Allylic-allylic alkylation with 3,5-dimethyl-4-nitroisoxazole. A route to dicarboxylic acid derivatives

by

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Supporting Information

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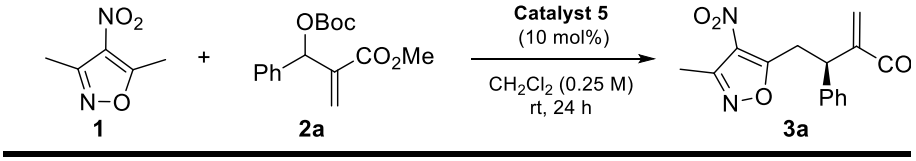
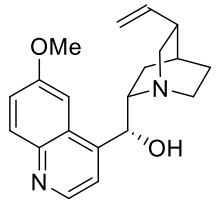
1. Screening results

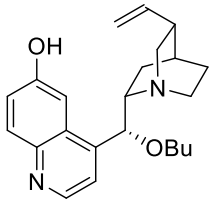
1.1. Catalyst screening



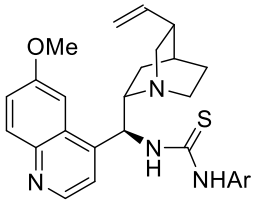
1 + 2a → 3a



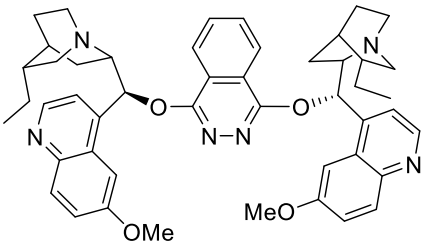
5a
3a: 26% yield
60:40 er



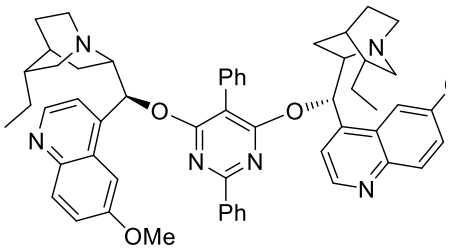
5b
3a: 22% yield
81:19 er



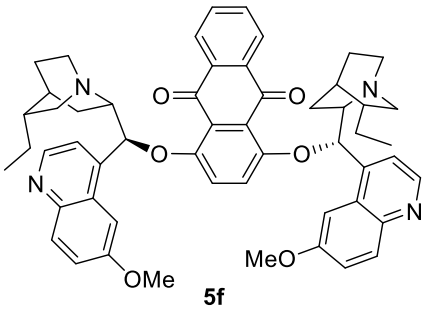
5c
Ar: 3,5-$(CF_3)_2C_6H_3$
3a: <5% conv.



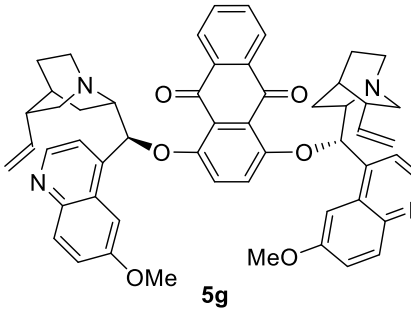
5d
3a: 22% yield
79:21 er



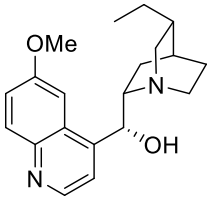
5e
3a: 41% yield
88:12 er



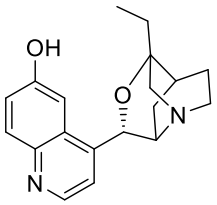
5f
3a: 43% yield
90:10 er



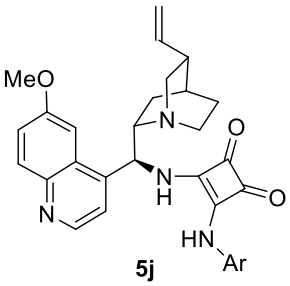
5g
3a: 38% yield
76:24 er



5h
3a: 22% yield
77:23 er

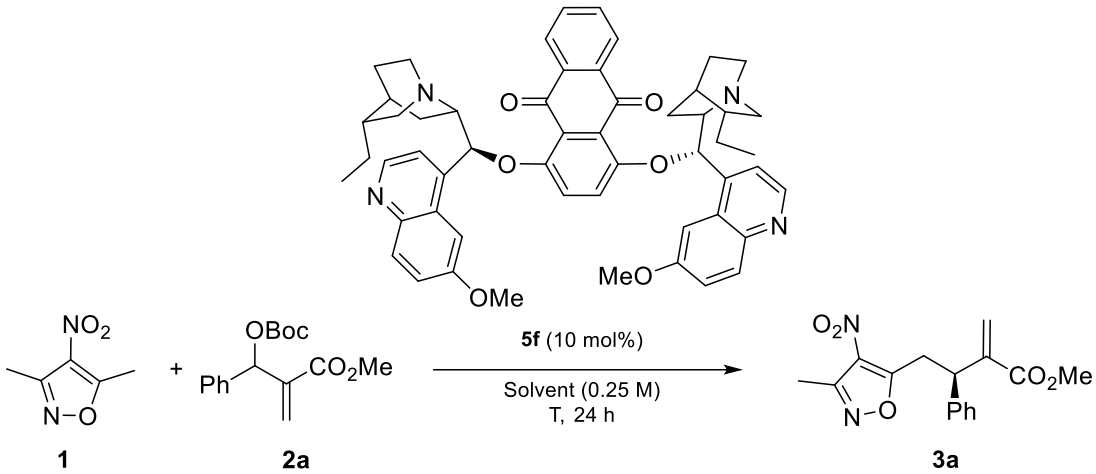


5i
3a: 32% yield
56:44 er



5j
Ar: 3,5-$(CF_3)_2C_6H_3$
3a: <5% conv.

1.2. Reaction conditions screening[a]

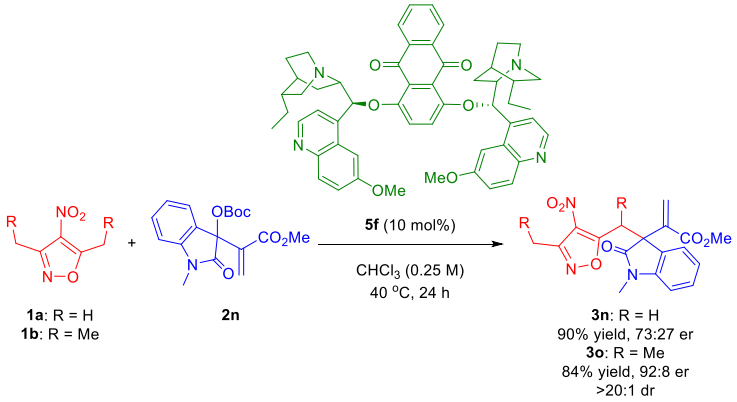


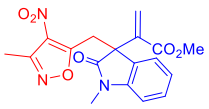
Entry	Solvent	T [°C][b]	Yield [%]	er[c]
1	CH_2Cl_2	rt	43	90:10
2	$CHCl_3$	rt	69	91:9
3	$ClCH_2CH_2Cl$	rt	40	86:14
4	Toluene	rt	19	89:11
5	THF	rt	36	87:13
6	1,4-Dioxane	rt	>5	nd
7	$AcOCH_3$	rt	39	84:16
8	CH_3CN	rt	80	89:11
9[d]	$CHCl_3$	rt	41	89:11
10[e]	$CHCl_3$	rt	66	90:10
11	$CHCl_3$	60	78	90:10
12	$CHCl_3$	50	85	92:8
13	$CHCl_3$	40	84	96:4
14	$CHCl_3$	10	20	92:8
15	$CHCl_3$	0	-	-
16[f]	$CHCl_3$	40	82	92:8
17[g]	$CHCl_3$	40	50	92:8
18[h]	$CHCl_3$	40	81	91:9
19[i]	$CHCl_3$	40	79	93:7

[a] Reactions performed on 0.1 mmol scale using **1** (1 equiv) and **2a** (1 equiv) in 0.4 mL of the solvent. [b] Isolated yields are given. [c] Determined by a chiral stationary phase HPLC. [d] Reaction was performed in 0.8 mL of CH_2Cl_2. [e] Reaction was performed in 0.2 mL of CH_2Cl_2. [f] Reaction was performed using **5f** (20 mol%). [g] Reaction was performed using **5f** (5 mol%). [h] Reaction was performed using **1** (1.5 equiv). [i] Reaction was performed using **2a** (1.5 equiv).

2. Additional scope experiments

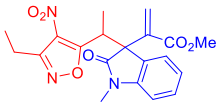
Following the general procedure (given in the manuscript file), further scope studies were performed to include isatin-derived MBH carbonate **2n** and 3,5-dimethyl-4-nitroisoxazole **1a** or 3,5-diethyl-4-nitroisoxazole **1b**. Absolute and relative configuration of the products was not assigned.





3n (*R*)-Methyl 2-(1-methyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)acrylate

Following the general procedure (given in the manuscript file), **3n** was isolated by FC on silica (hexane/ethyl acetate 20:1) in 90% yield as a pale-yellow oil. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.23 (td, *J* = 7.7, 1.2 Hz, 1H), 7.13 (d, *J* = 7.7 Hz, 1H), 6.94 (td, *J* = 7.7, 0.8 Hz, 1H), 6.75 (d, *J* = 7.7 Hz, 1H), 6.62 (s, 1H), 6.17 (s, 1H), 4.34 (d, *J* = 14.2 Hz, 1H), 3.80 (d, *J* = 14.2 Hz, 1H), 3.63 (s, 3H), 3.22 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 176.0, 169.5, 165.3, 155.2, 143.9, 138.5, 129.5, 129.2 (2C), 128.2, 123.5, 122.8, 108.4, 54.2, 52.4, 32.3, 26.8, 11.6. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{18}N_3O_6$ 372.1191; Found: 372.1204. The er was determined by UPC^2 using a chiral Chiralpack IA column gradient from 100% CO_2 up to 40%; *i*-PrOH, flow rate 2.5 mL/min; τ_{major} = 3.1 min, τ_{minor} = 2.8 min (73:27 er). $[\alpha]^{20}_D$ = -132.3 (*c* = 0.7, $CHCl_3$).



3o Methyl 2-((*R*)-3-((*S*)-1-(3-ethyl-4-nitroisoxazol-5-yl)ethyl)-1-methyl-2-oxoindolin-3-yl)acrylate

Following the general procedure (given in the manuscript file), **3o** was isolated by FC on silica (hexane/ethyl acetate 20:1) in 84% yield as a pale-yellow oil. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.25 (d, *J* = 7.7 Hz, 1H), 7.16 (td, *J* = 7.7, 1.2 Hz, 1H), 6.89 (td, *J* = 7.6, 1.0 Hz, 1H), 6.65 (d, *J* = 7.7 Hz, 1H), 6.58 (s, 1H), 6.12 (s, 1H), 5.28 (q, *J* = 7.2 Hz, 1H), 3.68 (s, 3H), 3.22 (s, 3H), 2.75 (q, *J* = 7.4 Hz, 2H), 1.58 (d, *J* = 7.2 Hz, 3H), 1.12 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 175.2, 174.1, 165.9, 159.5, 143.3, 137.8, 129.3, 129.2, 128.4 (2C), 123.8, 122.6, 108.1, 56.9, 52.4, 37.0, 26.6, 19.6, 12.8, 11.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{20}H_{22}N_3O_6$: 400.1504; Found: 400.1514. The er was determined by UPC^2 using a chiral Chiralpack IA column gradient from 100% CO_2 up to 40%; *i*-PrOH, flow rate 2.5 mL/min; τ_{major} = 5.6 min, τ_{minor} = 6.3 min (92:8 er). $[\alpha]^{20}_D$ = -121.3 (*c* = 0.8, $CHCl_3$).

3. Assignment of absolute configuration

Computational details

The theoretical approach we used in this work is common to all studied structures and includes (i) conformational search at molecular mechanics level (MM3); (ii) pre-optimization at the B3LYP/6-31G(d) level; (iii) re-optimization of conformers found at low-DFT level at B3LYP/6-311++G(d,p) level followed by frequency calculations to confirm stability of received structures; (iv) calculations on relative energies (ΔE_{DFT} and $\Delta\Delta G_{DFT}$) using Boltzmann distribution at T = 298.15 K; (v) rotator strengths calculations at the TD-DFT/6-311++G(d,p) level for all stable conformers of relative energies ranging from 0.0 to 2.0 kcal mol^{-1}.

Preliminary conformer distribution search was performed by the Scigress package[1] using the MM3 molecular mechanics force field. All possible conformers were analyzed using the systematic search methodology. Minimum energy conformers of relative steric energies (ΔE_{SE}) up to 10 kcal mol^{-1} found by molecular mechanics were further fully optimized at the B3LYP/6-31G(d) level as implemented in the Gaussian09 package.[2] Higher accuracy calculations were performed at the B3LYP/6-311++G(d,p) level.

The conformers obtained at the B3LYP/6-311++G(d,p) level were the real minima (no imaginary frequencies have been found). Total and free energy values have been calculated and used to obtain the Boltzmann population of conformers at 298.15 K. Only the results for conformers that differ from the most stable one by less than 2 kcal mol^{-1} have been taken into account for further calculations, following a generally accepted protocol.[3]

The TD-DFT/6-311++G(2d,2p) calculations of ECD of **3a** and **3g** were performed for all structures re-optimized at higher level of theory. We used two different density functionals for calculations of rotatory strengths, namely CAM-B3LYP[4] and M06-2X functional.[5] Rotatory strengths were calculated using both length and velocity representations. In the present study, the differences between the length and velocity representations of the calculated values of rotatory strengths were quite small, and for this reason only the velocity representations were further used. The CD spectra were simulated by overlapping Gaussian functions for each transition according to the procedure previously described and using half band width 0.4 eV.[6] It should be noted, that there are not substantial differences between ECD spectra calculated with these two functionals for the same molecule, therefore we discussed here only results obtained with the use of CAM-B3LYP functional. Many authors indicate CAM-B3LYP functional as the best suited for TD-DFT calculations. The results obtained with the use of CAM-B3LYP functional are comparable to results obtained with the use of more sophisticated EOM-CCSD method.[7-11]

The solvent effect on structure and ECD spectra was not taken into account, since the experimental ECD measurements were done in non-polar cyclohexane.

References:

[1] Scigress 2.5, Fujitsu Ltd.
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Table S1. Total and Gibbs free energies (*E*, *ΔG*, in Hartree), relative energies (*ΔE*, *ΔΔG*, in kcal mol^{-1}), *ΔE*- and *ΔΔG*-based percentage populations (%*ΔE*, %*ΔΔG*) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of **3a**.

Conf. no.[a]	*E*	*ΔG*	*ΔE*	%*ΔE*	*ΔΔG*	%*ΔΔG*	#ImFreq
1	-1105.15135	-1104.90364	0.62	8.41	0.19	12.6	0
2	-1105.14993	-1104.90229	1.51	1.87	1.04	3.01	0
3	-1105.15082	-1104.90249	0.95	4.8	0.92	3.71	0
4	-1105.15064	-1104.90307	1.07	3.96	0.55	6.85	0
5	-1105.15106	-1104.90255	0.80	6.21	0.88	3.98	0
6	-1105.15234	-1104.90395	0.00	24.05	0.00	17.47	0
7	-1105.14934	-1104.9026	1.88	1.01	0.85	4.18	0
8	-1105.15107	-1104.90294	0.79	6.28	0.63	5.98	0
9	-1105.15121	-1104.90325	0.71	7.3	0.44	8.30	0
10	-1105.14889	-1104.90088	2.16	-	1.93	0.68	0
11	-1105.15084	-1104.90266	0.94	4.93	0.81	4.46	0
13	-1105.15182	-1104.90349	0.33	13.85	0.29	10.76	0
14	-1105.14922	-1104.90112	1.96	0.88	1.77	0.88	0
15	-1105.15091	-1104.90307	0.89	5.31	0.55	6.92	0
17	-1105.15085	-1104.90268	0.93	4.96	0.8	4.55	0
21	-1105.15055	-1104.9023	1.12	3.6	1.03	3.05	0
23	-1105.14954	-1104.90083	1.75	1.24	1.96	0.64	0
24	-1105.14875	-1104.90132	2.25	-	1.65	1.08	0
25	-1105.1496	-1104.90118	1.72	1.32	1.74	0.93	0

[a] Conformers are numbered according to their appearance during conformational search.

Table S2. Total and Gibbs free energies (*E*, *ΔG*, in Hartree), relative energies (*ΔE*, *ΔΔG*, in kcal mol^{-1}), *ΔE*- and *ΔΔG*-based percentage populations (%*ΔE*, %*ΔΔG*) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP/6-311++G(d,p) level for individual conformers of **3g**

Conf. no.[a]	*E*	*ΔG*	*ΔE*	%*ΔE*	*ΔΔG*	%*ΔΔG*	#ImFreq
1	-1144.48094	-1144.20917	0.61	9.47	0.24	13.47	0
2	-1144.47951	-1144.20744	1.5	2.08	1.33	2.13	0
3	-1144.48042	-1144.20787	0.93	5.45	1.05	3.39	0
4	-1144.48021	-1144.20882	1.06	4.38	0.46	9.23	0
5	-1144.48069	-1144.2079	0.76	7.29	1.04	3.49	0
6	-1144.48191	-1144.20955	0	26.36	0	20.04	0
7	-1144.47891	-1144.20782	1.88	1.1	1.09	3.19	0
8	-1144.48058	-1144.20829	0.83	6.47	0.79	5.26	0
9	-1144.48075	-1144.20888	0.73	7.73	0.42	9.89	0
10	-1144.47848	-1144.20646	2.15	-	1.94	0.76	0
11	-1144.48047	-1144.20784	0.9	5.74	1.07	3.27	0
13	-1144.48133	-1144.20916	0.36	14.37	0.25	13.22	0
15	-1144.47869	-1144.20654	2.02	-	1.89	0.82	0
17	-1144.48042	-1144.20858	0.94	5.43	0.61	7.16	0
19	-1144.47795	-1144.20639	2.49	-	1.98	0.7	0
21	-1144.48016	-1144.20784	1.1	4.14	1.07	3.28	0
22	-1144.47688	-1144.20637	3.15	-	1.99	0.69	0

[a] Conformers are numbered according to their appearance during conformational search.

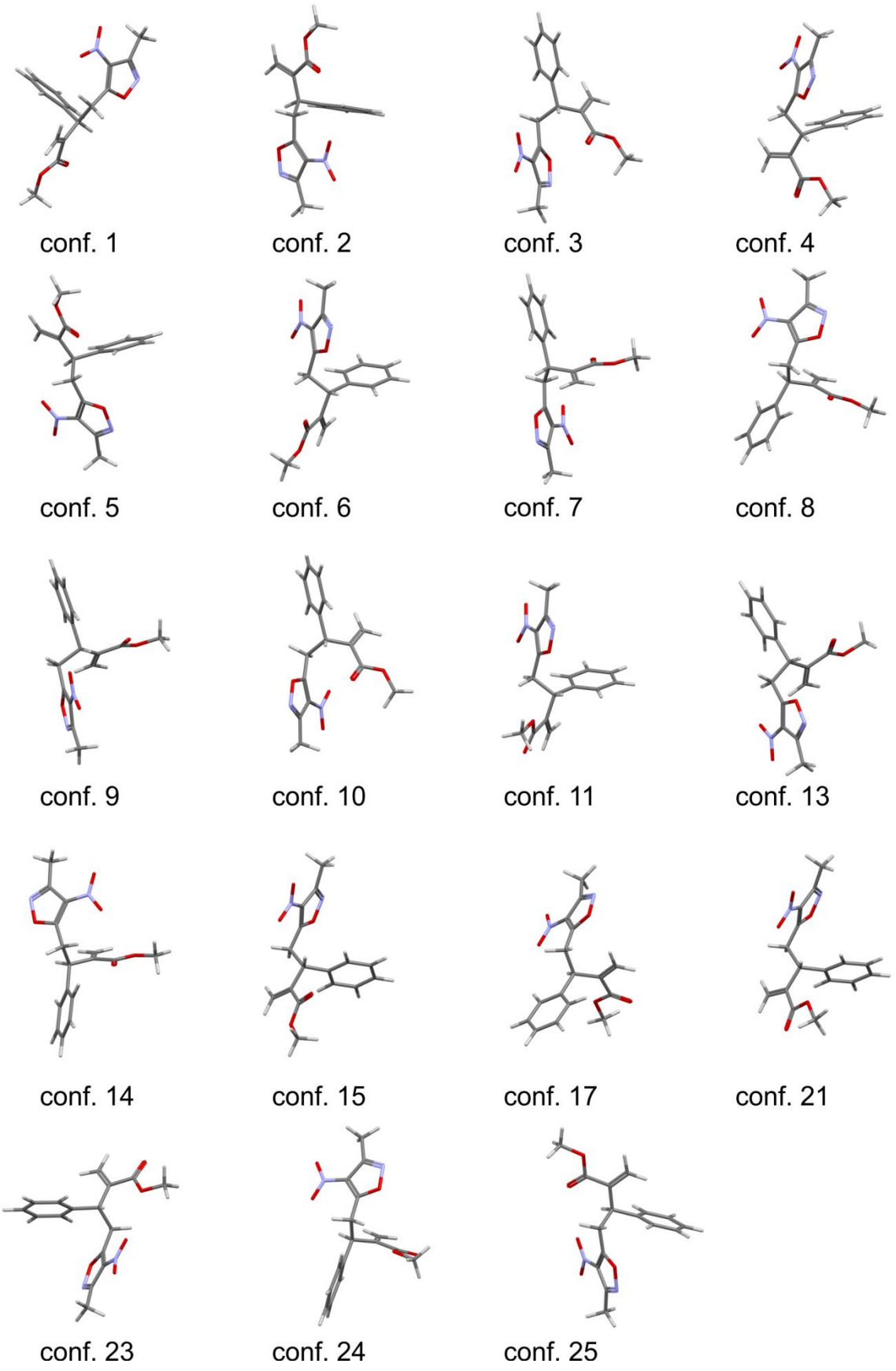

Figure S1. Structures of individual, low-energy conformers of **3a**, calculated at the B3LYP/6-311++G(d,p) level of theory

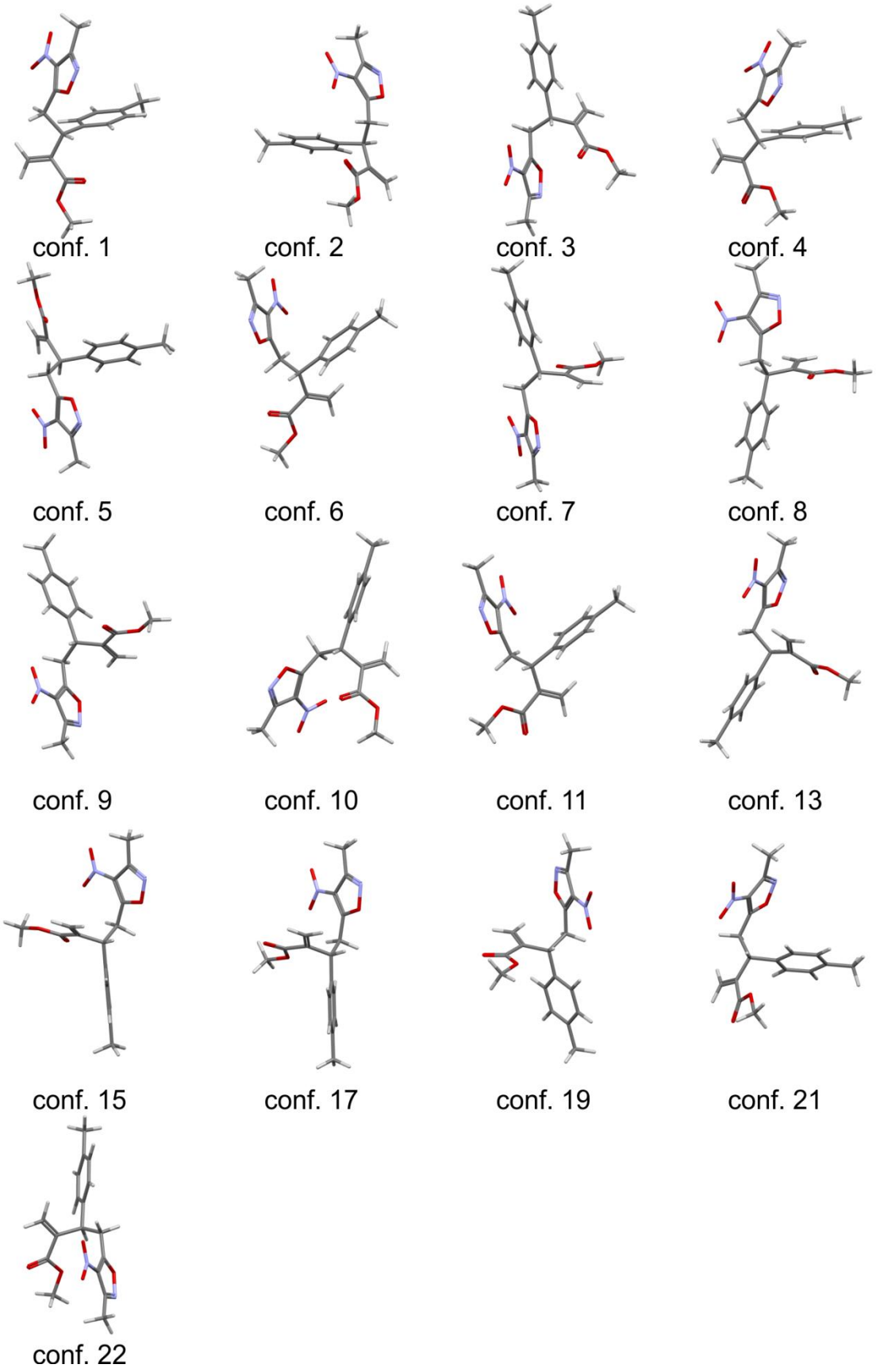

Figure S2. Structures of individual, low-energy conformers of **3g**, calculated at the B3LYP/6-311++G(d,p) level of theory

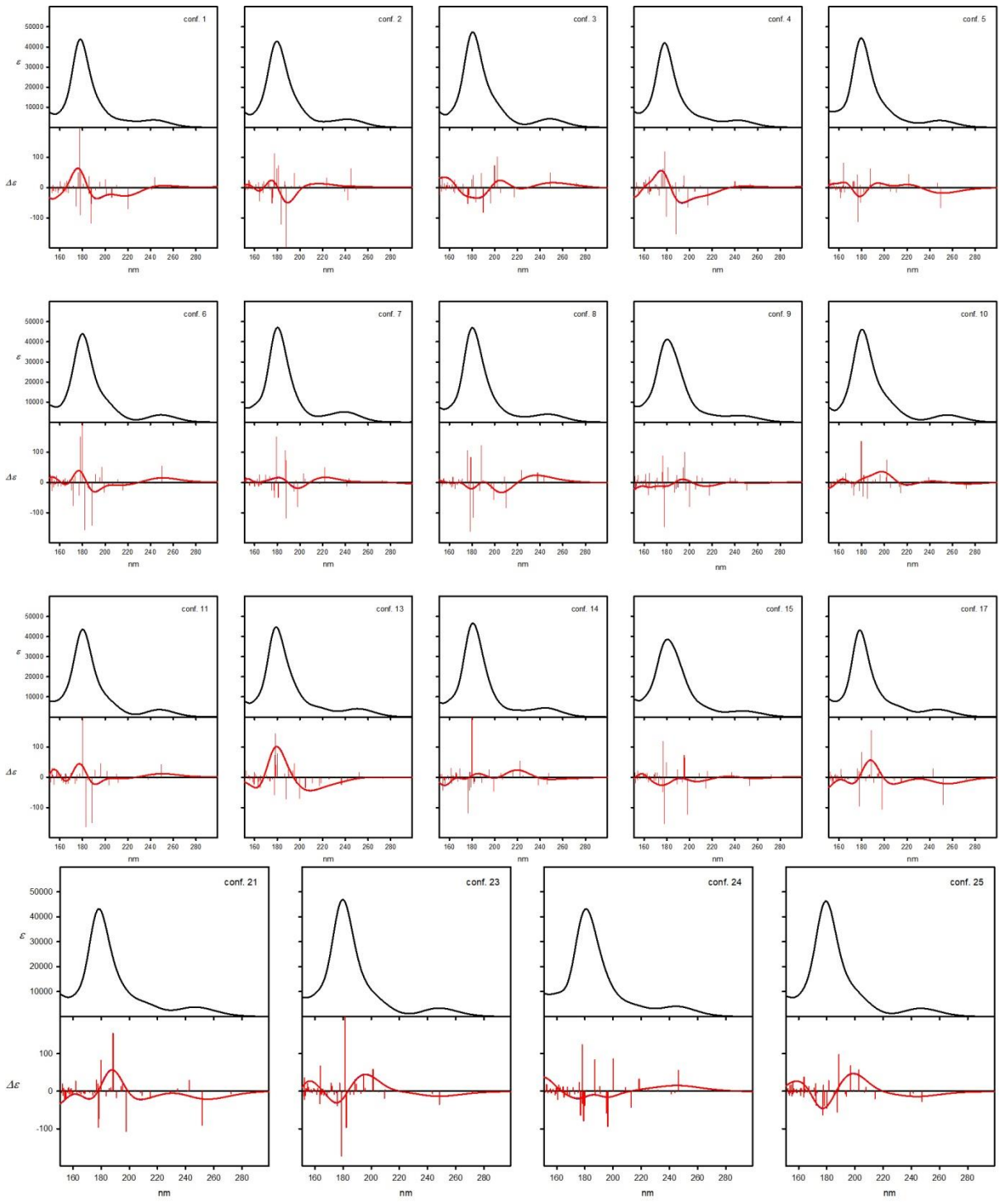

Figure S3. UV and ECD spectra of the low-energy conformers of compound **3a** calculated at TD-CAM-B3LYP/6-311++G(2d,2p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected

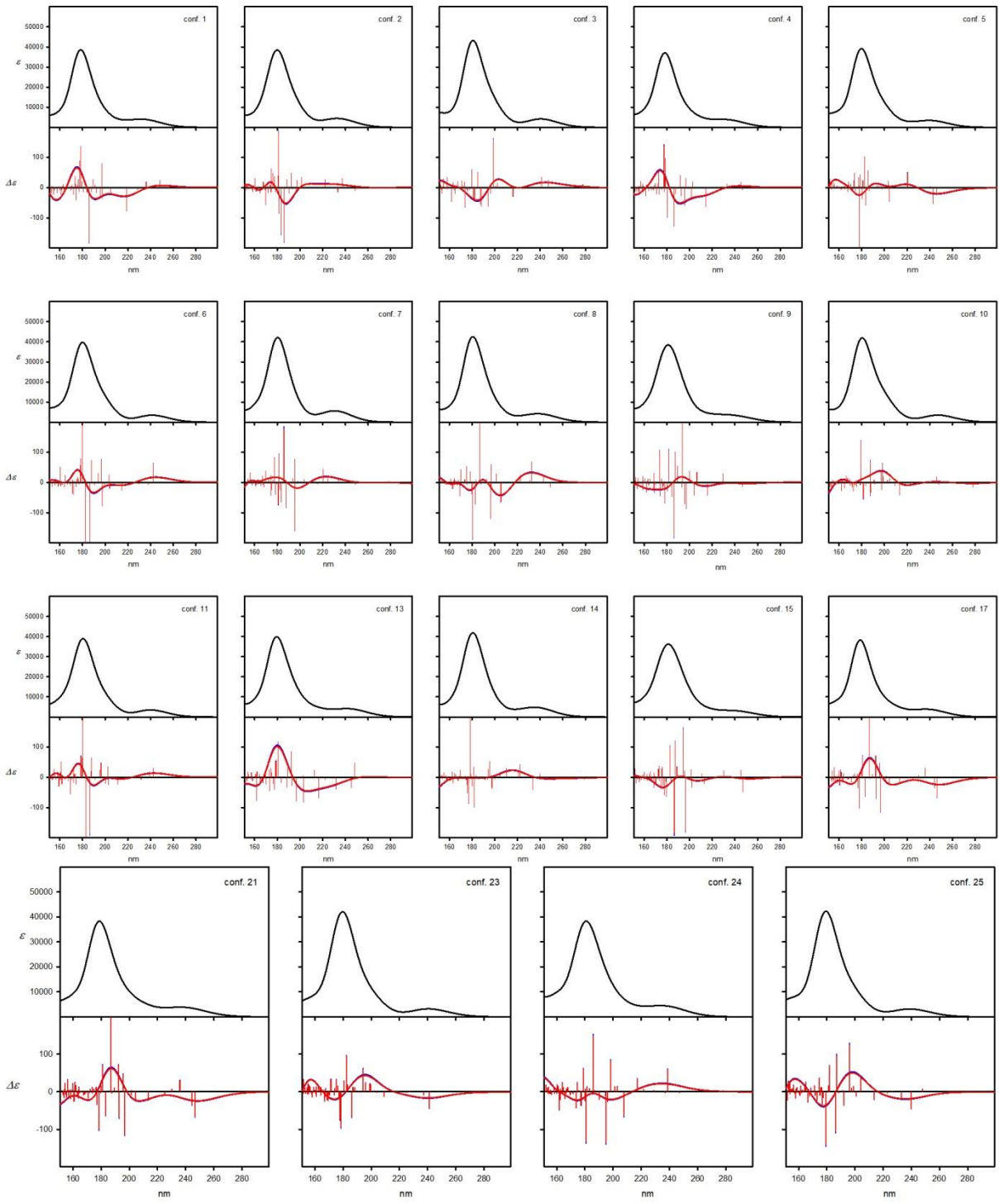

Figure S4. UV and ECD spectra of the low-energy conformers of compound **3a** calculated at TD-M06-2X/6-311++G(2d,2p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected

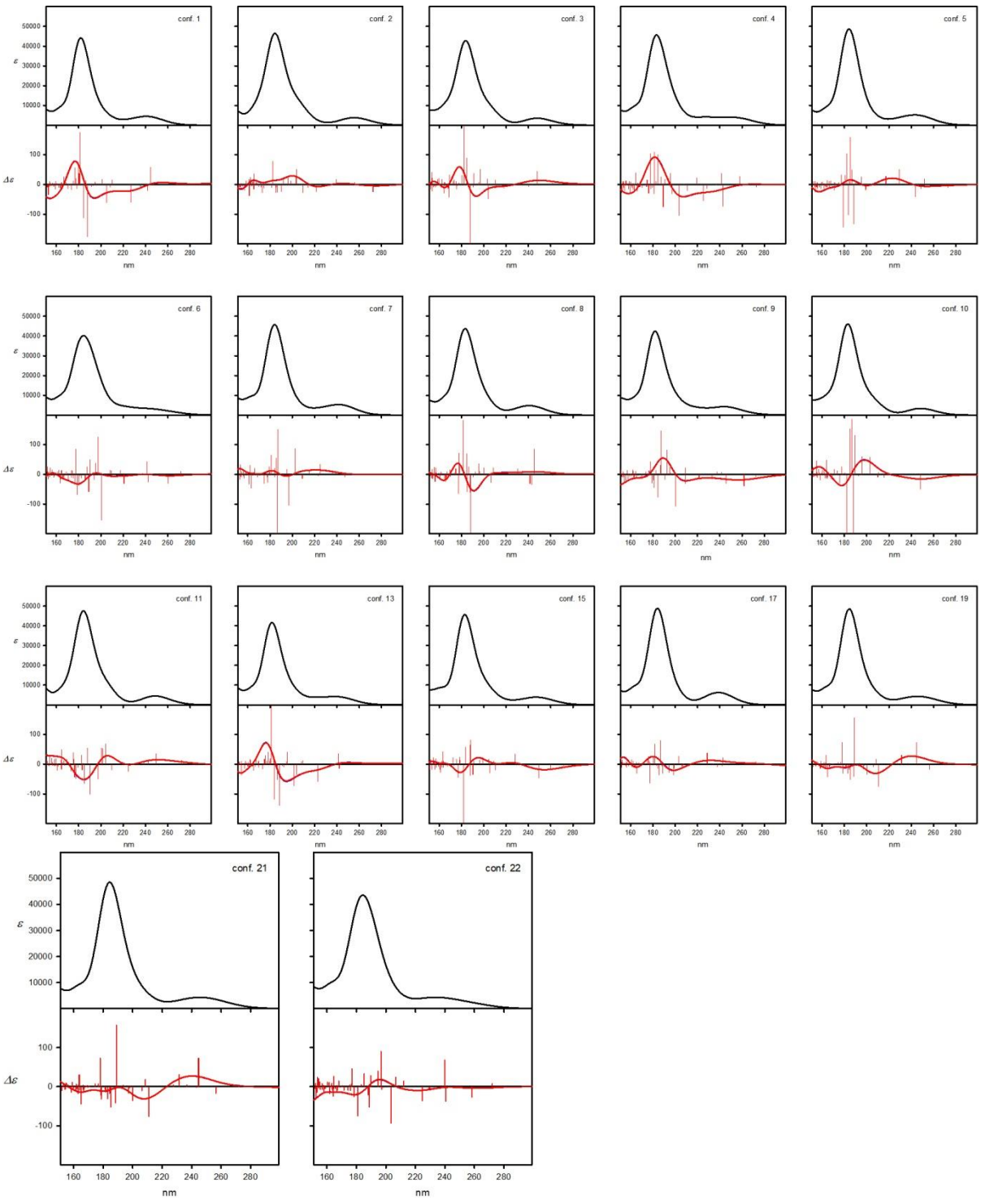

Figure S5. UV and ECD spectra of the low-energy conformers of compound **3g** calculated at TD-CAM-B3LYP/6-311++G(2d,2p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected

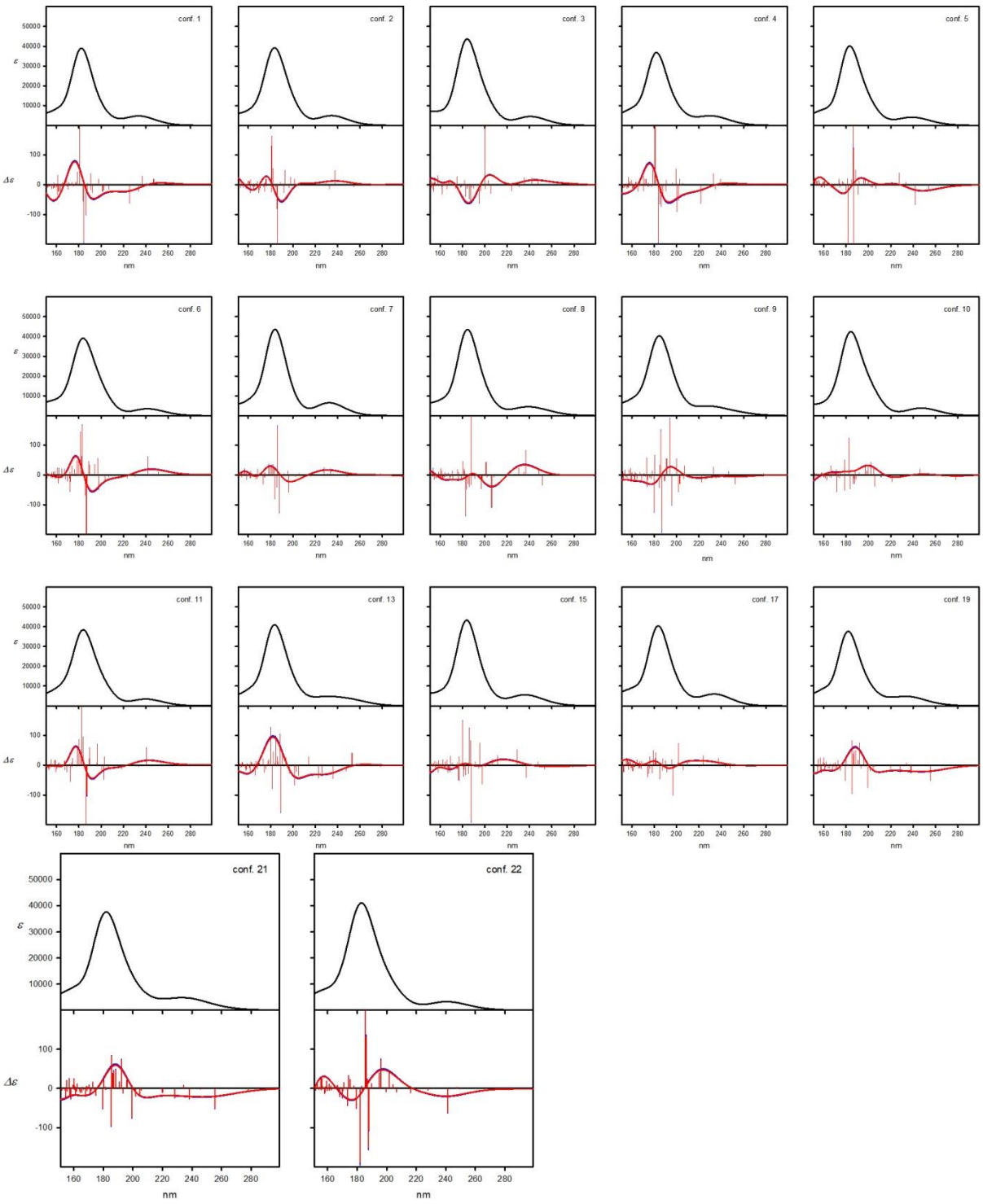

Figure S6. UV and ECD spectra of the low-energy conformers of compound **3g** calculated at TD-M06-2X/6-311++G(2d,2p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected

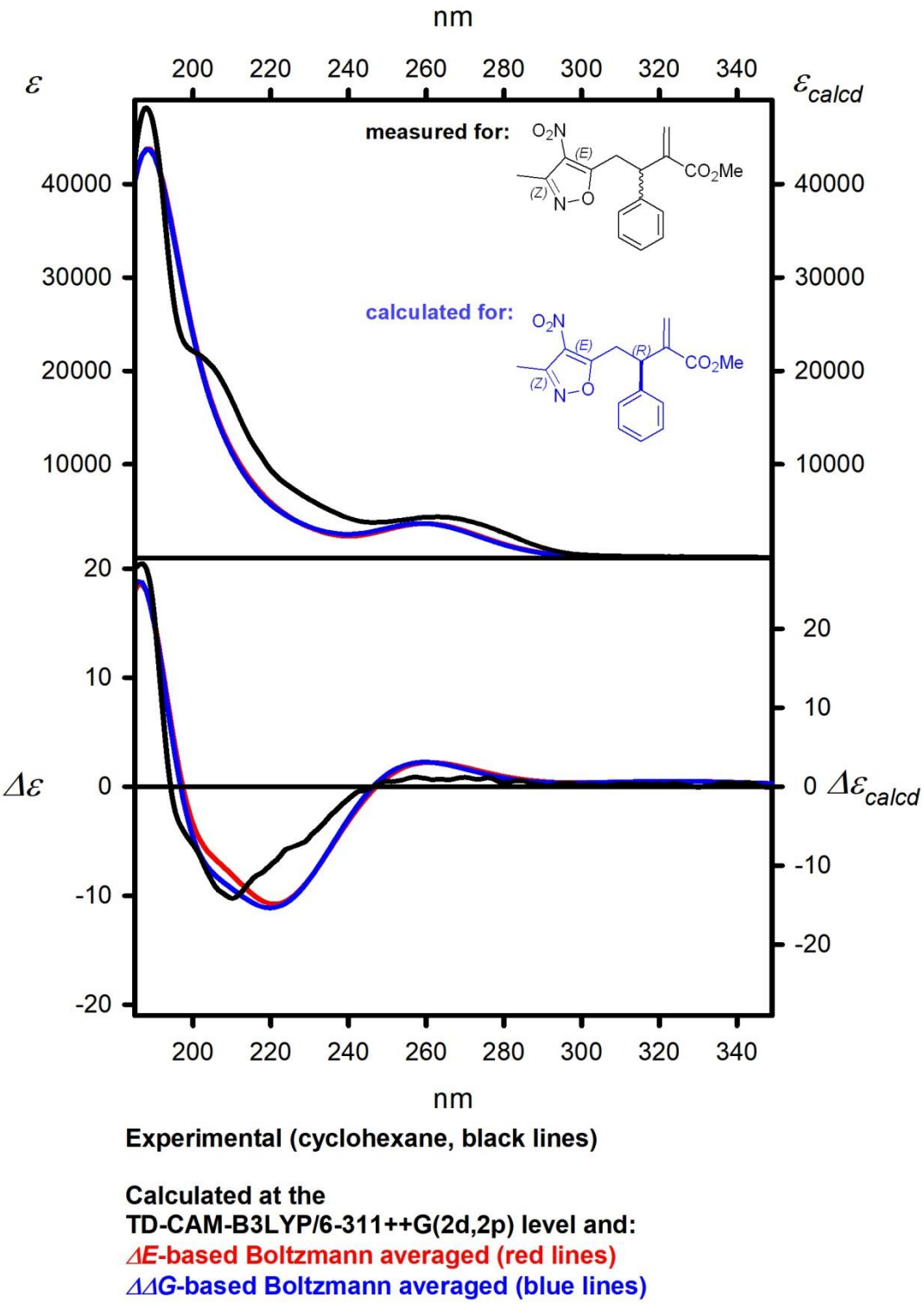

Figure S7. UV (upper panel) and ECD (lower panel) spectra of **3a**, measured in cyclohexane (solid black line) and calculated at TD-CAM-B3LYP/6-311++G(2d,2p) level and *ΔE*-based Boltzmann averaged (solid red lines) and *ΔΔG*-based Boltzmann averaged (solid blue lines). Wavelengths have been corrected to match experimental UV maximum

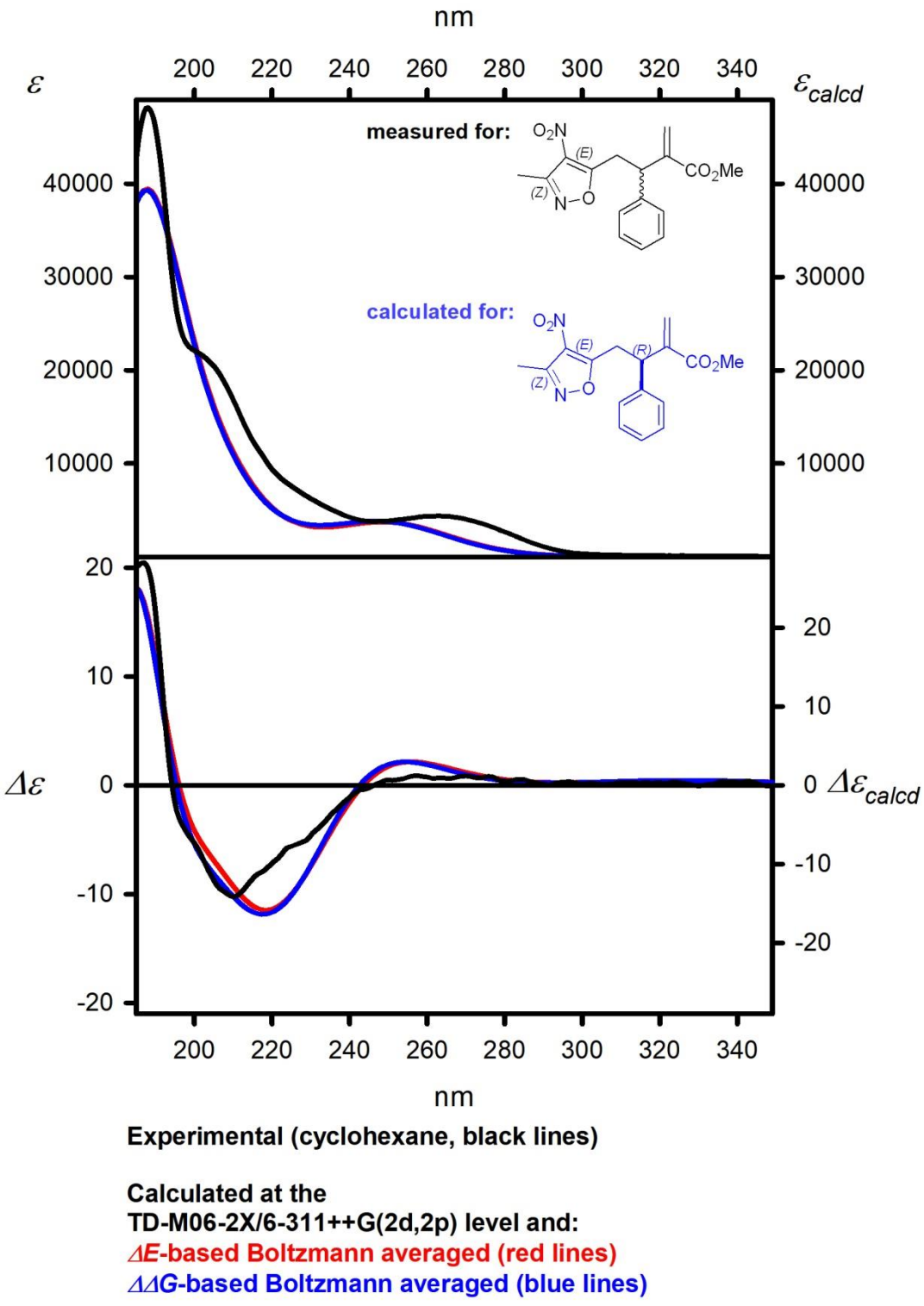

Figure S8. UV (upper panel) and ECD (lower panel) spectra of **3a**, measured in cyclohexane (solid black line) and calculated at TD-M06-2X/6-311++G(2d,2p) level and *ΔE*-based Boltzmann averaged (solid red lines) and *ΔΔG*-based Boltzmann averaged (solid blue lines). Wavelengths have been corrected to match experimental UV maximum

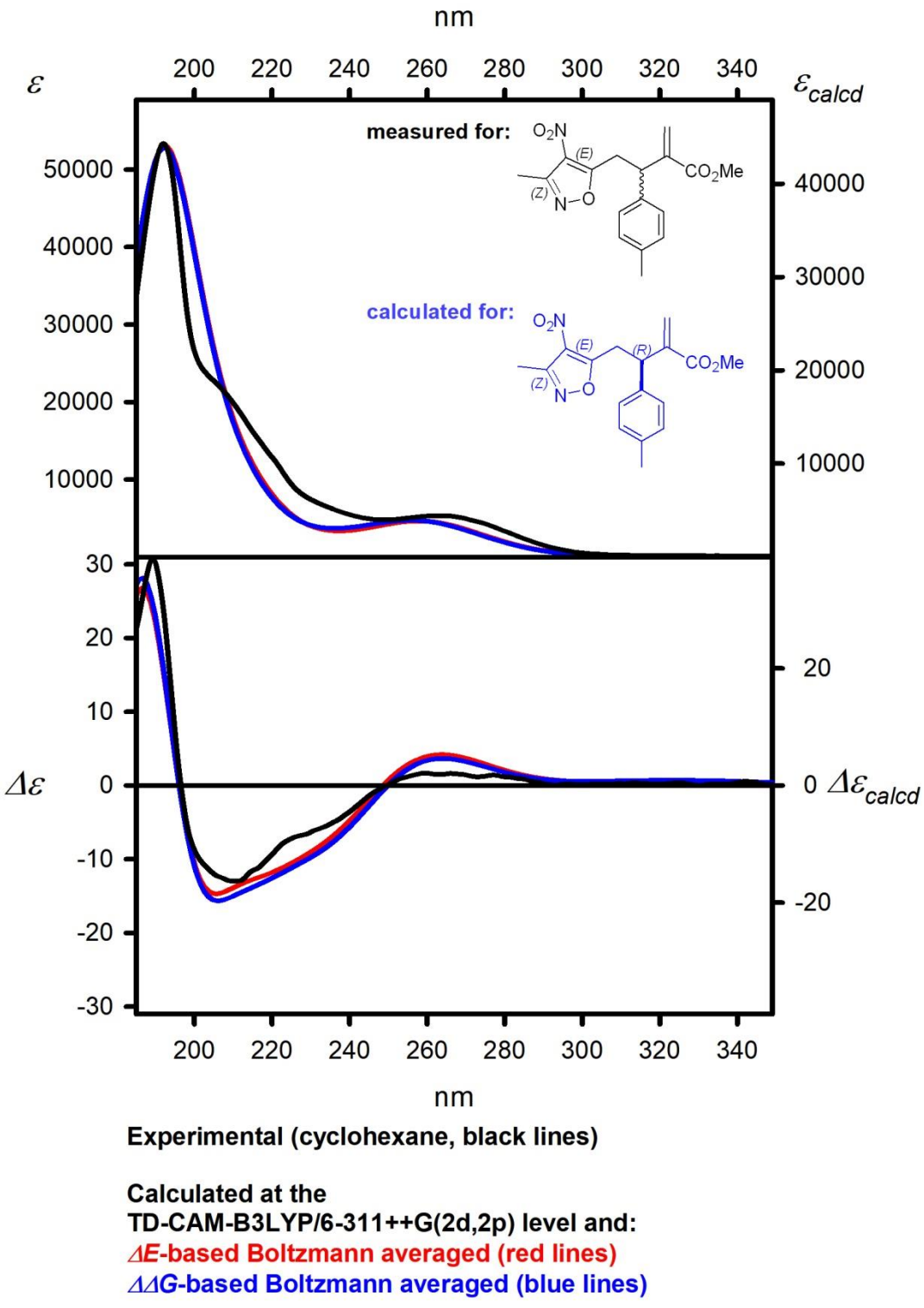

Figure S9. UV (upper panel) and ECD (lower panel) spectra of **3g**, measured in cyclohexane (solid black line) and calculated at TD-CAM-B3LYP/6-311++G(2d,2p) level and *ΔE*-based Boltzmann averaged (solid red lines) and *ΔΔG*-based Boltzmann averaged (solid blue lines). Wavelengths have been corrected to match experimental UV maximum

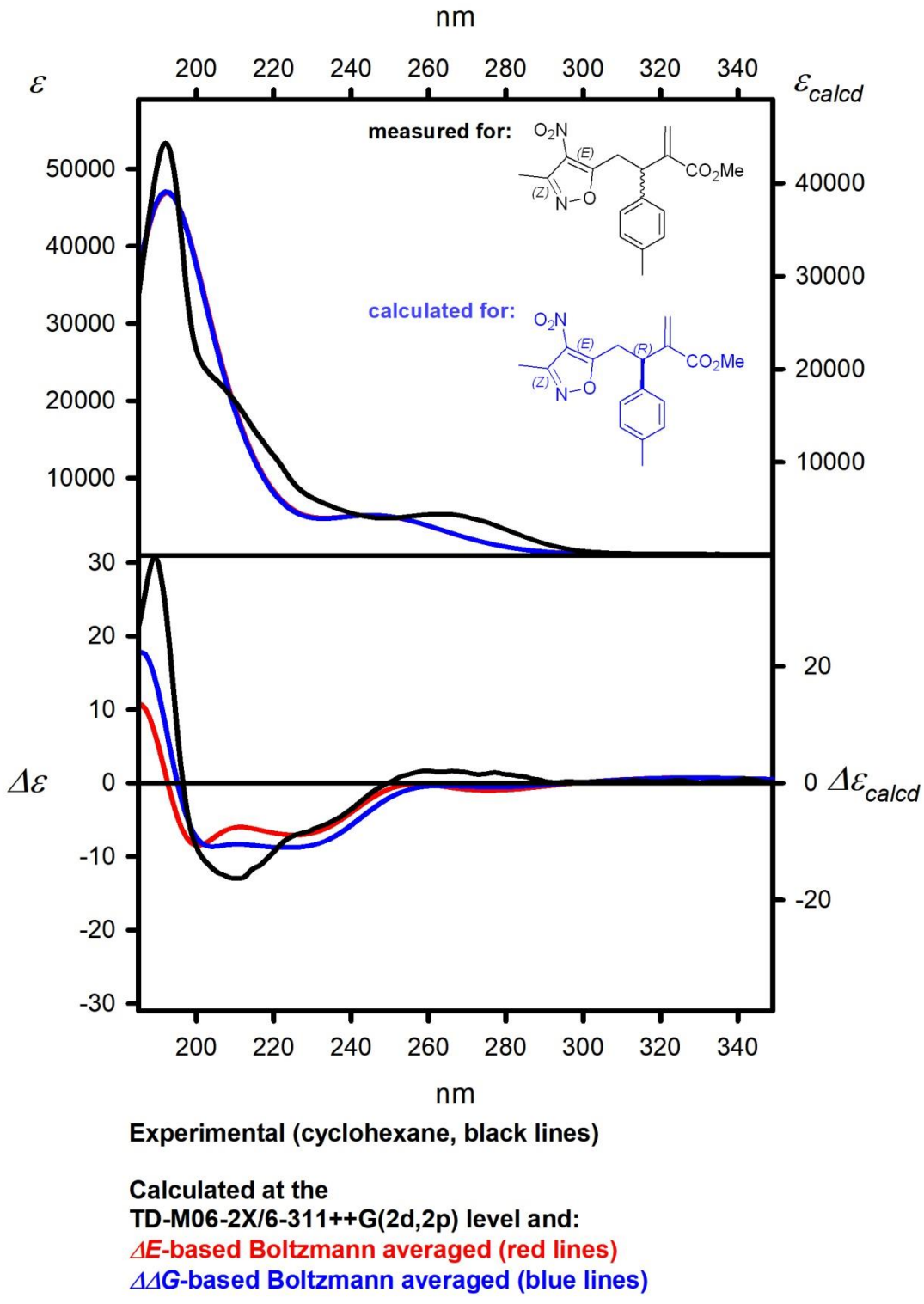

Figure S10. UV (upper panel) and ECD (lower panel) spectra of **3g**, measured in cyclohexane (solid black line) and calculated at TD-M06-2X/6-311++G(2d,2p) level and *ΔE*-based Boltzmann averaged (solid red lines) and *ΔΔG*-based Boltzmann averaged (solid blue lines). Wavelengths have been corrected to match experimental UV maximum

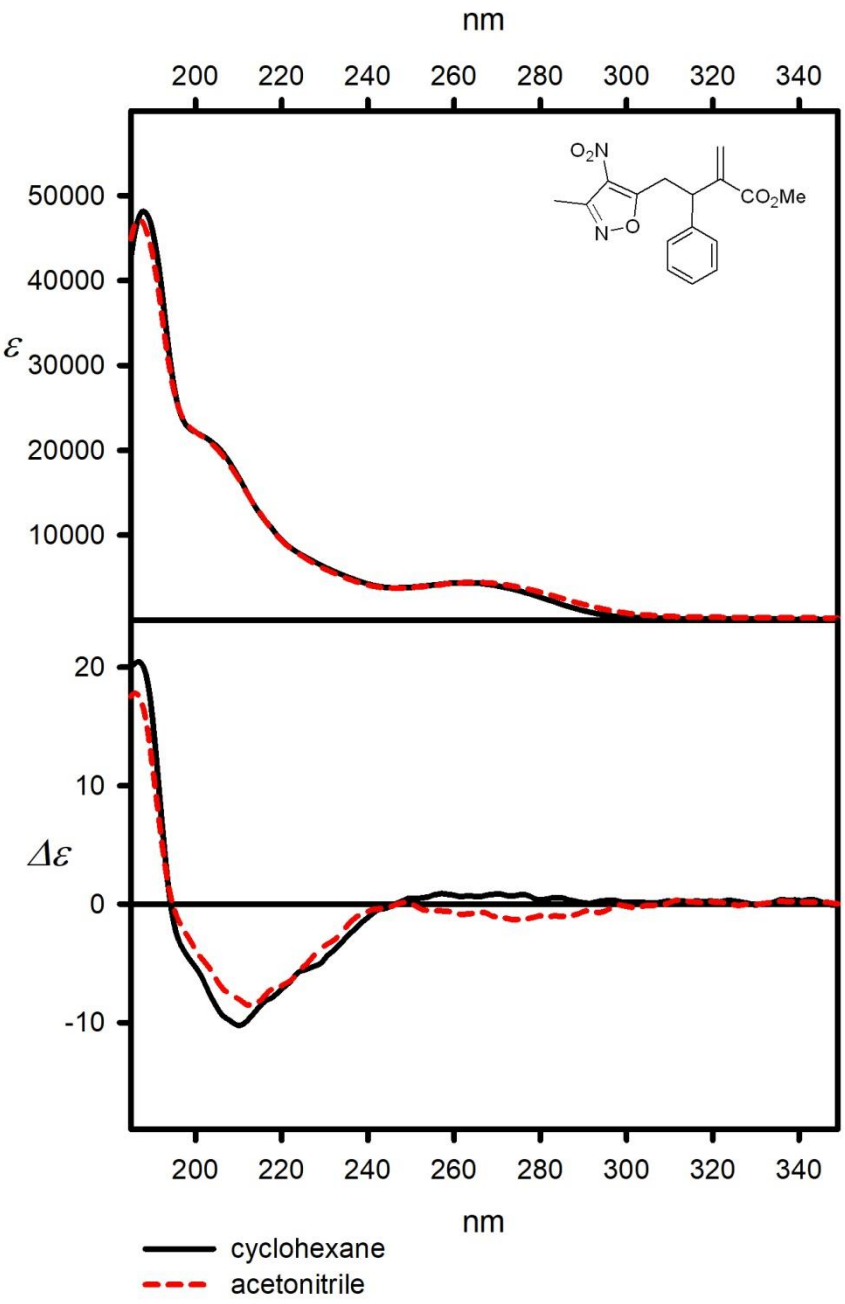

Figure S11. UV (upper panel) and ECD (lower panel) spectra of **3a**, measured in cyclohexane (solid black lines) and acetonitrile (red dashed lines) solution

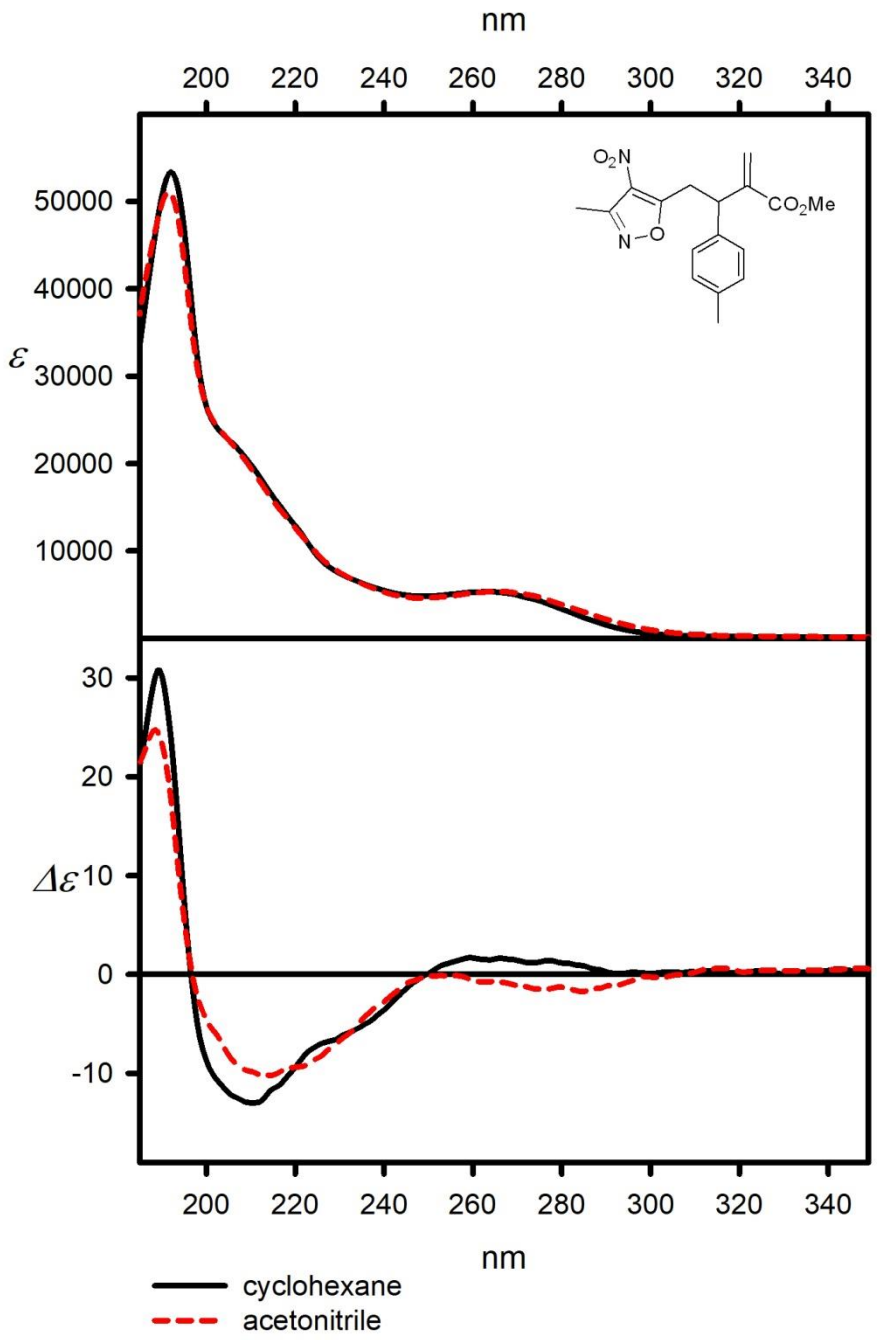

Figure S12. UV (upper panel) and ECD (lower panel) spectra of **3g**, measured in cyclohexane (solid black lines) and acetonitrile (red dashed lines) solution

Cartesian coordinates for all calculated structures

3a				
Conf. no.[a]				
1	N	-2.80040000	-1.08920000	2.08530000
	C	-3.51330000	-0.65420000	1.08480000
	C	-2.73000000	-0.67880000	-0.11500000
	C	-1.49470000	-1.15170000	0.24890000
	O	-1.52330000	-1.40110000	1.55510000
	C	-4.92600000	-0.23430000	1.30740000
	C	-0.22030000	-1.42550000	-0.46810000
	C	0.97900000	-0.64500000	0.12360000
	C	0.75550000	0.86730000	0.07550000
	C	0.64470000	1.54320000	-1.14150000
	C	0.41510000	2.91390000	-1.17450000
	C	0.29860000	3.63180000	0.01220000
	C	0.41350000	2.96940000	1.22910000
	C	0.64070000	1.59670000	1.25890000
	C	2.29150000	-1.02950000	-0.53670000
	C	2.41890000	-1.62250000	-1.72340000
	C	3.50210000	-0.71110000	0.28840000
	O	4.65450000	-0.78560000	-0.40360000
	O	3.45300000	-0.42910000	1.46320000
	C	5.84950000	-0.52790000	0.35580000
	N	-3.15850000	-0.28680000	-1.42330000
	O	-4.27860000	0.20880000	-1.52070000
	O	-2.39600000	-0.46970000	-2.37100000
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	H	-5.60240000	-0.81180000	0.67940000
	H	-5.05940000	0.81270000	1.04120000
	H	-0.01690000	-2.49680000	-0.39380000
	H	-0.37740000	-1.18850000	-1.51460000
	H	1.07110000	-0.91660000	1.17370000
	H	0.74000000	1.00090000	-2.07300000
	H	0.32810000	3.42020000	-2.12610000
	H	0.12190000	4.69840000	-0.01290000
	H	0.32900000	3.51850000	2.15700000
	H	0.73970000	1.08840000	2.20820000
	H	3.39310000	-1.85180000	-2.12590000
	H	1.56340000	-1.89620000	-2.32360000
	H	5.82170000	0.47490000	0.77590000
	H	6.66680000	-0.62480000	-0.35110000
	H	5.95040000	-1.25120000	1.16210000
2	N	3.24760000	-0.45570000	-1.96490000
	C	3.65590000	-0.47820000	-0.72750000
	C	2.55720000	-0.78370000	0.14050000
	C	1.46180000	-0.93610000	-0.67170000
	O	1.86100000	-0.74450000	-1.92790000
	C	5.08870000	-0.21020000	-0.41520000

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	C	-0.62960000	1.34550000	1.03530000
	C	-0.50420000	2.60660000	1.61060000
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	C	-0.63110000	3.62180000	-0.56280000
	C	-0.75450000	2.36140000	-1.13590000
	C	-2.36140000	-0.60340000	-1.12010000
	C	-2.99240000	-0.69940000	-2.29120000
	C	-3.06670000	-0.97110000	0.14670000
	O	-4.40350000	-1.04900000	0.00360000
	O	-2.50540000	-1.19600000	1.19500000
	C	-5.13050000	-1.44690000	1.18060000
	N	2.60590000	-0.90440000	1.56630000
	O	3.68250000	-0.66750000	2.11110000
	O	1.58440000	-1.23720000	2.16220000
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	H	5.53010000	-1.05230000	0.11500000
	H	5.18310000	0.65920000	0.23300000
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	H	-0.16160000	-1.42730000	0.58420000
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	H	-0.84330000	2.27320000	-2.21150000
	H	-4.02440000	-1.00790000	-2.35240000
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	C	-0.29060000	-0.70960000	-1.09460000
	C	-1.09630000	0.06520000	-0.00340000
	C	-2.56190000	-0.34180000	-0.00220000
	C	-3.27240000	-0.63900000	-1.16660000
	C	-4.62000000	-0.98690000	-1.11260000
	C	-5.28000000	-1.04460000	0.10870000
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	C	-3.23770000	-0.40910000	1.21900000
	C	-0.89830000	1.57460000	-0.12170000
	C	-1.73930000	2.39770000	-0.74700000
	C	0.31890000	2.11210000	0.56430000
	O	0.55940000	3.40700000	0.29800000

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	C	1.71760000	3.96870000	0.94280000
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	H	-5.15000000	-1.21620000	-2.02710000
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	H	-2.70080000	-0.19410000	2.13390000
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	H	1.75510000	5.00260000	0.61630000
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	C	-2.67970000	-0.62760000	-0.03250000
	C	-1.44230000	-1.13730000	0.26740000
	O	-1.40020000	-1.35740000	1.57910000
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	C	-0.22320000	-1.47110000	-0.51680000
	C	1.03880000	-0.72350000	-0.01250000
	C	0.85310000	0.79260000	-0.08920000
	C	0.84660000	1.45850000	-1.31620000
	C	0.63540000	2.83140000	-1.37810000
	C	0.43050000	3.56130000	-0.21130000
	C	0.43910000	2.90870000	1.01650000
	C	0.64980000	1.53450000	1.07500000
	C	2.29210000	-1.17910000	-0.74070000
	C	2.31750000	-1.85700000	-1.88750000
	C	3.62730000	-0.84290000	-0.13580000
	O	3.51210000	-0.40580000	1.13380000
	O	4.68850000	-0.96160000	-0.69920000
	C	4.74740000	-0.05730000	1.78500000
	N	-3.17250000	-0.24750000	-1.32220000
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	H	-0.05520000	-2.54780000	-0.43250000
	H	-0.43010000	-1.24550000	-1.55730000
	H	1.16890000	-0.97470000	1.03880000
	H	1.01290000	0.90570000	-2.23110000

	H	0.63250000	3.33020000	-2.33760000
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	H	3.26500000	-2.12060000	-2.33380000
	H	1.41990000	-2.16060000	-2.40460000
	H	4.46700000	0.27550000	2.77870000
	H	5.24880000	0.73880000	1.23940000
	H	5.40370000	-0.92290000	1.83900000
5	N	3.09390000	0.87200000	1.78370000
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	C	2.65910000	-0.67930000	0.23150000
	C	1.48240000	-0.43270000	0.89810000
	O	1.73090000	0.48720000	1.82420000
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	C	0.09320000	-0.95440000	0.80800000
	C	-0.67460000	-0.44510000	-0.44690000
	C	-0.80970000	1.07430000	-0.53310000
	C	-1.15460000	1.87670000	0.55690000
	C	-1.26880000	3.25590000	0.41320000
	C	-1.04330000	3.85790000	-0.81980000
	C	-0.69960000	3.06990000	-1.91290000
	C	-0.58390000	1.69240000	-1.76620000
	C	-2.00910000	-1.16260000	-0.61910000
	C	-2.23750000	-1.95060000	-1.67060000
	C	-3.05420000	-0.99790000	0.43680000
	O	-4.28470000	-1.35240000	0.02220000
	O	-2.82990000	-0.60390000	1.56020000
	C	-5.32450000	-1.26220000	1.01320000
	N	2.85760000	-1.61650000	-0.82460000
	O	3.98940000	-1.71620000	-1.29320000
	O	1.88670000	-2.27380000	-1.20560000
	H	5.51600000	1.08140000	1.19280000
	H	5.23140000	0.65170000	-0.50910000
	H	5.61960000	-0.60720000	0.64380000
	H	0.14230000	-2.04100000	0.74880000
	H	-0.43530000	-0.68630000	1.71760000
	H	-0.08050000	-0.75170000	-1.30520000
	H	-1.34300000	1.42950000	1.52090000
	H	-1.53200000	3.86030000	1.27060000
	H	-1.12980000	4.93050000	-0.92680000
	H	-0.51670000	3.52520000	-2.87680000
	H	-0.31190000	1.08740000	-2.62220000
	H	-3.18380000	-2.45130000	-1.80520000
	H	-1.47280000	-2.11670000	-2.41720000
	H	-6.23200000	-1.57390000	0.50690000
	H	-5.41690000	-0.23990000	1.37240000
	H	-5.10750000	-1.91910000	1.85270000
6	N	-2.42190000	-1.49900000	1.99710000
	C	-3.15790000	-1.37100000	0.92970000

	C	-2.32210000	-1.12960000	-0.20930000
	C	-1.03190000	-1.12130000	0.26240000
	O	-1.07840000	-1.34230000	1.57250000
	C	-4.64060000	-1.48450000	1.03380000
	C	0.31340000	-0.94490000	-0.34560000
	C	1.13470000	0.20310000	0.31330000
	C	0.43100000	1.54960000	0.26990000
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	C	0.48410000	2.38200000	1.39040000
	C	2.53790000	0.23150000	-0.28540000
	C	3.00830000	1.19490000	-1.07710000
	C	3.41050000	-0.91850000	0.11250000
	O	4.61940000	-0.90910000	-0.47930000
	O	3.06960000	-1.77580000	0.89750000
	C	5.49950000	-1.98650000	-0.11090000
	N	-2.75480000	-0.92980000	-1.55660000
	O	-3.96580000	-0.94580000	-1.76640000
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	H	0.86420000	-1.87530000	-0.20120000
	H	0.19280000	-0.78600000	-1.41110000
	H	1.25580000	-0.07210000	1.36100000
	H	-0.33220000	1.37820000	-1.73920000
	H	-1.40820000	3.57680000	-1.74670000
	H	-1.29050000	5.03790000	0.25170000
	H	-0.07810000	4.25500000	2.26820000
	H	1.00560000	2.04550000	2.27740000
	H	4.01490000	1.15130000	-1.46250000
	H	2.40310000	2.04750000	-1.34690000
	H	6.41170000	-1.81820000	-0.67360000
	H	5.05710000	-2.94460000	-0.37440000
	H	5.69790000	-1.96600000	0.95840000
7	N	3.06920000	-1.35490000	1.71740000
	C	3.69340000	-0.81750000	0.70700000
	C	2.76380000	-0.54680000	-0.34790000
	C	1.53580000	-0.95250000	0.11090000
	O	1.70480000	-1.43520000	1.34020000
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	C	0.16030000	-0.96710000	-0.45940000
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	C	-2.34570000	-0.96870000	0.05710000
	C	-2.72770000	-0.76760000	-1.27060000
	C	-4.02060000	-1.06860000	-1.68910000
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	C	-4.58570000	-1.77370000	0.53620000
	C	-3.29310000	-1.47530000	0.95070000

	C	-0.84810000	0.74600000	1.17150000
	C	-0.59700000	0.94290000	2.46640000
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	O	-1.20970000	3.07660000	0.89870000
	O	-0.99130000	1.83120000	-0.95730000
	C	-1.34170000	4.23820000	0.05880000
	N	3.06150000	0.01950000	-1.62810000
	O	4.19010000	0.48170000	-1.78810000
	O	2.18470000	0.00610000	-2.48820000
	H	5.54000000	-0.96220000	1.72810000
	H	5.39330000	0.46980000	0.68250000
	H	5.67220000	-1.09990000	-0.03970000
	H	0.13160000	-0.27620000	-1.29360000
	H	-0.01960000	-1.96630000	-0.86690000
	H	-0.78390000	-1.33290000	1.42280000
	H	-2.02620000	-0.35890000	-1.98180000
	H	-4.29670000	-0.90630000	-2.72220000
	H	-5.95740000	-1.80430000	-1.11870000
	H	-5.30010000	-2.16860000	1.24570000
	H	-3.01470000	-1.64050000	1.98410000
	H	-0.54440000	1.93570000	2.88560000
	H	-0.42980000	0.10860000	3.13380000
	H	-1.47920000	5.07150000	0.73980000
	H	-2.20160000	4.13380000	-0.59880000
	H	-0.44580000	4.37600000	-0.54250000
8	N	-3.28480000	1.49820000	0.81960000
	C	-3.75120000	0.39610000	0.30200000
	C	-2.71320000	-0.58820000	0.24950000
	C	-1.59410000	0.00620000	0.78110000
	O	-1.92330000	1.24810000	1.12380000
	C	-5.17680000	0.31890000	-0.12620000
	C	-0.19500000	-0.42710000	1.03430000
	C	0.68440000	-0.43140000	-0.25080000
	C	2.05130000	-1.06860000	-0.00280000
	C	2.52710000	-2.00190000	-0.92730000
	C	3.76270000	-2.61630000	-0.75790000
	C	4.54640000	-2.30820000	0.34860000
	C	4.08250000	-1.38390000	1.27810000
	C	2.84690000	-0.76780000	1.10540000
	C	0.77630000	0.92410000	-0.94270000
	C	0.35240000	1.08440000	-2.19740000
	C	1.33710000	2.08450000	-0.18270000
	O	1.56020000	3.16450000	-0.95410000
	O	1.56210000	2.07370000	1.00710000
	C	2.05810000	4.32640000	-0.26610000
	N	-2.81370000	-1.92390000	-0.24260000
	O	-3.91690000	-2.30730000	-0.62630000
	O	-1.79250000	-2.61250000	-0.25720000
	H	-5.66000000	1.27430000	0.06260000
	H	-5.69710000	-0.46840000	0.41650000
	H	-5.24790000	0.07600000	-1.18520000

	H	0.22890000	0.23530000	1.78290000
	H	-0.21440000	-1.44400000	1.42120000
	H	0.17670000	-1.08470000	-0.95790000
	H	1.91990000	-2.25740000	-1.78640000
	H	4.10710000	-3.33870000	-1.48540000
	H	5.50650000	-2.78620000	0.48700000
	H	4.68360000	-1.13780000	2.14310000
	H	2.51440000	-0.03910000	1.82860000
	H	0.42330000	2.03550000	-2.70150000
	H	-0.07570000	0.25790000	-2.74840000
	H	2.17110000	5.08720000	-1.03130000
	H	3.01510000	4.10770000	0.20220000
	H	1.35080000	4.64820000	0.49500000
9	N	3.58080000	0.61330000	-1.65730000
	C	3.85710000	0.12620000	-0.47960000
	C	2.72200000	-0.58280000	0.02840000
	C	1.74550000	-0.47970000	-0.93150000
	O	2.24620000	0.22720000	-1.94090000
	C	5.20160000	0.35130000	0.12300000
	C	0.34700000	-0.97260000	-1.05850000
	C	-0.68410000	-0.21620000	-0.17500000
	C	-2.00980000	-0.97720000	-0.18500000
	C	-2.91000000	-0.87000000	-1.24590000
	C	-4.08760000	-1.61100000	-1.25570000
	C	-4.38360000	-2.46720000	-0.20050000
	C	-3.49490000	-2.57680000	0.86420000
	C	-2.31770000	-1.83680000	0.87070000
	C	-0.86980000	1.24850000	-0.52430000
	C	-0.59320000	1.81490000	-1.69830000
	C	-1.40120000	2.07460000	0.60900000
	O	-1.82840000	3.29360000	0.22730000
	O	-1.43370000	1.69280000	1.75580000
	C	-2.31290000	4.13790000	1.28720000
	N	2.62860000	-1.29100000	1.26530000
	O	3.60920000	-1.27200000	2.00530000
	O	1.57760000	-1.88200000	1.51290000
	H	5.80750000	0.93970000	-0.56150000
	H	5.69450000	-0.59800000	0.32520000
	H	5.11200000	0.87270000	1.07450000
	H	0.06470000	-0.93430000	-2.10970000
	H	0.32950000	-2.01570000	-0.74920000
	H	-0.31790000	-0.25010000	0.84860000
	H	-2.70090000	-0.19550000	-2.06560000
	H	-4.77510000	-1.51430000	-2.08520000
	H	-5.30090000	-3.03990000	-0.20540000
	H	-3.71890000	-3.23450000	1.69300000
	H	-1.63320000	-1.92150000	1.70420000
	H	-0.77210000	2.86640000	-1.86020000
	H	-0.17090000	1.25870000	-2.52170000
	H	-2.61850000	5.06020000	0.80430000
	H	-1.52490000	4.32700000	2.01290000

	H	-3.15610000	3.66890000	1.78920000
10	N	2.38720000	-2.28390000	1.47760000
	C	3.12400000	-1.65150000	0.60850000
	C	2.28810000	-1.02100000	-0.36780000
	C	0.99710000	-1.31740000	-0.00950000
	O	1.04250000	-2.07830000	1.07880000
	C	4.60830000	-1.66640000	0.74280000
	C	-0.35260000	-1.05470000	-0.57540000
	C	-1.24250000	-0.06480000	0.25320000
	C	-2.71990000	-0.39270000	0.09850000
	C	-3.27790000	-0.80190000	-1.11470000
	C	-4.63880000	-1.07570000	-1.21910000
	C	-5.46630000	-0.94540000	-0.10970000
	C	-4.92240000	-0.54060000	1.10530000
	C	-3.56290000	-0.26800000	1.20500000
	C	-0.93280000	1.39640000	-0.06770000
	C	-1.68740000	2.17630000	-0.84110000
	C	0.29680000	1.94120000	0.58420000
	O	0.56860000	3.21410000	0.25080000
	O	0.98030000	1.30140000	1.35460000
	C	1.74320000	3.78090000	0.85840000
	N	2.70750000	-0.20730000	-1.46010000
	O	3.91730000	-0.09100000	-1.64970000
	O	1.84290000	0.33760000	-2.14850000
	H	4.88260000	-2.25380000	1.61560000
	H	4.99240000	-0.65330000	0.85010000
	H	5.07090000	-2.09130000	-0.14620000
	H	-0.23860000	-0.70580000	-1.59660000
	H	-0.86490000	-2.01730000	-0.59380000
	H	-0.98650000	-0.21560000	1.30130000
	H	-2.65350000	-0.91130000	-1.99120000
	H	-5.04960000	-1.39250000	-2.16810000
	H	-6.52260000	-1.16210000	-0.18920000
	H	-5.55440000	-0.44310000	1.97750000
	H	-3.14830000	0.04210000	2.15570000
	H	-1.40590000	3.19930000	-1.03490000
	H	-2.59970000	1.81350000	-1.29090000
	H	1.79130000	4.80160000	0.49400000
	H	2.62930000	3.22640000	0.55770000
	H	1.65700000	3.76240000	1.94250000
11	N	-2.16910000	-1.76220000	1.84420000
	C	-2.99980000	-1.47150000	0.88330000
	C	-2.27130000	-1.04080000	-0.27350000
	C	-0.94370000	-1.09360000	0.07270000
	O	-0.86960000	-1.52340000	1.32920000
	C	-4.46700000	-1.61810000	1.10250000
	C	0.34260000	-0.80950000	-0.61810000
	C	1.22870000	0.22050000	0.14260000
	C	0.55560000	1.57320000	0.32120000
	C	-0.20900000	2.17530000	-0.68100000

	C	-0.78900000	3.42520000	-0.48070000
	C	-0.61470000	4.09430000	0.72530000
	C	0.14080000	3.50320000	1.73290000
	C	0.71760000	2.25490000	1.52990000
	C	2.59660000	0.30760000	-0.53010000
	C	3.02190000	1.34110000	-1.25500000
	C	3.56210000	-0.83180000	-0.36270000
	O	3.10900000	-1.75930000	0.51010000
	O	4.62870000	-0.92490000	-0.92030000
	C	3.99130000	-2.87240000	0.74810000
	N	-2.82480000	-0.63740000	-1.52890000
	O	-4.04970000	-0.62630000	-1.62510000
	O	-2.05540000	-0.32720000	-2.43800000
	H	-4.64290000	-1.98340000	2.11120000
	H	-4.89540000	-2.31230000	0.38150000
	H	-4.97240000	-0.66380000	0.96520000
	H	0.89190000	-1.74970000	-0.68560000
	H	0.12960000	-0.47940000	-1.62820000
	H	1.39350000	-0.18900000	1.13820000
	H	-0.36510000	1.67440000	-1.62620000
	H	-1.37960000	3.87150000	-1.26910000
	H	-1.06790000	5.06350000	0.88120000
	H	0.27670000	4.01000000	2.67860000
	H	1.29910000	1.80060000	2.32190000
	H	4.00560000	1.31600000	-1.70010000
	H	2.41270000	2.21900000	-1.40710000
	H	3.47100000	-3.50730000	1.45740000
	H	4.93420000	-2.52340000	1.16280000
	H	4.18560000	-3.40630000	-0.17930000
13	N	3.07430000	0.36540000	2.07600000
	C	3.74660000	0.11060000	0.98940000
	C	2.89340000	-0.52800000	0.03080000
	C	1.66180000	-0.63610000	0.63020000
	O	1.75860000	-0.11100000	1.84780000
	C	5.18530000	0.49050000	0.90120000
	C	0.34310000	-1.21710000	0.25380000
	C	-0.84690000	-0.23600000	0.41470000
	C	-2.16280000	-0.99700000	0.26000000
	C	-2.94580000	-1.27020000	1.38160000
	C	-4.12720000	-1.99560000	1.26590000
	C	-4.54300000	-2.45830000	0.02210000
	C	-3.77180000	-2.18730000	-1.10380000
	C	-2.59250000	-1.45990000	-0.98490000
	C	-0.78610000	0.97070000	-0.50430000
	C	-0.09070000	1.04730000	-1.63910000
	C	-1.59420000	2.13770000	-0.02280000
	O	-1.71730000	3.11730000	-0.93870000
	O	-2.08120000	2.20220000	1.08230000
	C	-2.45670000	4.27500000	-0.51070000
	N	3.25870000	-0.95580000	-1.28290000
	O	4.43120000	-0.80830000	-1.61780000

	O	2.38740000	-1.44140000	-2.00610000
	H	5.48520000	0.97230000	1.82840000
	H	5.35290000	1.16800000	0.06560000
	H	5.80390000	-0.38840000	0.72790000
	H	0.40880000	-1.61410000	-0.75300000
	H	0.16000000	-2.06290000	0.92040000
	H	-0.82580000	0.14750000	1.43320000
	H	-2.63550000	-0.90020000	2.34990000
	H	-4.72380000	-2.19280000	2.14610000
	H	-5.46200000	-3.02060000	-0.07050000
	H	-4.08960000	-2.53840000	-2.07620000
	H	-2.01060000	-1.24440000	-1.87140000
	H	-0.11790000	1.94210000	-2.24140000
	H	0.52000000	0.23100000	-1.99810000
	H	-1.97250000	4.73980000	0.34540000
	H	-3.47260000	3.99660000	-0.23950000
	H	-2.45800000	4.94740000	-1.36220000
14	N	-3.02550000	-2.54830000	-0.49180000
	C	-3.60110000	-1.41660000	-0.19720000
	C	-2.63990000	-0.51890000	0.37140000
	C	-1.44880000	-1.20040000	0.39900000
	O	-1.66790000	-2.41150000	-0.11260000
	C	-5.05470000	-1.23030000	-0.47070000
	C	-0.05540000	-0.91380000	0.83330000
	C	0.89720000	-0.67440000	-0.37860000
	C	2.36810000	-0.90700000	-0.03320000
	C	2.92190000	-0.60960000	1.21260000
	C	4.26630000	-0.86030000	1.46880000
	C	5.08170000	-1.40770000	0.48430000
	C	4.54160000	-1.70630000	-0.76190000
	C	3.19690000	-1.45890000	-1.01330000
	C	0.64360000	0.66160000	-1.06480000
	C	0.20310000	0.72330000	-2.32220000
	C	0.89720000	1.91160000	-0.28050000
	O	0.67740000	3.03410000	-0.98980000
	O	1.25900000	1.92230000	0.87310000
	C	0.85970000	4.26600000	-0.26800000
	N	-2.88050000	0.81830000	0.81950000
	O	-4.03190000	1.24120000	0.73540000
	O	-1.93150000	1.46390000	1.25820000
	H	-5.45310000	-2.13700000	-0.91930000
	H	-5.21460000	-0.38820000	-1.14180000
	H	-5.59280000	-1.01030000	0.44970000
	H	-0.05190000	-0.06130000	1.50280000
	H	0.30070000	-1.79050000	1.37550000
	H	0.64760000	-1.43370000	-1.11990000
	H	2.31380000	-0.15920000	1.98160000
	H	4.67640000	-0.62150000	2.44070000
	H	6.12610000	-1.60170000	0.68670000
	H	5.16230000	-2.13760000	-1.53550000
	H	2.78490000	-1.70170000	-1.98490000

	H	0.02690000	1.66820000	-2.81210000
	H	0.01140000	-0.17750000	-2.89000000
	H	0.63480000	5.05270000	-0.98040000
	H	1.88480000	4.34970000	0.08590000
	H	0.18010000	4.30860000	0.58000000
15	N	-3.52160000	1.18510000	-0.81490000
	C	-3.76370000	0.14620000	-0.06490000
	C	-2.65150000	-0.75330000	-0.11390000
	C	-1.72800000	-0.17190000	-0.94710000
	O	-2.23500000	0.98010000	-1.37240000
	C	-5.05390000	0.04480000	0.67440000
	C	-0.37720000	-0.55080000	-1.43930000
	C	0.74080000	-0.32420000	-0.38720000
	C	0.84640000	1.14180000	0.02910000
	C	1.29360000	2.11690000	-0.86440000
	C	1.35630000	3.45310000	-0.48640000
	C	0.97620000	3.83470000	0.79670000
	C	0.53790000	2.87070000	1.69740000
	C	0.47640000	1.53430000	1.31500000
	C	2.08050000	-0.86620000	-0.85250000
	C	2.40040000	-1.18240000	-2.10670000
	C	3.06660000	-1.07080000	0.25870000
	O	4.32110000	-1.29770000	-0.17580000
	O	2.76620000	-1.04760000	1.42910000
	C	5.29610000	-1.53990000	0.85470000
	N	-2.52710000	-2.01530000	0.54190000
	O	-3.46680000	-2.38720000	1.24130000
	O	-1.49070000	-2.65630000	0.36580000
	H	-4.87630000	-0.03590000	1.74550000
	H	-5.59910000	-0.84820000	0.37370000
	H	-5.65490000	0.92710000	0.46890000
	H	-0.39580000	-1.60620000	-1.70610000
	H	-0.18560000	0.03540000	-2.33720000
	H	0.47280000	-0.89440000	0.50040000
	H	1.60360000	1.83380000	-1.86200000
	H	1.70330000	4.19520000	-1.19250000
	H	1.02500000	4.87390000	1.09180000
	H	0.24820000	3.15550000	2.69970000
	H	0.15380000	0.78650000	2.02700000
	H	3.38200000	-1.55800000	-2.34960000
	H	1.69860000	-1.08370000	-2.92200000
	H	6.23480000	-1.69460000	0.33320000
	H	5.02690000	-2.42160000	1.43210000
	H	5.36290000	-0.68260000	1.52070000
17	N	-3.67320000	0.30230000	1.70580000
	C	-3.87650000	-0.03410000	0.46260000
	C	-2.68160000	-0.60130000	-0.08570000
	C	-1.74770000	-0.57340000	0.92140000
	O	-2.32760000	-0.04080000	1.99270000
	C	-5.21040000	0.19360000	-0.16210000

	C	-0.32660000	-0.99860000	1.04570000
	C	0.68510000	-0.10950000	0.26720000
	C	2.04560000	-0.80730000	0.24620000
	C	2.96020000	-0.67120000	1.29090000
	C	4.17190000	-1.35590000	1.26760000
	C	4.48680000	-2.18510000	0.19700000
	C	3.58220000	-2.32520000	-0.85130000
	C	2.37230000	-1.64100000	-0.82540000
	C	0.78140000	1.32200000	0.76300000
	C	0.41280000	1.75760000	1.96680000
	C	1.36500000	2.35140000	-0.16610000
	O	1.48830000	1.88590000	-1.42480000
	O	1.67910000	3.47190000	0.15650000
	C	2.04620000	2.80850000	-2.37800000
	N	-2.50110000	-1.12760000	-1.40030000
	O	-3.44860000	-1.05070000	-2.17860000
	O	-1.41140000	-1.63160000	-1.67570000
	H	-5.87500000	0.64860000	0.56800000
	H	-5.63670000	-0.74600000	-0.50950000
	H	-5.11980000	0.84330000	-1.03090000
	H	-0.07390000	-1.04300000	2.10410000
	H	-0.24220000	-2.00650000	0.64340000
	H	0.34050000	-0.07690000	-0.76320000
	H	2.73520000	-0.01770000	2.12280000
	H	4.87050000	-1.23550000	2.08440000
	H	5.42990000	-2.71370000	0.17680000
	H	3.81920000	-2.96400000	-1.69130000
	H	1.67400000	-1.75260000	-1.64480000
	H	0.54760000	2.79800000	2.22390000
	H	-0.02960000	1.11350000	2.71070000
	H	2.07200000	2.27070000	-3.31980000
	H	3.04830000	3.10280000	-2.07450000
	H	1.42120000	3.69500000	-2.45690000
21	N	-3.41960000	1.32780000	-0.75870000
	C	-3.66920000	0.28320000	-0.01930000
	C	-2.59080000	-0.65200000	-0.12690000
	C	-1.67970000	-0.08600000	-0.98450000
	O	-2.16270000	1.09040000	-1.36860000
	C	-4.93420000	0.21030000	0.76540000
	C	-0.36470000	-0.50020000	-1.54070000
	C	0.80380000	-0.37700000	-0.52420000
	C	0.96860000	1.05900000	-0.02980000
	C	1.50150000	2.05200000	-0.85350000
	C	1.60770000	3.36470000	-0.40770000
	C	1.18520000	3.70500000	0.87350000
	C	0.65900000	2.72280000	1.70510000
	C	0.55450000	1.41050000	1.25510000
	C	2.09970000	-0.93430000	-1.08920000
	C	2.33290000	-1.20670000	-2.37210000
	C	3.22730000	-1.21270000	-0.13330000
	O	2.82160000	-1.18150000	1.15030000

	O	4.36340000	-1.45630000	-0.46210000
	C	3.84140000	-1.44620000	2.13080000
	N	-2.48290000	-1.92700000	0.50480000
	O	-3.40650000	-2.28060000	1.23430000
	O	-1.47360000	-2.59710000	0.28150000
	H	-5.51210000	1.11570000	0.59830000
	H	-4.72110000	0.10250000	1.82760000
	H	-5.51990000	-0.65810000	0.46840000
	H	-0.44120000	-1.53930000	-1.85760000
	H	-0.17610000	0.12120000	-2.41510000
	H	0.54040000	-0.99020000	0.33520000
	H	1.84520000	1.79980000	-1.84810000
	H	2.02300000	4.12060000	-1.06010000
	H	1.26860000	4.72550000	1.22080000
	H	0.33270000	2.97530000	2.70490000
	H	0.15580000	0.64910000	1.91290000
	H	3.29670000	-1.59010000	-2.67270000
	H	1.59020000	-1.06350000	-3.14240000
	H	3.34390000	-1.37540000	3.09220000
	H	4.63810000	-0.71000000	2.05350000
	H	4.25670000	-2.44070000	1.98430000
23	N	3.30000000	0.08110000	1.51530000
	C	3.36330000	-0.77800000	0.53670000
	C	2.04160000	-1.17880000	0.16040000
	C	1.18360000	-0.49080000	0.98350000
	O	1.92340000	0.25930000	1.79570000
	C	4.68800000	-1.19340000	-0.00540000
	C	-0.29230000	-0.41890000	1.16420000
	C	-1.05720000	0.33170000	0.02810000
	C	-0.48830000	1.70480000	-0.29020000
	C	-0.10460000	2.61380000	0.69890000
	C	0.39200000	3.86900000	0.36150000
	C	0.51340000	4.23920000	-0.97320000
	C	0.13740000	3.34340000	-1.96860000
	C	-0.35680000	2.08950000	-1.62680000
	C	-2.54850000	0.35770000	0.36510000
	C	-3.22770000	1.44600000	0.72390000
	C	-3.34080000	-0.91750000	0.26860000
	O	-2.63070000	-1.90720000	-0.30600000
	O	-4.48180000	-1.05280000	0.64130000
	C	-3.31630000	-3.16120000	-0.47570000
	N	1.68250000	-2.12750000	-0.84310000
	O	2.59150000	-2.64540000	-1.48860000
	O	0.48670000	-2.37490000	-0.99840000
	H	5.47500000	-0.67200000	0.53370000
	H	4.75640000	-0.96350000	-1.06730000
	H	4.82430000	-2.26870000	0.09740000
	H	-0.68140000	-1.43410000	1.20980000
	H	-0.47880000	0.06050000	2.12400000
	H	-0.94570000	-0.28210000	-0.86360000
	H	-0.18200000	2.34740000	1.74390000

	H	0.68840000	4.55450000	1.14370000
	H	0.90230000	5.21360000	-1.23490000
	H	0.23230000	3.61730000	-3.01050000
	H	-0.64390000	1.39780000	-2.40850000
	H	-4.28150000	1.36900000	0.94790000
	H	-2.76000000	2.41620000	0.78830000
	H	-3.63200000	-3.55300000	0.48870000
	H	-2.59420000	-3.82080000	-0.94450000
	H	-4.18970000	-3.02900000	-1.11020000
24	N	-3.29960000	1.60300000	0.68340000
	C	-3.78060000	0.46420000	0.26920000
	C	-2.74690000	-0.52630000	0.27490000
	C	-1.61450000	0.10520000	0.72660000
	O	-1.93130000	1.37260000	0.97420000
	C	-5.21570000	0.35850000	-0.11940000
	C	-0.21060000	-0.30740000	0.98780000
	C	0.64400000	-0.43260000	-0.30270000
	C	2.05460000	-0.96510000	-0.03460000
	C	2.60710000	-1.08480000	1.23970000
	C	3.89030000	-1.59650000	1.41720000
	C	4.64510000	-1.99600000	0.32180000
	C	4.10500000	-1.88260000	-0.95570000
	C	2.82440000	-1.37340000	-1.12820000
	C	0.65610000	0.83150000	-1.15280000
	C	0.08920000	0.86490000	-2.35900000
	C	1.32440000	2.09570000	-0.69260000
	O	1.69590000	2.03930000	0.60220000
	O	1.50920000	3.06500000	-1.38780000
	C	2.34950000	3.21750000	1.11080000
	N	-2.86170000	-1.90020000	-0.09400000
	O	-3.97070000	-2.30780000	-0.43170000
	O	-1.84510000	-2.59470000	-0.05310000
	H	-5.69160000	1.32870000	-0.00100000
	H	-5.72640000	-0.37790000	0.49870000
	H	-5.31060000	0.02820000	-1.15250000
	H	0.22280000	0.42360000	1.66480000
	H	-0.22670000	-1.28060000	1.47550000
	H	0.14830000	-1.18950000	-0.91090000
	H	2.04900000	-0.77750000	2.11160000
	H	4.29670000	-1.68120000	2.41600000
	H	5.64110000	-2.39330000	0.46050000
	H	4.67880000	-2.19350000	-1.81820000
	H	2.41670000	-1.28960000	-2.12710000
	H	0.12040000	1.76530000	-2.95480000
	H	-0.40900000	-0.00200000	-2.77060000
	H	2.58520000	2.99440000	2.14610000
	H	1.68550000	4.07590000	1.04260000
	H	3.25620000	3.41850000	0.54510000
25	N	3.18740000	-0.45970000	1.85660000
	C	3.35870000	-1.04200000	0.70270000

C	2.08890000	-1.27120000	0.08330000
C	1.14480000	-0.77690000	0.94960000
O	1.78960000	-0.29360000	2.00970000
C	4.73460000	-1.36550000	0.22950000
C	-0.34040000	-0.68200000	0.98380000
C	-0.97740000	0.24820000	-0.09760000
C	-0.25960000	1.57640000	-0.26420000
C	0.14630000	2.35530000	0.82270000
C	0.79150000	3.57250000	0.62740000
C	1.04160000	4.03410000	-0.66040000
C	0.64470000	3.26800000	-1.75130000
C	0.00180000	2.05120000	-1.55160000
C	-2.47250000	0.40000000	0.17750000
C	-3.07310000	1.54520000	0.50150000
C	-3.27910000	-0.85120000	0.00900000
O	-4.58450000	-0.69420000	0.30420000
O	-2.81380000	-1.90450000	-0.36350000
C	-5.40210000	-1.86610000	0.13500000
N	1.84870000	-1.90780000	-1.17180000
O	2.82850000	-2.27470000	-1.81840000
O	0.68130000	-2.05550000	-1.52860000
H	5.45540000	-1.04070000	0.97590000
H	4.93950000	-0.87060000	-0.71820000
H	4.84040000	-2.43550000	0.05920000
H	-0.75770000	-1.67700000	0.83860000
H	-0.61100000	-0.34230000	1.98300000
H	-0.89020000	-0.29370000	-1.03760000
H	-0.03170000	2.01370000	1.83320000
H	1.10270000	4.15620000	1.48300000
H	1.54640000	4.97830000	-0.81200000
H	0.83970000	3.61320000	-2.75760000
H	-0.29790000	1.45800000	-2.40610000
H	-4.13810000	1.58100000	0.66900000
H	-2.51870000	2.46690000	0.59380000
H	-5.36850000	-2.20700000	-0.89740000
H	-6.40670000	-1.55770000	0.40480000
H	-5.05810000	-2.66640000	0.78660000

[a] Conformers are numbered according to their appearance during conformational search.

3g

Conf. no.[a]				
1	N	-2.80020000	-1.35660000	2.07650000
	C	-3.51120000	-0.91040000	1.07960000
	C	-2.72720000	-0.92580000	-0.11980000
	C	-1.49310000	-1.40470000	0.24060000
	O	-1.52340000	-1.66610000	1.54430000
	C	-4.92330000	-0.48960000	1.30510000
	C	-0.21830000	-1.67290000	-0.47760000
	C	0.97930000	-0.89330000	0.11940000
	C	0.75350000	0.61810000	0.08180000
	C	0.64050000	1.30780000	-1.12770000
	C	0.40680000	2.67580000	-1.14870000
	C	0.28400000	3.40730000	0.03640000
	C	0.40270000	2.71610000	1.24060000
	C	0.63460000	1.34360000	1.26450000
	C	2.29230000	-1.27130000	-0.54340000
	C	2.42140000	-1.85230000	-1.73590000
	C	3.50230000	-0.96130000	0.28570000
	O	4.65450000	-1.01930000	-0.40890000
	O	3.45410000	-0.69970000	1.46520000
	C	5.84920000	-0.77110000	0.35400000
	N	-3.15400000	-0.52010000	-1.42430000
	O	-4.26980000	-0.01370000	-1.51630000
	O	-2.39480000	-0.70260000	-2.37470000
	H	-5.18140000	-0.64790000	2.34920000
	H	-5.60040000	-1.05890000	0.67030000
	H	-5.05400000	0.56040000	1.04980000
	H	-0.01370000	-2.74450000	-0.40990000
	H	-0.37550000	-1.42940000	-1.52270000
	H	1.07190000	-1.17200000	1.16770000
	H	0.73550000	0.77680000	-2.06590000
	H	0.31760000	3.18320000	-2.10110000
	C	0.04320000	4.89550000	0.00380000
	H	0.31400000	3.25390000	2.17590000
	H	0.73130000	0.83470000	2.21410000
	H	3.39620000	-2.07630000	-2.14020000
	H	1.56660000	-2.12110000	-2.33930000
	H	6.66620000	-0.85090000	-0.35540000
	H	5.95420000	-1.50930000	1.14610000
	H	5.81770000	0.22320000	0.79360000
	H	0.91530000	5.42770000	-0.38190000
	H	-0.79910000	5.14630000	-0.64250000
	H	-0.16870000	5.28450000	0.99860000
2	N	-3.28430000	-1.01820000	1.85200000
	C	-3.67960000	-0.79510000	0.63040000
	C	-2.57890000	-0.95630000	-0.27300000
	C	-1.49540000	-1.28480000	0.50220000
	O	-1.90370000	-1.32590000	1.76960000

	C	-5.10290000	-0.43940000	0.36560000
	C	-0.06010000	-1.58540000	0.25030000
	C	0.88190000	-0.61970000	1.02340000
	C	0.74590000	0.84200000	0.60040000
	C	0.66870000	1.24990000	-0.73320000
	C	0.55440000	2.59700000	-1.05720000
	C	0.51490000	3.58450000	-0.07130000
	C	0.58610000	3.17330000	1.25970000
	C	0.69880000	1.82750000	1.58790000
	C	2.33010000	-1.09700000	1.01900000
	C	2.95750000	-1.41220000	2.15280000
	C	3.03720000	-1.23130000	-0.29250000
	O	4.37460000	-1.32770000	-0.16440000
	O	2.47790000	-1.26830000	-1.36510000
	C	5.10300000	-1.50400000	-1.39330000
	N	-2.61420000	-0.79980000	-1.69550000
	O	-3.67170000	-0.41130000	-2.18920000
	O	-1.60200000	-1.06220000	-2.34000000
	H	-5.65060000	-0.43400000	1.30480000
	H	-5.55680000	-1.15400000	-0.31890000
	H	-5.17050000	0.53980000	-0.10490000
	H	0.13040000	-2.60350000	0.59910000
	H	0.12960000	-1.56370000	-0.81430000
	H	0.57700000	-0.66380000	2.06830000
	H	0.70210000	0.52030000	-1.52790000
	H	0.48960000	2.88200000	-2.09980000
	C	0.41530000	5.04430000	-0.43520000
	H	0.54340000	3.91100000	2.05100000
	H	0.74150000	1.54020000	2.63130000
	H	3.98720000	-1.73440000	2.15770000
	H	2.44820000	-1.35380000	3.10540000
	H	6.14720000	-1.55700000	-1.10370000
	H	4.93110000	-0.66130000	-2.05890000
	H	4.79430000	-2.42120000	-1.89000000
	H	-0.21570000	5.19300000	-1.31140000
	H	0.00130000	5.63080000	0.38420000
	H	1.39910000	5.45780000	-0.66980000
3	N	3.54290000	0.06910000	-1.43020000
	C	3.65660000	-0.88510000	-0.54820000
	C	2.36210000	-1.39010000	-0.21110000
	C	1.46530000	-0.66210000	-0.94990000
	O	2.15380000	0.20430000	-1.68790000
	C	5.00370000	-1.28310000	-0.05050000
	C	-0.01360000	-0.66060000	-1.09080000
	C	-0.76750000	0.18140000	-0.01230000
	C	-2.25920000	-0.11420000	-0.02460000
	C	-2.98510000	-0.35600000	-1.18980000
	C	-4.35610000	-0.60040000	-1.14420000
	C	-5.04910000	-0.61390000	0.06390000
	C	-4.31930000	-0.37350000	1.23150000
	C	-2.95430000	-0.13080000	1.18780000

	C	-0.45240000	1.67030000	-0.13830000
	C	-1.21140000	2.54710000	-0.79490000
	C	0.78760000	2.12100000	0.56860000
	O	1.11380000	3.40130000	0.32140000
	O	1.43300000	1.40710000	1.30510000
	C	2.29890000	3.87920000	0.98400000
	N	2.05080000	-2.42150000	0.72310000
	O	2.99060000	-3.00040000	1.26470000
	O	0.86360000	-2.67400000	0.93010000
	H	5.76120000	-0.67120000	-0.53410000
	H	5.19370000	-2.33460000	-0.25810000
	H	5.06320000	-1.15500000	1.02910000
	H	-0.24660000	-0.28590000	-2.08660000
	H	-0.35940000	-1.68820000	-1.01040000
	H	-0.38280000	-0.14070000	0.95330000
	H	-2.49210000	-0.36070000	-2.15240000
	H	-4.89050000	-0.78600000	-2.06730000
	C	-6.52890000	-0.89730000	0.12030000
	H	-4.82530000	-0.38350000	2.18890000
	H	-2.41570000	0.04370000	2.11050000
	H	-0.93040000	3.58650000	-0.85870000
	H	-2.13400000	2.24600000	-1.26990000
	H	2.40200000	4.91470000	0.67710000
	H	3.16420000	3.29870000	0.67230000
	H	2.18570000	3.80730000	2.06340000
	H	-7.05460000	-0.14430000	0.70910000
	H	-6.96850000	-0.91240000	-0.87590000
	H	-6.72680000	-1.86570000	0.58460000
4	N	-2.65160000	-1.30600000	2.13280000
	C	-3.40260000	-0.81230000	1.18900000
	C	-2.69680000	-0.84200000	-0.05770000
	C	-1.46550000	-1.38070000	0.21650000
	O	-1.42560000	-1.66260000	1.51640000
	C	-4.77760000	-0.33370000	1.50870000
	C	-0.25040000	-1.69070000	-0.58320000
	C	1.01760000	-0.97710000	-0.04570000
	C	0.84840000	0.54210000	-0.05340000
	C	0.84390000	1.26840000	-1.24560000
	C	0.64830000	2.64330000	-1.24180000
	C	0.45590000	3.34450000	-0.04870000
	C	0.46150000	2.61560000	1.14000000
	C	0.65590000	1.23770000	1.13870000
	C	2.26760000	-1.40980000	-0.79310000
	C	2.28920000	-2.03250000	-1.97090000
	C	3.60460000	-1.11390000	-0.17160000
	O	3.49330000	-0.75780000	1.12340000
	O	4.66460000	-1.19900000	-0.74350000
	C	4.73050000	-0.45330000	1.79210000
	N	-3.18580000	-0.39530000	-1.32700000
	O	-4.27790000	0.16790000	-1.33890000
	O	-2.49980000	-0.60140000	-2.32640000

	H	-4.97790000	-0.49900000	2.56440000
	H	-5.51750000	-0.86120000	0.90890000
	H	-4.87640000	0.72540000	1.27750000
	H	-0.09270000	-2.77170000	-0.54730000
	H	-0.45560000	-1.41660000	-1.61230000
	H	1.14460000	-1.27670000	0.99330000
	H	0.99730000	0.76040000	-2.18850000
	H	0.64500000	3.17970000	-2.18230000
	C	0.27130000	4.84090000	-0.05050000
	H	0.31110000	3.12840000	2.08160000
	H	0.65690000	0.69900000	2.07720000
	H	3.23500000	-2.28170000	-2.42910000
	H	1.38980000	-2.30460000	-2.50230000
	H	5.38660000	-1.32070000	1.78800000
	H	4.45340000	-0.18580000	2.80640000
	H	5.23100000	0.37650000	1.29830000
	H	1.22710000	5.35390000	-0.17930000
	H	-0.37910000	5.15940000	-0.86550000
	H	-0.16430000	5.18840000	0.88530000
5	N	3.10600000	0.78890000	1.80990000
	C	3.70310000	0.17020000	0.82990000
	C	2.78600000	-0.72890000	0.19800000
	C	1.59610000	-0.59950000	0.87460000
	O	1.77650000	0.29910000	1.83630000
	C	5.13420000	0.45810000	0.52900000
	C	0.25200000	-1.22390000	0.76190000
	C	-0.56470000	-0.69340000	-0.45370000
	C	-0.83430000	0.80880000	-0.41680000
	C	-1.32180000	1.47530000	0.71090000
	C	-1.55340000	2.84410000	0.68220000
	C	-1.31020000	3.60200000	-0.46590000
	C	-0.82310000	2.93590000	-1.58880000
	C	-0.58920000	1.56460000	-1.56320000
	C	-1.82630000	-1.51670000	-0.69110000
	C	-1.99080000	-2.21290000	-1.81680000
	C	-2.87010000	-1.56610000	0.37820000
	O	-4.06070000	-2.01080000	-0.06620000
	O	-2.67750000	-1.25960000	1.53450000
	C	-5.09130000	-2.13010000	0.93100000
	N	3.04980000	-1.60320000	-0.89680000
	O	4.18820000	-1.60940000	-1.36040000
	O	2.12480000	-2.30270000	-1.31490000
	H	5.50100000	1.21210000	1.22100000
	H	5.24680000	0.81410000	-0.49370000
	H	5.73480000	-0.44540000	0.62000000
	H	0.38620000	-2.29720000	0.63280000
	H	-0.28650000	-1.05550000	1.68930000
	H	0.05310000	-0.87530000	-1.33050000
	H	-1.53010000	0.92540000	1.61600000
	H	-1.92730000	3.33280000	1.57340000
	C	-1.56320000	5.08840000	-0.47970000

	H	-0.61800000	3.49280000	-2.49420000
	H	-0.20710000	1.07760000	-2.45190000
	H	-2.88540000	-2.78770000	-1.99920000
	H	-1.22350000	-2.22630000	-2.57880000
	H	-5.96550000	-2.49070000	0.39920000
	H	-5.29110000	-1.16290000	1.38650000
	H	-4.79320000	-2.83550000	1.70360000
	H	-2.61370000	5.31230000	-0.28490000
	H	-0.97780000	5.59560000	0.28920000
	H	-1.30190000	5.52620000	-1.44180000
6	N	-2.13180000	-1.97110000	2.02610000
	C	-2.87740000	-1.96980000	0.95750000
	C	-2.07770000	-1.66090000	-0.19090000
	C	-0.79900000	-1.47540000	0.27620000
	O	-0.81850000	-1.65960000	1.59250000
	C	-4.33420000	-2.26500000	1.07000000
	C	0.51450000	-1.15330000	-0.34210000
	C	1.20010000	0.09250000	0.29270000
	C	0.35050000	1.35040000	0.22500000
	C	-0.41710000	1.68850000	-0.89000000
	C	-1.16610000	2.86220000	-0.91400000
	C	-1.17490000	3.73900000	0.16950000
	C	-0.41060000	3.39530000	1.28740000
	C	0.33620000	2.22530000	1.31380000
	C	2.59040000	0.26500000	-0.31220000
	C	2.93910000	1.24350000	-1.14710000
	C	3.59380000	-0.75580000	0.12610000
	O	4.79830000	-0.61600000	-0.45910000
	O	3.35410000	-1.62400000	0.93610000
	C	5.80050000	-1.56420000	-0.05010000
	N	-2.53110000	-1.55840000	-1.54210000
	O	-3.72990000	-1.73660000	-1.74810000
	O	-1.70930000	-1.29990000	-2.42170000
	H	-4.58010000	-2.45950000	2.11090000
	H	-4.59910000	-3.12920000	0.46320000
	H	-4.92400000	-1.42620000	0.70440000
	H	1.16960000	-2.01200000	-0.18750000
	H	0.37240000	-1.02650000	-1.40940000
	H	1.35320000	-0.14640000	1.34510000
	H	-0.44890000	1.03650000	-1.75230000
	H	-1.75740000	3.09200000	-1.79120000
	C	-1.97070000	5.01940000	0.13720000
	H	-0.40660000	4.04640000	2.15260000
	H	0.91080000	1.98210000	2.19860000
	H	3.94260000	1.30600000	-1.53790000
	H	2.23270000	2.00310000	-1.44720000
	H	5.98510000	-1.48380000	1.01890000
	H	6.69030000	-1.30390000	-0.61350000
	H	5.48160000	-2.57790000	-0.28230000
	H	-2.71620000	5.00320000	-0.65640000
	H	-2.48650000	5.19030000	1.08250000

	H	-1.32160000	5.88050000	-0.03740000
7	N	3.35430000	-1.20360000	1.82470000
	C	3.96490000	-0.92170000	0.70790000
	C	3.00430000	-0.75510000	-0.34040000
	C	1.77300000	-0.94780000	0.23460000
	O	1.96850000	-1.21470000	1.52400000
	C	5.45240000	-0.83070000	0.67550000
	C	0.37310000	-0.93230000	-0.27260000
	C	-0.65950000	-0.40350000	0.75430000
	C	-2.09700000	-0.67590000	0.31370000
	C	-2.53750000	-0.52890000	-1.00270000
	C	-3.85910000	-0.79500000	-1.34410000
	C	-4.78910000	-1.21120000	-0.39090000
	C	-4.34530000	-1.36060000	0.92360000
	C	-3.02510000	-1.09780000	1.26770000
	C	-0.44150000	1.05430000	1.15110000
	C	-0.15070000	1.39670000	2.40690000
	C	-0.54090000	2.10350000	0.09010000
	O	-0.64420000	3.35120000	0.58680000
	O	-0.51650000	1.87290000	-1.09830000
	C	-0.69470000	4.40550000	-0.39160000
	N	3.27620000	-0.46280000	-1.71420000
	O	4.43160000	-0.15580000	-2.00470000
	O	2.35170000	-0.54110000	-2.51930000
	H	5.84770000	-1.06130000	1.66170000
	H	5.76750000	0.16760000	0.37740000
	H	5.86390000	-1.52560000	-0.05490000
	H	0.35310000	-0.36250000	-1.19400000
	H	0.10340000	-1.96040000	-0.53170000
	H	-0.51510000	-0.97180000	1.67190000
	H	-1.85560000	-0.19330000	-1.76930000
	H	-4.16970000	-0.67710000	-2.37470000
	C	-6.22720000	-1.46910000	-0.76340000
	H	-5.03670000	-1.69410000	1.68720000
	H	-2.71090000	-1.23030000	2.29570000
	H	-0.01440000	2.42800000	2.69280000
	H	-0.03450000	0.64520000	3.17560000
	H	-0.77620000	5.32430000	0.17950000
	H	-1.55830000	4.27880000	-1.04040000
	H	0.20980000	4.40690000	-0.99600000
	H	-6.31470000	-1.82270000	-1.79030000
	H	-6.68000000	-2.21330000	-0.10890000
	H	-6.82270000	-0.55660000	-0.68120000
8	N	-3.74280000	1.01730000	0.89820000
	C	-4.04170000	-0.13450000	0.36540000
	C	-2.86330000	-0.94130000	0.26950000
	C	-1.83940000	-0.18790000	0.79150000
	O	-2.35200000	0.97940000	1.16910000
	C	-5.44680000	-0.42760000	-0.03680000
	C	-0.38350000	-0.39910000	1.00420000

	C	0.45730000	-0.22850000	-0.29640000
	C	1.91750000	-0.62090000	-0.07910000
	C	2.51670000	-1.49940000	-0.98370000
	C	3.84050000	-1.89530000	-0.83640000
	C	4.61710000	-1.42860000	0.22430000
	C	4.01400000	-0.55730000	1.13240000
	C	2.69020000	-0.15720000	0.98730000
	C	0.29510000	1.13040000	-0.96890000
	C	-0.14330000	1.22420000	-2.22560000
	C	0.62560000	2.36710000	-0.19430000
	O	0.61170000	3.48260000	-0.94780000
	O	0.87100000	2.38340000	0.99140000
	C	0.87810000	4.70980000	-0.24530000
	N	-2.76420000	-2.26610000	-0.25120000
	O	-3.80260000	-2.81120000	-0.62010000
	O	-1.64830000	-2.78470000	-0.30350000
	H	-6.06930000	0.43730000	0.17900000
	H	-5.82560000	-1.29490000	0.50110000
	H	-5.50180000	-0.66250000	-1.09850000
	H	-0.05210000	0.30120000	1.76480000
	H	-0.23190000	-1.41650000	1.35900000
	H	0.05810000	-0.95080000	-1.00620000
	H	1.93790000	-1.89110000	-1.81060000
	H	4.27050000	-2.58460000	-1.55210000
	C	6.06140000	-1.83490000	0.37330000
	H	4.58680000	-0.18380000	1.97210000
	H	2.26670000	0.52960000	1.70410000
	H	-0.24700000	2.17800000	-2.71880000
	H	-0.40450000	0.33910000	-2.79000000
	H	1.86710000	4.68110000	0.20640000
	H	0.13320000	4.87160000	0.53070000
	H	0.82350000	5.48940000	-0.99790000
	H	6.23960000	-2.82790000	-0.03850000
	H	6.72030000	-1.14030000	-0.15350000
	H	6.36630000	-1.84210000	1.41940000
9	N	3.91470000	0.16890000	-1.65710000
	C	4.11540000	-0.37160000	-0.48750000
	C	2.88530000	-0.90120000	0.01770000
	C	1.93350000	-0.63380000	-0.93550000
	O	2.53500000	-0.00020000	-1.93860000
	C	5.48060000	-0.36720000	0.11060000
	C	0.47450000	-0.89950000	-1.05830000
	C	-0.41910000	0.01000000	-0.16880000
	C	-1.84710000	-0.53380000	-0.16090000
	C	-2.73520000	-0.29490000	-1.20910000
	C	-4.01220000	-0.84550000	-1.20110000
	C	-4.44740000	-1.64640000	-0.14440000
	C	-3.55520000	-1.88130000	0.90320000
	C	-2.27770000	-1.33460000	0.89700000
	C	-0.37870000	1.48400000	-0.52520000
	C	-0.04230000	1.99440000	-1.70940000

	C	-0.74990000	2.38980000	0.61080000
	O	-0.99950000	3.65600000	0.22460000
	O	-0.80910000	2.02780000	1.76290000
	C	-1.31960000	4.57370000	1.28550000
	N	2.68600000	-1.60050000	1.24690000
	O	3.66210000	-1.75320000	1.97760000
	O	1.55390000	-2.01320000	1.49820000
	H	6.16750000	0.13370000	-0.56700000
	H	5.82230000	-1.38480000	0.29240000
	H	5.47550000	0.14360000	1.07200000
	H	0.19700000	-0.81550000	-2.10810000
	H	0.29230000	-1.92670000	-0.74950000
	H	-0.05140000	-0.07650000	0.85140000
	H	-2.43690000	0.33410000	-2.03740000
	H	-4.68070000	-0.64600000	-2.02920000
	C	-5.84440000	-2.21340000	-0.11970000
	H	-3.86260000	-2.49910000	1.73750000
	H	-1.60750000	-1.53110000	1.72340000
	H	-0.05820000	3.06000000	-1.87710000
	H	0.27000000	1.37470000	-2.53660000
	H	-1.49370000	5.52780000	0.79900000
	H	-0.49210000	4.64590000	1.98800000
	H	-2.21040000	4.24400000	1.81530000
	H	-6.53730000	-1.52730000	0.37350000
	H	-6.22090000	-2.38760000	-1.12730000
	H	-5.88000000	-3.15730000	0.42360000
10	N	2.59300000	-2.39480000	1.45000000
	C	3.36010000	-1.79280000	0.58570000
	C	2.55650000	-1.10440000	-0.37840000
	C	1.25230000	-1.33310000	-0.01780000
	O	1.26020000	-2.11000000	1.06020000
	C	4.84180000	-1.89030000	0.71380000
	C	-0.08340000	-0.98710000	-0.57160000
	C	-0.90900000	0.04690000	0.27080000
	C	-2.40270000	-0.19930000	0.12840000
	C	-3.00070000	-0.55480000	-1.08120000
	C	-4.37590000	-0.74790000	-1.17220000
	C	-5.20350000	-0.59660000	-0.06000000
	C	-4.60360000	-0.23960000	1.14930000
	C	-3.23120000	-0.04620000	1.24140000
	C	-0.52040000	1.49000000	-0.04650000
	C	-1.24260000	2.31800000	-0.80070000
	C	0.74830000	1.96010000	0.58770000
	O	1.08990000	3.21550000	0.25140000
	O	1.40360000	1.28060000	1.34870000
	C	2.30340000	3.71220000	0.84350000
	N	3.01580000	-0.29940000	-1.46090000
	O	4.22930000	-0.24880000	-1.65600000
	O	2.18000000	0.30420000	-2.13570000
	H	5.08650000	-2.49940000	1.58040000
	H	5.28100000	-0.90050000	0.82800000

	H	5.27750000	-2.33230000	-0.18050000
	H	0.04260000	-0.63810000	-1.59130000
	H	-0.65180000	-1.91750000	-0.59250000
	H	-0.65160000	-0.12350000	1.31570000
	H	-2.39810000	-0.68200000	-1.97070000
	H	-4.80950000	-1.02010000	-2.12620000
	C	-6.68900000	-0.83860000	-0.15120000
	H	-5.21670000	-0.11440000	2.03290000
	H	-2.79640000	0.22830000	2.19420000
	H	-0.90630000	3.32460000	-0.99300000
	H	-2.18230000	2.01100000	-1.23500000
	H	2.40380000	4.73020000	0.48220000
	H	3.15240000	3.11030000	0.52740000
	H	2.23240000	3.69370000	1.92870000
	H	-7.24140000	-0.17200000	0.51070000
	H	-7.05420000	-0.68740000	-1.16630000
	H	-6.93770000	-1.86260000	0.13740000
11	N	-1.73980000	-2.25900000	1.91700000
	C	-2.58910000	-2.18390000	0.93160000
	C	-1.92560000	-1.70430000	-0.24490000
	C	-0.61730000	-1.49490000	0.11600000
	O	-0.49390000	-1.82300000	1.39900000
	C	-4.01110000	-2.57560000	1.14710000
	C	0.61120000	-1.02540000	-0.57910000
	C	1.27430000	0.20110000	0.11380000
	C	0.35880000	1.41280000	0.19350000
	C	-0.49870000	1.78910000	-0.84020000
	C	-1.30350000	2.92010000	-0.72640000
	C	-1.28080000	3.71460000	0.41840000
	C	-0.42550000	3.33250000	1.45510000
	C	0.37660000	2.20530000	1.34430000
	C	2.61420000	0.49630000	-0.55700000
	C	2.85070000	1.54170000	-1.34810000
	C	3.77200000	-0.42950000	-0.31290000
	O	3.49060000	-1.36270000	0.62420000
	O	4.84320000	-0.36140000	-0.86550000
	C	4.56160000	-2.27340000	0.93500000
	N	-2.51710000	-1.48560000	-1.52810000
	O	-3.72430000	-1.69100000	-1.63250000
	O	-1.79610000	-1.10850000	-2.45150000
	H	-4.13950000	-2.90400000	2.17550000
	H	-4.29610000	-3.37740000	0.46810000
	H	-4.67390000	-1.73600000	0.94500000
	H	1.32550000	-1.85000000	-0.57260000
	H	0.36570000	-0.81100000	-1.61290000
	H	1.49470000	-0.10230000	1.13630000
	H	-0.55860000	1.20180000	-1.74610000
	H	-1.96300000	3.18130000	-1.54410000
	C	-2.13890000	4.94880000	0.53610000
	H	-0.39190000	3.91980000	2.36420000
	H	1.02410000	1.93200000	2.16800000

	H	3.82830000	1.67260000	-1.78810000
	H	2.09000000	2.27760000	-1.55950000
	H	4.16450000	-2.93850000	1.69470000
	H	5.42280000	-1.72730000	1.31280000
	H	4.85410000	-2.83050000	0.04780000
	H	-1.53780000	5.85560000	0.43850000
	H	-2.90380000	4.97520000	-0.23850000
	H	-2.63720000	4.99490000	1.50500000
13	N	-3.40030000	0.07150000	-2.06260000
	C	-4.01950000	-0.29150000	-0.97540000
	C	-3.07590000	-0.81880000	-0.03390000
	C	-1.84720000	-0.74420000	-0.64450000
	O	-2.02870000	-0.21890000	-1.85240000
	C	-5.49650000	-0.11880000	-0.87090000
	C	-0.45650000	-1.13890000	-0.28740000
	C	0.58020000	0.00650000	-0.42910000
	C	1.99140000	-0.55880000	-0.28310000
	C	2.48290000	-0.98990000	0.94960000
	C	3.75010000	-1.54990000	1.05550000
	C	4.57410000	-1.69150000	-0.06290000
	C	4.08070000	-1.25430000	-1.29240000
	C	2.81180000	-0.69590000	-1.40130000
	C	0.34380000	1.17560000	0.51050000
	C	-0.33510000	1.12270000	1.65650000
	C	0.95100000	2.46220000	0.03910000
	O	0.93440000	3.43520000	0.97050000
	O	1.40490000	2.61970000	-1.07080000
	C	1.47970000	4.69930000	0.55290000
	N	-3.36520000	-1.31660000	1.27400000
	O	-4.54350000	-1.33850000	1.62060000
	O	-2.42810000	-1.69070000	1.98110000
	H	-5.86950000	0.32840000	-1.78900000
	H	-5.75010000	0.51740000	-0.02460000
	H	-5.98390000	-1.07810000	-0.70600000
	H	-0.45770000	-1.56360000	0.71030000
	H	-0.15800000	-1.93420000	-0.97400000
	H	0.50360000	0.40050000	-1.44090000
	H	1.87680000	-0.88500000	1.84000000
	H	4.10410000	-1.88110000	2.02380000
	C	5.96110000	-2.26980000	0.06180000
	H	4.69610000	-1.34860000	-2.17820000
	H	2.45950000	-0.35500000	-2.36610000
	H	-0.44030000	1.99970000	2.27630000
	H	-0.80170000	0.21310000	2.00760000
	H	1.39090000	5.35110000	1.41570000
	H	0.91640000	5.09690000	-0.28860000
	H	2.52190000	4.58490000	0.26320000
	H	6.00460000	-3.03380000	0.83790000
	H	6.29000000	-2.71900000	-0.87460000
	H	6.68630000	-1.49640000	0.32580000

15	N	-3.15460000	-2.72480000	-0.46270000
	C	-3.80640000	-1.63890000	-0.15480000
	C	-2.90250000	-0.67090000	0.39200000
	C	-1.66330000	-1.26150000	0.39280000
	O	-1.80300000	-2.48650000	-0.11380000
	C	-5.27560000	-1.56220000	-0.39520000
	C	-0.28570000	-0.87070000	0.79390000
	C	0.60960000	-0.53540000	-0.43910000
	C	2.10270000	-0.66910000	-0.14330000
	C	2.67660000	-0.37330000	1.09380000
	C	4.04160000	-0.53200000	1.30060000
	C	4.88580000	-0.98330000	0.28440000
	C	4.30970000	-1.27980000	-0.95040000
	C	2.94360000	-1.12720000	-1.15830000
	C	0.24090000	0.79530000	-1.08210000
	C	-0.24620000	0.85650000	-2.32210000
	C	0.43340000	2.04030000	-0.27300000
	O	0.12340000	3.16290000	-0.94820000
	O	0.82310000	2.04780000	0.87150000
	C	0.23980000	4.38560000	-0.19800000
	N	-3.23230000	0.64440000	0.84710000
	O	-4.41430000	0.97920000	0.79190000
	O	-2.32440000	1.36030000	1.26320000
	H	-5.61520000	-2.49680000	-0.83490000
	H	-5.51330000	-0.73540000	-1.06230000
	H	-5.80740000	-1.38170000	0.53730000
	H	-0.32970000	-0.03130000	1.47830000
	H	0.15460000	-1.72500000	1.30900000
	H	0.39050000	-1.29280000	-1.19200000
	H	2.06500000	0.00250000	1.89950000
	H	4.45680000	-0.29700000	2.27270000
	C	6.36940000	-1.12600000	0.51260000
	H	4.93210000	-1.64360000	-1.75810000
	H	2.52670000	-1.37510000	-2.12670000
	H	-0.50510000	1.79820000	-2.78040000
	H	-0.39430000	-0.04160000	-2.90700000
	H	-0.04880000	5.17360000	-0.88560000
	H	1.26390000	4.52680000	0.14030000
	H	-0.42490000	4.36300000	0.66250000
	H	6.58180000	-1.54570000	1.49620000
	H	6.82620000	-1.77190000	-0.23620000
	H	6.86980000	-0.15620000	0.45980000
17	N	-3.96410000	-0.10430000	1.72560000
	C	-4.13150000	-0.43870000	0.47650000
	C	-2.87720000	-0.83370000	-0.08980000
	C	-1.94660000	-0.70450000	0.91270000
	O	-2.58300000	-0.27450000	1.99810000
	C	-5.48880000	-0.37480000	-0.13590000
	C	-0.48160000	-0.94360000	1.02080000
	C	0.40340000	0.08140000	0.25460000
	C	1.84180000	-0.43450000	0.21990000

	C	2.74720000	-0.18360000	1.24860000
	C	4.03360000	-0.71470000	1.21140000
	C	4.45830000	-1.50860000	0.14710000
	C	3.54670000	-1.75700000	-0.88250000
	C	2.26300000	-1.22930000	-0.84840000
	C	0.31420000	1.50500000	0.77310000
	C	-0.10720000	1.87080000	1.98290000
	C	0.76030000	2.61540000	-0.13870000
	O	0.94310000	2.18970000	-1.40430000
	O	0.92760000	3.76210000	0.20160000
	C	1.37660000	3.19160000	-2.34150000
	N	-2.64040000	-1.30680000	-1.41550000
	O	-3.59610000	-1.33990000	-2.18690000
	O	-1.49640000	-1.65870000	-1.70700000
	H	-6.20280000	-0.03390000	0.60960000
	H	-5.78740000	-1.35300000	-0.50910000
	H	-5.49370000	0.30560000	-0.98570000
	H	-0.21660000	-0.97400000	2.07660000
	H	-0.27060000	-1.92480000	0.59950000
	H	0.05240000	0.08580000	-0.77430000
	H	2.45680000	0.43830000	2.08460000
	H	4.71680000	-0.50380000	2.02430000
	C	5.85980000	-2.06210000	0.09180000
	H	3.84520000	-2.37070000	-1.72330000
	H	1.57750000	-1.43800000	-1.65970000
	H	-0.10810000	2.91580000	2.25620000
	H	-0.46300000	1.16340000	2.71560000
	H	1.47650000	2.67580000	-3.29070000
	H	2.32970000	3.61220000	-2.02900000
	H	0.63970000	3.98860000	-2.41150000
	H	6.33310000	-2.04320000	1.07260000
	H	5.86600000	-3.09160000	-0.26720000
	H	6.48620000	-1.47900000	-0.58720000
19	N	-3.37100000	-2.35270000	-0.43150000
	C	-3.94010000	-1.25970000	-0.00770000
	C	-2.95300000	-0.38650000	0.55620000
	C	-1.75220000	-1.03960000	0.43300000
	O	-1.98830000	-2.21190000	-0.15190000
	C	-5.41350000	-1.08670000	-0.15450000
	C	-0.34110000	-0.74160000	0.79850000
	C	0.61630000	-0.78870000	-0.42200000
	C	2.09300000	-0.73010000	-0.02860000
	C	2.54590000	-0.36740000	1.23660000
	C	3.90670000	-0.35710000	1.53540000
	C	4.86170000	-0.70440000	0.58350000
	C	4.40540000	-1.06510000	-0.68770000
	C	3.05130000	-1.07830000	-0.98600000
	C	0.25400000	0.22640000	-1.50080000
	C	-0.19460000	-0.15820000	-2.69610000
	C	0.38680000	1.70730000	-1.27830000
	O	0.73050000	2.00590000	-0.01290000

	O	0.19630000	2.54520000	-2.12730000
	C	0.84410000	3.40950000	0.28880000
	N	-3.18600000	0.90310000	1.13340000
	O	-4.33870000	1.32790000	1.10800000
	O	-2.23310000	1.50880000	1.62010000
	H	-5.83210000	-1.97250000	-0.62590000
	H	-5.63780000	-0.20920000	-0.75820000
	H	-5.88070000	-0.93340000	0.81680000
	H	-0.31110000	0.22210000	1.29090000
	H	-0.02020000	-1.50320000	1.51330000
	H	0.46820000	-1.76410000	-0.88730000
	H	1.84690000	-0.07750000	2.00750000
	H	4.22520000	-0.07000000	2.52950000
	C	6.33460000	-0.70310000	0.90550000
	H	5.11930000	-1.34170000	-1.45360000
	H	2.73240000	-1.36090000	-1.98120000
	H	-0.43850000	0.57500000	-3.45090000
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	H	1.13780000	3.45800000	1.33180000
	H	6.52080000	-0.32320000	1.90890000
	H	6.75170000	-1.71050000	0.84850000
	H	6.89350000	-0.08300000	0.20280000
21	N	-3.33640000	1.40210000	-0.90480000
	C	-3.69680000	0.48260000	-0.05340000
	C	-2.74540000	-0.58670000	-0.06730000
	C	-1.79020000	-0.23490000	-0.98940000
	O	-2.13230000	0.94480000	-1.49560000
	C	-4.94310000	0.65390000	0.74610000
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	C	0.64820000	-0.77150000	-0.51810000
	C	0.99770000	0.67950000	-0.19710000
	C	1.64420000	1.49710000	-1.12620000
	C	1.91620000	2.82760000	-0.83830000
	C	1.55730000	3.39110000	0.38890000
	C	0.91670000	2.57100000	1.31610000
	C	0.64380000	1.23680000	1.02920000
	C	1.85400000	-1.54660000	-1.02210000
	C	2.02660000	-1.99100000	-2.26600000
	C	2.95930000	-1.84930000	-0.04770000
	O	2.58630000	-1.62470000	1.22660000
	O	4.05190000	-2.26290000	-0.35350000
	C	3.58700000	-1.89660000	2.22410000
	N	-2.78340000	-1.78990000	0.69880000
	O	-3.72570000	-1.94170000	1.47330000
	O	-1.87340000	-2.60440000	0.53910000
	H	-5.40640000	1.60310000	0.48870000
	H	-4.72120000	0.63140000	1.81170000
	H	-5.64000000	-0.15890000	0.54880000
	H	-0.75630000	-1.91850000	-1.69970000

	H	-0.30420000	-0.37670000	-2.44660000
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	H	1.94570000	1.09200000	-2.08350000
	H	2.41710000	3.43810000	-1.57920000
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	H	0.62760000	2.97700000	2.27710000
	H	0.15540000	0.62190000	1.77430000
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	H	1.29160000	-1.84640000	-3.04340000
	H	3.87630000	-2.94460000	2.19320000
	H	3.12230000	-1.65430000	3.17390000
	H	4.46510000	-1.27730000	2.05540000
	H	1.55050000	5.49070000	-0.11070000
	H	1.37310000	5.15870000	1.61180000
	H	2.94300000	4.98380000	0.83340000
22	N	3.11350000	0.11740000	2.09160000
	C	3.61800000	-0.48450000	1.05070000
	C	2.56570000	-1.06790000	0.27270000
	C	1.39760000	-0.76200000	0.92560000
	O	1.71140000	-0.06220000	2.01240000
	C	5.09310000	-0.48650000	0.83590000
	C	-0.04490000	-1.03580000	0.69130000
	C	-0.86760000	0.22060000	0.27440000
	C	-2.36370000	-0.06500000	0.28430000
	C	-2.91590000	-1.29520000	-0.06900000
	C	-4.29560000	-1.48860000	-0.06950000
	C	-5.17160000	-0.46500000	0.28420000
	C	-4.61620000	0.76690000	0.64100000
	C	-3.24270000	0.96100000	0.64320000
	C	-0.38670000	0.79280000	-1.06290000
	C	-0.79850000	0.34690000	-2.24820000
	C	0.60290000	1.92180000	-1.08320000
	O	0.86080000	2.39970000	0.15320000
	O	1.11480000	2.37440000	-2.07940000
	C	1.79140000	3.49610000	0.21600000
	N	2.71510000	-1.83710000	-0.92660000
	O	3.85210000	-1.95610000	-1.37650000
	O	1.71200000	-2.33800000	-1.43030000
	H	5.57320000	0.06120000	1.64310000
	H	5.34160000	-0.02780000	-0.11940000
	H	5.47530000	-1.50560000	0.80820000
	H	-0.11640000	-1.80860000	-0.06590000
	H	-0.46230000	-1.42060000	1.62350000
	H	-0.68830000	0.97870000	1.03220000
	H	-2.28000000	-2.12340000	-0.34960000
	H	-4.69230000	-2.45590000	-0.35070000
	C	-6.66400000	-0.67830000	0.30590000
	H	-5.26770000	1.58440000	0.92390000
	H	-2.84410000	1.92720000	0.92620000
	H	-0.40530000	0.77930000	-3.15620000
	H	-1.52950000	-0.44330000	-2.33620000

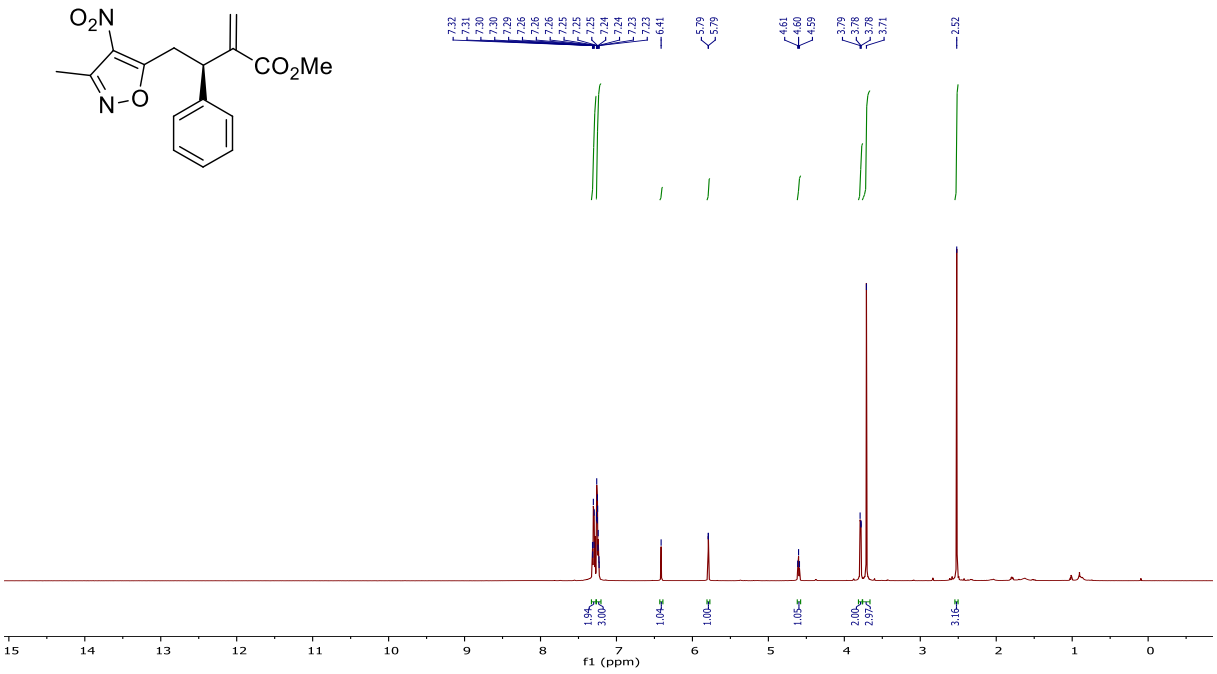
H	2.74250000	3.21120000	-0.22720000
H	1.90990000	3.71470000	1.27180000
H	1.39380000	4.35730000	-0.31640000
H	-7.19010000	0.15170000	-0.16690000
H	-6.94150000	-1.59370000	-0.21470000
H	-7.03540000	-0.75510000	1.33020000

[a] Conformers are numbered according to their appearance during conformational search.

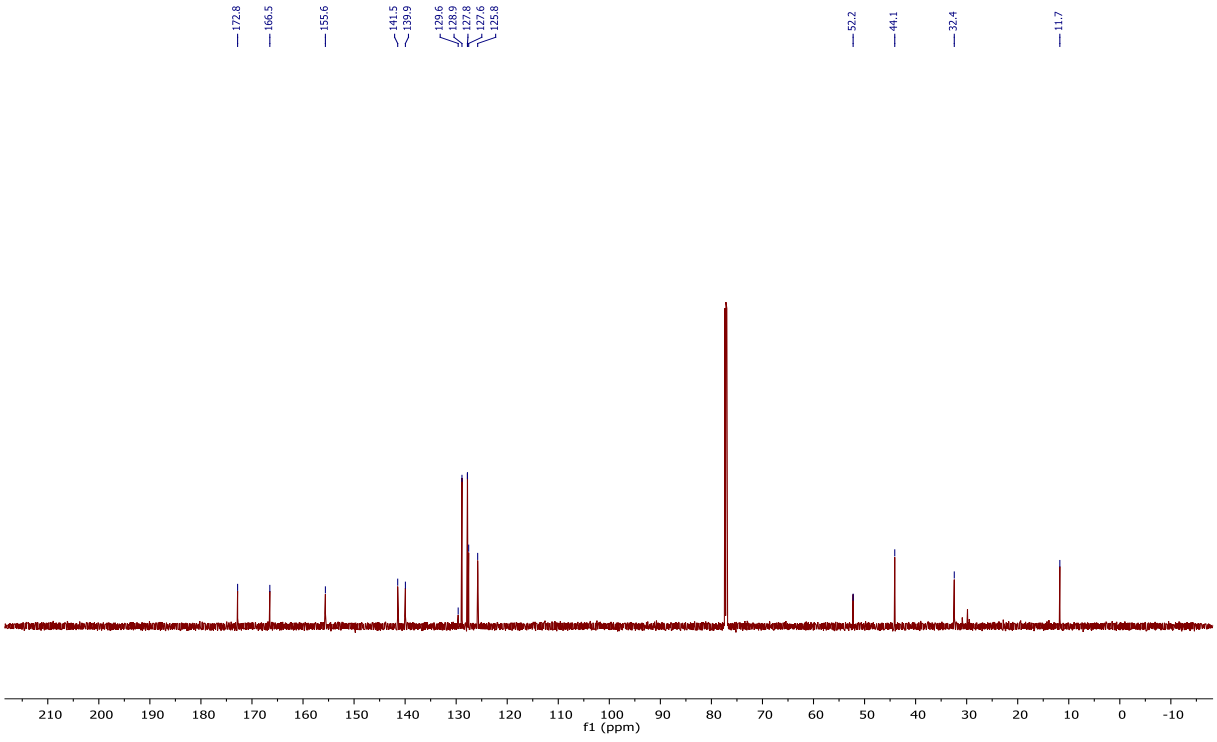
4. NMR Data

3a (*R*)-Methyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-phenylbutanoate (Table 2, entry 1)

^{1}H NMR

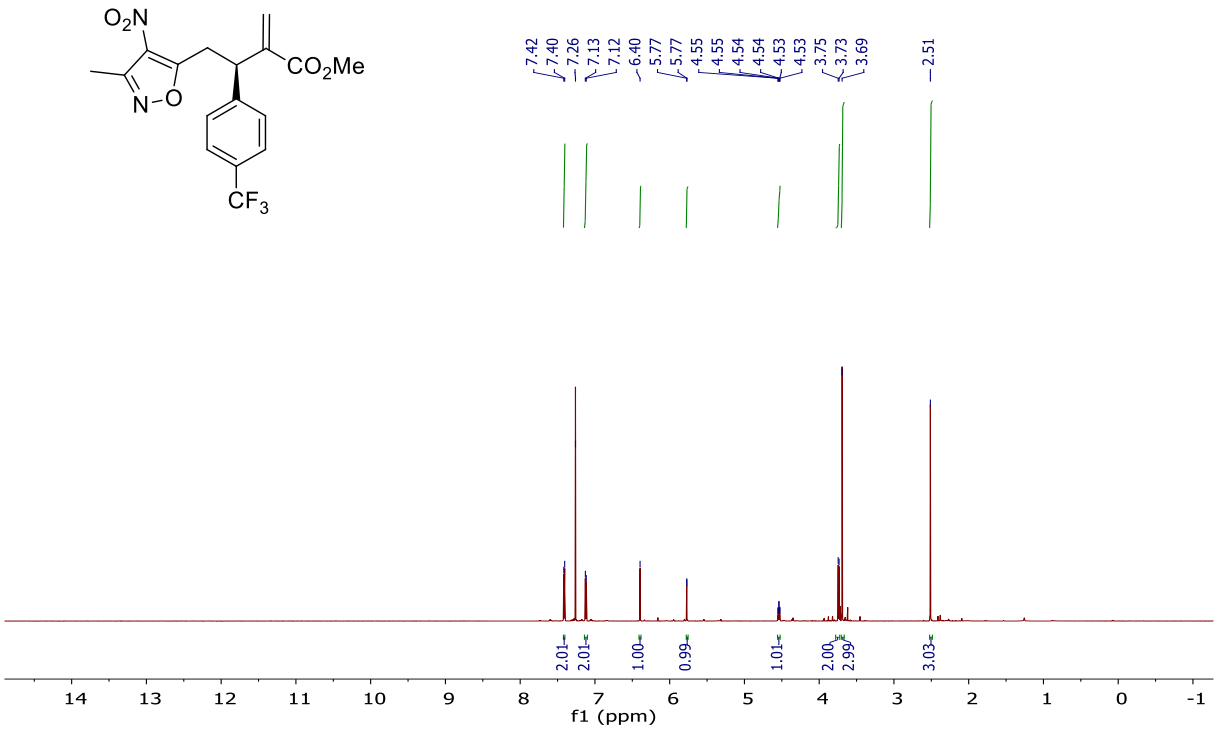


^{13}C NMR

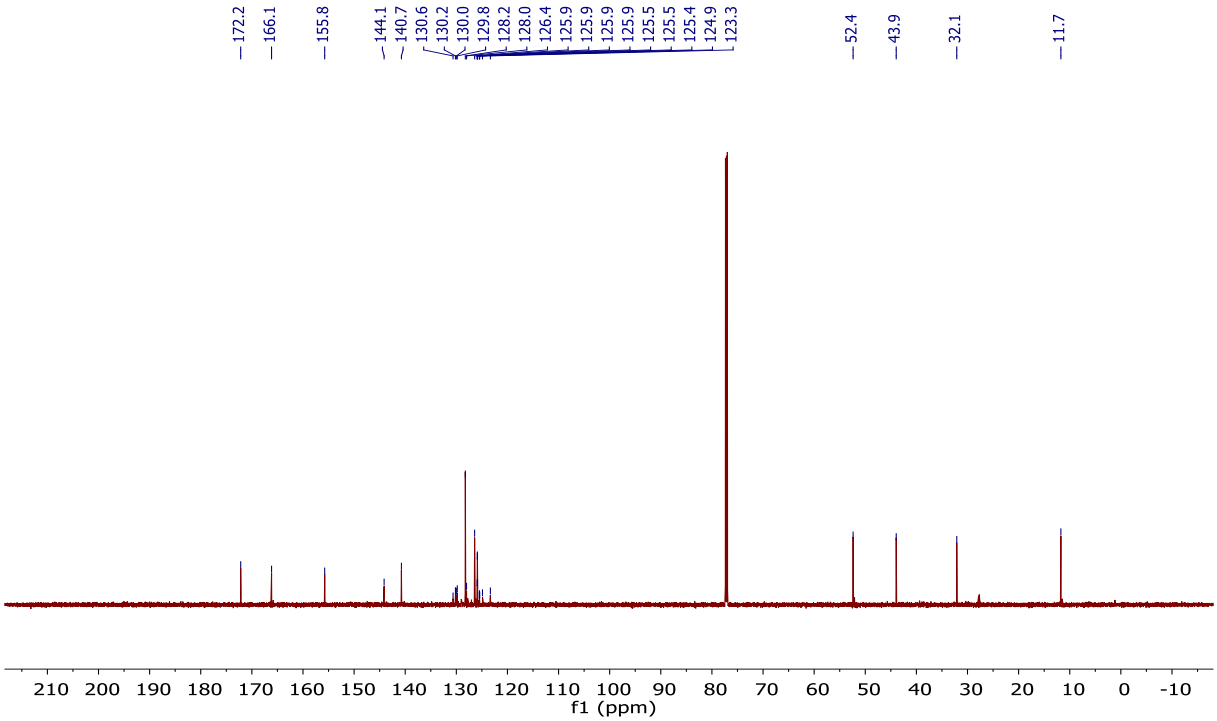


3b (*R*)-Methyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-(4-(trifluoromethyl)phenyl) butanoate (Table 2, entry 2)

^{1}H NMR

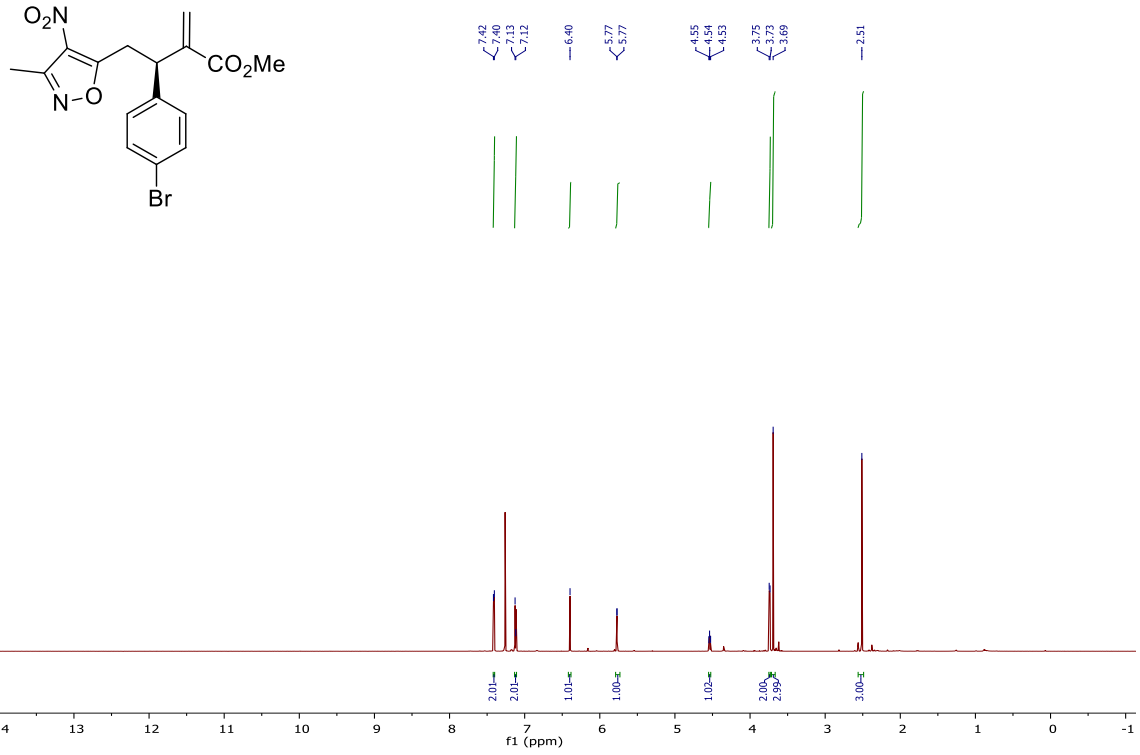


^{13}C NMR

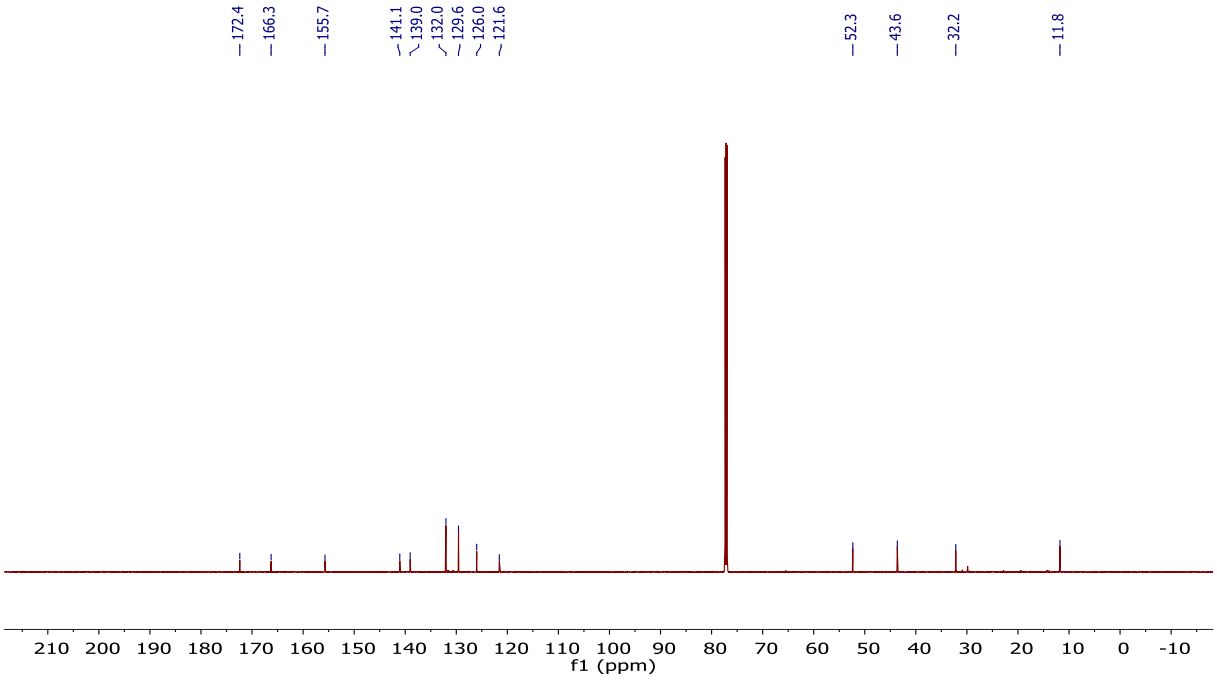


3c (*R*)-Methyl 3-(4-bromophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 3)

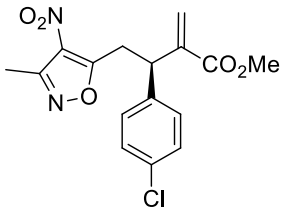
^{1}H NMR



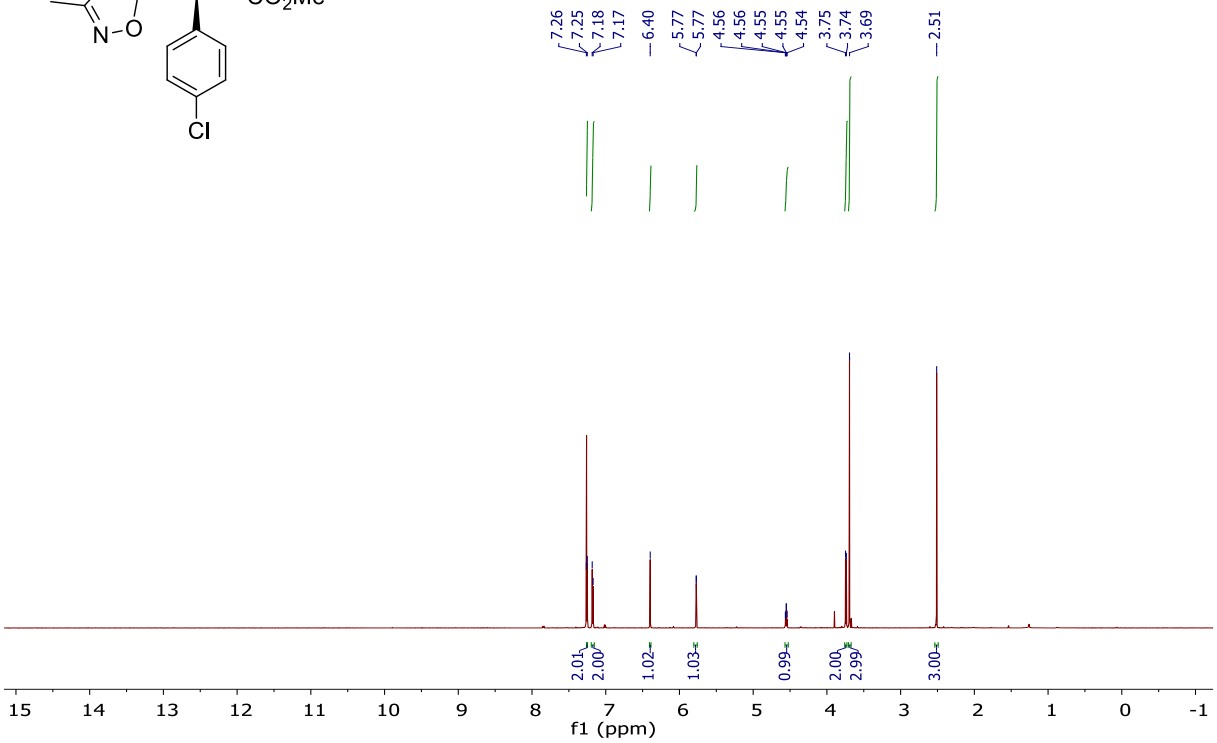
^{13}C NMR



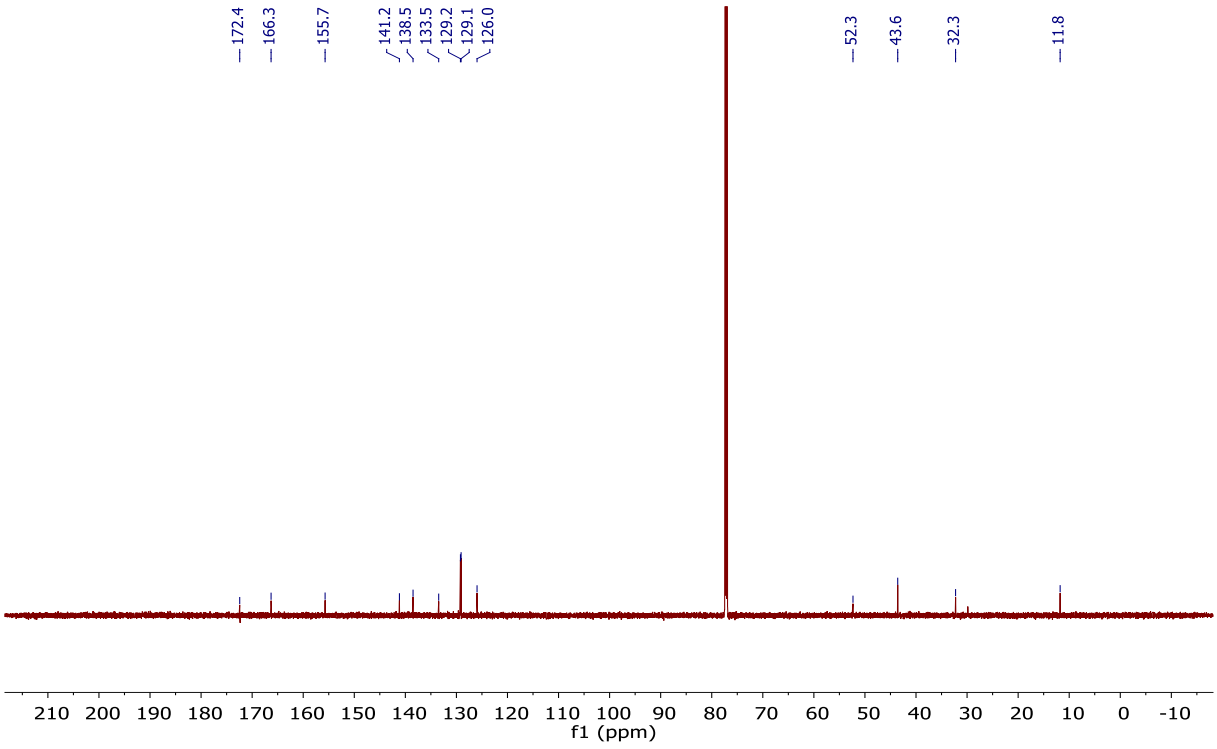
3d (*R*)-Methyl 3-(4-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 4)



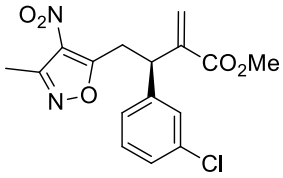
^{1}H NMR



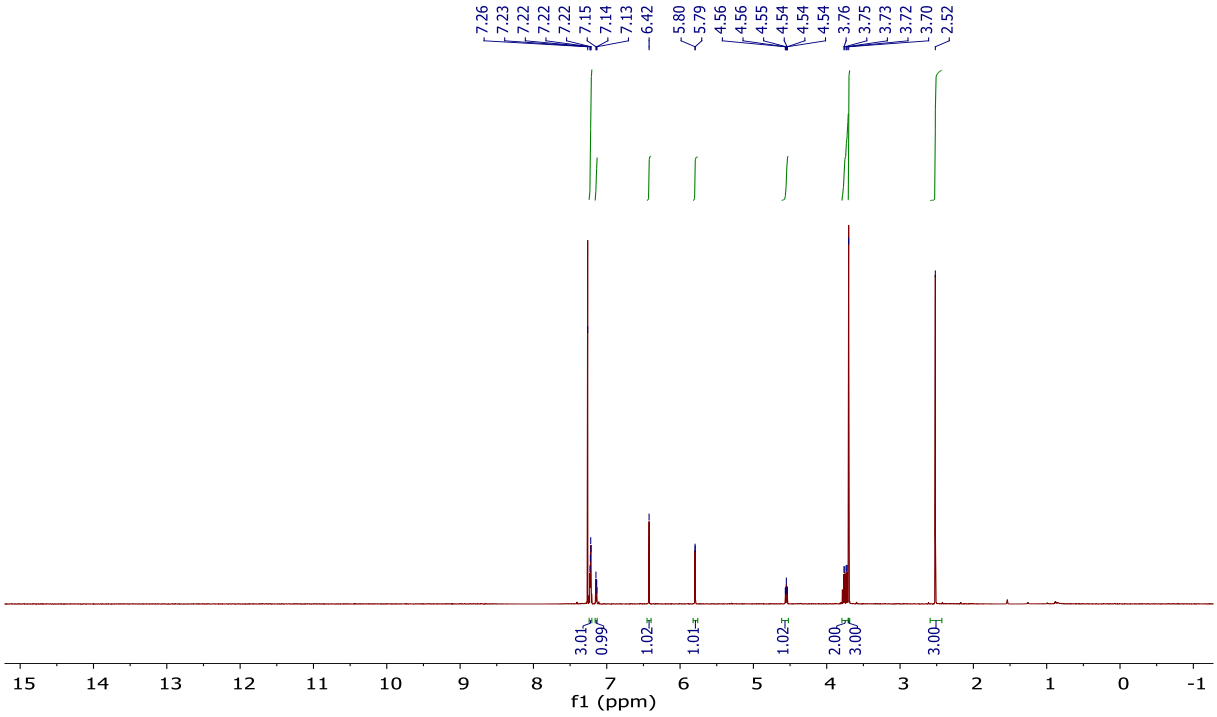
^{13}C NMR



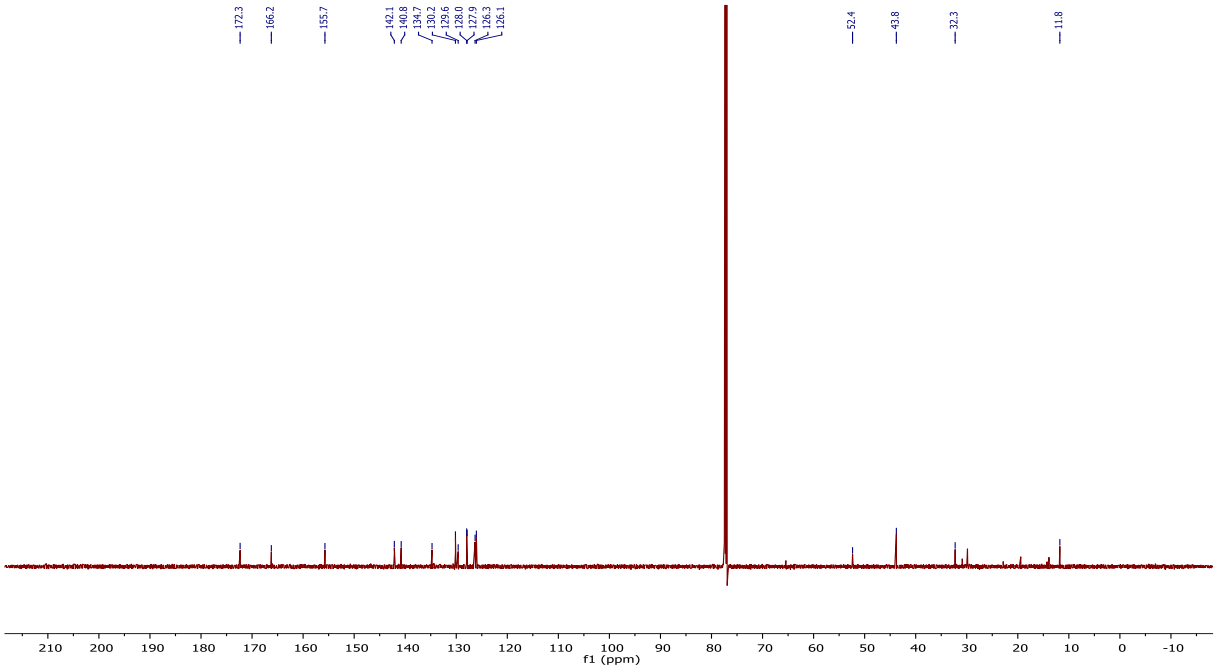
3e (*R*)-Methyl 3-(3-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 5)



^{1}H NMR

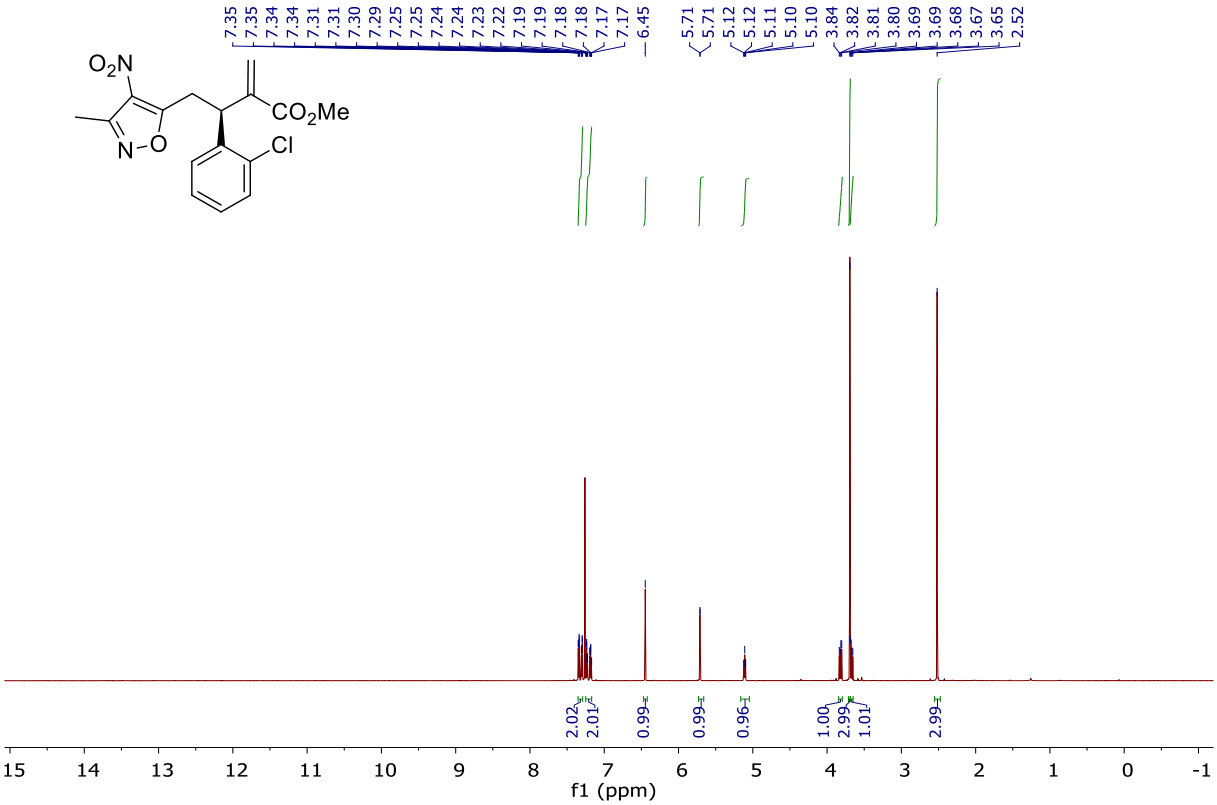


^{13}C NMR

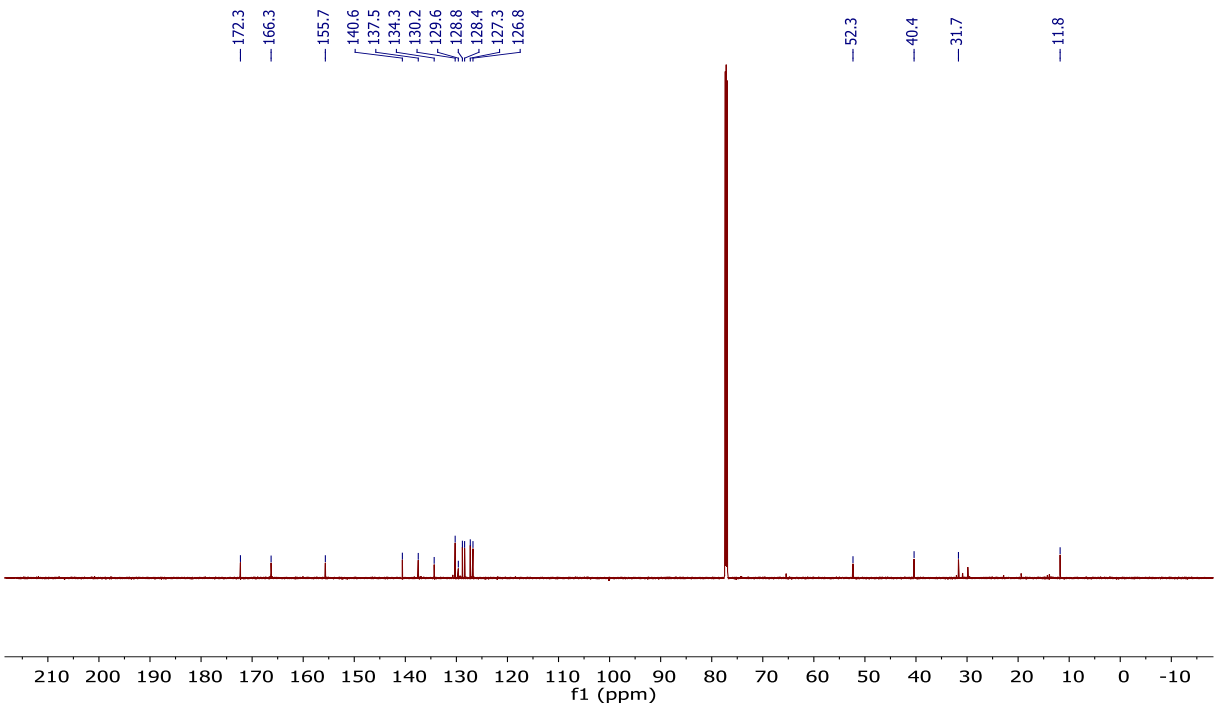


3f (*S*)-Methyl 3-(2-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 6)

^{1}H NMR

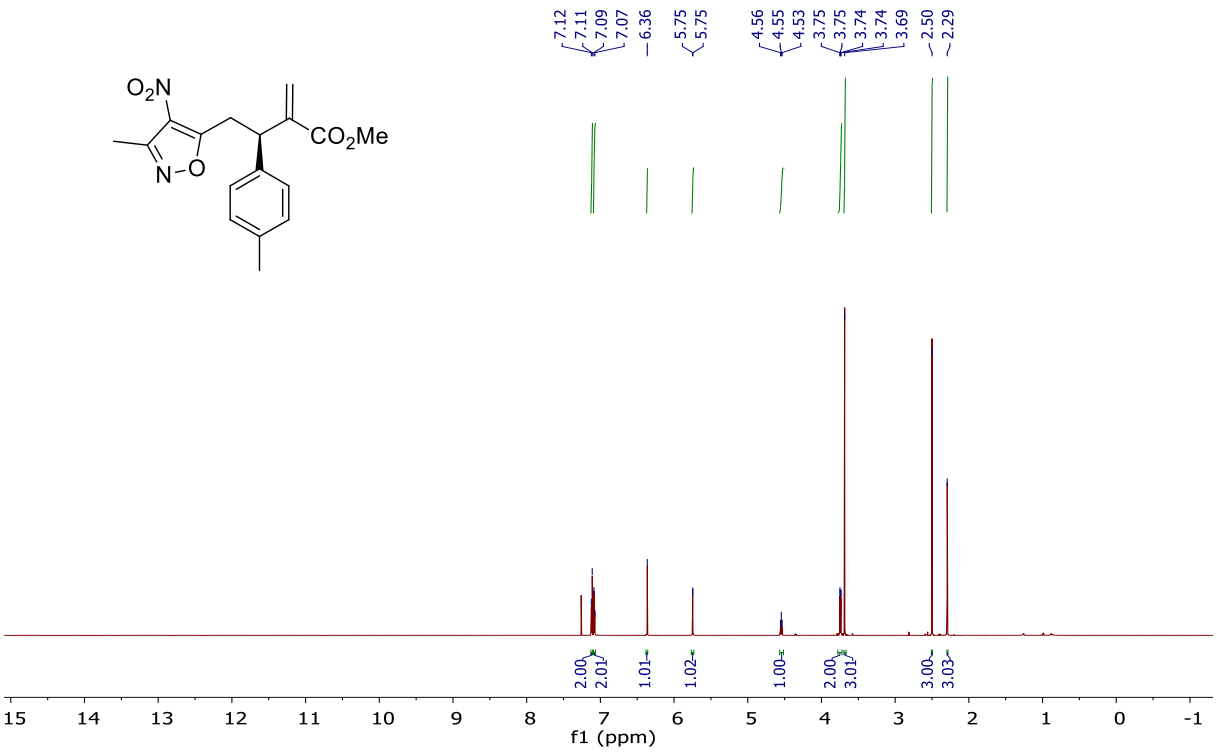


^{13}C NMR

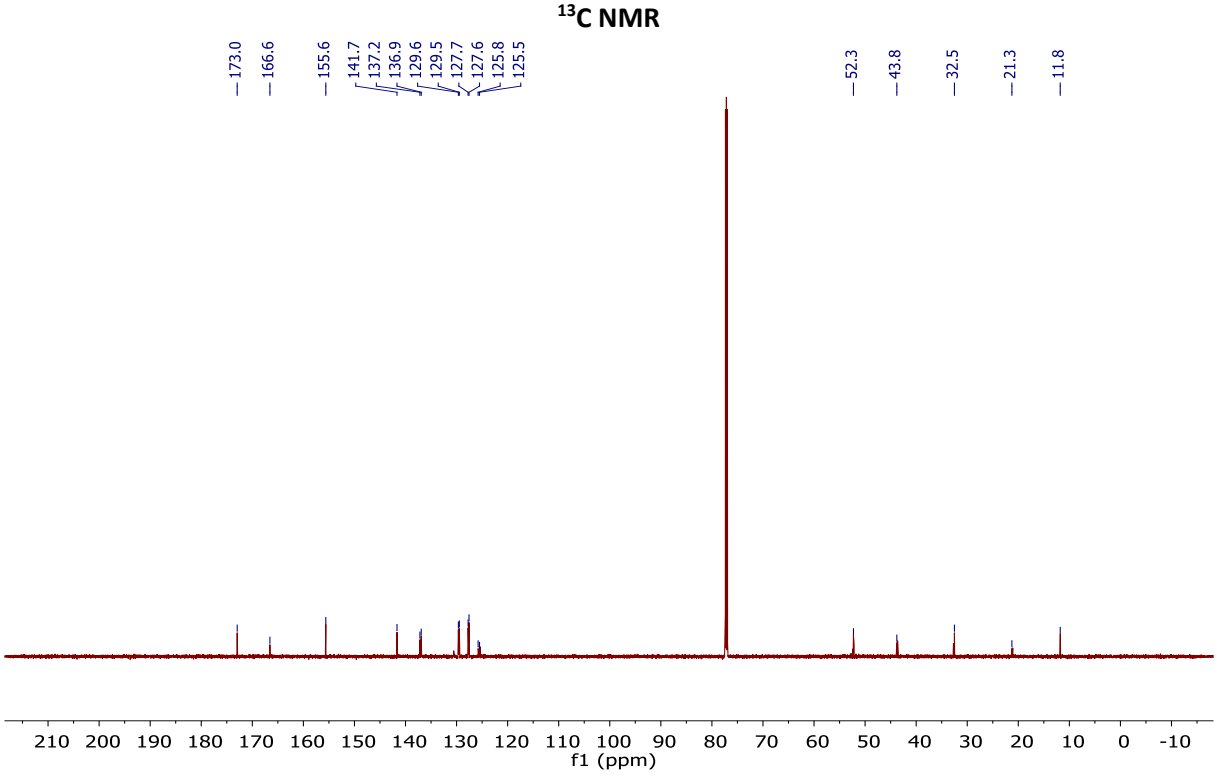


3g (*R*)-Methyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-(p-tolyl)butanoate (Table 2, entry 7)

^{1}H NMR

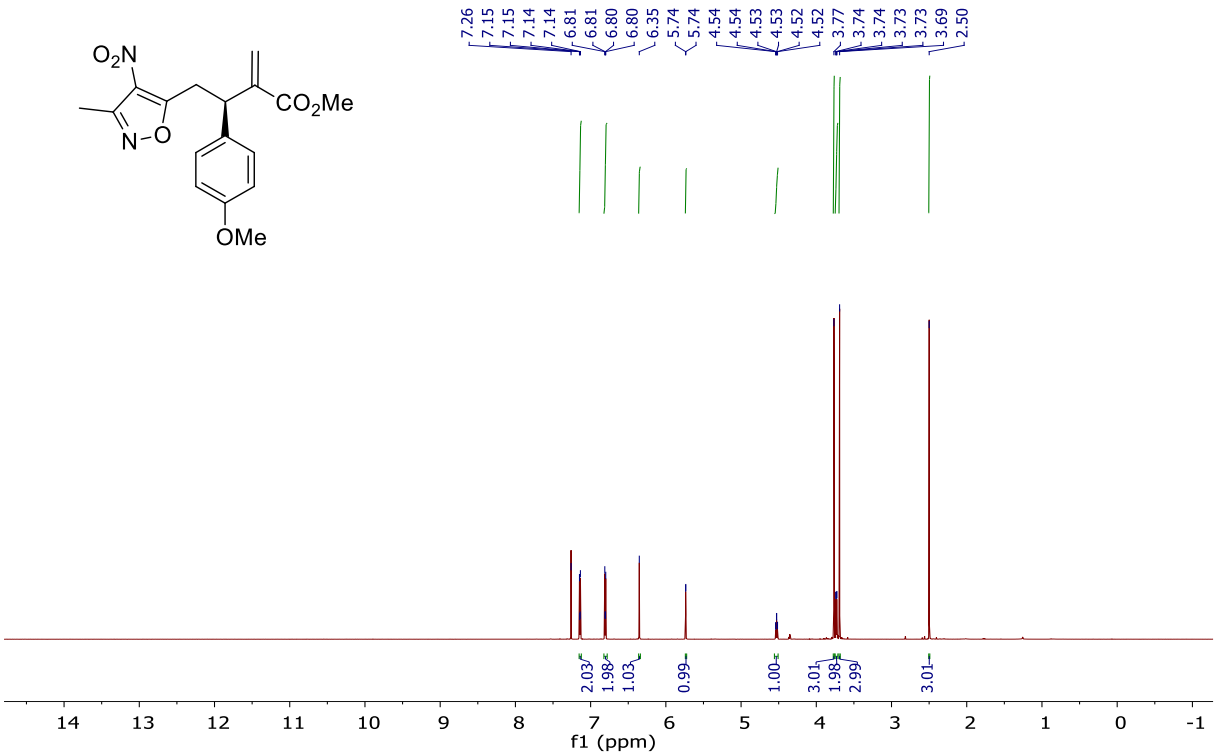


^{13}C NMR

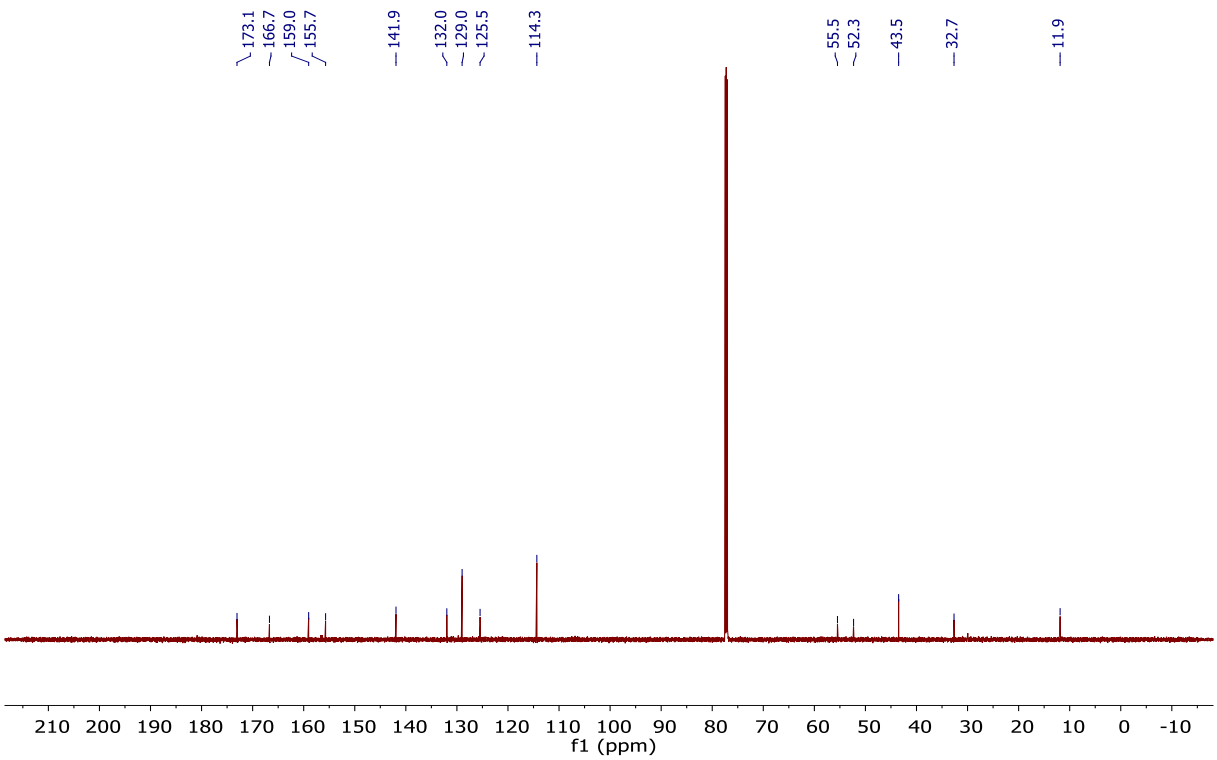


3h (*R*)-Methyl 3-(4-methoxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 8)

^{1}H NMR

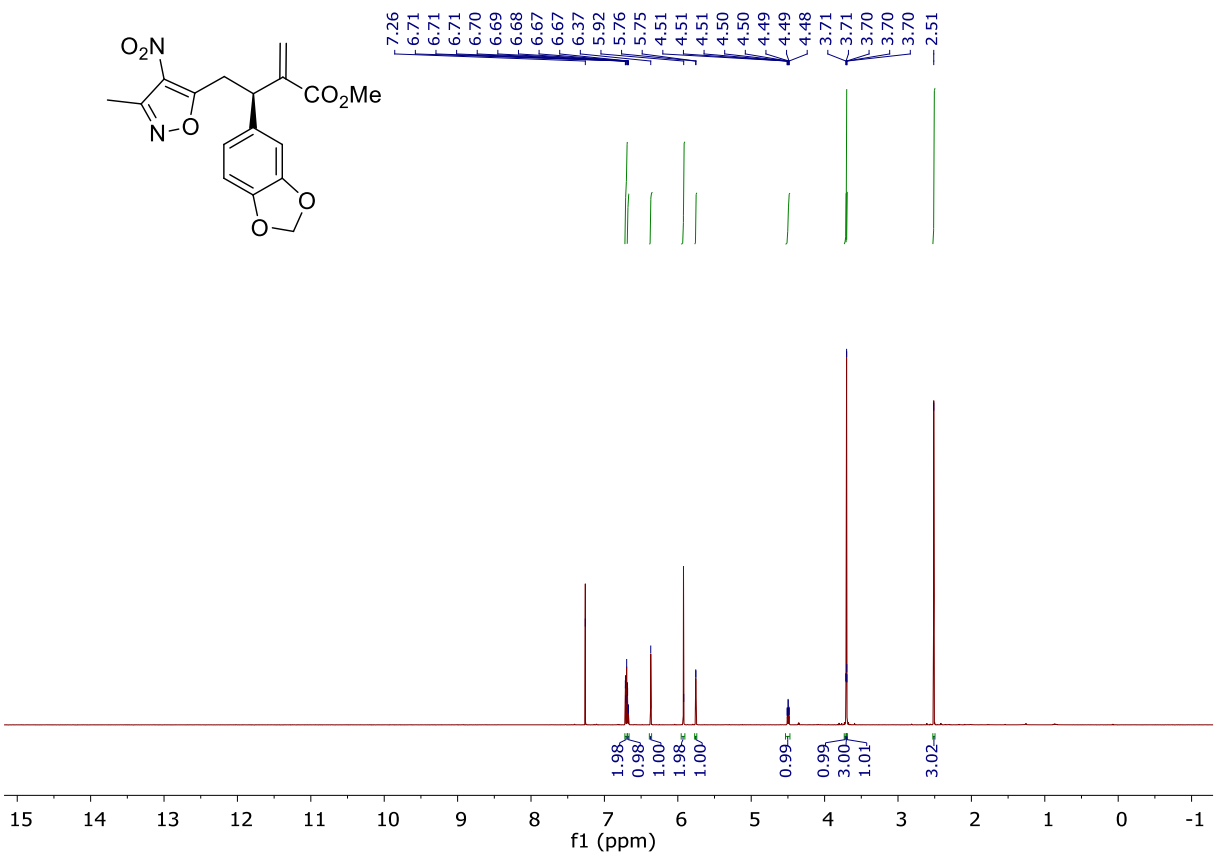


^{13}C NMR

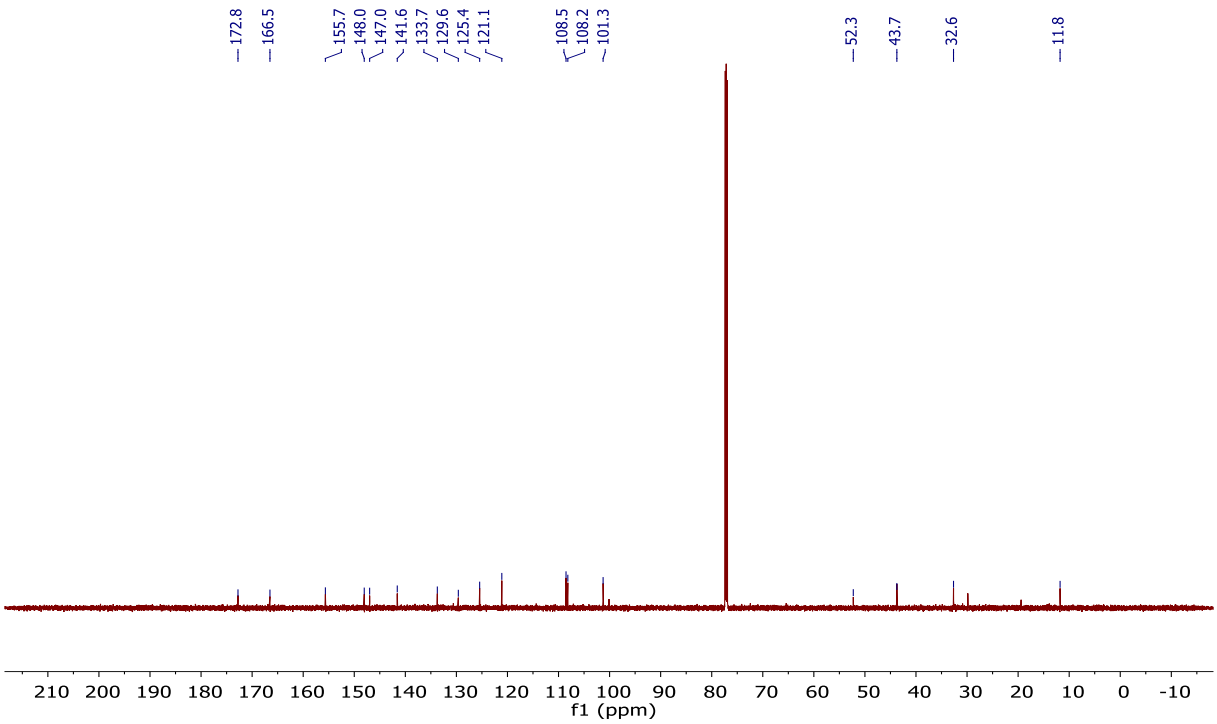


3i (*R*)-Methyl 3-(benzo[d][1,3]dioxol-5-yl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 9)

^{1}H NMR

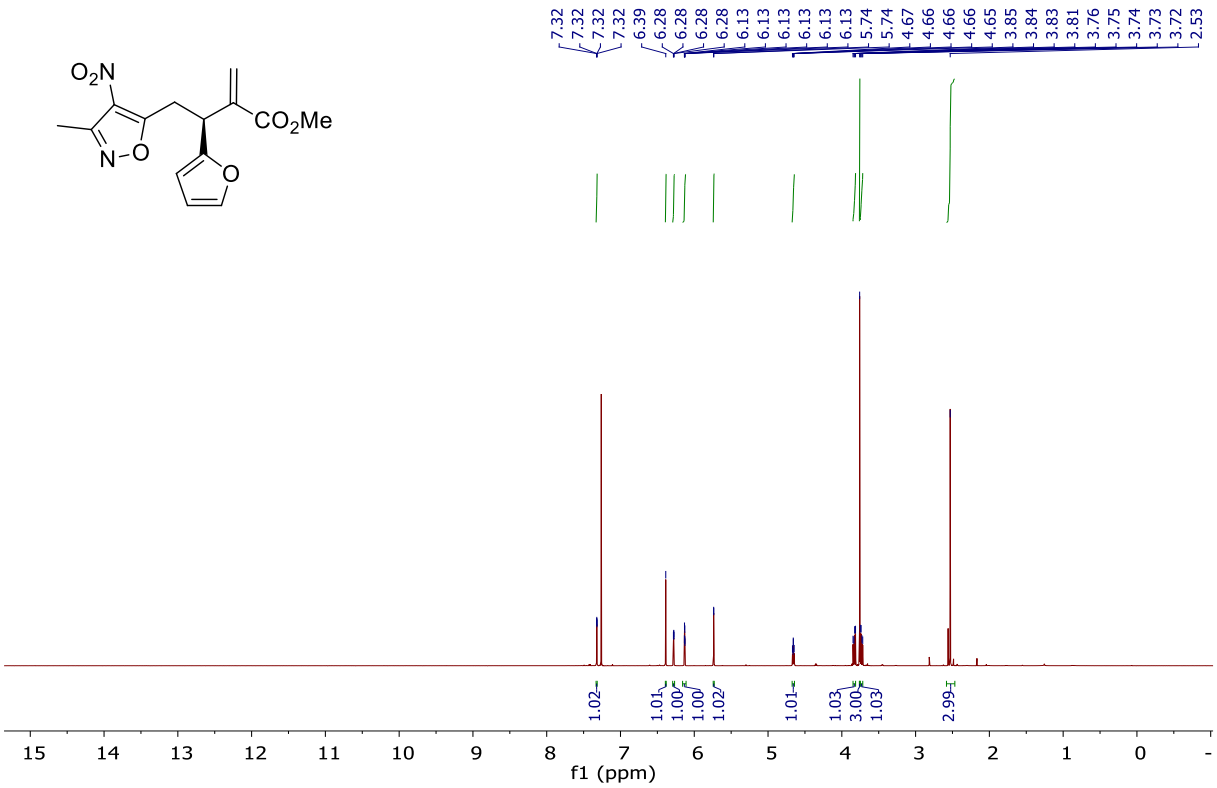


^{13}C NMR

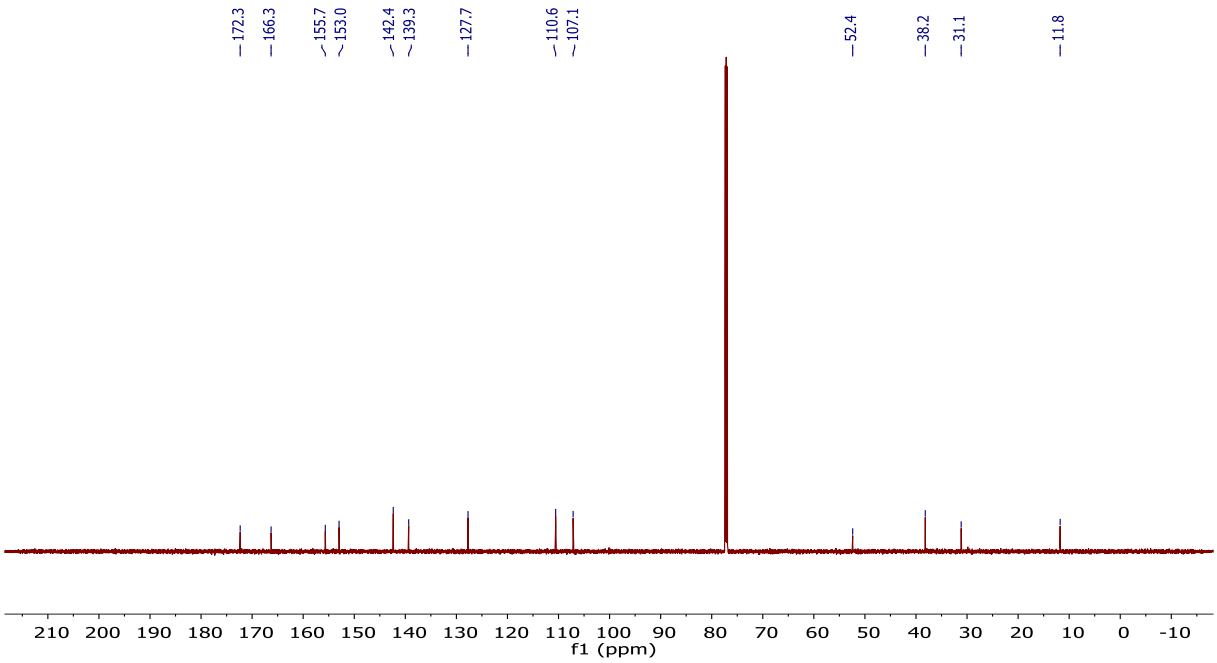


3j (*S*)-Methyl 3-(furan-2-yl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 10)

^{1}H NMR

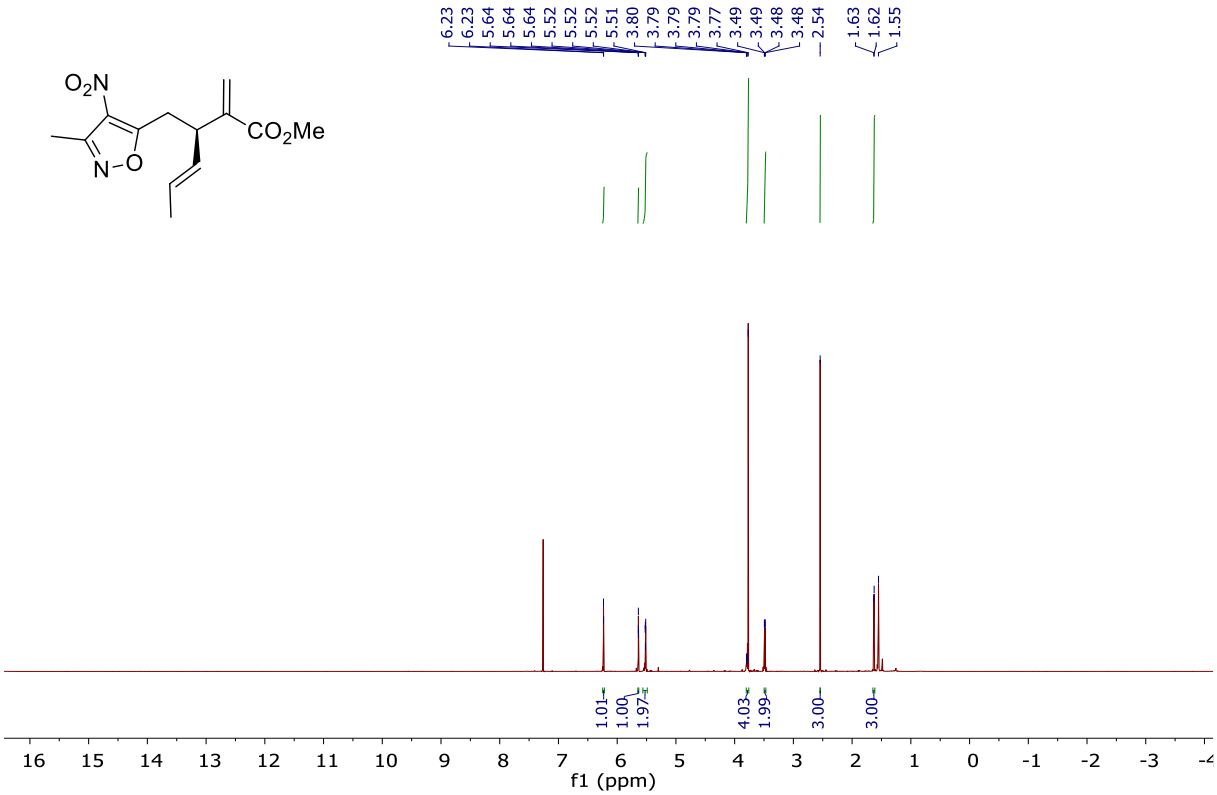


^{13}C NMR

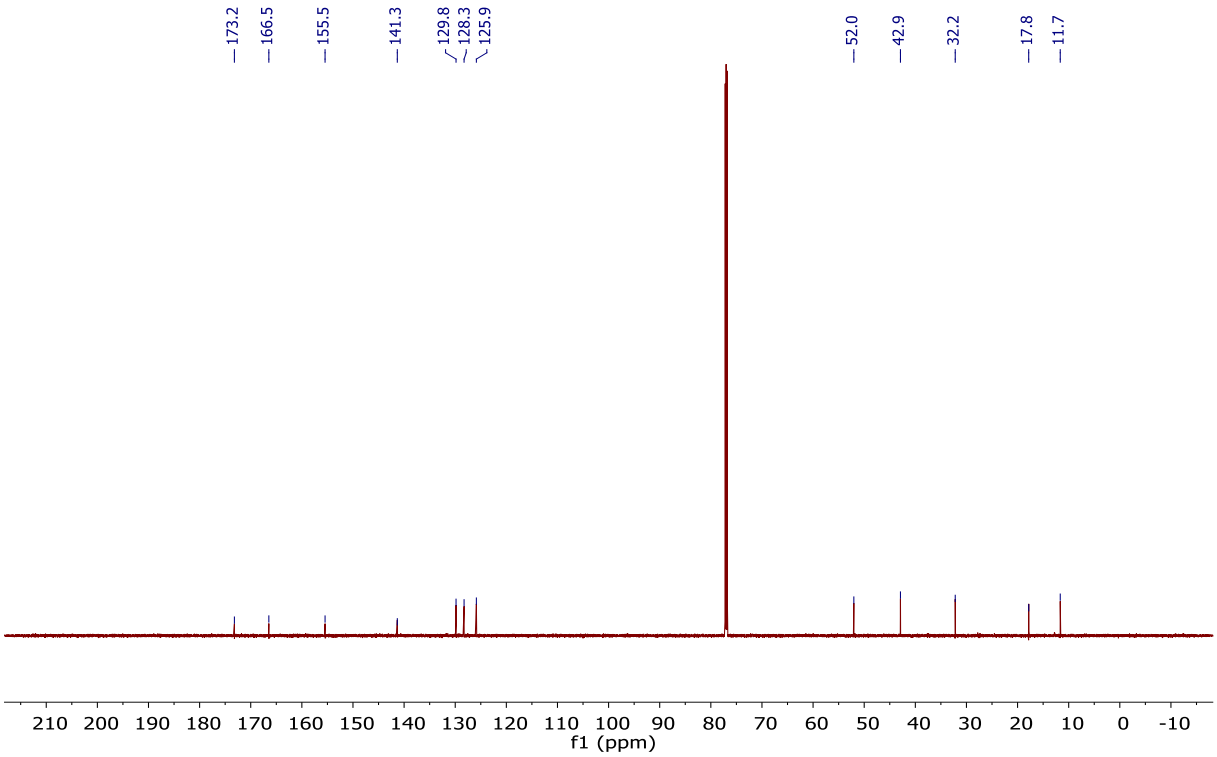


3k (*R,E*)-Methyl 3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-methylenehex-4-enoate (Table 2, entry 11)

^{1}H NMR

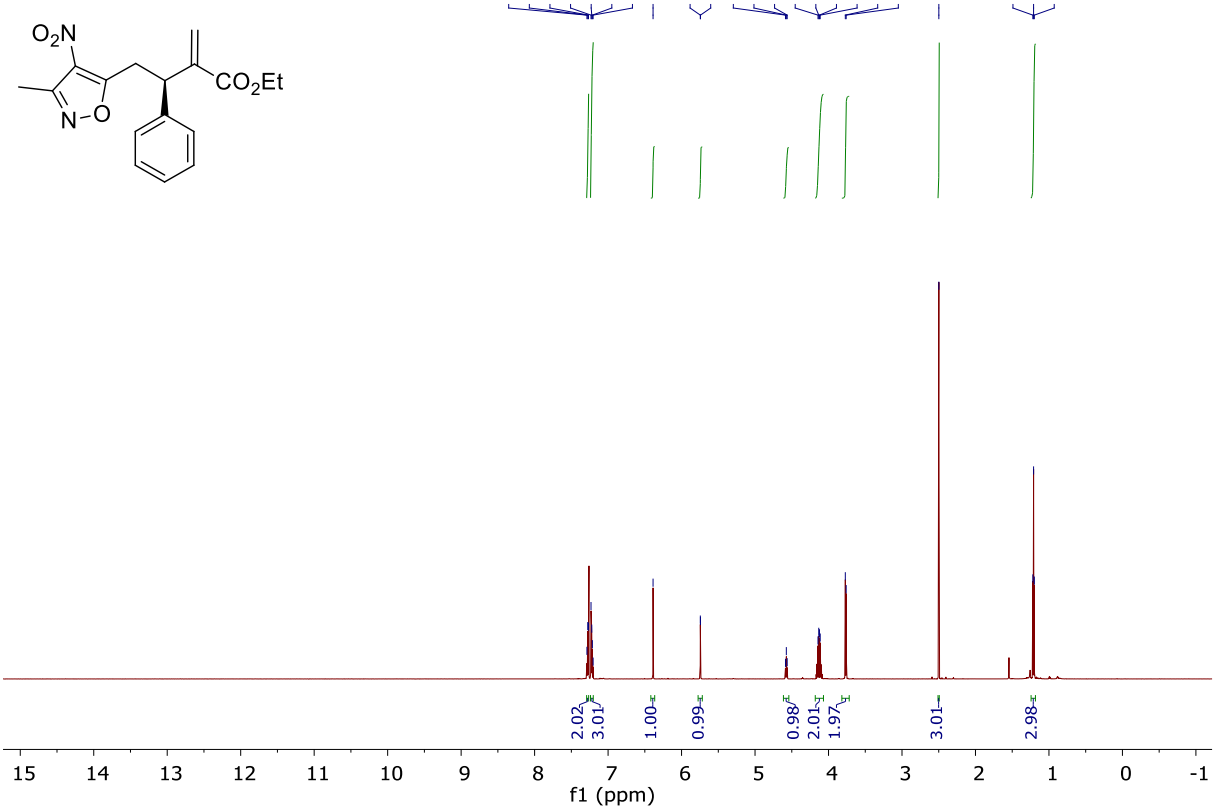


^{13}C NMR

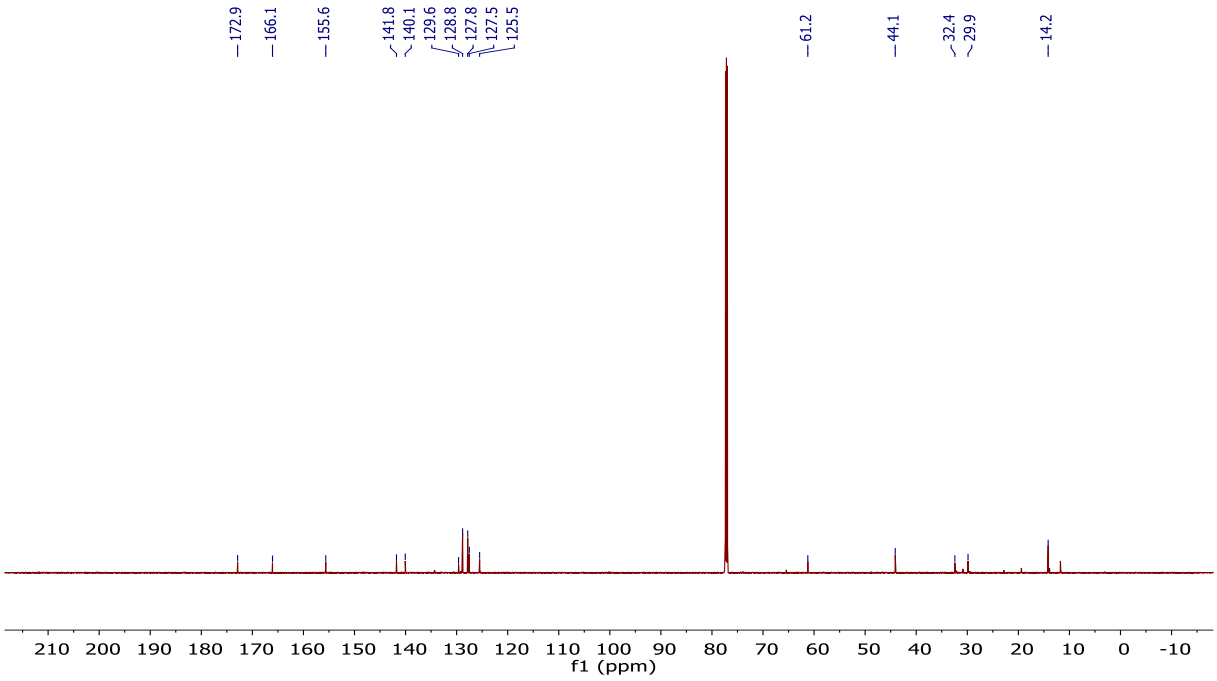


3l (*R*)-Ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-phenylbutanoate (Table 2, entry 12)

^{1}H NMR

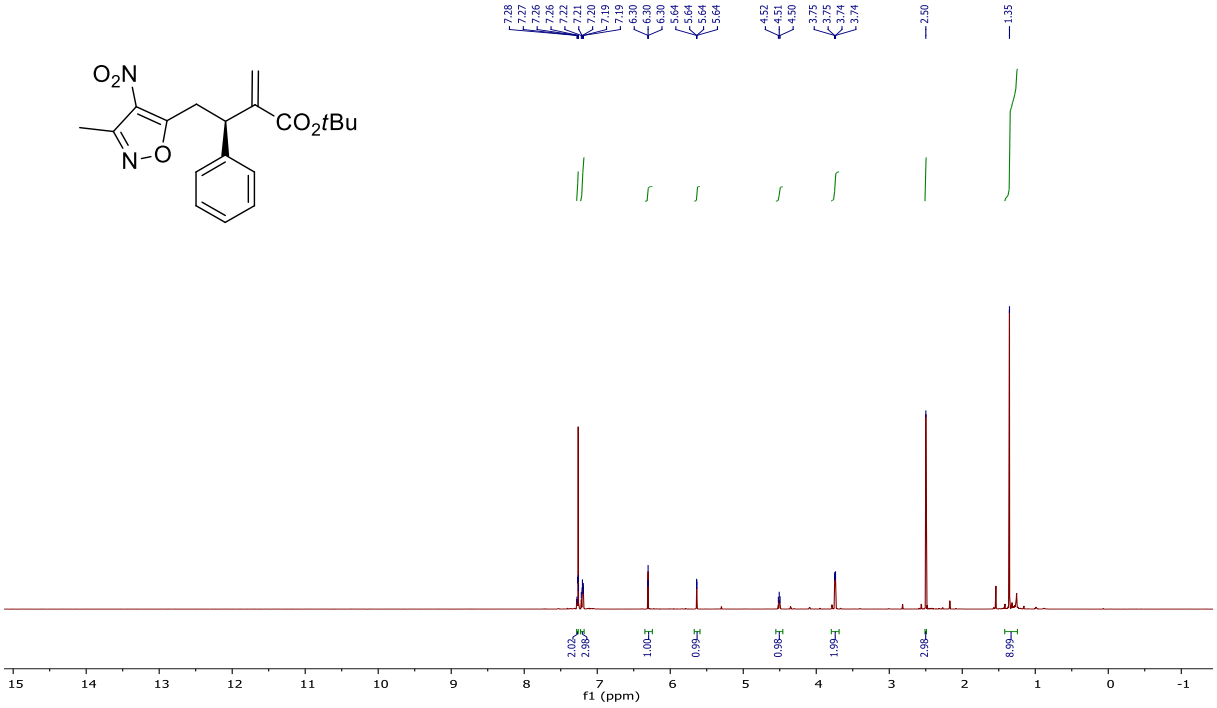


^{13}C NMR

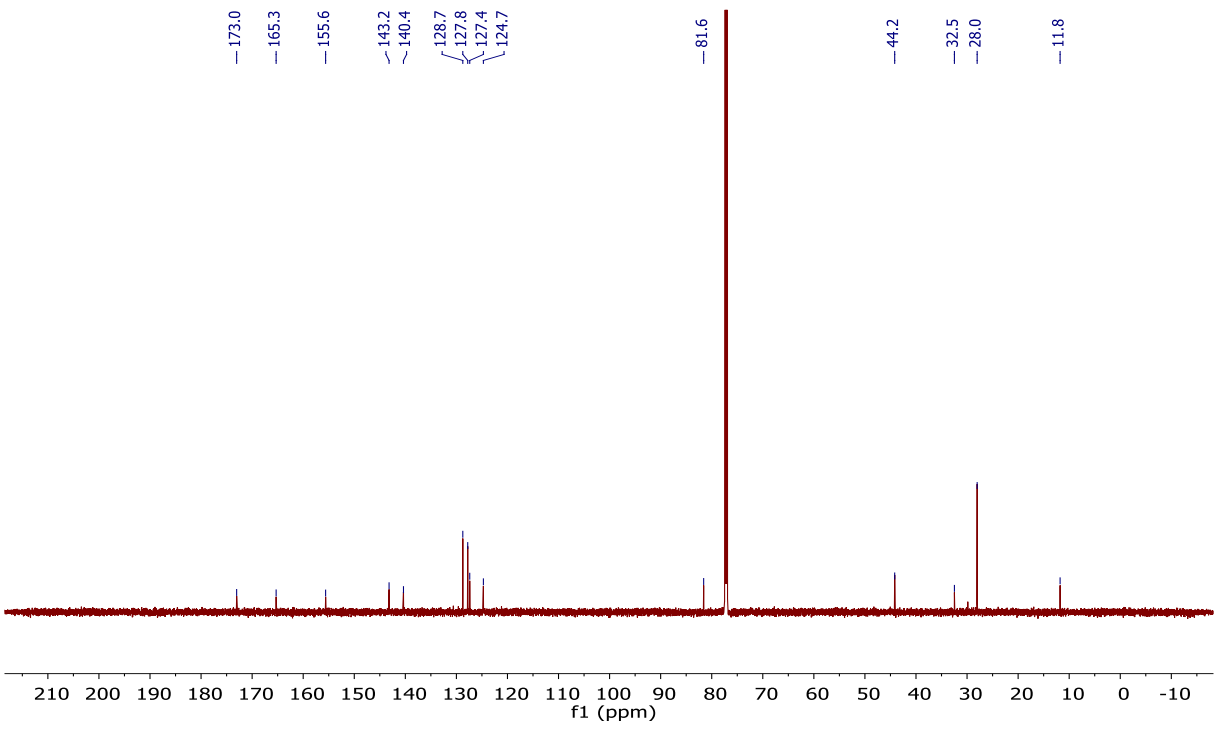


3m (*R*)-*tert*-Butyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-phenylbutanoate (Table 2, entry 13)

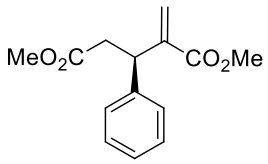
^{1}H NMR



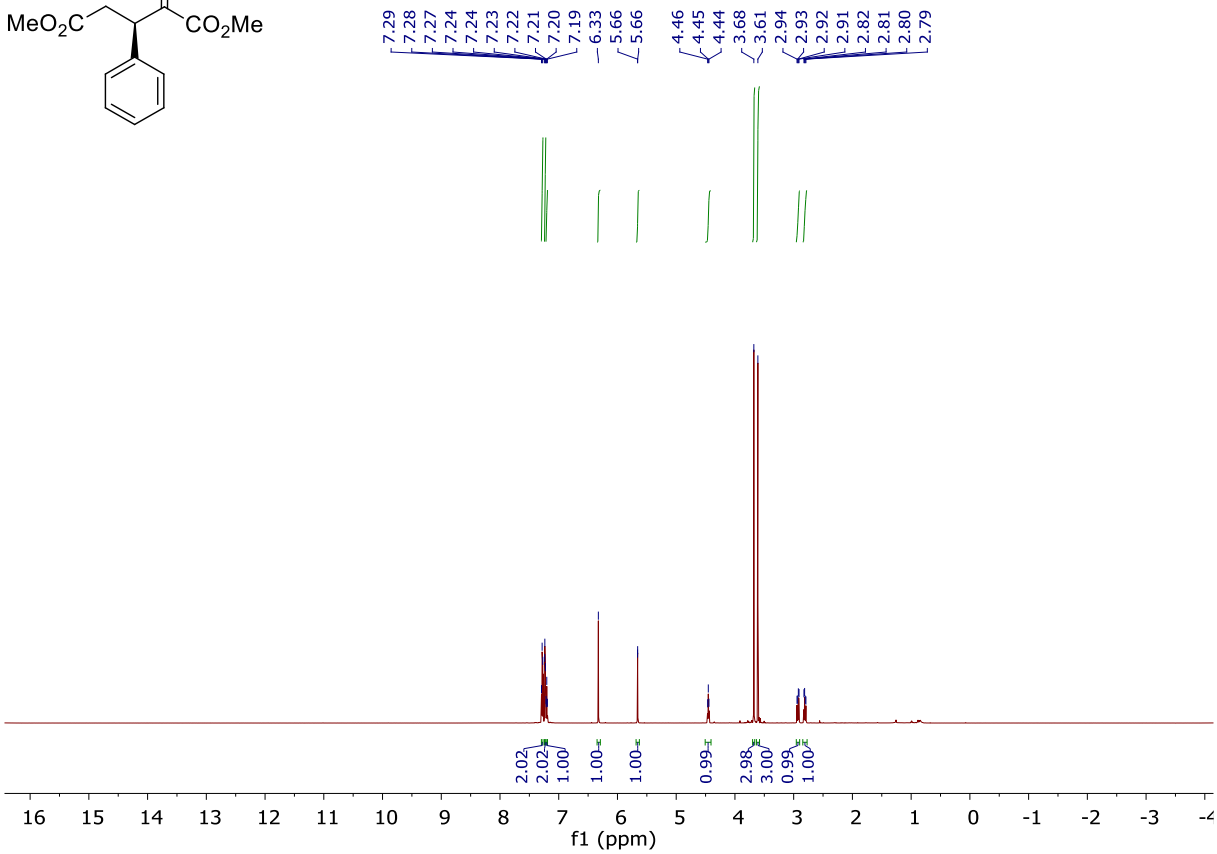
^{13}C NMR



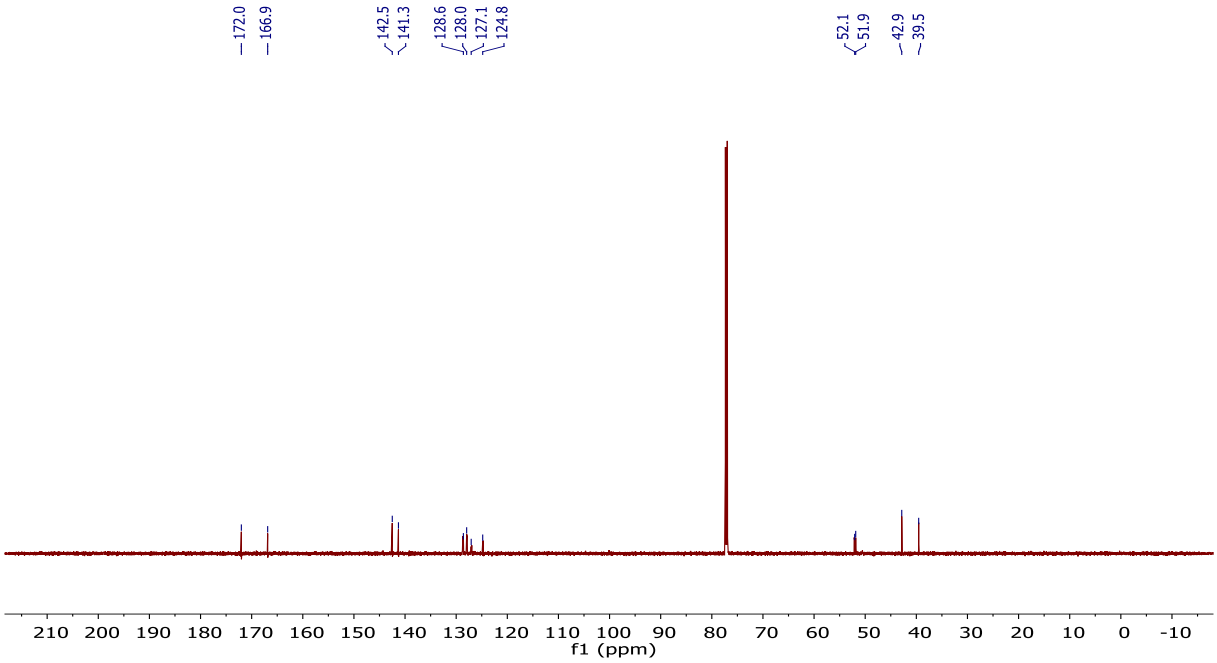
4a (*R*)-Dimethyl 2-methylene-3-phenylpentanedioate (Scheme 3)



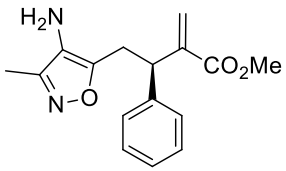
^{1}H NMR



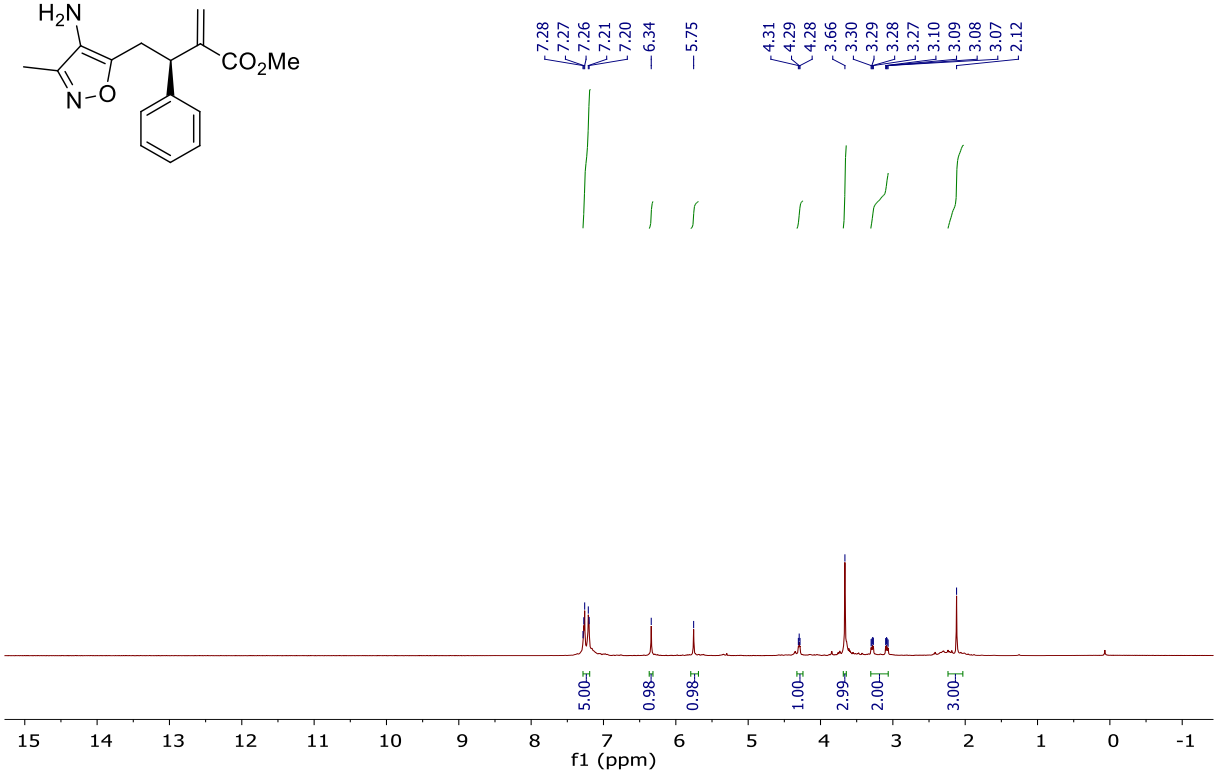
^{13}C NMR



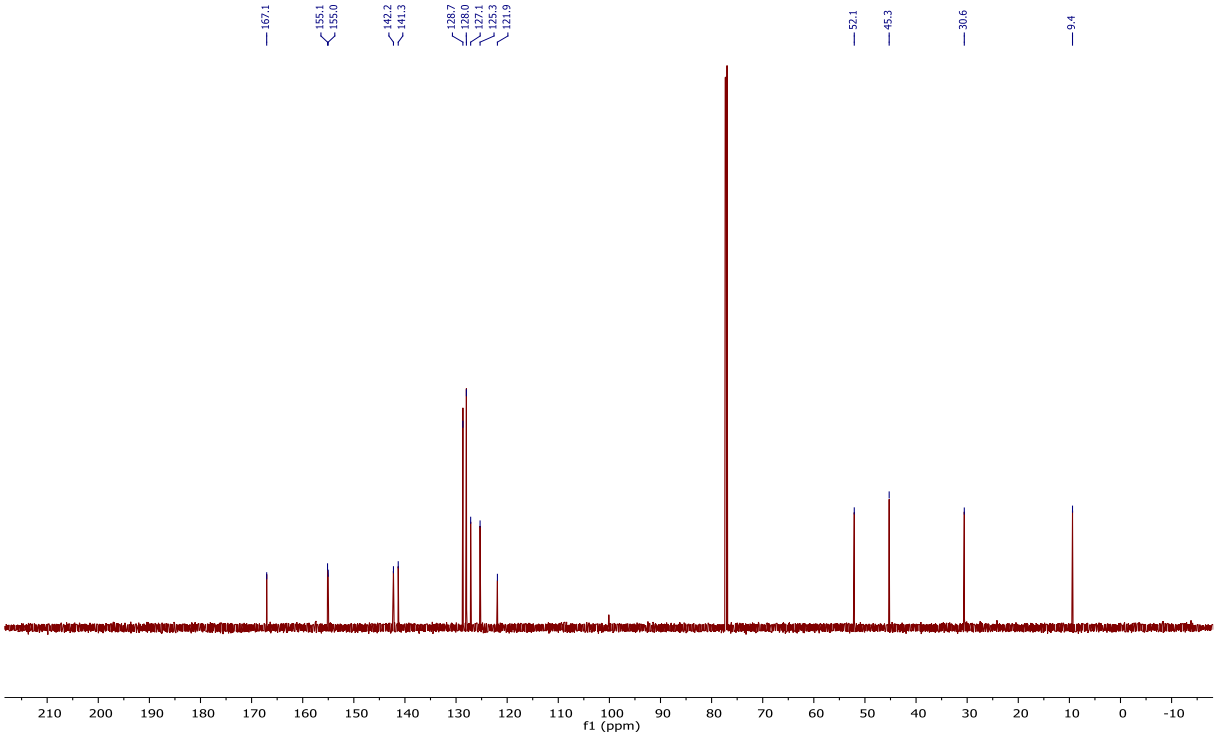
6a (*R*)-Methyl 4-(4-amino-3-methylisoxazol-5-yl)-2-methylene-3-phenylbutanoate (Scheme 3)



^{1}H NMR

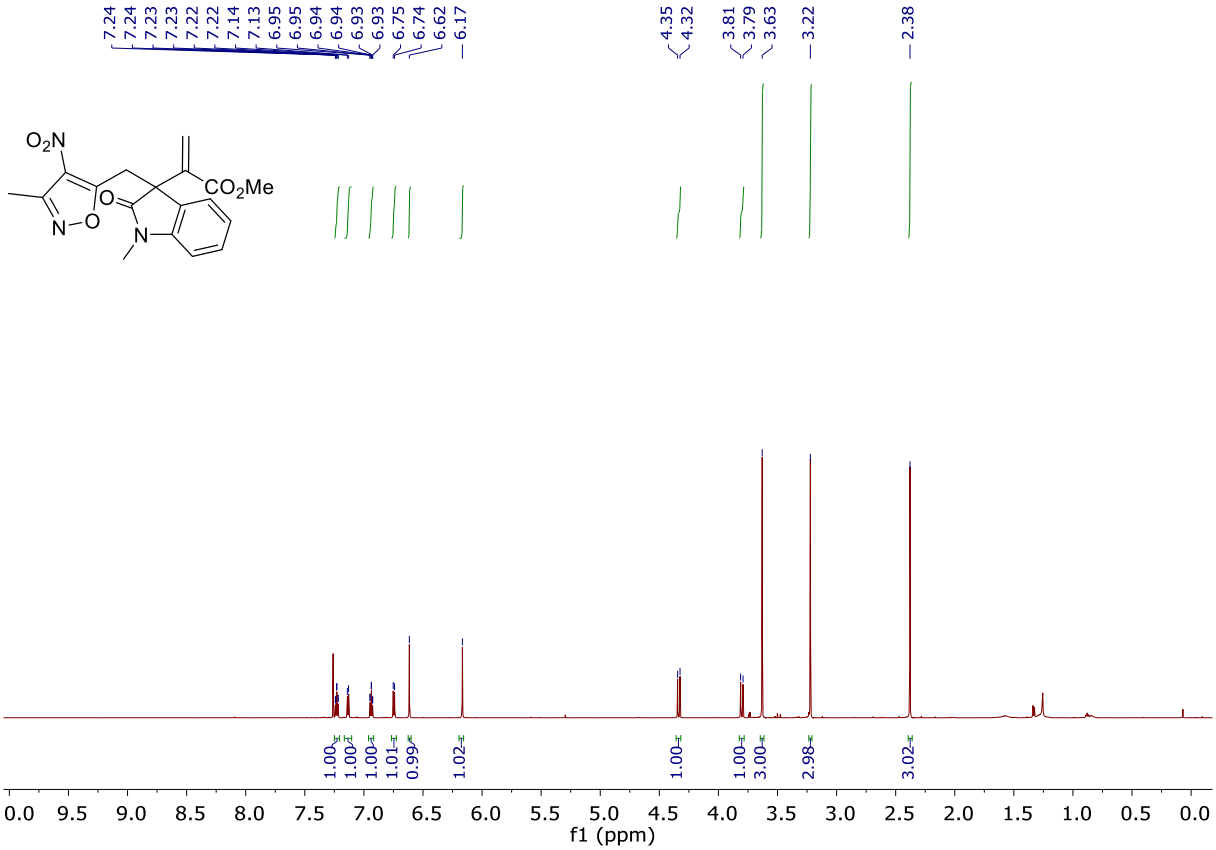


^{13}C NMR

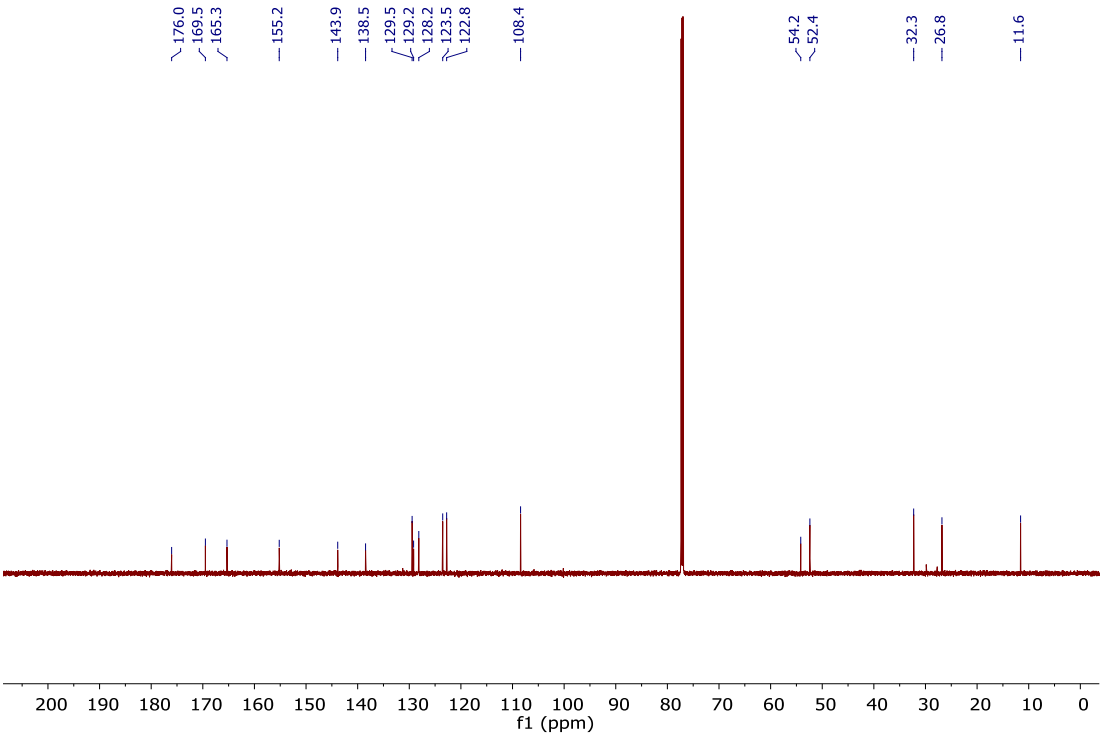


3n (*R*)-Methyl 2-(1-methyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)acrylate

^{1}H NMR

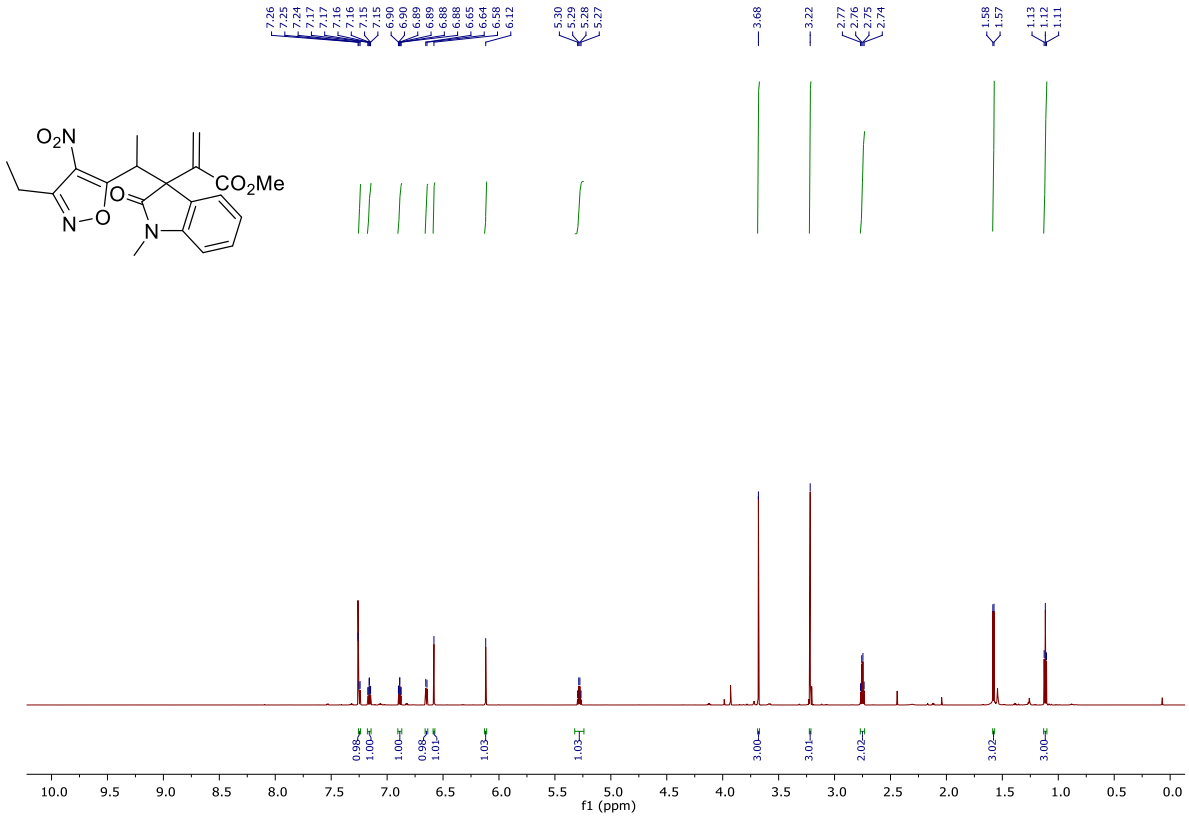


^{13}C NMR

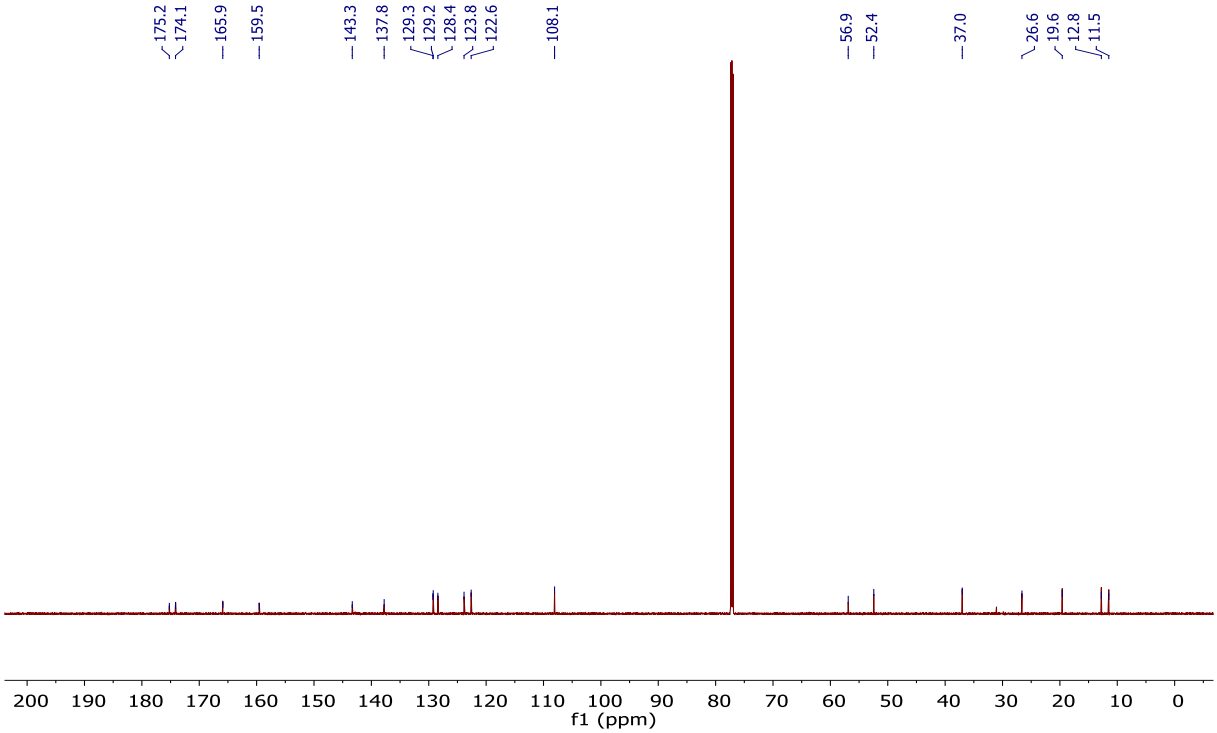


3o Methyl 2-((*R*)-3-((*S*)-1-(3-ethyl-4-nitroisoxazol-5-yl)ethyl)-1-methyl-2-oxoindolin-3-yl)acrylate

^{1}H NMR



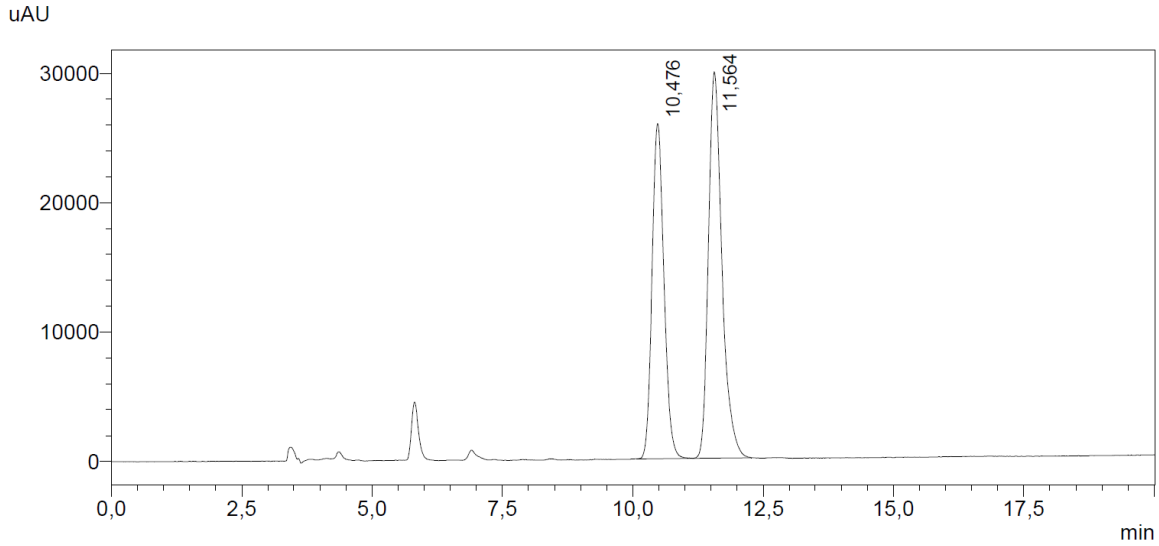
^{13}C NMR



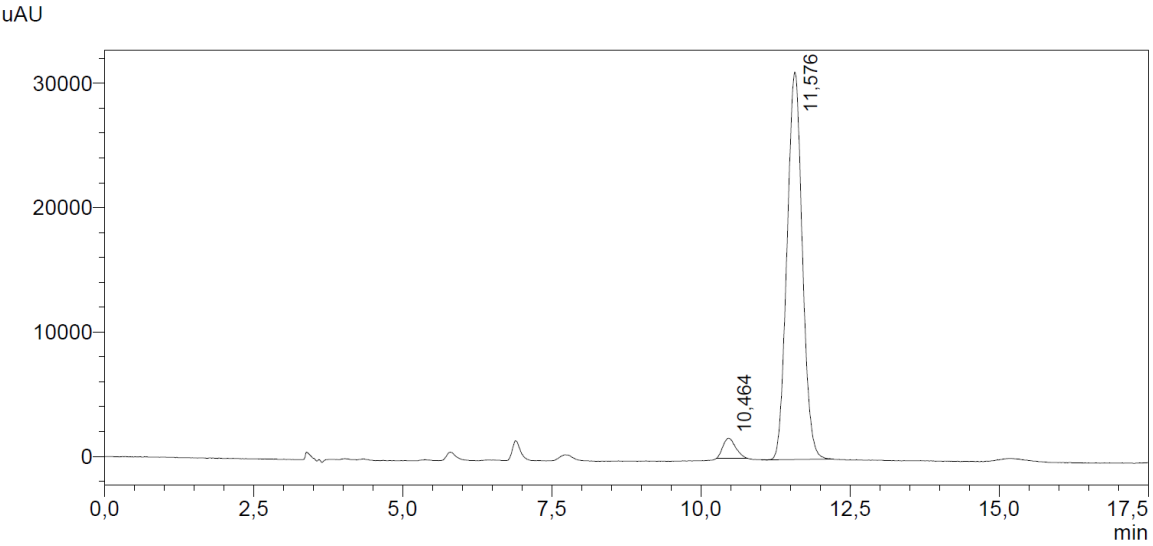
5. HPLC traces

3a (*R*)-Methyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-phenylbutanoate (Table 2, entry 1)

Racemic sample



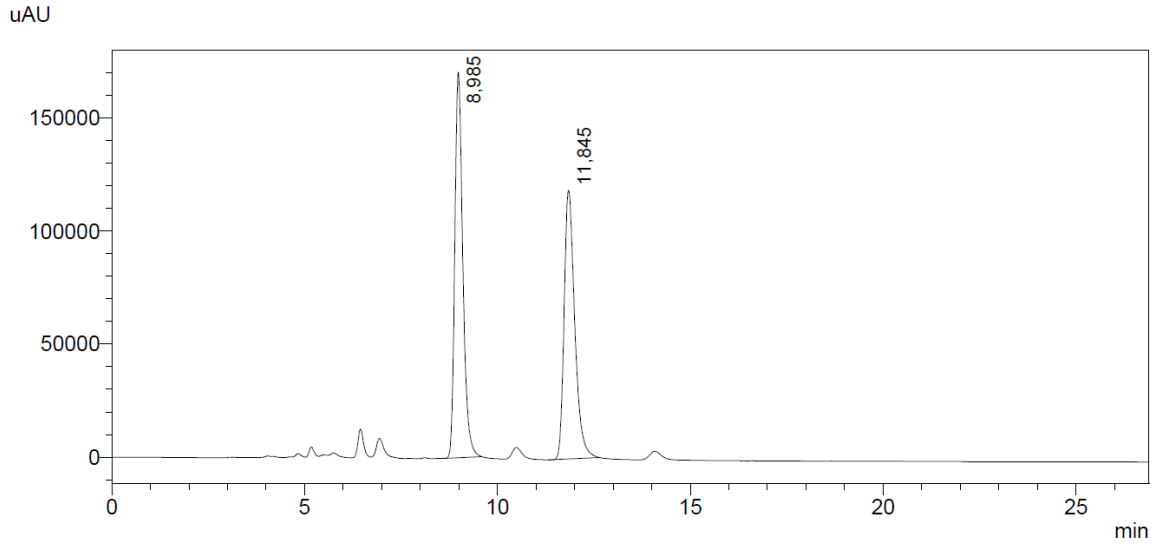
Enantiomerically enriched sample



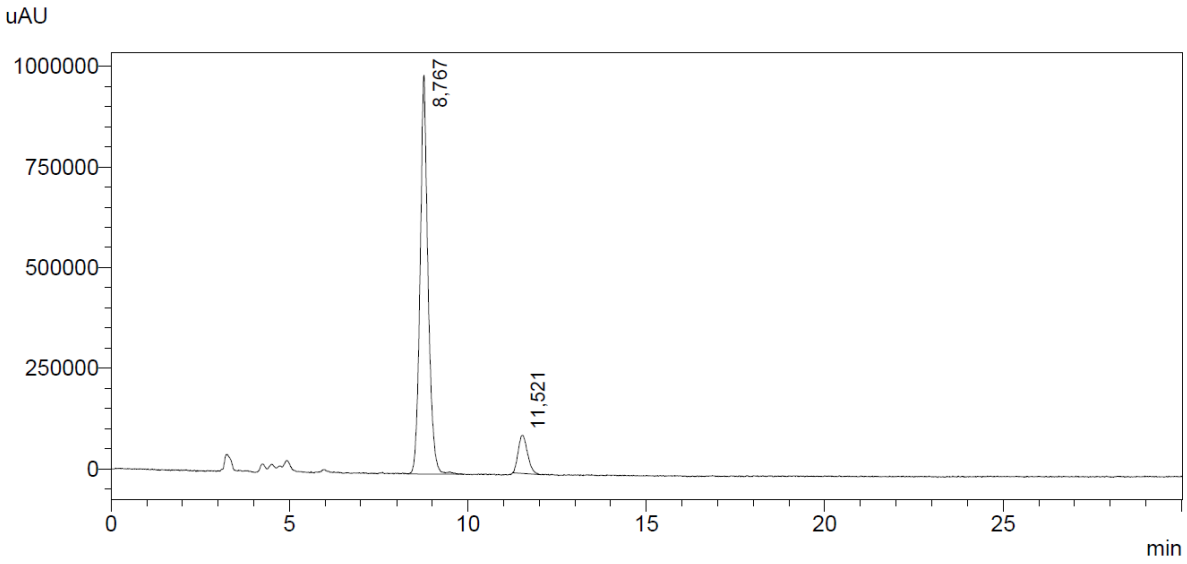
Peak#	Ret. Time	Area%
1	10,464	4,063
2	11,576	95,937
Total		100,000

3b (*R*)-Methyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-(4-(trifluoromethyl)phenyl) butanoate (Table 2, entry 2)

Racemic sample



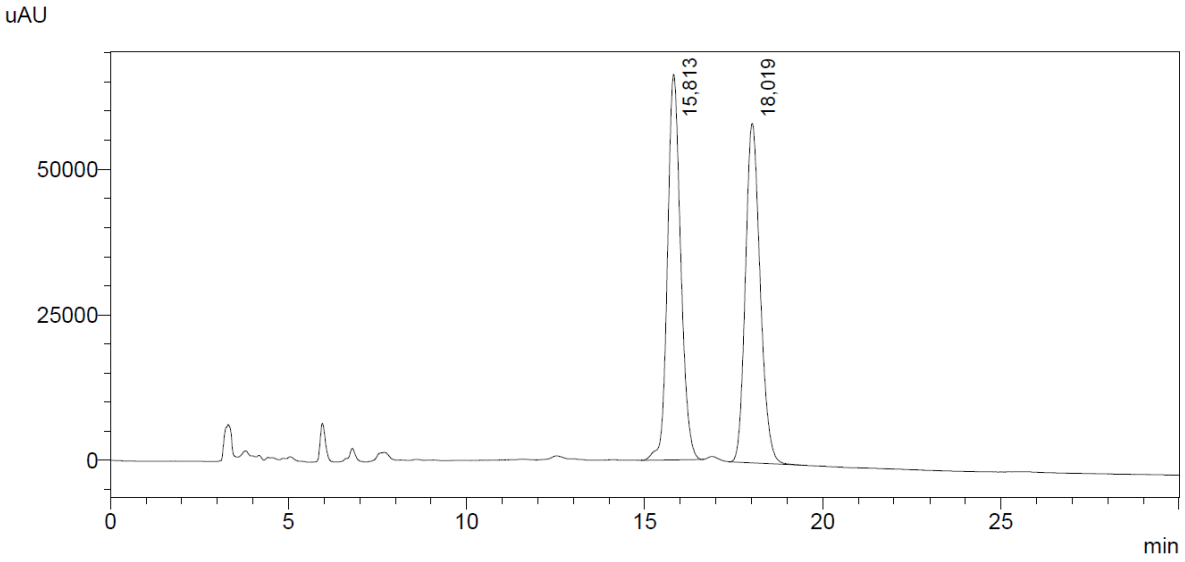
Enantiomerically enriched sample



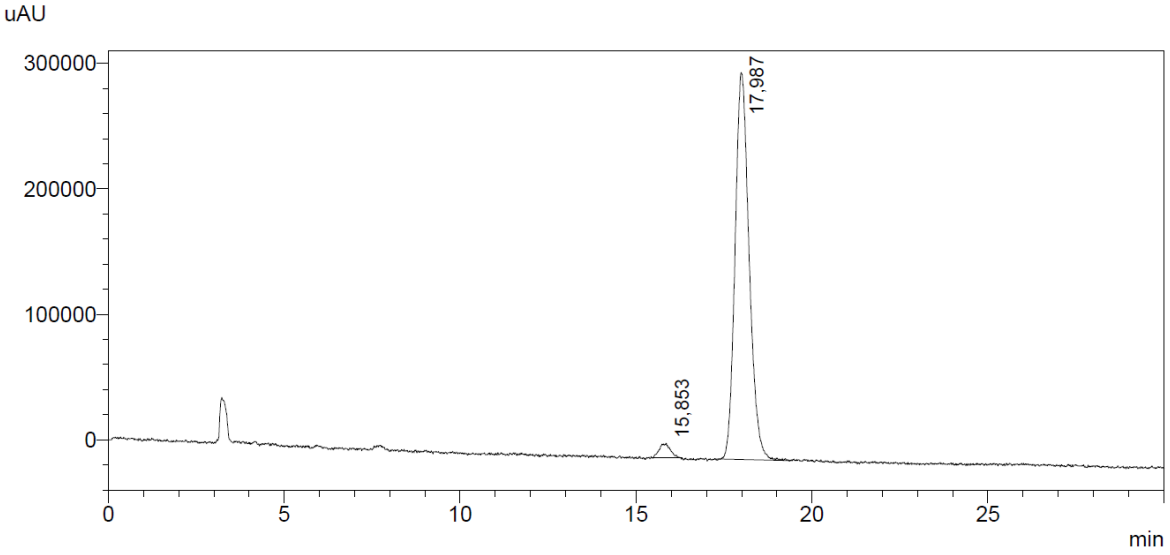
Peak#	Ret. Time	Area%
1	8,767	89,868
2	11,521	10,132
Total		100,000

3c (*R*)-Methyl 3-(4-bromophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 3)

Racemic sample



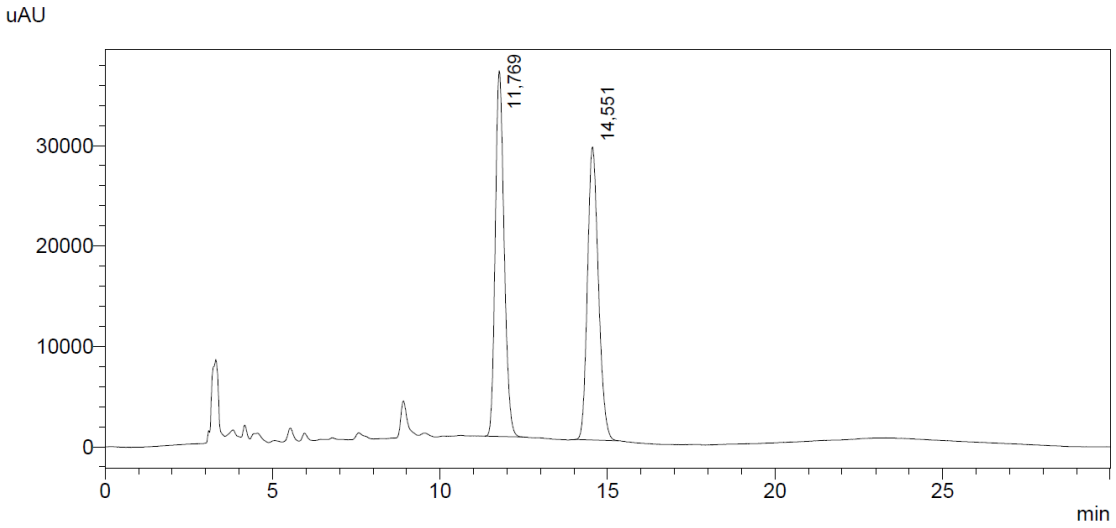
Enantiomerically enriched sample



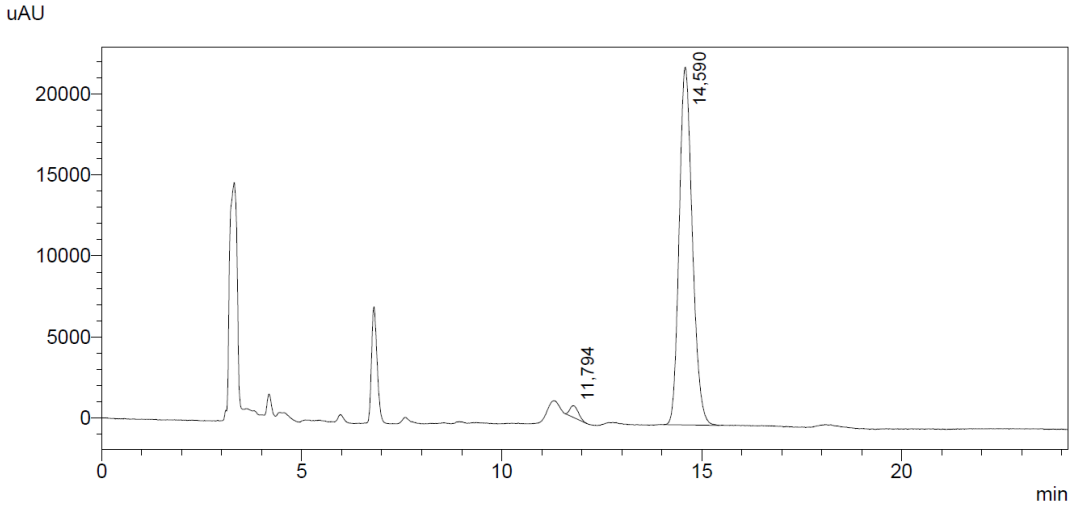
Peak#	Ret. Time	Area%
1	15,853	2,968
2	17,987	97,032
Total		100,000

3d (*R*)-Methyl 3-(4-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 4)

Racemic sample



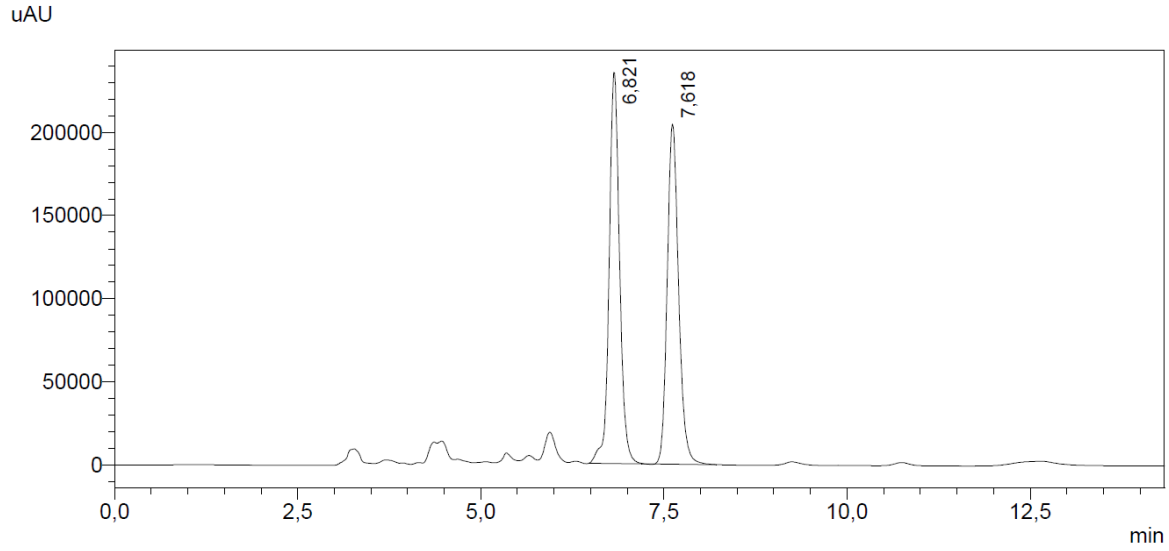
Enantiomerically enriched sample



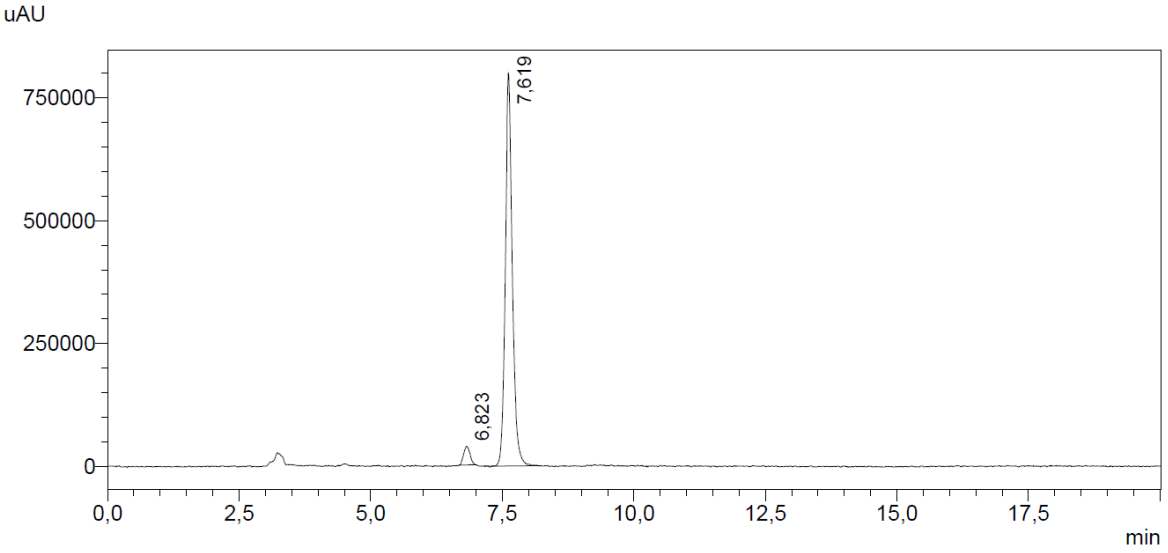
Peak#	Ret. Time	Area%
1	11,794	2,053
2	14,590	97,947
Total		100,000

3e (*R*)-Methyl 3-(3-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 5)

Racemic sample



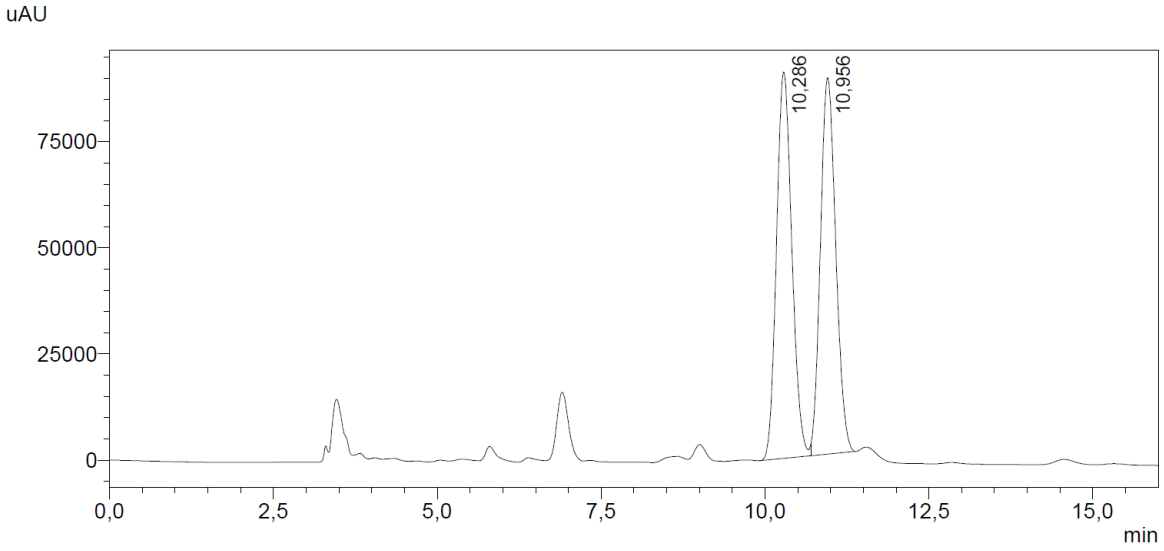
Enantiomerically enriched sample



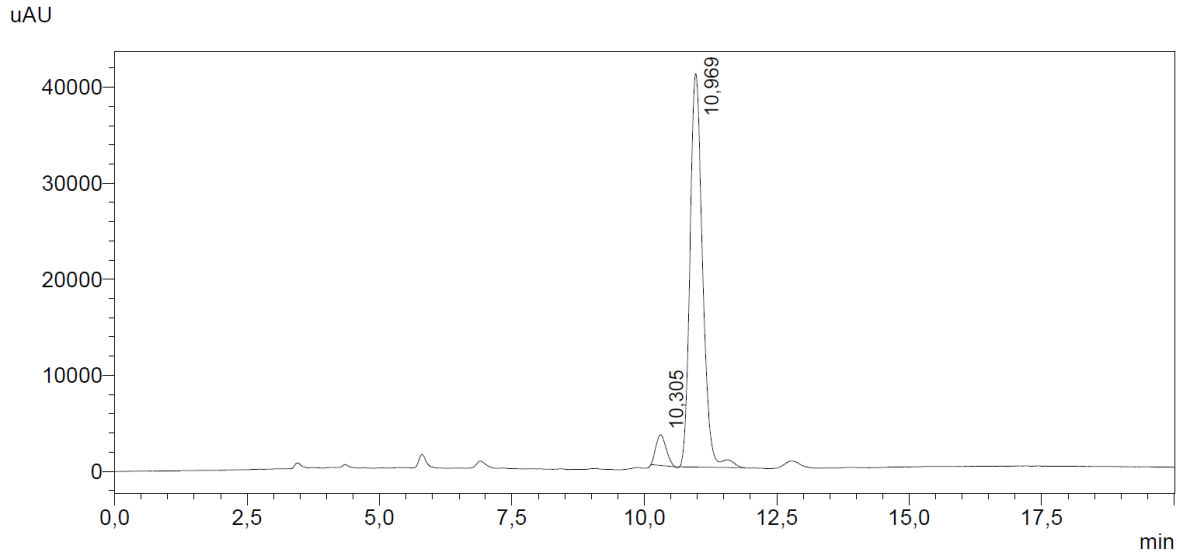
Peak#	Ret. Time	Area%
1	6,823	4,191
2	7,619	95,809
Total		100,000

3f (*S*)-Methyl 3-(2-chlorophenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 6)

Racemic sample



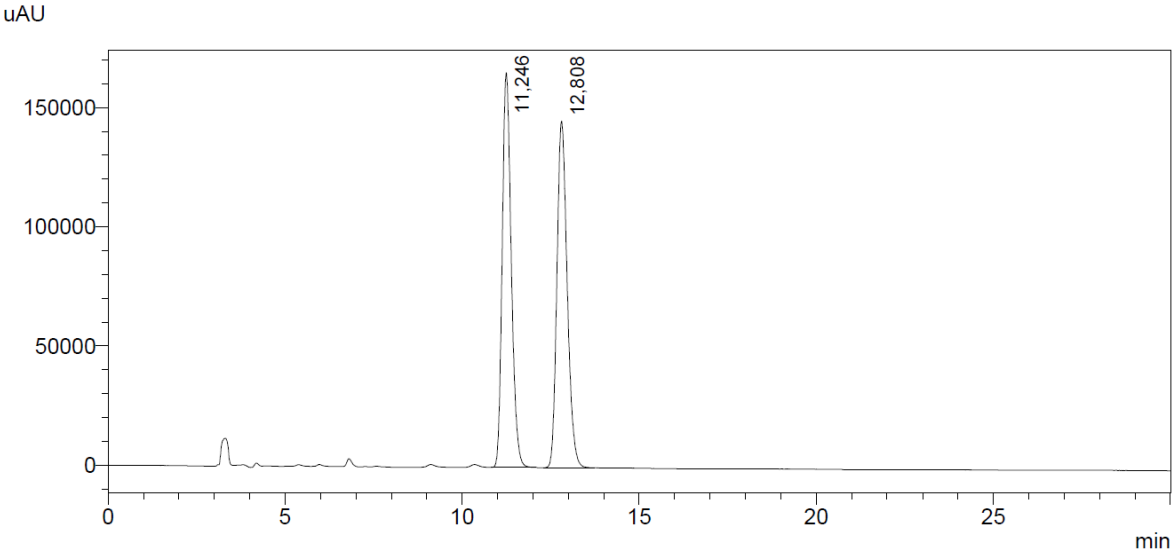
Enantiomerically enriched sample



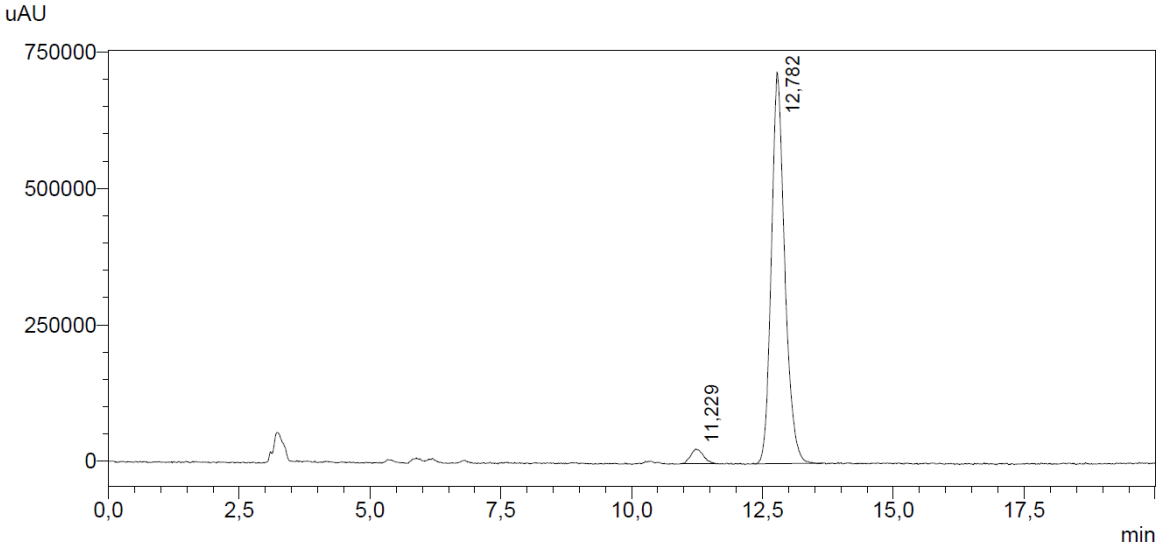
Peak#	Ret. Time	Area%
1	10,305	5,947
2	10,969	94,053
Total		100,000

3g (*R*)-Methyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-(p-tolyl)butanoate (Table 2, entry 7)

Racemic sample



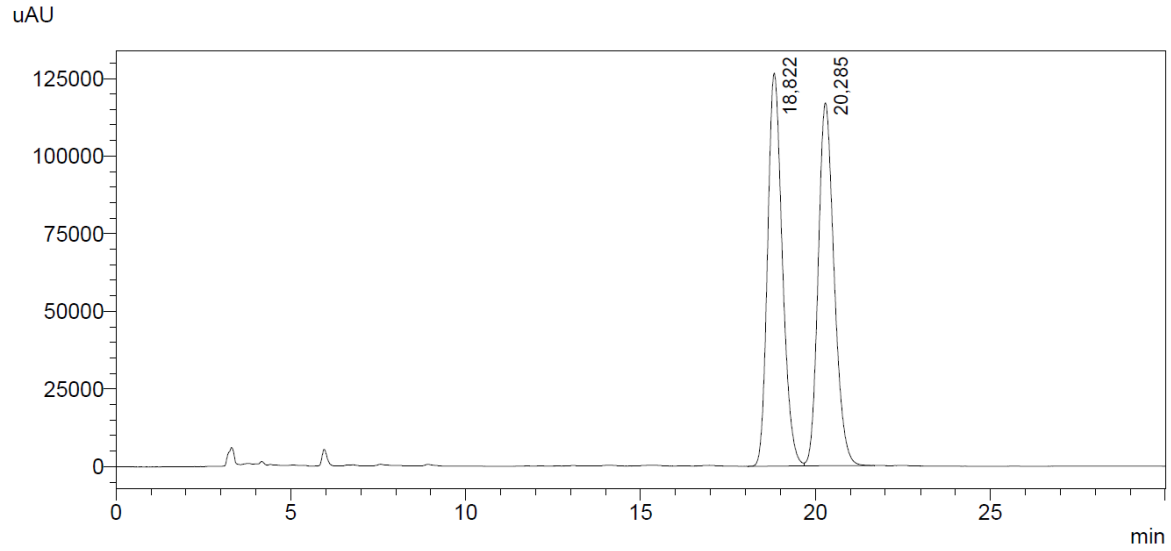
Enantiomerically enriched sample



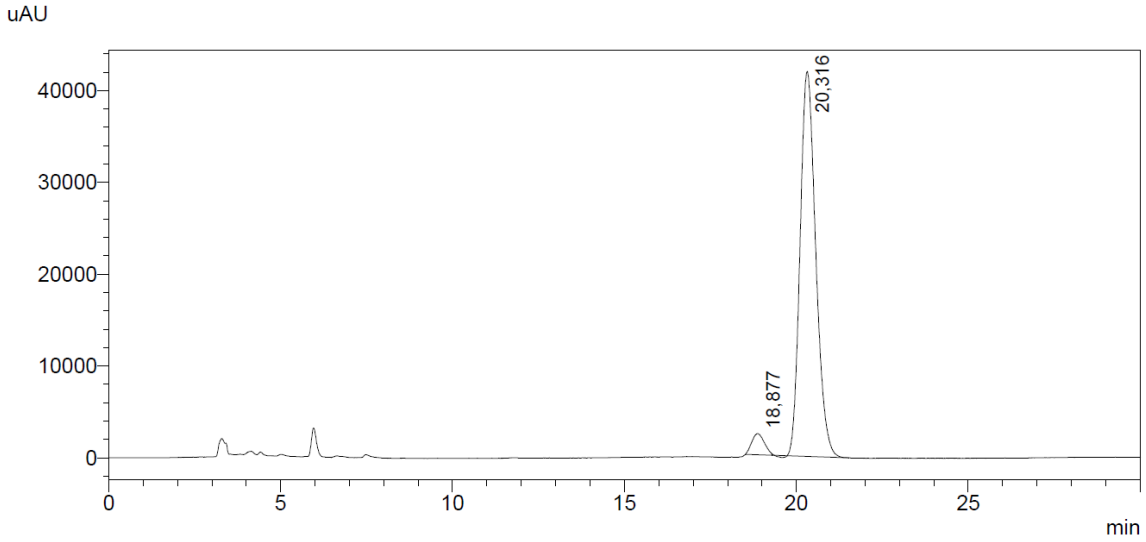
Peak#	Ret. Time	Area%
1	11,229	3,166
2	12,782	96,834
Total		100,000

3h (*R*)-Methyl 3-(4-methoxyphenyl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 8)

Racemic sample



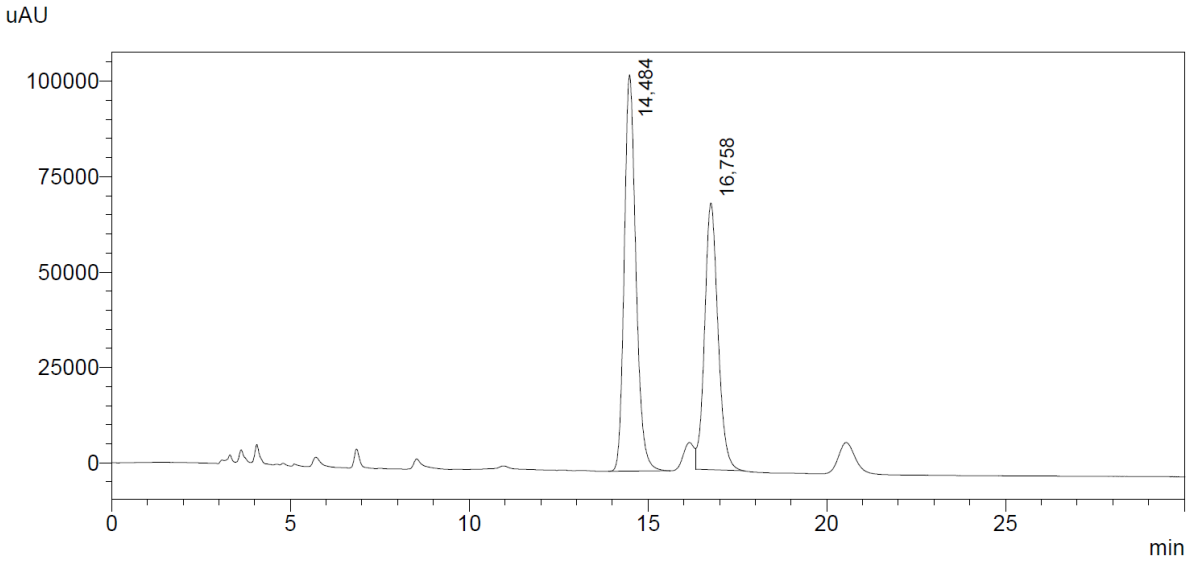
Enantiomerically enriched sample



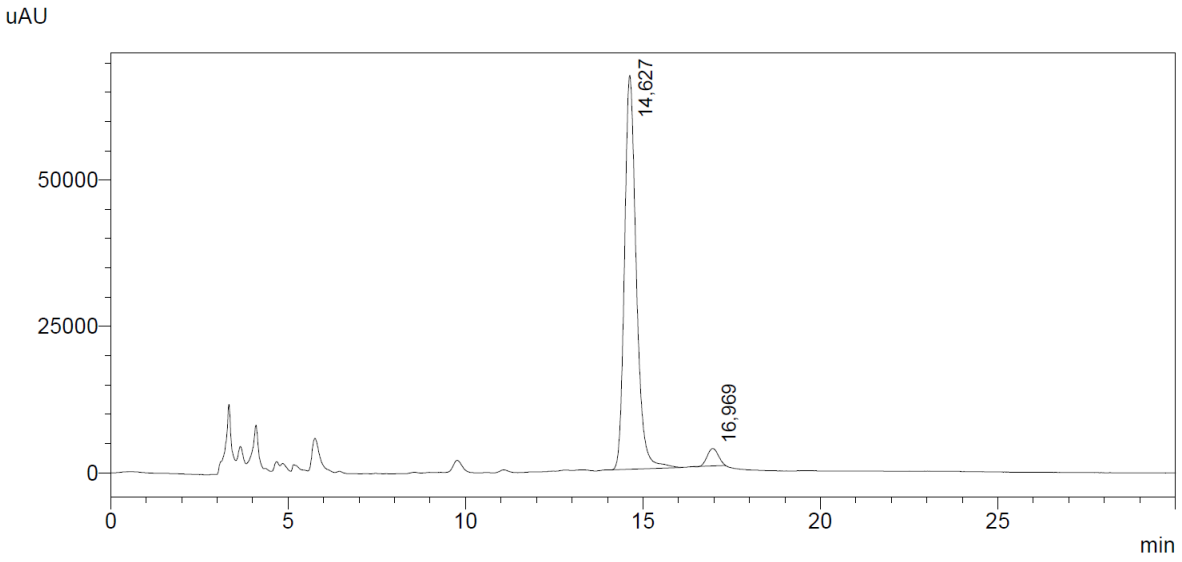
Peak#	Ret. Time	Area%
1	18,877	4,238
2	20,316	95,762
Total		100,000

3i (*R*)-Methyl 3-(benzo[d][1,3]dioxol-5-yl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 9)

Racemic sample



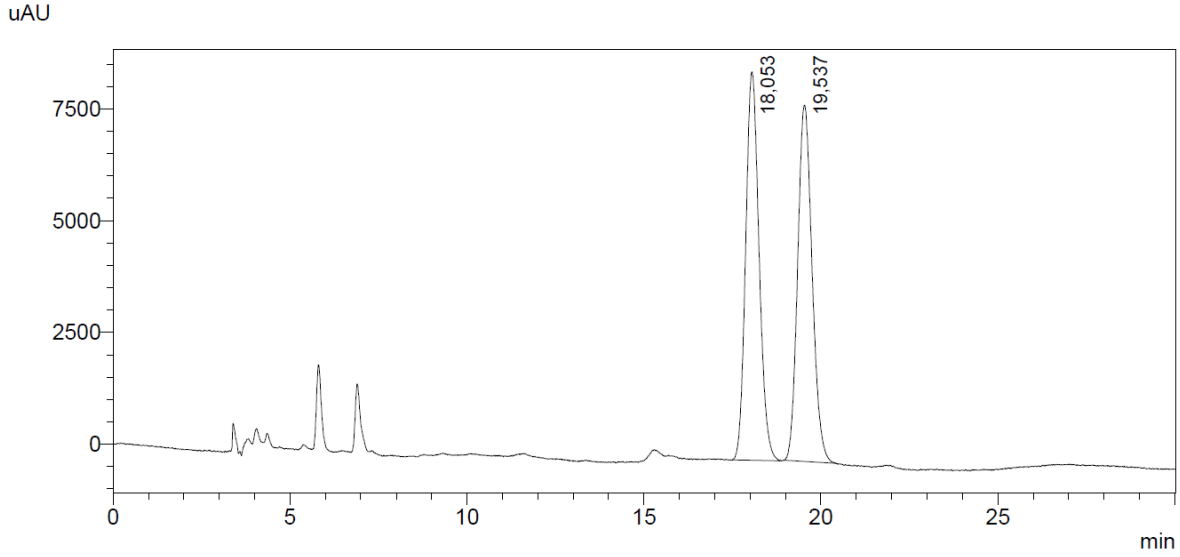
Enantiomerically enriched sample



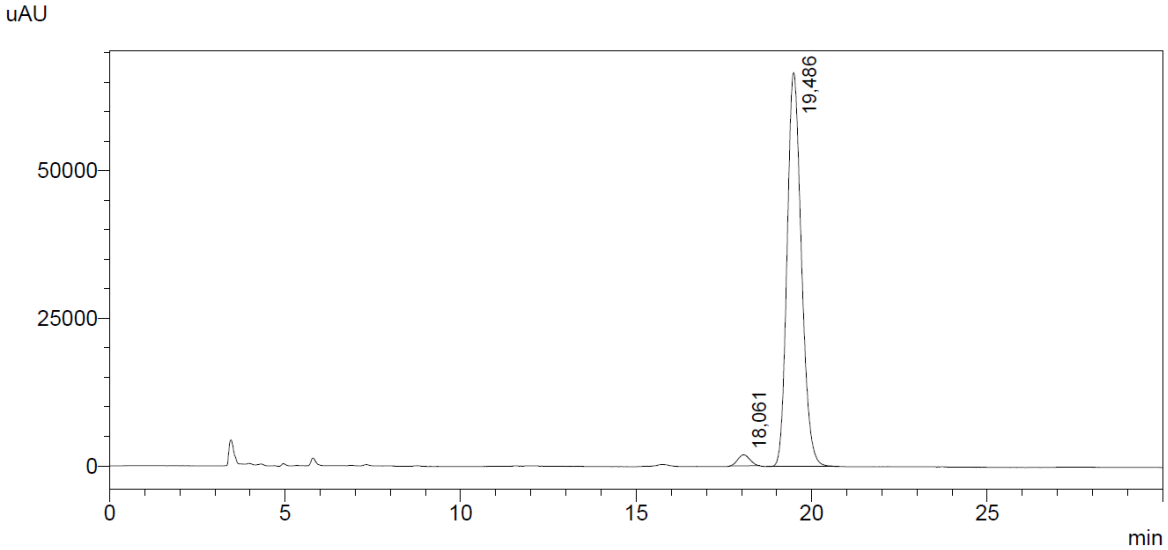
Peak#	Ret. Time	Area%
1	14,627	96,060
2	16,969	3,940
Total		100,000

3j (*S*)-Methyl 3-(furan-2-yl)-4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylenebutanoate (Table 2, entry 10)

Racemic sample



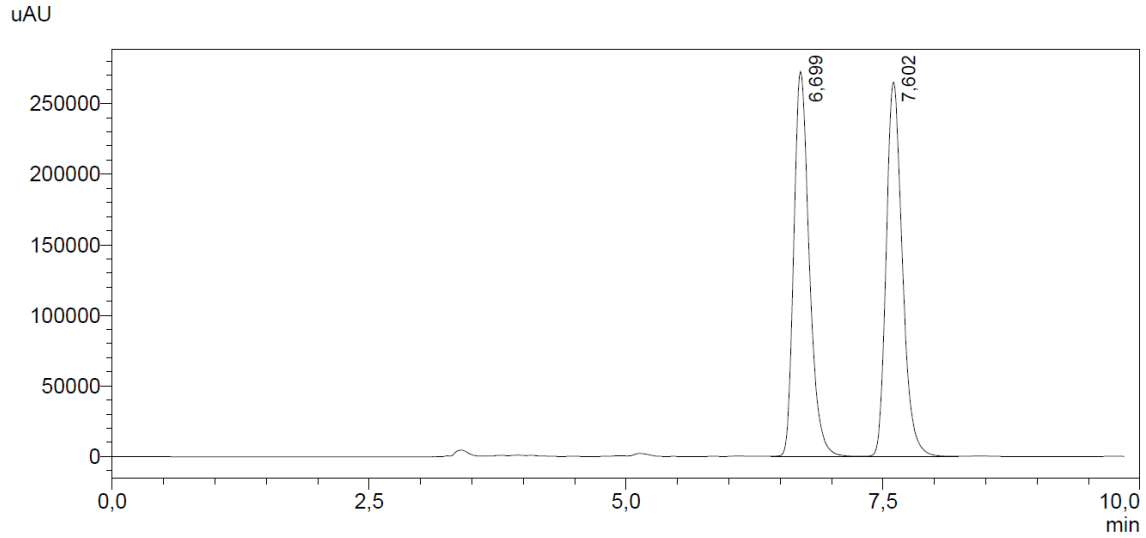
Enantiomerically enriched sample



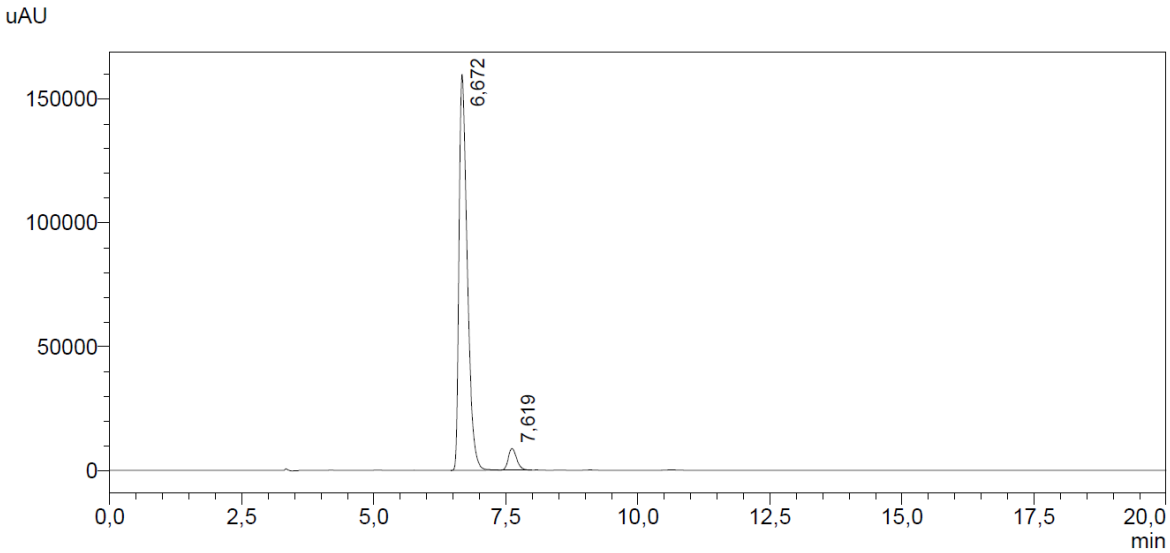
Peak#	Ret. Time	Area%
1	18,061	2,316
2	19,486	97,684
Total		100,000

3k (*R,E*)-Methyl 3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-methylenehex-4-enoate (Table 2, entry 11)

Racemic sample



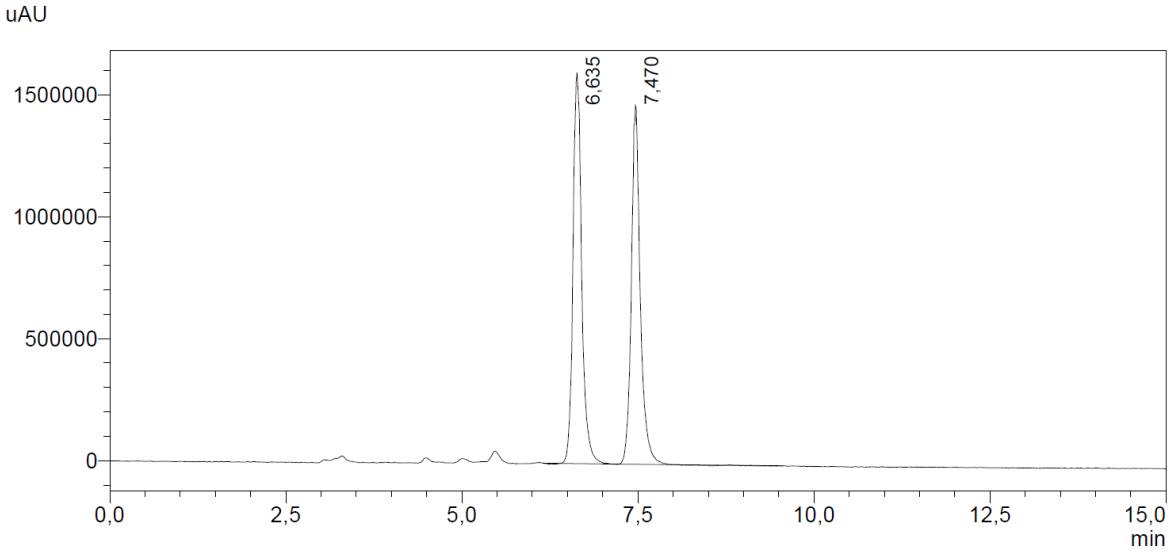
Enantiomerically enriched sample



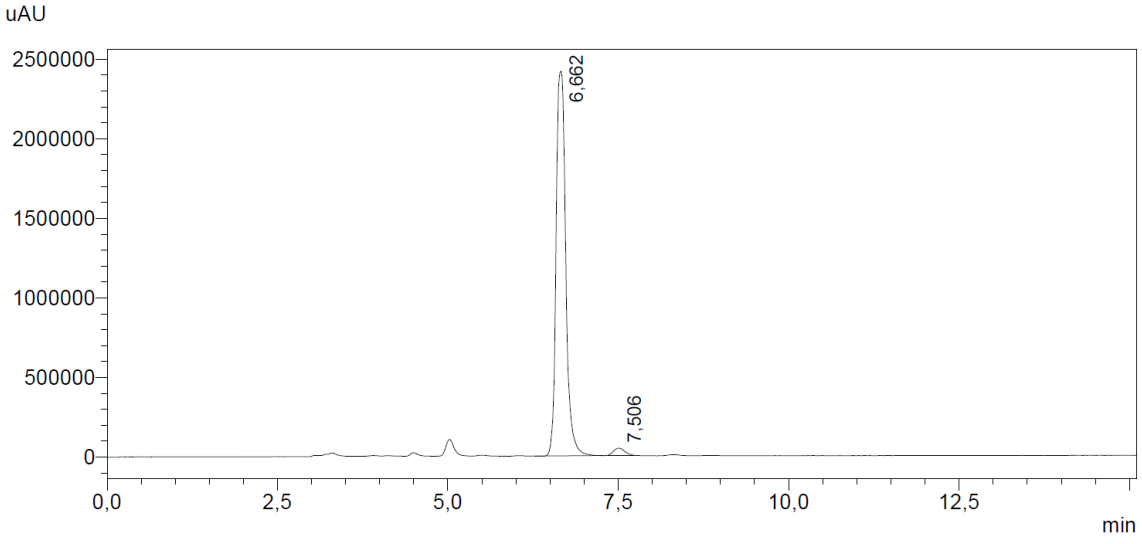
Peak#	Ret. Time	Area%
1	6,672	94,746
2	7,619	5,254
Total		100,000

3l (*R*)-Ethyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-phenylbutanoate (Table 2, entry 12)

Racemic sample



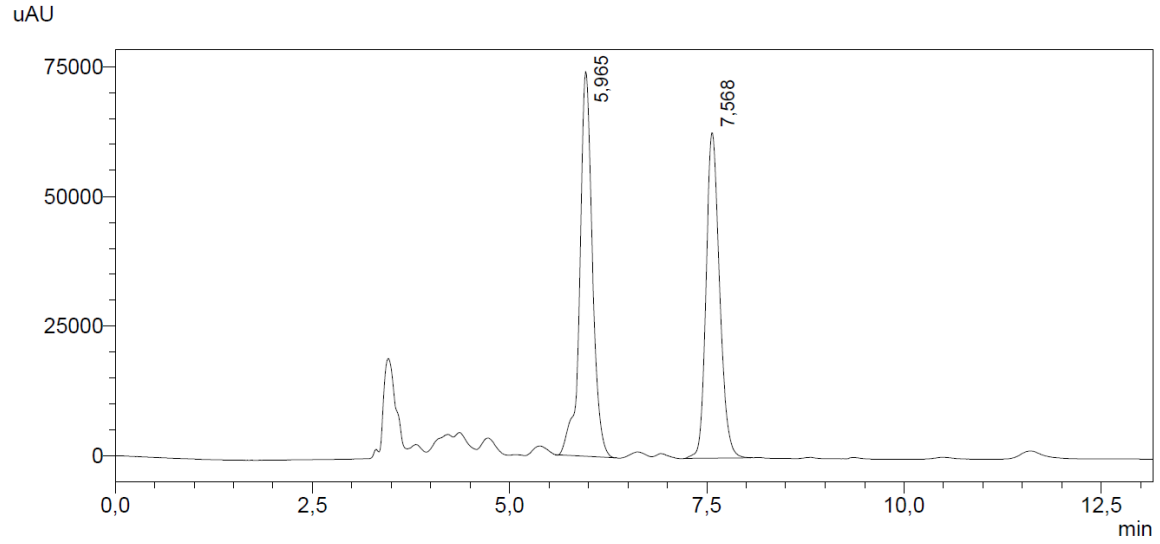
Enantiomerically enriched sample



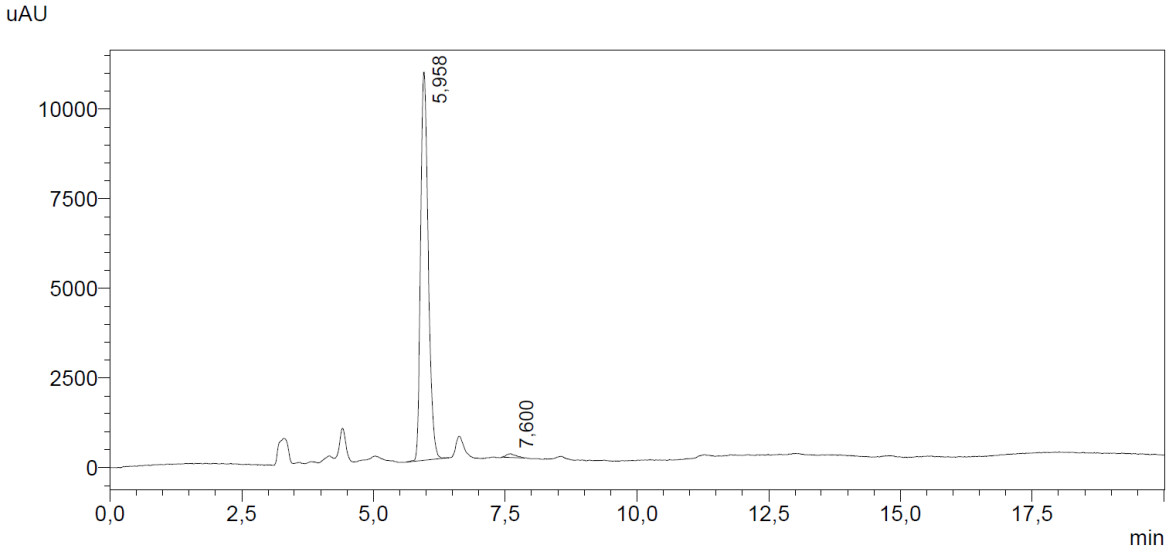
Peak#	Ret. Time	Area%
1	6,662	97,994
2	7,506	2,006
Total		100,000

3m (*R*)-*tert*-Butyl 4-(3-methyl-4-nitroisoxazol-5-yl)-2-methylene-3-phenylbutanoate (Table 2, entry 13)

Racemic sample



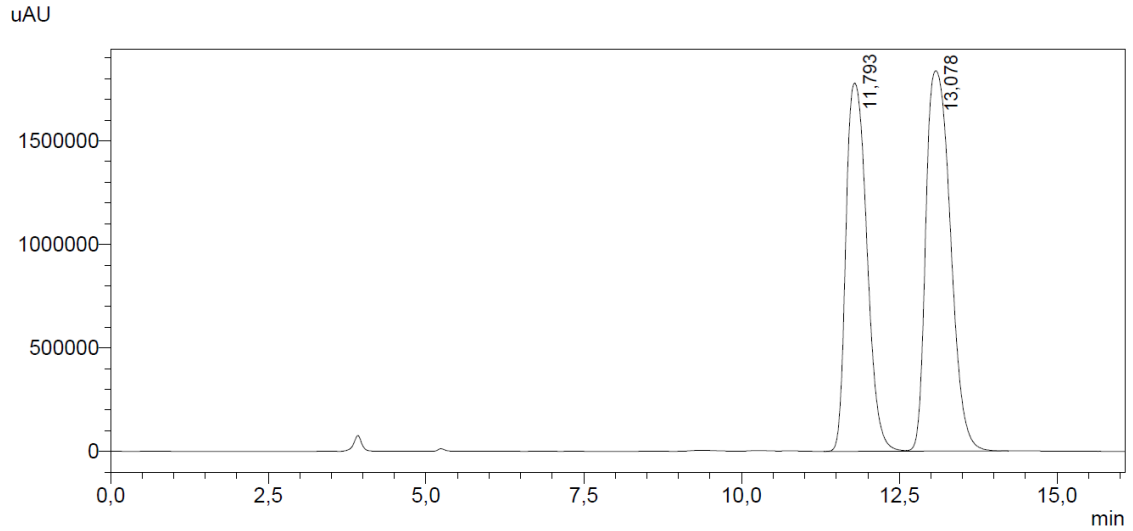
Enantiomerically enriched sample



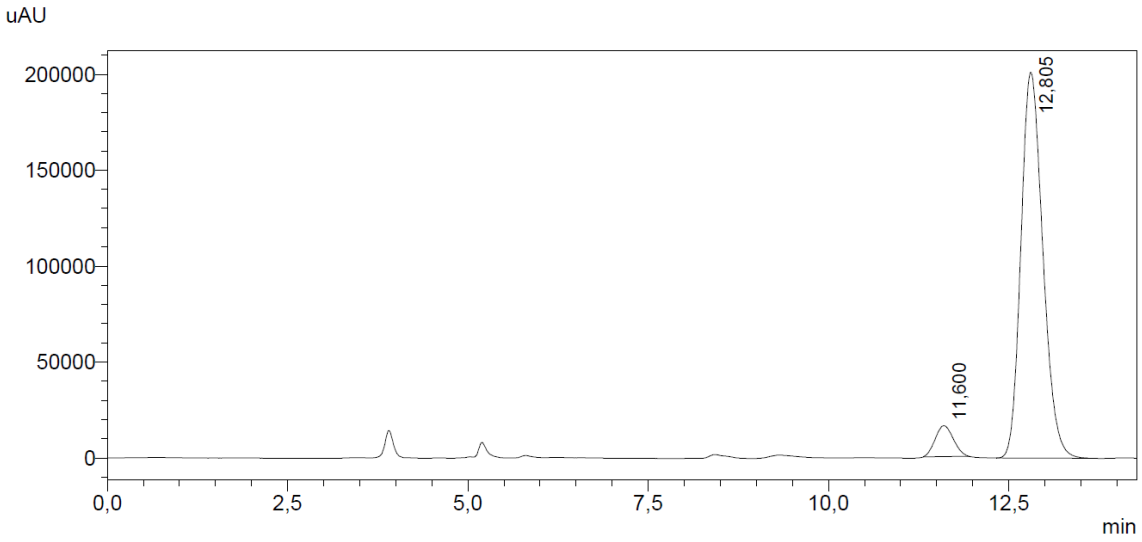
Peak#	Ret. Time	Area%
1	5,958	98,788
2	7,600	1,212
Total		100,000

4a (*R*)-Dimethyl 2-methylene-3-phenylpentanedioate (Scheme 3)

Racemic sample



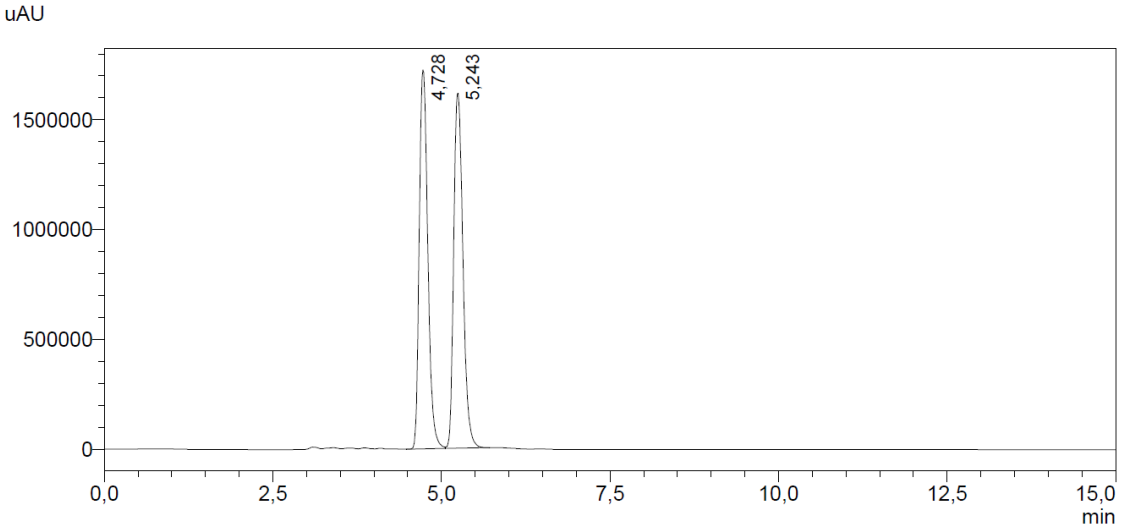
Enantiomerically enriched sample



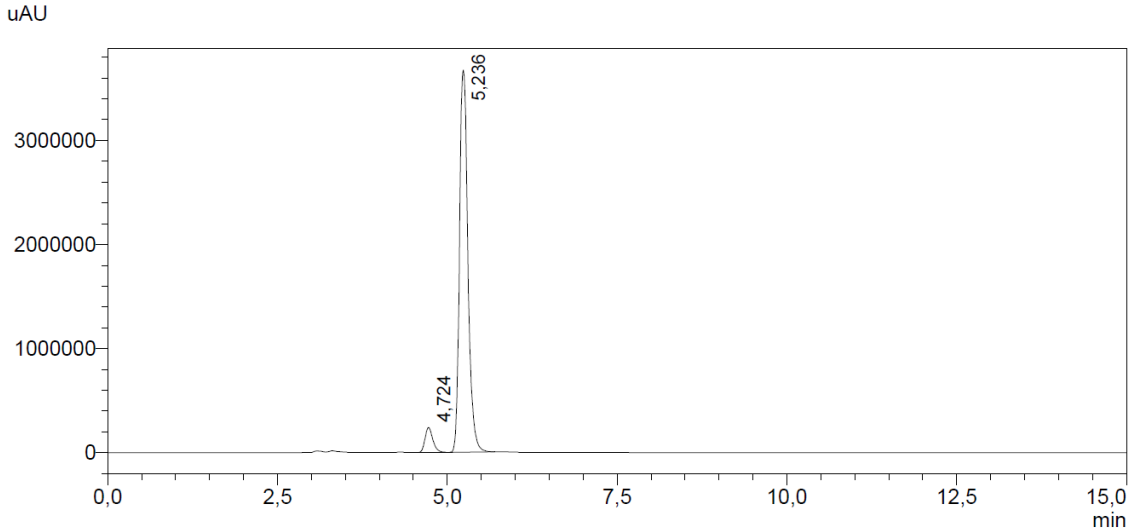
Peak#	Ret. Time	Area%
1	11,600	6,200
2	12,805	93,800
Total		100,000

6a (*R*)-Methyl 4-(4-amino-3-methylisoxazol-5-yl)-2-methylene-3-phenylbutanoate (Scheme 3)

Racemic sample



Enantiomerically enriched sample

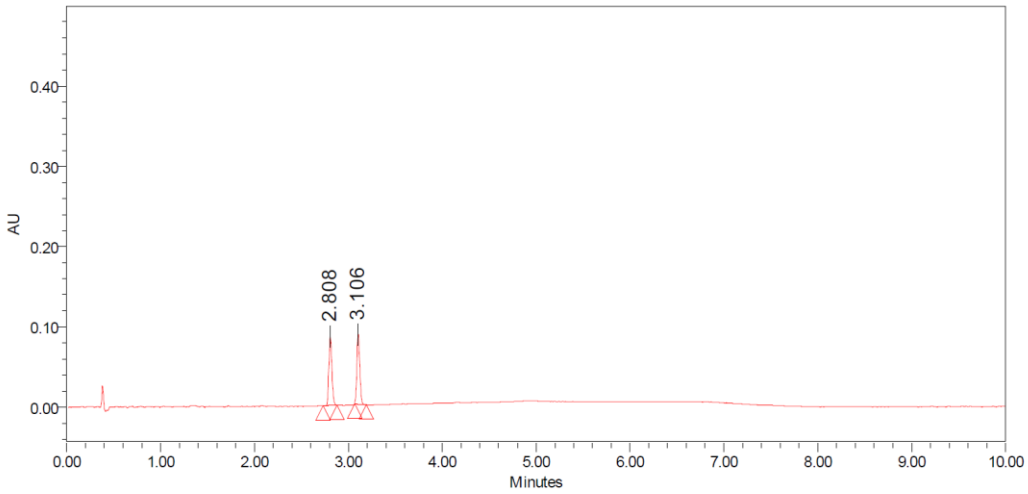


Peak#	Ret. Time	Area%
1	4,724	5,699
2	5,236	94,301
Total		100,000

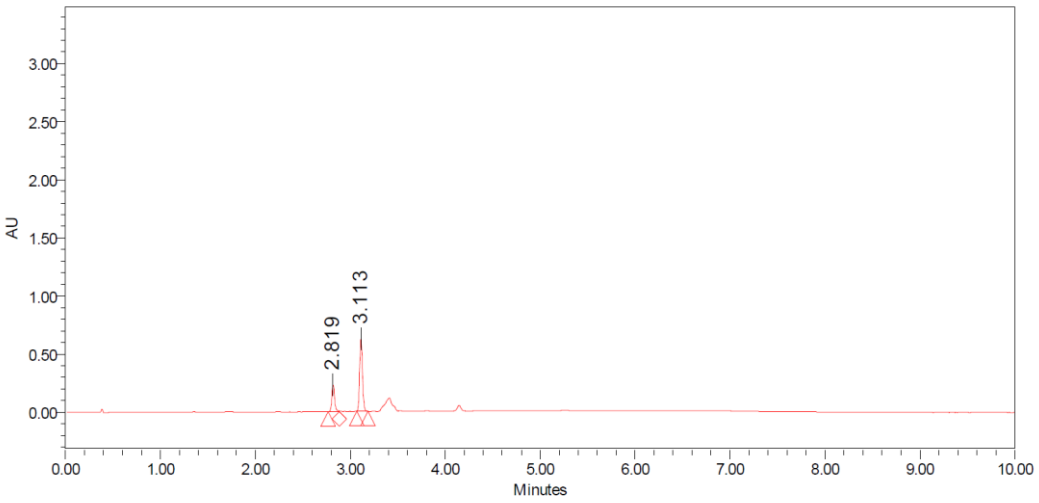
3n (*R*)-Methyl 2-(1-methyl-3-((3-methyl-4-nitroisoxazol-5-yl)methyl)-2-oxoindolin-3-yl)acrylate

(UPC^2 trace)

Racemic sample



Enantiomerically enriched sample



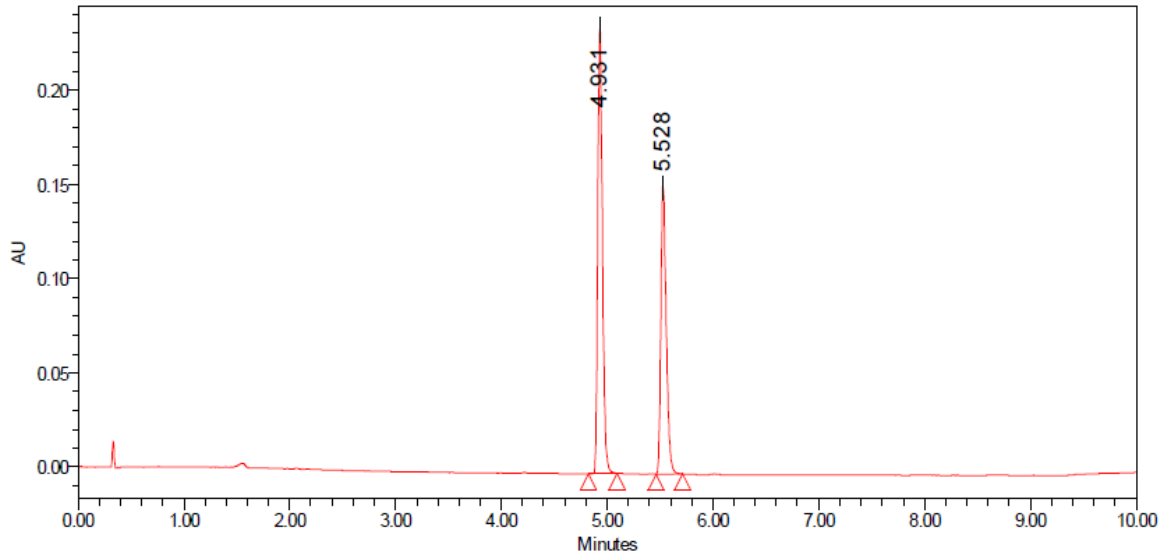
Peak Results

	RT	% Area
1	2.819	26.82
2	3.113	73.18

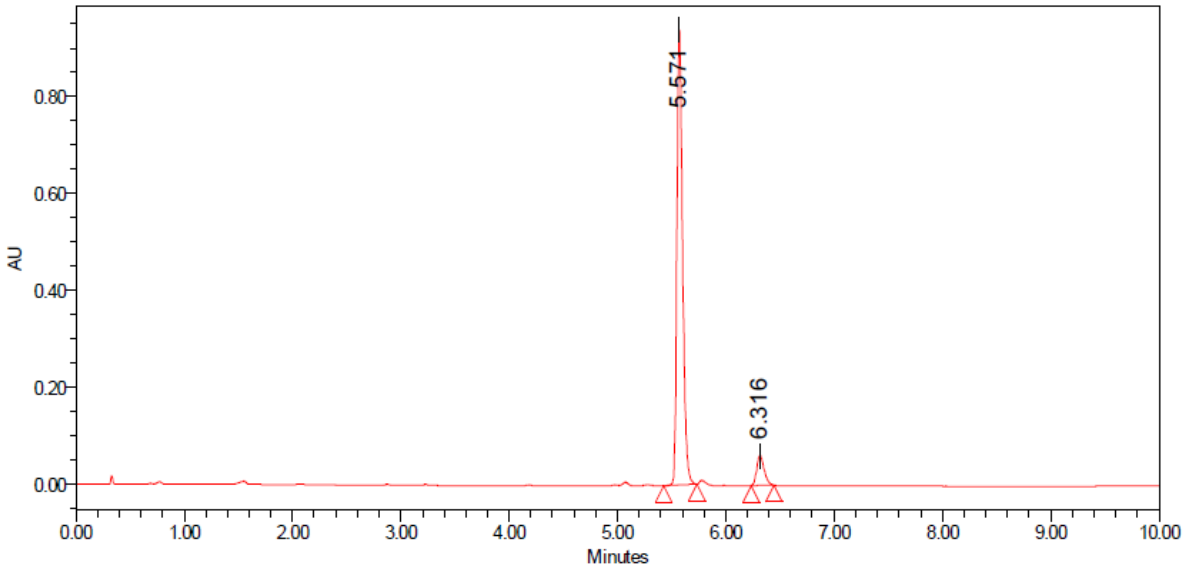
3o Methyl 2-((*R*)-3-((*S*)-1-(3-ethyl-4-nitroisoxazol-5-yl)ethyl)-1-methyl-2-oxoindolin-3-yl)acrylate

(UPC^2 trace)

Racemic sample



Enantiomerically enriched sample



	RT	Area	% Area
1	5.571	3256587	91.90
2	6.316	287092	8.10