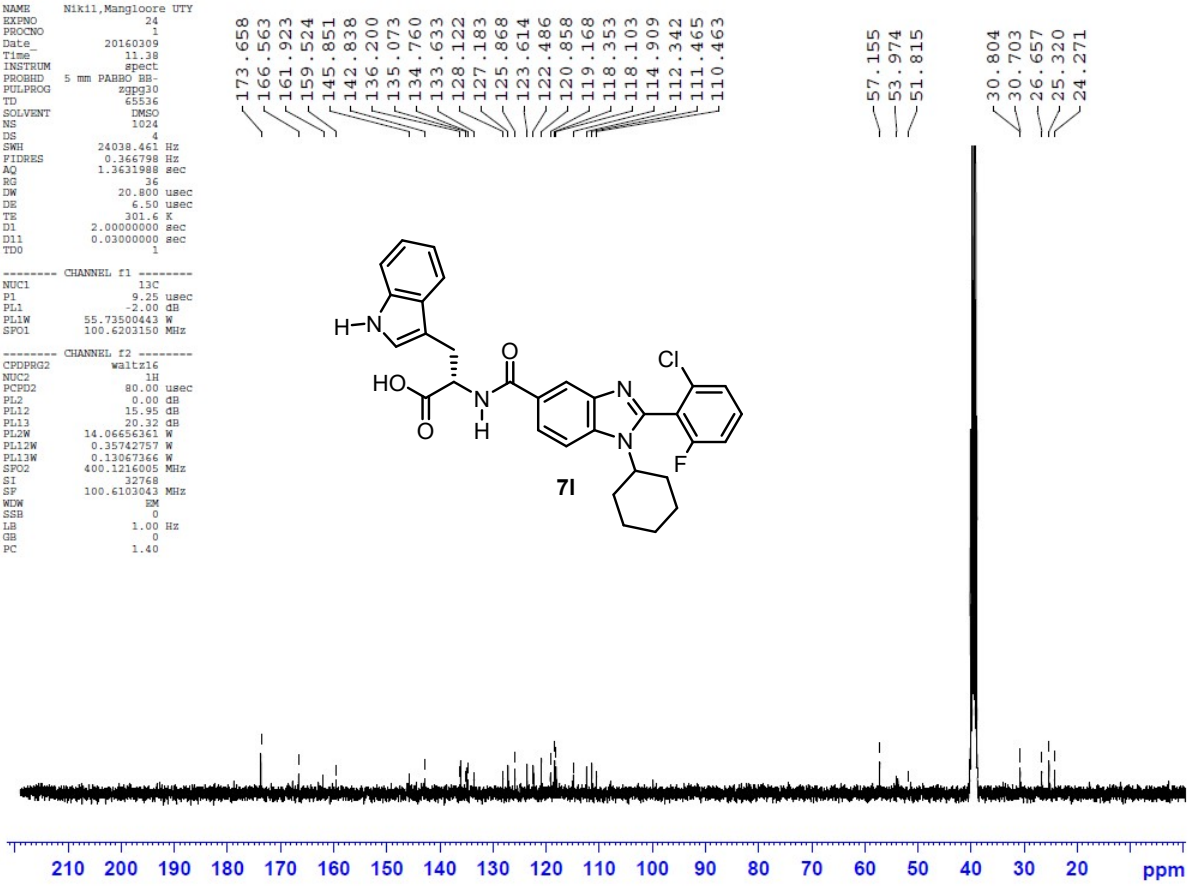

HO
O
N
H
O
Cl
N
N
F
7j
CHLOROFORM-d
Water
TMS
Chemical Shift (ppm)


HO
O
N
H
O
Cl
N
N
F
7j
CHLOROFORM-d
Chemical Shift (ppm)

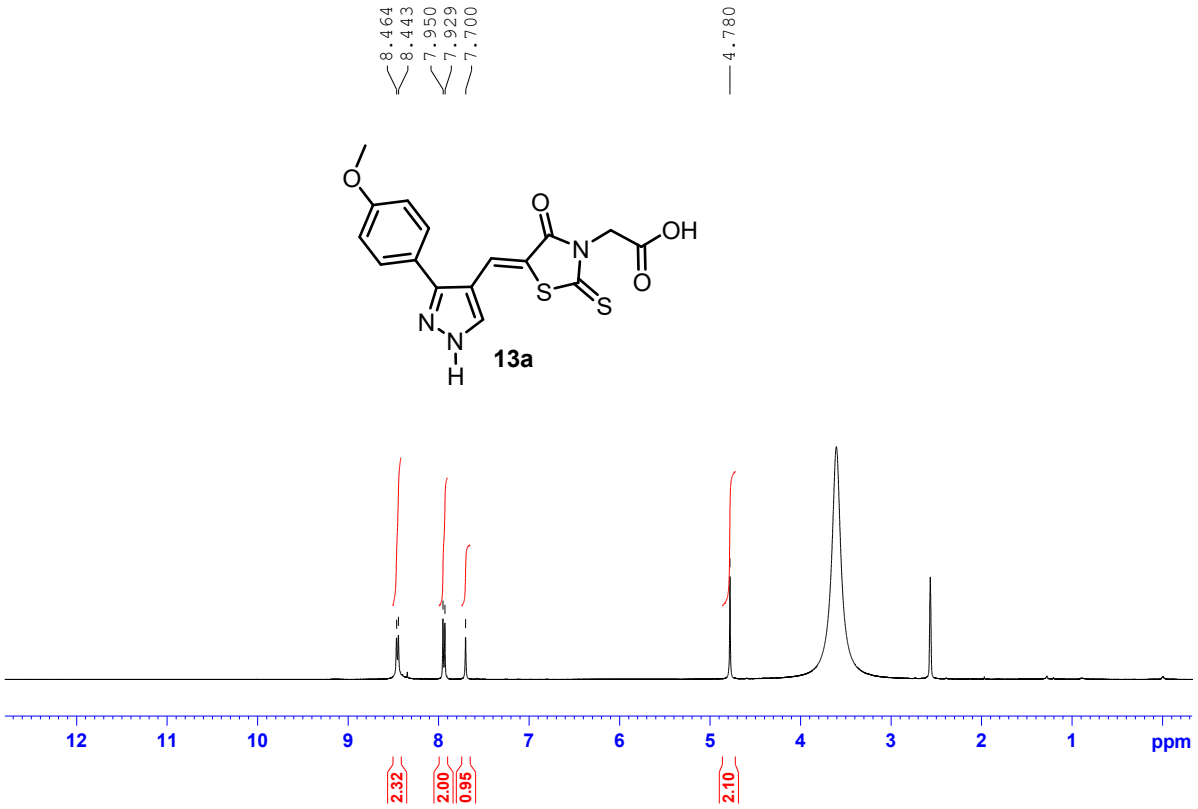

8.448
8.423
8.284
7.975
7.946
7.862
7.834
7.738
7.717
7.711
7.690
7.615
7.589
7.526
7.497
7.469
4.406
3.644
2.508
2.192
2.166
2.143
2.100
1.897
1.783
1.731
1.696
1.636
1.600
1.583
1.236
1.212
7-K
HO
O
N
H
O
N
N
Cl
F
7k
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.94
1.00
0.92
1.00
1.04
0.96
1.08
1.21
2.13
7.99
4.83
6.09


175.13
166.85
146.25
143.25
135.37
135.21
135.17
134.18
134.06
128.89
126.39
122.85
119.54
119.16
118.90
115.62
115.33
112.96
57.69
52.29
40.52
40.24
39.96
39.68
39.40
39.12
38.84
31.17
25.79
25.12
24.75
23.53
21.99
HO
O
O
N
H
N
N
Cl
F
7k
200
180
160
140
120
100
80
60
40
20
0
ppm

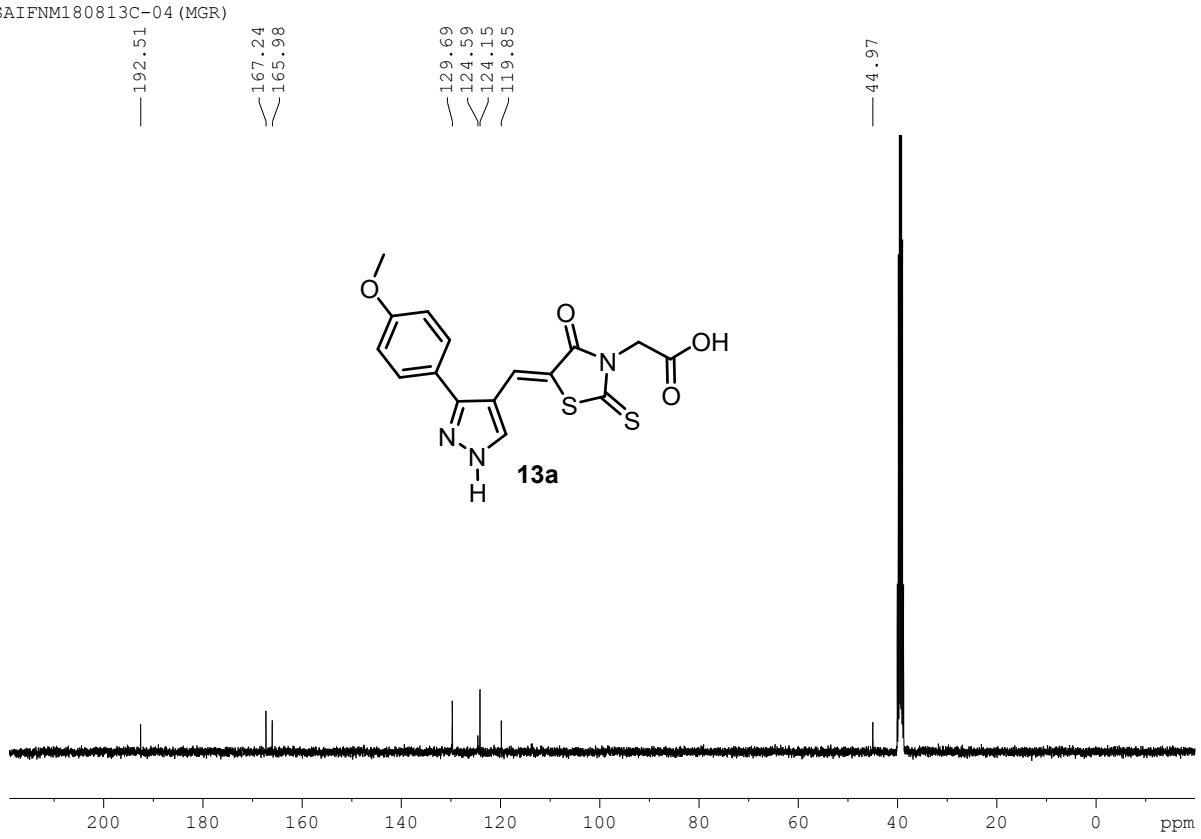

10.802
8.680
8.661
8.266
7.959
7.938
7.805
7.784
7.764
7.743
7.728
7.707
7.632
7.620
7.601
7.532
7.511
7.489
7.334
7.314
7.230
7.079
7.061
7.042
7.014
6.995
6.977
4.723
4.708
4.701
4.690
3.887
3.857
3.827
3.280
3.254
3.243
3.218
2.184
2.166
2.135
2.104
1.898
1.871
1.793
1.610
1.587
1.357
1.335
1.282
1.260
1.235
1.170
1.149
NAME Nikil,Mangloore UTY
EXPNO 23
PROCNO 1
Date_ 20160309
Time_ 11.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 22.6
DW 60.800 usec
DE 6.50 usec
TE 300.9 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 12.75 usec
PL1 0.00 dB
PL1W 14.06656361 W
SFO1 400.1224709 MHz
SI 32768
SF 400.1200032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7l
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.01 1.05 1.06 1.07 1.20 2.04 1.05 1.03 1.02 1.03 0.96 1.00 1.21 2.25 2.21 1.20 3.07 1.30 2.07 2.98


NAME Nikil,Mangloore UTY
EXPNO 24
PROCNO 1
Date_ 20160309
Time_ 11.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 36
DW 20.800 usec
DE 6.50 usec
TE 301.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.25 usec
PL1 -2.00 dB
PL1W 55.73500443 W
SFO1 100.6203150 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.95 dB
PL13 20.32 dB
PL2W 14.06656361 W
PL12W 0.35742757 W
PL13W 0.13067366 W
SFO2 400.1216005 MHz
SI 32768
SF 100.6103043 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
173.658
166.563
161.923
159.524
145.851
142.838
136.200
135.073
134.760
133.633
128.122
127.183
125.868
123.614
122.486
120.858
119.168
118.353
118.103
114.909
112.342
111.465
110.463
57.155
53.974
51.815
30.804
30.703
26.657
25.320
24.271
7l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

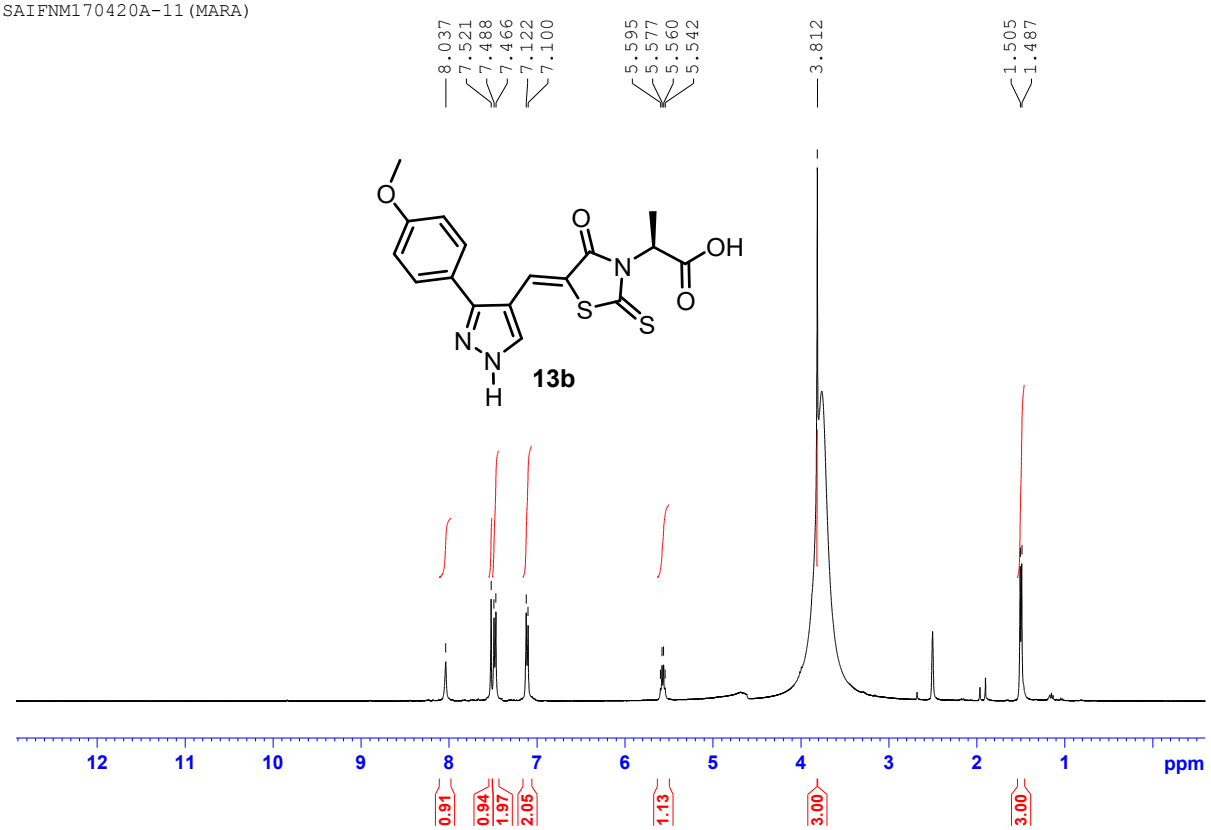
SAIFNM180813C-03(MGR)



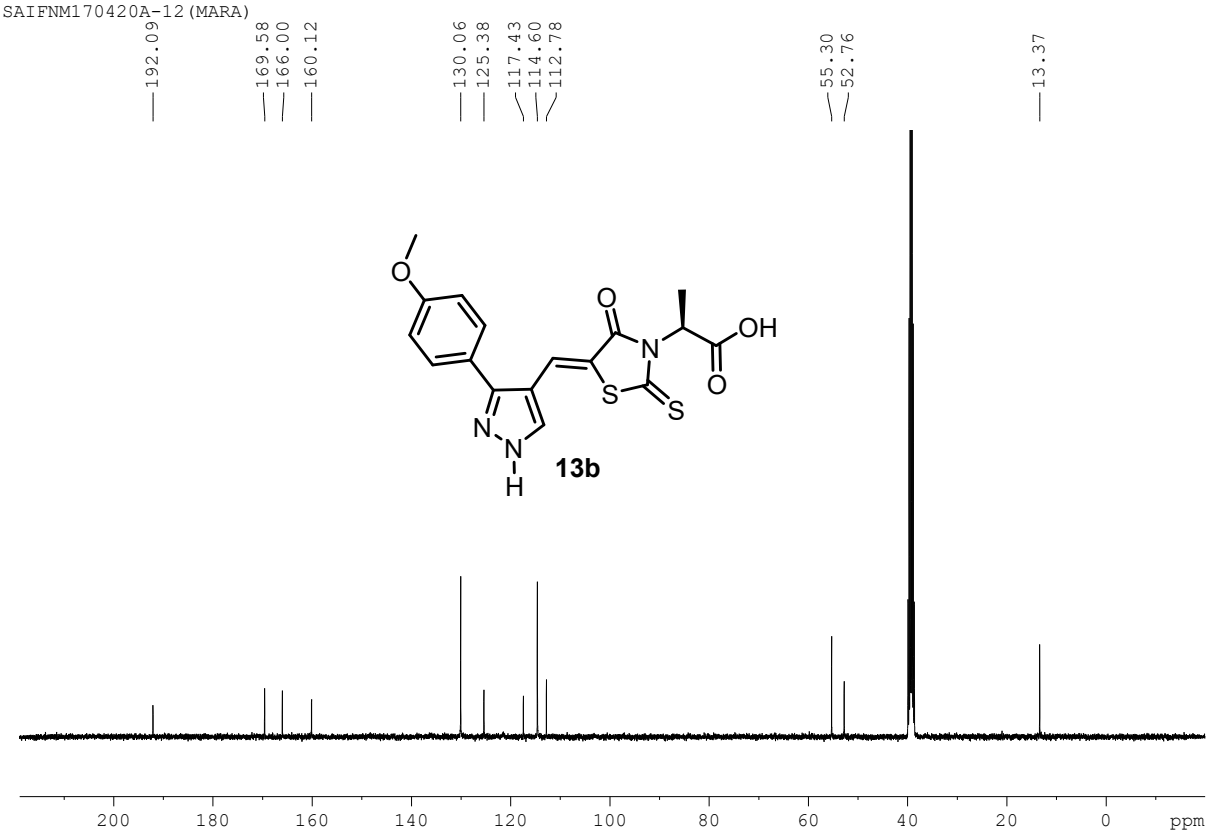
SAIFNM180813C-04(MGR)

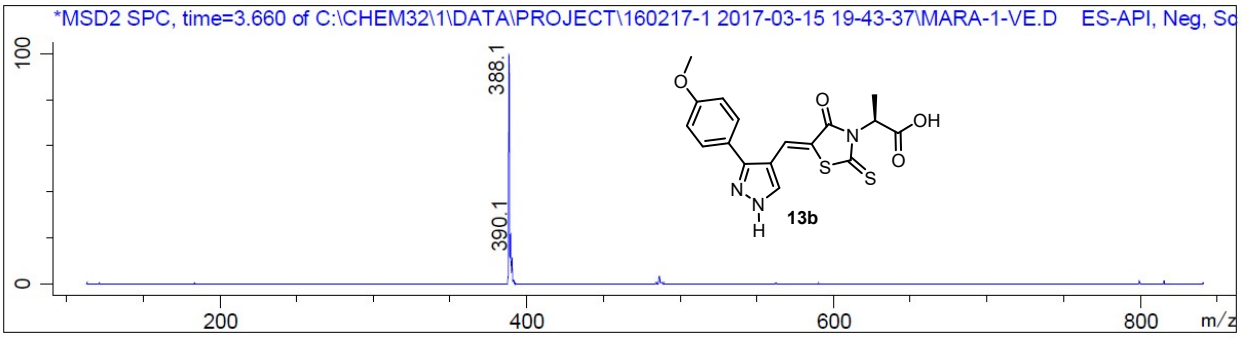


SAIFNM170420A-11(MARA)

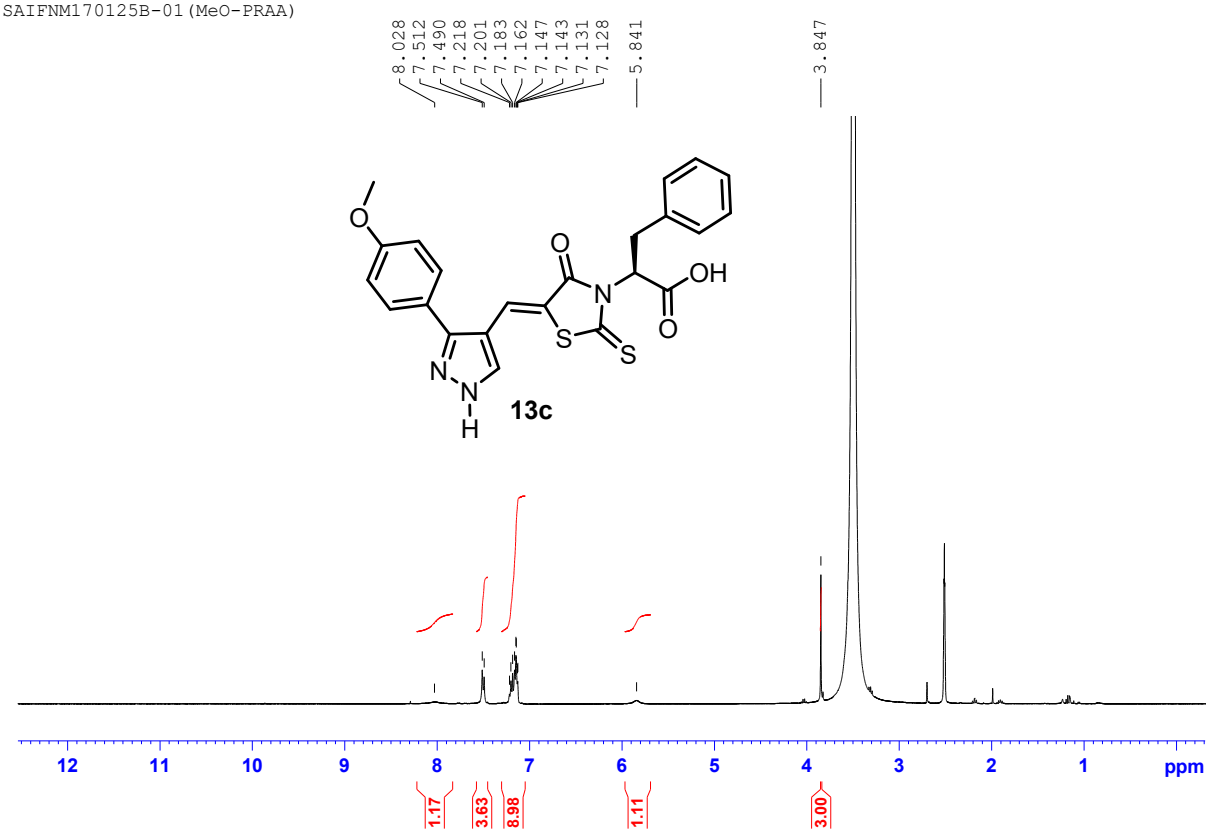


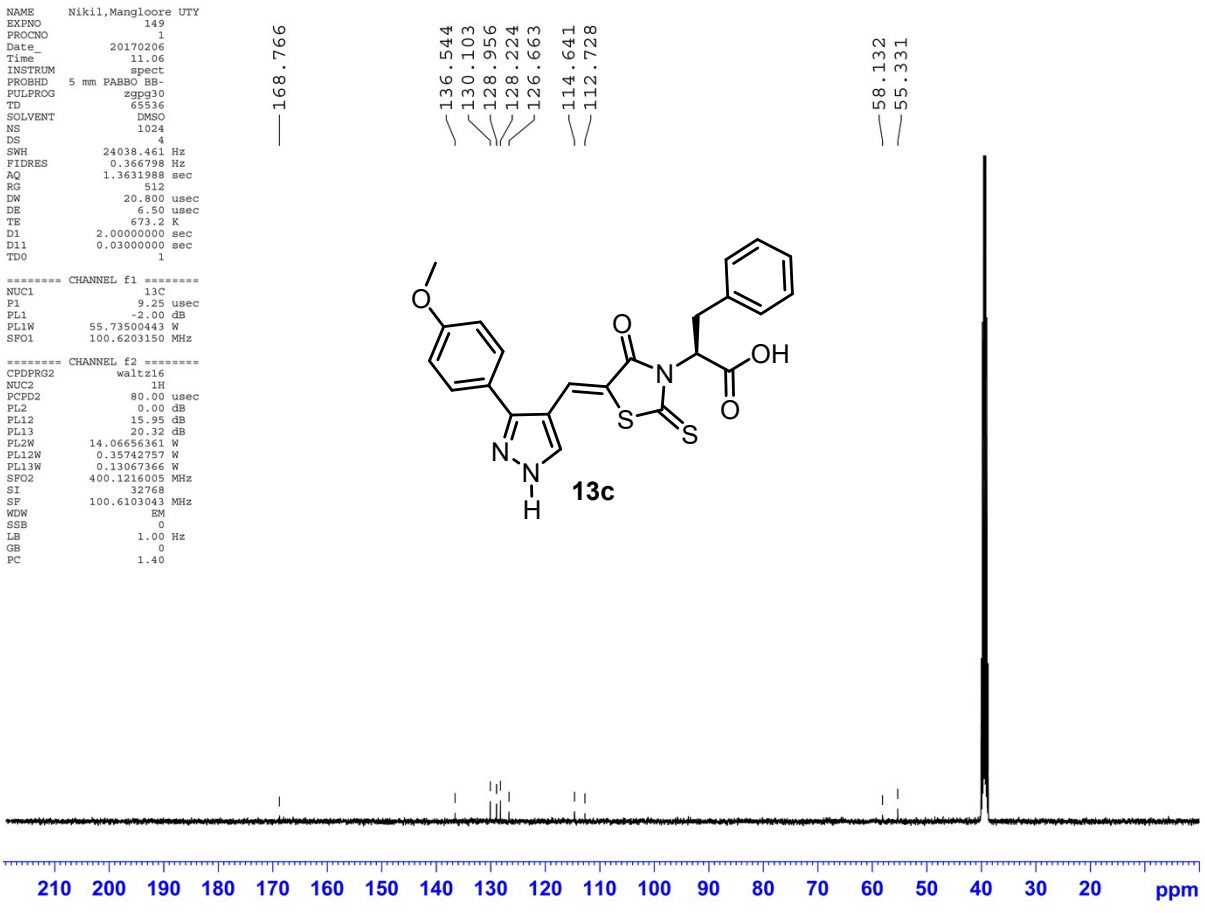
SAIFNM170420A-12(MARA)




*MSD2 SPC, time=3.660 of C:\CHEM32\1\DATA\PROJECT\160217-1 2017-03-15 19-43-37\MARA-1-VE.D ES-API, Neg, Sc
100
0
388.1
390.1
200
400
600
800
m/z
O
N
H
N
S
S
O
OH
O
13b

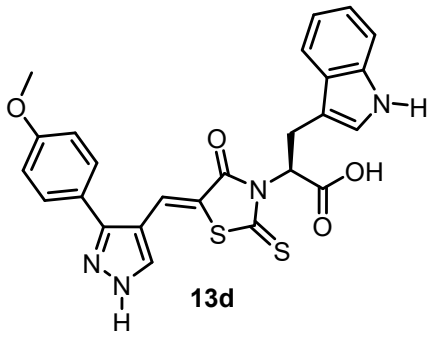
SAIFNM170125B-01(MeO-PRAA)



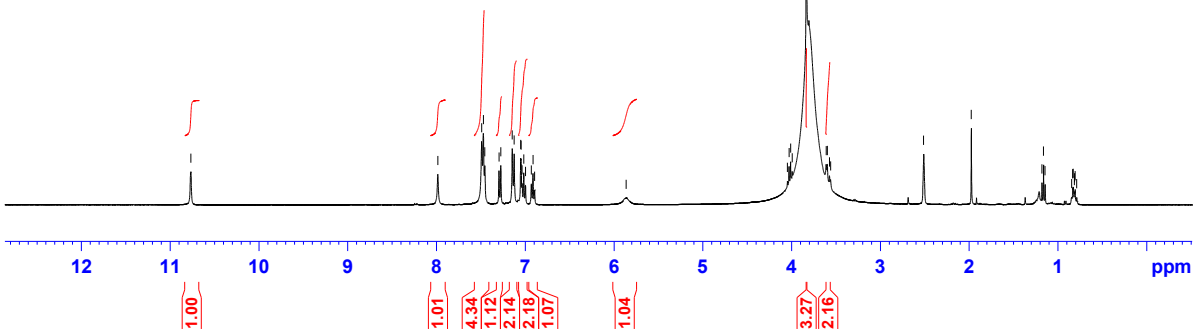


SAIFNM170420A-01(MT)

10.767
7.985
7.491
7.472
7.455
7.296
7.276
7.146
7.125
7.051
7.047
7.036
7.016
6.998
6.931
6.913
6.894
5.864
4.046
4.028
4.011
3.993
3.610
3.597
3.573
3.560
2.513
1.976
1.181
1.163
1.145
0.845
0.833
0.828
0.815
0.812
0.807
0.789



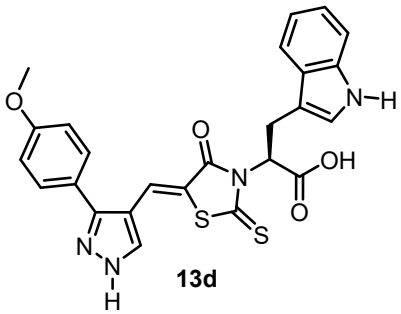
13d



1.00 1.01 4.34 1.12 2.14 2.18 1.07 1.04 3.27 2.16

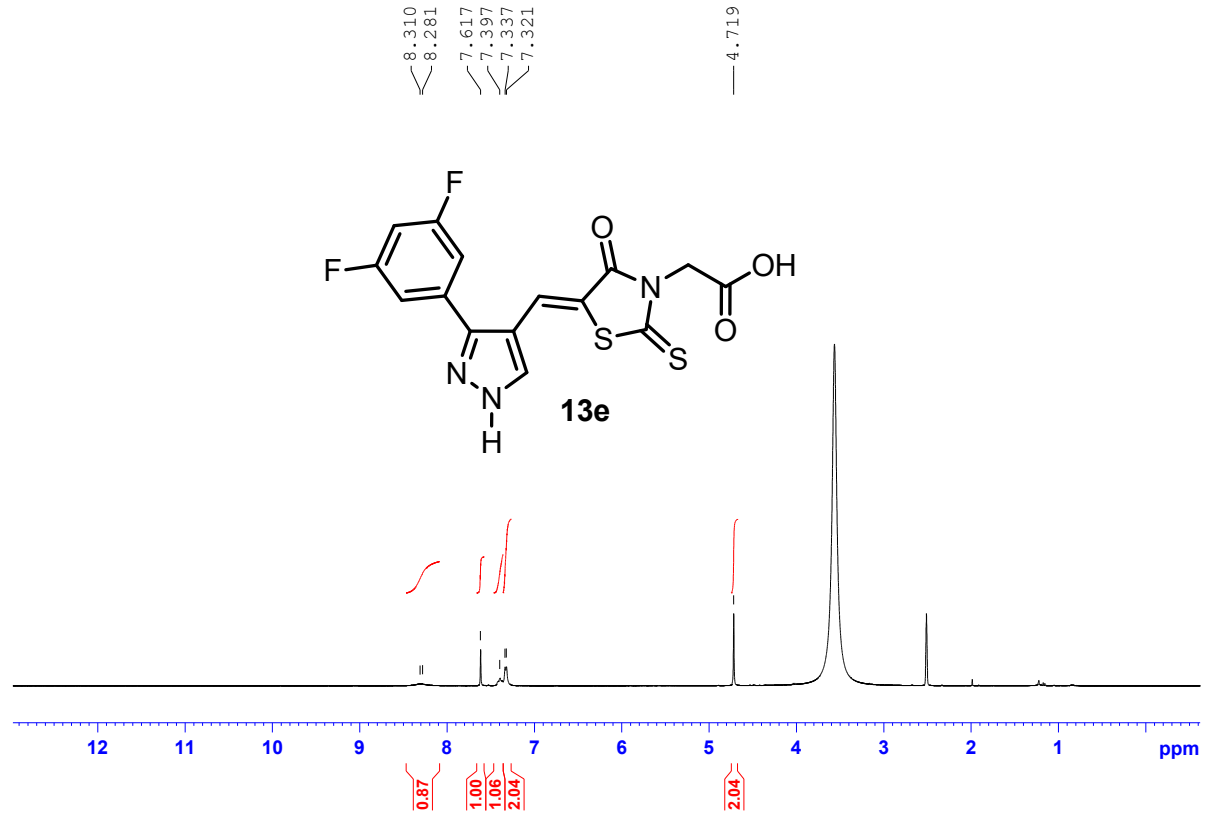
SAIFNM170420A-02(MT)

192.15
169.07
166.30
160.12
135.92
130.06
127.07
125.16
123.68
120.94
118.39
117.82
117.16
114.62
112.73
111.34
108.98
58.03
55.30
23.02

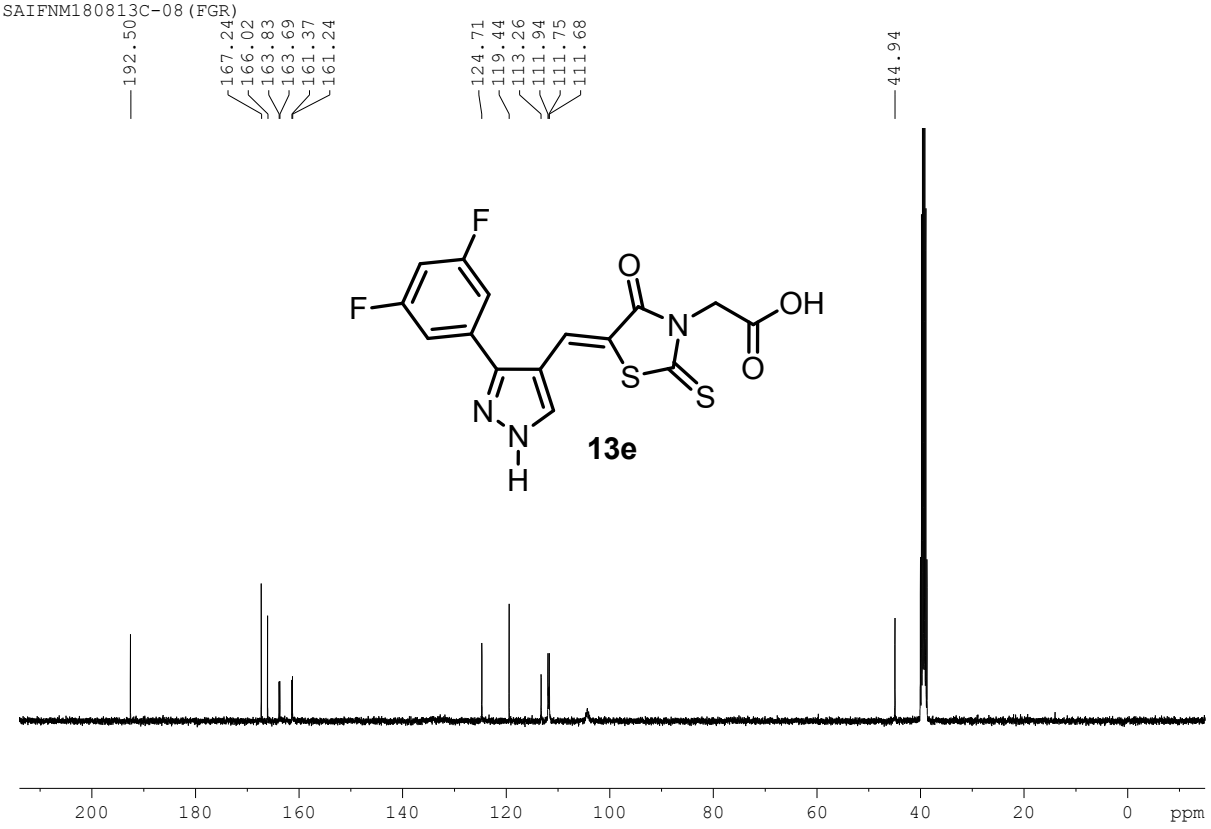


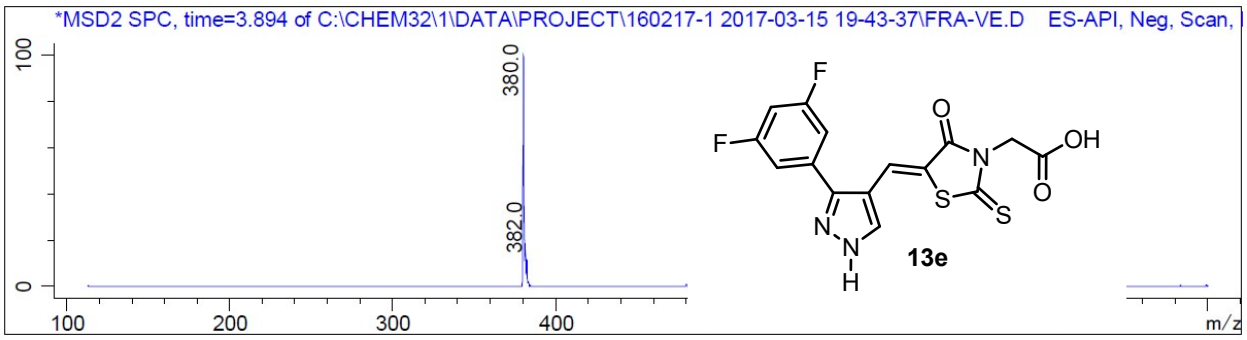
13d

SAIFNM180813C-07(FGR)

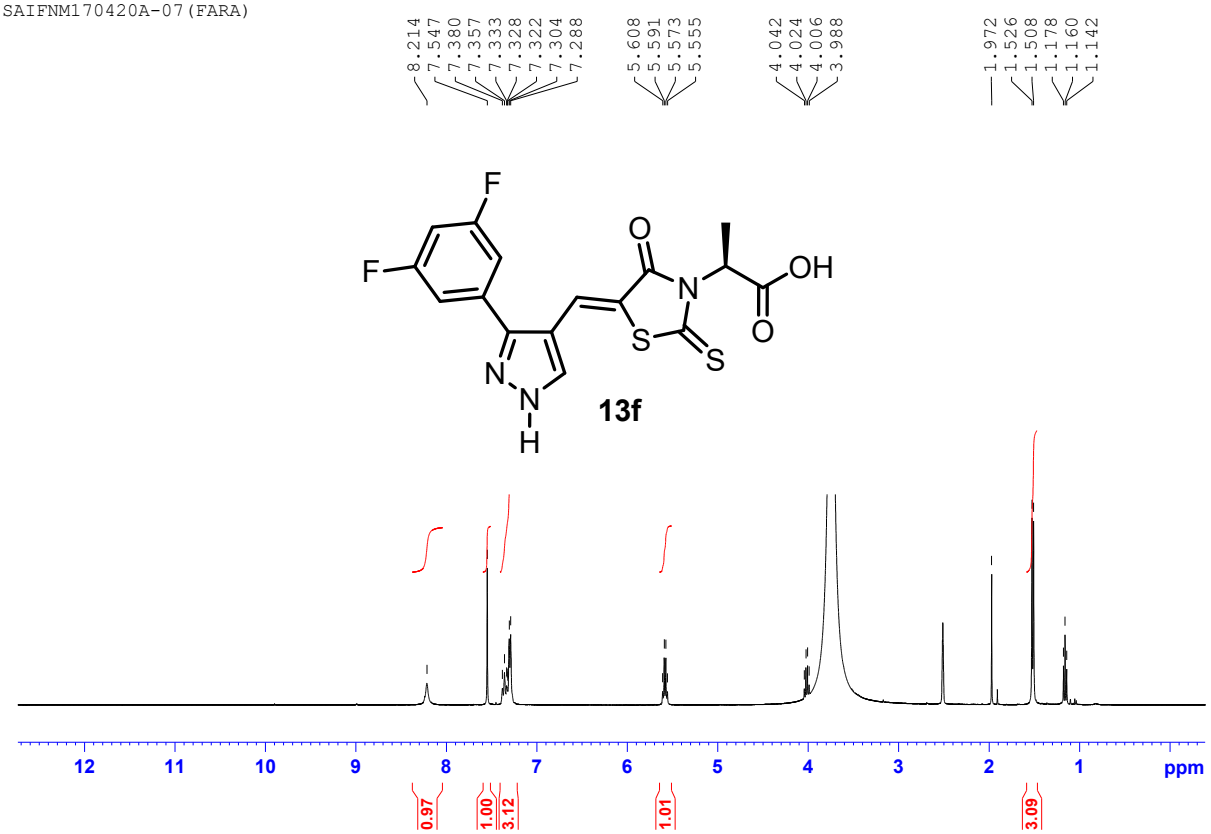


SAIFNM180813C-08(FGR)

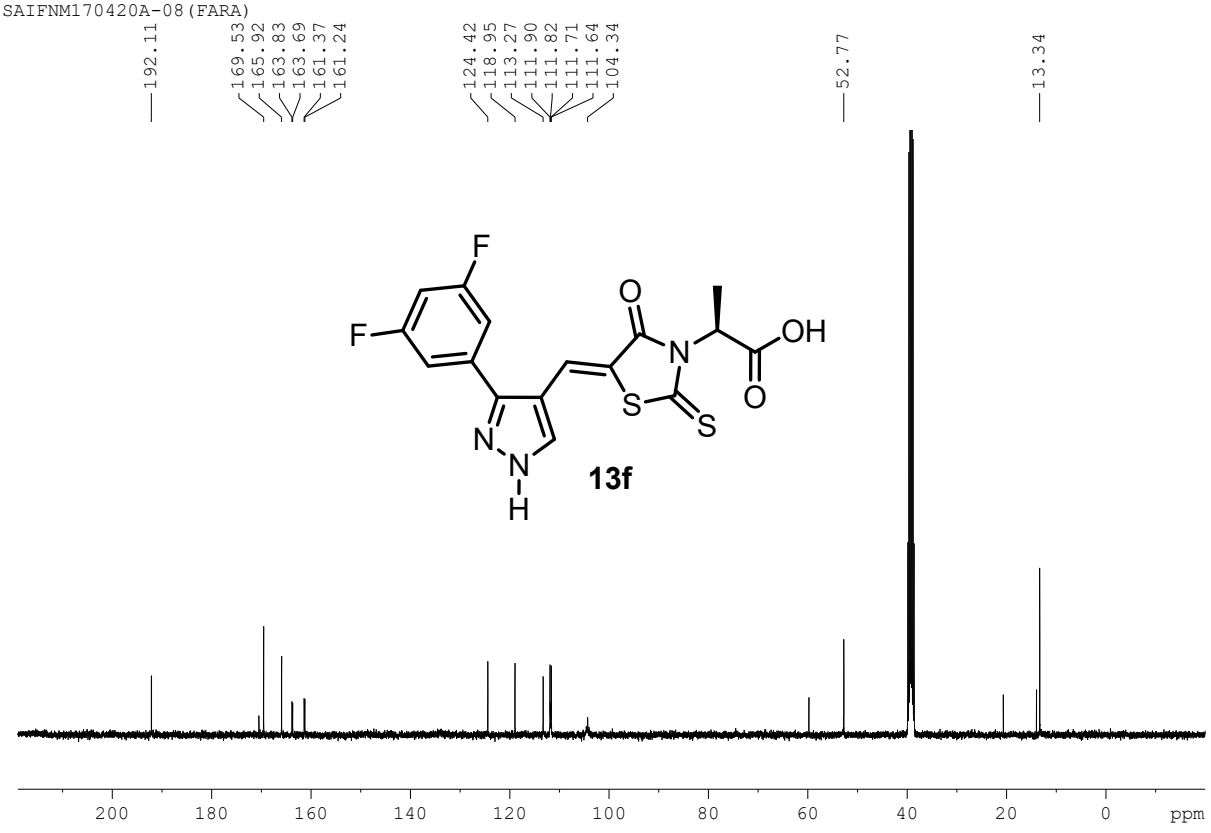


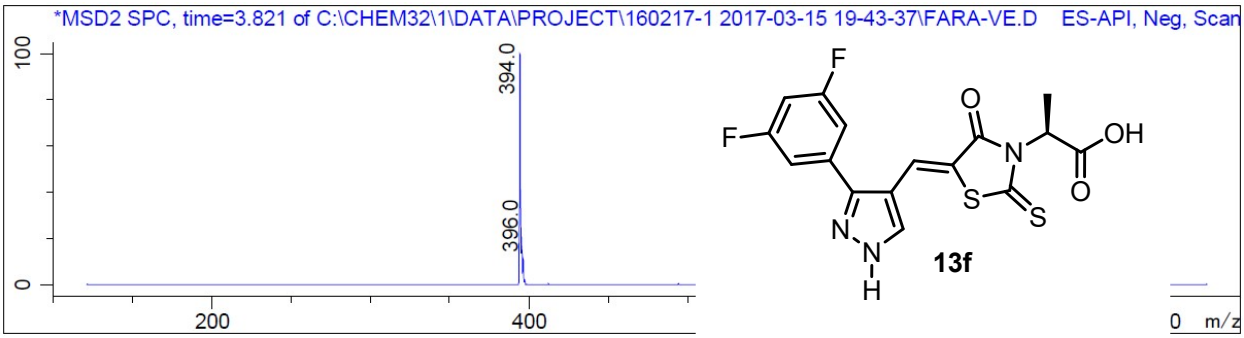

*MSD2 SPC, time=3.894 of C:\CHEM32\1\DATA\PROJECT\160217-1 2017-03-15 19-43-37\FRA-VE.D ES-API, Neg, Scan,
100
0
380.0
382.0
100
200
300
400
m/z
F
F
O
N
OH
O
S
S
N
N
H
13e

SAIFNM170420A-07(FARA)

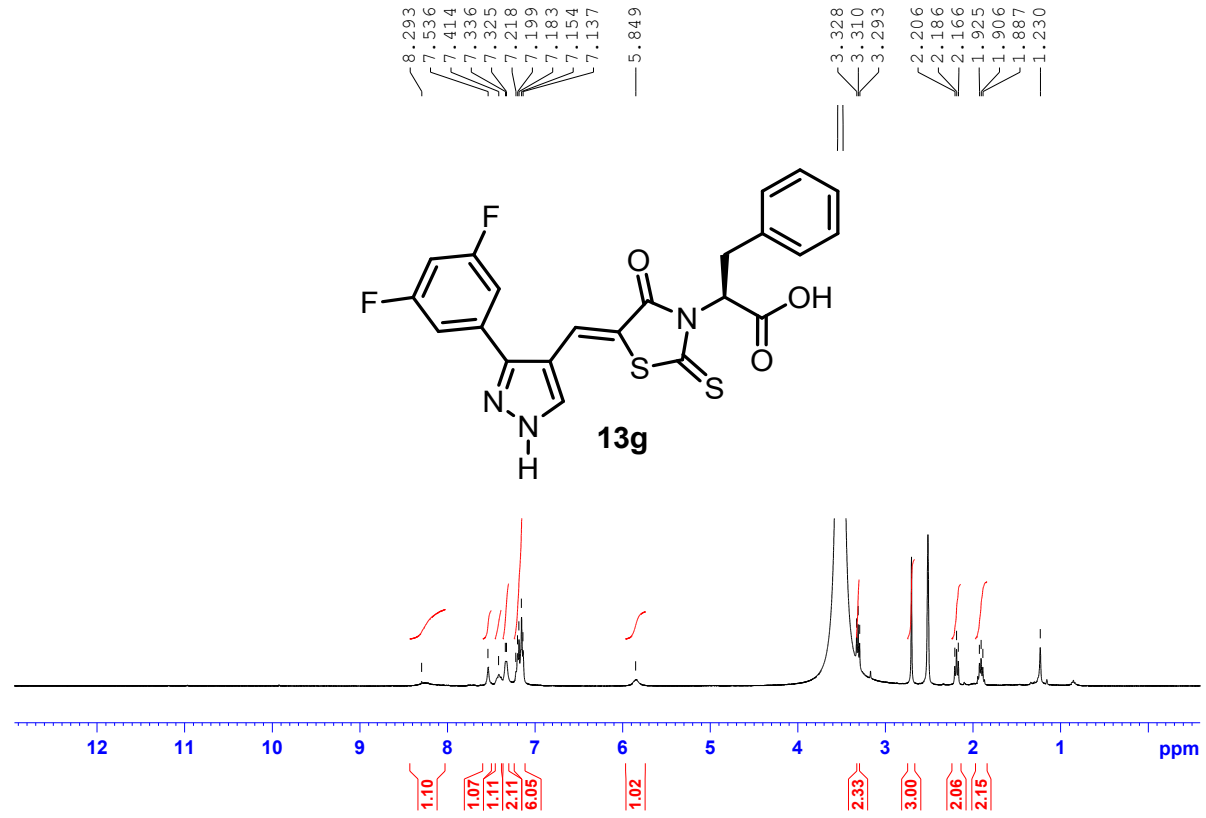


SAIFNM170420A-08(FARA)

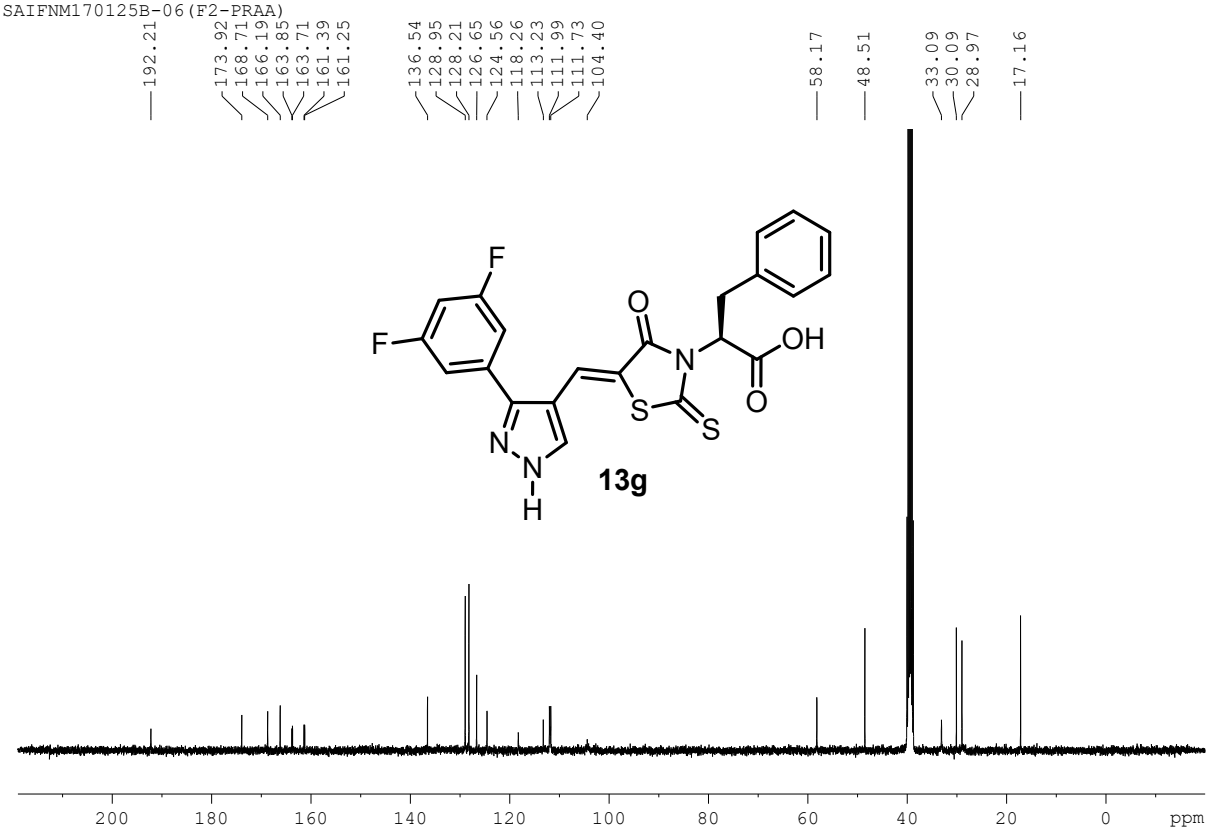



*MSD2 SPC, time=3.821 of C:\CHEM32\1\DATA\PROJECT\160217-1 2017-03-15 19-43-37\FARA-VE.D ES-API, Neg, Scan
100
0
394.0
396.0
200
400
F
F
O
N
OH
O
S
S
N
N
H
13f
0 m/z

SAIFNM170125B-05(F2-PRAA)

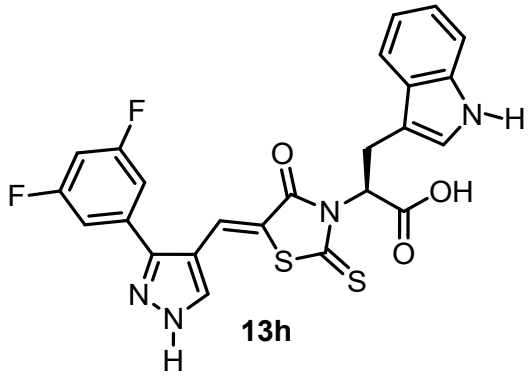


SAIFNM170125B-06(F2-PRAA)

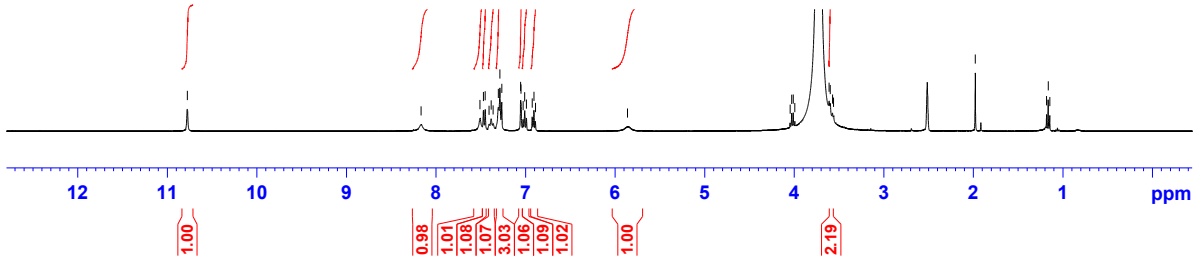


SAIFNM170420A-03(FT)

10.774
8.165
7.507
7.468
7.449
7.405
7.382
7.359
7.302
7.285
7.264
7.053
7.048
7.026
7.007
6.989
6.924
6.904
6.887
5.859
4.045
4.027
4.009
3.991
3.608
3.596
3.571
3.559
1.976
1.180
1.162
1.145



13h

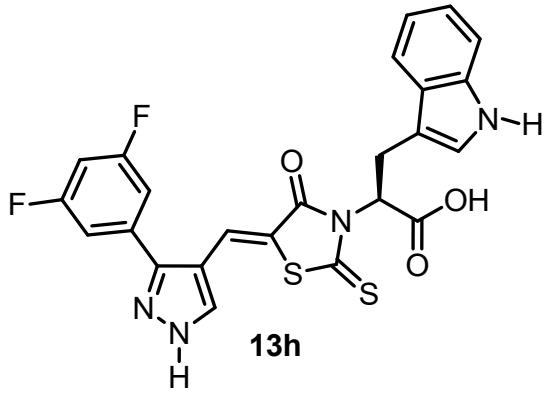


12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.00 0.98 1.01 1.08 1.07 3.03 1.06 1.09 1.02 1.00 2.19

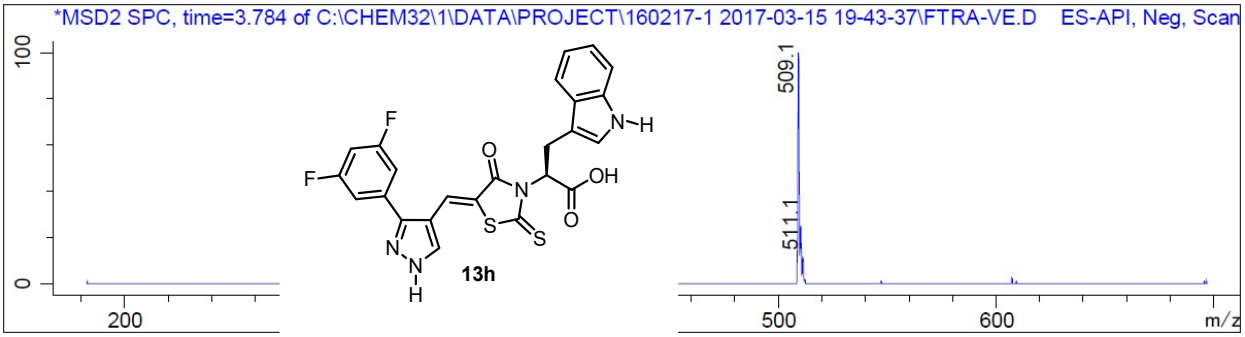
SAIFNM170420A-04(FT)

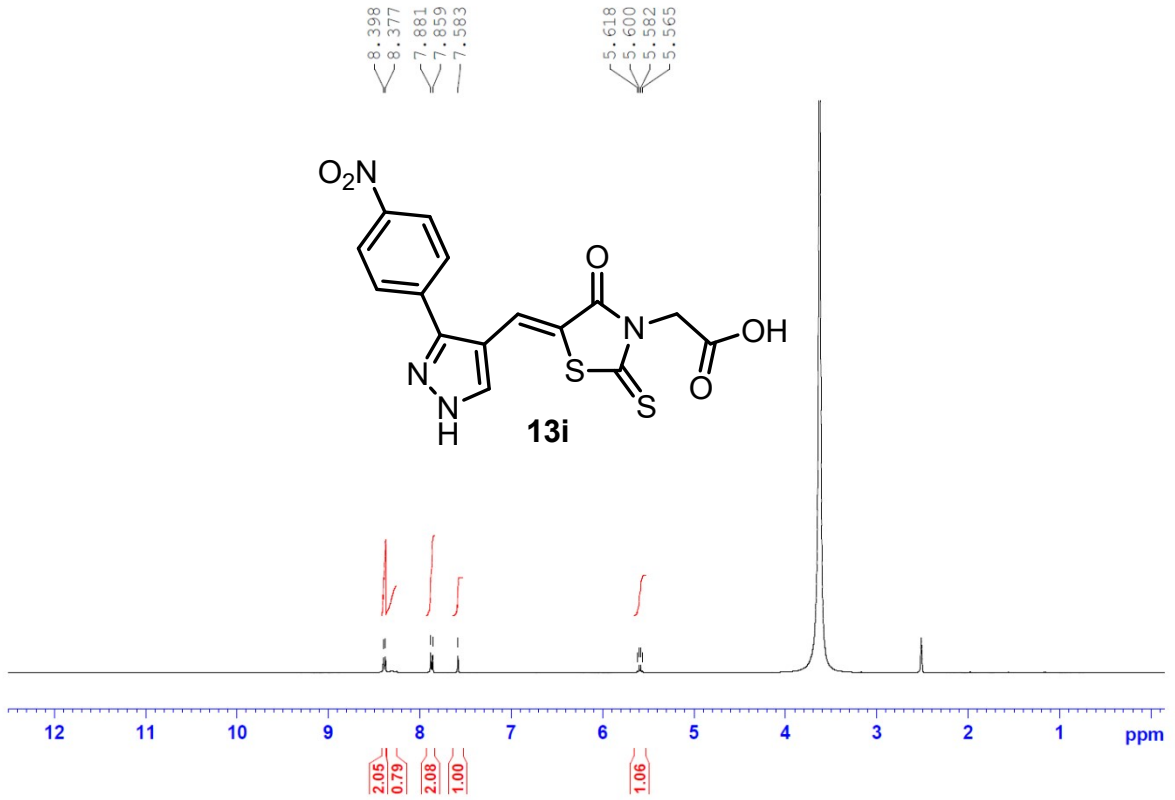
192.15
169.01
166.20
163.84
163.71
161.39
161.25
135.91
127.04
124.25
123.70
120.93
118.62
118.38
117.79
113.22
111.93
111.86
111.67
111.34
108.95
104.37
58.07
23.01

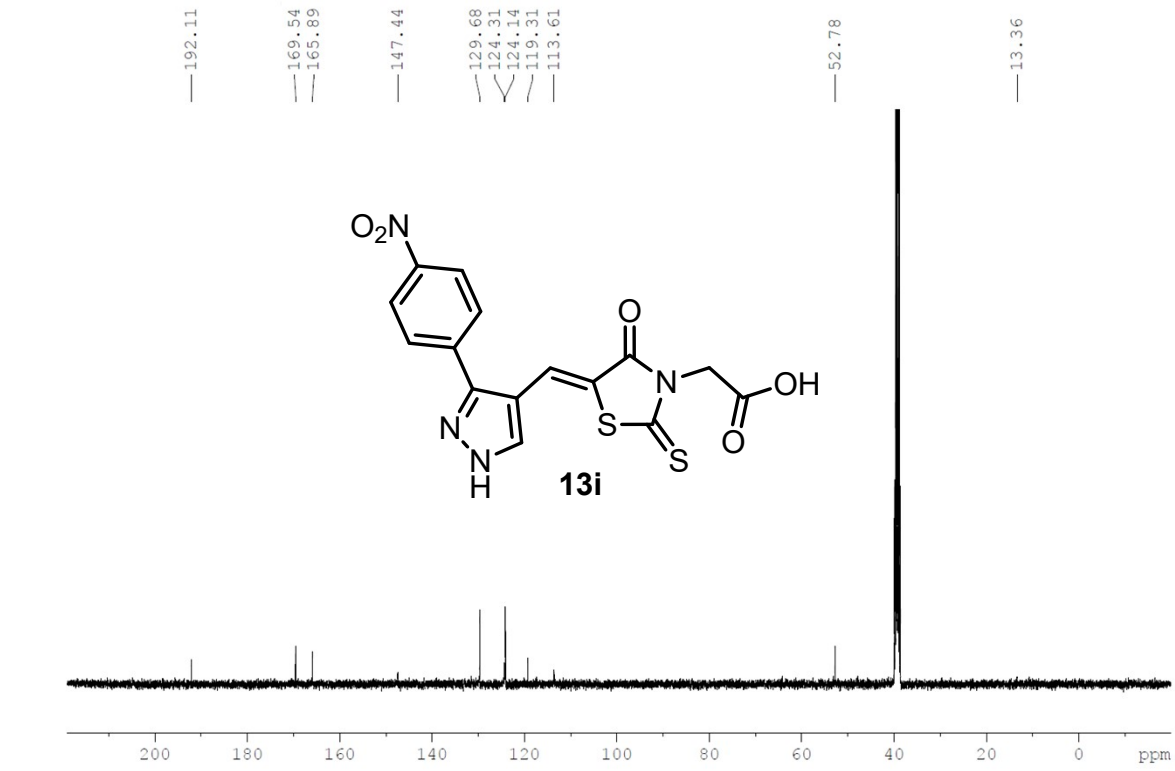


13h

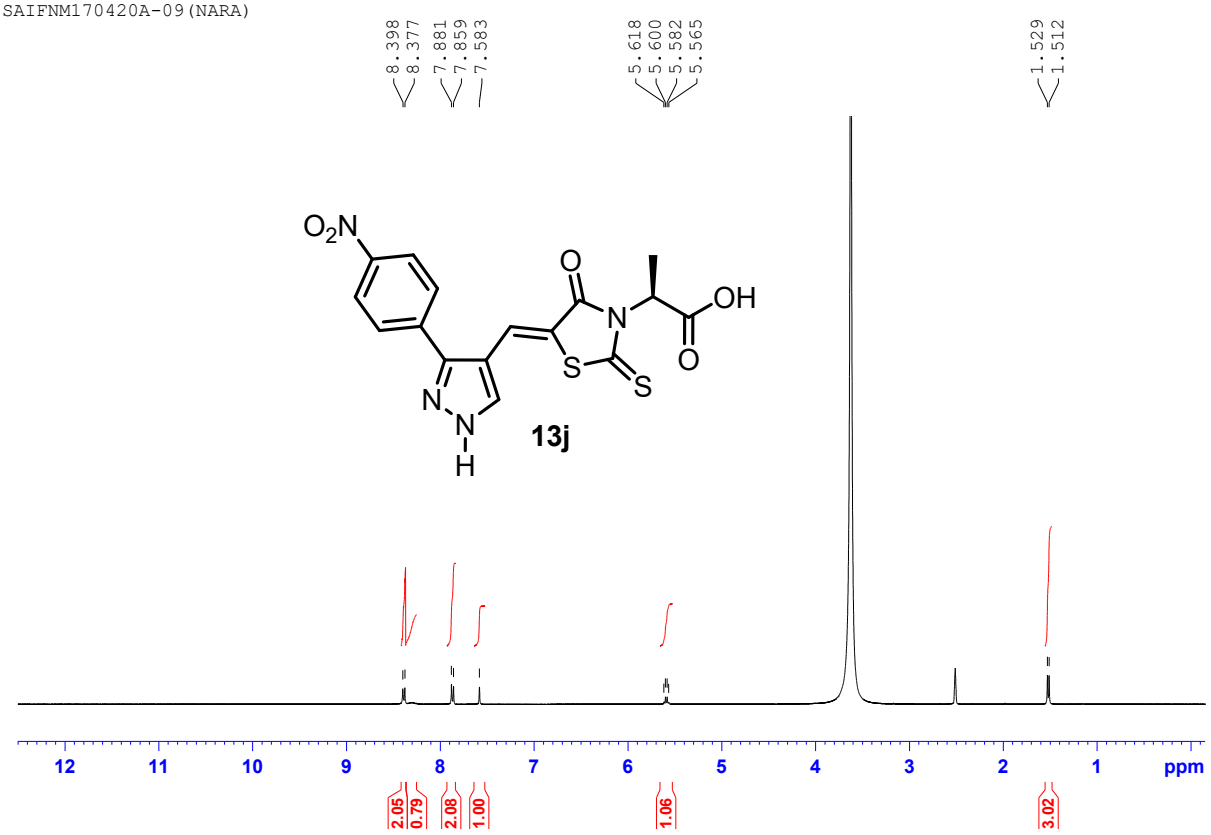
200 180 160 140 120 100 80 60 40 20 0 ppm


*MSD2 SPC, time=3.784 of C:\CHEM32\1\DATA\PROJECT\160217-1 2017-03-15 19-43-37\FTRA-VE.D ES-API, Neg, Scan
100
0
200
F
F
O
N
S
S
OH
O
N
H
N
N
H
13h
509.1
511.1
500
600
m/z

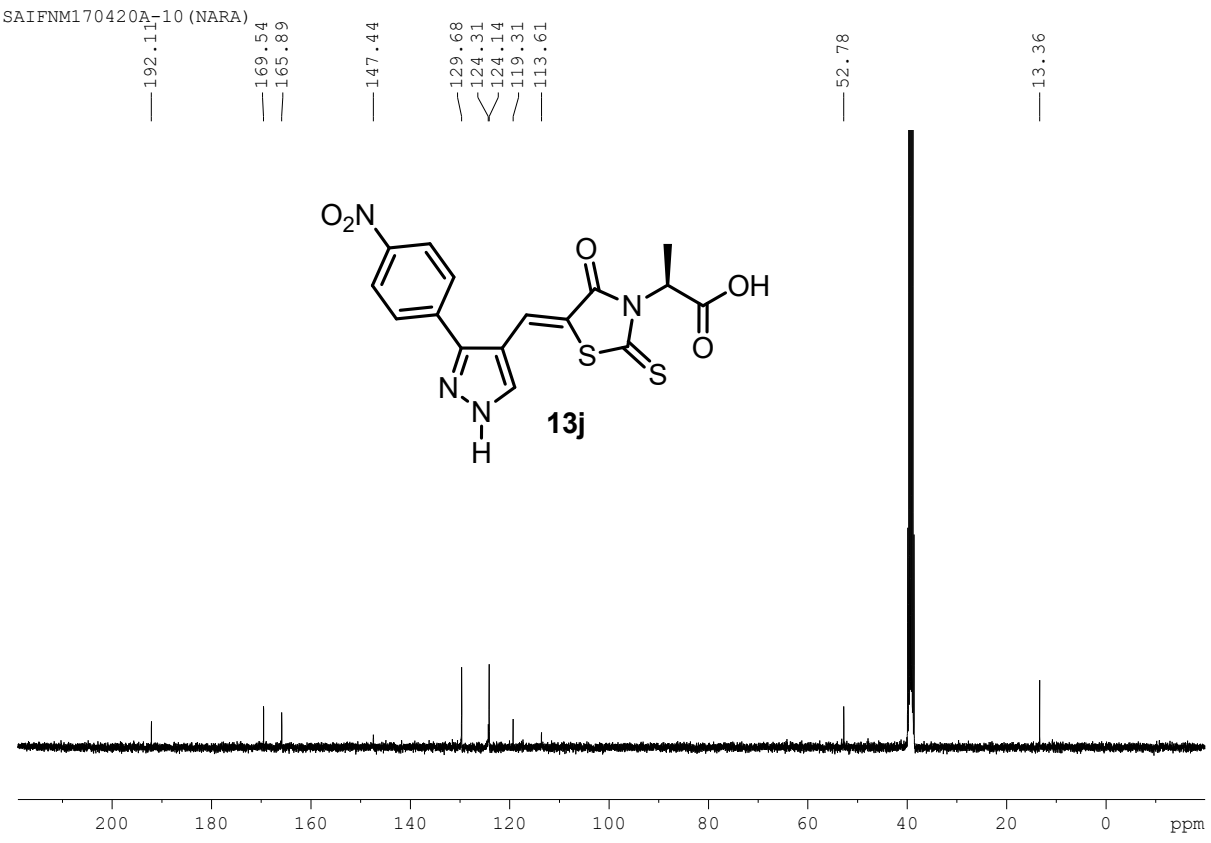

8.398
8.377
7.881
7.859
7.583
5.618
5.600
5.582
5.565
O2N
O
N
OH
S
O
N
N
H
S
13i
12
11
10
9
8
7
6
5
4
3
2
1
ppm
2.05
0.79
2.08
1.00
1.06


192.11
169.54
165.89
147.44
129.68
124.31
124.14
119.31
113.61
52.78
13.36
O2N
O
N
OH
S
O
N
N
H
S
13i
200
180
160
140
120
100
80
60
40
20
0
ppm

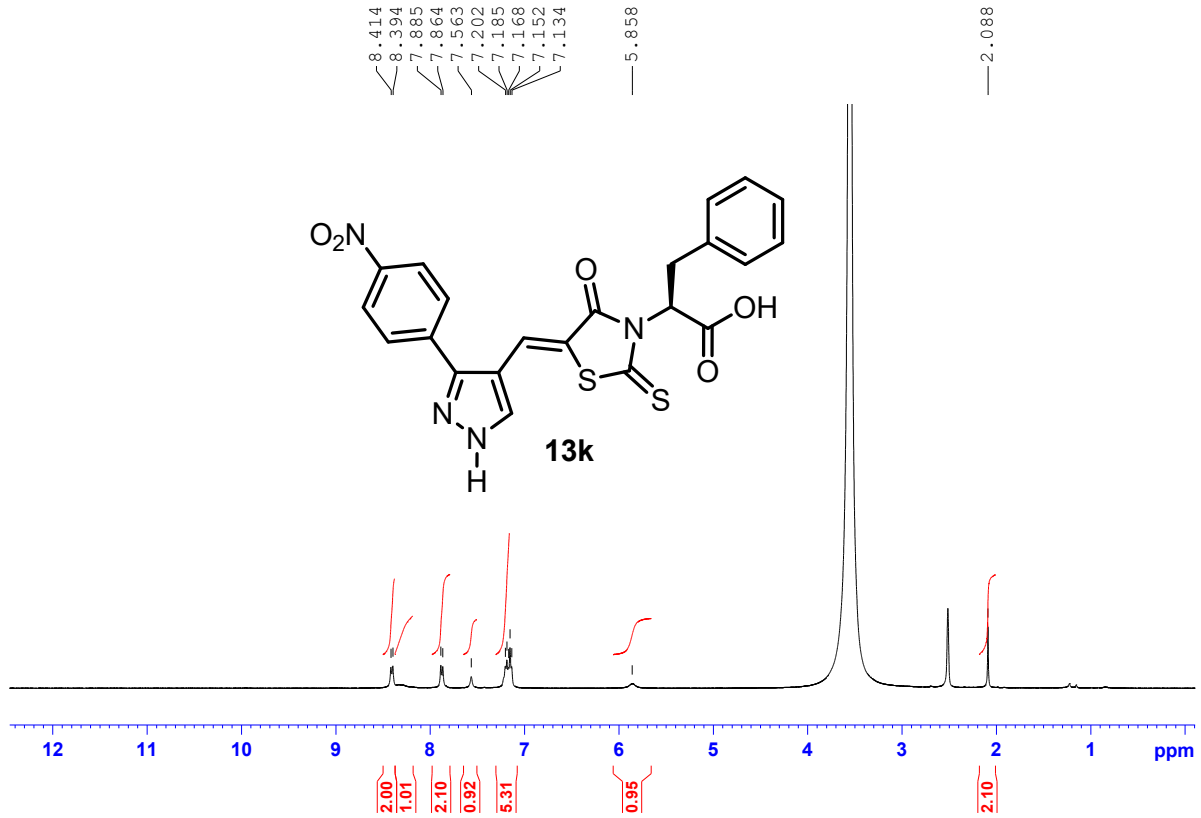
SAIFNM170420A-09(NARA)



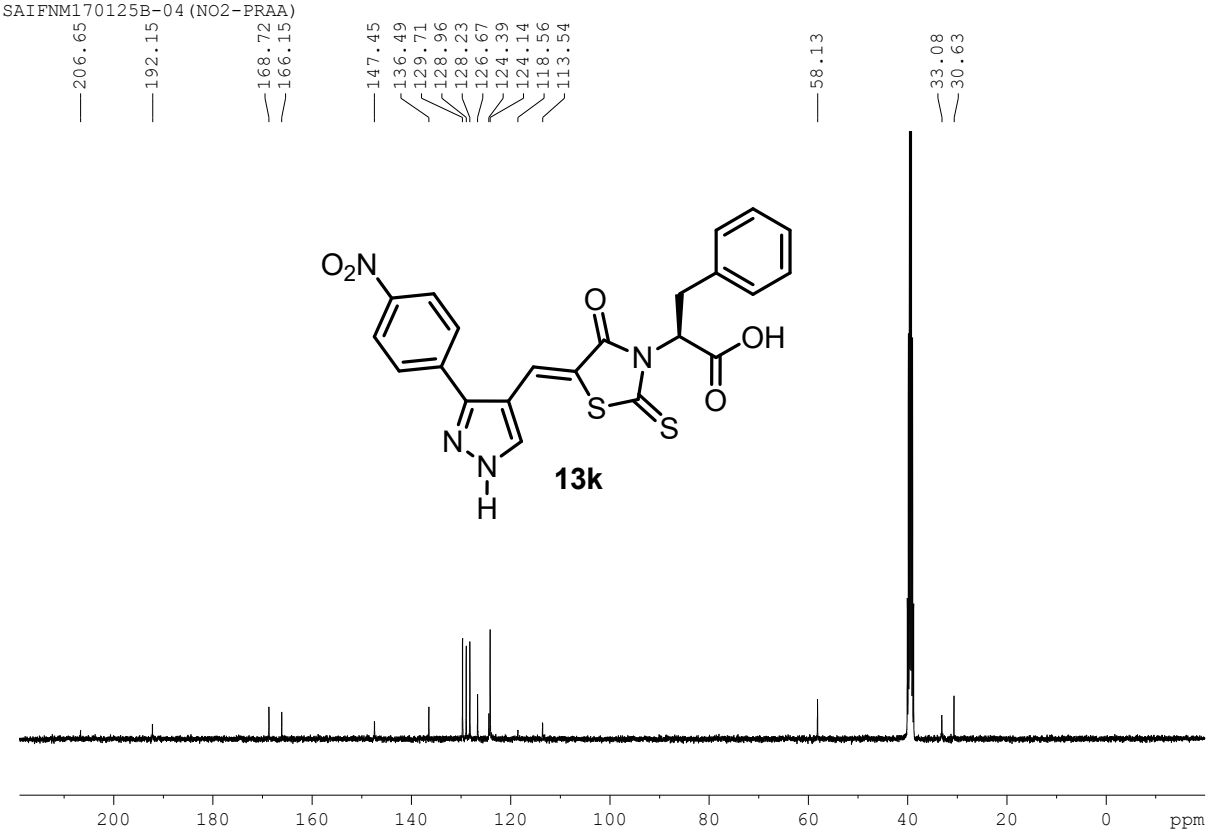
SAIFNM170420A-10(NARA)



SAIFNM170125B-03(NO2-PRAA)



SAIFNM170125B-04(NO2-PRAA)



SAIFNM180212A-13(NTRA)