Supplementary Material (ESI) for New Journal of Chemistry

Asymmetric Organocatalytic Michael Addition of Azlactones to *cis*-1,2-Bis(phenylsulfonyl)ethene. A Simple Entry to Quaternary α-Amino Acids.

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Supporting Information

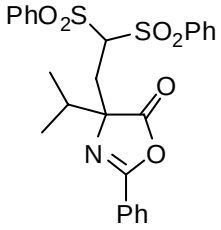
CONTENTS

General methods.

Chemicals and solvents were either purchased *puriss p.A.* from commercial suppliers or purified by standard techniques. For thin-layer chromatography (TLC), silica gel plates F254 were used and compounds were visualized by irradiation with UV light and/or by treatment with a solution of phosphomolybdic acid (25 g), $Ce(SO_4)_2 \cdot H_2O$ (10 g), conc. H_2SO_4 (60 mL), and H_2O (940 mL) followed by heating or by treatment with a solution of *p*-anisaldehyde (23 mL), conc. H_2SO_4 (35 mL), acetic acid (10 mL), and ethanol (900 mL) followed by heating. Flash chromatography was performed using silica gel (particle size 0.040-0.063 mm). Chemical shifts are given in ppm relative to tetramethylsilane (TMS) and the coupling constants *J* are given in Hz. The spectra were recorded in $CDCl_3$ as solvent at room temperature. TMS served as internal standard (δ = 0 ppm) for ^{1}H NMR, $CDCl_3$ was used as internal standard (δ = 77.0 ppm) for ^{13}C NMR and TFA was used as external standard for ^{19}F NMR. High-resolution mass spectra were recorded on a MicrOTOF spectrometer.

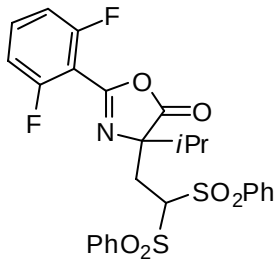
General procedure.

To a flask containing a solution of the oxazol-5-one (0.078 mmol, 1.5 equiv.) and the corresponding catalyst (0.0052 mmol, 0.1 equiv.) at the desired temperature in toluene (0.5 mL), 1,2-bis(phenylsulfonyl)ethylene (16 mg, 0.052 mmol, 1 equiv.) was added in one portion. The reaction mixture was stirred at this temperature after completion. The crude was purified by column chromatography to afford compound **3**.



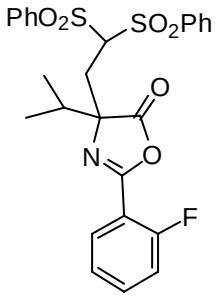
4-(2,2-Bis(phenylsulfonyl)ethyl)-4-isopropyl-2-phenyloxazol-5(4*H*)-one 3a

Colorless oil. **^{1}H NMR (300 MHz, $CDCl_3$): δ =** 8.08-8.05 (m, 2H), 8.01-7.98 (m, 2H), 7.83-7.81 (m, 2H), 7.64-7.51 (m, 6H), 7.44-7.39 (m, 2H), 5.05 (dd, *J*=8.2 Hz, *J'*=2.6 Hz, 1H), 2.89 (dd, *J*=16.4 Hz, *J'*=2.3 Hz, 1H), 2.74 (dd, *J*=16.1 Hz, *J'*=7.9 Hz, 1H), 2.08 (h, *J*=6.7 Hz, 1H), 0.98 (d *J*=6.7 Hz, 1H), 0.95 (d, *J*=6.7 Hz, 1H); **^{13}C NMR (75 MHz, $CDCl_3$): δ =** 206.9, 162.0, 137.3, 136.9, 134.7, 134.6, 133.1, 130.0, 129.7, 129.1, 128.8, 128.2, 79.3, 72.3, 37.4, 30.9, 29.5, 16.4,; **HRMS (ESI):** calcd. for $[M+H]^+$ ($C_{26}H_{26}NO_6S_2$) requires 512.1196, found 512.1198. **HPLC** (Chiralpak IA, *n*-hexane: *i*-PrOH = 80:20, λ=254 nm, 1.0 mL/min): t_R = 9.5, 12.4 min. $[\alpha]_D^{25}$= -11.2 (c=0.77, $CHCl_3$, 93% ee).



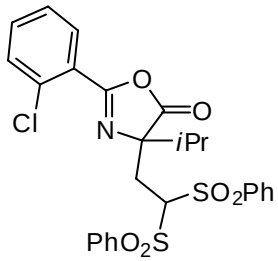
4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2,6-difluorophenyl)-4-isopropyloxazol-5(4*H*)-one 3b

Colorless oil. **^{1}H-RMN** (300 MHz. $CDCl_3$, TMS_{int}): δ(ppm)= 8.01-7.93 (m, 4H), 7.73-7.66 (m, 2H), 7.61-7.50 (m, 5H), 7.10-7.02 (m, 2H), 5.01 (dd, J_1=2.3 Hz, J_2=7.9 Hz, 1H), 2.95 (dd, J_1=2.5 Hz, J_2=16.4 Hz, 1H), 2.76 (dd, J_1=7.8 Hz, J_2=16.3 Hz, 1H), 2.15-2.03 (m, 1H), 0.97 (t, J=7.0 Hz, 6H). **^{19}F-NMR** (376 MHz. $CDCl_3$): δ(ppm)= -107.6- -107.7. **^{13}C-RMN** (100 MHz. $CDCl_3$): δ(ppm)= 178.2, 162.5 (d, J=5.4 Hz), 159.9 (d, J=5.4 Hz), 155.5, 137.8, 136.1, 134.8, 134.6, 134.1, 134.0, 133.9, 130.6, 129.3, 129.2, 129.0, 112.3 (dd, J_1=3.1 Hz, J_2=21.9 Hz), 78.7, 72.3, 37.1, 28.9, 16.4, 16.1. **HPLC** (Chiralpak® IA, 1 $mLmin^{-1}$, hexane:IPA 90:10, 254 nm): t_R= 25.7 (maj.), 27.3 min. **HRMS [2M+K]$^+$:** Calculated for $[C_{52}H_{46}F_4N_2KO_{12}S_4]^+$: 1133.1501; found: 1133.1503. $[\alpha]_D^{25}$= -12.7 (c=0.9, $CHCl_3$, 92% ee).



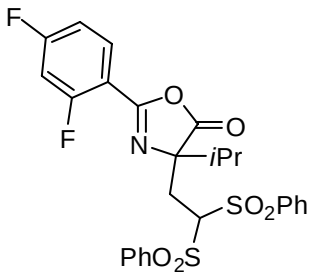
4-(2,2-Bisphenylsulfonyl)ethyl)-2-(2-fluorophenyl)-4-isopropyloxazol-5(4*H*)-one 3c

Colorless oil. **^{1}H NMR (300 MHz, $CDCl_3$, TMS_{int}): δ (ppm) =** 7.99-7.88 (m, 5H), 7.69-7.55 (m, 5H), 7.51-7.46 (m, 2H), 7.31-7.28 (m, 2H), 7.25-7.22 (m, 2H), 5.08 (dd, *J*=7.9 Hz, *J'*=2.6 Hz, 1H), 2.90 (dd, *J*=16.4 Hz, J'= 2,6 Hz, 1H), 2.76 (dd, *J*=16.4 Hz, J'= 7.9 Hz, 1H), 2.09 (h, *J*=6.7 Hz, 1H), 0.96 (d, *J*=6.7 Hz, 3H), 0.95 (d, *J*=6.7 Hz, 3H). **^{19}F-NMR** (376 MHz. $CDCl_3$): δ(ppm)= -107.9- -108.1. **^{13}C NMR (75 MHz, $CDCl_3$, TMS_{int}): δ (ppm) =** 178.6, 161.4 (d, *J*=261.5 Hz), 158.6 (d, *J*=5.7 Hz), 136.1 (d, *J*=90.1 Hz), 134.7 (d, *J*=4.6 Hz), 134.5 (d, *J*=8.8 Hz), 130.9, 130.2, 129.5, 129.2, 128.9, 124.5 (d, *J*=3.8 Hz), 117.1 (d, *J*=20.7 Hz), 78.9, 72.3, 37.4, 29.3, 16.4, 16.2; ^{19}F NMR (100 MHz, $CDCl_3$): δ (ppm) = -107.96-(-108.04). **HRMS (ESI):** $[2M+Na]^+$ calc. for $C_{52}H_{48}F_2N_2NaO_{12}S_4$ requires 1081.1950, found 1081.1935. **HPLC** (Chiralpak IA, *n*-hexane: *i*-PrOH = 90:10, λ=254 nm, 1.0 mL/min): t_R = 11.6 min, 14.2 min. $[\alpha]_D^{25}$= -9,6 (c=0.86, $CHCl_3$, 92% ee).



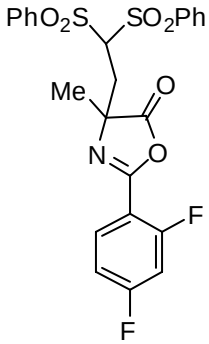
4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2-chlorophenyl)-4-isopropyloxazol-5(4*H*)-one 3d

Colorless oil. **^{1}H-RMN** (300 MHz. $CDCl_3$, TMS_{int}): δ(ppm)= 8.00-7.85 (m, 5H), 7.76-7.45 (m, 8H), 7.44-7.35 (m, 1H), 5.11 (dd, J_1=2.3 Hz, J_2=8.2 Hz, 1H), 2.92 (dd, J_1=2.3 Hz, J_2=16.4, 1H), 2.76 Hz (dd, J_1=8.2 Hz, J_2=16.4 Hz, 1H), 2.15-2.02 (m, 1H), 0.97 (d, J=6.7 Hz, 3H), 0.96 (d, J=6.7 Hz). **^{13}C-RMN** (100 MHz. $CDCl_3$): δ(ppm)= 178.7, 160.0, 140.3, 137.6, 136.5, 134.9, 134.7, 134.7, 133.9, 133.0, 131.7, 131.4, 130.3, 129.8, 129.4, 129.2, 128.9, 128.4, 127.0, 124.7, 79.1, 73.0, 37.5, 29.1, 16.4, 16.3. **HPLC** (Chiralpak® IA, 1 mLmin^{-1}, hexane:IPA 90:10, 254 nm): t_R= 21.9, 25.4 (maj.) min. **HRMS [M+H]$^+$:** Calculated for $[C_{26}H_{25}ClNO_6S_2]^+$: 546.0806; found: 546.0795. $[\alpha]_D^{25}$= -5,6 (c=0.9, $CHCl_3$, 84% ee).



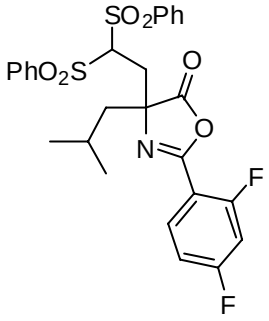
4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2,4-difluorophenyl)-4-isopropyloxazol-5(4*H*)-one 3e

Colorless oil. **^{1}H-RMN** (300 MHz. $CDCl_3$, TMS_{int}): δ(ppm)= 7.99-7.89 (m, 5H), 7.74-7.48 (m, 6H), 7.06-6.96 (m, 2H), 5.05 (dd, J_1=2.6 Hz, J_2=7.9 Hz, 1H), 2.89 (dd, J_1=2.6 Hz, J_2=16.4 Hz, 1H), 2.73 (dd, J_1=7.9 Hz, J_2=16.4 Hz, 1H), 2.15-2.00 (m, 1H), 0.95 (d, J=6.7 Hz, 6H). **^{19}F-NMR** (376 MHz. $CDCl_3$): δ(ppm)= -100.8- -101.0, -102.9- -103.1. **^{13}C-RMN** (100 MHz. $CDCl_3$): δ(ppm)= 178.3, 166.9 (d, J=11.9 Hz), 164.4 (d, J=11.5 Hz), 163.6 (d, J=12.3 Hz), 161.0 (d, J=12.7 Hz), 157.9 (d, J=6.5 Hz), 140.3, 137.5, 136.5, 134.7 (d, J=9.2 Hz), 132.5 (dd, J_1=2.3 Hz, J_2=10.4 Hz), 130.2, 129.8, 129.5, 128.9, 128.5, 112.2 (dd, J_1=3.8 Hz, J_2=21.9 Hz), 105.6 (t, J=25.1 Hz), 79.0, 72.3, 37.4, 29.2, 16.4, 16.2. **HPLC** (Chiralpak® IA, 1 mLmin^{-1}, hexane:IPA 80:20, 254 nm): t_R= 11.3, 13.6 (maj.) min. **HRMS [2M+Na]$^+$:** Calculated for $[C_{52}H_{46}F_4N_2NaO_{12}S_4]^+$: 1117.1762; found: 1117.1756. $[\alpha]_D^{25}$= -10.3 (c=1.1, $CHCl_3$, 88% ee).



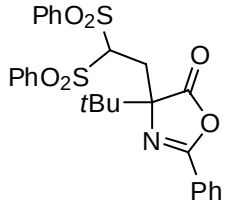
4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2,4-difluorophenyl)-4-methyloxazol-5(4*H*)-one 3g

Colorless oil. **^{1}H NMR (300 MHz, $CDCl_3$, TMS_{int}): δ (ppm) =** 8.03-7.87 (m, 4H), 7.60-7.48 (m, 6H), 7.06-6.94 (m, 3H), 5.05 (dd, J_1=5.71 J_1=5.71, J_2=4.10 Hz, 1H), 2.80-2.76 (m,2H), 1.52 (s, 3H); **^{13}C NMR (75 MHz, $CDCl_3$, TMS_{int}): δ (ppm) =** 179.8, 138.6, 137.6, 135.8, 133.6, 133.5, 131.2, 130.8, 130.2, 130.2, 130.1, 113.4, 113.2, 113.2, 106.7, 79.8, 67.3, 33.1, 26.7 **^{19F} NMR (300 MHz, $CDCl_3$): δ (ppm)=** -100,55 (m), -102.71 (m) **HRMS (ESI):** $[M+H]^+$ calc. for $C_{24}H_{20}F_2NO_6S_2$ requires 520.0695, found 520.0696. **HPLC** (Chiralpak IA, *n*-hexane: *i*-PrOH = 90:10, λ=254 nm, 1.0 mL/min): t_R = 26.8 min, 33.3 min.



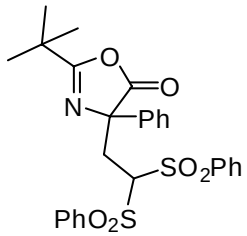
4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2,4-difluorophenyl)-4-isobutyloxazol-5(4*H*)-one 3h

Colorless oil. **^{1}H NMR (300 MHz, $CDCl_3$): δ =** 8.02-7.98 (m, 2H), 7.96-7.90 (m, 3H), 7.75-7.64 (m, 2H), 7.63-7.56 (m, 2H), 7.56-7.50 (m, 2H), 7.05-7.96 (m, 2H), 5.05 (dd, J_1=3.8 H, J_2=5.8 H, 1H), 2.78-2.74 (m, 2H), 1.79 (dd, J_1=5.6 H, J_2=14.2 H, 1H), 1.69 (dd, J_1=6.5 H, J_2=14.2 H, 1H, 1.55-1.45 (m, 1H), 0.84 (t, J=6.5 H, 6H). **^{19}F-NMR (376 MHz. $CDCl_3$): δ(ppm) =** -100.2- -100.3 (m, 1F), -102.5- -102.6 (m, 1F).**^{13}C NMR (75 MHz, $CDCl_3$): δ =** 179.0, 167.0, 166.9, 164.4, 164.3, 163.6, 163.5, 161.0, 160.9, 157.3, 157.2, 137.6, 136.7, 134.7 (d, J=6.1 Hz), 132.4 (d, J=10.0 Hz), 130.2, 129.7, 129.1 (d, J=12.7 Hz), 112.2 (d, J=22.2 Hz), 105.7 (t, J=25.3 Hz), 18.7, 69.6, 47.1, 32.1, 24.6, 24.0, 23.4. **HRMS (ESI):** calcd. for $[M+H]^+$ ($C_{27}H_{26}F_2NO_6S_2$) requires 562.1164, found 562.1158. **HPLC** (Chiralpak IA, *n*-hexane: *i*-PrOH = 90:10, λ=254 nm, 1.0 mL/min): t_R = 19.9, 23.2 (maj.) min. $[\alpha]_D^{25}$**=** 0.5 (c=1.33, $CHCl_3$, 74% ee).



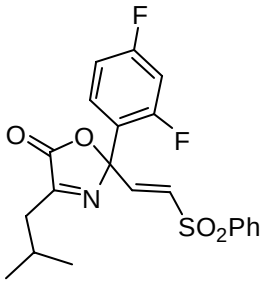
4-(2,2-Bis(phenylsulfonyl)ethyl)-4-*tert*-butyl-2-phenyloxazol-5(4*H*)-one 3i

Colorless oil. **^{1}H NMR (300 MHz, $CDCl_3$, TMS_{int}): δ (ppm) =** 8.08-7.98 (m, 4H), 7.79-7.76 (m, 2H), 7.71-7.52 (m, 7H), 7.41-7.36 (m, 2H), 5.03 (d, *J*=8.8 Hz, 1H), 2.99 (d, *J*=16.4 Hz, 1H), 2.68-2.59 (m, 1H), 0.98 (s, 9H); **^{13}C NMR (75 MHz, $CDCl_3$, TMS_{int}): δ (ppm) =** 178.7, 162.1, 137.3, 137.2, 134.7, 134.5, 133.1, 129.9, 129.7, 129.2, 128.9, 128.8, 128.2, 125.7, 79.6, 73.9, 40.2, 28.0, 23.9. **HRMS (ESI):** $[2M+Na]^+$ calc. for $C_{54}H_{54}N_2NaO_{12}S_4$ requires 1073.2452, found 1073.2447. **HPLC** (Chiralpak IA, *n*-hexane: *i*-PrOH = 90:10, λ=254 nm, 1.0 mL/min): t_R = 7.8 min, 11.1 min. $[\alpha]_D^{25}$**=** -5.2 (c=0.9, $CHCl_3$, 72% ee).



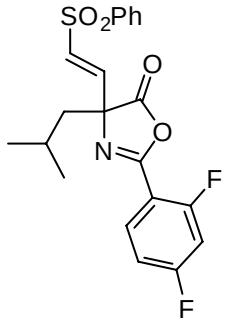
4-(2,2-Bis(phenylsulfonyl)ethyl)-2-tertbutyl-4-phenyloxazol-5(4*H*)-one 3j

Colorless oil. **^{1}H-RMN** (300 MHz. $CDCl_3$, TMS_{int}): δ(ppm)= 8.04-7.99 (m, 2H), 7.82-7.48 (m, 8H), 7.46-7.40 (m, 2H), 7.33-7.28 (m, 1H), 4.99-4.94 (m, 1H), 3.02-2.97 (m, 2H), 1.36 (s, 9H). **^{13}C-RMN** (100 MHz. $CDCl_3$): δ(ppm)= 178.3, 172.3, 138.4, 137.7, 136.9, 134.5, 130.3, 129.4, 129.4, 129.1, 129.0, 128.9, 128.7, 125.2, 79.2, 69.8, 34.4, 29.7, 26.8. **HPLC** (Chiralpak® IA, 1 $mLmin^{-1}$, hexane:IPA 80:20, 254 nm): t_R= 7.9, 9.7 (maj.) min. **HRMS $[2M+Na]^+$:** Calculated for $[C_{54}H_{54}N_2NaO_{12}S_4]^+$: 1073.2452; found: 1073.2450. $[\alpha]_D^{25}$**=** +10.3 (c=0.6, $CHCl_3$, 82% ee).



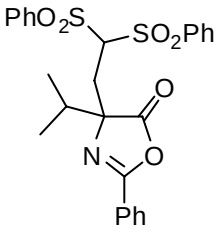
(*E*)-2-(2,4-Difluorophenyl)-4-isobutyl-2-(2-(phenylsulfonyl)vinyl)oxazol-5(2*H*)-one 5h

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.93-7.90 (m, 2H), 7.67-7.62 (m, 1H), 7.57-7.53 (m, 1H), 7.48-7.40 (m, 1H), 6.93-6.80 (m, 3H), 6.61 (dd, J_1=3.2 Hz, J_2=12.3 Hz, 1H), 6.52 (d, J=12.3 Hz, 1H), 2.57 (d, J=7.0 Hz, 2H), 2.33-2.23 (m, 1H), 1.00 (d, J=6.5 Hz, 6H). **^{19}F-NMR (376 MHz. $CDCl_3$): δ(ppm) =** -106.3- -106.5(m, 1F), -106.6- -106.8 (m, 1F). **^{13}C NMR (75 MHz, $CDCl_3$): δ =** 164.9, 137.1, 134.8, 133.8, 132.4, 129.2, 129.0, 126.7, 111.3 (d, J=22.2 Hz), 104.8 (t, J=24 H), 36.6, 26.1, 22.5, 22.4. **HRMS (ESI):** calcd. for $[M+H]^+$ ($C_{21}H_{20}F_2NO_4S$) requires 420.1076, found 420.1072



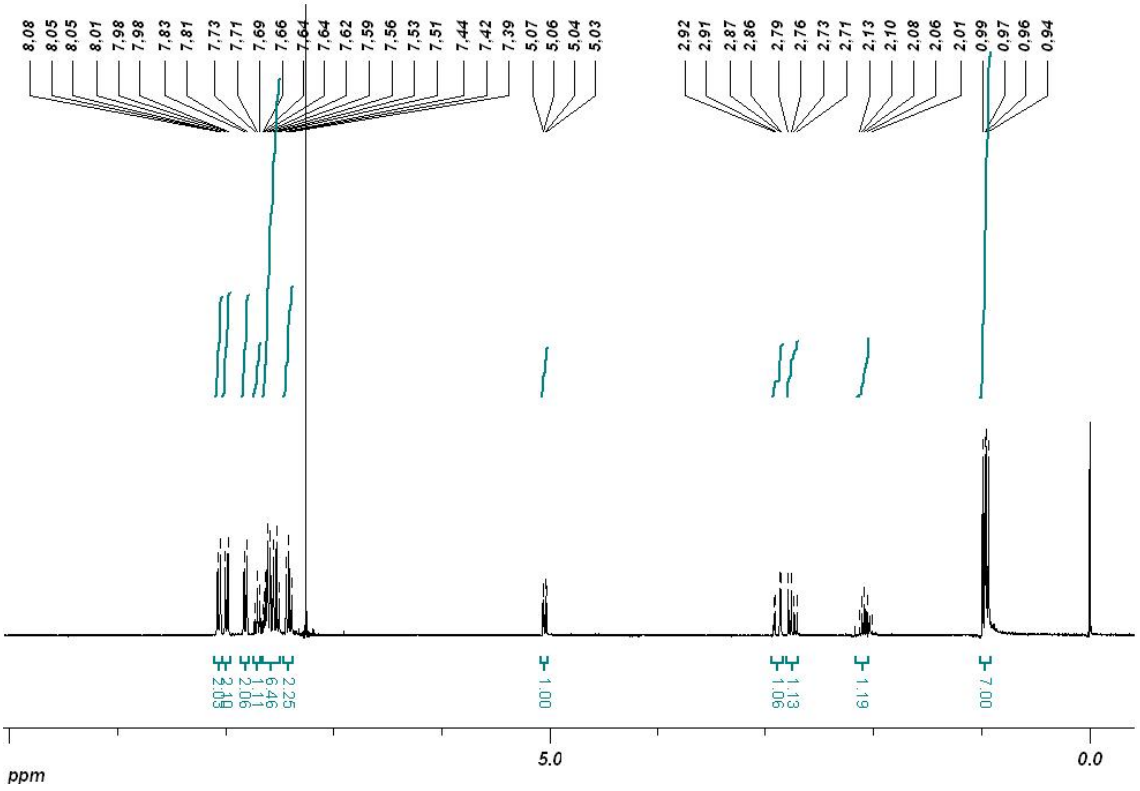
(*E*)-2-(2,4-Difluorophenyl)-4-isobutyl-4-(2-(phenylsulfonyl)vinyl)oxazol-5(4*H*)-one 4h

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.08-7.90 (m, 3H), 7.70-7.50 (m, 3H), 7.05-6.95 (m, 2H), 6.43 (d, J=11.9 Hz, 1H), 6.29 (d, J=11.9 Hz, 1H), 2.12 (dd, J_1=5.4 Hz, J_2=13.9 Hz, 1H), 1.96 (dd, J_1=6.5 Hz, J_2=13.9 Hz, 1H), 1.82-1.75 (m, 1H), 0.98 (d, J=6.5 Hz, 3H), 0.96 (d, J=6.5 Hz, 3H). **^{19}F-NMR (376 MHz. $CDCl_3$): δ(ppm) =** -101.0- -101.2 (m, 1F), -103.1- -103.2 (m, 1F). **HRMS (ESI):** calcd. for $[M+H]^+$ ($C_{21}H_{20}F_2NO_4S$) requires 420.1076, found 420.1073

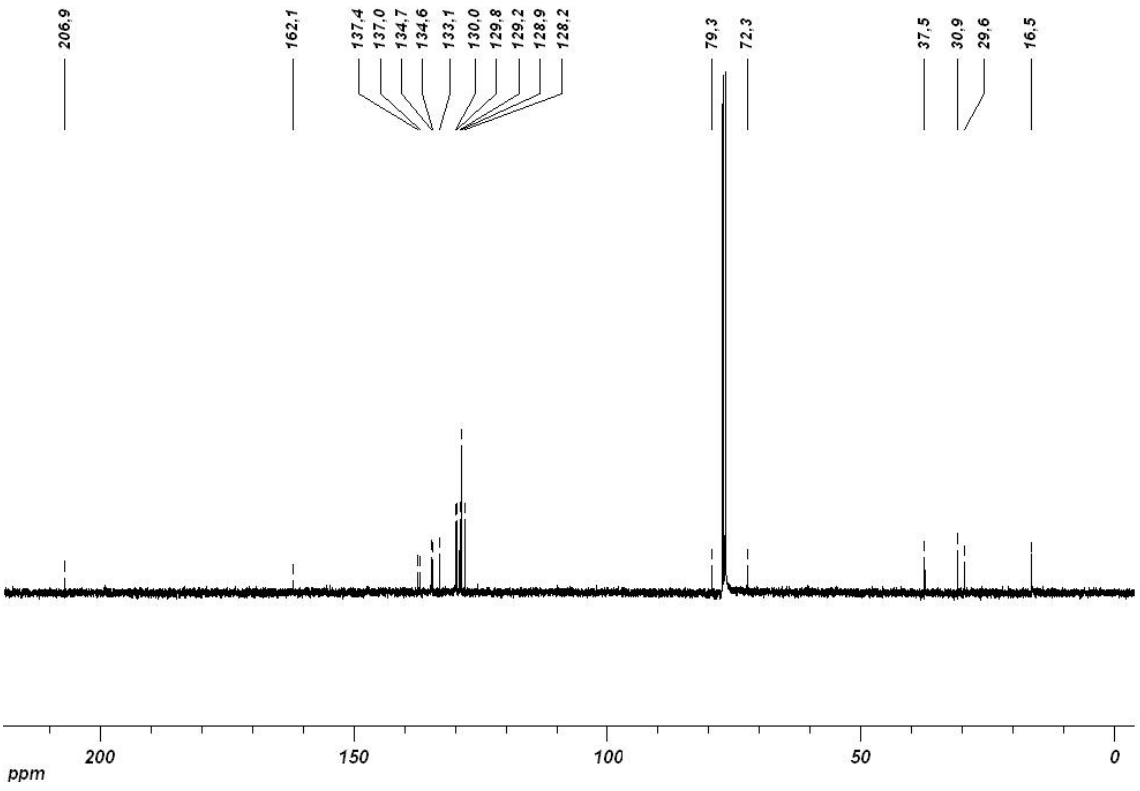


4-(2,2-Bis(phenylsulfonyl)ethyl)-4-isopropyl-2-phenyloxazol-5(4*H*)-one 3a

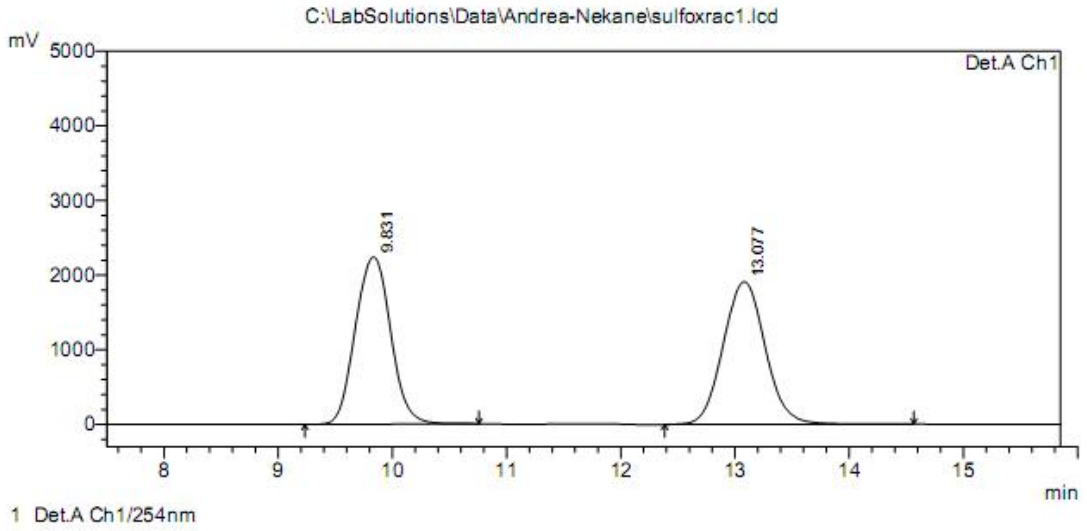
^{1}H-NMR



^{13}C-NMR



HPLC



PeakTable

Detector A Ch1 254nm

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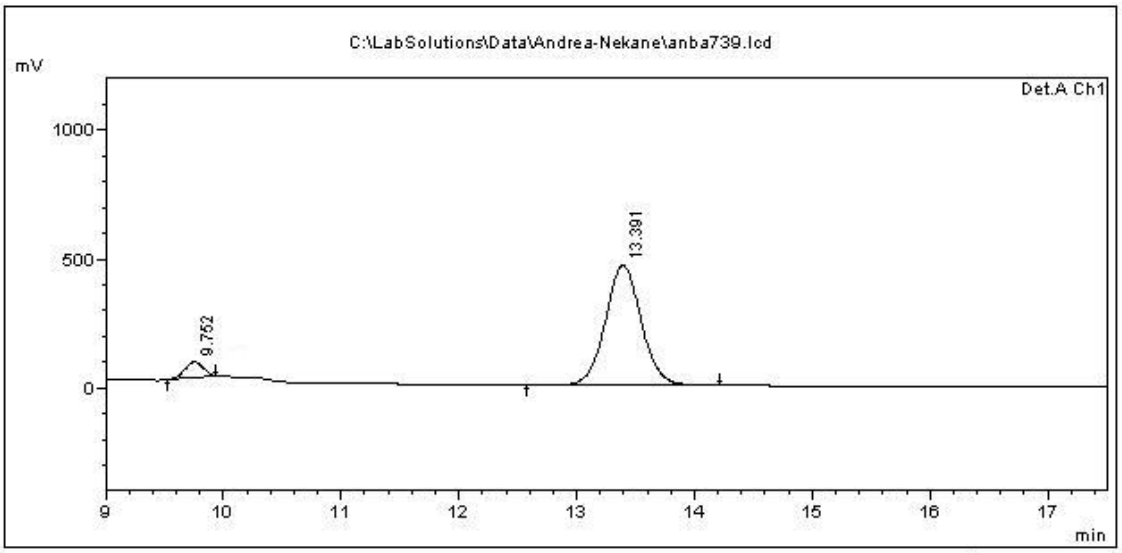
Total		97090683	4150180	100.000	100.000



PeakTable

Detector A Ch1 254nm

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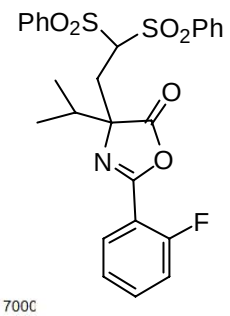
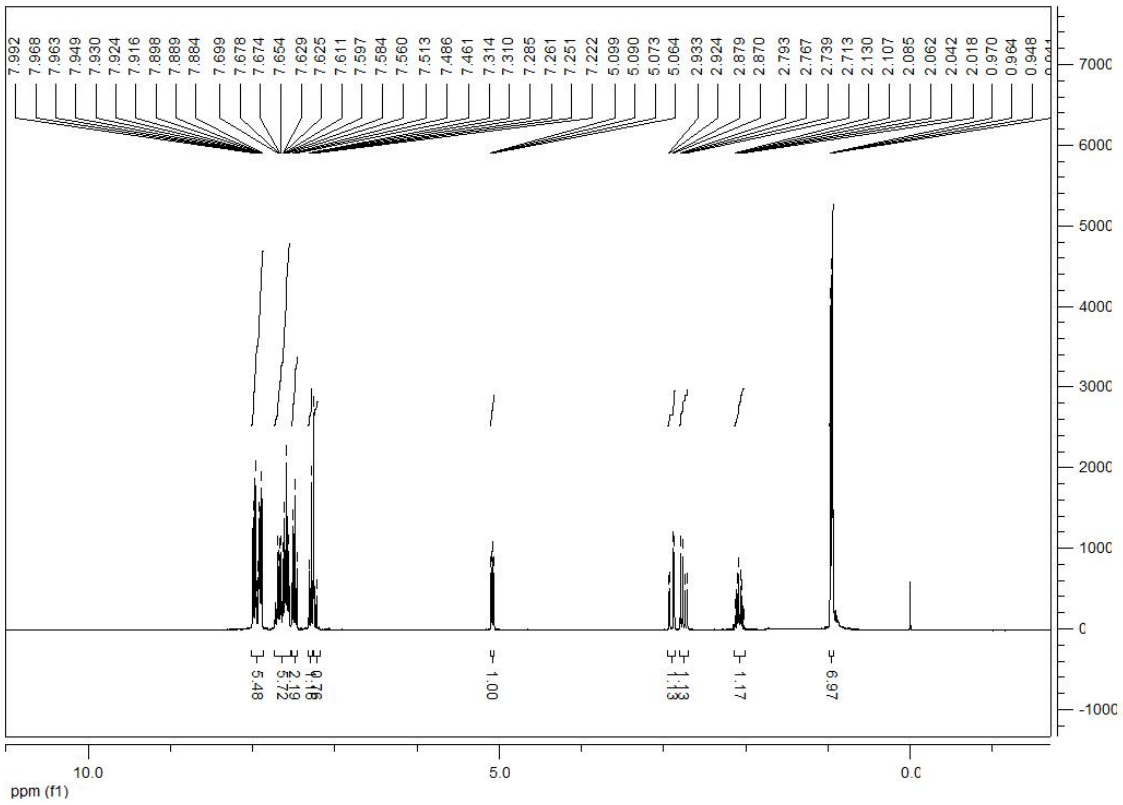
1	9.752	651968	6.165
2	13.391	9923405	93.835
Total		10575374	100.000

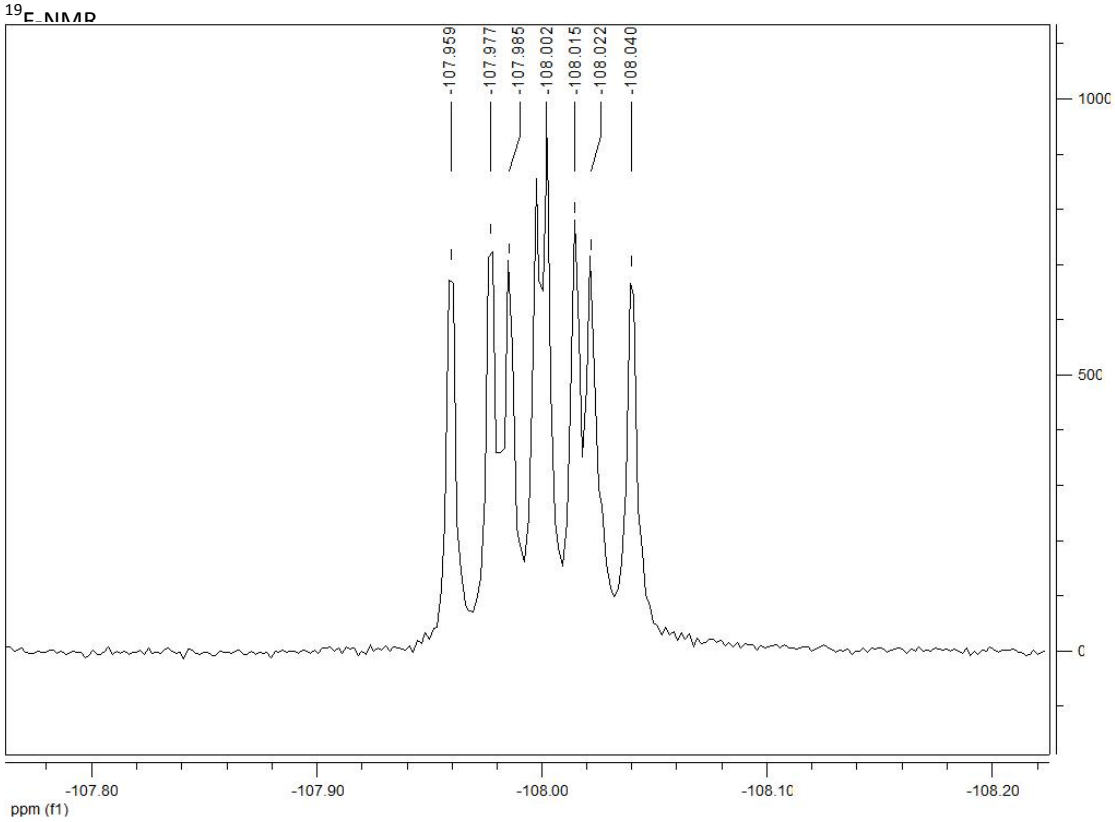


4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2-fluorophenyl)-4-isopropyloxazol-5(4H)-one 3c

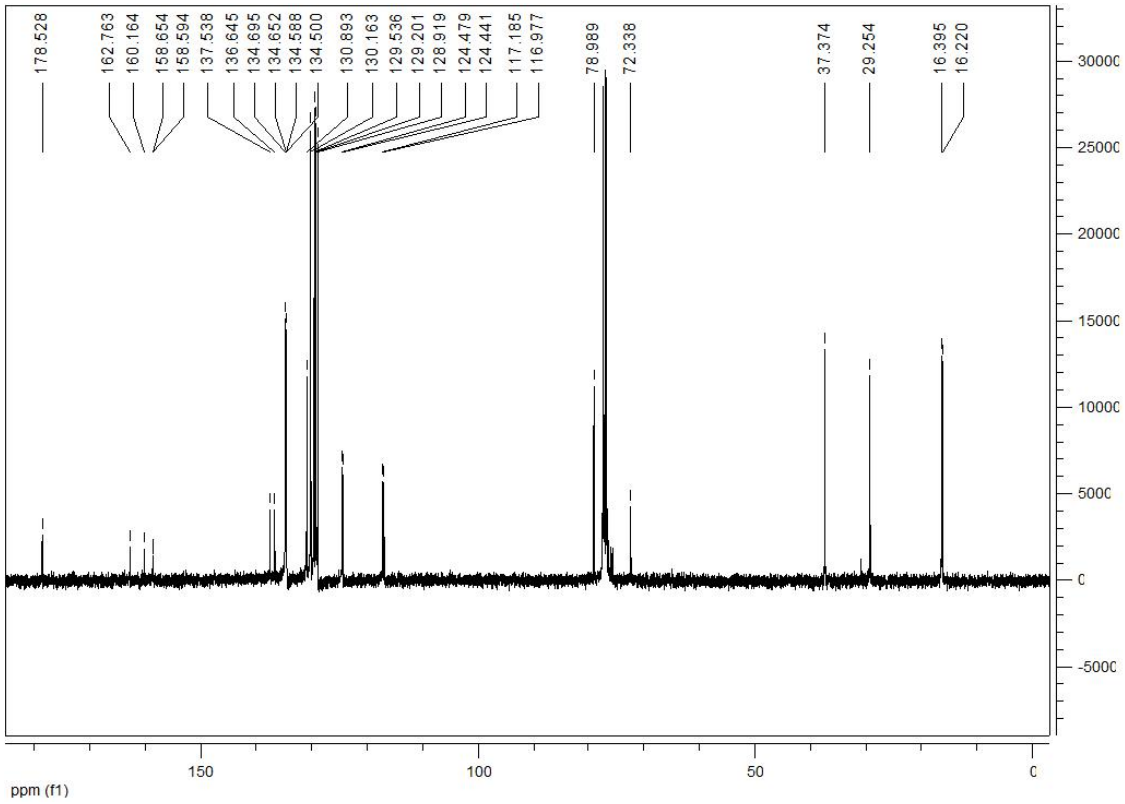
^{1}H-NMR



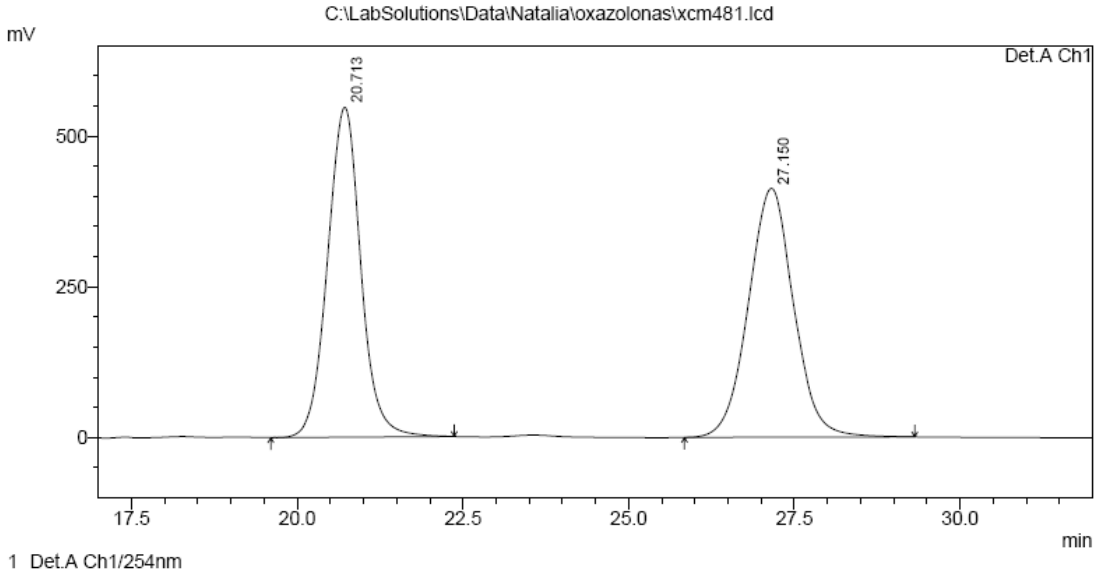
^{19}F-NMR



^{13}C-NMR



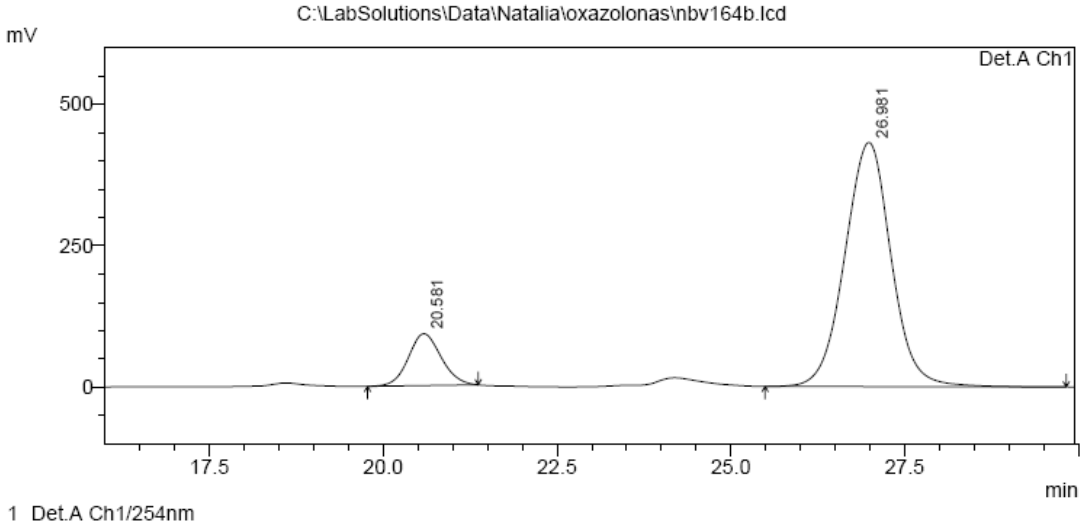
HPLC



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	20.713	19125365	49.348
2	27.150	19630616	50.652
Total		38755981	100.000

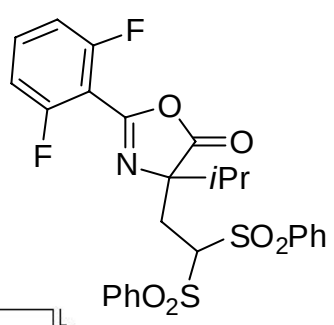


1 Det.A Ch1/254nm

PeakTable

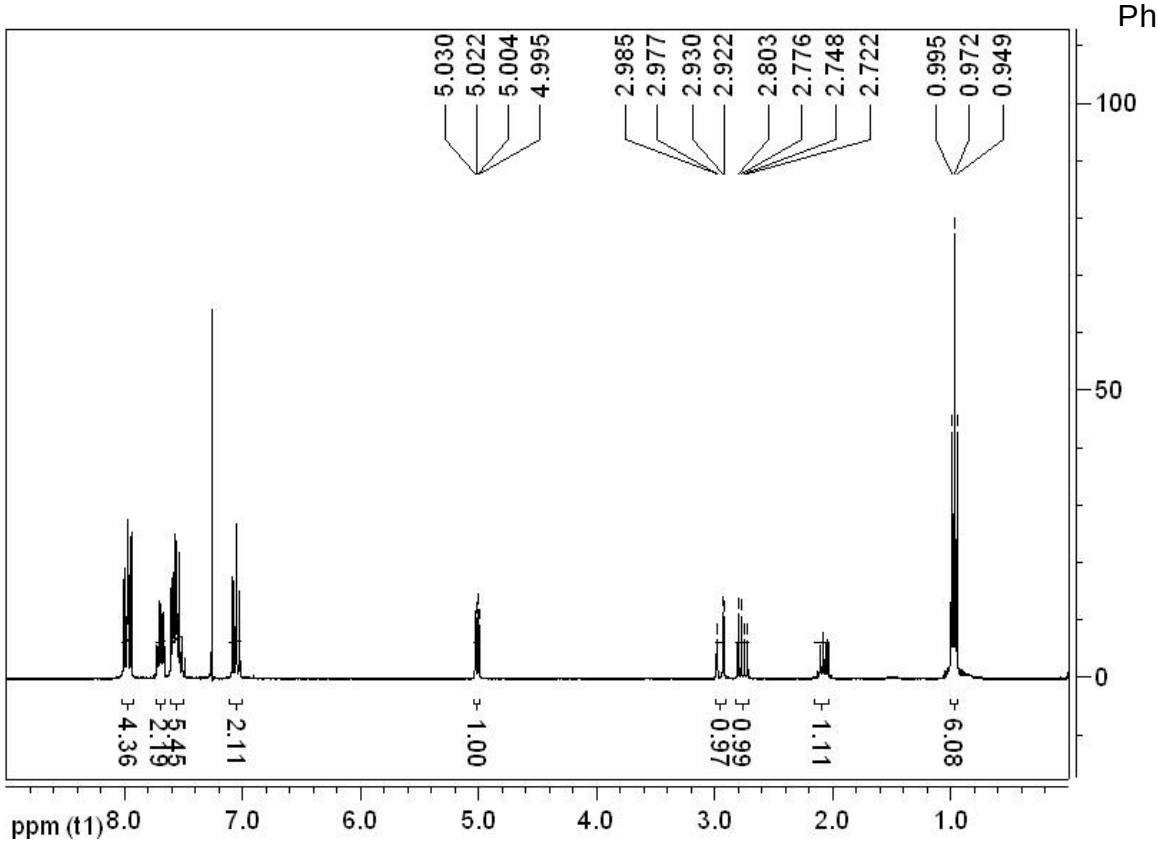
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	20.581	3012013	13.095
2	26.981	19989166	86.905
Total		23001178	100.000

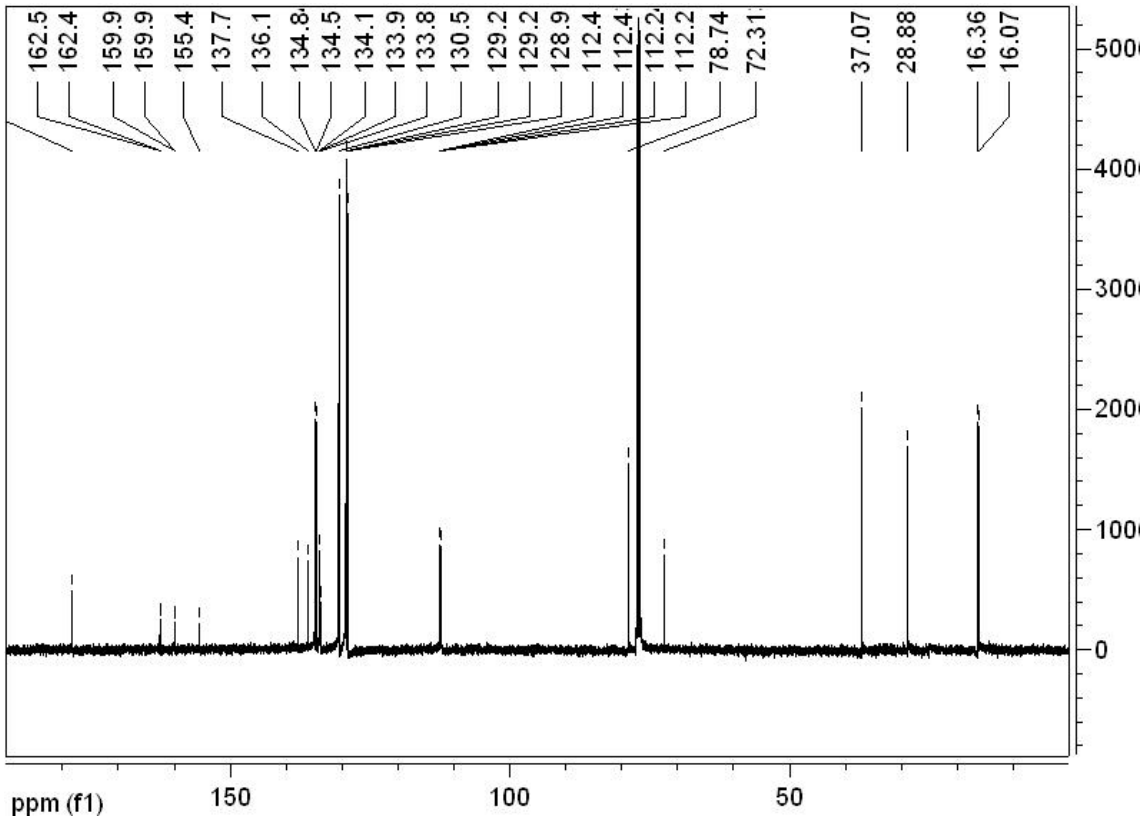


4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2,6-difluorophenyl)-4-isopropyloxazol-5(4*H*)-one 3b

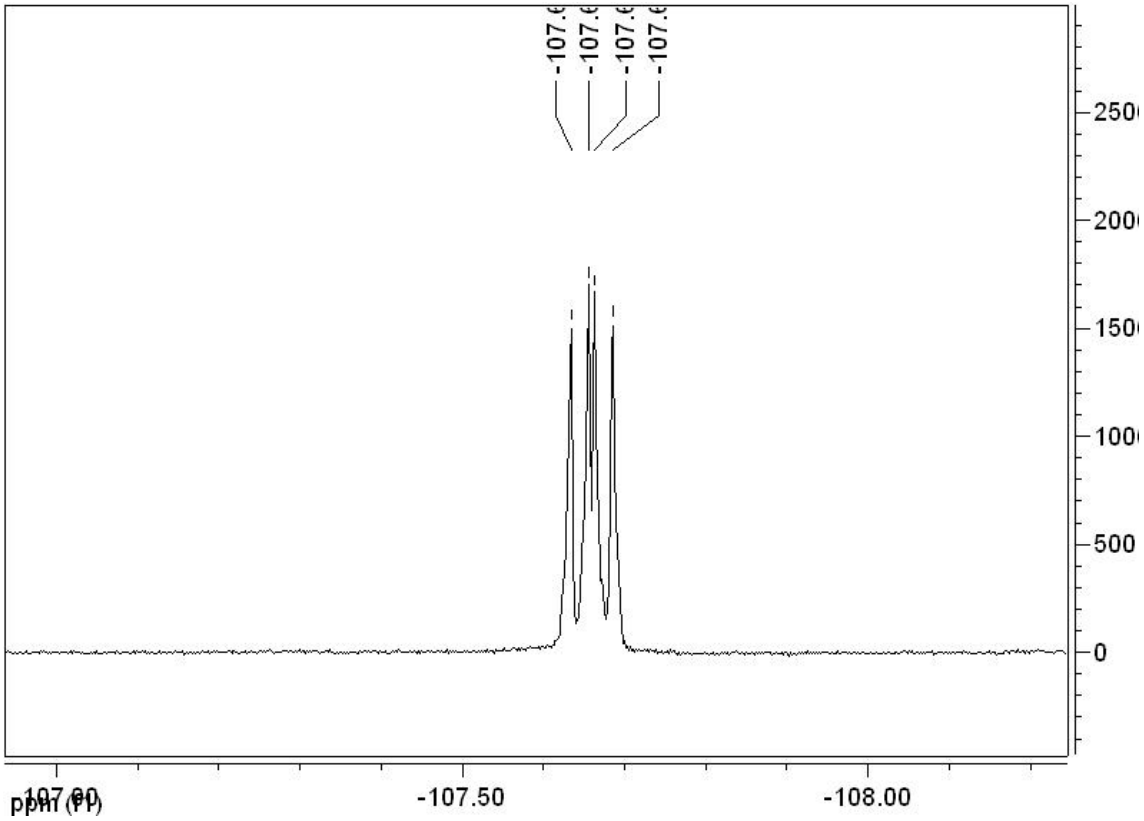
^{1}H-NMR



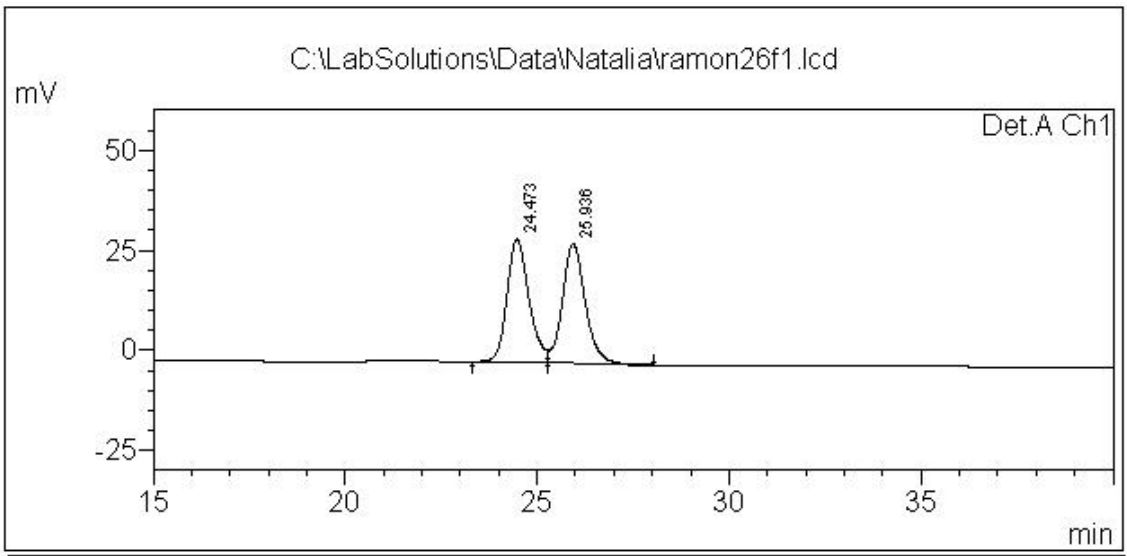
^{13}C-NMR



^{19}F-NMR



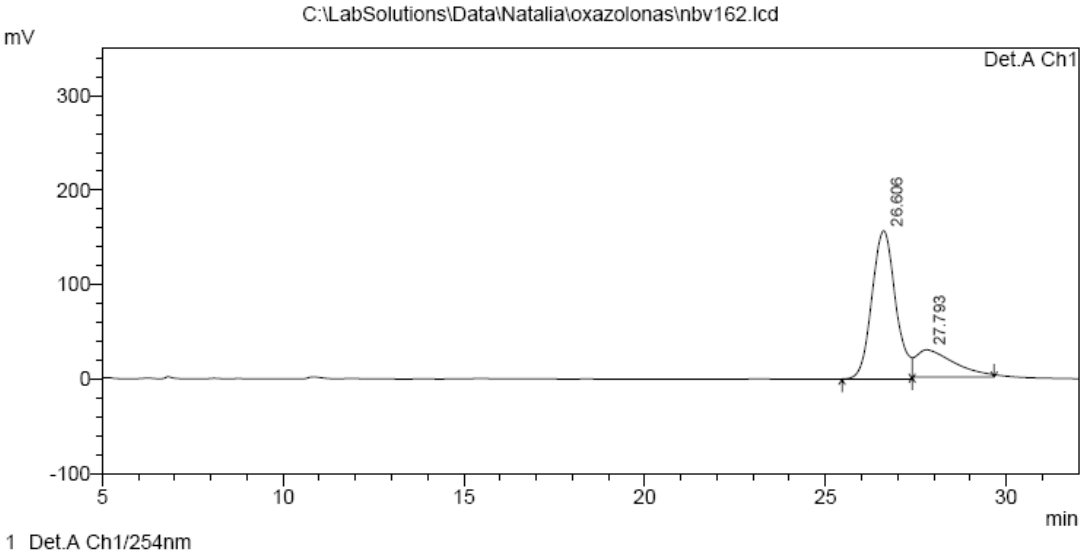
HPLC



PeakTable

Detector A Ch1 254nm

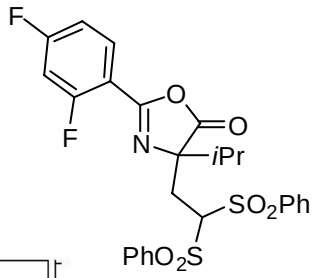
Peak#	Ret. Time	Area	Area %
1	24.473	1230422	49.890
2	25.936	1235861	50.110
Total		2466283	100.000



PeakTable

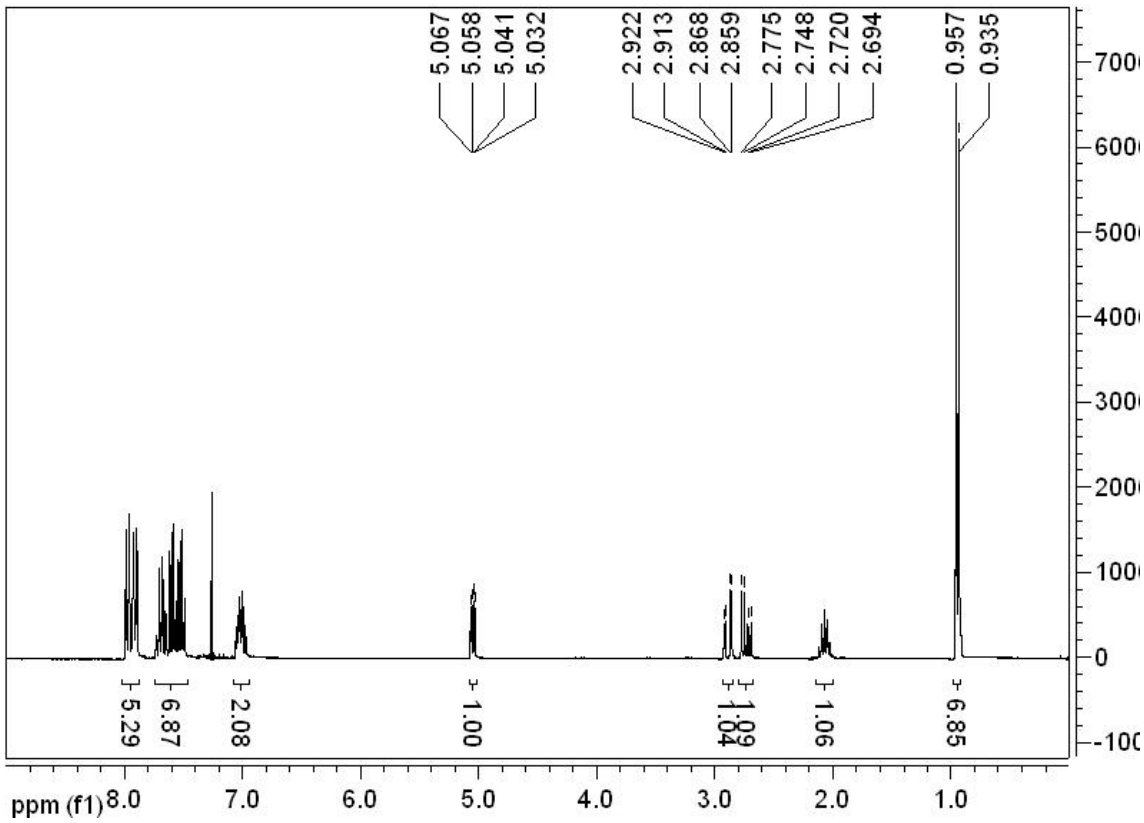
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	26.606	7184390	76.901
2	27.793	2158034	23.099
Total		9342424	100.000

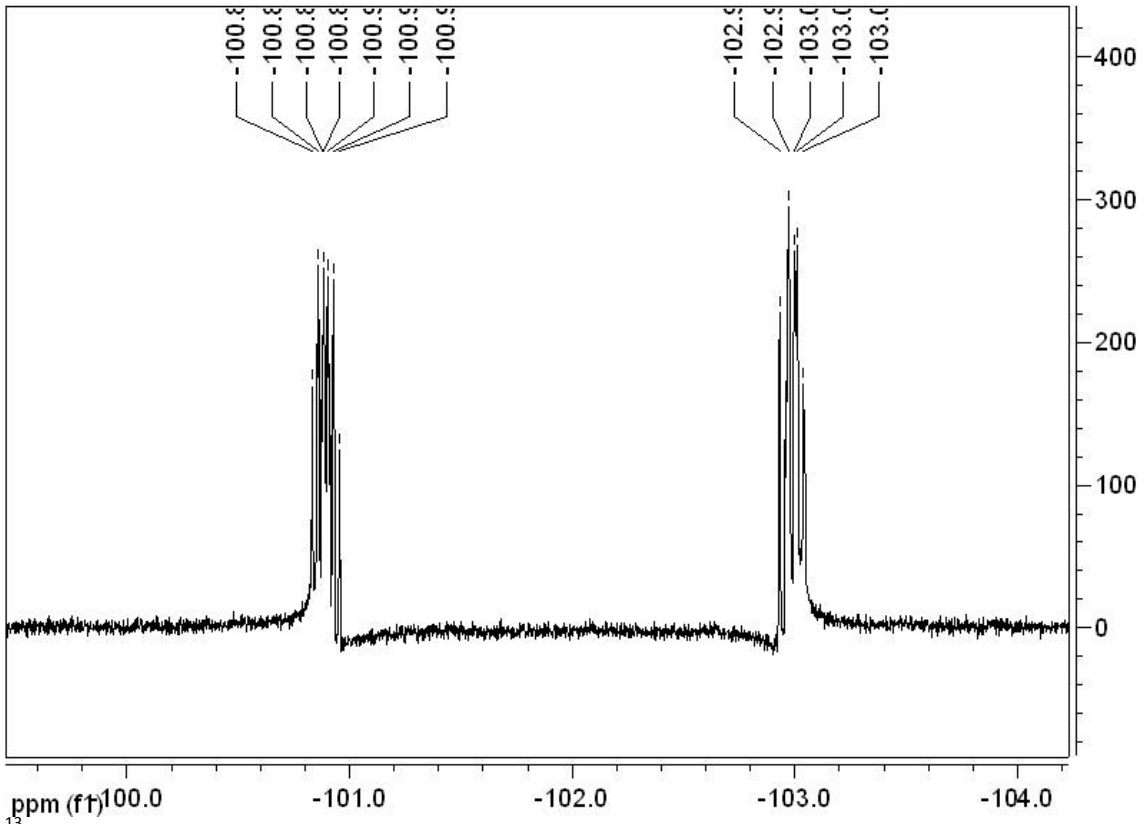


4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2,4-difluorophenyl)-4-isopropyloxazol-5(4*H*)-one 3e

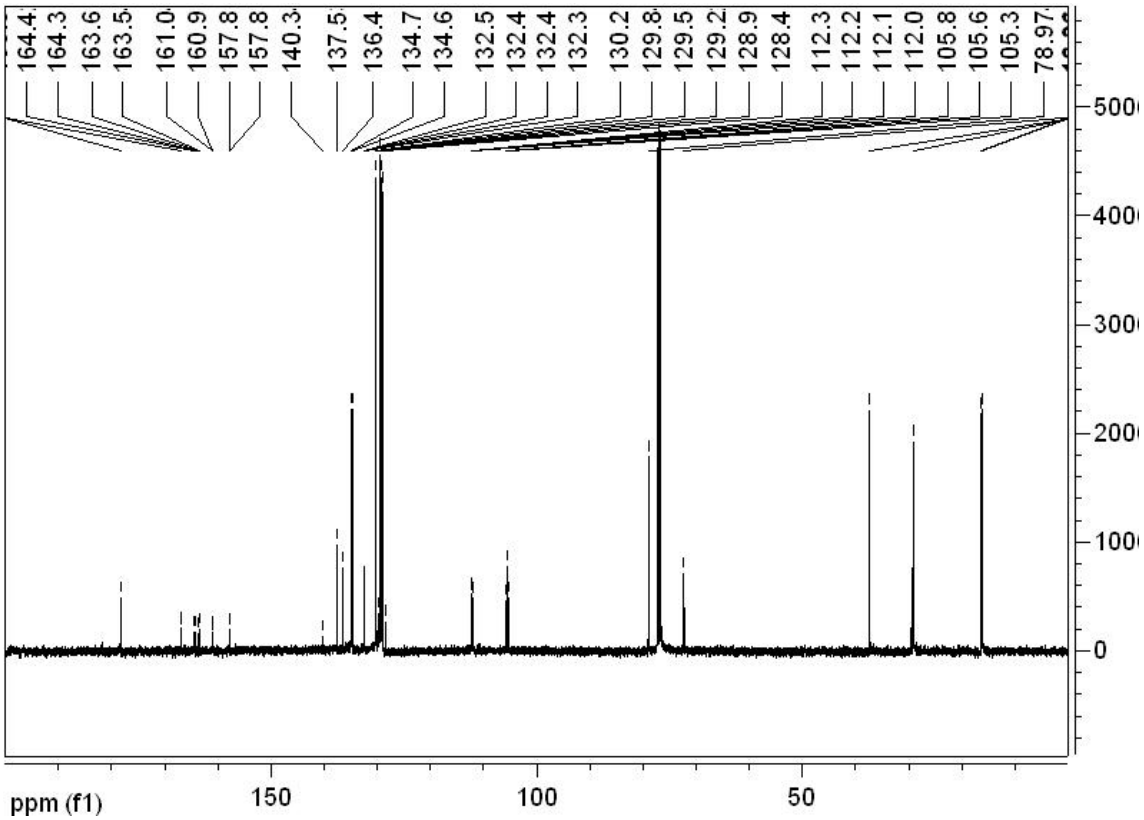
^{1}H-NMR



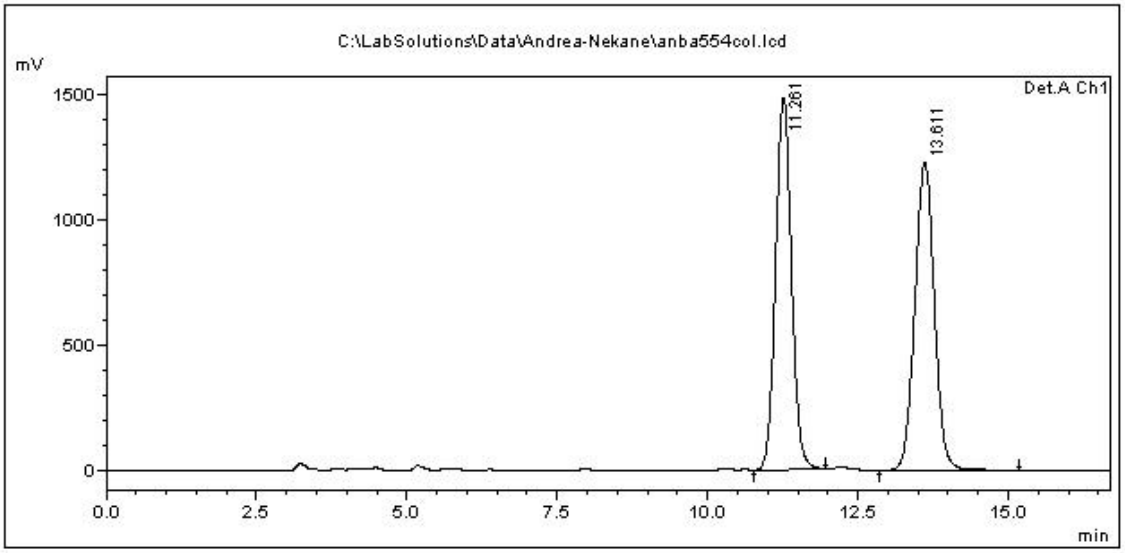
^{19}F-NMR



^{13}C-NMR



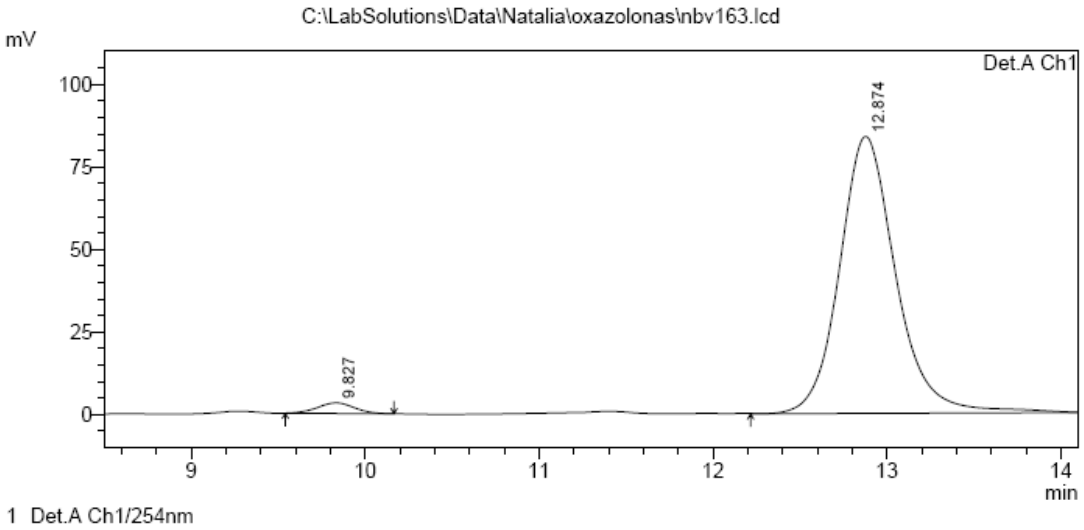
HPLC



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	11.261	27157702	49.558
2	13.611	27642134	50.442
Total		54799836	100.000

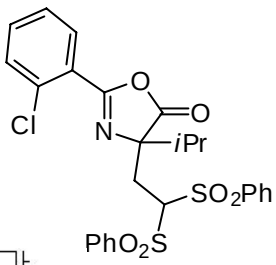


1 Det.A Ch1/254nm

PeakTable

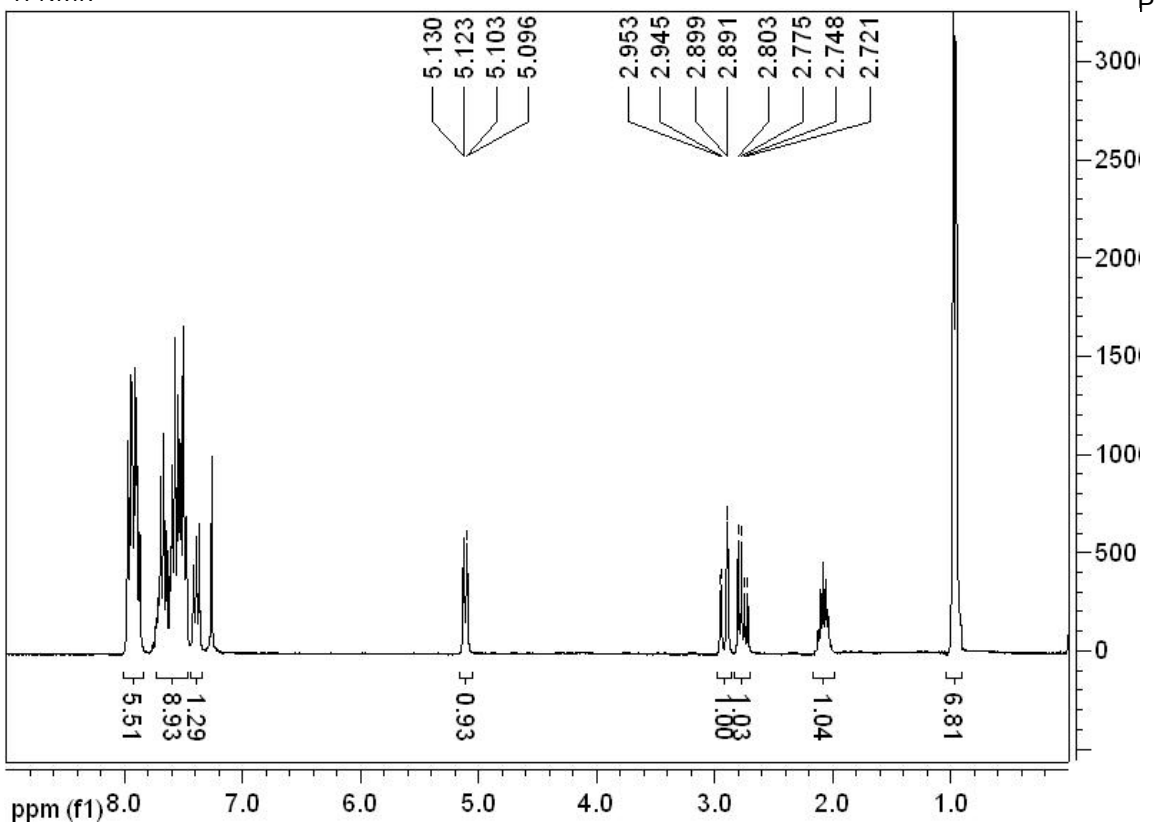
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	9.827	47140	2.430
2	12.874	1893157	97.570
Total		1940298	100.000

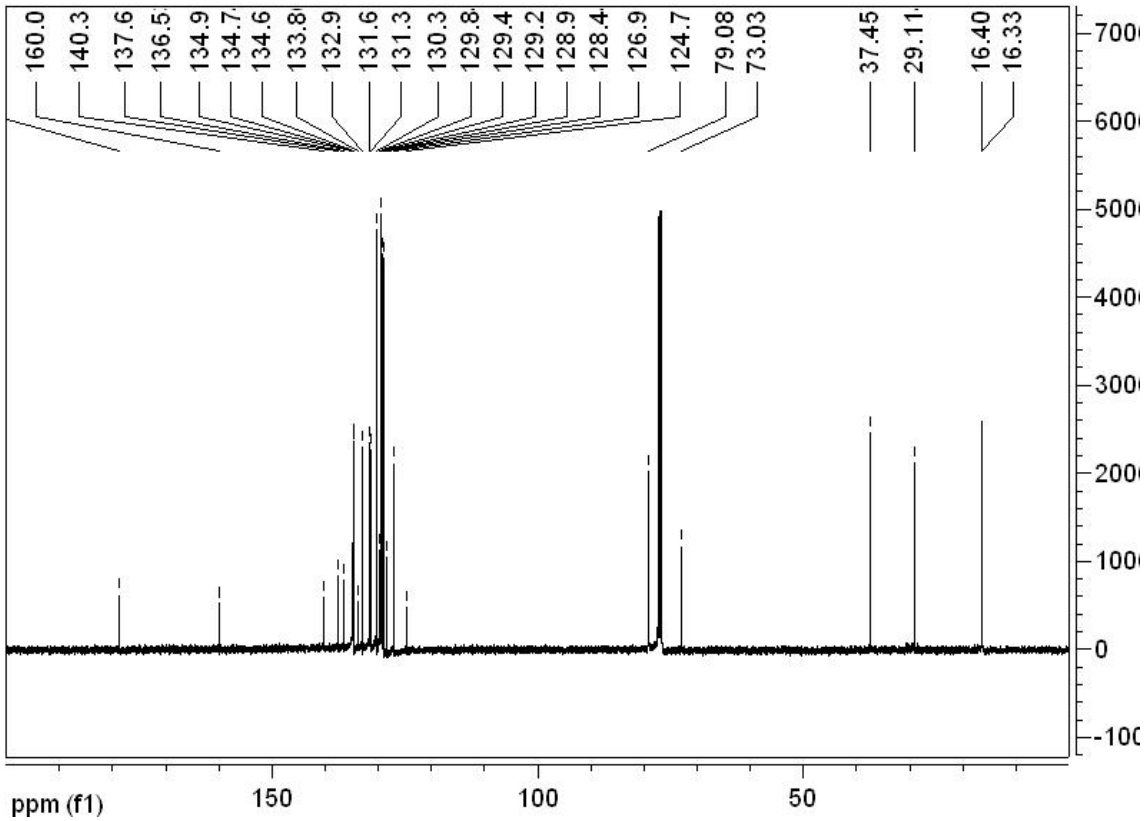


4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2-chlorophenyl)-4-isopropyloxazol-5(4*H*)-one 3d

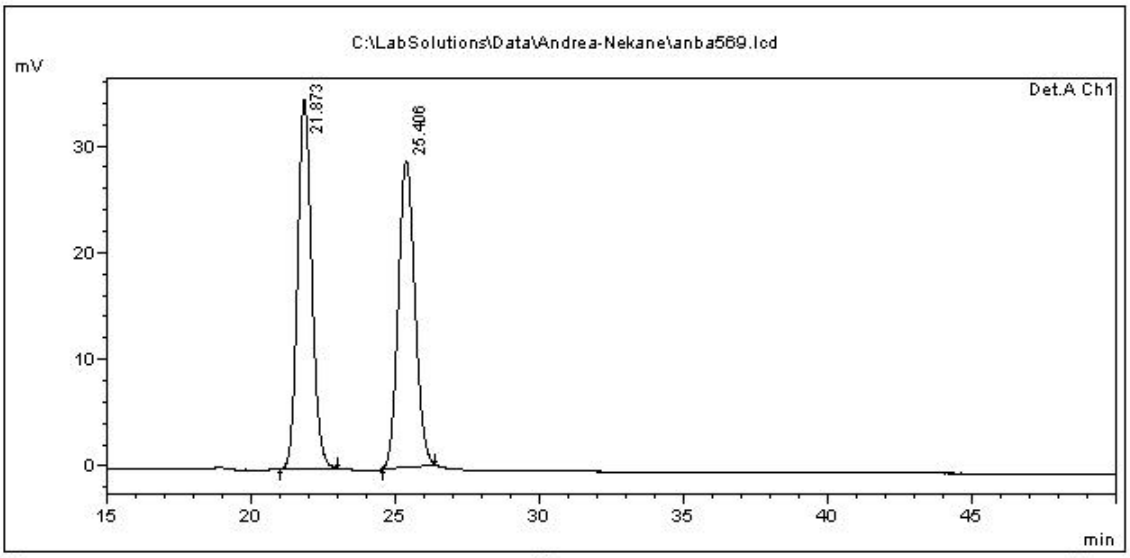
^{1}H-NMR



^{13}C-NMR



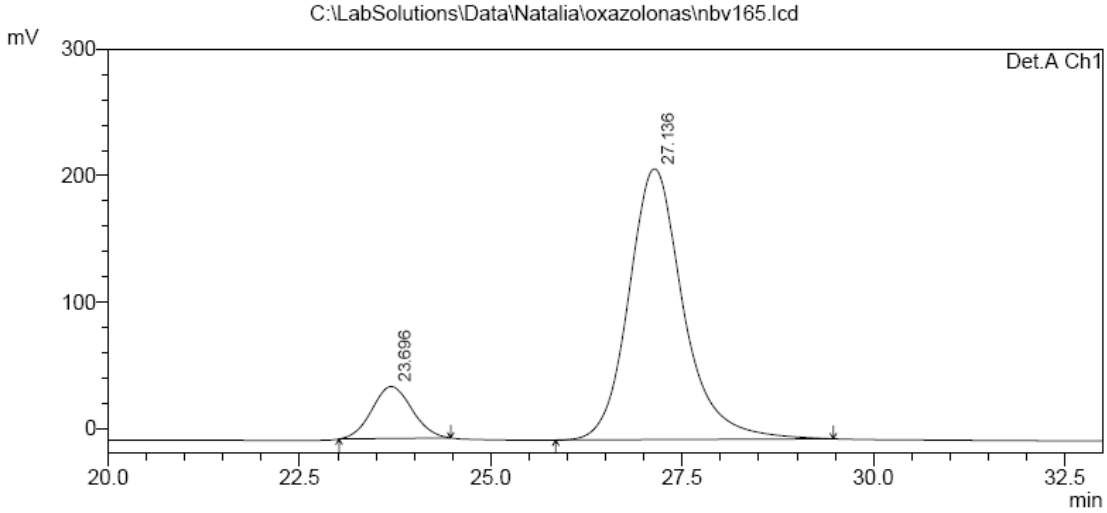
HPLC



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	21.873	1185966	50.866
2	25.406	1145579	49.134
Total		2331545	100.000

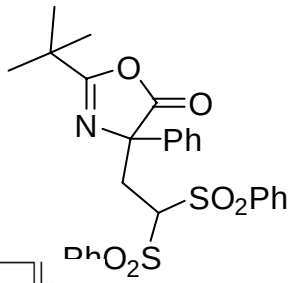


1 Det.A Ch1/254nm

PeakTable

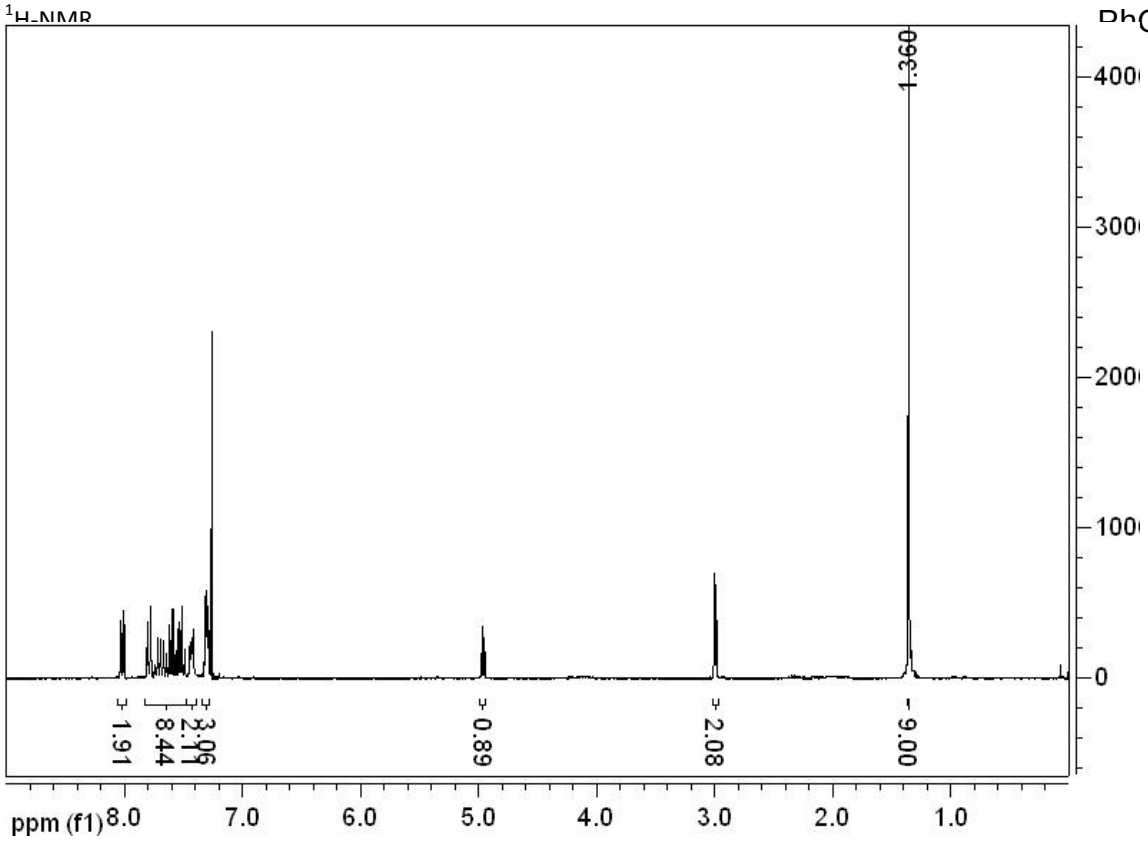
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	23.696	1502353	12.378
2	27.136	10634671	87.622
Total		12137025	100.000

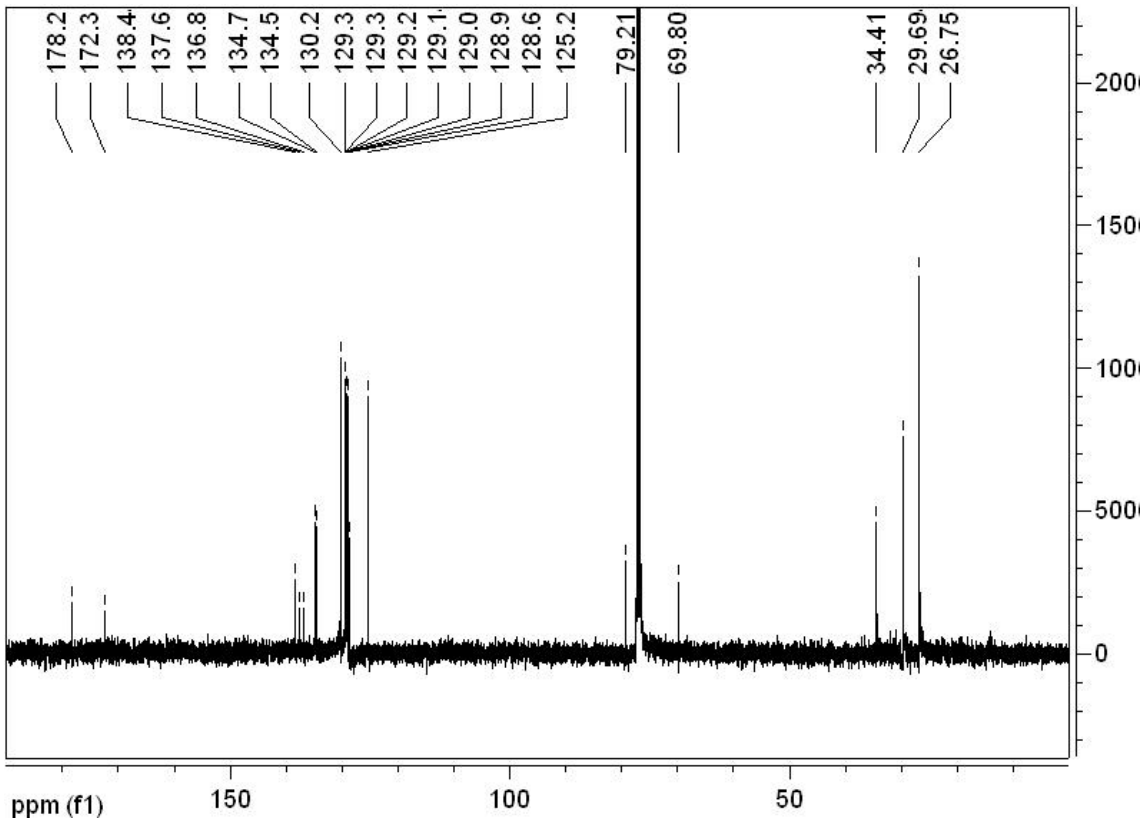


4-(2,2-Bis(phenylsulfonyl)ethyl)-2-tertbutyl-4-phenyloxazol-5(4*H*)-one 3j

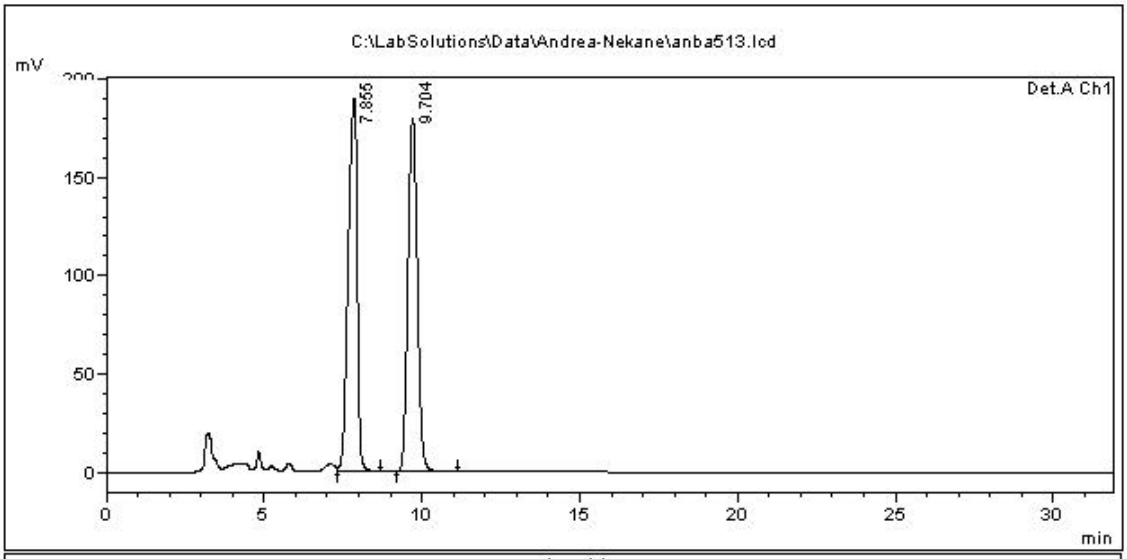
^{1}H-NMR



^{13}C-NMR



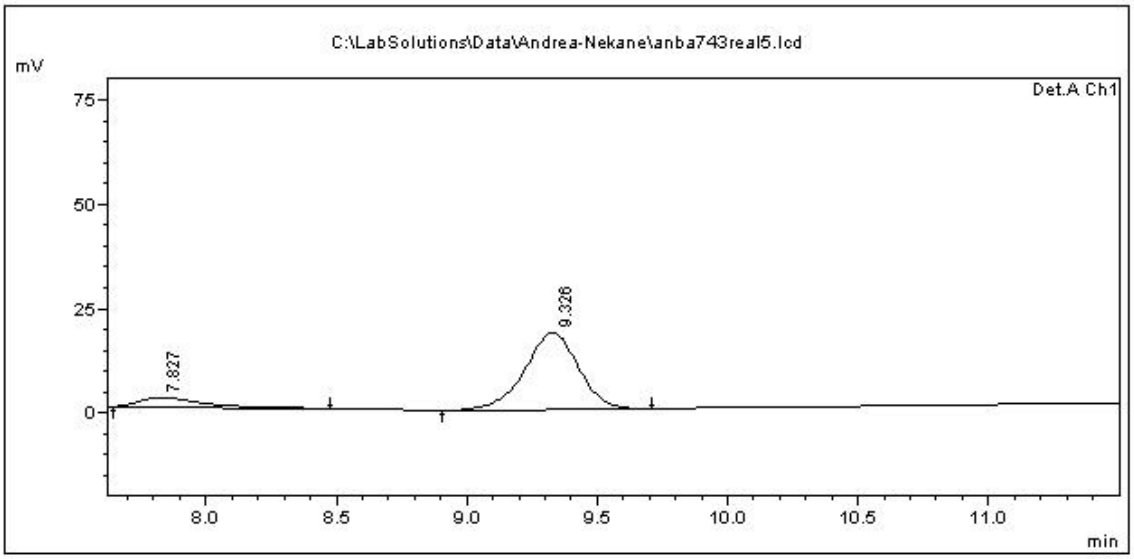
HPLC



PeakTable

Detector A Ch1 254nm

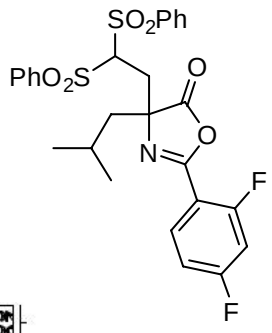
Peak#	Ret. Time	Area	Area %
1	7.855	3779727	50.161
2	9.704	3755397	49.839
Total		7535124	100.000



PeakTable

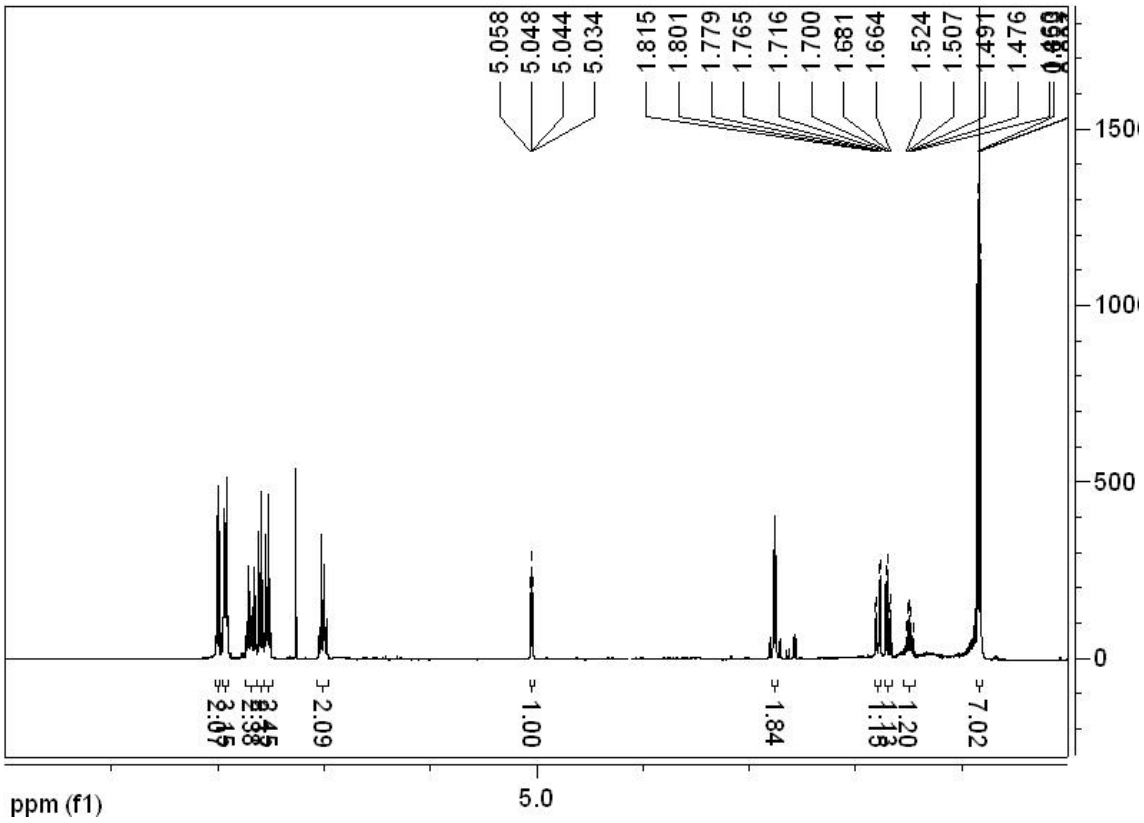
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	7.827	36345	12.088
2	9.326	264321	87.912
Total		300665	100.000

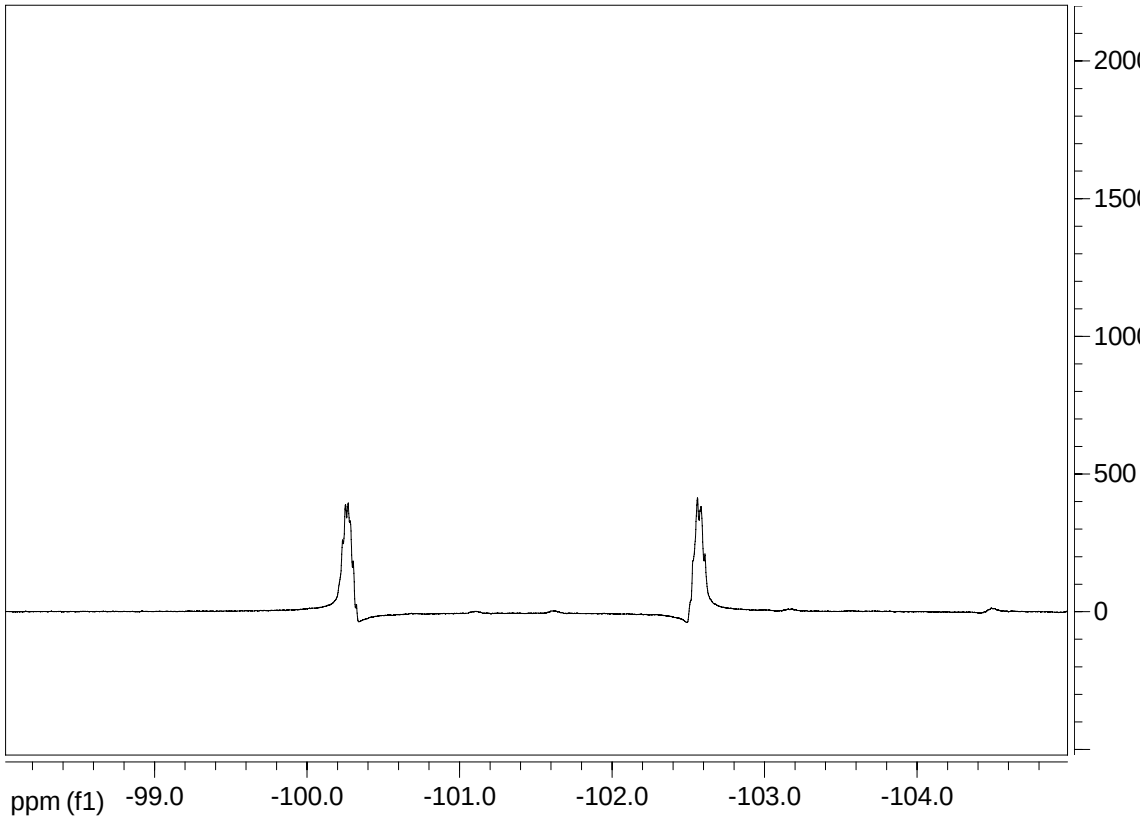


4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2,4-difluorophenyl)-4-isobutyloxazol-5(4*H*)-one 3h

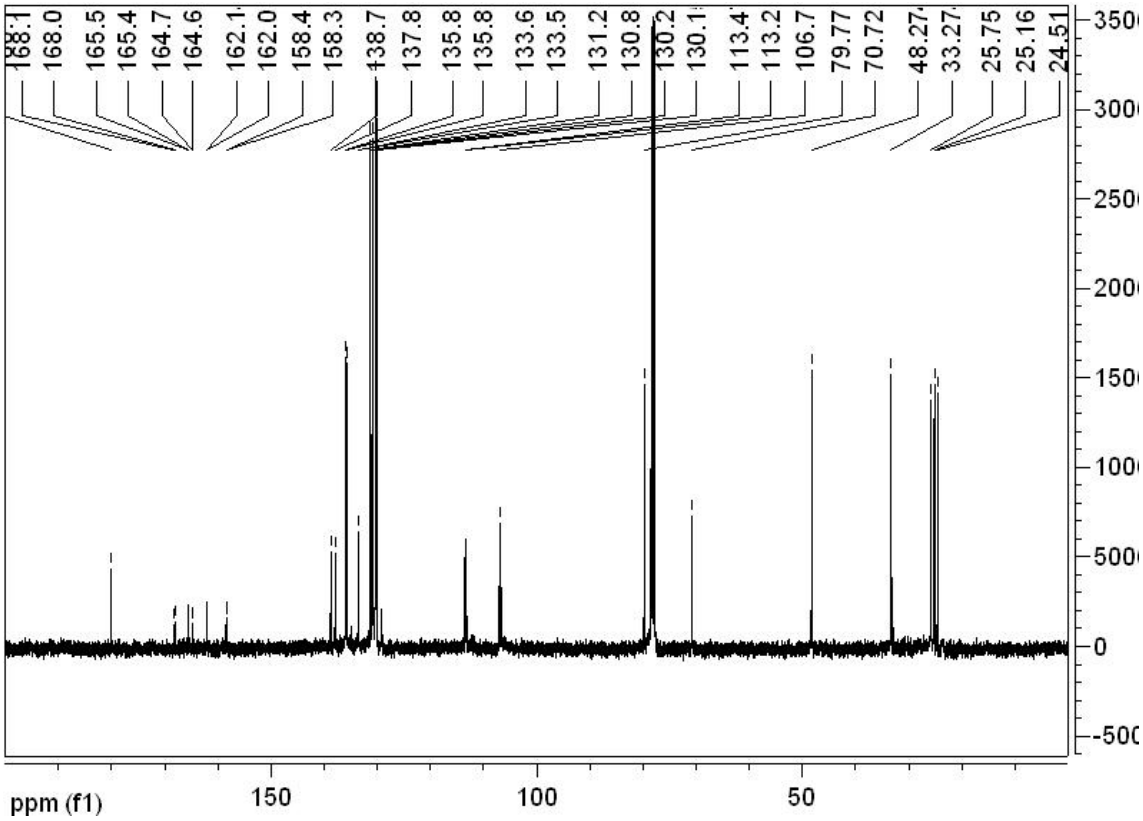
^{1}H-NMR



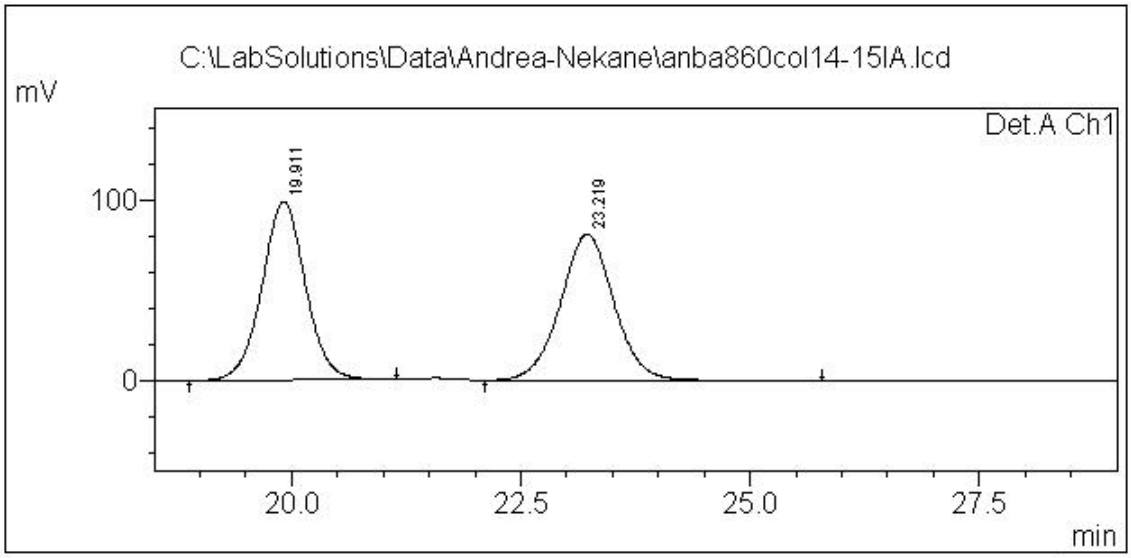
^{19}F-NMR



^{13}C-NMR



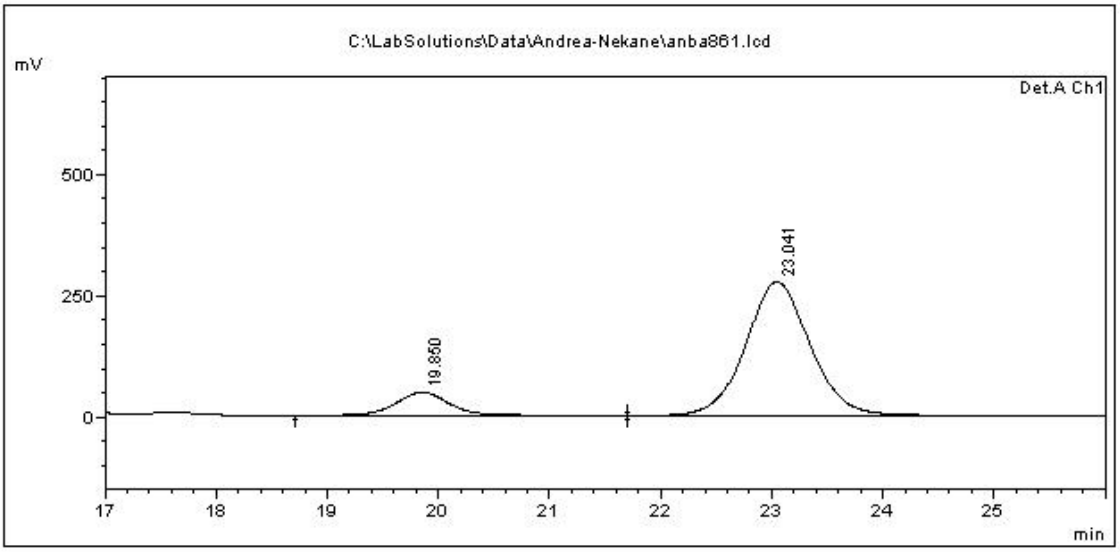
HPLC



PeakTable

Detector A Ch1 254nm

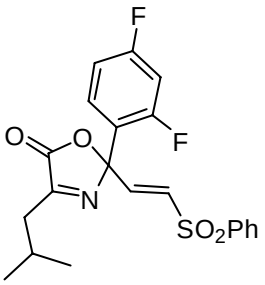
Peak#	Ret. Time	Area	Area %
1	19.911	3263672	49.842
2	23.219	3284365	50.158
Total		6548037	100.000



PeakTable

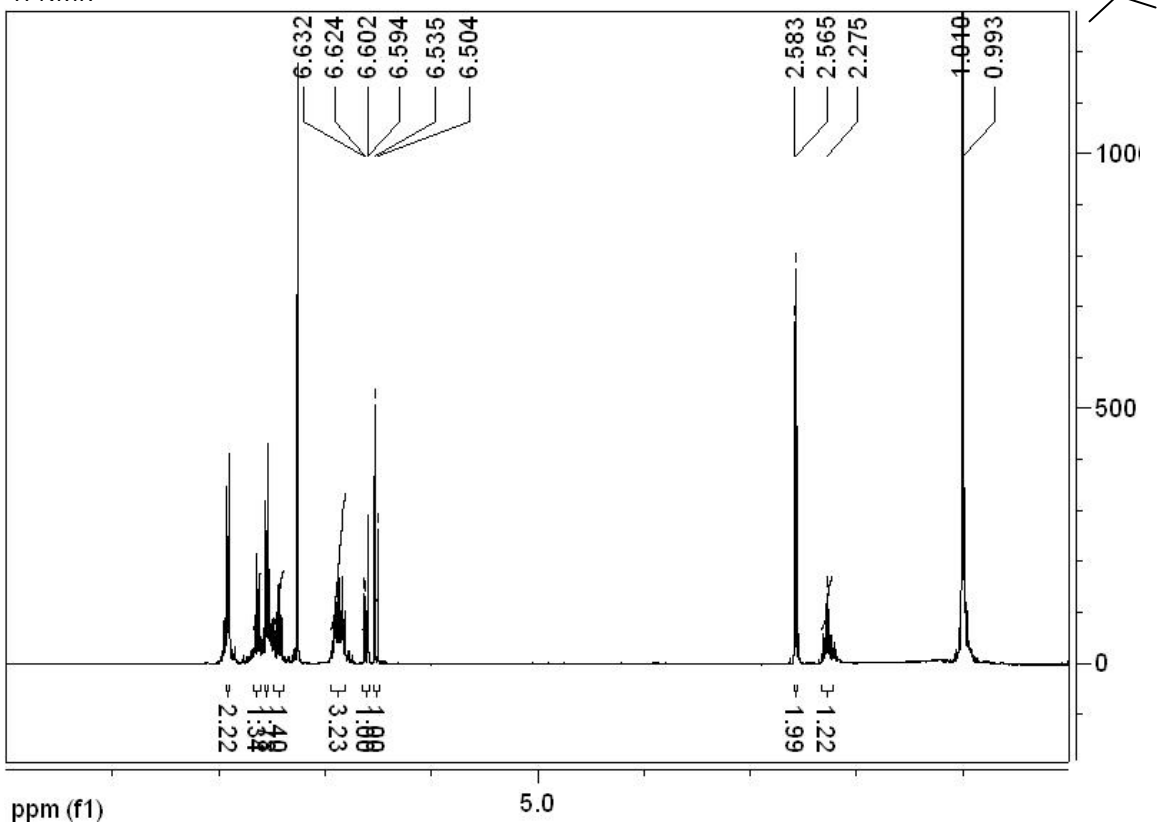
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	19.850	1613373	12.582
2	23.041	11209427	87.418
Total		12822799	100.000

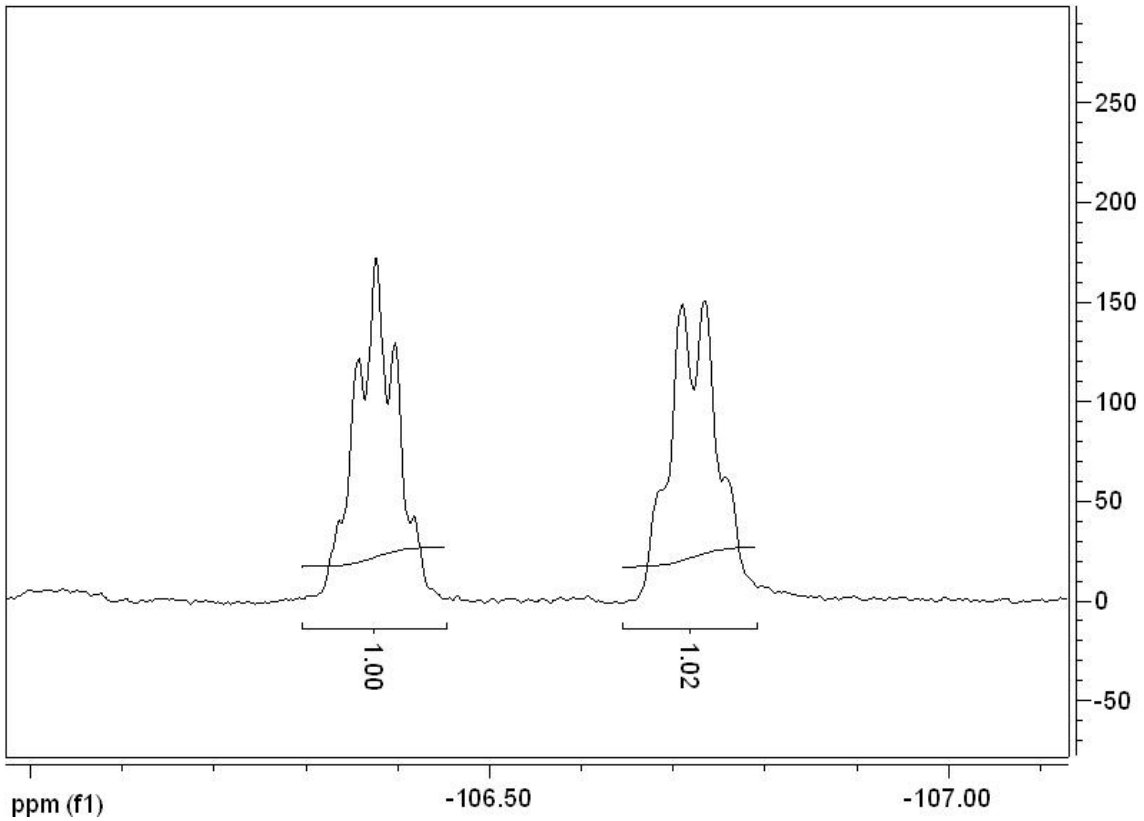


(*E*)-2-(2,4-Difluorophenyl)-4-isobutyl-2-(2-(phenylsulfonyl)vinyl)oxazol-5(2*H*)-one 5h

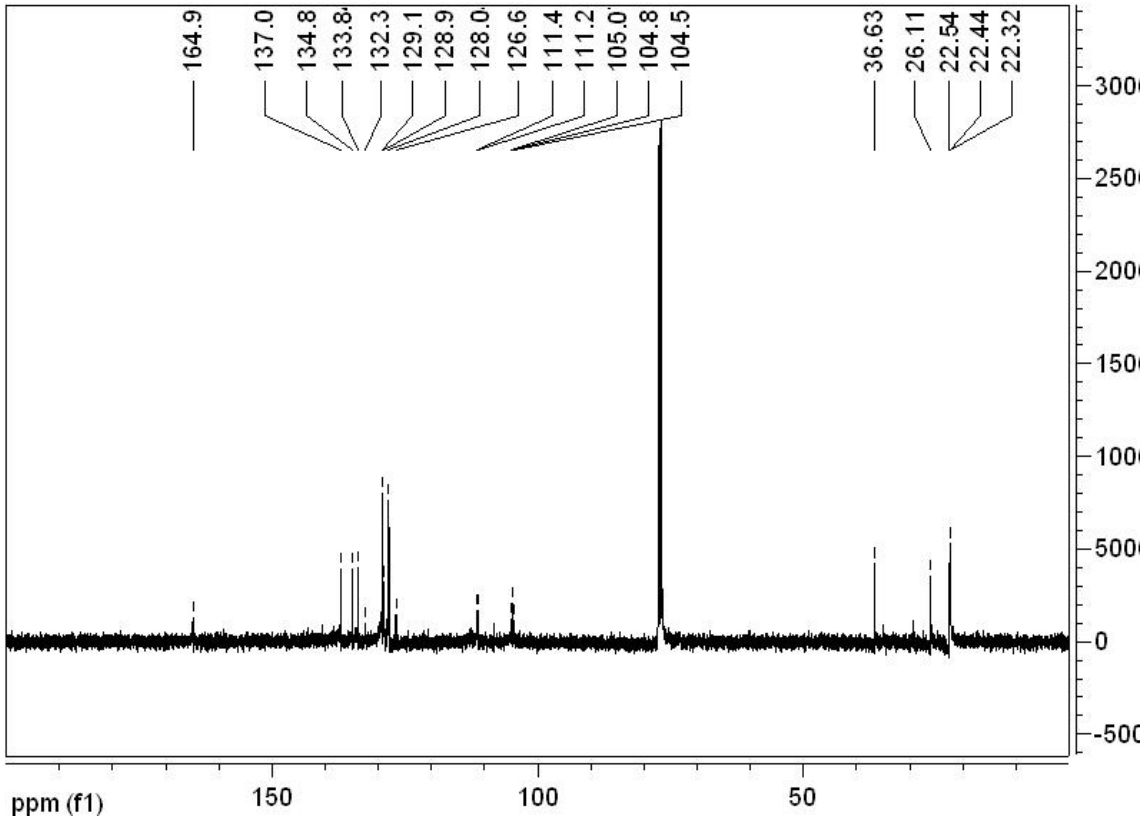
^{1}H-NMR

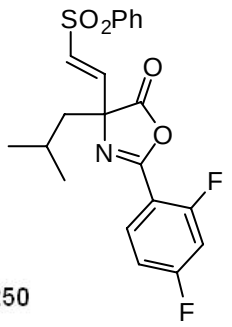


^{19}F-NMR



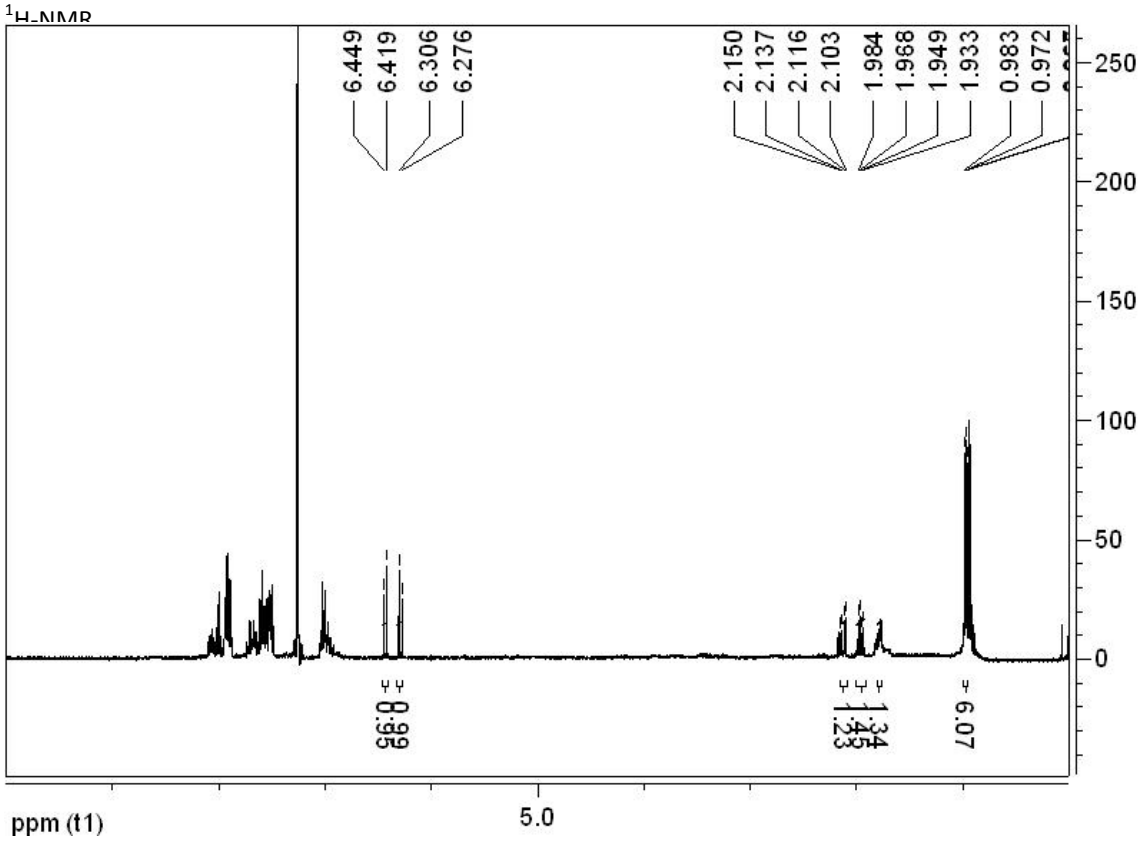
^{13}C-NMR


164.9
137.0
134.8
133.8
132.3
129.1
128.9
128.0
126.6
111.4
111.2
105.0
104.8
104.5
36.63
26.11
22.54
22.44
22.32
300
250
200
150
100
500
0
-500
ppm (f1)
150
100
50

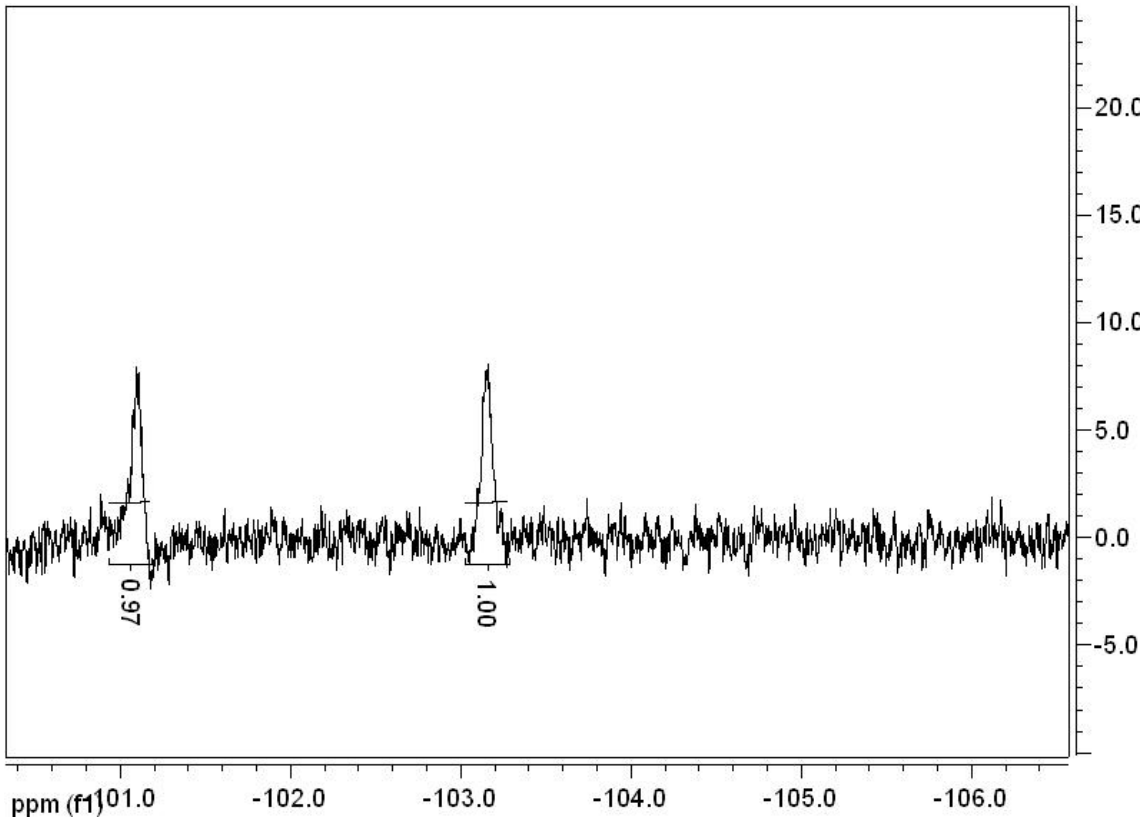


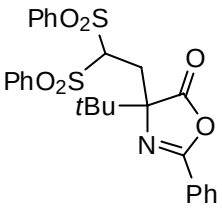
(*E*)-2-(2,4-Difluorophenyl)-4-isobutyl-4-(2-(phenylsulfonyl)vinyl)oxazol-5(4*H*)-one 4h

^{1}H-NMR



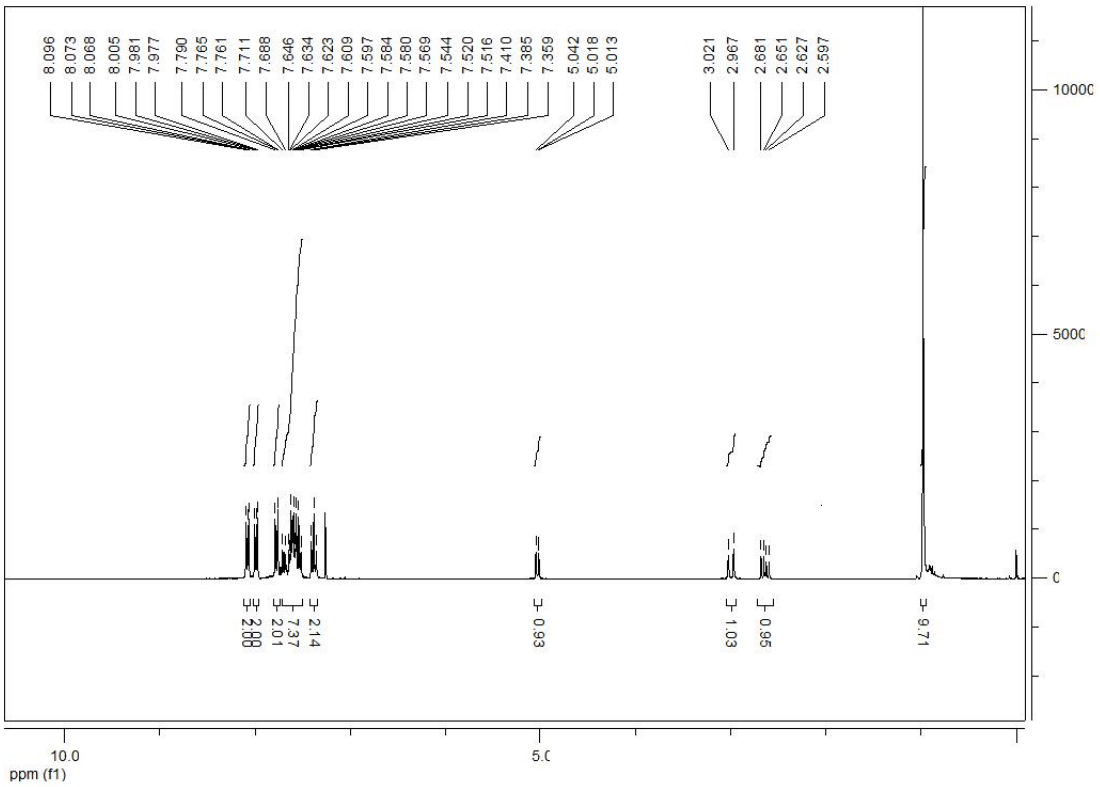
^{19}F-NMR



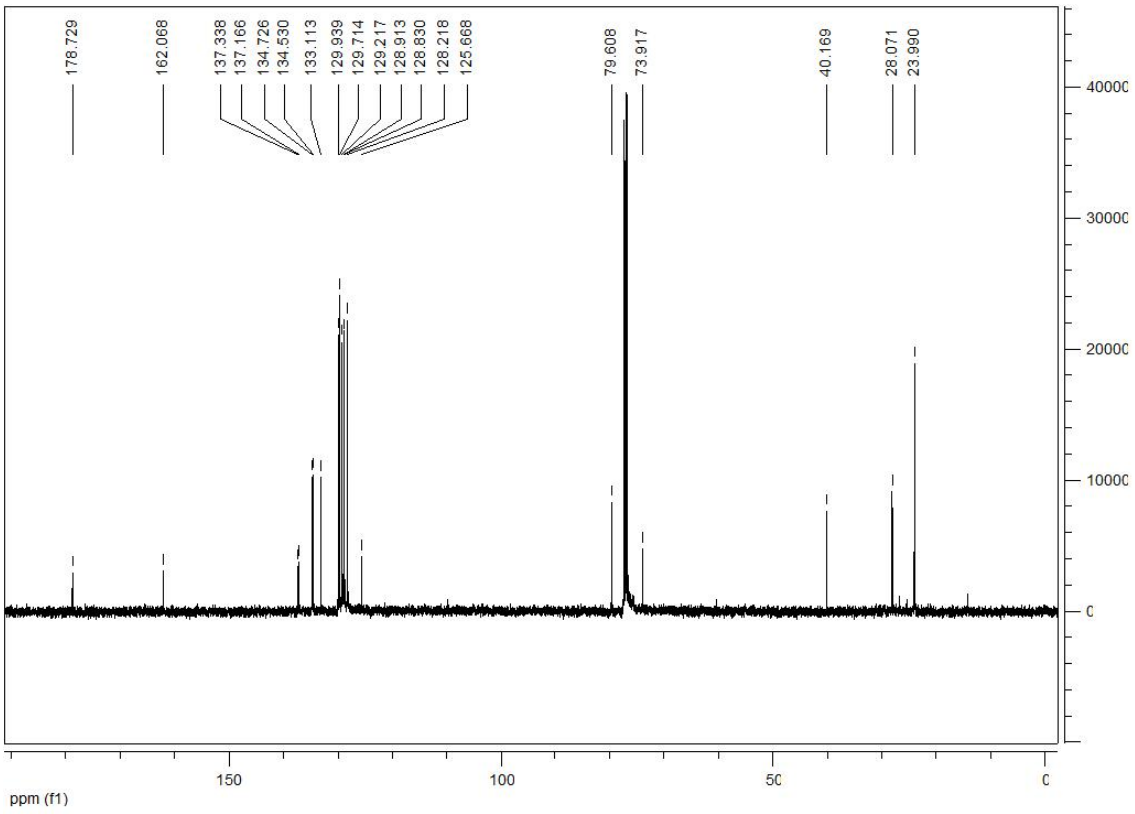


4-(2,2-Bis(phenylsulfonyl)ethyl)-4-*tert*-butyl-2-phenyloxazol-5(4*H*)-one 3i

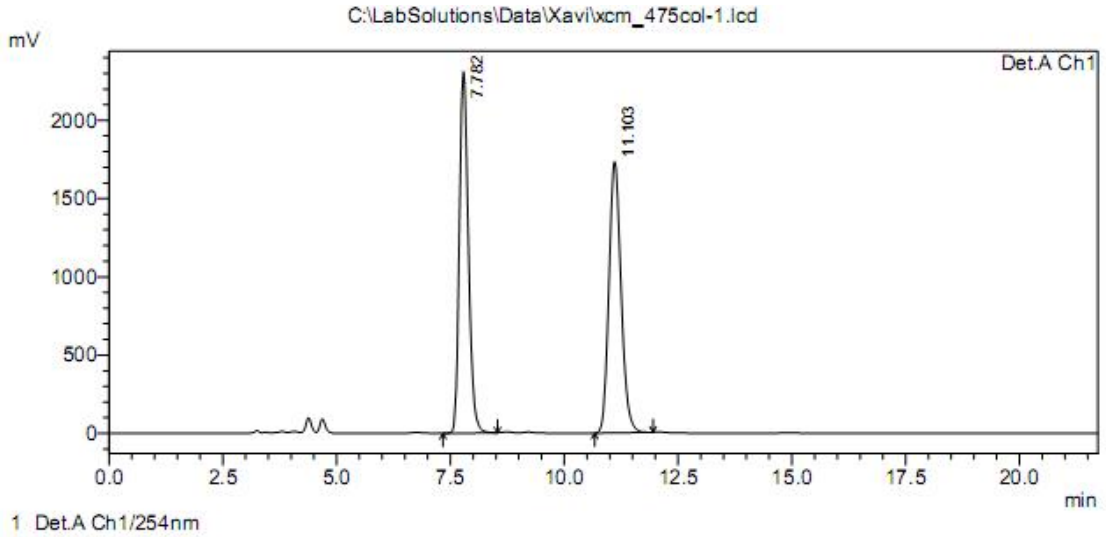
^{1}H-NMR



^{13}C-NMR



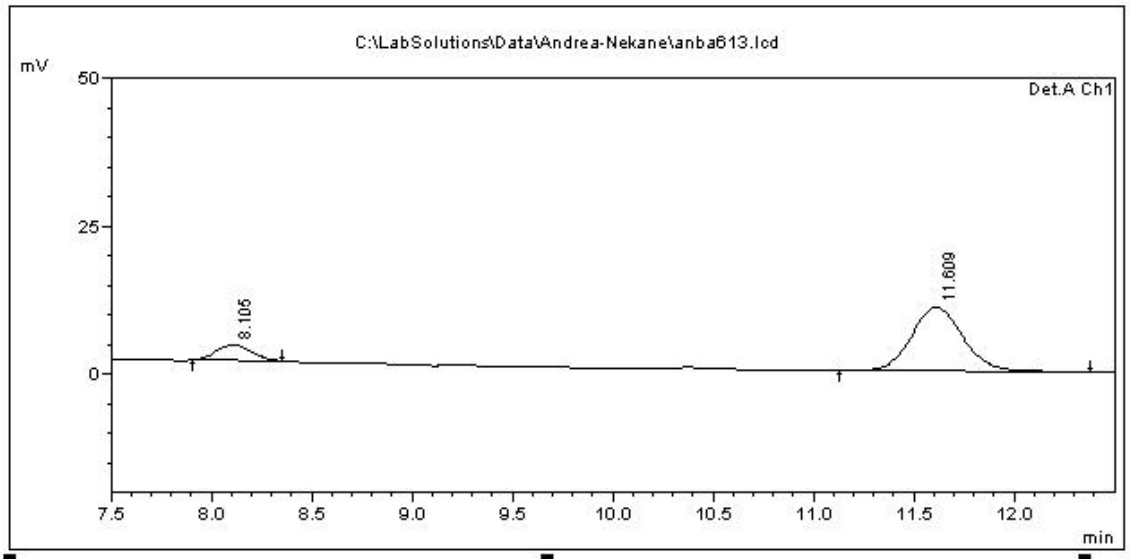
HPLC



PeakTable

Detector A Ch1 254nm

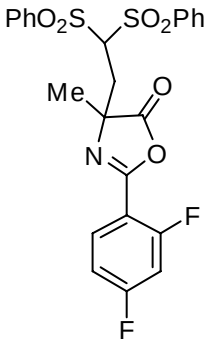
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.782	31774354	2310991	49.810	57.129
2	11.103	32016439	1734250	50.190	42.871
Total		63790793	4045241	100.000	100.000



PeakTable

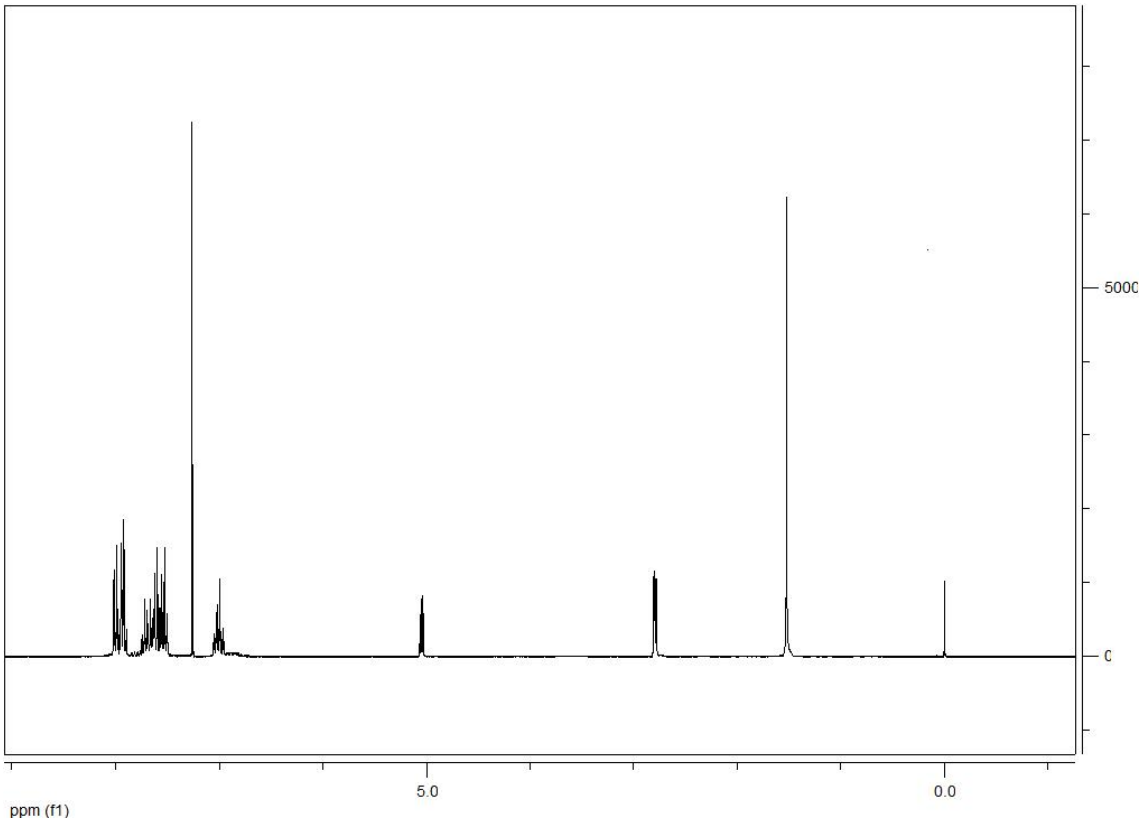
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Area %
1	8.105	31774	14.239
2	11.609	191371	85.761
Total		223145	100.000

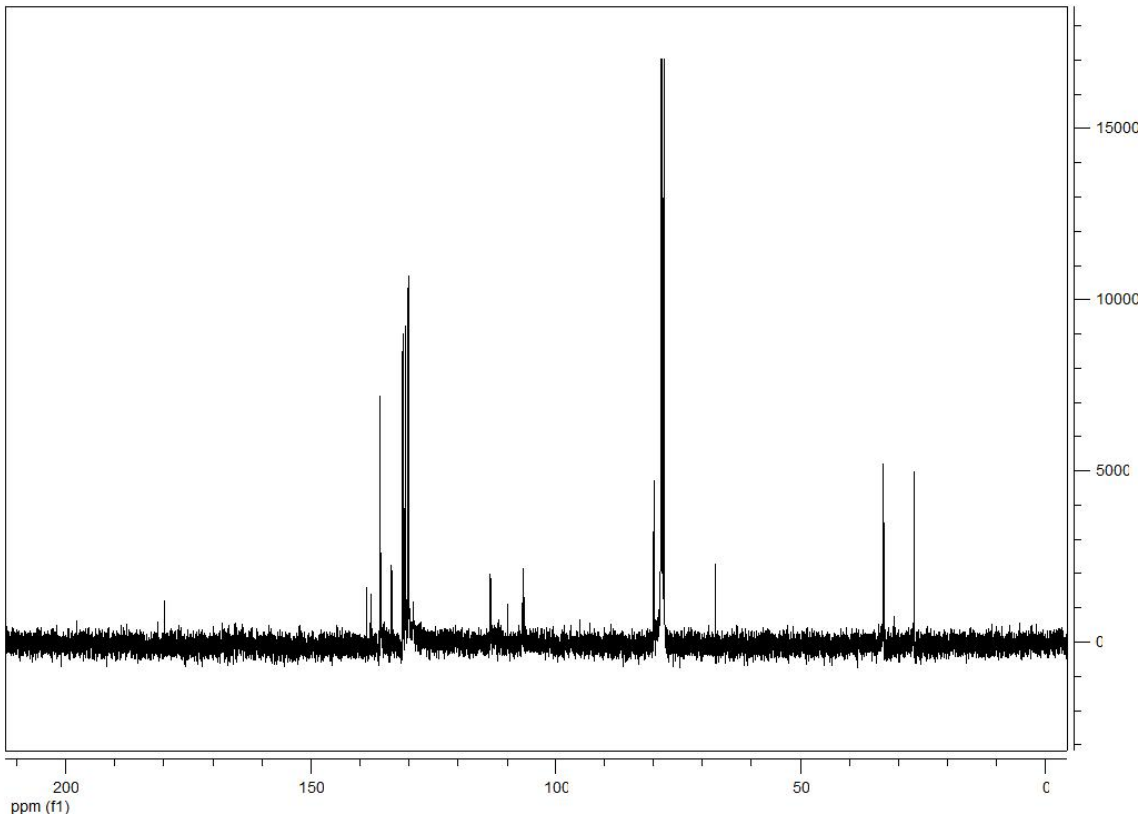


4-(2,2-Bis(phenylsulfonyl)ethyl)-2-(2,4-difluorophenyl)-4-methyloxazol-5(4*H*)-one 3g

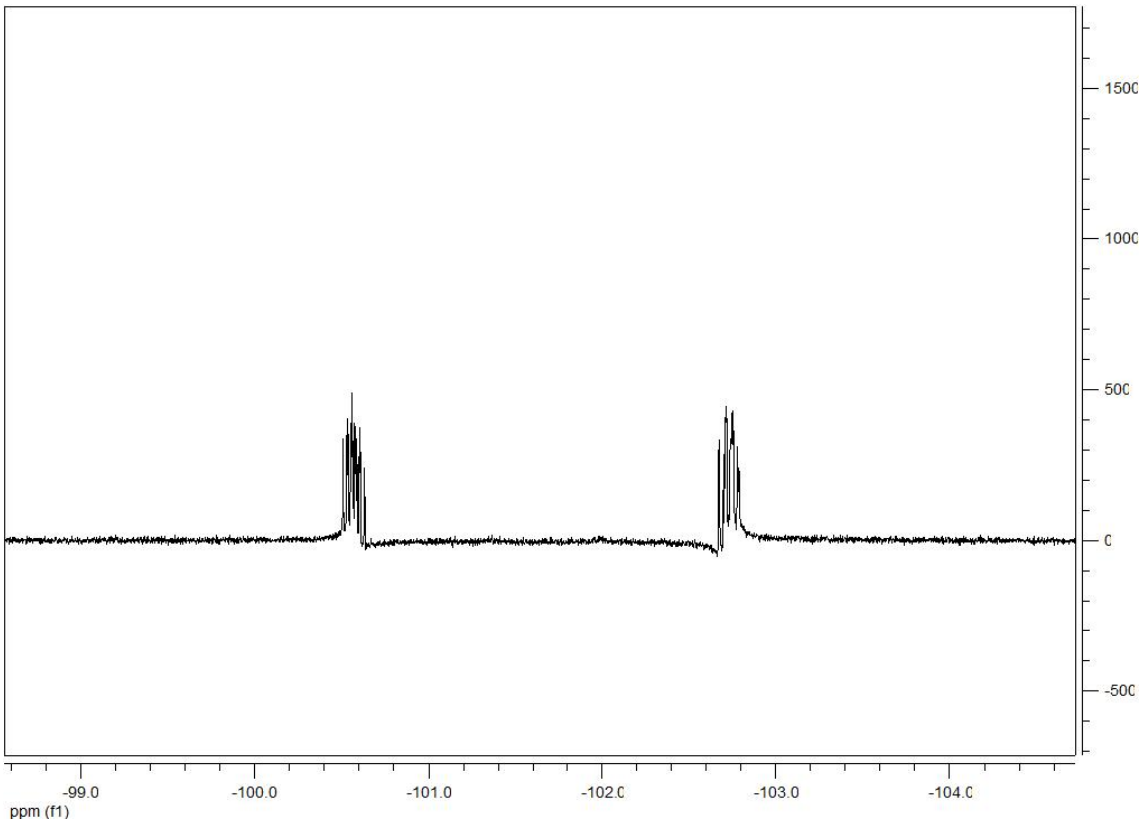
^{1}H-NMR



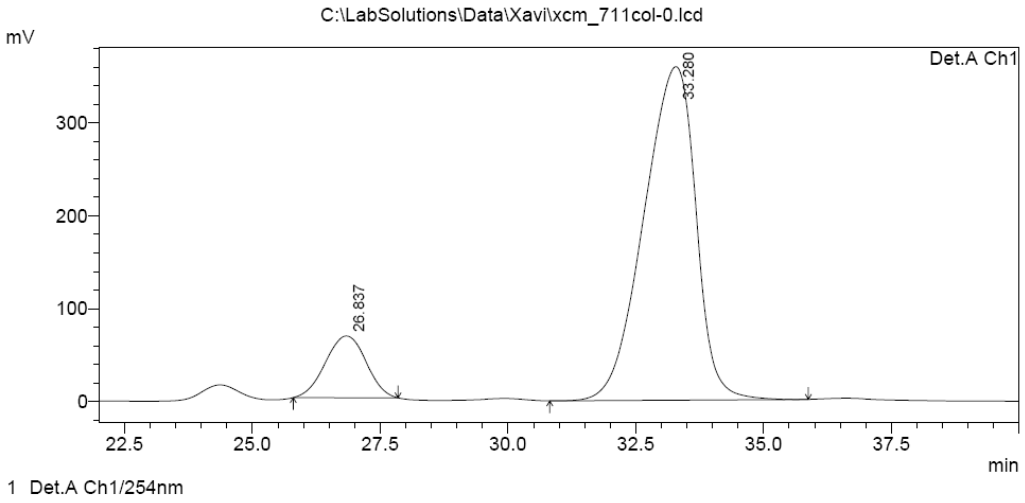
^{13}C-NMR


15000
10000
5000
0
200
150
100
50
0
ppm (f1)

^{19}F-NMR


1500
1000
500
0
-500
-99.0
-100.0
-101.0
-102.0
-103.0
-104.0
ppm (f1)

HPLC

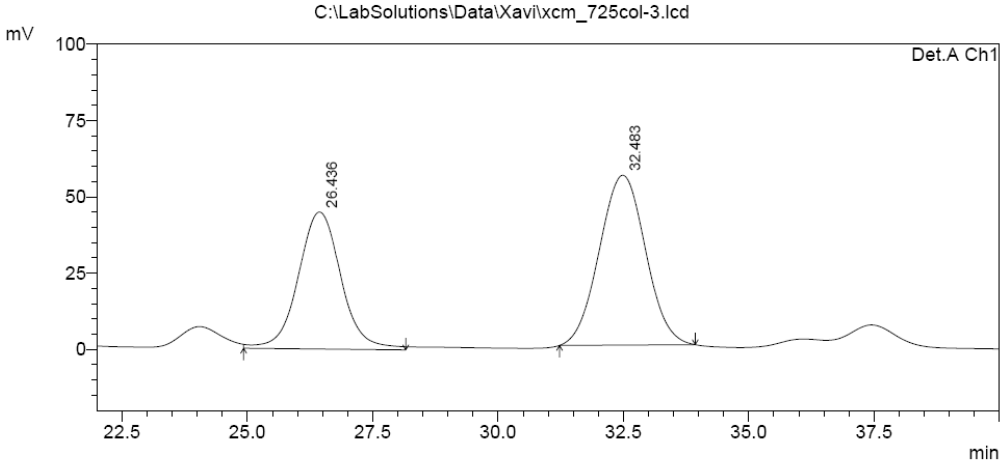


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.837	3680061	66454	12.649	15.615
2	33.280	25413186	359125	87.351	84.385
Total		29093247	425579	100.000	100.000



1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.436	2679608	44923	42.900	44.664
2	32.483	3566511	55657	57.100	55.336
Total		6246119	100580	100.000	100.000