Supporting Information

Organocatalytic sulfa-Michael/adol cascade: constructing functionalized 2,5-dihydrothiophenes bearing a quaternary carbon stereocenter

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1. General Information

Unless otherwise noted, materials were used as commercial suppliers and used without further purification. All the solvents were treated according to general methods. All reactions were monitored by TLC analysis with silica gel-coated plates. Flash column chromatography was performed using 200-300 mesh silica gel. ^{1}H NMR and ^{13}C NMR NMR spectra were recorded on Varian-Mercury 400/600 (400/600 MHz) spectrometers. Chemical shifts (δ) are reported in parts per million (ppm) relative to residual solvent signals ($CHCl_3$: 7.26 ppm for ^{1}H NMR; 77.0 ppm for ^{13}C NMR). Data are reported as follows: chemical shift (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet), coupling constants (Hz). Mass spectra were measured on a Finnigan Trace MS spectrometer (EI) or API 2000 LC/MS/MS (ESI-MS). Enantiomeric ratios were determined by HPLC with chiral columns (chiralpak AS-H column, chiralpak AD-H column, chiralpak OJ-H column or chiralcel OD-H column) with hexane and *i*-PrOH as solvents. Optical rotations were measured with a polarimeter.

2. Screening of the reaction conditions

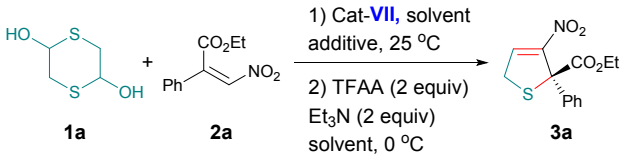


Table 1. Solvent screening

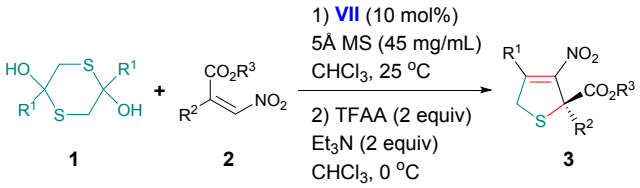
entry	**1a**	**2a**	**VII**	additive	Solvent	time	**3a**	
	(mmol)	(mmol)	(mmol)		(2 mL)	(h)	yield (%)	ee (%)
1	0.18	0.3	0.03	none	CH_2Cl_2	24	64	60
2	0.18	0.3	0.03	none	$ClCH_2CH_2Cl$	24	55	58
3	0.18	0.3	0.03	none	$CHCl_3$	24	69	71
4	0.18	0.3	0.03	none	toluene	24	56	62
5	0.18	0.3	0.03	none	benzene	24	54	68
6	0.18	0.3	0.03	none	xylene	24	61	60
7	0.18	0.3	0.03	none	THF	24	35	48
8	0.18	0.3	0.03	none	Et_2O	24	68	66
9	0.18	0.3	0.03	none	1,4-dioxane	24	67	64
10	0.18	0.3	0.03	none	CH_3OH	24	44	3
11	0.18	0.3	0.03	none	*i*-PrOH	24	46	5
12	0.18	0.3	0.03	none	CH_3CN	24	43	12

Table 2. Concentration, equivalent of additive and catalyst screening

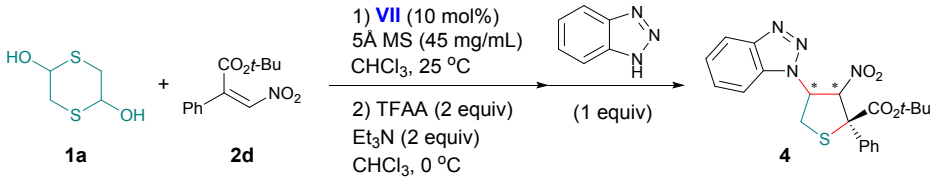
entry	**1a**	**2a**	**VII**	5Å MS	$CHCl_3$	time	**3a**	
	(mmol)	(mmol)	(mmol)	(mg)	(mL)	(h)	yield (%)	ee (%)
1	0.18	0.3	0.03	80	2 mL	24	68	75
2	0.18	0.3	0.03	90	2 mL	24	70	77
3	0.18	0.3	0.03	100	2 mL	24	69	74
4	0.18	0.3	0.015	90	2 mL	48	59	73
5	0.18	0.3	0.045	90	2 mL	24	68	75
6	0.18	0.3	0.03	90	1 mL	20	61	70
7	0.18	0.3	0.03	90	1.5 mL	24	70	75
8	0.18	0.3	0.03	90	3 mL	24	63	73

3. Experimental Procedures for the preparation of products 3 and 4

α-Aryl-β-nitroacrylates 2 were prepared according to the literature procedures.[1] The 2,5-dihydrothiophenes 3 and derivative 4 were prepared as the following procedure.



To a stirred solution of β-nitroacrylates **2** (0.3 mmol), catalyst **VII** (0.03 mmol), 5Å MS（45 mg/mL, 90 mg）in distilled chloroform (2 mL), the substrate **1** (0.18 mmol) was added at room temperature. After completed (monitored by TLC analysis), the mixture was cooled to 0 °C, then TFAA (0.6 mmol) was added and Et_3N (0.6 mmol) was dropped slowly. The reaction mixture was kept stirring until completed (monitored by TLC analysis), the crude product was washed with H_2O (2 mL × 3), dried with $MgSO_4$, then purified by column chromatography on silica gel (PE/EA = 20/1~10/1 as eluant) to afford the corresponding product **3**.

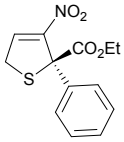


To a solution of β-nitroacrylate **2d** (0.3 mmol), catalyst **VII** (0.03 mmol), 5Å MS（45 mg/mL, 90 mg）in distilled chloroform (2 mL), the 1,4-dithiane-2,5-diol **1a** (0.18 mmol) was added at room temperature. After completed (monitored by TLC analysis), the mixture was cooled to 0 °C, then TFAA (0.6 mmol) was added and Et_3N (0.6 mmol) was dropped slowly. The reaction was kept stirring until completed (monitored by TLC analysis), then benzotriazole (0.3 mmol) was added directly. After

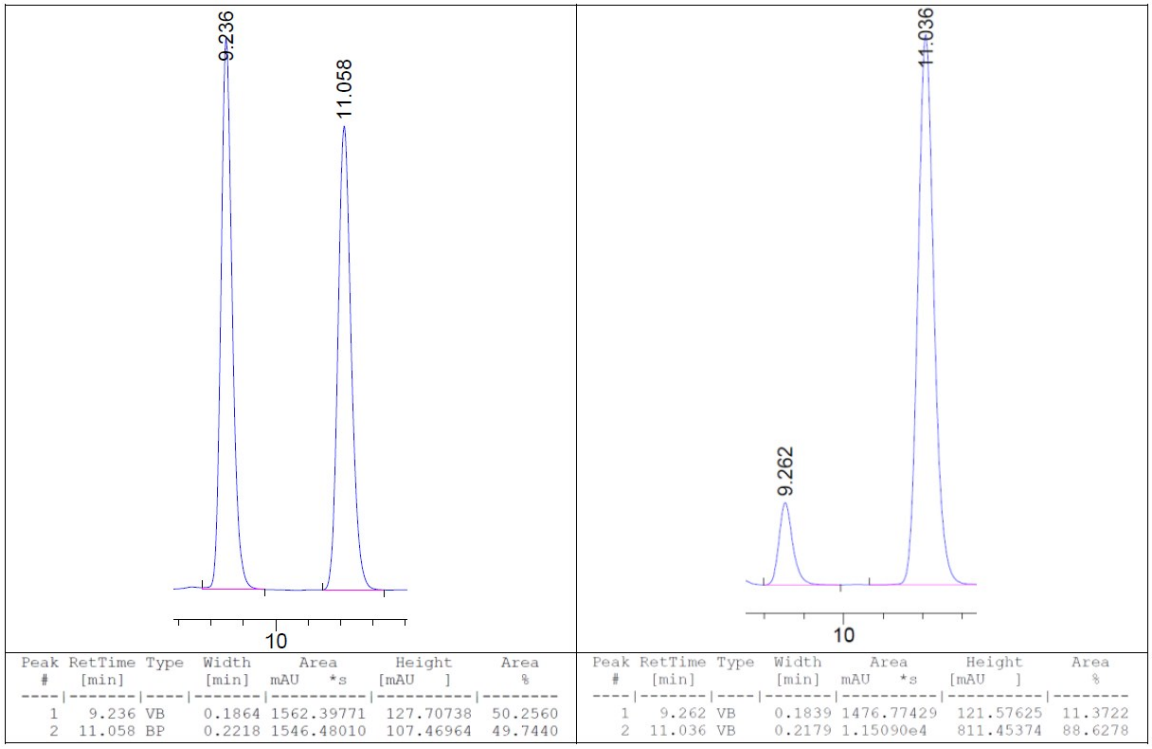
completed (monitored by TLC analysis), the mixture was washed with H_2O (2 mL × 3), dried with $MgSO_4$, then purified by column chromatography on silica gel (PE/EA = 10/1~5/1 as eluant) to afford the corresponding product **4**.

4. ^1H, ^{13}C NMR, HRMS date and HPLC traces of compounds 3 and 4

(*S*)-ethyl-3-nitro-2-phenyl-2, 5-dihydrothiophene-2-carboxylate (3a)



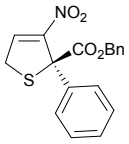
Pale yellow oil, yield: 70%, ee: 77%. ^1H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, *J* = 7.8 Hz, 2H), 7.39 (t, *J* = 2.8 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.28 (d, *J* = 6.7 Hz, 1H), 4.30-4.40 (m, 2H), 4.00-4.14 (m, 2H), 1.31 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.4, 153.7, 137.7, 128.6, 128.1, 127.9, 121.0, 65.9, 62.5, 33.2, 13.8 ppm. FTIR (KBr, cm^{-1}): 3036, 2984, 2932, 2908, 1736, 1664, 1540, 1425, 1334, 1264, 1020, 804, 749, 695. HRMS (ESI): Calcd for $C_{13}H_{13}NO_4S$ $[M+Na]^+$: 302.0463. Found: 302.0458. [α]16 D = +15.6 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 11.036 min, t_{minor} = 9.262 min)



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.236	VB	0.1864	1562.39771	127.70738	50.2560
2	11.058	BP	0.2218	1546.48010	107.46964	49.7440

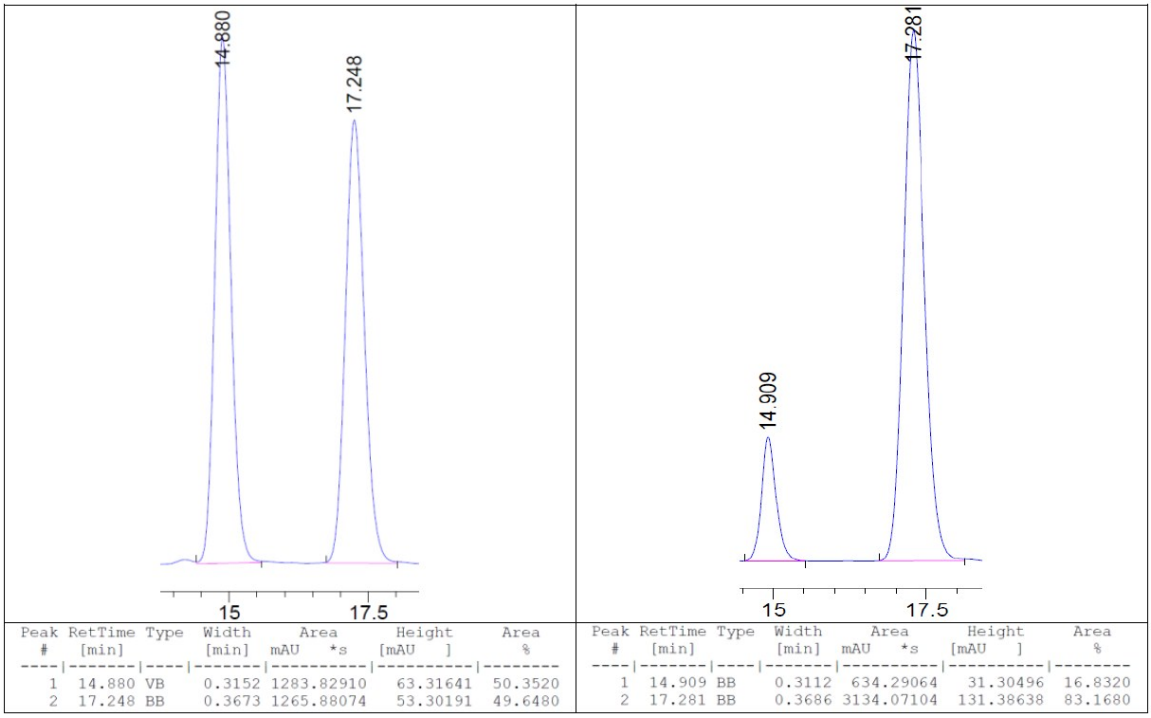
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.262	VB	0.1839	1476.77429	121.57625	11.3722
2	11.036	VB	0.2179	1.15090e4	811.45374	88.6278

(*S*)-benzyl-3-nitro-2-phenyl-2,5-dihydrothiophene-2-carboxylate (3b)



Colorless oil, yield: 68%, ee: 66%. ^1H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 7.4 Hz, 2H), 7.27-7.39 (m, 9H), 5.32 (d, *J* = 3.4 Hz, 2H), 3.99-4.14 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1, 143.2, 134.1, 131.9, 129.4, 129.3, 128.9, 127.4, 126.7, 70.6, 53.4, 21.3 ppm. FTIR (KBr, cm^{-1}): 3028, 2982, 2931, 2902, 1743, 1673, 1597, 1533,

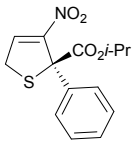
1348, 1262, 1100, 811, 751, 693. HRMS (ESI): Calcd for $C_{18}H_{15}NO_4S$ $[M+Na]^+$: 364.0619. Found: 364.0614. [α]16 D = +31.6 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, hexane/2-propanol = 90:10, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 17.281 min, t_{minor} = 14.909 min)



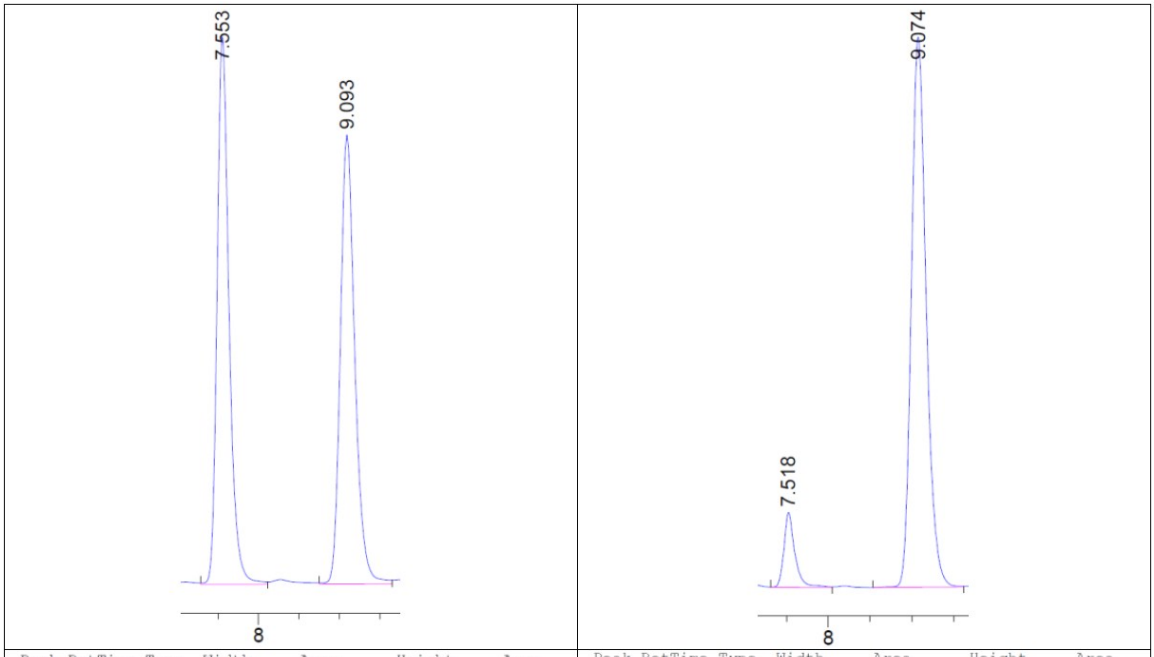
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.880	VB	0.3152	1283.82910	63.31641	50.3520
2	17.248	BB	0.3673	1265.88074	53.30191	49.6480

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.909	BB	0.3112	634.29064	31.30496	16.8320
2	17.281	BB	0.3686	3134.07104	131.38638	83.1680

(*S*)-isopropyl-3-nitro-2-phenyl-2, 5-dihydrothiophene-2-carboxylate (3c)



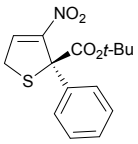
Pale yellow oil, yield: 67%, ee: 80%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 2.8 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.29 (d, *J* = 7.1 Hz, 1H), 5.19-5.25 (m, 1H), 4.02-4.16 (m, 2H), 1.34 (d, *J* = 6.3 Hz, 3H), 1.29 (d, *J* = 6.2 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.8, 153.7, 137.5, 128.6, 128.0, 127.8, 120.3, 70.3, 66.0, 33.1, 21.3 ppm. FTIR (KBr, cm^{-1}): 3030, 2975, 2934, 2843, 1738, 1641, 1539, 1371, 1246, 1018, 819, 758, 698. HRMS (ESI): Calcd for $C_{14}H_{15}NO_4S$ $[M+Na]^+$: 316.0619. Found: 316.0613. [α]16 D = +20.3 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 9.074 min, t_{minor} = 7.518 min)



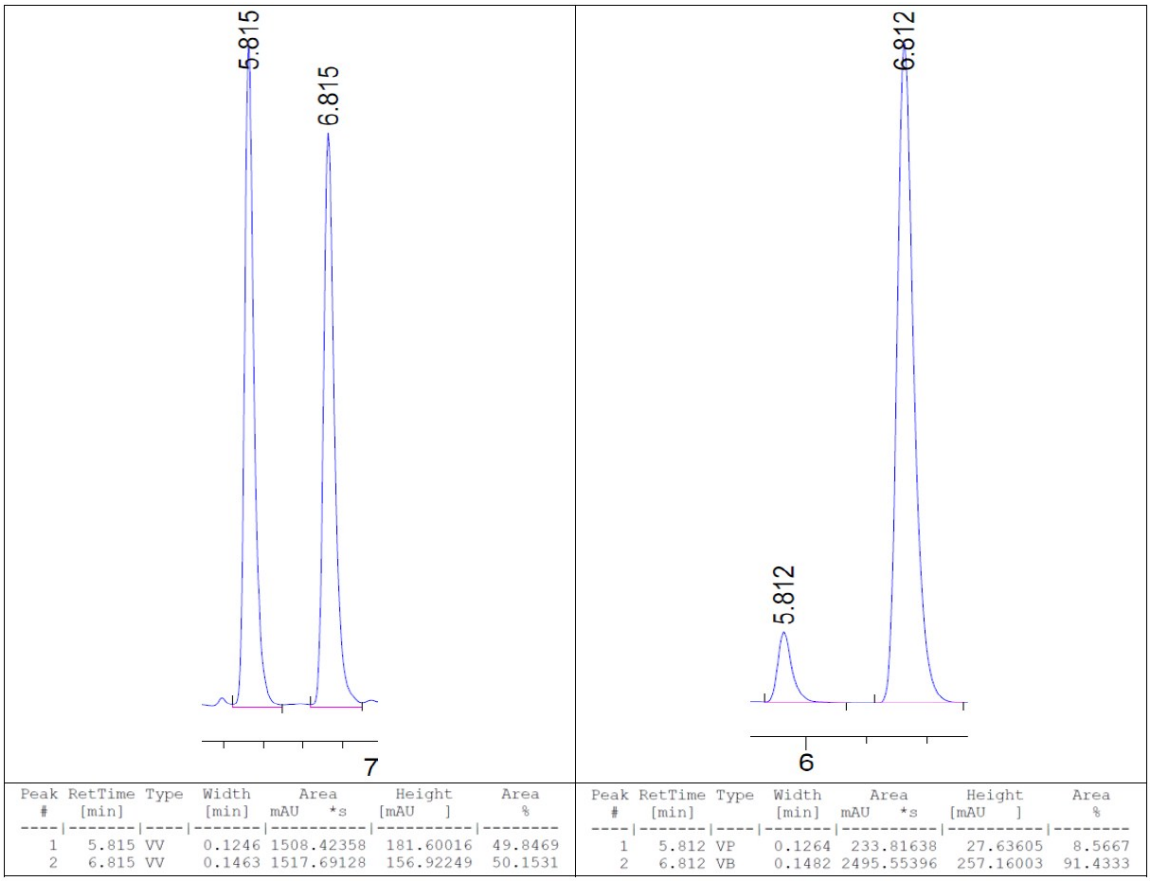
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.553	VV	0.1561	1684.88867	164.27077	50.0889
2	9.093	VV	0.1890	1678.90967	134.79648	49.9111

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.518	VV	0.1561	211.29002	22.01873	9.7668
2	9.074	VB	0.1872	1952.05945	158.73532	90.2332

(*S*)-tert-butyl-3-nitro-2-phenyl-2, 5-dihydrothiophene-2-carboxylate (3d)



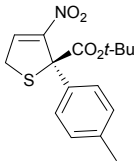
Pale yellow oil, yield: 73%, ee: 83%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 7.4 Hz, 2H), 7.31-7.36 (m, 3H), 7.27 (d, *J* = 7.2 Hz, 1H), 3.99-4.13 (m, 2H), 1.53 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 154.1, 137.4, 128.5, 128.2, 127.8, 120.1, 83.4, 67.1, 33.6, 28.5 ppm. FTIR (KBr, cm^{-1}): 3041, 2935, 2843, 1732, 1655, 1533, 1365, 1254, 1019, 816, 765, 694. HRMS (ESI): Calcd for $C_{15}H_{17}NO_4S$ $[M+H]^+$: 308.0957. Found: 308.0951. [α]16 D = +28.9 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 6.812 min, t_{minor} = 5.812 min)



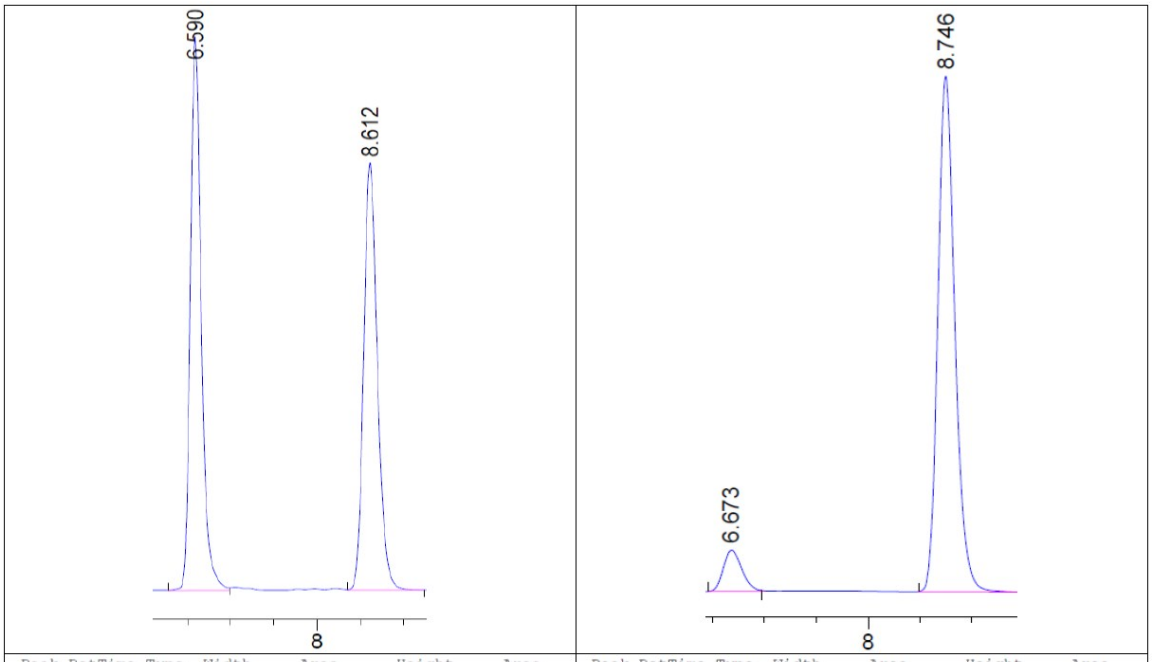
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.815	VV	0.1246	1508.42358	181.60016	49.8469
2	6.815	VV	0.1463	1517.69128	156.92249	50.1531

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.812	VP	0.1264	233.81638	27.63605	8.5667
2	6.812	VB	0.1482	2495.55396	257.16003	91.4333

(*S*)-tert-butyl-3-nitro-2-(*p*-tolyl)-2, 5-dihydrothiophene-2-carboxylate (3e)



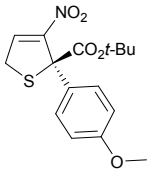
Pale yellow oil, yield: 65%, ee: 86%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.35 (t, *J* = 2.4 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 3.98-4.13 (m, 2H), 2.32(s, 3H), 1.52 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 154.1, 137.8, 137.0, 135.3, 128.6, 128.5, 83.3, 66.6, 33.0, 27.7, 21.0 ppm. FTIR (KBr, cm^{-1}): 3046, 2983, 2935, 2872, 1737, 1659, 1540, 1447, 1371, 1342, 1265, 1024, 831, 764, 689. HRMS (ESI): Calcd for $C_{16}H_{19}NO_4S$ $[M+Na]^+$: 344.0932. Found: 344.0927. [α]16 D = +37.3 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 8.746 min, t_{minor} = 6.673 min)



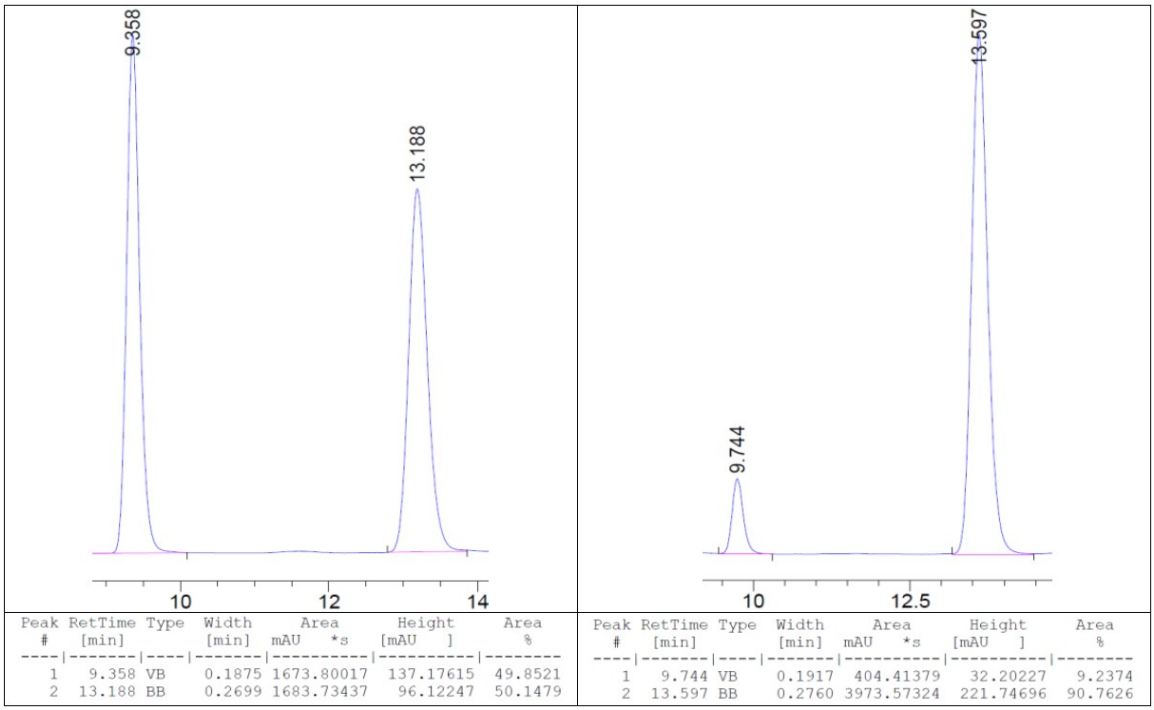
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.590	BV	0.1345	2589.25488	294.78839	50.6015
2	8.612	VB	0.1703	2527.69385	227.59038	49.3985

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.673	BV	0.1428	164.63414	15.00882	7.1066
2	8.746	BP	0.1739	2152.05005	188.63354	92.8934

(*S*)- tert-butyl-2-(4-methoxyphenyl)-3-nitro-2,5-dihydrothiophene-2-carboxylate (3f)



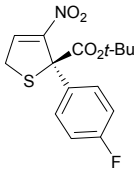
Pale yellow oil, yield: 71%, ee: 82%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.9 Hz, 2H), 7.32 (t, *J* = 2.9 Hz, 1H), 6.85 (d, *J* = 8.9 Hz, 2H), 3.79-4.07 (m, 2H), 3.72 (s, 3H), 1.52 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 159.0, 154.2, 136.7, 130.1, 130.0, 113.1, 83.3, 66.4, 55.2, 32.9, 27.7 ppm. FTIR (KBr, cm^{-1}): 3042, 2984, 2933, 2871, 1739, 1665, 1536, 1463, 1446, 1349, 1258, 1174, 1032, 828, 761, 693. HRMS (ESI): Calcd for $C_{16}H_{19}NO_5S$ $[M+Na]^+$: 360.0882. Found: 360.0871. [α]16 D = +13.2 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 13.597 min, t_{minor} = 9.744 min)



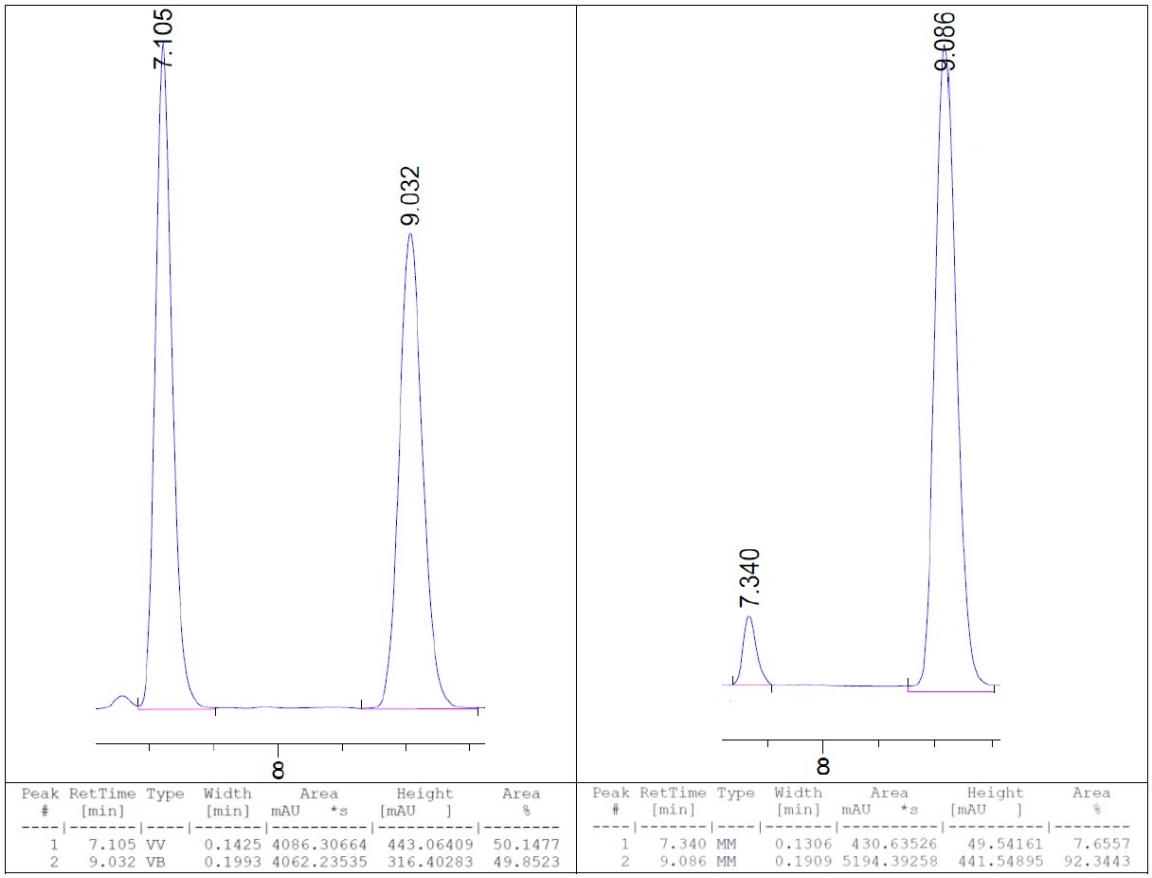
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.358	VB	0.1875	1673.80017	137.17615	49.8521
2	13.188	BB	0.2699	1683.73437	96.12247	50.1479

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.744	VB	0.1917	404.41379	32.20227	9.2374
2	13.597	BB	0.2760	3973.57324	221.74696	90.7626

(*S*)-tert-butyl-2-(4-fluorophenyl)-3-nitro-2, 5-dihydrothiophene-2-carboxylate (3g)



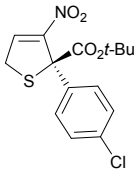
Pale yellow oil, yield: 68%, ee: 85%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62-7.64 (m, 2H), 7.32 (s, 1H), 6.70 (t, J = 7.8 Hz, 2H), 3.96-4.08 (m, 2H), 1.51 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.0, 162.7, 161.1, 153.8, 137.4, 134.0, 130.7, 114.6, 83.5, 66.1, 32.9, 27.5 ppm. FTIR (KBr, cm^{-1}): 3061, 2986, 2932, 1730, 1669, 1546, 1443, 1372, 1264, 1165, 1027, 832, 810, 692. HRMS (ESI): Calcd for $C_{15}H_{16}FNO_4S$ $[M+Na]^+$: 348.0682. Found: 348.0684. [α]16 D= +31.3 (C = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 9.086 min, t_{minor} = 7.340 min)



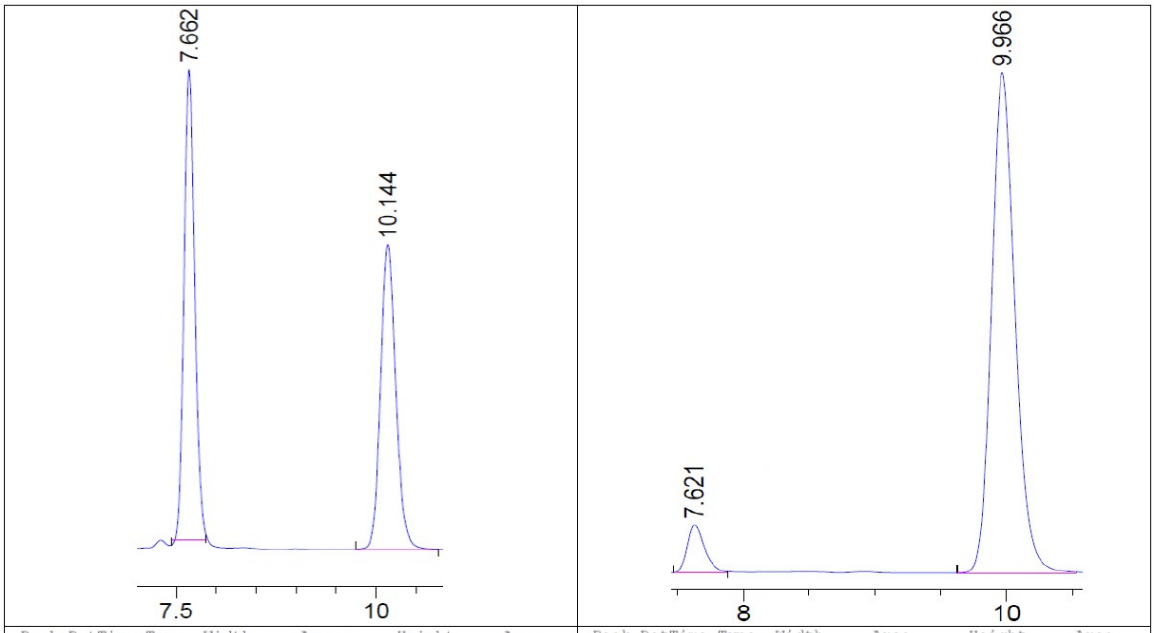
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.105	VV	0.1425	4086.30664	443.06409	50.1477
2	9.032	VB	0.1993	4062.23535	316.40283	49.8523

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.340	MM	0.1306	430.63526	49.54161	7.6557
2	9.086	MM	0.1909	5194.39258	441.54895	92.3443

(*S*)-tert-butyl-2-(4-chlorophenyl)-3-nitro-2, 5-dihydrothiophene-2-carboxylate (3h)



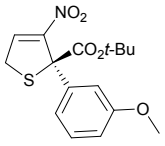
Pale yellow oil, yield: 75%, ee: 86%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, J = 7.8 Hz, 2H), 7.37 (s, 1H), 7.30 (d, J = 8.2 Hz, 2H), 4.02-4.13 (m, 2H), 1.52 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.9, 154.0, 137.4, 137.2, 136.8, 134.0, 130.3, 128.0, 83.8, 33.2, 27.7 ppm. FTIR (KBr, cm^{-1}): 3058, 2983, 2937, 1735, 1662, 1541, 1439, 1368, 1260, 1161, 1028, 828, 752, 692. HRMS (ESI): Calcd for $C_{15}H_{16}ClNO_4S$ $[M+Na]^+$: 364.0386. Found: 364.0377. [α]16 D= +78.2 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 9.966 min, t_{minor} = 7.621 min)



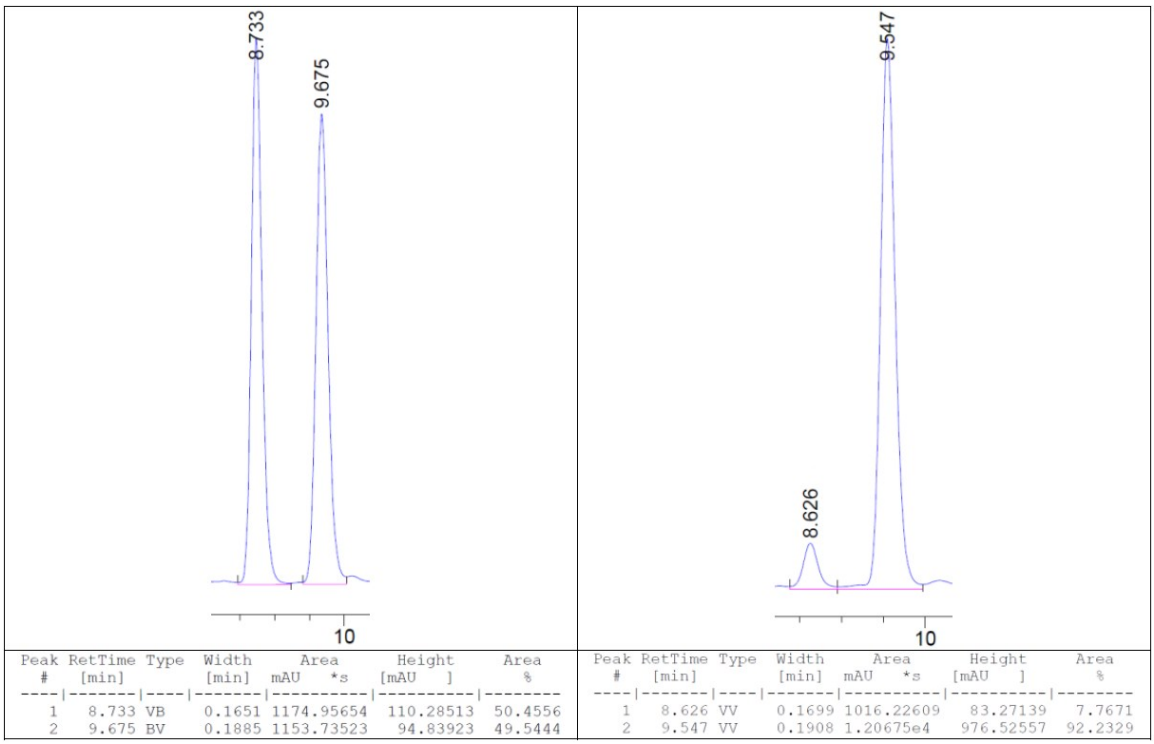
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.662	MM	0.1544	1765.12915	190.59787	51.7514
2	10.144	BB	0.2051	1645.65295	123.41629	48.2486

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.621	BB	0.1526	499.24069	45.02010	7.0964
2	9.966	BV	0.1939	5839.17480	462.48083	92.9036

(*S*)-tert-butyl-2-(3-methoxy phenyl)-3-nitro-2, 5-dihydrothiophene-2-carboxylate (3i)



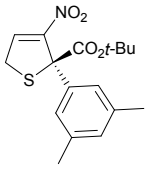
Pale yellow oil, yield: 71%, ee: 84%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 (s, 1H), 7.22-7.25 (m, 2H), 7.18 (d, *J* = 6.6 Hz, 1H), 6.80 (d, *J* = 7.8 Hz, 1H), 3.96-4.07 (m, 2H), 3.78 (s, 3H), 1.52 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.0, 159.0, 153.9, 139.9, 137.3, 128.8, 120.8, 115.1, 112.8, 83.4. 66.5, 55.2, 33.0, 27.6 ppm. FTIR (KBr, cm^{-1}): 3049, 2980, 2839, 1734, 1667, 1530, 1432, 1364, 1260, 1164, 1024, 798, 706, 664. HRMS (ESI): Calcd for $C_{16}H_{19}NO_5S$ $[M+Na]^+$: 360.0882. Found: 360.0871. [α]16 D= +28.5 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 9.547 min, t_{minor} = 8.626 min)



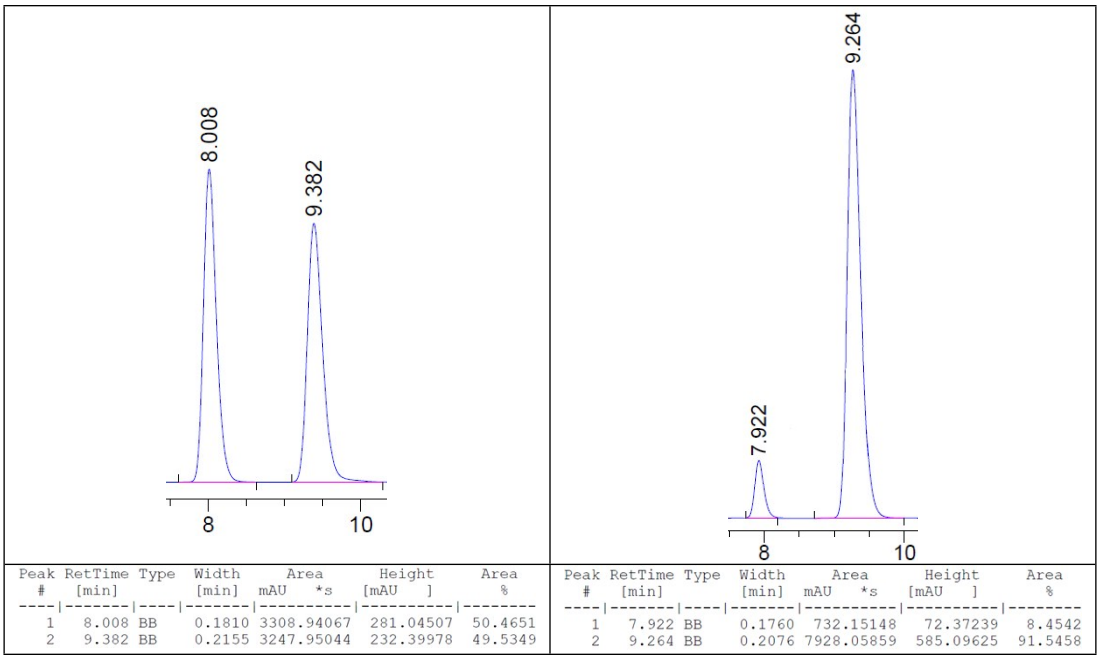
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.733	VB	0.1651	1174.95654	110.28513	50.4556
2	9.675	BV	0.1885	1153.73523	94.83923	49.5444

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.626	VV	0.1699	1016.22609	83.27139	7.7671
2	9.547	VV	0.1908	1.20675e4	976.52557	92.2329

(*S*)-tert-butyl-2-(3, 5-dimethylphenyl)-3-nitro-2, 5-dihydrothiophene-2-carboxylate (3j)



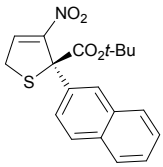
Pale yellow oil, yield: 67%, ee: 83%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 (s, 1H), 7.20 (s, 2H), 6.90 (s, 1H), 3.96-4.08 (m, 2H), 2.30 (s, 6H), 1.52 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.2, 154.1, 137.2, 131.0, 130.0, 129.5, 126.2, 83.1, 66.5, 33.0, 27.6, 21.4 ppm. FTIR (KBr, cm^{-1}): 3041, 2986, 2949, 1733, 1658, 1537, 1431, 1364, 1259, 1172, 1023, 818, 755, 692. HRMS (ESI): Calcd for $C_{17}H_{21}NO_4S$ $[M+Na]^+$: 358.1089. Found: 358.1083. [α]16 D= +44.9 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 9.264 min, t_{minor} = 7.922 min)



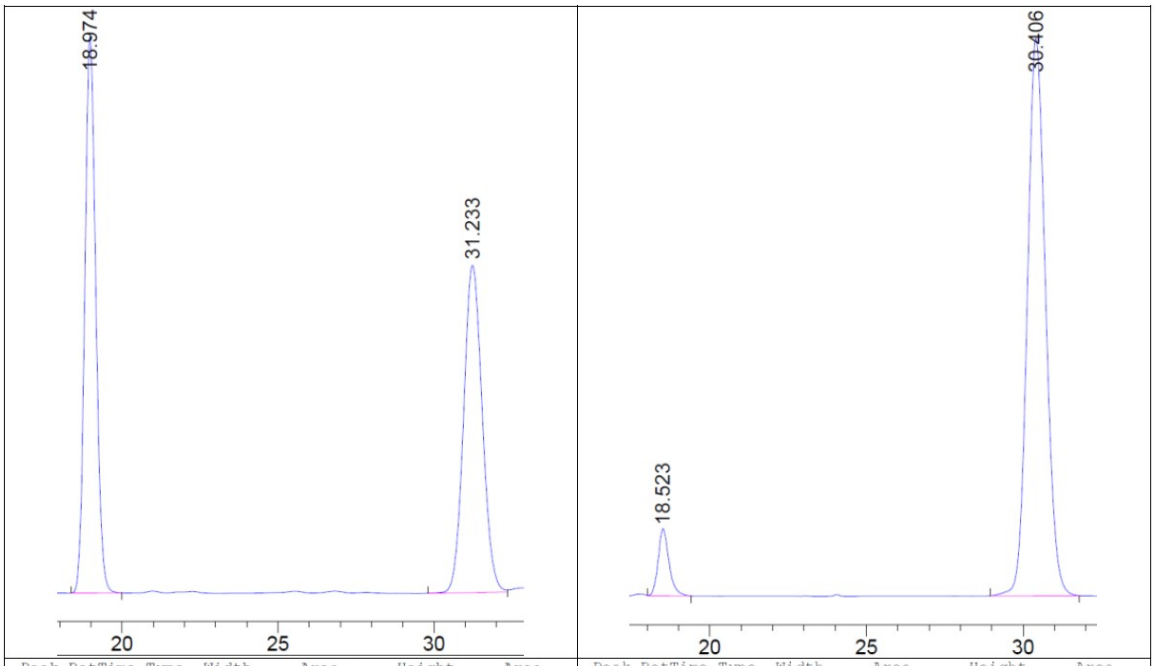
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.008	BB	0.1810	3308.94067	281.04507	50.4651
2	9.382	BB	0.2155	3247.95044	232.39978	49.5349

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.922	BB	0.1760	732.15148	72.37239	8.4542
2	9.264	BB	0.2076	7928.05859	585.09625	91.5458

(*S*)-tert-butyl-2-(naphthalen-2-yl)-3-nitro-2,5-dihydrothiophene-2-carboxylate (3k)



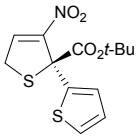
Pale yellow oil, yield: 72%, ee: 86%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.81 (d, *J* = 8.6 Hz, 3H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.45-7.49 (m, 3H), 4.08-4.19 (m, 2H), 1.53 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.4, 153.6, 137.9, 134.9, 132.6, 128.5, 127.8, 127.7, 127.6, 127.4, 126.7, 126.3, 126.0, 82.8, 66.1, 33.2, 28.6 ppm. FTIR (KBr, cm^{-1}): 3037, 2980, 2932, 1729, 1658, 1536, 1433, 1360, 1252, 1163, 1041, 775, 736. HRMS (ESI): Calcd for $C_{19}H_{19}NO_4S$ $[M+Na]^+$: 380.0932. Found: 380.0927. [α]16 D= +78.2 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 5:95, 0.8 mL/min, 25 °C, 254 nm, t_{major} = 30.406 min, t_{minor} = 18.523 min)



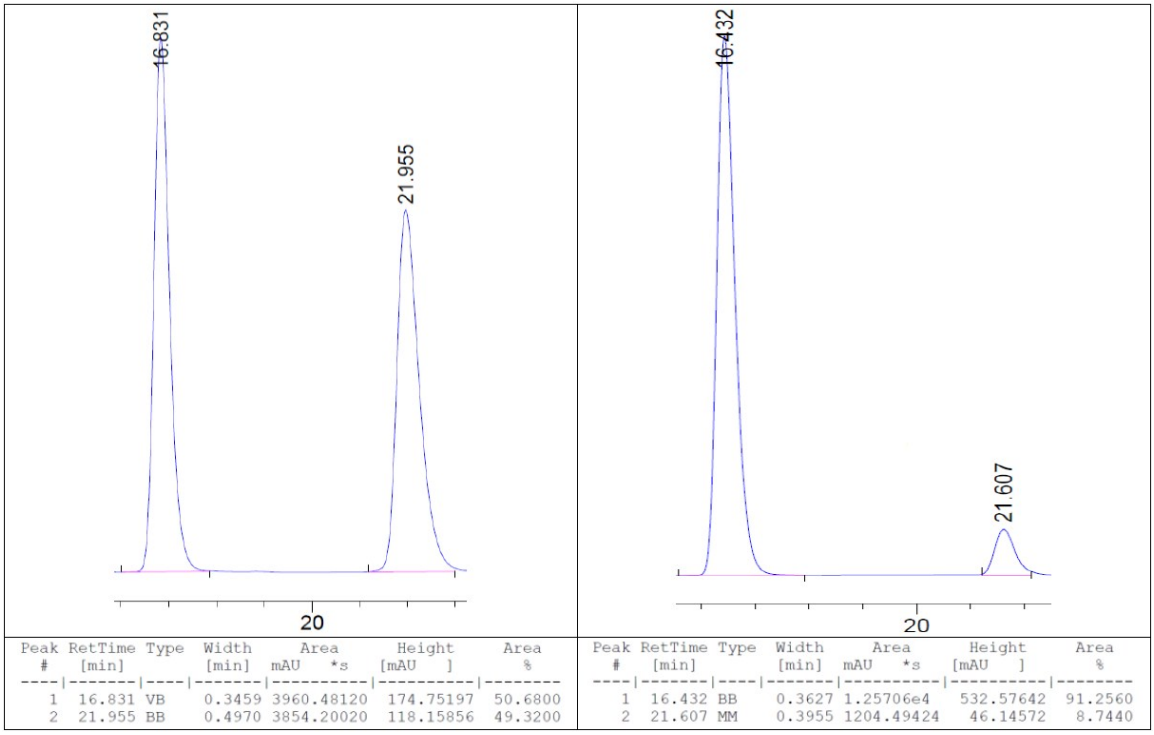
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.974	PB	0.3810	5981.92920	243.73344	50.0428
2	31.233	BB	0.6472	5971.68652	143.47978	49.9572

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.523	VB	0.3658	594.28921	24.99505	6.7672
2	30.406	BB	0.6272	8187.61768	202.63985	93.2328

(*S*)-tert-butyl-3-nitro-2, 5-dihydro-[2, 2'-bithiophene]-2-carboxylate (3l)



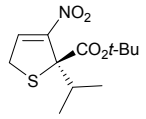
Pale yellow oil, yield: 62%, ee: 83%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 (d, *J* = 1.5 Hz, 1H), 7.30 (d, *J* = 4.8 Hz, 1H), 7.22-7.23 (m, 1H), 6.94-6.96 (m, 1H), 4.08 (dd, *J* = 51.5, 17.7 Hz, 2H), 1.53 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 168,7, 141.3, 137.8, 127.9, 127.7, 127.0, 126.8, 84.1, 62.8, 33.3, 27.6 ppm. FTIR (KBr, cm^{-1}): 3028, 2982, 2937, 1734, 1541, 1443, 1368, 1259, 1156, 1034, 802. HRMS (ESI): Calcd for $C_{13}H_{15}NO_4S$ $[M+Na]^+$: 336.0340. Found: 336.0331. [α]16 D= +38.2 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 5:95, 0.8 mL/min, 25 °C, 254 nm, t_{major} = 16.432 min, t_{minor} = 21.607 min)



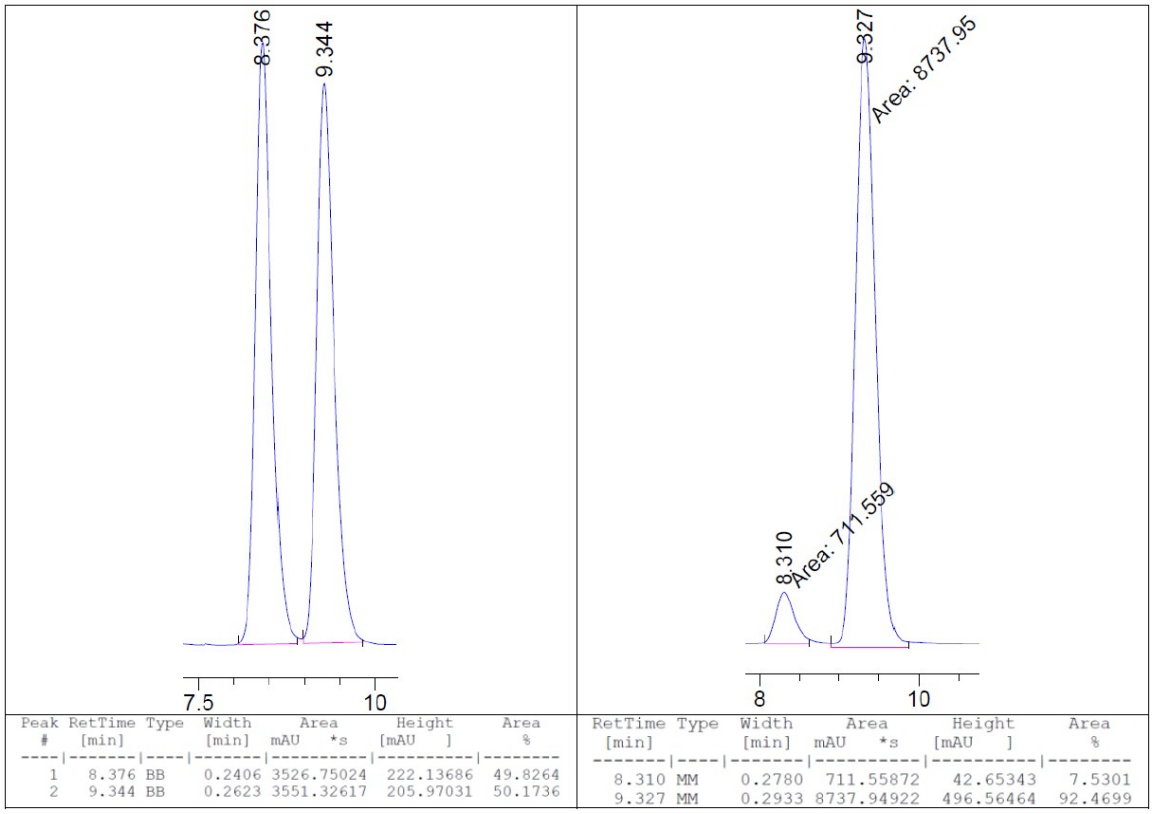
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.831	VB	0.3459	3960.48120	174.75197	50.6800
2	21.955	BB	0.4970	3854.20020	118.15856	49.3200

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.432	BB	0.3627	1.25706e4	532.57642	91.2560
2	21.607	MM	0.3955	1204.49424	46.14572	8.7440

(*S*)-tert-butyl-2-isopropyl-3-nitro-2, 5-dihydrothiophene-2-carboxylate (3m)



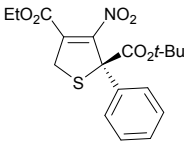
Pale yellow oil, yield: 69%, ee: 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 7.2 Hz, 1H), 3.87-4.01 (m, 2H), 2.19-2.26 (m, 1H), 1.51 (s, 9H), 1.04 (dd, *J* = 7.0, 1.4 Hz, 6H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 154.3, 123.9, 84.8, 70.5, 33.2, 27.7, 27.0, 16.8 ppm. FTIR (KBr, cm^{-1}): 3061, 2978, 2873, 1740, 1684, 1539, 1432, 1371, 1258, 1107, 1024, 778. HRMS (ESI): Calcd for $C_{12}H_{19}NO_4S$ $[M+Na]^+$: 296.0933. Found: 296.0927. [α]16 D= +28.9 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1.0 mL/min, 25 °C, 254 nm, t_{major} = 9.327 min, t_{minor} = 8.310 min)



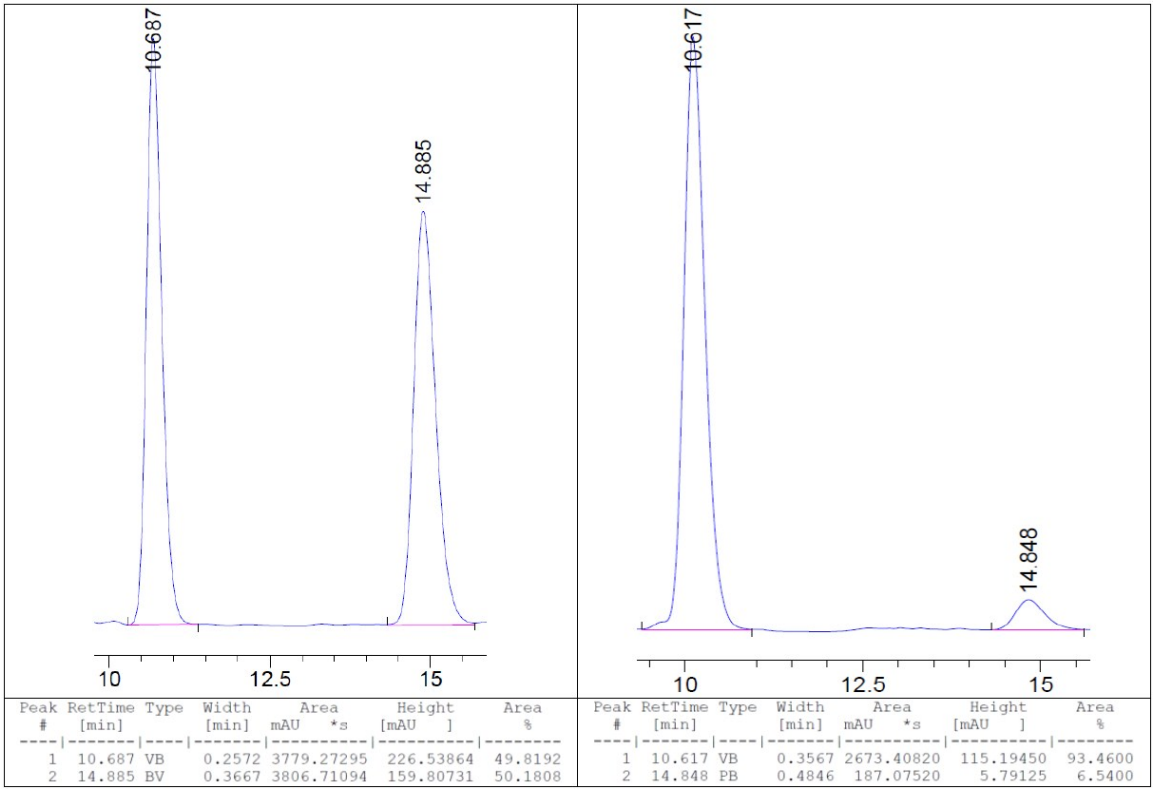
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.376	BB	0.2406	3526.75024	222.13686	49.8264
2	9.344	BB	0.2623	3551.32617	205.97031	50.1736

RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
8.310	MM	0.2780	711.55872	42.65343	7.5301
9.327	MM	0.2933	8737.94922	496.56464	92.4699

(*S*)-2-tert-butyl-4-ethyl 3-nitro-2-phenyl-2,5-dihydrothiophene-2, 4-dicarboxylate (3n)



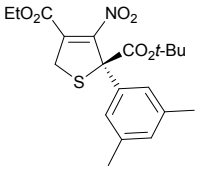
Pale yellow oil, yield: 65%, ee: 87%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, J = 7.8 Hz, 2H), 7.36 (t, J = 7.2 Hz, 2H), 7.31 (d, J = 6.6 Hz, 1H), 4.33 (dd, J = 14.1, 7.0 Hz, 2H), 4.13 (dd, J = 11.2 Hz, 2H), 1.54 (s, 9H), 1.32 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.6, 161.8, 151.1, 136.9, 128.5, 128.4, 128.3, 128.1, 84.1, 68.9, 62.8, 34.5, 27.8, 13.7 ppm. FTIR (KBr, cm^{-1}): 2983, 2939, 2877, 1738, 1694, 1532, 1447, 1362, 1249, 1036, 818, 760, 697. HRMS (ESI): Calcd for $C_{18}H_{21}NO_6S$ $[M+Na]^+$: 402.0987. Found: 402.0982. [α]16 D= +20.6 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 5:95, 1,0 mL/min, 25 °C, 254 nm, t_{major} = 10.617 min, t_{minor} = 14.848 min)



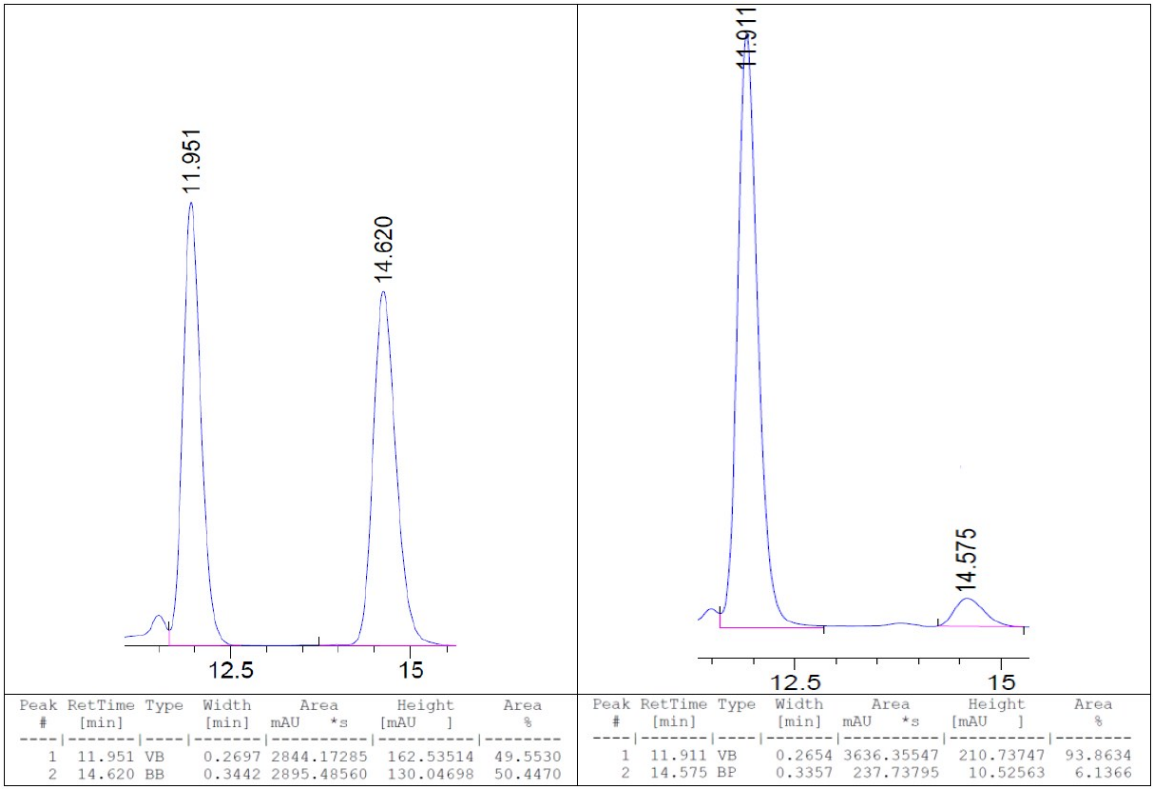
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.687	VB	0.2572	3779.27295	226.53864	49.8192
2	14.885	BV	0.3667	3806.71094	159.80731	50.1808

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.617	VB	0.3567	2673.40820	115.19450	93.4600
2	14.848	PB	0.4846	187.07520	5.79125	6.5400

(*S*)-2-tert-butyl-4-ethyl-2-(3,5-dimethylphenyl)-3-nitro-2,5-dihydrothiophene-2,4-dicarboxylate (3o)



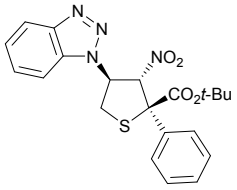
Pale yellow oil, yield: 64%, ee: 88%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.19 (s, 2H), 6.93 (s, 1H), 4.18 (dd, *J* = 14.0, 7.0 Hz, 2H), 4.13-4.22 (m, 2H), 2.31 (s, 6H), 1.53 (s, 9H), 1.32 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.6, 161.8, 151.3, 137.6, 136.6, 130.1, 126.1, 125.9, 83.8, 68.7, 62.7, 34.3, 27.6, 21.4, 13.6 ppm. FTIR (KBr, cm^{-1}): 2987, 2941, 2829, 1729, 1685, 1531, 1452, 1351, 1263, 1102, 1015, 820, 756, 693. HRMS (ESI): Calcd for $C_{20}H_{25}NO_6S$ $[M+Na]^+$: 430.1300. Found: 430.1296. [α]16 D= +26.1 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 5:95, 1,0 mL/min, 25 °C, 254 nm, t_{major} = 11.911 min, t_{minor} = 14.575 min)



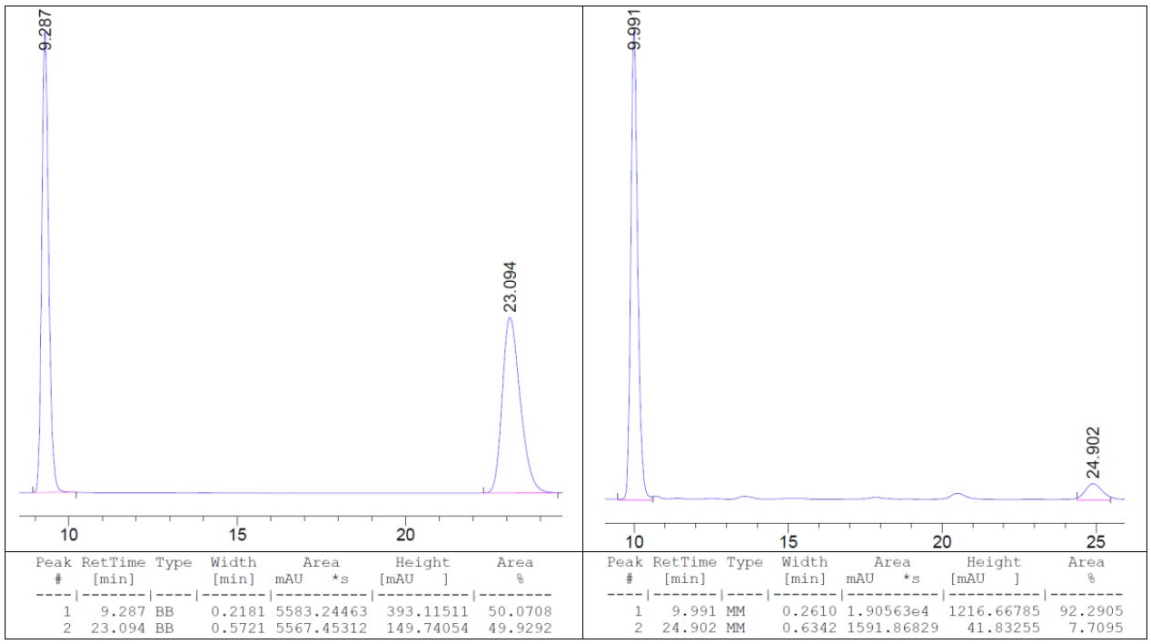
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.951	VB	0.2697	2844.17285	162.53514	49.5530
2	14.620	BB	0.3442	2895.48560	130.04698	50.4470

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.911	VB	0.2654	3636.35547	210.73747	93.8634
2	14.575	BP	0.3357	237.73795	10.52563	6.1366

(2*S*,3*S*,4*S*)-tert-butyl-4-(1*H*-benzo[d][1,2,3]triazol-1-yl)-3-nitro-2-phenyltetrahydrothiophene-2-carboxylate (4)



White solid, mp 119-121 °C, yield: 58%, dr: > 19:1, ee: 85%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 7.4 Hz, 2H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.41-7.44 (m, 3H), 7.38 (t, *J* = 7.3 Hz, 1H), 6.51 (dd, *J* = 14.8, 8.2 Hz, 1H), 6.10 (d, *J* = 8.1 Hz, 1H), 3.77 (dd, *J* = 11.7, 8.7 Hz, 1H), 3.61 (dd, *J* = 11.8, 6.4 Hz, 1H), 1.56 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.7, 145.9, 136.2, 132.8, 128.4, 128.3, 128.1, 124.5, 120.2, 109.3, 95.2, 84.5, 64.6, 63.0, 33.0, 27.6 ppm. FTIR (KBr, cm^{-1}): 2938, 2904, 1726, 1678, 1596, 1531, 1489, 1362, 1216, 1152, 1045, 814, 747, 695. HRMS (ESI): Calcd for $C_{21}H_{21}N_4O_4S$ $[M+H]^+$: 427.1440. Found: 427.1445. [α]16 D= +33.8 (*C* = 1.0, $CHCl_3$). HPLC (Chiralpak AD-H column, *i*-PrOH/hexane = 10:90, 1,0 mL/min, 25 °C, 254 nm, t_{major} = 9.991 min, t_{minor} = 24.902 min)



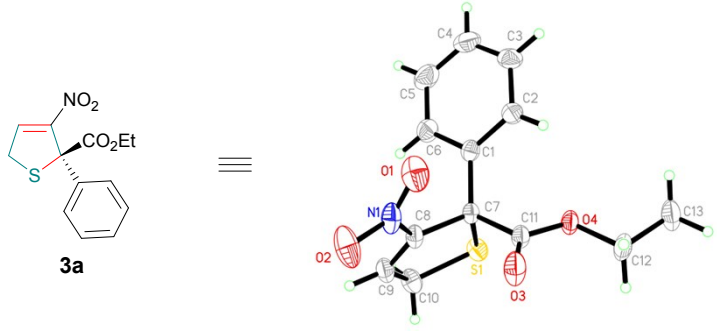
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.287	BB	0.2181	5583.24463	393.11511	50.0708
2	23.094	BB	0.5721	5567.45312	149.74054	49.9292

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.991	MM	0.2610	1.90563e4	1216.66785	92.2905
2	24.902	MM	0.6342	1591.86829	41.83255	7.7095

Procedure for a larger scale experiment

To a stirred solution of β-nitroacrylates **2a** (2 mmol, 442.4 mg), catalyst **VII** (0.2 mmol, 104.5 mg), 5Å MS（45 mg/mL, 607.5 mg）in distilled chloroform (13.5 mL), the substrate **1a** (1.2 mmol, 182.7 mg) was added at room temperature. After completed (monitored by TLC analysis), the mixture was cooled to 0 °C, then TFAA (4 mmol, 0.56 mL) was added and Et_3N (4 mmol, 0.56 mL) was dropped slowly. The reaction mixture was kept stirring until completed (monitored by TLC analysis), the crude product was washed with H_2O (10 mL × 3), dried with $MgSO_4$, then purified by column chromatography on silica gel (PE/EA = 20/1~10/1 as eluant) to afford the corresponding product **3a** in 67% yield. The enantioselectivity was 76%, determined by chiral HPLC analysis.

5. X-Ray Structure of 3a



6. DFT calculation

6.1 Computational methods

Spin-unrestricted density functional theory (DFT) calculations were performed using the Gaussian09 program package.[2] All structures were optimized without symmetry constrains at the B3LYP[3] level with the standard 6-31G (d, p) basis sets[4] for all atoms. The nature of all inter mediates was confirmed by performing normal-mode analysis, and the transition states (TSs) of reactions were confirmed by vibrational analysis and characterized by occurrence of only one imaginary frequency. All aromatic groups are replaced by methyl to save the calculation time.

The adsorption energy (Eads) was calculated as follows:

$E_{ads} = E_{total} - E_{cat} - E_{IS1} - E_{IS2}$

Where E_{total} is the calculated total energy of the adsorption system, E_{cat} is the energy of the catalyst, E_{IS1} and E_{IS2} are the energy of the reaction species.

6.2 Energy profile and calculated structures for the reaction pathway

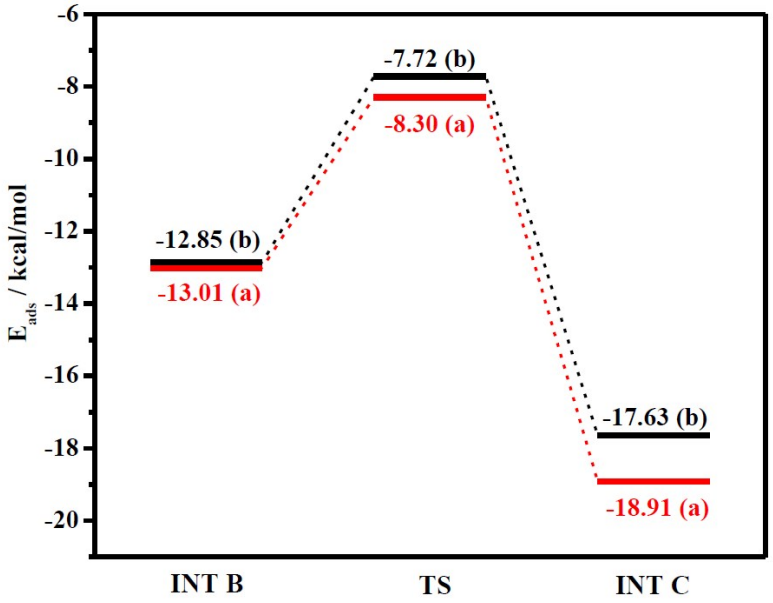
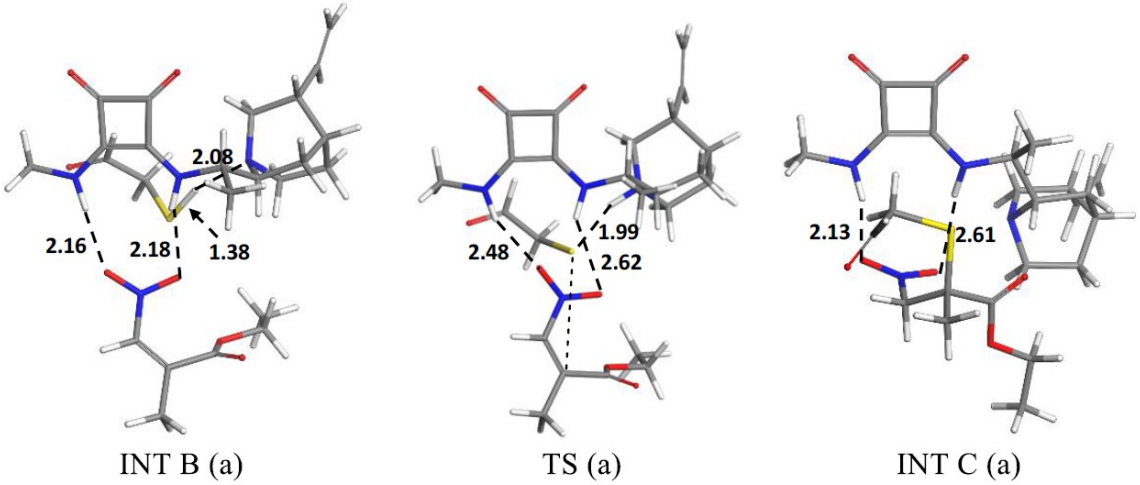
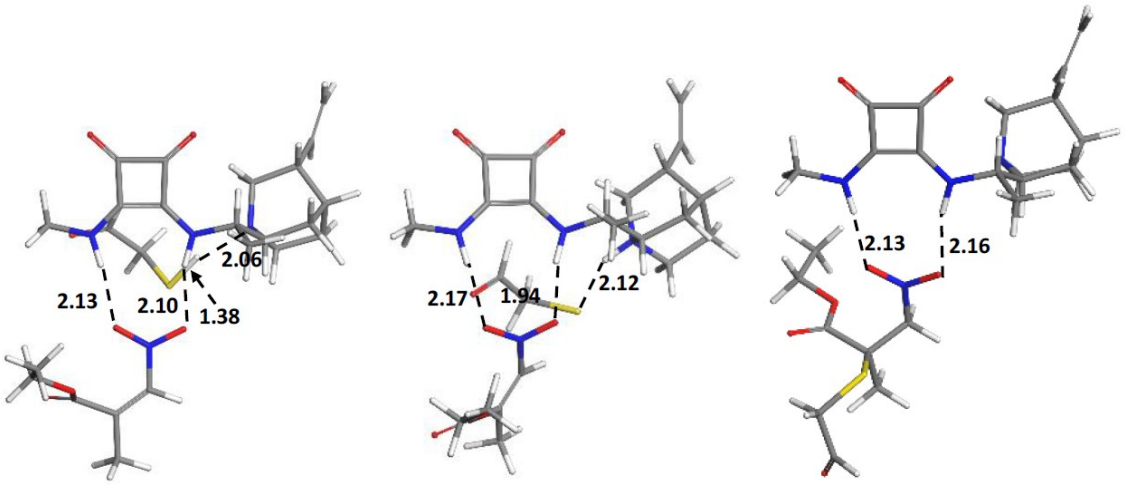


Fig S-1. The Gibbs free Energy profile of the reaction from INT B to INT



INT B (a) TS (a) INT C (a)

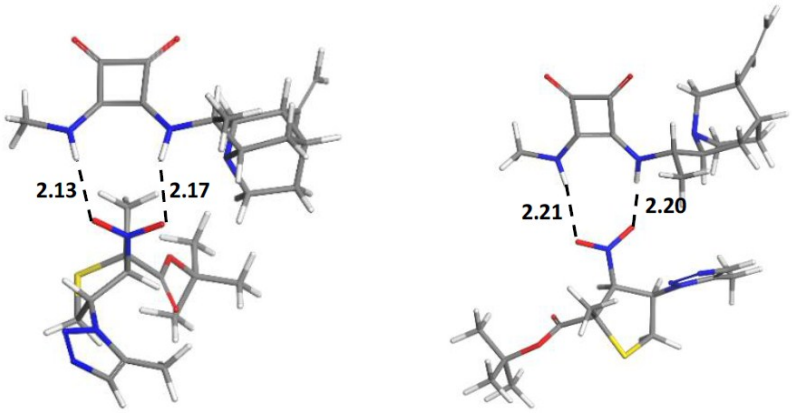


INT B (b) TS (b) INT C (b)

Fig S-2. Optimized structures on the reaction pathway, distances are in angstrom

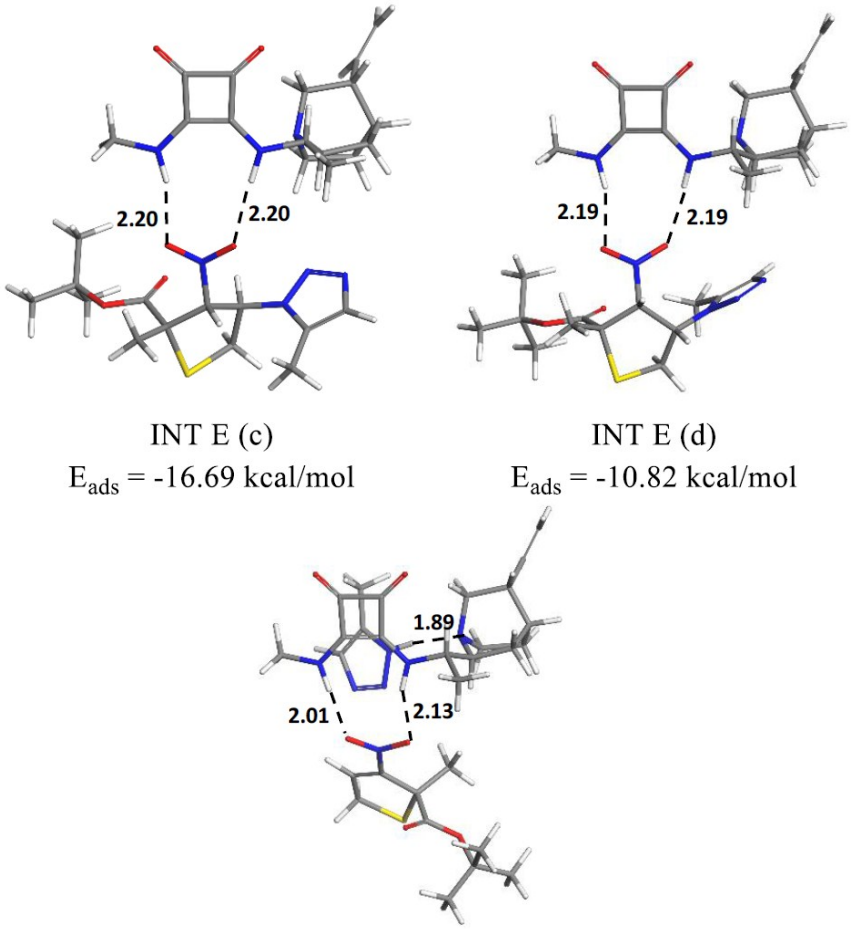
The Gibbs free Energy of the transition state is -8.30 kcal/mol for (a) and -7.72 kcal/mol for (b). This result predicts that (a) is the main reaction pathway, which is in agreement with the experimental results.

6.3 Energy profile and calculated structures for the compound 4



INT E (a)
E_{ads} = -17.97 kcal/mol

INT E (b)
E_{ads} = -14.31 kcal/mol



INT E (c)
E_{ads} = -16.69 kcal/mol

INT E (d)
E_{ads} = -10.82 kcal/mol

INT D (a)
Eads = -23.45 kcal/mol

Fig S-3. The Gibbs free Energy profile of optimized structures, distances are in angstrom

As in Fig S-3, the lowest Gibbs free Energy of the optimized structures of compound **4** is -17.97 kcal/mol for (a) and the energy of corresponding adsorption state is -23.45 kcal/mol. This result shows that this reaction is endothermic, based on the Brønsted–Evans–Polanyi (BEP) relationship, the less heat it absorbs, the lower the Gibbs free Energy of the transition state is. Thus, we deduce that the configurations of the compound 4 are (3*S*, 4*S*), which is in agreement with INT E (a).

References

1 (a) X. Creary. *J. Org. Chem*., 1987, **52**, 5026. (b) C. Christensen., K. Juhl., R. G. Hazell and K. A. Jørgensen., *J. Org. Chem*., 2002, **67**, 4875. (c) H. Li., L. Wang., L. Tang and L. Deng., *J. Am. Chem. Soc*., 2004, **126**, 9906. (d) N. J. A. Martin., X. Cheng and B. List., *J. Am. Chem. Soc*., 2008, **130**, 13862. (d) H.-H. Lu., F.-G. Zhang., S.-W. Duan and W.-J. Xiao., *Org. Lett*. 2009, **11**, 3946.

2 Gaussian 09, Revision E.01, Frisch, M. J. et al., Gaussian, Inc., Wallingford CT, 2013.

3 (a) A. D. Becke. *J. Chem. Phys.* **1993**, *98*, 5648. (b) C. Lee, W. Yang, R. G. *Parr. Phys. Rev. B* **1988**, *37*, 785.

4 W. J. Hehre, L. Radom, P. v. R. Schleyer, J. A. Pople. Ab Initio Molecular Orbital Theory; John Wiley & Sons, Inc.: New York, 1986.

Energies, thermal Free Energies, Z.P.E., negative eigenvalues (for TS structure) and Cartesian coordinates of all structures

INT B (a)
Zero-point correction=0.592054
Sum of electronic and zero-point Energies=-2079.277126
Sum of electronic and thermal Free Energies=-2079.359816
0 1

O	-3.04360000	4.75270000	-0.69620000
O	-3.79120000	1.62930000	-1.62410000
N	0.07200000	3.86390000	-0.33170000
N	-0.66670000	0.80740000	-1.33550000
C	-1.05000000	3.24330000	-0.71750000
C	-1.36360000	1.94160000	-1.14980000
C	-2.45970000	3.69740000	-0.86580000
C	-2.79760000	2.26970000	-1.30580000
H	0.92700000	3.32410000	-0.27800000
H	0.33270000	0.79680000	-1.16070000
C	0.06730000	5.21130000	0.23470000
H	0.18270000	5.17970000	1.32400000
H	0.88020000	5.80210000	-0.19880000
H	-0.88600000	5.68420000	-0.00450000
C	-3.88870000	-2.38110000	-0.14240000
C	-2.85190000	-3.45560000	-0.57660000
H	-4.42680000	-2.06200000	-1.04340000
C	-1.27480000	-2.57300000	1.15360000
C	-1.95960000	-2.83370000	-1.66740000
H	-3.37720000	-4.32960000	-0.97510000
H	-0.18450000	-2.67720000	1.16920000
H	-1.58600000	-2.36180000	2.18210000
H	-1.27300000	-3.58500000	-2.07370000
H	-2.59110000	-2.49900000	-2.49900000
N	-1.60980000	-1.38420000	0.33920000
C	-3.07110000	-1.16000000	0.41350000
H	-3.31670000	-0.98360000	1.46670000
H	-3.33180000	-0.25110000	-0.13220000
C	-1.96120000	-3.86070000	0.61160000
H	-2.55010000	-4.35230000	1.39220000
H	-1.21550000	-4.59120000	0.27690000
C	-4.90760000	-2.88560000	0.84220000
C	-6.21860000	-2.96640000	0.61190000
H	-4.52870000	-3.18950000	1.81950000
H	-6.91010000	-3.33170000	1.36540000
H	-6.64990000	-2.66240000	-0.33890000
C	4.42040000	-1.57530000	-0.58740000
O	4.34530000	-2.33570000	-1.52540000
C	5.15470000	-0.25700000	-0.68440000
C	6.65080000	-0.37920000	-0.68220000
H	6.98830000	-0.83040000	0.25790000
H	6.95810000	-1.05070000	-1.49130000
H	7.14260000	0.58690000	-0.80910000
C	4.55690000	0.93300000	-0.81950000
H	5.07900000	1.87560000	-0.90720000

N	3.12420000	1.10850000	-0.85450000
O	2.38670000	0.11720000	-0.89670000
O	2.72250000	2.27560000	-0.85820000
C	-0.67870000	2.64410000	2.94740000
O	-0.17760000	3.65900000	3.38280000
H	-1.41880000	2.67090000	2.12120000
C	-0.31850000	1.25900000	3.43510000
H	-1.21130000	0.66690000	3.65410000
H	0.30420000	1.33770000	4.32780000
S	0.68250000	0.40580000	2.13460000
H	-0.35180000	-0.08660000	1.37450000
C	-1.16630000	-1.63030000	-1.05690000
H	-0.10370000	-1.89740000	-0.97780000
C	-1.25270000	-0.37920000	-1.96380000
H	-2.30440000	-0.13790000	-2.14270000
C	-0.56070000	-0.63910000	-3.31250000
H	-0.68100000	0.22730000	-3.96810000
H	0.51210000	-0.81220000	-3.16790000
H	-0.97710000	-1.51130000	-3.82360000
O	4.01340000	-1.80800000	0.66050000
C	3.32930000	-3.07410000	0.88750000
H	3.98530000	-3.88480000	0.55740000
H	2.43300000	-3.08920000	0.26050000
C	3.00130000	-3.15210000	2.36410000
H	2.35260000	-2.32420000	2.66300000
H	2.48510000	-4.09420000	2.57370000
H	3.91190000	-3.12000000	2.96900000

INT B (b)
Zero-point correction=0.592170
Sum of electronic and zero-point Energies=-2079.276869
Sum of electronic and thermal Free Energies=-2079.360133
0 1

O	-0.66860000	4.94100000	-0.38460000
O	-2.95090000	2.78370000	-1.53120000
N	1.42460000	2.47180000	0.00190000
N	-0.80190000	0.37190000	-1.23730000
C	0.16960000	2.58600000	-0.45280000
C	-0.77750000	1.69140000	-0.98480000
C	-0.74960000	3.74620000	-0.60680000
C	-1.78820000	2.75960000	-1.14940000
H	1.83510000	1.54720000	0.06330000
H	0.02110000	-0.19150000	-1.04760000
C	2.10750000	3.56980000	0.68460000
H	2.09930000	3.42350000	1.77040000
H	3.14320000	3.63920000	0.33730000
H	1.58830000	4.50000000	0.45010000
C	-5.26350000	-0.57620000	-0.28080000
C	-4.98640000	-2.02060000	-0.78500000
H	-5.48750000	0.04020000	-1.16010000
C	-3.25320000	-2.27780000	1.00100000
C	-3.85400000	-1.94700000	-1.82710000
H	-5.89310000	-2.42620000	-1.24560000

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H	-3.42760000	-1.99520000	2.04450000
H	-3.68210000	-2.93360000	-2.27220000
H	-4.15990000	-1.28020000	-2.64220000
N	-2.84030000	-1.05430000	0.27690000
C	-3.93070000	-0.05840000	0.36930000
H	-4.08240000	0.15590000	1.43310000
H	-3.61830000	0.87430000	-0.10420000
C	-4.52320000	-2.92220000	0.37350000
H	-5.31570000	-3.04050000	1.11920000
H	-4.30390000	-3.92540000	-0.01000000
C	-6.43510000	-0.47500000	0.65660000
C	-7.55260000	0.21060000	0.41280000
H	-6.33870000	-0.99600000	1.61070000
H	-8.36460000	0.25530000	1.13250000
H	-7.69310000	0.75960000	-0.51520000
C	6.52090000	0.99620000	-2.52680000
C	6.37960000	0.66440000	-1.05590000
H	7.04250000	1.95150000	-2.63780000
H	7.09670000	0.22780000	-3.05020000
H	5.54090000	1.08230000	-3.00370000
H	7.34660000	0.56370000	-0.55470000
H	5.79560000	1.41380000	-0.51460000
O	5.67720000	-0.60880000	-0.96230000
C	5.44320000	-1.05380000	0.27410000
O	5.83730000	-0.55550000	1.30330000
C	4.71500000	-2.37850000	0.26380000
C	5.56320000	-3.55510000	0.64990000
H	6.38500000	-3.68050000	-0.06480000
H	6.01430000	-3.36210000	1.62900000
H	4.98660000	-4.48080000	0.69340000
C	3.40970000	-2.52250000	0.00280000
H	2.88390000	-3.46700000	0.00880000
N	2.53630000	-1.42490000	-0.33930000
O	2.92870000	-0.26460000	-0.19660000
O	1.41510000	-1.73810000	-0.75750000
C	-0.06310000	1.64980000	3.15310000
O	0.86300000	2.24050000	3.66690000
H	-0.63180000	2.08780000	2.30660000
C	-0.50250000	0.26310000	3.56500000
H	-1.58070000	0.22290000	3.74420000
H	0.03450000	-0.03660000	4.46640000
S	-0.05760000	-0.93670000	2.23120000
H	-1.14560000	-0.74340000	1.41210000
C	-2.55330000	-1.41670000	-1.13450000
H	-1.81430000	-2.22750000	-1.07840000
C	-1.90980000	-0.26910000	-1.95000000
H	-2.65480000	0.51380000	-2.11780000
C	-1.41420000	-0.78400000	-3.31190000
H	-1.01720000	0.04540000	-3.90300000
H	-0.61360000	-1.52100000	-3.17840000
H	-2.21610000	-1.25630000	-3.88590000

TS (a)
Zero-point correction= 0.595165
Sum of electronic and zero-point Energies= -2079.269622
Sum of electronic and thermal Free Energies= -2079.347208
0 1

O	-3.55510000	4.45360000	-0.39490000
O	-4.07600000	1.31280000	-1.44590000
N	-0.38090000	3.72850000	-0.01710000
N	-0.89210000	0.75150000	-1.29040000
C	-1.45490000	3.09080000	-0.48530000
C	-1.67920000	1.81360000	-1.02770000
C	-2.89640000	3.45680000	-0.62220000
C	-3.12840000	2.03310000	-1.13980000
H	0.46030000	3.18140000	0.12860000
H	0.11250000	0.85890000	-1.18460000
C	-0.46240000	5.03220000	0.64260000
H	-0.29030000	4.91810000	1.71710000
H	0.28650000	5.71190000	0.22290000
H	-1.45640000	5.44630000	0.46940000
C	-3.84520000	-2.19600000	-0.03730000
C	-2.95990000	-3.40460000	-0.45140000
H	-4.25490000	-1.74770000	-0.94930000
C	-1.15750000	-2.76580000	1.16260000
C	-1.99160000	-2.94080000	-1.55800000
H	-3.59560000	-4.21130000	-0.82800000
H	-0.11200000	-2.99580000	0.95280000
H	-1.21750000	-2.50750000	2.22140000
H	-1.32890000	-3.76280000	-1.84750000
H	-2.56380000	-2.66370000	-2.44880000
N	-1.47940000	-1.50670000	0.40140000
C	-2.91740000	-1.14400000	0.63440000
H	-3.05210000	-1.11000000	1.71880000
H	-3.10870000	-0.15030000	0.23550000
C	-2.12830000	-3.89410000	0.74800000
H	-2.77730000	-4.17280000	1.58270000
H	-1.56570000	-4.79180000	0.47330000
C	-5.00570000	-2.55980000	0.85140000
C	-6.28340000	-2.32850000	0.55130000
H	-4.76290000	-3.02940000	1.80580000
H	-7.08570000	-2.60510000	1.22830000
H	-6.57240000	-1.84390000	-0.37770000
C	4.91790000	-1.08580000	-0.65170000
O	5.21350000	-1.87410000	-1.52180000
C	5.15060000	0.40170000	-0.79340000
C	6.58190000	0.83070000	-0.65390000
H	6.95150000	0.57940000	0.34690000
H	7.19660000	0.27930000	-1.37370000
H	6.70760000	1.90250000	-0.81860000
C	4.18190000	1.28570000	-1.05920000
H	4.33390000	2.35130000	-1.15940000
N	2.79500000	0.92190000	-1.22650000
O	2.47310000	-0.26520000	-1.30430000
O	1.99490000	1.86310000	-1.30560000

C	-0.27690000	2.11440000	3.09120000
O	0.26370000	3.18470000	3.30620000
H	-1.27420000	2.06990000	2.59880000
C	0.33260000	0.77260000	3.37080000
H	-0.38430000	0.12390000	3.88760000
H	1.22570000	0.89680000	3.98700000
S	0.79510000	0.07050000	1.71680000
H	-0.79020000	-0.75500000	0.84100000
C	-1.16250000	-1.71800000	-1.06430000
H	-0.08940000	-1.93410000	-1.07490000
C	-1.39910000	-0.45400000	-1.93080000
H	-2.47480000	-0.30520000	-2.06420000
C	-0.73640000	-0.64770000	-3.30540000
H	-0.97150000	0.20410000	-3.94770000
H	0.35160000	-0.70730000	-3.19620000
H	-1.08150000	-1.55680000	-3.80670000
O	4.47250000	-1.37330000	0.56870000
C	4.16360000	-2.76740000	0.84250000
H	5.07150000	-3.36060000	0.69590000
H	3.42320000	-3.09580000	0.10700000
C	3.63470000	-2.83460000	2.26070000
H	2.76040000	-2.18520000	2.37050000
H	3.35300000	-3.86600000	2.49790000
H	4.39810000	-2.51700000	2.97680000

TS (b)
Zero-point correction=0.596347
Sum of electronic and zero-point Energies=-2079.268693
Sum of electronic and thermal Free Energies=-2079.346750
0 1

O	1.37163400	5.08848300	-0.75512800
O	3.40526500	2.68259600	0.38264200
N	-1.18194200	3.14892000	-0.19203600
N	0.87607900	0.77767900	0.92817500
C	0.13370500	3.03370900	-0.02887000
C	1.00595100	2.05010000	0.47443000
C	1.27368000	3.96818700	-0.29561400
C	2.20034100	2.86966100	0.23487900
H	-1.78329400	2.35696000	0.01358300
H	-0.06024000	0.38776200	1.02664300
C	-1.77700200	4.20882700	-1.00295700
H	-2.09481700	3.80427700	-1.96957000
H	-2.64625700	4.62964200	-0.48912200
H	-1.03640700	4.99356800	-1.15985700
C	4.91486000	-0.74763800	0.25499300
C	4.70073000	-1.99753900	1.15482400
H	5.02934100	0.12581300	0.90679300
C	2.86817200	-2.87369100	-0.30159600
C	3.58793200	-1.68126600	2.17354200
H	5.62985400	-2.23071000	1.68294400
H	2.06265600	-3.46295600	0.14110700
H	2.80573500	-3.01025100	-1.38170300
H	3.38486600	-2.55968300	2.79463700

H	3.92790700	-0.88822900	2.84593500
N	2.52404400	-1.42322000	-0.04740400
C	3.62433300	-0.54954200	-0.58699000
H	3.75625900	-0.84757200	-1.63003800
H	3.29981200	0.48987600	-0.56235500
C	4.25098400	-3.19636200	0.30231300
H	4.97796700	-3.40668800	-0.48684600
H	4.18906600	-4.09664300	0.92126600
C	6.13939200	-0.82568700	-0.61893200
C	7.14751700	0.04487100	-0.57813000
H	6.17744600	-1.64798500	-1.33441200
H	8.00887700	-0.05142900	-1.23179100
H	7.14242200	0.89198900	0.10301600
C	-5.96068100	-0.24743200	3.35693900
C	-6.33185400	-0.19736500	1.88851200
H	-6.70727000	0.29475200	3.94518100
H	-5.92205600	-1.27937700	3.71708200
H	-4.98474400	0.21565800	3.52607400
H	-7.30082600	-0.66400000	1.68709600
H	-6.36795800	0.82667400	1.50567600
O	-5.30823400	-0.92174500	1.15918600
C	-5.45123400	-0.95225400	-0.17516600
O	-6.41183200	-0.52483500	-0.77873200
C	-4.30498500	-1.64367600	-0.86125800
C	-4.69941600	-2.59698200	-1.95410600
H	-5.28610200	-3.43113200	-1.55205400
H	-5.33953200	-2.07122000	-2.66923500
H	-3.82466200	-2.99556600	-2.47023800
C	-3.01617700	-1.41973000	-0.58297600
H	-2.15886300	-1.90721000	-1.05810200
N	-2.55670900	-0.45165100	0.39197500
O	-3.06574000	0.66832900	0.45161200
O	-1.59009100	-0.80871700	1.08147600
C	-0.52824300	0.53011400	-2.60653600
O	-1.63784200	0.94533700	-2.31029400
H	0.38272800	1.07442900	-2.27369900
C	-0.25443600	-0.74335700	-3.33984200
H	0.57440600	-0.62344400	-4.04460300
H	-1.15014000	-1.07473100	-3.86982000
S	0.19599800	-1.97060600	-2.02155200
H	1.62735700	-1.26859900	-0.63125200
C	2.29228900	-1.22303800	1.43646000
H	1.44894700	-1.88217500	1.66634600
C	1.89805500	0.22239500	1.81667000
H	2.77697600	0.86504600	1.71378800
C	1.41099300	0.25864500	3.27679000
H	1.20278200	1.29184400	3.56532300
H	0.48656400	-0.31877400	3.38620100
H	2.15019700	-0.14360700	3.97550800

INT C (a)
Zero-point correction=0.596760
Sum of electronic and zero-point Energies=-2079.286521

Sum of electronic and thermal Free Energies=-2079.366371

0 1

O	1.16380000	5.77070000	0.12690000
O	-0.69810000	4.23050000	-2.16680000
N	1.15730000	3.06160000	1.93180000
N	-0.74110000	1.54190000	-0.25060000
C	0.61840000	3.41700000	0.75340000
C	-0.19800000	2.77160000	-0.19170000
C	0.65720000	4.67330000	-0.03310000
C	-0.21320000	3.96500000	-1.08110000
H	1.15230000	2.08570000	2.20410000
H	-0.83030000	1.00560000	0.60890000
C	1.99790000	3.96760000	2.70720000
H	1.61190000	4.07660000	3.72690000
H	3.02890000	3.59950000	2.76600000
H	1.99870000	4.94400000	2.22080000
N	-2.66670000	-0.20590000	0.60560000
C	-6.28220000	-0.32760000	0.95240000
C	-7.51880000	0.15440000	0.82070000
H	-6.06980000	-0.99970000	1.78540000
H	-8.31320000	-0.11070000	1.51200000
H	-7.78200000	0.83620000	0.01530000
C	0.27810000	-5.59090000	1.16330000
C	0.27410000	-4.55460000	0.05830000
H	-0.57770000	-6.26150000	1.04070000
H	1.19090000	-6.19250000	1.13560000
H	0.20350000	-5.11680000	2.14590000
H	0.35130000	-5.00470000	-0.93560000
H	-0.62570000	-3.93350000	0.07590000
O	1.42780000	-3.69460000	0.26280000
C	1.58590000	-2.69460000	-0.62020000
O	0.85430000	-2.48750000	-1.56140000
C	2.89220000	-1.92500000	-0.34010000
C	4.06060000	-2.86890000	-0.71680000
H	4.01440000	-3.78240000	-0.11580000
H	3.98690000	-3.14130000	-1.77180000
H	5.02450000	-2.38890000	-0.54620000
C	3.04010000	-1.56110000	1.14290000
H	2.94200000	-2.46490000	1.74970000
N	1.96390000	-0.63200000	1.64620000
O	0.79740000	-0.88520000	1.36840000
O	2.33170000	0.32060000	2.33760000
C	5.40610000	0.27450000	-0.79810000
O	5.99650000	-0.20910000	0.14800000
H	5.87680000	0.32930000	-1.80140000
C	3.98630000	0.77300000	-0.71770000
H	3.85030000	1.65670000	-1.34940000
H	3.71820000	1.02580000	0.30940000
S	2.80340000	-0.43220000	-1.46830000
H	3.99110000	-1.07240000	1.35030000
C	-4.59850000	-1.22060000	-0.76480000
H	-5.41760000	-1.65150000	-1.34950000
C	-4.00050000	-2.28180000	0.18160000

H	-4.77900000	-2.73030000	0.80730000
H	-3.57200000	-3.09580000	-0.41530000
C	-1.69960000	1.12040000	-1.28310000
H	-2.50780000	1.86360000	-1.35240000
C	-1.03680000	1.00330000	-2.66010000
H	-0.21840000	0.27770000	-2.62840000
H	-1.76660000	0.67530000	-3.40740000
H	-0.65680000	1.97720000	-2.97410000
C	-2.28670000	-0.23110000	-0.83000000
H	-1.47130000	-0.96120000	-0.90020000
C	-2.90550000	-1.58950000	1.05120000
H	-1.95340000	-2.12870000	1.00620000
H	-3.20320000	-1.55170000	2.10490000
C	-3.89430000	0.58020000	0.82610000
H	-4.09050000	0.58840000	1.90380000
H	-3.70880000	1.61750000	0.53480000
C	-3.48620000	-0.70780000	-1.70260000
H	-3.17120000	-1.49860000	-2.39180000
H	-3.87670000	0.11270000	-2.31730000
C	-5.12800000	-0.00240000	0.04460000
H	-5.47690000	0.74240000	-0.68170000

INT C (b)
Zero-point correction= 0.596378
Sum of electronic and zero-point Energies= -2079.284485
Sum of electronic and thermal Free Energies= -2079.366174
0 1

O	-2.63548400	5.04992800	0.31064300
O	-4.56056000	2.60891100	-0.92530200
N	-0.01840200	3.16635100	-0.12278400
N	-1.90431400	0.80359800	-1.43365900
C	-1.33278800	3.02937600	-0.36078100
C	-2.13764300	2.01452100	-0.90573200
C	-2.49412200	3.92609700	-0.14107200
C	-3.37308000	2.81227300	-0.71928300
H	0.59650200	2.37898100	-0.28530200
H	-0.97406500	0.40560400	-1.36754800
C	0.54087600	4.35404700	0.51018000
H	0.96007800	4.11988500	1.49669500
H	1.33471900	4.78698000	-0.10852800
H	-0.25562100	5.08902300	0.63393900
C	-5.58360500	-1.46515700	0.52895900
C	-5.00423500	-2.72421100	-0.17616100
H	-6.25067900	-0.96889300	-0.18698300
C	-2.87350400	-2.37489200	1.09592300
C	-4.29780300	-2.25295400	-1.46390600
H	-5.81938600	-3.41178100	-0.42518100
H	-1.87300300	-2.74878200	0.84774000
H	-2.87931500	-2.16110500	2.17060800
H	-3.98001900	-3.11338400	-2.06394100
H	-5.00873200	-1.68361000	-2.07601700
N	-3.07919100	-1.09953200	0.38893700
C	-4.36297400	-0.52001100	0.82782100

H	-4.28185500	-0.33007900	1.90389200
H	-4.51042800	0.44997500	0.34849900
C	-3.97012800	-3.42381000	0.72851500
H	-4.44938000	-3.82910800	1.62552500
H	-3.53546300	-4.27666600	0.19348000
C	-6.38949200	-1.77526800	1.75971200
C	-7.69629200	-1.54681300	1.89785300
H	-5.84321700	-2.20379400	2.60168400
H	-8.22479500	-1.78260900	2.81686800
H	-8.28537500	-1.10755600	1.09616400
C	-3.07120600	-1.36763800	-1.06429900
H	-2.14684800	-1.93360900	-1.24898700
C	-2.97313200	-0.07788500	-1.91330200
H	-3.90111900	0.49349500	-1.82207800
C	-2.73564500	-0.41032100	-3.39419600
H	-2.70417200	0.50775700	-3.98637900
H	-1.78091600	-0.93365700	-3.52612300
H	-3.52737700	-1.04890100	-3.79582400
C	2.83497400	0.24672300	4.45509900
C	3.70470200	0.75974400	3.32609500
H	2.87213000	0.94933200	5.29283800
H	1.79330800	0.15068600	4.13667100
H	3.18324200	-0.72723300	4.81040300
H	3.36645300	1.72818400	2.94778300
H	4.75335200	0.86046900	3.61947800
O	3.62435700	-0.20397500	2.23774200
C	4.31750500	0.10127700	1.12675700
O	5.02416300	1.07492900	1.01174600
C	4.16681300	-1.02906300	0.08239500
C	5.00471000	-2.23430400	0.56790600
H	6.05742600	-1.96283900	0.66026100
H	4.64746100	-2.56723700	1.54720200
H	4.92924800	-3.06238700	-0.14144000
C	2.71129800	-1.50768000	-0.03053300
H	2.35093800	-1.82763100	0.94988200
N	1.72894700	-0.44399000	-0.46588400
O	0.80917700	-0.80843300	-1.19212300
O	1.88101900	0.69471500	-0.03164700
C	7.29556300	-1.23386100	-1.73093900
O	7.98933000	-1.72312400	-0.86637400
H	7.25113900	-1.67239200	-2.75091100
C	6.41244700	-0.02340800	-1.51799300
H	6.55456300	0.69187900	-2.33525400
H	6.60649300	0.47002400	-0.56658100
S	4.62928500	-0.47516300	-1.63238700
H	2.60144700	-2.31568400	-0.75220200

INT D (a)
Zero-point correction=0.715679
Sum of electronic and zero-point Energies=-2362.956821
Sum of electronic and thermal Free Energies=-2363.043426
0 1

O	4.85650000	-3.47910000	-1.54710000

O	4.84720000	-0.17050000	-1.99810000
N	1.59780000	-3.45020000	-1.48860000
N	1.59820000	-0.18010000	-1.79930000
C	2.55050000	-2.52560000	-1.64400000
C	2.55090000	-1.12520000	-1.78660000
C	4.03260000	-2.58830000	-1.68420000
C	4.02630000	-1.07080000	-1.87570000
H	0.63350000	-3.14600000	-1.40730000
H	0.62170000	-0.43960000	-1.68680000
C	1.89790000	-4.85670000	-1.24950000
H	1.57450000	-5.15770000	-0.24650000
H	1.39170000	-5.49060000	-1.98550000
H	2.97550000	-5.00360000	-1.33250000
C	4.00540000	3.33540000	0.55410000
C	2.62830000	4.04970000	0.46900000
H	4.56140000	3.58810000	-0.35710000
C	1.64080000	2.12770000	1.73470000
C	1.93200000	3.56040000	-0.81560000
H	2.78060000	5.13300000	0.42550000
H	0.59930000	1.79640000	1.79230000
H	2.15230000	1.72830000	2.61690000
H	1.02290000	4.14120000	-1.00600000
H	2.60010000	3.72740000	-1.66950000
N	2.26040000	1.49290000	0.54360000
C	3.71370000	1.79390000	0.55400000
H	4.12980000	1.33010000	1.45580000
H	4.18890000	1.30630000	-0.29970000
C	1.74850000	3.67850000	1.67730000
H	2.16840000	4.07810000	2.60550000
H	0.75850000	4.13410000	1.56110000
C	4.84090000	3.76510000	1.72930000
C	6.01120000	4.39830000	1.64310000
H	4.45150000	3.51910000	2.71850000
H	6.57600000	4.67920000	2.52700000
H	6.45110000	4.65470000	0.68210000
C	1.59160000	2.04360000	-0.66970000
H	0.51700000	1.92890000	-0.47840000
C	1.89300000	1.24570000	-1.96150000
H	2.96010000	1.31510000	-2.19190000
C	1.08190000	1.79080000	-3.14740000
H	1.32750000	1.23180000	-4.05380000
H	0.00680000	1.68250000	-2.96300000
H	1.28960000	2.84760000	-3.33280000
S	-4.65480000	-0.93050000	2.15590000
C	-3.84700000	-2.58620000	2.26970000
H	-3.35240000	-2.71000000	3.23960000
H	-4.59810000	-3.37690000	2.16840000
C	-3.49110000	-0.28240000	0.82400000
C	-4.37540000	0.14610000	-0.36110000
O	-4.48260000	-0.50790000	-1.37720000
O	-4.99440000	1.29980000	-0.08510000
C	-5.96280000	1.91340000	-1.02710000
C	-5.24450000	2.28580000	-2.32660000

C	-7.13580000	0.95740000	-1.25750000
C	-6.41270000	3.16270000	-0.26840000
H	-4.38180000	2.92540000	-2.11600000
H	-4.90500000	1.39710000	-2.85900000
H	-5.92940000	2.84290000	-2.97350000
H	-7.58230000	0.66390000	-0.30290000
H	-7.90370000	1.46360000	-1.85100000
H	-6.81710000	0.06110000	-1.79000000
H	-7.14050000	3.72040000	-0.86490000
H	-6.87950000	2.89060000	0.68230000
H	-5.56170000	3.81740000	-0.06060000
C	-2.84740000	-2.64000000	1.16870000
H	-2.24560000	-3.52190000	0.99230000
C	-2.70210000	-1.52070000	0.45600000
N	-1.72520000	-1.47680000	-0.61120000
O	-1.41430000	-0.37380000	-1.07380000
O	-1.24470000	-2.54220000	-1.00700000
C	-2.64180000	0.87090000	1.38770000
H	-3.29380000	1.62790000	1.82520000
H	-1.96490000	0.48570000	2.15280000
H	-2.05030000	1.32930000	0.59270000
C	2.38880000	-2.18510000	2.04670000
N	0.19210000	-2.58190000	2.22360000
N	0.32980000	-1.44050000	1.59400000
C	3.88340000	-2.22390000	2.06140000
H	4.31110000	-1.22310000	2.17170000
H	4.23470000	-2.83370000	2.89740000
H	4.28760000	-2.65860000	1.14070000
C	1.42980000	-3.06530000	2.51790000
H	1.56740000	-3.99780000	3.04570000
N	1.65100000	-1.19620000	1.48270000
H	1.95070000	-0.30990000	1.02030000

INT E (a)
Zero-point correction= 0.718448
Sum of electronic and zero-point Energies= -2362.948082
Sum of electronic and thermal Free Energies= -2363.032676
0 1

O	-3.44800000	-3.96210000	-3.23850000
O	-4.96370000	-2.24370000	-0.80380000
N	-0.68050000	-3.89160000	-1.53230000
N	-2.19690000	-2.24560000	0.89790000
C	-1.92980000	-3.44310000	-1.32570000
C	-2.56780000	-2.72540000	-0.29920000
C	-3.16490000	-3.49950000	-2.14730000
C	-3.85980000	-2.71750000	-1.02750000
H	0.01560000	-3.75350000	-0.81140000
H	-1.21420000	-2.22520000	1.14820000
C	-0.31910000	-4.69710000	-2.69440000
H	0.55530000	-4.27370000	-3.19930000
H	-0.08850000	-5.72960000	-2.40600000
H	-1.16280000	-4.70550000	-3.38560000
C	-4.56330000	1.88710000	0.79290000

C	-3.93480000	2.11360000	2.19660000
H	-5.50340000	1.34110000	0.93980000
C	-1.67320000	1.90540000	1.14110000
C	-3.74370000	0.73070000	2.85050000
H	-4.60790000	2.72750000	2.80400000
H	-0.72170000	1.65300000	1.62260000
H	-1.43360000	2.42650000	0.20760000
H	-3.42330000	0.84080000	3.89270000
H	-4.70680000	0.20550000	2.86750000
N	-2.35120000	0.64740000	0.77700000
C	-3.56260000	0.97160000	-0.00320000
H	-3.23370000	1.47260000	-0.92040000
H	-4.05650000	0.04700000	-0.30970000
C	-2.55650000	2.79240000	2.07070000
H	-2.65580000	3.80870000	1.67520000
H	-2.10550000	2.88840000	3.06530000
C	-4.88570000	3.16050000	0.06110000
C	-6.11060000	3.55460000	-0.28930000
H	-4.03680000	3.79050000	-0.21070000
H	-6.28190000	4.48220000	-0.82750000
H	-6.98920000	2.95810000	-0.05530000
C	-2.68460000	-0.07340000	2.02650000
H	-1.74530000	-0.11330000	2.59420000
C	-3.12150000	-1.53760000	1.78990000
H	-4.09520000	-1.55570000	1.29230000
C	-3.22880000	-2.29810000	3.12090000
H	-3.57400000	-3.31980000	2.94360000
H	-2.25330000	-2.34990000	3.61870000
H	-3.93120000	-1.81520000	3.80600000
S	3.14130000	0.17930000	-2.39940000
C	4.47180000	-0.05000000	-1.17010000
H	5.31470000	-0.56170000	-1.63810000
H	4.80420000	0.91110000	-0.77160000
C	1.85920000	0.41710000	-1.04790000
C	1.93430000	1.92910000	-0.73970000
O	2.66630000	2.38440000	0.12430000
O	1.16820000	2.63350000	-1.56580000
C	1.26320000	4.11920000	-1.66610000
C	0.84010000	4.76270000	-0.34440000
C	2.68620000	4.50400000	-2.07600000
C	0.26420000	4.43280000	-2.77970000
H	-0.16640000	4.44160000	-0.06230000
H	1.53210000	4.51060000	0.45900000
H	0.82430000	5.85040000	-0.46560000
H	2.98040000	3.97140000	-2.98480000
H	2.72160000	5.57770000	-2.28380000
H	3.40320000	4.28230000	-1.28460000
H	0.23330000	5.51160000	-2.95700000
H	0.55200000	3.93700000	-3.71060000
H	-0.74060000	4.09940000	-2.50590000
C	3.81450000	-0.93840000	-0.10500000
H	3.65850000	-1.92500000	-0.54520000
C	2.42320000	-0.35290000	0.20370000

N	1.47130000	-1.45560000	0.61700000
O	0.64880000	-1.17370000	1.48700000
O	1.54180000	-2.54350000	0.04900000
C	0.48750000	-0.03950000	-1.55620000
H	0.21450000	0.54060000	-2.43790000
H	0.51760000	-1.09490000	-1.83310000
H	-0.29220000	0.10860000	-0.79990000
C	5.09500000	-0.41240000	2.09210000
N	5.99260000	-2.46710000	2.16310000
N	5.21390000	-2.44360000	1.12700000
C	4.68330000	0.99320000	2.39190000
H	3.72710000	1.02670000	2.92790000
H	5.43260000	1.45550000	3.03870000
H	4.56900000	1.61070000	1.49930000
C	5.94860000	-1.25170000	2.77700000
H	6.52060000	-1.04320000	3.66940000
N	4.64430000	-1.19900000	1.06350000
H	2.43260000	0.32280000	1.05420000

INT E (b)
Zero-point correction=0.718283
Sum of electronic and zero-point Energies= -2362.942252
Sum of electronic and thermal Free Energies= -2363.027313
0 1

O	2.92070000	5.69590000	-0.14590000
O	4.66960000	3.23630000	1.29920000
N	0.41800000	3.64460000	-0.53300000
N	2.12150000	1.23490000	0.89390000
C	1.64740000	3.55370000	0.00150000
C	2.38540000	2.51800000	0.59660000
C	2.75780000	4.52540000	0.15510000
C	3.55810000	3.39660000	0.81720000
H	-0.21830000	2.86300000	-0.43150000
H	1.34520000	0.79570000	0.41120000
C	-0.11860000	4.90140000	-1.03950000
H	-0.50290000	4.77640000	-2.05800000
H	-0.93240000	5.27450000	-0.40520000
H	0.68310000	5.64120000	-1.04980000
C	6.35510000	-0.64790000	-0.35090000
C	5.66230000	-1.99300000	0.00710000
H	6.81930000	-0.26660000	0.56720000
C	3.91740000	-1.45420000	-1.71040000
C	4.64490000	-1.70430000	1.12960000
H	6.41360000	-2.71050000	0.35370000
H	2.89950000	-1.85160000	-1.80420000
H	4.20760000	-1.08070000	-2.69860000
H	4.22970000	-2.63870000	1.52480000
H	5.16030000	-1.20930000	1.96230000
N	3.88270000	-0.30400000	-0.79310000
C	5.21080000	0.33790000	-0.79400000
H	5.39440000	0.70290000	-1.81050000
H	5.19200000	1.21700000	-0.14580000
C	4.90730000	-2.55460000	-1.21500000

H	5.60690000	-2.84610000	-2.00520000
H	4.37010000	-3.46530000	-0.92210000
C	7.43760000	-0.78040000	-1.38590000
C	8.73340000	-0.54520000	-1.17450000
H	7.11820000	-1.07570000	-2.38690000
H	9.47050000	-0.64690000	-1.96550000
H	9.10390000	-0.23380000	-0.20060000
C	3.51300000	-0.79360000	0.55180000
H	2.61110000	-1.40450000	0.40080000
C	3.11050000	0.34480000	1.51480000
H	3.98170000	0.96790000	1.73720000
C	2.54860000	-0.21160000	2.83220000
H	2.28730000	0.61130000	3.50250000
H	1.64790000	-0.81150000	2.66010000
H	3.28090000	-0.84380000	3.34300000
S	-4.54570000	-2.33760000	0.39600000
C	-3.45220000	-3.01990000	-0.90740000
H	-3.29570000	-4.08210000	-0.71140000
H	-3.90430000	-2.90420000	-1.89660000
C	-3.83810000	-0.60010000	0.27840000
C	-4.89860000	0.22610000	-0.49240000
O	-4.84590000	0.41000000	-1.69650000
O	-5.85820000	0.64680000	0.32360000
C	-7.05840000	1.37490000	-0.17380000
C	-6.62690000	2.70160000	-0.80230000
C	-7.82830000	0.47970000	-1.14660000
C	-7.85310000	1.60590000	1.11150000
H	-6.02470000	3.28090000	-0.09610000
H	-6.05020000	2.54200000	-1.71360000
H	-7.51660000	3.28890000	-1.04950000
H	-8.05230000	-0.48490000	-0.68150000
H	-8.77640000	0.96110000	-1.40550000
H	-7.26320000	0.30960000	-2.06330000
H	-8.77750000	2.14460000	0.88480000
H	-8.11330000	0.65440000	1.58330000
H	-7.27330000	2.19920000	1.82400000
C	-2.13580000	-2.22510000	-0.83600000
H	-1.60050000	-2.31220000	-1.78500000
C	-2.60570000	-0.76880000	-0.66730000
N	-1.49250000	0.21890000	-0.43970000
O	-1.81860000	1.37060000	-0.16200000
O	-0.34020000	-0.15550000	-0.63550000
C	-3.59490000	-0.07230000	1.69880000
H	-4.51250000	-0.17560000	2.27950000
H	-2.79910000	-0.64410000	2.17300000
H	-3.32880000	0.98580000	1.67590000
C	-0.28830000	-3.70890000	0.04850000
N	-0.27660000	-2.83540000	2.10830000
N	-1.19630000	-2.20370000	1.43930000
C	-0.03020000	-4.46980000	-1.20990000
H	-0.91010000	-5.02880000	-1.54750000
H	0.28110000	-3.80980000	-2.02810000
H	0.77400000	-5.18880000	-1.04270000

C	0.29820000	-3.76480000	1.29540000
H	1.09210000	-4.40990000	1.64120000
N	-1.22450000	-2.72270000	0.18710000
H	-2.98400000	-0.46080000	-1.65150000

INT E (c)
Zero-point correction=0.718185
Sum of electronic and zero-point Energies=-2362.946050
Sum of electronic and thermal Free Energies=-2363.032288
0 1

O	-2.85390000	5.40270000	-1.17550000
O	-4.91170000	2.77300000	-1.36860000
N	-0.30560000	3.39600000	-1.41710000
N	-2.33010000	0.81500000	-1.71030000
C	-1.64150000	3.23370000	-1.40610000
C	-2.50350000	2.13010000	-1.51050000
C	-2.76700000	4.19140000	-1.29210000
C	-3.70980000	2.98620000	-1.39260000
H	0.29180000	2.57920000	-1.39080000
H	-1.38830000	0.44450000	-1.65360000
C	0.31520000	4.68900000	-1.15890000
H	0.79190000	4.71770000	-0.17030000
H	1.07460000	4.91020000	-1.91710000
H	-0.45760000	5.45820000	-1.19370000
C	-5.50370000	-0.64220000	1.67520000
C	-4.85800000	-2.02310000	1.37100000
H	-6.36450000	-0.52680000	1.00420000
C	-2.64560000	-1.01660000	1.99170000
C	-4.44970000	-2.02460000	-0.11670000
H	-5.58680000	-2.81800000	1.56280000
H	-1.63660000	-1.35680000	1.73930000
H	-2.56910000	-0.39330000	2.89010000
H	-4.13000000	-3.02570000	-0.42630000
H	-5.32090000	-1.75830000	-0.73000000
N	-3.13830000	-0.15760000	0.89860000
C	-4.42090000	0.44090000	1.31100000
H	-4.21740000	1.08210000	2.17590000
H	-4.78810000	1.09720000	0.51850000
C	-3.59360000	-2.23270000	2.23010000
H	-3.85440000	-2.33470000	3.28900000
H	-3.10440000	-3.16720000	1.93260000
C	-6.00660000	-0.50720000	3.08540000
C	-7.28530000	-0.35470000	3.43350000
H	-5.25050000	-0.52230000	3.87200000
H	-7.58850000	-0.25260000	4.47150000
H	-8.07770000	-0.32040000	2.68930000
C	-3.28860000	-0.99810000	-0.30890000
H	-2.34620000	-1.55400000	-0.39580000
C	-3.42140000	-0.16260000	-1.60280000
H	-4.34810000	0.41820000	-1.58250000
C	-3.41670000	-1.05970000	-2.84830000
H	-3.52000000	-0.45320000	-3.75200000
H	-2.47750000	-1.62190000	-2.91770000

H	-4.23670000	-1.78210000	-2.82400000
S	4.96910000	-2.00760000	0.07890000
C	3.43520000	-2.68010000	0.84800000
H	3.44000000	-3.76450000	0.73350000
H	3.41800000	-2.43440000	1.90960000
C	4.10450000	-0.45340000	-0.48320000
C	3.96850000	0.44780000	0.76140000
O	3.11820000	0.25090000	1.61090000
O	4.91120000	1.38260000	0.78790000
C	5.03830000	2.34370000	1.92200000
C	3.77030000	3.19500000	2.01020000
C	5.32820000	1.57510000	3.21260000
C	6.24180000	3.18630000	1.49960000
H	3.56410000	3.67430000	1.04860000
H	2.90650000	2.59670000	2.30040000
H	3.91710000	3.98200000	2.75630000
H	6.20070000	0.92730000	3.08490000
H	5.55040000	2.28850000	4.01210000
H	4.47450000	0.96870000	3.51560000
H	6.44480000	3.94760000	2.25790000
H	7.13350000	2.56280000	1.38870000
H	6.04880000	3.68990000	0.54830000
C	2.20660000	-2.03540000	0.14620000
H	1.63530000	-1.48200000	0.88930000
C	2.74560000	-1.03180000	-0.91390000
N	1.69780000	0.02280000	-1.22070000
O	1.96140000	1.20550000	-1.01280000
O	0.64280000	-0.39170000	-1.68950000
C	4.88440000	0.17630000	-1.63970000
H	5.89300000	0.44230000	-1.32250000
H	4.95260000	-0.52450000	-2.47630000
H	4.38670000	1.08920000	-1.97410000
C	1.36810000	-3.95950000	-1.36590000
N	-0.65200000	-3.98140000	-0.39600000
N	0.02810000	-3.04190000	0.18640000
C	2.55850000	-4.21380000	-2.23500000
H	3.50430000	-4.15370000	-1.69000000
H	2.48250000	-5.21330000	-2.66900000
H	2.61220000	-3.50470000	-3.07040000
C	0.12890000	-4.56480000	-1.34770000
H	-0.23200000	-5.37760000	-1.96090000
N	1.26490000	-3.00580000	-0.38920000
H	2.87640000	-1.54030000	-1.87040000

INT E (d)
Zero-point correction=0.718434
Sum of electronic and zero-point Energies=-2362.936694
Sum of electronic and thermal Free Energies=-2363.022647
0 1

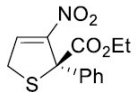
O	-2.65400000	5.41890000	-0.56710000
O	-4.66160000	2.92900000	-1.54120000
N	-0.19420000	3.30930000	-0.31780000
N	-2.16030000	0.85310000	-1.29240000

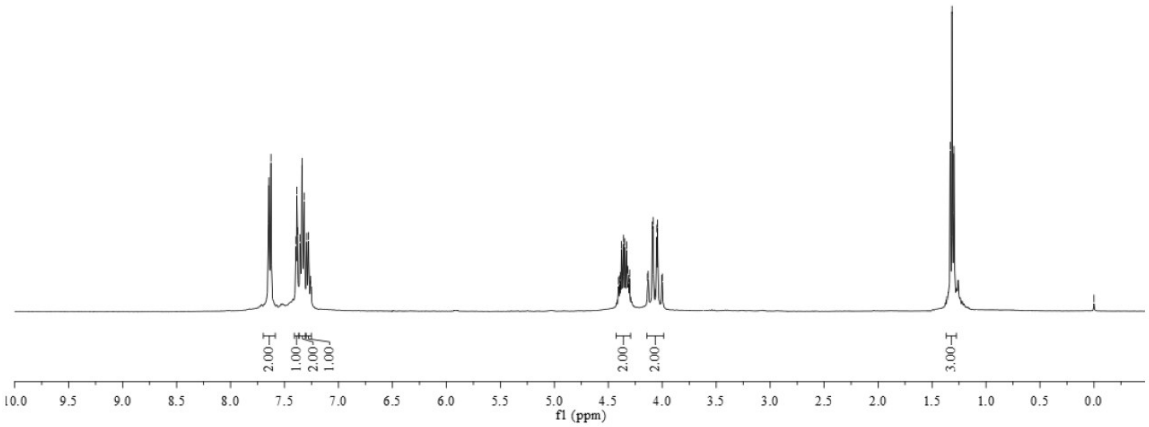
C	-1.48710000	3.21540000	-0.67220000
C	-2.33320000	2.16470000	-1.06430000
C	-2.57530000	4.21820000	-0.76750000
C	-3.49380000	3.07540000	-1.21390000
H	0.40290000	2.49390000	-0.37490000
H	-1.29210000	0.42850000	-0.98750000
C	0.43060000	4.58310000	0.01290000
H	0.89870000	4.54210000	1.00330000
H	1.19830000	4.85390000	-0.72270000
H	-0.33880000	5.35650000	0.01680000
C	-6.29650000	-0.57490000	0.84580000
C	-5.64550000	-1.97530000	0.66780000
H	-6.89700000	-0.37700000	-0.05110000
C	-3.70140000	-1.12990000	2.00780000
C	-4.79170000	-1.92620000	-0.61630000
H	-6.42870000	-2.73480000	0.57250000
H	-2.67460000	-1.51020000	2.06520000
H	-3.88320000	-0.55830000	2.92470000
H	-4.43760000	-2.92720000	-0.88680000
H	-5.41570000	-1.57350000	-1.44770000
N	-3.78870000	-0.19370000	0.87520000
C	-5.11160000	0.45930000	0.90780000
H	-5.16310000	1.04290000	1.83360000
H	-5.18300000	1.17510000	0.08610000
C	-4.72630000	-2.29810000	1.86410000
H	-5.31090000	-2.42990000	2.78070000
H	-4.21530000	-3.25140000	1.68060000
C	-7.21190000	-0.47900000	2.03480000
C	-8.52830000	-0.27240000	1.97500000
H	-6.74290000	-0.57110000	3.01600000
H	-9.13850000	-0.20170000	2.87060000
H	-9.04400000	-0.15970000	1.02410000
C	-3.58680000	-0.96290000	-0.37130000
H	-2.68620000	-1.56840000	-0.19840000
C	-3.26810000	-0.06470000	-1.58850000
H	-4.12980000	0.56680000	-1.82320000
C	-2.90690000	-0.90970000	-2.81860000
H	-2.68520000	-0.25980000	-3.66930000
H	-2.02840000	-1.53460000	-2.61960000
H	-3.72780000	-1.57370000	-3.10180000
S	5.37720000	-1.93790000	-0.99640000
C	3.99480000	-2.88490000	-0.26480000
H	4.18670000	-3.95200000	-0.39270000
H	3.90570000	-2.64700000	0.79360000
C	4.34030000	-0.38120000	-1.05420000
C	4.39070000	0.17350000	0.38140000
O	3.64640000	-0.23820000	1.25690000
O	5.35400000	1.07260000	0.52610000
C	5.67060000	1.69500000	1.84440000
C	4.45830000	2.48930000	2.33430000
C	6.10720000	0.60900000	2.82930000
C	6.83480000	2.62110000	1.49340000
H	4.14020000	3.20900000	1.57450000

H	3.62140000	1.83280000	2.57270000
H	4.73360000	3.04640000	3.23510000
H	6.92610000	0.01800000	2.40870000
H	6.46770000	1.08220000	3.74790000
H	5.28120000	-0.05560000	3.08340000
H	7.16770000	3.15340000	2.38880000
H	7.67900000	2.05020000	1.09680000
H	6.53190000	3.35890000	0.74550000
C	2.77630000	-2.44270000	-1.08400000
H	2.87280000	-2.90780000	-2.06650000
C	2.91130000	-0.89520000	-1.39310000
N	1.83900000	0.04740000	-0.85260000
O	2.15250000	1.23620000	-0.77710000
O	0.71540000	-0.38320000	-0.64290000
C	4.91310000	0.56380000	-2.11370000
H	5.94960000	0.81420000	-1.88530000
H	4.87610000	0.09080000	-3.09860000
H	4.33490000	1.48970000	-2.13860000
C	0.91200000	-3.06990000	0.61470000
N	-0.45550000	-3.74910000	-1.02990000
N	0.64480000	-3.36950000	-1.60030000
C	1.50650000	-2.71210000	1.93760000
H	1.97290000	-1.72500000	1.92540000
H	0.71630000	-2.71160000	2.69160000
H	2.26150000	-3.44030000	2.25590000
C	-0.33140000	-3.58650000	0.31750000
H	-1.12630000	-3.85120000	0.99940000
N	1.50150000	-2.95480000	-0.61570000
H	2.75530000	-0.77040000	-2.46800000

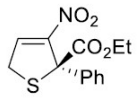
7. ^{1}H, ^{13}C NMR spectra of compounds 3 and 4

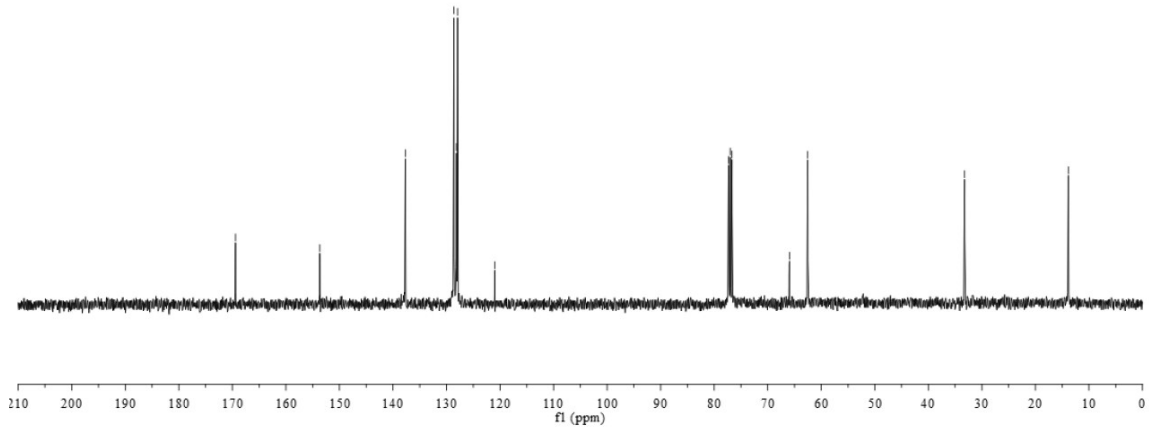
zxy1073 cdcl3



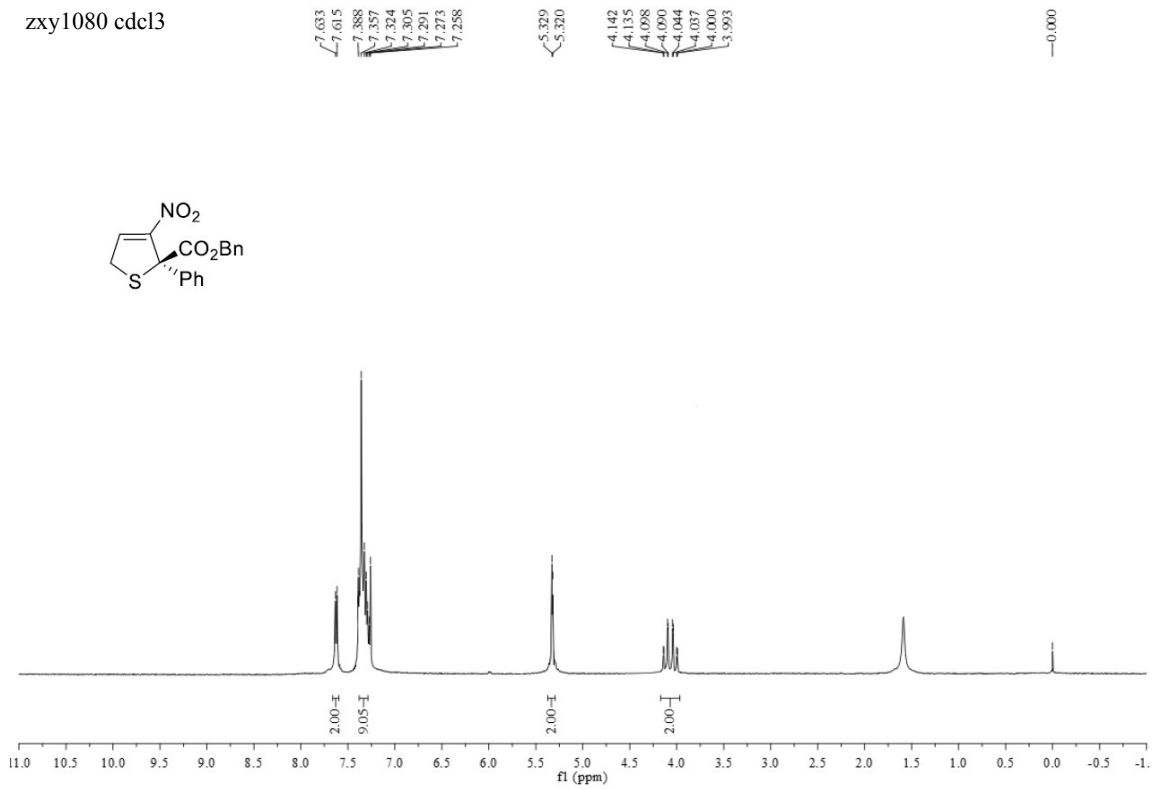


zxy1073 c13 cdcl3





zxy1080 cdcl3



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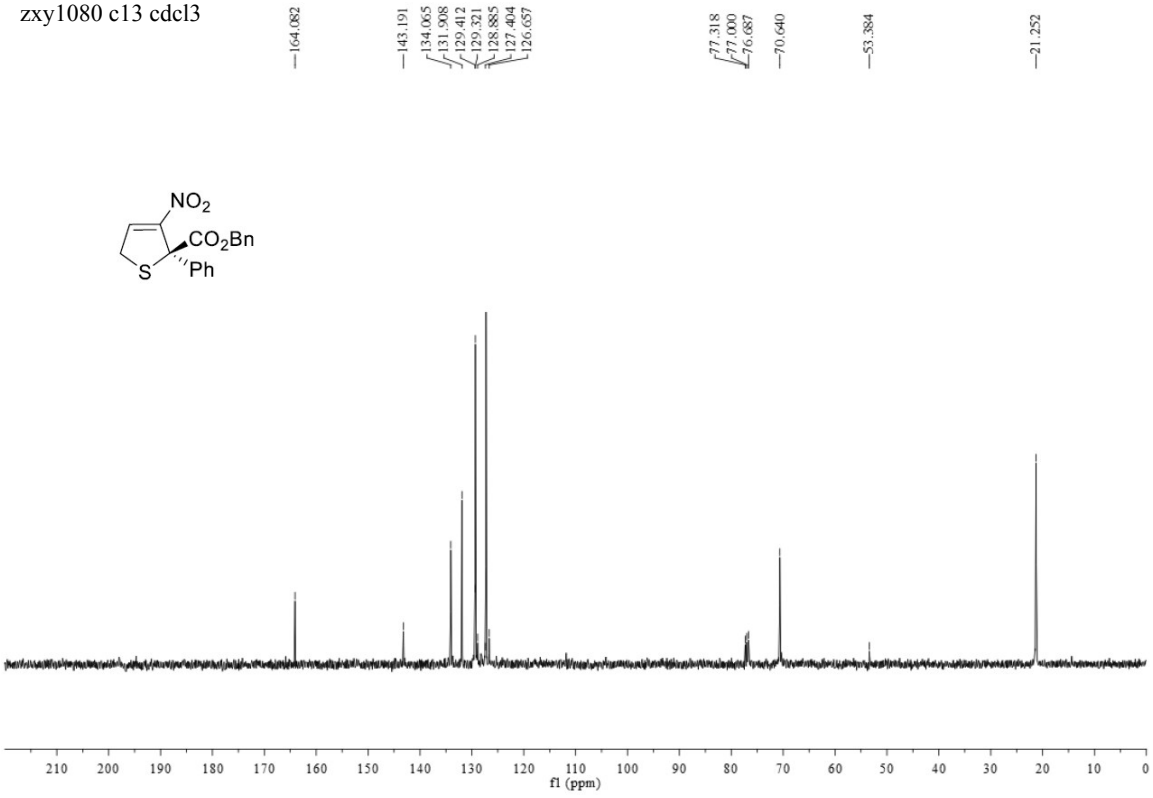

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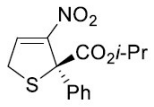

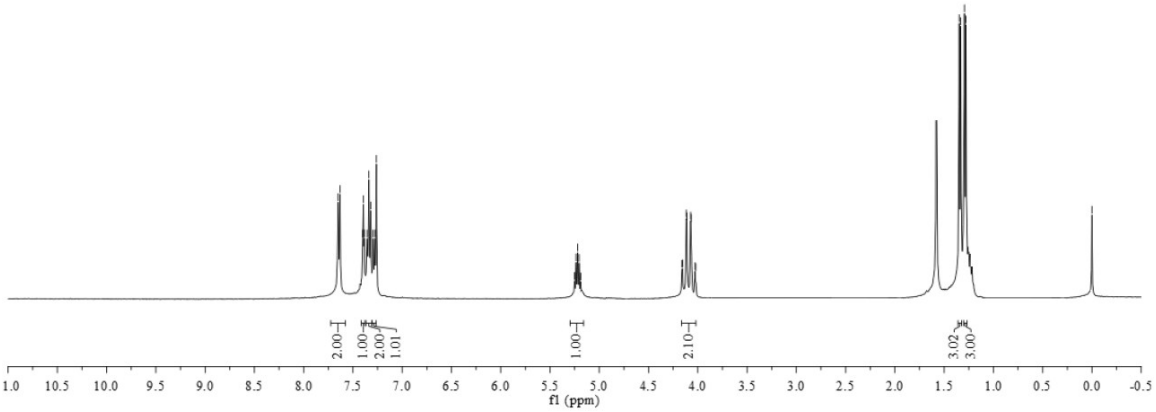

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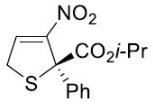

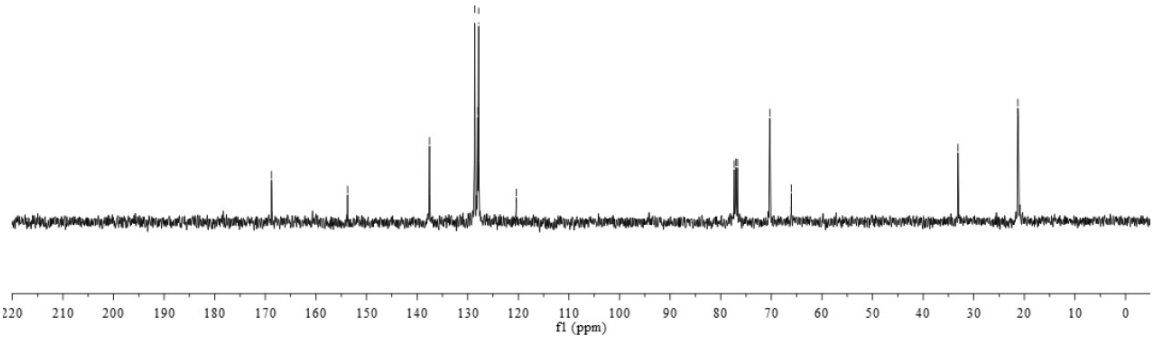

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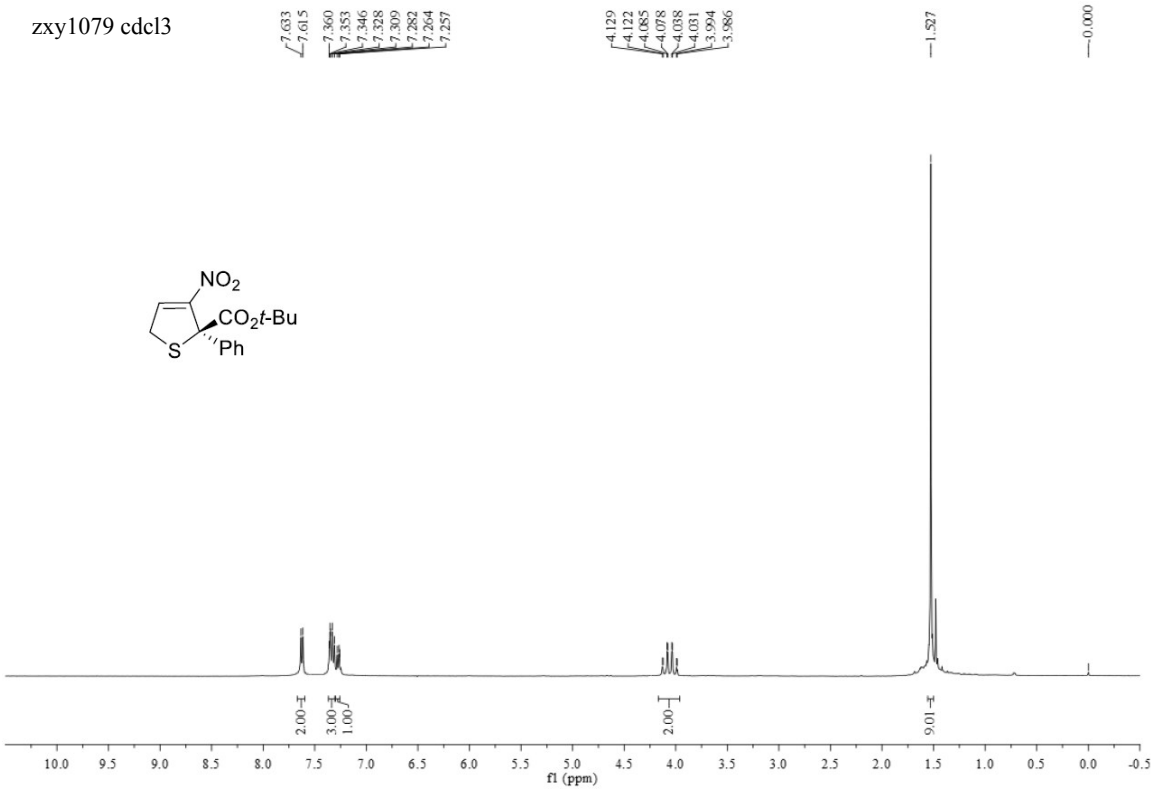

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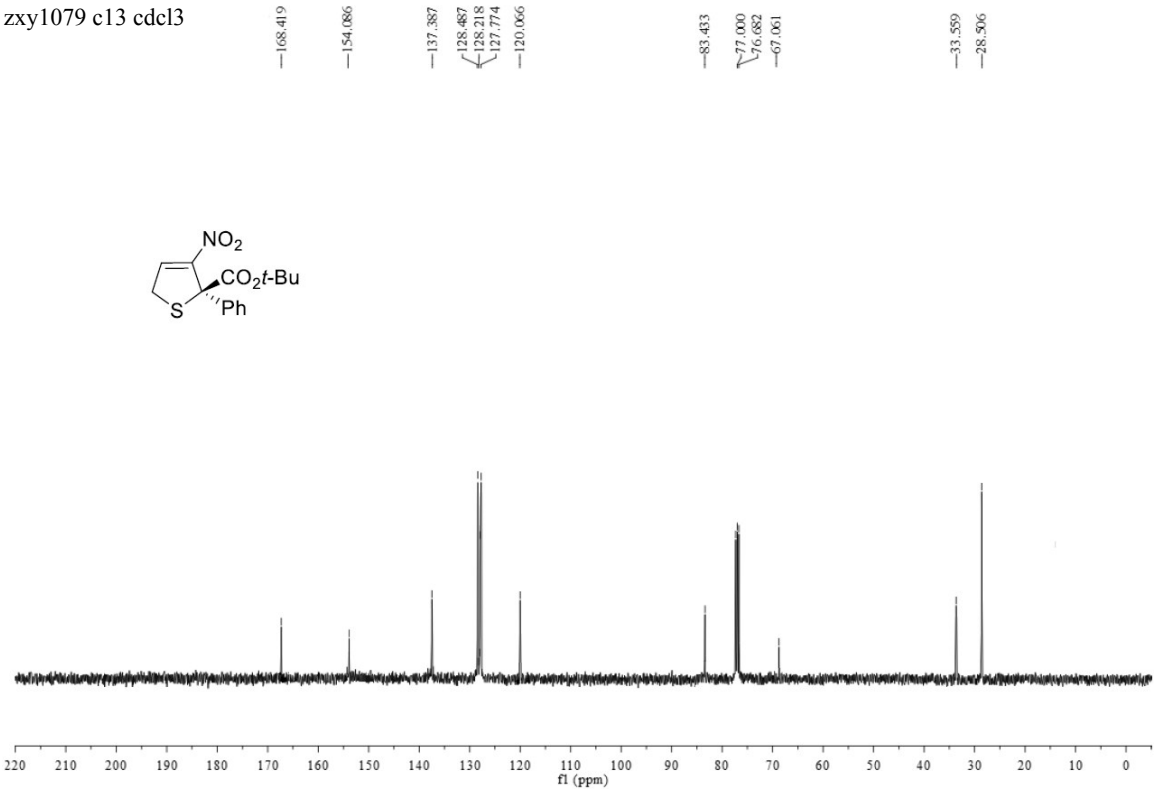

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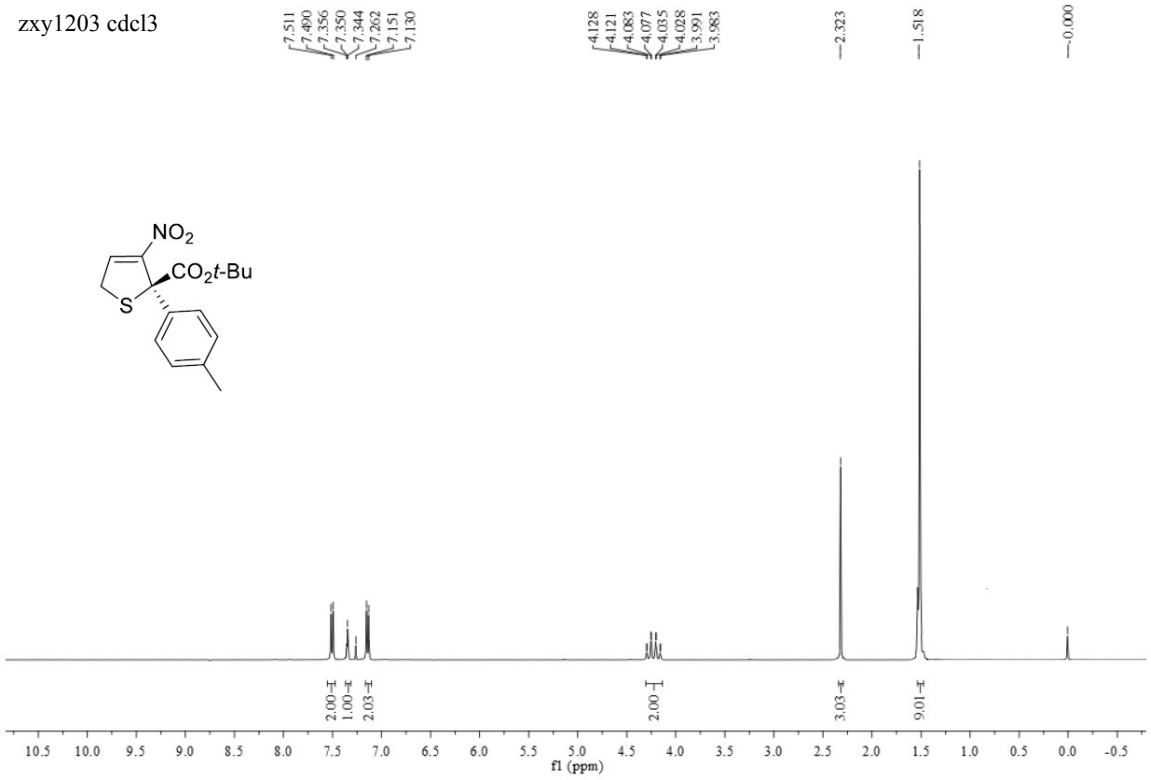

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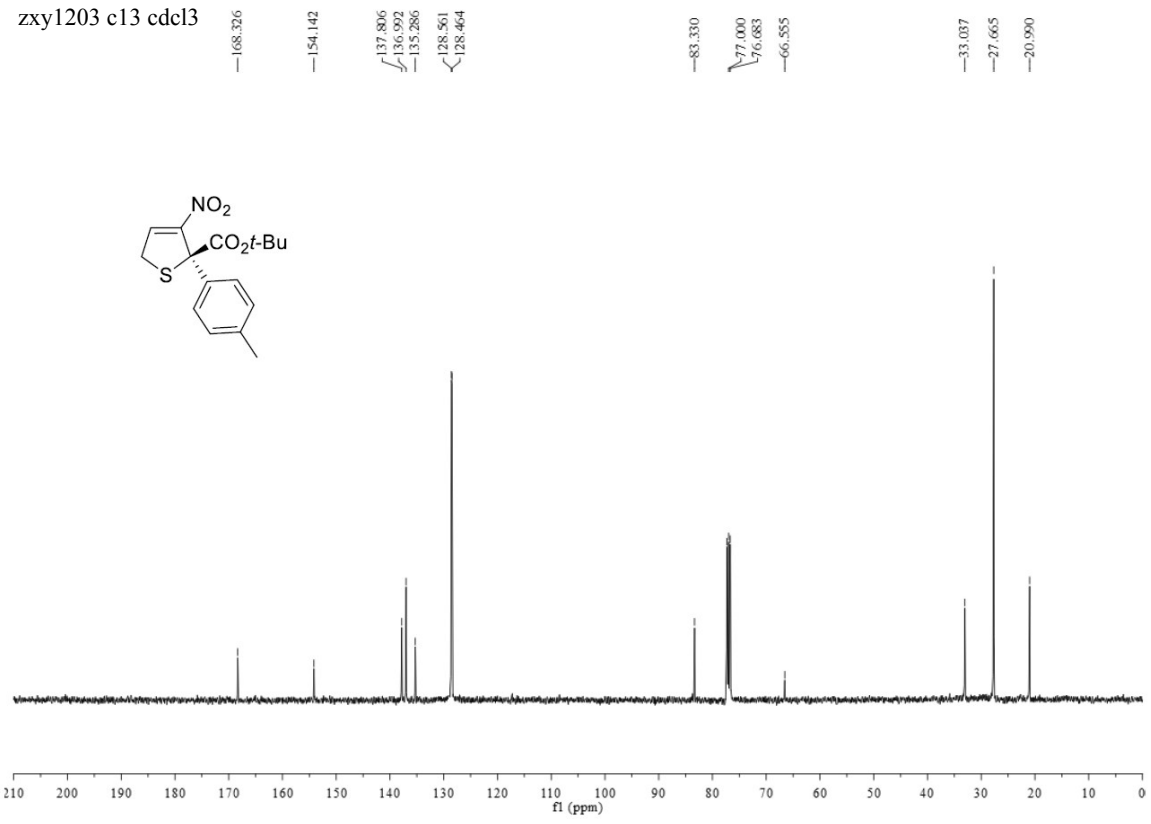

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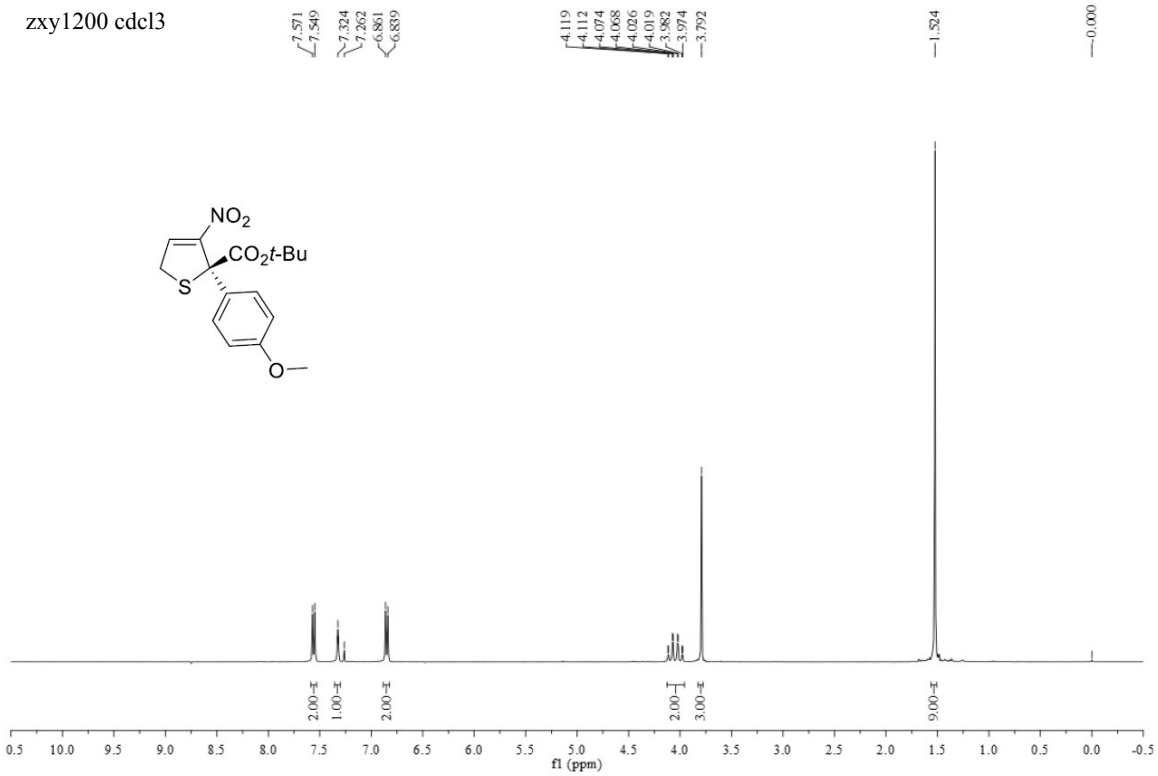

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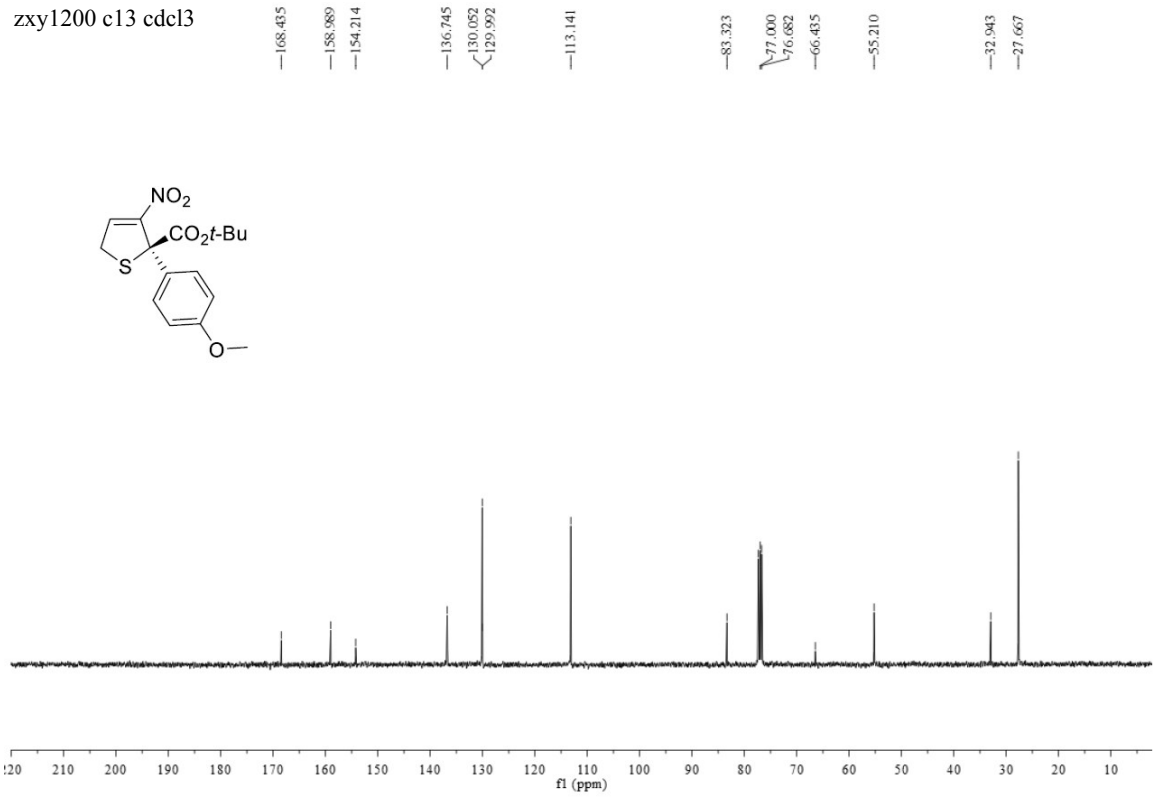

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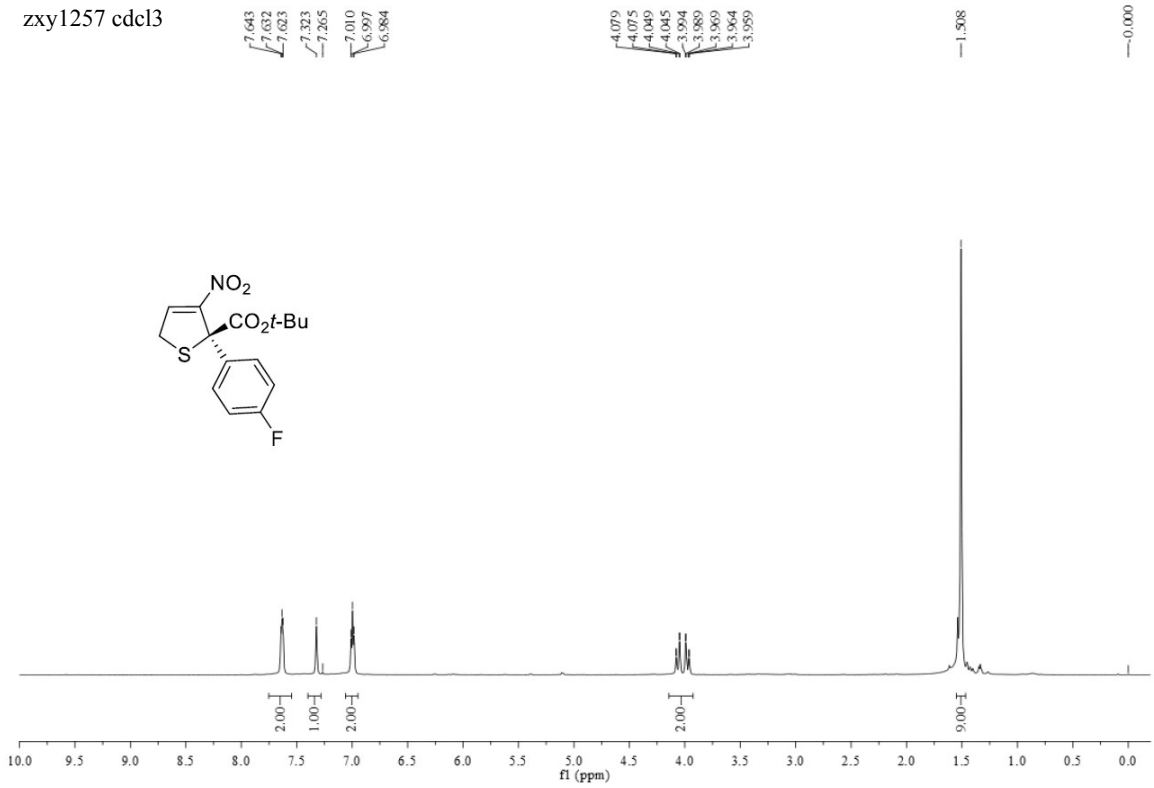

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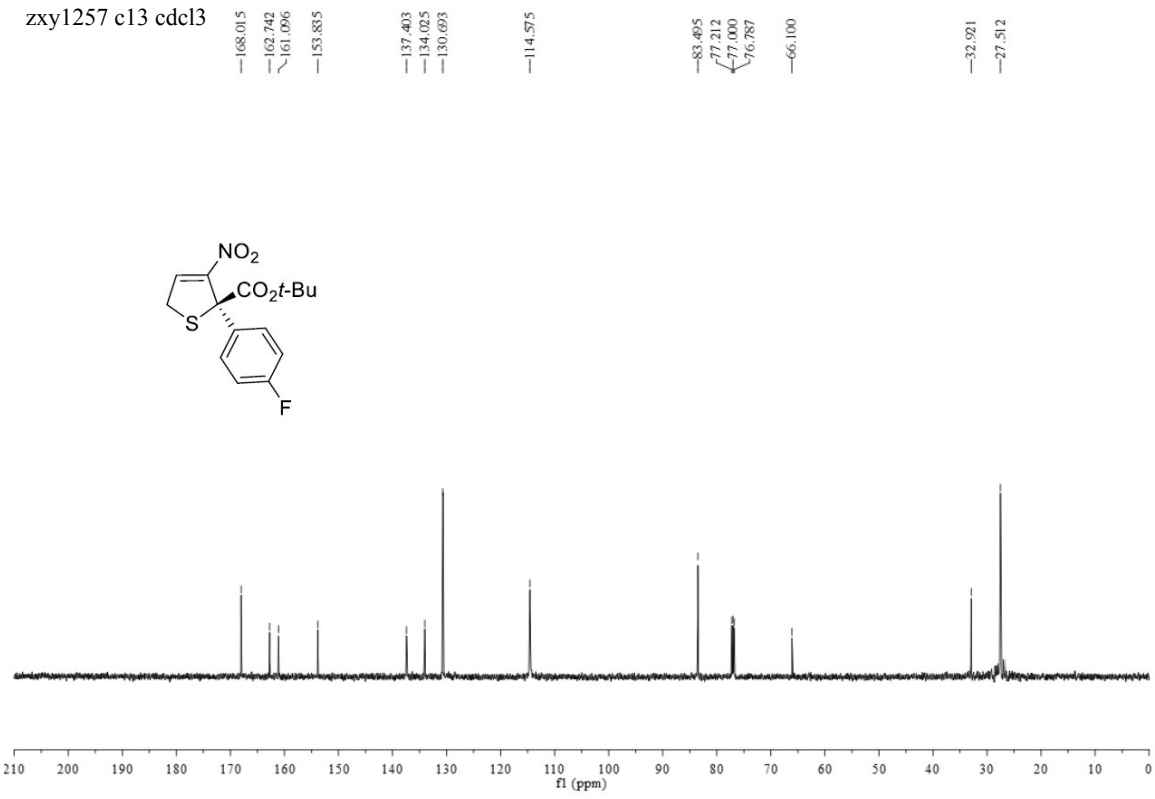

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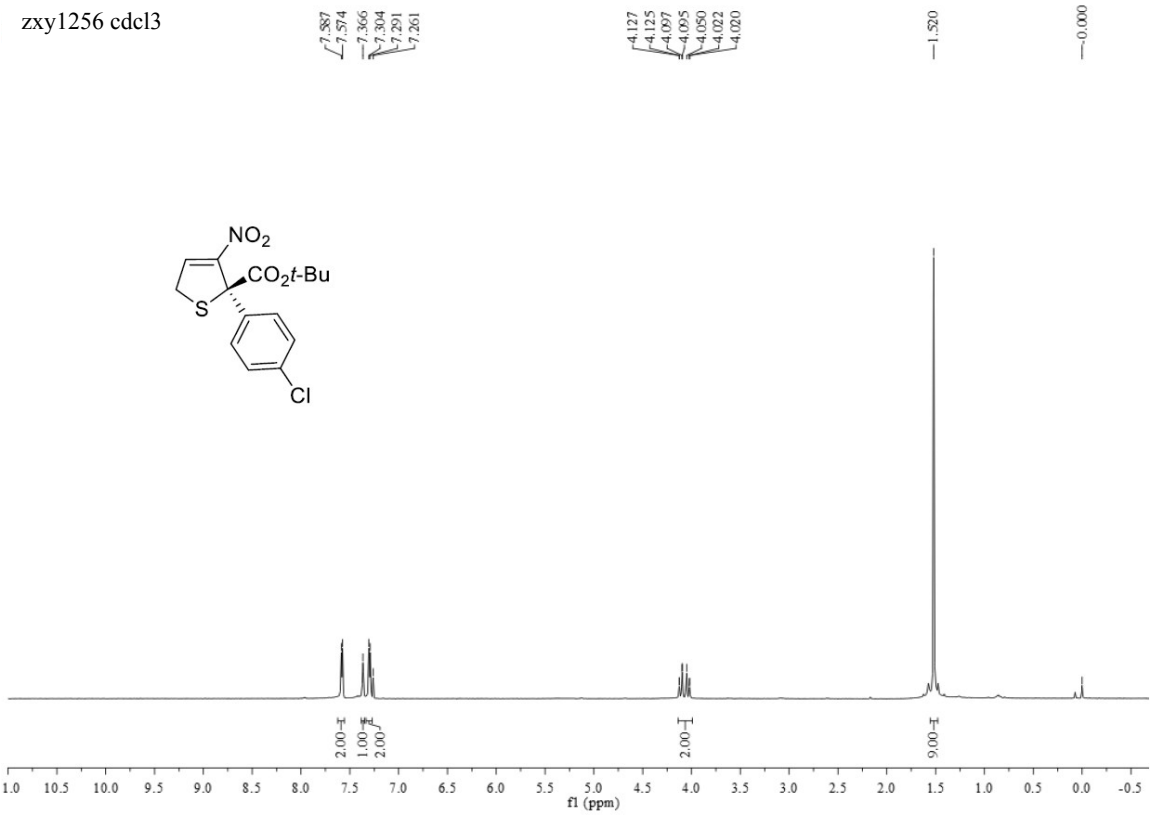

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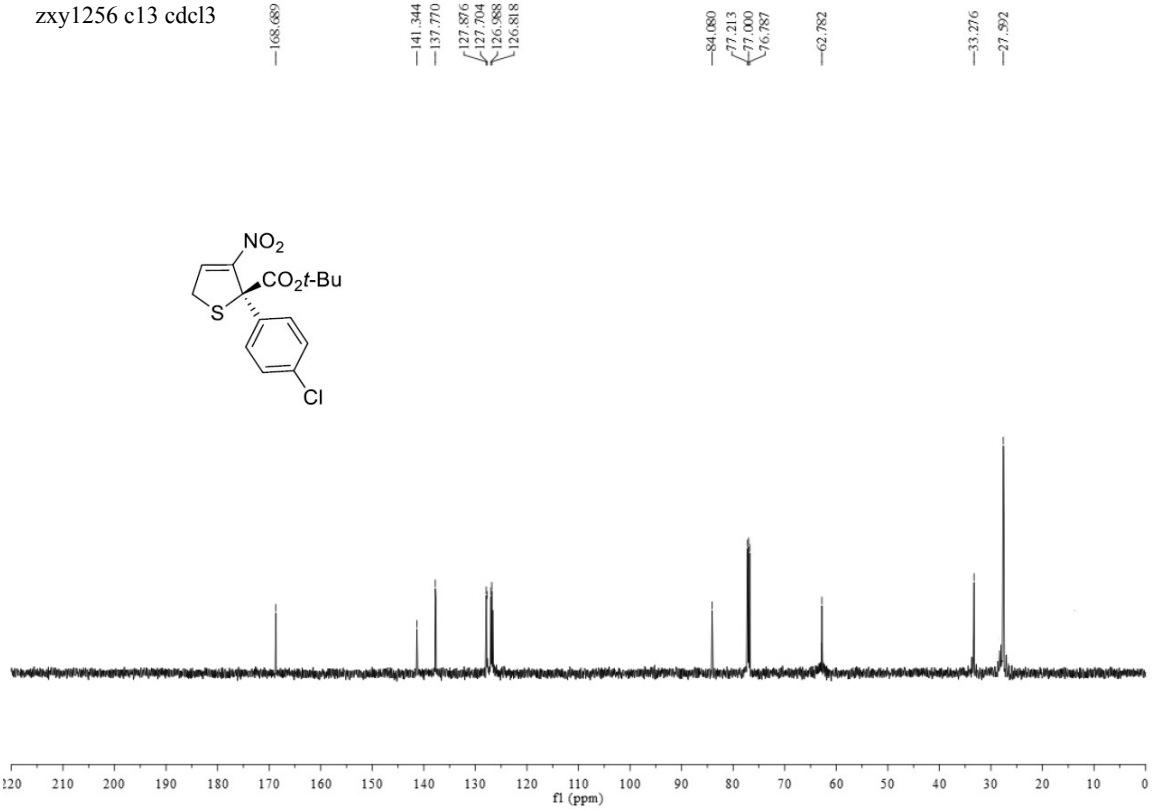

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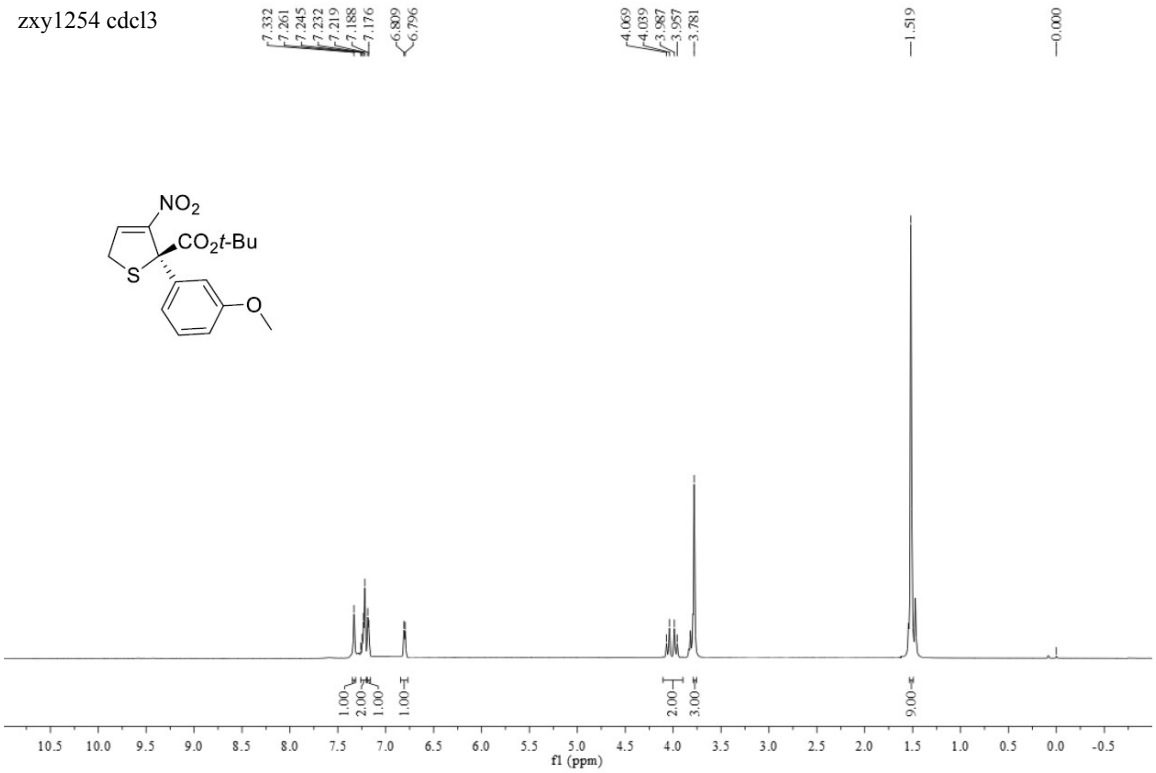

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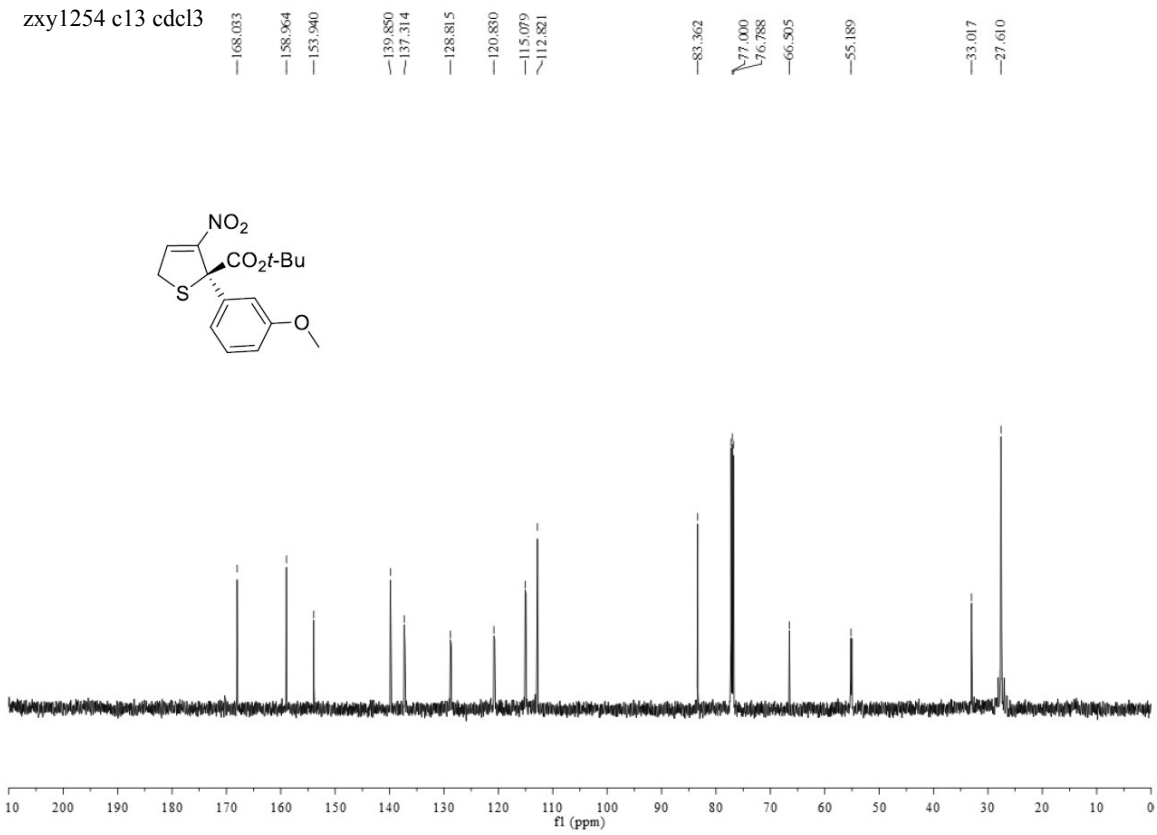

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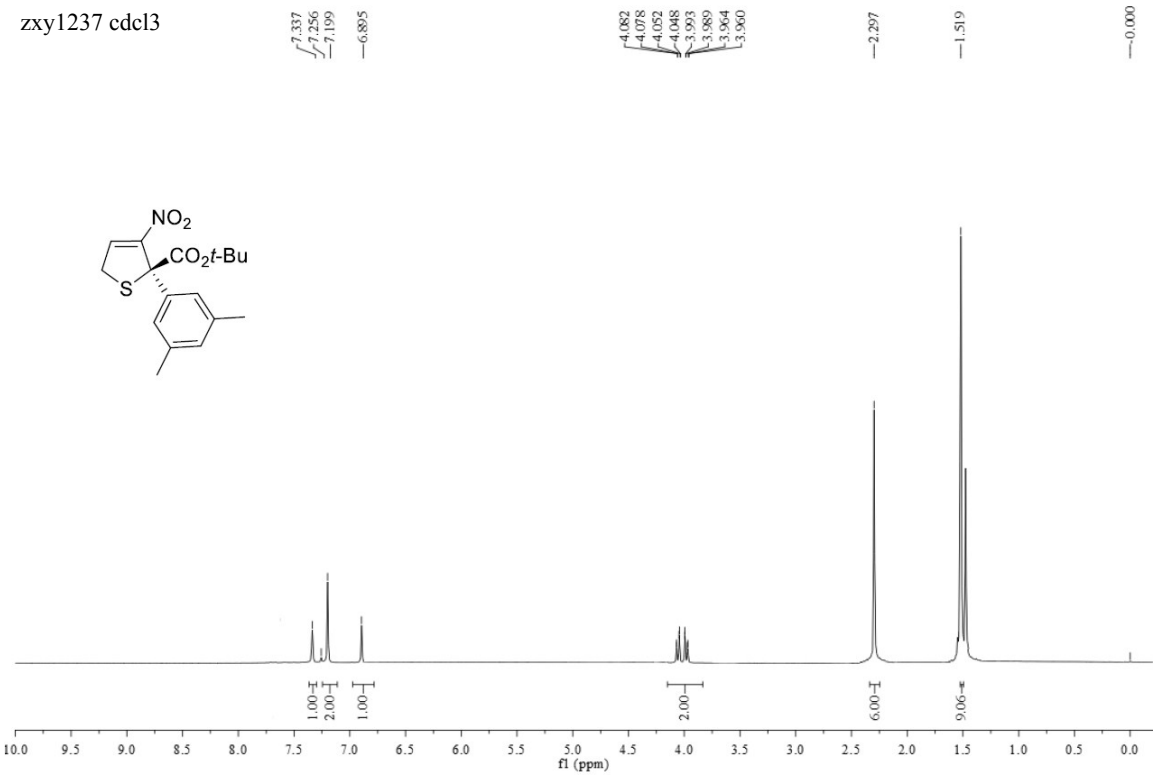

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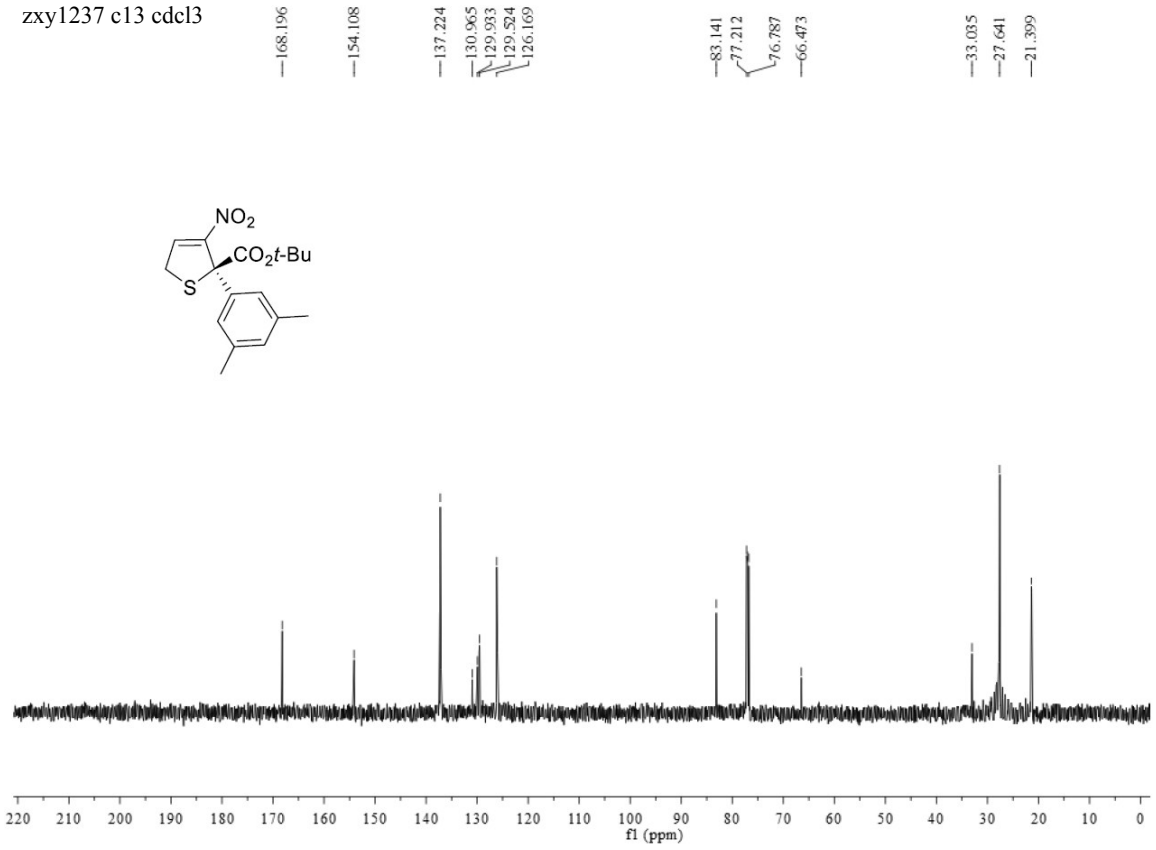

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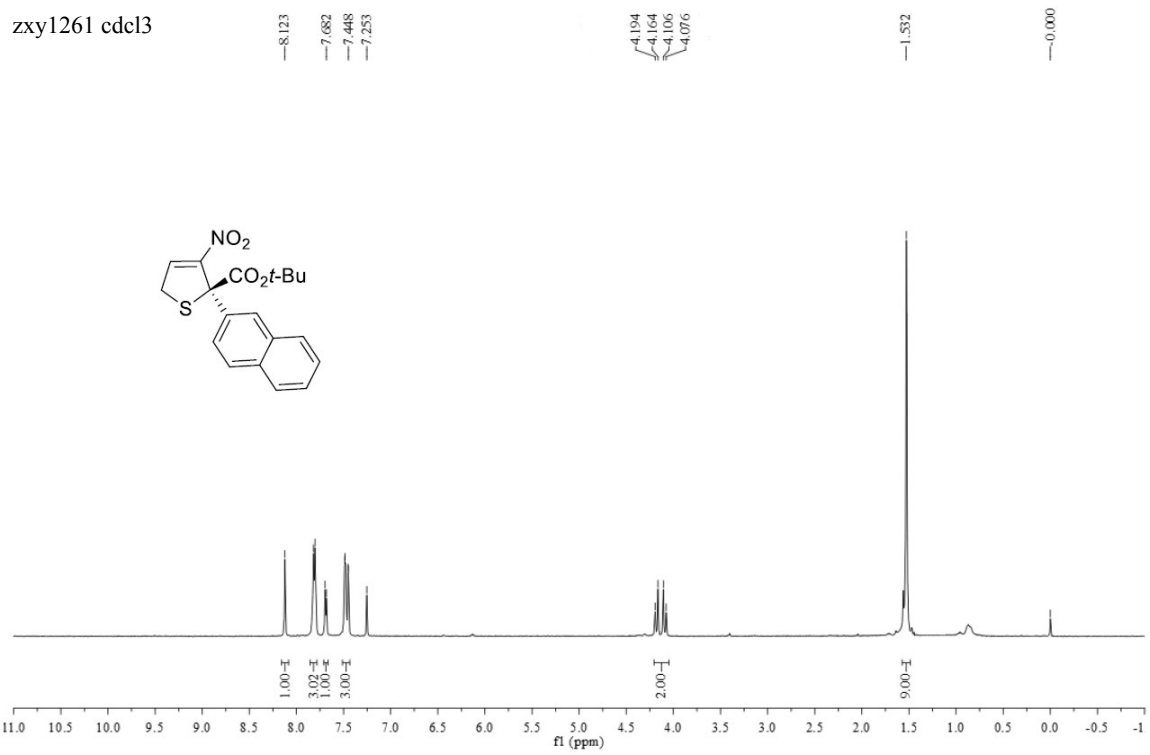

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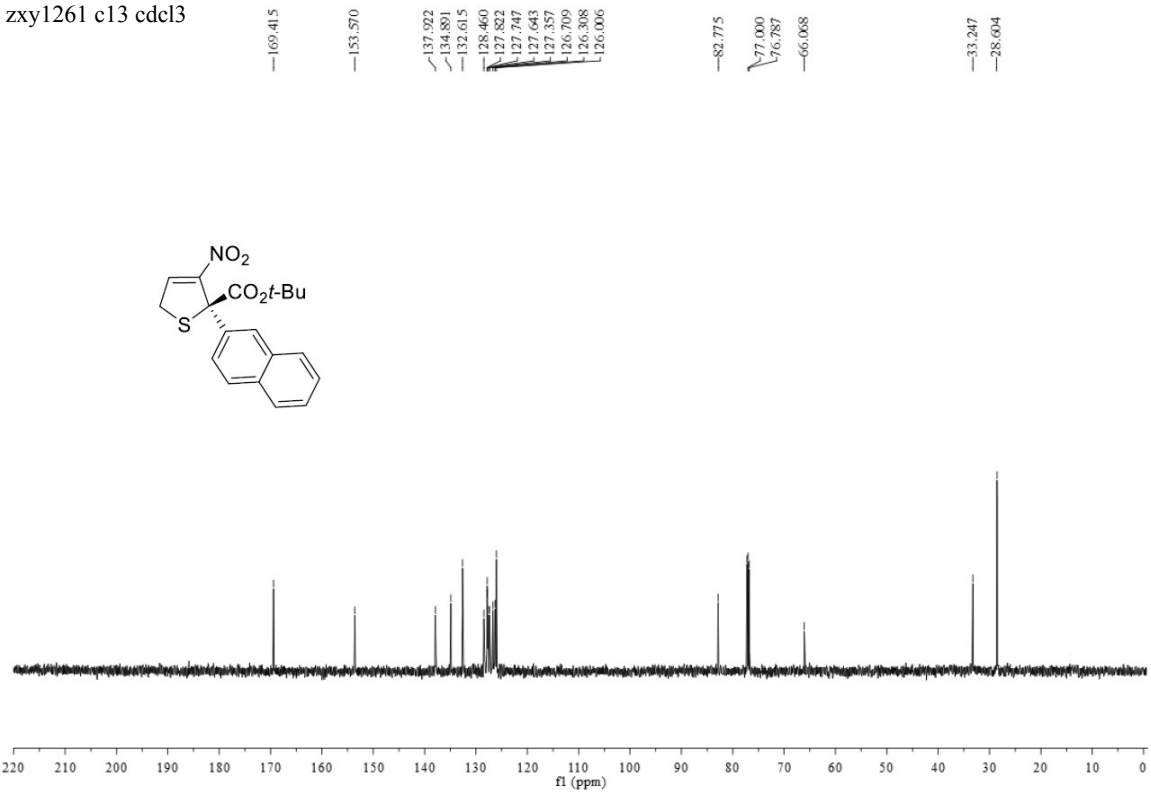

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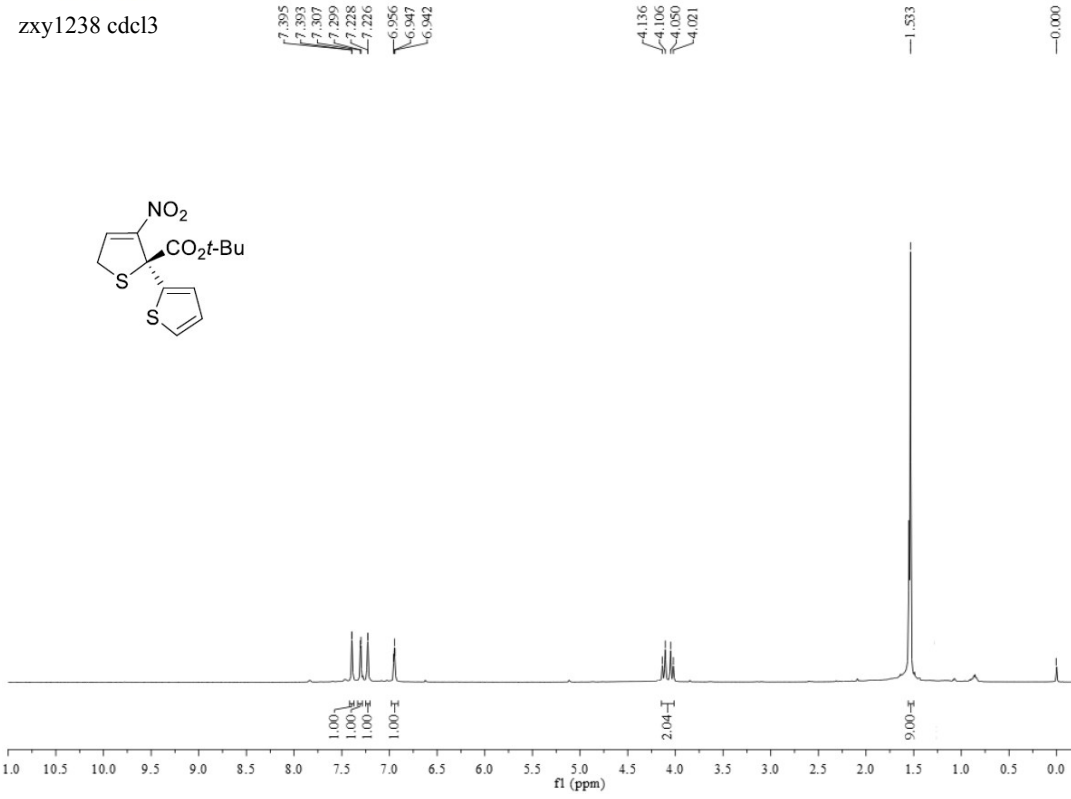

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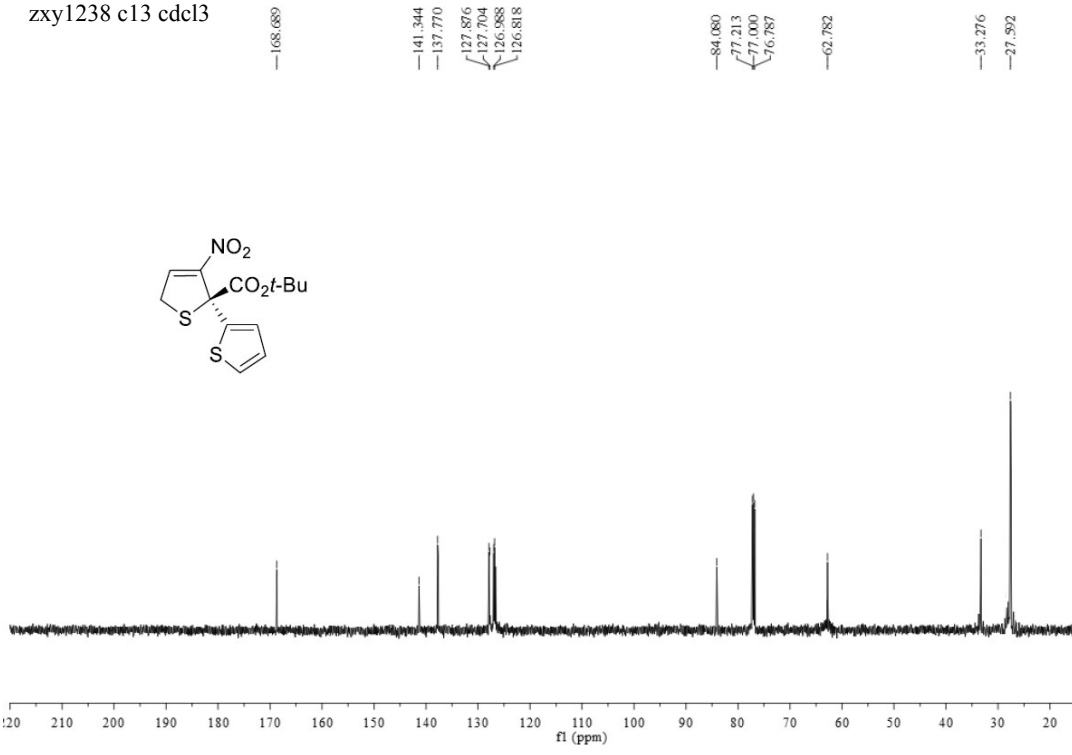

ZXY1260 cdcl3

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3.919
3.912
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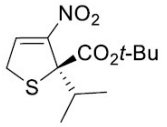
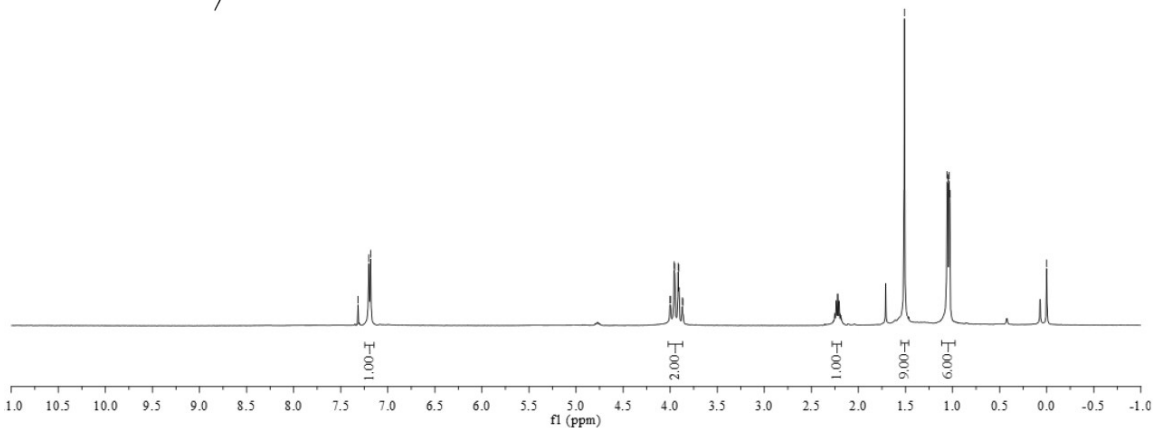
1.032
0.000





ZXY1260 C13 CDCl3

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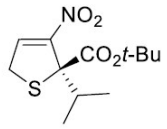
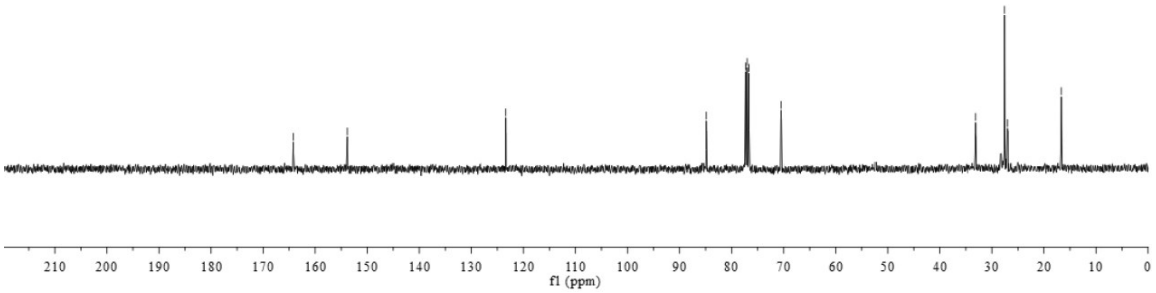
16.752





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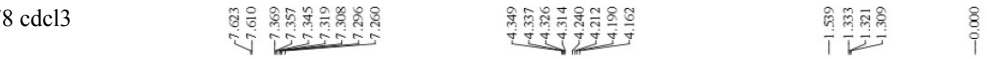

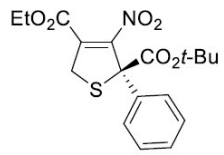

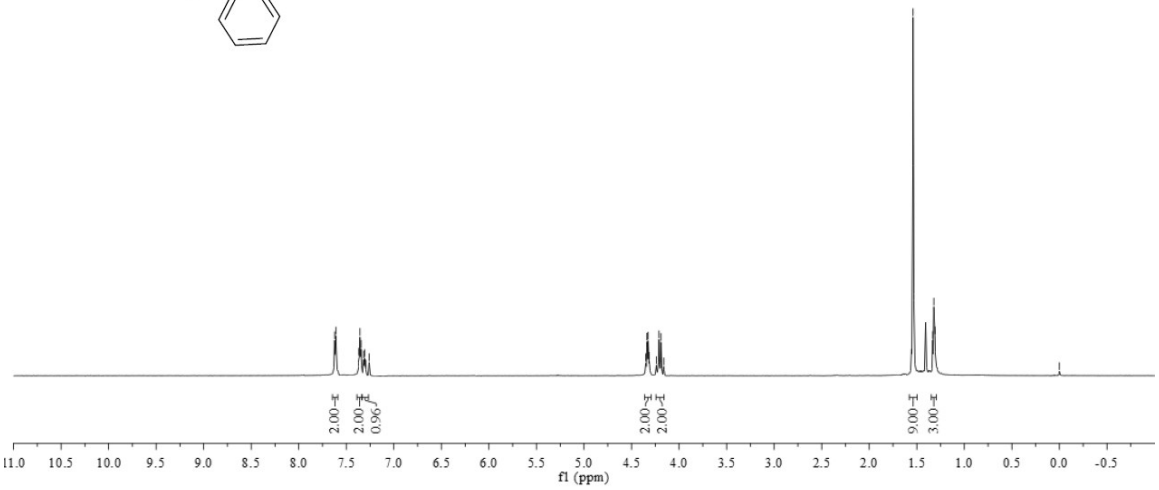

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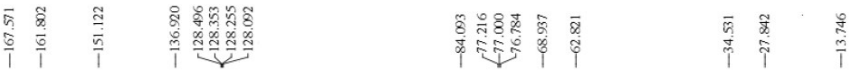

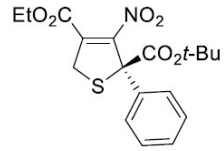

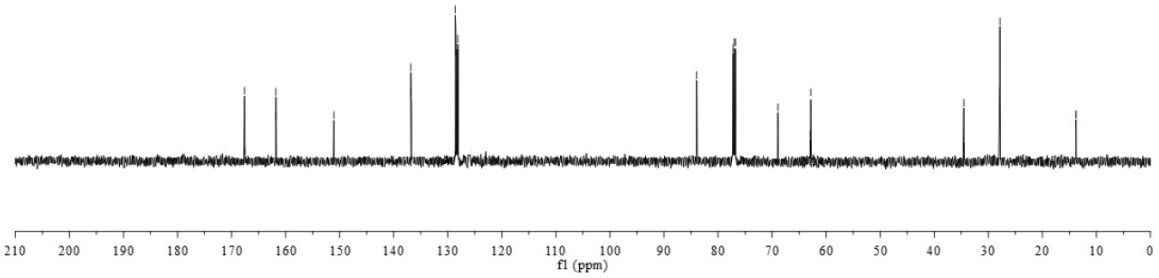

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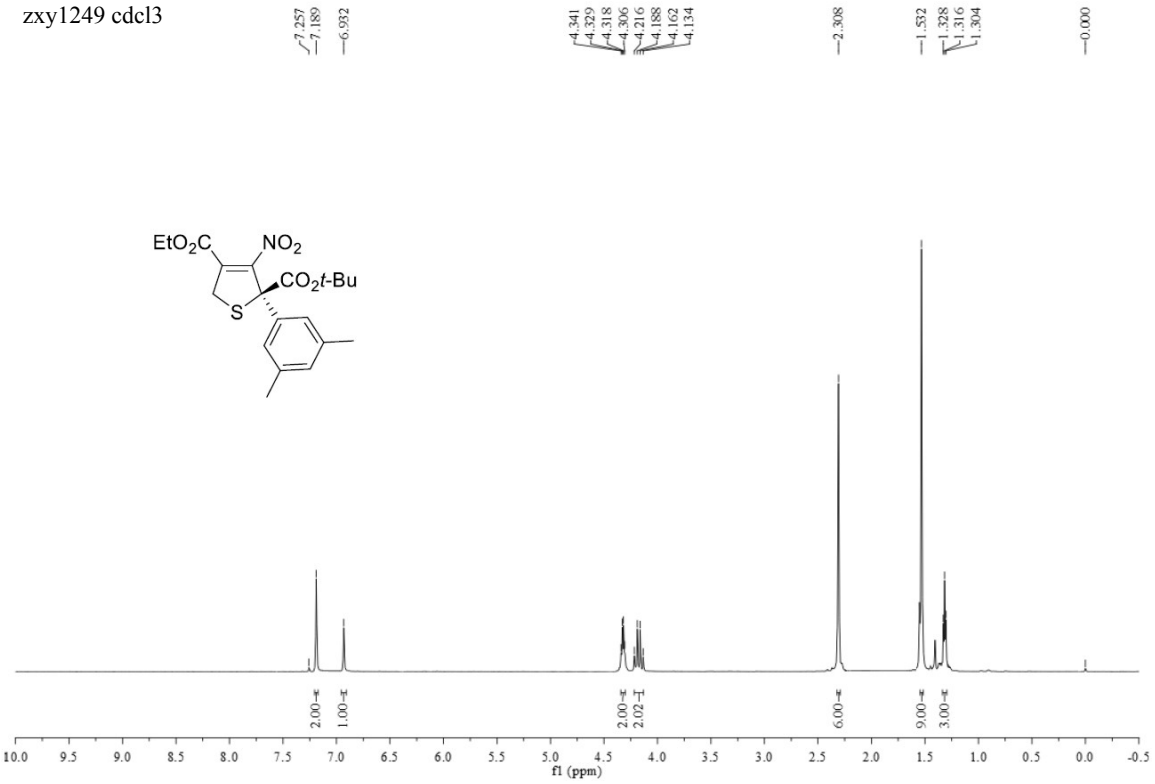

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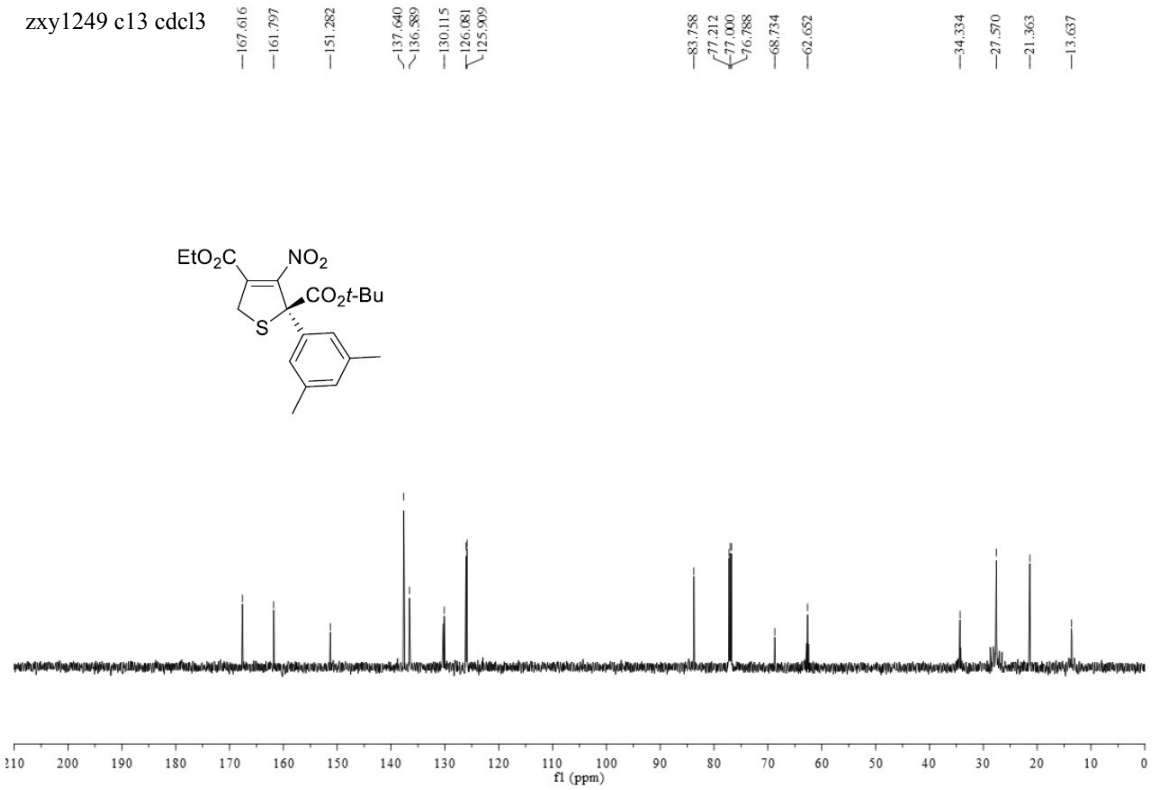

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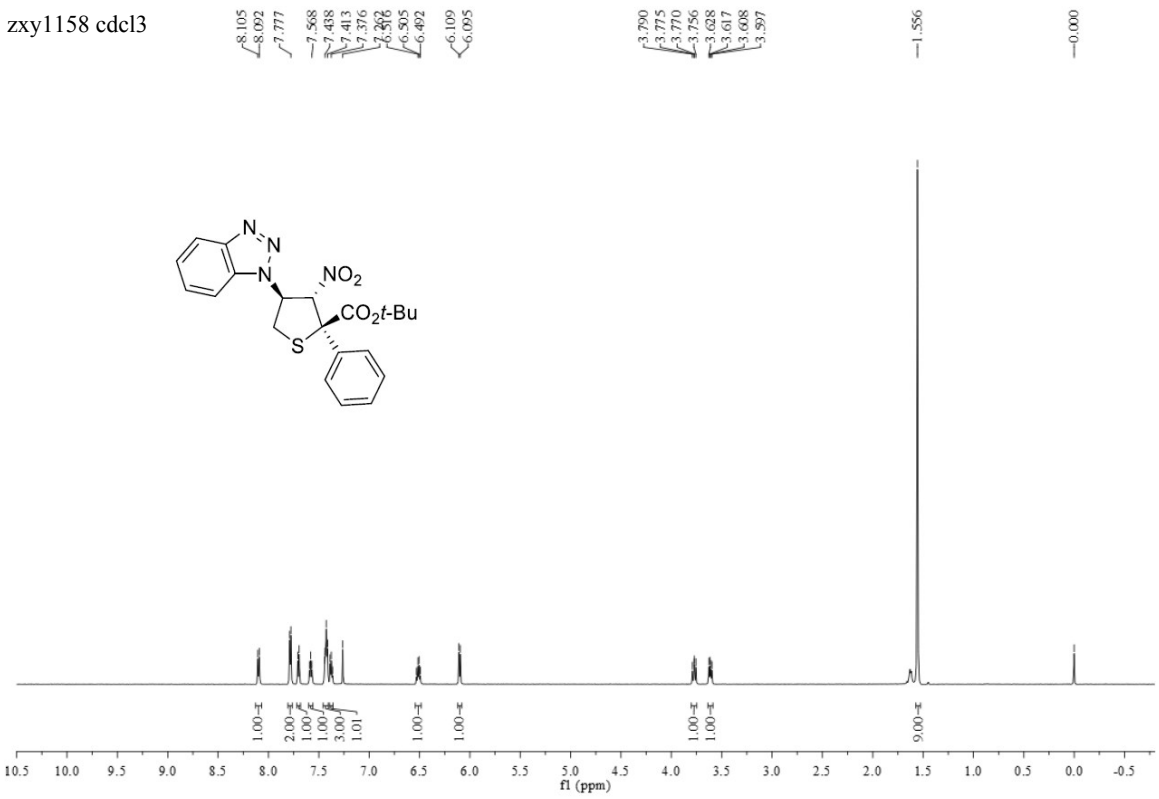

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