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Development of an *in situ* Culture-Free Screening Test for the Rapid Detection of *Staphylococcus aureus* within Healthcare Environments

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Bacterial Culture

Bacterial isolates were obtained from a clinical setting as a result of both MRSA (MRSA numbers 1-11,13,14,16,17 and 19) and MSSA (MSSA numbers 58,59.61,62, 63,64, 68, 69,71,72) infection, and were part of a cohort of bacteria taken from UK hospitals. E.coli samples were a combination of clinical isolates and wild type strains (*E.coli* 1-10), and coagulase negative Staphylococci include strains of *S.epidermidis, S. warneri, S.hominus* and *M. luteus,* and were obtained from clinical isolates from Sutton hospital. All bacteria were cultured initially on Brain Heart infusion agar, after which they were subcultured twice onto nutrient agar overnight at 37 °C, under aerobic conditions. Each bacterial isolate possesses individual characteristics, and thus displays a variance in the amount of coagulase produced, and therefore there is a degree of variance in results, lending to a greater amount of error in the results depicted.

Preparation of the LGX solution

A 100 μM and 50 μM solution of compound **3** was prepared by dissolving it in 2.5 % methanol followed by dilution in 1 x PBS. Solutions of Tris Base (0.05 M) and NaCl (0.1 M) in deionised H_2O were added to the solution until an optimum pH of 8.5 was achieved. The appropriate amount of human prothrombin in 1 x PBS was then added to produce final prothrombin concentrations of 83.6 nM and 41.8 nM, respectively. The resulting solution was termed "LGX". The concentrations of LGX, subsequently discussed, refer to the concentration of the active constituent compound **3**.

Testing procedure the efficacy of LGX as a selective and sensitive means of detecting *S. aureus*

In order to detect the presence of staphylocoagulase and thus the efficacy of LGX, varying cell concentrations (10^6, 10^5, 10^3, 10^2 CFU/mL (50 μM LGX) and 10^4, 10^3, 10^2, 10^0 CFU/mL (100 μM LGX) were added to a microtitre plate (Nunclon 96 well plates) in a 1:1 ratio with either 50 μM or 100 μM of prepared LGX solution. This provided a final LGX concentration of 25 μM or 50 μM, respectively. The relative fluorescence was then recorded every fifteen minutes over a six hour time period ($\lambda_{ex.}$ = 488 nm and $\lambda_{em.}$ = 525 nm). Positive controls used in each experiment were a control strain of MRSA (NCTC 12493), and the negative control was a clinical isolate of *E. coli*. A 1:1 ratio of both the 100 μM and 50 μM of LGX solution with 1 x PBS was used, and termed "LGX alone". Fluorescence intensity was determined at 15 minute intervals over a 6 hour time period and n=3 samples were assayed in each case. We assayed 15 Strains of MRSA at varying cell concentration (10^6, 10^5, 10^3, 10^2 CFU/mL (50 μM LGX) and 10^4, 10^3, 10^2, 10^0 CFU/mL (100 μM) LGX)) with equal volume of both 50 μM and 100 μM LGX, respectively, to give a final LGX concentration of 25 μM or 50 μM, respectively, in addition to a strain of *E-coli*, which served as a negative control as described above.

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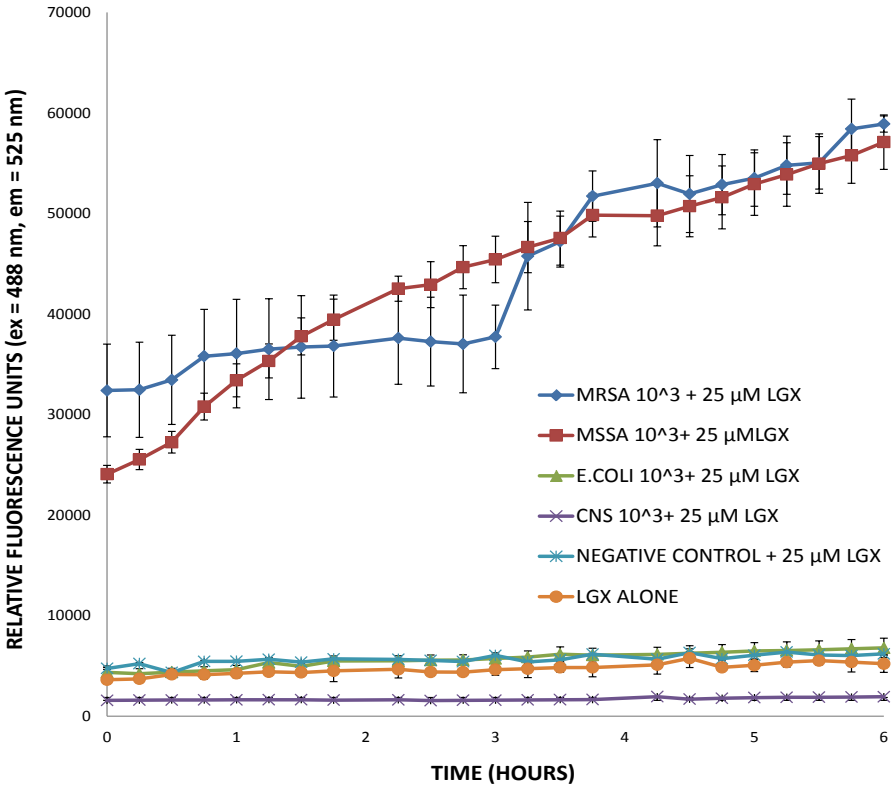

Figure 1 – The efficacy of 25µM LGX in detecting MRSA concentrations as low as 10^2 CFU/mL. Average of ten to fifteen bacterial strains (n=3). Error bars represent standard deviation.

As can be observed in figure 1, the results of all concentrations of MRSA (average of all 15 samples per data set illustrated) are plotted against a negative control and LGX alone, there is a significantly greater increase in fluorescence intensity in MRSA samples across the 6 hour time period. Taking a lower threshold limit of 20,000 relative fluorescence units (RFU) as a positive result, it can be seen that at a 25µM concentration of LGX, and at all 10^3 CFU/mL MRSA/MSSA, there is a clear positive result yet, however as expected, this is lower than the effect observed with the 50µM LGX. As with the 50 µM data an instantaneous positive reaction can also be observed. This data shows that the compound harbours the ability to rapidly detect SA at low concentrations.

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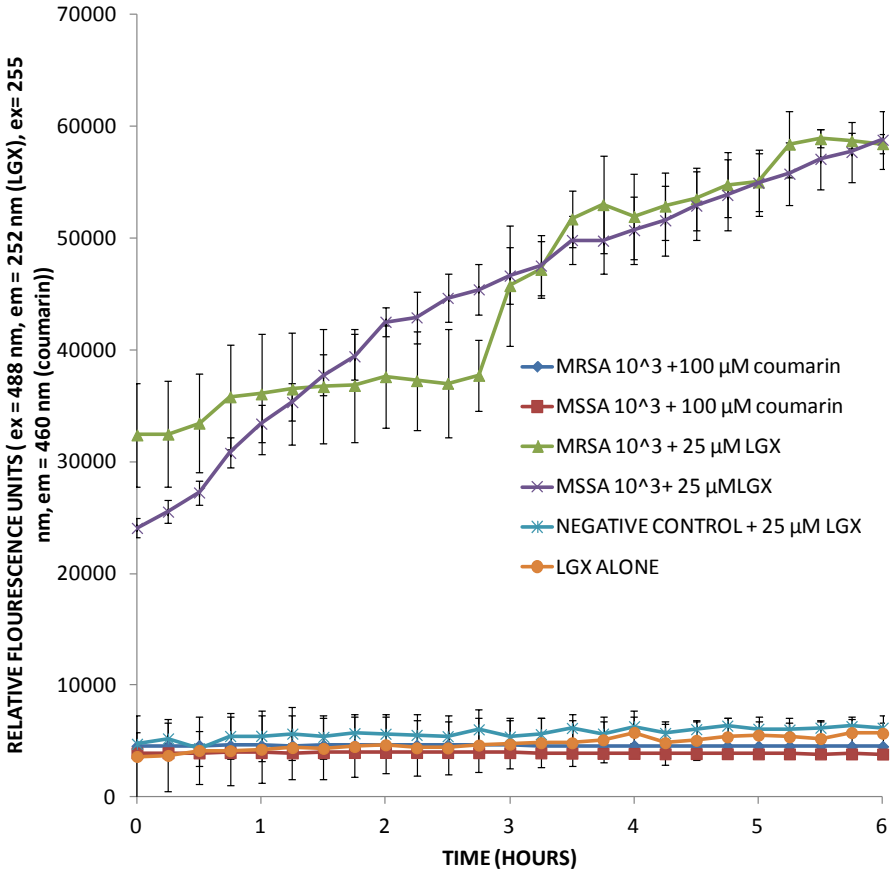

Figure 2 - The efficacy of 25 µM LGX at demonstrating both selectivity and sensitivity in detecting coagulase positive MRSA and MSSA, compared to the efficacy 100 µM coumarin, in bacterial concentrations of 10^3 CFU/mL. Average of ten to fifteen bacterial strains (n=3). Error bars represent standard deviation.

The data demonstrated in Figure 2 illustrates that, similarly to 50 µM LGX and 500 µM coumarin, there is significantly more fluorescence produced by LGX, when compared to the coumarin system. These results show that at low concentrations, the LGX system demonstrates considerable efficacy in terms of speed of detection, as well sensitivity, and is a vast improvement on the existing coumarin system.

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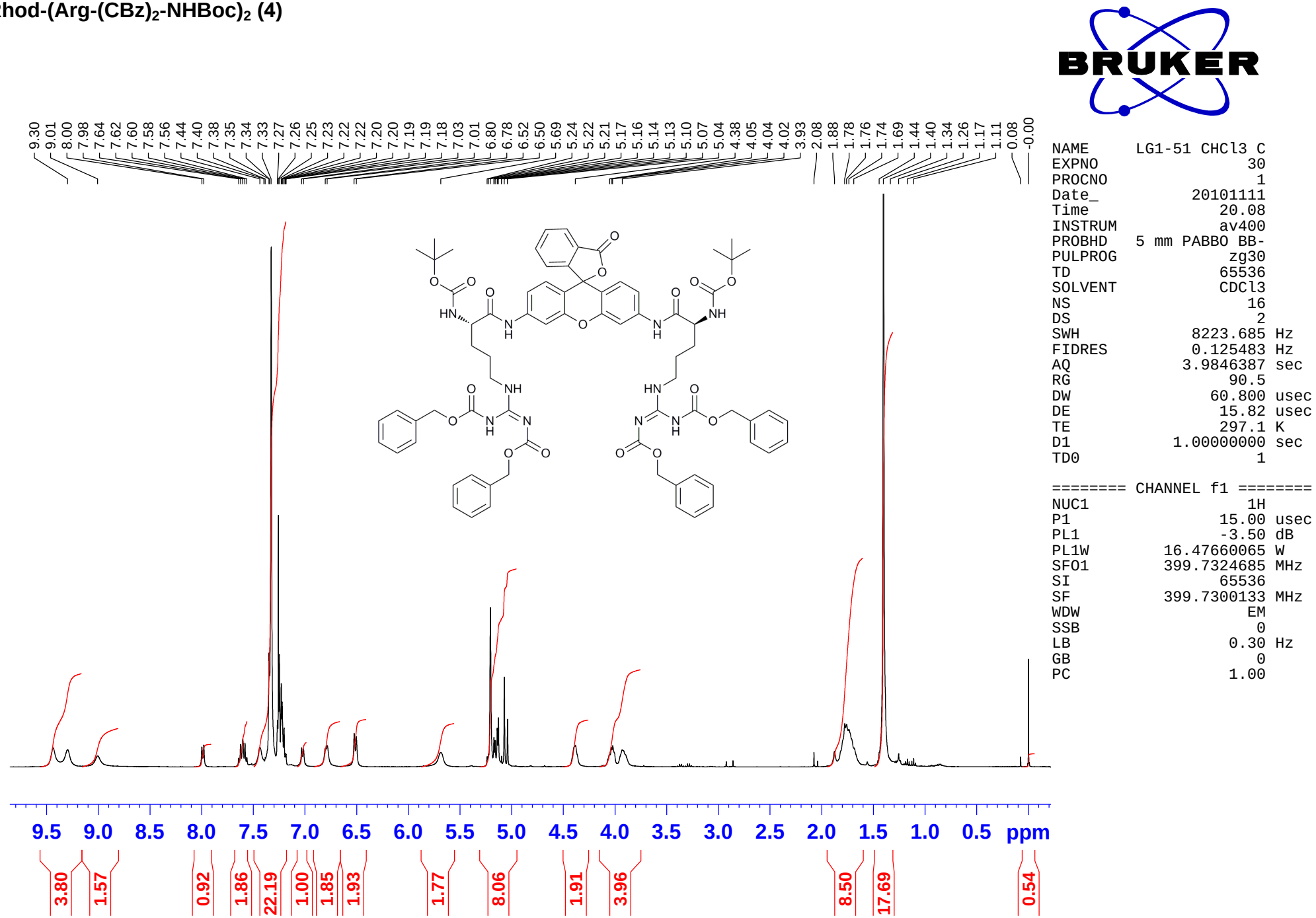
Rhod-(Arg-$(CBz)_2$-NHBoc)$_2$ (4)



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Time	20.08
INSTRUM	av400
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	15.82 usec
TE	297.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	15.00 usec
PL1	-3.50 dB
PL1W	16.47660065 W
SFO1	399.7324685 MHz
SI	65536
SF	399.7300133 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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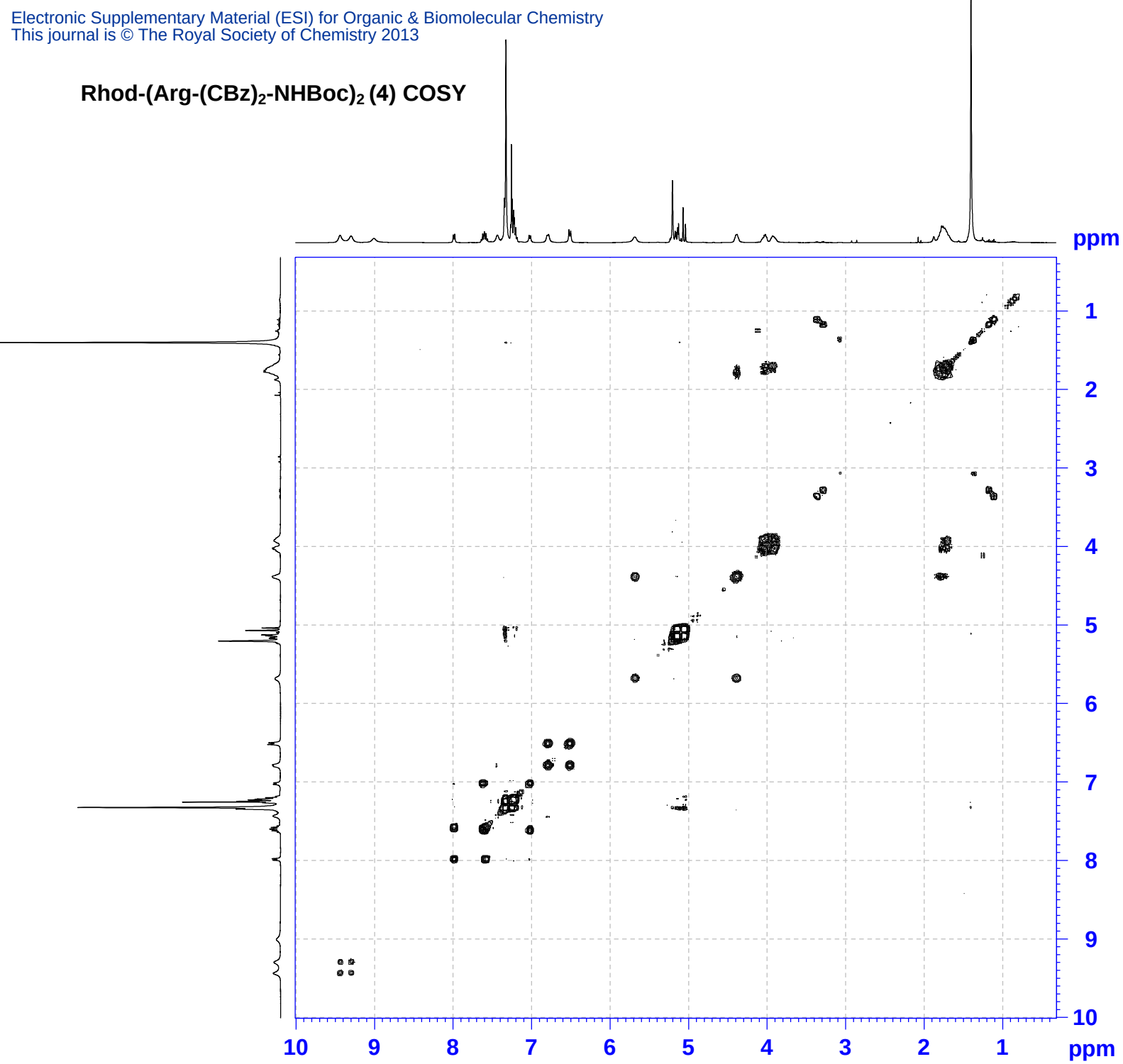
Rhod-(Arg-$(CBz)_2$-NHBoc)$_2$ (4) COSY

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PROCNO                1
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PULPROG      cosygpmfqf
TD                 2048
SOLVENT            CDCl3
NS                    2
DS                    8
SWH            3875.969 Hz
FIDRES         1.892563 Hz
AQ             0.2642420 sec
RG                 2050
DW              129.000 usec
DE                6.50 usec
TE                297.2 K
D0           0.00000300 sec
D1           1.92750096 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00025800 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1               -3.50 dB
PL1W        16.47660065 W
SFO1       399.7320771 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPNAM3          SINE.100
GPZ1              16.00 %
GPZ2              12.00 %
GPZ3              40.00 %
P16             1000.00 usec
ND0                   1
TD                  128
SFO1           399.7321 MHz
FIDRES        30.281008 Hz
SW                9.696 ppm
FnMODE               QF
SI                 1024
SF         399.7300133 MHz
WDW                SINE
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.40
SI                 1024
MC2                  QF
SF         399.7300133 MHz
WDW                SINE
SSB                   0
LB                 0.00 Hz
GB                    0
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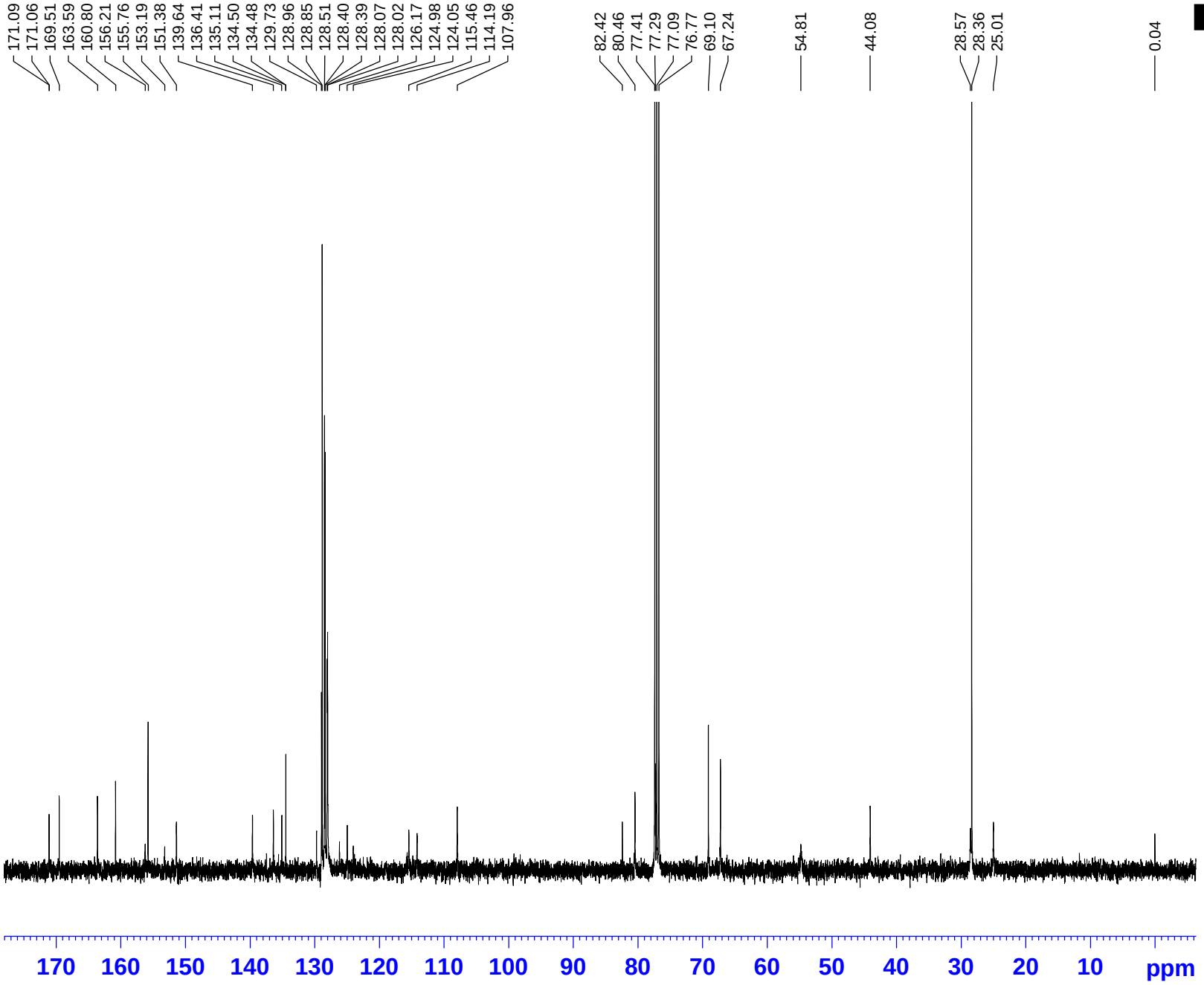
Rhod-(Arg-$(CBz)_2$-NHBoc)$_2$ (4)



BRUKER

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INSTRUM	av400
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	9.66 usec
TE	297.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-3.70 dB
PL1W	74.19429779 W
SFO1	100.5222397 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.50 dB
PL12	11.04 dB
PL13	14.00 dB
PL2W	16.47660065 W
PL12W	0.57925212 W
PL13W	0.29300001 W
SFO2	399.7315989 MHz
SI	65536
SF	100.5121880 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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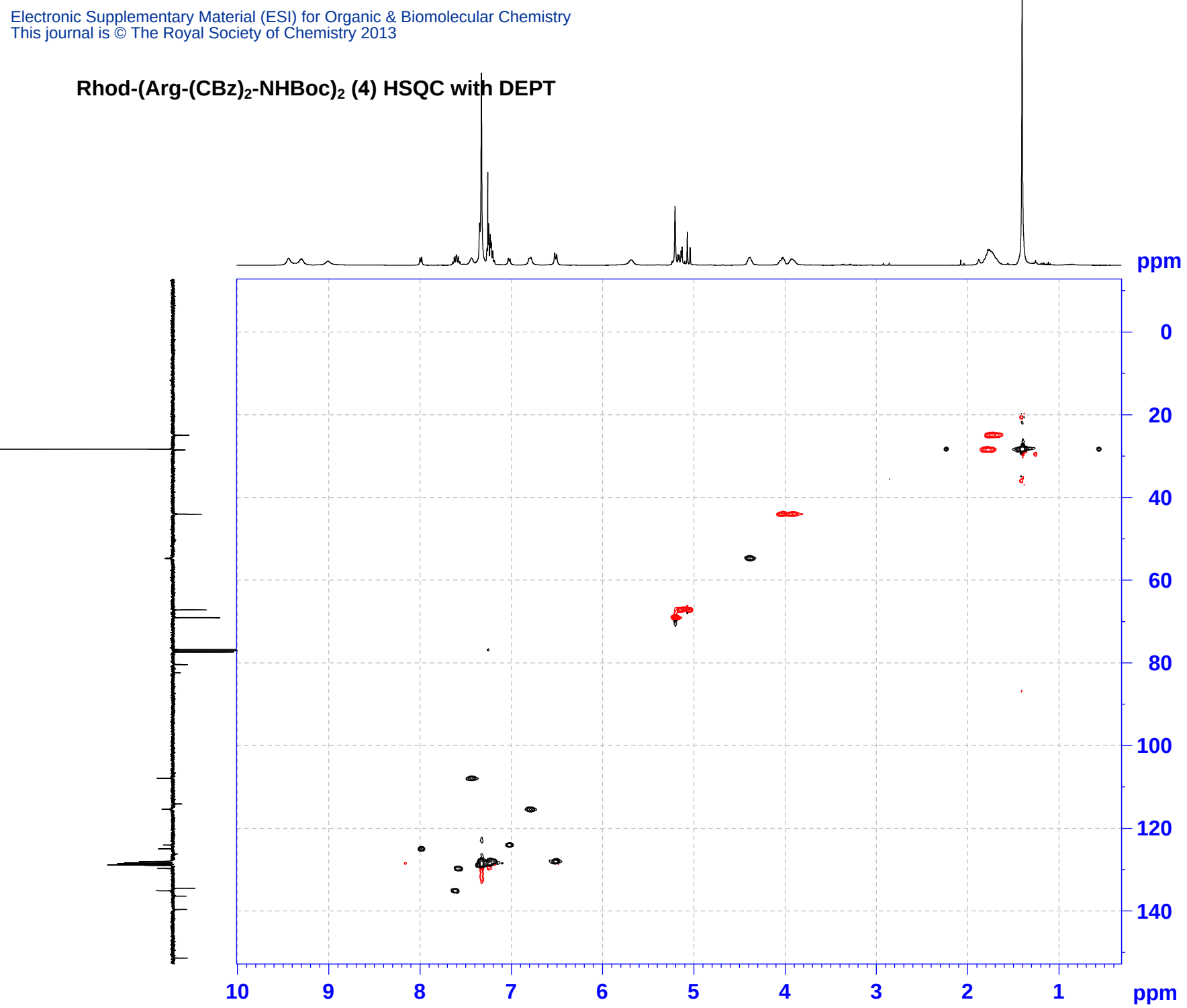
Rhod-(Arg-$(CBz)_2$-NHBoc)$_2$ (4) HSQC with DEPT

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EXPNO               31
PROCNO               1
Date_         20101111
Time             20.10
INSTRUM           av400
PROBHD    5 mm PABBO BB-
PULPROG   hsqcedetgpsp.3
TD                1024
SOLVENT           CDCl3
NS                   2
DS                  16
SWH           3875.969 Hz
FIDRES          3.785126 Hz
AQ            0.1321460 sec
RG                2050
DW              129.000 usec
DE                6.50 usec
TE               297.2 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.44777596 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D21           0.00360000 sec
IN0           0.00003005 sec
L31                  1

======== CHANNEL f1 ========
NUC1                1H
P1                15.00 usec
P2                30.00 usec
P28                1.00 usec
PL1               -3.50 dB
PL1W         16.47660065 W
SFO1         399.7320771 MHz

======== CHANNEL f2 ========
CPDPRG2   bi_p5m4sp_4sp.2
NUC2                13C
P3                 9.60 usec
P14              500.00 usec
P31             1900.00 usec
P63             1500.00 usec
PL0              120.00 dB
PL2               -3.70 dB
PL12              13.56 dB
PL0W          0.00000000 W
PL2W         74.19429779 W
PL12W         1.39434588 W
SFO2         100.5192243 MHz
SP3                4.81 dB
SP14               6.29 dB
SP18              11.02 dB
SP31              12.31 dB
SPNAM3    Crp60,0.5,20.1
SPNAM14   Crp32,1.5,20.2
SPNAM18    Crp60_xfilt.2
SPNAM31   Crp32,1.5,20.2
SPOAL3             0.500
SPOAL14            0.500
SPOAL18            0.500
SPOAL31            0.500
SPOFFS3            0.00 Hz
SPOFFS14           0.00 Hz
SPOFFS18           0.00 Hz
SPOFFS31           0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPZ1               80.00 %
GPZ2               20.10 %
P16              1000.00 usec
ND0                   2
TD                  256
SFO1           100.5192 MHz
FIDRES         65.046150 Hz
SW               165.658 ppm
FnMODE     Echo-Antiecho
SI                 1024
SF           399.7300133 MHz
WDW                QSINE
SSB                   2
LB                 0.00 Hz
GB                    0
PC                 1.40
SI                 1024
MC2         echo-antiecho
SF           100.5121880 MHz
WDW                QSINE
SSB                   2
LB                 0.00 Hz
GB                    0
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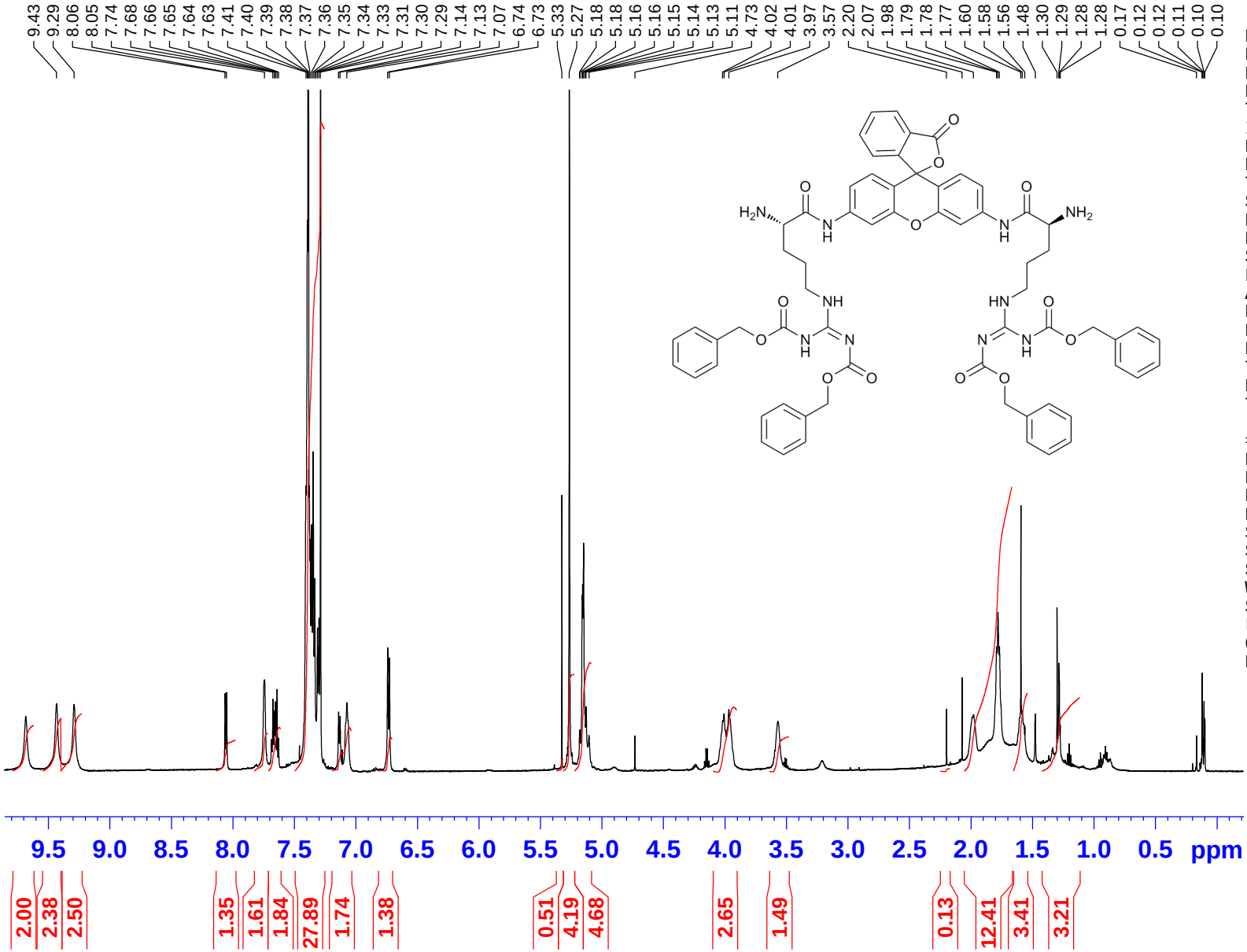
Rhodamine-(Arg-CBz)$_2$-NH$_2$)$_2$ (6)



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INSTRUM	av600
PROBHD	5 mm PATXI 1H/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12345.679 Hz
FIDRES	0.188380 Hz
AQ	2.6542580 sec
RG	228
DW	40.500 usec
DE	11.34 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	7.00 usec
PL1	0.25 dB
PL1W	16.59961510 W
SFO1	600.1337060 MHz
SI	65536
SF	600.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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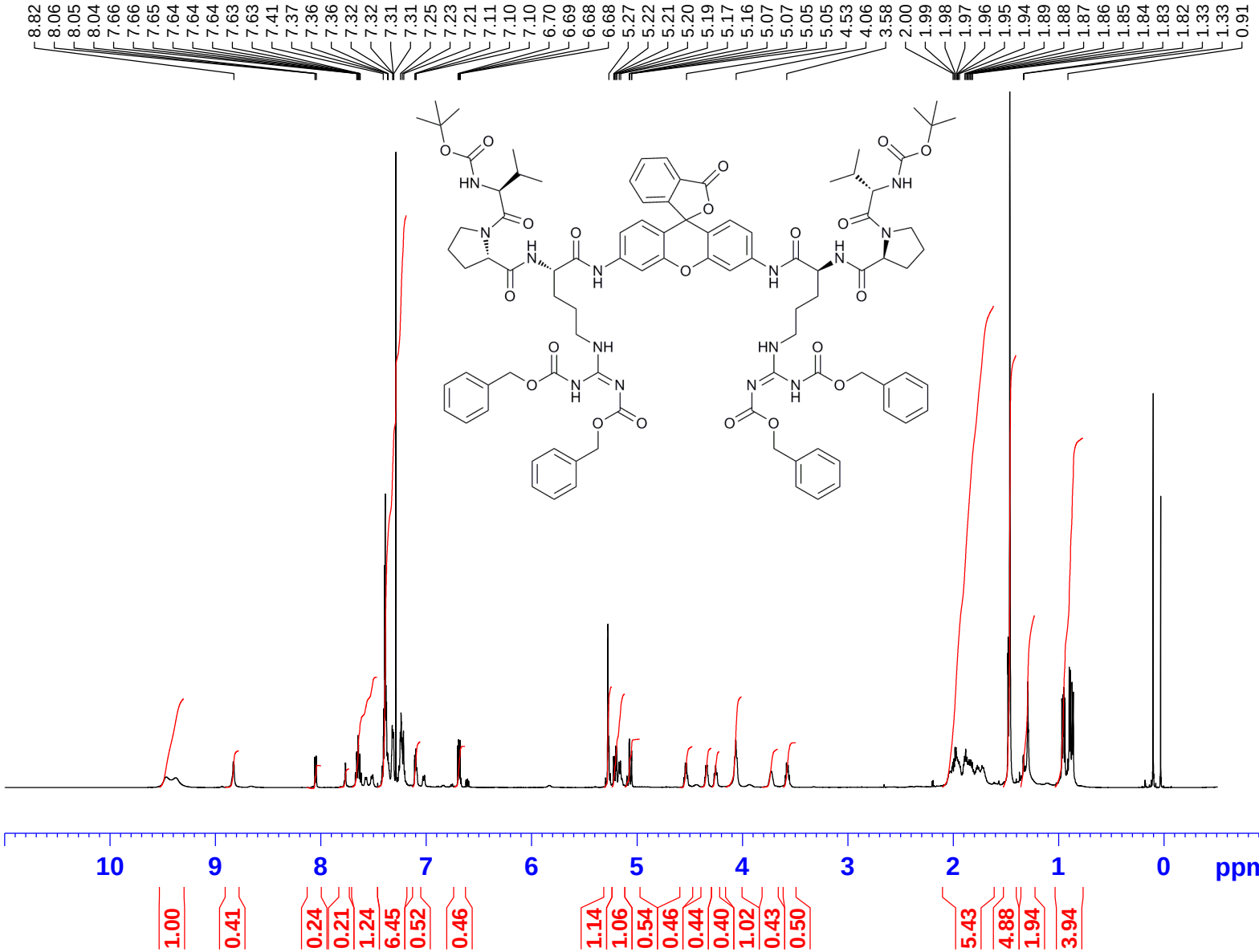
Rhodamine-(Arg-(Cbz)$_2$-Pro-Val-NHBoc)$_2$ (5)



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EXPNO	10
PROCNO	1
Date_	20101124
Time	14.54
INSTRUM	av600
PROBHD	5 mm PATXI 1H/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8417.509 Hz
FIDRES	0.128441 Hz
AQ	3.8928883 sec
RG	57
DW	59.400 usec
DE	6.50 usec
TE	308.0 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	7.00 usec
PL1	0.25 dB
PL1W	16.59961510 W
SFO1	600.1339008 MHz
SI	32768
SF	600.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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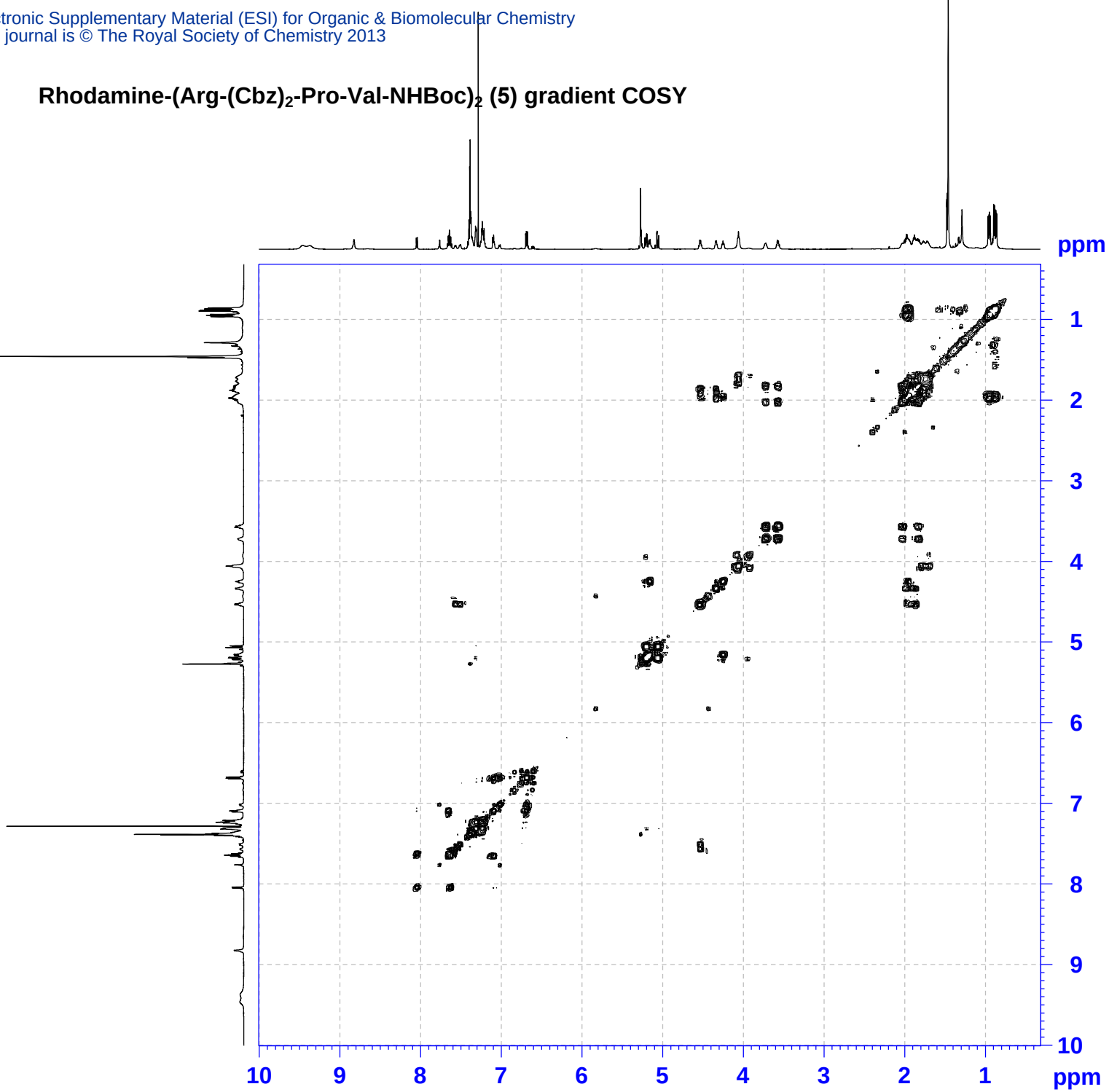
Rhodamine-(Arg-(Cbz)$_2$-Pro-Val-NHBoc)$_2$ (5) gradient COSY



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EXPNO	13
PROCNO	1
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INSTRUM	av600
PROBHD	5 mm PATXI 1H/
PULPROG	cosygpmfqf
TD	2048
SOLVENT	CDCl3
NS	2
DS	8
SWH	6009.615 Hz
FIDRES	2.934382 Hz
AQ	0.1704436 sec
RG	2050
DW	83.200 usec
DE	6.50 usec
TE	308.0 K
D0	0.00000300 sec
D1	2.00000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00016640 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	7.00 usec
PL1	0.25 dB
PL1W	16.59961510 W
SFO1	600.1330006 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPNAM3	SINE.100
GPZ1	16.00 %
GPZ2	12.00 %
GPZ3	40.00 %
P16	1000.00 usec
ND0	1
TD	128
SFO1	600.133 MHz
FIDRES	46.950092 Hz
SW	10.014 ppm
FnMODE	QF
SI	1024
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	QF
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

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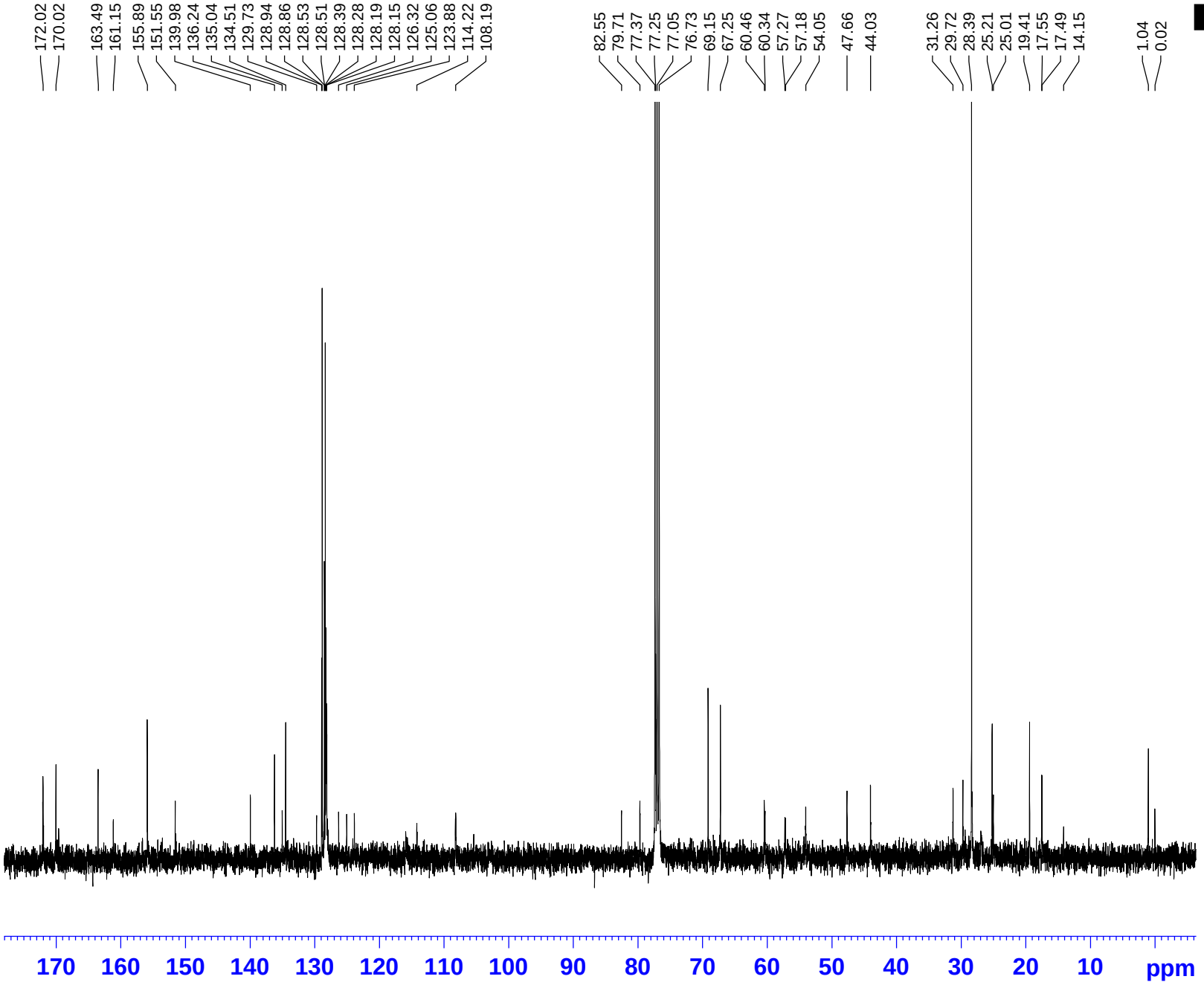
Rhodamine-(Arg-(Cbz)$_2$-Pro-Val-NHBoc)$_2$ (5)



BRUKER

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Time	9.42
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PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	9.66 usec
TE	296.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-3.70 dB
PL1W	74.19429779 W
SFO1	100.5222397 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.50 dB
PL12	11.04 dB
PL13	14.00 dB
PL2W	16.47660065 W
PL12W	0.57925212 W
PL13W	0.29300001 W
SFO2	399.7315989 MHz
SI	65536
SF	100.5121880 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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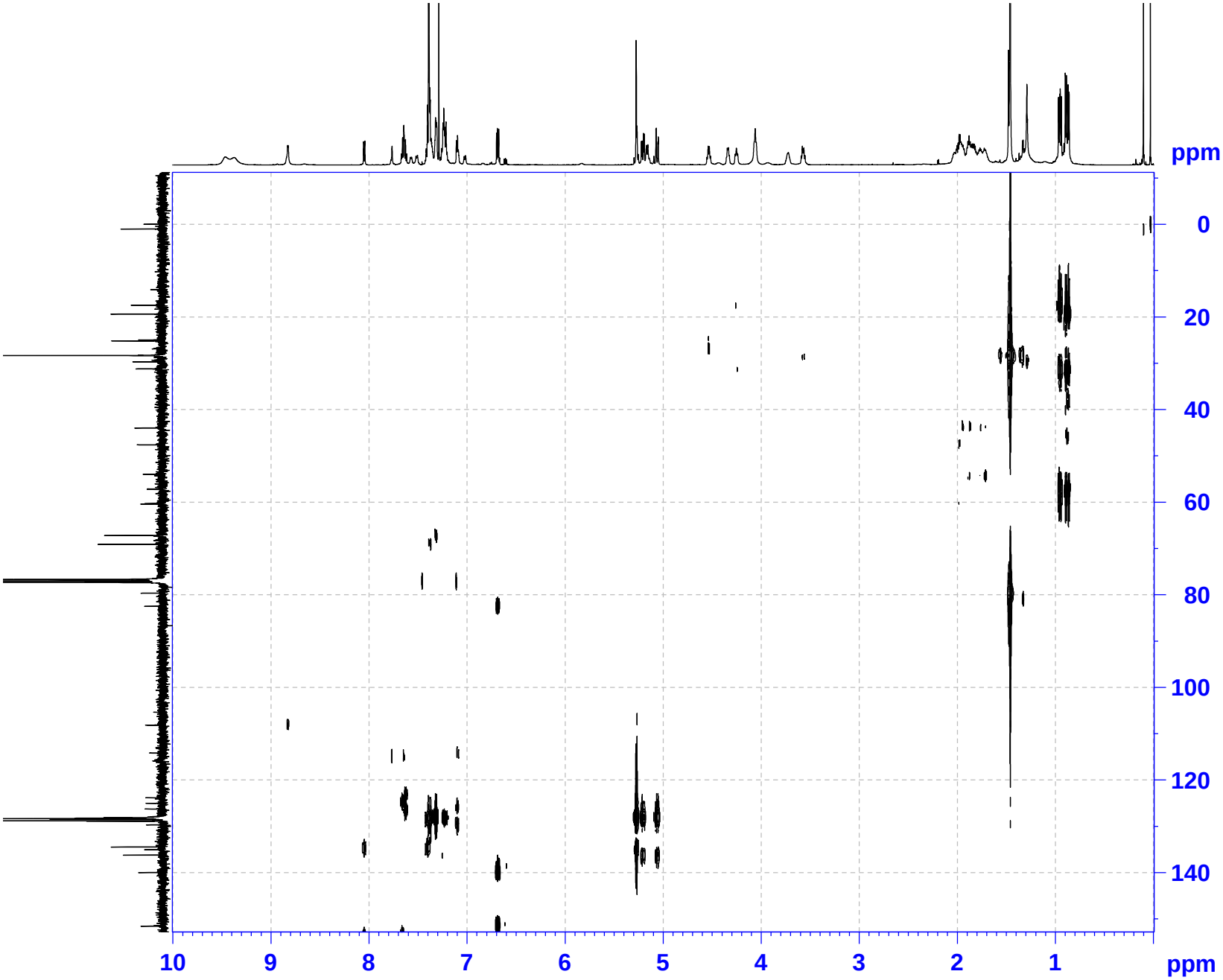
Rhodamine-(Arg-(Cbz)$_2$-Pro-Val-NHBoc)$_2$ (5) HMBC



BRUKER

NAME	LG1-57
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PROCNO	1
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Time	15.14
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PROBHD	5 mm PATXI 1H/
PULPROG	hmbcetgpl3nd
TD	4096
SOLVENT	CDCl3
NS	4
DS	16
SWH	6009.615 Hz
FIDRES	1.467191 Hz
AQ	0.3408372 sec
RG	2050
DW	83.200 usec
DE	6.50 usec
TE	307.8 K
CNST6	120.0000000
CNST7	165.0000000
CNST13	10.0000000
CNST30	0.5981154
D0	0.00000300 sec
D1	1.50000000 sec
D6	0.05000000 sec
D16	0.00020000 sec
IN0	0.00001490 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	7.00 usec
P2	14.00 usec
PL1	0.25 dB
PL1W	16.59961510 W
SFO1	600.1330006 MHz
======== CHANNEL f2 ========	
NUC2	13C
P3	12.00 usec
P24	2000.00 usec
PL2	-3.30 dB
PL2W	191.18331909 W
SFO2	150.9178750 MHz
SP7	3.28 dB
SPNAM7	Crp60comp.4
SPOAL7	0.500
SPOFFS7	0.00 Hz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM3	SINE.100
GPNAM4	SINE.100
GPNAM5	SINE.100
GPNAM6	SINE.100
GPZ1	80.00 %
GPZ3	14.00 %
GPZ4	-8.00 %
GPZ5	-4.00 %
GPZ6	-2.00 %
P16	1000.00 usec
ND0	2
TD	128
SFO1	150.9179 MHz
FIDRES	261.860260 Hz
SW	222.095 ppm
FnMODE	Echo-Antiecho
SI	2048
SF	600.1300000 MHz
WDW	SINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	echo-antiecho
SF	150.9028090 MHz
WDW	SINE
SSB	2
LB	0.00 Hz
GB	0

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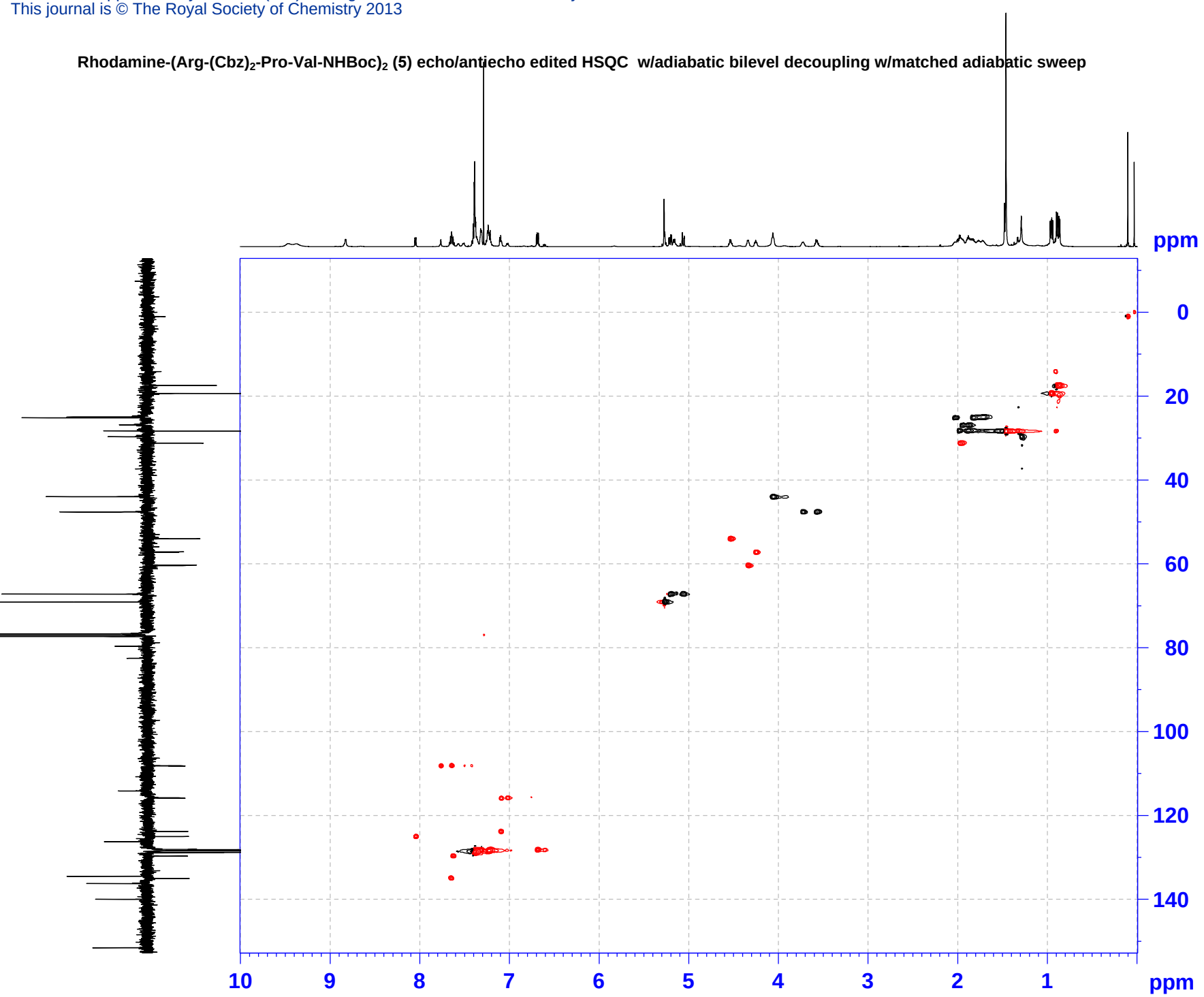
Rhodamine-(Arg-(Cbz)$_2$-Pro-Val-NHBoc)$_2$ (5) echo/antiecho edited HSQC w/adiabatic bilevel decoupling w/matched adiabatic sweep



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PROBHD	5 mm PATXI 1H/
PULPROG	hsqcedetgpsp.3
TD	1024
SOLVENT	CDCl3
NS	2
DS	16
SWH	6009.615 Hz
FIDRES	5.868765 Hz
AQ	0.0852468 sec
RG	2050
DW	83.200 usec
DE	6.50 usec
TE	308.3 K
CNST2	145.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D4	0.00172414 sec
D11	0.03000000 sec
D16	0.00020000 sec
D21	0.00360000 sec
IN0	0.00002000 sec
L31	1
======== CHANNEL f1 ========	
NUC1	1H
P1	7.00 usec
P2	14.00 usec
P28	0.00 usec
PL1	0.25 dB
PL1W	16.59961510 W
SFO1	600.1330006 MHz
======== CHANNEL f2 ========	
CPDPRG2	bi_p5m4sp_4sp.2
NUC2	13C
P3	12.00 usec
P14	500.00 usec
P31	1730.00 usec
P63	1500.00 usec
PL0	120.00 dB
PL2	-3.30 dB
PL12	12.02 dB
PL0W	0.00000000 W
PL2W	191.18331909 W
PL12W	5.61629534 W
SFO2	150.9133719 MHz
SP3	3.28 dB
SP14	4.76 dB
SP18	8.67 dB
SP31	10.78 dB
SPNAM3	Crp60,0.5,20.1
SPNAM14	Crp32,1.5,20.2
SPNAM18	Crp60_xfilt.2
SPNAM31	Crp32,1.5,20.2
SPOAL3	0.500
SPOAL14	0.500
SPOAL18	0.500
SPOAL31	0.500
SPOFFS3	0.00 Hz
SPOFFS14	0.00 Hz
SPOFFS18	0.00 Hz
SPOFFS31	0.00 Hz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	80.00 %
GPZ2	20.10 %
P16	1000.00 usec
ND0	2
TD	256
SFO1	150.9134 MHz
FIDRES	97.656288 Hz
SW	165.658 ppm
FnMODE	Echo-Antiecho
SI	2048
SF	600.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	echo-antiecho
SF	150.9028090 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

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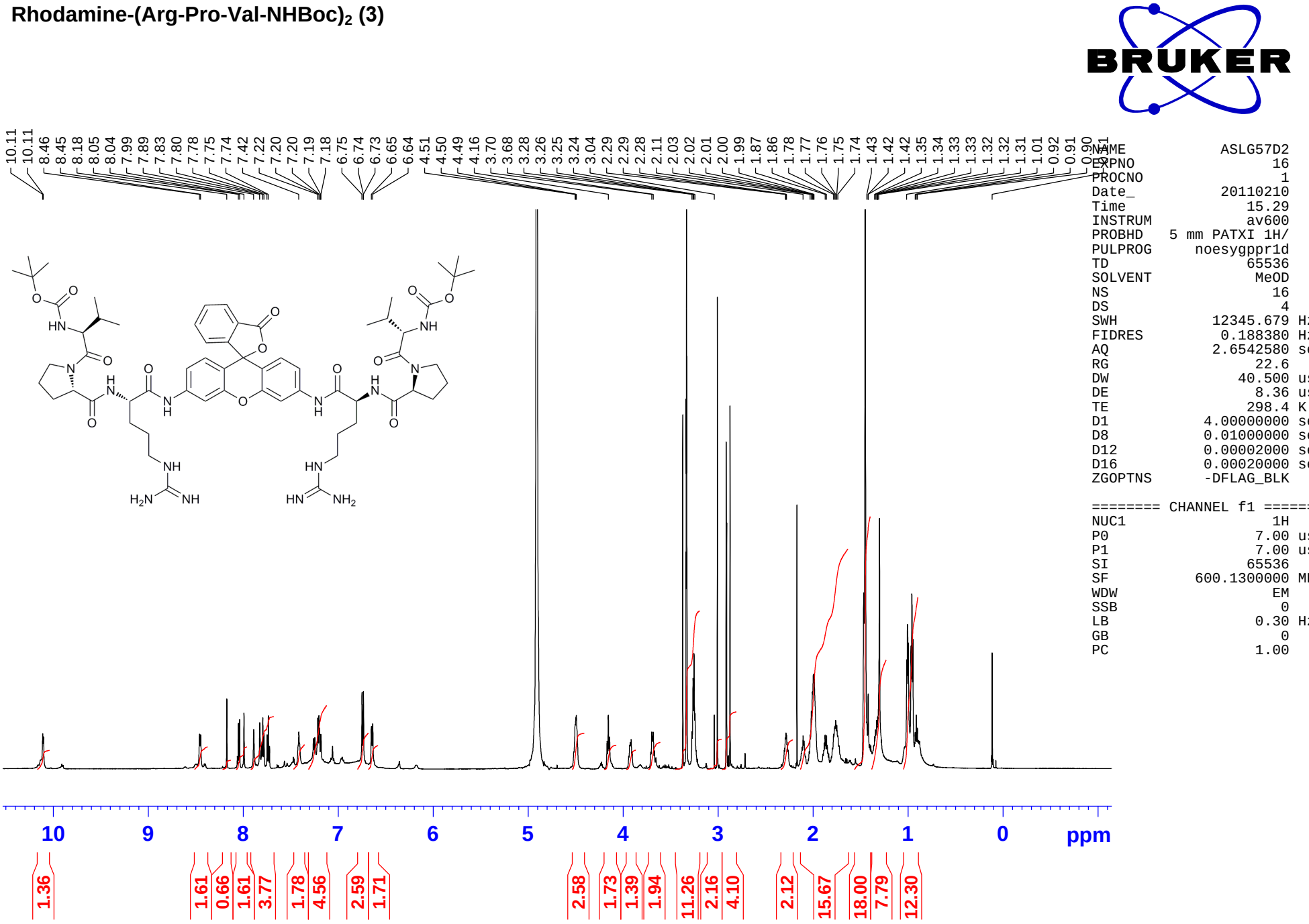
Rhodamine-(Arg-Pro-Val-NHBoc)$_2$ (3)



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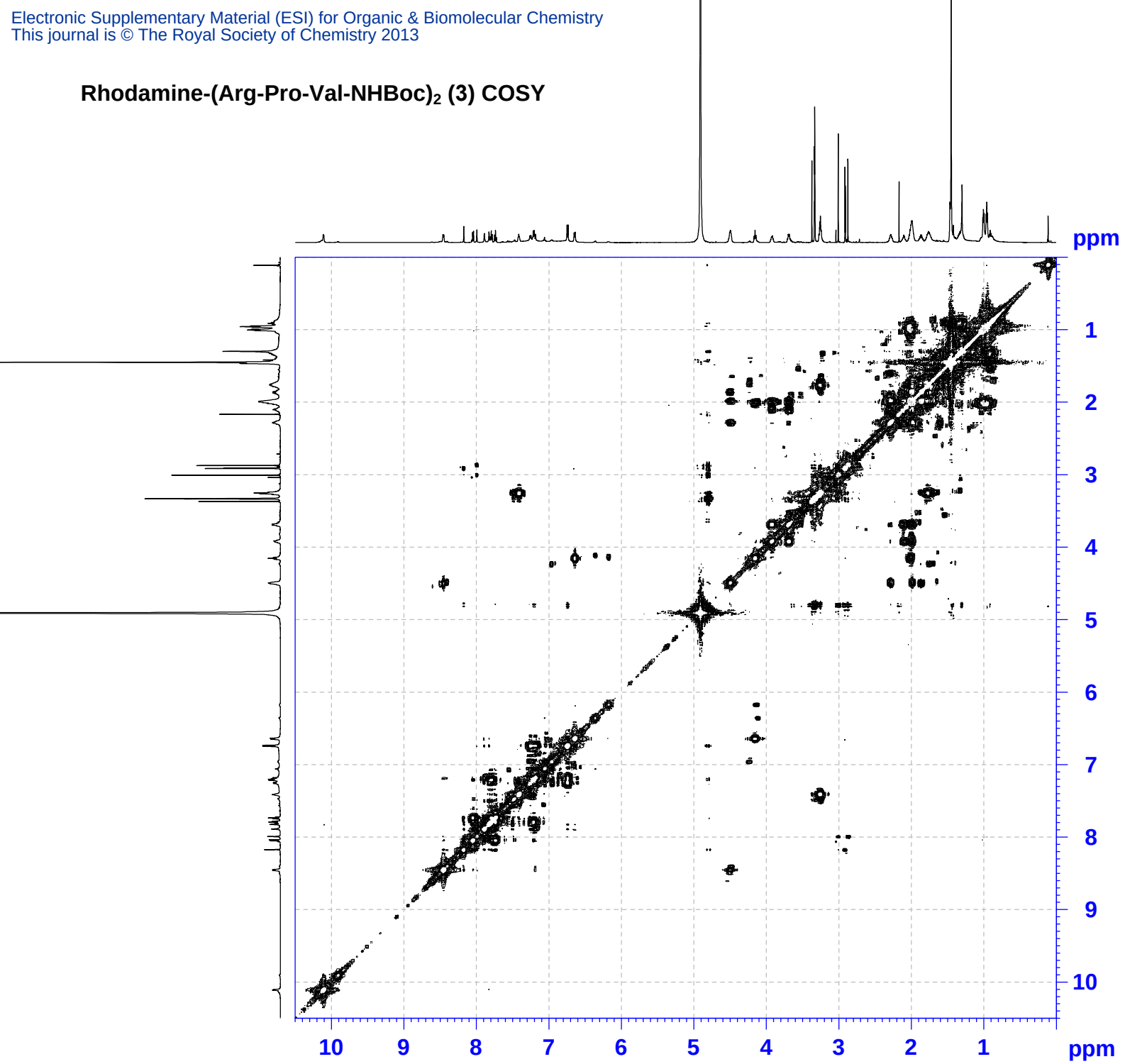
Rhodamine-(Arg-Pro-Val-NHBoc)$_2$ (3) COSY



BRUKER

NAME	ASLG57D2	
EXPNO	24	
PROCNO	1	
Date_	20110211	
Time	10.16	
INSTRUM	av600	
PROBHD	5 mm PATXI 1H/	
PULPROG	cosygpprqf	
TD	4096	
SOLVENT	MeOD	
NS	16	
DS	8	
SWH	9615.385	Hz
FIDRES	2.347506	Hz
AQ	0.2130420	sec
RG	128	
DW	52.000	usec
DE	6.50	usec
TE	298.4	K
D0	0.00000300	sec
D1	2.00000000	sec
D11	0.03000000	sec
D12	0.00002000	sec
D16	0.00020000	sec
IN0	0.00010395	sec
======== CHANNEL f1 ========		
NUC1	1H	
P0	7.00	usec
P1	7.00	usec
ND0	1	
TD	256	
SFO1	600.1329	MHz
FIDRES	37.576378	Hz
SW	16.029	ppm
FnMODE	QF	
SI	2048	
SF	600.1300000	MHz
WDW	SINE	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	
SI	2048	
MC2	QF	
SF	600.1300000	MHz
WDW	SINE	
SSB	0	
LB	0.00	Hz
GB	0	

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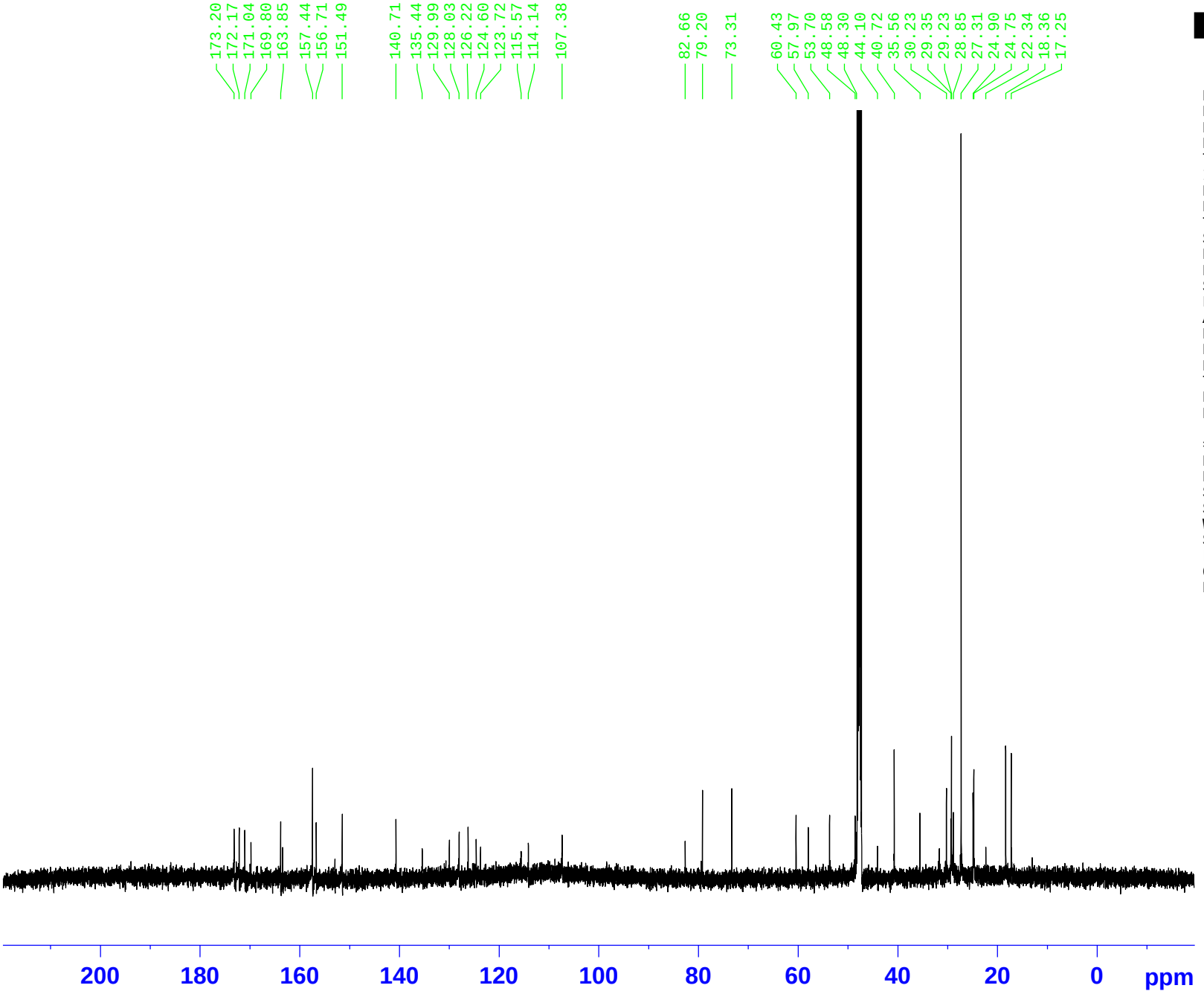
Rhodamine-(Arg-Pro-Val-NHBoc)$_2$ (3)



NAME	ASLG57D2
EXPNO	23
PROCNO	1
Date_	20110210
Time	20.51
INSTRUM	av600
PROBHD	5 mm PATXI 1H/
PULPROG	zgpg30
TD	65536
SOLVENT	MeOD
NS	5120
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	322
DW	13.867 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	12.00 usec
SI	32768
SF	150.9028090 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

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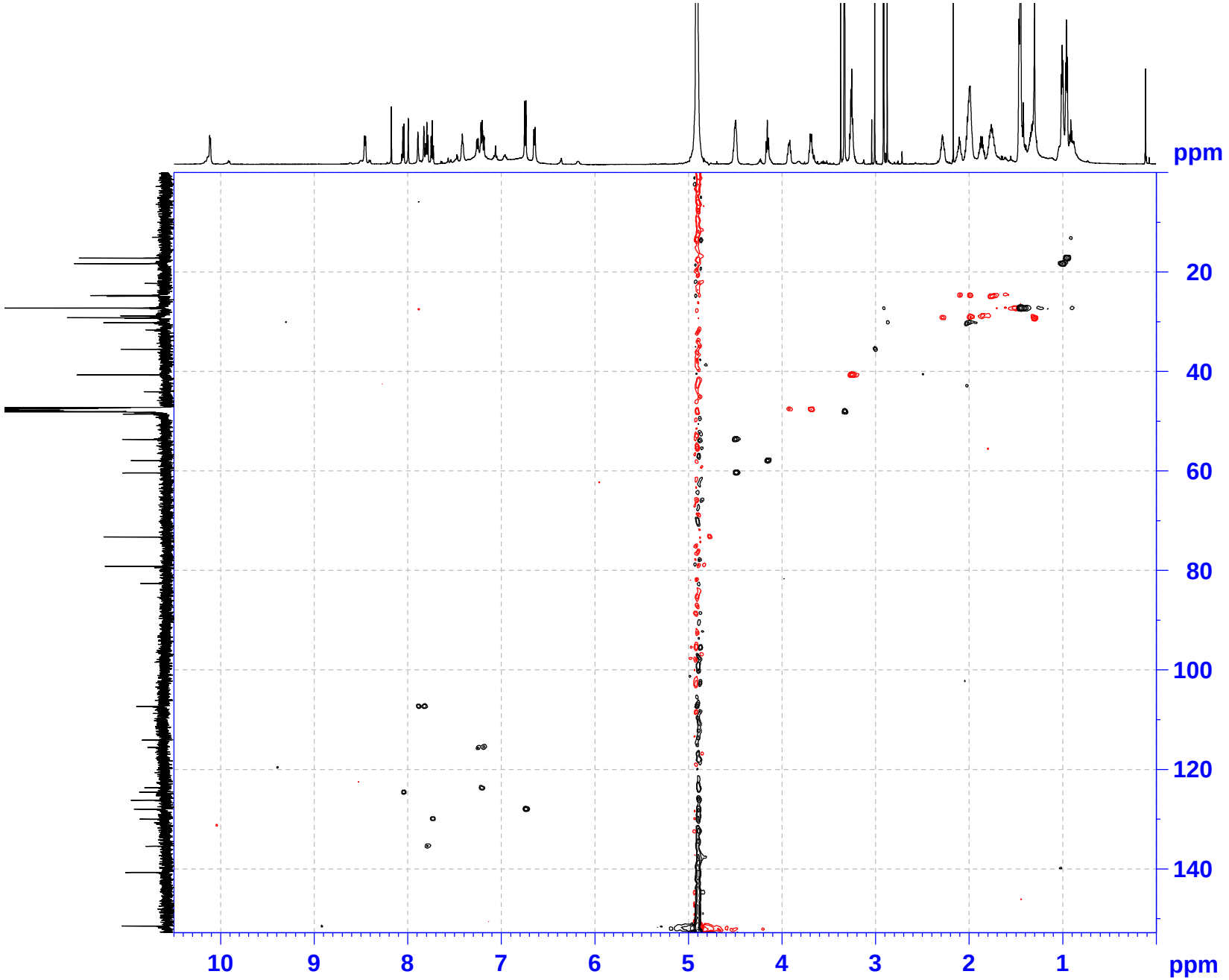
Rhodamine-(Arg-Pro-Val-NHBoc)$_2$ (3) HSQC



NAME	ASLG57D2
EXPNO	13
PROCNO	2
Date_	20110210
Time	13.21
INSTRUM	av600
PROBHD	5 mm PATXI 1H/
PULPROG	hsqcedetgpsisp2.4
TD	1024
SOLVENT	MeOD
NS	4
DS	32
SWH	9615.385 Hz
FIDRES	9.390024 Hz
AQ	0.0532980 sec
RG	1
DW	52.000 usec
DE	6.50 usec
TE	299.4 K
CNST2	145.0000000
CNST17	-0.5000000
D0	0.00000300 sec
D1	1.50000000 sec
D2	0.00344828 sec
D4	0.00172414 sec
D11	0.03000000 sec
D16	0.00020000 sec
D21	0.00360000 sec
D24	0.00089000 sec
IN0	0.00002000 sec
L0	0
TD0	2
======== CHANNEL f1 ========	
NUC1	1H
P1	7.00 usec
P2	14.00 usec
P28	0.00 usec
ND0	2
TD	256
SFO1	150.9134 MHz
FIDRES	97.656288 Hz
SW	165.658 ppm
FnMODE	Echo-Antiecho
SI	2048
SF	600.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	150.9028090 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

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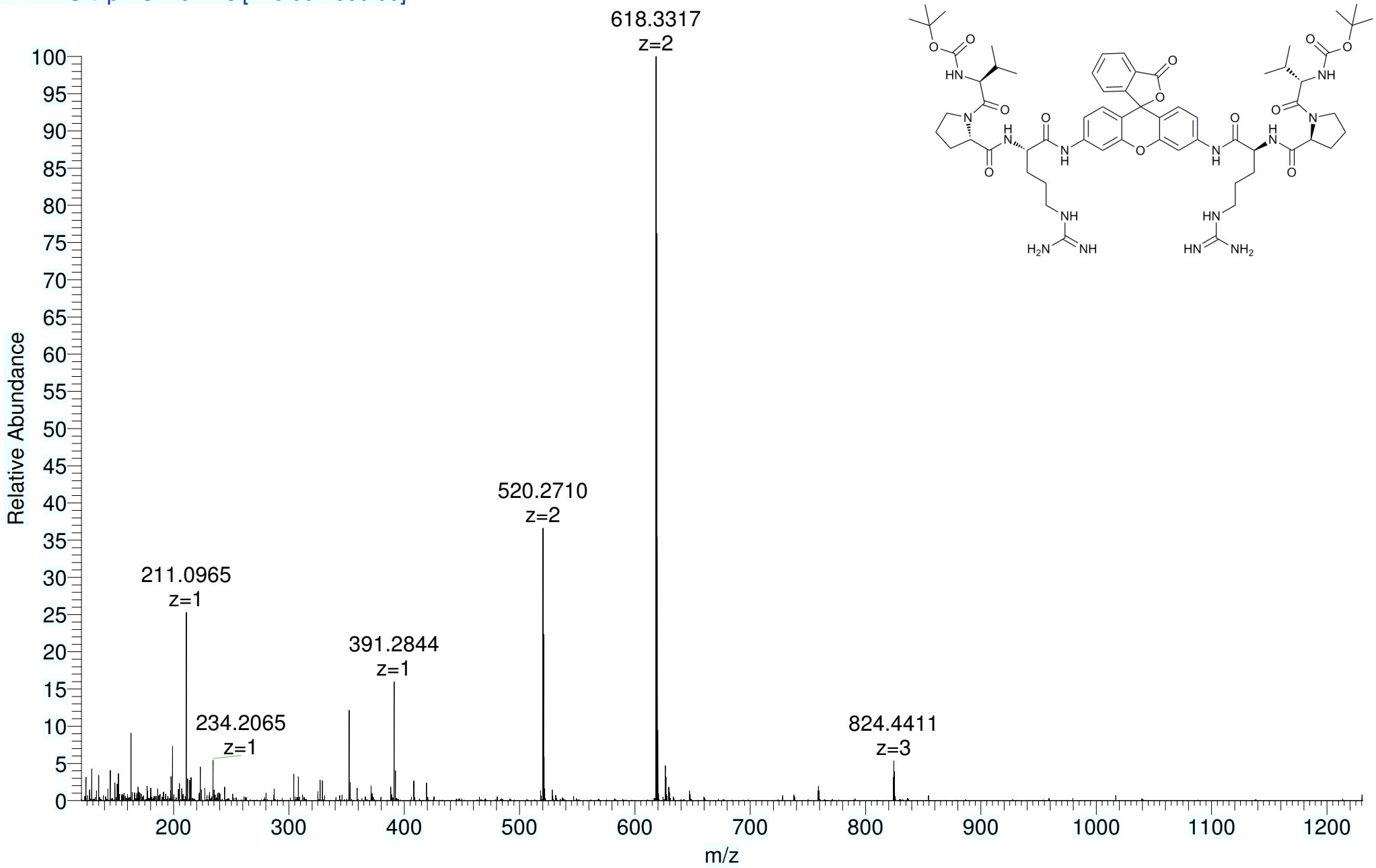
ASLG57D MW=1235?
(MeOH)/MeOH + NH4OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

Alex Sinclair
02/02/2011 12:47:25

KINSIN001-OE-HNESP #18-22 RT: 0.82-0.91 AV: 5 SM: 7G NL: 6.42E6
T: FTMS + p NSI Full ms [120.00-2000.00]



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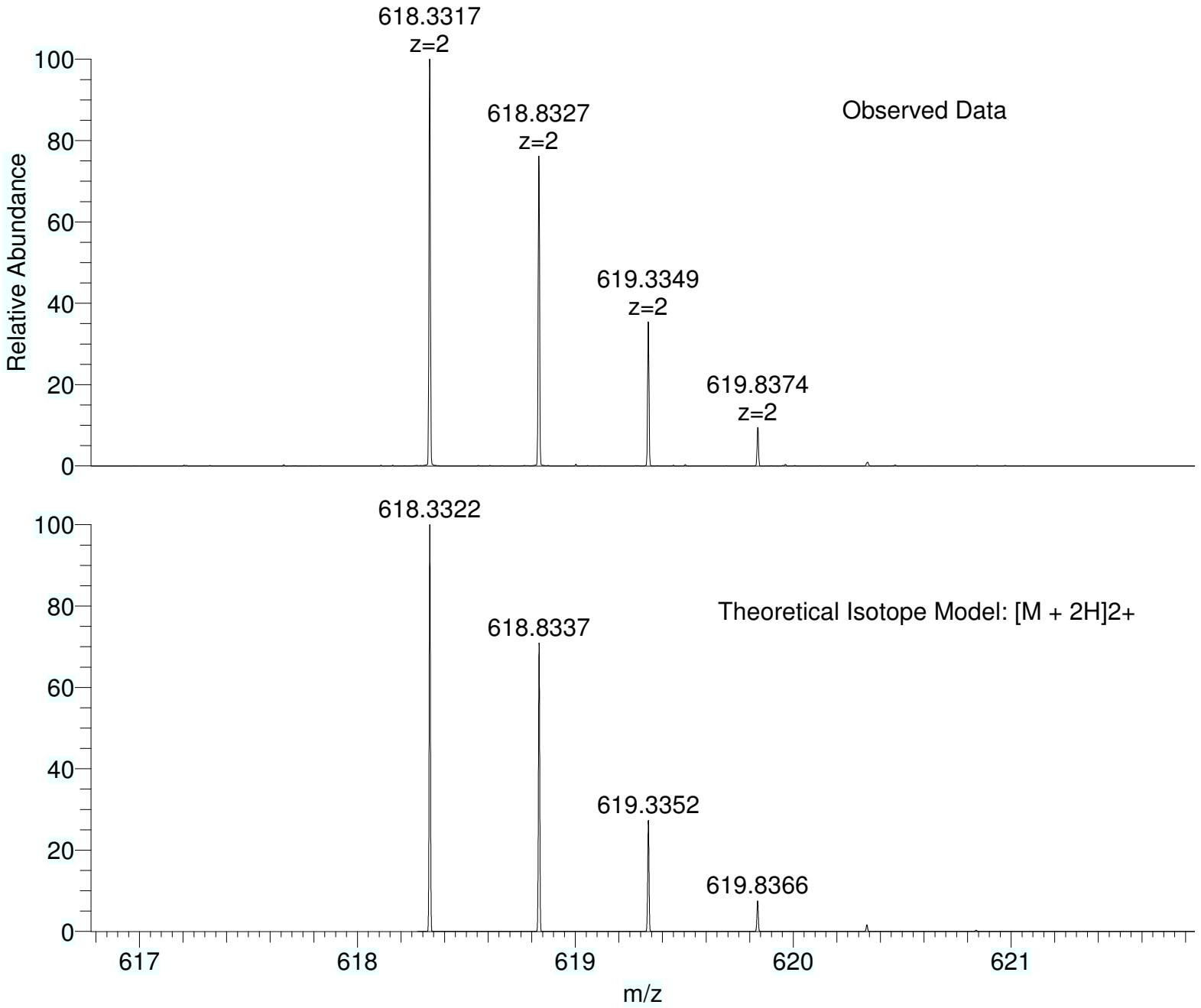
ASLG57D MW=1235?
(MeOH)/MeOH + NH4OAc

EPSRC National Centre Swansea
LTQ Orbitrap XL

Alex Sinclair
02/02/2011 12:47:25



NL:
6.42E6
KINSIN001-OE-HNESP#18-22
RT: 0.82-0.91 AV: 5 T: FTMS
+ p NSI Full ms
[120.00-2000.00]

NL:
1.10E4
$C_{62}H_{86}N_{14}O_{13}$ HH:
$C_{62}H_{88}N_{14}O_{13}$
p (gss, s /p:40) Chrg 2
R: 100000 Res .Pwr . @FWHM