

Rhodium(III)-Catalyzed Enantioselective C–H Activation/Annulation of Ferrocenecarboxamides with Internal Alkynes

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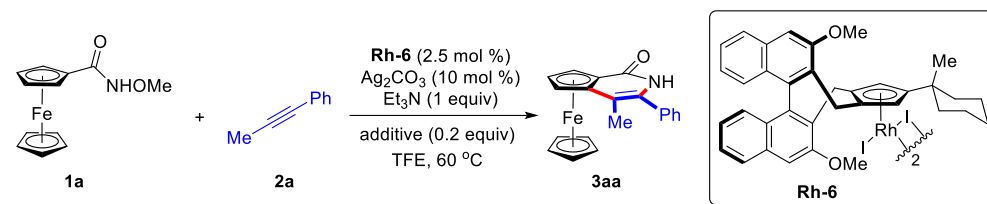
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1. General information

Unless otherwise noted, materials were purchased from commercial suppliers (Shanghai Bidepharm, Adamas-beta®, J&K Scientific, TCI Shanghai and others) and used without further purification. All the solvents were treated according to standard methods. Flash column chromatography was performed using 200–300 mesh silica gel. ^1H and ^{13}C NMR spectra were recorded on Bruker, Agilent, and Varian instruments (400 MHz and 100 MHz, respectively) and internally referenced to tetramethylsilane signal or residual protic solvent signals. Data for ^1H NMR are recorded as follows: chemical shift (δ , ppm), multiplicity (s = singlet, d = doublet, t = triplet, sept = septet, m = multiplet, br = broad singlet, coupling constant (s) in Hz, integration). Data for ^{13}C NMR and ^{19}F NMR are reported in terms of chemical shift (δ , ppm). All air- and moisture-sensitive reactions were performed under an atmosphere of argon in flame-dried glassware. **Rh-2**¹, and **Rh-3–Rh-7**² were prepared according to the known procedures.

2. Details for condition optimization

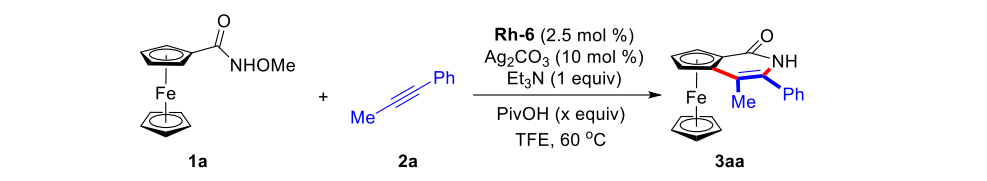
Table S1. Screening of additives.^[a]



Entry	Additive (0.2 equiv)	Yield ^[b]	Ee ^[c]
1	PhCO ₂ Na	60%	77%
2	NaTFA	68%	69%
3	NaOAc	72%	61%
4	Na ₂ CO ₃	60%	65%
5	NaOPiv	70%	80%
6	KOPiv	70%	80%
7	CsOPiv	58%	80%
8	HOPiv	42%	82%

[a] **1a** (0.05 mmol), **2a** (0.075 mmol), **Rh-6** (2.5 mol %), Ag₂CO₃ (10 mol %), and Et₃N (0.05 mmol) in TFE (0.5 mL) at 60 °C for 24 h under argon atmosphere. [b] The yields were detected by ¹H NMR spectra of crude reaction mixtures with 1,3,5-trimethoxybenzene as an internal standard. [c] The ee values were determined by HPLC analysis with a chiral stationary phase.

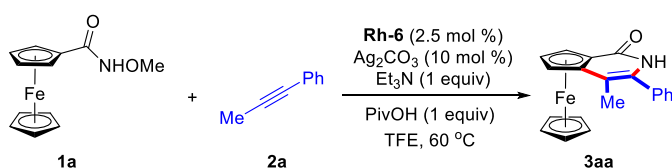
Table S2. Investigation of the equivalent of additives.^[a]



Entry	PivOH (x equiv)	Yield ^[b]	Ee ^[c]
1	0.2	42%	82%
2	0.6	40%	87%
3	1.0	37%	90%
4	1.4	24%	94%
5	1.8	<10%	-

[a] **1a** (0.05 mmol), **2a** (0.075 mmol), **Rh-6** (2.5 mol %), Ag₂CO₃ (10 mol %), and Et₃N (0.05 mmol) in TFE (0.5 mL) at 60 °C for 24 h under argon atmosphere. [b] The yields were detected by ¹H NMR spectra of crude reaction mixtures with 1,3,5-trimethoxybenzene as an internal standard. [c] The ee values were determined by HPLC analysis with a chiral stationary phase.

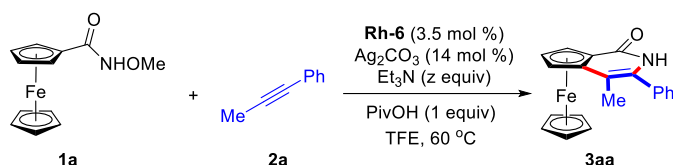
Table S3. Investigation of the equivalent of alkyne **2a**.^[a]



Entry	Alkyne 2a (y equiv)	Yield ^[c]	Ee ^[d]
1	1.5	37%	90%
2	2	43%	92%
3	2.5	43%	92%
4 ^[b]	2	49%	92%

[a] **1a** (0.05 mmol), **2a** (y × 0.05 mmol) **Rh-6** (2.5 mol %), Ag₂CO₃ (10 mol %), Et₃N (0.05 mmol), and PivOH (0.05 mmol) in TFE (0.5 mL) at 60 °C for 24 h under argon atmosphere. [b] [Rh] (3.5 mol %), Ag₂CO₃ (14 mol %). [c] The yields were detected by ¹H NMR spectra of crude reaction mixtures with 1,3,5-trimethoxybenzene as an internal standard. [d] The ee values were determined by HPLC analysis with a chiral stationary phase.

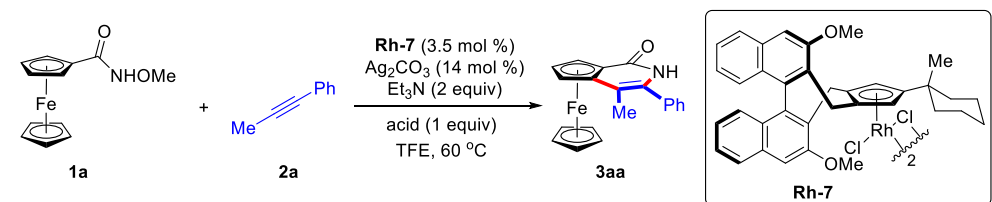
Table S4. Investigation of the equivalent of Et₃N.^[a]



Entry	Et ₃ N (z equiv)	Yield ^[c]	Ee ^[d]
1	1.0	49%	92%
2	2.0	70%	88%
3	2.5	69%	87%
4 ^[b]	2.0	82%	90%

[a] **1a** (0.05 mmol), **2a** (0.1 mmol), **Rh-6** (3.5 mol %), Ag₂CO₃ (14 mol %), Et₃N (z × 0.05 mmol), and PivOH (0.05 mmol) in TFE (0.5 mL) at 60 °C for 24 h under argon atmosphere. [b] **Rh-7** (3.5 mol %). [c] The yields were detected by ¹H NMR spectra of crude reaction mixtures with 1,3,5-trimethoxybenzene as an internal standard. [d] The ee values were determined by HPLC analysis with a chiral stationary phase.

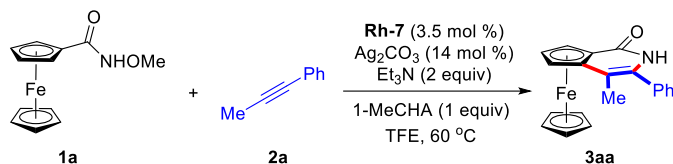
Table S5. Optimization of acids.^[a]



Entry	Acid	Yield ^[b]	Ee ^[c]
1	1-MeCHA	80% (77% ^[d])	94%
2	1-AdCO ₂ H	61%	92%
3	PhCO ₂ H	42%	85%
4	CH ₃ CO ₂ H	51%	83%

[a] **1a** (0.05 mmol), **2a** (0.1 mmol), **Rh-7** (3.5 mol %), Ag₂CO₃ (14 mol %), Et₃N (0.1 mmol), and acid (0.05 mmol) in TFE (0.5 mL) at 60 °C for 24 h under argon atmosphere. [b] The yields were detected by ¹H NMR spectra of crude reaction mixtures with 1,3,5-trimethoxybenzene as an internal standard. [c] The ee values were determined by HPLC analysis with a chiral stationary phase. [d] Isolated yield of 0.2 mmol scale reaction in parentheses. 1-MeCHA = 1-methylcyclohexane-1-carboxylic acid.

Table S6. Control experiments.^[a]



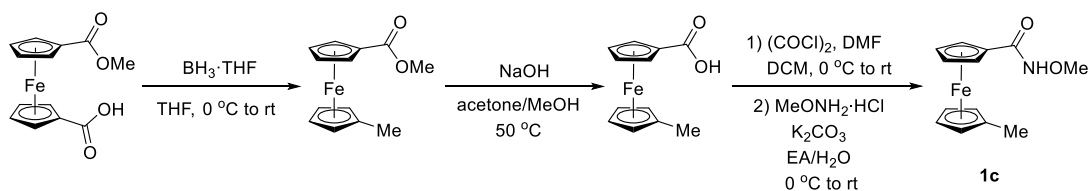
Entry	Conditions	Yield ^[b]	Ee ^[c]
1	No Rh-7	n.r.	-
2	No Ag ₂ CO ₃	60%	93%
3	No Et ₃ N	trace	-
4	No 1-MeCHA	84%	61%

[a] **1a** (0.05 mmol), **2a** (0.1 mmol), **Rh-7** (3.5 mol %), Ag₂CO₃ (14 mol %), Et₃N (0.1 mmol), and PivOH (0.05 mmol) in TFE (0.5 mL) at 60 °C for 24 h under argon atmosphere. [b] Detected by ¹H NMR integration methods with 1,3,5-trimethoxybenzene as an internal standard. [c] The ee values were determined by HPLC analysis with a chiral stationary phase.

3. Synthesis and Characterization of Substrates

Ferrocene carboxamides (**1a**, **1b**, **1f**, **1g**, **1i**, **1k**, **1l**)³ and internal alkynes (**2b-t**)⁴ were prepared according to the procedures reported in the literature.

Synthesis of **1c**



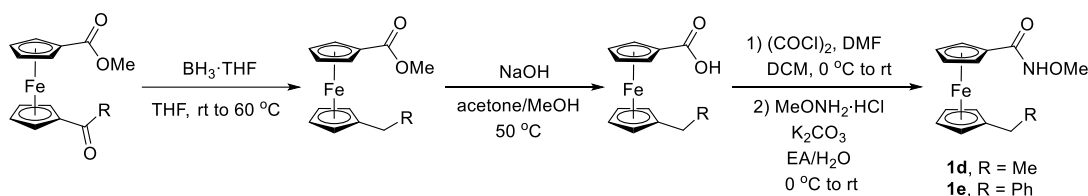
To a solution of 1,1'-ferrocene dicarboxylic acid mono-methyl ester (990 mg, 3.44 mmol) in dry THF (10 mL) at 0 °C under Ar was added dropwise BH₃·THF (6.88 mL, 2 equiv, 1 M in THF). The reaction mixture was warmed up to ambient temperature and stirred overnight. The reaction was quenched by HCl solution (1 N, 100 mL). The resultant mixture was extracted with ethyl acetate (3 × 15 mL). The combined organic phase was dried over anhydrous NaSO₄, filtered, and evaporated all the volatiles under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 10:1).

A mixture of the above crude product (500 mg, 1.94 mmol) and NaOH (88 mg, 1.1 equiv) in acetone/MeOH (11 mL, 10:1) was heated at 50 °C for 24 h. The reaction was quenched by HCl (1 N) solution. The resultant mixture was extracted with ethyl acetate (3 × 15 mL). The combined organic phase was dried over anhydrous NaSO₄, filtered, and evaporated all the volatiles under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 4:1).

To a solution of the above ferrocene carboxylic acid (300 mg, 1.23 mmol, 1 equiv) in dry CH₂Cl₂ (10 mL) at 0 °C under Ar was added dropwise oxalyl chloride (234 mg, 1.84 mmol, 1.5 equiv) followed by a catalytic amount of DMF (2 drops). The reaction was allowed to stir at rt until completion (typically 2 h). The solvent was then removed under reduced pressure to afford the corresponding crude acyl chloride. Methoxyamine hydrochloride (124 mg, 1.48 mmol, 1.2 equiv) was added to a biphasic mixture of K₂CO₃ (340 mg, 2.46 mmol, 2 equiv) in a mixture of EtOAc/H₂O (6 mL, 2:1). The resulting solution was cooled to 0 °C followed by dropwise addition of the unpurified acyl chloride dissolved in

a minimum amount of EtOAc. The flask containing the acyl chloride was then rinsed with additional EtOAc. The reaction was allowed to stir overnight at rt. Afterwards, the reaction was quenched with H₂O. The phases were separated and the aqueous phase was extracted with ethyl acetate (3 × 15 mL). The combined organic layers were dried over Na₂SO₄, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 1:1) to afford products **1c** (280 mg, 83% yield) as orange red solid. m.p. = 98-99 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.29 (s, 1H), 4.77 – 4.63 (m, 2H), 4.36 – 4.24 (m, 2H), 4.14 – 4.03 (m, 4H), 3.84 (s, 3H), 1.94 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 85.8, 73.1, 71.5, 70.9, 69.2, 68.9, 64.5, 13.8. IR (thin film): ν_{max} (cm⁻¹) = 3193, 3092, 3007, 2958, 2926, 2895, 2809, 2361, 2337, 2289, 2101, 1983, 1624, 1518, 1447, 1380, 1339, 1296, 1224, 1193, 1142, 1060, 1034, 1019, 937, 921, 868, 848, 820, 768, 638, 563, 531, 510, 497, 484, 454, 413. HRMS (ESI) calcd for C₁₃H₁₅FeNO₂Na [M+Na]⁺ 296.0344, found 296.0349.

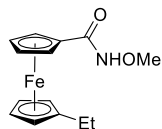
Typical procedure for the synthesis of **1d** and **1e** (**1d** as a representative example)



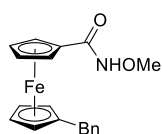
To a solution of 1'-acetyl-1-ferrocene carboxylic acid methyl ester (1.1 g, 4 mmol, 1.0 equiv) in dry THF (10 mL) at rt under Ar was added dropwise BH₃·THF (5 mL, 1.1 equiv, 1 M in THF). The reaction mixture was warmed up to 60 °C and stirred overnight. The reaction was quenched by HCl solution (1 N, 100 mL). The resultant mixture was extracted with ethyl acetate (3 × 15 mL). The combined organic phase was dried over anhydrous NaSO₄, filtered, and evaporated all the volatiles under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 10:1).

A mixture of the above crude product (684 mg, 2.5 mmol) and NaOH (111 mg, 1.1 equiv) in acetone/MeOH (11 mL, 10:1) was heated at 50 °C for 24 h. The reaction was quenched by HCl (1 N) solution. The resultant mixture was extracted with ethyl acetate (3 × 15 mL). The combined organic phase was dried over anhydrous NaSO₄, filtered, and evaporated all the volatiles under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 4:1).

To a solution of the above ferrocene carboxylic acid (570 mg, 2.2 mmol, 1 equiv) in dry CH₂Cl₂ (10 mL) at 0 °C under Ar was added dropwise oxalyl chloride (419 mg, 3.3 mmol, 1.5 equiv) followed by a catalytic amount of DMF (2 drops). The reaction was allowed to stir at rt until completion (typically 2 h). The solvent was then removed under reduced pressure to afford the corresponding crude acyl chloride. Methoxyamine hydrochloride (217 mg, 2.6 mmol, 1.2 equiv) was added to a biphasic mixture of K₂CO₃ (608 mg, 4.4 mmol, 2 equiv) in a mixture of EtOAc/H₂O (6 mL, 2:1). The resulting solution was cooled to 0 °C followed by dropwise addition of the unpurified acyl chloride dissolved in a minimum amount of EtOAc. The flask containing the acyl chloride was then rinsed with additional EtOAc. The reaction was allowed to stir overnight at rt. Afterwards, the reaction was quenched with H₂O. The phases were separated and the aqueous phase was extracted with ethyl acetate (3 × 15 mL). The combined organic layers were dried over Na₂SO₄, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 1:1) to afford products **1d**.

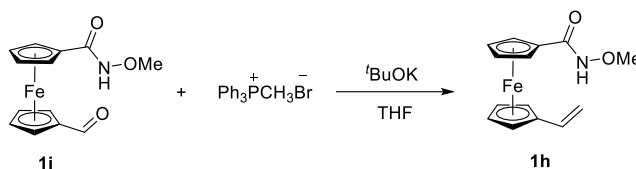


Compound **1d** was prepared from 1'-acetyl-1-ferrocene carboxylic acid methyl ester following the above procedure. 340 mg, 54% yield as orange red solid. m.p. = 63-65 °C. ^1H NMR (400 MHz, CDCl_3) δ 9.31 (s, 1H), 4.73 (s, 2H), 4.31 (s, 2H), 4.11 (s, 4H), 3.83 (s, 3H), 2.55 – 2.04 (m, 2H), 1.12 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 170.0, 92.9, 73.0, 71.4, 69.4, 69.2, 68.8, 64.5, 21.5, 14.8. IR (thin film): ν_{max} (cm^{-1}) = 3183, 3100, 3004, 2958, 2930, 2889, 2867, 2806, 2348, 2107, 2085, 1632, 1509, 1454, 1436, 1416, 1374, 1342, 1297, 1219, 1180, 1145, 1053, 1026, 943, 929, 906, 878, 853, 818, 649, 582, 526, 506, 483, 460, 443. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{17}\text{FeNO}_2\text{Na}$ $[\text{M}+\text{Na}]^+$ 310.0500, found 310.0509.



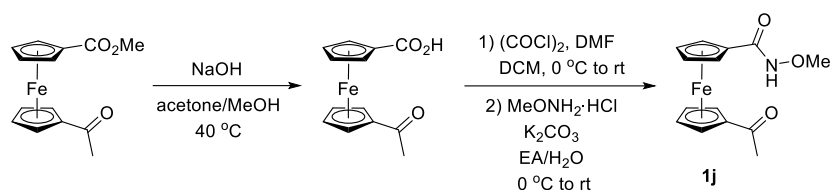
Compound **1e** was prepared from 1'-benzoyl-1-ferrocene carboxylic acid methyl ester following the above procedure. 1.5 g, 68% yield as yellow solid. m.p. = 100-102 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.81 (s, 1H), 7.32 – 7.21 (m, 2H), 7.22 – 7.07 (m, 3H), 4.71 (s, 2H), 4.34 (s, 2H), 4.17 (s, 2H), 4.16 (s, 2H), 3.84 (s, 3H), 3.66 (s, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 170.0, 141.2, 128.5, 128.4, 126.2, 89.8, 73.1, 71.6, 70.5, 69.7, 69.0, 64.7, 35.0. IR (thin film): ν_{max} (cm^{-1}) = 3224, 3075, 2995, 2928, 1641, 1604, 1583, 1501, 1454, 1429, 1394, 1375, 1340, 1297, 1222, 1179, 1159, 1061, 1027, 946, 927, 861, 818, 769, 745, 725, 697, 633, 581, 534, 513, 490, 462, 423. HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{19}\text{FeNO}_2$ $[\text{M}]^+$ 349.0760, found 349.0762.

Synthesis of 1h



To a solution of $t\text{BuOK}$ (269 mg, 2.4 mmol, 1.2 equiv) and methyltriphenylphosphonium bromide (786 mg, 2.2 mmol, 1.1 equiv) in dry THF (10 mL) under Ar was stirred for 1 h and then **1i** was added into this solution. The reaction mixture was stirred overnight at ambient temperature. The reaction was quenched by H_2O . The resultant mixture was extracted with ethyl acetate (3×15 mL). The combined organic phase was dried over anhydrous NaSO_4 , filtered, and evaporated all the volatiles under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 10:1) to afford **1h** (240 mg, 42% yield) as dark red liquid. ^1H NMR (400 MHz, CDCl_3) δ 8.59 (s, 1H), 6.42 (dd, J = 17.5 and 10.7 Hz, 1H), 5.39 (d, J = 17.5 Hz, 1H), 5.14 (d, J = 10.7 Hz, 1H), 4.62 (s, 2H), 4.38 (s, 2H), 4.32 (s, 2H), 4.27 (s, 2H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 169.8, 133.3, 113, 85.0, 73.5, 72.0, 70.7, 69.5, 68.44, 64.7. IR (thin film): ν_{max} (cm^{-1}) = 3176, 3004, 2975, 2937, 2896, 2809, 2290, 2097, 1800, 1634, 1513, 1455, 1437, 1415, 1378, 1338, 1298, 1241, 1220, 1199, 1180, 1146, 1053, 1028, 982, 942, 930, 898, 859, 841, 819, 722, 657, 585, 564, 532, 508, 479, 446. HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{15}\text{FeNO}_2$ $[\text{M}]^+$ 285.0447, found 285.0442.

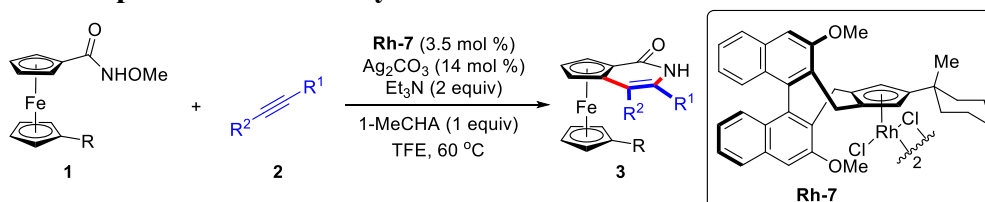
Synthesis of **1j**



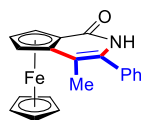
A mixture of 1'-acetyl-1-ferrocenediformic acid mono-methyl ester (2.29 g, 8 mmol), NaOH (360 mg, 9 mmol, 1.1 equiv) in acetone/MeOH (45 mL, 8/1) was heated at 40 °C for 24 h. The reaction was quenched by HCl solution (1 N). The resultant mixture was extracted with ethyl acetate (3 × 30 mL). The combined organic phase was dried over anhydrous NaSO₄, filtered, and evaporated all the volatiles under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 10:1).

To a solution of the above ferrocene carboxylic acid (1.8 g, 6.6 mmol, 1 equiv) in dry CH₂Cl₂ (10 mL) at 0 °C under Ar was added dropwise oxalyl chloride (1.4 equiv) followed by a catalytic amount of DMF (3 drops). The reaction was allowed to stir at rt until completion (typically 2 h). The solvent was then removed under reduced pressure to afford the corresponding crude acyl chloride. Methoxyamine hydrochloride (1.1 equiv) was added to a biphasic mixture of K₂CO₃ (1.8 equiv) in a mixture of EtOAc/H₂O (18 mL, 2:1). The resulting solution was cooled to 0 °C followed by dropwise addition of the unpurified acyl chloride dissolved in a minimum amount of EtOAc. The flask containing the acyl chloride was then rinsed with additional EtOAc. The reaction was allowed to stir overnight at rt. Afterwards, the reaction was quenched with H₂O. The phases were separated and the aqueous phase was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were dried over Na₂SO₄, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 1:1) to afford **1j** (1.0 g, 56% yield) as dark red liquid. ¹H NMR (400 MHz, CDCl₃) δ 10.01 (s, 1H), 4.73 (m, 4H), 4.52 (s, 2H), 4.34 (s, 2H), 3.82 (s, 3H), 2.38 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 202.8, 168.0, 79.9, 74.9, 73.9, 71.9, 71.2, 70.0, 64.2, 27.6. IR (thin film): ν_{max} (cm⁻¹) = 3473, 3197, 3101, 2936, 2814, 2415, 2350, 2318, 2246, 2075, 1645, 1508, 1453, 1399, 1373, 1356, 1275, 1222, 1186, 1147, 1114, 1057, 1025, 942, 926, 893, 818, 767, 730, 700, 667, 645, 690, 593, 528, 480. HRMS (ESI) calcd for C₁₄H₁₅FeNO₃Na [M+Na]⁺ 324.0294, found 324.0298.

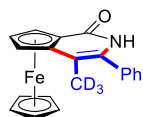
4. General procedure for the synthesis of **3**



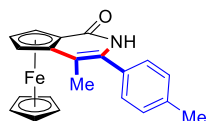
Under Ar atmosphere, a Schlenk tube (15 mL) with a magnetic stir bar were charged with **Rh-7** (9.4 mg, 0.007 mmol, 3.5 mol %), Ag₂CO₃ (7.7 mg, 0.028 mmol, 14 mol %), and TFE (2.0 mL). The mixture was stirred at room temperature for 30 min before the addition of ferrocenecarboxamide **1** (0.2 mmol, 1.0 equiv), 1-MeCHA (0.2 mmol, 1.0 equiv), Et₃N (0.4 mmol, 2 equiv), and internal alkyne **2** (0.4 mmol, 2 equiv). The reaction was stirred at 60 °C for 24 h. The mixture was diluted with EtOAc (15 mL), and filtered through a celite pad. The filter cake was washed with EtOAc and the filtrate was concentrated under reduced pressure. The crude residue was purified by column chromatography on silica gel (PE/EA/Et₃N) to afford products **3**.



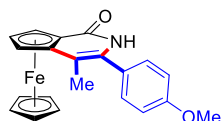
Compound **3aa**³, 53 mg, 77% yield, red solid. ¹H NMR (400 MHz, CDCl₃) δ 7.73 (s, 1H), 7.54 – 7.35 (m, 5H), 5.18 (dd, *J* = 2.7, 1.2 Hz, 1H), 4.79 (dd, *J* = 2.6, 1.2 Hz, 1H), 4.44 – 4.35 (m, 1H), 4.08 (s, 5H), 2.17 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 95:05 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t*_R (minor) = 18.54 min, *t*_R (major) = 23.41 min, 94% ee. [α]_D²⁵ = +1986.0 (*c* = 0.025, CHCl₃). A 2-mmol scale reaction afforded **3aa** in 505 mg (74% yield, 94% ee).



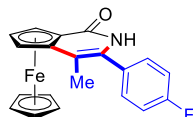
Compound **3ab**, 51 mg, 74% yield, red solid, m.p. = 181–182 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.99 (s, 1H), 7.52 – 7.30 (m, 5H), 5.13 (d, *J* = 1.2 Hz, 1H), 4.77 (d, *J* = 1.2 Hz, 1H), 4.42 – 4.32 (m, 1H), 4.05 (s, 5H). ¹³C NMR (100 MHz, CDCl₃) δ 169.3, 135.6, 132.6, 128.9, 128.8, 128.6, 110.2, 90.9, 71.7, 69.9, 65.7, 64.8. IR (thin film): ν_{max} (cm⁻¹) = 3024, 2922, 2852, 1643, 1496, 1432, 1411, 1363, 1333, 1304, 1260, 1172, 1103, 1049, 1001, 911, 815, 788, 758, 700, 688, 669, 646, 610, 507, 480, 446, 430. HRMS (ESI) calcd for C₂₀H₁₅D₃FeNO [M+H]⁺ 347.0921, found 347.0927. HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 95:05 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t*_R (minor) = 18.49 min, *t*_R (major) = 23.27 min, 94% ee. [α]_D²⁸ = +2042.7 (*c* = 0.025, CHCl₃).



Compound **3ac**³, 55 mg, 78% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 7.83 (s, 1H), 7.37 – 7.20 (m, 4H), 5.18 (br, 1H), 4.83 – 4.73 (m, 1H), 4.44 – 4.32 (m, 1H), 4.07 (s, 5H), 2.42 (s, 3H), 2.18 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 97:03 v/v, flow rate 0.7 mL/min, λ = 254 nm, 40 °C. *t*_R (minor) = 51.34 min, *t*_R (major) = 57.17 min, 95% ee. [α]_D²⁹ = +1907.1 (*c* = 0.025, CHCl₃).

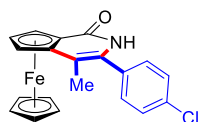


Compound **3ad**³, 64 mg, 85% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 7.75 (s, 1H), 7.31 (d, *J* = 8.3 Hz, 2H), 6.98 (d, *J* = 8.2 Hz, 2H), 5.16 (br, 1H), 4.77 (br, 1H), 4.43 – 4.31 (m, 1H), 4.06 (s, 5H), 3.86 (s, 3H), 2.16 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 85:15 v/v, flow rate 1 mL/min, λ = 254 nm, 40 °C. *t*_R (minor) = 10.90 min, *t*_R (major) = 12.77 min, 94% ee. [α]_D²⁹ = +1616.8 (*c* = 0.025, CHCl₃).

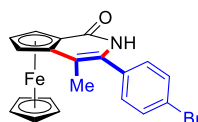


Compound **3ae**³, 57 mg, 79% yield, red solid. ¹H NMR (400 MHz, CDCl₃) δ 8.32 (s, 1H), 7.36 (dd, *J* = 7.9, 5.6 Hz, 2H), 7.14 (m, 2H), 5.19 – 5.06 (m, 1H), 4.81 – 4.70 (m, 1H), 4.41 – 4.31 (m, 1H), 4.04 (s, 5H), 2.12 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t*_R (minor) = 11.53 min, *t*_R (major) =

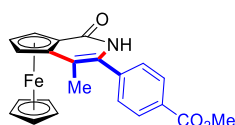
13.17 min, 91% ee. $[\alpha]_D^{28} = +1669.0$ ($c = 0.025$, CHCl_3).



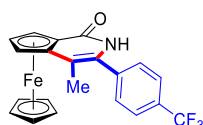
Compound **3af**, 61 mg, 81% yield, red foam. ^1H NMR (400 MHz, CDCl_3) δ 8.46 (s, 1H), 7.42 (d, $J = 7.7$ Hz, 2H), 7.33 (d, $J = 7.8$ Hz, 2H), 5.13 (br, 1H), 4.76 (br, 1H), 4.37 (br, 1H), 4.06 (s, 5H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 169.5, 134.6, 133.8, 131.5, 130.4, 129.0, 110.9, 90.6, 71.8, 69.9, 65.7, 64.9, 14.3. IR (thin film): ν_{max} (cm^{-1}) = 3141, 3094, 2916, 2854, 2321, 2293, 2115, 2082, 1780, 1714, 1639, 1494, 1446, 1431, 1399, 1362, 1332, 1301, 1274, 1256, 1173, 1133, 1105, 1089, 1015, 999, 895, 879, 818, 770, 732, 694, 656, 637, 616, 592, 574, 517, 497, 484, 459, 442. HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{17}\text{ClFeNO}$ $[\text{M}+\text{H}]^+$ 378.0343, found 378.0347. HPLC conditions: Chiralpak AD-H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 95:05 v/v, flow rate 1 mL/min, $\lambda = 254$ nm, 40 $^\circ\text{C}$. t_R (minor) = 21.15 min, t_R (major) = 23.48 min, 95% ee. $[\alpha]_D^{29} = +1686.0$ ($c = 0.025$, CHCl_3).



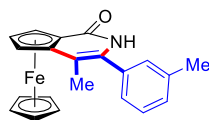
Compound **3ag**³, 66 mg, 79% yield, red solid. ^1H NMR (400 MHz, CDCl_3) δ 8.51 (s, 1H), 7.58 (d, $J = 8.3$ Hz, 2H), 7.26 (d, $J = 8.2$ Hz, 2H), 5.13 (d, $J = 1.2$ Hz, 1H), 4.76 (d, $J = 1.2$ Hz, 1H), 4.42 – 4.33 (m, 1H), 4.03 (s, 5H), 2.13 (s, 3H). HPLC conditions: Chiralpak AD-H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 95:05 v/v, flow rate 1 mL/min, $\lambda = 254$ nm, 40 $^\circ\text{C}$. t_R (minor) = 22.44 min, t_R (major) = 25.25 min, 94% ee. $[\alpha]_D^{28} = +2515.0$ ($c = 0.025$, CHCl_3).



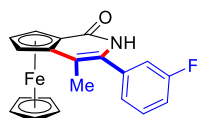
Compound **3ah**³, 64 mg, 80% yield, red foam. ^1H NMR (400 MHz, CDCl_3) δ 8.45 (s, 1H), 8.11 (d, $J = 7.8$ Hz, 2H), 7.47 (d, $J = 7.7$ Hz, 2H), 5.14 (br, 1H), 4.78 (br, 1H), 4.38 (br, 1H), 4.04 (s, 5H), 3.93 (s, 3H), 2.16 (s, 3H). HPLC conditions: Chiralpak AD-H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, $\lambda = 254$ nm, 25 $^\circ\text{C}$. t_R (minor) = 19.90 min, t_R (major) = 24.81 min, 93% ee. $[\alpha]_D^{28} = +1753.4$ ($c = 0.025$, CHCl_3).



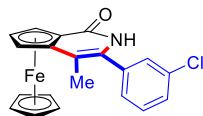
Compound **3ai**, 74 mg, 90% yield, red foam. ^1H NMR (400 MHz, CDCl_3) δ 8.62 (s, 1H), 7.73 (d, $J = 7.9$ Hz, 2H), 7.54 (d, $J = 7.9$ Hz, 2H), 5.14 (br, 1H), 4.80 (br, 1H), 4.48 – 4.33 (m, 1H), 4.05 (s, 5H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) 169.7, 138.9, 131.3, 130.5 (q, $J = 33.4$ Hz), 129.6, 125.7 (q, $J = 3.8$ Hz), 124.0 (q, $J = 270.4$ Hz), 111.8, 90.4, 72.0, 71.8, 69.9, 65.9, 65.1, 14.3. ^{19}F NMR (376 MHz, CDCl_3) δ -62.6. IR (thin film): ν_{max} (cm^{-1}) = 3163, 2921, 2853, 2317, 2100, 1747, 1645, 1617, 1458, 1408, 1377, 1322, 1263, 1193, 1165, 1129, 1110, 1067, 1017, 999, 904, 869, 837, 814, 769, 752, 706, 691, 662, 643, 620, 598, 513, 482, 453, 439, 409. HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{17}\text{F}_3\text{FeNO}$ $[\text{M}+\text{H}]^+$ 412.0606, found 412.0607. HPLC conditions: Chiralpak IC column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, $\lambda = 254$ nm, 25 $^\circ\text{C}$. t_R (minor) = 27.01 min, t_R (major) = 29.98 min, 95% ee. $[\alpha]_D^{28} = +1380.7$ ($c = 0.025$, CHCl_3).



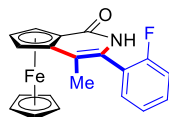
Compound **3aj**³, 59 mg, 83% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 8.02 (s, 1H), 7.37 – 7.29 (m, 1H), 7.24 – 7.13 (m, 3H), 5.15 (d, *J* = 0.8 Hz, 1H), 4.77 (d, *J* = 0.8 Hz, 1H), 4.42 – 4.31 (m, 1H), 4.05 (s, 5H), 2.41 (s, 3H), 2.16 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 85:15 v/v, flow rate 1 mL/min, λ = 254 nm, 40 °C. *t*_R (minor) = 6.38 min, *t*_R (major) = 8.65 min, 97% ee. [α]_D²⁸ = +1757.5 (*c* = 0.025, CHCl₃).



Compound **3ak**, 48 mg, 67% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 8.31 (s, 1H), 7.50 – 7.36 (m, 1H), 7.24 – 7.05 (m, 3H), 5.15 (br, 1H), 4.78 (br, 1H), 4.46 – 4.33 (m, 1H), 4.05 (s, 5H), 2.16 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 169.3, 162.7 (d, *J* = 247.8 Hz), 137.5 (d, *J* = 7.7 Hz), 131.3, 130.5 (d, *J* = 8.5 Hz), 124.7 (d, *J* = 3.1 Hz), 116.2 (d, *J* = 22.0 Hz), 115.6 (d, *J* = 21.0 Hz), 111.1, 90.5, 71.8, 71.8, 69.9, 65.8, 65.0, 14.3. ¹⁹F NMR (376 MHz, CDCl₃) δ -111.85 (m). IR (thin film): ν_{max} (cm⁻¹) = 3168, 3035, 2915, 2854, 1642, 1609, 1578, 1491, 1433, 1379, 1331, 1305, 1267, 1192, 1168, 1122, 1104, 1061, 1000, 906, 875, 817, 786, 734, 712, 687, 664, 624, 520, 501, 485, 448. HRMS (ESI) calcd for C₂₀H₁₇FFeNO [M+H]⁺ 362.0638, found 362.0644. HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t*_R (minor) = 8.45 min, *t*_R (major) = 12.14 min, 92% ee. [α]_D²⁸ = +1889.4 (*c* = 0.025, CHCl₃).

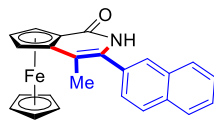


Compound **3al**, 59 mg, 78% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 8.51 (s, 1H), 7.44 – 7.34 (m, 3H), 7.32 – 7.25 (m, 1H), 5.16 (br, 1H), 4.78 (br, 1H), 4.45 – 4.33 (m, 1H), 4.05 (s, 5H), 2.16 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 169.5, 137.1, 134.6, 131.2, 130.1, 129.2, 128.6, 127.3, 111.2, 90.5, 71.8, 71.8, 69.9, 65.8, 65.0, 14.3. IR (thin film): ν_{max} (cm⁻¹) = 3177, 3097, 3059, 2912, 2285, 2110, 1643, 1594, 1563, 1484, 1444, 1427, 1408, 1379, 1353, 1330, 1300, 1173, 1135, 1105, 1078, 1060, 1024, 1005, 925, 892, 872, 848, 805, 785, 754, 708, 687, 660, 623, 584, 568, 540, 490, 473, 451. HRMS (ESI) calcd for C₂₀H₁₇ClFeNO [M+H]⁺ 378.0343, found 378.0348. HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t*_R (minor) = 8.64 min, *t*_R (major) = 13.74 min, 95% ee. [α]_D²⁷ = +1888.6 (*c* = 0.025, CHCl₃).

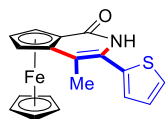


Compound **3am**, 60 mg, 83% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 8.42 (s, 1H), 7.37 (m, 2H), 7.19 (m, 2H), 5.12 (br, 1H), 4.76 (br, 1H), 4.42 – 4.31 (m, 1H), 4.05 (s, 5H), 2.04 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 169.4, 159.7 (d, *J* = 248.3 Hz), 131.2 (d, *J* = 2.1 Hz), 130.9 (d, *J* = 8.3 Hz), 126.3, 124.5 (d, *J* = 3.5 Hz), 123.0 (d, *J* = 15.8 Hz), 116.2 (d, *J* = 22.0 Hz), 112.9, 90.2, 72.0, 71.7, 70.0, 65.7, 64.8, 14.1. ¹⁹F NMR (376 MHz, CDCl₃) δ -113.4 (m). IR (thin film): ν_{max} (cm⁻¹) = 3091, 3000, 2852, 2287, 2243, 2119, 1639, 1533, 1515, 1495, 1443, 1381, 1363, 1334, 1306, 1252, 1219, 1177, 1136, 1101, 1062, 1027, 999, 950, 865, 823, 760, 743, 700, 684, 659, 624, 574, 535, 507, 481, 452. HRMS (ESI) calcd for C₂₀H₁₇FFeNO [M+H]⁺ 362.0638, found 362.0641. HPLC conditions: Chiralpak

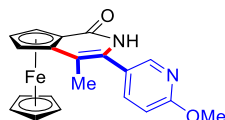
AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 95:05 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (minor) = 21.12 min, t_R (major) = 23.11 min, 96% ee. $[\alpha]_D^{28} = +2158.5$ ($c = 0.025$, CHCl₃).



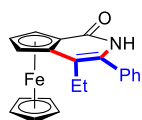
Compound **3an**, 65 mg, 82% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 8.26 (s, 1H), 7.94 – 7.83 (m, 4H), 7.54 (m, 2H), 7.49 (dd, $J = 8.4, 1.7$ Hz, 1H), 5.21 – 5.13 (m, 1H), 4.80 (dd, $J = 2.4, 1.1$ Hz, 1H), 4.43 – 4.34 (m, 1H), 4.08 (s, 5H), 2.21 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 169.4, 133.1, 133.0, 132.8, 132.5, 128.5, 128.3, 128.2, 127.8, 126.8, 126.8, 126.4, 110.8, 90.9, 71.7, 69.9, 65.7, 64.8, 14.4. IR (thin film): $\nu_{\max}$ (cm⁻¹) = 3377, 3166, 3048, 2915, 2853, 2301, 2117, 1917, 1775, 1641, 1596, 1503, 1426, 1378, 1350, 1326, 1297, 1264, 1228, 1170, 1136, 1118, 1104, 1060., 1021, 1000, 946, 896, 858, 817, 790, 770, 747, 731, 697, 669, 645, 620, 586, 548, 519, 476, 451. HRMS (ESI) calcd for C₂₄H₂₀FeNO [M+H]⁺ 394.0889, found 394.0893. HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 95:05 v/v, flow rate 1 mL/min, λ = 254 nm, 40 °C. t_R (minor) = 30.71 min, t_R (major) = 37.87 min, 96% ee. $[\alpha]_D^{28} = +1659.5$ ($c = 0.025$, CHCl₃).



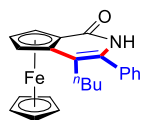
Compound **3ao**³, 28 mg, 40% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 7.84 (s, 1H), 7.42 (d, $J = 3.9$ Hz, 1H), 7.21 – 7.07 (m, 2H), 5.18 (br, 1H), 4.79 (br, 1H), 4.41 (br, 1H), 4.07 (s, 5H), 2.30 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (minor) = 12.47 min, t_R (major) = 13.82 min, 93% ee. $[\alpha]_D^{28} = +1458.5$ ($c = 0.025$, CHCl₃).



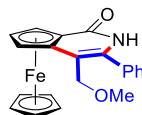
Compound **3ap**, 63 mg, 84% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 8.74 (s, 1H), 8.18 (s, 1H), 7.60 (d, $J = 7.2$ Hz, 1H), 6.83 (d, $J = 7.8$ Hz, 1H), 5.12 (br, 1H), 4.76 (br, 1H), 4.36 (br, 1H), 4.03 (s, 5H), 3.97 (s, 3H), 2.13 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 169.6, 164.1, 147.3, 139.0, 129.5, 124.5, 111.4, 111.1, 90.6, 71.8, 71.8, 69.9, 65.8, 64.9, 53.8, 14.3. IR (thin film): $\nu_{\max}$ (cm⁻¹) = 3169, 3085, 3013, 2926, 2853, 2322, 2088, 1782, 1642, 1602, 1564, 1494, 1464, 1411, 1372, 1333, 1285, 1173, 1128, 1105, 1061, 1027, 1017, 931, 826, 766, 734, 685, 618, 588, 570, 542, 488, 450. HRMS (ESI) calcd for C₂₀H₁₉FeN₂O₂ [M+H]⁺ 375.0790, found 375.0794. HPLC conditions: Chiralpak IG column (4.6 mm × 250 mm), hexane/*i*-PrOH, 80:20 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (minor) = 19.10 min, t_R (major) = 24.08 min, 83% ee. $[\alpha]_D^{29} = +1406.6$ ($c = 0.025$, CHCl₃).



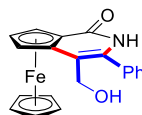
Compound **3aq**³, 42 mg, 59% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 7.93 (s, 1H), 7.53 – 7.33 (m, 5H), 5.29 – 5.03 (m, 1H), 4.91 – 4.73 (m, 1H), 4.48 – 4.33 (m, 1H), 4.06 (s, 5H), 2.72 – 2.36 (m, 2H), 1.32 (t, $J = 7.5$ Hz, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (minor) = 9.13 min, t_R (major) = 14.29 min, 94% ee. $[\alpha]_D^{29} = +2042.5$ ($c = 0.025$, CHCl₃).



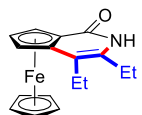
Compound **3ar**³, 42 mg, 55% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 7.98 (s, 1H), 7.49 – 7.32 (m, 5H), 5.20 – 5.07 (m, 1H), 4.83 – 4.71 (m, 1H), 4.44 – 4.33 (m, 1H), 4.05 (s, 5H), 2.56 – 2.33 (m, 2H), 1.85 – 1.56 (m, 2H), 1.33 (q, *J* = 7.4 Hz, 2H), 0.88 (t, *J* = 7.3 Hz, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t_R* (minor) = 6.75 min, *t_R* (major) = 8.58 min, 93% ee. [α]_D²⁸ = +1781.6 (*c* = 0.025, CHCl₃).



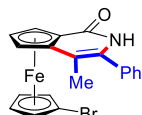
Compound **3as**³, 41 mg, 55% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 8.05 (s, 1H), 7.50 – 7.42 (m, 5H), 5.14 (br, 1H), 4.92 (br, 1H), 4.45 – 4.39 (m, 1H), 4.34 (d, *J* = 10.7 Hz, 1H), 4.18 (d, *J* = 10.7 Hz, 1H), 4.07 (s, 5H), 3.38 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t_R* (minor) = 12.39 min, *t_R* (major) = 14.31 min, 98% ee. [α]_D²⁸ = +1457.7 (*c* = 0.05, CHCl₃).



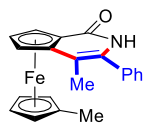
Compound **3at**³, 50 mg, 70% yield, red foam. ¹H NMR (400 MHz, CD₃OD) δ 7.66 – 7.37 (m, 5H), 5.11 (br, 2H), 4.59 (d, *J* = 11.8 Hz, 1H), 4.49 (br, 1H), 4.38 (d, *J* = 11.8 Hz, 1H), 4.08 (s, 5H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t_R* (major) = 24.66 min, *t_R* (minor) = 30.19 min, 97% ee. [α]_D²⁸ = +1891.6 (*c* = 0.05, CHCl₃).



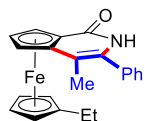
Compound **3au**, 52 mg, 84% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 9.32 (s, 1H), 5.10 (br, 1H), 4.70 (br, 1H), 4.30 (br, 1H), 3.97 (s, 5H), 2.60 – 2.41 (m, 4H), 1.31 – 1.18 (m, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 134.7, 113.4, 91.1, 71.3, 71.1, 69.8, 64.7, 63.8, 23.5, 21.2, 15.0, 14.3. IR (thin film): ν_{max} (cm⁻¹) = 3305, 3166, 3096, 3036, 2964, 2927, 2870, 1650, 1630, 1487, 1448, 1410, 1375, 1342, 1322, 1295, 1260, 1217, 1179, 1105, 1078, 1057, 1030, 1000, 878, 850, 821, 772, 718, 685, 650, 631, 592, 576, 543, 506, 476, 446. HRMS (ESI) calcd for C₁₇H₂₀FeNO [M+H]⁺ 310.0894, found 310.0884. HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 95:05 v/v, flow rate 0.7 mL/min, λ = 254 nm, 40 °C. *t_R* (minor) = 15.57 min, *t_R* (major) = 17.36 min, 41% ee. [α]_D²⁸ = +627.3 (*c* = 0.025, CHCl₃).



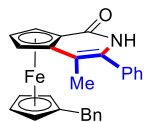
Compound **3ba**³, 61 mg, 73% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 8.05 (s, 1H), 7.53 – 7.34 (m, 5H), 5.20 (br, 1H), 4.78 (br, 1H), 4.43 (br, 1H), 4.33 (br, 1H), 4.19 – 4.01 (m, 3H), 2.15 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. *t_R* (minor) = 11.43 min, *t_R* (major) = 12.78 min, 96% ee. [α]_D²⁹ = +1740.4 (*c* = 0.025, CHCl₃).



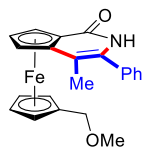
Compound **3ca**, 50 mg, 70% yield, red foam. ^1H NMR (400 MHz, CD_2Cl_2) δ 8.81 (s, 1H), 7.55 – 7.38 (m, 5H), 5.01 (br, 1H), 4.73 (br, 1H), 4.40 – 4.29 (m, 1H), 4.01 (br, 2H), 3.96 – 3.81 (m, 2H), 2.15 (s, 3H), 1.74 (s, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 169.1, 1369, 133.2, 129.5, 128.9, 128.7, 109.7, 91.7, 84.8, 72.8, 72.3, 70.9, 70.8, 68.9, 68.6, 65.9, 65.4, 14.5, 12.3. IR (thin film): ν_{max} (cm^{-1}) = 3169, 3028, 2919, 2853, 2316, 2116, 2086, 1893, 1713, 1639, 1495, 1442, 1380, 1364 1332, 1300, 1260, 1228, 1172, 1132, 1059, 1025, 1003, 921, 883, 811, 769, 702, 627, 584, 569, 484, 452. HRMS (ESI) calcd for $\text{C}_{21}\text{H}_{20}\text{FeNO}$ $[\text{M}+\text{H}]^+$ 358.0889, found 358.0886. HPLC conditions: Chiralpak AD–H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 $^\circ\text{C}$. t_{R} (minor) = 8.84 min, t_{R} (major) = 11.27 min, 94% ee. $[\alpha]_{\text{D}}^{28}$ = +1319.9 (c = 0.020, CHCl_3).



Compound **3da**, 46 mg, 62% yield, red foam. ^1H NMR (400 MHz, CD_2Cl_2) δ 9.20 (s, 1H), 7.52 – 7.39 (m, 5H), 5.05 – 4.94 (m, 1H), 4.79 – 4.68 (m, 1H), 4.39 – 4.28 (m, 1H), 4.03 – 3.89 (m, 4H), 2.24 – 2.10 (m, 5H), 1.08 (t, J = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 169.4, 135.9, 133.3, 129.6, 128.8, 128.6, 109.9, 91.7, 91.6, 72.7, 72.3, 69.3, 69.1, 69.1, 69.0, 65.9, 65.3, 20.8, 15.2, 14.5. IR (thin film): ν_{max} (cm^{-1}) = 3165, 3052, 2963, 2925, 2107, 1725, 1641, 1571, 1496, 1442, 1358, 1333, 1299, 1262, 1173, 1131, 1061, 1039, 1022, 1003, 905, 813, 770, 733, 701, 585, 483. HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{22}\text{FeNO}$ $[\text{M}+\text{H}]^+$ 372.1045, found 372.1048. HPLC conditions: Chiralpak OD–H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 $^\circ\text{C}$. t_{R} (minor) = 7.38 min, t_{R} (major) = 10.52 min, 94% ee. $[\alpha]_{\text{D}}^{26}$ = +1359.9 (c = 0.025, CHCl_3).

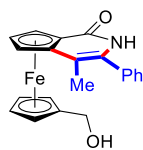


Compound **3ea**, 53 mg, 61% yield, red foam. ^1H NMR (400 MHz, CD_2Cl_2) δ 8.55 (s, 1H), 7.54 – 7.40 (m, 5H), 7.27 – 7.06 (m, 5H), 5.13 – 5.04 (m, 1H), 4.84 – 4.75 (m, 1H), 4.45 – 4.35 (m, 1H), 4.11 – 3.95 (m, 4H), 3.58 – 3.43 (m, 2H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 169.1, 141.9, 136.0, 133.3, 129.5, 129.0, 128.8, 128.6, 128.5, 126.3, 109.8, 91.9, 88.6, 72.5, 70.6, 70.3, 69.6, 69.5, 66.2, 65.6, 34.2, 14.5. IR (thin film): ν_{max} (cm^{-1}) = 3163, 3025, 2913.89, 1642, 1600, 1494, 1442, 1378, 1332, 1300, 1260, 1172, 1132, 1073, 1025, 1002, 924, 812, 769, 701, 619, 566, 482, 464. HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{24}\text{FeNO}$ $[\text{M}+\text{H}]^+$ 434.1202, found 434.1201. HPLC conditions: Chiralpak OD–H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 85:15 v/v, flow rate 1 mL/min, λ = 254 nm, 25 $^\circ\text{C}$. t_{R} (minor) = 7.15 min, t_{R} (major) = 10.19 min, 91% ee. $[\alpha]_{\text{D}}^{28}$ = +1317.9 (c = 0.025, CHCl_3).

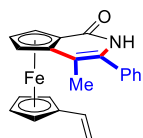


Compound **3fa**³, 42 mg, 55% yield, red foam. ^1H NMR (400 MHz, CDCl_3) δ 7.95 (s, 1H), 7.53 – 7.34 (m, 5H), 5.13 (br, 1H), 4.75 (br, 1H), 4.37 (br, 1H), 4.19 – 4.02 (m, 6H), 3.24 (s, 3H), 2.15 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 $^\circ\text{C}$. t_{R} (minor) = 12.53 min, t_{R} (major) = 14.49 min, 96% ee. $[\alpha]_{\text{D}}^{28}$ =

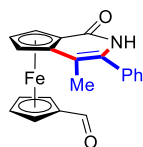
+1534.7 ($c = 0.025$, CHCl_3).



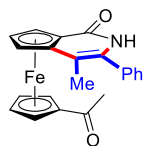
Compound **3ga**³, 40 mg, 53% yield, red foam. ¹H NMR (400 MHz, CDCl_3) δ 8.05 (s, 1H), 7.52 – 7.36 (m, 5H), 5.19 (br, 1H), 4.87 – 4.77 (m, 1H), 4.43 (br, 1H), 4.40 – 4.18 (m, 3H), 4.15 (br, 2H), 3.70 (br, 1H), 3.17 (br, 1H), 2.17 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, $\lambda = 254$ nm, 25 °C. t_R (minor) = 18.90 min, t_R (major) = 22.41 min, 90% ee. $[\alpha]_D^{28} = +1659.1$ ($c = 0.025$, CHCl_3).



Compound **3ha**, 35 mg, 47% yield, red foam. ¹H NMR (400 MHz, CD_2Cl_2) δ 8.75 (s, 1H), 7.53 – 7.36 (m, 5H), 6.16 (dd, $J = 17.5, 10.7$ Hz, 1H), 5.24 (dd, $J = 17.5, 1.2$ Hz, 1H), 5.08 (dd, $J = 10.8, 1.2$ Hz, 1H), 5.04 – 4.98 (m, 1H), 4.77 – 4.68 (m, 1H), 4.36 – 4.29 (m, 1H), 4.24 – 4.16 (m, 3H), 4.14 (br, 1H), 2.09 (s, 3H). ¹³C NMR (100 MHz, CD_2Cl_2) δ 168.5, 135.9, 133.8, 132.1, 129.6, 128.8, 128.7, 113.1, 109.4, 92.4, 84.6, 73.3, 72.6, 70.4, 69.9, 68.6, 67.9, 66.2, 65.9, 14.6. IR (thin film): ν_{max} (cm^{-1}) = 3165, 3081, 3052, 2920, 2852, 2116, 1893, 1786, 1729, 1642, 1495, 1442, 1377, 1332, 1300, 1261, 1241, 1172, 1131, 1061, 1028, 983, 894, 867, 814, 770, 724, 702, 636, 620, 586, 566, 506, 480, 461, 416. HRMS (ESI) calcd for $\text{C}_{22}\text{H}_{20}\text{FeNO}$ $[\text{M}+\text{H}]^+$ 370.0889, found 370.0884. HPLC conditions: Chiralpak AD–H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, $\lambda = 254$ nm, 25 °C. t_R (minor) = 9.11 min, t_R (major) = 11.06 min, 90% ee. $[\alpha]_D^{28} = +1938.1$ ($c = 0.025$, CHCl_3).

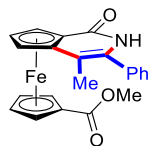


Compound **3ia**³, 30 mg, 41% yield, dark red foam. ¹H NMR (400 MHz, CDCl_3) δ 9.73 (s, 1H), 8.06 (s, 1H), 7.52 – 7.38 (m, 5H), 5.21 (br, 1H), 4.88 (br, 1H), 4.76 (br, 1H), 4.66 – 4.49 (m, 3H), 4.40 (br, 1H), 2.07 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, $\lambda = 254$ nm, 25 °C. t_R (minor) = 25.07 min, t_R (major) = 28.90 min, 96% ee. $[\alpha]_D^{28} = +3665.5$ ($c = 0.025$, CHCl_3).

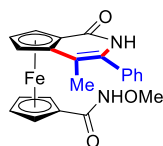


Compound **3ja**, 45 mg, 58% yield, red foam. ¹H NMR (400 MHz, CD_2Cl_2) δ 8.57 (s, 1H), 7.55 – 7.38 (m, 5H), 5.11 – 5.06 (m, 1H), 4.85 – 4.80 (m, 1H), 4.66 – 4.58 (m, 2H), 4.49 – 4.41 (m, 2H), 4.40 – 4.36 (m, 1H), 2.25 (s, 3H), 2.08 (s, 3H). ¹³C NMR (100 MHz, CD_2Cl_2) δ 202.5, 169.8, 137.6, 136.8, 131.6, 131.0, 130.9, 110.8, 95.0, 82.7, 75.6, 75.4, 75.3, 74.8, 73.2, 73.1, 68.8, 68.0, 56.4, 56.1, 30.0, 16.4. IR (thin film): ν_{max} (cm^{-1}) = 3168, 3102, 3024, 2921, 2853, 2338, 2100, 1898, 1807, 1731, 1643, 1495, 1451, 1398, 1375, 1353, 1333, 1304, 1273, 1211, 1175, 1135, 1113, 1080, 1061, 1034, 1018, 958, 891, 853, 821, 806, 789, 773, 707, 665, 619, 588, 569, 526, 491, 459, 425. HRMS (ESI) calcd for

C₂₂H₂₀FeNO₂ [M+H]⁺ 386.0838, found 386.0834. HPLC conditions: Chiralpak OD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 80:20 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (minor) = 8.32 min, t_R (major) = 9.46 min, 97% ee. [α]_D²⁶ = +3237.1 (*c* = 0.025, CHCl₃).

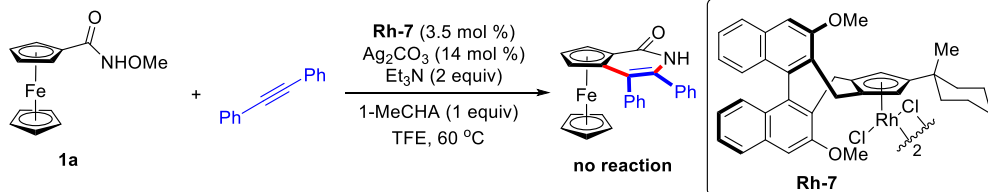


Compound **3ka**³, 52 mg, 65% yield, red solid. ¹H NMR (400 MHz, CDCl₃) δ 7.98 (s, 1H), 7.58 – 7.32 (m, 5H), 5.16 (br, 1H), 4.78 (br, 1H), 4.71 (br, 1H), 4.58 (br, 1H), 4.49 – 4.25 (m, 3H), 3.67 (s, 3H), 2.09 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 90:10 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (minor) = 16.91 min, t_R (major) = 24.16 min, 99% ee. [α]_D²⁸ = +2796.4 (*c* = 0.025, CHCl₃).

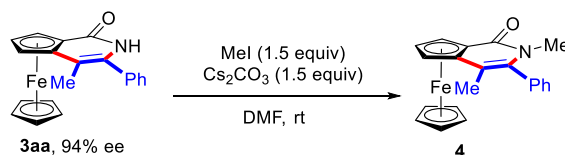


Compound **3la**³, 44 mg, 59% yield, red foam. ¹H NMR (400 MHz, CDCl₃) δ 9.96 (s, 1H), 8.42 (s, 1H), 7.49 – 7.34 (m, 5H), 5.13 (br, 1H), 4.83 (br, 1H), 4.66 (br, 1H), 4.58 (br, 1H), 4.45 (br, 1H), 4.36 (br, 1H), 4.15 (br, 1H), 3.78 (s, 3H), 2.13 (s, 3H). HPLC conditions: Chiralpak AD–H column (4.6 mm × 250 mm), hexane/*i*-PrOH, 80:20 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (minor) = 6.42 min, t_R (major) = 10.36 min, 95% ee. [α]_D²⁸ = +2360.6 (*c* = 0.025, CHCl₃).

Unsuccessful substrate

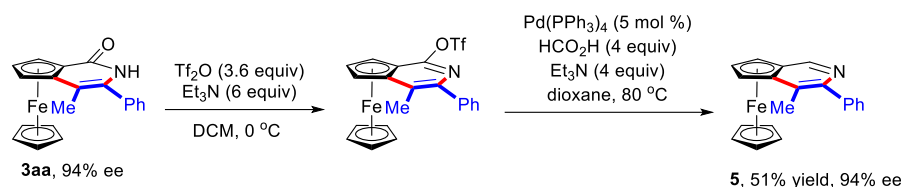


5. Derivatization reactions

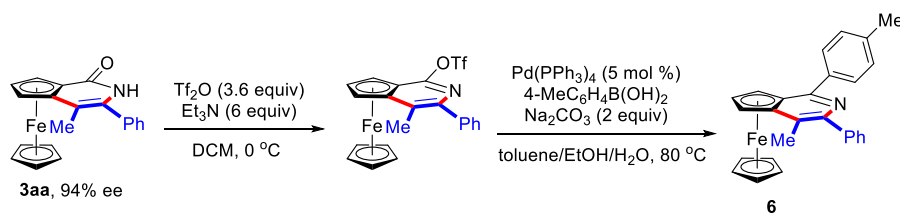


Under argon atmosphere, to a mixture of **3aa** (69 mg, 0.2 mmol, 1.0 equiv) and Cs₂CO₃ (100 mg, 0.3 mmol, 1.5 equiv) in anhydrous DMF (2.0 mL) was added MeI (43 mg, 0.3 mmol, 1.5 equiv). The reaction was stirred at room temperature for 24 h. Afterwards, the reaction was quenched with H₂O. The phases were separated and the aqueous phase was extracted with ethyl acetate (3 × 10 mL). The combined organic layers were dried over Na₂SO₄, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (PE/EtOAc = 1:1) to afford **4** (68 mg, 96% yield) as red foam. ¹H NMR (400 MHz, CD₂Cl₂) δ 7.55 – 7.42 (m, 3H), 7.30 – 7.16 (m, 2H), 5.12 (dd, *J* = 2.5, 1.1 Hz, 1H), 4.75 (dd, *J* = 2.4, 1.1 Hz, 1H), 4.35 – 4.30 (m, 1H), 4.05 (s, 5H), 3.08 (s, 3H), 1.90 (s, 3H). ¹³C NMR (100 MHz, CD₂Cl₂) δ 168.7, 137.1, 136.6, 130.2, 130.1, 129.1, 129.0, 128.6, 111.7, 89.5, 73.0, 71.2, 69.9, 66.0, 64.4, 33.4, 15.3. IR (thin film): ν_{max} (cm⁻¹) = 3439, 3082,

2914, 2857, 2735, 2697, 2648, 2390, 2316, 2112, 1887, 1773, 1709, 1645, 1610, 1593, 1494, 1443, 1409, 1376, 1319, 1275, 1210, 1178, 1147, 1104, 1084, 1053, 1023, 1000, 941, 919, 884, 869, 817, 780, 766, 711, 652, 637, 597, 530, 486, 435. HRMS (ESI) calcd for $C_{21}H_{20}FeNO$ $[M+H]^+$ 358.0889, found 358.0892. HPLC conditions: Chiralpak IG column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 85:15 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (minor) = 5.82 min, t_R (major) = 6.85 min, 94% ee. $[\alpha]_D^{27}$ = +3263.3 (c = 0.025, $CHCl_3$).



To a stirred mixture of **3aa** (98 mg, 0.3 mmol) and Et_3N (182 mg, 1.8 mmol, 6 equiv) in dry DCM (3 mL) at 0 °C was added Tf_2O (304 mg, 1.08 mmol). The mixture was stirred for 30 min at 0 °C and diluted successively with DCM (3 mL), and sat. $NaHCO_3$ aq. (6 mL). Then the organic layer was separated, dried with Na_2SO_4 , filtered and concentrated under reduced pressure. The residue was purified by column chromatography (neutral aluminum oxide) to afford trifluoromethanesulfonate, which was used for the next step without further purification. To a stirred mixture of the above trifluoromethanesulfonate, $Pd(PPh_3)_4$ (17 mg, 0.015 mmol), Et_3N (121 mg, 1.2 mmol, 4 equiv) in dry dioxane (3 mL) at rt was added HCO_2H (41 mg, 0.9 mmol). The mixture was stirred for 40 min at 80 °C and then was allowed to cool to rt. The reaction mixture was diluted with saturated aqueous $NaCl$ solution and extracted with ethyl acetate. The organic layer was dried with Na_2SO_4 , concentrated in vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/ Et_3N = 8/1/1, v/v/v) to afford red purple sticky oil (50 mg, 51% yield). 1H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 7.60 – 7.31 (m, 5H), 5.08 (d, J = 5.9 Hz, 2H), 4.31 (br, 1H), 3.91 (s, 5H), 2.52 (s, 3H). HPLC conditions: Chiralpak OD–H column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 95/05 v/v, flow rate 1 mL/min, λ = 254 nm, 25 °C. t_R (major) = 8.61 min, t_R (minor) = 10.68 min, 94% ee. $[\alpha]_D^{27}$ = -359.7 (c = 0.025, $CHCl_3$).

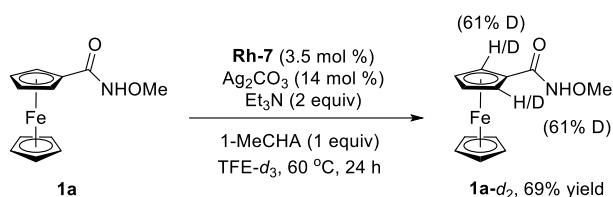


To a stirred mixture of **3aa** (34 mg, 0.1 mmol) and Et_3N (61 mg, 0.6 mmol, 6 equiv) in dry DCM (1 mL) at 0 °C was added Tf_2O (102 mg, 0.36 mmol). The mixture was stirred for 30 min at 0 °C and diluted successively with DCM (3 mL), and sat. $NaHCO_3$ aq. (2 mL). Then the organic layer was separated, dried with Na_2SO_4 , filtered and concentrated under reduced pressure. The residue was purified by column chromatography (neutral aluminum oxide) to afford trifluoromethanesulfonate, which was used for the next step without further purification. The mixture of the above trifluoromethanesulfonate, $Pd(PPh_3)_4$ (6 mg, 0.005 mmol), 4-MeC₆H₄B(OH)₂ (27 mg, 0.2 mmol, 2 equiv), Na_2CO_3 (21 mg, 0.2 mmol, 2 equiv) in 1.2 mL toluene/EtOH/ H_2O (10/1/1) under Ar was stirred for 24 h at 80 °C and then was allowed to cool to rt. The reaction mixture was diluted with brine and extracted with ethyl acetate. The organic layer was dried with Na_2SO_4 , concentrated in vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/ Et_3N = 100/1/2, v/v/v) to afford red purple

sticky oil (28 mg, 67% yield). ^1H NMR (400 MHz, CDCl_3) δ 8.11 (d, $J = 8.0$ Hz, 2H), 7.66 (d, $J = 7.3$ Hz, 2H), 7.51 – 7.43 (m, 2H), 7.39 – 7.32 (m, 3H), 5.26 (d, $J = 1.9$ Hz, 1H), 5.17 – 5.09 (m, 1H), 4.40 – 4.33 (m, 1H), 3.90 (s, 5H), 2.58 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 162.9, 145.6, 141.5, 139.1, 137.8, 130.1, 129.3, 128.4, 128.0, 127.0, 124.9, 93.0, 78.5, 73.3, 68.6, 63.8, 62.3, 21.6, 16.5. IR (thin film): ν_{max} (cm^{-1}) = 3368, 3028, 2918, 2851, 2729, 2330, 2111, 1891, 1774, 1710, 1647, 1612, 1578, 1556, 1509, 1490, 1451, 1405, 1383, 1358, 1329, 1244, 1212, 1180, 1158, 1124, 1105, 1074, 1040, 1019, 1000, 986, 912, 882, 858, 821, 778, 756, 728, 700, 649, 584, 568, 531, 508, 478, 455. HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{24}\text{FeN}$ $[\text{M}+\text{H}]^+$ 418.1253, found 418.1258. HPLC conditions: Chiralpak IG column (4.6 mm $\times$ 250 mm), hexane/*i*-PrOH, 97:03 v/v, flow rate 1 mL/min, $\lambda = 254$ nm, 25 $^\circ\text{C}$. t_{R} (minor) = 9.87 min, t_{R} (major) = 10.97 min, 94% ee. $[\alpha]_{\text{D}}^{27} = +1688.8$ ($c = 0.025$, CHCl_3).

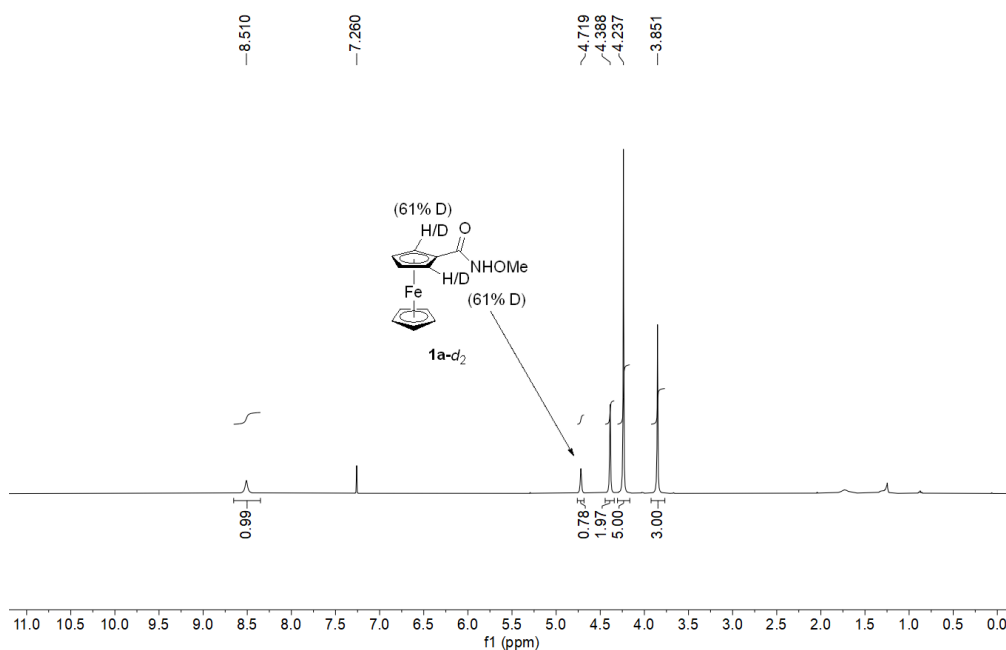
6. Mechanistic experiments

(1) Deuterium-labeling experiments

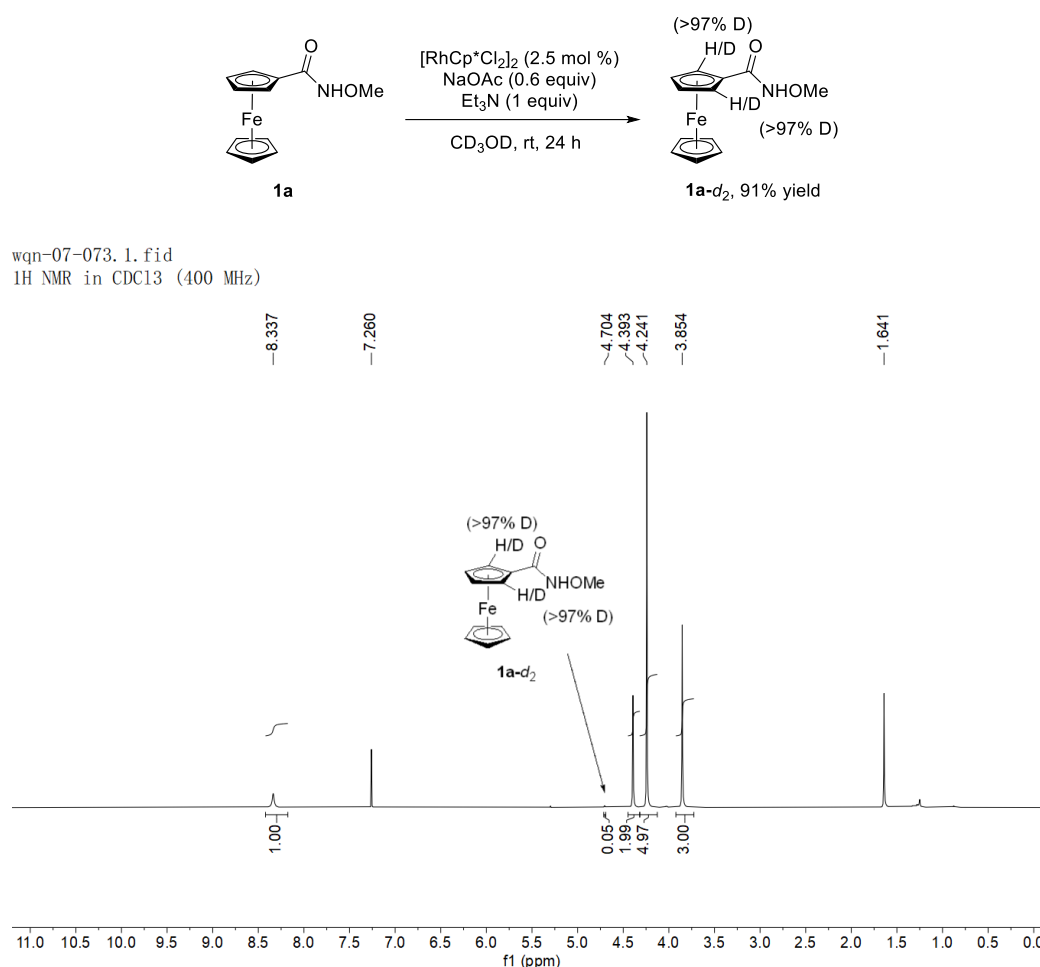


Under Ar atmosphere, a 15 mL Schlenk tube with a magnetic stir bar were charged with **Rh-7** (4.7 mg, 0.0035 mmol, 3.5 mol %), Ag_2CO_3 (3.8 mg, 0.014 mmol, 14 mol %), and TFE (1.0 mL). The mixture was stirred at room temperature for 30 min before the addition of ferrocenecarboxamide **1a** (0.1 mmol, 1.0 equiv), 1-MeCHA (0.1 mmol, 1.0 equiv), and Et_3N (0.2 mmol, 2 equiv). The reaction was stirred at 60 $^\circ\text{C}$ for 24 h. The mixture was diluted with EtOAc (15 mL), and filtered through a celite pad. The filter cake was washed with EtOAc and the filtrate was concentrated under reduced pressure. The remaining residue was purified by column chromatography on silica gel (PE/EA = 2/1, v/v) to afford **1a- d_2** as an orange solid (18 mg, 69% yield).

wqn-07-065-H1. 1. fid
 ^1H NMR in CDCl_3 (400 MHz)



(2) Synthesis of **1a-d₂**



Under Ar atmosphere, a 15 mL Schlenk tube with a magnetic stir bar were charged with $[\text{RhCp}^*\text{Cl}_2]_2$ (26 mg, 0.0423 mmol), **1a** (438 mg, 1.69 mmol), NaOAc (83 mg, 1.0 mmol), Et_3N (172 mg, 1.69 mmol) and CD_3OD (10 mL). The mixture was stirred at rt for 24 h. The mixture was quenched with $\text{CH}_3\text{CO}_2\text{D}$ (1.5 mL) and stirred for 5 min. Then, the mixture was diluted with H_2O and extracted with ethyl acetate. The organic layer was dried with Na_2SO_4 , concentrated in vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 2/1, v/v) to afford **1a-d₂** as orange solid (400 mg, 91% yield).

(3) Parallel kinetic isotope effect experiment

Under Ar atmosphere, a Schlenk tube (15 mL) with a magnetic stir bar were charged with **Rh-7** (9.4 mg, 0.0035 mmol, 3.5 mol %), Ag_2CO_3 (7.7 mg, 0.014 mmol, 14 mol %), and TFE (2.0 mL). The mixture was stirred at room temperature for 30 min before the addition of ferrocenecarboxamide **1a** or **1a-d₂** (0.2 mmol, 1.0 equiv), 1-MeCHA (0.2 mmol, 1.0 equiv), Et_3N (0.4 mmol, 2 equiv), and **2a** (0.4 mmol, 2.0 equiv). The reaction was stirred at 60 °C. For each 10 min, 200 μL of the reaction mixture was transferred to a short pad of silica gel and washed with ethyl acetate. The solvent was evaporated, and analyzed by ^1H NMR using dibromomethane as an internal standard. The initial rates of the two reactions were calculated based on the slopes of the straight lines obtained by fitting the four points. The KIE value (k_H/k_D) was calculated to be 1.0 (**Figure S1** and **Figure S2**).

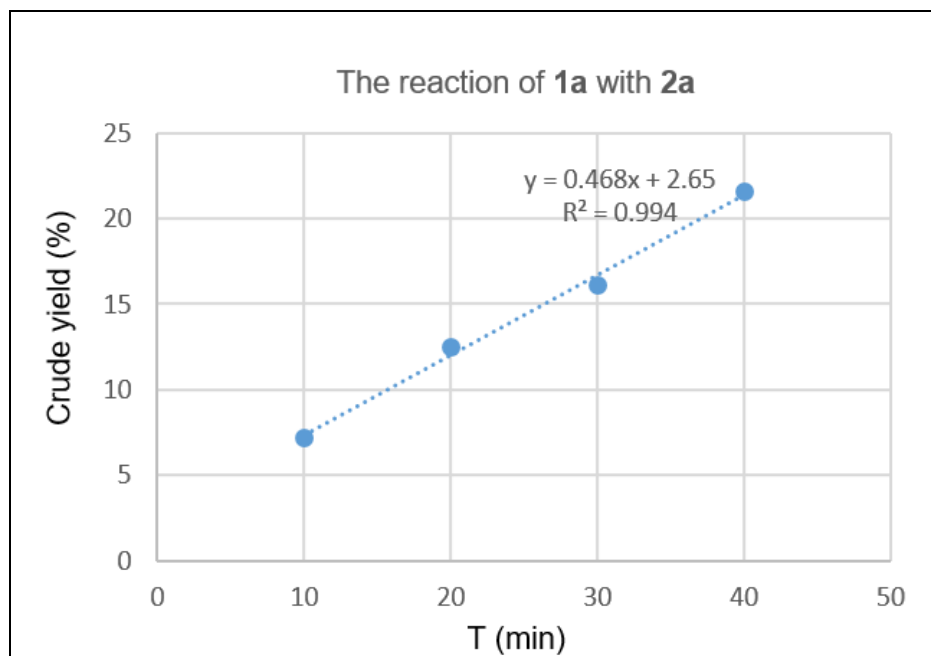
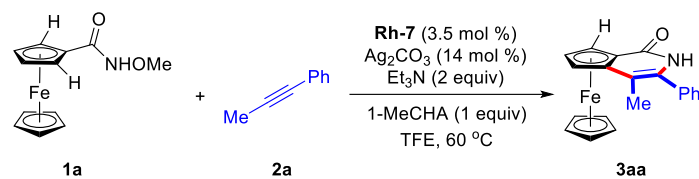


Figure S1. The rate of the reaction of **1a** and **2a**

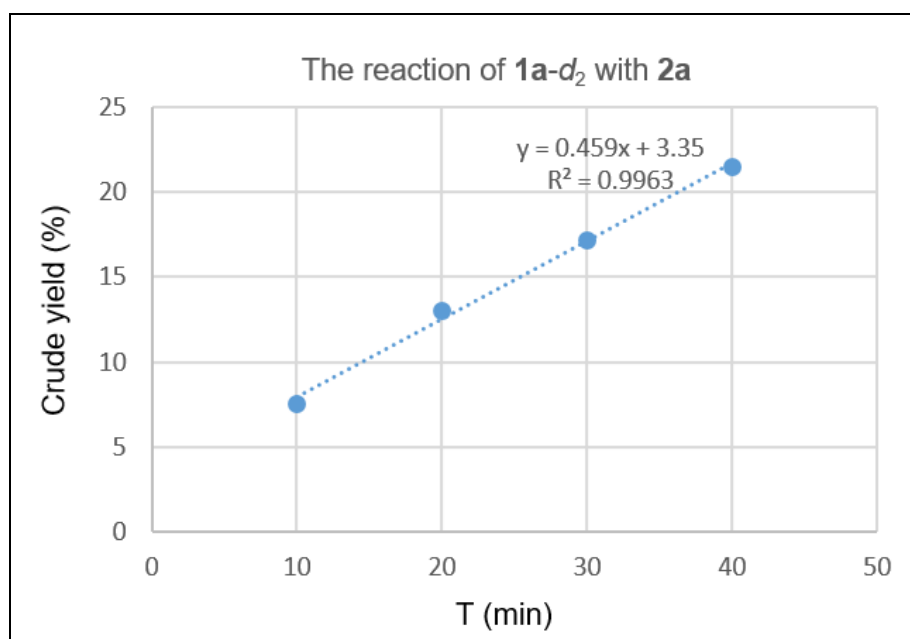
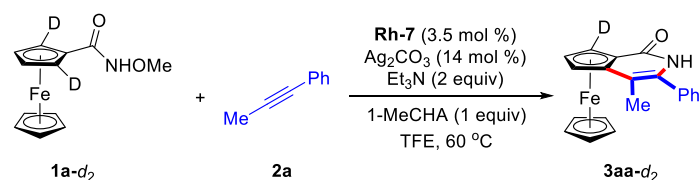


Figure S2. The rate of the reaction of **1a-d₂** and **2a**

7. X-Ray crystal structures

The crystal of enantiopure **3ka** was obtained through slow vapor diffusion of *n*-hexane into the ethyl acetate solution of **3ka**. The structure and absolute configuration (R_p) of **3ka** were then determined by X-ray crystallographic analysis (**Figure S3**).

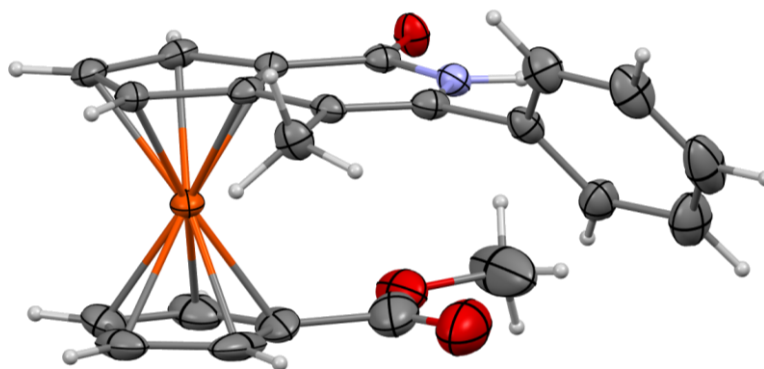


Figure S3. The X-ray crystal structure of enantiopure **3ka** with thermal ellipsoids at the 30% probability level (CCDC: 2086642).

Table S7. Crystal data and structure refinement for mj21281_0m.

Identification code	mj21281_0m	
Empirical formula	C ₂₂ H ₁₉ Fe N O ₃	
Formula weight	401.23	
Temperature	193.0 K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 6.78120(10) Å	a = 90°.
	b = 22.3955(5) Å	b = 105.1970(10)°.
	c = 12.8222(2) Å	g = 90°.
Volume	1879.19(6) Å ³	
Z	4	
Density (calculated)	1.418 Mg/m ³	
Absorption coefficient	4.439 mm ⁻¹	
F(000)	832	
Crystal size	0.05 x 0.02 x 0.01 mm ³	
Theta range for data collection	3.107 to 54.885°.	
Index ranges	-7 ≤ h ≤ 8, -27 ≤ k ≤ 27, -15 ≤ l ≤ 15	
Reflections collected	17175	
Independent reflections	6785 [R(int) = 0.0569]	
Completeness to theta = 53.594°	99.9 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.7508 and 0.4784
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6785 / 85 / 484
Goodness-of-fit on F ²	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0495, wR2 = 0.1203
R indices (all data)	R1 = 0.0621, wR2 = 0.1294
Absolute structure parameter	-0.005(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.531 and -0.436 e.Å ⁻¹

8. DFT calculations

Computational methods. All the computational works were performed with Gaussian16⁵ or ORCA 4.1.0 packages.⁶ DFT calculations were carried out using the B3LYP-D3(BJ) functional⁷ including the D3 version of Grimme's empirical dispersion correction with Becke–Johnson damping.⁸ The def2-SVP basis sets⁹ were applied for all atoms. Optimizations were conducted without any constraint in gas phase. Frequency analyses were carried out to confirm each structure being a minimum (no imaginary frequency) or a transition state (only one imaginary frequency). Single-point calculations with RI-PWPB95-D3(BJ) method and def2-TZVPP basis sets in ORCA 4.1.0 (with auxiliary basis sets def2-TZVPP/C¹⁰ and def2/JK¹¹) were performed using the geometries obtained at the B3LYP-D3(BJ)/def2-SVP level of theory. The calculated structures were visualized with VMD.¹²

Alternative pathway for the formation of 2-pyridone ring. An alternative reaction pathway for the formation of 2-pyridone ring, in which the C–N bond-formation occurred prior to the N–O bond-cleavage, was considered (**Figure S4**). Starting from **INT-4**, a transition state corresponding to the C–N bond reductive elimination process was located [**TS-6**, 4.9 kcal/mol, B(N–C3) = 1.88 Å]. It delivered a Rh(I) species coordinated by a cyclic N-methoxy amide **INT-8** (–7.7 kcal/mol). The regeneration of the Rh(III) catalyst required the oxidative addition of the Rh(I) center with N-methoxy group as the internal oxidant. The cleavage of the N–O bond was facilitated by one molecule of 1-MeCHA from the acid-coordinated intermediate **INT-9** (2.4 kcal/mol). The N–O cleavage proceeded with the concurrent protonation of the leaving methoxy anion via a seven-membered-ring transition state **TS-7** (6.6 kcal/mol), producing Rh(III) intermediate **INT-10** (–69.8 kcal/mol) with significant energy release. The initial complex **INT-0** could be regenerated by the dissociation of (*R_p*)-**3aa** and the coordination of another molecule of **1a**.

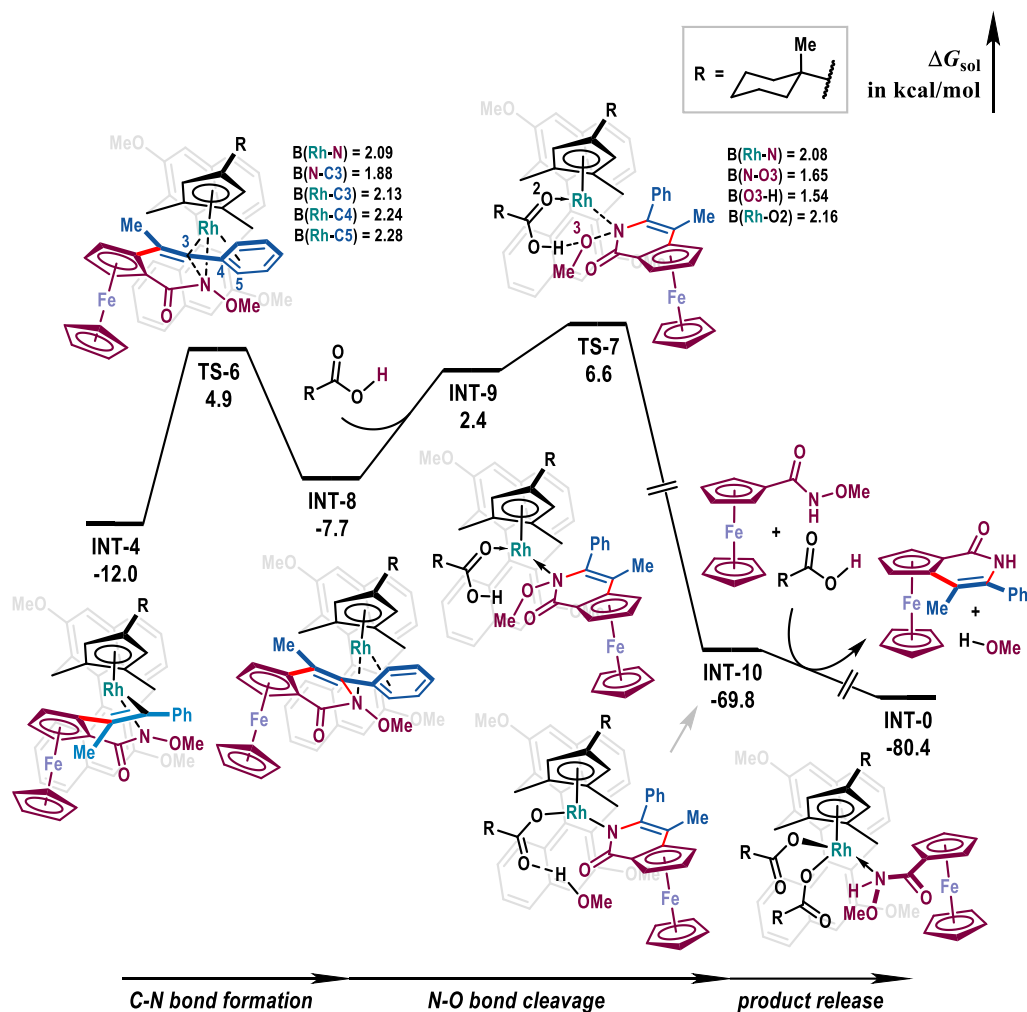


Figure S4. The profile of the alternative reaction pathway for the formation of 2-pyridone ring calculated at the PWPB95-D3(BJ)/def2-TZVPP (SMD, TFE)//B3LYP-D3(BJ)/def2-SVP (gas) level of theory. The relative Gibbs free energies (ΔG_{sol}) are in kcal/mol. The distances of forming/cleaving bonds are in Å.

The cleavage of the enantiotopic C–H bond and all possible regio- and enantio-selective alkyne insertion. DFT calculations on the reaction profiles leading to the minor enantiomer and regio-isomers have been performed (Figure S5). The computational results have confirmed that the cleavage of the enantiotopic C–H bond proceed by a CMD mechanism from INT-1-(S_p) (3.6 kcal/mol) via transition state TS-2-(S_p) (13.5 kcal/mol) to INT-2-(S_p) (2.8 kcal/mol). The precursors for all the alkyne insertion transition states have been located as INT-3-(S_p) (6.6 kcal/mol), INT-3'-(R_p) (2.5 kcal/mol) and INT-3'-(S_p) (6.7 kcal/mol). The additional isomers of the rhodacyclic intermediates have also been found as INT-4-(S_p) (–8.3 kcal/mol), INT-4'-(R_p) (–8.6 kcal/mol) and INT-4'-(S_p) (–12.6 kcal/mol). All these results support the alkyne insertion being the enantio- and regio-selectivity-determining step.

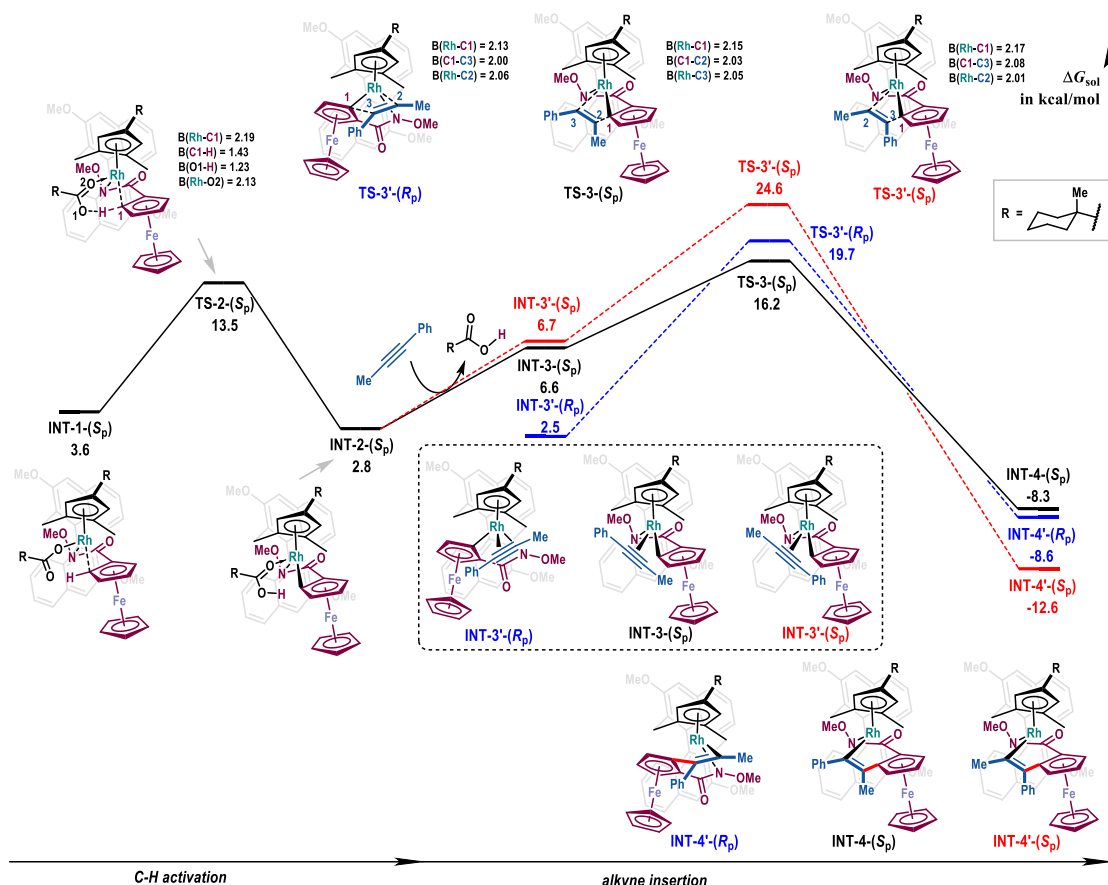


Figure S5. The profile of the cleavage of the enantiotopic C–H bond and all possible regio- and enantio-selective alkyne insertion. Calculations have been performed at the PWPB95-D3(BJ)/def2-TZVPP (SMD, TFE)//B3LYP-D3(BJ)/def2-SVP (gas) level of theory. The relative Gibbs free energies (ΔG_{sol}) are in kcal/mol. The distances of forming/cleaving bonds are in Å.

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10. Cartesian coordinates of the calculated structures

- (1) Optimized at B3LYP-D3(BJ)/def2-SVP level of theory

1a

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
 SCF Done: E(RB3LYP) = -1933.42151889 a.u.
 Zero-point correction = 0.228387 Hartree/Particle
 Sum of electronic and thermal Free Energies = -1933.236047 a.u.
 Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol

FINAL SINGLE POINT ENERGY = -1933.820190834415 a.u.

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2a

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -347.501145695 a.u.
Zero-point correction = 0.137773 Hartree/Particle
Sum of electronic and thermal Free Energies = -347.397689 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -347.581355190954 a.u.

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3aa

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
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Zero-point correction = 0.318513 Hartree/Particle
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Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -2165.843845166578 a.u.

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C,0,-3.1234677493,1.4454447716,0.1726609948
H,0,-4.6640205687,1.924301751,1.7302109485
C,0,-4.577571412,0.3898083361,-1.2780502263
H,0,-6.3869004923,0.7020251477,0.0137279779
C,0,-3.2087758902,0.771475907,-1.0972626342
H,0,-4.9827002351,-0.1604823194,-2.1244698843
C,0,-1.836593877,1.8549320738,0.7300932512
O,0,-1.6486830246,2.3745158814,1.8182663252
N,0,-0.780780434,1.5722852251,-0.1328608267
C,0,0.4851442732,0.7895759358,-2.0390699704
C,0,1.356116907,1.8886588814,-2.1504827305
C,0,0.9111162541,-0.4579226023,-2.5263258156
C,0,2.6099582641,1.7465737264,-2.7466171915
H,0,1.0364108612,2.8671803574,-1.783835873
C,0,2.1648840137,-0.5984242879,-3.1239036173
H,0,0.2586951365,-1.325859469,-2.4156676595
C,0,3.0177750956,0.502947676,-3.2376251606
H,0,3.2694076085,2.6133176513,-2.8339599155
H,0,2.4817914458,-1.5766798799,-3.4932454597
H,0,3.9995178558,0.3916250542,-3.7037102114
C,0,-0.8358104213,0.9456410677,-1.3819970214
C,0,-2.0305980423,0.5368448602,-1.9088594709
C,0,-2.2068390636,-0.100462613,-3.2574631581
H,0,-2.483082919,-1.1658847291,-3.1637312779
H,0,-3.0278352482,0.3900730681,-3.8058191702
H,0,-1.3027262775,-0.0385354021,-3.8752334125
H,0,0.1343298538,1.7986225919,0.2433555212

1-MeCHA

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -463.468059924 a.u.
Zero-point correction = 0.213108 Hartree/Particle
Sum of electronic and thermal Free Energies = -463.289745 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -463.617489113127 a.u.

```

H,0,-0.6259881688,0.1732615842,-1.3765589796
C,0,-1.825134224,-0.1005890607,0.0373041993
O,0,-0.9412305545,-0.4985432281,0.7560193266
O,0,-1.5806511929,0.2897494457,-1.2344690741
C,0,-3.7265184934,1.5104692946,0.2551218868
C,0,-4.1381189454,-0.8519954935,-0.5502200931
C,0,-5.2350453536,1.71604988,0.4247192336
H,0,-3.4310104732,1.8485503504,-0.750602083
H,0,-3.1686064027,2.1306163671,0.9764797556
C,0,-5.6467998659,-0.6473794803,-0.3808899917
H,0,-3.8567291497,-0.5954402286,-1.5836810598
H,0,-3.872886103,-1.9120447525,-0.4015043043
C,0,-6.0312065947,0.8273240912,-0.5359351973
H,0,-5.4785917725,2.7776533976,0.2542189421
H,0,-5.5339189715,1.4969503132,1.4640947428
H,0,-6.1825113014,-1.26223558,-1.1227417483
H,0,-5.9707976691,-1.0114369647,0.6091206947
H,0,-7.1138179943,0.9617494875,-0.3769262303
H,0,-5.8243165828,1.1452430302,-1.5743240802
C,0,-3.2982883137,0.0258234651,0.4186452912
C,0,-3.4510774719,-0.4426255094,1.8709096929
H,0,-4.4943098567,-0.3751004746,2.206193106
H,0,-3.1208372073,-1.4856714103,1.9794722318
H,0,-2.8325343371,0.1688624758,2.543431738

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MeOH

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -115.63499559 a.u.
Zero-point correction = 0.051041 Hartree/Particle
Sum of electronic and thermal Free Energies = -115.606675 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -115.696078379390 a.u.

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-----
C,0,-10.5977818687,2.0361330581,-0.0000019802
H,0,-10.960834381,3.0755795781,-0.0000104206
H,0,-11.0199807836,1.5377608416,-0.8960986561
H,0,-11.020058098,1.5377499437,0.8960508633
O,0,-9.1908498814,2.0770710136,0.0000573059
H,0,-8.8636980773,1.168867895,0.0001902777

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INT-0

```

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4512.33739582 a.u.
Zero-point correction = 1.257761 Hartree/Particle
Sum of electronic and thermal Free Energies = -4511.185601 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4513.275916120363 a.u.

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-----
O,0,-1.3179744302,-2.4816888873,-1.9076196742
O,0,-4.0544718383,4.3782815163,-0.9127706404
C,0,-0.6207824821,3.0985720922,-1.1732101054
C,0,0.2757398595,2.7017826817,-2.2243124806
C,0,-0.1941939461,1.4406756729,-2.6994178442
C,0,-1.4273128034,1.0953424541,-2.0314475318
C,0,-1.6755459265,2.1153119841,-1.0591954404
C,0,-2.3334476184,-0.0274468804,-2.4559226018
C,0,-2.9327739648,-0.8694800647,-1.3549965644
C,0,-2.3570062503,-2.1589924883,-1.107622618

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C,0,-2.8897409991,-2.9917952061,-0.1441002357
 C,0,-3.988180039,-2.5647813342,0.649635083
 C,0,-4.5154833454,-3.3799694449,1.6880467511
 C,0,-5.5615245266,-2.9411978419,2.472677972
 C,0,-6.1323990951,-1.6653134868,2.2500860857
 C,0,-5.650079971,-0.8563103592,1.2415713531
 C,0,-4.5728715189,-1.2790019732,0.4172944794
 C,0,-4.0440490674,-0.4595149112,-0.6360369168
 C,0,-0.740028249,-3.765254233,-1.8048039861
 C,0,-2.7954281526,2.1258641016,-0.0556064697
 C,0,-4.1357053176,2.0371299479,-0.7436027976
 C,0,-4.7304630624,0.8155658567,-1.0085497228
 C,0,-5.9903252907,0.7555843415,-1.6993719384
 C,0,-6.6260286181,-0.4733090183,-2.0266795947
 C,0,-7.8372533334,-0.4933004672,-2.6873908406
 C,0,-8.4691041872,0.7179368295,-3.0559148777
 C,0,-7.8710534155,1.9262398843,-2.7661122595
 C,0,-6.6212712485,1.9802299615,-2.0909612395
 C,0,-5.9823934125,3.2213041708,-1.8191152099
 C,0,-4.7610454426,3.2483353249,-1.179468517
 C,0,-4.5920305446,5.6244692841,-1.2952865027
 H,0,-0.5387985928,3.9938145744,-0.5623294189
 H,0,0.2800998309,0.8346645168,-3.467975559
 H,0,-1.774187648,-0.6771367517,-3.137533034
 H,0,-3.1476619043,0.4392171075,-3.0358225571
 H,0,-2.468601861,-3.9786441684,0.0406990791
 H,0,-4.0690650628,-4.3619618912,1.8614180754
 H,0,-5.9502230244,-3.5781693513,3.2707458443
 H,0,-6.956168221,-1.3211591513,2.879324663
 H,0,-6.0904139066,0.1268607194,1.0700239338
 H,0,-0.3512173794,-3.9472574681,-0.7926046209
 H,0,0.1002837089,-3.7902005438,-2.507795577
 H,0,-1.4708776617,-4.5523414879,-2.0618874613
 H,0,-2.7296280445,3.0432070676,0.5402515206
 H,0,-2.66316719,1.2750352299,0.6254240165
 H,0,-6.1436418573,-1.4096974762,-1.7466096721
 H,0,-8.3102857697,-1.4480016376,-2.92798356
 H,0,-9.4295853296,0.6933663129,-3.576140881
 H,0,-8.350012147,2.8645980825,-3.0575582213
 H,0,-6.4743970697,4.1382726051,-2.1415704346
 H,0,-4.7398533161,5.6838952885,-2.3880821215
 H,0,-3.8654118691,6.387710755,-0.9879475287
 H,0,-5.5566352924,5.8209533686,-0.7950133569
 C,0,5.9234657945,-2.9084958493,0.8073512348
 C,0,4.7618569185,-2.6415064391,1.5964611276
 C,0,4.2759260973,-3.8924494834,2.0882831726
 C,0,5.1326268204,-4.928104589,1.6028063255
 C,0,6.1536669771,-4.318238667,0.8105758141
 H,0,6.5051704101,-2.1710026589,0.2578340369
 H,0,4.2947173465,-1.6677612998,1.7347759992
 H,0,3.3900267886,-4.0354841309,2.7034783236
 H,0,5.0159555687,-5.9949507878,1.7858828003
 H,0,6.9482983689,-4.8372027628,0.27748714
 Fe,0,4.294730581,-3.8924742675,0.0208286285
 C,0,4.3573425657,-4.2594944494,-2.010664679
 C,0,3.5312752631,-5.2252772643,-1.3694918348
 C,0,3.8096363361,-2.9629977944,-1.7429669436
 H,0,5.2638184695,-4.4372354433,-2.5839637792

C,0,2.4728097849,-4.5301417317,-0.7035545302
 H,0,3.6935791331,-6.3016879645,-1.360605447
 C,0,2.6364704868,-3.1301759715,-0.9327124403
 H,0,1.6927958938,-4.9889966721,-0.099008077
 C,0,4.5020223533,-1.710517135,-2.1517445104
 O,0,5.4307306019,-1.7037955778,-2.9458761916
 N,0,4.0195892655,-0.582998256,-1.5405459893
 O,0,4.7146010269,0.6017958442,-1.7016372898
 C,0,5.9747483273,0.5827482724,-1.0376788279
 H,0,5.8466594431,0.3818114106,0.0392764492
 H,0,6.3961273828,1.5884868767,-1.1743336238
 H,0,6.6436032408,-0.1636262668,-1.4919738235
 Rh,0,0.211178883,1.2337646637,-0.5851201248
 H,0,1.9915216751,-2.3369500128,-0.5588033872
 C,0,2.8270008477,1.2461493064,1.0262103197
 O,0,2.0162040547,1.861140988,0.2373906804
 O,0,3.0521264678,0.0306864994,1.0084769971
 C,0,0.1123036892,-0.5104995417,1.261589716
 O,0,0.4376051354,-0.8366138875,0.0817058938
 O,0,-0.2384266725,0.7004803291,1.4492069135
 C,0,1.4630515386,3.4616151214,-2.7673739981
 C,0,1.9890518467,4.4630674888,-1.7130605169
 C,0,2.5846959833,2.4666759178,-3.1501051013
 C,0,3.309348438,5.1301664807,-2.1147562888
 H,0,2.135169227,3.9098634053,-0.7745221921
 H,0,1.2243491528,5.2360106967,-1.5245420266
 C,0,3.8921407637,3.1435016789,-3.562992213
 H,0,2.7933857868,1.8288434261,-2.2808898891
 H,0,2.2386138383,1.8065220322,-3.9617567661
 C,0,4.3806617286,4.0955447071,-2.4707783462
 H,0,3.6543021213,5.7695055889,-1.2849667536
 H,0,3.1504750645,5.8059295325,-2.9738302442
 H,0,4.6404503558,2.358109689,-3.7463951175
 H,0,3.7651514227,3.6959794777,-4.511357739
 H,0,5.3109982839,4.5996237652,-2.7811150047
 H,0,4.6200949698,3.5027875112,-1.5738618252
 C,0,0.9364064478,4.2082336085,-4.0150523346
 H,0,0.5664749296,3.4994055426,-4.7721225329
 H,0,0.1112966796,4.8881351746,-3.7497199204
 H,0,1.7321983811,4.8082377518,-4.4773312725
 C,0,3.5316674569,2.1674483746,2.0486073704
 C,0,4.4976382607,1.3386893678,2.9204016162
 C,0,4.3341065441,3.240314689,1.2712548512
 C,0,5.3936203366,2.1958928289,3.8200433604
 H,0,5.135275869,0.7358583874,2.2544393432
 H,0,3.9243272443,0.6155856952,3.5204875399
 C,0,5.2359057134,4.0948349962,2.1666685933
 H,0,4.9619760622,2.7287682491,0.5239687705
 H,0,3.637575493,3.8762058813,0.7081717755
 C,0,6.1784270573,3.2277209151,3.0051769569
 H,0,6.0843853326,1.5428265835,4.3787060344
 H,0,4.7847986711,2.7169868659,4.5796738602
 H,0,5.8117836515,4.7973360416,1.5409744464
 H,0,4.6187601515,4.7181050124,2.837143694
 H,0,6.7982275846,3.8561560109,3.6663262304
 H,0,6.8762752952,2.6979714844,2.330472391
 C,0,0.1050806549,-1.4867468126,2.4259492811
 C,0,-1.3601286609,-1.5625904895,2.9367838056

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C,0,0.5732094165,-2.8750522898,1.9504416141
C,0,-1.5815345404,-2.6744898069,3.9659968299
H,0,-2.0191998576,-1.7452858877,2.0756925069
H,0,-1.6486137429,-0.584151654,3.3496592173
C,0,0.3596709238,-3.9719372208,2.9952821669
H,0,0.0064045985,-3.1337055264,1.0436375717
H,0,1.6276595752,-2.8209416525,1.6500366286
C,0,-1.1025057985,-4.0334122703,3.4459228439
H,0,-2.6533138501,-2.7191303202,4.21920305
H,0,-1.0499842029,-2.4352111531,4.9033939099
H,0,0.676716916,-4.9419389788,2.5765727269
H,0,1.0072130652,-3.7944143984,3.8716467802
H,0,-1.2408095541,-4.8108392891,4.2155533462
H,0,-1.7290618872,-4.328725294,2.5852984723
C,0,2.4297205671,2.8237556975,2.9027788013
H,0,1.7543176358,3.4122946121,2.266741409
H,0,1.8262002051,2.0587986715,3.4129076261
H,0,2.8530780618,3.4872368887,3.6703002764
C,0,1.0414646255,-0.9289609489,3.5156005449
H,0,2.0635599721,-0.8319662856,3.1253272323
H,0,0.699486634,0.0628483258,3.8428815011
H,0,1.0623024971,-1.5902268285,4.3925757126
H,0,3.4880787403,-0.6018734137,-0.6565765324

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TS-1

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4512.33257514 a.u.
Imaginary frequency = -846.6177 cm-1
Zero-point correction = 1.253405 Hartree/Particle
Sum of electronic and thermal Free Energies = -4511.182822 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4513.261157898510 a.u.

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```

O,0,0.1721015351,-2.8620320525,-0.3474392647
O,0,-4.0566469123,3.3691621847,-0.2047753339
C,0,-0.7096164516,2.9328264085,-0.3650321533
C,0,0.313372126,2.7988115303,-1.3526627482
C,0,0.2810725085,1.4070522664,-1.7637000981
C,0,-0.7333726601,0.7184259307,-1.0479885121
C,0,-1.3224266079,1.6674664675,-0.1158359329
C,0,-1.1920482827,-0.6812935285,-1.3768008279
C,0,-1.8025849909,-1.5578221176,-0.2987625788
C,0,-1.0736916705,-2.7013148463,0.1693629543
C,0,-1.6355660632,-3.5841588187,1.0689483289
C,0,-2.9272740145,-3.3496816493,1.604044527
C,0,-3.4979814392,-4.2122359308,2.5796072795
C,0,-4.7471564024,-3.9566292548,3.1040475248
C,0,-5.4821285706,-2.8263517619,2.6719664895
C,0,-4.9572540689,-1.9779080949,1.7191774134
C,0,-3.6722184586,-2.2140801361,1.1580626809
C,0,-3.0968537416,-1.3558550486,0.1619758999
C,0,0.8756829885,-4.0654206769,-0.107009849
C,0,-2.467228212,1.4018522699,0.8156356132
C,0,-3.6664334554,1.0599507205,-0.0343204661
C,0,-3.9324622351,-0.2486349417,-0.3926346575
C,0,-5.004098737,-0.5543482579,-1.2994039091
C,0,-5.2971832868,-1.8808788852,-1.7172936968

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C,0,-6.3343200518,-2.1377079359,-2.5907734377
 C,0,-7.1270871507,-1.0762045935,-3.087749121
 C,0,-6.8616686184,0.2230633326,-2.7082072562
 C,0,-5.797628078,0.5210039826,-1.8141855359
 C,0,-5.4992309021,1.860112488,-1.4379143434
 C,0,-4.4484834967,2.1249243907,-0.5845853773
 C,0,-4.7560990899,4.487350091,-0.7028921352
 H,0,-0.918005615,3.8303911026,0.2129807026
 H,0,0.9212762146,0.9522192242,-2.5135215902
 H,0,-0.3564432981,-1.2123657137,-1.8461313688
 H,0,-1.9562162507,-0.5410599392,-2.162527203
 H,0,-1.0905304505,-4.4641005672,1.406280277
 H,0,-2.9227574889,-5.0789524388,2.9145042274
 H,0,-5.1709138413,-4.623764079,3.8583793375
 H,0,-6.4679978033,-2.6252218957,3.0970325791
 H,0,-5.5255507198,-1.1071987267,1.3907842486
 H,0,1.0601267575,-4.222686991,0.9658137305
 H,0,1.841033155,-3.9623748775,-0.6156314195
 H,0,0.3257876905,-4.9329415599,-0.5114673231
 H,0,-2.6518836236,2.295020078,1.4229392463
 H,0,-2.2161929491,0.5719424038,1.487208432
 H,0,-4.6891091915,-2.7013458055,-1.3351201454
 H,0,-6.5451219731,-3.1640032114,-2.8998006595
 H,0,-7.9483480278,-1.2880276901,-3.7765702537
 H,0,-7.467146205,1.0467845467,-3.0953021277
 H,0,-6.1085784914,2.6622242245,-1.8530632826
 H,0,-4.705647451,4.5384567486,-1.8049216852
 H,0,-4.271008808,5.3756672487,-0.2779811489
 H,0,-5.8165885375,4.4725337062,-0.395552867
 C,0,5.4044081756,-1.6389884583,0.3778548597
 C,0,4.564031829,-2.7917867211,0.3998562715
 C,0,4.9133895776,-3.6128827523,-0.7171059877
 C,0,5.9692996223,-2.9637351922,-1.4297137425
 C,0,6.2723123918,-1.7421782638,-0.7522205266
 H,0,5.3543025482,-0.8120432281,1.082304055
 H,0,3.7742849509,-2.9708519385,1.1251986413
 H,0,4.4477851268,-4.5583085372,-0.9911138455
 H,0,6.4428629807,-3.3253302993,-2.3408288787
 H,0,7.0106416844,-1.0036532809,-1.0589186861
 Fe,0,4.3031815306,-1.7476482792,-1.3612327697
 C,0,4.0713496835,-0.2492597473,-2.7587918915
 C,0,3.5647255437,-1.4668649157,-3.2884669831
 C,0,3.3473135709,0.0459573953,-1.5539738185
 H,0,4.873008544,0.3672499787,-3.1567671942
 C,0,2.5297552684,-1.9322641067,-2.4188691393
 H,0,3.9180650974,-1.9701485989,-4.1865598336
 C,0,2.4007755792,-1.0120156793,-1.3372219441
 H,0,1.949071816,-2.8419626887,-2.5507451741
 C,0,3.6853544162,1.2259875828,-0.7267974464
 O,0,4.5845042933,1.9808812182,-1.0578494453
 N,0,2.9455306212,1.3939444894,0.4608632339
 O,0,3.4414256116,2.5058736267,1.175140452
 C,0,4.5782849331,2.1732687059,1.9571694608
 H,0,4.3221660473,1.420120656,2.7177157738
 H,0,4.8649376185,3.1071179503,2.4593043525
 H,0,5.4138257413,1.8363591449,1.3216132675
 Rh,0,0.7538986341,1.5573341344,0.3887913441
 H,0,1.7143937812,-1.1095785566,-0.5045014128

C,0,1.342703222,2.7107223958,3.16209347
 O,0,0.7782197035,2.8234109136,2.0093820778
 O,0,1.946312212,1.731438814,3.5932555136
 C,0,1.5872642401,-0.5679030113,2.4109781832
 O,0,2.7975599405,-0.5547919391,2.0051541768
 O,0,0.6361663917,-0.0825795149,1.743799851
 H,0,2.9182260136,0.3176232937,1.219296977
 C,0,1.1086433811,3.9397767337,-1.956926507
 C,0,1.8586356809,4.7053826182,-0.8350651333
 C,0,2.1201360448,3.3959677652,-2.9917063634
 C,0,2.8250897506,5.7656354323,-1.3685038604
 H,0,2.4328337529,3.9848473804,-0.2370769666
 H,0,1.1256115782,5.1590768582,-0.1481346295
 C,0,3.1070530935,4.4518620599,-3.5003095763
 H,0,2.7033222578,2.5906434868,-2.5295470657
 H,0,1.57182553,2.9478722149,-3.837923333
 C,0,3.8303056832,5.1428699631,-2.3406878767
 H,0,3.3514624105,6.2276484769,-0.5172586908
 H,0,2.2745751769,6.5819875207,-1.870248303
 H,0,3.8348786866,3.9661926752,-4.1706427852
 H,0,2.58017184,5.2052862076,-4.112774226
 H,0,4.5240999602,5.9089374449,-2.7251634969
 H,0,4.4323215143,4.3928636401,-1.8010829512
 C,0,0.084256172,4.8612934,-2.6567366295
 H,0,-0.4919027789,4.303902411,-3.4125368419
 H,0,-0.626145832,5.2856509686,-1.9304704606
 H,0,0.581699117,5.6988637112,-3.164618097
 C,0,1.2310091053,3.9854657704,4.0399337846
 C,0,0.7317448734,3.5572043162,5.4406962203
 C,0,2.6711799776,4.547005381,4.1694536176
 C,0,0.8525483889,4.6637709675,6.4933842663
 H,0,1.3320185321,2.6893316826,5.7548518145
 H,0,-0.3128624164,3.2086899027,5.3654856806
 C,0,2.7946216645,5.6603692418,5.2137979564
 H,0,3.3272006134,3.7100010719,4.4574309761
 H,0,3.0134195237,4.8961631443,3.1810402976
 C,0,2.2869510645,5.1949226346,6.5821966046
 H,0,0.5281873104,4.2765452523,7.473962159
 H,0,0.1683875811,5.4965662824,6.2527736031
 H,0,3.8470505084,5.9827927642,5.2860105453
 H,0,2.2241197364,6.5494222621,4.892565003
 H,0,2.3509607903,6.0141533064,7.3181095747
 H,0,2.9454354559,4.3874452892,6.9518833077
 C,0,1.2756575197,-1.3170809533,3.7099148588
 C,0,-0.039240187,-0.7787577742,4.3184840328
 C,0,1.0758815798,-2.8032015932,3.313123897
 C,0,-0.5597594553,-1.6380220629,5.4734860389
 H,0,-0.7999993919,-0.7537617913,3.5233141277
 H,0,0.1212867005,0.2615445777,4.6360176964
 C,0,0.5430529833,-3.671768798,4.4562559339
 H,0,0.3486884558,-2.8298011764,2.4901689996
 H,0,2.026752819,-3.209090519,2.929277397
 C,0,-0.7494489161,-3.0948840909,5.041681916
 H,0,-1.5153681817,-1.2232086118,5.8347755946
 H,0,0.1359568936,-1.5931341324,6.3293723278
 H,0,0.3714716063,-4.697051427,4.0844716395
 H,0,1.3045065545,-3.75893169,5.2500167203
 H,0,-1.0947747254,-3.7112308063,5.8886764443

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H,0,-1.5435564817,-3.1392017389,4.276165841
C,0,0.2933627248,5.0206797165,3.407116461
H,0,0.6620161476,5.3246725653,2.417323173
H,0,-0.7156784811,4.6022985845,3.2734746617
H,0,0.2056468246,5.9213584464,4.0322123399
C,0,2.4558022311,-1.1592415921,4.6812782107
H,0,3.3771777886,-1.5637833571,4.2396927615
H,0,2.615614978,-0.0958388861,4.8998480258
H,0,2.2634882706,-1.6919071284,5.6229060488

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INT-1

```

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4048.82478105 a.u.
Zero-point correction = 1.041509 Hartree/Particle
Sum of electronic and thermal Free Energies = -4047.877117 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4049.630485035613 a.u.

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O,0,-1.4096900564,-1.8349156703,-3.1034959514
O,0,-3.4346850955,3.6218671426,1.4554466944
C,0,-0.2652419677,2.3279620184,0.3545620728
C,0,0.568528669,2.6360384327,-0.7801241189
C,0,-0.0430247263,1.9793349745,-1.8909796832
C,0,-1.2804067725,1.3496806902,-1.4948971616
C,0,-1.4134961986,1.5837420317,-0.0889385742
C,0,-2.2671749708,0.7071518861,-2.4356485975
C,0,-2.9733838387,-0.5253933292,-1.9110867106
C,0,-2.492364729,-1.82079916,-2.2889061298
C,0,-3.1330638694,-2.9624332837,-1.8496776757
C,0,-4.2538579796,-2.8797533535,-0.9851950548
C,0,-4.8876365161,-4.0463108549,-0.4752081279
C,0,-5.9413125906,-3.9507532125,0.4086441017
C,0,-6.4137219007,-2.6803874726,0.8185355744
C,0,-5.826791274,-1.5308629583,0.3313701465
C,0,-4.7388349071,-1.5964147249,-0.5815277078
C,0,-4.0843389425,-0.4253994477,-1.0867147076
C,0,-0.8800404396,-3.0942981876,-3.480418817
C,0,-2.5397860421,1.1296618493,0.7890715179
C,0,-3.8423922111,1.6571334644,0.234985972
C,0,-4.5779437728,0.9230644971,-0.6786857158
C,0,-5.7853080416,1.4559247839,-1.2419478516
C,0,-6.5611620067,0.7417783341,-2.1947035471
C,0,-7.7194279186,1.282491718,-2.7145761797
C,0,-8.1522519463,2.566480925,-2.3056331596
C,0,-7.4150791767,3.2883122186,-1.3900605015
C,0,-6.2161930051,2.7605023562,-0.8380595413
C,0,-5.4340985561,3.5048227747,0.0881572342
C,0,-4.2672674528,2.97398609,0.5987984048
C,0,-3.7645701451,4.928090078,1.8700001204
H,0,-0.093681808,2.6408709626,1.3812160953
H,0,0.3628267524,1.945722466,-2.9001964187
H,0,-1.7371200048,0.4498311324,-3.3607950877
H,0,-3.0249934034,1.4662292956,-2.6925767346
H,0,-2.7706998115,-3.9486357702,-2.1307011022
H,0,-4.5139272315,-5.0248184754,-0.7863671595
H,0,-6.4115590595,-4.8565168794,0.7987512906
H,0,-7.2440817798,-2.611719206,1.524874016

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H,0,-6.1899137091,-0.5537430757,0.651579952
H,0,-0.5392925642,-3.644421792,-2.5909195285
H,0,-0.0199836306,-2.8900712359,-4.1276921579
H,0,-1.6244639891,-3.6846777486,-4.0423321736
H,0,-2.3722158226,1.5012781713,1.8062236453
H,0,-2.5439930387,0.0342571379,0.8266630937
H,0,-6.2280996176,-0.2479178269,-2.5093359523
H,0,-8.3050019002,0.7187199843,-3.4442787343
H,0,-9.0715949171,2.9867935631,-2.7204122493
H,0,-7.7431900678,4.28300945,-1.077139239
H,0,-5.7736863016,4.5013243185,0.3686260136
H,0,-3.8246921554,5.6222823813,1.0131064262
H,0,-2.9623034215,5.2559956165,2.5437456942
H,0,-4.7255054934,4.9513482067,2.4137162267
C,0,1.7493733342,3.5836982808,-0.81538792
C,0,2.4454829492,3.6267897881,0.5671083816
C,0,2.7442985049,3.1359805249,-1.9101907489
C,0,3.7872124584,4.3647683694,0.5613057011
H,0,2.6161052494,2.6027301545,0.9213971385
H,0,1.7655934016,4.0967544907,1.2978488618
C,0,4.086945319,3.86934487,-1.8797722271
H,0,2.9346221237,2.0654766686,-1.7777863284
H,0,2.2771931845,3.2480551848,-2.9028808375
C,0,4.7300003129,3.7837347692,-0.4940623147
H,0,4.2381870092,4.2881670701,1.5637673029
H,0,3.6390941077,5.4430539993,0.3696735321
H,0,4.7493365232,3.4290819959,-2.6435521761
H,0,3.9542926191,4.9293499325,-2.1618640019
H,0,5.6962264119,4.3146531582,-0.4843702676
H,0,4.9381996426,2.7269331075,-0.2496590253
C,0,1.164090076,4.9733226624,-1.1592611993
H,0,0.6627494944,4.9586594721,-2.139739839
H,0,0.4265299965,5.2863096062,-0.4036290244
H,0,1.9544611244,5.7366573713,-1.1949105325
C,0,2.7424981065,-4.0099773073,-3.020163689
C,0,3.9381193199,-3.6318863316,-3.7057342651
C,0,4.8881152124,-3.205322689,-2.7275960301
C,0,4.2789889236,-3.319832551,-1.4390233403
C,0,2.9536205381,-3.8180932217,-1.6200509352
H,0,1.8250869097,-4.3678431983,-3.4813133886
H,0,4.0922059334,-3.6449089929,-4.783442523
H,0,5.8875702594,-2.8236892469,-2.9284292701
H,0,4.7247274262,-3.0074251159,-0.4960238265
H,0,2.1942036378,-3.9377328098,-0.8500329488
Fe,0,3.1991378104,-2.0324088095,-2.6222784964
C,0,3.8568757679,-0.0850982863,-2.6466927745
C,0,3.0870543092,-0.3304754764,-3.8248392553
C,0,3.0289640014,-0.348015227,-1.518957734
H,0,4.8916695556,0.2443488946,-2.5885232725
C,0,1.77871983,-0.73415979,-3.4327565483
H,0,3.448565198,-0.2518539981,-4.8488368519
C,0,1.7192102094,-0.7428345688,-1.9963789752
H,0,0.9663013421,-1.0140677079,-4.0975488623
C,0,3.3603255848,-0.0505646805,-0.0961948587
O,0,4.5078419745,0.0591017597,0.3215499437
N,0,2.2034274859,0.1234915951,0.6001501377
O,0,2.3705191553,0.6465655768,1.8725129312
C,0,2.0184176244,-0.2920027879,2.8723585583

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H,0,0.9489160016,-0.5454206059,2.8119542998
H,0,2.2394622444,0.1946672542,3.8338034074
H,0,2.6185842825,-1.212961809,2.7795472725
Rh,0,0.4338526553,0.4533036487,-0.4183302233
H,0,0.9924572835,-1.3858630361,-1.4344530287
C,0,-0.3623027368,-2.3331560884,0.4936165203
O,0,-0.3739012491,-1.0775334066,0.7784000841
O,0,0.1449870945,-2.8199617577,-0.5227166623
C,0,0.0817632475,-3.4945080574,2.6459079963
C,0,-1.3899776076,-4.5993432003,0.928370462
C,0,-0.3175462272,-4.5590710872,3.6732751159
H,0,1.0065229624,-3.8179878572,2.1363940853
H,0,0.3162941301,-2.5467966123,3.1511272516
C,0,-1.8001530318,-5.6613398653,1.9521986643
H,0,-0.5229325358,-4.9619037443,0.3558171329
H,0,-2.1974341641,-4.4383108423,0.2017479688
C,0,-0.7038784603,-5.878262705,2.9990306331
H,0,0.5155263548,-4.7172290056,4.3785248541
H,0,-1.1656133363,-4.1945513287,4.278622478
H,0,-2.021677728,-6.6075134816,1.430162571
H,0,-2.7375183825,-5.3647135758,2.4544323577
H,0,-1.0245232141,-6.6173672155,3.7522732342
H,0,0.1880227504,-6.3022546849,2.5018897934
C,0,-1.0071455711,-3.2465666623,1.5667534466
C,0,-2.2351831715,-2.5526679833,2.1766183044
H,0,-2.7275750682,-3.1887440644,2.9251405751
H,0,-2.9806032394,-2.3250397687,1.4017525059
H,0,-1.947592146,-1.6107618995,2.6623164489

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INT-1- (S_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4048.82199430 a.u.
Zero-point correction = 1.041452 Hartree/Particle
Sum of electronic and thermal Free Energies = -4047.873058 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4049.628110061751 a.u.

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O,0,-1.7184738347,-2.7517370861,-2.1187764402
O,0,-3.1926054103,3.7603414023,1.2352354804
C,0,-0.2466287708,2.4461371995,-0.2770074813
C,0,0.3078728455,2.3548504032,-1.5736782755
C,0,-0.4235963379,1.2836381003,-2.2346474489
C,0,-1.4468476228,0.7831487286,-1.3878943785
C,0,-1.281219714,1.4504328877,-0.1054246582
C,0,-2.540776494,-0.1563294875,-1.8229806856
C,0,-2.9590162973,-1.2165985622,-0.830273027
C,0,-2.4735266598,-2.5506155898,-1.0080230493
C,0,-2.7794836067,-3.5378126493,-0.0965078466
C,0,-3.5790072242,-3.2458396177,1.0366691418
C,0,-3.8617427304,-4.2332039939,2.0199698494
C,0,-4.6400703103,-3.9383634763,3.1194539564
C,0,-5.1744233987,-2.6374495136,3.2852080035
C,0,-4.9175845903,-1.6575668048,2.3482524389
C,0,-4.1165928308,-1.9301741187,1.2060862847
C,0,-3.8009934776,-0.9287531327,0.2322875763
C,0,-1.3738789754,-4.0794865623,-2.4713298394
C,0,-2.1191706255,1.2467326683,1.1217075823

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C,0,-3.5736786513,1.4835369582,0.7973901475
 C,0,-4.377742318,0.4434530907,0.3667116942
 C,0,-5.748935862,0.6826460017,0.0148854555
 C,0,-6.6078701114,-0.3522967173,-0.4445614689
 C,0,-7.9226479195,-0.0901075329,-0.7716429022
 C,0,-8.437382412,1.2232206699,-0.6564788854
 C,0,-7.625826103,2.250825611,-0.222627013
 C,0,-6.2666523061,2.0140364989,0.1194807573
 C,0,-5.4134651541,3.0704026521,0.5441459192
 C,0,-4.0948994384,2.8139130539,0.8585762889
 C,0,-3.6159203963,5.1004040633,1.3368391799
 H,0,0.0987649842,3.0961106741,0.5229940275
 H,0,-0.2363892415,0.9219710327,-3.2447387666
 H,0,-2.2276738405,-0.6371232174,-2.7570704526
 H,0,-3.4096292896,0.4829730909,-2.0557759831
 H,0,-2.3691935836,-4.5397488228,-0.2003078827
 H,0,-3.4415848077,-5.2337327895,1.8902346953
 H,0,-4.8440057151,-4.7080592779,3.8679302417
 H,0,-5.7882921823,-2.4092675248,4.1597262522
 H,0,-5.3238547658,-0.6538030828,2.4811383388
 H,0,-0.7242361679,-4.531694765,-1.7066156372
 H,0,-0.8316499951,-4.0118349333,-3.4230265971
 H,0,-2.280362832,-4.6956696788,-2.6077527989
 H,0,-1.7774321901,1.9348225091,1.9039302906
 H,0,-1.969788112,0.216692724,1.4719147298
 H,0,-6.2109480686,-1.3642174291,-0.5317105526
 H,0,-8.5694511479,-0.8983802123,-1.1203706966
 H,0,-9.4801579319,1.4222192024,-0.9154408731
 H,0,-8.0185172177,3.267617233,-0.1382730623
 H,0,-5.8253971468,4.0775429727,0.5999182432
 H,0,-3.9788619564,5.4867809022,0.367738562
 H,0,-2.7410446622,5.6841345684,1.6520153231
 H,0,-4.4177924519,5.2177580999,2.0871317237
 C,0,1.3633966858,3.2482479721,-2.1921451794
 C,0,2.0424019794,4.0940707601,-1.0897182553
 C,0,2.4391737319,2.3870229449,-2.8987466741
 C,0,3.2512181631,4.8933950659,-1.585505051
 H,0,2.38626606,3.406803315,-0.3031216554
 H,0,1.3011336322,4.7736579113,-0.6366853811
 C,0,3.6358596035,3.1956092832,-3.4057669811
 H,0,2.8093057748,1.6647989733,-2.1605170986
 H,0,1.9803614261,1.8168991359,-3.7230722407
 C,0,4.2795004434,3.9822813444,-2.2610141046
 H,0,3.7082397367,5.4204199661,-0.7317157227
 H,0,2.9290940444,5.678289114,-2.2925569379
 H,0,4.3696664763,2.5070482998,-3.8568657153
 H,0,3.3296100371,3.886912334,-4.2108067878
 H,0,5.135401678,4.572433151,-2.6279211637
 H,0,4.6684108359,3.2686170193,-1.5143667002
 C,0,0.6298070497,4.1556614139,-3.2037913369
 H,0,0.1439757705,3.5570240808,-3.9902829901
 H,0,-0.1484097928,4.7511129441,-2.7010010377
 H,0,1.3224223095,4.8524156333,-3.6961208092
 C,0,5.1707024847,-1.6187778597,-0.3654440671
 C,0,5.6423230386,-2.5798589661,-1.310422098
 C,0,5.0175199758,-3.8326687922,-1.0200324422
 C,0,4.1596657468,-3.6479275447,0.1075279392
 C,0,4.2562381779,-2.2814154794,0.5119870612

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H,0,5.3990015547,-0.5552087525,-0.3456727142
H,0,6.3319381335,-2.384888667,-2.1300446037
H,0,5.1469888799,-4.7575561597,-1.5794858586
H,0,3.4889192266,-4.3897538511,0.5374498955
H,0,3.6807774588,-1.8131506539,1.3081090604
Fe,0,3.5803621926,-2.3977574481,-1.419360851
C,0,1.9668858933,-3.1669955786,-2.4492868056
C,0,2.8057542528,-2.4498802159,-3.3547380748
C,0,1.5565511315,-2.2713831354,-1.4189249993
H,0,1.7004135402,-4.2193470318,-2.4976074259
C,0,2.9153215289,-1.1039344676,-2.8969346554
H,0,3.3039089797,-2.8665220182,-4.2284335017
C,0,2.1449436785,-0.9852357219,-1.6936706232
H,0,3.5288494514,-0.3225683103,-3.3385695829
C,0,0.6771921087,-2.591472424,-0.2623551993
O,0,0.4710063746,-3.7469850584,0.1222849905
N,0,0.166781335,-1.4616824199,0.2688787531
O,0,-0.6759929617,-1.595381056,1.3553825977
C,0,0.0161013418,-1.9533354224,2.548818085
H,0,0.802947824,-1.2182354112,2.7723796065
H,0,-0.746686805,-1.9496873859,3.3407079233
H,0,0.4431473109,-2.9631080267,2.4496992091
Rh,0,0.5343512361,0.4221012291,-0.4687339404
C,0,2.9104404266,1.055646008,1.1489597016
O,0,1.6972490672,0.6234300171,1.2473525156
O,0,3.5155255553,1.2191496285,0.0848547899
C,0,5.1001083304,1.386461897,2.3477082455
C,0,3.1213252536,0.4473643477,3.6053481361
C,0,5.8411206404,1.5999242112,3.6713493277
H,0,5.3794742726,0.3997402011,1.942126266
H,0,5.4131474755,2.1238060475,1.5940473749
C,0,3.8666783334,0.6537674227,4.9281882469
H,0,3.3084133554,-0.5818962127,3.2528865154
H,0,2.0349868419,0.5283050656,3.7527294547
C,0,5.3846172753,0.5973473045,4.7351574168
H,0,6.9271106442,1.5116690032,3.5020498658
H,0,5.6732073336,2.6272013727,4.0402619993
H,0,3.5425211841,-0.1100808859,5.6544172094
H,0,3.5901903367,1.6280938981,5.3682066751
H,0,5.9034719514,0.7814804649,5.690659305
H,0,5.6692624268,-0.4216833658,4.4142547817
C,0,3.5639675052,1.4287420711,2.4963358085
C,0,3.0742652703,2.8605672841,2.8025805497
H,0,3.4921870865,3.2419880106,3.7449623674
H,0,1.9768460275,2.8812294976,2.8863721354
H,0,3.3749856952,3.5517610599,1.9995131481
H,0,2.3857176858,-0.1616538222,-0.979404763

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TS-2

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4048.81346423 a.u.
Imaginary frequency = -1422.8918 cm-1
Zero-point correction = 1.036917 Hartree/Particle
Sum of electronic and thermal Free Energies = -4047.867948 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = 4049.617773928835 a.u.

```

O,0,1.1392497283,1.5960643849,-2.6344880161
 O,0,2.7368507086,-4.3638500465,1.5379125467
 C,0,-0.3183842866,-2.5671751778,0.8380950504
 C,0,-1.3324371101,-2.571550108,-0.1882013797
 C,0,-0.7334347928,-1.9523008783,-1.3359653694
 C,0,0.6184043566,-1.578083226,-1.0517042121
 C,0,0.8612486289,-1.9629410315,0.3216384567
 C,0,1.6070473166,-1.0703906028,-2.0706052157
 C,0,2.5537054238,0.0108693558,-1.5974928335
 C,0,2.2744286925,1.3778437595,-1.9256596735
 C,0,3.144883571,2.3830235098,-1.5540425237
 C,0,4.2998046322,2.0944497324,-0.7821425777
 C,0,5.1642501141,3.1254125819,-0.3227724685
 C,0,6.2527380154,2.8340544043,0.4722968978
 C,0,6.5286150156,1.4944237844,0.8374152622
 C,0,5.7147289808,0.4716394331,0.394734774
 C,0,4.5844567132,0.7395965022,-0.4242083778
 C,0,3.7028437554,-0.2946442026,-0.8837213224
 C,0,0.8227443669,2.9271772487,-2.9916393652
 C,0,2.1351144629,-1.7413344852,1.085108761
 C,0,3.2867428408,-2.4034127662,0.3674620905
 C,0,4.0270039544,-1.721129616,-0.581654413
 C,0,5.0842157457,-2.3790469919,-1.2969187754
 C,0,5.8542492217,-1.7231237486,-2.2954034789
 C,0,6.8650988356,-2.3853005865,-2.9618587498
 C,0,7.1499308103,-3.7384171533,-2.6608624545
 C,0,6.4127625948,-4.4056573994,-1.7048827231
 C,0,5.363036049,-3.7525994413,-1.0033265896
 C,0,4.5803276868,-4.4379727459,-0.0336142688
 C,0,3.5575842478,-3.7853984672,0.623542711
 C,0,2.911453491,-5.7279694588,1.8457275078
 H,0,-0.4297517842,-2.9435053882,1.8514161309
 H,0,-1.2337652431,-1.7736873152,-2.2851408841
 H,0,1.041900859,-0.6983785091,-2.9335777825
 H,0,2.2045119532,-1.9303894413,-2.4168783696
 H,0,2.9509478363,3.4189781897,-1.8232056805
 H,0,4.9419824473,4.1591142086,-0.5994378218
 H,0,6.9028733006,3.6379233483,0.825674298
 H,0,7.3883316977,1.2709526478,1.4730557428
 H,0,5.9275942281,-0.5594924872,0.6790106812
 H,0,0.7242702754,3.5563544049,-2.0946148668
 H,0,-0.1437244506,2.8947780213,-3.5078812164
 H,0,1.5866871175,3.3508927617,-3.6665357093
 H,0,2.0215113697,-2.1544806216,2.0939611389
 H,0,2.3122641736,-0.6627162446,1.1789999979
 H,0,5.6362838739,-0.6807175442,-2.5298133755
 H,0,7.4475809653,-1.8642096604,-3.7250287808
 H,0,7.9532901753,-4.2552146508,-3.1913645959
 H,0,6.6245277909,-5.4531564284,-1.4748772509
 H,0,4.8022127033,-5.4863060136,0.1632246363
 H,0,2.7808797956,-6.3647548276,0.9528771684
 H,0,2.1423454993,-5.9837496224,2.586056431
 H,0,3.9088751676,-5.9230775299,2.2780971066
 C,0,-2.6689829354,-3.2843660289,-0.1397439531
 C,0,-3.2146488883,-3.3041341865,1.3092995295
 C,0,-3.6702822187,-2.5814285874,-1.0851773663
 C,0,-4.6636277437,-3.7868099273,1.4195258189
 H,0,-3.1537569835,-2.2949488321,1.7341566525

H,0,-2.5620198732,-3.939035677,1.9319243539
 C,0,-5.1168032767,-3.0594461079,-0.9390307877
 H,0,-3.6400009831,-1.5063641303,-0.8757794065
 H,0,-3.3394184222,-2.7035836251,-2.1299772207
 C,0,-5.5856683946,-2.9674700041,0.5145941463
 H,0,-4.9857584653,-3.7060890155,2.4702593763
 H,0,-4.7402008406,-4.8566070935,1.1526532772
 H,0,-5.7605624581,-2.4488060707,-1.5938670066
 H,0,-5.2166740384,-4.101060608,-1.2941438543
 H,0,-6.6278435775,-3.3160122609,0.6058955514
 H,0,-5.5664655737,-1.9131797876,0.8427580427
 C,0,-2.3993691274,-4.727487806,-0.6252429631
 H,0,-2.0041537653,-4.7294816749,-1.6532611209
 H,0,-1.6634521539,-5.2278166331,0.0235622343
 H,0,-3.3204338018,-5.3278788899,-0.6161202014
 C,0,-2.2021038863,4.4583140956,-1.1957557661
 C,0,-3.2386192538,4.4620634234,-2.1746703418
 C,0,-4.4703674144,4.1662891669,-1.5131908855
 C,0,-4.1938258042,3.9856187427,-0.1224653926
 C,0,-2.7933516933,4.1644637244,0.072329894
 H,0,-1.1432334929,4.6182626827,-1.3752066605
 H,0,-3.1124254425,4.6297050566,-3.2430541633
 H,0,-5.4435913643,4.0607360202,-1.9893588346
 H,0,-4.9102187248,3.6895409522,0.6419911861
 H,0,-2.2572110507,4.0451041603,1.0099760539
 Fe,0,-3.1458442255,2.6092788867,-1.2390454437
 C,0,-4.2813950509,0.9030719542,-1.3408063948
 C,0,-3.5872399944,1.0823452642,-2.5777560227
 C,0,-3.2996828037,0.8047057593,-0.318585641
 H,0,-5.3577436337,0.8624074929,-1.1869002429
 C,0,-2.1874556941,1.0751272078,-2.3100075705
 H,0,-4.0512511216,1.2377882095,-3.5511444841
 C,0,-1.9740421572,0.9001771914,-0.8951331832
 H,0,-1.4006518625,1.2049490385,-3.0491613603
 C,0,-3.4865569549,0.4465278883,1.114118295
 O,0,-4.5587807113,0.4768457696,1.70738308
 N,0,-2.2738566409,0.0485935152,1.6023764256
 O,0,-2.319704154,-0.5471033941,2.8561468954
 C,0,-1.6827736936,0.2562674488,3.8284511979
 H,0,-0.6101963806,0.3780399226,3.602382968
 H,0,-1.8031697144,-0.2709364295,4.786630313
 H,0,-2.1579558322,1.2503040904,3.8959455504
 Rh,0,-0.7884357726,-0.4867523058,0.2698613971
 H,0,-0.9825122465,1.7741378731,-0.3712662016
 C,0,0.4890919464,2.1072171597,1.0360149063
 O,0,0.4408208358,0.8899615232,1.3382479123
 O,0,-0.1698145226,2.6055061167,0.071078447
 C,0,0.3602679007,3.4528651614,3.0849124672
 C,0,1.7309231624,4.3110645982,1.1489788421
 C,0,0.9501015981,4.5416732864,3.9859221747
 H,0,-0.5802052564,3.8264615112,2.6443052216
 H,0,0.0985667038,2.5611059387,3.6724713194
 C,0,2.3257133093,5.3986362515,2.0480975066
 H,0,0.8392335501,4.7118237173,0.6427520037
 H,0,2.4442455427,4.0333649579,0.3616421955
 C,0,1.365278079,5.7753092011,3.1796613007
 H,0,0.2095918951,4.8159421345,4.7552628027
 H,0,1.8243487058,4.1445620917,4.5297312676

H,0,2.5632804899,6.2859349378,1.4379832217
H,0,3.2845259519,5.0561416286,2.474061744
H,0,1.8209032363,6.5316384442,3.8399271205
H,0,0.4620599406,6.2409369336,2.7443290466
C,0,1.315813269,3.0423801856,1.9260800078
C,0,2.5366997238,2.2801418353,2.4639895975
H,0,3.1519721963,2.918739367,3.1112077011
H,0,3.1743367877,1.931876345,1.640317399
H,0,2.2205691747,1.4034532913,3.0448655371

TS-2- (S_p)

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4048.80525361 a.u.
Imaginary frequency = -1373.2092 cm⁻¹
Zero-point correction = 1.036821 Hartree/Particle
Sum of electronic and thermal Free Energies = -4047.860067 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4049.608660280212 a.u.

O,0,-1.1258689428,-2.4303900928,-2.4147058944
O,0,-3.9521963875,3.1833521176,1.7293700238
C,0,-0.5860732458,2.3836671668,0.6964097221
C,0,0.2461490452,2.609441695,-0.4434674399
C,0,-0.2077368552,1.6664156177,-1.4358828133
C,0,-1.3171658928,0.9166176182,-0.9310887103
C,0,-1.5310427719,1.3449365784,0.4362582888
C,0,-2.183542167,0.0156908462,-1.7752859114
C,0,-2.7017852456,-1.2459301852,-1.1222567849
C,0,-2.0781694583,-2.4919951155,-1.4488178109
C,0,-2.4561034001,-3.6574609588,-0.8177657157
C,0,-3.4850131411,-3.6450904543,0.1563707761
C,0,-3.8580301717,-4.8234189589,0.8593505911
C,0,-4.8685412613,-4.8011347645,1.7975309351
C,0,-5.5557620043,-3.5943712883,2.0745245043
C,0,-5.2156402977,-2.4340970019,1.4093753497
C,0,-4.1753979866,-2.4241815727,0.4407636852
C,0,-3.769982089,-1.2300868226,-0.2388856289
C,0,-0.6350447688,-3.6422034197,-2.9579854502
C,0,-2.5764886746,0.8365565509,1.3871699987
C,0,-3.9496780293,1.027031175,0.7937296283
C,0,-4.5142914035,0.042598202,0.0041227396
C,0,-5.7973420125,0.245940475,-0.6079648147
C,0,-6.4086182998,-0.7324477538,-1.4379061989
C,0,-7.644850363,-0.507049768,-2.0086263125
C,0,-8.3253672931,0.7118299482,-1.7763597366
C,0,-7.7536240394,1.6848192385,-0.9829414423
C,0,-6.4807678438,1.4842063934,-0.3829873624
C,0,-5.8709419799,2.4892237225,0.4184926141
C,0,-4.6292808315,2.2718999403,0.9792582513
C,0,-4.5436706849,4.4385943352,1.9688889886
H,0,-0.4857061582,2.8780915937,1.6616913091
H,0,0.2065858528,1.5392041879,-2.4332082122
H,0,-1.6234422253,-0.2502987819,-2.6791259639
H,0,-3.0404509105,0.636307688,-2.090076658
H,0,-1.9395529824,-4.5929318726,-1.0202359538
H,0,-3.3214819487,-5.7509782056,0.644026366
H,0,-5.1402699152,-5.7152692568,2.3313084625

H,0,-6.3545470149,-3.5823231025,2.8199064572
 H,0,-5.7406040657,-1.5034583639,1.6297584544
 H,0,-0.049643428,-4.1951030066,-2.2075328612
 H,0,0.0100606939,-3.3604207632,-3.800067168
 H,0,-1.4650605129,-4.2689163699,-3.3295483333
 H,0,-2.4867439786,1.3805451702,2.335148604
 H,0,-2.3907050739,-0.2284847186,1.5788083979
 H,0,-5.8842920158,-1.6719003576,-1.6157689185
 H,0,-8.100697471,-1.2716970596,-2.6417944455
 H,0,-9.3047977137,0.8819824191,-2.2301337337
 H,0,-8.2736966895,2.6301055564,-0.8060424138
 H,0,-6.4036241656,3.4285747014,0.5635868486
 H,0,-4.7296142432,4.9872182609,1.0282156022
 H,0,-3.8348778295,5.0091834051,2.5835415282
 H,0,-5.4985974399,4.3417445848,2.5156269665
 C,0,1.2666671129,3.7223507907,-0.5931734425
 C,0,2.3079793285,3.6354438147,0.5503524114
 C,0,1.9958627203,3.5939070319,-1.9491783897
 C,0,3.4737124317,4.6150226029,0.4006812927
 H,0,2.7136986101,2.6140206683,0.5576783412
 H,0,1.8053136466,3.7782131686,1.5211813387
 C,0,3.1775819873,4.5565776663,-2.1061557644
 H,0,2.36525137,2.5621248728,-2.0432452737
 H,0,1.2747407471,3.744160653,-2.7697008382
 C,0,4.1715716956,4.4237969673,-0.9485041894
 H,0,4.1860885304,4.4585580501,1.2273763654
 H,0,3.1202865881,5.6570524694,0.4911663929
 H,0,3.6803239096,4.3620390064,-3.0678056595
 H,0,2.8147591468,5.5977736488,-2.1579215007
 H,0,4.9975427199,5.1444640965,-1.0655862217
 H,0,4.6268920512,3.4166594291,-0.974777931
 C,0,0.4923340604,5.0569590463,-0.5286179607
 H,0,-0.2767473004,5.0965373388,-1.3157563779
 H,0,-0.0132521938,5.1701966643,0.4428678414
 H,0,1.1557077117,5.9231546387,-0.6619897057
 C,0,5.406343912,-1.4839057019,0.4381614745
 C,0,5.8599197522,-2.0291267828,-0.7986972195
 C,0,5.173455939,-3.263880267,-1.0156896935
 C,0,4.2988910871,-3.4865282131,0.0929204618
 C,0,4.4438051363,-2.388054284,0.9895880744
 H,0,5.7001893568,-0.5307227087,0.8699753448
 H,0,6.5769379593,-1.5691765015,-1.4767537029
 H,0,5.2711420493,-3.9048680421,-1.8902205066
 H,0,3.5807654532,-4.2983436716,0.196097355
 H,0,3.8818761145,-2.2409469769,1.9082262285
 Fe,0,3.8049364166,-1.7291594142,-0.8562316487
 C,0,2.3809848097,-2.1294085768,-2.2729582344
 C,0,3.2193277203,-1.0653472352,-2.730352426
 C,0,1.7912152691,-1.7087556374,-1.0499860765
 H,0,2.2539234061,-3.1028666552,-2.7392679165
 C,0,3.1226175312,0.0089327045,-1.7976288223
 H,0,3.8562296486,-1.0908554641,-3.6137274824
 C,0,2.2191958152,-0.3606085723,-0.7349769559
 H,0,3.7005138999,0.9304134785,-1.8466903769
 C,0,0.8322360257,-2.4231539841,-0.1641740217
 O,0,0.6906279188,-3.6484896364,-0.1174633217
 N,0,0.1855435942,-1.4962467122,0.5784102453
 O,0,-0.8125917679,-1.9365182065,1.4292595025

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C,0,-0.2858593694,-2.4989930928,2.6221954072
H,0,0.3300366476,-1.7614354273,3.1638682618
H,0,-1.1579516676,-2.7779557878,3.2313295454
H,0,0.3065245822,-3.3986720095,2.3912894956
Rh,0,0.4914168798,0.5154725935,0.2782645749
C,0,2.521432953,0.614637818,2.4425841453
O,0,1.2836977355,0.5522042543,2.2501647796
O,0,3.3742056501,0.4629183324,1.5112010132
C,0,3.8858856175,2.2121288014,3.7674502683
C,0,3.9898289899,-0.2663057408,4.2540839122
C,0,4.6749068301,2.4967525875,5.048688587
H,0,4.5879965921,2.118330425,2.9239217621
H,0,3.2160357822,3.0552100259,3.5303676681
C,0,4.7760466933,0.0161418459,5.5375372396
H,0,4.7007922228,-0.4376137526,3.4313805199
H,0,3.3949641342,-1.1891474595,4.3593205237
C,0,5.5770358935,1.316828903,5.423340046
H,0,5.2768990372,3.4098157972,4.9091488145
H,0,3.9829414942,2.7111732378,5.8812991628
H,0,5.4500291561,-0.8312169698,5.7441109441
H,0,4.0899950737,0.07886419,6.3996397005
H,0,6.1112081633,1.5246440247,6.3650229343
H,0,6.3507783619,1.1944799517,4.6433845207
C,0,3.052955471,0.9029631277,3.8483187588
C,0,1.8814641217,1.0465796827,4.8266900244
H,0,2.2368382339,1.2532655094,5.8449702042
H,0,1.2790440561,0.1274022683,4.8544657185
H,0,1.2161872048,1.8674975148,4.5229690212
H,0,2.7951823912,0.0667782227,0.4992446916

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INT-2

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4048.83107668 a.u.
Zero-point correction = 1.042798 Hartree/Particle
Sum of electronic and thermal Free Energies = -4047.877847 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4049.633429699099 a.u.

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C,0,-2.0445754036,3.5435359719,-0.8154973011
C,0,-2.7626883241,4.0439513032,-1.9472348102
C,0,-4.1477774174,4.099560964,-1.6020868154
C,0,-4.2877507472,3.6368439657,-0.2577778034
C,0,-2.9881466946,3.2954424957,0.2266139524
H,0,-0.9840131578,3.3150499916,-0.7621030968
H,0,-2.339223118,4.3166409164,-2.9117700298
H,0,-4.9579597581,4.4123787165,-2.2586001974
H,0,-5.222613993,3.5207419817,0.2876367976
H,0,-2.7684971674,2.8423032677,1.1896869955
Fe,0,-3.441255273,2.1597100596,-1.4237191832
C,0,-4.8646089143,0.7287976172,-1.8428298903
C,0,-4.042904695,0.9578722062,-2.9902412366
C,0,-3.9951428322,0.2981993132,-0.7953662478
H,0,-5.9399055127,0.8769919048,-1.766071504
C,0,-2.6789373707,0.6610403902,-2.6415520683
H,0,-4.3897766476,1.3198148173,-3.9576319359
C,0,-2.6487244941,0.2523200958,-1.2778381681
H,0,-1.8160058748,0.7520604618,-3.2970515286

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C,0,-4.230819688,-0.0724706274,0.6225777761
O,0,-5.3238522776,-0.2581153512,1.153718371
N,0,-2.9971717799,-0.1626472355,1.2104028984
O,0,-2.9412614751,-0.6163563099,2.5598506281
C,0,-3.6781286728,0.2140935809,3.4670556945
H,0,-3.3925948286,1.2716821196,3.3331786542
H,0,-3.3907000631,-0.1239429146,4.473033705
H,0,-4.7542448665,0.0954526226,3.2962769955
Rh,0,-1.352886783,-0.5845293538,0.0276154052
O,0,0.6325798942,1.5969324671,-2.8285408927
O,0,2.6309757912,-3.7225800446,1.9630143869
C,0,-0.4798143176,-2.516673412,0.881315372
C,0,-1.435923111,-2.7299763034,-0.1933770161
C,0,-0.8509278308,-2.14351139,-1.3725647625
C,0,0.3694273823,-1.4993065972,-1.031459395
C,0,0.5891549602,-1.7519437263,0.3903041184
C,0,1.3458526222,-0.941887097,-2.0351335864
C,0,2.1623619295,0.2646533215,-1.6259853997
C,0,1.7766594505,1.5604508836,-2.1034156958
C,0,2.5646541741,2.6676983038,-1.8578335616
C,0,3.7486027786,2.5553725935,-1.0825977237
C,0,4.5723374889,3.682913455,-0.8146551492
C,0,5.7112931083,3.5631609269,-0.0468633157
C,0,6.0711862394,2.307676619,0.4988866494
C,0,5.2937102923,1.1944393409,0.2528128603
C,0,4.125012625,1.2809466411,-0.5525641292
C,0,3.3196263105,0.1356445598,-0.8718183767
C,0,0.2651881346,2.8048215542,-3.4595866244
C,0,1.7785004534,-1.2656419712,1.1682879078
C,0,3.0364022656,-1.8653831594,0.5849354944
C,0,3.7524195618,-1.2173467603,-0.4072840326
C,0,4.8910877113,-1.8495045205,-1.0147557457
C,0,5.6310073689,-1.2436521586,-2.0665392896
C,0,6.7199703255,-1.8790167915,-2.6275062169
C,0,7.1189694032,-3.1543957708,-2.1620839587
C,0,6.4137954911,-3.7742802976,-1.1518664451
C,0,5.2842756758,-3.1483843632,-0.5575867756
C,0,4.5340770926,-3.7926490099,0.4643822679
C,0,3.4281719556,-3.1747558428,1.0100276062
C,0,2.9150536742,-5.0228992178,2.4264519846
H,0,-0.593048354,-2.8436871153,1.911669682
H,0,-1.2897809143,-2.1537814487,-2.3674016695
H,0,0.7861492459,-0.6968509313,-2.9456905194
H,0,2.0471348995,-1.7541287253,-2.2921366399
H,0,2.2900299661,3.6497852969,-2.2394878318
H,0,4.2840120053,4.6521357488,-1.2293918023
H,0,6.3327358821,4.4395650174,0.1509260638
H,0,6.9660278383,2.2214338567,1.1191663873
H,0,5.5743204951,0.2285090864,0.6736715936
H,0,0.1135935299,3.6148033635,-2.7287296089
H,0,-0.6851021639,2.6134178603,-3.9712341752
H,0,1.0294785935,3.1184654068,-4.1921333596
H,0,1.6655212039,-1.5445725727,2.2221987058
H,0,1.8351377171,-0.1725375295,1.1012162843
H,0,5.3263156574,-0.2617006248,-2.429134133
H,0,7.2759887404,-1.3966403213,-3.4345719825
H,0,7.9841718569,-3.6497017656,-2.6092304098
H,0,6.7122825013,-4.7636654732,-0.7955351848


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H,0,4.8469154146,-4.7844632066,0.7890310448
H,0,2.8776333561,-5.7618898461,1.6066966283
H,0,2.1430400411,-5.2675870074,3.1674677728
H,0,3.9078701084,-5.0755091697,2.9074492394
C,0,-2.6380023657,-3.6541782455,-0.1574432647
C,0,-3.2736013275,-3.6548312022,1.25423736
C,0,-3.6814707664,-3.2095743142,-1.2109957523
C,0,-4.6151331236,-4.3902146373,1.3287198558
H,0,-3.4275210188,-2.6180785287,1.5782015328
H,0,-2.564257459,-4.1016087801,1.9713490664
C,0,-5.0201513201,-3.9455634989,-1.1101036977
H,0,-3.8656746652,-2.1348820996,-1.0864108797
H,0,-3.260646368,-3.3352766885,-2.2223020038
C,0,-5.6048362565,-3.839156332,0.3000652663
H,0,-5.0226327265,-4.2862003566,2.3477089754
H,0,-4.47362223,-5.4735314622,1.1623207002
H,0,-5.717320648,-3.5194981474,-1.8501111177
H,0,-4.8963560098,-5.0098753143,-1.3802531688
H,0,-6.5648869766,-4.3783949433,0.360636822
H,0,-5.8123958269,-2.7797730807,0.5311043086
C,0,-2.0988779637,-5.0624920518,-0.4992335556
H,0,-1.6404780291,-5.0747974524,-1.500519513
H,0,-1.3339698705,-5.3754429482,0.2288160711
H,0,-2.9026478993,-5.8123097365,-0.4869368593
C,0,1.2050960836,3.375363484,1.4029668193
C,0,0.6013794181,2.5855602758,2.5795732
C,0,1.7417873715,1.992999788,3.4521930003
C,0,2.7558097174,3.0500266848,3.8973569546
C,0,3.3361332715,3.8021719968,2.6978828024
C,0,2.2273978951,4.4244504047,1.8468578531
H,0,1.3069778603,1.4726156057,4.3181331675
H,0,1.6944581311,2.6650346142,0.7218144364
H,0,0.3969400753,3.8459778302,0.8245217107
H,0,2.2771047749,3.7624399392,4.5914661214
H,0,3.5599733673,2.5591507913,4.4699322291
H,0,4.0472210896,4.5754459288,3.0322566368
H,0,3.9119408879,3.0977577895,2.0758772291
H,0,1.7275591557,5.2277096941,2.4161809743
H,0,2.6597358619,4.9040088347,0.9549124274
H,0,2.2721712634,1.2292003633,2.857670288
C,0,-0.3432013388,3.4686715325,3.4241708449
H,0,-1.1701294165,3.8522746276,2.8067108632
H,0,-0.768049635,2.8976754796,4.2616891498
H,0,0.193183324,4.3344262802,3.8344528657
C,0,-0.240452734,1.431340226,2.049612751
O,0,-0.4695339697,1.2807019271,0.8484533596
O,0,-0.681281852,0.6329192982,2.9952712956
H,0,-1.4128234428,0.0029983204,2.7114311761
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INT-2- (S_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4048.82661494 a.u.
Zero-point correction = 1.042461 Hartree/Particle
Sum of electronic and thermal Free Energies = -4047.876085 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4049.630959035521 a.u.
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```

O,0,-1.3195230633,-3.8846088228,-0.2924047817
 O,0,-5.7912533881,2.0012958461,-1.5662470384
 C,0,-2.1959429861,1.6366384227,-1.1543143646
 C,0,-1.0560408722,1.3186233658,-2.0052511861
 C,0,-1.1532108654,-0.0713239908,-2.2877417484
 C,0,-2.2519927001,-0.6377215332,-1.5372829585
 C,0,-2.9279928343,0.4815711005,-0.8733717833
 C,0,-2.7767615163,-2.0424353354,-1.7125887296
 C,0,-3.3398392669,-2.6864173733,-0.4641317835
 C,0,-2.5170160177,-3.5994777827,0.2711920283
 C,0,-2.9536712418,-4.1417182555,1.4623486082
 C,0,-4.2318471357,-3.8118682344,1.9776084056
 C,0,-4.6804624644,-4.3116678415,3.231359964
 C,0,-5.9282575816,-3.9858680554,3.7198940375
 C,0,-6.7878970361,-3.1446180362,2.9723664484
 C,0,-6.3804034673,-2.6437444548,1.7526737522
 C,0,-5.0984064377,-2.9573277628,1.2244740935
 C,0,-4.6248547475,-2.4199047972,-0.0167974388
 C,0,-0.5487401729,-4.9462177931,0.2427920875
 C,0,-4.1647393241,0.4130497886,-0.0237031999
 C,0,-5.3086652864,-0.1722771833,-0.8137869212
 C,0,-5.5219013146,-1.5381293822,-0.821935436
 C,0,-6.5766849106,-2.1077592863,-1.6100289579
 C,0,-6.8230584439,-3.5065633587,-1.6542469673
 C,0,-7.8487597191,-4.0219041972,-2.4203029097
 C,0,-8.6731262857,-3.1583568215,-3.180551718
 C,0,-8.4530404354,-1.7965759845,-3.1648411402
 C,0,-7.4040161438,-1.2346567361,-2.3874585402
 C,0,-7.1545947389,0.1660521477,-2.3766579183
 C,0,-6.1232788382,0.6833704559,-1.6193979543
 C,0,-6.5360317289,2.9204161453,-2.3302219101
 H,0,-2.4262197239,2.6179526222,-0.7456422421
 H,0,-0.4814829984,-0.6509279258,-2.9171172139
 H,0,-1.9643371363,-2.6650235382,-2.1052906704
 H,0,-3.5638911771,-1.9949659969,-2.4840414707
 H,0,-2.3073411197,-4.7929309634,2.0461287656
 H,0,-4.0112125281,-4.9583101229,3.8045826537
 H,0,-6.2565270952,-4.3757266874,4.6866363191
 H,0,-7.7751081103,-2.8895633678,3.3648926754
 H,0,-7.0413396682,-1.9901201282,1.1816338716
 H,0,-0.2321493844,-4.7246302489,1.2727397379
 H,0,0.3360981401,-5.0332258652,-0.3988073754
 H,0,-1.1221509391,-5.8902476458,0.2206005604
 H,0,-4.4116356173,1.4252973691,0.3190867456
 H,0,-3.96834926,-0.2119422227,0.8563283695
 H,0,-6.1870287255,-4.1703957973,-1.0674657553
 H,0,-8.0259602082,-5.0996297814,-2.441031461
 H,0,-9.4841157678,-3.5740413282,-3.7835517933
 H,0,-9.0848277434,-1.1276283792,-3.7552818493
 H,0,-7.7896503418,0.8088226405,-2.9855192073
 H,0,-6.4764171825,2.6946330246,-3.4099099737
 H,0,-6.0992435374,3.9107853095,-2.1456277264
 H,0,-7.5990953836,2.933231462,-2.0302790118
 C,0,-0.0856667751,2.318628733,-2.608520127
 C,0,-0.0448863352,3.5945294048,-1.733045122
 C,0,1.3327033244,1.7031887741,-2.6615553399
 C,0,1.0559511038,4.584960835,-2.1233649978
 H,0,0.1178051957,3.2787108944,-0.6926176308

H,0,-1.024937275,4.0984393875,-1.7661575967
C,0,2.4270547939,2.6937211791,-3.0653871081
H,0,1.5637200491,1.3071278358,-1.6612257802
H,0,1.3334306341,0.8410660173,-3.3478755122
C,0,2.4313885233,3.9145424555,-2.1427313998
H,0,1.0499786066,5.4302706744,-1.4149211502
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H,0,3.4045815522,2.1850506926,-3.0336033514
H,0,2.285081043,3.0224503555,-4.1099664916
H,0,3.2080390732,4.6336021507,-2.4506368748
H,0,2.691114748,3.5905623628,-1.1186468206
C,0,-0.5974636316,2.651164378,-4.0261559037
H,0,-0.6160506786,1.7471440884,-4.6542664369
H,0,-1.6218082514,3.0538884954,-3.9842548419
H,0,0.0370676146,3.3966922035,-4.5269732387
C,0,3.0618258198,1.0472699241,1.0842047344
C,0,4.21967634,0.3693950008,0.5925329607
C,0,4.5442588416,-0.6745691604,1.5124927118
C,0,3.586674735,-0.6433009022,2.5727598474
C,0,2.6705622487,0.420018916,2.3064657806
H,0,2.5344122797,1.8624794285,0.5986633141
H,0,4.7456631361,0.5921517951,-0.3343778633
H,0,5.3591863068,-1.3889152283,1.4076372087
H,0,3.5399359295,-1.3309041187,3.4152947136
H,0,1.7931114505,0.6691471904,2.897677969
Fe,0,2.635558877,-0.947642433,0.7661650829
C,0,2.0237840762,-2.9099575772,0.682911188
C,0,2.6551807496,-2.5324817319,-0.5421047652
C,0,0.8999621282,-2.047020898,0.8508316526
H,0,2.3397464102,-3.6936428877,1.3684704479
C,0,1.9207728997,-1.4355892895,-1.1102594815
H,0,3.5592400468,-2.9760225874,-0.957909958
C,0,0.8298363708,-1.1296991064,-0.2402329748
H,0,2.1879837111,-0.9205722263,-2.0297022983
C,0,-0.1871972154,-2.0307000413,1.8584324642
O,0,-0.3455301451,-2.8785898256,2.7401322749
N,0,-0.966889337,-0.9463806398,1.5880863886
O,0,-2.1895126416,-0.7603287085,2.286826274
C,0,-2.1324393355,-0.9299779873,3.7099639981
H,0,-1.2881913747,-0.3574931766,4.1309437247
H,0,-3.0847368649,-0.5229493763,4.0793312319
H,0,-2.0214352031,-1.9874898856,3.9682755245
Rh,0,-0.7759014138,0.1002161943,-0.1820105189
C,0,-0.6656112271,2.3241662221,1.985537361
O,0,0.0561543989,1.7526380818,1.1710781178
O,0,-1.81795517,1.8531933188,2.4114355063
C,0,-0.448281037,3.6598201459,4.0994751534
C,0,-1.3607653453,4.6997440122,1.9771435345
C,0,-0.3510264162,5.0491076237,4.7371816579
H,0,-1.4226562382,3.2163408539,4.3543646791
H,0,0.3249012971,2.9902909068,4.5120129156
C,0,-1.2608534384,6.0883313971,2.6155024624
H,0,-2.3684863544,4.2935852783,2.1601732483
H,0,-1.2333124298,4.7660962949,0.8840582882
C,0,-1.3828964331,6.0114186005,4.1404884531
H,0,-0.4984106926,4.9586226938,5.8256710414
H,0,0.6627700386,5.4623219228,4.6000509513
H,0,-2.0507790213,6.7352980884,2.1998412987

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H,0,-0.3024178792,6.5622569834,2.3432555585
H,0,-1.2759184365,7.0143783377,4.5850734321
H,0,-2.3972406413,5.65834379,4.4018323621
C,0,-0.3171904346,3.69775863,2.5532826924
C,0,1.1070995113,4.0758630678,2.1284465297
H,0,1.3862585649,5.0607324416,2.5238552535
H,0,1.197434294,4.1136722516,1.0346175428
H,0,1.8366677788,3.3423281511,2.4979170804
H,0,-1.9963395061,0.8956597398,2.1631988515

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INT-3

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.85150500 a.u.
Zero-point correction = 0.968082 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.972969 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.598559557539 a.u.

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C,0,-2.7538866141,-3.7525279795,-2.5689946976
C,0,-1.8105642779,-4.8225016338,-2.6372538979
C,0,-1.531679524,-5.2476482898,-1.3020297876
C,0,-2.298136519,-4.4386254882,-0.4092617559
C,0,-3.0571979896,-3.5161088309,-1.1908985322
H,0,-3.1705759607,-3.2190221341,-3.4210418416
H,0,-1.3679243295,-5.2284660837,-3.5451729842
H,0,-0.8263360021,-6.0231081755,-1.0095199353
H,0,-2.2510417532,-4.4787410942,0.6771763864
H,0,-3.7227045774,-2.751844474,-0.7972944242
Fe,0,-1.0257483895,-3.2646396998,-1.5204027026
C,0,0.9354233462,-3.2516690922,-0.9273646165
C,0,0.8301087667,-2.7988827391,-2.2789197888
C,0,0.1582131072,-2.3561682693,-0.1334599114
H,0,1.4803529842,-4.1204168516,-0.5661193012
C,0,-0.0101299786,-1.6319243603,-2.3058844284
H,0,1.291462408,-3.2697866662,-3.1457623304
C,0,-0.402532781,-1.3435826191,-0.9644116474
H,0,-0.2591306085,-1.0596663342,-3.1975926929
C,0,-0.2698321726,-2.3915251347,1.2780906224
O,0,-0.0946941231,-3.3370447017,2.0530612013
N,0,-0.9374639184,-1.2366104202,1.5430564336
O,0,-1.5137977461,-1.117817535,2.7966281128
C,0,-2.5401247122,-2.0806398205,3.0273299775
H,0,-3.246075155,-2.1079475745,2.1820192283
H,0,-3.0718308645,-1.7475689775,3.9297302823
H,0,-2.1043440393,-3.0785320585,3.1790604594
Rh,0,-1.1044524258,0.2487982018,0.0996110495
C,0,-4.2440728144,0.273422803,1.2174006777
C,0,-3.9226608043,0.7035623781,2.5168734104
C,0,-5.6032707822,0.1563222627,0.8557562264
C,0,-4.9342404238,1.0169970107,3.4246181183
H,0,-2.8737739415,0.7624633292,2.8028587341
C,0,-6.6085577719,0.4729129982,1.7672433473
H,0,-5.8598412466,-0.1769485009,-0.1519820752
C,0,-6.2780994686,0.9081515104,3.0556782989
H,0,-4.6692120304,1.3501474654,4.4308990623
H,0,-7.6563005661,0.3818652853,1.4709905265
H,0,-7.0666013098,1.1574112429,3.7694904643

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C,0,-3.2448347,0.0202372944,0.2090058306
C,0,-2.9053070161,-0.154654642,-0.9917985717
C,0,-3.1108733611,-0.2866960815,-2.4369319786
H,0,-2.5222618964,-1.1197999584,-2.8392950048
H,0,-2.8019073205,0.6359194094,-2.9545274358
H,0,-4.1759627982,-0.4678290534,-2.6552641472
O,0,1.4479996965,-0.8989156546,3.521091678
O,0,2.6107652016,3.082685185,-2.7296796858
C,0,-0.4226397743,2.0139074723,-1.1053820939
C,0,-1.1541748735,2.5973677972,-0.0121907241
C,0,-0.4782977892,2.2160772476,1.1765919751
C,0,0.7135906658,1.4867199834,0.8318370204
C,0,0.7502967652,1.3745130887,-0.5949183045
C,0,1.8155610473,1.1978351049,1.8220540639
C,0,2.5842443195,-0.0892150608,1.6345364046
C,0,2.2997662481,-1.1841155443,2.5146931571
C,0,2.8963105907,-2.4139218185,2.318663778
C,0,3.8113167963,-2.606840401,1.2532486237
C,0,4.3824904096,-3.8815726059,0.9841098712
C,0,5.2783162344,-4.0546046992,-0.0501409075
C,0,5.6500468239,-2.9559267812,-0.8628079364
C,0,5.1140788383,-1.7065463715,-0.6261858035
C,0,4.1814009754,-1.4981707346,0.4254837008
C,0,3.5646168722,-0.2272715891,0.6639231507
C,0,1.1416912179,-1.8920667923,4.4839081901
C,0,1.8579103462,0.7871353314,-1.4245483676
C,0,3.1671444035,1.4664293305,-1.1174289694
C,0,3.9899058116,0.9693189082,-0.1243016761
C,0,5.2281593256,1.6247419526,0.1908920349
C,0,6.1003984461,1.1570086013,1.2107540471
C,0,7.2852002729,1.8092848411,1.4855420869
C,0,7.6493479168,2.9642567605,0.7533880836
C,0,6.8184697002,3.448853506,-0.2354613085
C,0,5.5907921718,2.8011150384,-0.5414068856
C,0,4.7152138364,3.3059567638,-1.5431082628
C,0,3.5256266705,2.6620369533,-1.8143019637
C,0,2.8739881466,4.2570001761,-3.4608729782
H,0,-0.639645315,2.1400101054,-2.163446859
H,0,-0.7555869797,2.4876717971,2.1916362081
H,0,1.3843780365,1.213073478,2.8289070119
H,0,2.5138490364,2.0498416064,1.7494252162
H,0,2.6348331448,-3.2633845667,2.9458092511
H,0,4.0918298449,-4.7263647646,1.6138034109
H,0,5.7039477013,-5.042059881,-0.245544498
H,0,6.3596017387,-3.1002368243,-1.6809310339
H,0,5.3936882574,-0.8613663546,-1.2572227067
H,0,0.657842154,-2.7542933032,4.0039404673
H,0,0.4411737452,-1.4237468153,5.1866204406
H,0,2.0533569559,-2.20567475,5.0244619425
H,0,1.6047209431,0.9007958366,-2.4845343663
H,0,1.9533738418,-0.2833401183,-1.2183979327
H,0,5.8199116421,0.2672508755,1.7752589522
H,0,7.9447457177,1.4336634761,2.271195356
H,0,8.5898634887,3.4741817159,0.9759410673
H,0,7.0933489609,4.3446539511,-0.7987445372
H,0,5.0058924633,4.2111843827,-2.075342114
H,0,2.9819207414,5.1336447064,-2.7974380312
H,0,2.0145716332,4.413629183,-4.1261723095

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H,0,3.7898240226,4.1610232084,-4.0710006758
C,0,-2.2659667304,3.6238139729,-0.1397986715
C,0,-3.2815084236,3.2194590368,-1.2357968638
C,0,-2.9935133274,3.8066576511,1.2109256946
C,0,-4.5141077957,4.1260782753,-1.3006972753
H,0,-3.6184264794,2.1964561893,-1.0277474827
H,0,-2.7756764581,3.195814538,-2.2151391919
C,0,-4.2409539801,4.6915772391,1.1363710273
H,0,-3.2927643449,2.8171728149,1.578435638
H,0,-2.2891694351,4.2180883693,1.9519939532
C,0,-5.2116352295,4.201562941,0.0596968032
H,0,-5.2060144345,3.7407203578,-2.0679695808
H,0,-4.2311506979,5.1422359883,-1.6267287801
H,0,-4.7341542201,4.6996988627,2.1220788938
H,0,-3.9575630902,5.7378474068,0.9255203684
H,0,-6.0939287104,4.8604970601,0.0063726859
H,0,-5.5806034688,3.1974741549,0.336228286
C,0,-1.5539600327,4.9404243172,-0.5359216732
H,0,-0.808505559,5.2210055201,0.2238338951
H,0,-1.0312726879,4.8301675894,-1.4982818068
H,0,-2.2688630015,5.769988654,-0.6315361088

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INT-3' - (R_p)

```

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.84991925 a.u.
Zero-point correction = 0.967923 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.971988 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.597618991909 a.u.

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C,0,-3.357172878,-3.0617626431,-2.0142314271
C,0,-2.5794801849,-4.220918389,-2.3147116562
C,0,-2.251465062,-4.8660353498,-1.081975225
C,0,-2.8260891956,-4.1056076573,-0.0177438702
C,0,-3.5133977282,-2.9944314752,-0.5946842438
H,0,-3.7449005096,-2.3470715767,-2.7354268104
H,0,-2.2678152925,-4.5417617054,-3.3072491507
H,0,-1.6373184715,-5.7575728747,-0.9685706777
H,0,-2.7007772598,-4.3038582786,1.0456100419
H,0,-4.0289533628,-2.2124035361,-0.0451791963
Fe,0,-1.5056265702,-2.9482840075,-1.0895124529
C,0,0.4638790337,-3.1851561618,-0.5738006084
C,0,0.3607515573,-2.7087302128,-1.9150592655
C,0,-0.1632010254,-2.210802056,0.2573540306
H,0,0.9152782934,-4.11580483,-0.24043679
C,0,-0.3366734739,-1.4521366994,-1.9004348558
H,0,0.7218632369,-3.2236526265,-2.8039962797
C,0,-0.6349861292,-1.1272534149,-0.5402609145
H,0,-0.575308937,-0.8692546649,-2.784734758
C,0,-0.4346277677,-2.1892362585,1.7052520895
O,0,-0.2355836116,-3.1308440576,2.480337643
N,0,-0.9608610122,-0.9748679665,2.0125905511
O,0,-1.3010639929,-0.7086015067,3.3324908913
C,0,-2.1678640868,-1.6715077329,3.9248342538
H,0,-2.9190919473,-2.025056949,3.2008108343
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H,0,-1.605268923,-2.5430020075,4.2848235767

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Rh,0,-1.1348284086,0.5107649498,0.5718845074
C,0,-4.0527367966,0.2519290163,2.1123209095
C,0,-3.2473086871,0.2913465517,0.8853270344
C,0,-3.0587615603,0.3182933599,-0.359007753
O,0,1.855890211,-1.0354728167,3.4907366242
O,0,2.3361782432,3.4345453803,-2.5544718196
C,0,-0.5580923912,2.3815145282,-0.5402327429
C,0,-1.0825299653,2.8570502635,0.7179390767
C,0,-0.2525909252,2.3193328362,1.7249812241
C,0,0.829092954,1.5816930926,1.1131201157
C,0,0.6422674716,1.6457189935,-0.303863343
C,0,2.0556458904,1.1470582764,1.8775178395
C,0,2.6759216971,-0.1676242012,1.4704459057
C,0,2.4785113905,-1.3029369079,2.3233583755
C,0,2.938286508,-2.5496678605,1.9500355022
C,0,3.6206674905,-2.7230747003,0.7189518319
C,0,4.034912553,-4.0077840209,0.2715798157
C,0,4.7033616139,-4.1624043844,-0.924894763
C,0,4.9970200759,-3.0339972421,-1.7282674598
C,0,4.6126097614,-1.7733950111,-1.3187926669
C,0,3.9115772311,-1.5833601007,-0.0978960414
C,0,3.4533707617,-0.2946168342,0.3298674451
C,0,1.7498474525,-2.0473019997,4.4754312963
C,0,1.5527245994,1.0900250596,-1.3632081135
C,0,2.9570634479,1.611068617,-1.2083946211
C,0,3.865882212,0.9339711154,-0.4169843332
C,0,5.2029291896,1.4353119512,-0.2547943559
C,0,6.1684155823,0.7852668044,0.5610454706
C,0,7.4456049453,1.2918650332,0.6908831356
C,0,7.8149594387,2.477305211,0.0122579583
C,0,6.8969326974,3.1378848011,-0.7774122529
C,0,5.5730722594,2.6433091482,-0.9296214957
C,0,4.6121029083,3.3316986603,-1.7215217885
C,0,3.3311279008,2.8353349932,-1.8450739638
C,0,2.6109336418,4.6465828176,-3.2166961919
H,0,-0.9308101524,2.6519613828,-1.5236557493
H,0,-0.3635487329,2.4551325131,2.7980268089
H,0,1.7980775884,1.1053381984,2.9410627527
H,0,2.7967559227,1.9549461822,1.7481264049
H,0,2.7428014253,-3.4217404151,2.5708979023
H,0,3.8059374236,-4.8760365879,0.8949543696
H,0,5.0084887212,-5.158151705,-1.2561631911
H,0,5.5262635946,-3.1635387595,-2.6752220099
H,0,4.8324927542,-0.9035761108,-1.9400701618
H,0,1.1360079634,-2.8799325188,4.1050933675
H,0,1.2505205254,-1.5800507606,5.3341486948
H,0,2.7512714091,-2.4024699178,4.7796673341
H,0,1.1525565102,1.3572669753,-2.3486063808
H,0,1.5716978999,-0.0025819929,-1.2975660869
H,0,5.8858462881,-0.1278388359,1.0853775604
H,0,8.1746448678,0.7764295182,1.3203091852
H,0,8.8287963631,2.8709124554,0.1186655987
H,0,7.1756837796,4.0581761586,-1.2976568633
H,0,4.9134811291,4.2565780888,-2.2123804517
H,0,2.9182718144,5.4365895947,-2.5083765379
H,0,1.6809523927,4.9521230848,-3.7141794096
H,0,3.403801518,4.5256534296,-3.97629336
C,0,-2.181415175,3.8866398934,0.8928004307

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C,0,-3.2421409857,3.7595100739,-0.2279850938
C,0,-2.8548460148,3.7256543435,2.2754469234
C,0,-4.4675066642,4.6541996502,-0.0213089419
H,0,-3.5767907813,2.7149792496,-0.272400141
H,0,-2.7782027791,3.9790163312,-1.2028375042
C,0,-4.0898816517,4.6104605569,2.4698522938
H,0,-3.1470501941,2.6731351289,2.3933417404
H,0,-2.1197961561,3.9327612973,3.0694912768
C,0,-5.1088038379,4.4077808765,1.3459923069
H,0,-5.1942625819,4.4632258747,-0.827776381
H,0,-4.187867038,5.7187379486,-0.106538565
H,0,-4.5456408035,4.3895883949,3.4491412289
H,0,-3.7935342953,5.6732729709,2.5047863886
H,0,-5.9806480494,5.0666572709,1.4910275051
H,0,-5.4900352511,3.3703716178,1.383626557
C,0,-1.4764542728,5.261380986,0.8004857719
H,0,-0.7170837301,5.3618800513,1.590819276
H,0,-0.9703801705,5.3729354326,-0.1707820574
H,0,-2.1896863528,6.0913065986,0.9066160312
C,0,-3.5448105809,0.345584884,-1.714514408
C,0,-2.7409484831,0.6967189671,-2.8108470063
C,0,-4.9038358222,0.0431821521,-1.9418535895
C,0,-3.271635515,0.7267083032,-4.099895831
H,0,-1.695031702,0.937994829,-2.6376857731
C,0,-5.4317724547,0.076579075,-3.2306290449
H,0,-5.5366974692,-0.2312233005,-1.0958423699
C,0,-4.6166456501,0.4133820453,-4.3169914245
H,0,-2.6293302258,0.9940989534,-4.942281065
H,0,-6.4844382675,-0.1683044931,-3.3904564938
H,0,-5.029546101,0.4328516409,-5.3280985024
H,0,-4.9005453232,0.9516885088,2.022116783
H,0,-4.4646336371,-0.7568275302,2.2752525281
H,0,-3.4602445757,0.5203375095,2.9945081602

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INT-3- (S_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.84850459 a.u.
Zero-point correction = 0.968392 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.968193 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.593451046365 a.u.

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O,0,-0.7705573997,-2.6163678159,-2.3902922773
O,0,-3.406684432,3.4177766159,1.2743271493
C,0,-0.1623590778,2.5017674402,0.343276794
C,0,0.6323239465,2.6763120776,-0.845281511
C,0,0.1989156029,1.6678912019,-1.7592129779
C,0,-0.8319076686,0.8829224289,-1.161233153
C,0,-1.0518674606,1.4196186234,0.1695658982
C,0,-1.6990796919,-0.079126989,-1.9393478962
C,0,-2.2824003929,-1.2620782845,-1.1988711154
C,0,-1.7223310518,-2.5591589751,-1.4271653198
C,0,-2.1609347763,-3.6542613253,-0.7128728714
C,0,-3.1989591292,-3.521238476,0.2420792211
C,0,-3.6357838499,-4.6236686719,1.02722962
C,0,-4.6594848712,-4.483800961,1.9403951814
C,0,-5.2965844228,-3.2302597407,2.10894924

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C,0,-4.893966872,-2.1416275486,1.3626930556
 C,0,-3.8379437636,-2.2527432368,0.4175143096
 C,0,-3.3672072841,-1.1350281021,-0.3445661035
 C,0,-0.3082562397,-3.8844295792,-2.8169449194
 C,0,-2.1210962294,0.9997778182,1.1371316672
 C,0,-3.4739335284,1.1983061843,0.5013160095
 C,0,-4.0635688379,0.1796800777,-0.2218704045
 C,0,-5.3239038338,0.385951478,-0.8779694412
 C,0,-5.9597145575,-0.6296515197,-1.6420064432
 C,0,-7.1726798116,-0.3990830083,-2.258718889
 C,0,-7.8037664638,0.8620813268,-2.1406452286
 C,0,-7.2069253254,1.8708770213,-1.4131068101
 C,0,-5.9570733781,1.6657820707,-0.7681320735
 C,0,-5.3216830147,2.7047692118,-0.0322194207
 C,0,-4.1035309672,2.4805856355,0.5750994141
 C,0,-3.9457217287,4.7127350055,1.3981674046
 H,0,-0.0998726852,3.1036973798,1.2465883713
 H,0,0.5766433918,1.5134953582,-2.7677399795
 H,0,-1.1200041412,-0.443272953,-2.7958731589
 H,0,-2.5277487452,0.5292930083,-2.3424627599
 H,0,-1.6919853672,-4.6267980242,-0.843206046
 H,0,-3.138594071,-5.5879655804,0.8946160823
 H,0,-4.9808432195,-5.3405339211,2.5379938352
 H,0,-6.1064473105,-3.1253089122,2.8348463211
 H,0,-5.3806558423,-1.174781834,1.4993097946
 H,0,0.239158601,-4.3875024084,-2.0056447008
 H,0,0.3682660537,-3.6942451503,-3.6595551902
 H,0,-1.1504519136,-4.5131192812,-3.1568806169
 H,0,-2.0441950985,1.6206872004,2.0374087207
 H,0,-1.9748621192,-0.0506495337,1.4166566466
 H,0,-5.4731665062,-1.6014365583,-1.7317666687
 H,0,-7.6482791722,-1.1922298606,-2.8401661915
 H,0,-8.7649950214,1.0362210003,-2.6303945783
 H,0,-7.6888985464,2.8482078157,-1.3244549329
 H,0,-5.8165911192,3.6736507784,0.0269463518
 H,0,-4.0826188489,5.1919935717,0.4123217979
 H,0,-3.2269392479,5.2985634288,1.98627459
 H,0,-4.9174714181,4.7015220385,1.9232290069
 C,0,1.4627508361,3.8954423281,-1.1947463102
 C,0,1.9755191448,4.5918274277,0.0879103405
 C,0,2.655960028,3.5039723057,-2.0965710101
 C,0,2.9546763069,5.7389893917,-0.1867405109
 H,0,2.4585789368,3.8388464572,0.7295524273
 H,0,1.1169530879,4.9740219073,0.6630883983
 C,0,3.6202752159,4.6612021716,-2.3748129923
 H,0,3.2010346173,2.6876557658,-1.6040639771
 H,0,2.2810647347,3.0915387865,-3.0467932598
 C,0,4.1212994916,5.301179086,-1.076982585
 H,0,3.330773934,6.1352950729,0.7707162533
 H,0,2.4235539692,6.5752848302,-0.6730953987
 H,0,4.4697923602,4.2936863071,-2.9736134874
 H,0,3.1224470028,5.4287876143,-2.9922204587
 H,0,4.7764408383,6.159506197,-1.2986397361
 H,0,4.7456267325,4.5719895472,-0.5300546034
 C,0,0.5070797916,4.8454457781,-1.9564764438
 H,0,0.1426304874,4.3708126088,-2.8800875949
 H,0,-0.3683320115,5.0902108245,-1.3353405102
 H,0,0.9996240879,5.7884786845,-2.2331547021

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C,0,5.8290919264,-1.2695733715,0.0686672654
C,0,6.0180566779,-2.3770219615,-0.8117751786
C,0,5.1304370595,-3.4194270419,-0.4037425492
C,0,4.3893375402,-2.9559665809,0.7255366064
C,0,4.8240137211,-1.6289173657,1.0210725399
H,0,6.3668517232,-0.3254692135,0.0217602083
H,0,6.7041646001,-2.4134433957,-1.6561892737
H,0,5.007162735,-4.3839724168,-0.8926998285
H,0,3.5883031411,-3.4975747531,1.225828374
H,0,4.4296163736,-1.0031847782,1.8155464289
Fe,0,4.0458706583,-1.7424008064,-0.897587978
C,0,2.7462845287,-2.5174432869,-2.2509296569
C,0,3.5450502321,-1.5087634231,-2.8744350981
C,0,2.03326735,-1.8813327592,-1.1889877995
H,0,2.7161016685,-3.5747082796,-2.5026066808
C,0,3.3126568666,-0.2636044423,-2.1936162798
H,0,4.2281406006,-1.6585575031,-3.7095943002
C,0,2.3473712923,-0.4923050618,-1.1692736368
H,0,3.7782930689,0.6850972488,-2.4529177237
C,0,1.1276546718,-2.4094352958,-0.1482688819
O,0,0.8678254568,-3.6027502532,0.0357432532
N,0,0.6598526907,-1.3563000275,0.5722030496
O,0,-0.2900000894,-1.6031953271,1.5483064625
C,0,0.153861523,-2.4626777804,2.5961014034
H,0,1.1517902253,-2.1622264541,2.9516044273
H,0,-0.5744881574,-2.3381217725,3.4093348968
H,0,0.1819757828,-3.5038877437,2.2476207828
Rh,0,1.0962107629,0.6005718411,0.0188500554
C,0,1.7024636532,0.4424911042,3.2578164152
C,0,0.3748386169,0.5961780689,3.6892306164
C,0,2.6659446472,-0.0264462061,4.1751505434
C,0,0.0174554078,0.2880257213,5.0006533923
H,0,-0.3740737886,0.9337991162,2.9802857693
C,0,2.3029707733,-0.3365577873,5.4845136259
H,0,3.6990864997,-0.1549230605,3.8472799775
C,0,0.9764676051,-0.1830299134,5.9020249896
H,0,-1.0214707419,0.4054205426,5.3176950643
H,0,3.0583430955,-0.7059434354,6.1821299529
H,0,0.6915577417,-0.4339239752,6.926397233
C,0,2.1136831882,0.7571051441,1.9132321899
C,0,2.945892746,1.112797064,1.0402449714
C,0,4.2473884605,1.6268659895,0.5967406024
H,0,4.5754785207,1.1345326632,-0.3254519301
H,0,4.2063031185,2.7102975711,0.4203909567
H,0,5.004192881,1.4404146895,1.3752846392

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INT-3' - (S_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.84659102 a.u.
Zero-point correction = 0.968179 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.965977 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.593645667237 a.u.

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```

O,0,-1.1830499724,-2.5585309912,-2.3845248622
O,0,-3.5440909227,3.4430704474,1.5003200765
C,0,-0.3501033719,2.4568561166,0.4321926311

```

C,0,0.4324476024,2.615584573,-0.7626346506
 C,0,-0.0497492282,1.6231847688,-1.6734699764
 C,0,-1.1182212079,0.8905927291,-1.07552546
 C,0,-1.2875851358,1.40805063,0.2661586003
 C,0,-2.0396163287,-0.0210237651,-1.8486797786
 C,0,-2.634555837,-1.2054175259,-1.1209531554
 C,0,-2.1155565298,-2.5092504404,-1.4024997848
 C,0,-2.5695477425,-3.613970018,-0.7135558125
 C,0,-3.5756404954,-3.480351563,0.2751564548
 C,0,-4.0242199541,-4.5947010167,1.0365501389
 C,0,-5.0137111974,-4.4540648024,1.9866614956
 C,0,-5.6034101592,-3.1874323893,2.2178162956
 C,0,-5.1888933956,-2.0871744679,1.4953798356
 C,0,-4.1675506726,-2.1989720912,0.5129733162
 C,0,-3.6872646613,-1.0711351187,-0.2284636966
 C,0,-0.7502152169,-3.8214849623,-2.8563886739
 C,0,-2.3322149672,0.9954457032,1.2633803942
 C,0,-3.7013295749,1.2441663575,0.6829223839
 C,0,-4.3416099623,0.2591736474,-0.0450670276
 C,0,-5.6181104935,0.515351216,-0.651128405
 C,0,-6.3065099078,-0.4626216371,-1.4188179898
 C,0,-7.5341762357,-0.1852917318,-1.9850646075
 C,0,-8.1282093736,1.0872810917,-1.8108725833
 C,0,-7.4799778877,2.0607521462,-1.0792672031
 C,0,-6.2136931884,1.8072108382,-0.48556238
 C,0,-5.5254376641,2.8107420528,0.2519742956
 C,0,-4.2927195951,2.540323897,0.808842635
 C,0,-4.0410336155,4.7501884058,1.6670067244
 H,0,-0.2529962638,3.0523658459,1.3371359706
 H,0,0.311813409,1.4552177245,-2.685439891
 H,0,-1.5040851276,-0.3773863954,-2.7360038145
 H,0,-2.8612537988,0.6263253735,-2.2029144676
 H,0,-2.1343334247,-4.5953108204,-0.8879190542
 H,0,-3.5635772063,-5.5692514634,0.8556064125
 H,0,-5.344510363,-5.3204058532,2.5649561229
 H,0,-6.3862736741,-3.0817692634,2.9726471934
 H,0,-5.6393853163,-1.1107334739,1.6796403713
 H,0,-0.2099726659,-4.3633137857,-2.0657208913
 H,0,-0.0723675231,-3.6165181873,-3.6946253993
 H,0,-1.607151564,-4.4196242072,-3.2141950964
 H,0,-2.1959334938,1.5799034908,2.1809974537
 H,0,-2.2098906956,-0.0676370672,1.5033416552
 H,0,-5.8488714505,-1.4433435594,-1.5521936031
 H,0,-8.0501052849,-0.9502246044,-2.5699108142
 H,0,-9.1014473937,1.298423354,-2.2606995536
 H,0,-7.9329417014,3.0470739154,-0.9477286383
 H,0,-5.9918570762,3.7903761009,0.3516382383
 H,0,-4.2005346423,5.2515552626,0.6956984159
 H,0,-3.2845877904,5.3049687587,2.2378169866
 H,0,-4.9924807805,4.7565365432,2.2280726931
 C,0,1.2694279955,3.831384736,-1.1076449909
 C,0,2.0440601234,4.3366554224,0.1319391058
 C,0,2.2543038405,3.5137682457,-2.2546883113
 C,0,3.0172397869,5.4791560363,-0.1774790212
 H,0,2.6037330479,3.4943508528,0.5612245225
 H,0,1.3286082605,4.6599669221,0.9054230633
 C,0,3.231927989,4.6539312556,-2.5579544386
 H,0,2.8190185803,2.6093592225,-1.9854843368

H,0,1.6898854899,3.2571681391,-3.1653145561
 C,0,3.9848226461,5.107957837,-1.3045705683
 H,0,3.578093755,5.7349264034,0.7362834761
 H,0,2.4582566208,6.3888189731,-0.4584066872
 H,0,3.9423238971,4.3276464218,-3.3353936493
 H,0,2.685584627,5.5114737141,-2.9875800506
 H,0,4.6430911646,5.960103078,-1.5413124504
 H,0,4.6411582741,4.2930470598,-0.9572260009
 C,0,0.2547344397,4.9061499892,-1.5703240266
 H,0,-0.3142952699,4.5512141553,-2.4432404652
 H,0,-0.4646826446,5.1300940052,-0.7677116118
 H,0,0.7523467515,5.8455330047,-1.8499475686
 C,0,5.3078044493,-1.5646654282,0.5081849812
 C,0,5.6728334685,-2.5009351931,-0.5038001317
 C,0,4.8007698817,-3.6277840351,-0.3972203455
 C,0,3.8929043791,-3.3860099342,0.6789551394
 C,0,4.206938037,-2.1097749727,1.2383874685
 H,0,5.7837309285,-0.6059928002,0.6837768717
 H,0,6.4653277956,-2.3711131547,-1.2389018449
 H,0,4.7983817055,-4.5004376759,-1.0481000459
 H,0,3.057457583,-4.0241132011,0.9626291288
 H,0,3.6723107263,-1.6249186362,2.050821986
 Fe,0,3.6888160172,-1.9348789979,-0.7558476097
 C,0,2.4236564014,-2.5620639647,-2.2178287462
 C,0,3.3109177998,-1.5758407749,-2.7471761343
 C,0,1.6989007954,-1.9352927257,-1.1587259417
 H,0,2.3437000445,-3.6026962781,-2.523143242
 C,0,3.1196622114,-0.35533915,-2.01343122
 H,0,4.0280137657,-1.7252801029,-3.5533680292
 C,0,2.0963724001,-0.568750741,-1.0420343143
 H,0,3.6692136999,0.5629789837,-2.2018023575
 C,0,0.7509526146,-2.480545769,-0.1702282166
 O,0,0.4663514634,-3.6746427466,-0.0290607138
 N,0,0.2839290521,-1.4468547331,0.5781216868
 O,0,-0.6472719794,-1.7374427114,1.5635502588
 C,0,-0.1491919912,-2.6025759753,2.580404453
 H,0,0.8231429128,-2.241922334,2.9588483381
 H,0,-0.8975832174,-2.5776984933,3.3861738387
 H,0,-0.0340549386,-3.6224868084,2.189857395
 Rh,0,0.7976584071,0.522568058,0.1274411721
 C,0,1.4119304061,0.634754068,2.1739312008
 C,0,2.4528819683,0.8661225106,1.5043688527
 C,0,3.8498897373,1.2256329097,1.4750169911
 C,0,4.5964985032,1.1179571149,2.6671451769
 C,0,4.4887239222,1.7149204946,0.3270403233
 C,0,5.9387674631,1.4902171278,2.7006275556
 H,0,4.1122781766,0.7302806181,3.5655875562
 C,0,5.8308089465,2.0901304088,0.3622222598
 H,0,3.9182797288,1.7918615731,-0.5915753782
 C,0,6.5634996735,1.9779484874,1.5472069499
 H,0,6.5037321079,1.3938968074,3.6306813281
 H,0,6.3112933422,2.462747594,-0.5452930842
 H,0,7.6173221399,2.264136149,1.5722310562
 C,0,0.5304899395,0.5781315434,3.3460087192
 H,0,0.1558375532,1.5881351819,3.5851623515
 H,0,-0.3357999312,-0.0674145382,3.159769821
 H,0,1.075902215,0.1978152432,4.2251561606

TS-3- (R_p)

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.83291661 a.u.
Imaginary frequency = -288.8546 cm⁻¹
Zero-point correction = 0.967792 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.952415 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.580554185232 a.u.

C,0,3.6203029068,1.3742319678,1.3823257134
C,0,4.6278454277,1.0076066955,0.4378100061
C,0,4.201197992,1.4472201037,-0.8529025099
C,0,2.927663601,2.0780339742,-0.7099526379
C,0,2.5723801351,2.0373971892,0.6719294473
H,0,3.6539275501,1.1861403435,2.4539337053
H,0,5.5492452878,0.4720420795,0.6595660758
H,0,4.7284074533,1.2881778654,-1.7915515464
H,0,2.3125676867,2.4520407104,-1.5262923957
H,0,1.6430116977,2.4119227365,1.0952411855
Fe,0,2.8317028037,0.1226144296,-0.0828813816
C,0,2.7702815729,-1.2979408606,-1.5588410384
C,0,3.1738621369,-1.9056083626,-0.333047453
C,0,1.4869300257,-0.7221552708,-1.3416299577
H,0,3.3303383667,-1.259653699,-2.4892353368
C,0,2.1364256414,-1.7169790651,0.6327840618
H,0,4.1216016088,-2.4105439554,-0.1540352628
C,0,1.0587899362,-1.0042955481,0.0074320326
H,0,2.1655763249,-2.0812320824,1.656402256
C,0,0.6172970327,0.0287535584,-2.2736901386
O,0,1.0221501611,0.6090598203,-3.2893874677
N,0,-0.6419377761,-0.0167598856,-1.7911480454
O,0,-1.6298819292,0.6934545948,-2.4580026569
C,0,-1.3575515787,2.0904178129,-2.5527254781
H,0,-1.0320413443,2.4914929298,-1.5804036893
H,0,-2.3090859756,2.5624067764,-2.8367656053
H,0,-0.5820632711,2.2886510329,-3.3061683378
Rh,0,-1.0504193332,-1.1587990118,-0.1057932296
C,0,-1.9340129864,1.8033835775,0.9303450625
C,0,-3.0898298436,1.9022438447,0.1296340915
C,0,-1.6935223008,2.8139945996,1.8899081696
C,0,-3.9878818512,2.953573974,0.3035488546
H,0,-3.2435191844,1.1527264721,-0.6458168663
C,0,-2.5962716,3.8611452528,2.0602550698
H,0,-0.7925045238,2.7650848836,2.5048939748
C,0,-3.7521219285,3.9335598964,1.2730940892
H,0,-4.8789816791,3.011125404,-0.3262915286
H,0,-2.398445212,4.6283005571,2.8128964949
H,0,-4.4586464964,4.7553903274,1.4092758735
C,0,-1.024370317,0.7000406366,0.798261308
C,0,0.015995318,0.1102434023,1.2993539001
C,0,0.6212413006,-0.0776115765,2.6450712451
H,0,1.7123701565,0.0245273783,2.6343665712
H,0,0.3774752218,-1.0773888798,3.0368522713
H,0,0.1916619741,0.6632450935,3.3364821782
O,0,-1.2923216711,-1.580741943,-4.3752418666
O,0,-0.6277642657,-6.4748769523,1.2817119986
C,0,-1.5971464929,-2.8808409804,1.1862608319

C,0,-2.8339910305,-2.2175525778,0.9097292199
 C,0,-2.9817668118,-2.2390760287,-0.5074963843
 C,0,-1.9144682339,-3.0358621696,-1.0905701175
 C,0,-1.0591978221,-3.4310145156,-0.030402988
 C,0,-1.8935986496,-3.497871553,-2.528299112
 C,0,-0.5425437255,-3.4737322766,-3.2073396914
 C,0,-0.2545547794,-2.4004451706,-4.1138783501
 C,0,1.0009608534,-2.2727895944,-4.6748436596
 C,0,2.0222211162,-3.207785614,-4.3711171672
 C,0,3.3439162677,-3.0562404537,-4.8748476875
 C,0,4.3302050917,-3.970723044,-4.5686662125
 C,0,4.0369983325,-5.0870267612,-3.7480655433
 C,0,2.7624541187,-5.2640910258,-3.2487984237
 C,0,1.7277908004,-4.3340217105,-3.537476094
 C,0,0.4090660653,-4.457923348,-2.9895128154
 C,0,-1.1283330974,-0.5209784844,-5.3015623379
 C,0,0.1922334848,-4.2609907808,-0.1217052674
 C,0,-0.0709469503,-5.5720105144,-0.815490384
 C,0,0.0461734214,-5.6667950857,-2.1892827004
 C,0,-0.223744033,-6.9074999266,-2.8601236592
 C,0,-0.1267689991,-7.0486664297,-4.2708898467
 C,0,-0.3894006431,-8.2574692655,-4.8829807807
 C,0,-0.7663312894,-9.380939129,-4.109497142
 C,0,-0.8796381481,-9.2724641707,-2.7389240013
 C,0,-0.617508629,-8.041330112,-2.0787109703
 C,0,-0.7529670614,-7.9121502095,-0.668166193
 C,0,-0.4996943861,-6.7033216639,-0.0533847246
 C,0,-1.0544934152,-7.5289261064,2.1122343513
 H,0,-1.1676512792,-3.0483129153,2.1718889688
 H,0,-3.8092124276,-1.8220053246,-1.0761415724
 H,0,-2.5915580965,-2.8769539189,-3.1002511849
 H,0,-2.2858605131,-4.5289832465,-2.5334681186
 H,0,1.2385600441,-1.4277580227,-5.3172505281
 H,0,3.5648174176,-2.192475258,-5.5072552569
 H,0,5.3417137135,-3.8359692673,-4.9599792148
 H,0,4.8226023296,-5.8077103281,-3.5091639671
 H,0,2.5372524981,-6.1209032123,-2.611738533
 H,0,-0.3425882545,0.1695378342,-4.9632918405
 H,0,-2.0901953452,0.005459422,-5.3306664992
 H,0,-0.8915008048,-0.9160937111,-6.3063117079
 H,0,0.5731978338,-4.4362125424,0.8911988182
 H,0,0.963139729,-3.7128496828,-0.6747477635
 H,0,0.1627534057,-6.1830267923,-4.8674429627
 H,0,-0.3070846592,-8.3480694795,-5.9685097124
 H,0,-0.9714060211,-10.3349078258,-4.6014436774
 H,0,-1.1770747845,-10.1364634794,-2.1386277508
 H,0,-1.0683336021,-8.7849172134,-0.0972102193
 H,0,-2.0570519942,-7.8928717717,1.8247635767
 H,0,-1.0971688623,-7.1282483759,3.1336815219
 H,0,-0.3496524408,-8.3791882502,2.0871958411
 C,0,-3.8226935556,-1.733161028,1.9531158817
 C,0,-3.0818048284,-0.9701950925,3.0803618759
 C,0,-4.8845690752,-0.8169876342,1.3061370694
 C,0,-4.0149839993,-0.2827050654,4.0803161567
 H,0,-2.4471045981,-0.205393681,2.6143437271
 H,0,-2.4051856565,-1.6620500786,3.6085075757
 C,0,-5.7984792792,-0.109908497,2.3114094127
 H,0,-4.361056154,-0.0533110897,0.7180640805

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H,0,-5.4895261805,-1.4051774892,0.5966665
C,0,-4.9925613075,0.6528934162,3.3658096693
H,0,-3.4104504045,0.2794191447,4.8113960988
H,0,-4.5788728982,-1.0338220638,4.6611056521
H,0,-6.4655080764,0.5793170561,1.7677817148
H,0,-6.4564605691,-0.8423770675,2.8116532208
H,0,-5.668479979,1.1333853384,4.0924033919
H,0,-4.4267632102,1.4634575552,2.8752031966
C,0,-4.4988244601,-3.0023788576,2.5217490194
H,0,-4.9941089194,-3.5698886538,1.7187394115
H,0,-3.7570461879,-3.6637811723,2.995194006
H,0,-5.2581977139,-2.7510897132,3.2761556762
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TS-3' - (R_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.82302613 a.u.
Imaginary frequency = -324.8618 cm-1
Zero-point correction = 0.966962 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.944493 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.570835569605 a.u.
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C,0,3.5607498325,1.2795170502,1.4814755634
C,0,4.6551005596,0.8406375853,0.6768351067
C,0,4.4303513438,1.2901117169,-0.6609449808
C,0,3.1948855878,2.0067758472,-0.6871794148
C,0,2.6616760972,2.002316482,0.6366919959
H,0,3.4262485263,1.0812607358,2.5413948761
H,0,5.4996073326,0.2439459744,1.0172915953
H,0,5.0644741615,1.0833379984,-1.5211352717
H,0,2.709303741,2.4081266549,-1.5751672235
H,0,1.7092594212,2.435303607,0.9318302771
Fe,0,2.8830795343,0.0719900262,-0.0663514433
C,0,2.7222932931,-1.2283662668,-1.6373622121
C,0,3.1904351028,-1.9260283971,-0.4871175234
C,0,1.4561493768,-0.6694219082,-1.3052072097
H,0,3.2285743392,-1.1188131078,-2.5919194135
C,0,2.2147816455,-1.8011885994,0.5504374765
H,0,4.1451703268,-2.4413614939,-0.3977851035
C,0,1.1017524108,-1.0464287183,0.0429939894
H,0,2.3237696399,-2.2146013784,1.5467378453
C,0,0.5353733466,0.1115354767,-2.1579702024
O,0,0.8802593032,0.7394641581,-3.1677281714
N,0,-0.7002348309,0.0149696917,-1.6241510812
O,0,-1.7536434645,0.6803034868,-2.2326553334
C,0,-1.5626279332,2.0869605512,-2.3330839854
H,0,-1.2585943454,2.5163105701,-1.3652301709
H,0,-2.5398756959,2.4994573285,-2.6250653198
H,0,-0.7974770314,2.3301049273,-3.0840647962
Rh,0,-1.0193341379,-1.1977527383,0.0240619087
C,0,-1.8269135516,1.8037302803,1.1257166446
C,0,-0.9402498061,0.6410706326,0.9481763974
C,0,0.1030536282,0.0238646178,1.4052553374
O,0,-1.3216211858,-1.5153687674,-4.2603070369
O,0,-0.6732074826,-6.5789286645,1.2546713831
C,0,-1.6256824403,-2.9458914948,1.2744352916
C,0,-2.830787793,-2.2274833777,0.9991476541

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C,0,-2.9641674727,-2.2126571444,-0.4184698137
 C,0,-1.9211896885,-3.0352116544,-1.0091554943
 C,0,-1.0876785806,-3.4771566652,0.048437087
 C,0,-1.9054907658,-3.4689827864,-2.4549275982
 C,0,-0.5573244765,-3.4279685274,-3.1368224648
 C,0,-0.2793626546,-2.338010417,-4.0266504895
 C,0,0.9678535301,-2.202313108,-4.603228119
 C,0,1.9925770085,-3.1426135211,-4.3262956603
 C,0,3.3066655089,-2.9858501676,-4.8474555318
 C,0,4.2982201951,-3.901630092,-4.5630245741
 C,0,4.0176765681,-5.0253513464,-3.7483848303
 C,0,2.7497279896,-5.2092242663,-3.2348895149
 C,0,1.710220045,-4.2782059507,-3.5011762043
 C,0,0.3968492063,-4.4142852898,-2.9425416062
 C,0,-1.1809963312,-0.4514676854,-5.1852681152
 C,0,0.1557464645,-4.3179050477,-0.0574715952
 C,0,-0.0999025312,-5.6007851064,-0.8043608508
 C,0,0.03327933,-5.6476311006,-2.1795804263
 C,0,-0.2275539435,-6.8660594732,-2.8951366293
 C,0,-0.119971857,-6.95887343,-4.3093074628
 C,0,-0.3737056113,-8.1467237721,-4.9646400017
 C,0,-0.7521427165,-9.2976143565,-4.2335461986
 C,0,-0.876741664,-9.2362971957,-2.8611221673
 C,0,-0.6245163492,-8.027526112,-2.1571660604
 C,0,-0.7737718816,-7.9478169927,-0.7445188897
 C,0,-0.5317461172,-6.759883261,-0.086522545
 C,0,-1.0985628608,-7.6643891063,2.0443930745
 H,0,-1.2248523335,-3.158756496,2.2615306887
 H,0,-3.7620775844,-1.7428244104,-0.988528458
 H,0,-2.6056232296,-2.8368991517,-3.0113631395
 H,0,-2.2962928752,-4.5002142049,-2.480298038
 H,0,1.1958460675,-1.3493132887,-5.2390920718
 H,0,3.5184947121,-2.1159812188,-5.4747001346
 H,0,5.3040908975,-3.7619042293,-4.9668651082
 H,0,4.8075034949,-5.7466445346,-3.5258719114
 H,0,2.5336745331,-6.0724137851,-2.6032190306
 H,0,-0.4005943522,0.248157827,-4.8531286985
 H,0,-2.149998268,0.0628760905,-5.2013614045
 H,0,-0.9521469746,-0.8401746677,-6.194321189
 H,0,0.521487762,-4.5351163017,0.9532908148
 H,0,0.9385097763,-3.7529180087,-0.5766776814
 H,0,0.1702682801,-6.0729005683,-4.8745430637
 H,0,-0.283119161,-8.1991525658,-6.0520263706
 H,0,-0.9497656719,-10.2348233809,-4.7595725327
 H,0,-1.176067007,-10.1210963913,-2.2929258162
 H,0,-1.0907572014,-8.8409733086,-0.2069985692
 H,0,-2.0964656709,-8.024796418,1.7369098427
 H,0,-1.1513308065,-7.3002327542,3.0789529839
 H,0,-0.3876344876,-8.5084669133,1.9946109367
 C,0,-3.8051834404,-1.7030509266,2.0326042192
 C,0,-3.0409570851,-1.1662440514,3.2685337684
 C,0,-4.6770153011,-0.5783520608,1.4294291595
 C,0,-3.9419450144,-0.4695573418,4.2923364769
 H,0,-2.2728127178,-0.4594123487,2.9224840348
 H,0,-2.4956379414,-1.9906779921,3.7544457772
 C,0,-5.5724587799,0.122822085,2.4561237803
 H,0,-4.0084461021,0.1610908071,0.9643200242
 H,0,-5.2960471252,-0.9897601696,0.6160636763


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C,0,-4.7673064505,0.6472296086,3.6480941171
H,0,-3.3193625321,-0.0660791785,5.1076351978
H,0,-4.6225183084,-1.201665122,4.7608650244
H,0,-6.113745755,0.9483671656,1.9652866516
H,0,-6.3470744895,-0.5748658294,2.8191353946
H,0,-5.4371201175,1.110341463,4.3912040461
H,0,-4.0874423339,1.4463719495,3.3021223728
C,0,-4.6896320495,-2.9071844606,2.4323920389
H,0,-5.2183065969,-3.3071666102,1.5535315113
H,0,-4.0741266497,-3.7168355806,2.8535655992
H,0,-5.4429764215,-2.62992375,3.1836115773
C,0,0.6822979728,-0.0881117133,2.7423284336
C,0,0.9090400796,1.09300119,3.4766424641
C,0,0.890947032,-1.3199433088,3.3854369184
C,0,1.3620450331,1.040325936,4.7939147644
H,0,0.7320000907,2.0588979951,3.0015361428
C,0,1.3447672007,-1.3702166564,4.7042936283
H,0,0.6758266916,-2.2424257832,2.8496805673
C,0,1.5908740362,-0.1922974023,5.4142643852
H,0,1.5388698333,1.9701162455,5.3401000899
H,0,1.5014264523,-2.3403889949,5.1822811556
H,0,1.9489991333,-0.2333336273,6.4452954355
H,0,-1.2691562281,2.7398653998,0.957336587
H,0,-2.6742733145,1.7885630359,0.4278953475
H,0,-2.2274608373,1.8431374277,2.1550199275

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TS-3- (S_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.82985642 a.u.
Imaginary frequency = -257.0038 cm-1
Zero-point correction = 0.967551 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.950153 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.577617171878 a.u.

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O,0,1.829100222,-1.5717425771,-2.4348181289
O,0,-0.0211457934,5.6353305694,-1.5616194337
C,0,-0.7853876727,2.7221497786,0.318996095
C,0,-0.1416186084,1.9823993747,1.3562578447
C,0,0.917696407,1.2333086456,0.7232705955
C,0,0.9148624482,1.4841036765,-0.6669379716
C,0,-0.192930451,2.3966912861,-0.9312222408
C,0,2.0047208434,1.0435548057,-1.6146699326
C,0,1.5857376106,0.6970839061,-3.0256221736
C,0,1.4666027593,-0.6802442827,-3.3931235758
C,0,1.0227077534,-1.0411583423,-4.647324156
C,0,0.6810441003,-0.0507440917,-5.6012315232
C,0,0.1662747855,-0.3962472186,-6.8809351475
C,0,-0.1590169688,0.5771096717,-7.8021052756
C,0,0.0189660532,1.9455917935,-7.4841351039
C,0,0.5161897814,2.3121391149,-6.2500926617
C,0,0.8560111055,1.3322585122,-5.2780463372
C,0,1.3368547861,1.6771052619,-3.9740429768
C,0,1.9683576466,-2.9327297477,-2.7972062792
C,0,-0.5327128772,3.0309481962,-2.2514200554
C,0,0.6651212313,3.7616704288,-2.8045174698
C,0,1.5655403915,3.1114276515,-3.6274302129

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C,0,2.7300241237,3.7927678028,-4.1175008445
 C,0,3.6868275758,3.1582613421,-4.9550310218
 C,0,4.7948708344,3.8426694053,-5.4117567941
 C,0,4.9973313266,5.1950240065,-5.0469609578
 C,0,4.0910788039,5.8354542343,-4.2273607632
 C,0,2.9411664768,5.1576954296,-3.7387707986
 C,0,2.0100561137,5.8006202508,-2.8762335239
 C,0,0.9073159024,5.1149749422,-2.4097712517
 C,0,0.13459615,6.9611082967,-1.1141159413
 H,0,-1.6219530736,3.4058755952,0.4402400948
 H,0,1.6165764005,0.5685255955,1.2266152364
 H,0,2.5165786676,0.1824624836,-1.1690858131
 H,0,2.7316418149,1.8726748088,-1.6544793739
 H,0,0.8772634393,-2.0870466188,-4.9069078533
 H,0,0.0268407654,-1.4539055681,-7.118729694
 H,0,-0.557398404,0.2944775245,-8.7797617008
 H,0,-0.2419496239,2.7124416211,-8.2174233812
 H,0,0.6457081482,3.367071354,-6.0037315496
 H,0,0.9938442551,-3.3651567991,-3.0708657881
 H,0,2.3679799102,-3.4455281111,-1.9128695965
 H,0,2.6785445761,-3.0436300774,-3.6359548323
 H,0,-1.3562338517,3.7382236328,-2.0972486361
 H,0,-0.8629048087,2.2543028977,-2.952295845
 H,0,3.5293135795,2.1163796928,-5.2360152374
 H,0,5.5187639232,3.3398785587,-6.0571901718
 H,0,5.8762285848,5.7306958943,-5.4140809848
 H,0,4.2473787261,6.8783773941,-3.9388277354
 H,0,2.1982418607,6.8353451237,-2.5914117069
 H,0,1.0790895939,7.093898258,-0.5567449636
 H,0,-0.710395066,7.16913165,-0.444457167
 H,0,0.1157607591,7.6797032699,-1.9528983868
 C,0,-0.3178233298,2.2025333186,2.8448814093
 C,0,-1.7752201345,2.6179592522,3.1585808702
 C,0,0.0431723322,0.9194683415,3.6276301856
 C,0,-2.0833545067,2.6943331634,4.6579861564
 H,0,-2.4548507713,1.8965832162,2.6795399857
 H,0,-1.9868653813,3.592374056,2.6902994221
 C,0,-0.2680114269,1.0009150893,5.125420669
 H,0,-0.5111584054,0.0807295574,3.1824400393
 H,0,1.1099563836,0.6863904332,3.4820924112
 C,0,-1.7253417694,1.3939370871,5.382353379
 H,0,-3.1506450684,2.9310081226,4.7999678656
 H,0,-1.5236228026,3.5291002891,5.1143478795
 H,0,-0.042227925,0.0313639214,5.5994630741
 H,0,0.3977739761,1.7370125237,5.608280197
 H,0,-1.9116788457,1.4929333754,6.4643467769
 H,0,-2.3897458442,0.5853418193,5.0286008451
 C,0,0.6530921357,3.3458520143,3.2240617063
 H,0,1.6910156168,3.0670581891,2.9860960337
 H,0,0.4117221529,4.2593028402,2.6592533054
 H,0,0.605587359,3.5873580925,4.2956825785
 C,0,-3.8075918679,-4.0821638852,1.4892913246
 C,0,-3.0145288299,-5.1953351438,1.0744734691
 C,0,-2.8668683004,-5.1248562609,-0.3447004583
 C,0,-3.5590549673,-3.964941231,-0.8079546693
 C,0,-4.1443650209,-3.3248580389,0.3248338456
 H,0,-4.1086747879,-3.8624382353,2.5119479789
 H,0,-2.5859771153,-5.9545622316,1.7263682274

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H,0,-2.2884782103,-5.8071264996,-0.9646070305
H,0,-3.571740568,-3.6044814104,-1.8348248625
H,0,-4.7152518722,-2.4000774342,0.2993058901
Fe,0,-2.0783664553,-3.4338941591,0.518449235
C,0,-0.1764625642,-3.5147555144,-0.1949920483
C,0,-0.1391094856,-3.5075240956,1.2316741743
C,0,-0.8207330523,-2.3126643,-0.60866229
H,0,0.177495555,-4.3015725249,-0.8556979132
C,0,-0.7453788262,-2.2970104715,1.6916691093
H,0,0.2587168236,-4.297381142,1.8670544426
C,0,-1.137094131,-1.5199808546,0.5530032656
H,0,-0.8681869011,-2.0260987404,2.736832411
C,0,-1.1223566049,-1.8304784885,-1.9760874921
O,0,-1.1590409835,-2.55256944,-2.9796298266
N,0,-1.3683257018,-0.5063585376,-1.9016816641
O,0,-1.6611084843,0.1779414592,-3.067690973
C,0,-2.8646792973,-0.2477626753,-3.6994445464
H,0,-3.7024878851,-0.2524812383,-2.9841251275
H,0,-3.0596339653,0.4935372139,-4.4873662617
H,0,-2.7335154833,-1.2479096695,-4.136683107
Rh,0,-1.0818697778,0.5188013202,-0.1226406139
C,0,-4.2253693574,1.075687381,-0.6539546597
C,0,-4.0285703094,2.1863042766,-1.4980985882
C,0,-5.5468861737,0.6173439348,-0.4442385091
C,0,-5.1126338884,2.8265178421,-2.0954437454
H,0,-3.0134522474,2.5186885777,-1.6966676626
C,0,-6.625823867,1.2601486762,-1.0459028612
H,0,-5.7146712093,-0.25560635,0.1897721106
C,0,-6.4156962869,2.3698395966,-1.8734929212
H,0,-4.9375858385,3.6832341438,-2.7508619438
H,0,-7.6395890753,0.890122769,-0.8738495574
H,0,-7.2629956514,2.8682072834,-2.3499453674
C,0,-3.1274571619,0.3988811913,-0.0245471594
C,0,-2.7928438234,-0.4052424832,0.9323026942
C,0,-3.2492820513,-0.7253971974,2.3081600379
H,0,-3.3126668265,-1.8038882443,2.4853800924
H,0,-2.5637472968,-0.3076183886,3.056709481
H,0,-4.2368365384,-0.2644034757,2.4669101246
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TS-3' - (S_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.81984776 a.u.
Imaginary frequency = -273.0431 cm-1
Zero-point correction = 0.967357 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.939392 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.564894010384 a.u.
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O,0,-1.4719873044,-1.8214108258,-3.1655761626
O,0,-2.4927601128,3.15305839,2.3439953527
C,0,0.4343226651,1.9055967371,0.72365464
C,0,1.1807335788,2.1899688586,-0.4585097952
C,0,0.4080814734,1.6687762464,-1.5638935574
C,0,-0.7634723674,1.0565176977,-1.0748831071
C,0,-0.7244891358,1.1542901668,0.3836846931
C,0,-1.909173209,0.590965498,-1.9396661091
C,0,-2.6441293595,-0.6508248374,-1.4898131412

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C,0,-2.3552048494,-1.8937870829,-2.1369609467
 C,0,-2.9575092859,-3.0623694297,-1.7226555785
 C,0,-3.870530601,-3.0540188019,-0.6389796831
 C,0,-4.4529732104,-4.2548916868,-0.1484983887
 C,0,-5.3366470074,-4.2353888058,0.9102883722
 C,0,-5.6816655184,-3.0078613719,1.5263250626
 C,0,-5.133447006,-1.8255346109,1.0718694759
 C,0,-4.215542055,-1.8139977645,-0.0132018869
 C,0,-3.5963520344,-0.6111117414,-0.4832905439
 C,0,-1.2977195807,-2.9586918112,-3.9903094917
 C,0,-1.786425654,0.6967413227,1.3446606992
 C,0,-3.1138167406,1.3254149239,1.0015662186
 C,0,-3.9784625842,0.7010745926,0.1209535329
 C,0,-5.2208956061,1.3209956052,-0.2441754825
 C,0,-6.1320943494,0.7212113904,-1.1551170859
 C,0,-7.3202826398,1.3420638225,-1.4829302868
 C,0,-7.6493233399,2.5959848481,-0.91522138
 C,0,-6.7808440511,3.2080656992,-0.0353414336
 C,0,-5.5485458502,2.5955818811,0.3206907591
 C,0,-4.6346624212,3.2269572274,1.2095688098
 C,0,-3.4408466529,2.6137475142,1.5299296471
 C,0,-2.7226673795,4.4243936634,2.9035268298
 H,0,0.7100213485,2.1807575516,1.7389649535
 H,0,0.6789735647,1.728509188,-2.6155764641
 H,0,-1.5306188164,0.4389090893,-2.9571292363
 H,0,-2.6230781206,1.4314980393,-1.9764992173
 H,0,-2.6985888862,-4.0149225156,-2.1788448802
 H,0,-4.1792698297,-5.1996747347,-0.625116688
 H,0,-5.7717339098,-5.1682357474,1.2776125098
 H,0,-6.3814320307,-2.9983946664,2.365424139
 H,0,-5.3945287989,-0.8811824548,1.55189385
 H,0,-0.8448602622,-3.7863048725,-3.423309614
 H,0,-0.6234078634,-2.6490976781,-4.7991996128
 H,0,-2.262037183,-3.280779006,-4.4222931739
 H,0,-1.4822352935,0.9776153721,2.3607622427
 H,0,-1.865475028,-0.3961419114,1.2961281974
 H,0,-5.8781110671,-0.2452051903,-1.5917937831
 H,0,-8.0099228858,0.864844903,-2.1829773623
 H,0,-8.5928325078,3.0804476345,-1.1783979405
 H,0,-7.028857789,4.1796058513,0.400505922
 H,0,-4.899261746,4.2028743338,1.6154563551
 H,0,-2.847894492,5.196035344,2.1229603841
 H,0,-1.8397148161,4.6667117325,3.5097609087
 H,0,-3.6173666204,4.4296571455,3.5514702786
 C,0,2.3430439539,3.1577875783,-0.5531849972
 C,0,3.2531604734,3.0451947241,0.6921751656
 C,0,3.1804105017,2.8912990935,-1.8236181119
 C,0,4.5103936223,3.9183670787,0.6090311533
 H,0,3.5467664988,1.9911507129,0.8131016669
 H,0,2.6802618092,3.3123820571,1.5947396766
 C,0,4.437304819,3.7629814565,-1.9201570552
 H,0,3.4641122232,1.8279309336,-1.8299486169
 H,0,2.55661618,3.0432742841,-2.7187092144
 C,0,5.3122583453,3.6505275984,-0.6683112957
 H,0,5.1394269258,3.7354393401,1.4955030635
 H,0,4.2299165461,4.9852421099,0.6481862057
 H,0,5.0135895311,3.4758817097,-2.8152765005
 H,0,4.1490269021,4.8173225004,-2.0722046263

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H,0,6.1664347441,4.3443514191,-0.7357024233
H,0,5.7423736941,2.6374127319,-0.614055894
C,0,1.7014499432,4.5648199505,-0.6249494909
H,0,1.0322359167,4.6398958648,-1.4957498878
H,0,1.1028139976,4.7617636066,0.2774808715
H,0,2.4565824863,5.3588438165,-0.7101929775
C,0,5.3052743905,-3.4885213268,-0.8393000062
C,0,5.3462518502,-3.9564959394,-2.1858274689
C,0,4.2216377947,-4.8140451791,-2.3914228764
C,0,3.4811984717,-4.8758987342,-1.1711562782
C,0,4.1524496405,-4.0577371019,-0.2139243281
H,0,6.0171341945,-2.8089704273,-0.3799959411
H,0,6.0904058059,-3.6871507646,-2.9334426238
H,0,3.9496095901,-5.2998765832,-3.326908627
H,0,2.5275205923,-5.3807807798,-1.0254777119
H,0,3.8146862562,-3.8714433943,0.8017018257
Fe,0,3.568678841,-2.9410816282,-1.8516242129
C,0,2.0737944496,-2.6164856827,-3.1942028954
C,0,3.172029578,-1.7581839421,-3.4938796021
C,0,1.6405885067,-2.3040738639,-1.8733107054
H,0,1.6587040847,-3.3975609919,-3.8258474354
C,0,3.4054213449,-0.9135120161,-2.3642596817
H,0,3.7599603007,-1.7622930288,-4.4105628532
C,0,2.4274888338,-1.210439876,-1.359418866
H,0,4.1942021629,-0.172347151,-2.3176595356
C,0,0.5071786653,-2.872041706,-1.1102371451
O,0,0.0165263643,-3.9902067629,-1.3117393698
N,0,0.1459714607,-1.9648065702,-0.1798336388
O,0,-0.8995957556,-2.2675578336,0.6786767925
C,0,-0.694053825,-3.4377212561,1.4609335412
H,0,0.2722463773,-3.3919646759,1.9932701656
H,0,-1.5203068736,-3.4517109112,2.1863339225
H,0,-0.7212175598,-4.3358991174,0.8288184197
Rh,0,1.0158827439,-0.0717194579,-0.1698716157
C,0,1.9374673118,-0.8536314416,1.4380167049
C,0,2.9484143758,-0.9165371331,0.6354725113
C,0,4.3936544913,-0.8480239195,0.8239331899
C,0,4.9423125394,-1.6027913957,1.8821644921
C,0,5.2545879552,-0.0169264346,0.0924219083
C,0,6.304371886,-1.550371356,2.1699058164
H,0,4.2886999741,-2.248353184,2.470598255
C,0,6.6192704885,0.0329257037,0.3793813192
H,0,4.8488309212,0.6141116947,-0.6909202622
C,0,7.155960788,-0.7392578347,1.412291088
H,0,6.705822889,-2.1555024829,2.9862718727
H,0,7.2672757669,0.6872315982,-0.2089312356
H,0,8.2254751967,-0.7045867555,1.6307540751
C,0,1.4781151852,-0.8891072922,2.8378458662
H,0,2.1336256522,-1.5091741785,3.4700113063
H,0,1.4672783338,0.1335172103,3.2534578935
H,0,0.4500477271,-1.2744977055,2.9069377788
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INT-4

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.89017775 a.u.
Zero-point correction = 0.969569 Hartree/Particle
Sum of electronic and thermal Free Energies = -3932.009646 a.u.

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Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.623272998848 a.u.

O,0,-1.95114403,-1.9727893803,-3.3871675025
O,0,-2.5417595142,3.5180406327,1.5432617041
C,0,0.0565492001,2.3782290599,-0.2632316901
C,0,0.6208744179,2.5761412291,-1.5392613486
C,0,-0.1969582131,1.8341418827,-2.4990246296
C,0,-1.227238382,1.1859647482,-1.8306129684
C,0,-1.0119841495,1.407707383,-0.3885596638
C,0,-2.4111061599,0.5542982714,-2.5084457526
C,0,-3.0898808431,-0.6215178605,-1.8466403029
C,0,-2.8341973462,-1.9302287707,-2.3697237556
C,0,-3.4876411553,-3.0316390034,-1.8530778766
C,0,-4.3946122123,-2.8878449346,-0.7731851353
C,0,-5.0280420595,-4.0168681036,-0.1827645544
C,0,-5.8567187367,-3.8756797307,0.9102595765
C,0,-6.0941546151,-2.5935327854,1.4629403302
C,0,-5.5035274805,-1.4781880223,0.9051143283
C,0,-4.6460567491,-1.5897256881,-0.2223473356
C,0,-3.9926758151,-0.4559530169,-0.8072773941
C,0,-1.5342009116,-3.2303399022,-3.8899879524
C,0,-1.9635389653,0.9887993286,0.6940409188
C,0,-3.3201930388,1.5992881431,0.4326037297
C,0,-4.2830956505,0.9175561828,-0.2941113668
C,0,-5.5454013556,1.5372391368,-0.5887677786
C,0,-6.5514330047,0.890274602,-1.3571341155
C,0,-7.7542847149,1.5127918393,-1.6215639005
C,0,-8.0058177785,2.8158828943,-1.1303505776
C,0,-7.0451661763,3.4749273979,-0.3919502117
C,0,-5.7945588406,2.8625700992,-0.1063965395
C,0,-4.7873429132,3.5446010247,0.630617781
C,0,-3.5754277725,2.9344302825,0.878917758
C,0,-2.6947223371,4.8352922476,2.0174146876
H,0,0.3892098649,2.8090809297,0.67633784
H,0,-0.0395562698,1.8061276865,-3.5753500944
H,0,-2.1103147871,0.2699360128,-3.5235063156
H,0,-3.1529278227,1.3667798573,-2.6024813799
H,0,-3.2808494161,-4.0305239684,-2.2319066894
H,0,-4.8298721844,-5.0056955631,-0.6040059233
H,0,-6.3281476403,-4.7547656232,1.356469021
H,0,-6.7448465587,-2.4889562453,2.3341948989
H,0,-5.6819792033,-0.492244618,1.3359889701
H,0,-1.0891645033,-3.828981719,-3.0818649818
H,0,-0.7723607044,-3.0145497086,-4.6491876551
H,0,-2.3786799997,-3.7657046411,-4.3606895193
H,0,-1.5679373012,1.3046743186,1.6653893745
H,0,-2.0491336227,-0.1011907793,0.7061709376
H,0,-6.3600434053,-0.1138366446,-1.7362376591
H,0,-8.5155557416,0.9984058674,-2.2124551837
H,0,-8.9619507553,3.3009192294,-1.3414861093
H,0,-7.2319141263,4.4848350719,-0.0172556444
H,0,-4.9956979918,4.5563065883,0.9772142138
H,0,-2.8891446107,5.5442565727,1.1929138341
H,0,-1.7502578659,5.1047414974,2.5082584873
H,0,-3.517106773,4.9114486626,2.7507625363
C,0,1.7203051587,3.5301102777,-1.9523460402
C,0,2.3961215575,4.1581343221,-0.7166819599

C,0,2.7872463463,2.7731349701,-2.7834243819
C,0,3.6090867752,5.0285046354,-1.0626516837
H,0,2.7250324812,3.3445423587,-0.0548854329
H,0,1.6549045808,4.7489477915,-0.1529494917
C,0,3.9897621241,3.6466535353,-3.1538092717
H,0,3.139492723,1.9175610338,-2.1844093616
H,0,2.3255809276,2.3525251069,-3.6914458312
C,0,4.6320453912,4.2652652145,-1.9093835626
H,0,4.0792948035,5.3800704805,-0.1293300974
H,0,3.2848259767,5.9363795369,-1.6003593572
H,0,4.7285027235,3.0357916314,-3.6984005057
H,0,3.6787465332,4.4434747972,-3.851657482
H,0,5.4643388503,4.9295744472,-2.1955113307
H,0,5.065129906,3.4577096318,-1.2978900279
C,0,1.0375212055,4.6267741237,-2.8026704178
H,0,0.5824430848,4.2050497169,-3.7112541905
H,0,0.2426481337,5.1228777657,-2.2242723665
H,0,1.754420744,5.3968811887,-3.1178363393
C,0,1.0014591719,-4.267854546,3.8145221773
C,0,-0.3072131758,-4.8109301833,3.9902084858
C,0,-0.7225490213,-5.3711706901,2.7422712127
C,0,0.3258736775,-5.1721605908,1.7946583714
C,0,1.3926748734,-4.4905262118,2.4569094991
H,0,1.58659889,-3.7593370515,4.5783200909
H,0,-0.8941086193,-4.7818501154,4.9067038763
H,0,-1.6894607419,-5.826570383,2.5353767155
H,0,0.275687419,-5.3978862861,0.7314072603
H,0,2.3239262133,-4.1673522659,1.9945533653
Fe,0,-0.3318106165,-3.3605358585,2.5102683702
C,0,-1.8495062175,-2.6248120984,1.3719782592
C,0,-2.0002494049,-2.1624415264,2.7089234313
C,0,-0.5908404645,-2.1559275782,0.869699311
H,0,-2.539228964,-3.2497711133,0.8185000493
C,0,-0.8259217,-1.4309878836,3.0556861817
H,0,-2.850957229,-2.3611167953,3.3576003559
C,0,0.0517514853,-1.3977278302,1.9187013883
H,0,-0.6258360814,-0.9668424027,4.0192906387
C,0,-0.1160891529,-2.5449471106,-0.4941735497
O,0,-0.3998818832,-3.6512259205,-0.9718387955
N,0,0.6011793843,-1.5987661898,-1.1394989027
O,0,0.9493862482,-1.9175289431,-2.4664370228
C,0,2.0399989226,-2.8223942677,-2.5138593992
H,0,2.9158166683,-2.4282079695,-1.9686132426
H,0,2.2945787825,-2.9342704097,-3.5783033975
H,0,1.7549426273,-3.7989082649,-2.0924460713
Rh,0,0.7620545343,0.4010941667,-0.8918054256
C,0,3.1210422392,0.5648828556,0.6683602106
C,0,3.5786444766,1.616870766,1.4888520356
C,0,4.0005920329,0.0674307647,-0.3162001521
C,0,4.8726912908,2.1205287281,1.3573250473
H,0,2.9047403511,2.0251032936,2.245201846
C,0,5.291181858,0.5815107266,-0.457082825
H,0,3.6661800544,-0.7532736053,-0.9538308626
C,0,5.7367686634,1.6039676187,0.385183926
H,0,5.2105294202,2.9253899493,2.0150914779
H,0,5.9564747366,0.1721877349,-1.2212371882
H,0,6.7501016118,1.9989366715,0.2842994392
C,0,1.7707960118,-0.0185134647,0.8079288133

C,0,1.3694437445,-0.7345057408,1.8796979201
 C,0,2.237787884,-0.9312996951,3.1046406105
 H,0,2.476584609,-1.9967349845,3.2350480488
 H,0,1.7097243767,-0.6156827318,4.0197755369
 H,0,3.178654168,-0.3719230245,3.0468608852

INT-4' - (R_p)

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
 SCF Done: E(RB3LYP) = -3932.88045683 a.u.
 Zero-point correction = 0.969222 Hartree/Particle
 Sum of electronic and thermal Free Energies = -3932.000211 a.u.
 Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
 FINAL SINGLE POINT ENERGY = -3933.617562632341 a.u.

C,0,-2.5253824467,-3.9946411765,-1.7173512963
 C,0,-1.4341128835,-4.9073031728,-1.8364965657
 C,0,-1.1404961399,-5.4197730479,-0.5338329189
 C,0,-2.0483058447,-4.8232054748,0.3919116631
 C,0,-2.9042129632,-3.9447377743,-0.3400187777
 H,0,-2.9680918948,-3.4143425359,-2.52352344
 H,0,-0.8991897727,-5.1470379007,-2.7539895851
 H,0,-0.3333596781,-6.1062488705,-0.2833475664
 H,0,-2.0290596664,-4.9287310267,1.4746900747
 H,0,-3.6848729298,-3.3205083703,0.0871465204
 Fe,0,-0.9347657463,-3.3686902951,-0.5444793649
 C,0,0.6991090373,-2.9124954187,0.5811608567
 C,0,1.0285180706,-2.8017684965,-0.7989298628
 C,0,-0.3611182346,-1.9909085085,0.8652789609
 H,0,1.1404471439,-3.5899933264,1.3018349682
 C,0,0.1569994794,-1.8362634347,-1.3852221056
 H,0,1.7896092947,-3.3801253574,-1.3188179564
 C,0,-0.7000247759,-1.3059071324,-0.3618403512
 H,0,0.1361974227,-1.5565449505,-2.4350857475
 C,0,-0.9885945006,-1.8980737246,2.218974625
 O,0,-1.1708997535,-2.9011937503,2.9205240829
 N,0,-1.3002186618,-0.6383425949,2.5890953086
 O,0,-1.8646111198,-0.4978248467,3.8685315156
 C,0,-3.2374481362,-0.8588408502,3.857392467
 H,0,-3.803356729,-0.2565135243,3.1239850954
 H,0,-3.6150498218,-0.6520613596,4.869852358
 H,0,-3.3535630911,-1.930037824,3.6284078188
 Rh,0,-0.7949558078,1.192860606,1.9099767872
 C,0,-3.0876438989,1.7099375802,0.2355101114
 C,0,-1.9339094729,0.7404023457,0.3143532319
 C,0,-1.7633355571,-0.291154973,-0.539595583
 O,0,0.8174626057,-1.1562970283,5.1056630239
 O,0,3.4356667419,2.3695181468,-0.81163396
 C,0,0.5262862828,2.6017330345,0.8891851827
 C,0,0.0269066719,3.3000792328,2.0046983322
 C,0,0.5511704739,2.635893513,3.2029781221
 C,0,1.3308758918,1.5491983036,2.8347420113
 C,0,1.2230045794,1.4242823358,1.3686704144
 C,0,2.2098487696,0.7647311574,3.7690611225
 C,0,2.4389733033,-0.6993082481,3.4727025616
 C,0,1.6993763781,-1.6687917697,4.2239833445
 C,0,1.9229371903,-3.018807833,4.0370102284
 C,0,2.8647478154,-3.4655857397,3.0766198326

C,0,3.0651892046,-4.8517728223,2.8259841031
 C,0,3.9315913409,-5.2774509318,1.8414080462
 C,0,4.6424757603,-4.3330251904,1.0612930742
 C,0,4.4775960068,-2.9820149231,1.288125102
 C,0,3.5949213004,-2.5111677429,2.2972699768
 C,0,3.3745243525,-1.1158018593,2.5378223309
 C,0,-0.0420552278,-2.0370961618,5.8108325864
 C,0,2.0091254945,0.462545069,0.5267703121
 C,0,3.4845555778,0.6518010965,0.7907494594
 C,0,4.1378855282,-0.0945868089,1.75838047
 C,0,5.527944182,0.1333946079,2.0371859744
 C,0,6.2321897801,-0.5888772927,3.0387448501
 C,0,7.5690081047,-0.3473022981,3.281125816
 C,0,8.2633847416,0.6326751277,2.5325153499
 C,0,7.6049999082,1.3584059576,1.5617332864
 C,0,6.2274281225,1.1359353364,1.2908095982
 C,0,5.5324295601,1.8967399232,0.31037754
 C,0,4.1912515316,1.6713315884,0.0785748798
 C,0,4.0433466303,3.3929405949,-1.5644871598
 H,0,0.3755969118,2.8374353939,-0.1601009771
 H,0,0.3624651032,2.9459070611,4.2293159062
 H,0,1.8069540312,0.8670976774,4.7837624678
 H,0,3.1887205776,1.2744255236,3.7517926618
 H,0,1.3464291293,-3.760333862,4.5860631577
 H,0,2.5017734051,-5.5758978609,3.4197276424
 H,0,4.0667071426,-6.3458777645,1.6561870546
 H,0,5.3204944805,-4.6762993542,0.2765209612
 H,0,5.0201374195,-2.2560545268,0.6813638914
 H,0,-0.6384229683,-2.6313205959,5.102702137
 H,0,-0.7083632555,-1.3987341247,6.4035197799
 H,0,0.5372580873,-2.6918890403,6.4867748163
 H,0,1.7721681018,0.6295068326,-0.5293860786
 H,0,1.7218234569,-0.5627632346,0.7743751879
 H,0,5.6982622144,-1.3446492332,3.6154446839
 H,0,8.0939741363,-0.9139853816,4.0534914788
 H,0,9.3226120429,0.8161464167,2.7285082402
 H,0,8.1359136709,2.1214901216,0.9863848258
 H,0,6.0826185443,2.6621042622,-0.2361090161
 H,0,4.4509237128,4.1883868757,-0.9152853917
 H,0,3.260891199,3.8183338069,-2.2066491546
 H,0,4.8584035284,3.0024368132,-2.1993517498
 C,0,-0.7473135272,4.602317274,2.0349986533
 C,0,-1.0784908277,5.0704849867,0.60001909
 C,0,-2.0614341225,4.4017464463,2.8350654793
 C,0,-2.0255820183,6.2735078766,0.5486535269
 H,0,-1.5475941109,4.2356897146,0.057299585
 H,0,-0.1409422317,5.2981765276,0.066754515
 C,0,-3.0004017658,5.6106956027,2.7821668585
 H,0,-2.5866698943,3.5284617671,2.4153875704
 H,0,-1.82255987,4.1454802916,3.879879671
 C,0,-3.3115825657,6.0085172925,1.3368057104
 H,0,-2.2608793933,6.5073171906,-0.5024589378
 H,0,-1.5251348716,7.1692781118,0.9551414596
 H,0,-3.9301422012,5.374052671,3.3248716798
 H,0,-2.5469960887,6.467071719,3.3108574373
 H,0,-3.9671213222,6.894301089,1.3127839283
 H,0,-3.8723137658,5.1898377278,0.8499783837
 C,0,0.1570064164,5.6450273422,2.7291390076

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H,0,0.3820738072,5.3527059385,3.7655590485
H,0,1.1120466282,5.7466202652,2.190753032
H,0,-0.3186783345,6.6348961123,2.7607699866
C,0,-2.6763249346,-0.4926344671,-1.7117526703
C,0,-3.9927677225,-0.9422538345,-1.5196370828
C,0,-2.2430132477,-0.2552595909,-3.0251677688
C,0,-4.8431582435,-1.1688101497,-2.6031976148
H,0,-4.3419280305,-1.1241828569,-0.5014127025
C,0,-3.0874926751,-0.4885478398,-4.1141310333
H,0,-1.2333889346,0.1251921808,-3.1936647002
C,0,-4.3899077371,-0.9512052399,-3.9079267394
H,0,-5.861363464,-1.5257892381,-2.4292767513
H,0,-2.7277420995,-0.3018450782,-5.1292518552
H,0,-5.0504035447,-1.1353622539,-4.7586052711
H,0,-3.8175225295,1.4339518103,-0.5408265218
H,0,-3.6367492322,1.7562932288,1.1941053635
H,0,-2.7441129178,2.7337802968,0.024635301

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INT-4- (S_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.87834445 a.u.
Zero-point correction = 0.969020 Hartree/Particle
Sum of electronic and thermal Free Energies = -3932.000971 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.614231514816 a.u.

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O,0,-0.6297096726,-3.837681476,-2.7185384922
O,0,-5.8959750363,0.615859033,0.2414850202
C,0,-2.357728596,1.1294393674,-0.2701456672
C,0,-1.4545140898,1.4878465252,-1.2971369874
C,0,-1.2789186128,0.2825339947,-2.0966102649
C,0,-2.2250366387,-0.7245716874,-1.6833221364
C,0,-2.8039316754,-0.2395279811,-0.4906978904
C,0,-2.5790077089,-1.9520566682,-2.4855985946
C,0,-2.6780371639,-3.2570215579,-1.7306047129
C,0,-1.5960786794,-4.1909586761,-1.8495365848
C,0,-1.6109706893,-5.3718954617,-1.1333688384
C,0,-2.6970391039,-5.6815137737,-0.2724990854
C,0,-2.7156346955,-6.8717719365,0.5059663469
C,0,-3.7805234893,-7.165173609,1.332363419
C,0,-4.8805543278,-6.2786985699,1.4180445193
C,0,-4.893301509,-5.1168292461,0.6728449297
C,0,-3.8115002769,-4.7859629939,-0.1867598847
C,0,-3.784631101,-3.5780093437,-0.9617254266
C,0,0.5133498229,-4.661016832,-2.8509869092
C,0,-3.7156333107,-1.005523871,0.4264684547
C,0,-4.9476896553,-1.4606011244,-0.3176620055
C,0,-4.9789250933,-2.6780909525,-0.9740525895
C,0,-6.1467537487,-3.0724689601,-1.7141528434
C,0,-6.2199005592,-4.3012642099,-2.4249109985
C,0,-7.3575738252,-4.6519427808,-3.1229240821
C,0,-8.4760128578,-3.7855138333,-3.1452170306
C,0,-8.4314209503,-2.5802705767,-2.4760008951
C,0,-7.2731313032,-2.1889859259,-1.7510574522
C,0,-7.2078568028,-0.9353961163,-1.0818367807
C,0,-6.0670408156,-0.5727468358,-0.3975461112
C,0,-6.942007115,1.5590401835,0.2138806927

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H,0,-2.7199628901,1.7623977778,0.5349921347
H,0,-0.6379768582,0.1967346928,-2.9719508403
H,0,-1.8398119298,-2.0614734537,-3.2863642773
H,0,-3.5509252432,-1.7422938771,-2.9645938192
H,0,-0.7863875067,-6.0795140373,-1.2070375456
H,0,-1.8642591976,-7.5542332973,0.4376866172
H,0,-3.7763677031,-8.0838686878,1.9241966598
H,0,-5.719632795,-6.5146784106,2.0766103104
H,0,-5.740109749,-4.432316202,0.7415869749
H,0,1.0647609593,-4.7150244468,-1.9024685542
H,0,1.1628774379,-4.1708751444,-3.5850954173
H,0,0.2339827482,-5.6681338197,-3.2092706053
H,0,-3.9916174557,-0.3706892785,1.27641456
H,0,-3.1794232823,-1.8832680793,0.8131970723
H,0,-5.3593894971,-4.97033789,-2.4106817313
H,0,-7.3950520229,-5.6016865042,-3.6612779118
H,0,-9.3739738266,-4.0714468236,-3.6983151568
H,0,-9.2898288429,-1.9036335942,-2.4972887847
H,0,-8.0715554191,-0.2736058686,-1.1372129695
H,0,-7.1850976303,1.8658213262,-0.8189637351
H,0,-6.5913943918,2.434516898,0.7760876879
H,0,-7.8573549207,1.1661834079,0.6911228564
C,0,-0.9115842477,2.8595302541,-1.63630393
C,0,-0.6639126858,3.6783568108,-0.3495597994
C,0,0.4080900432,2.7259136211,-2.4308922021
C,0,0.0411030343,5.0144078897,-0.5949370622
H,0,-0.03055585,3.0682566357,0.3105521714
H,0,-1.6206753806,3.8445832882,0.173253695
C,0,1.1413707118,4.0524833782,-2.648370711
H,0,1.0696524645,2.0411483695,-1.8854471833
H,0,0.205192688,2.2560668738,-3.4065644432
C,0,1.3645030088,4.8006888557,-1.332208378
H,0,0.2149155674,5.5164976503,0.3711513349
H,0,-0.6046951123,5.6917064867,-1.1809728199
H,0,2.1057640901,3.8467505711,-3.1400467643
H,0,0.5718847302,4.6974072639,-3.3409832959
H,0,1.8674259029,5.7644381569,-1.5163776099
H,0,2.0381463094,4.2071696845,-0.689831093
C,0,-1.997835557,3.5325005305,-2.5075091848
H,0,-2.2043064499,2.9313377367,-3.4066402659
H,0,-2.9393689593,3.6381505422,-1.9466673737
H,0,-1.684471662,4.5330273501,-2.8381643782
C,0,5.9783365647,0.1183715736,0.6062954986
C,0,6.6328406949,0.0272088139,-0.6594501411
C,0,6.2413775799,-1.2049034129,-1.2694866003
C,0,5.3448457726,-1.8746554843,-0.3839740152
C,0,5.182224091,-1.0578417063,0.776418899
H,0,6.0585933331,0.9478352495,1.3061889105
H,0,7.2942401934,0.7756775361,-1.0925779325
H,0,6.5400329357,-1.5537440453,-2.2564801684
H,0,4.7973233722,-2.7892896198,-0.6022319756
H,0,4.5334801063,-1.2771410673,1.6229048805
Fe,0,4.5768057763,-0.038205178,-0.9088893708
C,0,3.3673416294,-0.1569484827,-2.5602774013
C,0,3.9896956991,1.1230510976,-2.5130006165
C,0,2.5946711279,-0.3310384207,-1.365714496
H,0,3.4776093727,-0.91439656,-3.3323735032
C,0,3.6260913128,1.744170287,-1.2810703953

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H,0,4.655852859,1.5404828141,-3.2659789682
C,0,2.7405745108,0.8666110473,-0.5662816304
H,0,3.9550454989,2.7235587309,-0.9408009343
C,0,1.95169919,-1.6541647425,-1.0642954959
O,0,2.4440647862,-2.6959661965,-1.5043656481
N,0,0.832396253,-1.6073835861,-0.2957403038
O,0,0.2021013167,-2.8588209956,-0.1567538146
C,0,0.668301594,-3.5558025703,0.98096534
H,0,0.4517630919,-3.0045542035,1.9117815573
H,0,0.1167298183,-4.5069465896,0.9926819473
H,0,1.7501697039,-3.756711898,0.9052326279
Rh,0,-0.5599389971,-0.1490171904,-0.136024918
C,0,0.1772640532,0.6918382876,2.2898077007
C,0,-0.7829356325,1.6178094958,2.7601456479
C,0,0.4721128088,-0.4241436357,3.1062164033
C,0,-1.4106242334,1.434957679,3.9896486712
H,0,-1.0184815708,2.4902164296,2.1517793757
C,0,-0.1676641073,-0.6106423735,4.333244231
H,0,1.2202679912,-1.1353535002,2.7542370973
C,0,-1.1136817431,0.3154727071,4.7785270077
H,0,-2.138815368,2.1708974395,4.339819485
H,0,0.0769312872,-1.4826223242,4.9447860762
H,0,-1.6162765979,0.1712588861,5.737781987
C,0,0.8377079113,0.7876169833,0.9713468624
C,0,2.1154513893,1.1360255531,0.7399357697
C,0,2.9600350823,1.8161395398,1.793226778
H,0,3.7770556648,1.16016048,2.1320769661
H,0,3.4335955931,2.7278276277,1.3923220118
H,0,2.3595938659,2.1018890534,2.6675614269

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INT-4' - (S_p)

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.88669211 a.u.
Zero-point correction = 0.968976 Hartree/Particle
Sum of electronic and thermal Free Energies = -3932.006881 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.623558843302 a.u.

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O,0,0.0134737021,-2.2869079588,-4.1668825174
O,0,-4.9605743382,1.8833113863,-0.6120171162
C,0,-1.2958032285,2.0332076367,-0.9688914365
C,0,-0.328444982,2.4548818877,-1.9133932227
C,0,-0.4664745929,1.5636916596,-3.0627925746
C,0,-1.4518909955,0.6068595677,-2.824806351
C,0,-1.9112414464,0.8142334964,-1.4457788837
C,0,-1.9499608881,-0.4053566541,-3.8225715461
C,0,-2.1177739718,-1.8079160752,-3.2851694507
C,0,-1.0605480108,-2.7528239797,-3.476738017
C,0,-1.1621163796,-4.0340438647,-2.979730502
C,0,-2.3040217926,-4.4244274073,-2.2352088031
C,0,-2.3995952529,-5.7155326972,-1.6482940824
C,0,-3.5002932221,-6.0768384402,-0.8991732253
C,0,-4.5611653032,-5.1593564921,-0.7054132503
C,0,-4.4986507015,-3.8990071182,-1.2650809961
C,0,-3.3768740142,-3.4970690281,-2.038881819
C,0,-3.261964361,-2.1848586786,-2.6010008096
C,0,1.0463356478,-3.1950948526,-4.5031392197

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C,0,-2.9668211081,0.0119675492,-0.732643648
 C,0,-4.220939166,-0.1360086016,-1.5608131533
 C,0,-4.3715396285,-1.1955095529,-2.4400324801
 C,0,-5.5593335553,-1.3167526845,-3.2372179218
 C,0,-5.7485625939,-2.3779298344,-4.1638250523
 C,0,-6.9037725596,-2.4687861697,-4.9132013623
 C,0,-7.922928164,-1.4968813289,-4.7723108649
 C,0,-7.7640992129,-0.4488146255,-3.8897065776
 C,0,-6.5850350221,-0.3259521394,-3.1052023137
 C,0,-6.3990893447,0.7637124984,-2.2103588654
 C,0,-5.2398695647,0.8636830943,-1.4685357888
 C,0,-5.9058779004,2.9150184635,-0.4528031459
 H,0,-1.5133540386,2.4942473264,-0.0096507913
 H,0,0.137545733,1.6091680143,-3.9673818132
 H,0,-1.2540814331,-0.4202724083,-4.6699083491
 H,0,-2.922489191,-0.0482036531,-4.1985835989
 H,0,-0.3424467941,-4.7419210859,-3.0824246004
 H,0,-1.574112881,-6.4170112065,-1.793730564
 H,0,-3.5545443343,-7.0720041785,-0.4507797884
 H,0,-5.4294357293,-5.4498688726,-0.1091959042
 H,0,-5.3134962463,-3.1901196578,-1.1101788747
 H,0,1.5424823881,-3.5791201008,-3.598077982
 H,0,1.7646046536,-2.6303518744,-5.1127302475
 H,0,0.6534489939,-4.036425544,-5.1013896911
 H,0,-3.1969895127,0.5029717724,0.2209509769
 H,0,-2.554179859,-0.9830282139,-0.5169636558
 H,0,-4.9633679727,-3.1267159753,-4.2722697535
 H,0,-7.0329487556,-3.2932216929,-5.6181720772
 H,0,-8.8355496189,-1.5767348119,-5.3680275796
 H,0,-8.5460427126,0.3078139556,-3.7831558165
 H,0,-7.1861586521,1.5136554104,-2.1381132962
 H,0,-6.0973129083,3.4419086529,-1.4046279288
 H,0,-5.4806678771,3.6231688431,0.2705934327
 H,0,-6.865319432,2.5318383204,-0.0618880306
 C,0,0.5480403098,3.6894391734,-1.8408163429
 C,0,0.8610427093,4.0183242443,-0.3605818527
 C,0,1.8733361327,3.4206187222,-2.594484306
 C,0,1.906001511,5.1221936627,-0.1803606454
 H,0,1.2291622204,3.098463512,0.1220766328
 H,0,-0.069753117,4.2969219904,0.160131312
 C,0,2.9336671675,4.5085234192,-2.3993231983
 H,0,2.2782687987,2.4610206471,-2.2391267057
 H,0,1.6688068005,3.2942770559,-3.6699527511
 C,0,3.2021379268,4.7783494209,-0.9168214088
 H,0,2.1016726124,5.2664806691,0.8950125791
 H,0,1.5163701488,6.085578007,-0.5533481649
 H,0,3.8628271114,4.2032394501,-2.9085978332
 H,0,2.6122830129,5.4459459857,-2.8864059174
 H,0,3.9435874384,5.5855925387,-0.7985579056
 H,0,3.6438221485,3.8751686927,-0.4588385761
 C,0,-0.2294648678,4.8458701393,-2.5051994356
 H,0,-0.4826489931,4.5952052572,-3.5472262928
 H,0,-1.1702748744,5.0397718868,-1.9668696099
 H,0,0.3525961615,5.7789451634,-2.5168127111
 C,0,5.500543201,-1.4977863881,0.7947441376
 C,0,6.3190938682,-1.4325223376,-0.3736966144
 C,0,5.8846748825,-2.4534995856,-1.2754682945
 C,0,4.7955007655,-3.1474040546,-0.6678403946

C,0,4.5596573561,-2.555773013,0.609308252
 H,0,5.5581647036,-0.8380557289,1.6572934105
 H,0,7.1158957833,-0.7133925101,-0.5565104096
 H,0,6.2868665206,-2.6402362221,-2.2699578762
 H,0,4.177648253,-3.9198617472,-1.1191038374
 H,0,3.7652571176,-2.833474257,1.2977760344
 Fe,0,4.3315061077,-1.1499761017,-0.8817802082
 C,0,3.2142180164,-0.8677046093,-2.5749125878
 C,0,4.0839479128,0.2428912831,-2.3824676708
 C,0,2.3624931216,-0.9851055134,-1.4277357955
 H,0,3.2020615896,-1.5434240505,-3.4253674958
 C,0,3.8033361924,0.8214354942,-1.1090605581
 H,0,4.8564256223,0.5749635886,-3.0738315187
 C,0,2.7274601551,0.0973749415,-0.4925910234
 H,0,4.3218492837,1.6685187336,-0.6688275141
 C,0,1.3993350598,-2.1262814449,-1.1747133663
 O,0,1.6872664143,-3.319387549,-1.3188746746
 N,0,0.2409859785,-1.5892844347,-0.7846018235
 O,0,-0.8169308182,-2.4015880716,-0.4241642138
 C,0,-0.5639776135,-3.1299338641,0.767951168
 H,0,-0.3482245366,-2.4478436995,1.6095122593
 H,0,-1.4855950212,-3.6945942056,0.9683254958
 H,0,0.2766708298,-3.8261757104,0.6237040099
 Rh,0,0.1444864541,0.4249115957,-1.0981596411
 C,0,0.7612543706,0.5006730018,0.8134993995
 C,0,2.0995761063,0.3533426217,0.8370147621
 C,0,2.9543698518,0.4143639082,2.0552595048
 C,0,2.8862907047,-0.6053681577,3.0185158453
 C,0,3.8640055978,1.4650249764,2.2585464758
 C,0,3.7157097906,-0.587467993,4.1421850484
 H,0,2.184218367,-1.4279187238,2.864652139
 C,0,4.6979732161,1.4837620424,3.3786439746
 H,0,3.9127463526,2.2786598363,1.5321873877
 C,0,4.6302648503,0.4542644051,4.3225589087
 H,0,3.6544482937,-1.3950916098,4.8758490275
 H,0,5.4019547616,2.3080814569,3.5178090185
 H,0,5.2848228187,0.4662606622,5.1972688207
 C,0,-0.1545980506,0.7052720638,1.9733002168
 H,0,0.3669145632,0.6200607848,2.9401360049
 H,0,-0.6291992318,1.7001322489,1.9327129713
 H,0,-0.9736431191,-0.032719745,1.9513160899

INT-5

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
 SCF Done: E(RB3LYP) = -4396.40276053 a.u.
 Zero-point correction = 1.185616 Hartree/Particle
 Sum of electronic and thermal Free Energies = -4395.316970 a.u.
 Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
 FINAL SINGLE POINT ENERGY = -4397.264672397457 a.u.

O,0,2.9787385221,-0.0957754049,3.5245636989
 O,0,0.2495183285,3.1049022971,-2.572133986
 C,0,-1.1785650903,1.8325016517,0.1148590582
 C,0,-1.5720350355,2.4003431139,1.3429799373
 C,0,-0.3818519536,2.4070756635,2.1936732559
 C,0,0.7068576419,1.8875730833,1.4911321683
 C,0,0.194842257,1.4100913852,0.2024963851

C,0,2.1378994336,1.9864126025,1.9540274734
 C,0,3.1291566555,0.9710280403,1.4328016401
 C,0,3.5427549202,-0.0940807485,2.2942968092
 C,0,4.4636148481,-1.0286320558,1.8645324127
 C,0,4.9966410473,-0.9649439978,0.553666065
 C,0,5.8881619564,-1.9608657887,0.0661115159
 C,0,6.3571119942,-1.9200521266,-1.2299028885
 C,0,5.9581392925,-0.8751227379,-2.0991090669
 C,0,5.1011044348,0.1095253369,-1.6525455269
 C,0,4.5989765722,0.0946836114,-0.322853775
 C,0,3.6705142851,1.0723904206,0.1593387265
 C,0,3.2682594661,-1.1717371032,4.3992331215
 C,0,1.033459692,1.0124687473,-0.9781952111
 C,0,1.9769170287,2.1454263907,-1.3010936782
 C,0,3.2408202782,2.1869629444,-0.7381277896
 C,0,4.1175754614,3.2943392883,-0.9904243774
 C,0,5.4172942249,3.3814667788,-0.4222716504
 C,0,6.2363422164,4.4604916548,-0.6861001293
 C,0,5.7889561612,5.5046213761,-1.5302774811
 C,0,4.5288793785,5.4527715772,-2.0895834676
 C,0,3.6604988505,4.3565322588,-1.8355761367
 C,0,2.3509654772,4.3014969661,-2.3890861253
 C,0,1.5254221878,3.2296866128,-2.1170182257
 C,0,-0.2936230033,4.1331220131,-3.3660097883
 H,0,-1.7952934777,1.6991358915,-0.7679342154
 H,0,-0.3352990124,2.7922938148,3.2111600017
 H,0,2.1496269266,1.9749538473,3.0507876999
 H,0,2.479590819,2.9875202525,1.6388464509
 H,0,4.7538210656,-1.8609011714,2.5015324715
 H,0,6.1820431399,-2.7717775363,0.7372254328
 H,0,7.0340882743,-2.6978926134,-1.5916013276
 H,0,6.3280231385,-0.8521623635,-3.126792017
 H,0,4.787517176,0.9083609512,-2.325653023
 H,0,2.9846154995,-2.1261514923,3.931614914
 H,0,2.662999504,-1.0055868333,5.29973154
 H,0,4.3374097078,-1.1758337158,4.6778287676
 H,0,0.3784762924,0.788428986,-1.8266981708
 H,0,1.6086877654,0.1128530224,-0.7569807566
 H,0,5.7615739332,2.5755726184,0.2270115448
 H,0,7.2335126687,4.5097807797,-0.2426968144
 H,0,6.4439661447,6.3547566184,-1.7360404213
 H,0,4.1782008132,6.260372818,-2.7377436073
 H,0,2.0207148926,5.1274241936,-3.018399385
 H,0,-0.311964409,5.0967999489,-2.8262354365
 H,0,-1.3230861695,3.8355286675,-3.605412293
 H,0,0.2717228856,4.2649424485,-4.3057154417
 C,0,-2.8554763933,3.1589395525,1.6379965563
 C,0,-3.7661680336,3.1772856392,0.3906259182
 C,0,-3.6281624431,2.5015699029,2.8016812193
 C,0,-5.1379897216,3.8131977636,0.6414864673
 H,0,-3.9221422572,2.1386131159,0.0703764195
 H,0,-3.2495647526,3.6957737932,-0.4344161401
 C,0,-4.9851623083,3.1527102567,3.0786515817
 H,0,-3.7783647719,1.4414391011,2.5518077815
 H,0,-3.0017952152,2.5210080178,3.7059851363
 C,0,-5.8592936486,3.155678938,1.822340651
 H,0,-5.749433244,3.7252236274,-0.2720143326
 H,0,-5.0290781131,4.895286383,0.8299533343

H,0,-5.4923275118,2.6047843104,3.8897267367
H,0,-4.8487207871,4.1847641136,3.4460922277
H,0,-6.8175511674,3.664742351,2.018482406
H,0,-6.0992665399,2.1120459569,1.5600171842
C,0,-2.4341508032,4.6005039765,2.0031539111
H,0,-1.8459164264,4.6231332583,2.9327764065
H,0,-1.8176812181,5.037609646,1.2022384838
H,0,-3.3056730116,5.2524980874,2.1504451208
C,0,-0.2172807266,-5.5279863941,-1.7466050981
C,0,1.1284597872,-5.6242758957,-2.2136480384
C,0,1.9940501418,-5.5498344995,-1.0784929659
C,0,1.1853923989,-5.4035083018,0.0882505471
C,0,-0.1828838699,-5.3892821747,-0.3235461086
H,0,-1.1092505938,-5.5436735963,-2.3701884261
H,0,1.4398599674,-5.7153901337,-3.2528539261
H,0,3.0823727201,-5.554376915,-1.1010261784
H,0,1.5556788136,-5.2213971801,1.0948106329
H,0,-1.0452698478,-5.2555549961,0.3275570051
Fe,0,0.8543218885,-3.8366799543,-1.2005231465
C,0,2.1514806348,-2.2928454152,-0.9243614503
C,0,1.7006284662,-2.2919161775,-2.2735270333
C,0,1.0078217932,-2.1298709885,-0.0724385793
H,0,3.1715395772,-2.4096090461,-0.5747837021
C,0,0.2798499478,-2.161924244,-2.2619991285
H,0,2.3284524267,-2.4022461563,-3.1554648256
C,0,-0.1687738552,-2.035726487,-0.9013236881
H,0,-0.3640227363,-2.1553629137,-3.1387852127
C,0,1.1351595507,-2.1832089476,1.4083635443
O,0,1.9704687331,-2.9218930603,1.9488258721
N,0,0.2892285958,-1.3772630494,2.085714178
O,0,0.4454277544,-1.5261674037,3.4850708889
C,0,-0.1745887744,-2.716840465,3.9646966021
H,0,-1.2295686067,-2.7527065323,3.6508463003
H,0,-0.1067683866,-2.6764953142,5.0615758626
H,0,0.3702589552,-3.5928700427,3.5869637977
Rh,0,-0.9217854515,0.2169209867,1.5989876013
C,0,-3.4859620562,-0.9393535683,0.7369787048
C,0,-4.310663968,-0.2744748269,-0.1918936389
C,0,-4.0985872954,-1.4894405658,1.8773445807
C,0,-5.6857317941,-0.1543142392,0.0115592714
H,0,-3.8561499747,0.1302532004,-1.0987359731
C,0,-5.4728612974,-1.3645852641,2.0878220964
H,0,-3.4815797297,-2.0222269157,2.5988178376
C,0,-6.2742498691,-0.6922889185,1.1600242171
H,0,-6.3009638679,0.3629000225,-0.7292439869
H,0,-5.9242858043,-1.8030572093,2.9815155349
H,0,-7.3498491177,-0.5961596644,1.3259801692
C,0,-2.0318608005,-1.0819824259,0.4774929514
C,0,-1.5876512793,-1.8896044826,-0.5136455077
C,0,-2.5523616316,-2.6758128321,-1.3874945923
H,0,-2.158508961,-3.6818488997,-1.5796329945
H,0,-2.6845209518,-2.1924849113,-2.3716946442
H,0,-3.5458189686,-2.7653722147,-0.9330740499
C,0,-2.598219186,1.5318494655,6.5005233312
C,0,-3.662962939,1.7935150062,7.5694348606
C,0,-5.0753971481,1.5932636513,7.0136410048
C,0,-5.2381115445,0.1944031199,6.4120050149
C,0,-4.1788667215,-0.087921706,5.3423389526


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C,0,-2.7373445964,0.1307187012,5.8436021075
H,0,-5.8269358187,1.7641425599,7.8016395992
H,0,-3.5064458195,1.120784516,8.4302840806
H,0,-3.5422002324,2.8181962629,7.9574490833
H,0,-2.6963666629,2.2990038008,5.7141836982
H,0,-1.5854060385,1.6378328424,6.9169540806
H,0,-5.1794999304,-0.5580293515,7.2178149367
H,0,-6.239609661,0.0836005596,5.9651324695
H,0,-4.2781861044,-1.1157226148,4.9620748003
H,0,-4.35562332,0.5639242455,4.4772362634
H,0,-5.2646964725,2.3492229085,6.2302181088
C,0,-2.3276056395,-0.9783311501,6.8375182667
H,0,-2.3694253963,-1.9667007286,6.3535185727
H,0,-1.3055263966,-0.8160016228,7.2062087294
H,0,-3.0068844178,-1.0036841499,7.6999204205
C,0,-1.7584588249,0.054553412,4.676050575
O,0,-2.112252874,-0.1956594363,3.5240045556
O,0,-0.5010439206,0.2419030202,5.0120956475
H,0,0.061997249,-0.2336220837,4.3160105527

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TS-4

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4396.36259366 a.u.
Imaginary frequency = -91.4668 cm-1
Zero-point correction = 1.182321 Hartree/Particle
Sum of electronic and thermal Free Energies = -4395.281709 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4397.234463494110 a.u.

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O,0,2.1432267322,-0.0331854604,3.8258516172
O,0,1.5851974058,3.2323733531,-2.9186161017
C,0,-0.7246683005,1.9217996554,-0.9569967955
C,0,-1.53679363,2.4260759275,0.0870120367
C,0,-0.7979759618,2.2304669454,1.2968012342
C,0,0.5155024868,1.7410721614,0.9843622304
C,0,0.5408011789,1.4703847435,-0.4211210199
C,0,1.6555823565,1.8509694291,1.9600102276
C,0,2.8607141758,0.9488524963,1.826382403
C,0,3.0651486486,-0.0369550947,2.8494562754
C,0,4.165706693,-0.8710165762,2.8118039163
C,0,5.0940700076,-0.7887571897,1.7431611947
C,0,6.1881839809,-1.691334714,1.635975973
C,0,7.0636604063,-1.6240679108,0.572430104
C,0,6.8893792048,-0.6421505053,-0.4328173276
C,0,5.8442604583,0.2551406141,-0.349964291
C,0,4.9214443245,0.2074635615,0.7292772638
C,0,3.8072132282,1.1058155839,0.8251491003
C,0,2.1722803794,-1.0261310718,4.8312358181
C,0,1.7492108604,1.0934314054,-1.2271332382
C,0,2.7394869301,2.2265433502,-1.1363032307
C,0,3.6994973774,2.2428570949,-0.1405931052
C,0,4.5864113416,3.366282455,-0.0065226285
C,0,5.5737736547,3.4427012817,1.0131614427
C,0,6.4098831118,4.53617531,1.1122445766
C,0,6.2950370357,5.6073246593,0.1949658073
C,0,5.3392936607,5.5681452909,-0.7988033276
C,0,4.4603718829,4.4583176375,-0.9248355887

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C,0,3.4534682611,4.4231255941,-1.9296771795
 C,0,2.6033379692,3.3415358028,-2.0214838938
 C,0,1.3510197279,4.2951947503,-3.8135320622
 H,0,-0.9792808067,1.9083564494,-2.0101684626
 H,0,-1.1434754451,2.4675079872,2.2989721407
 H,0,1.2495174534,1.7530043899,2.9728443548
 H,0,1.9947318914,2.8979129535,1.847299704
 H,0,4.3162948624,-1.6261281657,3.5818057546
 H,0,6.3162390732,-2.4516249638,2.4109231335
 H,0,7.8946724227,-2.3303612516,0.5028955719
 H,0,7.5836402445,-0.5964073583,-1.2749910626
 H,0,5.7076094632,1.0085713673,-1.1268482923
 H,0,2.1426768322,-2.0262995398,4.3780072479
 H,0,1.2626197495,-0.8750776099,5.4228316772
 H,0,3.0668426539,-0.9136327996,5.4703459098
 H,0,1.4511069347,0.9047913031,-2.2639628159
 H,0,2.198670075,0.1796254613,-0.831412271
 H,0,5.6651279141,2.6192025105,1.7216786534
 H,0,7.1634111518,4.5756030333,1.9021000224
 H,0,6.9626815203,6.4682548734,0.2785088297
 H,0,5.2415207522,6.3969158829,-1.5049974186
 H,0,3.3677402196,5.2729774587,-2.6060995195
 H,0,1.1184679384,5.2325188741,-3.2776773677
 H,0,0.4862378497,4.0065343506,-4.4254563488
 H,0,2.2184122881,4.4699097763,-4.4743466601
 C,0,-2.8578866653,3.1517813097,-0.0713358048
 C,0,-3.8327562686,2.3238485583,-0.9406481862
 C,0,-3.5010258834,3.4240549423,1.3079205526
 C,0,-5.2292214021,2.9400761364,-1.045751794
 H,0,-3.9110709457,1.3199038297,-0.5018369477
 H,0,-3.4093519714,2.1851826967,-1.9442137266
 C,0,-4.9045435043,4.0334196005,1.2126643028
 H,0,-3.5539083964,2.47865296,1.8679939176
 H,0,-2.8473830626,4.0918951999,1.8934249767
 C,0,-5.8350393181,3.1902124633,0.3366659424
 H,0,-5.8715441242,2.2617895535,-1.6307891475
 H,0,-5.1901394259,3.8880526895,-1.6108278651
 H,0,-5.3232824825,4.1323452383,2.2276700399
 H,0,-4.8475748379,5.0582400158,0.8062366539
 H,0,-6.8223512318,3.6730345098,0.248241016
 H,0,-6.0071079948,2.2195986266,0.8296693414
 C,0,-2.5066796047,4.4877535967,-0.7697111
 H,0,-1.7736227134,5.0572777625,-0.1770477876
 H,0,-2.0723841777,4.3066895428,-1.7649409478
 H,0,-3.3962712749,5.1186683778,-0.9013767493
 C,0,0.944610167,-5.5768284157,-1.8954967435
 C,0,2.2300553088,-5.9118132436,-1.3710684042
 C,0,2.1827418129,-5.7484453861,0.0483036674
 C,0,0.8709345326,-5.3093214546,0.4001035269
 C,0,0.1041000717,-5.2011533297,-0.8010746748
 H,0,0.6613268696,-5.5925156731,-2.9463699484
 H,0,3.0984888609,-6.2172761992,-1.9521002572
 H,0,3.0117655324,-5.8935646093,0.7384693297
 H,0,0.5411770558,-5.0315616815,1.399686995
 H,0,-0.9243234481,-4.8505766464,-0.8711475966
 Fe,0,1.7432118789,-3.9586345241,-0.8790344108
 C,0,2.8775388793,-2.5414456858,0.051902146
 C,0,3.3311600853,-2.6759965183,-1.2847788729

C,0,1.4971448037,-2.148717918,0.0204271524
 H,0,3.4392937158,-2.7075605127,0.9624167342
 C,0,2.2330416589,-2.4079001972,-2.1510881955
 H,0,4.3366056832,-2.9577390039,-1.5901896535
 C,0,1.0810245693,-2.0577860553,-1.3603418723
 H,0,2.2616942798,-2.4522387339,-3.2366739176
 C,0,0.7511103058,-2.0149968113,1.3092163346
 O,0,1.2291633253,-2.4772041819,2.3401461912
 N,0,-0.4787949643,-1.4474416467,1.1815825335
 O,0,-0.7534396164,-1.0239413564,3.6658317368
 C,0,-1.2549161489,-2.2464351294,4.1369569114
 H,0,-1.8608186772,-2.7736494883,3.3780594579
 H,0,-1.877201984,-2.1174863633,5.0457544344
 H,0,-0.4015629,-2.8930990298,4.3844308287
 Rh,0,-1.0194753793,0.1394865594,0.3973986022
 C,0,-2.403110757,-0.6105984517,-2.1960049354
 C,0,-2.3423003599,0.2056083028,-3.3439492312
 C,0,-3.6396764073,-1.1812774535,-1.8562737431
 C,0,-3.4820115254,0.4704821449,-4.1025798801
 H,0,-1.3780454943,0.6151419294,-3.6539953463
 C,0,-4.7834722335,-0.9094877724,-2.608772852
 H,0,-3.6868048008,-1.8319136832,-0.9880265752
 C,0,-4.7141785001,-0.0753674651,-3.7279093104
 H,0,-3.4093722484,1.1041667087,-4.9900716967
 H,0,-5.7372502869,-1.3565312629,-2.317869607
 H,0,-5.6114924703,0.1373890265,-4.3138162489
 C,0,-1.1704846871,-0.9151176469,-1.4381060554
 C,0,-0.2250674781,-1.728355625,-1.9549723991
 C,0,-0.4416165171,-2.3643511712,-3.3230771161
 H,0,-0.042033724,-3.3867058352,-3.3275736654
 H,0,0.0875939745,-1.8019263872,-4.1109667618
 H,0,-1.5006410235,-2.3990939733,-3.5995375521
 C,0,-5.6343475193,0.2749300436,3.172451367
 C,0,-7.1193604128,-0.025605802,3.3925958227
 C,0,-7.8720114768,-0.1262623169,2.0630480014
 C,0,-7.2246114805,-1.169297693,1.1489602141
 C,0,-5.7329464841,-0.8929999461,0.9275389659
 C,0,-4.9327183194,-0.7393059178,2.2375819922
 H,0,-8.9339412933,-0.3691349352,2.2346921556
 H,0,-7.2364250869,-0.9705335269,3.9516025164
 H,0,-7.5622028143,0.7601545995,4.0271213454
 H,0,-5.5410967134,1.2797417749,2.7278767712
 H,0,-5.0886460381,0.3179211809,4.1252950534
 H,0,-7.3598781111,-2.171871467,1.591212062
 H,0,-7.7379366567,-1.1973067687,0.1729439042
 H,0,-5.290402441,-1.697297058,0.3253876219
 H,0,-5.6219976767,0.026369095,0.3311003112
 H,0,-7.8532359288,0.8583988359,1.5612492103
 C,0,-4.7769284937,-2.1064773364,2.9361956101
 H,0,-4.2197373049,-2.8059604885,2.2942115874
 H,0,-4.2288507776,-1.9966890245,3.8824747896
 H,0,-5.7542067776,-2.5578415157,3.1595321591
 C,0,-3.492319654,-0.2377771877,1.9769091607
 O,0,-3.0028560985,-0.492224901,0.8192432128
 O,0,-2.889442649,0.3503639922,2.8898240769
 H,0,-1.5107938031,-0.4414960783,3.4280496206

INT-6

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4280.69877755 a.u.
Zero-point correction = 1.129196 Hartree/Particle
Sum of electronic and thermal Free Energies = -4279.667511 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4281.527825642256 a.u.

O,0,1.4529220485,-0.1678680442,3.7828369093
O,0,1.9082095526,3.7027126316,-2.6606057039
C,0,-0.8146235346,2.3903608078,-1.0183332068
C,0,-1.6878075748,2.7778975442,0.0252300566
C,0,-1.0287577441,2.4203908585,1.2425101017
C,0,0.292712575,1.9217945744,0.9576242021
C,0,0.400904526,1.8258144049,-0.4637235185
C,0,1.3760183768,1.8719798487,2.0010965781
C,0,2.449477652,0.8165792175,1.8973476871
C,0,2.4375574999,-0.2441341102,2.8620786966
C,0,3.4105200184,-1.2228835758,2.8380768829
C,0,4.4108919386,-1.2184885373,1.8328225992
C,0,5.3731349843,-2.2612781637,1.7368329971
C,0,6.3212261324,-2.2626447752,0.735795949
C,0,6.3562924709,-1.2127695133,-0.2139059455
C,0,5.445402998,-0.1795311488,-0.1379282907
C,0,4.4519773746,-0.1533269743,0.8776281717
C,0,3.4780103362,0.894777547,0.9697052929
C,0,1.3505934071,-1.1738733947,4.7723325529
C,0,1.6208816273,1.4039617621,-1.2309641121
C,0,2.7520085264,2.3536355981,-0.9330072442
C,0,3.6229871937,2.1141233799,0.1144220888
C,0,4.6611138004,3.060832087,0.4235254943
C,0,5.5654754986,2.8788088769,1.5051616709
C,0,6.5510425128,3.8072376628,1.7719948377
C,0,6.6766274142,4.9653070911,0.9690379612
C,0,5.8066513822,5.177319351,-0.0799540215
C,0,4.7781598947,4.2425541277,-0.3776425111
C,0,3.8584937644,4.4708851834,-1.4390095039
C,0,2.8587367473,3.5577259039,-1.6978203314
C,0,1.9242899299,4.8609388745,-3.4639506456
H,0,-1.0147956845,2.4924917905,-2.07741515
H,0,-1.4301944305,2.5484637579,2.2452130262
H,0,0.9019385241,1.8039202002,2.9861852639
H,0,1.8551789971,2.8664768089,1.9410973044
H,0,3.4025300119,-2.0343076804,3.5639415486
H,0,5.3394445606,-3.0730052319,2.468261055
H,0,7.0484554251,-3.075825936,0.6724551452
H,0,7.1065451739,-1.2226413802,-1.0077740429
H,0,5.470914822,0.6285399963,-0.8704155286
H,0,1.2035763382,-2.1576897623,4.3061460291
H,0,0.4671411469,-0.9237608331,5.3731744061
H,0,2.2446116963,-1.1816498646,5.4210486054
H,0,1.3886056319,1.393732905,-2.3008826802
H,0,1.9061835177,0.3875909119,-0.9394304998
H,0,5.4729842922,1.9885978106,2.1272953801
H,0,7.2371535029,3.6478735264,2.6068815473
H,0,7.4615497741,5.6940562196,1.1850607725
H,0,5.8938246593,6.0747555133,-0.6980312336
H,0,3.9590183487,5.3849301199,-2.0233669084

H,0,1.8050544315,5.7764021489,-2.8578625729
 H,0,1.0768826848,4.7748227734,-4.1565708775
 H,0,2.8600182744,4.9393180476,-4.0450911697
 C,0,-3.0430901154,3.44159739,-0.0997951591
 C,0,-3.7548893188,2.9428227073,-1.3785211044
 C,0,-3.9104394155,3.1005154167,1.1376566903
 C,0,-5.2078984311,3.4045610383,-1.4973034315
 H,0,-3.7444856648,1.8456052418,-1.360275271
 H,0,-3.1879742643,3.2533146829,-2.2693380343
 C,0,-5.3678566716,3.5536442977,1.0092647294
 H,0,-3.8907478123,2.007842993,1.2630652158
 H,0,-3.4624794829,3.5479362631,2.0407140287
 C,0,-6.0132637663,2.9974951887,-0.261986477
 H,0,-5.64355598,2.9613798366,-2.4072030998
 H,0,-5.2613719707,4.5001990428,-1.6295862275
 H,0,-5.9252315784,3.2223725948,1.9009415245
 H,0,-5.4307376544,4.6565283846,1.0012891096
 H,0,-7.0579344859,3.3398553726,-0.3468217758
 H,0,-6.0395261846,1.8951551397,-0.1995316104
 C,0,-2.7682564445,4.960389381,-0.1783466517
 H,0,-2.2387909253,5.3126110031,0.7209756827
 H,0,-2.1478251217,5.2006161866,-1.05601922
 H,0,-3.7051188428,5.5288506183,-0.261897233
 C,0,-0.6261399315,-4.9352299775,-2.0305588734
 C,0,0.4998194641,-5.7887372515,-1.8209742548
 C,0,0.7065011705,-5.9000194813,-0.4108929884
 C,0,-0.2875701617,-5.1108254464,0.2437340477
 C,0,-1.1126601309,-4.5094927935,-0.7571731855
 H,0,-1.0335775345,-4.6379241714,-2.9947299843
 H,0,1.1030257167,-6.2579109317,-2.5963652197
 H,0,1.5030070659,-6.4593990962,0.0769446995
 H,0,-0.3649070365,-4.9346799523,1.3153693112
 H,0,-1.9338149494,-3.8125411535,-0.5798800977
 Fe,0,0.8531845092,-3.9203052784,-0.9858803672
 C,0,2.2628099315,-2.9440891096,0.1390728436
 C,0,2.8251653719,-3.2183135851,-1.1310382453
 C,0,1.0961587717,-2.1351839487,-0.0568780221
 H,0,2.6123949882,-3.285605486,1.106125988
 C,0,2.003010096,-2.6116105903,-2.1203583555
 H,0,3.7193916043,-3.8082732914,-1.3197292253
 C,0,0.9082525054,-1.9233081394,-1.4834771083
 H,0,2.1768250999,-2.6698353291,-3.1905667084
 C,0,0.1733428061,-1.8596357544,1.0541192356
 O,0,0.3398929662,-2.2729916591,2.2064320261
 N,0,-0.9667687754,-1.2215623434,0.7212935895
 Rh,0,-1.2538778142,0.4854119089,0.1162086467
 C,0,-2.1907893739,0.0869952415,-2.7339832712
 C,0,-1.8581900487,1.0075027151,-3.7494064136
 C,0,-3.5150945984,-0.3788292123,-2.6595245338
 C,0,-2.8227035101,1.4762103813,-4.640930812
 H,0,-0.8210059155,1.3351465552,-3.854428503
 C,0,-4.4770010722,0.0919395578,-3.5560001376
 H,0,-3.7700230938,-1.109066704,-1.8899599473
 C,0,-4.1435207792,1.0278774863,-4.5390545844
 H,0,-2.5415621784,2.1880500177,-5.4212363035
 H,0,-5.5019927879,-0.2799731798,-3.4819890831
 H,0,-4.9042428521,1.3975641695,-5.2309893927
 C,0,-1.1352330927,-0.4242528821,-1.830962373

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C,0,-0.1871263207,-1.2915132743,-2.2477272634
C,0,-0.197366732,-1.7156058394,-3.7141954289
H,0,0.0042645509,-2.7909352821,-3.799437431
H,0,0.588954601,-1.1859374754,-4.2781988873
H,0,-1.1550342099,-1.5054755972,-4.1987120019
C,0,-3.3699594945,-2.8975106453,2.544392988
C,0,-3.4720381187,-3.2220573531,4.036916794
C,0,-2.7608799975,-2.1610406884,4.8811418591
C,0,-3.3220817659,-0.7677732776,4.5840190192
C,0,-3.2197654124,-0.435804073,3.0906638791
C,0,-3.8951800359,-1.4865672403,2.1815454208
H,0,-2.8472233728,-2.3935870964,5.9563191851
H,0,-4.5302998258,-3.2893516232,4.3466514417
H,0,-3.0351080043,-4.2173003985,4.2250693613
H,0,-2.3097649721,-2.9457082204,2.2491377077
H,0,-3.901500155,-3.643372241,1.9361223668
H,0,-4.3729222598,-0.7157532873,4.9199977677
H,0,-2.778780216,-0.0027566122,5.165393237
H,0,-3.6444347275,0.5588981773,2.8879057578
H,0,-2.1526425922,-0.3850746784,2.8301706102
H,0,-1.6850063835,-2.1740965893,4.6308289753
C,0,-5.4313066063,-1.4127445981,2.3121309136
H,0,-5.7959681472,-0.4116446638,2.0295745632
H,0,-5.90346099,-2.1507953068,1.6468355174
H,0,-5.765598043,-1.6133011695,3.3404248276
C,0,-3.6008608001,-1.244353676,0.6797344924
O,0,-3.2679763654,-0.0191435521,0.3329652031
O,0,-3.7627167613,-2.1572889703,-0.1182222435
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TS-5

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4280.69699187 a.u.
Imaginary frequency = -116.3978 cm-1
Zero-point correction = 1.128784 Hartree/Particle
Sum of electronic and thermal Free Energies = -4279.664912 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4281.527018156072 a.u.
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O,0,-1.3247667215,1.2786304316,3.5875085128
O,0,-2.2822269967,-3.8144863244,-1.8407254157
C,0,0.5721211954,-2.6299291456,-0.3181725514
C,0,1.3138258202,-2.9358944815,0.8504091966
C,0,0.6717427489,-2.2314087818,1.9189241208
C,0,-0.5224156137,-1.591735877,1.4363649961
C,0,-0.5501259676,-1.7748123913,0.0192181127
C,0,-1.6134605862,-1.1187170781,2.3561191829
C,0,-2.4649122414,0.0550204787,1.9383113344
C,0,-2.2736150251,1.2976829813,2.6277302029
C,0,-3.0622532685,2.3912766895,2.3316417441
C,0,-4.0392979236,2.3177500026,1.3058267494
C,0,-4.8088441106,3.4529459513,0.9299473334
C,0,-5.7237375622,3.3815581608,-0.0992749615
C,0,-5.9170945745,2.1647491782,-0.7971424925
C,0,-5.1968645726,1.0420980462,-0.4443882319
C,0,-4.2438926069,1.0850972161,0.6085102364
C,0,-3.4685799464,-0.0601956281,0.9882537334
C,0,-1.0537519294,2.4630467122,4.3117431695

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C,0,-1.6478221752,-1.3357051508,-0.9078630895
 C,0,-2.939067598,-1.9997284704,-0.5021312673
 C,0,-3.7941562377,-1.3985920799,0.4044416686
 C,0,-4.9914451836,-2.0732330351,0.8290872558
 C,0,-5.8888683414,-1.5140345409,1.7792912754
 C,0,-7.0301389965,-2.1887275469,2.1624186553
 C,0,-7.3262889229,-3.4587326647,1.6136980098
 C,0,-6.4688977163,-4.0341780831,0.6994132926
 C,0,-5.283159324,-3.3670448775,0.2880820192
 C,0,-4.3789958334,-3.96844972,-0.6310848493
 C,0,-3.2265789414,-3.3088930238,-1.00203794
 C,0,-2.4697954686,-5.1038736397,-2.3784843097
 H,0,0.8068160065,-2.9663150587,-1.3218357298
 H,0,0.9933908616,-2.219173028,2.9570289526
 H,0,-1.1702457272,-0.9091302197,3.3358027963
 H,0,-2.2700587652,-1.9994348218,2.4795398784
 H,0,-2.923242025,3.3370047857,2.8529612442
 H,0,-4.6516317405,4.3925503064,1.4661809314
 H,0,-6.3016583222,4.26562486,-0.3796093467
 H,0,-6.6388724508,2.1160791899,-1.6156018199
 H,0,-5.3453118775,0.1047587079,-0.9822848639
 H,0,-0.7023113058,3.2539208612,3.6339100752
 H,0,-0.255973621,2.2125059921,5.0207587055
 H,0,-1.9458372545,2.7991364591,4.8693220831
 H,0,-1.378524606,-1.5996147322,-1.9362545823
 H,0,-1.7632859057,-0.2481738689,-0.8585339524
 H,0,-5.6653060638,-0.5360473469,2.2055486464
 H,0,-7.7077977154,-1.7409146635,2.8927798802
 H,0,-8.2334778796,-3.9850605738,1.9200038969
 H,0,-6.6883954891,-5.0192026527,0.279236489
 H,0,-4.6155472601,-4.959796404,-1.0162191564
 H,0,-2.5330320405,-5.8689686707,-1.5846154627
 H,0,-1.5958685163,-5.3115487472,-3.0096547941
 H,0,-3.3832837863,-5.1573981411,-2.996709678
 C,0,2.5368301982,-3.822601888,0.962634104
 C,0,3.4178681903,-3.6632846784,-0.2991678559
 C,0,3.3546525362,-3.4306051898,2.2183194889
 C,0,4.7731508486,-4.3647057724,-0.1975270757
 H,0,3.5978570511,-2.5910254156,-0.4515757389
 H,0,2.8724301541,-4.0279777773,-1.1824975733
 C,0,4.7177851829,-4.12302804,2.3058092782
 H,0,3.5148503654,-2.3435364214,2.1780268333
 H,0,2.7683423033,-3.6505135072,3.1263133238
 C,0,5.5417517716,-3.8905150818,1.0372209319
 H,0,5.3461670463,-4.1543174742,-1.1147981587
 H,0,4.6451538743,-5.4614350134,-0.1550066016
 H,0,5.2559369439,-3.7419667443,3.1895444951
 H,0,4.5915379265,-5.2084293839,2.4685896165
 H,0,6.5161624143,-4.4013976521,1.1103818389
 H,0,5.7499190983,-2.8109056006,0.9358161129
 C,0,2.0054960151,-5.2687167541,1.0827408519
 H,0,1.3545628974,-5.3776073681,1.9646224005
 H,0,1.421664749,-5.5467575582,0.1911480947
 H,0,2.8310139477,-5.9873324259,1.182889686
 C,0,1.5653901835,4.1568379869,-2.9685652862
 C,0,0.5385993641,5.1150144295,-3.2306690928
 C,0,0.1829121401,5.7260495153,-1.9883442857
 C,0,0.9860287153,5.1398586335,-0.9623398802

C,0,1.8405657909,4.1671194756,-1.568276264
 H,0,2.0407383571,3.5071348961,-3.7006371364
 H,0,0.0946908127,5.3307105252,-4.2010084021
 H,0,-0.5875685893,6.4817569902,-1.8450876384
 H,0,0.9234931458,5.3461423826,0.1046463969
 H,0,2.5353184076,3.5087648937,-1.0454592832
 Fe,0,-0.1394115323,3.6876125014,-1.8843918434
 C,0,-1.6432623364,3.1781366804,-0.5908119032
 C,0,-2.177208468,3.2049274703,-1.9045995797
 C,0,-0.5853056074,2.2136202562,-0.5671177368
 H,0,-1.9450250385,3.7838417107,0.2547112203
 C,0,-1.4391969501,2.2877275216,-2.7067107813
 H,0,-2.9951299206,3.8354536348,-2.2459914698
 C,0,-0.4394423657,1.6519615022,-1.8901077552
 H,0,-1.6066519186,2.1065450492,-3.7647116443
 C,0,0.3407831016,2.0434661424,0.5502275727
 O,0,0.2838355774,2.6884135518,1.6024922797
 N,0,1.3811246227,1.182135806,0.3967696951
 Rh,0,1.30561227,-0.6879134878,0.4401610817
 C,0,2.5696804312,-0.7719578571,-2.2495820467
 C,0,2.2517837455,-1.8643358598,-3.0845374174
 C,0,3.9211685851,-0.433929811,-2.0695867571
 C,0,3.2525108795,-2.6030602842,-3.714375711
 H,0,1.2036670046,-2.1172609353,-3.2590415725
 C,0,4.9185160958,-1.1828541198,-2.6975643152
 H,0,4.1848275156,0.3926571198,-1.4068119247
 C,0,4.5955662548,-2.2700368419,-3.5146114156
 H,0,2.9822369718,-3.4416892413,-4.3610366487
 H,0,5.9647599989,-0.9101303568,-2.5389039076
 H,0,5.3840907412,-2.8527796214,-3.9970458867
 C,0,1.4653843499,0.0059253551,-1.647830908
 C,0,0.6103793439,0.7548869899,-2.3832776926
 C,0,0.718984362,0.7386688266,-3.9019347338
 H,0,0.5948678322,1.754566892,-4.3000954221
 H,0,-0.0787769191,0.1148301818,-4.3396286233
 H,0,1.6795348121,0.3445588945,-4.2469366404
 C,0,4.0205495625,2.5720388136,2.7655810263
 C,0,4.0080554812,3.068022749,4.2138310569
 C,0,2.7910547597,2.5287416436,4.9696654936
 C,0,2.7337668426,0.999785541,4.8999207555
 C,0,2.7599236114,0.5029368591,3.4490309915
 C,0,3.9687110349,1.0323069381,2.6454448231
 H,0,2.7981947496,2.8688410468,6.019536276
 H,0,4.9320814606,2.7591270612,4.73422647
 H,0,4.0061297489,4.1710648503,4.226009336
 H,0,3.1360377577,2.974611827,2.244154025
 H,0,4.90014556,2.9458109297,2.2229129327
 H,0,3.579452761,0.575321054,5.469208503
 H,0,1.8189081383,0.627743813,5.3938064139
 H,0,2.7546799552,-0.5966646921,3.4244140571
 H,0,1.8361182962,0.8426627428,2.9587826666
 H,0,1.8798711273,2.9416425943,4.5032534709
 C,0,5.278772182,0.3846391789,3.1466836
 H,0,5.2377946146,-0.7100907885,3.0305330952
 H,0,6.1351082022,0.7587216916,2.5652268528
 H,0,5.4669746635,0.6025557165,4.2079494317
 C,0,3.8987802539,0.6603597949,1.1415608151
 O,0,3.3544976072,-0.5002202588,0.8458956166

O,0,4.440051584,1.3890615508,0.3225939514

INT-7

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4280.84008237 a.u.
Zero-point correction = 1.132143 Hartree/Particle
Sum of electronic and thermal Free Energies = -4279.804072 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4281.660101845743 a.u.

O,0,2.1579931053,-1.4118938535,4.0902535004
O,0,1.7834047059,4.3888891071,-0.5232303558
C,0,-0.828274463,2.2907691228,1.3233279805
C,0,-1.3129074742,2.2926956907,2.6775643534
C,0,-0.2539725709,1.7934883023,3.4921063429
C,0,0.9074441145,1.5530308392,2.6651205195
C,0,0.5512842857,1.8557579997,1.3131076425
C,0,2.2590289889,1.1571479015,3.1964002572
C,0,2.9331276257,0.0493172158,2.4222472165
C,0,2.8035910815,-1.2913565338,2.9082685462
C,0,3.3363429879,-2.3448322195,2.1941269583
C,0,4.0066941439,-2.1184796987,0.9632920048
C,0,4.5195925938,-3.1926901913,0.1866389684
C,0,5.1542398984,-2.9605733979,-1.0149464156
C,0,5.3092499271,-1.6383215401,-1.4961713544
C,0,4.8308486382,-0.5730229552,-0.7612108318
C,0,4.1718593881,-0.7807202033,0.4805834327
C,0,3.6387792241,0.2996950927,1.2566777671
C,0,1.8202023319,-2.7003934311,4.5601571655
C,0,1.4249956429,1.7502976115,0.0907382757
C,0,2.7651247695,2.4136708865,0.2827871469
C,0,3.8330330852,1.7138575783,0.8148083163
C,0,5.1056505466,2.3524994565,0.9972965373
C,0,6.2255781049,1.6760380649,1.5524146574
C,0,7.4359965951,2.3195481078,1.710726284
C,0,7.5792489438,3.6734935391,1.3242939472
C,0,6.5075353784,4.3602690701,0.7929204442
C,0,5.2471076547,3.726585706,0.6184619792
C,0,4.1286490826,4.4315987442,0.0933018522
C,0,2.9137898486,3.7950119487,-0.0574352017
C,0,1.8299756888,5.7458311277,-0.8994377985
H,0,-1.3887946357,2.5867266713,0.4400758214
H,0,-0.2897562516,1.6310570439,4.5659633884
H,0,2.1454988546,0.8562844053,4.2435633956
H,0,2.8871430112,2.0625788426,3.1729987438
H,0,3.2312953171,-3.3689935988,2.5461839911
H,0,4.3892185315,-4.2119831007,0.5552392842
H,0,5.5340908798,-3.7996793727,-1.6027924415
H,0,5.8084139185,-1.4624443301,-2.4518719638
H,0,4.9490871449,0.4466211427,-1.1309969768
H,0,1.1891172823,-3.2208369968,3.8245666094
H,0,1.2459986328,-2.553076467,5.4839599706
H,0,2.722128568,-3.2966502166,4.7863381121
H,0,0.8938050861,2.213106941,-0.7461543311
H,0,1.5769637153,0.6923231447,-0.1580673389
H,0,6.1160143491,0.6328552487,1.8504991481
H,0,8.2871350221,1.7831163578,2.1362037262

H,0,8.5414427784,4.1754185552,1.4516639957
 H,0,6.6127352579,5.4081365659,0.4996695809
 H,0,4.2567223267,5.4800509029,-0.1740778174
 H,0,2.1061782637,6.3939646885,-0.0488048996
 H,0,0.8212248705,6.0110123255,-1.2417911944
 H,0,2.5478653237,5.9153386065,-1.7215373023
 C,0,-2.6804725728,2.7435348166,3.1408975451
 C,0,-3.7363411745,2.4304490909,2.0514101843
 C,0,-3.052682536,2.0235216736,4.4607981074
 C,0,-5.1772101137,2.6661129592,2.5107375707
 H,0,-3.6233501868,1.3742834309,1.7695550114
 H,0,-3.5269161153,3.0305262949,1.1521857204
 C,0,-4.5009696742,2.2586201892,4.8994496907
 H,0,-2.900220912,0.9458048015,4.3047042439
 H,0,-2.3661253258,2.345834145,5.2613456898
 C,0,-5.4857784729,1.8849216039,3.7895083071
 H,0,-5.864439184,2.3675795743,1.7018216008
 H,0,-5.3585979527,3.7418302518,2.6850601041
 H,0,-4.7017374645,1.6663369752,5.8074367238
 H,0,-4.6526745056,3.3153192175,5.1835800704
 H,0,-6.5231766967,2.0675782345,4.1150947873
 H,0,-5.4006177965,0.8039629458,3.5806346466
 C,0,-2.5633474845,4.2691984818,3.3612677455
 H,0,-1.7991523163,4.4996674523,4.1199243541
 H,0,-2.2828587486,4.7803635664,2.4270049673
 H,0,-3.5175059471,4.6935466188,3.7039188175
 C,0,-2.1054069764,-4.6075233387,-1.8896570445
 C,0,-1.3656748541,-5.796497824,-2.1729142216
 C,0,-1.2027170182,-6.5135907216,-0.9469857126
 C,0,-1.8457310733,-5.7660120107,0.0884151619
 C,0,-2.4005334711,-4.585113978,-0.492333845
 H,0,-2.366995965,-3.826932247,-2.6019381298
 H,0,-0.9699330635,-6.0913135766,-3.1434715961
 H,0,-0.6657073913,-7.4524757082,-0.8219981874
 H,0,-1.8804740215,-6.0363942701,1.1410363443
 H,0,-2.900701546,-3.7766015102,0.0418691068
 Fe,0,-0.3555534211,-4.6436158755,-0.7993433342
 C,0,1.1640130952,-4.3193619444,0.5572503205
 C,0,1.686904103,-4.8757250407,-0.6469800457
 C,0,0.5533123179,-3.0693479331,0.2165577479
 H,0,1.229975943,-4.7457741351,1.5545599606
 C,0,1.3665239343,-4.0076508936,-1.7378341238
 H,0,2.2140774881,-5.8243879506,-0.7302630689
 C,0,0.6711412038,-2.8703131261,-1.2114732635
 H,0,1.6140452123,-4.1804386995,-2.7824226935
 C,0,-0.0279364043,-1.9998307569,0.9836311809
 O,0,0.0012095057,-1.8499433348,2.255468001
 N,0,-0.5693326468,-0.9720282407,0.3262021548
 Rh,0,-0.7568807165,0.2829185999,1.9965470093
 C,0,-1.4083653624,0.3127812182,-1.5237531287
 C,0,-0.9107705728,1.2684862536,-2.4235424521
 C,0,-2.7099798433,0.4660988679,-1.0112460129
 C,0,-1.6903669138,2.3671795184,-2.7956192992
 H,0,0.10344157,1.1639297772,-2.8135138824
 C,0,-3.4891649563,1.5579993457,-1.3959077229
 H,0,-3.090558832,-0.2827280191,-0.310467268
 C,0,-2.9816272411,2.5163294307,-2.2807309644
 H,0,-1.2849624702,3.1110717989,-3.4859711384

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H,0,-4.5010054129,1.6634624973,-0.9974724415
H,0,-3.5924299381,3.3745032595,-2.5720501425
C,0,-0.5942741993,-0.8324252871,-1.0471037907
C,0,0.0415539271,-1.7445528184,-1.8628900944
C,0,0.0345333715,-1.7066290633,-3.3645647287
H,0,-0.2400655966,-2.6963989911,-3.7664945059
H,0,1.0338943258,-1.4660013355,-3.7676970036
H,0,-0.6765771696,-0.9714932617,-3.7608088456
C,0,-2.7922473031,-4.0766461254,3.0263445037
C,0,-2.7576646385,-5.1053647305,4.159532872
C,0,-1.8821573478,-4.6292290443,5.3209042572
C,0,-2.3523102164,-3.2625989885,5.8256156232
C,0,-2.3813712488,-2.2275714845,4.695694274
C,0,-3.229633598,-2.6647684516,3.4805390687
H,0,-1.8822929673,-5.3693646692,6.1389111345
H,0,-3.7800320445,-5.2981899707,4.5298321907
H,0,-2.3897579355,-6.0702286301,3.7698213955
H,0,-1.7827866292,-3.9932465568,2.5908417709
H,0,-3.4559827109,-4.4137610172,2.2185234653
H,0,-3.3552428165,-3.3684790986,6.2763626962
H,0,-1.6925531872,-2.904492072,6.6346672265
H,0,-2.7489211805,-1.260986994,5.0718835816
H,0,-1.353718806,-2.0521837494,4.343436442
H,0,-0.8365938515,-4.5434475516,4.9710115519
C,0,-4.73553782,-2.6288681977,3.8043855773
H,0,-5.0404033691,-1.6165101924,4.1154354951
H,0,-5.3213446197,-2.9057892319,2.9150384086
H,0,-4.9979298827,-3.3209143623,4.618327219
C,0,-3.0150551513,-1.7020781451,2.2854321356
O,0,-2.5439522718,-0.5353354742,2.6065224556
O,0,-3.3259913441,-2.0416267696,1.1481622469

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TS-6

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.84981251 a.u.
Imaginary frequency = -333.3953 cm-1
Zero-point correction = 0.968043 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.969653 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.595945917548 a.u.

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```

C,0,-5.5518866773,-8.9396464324,9.4812810676
C,0,-6.3294340688,-8.4701829002,10.5845077548
C,0,-7.6974204867,-8.8000750989,10.3302779753
C,0,-7.7677509113,-9.4658674644,9.0696401394
C,0,-6.4397390632,-9.5514536795,8.5453620566
H,0,-4.4752565016,-8.8301998291,9.3650199955
H,0,-5.9495163705,-7.9382081345,11.4549924498
H,0,-8.5443725876,-8.5521400247,10.9677518192
H,0,-8.6783915362,-9.7743224945,8.5594182977
H,0,-6.1584772522,-9.9700574931,7.5812319585
Fe,0,-6.977729732,-7.5823429064,8.8328076442
C,0,-8.4143569963,-6.2205490174,8.3231023133
C,0,-7.4062350071,-5.5849096083,9.1042099711
C,0,-7.7866151348,-6.7244983736,7.1335106851
H,0,-9.468521425,-6.3303416868,8.565463859
C,0,-6.1513599796,-5.7285585502,8.4300415062

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H,0,-7.5563478605,-5.1014834944,10.0680011889
C,0,-6.378813394,-6.4040588392,7.185524116
H,0,-5.188686218,-5.3690222531,8.7878065845
C,0,-8.4151383962,-7.6563616138,6.1890065097
O,0,-9.4436118168,-8.2774231516,6.4297226041
N,0,-7.7101134018,-7.8316900745,4.9840325501
O,0,-8.1130218277,-8.9771038173,4.2818585554
C,0,-7.6864911049,-10.1715771505,4.9193309266
H,0,-6.5905627837,-10.1777140841,5.0488018632
H,0,-7.9844061692,-10.9857865415,4.243463392
H,0,-8.1887466424,-10.3032285192,5.8892191424
Rh,0,-7.5343607506,-6.1180464919,3.7969569082
C,0,-5.5099987425,-7.0613961342,3.5794089782
C,0,-4.3238406313,-6.328140285,3.2230557242
C,0,-6.3410975092,-7.5682257515,2.5128798614
C,0,-4.002667164,-6.0996448666,1.9085633488
H,0,-3.6784524371,-5.9537595513,4.0155229456
C,0,-6.0008587724,-7.2394099103,1.1668805701
H,0,-7.0382394596,-8.3821928308,2.6824917922
C,0,-4.866314348,-6.5250460013,0.8624892554
H,0,-3.0851405564,-5.5584258902,1.6649398582
H,0,-6.6535553057,-7.5996058552,0.3701585011
H,0,-4.6130611489,-6.3014255764,-0.1762045489
C,0,-5.9960509318,-7.0615901584,4.9329618772
C,0,-5.4495332575,-6.7950206628,6.1544227845
C,0,-3.9796651676,-6.9106845987,6.4625945337
H,0,-3.8280496663,-7.3842681244,7.4468534962
H,0,-3.4788130369,-5.9246978226,6.5032983183
H,0,-3.4526578442,-7.5175583427,5.7126607266
O,0,-9.2488625365,-8.4198710828,1.1548950508
O,0,-11.6208390672,-3.1395157299,5.7388967444
C,0,-8.4081565154,-4.2329222139,4.6640990692
C,0,-7.5995061883,-3.8545398757,3.5661614261
C,0,-8.1514377972,-4.5325556748,2.4114821228
C,0,-9.3498726475,-5.23059308,2.7711331705
C,0,-9.4688090554,-5.0920563957,4.1925840177
C,0,-10.2901944652,-5.9268024285,1.8177665941
C,0,-10.9023519918,-7.2114599361,2.3403587791
C,0,-10.3233751212,-8.4728522636,1.9904794245
C,0,-10.8509273547,-9.6525813599,2.4731963512
C,0,-11.9737646673,-9.6446935984,3.339382951
C,0,-12.5154760729,-10.8469946454,3.8698387206
C,0,-13.6010105771,-10.8204515825,4.7194466948
C,0,-14.1925639134,-9.5855050487,5.0788211338
C,0,-13.6893644406,-8.4025082677,4.578475445
C,0,-12.5763459516,-8.3977889265,3.6943992024
C,0,-12.0175005977,-7.1891736745,3.1653795054
C,0,-8.6863172419,-9.6349565465,0.7195430569
C,0,-10.5932420275,-5.5924041845,5.0589216624
C,0,-11.9093609363,-5.1116709128,4.4961849109
C,0,-12.5976362984,-5.8740708891,3.5694967719
C,0,-13.823575391,-5.4014875601,2.9955454824
C,0,-14.5533646616,-6.151602818,2.0345771346
C,0,-15.7322984076,-5.66854306,1.5038568697
C,0,-16.2319869459,-4.4081957131,1.910194867
C,0,-15.5407743433,-3.6527984052,2.8349313474
C,0,-14.3231027871,-4.1213948815,3.3989880226
C,0,-13.5894777723,-3.3445086239,4.3383499946

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C,0,-12.4049613914,-3.821125541,4.8629859323
C,0,-12.015622612,-1.8513097062,6.1472005892
H,0,-8.286800306,-3.9338999847,5.7023259713
H,0,-7.7528725544,-4.4777809746,1.4003573387
H,0,-9.7427844532,-6.1390412936,0.8907064612
H,0,-11.1064543035,-5.2302743058,1.5624276983
H,0,-10.4078033582,-10.6140067345,2.218964967
H,0,-12.0503750391,-11.7976043958,3.5953560181
H,0,-14.0040502919,-11.7529020588,5.1222491537
H,0,-15.0473677999,-9.5703351088,5.7589013426
H,0,-14.1419705837,-7.451933107,4.8626613662
H,0,-8.2766504787,-10.2171373165,1.5628687675
H,0,-7.8687550429,-9.3808962569,0.0332063168
H,0,-9.4263760353,-10.2554867647,0.1839853995
H,0,-10.4495281371,-5.2122429865,6.0765598011
H,0,-10.5923818406,-6.6866967843,5.1150332566
H,0,-14.1666273397,-7.1230131059,1.7235123834
H,0,-16.2824656799,-6.2595784445,0.7680257747
H,0,-17.1668757643,-4.0328505046,1.4868079441
H,0,-15.9216052796,-2.6764865468,3.1465654562
H,0,-13.9818307697,-2.3677541941,4.619838012
H,0,-12.0923911019,-1.1589931332,5.2898158835
H,0,-11.2404087611,-1.4880057312,6.8346004757
H,0,-12.9861327716,-1.8701171018,6.6746018124
C,0,-6.4539337574,-2.8640327303,3.612225915
C,0,-5.5410662196,-3.1841615159,4.8233624121
C,0,-5.6315634838,-2.9408353396,2.3068929817
C,0,-4.2514747453,-2.3599650619,4.8574273569
H,0,-5.287359089,-4.253969899,4.7865070462
H,0,-6.1049827022,-3.0428425714,5.7589706851
C,0,-4.3332855485,-2.1283086121,2.3447075606
H,0,-5.3842105955,-3.9947463543,2.11920144
H,0,-6.2558746261,-2.6079011671,1.461391498
C,0,-3.4660988106,-2.5001734817,3.5508367591
H,0,-3.6345287793,-2.6826079769,5.7127304541
H,0,-4.482590177,-1.2945701526,5.0326535407
H,0,-3.7750489646,-2.2903463633,1.4074208698
H,0,-4.5610628857,-1.0485746826,2.3800487022
H,0,-2.5558742139,-1.8783166982,3.5768305464
H,0,-3.1295654161,-3.5463297197,3.4440689697
C,0,-7.0821879709,-1.4605132997,3.7648485099
H,0,-7.7643742372,-1.2495378307,2.9264848823
H,0,-7.6631332873,-1.3939598214,4.6973484336
H,0,-6.3182954452,-0.6694863631,3.7853566229

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INT-8

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -3932.87250621 a.u.
Zero-point correction = 0.969655 Hartree/Particle
Sum of electronic and thermal Free Energies = -3931.991643 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -3933.616803117728 a.u.

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O,0,-1.0521706114,-2.0064358276,-2.2600214435
O,0,-3.3362647165,3.7607989335,1.8059554876
C,0,-0.1451084437,2.509663437,0.9053976709
C,0,0.7043585058,2.7637771855,-0.1906771051

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C,0,0.1827301776,1.9763847259,-1.2930865859
 C,0,-1.055917277,1.3480703022,-0.9060236109
 C,0,-1.2077965078,1.6176546586,0.485330291
 C,0,-1.9844227326,0.5911589502,-1.8247830996
 C,0,-2.6614528899,-0.6192482713,-1.2105689308
 C,0,-2.132386401,-1.9321603109,-1.4350906196
 C,0,-2.7186239559,-3.0414965095,-0.8593436278
 C,0,-3.8633297072,-2.911470042,-0.0312155387
 C,0,-4.4719357654,-4.0388233537,0.5845777065
 C,0,-5.5813402666,-3.8926402638,1.3905566206
 C,0,-6.1296879203,-2.607662969,1.6187051426
 C,0,-5.5608192769,-1.4953728945,1.0329891013
 C,0,-4.4220909998,-1.6145530915,0.1905098554
 C,0,-3.7968770693,-0.4810591629,-0.4255795971
 C,0,-0.5383012046,-3.2799727106,-2.5753576845
 C,0,-2.3677822381,1.2283588855,1.3633883821
 C,0,-3.6520114278,1.6989550002,0.7243191508
 C,0,-4.3378578558,0.8844215308,-0.1584331493
 C,0,-5.5259567632,1.3462749569,-0.815150076
 C,0,-6.2503619729,0.5415730927,-1.7350844945
 C,0,-7.3918892557,1.0169955804,-2.3483843695
 C,0,-7.8579007141,2.3239428231,-2.0696008063
 C,0,-7.1706085936,3.1320354677,-1.1873051165
 C,0,-5.9911589129,2.6724873711,-0.5408522523
 C,0,-5.2612212718,3.5015748737,0.3558709044
 C,0,-4.113450653,3.0321998082,0.9622395794
 C,0,-3.6894376705,5.0964754502,2.074780158
 H,0,-0.0516241181,2.9100462663,1.9124454241
 H,0,0.6010825636,1.9423111043,-2.296615904
 H,0,-1.4115340512,0.2749370592,-2.7056488398
 H,0,-2.7676105361,1.2835384677,-2.1785443778
 H,0,-2.3160815233,-4.039827344,-1.0225430025
 H,0,-4.0407918054,-5.0282622507,0.4099227501
 H,0,-6.037295,-4.7684766104,1.8587987595
 H,0,-7.0043380306,-2.4970768085,2.2638753846
 H,0,-5.9812288739,-0.5058169238,1.2150046841
 H,0,-0.1687073592,-3.8023710619,-1.6758798521
 H,0,0.3024440404,-3.1221570896,-3.2623446819
 H,0,-1.2978180018,-3.9116272464,-3.0688032325
 H,0,-2.2385836091,1.6910595953,2.3483604057
 H,0,-2.3924553897,0.1438180496,1.5165509807
 H,0,-5.8896711061,-0.4655448019,-1.9487780722
 H,0,-7.9380179994,0.3838344156,-3.0514984109
 H,0,-8.7630448691,2.6932916618,-2.5579414121
 H,0,-7.5248815099,4.1442049999,-0.9742179773
 H,0,-5.6267687506,4.5115559808,0.5390937089
 H,0,-3.7072104963,5.7055437834,1.1533535638
 H,0,-2.9232424363,5.494054407,2.7533777063
 H,0,-4.6773072861,5.167350782,2.5644480025
 C,0,1.9070770234,3.6870724439,-0.1830060267
 C,0,2.7966541819,3.3647936023,1.0469028172
 C,0,2.7299200404,3.4933170425,-1.475738978
 C,0,4.1370889826,4.1042470943,1.0512726167
 H,0,2.9816559656,2.2797713359,1.0525916319
 H,0,2.2403590996,3.5817894941,1.9726529969
 C,0,4.0759821017,4.2246830202,-1.4693543541
 H,0,2.914985723,2.4179527185,-1.604720015
 H,0,2.1302997272,3.8174047787,-2.3423191278

C,0,4.9146401183,3.8526903785,-0.2432248655
 H,0,4.7290990257,3.7809079521,1.9241473025
 H,0,3.975848155,5.1893975822,1.1772013238
 H,0,4.6251762951,3.9842787585,-2.3950699887
 H,0,3.9175395135,5.3173664493,-1.4841733227
 H,0,5.864333832,4.4132630869,-0.2406567806
 H,0,5.1793863997,2.7823036712,-0.3007222051
 C,0,1.3722645023,5.1335043321,-0.0987782376
 H,0,0.7099631298,5.3501981847,-0.95149097
 H,0,0.7914313011,5.2806247687,0.8246015973
 H,0,2.1862087183,5.8734383515,-0.1073292773
 C,0,3.0037672177,-2.0161815211,6.4499767405
 C,0,2.2050373843,-1.3451118267,7.4263151533
 C,0,0.8310270148,-1.5956569855,7.1195742468
 C,0,0.7803824376,-2.4122863281,5.951050903
 C,0,2.1262171717,-2.6745673802,5.5388529207
 H,0,4.0907852736,-2.0028562989,6.3936648666
 H,0,2.5765600027,-0.7325809988,8.2458821422
 H,0,-0.028302928,-1.2029449815,7.6600495998
 H,0,-0.1269419844,-2.7326135146,5.4414817983
 H,0,2.4342611984,-3.2510141336,4.670261281
 Fe,0,1.7510896509,-0.6418676635,5.5409264865
 C,0,0.5691052723,0.9333836312,4.9962869123
 C,0,1.7519917026,1.4112887754,5.6302309421
 C,0,0.983780647,0.2350435042,3.8124102777
 H,0,-0.4593516598,1.0784837114,5.3174632444
 C,0,2.8891866209,0.9580775096,4.8851856136
 H,0,1.7911498226,1.9912836397,6.5505836533
 C,0,2.4208964609,0.2453181713,3.731758888
 H,0,3.9297786968,1.1480037979,5.1379524666
 C,0,0.1844586489,-0.5650854264,2.9110402592
 O,0,-0.9581579143,-0.9353555975,3.0696878859
 N,0,0.9161761851,-0.9736811278,1.7121810551
 O,0,0.5071177897,-2.2730557968,1.2983908999
 C,0,0.9357115427,-3.2845094061,2.1963063777
 H,0,2.0282884654,-3.2516495732,2.3424140844
 H,0,0.657155254,-4.2310219952,1.7129019692
 H,0,0.4182484372,-3.2067402051,3.1641931704
 Rh,0,0.7314078318,0.5222404395,0.2028377121
 C,0,2.6618999404,-0.587811692,0.0912696502
 C,0,3.8703393077,0.0372690073,-0.385899603
 C,0,1.7199485483,-1.077621005,-0.906206807
 C,0,4.1074005183,0.2085681224,-1.7247481648
 H,0,4.6012943201,0.4076849522,0.3254330125
 C,0,1.998123889,-0.8201214965,-2.2916414481
 H,0,1.0497876319,-1.8995292068,-0.6797135056
 C,0,3.1478765202,-0.1965630529,-2.6987998399
 H,0,5.031125431,0.6958067536,-2.0461135802
 H,0,1.2638973966,-1.1576775114,-3.0244441556
 H,0,3.3408641446,-0.0212065247,-3.7596416664
 C,0,2.3482549112,-0.6861587885,1.5258282813
 C,0,3.1287292813,-0.3056086693,2.607713361
 C,0,4.6301821625,-0.2411214748,2.6204987211
 H,0,4.9959331634,-0.5359852788,3.6181821072
 H,0,5.0283736696,0.7732914987,2.4277866936
 H,0,5.0829077048,-0.9264460111,1.8926568063

INT-9

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4396.38289736 a.u.
Zero-point correction = 1.185862 Hartree/Particle
Sum of electronic and thermal Free Energies = -4395.295318 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4397.246593920594 a.u.

O,0,-3.9390345318,-0.1221491305,-2.0443795914
O,0,-4.6954288543,5.5563842611,2.5016445472
C,0,-1.9638233783,4.0322769195,0.8668687507
C,0,-1.3472326338,4.183694454,-0.4063608209
C,0,-2.2492596869,3.5759396055,-1.3786279056
C,0,-3.3868233883,3.077667598,-0.7335944366
C,0,-3.1628978016,3.2860351904,0.6913112079
C,0,-4.5989420628,2.4902192593,-1.4086159896
C,0,-5.2391376116,1.3169026385,-0.7005364312
C,0,-4.8907172782,-0.0185943276,-1.0824472608
C,0,-5.5067965024,-1.1051661325,-0.4929316781
C,0,-6.4586985818,-0.9207482266,0.544469682
C,0,-7.0776295248,-2.024008305,1.1939140348
C,0,-7.9438808909,-1.831960605,2.2498613231
C,0,-8.2371794283,-0.5222448121,2.6997070416
C,0,-7.6697016662,0.5693486769,2.0744516592
C,0,-6.7770595296,0.403988583,0.980769955
C,0,-6.1589481473,1.5141037694,0.3175216695
C,0,-3.5473647183,-1.4101039033,-2.4751025784
C,0,-4.1506056729,2.9711483696,1.7811651376
C,0,-5.4891511092,3.5997521861,1.4724169542
C,0,-6.4579049654,2.9077782337,0.7646094794
C,0,-7.7084777876,3.526958416,0.4312017891
C,0,-8.7181957124,2.8561229697,-0.3104329688
C,0,-9.9115041066,3.4805482782,-0.6122620787
C,0,-10.1467274337,4.809915969,-0.1875647901
C,0,-9.1811001288,5.4913006934,0.5241493841
C,0,-7.9410217785,4.8768727927,0.8485348364
C,0,-6.9278947877,5.575869991,1.5610104251
C,0,-5.7283228703,4.9585081959,1.8531058618
C,0,-4.8177222994,6.9065475332,2.8805401329
H,0,-1.6130670061,4.4272976071,1.8164725487
H,0,-2.0813492109,3.5552670546,-2.4532842494
H,0,-4.3132681648,2.1854771644,-2.4237502877
H,0,-5.3604583001,3.2814659367,-1.5104407048
H,0,-5.2568081739,-2.1224913351,-0.7889124943
H,0,-6.8435400655,-3.0343008572,0.8489230497
H,0,-8.4025703943,-2.6916103444,2.7442872321
H,0,-8.9158645075,-0.376507593,3.5430990792
H,0,-7.8963923281,1.5782380075,2.4206504261
H,0,-3.1901410336,-2.0208675738,-1.6314014556
H,0,-2.727788829,-1.261816555,-3.187270383
H,0,-4.3829098389,-1.9343613406,-2.9722177595
H,0,-3.7613464151,3.3493875622,2.7342202925
H,0,-4.2622298057,1.887428166,1.8701783669
H,0,-8.5366538923,1.8319841377,-0.6387056764
H,0,-10.6771929122,2.9482959336,-1.181391054
H,0,-11.0945223595,5.2974231431,-0.4287226171
H,0,-9.356281857,6.5209033959,0.8474945057
H,0,-7.1214728948,6.6066629319,1.8562452905

H,0,-4.9856727738,7.560002462,2.0059099799
 H,0,-3.8704911081,7.185202564,3.3607229939
 H,0,-5.6442281165,7.0565207421,3.5982120219
 C,0,-0.3205139167,5.2482297146,-0.7463082557
 C,0,0.7349989323,5.3761808245,0.3718032817
 C,0,0.3806777617,4.9438280094,-2.0867467722
 C,0,1.8500497621,6.3749508838,0.0454816839
 H,0,1.1718419667,4.3850386946,0.5463743008
 H,0,0.2418157915,5.6679544206,1.3127121748
 C,0,1.4980460039,5.9355507355,-2.428653209
 H,0,0.7913786971,3.9274381853,-2.0298589952
 H,0,-0.3609274494,4.9317282878,-2.9013508691
 C,0,2.5199164333,6.0610114661,-1.2951688339
 H,0,2.6002115753,6.3595419152,0.8534498873
 H,0,1.445761586,7.4020894469,0.0223429935
 H,0,1.9985659999,5.6171108328,-3.3586126
 H,0,1.0661751736,6.9281240328,-2.6437310992
 H,0,3.2728898926,6.8288189507,-1.540102862
 H,0,3.0646356941,5.1088902751,-1.1973334204
 C,0,-1.1344500507,6.5615262213,-0.8659416653
 H,0,-1.914939958,6.4632808253,-1.6361754568
 H,0,-1.6318607578,6.7927310467,0.088027293
 H,0,-0.5009008539,7.4185288118,-1.1360513856
 C,0,5.0363892902,-0.047788528,0.2621301865
 C,0,5.2844916385,0.2785376887,1.630398151
 C,0,4.2356196943,-0.2914818589,2.416485636
 C,0,3.3373940755,-0.9698614628,1.5373439583
 C,0,3.834632408,-0.8190722534,0.206434544
 H,0,5.6448720322,0.2531987025,-0.5889649267
 H,0,6.1116573055,0.8786724012,2.0056477923
 H,0,4.1183330845,-0.1943879032,3.4942655468
 H,0,2.3957590269,-1.4310402594,1.8284654769
 H,0,3.3653763594,-1.1900718558,-0.7014351836
 Fe,0,3.4515355075,1.0270934846,1.0424838417
 C,0,2.1139786753,2.2312111438,2.0470077185
 C,0,3.2843814191,2.9699865069,1.6860965643
 C,0,1.5080641597,1.7663328975,0.8450902636
 H,0,1.7382939935,2.0458785055,3.0500385722
 C,0,3.4304542562,2.9192950564,0.2658671784
 H,0,3.9692003252,3.4585217149,2.3765313123
 C,0,2.3176926324,2.1750860829,-0.2625664846
 H,0,4.241237965,3.3619869986,-0.3066634889
 C,0,0.3369015702,0.8857553646,0.6991930958
 O,0,0.114334517,-0.0697601446,1.4703859387
 N,0,-0.0164316926,0.7060293151,-0.7827279012
 O,0,-0.4877128762,-0.6173212724,-1.0640152512
 C,0,0.5527136171,-1.6021383871,-1.0532673698
 H,0,1.264364298,-1.4165148518,-1.8709132348
 H,0,0.0376802087,-2.5561655277,-1.2284138934
 H,0,1.050058164,-1.6136948766,-0.0772030351
 Rh,0,-1.4910571882,1.9475653519,0.0731914619
 C,0,0.2886939694,0.8123115868,-3.2181610086
 C,0,-1.0792115356,0.9724953342,-3.5092860168
 C,0,1.1253033068,0.2915425302,-4.2213712472
 C,0,-1.578166788,0.6712197135,-4.775270424
 H,0,-1.753072829,1.3138707412,-2.7253793193
 C,0,0.6233349557,-0.0135702836,-5.4890015245
 H,0,2.1768059758,0.1019744087,-4.001288765

C,0,-0.7291341278,0.1846504591,-5.7753892909
 H,0,-2.6431019295,0.8109939459,-4.976774454
 H,0,1.2929397554,-0.4169212005,-6.2525206926
 H,0,-1.1224905956,-0.0514625598,-6.7670088139
 C,0,0.8162779296,1.1552552939,-1.8750729611
 C,0,1.9648696017,1.8509660246,-1.6347666051
 C,0,2.8625007654,2.3887961503,-2.7165287888
 H,0,3.7695104494,1.7675998697,-2.8125591691
 H,0,3.2001261669,3.4031193441,-2.462890055
 H,0,2.3712390671,2.4291552891,-3.6951404899
 C,0,-4.4778838576,-0.8426258238,4.920755554
 C,0,-4.1401685609,-0.4306168686,3.4861633729
 C,0,-3.1185824112,-1.3712047865,2.8124723116
 C,0,-1.8496715539,-1.4758815412,3.7141127876
 C,0,-2.1856040187,-1.8859327752,5.1506607397
 C,0,-3.2152917612,-0.9434838965,5.7819129073
 H,0,-3.7091307987,0.5807579551,3.5020764371
 H,0,-5.0530251647,-0.3772628022,2.8767578408
 H,0,-5.009566032,-1.8098927547,4.9253316277
 H,0,-5.1801569706,-0.1099503368,5.3511250454
 H,0,-1.3439889279,-0.4976189008,3.7137127244
 H,0,-1.1388187226,-2.1808472836,3.256831906
 H,0,-1.2588071659,-1.8966276868,5.7481413
 H,0,-2.5733217098,-2.9193991823,5.1702062962
 H,0,-2.7671911819,0.0624800438,5.8788545054
 H,0,-3.4668029738,-1.2755957937,6.8030996368
 C,0,-2.6131380122,-0.756490022,1.5145919445
 O,0,-2.5705785358,0.4586791072,1.3365759382
 O,0,-2.170283485,-1.6230482227,0.6343142614
 H,0,-1.612813144,-1.1346596063,-0.0353758763
 C,0,-3.7165246746,-2.7613448515,2.5470874831
 H,0,-2.9680921466,-3.4335512024,2.1068595548
 H,0,-4.5687214257,-2.6916955485,1.8586423033
 H,0,-4.0805295954,-3.2153356919,3.478131377

TS-7

Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
 SCF Done: E(RB3LYP) = -4396.37580423 a.u.
 Imaginary frequency = -444.8774 cm⁻¹
 Zero-point correction = 1.183641 Hartree/Particle
 Sum of electronic and thermal Free Energies = -4395.291094 a.u.
 Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
 FINAL SINGLE POINT ENERGY = -4397.237088284683 a.u.

O,0,-0.9853974922,-2.0928122638,-2.2892616239
 O,0,-3.0754666039,3.8620372485,1.4818049228
 C,0,0.023342833,2.578777557,0.4553998105
 C,0,0.8264203563,2.7119418982,-0.7067856858
 C,0,0.214528163,1.8887861604,-1.7343955768
 C,0,-0.9628172915,1.2827892792,-1.2307897975
 C,0,-1.0263276953,1.6559257665,0.1671621973
 C,0,-1.9721629184,0.4894740737,-2.023015057
 C,0,-2.5981317764,-0.6835944417,-1.2956819678
 C,0,-2.0609034406,-2.000909059,-1.4693021046
 C,0,-2.6307615768,-3.087254803,-0.8341205062
 C,0,-3.7389121983,-2.9187196736,0.0353213536
 C,0,-4.3135772297,-4.0165140978,0.7335037642

C,0,-5.3528615169,-3.8278192326,1.6202122951
 C,0,-5.8703067443,-2.5289623286,1.8428520521
 C,0,-5.3446341943,-1.4468274302,1.1668893858
 C,0,-4.2747764542,-1.6092722415,0.2447346797
 C,0,-3.6886298408,-0.5051528269,-0.4573663302
 C,0,-0.4094580361,-3.3634435284,-2.5153873011
 C,0,-2.1331393659,1.3111587441,1.1255056376
 C,0,-3.4617713462,1.7404096982,0.5506286964
 C,0,-4.21152667,0.8740682452,-0.2257179841
 C,0,-5.4473400932,1.2976237366,-0.8176125621
 C,0,-6.2362464914,0.4408323878,-1.6315784172
 C,0,-7.422166333,0.880310537,-2.1843816951
 C,0,-7.8702270155,2.2020531122,-1.949451301
 C,0,-7.1207531434,3.0605337786,-1.1717145848
 C,0,-5.8943805238,2.6388239992,-0.5898680265
 C,0,-5.1012703844,3.5194429565,0.196929043
 C,0,-3.9095517598,3.0859080685,0.7423387777
 C,0,-3.4062902413,5.2145939166,1.6879463407
 H,0,0.1559079975,3.0863677732,1.4072238357
 H,0,0.5673923045,1.8117336605,-2.7595868461
 H,0,-1.4889307896,0.1288483764,-2.9400451945
 H,0,-2.7841166149,1.1686322269,-2.3342666686
 H,0,-2.2243886039,-4.0885861528,-0.9628477227
 H,0,-3.9075569775,-5.0167001615,0.5624633302
 H,0,-5.7770930316,-4.6808279751,2.1552878334
 H,0,-6.6883451406,-2.3842135261,2.5521785124
 H,0,-5.7431196339,-0.4466989189,1.3402788543
 H,0,-0.0964046695,-3.8326497727,-1.5701913592
 H,0,0.4717411164,-3.19455962,-3.1439188699
 H,0,-1.1184882693,-4.0317834023,-3.035686565
 H,0,-1.9472999994,1.8175547392,2.0801366441
 H,0,-2.1402953498,0.2351833908,1.3155779053
 H,0,-5.889709965,-0.5774626778,-1.8129783712
 H,0,-8.017213913,0.2071685204,-2.8059011791
 H,0,-8.8107889347,2.5427313164,-2.3892600433
 H,0,-7.4607947346,4.0842535756,-0.9936674055
 H,0,-5.4548146577,4.5392398603,0.3460357354
 H,0,-3.4908194855,5.7619104371,0.732187519
 H,0,-2.5916028906,5.6506066585,2.280960942
 H,0,-4.3552723275,5.3233773478,2.2431751297
 C,0,1.8414551312,3.8155295284,-0.9277376365
 C,0,2.7739738588,3.9535178585,0.2967039103
 C,0,2.6919803888,3.5512127316,-2.1877450893
 C,0,3.8700770643,5.0064010179,0.1066728202
 H,0,3.2342207304,2.973140801,0.4877733651
 H,0,2.1772087902,4.1929097264,1.1910190157
 C,0,3.8011310126,4.5881164962,-2.3990264906
 H,0,3.1329889805,2.5492518678,-2.0949890244
 H,0,2.0414349614,3.5235059468,-3.0765034415
 C,0,4.6887452548,4.7461569857,-1.1607893143
 H,0,4.5326949055,5.0070692306,0.9879434395
 H,0,3.4234762784,6.0148163362,0.0578347725
 H,0,4.4132409719,4.2973720033,-3.2693393779
 H,0,3.3561693534,5.5644096496,-2.6569637203
 H,0,5.4255044066,5.5518055487,-1.3178611797
 H,0,5.2660113988,3.8204415362,-1.01392224
 C,0,1.0039678819,5.1041829408,-1.1199855473
 H,0,0.3031973804,4.9833108401,-1.9607039389

H,0,0.4114065062,5.3175523394,-0.2178070062
 H,0,1.6329519377,5.9813164249,-1.3291723658
 C,0,7.6747800445,-1.0932655445,0.4041914058
 C,0,7.9548673418,-0.7695911066,1.767060699
 C,0,6.9917827768,-1.4370912557,2.5858332029
 C,0,6.1140966828,-2.1709935668,1.7312910024
 C,0,6.5376409543,-1.9576917787,0.3834121233
 H,0,8.2186246027,-0.7282420101,-0.4653291626
 H,0,8.7467889442,-0.1107375178,2.118959689
 H,0,6.9162945399,-1.3692296416,3.6696022947
 H,0,5.2342450821,-2.7275650726,2.0486310321
 H,0,6.0535571869,-2.3490589707,-0.5079294302
 Fe,0,6.042973206,-0.1643014996,1.2711904694
 C,0,4.6005252933,0.8676135211,2.3132641405
 C,0,5.6912034465,1.7332420722,1.9942940341
 C,0,4.052177555,0.4049455841,1.078997548
 H,0,4.233784705,0.6065590813,3.3024922227
 C,0,5.8554098633,1.7586766622,0.5743195519
 H,0,6.3199246587,2.2557813132,2.7126746614
 C,0,4.8231428123,0.940683456,-0.0000808852
 H,0,6.6276333839,2.2999151291,0.0342333682
 C,0,3.0061728833,-0.5853733374,0.8502033662
 O,0,2.6812887597,-1.4572457749,1.6489939391
 N,0,2.5377821606,-0.6089411947,-0.5405204973
 O,0,2.155427462,-2.1739405975,-0.9145884495
 C,0,3.2610002265,-3.0471959026,-0.869864011
 H,0,4.0674308972,-2.7006187303,-1.5370926875
 H,0,2.9010719027,-4.0164696539,-1.2541465936
 H,0,3.6409512185,-3.1760273597,0.1546053274
 Rh,0,0.8629617392,0.5152465875,-0.0501043857
 C,0,2.9910622156,-0.6200233135,-2.9729956305
 C,0,1.6409330312,-0.6633944282,-3.3613853299
 C,0,3.954589214,-1.0694542333,-3.8957001373
 C,0,1.2759199821,-1.0695592015,-4.6432656613
 H,0,0.8730455549,-0.4163800098,-2.6343133227
 C,0,3.5895542059,-1.4819731746,-5.1792646253
 H,0,5.001767088,-1.1276110072,-3.5993544924
 C,0,2.2479690861,-1.4686640943,-5.5663491551
 H,0,0.2170620933,-1.0910775898,-4.911952907
 H,0,4.3594921985,-1.825831992,-5.874236501
 H,0,1.9600324913,-1.7877537489,-6.5709319385
 C,0,3.4023197368,-0.1729631486,-1.6167817114
 C,0,4.513514836,0.5906526422,-1.3710014829
 C,0,5.4120252179,1.1582783243,-2.4371976185
 H,0,6.3373088123,0.5644597738,-2.5314796233
 H,0,5.718459033,2.1776281056,-2.1657031762
 H,0,4.9327515357,1.199689187,-3.4216423
 H,0,1.055939175,-2.5467646205,0.0932501237
 C,0,-0.0571137834,-2.0644017419,1.5885175957
 O,0,0.0405542184,-0.8459164605,1.4166725583
 O,0,0.4129385939,-2.9575319017,0.7652645659
 C,0,-1.1316742851,-4.0865145766,2.6790921067
 C,0,0.4228534252,-2.5356250098,3.9342345791
 C,0,-1.5364001041,-4.7524154623,3.9973409977
 H,0,-0.2894962501,-4.6443614642,2.2438421351
 H,0,-1.9565434051,-4.1384301755,1.9542690143
 C,0,0.0272722311,-3.2100968437,5.2508881449
 H,0,1.3249403412,-3.0209940055,3.52751498

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H,0,0.6918673763,-1.4806440531,4.0948665744
C,0,-0.4131007873,-4.6611199746,5.0346260739
H,0,-1.795610793,-5.8073343184,3.8073240942
H,0,-2.4513985402,-4.2826567785,4.3975499718
H,0,0.8793211005,-3.1680677905,5.9496868635
H,0,-0.7906918248,-2.6465849471,5.732197561
H,0,-0.7282676927,-5.1146986969,5.9892163239
H,0,0.4524244841,-5.2490962299,4.6774011399
C,0,-0.7024140579,-2.6129385985,2.8584542362
C,0,-1.8961097647,-1.7279447578,3.2465074917
H,0,-2.3544507691,-2.0700247654,4.1833475108
H,0,-1.5775973809,-0.6864093103,3.381419081
H,0,-2.6740000781,-1.7560894615,2.470394513
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INT-10

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Opt @ B3LYP-D3(BJ)/def2-SVP in gas phase
SCF Done: E(RB3LYP) = -4396.49617696 a.u.
Zero-point correction = 1.186124 Hartree/Particle
Sum of electronic and thermal Free Energies = -4395.411975 a.u.
Sp @ RI-PWPB95-D3(BJ)/def2-TZVPP in 2,2,2-trifluoroethanol
FINAL SINGLE POINT ENERGY = -4397.358297853446 a.u.
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O,0,1.6557015991,-0.3434173587,2.9277580098
O,0,4.0700441272,3.145564559,-3.163232078
C,0,0.7895845294,2.6641596996,-1.6977785314
C,0,-0.0473547015,3.2699268147,-0.693882756
C,0,0.5512360044,2.9017934547,0.5636112282
C,0,1.7081747288,2.0941496256,0.3513424177
C,0,1.8405957033,1.9231868833,-1.0841612306
C,0,2.6812196839,1.6738166042,1.4199790808
C,0,3.2345520535,0.2711671957,1.3035595172
C,0,2.6463571561,-0.7542704049,2.112439874
C,0,3.1135850549,-2.0520499256,2.0495975254
C,0,4.1624742595,-2.3997496816,1.1599126296
C,0,4.6186213497,-3.7408806153,1.035484548
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C,0,6.1981187888,-3.073461174,-0.6757883217
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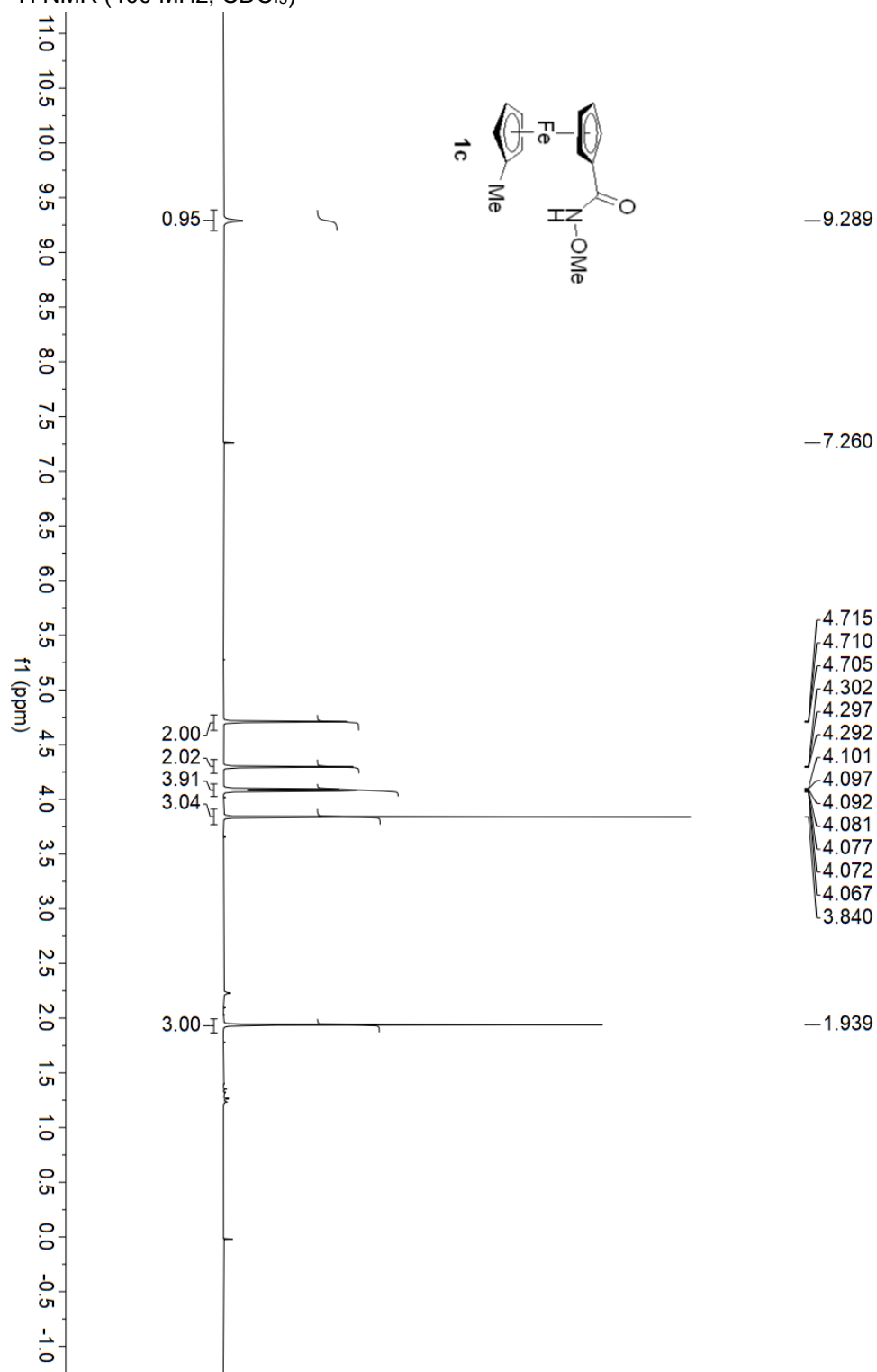
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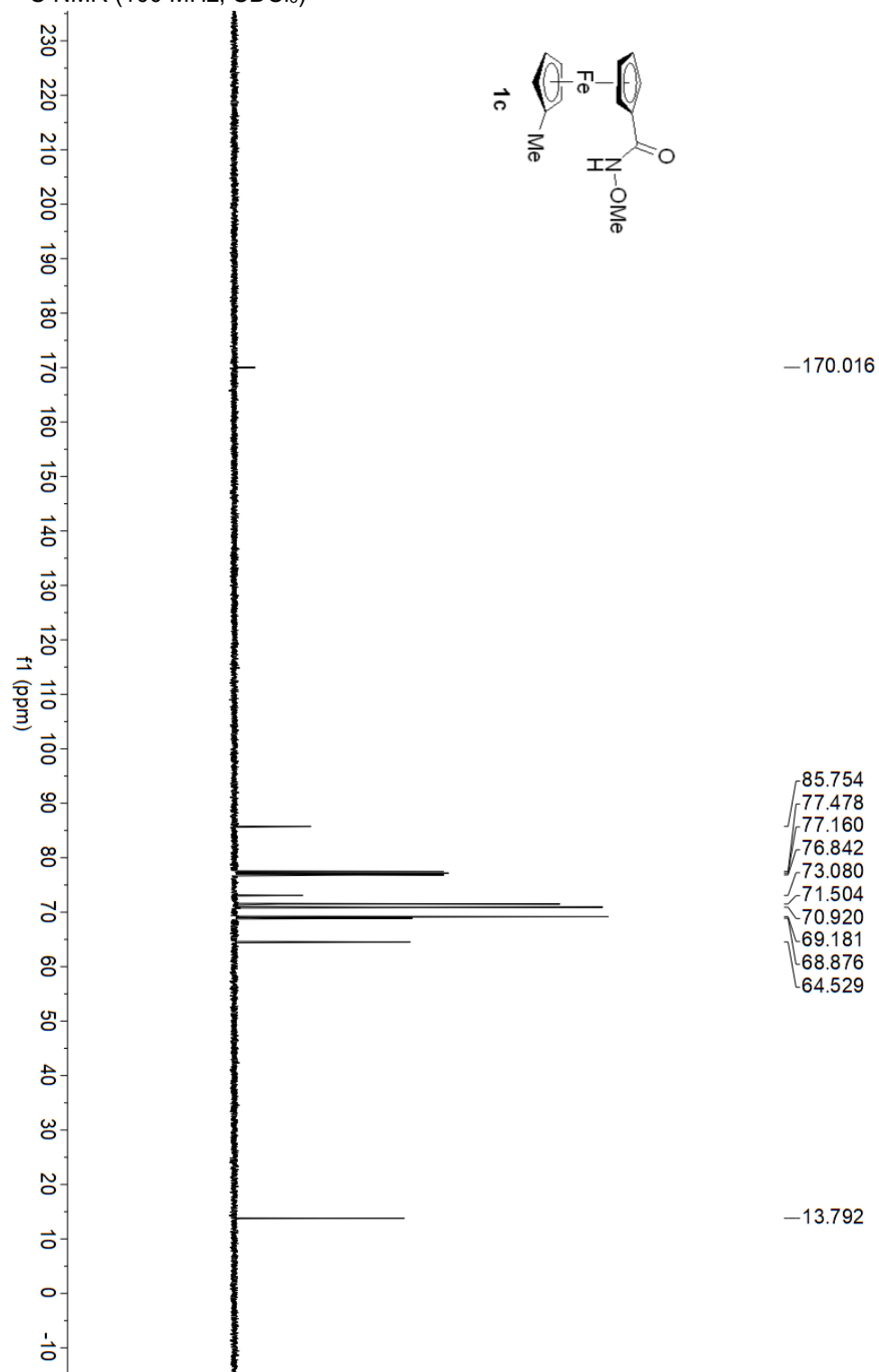
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11. Copies of NMR spectra

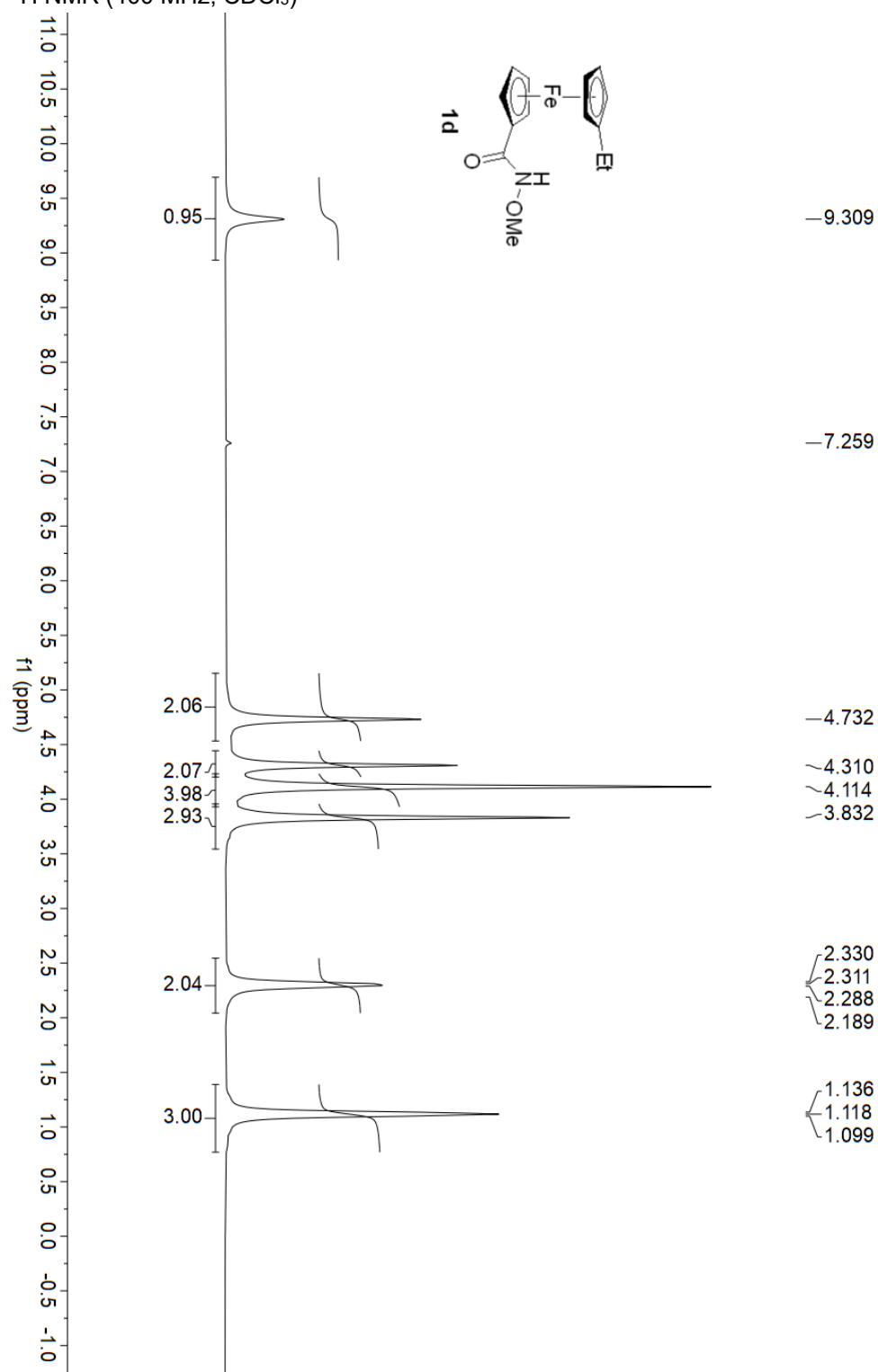
^1H NMR (400 MHz, CDCl_3)



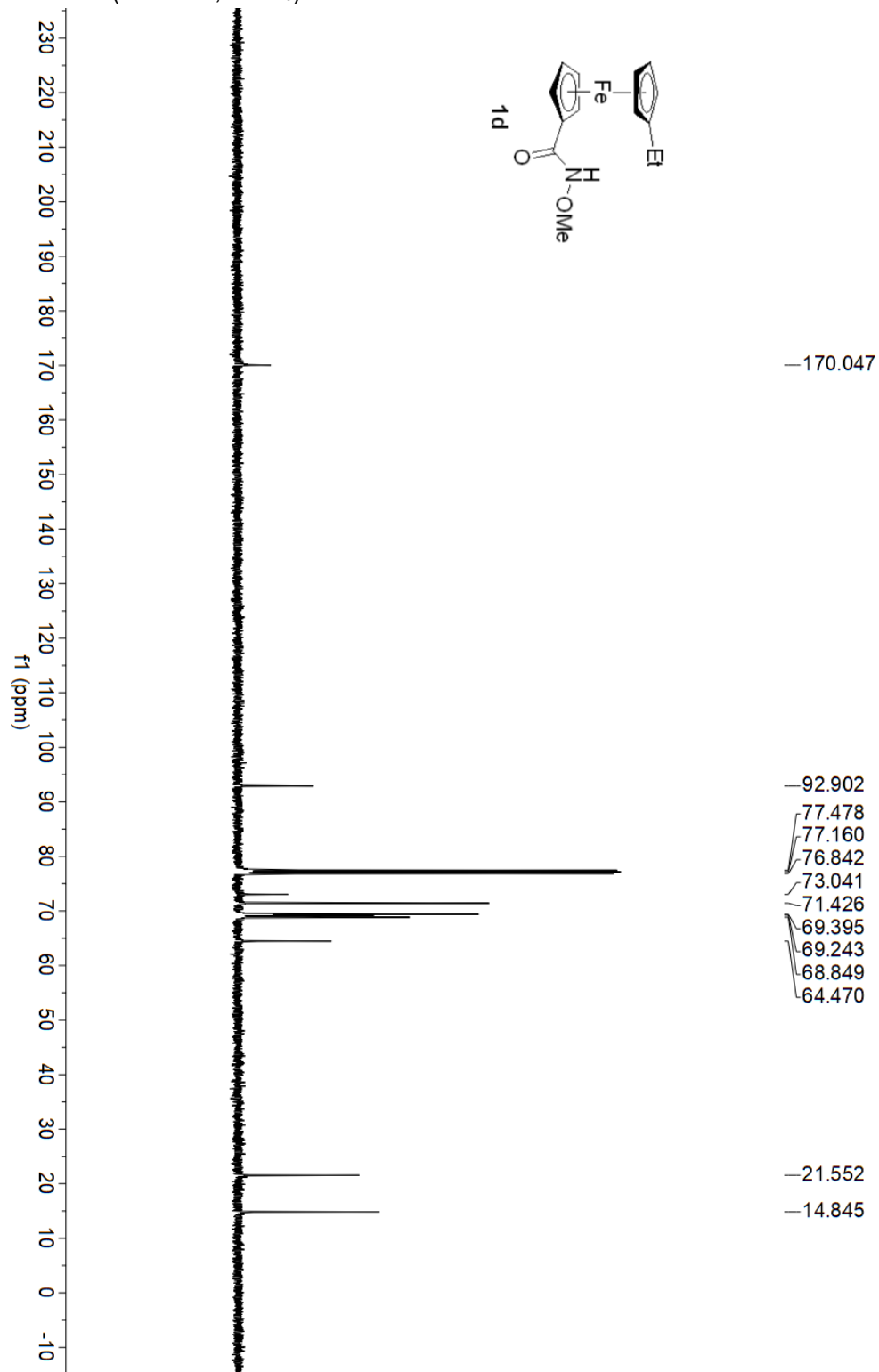
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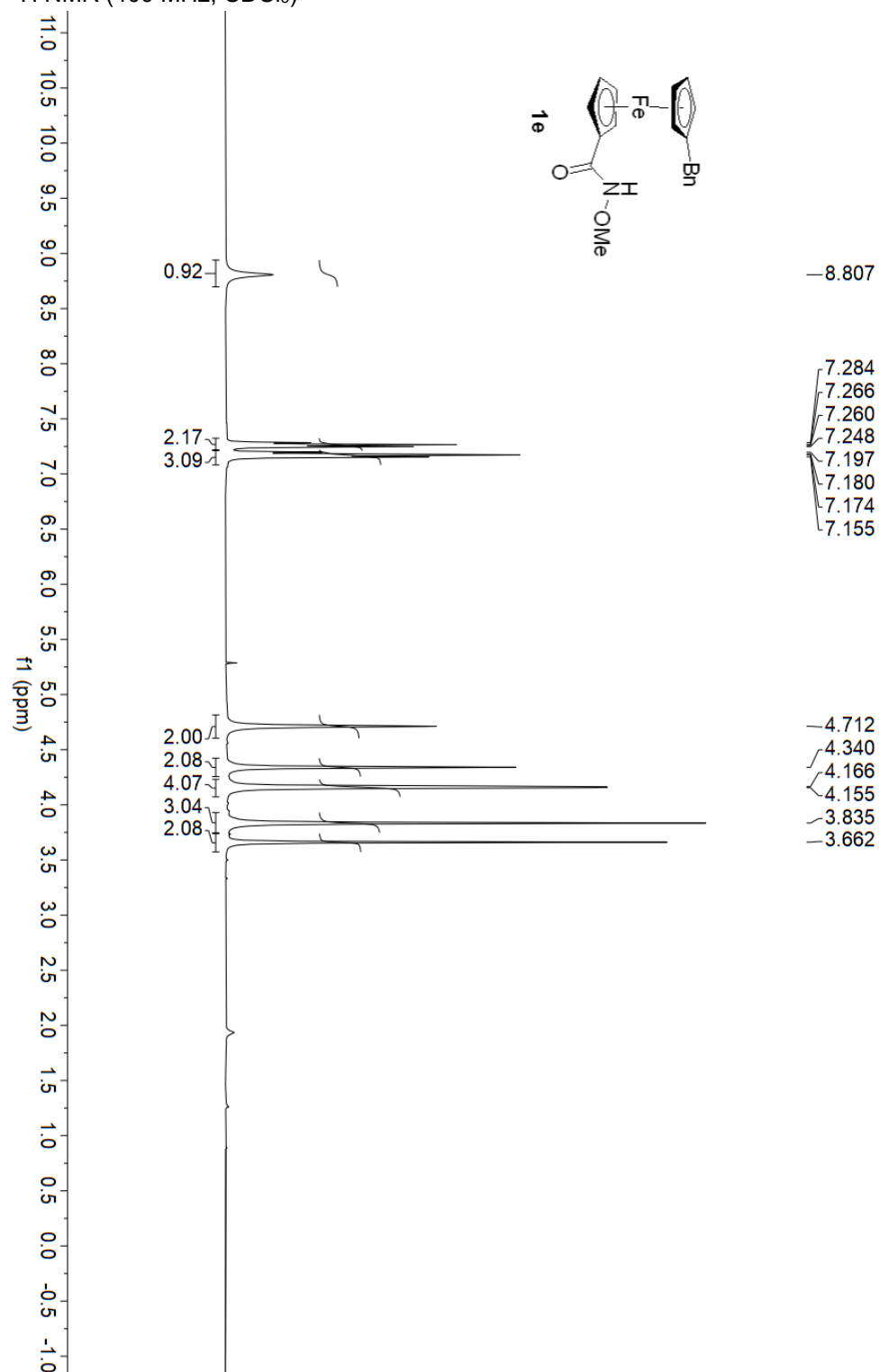
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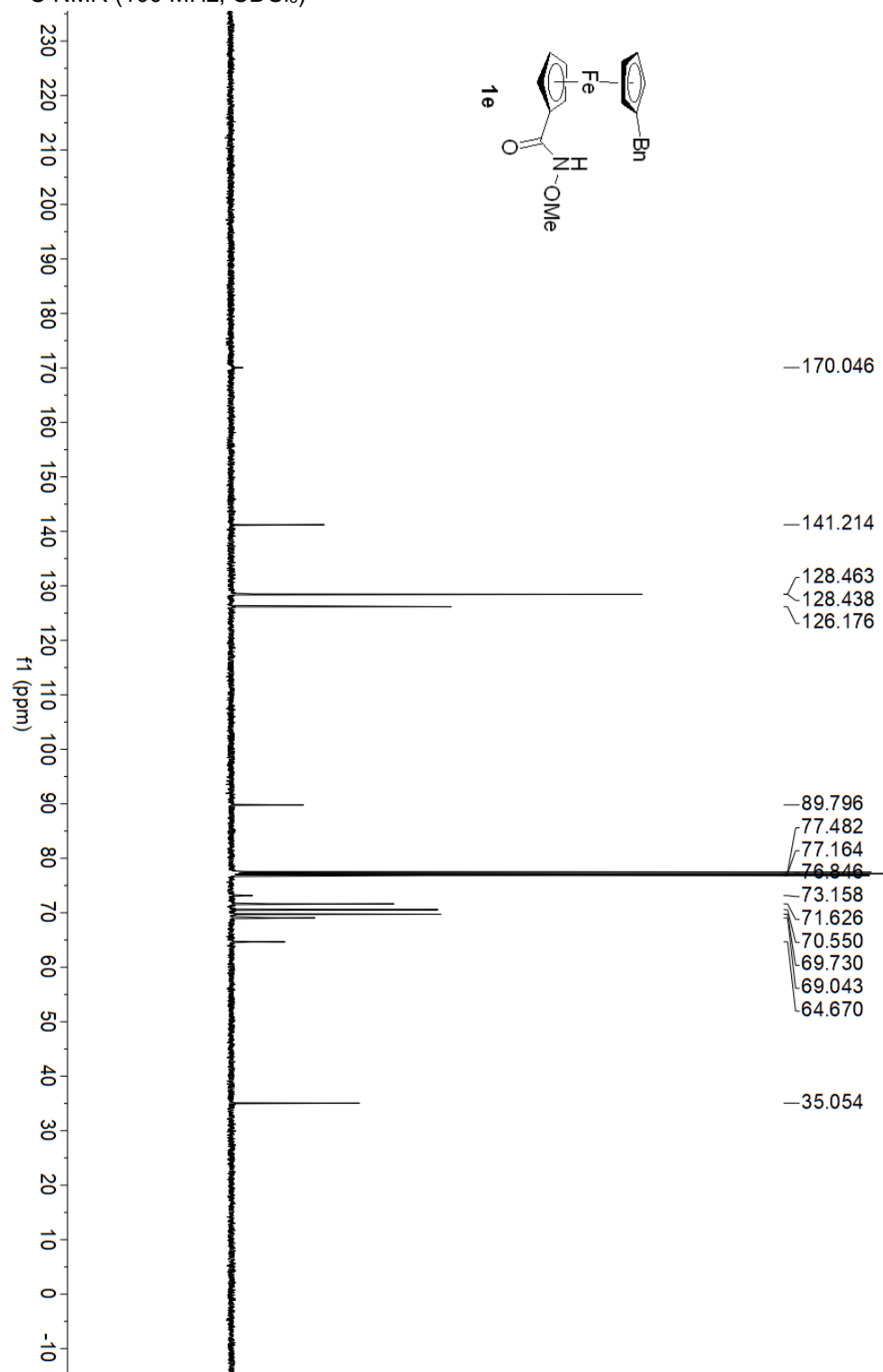
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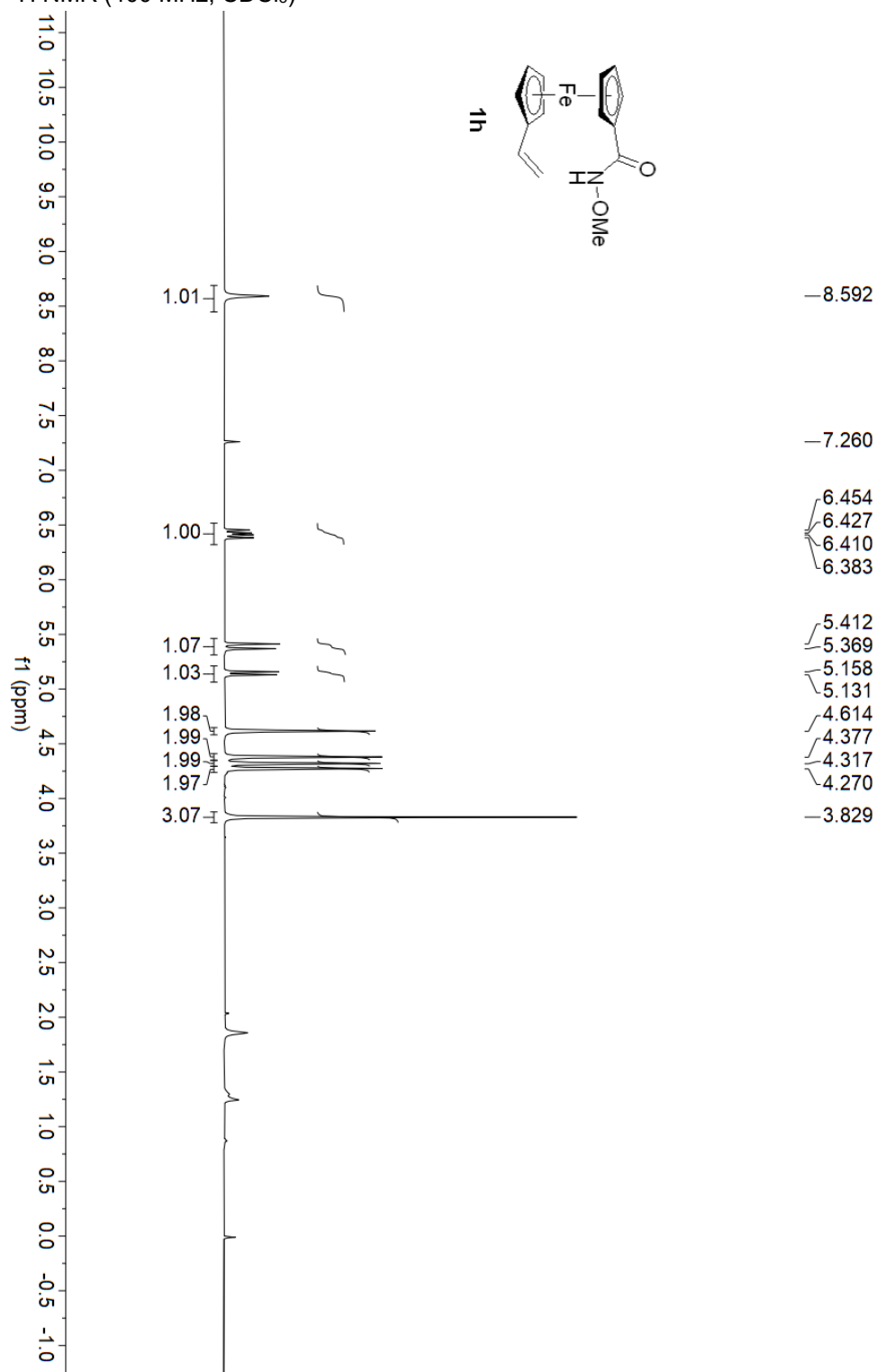
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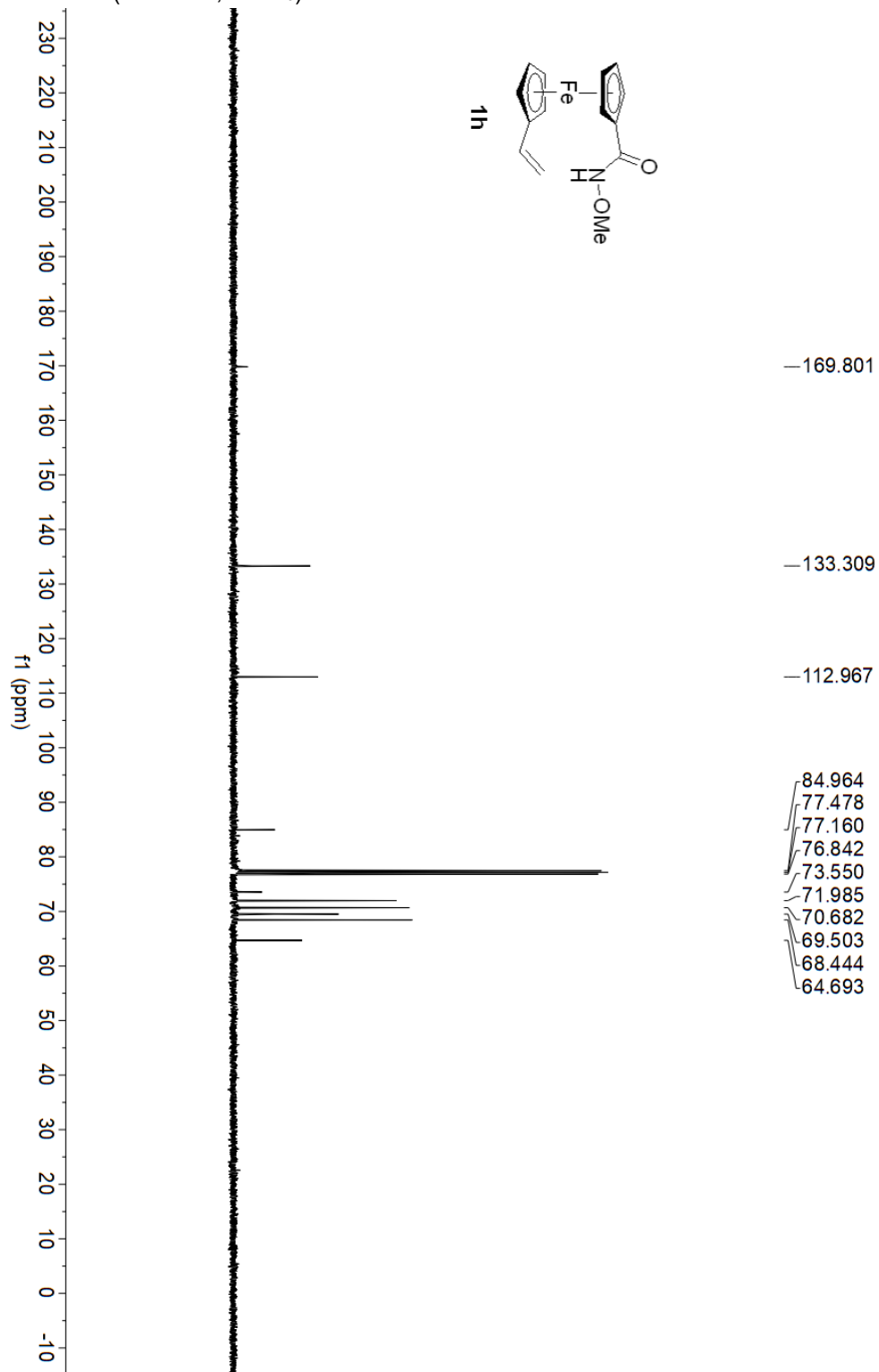
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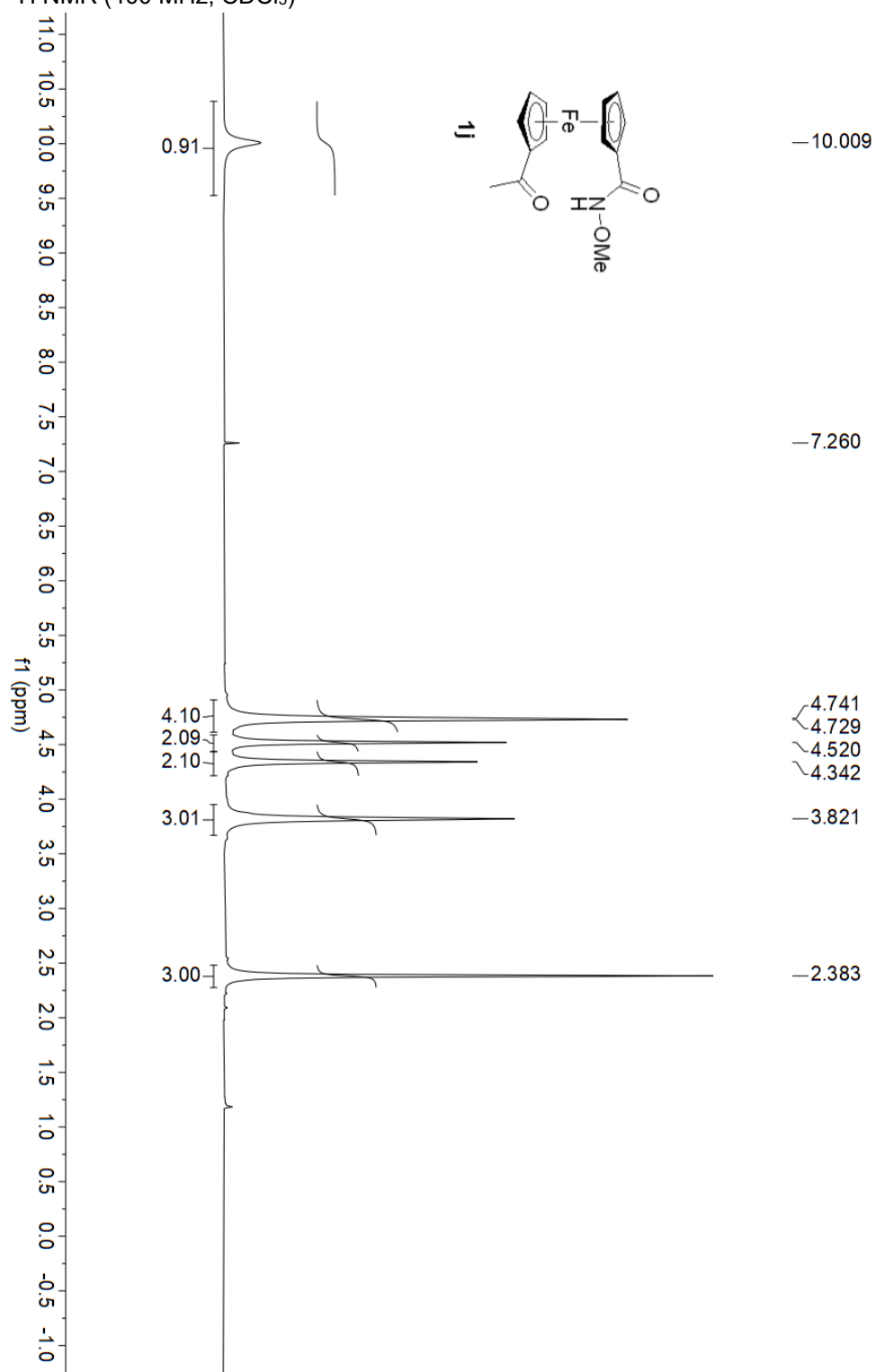
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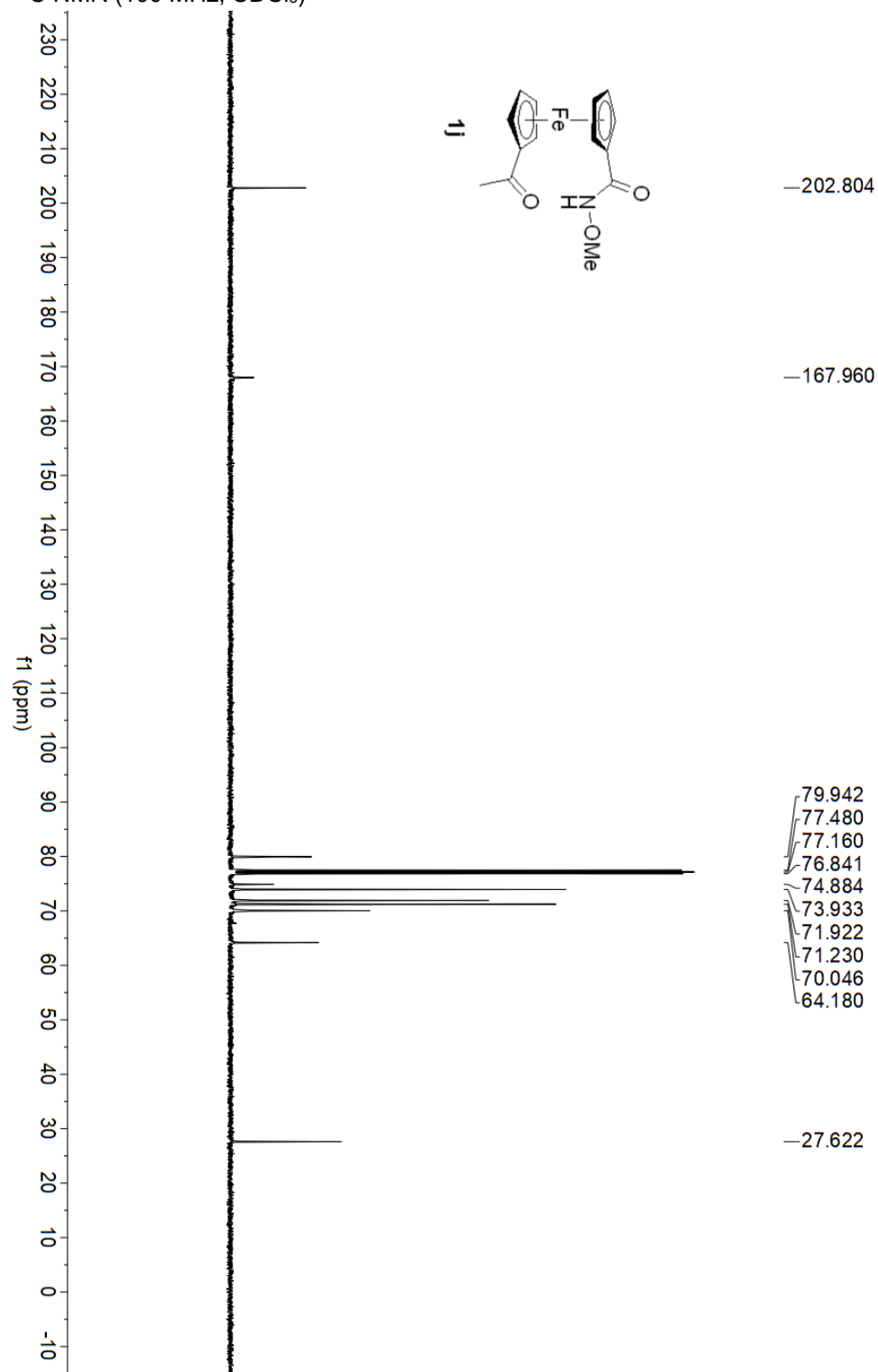
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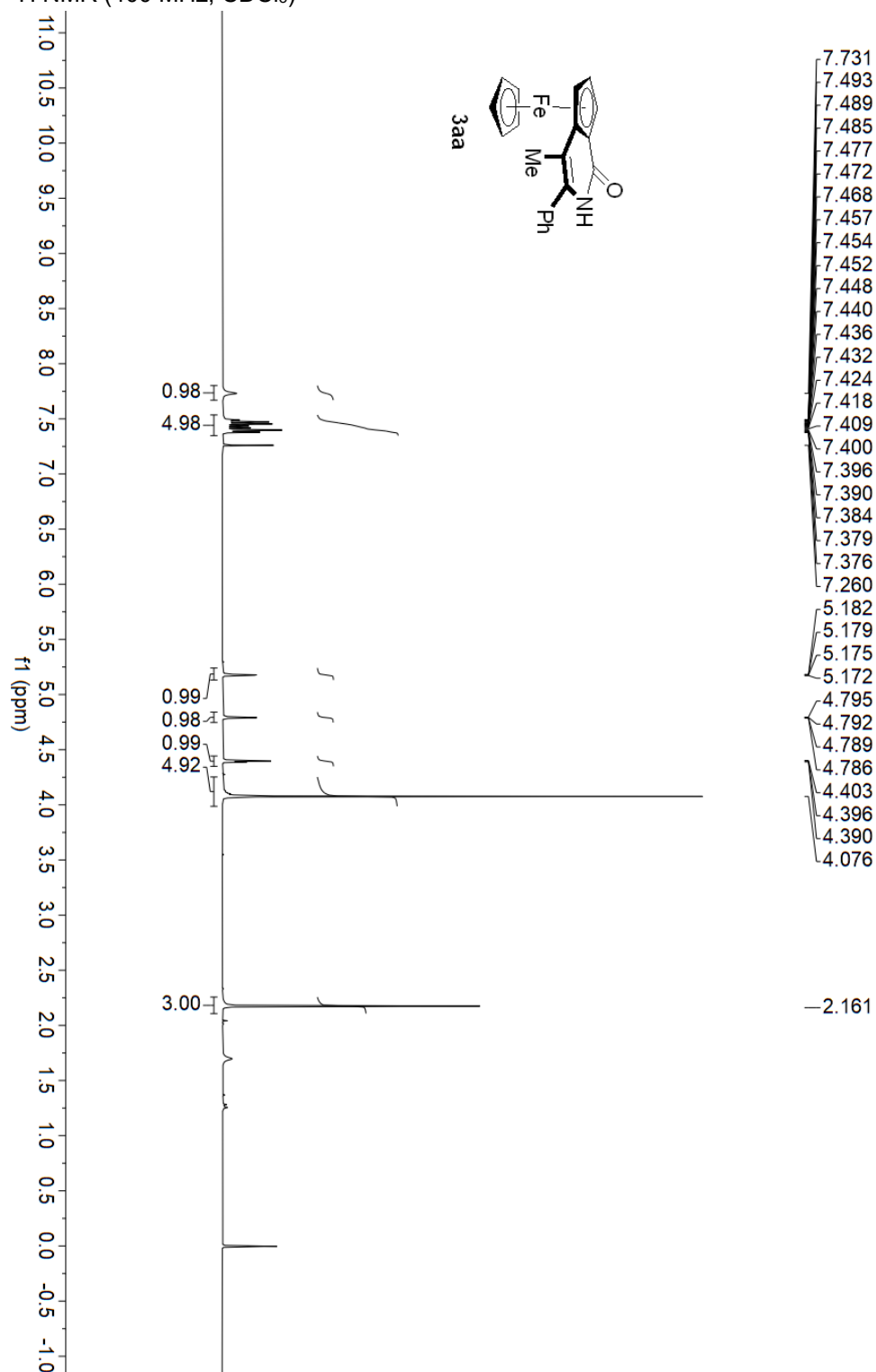
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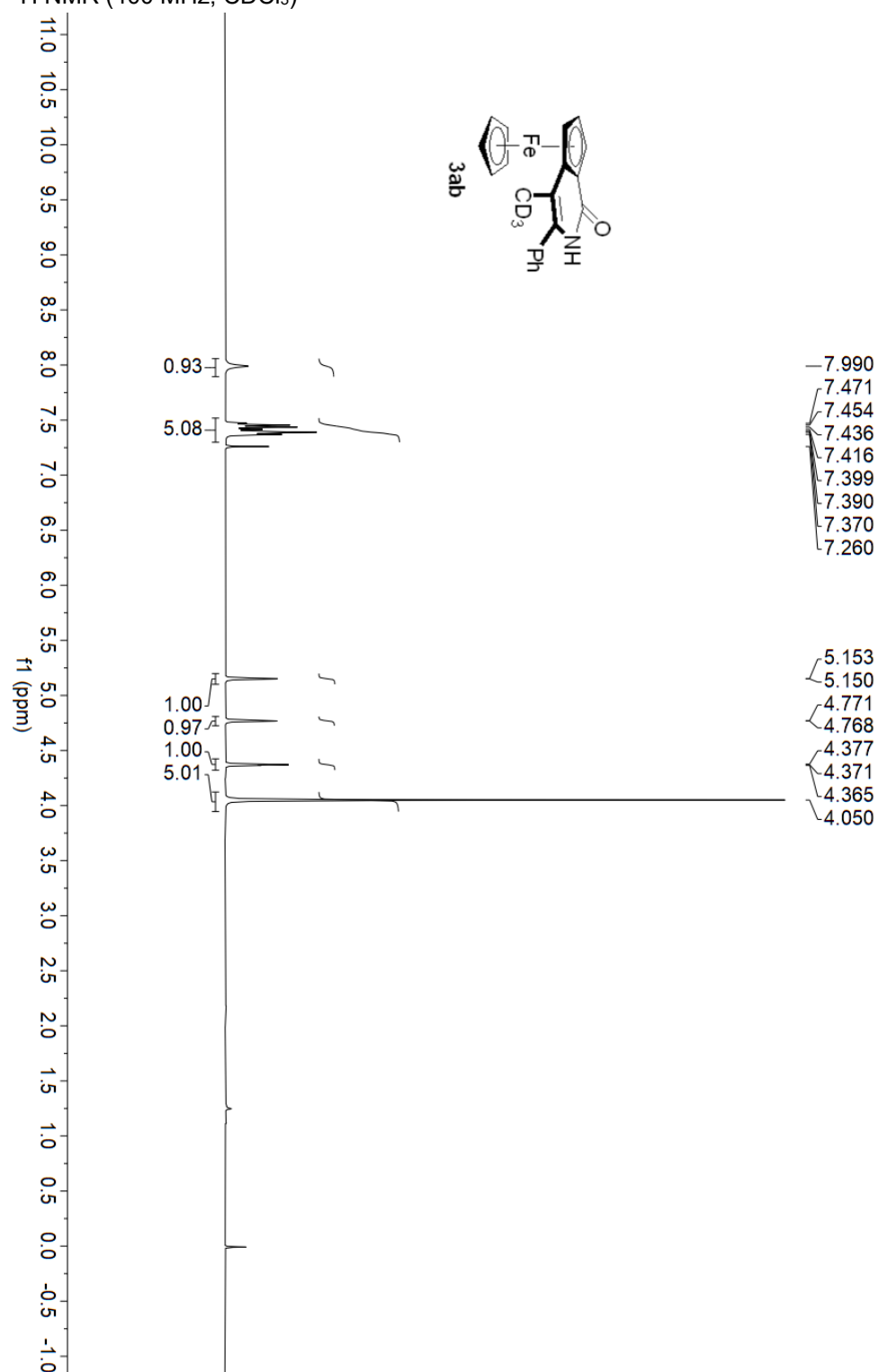
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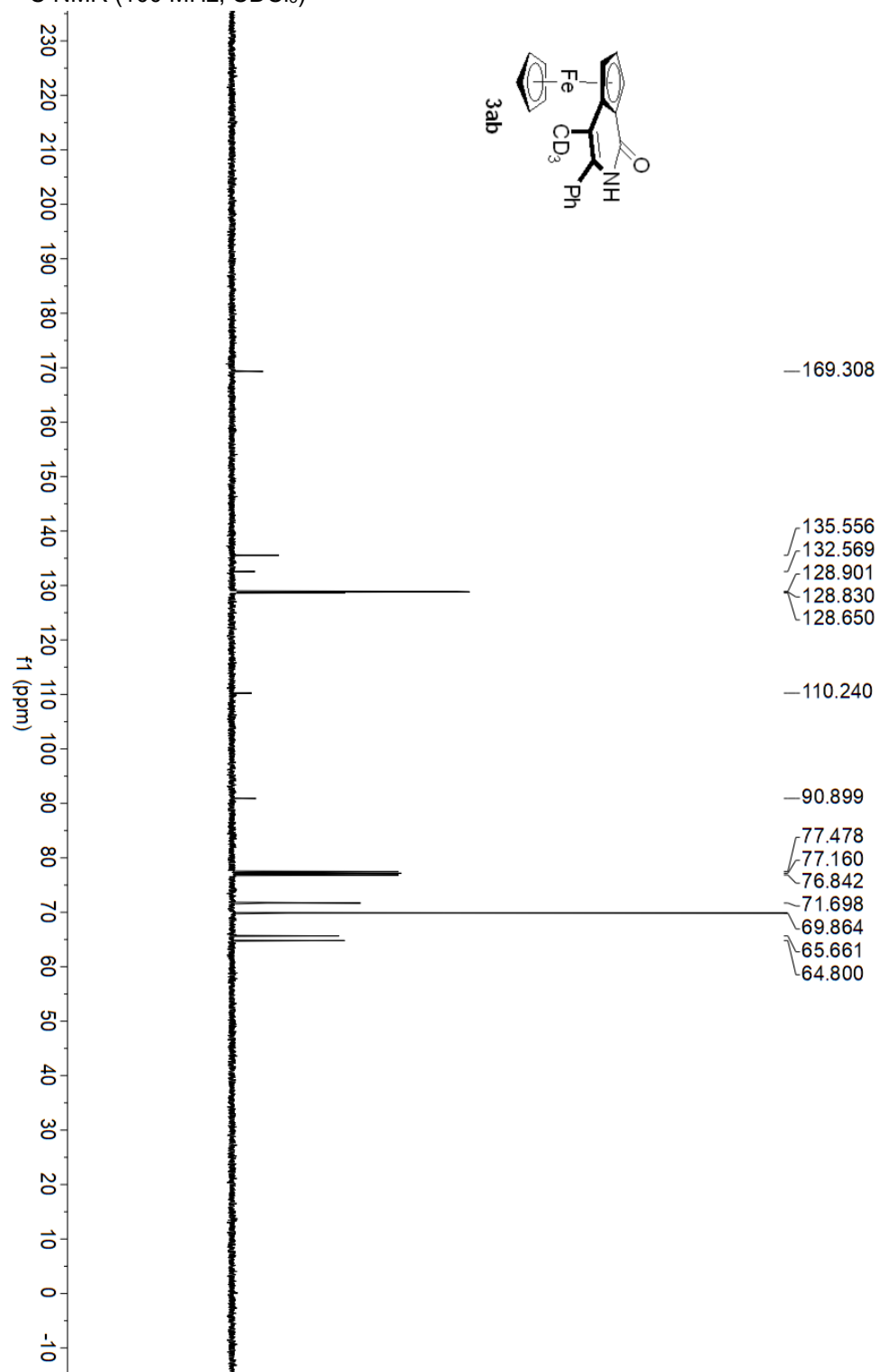
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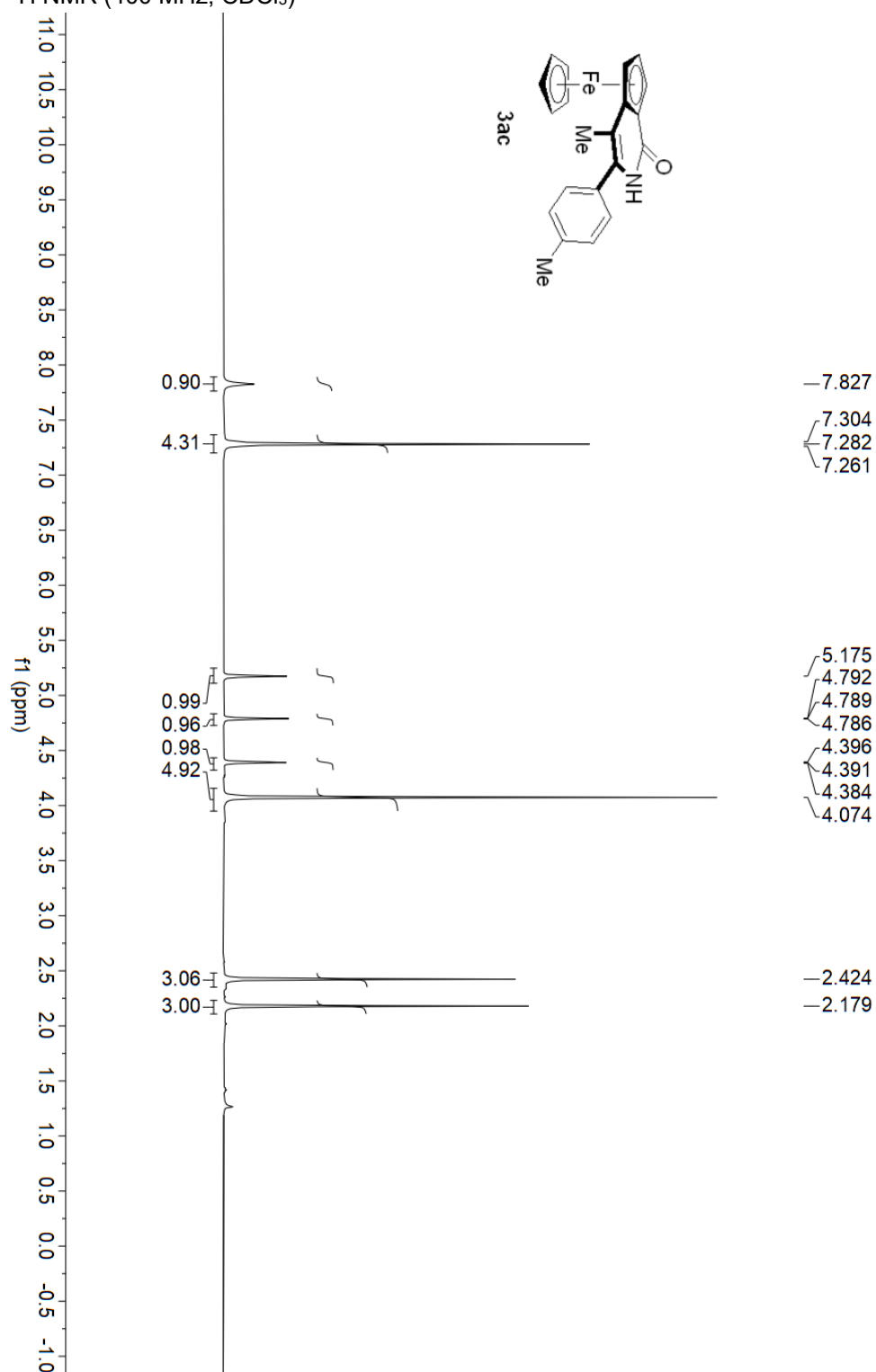
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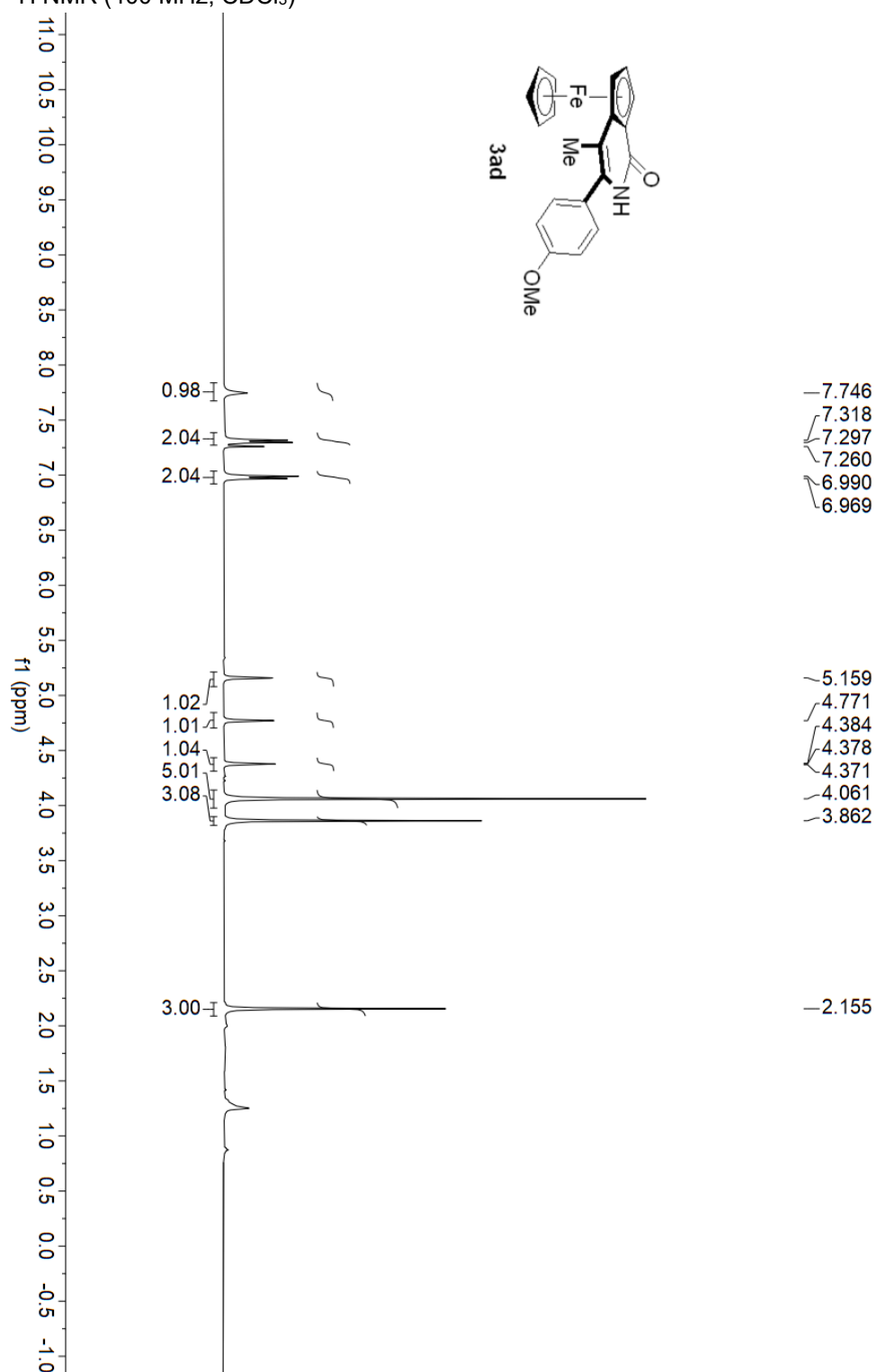
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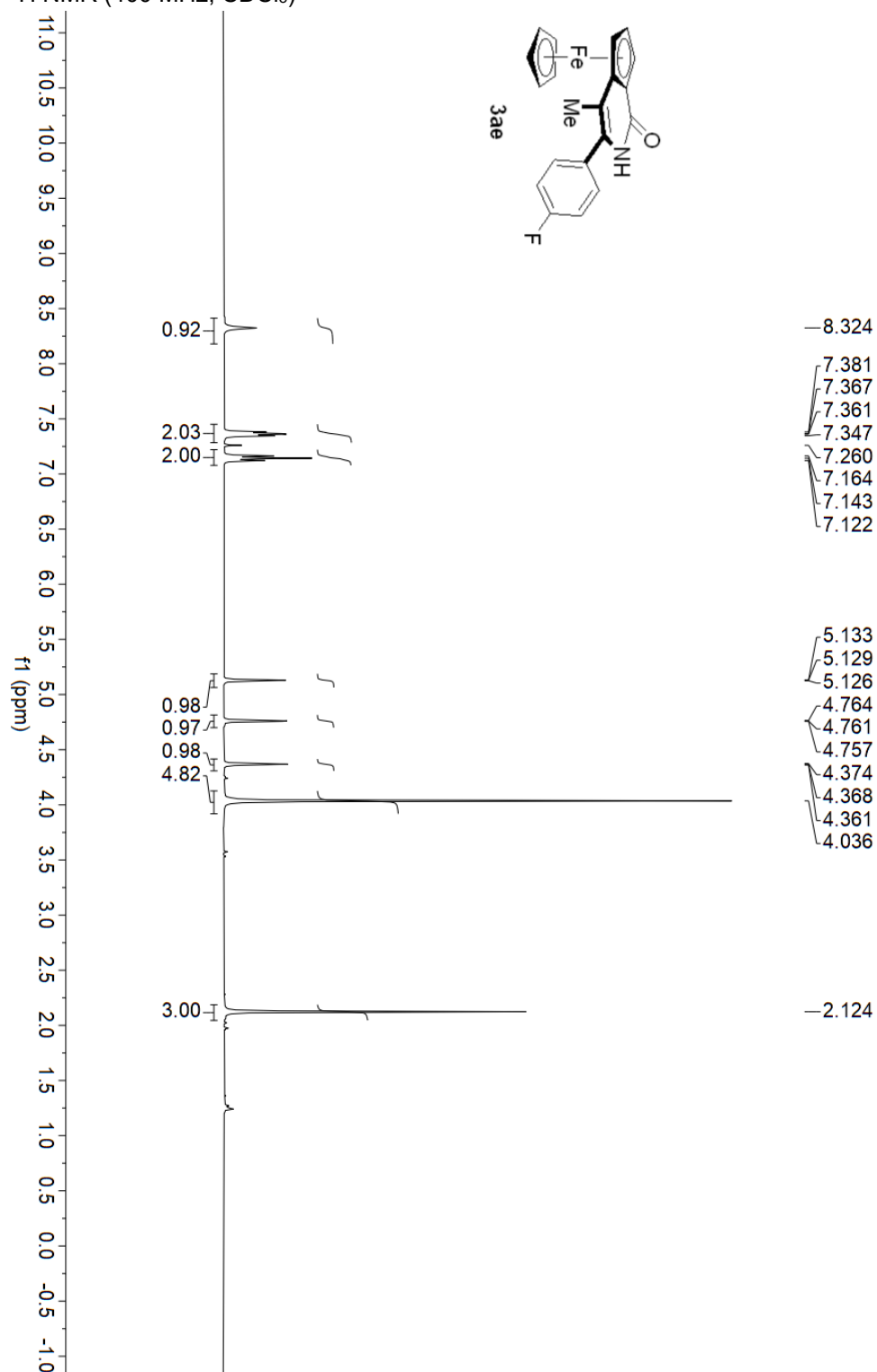
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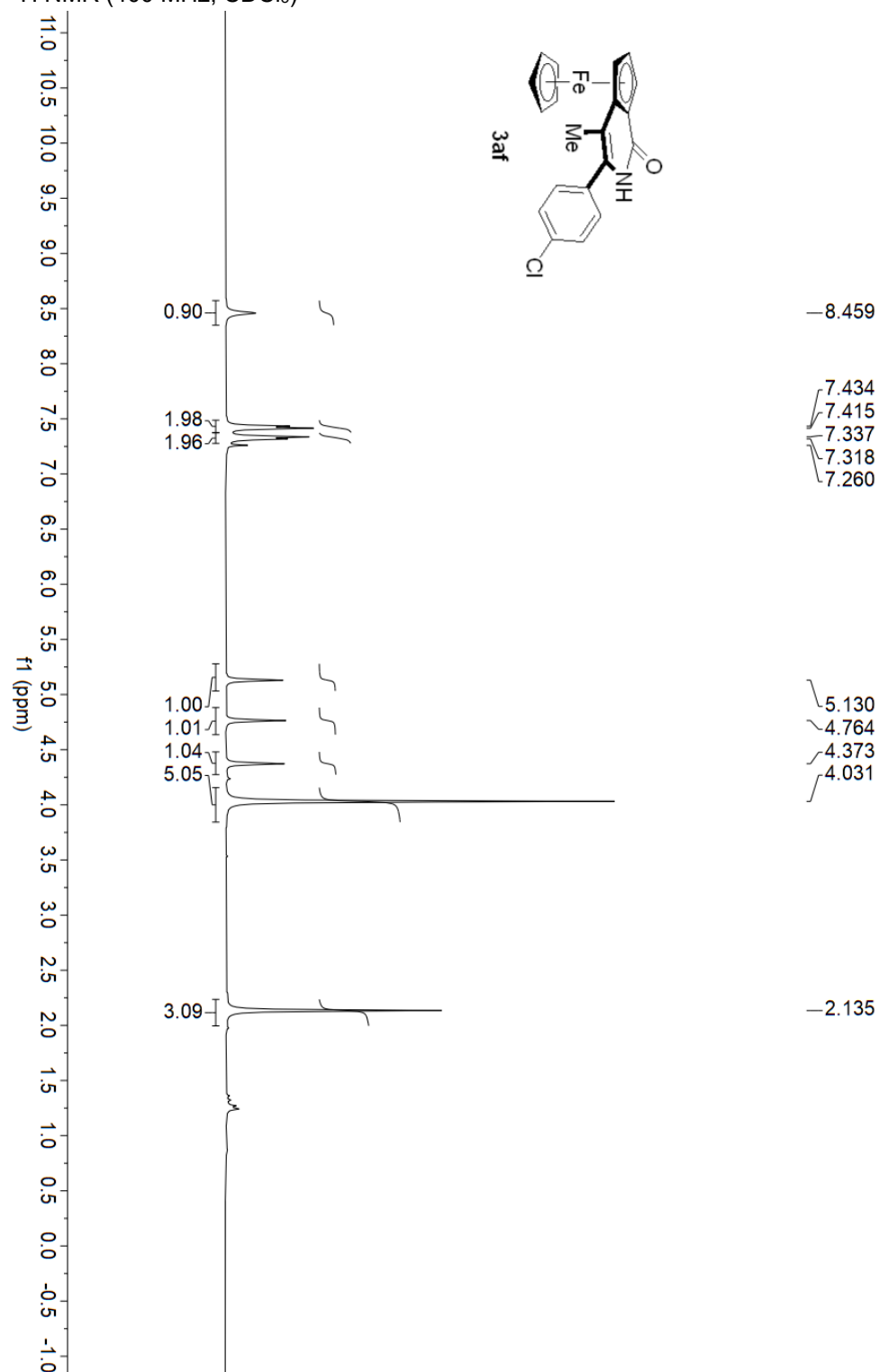
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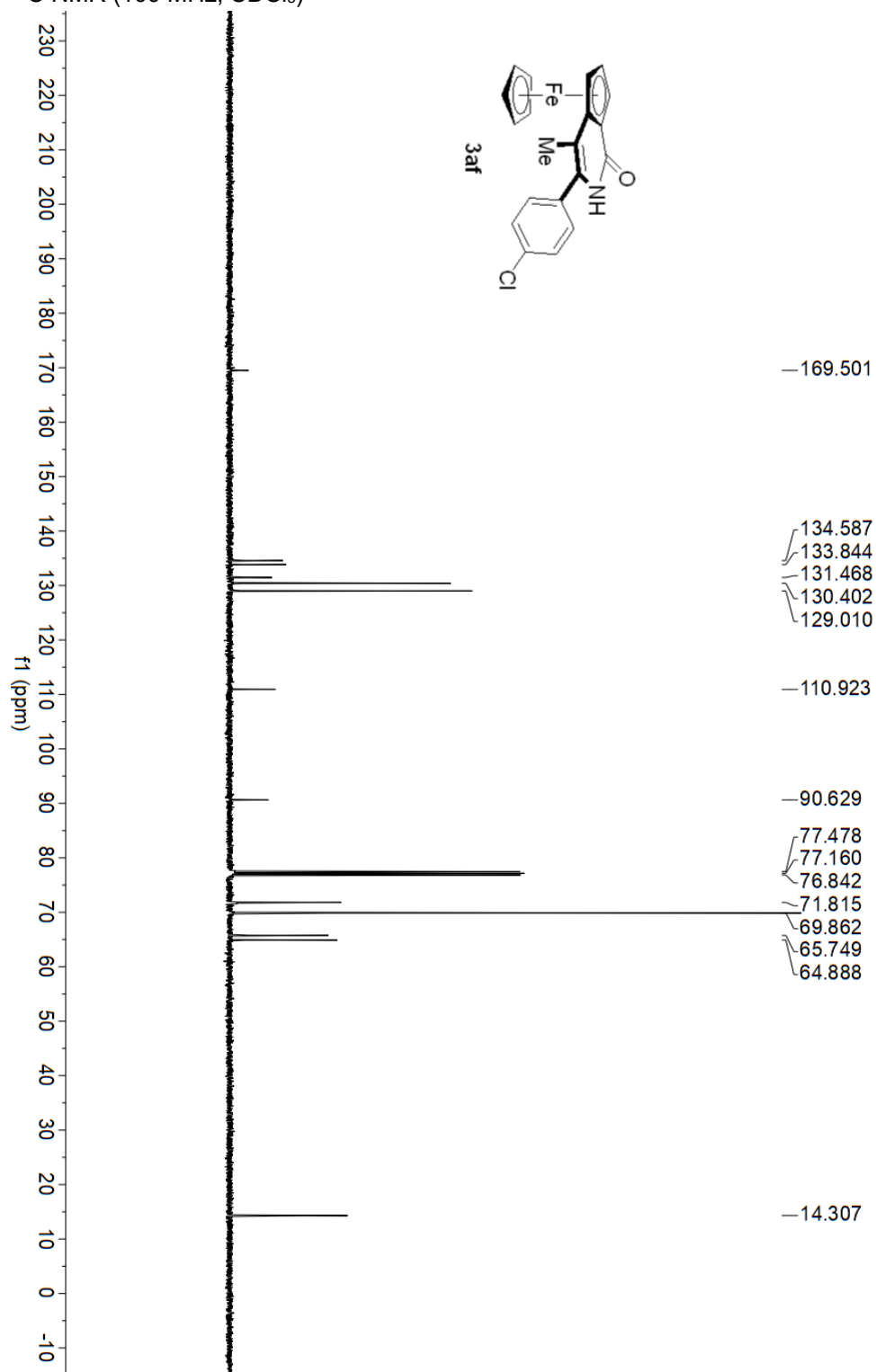
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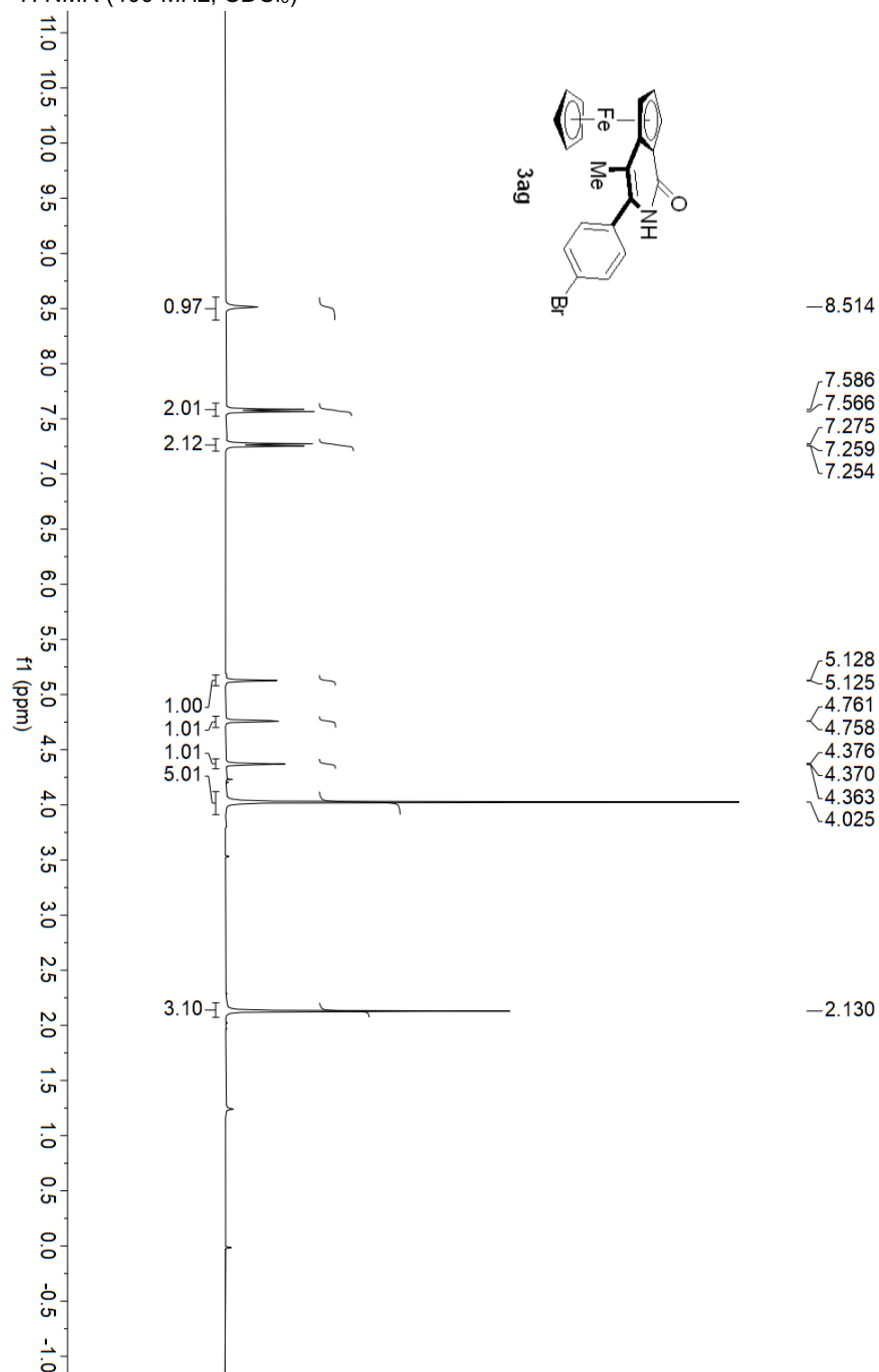
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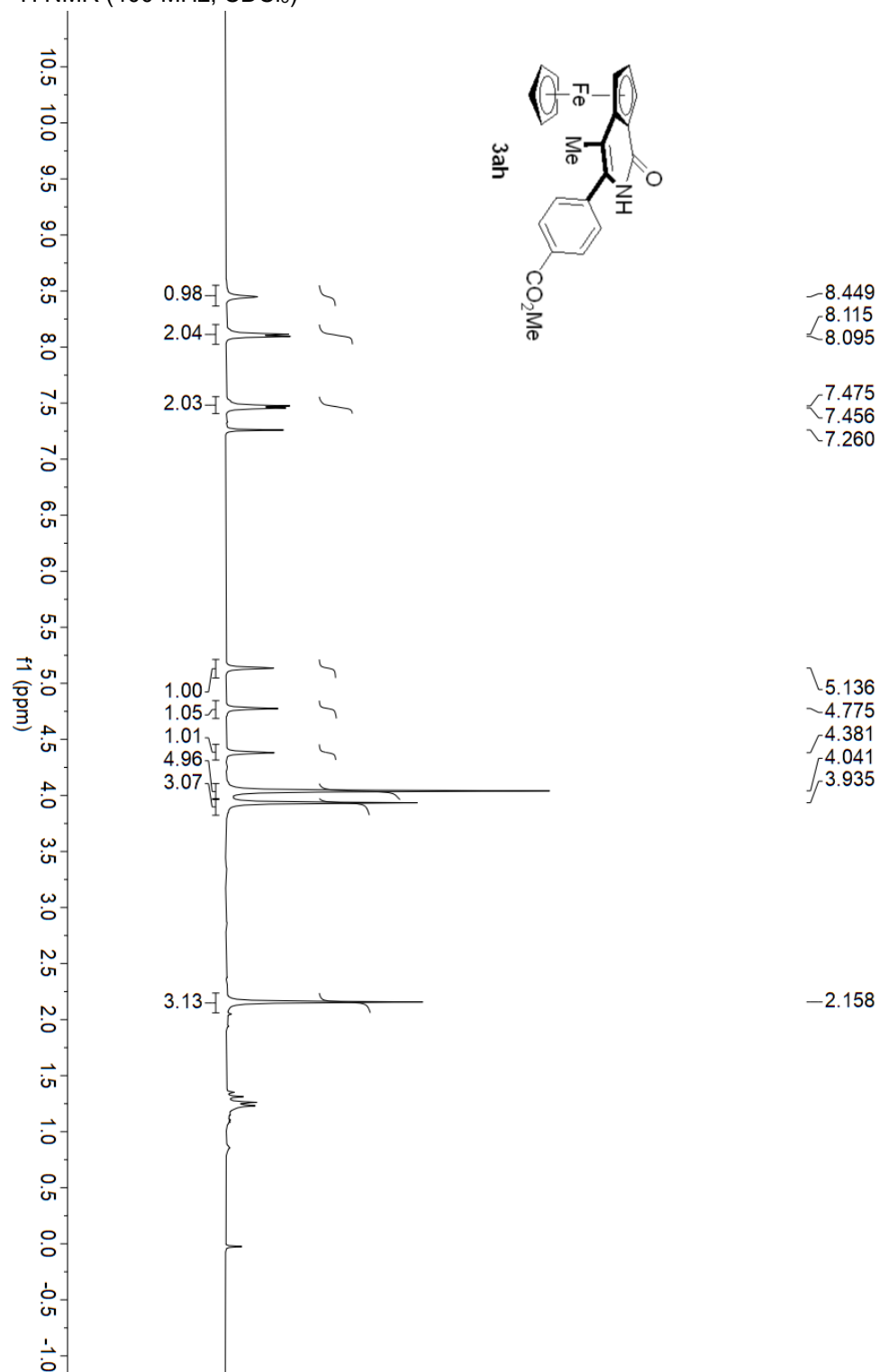
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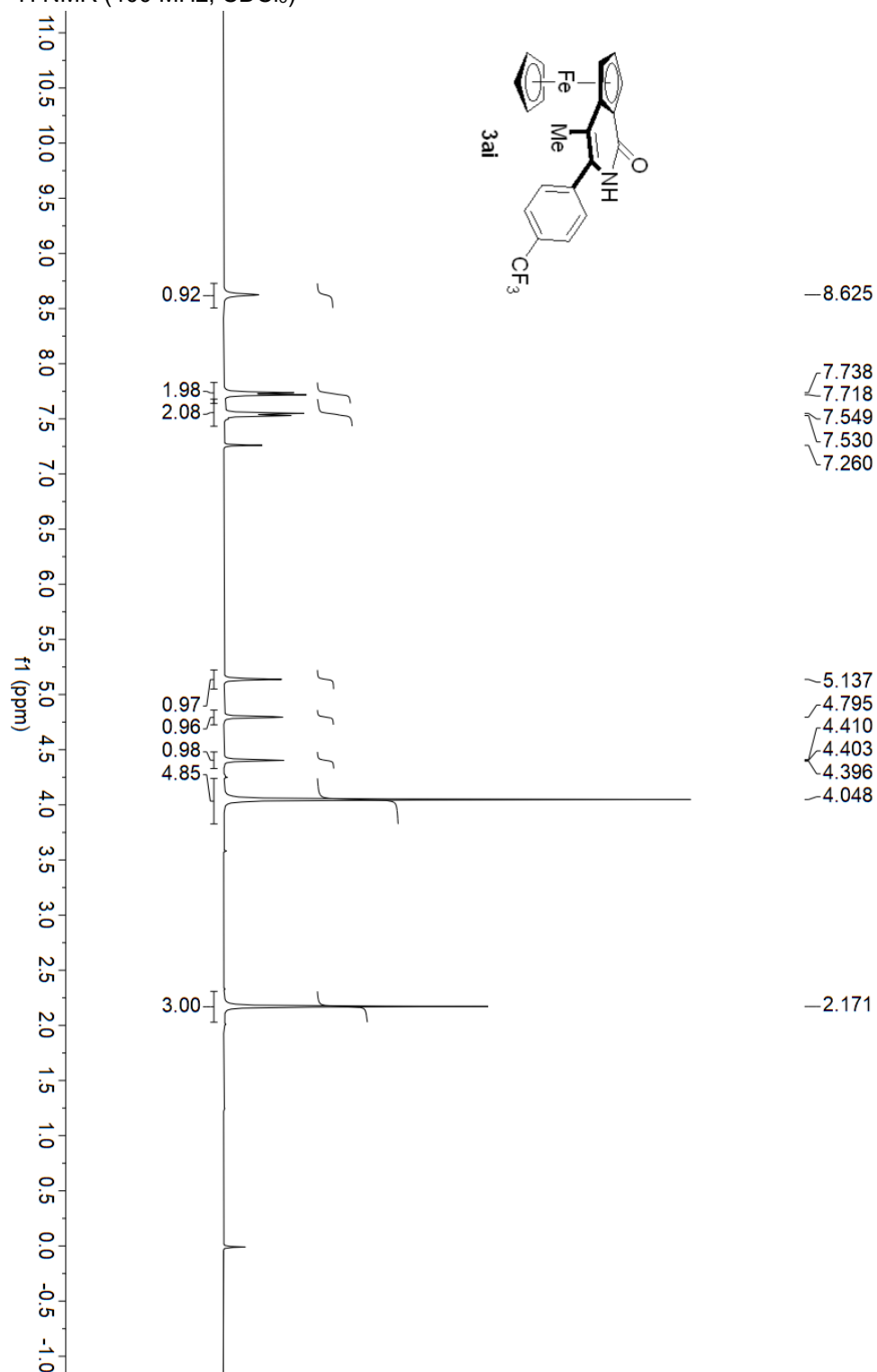
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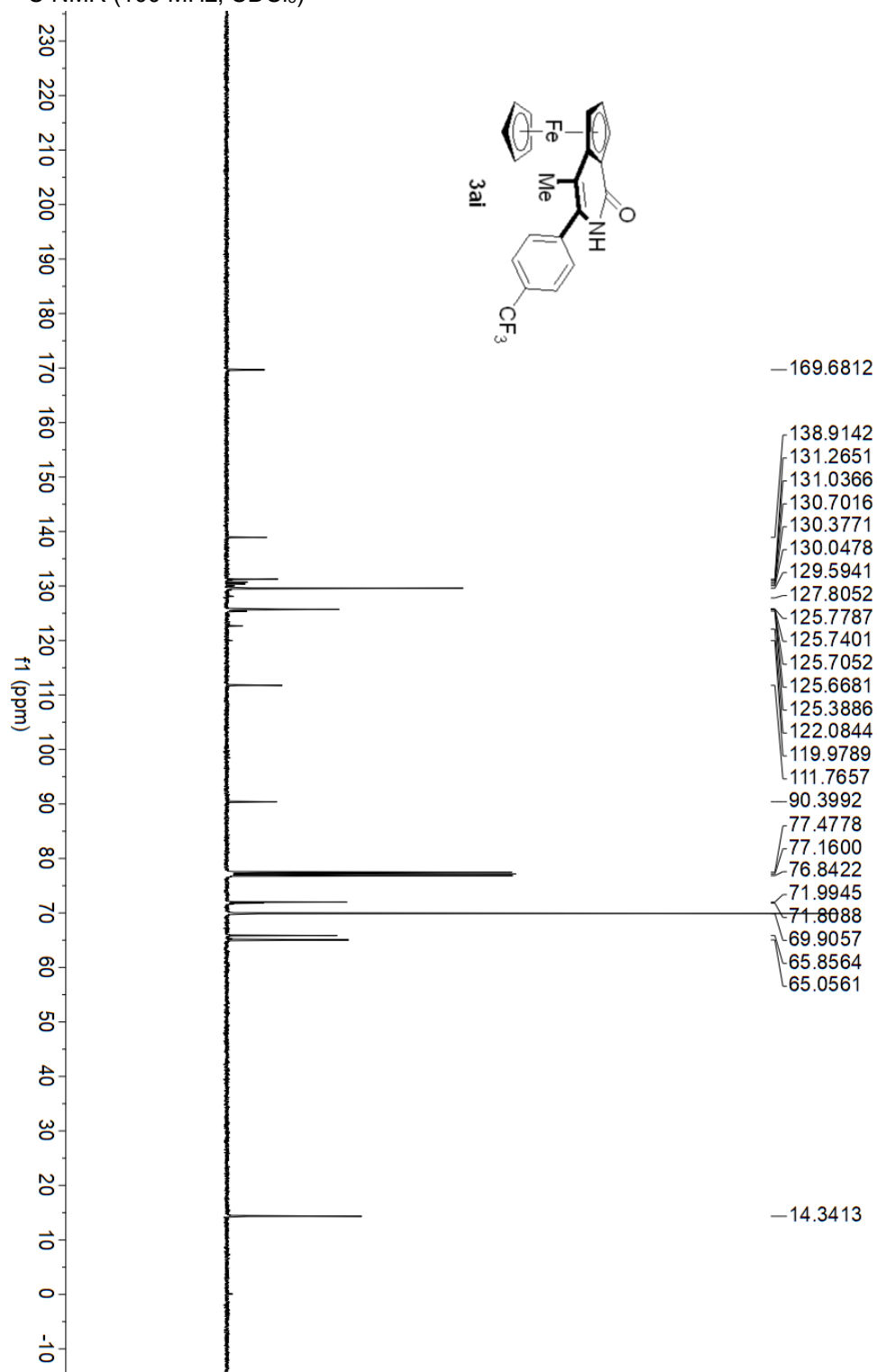
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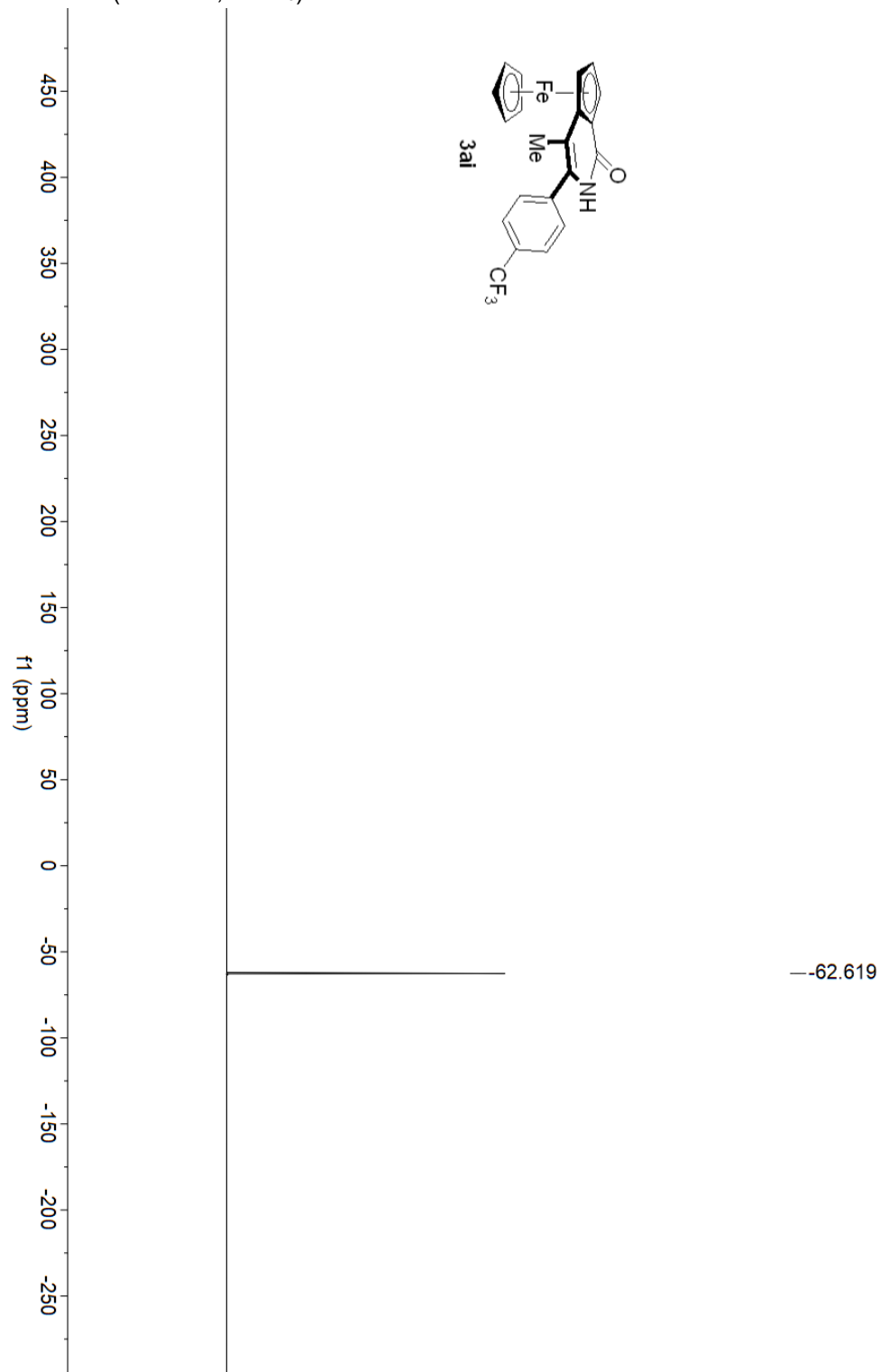
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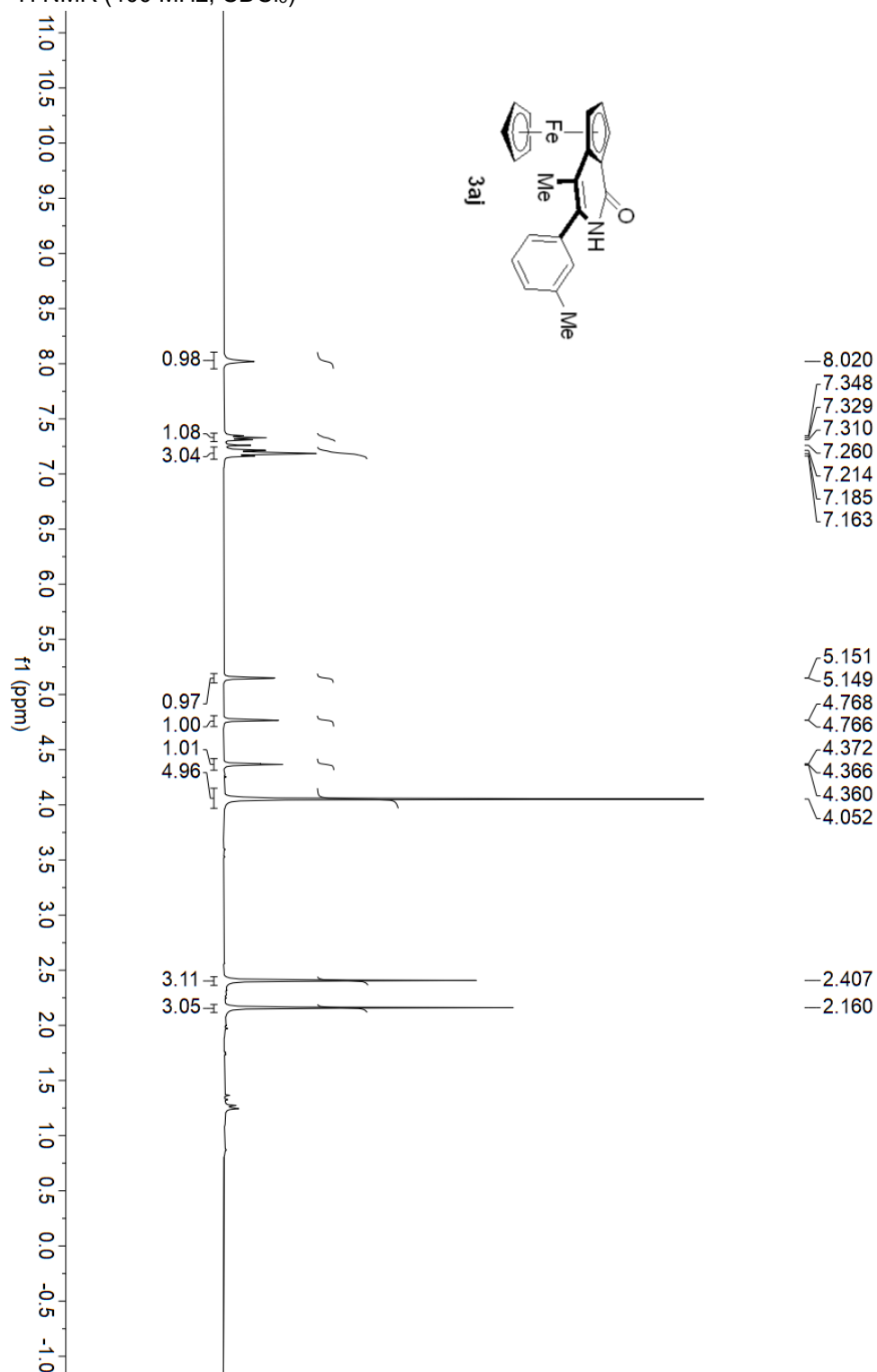
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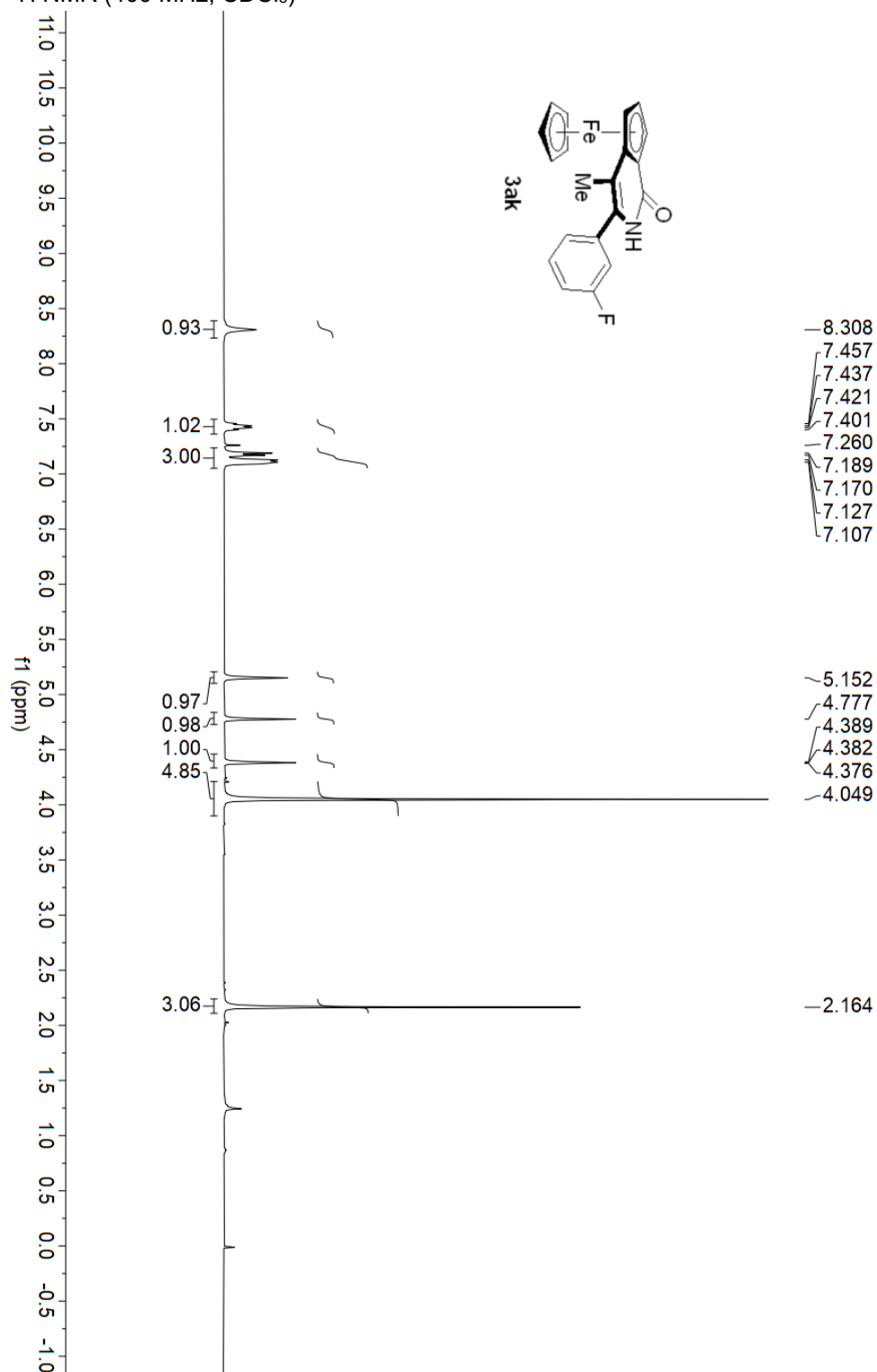
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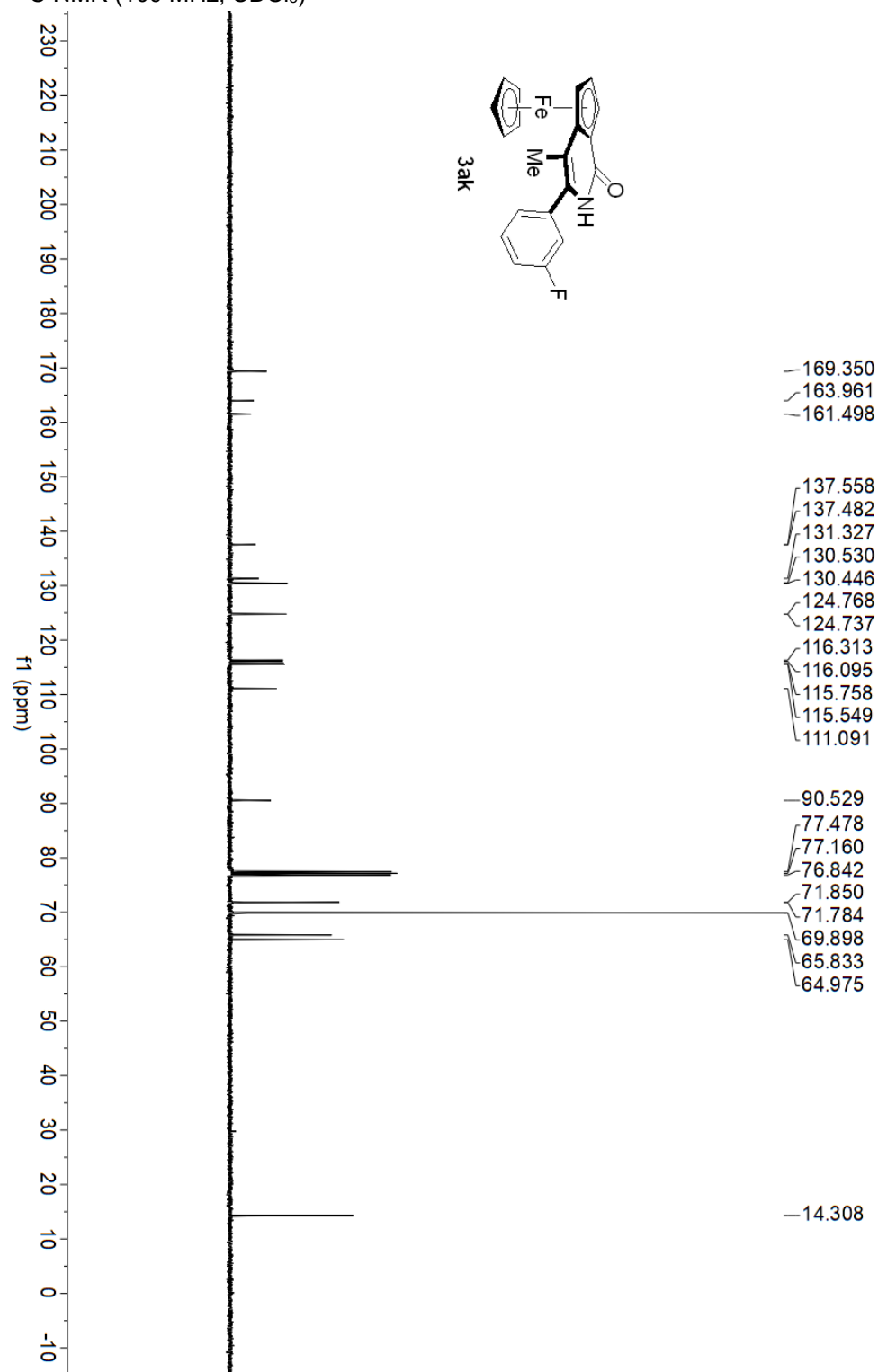
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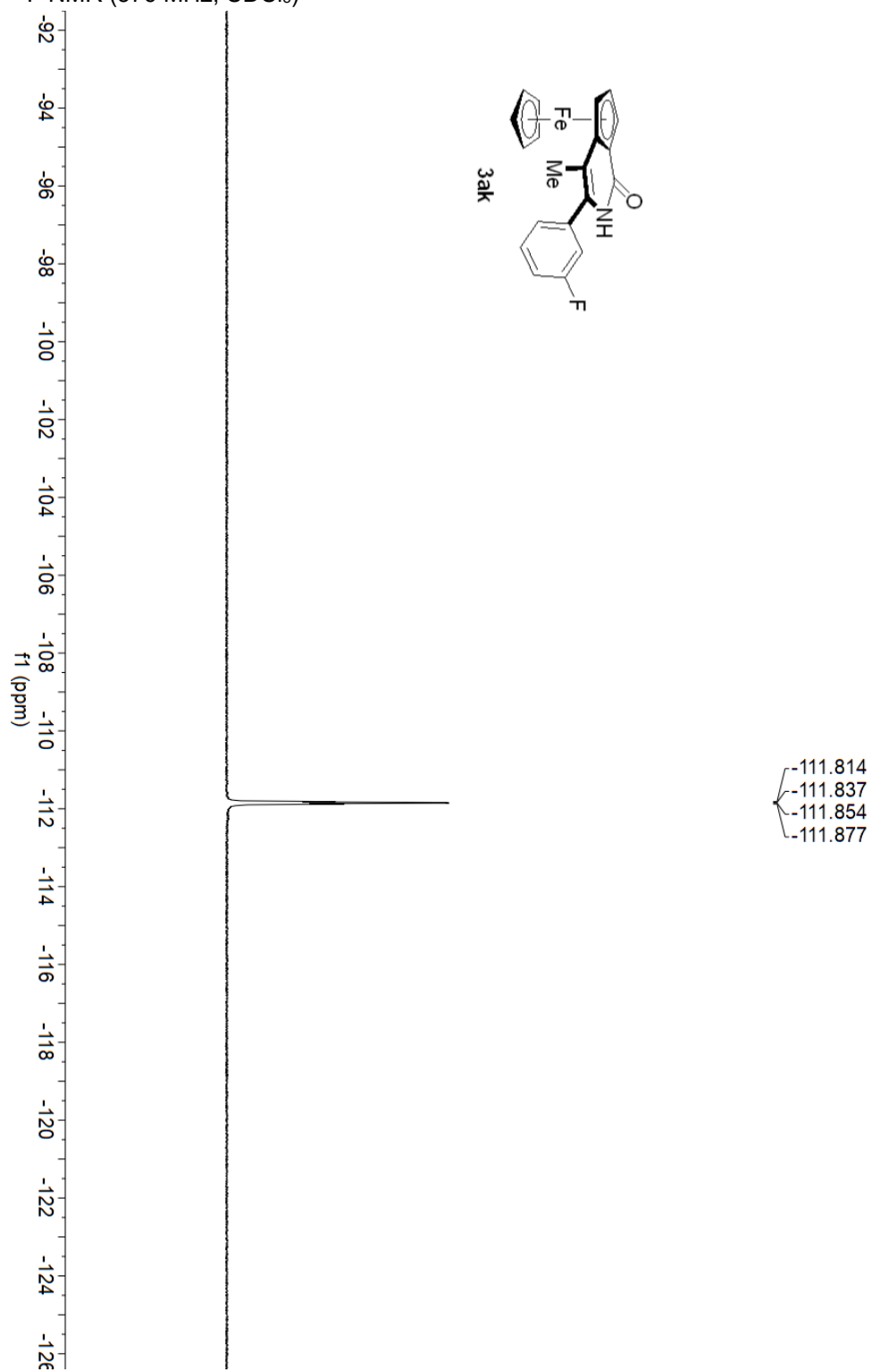
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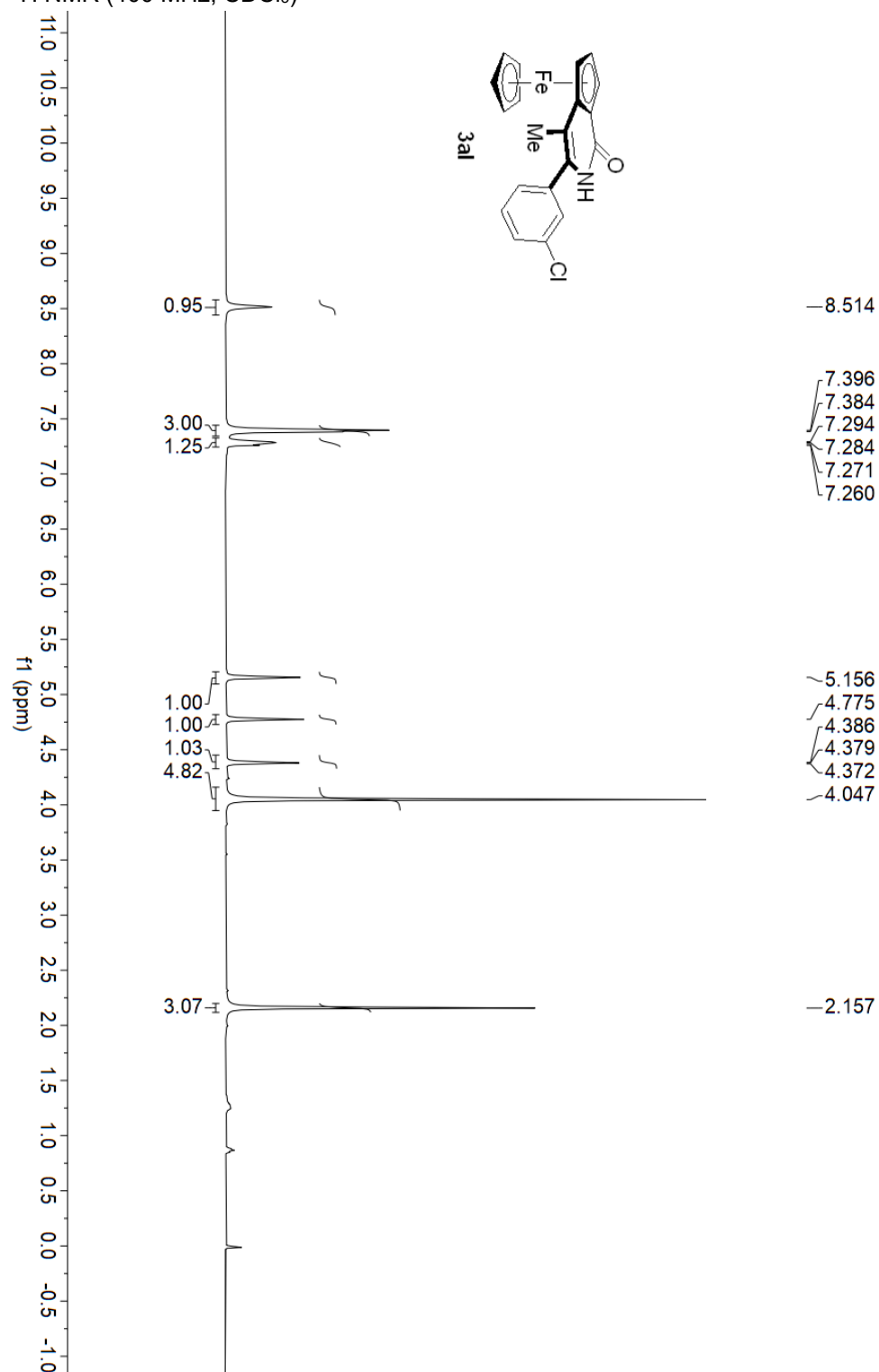
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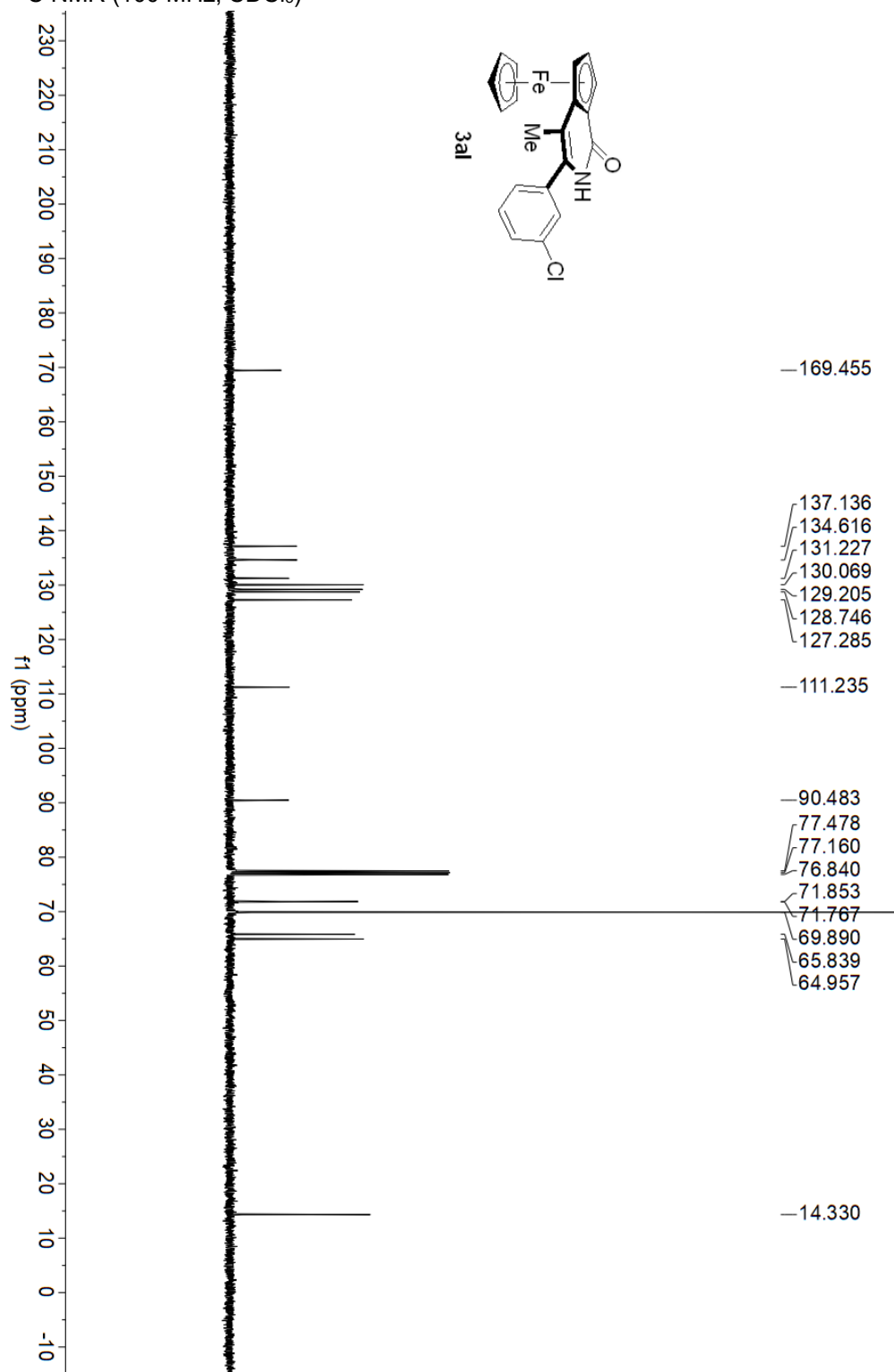
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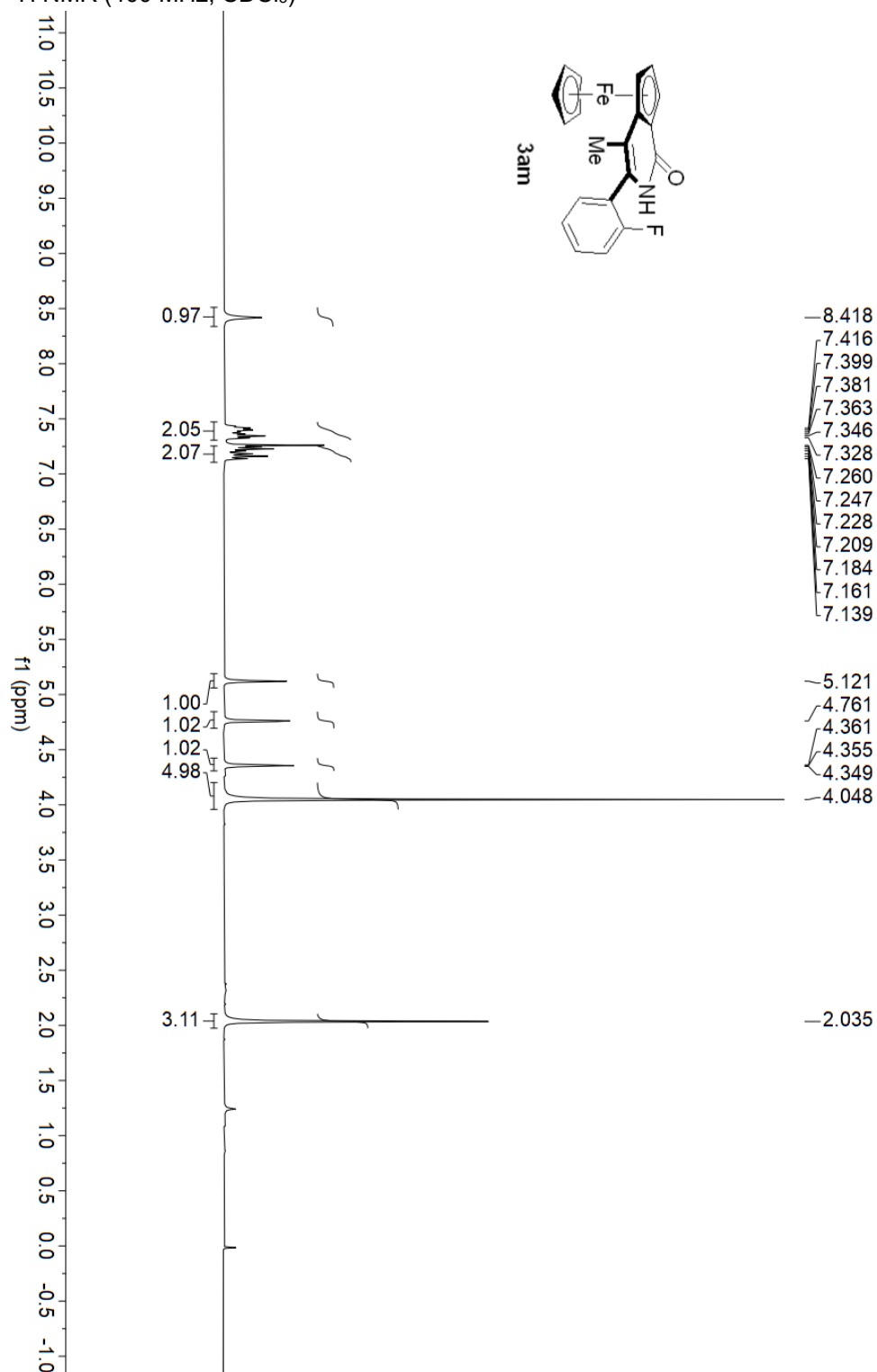
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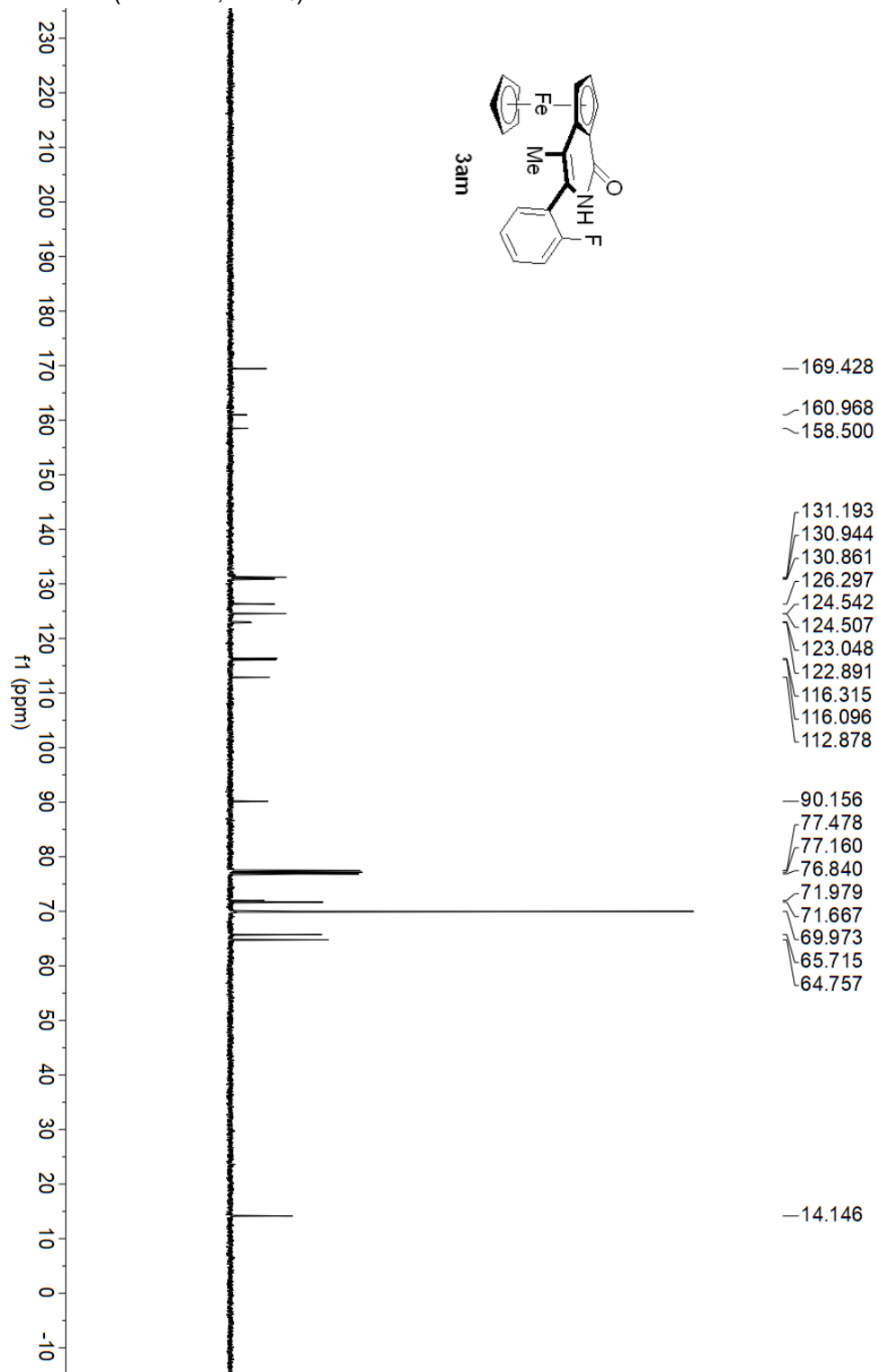
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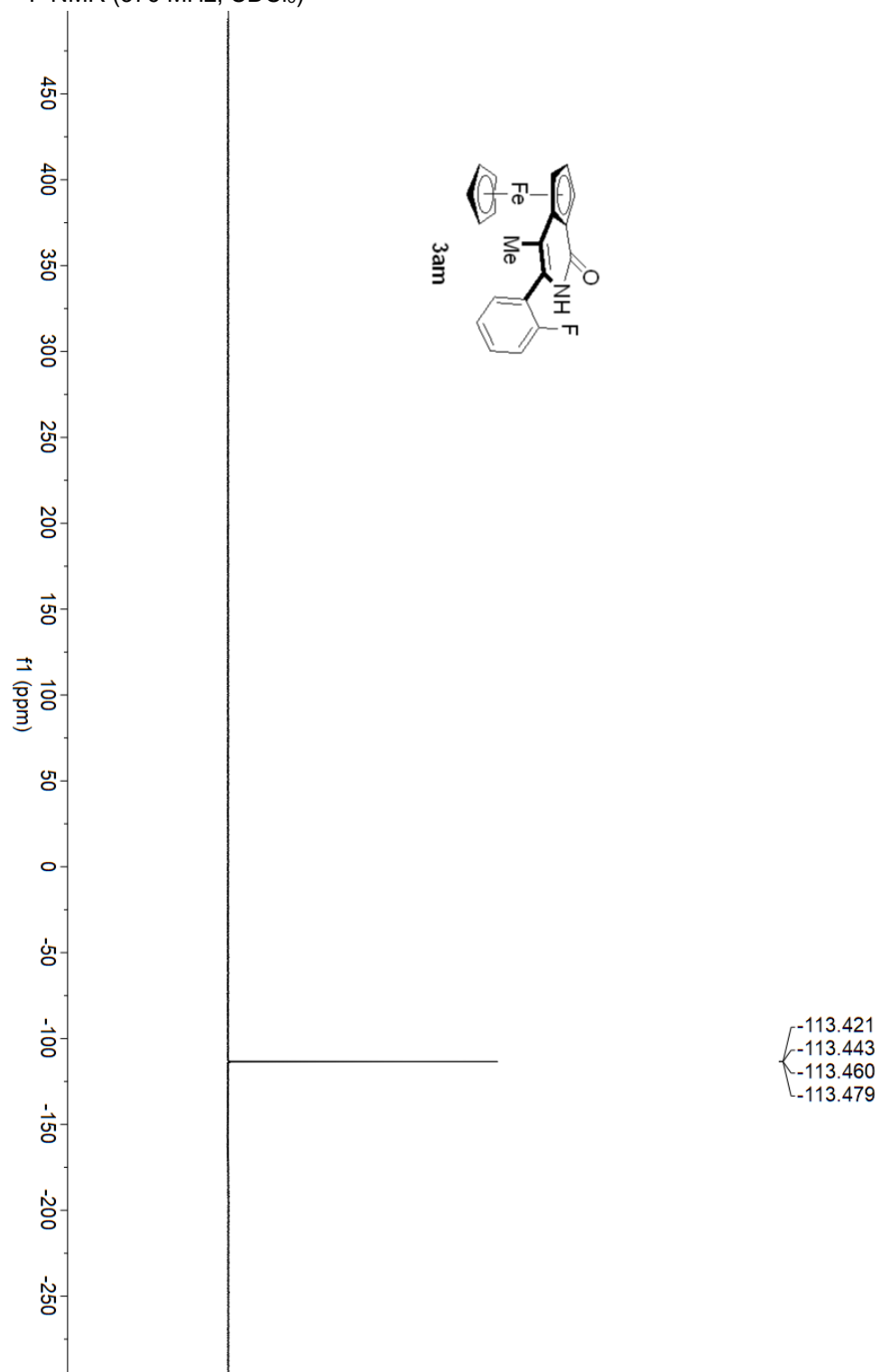
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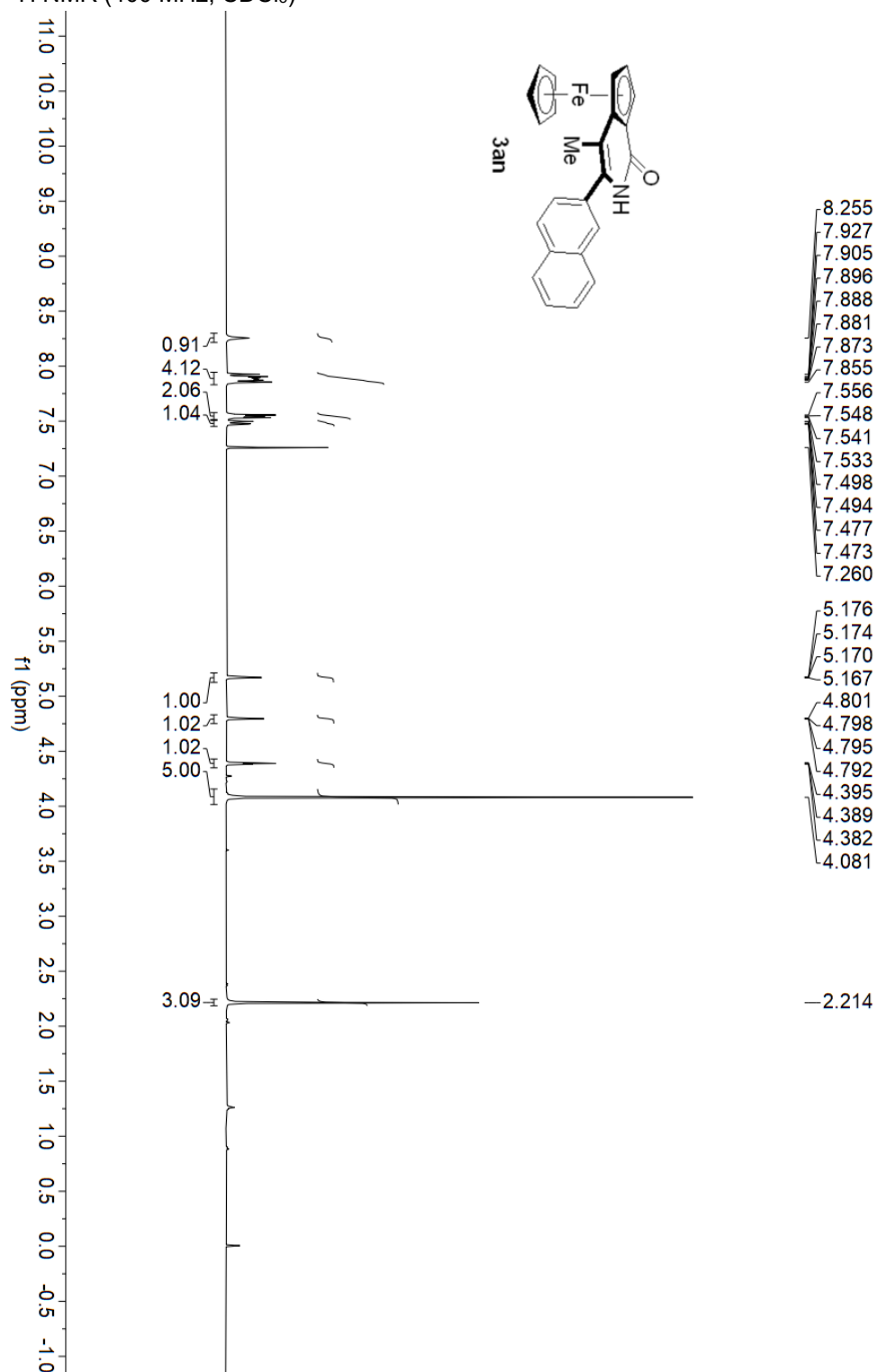
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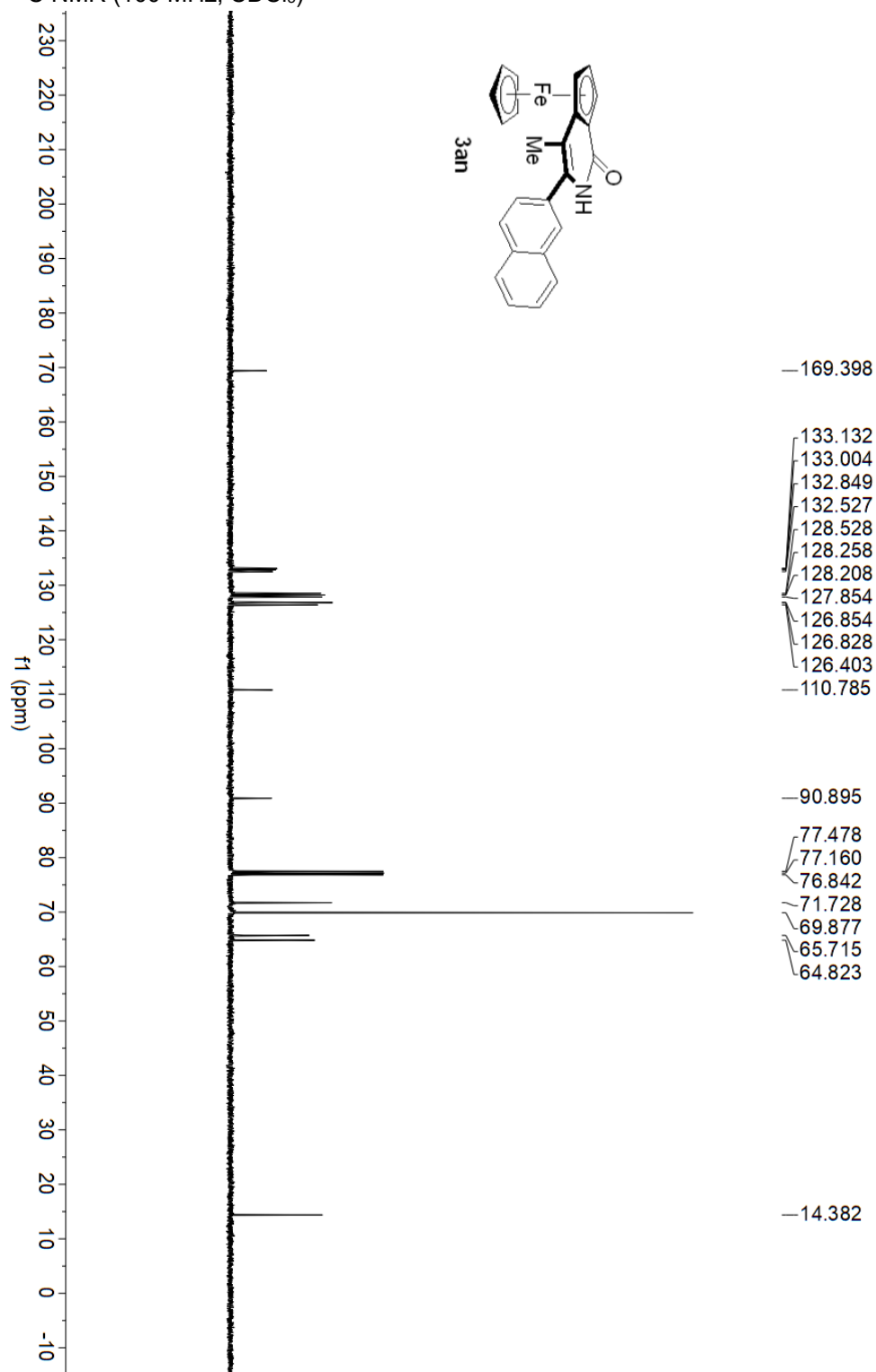
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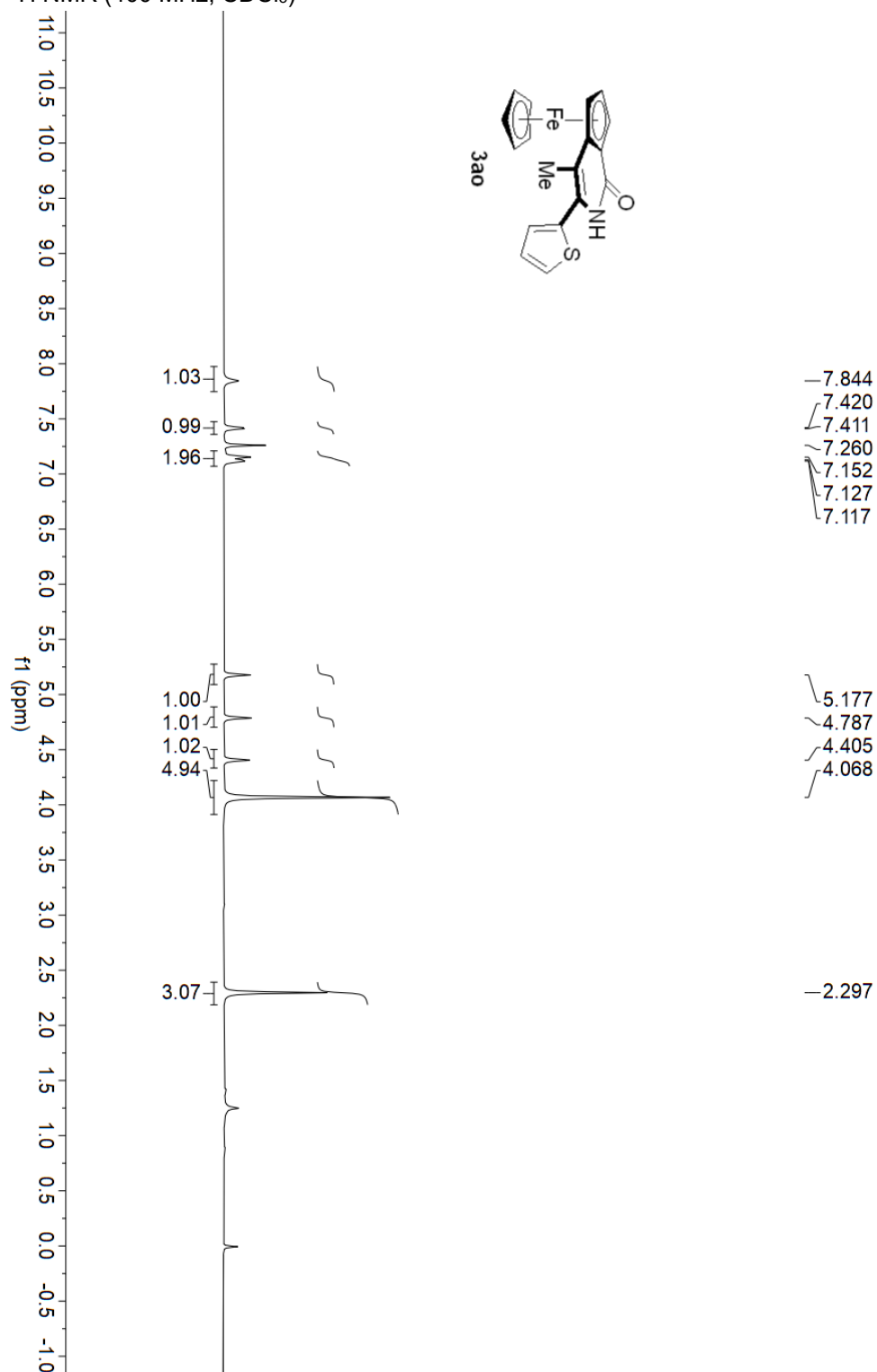
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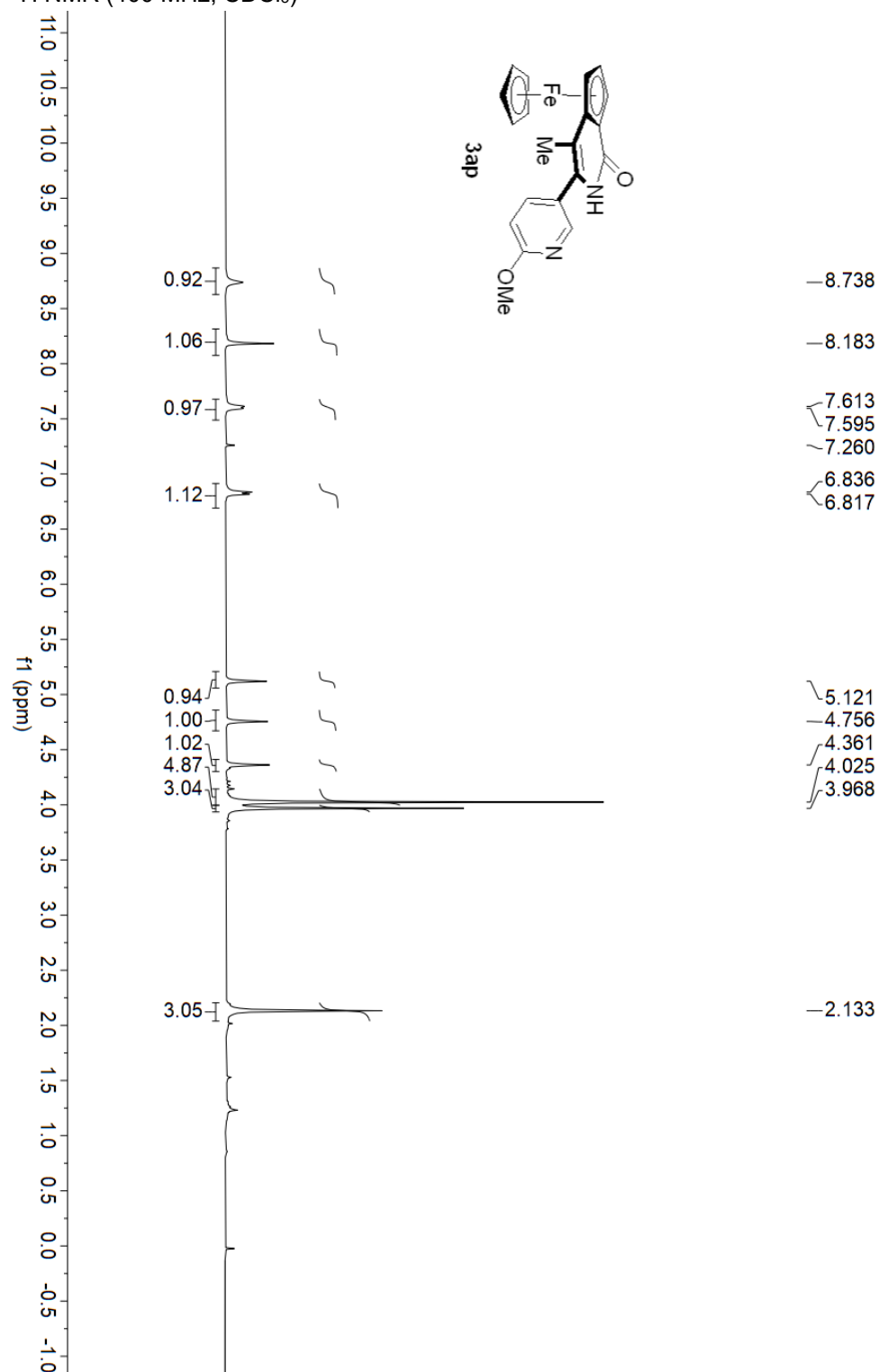
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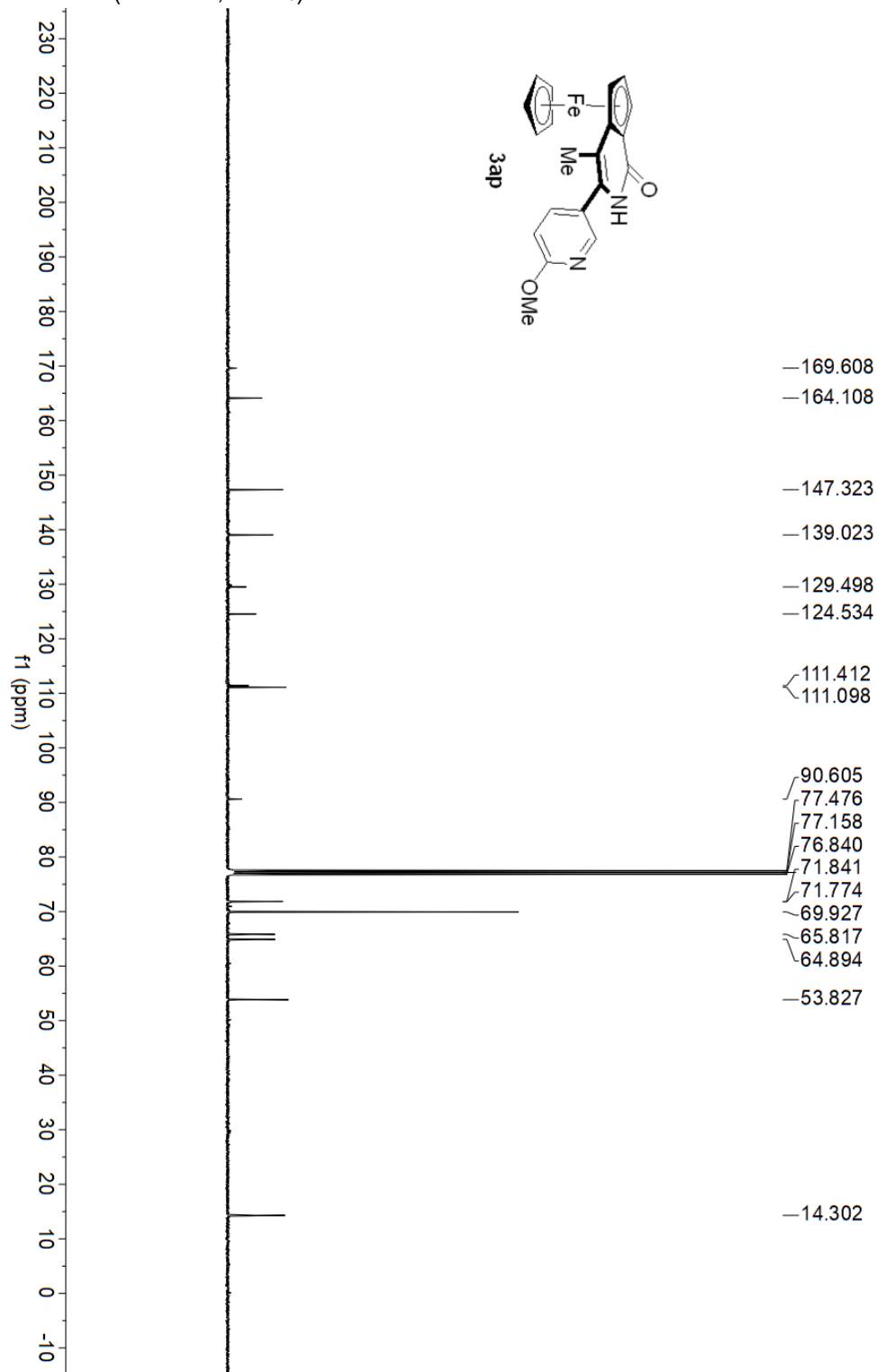
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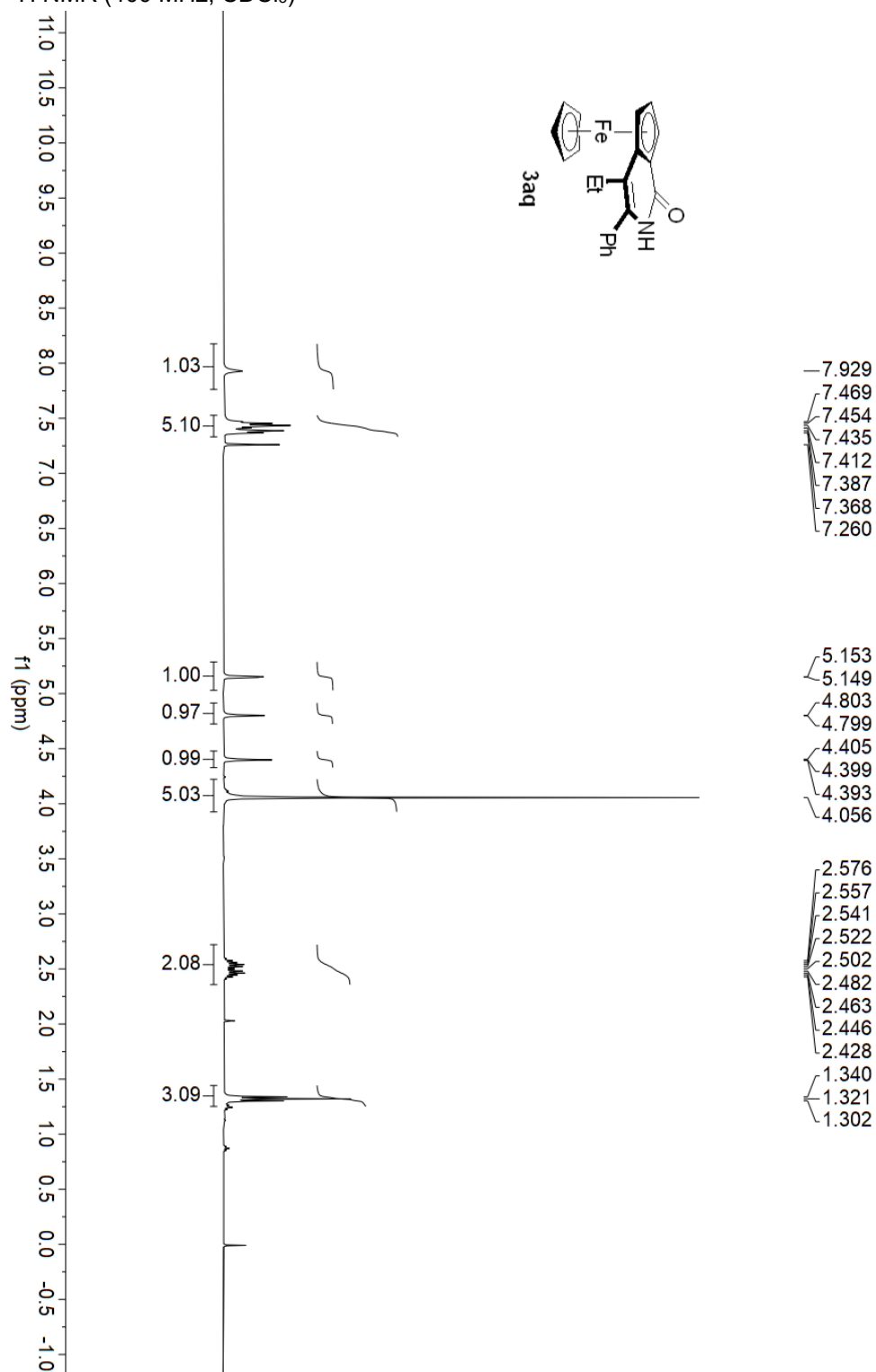
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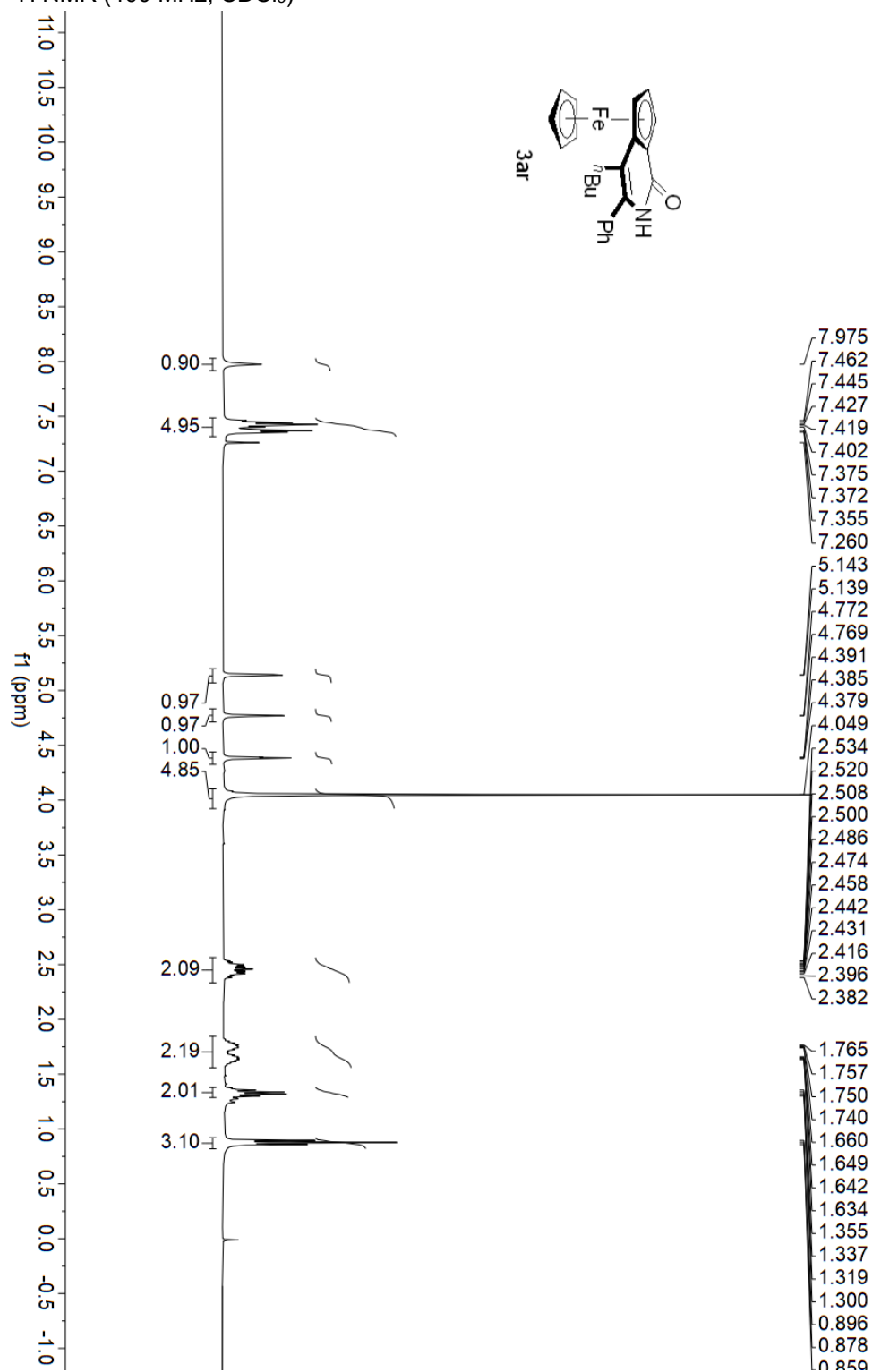
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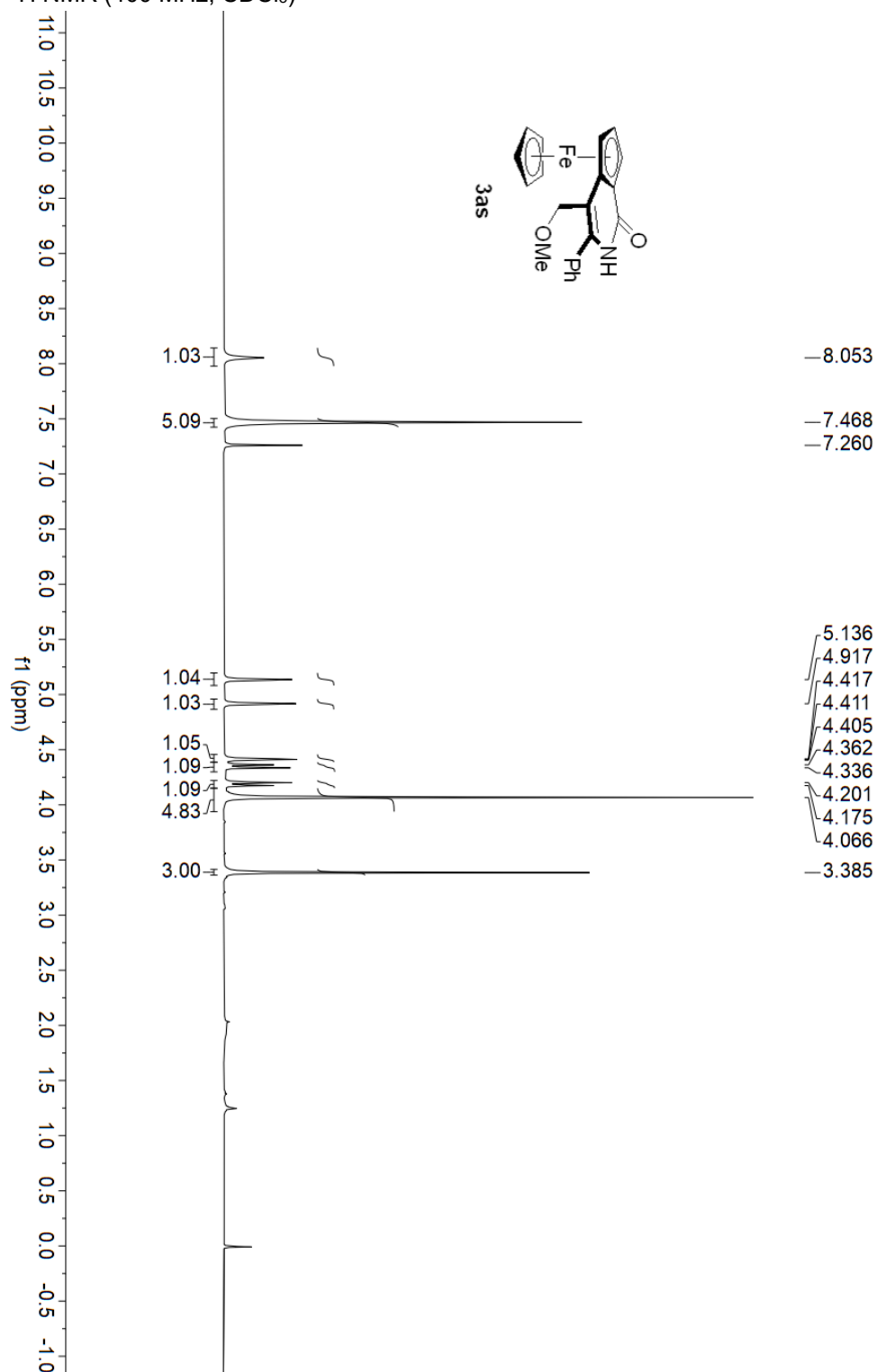
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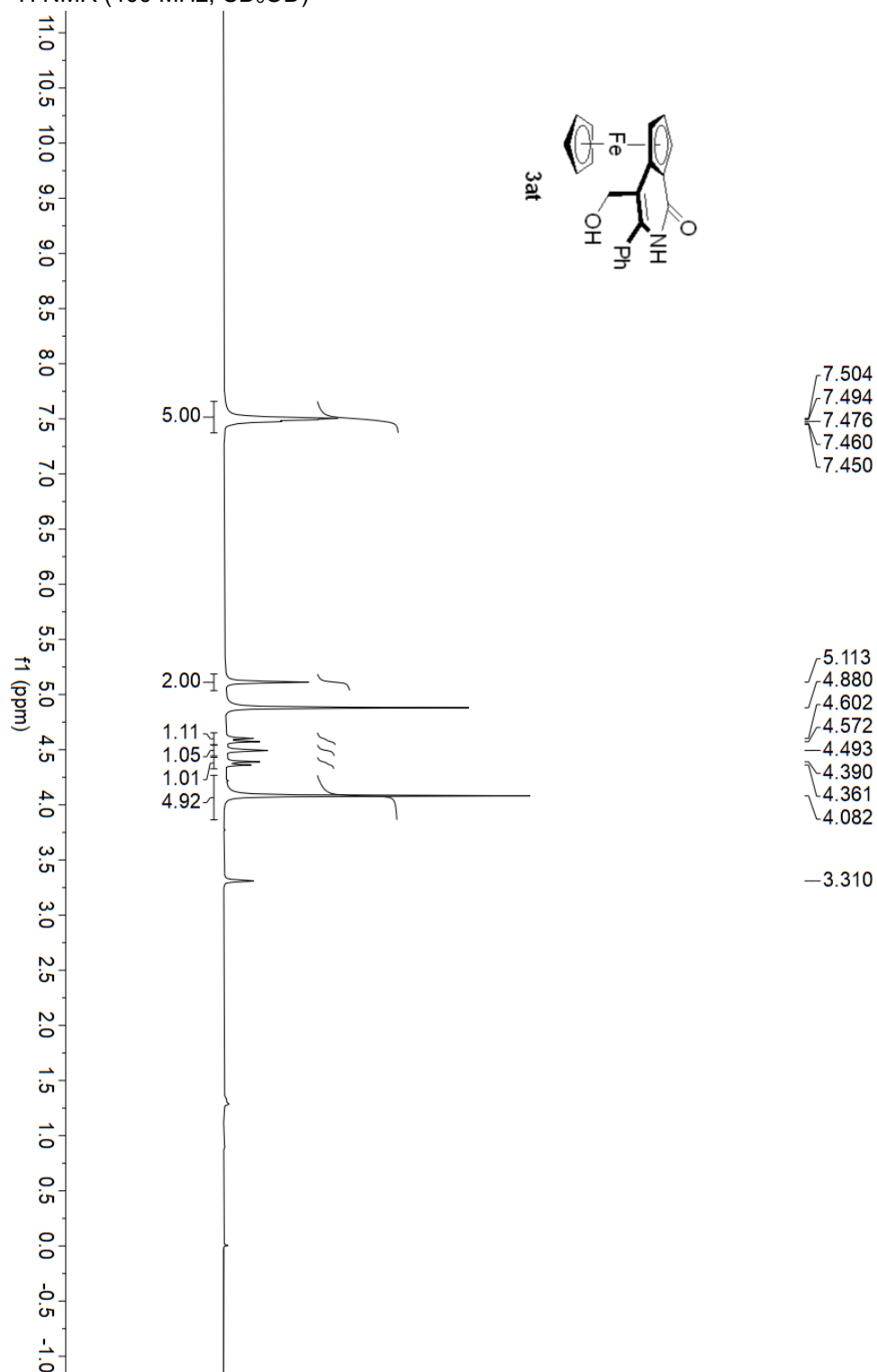
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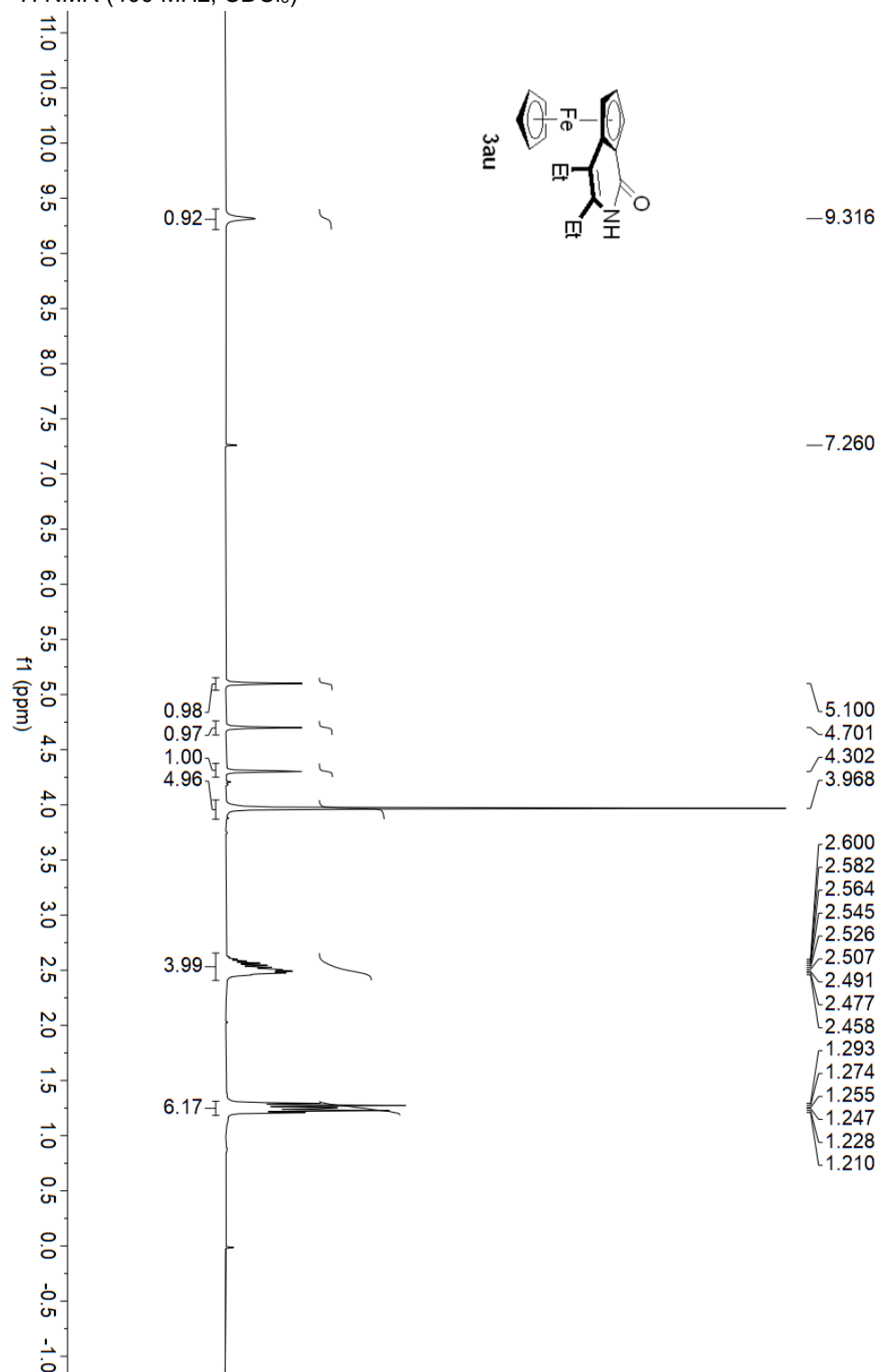
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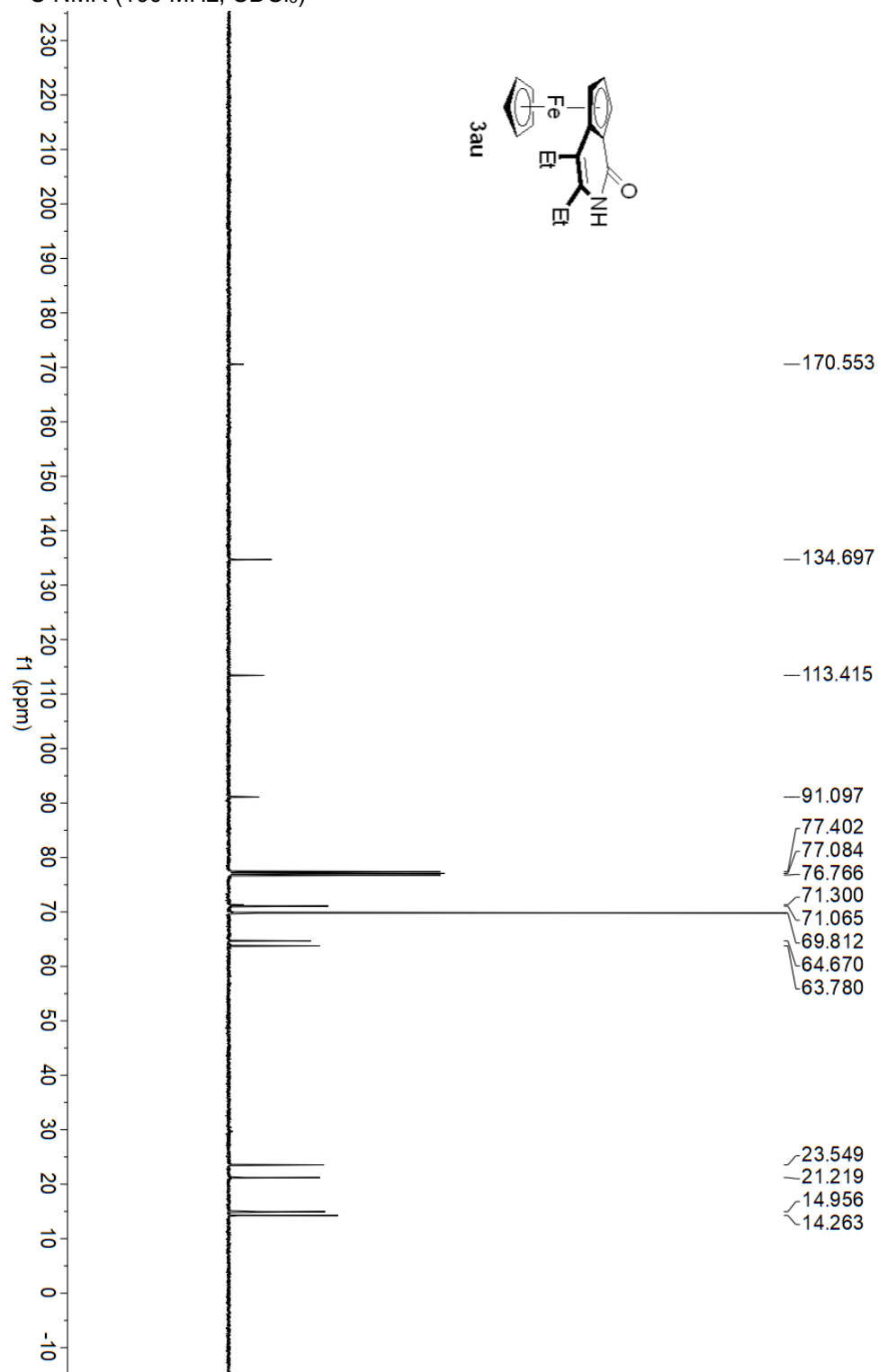
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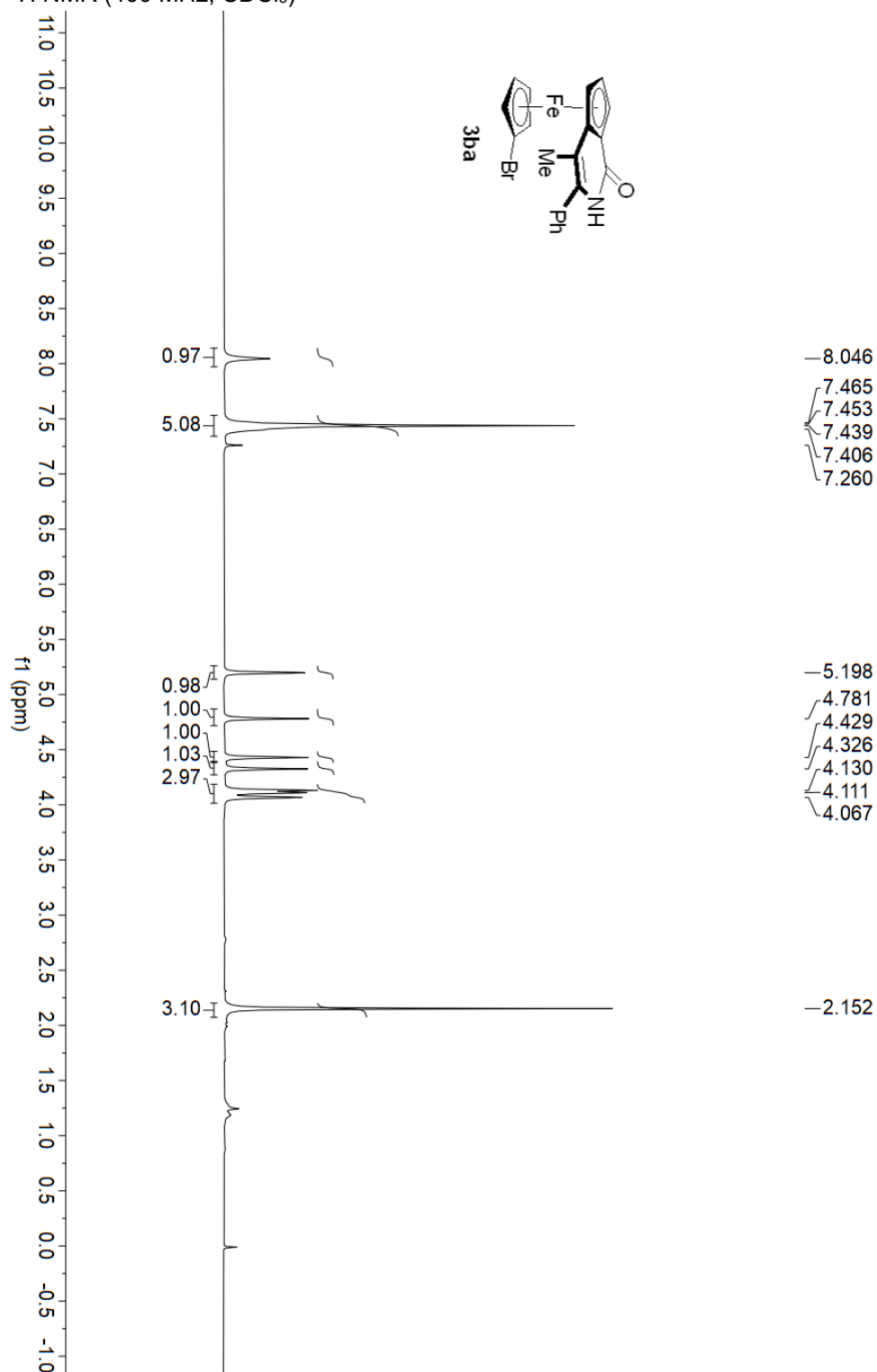
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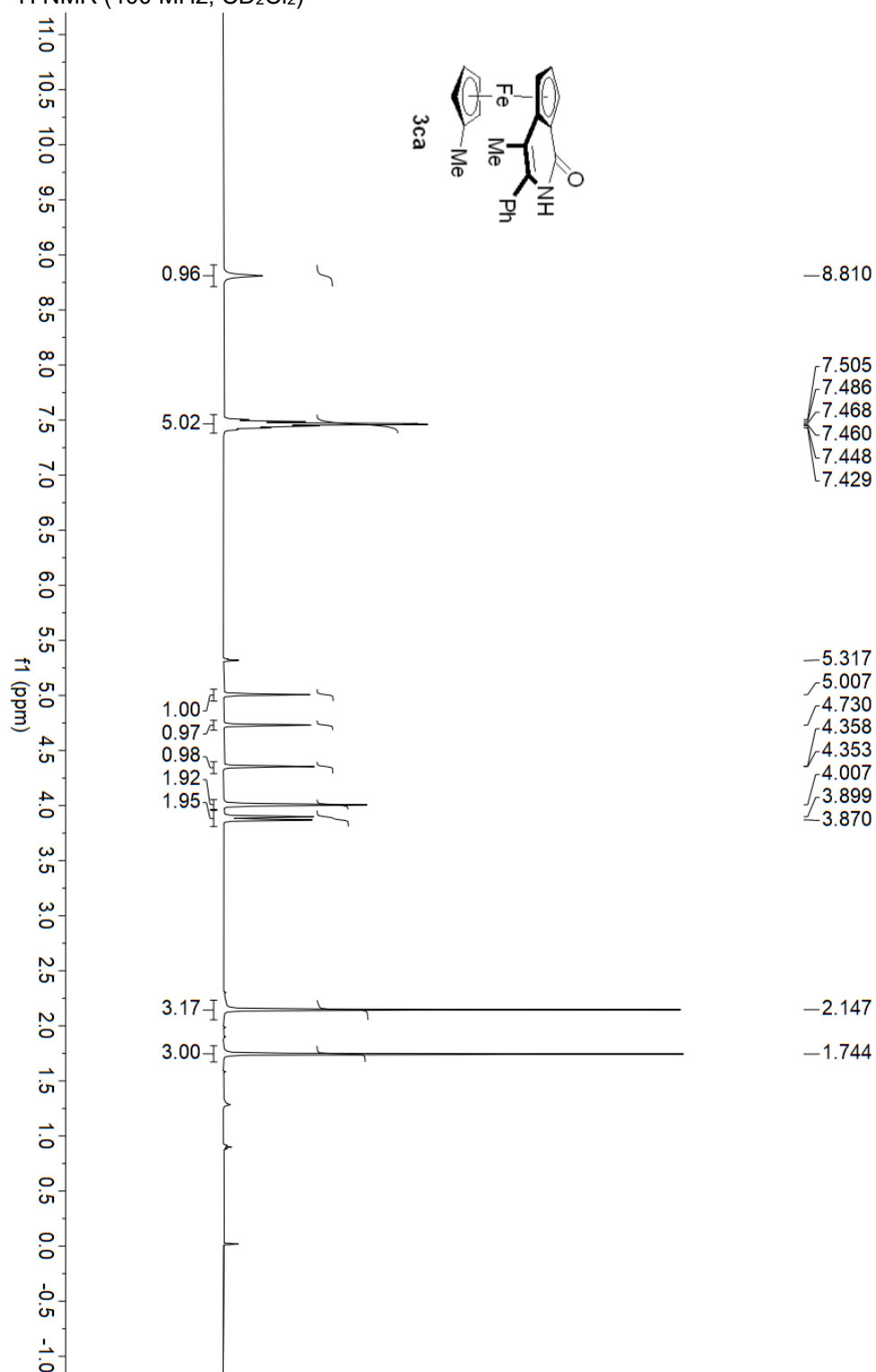
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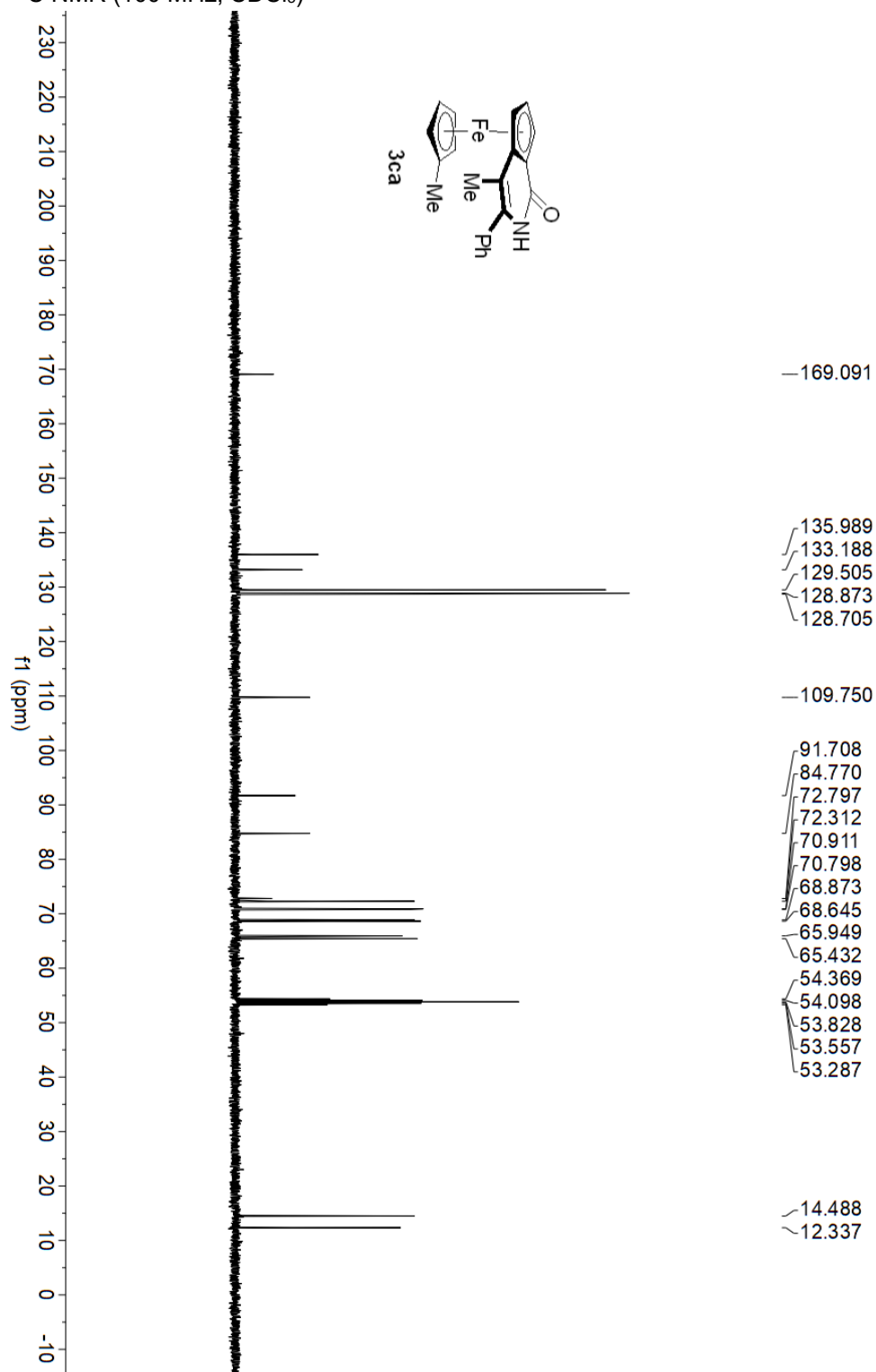
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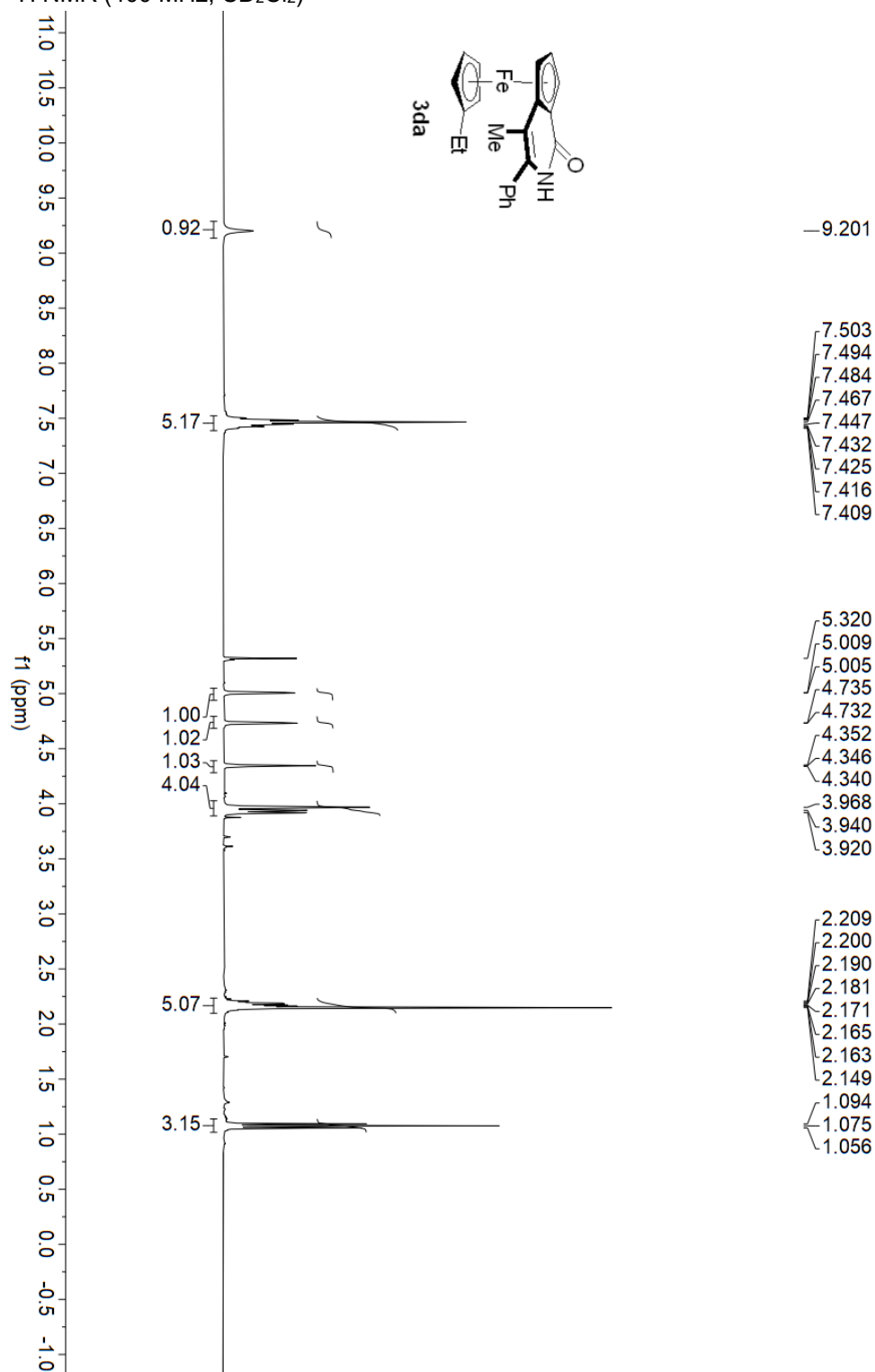
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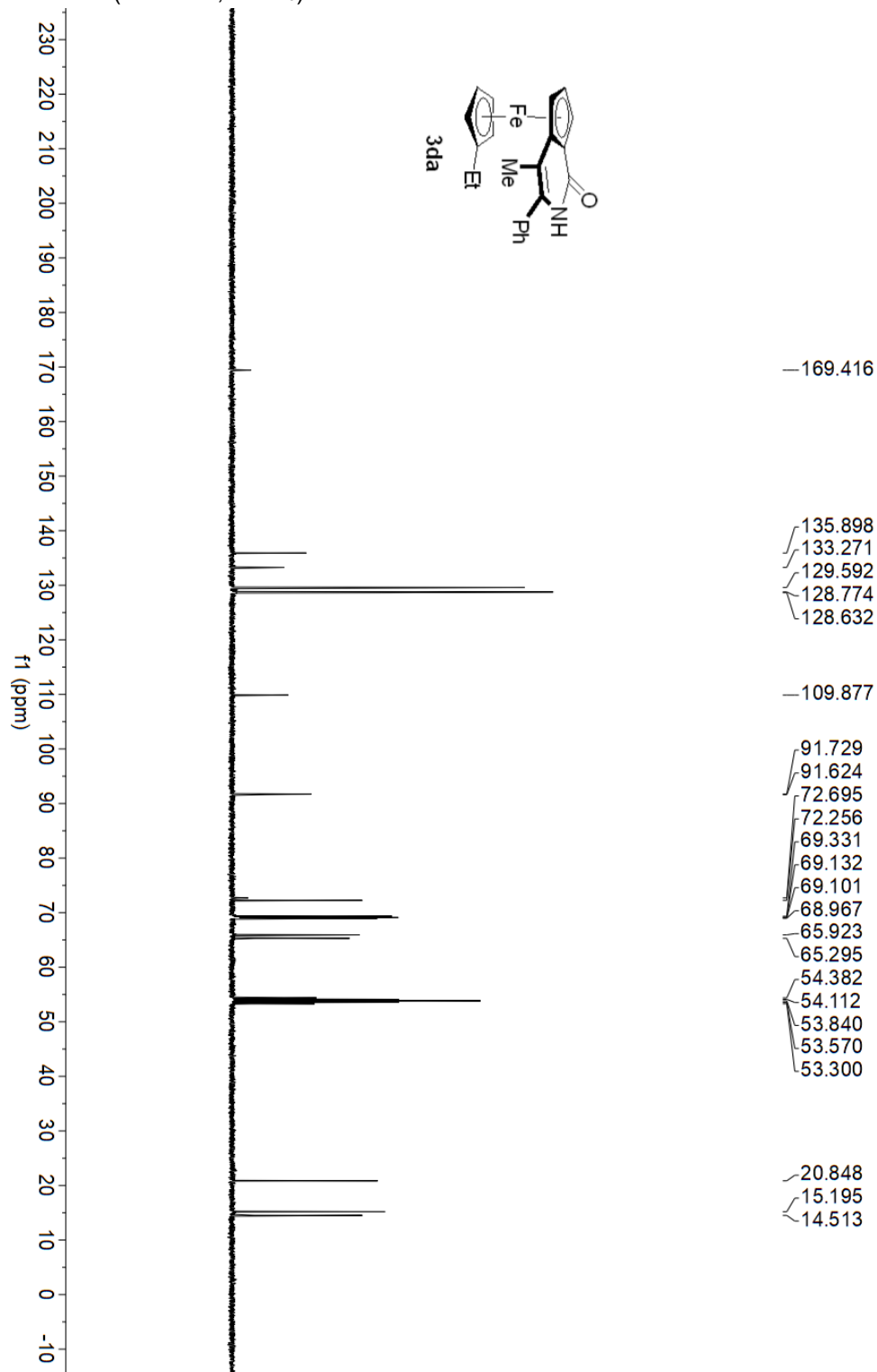
¹³C NMR (100 MHz, CDCl₃)



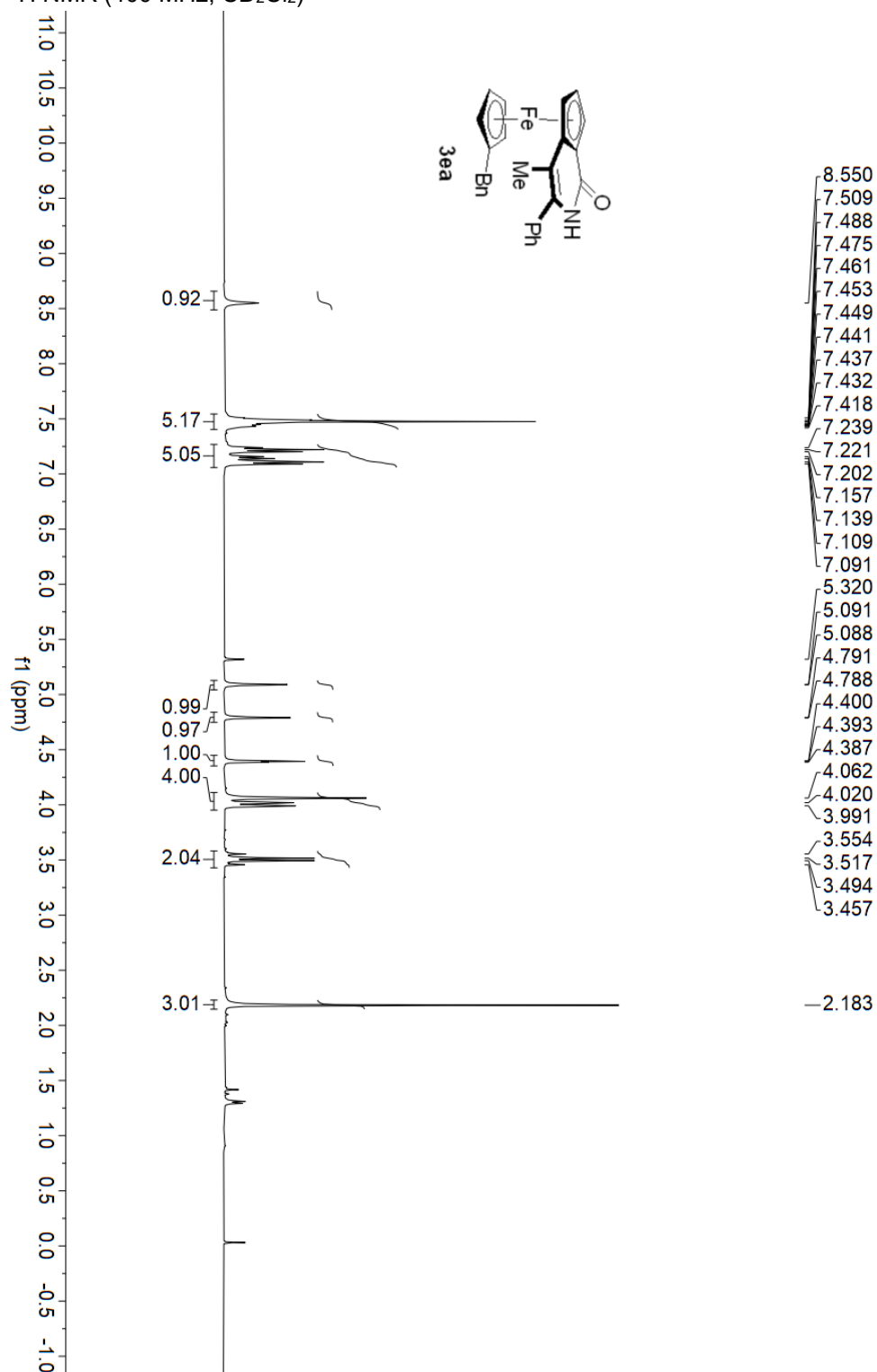
^1H NMR (400 MHz, CD_2Cl_2)



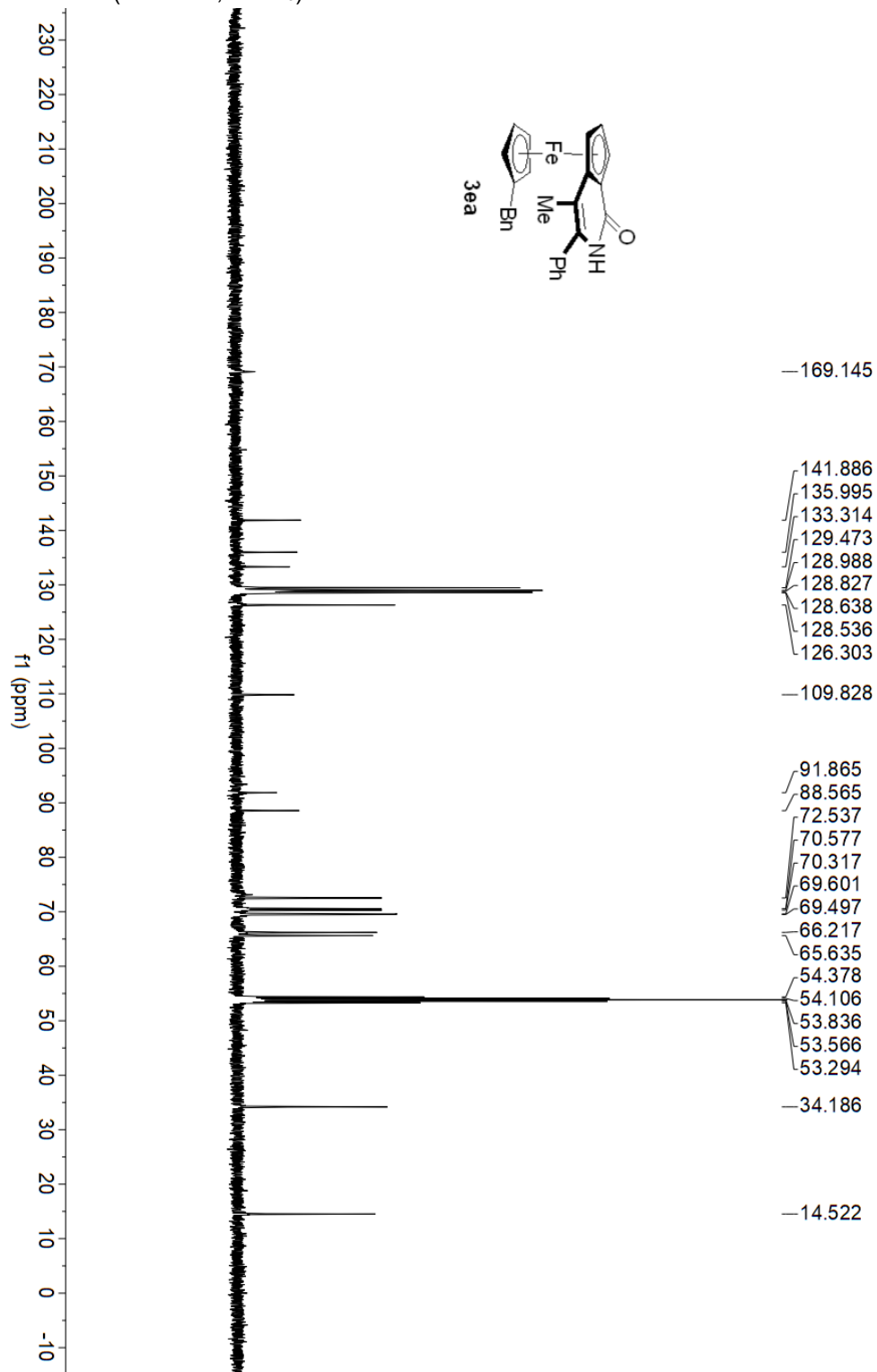
¹³C NMR (100 MHz, CDCl₃)



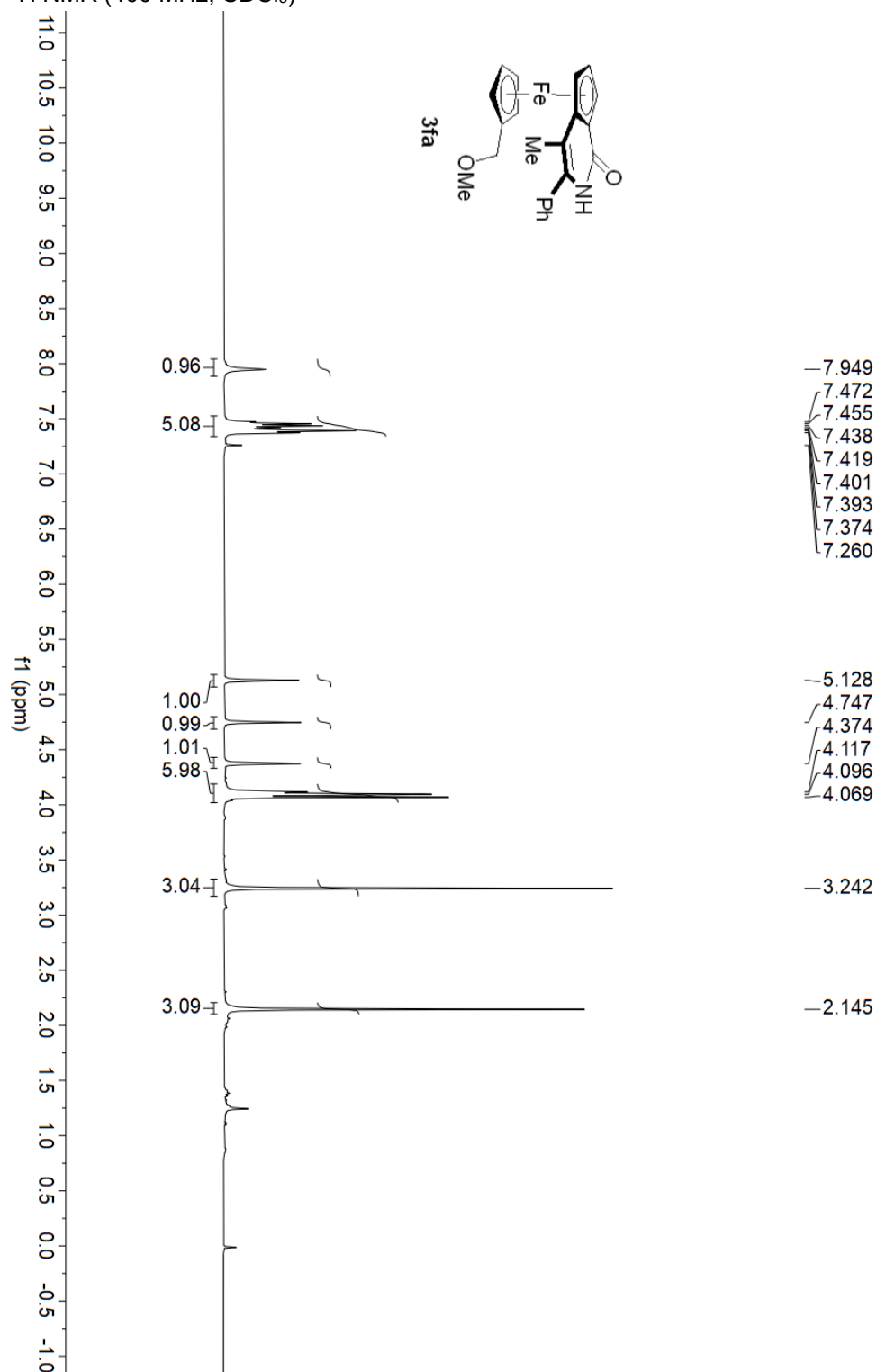
^1H NMR (400 MHz, CD_2Cl_2)



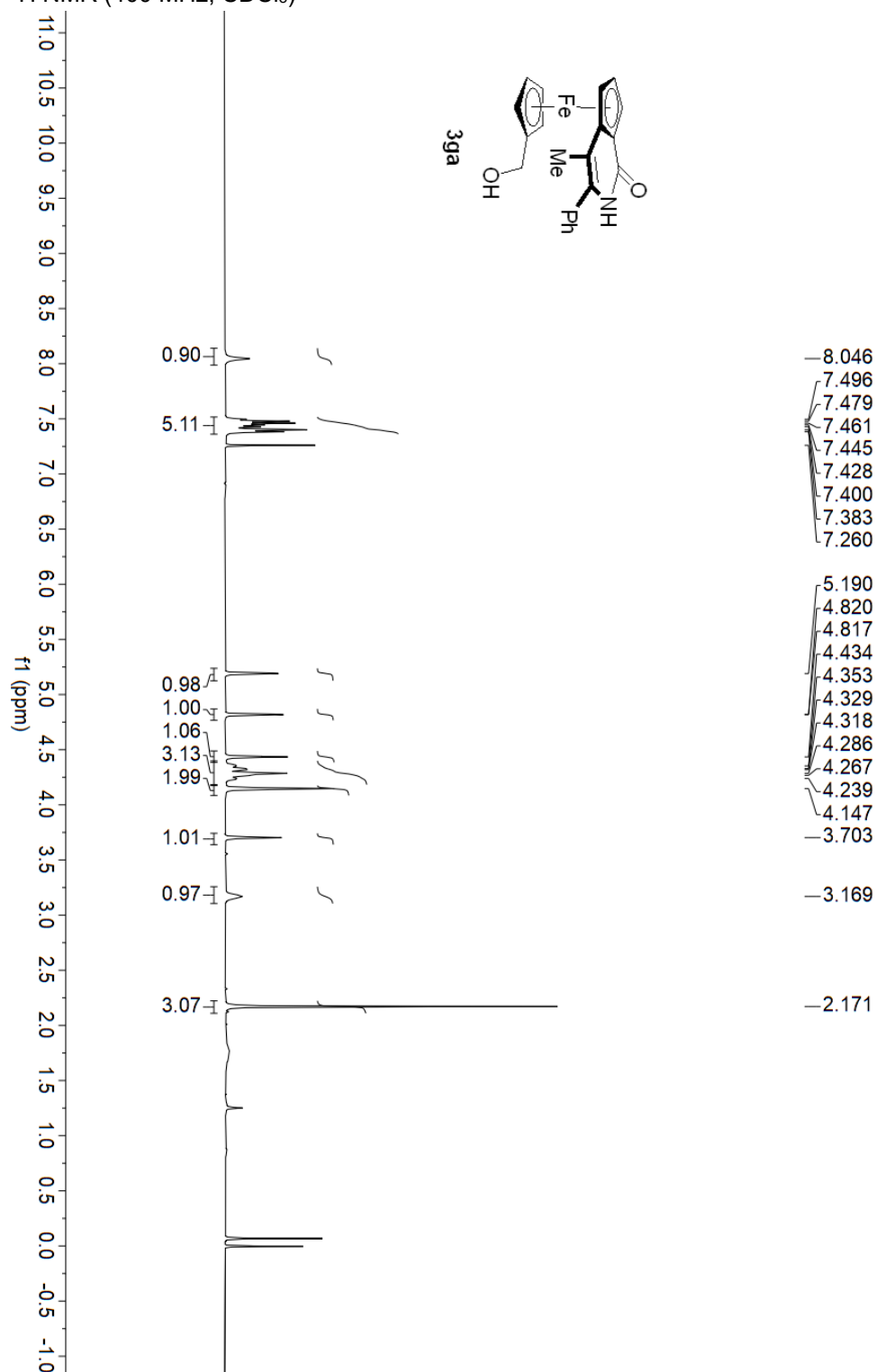
^{13}C NMR (100 MHz, CDCl_3)



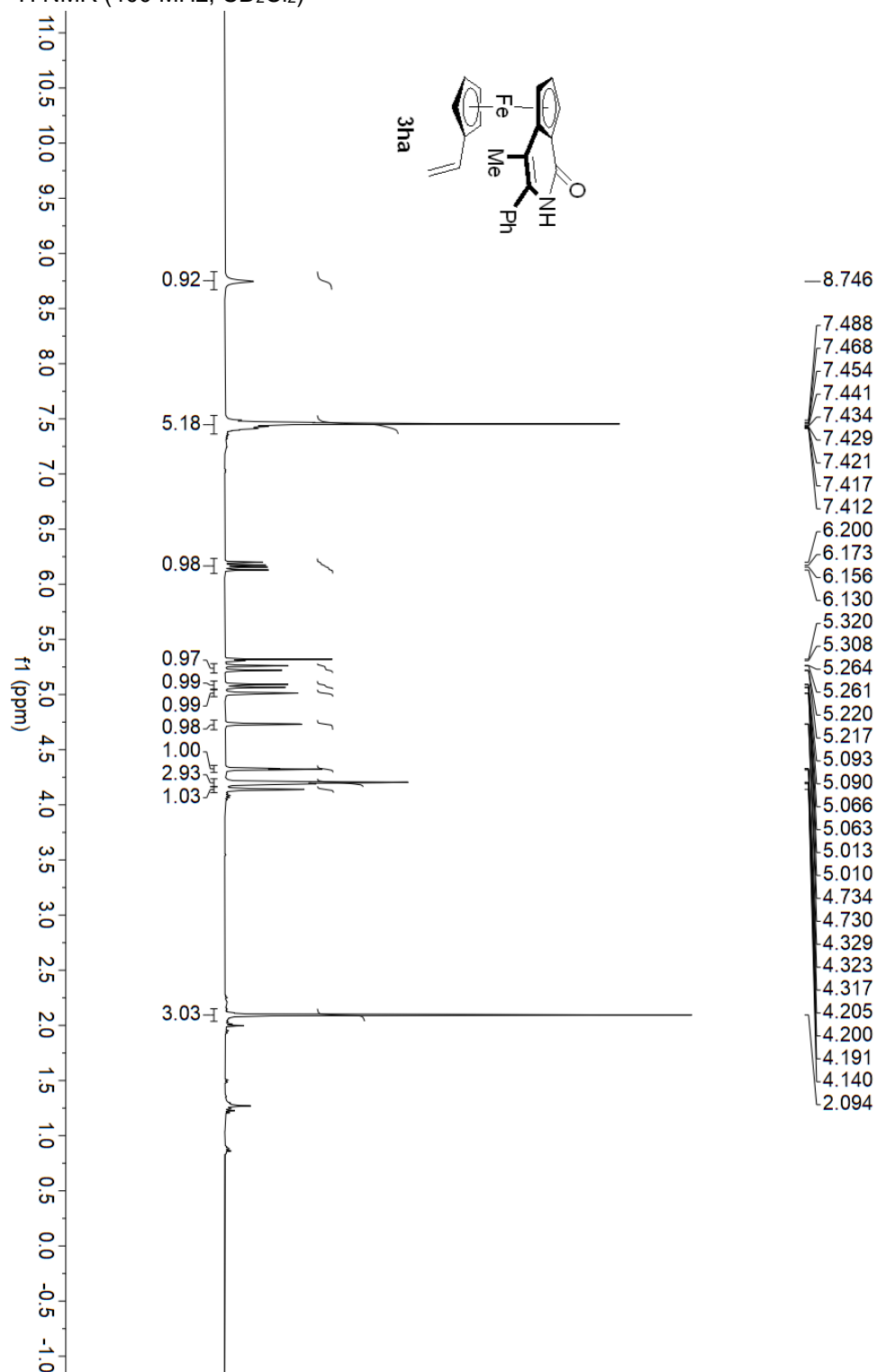
¹H NMR (400 MHz, CDCl₃)



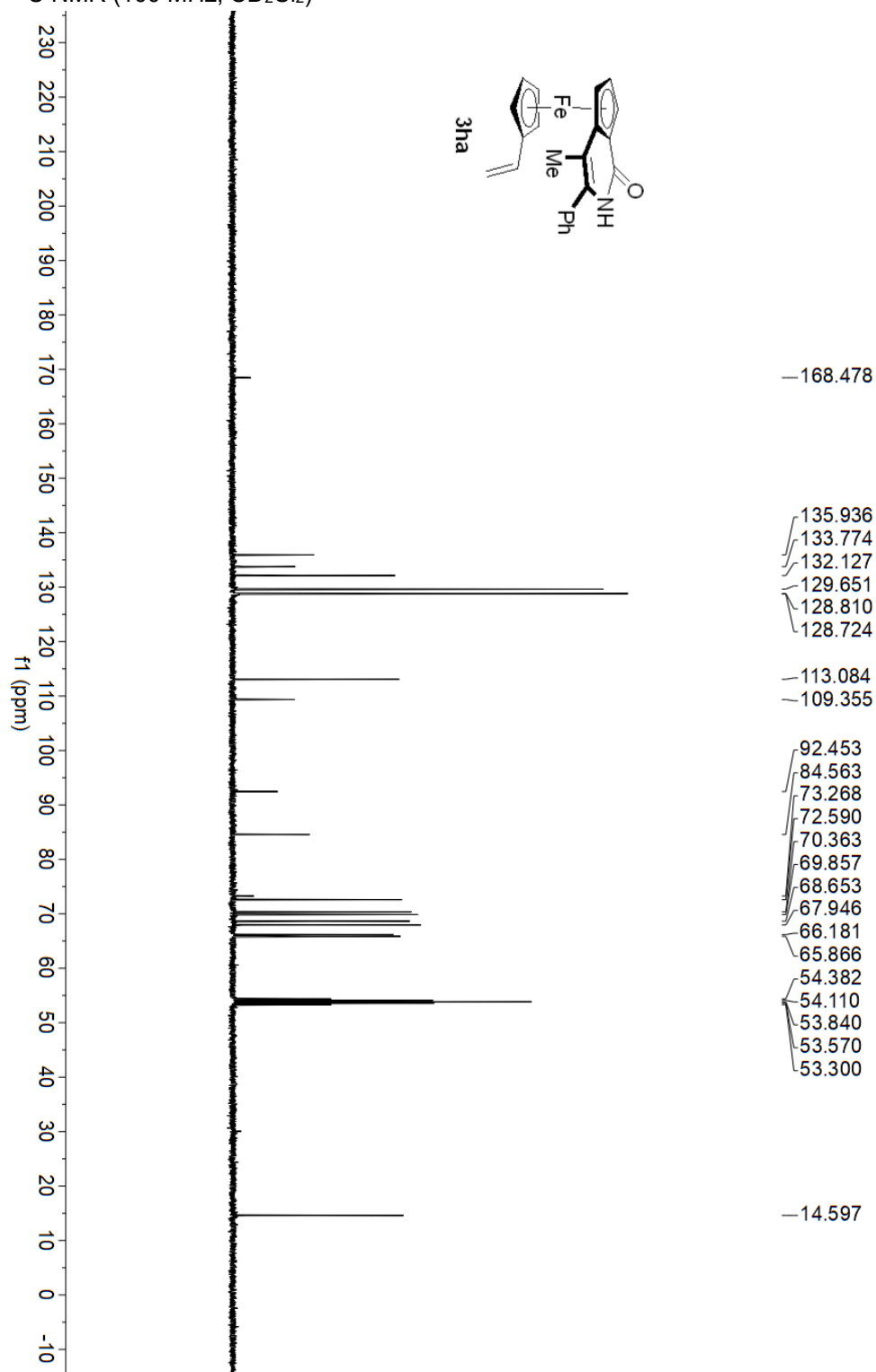
¹H NMR (400 MHz, CDCl₃)



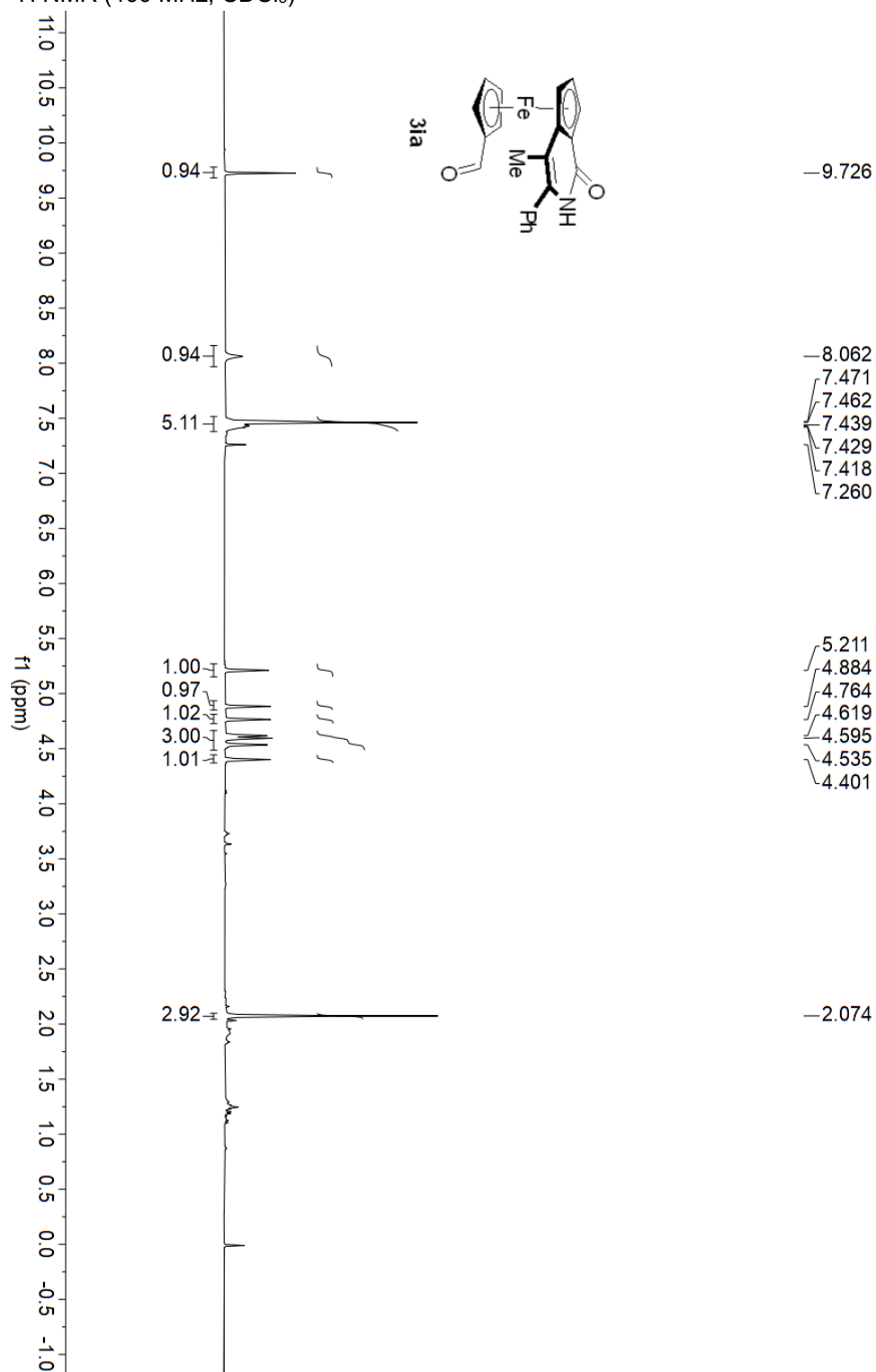
^1H NMR (400 MHz, CD_2Cl_2)



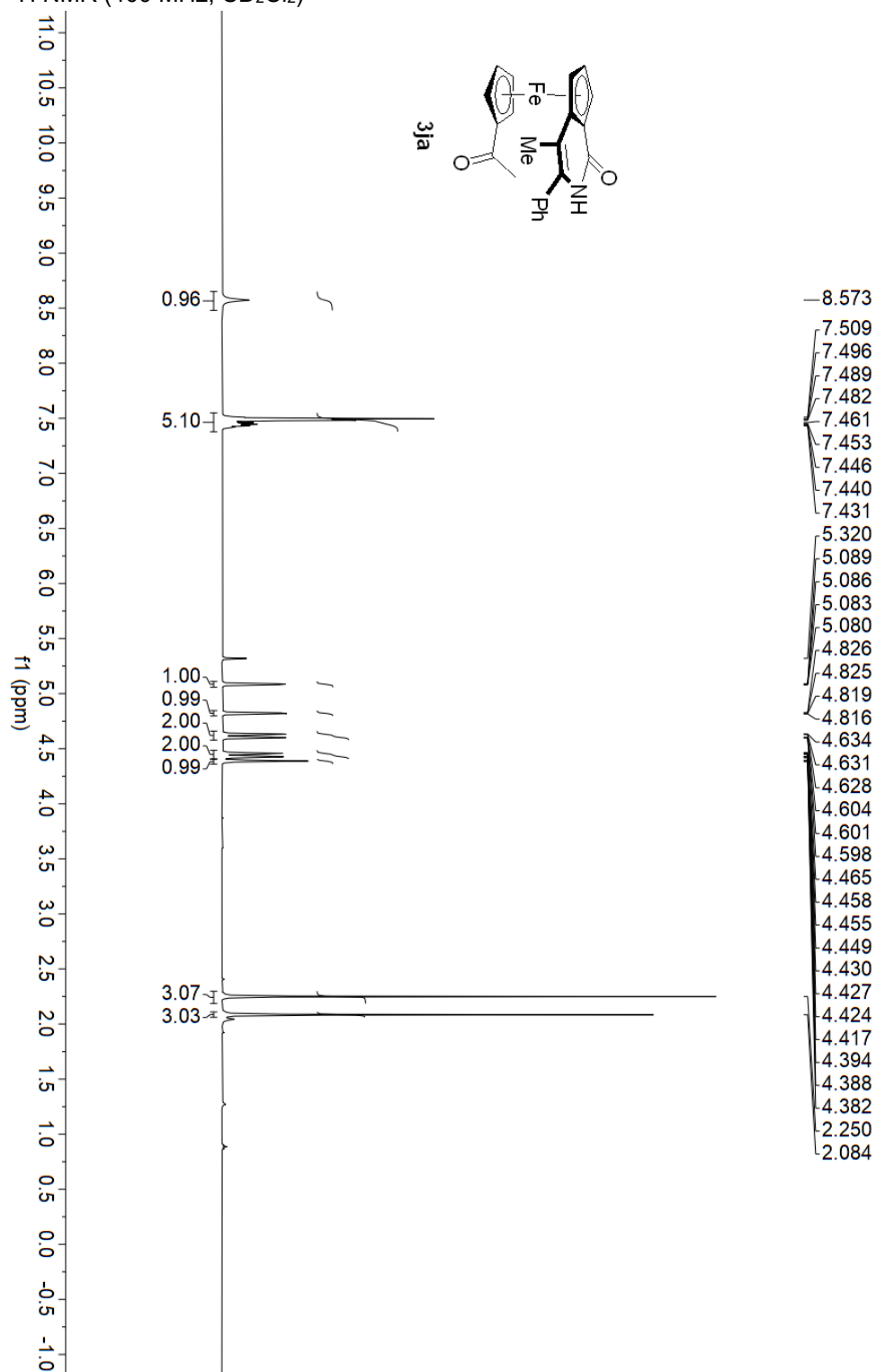
^{13}C NMR (100 MHz, CD_2Cl_2)



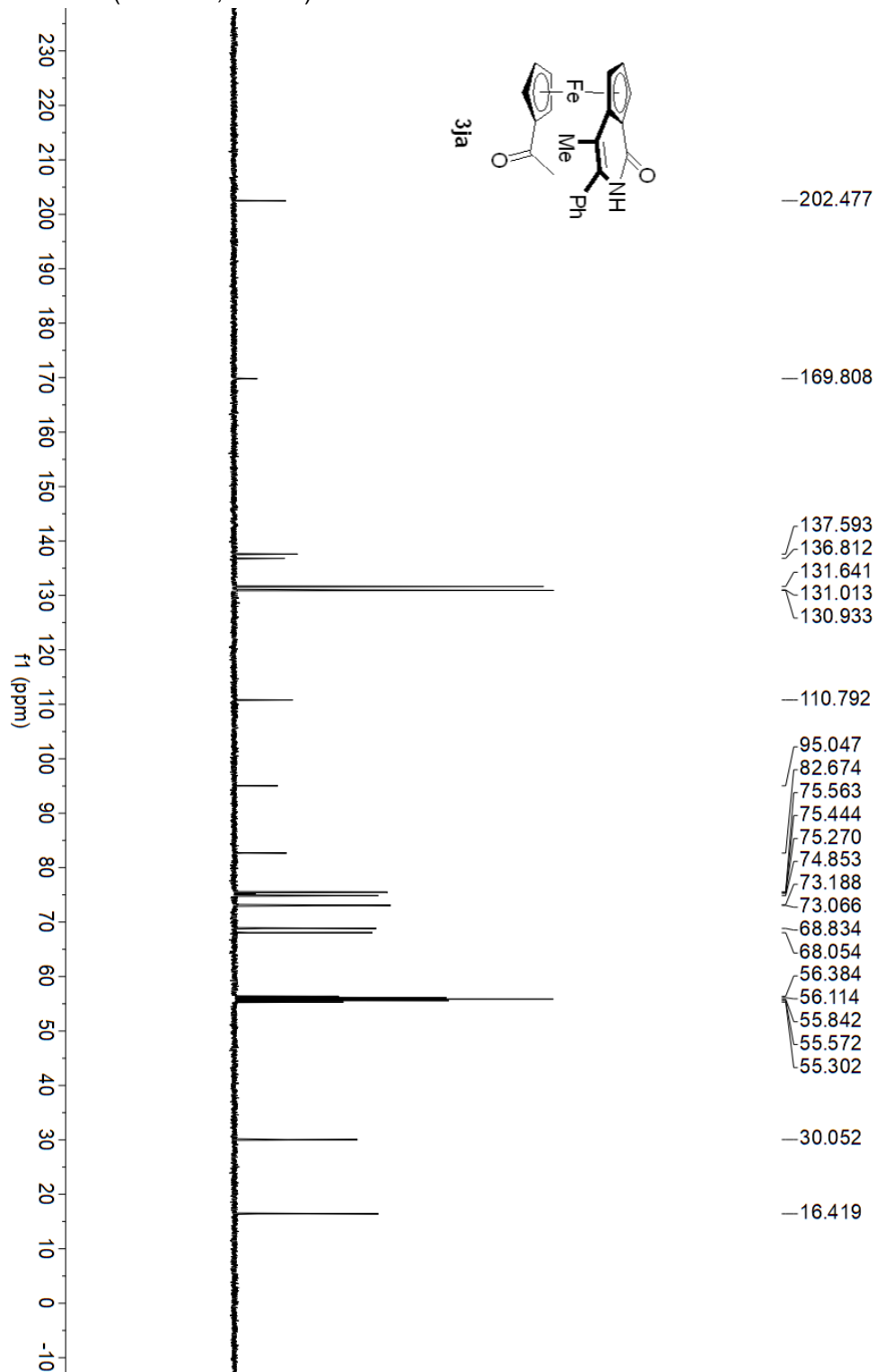
¹H NMR (400 MHz, CDCl₃)



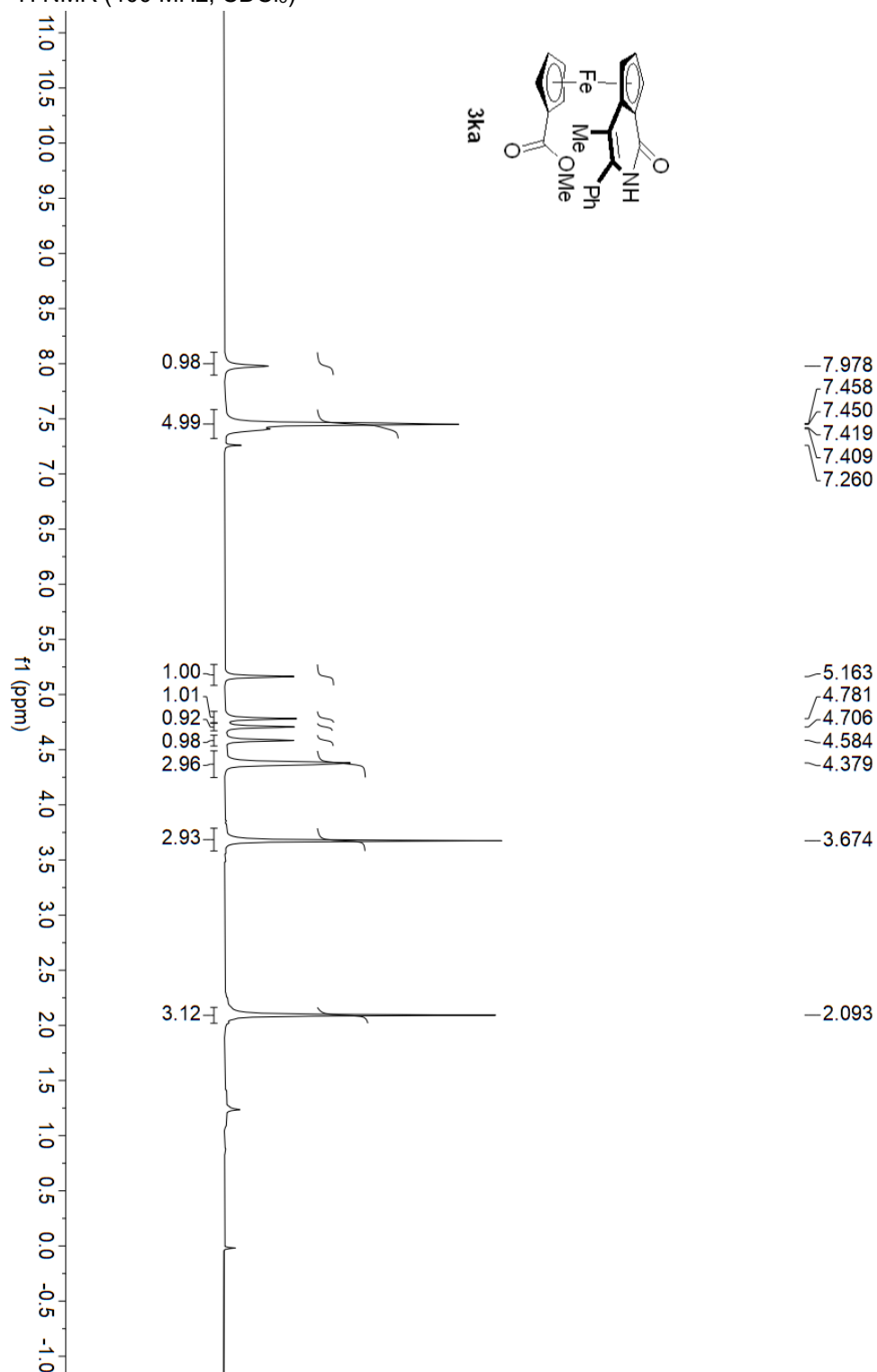
¹H NMR (400 MHz, CD₂Cl₂)



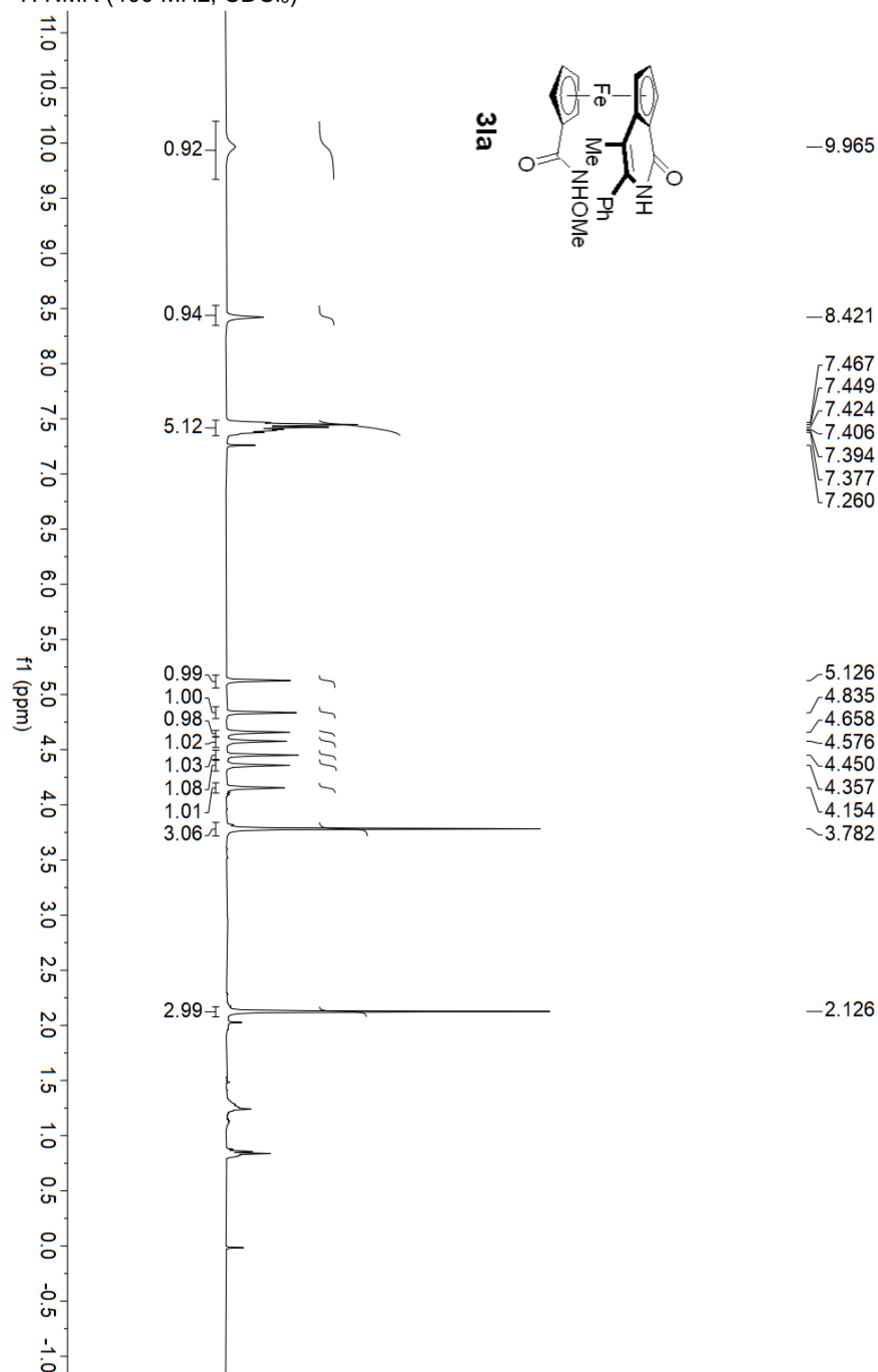
¹³C NMR (100 MHz, CD₂Cl₂)



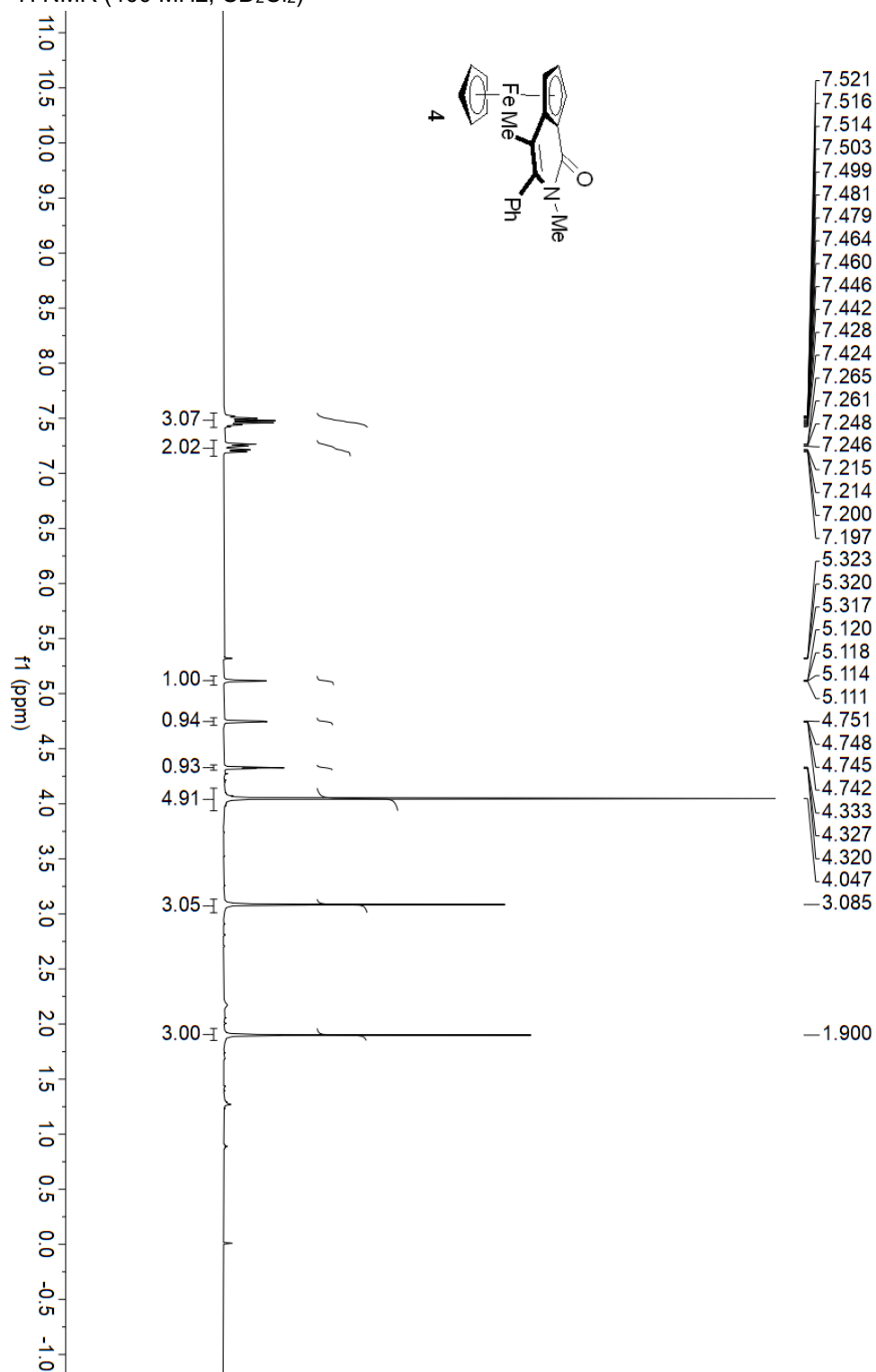
^1H NMR (400 MHz, CDCl_3)



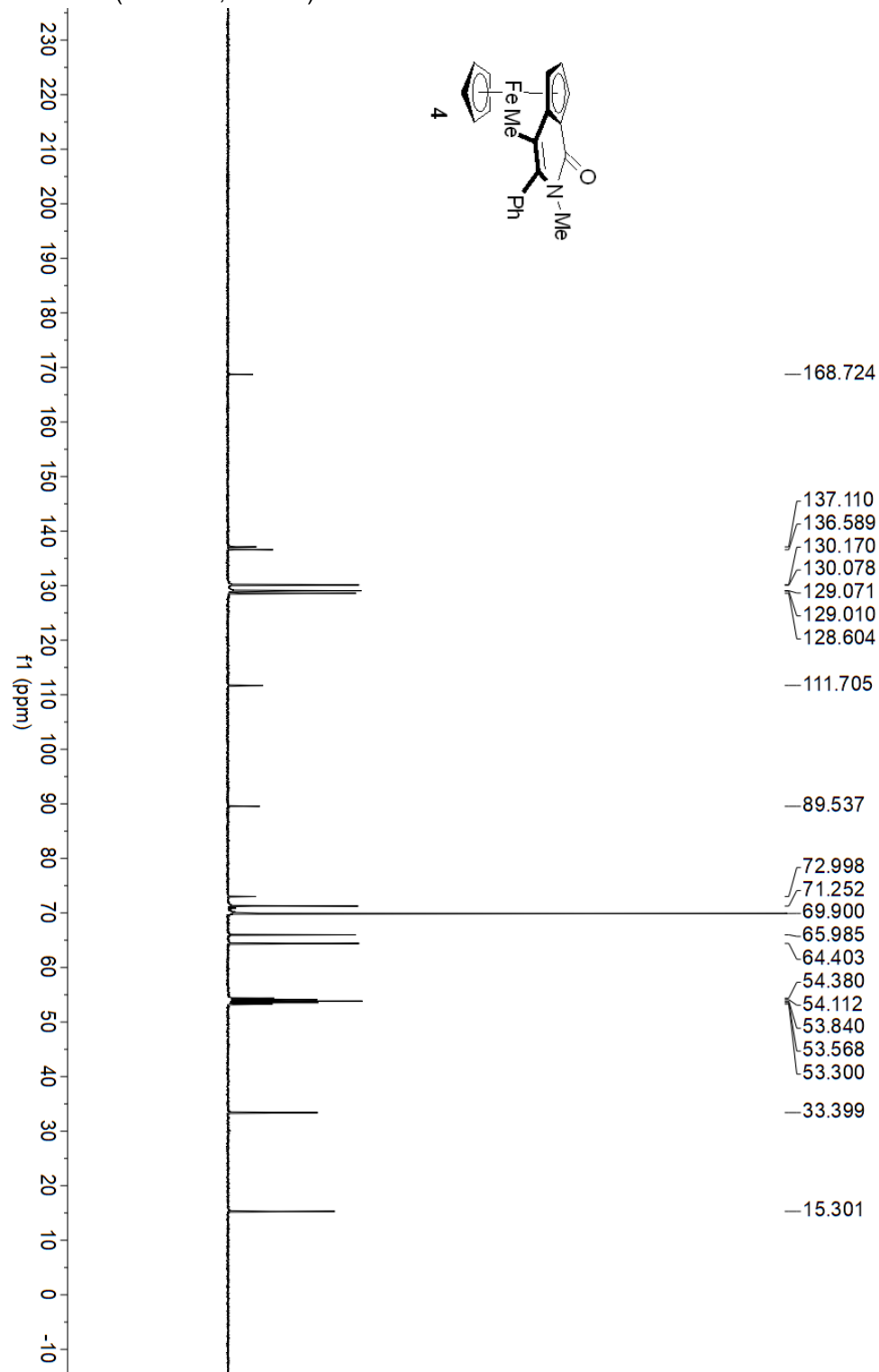
¹H NMR (400 MHz, CDCl₃)



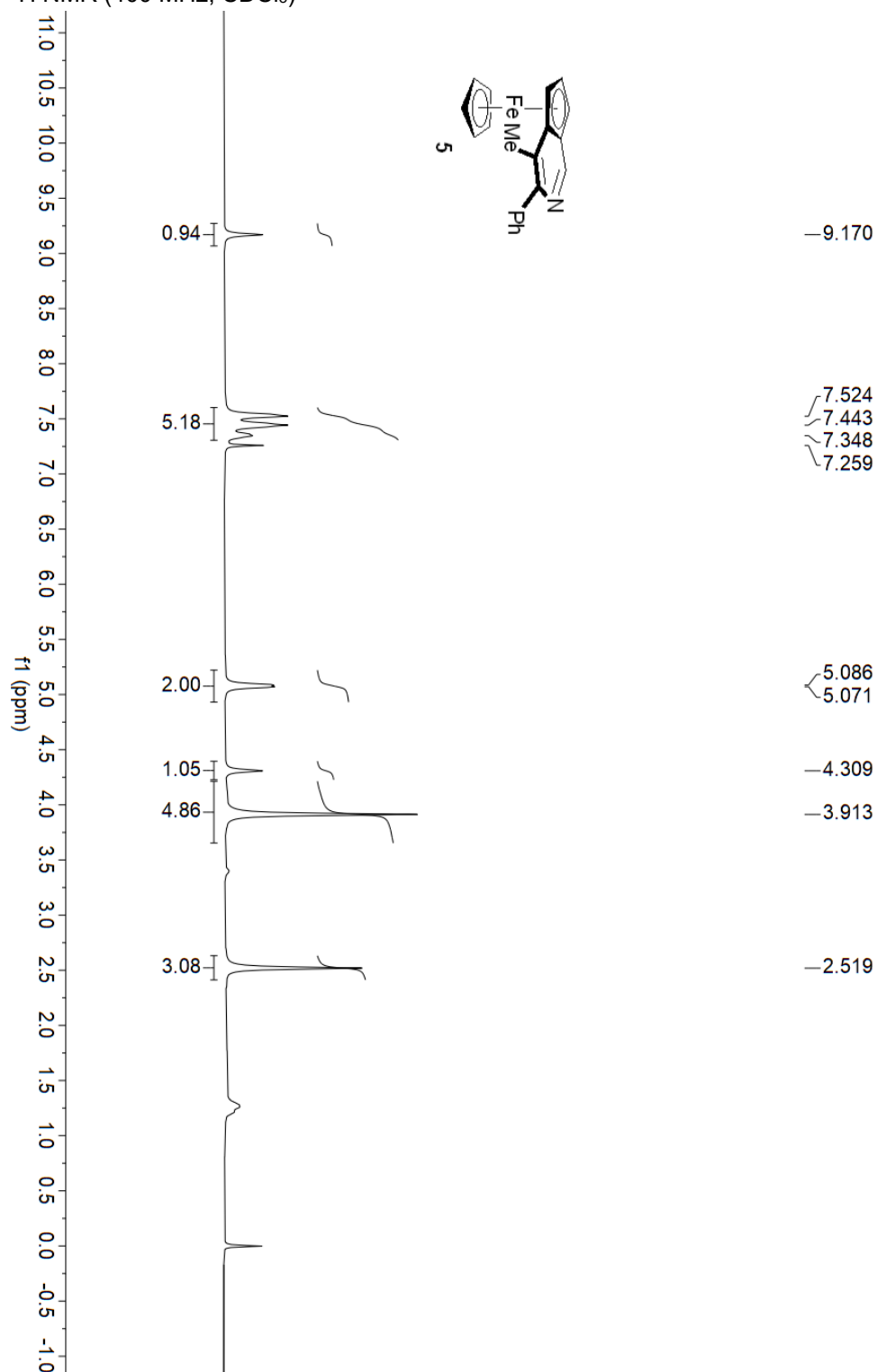
^1H NMR (400 MHz, CD_2Cl_2)



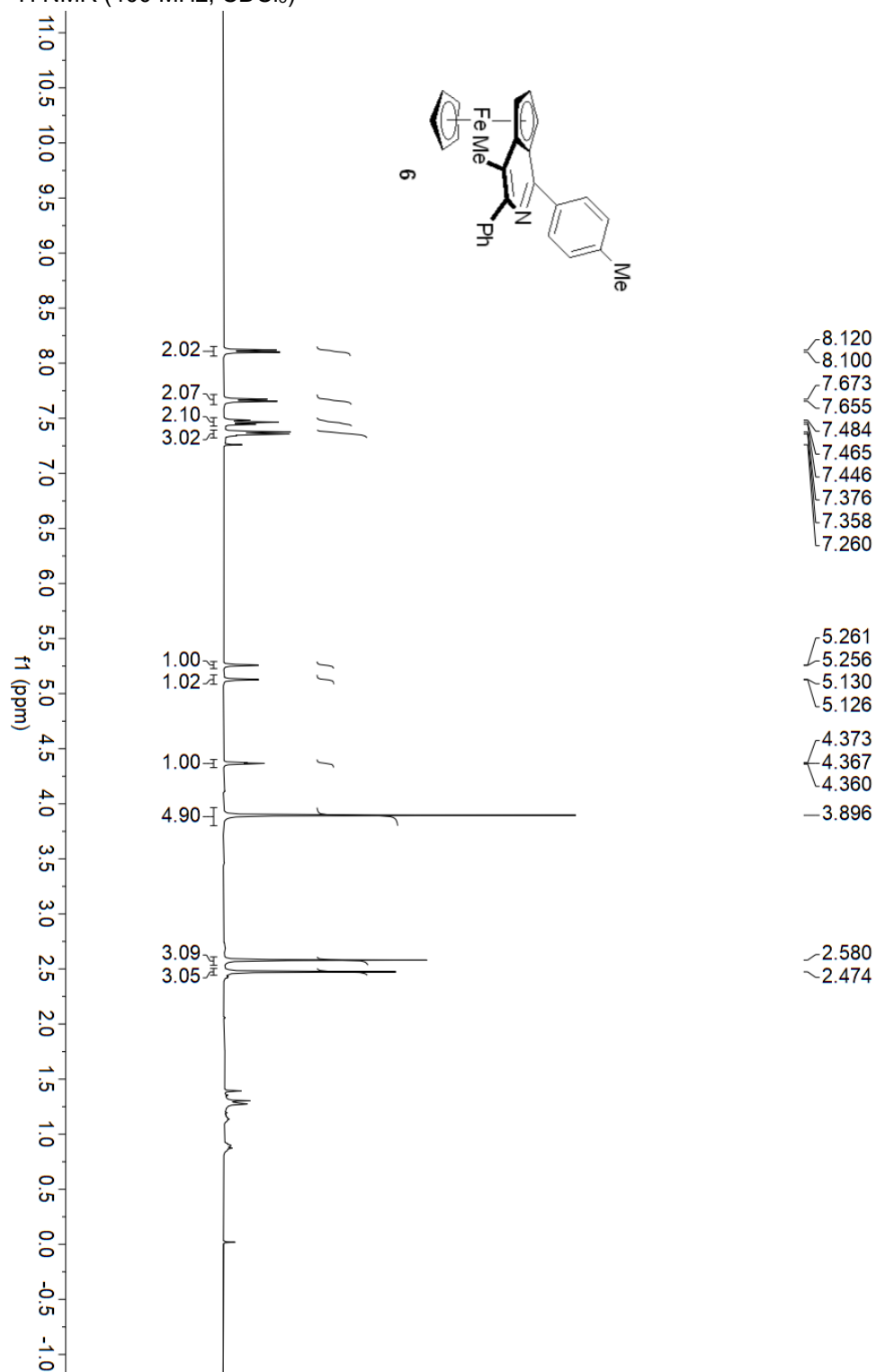
¹³C NMR (100 MHz, CD₂Cl₂)



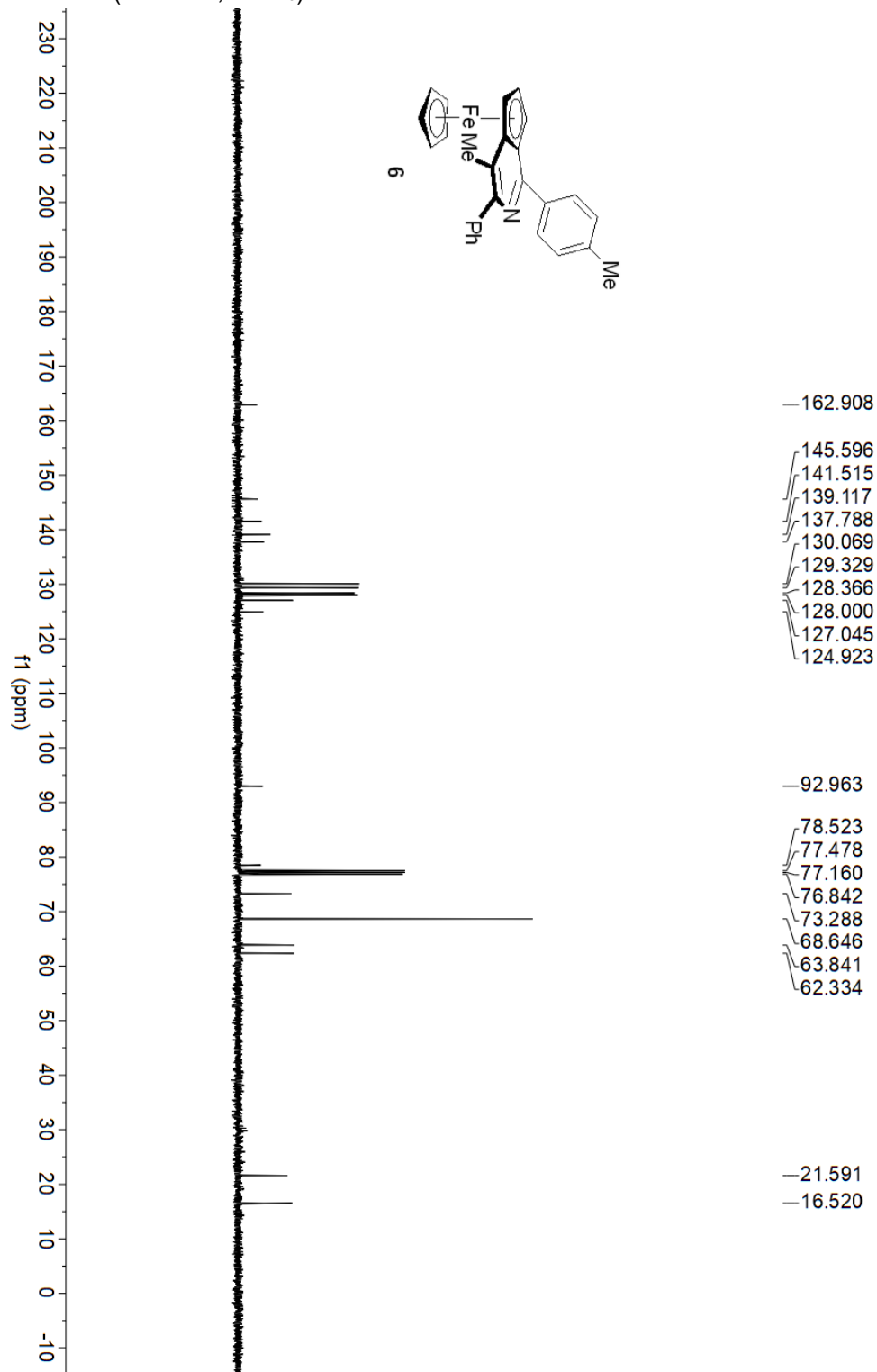
^1H NMR (400 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3)

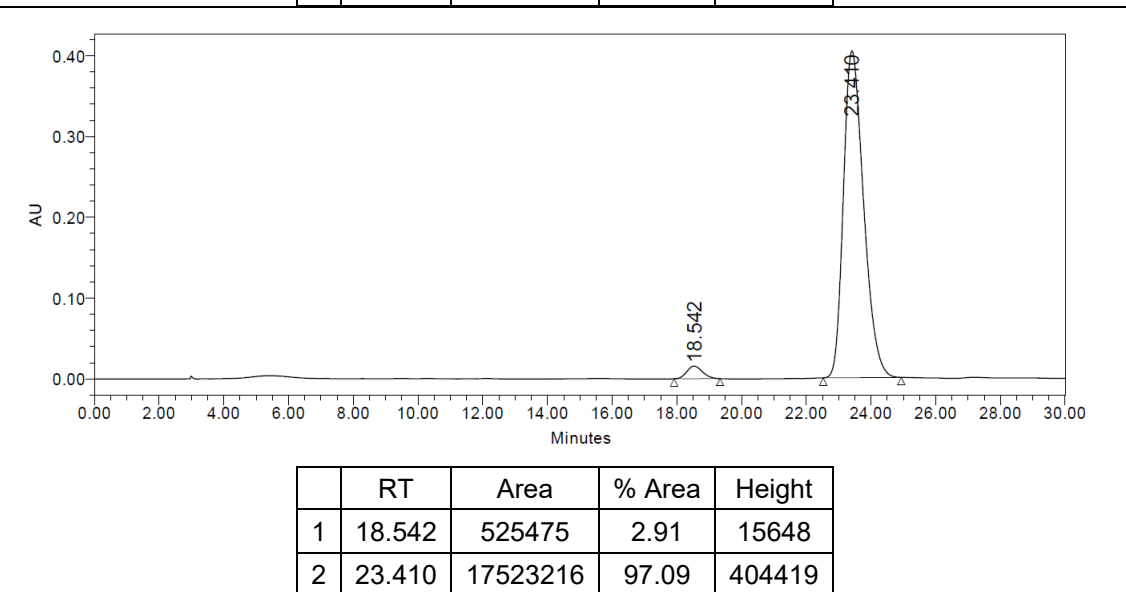
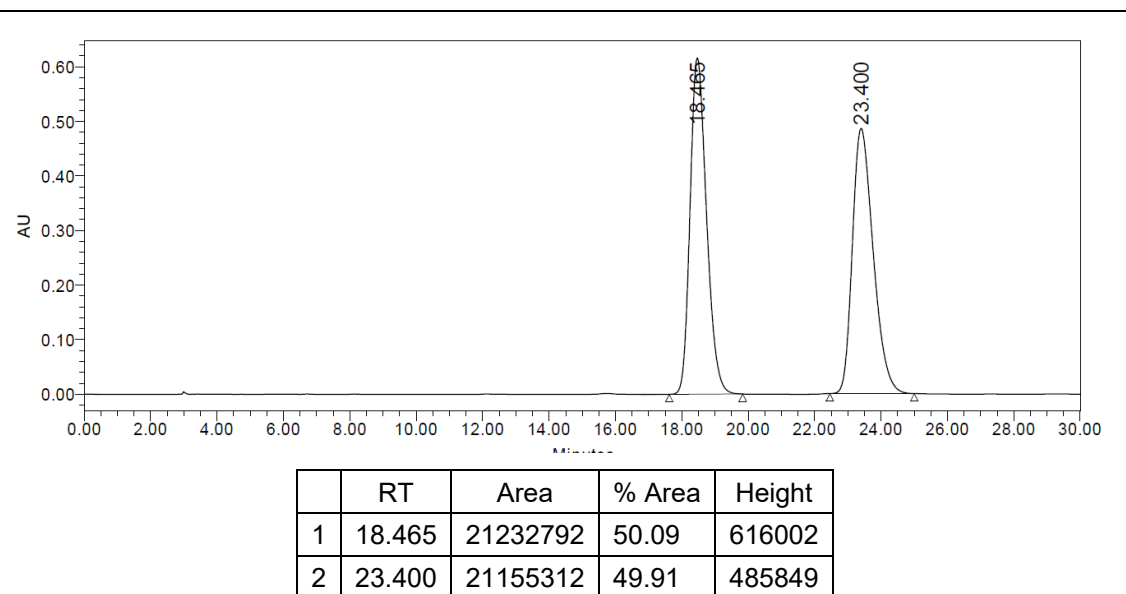
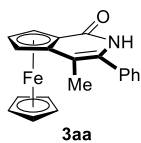


¹³C NMR (100 MHz, CDCl₃)

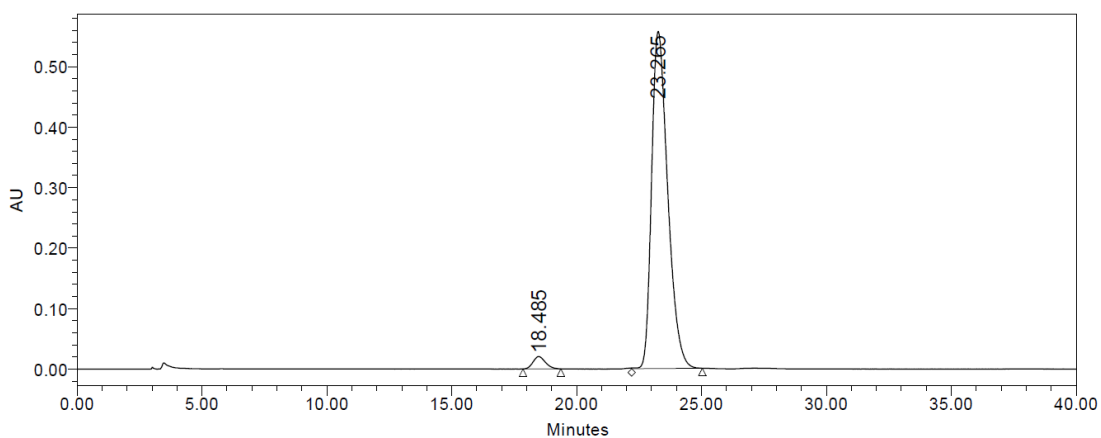
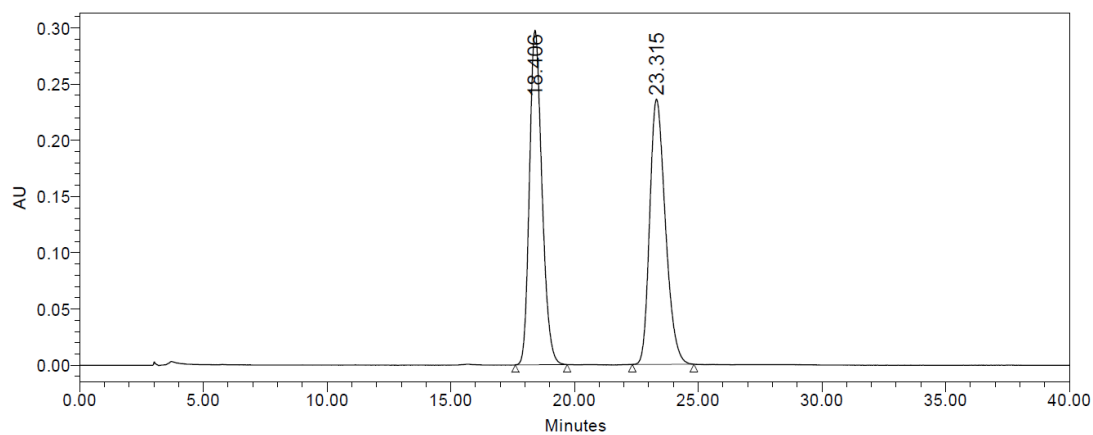
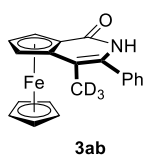


12. Copies of HPLC chromatogram

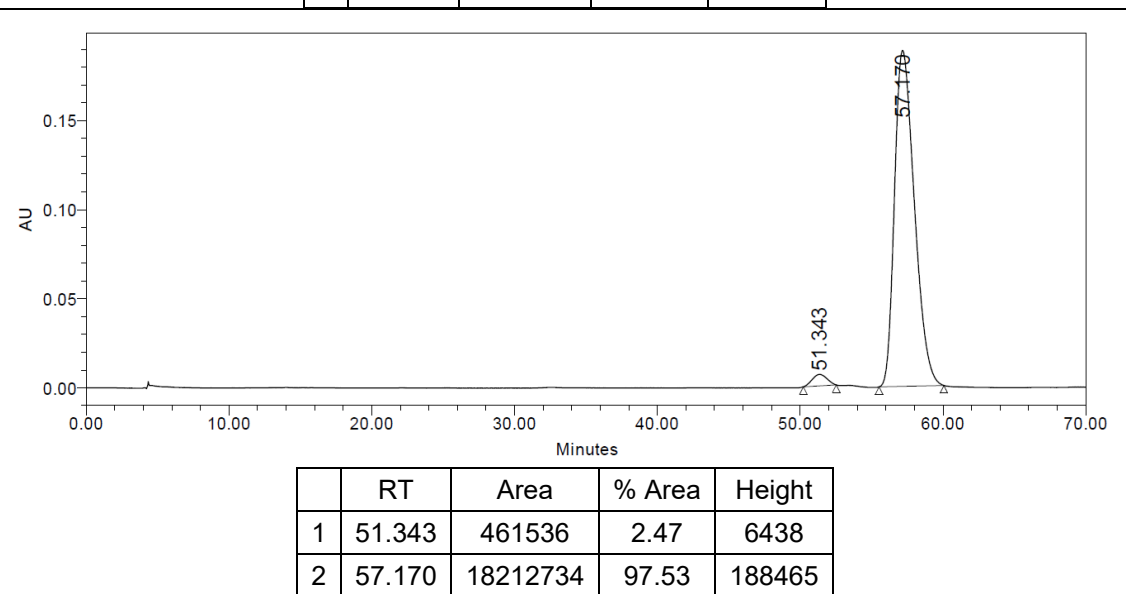
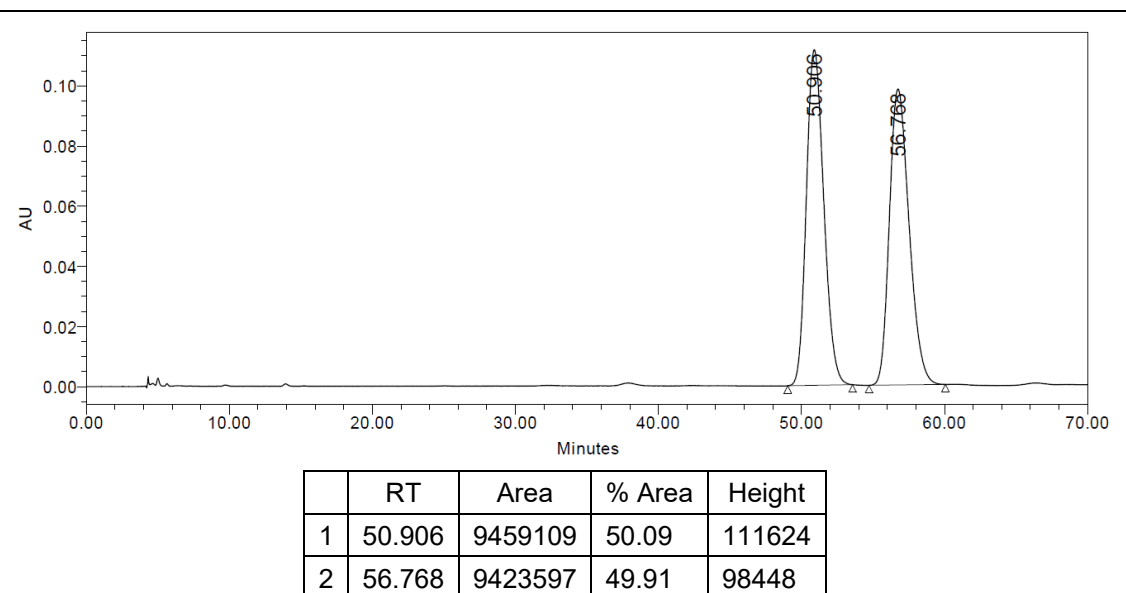
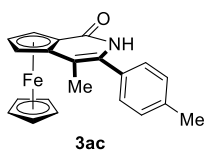
HPLC analysis of **3aa**



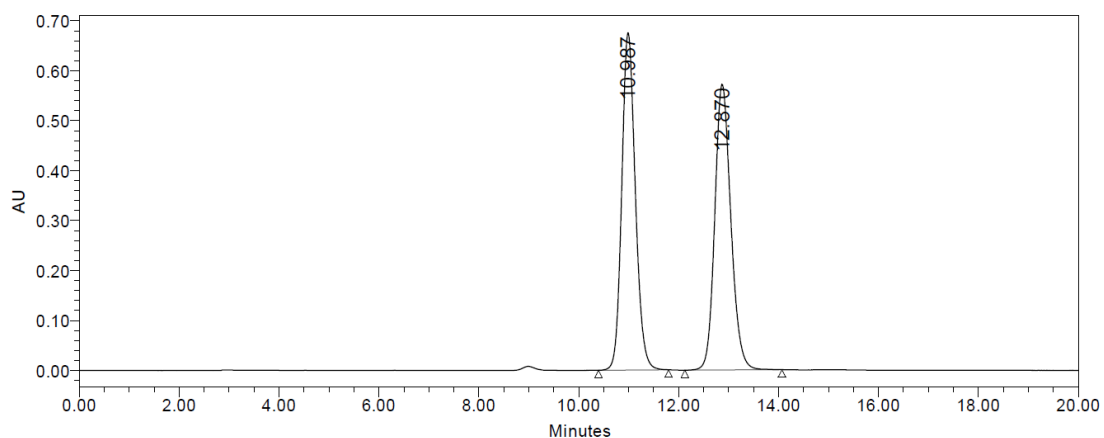
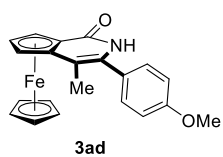
HPLC analysis of **3ab**



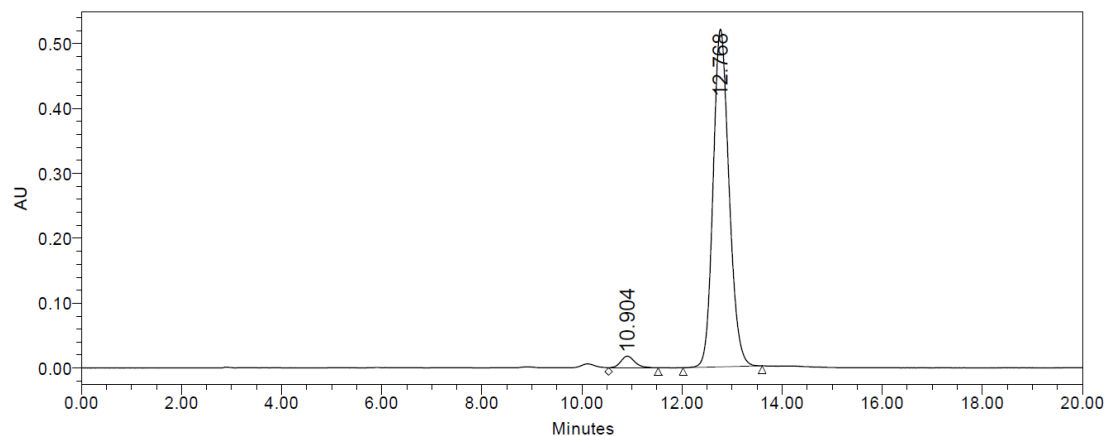
HPLC analysis of **3ac**



HPLC analysis of **3ad**

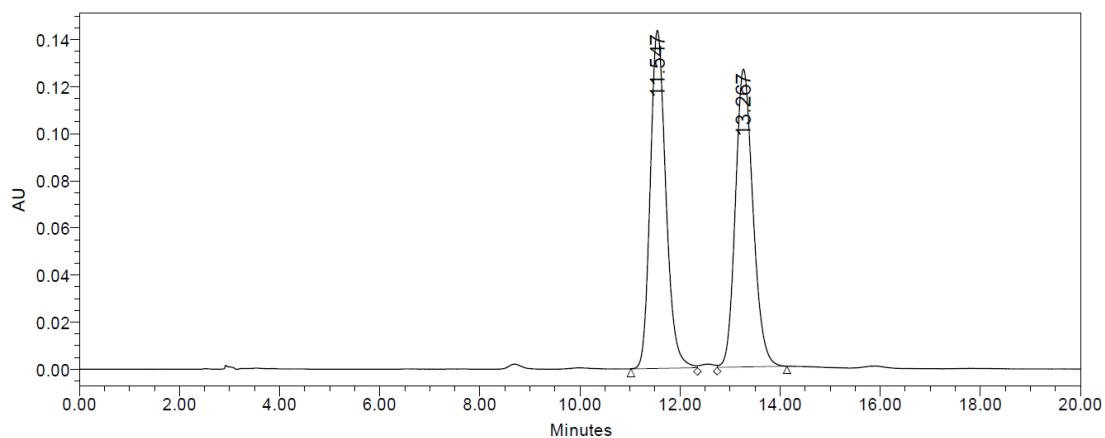
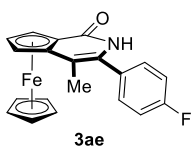


	RT	Area	% Area	Height
1	10.987	12736284	49.92	675064
2	12.870	12774972	50.08	571554

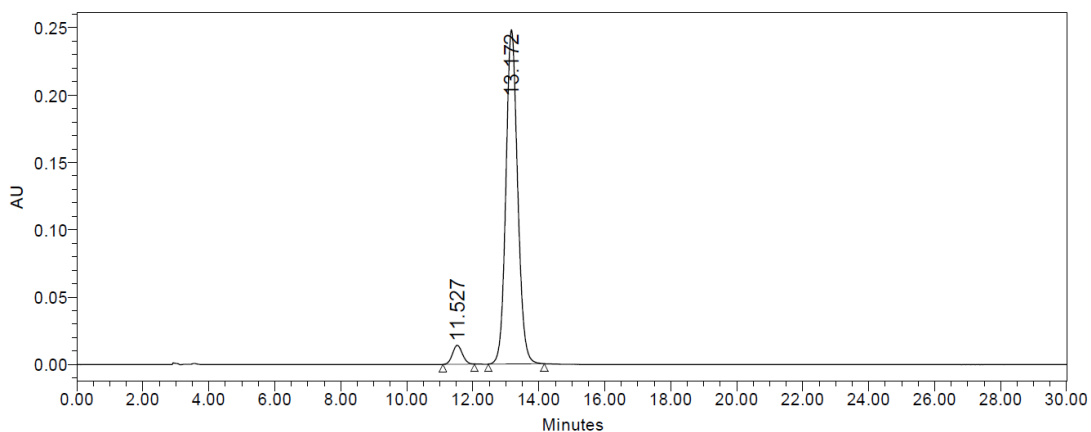


	RT	Area	% Area	Height
1	10.904	341252	2.88	17824
2	12.768	11528316	97.12	520496

HPLC analysis of **3ae**

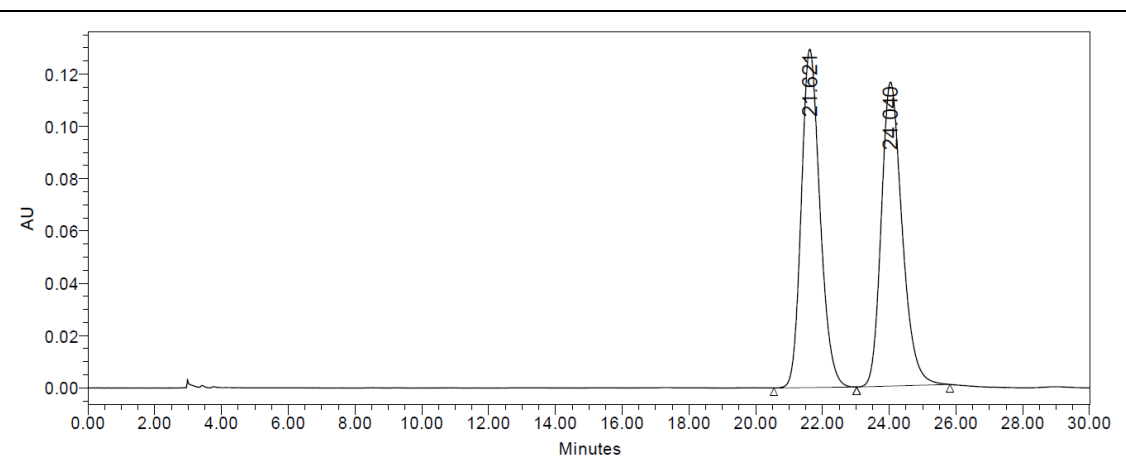
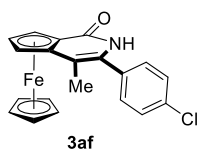


	RT	Area	% Area	Height
1	11.547	3111085	50.14	143519
2	13.267	3093265	49.86	126455

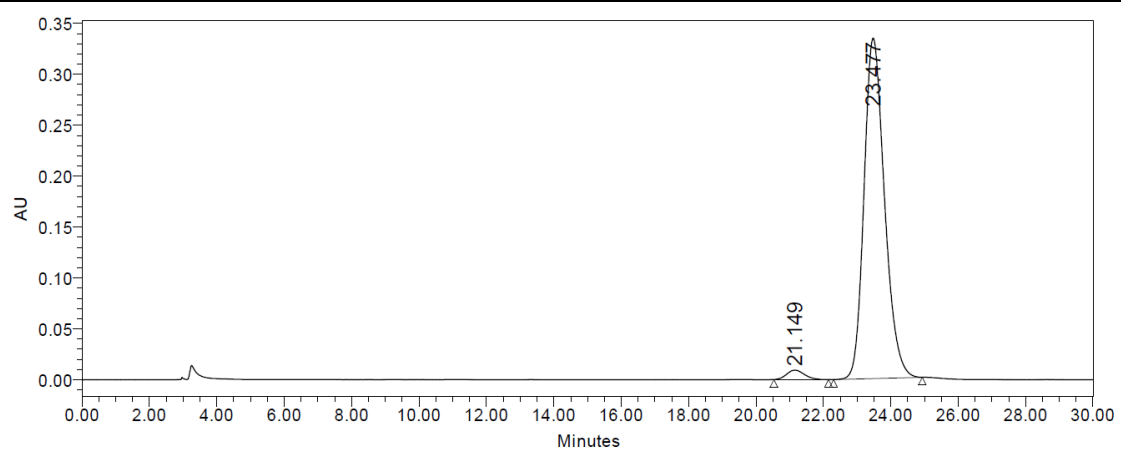


	RT	Area	% Area	Height
1	11.527	292730	4.56	14011
2	13.172	6131668	95.44	247958

HPLC analysis of **3af**

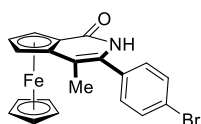


	RT	Area	% Area	Height
1	21.621	5028402	49.88	129392
2	24.040	5052442	50.12	116253

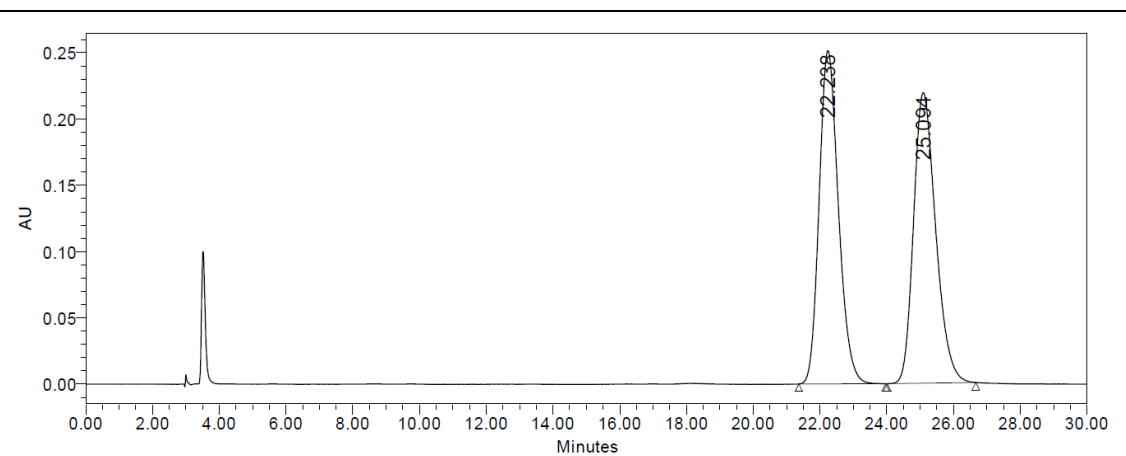


	RT	Area	% Area	Height
1	21.149	340814	2.36	9322
2	23.477	14106509	97.64	334281

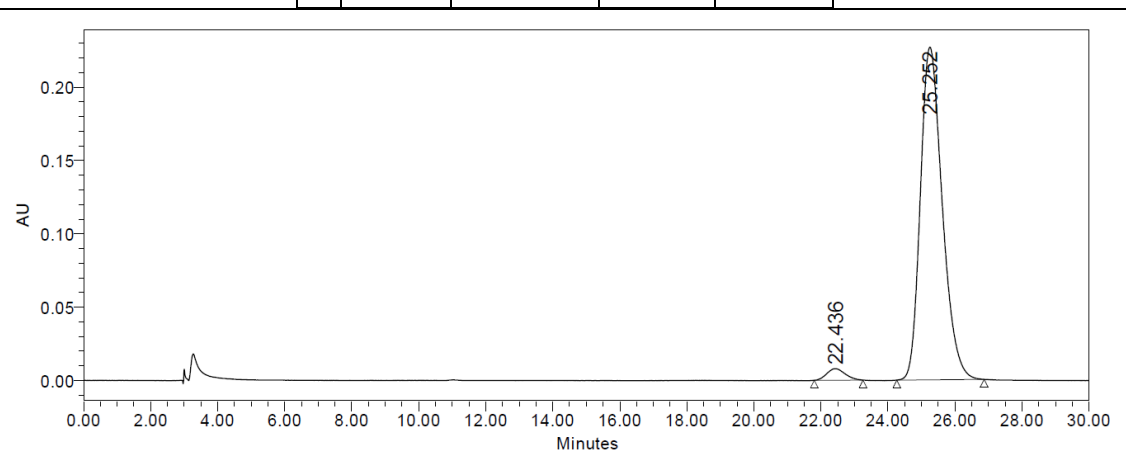
HPLC analysis of **3ag**



3ag

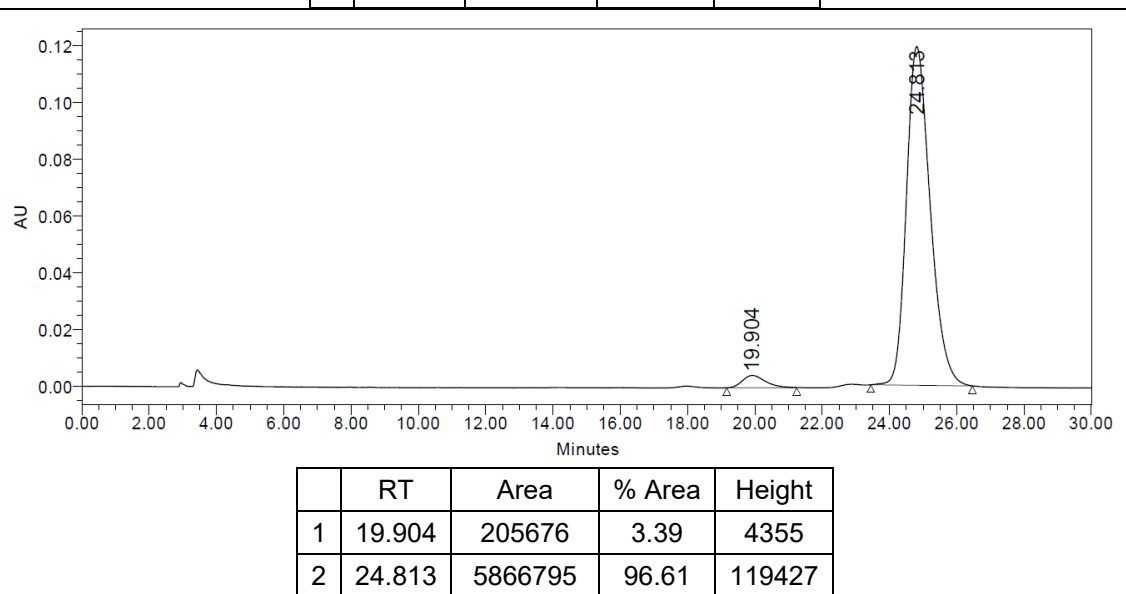
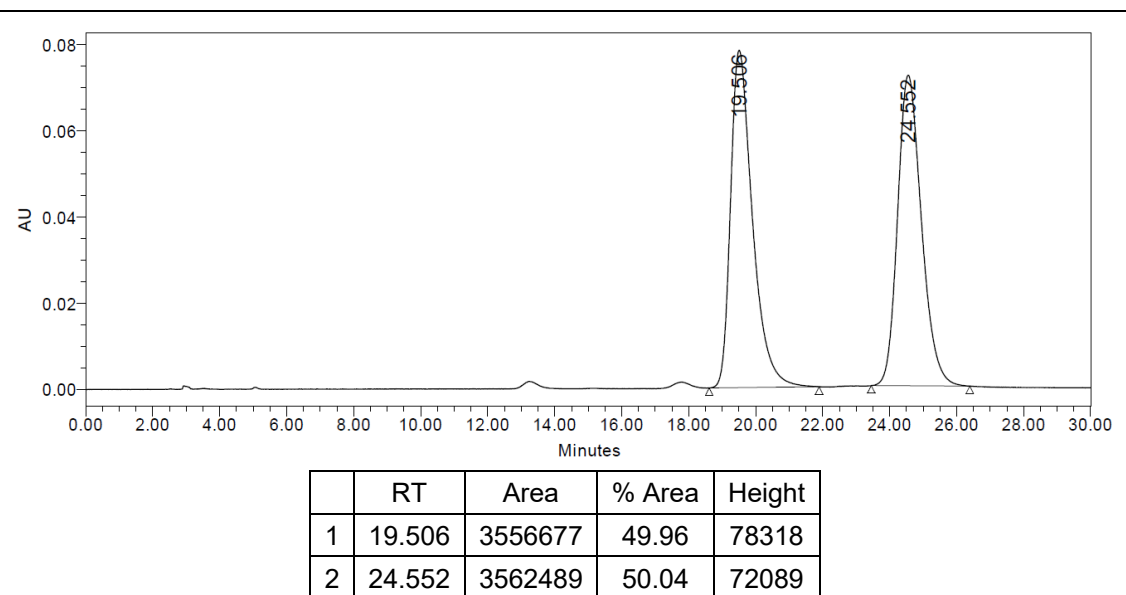
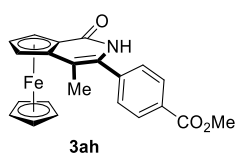


	RT	Area	% Area	Height
1	22.238	10079235	49.99	251438
2	25.094	10083835	50.01	219166

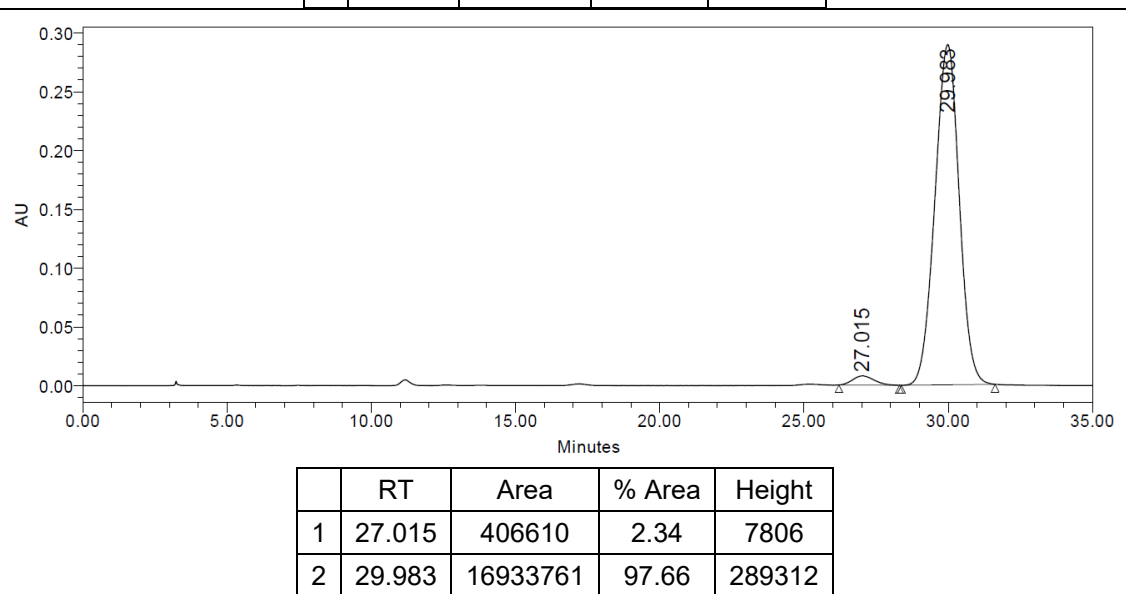
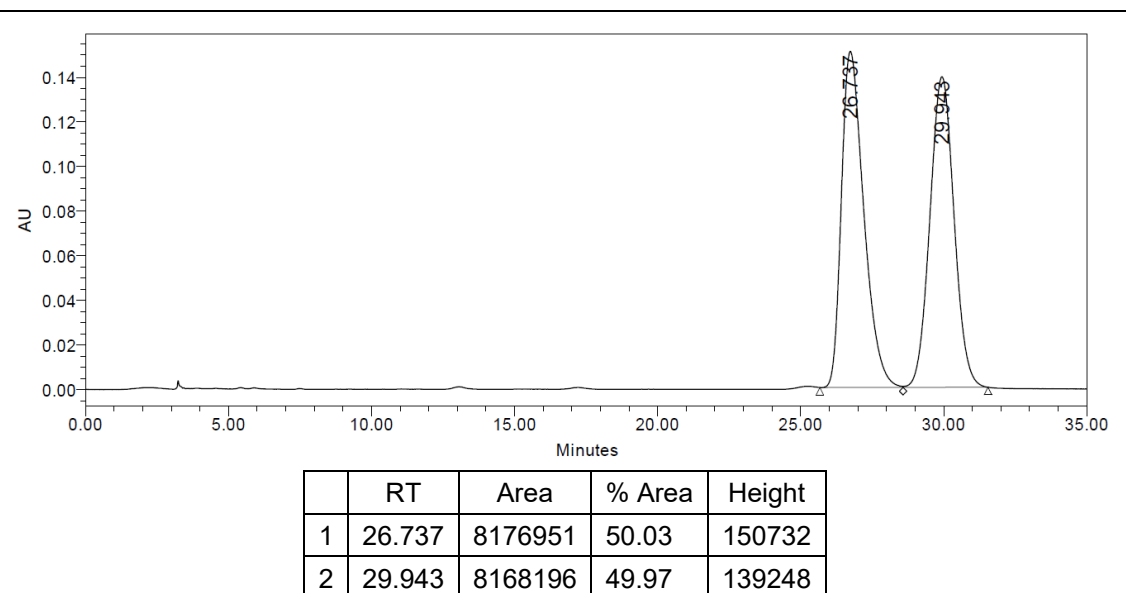
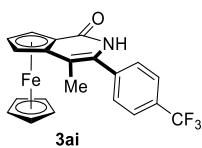


	RT	Area	% Area	Height
1	22.436	299996	2.83	7927
2	25.252	10286206	97.17	227011

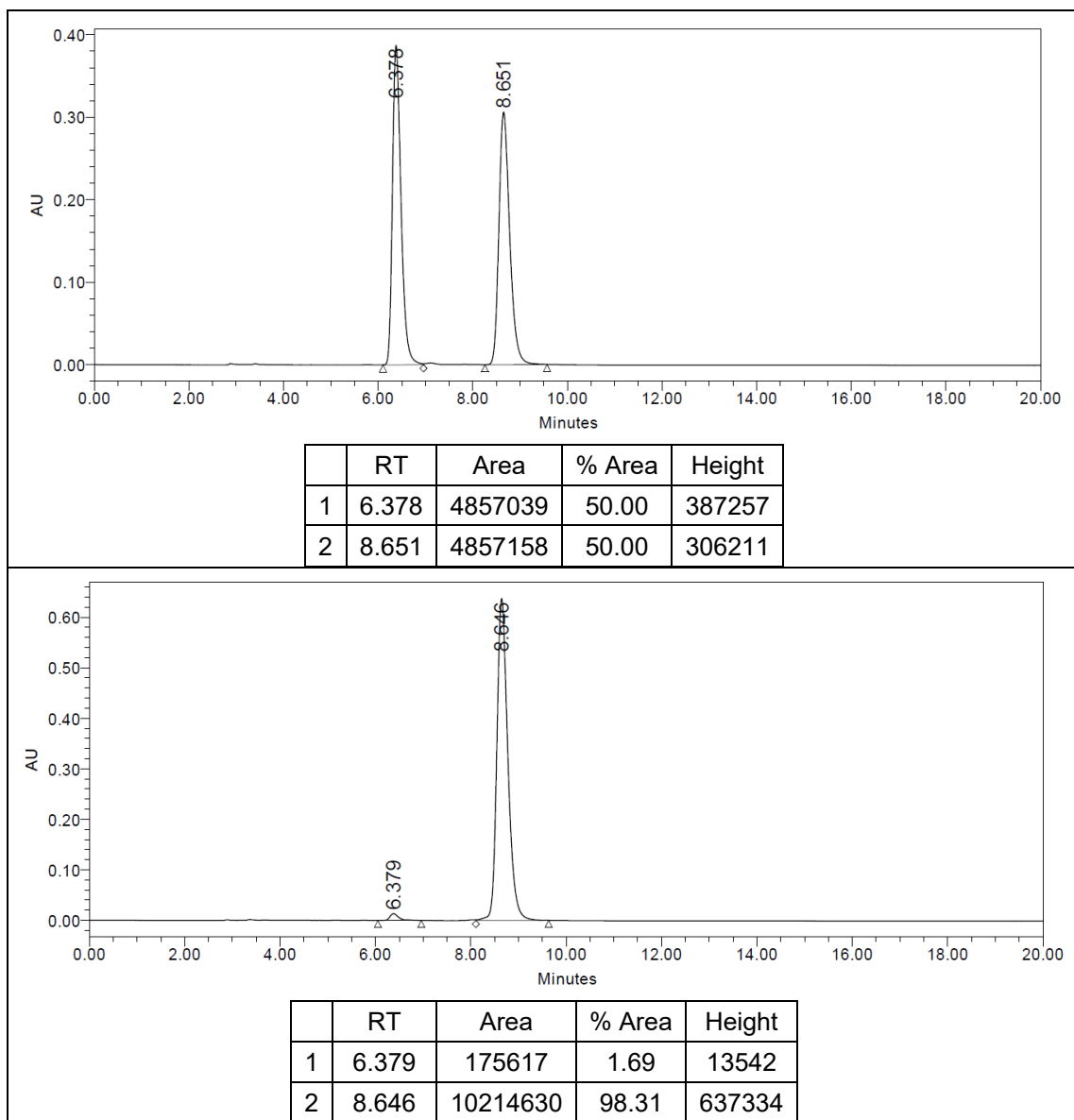
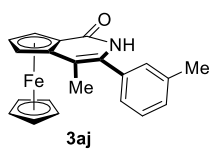
HPLC analysis of **3ah**



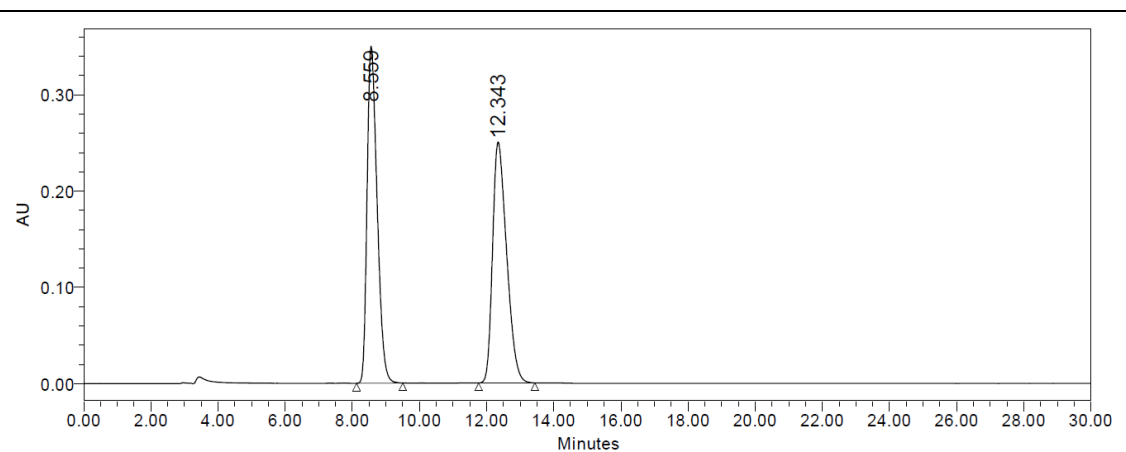
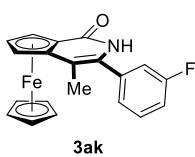
HPLC analysis of **3ai**



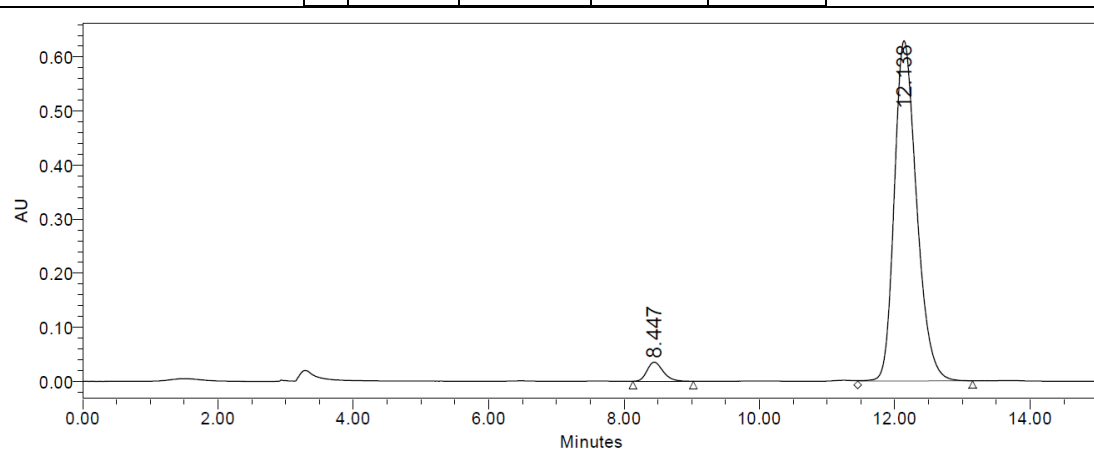
HPLC analysis of **3aj**



HPLC analysis of **3ak**

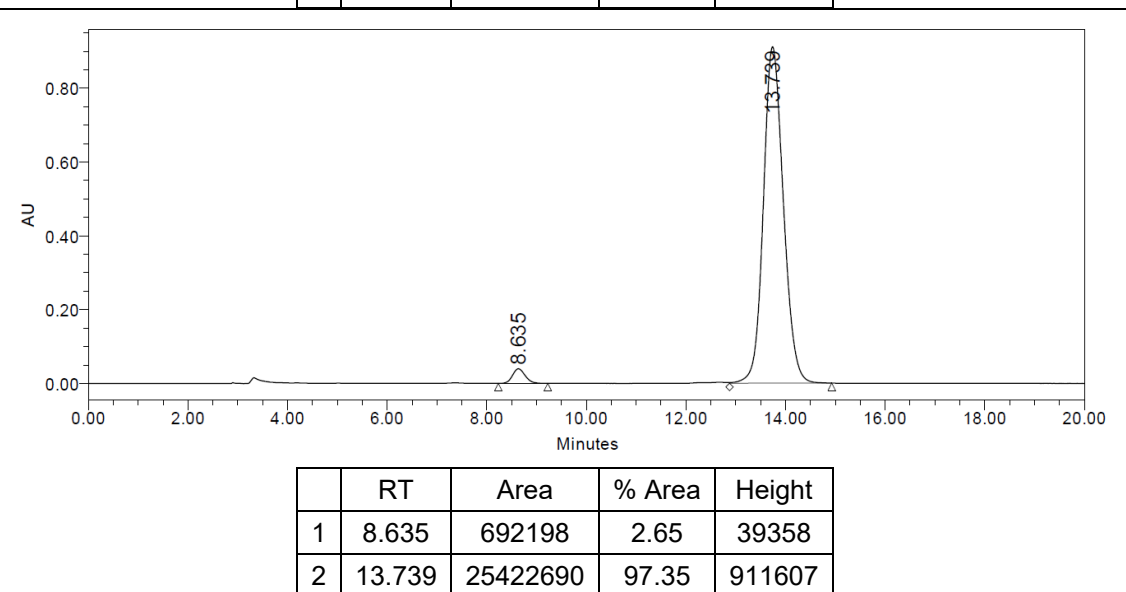
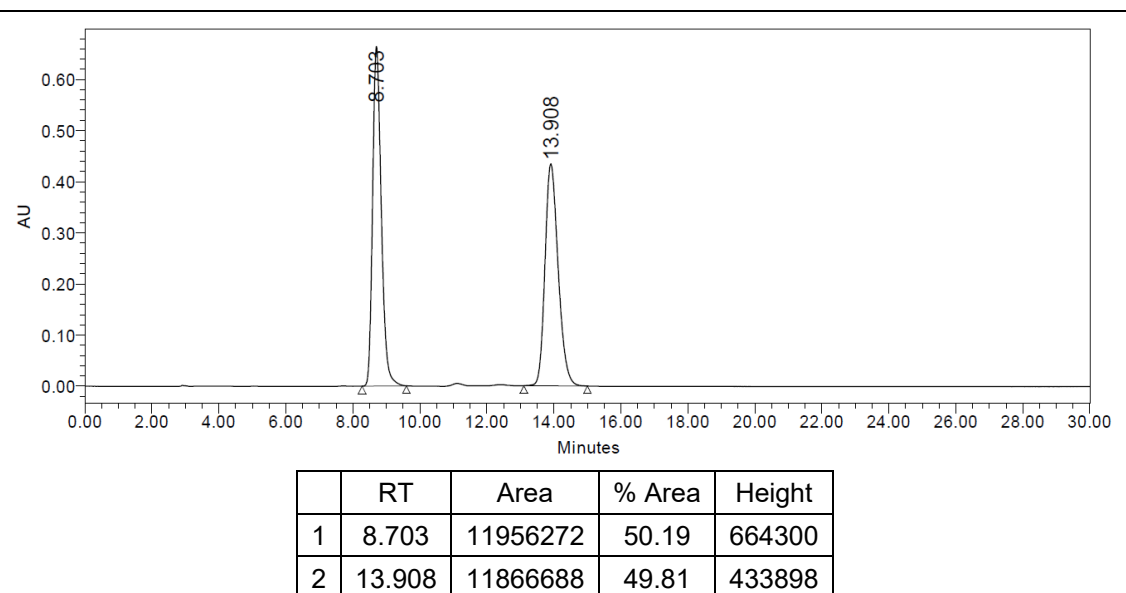
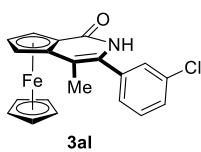


	RT	Area	% Area	Height
1	8.559	7249754	49.93	350108
2	12.343	7271467	50.07	250463

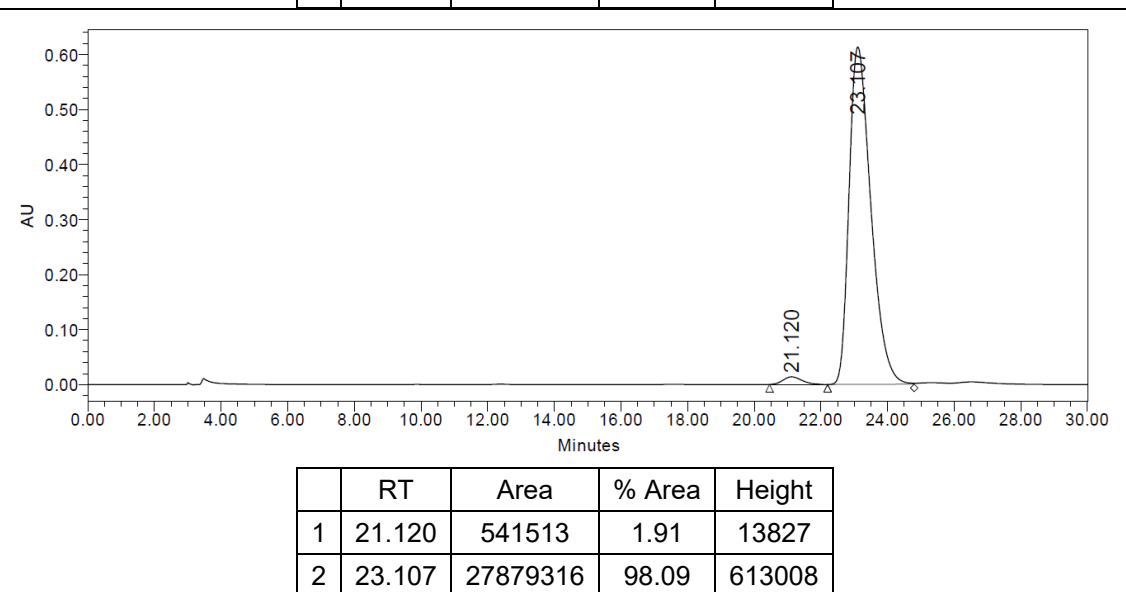
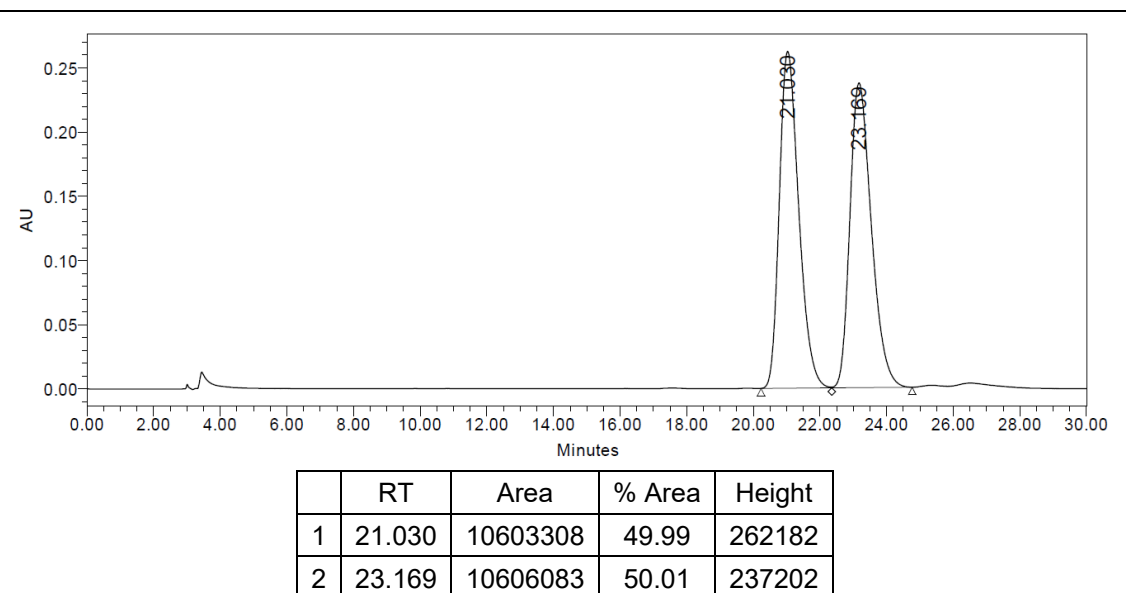
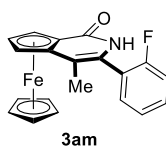


	RT	Area	% Area	Height
1	8.447	578929	3.86	35269
2	12.138	14426449	96.14	629336

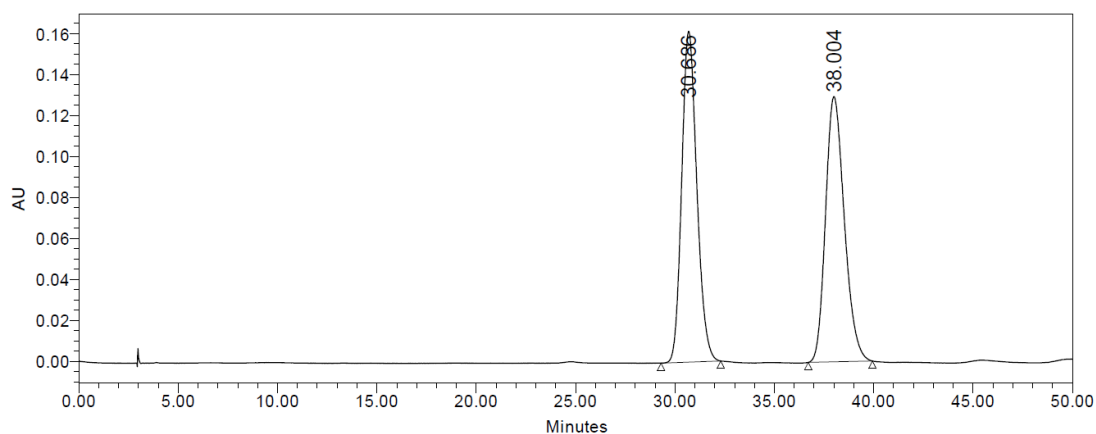
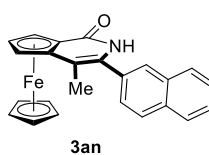
HPLC analysis of **3al**



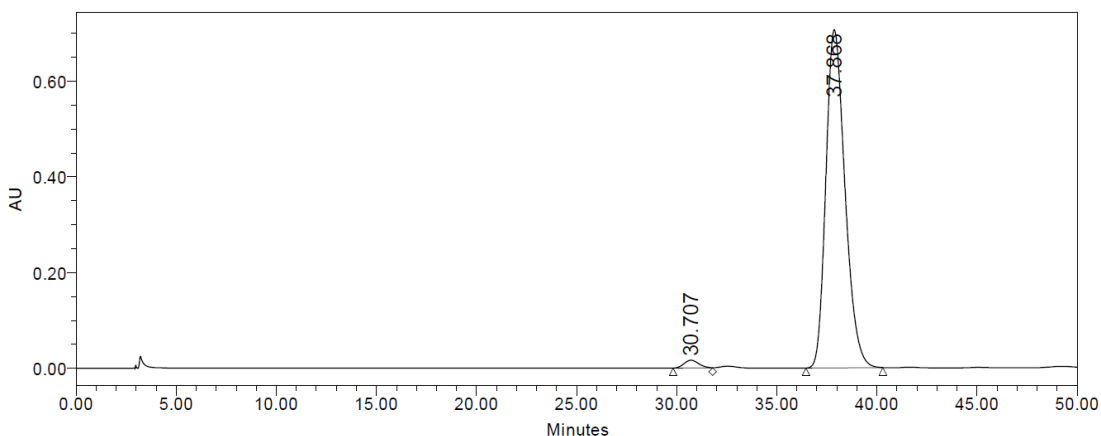
HPLC analysis of **3am**



HPLC analysis of **3an**

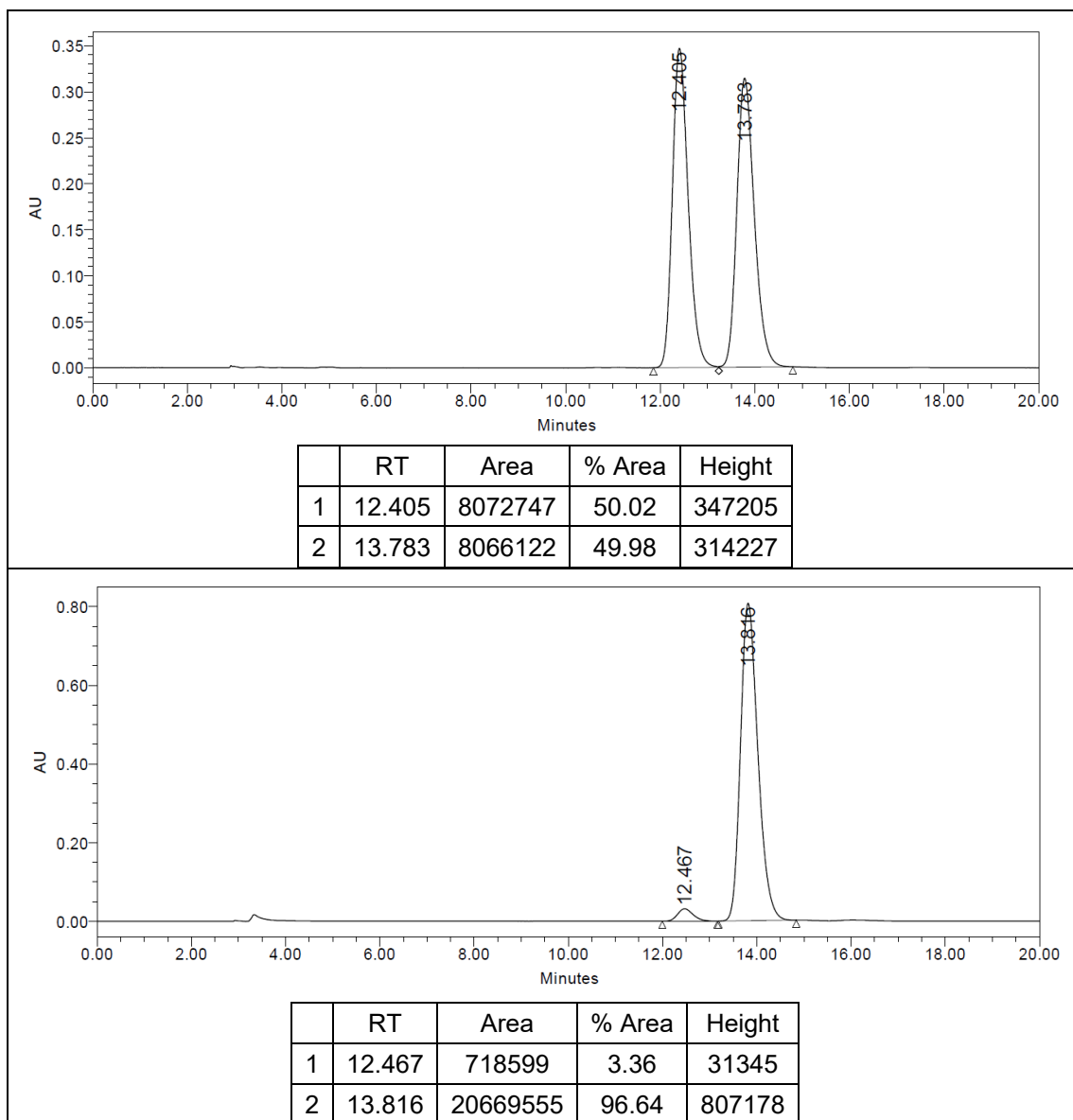
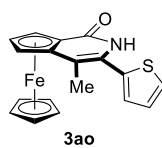


	RT	Area	% Area	Height
1	30.686	8528813	50.03	161555
2	38.004	8517972	49.97	129518

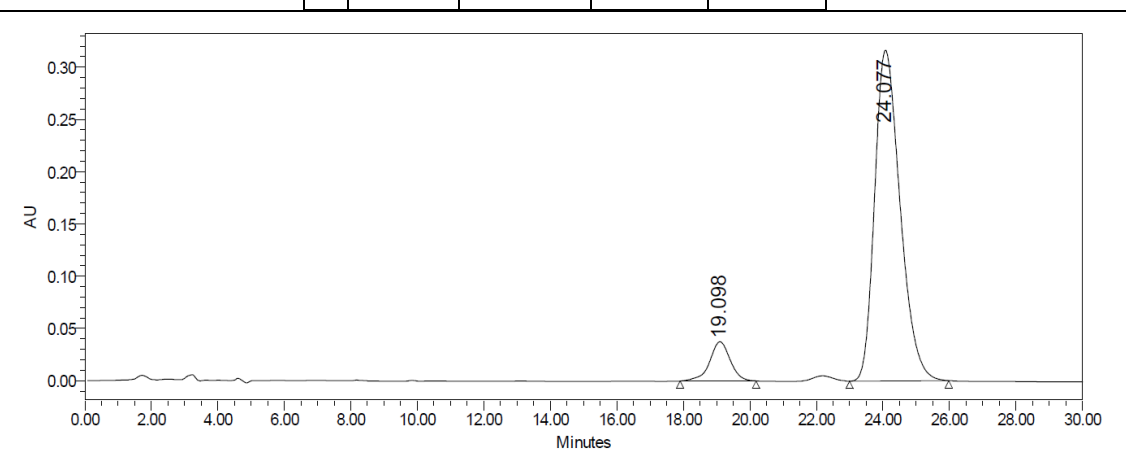
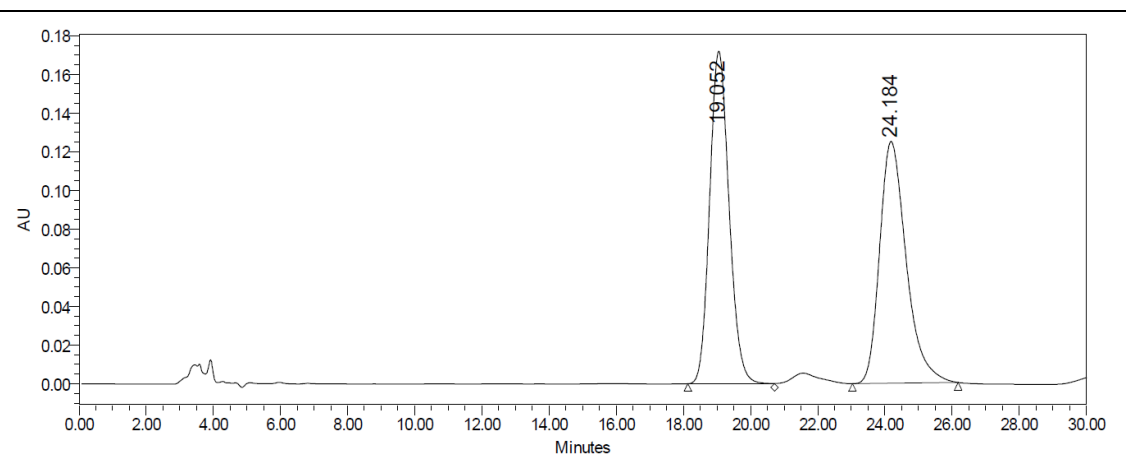
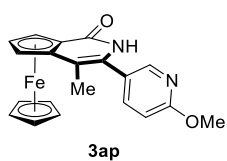


	RT	Area	% Area	Height
1	30.707	836252	1.75	16382
2	37.868	46868473	98.25	706429

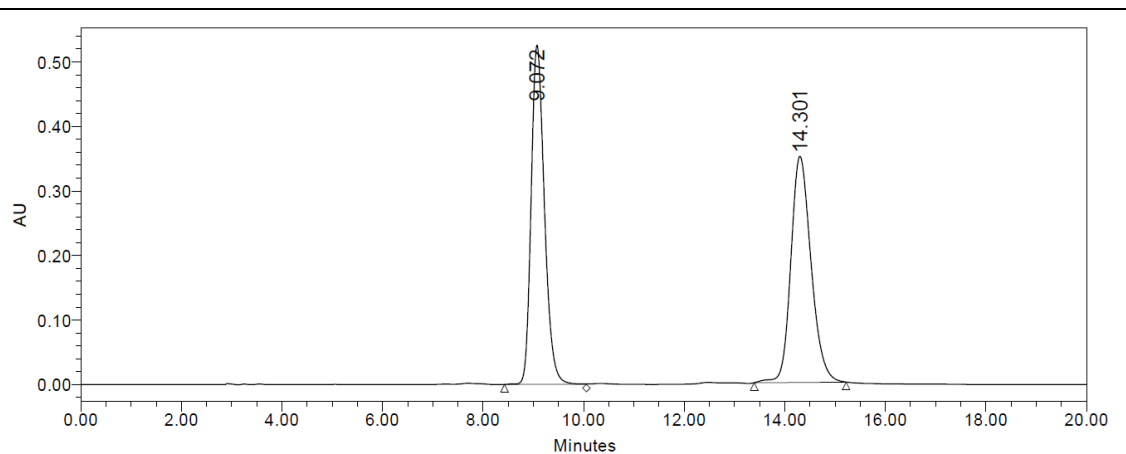
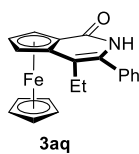
HPLC analysis of **3ao**



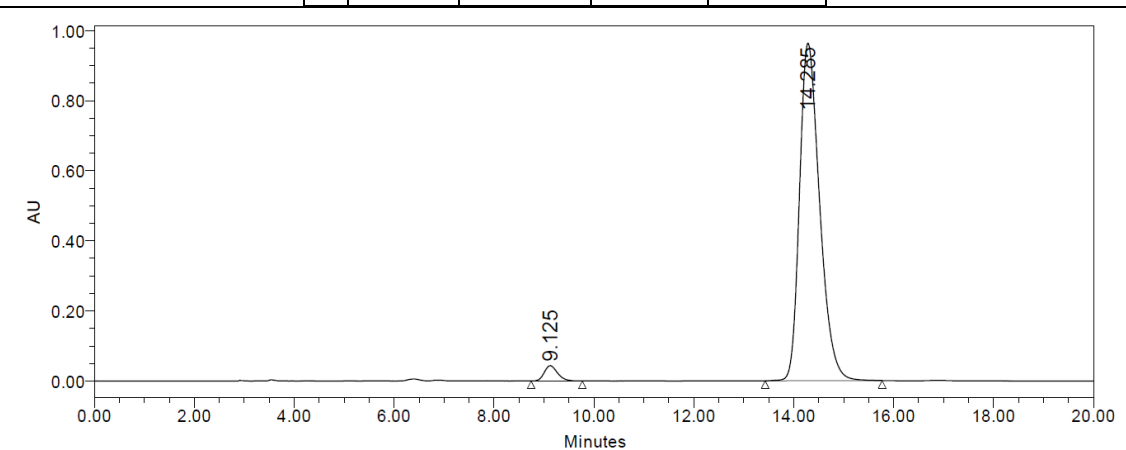
HPLC analysis of **3ap**



HPLC analysis of **3aq**

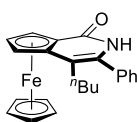


	RT	Area	% Area	Height
1	9.072	9641800	49.63	525191
2	14.301	9784825	50.37	350302

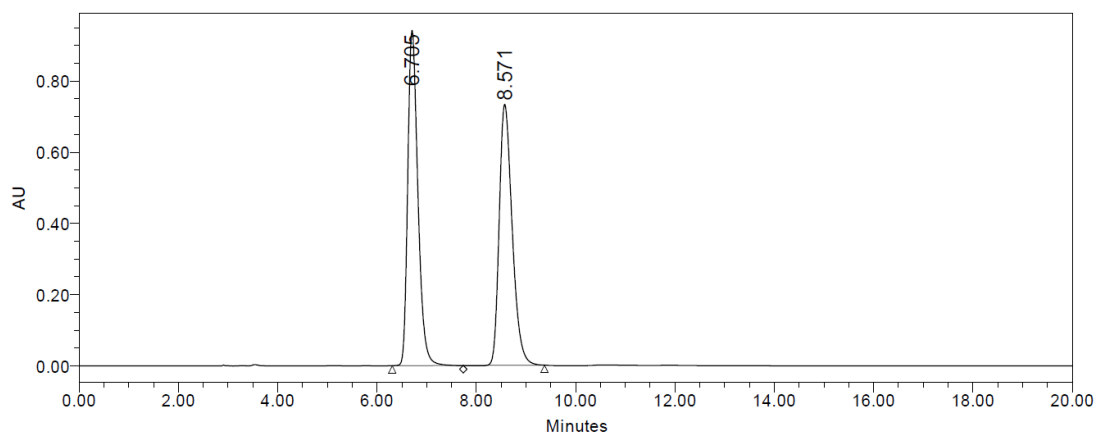


	RT	Area	% Area	Height
1	9.125	798655	2.88	2.88
2	14.285	26908211	97.12	97.12

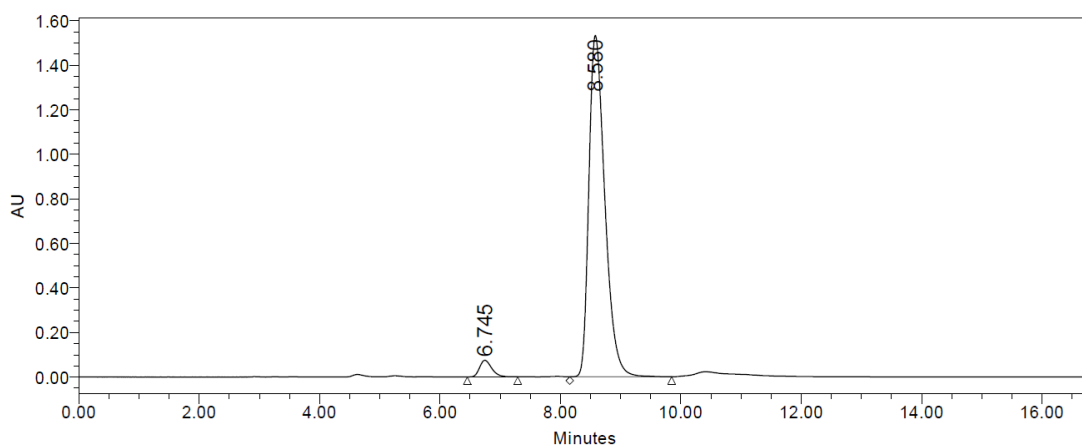
HPLC analysis of **3ar**



3ar

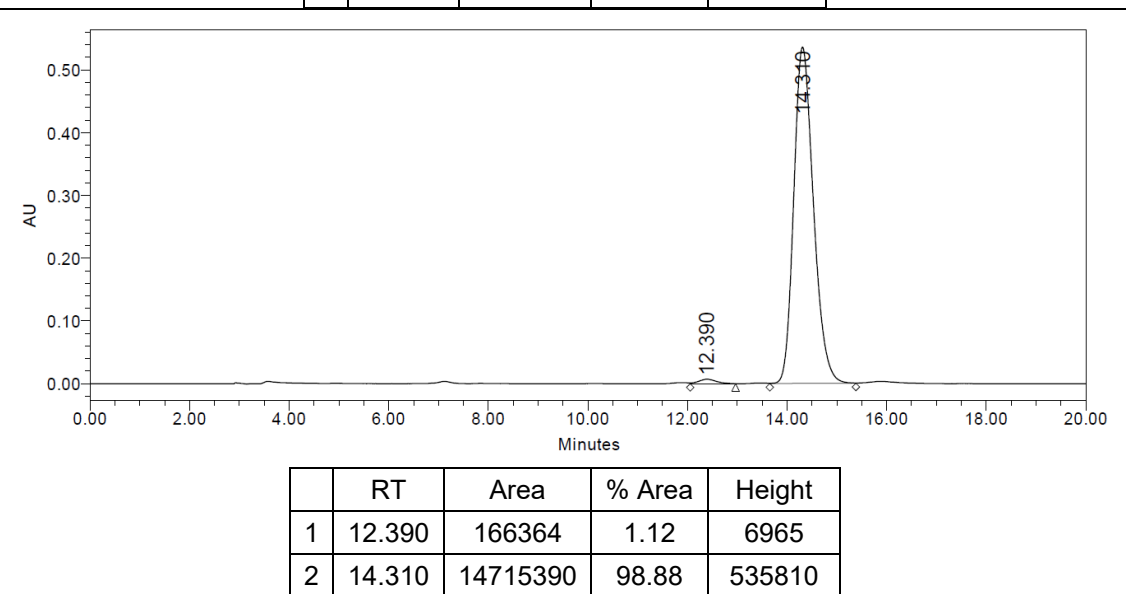
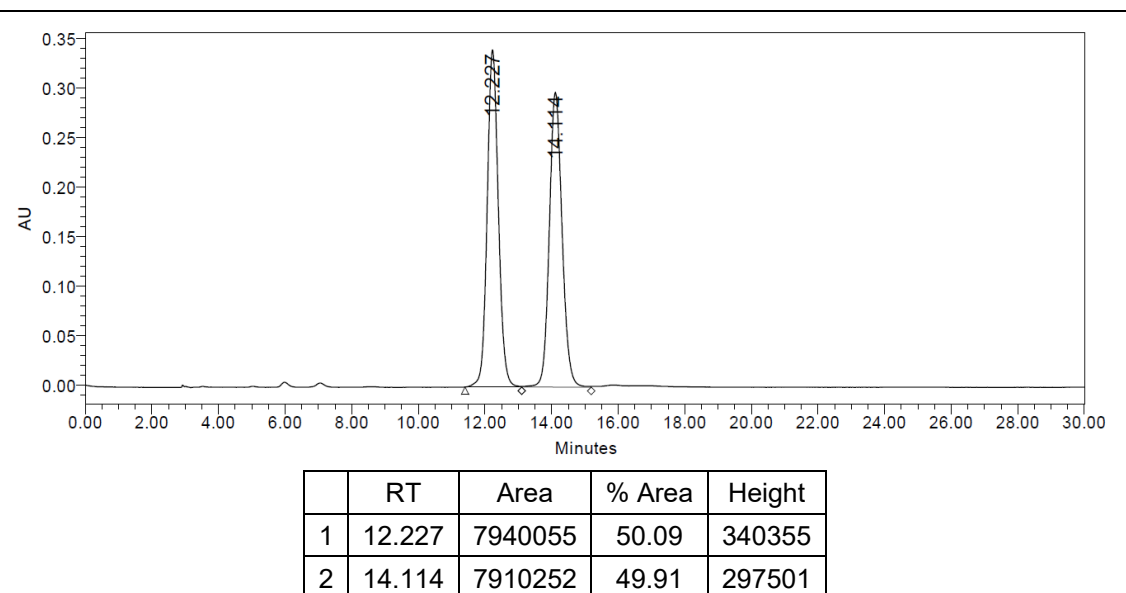
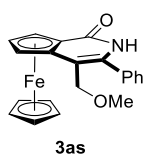


	RT	Area	% Area	Height
1	6.705	13375157	50.10	941153
2	8.571	13319865	49.90	733016

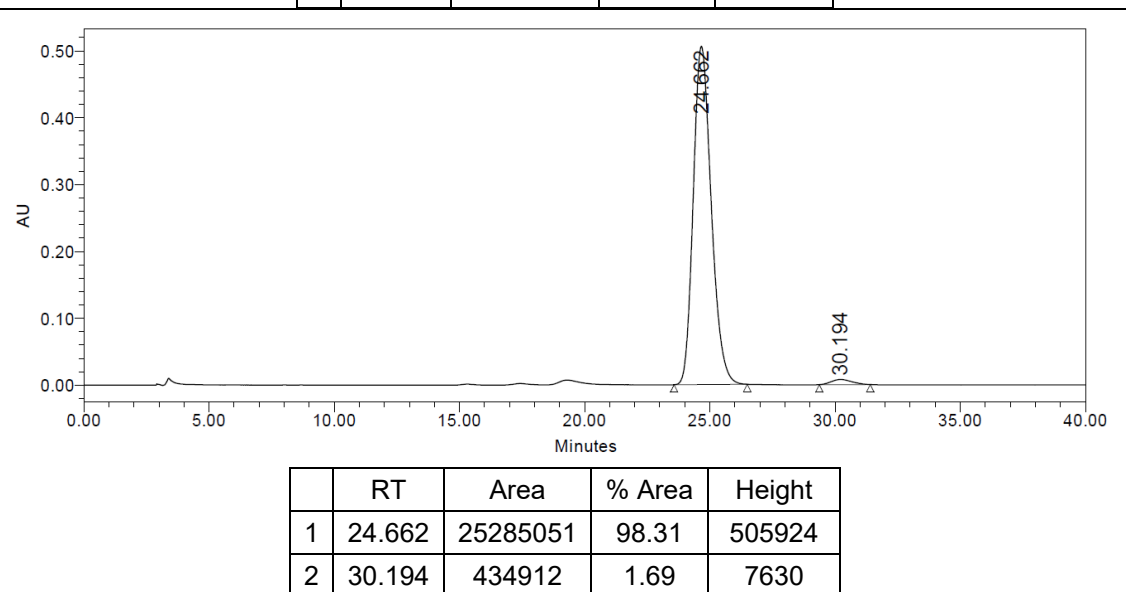
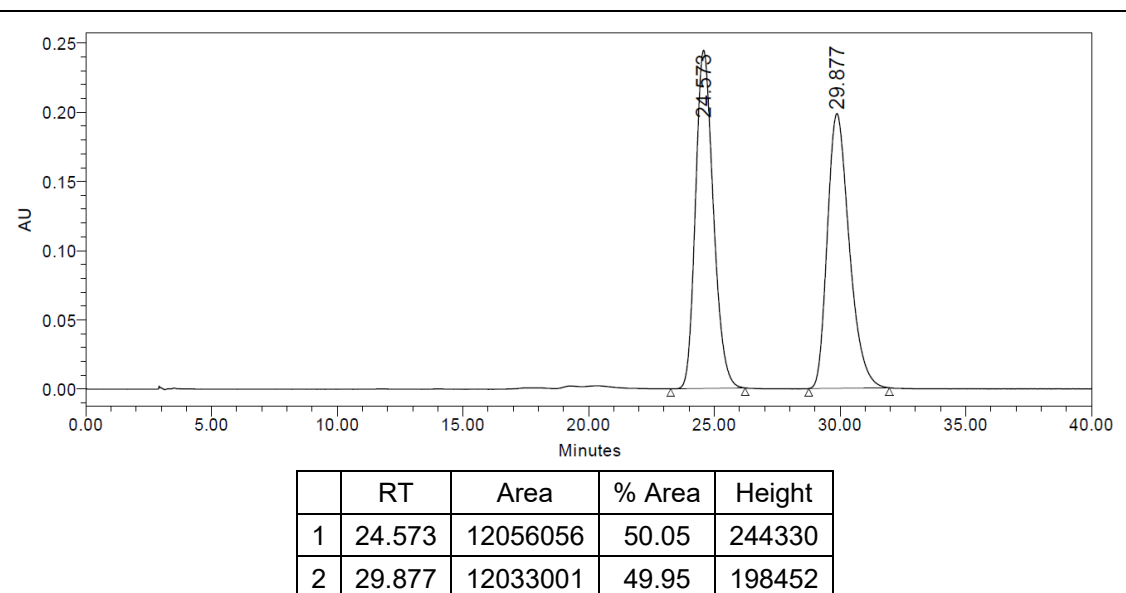
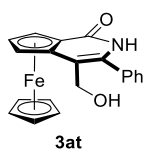


	RT	Area	% Area	Height
1	6.745	1039032	3.55	74492
2	8.580	28196487	96.45	1533179

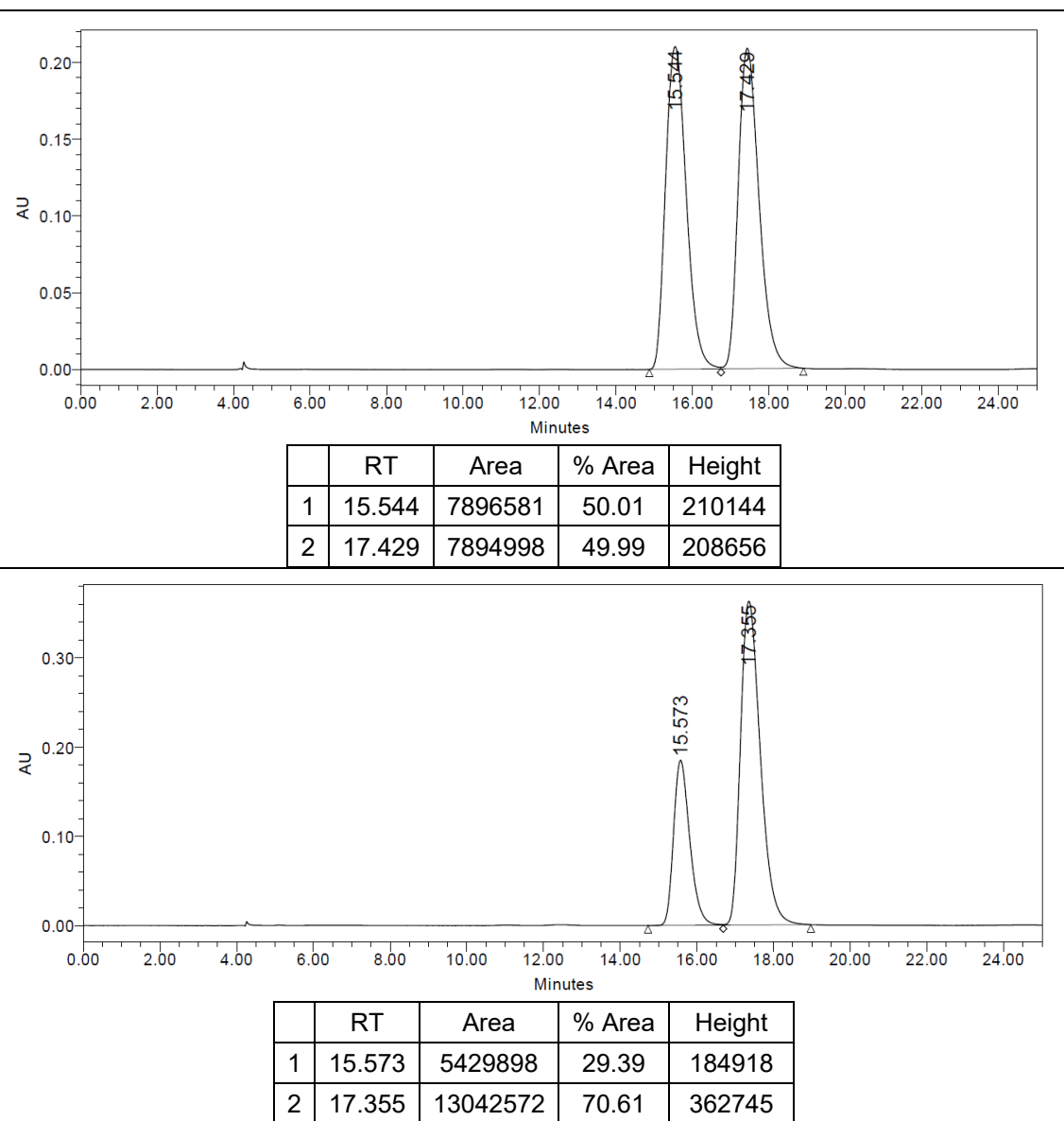
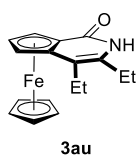
HPLC analysis of **3as**



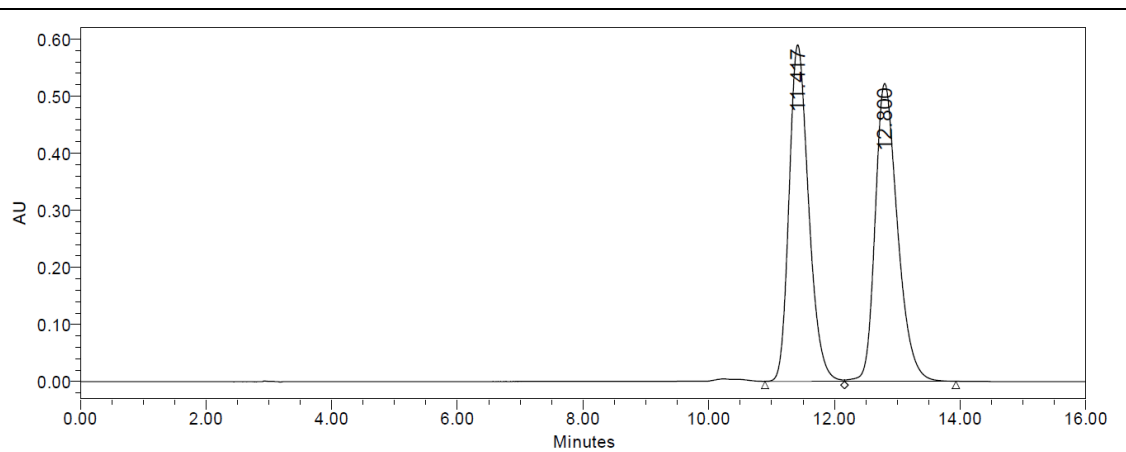
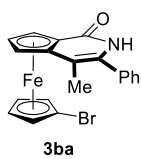
HPLC analysis of **3at**



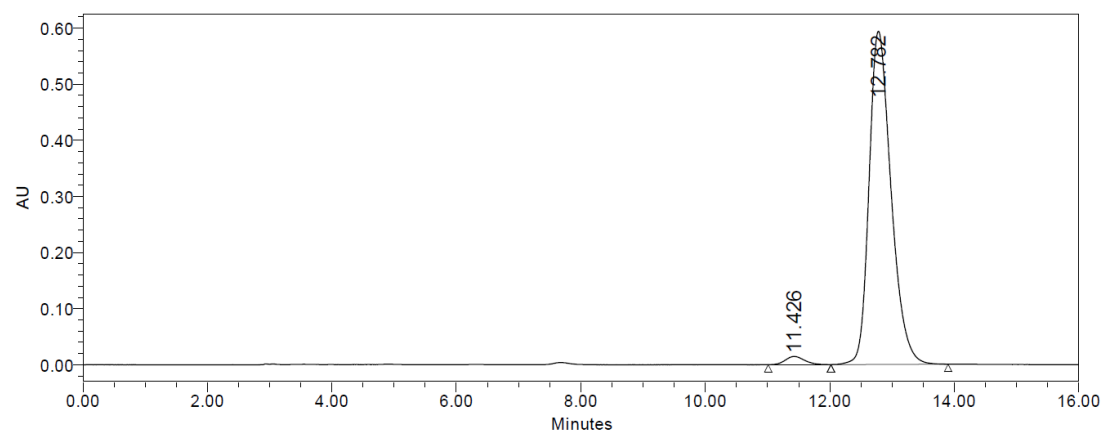
HPLC analysis of **3au**



HPLC analysis of **3ba**

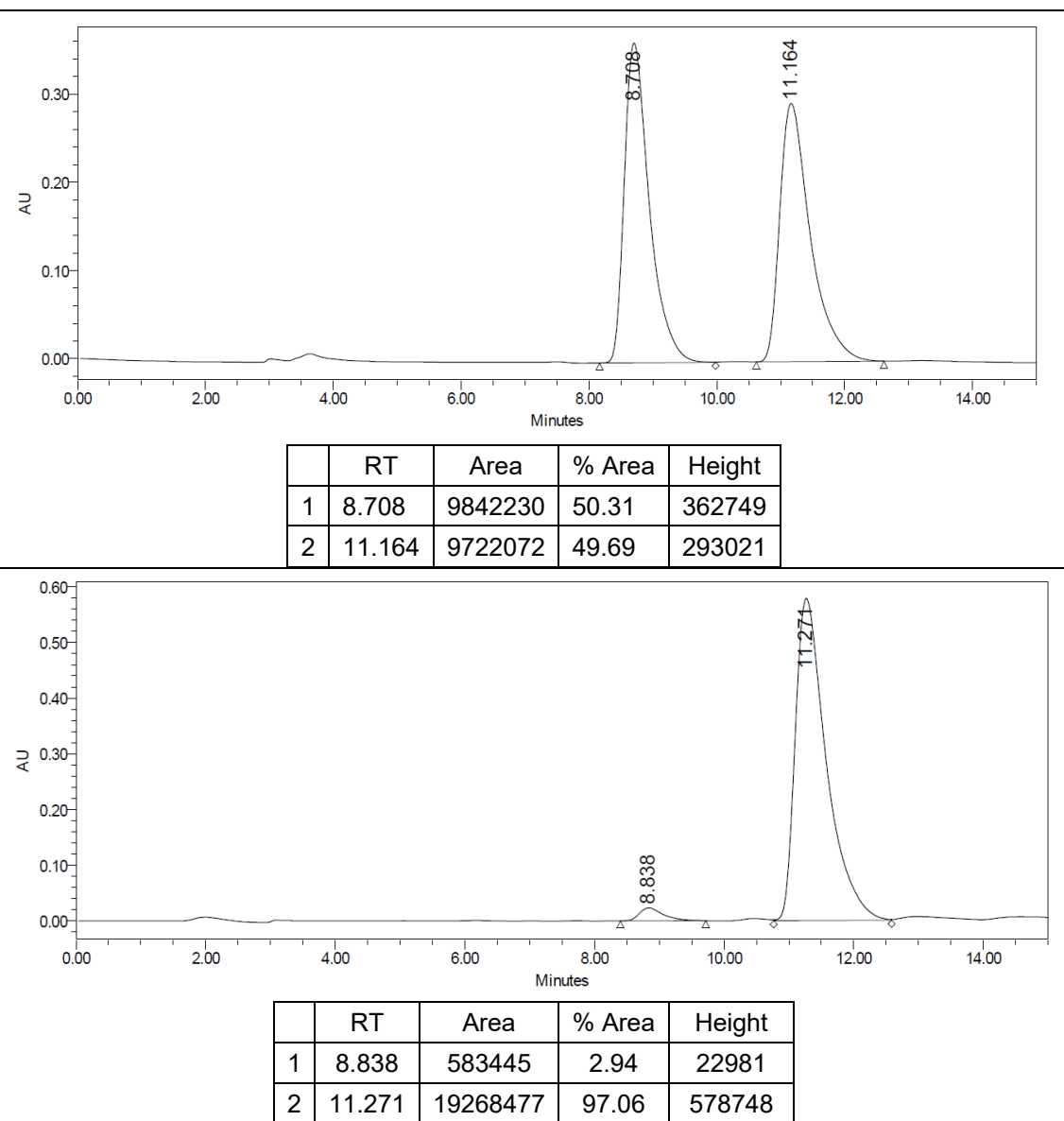
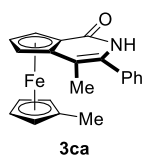


	RT	Area	% Area	Height
1	11.417	12746339	49.69	589383
2	12.800	12903307	50.31	521620

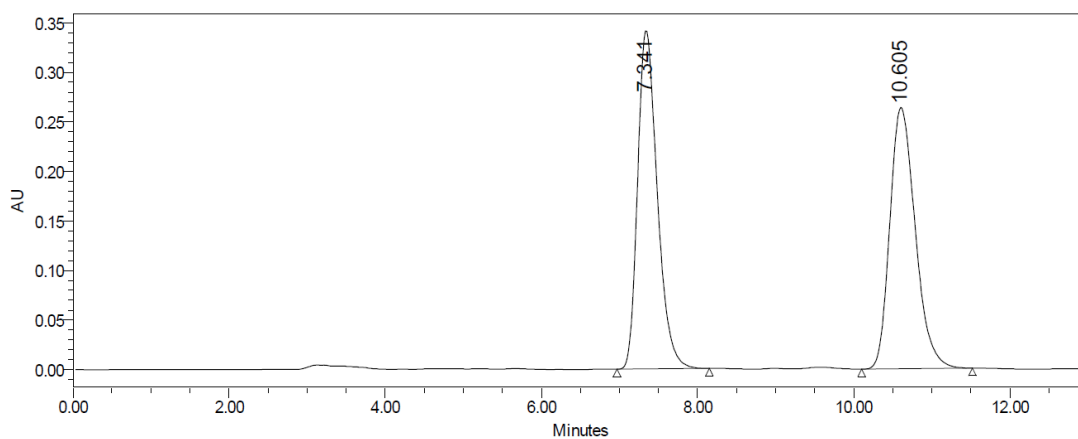
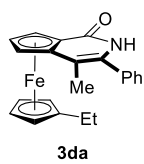


	RT	Area	% Area	Height
1	11.426	311757	2.09	14637
2	12.782	14585692	97.91	593840

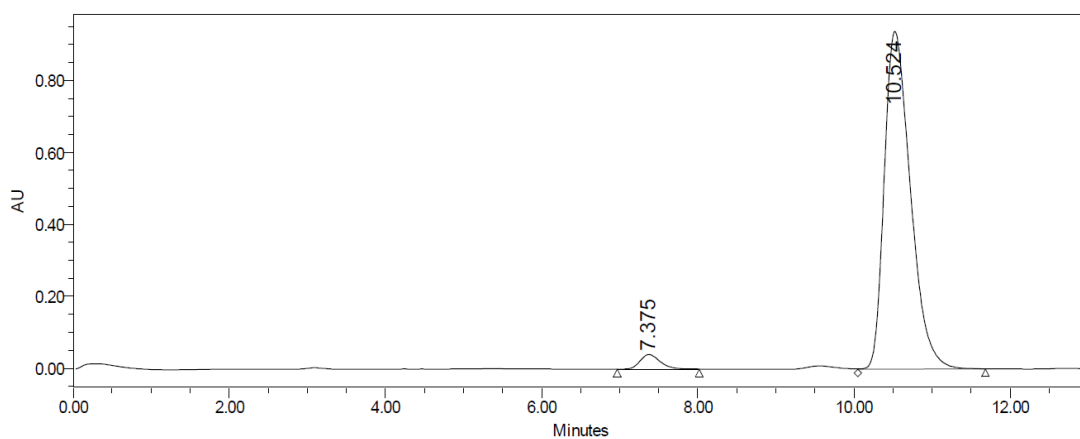
HPLC analysis of **3ca**



HPLC analysis of **3da**

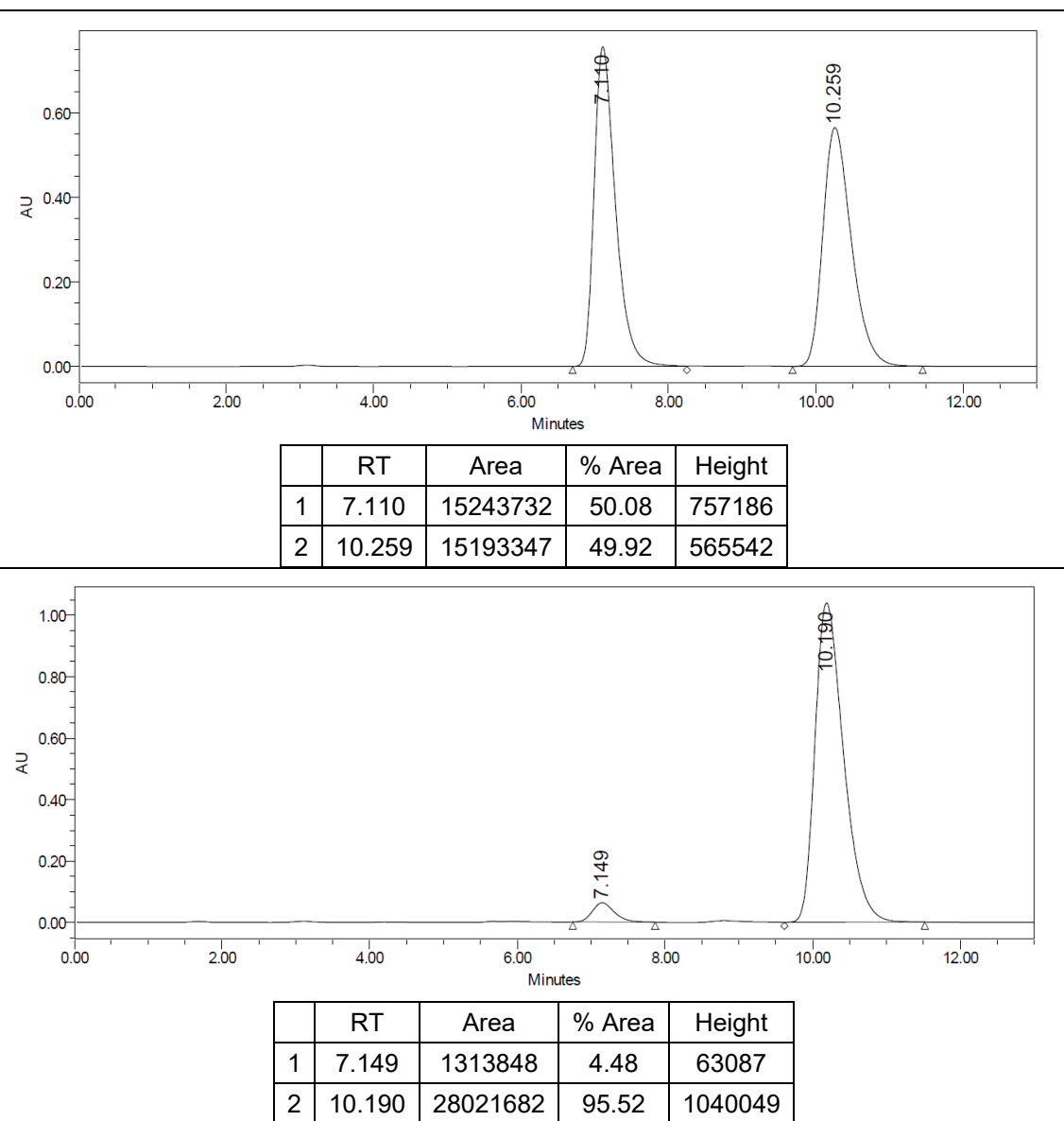
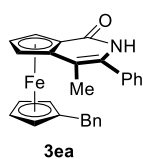


	RT	Area	% Area	Height
1	7.341	5975930	50.06	341804
2	10.605	5962001	49.94	263719

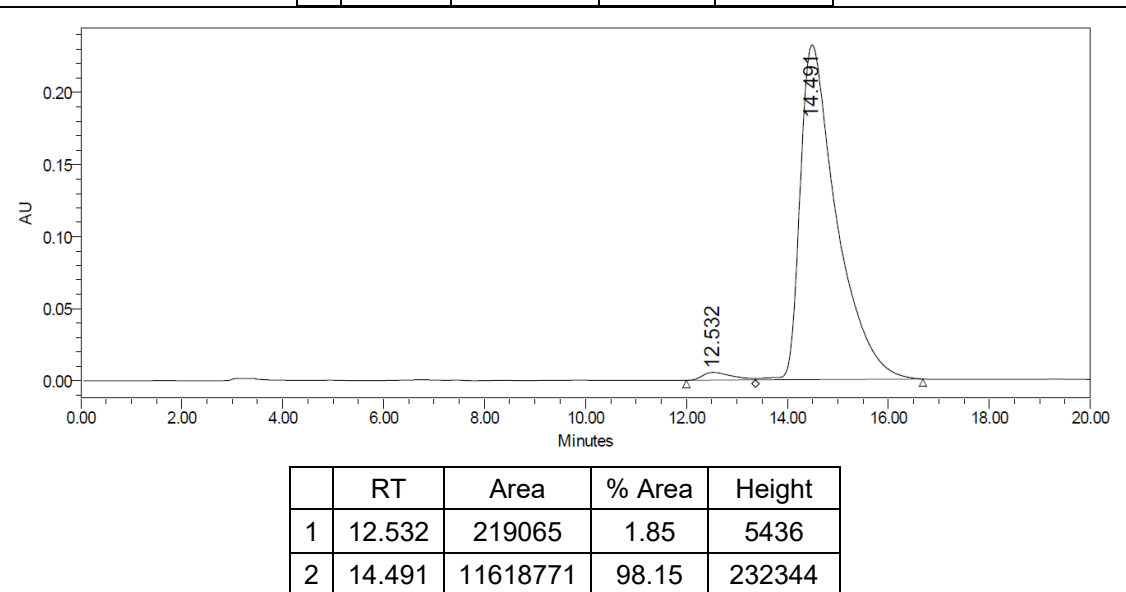
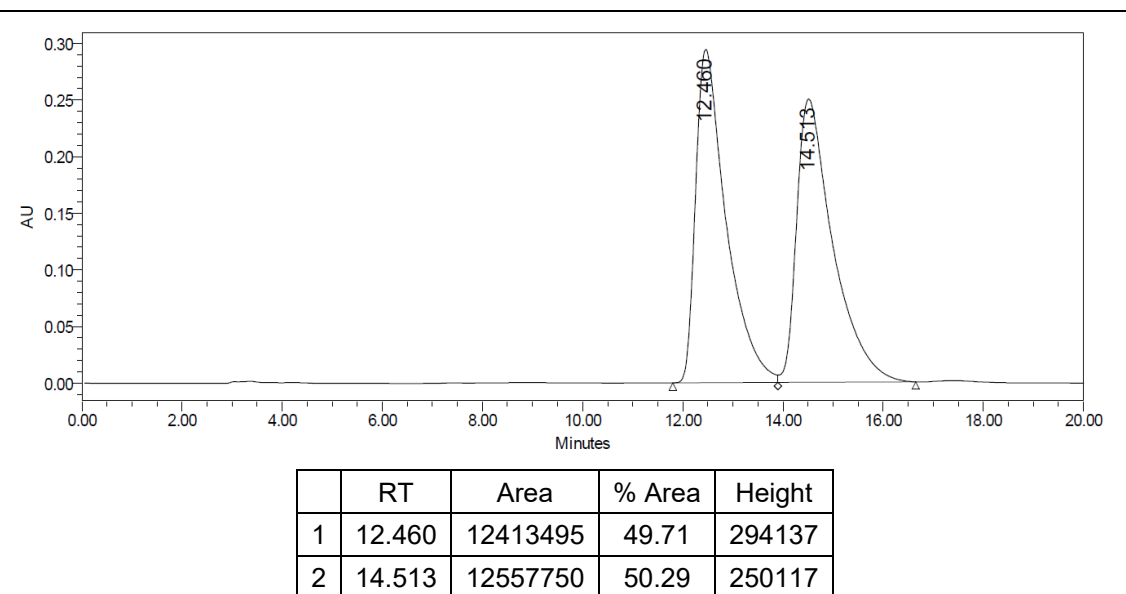
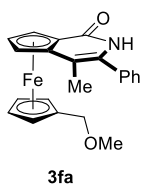


	RT	Area	% Area	Height
1	7.375	718834	3.19	40470
2	10.524	21819312	96.81	938993

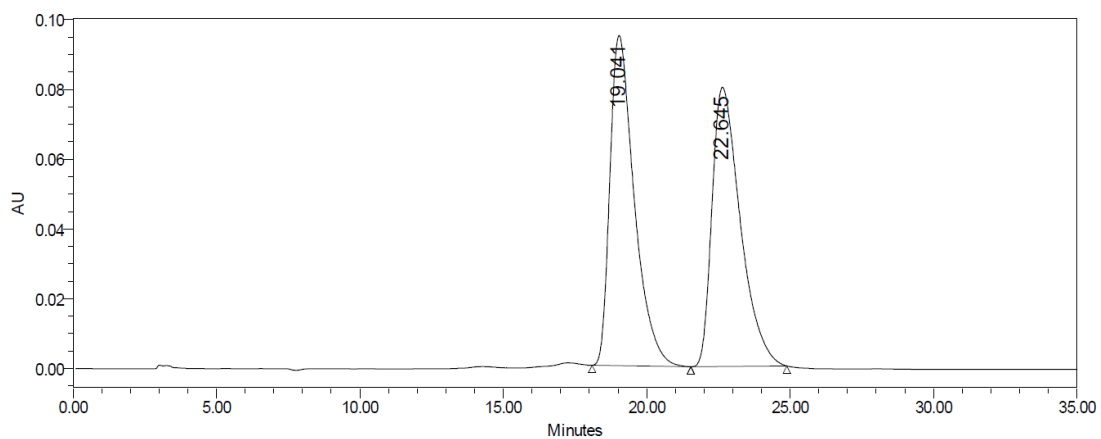
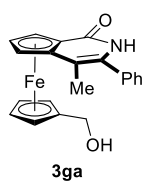
HPLC analysis of **3ea**



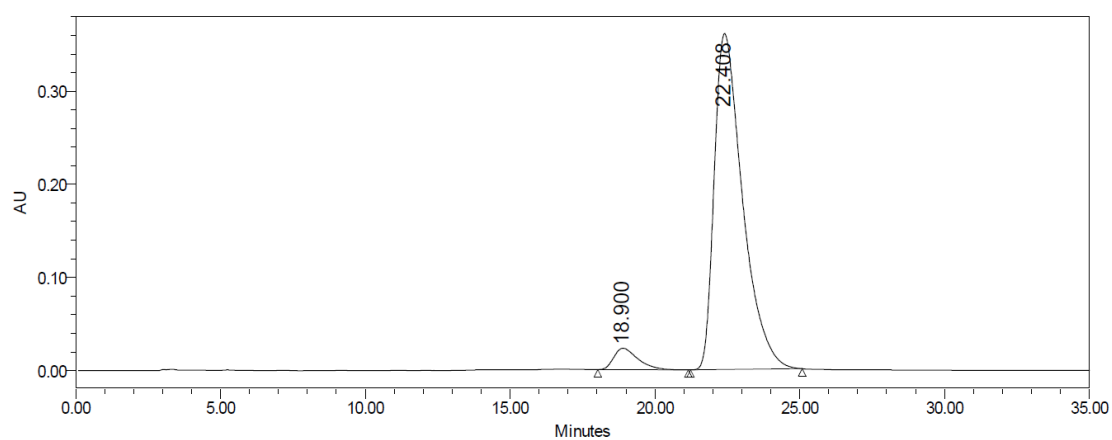
HPLC analysis of **3fa**



HPLC analysis of **3ga**

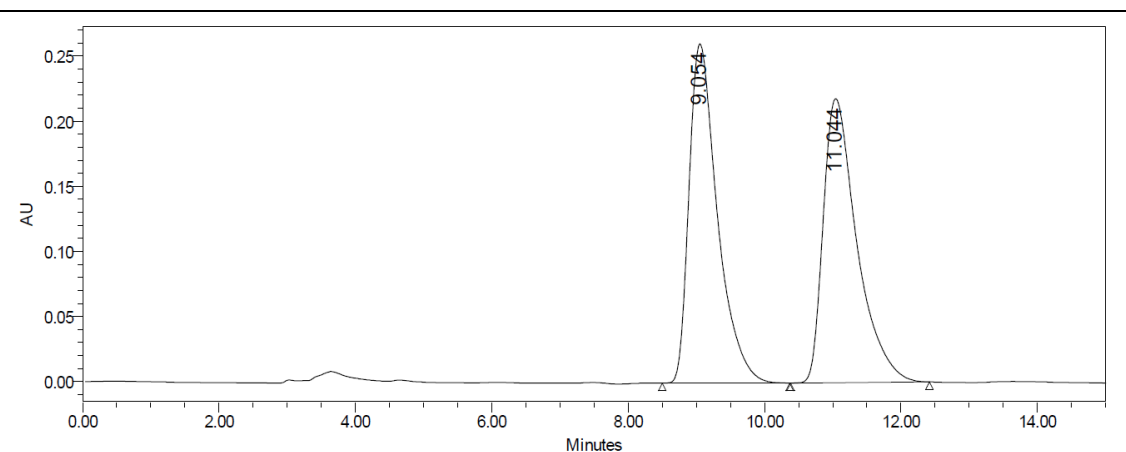
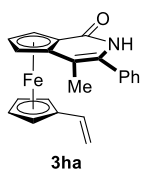


	RT	Area	% Area	Height
1	19.041	5580360	50.38	94688
2	22.645	5495684	49.62	80079

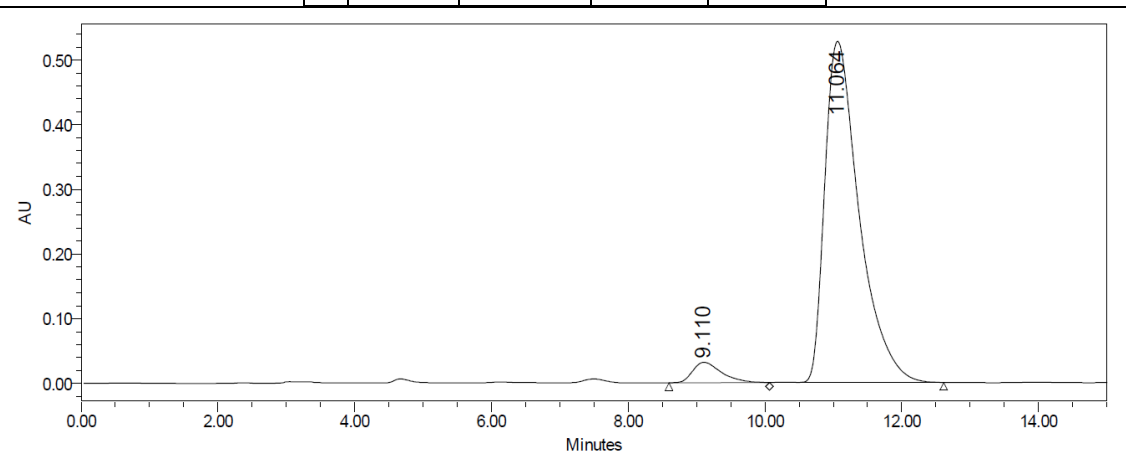


	RT	Area	% Area	Height
1	18.900	1331224	5.16	23026
2	22.408	24490455	94.84	361050

HPLC analysis of **3ha**

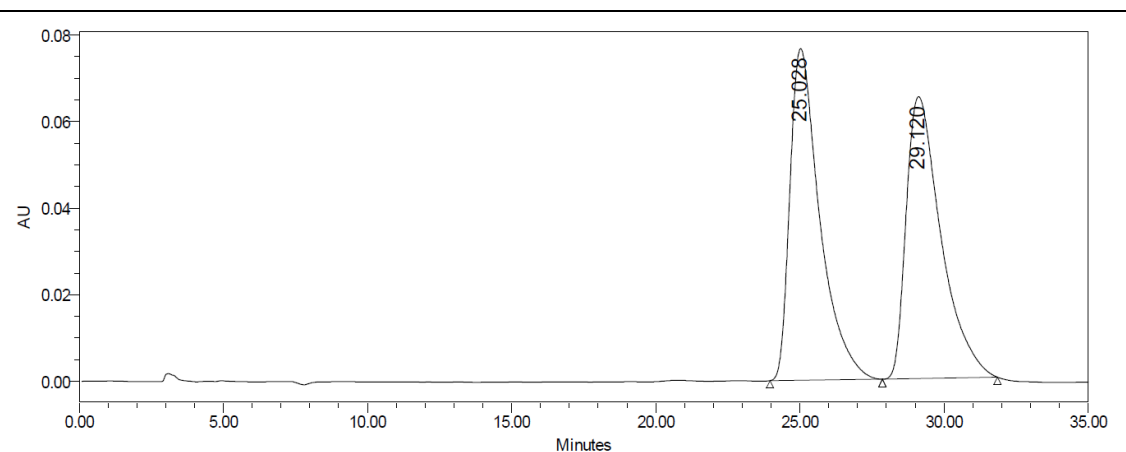
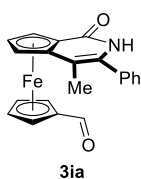


	RT	Area	% Area	Height
1	9.054	7509822	50.13	260671
2	11.044	7470831	49.87	218178

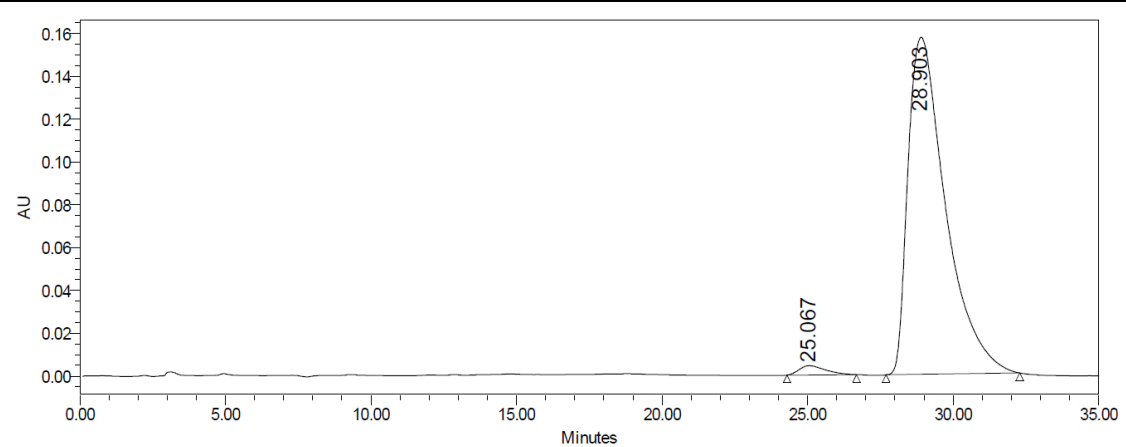


	RT	Area	% Area	Height
1	9.110	920912	4.75	31499
2	11.064	18470337	95.25	527681

HPLC analysis of **3ia**

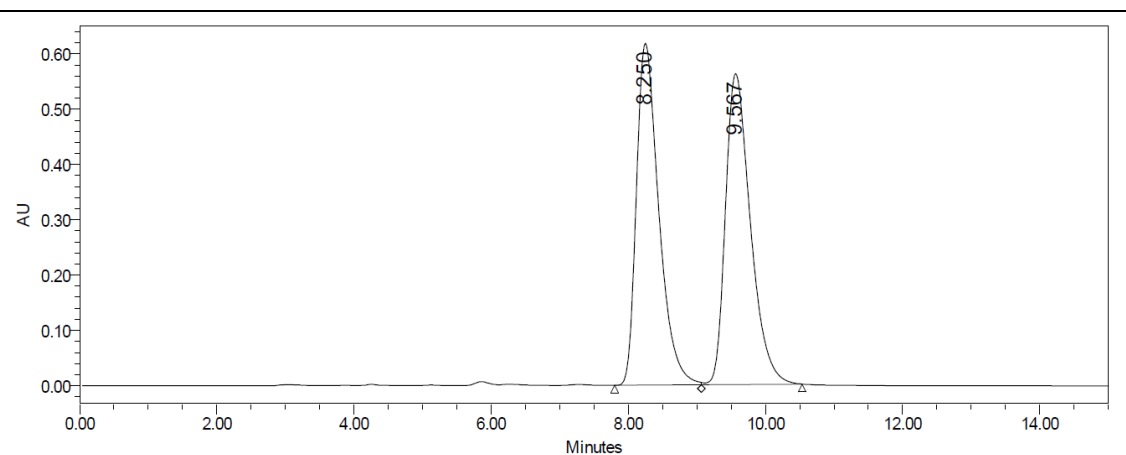
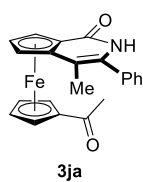


	RT	Area	% Area	Height
1	25.028	5513933	50.23	76575
2	29.120	5463504	49.77	65106

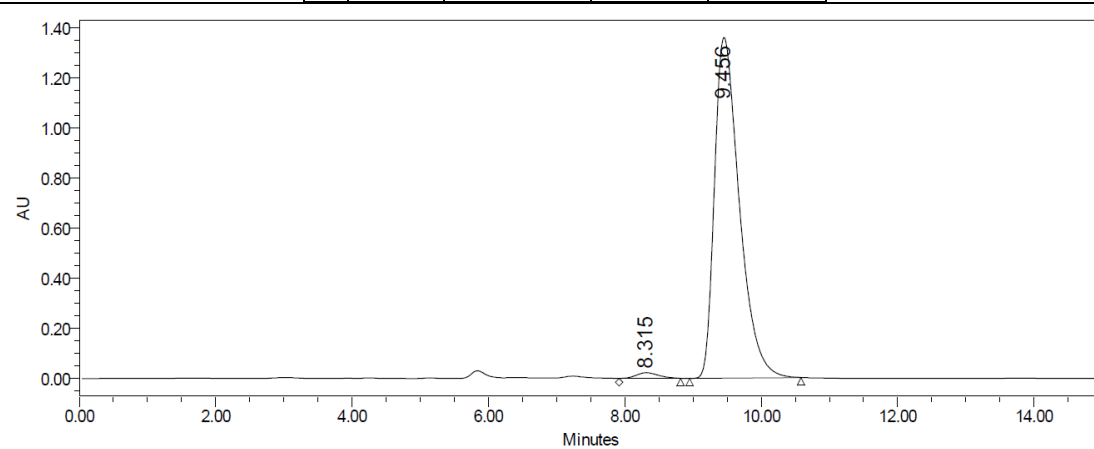


	RT	Area	% Area	Height
1	25.067	267720	1.85	4290
2	28.903	14184673	98.15	157467

HPLC analysis of 3ja

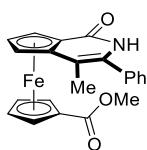


	RT	Area	% Area	Height
1	8.250	14071541	49.70	618601
2	9.567	14241039	50.30	562578

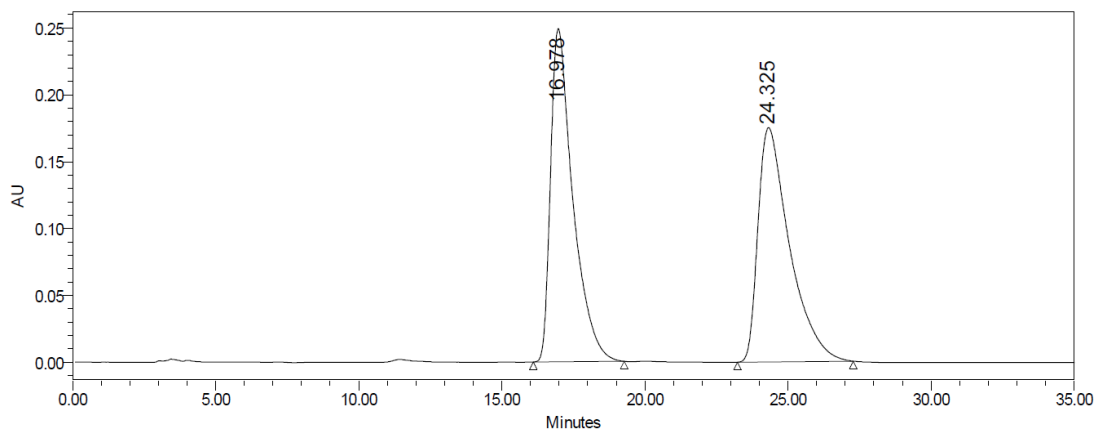


	RT	Area	% Area	Height
1	8.315	491141	1.40	22006
2	9.456	34544105	98.60	1360379

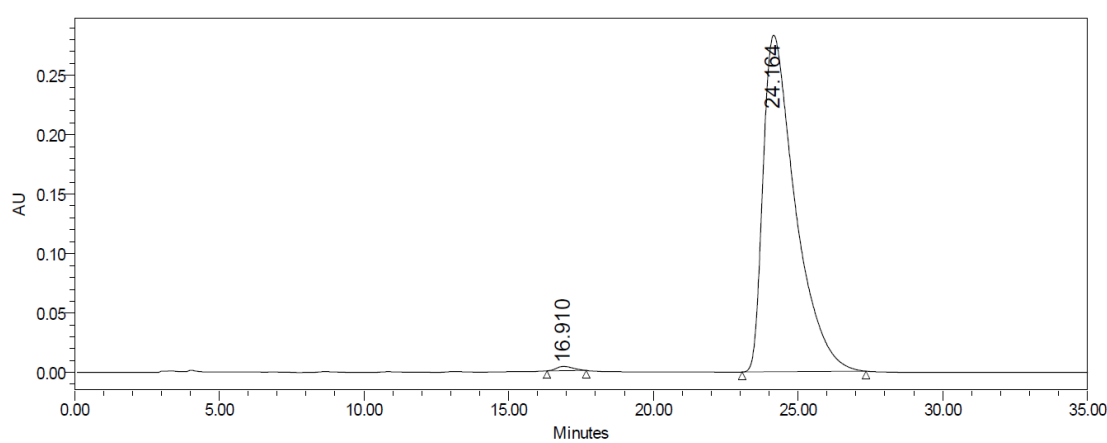
HPLC analysis of **3ka**



3ka

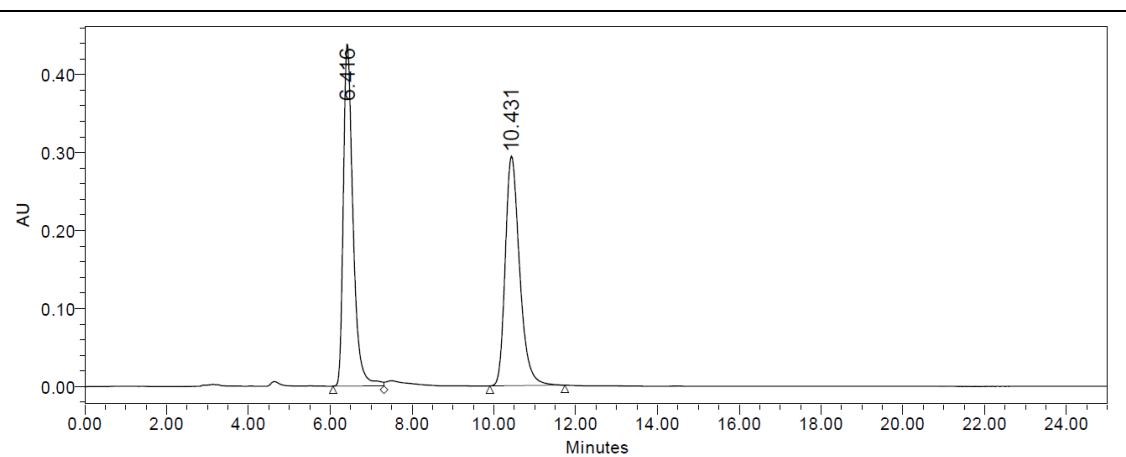
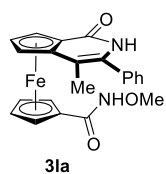


	RT	Area	% Area	Height
1	16.978	13501374	50.19	249314
2	24.325	13399850	49.81	175276

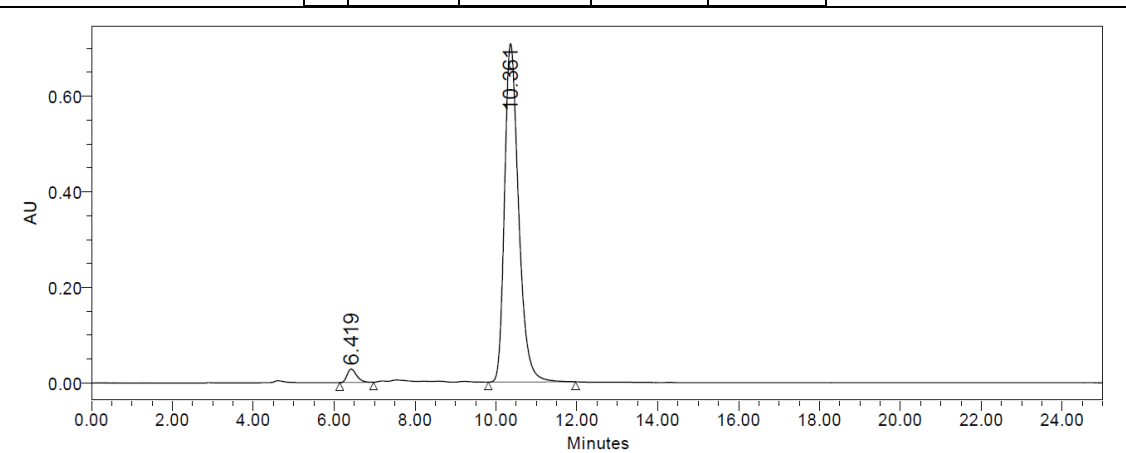


	RT	Area	% Area	Height
1	16.910	140417	0.64	3557
2	24.164	21931889	99.36	283287

HPLC analysis of **3la**

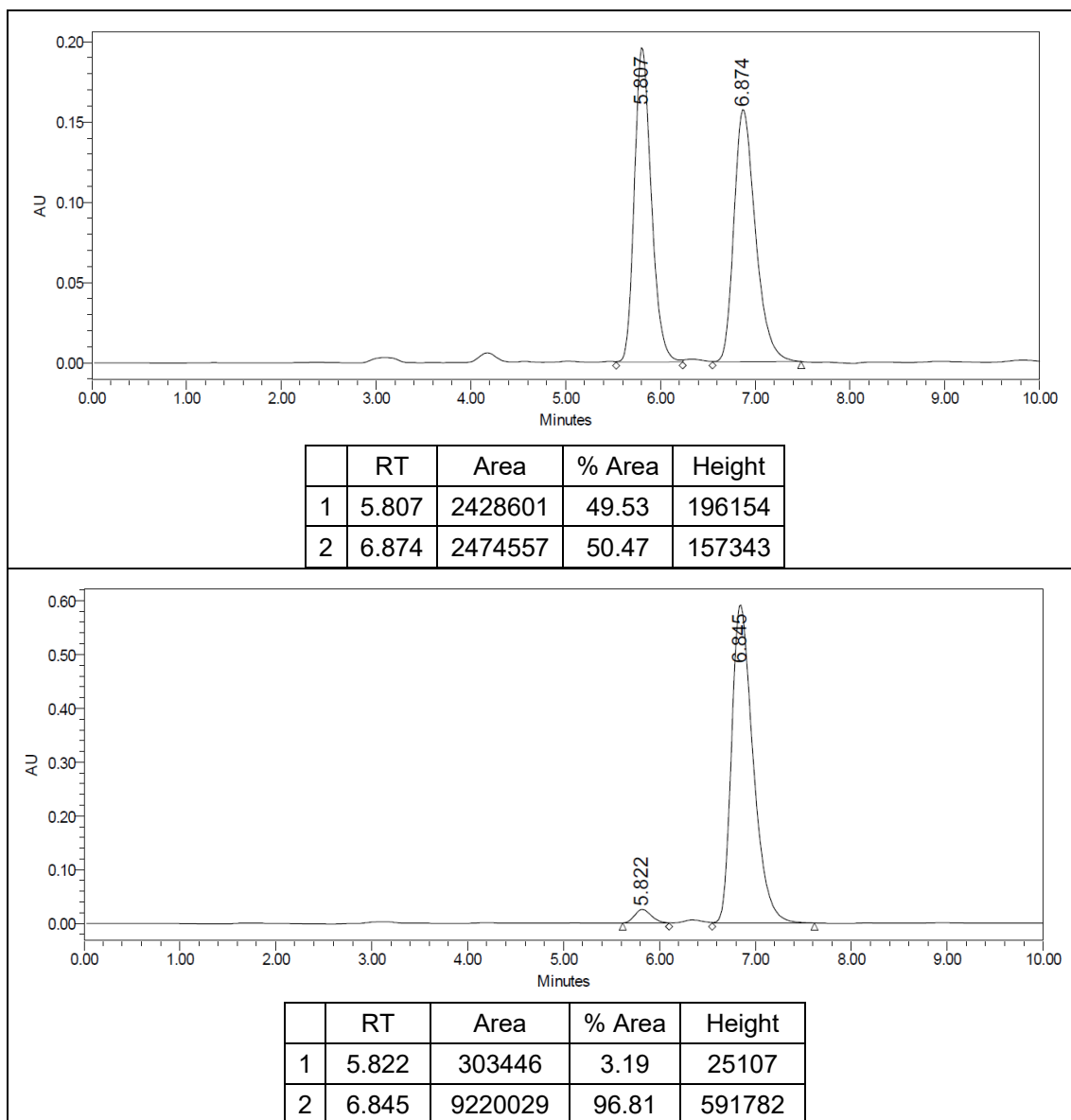
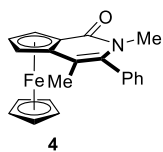


	RT	Area	% Area	Height
1	6.416	7210571	50.13	438401
2	10.431	7174151	49.87	294380

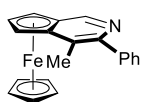


	RT	Area	% Area	Height
1	6.419	461115	2.62	28139
2	10.361	17106702	97.38	708189

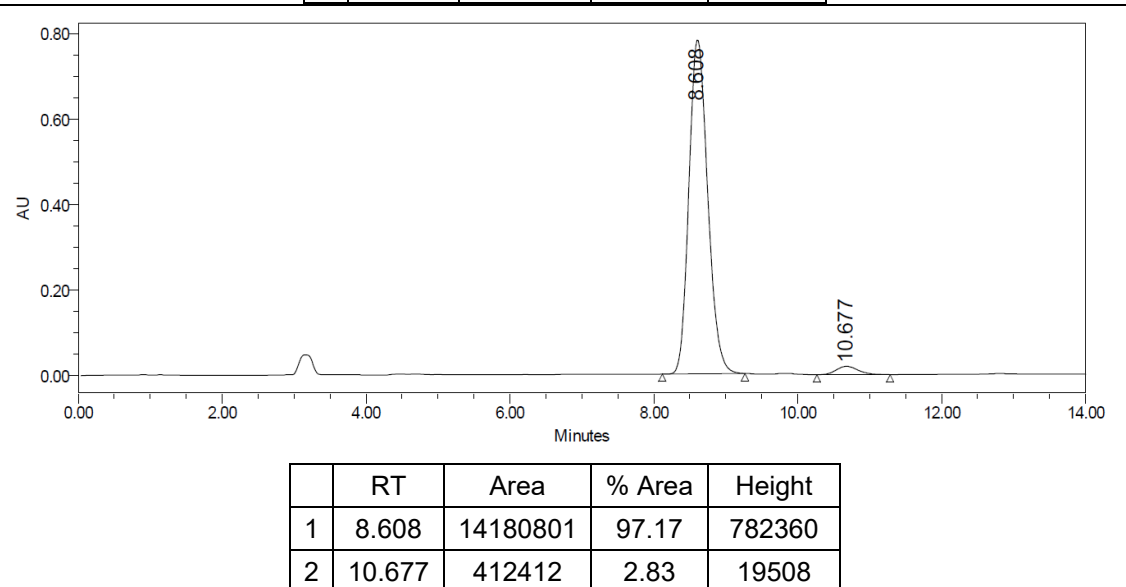
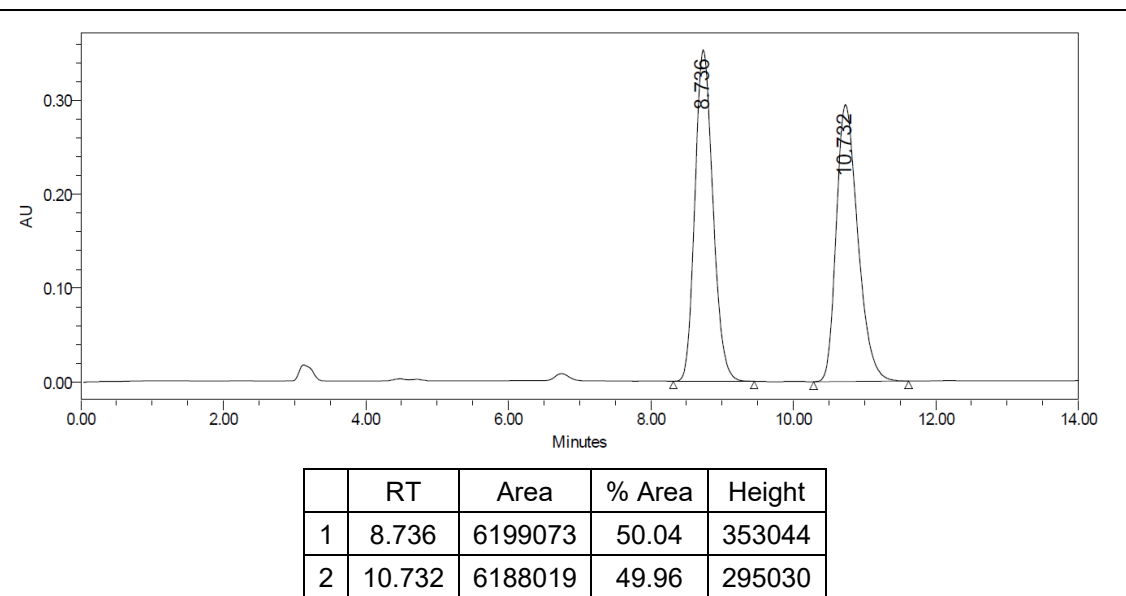
HPLC analysis of 4



HPLC analysis of **5**



5



HPLC analysis of **6**

