

Supporting Information

Phragmalin-Type limonoids from the roots of *Trichilia sinensis*

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Figure S1. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **1**

Figure S2. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **1**

Figure S3. HSQC spectrum of compound **1** in CDCl_3

Figure S4. ^1H - ^1H COSY spectrum of compound **1** in CDCl_3

Figure S5. HMBC spectrum of compound **1** in CDCl_3

Figure S6. ROESY spectrum of compound **1** in CDCl_3

Figure S7. HREI-MS spectrum of compound **1**

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Figure S13. ROESY spectrum of compound **2** in CDCl_3

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Figure S20. ROESY spectrum of compound **3** in CDCl_3

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Figure S29. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **5**

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Figure S33. HMBC spectrum of compound **5** in CDCl_3

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Figure S36. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **6**

Figure S37. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **6**

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Figure S39. ^1H - ^1H COSY spectrum of compound **6** in CDCl_3

Figure S40. HMBC spectrum of compound **6** in CDCl_3

Figure S41. ROESY spectrum of compound **6** in CDCl_3

Figure S42. HRESI-MS spectrum of compound **6**

Figure S43. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **7**

Figure S44. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **7**

Figure S45. HSQC spectrum of compound **7** in CDCl_3

Figure S46. ^1H - ^1H COSY spectrum of compound **7** in CDCl_3

Figure S47. HMBC spectrum of compound **7** in CDCl_3

Figure S48. ROESY spectrum of compound **7** in CDCl_3

Figure S49. HRESI-MS spectrum of compound **7**

Figure S50. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **9**

Figure S51. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **9**

Figure S52. HSQC spectrum of compound **9** in CDCl_3

Figure S53. ^1H - ^1H COSY spectrum of compound **9** in CDCl_3

Figure S54. HMBC spectrum of compound **9** in CDCl_3

Figure S55. ROESY spectrum of compound **9** in CDCl_3

Figure S56. HRESI-MS spectrum of compound **9**

Figure S57. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **10**

Figure S58. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **10**

Figure S59. HSQC spectrum of compound **10** in CDCl_3

Figure S60. ^1H - ^1H COSY spectrum of compound **10** in CDCl_3

Figure S61. HMBC spectrum of compound **10** in CDCl_3

Figure S62. ROESY spectrum of compound **10** in CDCl_3

Figure S63. HRESI-MS spectrum of compound **10**

Figure S64. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **11**

Figure S65. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **11**

Figure S66. HSQC spectrum of compound **11** in CDCl₃

Figure S67. ¹H-¹H COSY spectrum of compound **11** in CDCl₃

Figure S68. HMBC spectrum of compound **11** in CDCl₃

Figure S69. ROESY spectrum of compound **11** in CDCl₃

Figure S70. HRESI-MS spectrum of compound **11**

Figure S71. ¹H NMR (500 MHz, CDCl₃) spectrum of compound **12**

Figure S72. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **12**

Figure S73. HSQC spectrum of compound **12** in CDCl₃

Figure S74. ¹H-¹H COSY spectrum of compound **12** in CDCl₃

Figure S75. HMBC spectrum of compound **12** in CDCl₃

Figure S76. ROESY spectrum of compound **12** in CDCl₃

Figure S77. HRESI-MS spectrum of compound **12**

Figure S78. ¹H NMR (500 MHz, CDCl₃) spectrum of compound **13**

Figure S79. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **13**

Figure S80. HSQC spectrum of compound **13** in CDCl₃

Figure S81. ¹H-¹H COSY spectrum of compound **13** in CDCl₃

Figure S82. HMBC spectrum of compound **13** in CDCl₃

Figure S83. ROESY spectrum of compound **13** in CDCl₃

Figure S84. HRESI-MS spectrum of compound **13**

Figure S85. ¹H NMR (500 MHz, CDCl₃) spectrum of compound **14**

Figure S86. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **14**

Figure S87. HSQC spectrum of compound **14** in CDCl₃

Figure S88. ^1H - ^1H COSY spectrum of compound **14** in CDCl_3

Figure S89. HMBC spectrum of compound **14** in CDCl_3

Figure S90. ROESY spectrum of compound **14** in CDCl_3

Figure S91. HRESI-MS spectrum of compound **14**

Figure S1. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **1**

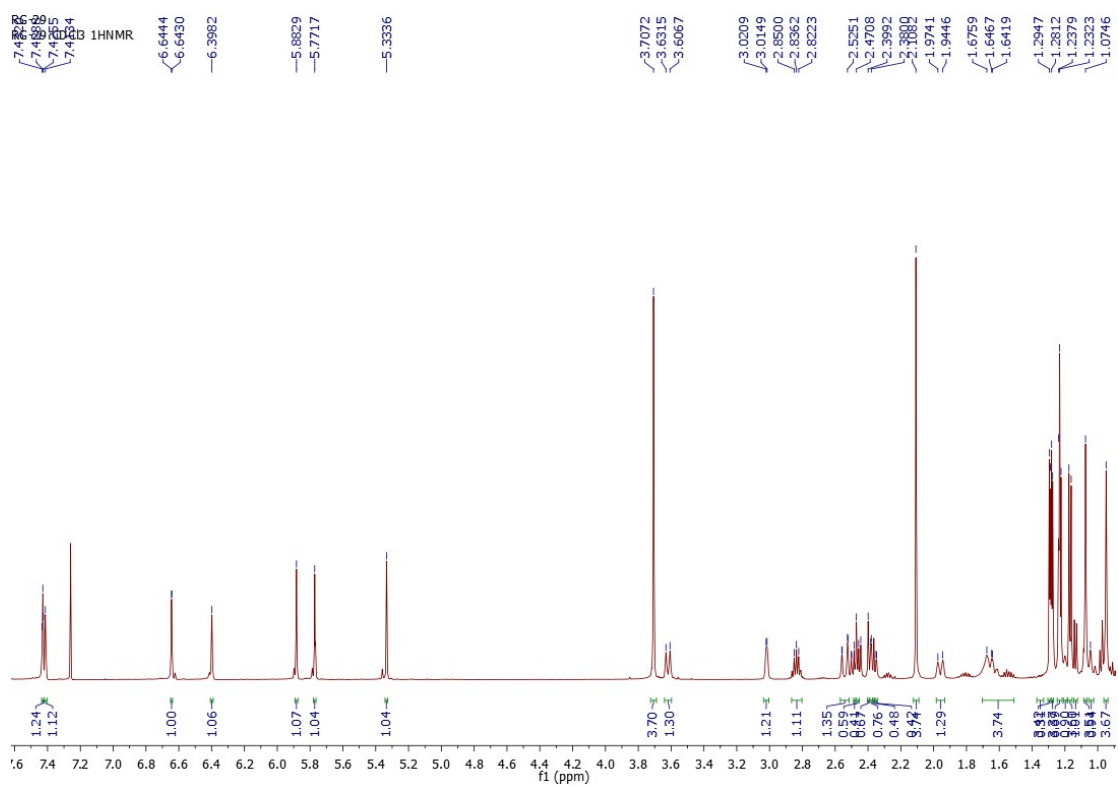


Figure S2. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **1**

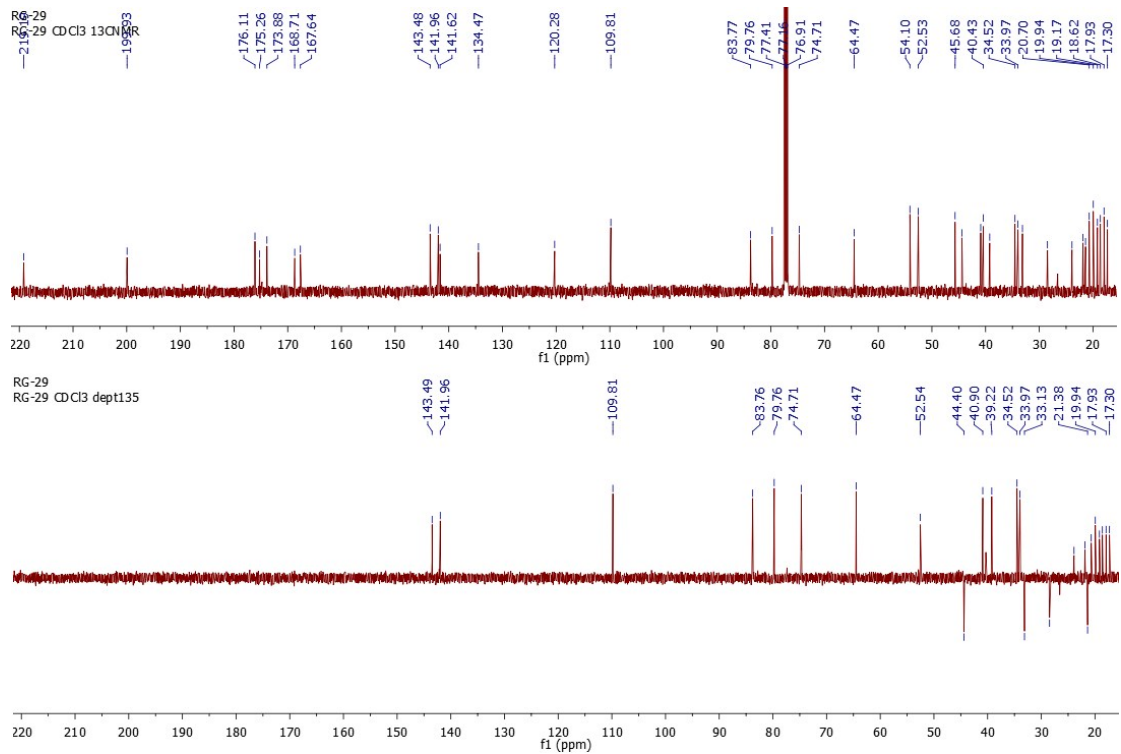


Figure S3. HSQC spectrum of compound **1** in CDCl₃

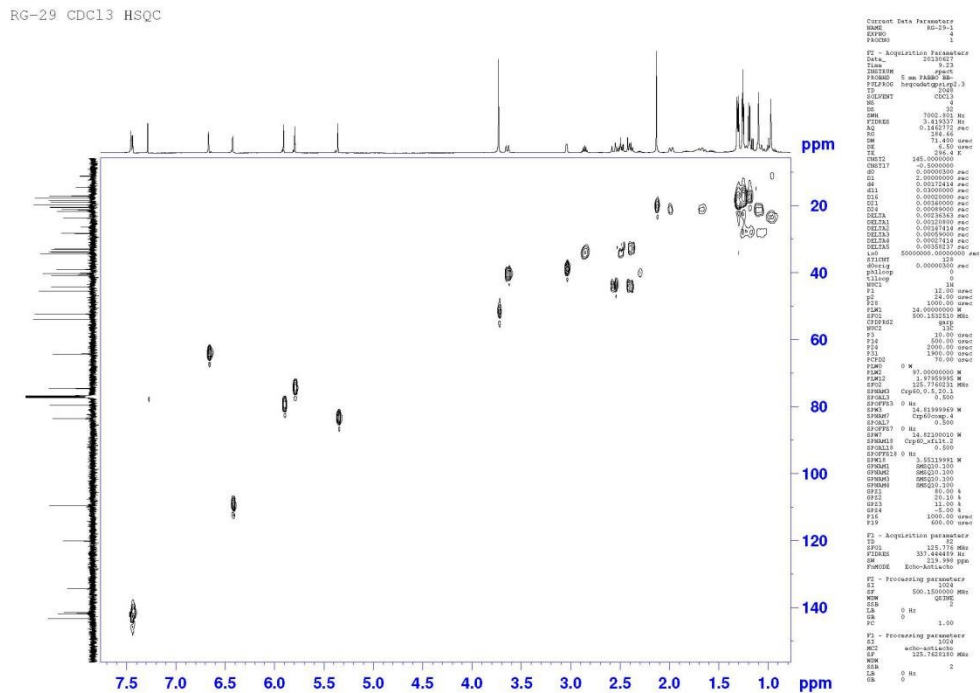


Figure S4. ¹H-¹H COSY spectrum of compound **1** in CDCl₃

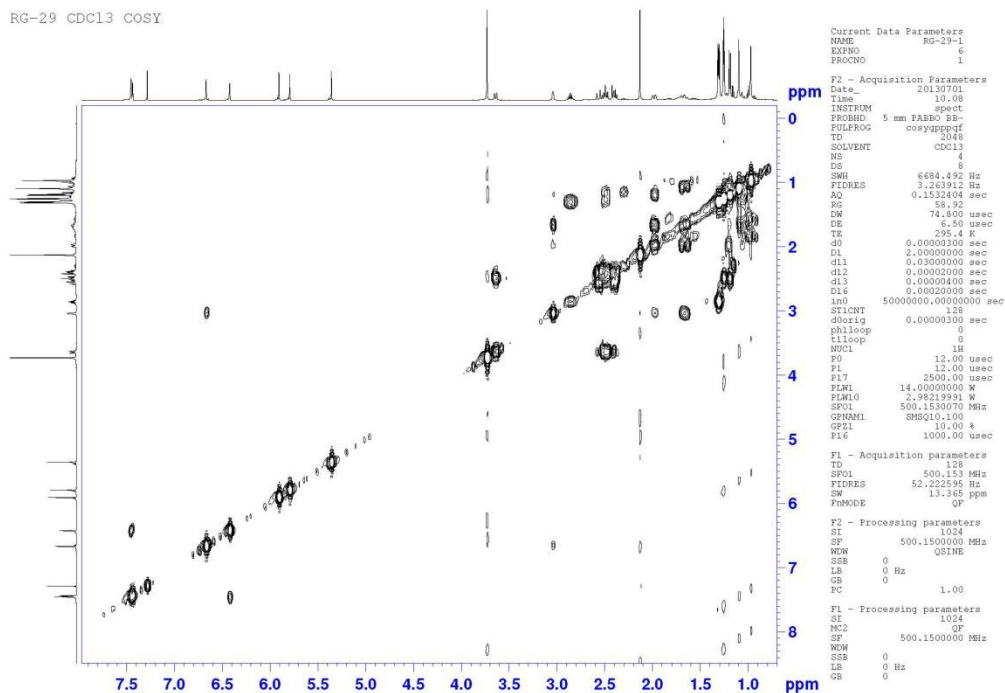


Figure S5. HMBC spectrum of compound **1** in CDCl₃

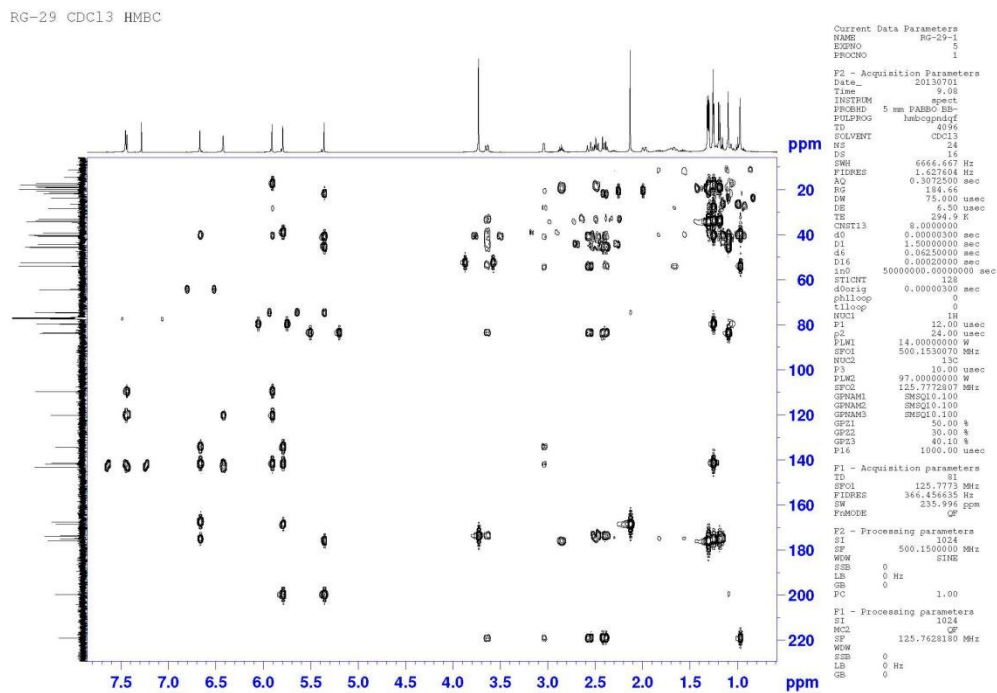


Figure S6. ROESY spectrum of compound **1** in CDCl₃

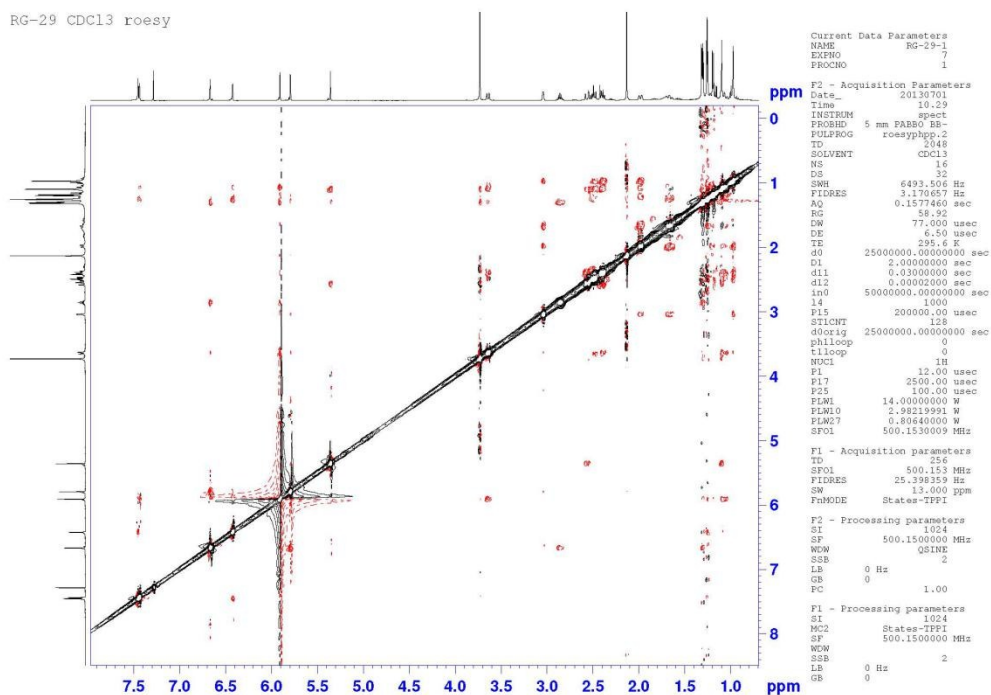


Figure S7. HREI-MS spectrum of compound 1

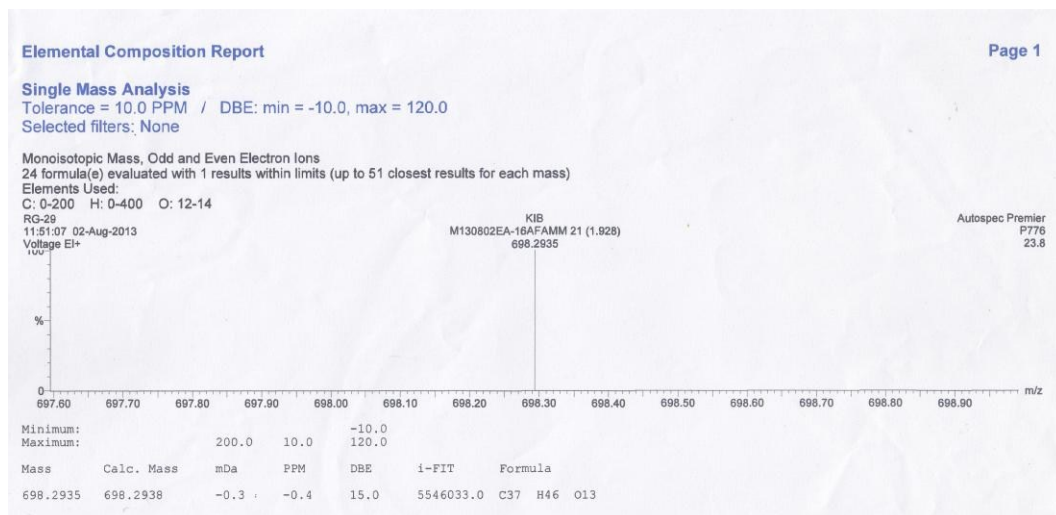


Figure S8. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 2

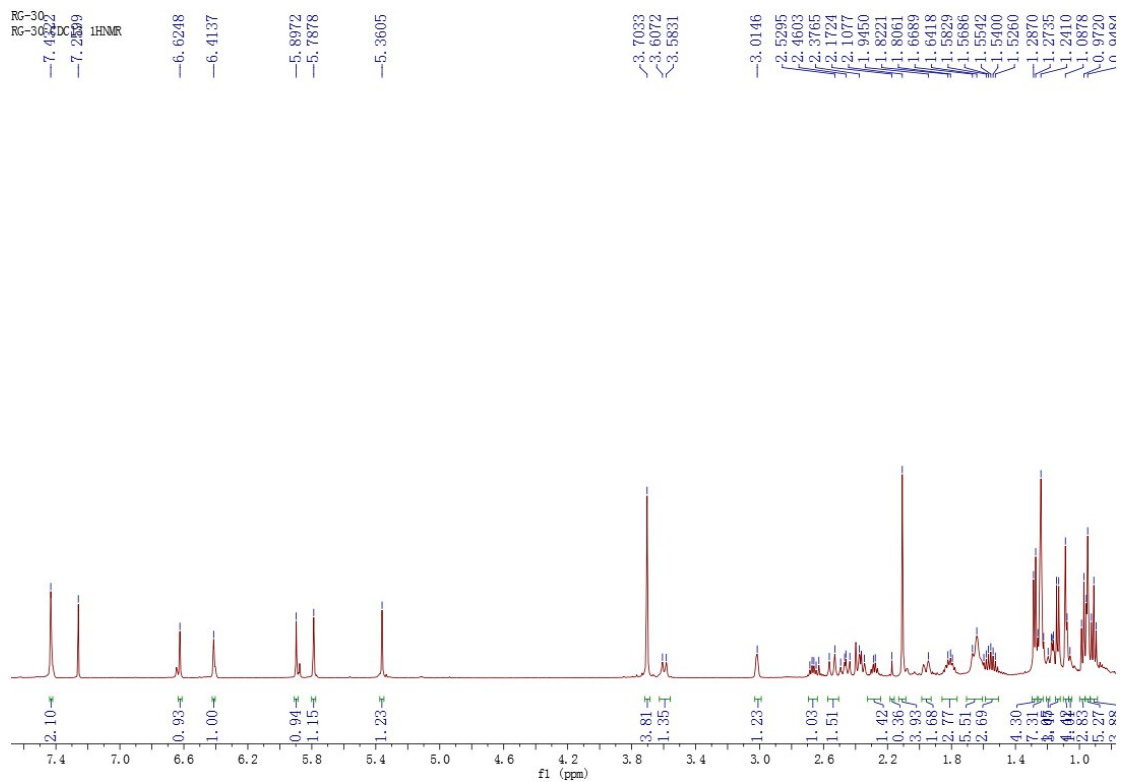


Figure S9. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **2**

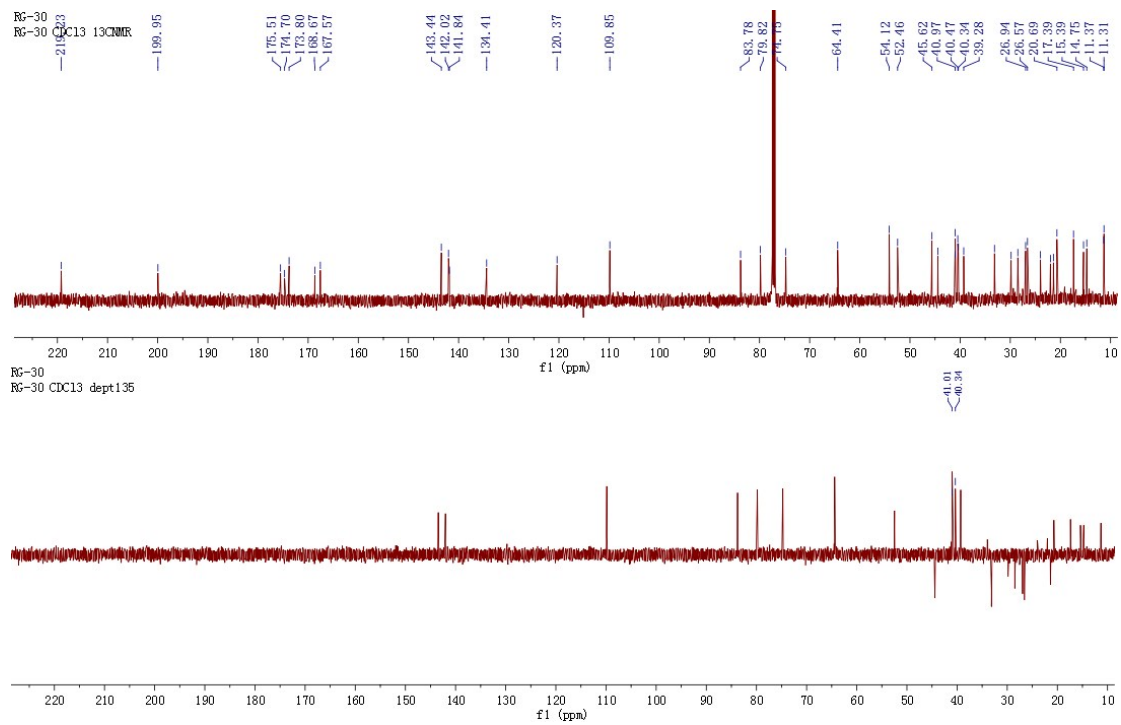


Figure S10. HSQC spectrum of compound **2** in CDCl₃

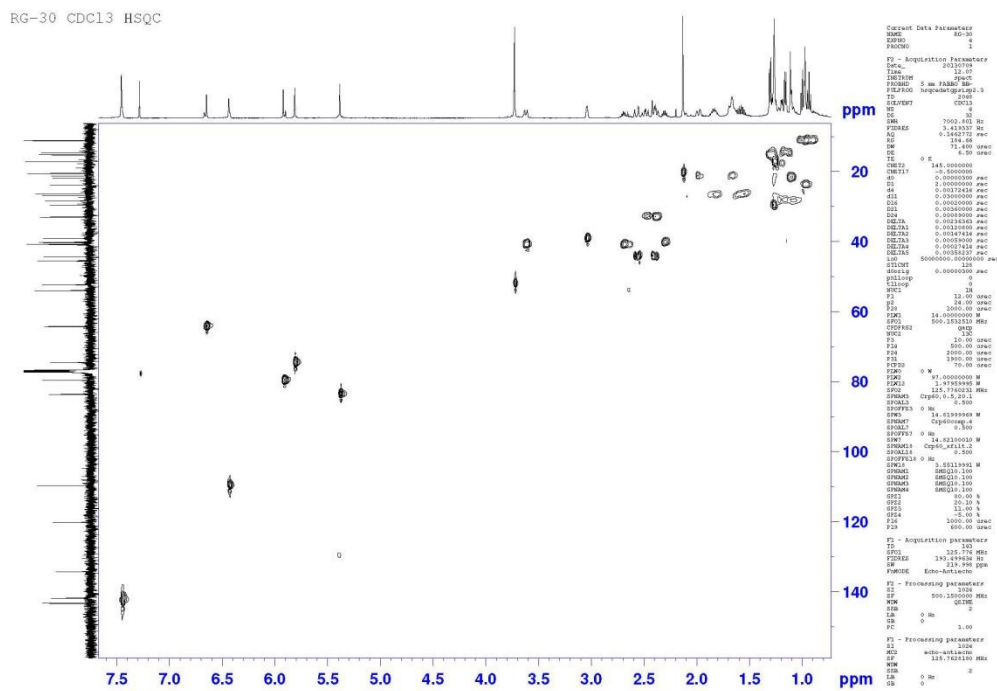


Figure S11. ¹H-¹H COSY spectrum of compound **2** in CDCl₃

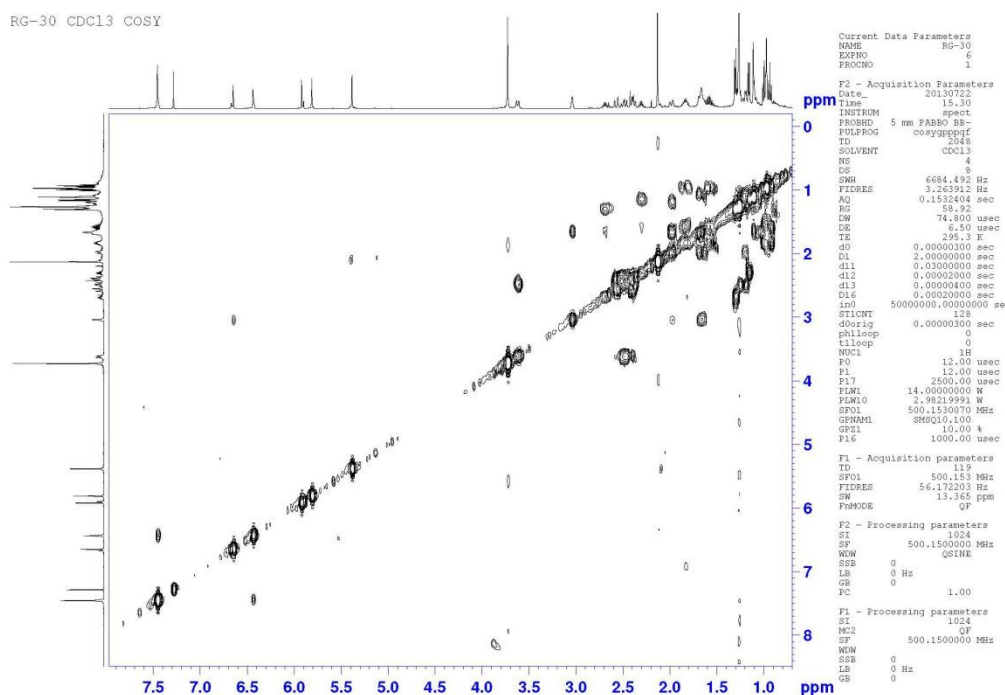


Figure S12. HMBC spectrum of compound **2** in CDCl₃

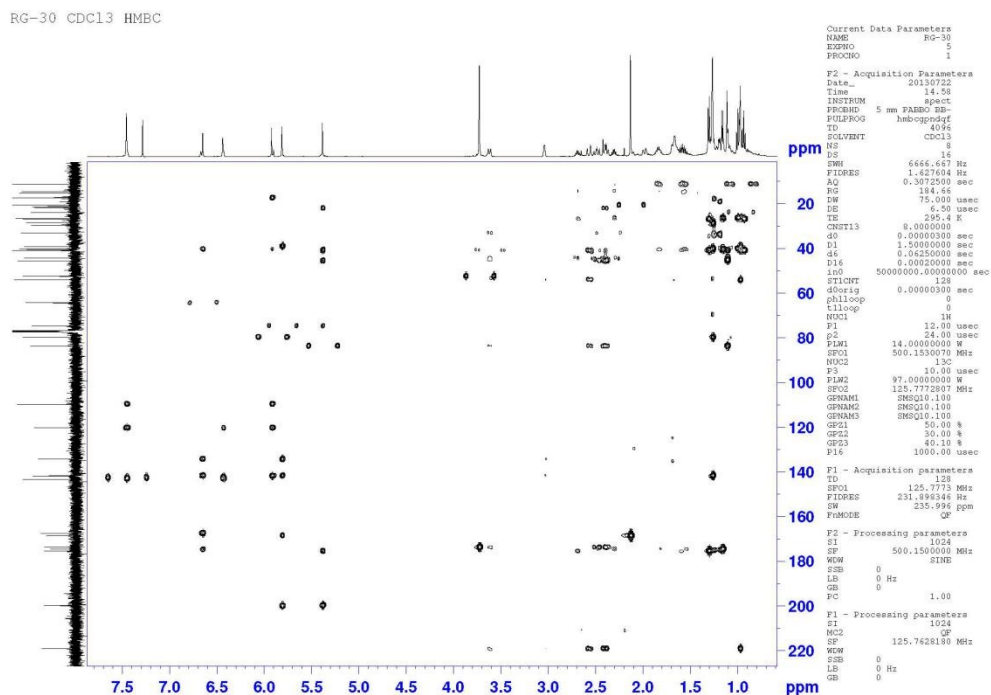


Figure S13. ROESY spectrum of compound **2** in CDCl₃

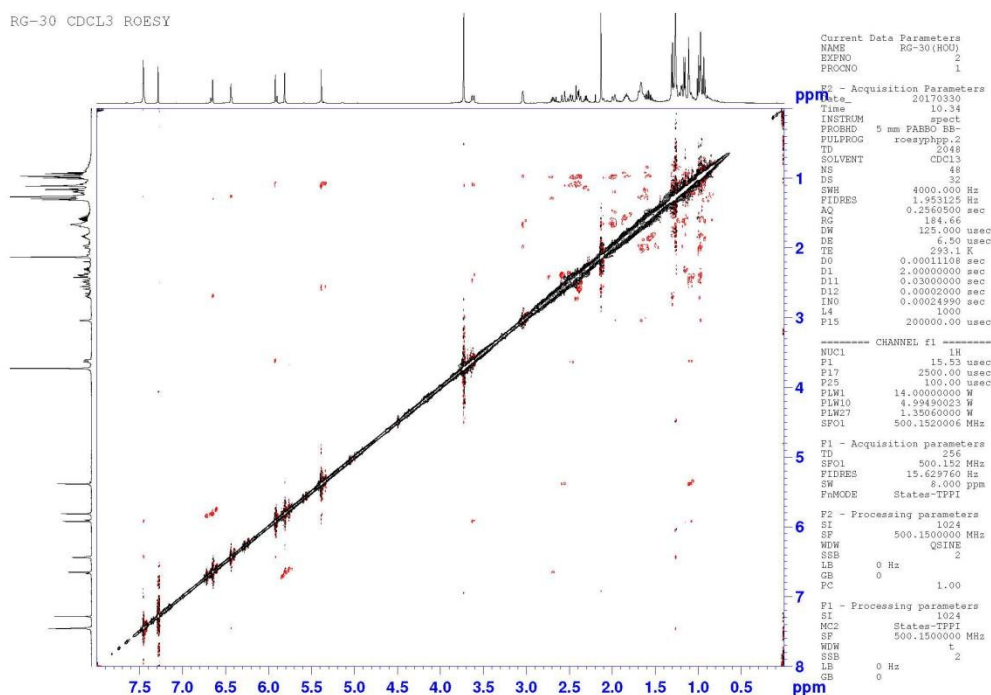


Figure S14. HRESI-MS spectrum of compound 2

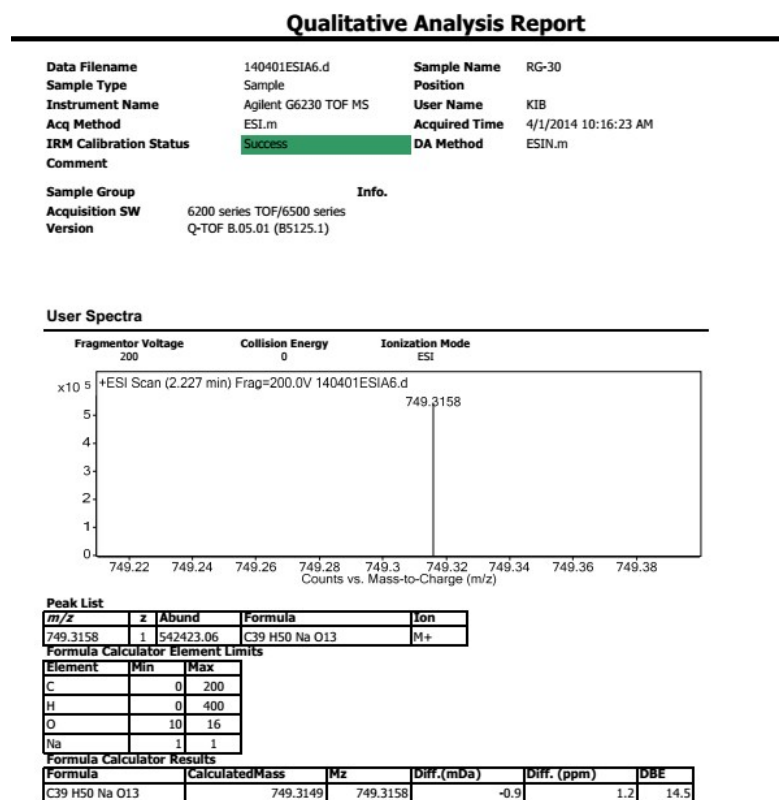


Figure S15. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 3

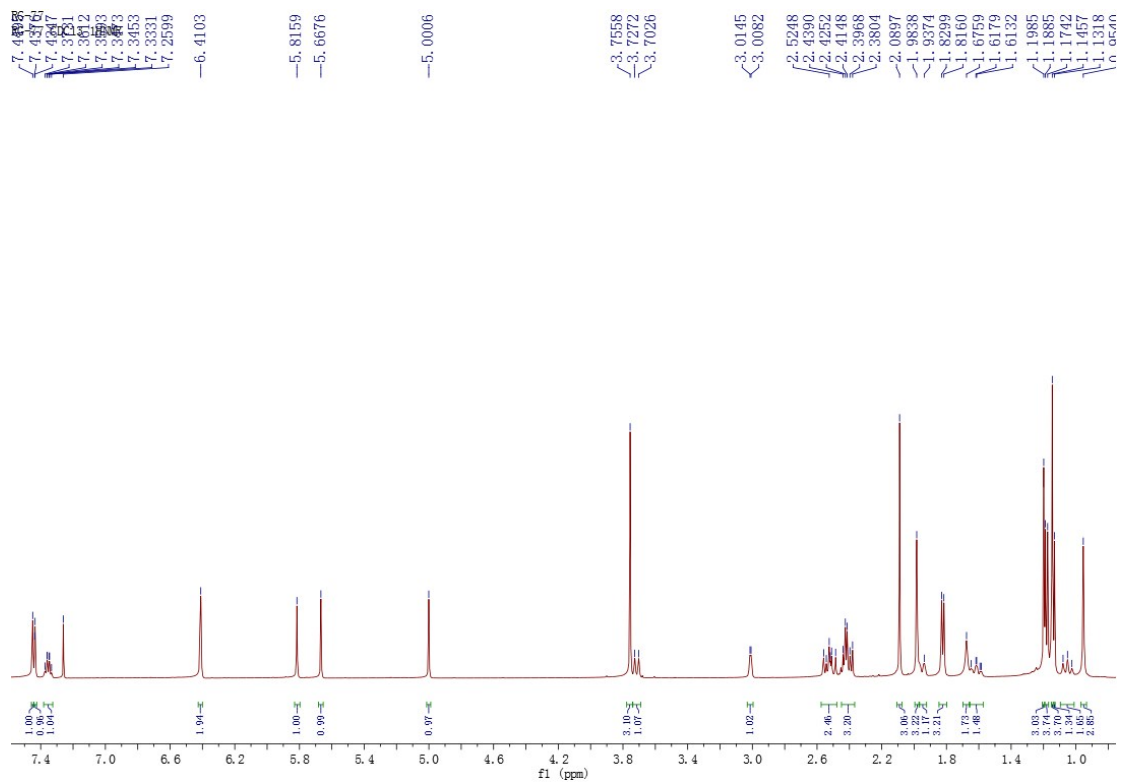


Figure S16. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **3**

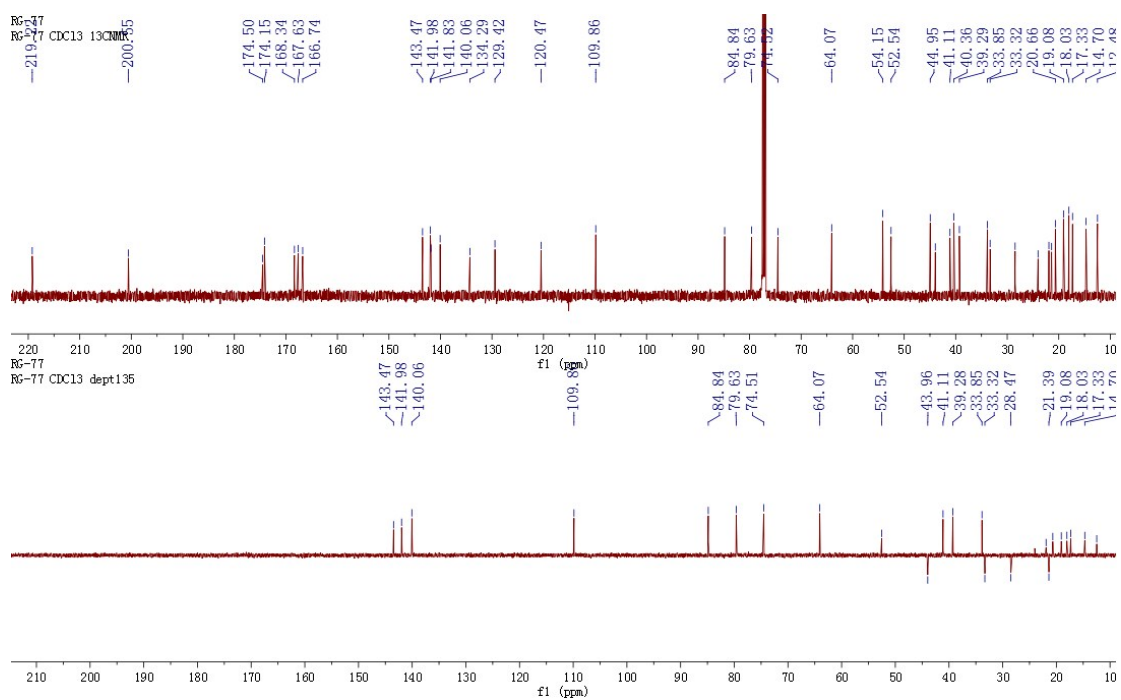


Figure S17. HSQC spectrum of compound **3** in CDCl_3

RG-77 CDCl3 HSQC

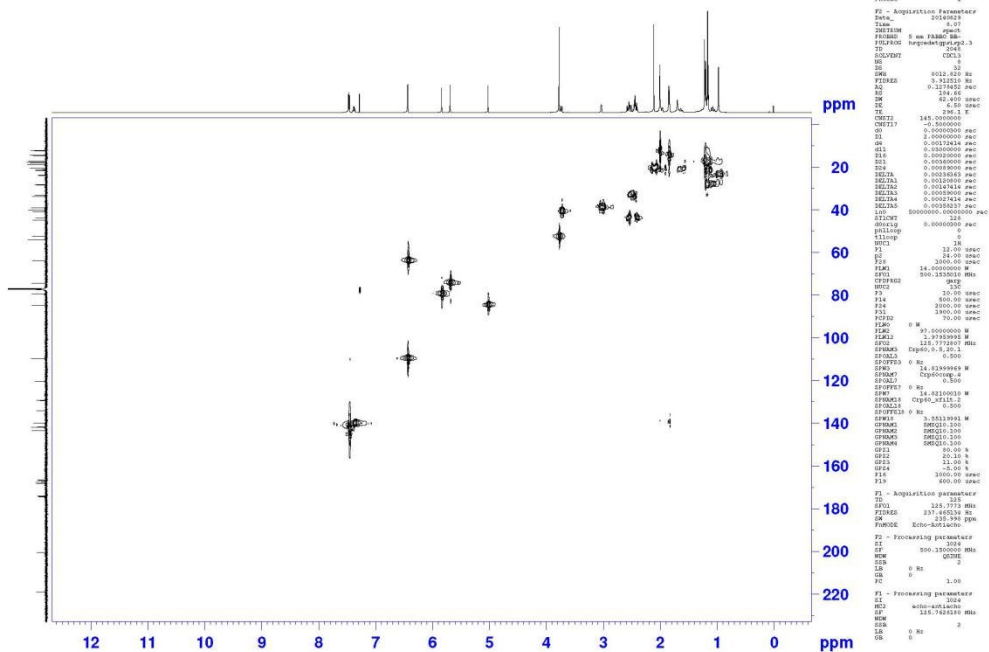


Figure S18. ^1H - ^1H COSY spectrum of compound **3** in CDCl_3

RG-77 CDCl3 COSY

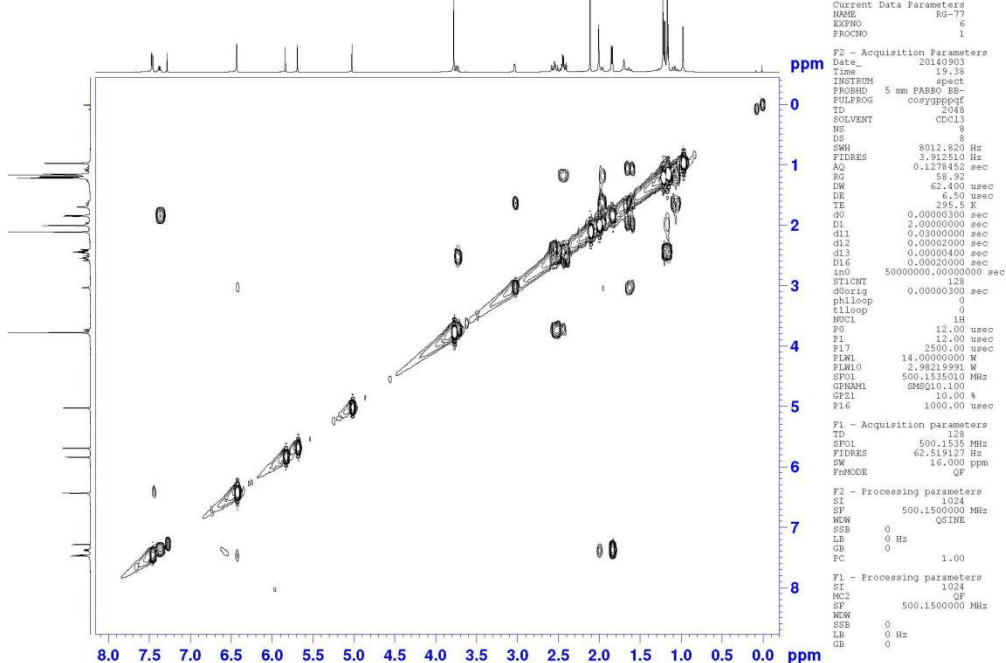


Figure S19. HMBC spectrum of compound **3** in CDCl_3

RG-77 CDCL3 HMBC

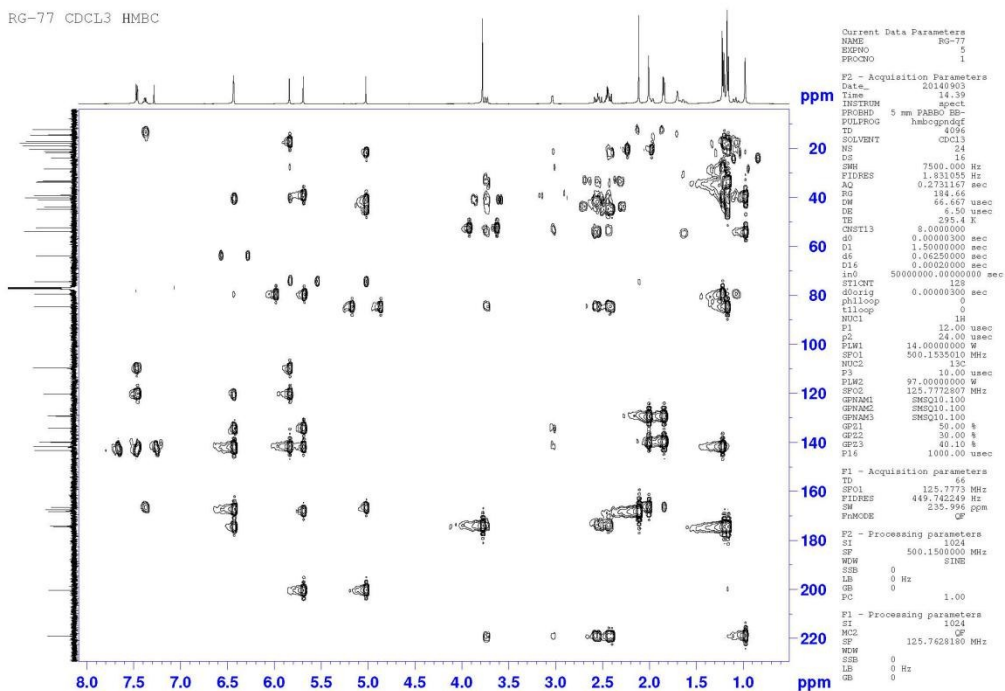


Figure S20. ROESY spectrum of compound 3 in CDCl₃

RG-77 CDCL3 roesy

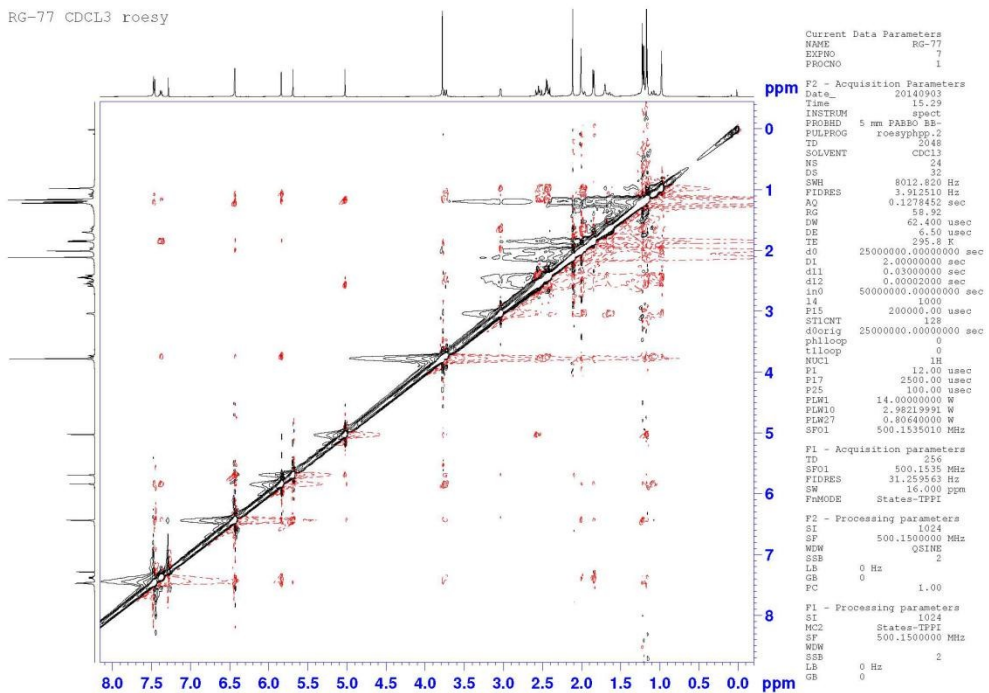


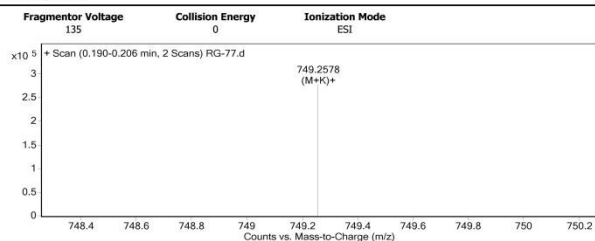
Figure S21. HRESI-MS spectrum of compound 3

Qualitative Analysis Report

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IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.2)

User Spectra



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729.3316	1	51852.3		
733.2836	1	131878.3		
734.2868	1	52848.45		
749.2578	1	276760.53	C38 H46 O13	(M+K)+
750.2609	1	106024.8	C38 H46 O13	(M+K)+
751.261	1	45067.43	C38 H46 O13	(M+K)+
922.0098	1	42019.98		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
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Figure S22. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 4

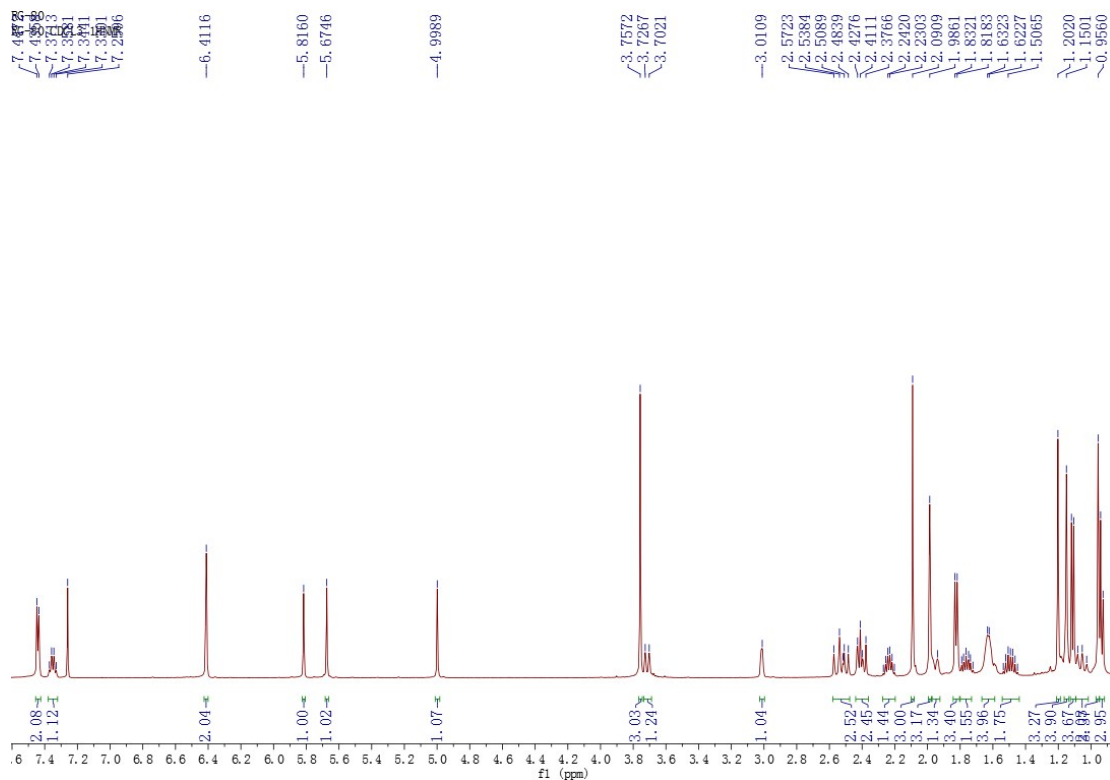


Figure S23. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound 4

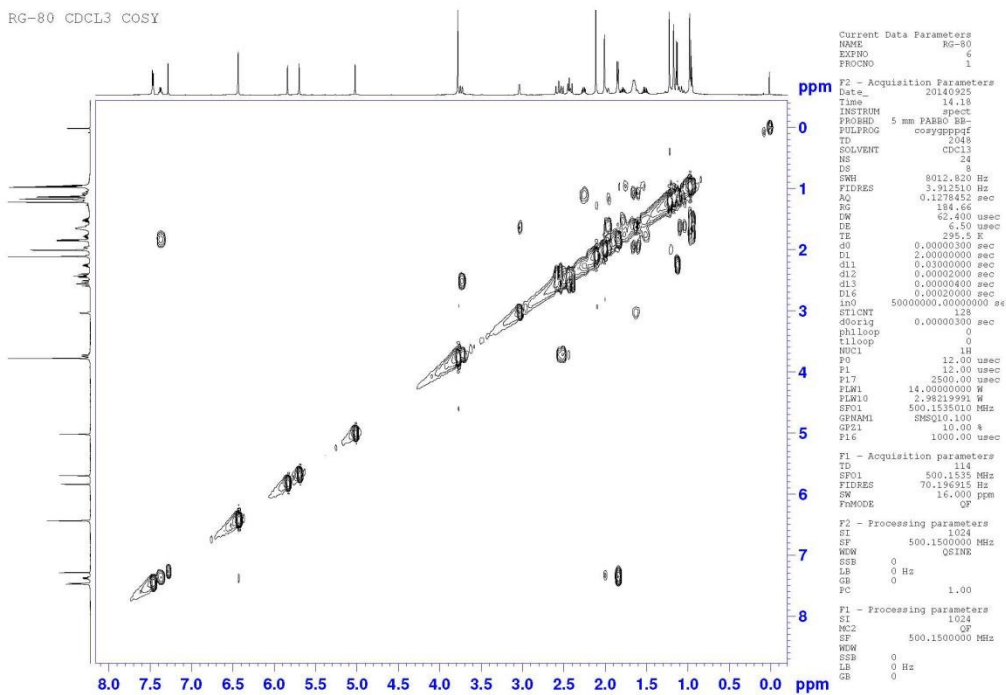


Figure S26. HMBC spectrum of compound 4 in CDCl₃

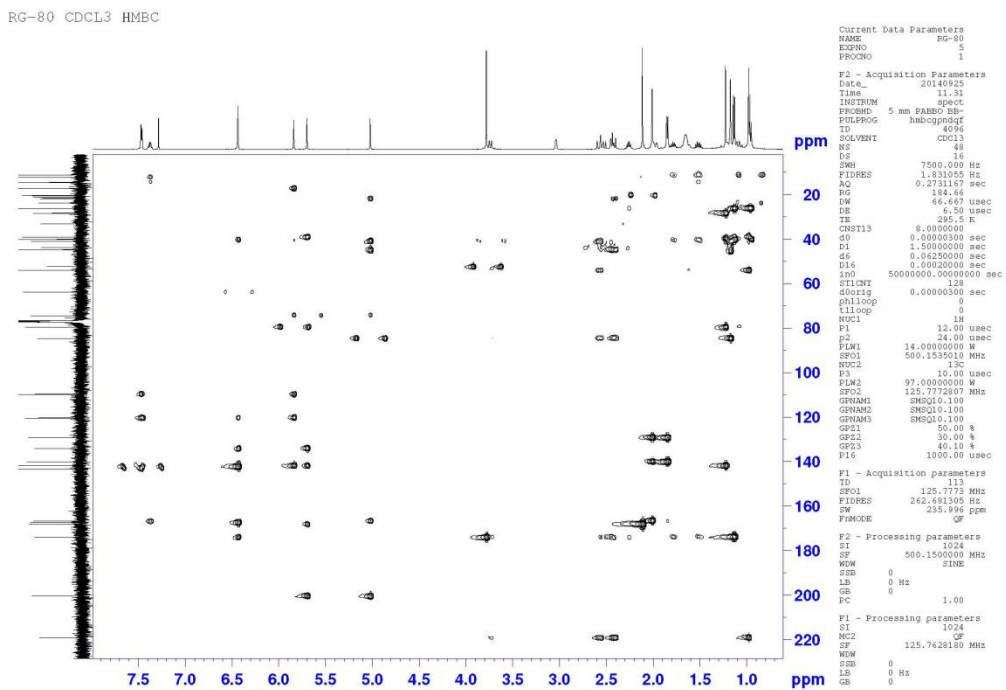
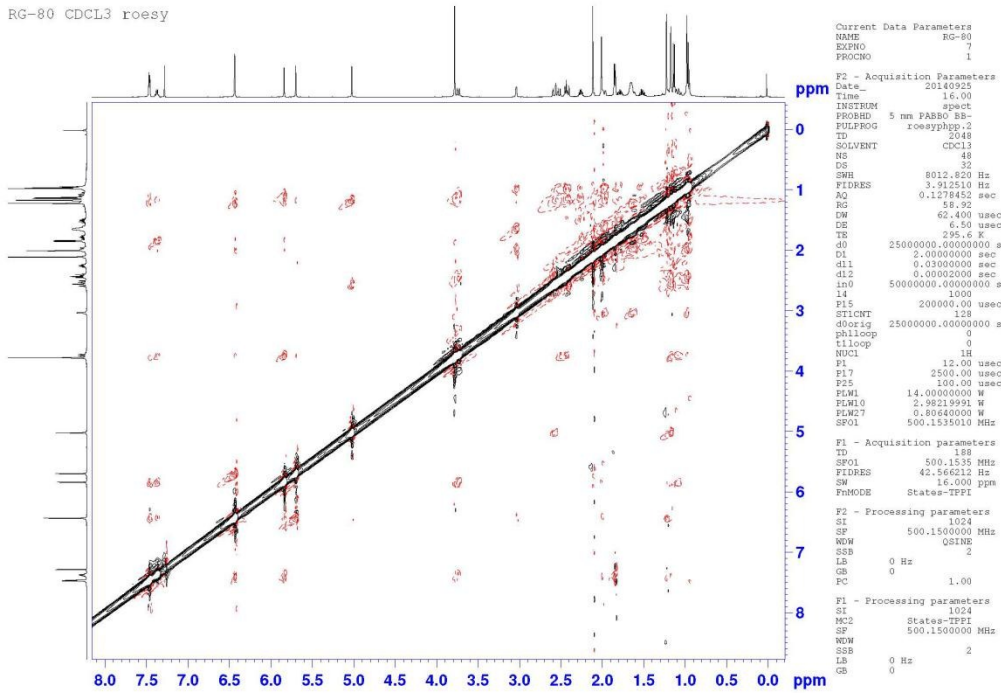


Figure S27. ROESY spectrum of compound 4 in CDCl₃

RG-80 CDCL3 roesy



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PROCNO   1

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PULPROG  roesypphg.2
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SOLVENT  CDCL3
NS        48
DS        32
SWH       8012.820 Hz
FIDRES    3.912510 Hz
AQ        0.1278452 sec
RG         58.92
DM        62.400 usec
DE         6.50 usec
TE        295.6 K
d0        25000000.00000000 s
d1        2.00000000 sec
d11       0.03000000 sec
d12       0.00020000 sec
in0       50000000.00000000 s
I1        1000
P15       2000000.00 usec
STICNT    128
d0org    25000000.00000000 s
ph1loop  0
tilloop  0
NUCL     1H
P1        12.00 usec
P17       2500.00 usec
P25       100.00 usec
PLWL     14.00000000 W
PLW10    2.98219991 W
PLW27    0.80640000 W
SP01     500.1535010 MHz

F1 - Acquisition parameters
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SP01     500.1535 MHz
FIDRES    42.566212 Hz
SW        16.000 ppm
FhMODE    States-TPPI

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WDW       QSINE
SSB       2
LB        0 Hz
GB        0
PC        1.00

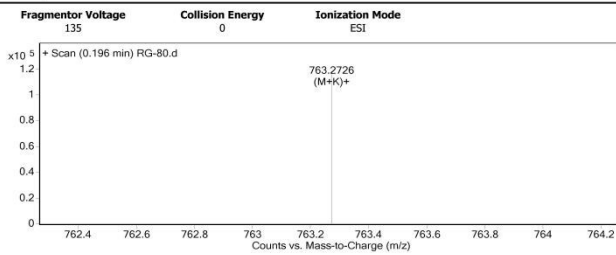
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SSB       2
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GB        0
    
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Figure S28. HRESI-MS spectrum of compound 4

Qualitative Analysis Report

Data Filename	RG-80.d	Sample Name	RG-80
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IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

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743.3462	1	20618.83		
747.2987	1	56817.65		
748.302	1	22202.19		
763.2726	1	117563.34	C39 H48 O13	(M+K)+
764.2755	1	54507.08	C39 H48 O13	(M+K)+
922.0098	1	55172.08		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C39 H48 O13	724.3095	763.2726	763.2726	0.2	0.2	16.0000

Figure S29. ¹H NMR (500 MHz, CDCl₃) spectrum of compound **5**

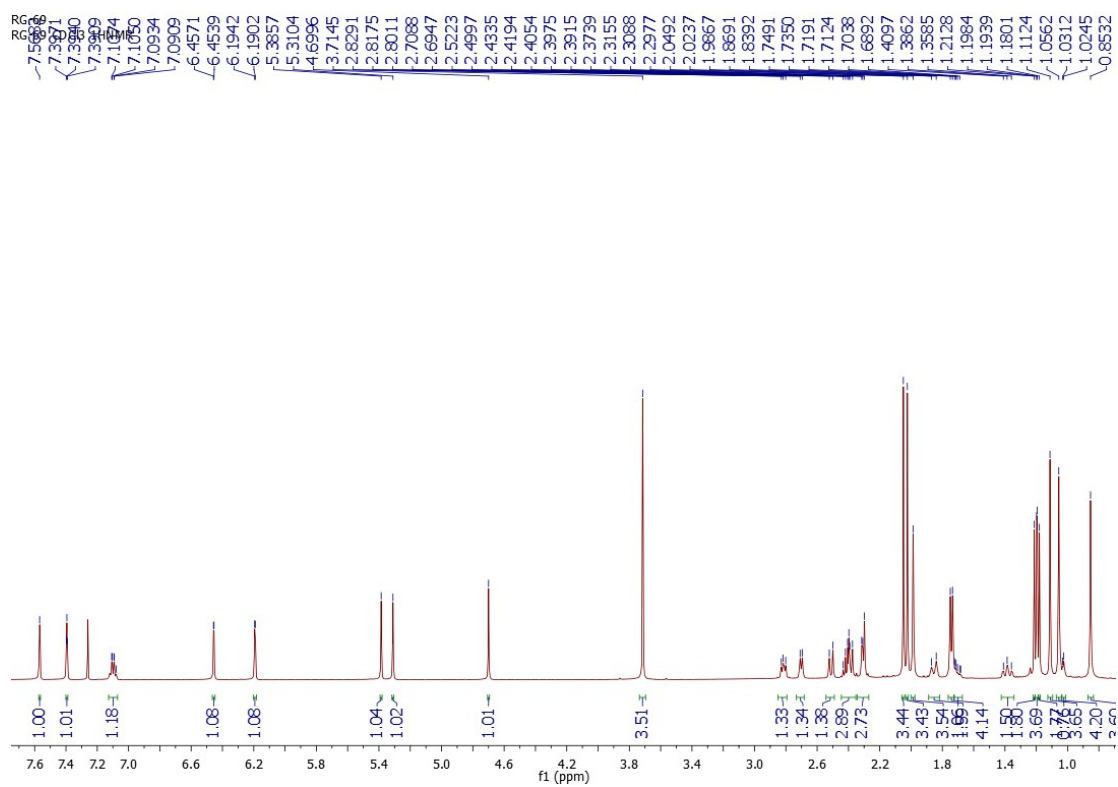


Figure S30. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **5**

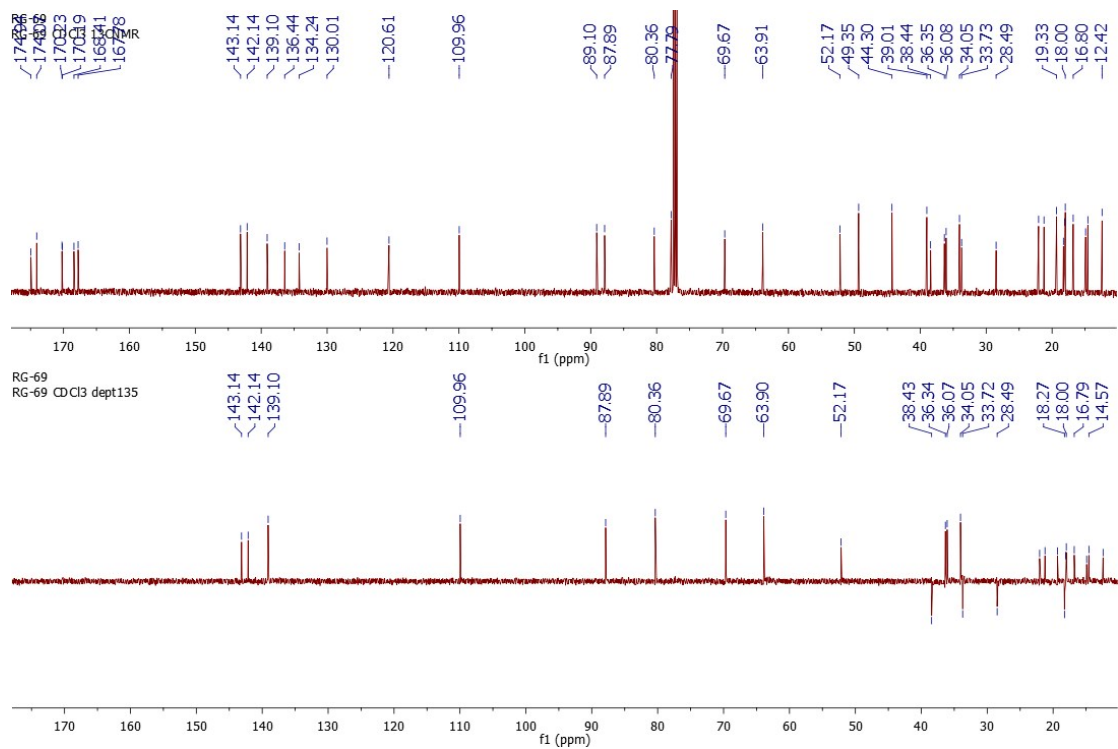


Figure S31. HSQC spectrum of compound **5** in CDCl₃

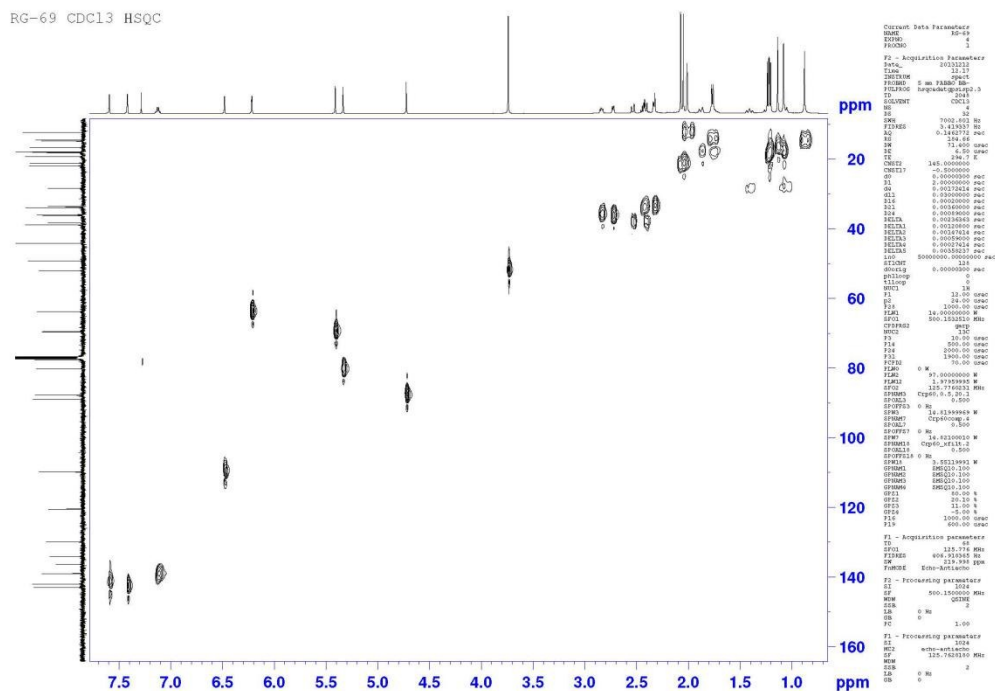


Figure S32. ¹H-¹H COSY spectrum of compound **5** in CDCl₃

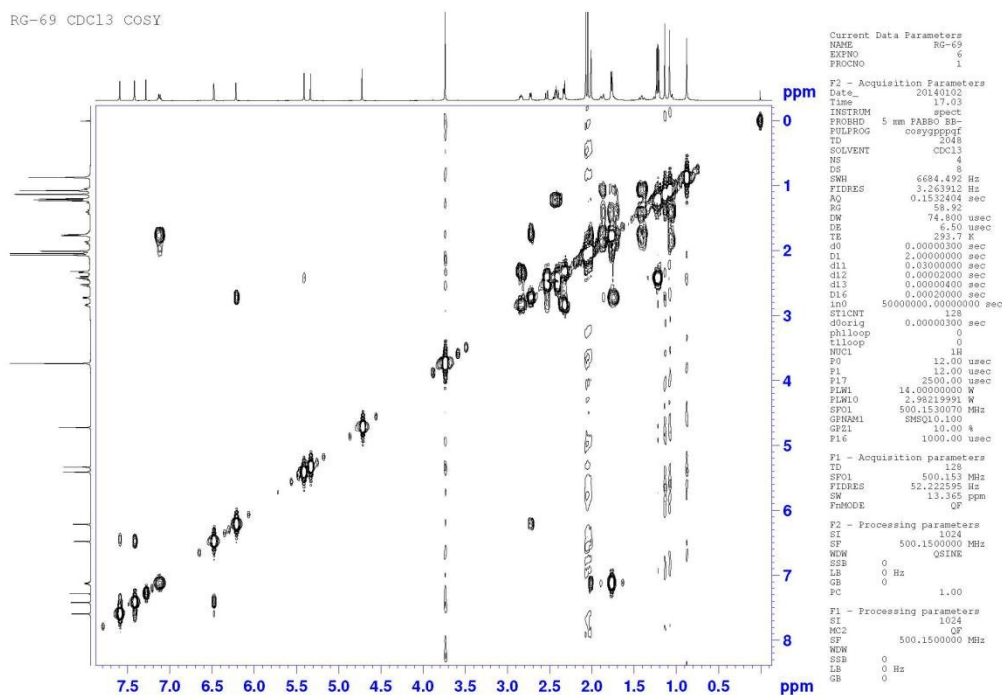


Figure S33. HMBC spectrum of compound **5** in CDCl₃

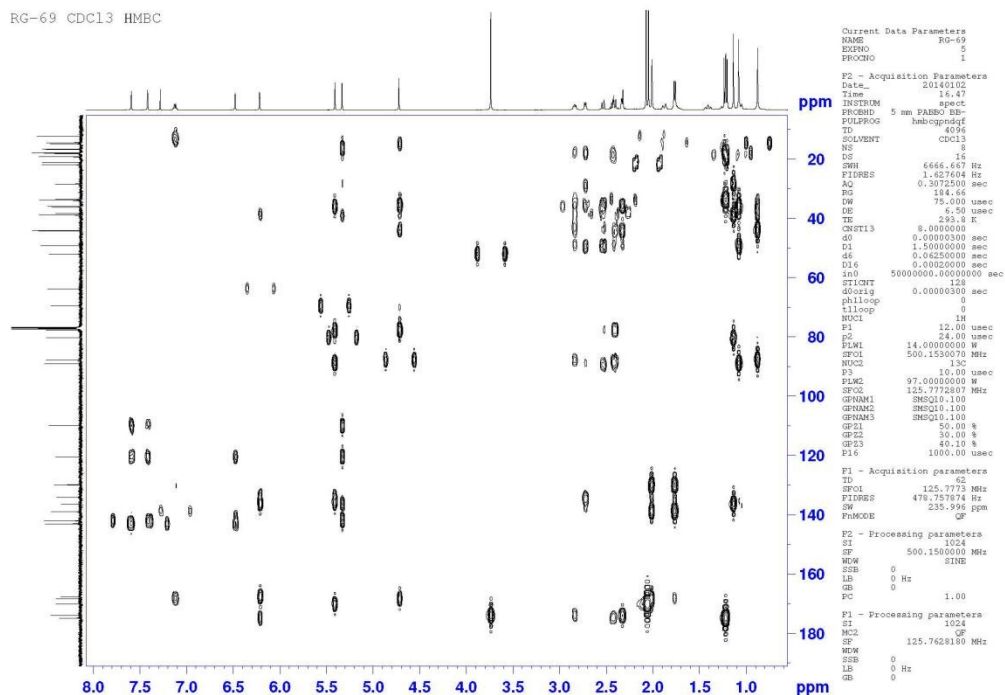


Figure S34. ROESY spectrum of compound **5** in CDCl₃

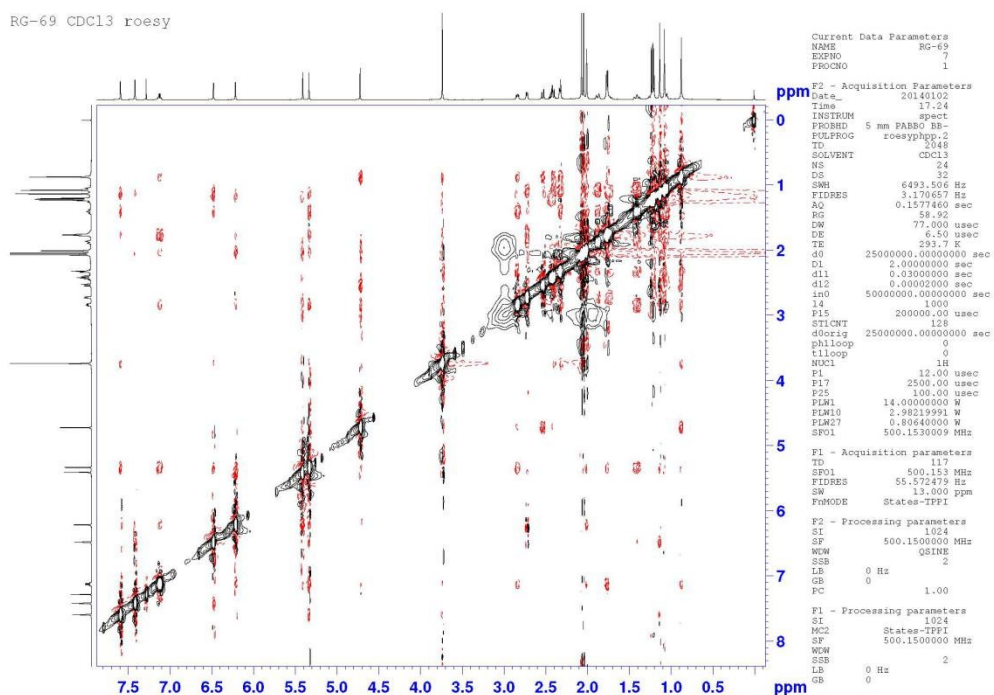


Figure S35. HRESI-MS spectrum of compound 5

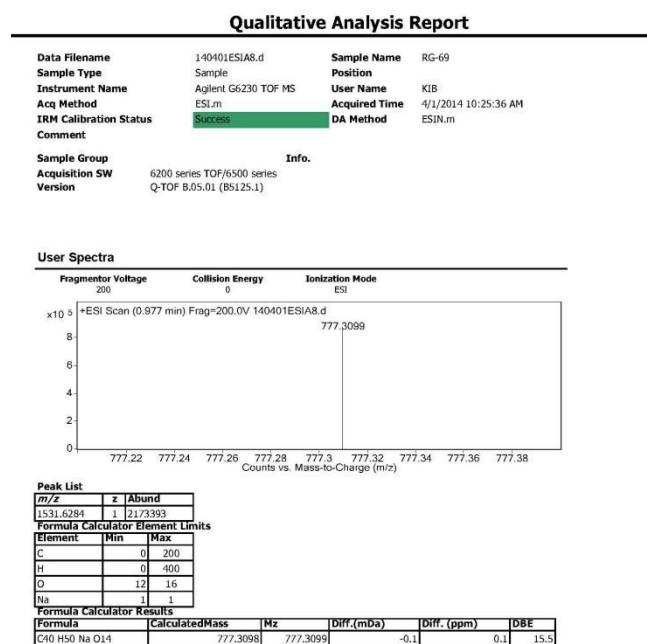


Figure S36. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 6

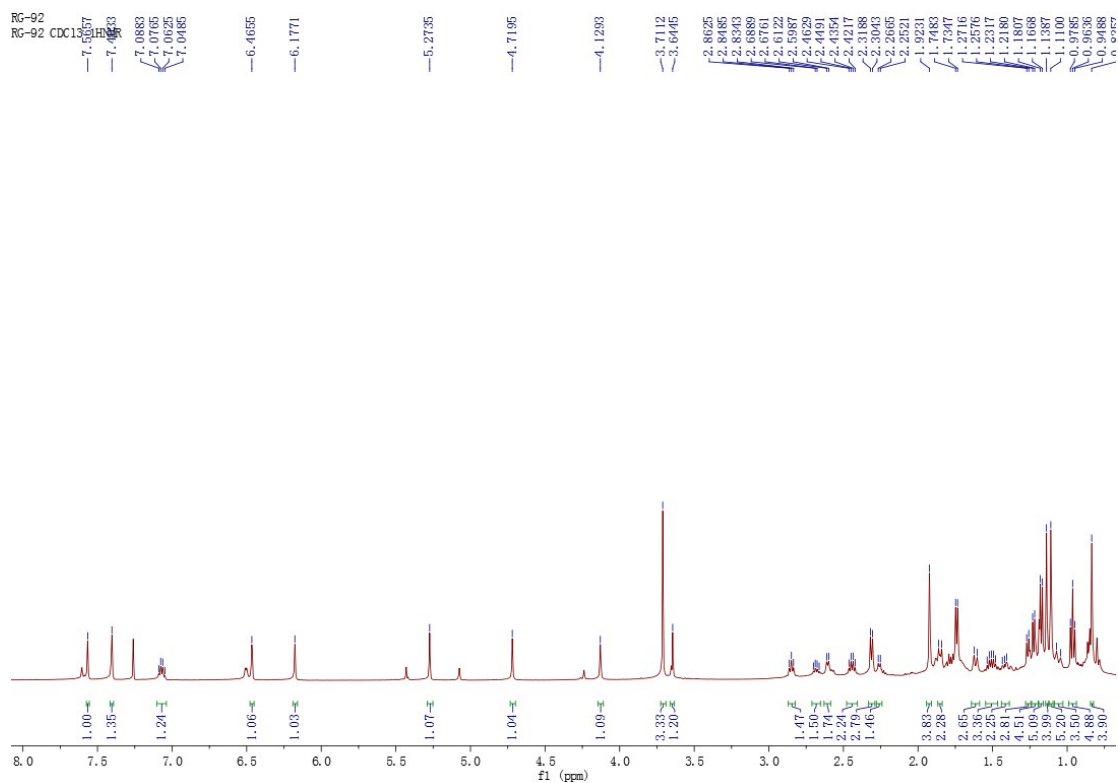


Figure S37. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound 6

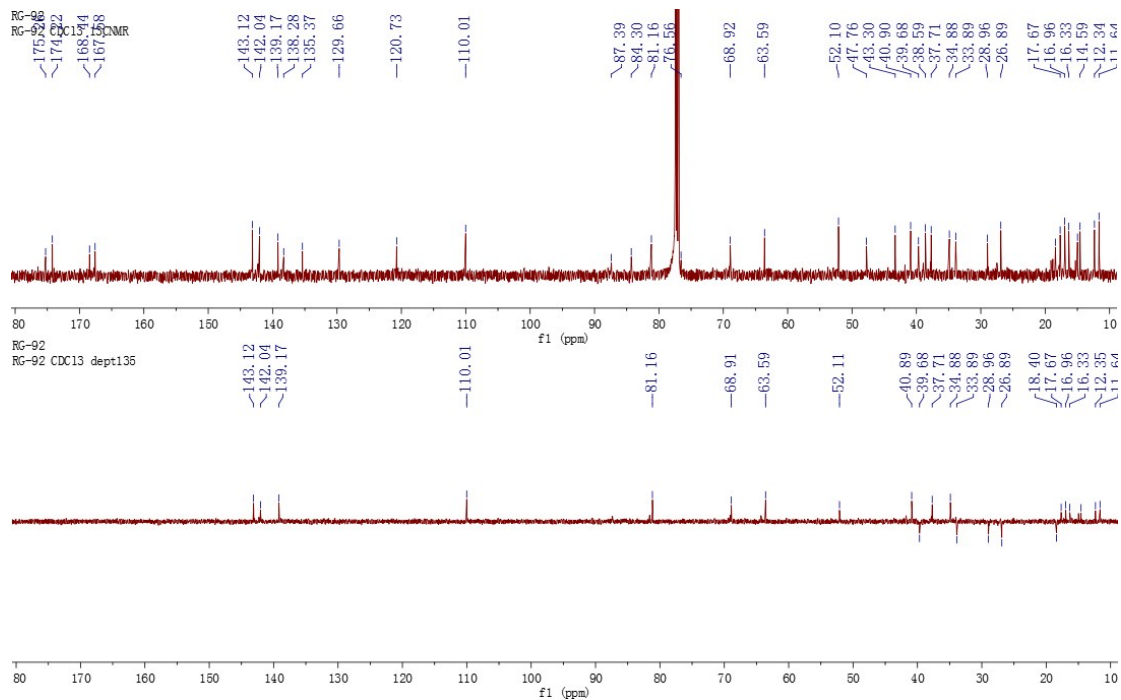


Figure S38. HSQC spectrum of compound **6** in CDCl_3

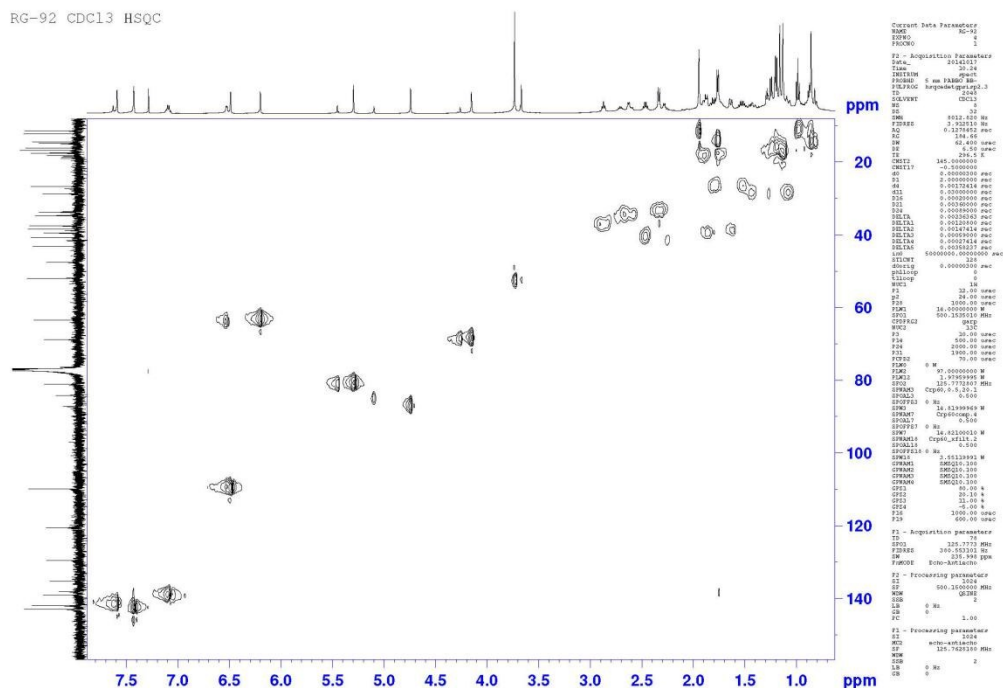


Figure S39. ^1H - ^1H COSY spectrum of compound **6** in CDCl_3

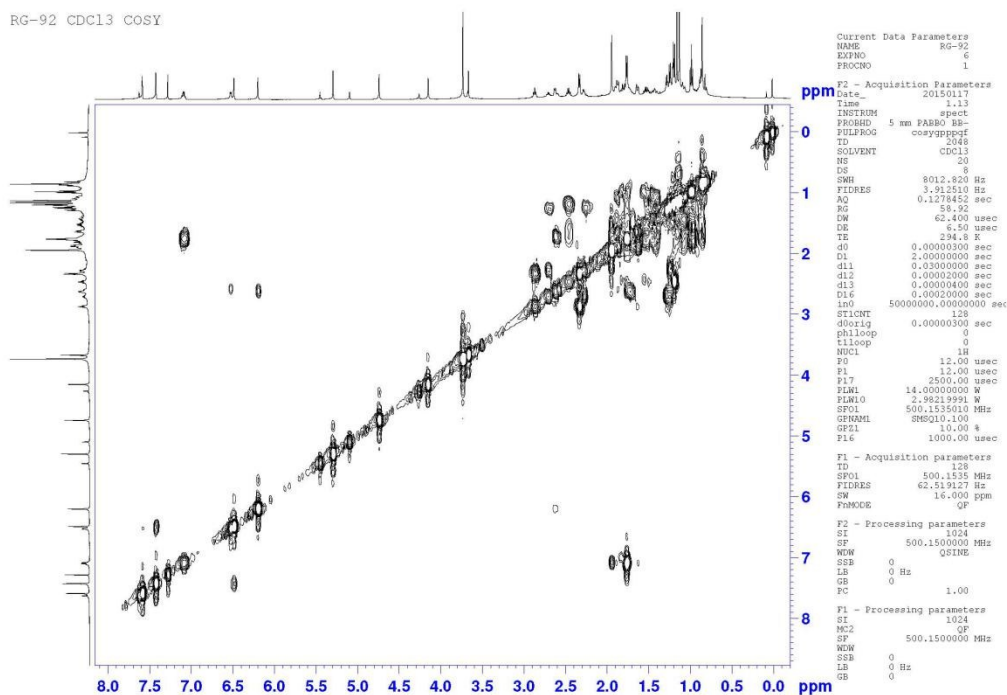


Figure S40. HMBC spectrum of compound **6** in CDCl_3

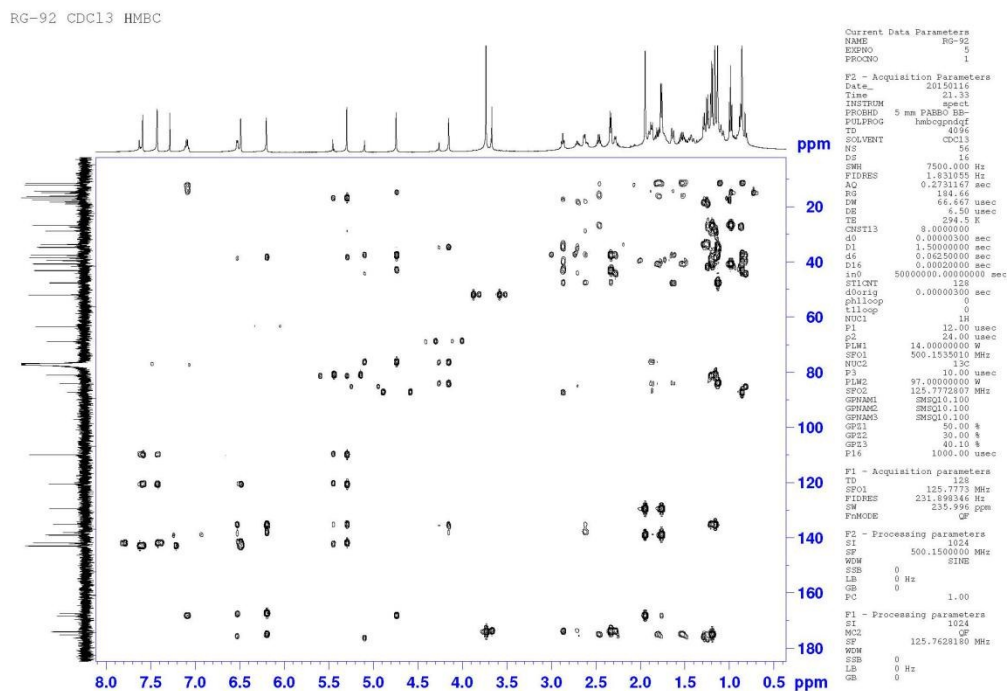


Figure S41. ROESY spectrum of compound 6 in CDCl₃

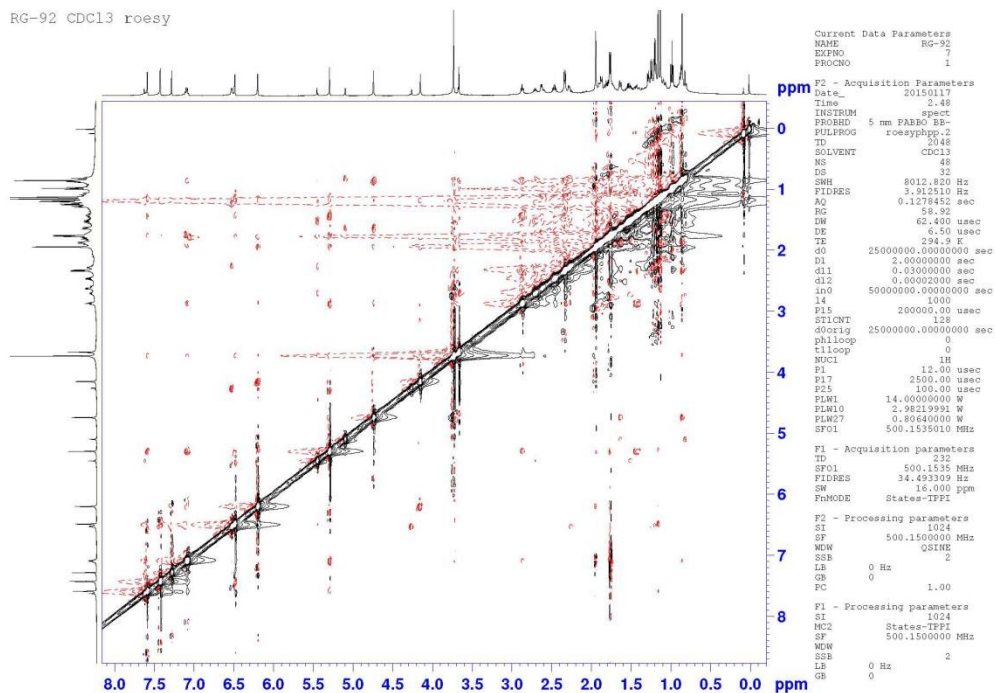


Figure S42. HRESI-MS spectrum of compound 6

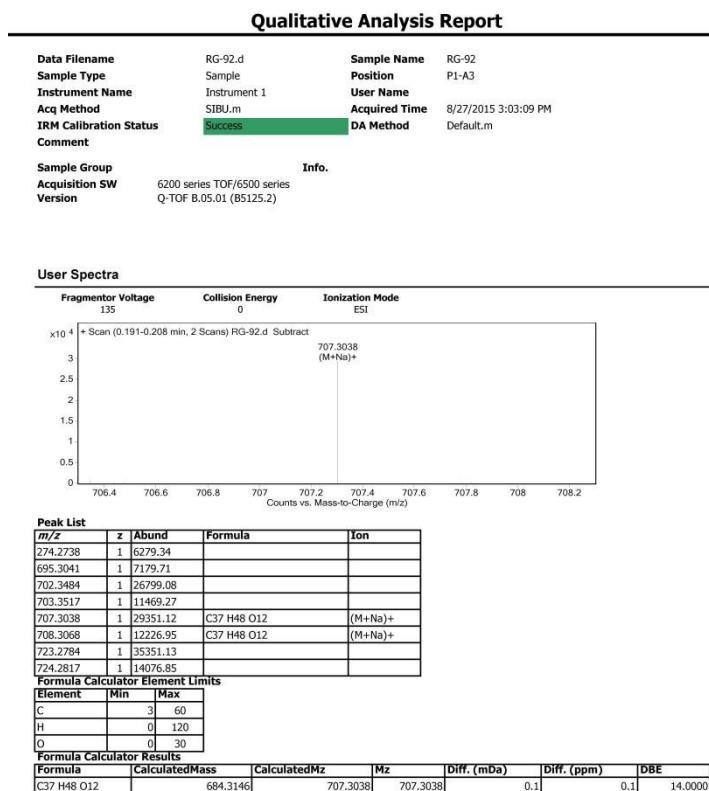


Figure S43. ^1H NMR (500 MHz, CDCl_3) spectrum of compound 7

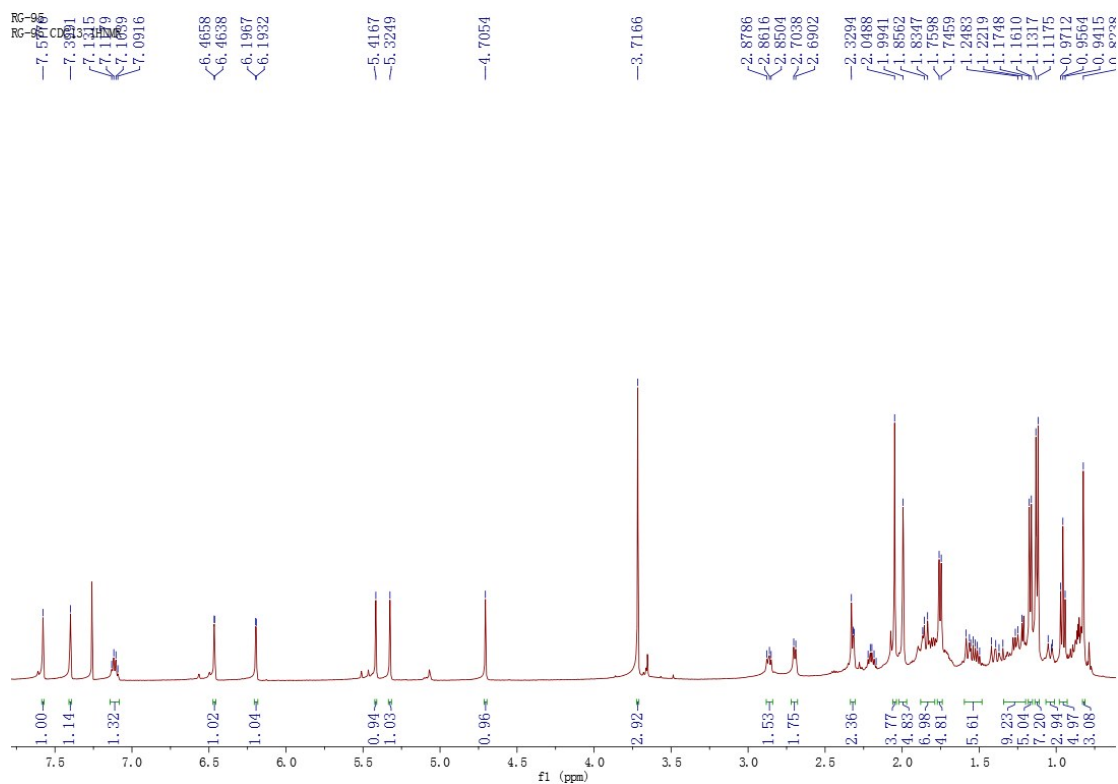
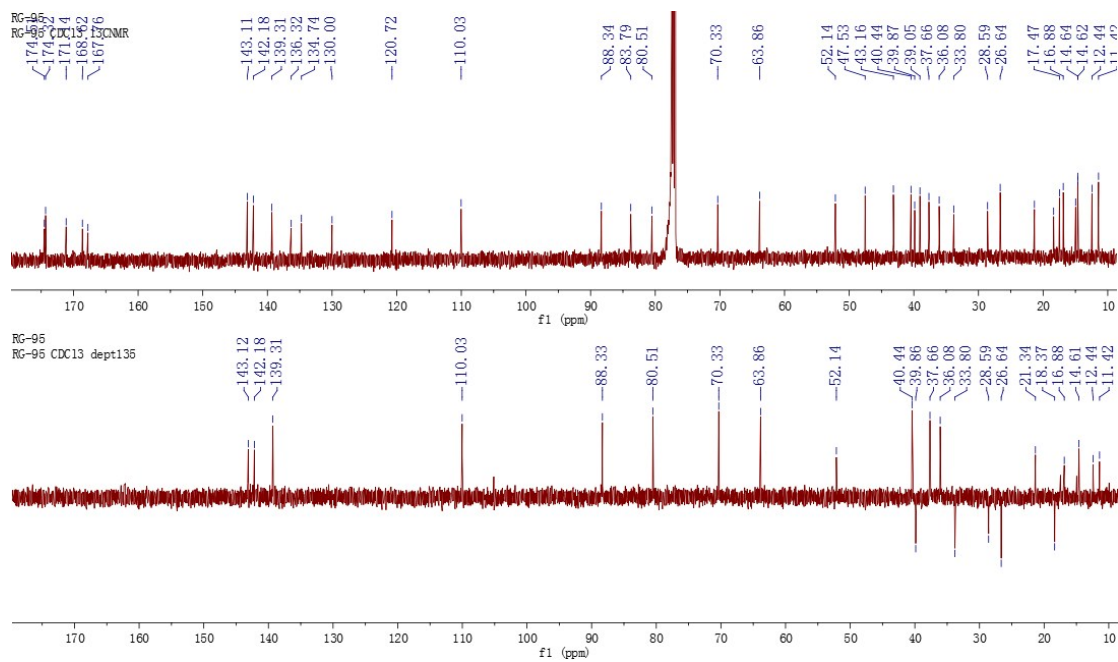


Figure S44. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 7



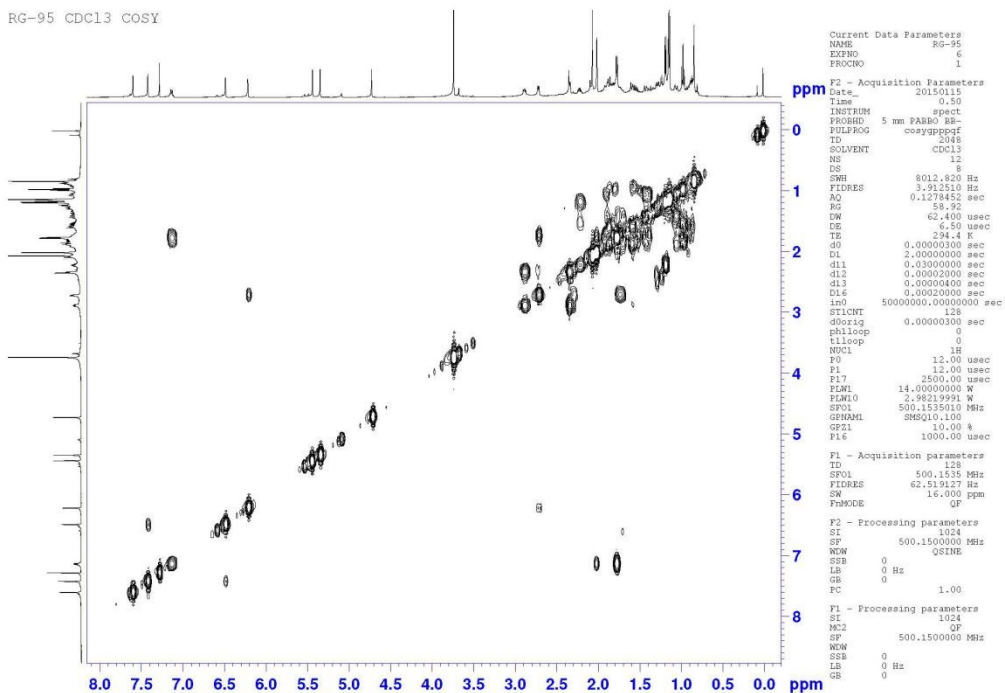


Figure S47. HMBC spectrum of compound 7 in CDCl₃

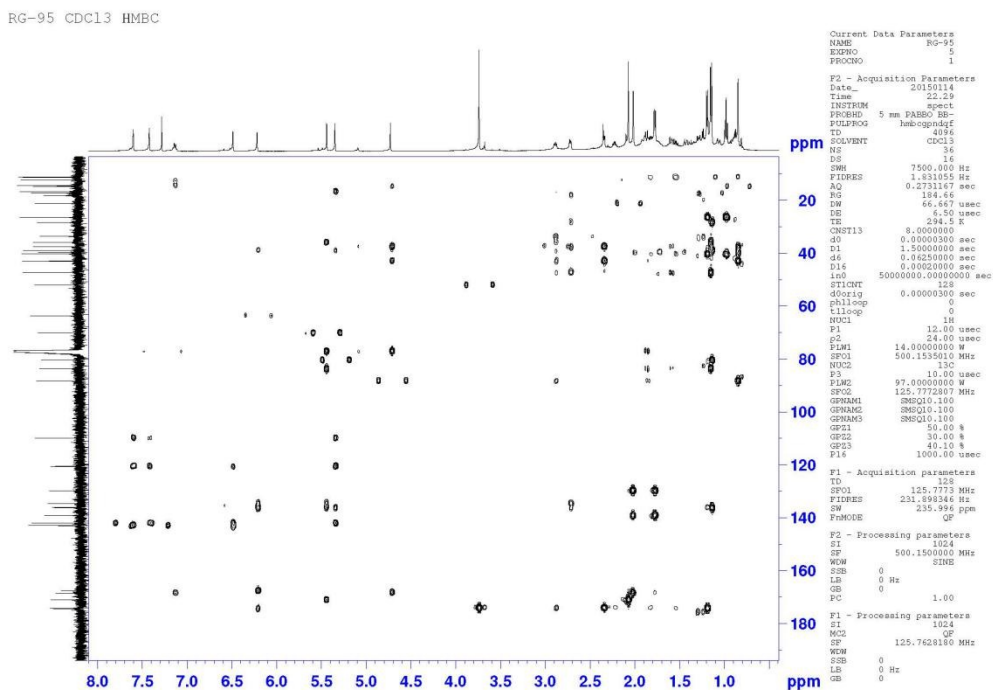
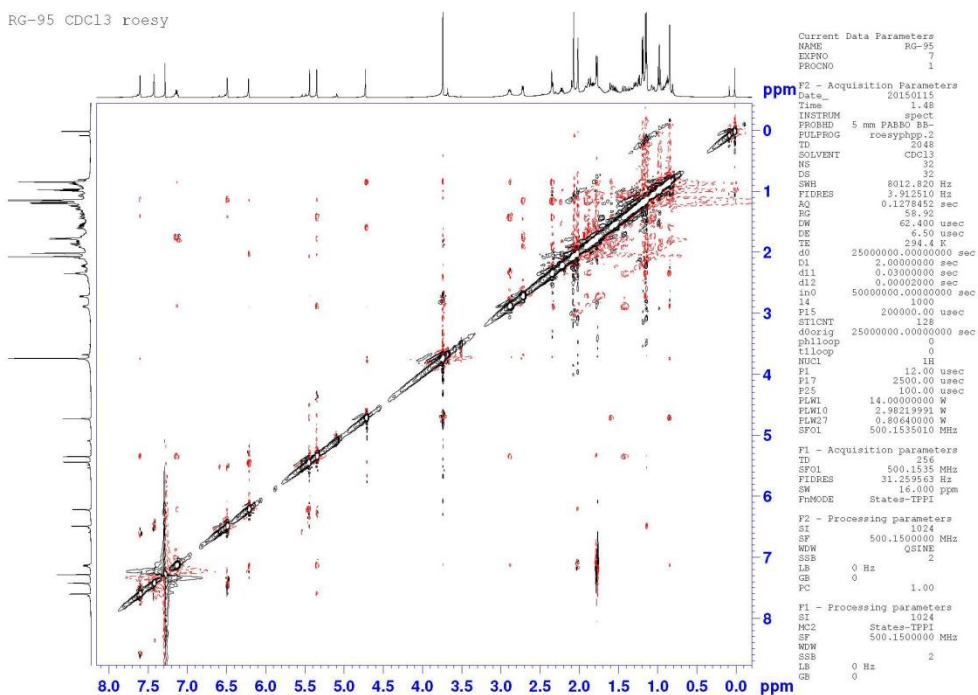


Figure S48. ROESY spectrum of compound 7 in CDCl₃

RG-95 CDC13 roesy



```

Current Data Parameters
NAME      RG-95
EXPERNO   7
PROCNO    1

F2 - Acquisition Parameters
Date_     20150115
Time      1.48
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   roesyppg.2
TD         2048
SOLVENT   CDC13
NS         32
DS         32
SMH       8012.820 Hz
FIDRES    3.912510 Hz
AQ         0.1276452 sec
RG         58.92
DW         62.400 usec
DE         6.50 usec
TE         294.4 K
d0         25000000.00000000 sec
d1         2.00000000 sec
d11        0.03000000 sec
d12        0.00002000 sec
in0        50000000.00000000 sec
I4         1500
P15        200000.00 usec
STICNT    128
d0orig    25000000.00000000 sec
p1loop    0
t1loop    0
NUC1      1H
P17        12.00 usec
P17        2500.00 usec
P25        100.00 usec
PLW1       14.00000000 W
PLW10      2.98219291 W
PLW27      0.80640000 W
SFOL       500.1535010 MHz

F1 - Acquisition parameters
TD         256
SFOL       500.1535 MHz
FIDRES    31.253663 Hz
SW         16.900 PPM
PnMODE    States-TPPI

F2 - Processing parameters
SI         1024
SF         500.1500000 MHz
WDW        QSINE
SSB        0
LB         0 Hz
GB         0
PC         1.00

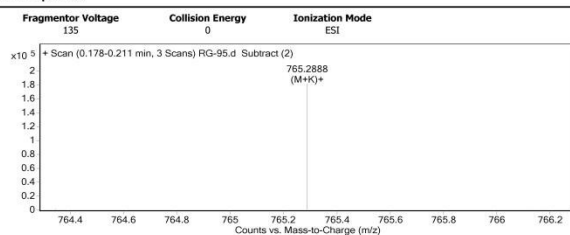
F1 - Processing parameters
SI         1024
MC2        States-TPPI
SF         500.1500000 MHz
WDW        QSINE
SSB        0
LB         0 Hz
GB         0
    
```

Figure S49. HRESI-MS spectrum of compound 7

Qualitative Analysis Report

Data Filename	RG-95.d	Sample Name	RG-95
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	8/27/2015 3:14:54 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
744.3593	1	105860.16		
745.3624	1	43446.01		
749.3148	1	88989.13		
750.318	1	35364.75		
765.2888	1	181052.48	C39 H50 O13	(M+K)+
766.2921	1	77883.64	C39 H50 O13	(M+K)+
767.2918	1	30469.57	C39 H50 O13	(M+K)+
772.3905	1	17044.38		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C39 H50 O13	726.3251	765.2883	765.2888	-0.5	-0.6	15.0000

--- End Of Report ---

Figure S50. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 9

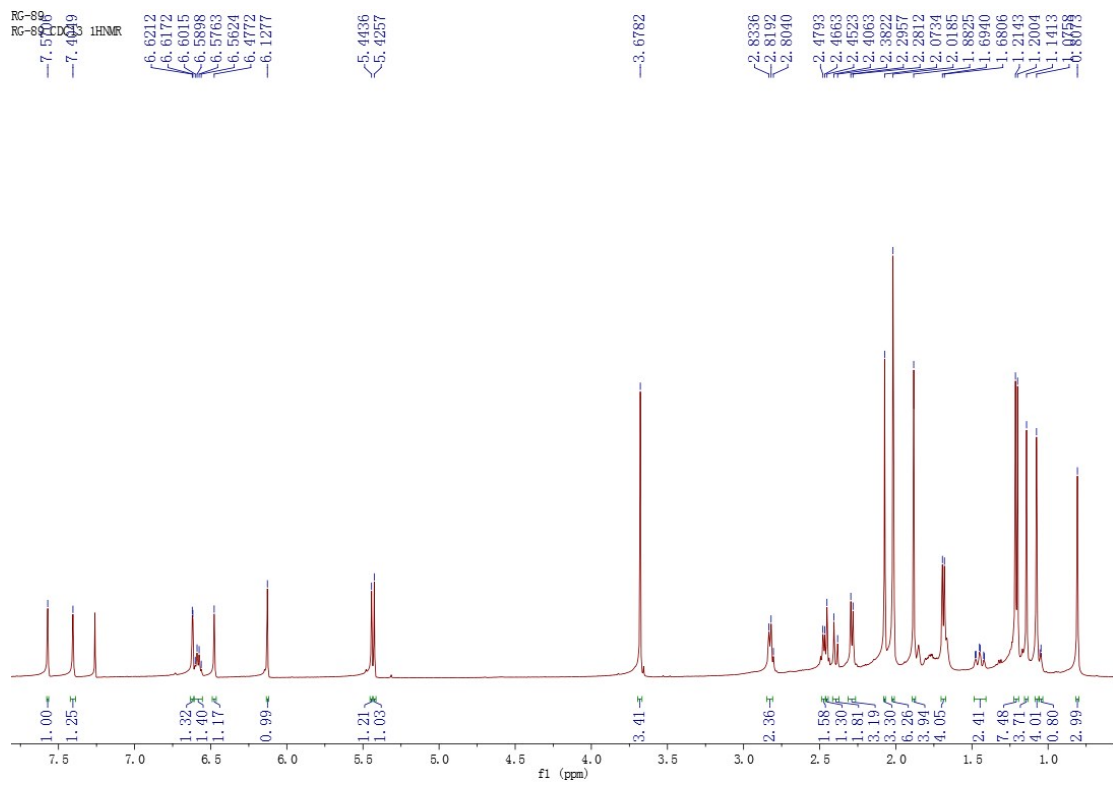


Figure S51. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **9**

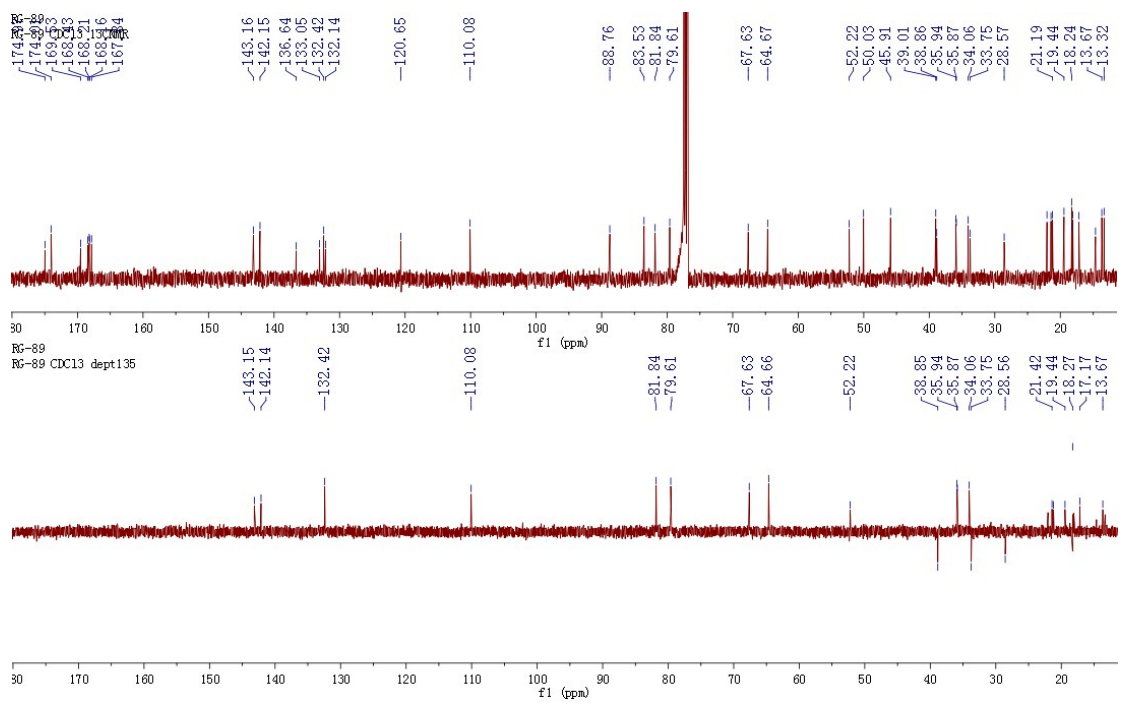


Figure S52. HSQC spectrum of compound **9** in CDCl₃

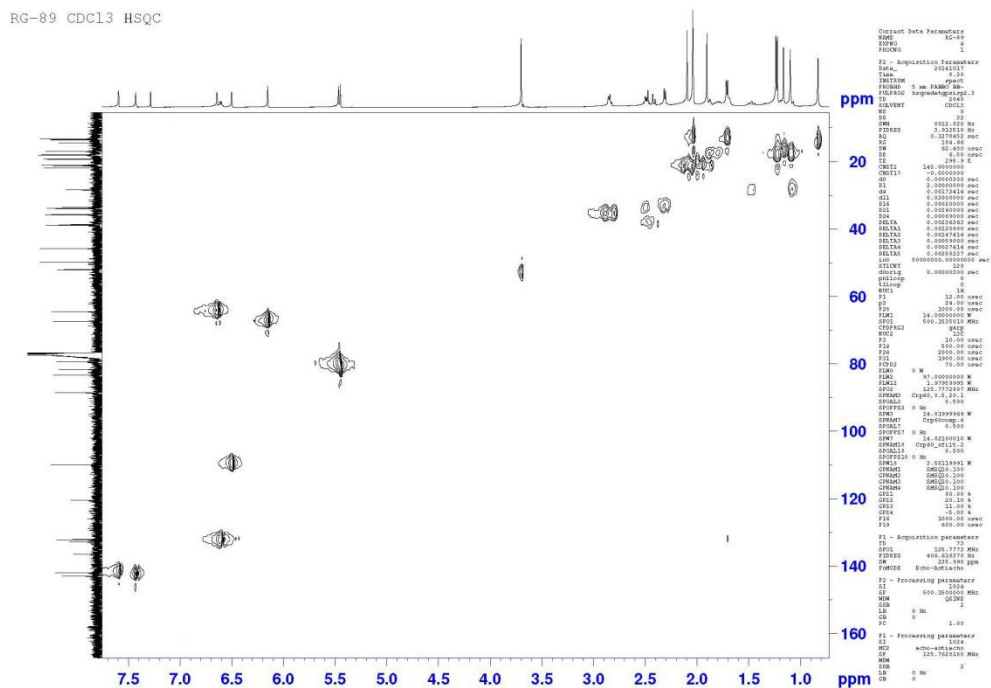


Figure S53. ¹H-¹H COSY spectrum of compound **9** in CDCl₃

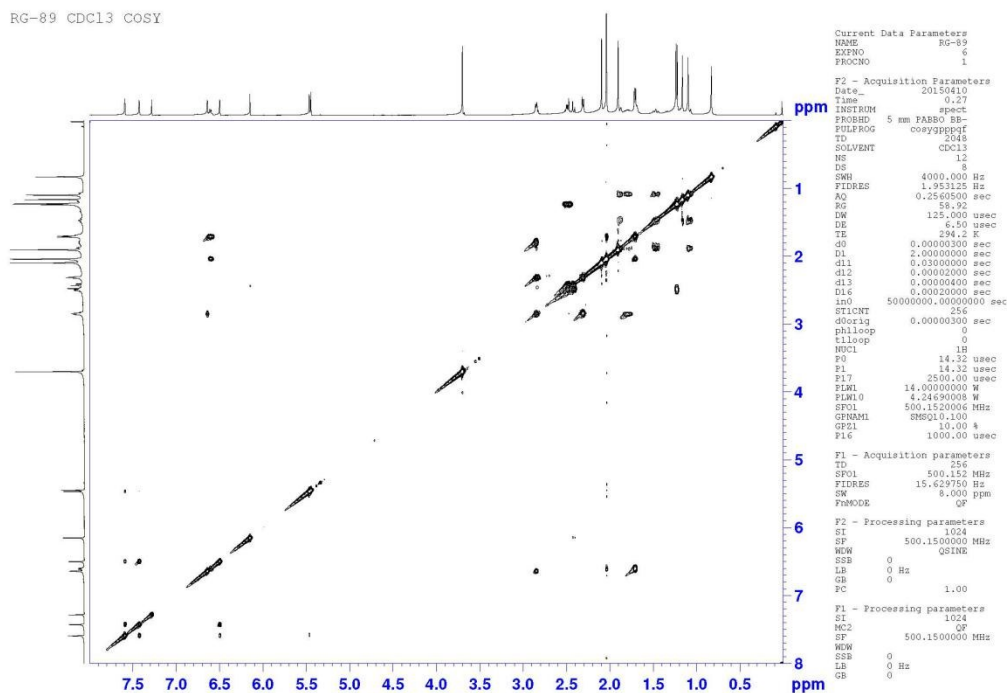


Figure S54. HMBC spectrum of compound **9** in CDCl₃

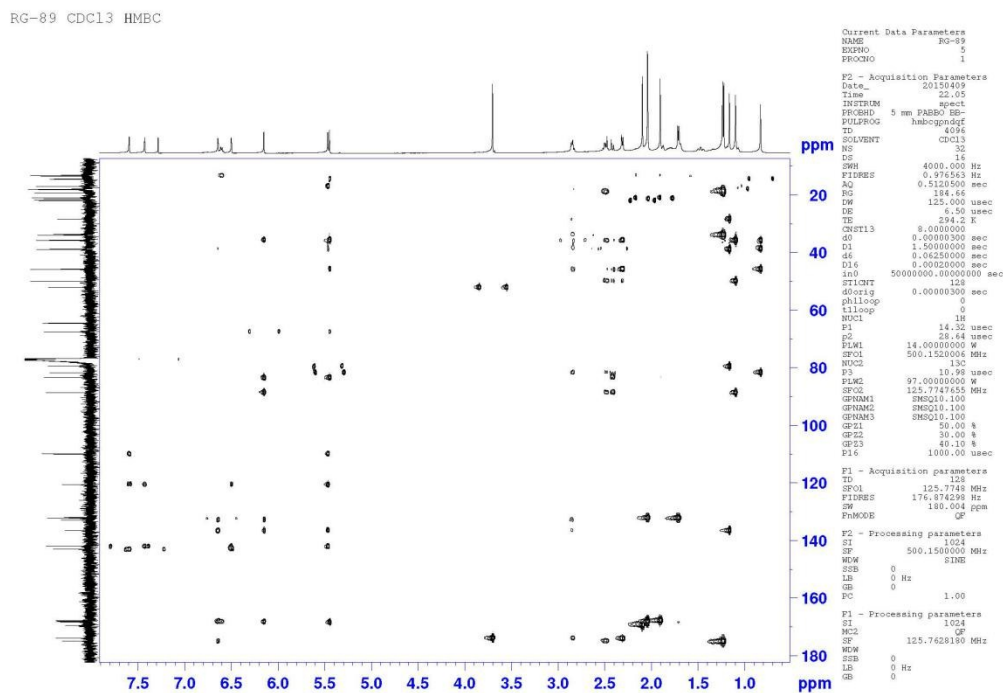


Figure S55. ROESY spectrum of compound **9** in CDCl₃

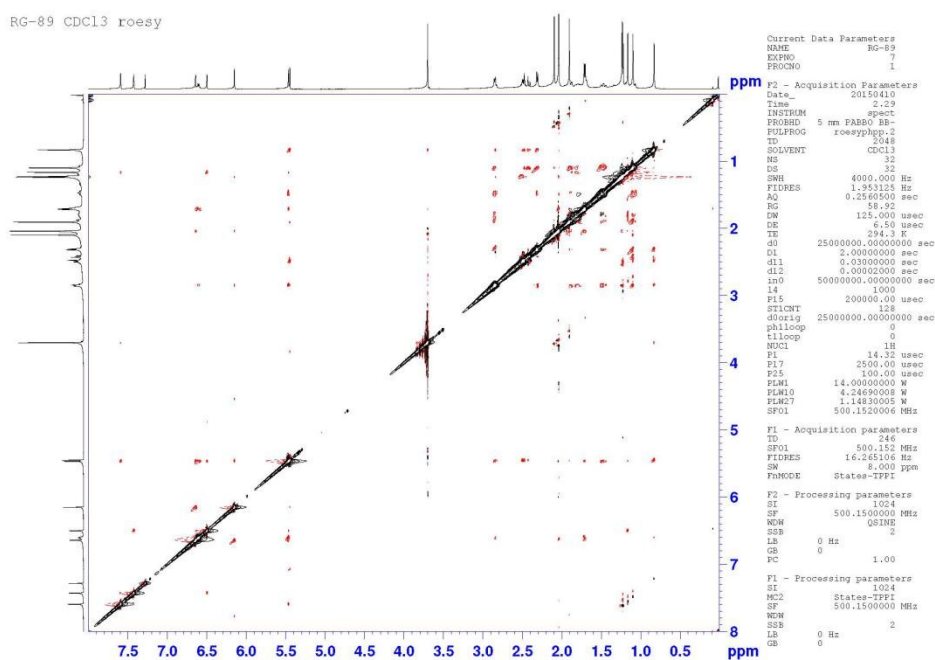


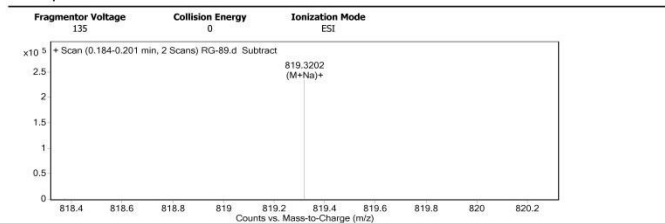
Figure S56. HRESI-MS spectrum of compound **9**

Qualitative Analysis Report

Data Filename	RG-89.d	Sample Name	RG-89
Sample Type	Sample	Position	P1-A8
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	8/27/2015 3:10:31 PM
IRM Calibration Status	Success	DA Method	Default.m

Sample Group: Info.
 Acquisition SW: 6200 series TOF/6500 series
 Version: Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
814.365	1	145966.16		
815.3679	1	63599.23		
819.3202	1	234960.58	C42 H52 O15	(M+Na)+
820.3235	1	105680.58	C42 H52 O15	(M+Na)+
821.3261	1	29166.88	C42 H52 O15	(M+Na)+
835.2941	1	199694.77		
836.2974	1	92325.59		
837.2975	1	37021.72		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C42 H52 O15	796.3306	819.3198	819.3202	-0.3	-0.4	17.0000

Figure S57. ¹H NMR (500 MHz, CDCl₃) spectrum of compound **10**

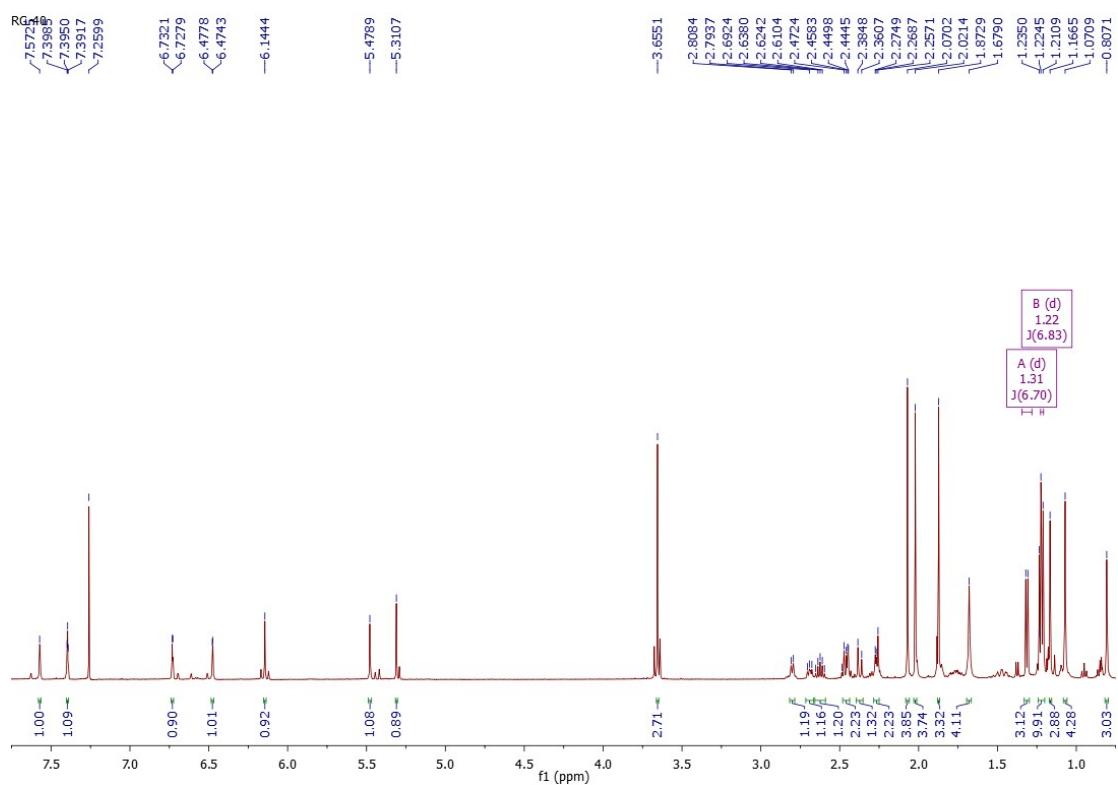


Figure S58. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **10**

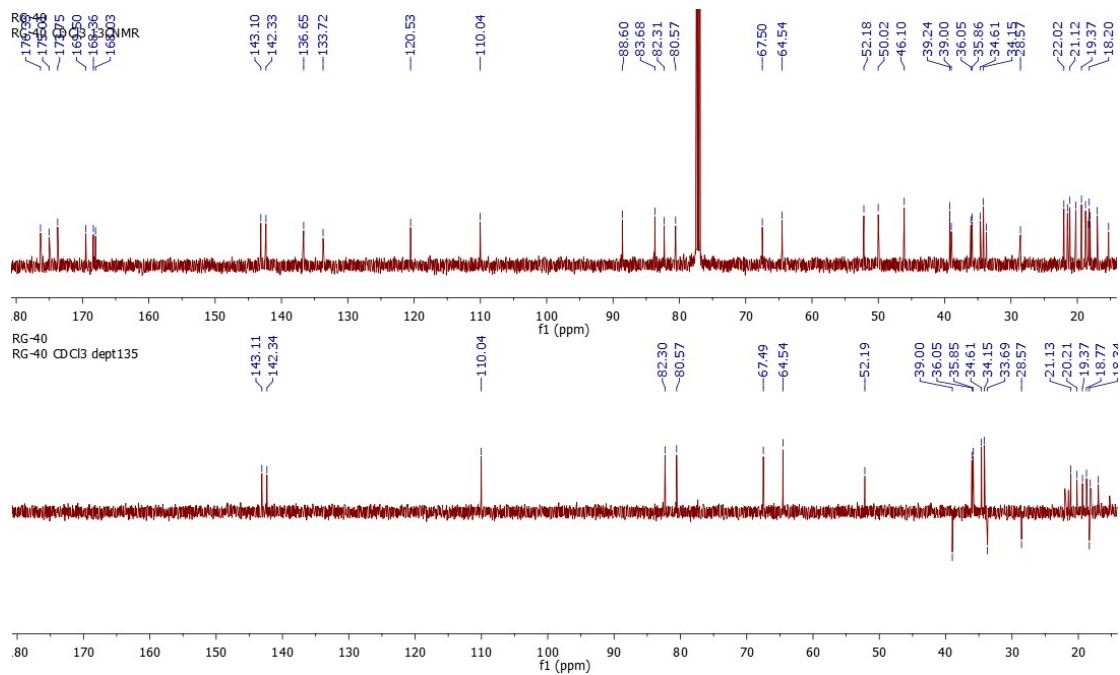


Figure S59. HSQC spectrum of compound **10** in $CDCl_3$

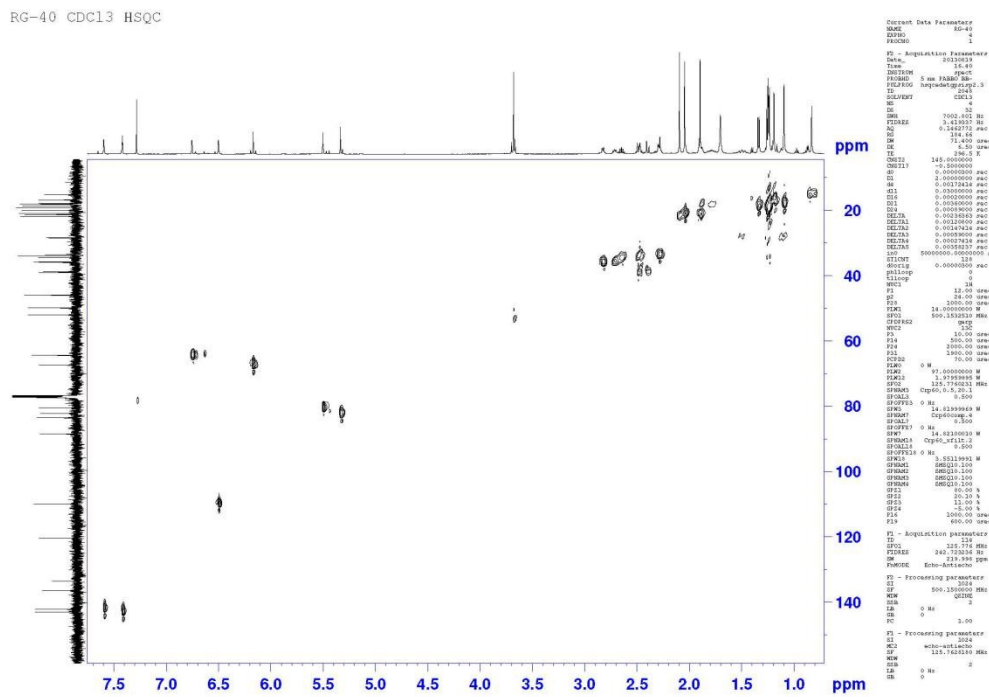


Figure S60. 1H - 1H COSY spectrum of compound **10** in $CDCl_3$

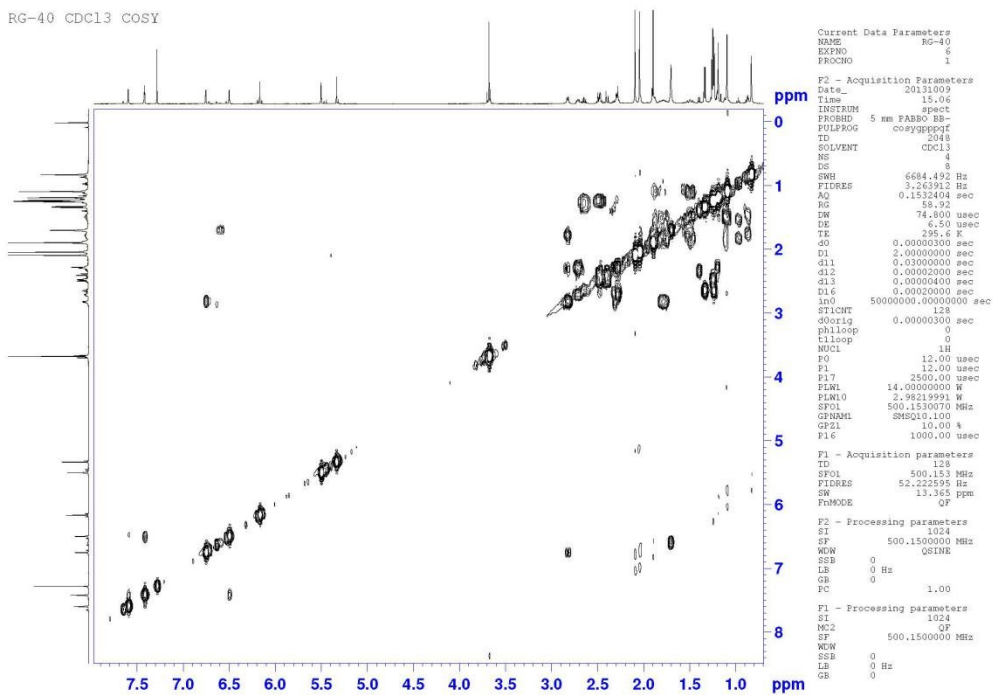


Figure S61. HMBC spectrum of compound **10** in CDCl₃

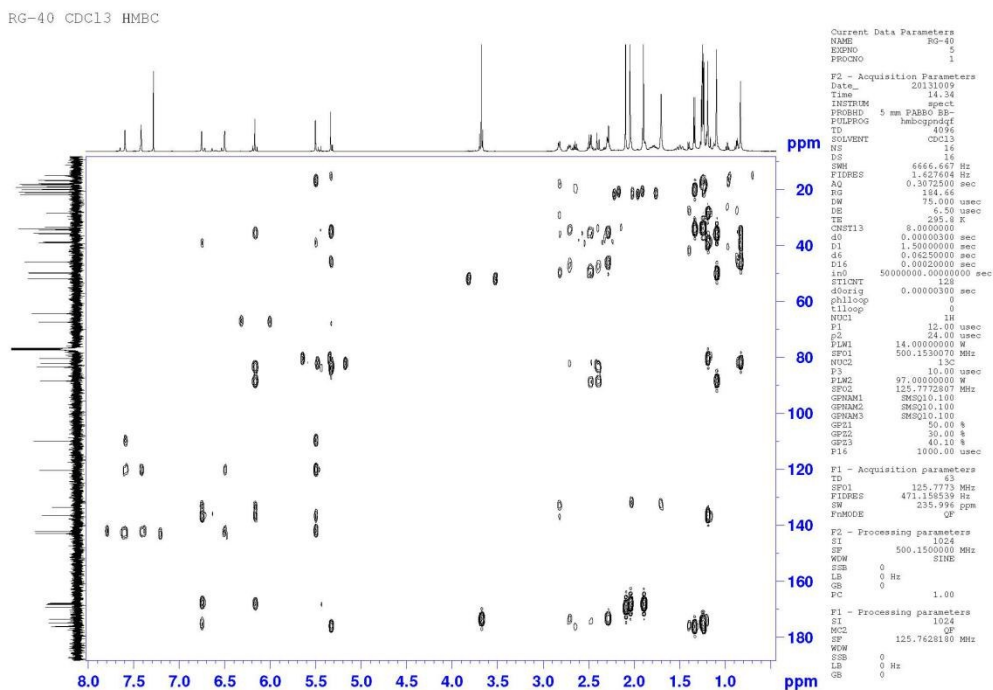


Figure S62. ROESY spectrum of compound **10** in CDCl₃

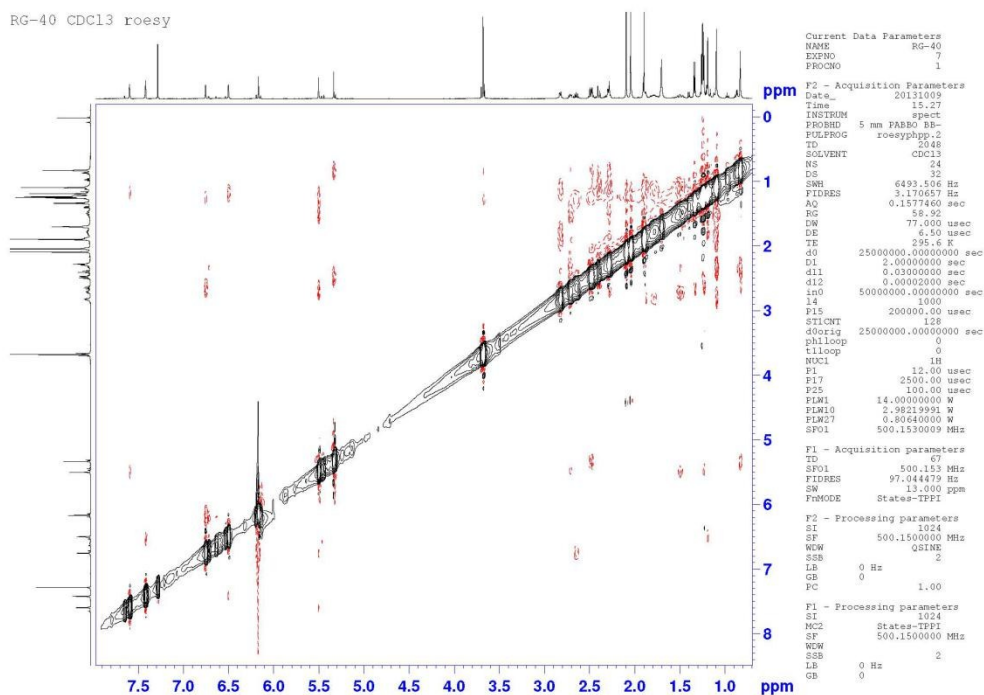


Figure S63. HRESI-MS spectrum of compound 10

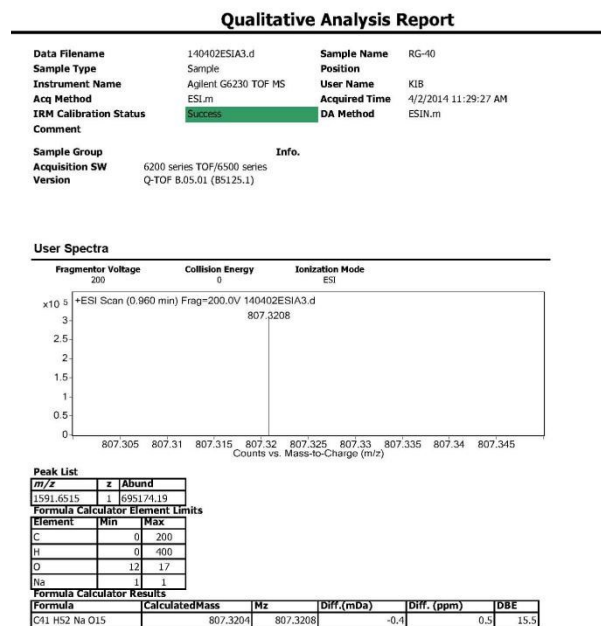


Figure S64. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 11

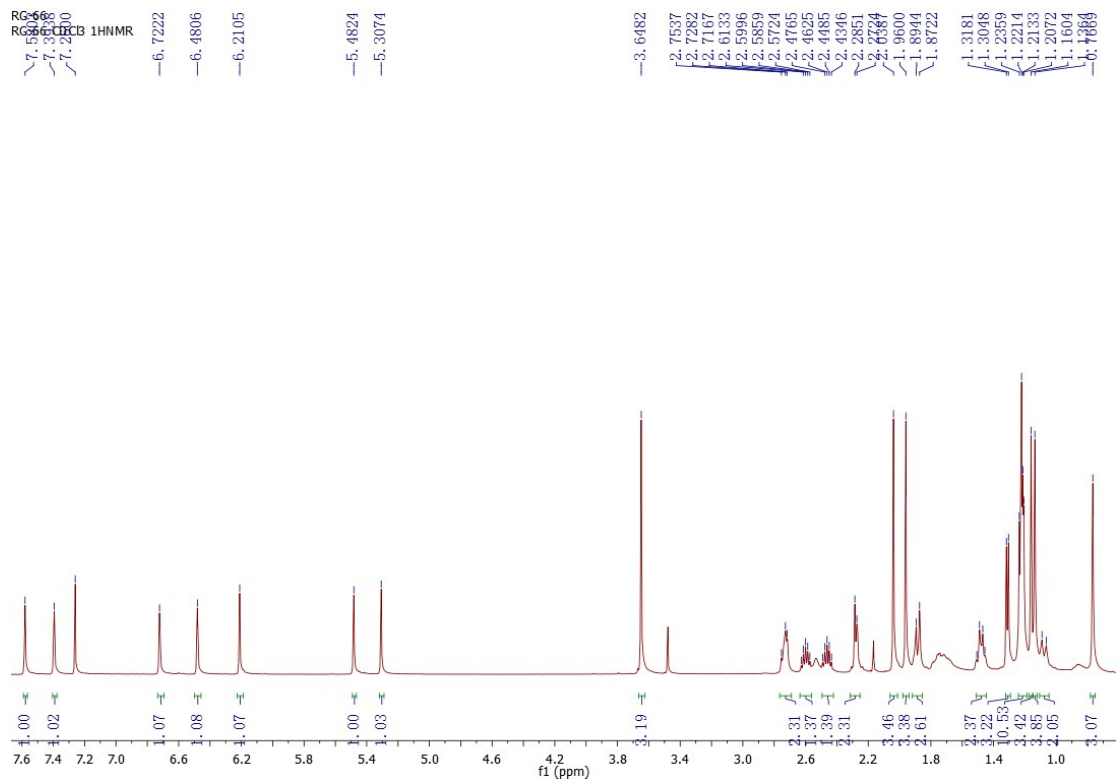


Figure S65. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **11**

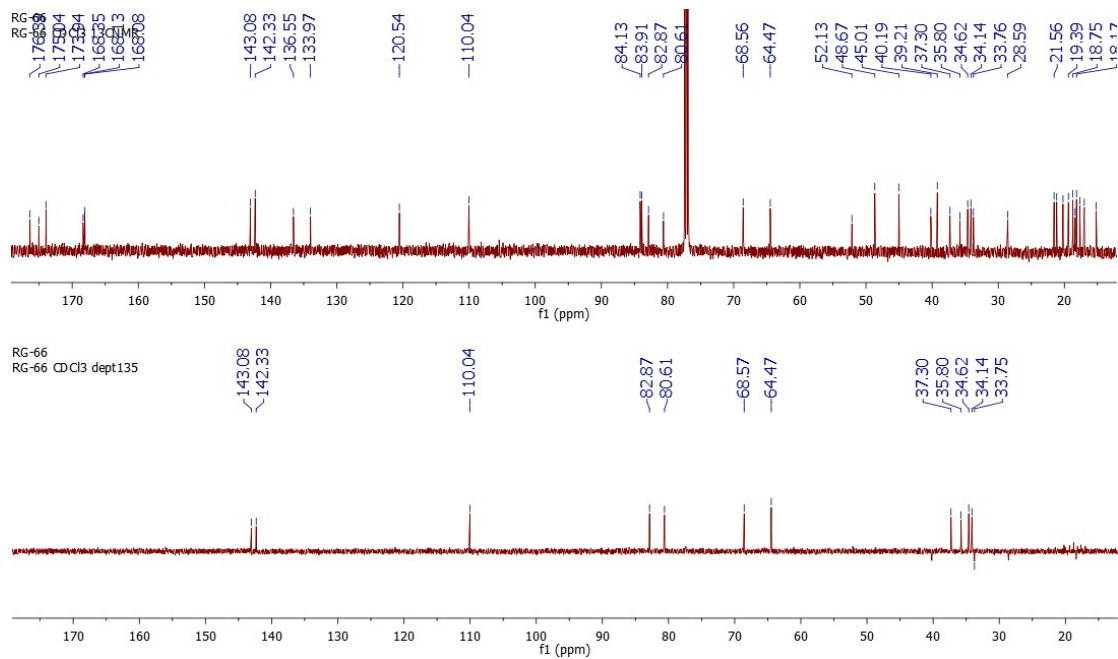


Figure S66. HSQC spectrum of compound **11** in CDCl₃

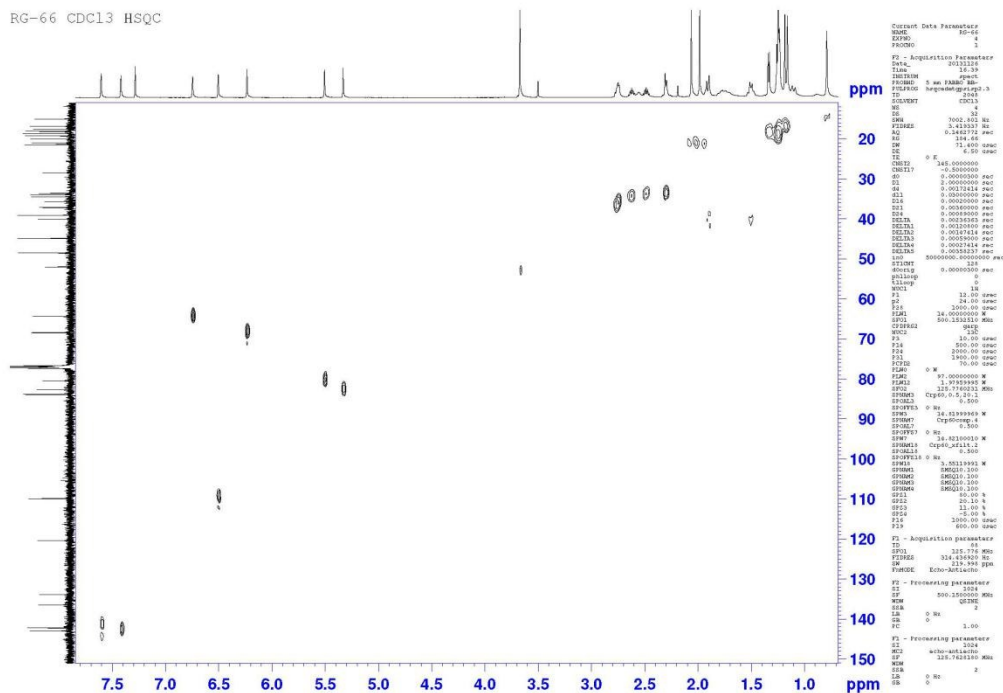


Figure S67. ¹H-¹H COSY spectrum of compound **11** in CDCl₃

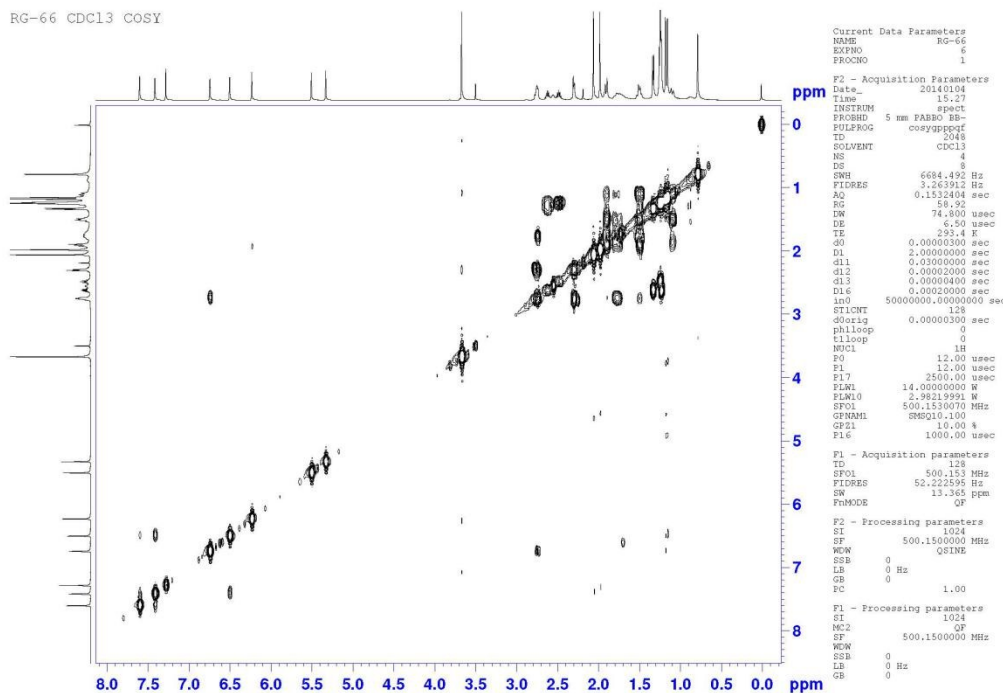


Figure S68. HMBC spectrum of compound **11** in CDCl₃

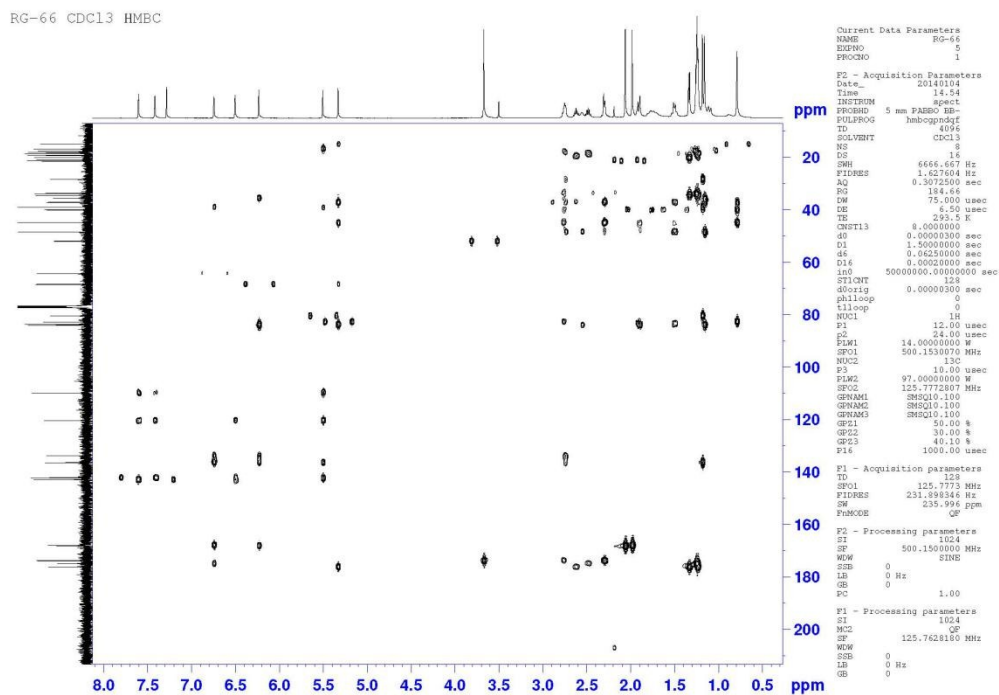


Figure S69. ROESY spectrum of compound **11** in CDCl₃

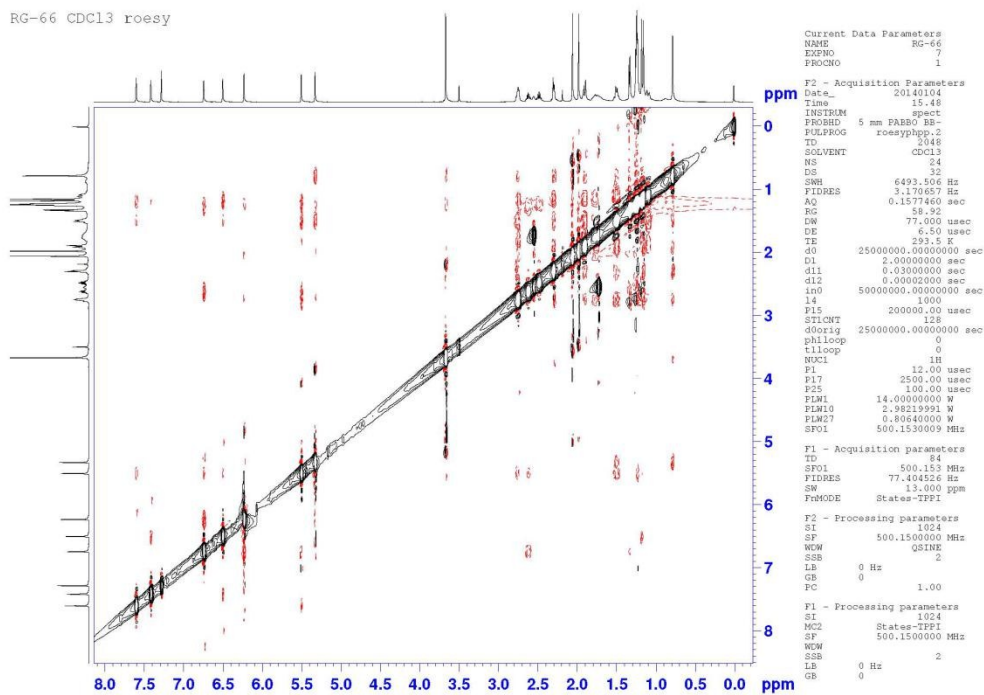


Figure S70. HRESI-MS spectrum of compound 11

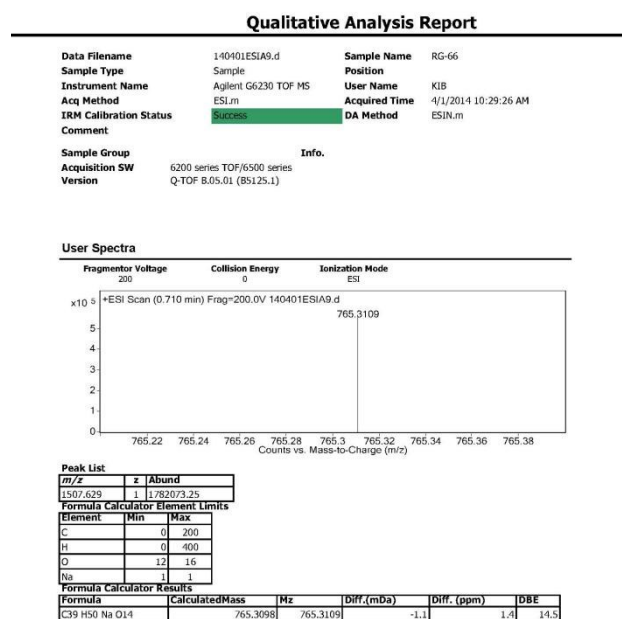


Figure S71. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 12

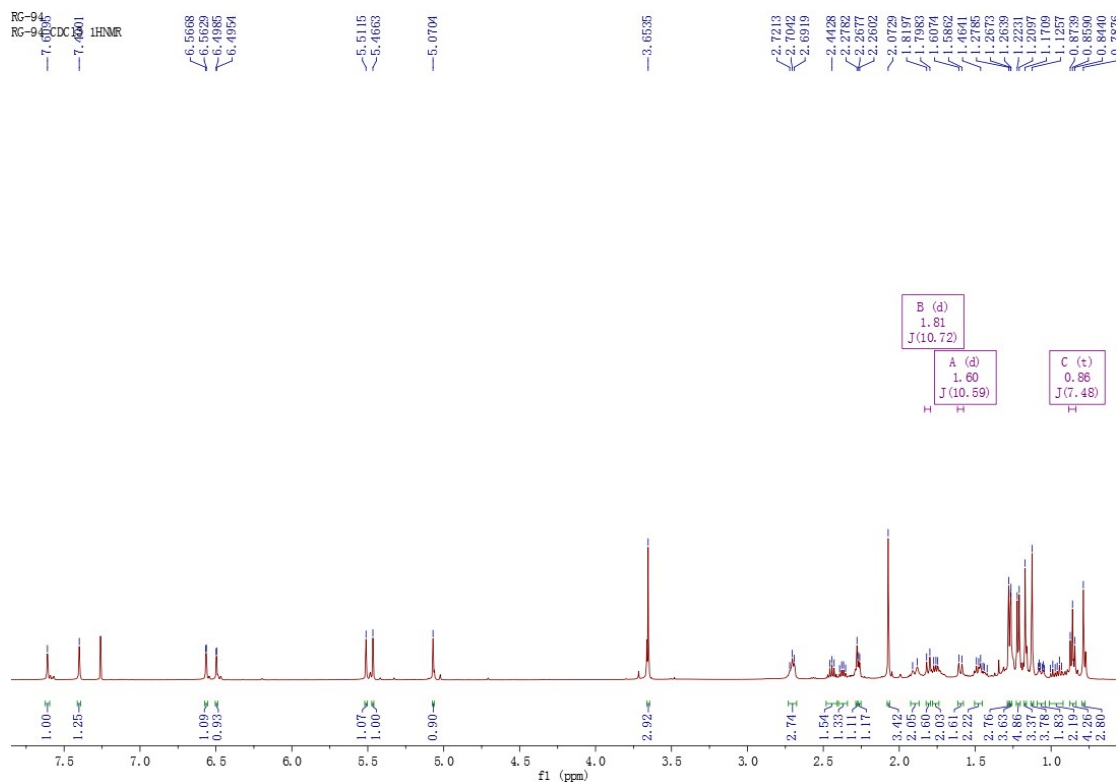


Figure S72. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 12

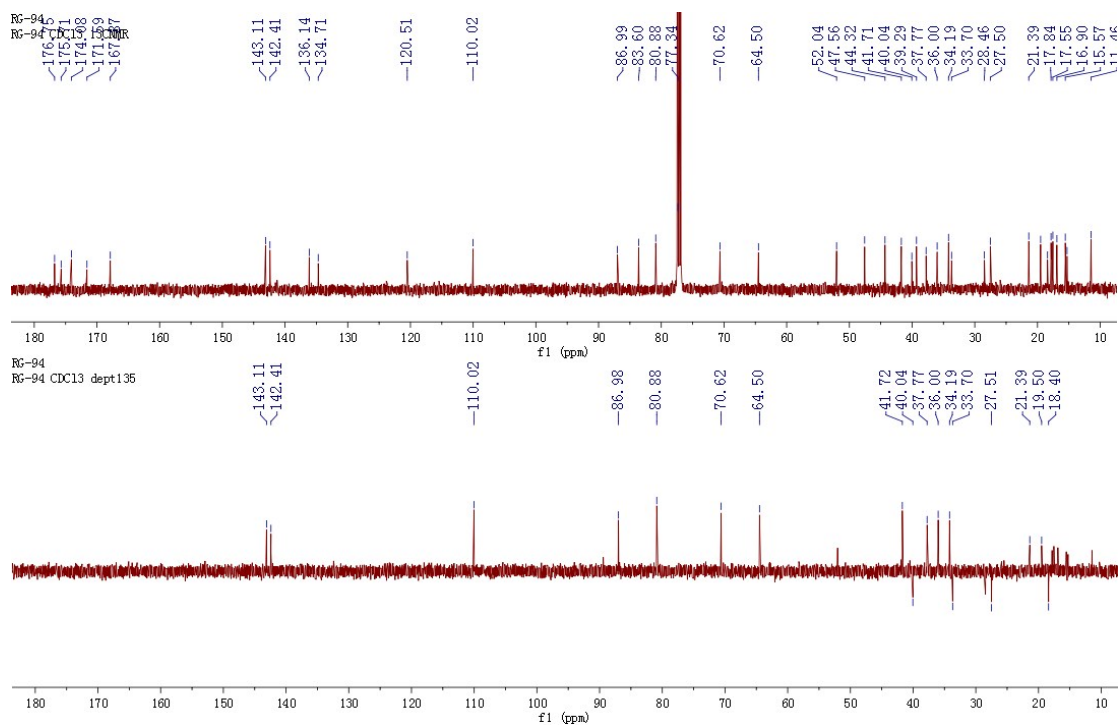


Figure S73. HSQC spectrum of compound 12 in CDCl_3

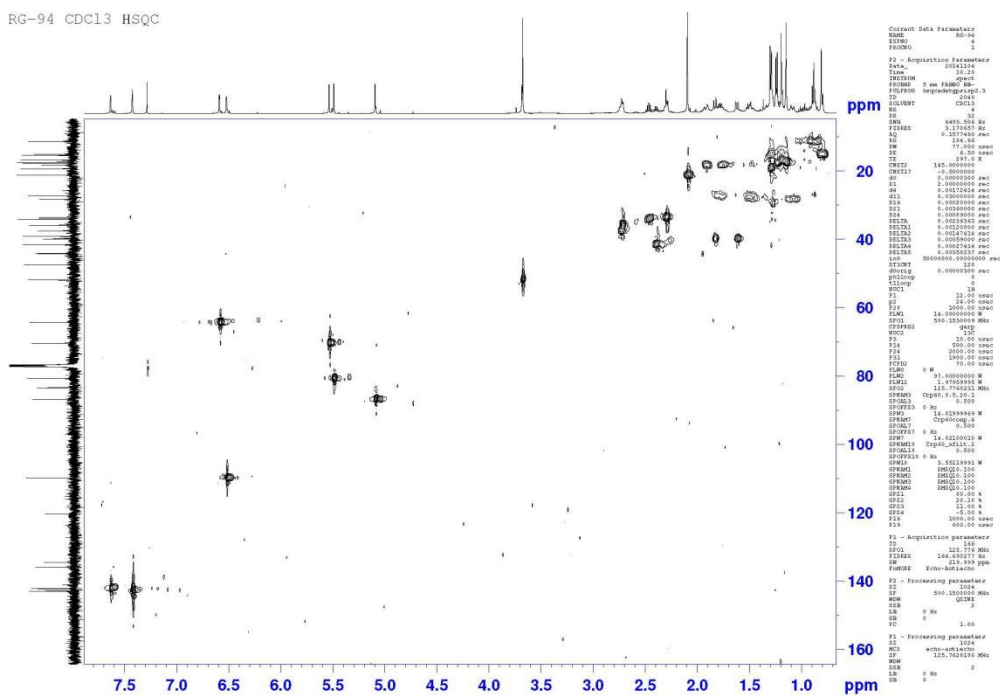


Figure S74. ^1H - ^1H COSY spectrum of compound 12 in CDCl_3

RG-94 CDC13 COSY

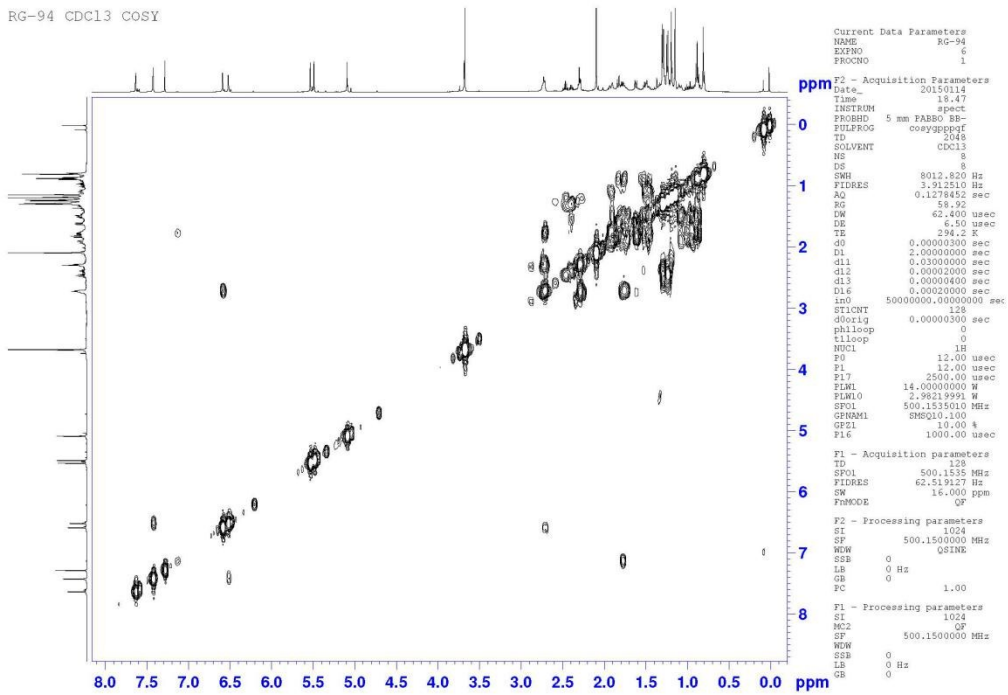


Figure S75. HMBC spectrum of compound 12 in CDCl₃

RG-94 CDC13 HMBC

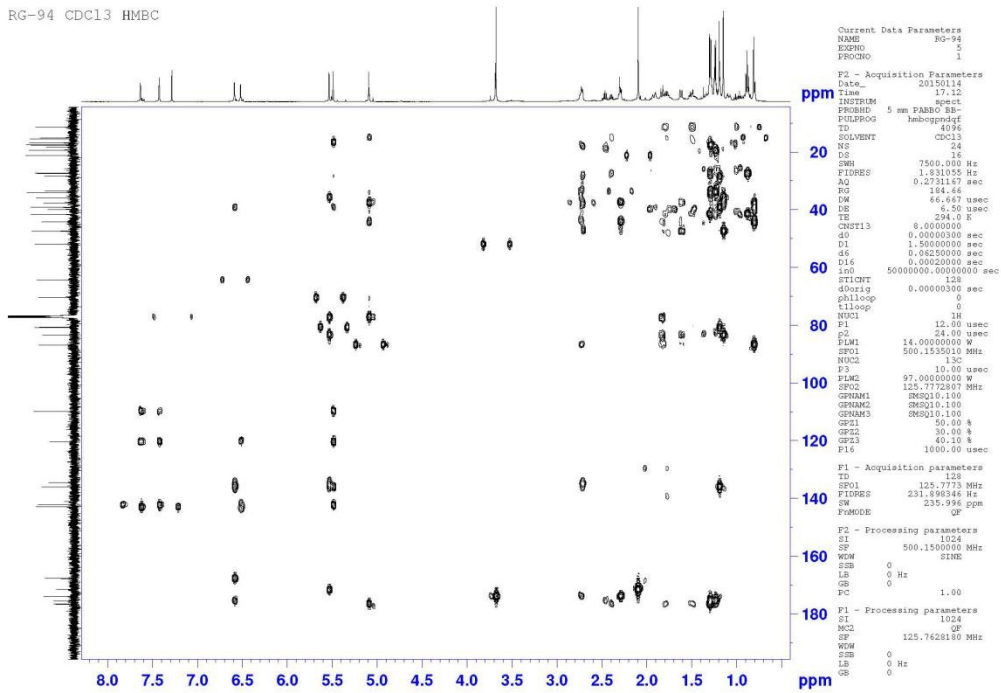
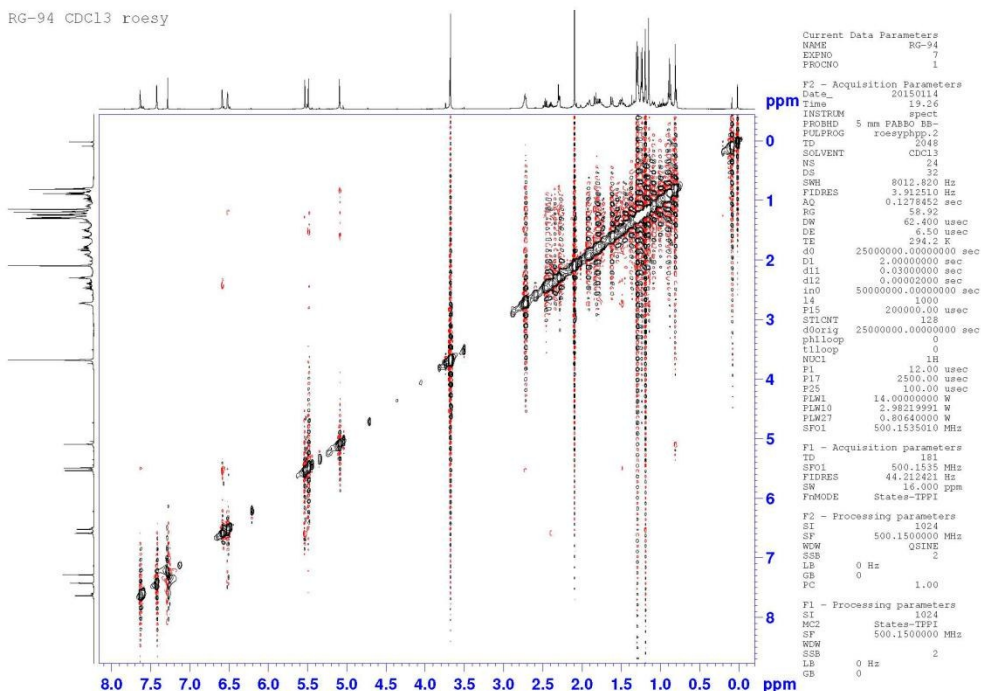


Figure S76. ROESY spectrum of compound 12 in CDCl₃

RG-94 CDC13 roesy



```

Current Data Parameters
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EXPNO    7
PROCNO   1

F2 - Acquisition Parameters
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Time     15:26
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PROBHD   5 mm F400 BB-
PULPROG  roesypph2
TD        2048
SOLVENT  CDCl3
NS        24
DS        32
SWH       8012.820 Hz
FIDRES    3.912510 Hz
AQ        0.1278452 sec
RG        58.92
DW        62.400 usec
DE        6.50 usec
TE        294.2 K
d0        25000000.00000000 sec
D1        2.00000000 sec
d11       0.03000000 sec
d12       0.00020000 sec
in0       50000000.00000000 sec
I4        1000
F15       200000.00 usec
STICHT    128
dloopip  25000000.00000000 sec
philoop   0
tilloop   0
MAGIC     1B
P1         12.00 usec
P17       2500.00 usec
F25       100.00 usec
PLM1      14.00000000 W
PLM0      2.38219921 W
PLM27     0.80640000 W
SFO1      500.1535010 MHz

F1 - Acquisition parameters
TD         181
SFO1      500.1535 MHz
FIDRES    44.212423 Hz
SW        16.008 ppm
FRMODE    States-TPPI

F2 - Processing parameters
SI         1024
SF        500.1500000 MHz
WDM       QSINE
SSB       2
LB         0 Hz
GB         0
PC         1.00

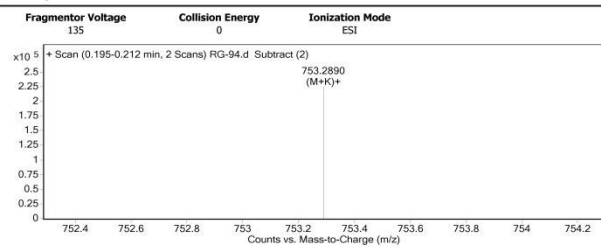
F1 - Processing parameters
SI         1024
MCC       States-TPPI
SF        500.1500000 MHz
WDM       QSINE
SSB       2
LB         0 Hz
GB         0
    
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Figure S77. HRESI-MS spectrum of compound 12

Qualitative Analysis Report

Data Filename	RG-94.d	Sample Name	RG-94
Sample Type	Sample	Position	P1-B1
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	8/27/2015 3:13:26 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List	m/z	z	Abund	Formula	Ion
	732.3595	1	161274.03		
	733.3625	1	64639.16		
	737.3148	1	124471.61		
	738.3182	1	47153.57		
	753.289	1	225409.59	C38 H50 O13	(M+K)+
	754.292	1	94869.48	C38 H50 O13	(M+K)+
	755.2919	1	35233.45	C38 H50 O13	(M+K)+
	760.3903	1	29949.78		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mBa)	Diff. (ppm)	DBE
C38 H50 O13	714.3251	753.2883	753.2890	-0.6	-0.8	14.0000

Figure S78. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 13

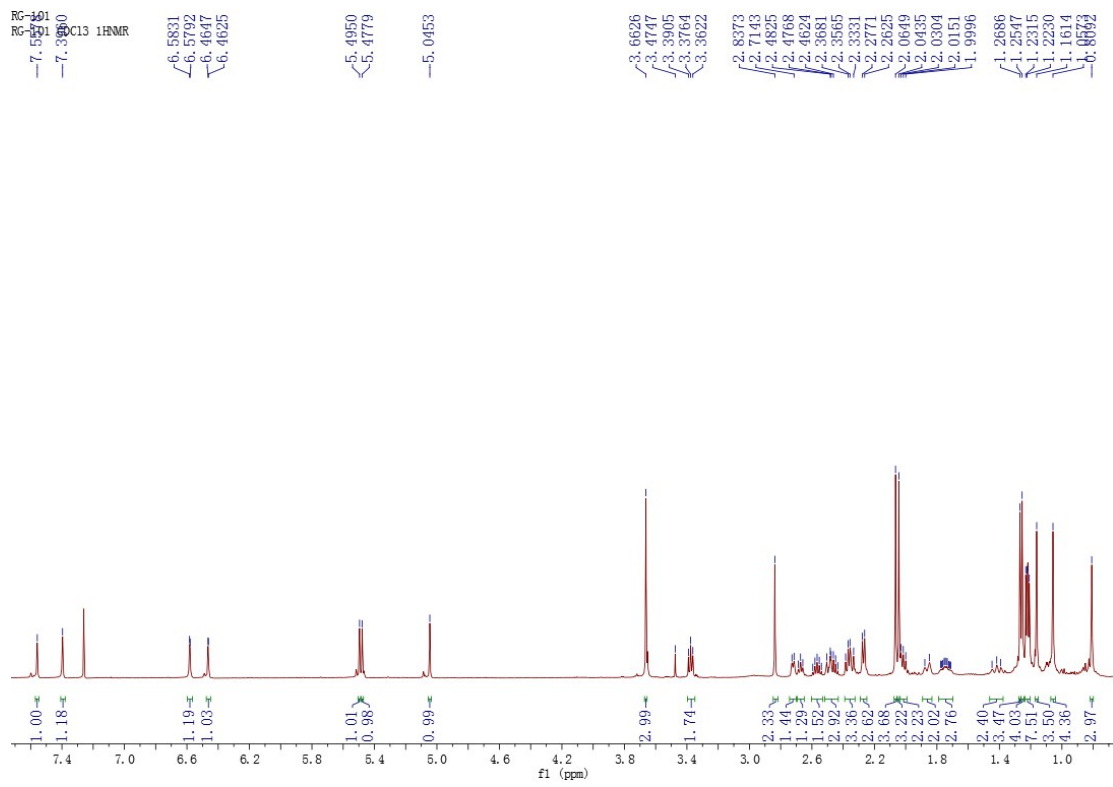


Figure S79. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **13**

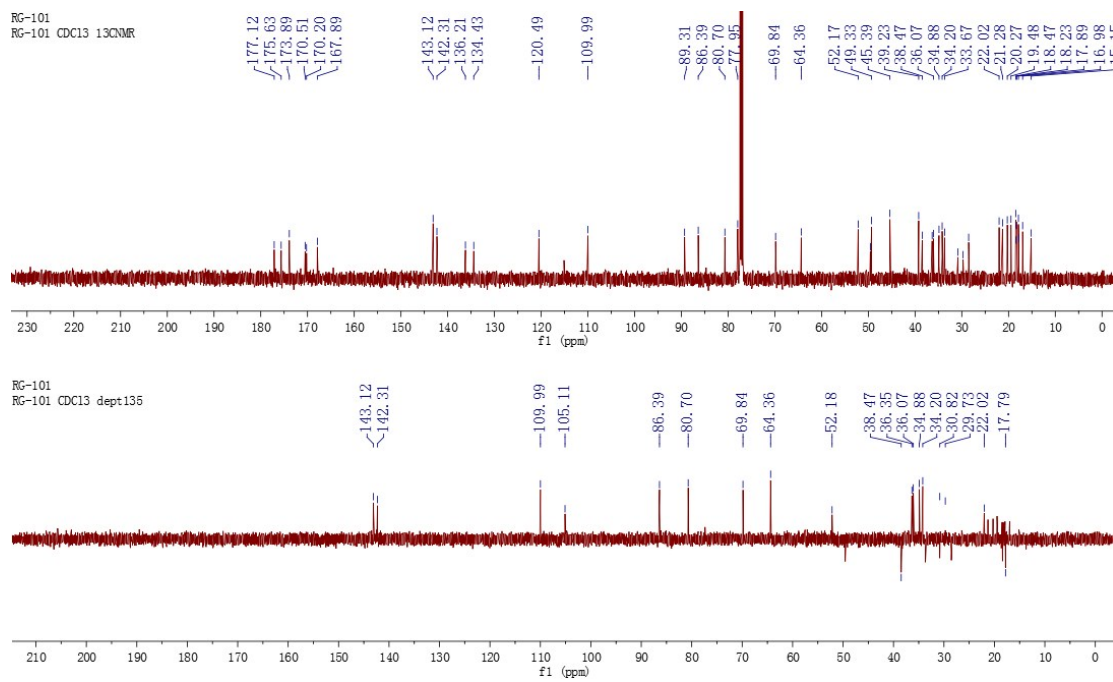


Figure S80. HSQC spectrum of compound **13** in CDCl₃

RG-101 CDCl3 HSQC

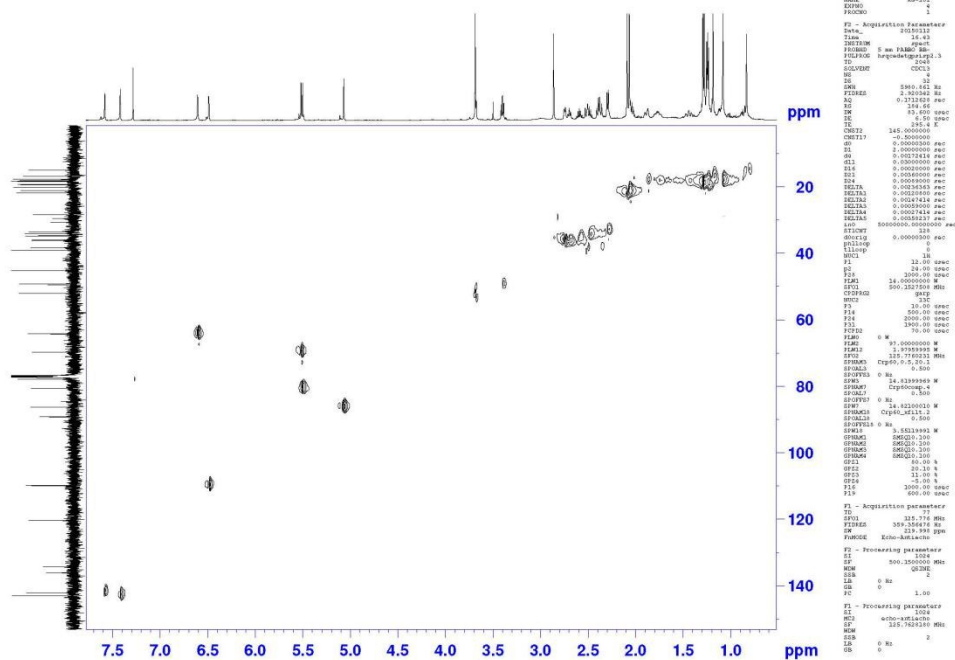


Figure S81. ^1H - ^1H COSY spectrum of compound **13** in CDCl_3

RG-101 CDCl3 COSY

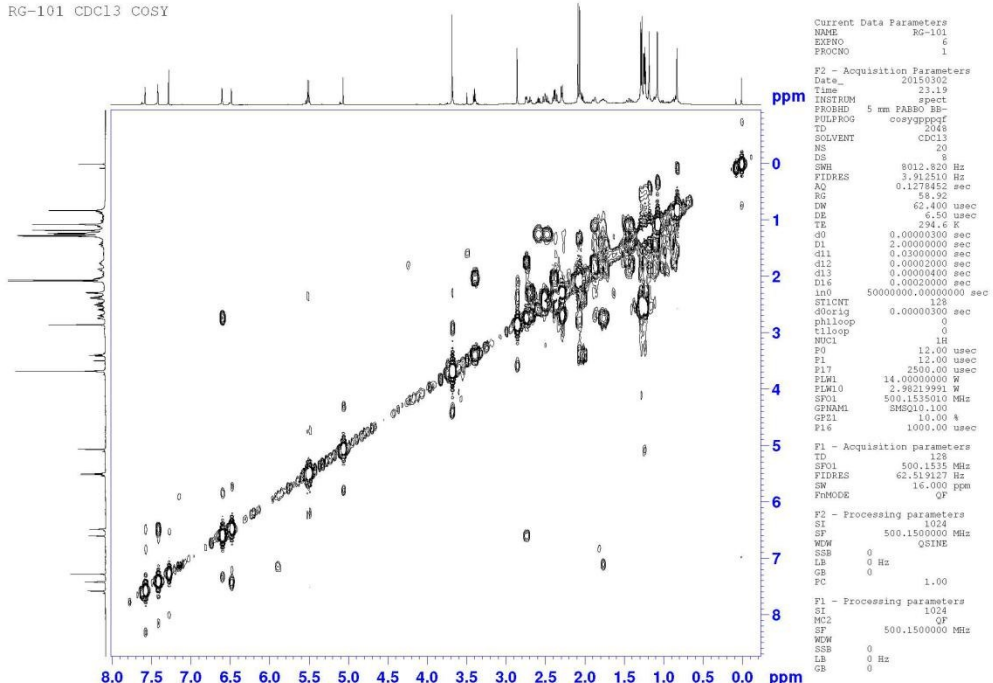


Figure S82. HMBC spectrum of compound **13** in CDCl_3

RG-101 CDCl3 HMBC

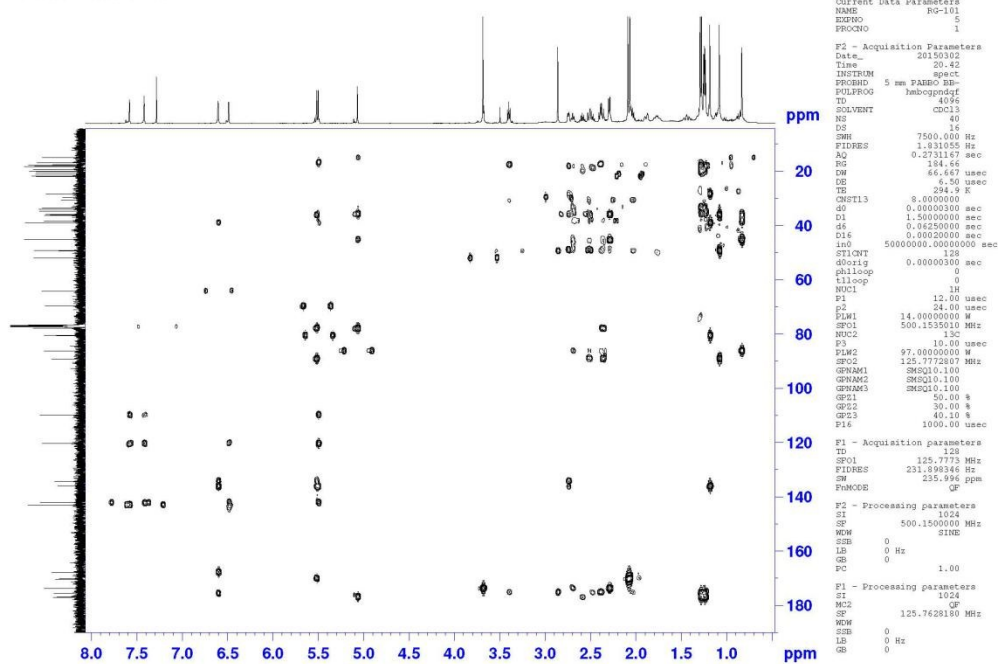


Figure S83. ROESY spectrum of compound 13 in CDCl₃

RG-101 CDCl3 roesy

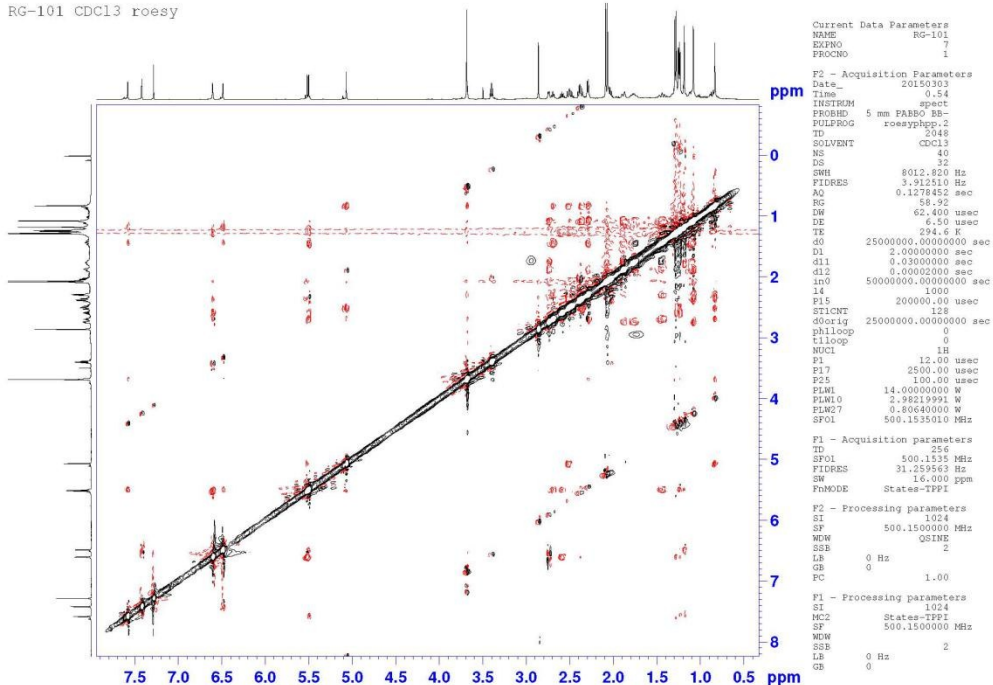


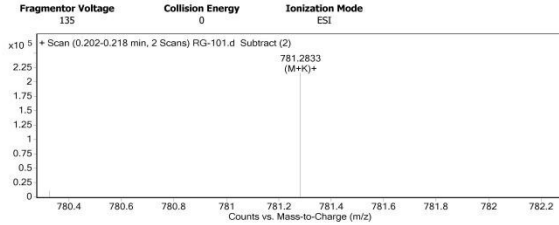
Figure S84. HRESI-MS spectrum of compound 13

Qualitative Analysis Report

Data Filename	RG-101.d	Sample Name	RG-101
Sample Type	Sample	Position	P1-B4
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	8/27/2015 3:17:48 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.2)	

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
760.3542	1	185482.25		
761.3571	1	75008.16		
765.3091	1	144866.84		
766.3125	1	58542.14		
781.2833	1	215877.2	C39 H50 O14	(M+K)+
782.2867	1	90177.84	C39 H50 O14	(M+K)+
783.2864	1	38459.95	C39 H50 O14	(M+K)+
788.3852	1	39626.17		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C39 H50 O14	742.3201	781.2832	781.2833	-0.1	-0.1	15.0000

Figure S85. ¹H NMR (500 MHz, CDCl₃) spectrum of compound **14**

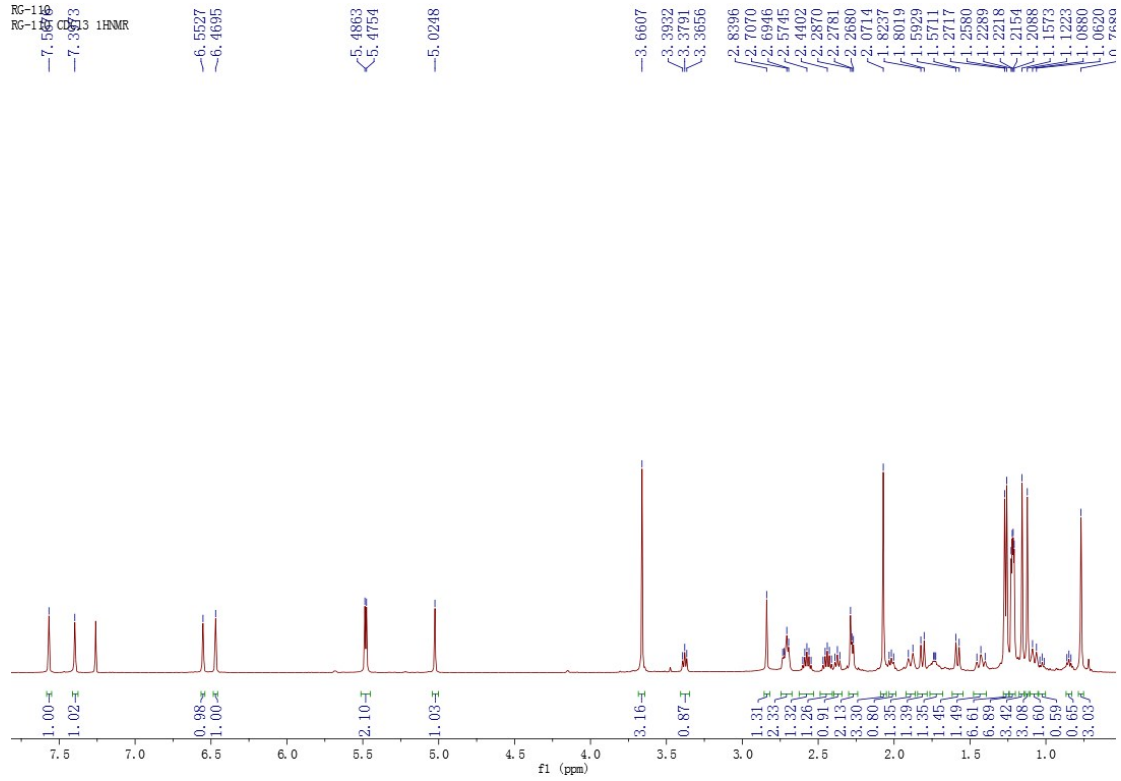


Figure S86. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound **14**

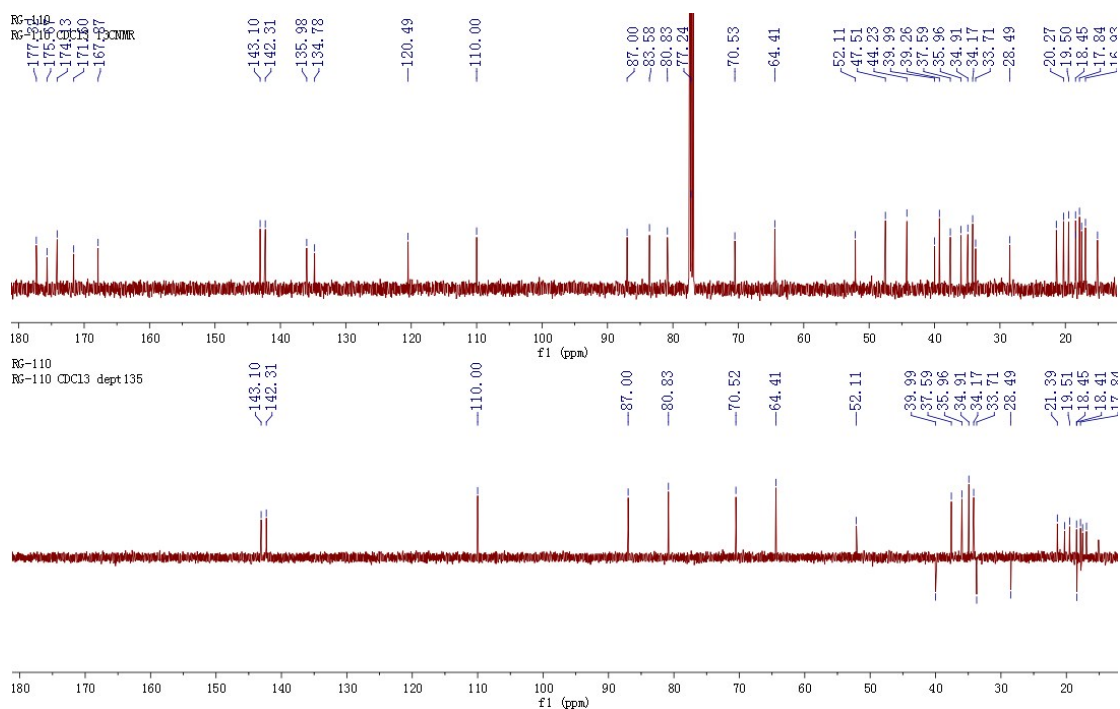


Figure S87. HSQC spectrum of compound **14** in CDCl₃

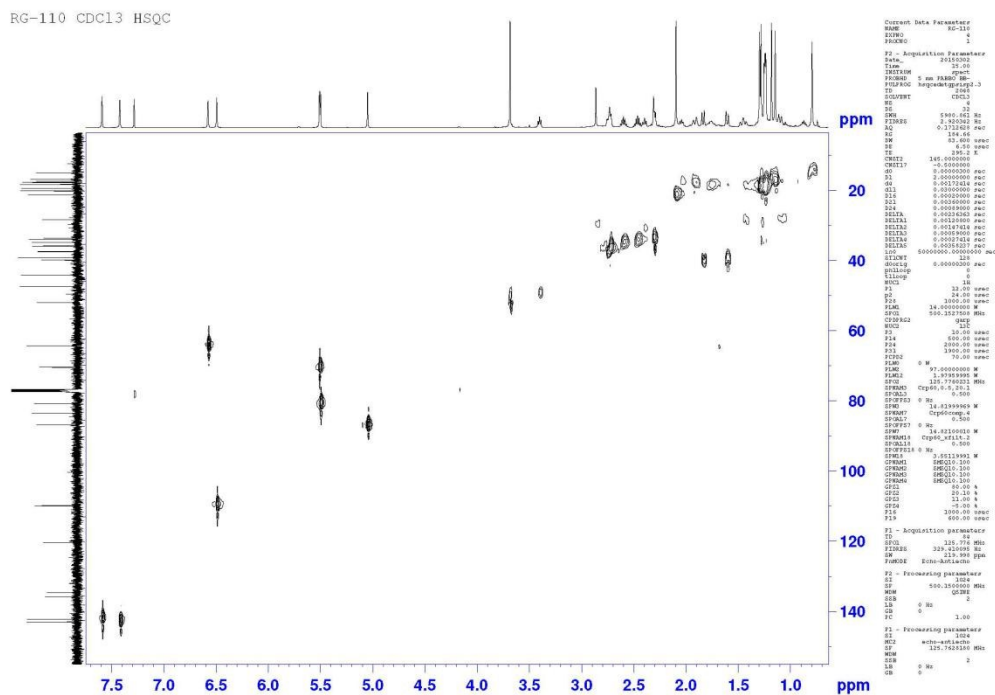


Figure S88. ^1H - ^1H COSY spectrum of compound **14** in CDCl_3

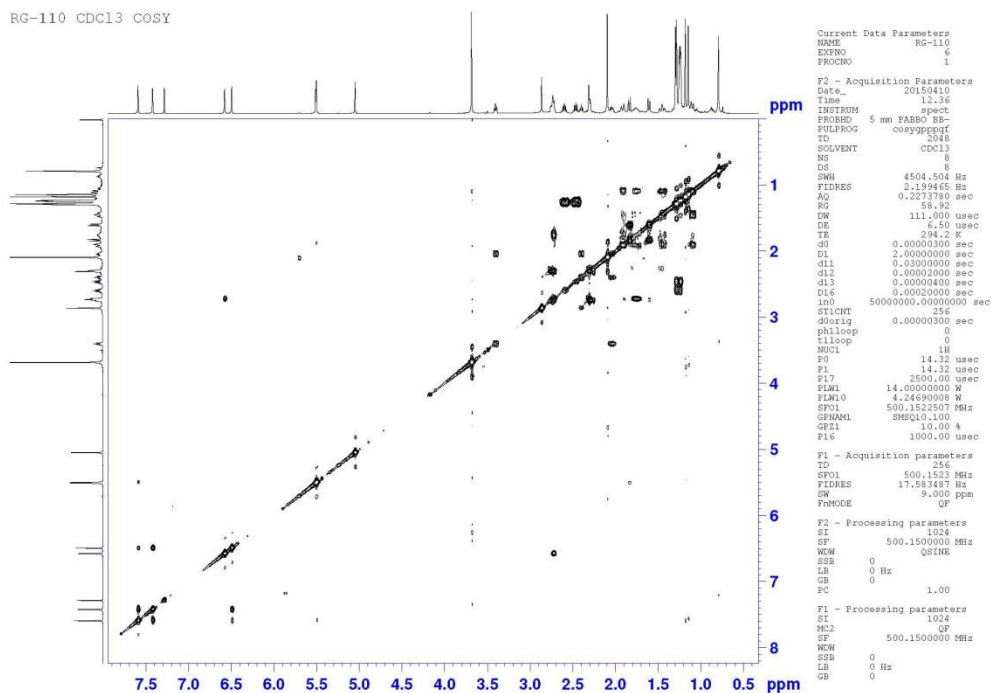


Figure S89. HMBC spectrum of compound **14** in CDCl_3

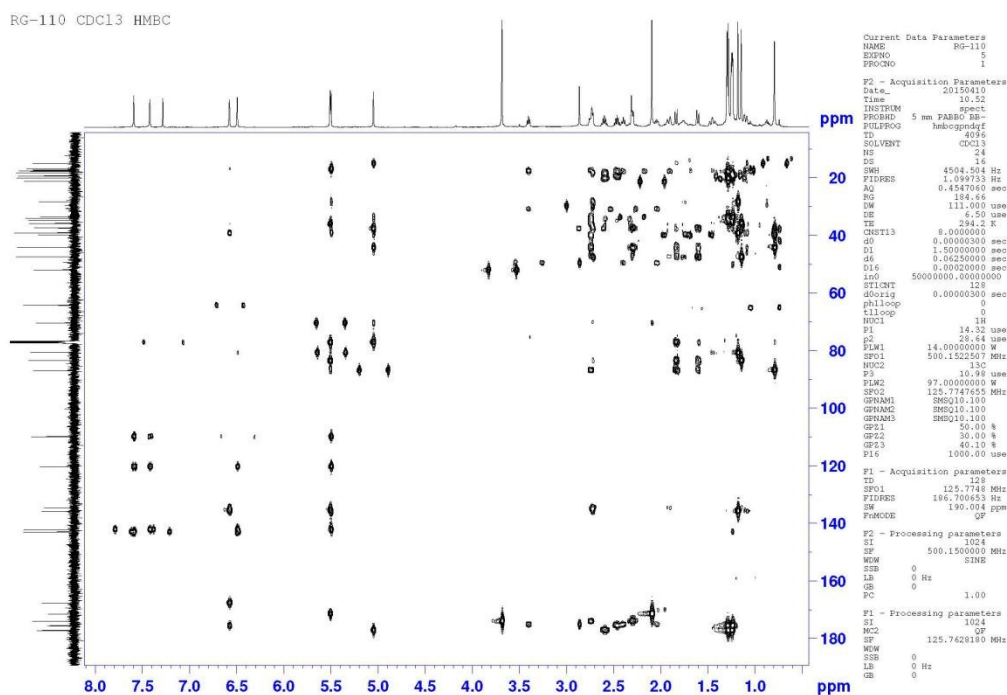


Figure S90. ROESY spectrum of compound 14 in CDCl₃

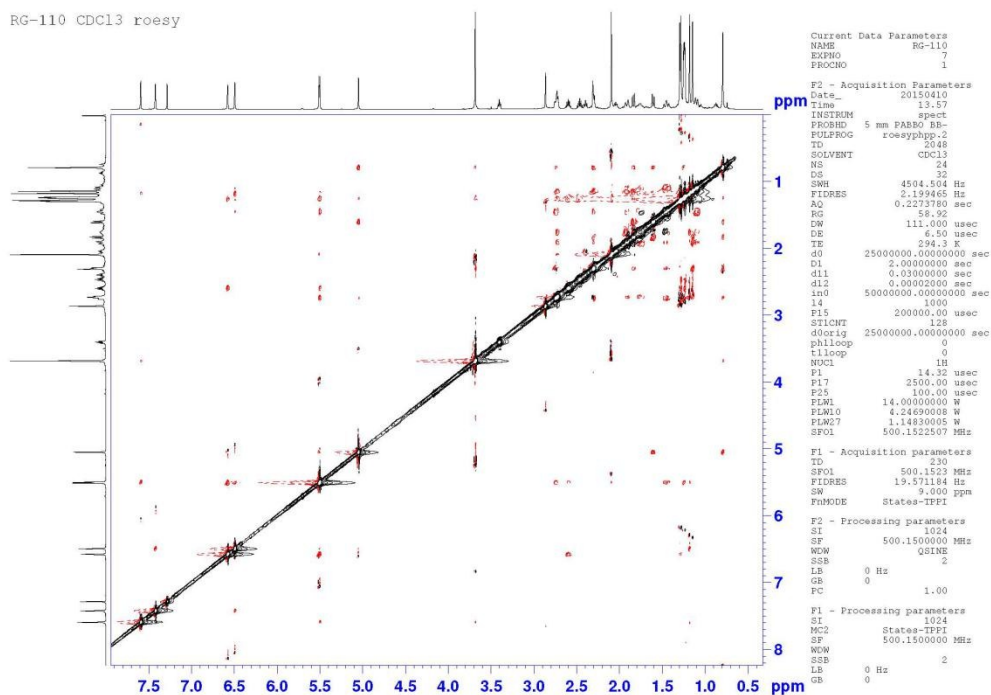


Figure S91. HRESI-MS spectrum of compound 14

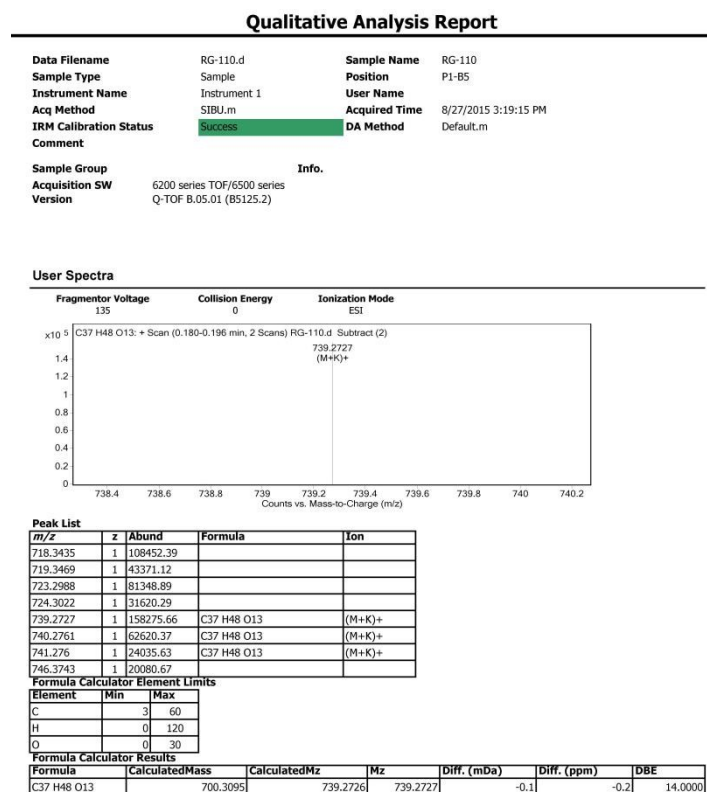
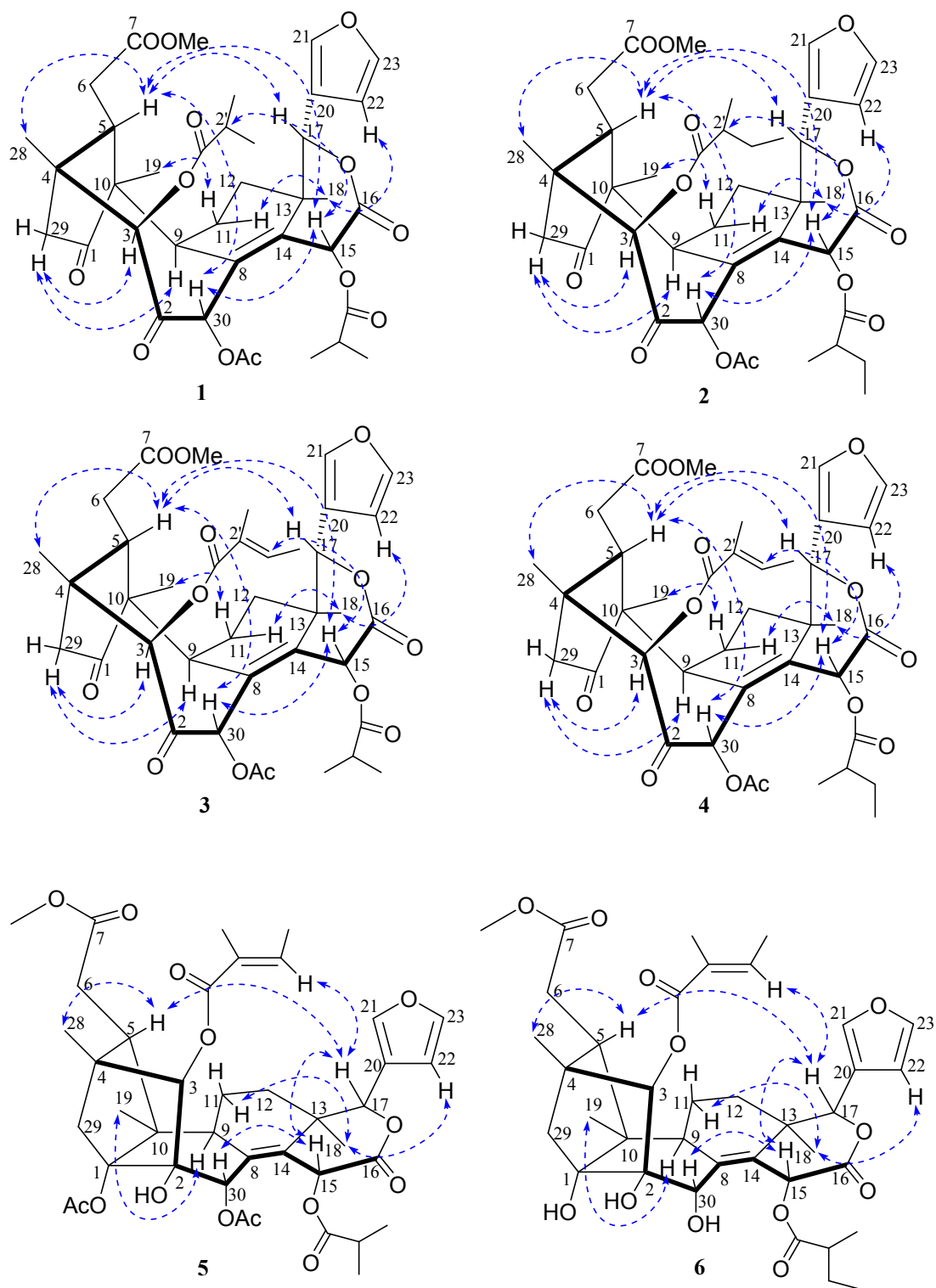
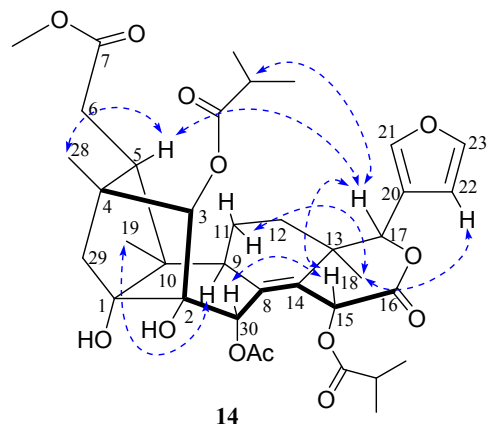
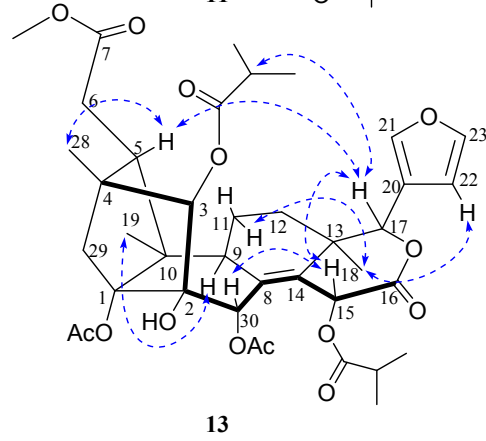
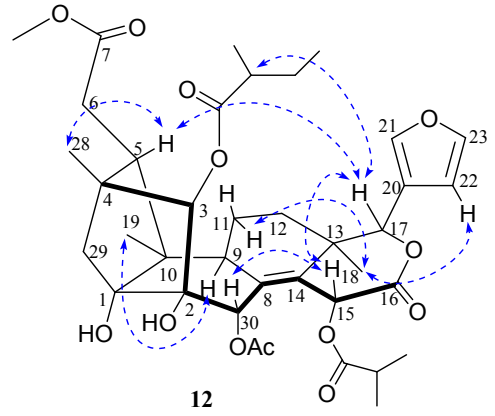
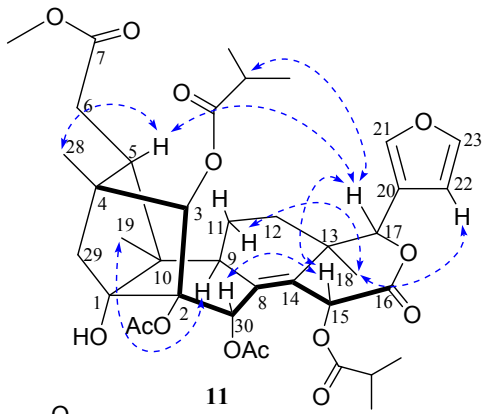
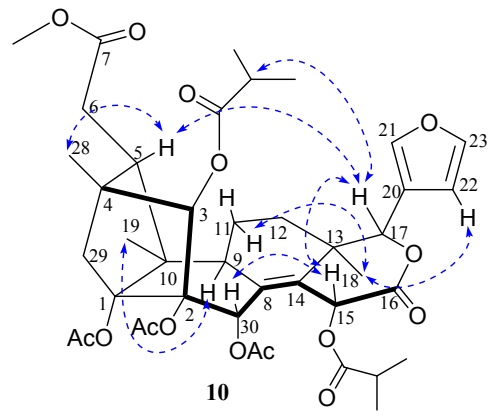
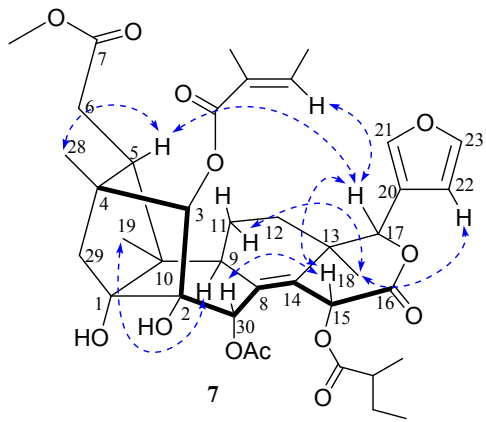


Figure S92. Key ROESY correlations of **1-4**, **5-7** and **10-14**





Experimental parameters of all 2D NMR

Table 1 HSQC experimental parameters of compound **1**

Table 2 ^1H - ^1H COSY experimental parameters of compound **1**

Table 3 HMBC experimental parameters of compound **1**

Table 4 ROESY experimental parameters of compound **1**

Table 5 HSQC experimental parameters of compound **2**

Table 6 ^1H - ^1H COSY experimental parameters of compound **2**

Table 7 HMBC experimental parameters of compound **2**

Table 8 ROESY experimental parameters of compound **2**

Table 9 HSQC experimental parameters of compound **3**

Table 10 ^1H - ^1H COSY experimental parameters of compound **3**

Table 11 HMBC experimental parameters of compound **3**

Table 12 ROESY experimental parameters of compound **3**

Table 13 HSQC experimental parameters of compound **4**

Table 14 ^1H - ^1H COSY experimental parameters of compound **4**

Table 15 HMBC experimental parameters of compound **4**

Table 16 ROESY experimental parameters of compound **4**

Table 17 HSQC experimental parameters of compound **5**

Table 18 ^1H - ^1H COSY experimental parameters of compound **5**

Table 19 HMBC experimental parameters of compound **5**

Table 20 ROESY experimental parameters of compound **5**

Table 17 HSQC experimental parameters of compound **5**

Table 18 ^1H - ^1H COSY experimental parameters of compound **5**

Table 19 HMBC experimental parameters of compound **5**

Table 20 ROESY experimental parameters of compound **5**

Table 21 HSQC experimental parameters of compound **6**

Table 22 ^1H - ^1H COSY experimental parameters of compound **6**

Table 23 HMBC experimental parameters of compound **6**

Table 24 ROESY experimental parameters of compound **6**

Table 25 HSQC experimental parameters of compound **7**

Table 26 ^1H - ^1H COSY experimental parameters of compound **7**

Table 27 HMBC experimental parameters of compound **7**

Table 28 ROESY experimental parameters of compound **7**

Table 29 HSQC experimental parameters of compound **9**

Table 30 ^1H - ^1H COSY experimental parameters of compound **9**

Table 31 HMBC experimental parameters of compound **9**

Table 32 ROESY experimental parameters of compound **9**

Table 33 HSQC experimental parameters of compound **10**

Table 34 ^1H - ^1H COSY experimental parameters of compound **10**

Table 35 HMBC experimental parameters of compound **10**

Table 36 ROESY experimental parameters of compound **10**

Table 37 HSQC experimental parameters of compound **11**

Table 38 ^1H - ^1H COSY experimental parameters of compound **11**

Table 39 HMBC experimental parameters of compound **11**

Table 40 ROESY experimental parameters of compound **11**

Table 41 HSQC experimental parameters of compound **12**

Table 42 ^1H - ^1H COSY experimental parameters of compound **12**

Table 43 HMBC experimental parameters of compound **12**

Table 44 ROESY experimental parameters of compound **12**

Table 45 HSQC experimental parameters of compound **13**

Table 46 ^1H - ^1H COSY experimental parameters of compound **13**

Table 47 HMBC experimental parameters of compound **13**

Table 48 ROESY experimental parameters of compound **13**

Table 49 HSQC experimental parameters of compound **14**

Table 50 ^1H - ^1H COSY experimental parameters of compound **14**

Table 51 HMBC experimental parameters of compound **14**

Table 52 ROESY experimental parameters of compound **14**

Table 1 HSQC experimental parameters of compound **1**

	Parameter	Value (f2, f1)
1	Comment	RG-29 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	296.4 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1462 sec
16	Acquisition Date	2013-06-27T09:23:53
17	Modification Date	2013-06-27T09:35:40
18	Spectrometer Frequency	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7002.8 Hz, 27670.4 Hz)
20	Lowest Frequency	(-250.4 Hz, -630.1 Hz)
21	Nucleus	(¹ H, ¹³ C)
22	Acquired Size	(1024, 82)
23	Spectral Size	(1024, 512)

Table 2 ¹H-¹H COSY experimental parameters of compound **1**

	Parameter	Value (f2, f1)
2	Comment	RG-29 CDCl ₃ COSY
3	Origin	Bruker BioSpin GmbH

4	Owner	nmrsu
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl ₃
9	Temperature	295.4 K
10	Pulse Sequence	cosygpppqf
11	Experiment	2D-COSY
12	Number of Scans	4
13	Receiver Gain	59
14	Relaxation Delay	2.0000 sec
15	Pulse Width	12.0000 μ sec
16	Acquisition Time	0.1532 sec
17	Acquisition Date	2013-07-01T10:08:52
18	Modification Date	2013-07-01T10:27:34
19	Spectrometer Frequency	(500.15 MHz, 500.15MHz)
20	Spectral Width	(6684.5 Hz, 6684.5 Hz)
21	Lowest Frequency	(-335.2 Hz, -335.2 Hz)
22	Nucleus	(1H, 1H)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 1024)

Table 3 HMBC experimental parameters of compound 1

	Parameter	Value (f2, f1)
1	Comment	RG-29 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.9 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	24

12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.3072 sec
16	Acquisition Date	2013-07-01T09:08:03
17	Modification Date	2013-07-01T10:08:18
18	Spectrometer Frequency	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(6666.7 Hz, 29683.0 Hz)
20	Lowest Frequency	(-326.3 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 81)
23	Spectral Size	(2048, 512)

Table 4 ROESY experimental parameters of compound **1**

	Parameter	Value (f2, f1)
1	Comment	RG-29 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.6 K
9	Pulse Sequence	roesyphpp.2
10	Experiment	2D-ROESY
11	Number of Scans	16
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1577 sec
16	Acquisition Date	2013-07-01T10:29:34
17	Modification Date	2013-07-01T13:13:20
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(6493.5 Hz, 6502.0 Hz)

20	Lowest Frequency	(-245.9 Hz, -250.1 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 256)
23	Spectral Size	(1024, 1024)

Table 5 HSQC experimental parameters of compound 2

	Parameter	Value (f2, f1)
1	Comment	RG-30 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	0.0 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1462 sec
16	Acquisition Date	2013-07-09T12:07:57
17	Modification Date	2013-07-09T12:28:40
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7002.8 Hz, 27670.4 Hz)
20	Lowest Frequency	(-250.4 Hz, -630.1 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 143)
23	Spectral Size	(1024, 1024)

Table 6 ¹H-¹H COSY experimental parameters of compound 2

	Parameter	Value (f2, f1)
1	Comment	RG-30 CDCl ₃ COSY

2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.3 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	4
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1532 sec
16	Acquisition Date	2013-07-22T15:30:57
17	Modification Date	2013-07-22T15:48:24
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(6684.5 Hz, 6684.5 Hz)
20	Lowest Frequency	(-335.2 Hz, -335.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 119)
23	Spectral Size	(1024, 1024)

Table 7 HMBC experimental parameters of compound 2

	Parameter	Value (f2, f1)
1	Comment	RG-30 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.4 K
9	Pulse Sequence	hmbcgpndqf

10	Experiment	2D-HMBC
11	Number of Scans	8
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.3072 sec
16	Acquisition Date	2013-07-22T14:58:32
17	Modification Date	2013-07-22T15:30:24
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(6666.7 Hz, 29683.0 Hz)
20	Lowest Frequency	(-326.3 Hz, -378.8 Hz)
21	Nucleus	(¹ H, ¹³ C)
22	Acquired Size	(2048, 128)
23	Spectral Size	(2048, 512)

Table 8 ROESY experimental parameters of compound 2

	Parameter	Value (f2, f1)
1	Comment	RG-30 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.4 K
9	Pulse Sequence	roesyhpp.2
10	Experiment	2D-ROESY
11	Number of Scans	24
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1577 sec
16	Acquisition Date	2013-07-22T15:50:43
17	Modification Date	2013-07-22T16:51:44
18	Spectrometer	(500.15 MHz, 500.15 MHz)

19	Spectral Width	(6493.5 Hz, 6502.0 Hz)
20	Lowest Frequency	(-245.9 Hz, -250.1 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 64)
23	Spectral Size	(1024, 1024)

Table 9 HSQC experimental parameters of compound **3**

	Parameter	Value (f2, f1)
3	Comment	RG-77 CDCl ₃ HSQC
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl ₃
10	Temperature	296.1 K
11	Pulse Sequence	hsqcedetgpsisp2.3
12	Experiment	2D-HSQC-EDITED
13	Number of Scans	8
14	Receiver Gain	185
15	Relaxation Delay	2.0000 sec
16	Pulse Width	12.0000 μ sec
17	Acquisition Time	0.1278 sec
18	Acquisition Date	2014-08-29T08:07:22
19	Modification Date	2014-08-29T08:43:06
20	Spectrometer	(500.15 MHz, 125.76 MHz)
21	Spectral Width	(8012.8 Hz, 29683.1 Hz)
22	Lowest Frequency	(-505.4 Hz, -378.8 Hz)
23	Nucleus	(1H, 13C)
24	Acquired Size	(1024, 125)
25	Spectral Size	(1024, 512)

Table 10 ¹H-¹H COSY experimental parameters of compound **3**

	Parameter	Value (f2, f1)
1	Comment	RG-77 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.5 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	8
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2014-09-03T19:38:08
17	Modification Date	2014-09-03T20:15:02
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 128)
23	Spectral Size	(1024, 1024)

Table 11 HMBC experimental parameters of compound **3**

	Parameter	Value (f2, f1)
1	Comment	RG-77 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.4 K

9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	24
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.2731 sec
16	Acquisition Date	2014-09-03T14:39:02
17	Modification Date	2014-09-03T15:27:14
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7500.0, 29683.0)
20	Lowest Frequency	(-249.0 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 66)
23	Spectral Size	(2048, 512)

Table 12 ROESY experimental parameters of compound **3**

	Parameter	Value (f2, f1)
1	Comment	RG-77 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.8 K
9	Pulse Sequence	roesyhpp.2
10	Experiment	2D-ROESY
11	Number of Scans	24
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2014-09-03T15:29:32

17	Modification Date	2014-09-03T19:31:56
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 256)
23	Spectral Size	(1024, 1024)

Table 13 HSQC experimental parameters of compound 4

	Parameter	Value (f2, f1)
1	Comment	RG-80 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	296.1 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1577 sec
16	Acquisition Date	2014-09-12T13:43:50
17	Modification Date	2014-09-12T14:21:06
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(6493.5 Hz, 27670.6 Hz)
20	Lowest Frequency	(-245.9 Hz, -630.2 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 256)
23	Spectral Size	(1024, 1024)

Table 14 ¹H-¹H COSY experimental parameters of compound 4

	Parameter	Value (f2, f1)
1	Comment	RG-80 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.5 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	24
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2014-09-25T14:18:16
17	Modification Date	2014-09-25T15:56:58
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 114)
23	Spectral Size	(1024, 1024)

Table 15 HMBC experimental parameters of compound 4

	Parameter	Value (f2, f1)
1	Comment	RG-80 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH

3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.5 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	48
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.2731 sec
16	Acquisition Date	2014-09-25T11:31:18
17	Modification Date	2014-09-25T14:17:00
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7500.0 Hz, 29683.0 Hz)
20	Lowest Frequency	(-249.0 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 113)
23	Spectral Size	(2048, 512)

Table 16 ROESY experimental parameters of compound **4**

	Parameter	Value (f2, f1)
1	Comment	RG-80 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.6 K
9	Pulse Sequence	roesyhpp.2
10	Experiment	2D-ROESY

11	Number of Scans	48
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2014-09-25T16:00:11
17	Modification Date	2014-09-25T21:55:58
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 188)
23	Spectral Size	(1024, 1024)

Table 17 HSQC experimental parameters of compound **5**

	Parameter	Value (f2, f1)
1	Comment	RG-69 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.7 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1462 sec
16	Acquisition Date	2013-12-12T12:17:59
17	Modification Date	2013-12-12T12:27:48
18	Spectrometer	(500.15 MHz, 125.76 MHz)

19	Spectral Width	(7002.8 Hz, 27670.4 Hz)
20	Lowest Frequency	(-250.4 Hz, -630.1 Hz)
21	Nucleus	(¹ H, ¹³ C)
22	Acquired Size	(1024, 68)
23	Spectral Size	(1024, 512)

Table 18 ¹H-¹H COSY experimental parameters of compound **5**

	Parameter	Value (f2, f1)
1	Comment	RG-69 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	293.7 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	4
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1532 sec
16	Acquisition Date	2014-01-02T17:03:07
17	Modification Date	2014-01-02T17:21:48
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(6684.5 Hz, 6684.5 Hz)
20	Lowest Frequency	(-335.2 Hz, -335.2 Hz)
21	Nucleus	(¹ H, ¹ H)
22	Acquired Size	(1024, 128)
23	Spectral Size	(1024, 1024)

Table 19 HMBC experimental parameters of compound 5

	Parameter	Value (f2, f1)
1	Comment	RG-69 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	293.8 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	8
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.3072 sec
16	Acquisition Date	2014-01-02T16:47:11
17	Modification Date	2014-01-02T17:02:34
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(6666.7 Hz, 29683.0 Hz)
20	Lowest Frequency	(-326.3 Hz, -378.8Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 62)
23	Spectral Size	(2048, 256)

Table 20 ROESY experimental parameters of compound 5

	Parameter	Value (f2, f1)
1	Comment	RG-69 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	

5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	293.7 K
9	Pulse Sequence	roesyphpp.2
10	Experiment	2D-ROESY
11	Number of Scans	24
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1577 sec
16	Acquisition Date	2014-01-02T17:24:07
17	Modification Date	2014-01-02T19:16:14
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(6493.5 Hz, 6502.0 Hz)
20	Lowest Frequency	(-245.9 Hz, -250.1 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 117)
23	Spectral Size	(1024, 1024)

Table 21 HSQC experimental parameters of compound 6

	Parameter	Value (f2, f1)
1	Comment	RG-92 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	296.5 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	8
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec

14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2014-10-17T10:24:57
17	Modification Date	2014-10-17T10:47:13
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(8012.8 Hz, 29683.1Hz)
20	Lowest Frequency	(-505.4 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 78)
23	Spectral Size	(1024, 512)

Table 22 ^1H - ^1H COSY experimental parameters of compound **6**

	Parameter	Value (f2, f1)
1	Comment	RG-92 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.8 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	20
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2015-01-17T01:13:00
17	Modification Date	2015-01-17T02:45:14
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)

22	Acquired Size	(1024, 128)
23	Spectral Size	(1024, 1024)

Table 23 HMBC experimental parameters of compound **6**

	Parameter	Value (f2, f1)
1	Comment	RG-92 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.5 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	56
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.2731 sec
16	Acquisition Date	2015-01-16T21:33:11
17	Modification Date	2015-01-17T01:11:52
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7500.0 Hz, 29683.0 Hz)
20	Lowest Frequency	(-249.0 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 128)
23	Spectral Size	(2048, 512)

Table 24 ROESY experimental parameters of compound **6**

	Parameter	Value (f2, f1)
1	Comment	RG-92 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu

4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.9 K
9	Pulse Sequence	roesyphpp.2
10	Experiment	2D-ROESY
11	Number of Scans	48
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2015-01-17T02:48:27
17	Modification Date	2015-01-17T10:08:39
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 232)
23	Spectral Size	(1024, 1024)

Table 25 HSQC experimental parameters of compound 7

	Parameter	Value (f2, f1)
1	Comment	RG-95 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.7 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	8

12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2014-11-05T09:04:11
17	Modification Date	2014-11-05T09:25:53
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(8012.8 Hz, 29683.1 Hz)
20	Lowest Frequency	(-505.4 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 76)
23	Spectral Size	(1024, 512)

Table 26 ^1H - ^1H COSY experimental parameters of compound **7**

	Parameter	Value (f2, f1)
1	Comment	RG-95 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.4 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	12
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2015-01-15T00:50:50
17	Modification Date	2015-01-15T01:46:11
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)

21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 128)
23	Spectral Size	(1024, 1024)

Table 27 HMBC experimental parameters of compound 7

	Parameter	Value (f2, f1)
1	Comment	RG-95 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.5 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	36
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.2731 sec
16	Acquisition Date	2015-01-14T22:29:24
17	Modification Date	2015-01-15T00:50:00
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7500.0 Hz, 29683.0 Hz)
20	Lowest Frequency	(-249.0 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 128)
23	Spectral Size	(2048, 512)

Table 28 ROESY experimental parameters of compound 7

	Parameter	Value (f2, f1)
1	Comment	RG-95 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	

5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.4 K
9	Pulse Sequence	roesyphpp.2
10	Experiment	2D-ROESY
11	Number of Scans	32
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2015-01-15T01:48:46
17	Modification Date	2015-01-15T07:11:57
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 256)
23	Spectral Size	(1024, 1024)

Table 29 HSQC experimental parameters of compound **9**

	Parameter	Value (f2, f1)
1	Comment	RG-89 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.9 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	8
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec

14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2014-10-17T08:20:06
17	Modification Date	2014-10-17T08:40:53
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(8012.8 Hz, 29683.1 Hz)
20	Lowest Frequency	(-505.4 Hz, -378.8 Hz)
21	Nucleus	(¹ H, ¹³ C)
22	Acquired Size	(1024, 73)
23	Spectral Size	(1024, 512)

Table 30 ¹H-¹H COSY experimental parameters of compound **9**

	Parameter	Value (f2, f1)
1	Comment	RG-89 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.2
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	12
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	14.3200 μ sec
15	Acquisition Time	0.2560 sec
16	Acquisition Date	2015-04-10T00:27:37
17	Modification Date	2015-04-10T02:26:31
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(4000.0 Hz, 4001.2 Hz)
20	Lowest Frequency	(0.6 Hz, 0.0 Hz)
21	Nucleus	(¹ H, ¹ H)
22	Acquired Size	(1024, 256)
23	Spectral Size	(1024, 1024)

Table 31 HMBC experimental parameters of compound **9**

	Parameter	Value (f2, f1)
1	Comment	RG-89 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.2 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	32
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	14.3200 μ sec
15	Acquisition Time	0.5120 sec
16	Acquisition Date	2015-04-09T22:05:11
17	Modification Date	2015-04-10T00:26:23
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(4000.0 Hz, 22639.9 Hz)
20	Lowest Frequency	(0.6 Hz, 627.5 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 128)
23	Spectral Size	(2048, 512)

Table 32 ROESY experimental parameters of compound **9**

	Parameter	Value (f2, f1)
1	Comment	RG-89 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect

6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.3 K
9	Pulse Sequence	roesyphpp.2
10	Experiment	2D-ROESY
11	Number of Scans	32
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	14.3200 μ sec
15	Acquisition Time	0.2560 sec
16	Acquisition Date	2015-04-10T02:29:19
17	Modification Date	2015-04-10T07:58:06
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(4000.0 Hz, 4001.2 Hz)
20	Lowest Frequency	(0.6 Hz, 0.0 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 246)
23	Spectral Size	(1024, 1024)

Table 33 HSQC experimental parameters of compound **10**

	Parameter	Value (f2, f1)
1	Comment	RG-40 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	296.5 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec

15	Acquisition Time	0.1462 sec
16	Acquisition Date	2013-08-19T16:40:42
17	Modification Date	2013-08-19T17:06:36
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7002.8 Hz, 27670.4 Hz)
20	Lowest	(-250.4 Hz, -630.1 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 114)
23	Spectral Size	(1024, 512)

Table 34 ¹H-¹H COSY experimental parameters of compound **10**

	Parameter	Value (f2, f1)
1	Comment	RG-40 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.6 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	4
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1532 sec
16	Acquisition Date	2013-10-09T15:06:08
17	Modification Date	2013-10-09T15:24:50
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(6684.5 Hz, 6684.5 Hz)
20	Lowest Frequency	(-335.2 Hz, -335.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 128)
23	Spectral Size	(1024, 1024)

Table 35 HMBC experimental parameters of compound **10**

	Parameter	Value (f2, f1)
1	Comment	RG-40 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.8 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	16
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.3072 sec
16	Acquisition Date	2013-10-09T14:34:22
17	Modification Date	2013-10-09T15:05:36
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(6666.7 Hz, 29683.0 Hz)
20	Lowest Frequency	(-326.3 Hz, -378.8 Hz)
21	Nucleus	(¹ H, ¹³ C)
22	Acquired Size	(2048, 63)
23	Spectral Size	(2048, 256)

Table 36 ROESY experimental parameters of compound **10**

	Parameter	Value (f2, f1)
1	Comment	RG-40 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	

5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.6 K
9	Pulse Sequence	roesyphpp.2
10	Experiment	2D-ROESY
11	Number of Scans	24
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1577 sec
16	Acquisition Date	2013-10-09T15:27:08
17	Modification Date	2013-10-09T16:31:04
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(6493.5 Hz, 6502.0 Hz)
20	Lowest Frequency	(-245.9 Hz, -250.1 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 67)
23	Spectral Size	(1024, 1024)

Table 37 HSQC experimental parameters of compound **11**

	Parameter	Value (f2, f1)
1	Comment	RG-66 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	0.0 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec

14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1462 sec
16	Acquisition Date	2013-11-26T16:39:31
17	Modification Date	2013-11-26T16:52:12
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7002.8 Hz, 27670.4 Hz)
20	Lowest Frequency	(-250.4 Hz, -630.1 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 88)
23	Spectral Size	(1024, 512)

Table 38 ^1H - ^1H COSY experimental parameters of compound **11**

	Parameter	Value (f2, f1)
1	Comment	RG-66 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	293.4 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	4
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1532 sec
16	Acquisition Date	2014-01-04T15:27:11
17	Modification Date	2014-01-04T15:45:52
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(6684.5 Hz, 6684.5 Hz)
20	Lowest Frequency	(-335.2 Hz, -335.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 128)

23	Spectral Size	(1024, 1024)
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Table 39 HMBC experimental parameters of compound **11**

	Parameter	Value (f2, f1)
3	Comment	RG-66 CDCl ₃ HMBC
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl ₃
10	Temperature	293.5 K
11	Pulse Sequence	hmbcgpndqf
12	Experiment	2D-HMBC
13	Number of Scans	8
14	Receiver Gain	185
15	Relaxation Delay	1.5000 sec
16	Pulse Width	12.0000 μ sec
17	Acquisition Time	0.3072 sec
18	Acquisition Date	2014-01-04T14:54:47
19	Modification	2014-01-04T15:26:38
20	Spectrometer	(500.15 MHz, 125.76 MHz)
21	Spectral Width	(6666.7 Hz, 29683.0 Hz)
22	Lowest	(-326.3 Hz, -378.8 Hz)
23	Nucleus	(¹ H, ¹³ C)
24	Acquired Size	(2048, 128)
25	Spectral Size	(2048, 512)

Table 40 ROESY experimental parameters of compound **11**

	Parameter	Value (f2, f1)
1	Comment	RG-66 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	

5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	293.5 K
9	Pulse Sequence	roesyhpp.2
10	Experiment	2D-ROESY
11	Number of Scans	24
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1577 sec
16	Acquisition Date	2014-01-04T15:48:12
17	Modification Date	2014-01-04T17:08:44
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(6493.5 Hz, 6502.0Hz)
20	Lowest Frequency	(-245.9 Hz, -250.1 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 84)
23	Spectral Size	(1024, 1024)

Table 41 HSQC experimental parameters of compound **12**

	Parameter	Value (f2, f1)
1	Comment	RG-94 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	297.0 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec

14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1577 sec
16	Acquisition Date	2014-11-04T10:20:46
17	Modification Date	2014-11-04T10:44:55
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(6493.5 Hz, 27670.6 Hz)
20	Lowest Frequency	(-245.9 Hz, -630.2 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 166)
23	Spectral Size	(1024, 1024)

Table 42 ^1H - ^1H COSY experimental parameters of compound **12**

	Parameter	Value (f2, f1)
1	Comment	RG-94 CDCl_3 COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl_3
8	Temperature	294.2
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	8
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2015-01-14T18:47:07
17	Modification Date	2015-01-14T19:24:01
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)

22	Acquired Size	(1024, 128)
23	Spectral Size	(1024, 1024)

Table 43 HMBC experimental parameters of compound **12**

	Parameter	Value (f2, f1)
1	Comment	RG-94 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.0 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	24
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.2731 sec
16	Acquisition Date	2015-01-14T17:12:41
17	Modification Date	2015-01-14T18:46:26
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7500.0 Hz, 29683.0 Hz)
20	Lowest Frequency	(-249.0 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 128)
23	Spectral Size	(2048, 512)

Table 44 ROESY experimental parameters of compound **12**

	Parameter	Value (f2, f1)
1	Comment	RG-94 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect

6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.2 K
9	Pulse Sequence	roesyphpp.2
10	Experiment	2D-ROESY
11	Number of Scans	24
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2015-01-14T19:26:17
17	Modification Date	2015-01-14T22:17:14
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 181)
23	Spectral Size	(1024, 1024)

Table 45 HSQC experimental parameters of compound **13**

	Parameter	Value (f2, f1)
1	Comment	RG-101 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.4 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1712 sec

16	Acquisition Date	2015-01-12T16:43:06
17	Modification Date	2015-01-12T16:54:24
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(5980.9 Hz, 27670.4 Hz)
20	Lowest Frequency	(-239.6 Hz, -630.1 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 77)
23	Spectral Size	(1024, 512)

Table 46 ¹H-¹H COSY experimental parameters of compound **13**

	Parameter	Value (f2, f1)
1	Comment	RG-101 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.6 K
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	20
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2015-03-02T23:19:26
17	Modification Date	2015-03-03T00:51:40
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 MHz, 8002.4 MHz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 128)
23	Spectral Size	(1024, 1024)

Table 47 HMBC experimental parameters of compound **13**

	Parameter	Value (f2, f1)
1	Comment	RG-101 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.9 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	40
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.2731 sec
16	Acquisition Date	2015-03-02T20:42:06
17	Modification Date	2015-03-02T23:18:18
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(7500.0 Hz, 29683.0 Hz)
20	Lowest Frequency	(-249.0 Hz, -378.8 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 128)
23	Spectral Size	(2048, 512)

Table 48 ROESY experimental parameters of compound **13**

	Parameter	Value (f2, f1)
1	Comment	RG-101 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect

6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.6 K
9	Pulse Sequence	roesyhpp.2
10	Experiment	2D-ROESY
11	Number of Scans	40
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec
15	Acquisition Time	0.1278 sec
16	Acquisition Date	2015-03-03T00:54:34
17	Modification Date	2015-03-03T07:38:33
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(8012.8 Hz, 8002.4 Hz)
20	Lowest Frequency	(-505.4 Hz, -500.2 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 256)
23	Spectral Size	(1024, 1024)

Table 49 HSQC experimental parameters of compound **14**

	Parameter	Value (f2, f1)
1	Comment	RG-110 CDCl ₃ HSQC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	295.2 K
9	Pulse Sequence	hsqcedetgpsisp2.3
10	Experiment	2D-HSQC-EDITED
11	Number of Scans	4
12	Receiver Gain	185
13	Relaxation Delay	2.0000 sec
14	Pulse Width	12.0000 μ sec

15	Acquisition Time	0.1712 sec
16	Acquisition Date	2015-03-02T15:00:22
17	Modification Date	2015-03-02T15:12:38
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(5980.9 Hz, 27670.4 Hz)
20	Lowest Frequency	(-239.6 Hz, -630.1 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(1024, 84)
23	Spectral Size	(1024, 512)

Table 50 ¹H-¹H COSY experimental parameters of compound 14

	Parameter	Value (f2, f1)
1	Comment	RG-110 CDCl ₃ COSY
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.2
9	Pulse Sequence	cosygpppqf
10	Experiment	2D-COSY
11	Number of Scans	8
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	14.3200 μ sec
15	Acquisition Time	0.2273 sec
16	Acquisition Date	2015-04-10T12:36:32
17	Modification Date	2015-04-10T13:54:42
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(4504.5 Hz, 4501.4 Hz)
20	Lowest Frequency	(-1.6 Hz, 0.0 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 256)
23	Spectral Size	(1024, 1024)

Table 51 HMBC experimental parameters of compound **14**

	Parameter	Value (f2, f1)
1	Comment	RG-110 CDCl ₃ HMBC
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	
5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.2 K
9	Pulse Sequence	hmbcgpndqf
10	Experiment	2D-HMBC
11	Number of Scans	24
12	Receiver Gain	185
13	Relaxation Delay	1.5000 sec
14	Pulse Width	14.3200 μ sec
15	Acquisition Time	0.4547 sec
16	Acquisition Date	2015-04-10T10:52:50
17	Modification Date	2015-04-10T12:35:49
18	Spectrometer	(500.15 MHz, 125.76 MHz)
19	Spectral Width	(4504.5 Hz, 23897.7 Hz)
20	Lowest Frequency	(-1.6 Hz, -1.4 Hz)
21	Nucleus	(1H, 13C)
22	Acquired Size	(2048, 128)
23	Spectral Size	(2048, 512)

Table 52 ROESY experimental parameters of compound **14**

	Parameter	Value (f2, f1)
1	Comment	RG-110 CDCl ₃ roesy
2	Origin	Bruker BioSpin GmbH
3	Owner	nmrsu
4	Site	

5	Spectrometer	spect
6	Author	
7	Solvent	CDCl ₃
8	Temperature	294.3 K
9	Pulse Sequence	roesyphpp.2
10	Experiment	2D-ROESY
11	Number of Scans	24
12	Receiver Gain	59
13	Relaxation Delay	2.0000 sec
14	Pulse Width	14.3200 μ sec
15	Acquisition Time	0.2273 sec
16	Acquisition Date	2015-04-10T13:57:04
17	Modification Date	2015-04-10T17:44:24
18	Spectrometer	(500.15 MHz, 500.15 MHz)
19	Spectral Width	(4504.5 Hz, 4501.4 Hz)
20	Lowest Frequency	(-1.6 Hz, 0.0 Hz)
21	Nucleus	(1H, 1H)
22	Acquired Size	(1024, 230)
23	Spectral Size	(1024, 1024)