

Expanding the scope of primary amine catalysis:

Stereoselective synthesis of indanedione-fused

2,6-disubstituted *trans*-spirocyclohexanones

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Das[§] and Wenwei Lin^{*,§}

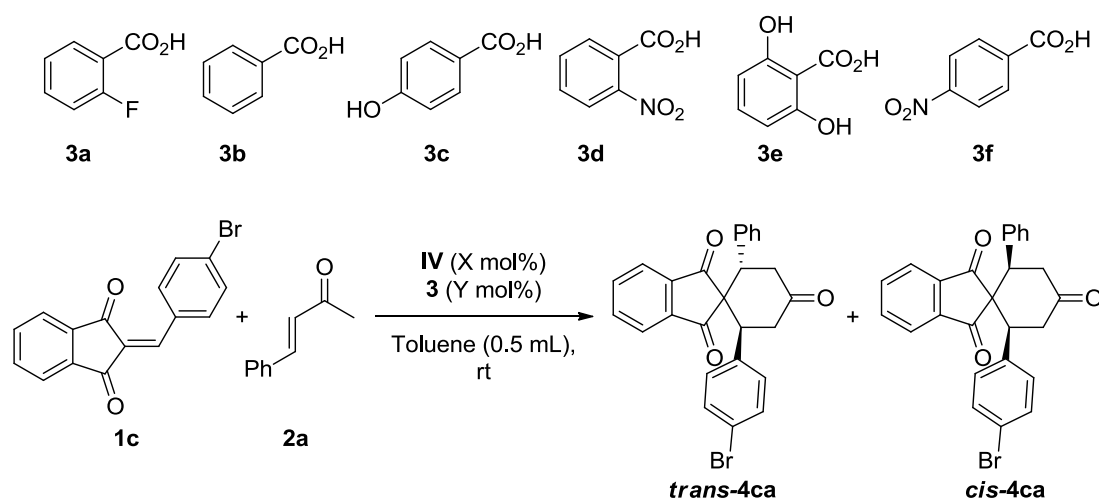
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1. Optimization of additional reaction parameters:

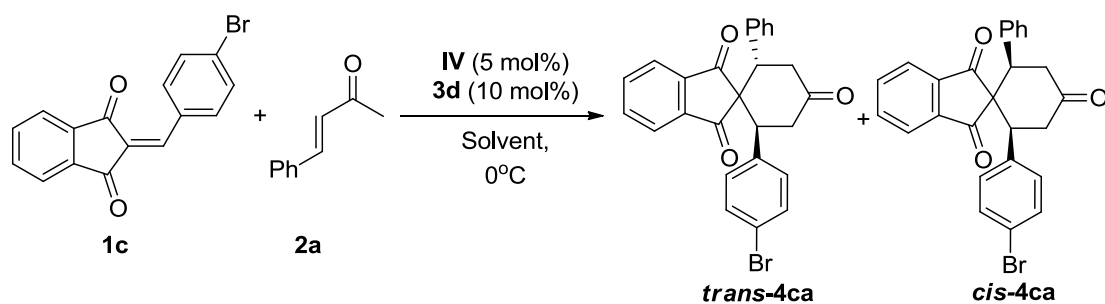
Table S1 : Screening of additives, loadings and dilutions:^a



Entry	Additive	X / Y	Time (d)	Yield (%) ^[b]	dr ^[b]	ee (%) ^[c]
1	None	10/-	3	50	1.7:1	99/49
2	3a	10/10	1	97	3.6:1	99/85
3	3a	20/10	1	98	1.7:1	99/56
4	3a	5/10	1	99	3.3:1	98/86
5	3a	10/20	1	96	3.6:1	98/87
6	3a	10/5	5	92	1:1.1	98/39
7	3b	5/10	1.5	97	2.7:1	98/85
8	3c	5/10	10	65	2.4:1	ND
9	3d	5/10	0.5	99	3:1	98/96
10	3e	5/10	4.5	93	1.3:1	96/99
11	3f	5/10	1	94	3:1	99/97
12 ^[d]	3a	5/10	1.5	94	2.7:1	98/89
13 ^[e]	3a	5/10	0.25	98	3.9:1	98/90
14^[e]	3d	5/10	0.25	94	4.5:1	98/97
15 ^[f]	3d	5/10	0.25	99	1.1:1	98/59
16^[f]	3e	5/10	1	99	1.3:1	97/97

[a] Unless otherwise specified, all the reactions were carried out using **1c** (0.1 mmol), **2a** (1.0 equiv), **3** (Y mol%) and **IV** (X mol%) in toluene (0.5 mL) and stirred at 30 °C. [b] Yield and diastereomeric ratio of **trans/cis 4ca** as determined by ¹H NMR analysis of the crude reaction mixture using Ph₃CH as internal standard. [c] ee of trans/cis as determined by HPLC analysis on a chiral stationary phase. [d] 1 mL of toluene was used. [e] 0.25 mL toluene was used. [f] Reaction carried out at 50 °C (for *cis* isomer)

Table S2 : Finalizing the optimal reaction conditions^a:

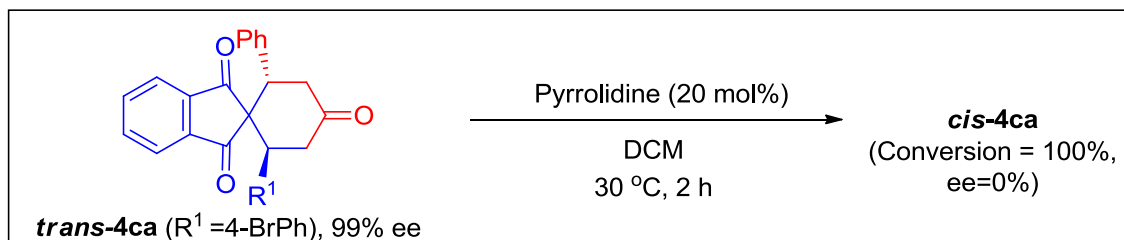


Entry	Solvent	Time (d)	Yield(%) ^b	dr ^b	ee% ^c
1	Toluene	27h	98	7:1	98/97
2 ^d	Toluene	6	54	12:1	ND
3	DCM	4	90	16:1	98/79
4	DCM : Toluene (4 : 1)	2.5	83	8:1	ND
5 ^f	DCM	2	76	11:1	ND
6 ^g	DCM	4	24	>30:1	ND
7 ^e	DCM	4	84	>20:1	ND
8 ^{e,h}	DCM	1.5	88	7:1	ND
9^{e,g,h}	DCM	4	85	>20:1	98/97

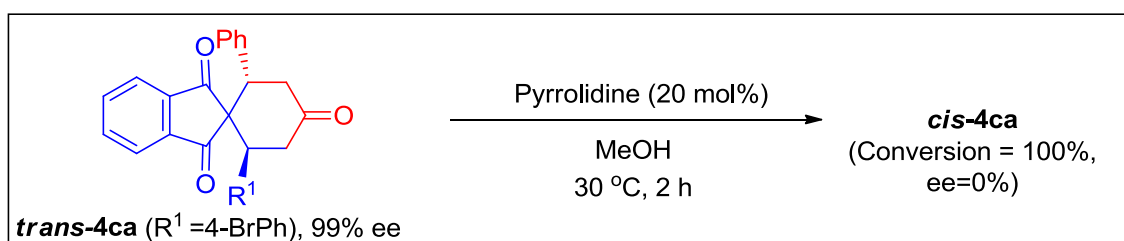
[a] Unless otherwise specified, all the reactions were carried out using **1c** (1.0 equiv), **2a** (0.1 mmol), **3d** (10 mol%) and **IV** (5 mol%) in the solvent (0.25 mL) and stirred at 0 °C. [b] Yield and diastereomeric ratio of **trans/cis 4ca** as determined by ¹H NMR analysis of the crude reaction mixture using Ph₃CH as an internal standard. [c] Determined by HPLC analysis on a chiral stationary phase. [d] Reaction at -20 °C. [e] 1.2 eq of **1a** was used. [f] 10 mol% of **IV** was used. [g] 20 mol% of **3d** was used. [h] Reaction at 10 °C.

2. Segregated control experiments of the scheme 8 of manuscript:

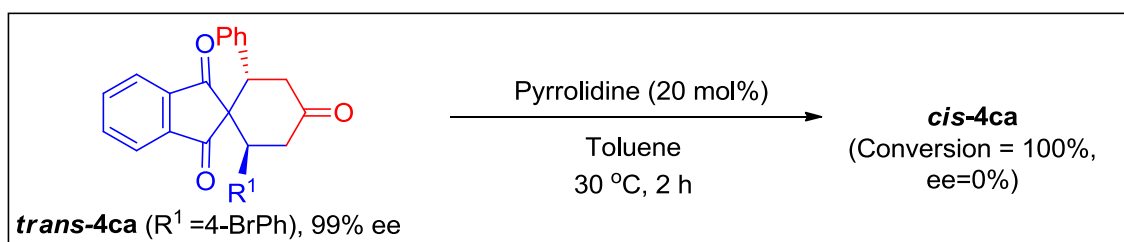
Scheme 8a-1:



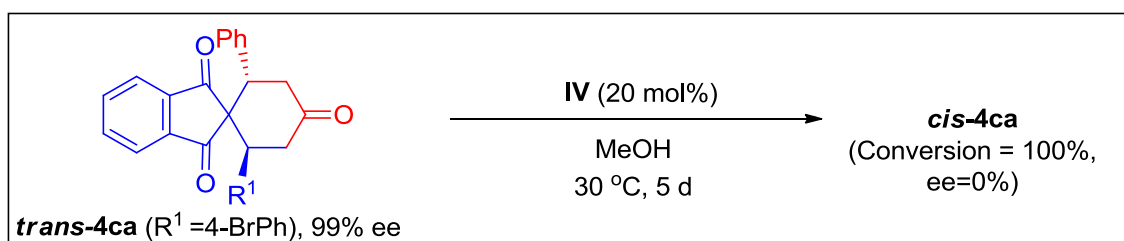
Scheme 8a-2:



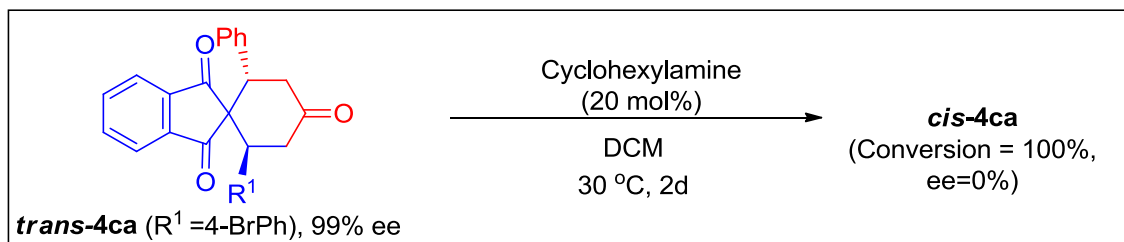
Scheme 8a-3:



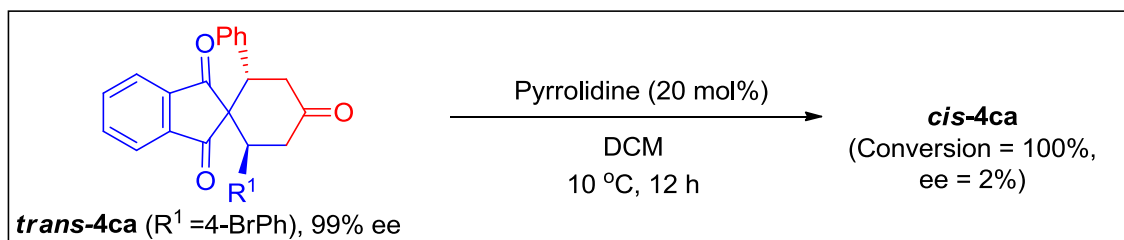
Scheme 8a-4:



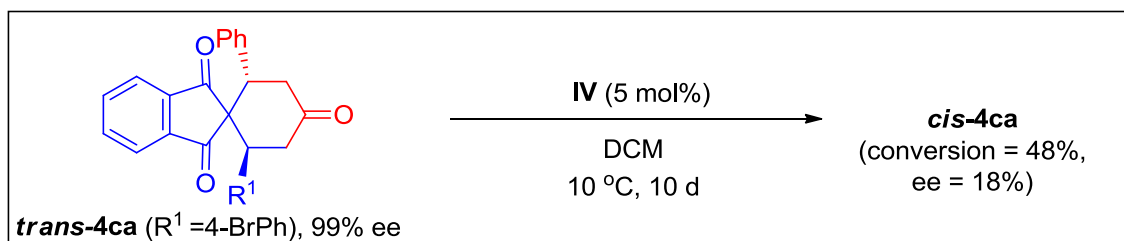
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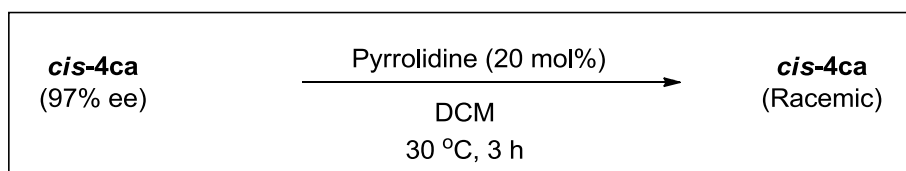
Scheme 8a-6:



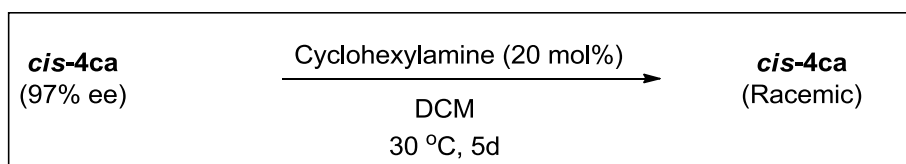
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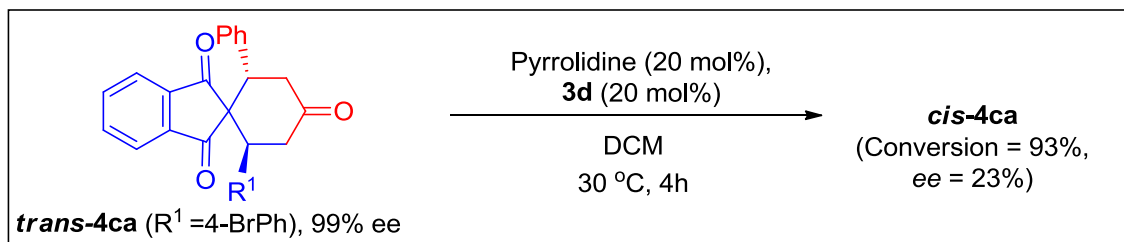
Scheme 8b-1:



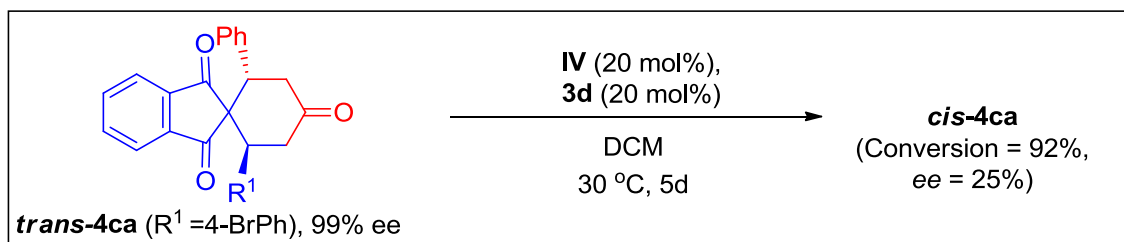
Scheme 8b-2:



Scheme 8c-1:

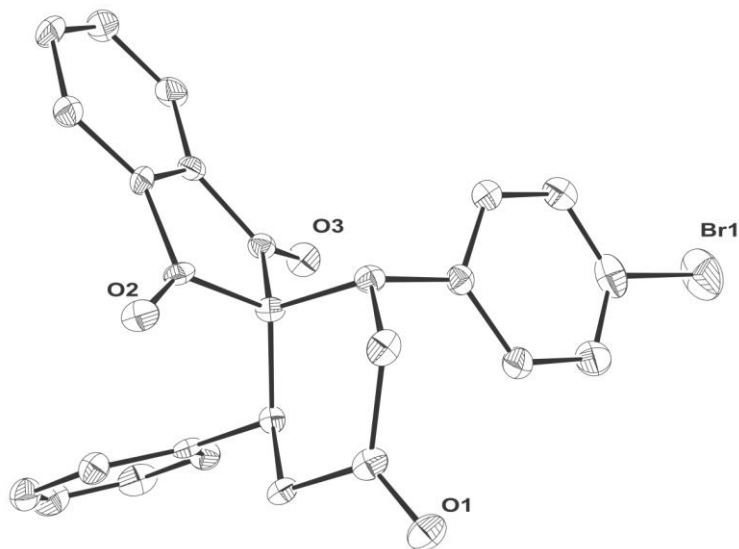


Scheme 8c-2:



3. ORTEP diagrams:

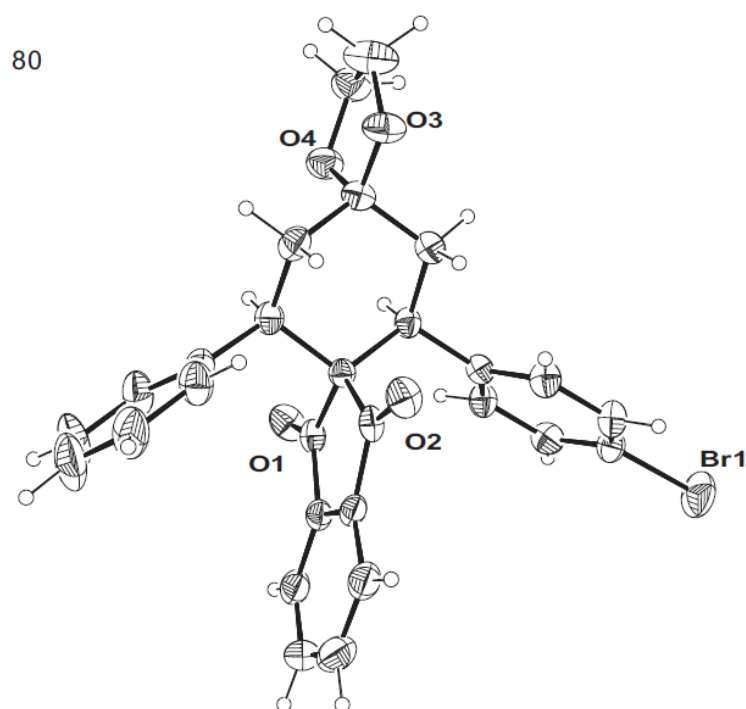
a) ***trans*-4ca** (CCDC: 1021314): The thermal ellipsoid was drawn at 30% probability level.



Empirical formula	C ₂₆ H ₁₉ Br O ₃	
Formula weight	459.32	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 9.121(3) Å	α = 90°.
	b = 10.294(3) Å	β = 90°.
	c = 45.103(12) Å	γ = 90°.
Volume	4235(2) Å ³	
Z	8	
Density (calculated)	1.441 Mg/m ³	
Absorption coefficient	1.966 mm ⁻¹	
F(000)	1872	
Crystal size	0.52 x 0.47 x 0.02 mm ³	
Theta range for data collection	2.28 to 25.05°.	
Index ranges	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, -52 ≤ l ≤ 53	
Reflections collected	28294	
Independent reflections	7416 [R(int) = 0.0701]	
Completeness to theta = 25.05°	99.8 %	
Absorption correction	multi-scan	

Max. and min. transmission	0.9617 and 0.4279
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7416 / 0 / 545
Goodness-of-fit on F^2	1.055
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0515$, $wR2 = 0.1018$
R indices (all data)	$R1 = 0.0999$, $wR2 = 0.1159$
Absolute structure parameter	0.017(10)
Largest diff. peak and hole	0.608 and $-0.657 \text{ e.}\text{\AA}^{-3}$

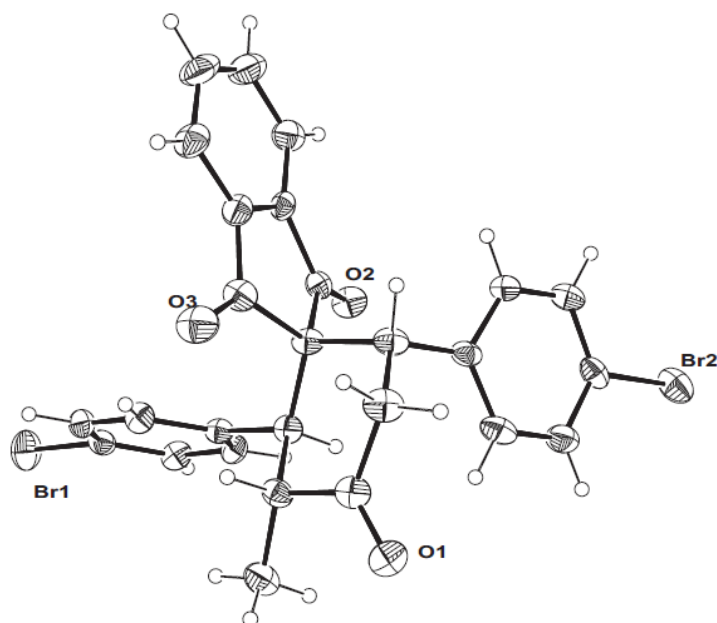
b) **cis-15ca** (CCDC: 1429053) : The thermal ellipsoid was drawn at 30% probability level.



Empirical formula	C ₂₈ H ₂₃ Br O ₄	
Formula weight	503.37	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁	
Unit cell dimensions	$a = 10.1259(2) \text{ Å}$	$\alpha = 90^\circ$.
	$b = 21.6147(4) \text{ Å}$	$\beta = 112.394(2)^\circ$.
	$c = 11.8647(3) \text{ Å}$	$\gamma = 90^\circ$.
Volume	$2400.97(9) \text{ Å}^3$	

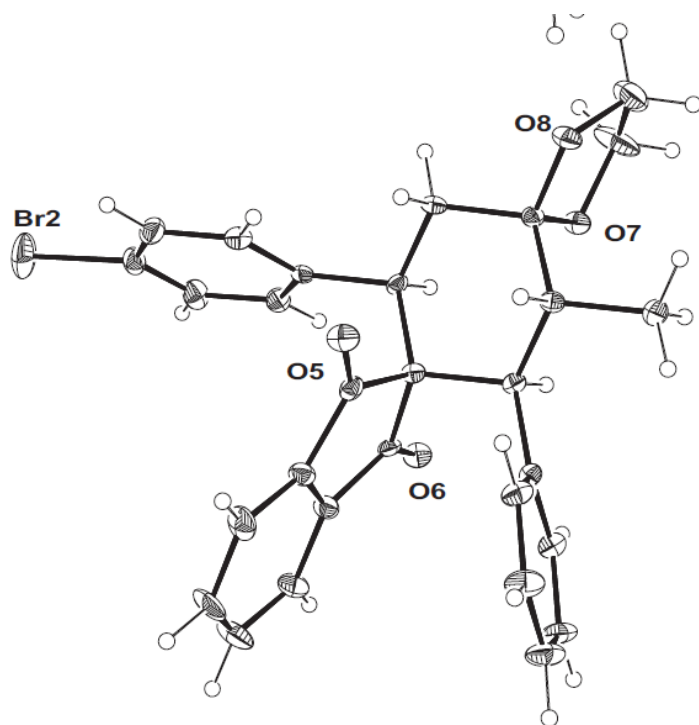
Z	4
Density (calculated)	1.393 Mg/m ³
Absorption coefficient	1.744 mm ⁻¹
F(000)	1032
Crystal size	0.42 x 0.25 x 0.13 mm ³
Theta range for data collection	1.86 to 25.00°.
Index ranges	-12<= <i>h</i> <=11, -25<= <i>k</i> <=25, -12<= <i>l</i> <=14
Reflections collected	16965
Independent reflections	8005 [R(int) = 0.0419]
Completeness to theta = 24.95°	99.4 %
Absorption correction	multi-scan
Max. and min. transmission	0.8051 and 0.5279
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8005 / 1 / 595
Goodness-of-fit on F ²	0.959
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.0780
R indices (all data)	R1 = 0.0832, wR2 = 0.0920
Absolute structure parameter	0.016(7)
Largest diff. peak and hole	0.269 and -0.264 e.Å ⁻³

(c) ***trans*-5cca** (CCDC: 1402038) : The thermal ellipsoid was drawn at 30% probability level.



Empirical formula	C27 H20 Br2 O3	
Formula weight	552.25	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P 1	
Unit cell dimensions	a = 8.1158(3) Å	$\alpha = 95.530(3)^\circ$.
	b = 8.6369(3) Å	$\beta = 104.286(3)^\circ$.
	c = 9.1898(4) Å	$\gamma = 108.675(3)^\circ$.
Volume	580.48(4) Å ³	
Z	1	
Density (calculated)	1.580 Mg/m ³	
Absorption coefficient	3.518 mm ⁻¹	
F(000)	276	
Crystal size	0.36 x 0.07 x 0.02 mm ³	
Theta range for data collection	2.33 to 25.01°.	
Index ranges	-9 ≤ h ≤ 9, -10 ≤ k ≤ 10, -10 ≤ l ≤ 10	
Reflections collected	5000	
Independent reflections	3414 [R(int) = 0.0215]	
Completeness to theta = 25.01°	99.1 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9330 and 0.3640	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3414 / 3 / 289	
Goodness-of-fit on F ²	0.861	
Final R indices [I > 2σ(I)]	R1 = 0.0302, wR2 = 0.0561	
R indices (all data)	R1 = 0.0435, wR2 = 0.0597	
Absolute structure parameter	0.013(6)	
Largest diff. peak and hole	0.445 and -0.305 e.Å ⁻³	

(d) **cis-16aca** (CCDC: 1431465) : The thermal ellipsoid was drawn at 30% probability level.



Empirical formula	C ₂₉ H ₂₅ Br O ₄	
Formula weight	517.40	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P 1	
Unit cell dimensions	a = 8.444 Å	α = 98.62°.
	b = 11.055 Å	β = 107.12°.
	c = 13.733 Å	γ = 93.00°.
Volume	1204.9 Å ³	
Z	2	
Density (calculated)	1.426 Mg/m ³	
Absorption coefficient	1.739 mm ⁻¹	
F(000)	532	
Crystal size	0.79 x 0.75 x 0.57 mm ³	
Theta range for data collection	1.58 to 25.17°.	
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 12, -16 ≤ l ≤ 16	
Reflections collected	10163	
Independent reflections	6442 [R(int) = 0.0374]	

Completeness to theta = 25.17°	98.8 %
Absorption correction	multi-scan
Max. and min. transmission	0.4372 and 0.3403
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6442 / 54 / 613
Goodness-of-fit on F ²	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0904
R indices (all data)	R1 = 0.0487, wR2 = 0.1143
Absolute structure parameter	0.058(9)
Largest diff. peak and hole	0.446 and -0.638 e.Å ⁻³

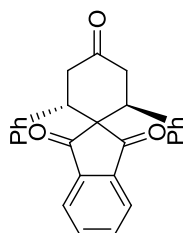
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PROCNO 1

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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
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FIDRES 0.220079 Hz
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RG 71.42
DW 69.333 usec
DE 10.52 usec
TE 297.6 K
D1 2.00000000 sec
TD0 1

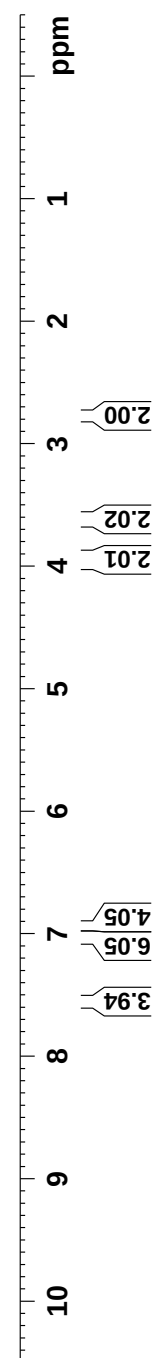
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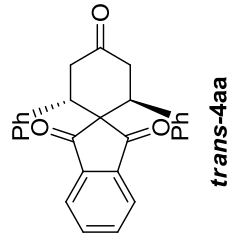


trans-4aa

S13



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202.88



142.13
137.32
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128.21
127.39
122.48

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77.00
76.69
61.67
43.54
41.64

Current Data Parameters
NAME Chris-120
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters

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DS 0
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FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
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TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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PLW1 46.00000000 W

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NUC2 1H
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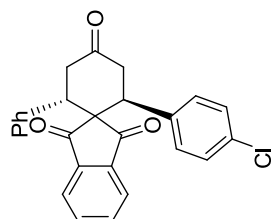
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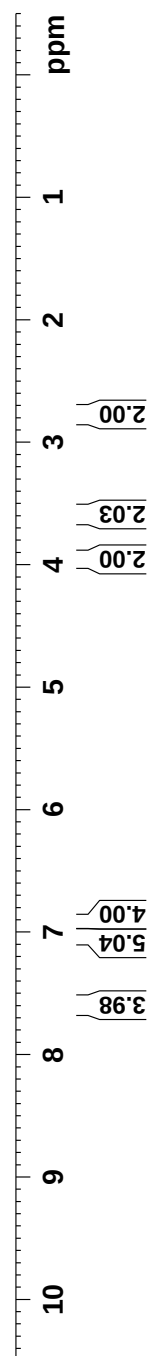
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RG 114
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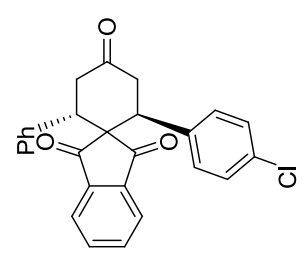
trans-4ba



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202.56

141.98
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128.32
128.23
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41.59
41.56



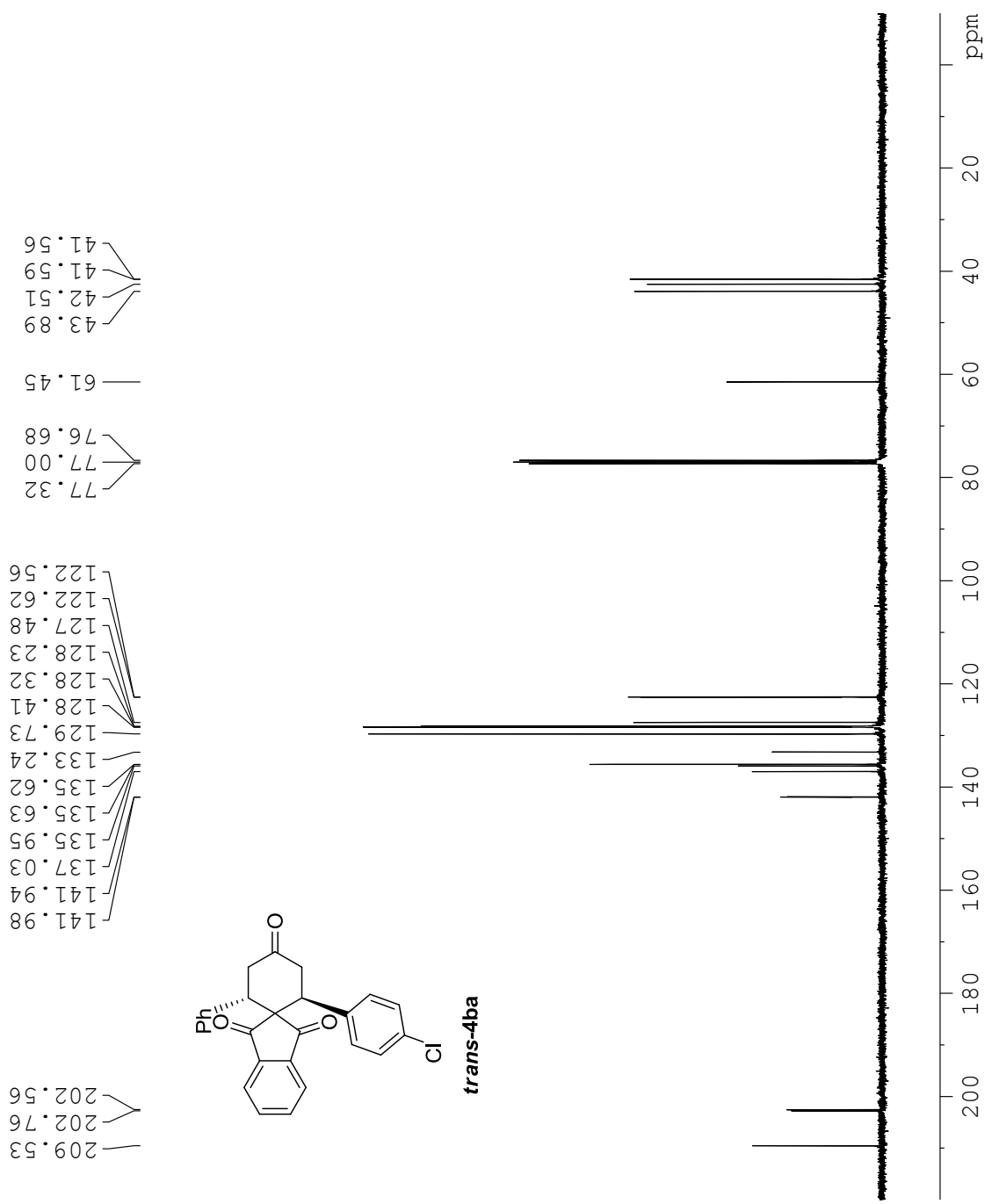
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TE         295.7 K
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SFO1       100.6233325 MHz

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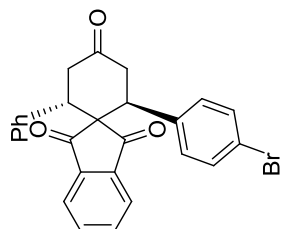


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 PROCNO 1

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 PULPROG zg30
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 FIDRES 0.220079 Hz
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 D1 2.00000000 sec
 TD0 1

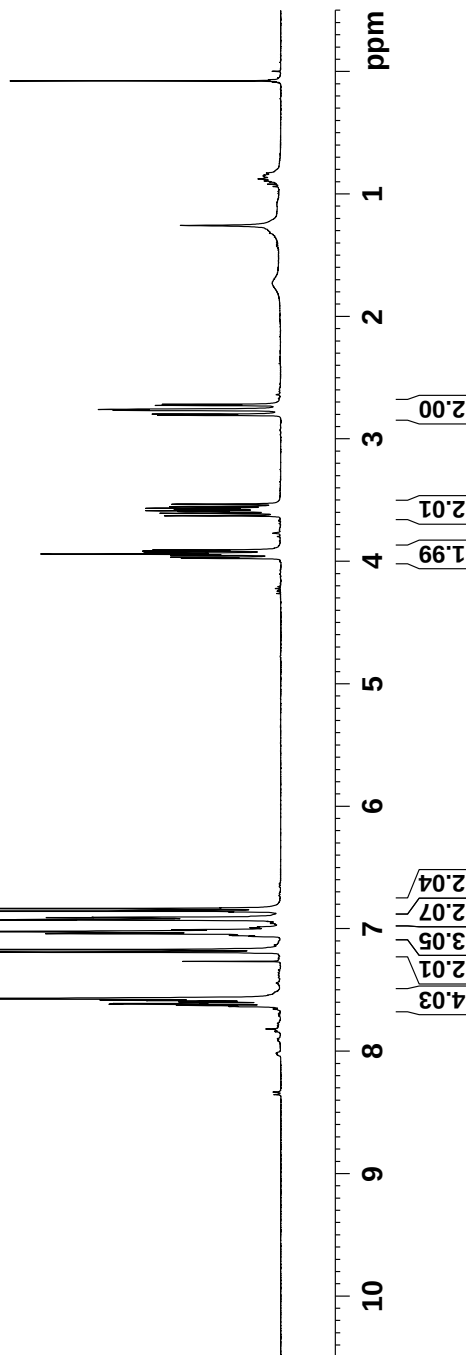
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trans-4ca

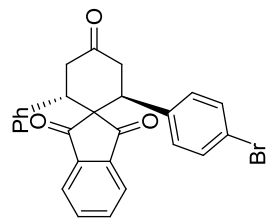
S17



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202.49

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135.63
135.61
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128.33
128.23
127.49
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122.57
121.43

77.32
77.00
76.68
61.40
43.97
42.56
41.57
41.56



trans-4ca

Current Data Parameters
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EXPNO 5
PROCNO 1

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PULPROG zgpg30
TD 32768
SOLVENT CDC13
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DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
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NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

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NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
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LB 2.00 Hz
GB 0
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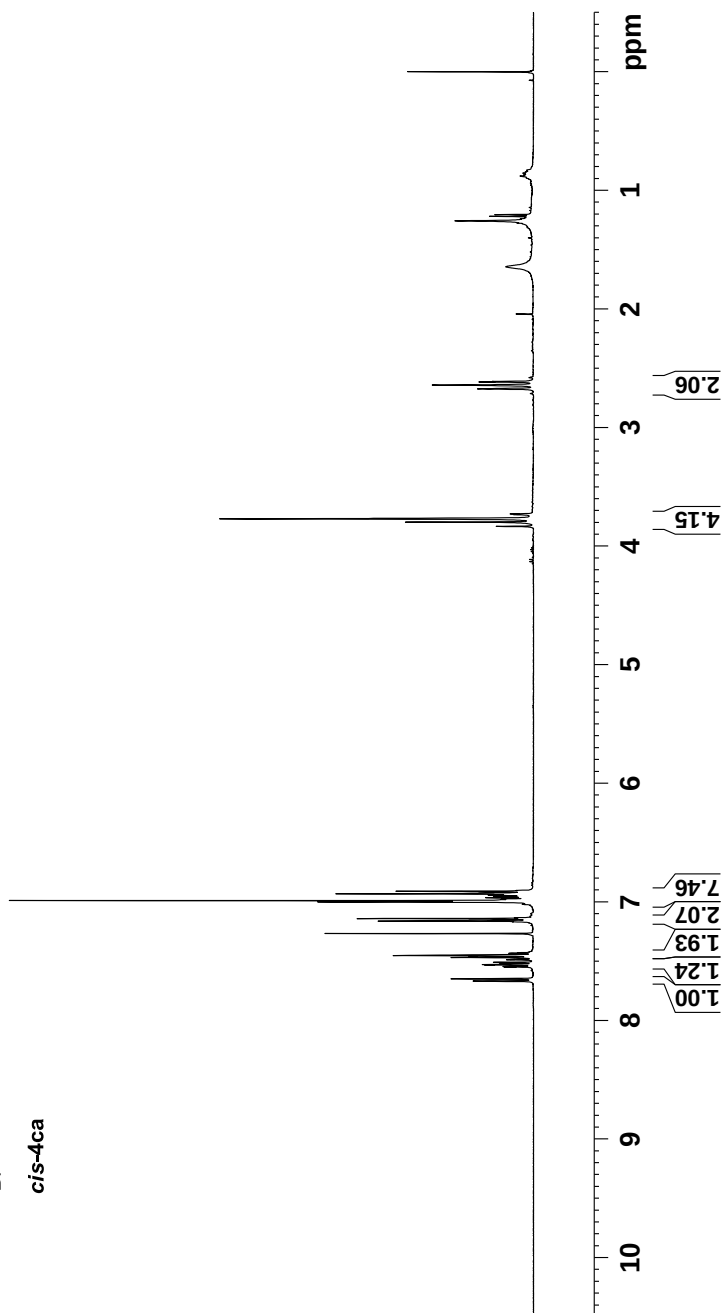
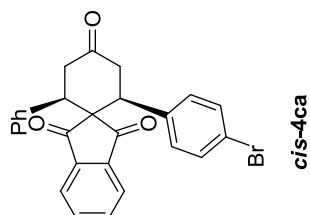
ppm

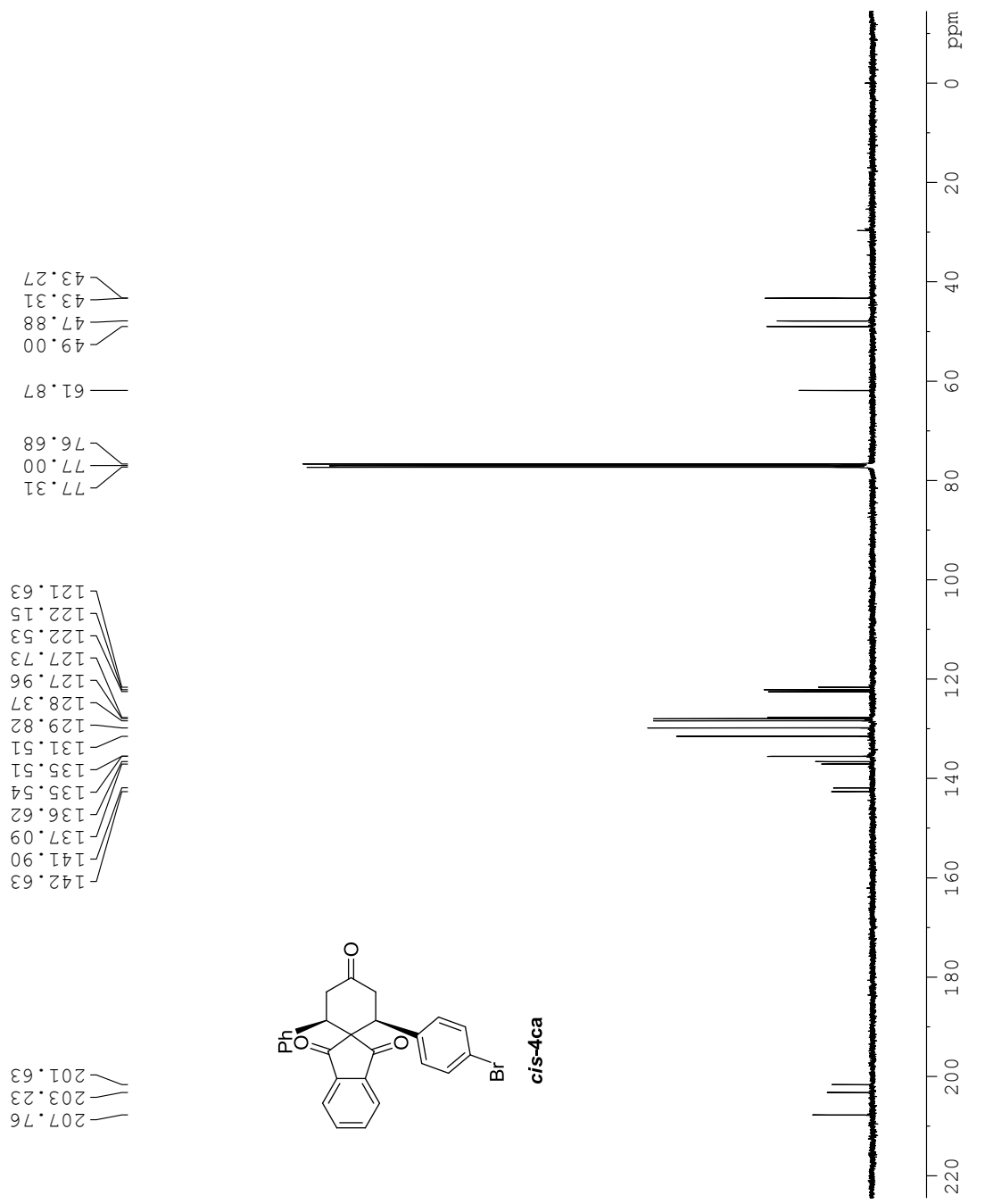
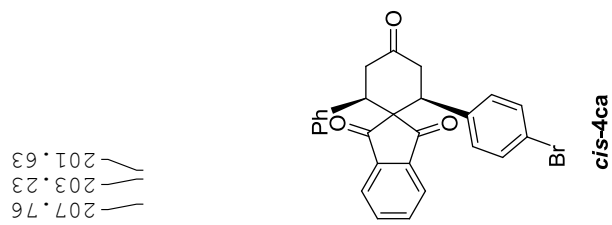
Current Data Parameters
NAME 218
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150728
Time_ 15.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 20
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.260921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 298.4 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 5.30 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300066 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00





Current Data Parameters
NAME 218
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150729
Time 17.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 959
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.60 dB
PL12 20.40 dB
PL13 23.40 dB
SFO2 400.1316005 MHz

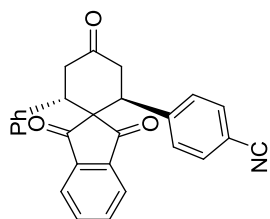
F2 - Processing parameters
SI 32768
SF 100.6127716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME Chris-128
 EXPNO 9
 PROCNO 1

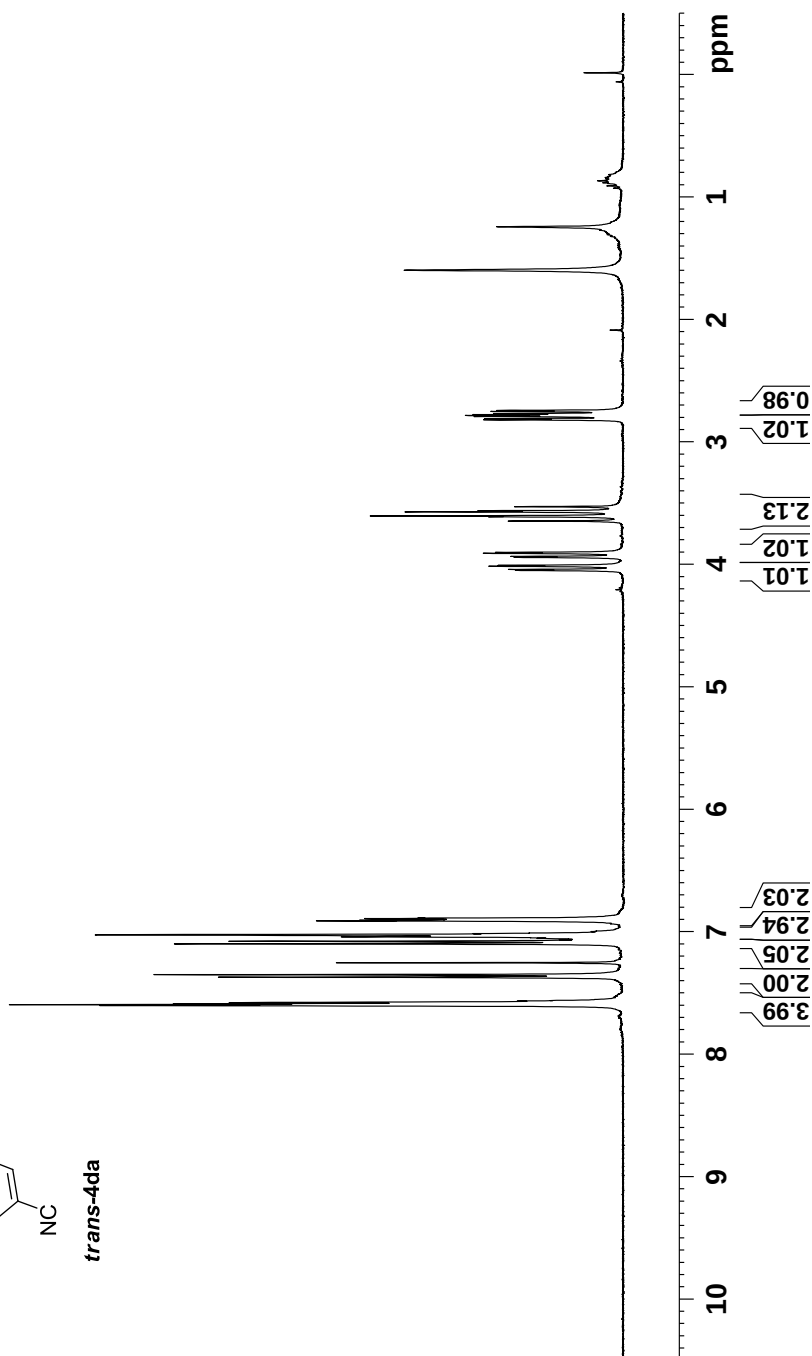
F2 - Acquisition Parameters
 Date_ 20150514
 Time_ 17.45
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 362
 DW 69.000 usec
 DE 6.50 usec
 TE 297.1 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 21.45 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300118 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



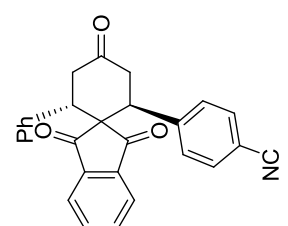
trans-4da



208.81
202.44
202.17

143.00
141.91
141.79
136.71
135.92
135.87
132.06
129.28
128.34
127.68
122.72
122.70
118.24
111.50

77.32
77.00
76.68
61.35
44.17
42.97
41.57
41.13



trans-4da

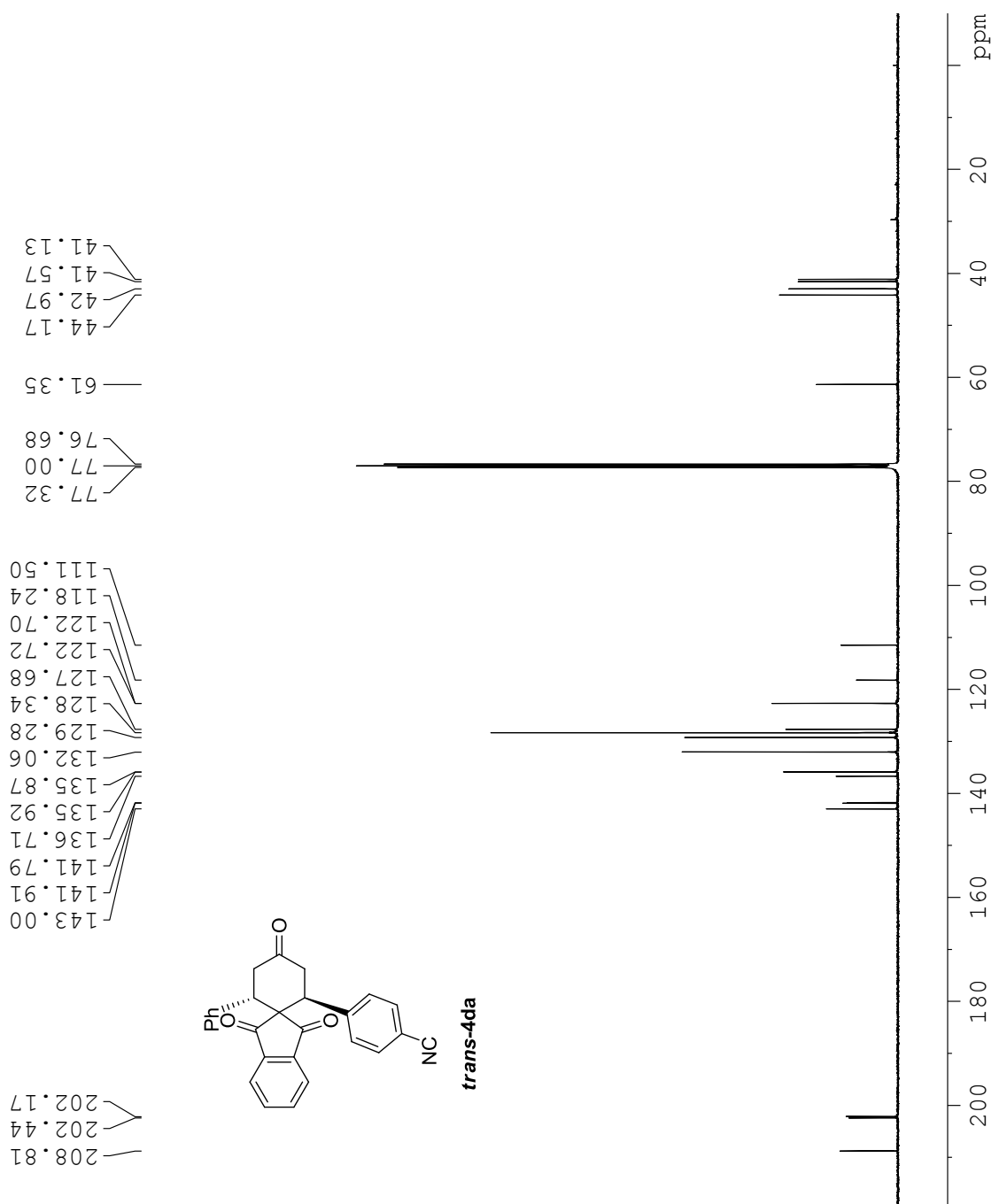
Current Data Parameters
NAME Chris-128
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150303
Time 8.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 13411
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127709 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME Chris-148
 EXPNO 1
 PROCNO 1

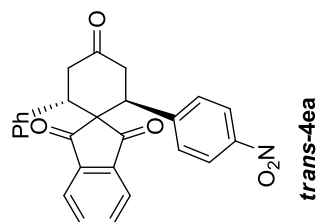
F2 - Acquisition Parameters

Date_ 20150417
 Time_ 18.11
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 228.1
 DW 69.000 usec
 DE 6.50 usec
 TE 299.4 K
 D1 2.00000000 sec
 TD0 1

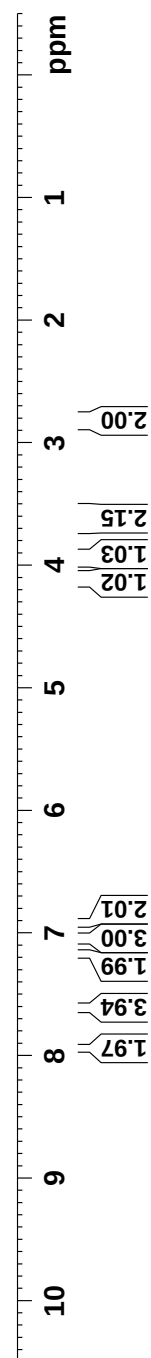
===== CHANNEL f1 =====
 NUC1 1H
 P1 21.45 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters

SI 16384
 SF 400.1300065 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



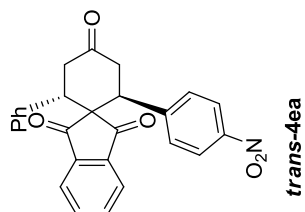
S23



208.61
202.37
202.05

147.10
145.09
141.88
141.75
136.66
135.98
135.90
129.46
128.34
127.71
123.44
122.76
122.75

77.31
77.00
76.68
61.33
44.36
42.62
41.58
41.25



```

Current Data Parameters
NAME      Chris-148
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20150417
Time      18.49
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS         1042
DS         0
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         0.6815744 sec
RG         8192
DW         20.800 usec
DE         6.50 usec
TE         300.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.00 usec
PL1        6.70 dB
SFO1       100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2]  waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -5.85 dB
PL12       6.00 dB
PL13       9.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6127716 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00

```

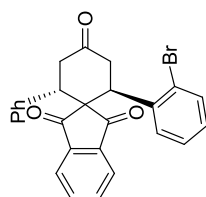
ppm

Current Data Parameters
 NAME 211
 EXPNO 8
 PROCNO 1

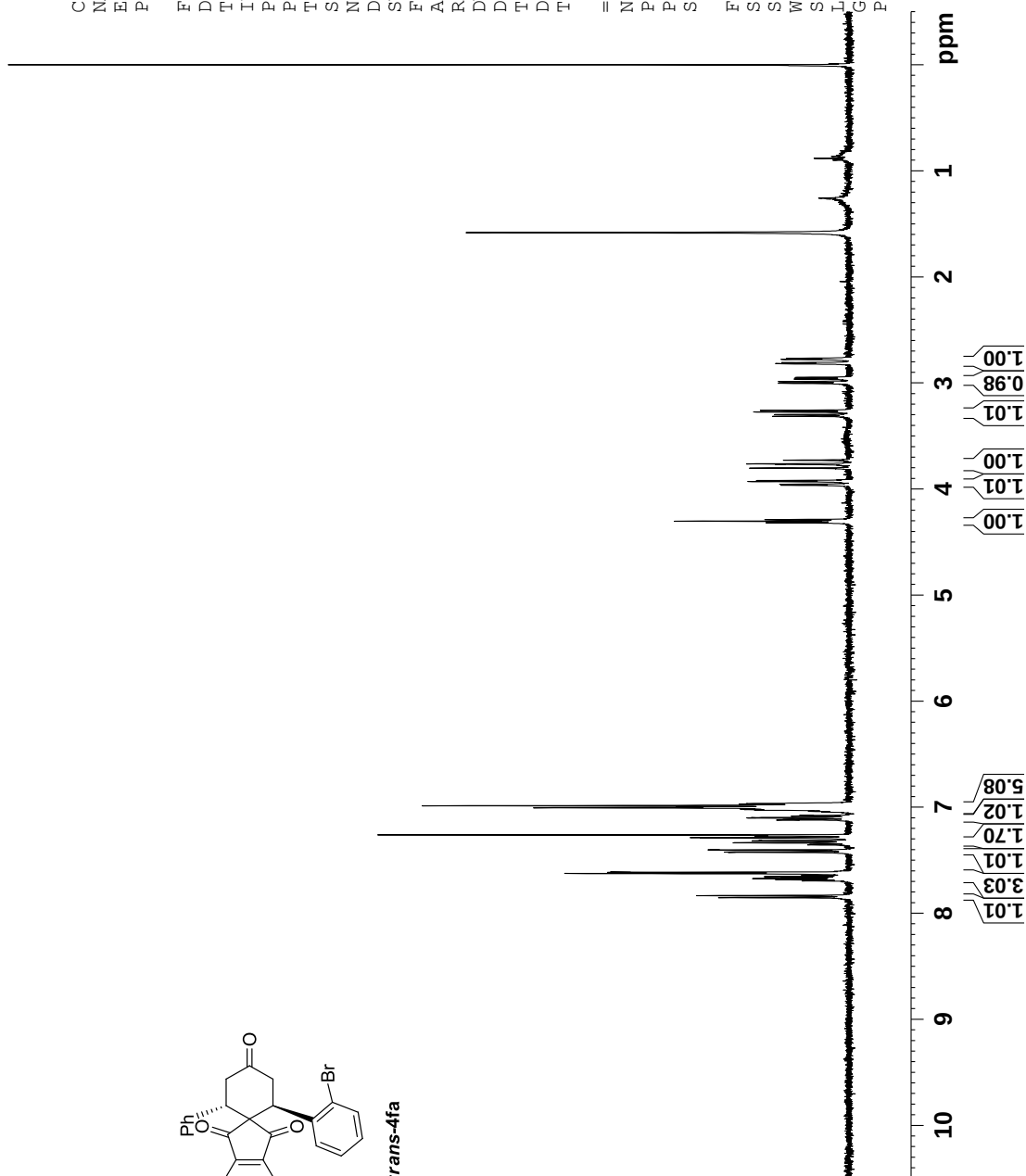
F2 - Acquisition Parameters
 Date_ 20150704
 Time_ 14.47
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 30
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.260921 sec
 RG 3649.1
 DW 69.000 usec
 DE 6.50 usec
 TE 298.9 K
 D1 2.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 11.90 usec
 PL1 3.00 dB
 SFO1 400.1324008 MHz

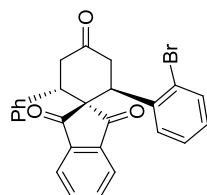
F2 - Processing parameters
 SI 16384
 SF 400.1300087 MHz
 EM
 WDW 0
 SSB 0 Hz
 LB 0
 GB 0
 PC 1.00



trans-4fa

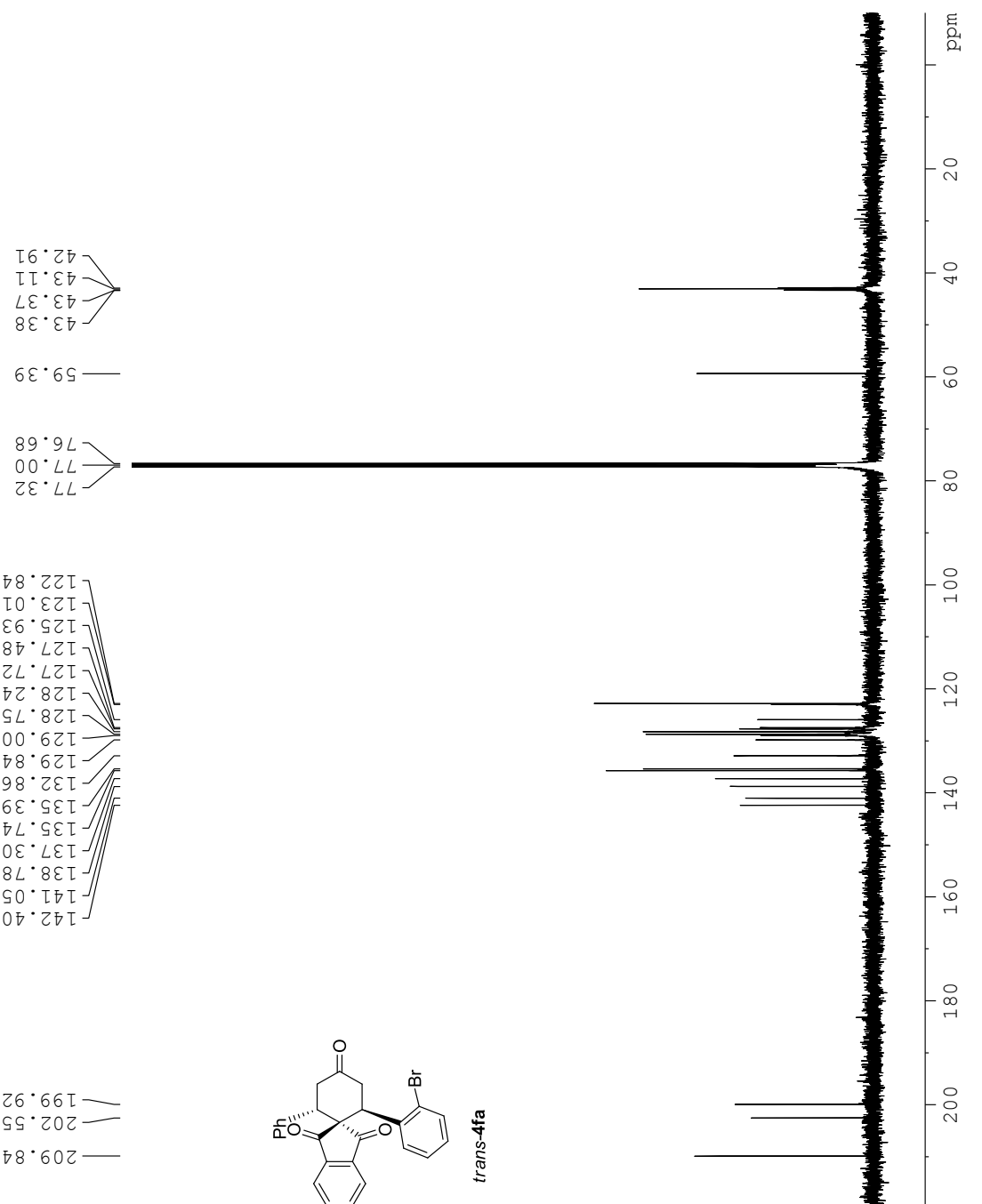


209.84
202.55
199.92



142.40
141.05
138.78
137.30
135.74
135.39
132.86
129.84
129.00
128.75
128.24
127.72
127.48
125.93
123.01
122.84

77.32
77.00
76.68
59.39
43.38
43.37
43.11
42.91



Current Data Parameters
NAME 211
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20150705
Time 22.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 3463
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 9195.2
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

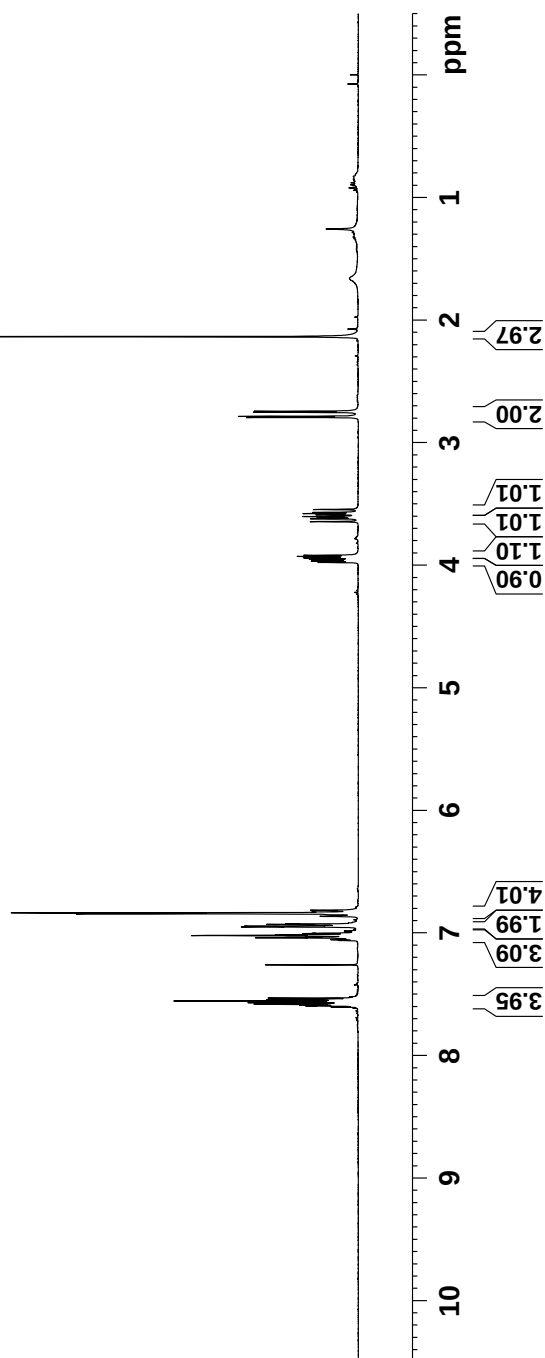
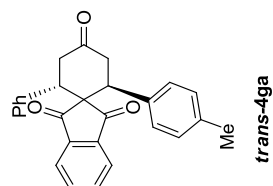
SI 32768
SF 100.6127709 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

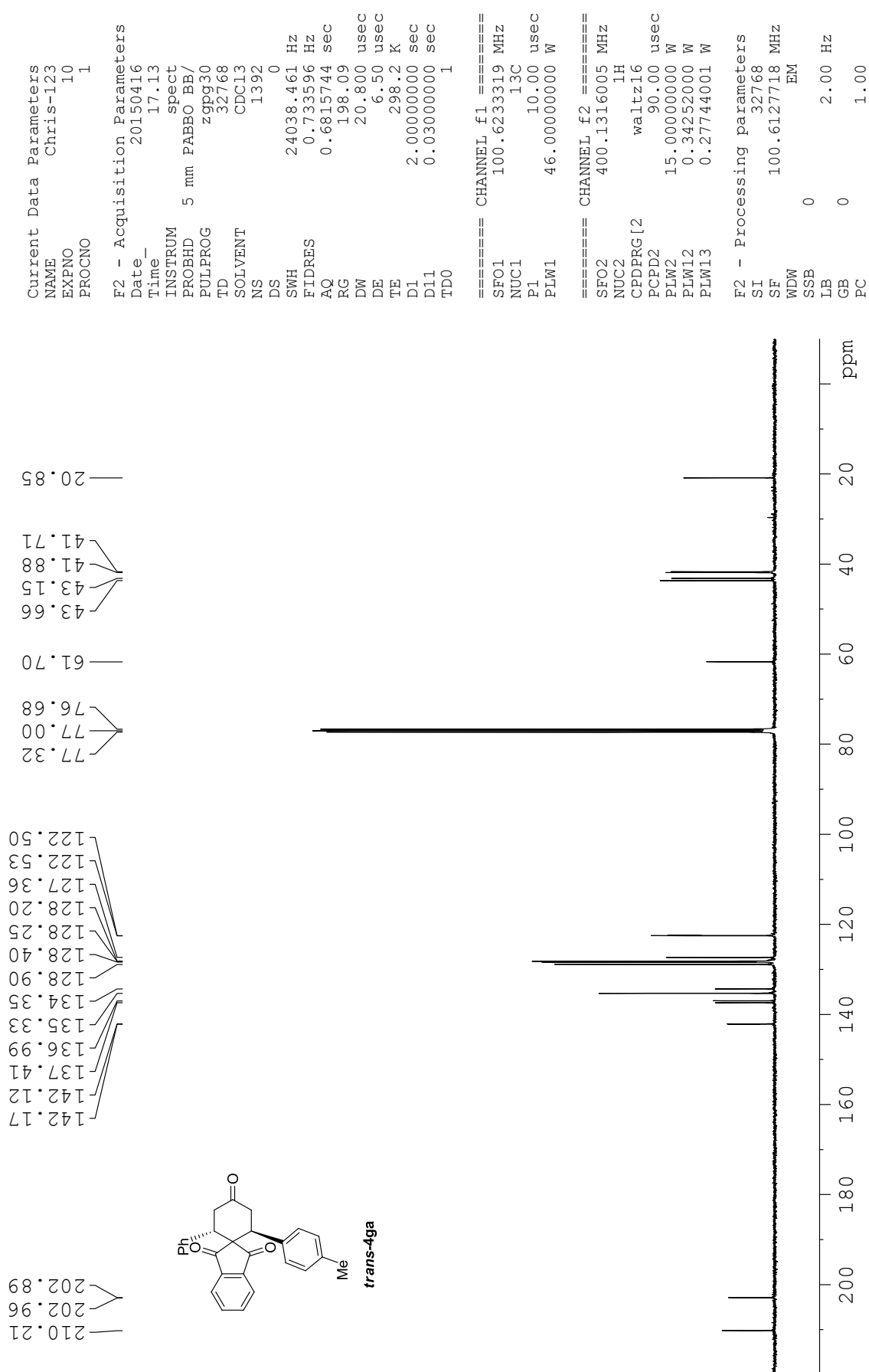
Current Data Parameters
 NAME Chris-123
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150416
 Time_ 17.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 78.51
 DW 69.333 usec
 DE 10.52 usec
 TE 297.6 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300079 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



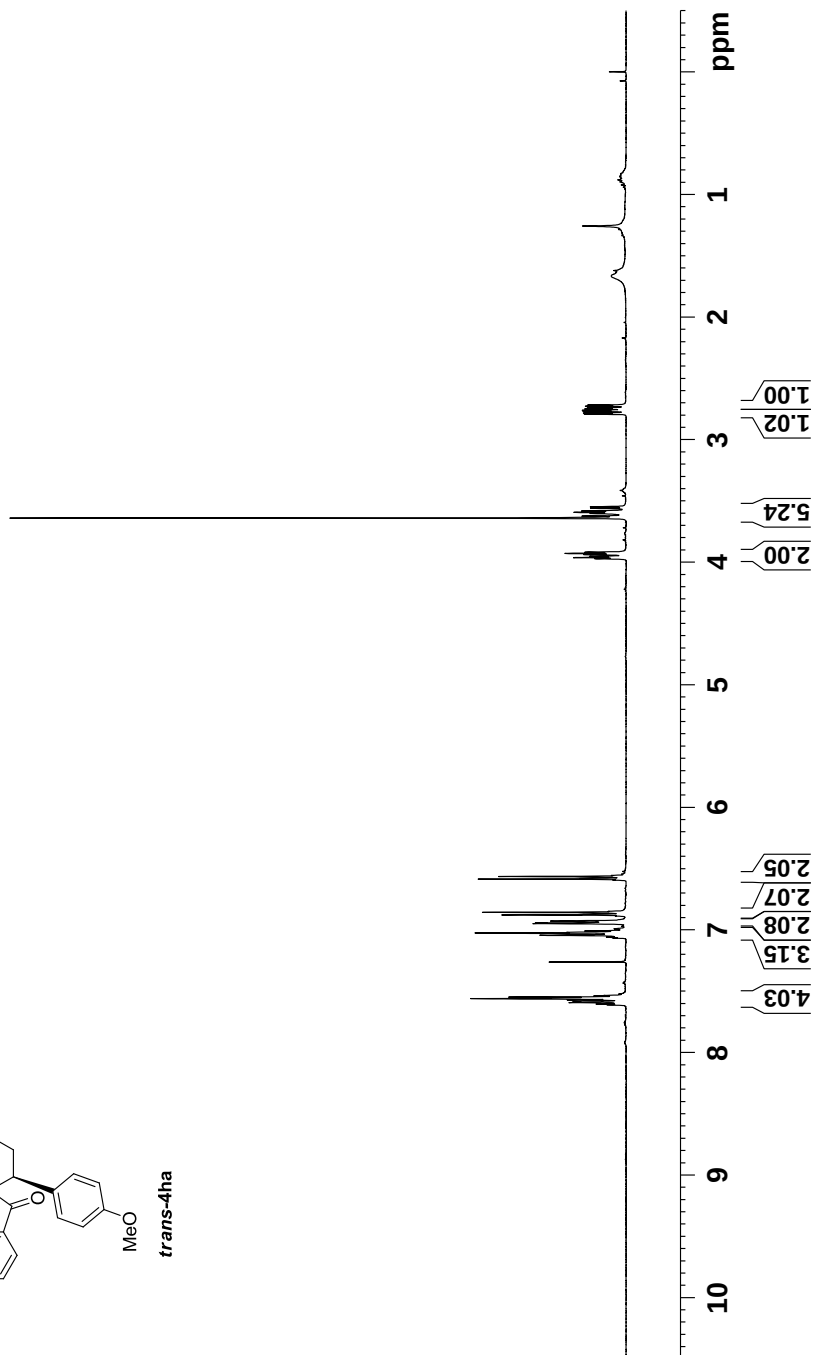
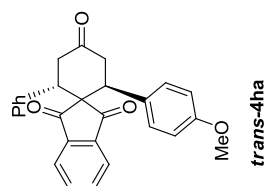


Current Data Parameters
 NAME Chris-147
 EXPNO 13
 PROCNO 1

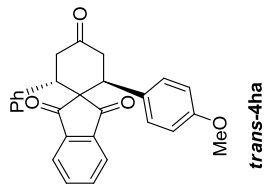
F2 - Acquisition Parameters
 Date_ 20150331
 Time_ 17.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 144.49
 DW 69.333 usec
 DE 10.52 usec
 TE 298.1 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300074 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



210.21
203.10
203.04



158.61
142.18
137.41
135.38
135.36
129.47
129.36
128.38
128.21
127.37
122.54
122.49
113.59

77.31
77.00
76.68
61.80
55.04
43.62
42.79
42.02
41.65

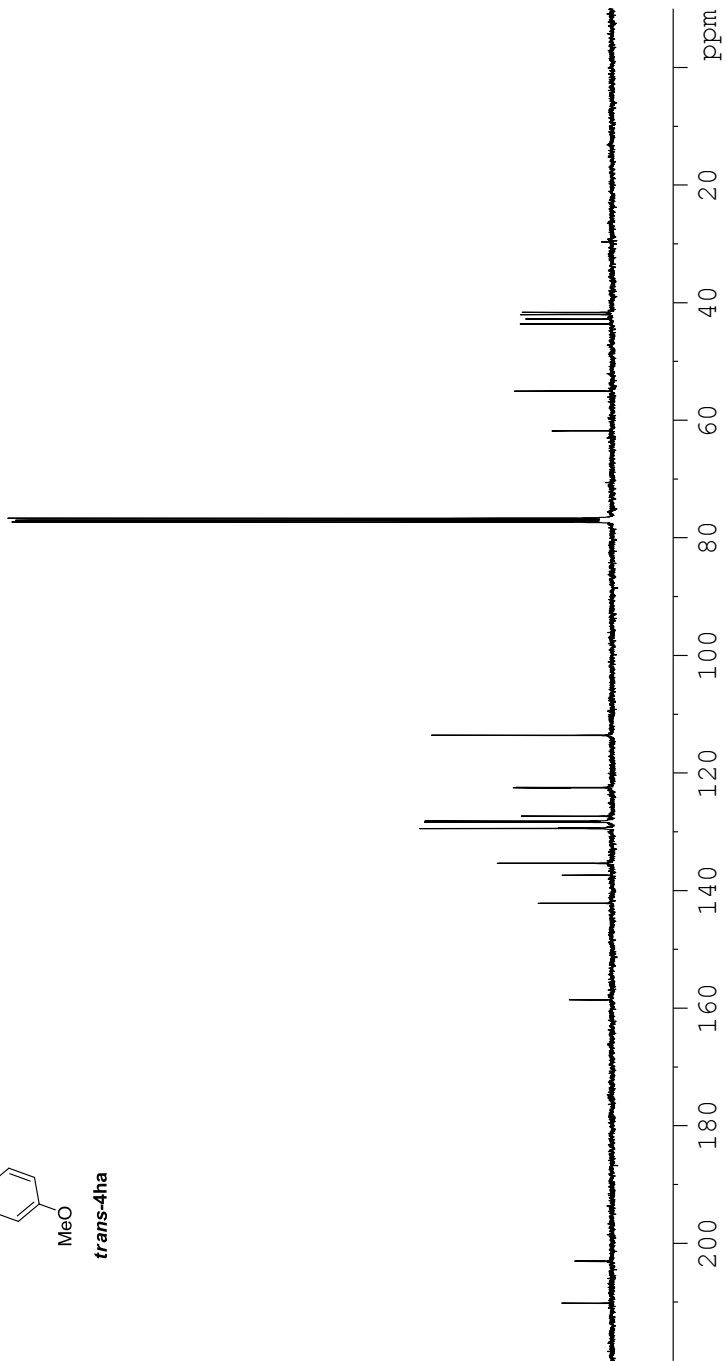
Current Data Parameters
NAME Chris-147
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150331
Time_ 17.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 734
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127710 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

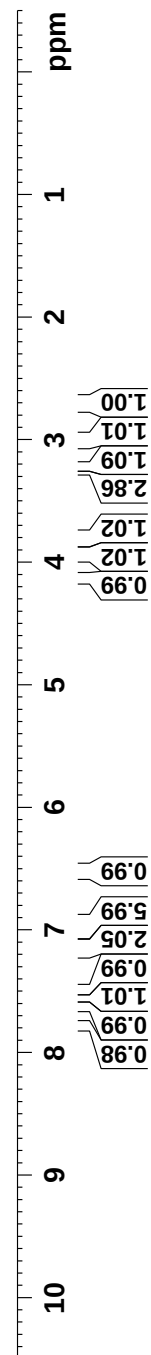
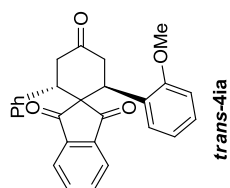


Current Data Parameters
 NAME Chris-171
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150331
 Time_ 13.37
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 45.15
 DW 69.333 usec
 DE 10.52 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 12.80 usec
 PLW1 15.00000000 W

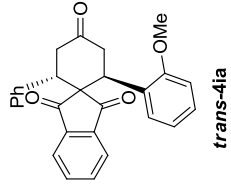
F2 - Processing parameters
 SI 16384
 SF 400.1300061 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



210.64
202.49
200.50

155.89
141.79
141.59
137.72
135.02
134.85
128.73
128.64
128.51
128.05
127.15
122.36
122.14
120.66
109.47

77.32
77.00
76.68
60.01
53.79
42.72
42.24
41.87
37.20



```

Current Data Parameters
NAME      Chris-171
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20150331
Time      13.42
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         32768
SOLVENT    CDCl3
NS         500
DS         0
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         0.6815744 sec
RG         198.09
DW         20.800 usec
DE         6.50 usec
TE         298.9 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      100.6233319 MHz
NUC1       13C
P1         10.00 usec
PLW1      46.00000000 W

===== CHANNEL f2 =====
SFO2      400.1316005 MHz
NUC2       1H
PCPDPRG[2] waltz16
PCPD2      90.00 usec
PLW2      15.00000000 W
PLW12     0.34252000 W
PLW13     0.27744001 W

F2 - Processing parameters
SI         32768
SF         100.6127776 MHz
WDW         EM
SSB         0
LB         2.00 Hz
GB         0
PC         1.00

```

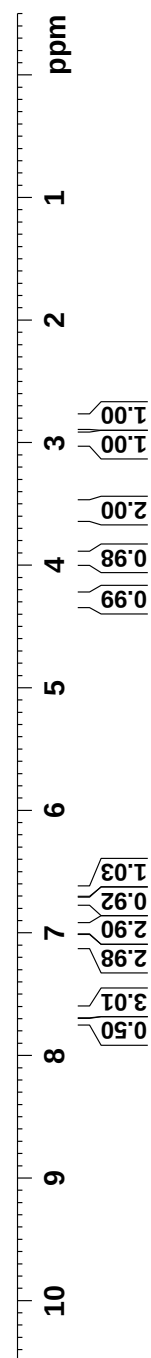
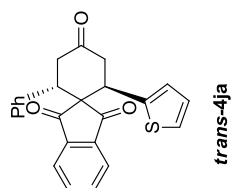
ppm

Current Data Parameters
 NAME Allen-406
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150327
 Time_ 19.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 198.09
 DW 69.333 usec
 DE 10.52 usec
 TE 297.4 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 12.80 usec
 PLW1 15.00000000 W

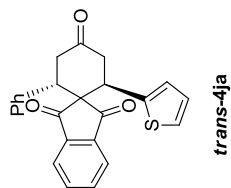
F2 - Processing parameters
 SI 16384
 SF 400.1300083 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



208.88
202.34
202.24

142.20
142.10
140.21
137.36
135.53
128.42
128.29
127.53
126.58
126.46
124.49
122.75

77.32
77.00
76.68
61.41
44.14
43.11
41.94
38.90



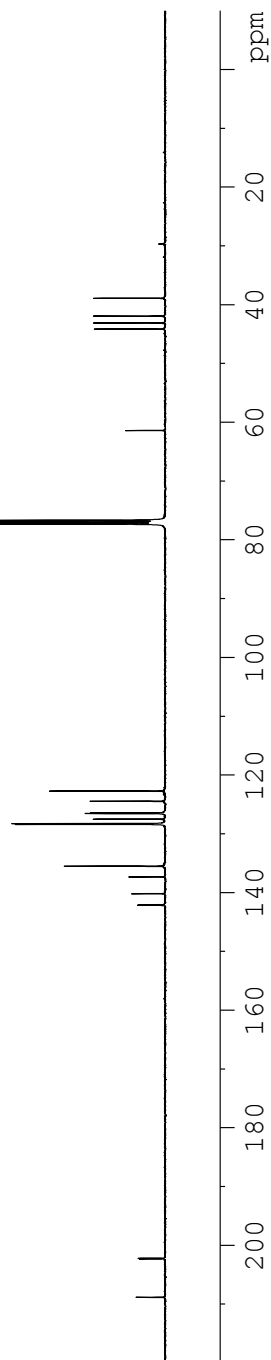
Current Data Parameters
NAME Allen-406
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150331
Time_ 22.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 14338
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127703 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

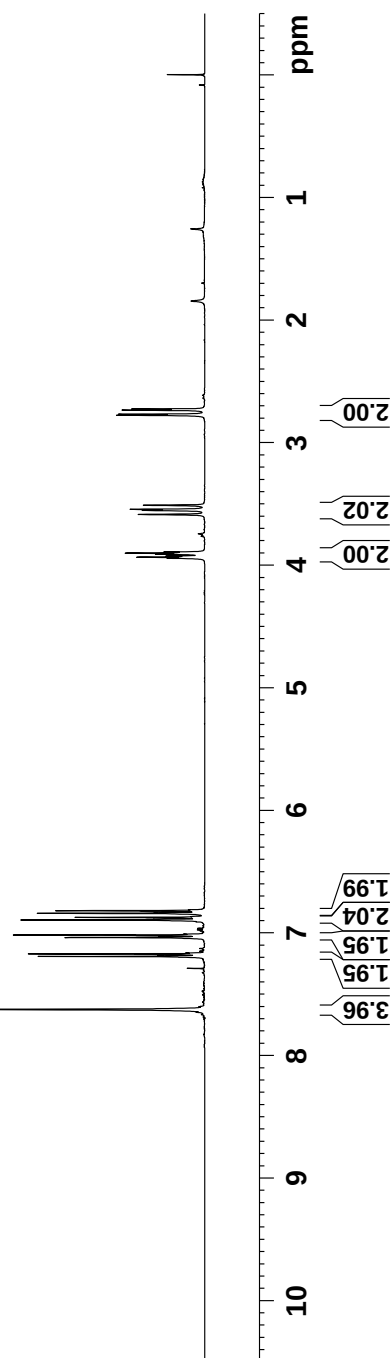
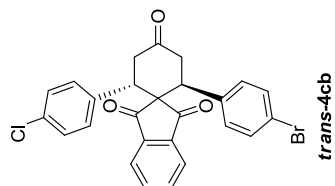


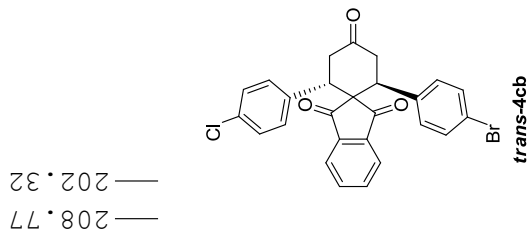
Current Data Parameters
 NAME Allen-278
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141004
 Time_ 15.34
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 35.9
 DW 69.000 usec
 DE 6.50 usec
 TE 297.7 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1299968 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





141.77
136.23
135.84
135.67
133.31
131.34
129.99
129.65
128.38
122.67
121.49

77.32
77.00
76.68

61.12

42.93
42.90
41.51
41.45

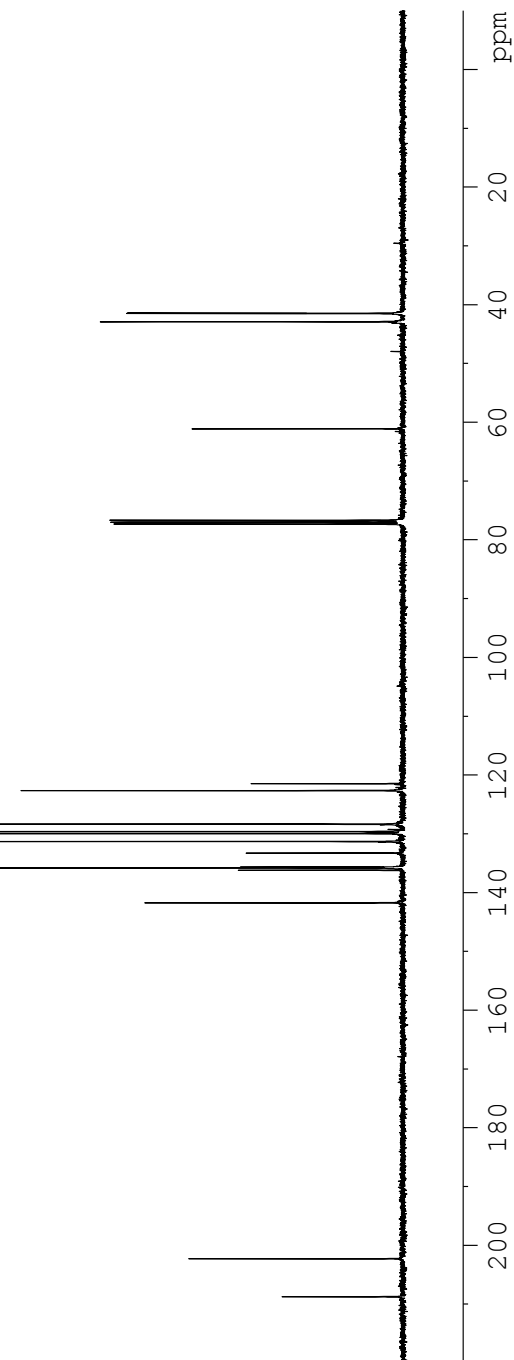
Current Data Parameters
NAME Allen-278
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141009
Time_ 18.12
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127797 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

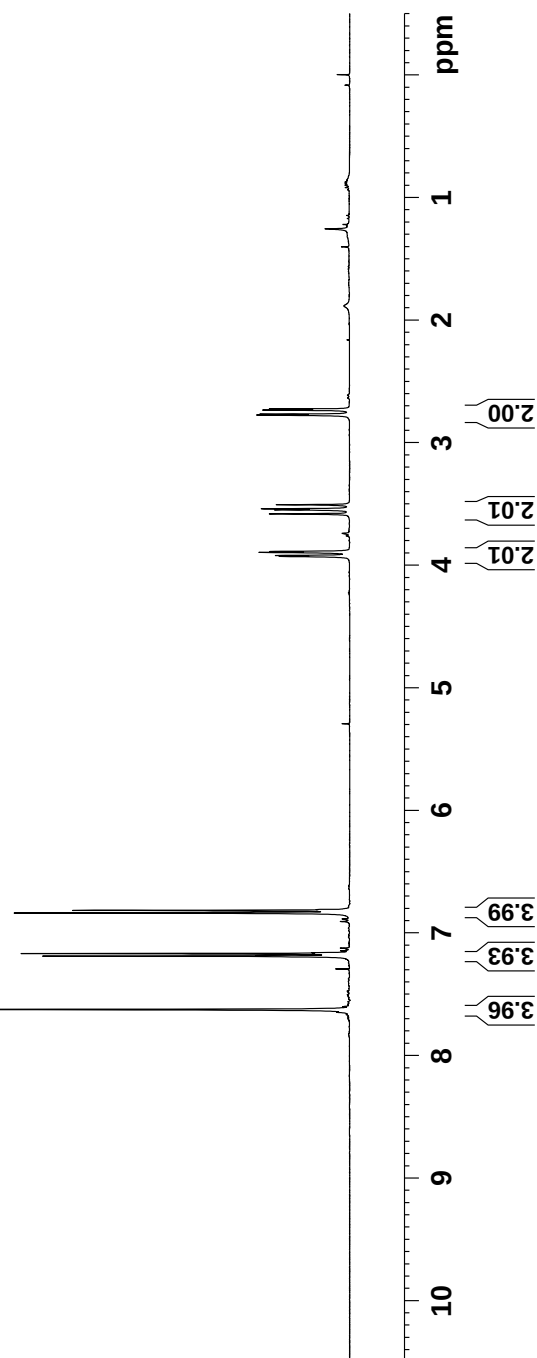
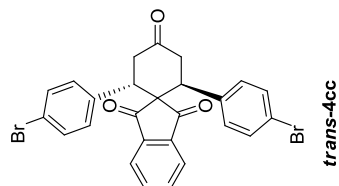


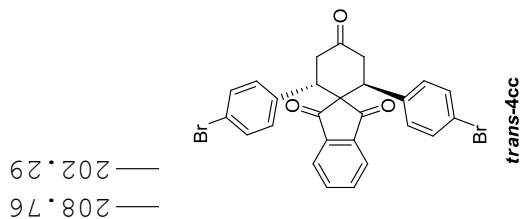
Current Data Parameters
 NAME Allen-279
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141006
 Time_ 21.08
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 35.9
 DW 69.000 usec
 DE 6.50 usec
 TE 297.8 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1299950 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





141.76
136.22
135.86
131.35
130.00
122.69
121.51

77.32
77.00
76.69

61.06

42.96
41.47

```

Current Data Parameters
NAME      Allen-279
EXPNO     5
PROCNO    1

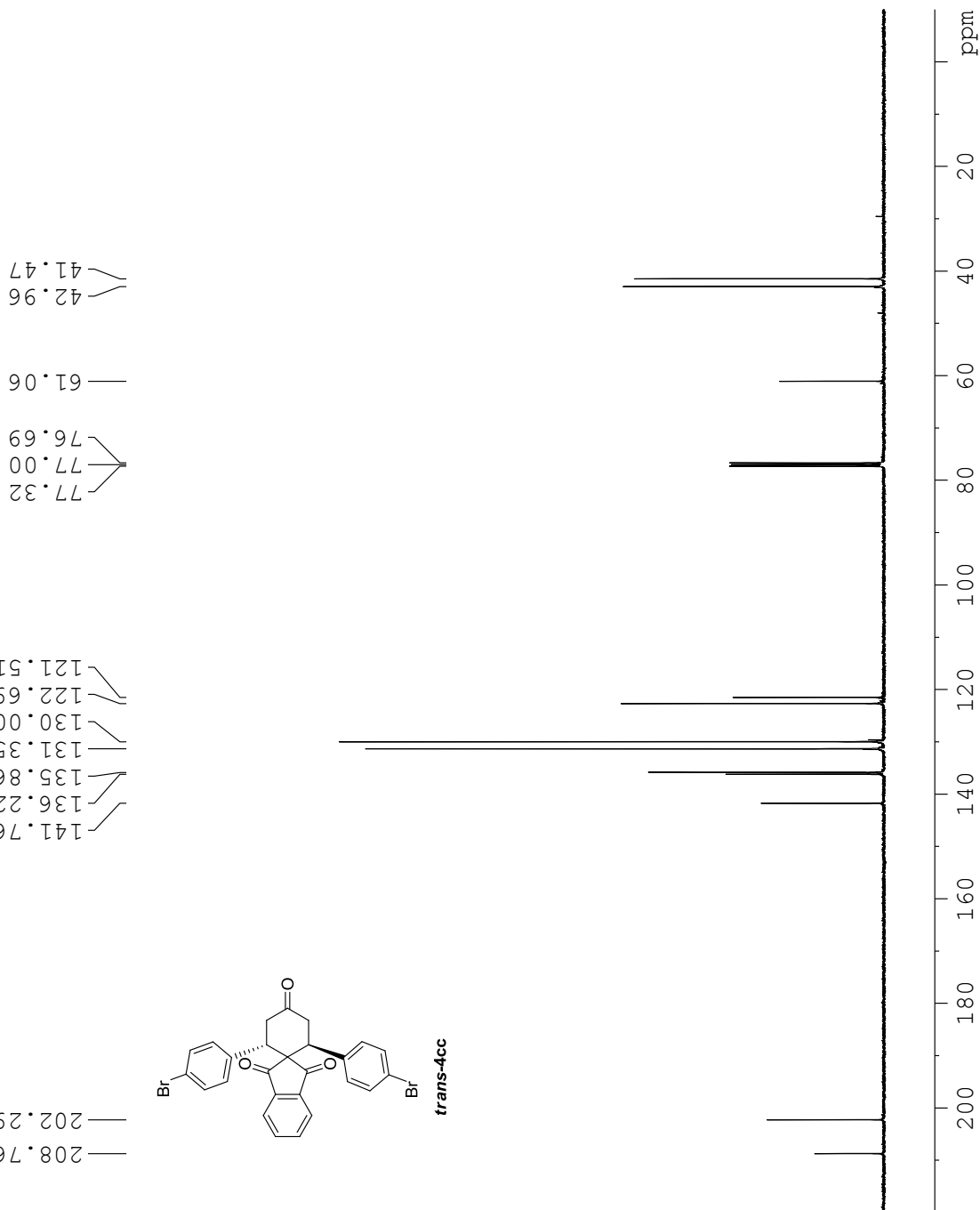
F2 - Acquisition Parameters
Date_     20141009
Time      18.38
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS        500
DS        0
SWH       24038.461 Hz
FIDRES    0.733596 Hz
AQ        0.6815744 sec
RG        4096
DW        20.800 usec
DE        6.50 usec
TE        300.0 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PL1       6.70 dB
SFO1      100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2  waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -5.85 dB
PL12      9.10 dB
PL13      12.10 dB
SFO2      400.1316005 MHz

F2 - Processing parameters
SI        32768
SF        100.6127789 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00

```

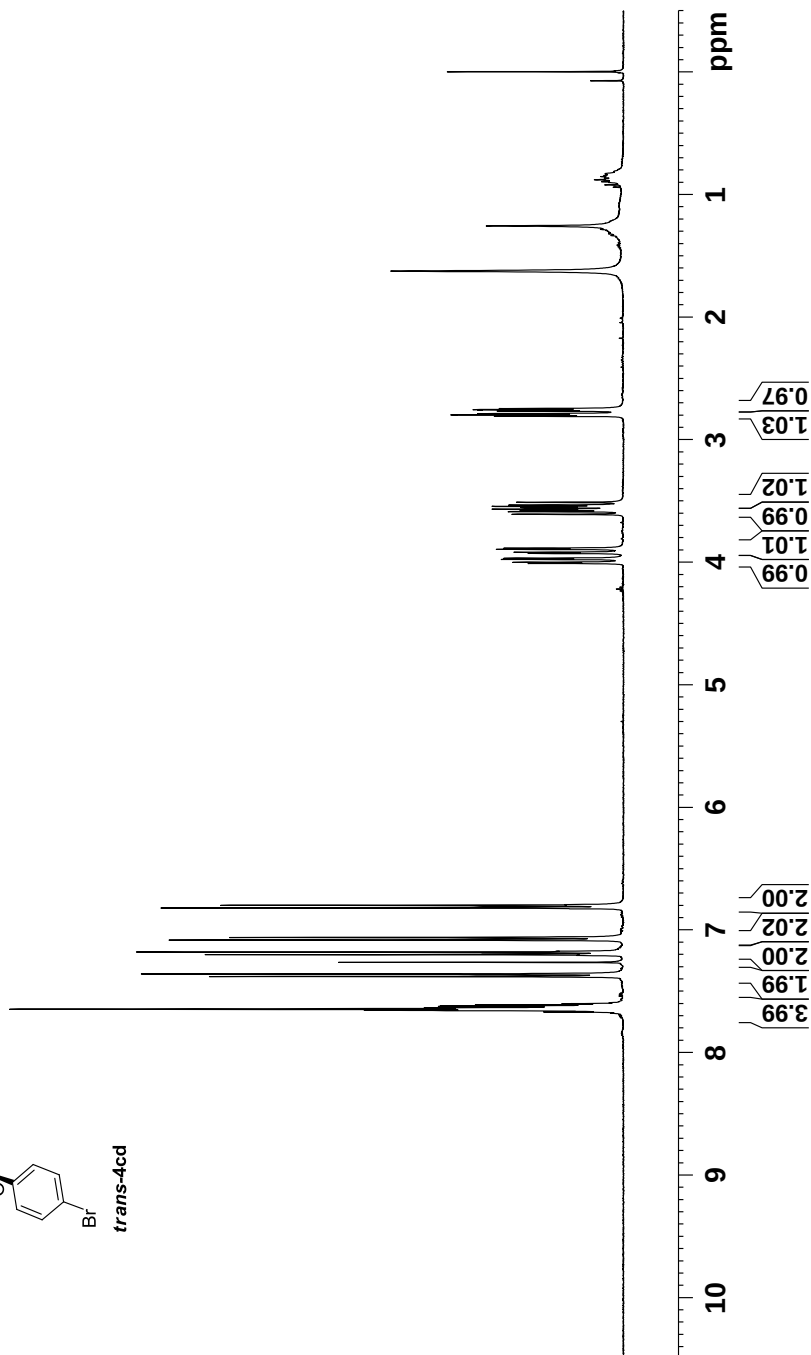
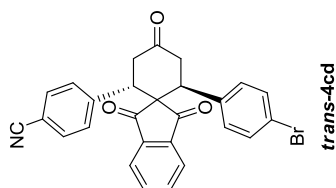


Current Data Parameters
 NAME Chris-157
 EXPNO 4
 PROCNO 1

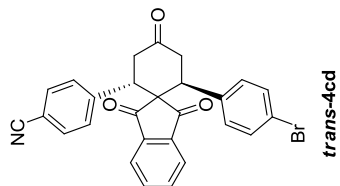
F2 - Acquisition Parameters
 Date_ 20150312
 Time_ 16.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 158.74
 DW 69.333 usec
 DE 10.52 usec
 TE 297.3 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300061 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



208.23
202.12
202.03



142.70
141.75
141.66
136.21
136.19
135.90
132.08
131.53
130.03
129.24
122.90
122.80
121.78
118.15
111.64

77.32
77.00
76.68

61.04

43.40
43.21
41.51
41.10

```

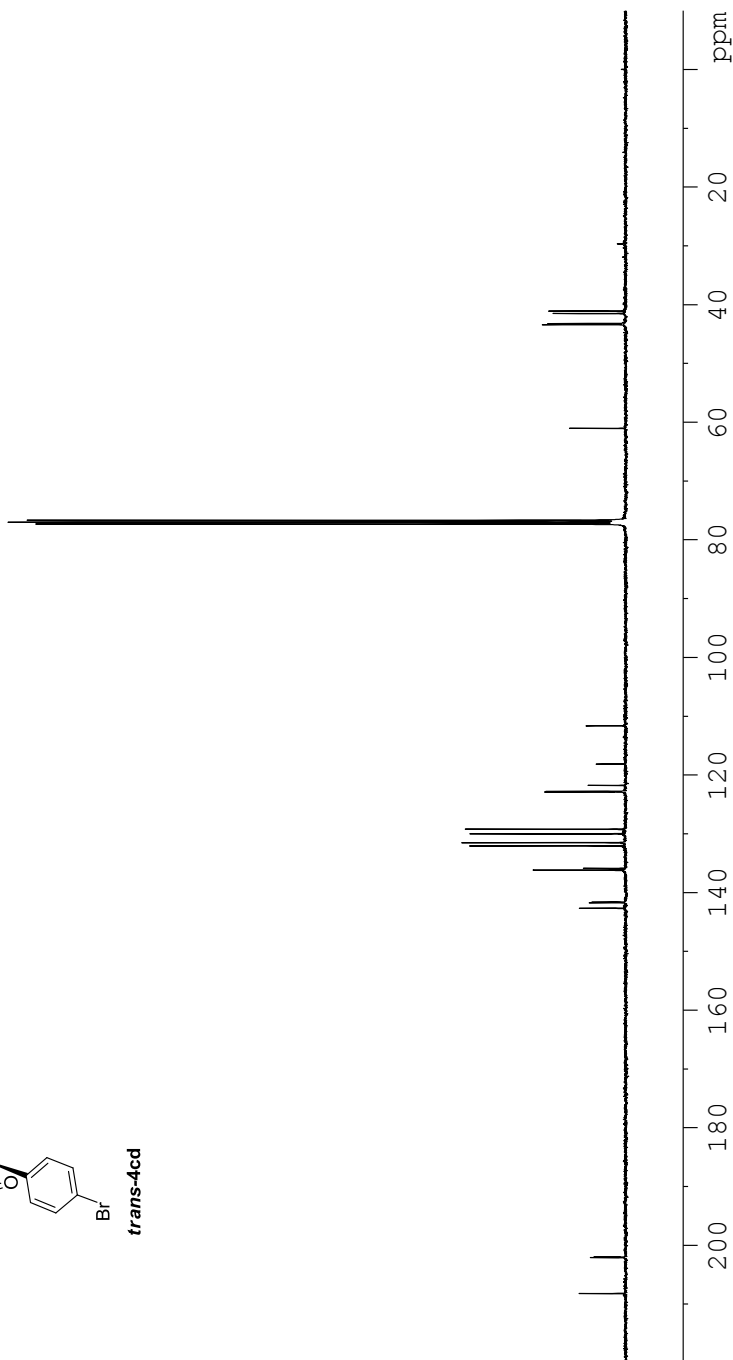
Current Data Parameters
NAME      Chris-157
EXPNO     5
PROCNO    1

F2 - Acquisition Parameters
Date_     20150312
Time      17.00
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS         2187
DS         0
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         0.6815744 sec
RG         198.09
DW         20.800 usec
DE         6.50 usec
TE         297.8 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SF01      100.6233319 MHz
NUC1       13C
P1         10.00 usec
PLW1       46.00000000 W

===== CHANNEL f2 =====
SF02      400.1316005 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2      90.00 usec
PLW2       15.00000000 W
PLW12      0.34252000 W
PLW13      0.27744001 W

F2 - Processing parameters
SI          32768
SF          100.6127710 MHz
WDW         EM
SSB         0
LB          2.00 Hz
GB          0
PC          1.00
  
```

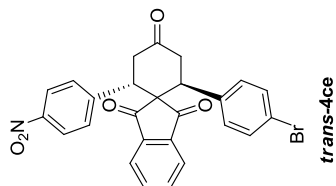


Current Data Parameters
 NAME Chris-162
 EXPNO 1
 PROCNO 1

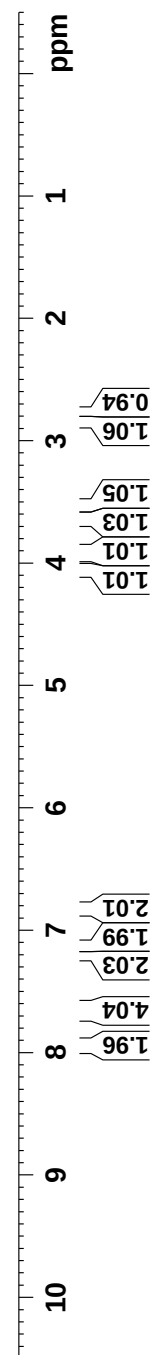
F2 - Acquisition Parameters
 Date_ 20150507
 Time_ 15.13
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.260921 sec
 RG 181
 DW 69.000 usec
 DE 6.50 usec
 TE 298.6 K
 D1 2.00000000 sec
 TD0 1

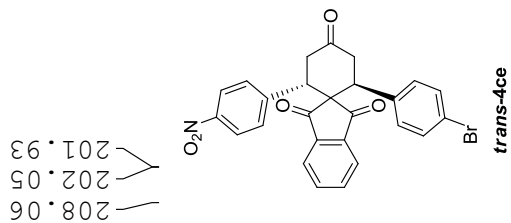
==== CHANNEL f1 =====
 NUC1 1H
 P1 21.45 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300047 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



S41





147.15
144.78
141.70
141.61
136.29
136.23
135.84
131.53
130.03
129.44
123.47
122.94
122.85
121.81

77.32
77.00
76.68

43.40
43.03
41.52
41.21

61.00

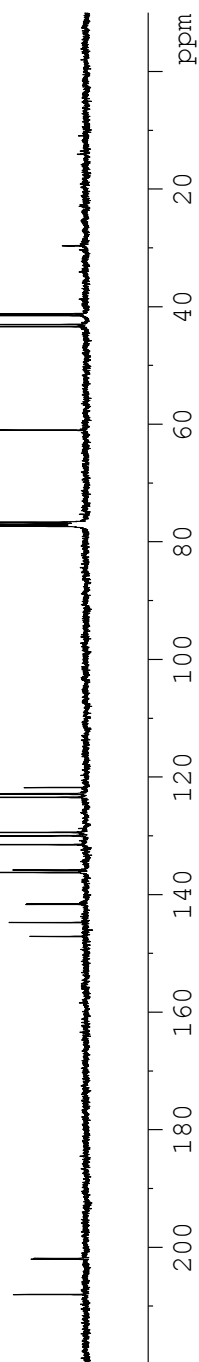
Current Data Parameters
NAME Chris-162
EXPNO 4
PROCNO 1

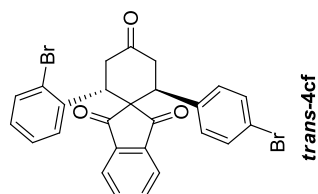
F2 - Acquisition Parameters
Date_ 20150426
Time_ 8.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127718 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



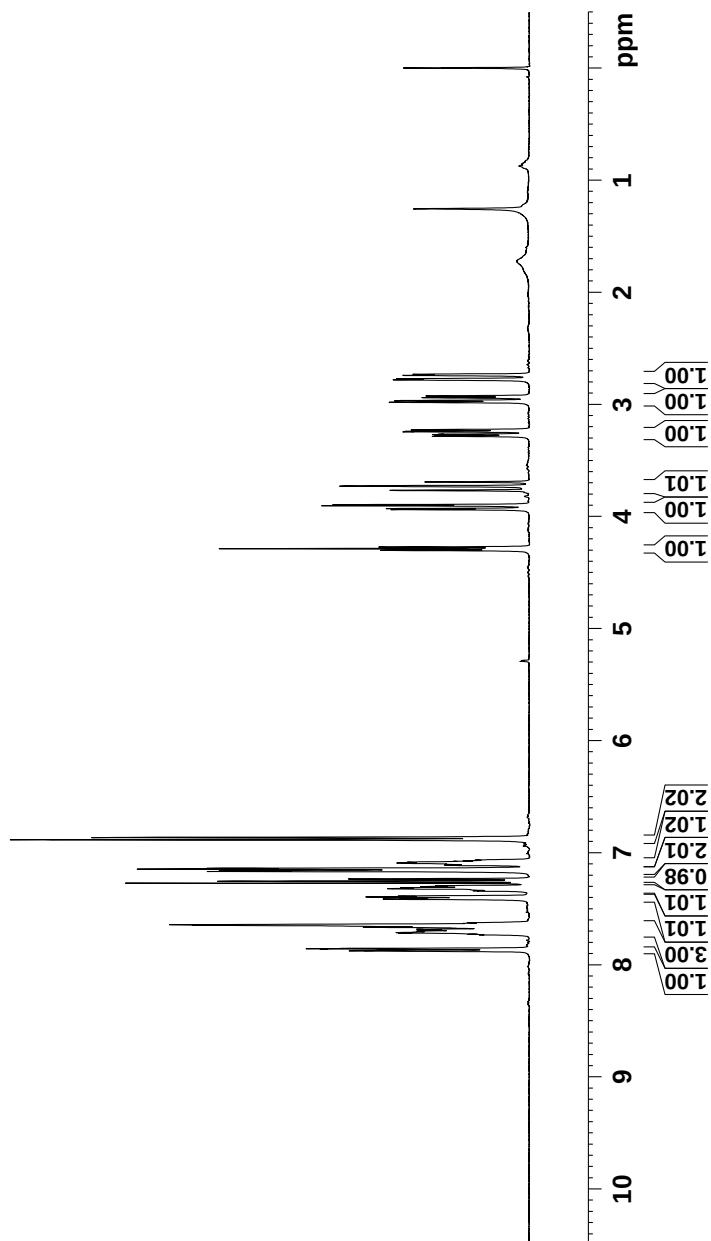


Current Data Parameters
NAME 216
EXNO 3
PROCNO 1

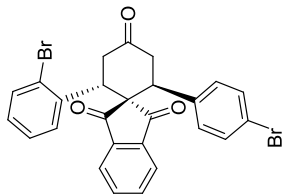
F2 - Acquisition Parameters
Date_ 20150629
Time_ 15.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.260921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 21.45 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300044 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



209.18
202.27
199.63



142.29
140.83
138.46
136.45
136.00
135.61
132.87
131.38
130.45
129.70
129.06
127.70
125.89
123.13
122.95
121.51

77.32
77.00
76.68

59.23

43.45
42.95
42.72
42.15

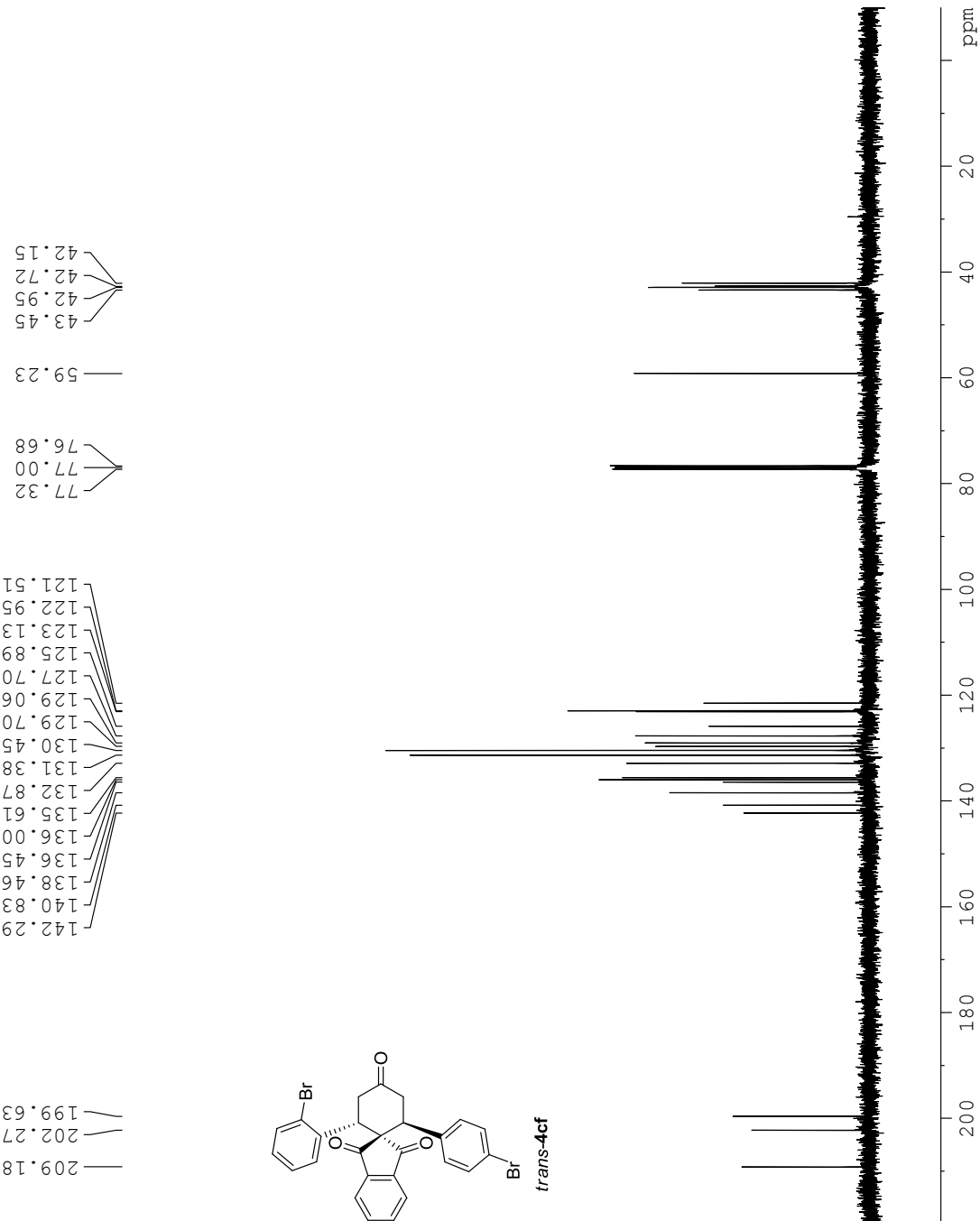
```
Current Data Parameters
NAME                216
EXPNO               4
PROCNO             1

F2 - Acquisition Parameters
Date_              20150629
Time_             15.19
INSTRUM            spect
PROBHD             5 mm BBO BB-1H
PULPROG            zgpg30
TD                 32768
SOLVENT            CDC13
NS                  109
DS                   0
SWH                 24038.461 Hz
FIDRES             0.733596 Hz
AQ                  0.6815744 sec
RG                  4597.6
DW                  20.800 usec
DE                   6.50 usec
TE                  299.0 K
D1                  2.0000000 sec
D11                 0.0300000 sec
TD0                 1

===== CHANNEL f1 =====
NUC1                 13C
P1                   10.00 usec
PL1                   6.70 dB
SFO1                 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2]           waltz16
NUC2                  1H
PCPD2                90.00 usec
PL2                   -5.85 dB
PL12                  6.00 dB
PL13                   9.00 dB
SFO2                 400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF                  100.6127757 MHz
WDW                   EM
SSB                   0
LB                   1.00 Hz
GB                   0
PC                   1.00
```

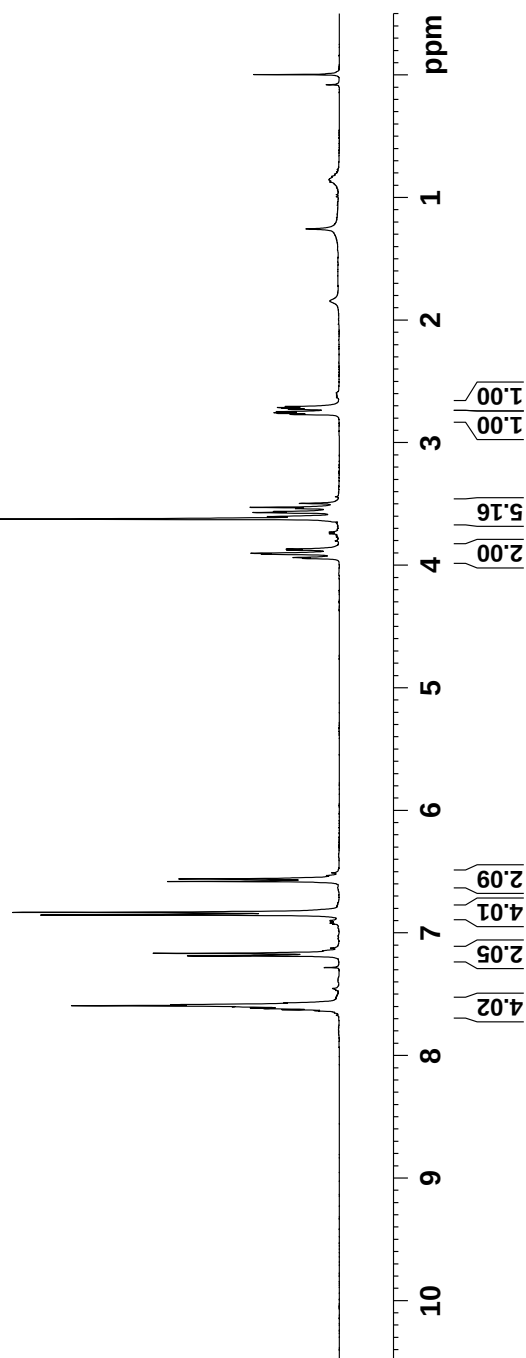
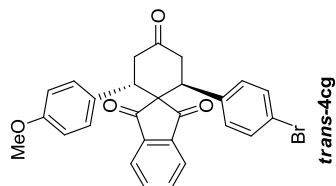


Current Data Parameters
 NAME Allen-285
 EXPNO 5
 PROCNO 1

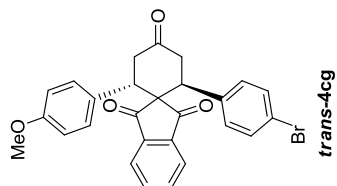
F2 - Acquisition Parameters
 Date_ 20141023
 Time_ 12.04
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 35.9
 DW 69.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1299999 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



209.51
202.80
202.64



158.60
141.97
141.92
136.57
135.61
135.56
131.30
130.03
129.36
129.00
122.59
122.56
121.34
113.54

77.32
77.00
76.68
61.45
54.95
43.15
42.57
41.91
41.51

```

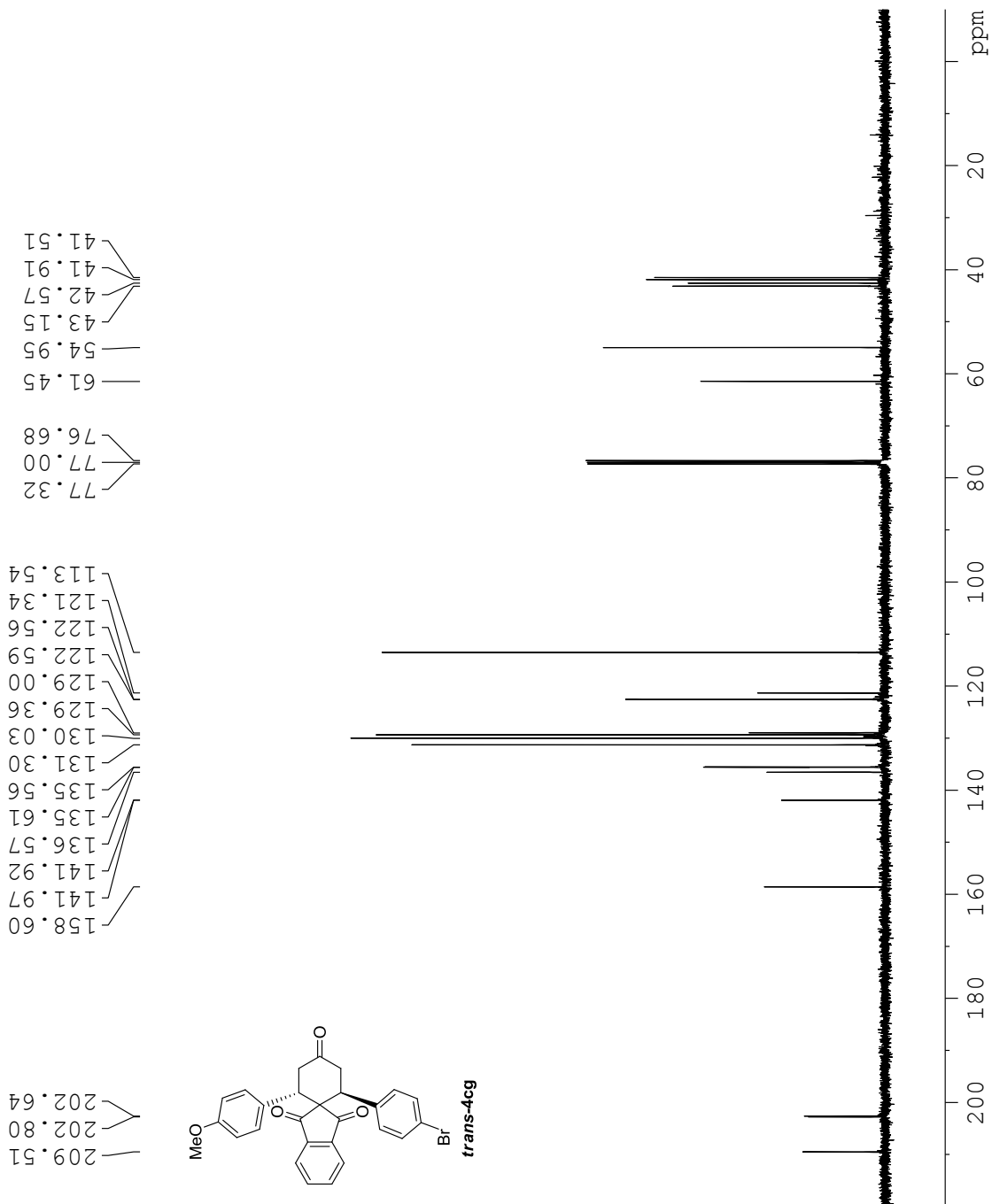
Current Data Parameters
NAME      Allen-285
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20141018
Time      16.45
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS         502
DS         0
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         0.6815744 sec
RG         2048
DW         20.800 usec
DE         6.50 usec
TE         297.7 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.00 usec
PL1        6.70 dB
SFO1       100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2]  waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -5.85 dB
PL12       9.10 dB
PL13       12.10 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI          32768
SF          100.6127782 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.00
  
```

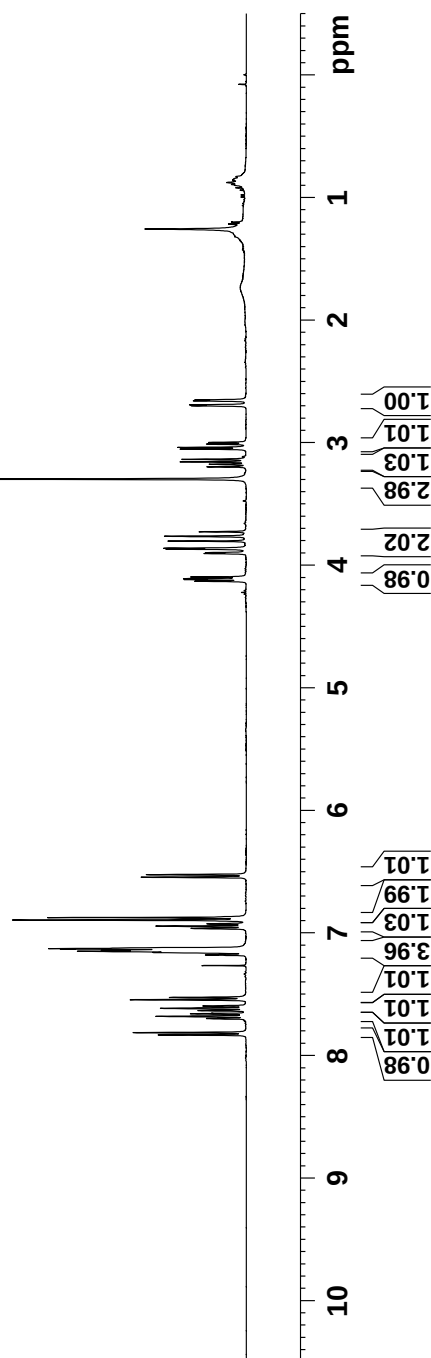
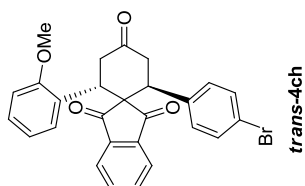


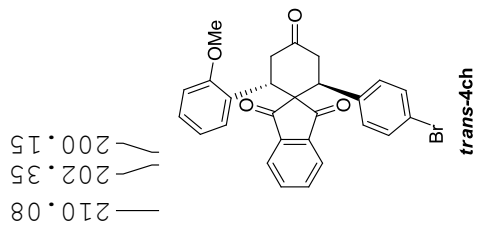
Current Data Parameters
 NAME Chris-172
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150331
 Time_ 16.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 57.42
 DW 69.333 usec
 DE 10.52 usec
 TE 297.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300052 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

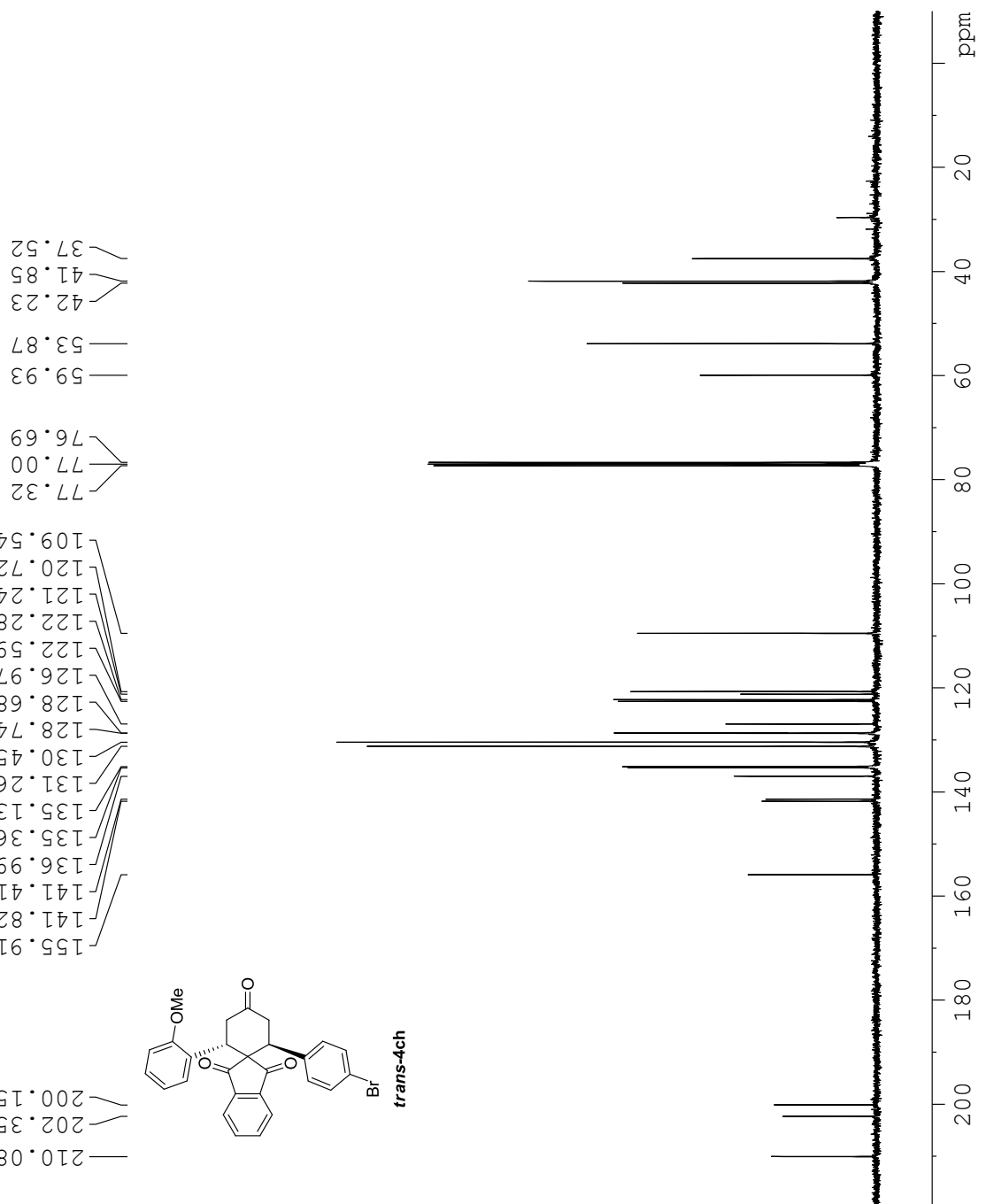




155.91
141.82
141.41
136.99
135.36
135.13
131.26
130.45
128.74
128.68
126.97
122.59
122.28
121.24
120.72
109.54

77.32
77.00
76.69

59.93
53.87
42.23
41.85
37.52



Current Data Parameters
NAME Chris-172
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150331
Time_ 17.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

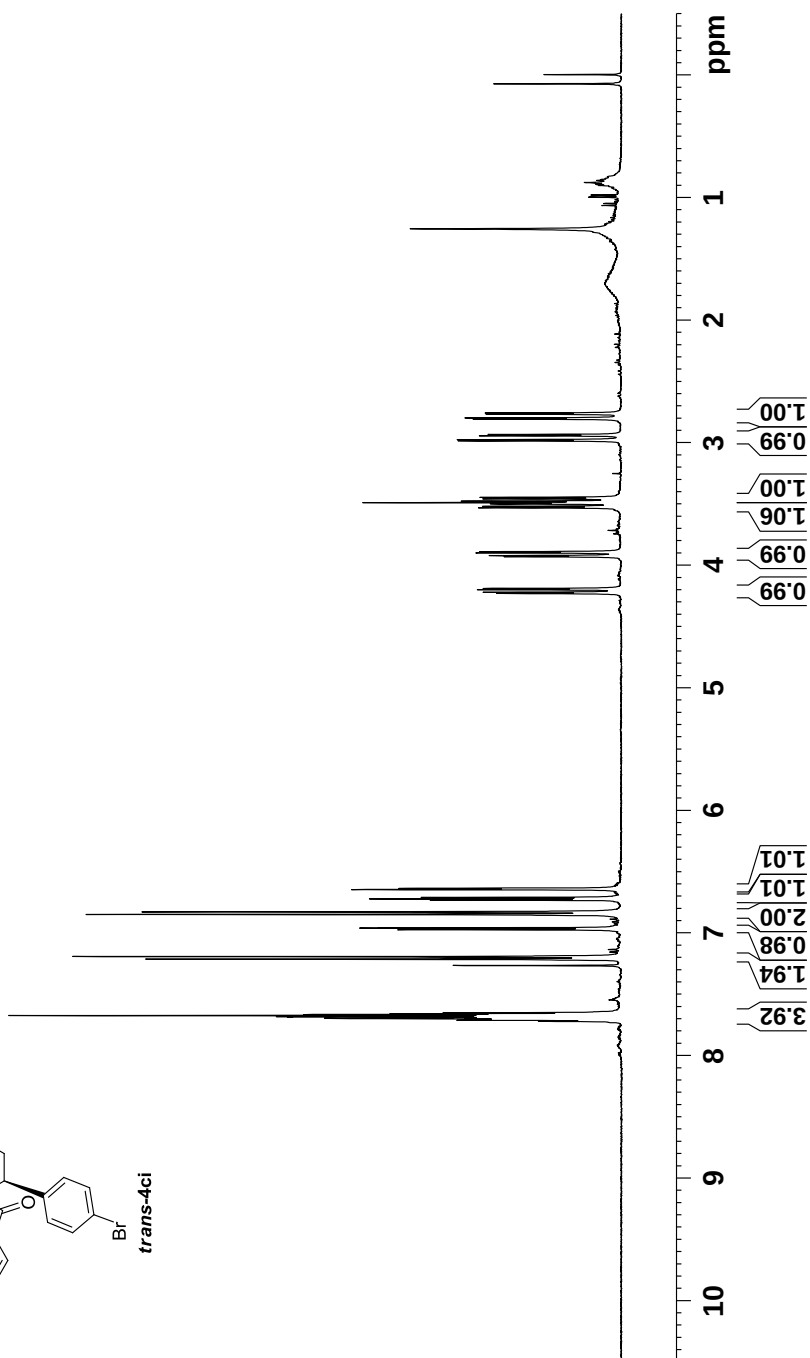
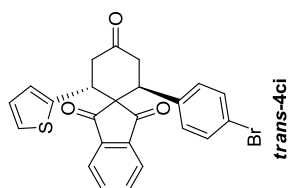
F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME Allen-370
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150326
 Time_ 12.08
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 228.1
 DW 69.000 usec
 DE 6.50 usec
 TE 298.6 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

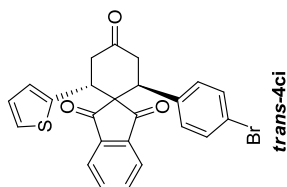
F2 - Processing parameters
 SI 16384
 SF 400.1300065 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



208.34
202.12
201.93

141.98
141.94
139.87
136.55
135.83
135.81
131.45
130.12
126.61
126.57
124.61
122.91
122.87
121.59

77.32
77.00
76.69
61.10
43.16
43.08
41.87
39.31



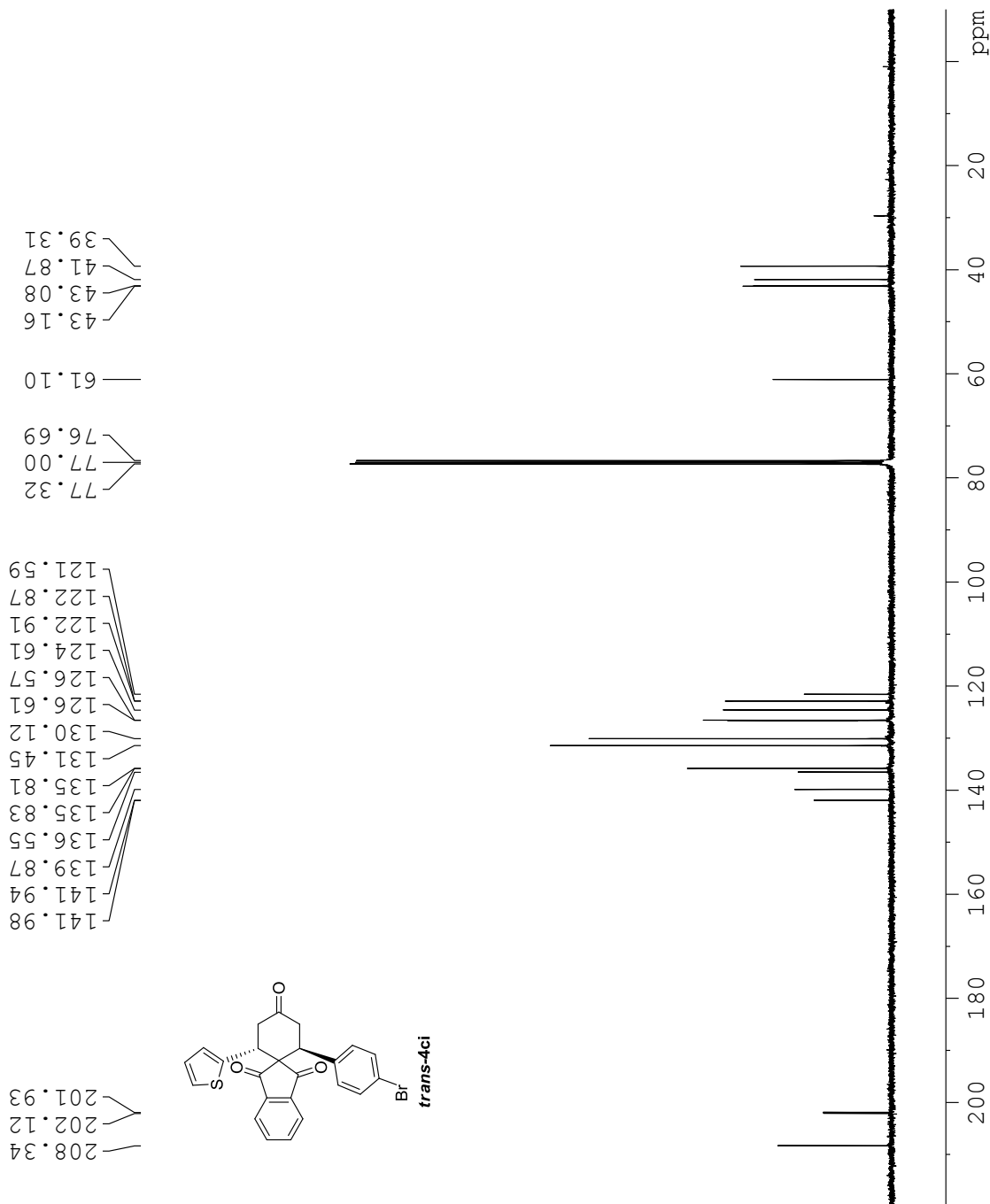
Current Data Parameters
NAME Allen-370
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150326
Time_ 12.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1284
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127723 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

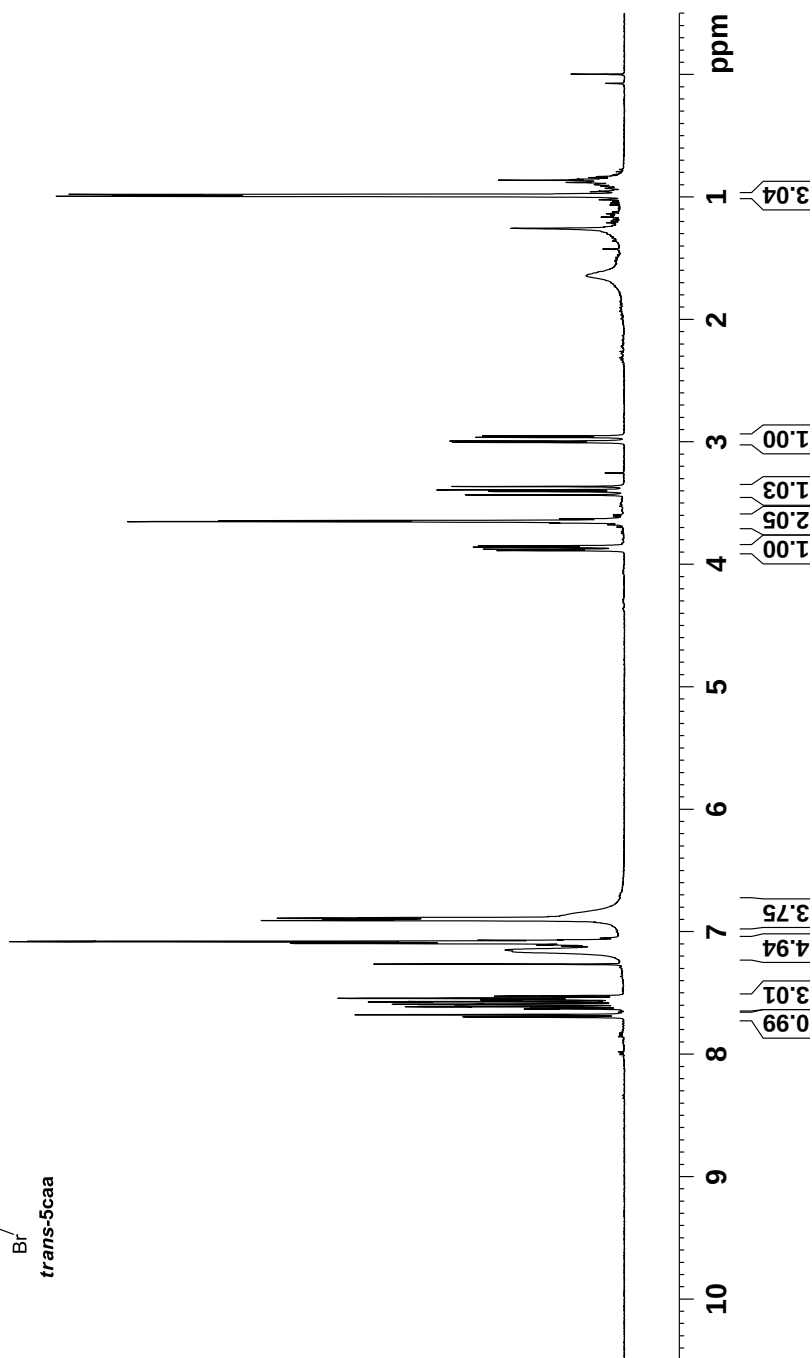
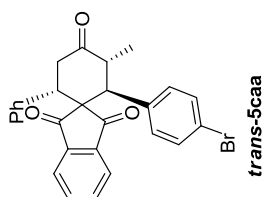


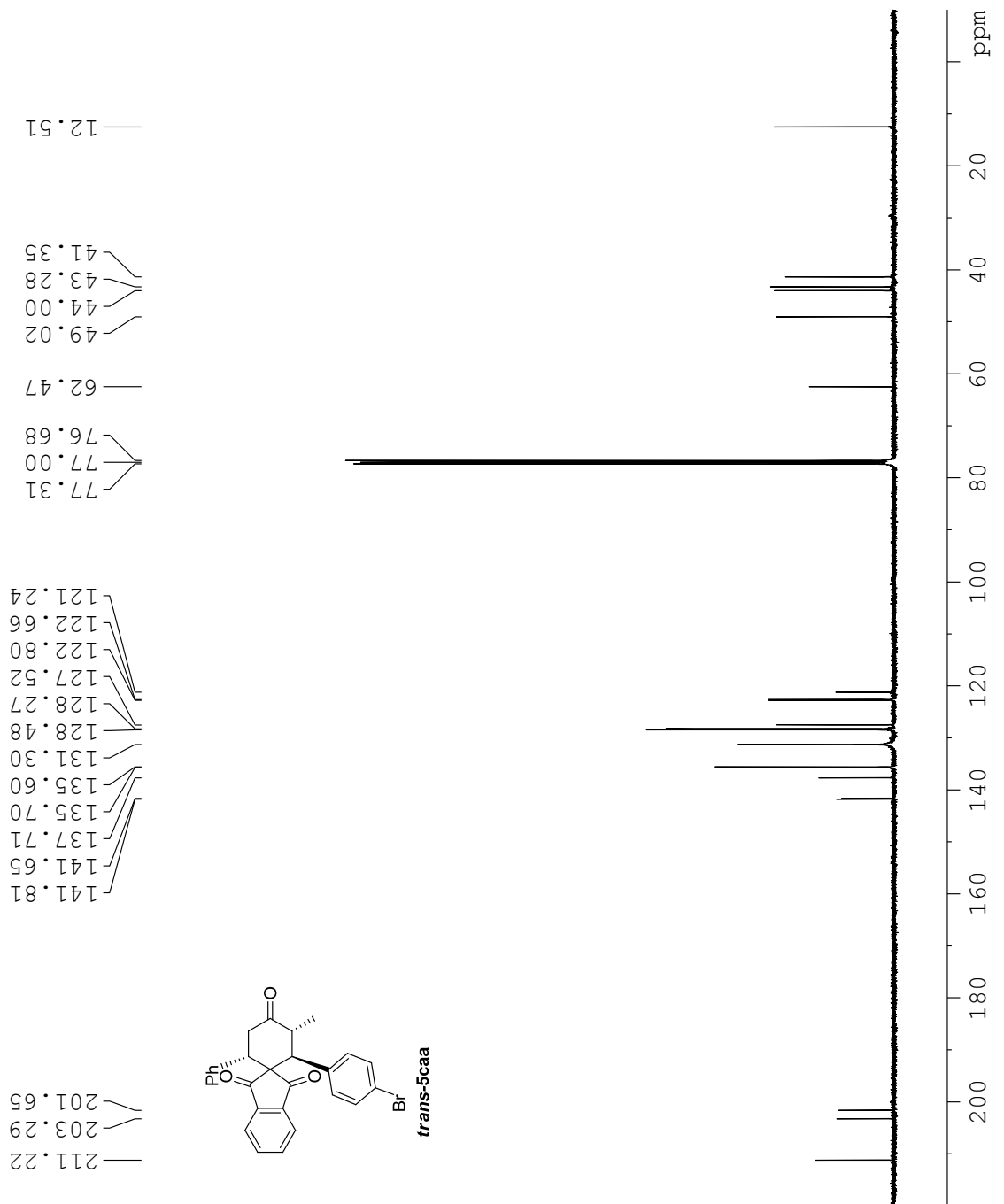
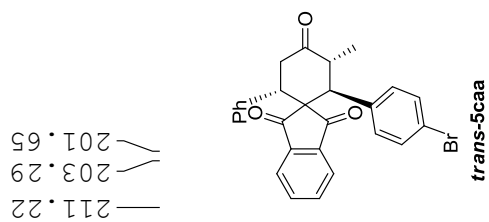
Current Data Parameters
 NAME 132-R
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150403
 Time_ 20.17
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 42
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 256
 DW 69.000 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300069 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





```

Current Data Parameters
NAME      132-R
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20150403
Time      20.21
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS         1449
DS         0
SWH        24038.461 Hz
FIDRES     0.733596 Hz
AQ         0.6815744 sec
RG         8192
DW         20.800 usec
DE         6.50 usec
TE         299.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.00 usec
PL1        6.70 dB
SFO1       100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2]  waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -5.85 dB
PL12       9.10 dB
PL13       12.10 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6127716 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
  
```

Current Data Parameters
NAME 187
EXPNO 3
PROCNO 1

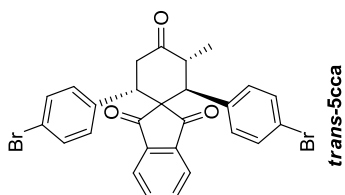
F2 - Acquisition Parameters

Date_ 20150519
Time 17.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 71
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
TD0 1

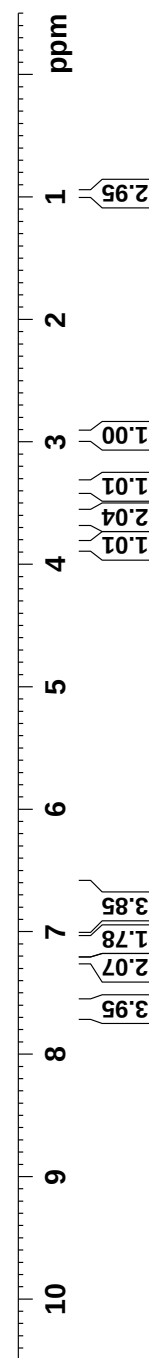
===== CHANNEL f1 =====
NUC1 1H
P1 21.45 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

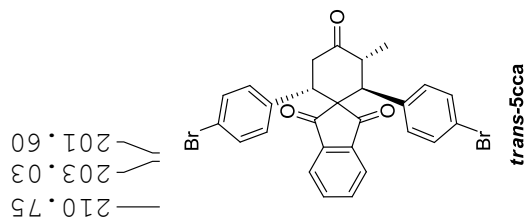
F2 - Processing parameters

SI 16384
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



S53





141.68
141.57
136.85
135.95
135.87
135.28
131.44
131.35
130.15
122.86
122.78
121.61
121.36

77.32
77.00
76.68

62.16

49.33
43.26
43.10
41.23

12.45

```

Current Data Parameters
NAME          187
EXPNO         5
PROCNO        1

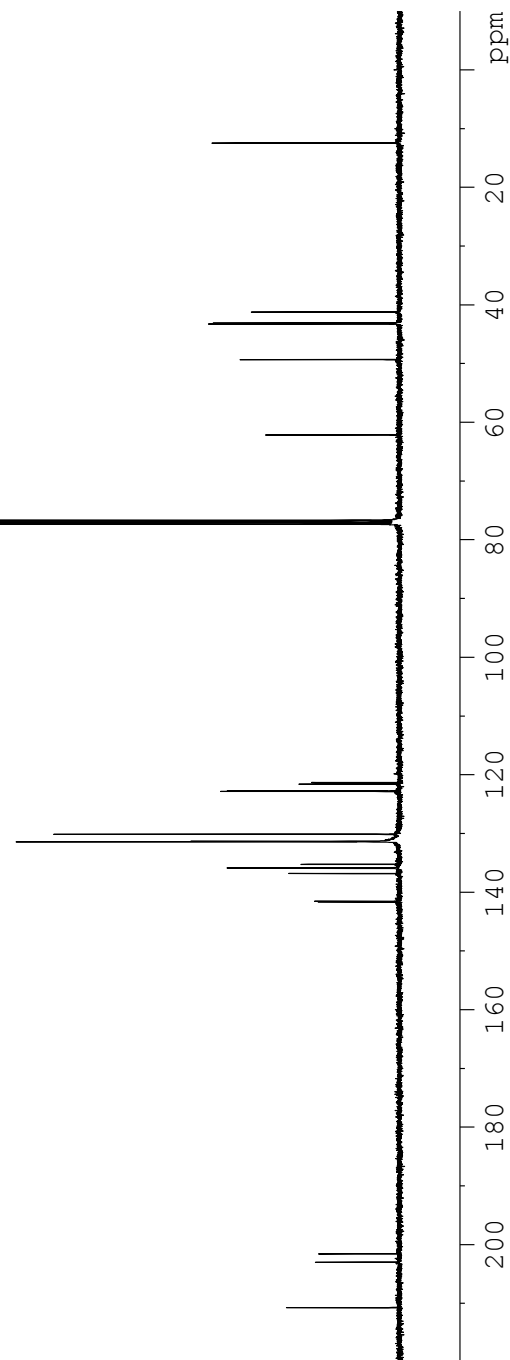
F2 - Acquisition Parameters
Date_         20150519
Time          18.10
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDC13
NS            1074
DS            0
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG            4597.6
DW            20.800 usec
DE            6.50 usec
TE            297.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            10.00 usec
PL1           6.70 dB
SFO1          100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2     waltz16
NUC2          1H
PCPD2         90.00 usec
PL2           -5.85 dB
PL12          6.00 dB
PL13          9.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI            32768
SF            100.6127723 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00

```

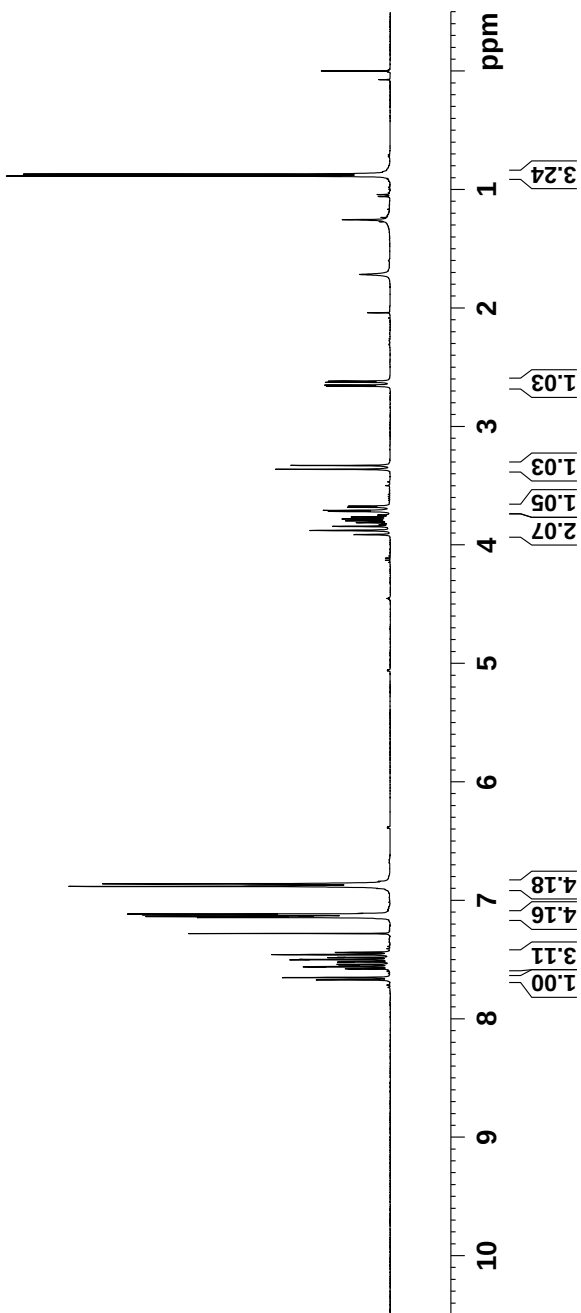
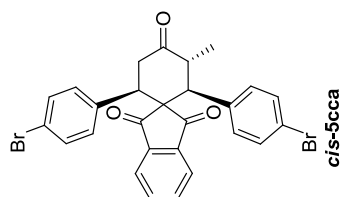


Current Data Parameters
 NAME 217
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150728
 Time 20.13
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 64
 DW 69.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 5.30 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300011 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



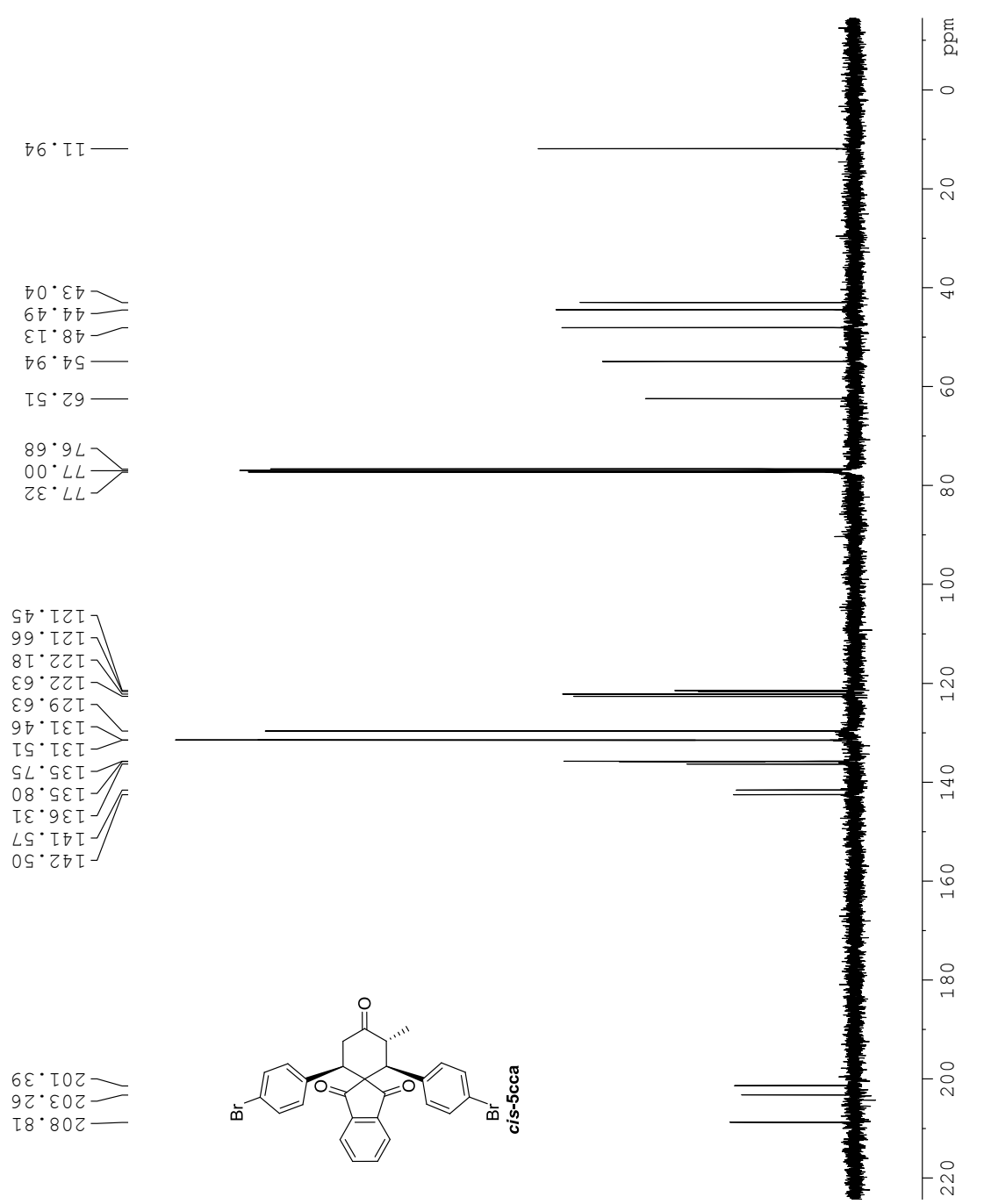
Current Data Parameters
NAME 217
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150728
Time 20.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 151
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.60 dB
PL12 20.40 dB
PL13 23.40 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127739 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Maddy-250
EXPNO 3
PROCNO 1

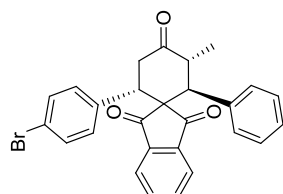
F2 - Acquisition Parameters

Date_ 20151010
Time_ 20.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 20
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 63.58
DW 69.333 usec
DE 10.50 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

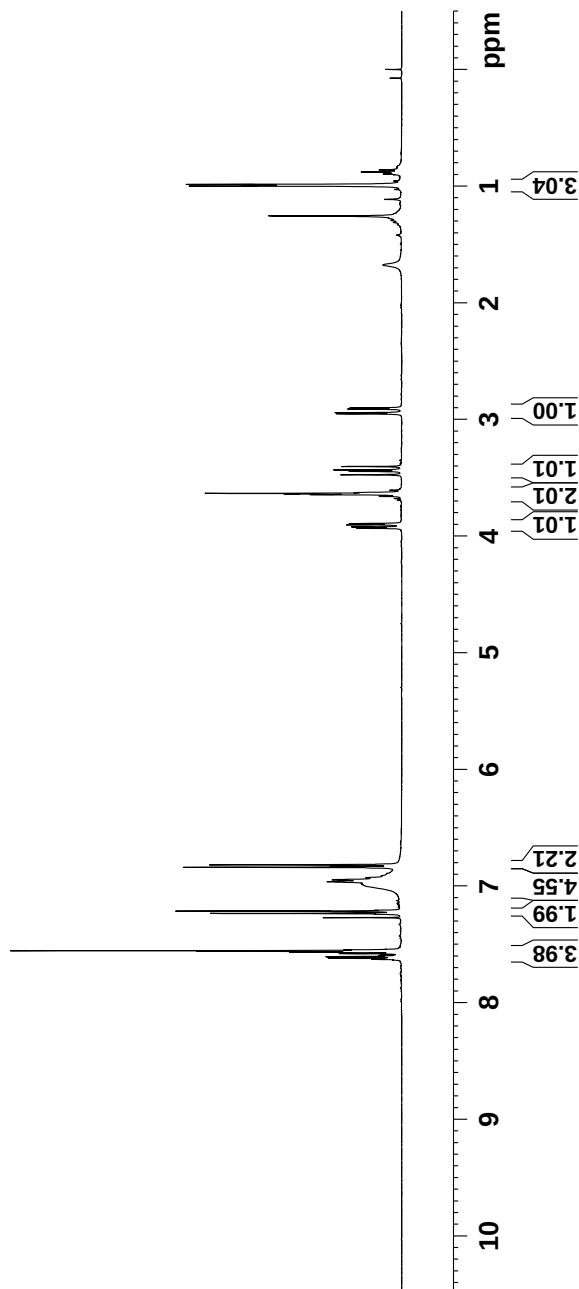
===== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

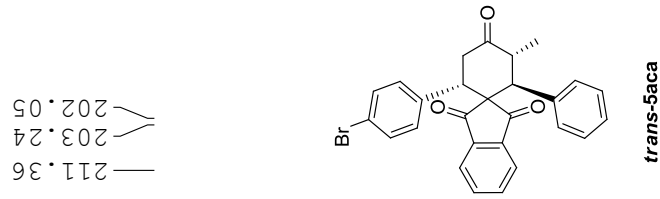
F2 - Processing parameters

SI 16384
SF 400.1300057 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



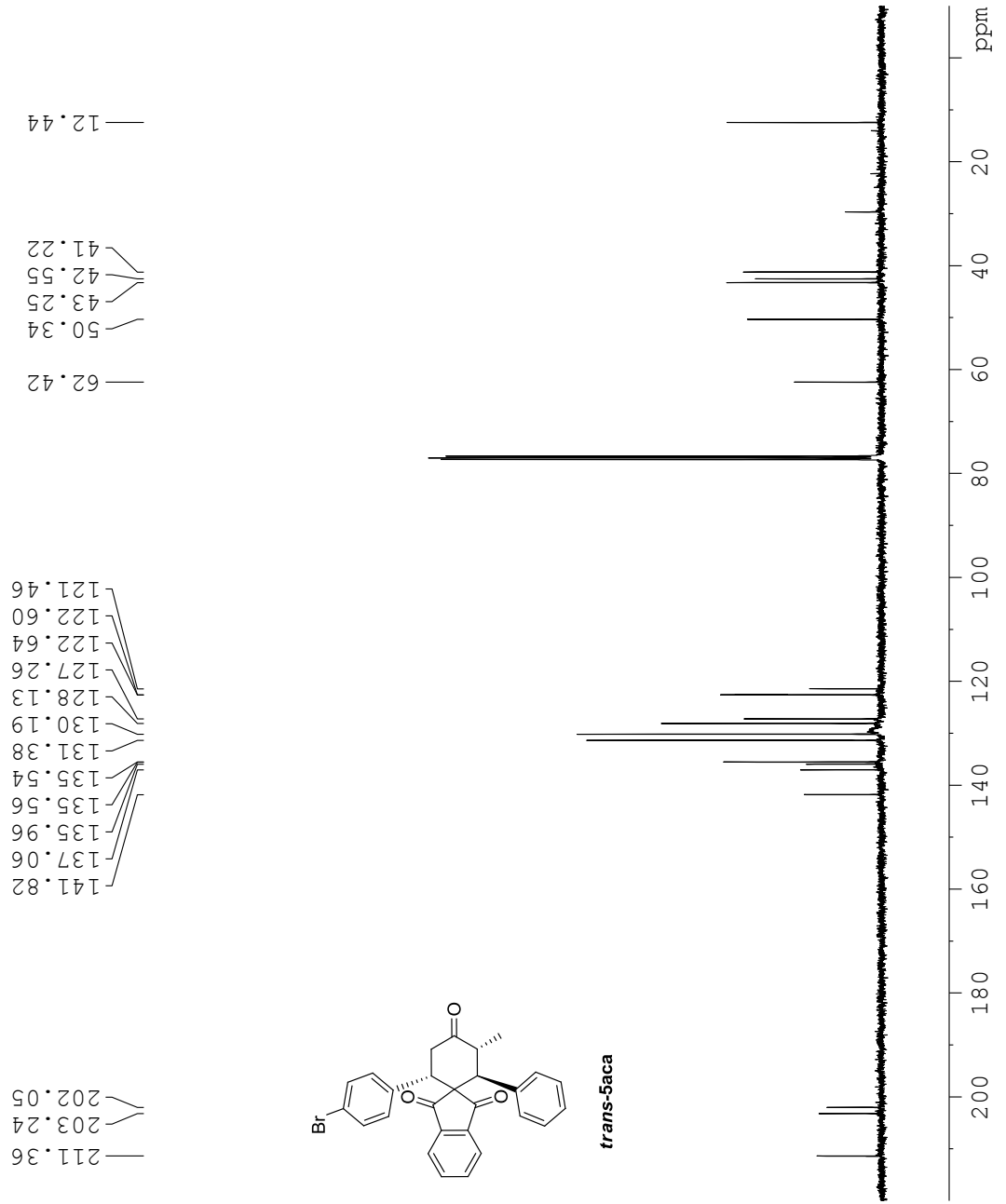
trans-5aca





141.82
137.06
135.96
135.56
135.54
131.38
130.19
128.13
127.26
122.64
122.60
121.46

62.42
50.34
43.25
42.55
41.22
12.44



Current Data Parameters
NAME Maddy-250
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151010
Time_ 20.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 225
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.5000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.33750001 W
PLW13 0.27338001 W

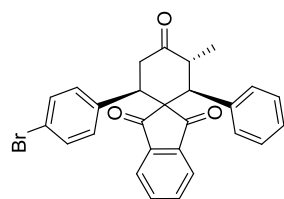
F2 - Processing parameters
SI 32768
SF 100.6127723 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME Maddy-250
EXPNO 1
PROCNO 1

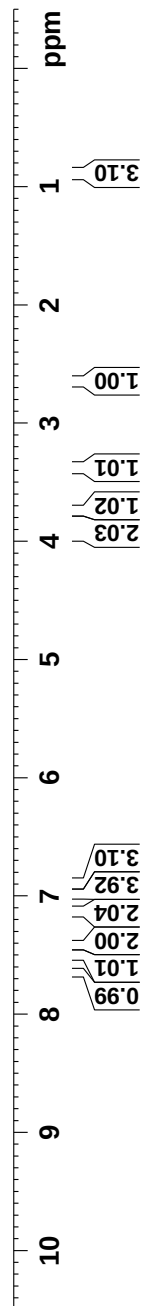
F2 - Acquisition Parameters
Date_ 20151010
Time 20.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 36.64
DW 69.333 usec
DE 10.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

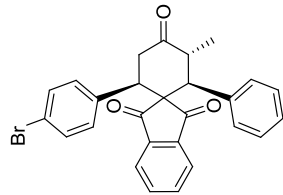
F2 - Processing parameters
SI 16384
SF 400.1299951 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



cis-5a



209.33
203.39
201.52



142.61
141.62
136.59
136.42
135.38
131.36
129.71
128.26
127.40
122.41
122.03
121.49

62.66
55.76
47.86
44.51
43.11

11.89

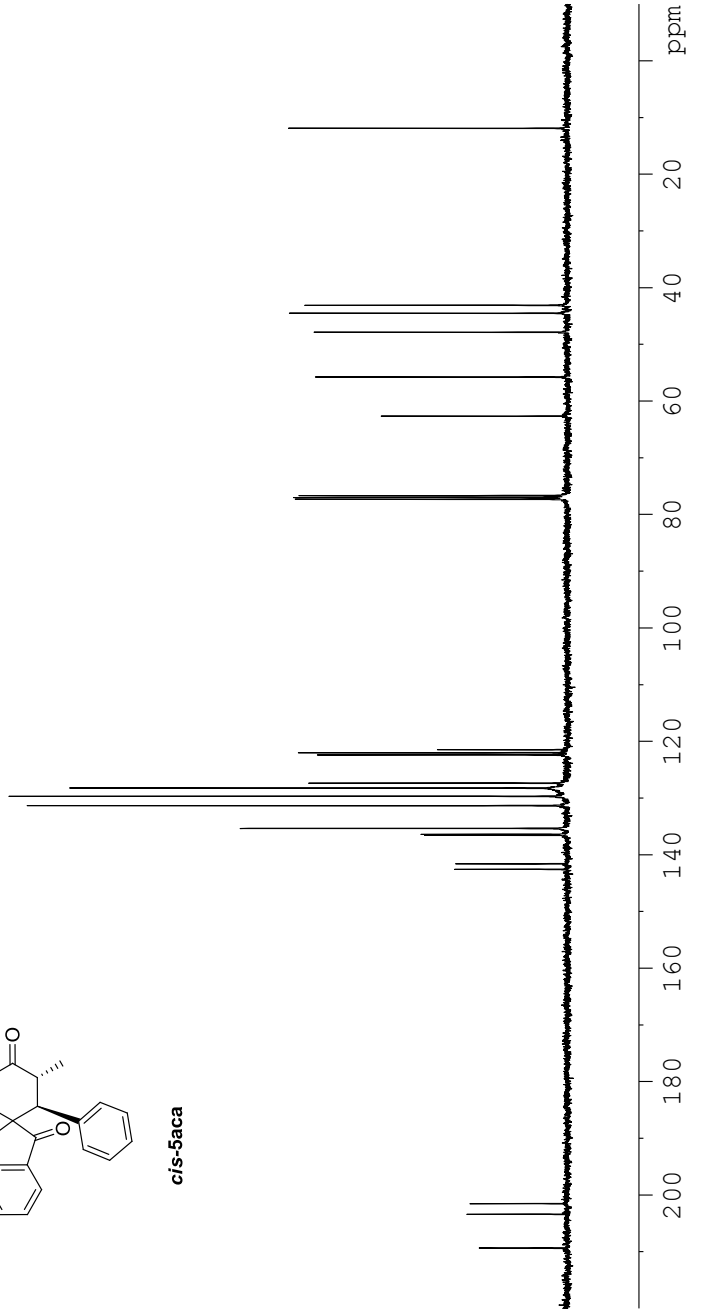
Current Data Parameters
NAME Maddy-250
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151010
Time_ 20.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 120
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.5000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.33750001 W
PLW13 0.27338001 W

F2 - Processing parameters
SI 32768
SF 100.6127786 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.00



Current Data Parameters
 NAME 181
 EXPNO 6
 PROCNO 1

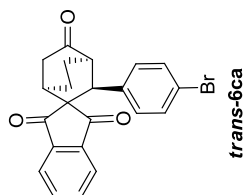
F2 - Acquisition Parameters

Date_ 20150509
 Time_ 15.36
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 30
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 114
 DW 69.000 usec
 DE 6.50 usec
 TE 299.1 K
 D1 2.0000000 sec
 TD0 1

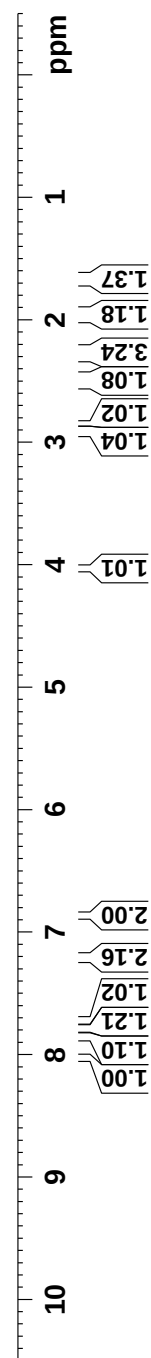
===== CHANNEL f1 =====
 NUC1 1H
 P1 21.45 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

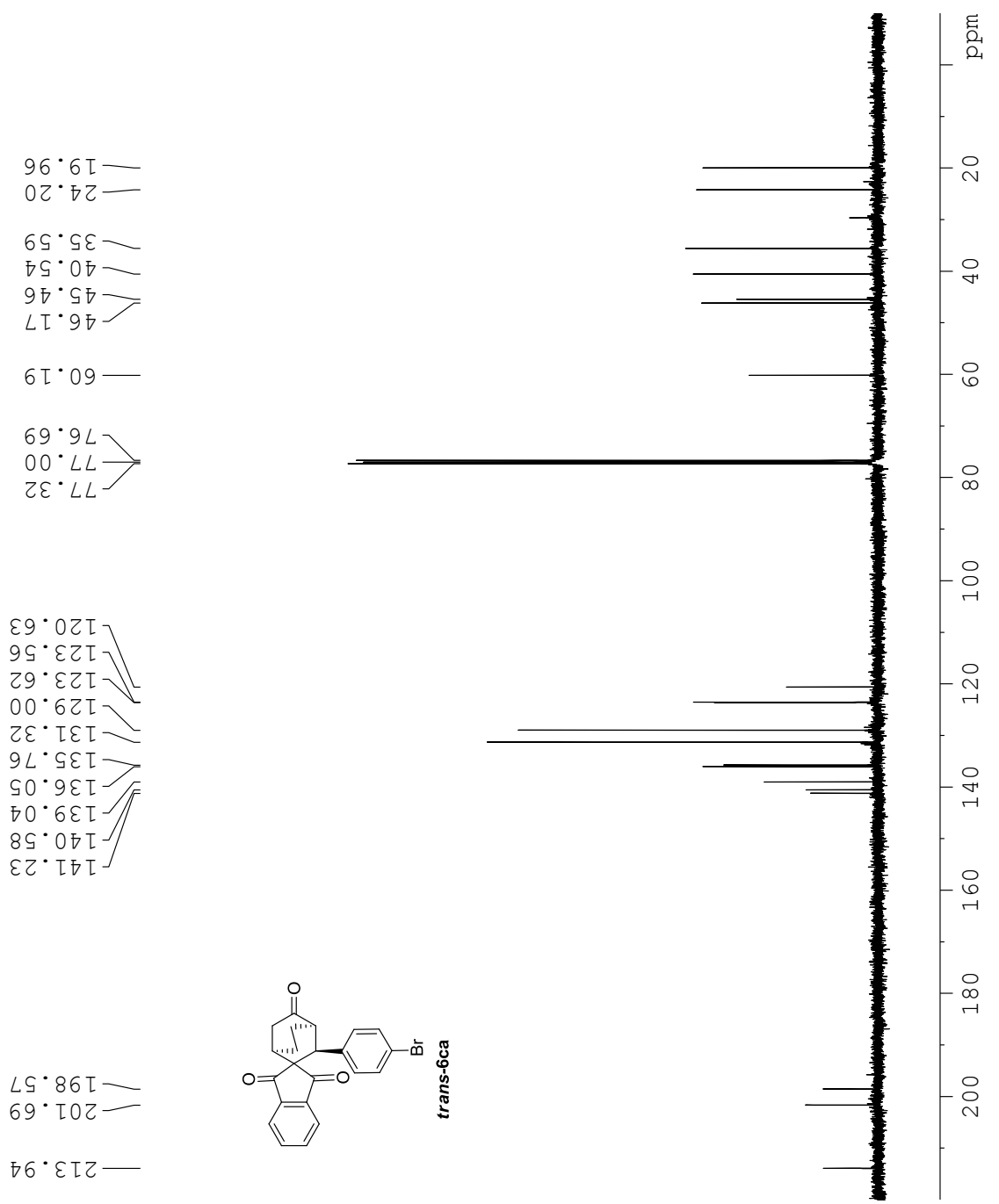
F2 - Processing parameters

SI 16384
 SF 400.1300030 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



S61





Current Data Parameters

NAME 181

EXPNO 7

PROCNO 1

F2 - Acquisition Parameters

Date_ 20150509

Time 15.40

INSTRUM spect

PROBHD 5 mm BBO BB-1H

PULPROG zgpg30

TD 32768

SOLVENT CDCl3

NS 152

DS 0

SWH 24038.461 Hz

FIDRES 0.733596 Hz

AQ 0.6815744 sec

RG 4597.6

DW 20.800 usec

DE 6.50 usec

TE 299.3 K

D1 2.00000000 sec

D11 0.03000000 sec

TD0 1

==== CHANNEL f1 =====

NUC1 13C

P1 10.00 usec

PL1 6.70 dB

SFO1 100.6233325 MHz

==== CHANNEL f2 =====

CPDPRG[2] waltz16

NUC2 1H

PCPD2 90.00 usec

PL2 -5.85 dB

PL12 6.00 dB

PL13 9.00 dB

SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768

SF 100.6127738 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.00

Current Data Parameters
NAME 214
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

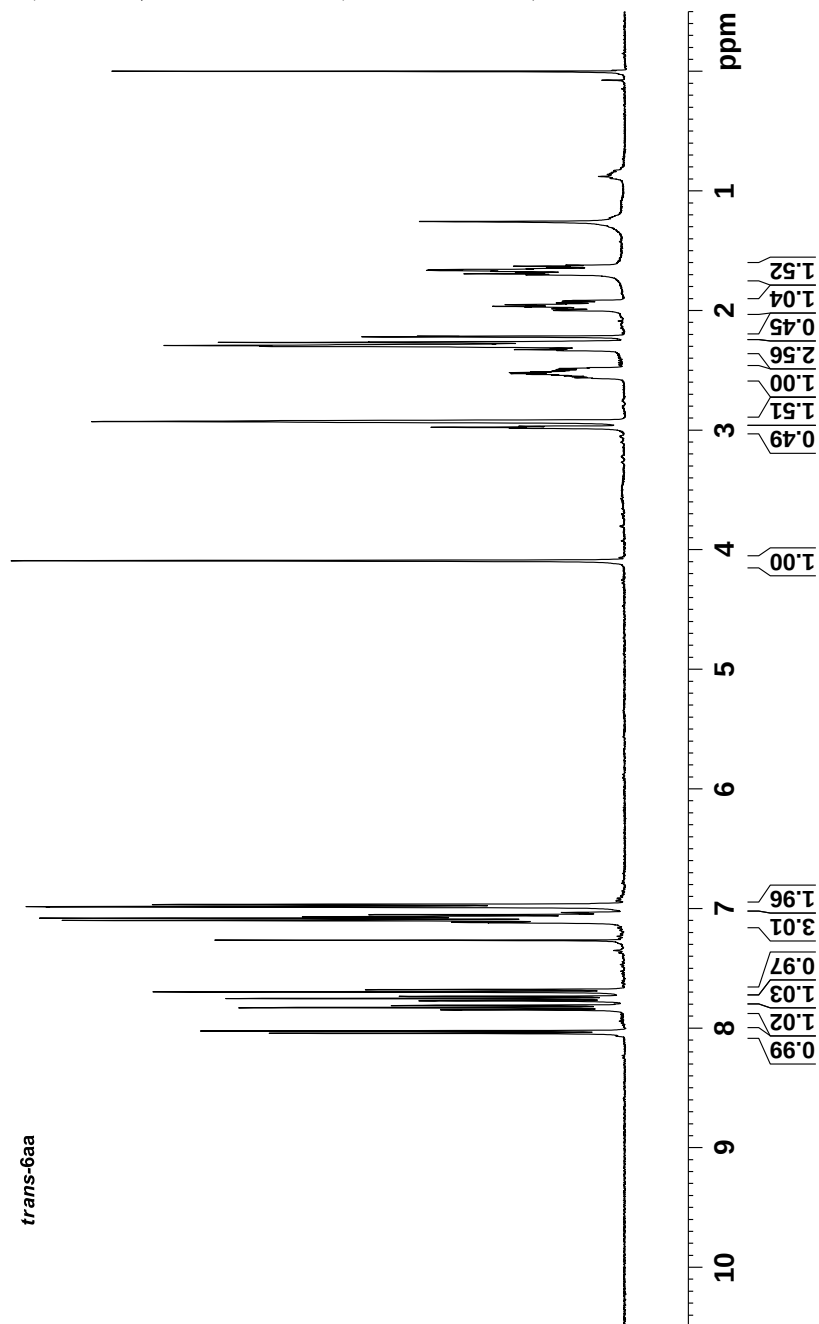
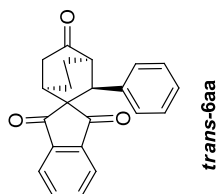
Date_ 20150701
Time_ 15.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.260921 sec
RG 362
DW 69.000 usec
DE 6.50 usec
TE 299.1 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====

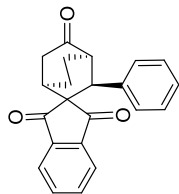
NUC1 1H
P1 21.45 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters

SI 16384
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



214.38
202.16
198.77



trans-6aa

141.42
140.69
140.07
135.93
135.62
128.30
127.20
126.68
123.60
123.48

77.36
77.04
76.72

60.33

46.30
46.18
40.65
35.63

24.41
20.16

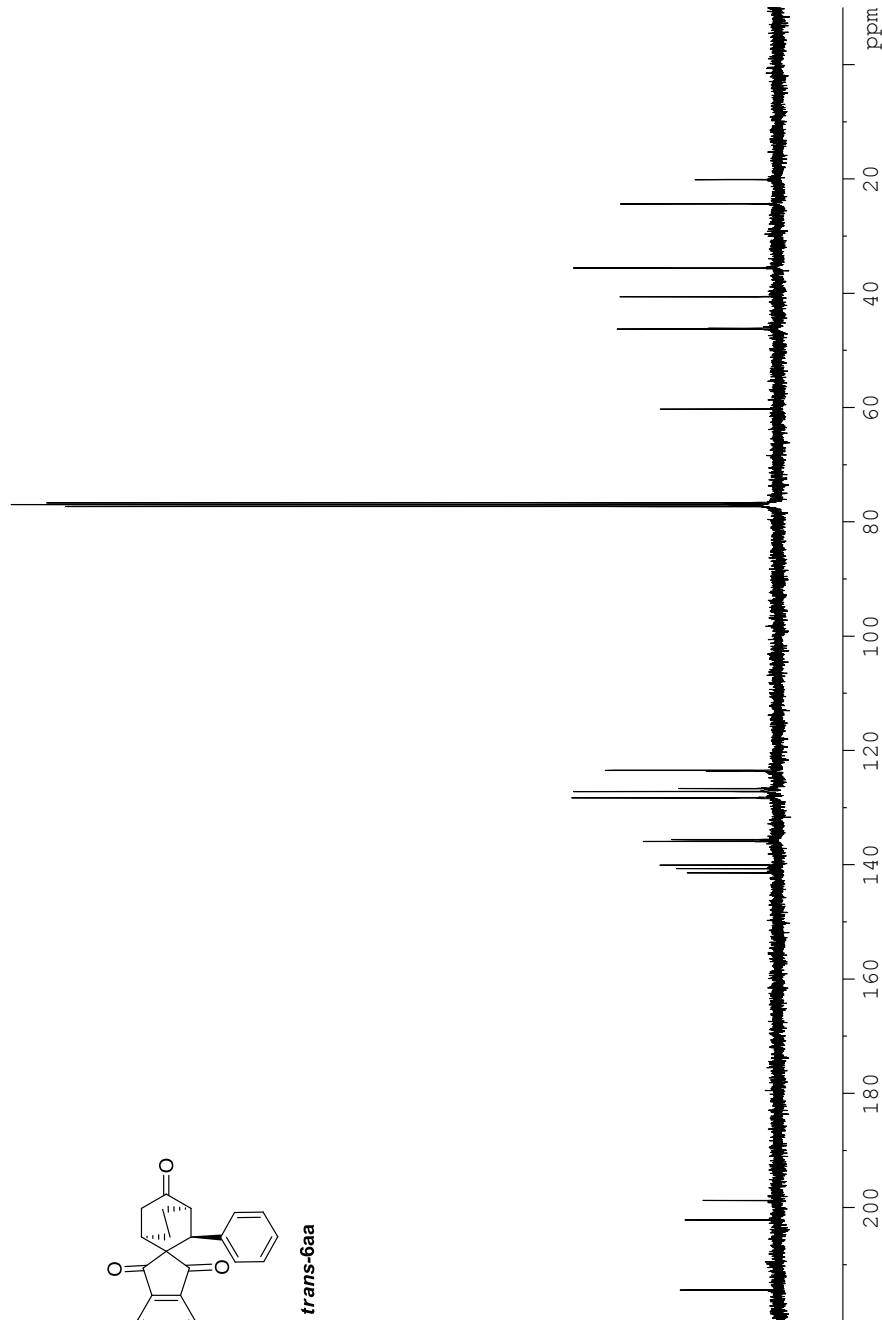
Current Data Parameters
NAME 214
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150701
Time_ 15.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 445
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 9195.2
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

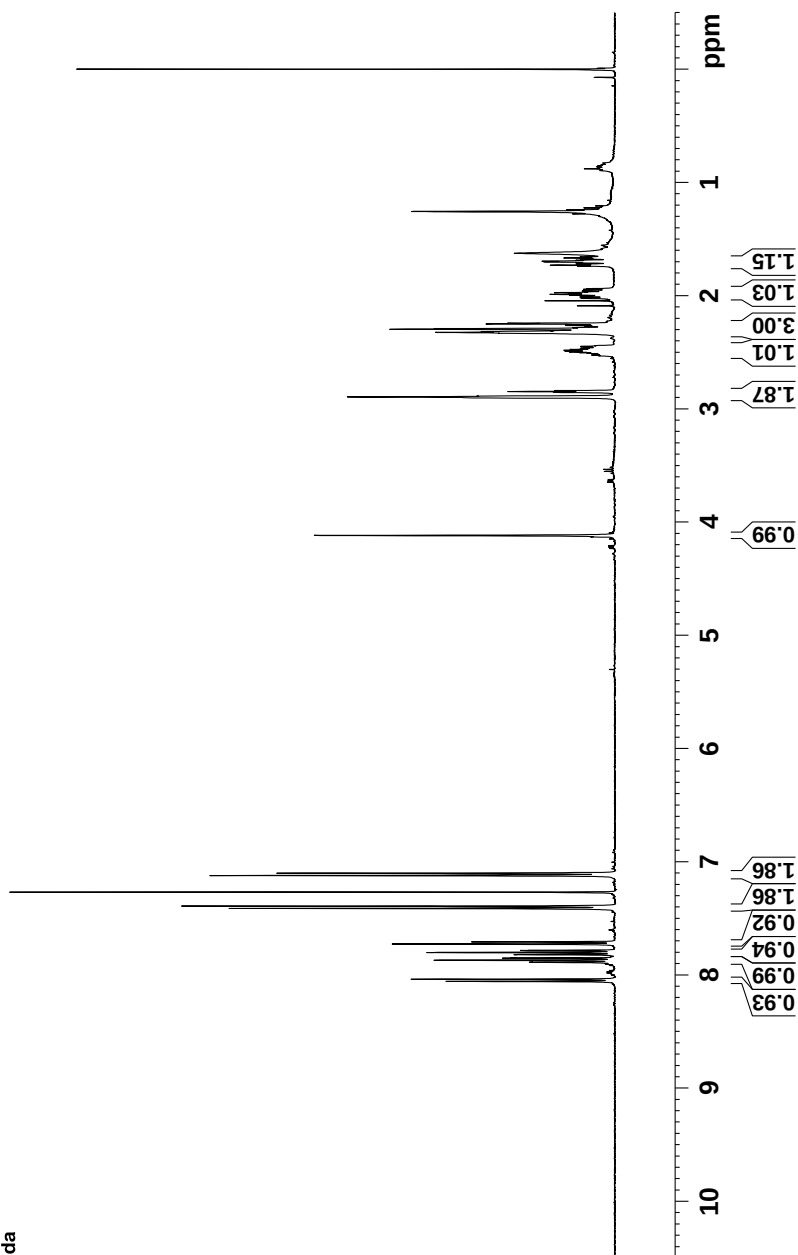
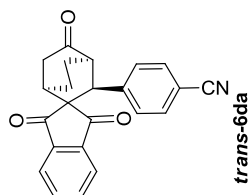


Current Data Parameters
NAME 215
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150703
Time 20.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 574.7
DW 69.000 usec
DE 6.50 usec
TE 298.9 K
D1 2.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 21.45 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300060 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



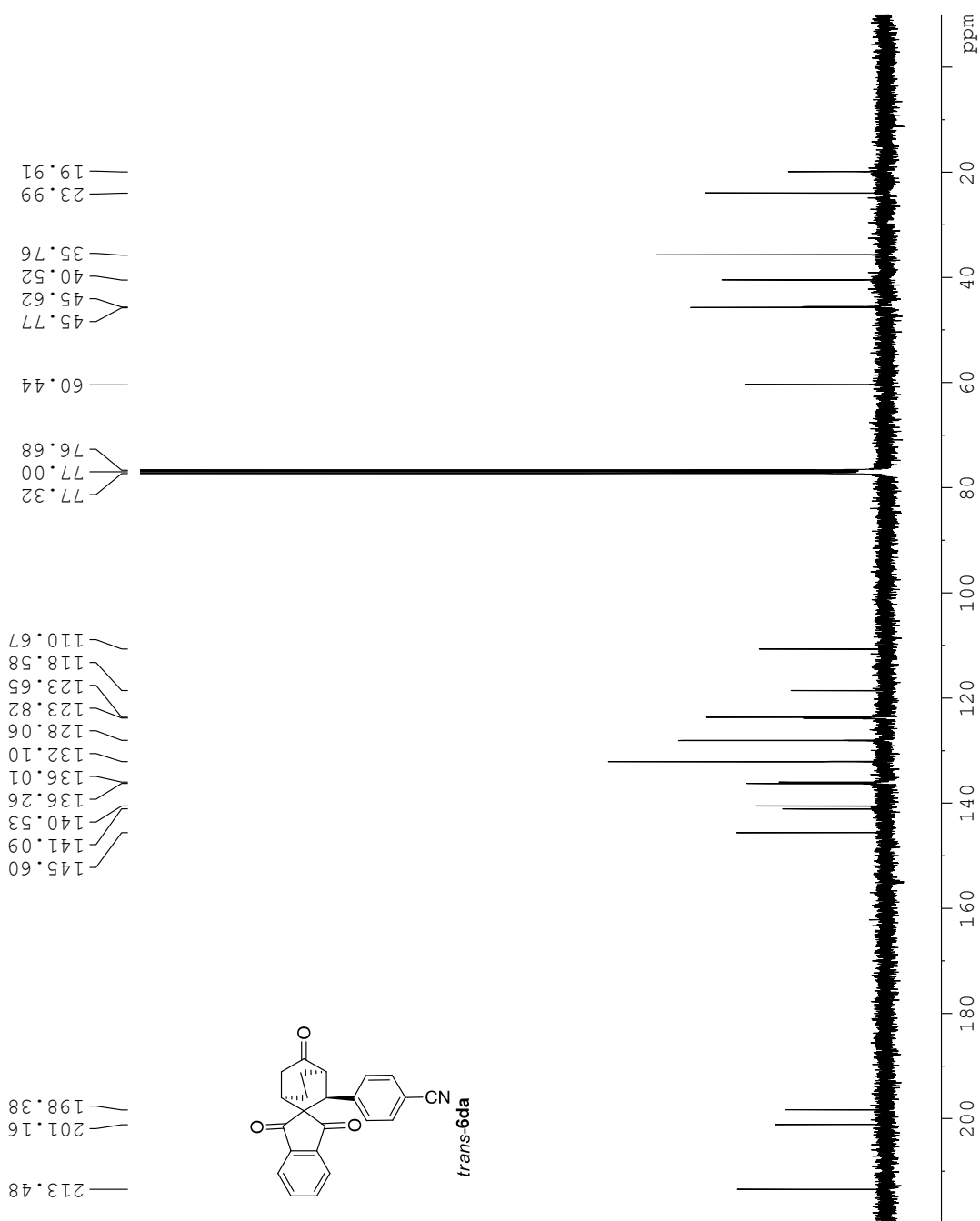
Current Data Parameters
NAME 215
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150703
Time_ 20.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 877
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 9195.2
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

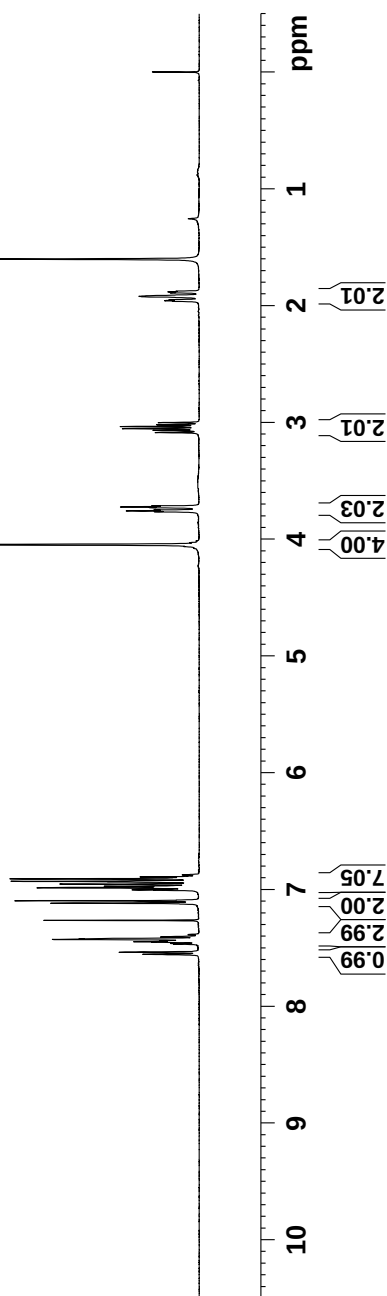
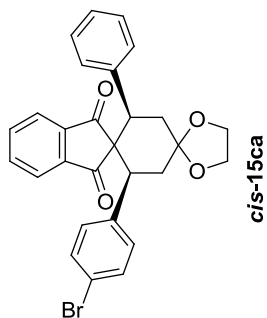


Current Data Parameters
NAME 244
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150930
Time_ 16.36
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 50
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.260921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PL1 1.80 dB
SFO1 400.1324008 MHz

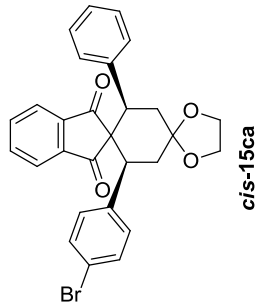
F2 - Processing parameters
SI 16384
SF 400.1300079 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



203.18
203.08

142.61
141.91
138.70
138.24
135.14
135.03
131.19
130.24
128.34
128.10
127.15
122.17
121.93
121.00
108.39

64.67
64.61
62.31
46.99
45.84
36.40
36.23



S68

```

Current Data Parameters
NAME                244
EXPNO                2
PROCNO              1

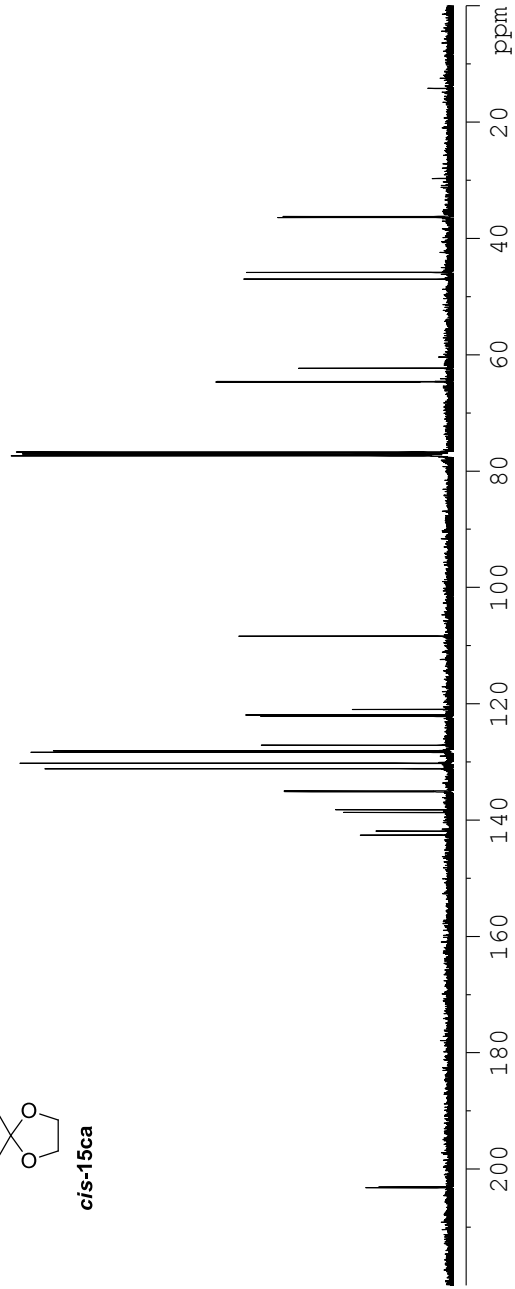
F2 - Acquisition Parameters
Date_                20150926
Time_                16.58
INSTRUM              spect
PROBHD               5 mm BBO BB-1H
PULPROG              zgpg30
TD                   32768
SOLVENT              CDCl3
NS                   162
DS                    0
SWH                  24038.461 Hz
FIDRES               0.733596 Hz
AQ                   0.6815744 sec
RG                    4096
DW                   20.800 usec
DE                   6.50 usec
TE                   296.7 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                  1

===== CHANNEL f1 =====
NUC1                  13C
P1                    9.00 usec
PL1                   7.00 dB
SFO1                 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2]            waltz16
NUC2                  1H
PCPD2                90.00 usec
PL2                   1.80 dB
PL12                 17.00 dB
PL13                 20.00 dB
SFO2                 400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF                  100.6127690 MHz
WDW                   EM
SSB                   0
LB                   1.00 Hz
GB                   0
PC                   1.00

```

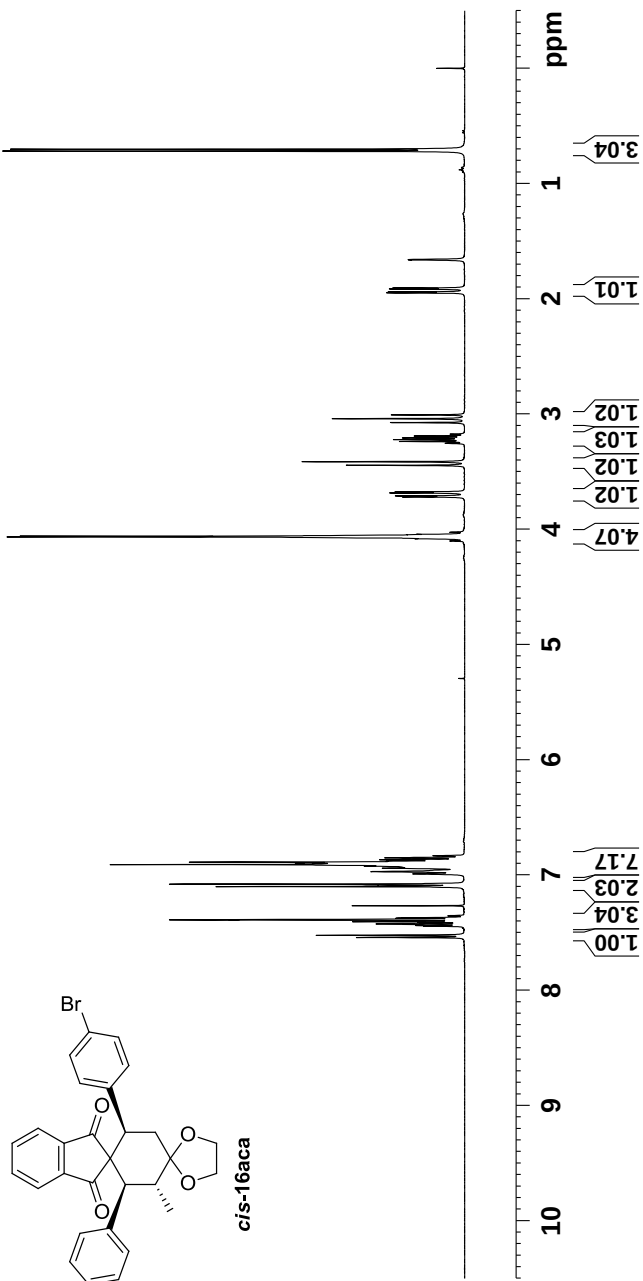


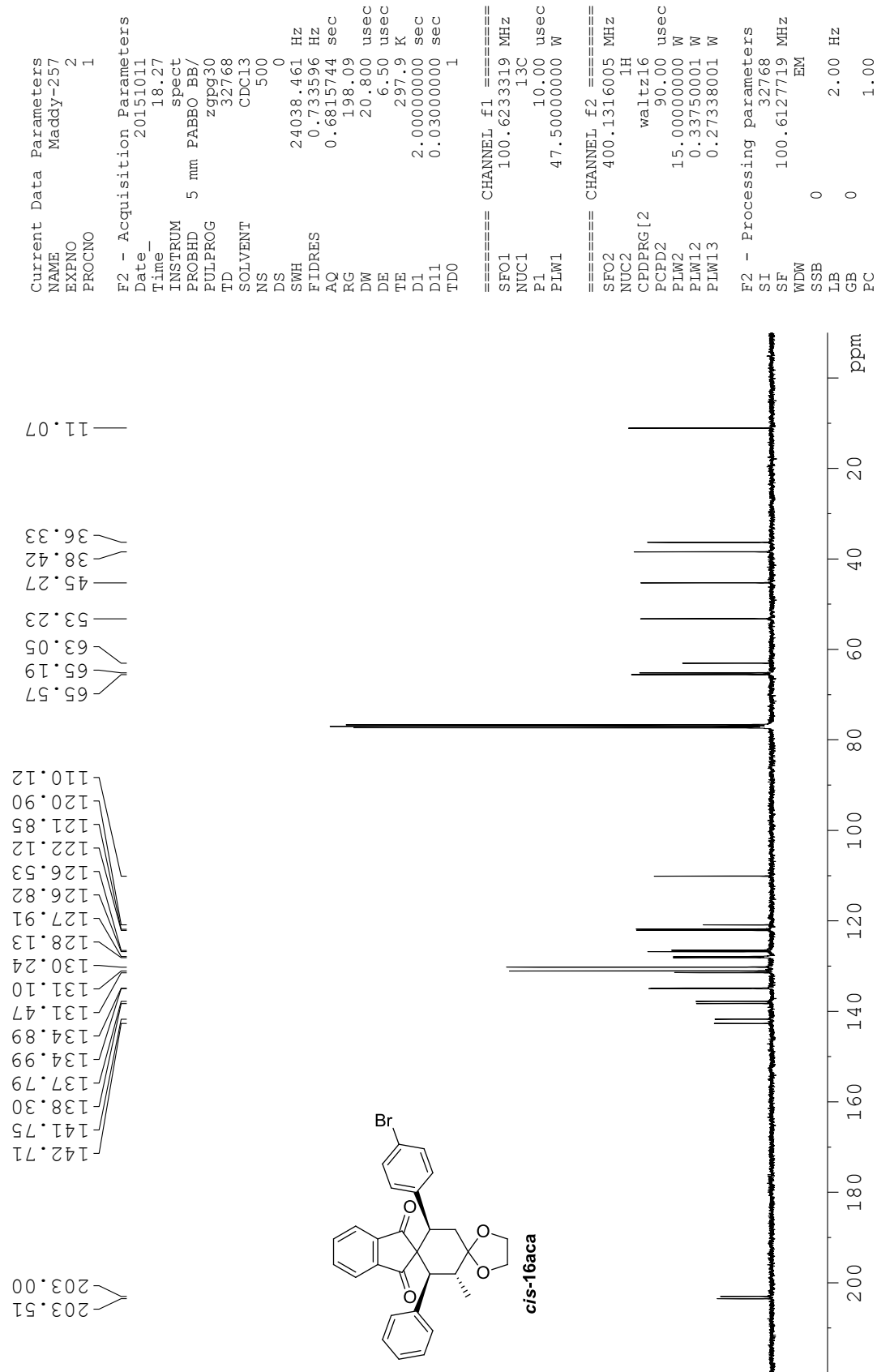
Current Data Parameters
NAME Maddy-257
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151011
Time_ 18.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 63.58
DW 69.333 usec
DE 10.50 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

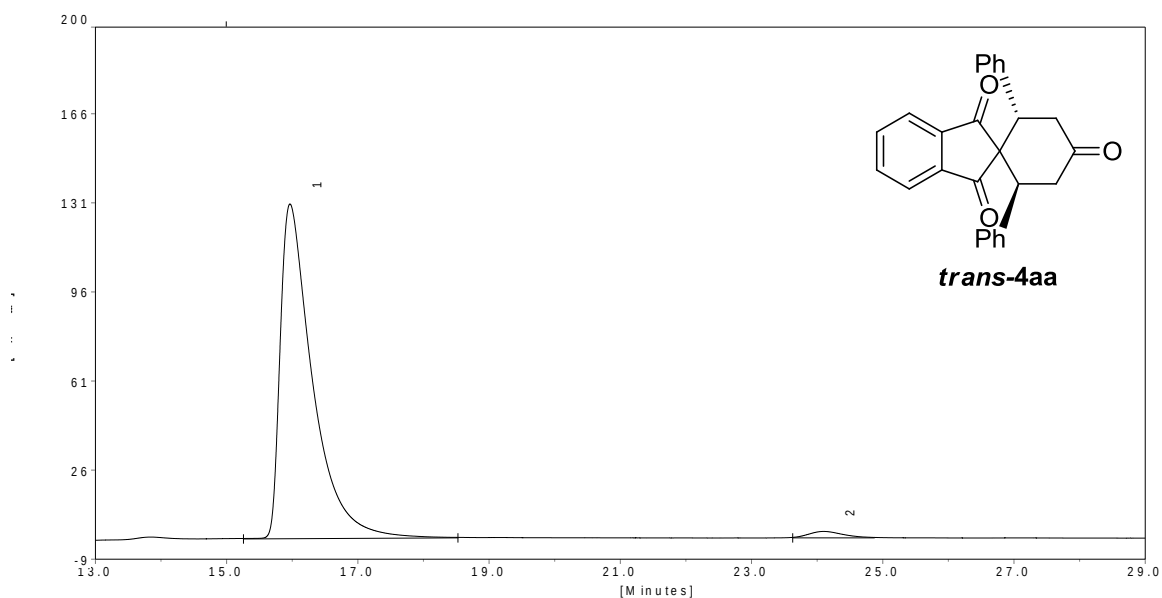




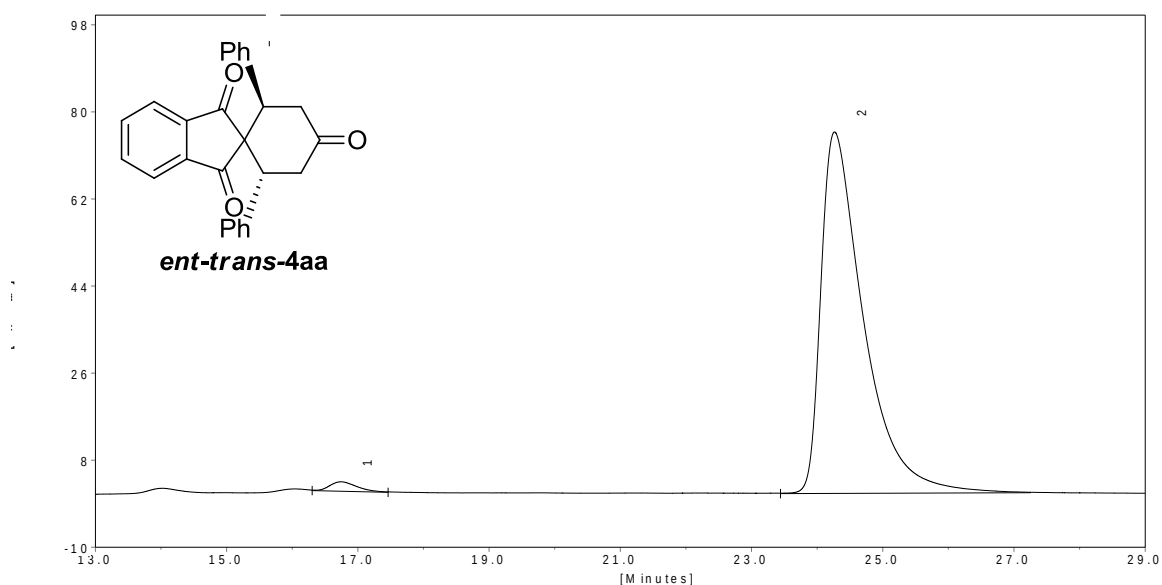
5. HPLC Chromatograms for all compounds:

HPLC chromatogram for **trans-4aa**:

Column : Chiralpak IB	Flow Rate:1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



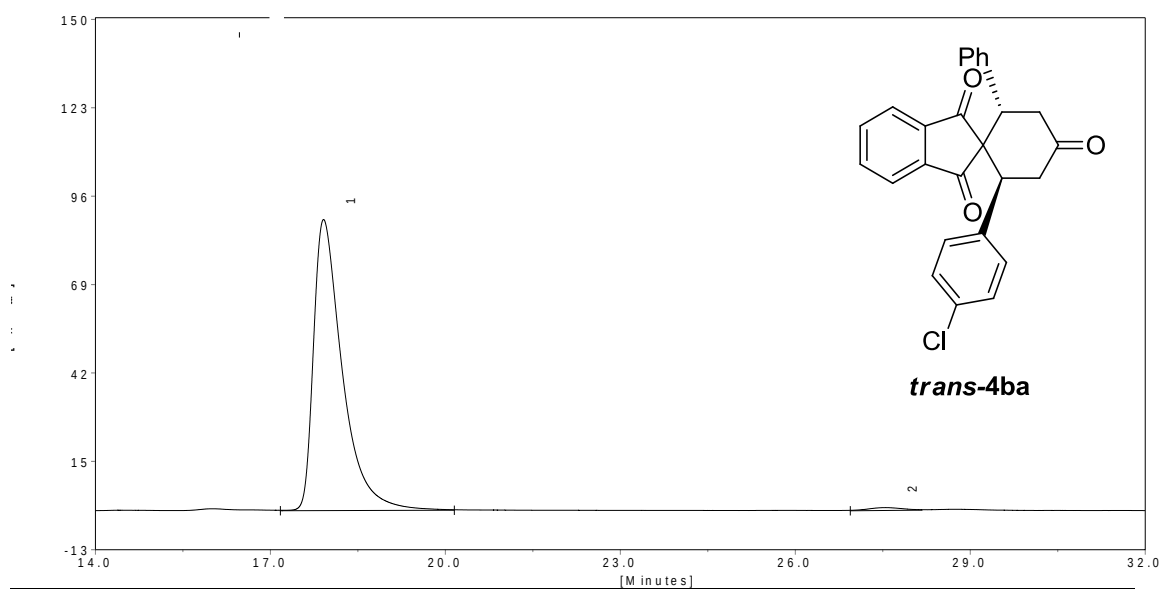
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
15.97	131.33	4468.13	98.2495
24.09	2.35	79.61	1.7505



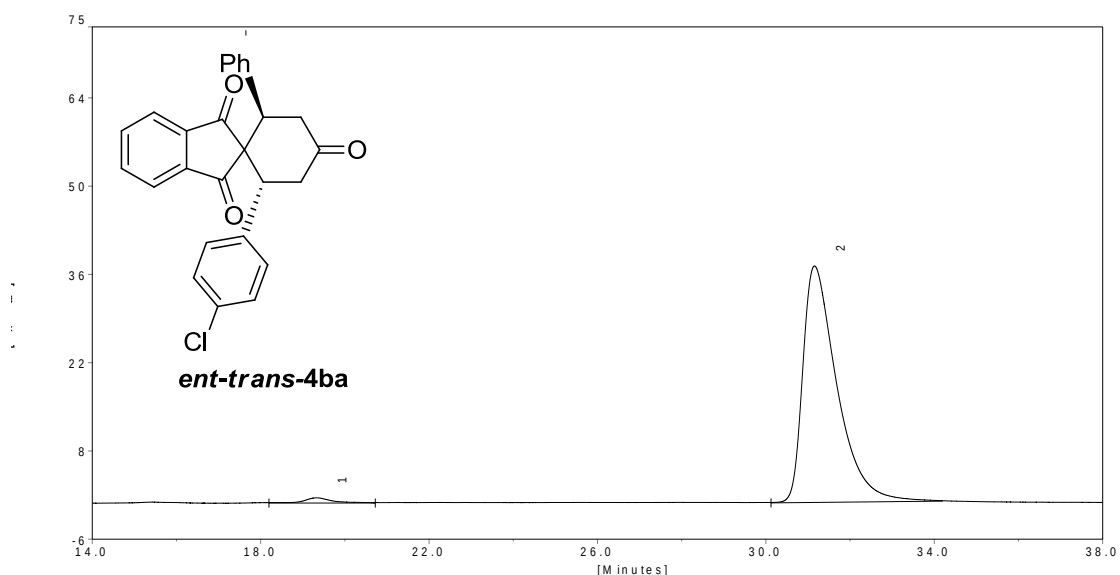
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
16.73	1.85	50.12	1.4706
24.27	74.64	3357.93	98.5294

HPLC chromatogram for **trans-4ba**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



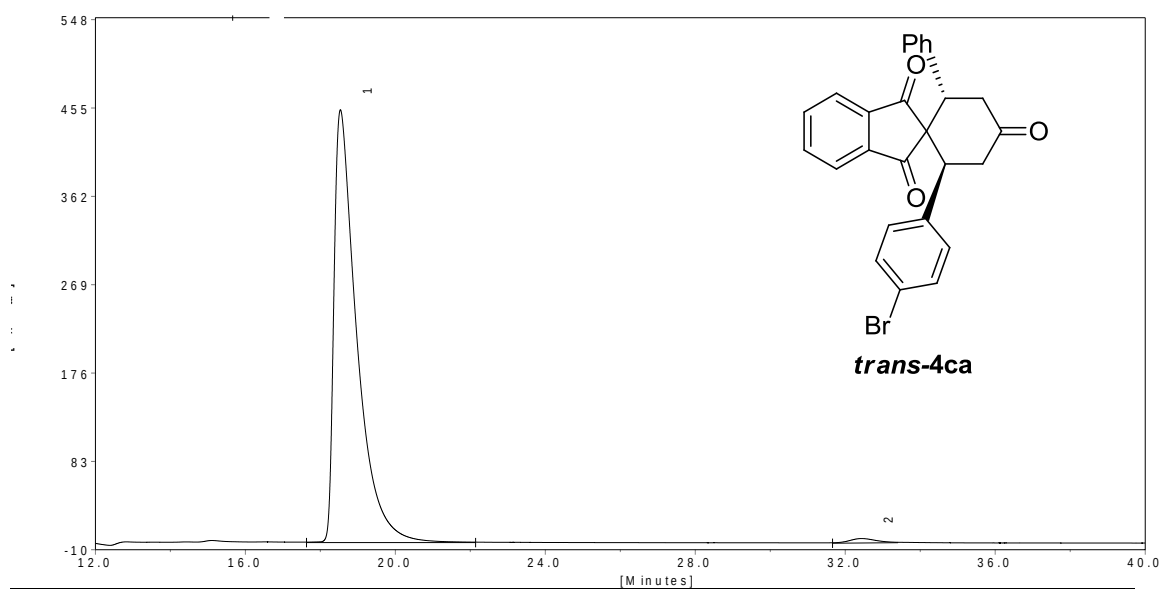
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
17.91	88.78	3029.24	99.1417
27.54	0.73	26.23	0.8583



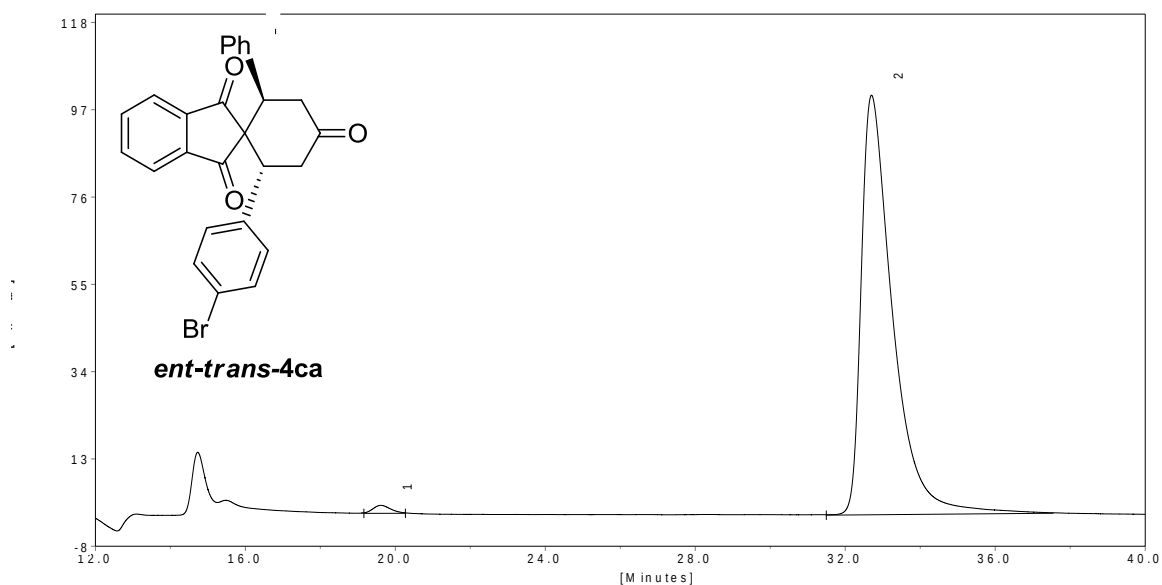
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
19.32	0.75	29.11	1.3726
31.16	37.44	2091.37	98.6274

HPLC chromatogram for **trans-4ca**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



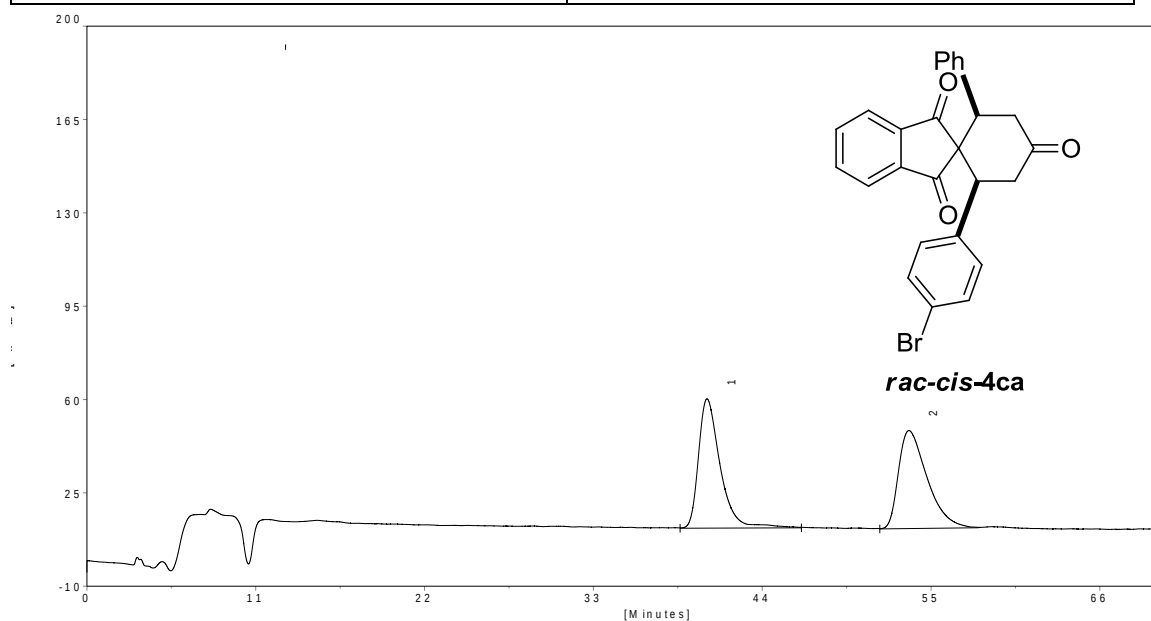
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
18.53	455.17	19126.61	99.0186
32.43	4.21	189.57	0.9814



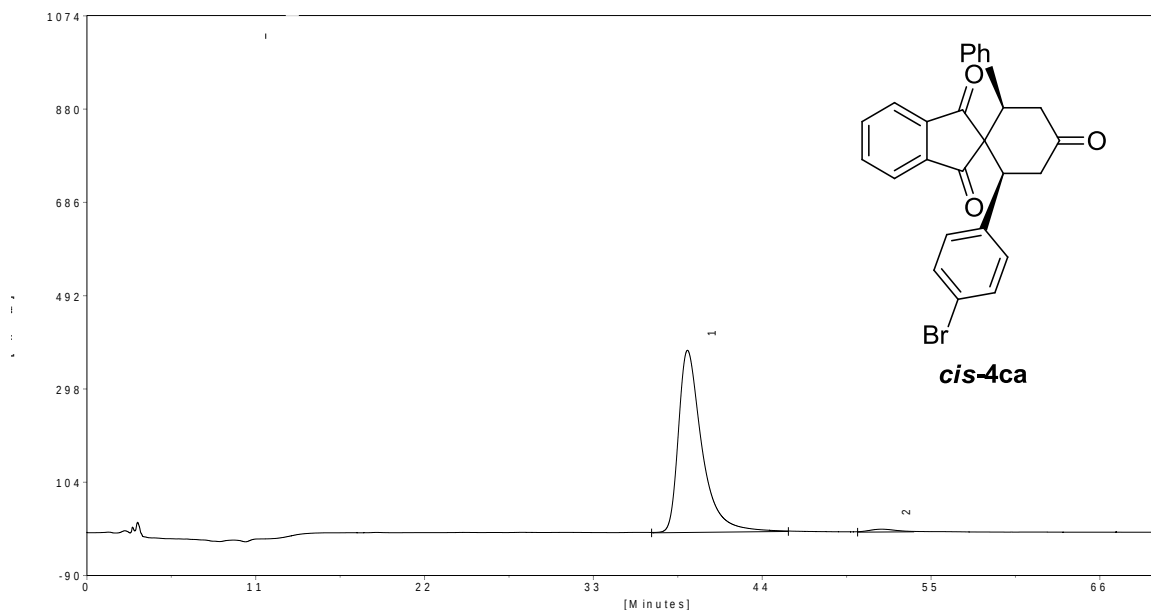
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
19.61	1.81	55.69	0.9429
32.70	100.82	5850.68	99.0571

HPLC chromatogram for *cis-4ca*:

Column : Chiralpak AD-H	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



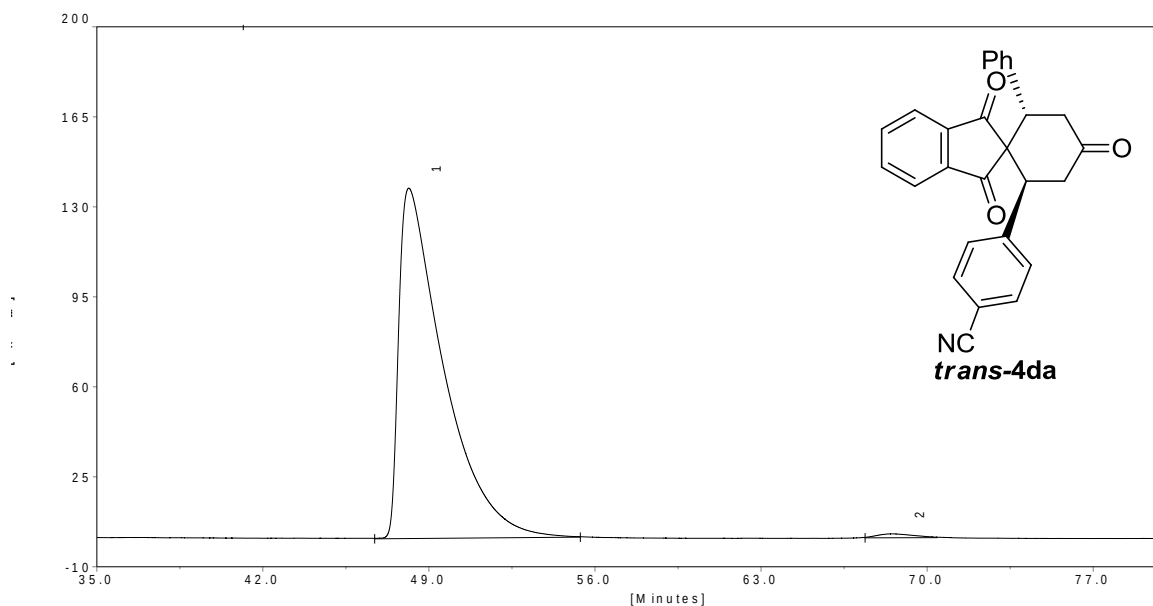
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
38.63	40.40	4696.46	49.9903
51.63	53.56	4698.29	50.0097



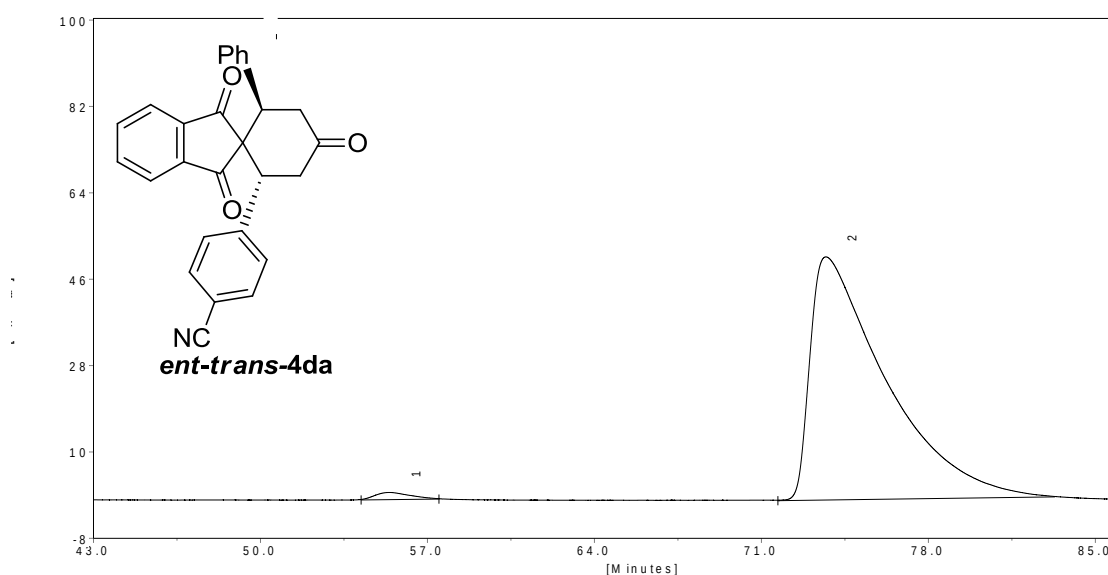
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
39.13	378.07	39948.79	98.6835
51.80	4.99	532.95	1.3165

HPLC chromatogram for **trans-4da**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



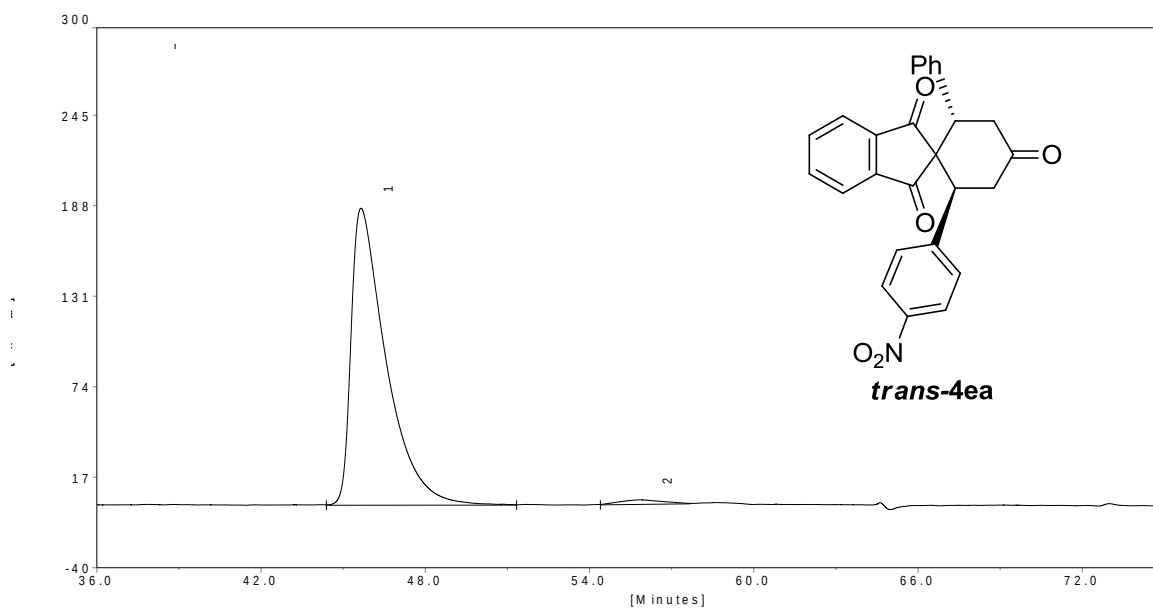
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
48.15	136.10	17759.41	99.2701
68.52	1.34	130.58	0.7299



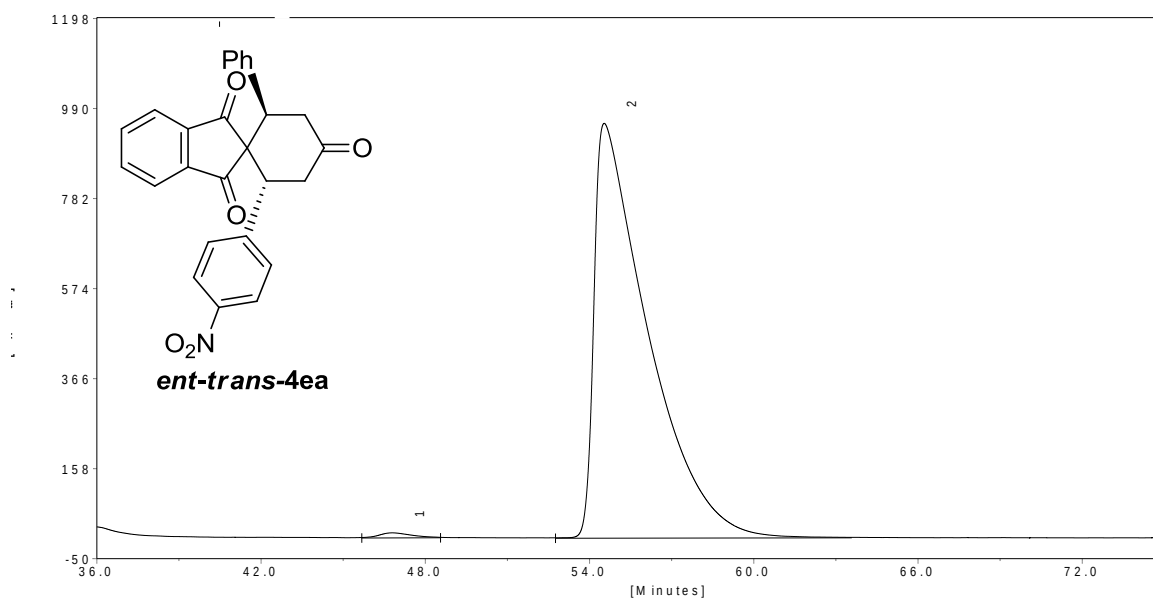
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
55.43	1.40	137.26	1.2233
73.71	50.57	11082.81	98.7767

HPLC chromatogram for **trans-4ea**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 229 nm



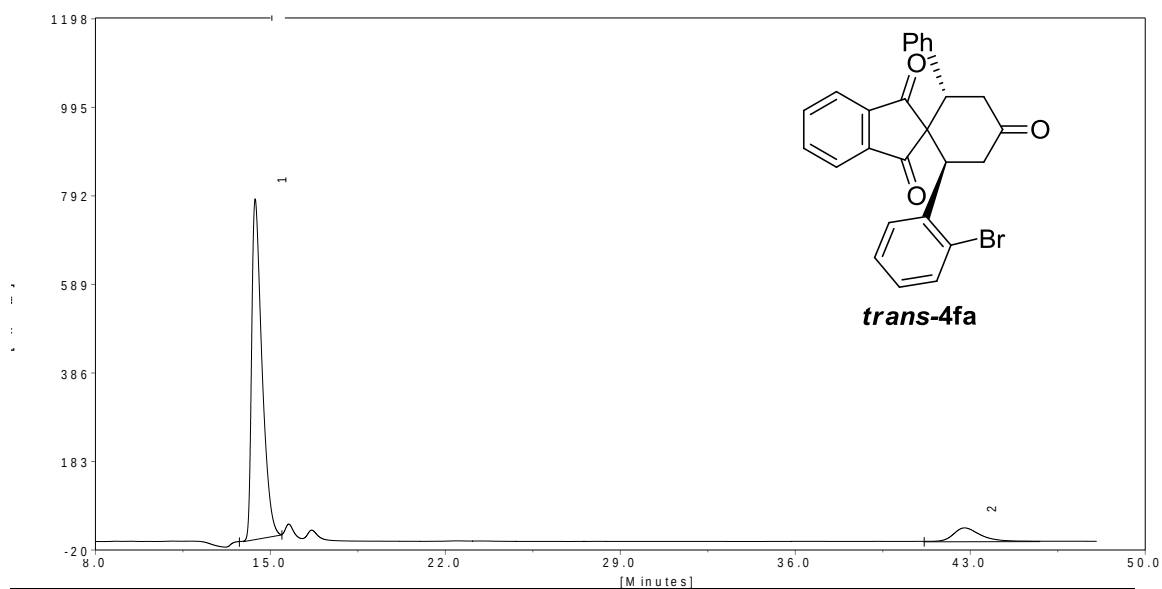
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
45.65	186.72	16531.17	98.4324
55.84	2.54	263.27	1.5676



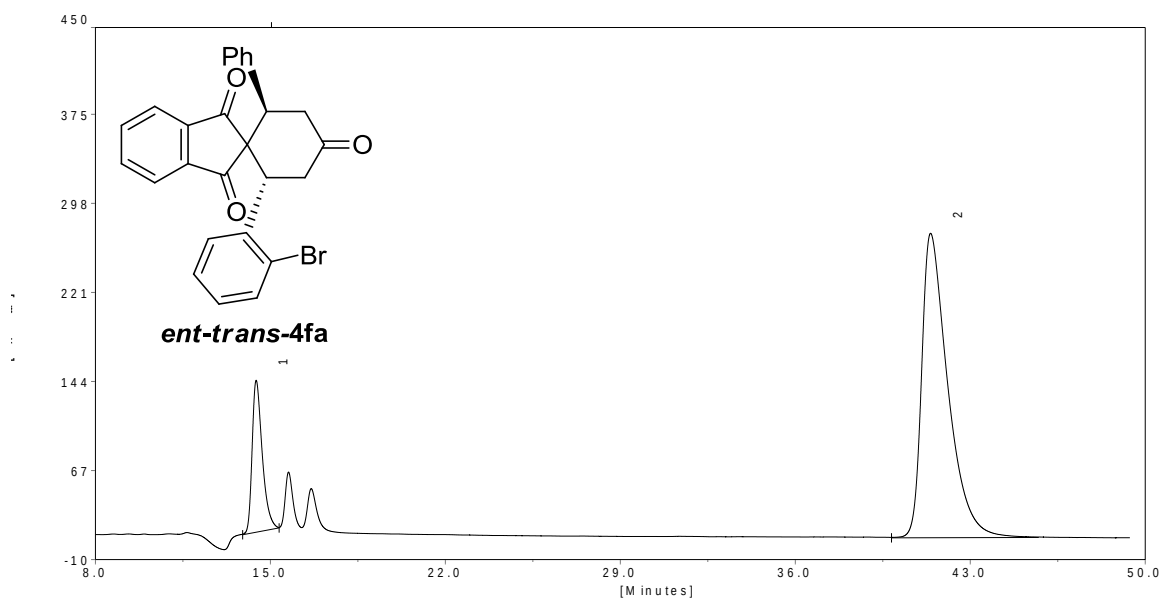
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
46.79	10.64	802.44	0.6121
54.54	957.42	130300.43	99.3879

HPLC chromatogram for **trans-4fa**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



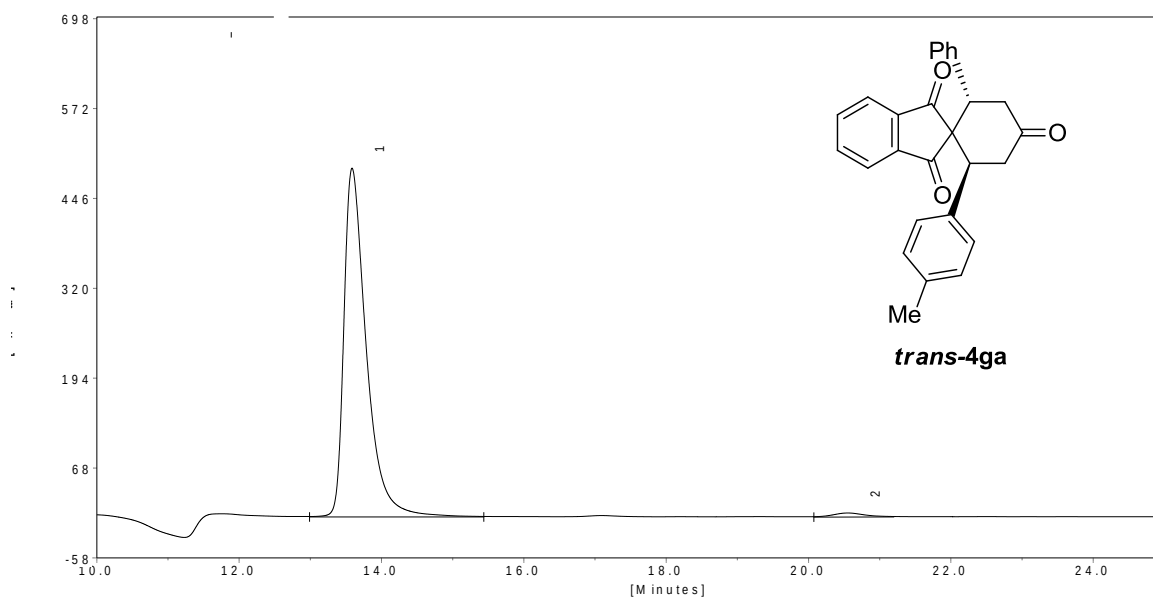
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
14.39	779.69	22277.78	90.8460
42.78	30.75	2244.78	9.1540



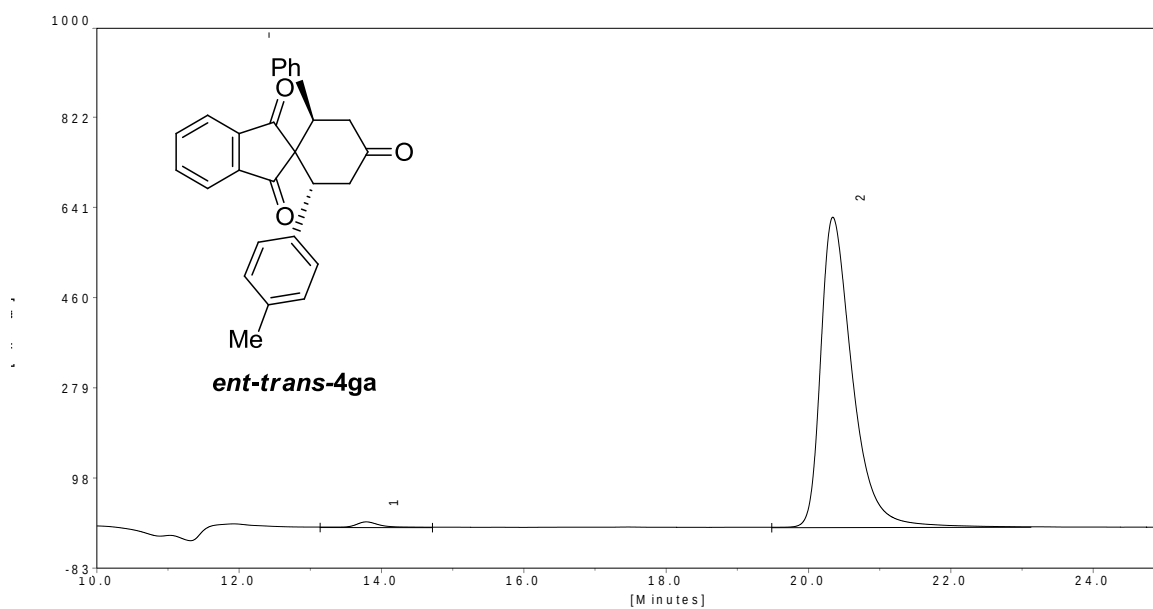
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
14.43	130.94	3660.57	16.1541
41.42	262.82	18999.81	83.8459

HPLC chromatogram for **trans-4ga**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



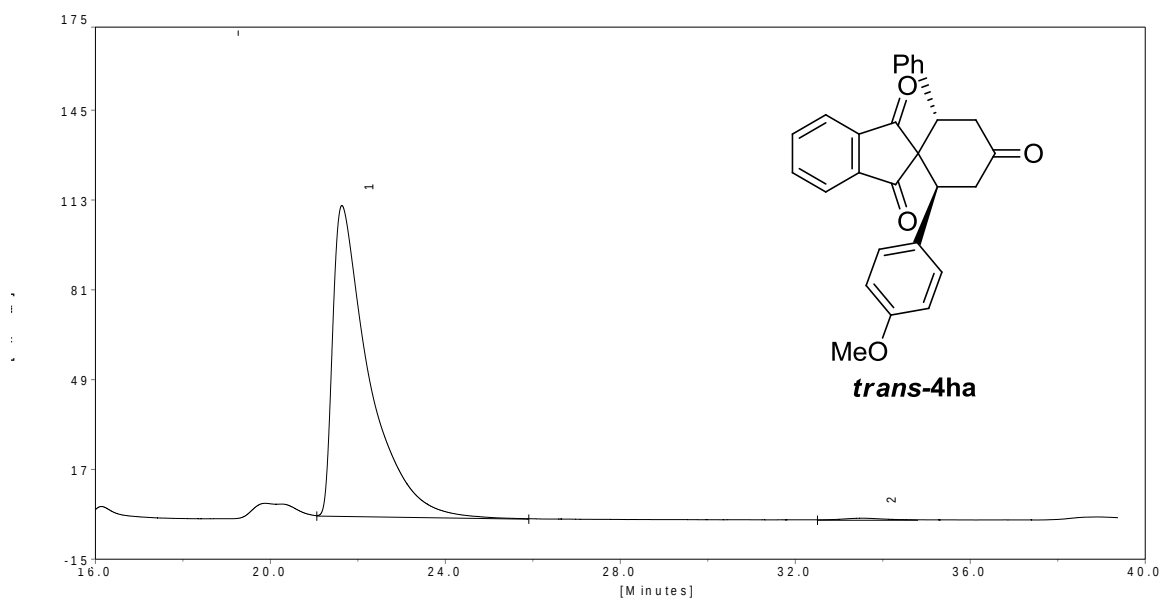
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
13.59	488.40	10632.58	98.6901
20.55	5.08	141.12	1.3099



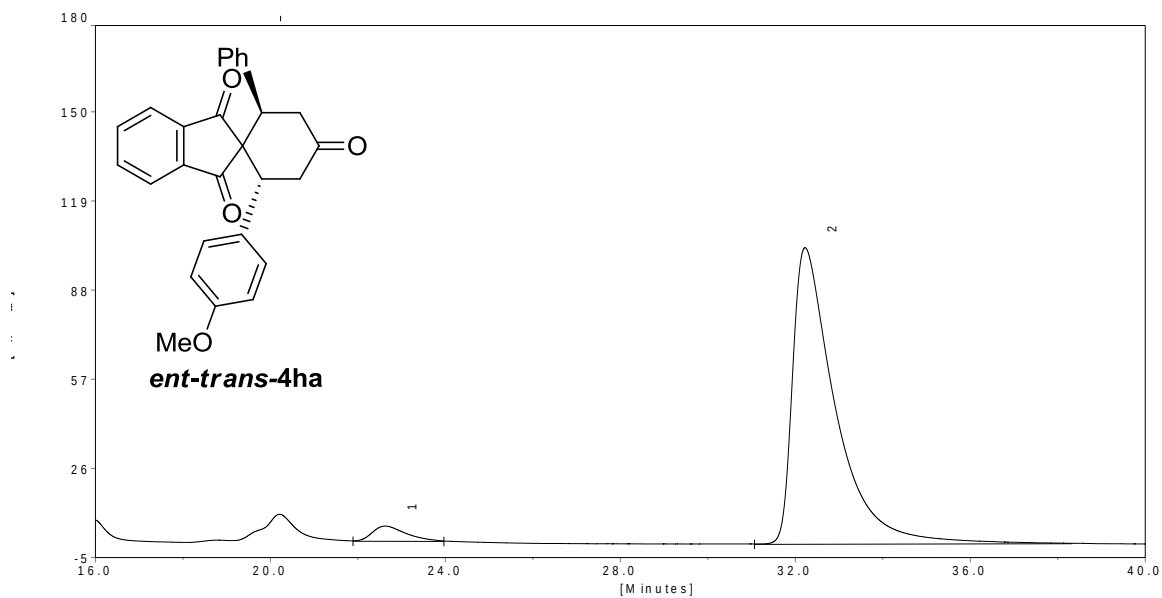
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
13.79	10.55	218.02	1.1262
20.34	622.05	19140.66	98.8738

HPLC chromatogram for **trans-4ha**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



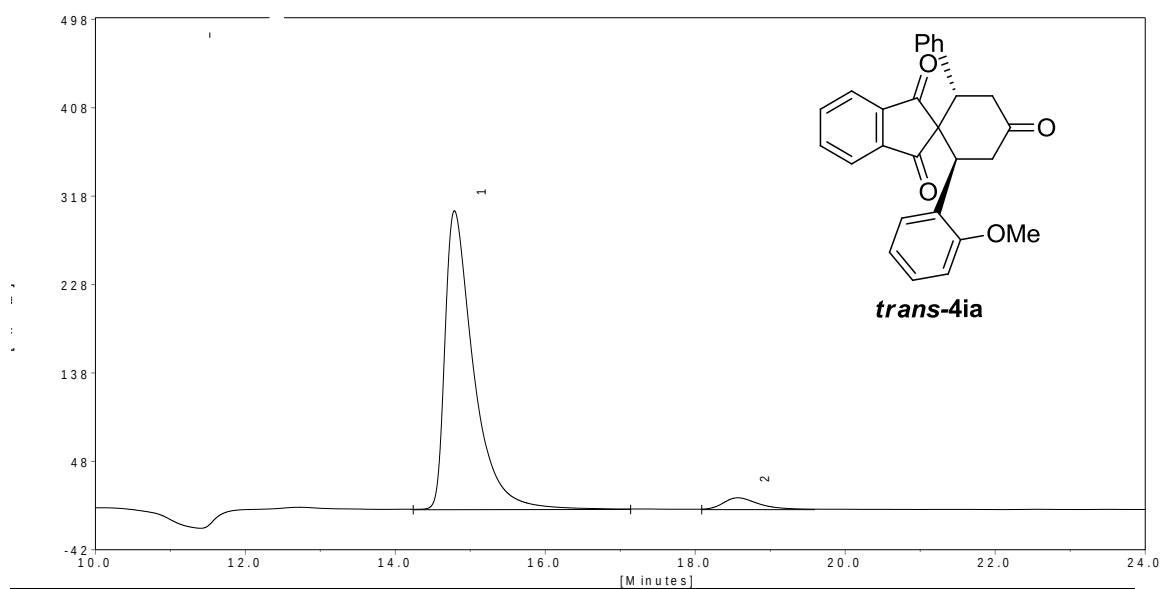
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
21.64	110.64	6366.75	99.4984
33.58	0.56	32.10	0.5016



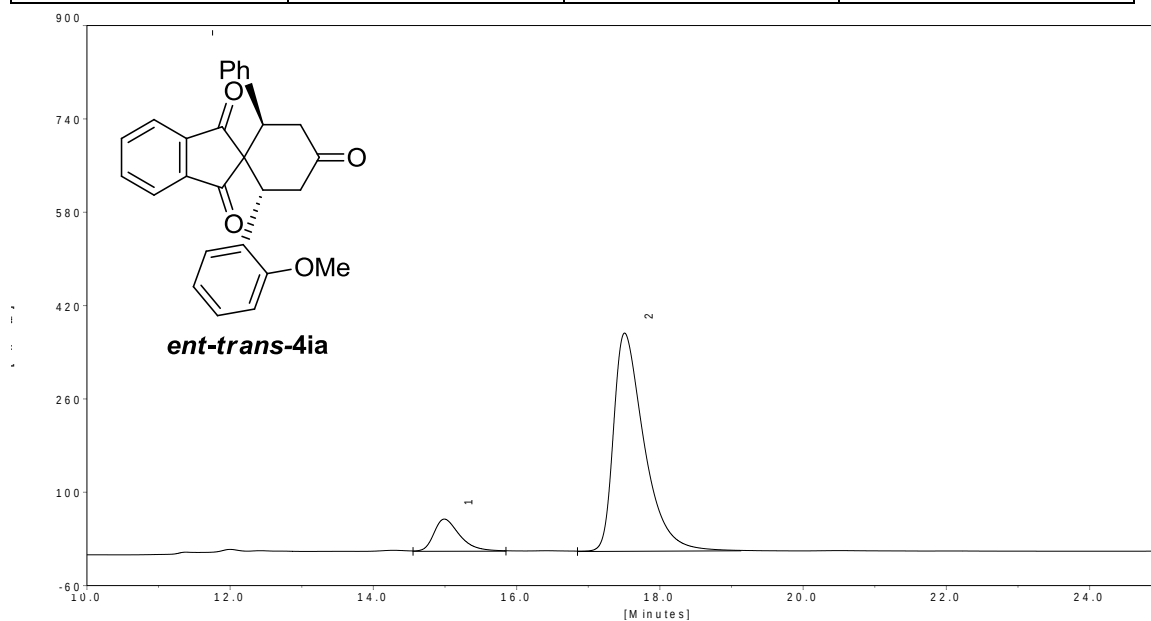
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
22.62	5.14	266.87	3.6820
32.23	103.00	6981.29	96.3180

HPLC chromatogram for **trans-4ia**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



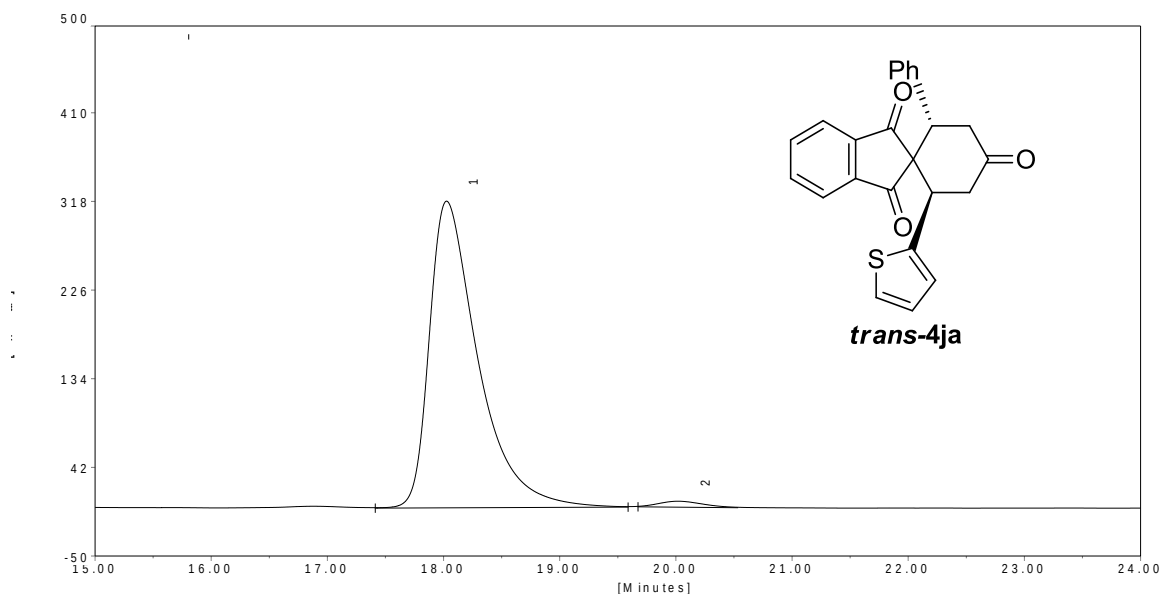
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
14.79	303.97	8006.50	95.6488
18.57	11.60	364.22	4.3512



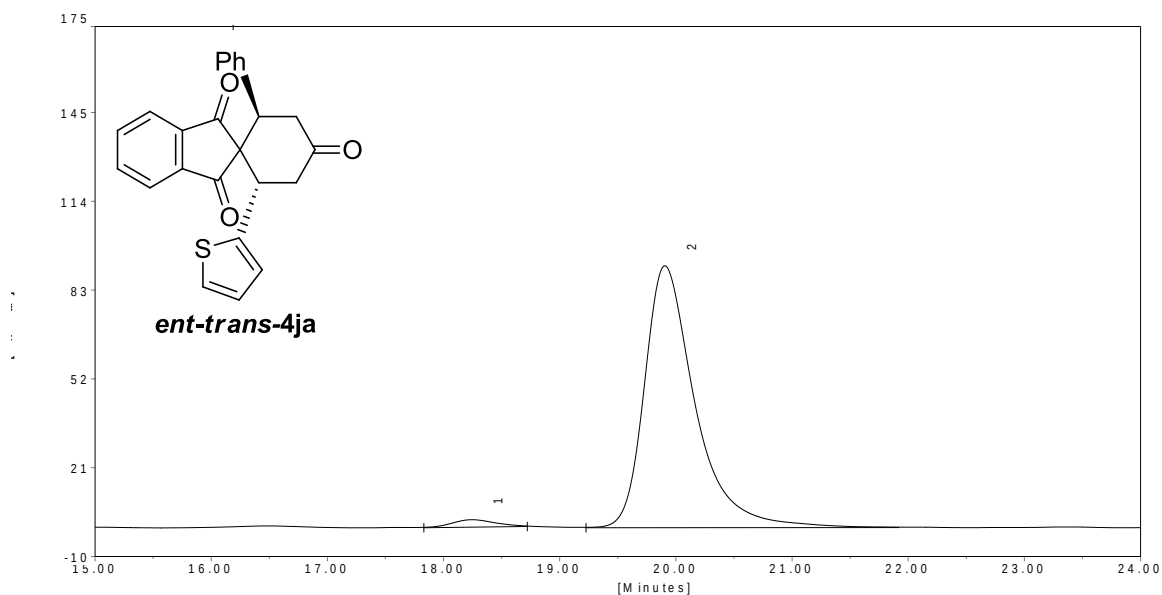
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
14.99	54.53	1332.41	10.7947
17.51	373.44	11010.76	89.2053

HPLC chromatogram for **trans-4ja**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



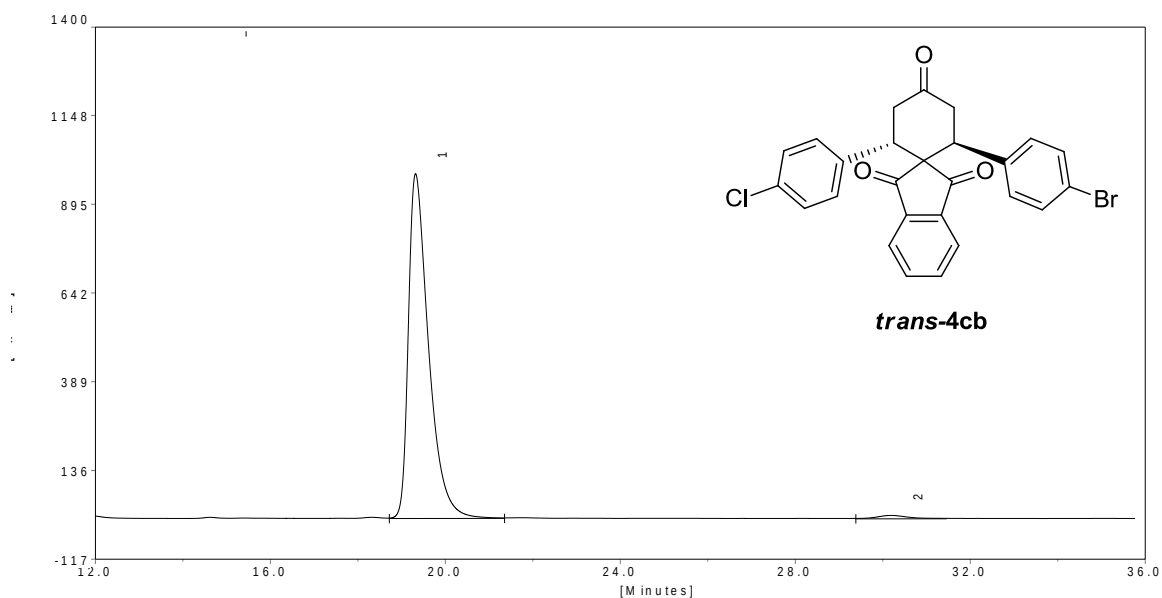
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
18.03	317.81	9194.41	98.4945
20.02	5.70	140.53	1.5055



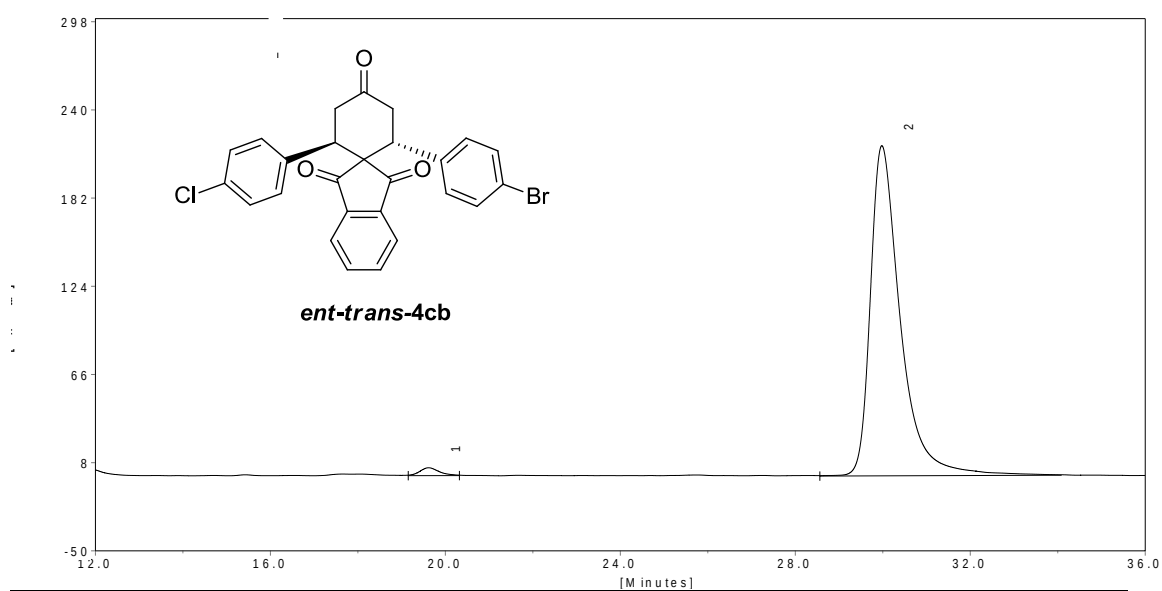
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
18.24	2.45	59.99	2.1321
19.90	91.28	2753.70	97.8679

HPLC chromatogram for **trans-4cb**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



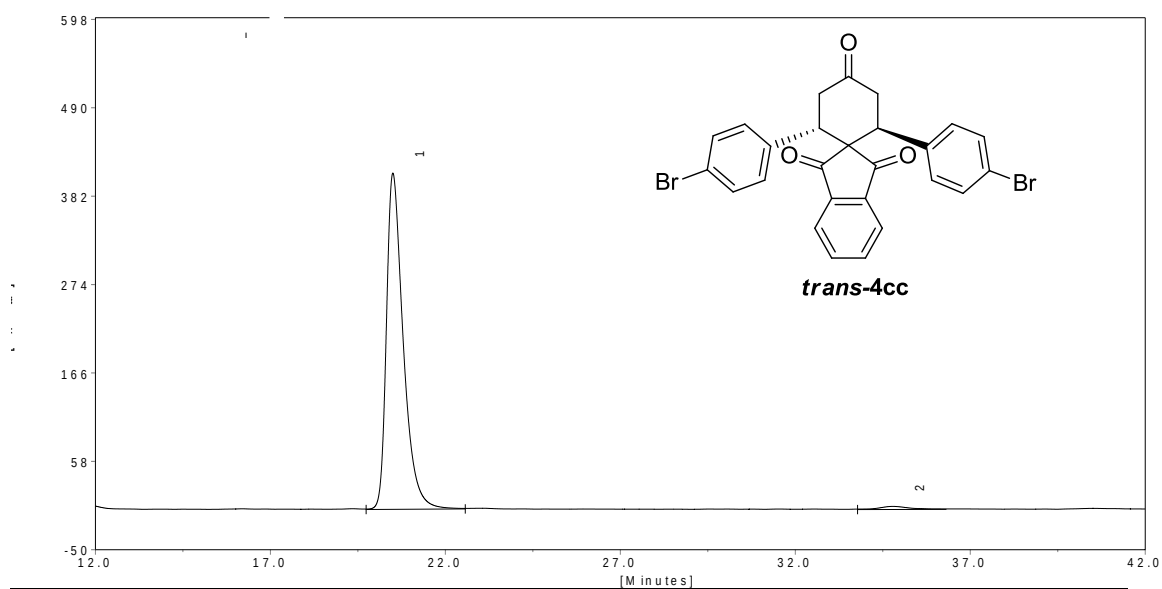
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
19.32	981.89	31309.14	98.8591
30.19	8.43	361.33	1.1409



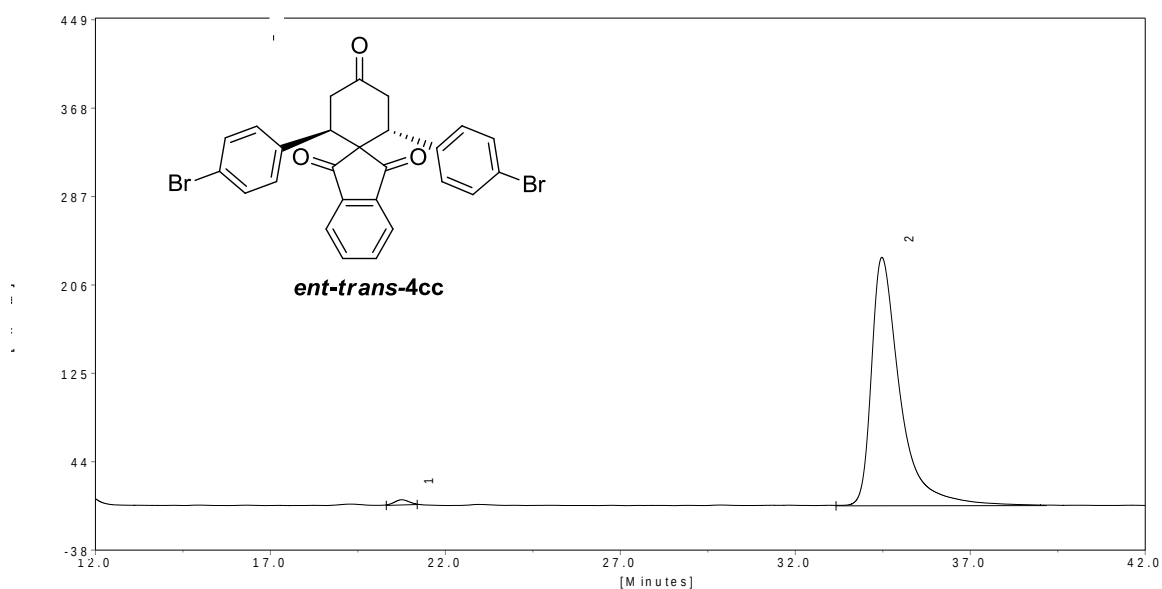
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
19.62	4.87	139.16	1.3344
29.98	216.86	10289.31	98.6656

HPLC chromatogram for **trans-4cc**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



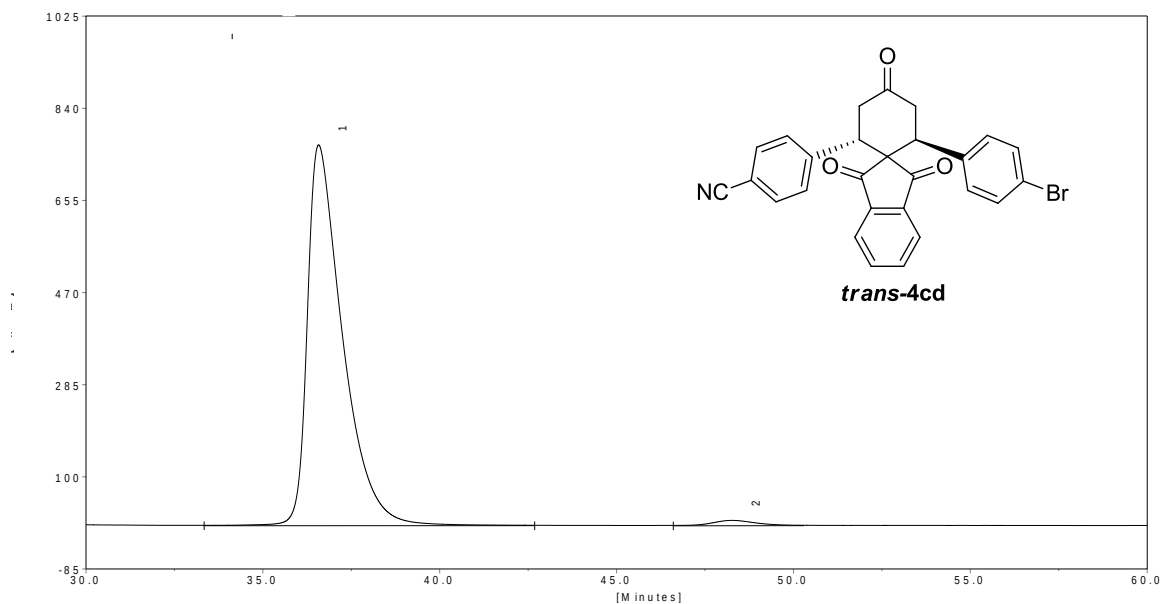
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
20.50	410.39	13609.98	98.8268
34.79	3.23	161.57	1.1732



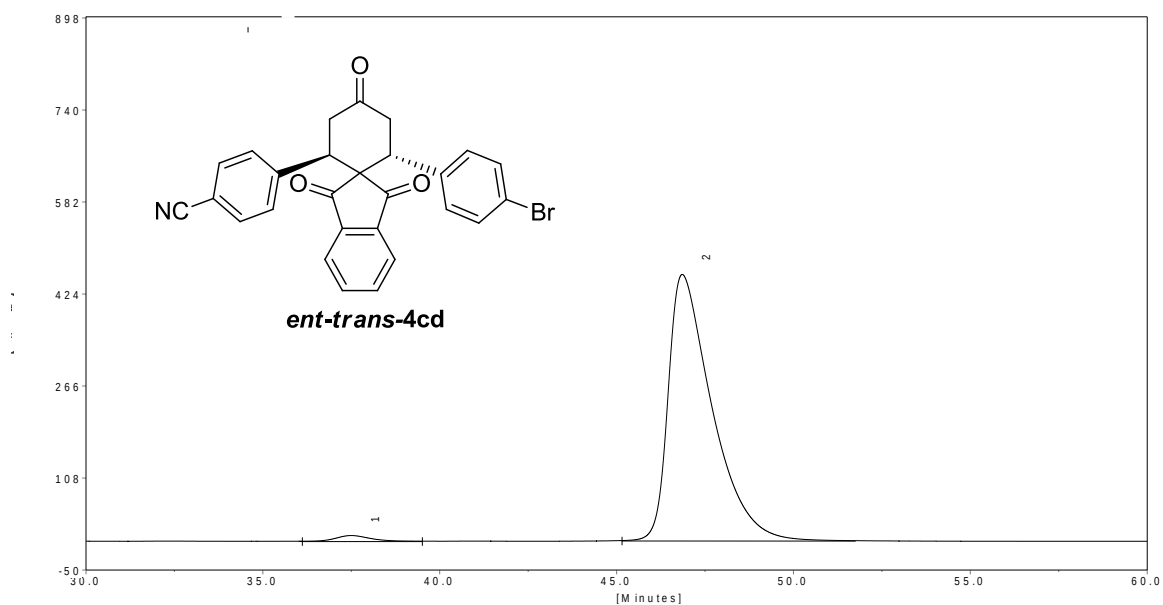
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
20.75	4.36	117.67	0.9085
34.48	227.31	12835.29	99.0915

HPLC chromatogram for **trans-4cd**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=85:15	Detector : UV 226 nm



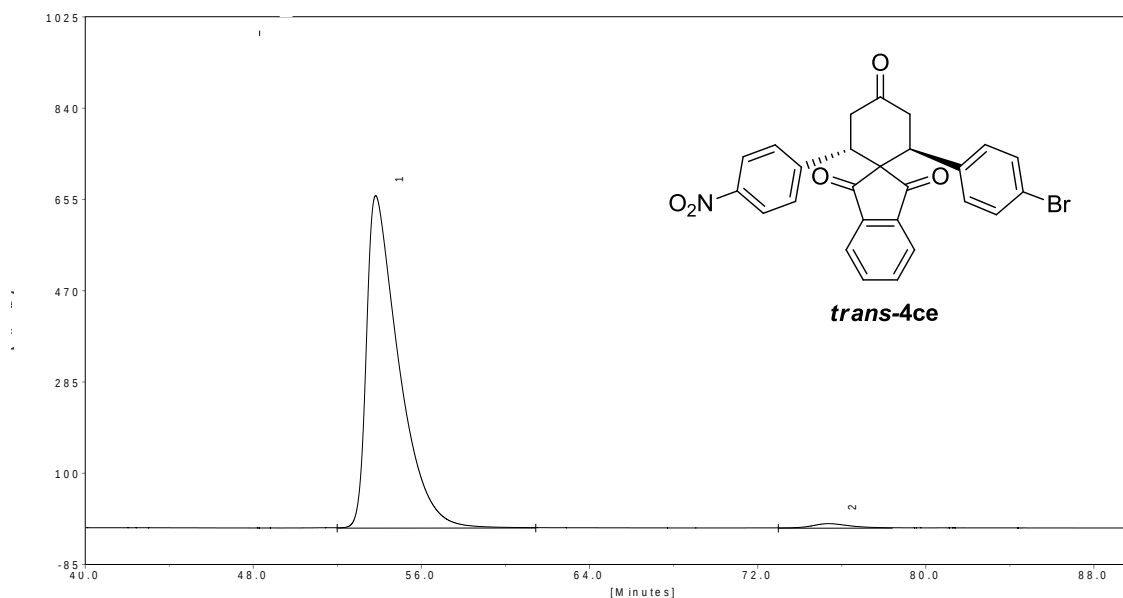
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
36.58	764.02	52692.32	98.5195
48.26	9.98	791.85	1.4805



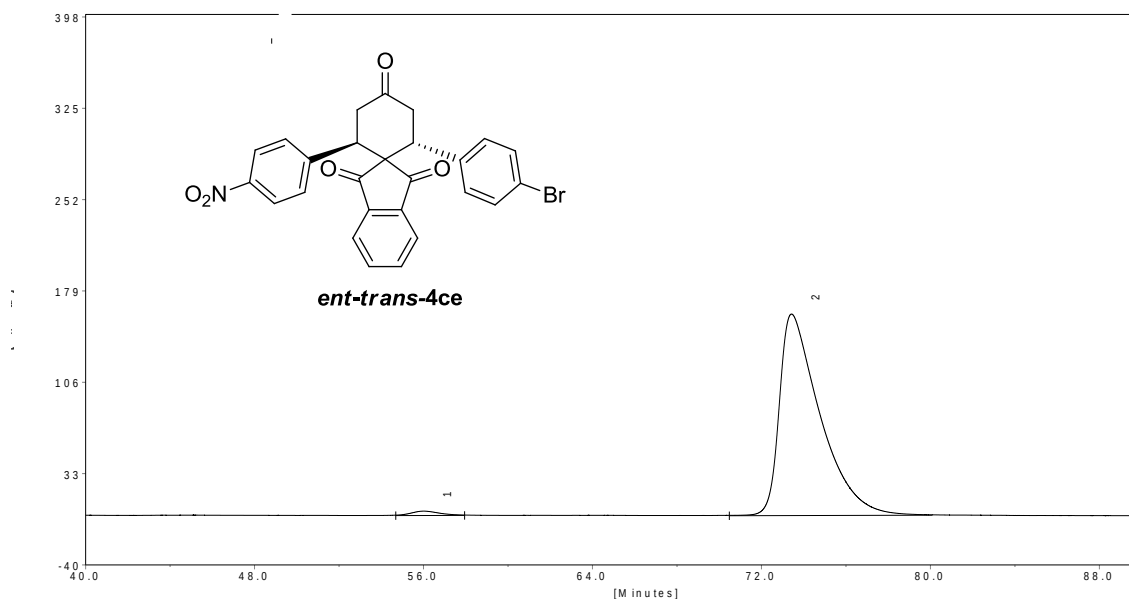
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
37.50	9.67	633.09	1.5910
46.86	457.06	39158.88	98.4090

HPLC chromatogram for **trans-4ce**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



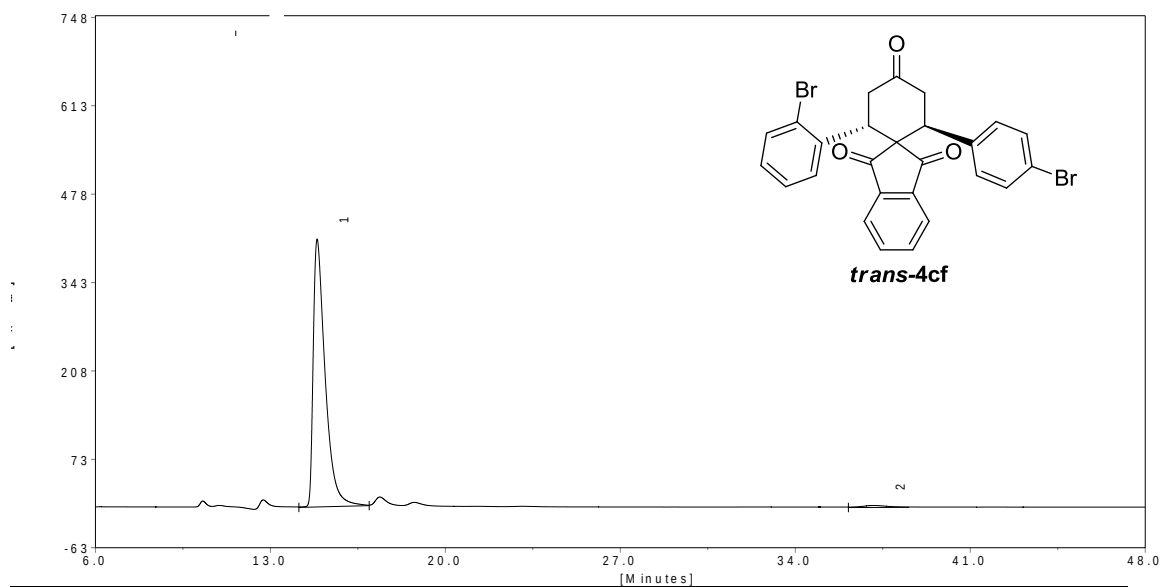
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
53.82	762.52	71701.36	98.6120
75.37	97.37	1009.19	1.3879



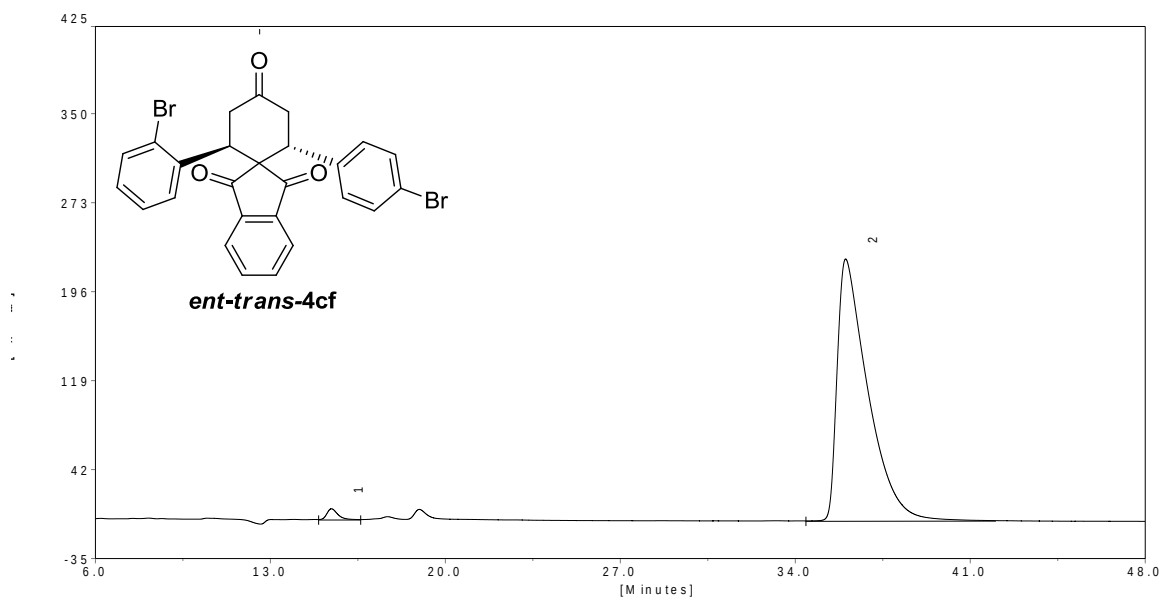
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
56.00	3.17	271.50	1.2530
73.43	160.79	21396.14	98.7470

HPLC chromatogram for **trans-4cf**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



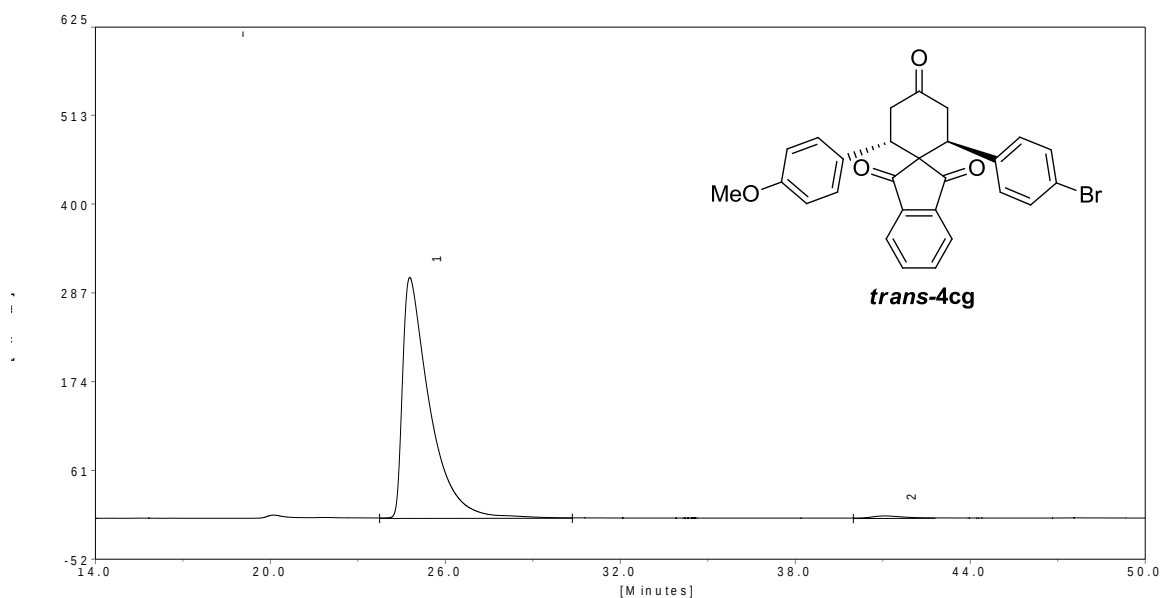
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
14.87	408.57	13462.68	99.0054
37.13	2.34	135.24	0.9946



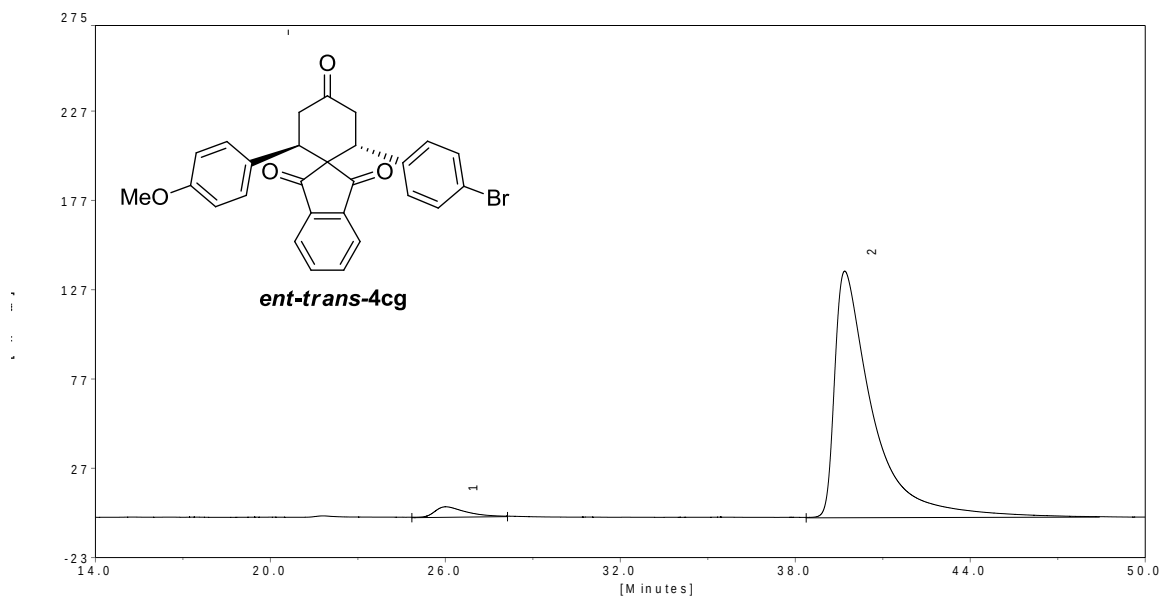
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
15.45	9.35	276.56	1.4164
36.02	226.65	19248.46	98.5836

HPLC chromatogram for **trans-4cg**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



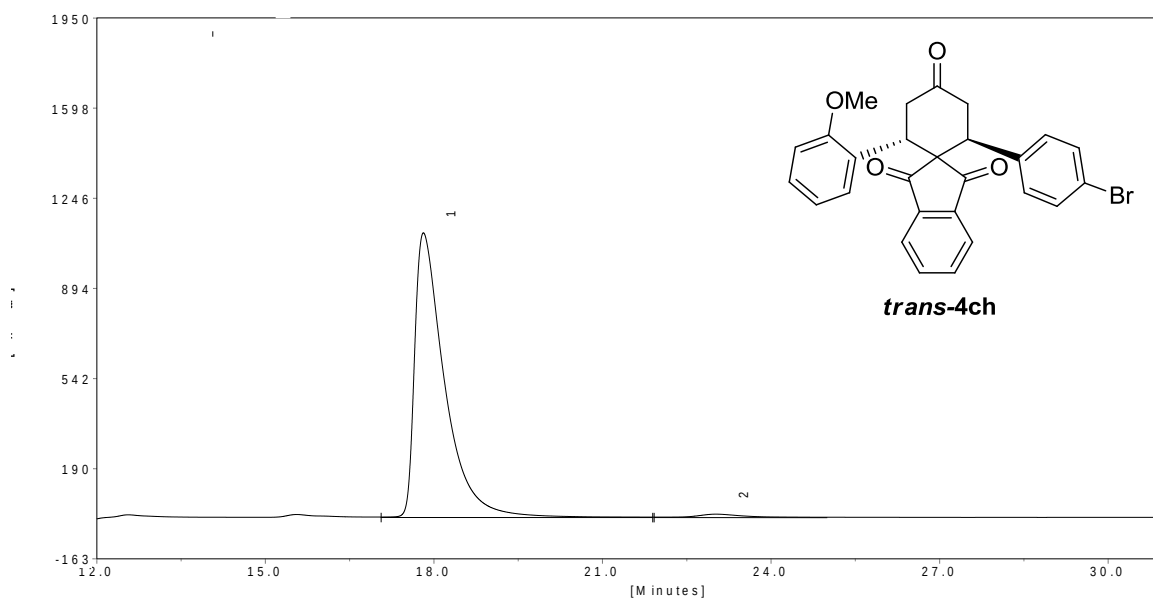
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
24.78	306.14	19618.78	99.1075
41.05	2.63	176.68	0.8925



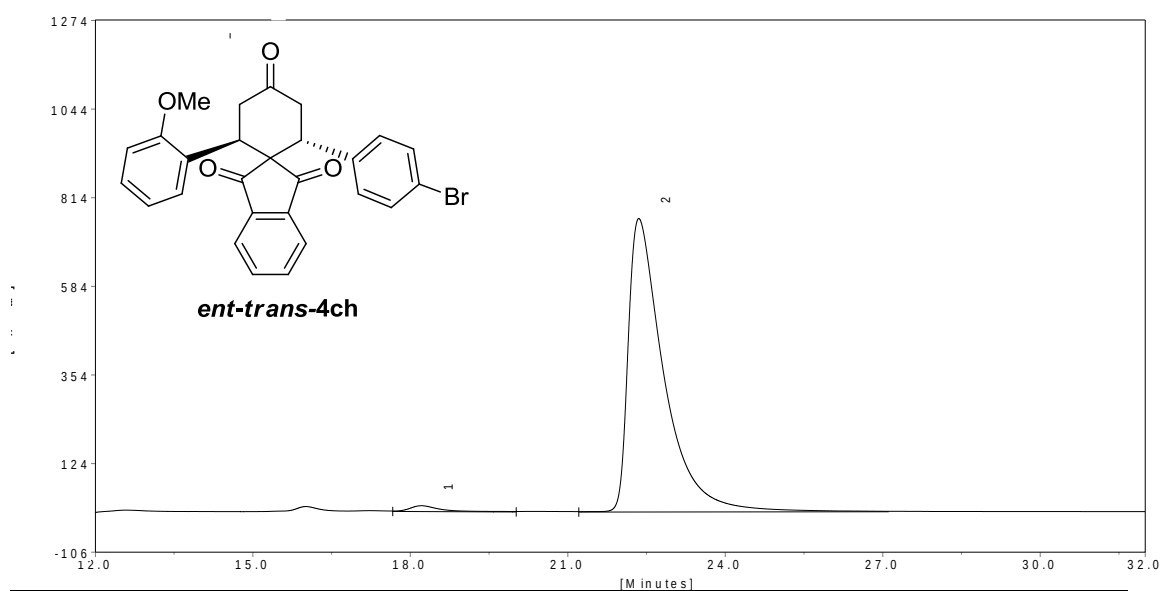
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
26.02	5.63	392.74	3.0711
39.70	137.87	12395.60	96.9289

HPLC chromatogram for **trans-4ch**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 227 nm



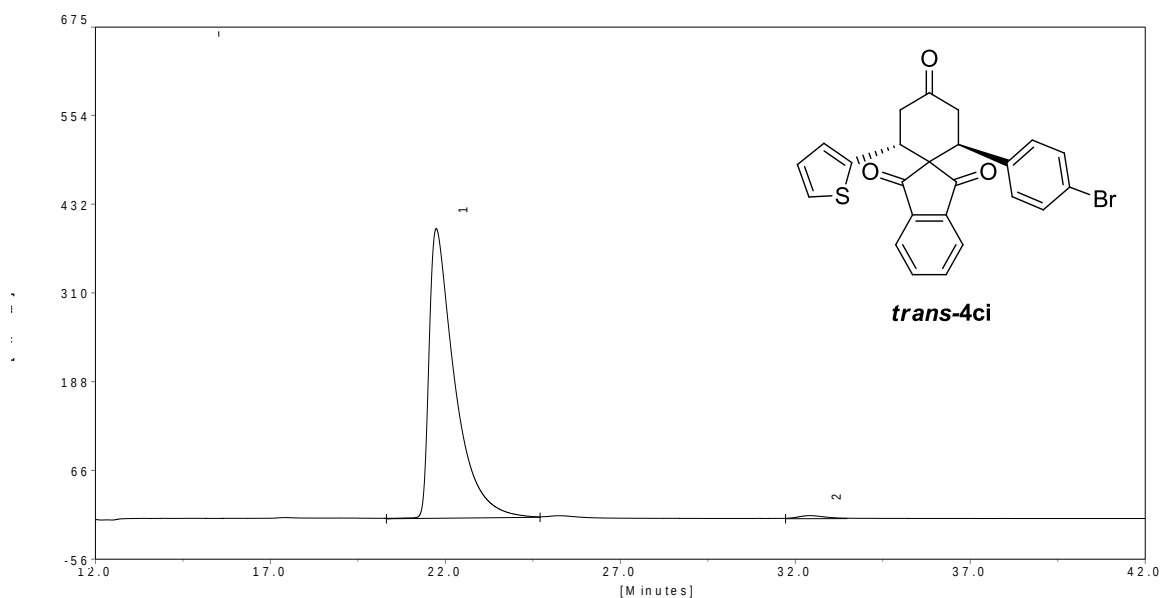
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
17.81	1110.23	40905.77	98.5976
23.02	11.71	581.82	1.4024



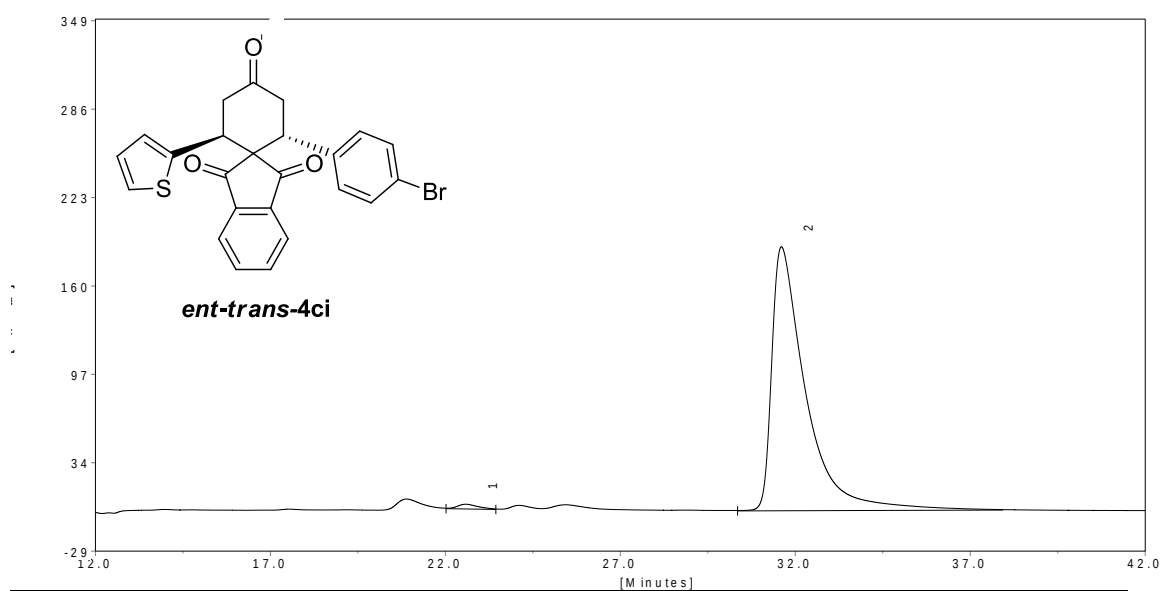
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
18.21	14.08	477.82	1.3195
22.35	760.70	35733.42	98.6805

HPLC chromatogram for **trans-4ci**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



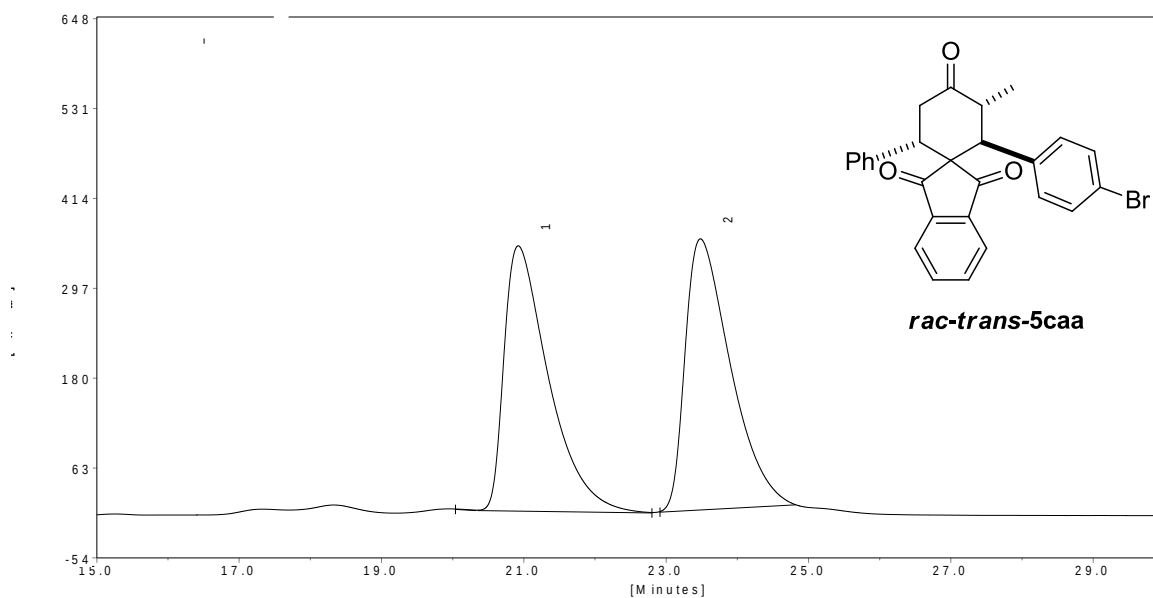
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
21.74	397.63	20088.11	99.1539
32.40	3.58	171.42	0.8461



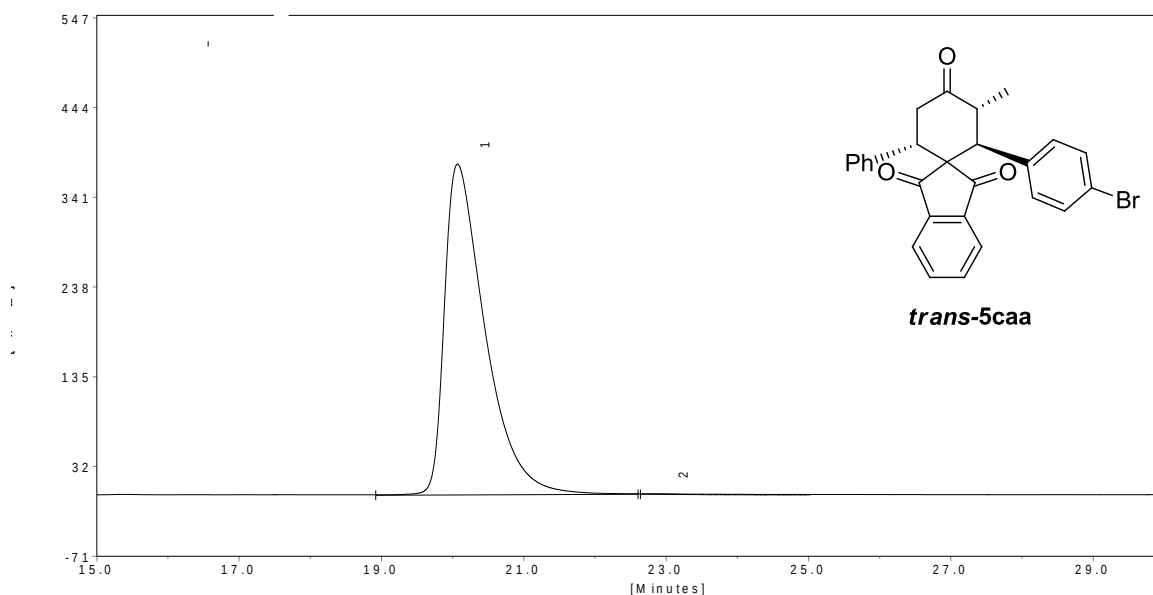
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
22.58	3.06	114.75	0.9016
31.60	187.89	12612.40	99.0984

HPLC chromatogram for **trans-5caa**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=98:02	Detector : UV 227 nm



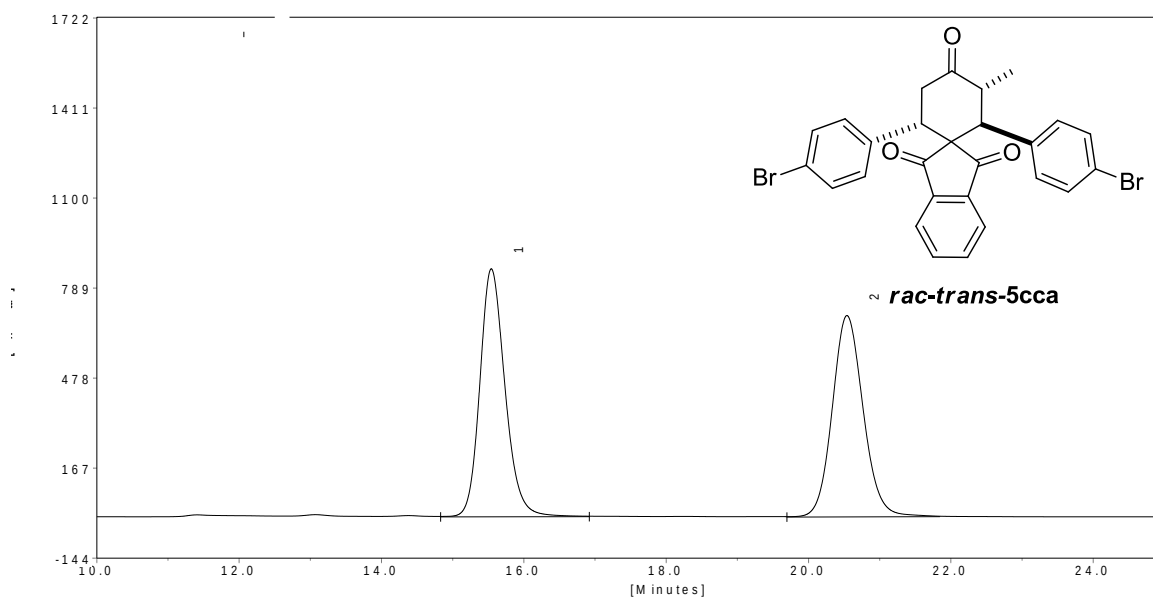
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
20.92	344.01	14833.66	48.8661
23.48	352.35	15522.08	51.1339



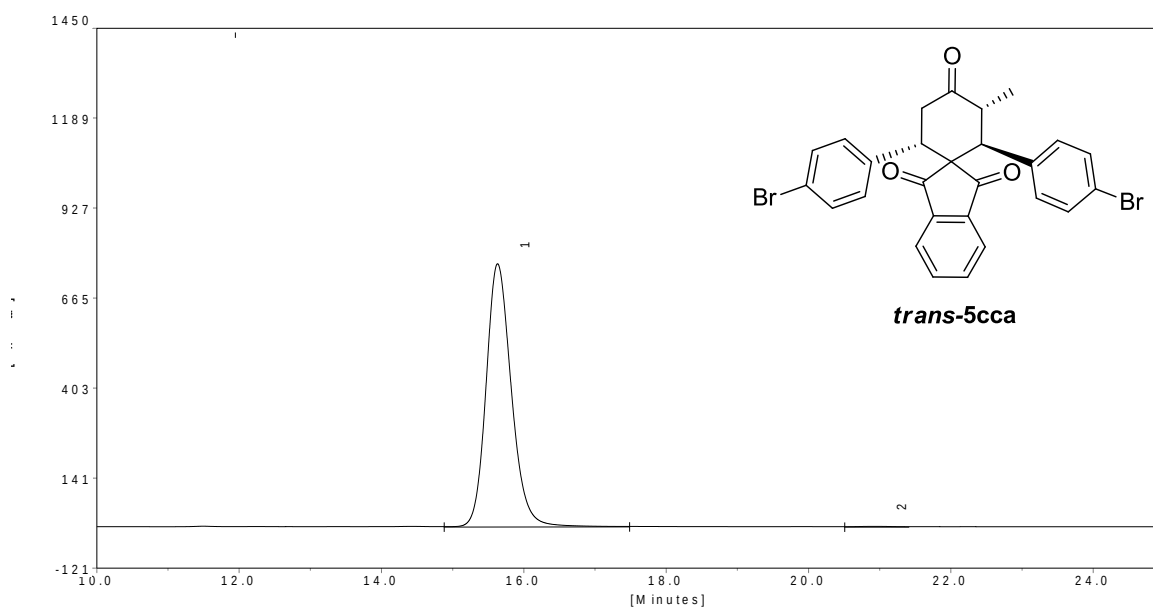
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
20.07	379.27	14973.34	99.9183
22.86	0.12	12.24	0.0817

HPLC chromatogram for **trans-5cca**:

Column : CHIRALPAK IA	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=80:20	Detector : UV 226 nm



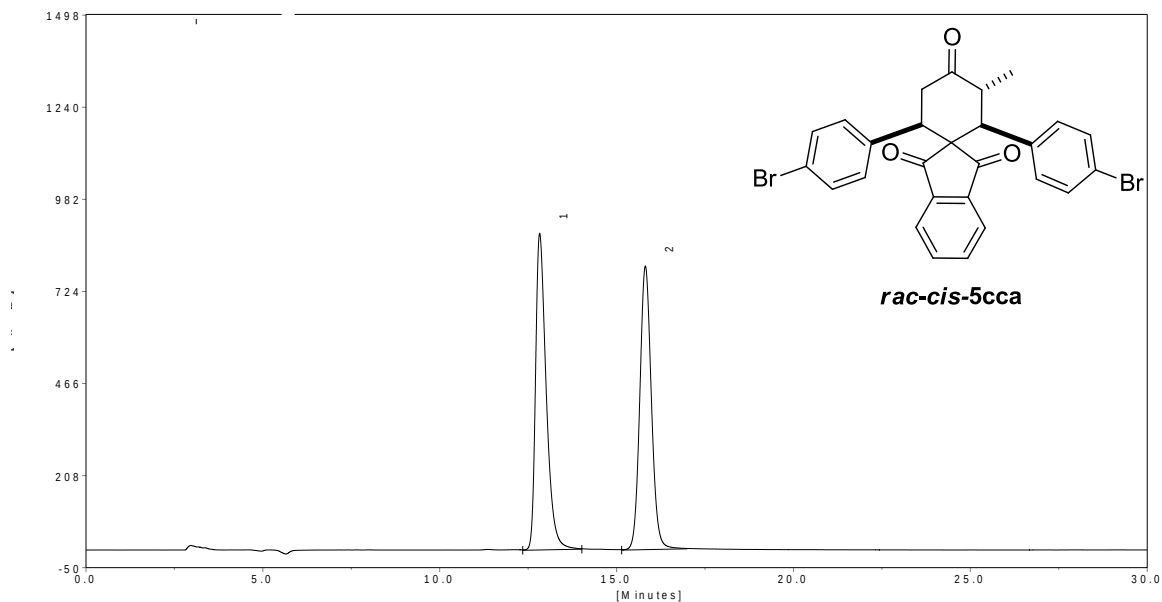
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
15.54	855.40	20900.46	50.1036
20.54	694.21	20814.01	49.8964



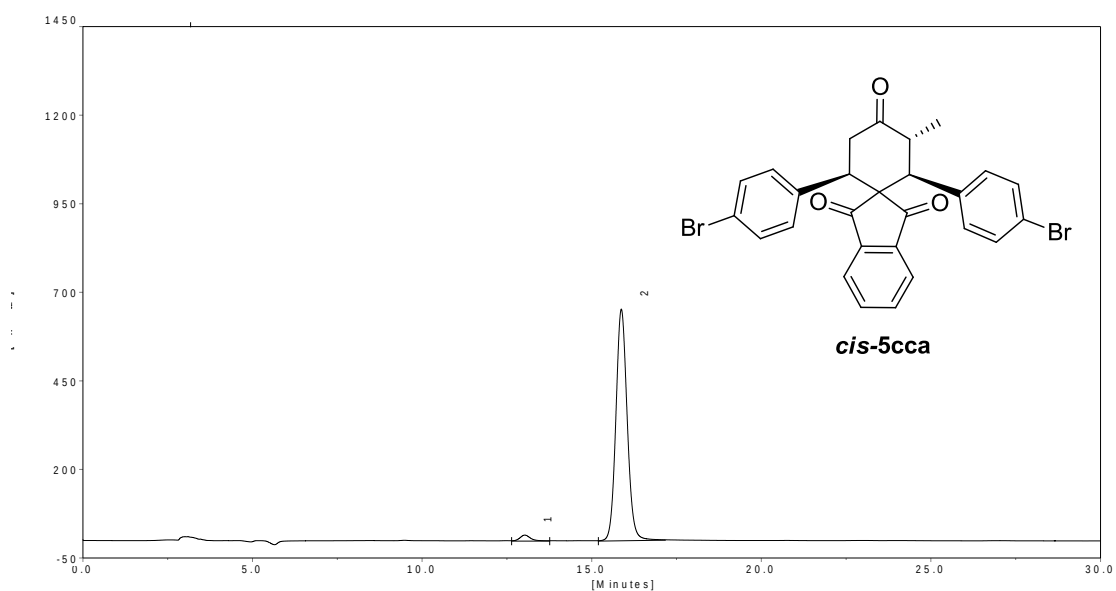
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
15.63	764.97	18786.07	99.8760
20.92	0.91	23.32	0.1240

HPLC chromatogram for **cis-5cca** (obtained as minor diastereomer along with trans-5cca):

Column : CHIRALPAK IA	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=80:20	Detector : UV 226 nm

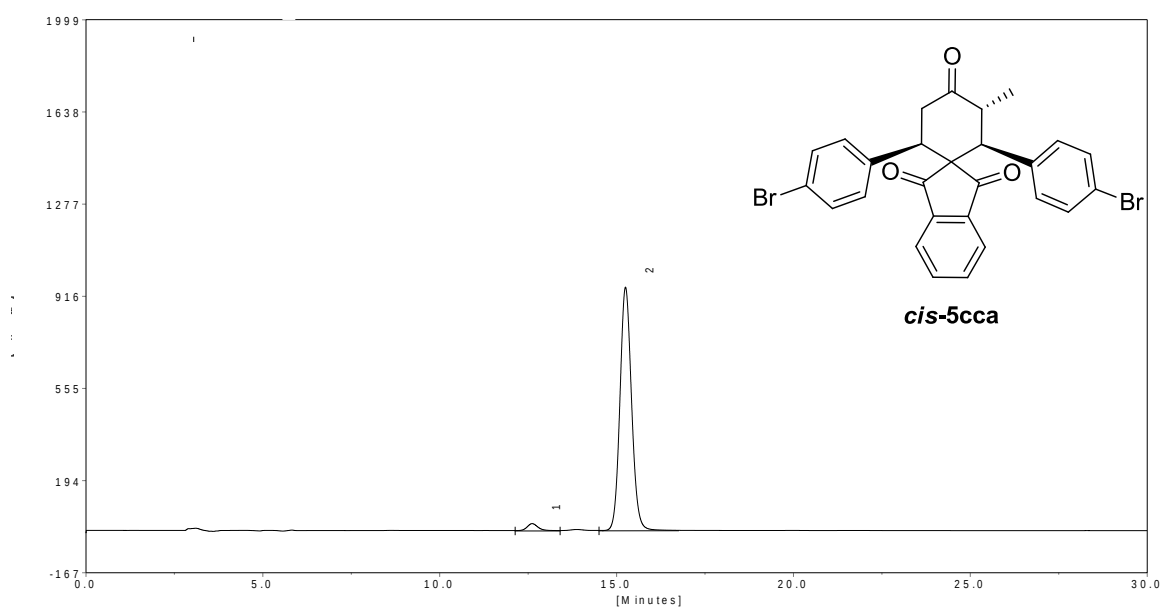


Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
12.83	886.32	18460.80	50.7232
15.81	793.77	17934.37	49.2768



Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
13.03	15.97	322.28	2.1022
15.87	652.93	15008.41	97.8978

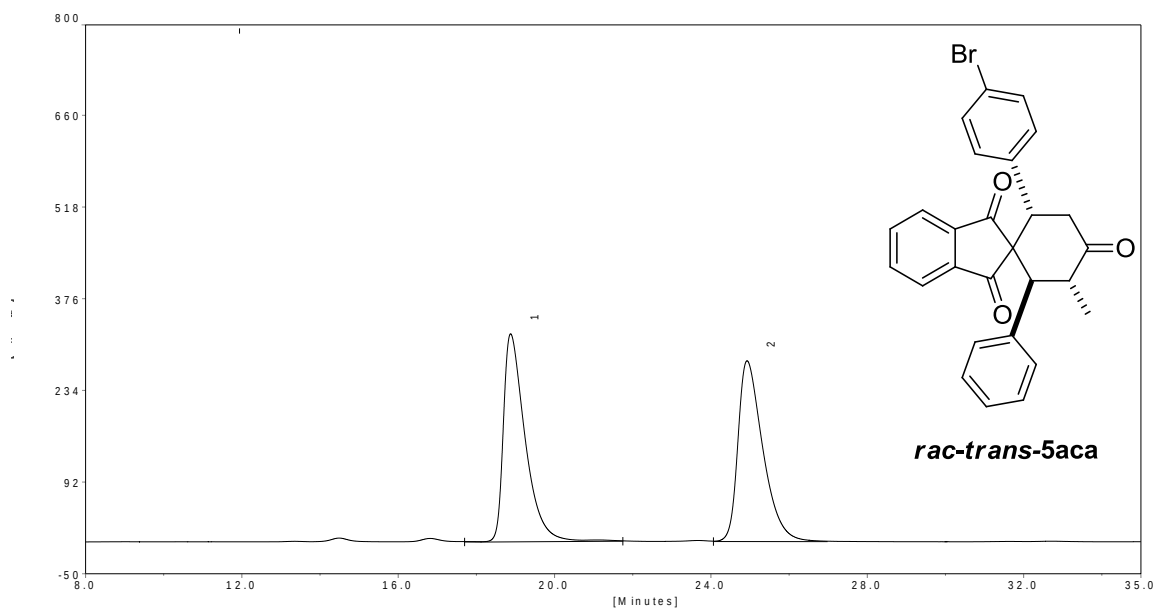
HPLC chromatogram for *cis*-5cca (obtained by epimerization of *trans*-5cca):



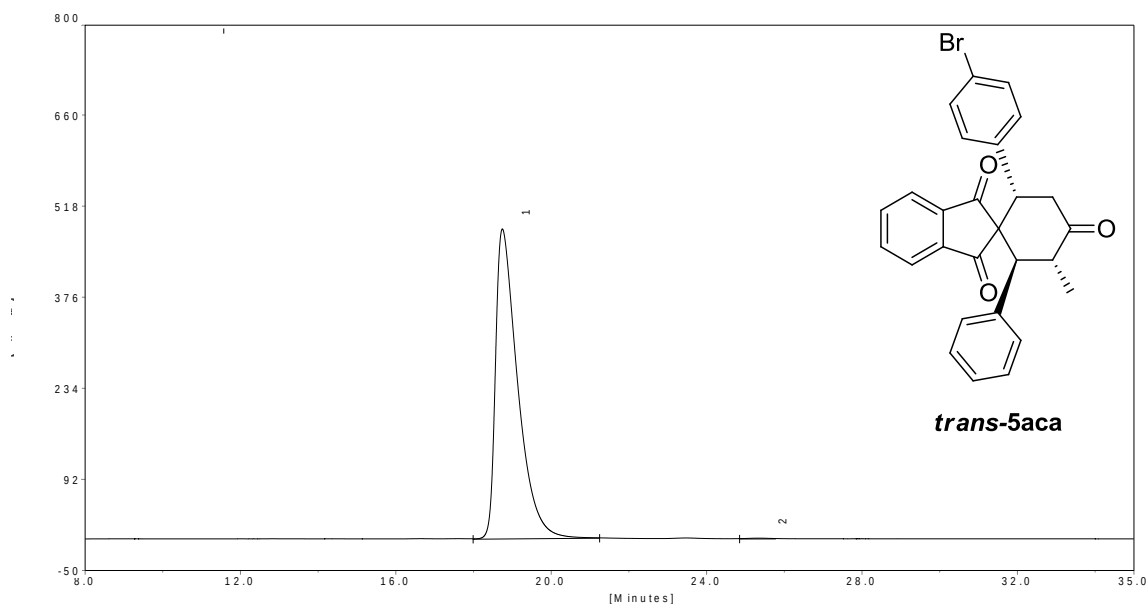
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
12.61	27.16	555.45	2.4989
15.25	953.10	21671.94	97.5011

HPLC chromatogram for **trans-5aca**:

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=98:02	Detector : UV 226 nm



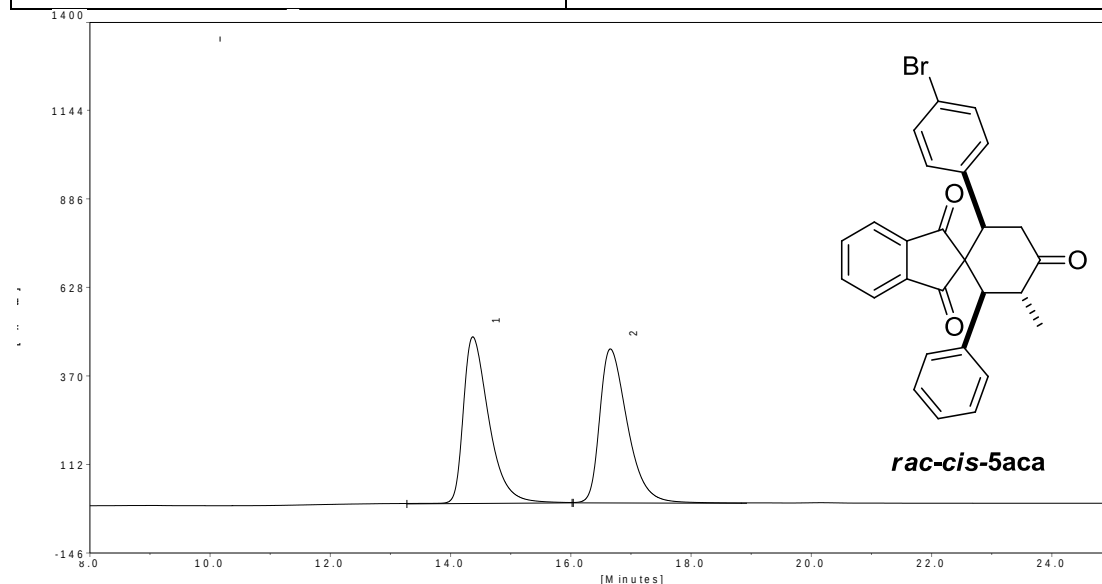
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
18.87	321.50	12356.18	50.1293
24.92	279.41	12292.44	49.8707



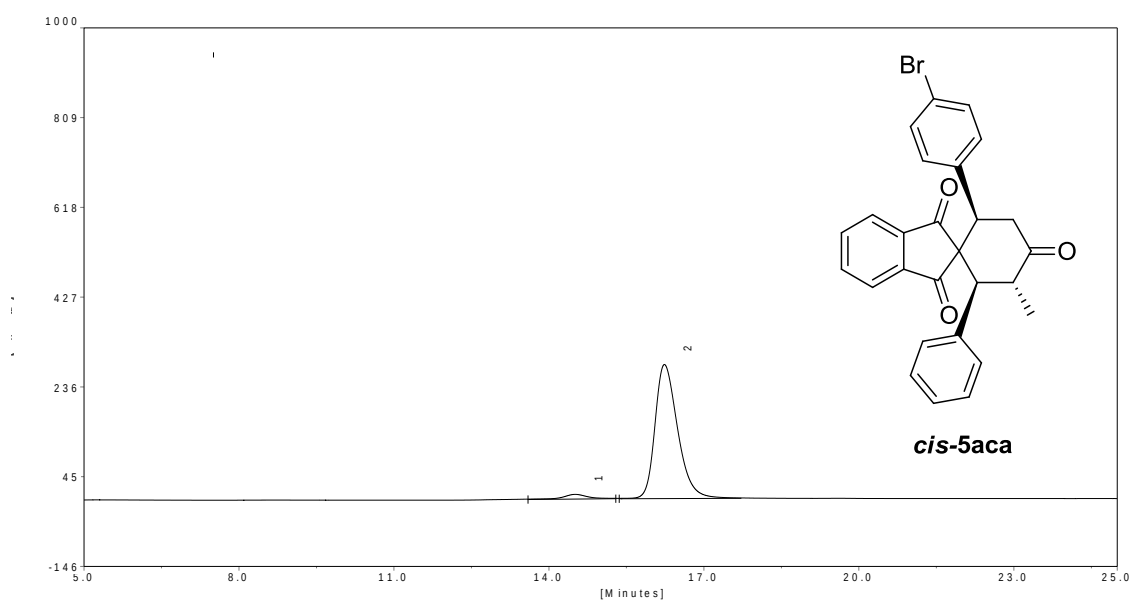
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
18.74	482.70	19025.28	99.8972
25.34	0.62	19.58	0.1028

HPLC chromatogram for **cis-5aca** (minor diastereomer that is obtained along with **trans-5aca**):

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=98:02	Detector : UV 226 nm

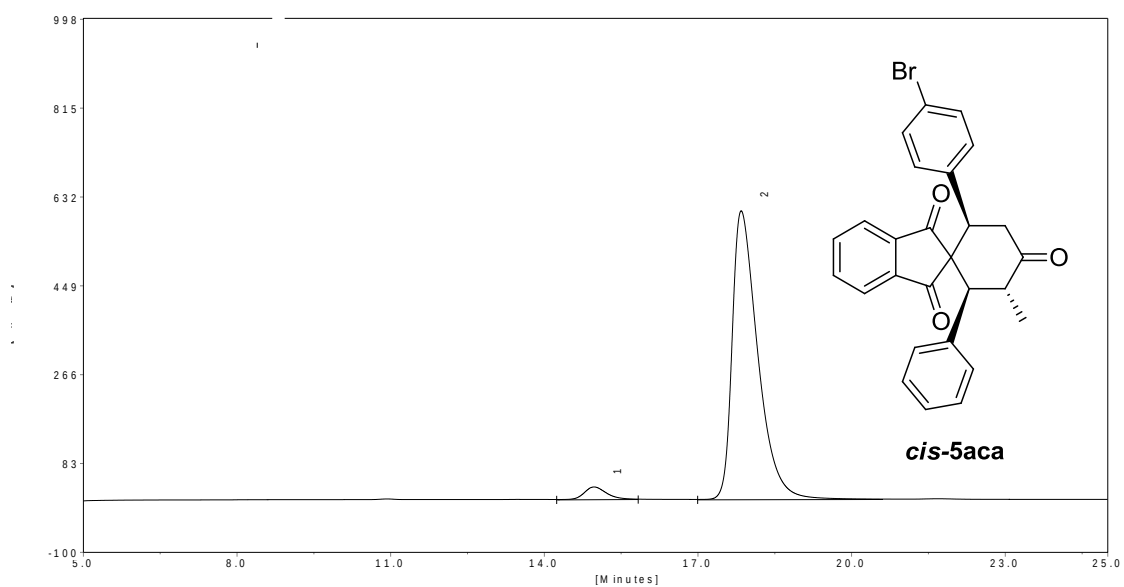


Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
14.37	484.54	14202.08	49.9324
16.66	447.78	14240.55	50.0676



Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
14.51	9.13	263.49	2.9758
16.24	284.48	8591.04	97.0242

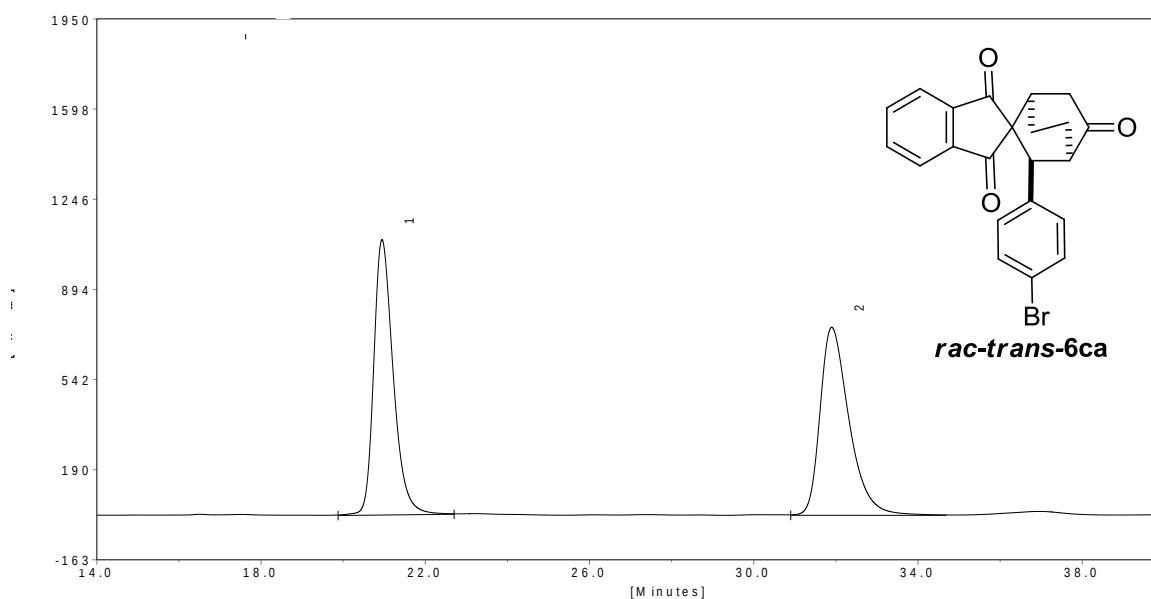
HPLC chromatogram for *cis*-5aca (obtained after epimerization of *trans*-5aca):



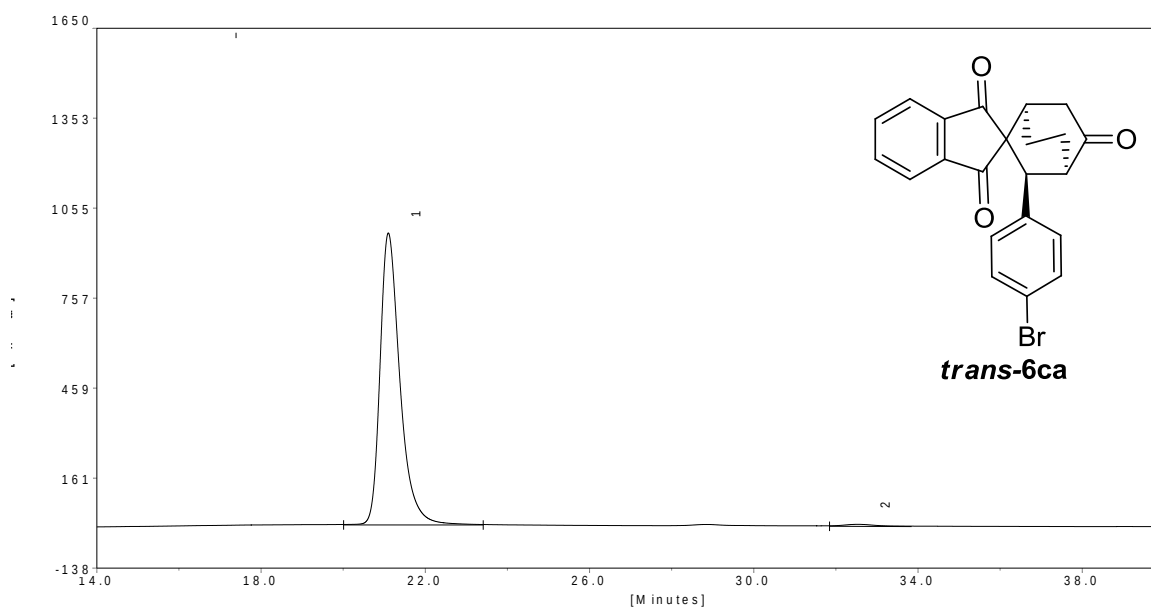
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
14.97	25.48	748.20	3.5010
17.84	594.43	20622.41	96.4990

HPLC chromatogram for **trans-6ca**:

Column : Chiralpak IA	Flow Rate :1.0 ml/min
Solvent : Hex:IPA=90:10	Detector : UV 226 nm



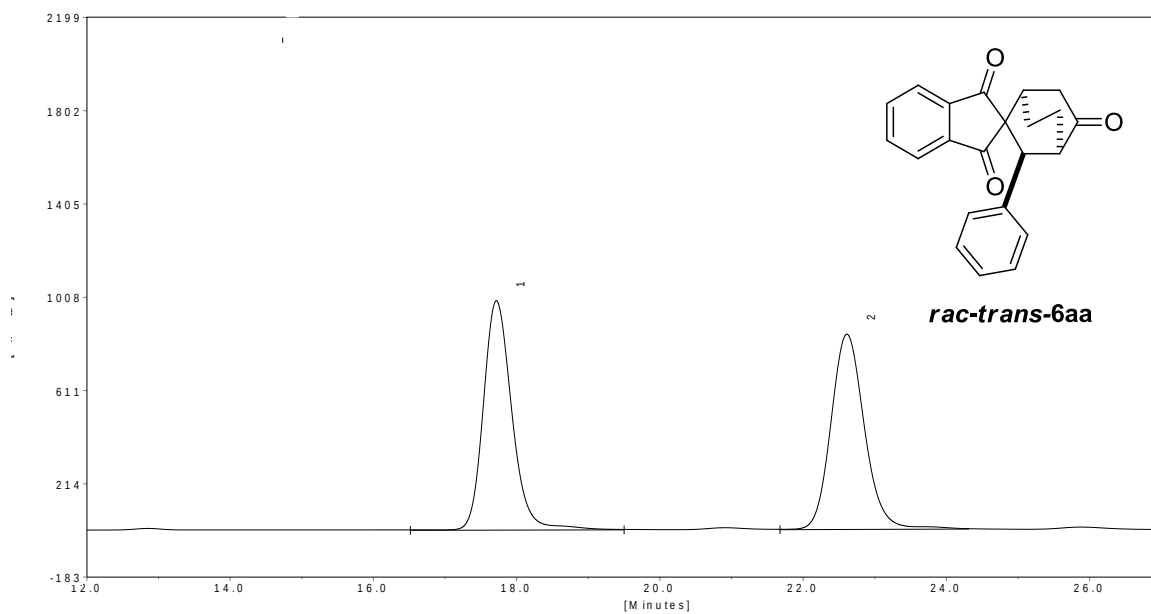
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
20.94	1073.94	35289.65	49.6943
31.90	732.61	35723.82	50.3057



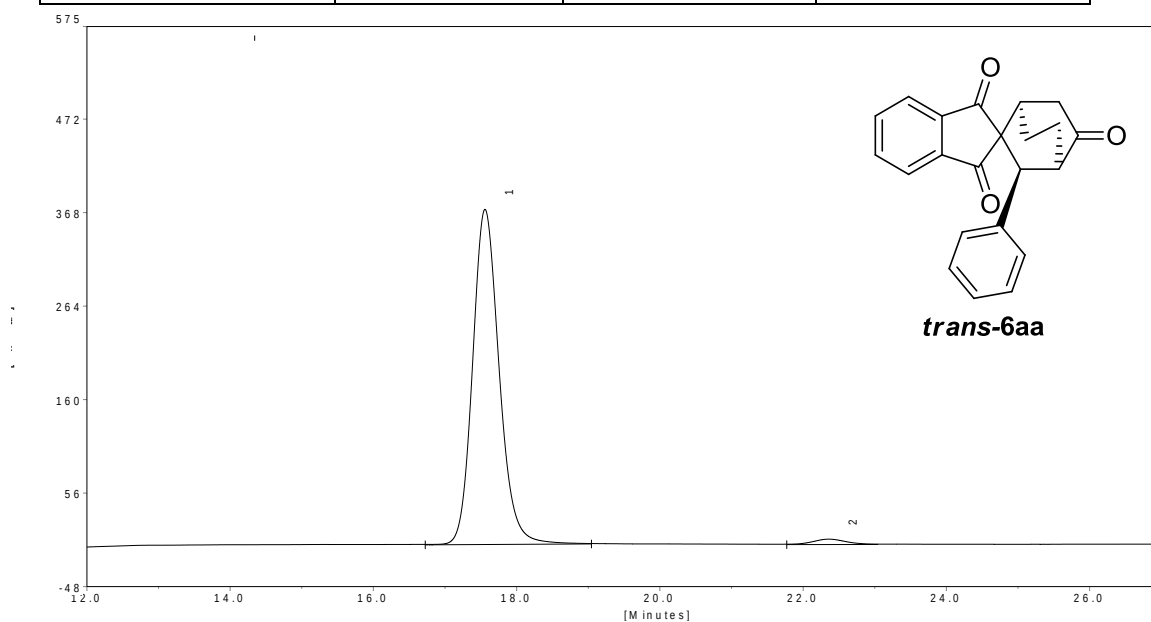
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
21.10	965.33	32288.21	99.2736
32.53	5.25	236.27	0.7264

HPLC chromatogram for **trans-6aa**:

Column : Chiralpak IA	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90 : 10	Detector : UV 226 nm



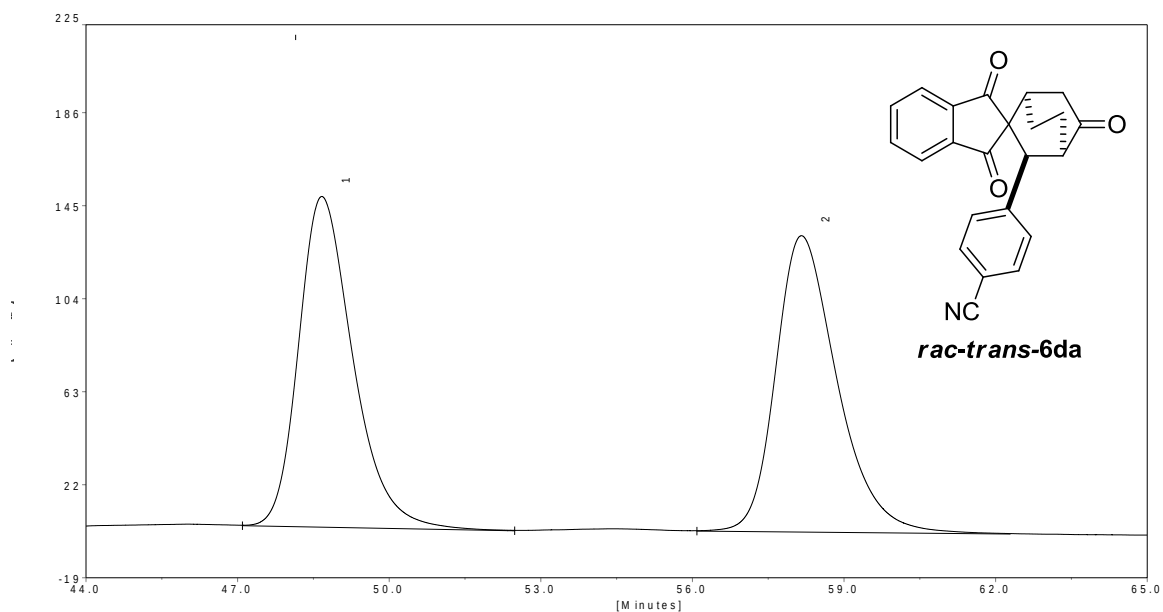
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
17.72	974.89	26827.79	49.9694
22.61	829.77	26860.59	50.0306



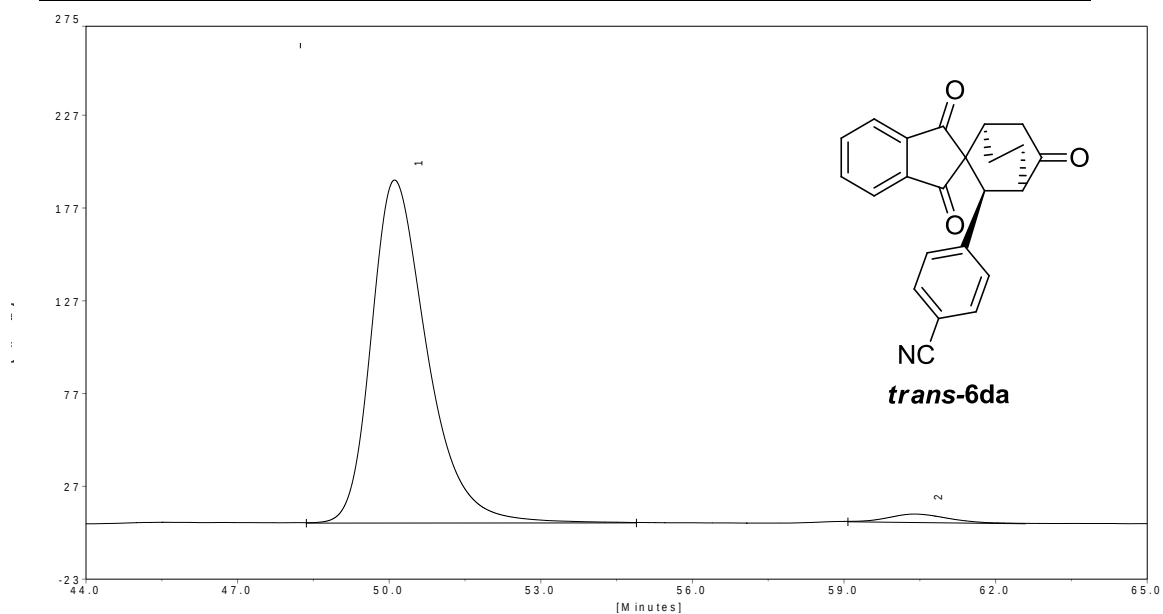
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
17.56	372.33	9540.79	98.2897
22.36	5.57	166.01	1.7103

HPLC chromatogram for **trans-6da**:

Column : Chiralpak IA	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=90 : 10	Detector : UV 226 nm



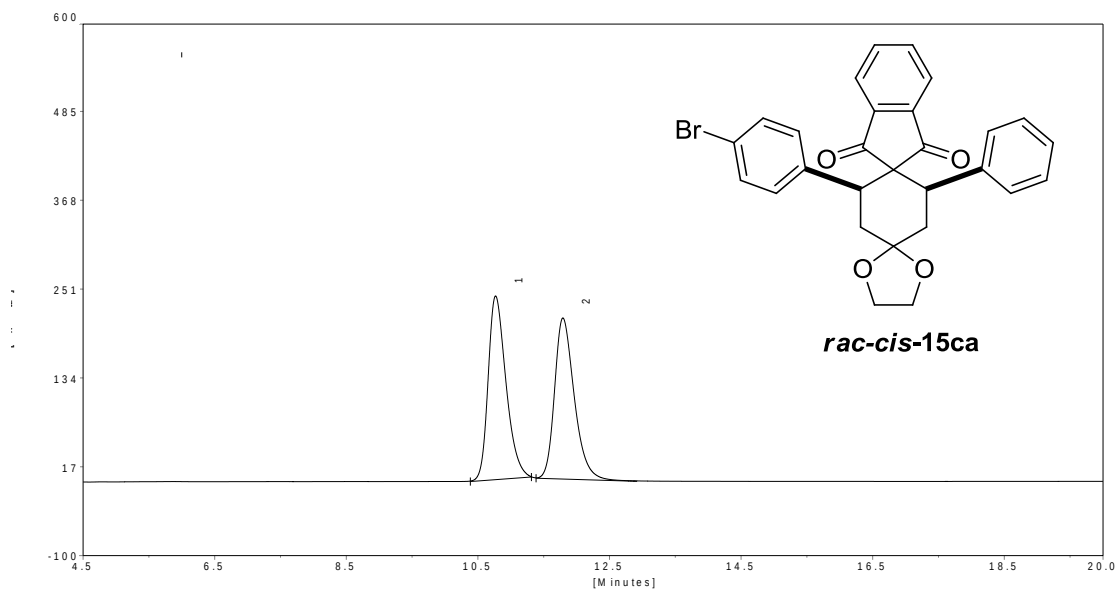
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
48.67	145.58	10857.37	49.6943
58.16	130.45	10990.95	50.3057



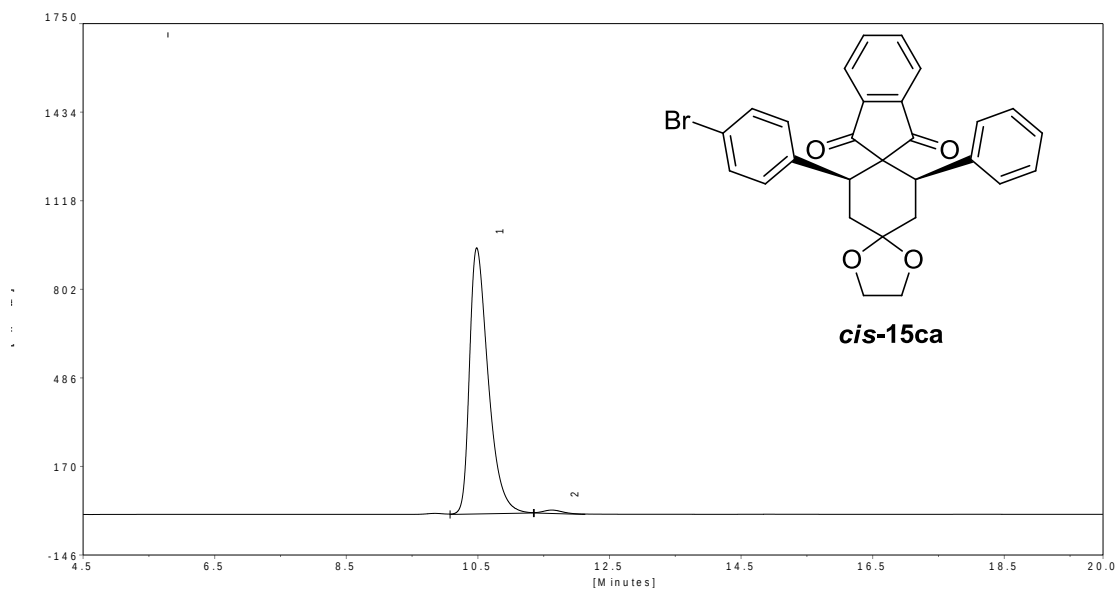
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
50.11	184.60	14119.18	97.6691
60.39	4.34	336.96	2.3309

HPLC chromatogram for *cis*-15ca :

Column : Chiralpak IB	Flow Rate : 1.0 ml/min
Solvent : Hex:IPA=95:05	Detector : UV 227 nm



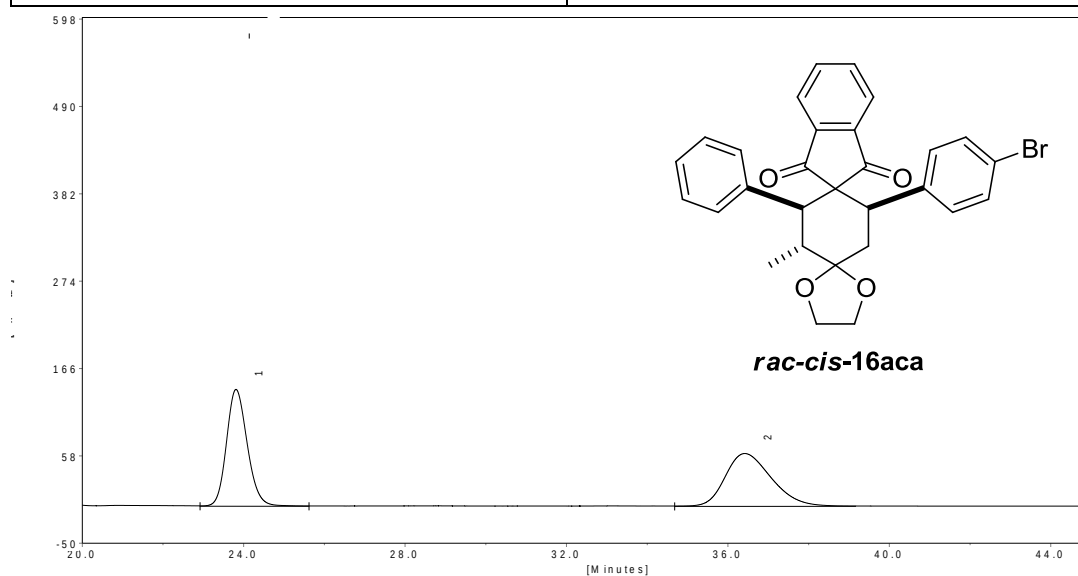
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
10.77	241.48	4527.65	50.8588
11.79	211.72	4374.74	49.1412



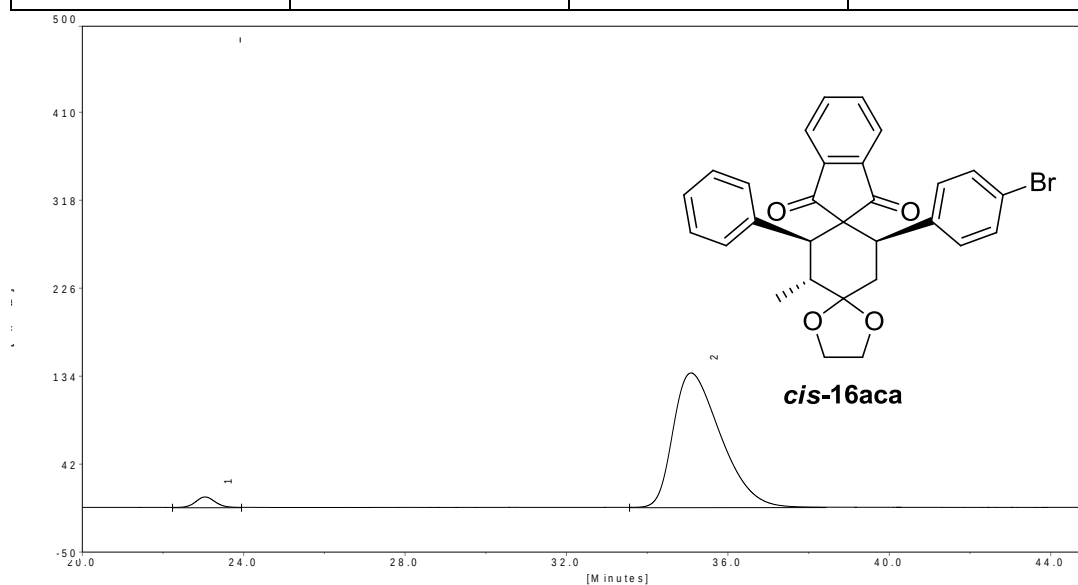
Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
10.48	948.37	18669.61	98.9760
11.62	10.80	193.15	1.0240

HPLC chromatogram for **cis-16aca** (Obtained from **cis-5aca**):

Column : Chiralpak IA	Flow Rate : 1.0 ml/min
Solvent : Hex:EtOH=90:10	Detector : UV 254 nm

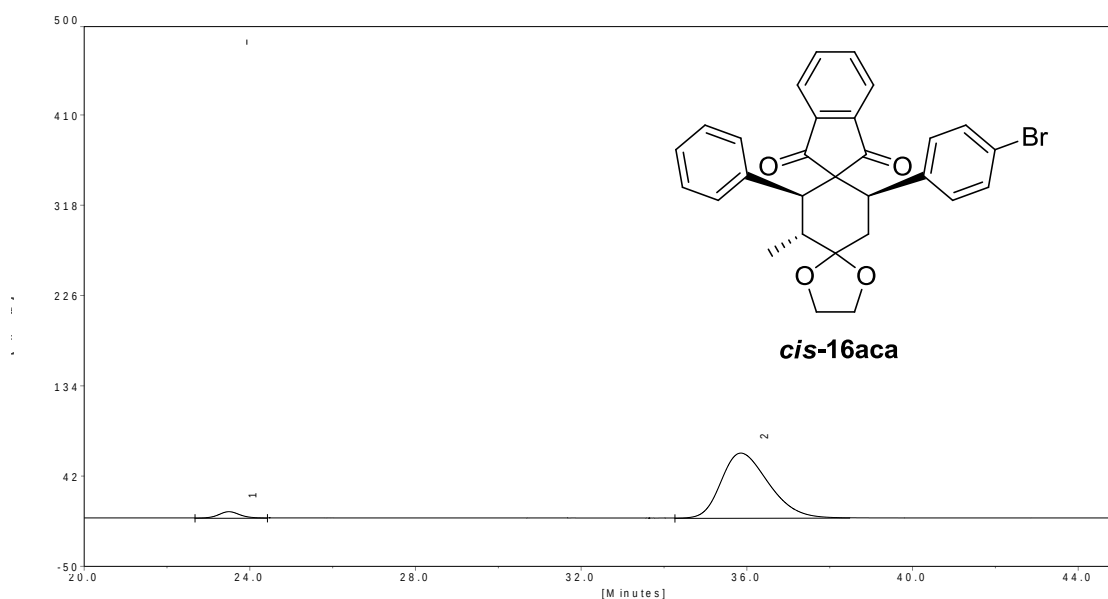


Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
23.81	144.06	5110.45	50.0757
36.42	64.87	5095.00	49.9243



Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
23.05	107.69	363.32	3.0657
35.09	237.38	11487.57	96.9343

HPLC chromatogram for **cis-16aca** (Obtained after epimerization of **trans-5aca** and derivatization):



Ret. Time (min)	Height (mv)	Area (mv.sec)	Rel. Area (%)
23.50	105.74	215.30	3.9323
35.86	165.46	5259.87	96.0677