Electronic Supplementary Information

Highly Enantioselective Organocatalytic Strecker Reaction of Cyclic *N*-Acyl Trifluoromethylketimines: Synthesis of Anti-HIV Drug DPC 083

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1. General information:

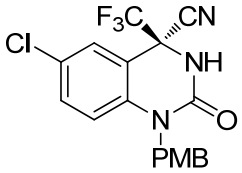
^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker AV 400 MHz spectrometer at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR), as well as 376 MHz (^{19}F NMR). Chemical shifts were reported in parts per million (ppm) from the solvent resonance as the internal standard ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; d_6-DMSO: δ_H = 2.50 ppm, δ_C = 39.52 ppm; CD_3OD, δ_H = 3.31 ppm). High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF-QII Instrument. IR spectra were recorded on an AVATAR 360 FT-IR spectrometer. High Pressure Liquid chromatography (HPLC) analyses were carried out on a Hewlett Packard Model HP 1200 instrument. Melting points (MP) were measured on a WRS-1A digital melting point apparatus and are uncorrected. Optical rotations were determined using an Autopol IV automatic polarimeter.

Materials:

Tetrahydrofuran (THF), diethyl ether and toluene were distilled from sodium / benzophenone prior to use; CH_2Cl_2 were distilled from CaH_2; CH_3OH were distilled from sodium; CH_3CN were distilled from P_2O_5. All purchased reagents were used without further purification. Analytical thin layer chromatography was performed on 0.20 mm Qingdao Haiyang silica gel plates. Silica gel (200-300 mesh) (from Qingdao Haiyang Chem. Company, Ltd.) was used for flash chromatography. Ketimines **1a** – **1l** were synthesized according to the known procedures.[1] Thioureas **2a** – **2d** were synthesized in our laboratory as before.[2] Thioureas **2f** – **2i** were synthesized according to the literatures.[3] TMSCN was purchased from ACROS Organics. Standard reagents and solvents were purified according to known procedures.

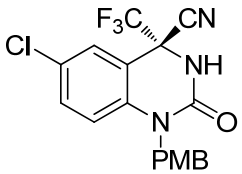
2. General procedure for the asymmetric strecker reactions

To the reaction mixture of trifluoromethyl ketimines **1** (0.1 mmol) and catalyst (**2g** or **2i**, 0.001 mmol) in toluene (2 mL) at 0 °C was added TMSCN (0.2 mmol). The resulting mixture was then stirred at 0 °C until reaction completed (detected by TLC). Purification by column chromatography on silica gel (petroleum ether / ethyl acetate = 10:1) afforded the product **3** or *ent*-**3**.

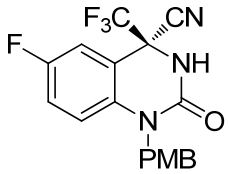


(*R*)-6-chloro-1-(4-methoxybenzyl)-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3a)

40 mg, white solid, mp 122–124 °C, 99% yield, 96% ee, $[\alpha]_D^{25}$ –23.4 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.56 (s, 1H), 7.34 (d, *J* = 8.8 Hz, 1H), 7.17 (d, *J* = 8.3 Hz, 2H), 6.92 (d, *J* = 8.9 Hz, 1H), 6.86 (d, *J* = 8.3 Hz, 2H), 5.20 (d, *J* = 16.3 Hz, 1H), 5.04 (d, *J* = 16.3 Hz, 1H), 3.78 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –80.71 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.3, 151.4, 136.3, 132.5, 129.0, 128.1, 127.9, 127.4, 122.1 (q, $^1J_{F\text{-}C}$ = 288.1 Hz), 117.1, 114.6, 113.4, 111.9, 59.4 (q, $^2J_{F\text{-}C}$ = 34.8 Hz), 55.4, 46.0. **HRMS** (ESI) found: m/z 418.0546 $[M+Na]^+$; calcd. for $C_{18}H_{13}ClF_3N_3O_2$+Na 418.0648; **IR** (KBr): ν 3208, 3092, 2937, 1688, 1514, 1429, 1388, 1250, 1193, 1026, 809, 743, 509 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / ^{i}PrOH (IPA) = 80:20, 1.0 mL / min, 254 nm) t_R (major) = 26.1 min, t_R (minor) = 6.5 min.

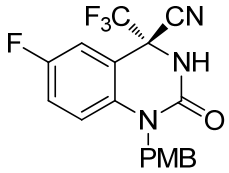


(*S*)-**3a**, 40 mg, white solid, mp 130–132 °C, 99% yield, 95% ee, $[\alpha]_D^{25}$ +22.4 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 1.0 mL / min, 254 nm) t_R (major) = 6.5 min, t_R (minor) = 27.0 min.

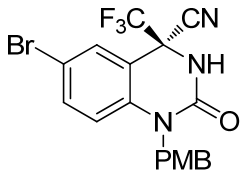


(*R*)-6-fluoro-1-(4-methoxybenzyl)-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3b)

38 mg, white solid, mp 128–130 °C, 99% yield, 96% ee, $[\alpha]_D^{25}$ –16.0 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.32 (d, *J* = 6.8 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.13 – 7.08 (m, 1H), 6.96 (dd, *J* = 9.1, 4.3 Hz, 1H), 6.87 (d, *J* = 8.5 Hz, 2H), 5.21 (d, *J* = 16.3 Hz, 1H), 5.06 (d, *J* = 16.3 Hz, 1H), 3.78 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –80.64 (s, 3F), –118.15 ~ –118.20 (m, 1F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.3, 158.3 (d, $^1J_{F\text{-}C}$ = 244.4 Hz), 151.8, 134.0, 128.0, 127.6, 122.1 (q, $^1J_{F\text{-}C}$ = 287.9 Hz), 119.4 (d, $^2J_{F\text{-}C}$ = 22.3 Hz), 117.3 (d, $^3J_{F\text{-}C}$ = 7.6 Hz), 115.3 (d, $^2J_{F\text{-}C}$ = 25.1 Hz), 114.6, 113.4, 111.7 (d, $^3J_{F\text{-}C}$ = 7.6 Hz), 59.5 (q, $^2J_{F\text{-}C}$ = 34.2 Hz), 55.4, 46.1. **HRMS** (ESI) found: m/z 378.1111 $[M]^-$; calcd. for $C_{18}H_{13}F_4N_3O_2$–H 378.0944; **IR** (KBr): ν 3209, 3088, 2931, 1689, 1518, 1447, 1394, 1250, 1195, 1027, 868, 744, 622, 516 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 75:25, 0.8 mL / min, 254 nm) t_R (major) = 27.0 min, t_R (minor) = 7.8 min.

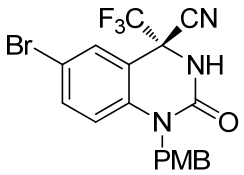


(*S*)-**3b**, 36 mg, white solid, mp 142–144 °C, 96% yield, 95% ee, $[\alpha]_D^{25}$ +18.2 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 75:25, 0.8 mL / min, 254 nm) t_R (major) = 7.9 min, t_R (minor) = 29.5 min.

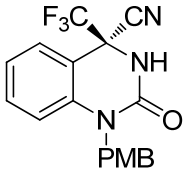


(*R*)-6-bromo-1-(4-methoxybenzyl)-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3c)

42 mg, white solid, mp 140–142 °C, 95% yield, 94% ee, $[\alpha]_D^{25}$ –28.4 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, d_6-DMSO) δ 9.90 (s, 1H), 7.70 – 7.63 (m, 2H), 7.16 (d, *J* = 8.5 Hz, 2H), 7.06 (d, *J* = 8.8 Hz, 1H), 6.87 (d, *J* = 8.5 Hz, 2H), 5.17 (d, *J* = 16.4 Hz, 1H), 4.96 (d, *J* = 16.5 Hz, 1H), 3.69 (s, 3H). **^{19}F NMR** (376 MHz, d_6-DMSO) δ –80.04 (s, 3F). **^{13}C NMR** (100 MHz, d_6-DMSO) δ 158.4, 149.9, 137.0, 135.2, 129.5, 127.8, 127.7, 121.9 (q, $^1J_{F\text{-}C}$ = 288.6 Hz), 117.8, 114.2, 114.0, 113.4, 111.4, 58.5 (q, $^2J_{F\text{-}C}$ = 33.6 Hz), 55.0, 44.1. **HRMS** (ESI) found: m/z 438.0255 $[M]^-$; calcd. for $C_{18}H_{13}BrF_3N_3O_2$–H 438.0143; **IR** (KBr): ν 3213, 3097, 2938, 1689, 1513, 1425, 1385, 1250, 1200, 1027, 808, 744, 536, 507 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 0.8 mL / min, 254 nm) t_R (major) = 22.0 min, t_R (minor) = 7.4 min.



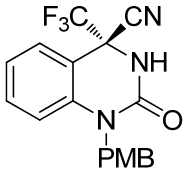
(*S*)-**3c**, 42 mg, white solid, mp 143–145 °C, 96% yield, 92% ee, $[\alpha]_D^{25}$ +31.6 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 0.8 mL / min, 254 nm) t_R (major) = 7.4 min, t_R (minor) = 22.3 min.



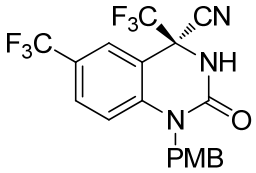
(*R*)-1-(4-methoxybenzyl)-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline -4-carbonitrile (3d)

33 mg, white solid, mp 138–140 °C, 93% yield, 95% ee, $[\alpha]_D^{25}$ –15.6 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.88 (d, *J* = 8.5 Hz, 2H), 5.24 (d, *J* = 16.2 Hz, 1H), 5.09 (d, *J* = 16.3 Hz, 1H), 3.78 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –80.86 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.1, 152.0, 137.6, 132.3, 128.2, 128.0, 127.9, 123.4, 122.3 (q, $^1J_{F\text{-}C}$ = 287.5 Hz), 115.6, 114.5, 113.9, 110.4, 59.7 (q, $^2J_{F\text{-}C}$ = 34.1 Hz), 55.3, 45.8. **HRMS** (ESI) found:

m/z 384.1024 $[M+Na]^+$; calcd. for $C_{18}H_{14}F_3N_3O_2$+Na 384.1038; **IR** (KBr): ν 3444, 3211, 3092, 2933, 1683, 1606, 1514, 1460, 1399, 1249, 1096, 1037, 826, 753, 499 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 0.8 mL / min, 254 nm) t_R (major) = 38.4 min, t_R (minor) = 11.8 min.

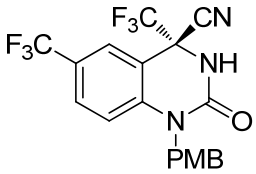


(*S*)-**3d**, 33 mg, white solid, mp 141–142 °C, 91% yield, 95% ee, $[\alpha]_D^{25}$ +17.4 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 0.8 mL / min, 254 nm) t_R (major) = 11.8 min, t_R (minor) = 39.0 min.

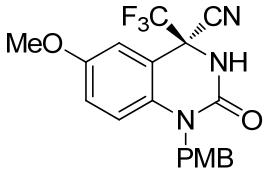


(*R*)-1-(4-methoxybenzyl)-2-oxo-4,6-bis(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3e)

40 mg, white solid, mp 128–129 °C, 94% yield, 92% ee, $[\alpha]_D^{25}$ –7.4 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 7.83 (s, 1H), 7.65 (d, *J* = 8.7 Hz, 1H), 7.20 (d, *J* = 8.5 Hz, 2H), 7.12 (d, *J* = 8.8 Hz, 1H), 6.89 (d, *J* = 8.6 Hz, 2H), 5.27 (d, *J* = 17.6 Hz, 1H), 5.11 (d, *J* = 16.3 Hz, 1H), 3.79 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –62.34 (s, 3F), –80.88 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.5, 151.7, 140.5, 129.6, 128.0, 127.0, 125.9 (q, $^2J_{F\text{-}C}$ = 33.9 Hz), 125.5, 123.3 (q, $^1J_{F\text{-}C}$ = 270.3 Hz), 122.1 (q, $^1J_{F\text{-}C}$ = 287.8 Hz), 116.2, 114.7, 113.2, 111.0, 59.5 (q, $^2J_{F\text{-}C}$ = 34.2 Hz), 55.4, 46.2. **HRMS** (ESI) found: m/z 428.1123 $[M]^-$; calcd. for $C_{19}H_{13}F_6N_3O_2$–H 428.0912; **IR** (KBr): ν 3451, 3204, 2938, 1703, 1626, 1518, 1390, 1333, 1250, 1200, 1129, 1090, 826, 749, 538 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 0.8 mL / min, 254 nm) t_R (major) = 11.1 min, t_R (minor) = 5.7 min.

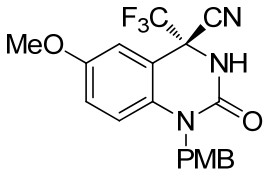


(*S*)-**3e**, 40 mg, white solid, mp 122–124 °C, 93% yield, 90% ee, $[\alpha]_D^{25}$ +10.0 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 0.8 mL / min, 254 nm) t_R (major) = 5.7 min, t_R (minor) = 11.2 min.

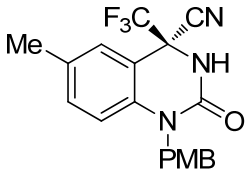


(*R*)-6-methoxy-1-(4-methoxybenzyl)-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydro quinazoline-4-carbonitrile (3f)

37 mg, white solid, mp 115–116 °C, 95% yield, 94% ee, $[\alpha]_D^{25}$ –25.0 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.19 (d, *J* = 8.5 Hz, 2H), 7.09 (s, 1H), 6.91 (s, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 5.19 (d, *J* = 16.3 Hz, 1H), 5.03 (d, *J* = 16.3 Hz, 1H), 3.79 (s, 3H), 3.77 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –80.52 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.1, 155.6, 151.7, 131.0, 129.0, 128.1, 128.0, 122.3 (q, $^1J_{F\text{-}C}$ = 287.7 Hz), 118.0, 116.9, 114.5, 113.4, 111.3, 59.8 (q, $^2J_{F\text{-}C}$ = 34.0 Hz), 55.9, 55.4, 45.8. **HRMS** (ESI) found: m/z 414.1082 $[M+Na]^+$; calcd. for $C_{19}H_{16}F_3N_3O_3$+Na 414.1144; **IR** (KBr): ν 3210, 3092, 2943, 1727, 1682, 1517, 1459, 1392, 1253, 1196, 1022, 748, 623, 507 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 1.0 mL / min, 254 nm) t_R (major) = 40.3 min, t_R (minor) = 8.6 min.

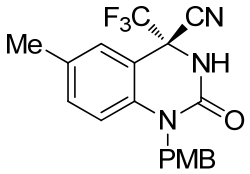


(*S*)-**3f**, 36 mg, white solid, mp 115–117 °C, 93% yield, 97% ee, $[\alpha]_D^{25}$ +26.6 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 1.0 mL / min, 254 nm) t_R (major) = 8.8 min, t_R (minor) = 46.1 min.

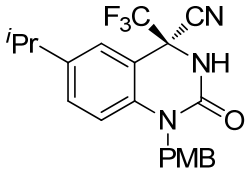


(*R*)-1-(4-methoxybenzyl)-6-methyl-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3g)

36 mg, white solid, mp 128–130 °C, 96% yield, 94% ee, $[\alpha]_D^{25}$ –18.8 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.38 (s, 1H), 7.19 (t, *J* = 10.0 Hz, 3H), 6.88 (t, *J* = 7.3 Hz, 3H), 5.21 (d, *J* = 16.2 Hz, 1H), 5.05 (d, *J* = 16.2 Hz, 1H), 3.77 (s, 3H), 2.33 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –80.78 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.1, 151.9, 135.2, 133.4, 132.9, 128.5, 128.1, 128.0, 122.3 (q, $^1J_{F\text{-}C}$ = 287.5 Hz), 115.6, 114.4, 114.0, 110.2, 59.8 (q, $^2J_{F\text{-}C}$ = 34.2 Hz), 55.4, 45.7, 20.5. **HRMS** (ESI) found: m/z 398.1046 $[M+Na]^+$; calcd. for $C_{19}H_{16}F_3N_3O_2$+Na 398.1195; **IR** (KBr): ν 3203, 3079, 2931, 1679, 1517, 1397, 1248, 1187, 1024, 804, 742, 623, 511, 438 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 0.8 mL / min, 254 nm) t_R (major) = 28.2 min, t_R (minor) = 9.8 min.

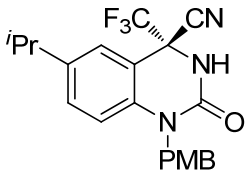


(*S*)-**3g**, 35 mg, white solid, mp 130–131 °C, 93% yield, 94% ee, $[\alpha]_D^{25}$ +22.0 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 0.8 mL / min, 254 nm) t_R (major) = 9.8 min, t_R (minor) = 28.4 min.

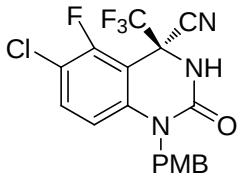


(*R*)-6-isopropyl-1-(4-methoxybenzyl)-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3h)

38 mg, white solid, mp 152–153 °C, 96% yield, 94% ee, $[\alpha]_D^{25}$ –26.0 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.40 (s, 1H), 7.25 (d, *J* = 1.5 Hz, 1H), 7.21 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.6 Hz, 1H), 6.87 (d, *J* = 8.6 Hz, 2H), 5.19 (d, *J* = 16.2 Hz, 1H), 5.06 (d, *J* = 16.2 Hz, 1H), 3.78 (s, 3H), 2.94 – 2.87(m, 1H), 1.24 (s, 3H), 1.22 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –80.90 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.2, 151.7, 144.4, 135.5, 130.3, 128.2, 128.0, 126.2, 122.3 (q, $^1J_{F\text{-}C}$ = 287.6 Hz), 115.6, 114.5, 114.0, 110.1, 59.9 (q, $^2J_{F\text{-}C}$ = 34.0 Hz), 55.4, 45.8, 33.4, 23.9, 23.8. **HRMS** (ESI) found: m/z 426.1382 $[M+Na]^+$; calcd. for $C_{21}H_{20}F_3N_3O_2$+Na 426.1508; **IR** (KBr): ν 3213, 3088, 2959, 1686, 1517, 1445, 1395, 1246, 1196, 1038, 820, 619, 442 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 1.0 mL / min, 254 nm) t_R (major) = 12.3 min, t_R (minor) = 6.4 min.



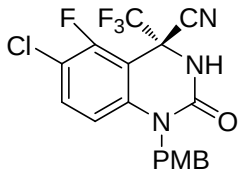
(*S*)-**3h**, 38 mg, white solid, mp 132–134 °C, 95% yield, 96% ee, $[\alpha]_D^{25}$ +22.8 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 1.0 mL / min, 254 nm) t_R (major) = 6.6 min, t_R (minor) = 13.3 min.



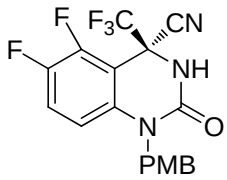
(*R*)-6-chloro-5-fluoro-1-(4-methoxybenzyl)-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3i)

40 mg, white solid, mp 140–142 °C, 98% yield, 96% ee, $[\alpha]_D^{25}$ –20.4 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, d_6-DMSO) δ 10.11 (s, 1H), 7.72 (d, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 8.5 Hz, 2H), 6.97 (d, *J* = 9.2 Hz, 1H), 6.88 (d, *J* = 8.5 Hz, 2H), 5.19 (d, *J* = 16.5 Hz, 1H), 4.98 (d, *J* = 16.5 Hz, 1H), 3.70 (s, 3H). **^{19}F NMR** (376 MHz, d_6-DMSO) δ –80.29 (d, *J* = 15.4 Hz, 3F), –111.92 ~ –111.97 (m, 1F). **^{13}C NMR** (100 MHz,

d_6-DMSO) δ 166.9, 158.5, 154.0 (d, $^1J_{F-C}$ = 250.2 Hz), 134.0, 131.4, 128.6, 127.7, 122.0 (q, $^1J_{F-C}$ = 288.7 Hz), 114.1, 113.7 (d, $^2J_{F-C}$ = 17.9 Hz), 112.6 (d, $^3J_{F-C}$ = 3.5 Hz), 111.8, 99.6 (d, $^2J_{F-C}$ = 14.9 Hz), 55.3 (q, $^2J_{F-C}$ = 34.8 Hz), 55.0, 44.4. **HRMS** (ESI) found: m/z 412.0759 $[M]^-$; calcd. for $C_{21}H_{20}F_3N_3O_2$–H 412.0554; **IR** (KBr): ν 3211, 3088, 2929, 1683, 1614, 1510, 1461, 1387, 1245, 1200, 1040, 812, 616, 507 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 75:25, 0.8 mL / min, 254 nm) t_R (major) = 64.0 min, t_R (minor) = 7.4 min.



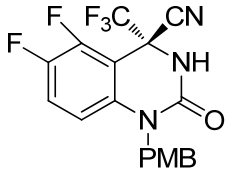
(*S*)-**3i**, 37 mg, white solid, mp 145–146 °C, 91% yield, 94% ee, $[\alpha]_D^{25}$ +21.6 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 75:25, 1.0 mL / min, 254 nm) t_R (major) = 7.4 min, t_R (minor) = 69.0 min.



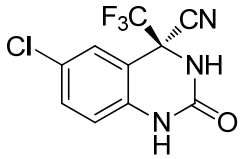
(*R*)-5,6-difluoro-1-(4-methoxybenzyl)-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3j)

38 mg, white solid, mp 174–176 °C, 96% yield, 96% ee, $[\alpha]_D^{25}$ –11.2 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, d_6-DMSO) δ 10.04 (s, 1H), 7.65 (dd, *J* = 18.7, 9.4 Hz, 1H), 7.16 (d, *J* = 8.5 Hz, 2H), 6.94 (dd, *J* = 12.1, 4.3 Hz, 1H), 6.88 (d, *J* = 8.6 Hz, 2H), 5.18 (d, *J* = 16.4 Hz, 1H), 4.97 (d, *J* = 16.5 Hz, 1H), 3.70 (s, 3H). **^{19}F NMR** (376 MHz, d_6-DMSO) δ –80.28 (d, *J* = 14.7 Hz, 3F), –135.09 ~ –135.29 (m, 1F), –144.63 ~ –144.72 (m, 1F). **^{13}C NMR** (100 MHz, d_6-DMSO) δ 158.5, 149.6, 146.8 (dd, $^1J_{F-C}$ = 250.5 Hz, $^2J_{F-C}$ = 16.2 Hz), 145.0 (dd, $^1J_{F-C}$ = 241.6 Hz, $^2J_{F-C}$ = 12.2 Hz), 134.9, 127.8, 127.7, 122.0 (q, $^1J_{F-C}$ = 289.3 Hz), 121.2 (d, $^2J_{F-C}$ = 17.7 Hz), 114.1, 111.8, 111.6 (d, $^3J_{F-C}$ = 2.8 Hz), 99.7 (d, $^2J_{F-C}$ = 11.9 Hz), 55.2 (q, $^2J_{F-C}$ = 30.1 Hz), 55.0, 44.4. **HRMS**

(ESI) found: m/z 420.0716 $[M+Na]^+$; calcd. for $C_{18}H_{12}F_5N_3O_2$+Na 420.0850; **IR** (KBr): ν 3211, 3088, 2926, 1684, 1613, 1516, 1483, 1394, 1245, 1200, 1033, 963, 811, 650, 507 cm^{-1}; **HPLC** (DAICEL Chiralpak IB, hexane / IPA = 90:10, 1.0 mL / min, 254 nm) t_R (major) = 15.4 min, t_R (minor) = 11.9 min.

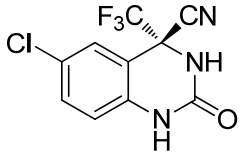


(*S*)-**3j**, 36 mg, white solid, mp 156–158 °C, 91% yield, 94% ee, $[\alpha]_D^{25}$ +12.6 (*c* 1.0, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IB, hexane / IPA = 90:10, 1.0 mL / min, 254 nm) t_R (major) = 11.7 min, t_R (minor) = 15.7 min.



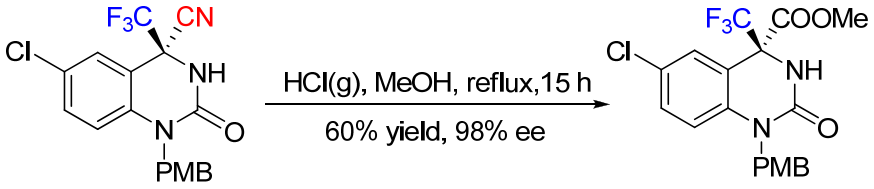
(*R*)-6-chloro-2-oxo-4-(trifluoromethyl)-1,2,3,4-tetrahydroquinazoline-4-carbonitrile (3k)

25 mg, white solid, mp 168–170 °C, 93% yield, 94% ee, $[\alpha]_D^{25}$ –18.0 (*c* 0.5, CH_2Cl_2), **^{1}H NMR** (400 MHz, d_6-DMSO) δ 10.32 (s, 1H), 9.43 (s, 1H), 7.53 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.46 (s, 1H), 7.02 (d, *J* = 8.7 Hz, 1H). **^{19}F NMR** (376 MHz, d_6-DMSO) δ –80.21 (s, 3F). **^{13}C NMR** (100 MHz, d_6-DMSO) δ 149.5, 136.8, 132.5, 126.4, 126.0, 122.1 (q, $^1J_{F\text{-}C}$ = 287.9 Hz), 117.3, 113.5, 109.0, 59.1 (q, $^2J_{F\text{-}C}$ = 33.5 Hz). **HRMS** (APCI) found: m/z 276.0108 $[M+H]^+$; calcd. for $C_{18}H_{12}F_5N_3O_2$+H 276.0073; **IR** (KBr): ν 3370, 3211, 3068, 2950, 1718, 1608, 1571, 1442, 1389, 1242, 1200, 1048, 952, 829, 742, 563, 458 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 90:10, 0.8 mL / min, 254 nm) t_R (major) = 6.8 min, t_R (minor) = 5.9 min.



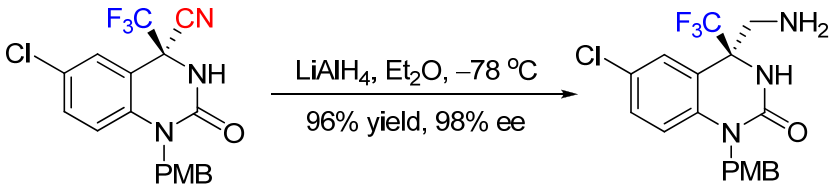
(*S*)-**3k**, 26 mg, white solid, mp 167–168 °C, 95% yield, 90% ee, $[\alpha]_D^{25}$ +20.0 (*c* 0.5, CH_2Cl_2), **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 90:10, 0.8 mL / min, 254 nm) t_R (major) = 5.9 min, t_R (minor) = 6.8 min.

3. Procedures for the further transformations



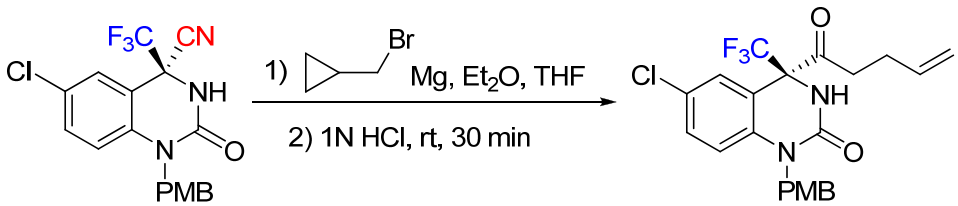
(*R*)-**3a** (98% ee) (*R*)-**4**

To a solution of **3a** (200 mg, 0.5 mmol) in dry methanol (20 mL) at 0 °C was added a saturated solution of dry HCl in methanol (10 mL). The mixture was refluxed for 15 hours and concentrated under reduced pressure. The crude mixture was treated with a saturated aqueous solution of $NaHCO_3$ (30 mL), and the aqueous layer was extracted with EtOAc (3 × 10 mL). The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. Purification by flash chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) gave the product (*R*)-**4**. 129 mg, white solid, mp 131–132 °C, 60% yield, 98% ee, $[\alpha]_D^{25}$ +29.2 (*c* 0.5, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.23 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 2H), 6.83 (dd, *J* = 11.7, 8.8 Hz, 3H), 6.64 (d, *J* = 32.4 Hz, 1H), 5.17 (d, *J* = 16.4 Hz, 1H), 5.02 (d, *J* = 16.4 Hz, 1H), 3.94 (s, 3H), 3.77 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –77.50 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.5, 159.1, 151.5, 136.9, 131.2, 128.0, 127.8, 123.3 (q, $^1J_{F\text{-}C}$ = 286.7 Hz), 116.6, 114.5, 113.7, 65.6 (q, $^2J_{F\text{-}C}$ = 29.8 Hz), 55.4, 54.6, 45.8. **HRMS** (ESI) found: m/z 451.0601 $[M+Na]^+$; calcd. for $C_{19}H_{16}ClF_3N_2O_4$+Na 451.0751; **IR** (KBr): ν 3276, 2957, 2933, 1760, 1692, 1511, 1426, 1249, 1200, 1034, 819, 567 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 1.0 mL / min, 254 nm) t_R (major) = 14.3 min, t_R (minor) = 9.5 min.



(*R*)-**3a** (98% ee) (*R*)-**5**

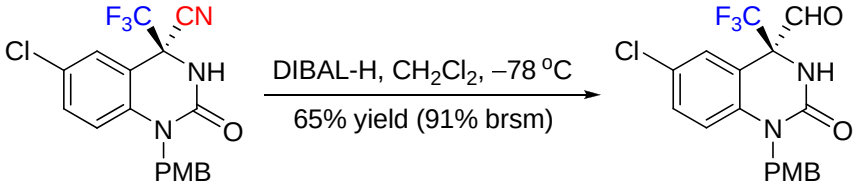
To a solution of **3a** (79 mg, 0.2 mmol) in dry diethyl ether (10 mL) was added $LiAlH_4$ (32 mg, 0.4 mmol, 4.0 equiv.) at 0 °C. The mixture was stirred for 24 h at room temperature, and the reaction mixture was hydrolyzed by successive addition of water (1 mL). The resulting precipitate was filtered on Celite. The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The crude was purified by column chromatography on silica gel to give the product (*R*)-**5**. 66 mg, white solid, mp 80–81 °C, 96% yield, 98% ee, $[\alpha]_D^{25}$ –24.6 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 (s, 1H), 7.18 (dd, *J* = 15.9, 7.0 Hz, 4H), 6.87 – 6.78 (m, 3H), 5.21 (d, *J* = 15.6 Hz, 1H), 4.98 (d, *J* = 15.9 Hz, 1H), 3.76 (s, 3H), 3.40 (d, *J* = 13.7 Hz, 1H), 3.28 (d, *J* = 12.9 Hz, 1H), 1.46 (s, 2H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –79.38 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.0, 153.6, 138.1, 130.4, 128.4, 128.0, 127.7, 126.3, 125.3 (q, $^1J_{F\text{-}C}$ = 287.4 Hz), 117.7, 116.5, 114.4, 62.5 (q, $^2J_{F\text{-}C}$ = 27.0 Hz), 55.4, 45.6, 45.0. **HRMS** (ESI) found: m/z 400.1005 $[M+H]^+$; calcd. for $C_{18}H_{17}ClF_3N_3O_2$+H 400.0961; **IR** (KBr): ν 3232, 3116, 2957, 1683, 1510, 1433, 1251, 1172, 1031, 816, 555, 422 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 80:20, 1.0 mL / min, 254 nm) t_R (major) = 49.9 min, t_R (minor) = 21.6 min.



(*R*)-**3a** (98% ee) (*R*)-**6**: 90% yield, 99% ee

To a solution of **3a** (200 mg, 0.5 mmol) in dry Et_2O (10 mL) and dry THF (2.5 mL) was added dropwise a solution of (cyclopropylmethyl)magnesium bromide (3.0 M in ether, 1.0 mL, 2.25 mmol, 4.5 eq.) in diethyl ether at 0 °C slowly. The resulting suspension was stirred at 0 °C for an additional 1 hour and then at room temperature for 4 hours. The mixture was cooled to 0 °C and slowly added an aqueous solution of

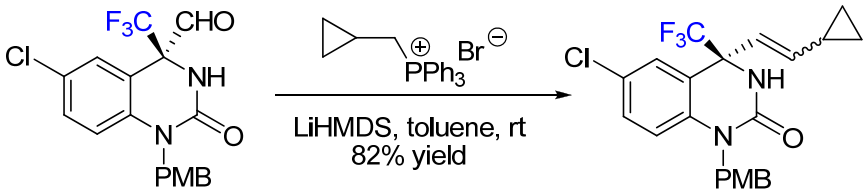
1M HCl (30 mL). The mixture was vigorously stirred at room temperature for 30 min, and then extracted with ethyl acetate (3 × 20 mL). The extracts were washed with 5% $NaHCO_3$, brine, dried over Na_2SO_4 and concentrated. The residue was subjected to column chromatography on silica gel (petroleum ether / ethyl acetate = 5:1) to give the product (*R*)-**6**. 200 mg, white solid, mp 156–157 °C, 90% yield, 99% ee, $[\alpha]_D^{25}$ +120.0 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 5.8 Hz, 1H), 7.26 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.19 (d, *J* = 8.5 Hz, 2H), 7.15 (s, 1H), 6.90 (t, *J* = 7.9 Hz, 3H), 5.72 – 5.62 (m, 1H), 5.26 (d, *J* = 16.2 Hz, 1H), 5.01 – 4.95 (m, 3H), 3.80 (s, 3H), 3.01 – 2.93 (m, 1H), 2.74 – 2.66 (m, 1H), 2.38 – 2.29 (m, 2H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –76.39 (d, *J* = 10.9 Hz, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.2, 159.2, 153.4, 137.1, 136.1, 131.3, 128.4, 127.9, 127.8, 127.5, 123.6 (q, $^1J_{F\text{-}C}$ = 286.6 Hz), 117.0, 116.1, 114.5, 113.6, 69.1 (q, $^2J_{F\text{-}C}$ = 26.9 Hz), 55.4, 45.6, 37.7, 27.5. **HRMS** (APCI) found: m/z 451.1232 $[M–H]^-$; calcd. for $C_{22}H_{20}ClF_3N_2O_3$–H 451.1115; **IR** (KBr): ν 3203, 3078, 2936, 1732, 1687, 1512, 1425, 1393, 1200, 1032, 919, 811, 561, 510 cm^{-1}; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 90:10, 1.0 mL / min, 254 nm) t_R (major) = 6.4 min, t_R (minor) = 9.2 min.



(*R*)-**3a** (98% ee) (*R*)-**7**

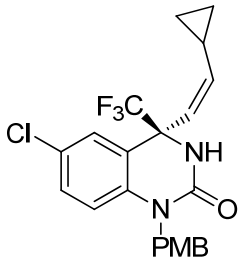
To a well-stirred solution of the **3a** (0.25 mmol) in dry dichloromethane (3 mL) under argon atmosphere was added DIBAL-H (2.0 equiv., 1.2 M in toluene) and stirred overnight at –78 °C. The reaction was then quenched after 1 hour of further stirring by slow addition of 2M HCl and ethyl acetate. The organic phase was washed with brine, dried over sodium sulfate and concentrated. The crude was then purified by column chromatography on silica gel (petroleum ether / ethyl acetate = 10:1 to 2:1) to give the corresponding aldehyde **7** and recovered **3a** as well. 65 mg, white solid, mp 76–77 °C, 65% yield (91% brsm), $[\alpha]_D^{25}$ –23.4 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 7.39 (s, 1H), 7.34 (s, 1H), 7.13 (dd, *J* = 14.5, 8.9 Hz, 3H), 6.86 (t, *J* = 9.5

Hz, 3H), 5.18 (d, J = 16.4 Hz, 1H), 5.01 (d, J = 16.4 Hz, 1H), 3.77 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –76.37 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 188.6, 159.2, 152.4, 137.4, 131.5, 128.4, 127.8, 127.8, 127.2, 123.1 (q, $^1J_{F\text{-}C}$ = 286.8 Hz), 117.2, 114.6, 112.1, 67.2 (q, $^2J_{F\text{-}C}$ = 28.2 Hz), 55.4, 45.8. **HRMS** (ESI) found: m/z 397.0442 $[M–H]^-$; calcd. for $C_{18}H_{14}ClF_3N_2O_3$–H 397.0645; **IR** (KBr): ν 3288, 2934, 1674, 1511, 1571, 1435, 1249, 1183, 1032, 813, 743, 561 cm^{-1}.



(*R*)-**7** (*S*)-**8** (*Z*/*E* = 8/1)

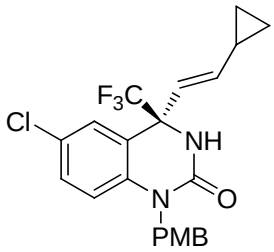
LiHMDS (1.0 M in THF, 0.4 mmol) was added dropwise to a suspension of (cyclopropylmethyl)triphenylphosphonium bromide (0.3 mmol) in anhydrous toluene (2.5 mL) under argon atmosphere, and the resulting mixture was stirred at rt for 15 min. A solution of **7** (80 mg, 0.2 mmol) in anhydrous toluene (1.5 mL) was added and the resulting mixture was stirred at rt for 1 h. The reaction was quenched with 1M HCl (10 mL), and the aqueous layer was extracted with ethyl acetate. The combined organic extracts were dried by $MgSO_4$ and concentrated. Column chromatography (petroleum ether / ethyl acetate = 10/1) afforded **8a** and **8b** (62 mg + 8 mg, 82% yield; *Z*/*E* = 8/1, determined by ^{19}F-NMR of the crude product).



(*S*,*Z*)-6-chloro-4-(2-cyclopropylvinyl)-1-(4-methoxybenzyl)-4-(trifluoromethyl)-3,4-dihydroquinazolin-2(1*H*)-one (8a)

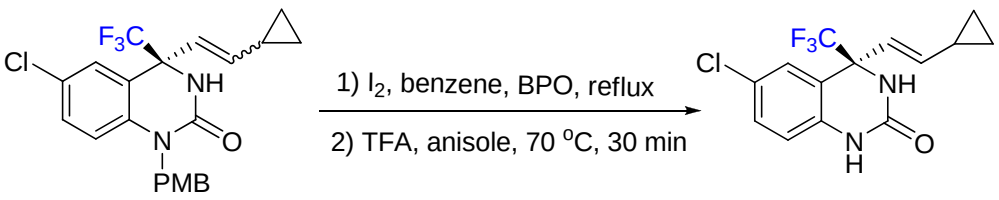
62 mg, white solid, 73% yield, 99% ee, $[\alpha]_D^{25}$ –35.7 (*c* 2.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (s, 1H), 7.16 (d, J = 8.3 Hz, 3H), 6.83 (d, J = 8.5 Hz, 2H), 6.79 (d, J = 8.9 Hz, 1H), 5.88 (d, J = 11.1 Hz, 1H), 5.60 (s, 1H), 5.30 (dd, J = 13.4, 8.4 Hz,

2H), 4.94 (d, J = 16.3 Hz, 1H), 3.77 (s, 3H), 1.37 – 1.30 (m, 1H), 0.84 – 0.78 (m, 1H), 0.58 – 0.51 (m, 1H), 0.48 – 0.41 (m, 1H), 0.35 – 0.29 (m, 1H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –82.89 (s, 3F). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.0, 152.6, 145.8, 136.9, 130.2, 128.9, 128.5, 127.8, 127.8, 125.4 (q, $^1J_{F\text{-}C}$ = 286.8 Hz), 122.6, 120.3, 116.0, 114.4, 62.0 (q, $^2J_{F\text{-}C}$ = 28.7 Hz), 55.39, 45.65, 11.38, 8.23, 8.08. **HRMS** (ESI) found: m/z 437.2030 $[M+H]^+$; calcd. for $C_{22}H_{20}ClF_3N_2O_2$+H 437.1165; **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 95:5, 1.0 mL / min, 254 nm) t_R (major) = 18.1 min, t_R (minor) = 20.3 min.



(*S*,*E*)-6-chloro-4-(2-cyclopropylvinyl)-1-(4-methoxybenzyl)-4-(trifluoromethyl)-3, 4-dihydroquinazolin-2(1*H*)-one (8b)

8 mg, slight yellow solid, 9% yield, 98% ee, $[\alpha]_D^{25}$ –28.6 (*c* 1.0, CH_2Cl_2), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.26 (s, 1H), 7.24 – 7.10 (m, 3H), 6.85 (d, J = 8.4 Hz, 2H), 6.82 – 6.72 (m, 1H), 6.03 (d, J = 15.5 Hz, 1H), 5.95 (s, 1H), 5.54 (dd, J = 15.3, 9.3 Hz, 1H), 5.17 (d, J = 15.6 Hz, 1H), 5.02 (d, J = 15.8 Hz, 1H), 3.77 (s, 3H), 1.64 – 1.48 (m, 1H), 0.88 – 0.78 (m, 2H), 0.54 – 0.44 (m, 2H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –80.55 (s, 3F). **HRMS** (ESI) found: m/z 437.2030 $[M+H]^+$; calcd. for $C_{22}H_{20}ClF_3N_2O_2$+H 437.1165; **HPLC** (DAICEL Chiralpak IB, hexane / IPA = 95:5, 1.0 mL / min, 254 nm) t_R (major) = 12.0 min, t_R (minor) = 10.0 min.



(*S*)-**8** (*Z*/*E* = 8/1) **DPC 083**

A mixture of **8** (100 mg, 0.23 mmol), iodine (115 mg, 4 portions, 2.0 equiv.), and BPO (55 mg, 4 portions, 1.0 equiv) in benzene (10 mL) was refluxed for 4 days. The reaction mixture was shaken with saturated sodium thiosulfate solution and the water layer was extracted with EtOAc. The combined organic extracts were dried over $MgSO_4$ and concentrated. The crude was separated by column chromatography on silica gel to yield the *trans*-isomer **8b** (70 mg).

To a solution of **8b** (70 mg, 0.16 mmol) in anisole (0.6 mL) was added TFA (3 mL). The reaction mixture was stirred at 70 ^oC for 30 min. Water was added and extracted with ethyl acetate. The combined organic extracts were washed with aqueous $NaHCO_3$ and brine, dried over Na_2SO_4 and concentrated. The crude was then purified by column chromatography on silica gel to give the product DPC-083(42 mg): slight yellow solid, 60% yield (two steps), 98% ee, $[\alpha]_D^{20}$ –22.0^o (*c* 0.40, CH_3OH) { lit.[4a]: $[\alpha]_D^{20}$ –22.5^o (*c* 0.40, CH_3OH), > 99.9% ee; lit.[4b]: $[\alpha]_D^{28}$ –19.8^o (*c* 0.40, CH_3OH), 95% ee}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.41 (s, 1H), 7.24 (s, 1H), 7.20 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.76 (d, *J* = 8.5 Hz, 1H), 6.01 (d, *J* = 15.5 Hz, 2H), 5.48 (dd, *J* = 15.4, 9.3 Hz, 1H), 1.56 – 1.49 (m, 1H), 0.86 – 0.76 (m, 2H), 0.52 – 0.40 (m, 2H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –80.59 (s, 3F). **HPLC** (DAICEL Chiralpak IC, hexane / IPA = 96:4, 0.6 mL / min, 254 nm) t_R (major) = 21.1 min, t_R (minor) = 17.0 min.

4. References:

[1] (*a*) J. W. Corbett, S. S. Ko, J. D. Rodgers, L. A. Gearhart, N. A. Magnus, L. T. Bacheler, S. Diamond, S. Jeffrey, R. M. Klabe, B. C. Cordova, S. Garber, K. Logue, G. L. Trainor, P. S. Anderson, S. K. Erickson-Viitanen, *J. Med. Chem.*, 2000, **43**, 2019; (*b*) N. A. Magnus, P. N. Confalone, L. Storace, M. Patel, C. C. Wood, W. P. Davis, R. L. Parsons, Jr. *J. Org. Chem.*, 2003, **68**, 754.

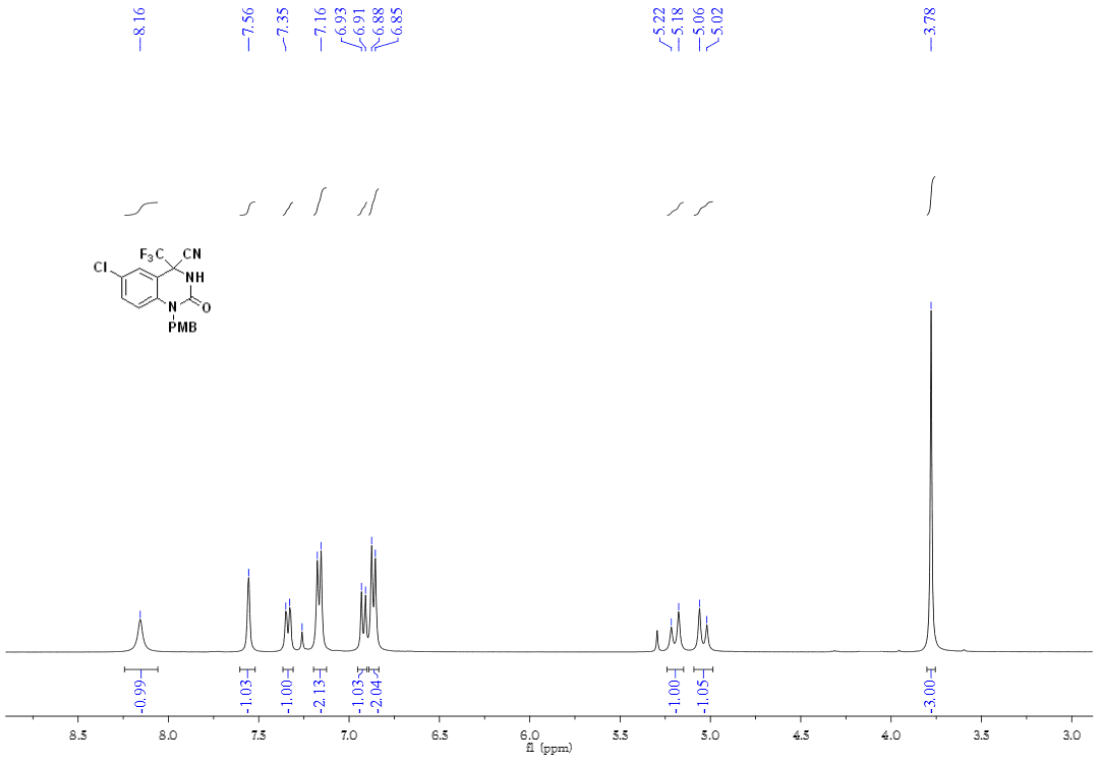
[2] (*a*) K. Liu, H.-F. Cui, J. Nie, K.-Y. Dong, X.-J. Li and J.-A. Ma, *Org. Lett.*, 2007, **9**, 923; (*b*) X.-J. Li, K. Liu, H. Ma, J. Nie and J.-A. Ma, *Synlett*, 2008, 3242; (*c*) H.

Ma, K. Liu, F.-G. Zhang, C.-L. Zhu, J. Nie and J.-A. Ma, *J. Org. Chem.*, 2010, **75**, 1402.

[3] (*a*) J. Ye, D. J. Dixon and P. S. Hynes, *Chem. Commun.*, 2005**,** 4481; (*b*) B. Vakulya, S. Varga, A. Csámpai and T. Soós, *Org. Lett.*, 2005, **7**, 1967.

[4] (*a*) B. Jiang, J. J. Dong, Y. G. Si, X. L. Zhao, Z. G. Huang and M. Xu, *Adv. Synth. Catal.*, 2008, **350**, 1360; (*b*) H. Xie, Y. Zhang, S. Zhang, X. Chen and W. Wang, *Angew. Chem. Int. Ed.*, 2011, **50**, 11773.

NMR spectra of the addition products and related compounds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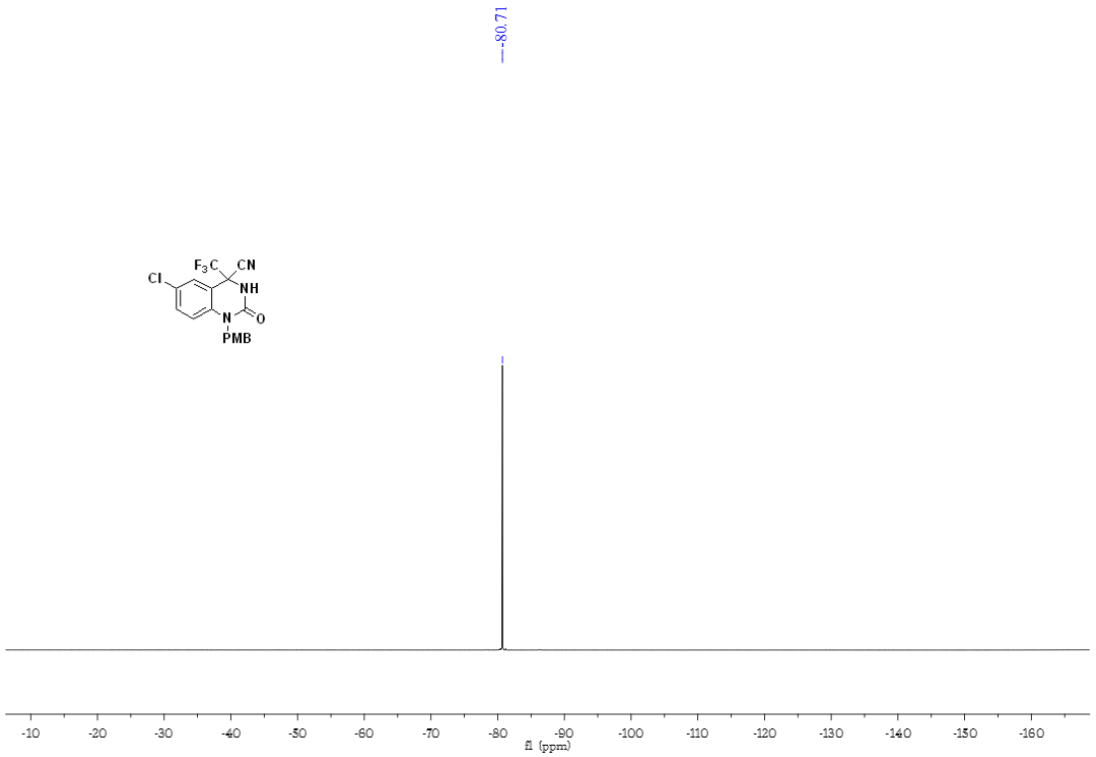
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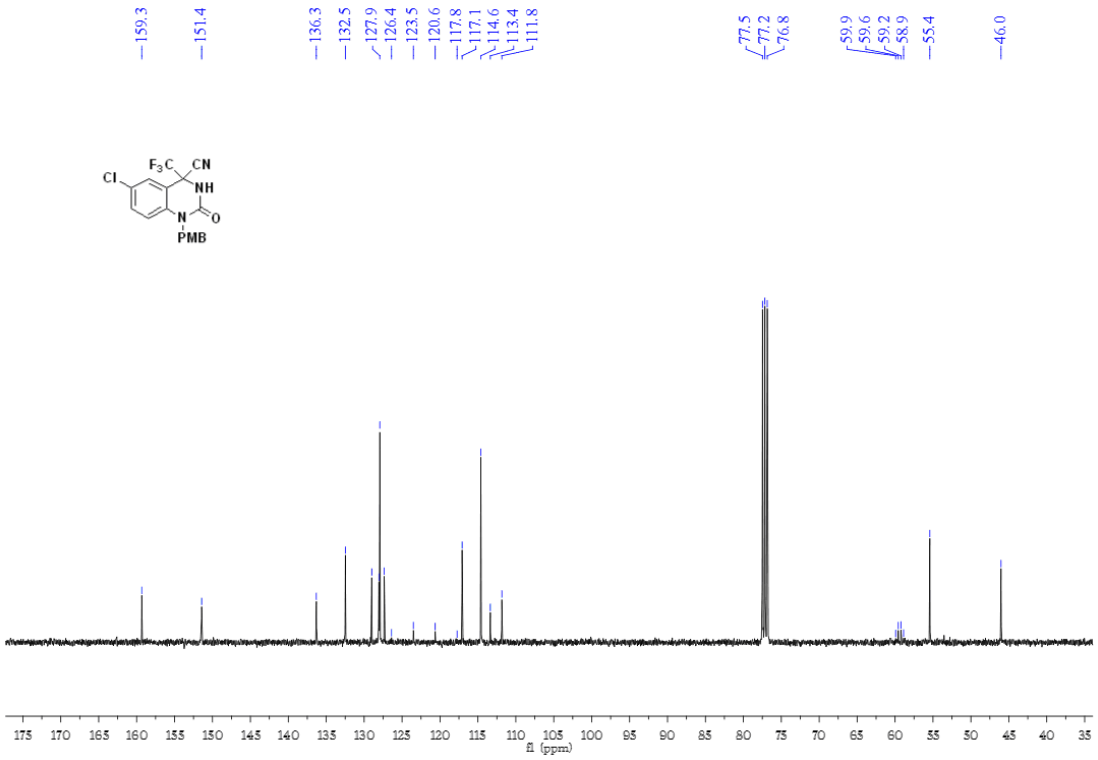

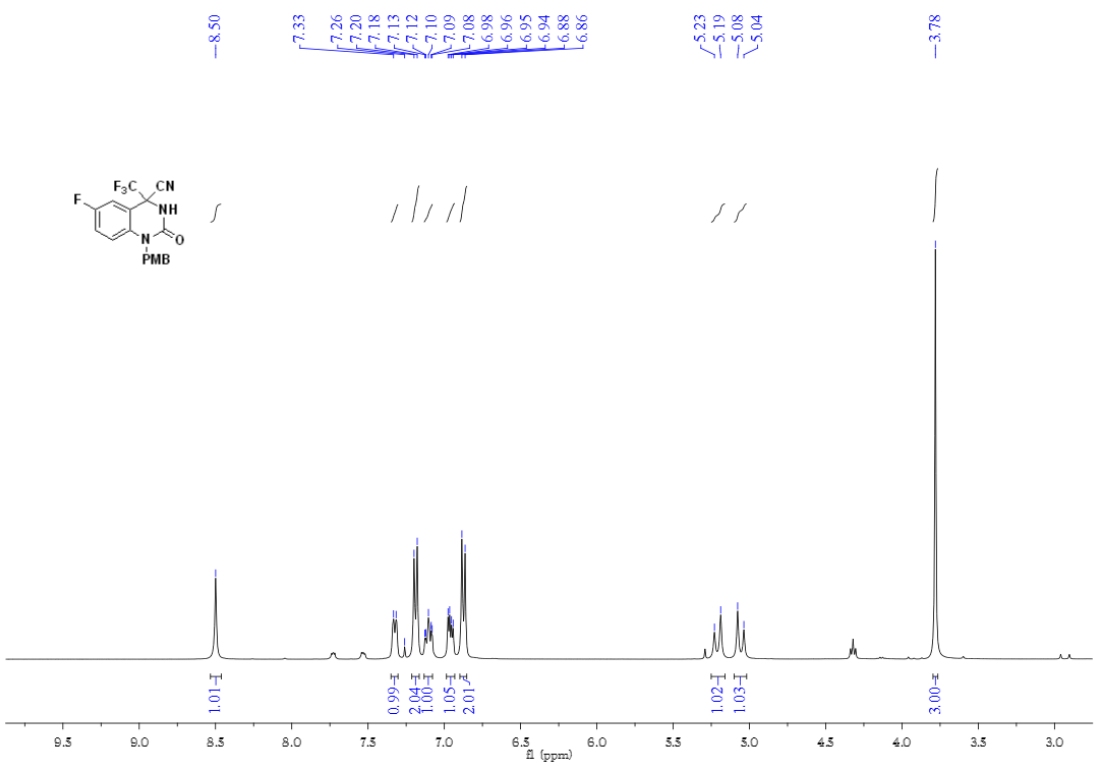

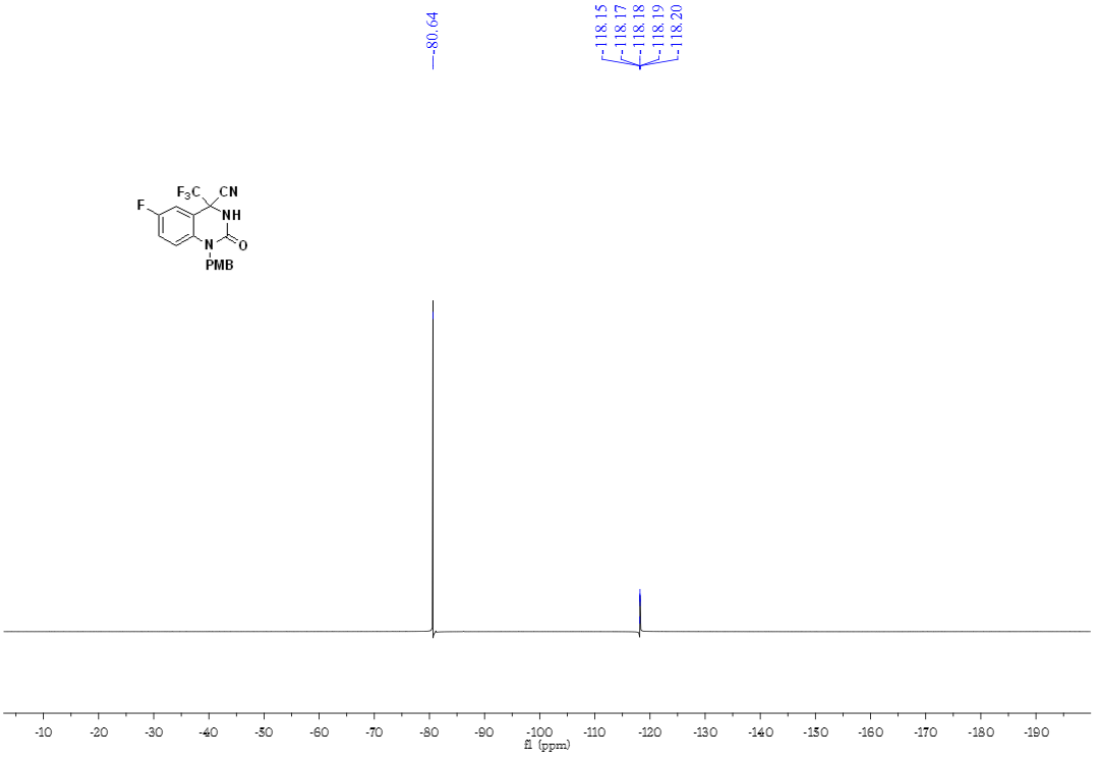

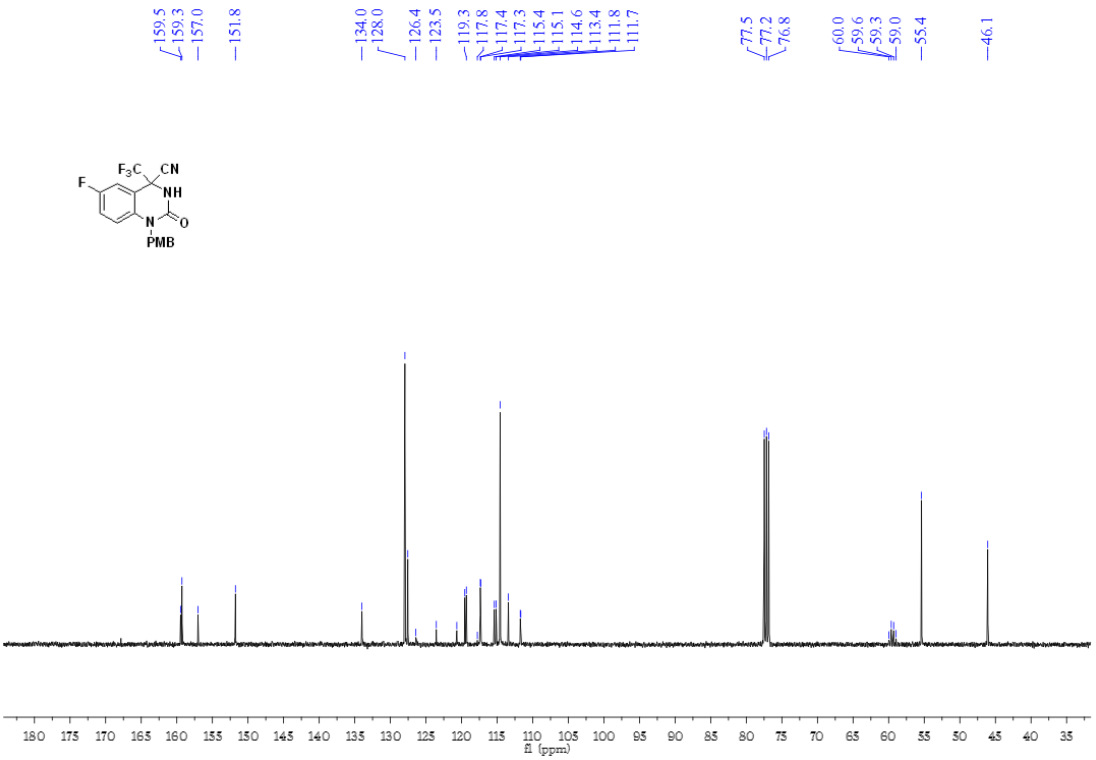

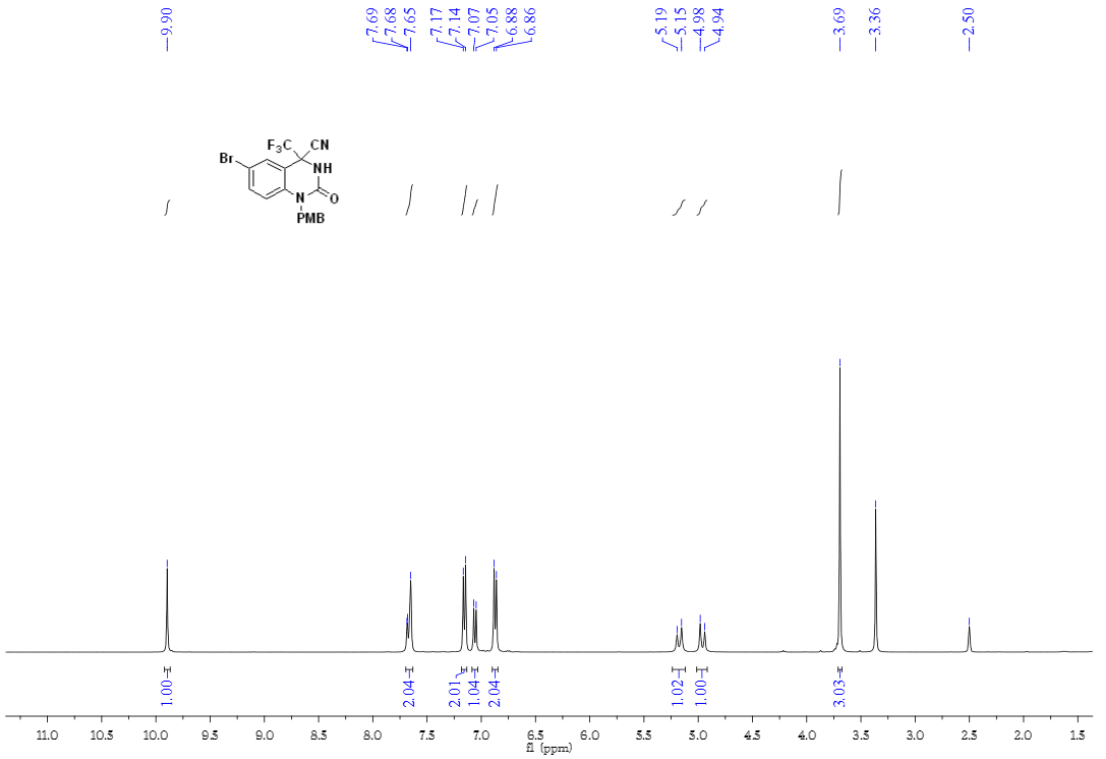
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CN
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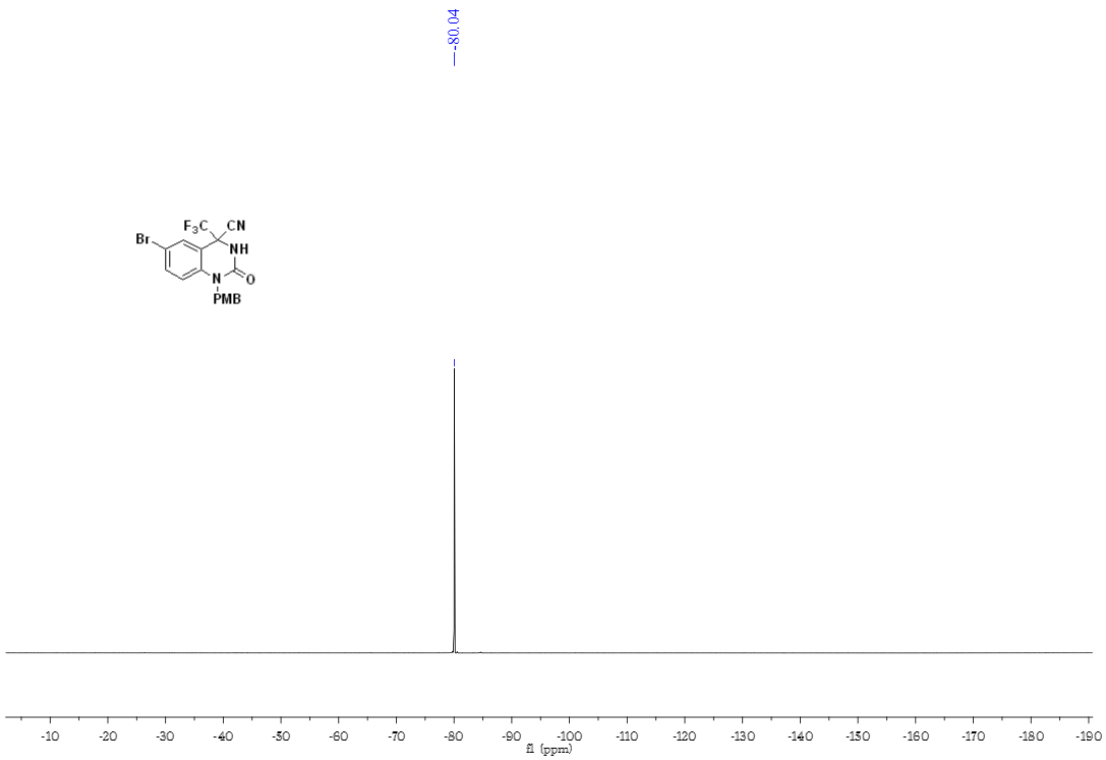
f1 (ppm)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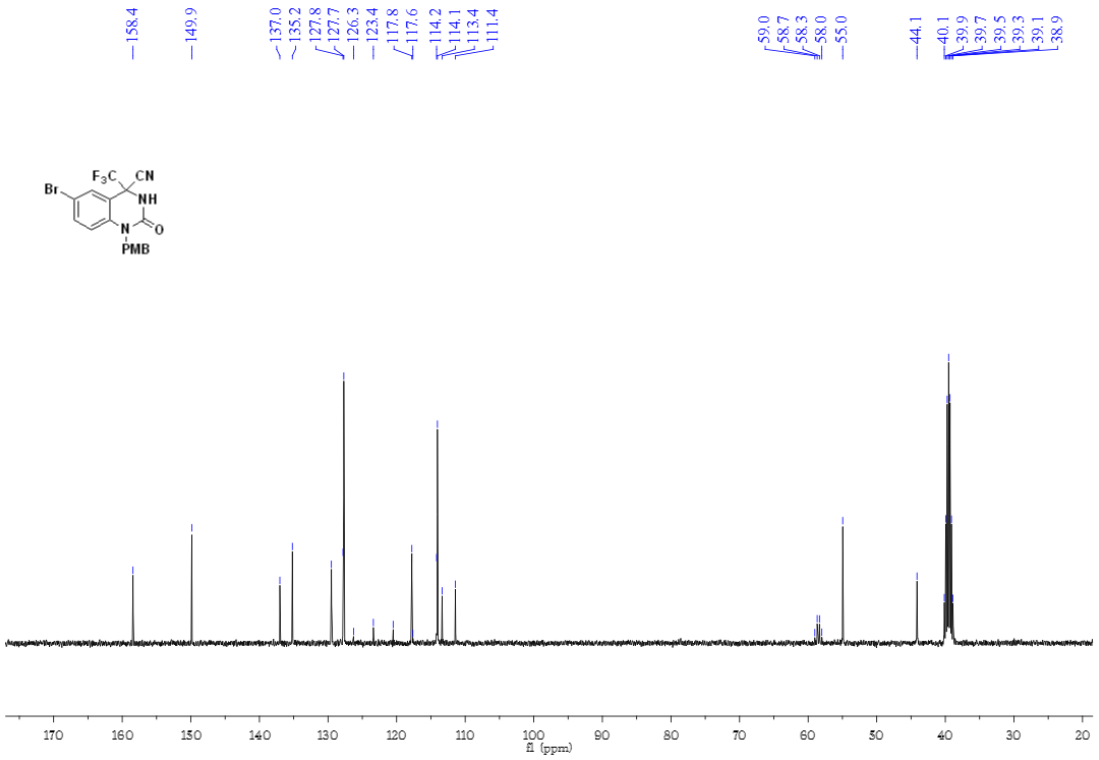
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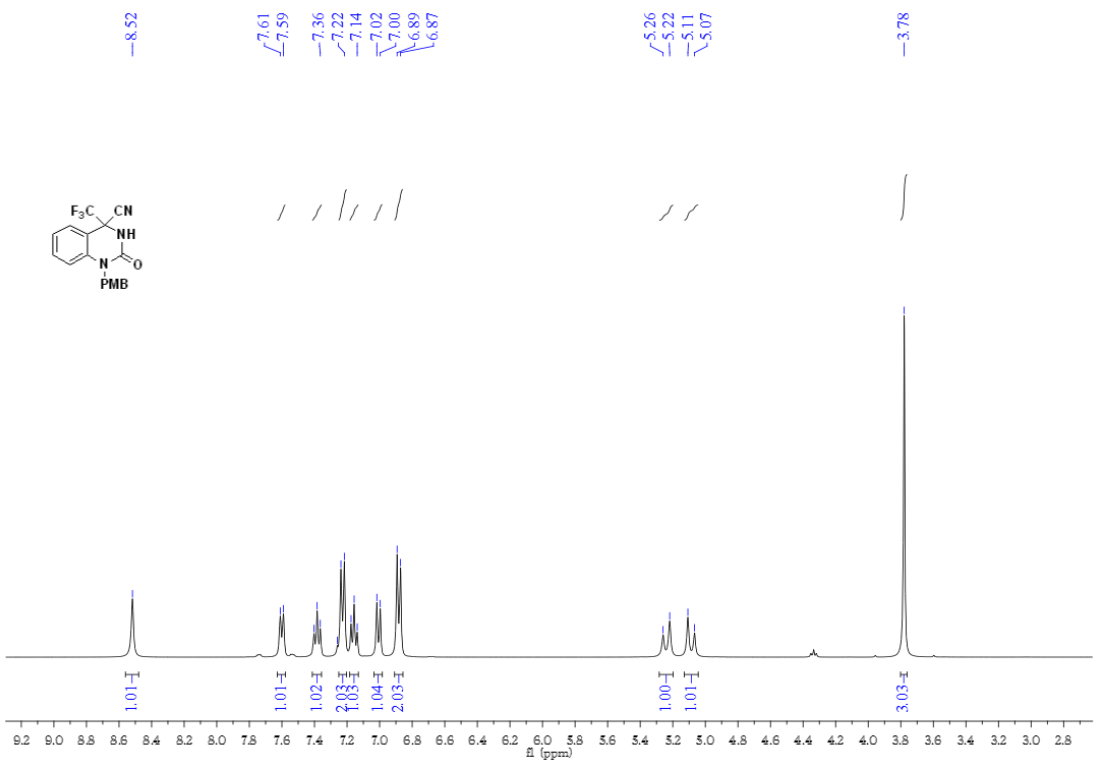
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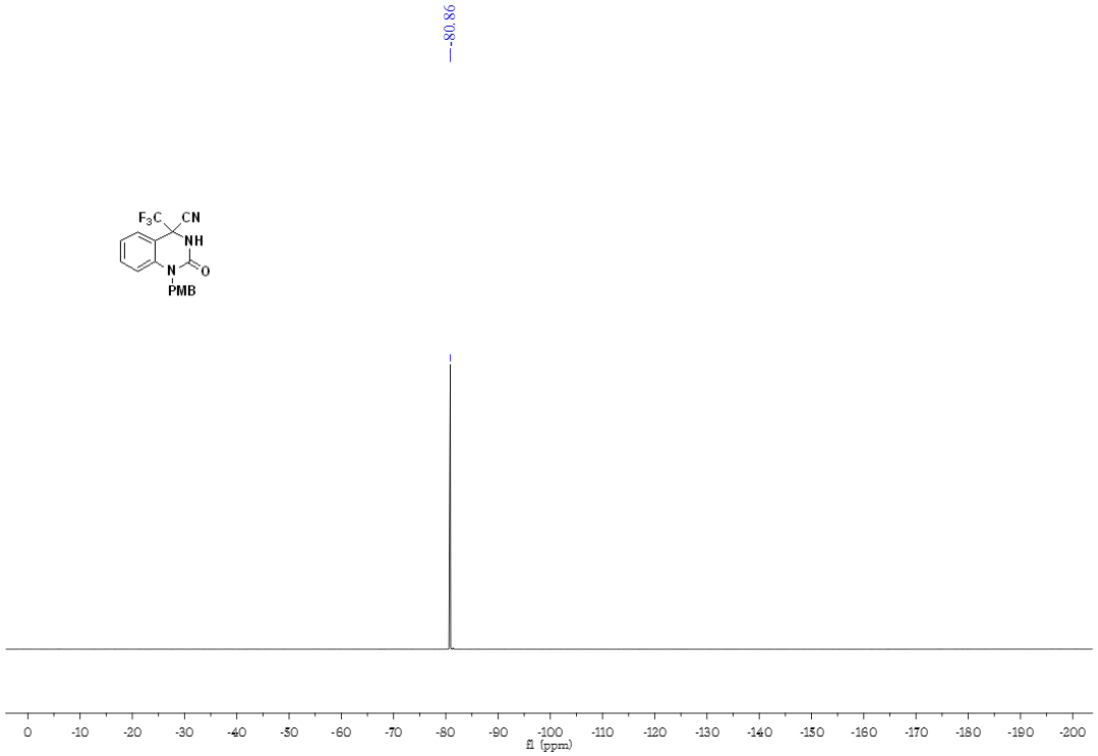

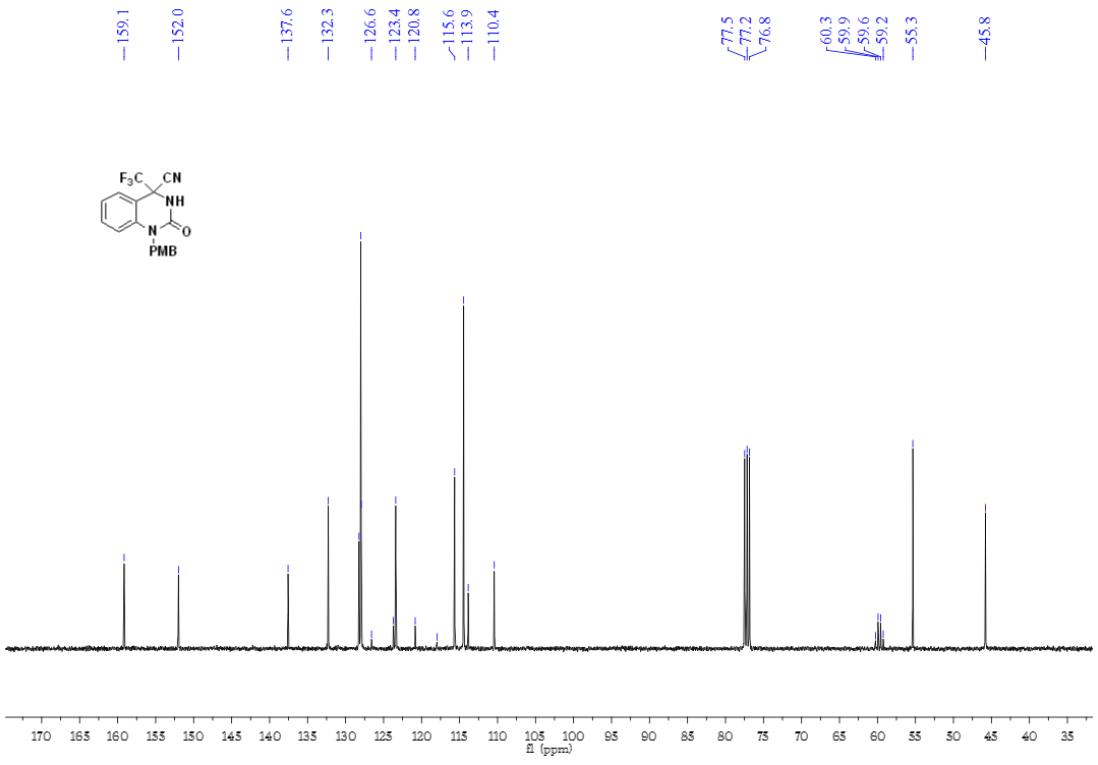

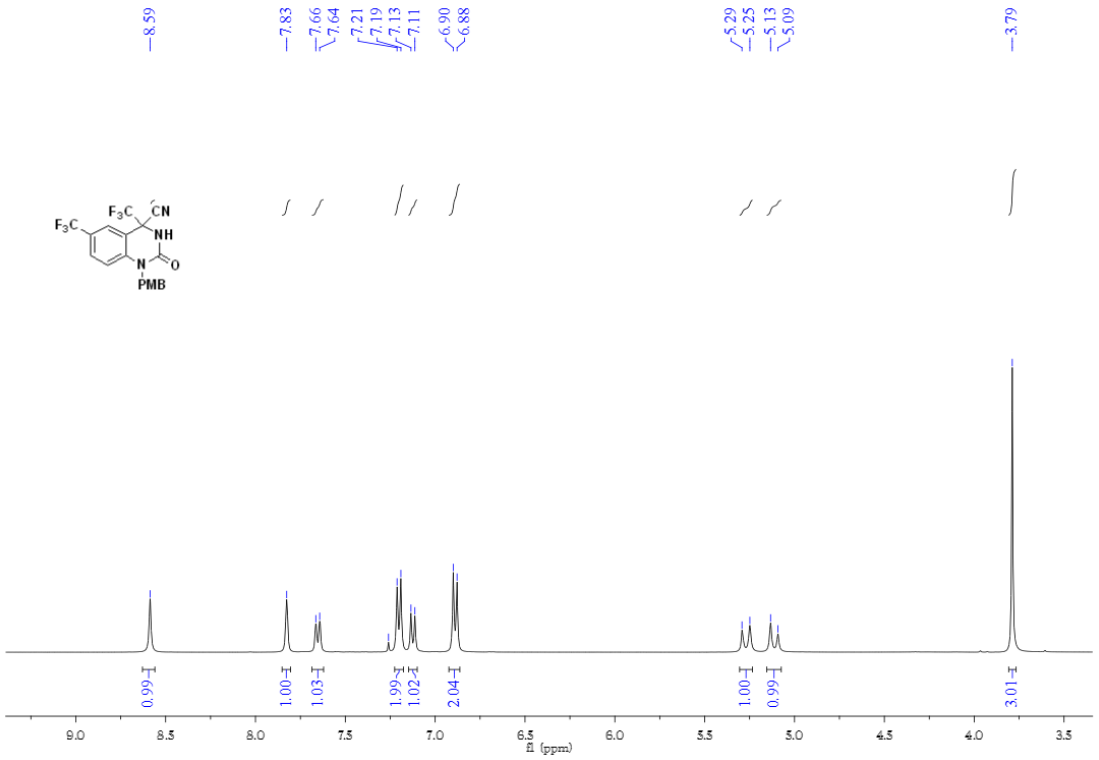
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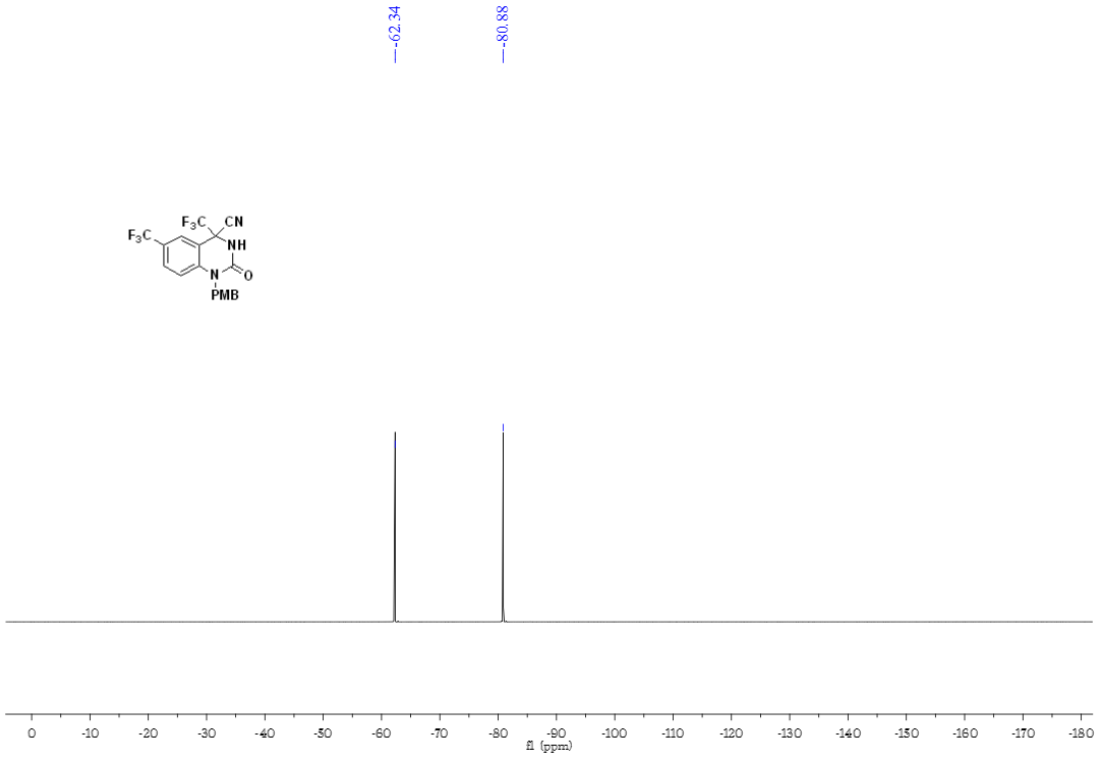
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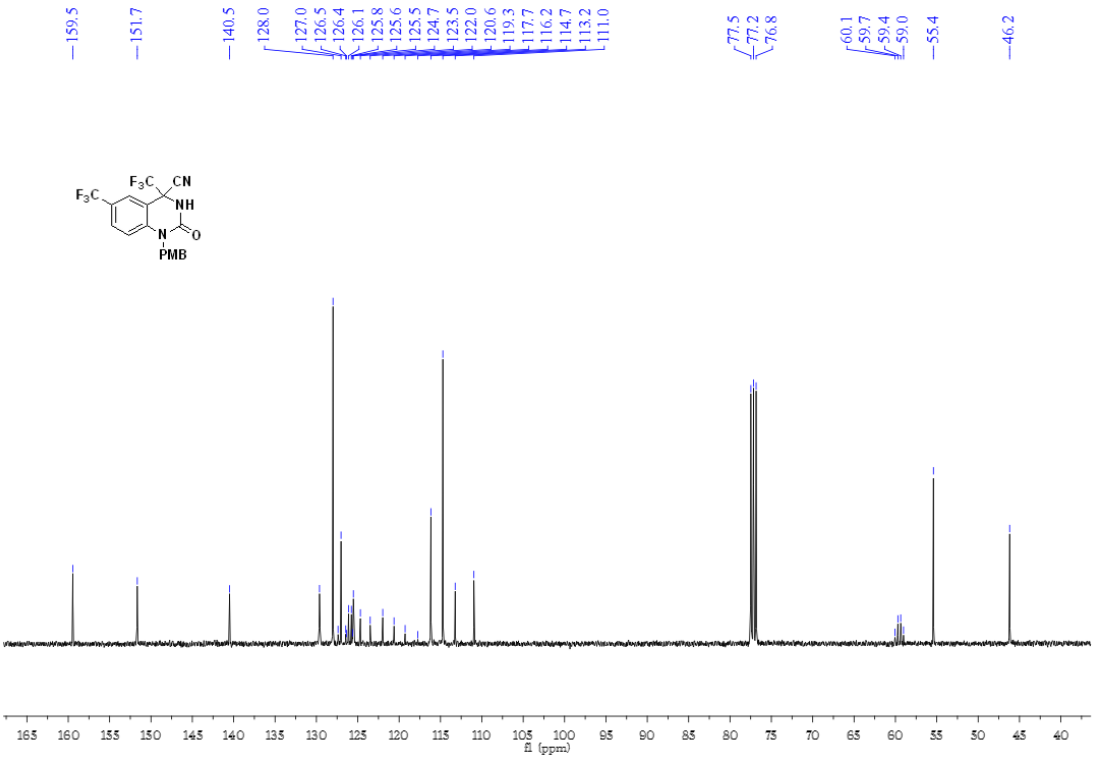
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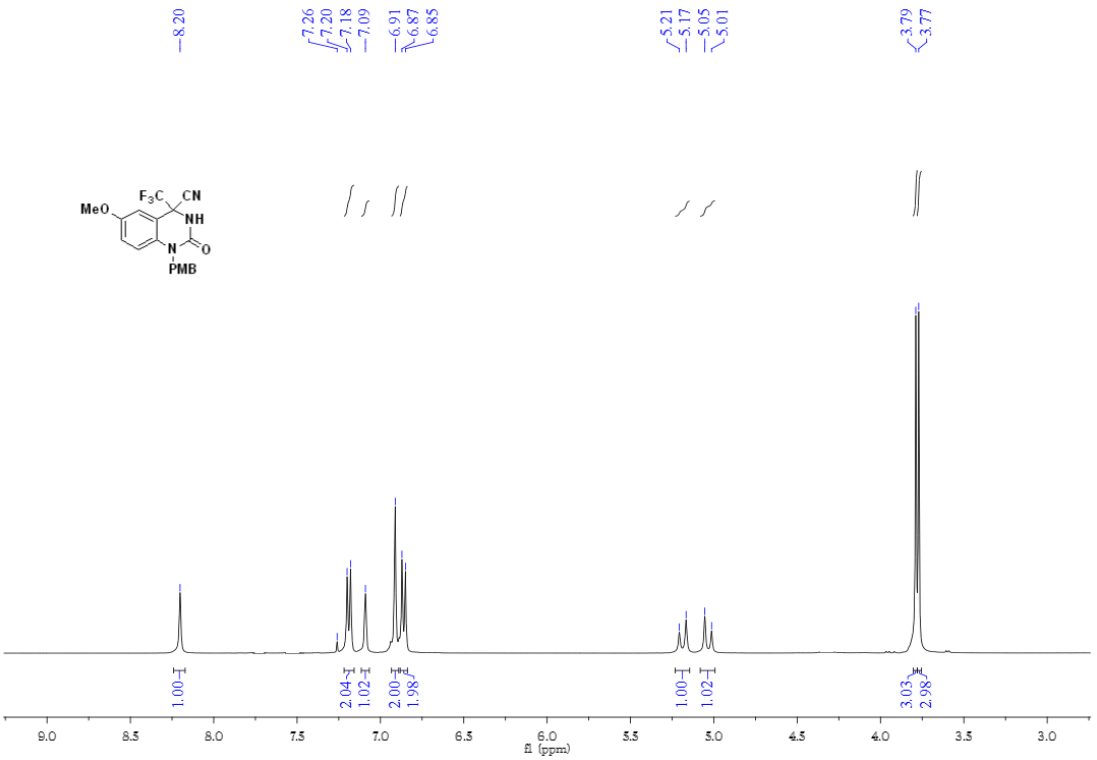
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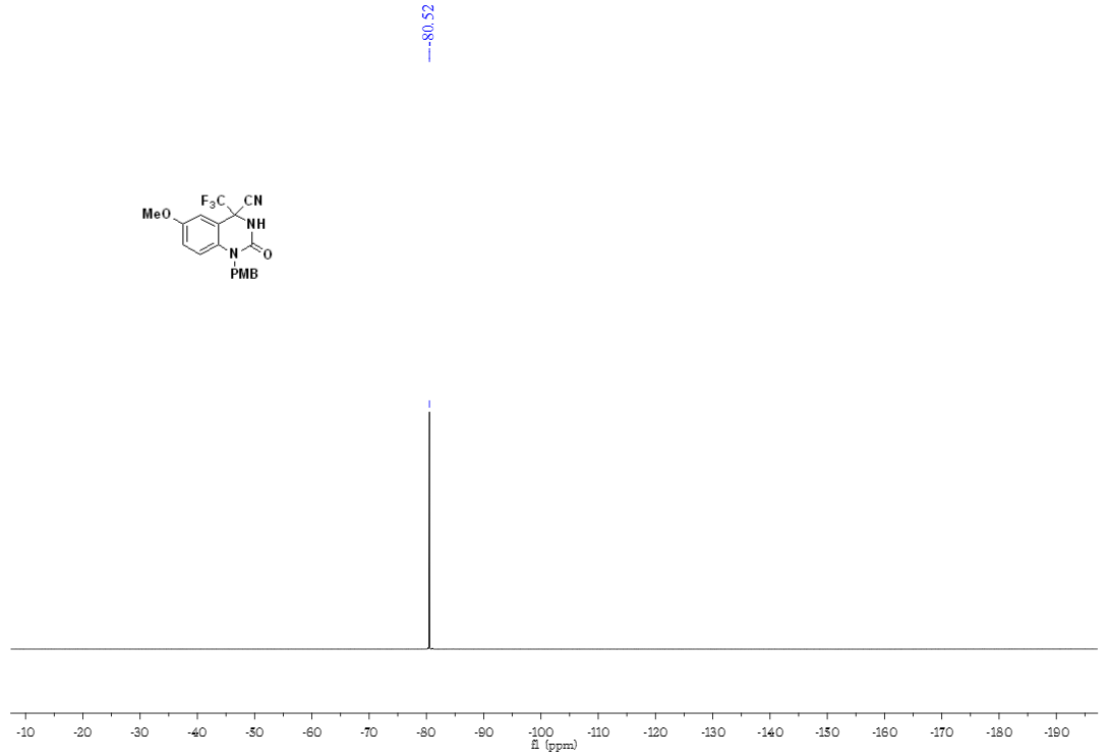

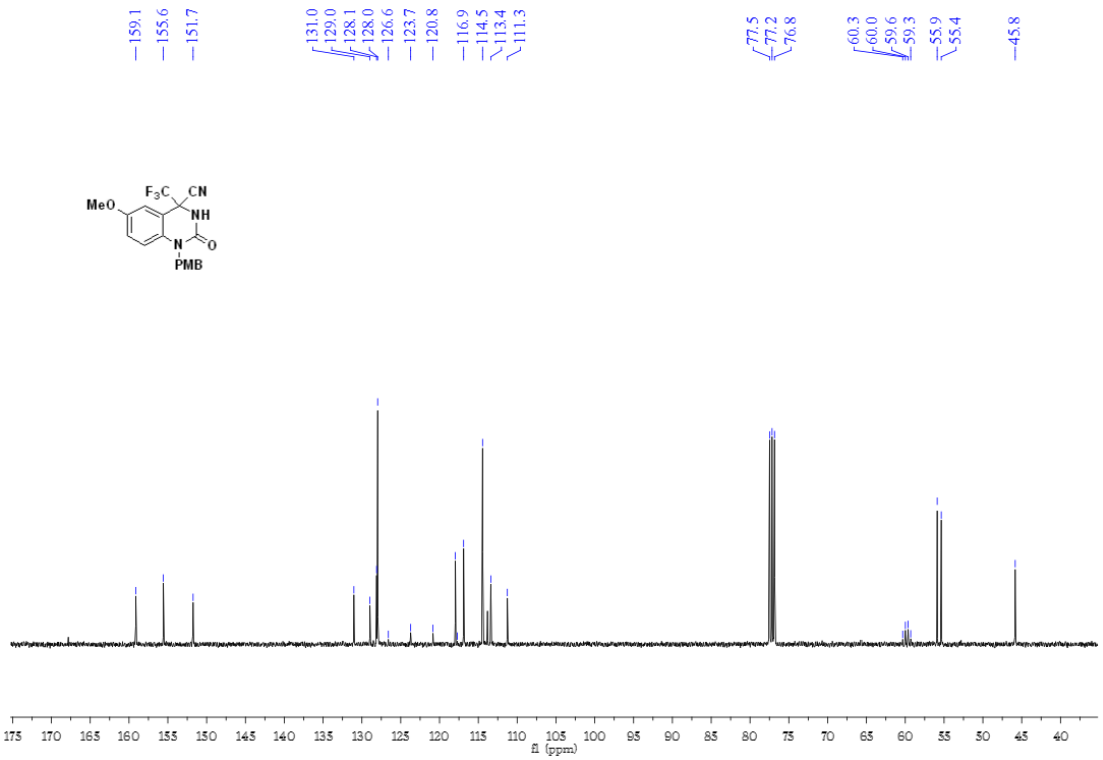

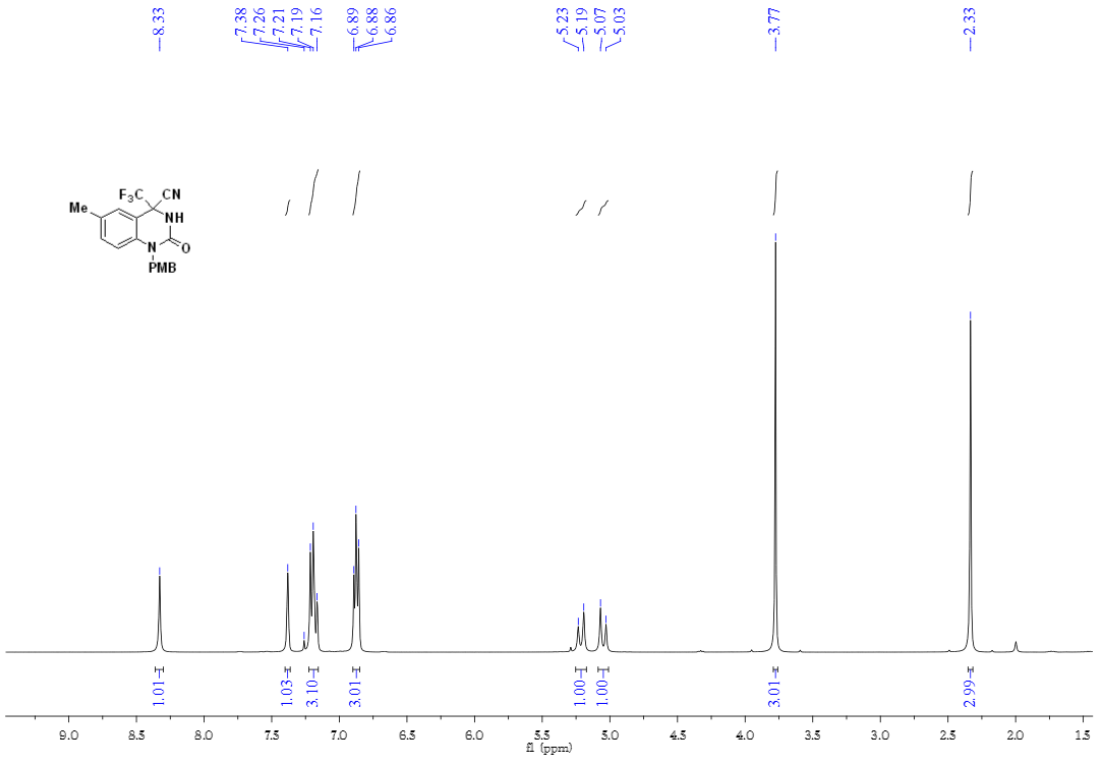

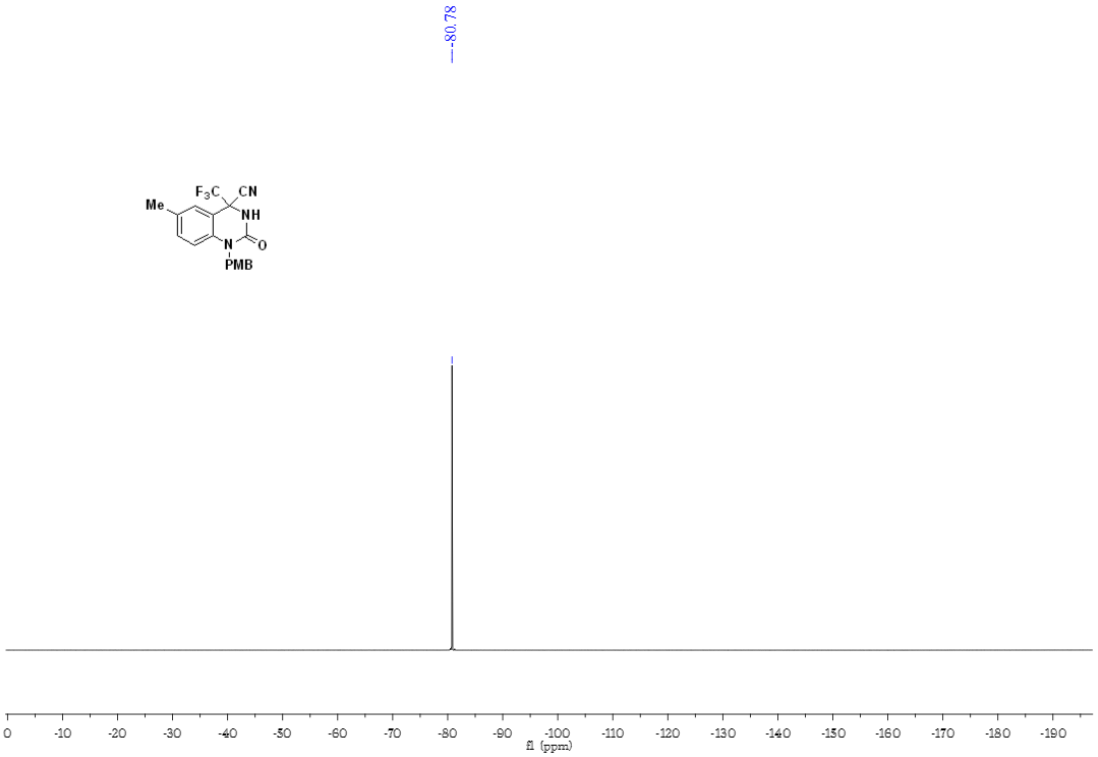

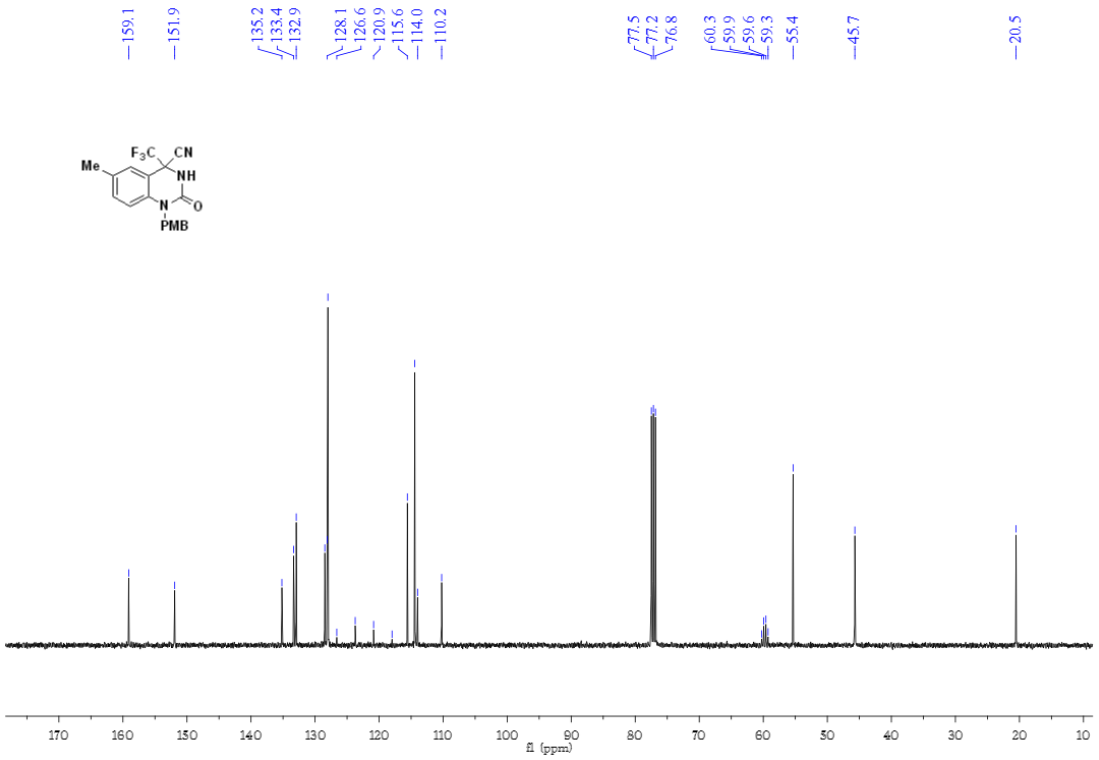

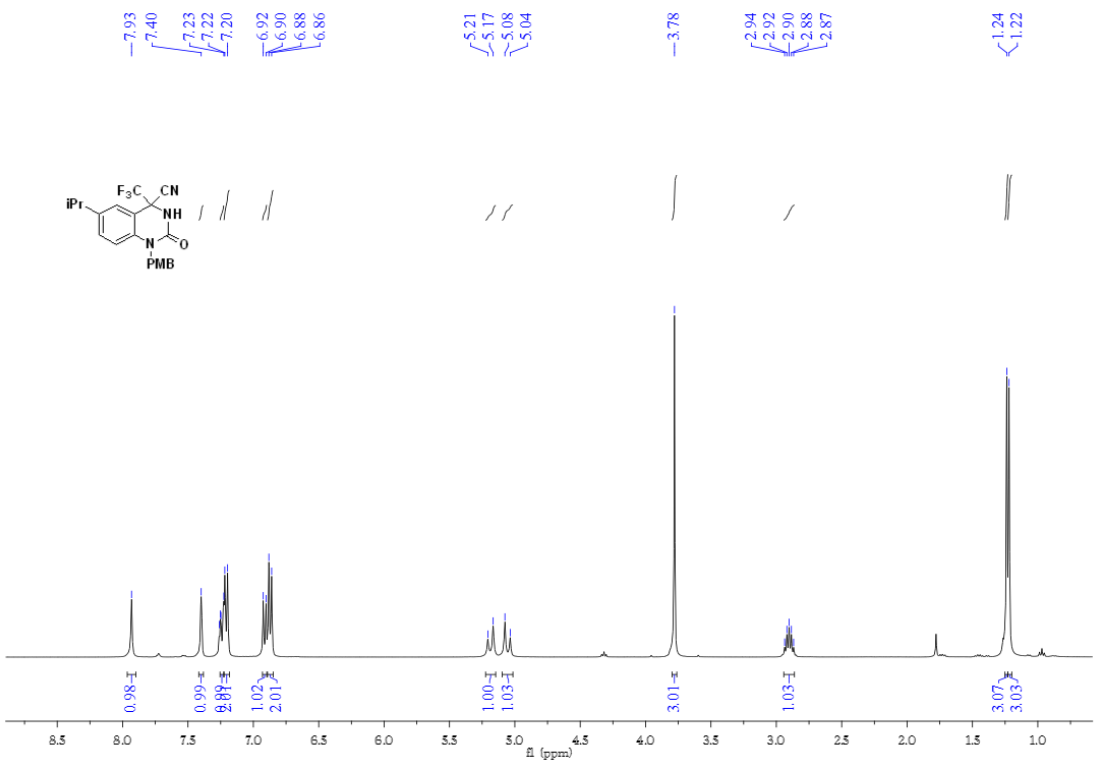

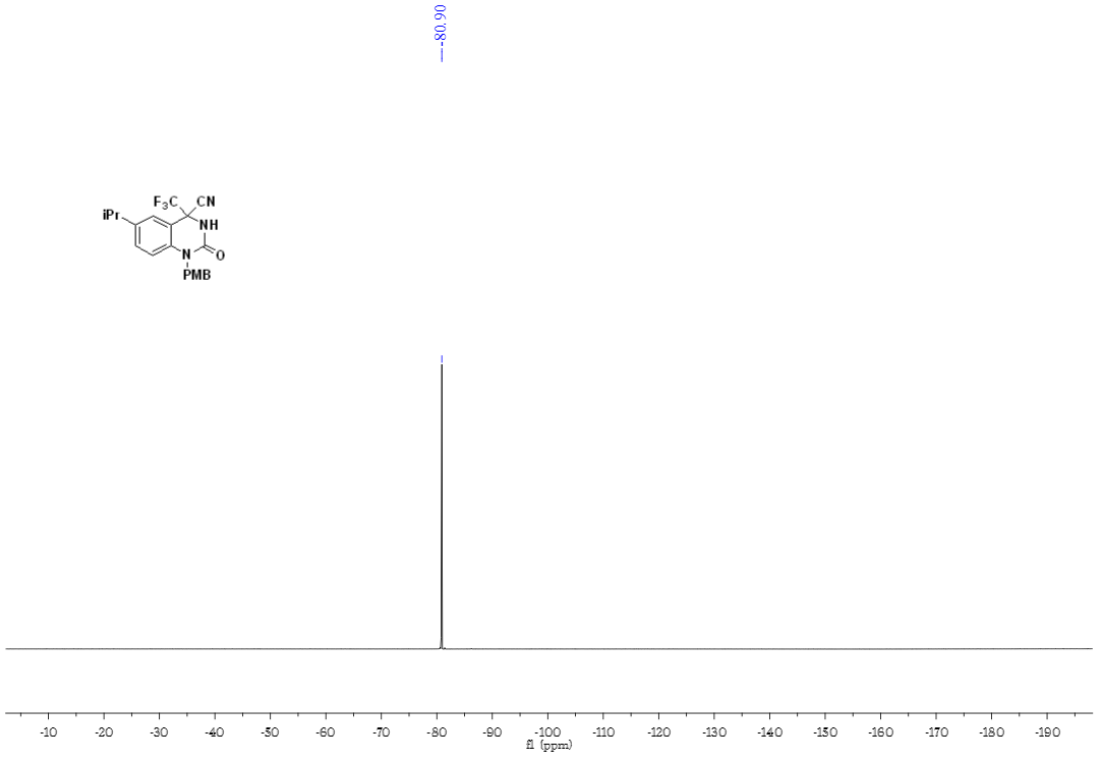
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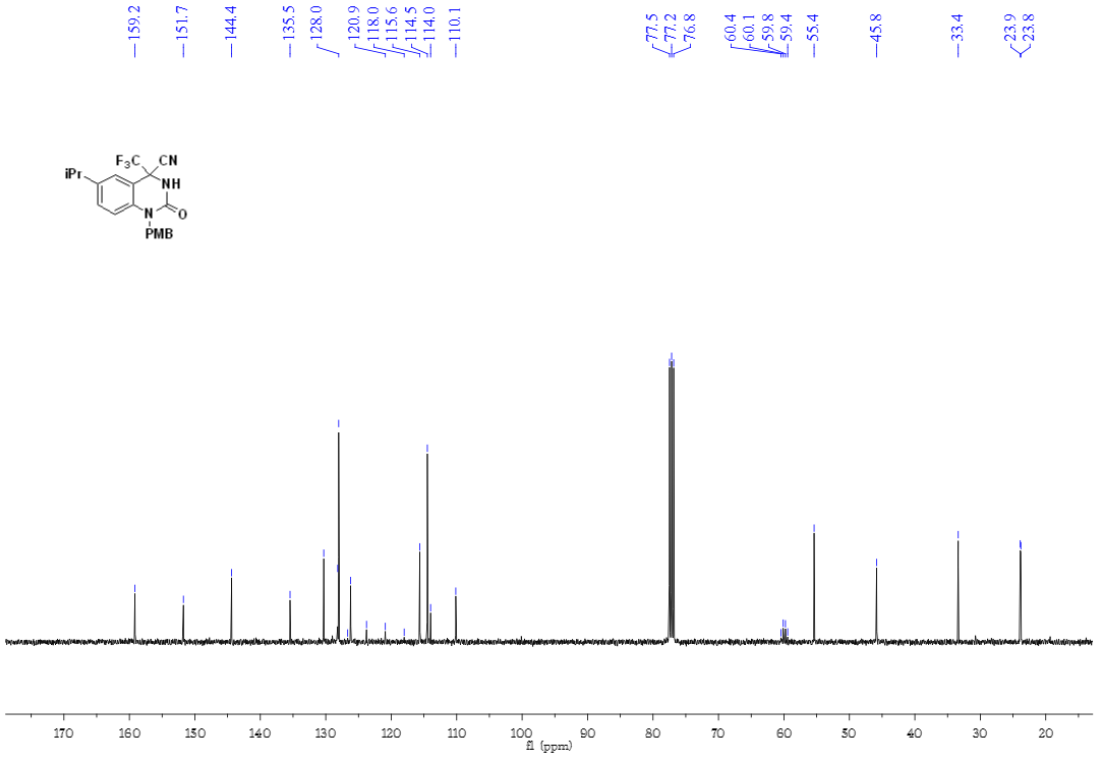
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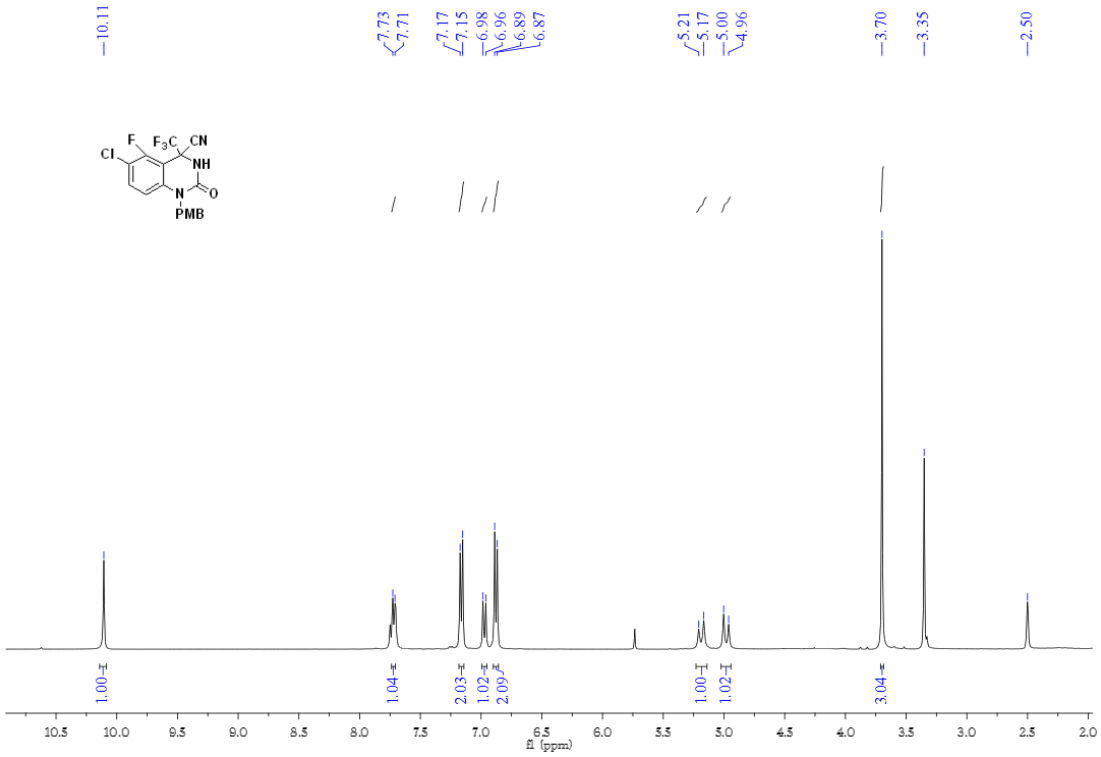
f1 (ppm)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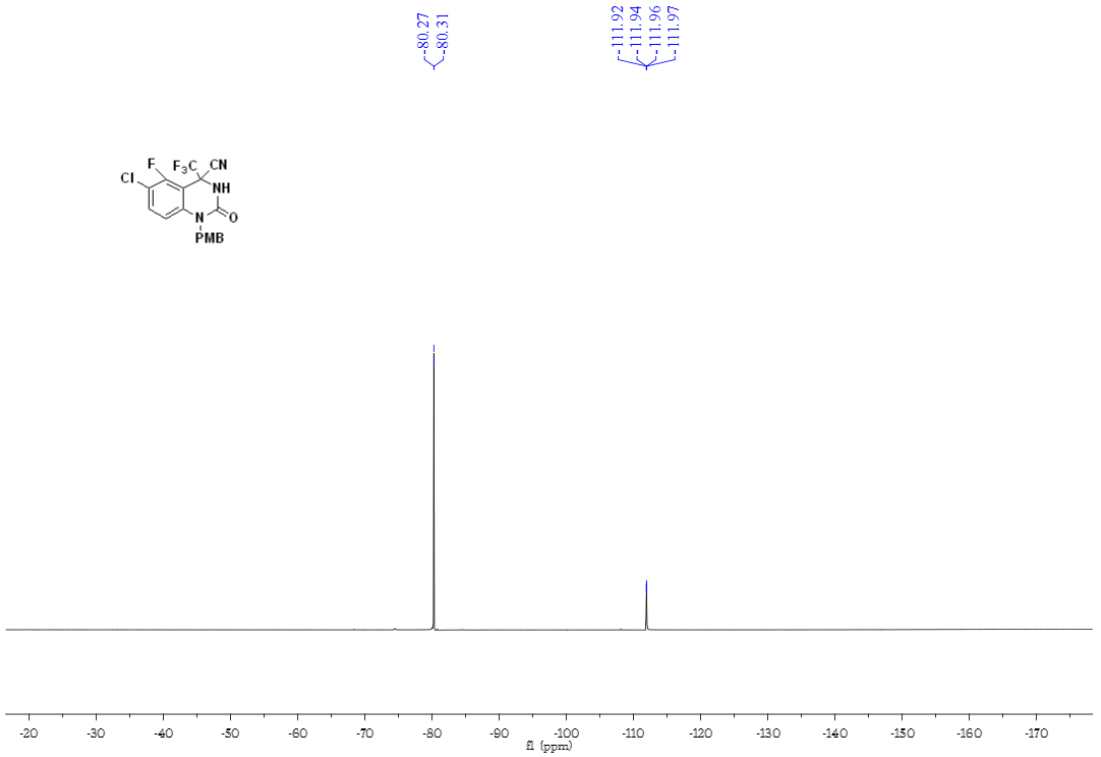
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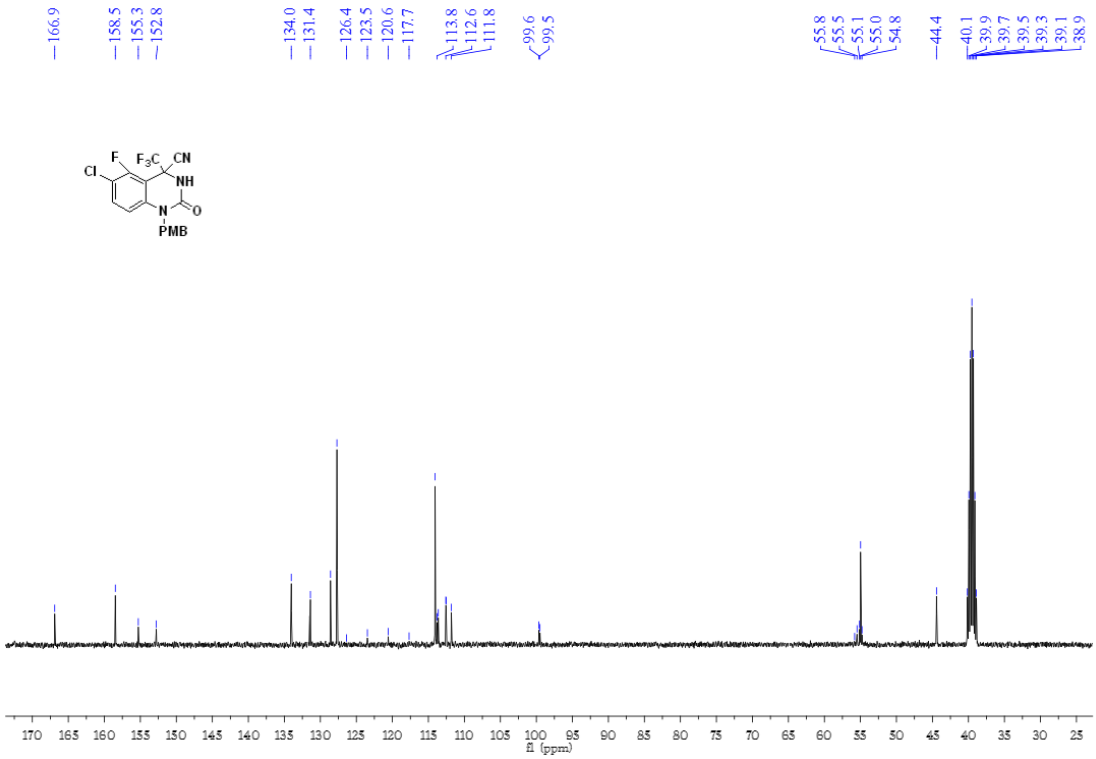
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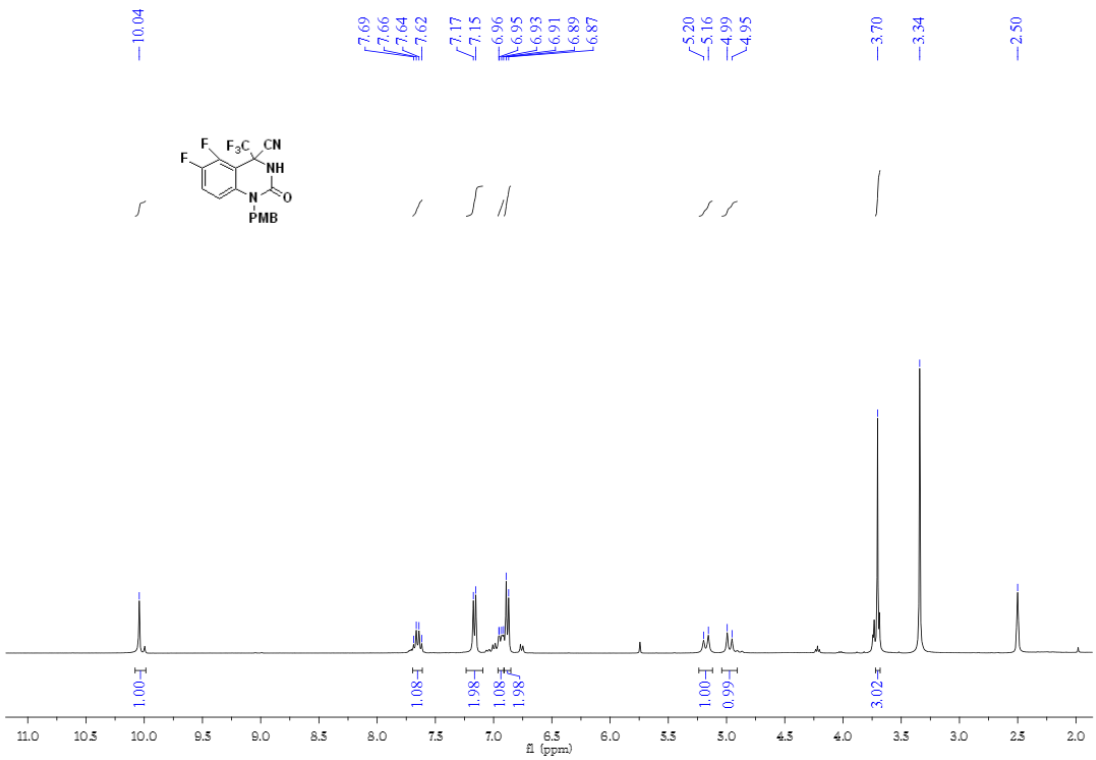
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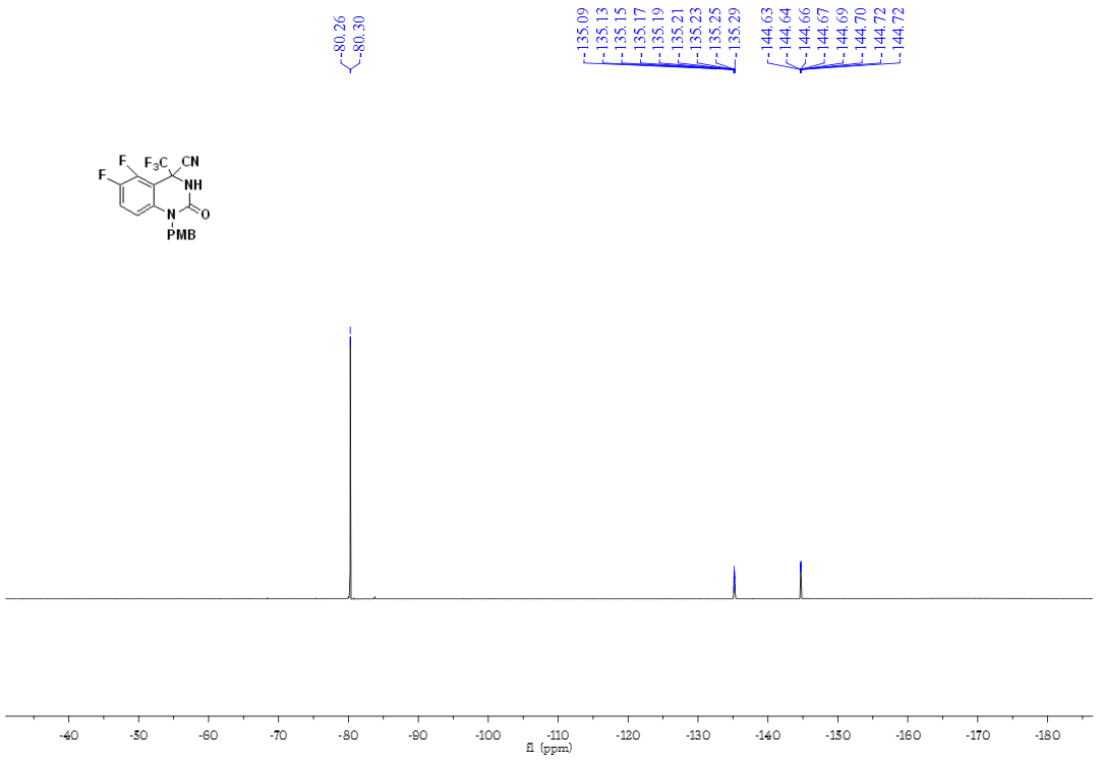
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-144.63
-144.64
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-144.67
-144.69
-144.70
-144.72
-144.72
F
F3C
CN
NH
N
O
PMB
-40
-50
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-70
-80
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-100
-110
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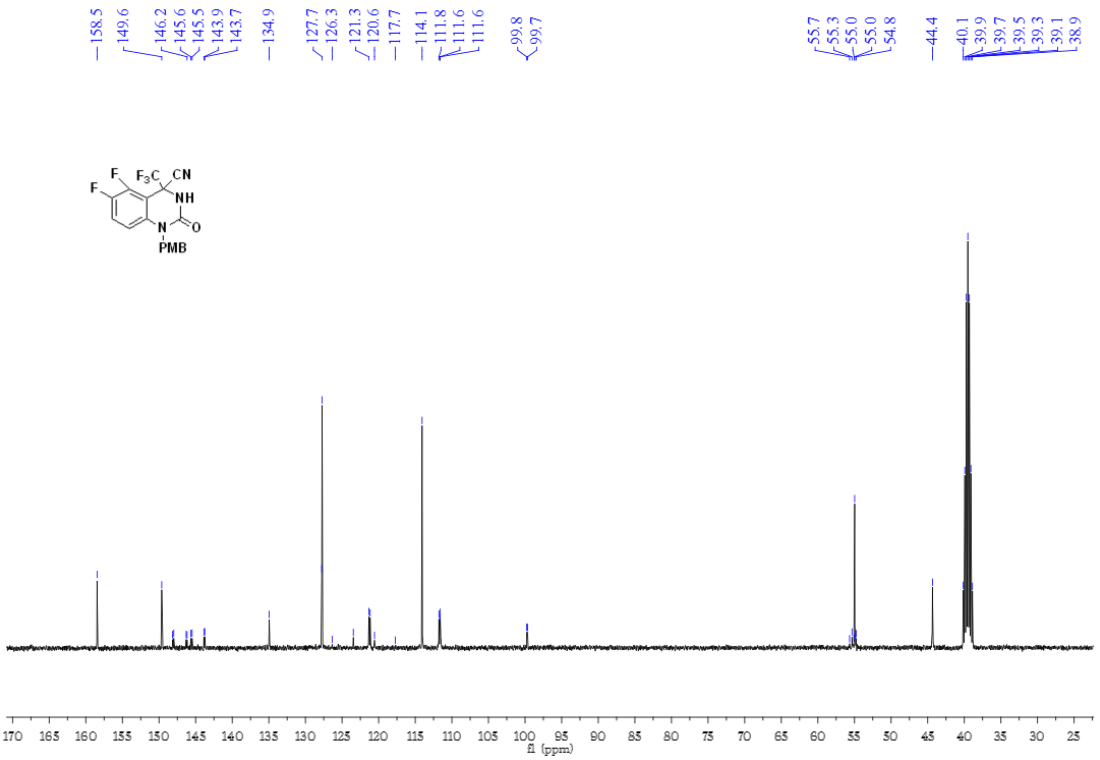
-130
-140
-150
-160
-170
-180
f1 (ppm)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55.3
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55.0
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39.7
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39.3
39.1
38.9
F
F3C
CN
NH
N
O
PMB
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155
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125
120
115
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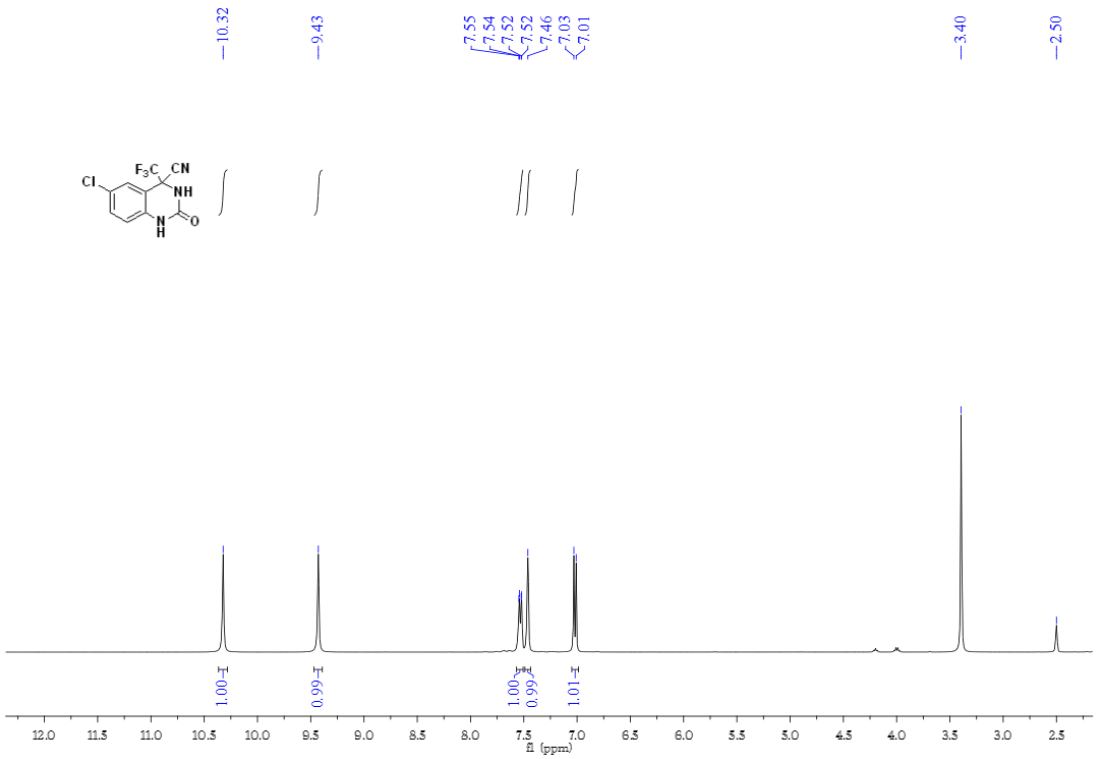
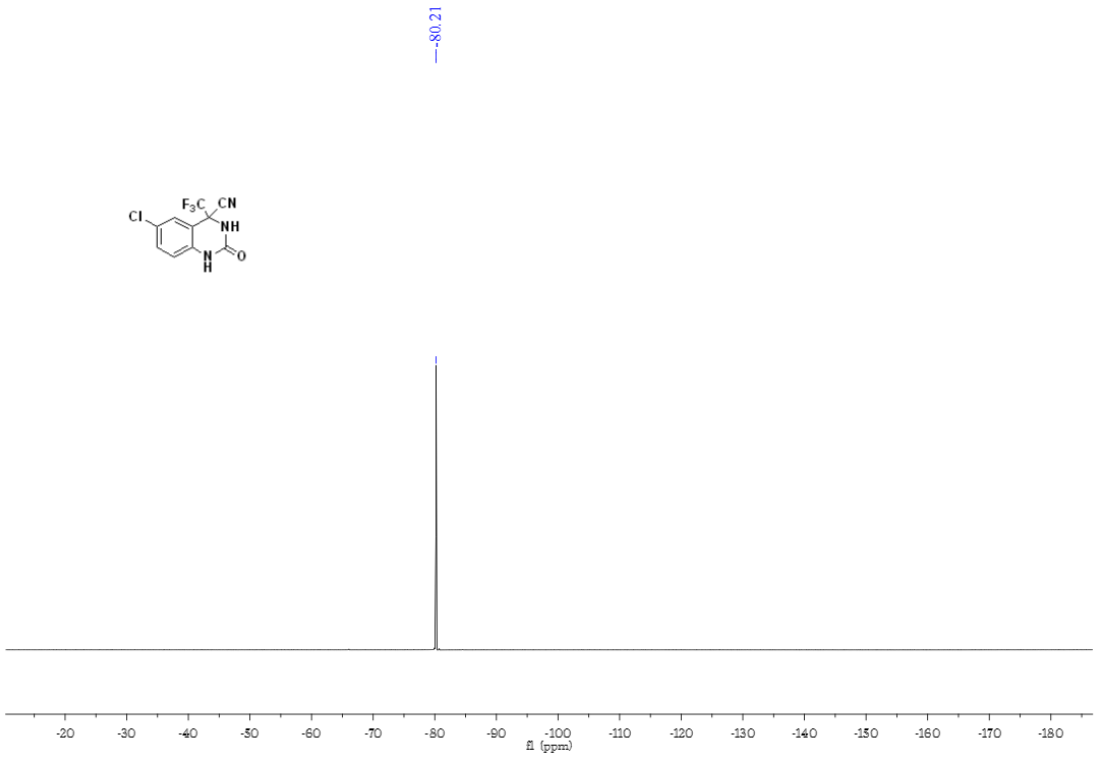
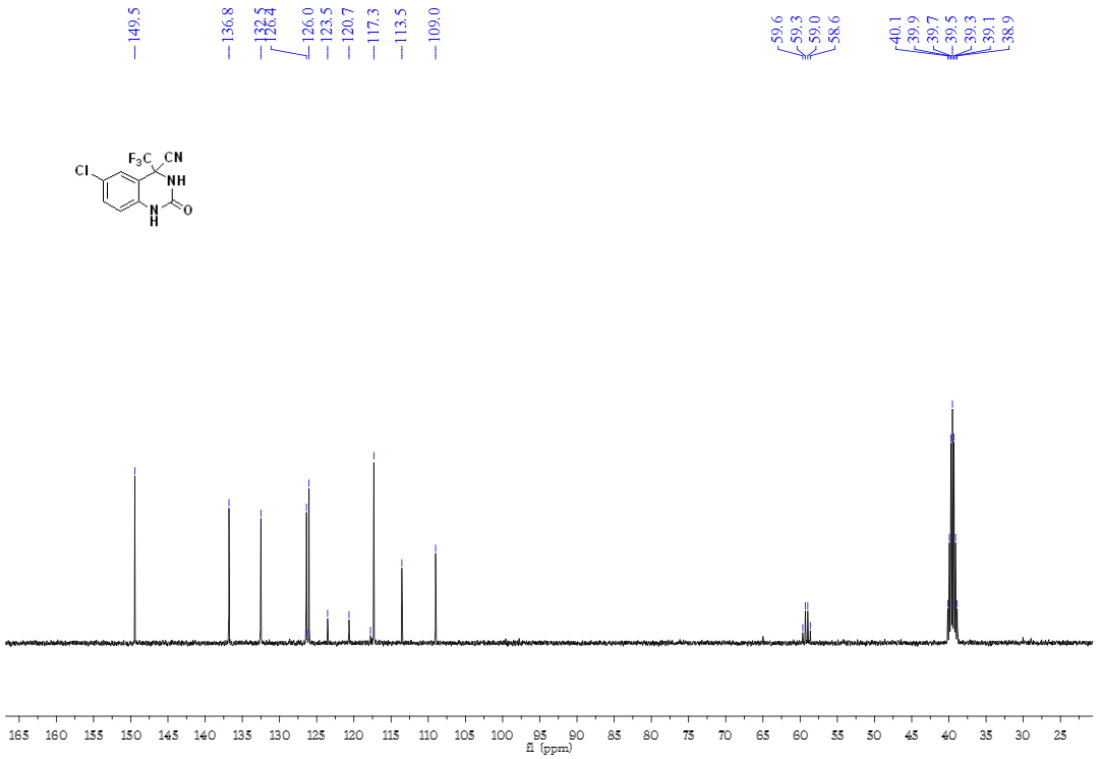
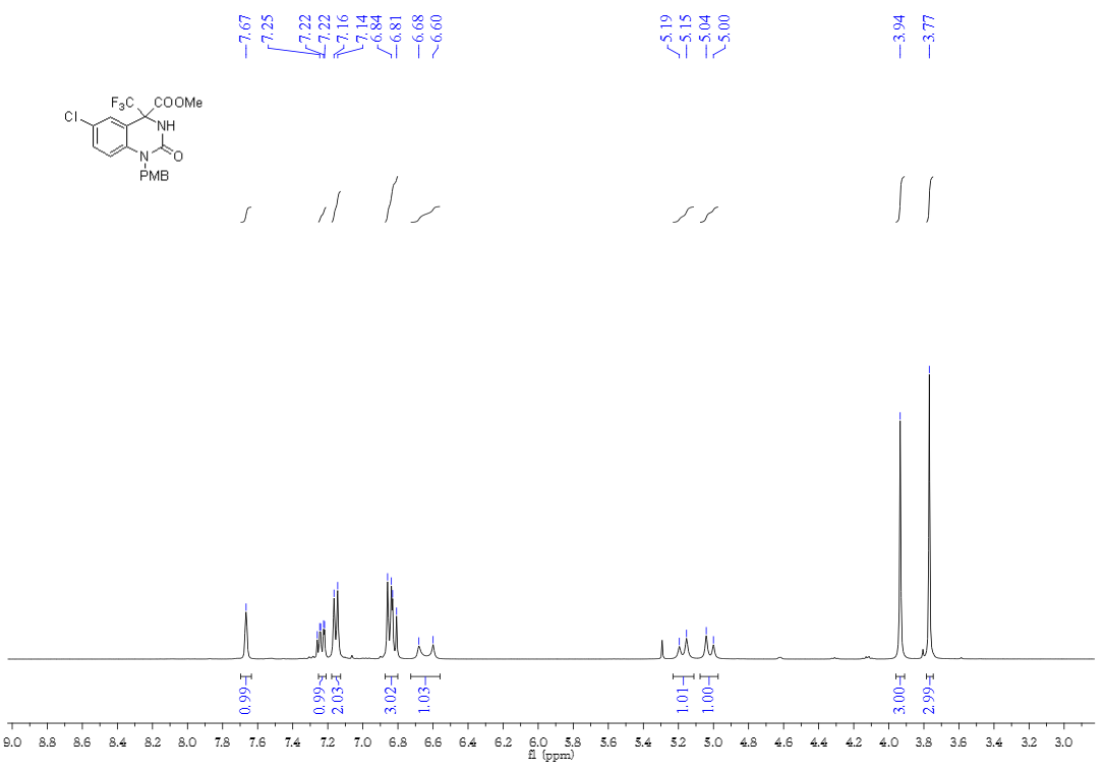
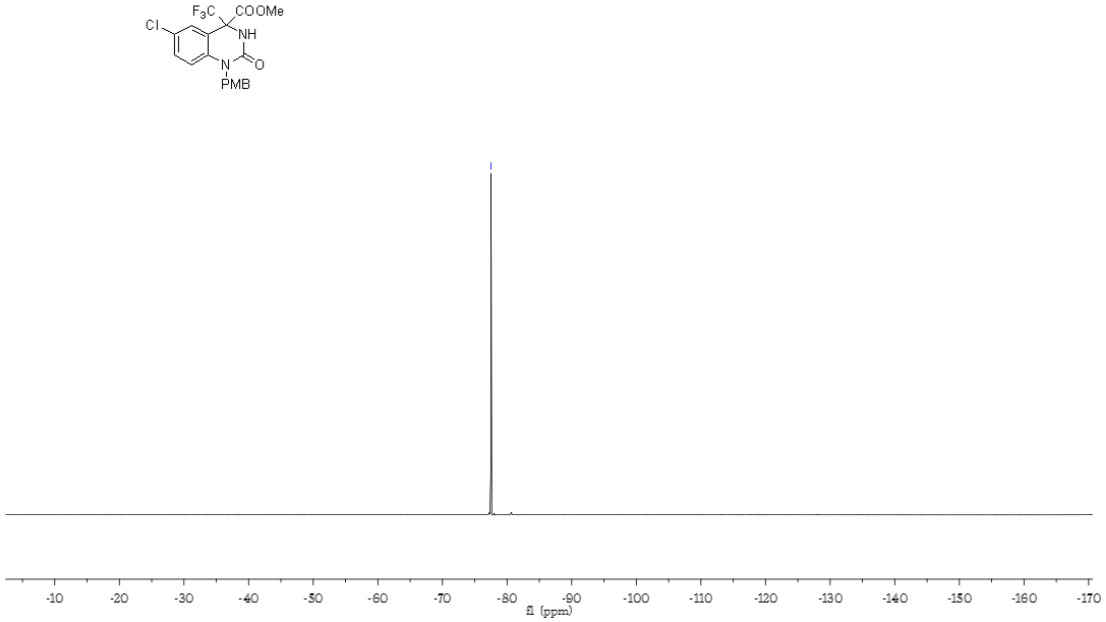
f1 (ppm)

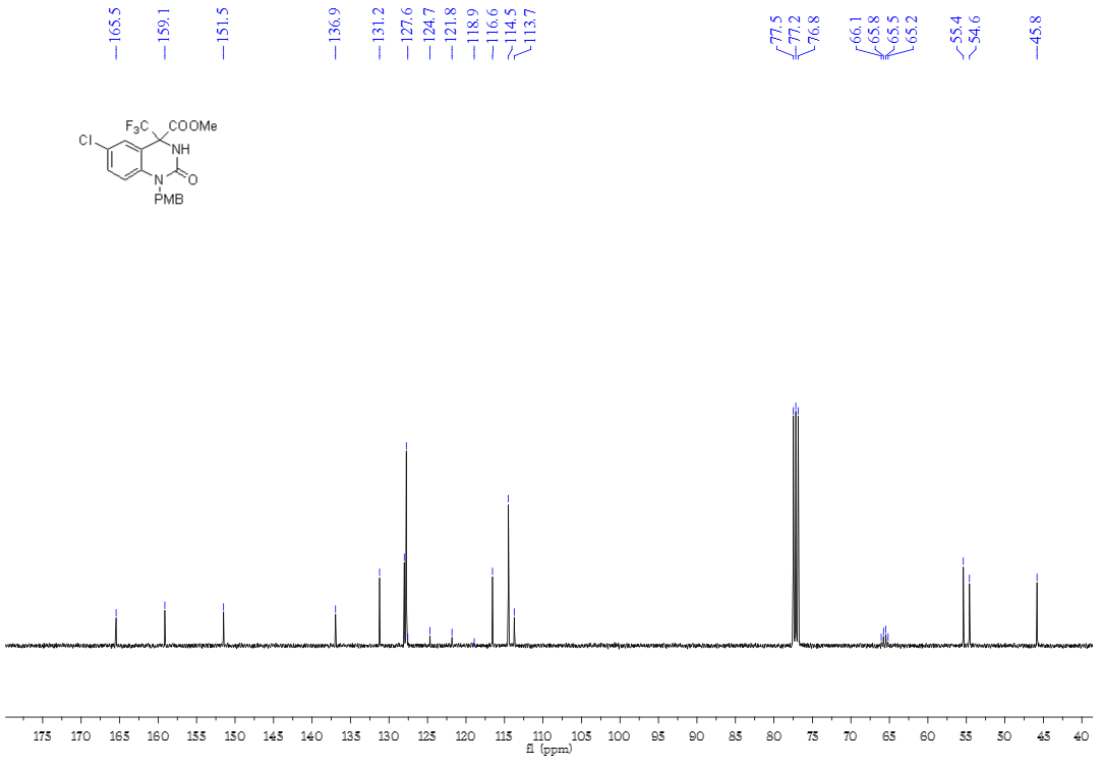


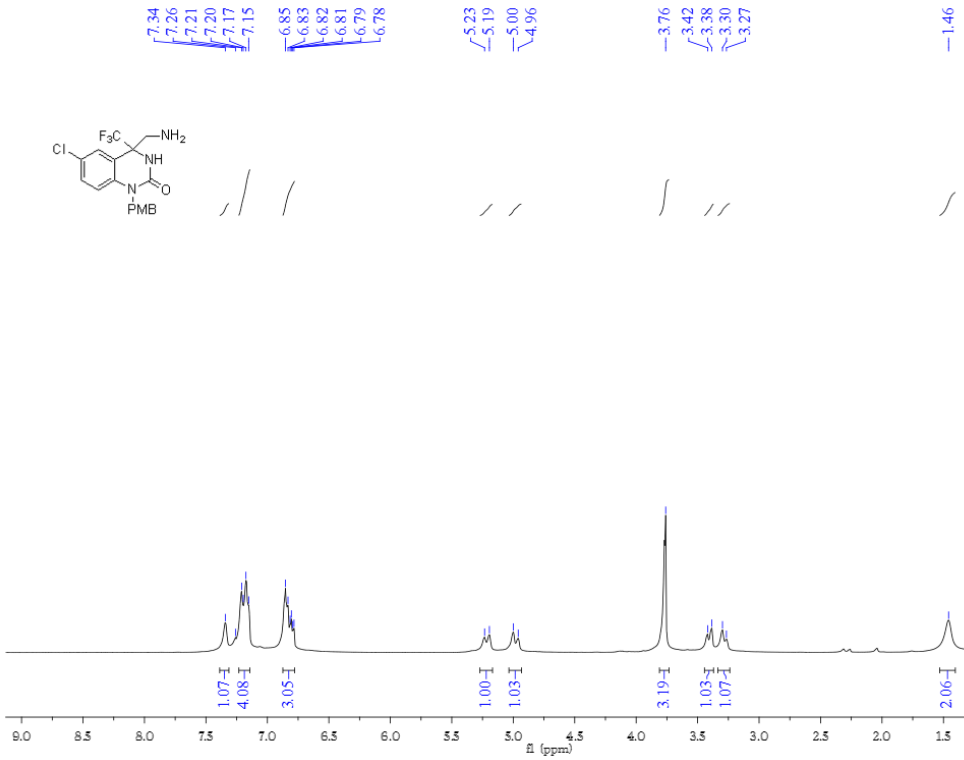








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3.30
3.27
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NH2
Cl
NH
N
O
PMB
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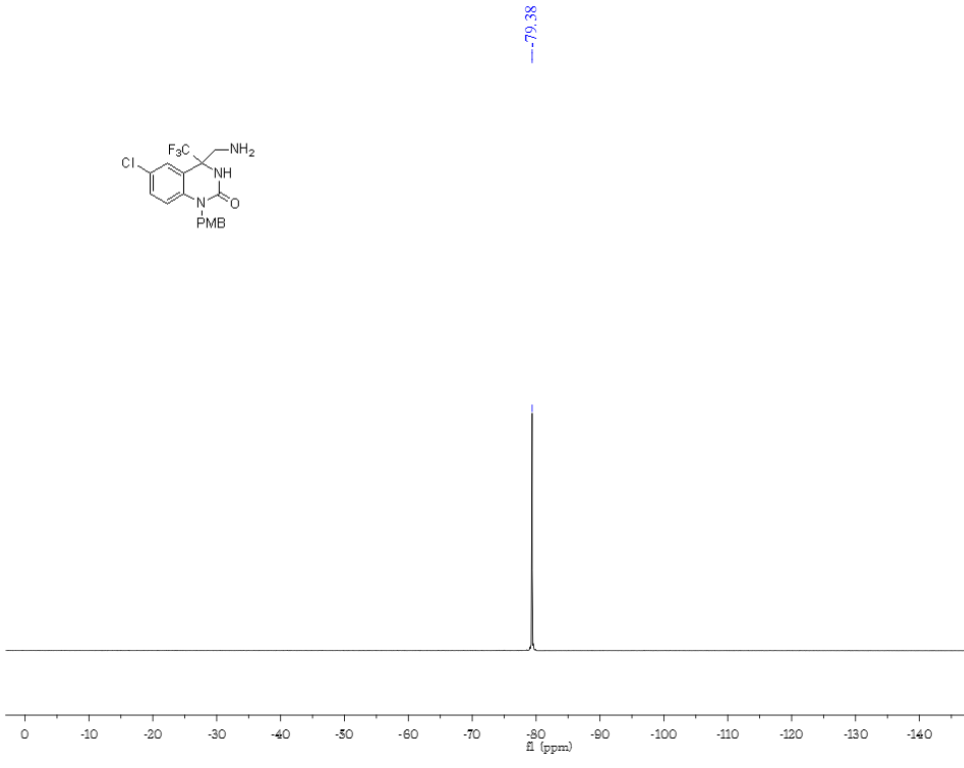
f1 (ppm)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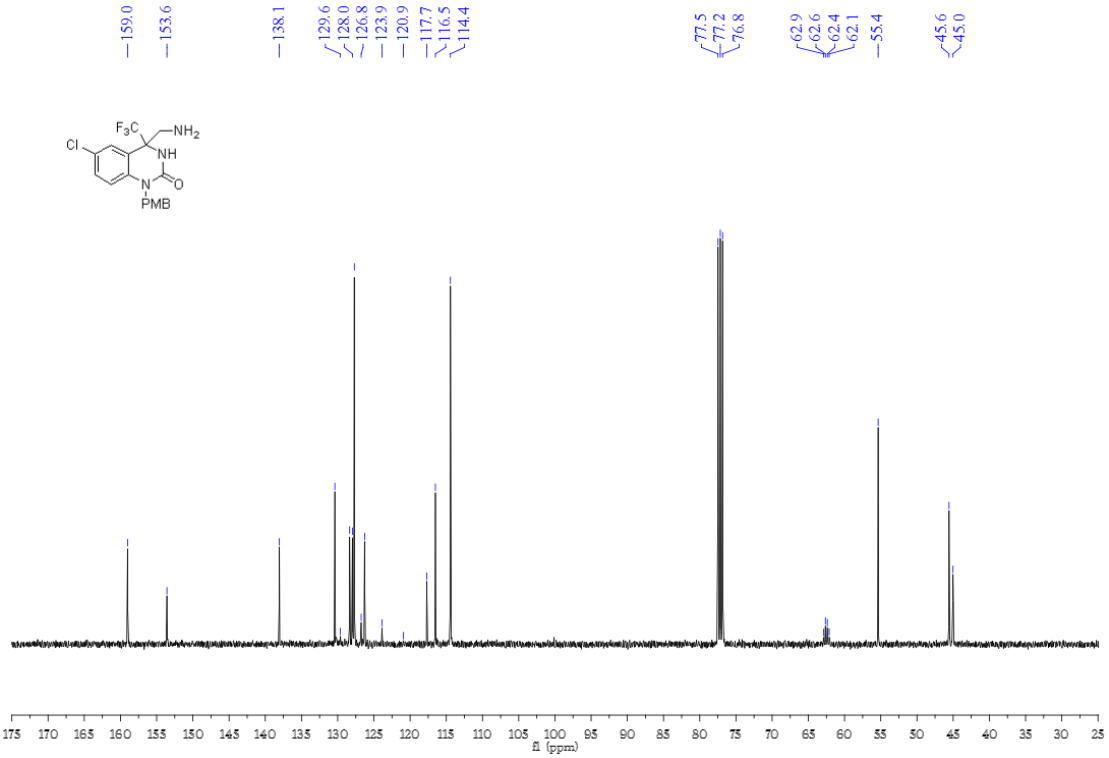
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116.5
114.4
77.5
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76.8
62.9
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55.4
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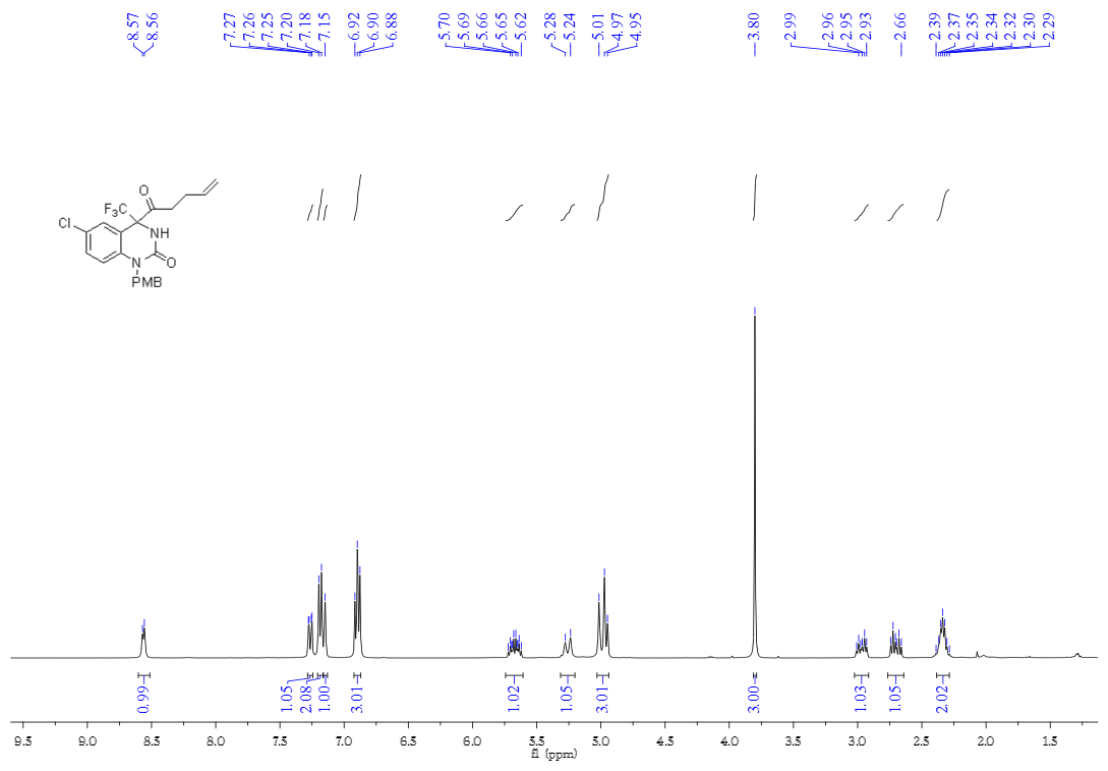
45.0
F3C
NH2
Cl
NH
N
O
PMB
f1 (ppm)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2.66
2.39
2.37
2.35
2.34
2.32
2.30
2.29
O
F3C
Cl
NH
N
O
PMB
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2.08
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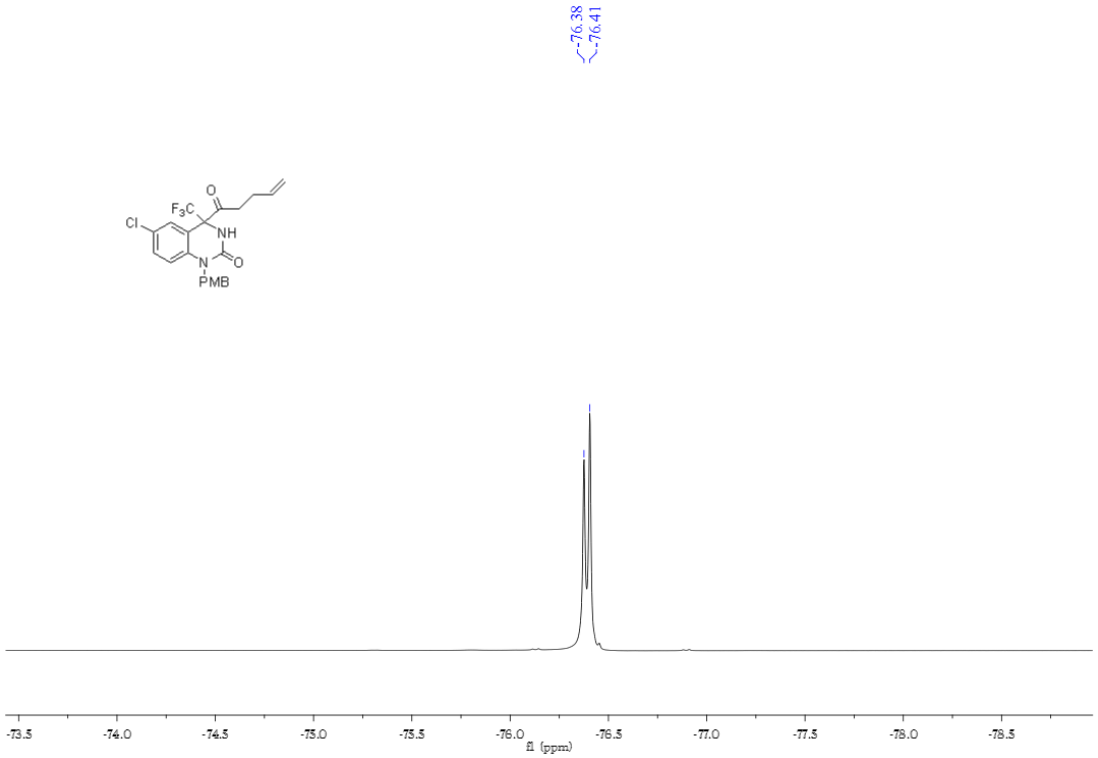
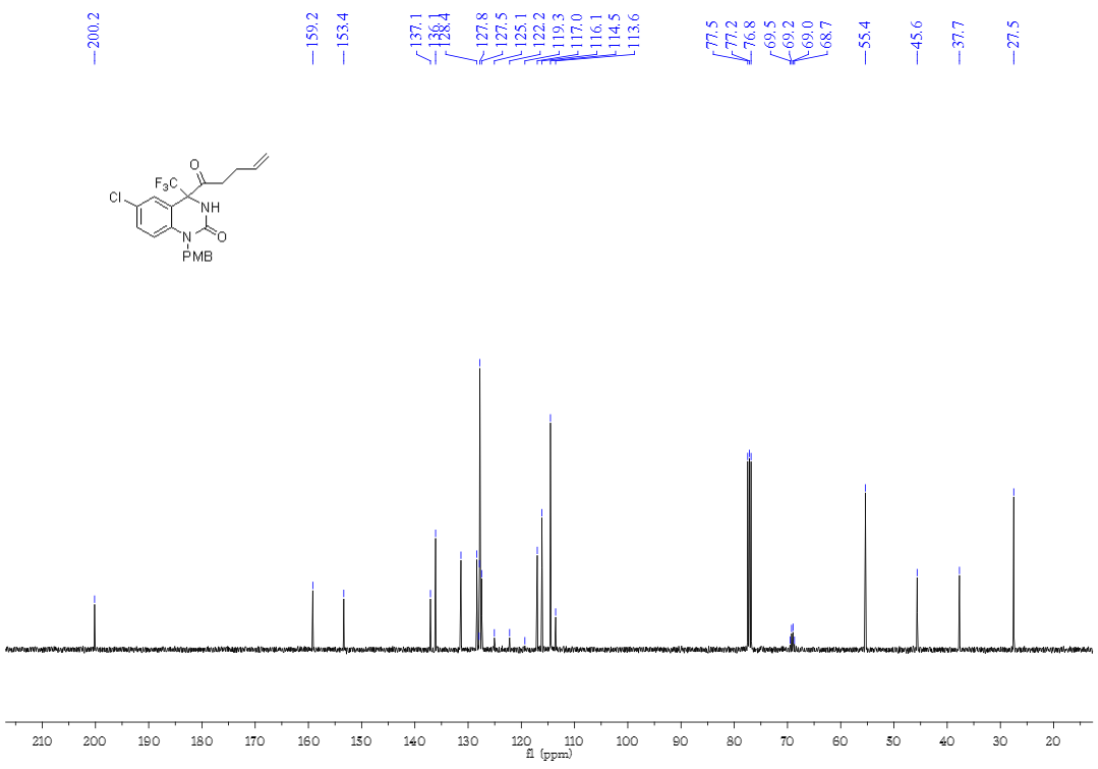
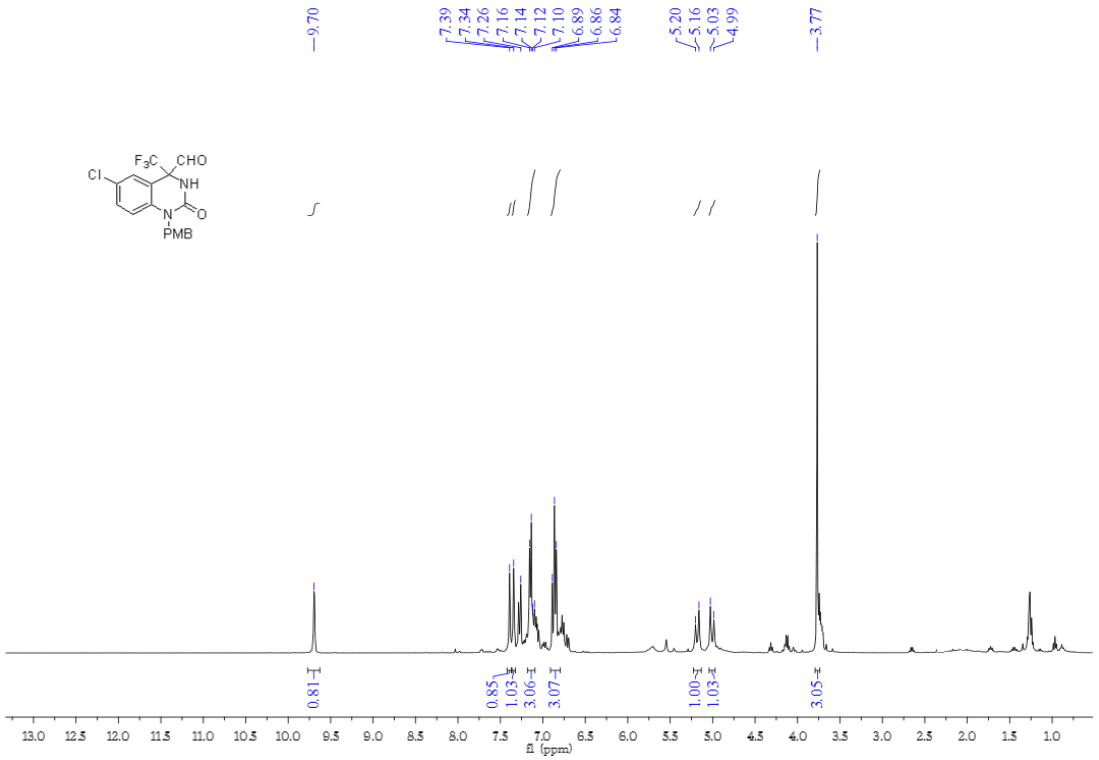
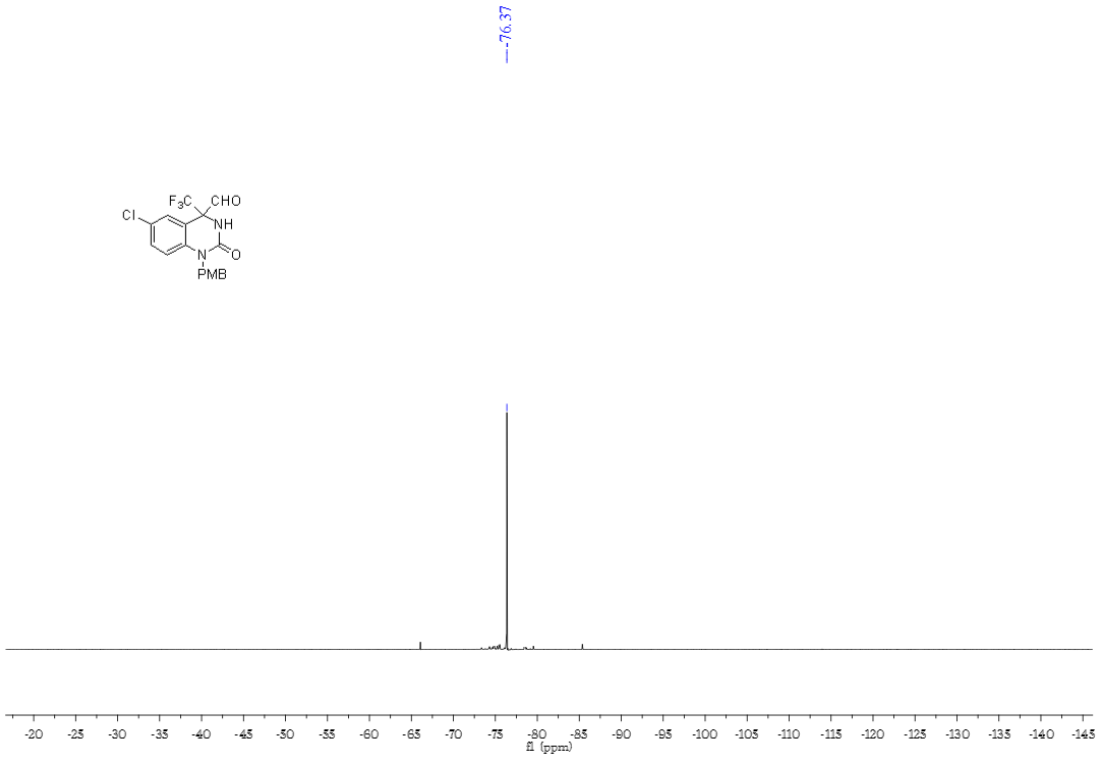
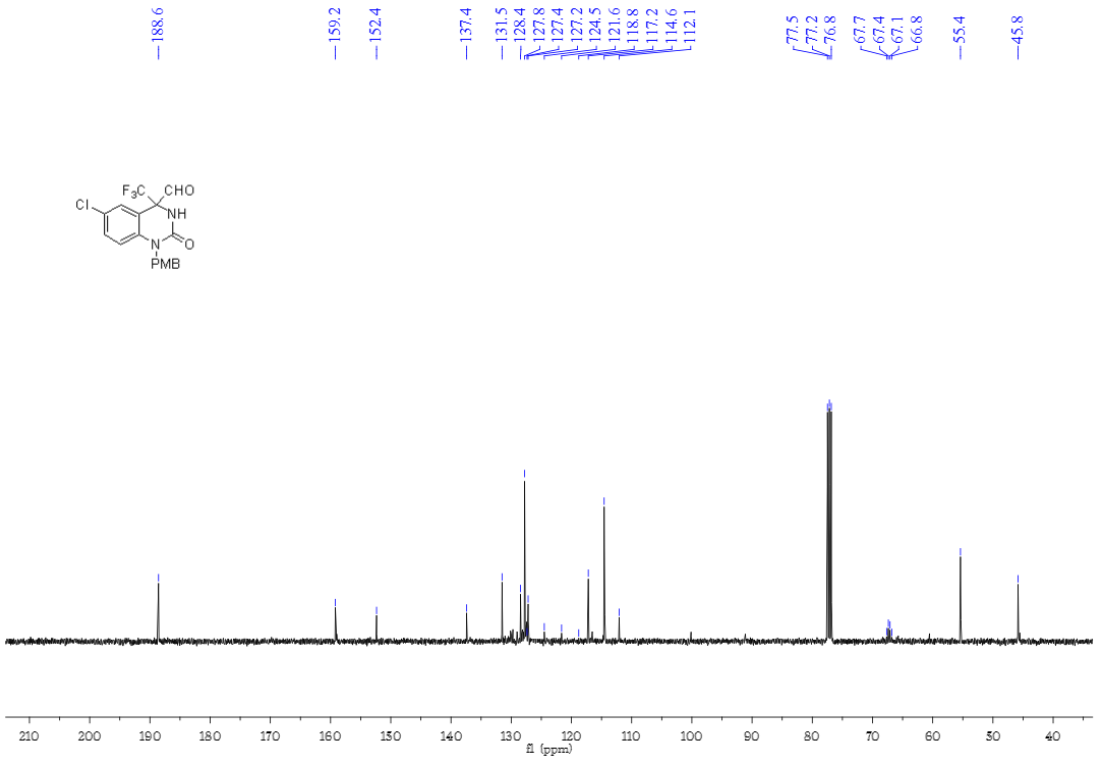
1.02
1.05
3.01
3.00
1.03
1.05
2.02
f1 (ppm)

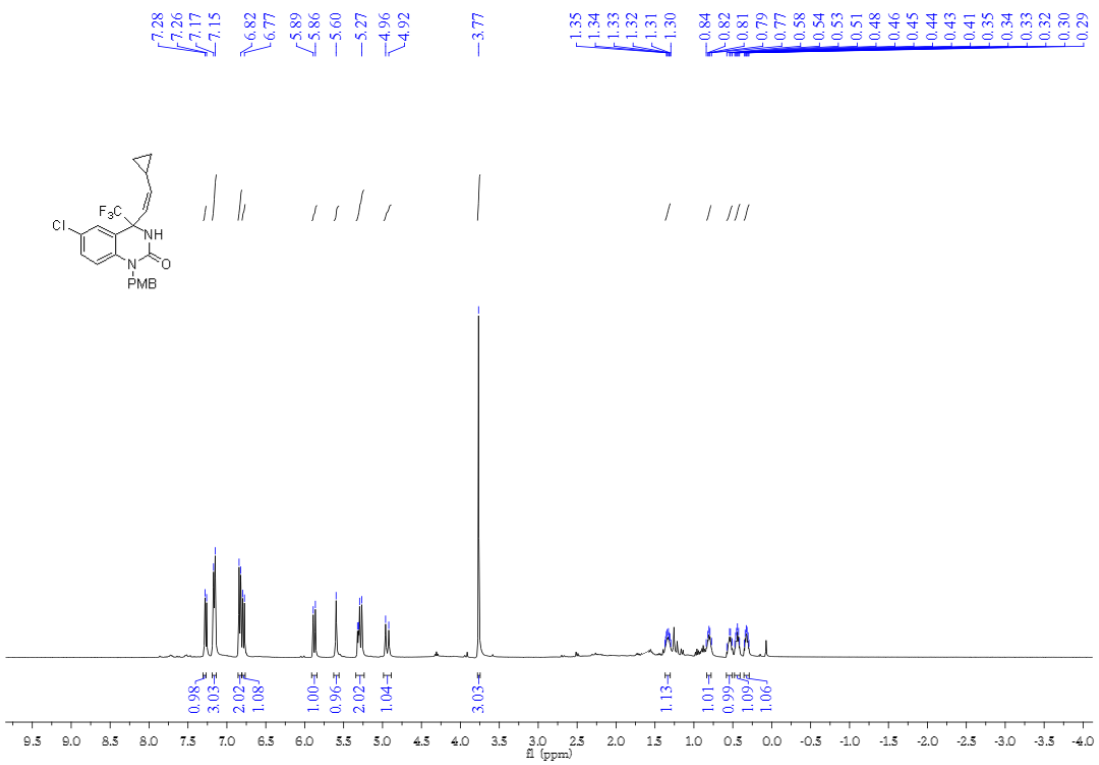


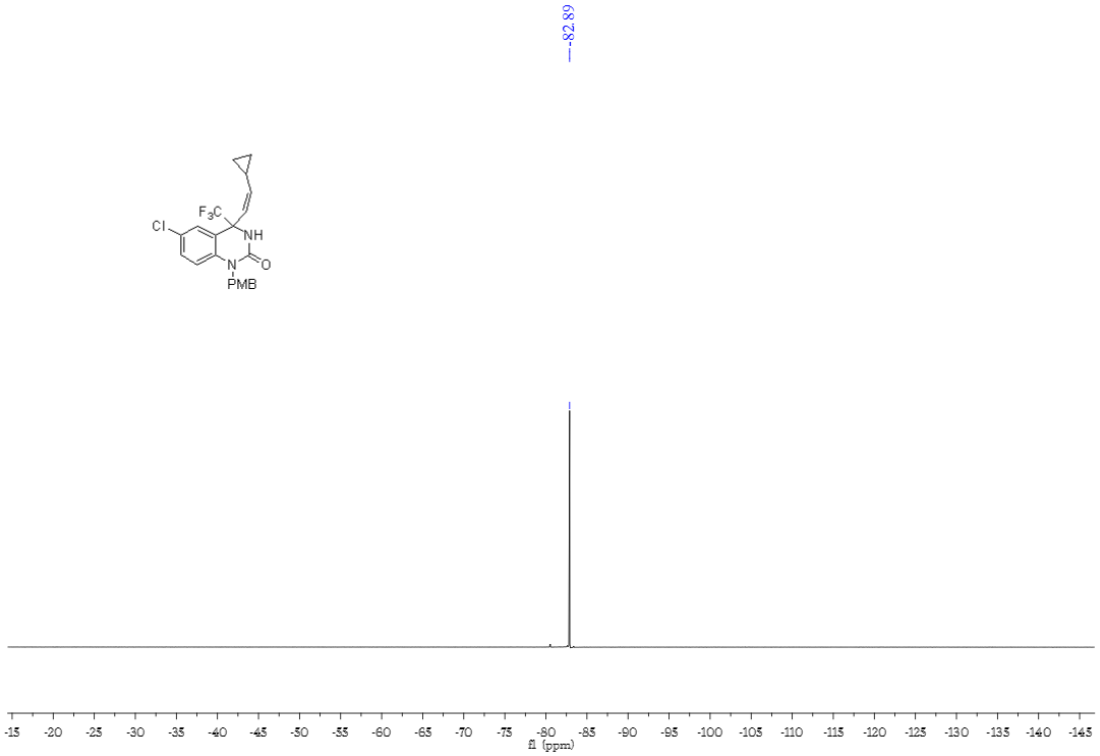


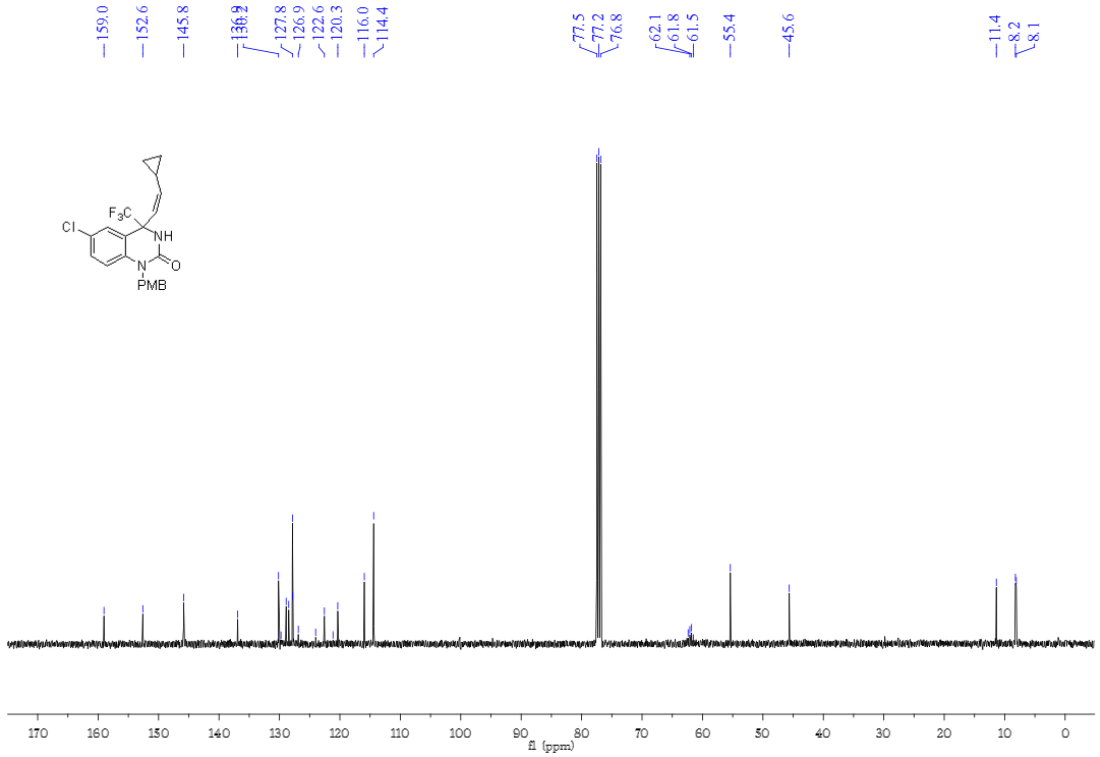


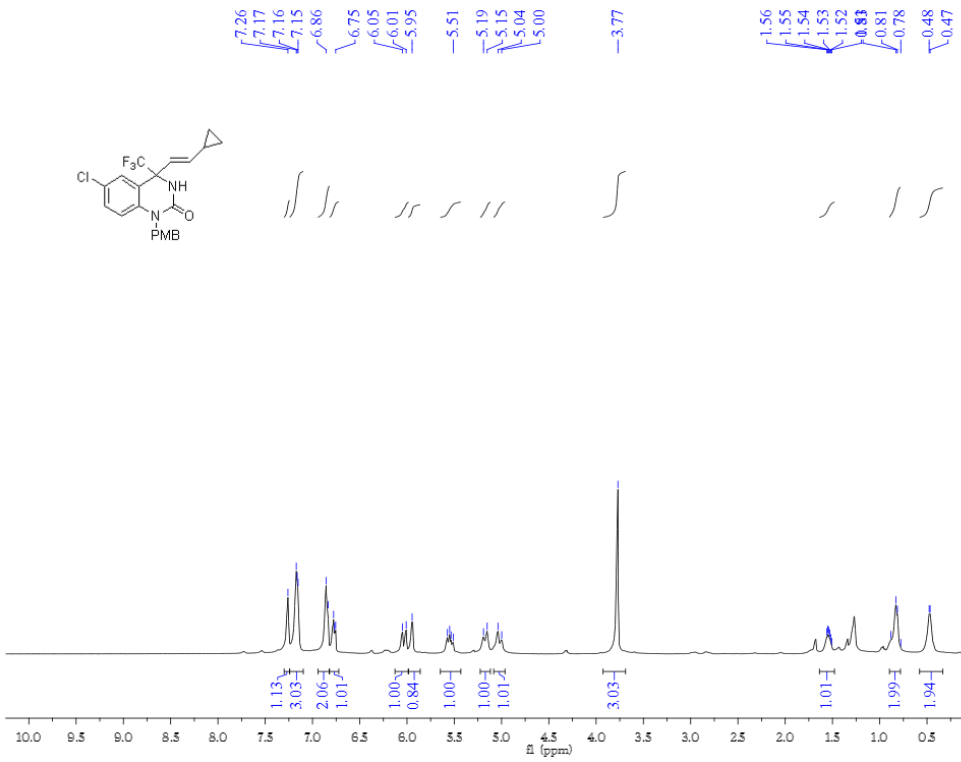


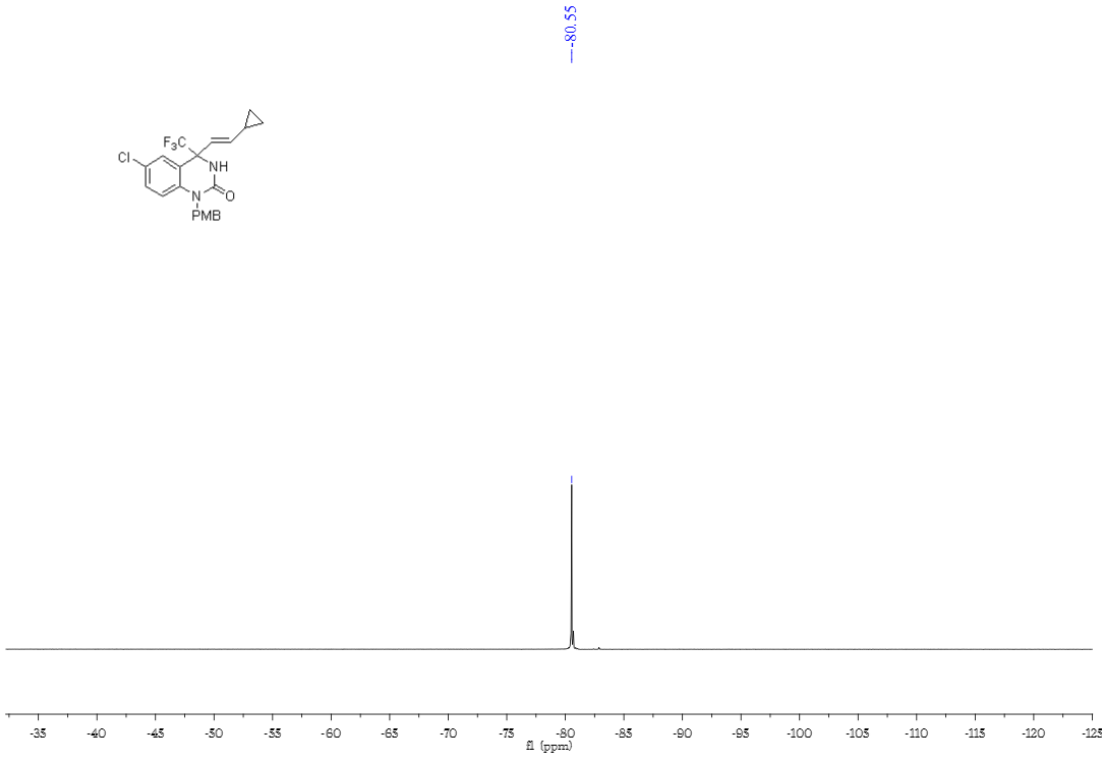


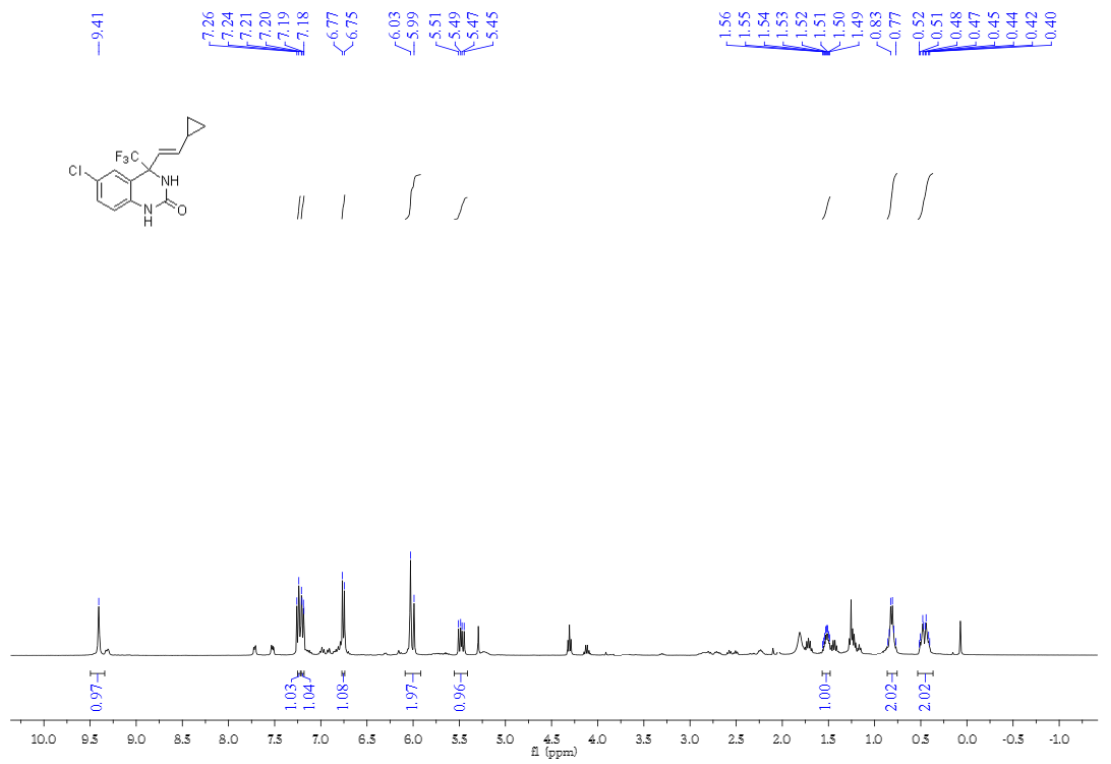


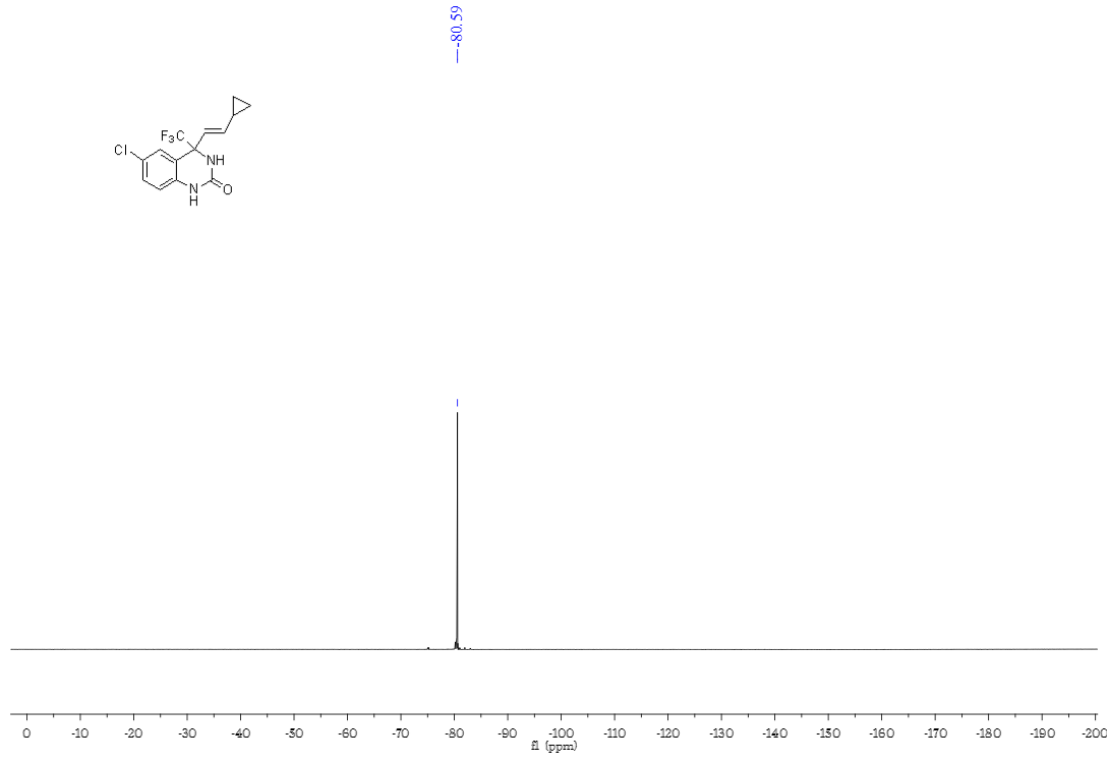






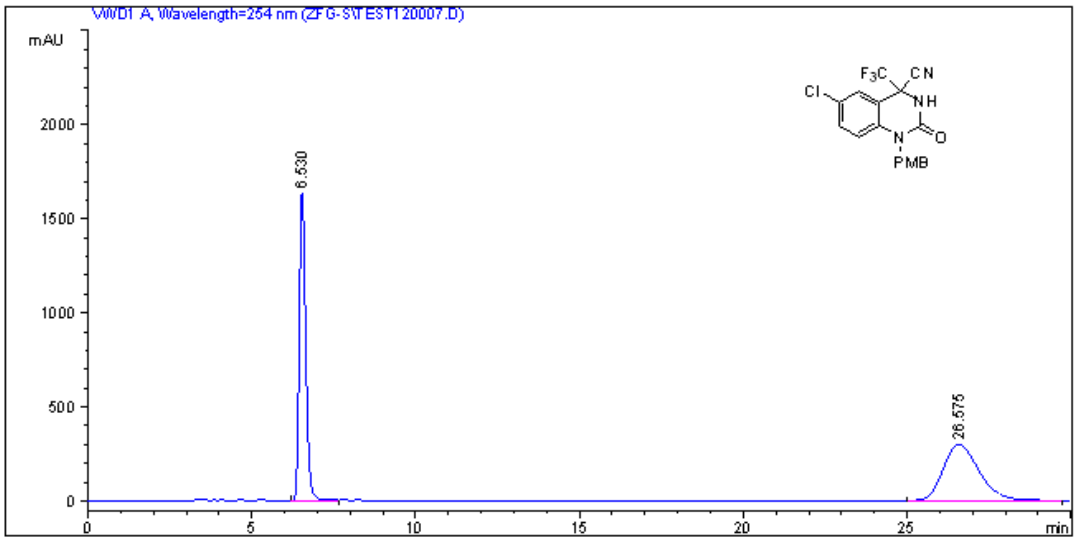






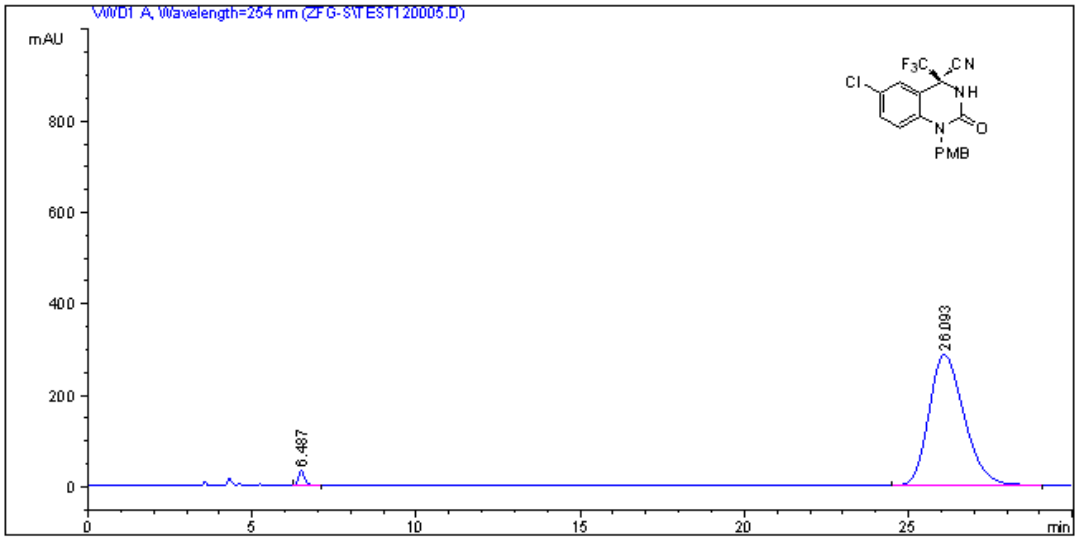
HPLC Charts of the Addition products and related compounds

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



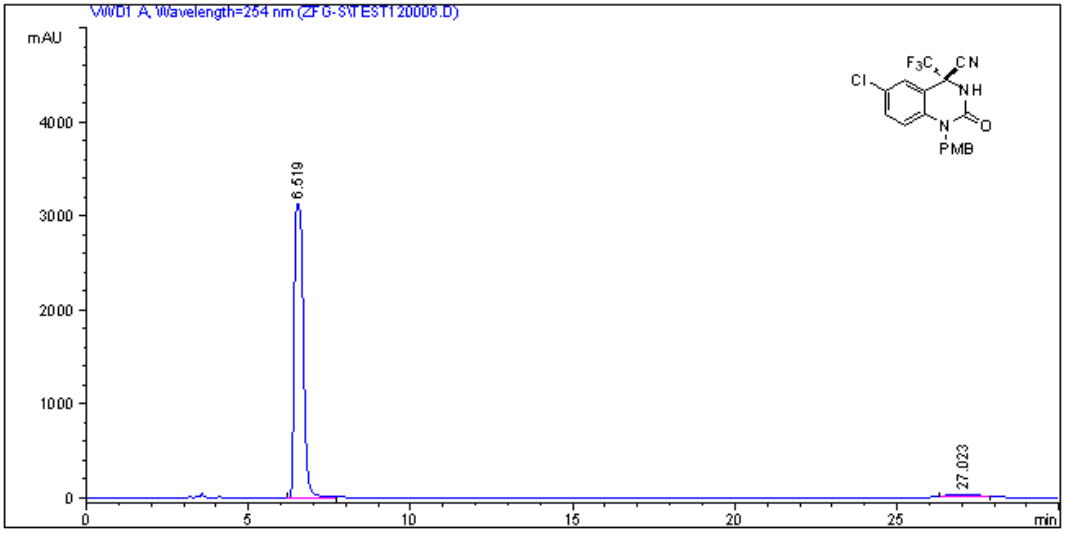
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.530	BV	0.2133	2.25682e4	1636.85852	49.9098
2	26.575	BB	1.1719	2.26498e4	300.04254	50.0902

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



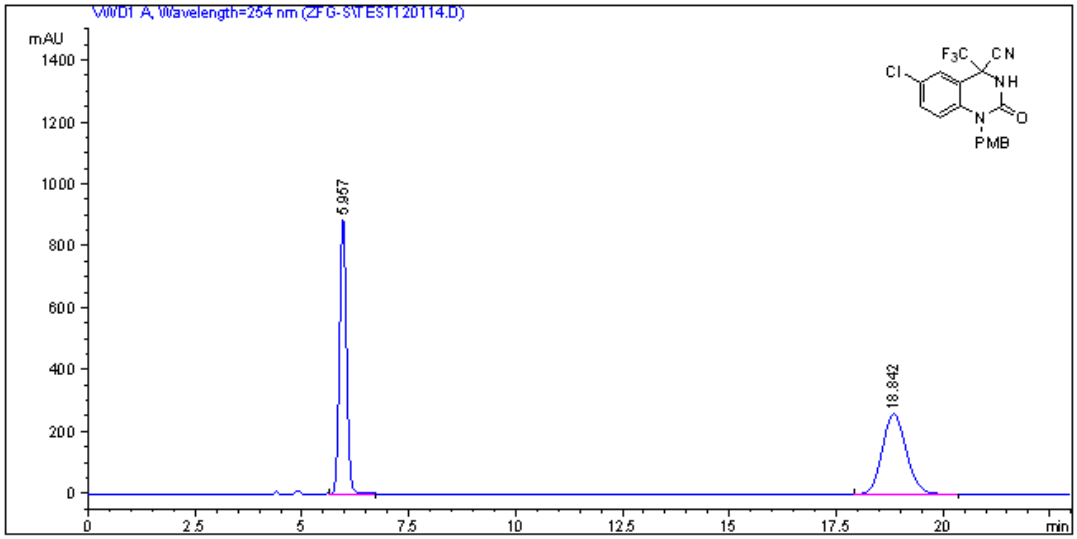
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.487	BB	0.2073	431.60437	31.90079	1.9875
2	26.093	BB	1.1486	2.12843e4	285.73413	98.0125

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



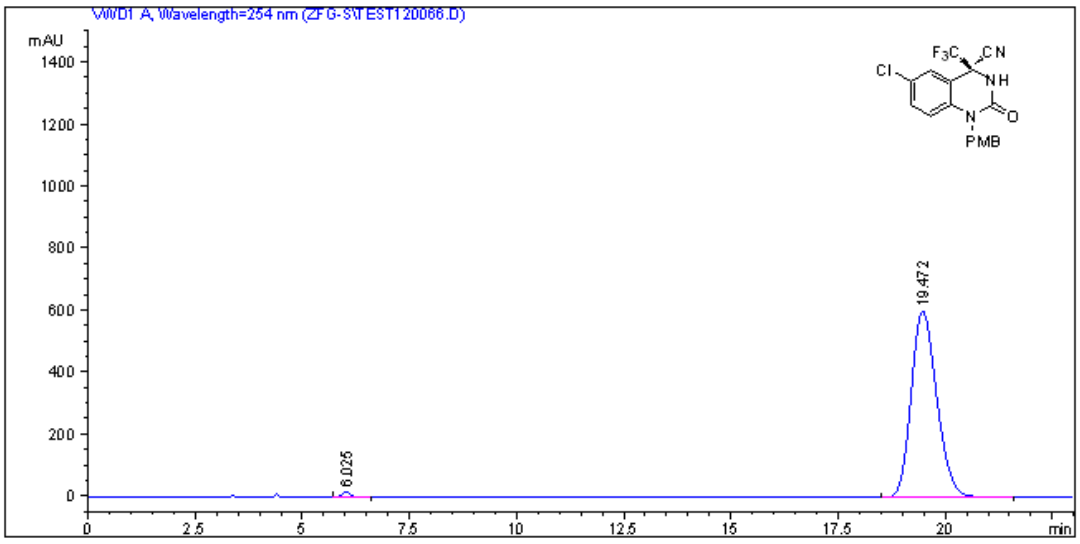
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.519	VV	0.3083	6.01130e4	3133.62402	97.6564
2	27.023	PP	0.9225	1442.64807	26.06297	2.3436

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



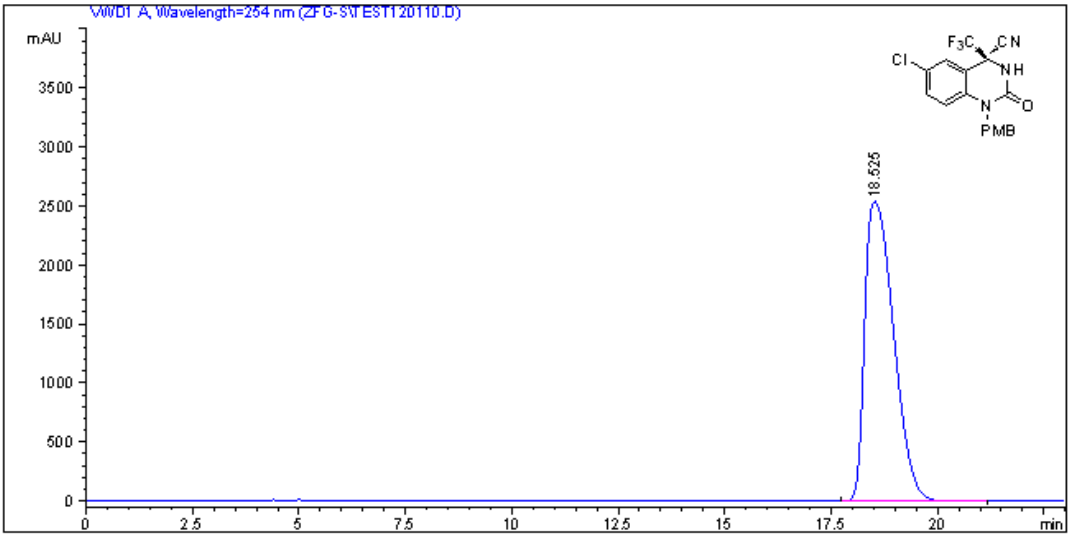
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.957	VB	0.1764	1.00788e4	886.22485	49.9581
2	18.842	BB	0.6034	1.00957e4	258.95340	50.0419

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



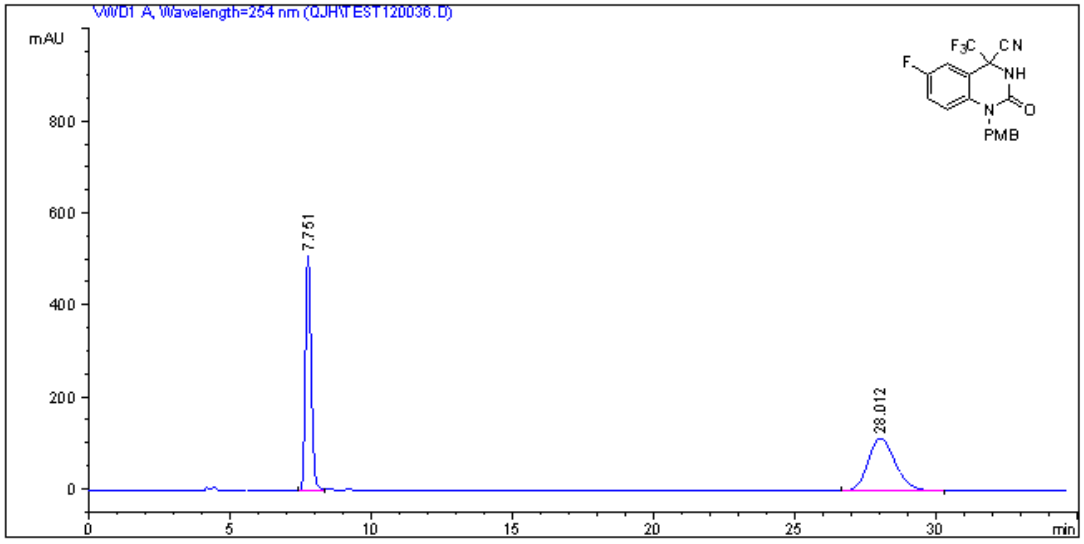
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.025	VV	0.2185	278.78836	18.92403	1.1011
2	19.472	BB	0.6432	2.50413e4	601.23950	98.8989

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



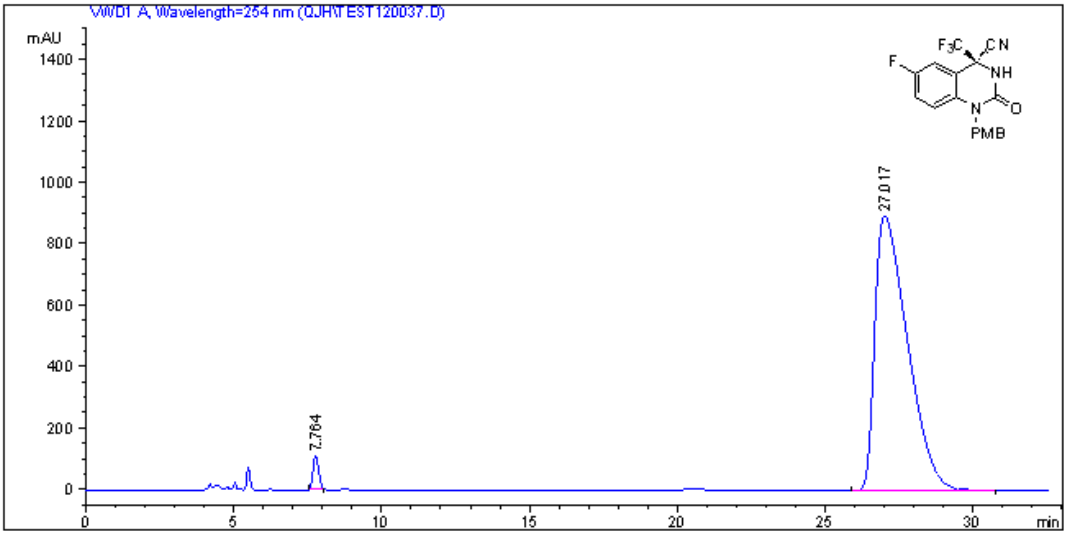
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.525	BB	0.7448	1.19660e5	2539.82446	100.0000

Sample Info : 254 nm, IC, i-PrOH : Hexane =25:75, 0.8mL/min



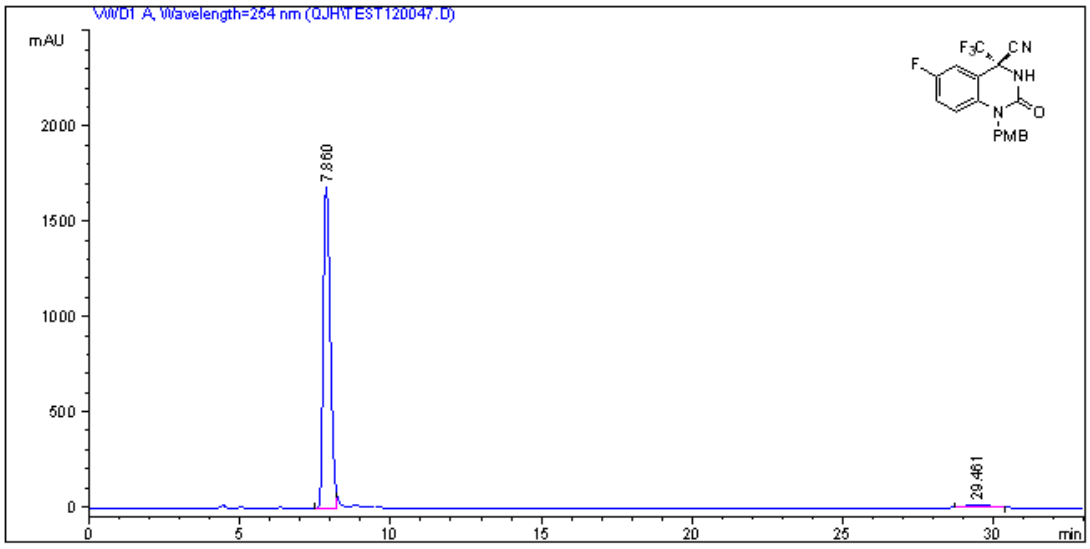
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.751	VV	0.2218	7301.42285	511.66769	48.8391
2	28.012	BB	1.0393	7648.53467	113.95336	51.1609

Sample Info : 254 nm, IC, i-PrOH : Hexane =25:75, 0.8mL/min



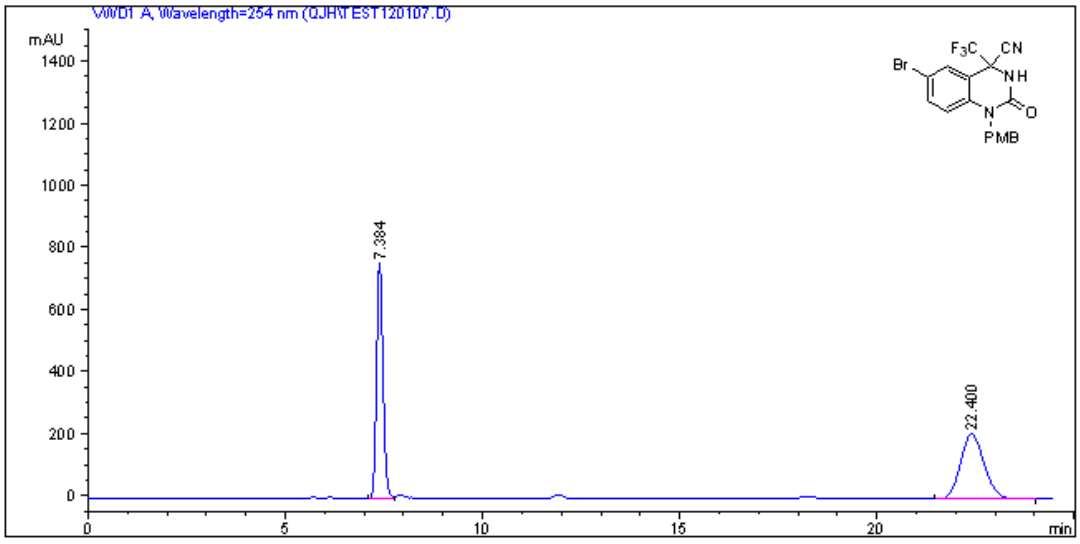
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.764	MM	0.2167	1411.40271	108.56749	2.0171
2	27.017	BB	1.1825	6.85597e4	894.45624	97.9829

Sample Info : 254 nm, IC, i-PrOH : Hexane =25:75, 0.8 mL/min



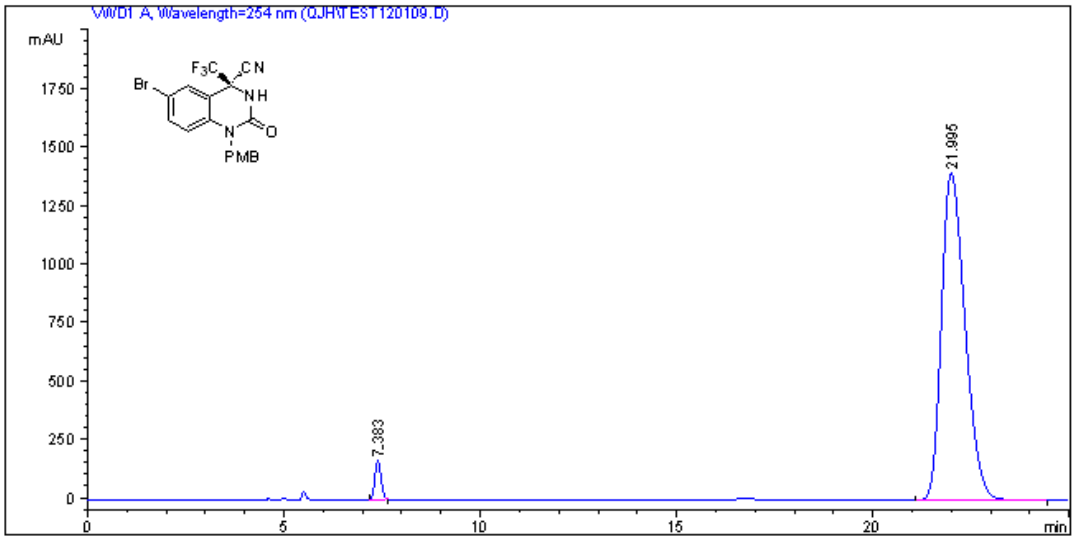
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.860	VBA	0.2597	2.74443e4	1686.77698	97.5284
2	29.461	MM	0.9472	695.49005	12.23808	2.4716

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



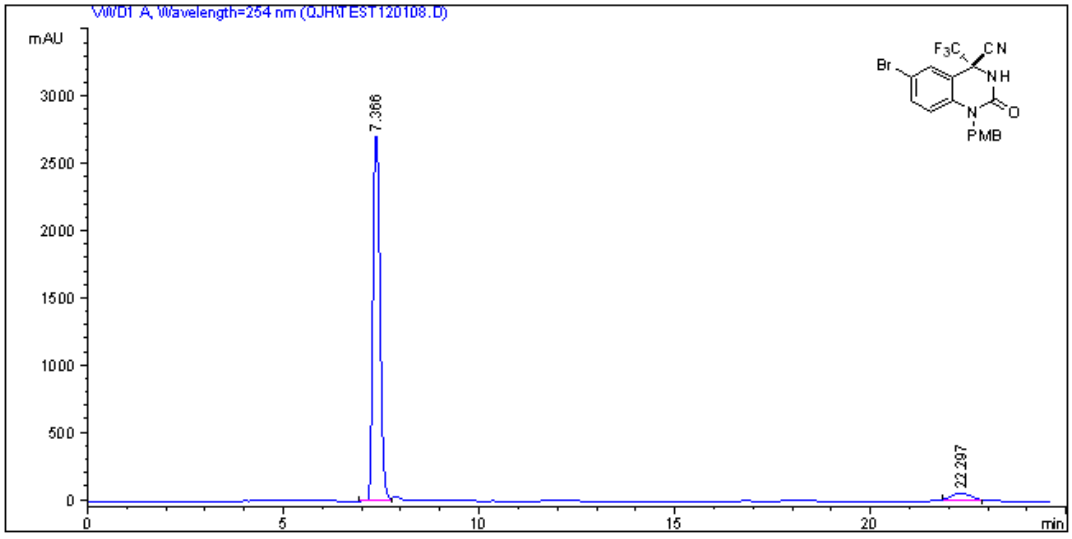
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.384	VV	0.1765	8628.00879	758.04370	49.7068
2	22.400	BB	0.6501	8729.77930	209.14067	50.2932

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



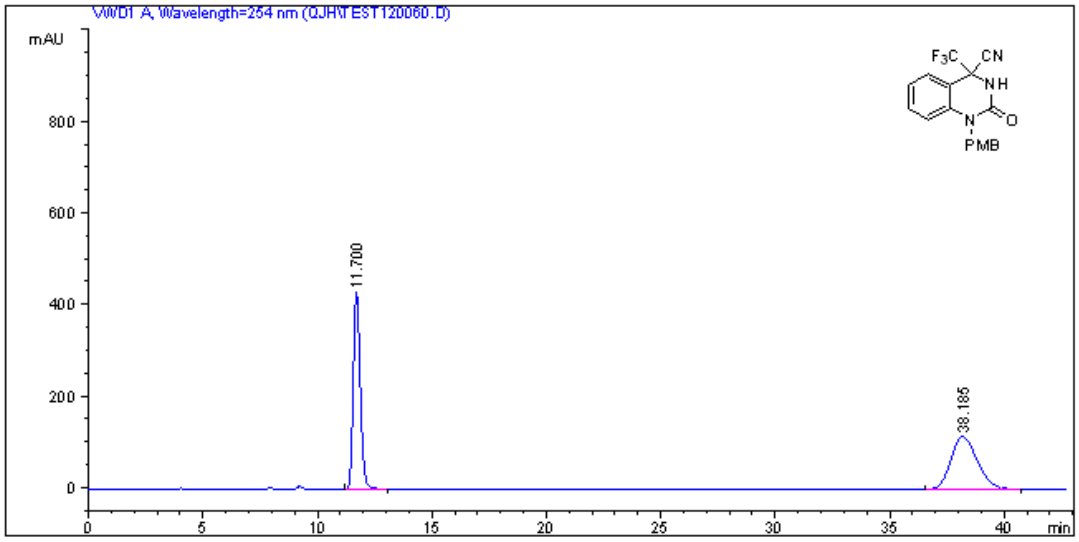
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.383	MM	0.1828	1813.05005	165.28615	3.0094
2	21.995	BB	0.6505	5.84338e4	1398.61169	96.9906

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



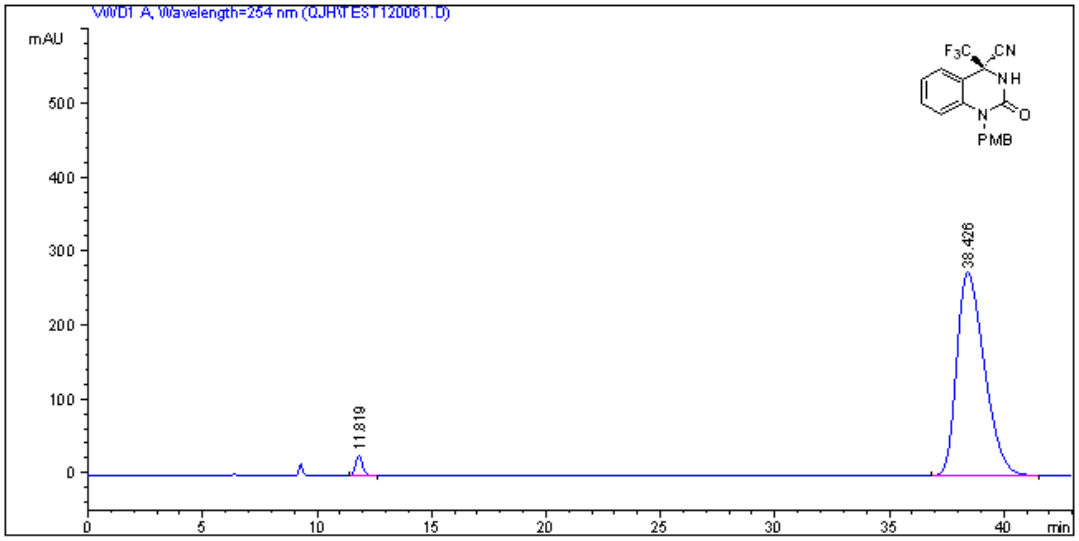
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.366	BV	0.2001	3.43692e4	2714.73584	95.9488
2	22.297	MM	0.5453	1451.14404	44.35538	4.0512

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



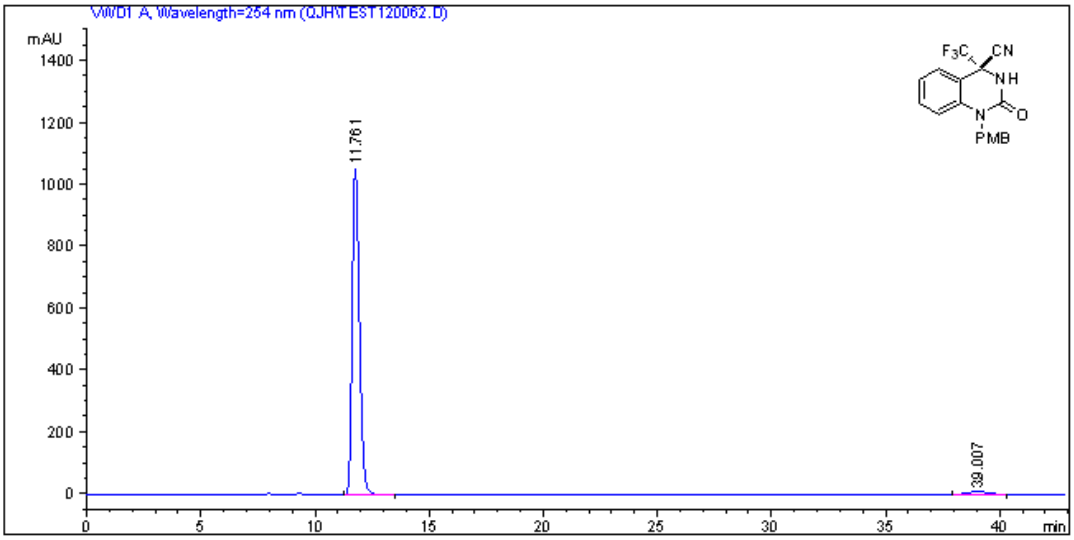
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.700	BB	0.3307	9163.86719	429.06561	49.7419
2	38.185	BB	1.2423	9258.95996	114.98464	50.2581

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



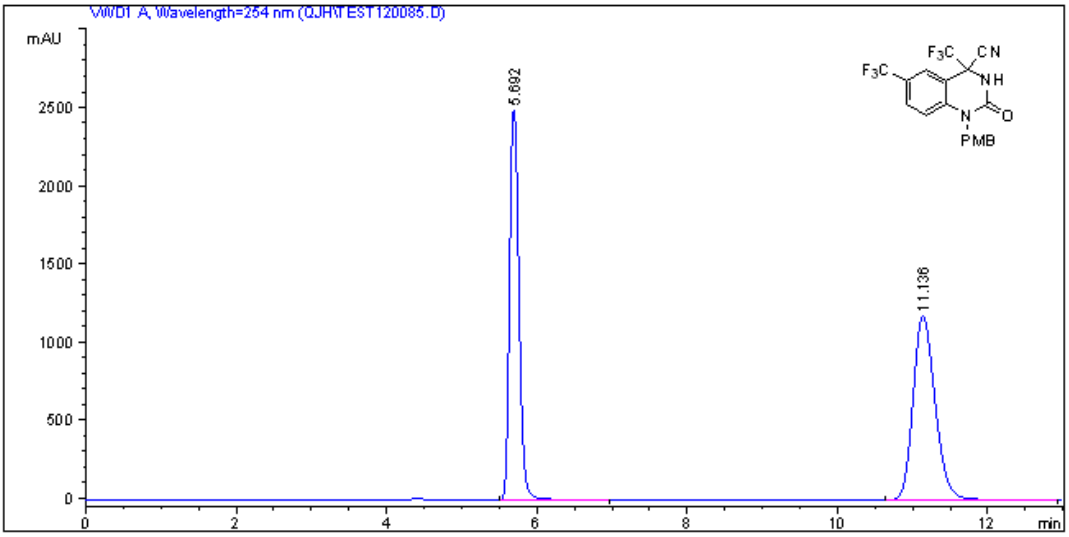
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.819	BB	0.3365	599.44757	27.43248	2.5284
2	38.426	BB	1.2988	2.31088e4	274.71786	97.4716

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



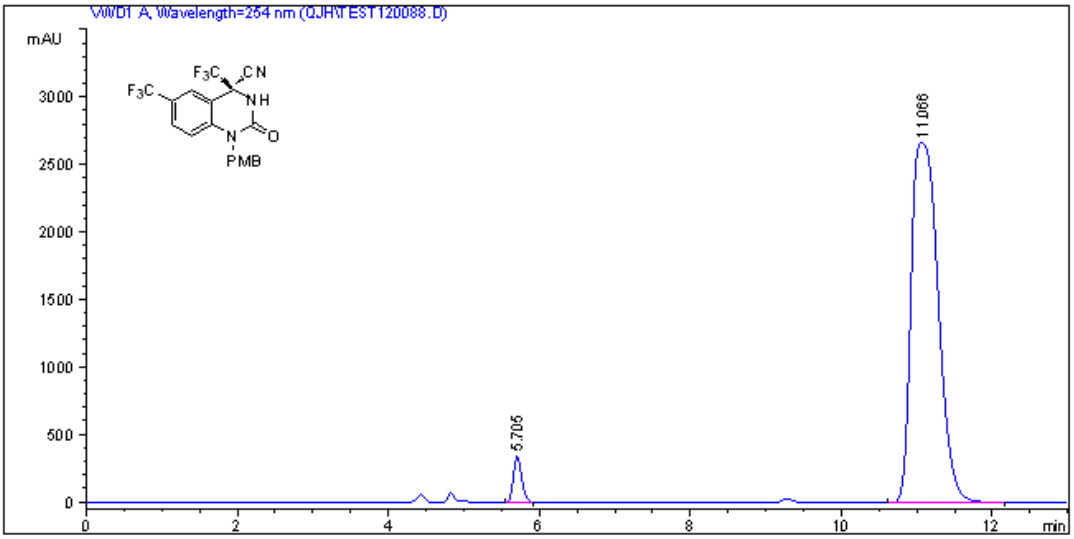
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.761	BB	0.3432	2.33751e4	1053.77136	97.5642
2	39.007	MM	1.1419	583.59222	8.51772	2.4358

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



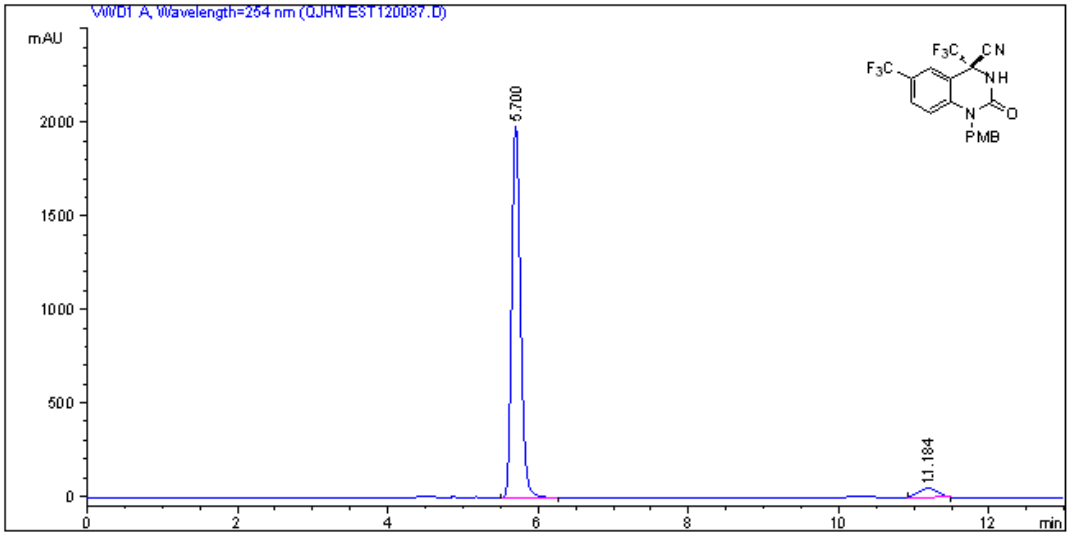
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.692	BB	0.1368	2.18040e4	2496.25049	47.6171
2	11.136	BB	0.3167	2.39863e4	1175.58936	52.3829

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



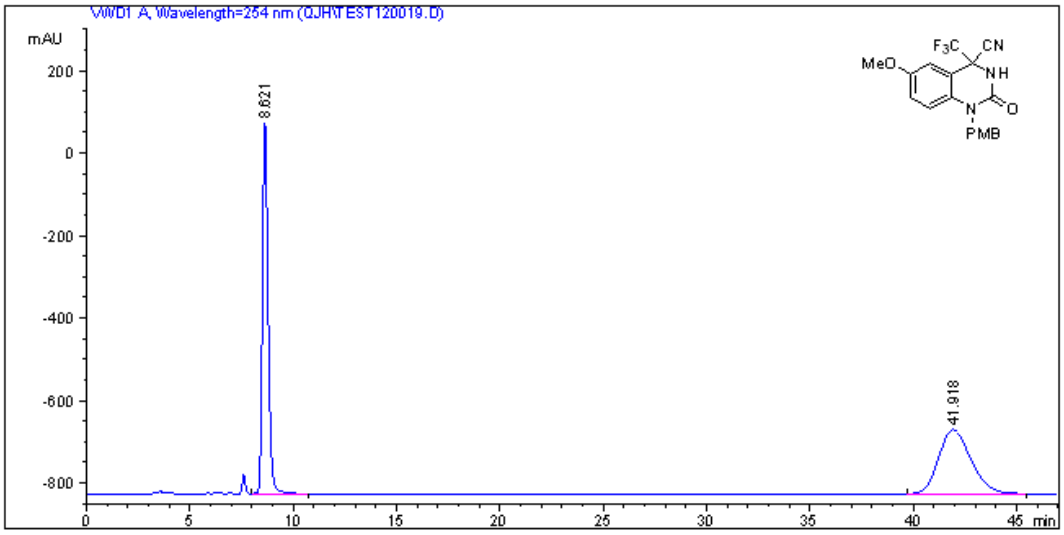
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.705	MM	0.1306	2698.89746	344.40182	3.8966
2	11.066	BV	0.3956	6.65642e4	2670.52612	96.1034

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



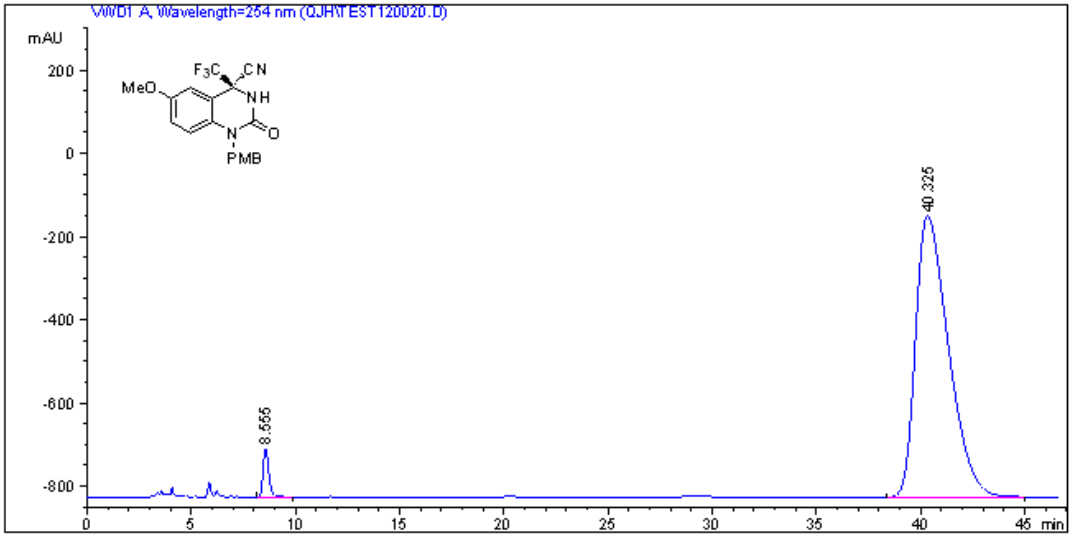
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.700	BV	0.1279	1.63408e4	1989.28223	94.9664
2	11.184	MM	0.3016	866.13324	47.85833	5.0336

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



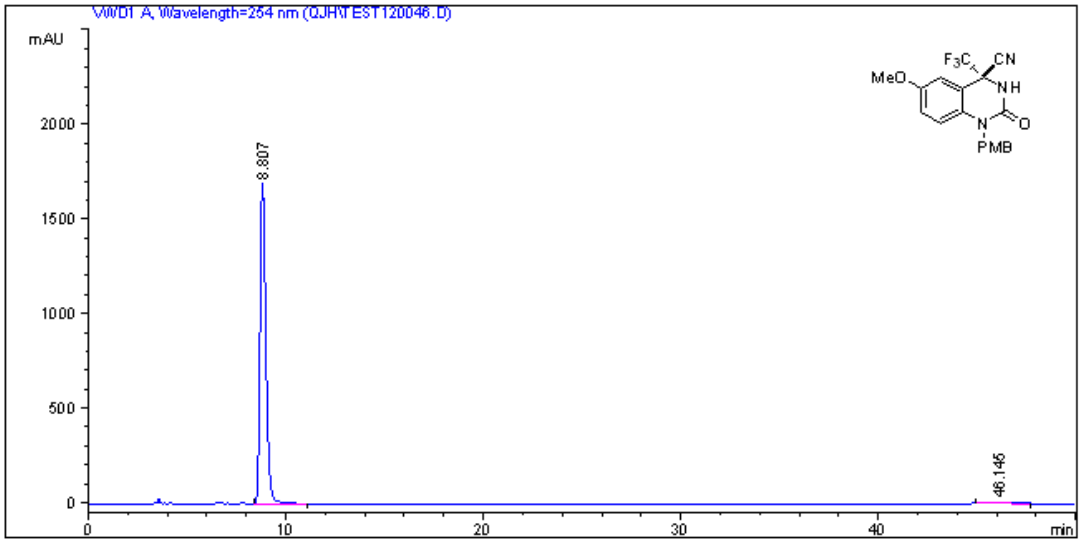
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.621	BB	0.2930	1.71891e4	898.80444	50.3424
2	41.918	BB	1.6036	1.69553e4	155.55782	49.6576

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



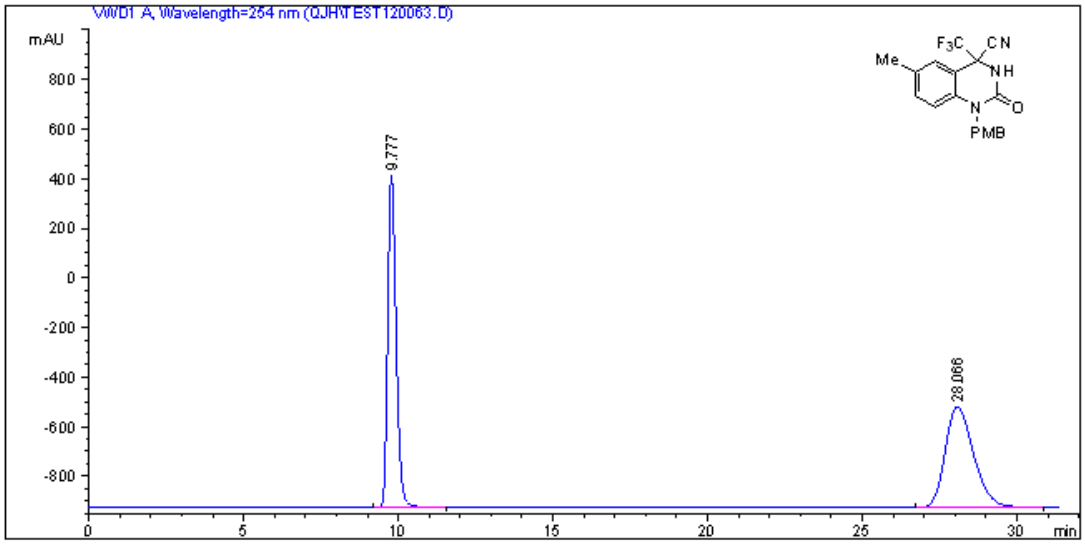
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.555	BB	0.2876	2220.84253	117.45379	2.9049
2	40.325	BB	1.6066	7.42299e4	676.35443	97.0951

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



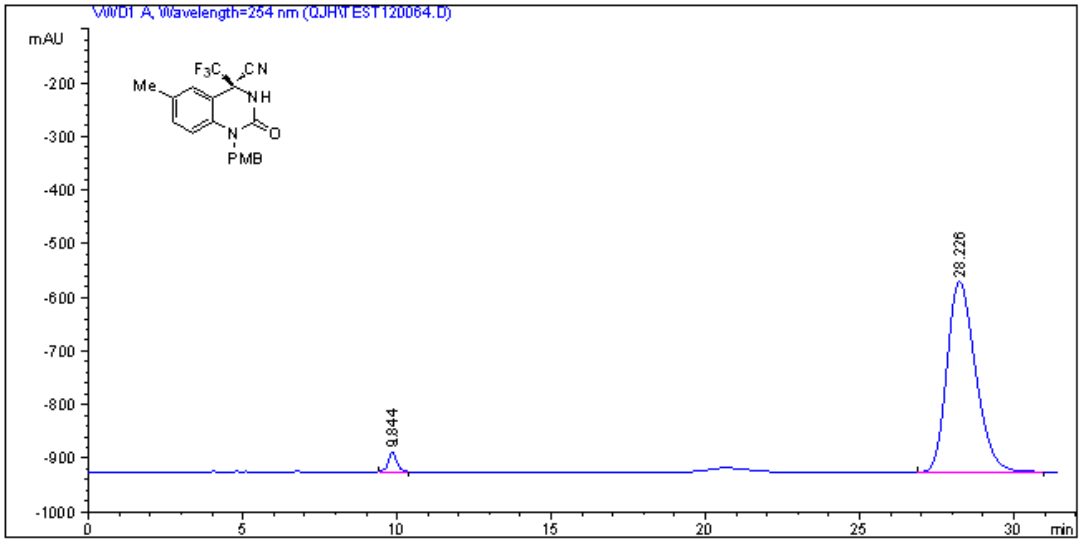
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.807	BB	0.3175	3.50376e4	1690.32544	98.5709
2	46.145	MM	1.6147	507.97986	5.24337	1.4291

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



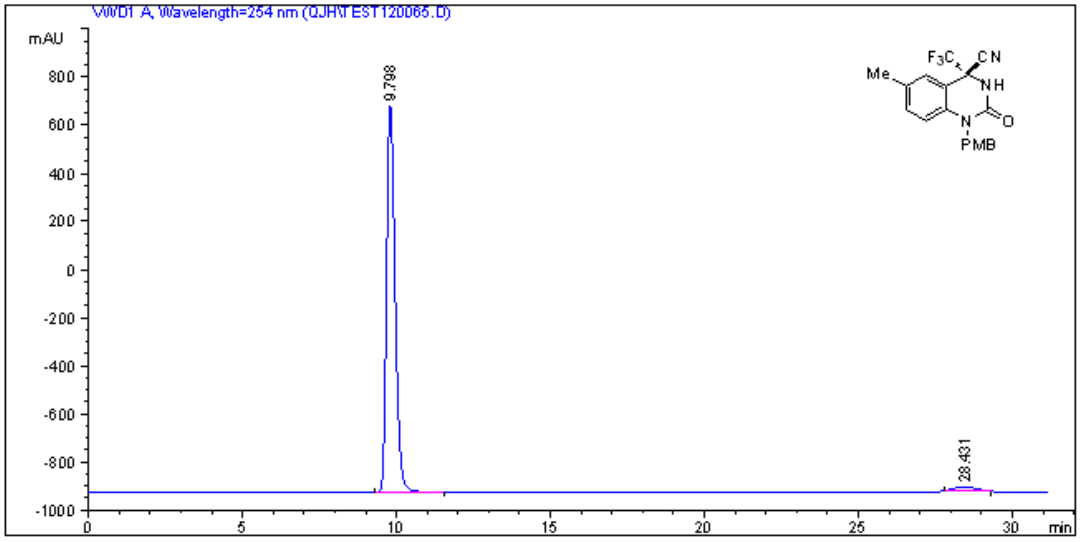
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.777	VB	0.2936	2.53223e4	1337.68286	49.5332
2	28.066	BB	0.9876	2.57995e4	405.11685	50.4668

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



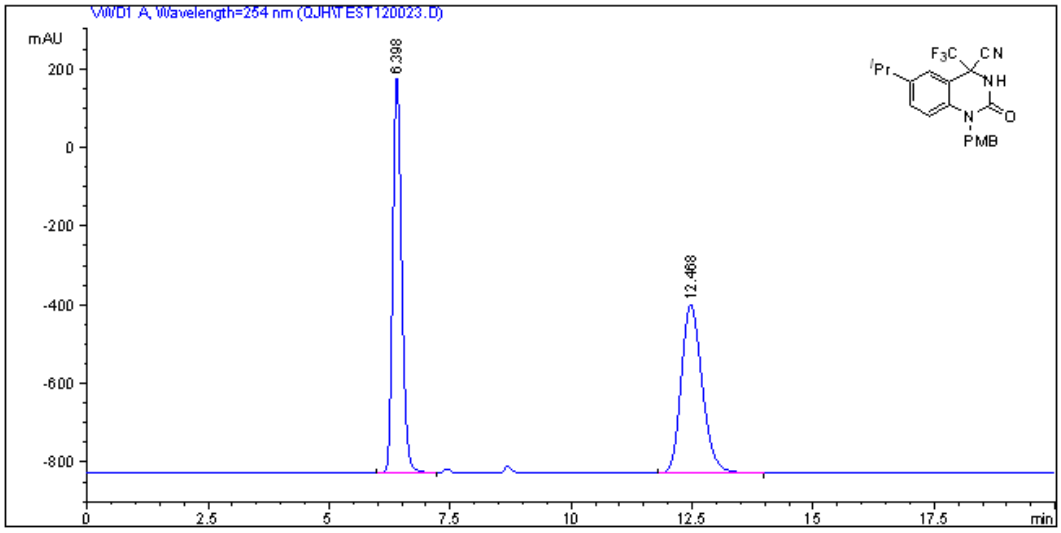
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.844	MM	0.3254	727.14117	37.24672	3.0857
2	28.226	BB	0.9918	2.28377e4	355.19577	96.9143

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 0.8mL/min



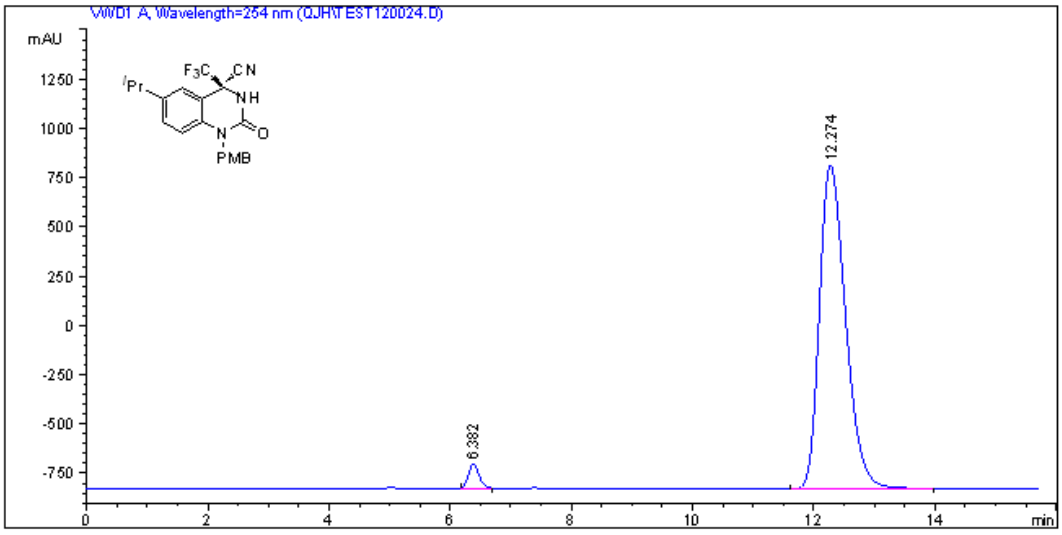
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.798	VB	0.3003	3.09207e4	1605.97424	97.1633
2	28.431	MM	0.8745	902.72925	17.20549	2.8367

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



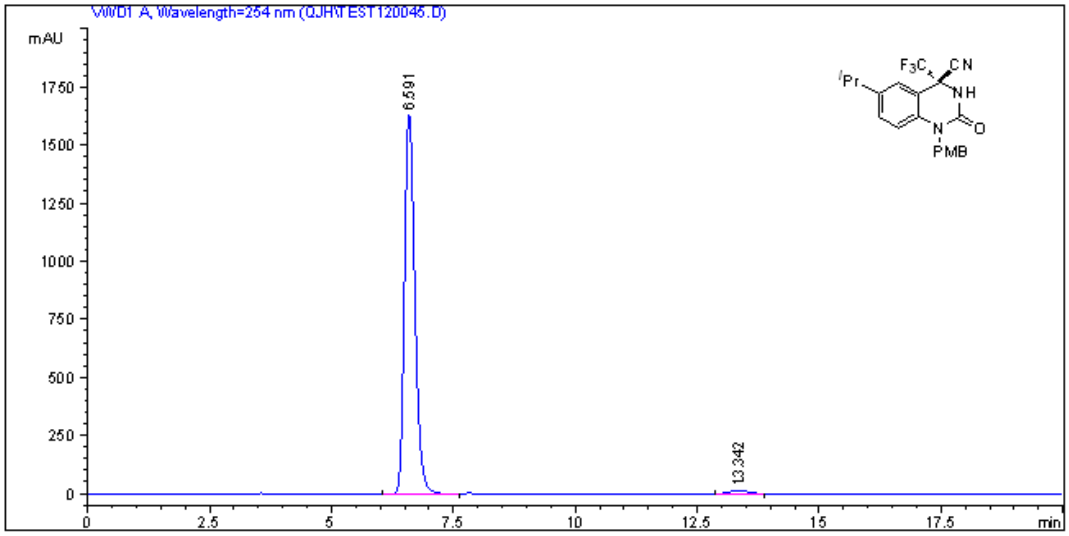
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.398	VV	0.1996	1.28889e4	1001.89069	49.9240
2	12.468	BBA	0.4685	1.29282e4	428.46793	50.0760

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



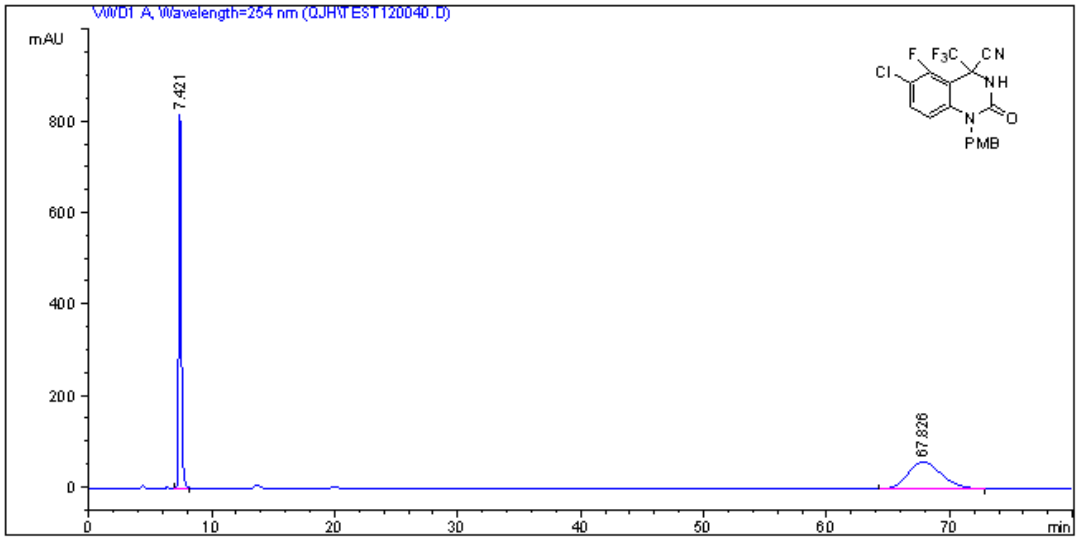
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.382	MM	0.2045	1520.45166	123.89207	3.0012
2	12.274	BBA	0.4631	4.91411e4	1640.28943	96.9988

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



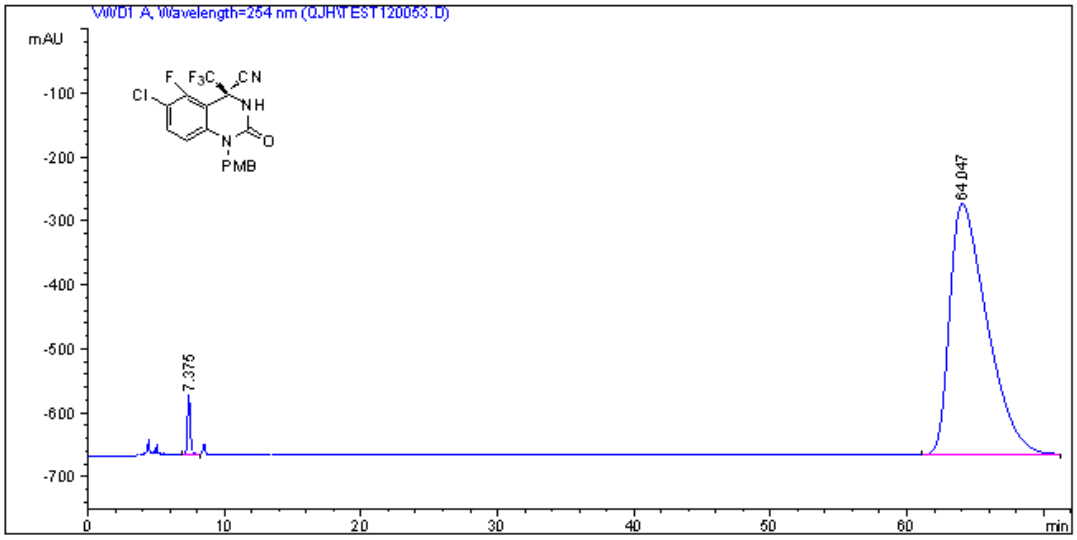
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.591	VV	0.2302	2.45402e4	1637.19055	98.1170
2	13.342	MM	0.5133	470.96539	15.29134	1.8830

Sample Info : 254 nm, IC, i-PrOH : Hexane =25:75, 0.8mL/min



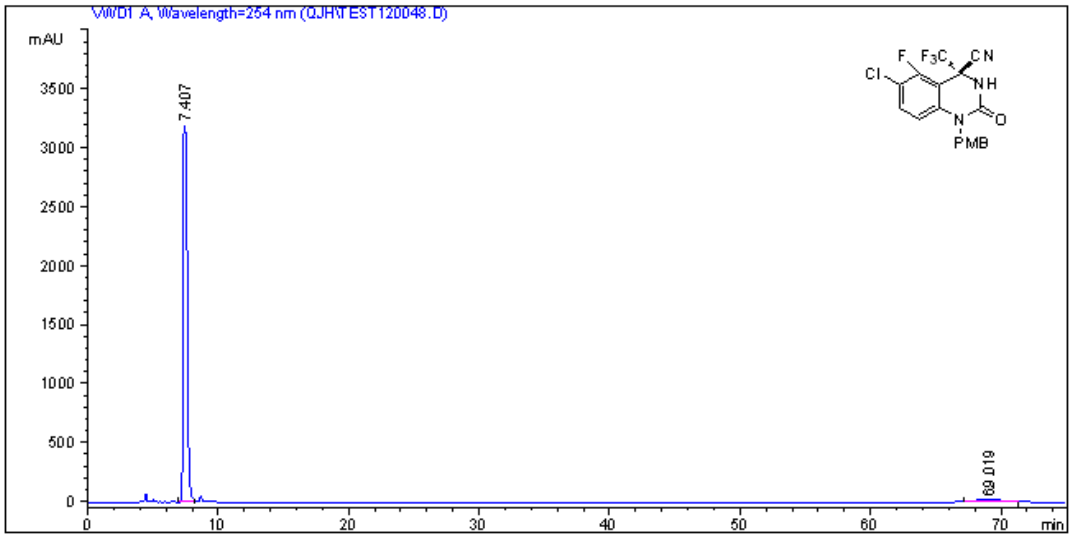
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.421	BBA	0.2165	1.15087e4	818.20526	50.4472
2	67.826	BB	2.8396	1.13047e4	58.96277	49.5528

Sample Info : 254 nm, IC, i-PrOH : Hexane =25:75, 0.8 mL/min



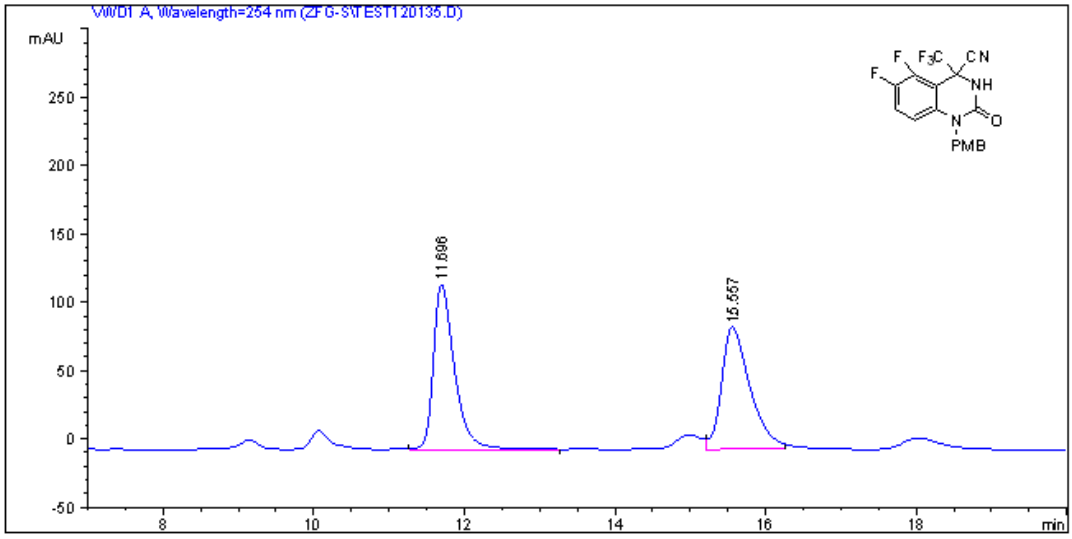
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.375	VBA	0.2176	1314.09058	92.80611	1.7245
2	64.047	BBA	2.7916	7.48877e4	392.88162	98.2755

Sample Info : 254 nm, IC, i-PrOH : Hexane =25:75, 0.8 mL/min



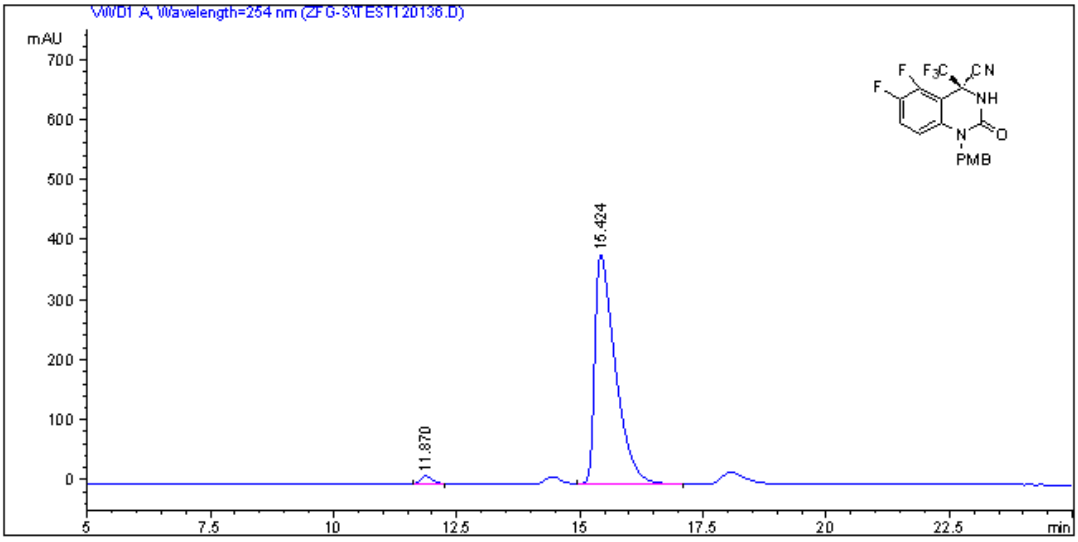
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.407	VBA	0.3608	7.16808e4	3194.21118	96.8254
2	69.019	MM	2.4631	2350.20459	15.90252	3.1746

Sample Info : 254nm, IB, i-PrOH : Hexane =10:90, 1.0 mL/min



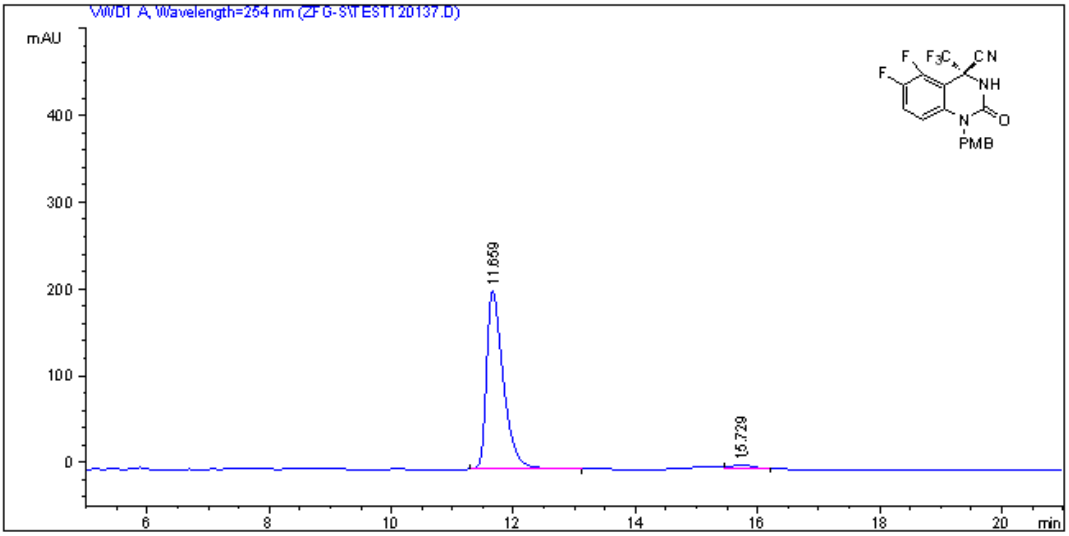
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.696	VB	0.2947	2348.64771	120.35042	50.1243
2	15.557	MM	0.4363	2336.99731	89.26569	49.8757

Sample Info : 254nm, IB, i-PrOH : Hexane =10:90, 1.0 mL/min



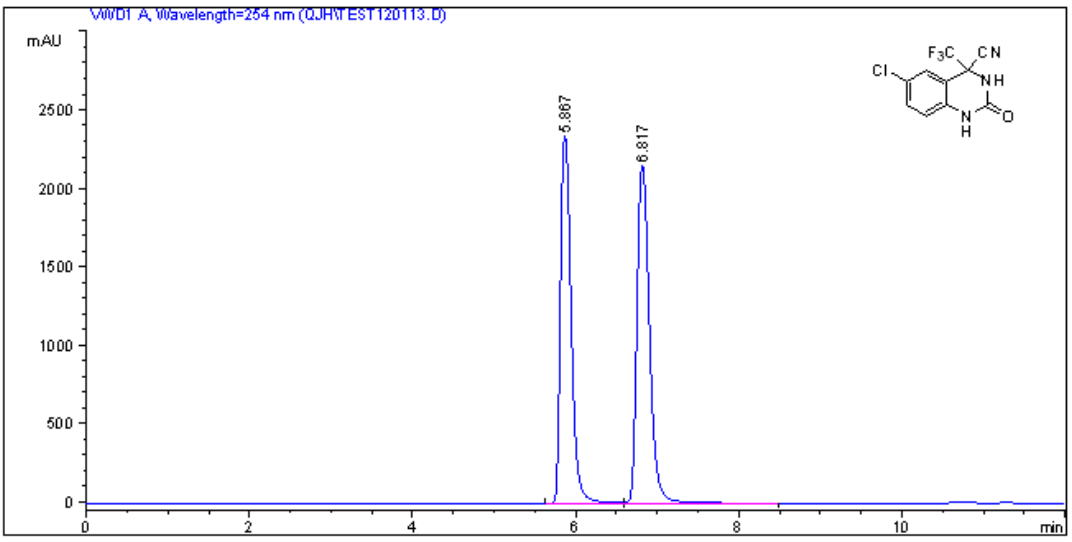
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.870	MM	0.2888	232.03041	13.38831	2.0304
2	15.424	VBA	0.4373	1.11957e4	382.82965	97.9696

Sample Info : 254nm, IB, i-PrOH : Hexane =10:90, 1.0 mL/min



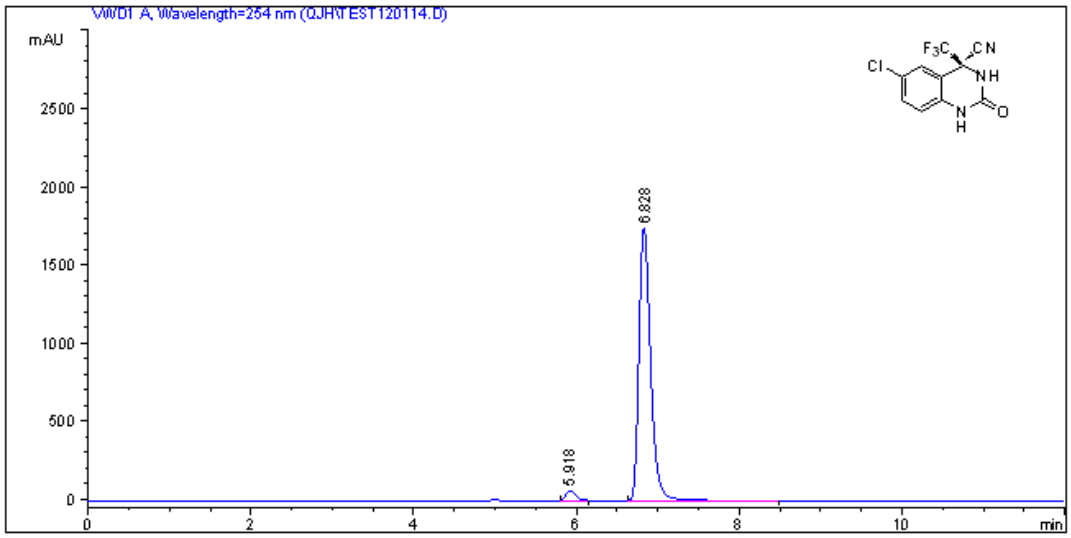
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.659	BB	0.2878	3944.17163	205.63376	97.0216
2	15.729	MM	0.4225	121.07977	4.77579	2.9784

Sample Info : 254 nm, IC, i-PrOH : Hexane =10:90, 0.8mL/min



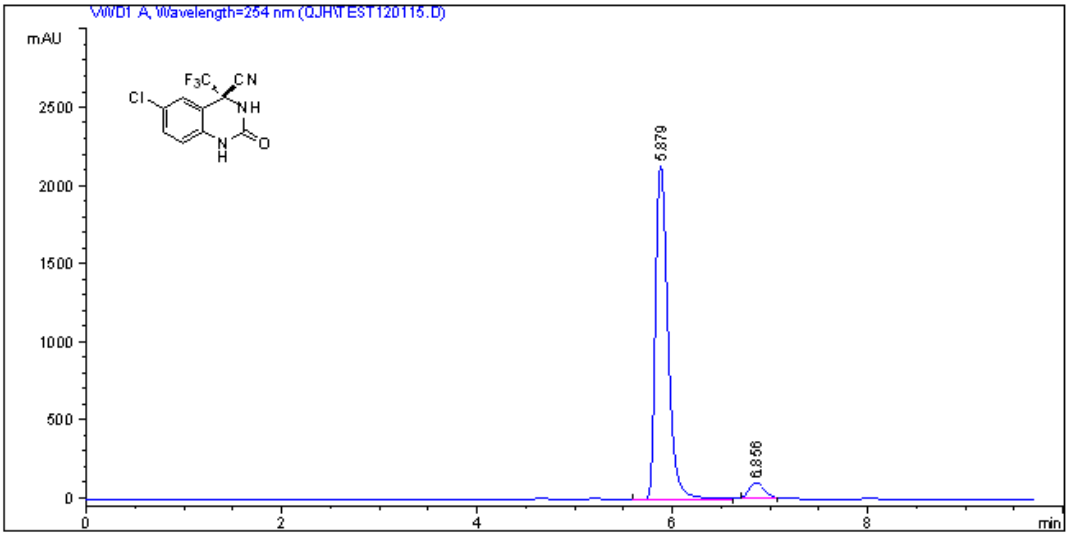
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.867	BV	0.1417	2.13967e4	2337.73901	48.1173
2	6.817	VB	0.1689	2.30711e4	2149.96631	51.8827

Sample Info : 254 nm, IC, i-PrOH : Hexane =10:90, 0.8mL/min



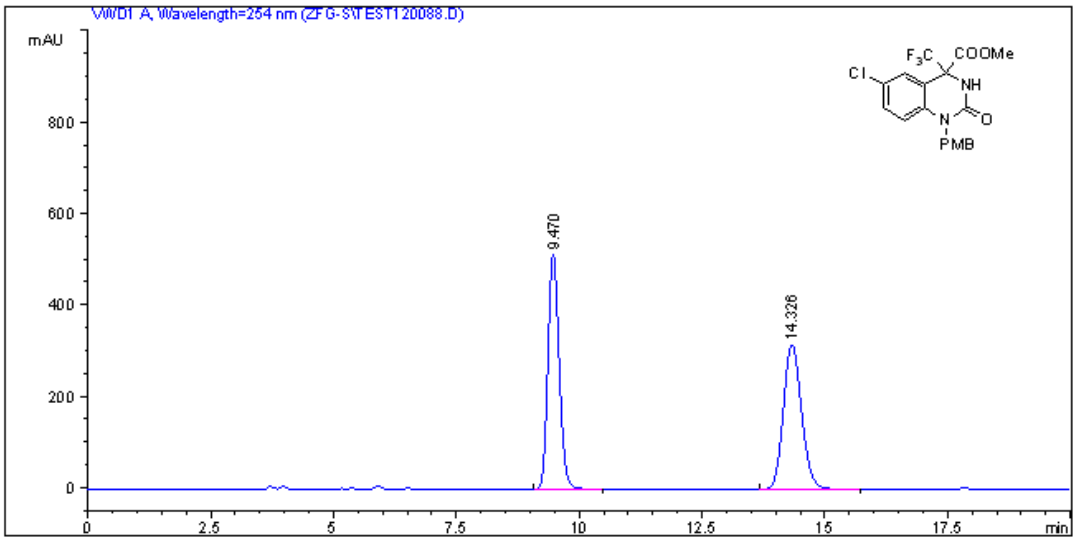
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.918	MM	0.1380	532.51129	64.30142	2.9504
2	6.828	BB	0.1551	1.7516le4	1742.47339	97.0496

Sample Info : 254 nm, IC, i-PrOH : Hexane =10:90, 0.8mL/min



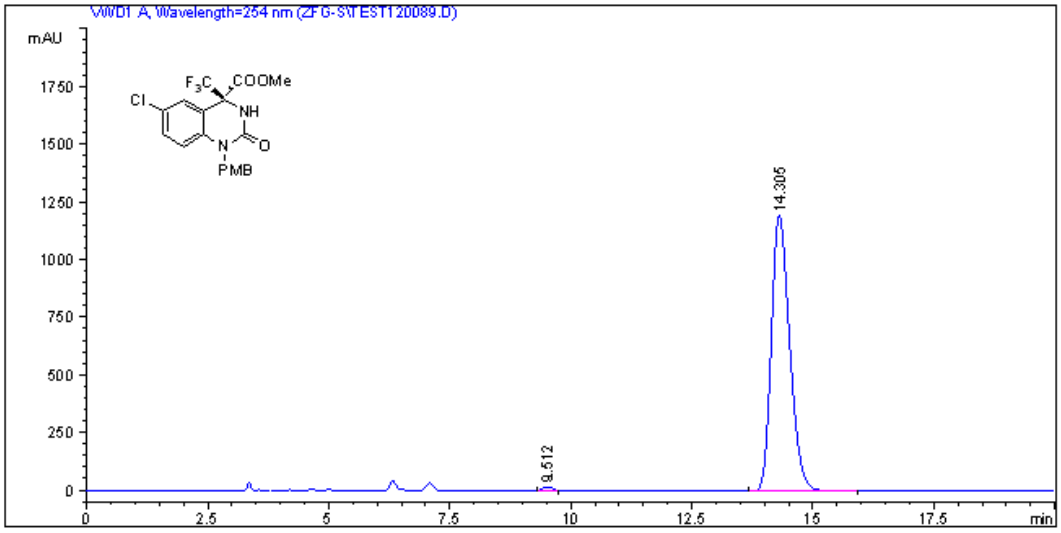
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.879	VV	0.1387	1.8961le4	2132.32056	94.9577
2	6.856	MM	0.1715	1006.84100	97.86214	5.0423

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



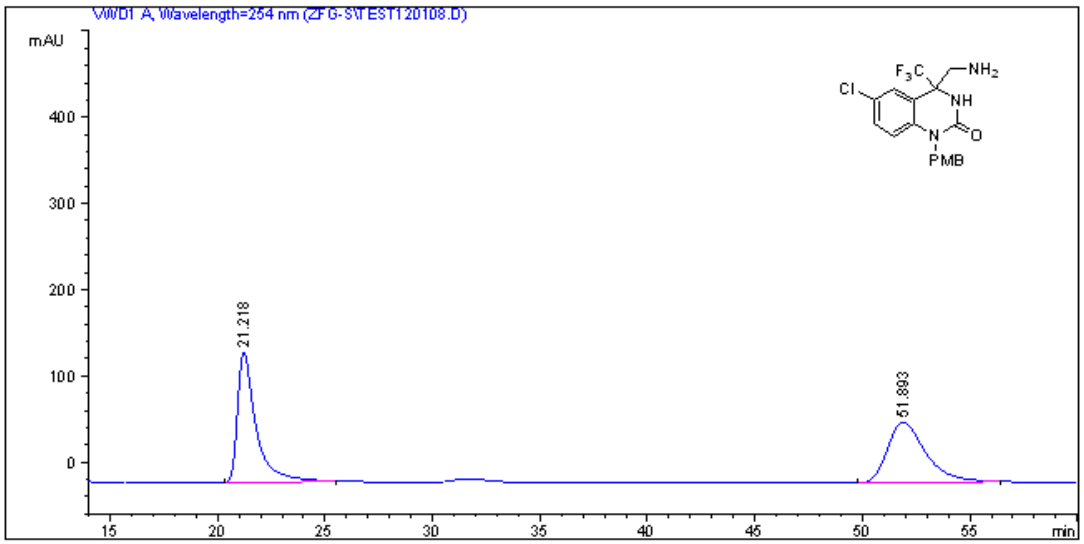
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.470	BB	0.2470	8186.90430	513.86078	50.0335
2	14.326	VB	0.3995	8175.95459	317.39954	49.9665

Sample Info : 254 nm, IC, i-PrOH : Hexane =20:80, 1.0 mL/min



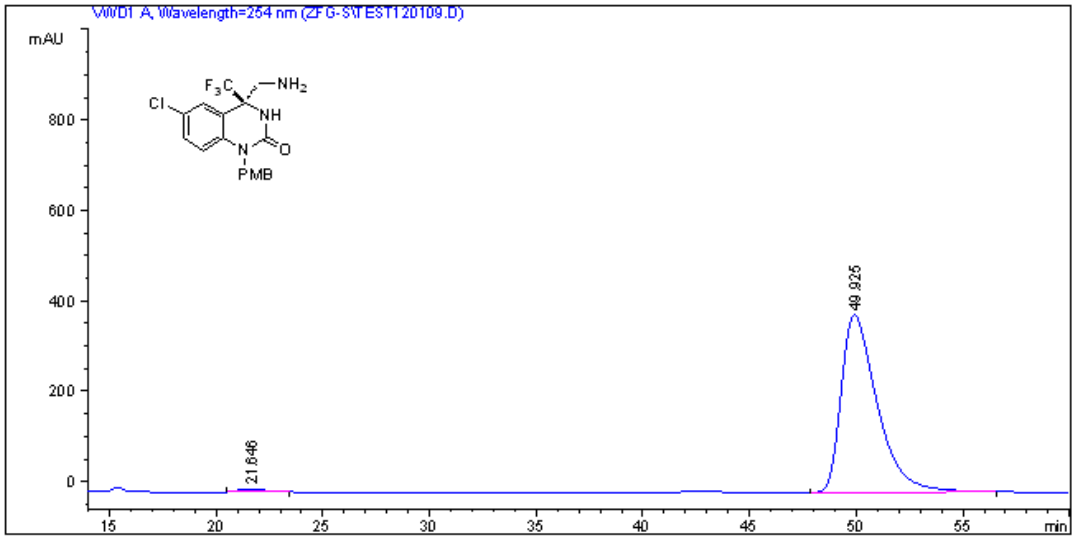
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.512	MM	0.2415	257.41647	17.76429	0.8119
2	14.305	BB	0.4065	3.14473e4	1193.20544	99.1881

Sample Info : 254nm, IC, i-PrOH : Hexane = 20:80, 1.0 mL/min



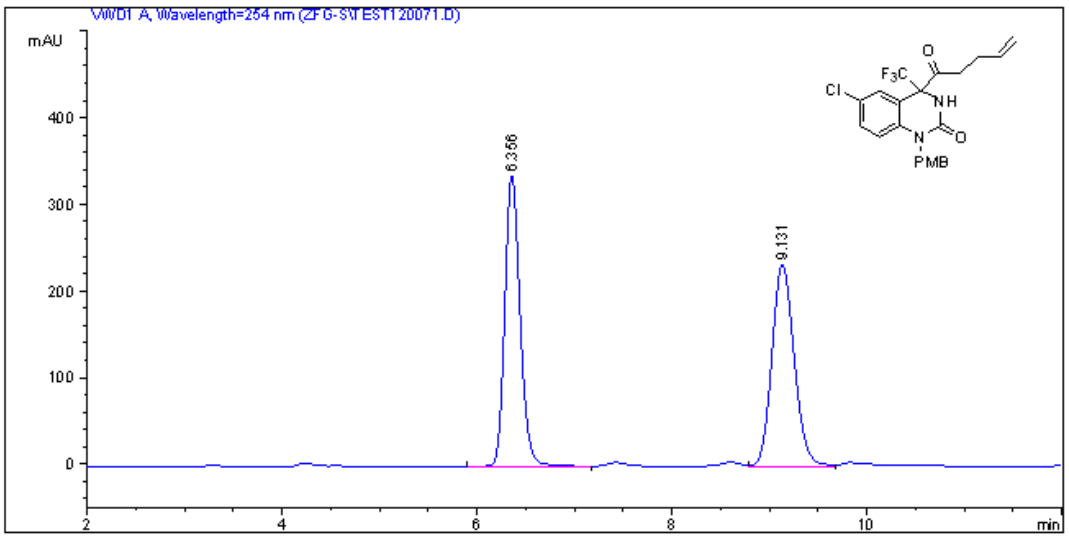
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.218	BB	0.8730	9119.36230	151.72989	51.1482
2	51.893	BB	1.8653	8709.92480	70.41467	48.8518

Sample Info : 254nm, IC, i-PrOH : Hexane = 20:80, 1.0 mL/min



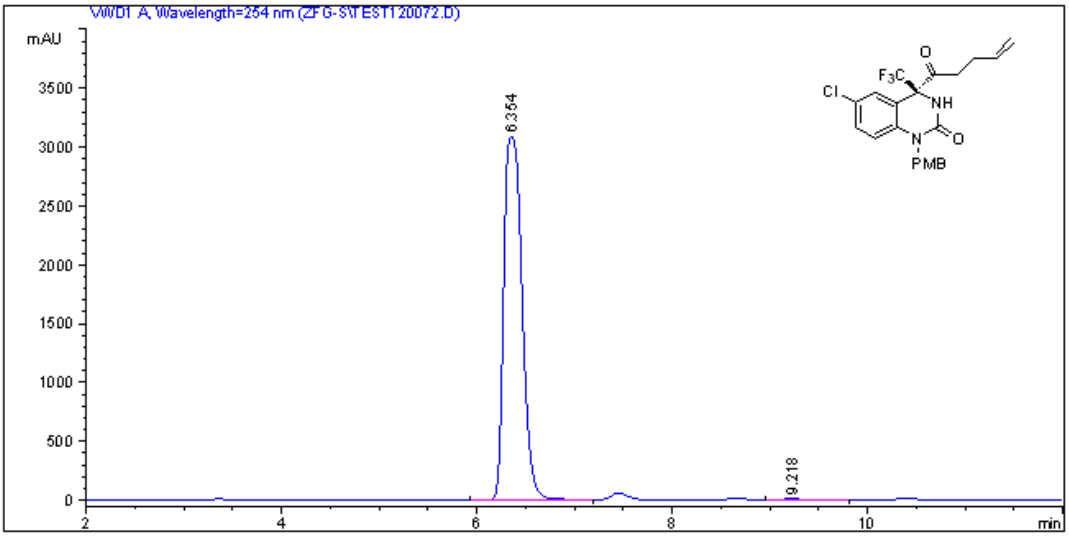
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.646	MM	1.5954	529.04047	5.52668	1.1297
2	49.925	BB	1.7665	4.63005e4	393.32858	98.8703

Sample Info : 254 nm, IC, i-PrOH : Hexane =10:90, 1.0 mL/min



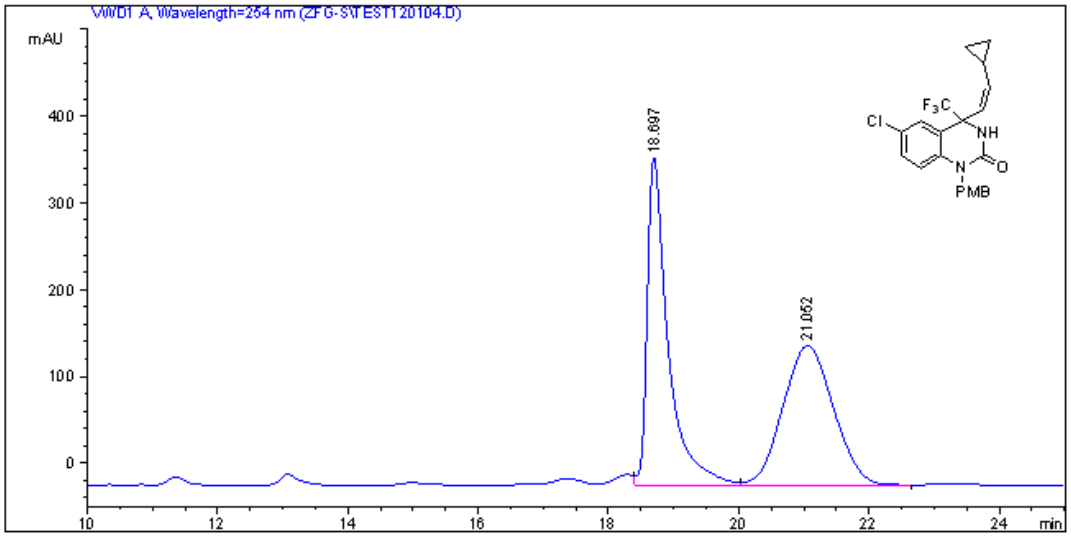
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.356	BV	0.1683	3670.88818	335.85965	49.7294
2	9.131	VV	0.2499	3710.83594	233.01689	50.2706

Sample Info : 254 nm, IC, i-PrOH : Hexane =10:90, 1.0 mL/min



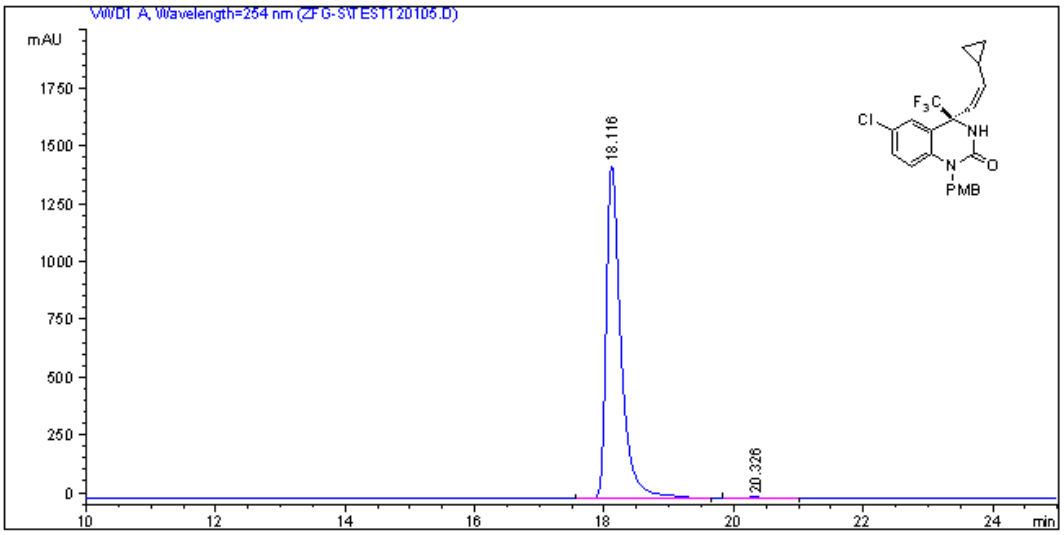
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.354	VBA	0.2072	4.02460e4	3092.43555	99.4277
2	9.218	BBA	0.2524	231.64531	14.34936	0.5723

Sample Info : 254nm, IC, i-PrOH : Hexane = 5:95, 1.0 mL/min



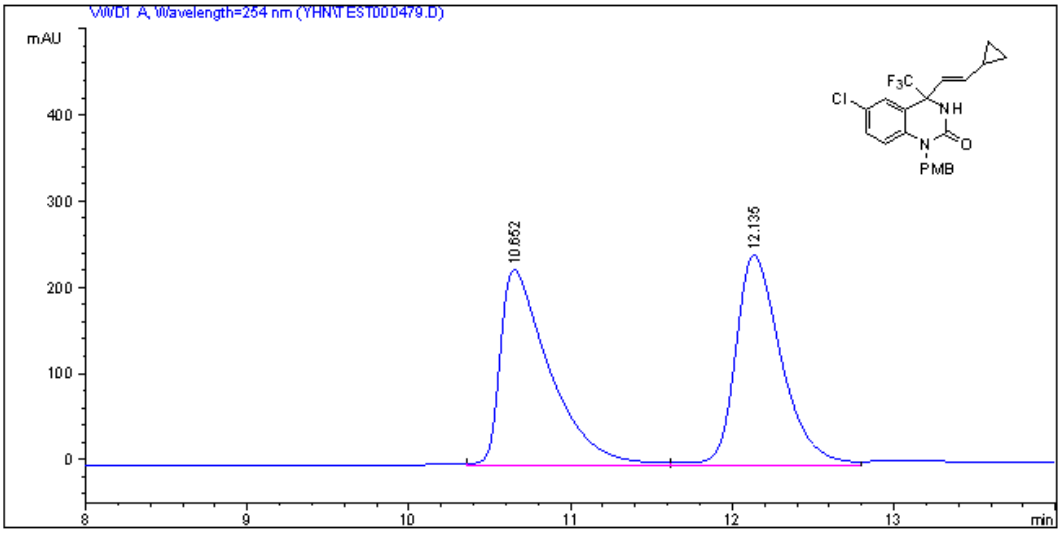
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.697	VV	0.3204	8386.72559	377.43066	49.3789
2	21.052	VB	0.8635	8597.70313	160.56996	50.6211

Sample Info : 254nm, IC, i-PrOH : Hexane = 5:95, 1.0 mL/min



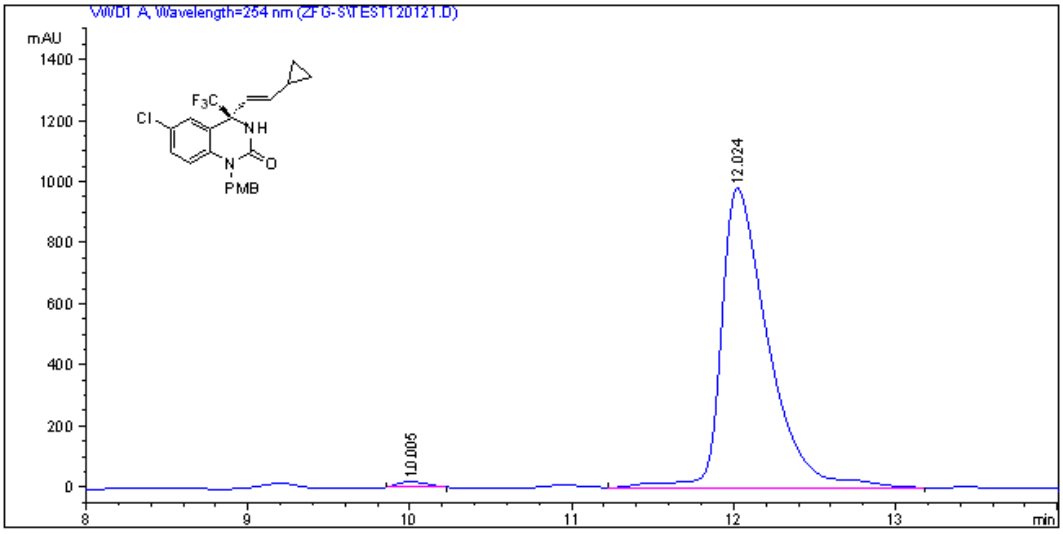
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.116	BV	0.2376	2.28373e4	1438.76392	99.4004
2	20.326	MM	0.6784	137.76416	3.38438	0.5996

Sample Info : 254 nm, IB, i-PrOH : Hexane =5:95 1.0 mL/min



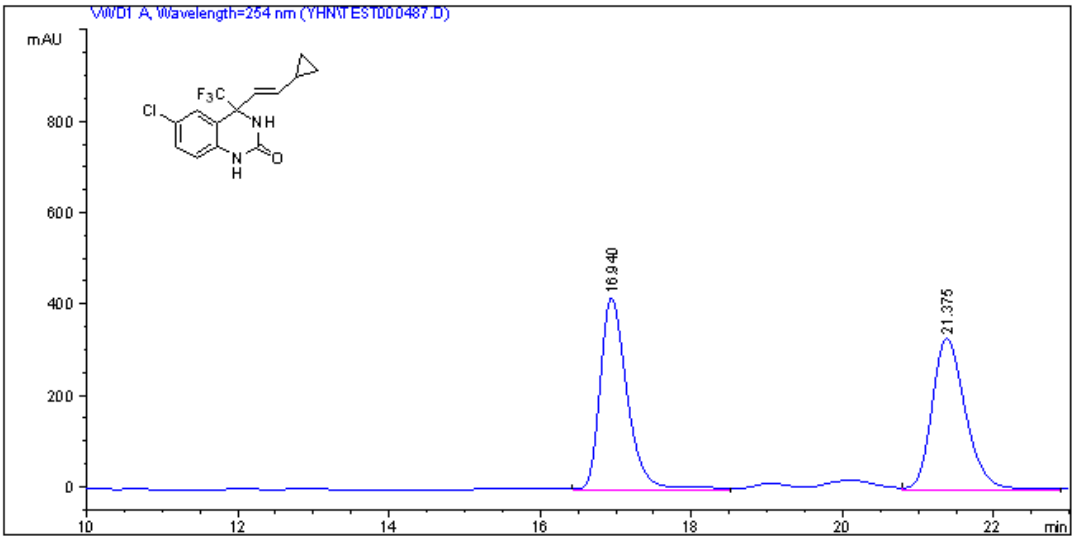
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.652	VV	0.3117	4898.34131	228.13379	50.1320
2	12.135	VV	0.3018	4872.55029	245.13243	49.8680

Sample Info : 254 nm, IB, i-PrOH : Hexane =5:95 1.0 mL/min



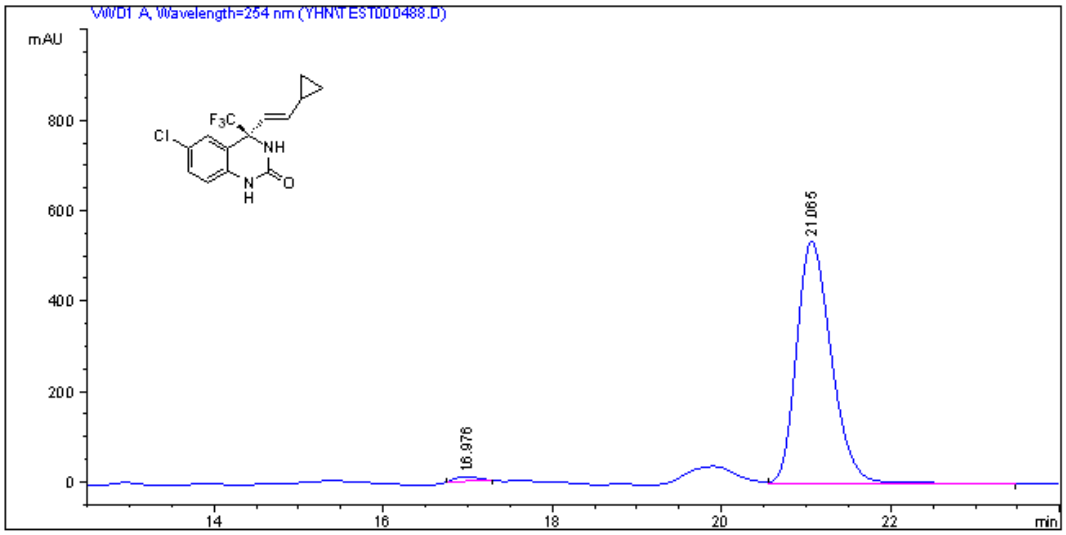
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.005	MM	0.2026	208.85275	17.18270	1.0236
2	12.024	VBA	0.3033	2.01955e4	985.02368	98.9764

Sample Info : 254nm, IC, i-PrOH : Hexane =4:96 0.6mL/min



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.940	VV	0.3774	1.04257e4	419.40494	50.7078
2	21.375	VBA	0.4744	1.01347e4	330.30594	49.2922

Sample Info : 254nm, IC, i-PrOH : Hexane =4:96 0.6mL/min



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.976	MM	0.3119	196.75024	10.51227	1.2505
2	21.065	BB	0.4481	1.55368e4	537.22314	98.7495