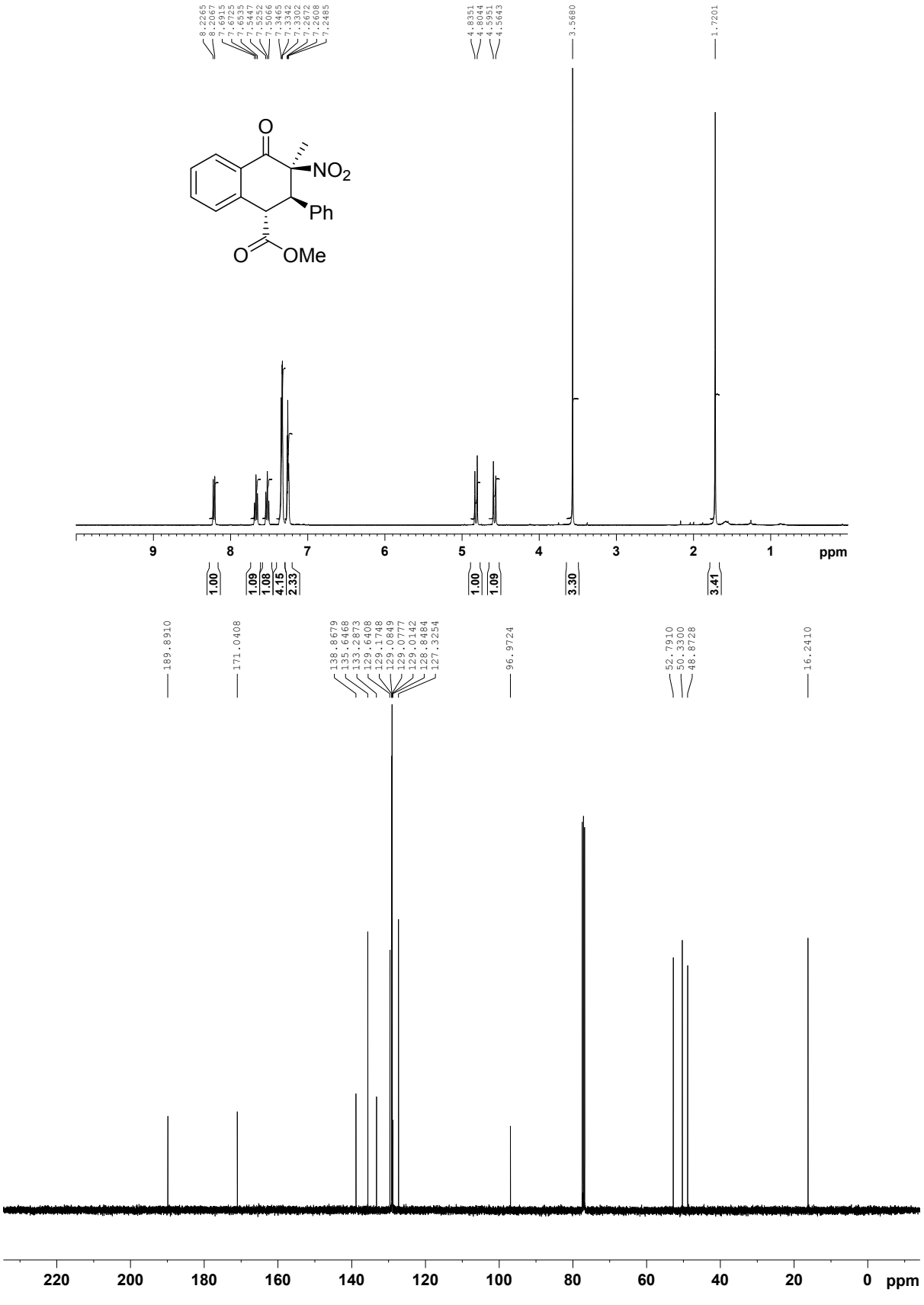
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Catalytic asymmetric Tamura cycloadditions involving nitroalkenes

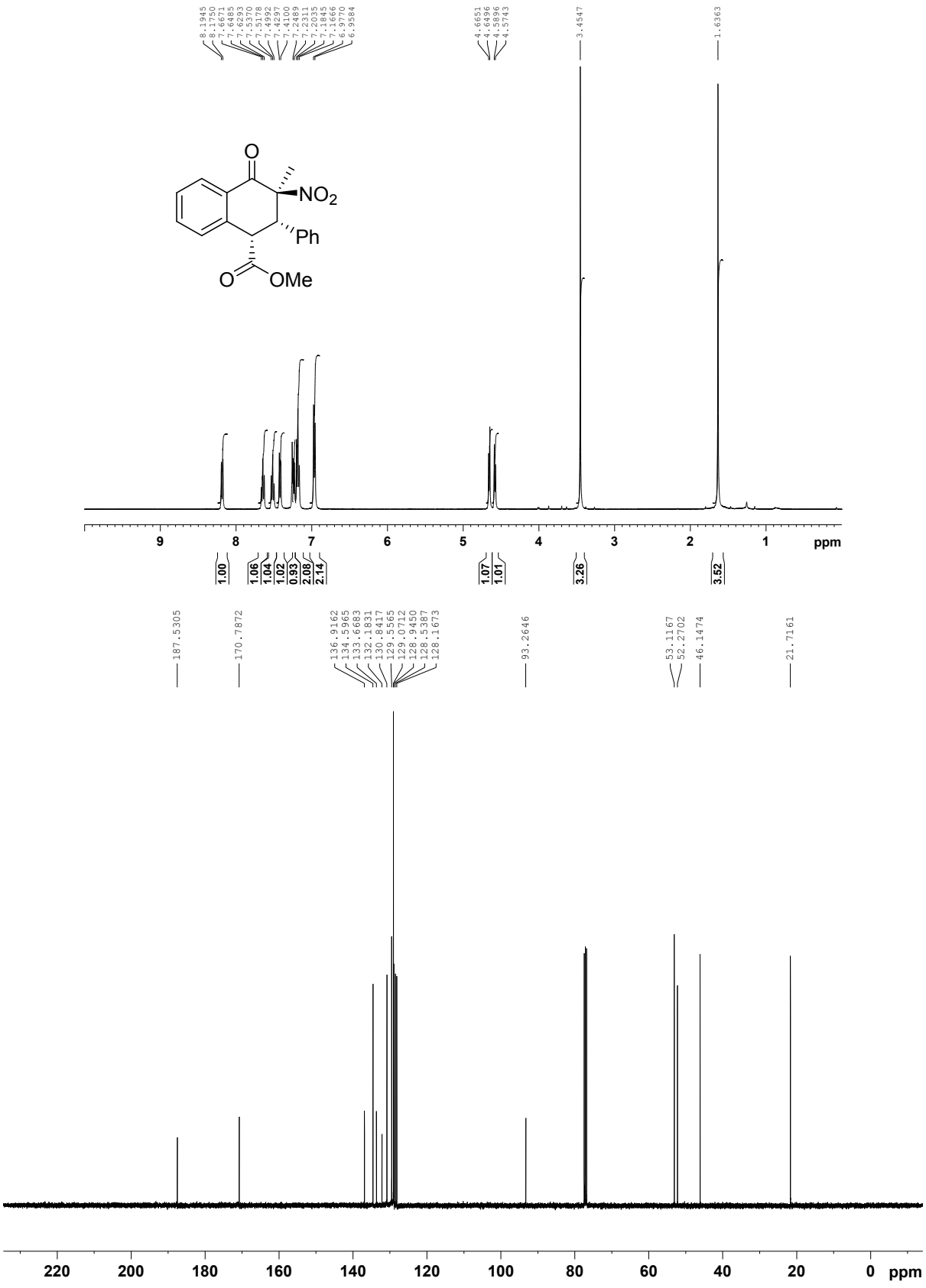
F. Manoni,[a] U. Farid,[a] C. Trujillo[a] and S. J. Connon* [a]

Electronic Supplementary Information

13a



13b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7.2311
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4.5896
4.5743
3.4547
1.6363
O
NO2
Ph
O
OMe
9
8
7
6
5
4
3
2
1
ppm
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1.06
1.04
1.02
0.93
2.08
2.14
1.07
1.01
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133.6683
132.1831
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129.5565
129.0712
128.9450
128.5387
128.1673
93.2646
53.1167
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140
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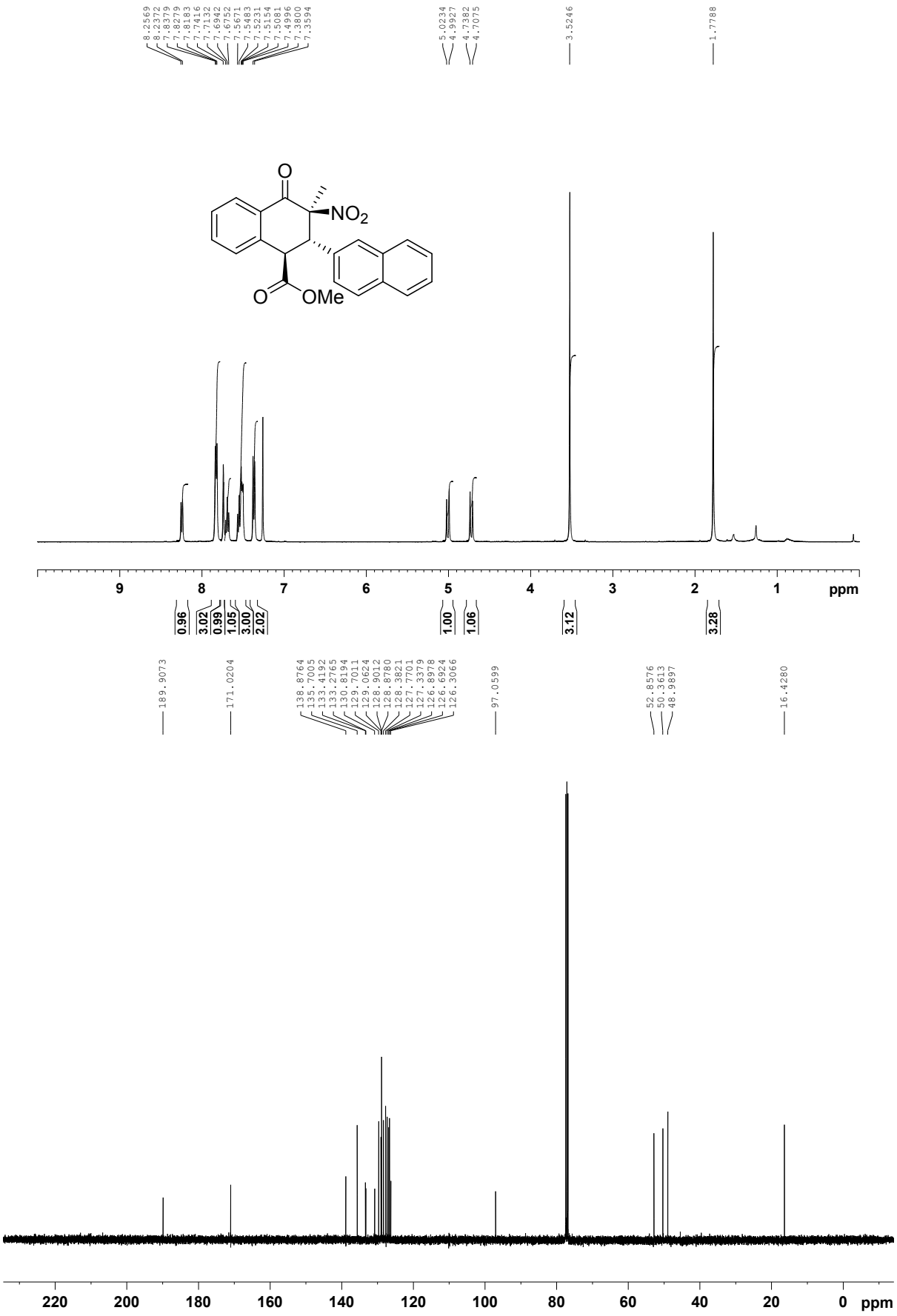
100
80
60
40
20
0
ppm

18a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7.4996
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7.3594
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4.7382
4.7075
3.5246
1.7788
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O
OMe
9
8
7
6
5
4
3
2
1
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1.05
3.00
2.02
1.00
1.06
3.12
3.28
189.9073
171.0204
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135.7005
133.4192
133.2765
130.8194
129.7011
129.0624
128.9012
128.8780
128.3821
127.7701
127.3379
126.8978
126.6924
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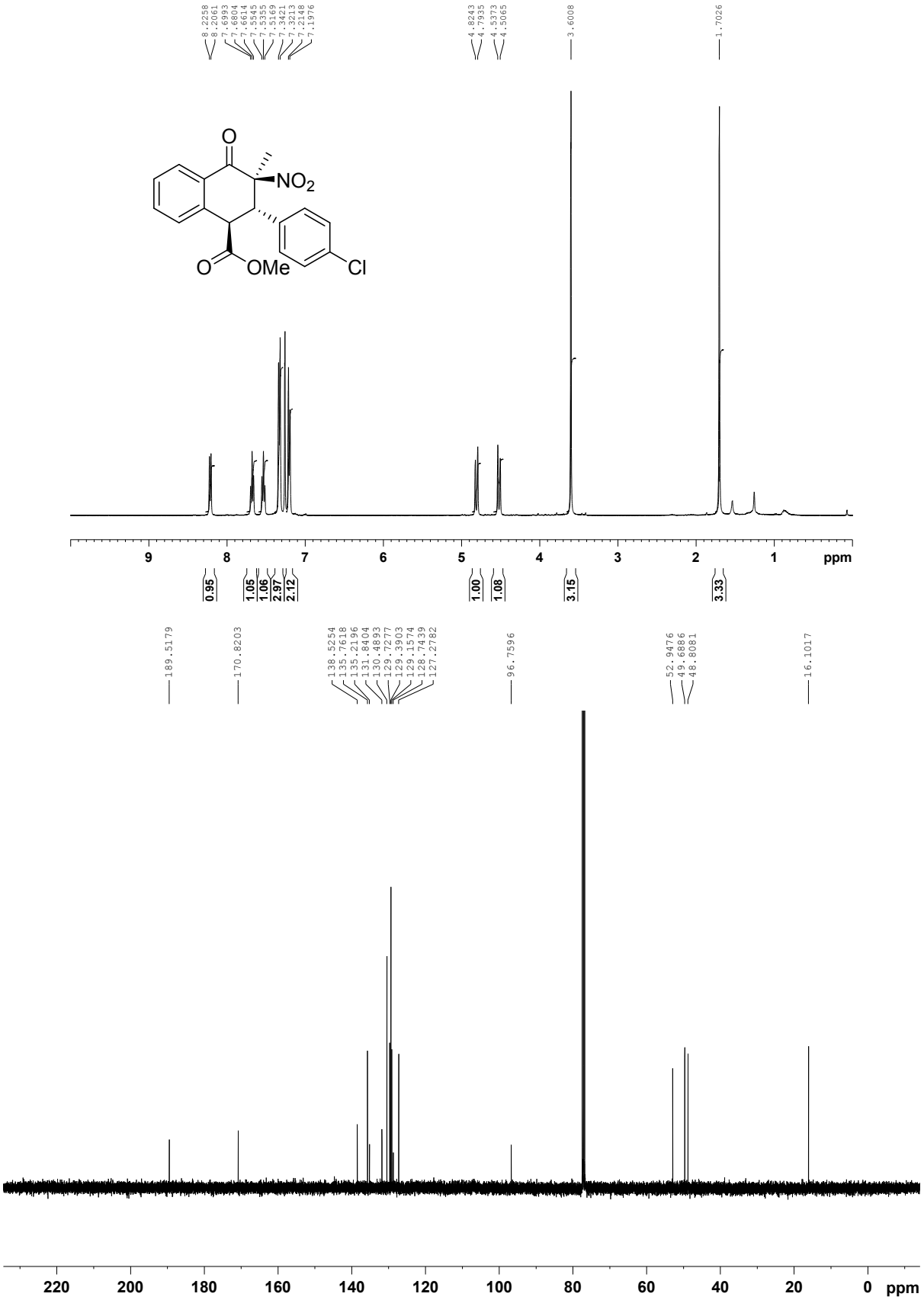
0
ppm

19a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7.1976
4.8243
4.7935
4.5373
4.5065
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NO2
O
OMe
Cl
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8
7
6
5
4
3
2
1
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1.06
2.97
2.12
1.00
1.08
3.15
3.33
189.5179
170.8203
138.5254
135.7618
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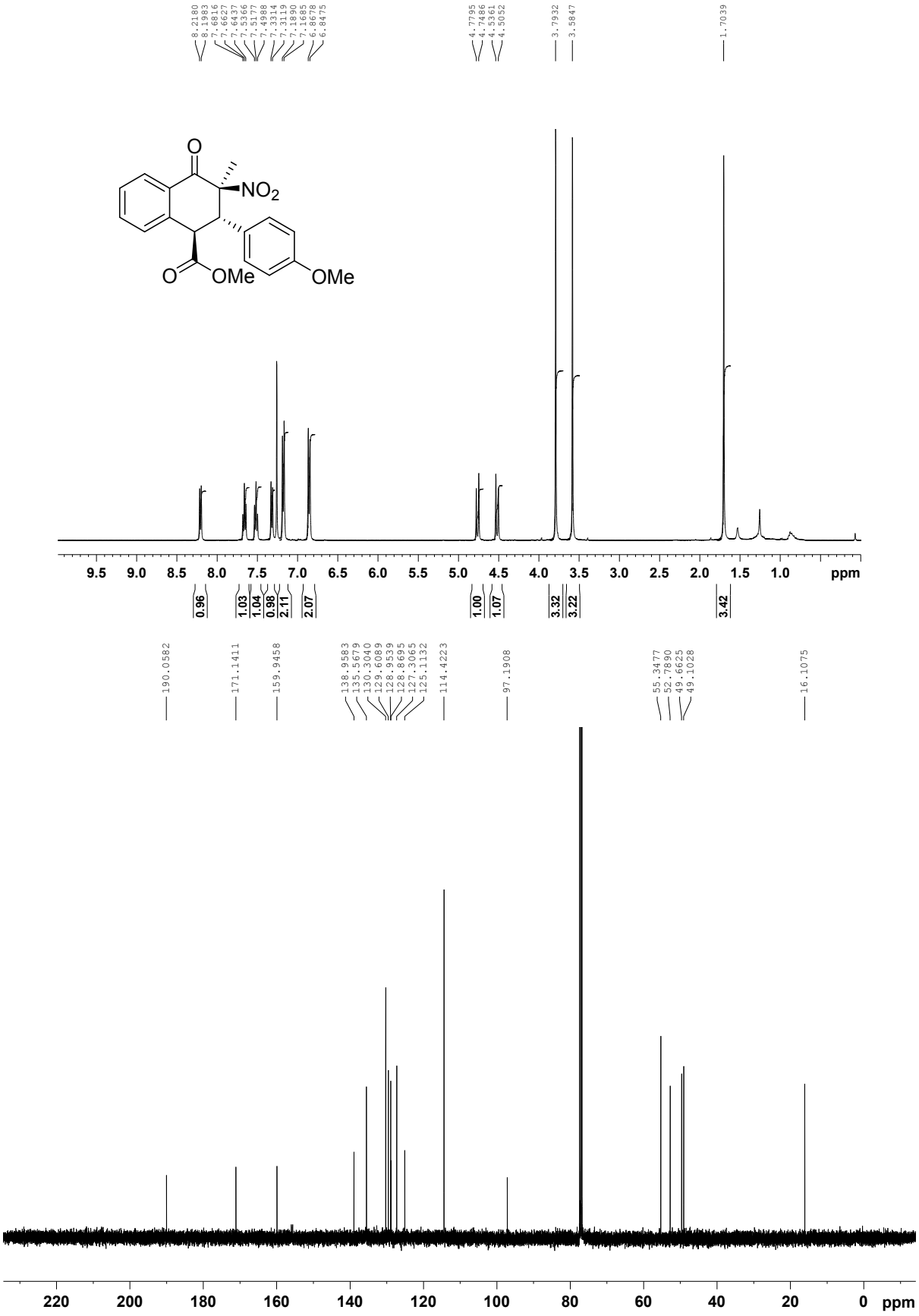
20a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7.1685
6.8678
6.8475
4.7795
4.7486
4.5361
4.5052
3.7932
3.5847
1.7039
O
NO2
O
OMe
OMe
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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1.03
1.04
0.98
2.11
2.07
1.00
1.07
3.32
3.22
3.42
190.0582
171.1411
159.9458
138.9583
135.5679
130.3040
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128.9539
128.8695
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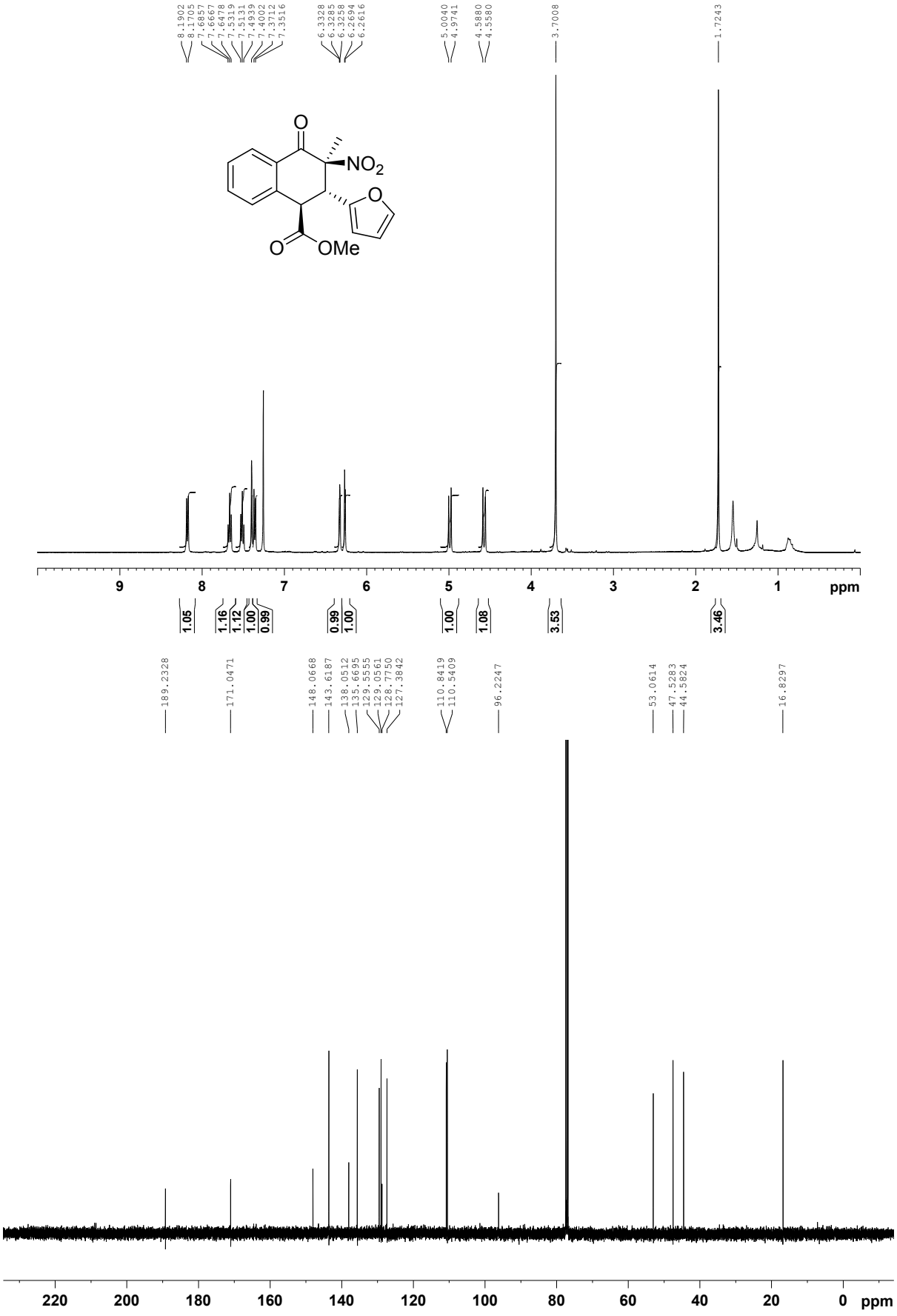
21a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6.3328
6.3285
6.3258
6.2694
6.2616
5.0040
4.9741
4.5880
4.5580
3.7008
1.7243
O
NO2
O
O
OMe
9
8
7
6
5
4
3
2
1
ppm
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1.16
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0.99
1.00
1.00
1.08
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143.6187
138.0512
135.6695
129.5555
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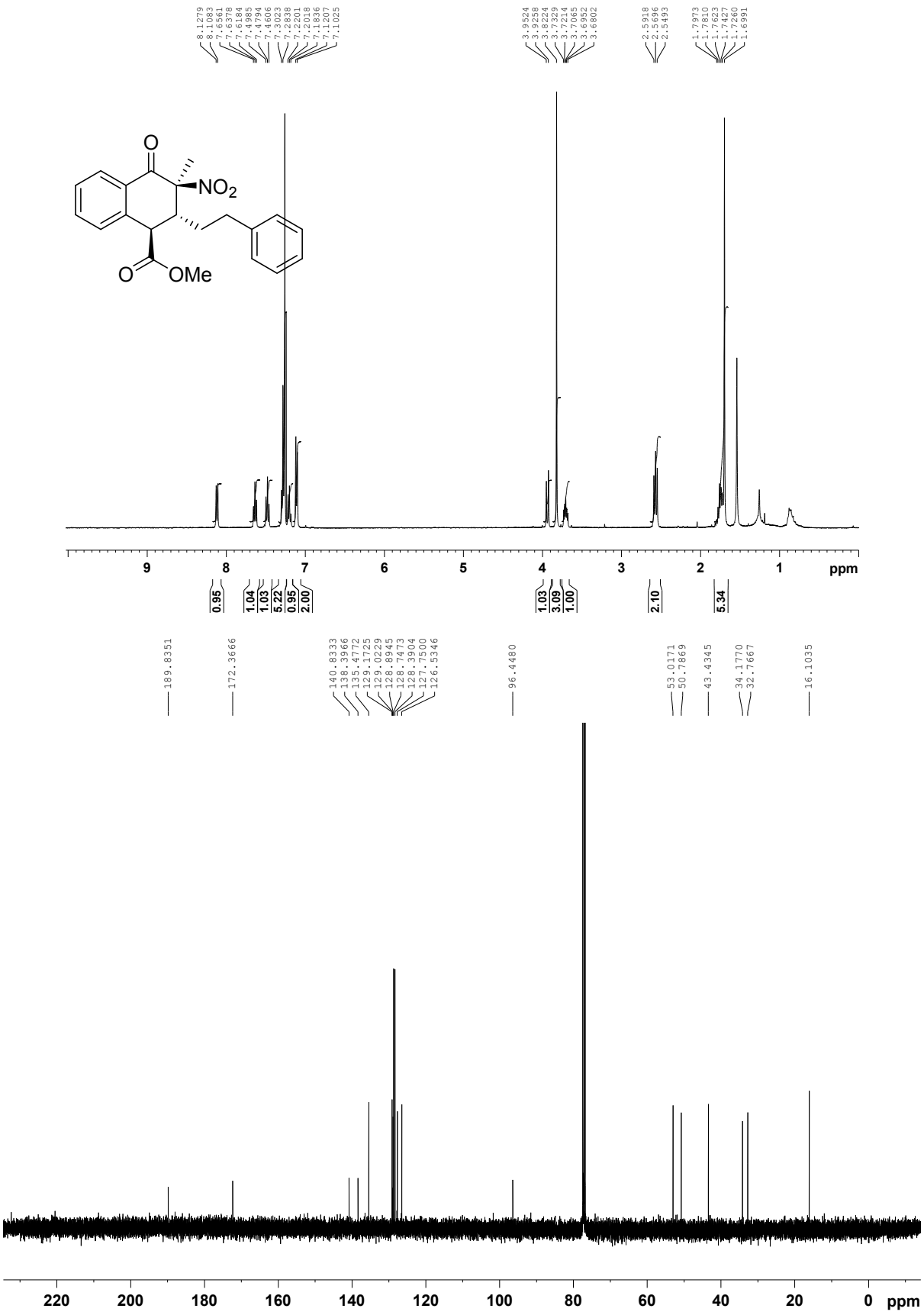
ppm

22a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7.2018
7.1836
7.1207
7.1025
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3.9258
3.8224
3.7329
3.7214
3.7065
3.6952
3.6802
2.5918
2.5696
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1.7810
1.7623
1.7427
1.7260
1.6991
O
NO2
O
OMe
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8
7
6
5
4
3
2
1
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1.03
5.22
0.95
2.00
1.03
3.09
1.00
2.10
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126.5346
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53.0171
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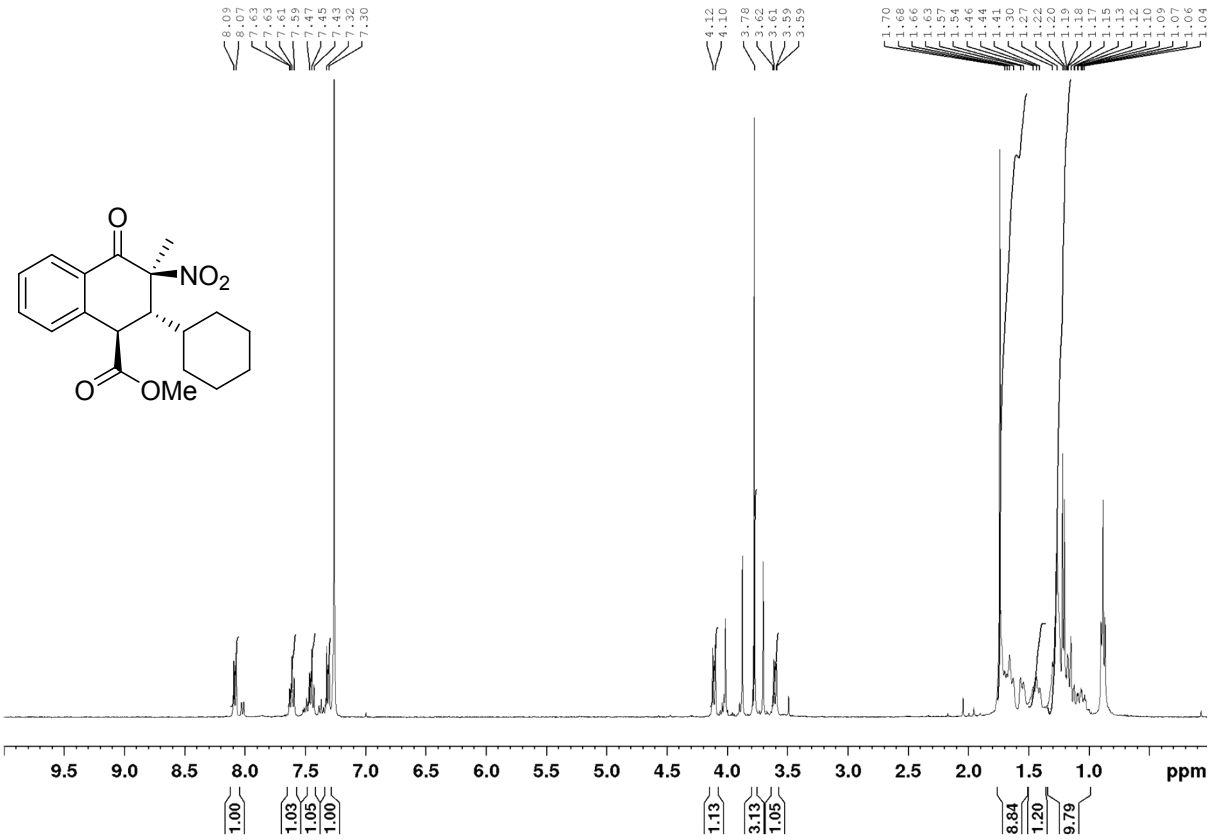
60
40
20
0
ppm

23a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7.32
7.30
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4.10
3.78
3.62
3.61
3.59
3.59
1.70
1.68
1.66
1.63
1.57
1.54
1.46
1.44
1.41
1.30
1.27
1.22
1.20
1.19
1.18
1.17
1.15
1.13
1.12
1.10
1.09
1.07
1.06
1.04
O
NO2
O
OMe
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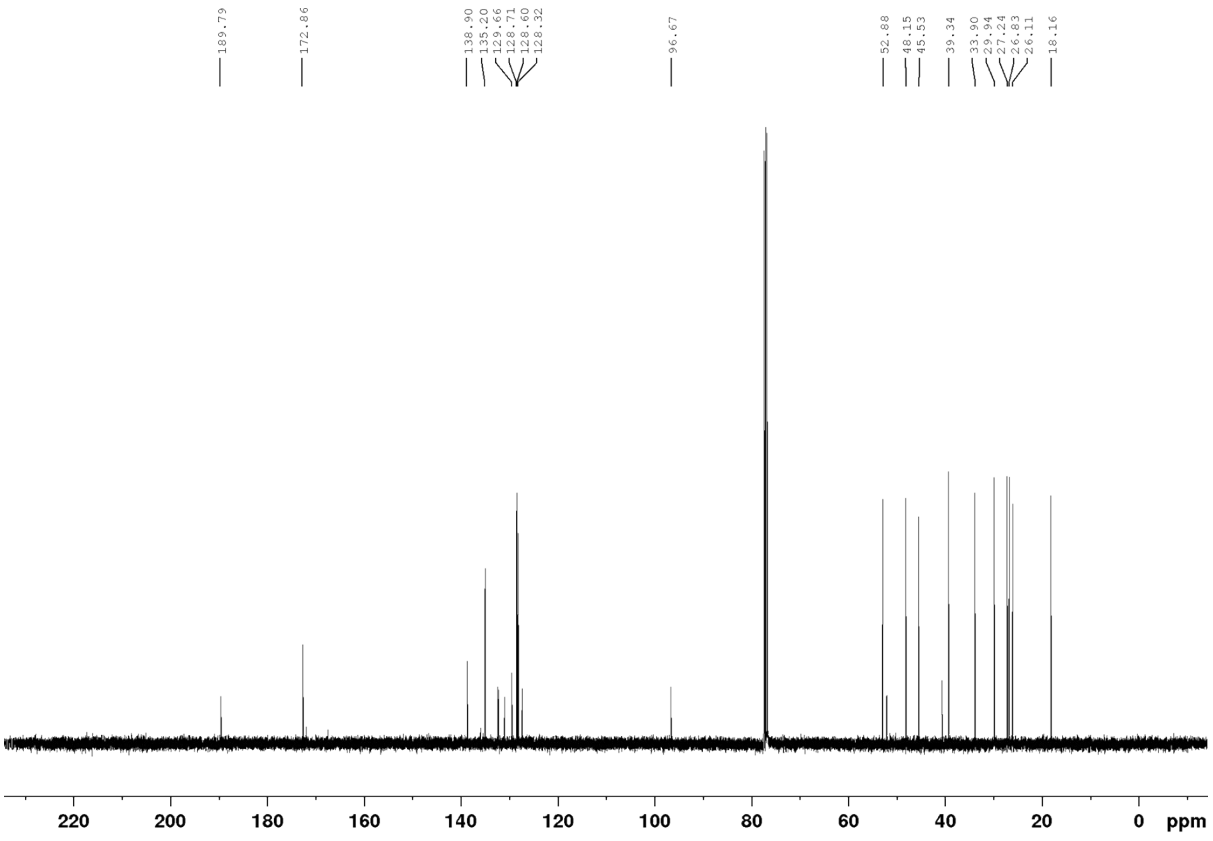
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29.94
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18.16
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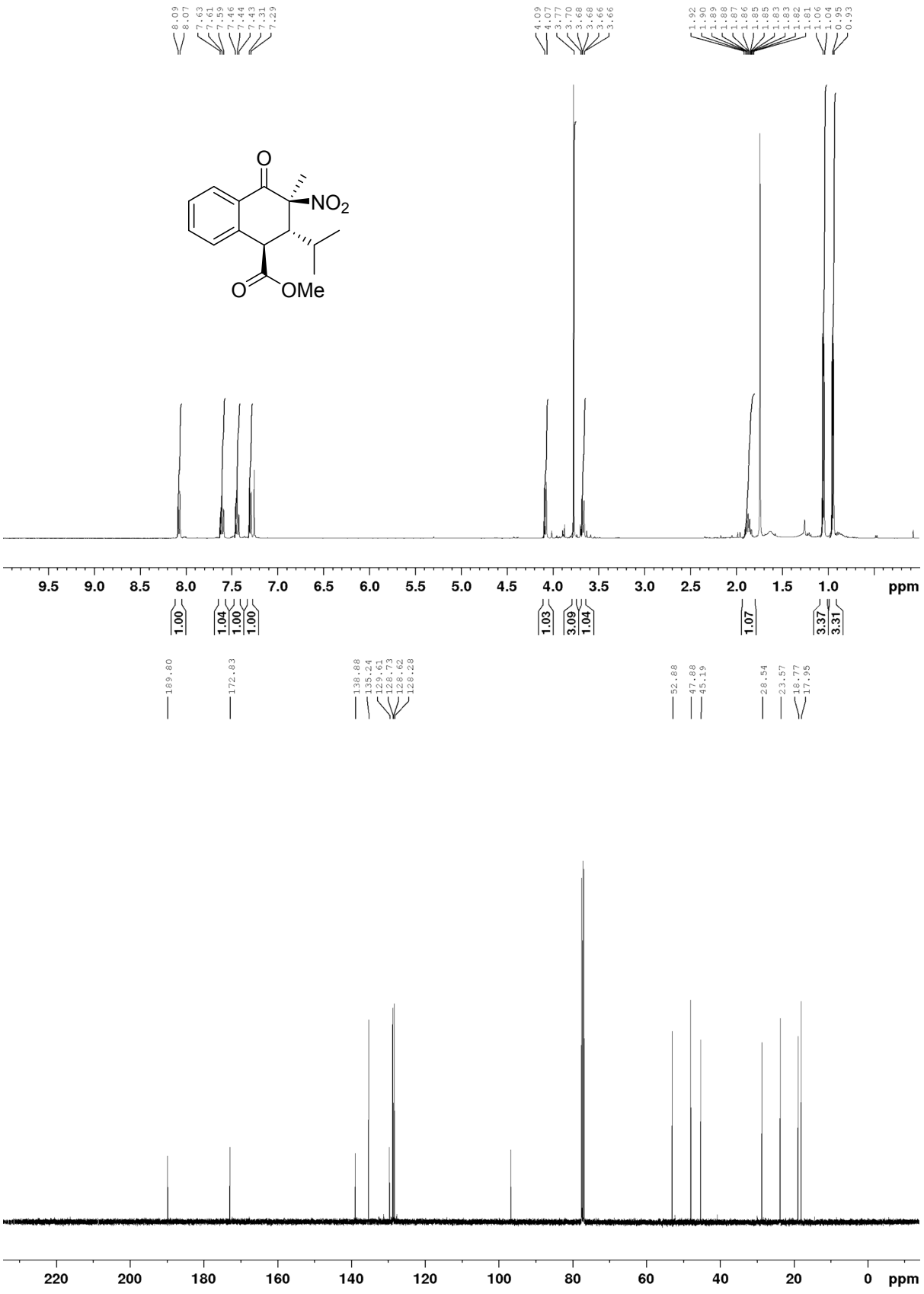
24a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7.43
7.31
7.29
4.09
4.07
3.77
3.70
3.68
3.68
3.66
3.66
1.92
1.90
1.89
1.88
1.87
1.86
1.85
1.85
1.83
1.83
1.82
1.81
1.06
1.04
0.95
0.93
O
NO2
O
OMe
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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1.04
1.00
1.00
1.03
3.09
1.04
1.07
3.37
3.31
189.80
172.83
138.88
135.24
129.71
128.73
128.62
128.28
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47.88
45.19
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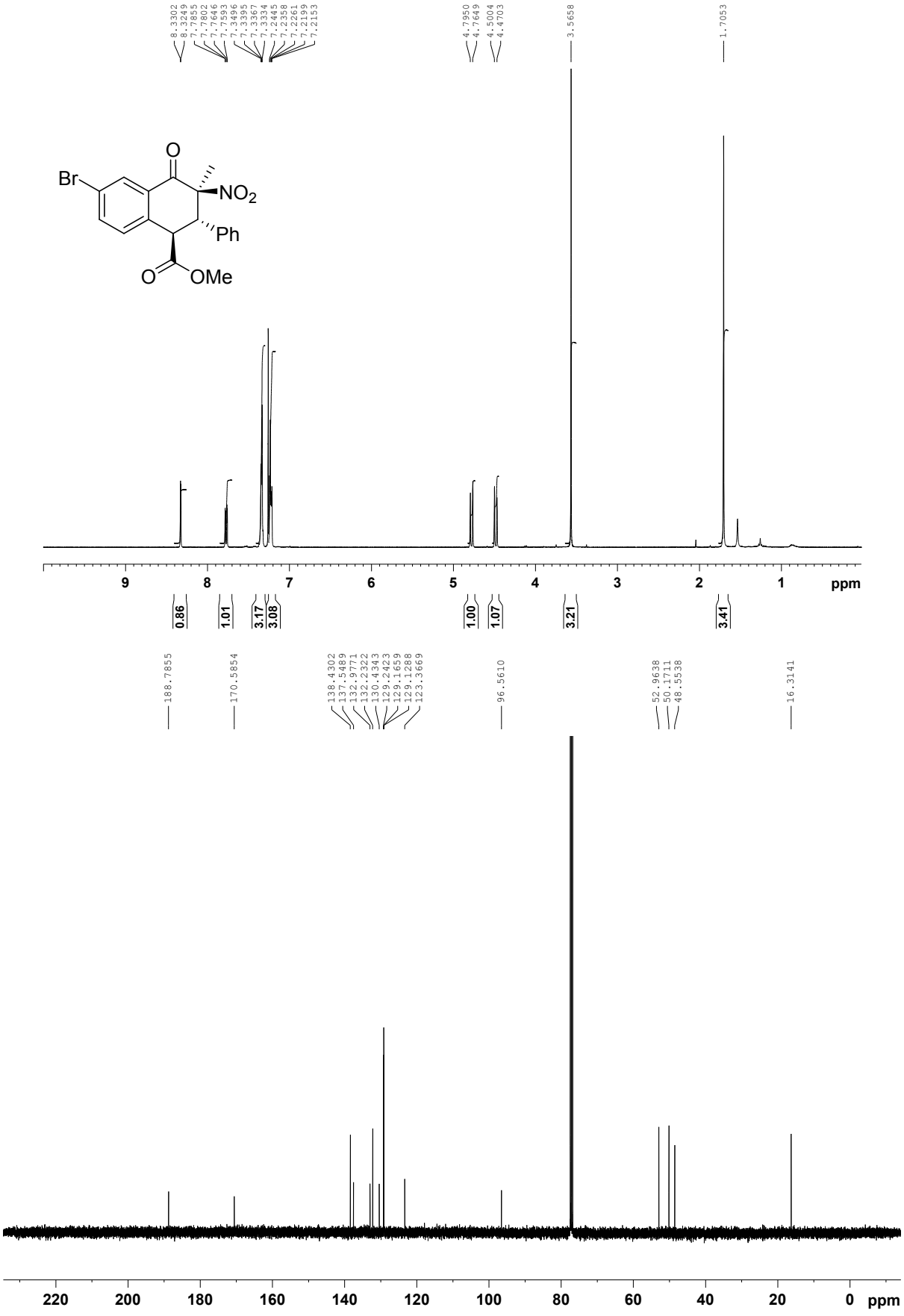
18.77
17.95
220 200 180 160 140 120 100 80 60 40 20 0 ppm

26a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7.3367
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7.2445
7.2358
7.2261
7.2199
7.2153
4.7950
4.7649
4.5004
4.4703
3.5658
1.7053
Br
O
NO2
Ph
O
OMe
9
8
7
6
5
4
3
2
1
ppm
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1.01
3.17
3.08
1.00
1.07
3.21
3.41
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132.2322
130.4343
129.2423
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96.5610
52.9638
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160
140
120
100
80
60
40
20
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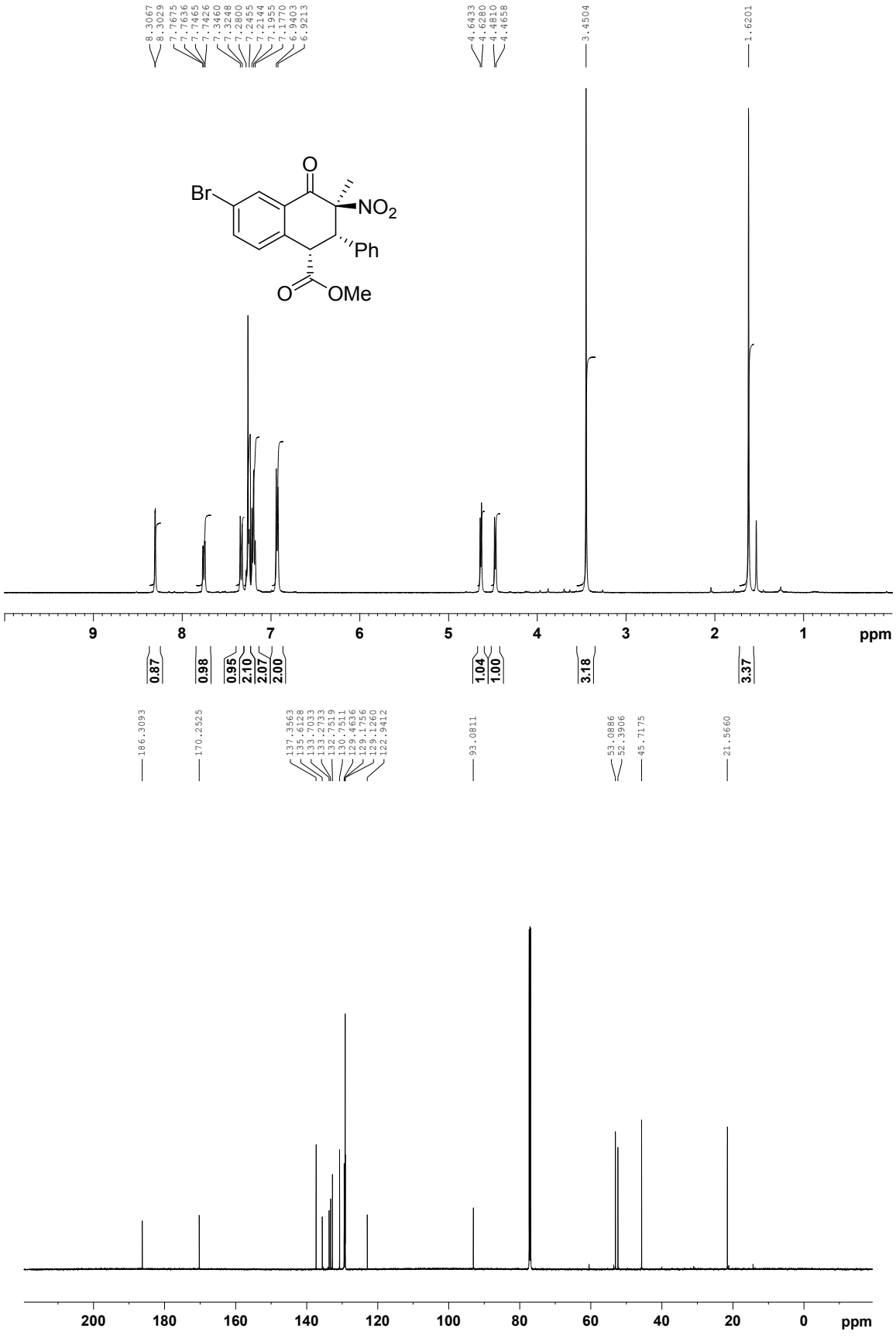
ppm

26b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Br
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NO2
Ph
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OMe
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5
4
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2
1
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0.98
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1.04
1.00
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186.3093
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120
100
80
60
40
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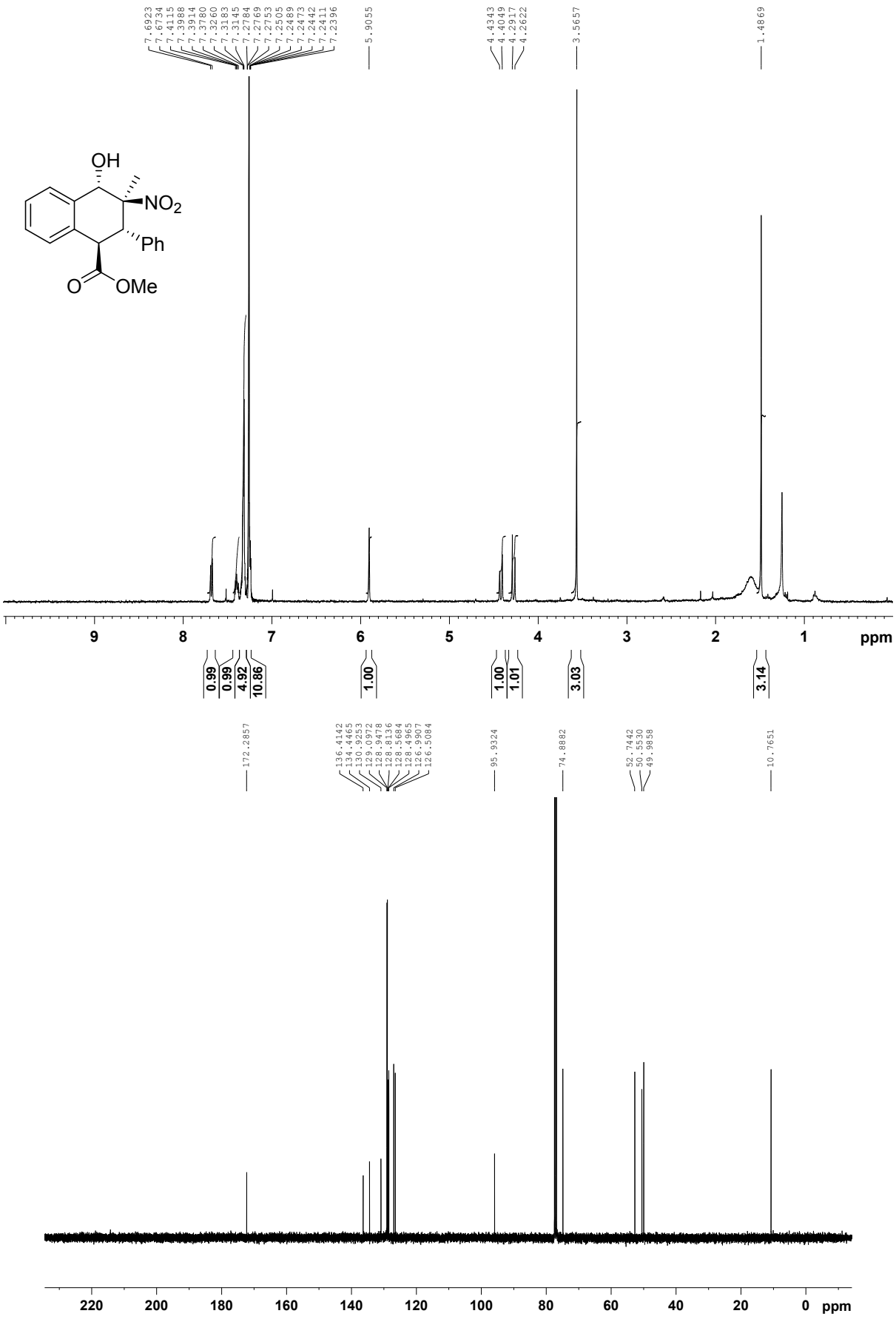
ppm

27a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7.2411
7.2396
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1.4869
OH
NO2
Ph
O
OMe
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8
7
6
5
4
3
2
1
ppm
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0.99
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1.00
1.00
1.01
3.03
3.14
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120
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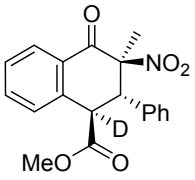
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MeO
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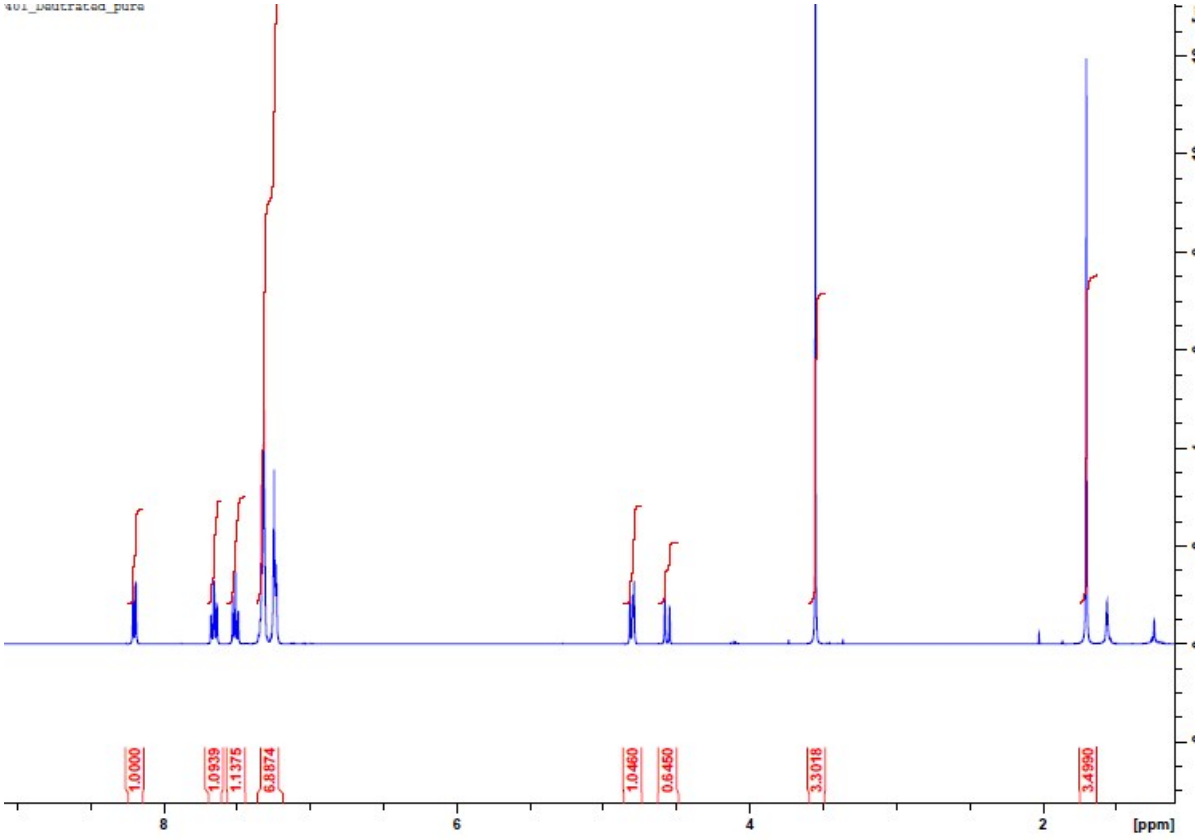
13a'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6
4
2
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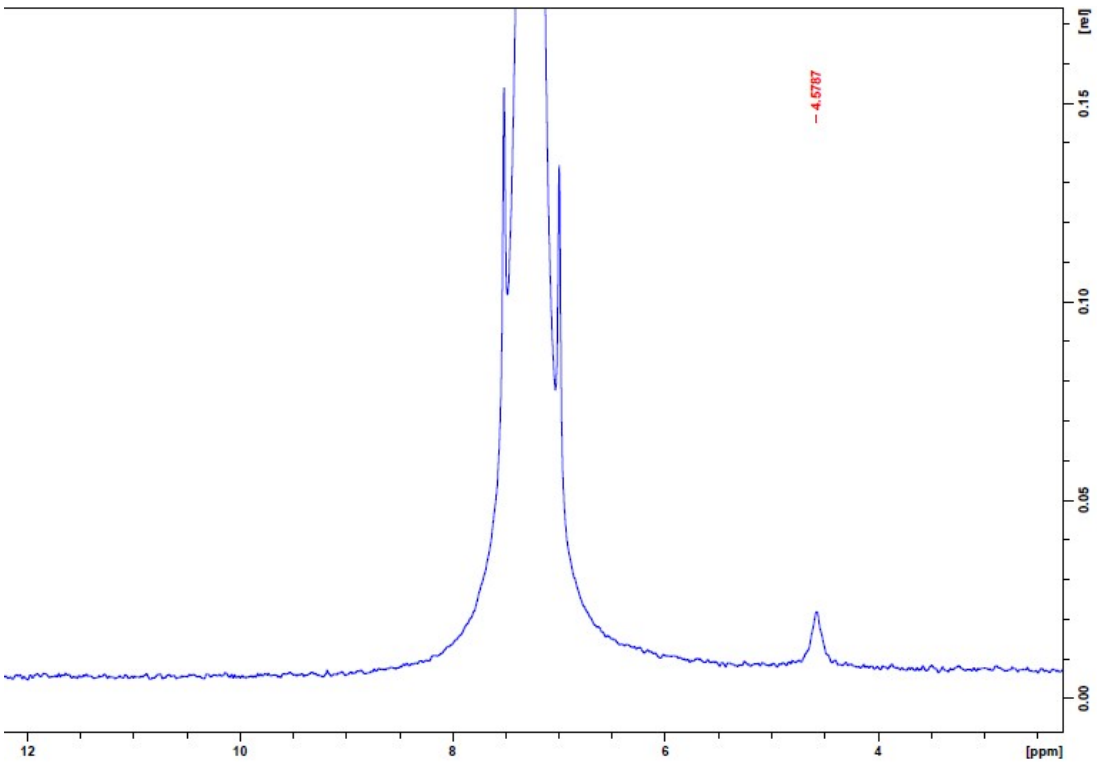
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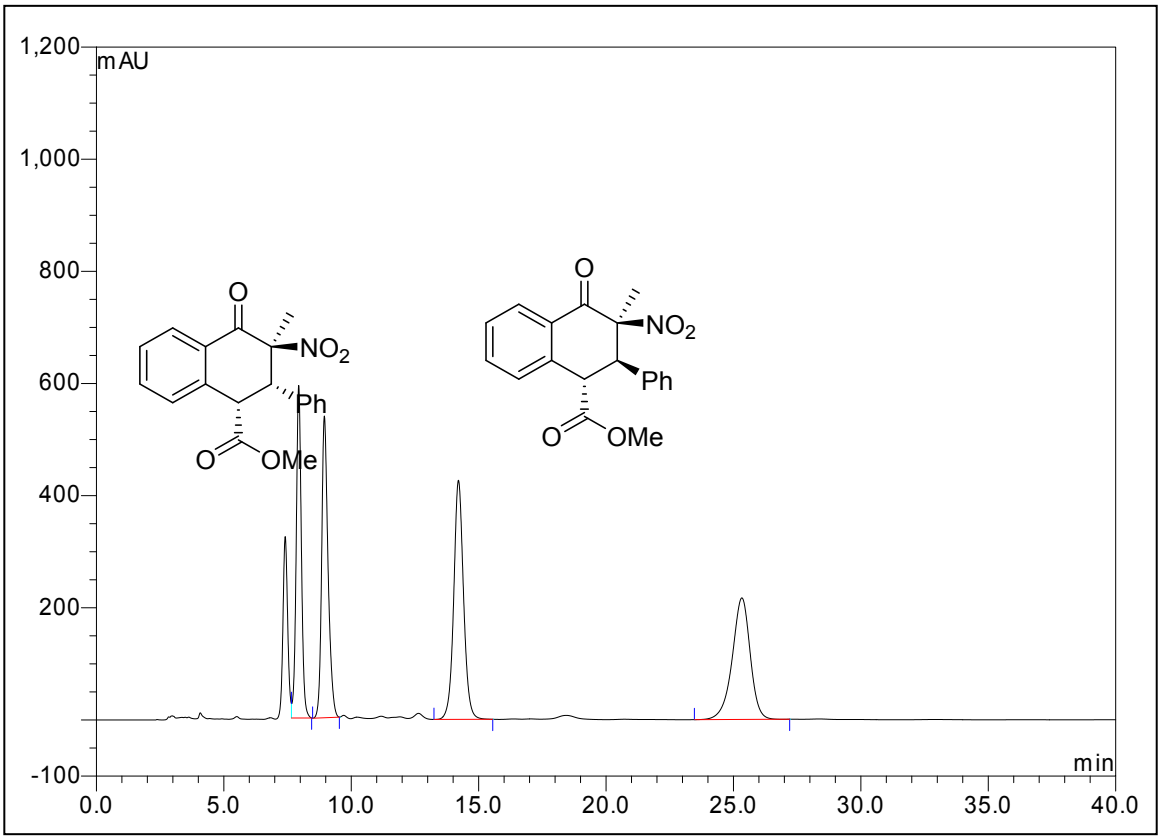
0.10
0.05
0.00
[rel]
12
10
8
6
4
[ppm]

HPLC Data

13a/13b
Rac.

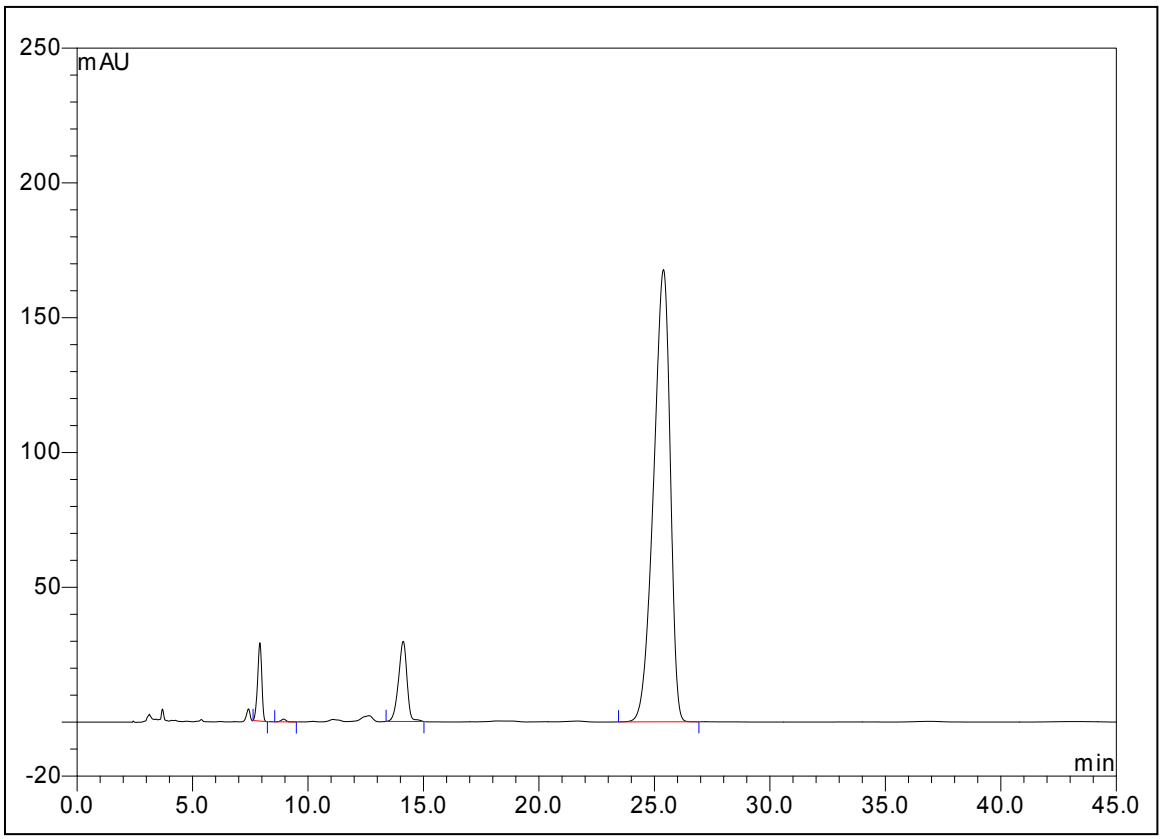
Sample Name:	**13a/13b, Racemic**	*Injection Volume:*	**20.0**
Vial Number:	**BA8**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**47.68**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.94	n.a.	593.040	139.392	21.01	n.a.	MB*
2	8.95	n.a.	538.107	156.473	23.59	n.a.	BMB*
3	14.21	n.a.	426.403	190.419	28.71	n.a.	BMB*
4	25.33	n.a.	216.801	177.031	26.69	n.a.	BMB*
Total:			1774.350	663.314	100.00	0.000	

13a/13b, table3 entry 1

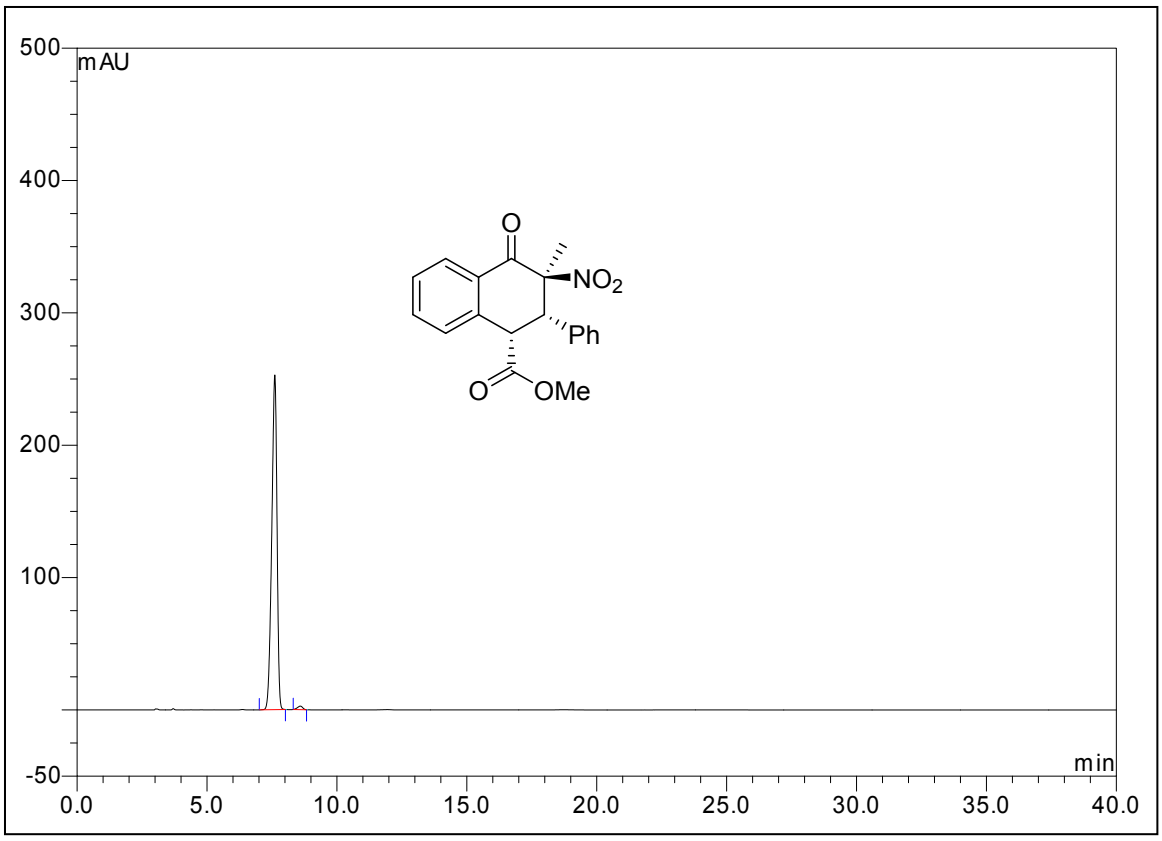
Sample Name:	**13a/13b**	*Injection Volume:*	**20.0**
Vial Number:	**GC1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 45min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**45.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.91	n.a.	29.028	6.078	3.83	n.a.	BMB*
2	8.95	n.a.	1.001	0.242	0.15	n.a.	BMB*
3	14.12	n.a.	29.710	12.674	7.99	n.a.	BMB*
4	25.39	n.a.	167.738	139.567	88.02	n.a.	BMB*
Total:			227.476	158.562	100.00	0.000	

13b
table3

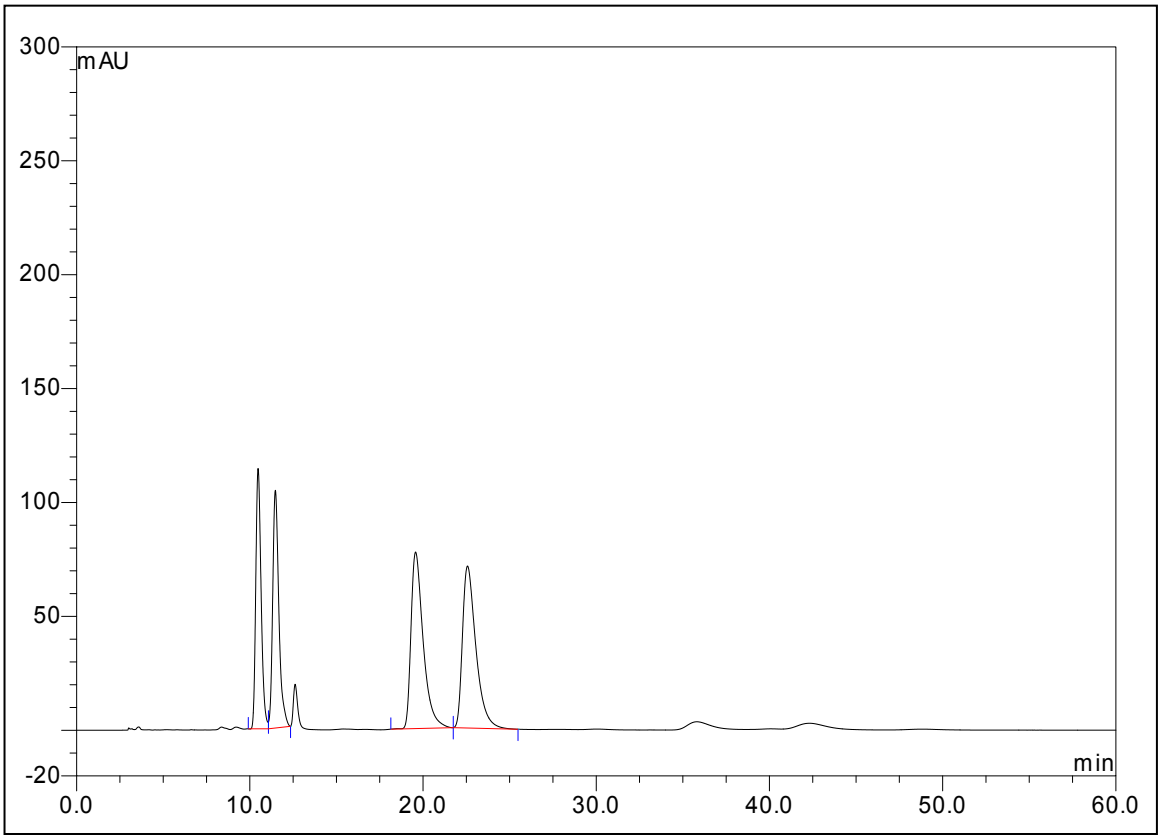
Sample Name:	**13b**	*Injection Volume:*	**20.0**
Vial Number:	**RA8**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 60min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.61	n.a.	252.849	59.074	98.97	n.a.	BMB*
2	8.59	n.a.	2.665	0.614	1.03	n.a.	BMB*
Total:			255.514	59.689	100.00	0.000	

18a/18b
rac.

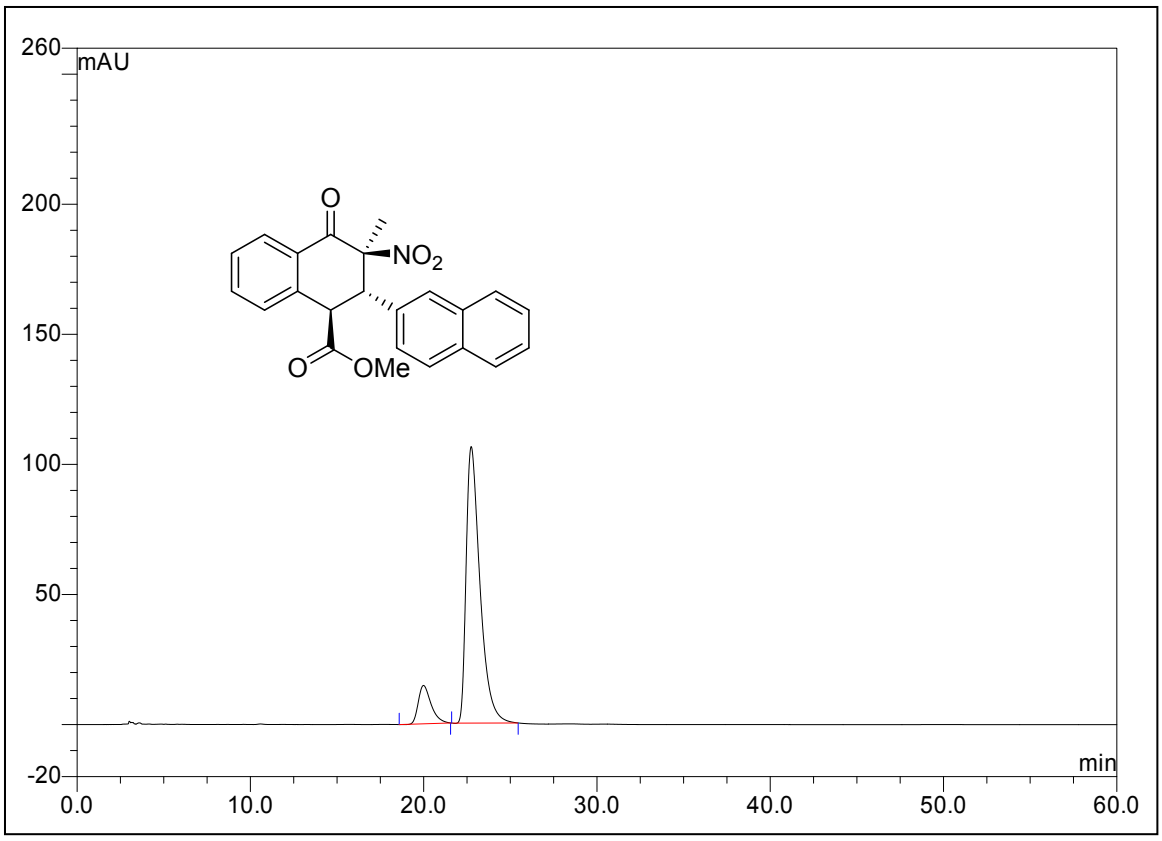
Sample Name:	**18a/18b**	*Injection Volume:*	**20.0**
Vial Number:	**RB7**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 60min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.48	n.a.	114.297	40.973	19.41	n.a.	BM *
2	11.47	n.a.	104.365	43.092	20.42	n.a.	MB*
3	19.57	n.a.	77.497	63.127	29.91	n.a.	BMb*
4	22.57	n.a.	71.112	63.864	30.26	n.a.	bMB*
Total:			367.271	211.056	100.00	0.000	

18a, table4

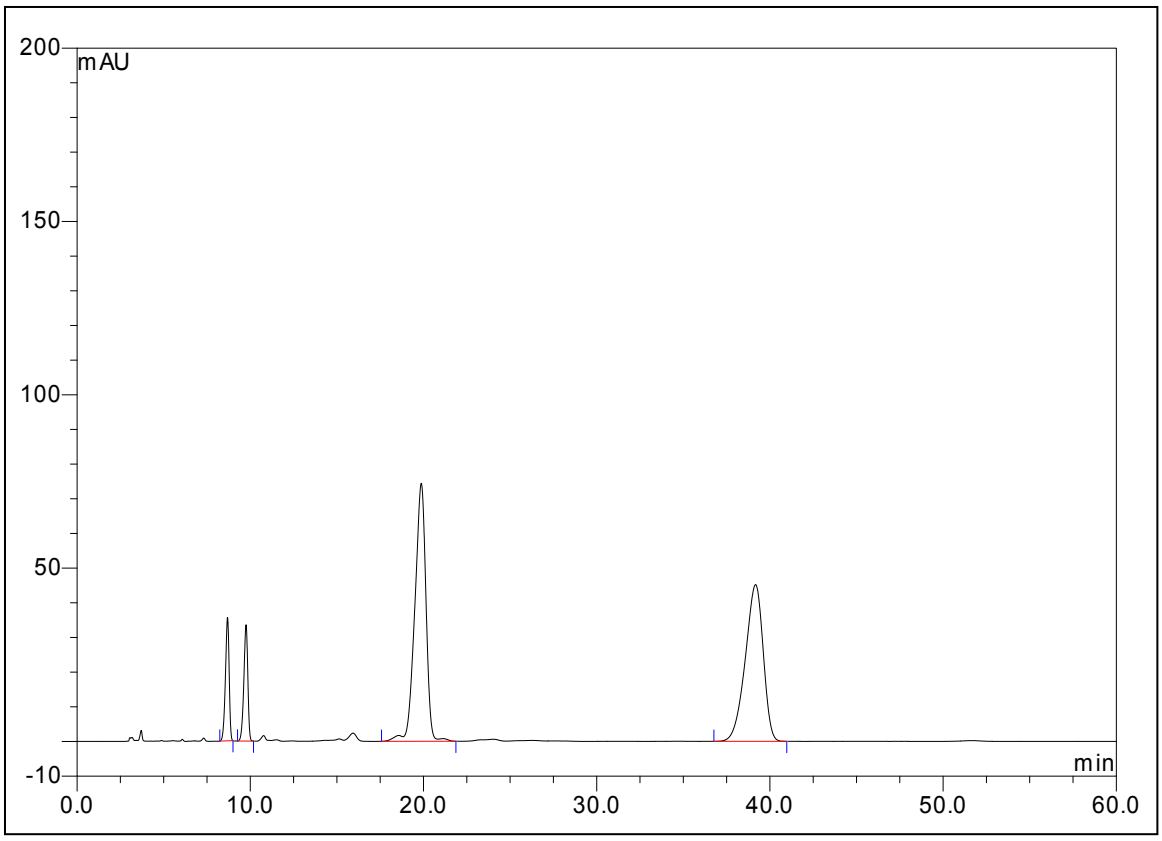
Sample Name:	**18a**	*Injection Volume:*	**20.0**
Vial Number:	**RC8**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 60min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.99	n.a.	14.746	12.559	11.34	n.a.	BMB*
2	22.74	n.a.	106.293	98.152	88.66	n.a.	BMB*
Total:			121.039	110.711	100.00	0.000	

19a/19b
rac.

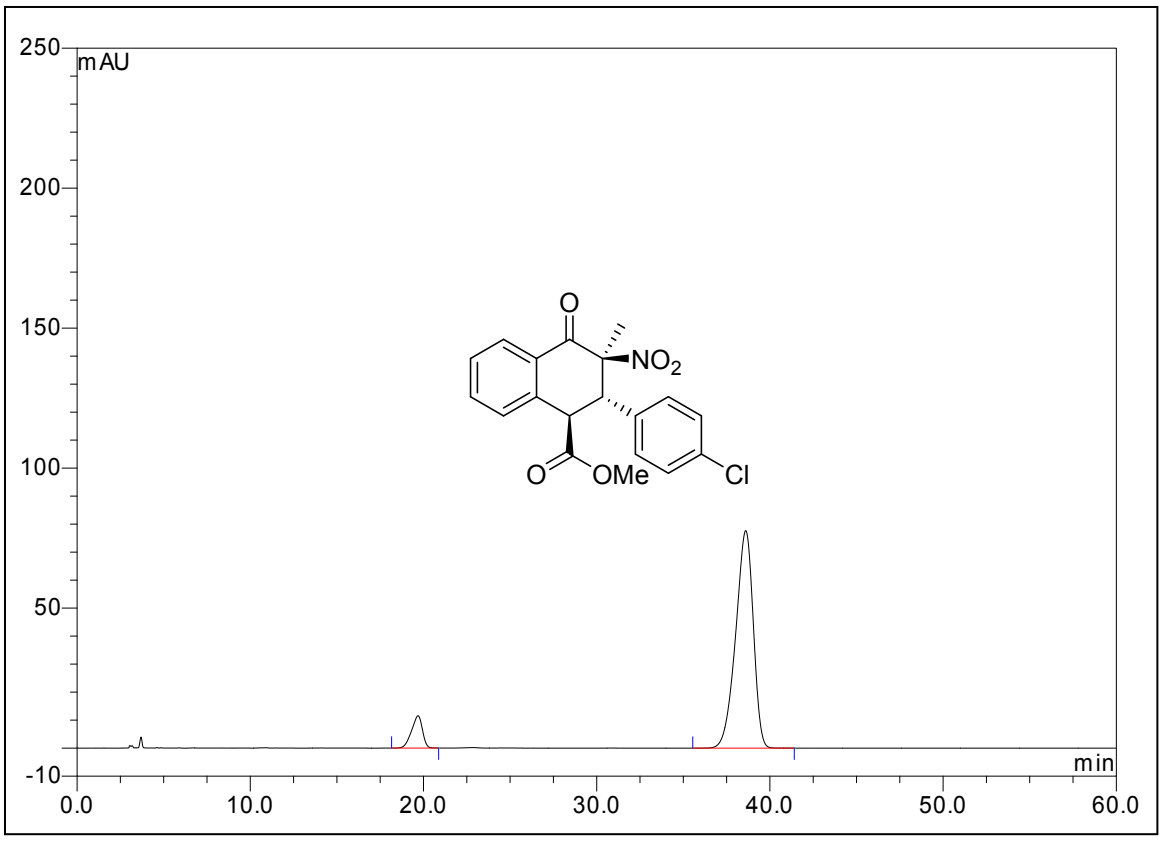
Sample Name:	**19a/19b**	*Injection Volume:*	**20.0**
Vial Number:	**RB1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 60min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.69	n.a.	35.589	8.844	6.93	n.a.	BMB*
2	9.75	n.a.	33.561	8.907	6.97	n.a.	BMB*
3	19.87	n.a.	74.434	55.740	43.65	n.a.	BMB*
4	39.17	n.a.	45.211	54.220	42.46	n.a.	BMB*
Total:			188.795	127.711	100.00	0.000	

19a, table4

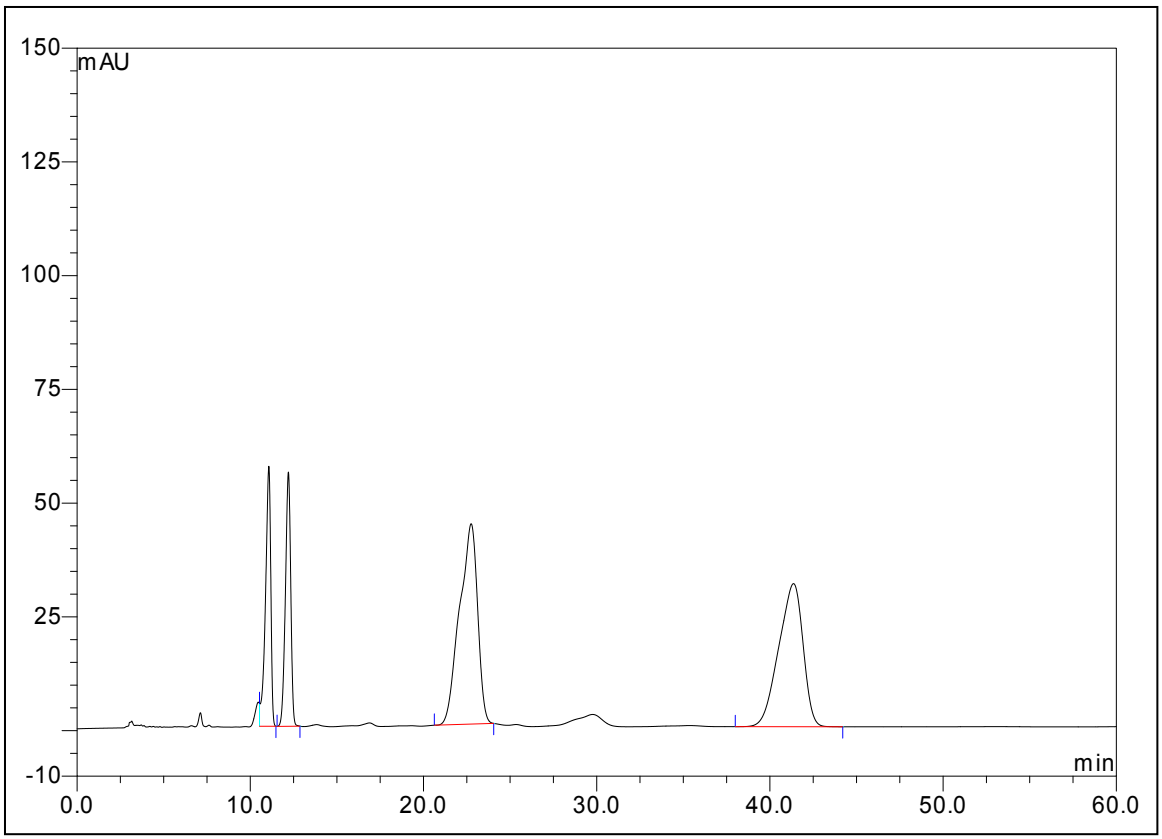
Sample Name:	**19a**	*Injection Volume:*	**20.0**
Vial Number:	**RB6**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 60min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.69	n.a.	11.554	8.404	8.41	n.a.	BMB*
2	38.61	n.a.	77.685	91.478	91.59	n.a.	BMB*
Total:			89.239	99.882	100.00	0.000	

20a/20b, rac.

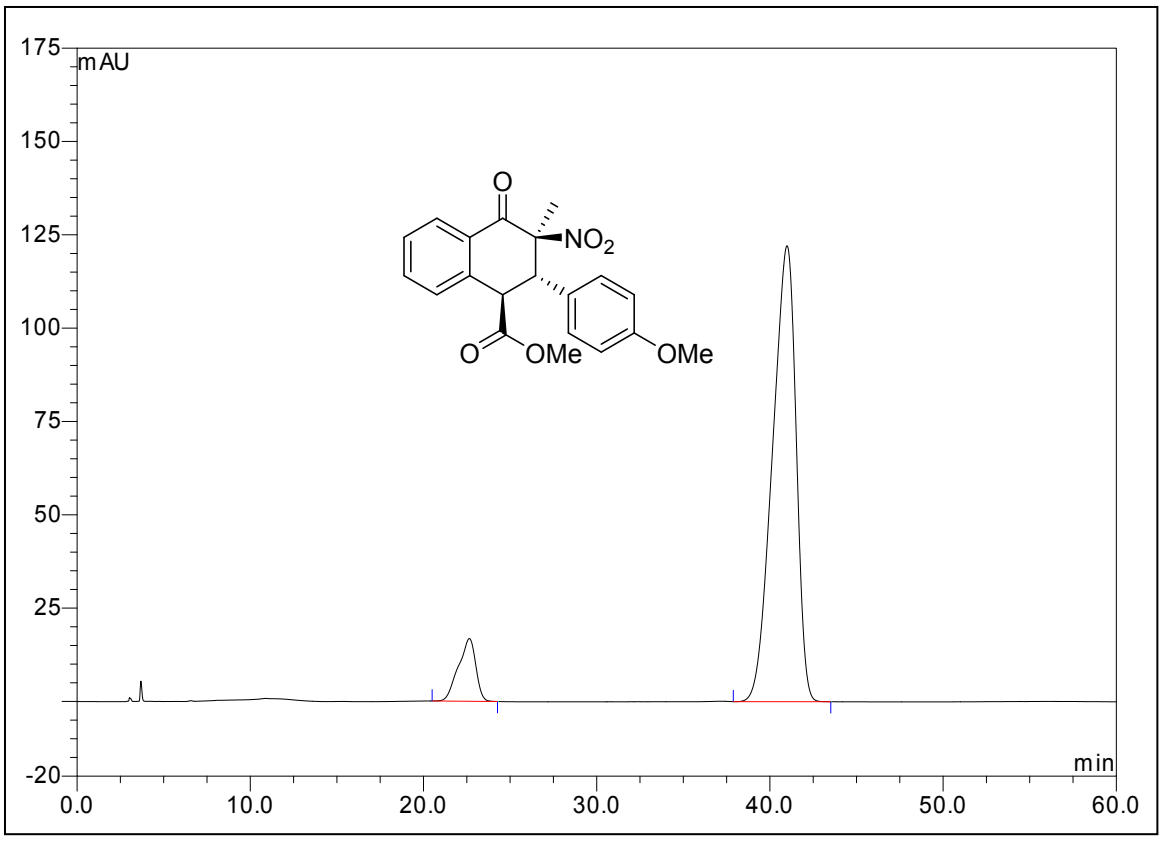
Sample Name:	**20a/20b**	*Injection Volume:*	**20.0**
Vial Number:	**RB1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 60min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.07	n.a.	57.150	20.170	13.96	n.a.	MB*
2	12.20	n.a.	55.881	19.902	13.78	n.a.	BMB*
3	22.75	n.a.	44.034	53.193	36.82	n.a.	BMB*
4	41.37	n.a.	31.456	51.201	35.44	n.a.	BMB*
Total:			188.522	144.466	100.00	0.000	

20a,
table4

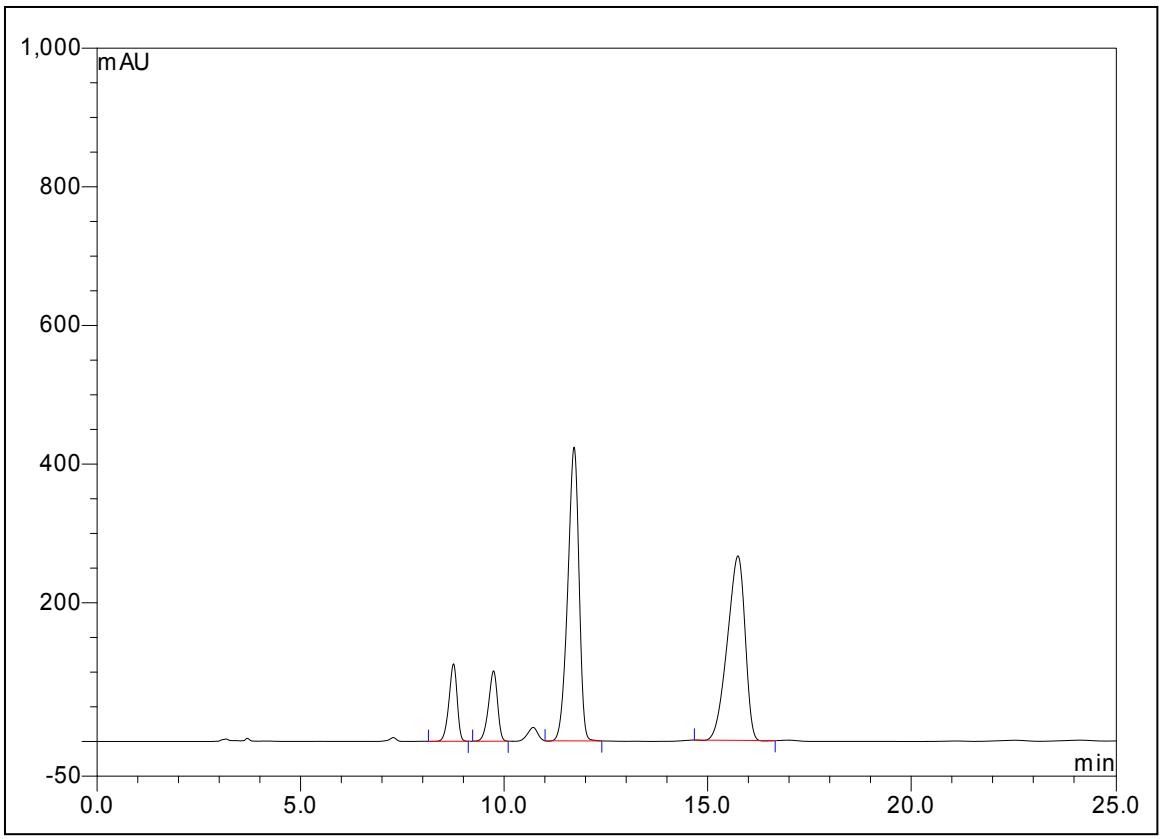
Sample Name:	**20a**	*Injection Volume:*	**20.0**
Vial Number:	**RA4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 60min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:	*Sample Weight:*	**1.0000**	
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	22.65	n.a.	16.791	19.477	9.17	n.a.	BMB*
2	40.99	n.a.	122.124	192.987	90.83	n.a.	BMB*
Total:			138.915	212.464	100.00	0.000	

21a/21b, rac.

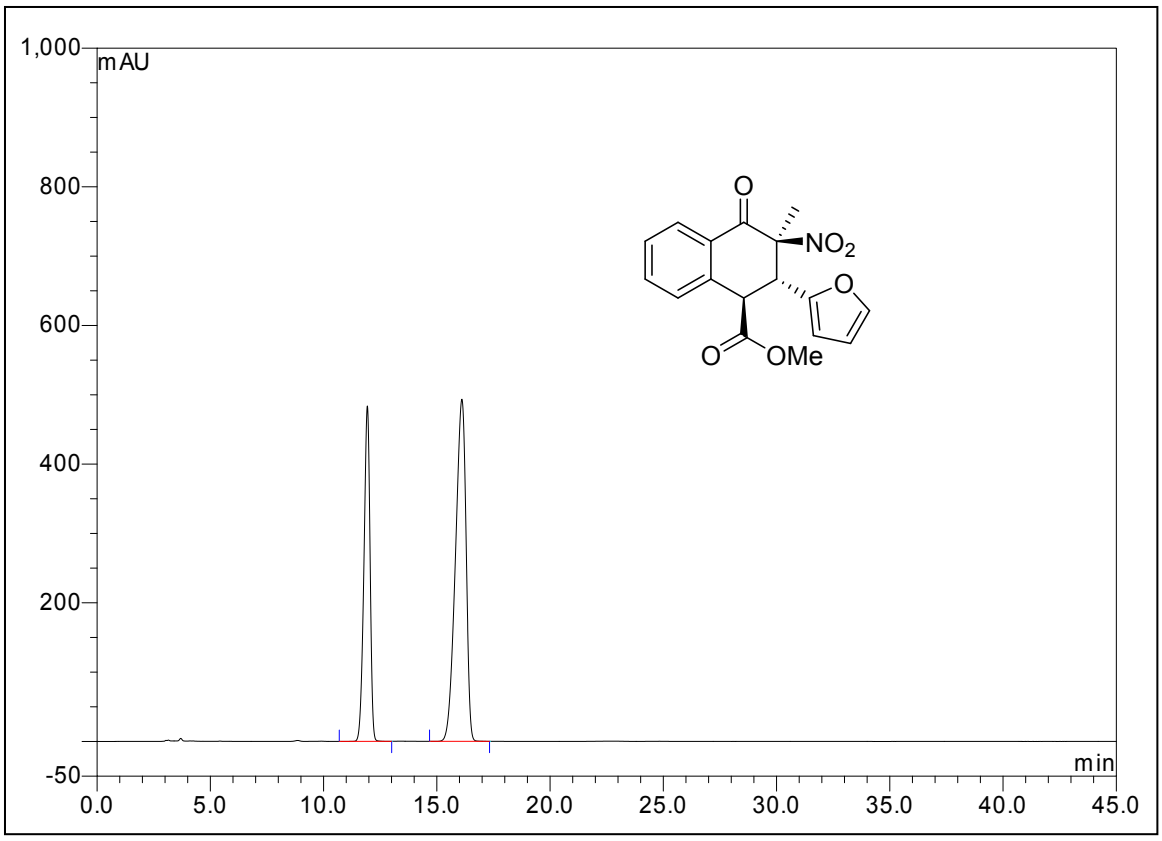
Sample Name:	**21a/21b**	*Injection Volume:*	**20.0**
Vial Number:	**GC5**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 30min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**25.04**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.75	n.a.	111.607	25.925	8.08	n.a.	BMB*
2	9.74	n.a.	101.400	25.919	8.07	n.a.	BMB*
3	11.72	n.a.	423.781	135.344	42.16	n.a.	BMB*
4	15.75	n.a.	266.098	133.826	41.69	n.a.	BMB*
Total:			902.886	321.013	100.00	0.000	

21a, table4

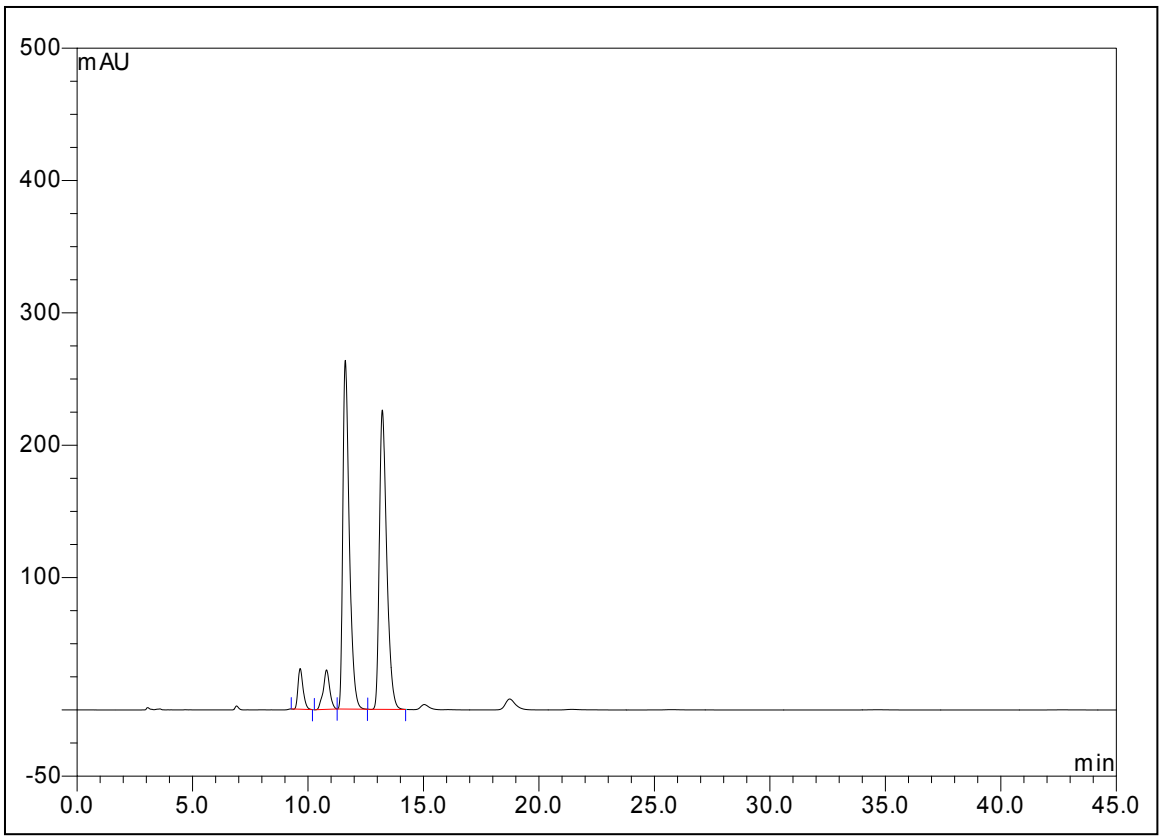
Sample Name:	**21a**	*Injection Volume:*	**20.0**
Vial Number:	**RA4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 45min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**45.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.93	n.a.	483.729	150.937	36.08	n.a.	BMB*
2	16.11	n.a.	493.425	267.430	63.92	n.a.	BMB*
Total:			977.154	418.366	100.00	0.000	

22a/22b
rac.

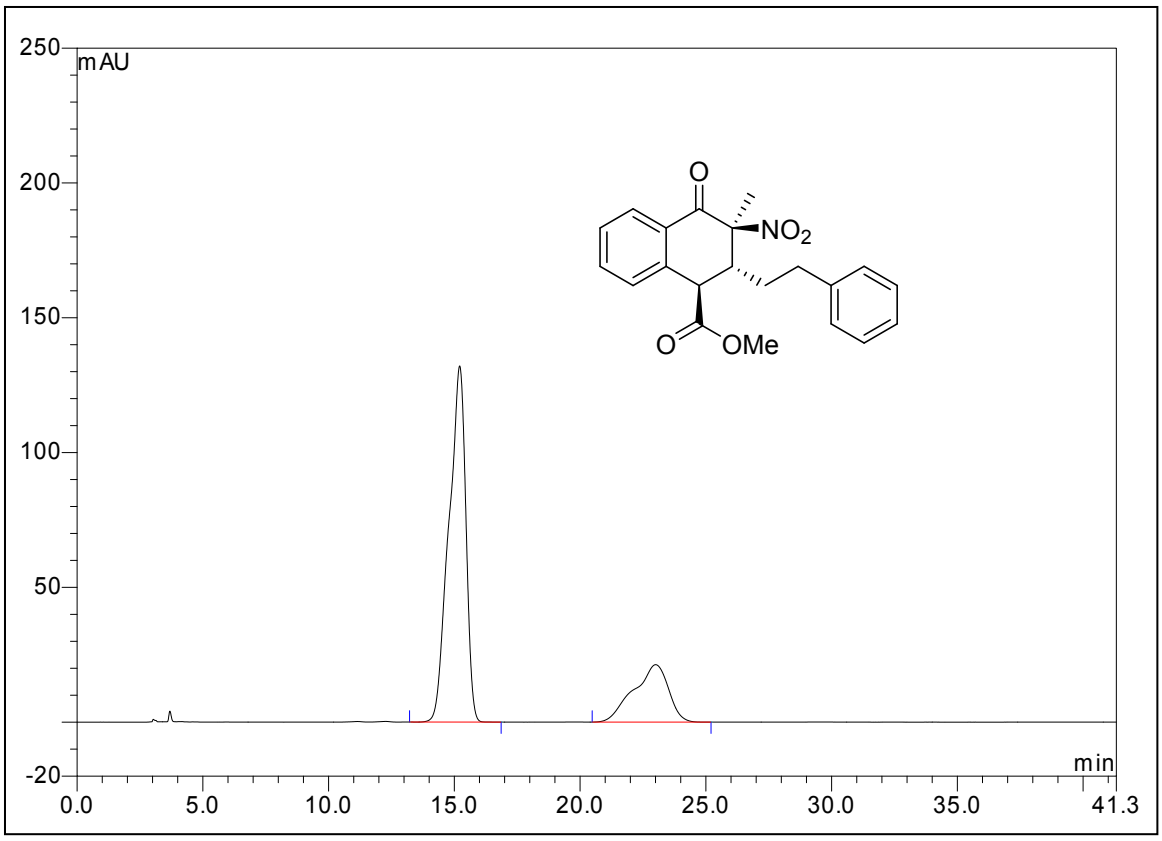
Sample Name:	**fmm1169**	*Injection Volume:*	**20.0**
Vial Number:	**RB8**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 45min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**45.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.66	n.a.	30.767	7.823	4.19	n.a.	BMB*
2	10.80	n.a.	29.790	9.674	5.18	n.a.	BMb*
3	11.61	n.a.	263.446	85.336	45.69	n.a.	bMB*
4	13.22	n.a.	226.144	83.922	44.94	n.a.	BMB*
Total:			550.147	186.755	100.00	0.000	

22a, table 4

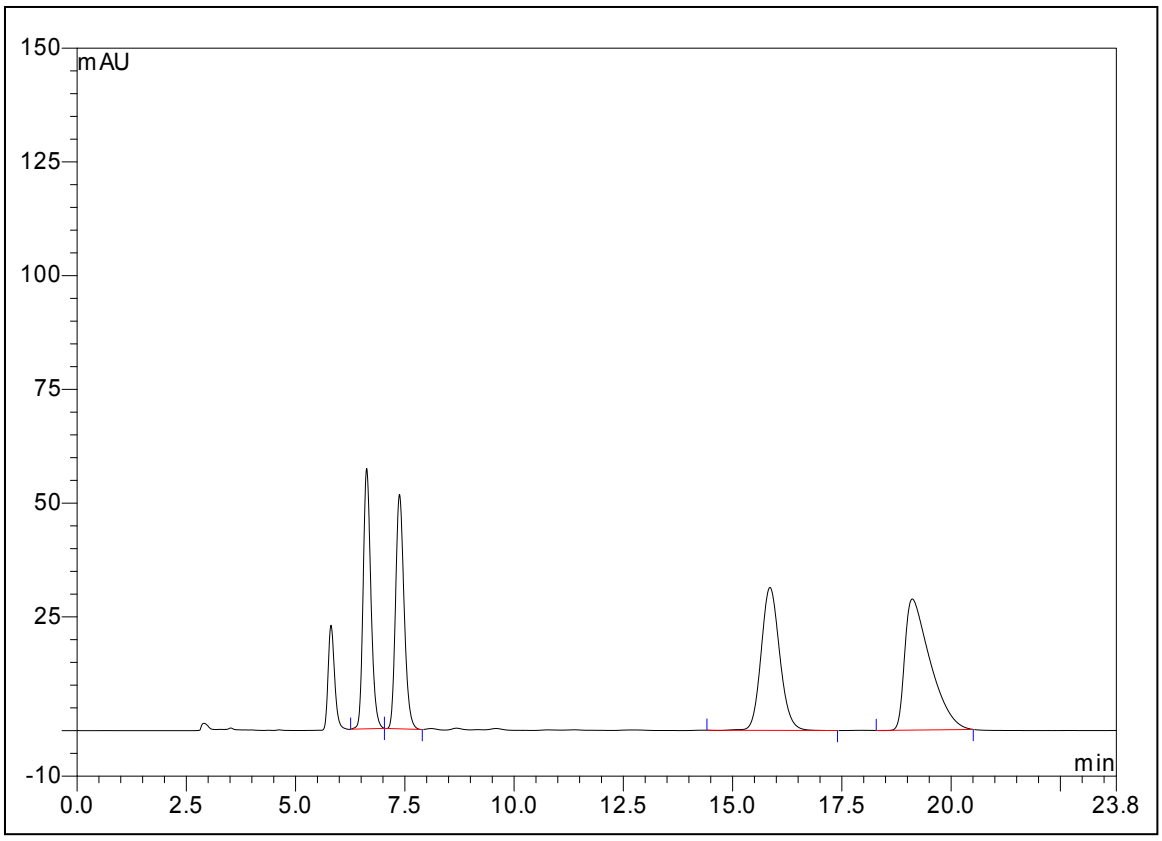
Sample Name:	**22a**	*Injection Volume:*	**20.0**
Vial Number:	**RA2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin45min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**41.32**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	15.21	n.a.	132.090	103.634	75.20	n.a.	BMB*
2	23.00	n.a.	21.297	34.181	24.80	n.a.	BMB*
Total:			153.387	137.815	100.00	0.000	

23a/23b, rac.

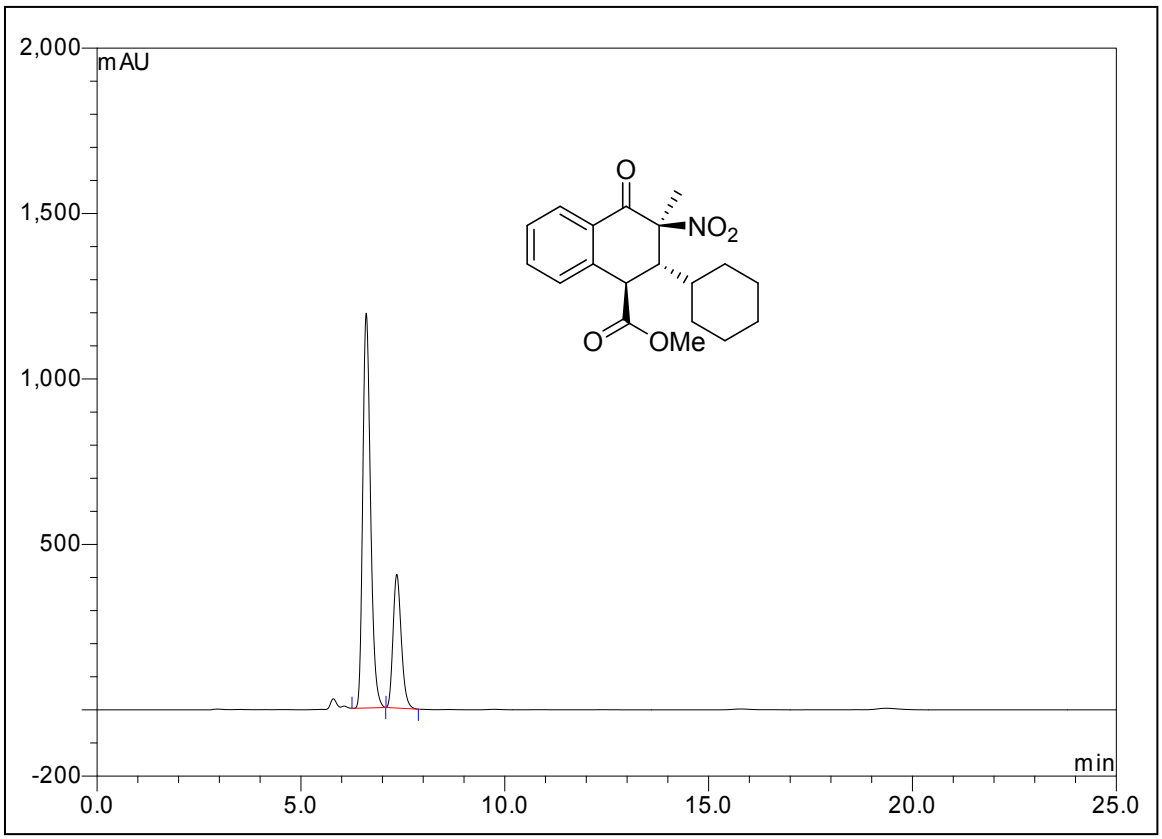
Sample Name:	**23a/23b**	*Injection Volume:*	**20.0**
Vial Number:	**RC1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**90H10IPA1mlmin 120min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**23.78**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.63	n.a.	57.215	11.763	20.17	n.a.	BMb*
2	7.38	n.a.	51.525	11.665	20.00	n.a.	bMB*
3	15.85	n.a.	31.426	15.469	26.52	n.a.	BMB*
4	19.11	n.a.	28.827	19.429	33.31	n.a.	BMB*
Total:			168.992	58.327	100.00	0.000	

23a, table 4

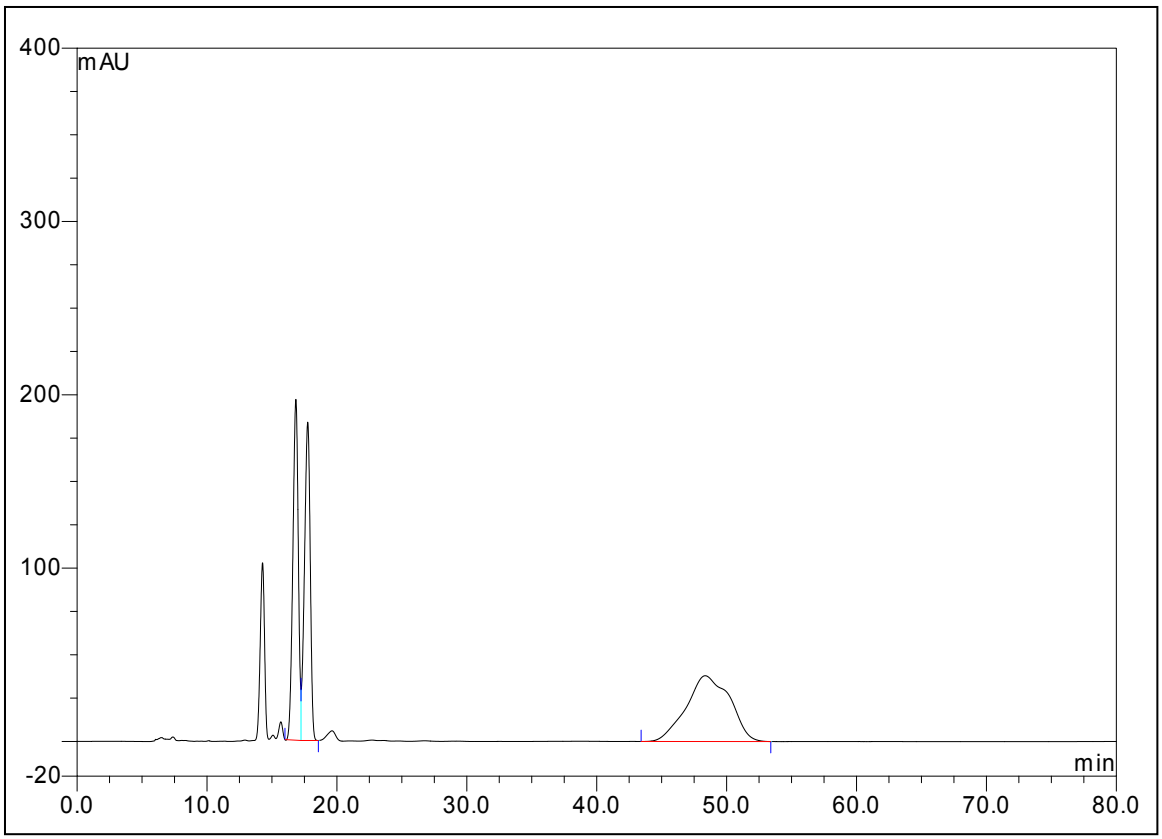
Sample Name:	**23a**	*Injection Volume:*	**20.0**
Vial Number:	**RD4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**90H10IPA1mlmin 25min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**25.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.60	n.a.	1192.963	263.725	73.53	n.a.	BMB*
2	7.35	n.a.	404.137	94.917	26.47	n.a.	BMB*
Total:			1597.100	358.643	100.00	0.000	

24a/24b, rac.

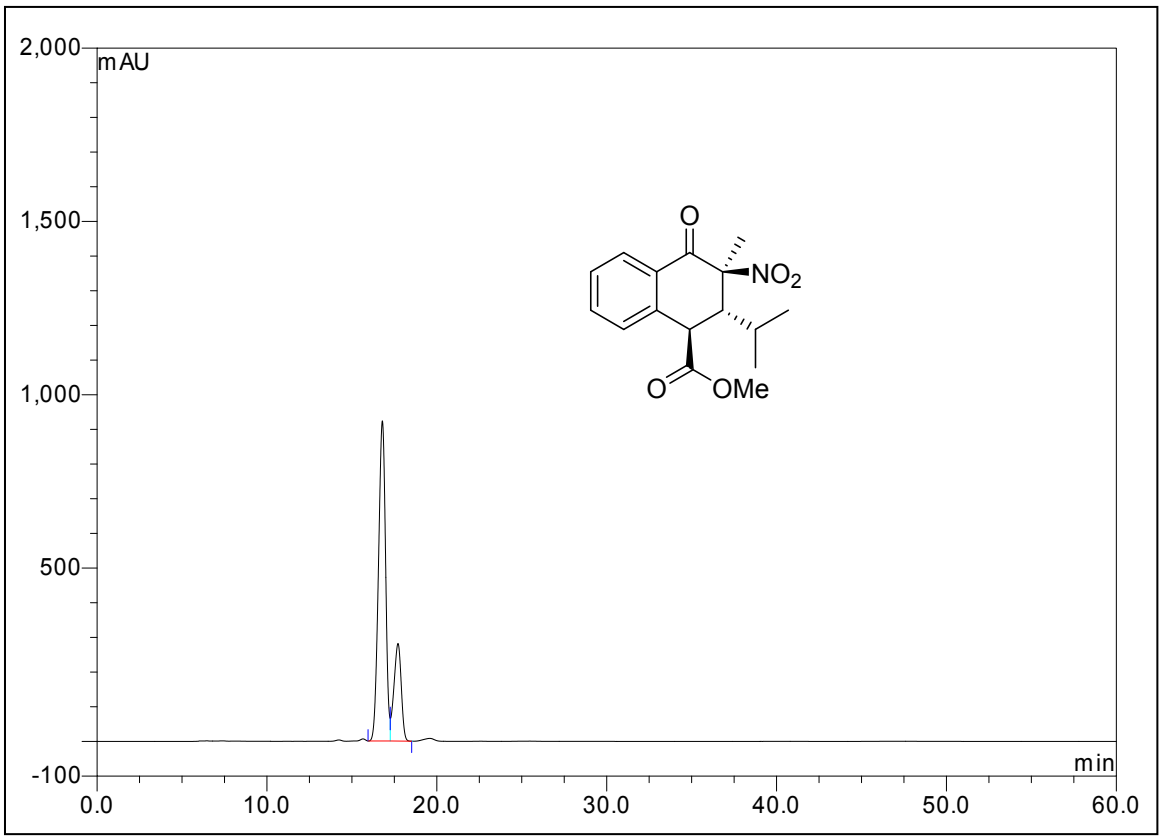
Sample Name:	**24a/24b**	*Injection Volume:*	**20.0**
Vial Number:	**RC2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA05mlmin 80min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**80.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.84	n.a.	196.645	95.340	28.21	n.a.	BM *
2	17.75	n.a.	183.646	94.762	28.04	n.a.	MB*
3	48.35	n.a.	37.955	147.862	43.75	n.a.	BMB*
Total:			418.246	337.965	100.00	0.000	

24a, table 4

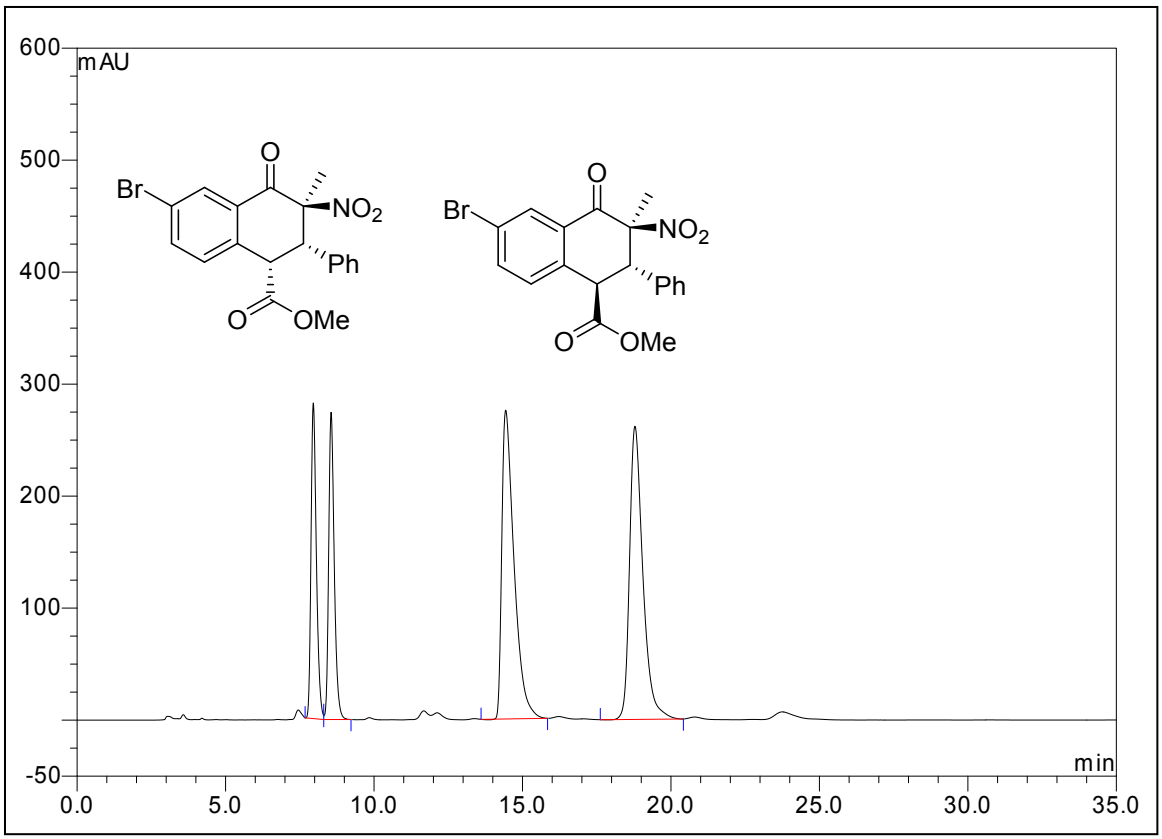
Sample Name:	**24a**	*Injection Volume:*	**20.0**
Vial Number:	**RE1**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA05mlmin 60min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**60.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.79	n.a.	923.543	447.627	76.01	n.a.	BM *
2	17.71	n.a.	281.605	141.256	23.99	n.a.	MB*
Total:			1205.148	588.883	100.00	0.000	

26a/26b, rac.

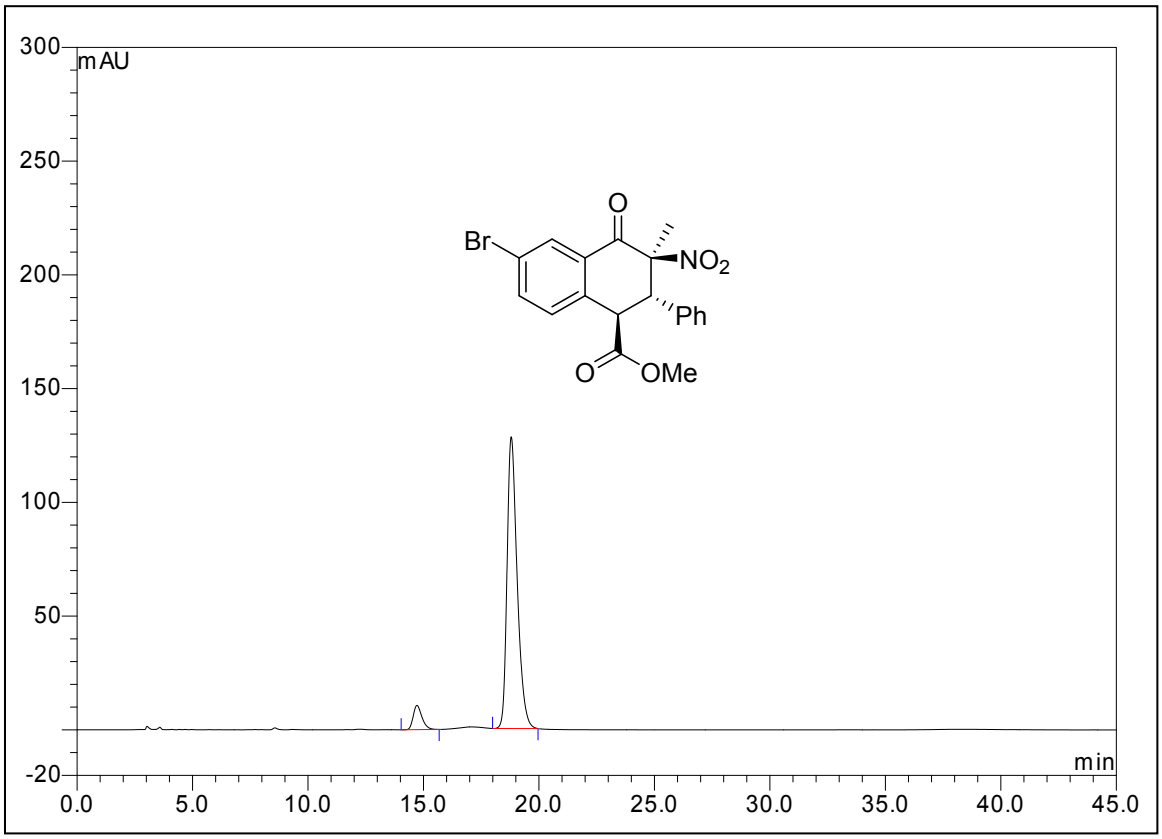
Sample Name:	**26a/26b**	*Injection Volume:*	**20.0**
Vial Number:	**RA3**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 45min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**45.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.95	n.a.	281.782	58.830	15.24	n.a.	BM *
2	8.55	n.a.	274.292	59.756	15.48	n.a.	MB*
3	14.43	n.a.	275.798	131.624	34.09	n.a.	BMB*
4	18.79	n.a.	261.788	135.866	35.19	n.a.	BMB*
Total:			1093.660	386.075	100.00	0.000	

26a, Scheme. 3

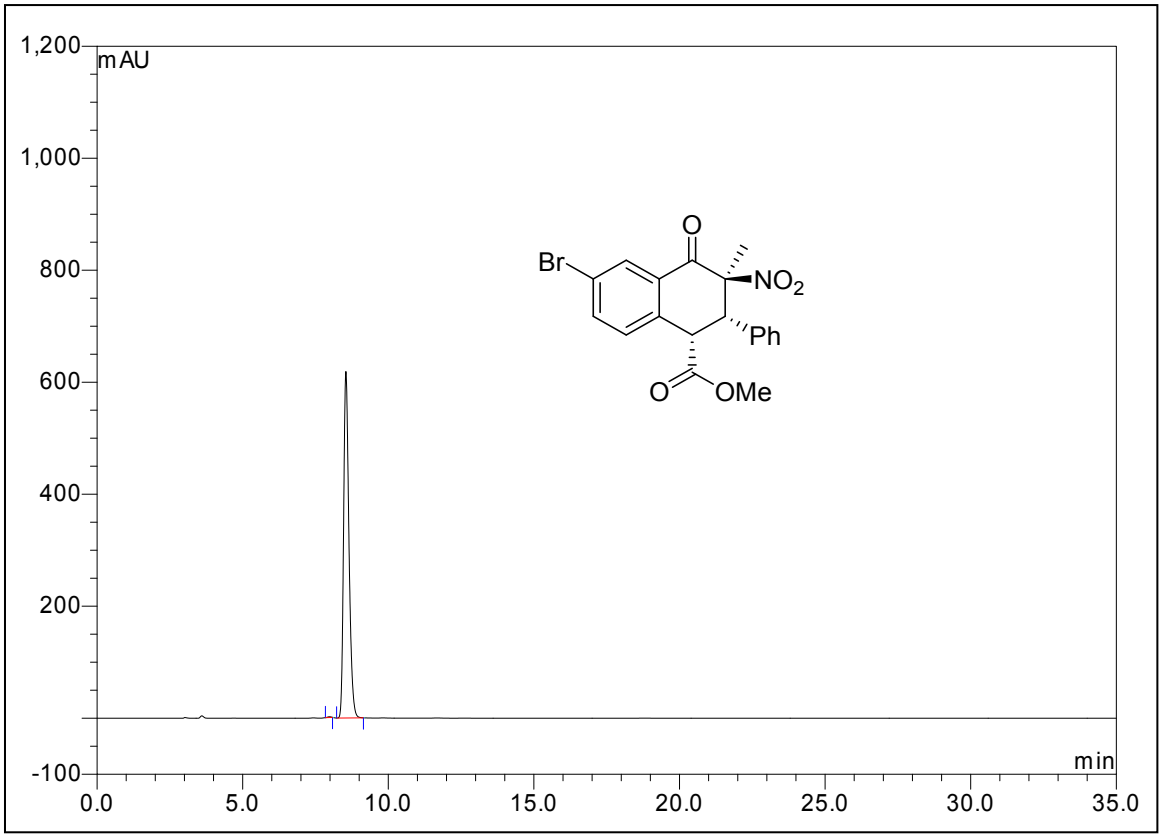
Sample Name:	**26a**	*Injection Volume:*	**20.0**
Vial Number:	**RB8**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 45min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**45.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	14.72	n.a.	10.650	4.677	6.71	n.a.	BMB*
2	18.80	n.a.	128.254	65.026	93.29	n.a.	BMB*
Total:			138.904	69.703	100.00	0.000	

26b, Scheme. 3

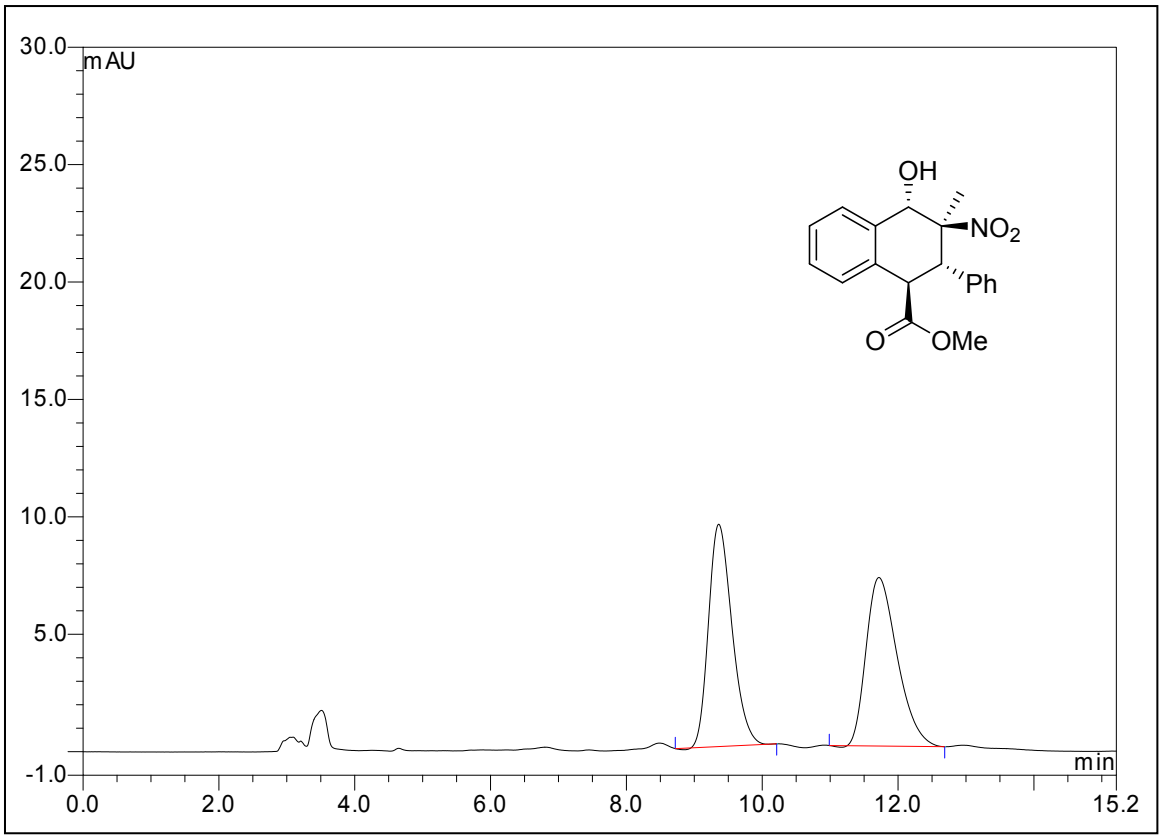
Sample Name:	**26b**	*Injection Volume:*	**20.0**
Vial Number:	**RC4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**95H5IPA1mlmin 45min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**45.00**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.98	n.a.	1.314	0.186	0.14	n.a.	BMB*
2	8.55	n.a.	618.750	131.494	99.86	n.a.	BMB*
Total:			620.063	131.680	100.00	0.000	

27a/27b

Sample Name:	**27a/27b**	*Injection Volume:*	**20.0**
Vial Number:	**RB2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**90H10IPA1mlmin 160min**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:		*Sample Weight:*	**1.0000**
Run Time (min):	**15.21**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.36	n.a.	9.467	3.781	49.83	n.a.	BMB*
2	11.72	n.a.	7.177	3.806	50.17	n.a.	BMB*
Total:			16.644	7.587	100.00	0.000	

Table 1. Crystal data and structure refinement for *cis*-26b.

Identification code	shelxl	
Empirical formula	$C_{3.45} H_{2.91} Br_{0.18} N_{0.18} O_{0.91}$	
Formula weight	76.04	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.415(2) Å	α= 90°.
	b = 11.469(2) Å	β= 90°.
	c = 15.047(3) Å	γ = 90°.
Volume	1797.4(6) $Å^3$	
Z	22	
Density (calculated)	1.546 Mg/m^3	
Absorption coefficient	2.317 mm^{-1}	
F(000)	848	
Crystal size	1.50 x 0.80 x 0.4 mm^3	
Theta range for data collection	2.23 to 25.00°.	
Index ranges	-12<=h<=12, -8<=k<=13, -17<=l<=13	
Reflections collected	7478	
Independent reflections	3106 [R(int) = 0.0693]	
Completeness to theta = 25.00°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.5272	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3106 / 0 / 237	
Goodness-of-fit on F^2	0.885	
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.1096	

R indices (all data)	R1 = 0.0448, wR2 = 0.1249
Absolute structure parameter	0.035(14)
Largest diff. peak and hole	0.490 and -0.687 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for *cis*-26b.

U(eq) is defined as one third of the trace of the orthogonalised U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-231(1)	6534(1)	1121(1)	34(1)
O(4)	2819(3)	9945(3)	-210(2)	22(1)
N(1)	2150(4)	12040(3)	1189(3)	21(1)
O(5)	4822(3)	10918(3)	3584(2)	24(1)
C(19)	4054(5)	11995(4)	236(3)	24(1)
C(15)	2787(4)	10164(4)	577(3)	17(1)
C(18)	2225(4)	9358(4)	1245(3)	16(1)
O(6)	4319(3)	9025(3)	3442(2)	25(1)
O(2)	1094(3)	11712(3)	940(3)	32(1)
C(6)	3275(4)	10493(4)	2504(3)	15(1)
C(5)	1467(4)	8443(4)	930(3)	21(1)
C(13)	5434(4)	9255(4)	1437(3)	19(1)
C(1)	815(4)	7763(4)	1543(3)	24(1)
C(4)	2381(4)	9558(4)	2152(3)	17(1)
C(7)	4126(4)	11099(4)	1789(3)	17(1)
C(3)	1688(4)	8865(4)	2746(3)	21(1)
C(9)	6508(5)	11090(4)	1571(4)	29(1)
C(17)	4171(4)	10037(4)	3229(3)	16(1)
C(2)	890(5)	7985(4)	2443(3)	24(1)
C(12)	6607(5)	8717(4)	1288(3)	25(1)
C(8)	5382(4)	10454(4)	1589(3)	17(1)
O(1)	2337(4)	12937(3)	1605(3)	39(1)

C(14)	3328(4)	11307(4)	936(3)	18(1)
C(16)	5826(6)	10597(5)	4200(4)	38(1)
C(10)	7680(5)	10544(5)	1425(5)	41(2)
C(11)	7733(5)	9350(5)	1289(4)	28(1)

Table 3. Bond lengths [Å] and angles [°] for *cis*-26b.

Br(1)-C(1)	1.891(5)
O(4)-C(15)	1.210(6)
N(1)-O(2)	1.220(5)
N(1)-O(1)	1.219(5)
N(1)-C(14)	1.536(5)
O(5)-C(17)	1.329(6)
O(5)-C(16)	1.445(6)
C(19)-C(14)	1.517(6)
C(15)-C(18)	1.486(6)
C(15)-C(14)	1.526(6)
C(18)-C(4)	1.394(7)
C(18)-C(5)	1.396(6)
O(6)-C(17)	1.214(6)
C(6)-C(4)	1.516(6)
C(6)-C(17)	1.527(6)
C(6)-C(7)	1.558(6)
C(5)-C(1)	1.385(7)
C(13)-C(12)	1.387(6)
C(13)-C(8)	1.395(6)
C(1)-C(2)	1.381(7)
C(4)-C(3)	1.397(7)
C(7)-C(8)	1.532(6)
C(7)-C(14)	1.548(6)
C(3)-C(2)	1.385(7)

C(9)-C(10)	1.390(7)
C(9)-C(8)	1.381(7)
C(12)-C(11)	1.380(7)
C(10)-C(11)	1.386(7)
O(2)-N(1)-O(1)	124.2(4)
O(2)-N(1)-C(14)	118.3(3)
O(1)-N(1)-C(14)	117.5(4)
C(17)-O(5)-C(16)	115.7(4)
O(4)-C(15)-C(18)	122.9(4)
O(4)-C(15)-C(14)	121.0(4)
C(18)-C(15)-C(14)	116.1(4)
C(4)-C(18)-C(5)	121.4(4)
C(4)-C(18)-C(15)	121.0(4)
C(5)-C(18)-C(15)	117.4(4)
C(4)-C(6)-C(17)	112.5(4)
C(4)-C(6)-C(7)	115.1(4)
C(17)-C(6)-C(7)	107.4(4)
C(1)-C(5)-C(18)	118.4(4)
C(12)-C(13)-C(8)	120.0(4)
C(2)-C(1)-C(5)	121.4(5)
C(2)-C(1)-Br(1)	119.9(4)
C(5)-C(1)-Br(1)	118.6(4)
C(18)-C(4)-C(3)	118.2(4)
C(18)-C(4)-C(6)	122.0(4)
C(3)-C(4)-C(6)	119.8(4)
C(8)-C(7)-C(14)	111.8(4)
C(8)-C(7)-C(6)	113.9(4)
C(14)-C(7)-C(6)	109.6(3)
C(4)-C(3)-C(2)	121.0(4)
C(10)-C(9)-C(8)	120.7(4)

O(6)-C(17)-O(5)	123.7(4)
O(6)-C(17)-C(6)	126.4(4)
O(5)-C(17)-C(6)	109.8(4)
C(1)-C(2)-C(3)	119.4(4)
C(13)-C(12)-C(11)	121.0(4)
C(13)-C(8)-C(9)	119.0(4)
C(13)-C(8)-C(7)	122.8(4)
C(9)-C(8)-C(7)	118.2(4)
C(15)-C(14)-C(19)	112.6(4)
C(15)-C(14)-N(1)	105.3(3)
C(19)-C(14)-N(1)	106.5(4)
C(15)-C(14)-C(7)	111.1(4)
C(19)-C(14)-C(7)	112.8(4)
N(1)-C(14)-C(7)	108.0(4)
C(9)-C(10)-C(11)	120.3(5)
C(10)-C(11)-C(12)	119.1(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *cis*-26b.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	35(1)	23(1)	44(1)	-7(1)	3(1)	-16(1)
O(4)	28(2)	19(2)	18(2)	-3(1)	0(1)	0(1)
N(1)	28(2)	17(2)	20(2)	2(2)	-5(2)	8(2)
O(5)	27(2)	20(2)	25(2)	-2(1)	-11(1)	-1(1)
C(19)	33(3)	16(2)	22(2)	4(2)	1(2)	-6(2)
C(15)	16(2)	14(2)	21(2)	2(2)	0(2)	4(2)
C(18)	15(2)	9(2)	22(2)	2(2)	1(2)	2(2)
O(6)	31(2)	17(2)	26(2)	6(1)	-2(1)	4(1)
O(2)	27(2)	29(2)	40(2)	-5(2)	-5(2)	9(2)

C(6)	18(2)	11(2)	17(2)	-2(2)	-3(2)	2(2)
C(5)	20(2)	18(2)	23(2)	-2(2)	-2(2)	0(2)
C(13)	18(2)	12(2)	27(2)	-2(2)	-1(2)	-2(2)
C(1)	16(2)	19(2)	36(3)	3(2)	-1(2)	-6(2)
C(4)	16(2)	13(2)	20(2)	1(2)	1(2)	3(2)
C(7)	21(2)	8(2)	21(2)	-1(2)	3(2)	-3(2)
C(3)	22(2)	23(2)	17(2)	1(2)	-4(2)	4(2)
C(9)	27(2)	14(2)	48(3)	-2(2)	9(2)	-3(2)
C(17)	20(2)	18(2)	11(2)	2(2)	0(2)	3(2)
C(2)	23(2)	19(2)	28(3)	10(2)	3(2)	-1(2)
C(12)	30(2)	17(2)	28(3)	-1(2)	3(2)	3(2)
C(8)	17(2)	13(2)	21(2)	2(2)	-3(2)	0(2)
O(1)	44(2)	20(2)	54(2)	-18(2)	-6(2)	11(2)
C(14)	18(2)	11(2)	25(2)	1(2)	1(2)	2(2)
C(16)	40(3)	34(3)	41(3)	-5(2)	-25(3)	2(3)
C(10)	18(2)	24(3)	81(5)	-1(3)	10(3)	-3(2)
C(11)	21(2)	26(2)	37(3)	-1(2)	6(2)	11(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *cis*-372.

	x	y	z	U(eq)
H(19A)	4751	11533	12	36
H(19B)	4386	12697	496	36
H(19C)	3483	12190	-242	36
H(6)	2738	11098	2774	18
H(5)	1401	8294	325	25
H(13)	4683	8817	1434	23
H(7)	4360	11867	2023	20
H(3)	1763	8997	3353	25
H(9)	6481	11893	1657	35

H(2A)	408	7547	2843	28
H(12)	6634	7917	1186	30
H(16A)	5469	10130	4669	57
H(16B)	6202	11288	4448	57
H(16C)	6473	10158	3893	57
H(10)	8432	10981	1419	49
H(11)	8518	8980	1200	34

Table 6. Torsion angles [°] for *cis*-26b.

O(4)-C(15)-C(18)-C(4)	170.1(4)
C(14)-C(15)-C(18)-C(4)	-10.2(6)
O(4)-C(15)-C(18)-C(5)	-14.1(6)
C(14)-C(15)-C(18)-C(5)	165.7(4)
C(4)-C(18)-C(5)-C(1)	3.1(7)
C(15)-C(18)-C(5)-C(1)	-172.7(4)
C(18)-C(5)-C(1)-C(2)	0.9(7)
C(18)-C(5)-C(1)-Br(1)	179.2(3)
C(5)-C(18)-C(4)-C(3)	-4.3(6)
C(15)-C(18)-C(4)-C(3)	171.4(4)
C(5)-C(18)-C(4)-C(6)	175.5(4)
C(15)-C(18)-C(4)-C(6)	-8.8(6)
C(17)-C(6)-C(4)-C(18)	-130.8(4)
C(7)-C(6)-C(4)-C(18)	-7.4(6)
C(17)-C(6)-C(4)-C(3)	49.1(5)
C(7)-C(6)-C(4)-C(3)	172.4(4)
C(4)-C(6)-C(7)-C(8)	-86.0(5)
C(17)-C(6)-C(7)-C(8)	40.1(5)
C(4)-C(6)-C(7)-C(14)	40.0(5)
C(17)-C(6)-C(7)-C(14)	166.1(4)
C(18)-C(4)-C(3)-C(2)	1.5(7)

C(6)-C(4)-C(3)-C(2)	-178.3(4)
C(16)-O(5)-C(17)-O(6)	5.4(7)
C(16)-O(5)-C(17)-C(6)	-172.4(4)
C(4)-C(6)-C(17)-O(6)	9.7(6)
C(7)-C(6)-C(17)-O(6)	-117.9(5)
C(4)-C(6)-C(17)-O(5)	-172.7(4)
C(7)-C(6)-C(17)-O(5)	59.7(4)
C(5)-C(1)-C(2)-C(3)	-3.6(7)
Br(1)-C(1)-C(2)-C(3)	178.2(4)
C(4)-C(3)-C(2)-C(1)	2.3(7)
C(8)-C(13)-C(12)-C(11)	0.1(7)
C(12)-C(13)-C(8)-C(9)	1.4(7)
C(12)-C(13)-C(8)-C(7)	-177.9(4)
C(10)-C(9)-C(8)-C(13)	-1.6(8)
C(10)-C(9)-C(8)-C(7)	177.7(5)
C(14)-C(7)-C(8)-C(13)	-77.8(5)
C(6)-C(7)-C(8)-C(13)	47.1(6)
C(14)-C(7)-C(8)-C(9)	102.9(5)
C(6)-C(7)-C(8)-C(9)	-132.2(5)
O(4)-C(15)-C(14)-C(19)	-8.7(6)
C(18)-C(15)-C(14)-C(19)	171.6(4)
O(4)-C(15)-C(14)-N(1)	107.0(5)
C(18)-C(15)-C(14)-N(1)	-72.7(4)
O(4)-C(15)-C(14)-C(7)	-136.3(4)
C(18)-C(15)-C(14)-C(7)	43.9(5)
O(2)-N(1)-C(14)-C(15)	-11.8(5)
O(1)-N(1)-C(14)-C(15)	170.4(4)
O(2)-N(1)-C(14)-C(19)	108.0(5)
O(1)-N(1)-C(14)-C(19)	-69.8(5)
O(2)-N(1)-C(14)-C(7)	-130.5(4)

O(1)-N(1)-C(14)-C(7)	51.6(5)
C(8)-C(7)-C(14)-C(15)	69.6(4)
C(6)-C(7)-C(14)-C(15)	-57.7(5)
C(8)-C(7)-C(14)-C(19)	-58.0(5)
C(6)-C(7)-C(14)-C(19)	174.7(4)
C(8)-C(7)-C(14)-N(1)	-175.5(3)
C(6)-C(7)-C(14)-N(1)	57.2(4)
C(8)-C(9)-C(10)-C(11)	0.5(10)
C(9)-C(10)-C(11)-C(12)	0.9(9)
C(13)-C(12)-C(11)-C(10)	-1.2(8)

Symmetry transformations used to generate equivalent atoms: