

Supporting Information for

Synthesis, leishmanicidal, trypanocidal, antiproliferative assay and apoptotic induction of (2-phenoxy pyridin-3-yl)naphthalene-1(2*H*)-one derivatives

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Figure S1

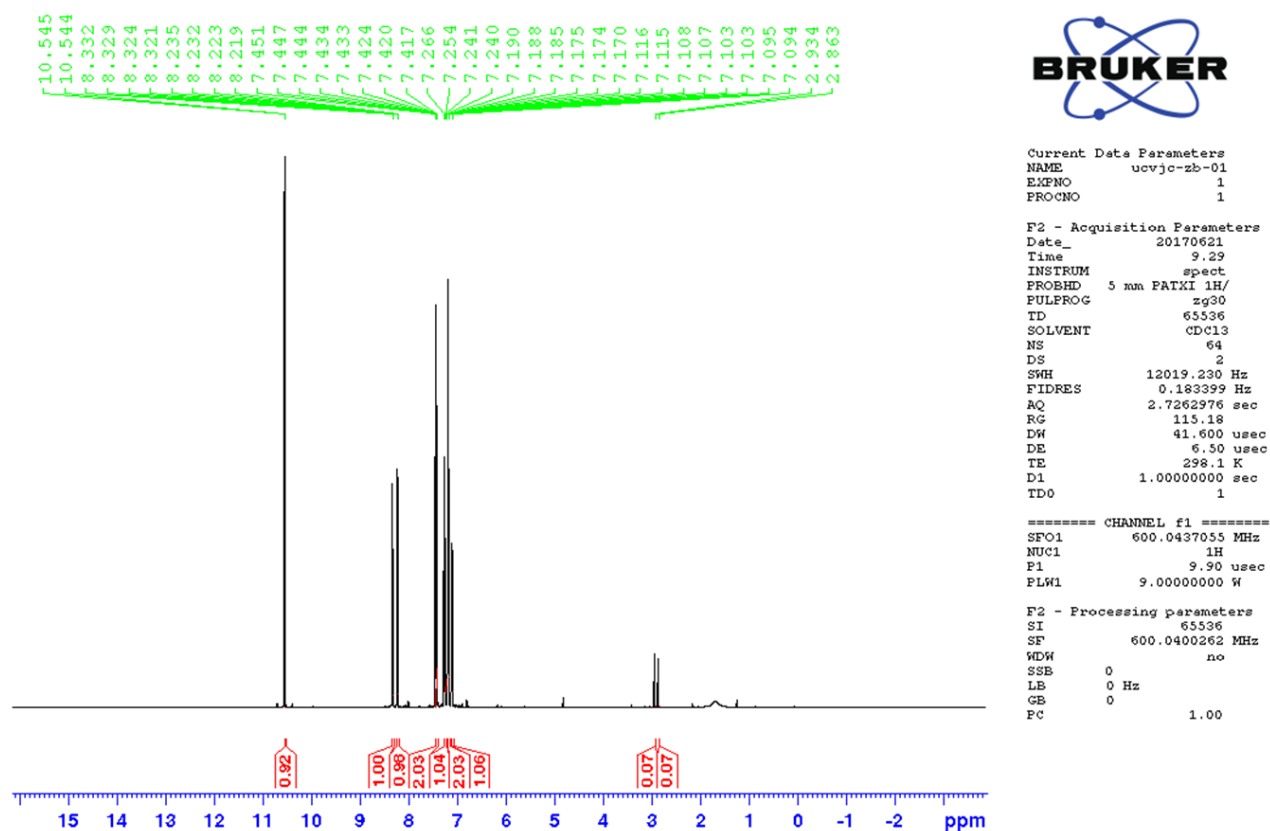


Figure S2

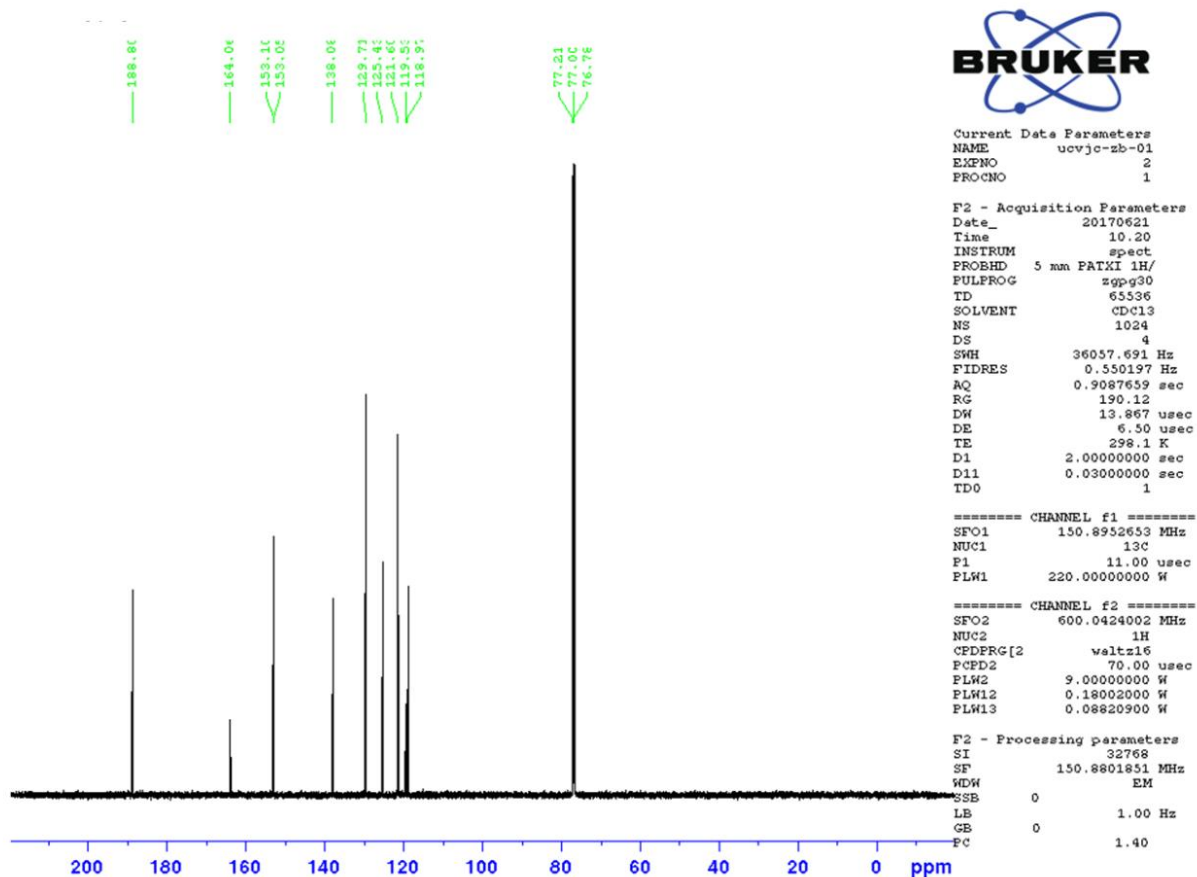


Figure S3

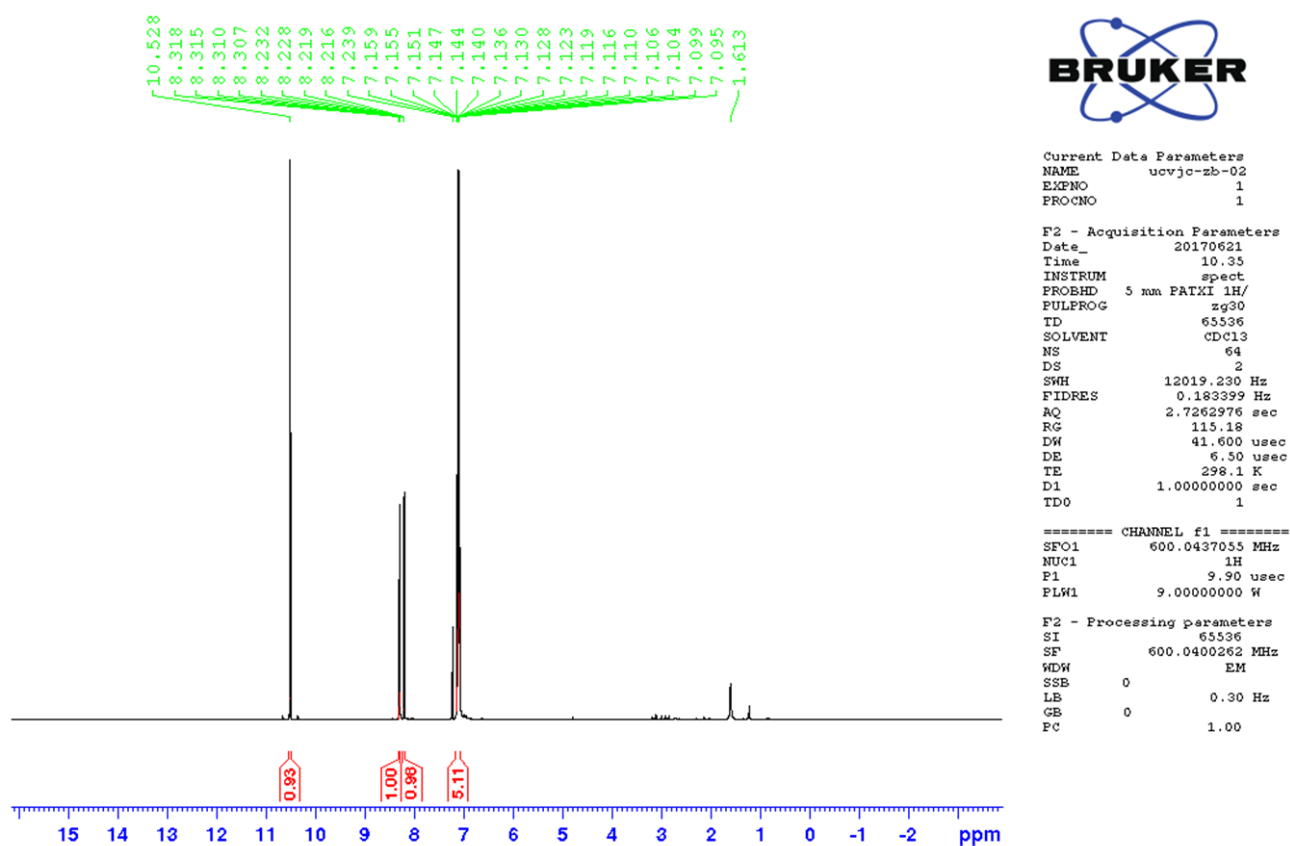


Figure S4

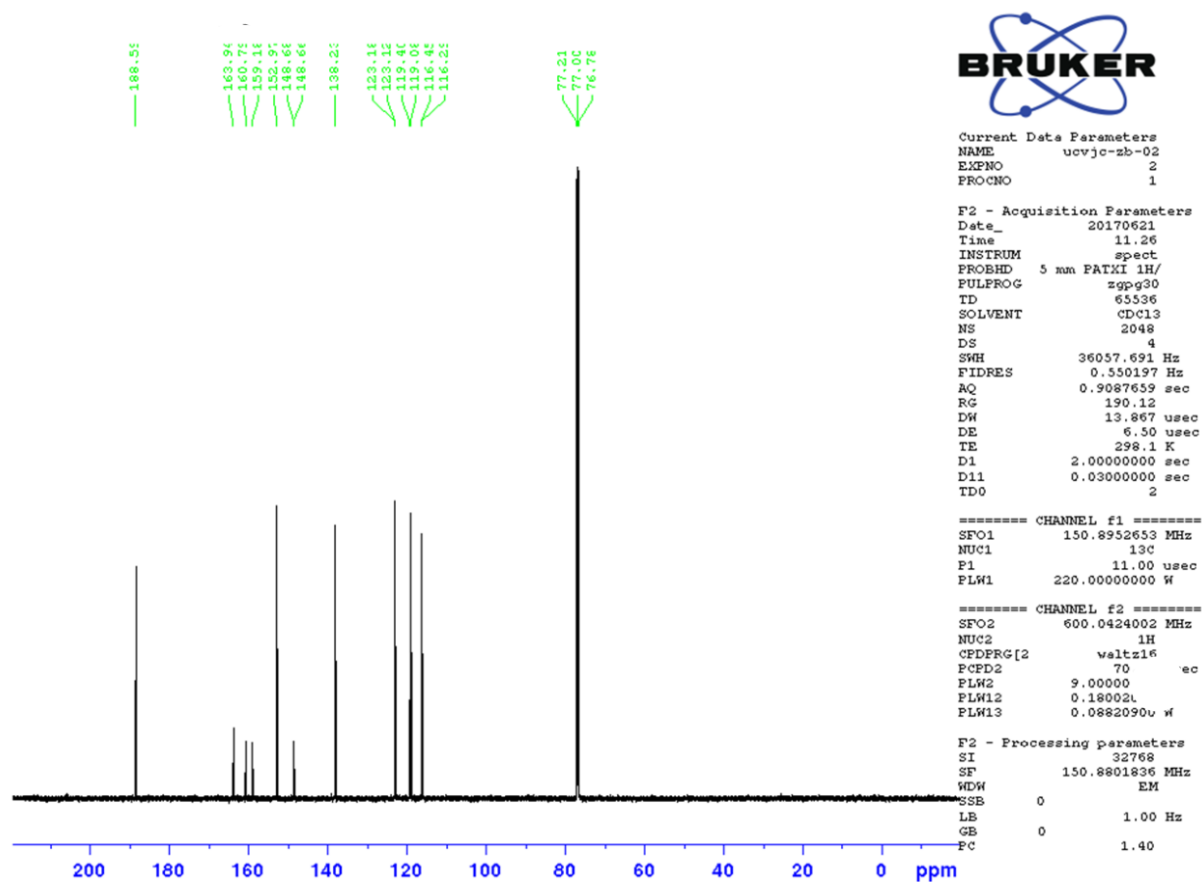


Figure S5

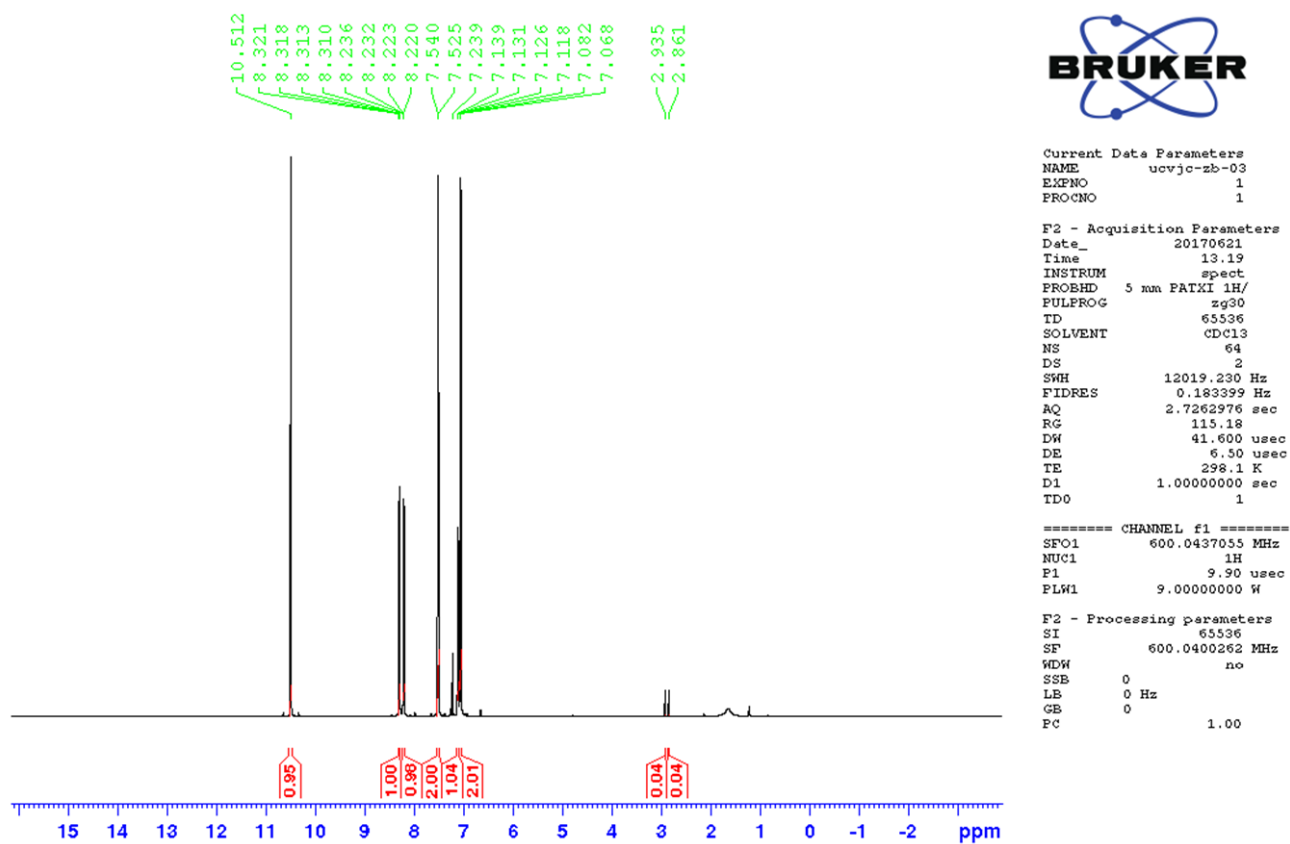


Figure S6

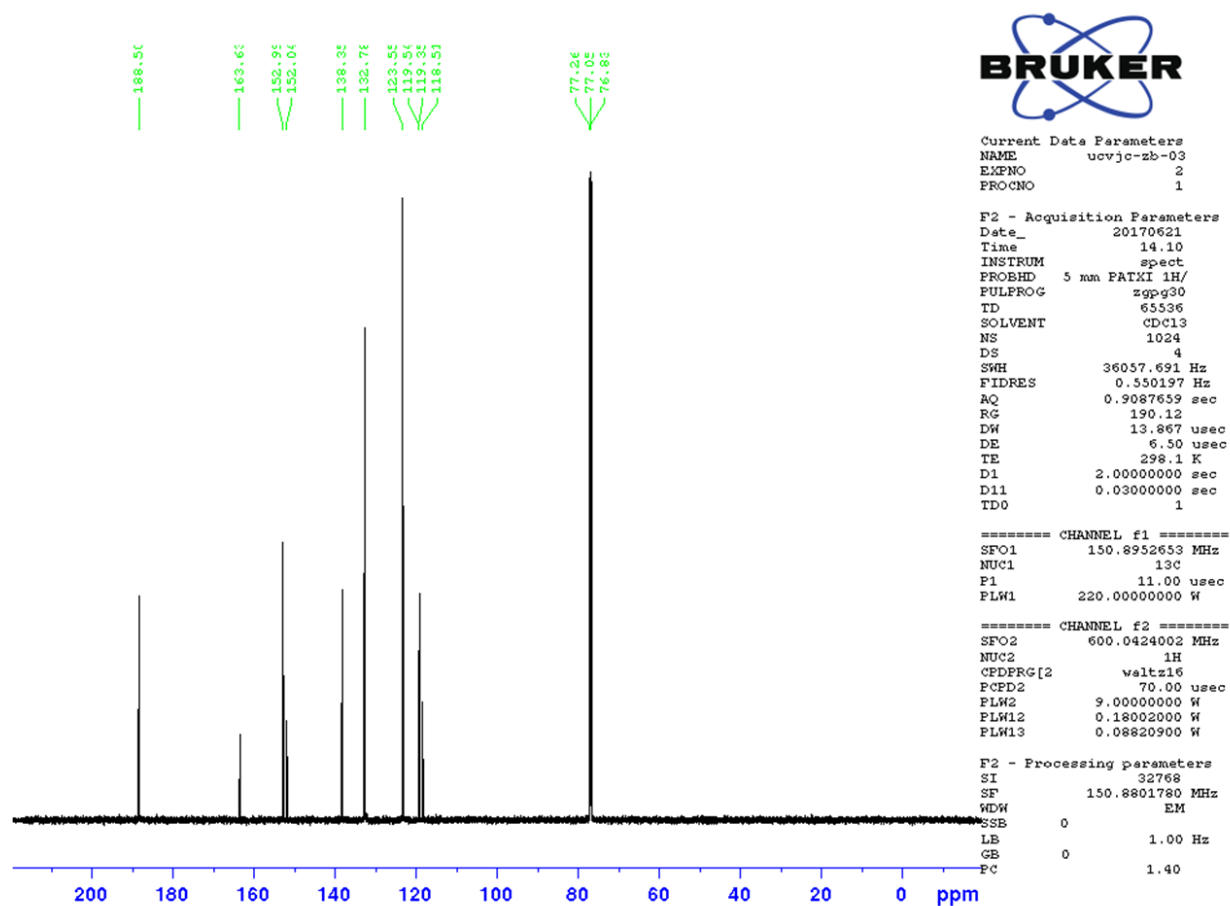


Figure S7

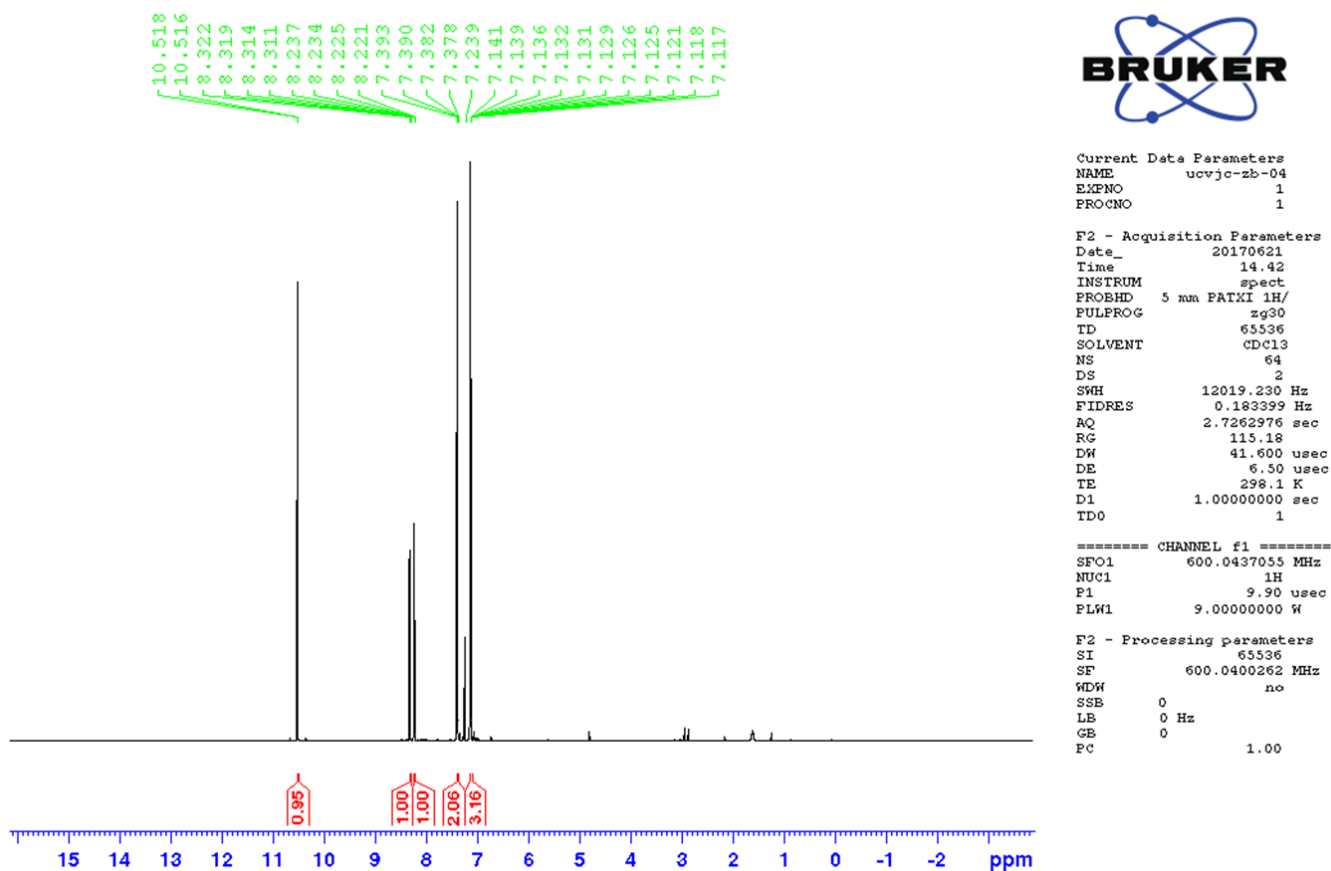


Figure S8

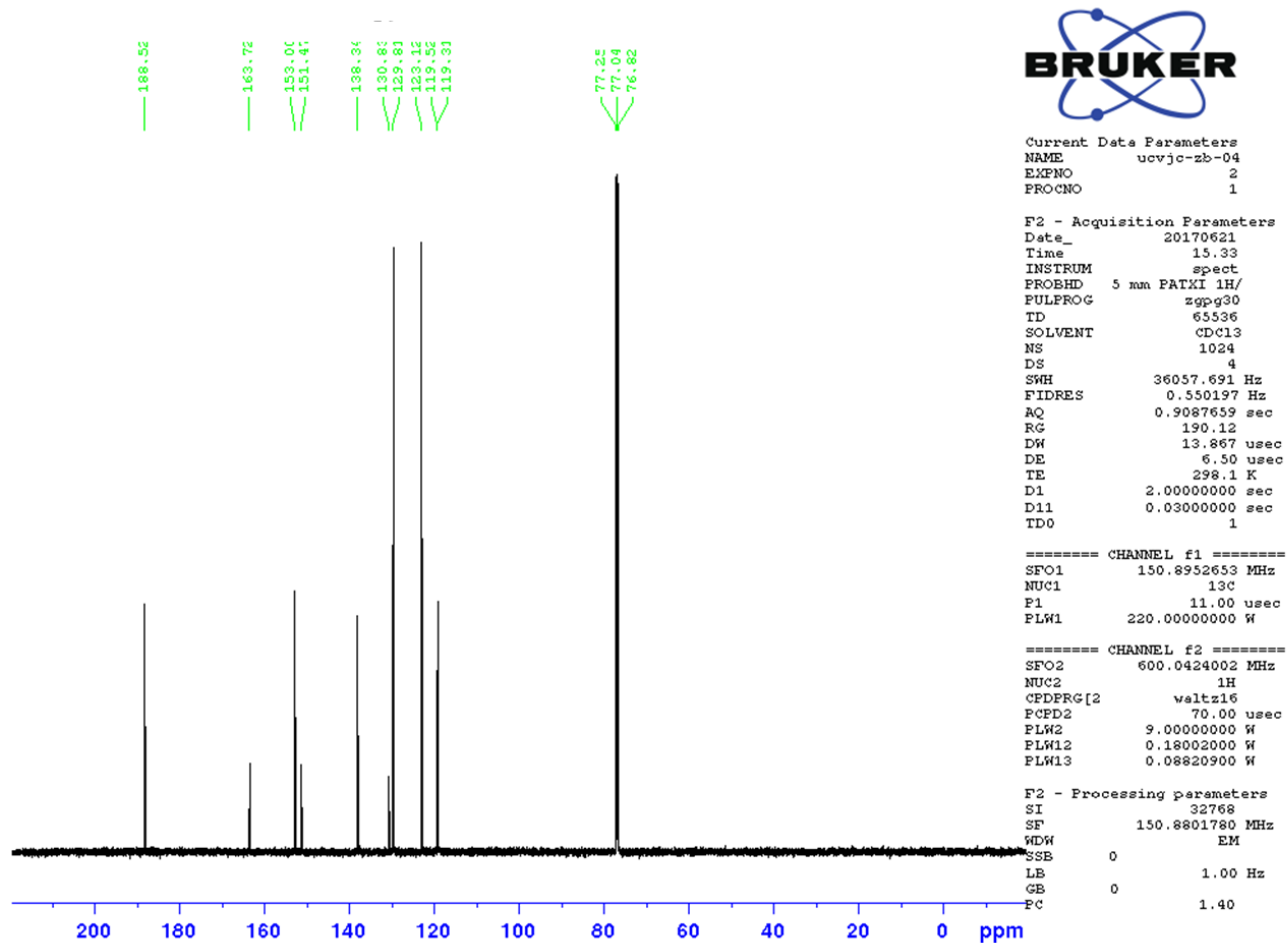


Figure S9

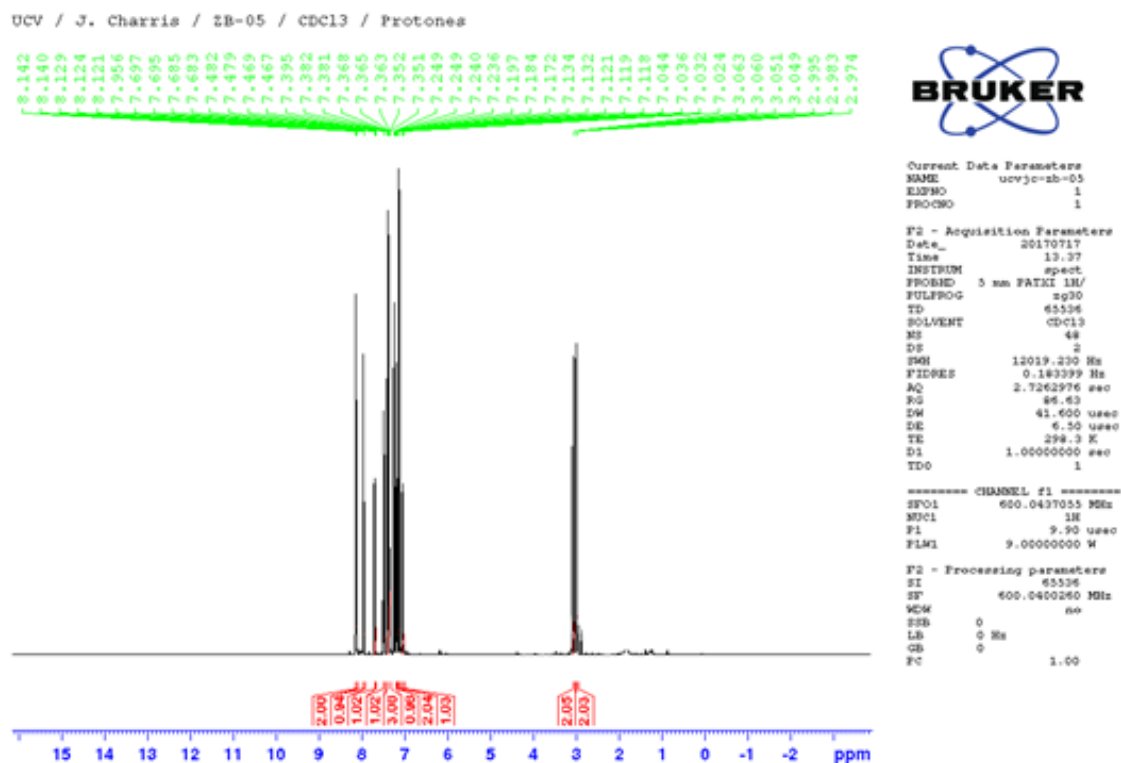
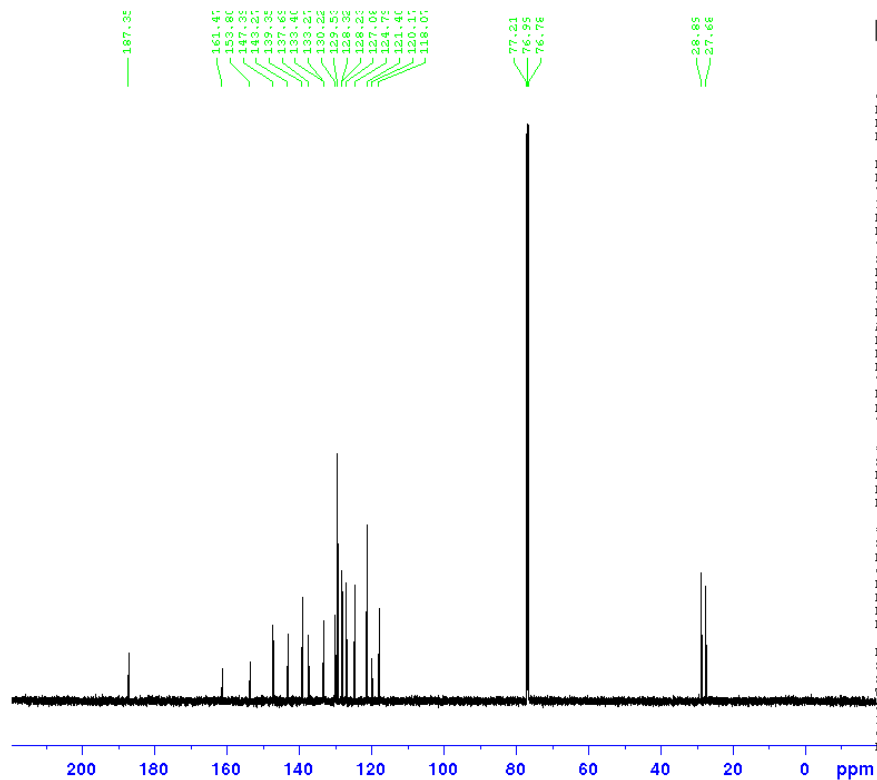


Figure S10

UCV / J. Charis / ZB-05 / CDCl₃ / Carbono



Current Data Parameters
NAME ucvjc-zb-05
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170717
Time 13.49
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 666
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 190.12
DM 13.867 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.8952653 MHz
NUC1 13C
P1 11.00 usec
PLW1 220.00000000 W

===== CHANNEL f2 =====
SFO2 600.0424002 MHz
NUC2 1H
CPDPRG2 valtz16
PCPD2 70.00 usec
PLW2 9.00000000 W
PLW12 0.18002000 W
PLW13 0.08820900 W

F2 - Processing parameters
SI 32768
SF 150.8801840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S11

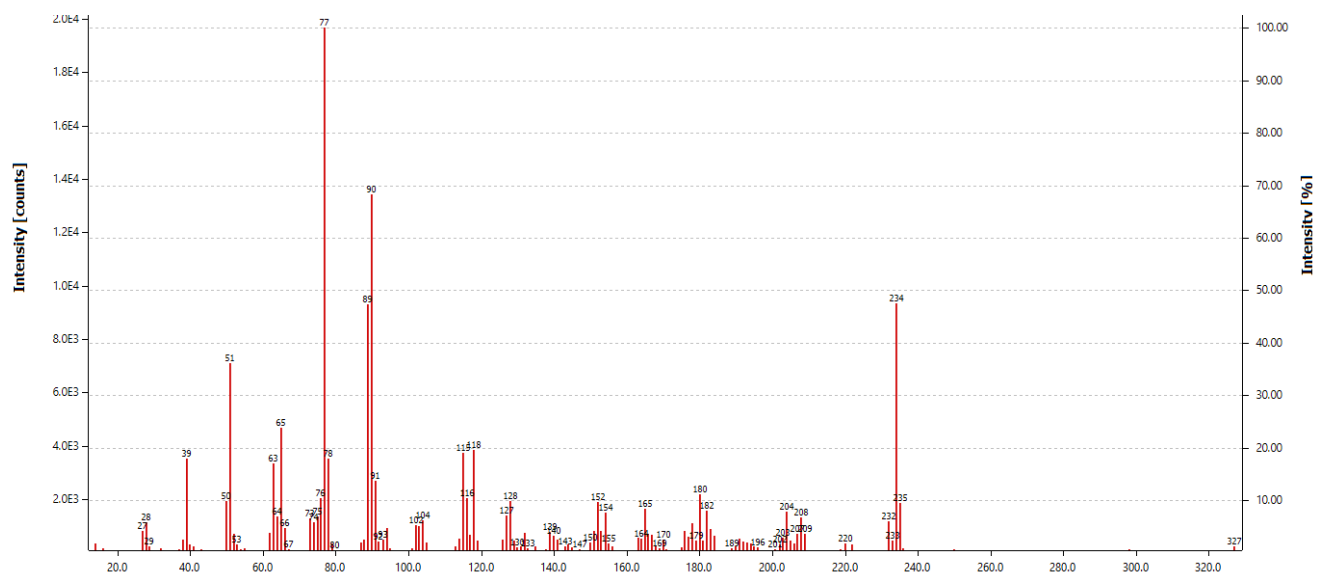
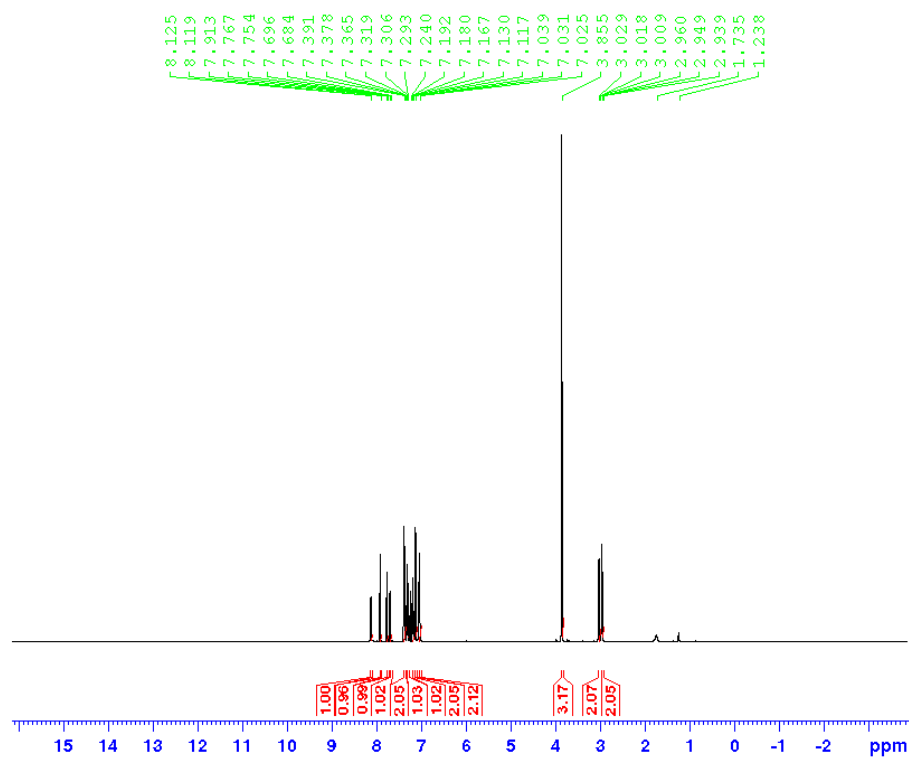


Figure S12

UCV / J. Charris / ZB-10 / CDCl₃ / Protones



Current Data Parameters
NAME ucvjc-zb-10
EXPNO 1
PROCNO 1

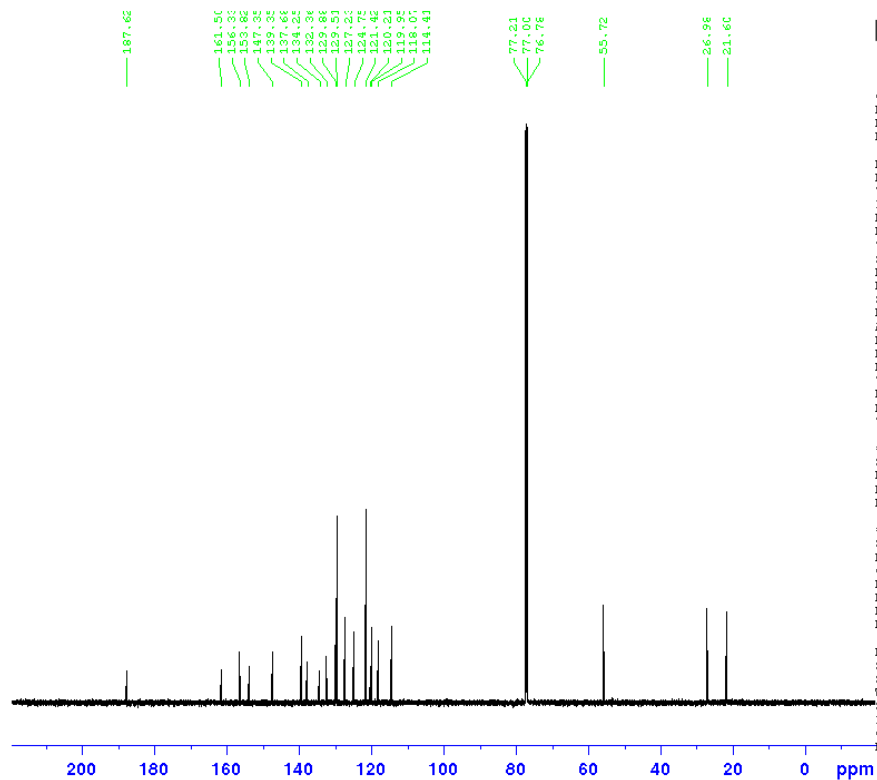
F2 - Acquisition Parameters
Date_ 20170717
Time 10.19
INSTRUM spect
PROBHD 5 mm FATHI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 48
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 86.63
DW 41.600 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.0437055 MHz
NUC1 1H
P1 9.90 usec
PLW1 9.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0400260 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
FC 1.00

Figure S13

UCV / J. Charis / ZB-10 / CDCl₃ / Carbono



Current Data Parameters
NAME ucvjc-zb-10
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170717
Time 10.20
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 190.12
DM 13.867 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.8952653 MHz
NUC1 13C
P1 11.00 usec
PLW1 220.00000000 W

===== CHANNEL f2 =====
SFO2 600.0424002 MHz
NUC2 1H
CPDPRG2 valtm16
PCPD2 70.00 usec
PLW2 9.00000000 W
PLW12 0.18002000 W
PLW13 0.08820900 W

F2 - Processing parameters
SI 32768
SF 150.8801845 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S14

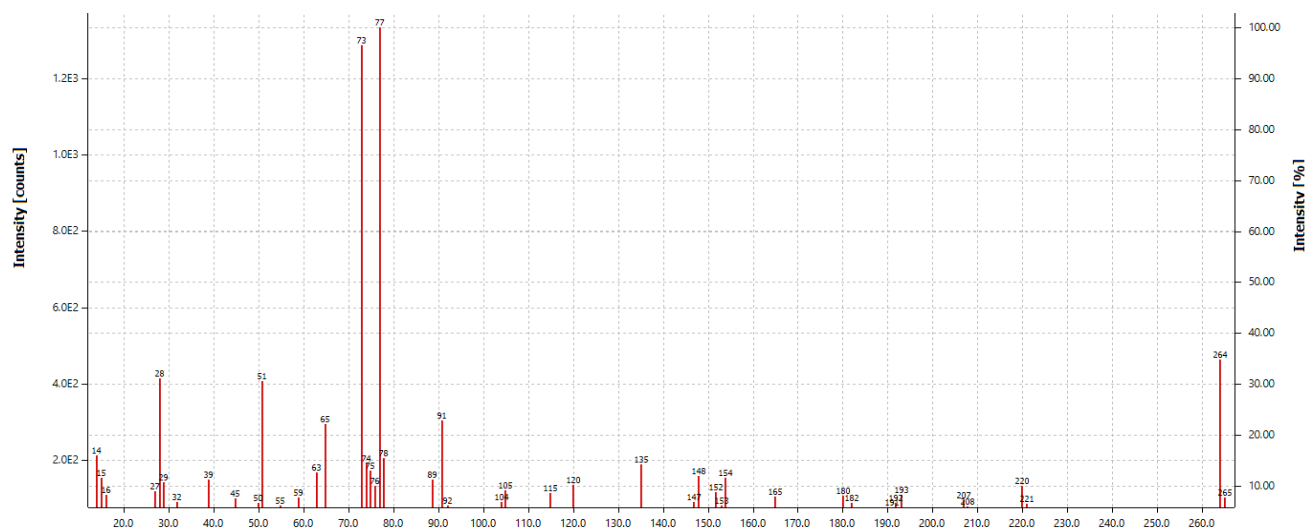
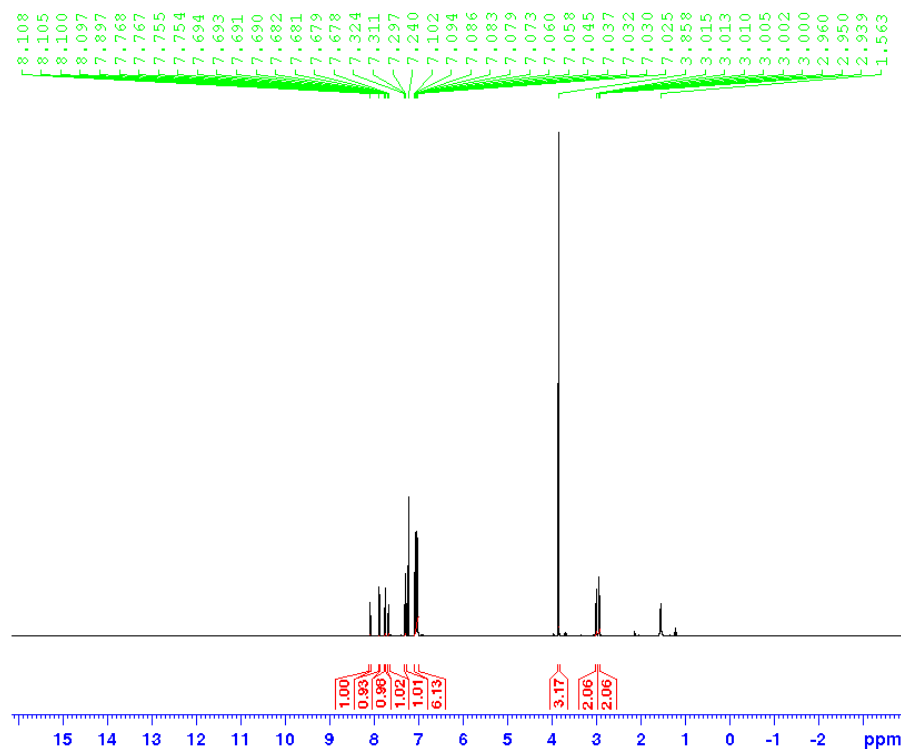


Figure S15

UCV / J. Charis / ZB-22 / CDCl3 / Protones



Current Data Parameters
NAME ucvjch-zb-22
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180303
Time 10.30
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 190.12
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.0437055 MHz
NUC1 1H
P1 9.90 usec
PLW1 9.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0400262 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S16

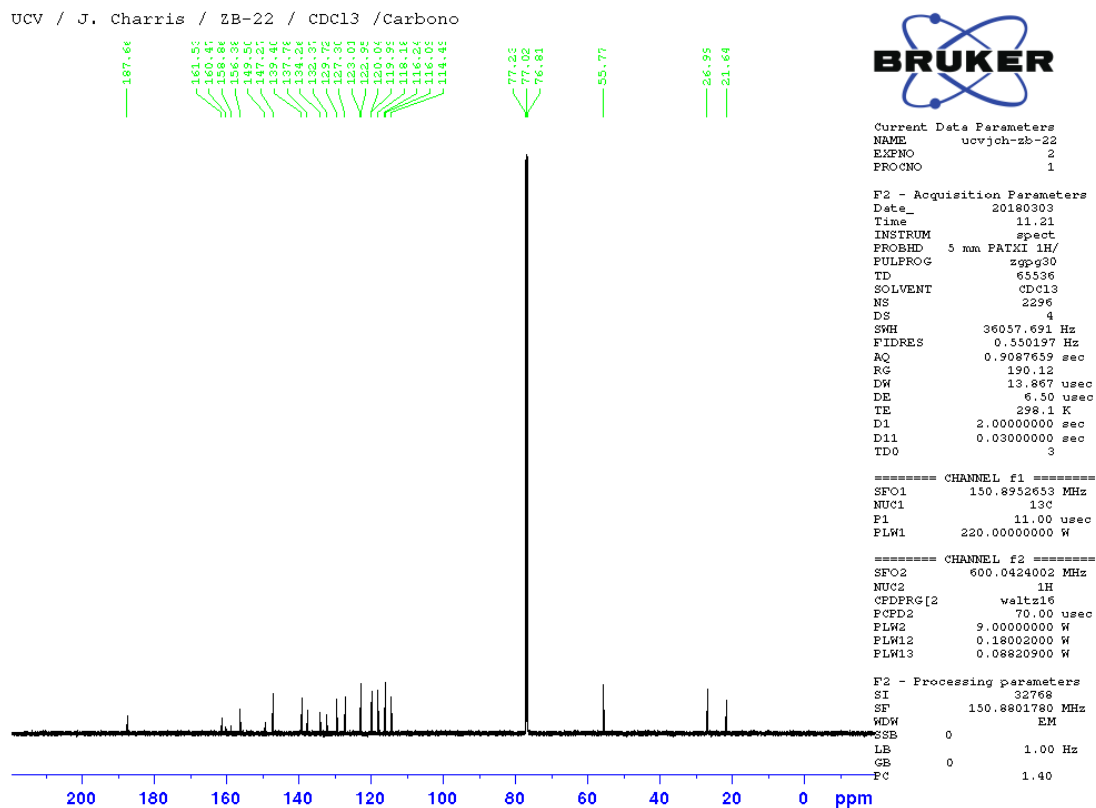


Figure S17

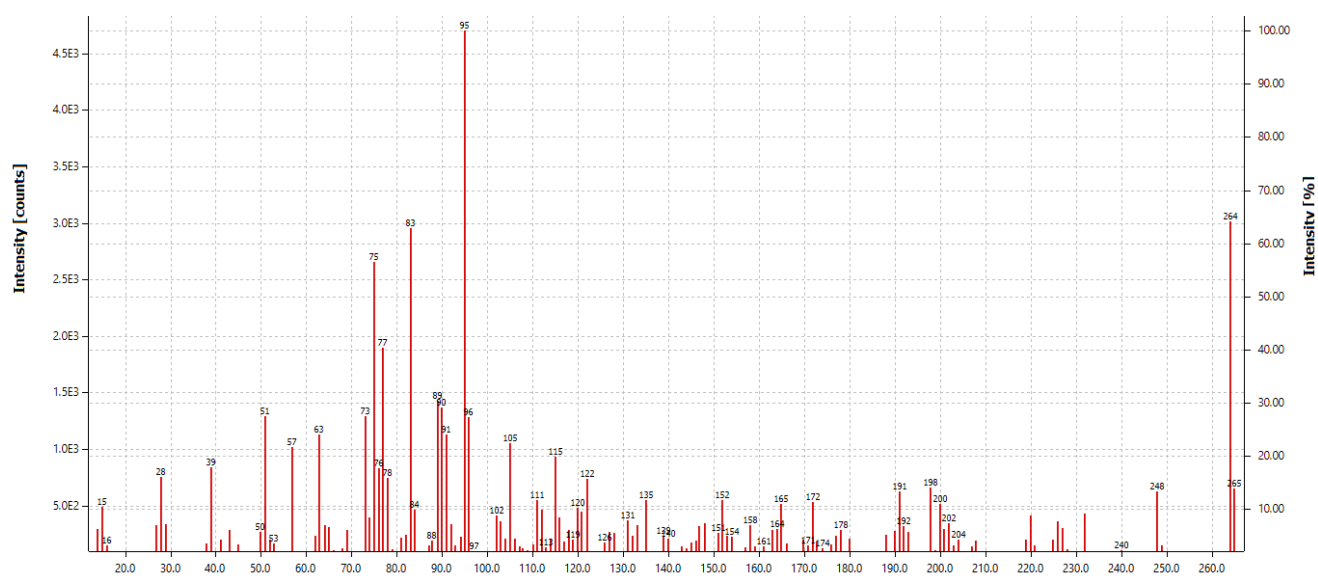
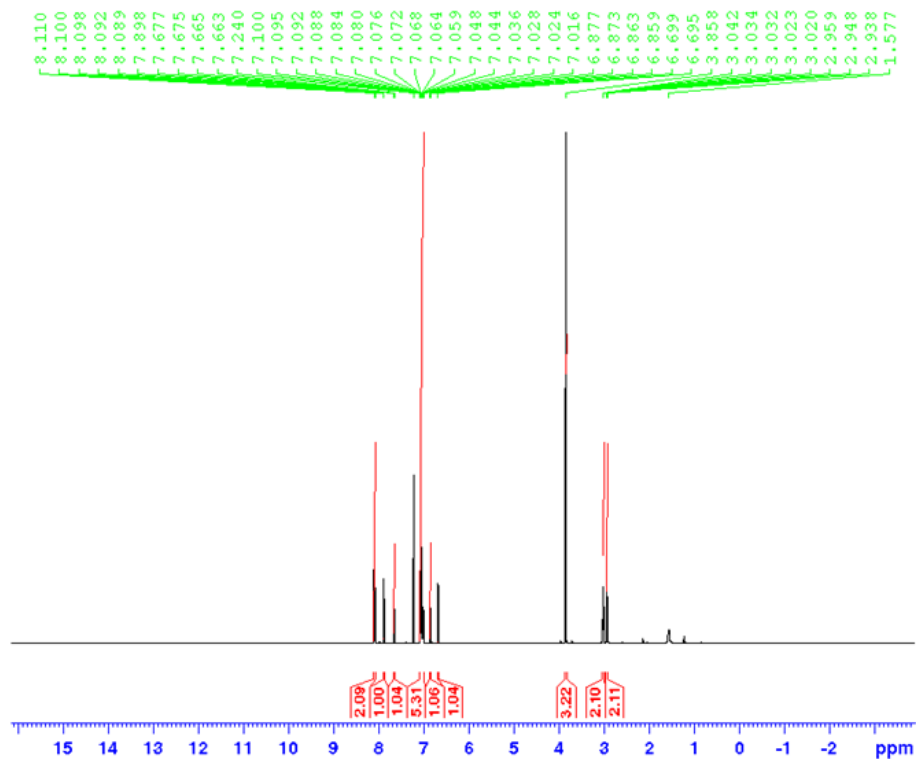


Figure S18

UCV / J. Charris / ZB-23 / CDCl₃ / Protones



Current Data Parameters
NAME ucvjch-zb-23
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180304
Time 11.31
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 96
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 190.12
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.0437055 MHz
NUC1 1H
P1 9.90 usec
PLW1 9.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0400262 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S19

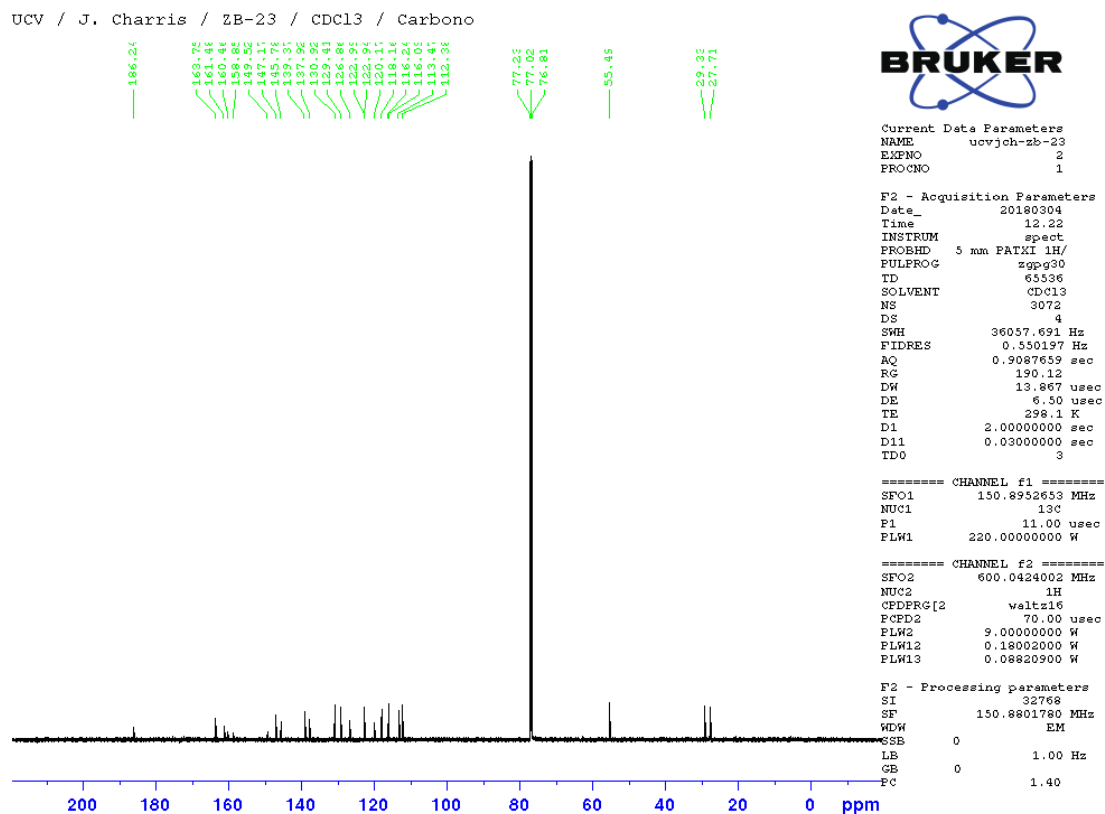


Figure S20

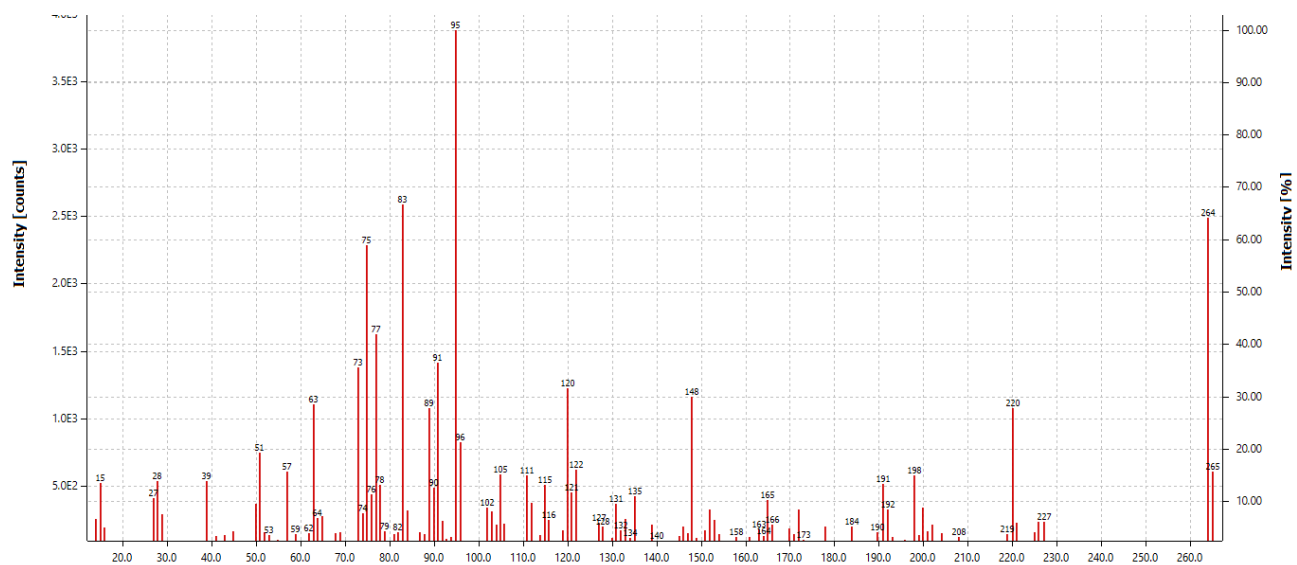
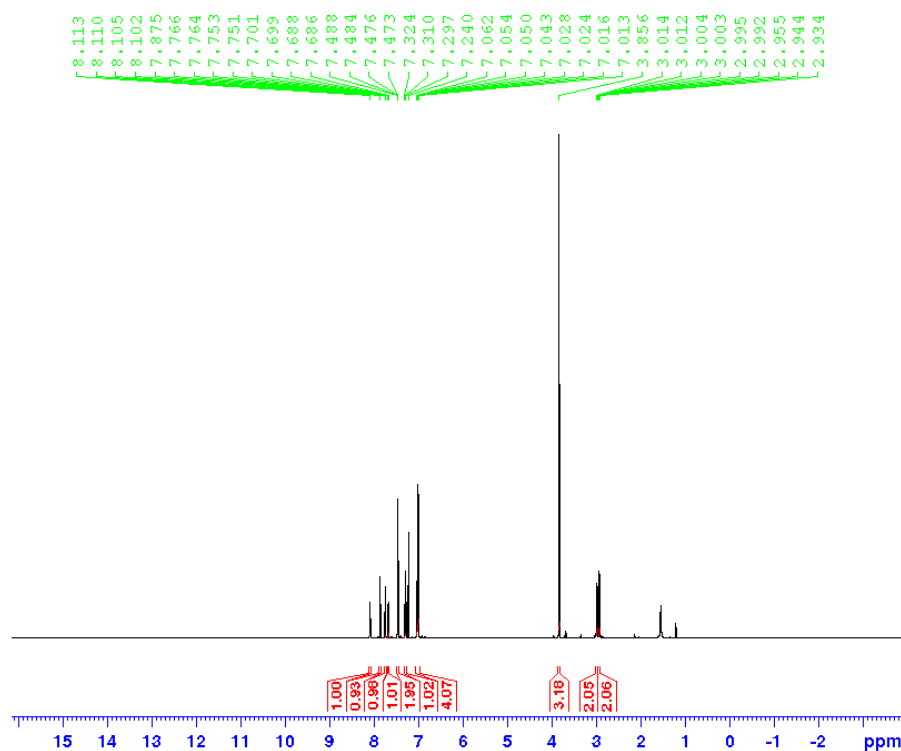


Figure S21

UCV / J. Charris / ZB-32 / CDCl3 / Protones



Current Data Parameters
NAME ucvjch-zb-32
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180301
Time 13.06
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 190.12
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.0437055 MHz
NUC1 1H
P1 9.90 usec
PLW1 9.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0400262 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S22

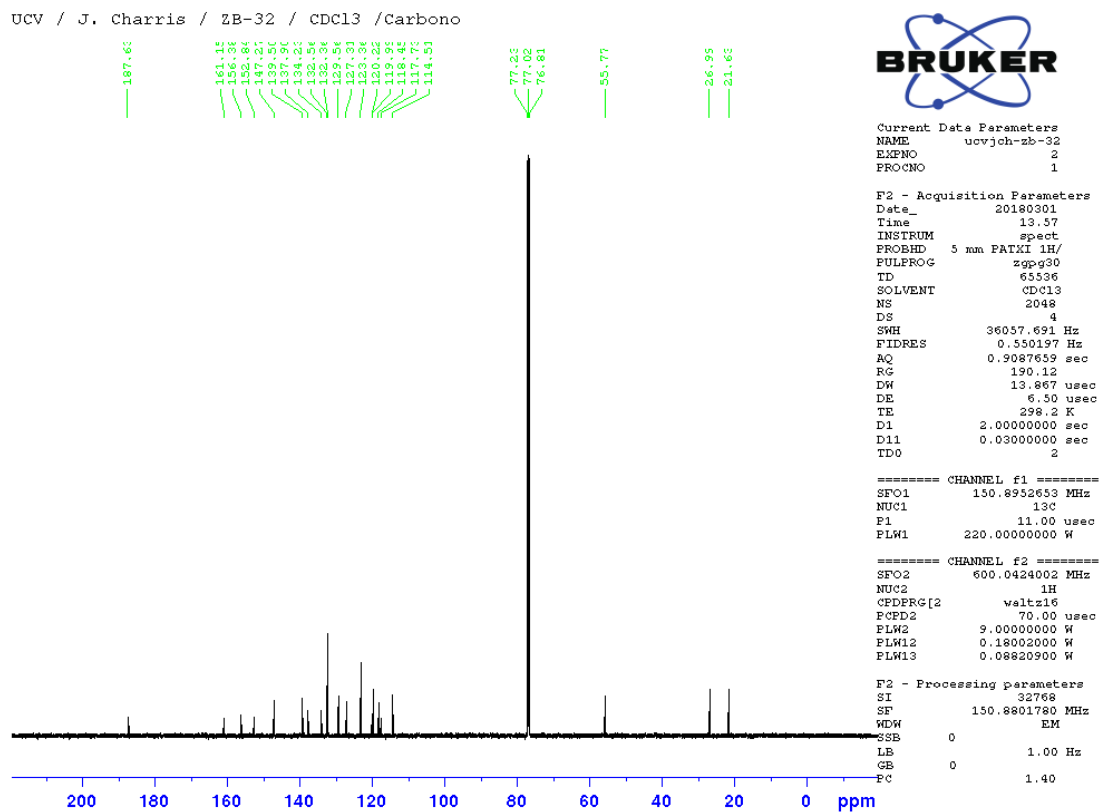


Figure S23

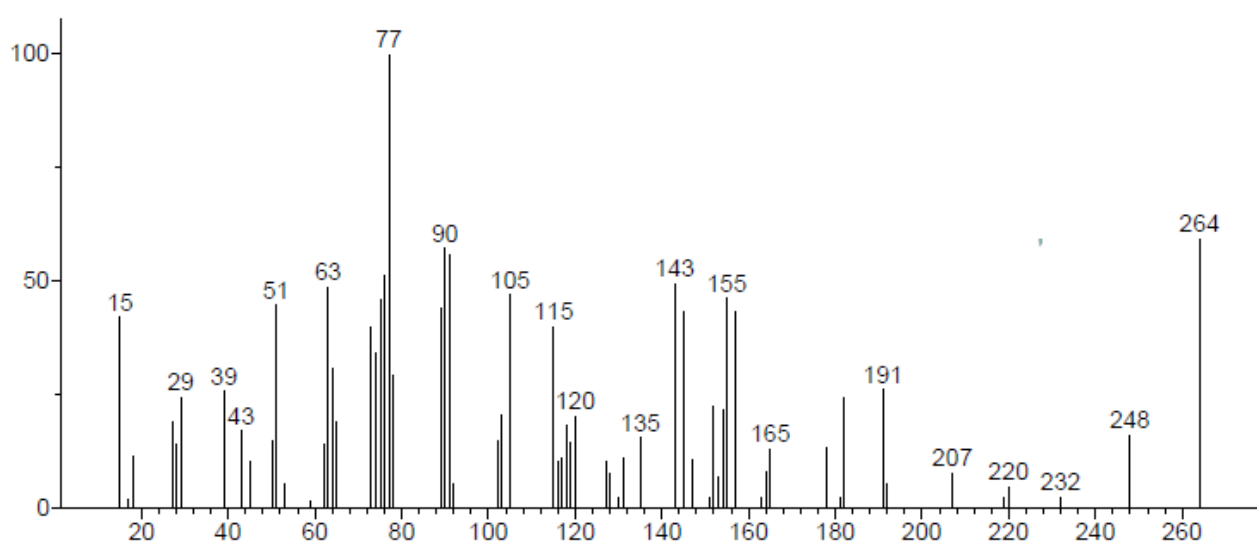
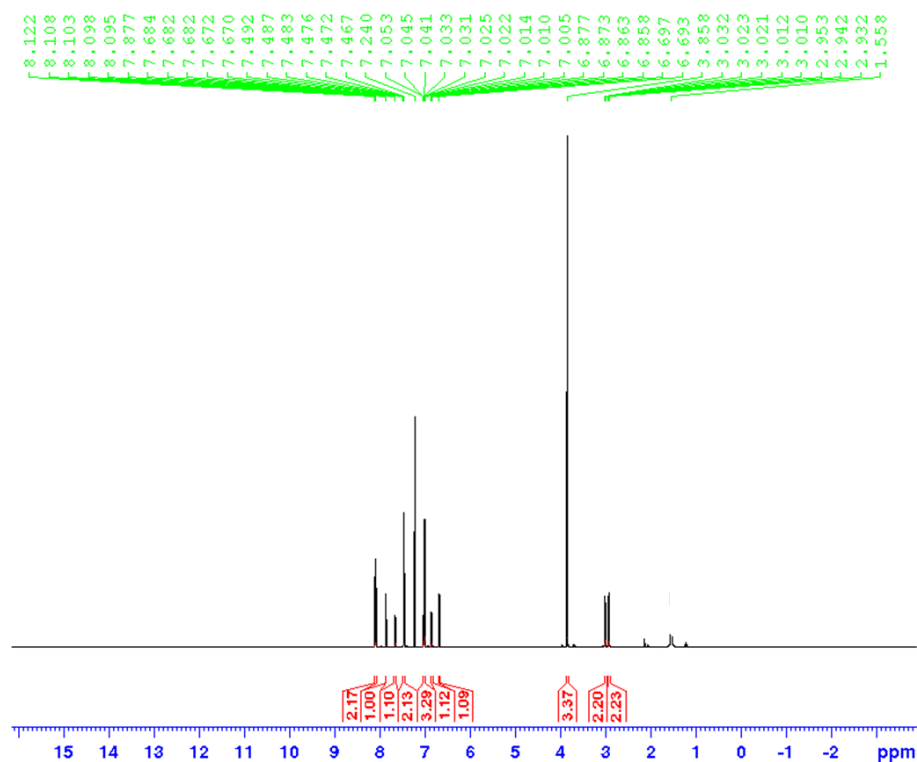


Figure S24

UCV / J. Charis / ZB-33 / CDCl₃ / Protones



Current Data Parameters
NAME ucvjch-zb-33
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180302
Time 7.54
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 96
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 190.12
DH 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.0437055 MHz
NUC1 1H
P1 9.90 usec
PLW1 9.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0400262 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S25

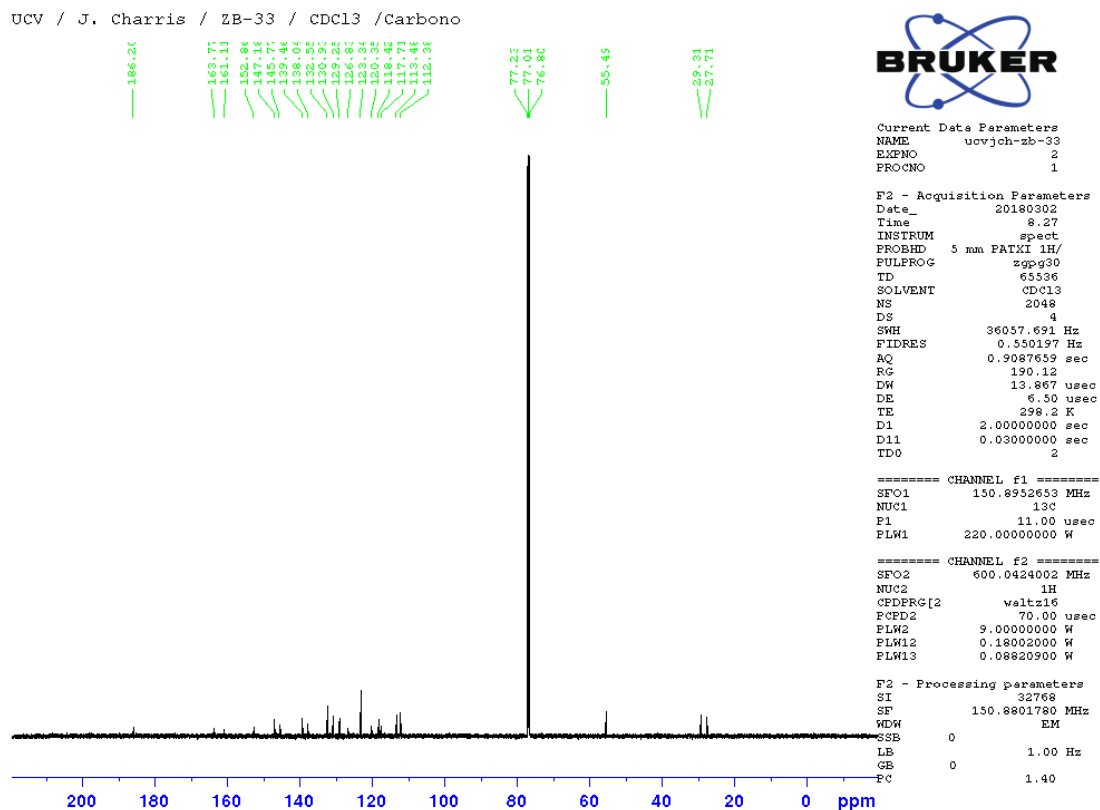


Figure S26

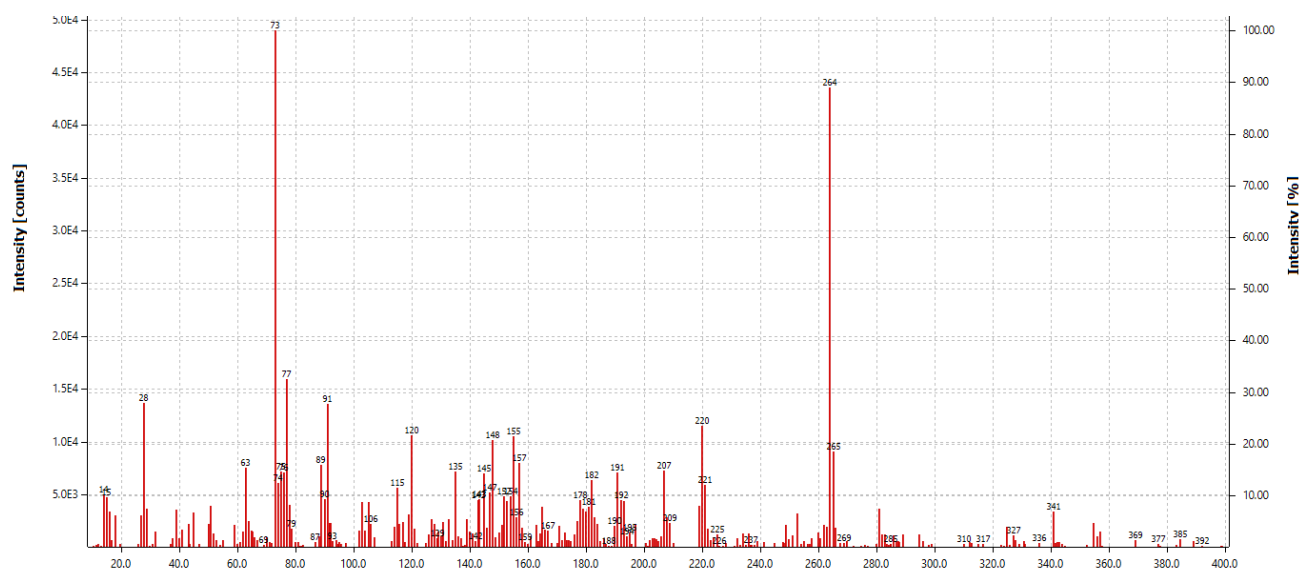
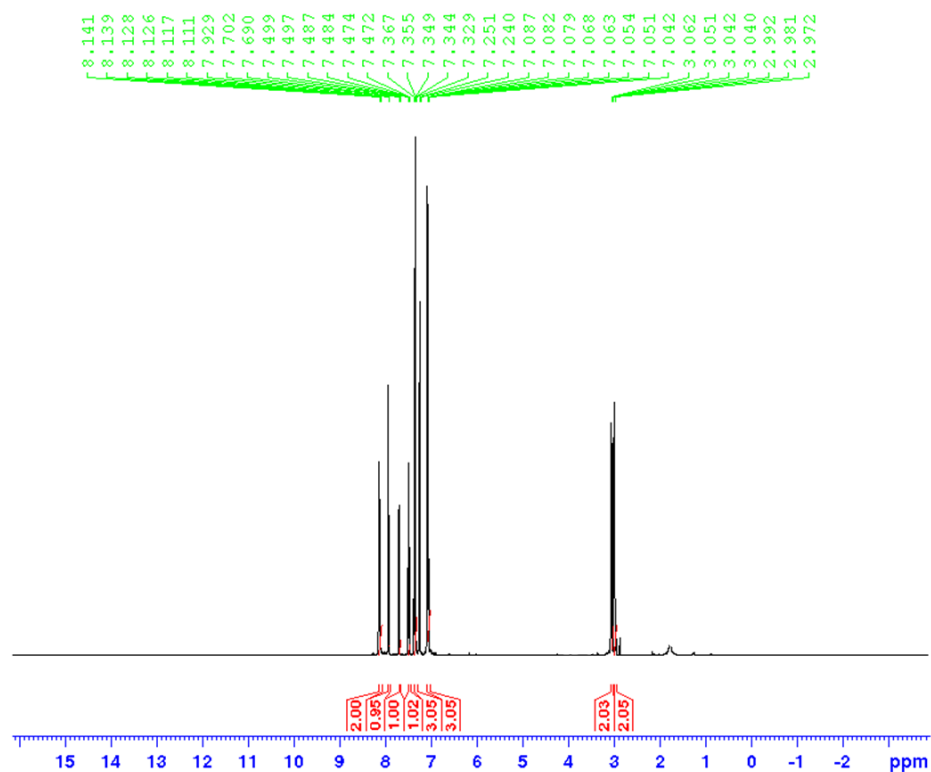


Figure S27

UCV / J. Charris / ZB-06 / CDCl₃ / Protones



Current Data Parameters
NAME ucvjc-zb-06
EXPNO 1
PROCNO 1

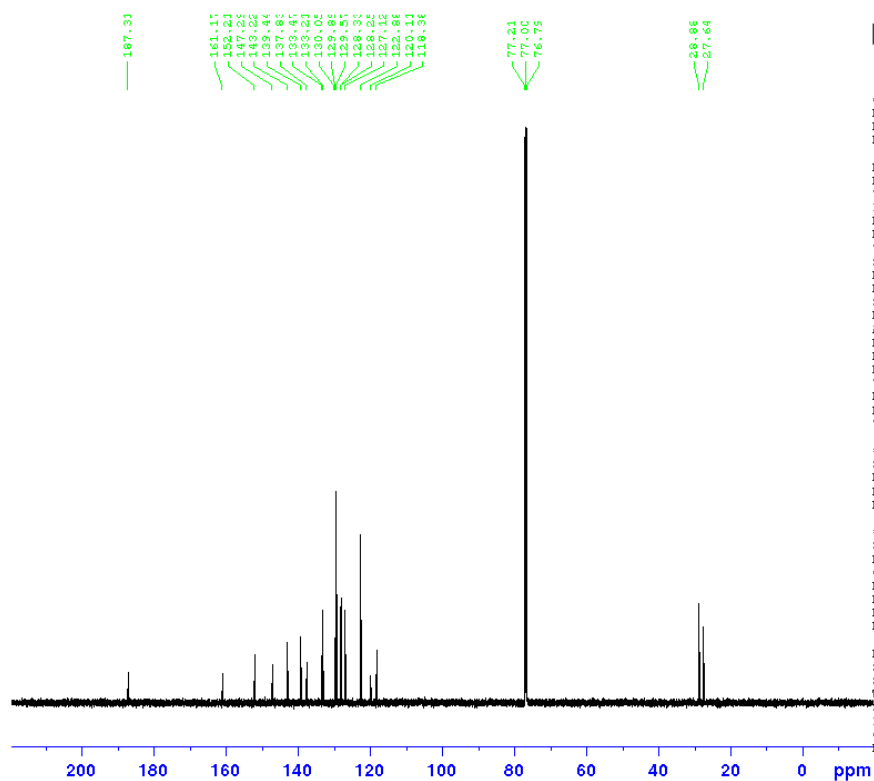
F2 - Acquisition Parameters
Date_ 20170717
Time 14.19
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 48
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 86.63
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.0437055 MHz
NUC1 1H
P1 9.90 usec
PLW1 9.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0400260 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S28

UCV / J. Charis / ZB-06 / CDCl₃ / Carbono



Current Data Parameters

NAME	ucvjc-zb-06
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20170717
Time	14.29
INSTRUM	spect
PROBHD	5 mm PATXI 1H/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	636
DS	4
SWH	36037.691 Hz
FIDRES	0.550197 Hz
AQ	0.9087659 sec
RG	190.12
DW	13.867 usec
DE	6.50 usec
TE	298.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

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

SFO1	150.8952653 MHz
NUC1	13C
F1	11.00 usec
PLW1	220.00000000 W

===== CHANNEL f2 =====

SFO2	600.0424002 MHz
NUC2	1H
CEDERG[2]	waltz16
PCPD2	70.00 usec
PLW2	9.00000000 W
PLW12	0.18002000 W
PLW13	0.08820900 W

F2 - Processing parameters

SI	32768
SF	150.8801837 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
FC	1.40

Figure S29

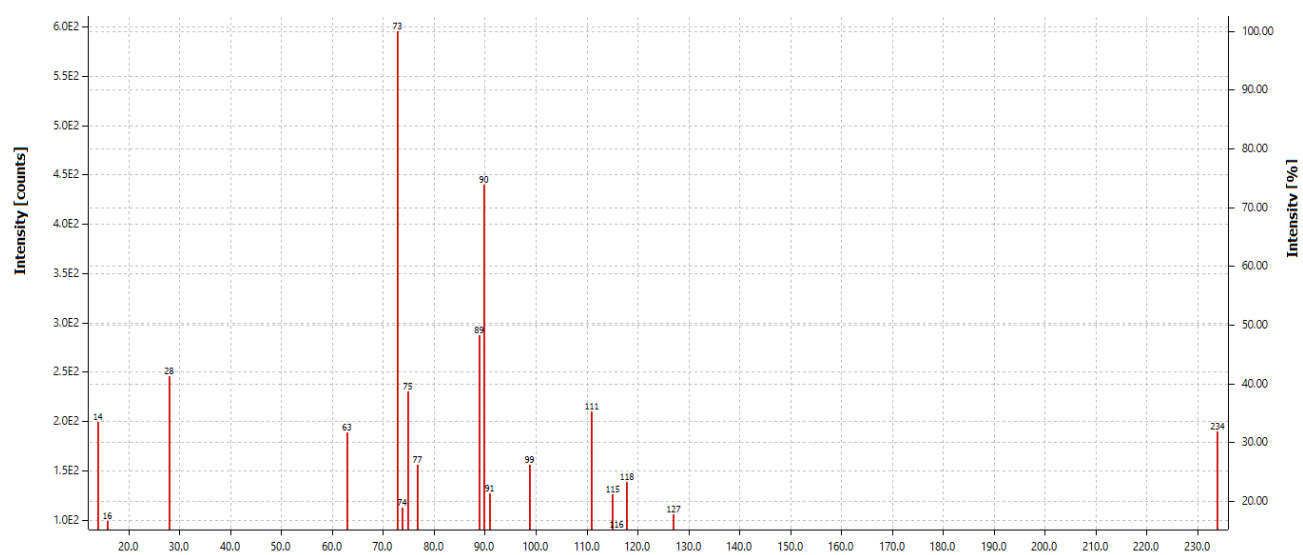
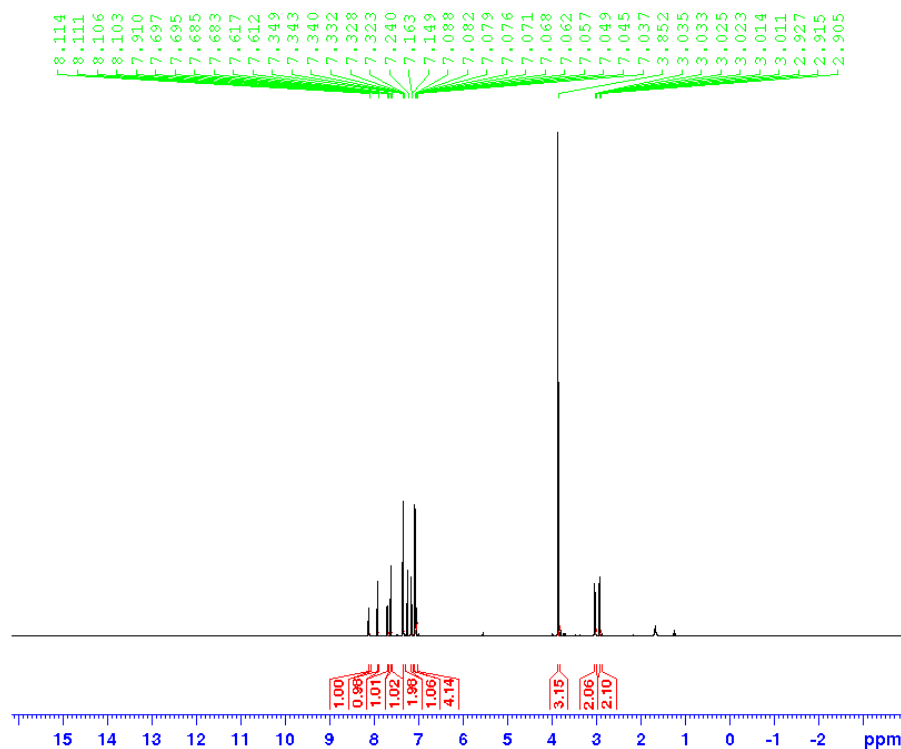


Figure S30

UCV / J. Charris / ZB-09 / CDCl₃ / Protones



Current Data Parameters
NAME ucvjc-zb-09
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170718
Time 7.35
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 48
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 86.63
DW 41.600 usec
DE 6.30 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.0437035 MHz
NUC1 1H
P1 9.90 usec
PLW1 9.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0400260 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S31

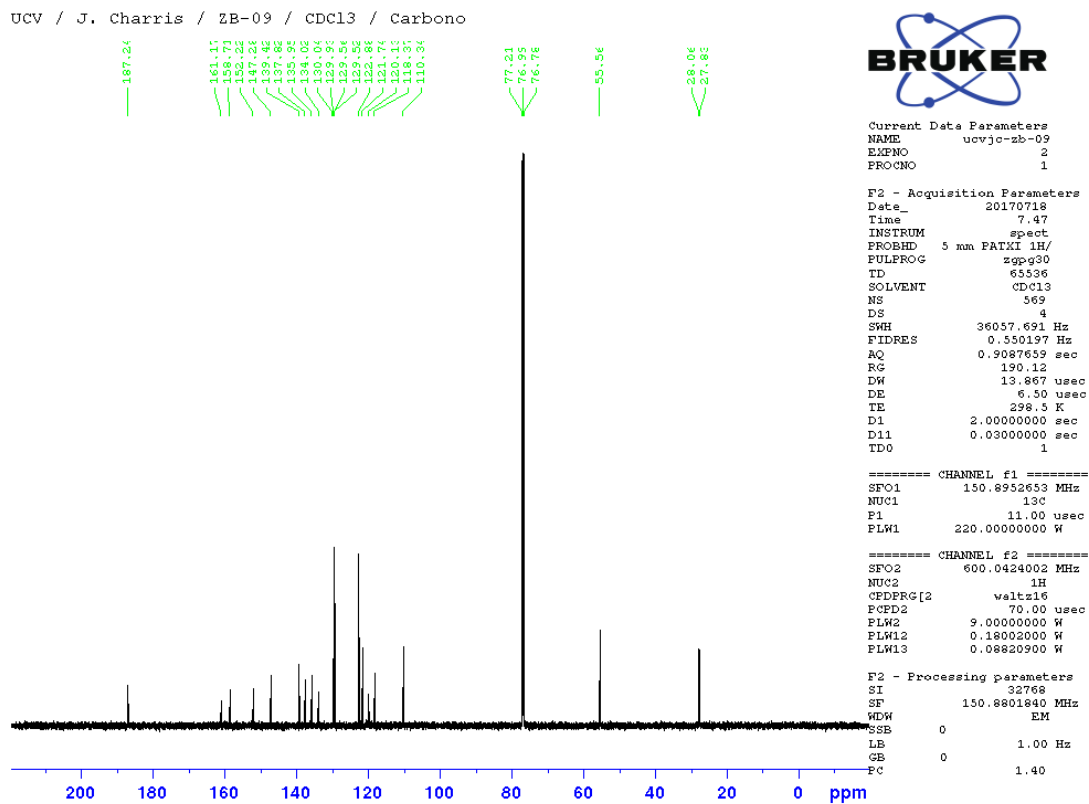
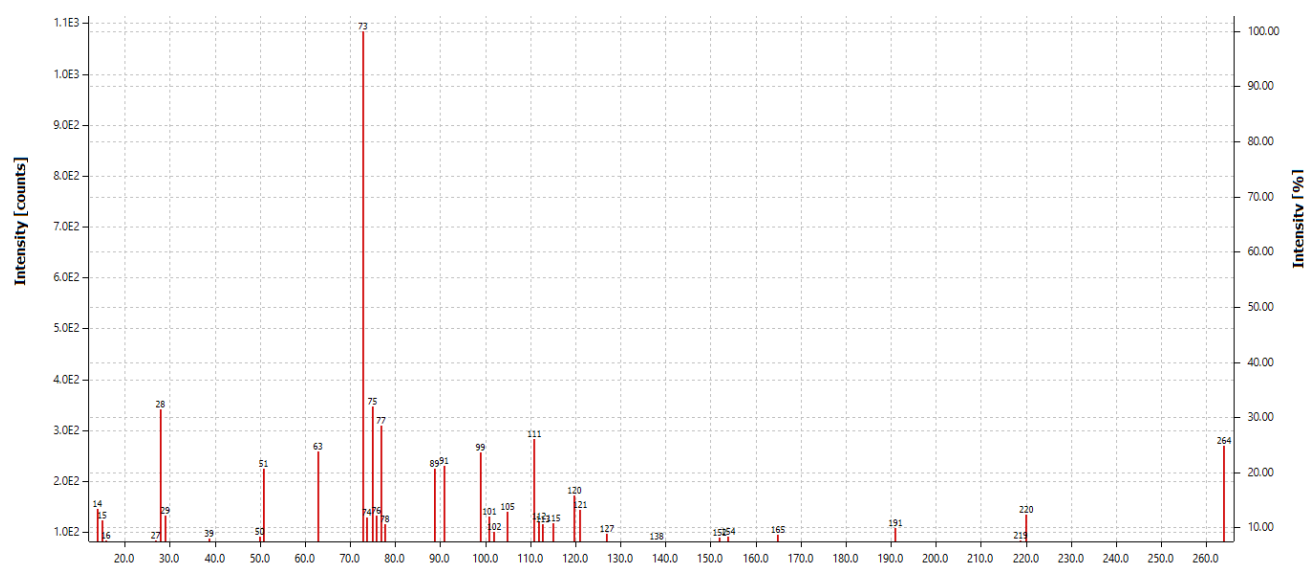


Figure S32



Supporting Information for Tables

Synthesis, leishmanicidal, trypanocidal, antiproliferative assay and apoptotic induction of (2-phenoxy pyridin-3-yl)naphthalen-1(2*H*)-one derivatives

Table S1 Quantitative analysis of percent of apoptotic effect on human K562 cell line induced by compounds **18** and **22**

Comp.	μM	K562		
		AV+/IP-	AV+/IP+	AV-/IP+
18	5	22.70	2.84	0.89
18	10	8.69	89.50	1.12
22	5	20.90	1.85	0.44
22	10	21.80	77.70	0.29
Dox	1	29.40	29.80	19.20
QC	50	34.30	6.25	1.57
Control		4.63	2.00	1.60

Data are expressed as a percentage of the total cellular population of at least three determinations, **Dox** = doxorubicin, **QC** = quercetin, **Control** = untreated cells, **AV+=** Annexin-V Positive, **IP+=** Propidium iodide Positive, *p <0.05, **p <0.01 vs control

Table S2 Quantitative analysis of percent of apoptotic effect on human A549 cell line induced by compounds **18** and **22**

Comp.	μM	A549		
		AV+/IP-	AV+/IP+	AV-/IP+
18	10	11.10	3.28	3.06
18	25	40.10	21.10	3.12
22	10	13.80	23.30	8.44
22	25	9.36	78.30	9.32
Dox	1	8.33	33.50	29.30
QC	50	26.10	21.70	5.60
Control		5.92	1.56	1.90

Data are expressed as a percentage of the total cellular population of at least three determinations, **Dox** = doxorubicin, **QC** = quercetin, **Control** = untreated cells, **AV+=** Annexin-V Positive, **IP+=** Propidium iodide Positive, *p <0.05, **p <0.01 vs control