Synthesis, Characterization and Biological Applications of Substituted Indolo[2,1-*b*]quinazolin-12(6*H*)-one Based Rhenium(I) Organometallic Compounds

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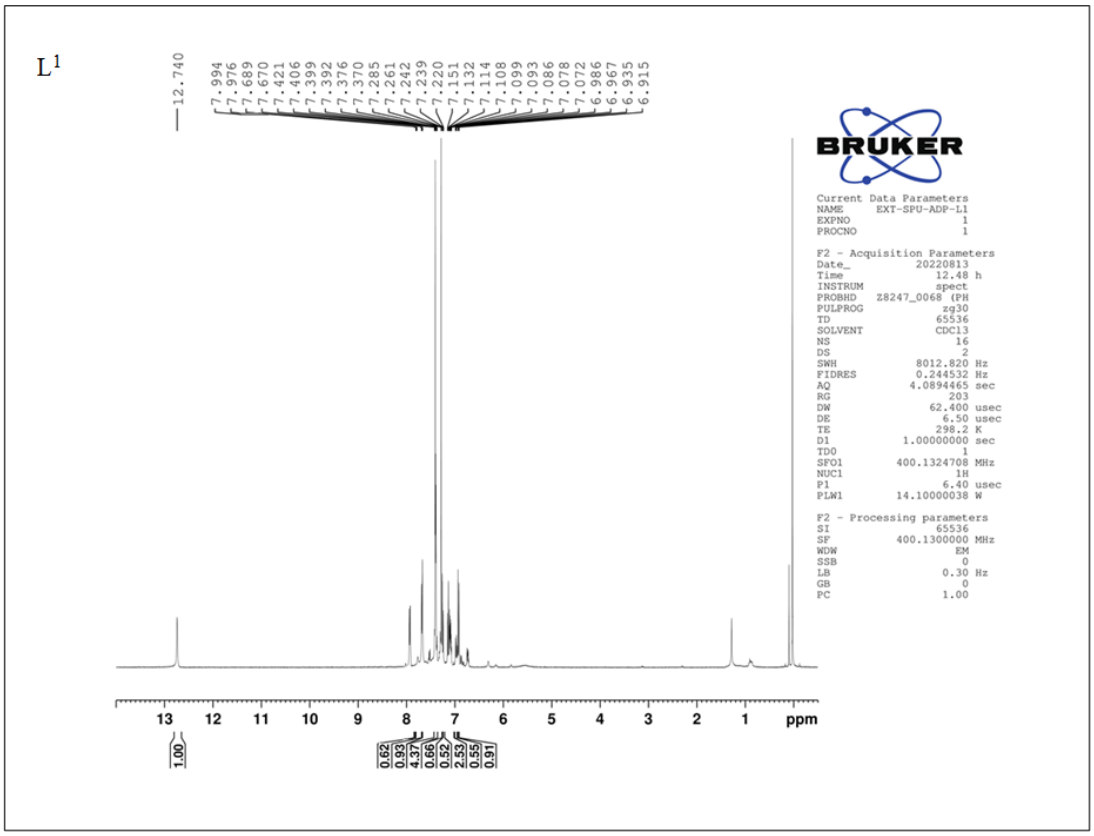
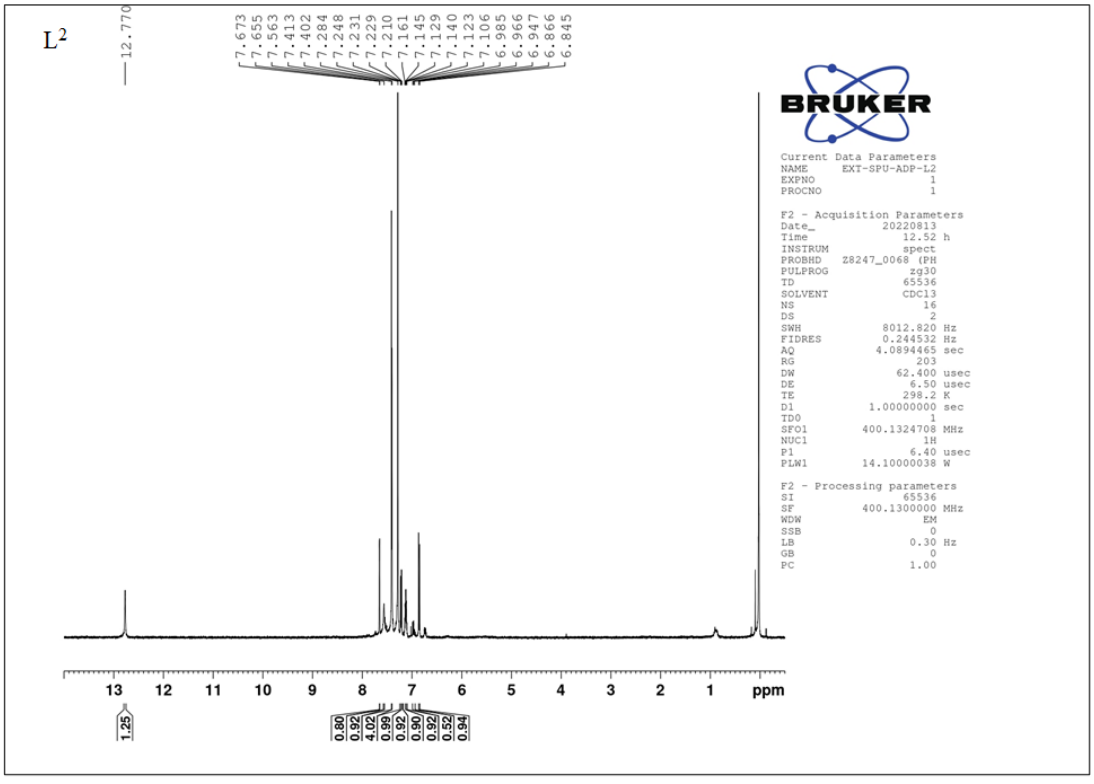
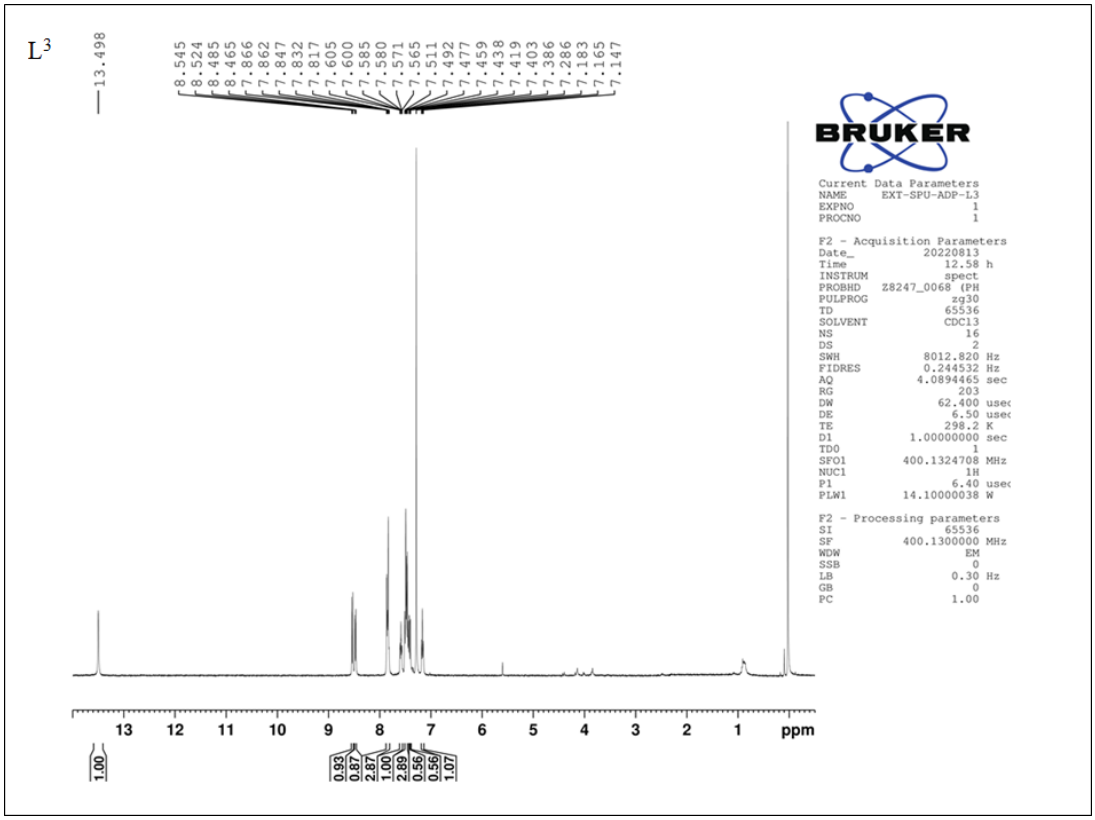
Electronic Supplementary Information (ESI) 1:

^{1}H NMR, ^{13}C NMR, Mass Spectra, and IR spectrum





L^3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7.580
7.571
7.565
7.511
7.492
7.477
7.459
7.438
7.419
7.403
7.386
7.286
7.183
7.165
7.147
BRUKER
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PROCNO 1
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 6.40 usec
PLW1 14.10000038 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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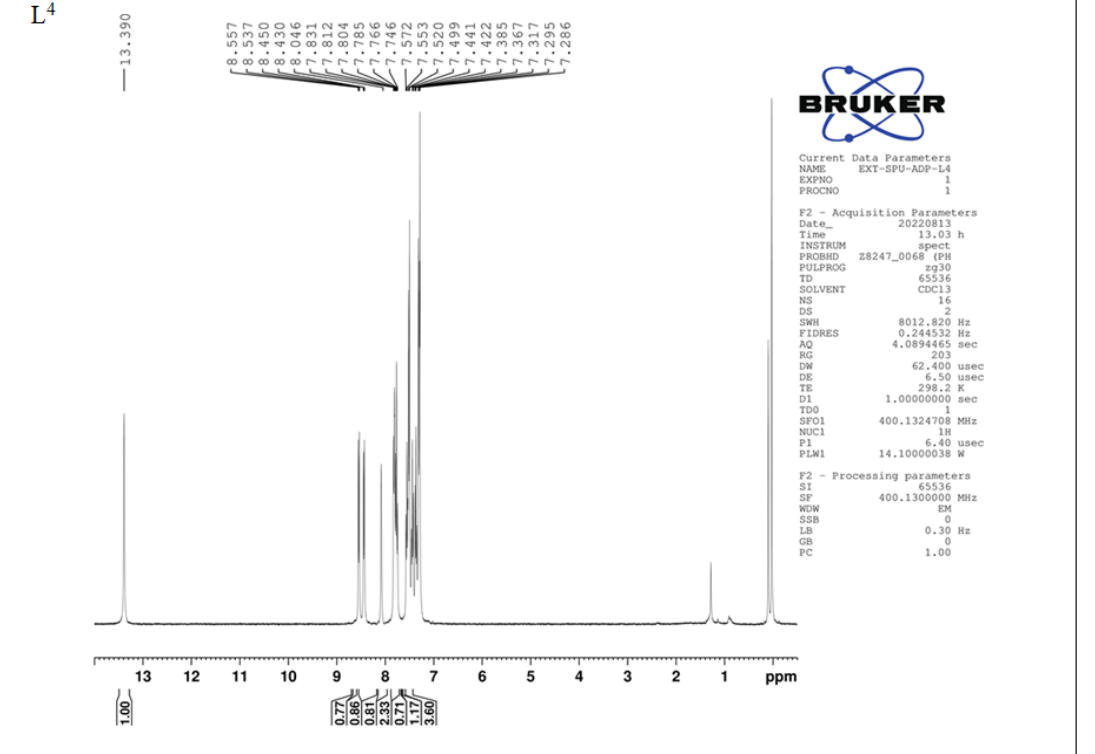
1.00
0.93 0.87 2.87 1.00 2.89 0.56 0.56 1.07

L^4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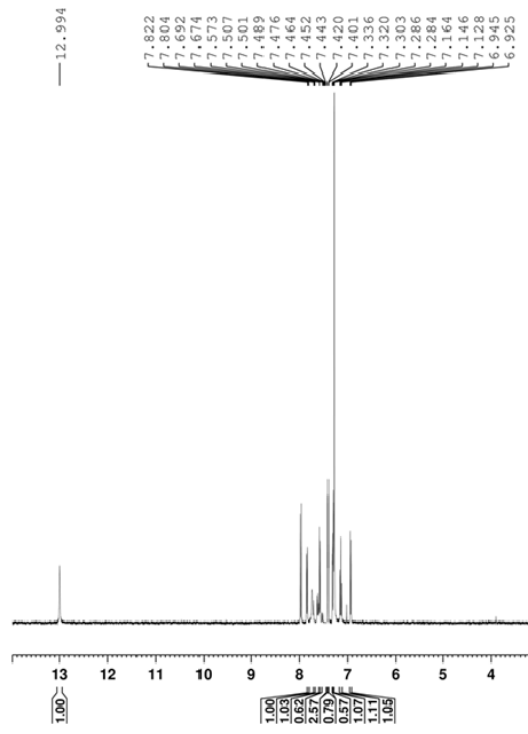
8.537
8.450
8.430
8.046
7.831
7.812
7.804
7.785
7.766
7.746
7.572
7.553
7.520
7.499
7.441
7.422
7.385
7.367
7.317
7.295
7.286
BRUKER
Current Data Parameters
NAME EXT-SPU-ADP-L4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220813
Time 13.03 h
INSTRUM spect
PROBHD Z8247_0068 (PH
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 6.40 usec
PLW1 14.10000038 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
0.77 0.86 0.81 2.33 0.71 1.17 3.60

L5



BRUKER

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EXPNO                  1
PROCNO                 1

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Date_           20220813
Time              13.07 h
INSTRUM             spect
PROBHD   Z8247_0068 (PH
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            4.0894465 sec
RG                   203
DW               62.400 usec
DE                6.50 usec
TE                298.2 K
D1            1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P1                 6.40 usec
PLW1         14.10000038 W

F2 - Processing parameters
SI                 65536
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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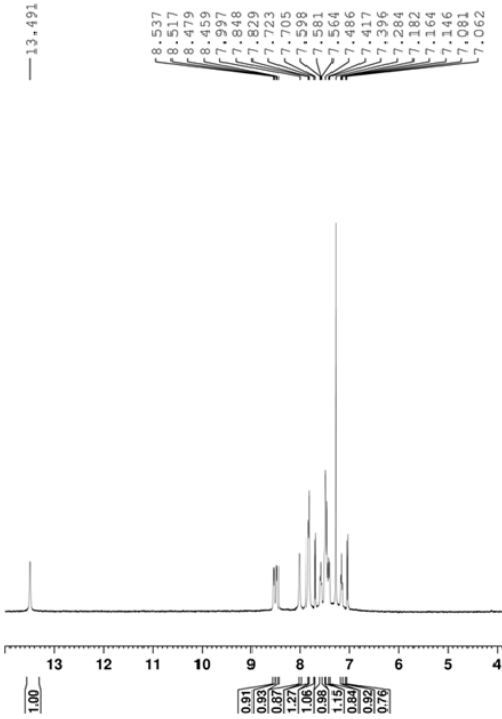
L6



BRUKER

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Current Data Parameters
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EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220813
Time              13.12 h
INSTRUM             spect
PROBHD   Z8247_0068 (PH
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            4.0894465 sec
RG                   203
DW               62.400 usec
DE                6.50 usec
TE                298.2 K
D1            1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P1                 6.40 usec
PLW1         14.10000038 W

F2 - Processing parameters
SI                 65536
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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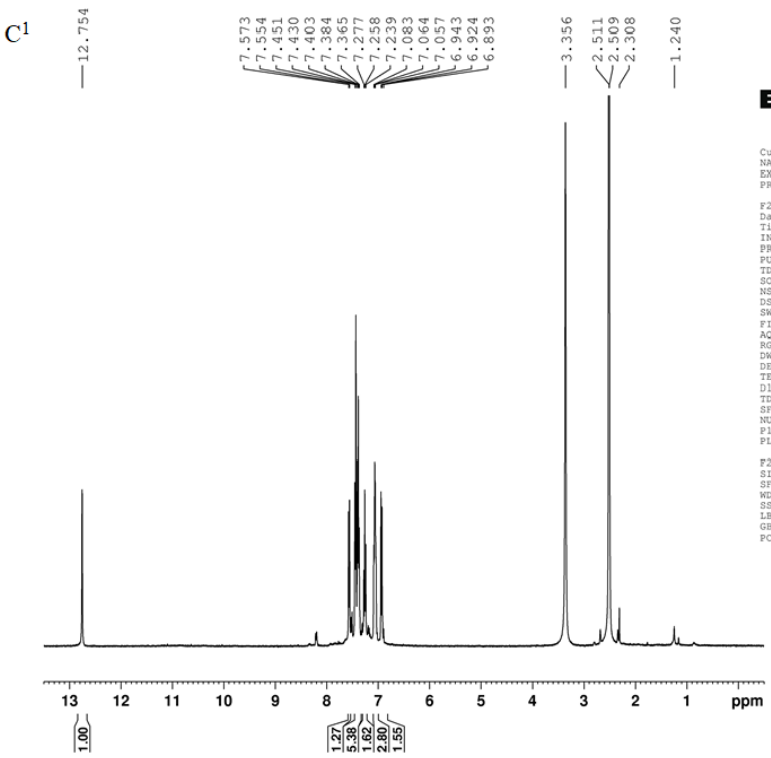
C[1]



BRUKER

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Current Data Parameters
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EXPNO                           3
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20230321
Time                        22.28 h
INSTRUM                      spect
PROBHD    Z8247_0068 (PH
PULPROG                     zg30
TD                         65536
SOLVENT                     DMSO
NS                            16
DS                             2
SWH                     8012.820 Hz
FIDRES                  0.244532 Hz
AQ                      4.0894465 sec
RG                           203
DW                        62.400 usec
DE                         6.50 usec
TE                        298.2 K
D1                     1.00000000 sec
TD0                            1
SFO1                400.1324708 MHz
NUC1                          1H
P1                         8.00 usec
PLW1                19.40600014 W

F2 - Processing parameters
SI                         65536
SF                  400.1300000 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
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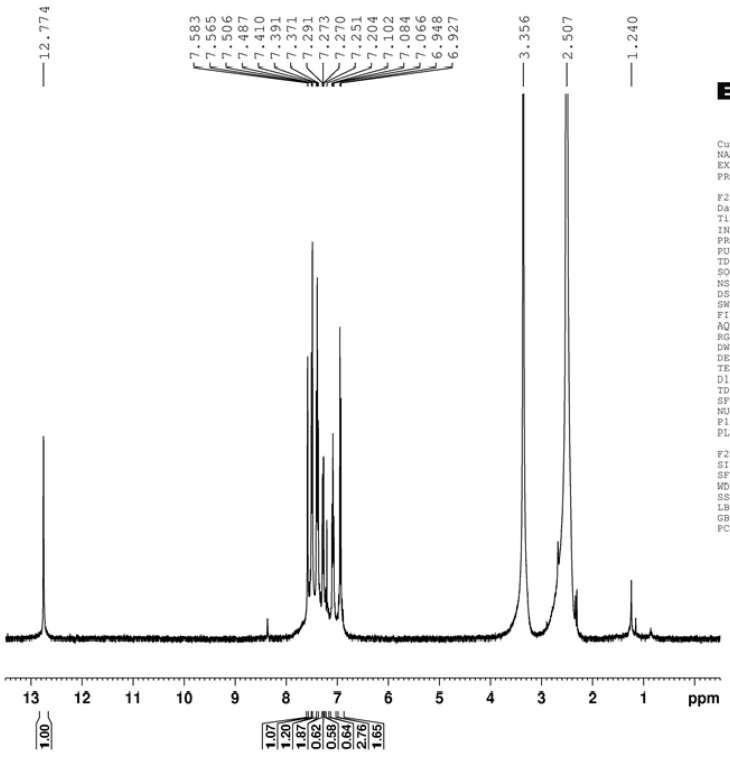
C[2]



BRUKER

```
Current Data Parameters
NAME        EXT-SPU-ADP-C2_210323
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20230321
Time                        17.13 h
INSTRUM                      spect
PROBHD    Z8247_0068 (PH
PULPROG                     zg30
TD                         65536
SOLVENT                     DMSO
NS                            16
DS                             2
SWH                     8012.820 Hz
FIDRES                  0.244532 Hz
AQ                      4.0894465 sec
RG                           203
DW                        62.400 usec
DE                         6.50 usec
TE                        298.2 K
D1                     1.00000000 sec
TD0                            1
SFO1                400.1324708 MHz
NUC1                          1H
P1                         8.00 usec
PLW1                19.40600014 W

F2 - Processing parameters
SI                         65536
SF                  400.1300000 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
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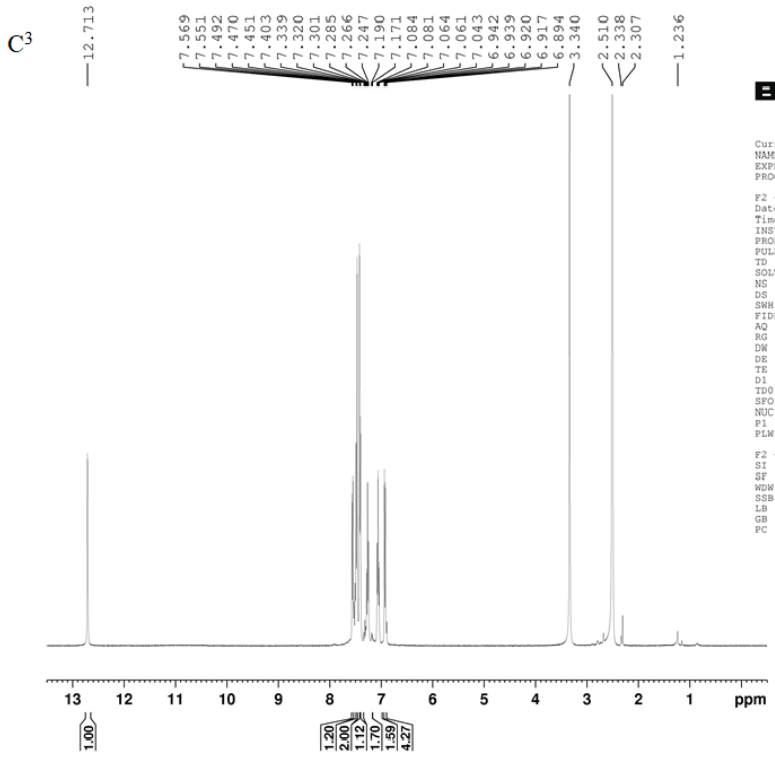
C3



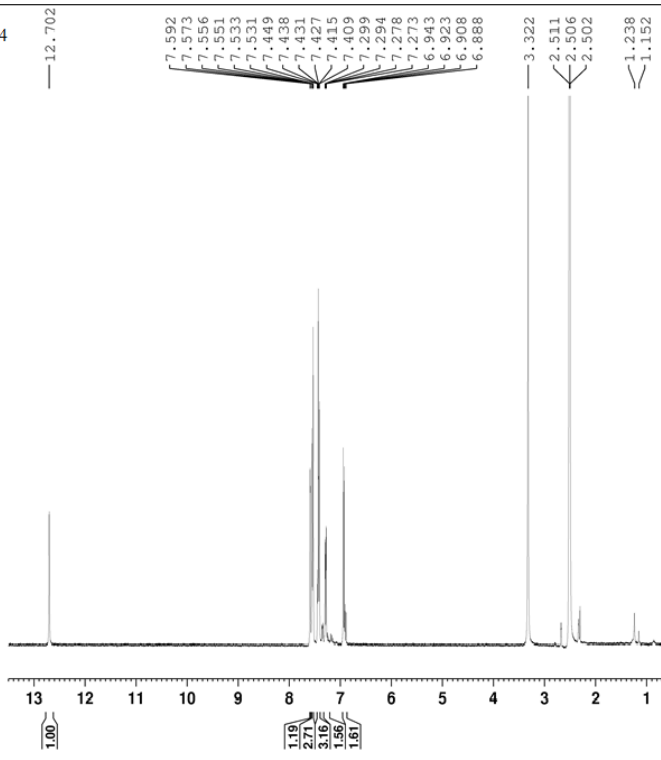
BRUKER

Current Data Parameters
NAME EXT-SPU-ADP-C3_210323
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230321
Time 22.08 h
INSTRUM spect
PROBHD Z8247_0068 (PH
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 8.00 usec
PLW1 19.40600014 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C4



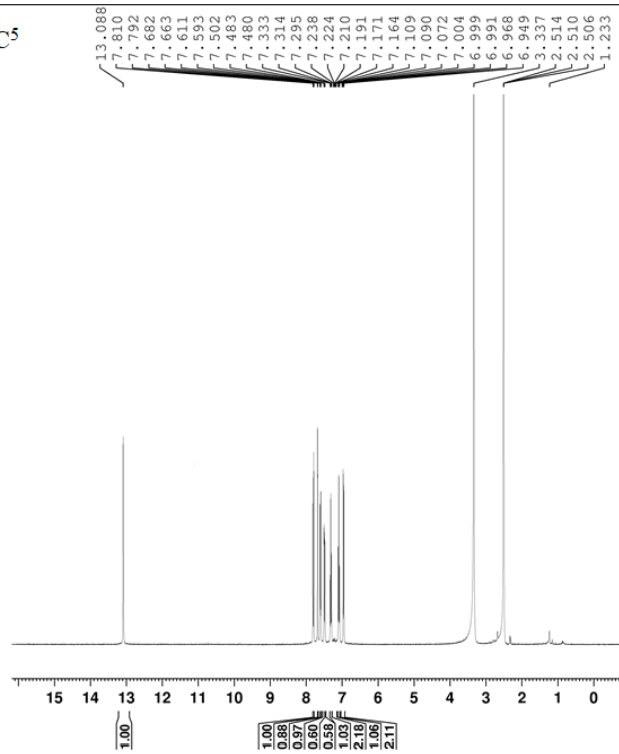
BRUKER

Current Data Parameters
NAME EXT-SPU-ADP-C4_210323
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230321
Time 17.22 h
INSTRUM spect
PROBHD Z8247_0068 (PH
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 8.00 usec
PLW1 19.40600014 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C5



BRUKER

```
Current Data Parameters
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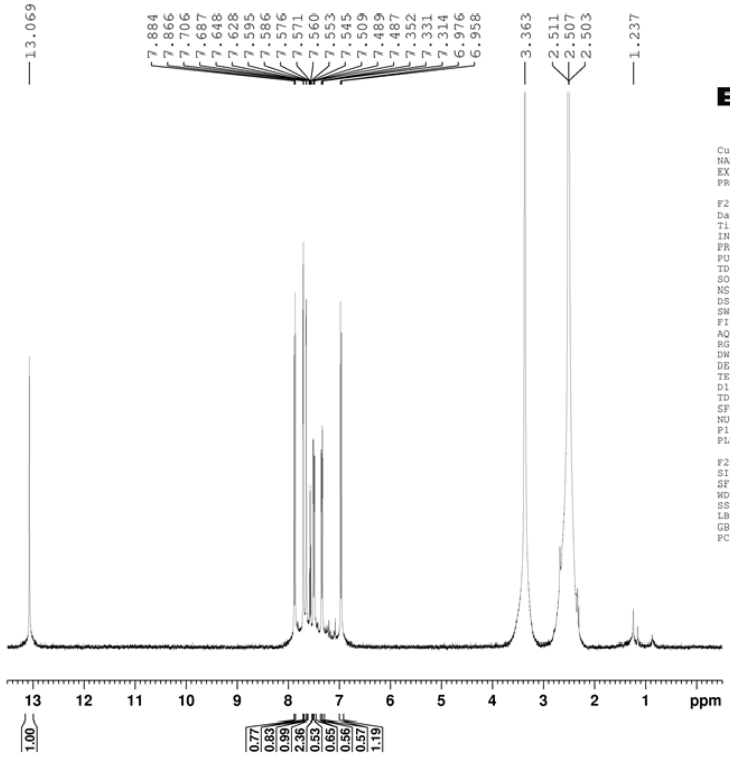
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20230321
Time                       22.18 h
INSTRUM                    spect
PROBHD     Z8247_0068 (PH
PULPROG                    zg30
TD                        65536
SOLVENT                    DMSO
NS                           16
DS                            2
SWH                    8012.820 Hz
FIDRES                 0.244532 Hz
AQ                     4.0894465 sec
RG                           203
DW                        62.400 usec
DE                         6.50 usec
TE                       298.2 K
D1                     1.00000000 sec
TD0                           1
SFO1                 400.1324708 MHz
NUC1                         1H
P1                         8.00 usec
PLW1                19.40600014 W

F2 - Processing parameters
SI                        65536
SF                   400.1300000 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

C6



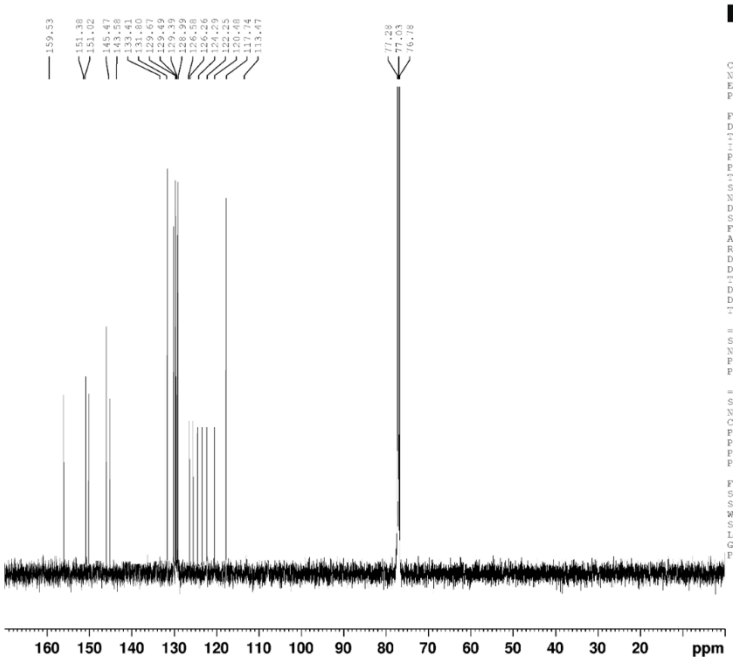
BRUKER

```
Current Data Parameters
NAME        EXT-SPU-ADP-C6_210323
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20230321
Time                       17.32 h
INSTRUM                    spect
PROBHD     Z8247_0068 (PH
PULPROG                    zg30
TD                        65536
SOLVENT                    DMSO
NS                           16
DS                            2
SWH                    8012.820 Hz
FIDRES                 0.244532 Hz
AQ                     4.0894465 sec
RG                           203
DW                        62.400 usec
DE                         6.50 usec
TE                       298.2 K
D1                     1.00000000 sec
TD0                           1
SFO1                 400.1324708 MHz
NUC1                         1H
P1                         8.00 usec
PLW1                19.40600014 W

F2 - Processing parameters
SI                        65536
SF                   400.1300000 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

L[1]



BRUKER

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Current Data Parameters
NAME        EXT-SPU-ADP-L1(500MHz)
EXPNO                1
PROCNO               1

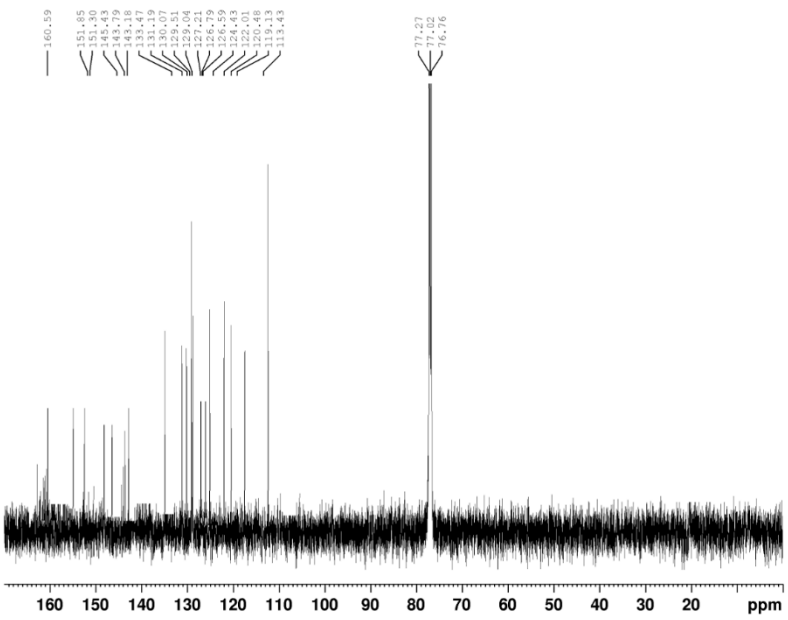
F2 - Acquisition Parameters
Date_          20231125
Time             16.50
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   4
SWH          29761.904 Hz
FIDRES         0.454131 Hz
AQ           1.1010048 sec
RG                 203
DW              16.800 usec
DE               6.50 usec
TE             298.6 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       125.7703637 MHz
NUC1             13C
P1             10.00 usec
PLW1       88.00000000 W

======== CHANNEL f2 ========
SFO2       500.1320005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2           80.00 usec
PLW2       16.00000000 W
PLW12       0.36000001 W
PLW13       0.18043999 W

F2 - Processing parameters
SI               32768
SF         125.7577890 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

L[2]



BRUKER

```
Current Data Parameters
NAME        EXT-SPU-ADP-L2(500MHz)
EXPNO                1
PROCNO               1

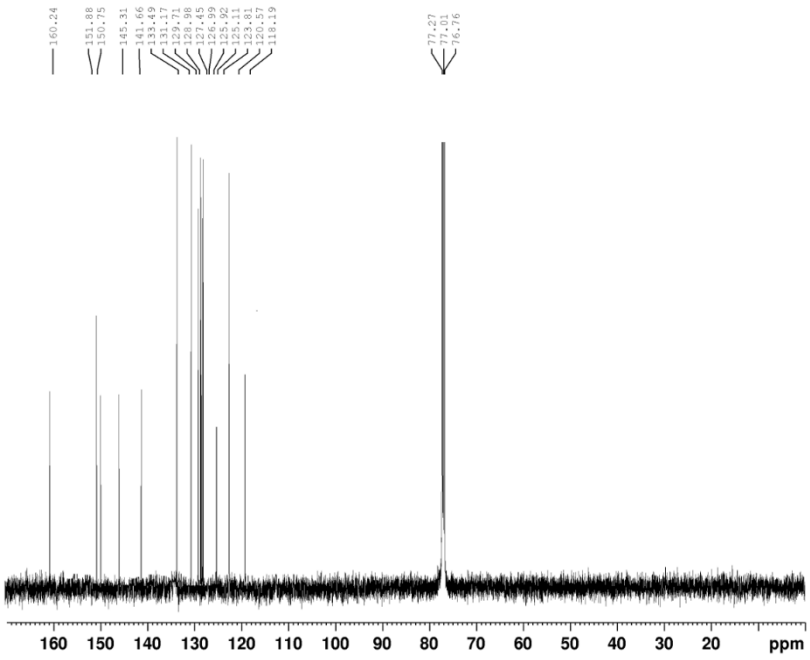
F2 - Acquisition Parameters
Date_          20231125
Time             17.22
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   4
SWH          29761.904 Hz
FIDRES         0.454131 Hz
AQ           1.1010048 sec
RG                 203
DW              16.800 usec
DE               6.50 usec
TE             297.5 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       125.7703637 MHz
NUC1             13C
P1             10.00 usec
PLW1       88.00000000 W

======== CHANNEL f2 ========
SFO2       500.1320005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2           80.00 usec
PLW2       16.00000000 W
PLW12       0.36000001 W
PLW13       0.18043999 W

F2 - Processing parameters
SI               32768
SF         125.7577890 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

L^3



BRUKER

```
Current Data Parameters
NAME        EXT-SPU-ADP-L3(500MHz)
EXPNO                    1
PROCNO                   1

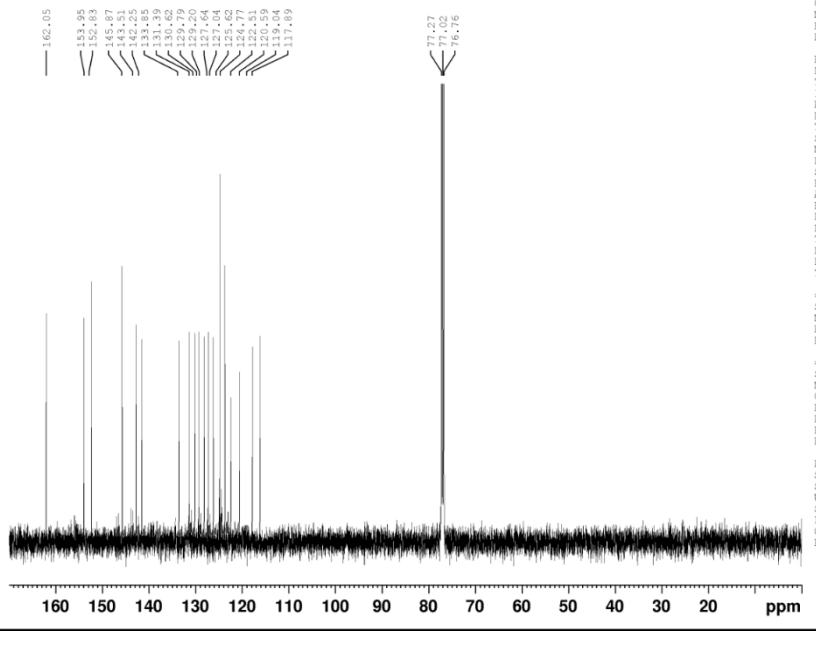
F2 - Acquisition Parameters
Date_             20231125
Time                22.58
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                   203
DW                16.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          125.7703637 MHz
NUC1                 13C
P1                 10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2          500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          16.00000000 W
PLW12          0.36000001 W
PLW13          0.18043999 W

F2 - Processing parameters
SI                   32768
SF            125.7577890 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

L^4



BRUKER

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Current Data Parameters
NAME        EXT-SPU-ADP-L4(500MHz)
EXPNO                    1
PROCNO                   1

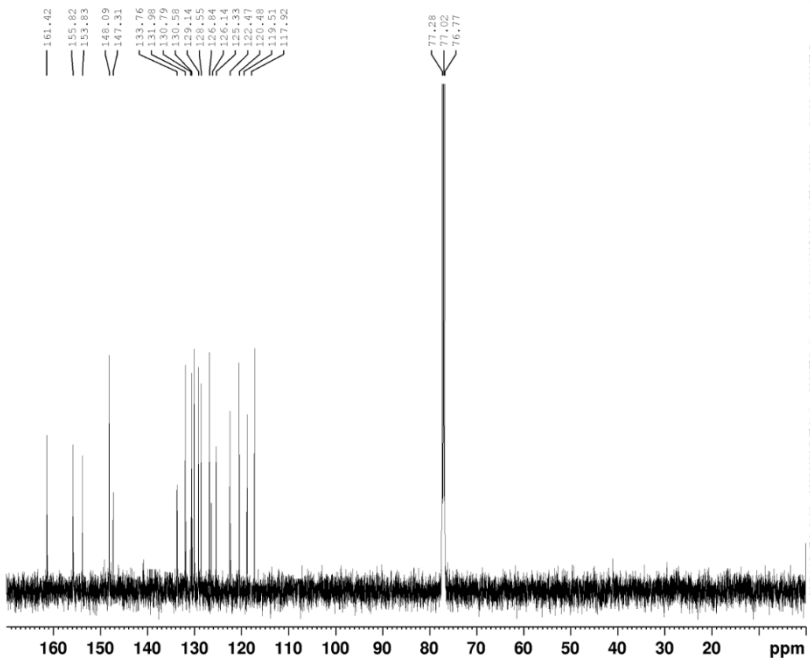
F2 - Acquisition Parameters
Date_             20231126
Time                 0.02
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                   203
DW                16.800 usec
DE                 6.50 usec
TE                297.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          125.7703637 MHz
NUC1                 13C
P1                 10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2          500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          16.00000000 W
PLW12          0.36000001 W
PLW13          0.18043999 W

F2 - Processing parameters
SI                   32768
SF            125.7577890 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

L[5]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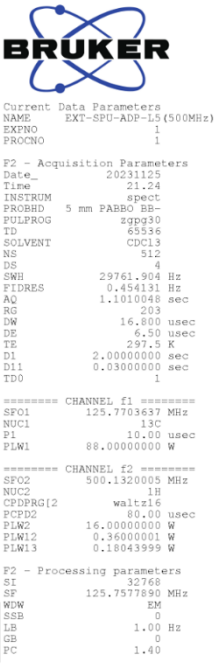
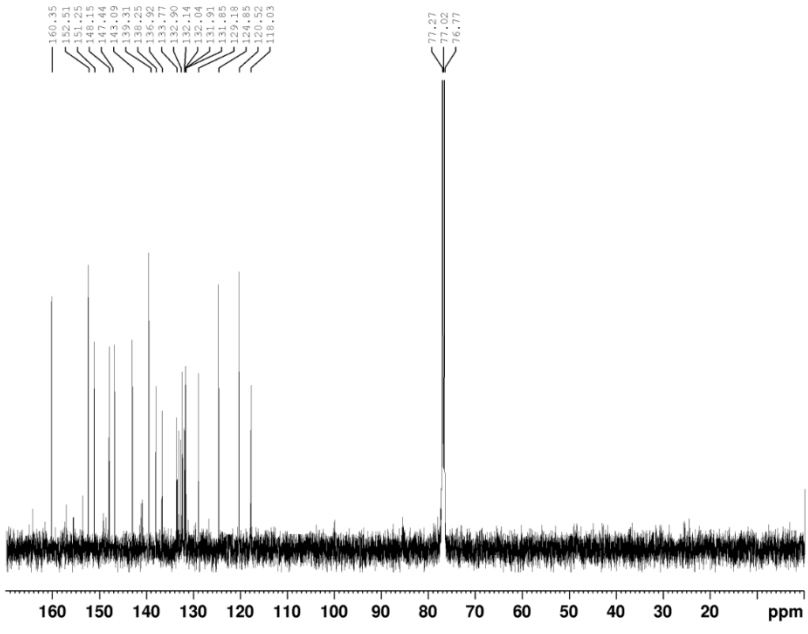
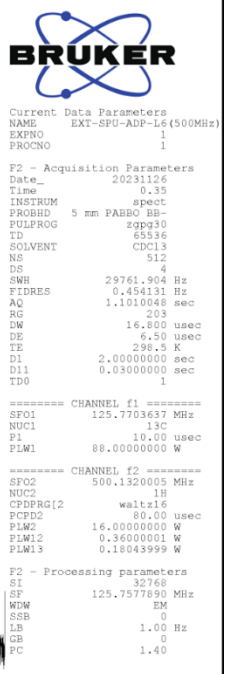
153.83
148.09
147.31
133.76
131.98
130.79
130.58
128.44
128.15
126.84
126.14
125.33
122.47
120.48
119.51
117.32
77.28
77.02
76.77
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

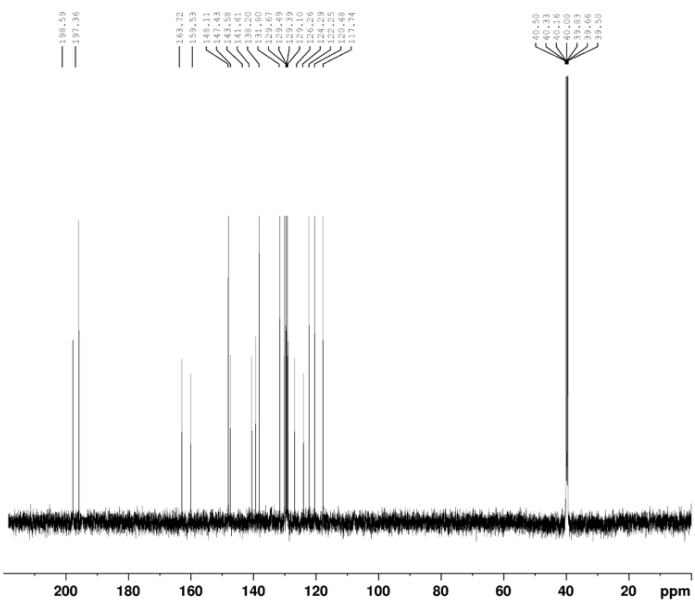

BRUKER
Current Data Parameters
NAME EXT-SPU-ADP-L5(500MHz)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231125
Time 21.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 10.00 usec
PLW1 88.00000000 W
======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.36000001 W
PLW13 0.18043999 W
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

L[6]


160.35
152.51
151.25
148.15
147.44
147.09
139.31
136.25
136.92
133.77
132.90
132.14
132.04
131.91
131.85
129.18
124.85
120.52
118.03
77.27
77.02
76.77
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


BRUKER
Current Data Parameters
NAME EXT-SPU-ADP-L6(500MHz)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231126
Time 0.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 10.00 usec
PLW1 88.00000000 W
======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 16.00000000 W
PLW12 0.36000001 W
PLW13 0.18043999 W
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C1



BRUKER

```
Current Data Parameters
NAME       EXT-SPU-ADP-C1(500MHz)
EXPNO                   1
PROCNO                  1

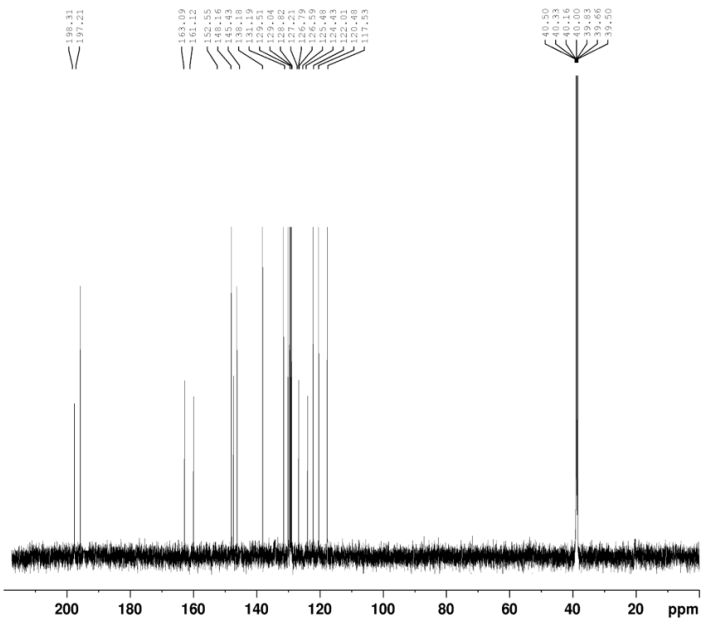
F2 - Acquisition Parameters
Date_           20231125
Time              16.50
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT            DMSO
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG                  203
DW              16.800 usec
DE               6.50 usec
TE              290.6 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7703637 MHz
NUC1              13C
P1              10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.1320005 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        16.00000000 W
PLW12        0.36000001 W
PLW13        0.18043999 W

F2 - Processing parameters
SI                32768
SF          125.7577890 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

C2



BRUKER

```
Current Data Parameters
NAME       EXT-SPU-ADP-C2(500MHz)
EXPNO                   1
PROCNO                  1

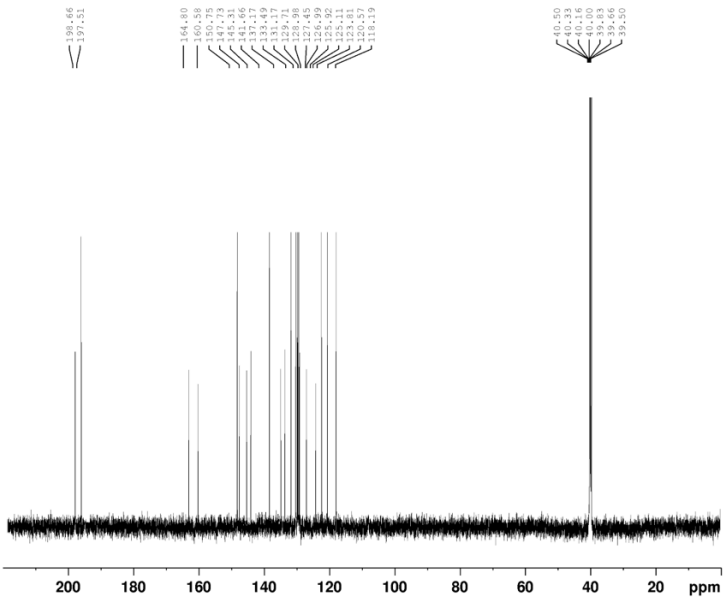
F2 - Acquisition Parameters
Date_           20231125
Time              17.22
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT            DMSO
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG                  203
DW              16.800 usec
DE               6.50 usec
TE              297.5 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7703637 MHz
NUC1              13C
P1              10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.1320005 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        16.00000000 W
PLW12        0.36000001 W
PLW13        0.18043999 W

F2 - Processing parameters
SI                32768
SF          125.7577890 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

C³



BRUKER

```
Current Data Parameters
NAME        EXT-SPU-ADP-C3(500MHz)
EXPNO                1
PROCNO               1

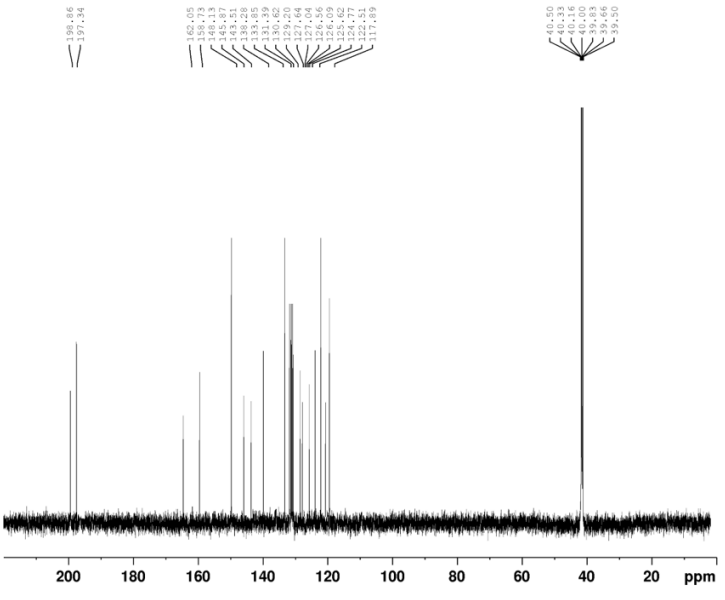
F2 - Acquisition Parameters
Date_          20231125
Time              22.58
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  203
DW               16.800 usec
DE                6.50 usec
TE              298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        125.7703637 MHz
NUC1              13C
P1              10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.1320005 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        16.00000000 W
PLW12        0.36000001 W
PLW13        0.18043999 W

F2 - Processing parameters
SI                32768
SF          125.7577890 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

C⁴



BRUKER

```
Current Data Parameters
NAME        EXT-SPU-ADP-C4(500MHz)
EXPNO                1
PROCNO               1

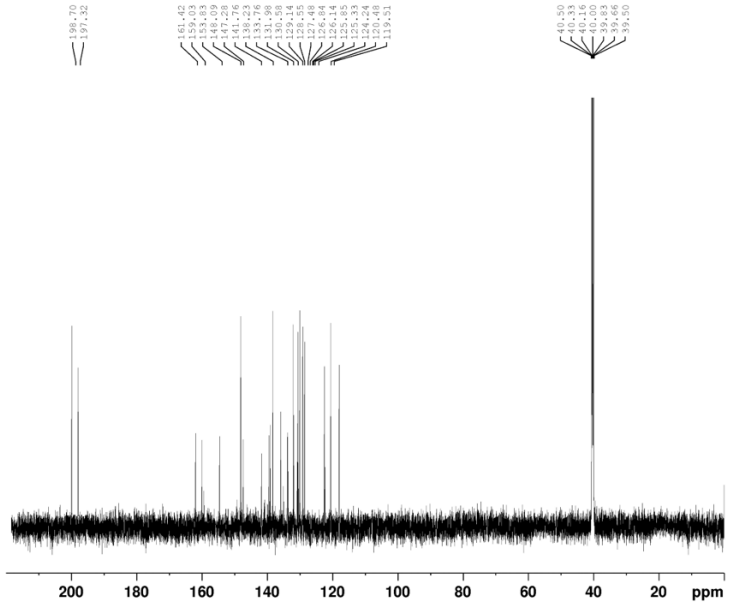
F2 - Acquisition Parameters
Date_          20231126
Time              0.02
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  203
DW               16.800 usec
DE                6.50 usec
TE              297.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        125.7703637 MHz
NUC1              13C
P1              10.00 usec
PLW1        88.00000000 W

======== CHANNEL f2 ========
SFO2        500.1320005 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        16.00000000 W
PLW12        0.36000001 W
PLW13        0.18043999 W

F2 - Processing parameters
SI                32768
SF          125.7577890 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

C5



BRUKER

```
Current Data Parameters
NAME        EXT-SPU-ADP-C5(500MHz)
EXPNO                          1
PROCNO                         1

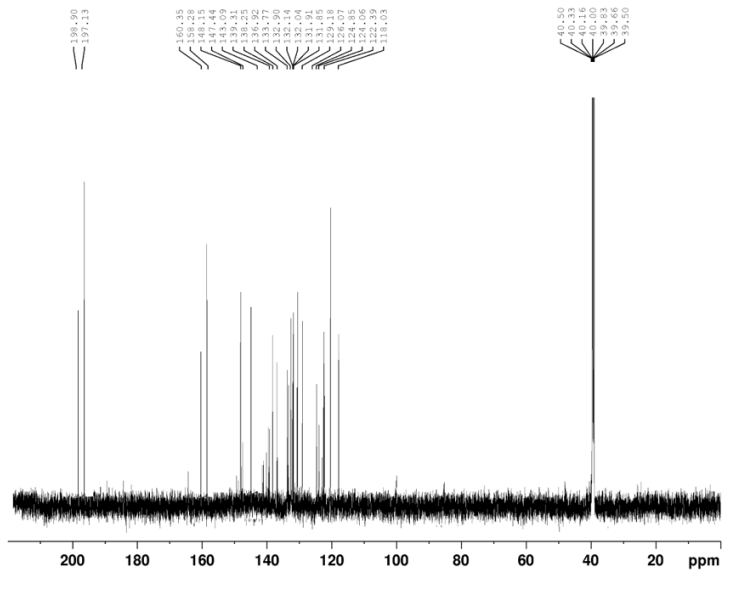
F2 - Acquisition Parameters
Date_                   20231125
Time                       21.24
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                    DMSO
NS                           512
DS                             4
SWH                   29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010048 sec
RG                           203
DW                        16.800 usec
DE                         6.50 usec
TE                        297.5 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                125.7703637 MHz
NUC1                        13C
P1                        10.00 usec
PLW1                88.00000000 W

======== CHANNEL f2 ========
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                16.00000000 W
PLW12                0.36000001 W
PLW13                0.18043999 W

F2 - Processing parameters
SI                         32768
SF                  125.7577890 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                          1.40
```

C6



BRUKER

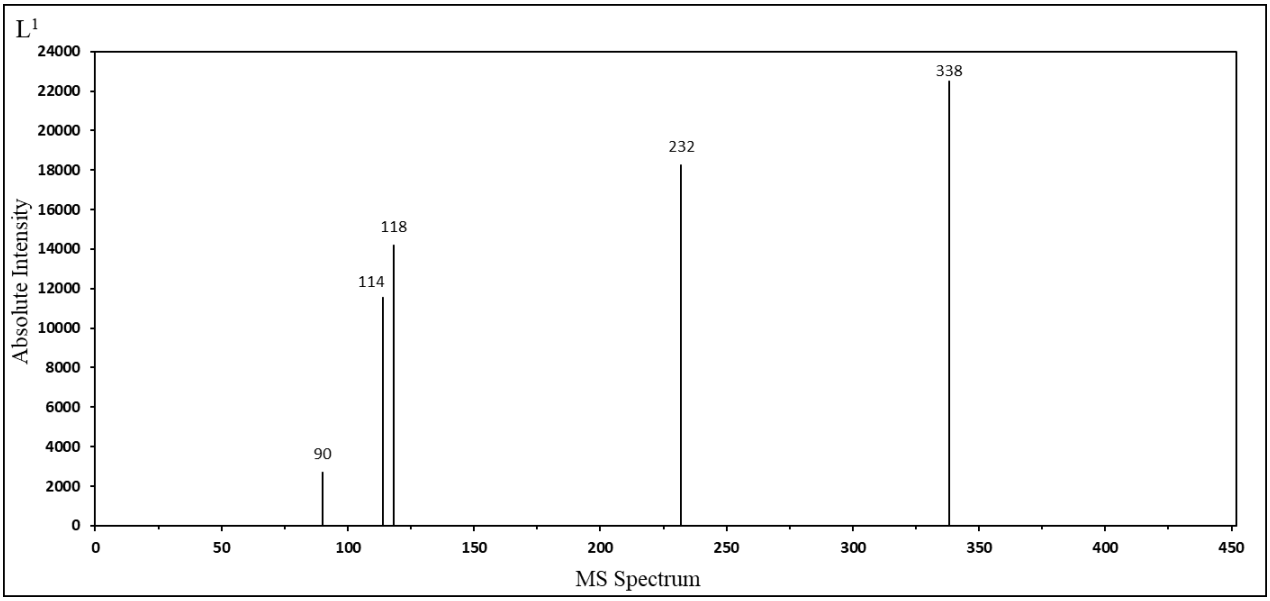
```
Current Data Parameters
NAME        EXT-SPU-ADP-C6(500MHz)
EXPNO                          1
PROCNO                         1

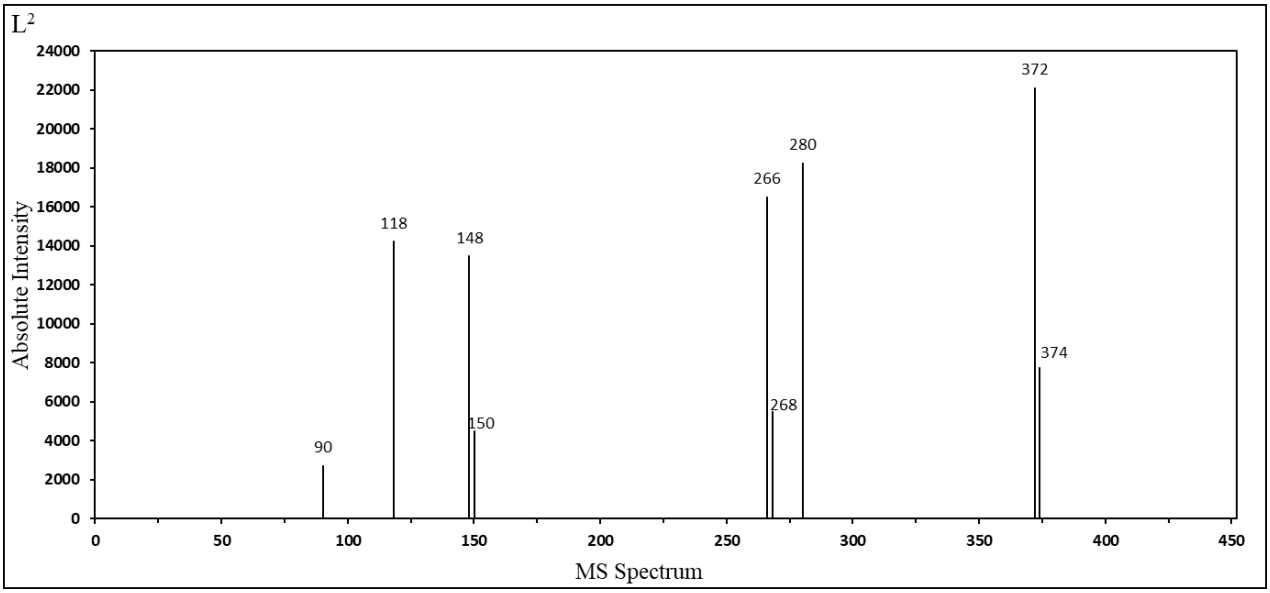
F2 - Acquisition Parameters
Date_                   20231126
Time                       0.35
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                    DMSO
NS                           512
DS                             4
SWH                   29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010048 sec
RG                           203
DW                        16.800 usec
DE                         6.50 usec
TE                        298.5 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                            1

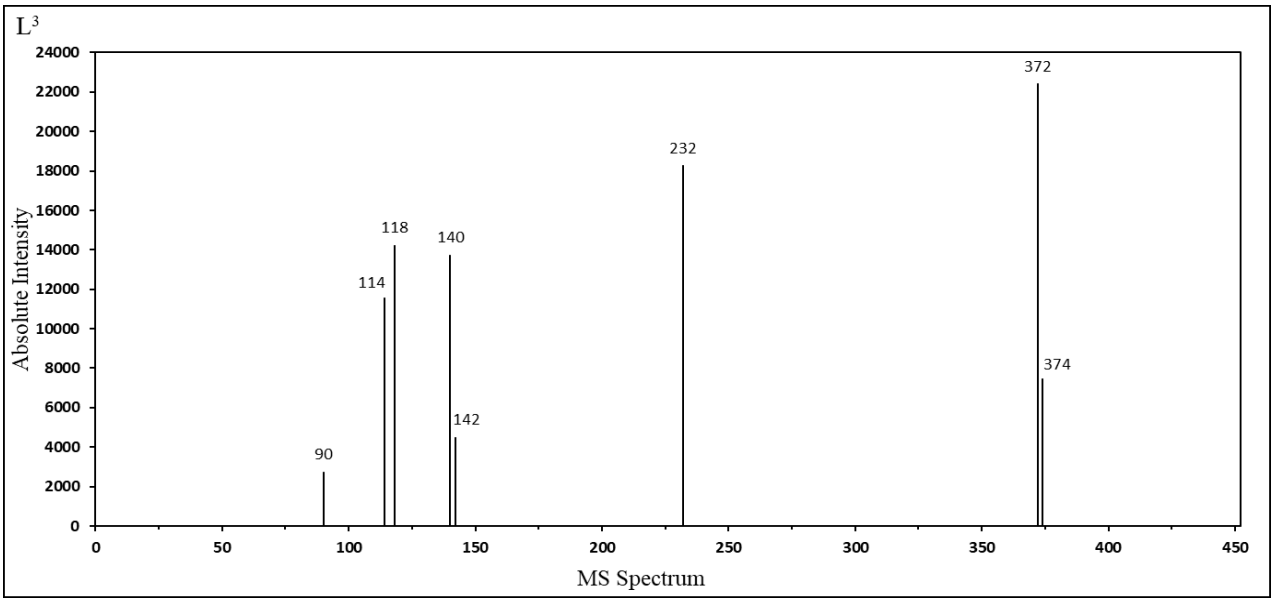
======== CHANNEL f1 ========
SFO1                125.7703637 MHz
NUC1                        13C
P1                        10.00 usec
PLW1                88.00000000 W

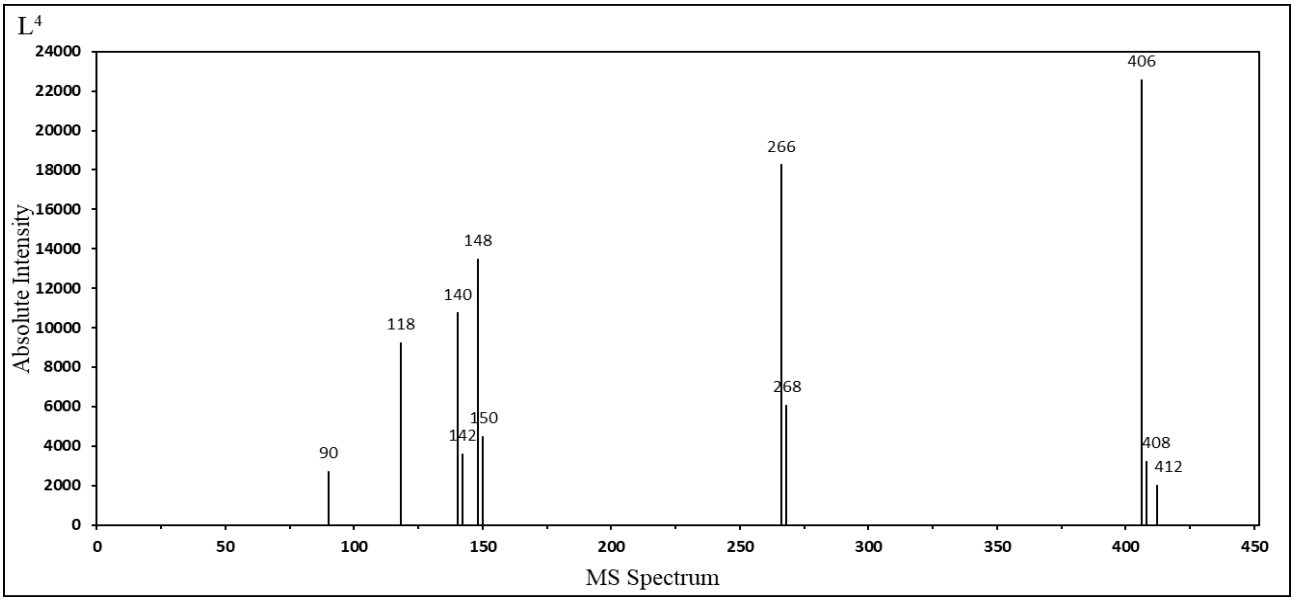
======== CHANNEL f2 ========
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                16.00000000 W
PLW12                0.36000001 W
PLW13                0.18043999 W

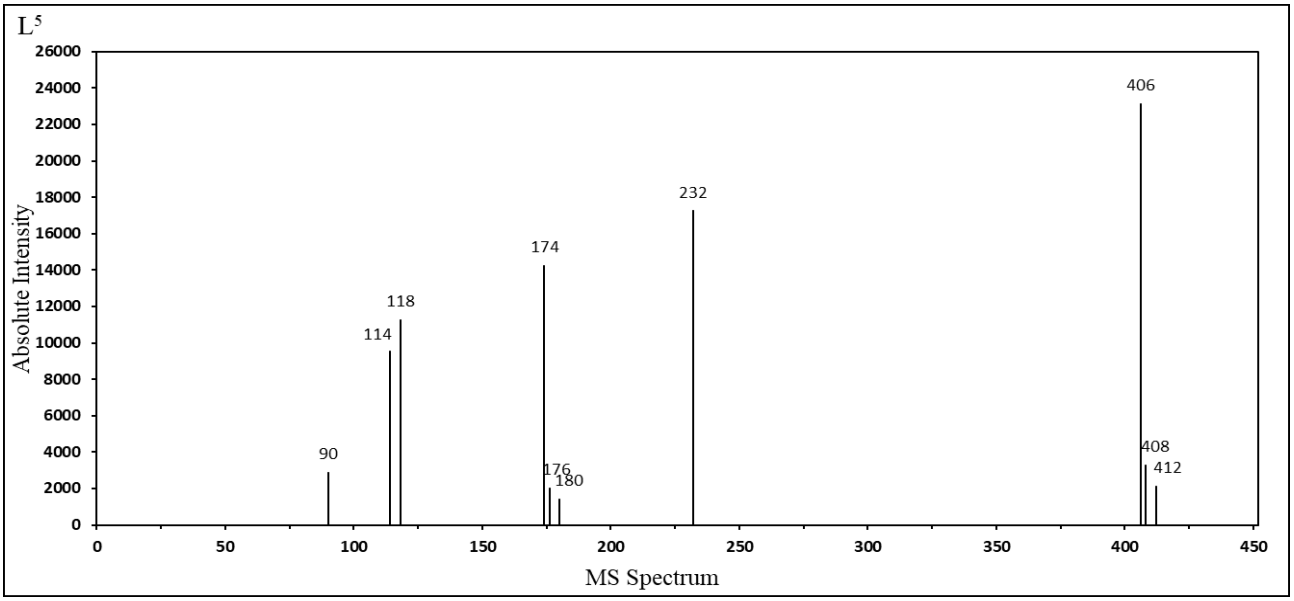
F2 - Processing parameters
SI                         32768
SF                  125.7577890 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                          1.40
```

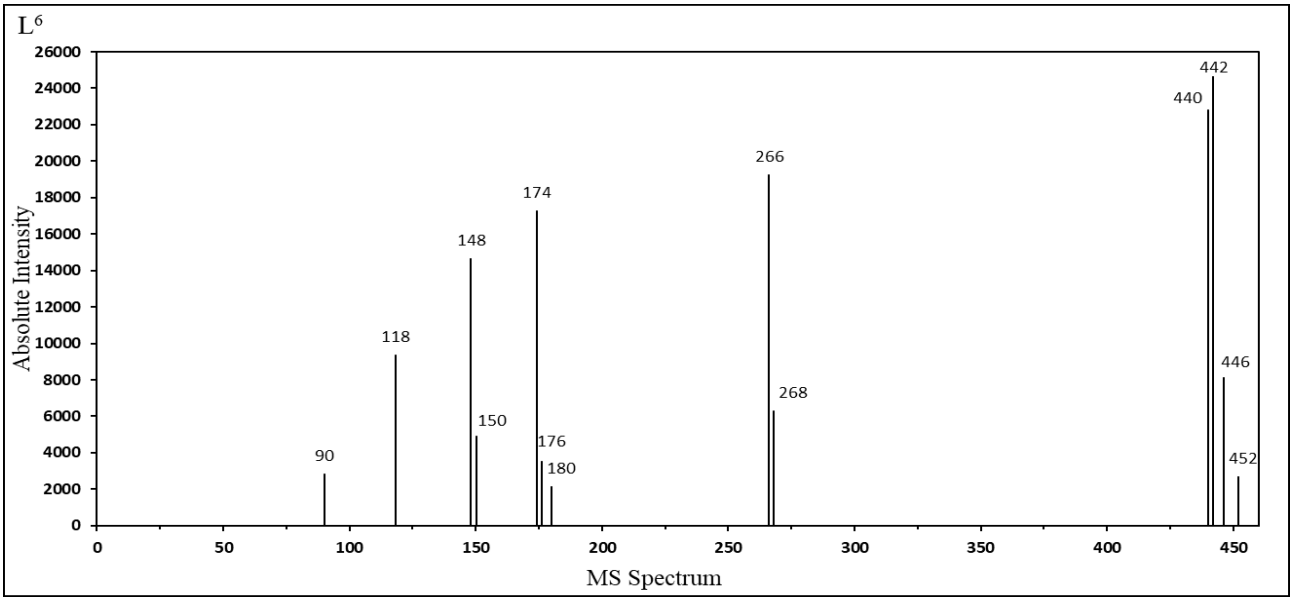

L1
Absolute Intensity
MS Spectrum
338
232
118
114
90

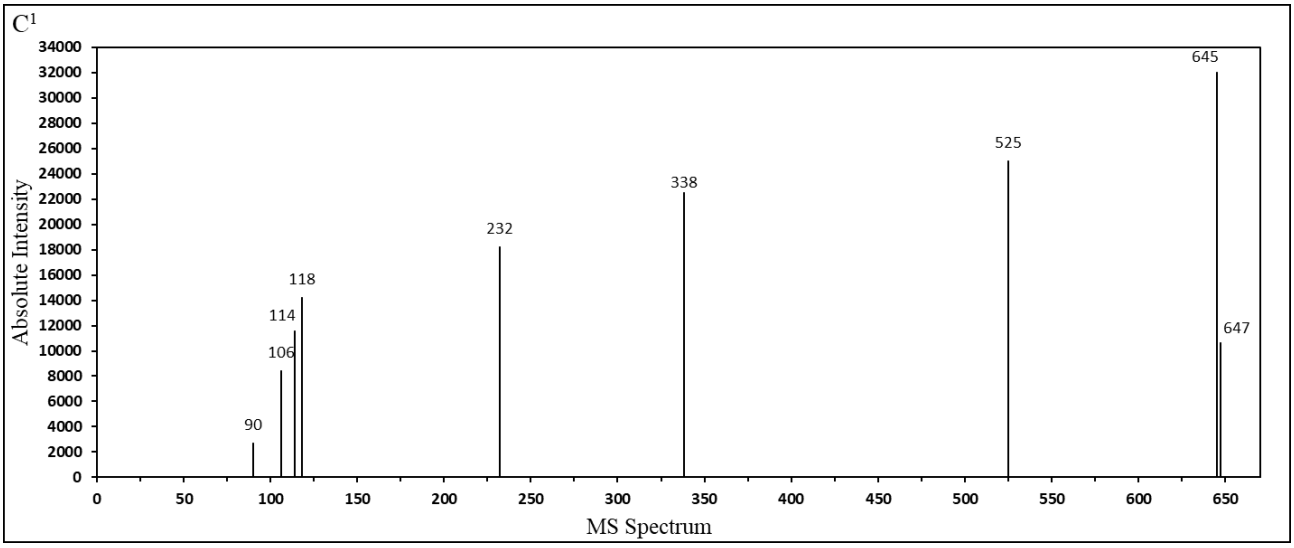

L2
Absolute Intensity
MS Spectrum
372
280
266
118
148
374
268
150
90

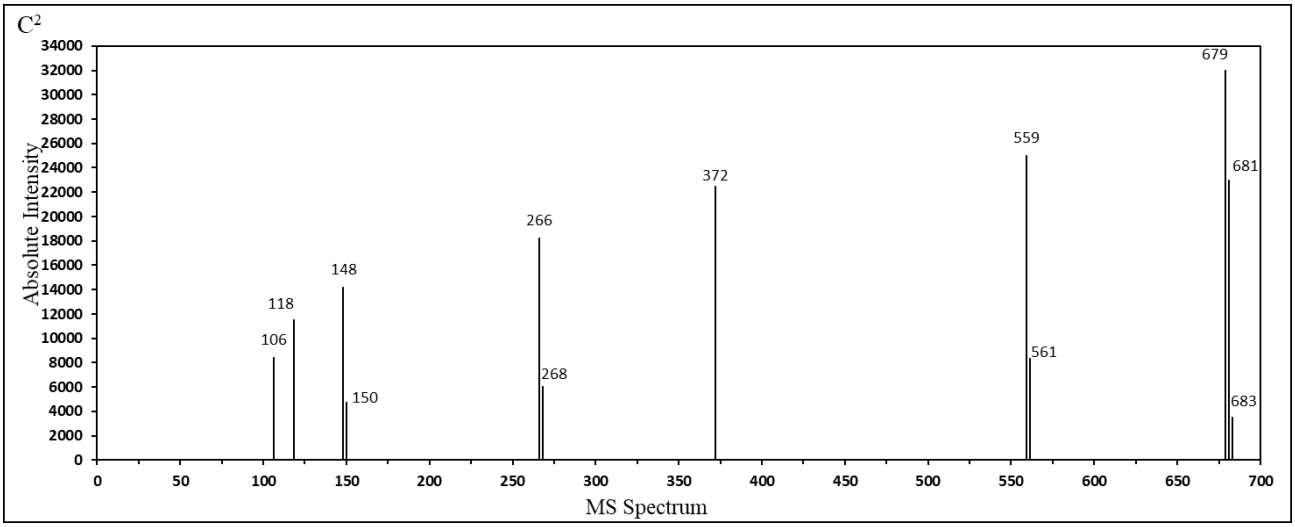

L3
Absolute Intensity
MS Spectrum
372
232
118
140
114
374
142
90

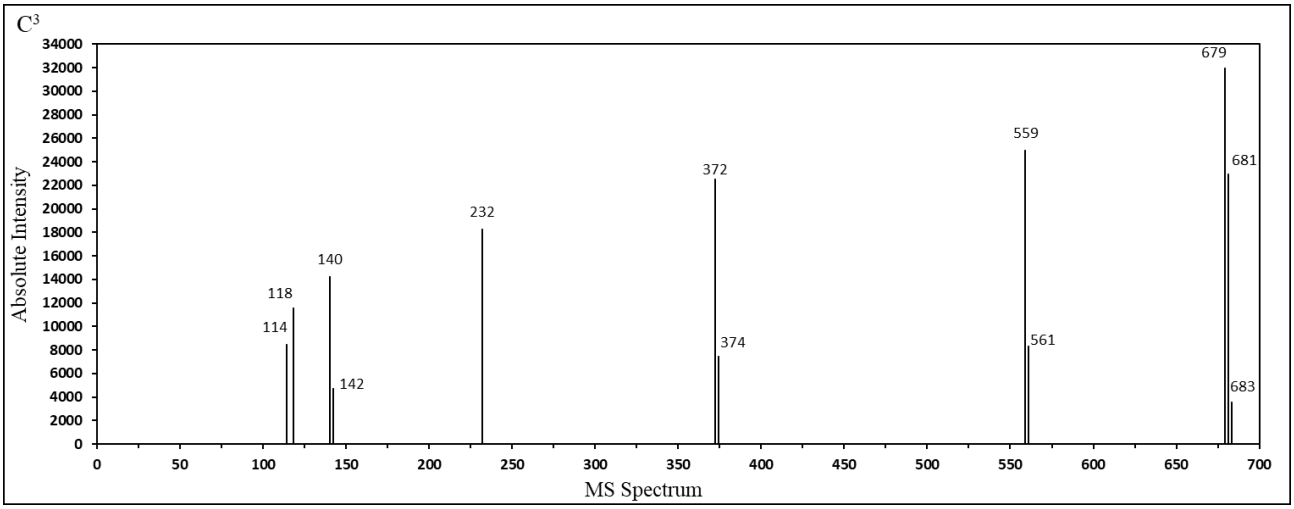

L4
Absolute Intensity
MS Spectrum
406
266
148
140
118
268
150
142
90
408
412

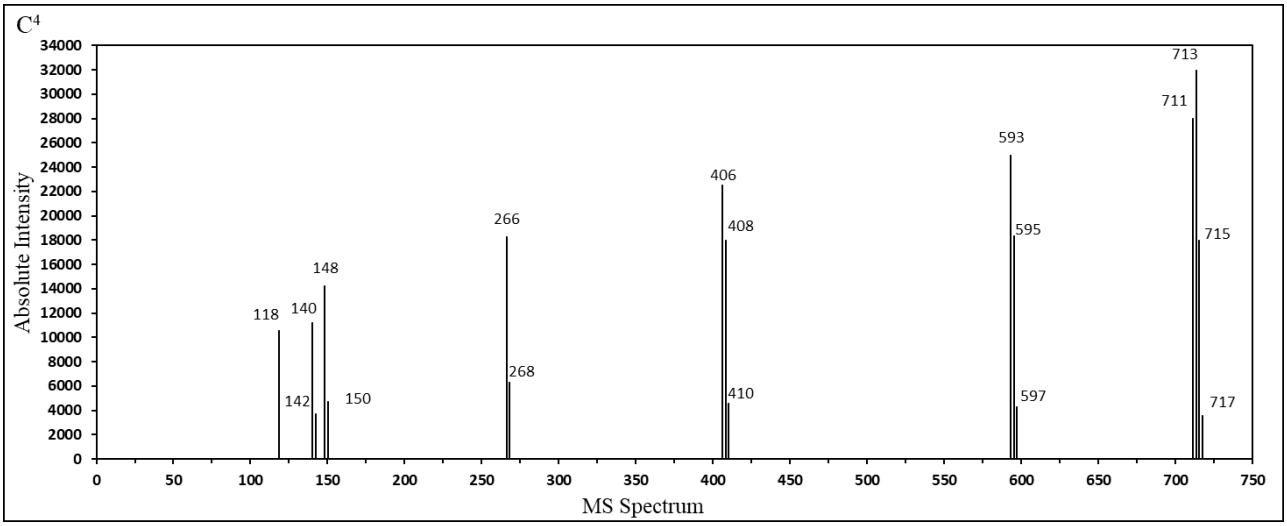

L5
Absolute Intensity
MS Spectrum
406
232
174
118
114
90
408
412
176
180

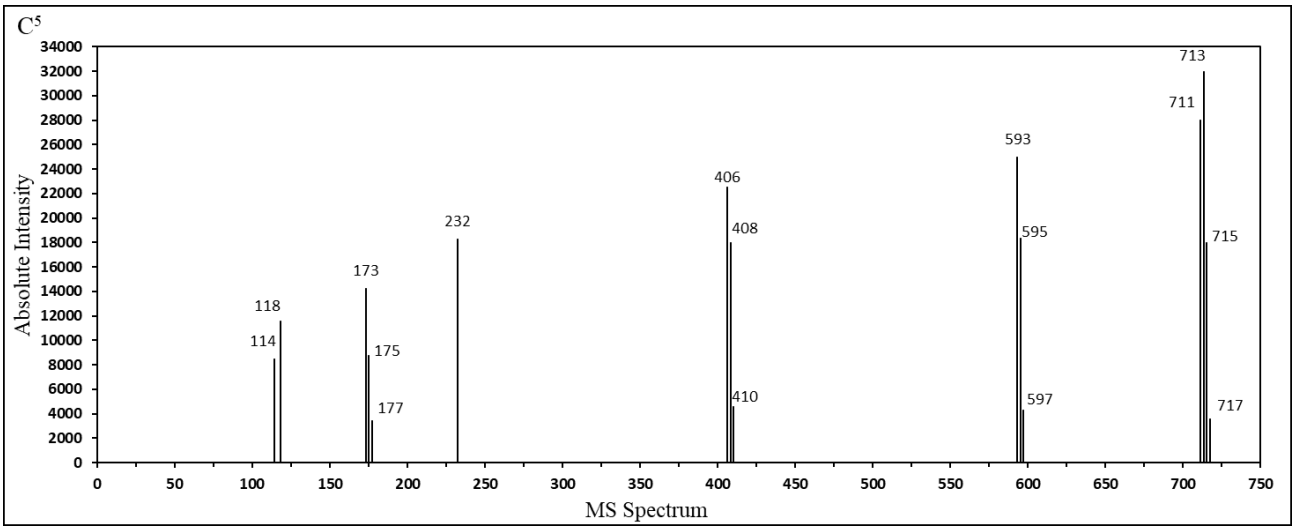

L6
Absolute Intensity
MS Spectrum
442
440
266
174
148
118
446
268
150
176
180
90
452

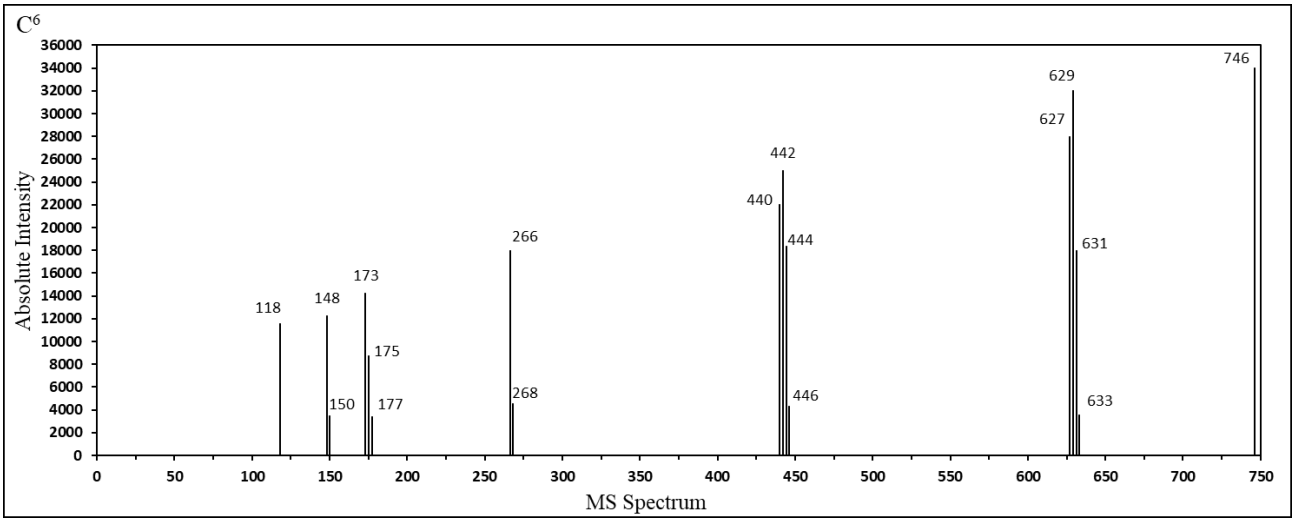

C1
Absolute Intensity
MS Spectrum
645
525
338
232
118
114
106
90
647

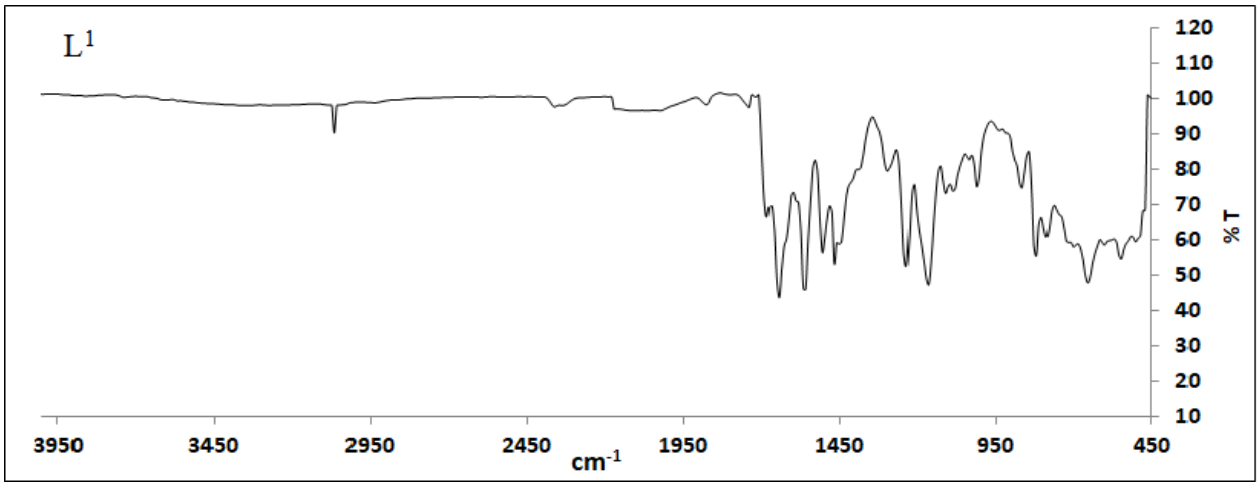

C2
Absolute Intensity
MS Spectrum
679
559
681
372
266
148
118
106
561
268
150
683

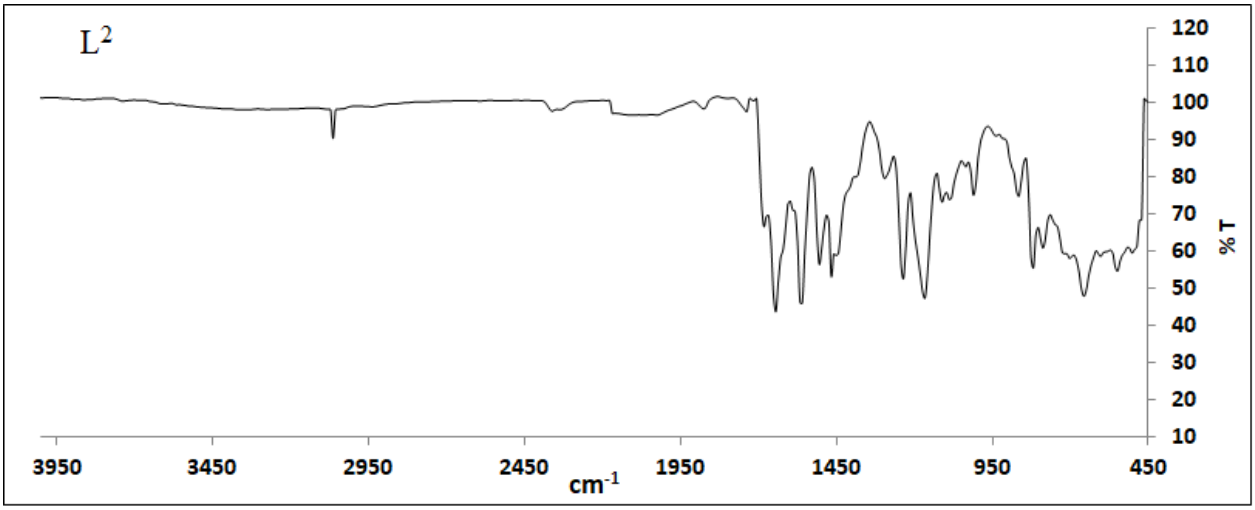

C3
Absolute Intensity
MS Spectrum
679
559
681
372
232
140
118
114
374
561
142
683


C4
Absolute Intensity
MS Spectrum
118
140
142
148
150
266
268
406
408
410
593
595
597
711
713
715
717

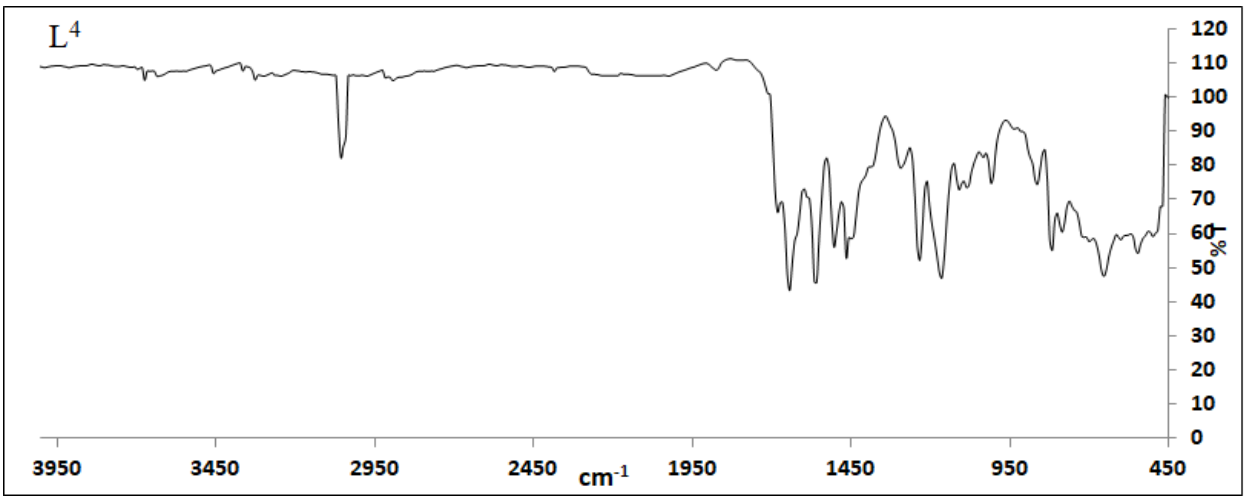

C5
Absolute Intensity
MS Spectrum
114
118
173
175
177
232
406
408
410
593
595
597
711
713
715
717

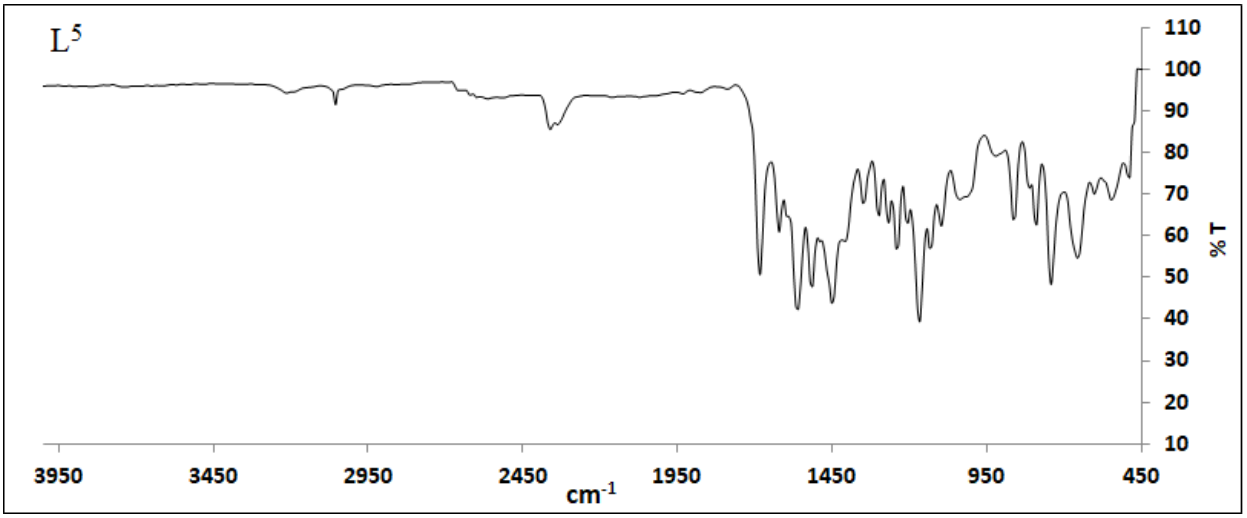

C6
Absolute Intensity
MS Spectrum
118
148
150
173
175
177
266
268
440
442
444
446
627
629
631
633
746

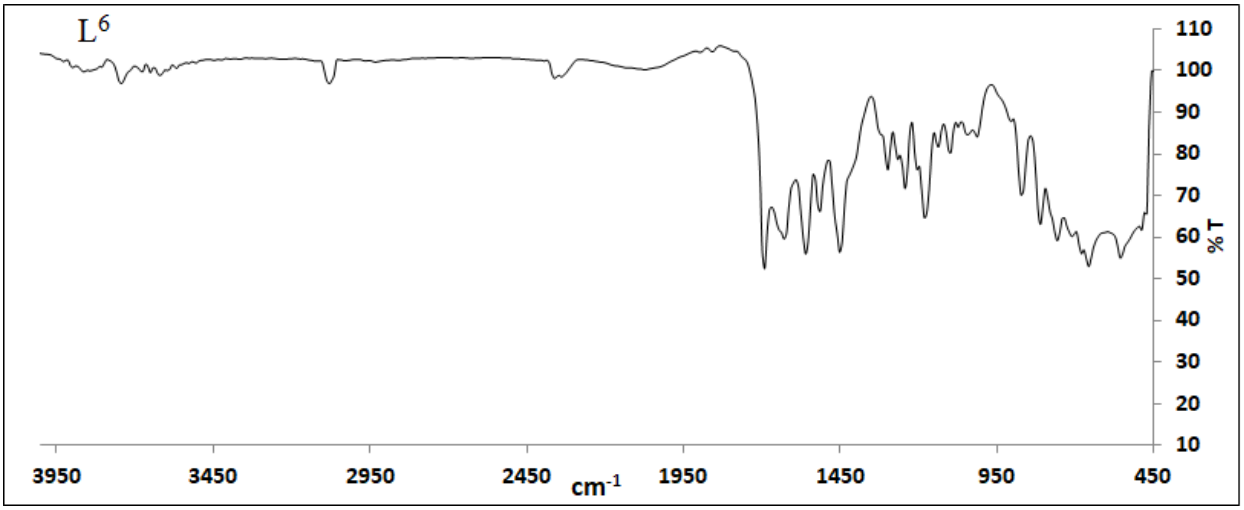

L1
120
110
100
90
80
70
60
50
40
30
20
10
% T
3950
3450
2950
2450
1950
1450
950
450
cm-1

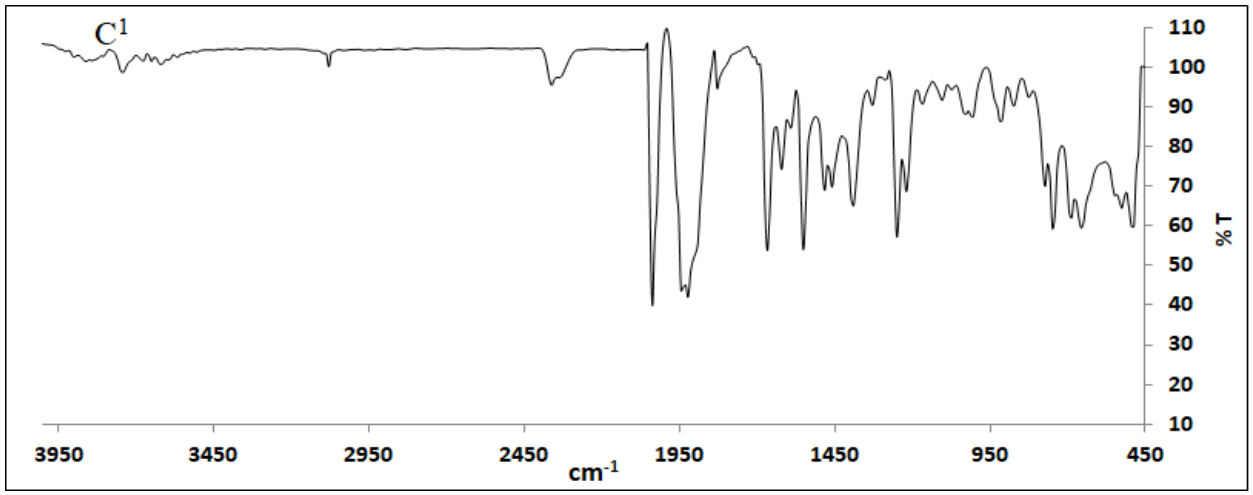

L2
120
110
100
90
80
70
60
50
40
30
20
10
% T
3950
3450
2950
2450
1950
1450
950
450
cm-1

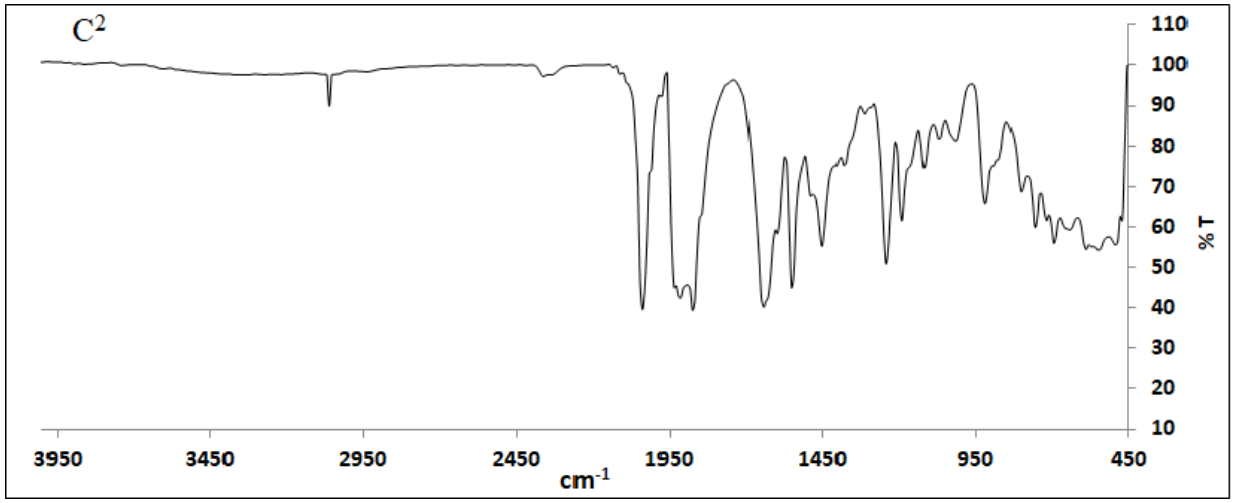

L3
110
100
90
80
70
60
50
40
30
20
10
% T
3950
3450
2950
2450
1950
1450
950
450
cm-1

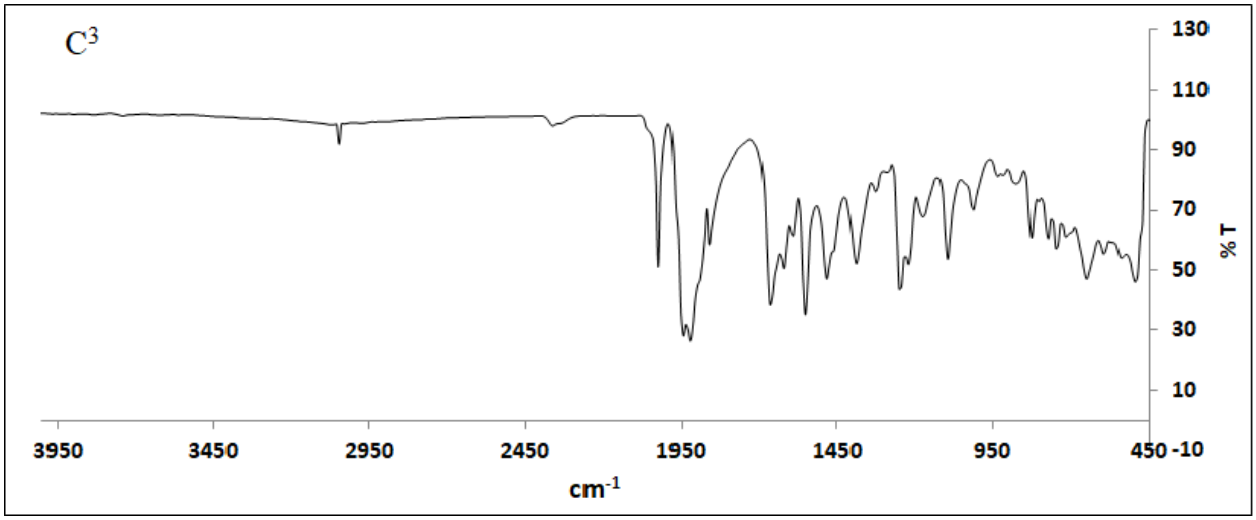

L4
120
110
100
90
80
70
60
50
40
30
20
10
0
%T
3950
3450
2950
2450
cm-1
1950
1450
950
450

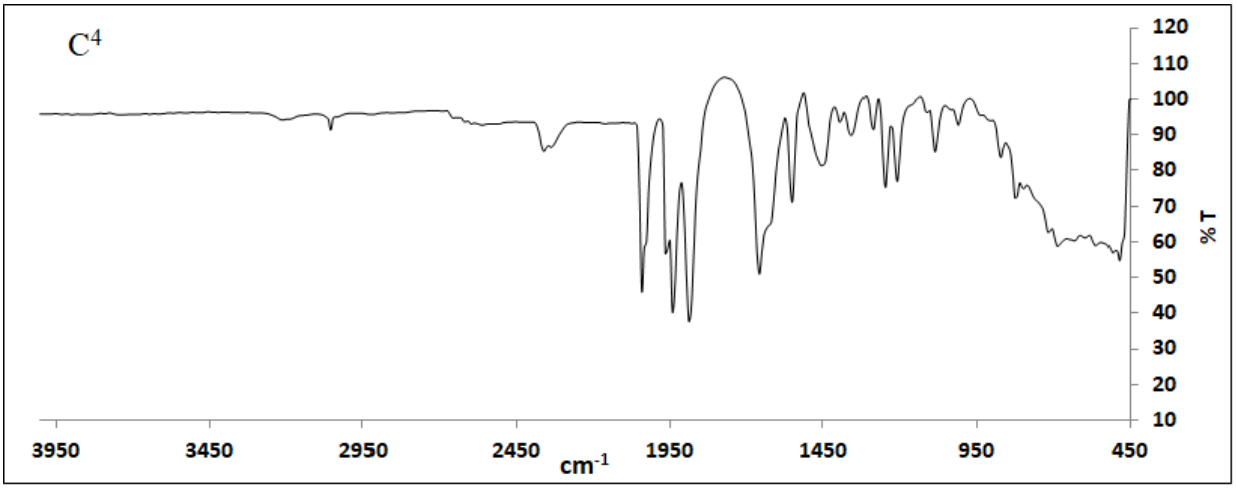

L5
110
100
90
80
70
60
50
40
30
20
10
% T
3950
3450
2950
2450
cm-1
1950
1450
950
450

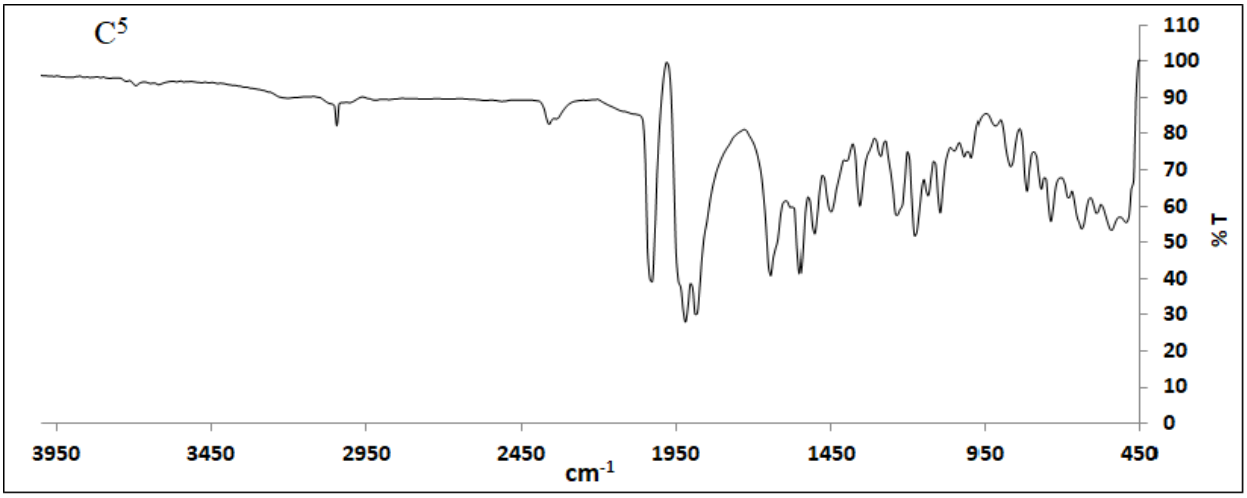

L6
110
100
90
80
70
60
50
40
30
20
10
% T
3950
3450
2950
2450
cm-1
1950
1450
950
450

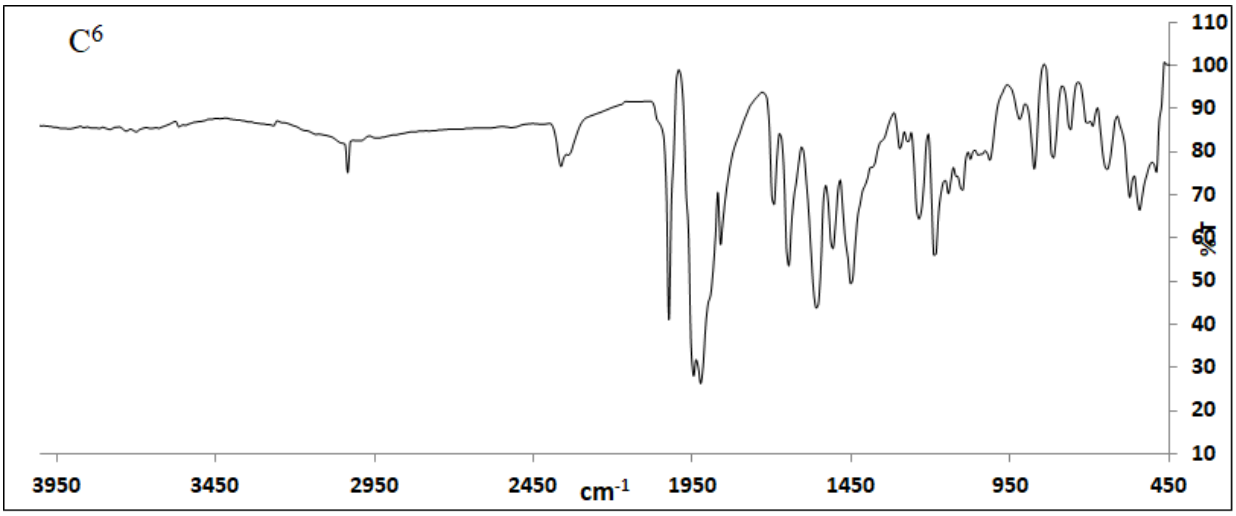

C1
110
100
90
80
70
60
50
40
30
20
10
% T
3950
3450
2950
2450
1950
1450
950
450
cm-1


C2
110
100
90
80
70
60
50
40
30
20
10
% T
3950
3450
2950
2450
1950
1450
950
450
cm-1


C3
130
110
90
70
50
30
10
-10
% T
3950
3450
2950
2450
1950
1450
950
450
cm-1


C4
120
110
100
90
80
70
60
50
40
30
20
10
% T
3950
3450
2950
2450
cm-1
1950
1450
950
450


C5
110
100
90
80
70
60
50
40
30
20
10
0
% T
3950
3450
2950
2450
cm-1
1950
1450
950
450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ESI 2: DFT data

(Table of bond length, bond angle, and Mulliken charges for ligands L^1–L^6 and complexes C^1–C^6)

L^1

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3938	R(15,20)	1.5995
R(1,6)	1.4115	R(17,18)	1.5011
R(1,7)	1.07	R(18,19)	1.2624
R(2,3)	1.3867	R(19,21)	1.5018
R(2,11)	1.4927	R(20,21)	1.3859
R(3,4)	1.3908	R(22,23)	1.2936
R(3,22)	1.5178	R(23,24)	1.4
R(4,5)	1.4086	R(24,25)	1
R(4,8)	1.07	R(24,26)	1.47
R(5,6)	1.4186	R(26,27)	1.54
R(5,9)	1.07	R(26,30)	1.3552
R(6,10)	1.07	R(27,28)	1.3552
R(11,12)	1.5159	R(27,32)	1.07
R(11,14)	1.4833	R(28,29)	1.54
R(12,13)	1.3183	R(28,33)	1.07
R(12,22)	1.5247	R(29,31)	1.3552
R(13,20)	1.4599	R(29,34)	1.07
R(14,15)	1.5177	R(30,31)	1.54
R(14,16)	1.2584	R(30,36)	1.07
R(15,17)	1.3854	R(31,35)	1.07

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.2335	A(17,18,19)	114.4711
A(2,1,7)	120.8846	A(18,19,21)	114.5781
A(6,1,7)	120.8803	A(13,20,15)	119.6016
A(1,2,3)	120.6161	A(13,20,21)	131.486
A(1,2,11)	126.7665	A(15,20,21)	108.8973
A(3,2,11)	112.6154	A(19,21,20)	136.4042
A(2,3,4)	122.3861	A(3,22,12)	104.6191
A(2,3,22)	108.7551	A(3,22,23)	127.6645
A(4,3,22)	128.8464	A(12,22,23)	127.7003
A(3,4,5)	117.7075	A(22,23,24)	120
A(3,4,8)	121.1479	A(23,24,25)	109.4712
A(5,4,8)	121.143	A(23,24,26)	109.4712

A(4,5,6)	120.245	A(25,24,26)	109.4712
A(4,5,9)	119.8769	A(24,26,27)	120
A(6,5,9)	119.8777	A(24,26,30)	120
A(1,6,5)	120.5107	A(27,26,30)	120
A(1,6,10)	119.7441	A(26,27,28)	120
A(5,6,10)	119.7449	A(26,27,32)	120
A(2,11,12)	103.0323	A(28,27,32)	120
A(2,11,14)	113.9795	A(27,28,29)	120
A(12,11,14)	114.567	A(27,28,33)	120
A(11,12,13)	127.2685	A(29,28,33)	120
A(11,12,22)	107.8991	A(28,29,31)	120
A(13,12,22)	124.8301	A(28,29,34)	120
A(12,13,20)	116.2261	A(31,29,34)	120
A(11,14,15)	115.0748	A(26,30,31)	120
A(11,14,16)	122.4471	A(26,30,36)	120
A(15,14,16)	122.4726	A(31,30,36)	120
A(14,15,17)	132.1974	A(29,31,30)	120
A(14,15,20)	118.419	A(29,31,35)	120
A(17,15,20)	109.3834	A(30,31,35)	120
A(15,17,18)	136.1971		

L^2

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3938	R(14,19)	1.5995
R(1,6)	1.4115	R(16,17)	1.5011
R(1,7)	1.07	R(17,18)	1.2624
R(2,3)	1.3867	R(18,20)	1.5018
R(2,10)	1.4927	R(19,20)	1.3859
R(3,4)	1.3908	R(21,22)	1.2936
R(3,21)	1.5178	R(22,23)	1.4
R(4,5)	1.4086	R(23,24)	1
R(4,8)	1.07	R(23,25)	1.47
R(5,6)	1.4186	R(25,26)	1.54
R(5,36)	1.76	R(25,29)	1.3552
R(6,9)	1.07	R(26,27)	1.3552
R(10,11)	1.5159	R(26,31)	1.07
R(10,13)	1.4833	R(27,28)	1.54
R(11,12)	1.3183	R(27,32)	1.07
R(11,21)	1.5247	R(28,30)	1.3552
R(12,19)	1.4599	R(28,33)	1.07
R(13,14)	1.5177	R(29,30)	1.54
R(13,15)	1.2584	R(29,35)	1.07
R(14,16)	1.3854	R(30,34)	1.07

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.2335	A(16,17,18)	114.4711
A(2,1,7)	120.8846	A(17,18,20)	114.5781
A(6,1,7)	120.8803	A(12,19,14)	119.6016
A(1,2,3)	120.6161	A(12,19,20)	131.486
A(1,2,10)	126.7665	A(14,19,20)	108.8973
A(3,2,10)	112.6154	A(18,20,19)	136.4042
A(2,3,4)	122.3861	A(3,21,11)	104.6191
A(2,3,21)	108.7551	A(3,21,22)	127.6645
A(4,3,21)	128.8464	A(11,21,22)	127.7003
A(3,4,5)	117.7075	A(21,22,23)	120
A(3,4,8)	121.1479	A(22,23,24)	109.4712
A(5,4,8)	121.143	A(22,23,25)	109.4712
A(4,5,6)	120.245	A(24,23,25)	109.4712
A(4,5,36)	119.8769	A(23,25,26)	120
A(6,5,36)	119.8777	A(23,25,29)	120
A(1,6,5)	120.5107	A(26,25,29)	120
A(1,6,9)	119.7441	A(25,26,27)	120
A(5,6,9)	119.7449	A(25,26,31)	120
A(2,10,11)	103.0323	A(27,26,31)	120
A(2,10,13)	113.9795	A(26,27,28)	120
A(11,10,13)	114.567	A(26,27,32)	120
A(10,11,12)	127.2685	A(28,27,32)	120
A(10,11,21)	107.8991	A(27,28,30)	120
A(12,11,21)	124.8301	A(27,28,33)	120
A(11,12,19)	116.2261	A(30,28,33)	120
A(10,13,14)	115.0748	A(25,29,30)	120
A(10,13,15)	122.4471	A(25,29,35)	120
A(14,13,15)	122.4726	A(30,29,35)	120
A(13,14,16)	132.1974	A(28,30,29)	120
A(13,14,19)	118.419	A(28,30,34)	120
A(16,14,19)	109.3834	A(29,30,34)	120
A(14,16,17)	136.1971		

L^3

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3938	R(14,19)	1.5995
R(1,6)	1.4115	R(16,17)	1.5011
R(1,7)	1.07	R(17,18)	1.2624
R(2,3)	1.3867	R(18,20)	1.5018
R(2,10)	1.4927	R(19,20)	1.3859

R(3,4)	1.3908	R(21,22)	1.2936
R(3,21)	1.5178	R(22,23)	1.4
R(4,5)	1.4086	R(23,24)	1
R(4,8)	1.07	R(23,25)	1.47
R(5,6)	1.4186	R(25,26)	1.54
R(5,35)	1.07	R(25,29)	1.3552
R(6,9)	1.07	R(26,27)	1.3552
R(10,11)	1.5159	R(26,31)	1.07
R(10,13)	1.4833	R(27,28)	1.54
R(11,12)	1.3183	R(27,32)	1.07
R(11,21)	1.5247	R(28,30)	1.3552
R(12,19)	1.4599	R(28,36)	1.76
R(13,14)	1.5177	R(29,30)	1.54
R(13,15)	1.2584	R(29,34)	1.07
R(14,16)	1.3854	R(30,33)	1.07

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.2335	A(16,17,18)	114.4711
A(2,1,7)	120.8846	A(17,18,20)	114.5781
A(6,1,7)	120.8803	A(12,19,14)	119.6016
A(1,2,3)	120.6161	A(12,19,20)	131.486
A(1,2,10)	126.7665	A(14,19,20)	108.8973
A(3,2,10)	112.6154	A(18,20,19)	136.4042
A(2,3,4)	122.3861	A(3,21,11)	104.6191
A(2,3,21)	108.7551	A(3,21,22)	127.6645
A(4,3,21)	128.8464	A(11,21,22)	127.7003
A(3,4,5)	117.7075	A(21,22,23)	120
A(3,4,8)	121.1479	A(22,23,24)	109.4712
A(5,4,8)	121.143	A(22,23,25)	109.4712
A(4,5,6)	120.245	A(24,23,25)	109.4712
A(4,5,35)	119.8769	A(23,25,26)	120
A(6,5,35)	119.8777	A(23,25,29)	120
A(1,6,5)	120.5107	A(26,25,29)	120
A(1,6,9)	119.7441	A(25,26,27)	120
A(5,6,9)	119.7449	A(25,26,31)	120
A(2,10,11)	103.0323	A(27,26,31)	120
A(2,10,13)	113.9795	A(26,27,28)	120
A(11,10,13)	114.567	A(26,27,32)	120
A(10,11,12)	127.2685	A(28,27,32)	120
A(10,11,21)	107.8991	A(27,28,30)	120
A(12,11,21)	124.8301	A(27,28,36)	120
A(11,12,19)	116.2261	A(30,28,36)	120
A(10,13,14)	115.0748	A(25,29,30)	120

A(10,13,15)	122.4471	A(25,29,34)	120
A(14,13,15)	122.4726	A(30,29,34)	120
A(13,14,16)	132.1974	A(28,30,29)	120
A(13,14,19)	118.419	A(28,30,33)	120
A(16,14,19)	109.3834	A(29,30,33)	120
A(14,16,17)	136.1971		

L^4

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3938	R(14,19)	1.5995
R(1,6)	1.4115	R(16,17)	1.5011
R(1,7)	1.07	R(17,18)	1.2624
R(2,3)	1.3867	R(18,20)	1.5018
R(2,10)	1.4927	R(19,20)	1.3859
R(3,4)	1.3908	R(21,22)	1.2936
R(3,21)	1.5178	R(22,23)	1.4
R(4,5)	1.4086	R(23,24)	1
R(4,8)	1.07	R(23,25)	1.47
R(5,6)	1.4186	R(25,26)	1.54
R(5,35)	1.76	R(25,29)	1.3552
R(6,9)	1.07	R(26,27)	1.3552
R(10,11)	1.5159	R(26,31)	1.07
R(10,13)	1.4833	R(27,28)	1.54
R(11,12)	1.3183	R(27,32)	1.07
R(11,21)	1.5247	R(28,30)	1.3552
R(12,19)	1.4599	R(28,36)	1.76
R(13,14)	1.5177	R(29,30)	1.54
R(13,15)	1.2584	R(29,34)	1.07
R(14,16)	1.3854	R(30,33)	1.07

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.2335	A(16,17,18)	114.4711
A(2,1,7)	120.8846	A(17,18,20)	114.5781
A(6,1,7)	120.8803	A(12,19,14)	119.6016
A(1,2,3)	120.6161	A(12,19,20)	131.486
A(1,2,10)	126.7665	A(14,19,20)	108.8973
A(3,2,10)	112.6154	A(18,20,19)	136.4042
A(2,3,4)	122.386	A(3,21,11)	104.6191
A(2,3,21)	108.7551	A(3,21,22)	127.6645
A(4,3,21)	128.8464	A(11,21,22)	127.7003
A(3,4,5)	117.7075	A(21,22,23)	120

A(3,4,8)	121.1479	A(22,23,24)	109.4712
A(5,4,8)	121.143	A(22,23,25)	109.4712
A(4,5,6)	120.245	A(24,23,25)	109.4712
A(4,5,35)	119.8769	A(23,25,26)	120
A(6,5,35)	119.8777	A(23,25,29)	120
A(1,6,5)	120.5107	A(26,25,29)	120
A(1,6,9)	119.7441	A(25,26,27)	120
A(5,6,9)	119.7449	A(25,26,31)	120
A(2,10,11)	103.0323	A(27,26,31)	120
A(2,10,13)	113.9795	A(26,27,28)	120
A(11,10,13)	114.567	A(26,27,32)	120
A(10,11,12)	127.2685	A(28,27,32)	120
A(10,11,21)	107.8991	A(27,28,30)	120
A(12,11,21)	124.8301	A(27,28,36)	120
A(11,12,19)	116.2261	A(30,28,36)	120
A(10,13,14)	115.0748	A(25,29,30)	120
A(10,13,15)	122.4471	A(25,29,34)	120
A(14,13,15)	122.4726	A(30,29,34)	120
A(13,14,16)	132.1974	A(28,30,29)	120
A(13,14,19)	118.419	A(28,30,33)	120
A(16,14,19)	109.3834	A(29,30,33)	120
A(14,16,17)	136.1971		

L^5

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3938	R(14,19)	1.5995
R(1,6)	1.4115	R(16,17)	1.5011
R(1,7)	1.07	R(17,18)	1.2624
R(2,3)	1.3867	R(18,20)	1.5018
R(2,10)	1.4927	R(19,20)	1.3859
R(3,4)	1.3908	R(21,22)	1.2936
R(3,21)	1.5178	R(22,23)	1.4
R(4,5)	1.4086	R(23,24)	1
R(4,8)	1.07	R(23,25)	1.47
R(5,6)	1.4186	R(25,26)	1.54
R(5,34)	1.07	R(25,29)	1.3552
R(6,9)	1.07	R(26,27)	1.3552
R(10,11)	1.5159	R(26,31)	1.07
R(10,13)	1.4833	R(27,28)	1.54
R(11,12)	1.3183	R(27,32)	1.07
R(11,21)	1.5247	R(28,30)	1.3552
R(12,19)	1.4599	R(28,35)	1.76
R(13,14)	1.5177	R(29,30)	1.54

R(13,15)	1.2584	R(29,36)	1.76
R(14,16)	1.3854	R(30,33)	1.07

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.2335	A(16,17,18)	114.4711
A(2,1,7)	120.8846	A(17,18,20)	114.5781
A(6,1,7)	120.8803	A(12,19,14)	119.6016
A(1,2,3)	120.6161	A(12,19,20)	131.486
A(1,2,10)	126.7665	A(14,19,20)	108.8973
A(3,2,10)	112.6154	A(18,20,19)	136.4042
A(2,3,4)	122.3861	A(3,21,11)	104.6191
A(2,3,21)	108.7551	A(3,21,22)	127.6645
A(4,3,21)	128.8464	A(11,21,22)	127.7003
A(3,4,5)	117.7075	A(21,22,23)	120
A(3,4,8)	121.1479	A(22,23,24)	109.4712
A(5,4,8)	121.143	A(22,23,25)	109.4712
A(4,5,6)	120.245	A(24,23,25)	109.4712
A(4,5,34)	119.8769	A(23,25,26)	120
A(6,5,34)	119.8777	A(23,25,29)	120
A(1,6,5)	120.5107	A(26,25,29)	120
A(1,6,9)	119.7441	A(25,26,27)	120
A(5,6,9)	119.7449	A(25,26,31)	120
A(2,10,11)	103.0323	A(27,26,31)	120
A(2,10,13)	113.9795	A(26,27,28)	120
A(11,10,13)	114.567	A(26,27,32)	120
A(10,11,12)	127.2685	A(28,27,32)	120
A(10,11,21)	107.8991	A(27,28,30)	120
A(12,11,21)	124.8301	A(27,28,35)	120
A(11,12,19)	116.2261	A(30,28,35)	120
A(10,13,14)	115.0748	A(25,29,30)	120
A(10,13,15)	122.4471	A(25,29,36)	120
A(14,13,15)	122.4726	A(30,29,36)	120
A(13,14,16)	132.1974	A(28,30,29)	120
A(13,14,19)	118.419	A(28,30,33)	120
A(16,14,19)	109.3834	A(29,30,33)	120
A(14,16,17)	136.1971		

L^6

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3938	R(14,19)	1.5995
R(1,6)	1.4115	R(16,17)	1.5011
R(1,7)	1.07	R(17,18)	1.2624

R(2,3)	1.3867	R(18,20)	1.5018
R(2,10)	1.4927	R(19,20)	1.3859
R(3,4)	1.3908	R(21,22)	1.2936
R(3,21)	1.5178	R(22,23)	1.4
R(4,5)	1.4086	R(23,24)	1
R(4,8)	1.07	R(23,25)	1.47
R(5,6)	1.4186	R(25,26)	1.54
R(5,34)	1.76	R(25,29)	1.3552
R(6,9)	1.07	R(26,27)	1.3552
R(10,11)	1.5159	R(26,31)	1.07
R(10,13)	1.4833	R(27,28)	1.54
R(11,12)	1.3183	R(27,32)	1.07
R(11,21)	1.5247	R(28,30)	1.3552
R(12,19)	1.4599	R(28,36)	1.76
R(13,14)	1.5177	R(29,30)	1.54
R(13,15)	1.2584	R(29,35)	1.76
R(14,16)	1.3854	R(30,33)	1.07

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.2335	A(16,17,18)	114.4711
A(2,1,7)	120.8846	A(17,18,20)	114.5781
A(6,1,7)	120.8803	A(12,19,14)	119.6016
A(1,2,3)	120.6161	A(12,19,20)	131.486
A(1,2,10)	126.7665	A(14,19,20)	108.8973
A(3,2,10)	112.6154	A(18,20,19)	136.4042
A(2,3,4)	122.3861	A(3,21,11)	104.6191
A(2,3,21)	108.7551	A(3,21,22)	127.6645
A(4,3,21)	128.8464	A(11,21,22)	127.7003
A(3,4,5)	117.7075	A(21,22,23)	120
A(3,4,8)	121.1479	A(22,23,24)	109.4712
A(5,4,8)	121.143	A(22,23,25)	109.4712
A(4,5,6)	120.245	A(24,23,25)	109.4712
A(4,5,34)	119.8769	A(23,25,26)	120
A(6,5,34)	119.8777	A(23,25,29)	120
A(1,6,5)	120.5107	A(26,25,29)	120
A(1,6,9)	119.7441	A(25,26,27)	120
A(5,6,9)	119.7449	A(25,26,31)	120
A(2,10,11)	103.0323	A(27,26,31)	120
A(2,10,13)	113.9795	A(26,27,28)	120
A(11,10,13)	114.567	A(26,27,32)	120
A(10,11,12)	127.2685	A(28,27,32)	120
A(10,11,21)	107.8991	A(27,28,30)	120
A(12,11,21)	124.8301	A(27,28,36)	120

A(11,12,19)	116.2261	A(30,28,36)	120
A(10,13,14)	115.0748	A(25,29,30)	120
A(10,13,15)	122.4471	A(25,29,35)	120
A(14,13,15)	122.4726	A(30,29,35)	120
A(13,14,16)	132.1974	A(28,30,29)	120
A(13,14,19)	118.419	A(28,30,33)	120
A(16,14,19)	109.3834	A(29,30,33)	120
A(14,16,17)	136.1971		

C[1]

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3922	R(20,21)	1.3845
R(1,6)	1.4141	R(22,23)	1.2851
R(1,7)	1.07	R(23,24)	1.4
R(2,3)	1.4087	R(23,37)	2.0157
R(2,11)	1.5096	R(24,25)	1
R(3,4)	1.3881	R(24,26)	1.47
R(3,22)	1.5169	R(26,27)	1.54
R(4,5)	1.4102	R(26,30)	1.3552
R(4,8)	1.07	R(27,28)	1.3552
R(5,6)	1.4227	R(27,32)	1.07
R(5,9)	1.07	R(28,29)	1.54
R(6,10)	1.07	R(28,33)	1.07
R(11,12)	1.4831	R(29,31)	1.3552
R(11,14)	1.487	R(29,34)	1.07
R(12,13)	1.2662	R(30,31)	1.54
R(12,22)	1.4573	R(30,36)	1.07
R(13,20)	1.4529	R(31,35)	1.07
R(13,37)	1.998	R(37,38)	2.27
R(14,15)	1.5408	R(37,39)	2.05
R(14,16)	1.2584	R(37,40)	2.05
R(15,17)	1.3853	R(37,41)	2.05
R(15,20)	1.6134	R(39,42)	1.1153
R(17,18)	1.5027	R(40,43)	1.1154
R(18,19)	1.2649	R(41,44)	1.1154
R(19,21)	1.5014		

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.0647	A(3,22,12)	105.1083
A(2,1,7)	120.9686	A(3,22,23)	138.119
A(6,1,7)	120.9648	A(12,22,23)	116.735

A(1,2,3)	120.2487	A(22,23,24)	124.0869
A(1,2,11)	127.4917	A(22,23,37)	111.8079
A(3,2,11)	112.2571	A(24,23,37)	124.1039
A(2,3,4)	122.6622	A(23,24,25)	109.4691
A(2,3,22)	106.9795	A(23,24,26)	109.4769
A(4,3,22)	130.3381	A(25,24,26)	109.4727
A(3,4,5)	117.3366	A(24,26,27)	119.9961
A(3,4,8)	121.3338	A(24,26,30)	120.0027
A(5,4,8)	121.3277	A(27,26,30)	120.0013
A(4,5,6)	120.482	A(26,27,28)	120.0005
A(4,5,9)	119.7593	A(26,27,32)	119.9995
A(6,5,9)	119.7582	A(28,27,32)	120.0001
A(1,6,5)	120.8474	A(27,28,29)	119.999
A(1,6,10)	119.5743	A(27,28,33)	120.0004
A(5,6,10)	119.5779	A(29,28,33)	120.0005
A(2,11,12)	100.9869	A(28,29,31)	120.0001
A(2,11,14)	118.1425	A(28,29,34)	119.9994
A(12,11,14)	112.5419	A(31,29,34)	120.0006
A(11,12,13)	132.4218	A(26,30,31)	119.9988
A(11,12,22)	111.841	A(26,30,36)	120.0004
A(13,12,22)	115.7254	A(31,30,36)	120.0009
A(12,13,20)	116.8549	A(29,31,30)	120.0004
A(12,13,37)	112.8283	A(29,31,35)	120.0001
A(20,13,37)	130.2951	A(30,31,35)	119.9995
A(11,14,15)	114.3067	A(13,37,23)	80.5387
A(11,14,16)	122.826	A(13,37,39)	90.1505
A(15,14,16)	122.8608	A(13,37,40)	98.6228
A(14,15,17)	132.3012	A(13,37,41)	91.2974
A(14,15,20)	118.9172	A(23,37,38)	85.0751
A(17,15,20)	108.7816	A(23,37,39)	97.3032
A(15,17,18)	136.1374	A(23,37,41)	96.0331
A(17,18,19)	114.8983	A(38,37,39)	90.7718
A(18,19,21)	114.7104	A(38,37,40)	95.7609
A(13,20,15)	116.9512	A(38,37,41)	91.1199
A(13,20,21)	133.3921	A(39,37,40)	82.5374
A(15,20,21)	109.6338	A(40,37,41)	84.1168
A(19,21,20)	135.7769		

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Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3923	R(19,20)	1.3845
R(1,6)	1.4142	R(21,22)	1.285
R(1,7)	1.07	R(22,23)	1.4001

R(2,3)	1.4087	R(22,36)	2.0159
R(2,10)	1.5097	R(23,24)	1
R(3,4)	1.3881	R(23,25)	1.4701
R(3,21)	1.5169	R(25,26)	1.5401
R(4,5)	1.4102	R(25,29)	1.3552
R(4,8)	1.07	R(26,27)	1.3552
R(5,6)	1.4227	R(26,31)	1.07
R(5,44)	1.76	R(27,28)	1.54
R(6,9)	1.07	R(27,32)	1.07
R(10,11)	1.4832	R(28,30)	1.3552
R(10,13)	1.487	R(28,33)	1.07
R(11,12)	1.2661	R(29,30)	1.54
R(11,21)	1.4569	R(29,35)	1.07
R(12,19)	1.453	R(30,34)	1.07
R(12,36)	1.9983	R(36,37)	2.27
R(13,14)	1.5408	R(36,38)	2.05
R(13,15)	1.2584	R(36,39)	2.05
R(14,16)	1.3853	R(36,40)	2.05
R(14,19)	1.6134	R(38,41)	1.1153
R(16,17)	1.5028	R(39,42)	1.1154
R(17,18)	1.2649	R(40,43)	1.1154
R(18,20)	1.5014		

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.0635	A(3,21,11)	105.1134
A(2,1,7)	120.9717	A(3,21,22)	138.1244
A(6,1,7)	120.9629	A(11,21,22)	116.7251
A(1,2,3)	120.2436	A(21,22,23)	124.0772
A(1,2,10)	127.5072	A(21,22,36)	111.8523
A(3,2,10)	112.2468	A(23,22,36)	124.0693
A(2,3,4)	122.6662	A(22,23,24)	109.4693
A(2,3,21)	106.981	A(22,23,25)	109.4773
A(4,3,21)	130.3327	A(24,23,25)	109.4703
A(3,4,5)	117.3393	A(23,25,26)	120.005
A(3,4,8)	121.3321	A(23,25,29)	119.9993
A(5,4,8)	121.3268	A(26,25,29)	119.9957
A(4,5,6)	120.4815	A(25,26,27)	120.0012
A(4,5,44)	119.7568	A(25,26,31)	120.0012
A(6,5,44)	119.7612	A(27,26,31)	119.9976
A(1,6,5)	120.8476	A(26,27,28)	120.0001
A(1,6,9)	119.5766	A(26,27,32)	120.0012
A(5,6,9)	119.5754	A(28,27,32)	119.9987
A(2,10,11)	100.9797	A(27,28,30)	119.9991

A(2,10,13)	118.1568	A(27,28,33)	120.0007
A(11,10,13)	112.5448	A(30,28,33)	120.0002
A(10,11,12)	132.4331	A(25,29,30)	120.0022
A(10,11,21)	111.8446	A(25,29,35)	119.9987
A(12,11,21)	115.7107	A(30,29,35)	119.9991
A(11,12,19)	116.8464	A(28,30,29)	120.0018
A(11,12,36)	112.8795	A(28,30,34)	119.9988
A(19,12,36)	130.2522	A(29,30,34)	119.9995
A(10,13,14)	114.3027	A(12,36,22)	80.4921
A(10,13,15)	122.8301	A(12,36,38)	90.3869
A(14,13,15)	122.8606	A(12,36,39)	98.5067
A(13,14,16)	132.3041	A(12,36,40)	95.3189
A(13,14,19)	118.9151	A(22,36,37)	87.2711
A(16,14,19)	108.7806	A(22,36,38)	95.9283
A(14,16,17)	136.1378	A(22,36,40)	94.732
A(16,17,18)	114.8983	A(37,36,38)	90.0673
A(17,18,20)	114.7089	A(37,36,39)	93.7262
A(12,19,14)	116.9604	A(37,36,40)	86.4464
A(12,19,20)	133.3835	A(38,36,39)	83.7991
A(14,19,20)	109.633	A(39,36,40)	85.6114
A(18,20,19)	135.7797		

C[3]

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3923	R(19,20)	1.3843
R(1,6)	1.4133	R(21,22)	1.2836
R(1,7)	1.0699	R(22,23)	1.3983
R(2,3)	1.4082	R(22,35)	2.0157
R(2,10)	1.5095	R(23,24)	0.9999
R(3,4)	1.3892	R(23,25)	1.4694
R(3,21)	1.5167	R(25,26)	1.5404
R(4,5)	1.4107	R(25,29)	1.3552
R(4,8)	1.0695	R(26,27)	1.3552
R(5,6)	1.4231	R(26,31)	1.0698
R(5,44)	1.0693	R(27,28)	1.5395
R(6,9)	1.0703	R(27,32)	1.0702
R(10,11)	1.4841	R(28,30)	1.3549
R(10,13)	1.4859	R(28,43)	1.7608
R(11,12)	1.2644	R(29,30)	1.5401
R(11,21)	1.4566	R(29,34)	1.0702
R(12,19)	1.4541	R(30,33)	1.0699
R(12,35)	1.9989	R(35,36)	2.2704
R(13,14)	1.5411	R(35,37)	2.0509

R(13,15)	1.2583	R(35,38)	2.0525
R(14,16)	1.3845	R(35,39)	2.0493
R(14,19)	1.6139	R(37,40)	1.1135
R(16,17)	1.5026	R(38,41)	1.1142
R(17,18)	1.2655	R(39,42)	1.1178
R(18,20)	1.5008		

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.0531	A(3,21,11)	105.1522
A(2,1,7)	120.959	A(3,21,22)	138.1144
A(6,1,7)	120.9862	A(11,21,22)	116.6952
A(1,2,3)	120.2742	A(21,22,23)	124.04
A(1,2,10)	127.5596	A(21,22,35)	111.9626
A(3,2,10)	112.1636	A(23,22,35)	123.9934
A(2,3,4)	122.6687	A(22,23,24)	109.5593
A(2,3,21)	107.0069	A(22,23,25)	109.5649
A(4,3,21)	130.3038	A(24,23,25)	109.4803
A(3,4,5)	117.2812	A(23,25,26)	120.068
A(3,4,8)	121.3485	A(23,25,29)	119.9569
A(5,4,8)	121.3686	A(26,25,29)	119.9751
A(4,5,6)	120.4737	A(25,26,27)	119.9945
A(4,5,44)	119.7047	A(25,26,31)	119.9798
A(6,5,44)	119.8213	A(27,26,31)	120.0253
A(1,6,5)	120.8816	A(26,27,28)	119.9983
A(1,6,9)	119.61	A(26,27,32)	119.9729
A(5,6,9)	119.508	A(28,27,32)	120.0287
A(2,10,11)	101.0181	A(27,28,30)	120.0458
A(2,10,13)	118.4069	A(27,28,43)	119.984
A(11,10,13)	112.5983	A(30,28,43)	119.9703
A(10,11,12)	132.4083	A(25,29,30)	120.022
A(10,11,21)	111.692	A(25,29,34)	119.9849
A(12,11,21)	115.8953	A(30,29,34)	119.993
A(11,12,19)	116.9091	A(28,30,29)	119.9643
A(11,12,35)	112.994	A(28,30,33)	120.0359
A(19,12,35)	130.0832	A(29,30,33)	119.9999
A(10,13,14)	114.1827	A(12,35,22)	80.5263
A(10,13,15)	122.9185	A(12,35,37)	92.5573
A(14,13,15)	122.8899	A(12,35,38)	89.1408
A(13,14,16)	132.3451	A(12,35,39)	96.7653
A(13,14,19)	118.869	A(22,35,36)	88.78
A(16,14,19)	108.7858	A(22,35,37)	91.2789
A(14,16,17)	136.1483	A(22,35,39)	97.9415
A(16,17,18)	114.9011	A(36,35,37)	87.1835
A(17,18,20)	114.6762	A(36,35,38)	101.5231

A(12,19,14)	116.8977	A(36,35,39)	85.1007
A(12,19,20)	133.4747	A(37,35,38)	86.7674
A(14,19,20)	109.5996	A(38,35,39)	85.573
A(18,20,19)	135.8228		

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Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.392	R(19,20)	1.3854
R(1,6)	1.4142	R(21,22)	1.2885
R(1,7)	1.0691	R(22,23)	1.4003
R(2,3)	1.4089	R(22,35)	2.0097
R(2,10)	1.5086	R(23,24)	0.9999
R(3,4)	1.3887	R(23,25)	1.4703
R(3,21)	1.5158	R(25,26)	1.5404
R(4,5)	1.411	R(25,29)	1.3537
R(4,8)	1.071	R(26,27)	1.355
R(5,6)	1.4222	R(26,31)	1.0704
R(5,44)	1.7609	R(27,28)	1.5396
R(6,9)	1.0691	R(27,32)	1.0698
R(10,11)	1.4827	R(28,30)	1.3557
R(10,13)	1.4883	R(28,43)	1.7603
R(11,12)	1.2701	R(29,30)	1.5397
R(11,21)	1.4645	R(29,34)	1.0703
R(12,19)	1.4533	R(30,33)	1.07
R(12,35)	1.9948	R(35,36)	2.2693
R(13,14)	1.5419	R(35,37)	2.054
R(13,15)	1.2583	R(35,38)	2.0462
R(14,16)	1.3849	R(35,39)	2.0484
R(14,19)	1.6116	R(37,40)	1.1154
R(16,17)	1.5019	R(38,41)	1.1212
R(17,18)	1.2642	R(39,42)	1.1151
R(18,20)	1.5013		

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.0813	A(3,21,11)	104.9445
A(2,1,7)	120.8908	A(3,21,22)	138.0068
A(6,1,7)	121.0246	A(11,21,22)	117.0102
A(1,2,3)	120.2998	A(21,22,23)	124.3991
A(1,2,10)	127.3791	A(21,22,35)	111.0554
A(3,2,10)	112.3177	A(23,22,35)	124.543
A(2,3,4)	122.582	A(22,23,24)	109.5596

A(2,3,21)	107.0546	A(22,23,25)	109.5189
A(4,3,21)	130.3442	A(24,23,25)	109.3706
A(3,4,5)	117.3506	A(23,25,26)	119.9478
A(3,4,8)	121.3734	A(23,25,29)	120.0003
A(5,4,8)	121.2747	A(26,25,29)	120.0519
A(4,5,6)	120.5	A(25,26,27)	120.0075
A(4,5,44)	119.6512	A(25,26,31)	119.9871
A(6,5,44)	119.8481	A(27,26,31)	120.0054
A(1,6,5)	120.8232	A(26,27,28)	119.9551
A(1,6,9)	119.6439	A(26,27,32)	120.0451
A(5,6,9)	119.5327	A(28,27,32)	119.9998
A(2,10,11)	100.9905	A(27,28,30)	119.995
A(2,10,13)	118.5697	A(27,28,43)	119.9845
A(11,10,13)	112.5908	A(30,28,43)	120.0202
A(10,11,12)	132.0181	A(25,29,30)	119.9573
A(10,11,21)	111.6702	A(25,29,34)	119.9498
A(12,11,21)	116.3069	A(30,29,34)	120.0928
A(11,12,19)	117.2891	A(28,30,29)	120.033
A(11,12,35)	111.9387	A(28,30,33)	120.0236
A(19,12,35)	130.7667	A(29,30,33)	119.9434
A(10,13,14)	114.282	A(12,35,22)	81.8069
A(10,13,15)	122.835	A(12,35,37)	88.8759
A(14,13,15)	122.8712	A(12,35,38)	98.1153
A(13,14,16)	132.3787	A(12,35,39)	91.5169
A(13,14,19)	118.8459	A(22,35,36)	91.7882
A(16,14,19)	108.7749	A(22,35,37)	87.925
A(14,16,17)	136.1816	A(22,35,39)	92.0291
A(16,17,18)	114.8848	A(36,35,37)	90.2429
A(17,18,20)	114.7306	A(36,35,38)	88.2894
A(12,19,14)	116.8042	A(36,35,39)	89.3552
A(12,19,20)	133.4886	A(37,35,38)	92.0548
A(14,19,20)	109.6705	A(38,35,39)	87.9916
A(18,20,19)	135.6945		

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Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3922	R(19,20)	1.3869
R(1,6)	1.4155	R(21,22)	1.2919
R(1,7)	1.0702	R(22,23)	1.4035
R(2,3)	1.4099	R(22,34)	2.0035
R(2,10)	1.5118	R(23,24)	1.0011

R(3,4)	1.3899	R(23,25)	1.4717
R(3,21)	1.5168	R(25,26)	1.5405
R(4,5)	1.4084	R(25,29)	1.3548
R(4,8)	1.0706	R(26,27)	1.3576
R(5,6)	1.4239	R(26,44)	1.7604
R(5,43)	1.0697	R(27,28)	1.5423
R(6,9)	1.0709	R(27,31)	1.0716
R(10,11)	1.4821	R(28,30)	1.356
R(10,13)	1.488	R(28,42)	1.7608
R(11,12)	1.2749	R(29,30)	1.5392
R(11,21)	1.475	R(29,33)	1.0699
R(12,19)	1.4521	R(30,32)	1.0706
R(12,34)	1.9817	R(34,35)	2.2707
R(13,14)	1.5437	R(34,36)	2.0488
R(13,15)	1.2587	R(34,37)	2.0517
R(14,16)	1.3841	R(34,38)	2.0521
R(14,19)	1.6125	R(36,39)	1.1169
R(16,17)	1.5031	R(37,40)	1.1161
R(17,18)	1.2652	R(38,41)	1.1158
R(18,20)	1.5013		

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	118.123	A(3,21,11)	104.9462
A(2,1,7)	120.8608	A(3,21,22)	137.6908
A(6,1,7)	121.0146	A(11,21,22)	117.3265
A(1,2,3)	120.1515	A(21,22,23)	124.8694
A(1,2,10)	127.3838	A(21,22,34)	109.9532
A(3,2,10)	112.461	A(23,22,34)	125.174
A(2,3,4)	122.6789	A(22,23,24)	109.4275
A(2,3,21)	106.9886	A(22,23,25)	109.5884
A(4,3,21)	130.3109	A(24,23,25)	109.298
A(3,4,5)	117.3393	A(23,25,26)	119.8457
A(3,4,8)	121.5016	A(23,25,29)	120.0969
A(5,4,8)	121.1568	A(26,25,29)	120.0574
A(4,5,6)	120.5089	A(25,26,27)	120.0247
A(4,5,43)	119.5588	A(25,26,44)	119.7114
A(6,5,43)	119.9317	A(27,26,44)	120.2639
A(1,6,5)	120.8043	A(26,27,28)	119.8375
A(1,6,9)	119.5892	A(26,27,31)	120.1059
A(5,6,9)	119.6059	A(28,27,31)	120.0566
A(2,10,11)	101.026	A(27,28,30)	120.0215
A(2,10,13)	118.6394	A(27,28,42)	120.1733
A(11,10,13)	112.4698	A(30,28,42)	119.8052

A(10,11,12)	131.8649	A(25,29,30)	120.0056
A(10,11,21)	111.4677	A(25,29,33)	120.0514
A(12,11,21)	116.6627	A(30,29,33)	119.943
A(11,12,19)	117.6913	A(28,30,29)	120.0523
A(11,12,34)	111.0472	A(28,30,32)	120.0106
A(19,12,34)	131.2464	A(29,30,32)	119.9371
A(10,13,14)	114.344	A(12,34,22)	83.3415
A(10,13,15)	122.8148	A(12,34,36)	89.7915
A(14,13,15)	122.8301	A(12,34,37)	94.6253
A(13,14,16)	132.3209	A(12,34,38)	89.5535
A(13,14,19)	119.0404	A(22,34,35)	96.3965
A(16,14,19)	108.6381	A(22,34,36)	88.1948
A(14,16,17)	136.1966	A(22,34,38)	90.9831
A(16,17,18)	115.0373	A(35,34,36)	90.7629
A(17,18,20)	114.6138	A(35,34,37)	85.6261
A(12,19,14)	116.3825	A(35,34,38)	89.8884
A(12,19,20)	133.7182	A(36,34,37)	92.8674
A(14,19,20)	109.8582	A(37,34,38)	87.9342
A(18,20,19)	135.5889		

C^{6}

Atom number	Bond length (Å)	Atom number	Bond length (Å)
R(1,2)	1.3912	R(19,20)	1.3846
R(1,6)	1.4119	R(21,22)	1.293
R(1,7)	1.0703	R(22,23)	1.4
R(2,3)	1.4081	R(22,34)	2.0059
R(2,10)	1.5114	R(23,24)	1
R(3,4)	1.3865	R(23,25)	1.4696
R(3,21)	1.5162	R(25,26)	1.5411
R(4,5)	1.4116	R(25,29)	1.3545
R(4,8)	1.0707	R(26,27)	1.3546
R(5,6)	1.4201	R(26,43)	1.7603
R(5,44)	1.7645	R(27,28)	1.5394
R(6,9)	1.0714	R(27,31)	1.0692
R(10,11)	1.4833	R(28,30)	1.3559
R(10,13)	1.4889	R(28,42)	1.7603
R(11,12)	1.2758	R(29,30)	1.5406
R(11,21)	1.475	R(29,33)	1.0697
R(12,19)	1.4503	R(30,32)	1.0689
R(12,34)	1.9885	R(34,35)	2.2685
R(13,14)	1.5419	R(34,36)	2.0454
R(13,15)	1.2586	R(34,37)	2.049
R(14,16)	1.3855	R(34,38)	2.0538

R(14,19)	1.6139	R(36,39)	1.116
R(16,17)	1.5034	R(37,40)	1.1155
R(17,18)	1.2643	R(38,41)	1.1159
R(18,20)	1.5027		

Atom number	Bond angle (Degree)	Atom number	Bond angle (Degree)
A(2,1,6)	117.9707	A(3,21,11)	104.8386
A(2,1,7)	121.0328	A(3,21,22)	137.8777
A(6,1,7)	120.9937	A(11,21,22)	117.2508
A(1,2,3)	120.3029	A(21,22,23)	124.8143
A(1,2,10)	127.3056	A(21,22,34)	110.0771
A(3,2,10)	112.3884	A(23,22,34)	125.1048
A(2,3,4)	122.6032	A(22,23,24)	109.4611
A(2,3,21)	107.219	A(22,23,25)	109.6946
A(4,3,21)	130.1625	A(24,23,25)	109.4443
A(3,4,5)	117.3285	A(23,25,26)	119.8363
A(3,4,8)	121.4252	A(23,25,29)	120.1058
A(5,4,8)	121.2429	A(26,25,29)	120.0578
A(4,5,6)	120.4075	A(25,26,27)	119.9741
A(4,5,44)	120.0353	A(25,26,43)	120.0491
A(6,5,44)	119.557	A(27,26,43)	119.9769
A(1,6,5)	120.9802	A(26,27,28)	120.0238
A(1,6,9)	119.7818	A(26,27,31)	119.9668
A(5,6,9)	119.2377	A(28,27,31)	120.0094
A(2,10,11)	101.0953	A(27,28,30)	119.9933
A(2,10,13)	118.6827	A(27,28,42)	120.036
A(11,10,13)	112.5888	A(30,28,42)	119.9708
A(10,11,12)	131.6937	A(25,29,30)	119.9266
A(10,11,21)	111.4864	A(25,29,33)	120.0626
A(12,11,21)	116.8194	A(30,29,33)	120.0107
A(11,12,19)	117.43	A(28,30,29)	120.024
A(11,12,34)	110.8457	A(28,30,32)	119.9942
A(19,12,34)	131.7134	A(29,30,32)	119.9818
A(10,13,14)	114.216	A(12,34,22)	83.159
A(10,13,15)	122.8407	A(12,34,36)	89.2059
A(14,13,15)	122.9296	A(12,34,37)	96.8054
A(13,14,16)	132.3758	A(12,34,38)	90.7825
A(13,14,19)	118.9269	A(22,34,35)	96.8401
A(16,14,19)	108.6971	A(22,34,36)	88.08
A(14,16,17)	136.114	A(22,34,38)	92.0508
A(16,17,18)	115.014	A(35,34,36)	90.794
A(17,18,20)	114.6544	A(35,34,37)	83.1956
A(12,19,14)	116.7379	A(35,34,38)	89.2177
A(12,19,20)	133.4734	A(36,34,37)	91.1289

A(14,19,20)	109.7635	A(37,34,38)	88.7403
A(18,20,19)	135.6881		

MULLIKEN CHARGES:

L^1

	Atom	Charge		Atom	Charge
1	C	-0.28117	18	C	0.03218
2	C	0.223222	19	C	0.025306
3	C	0.165106	20	C	-0.03574
4	C	-0.24556	21	C	-0.07959
5	C	-0.29061	22	C	-0.1457
6	C	-0.22875	23	N	0.05452
11	N	-0.26756	24	N	-0.35335
12	C	-0.02879	26	C	0.291981
13	N	0.077823	27	C	-0.32411
14	C	0.144107	28	C	-0.18861
15	C	0.037654	29	C	-0.22728
16	O	-0.21627	30	C	-0.31968
17	C	-0.03896	31	C	-0.21497

L^2

	Atom	Charge		Atom	Charge
1	C	-0.26943	18	C	0.027844
2	C	0.219801	19	C	-0.03551
3	C	0.18246	20	C	-0.07734
4	C	-0.15193	21	C	-0.14755
5	C	-0.22326	22	N	0.060625
6	C	-0.22424	23	N	-0.35247
10	N	-0.26317	25	C	0.292644
11	C	-0.0262	26	C	-0.32197
12	N	0.079358	27	C	-0.18778
13	C	0.144761	28	C	-0.2262
14	C	0.037573	29	C	-0.31943

15	O	-0.2161	30	C	-0.21453
16	C	-0.03708	36	Cl	-0.02984
17	C	0.034709			

L^3

	Atom	**Charge**		**Atom**	**Charge**
1	C	-0.28042	18	C	0.026877
2	C	0.224026	19	C	-0.03596
3	C	0.165184	20	C	-0.07797
4	C	-0.24481	21	C	-0.14453
5	C	-0.29016	22	N	0.051848
6	C	-0.22792	23	N	-0.35163
10	N	-0.26724	25	C	0.297384
11	C	-0.029	26	C	-0.30206
12	N	0.078442	27	C	-0.15834
13	C	0.144415	28	C	-0.11224
14	C	0.037799	29	C	-0.31503
15	O	-0.2154	30	C	-0.19352
16	C	-0.03795	36	Cl	-0.04139
17	C	0.03397			

L^4

	Atom	**Charge**		**Atom**	**Charge**
1	C	-0.26893	18	C	0.029353
2	C	0.220697	19	C	-0.0357
3	C	0.182562	20	C	-0.07574
4	C	-0.15084	21	C	-0.14653
5	C	-0.22368	22	N	0.058038
6	C	-0.2232	23	N	-0.35083
10	N	-0.2629	25	C	0.297916
11	C	-0.02634	26	C	-0.29992
12	N	0.079955	27	C	-0.15734
13	C	0.145095	28	C	-0.11189
14	C	0.03773	29	C	-0.31482
15	O	-0.21527	30	C	-0.19302
16	C	-0.03607	35	Cl	-0.02818
17	C	0.036423	36	Cl	-0.03948

L[5]

	Atom	Charge		Atom	Charge
1	C	-0.2824	18	C	0.025209
2	C	0.221979	19	C	-0.03862
3	C	0.167644	20	C	-0.08019
4	C	-0.24914	21	C	-0.09737
5	C	-0.29133	22	N	0.028589
6	C	-0.22992	23	N	-0.34009
10	N	-0.26667	25	C	0.407084
11	C	-0.03672	26	C	-0.2888
12	N	0.078014	27	C	-0.16695
13	C	0.143469	28	C	-0.10335
14	C	0.037896	29	C	-0.25228
15	O	-0.21648	30	C	-0.19254
16	C	-0.03907	35	Cl	-0.02736
17	C	0.032221	36	Cl	0.025791

L[6]

	Atom	Charge		Atom	Charge
1	C	-0.27076	19	C	-0.03838
2	C	0.218867	20	C	-0.07797
3	C	0.184463	21	C	-0.09984
4	C	-0.15502	22	N	0.034541
5	C	-0.22317	23	N	-0.33941
6	C	-0.22592	25	C	0.408239
10	N	-0.26241	26	C	-0.2867
11	C	-0.03401	27	C	-0.16593
12	N	0.079486	28	C	-0.10308
13	C	0.144145	29	C	-0.25226
14	C	0.037837	30	C	-0.19187
15	O	-0.21635	34	Cl	-0.03194
16	C	-0.03719	35	Cl	0.026004
17	C	0.034655	36	Cl	-0.02535
18	C	0.027681			

C[1]

	Atom	Charge		Atom	Charge
1	C	-0.31561	22	C	0.000168
2	C	0.209702	23	N	-0.29971
3	C	0.278755	24	N	-0.25156
4	C	-0.36207	26	C	0.052024
5	C	-0.25584	27	C	-0.28049
6	C	-0.23319	28	C	-0.22839
11	N	-0.23316	29	C	-0.22802
12	C	0.126637	30	C	-0.26568
13	N	-0.30104	31	C	-0.23603
14	C	0.081234	37	Re	0.284896
15	C	-0.00096	38	Cl	0.287582
16	O	-0.20603	39	C	0.013614
17	C	-0.06796	40	C	0.086446
18	C	0.004937	41	C	-0.0552
19	C	-0.02094	42	O	-0.04617
20	C	0.060046	43	O	-0.05788
21	C	-0.12824	44	O	-0.05231

C[2]

	Atom	Charge		Atom	Charge
1	C	-0.30591	22	N	-0.29183
2	C	0.209034	23	N	-0.26301
3	C	0.297713	25	C	0.072062
4	C	-0.30586	26	C	-0.28169
5	C	-0.16486	27	C	-0.22423
6	C	-0.21216	28	C	-0.23043
10	N	-0.22918	29	C	-0.25274
11	C	0.136129	30	C	-0.21463
12	N	-0.30256	36	Re	0.294852
13	C	0.082847	37	Cl	0.233844
14	C	0.000997	38	C	0.020221

15	O	-0.20401	39	C	0.085697
16	C	-0.06454	40	C	-0.04928
17	C	0.010969	41	O	-0.04474
18	C	-0.01405	42	O	-0.05795
19	C	0.066551	43	O	-0.05104
20	C	-0.12137	44	Cl	-0.03669
21	C	0.002126			

C[3]

	Atom	**Charge**		**Atom**	**Charge**
1	C	-0.31318	22	N	-0.27595
2	C	0.213229	23	N	-0.27324
3	C	0.278259	25	C	0.101475
4	C	-0.3562	26	C	-0.26324
5	C	-0.25361	27	C	-0.1929
6	C	-0.22693	28	C	-0.14012
10	N	-0.235	29	C	-0.26757
11	C	0.139457	30	C	-0.16549
12	N	-0.3022	35	Re	0.300503
13	C	0.086174	36	Cl	0.168126
14	C	0.005136	37	C	0.033182
15	O	-0.20177	38	C	0.070194
16	C	-0.06497	39	C	-0.04539
17	C	0.015083	40	O	-0.04003
18	C	-0.02962	41	O	-0.04686
19	C	0.086248	42	O	-0.05253
20	C	-0.11493	43	Cl	-0.03504
21	C	-0.00242			

C[4]

	Atom	**Charge**		**Atom**	**Charge**
1	C	-0.30386	22	N	-0.28706
2	C	0.212772	23	N	-0.28844
3	C	0.299422	25	C	0.156338

4	C	-0.30263	26	C	-0.26583
5	C	-0.16283	27	C	-0.18594
6	C	-0.20633	28	C	-0.13672
10	N	-0.23012	29	C	-0.24279
11	C	0.146751	30	C	-0.15779
12	N	-0.30723	35	Re	0.307894
13	C	0.089477	36	Cl	0.102974
14	C	0.006886	37	C	0.035749
15	O	-0.19938	38	C	0.091718
16	C	-0.06006	39	C	-0.03486
17	C	0.023644	40	O	-0.0409
18	C	-0.00154	41	O	-0.06592
19	C	0.067291	42	O	-0.04455
20	C	-0.10448	43	Cl	-0.03784
21	C	0.00548	44	Cl	-0.02934

C^5

	Atom	**Charge**		**Atom**	**Charge**
1	C	-0.31239	22	N	-0.30076
2	C	0.213184	23	N	-0.28999
3	C	0.280675	26	C	-0.20282
4	C	-0.35094	27	C	-0.21446
5	C	-0.24937	28	C	-0.12822
6	C	-0.22526	29	C	-0.24084
10	N	-0.23444	30	C	-0.16143
11	C	0.143834	34	Re	0.316429
12	N	-0.31432	35	Cl	0.050308
13	C	0.092955	36	C	0.030292
14	C	0.015414	37	C	0.100369
15	O	-0.1968	38	C	-0.02785
16	C	-0.0568	39	O	-0.04185
17	C	0.030206	40	O	-0.05721
18	C	-0.00041	41	O	-0.03878
19	C	0.073103	42	Cl	-0.03861
20	C	-0.09639	44	Cl	-0.02058

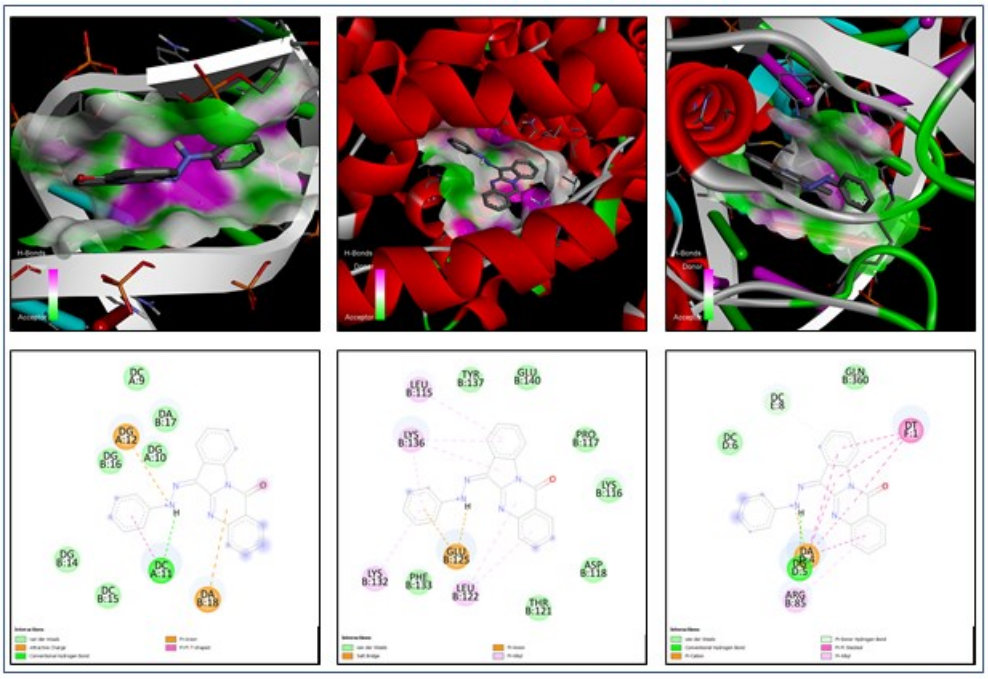
21	C	0.016829			

C[6]

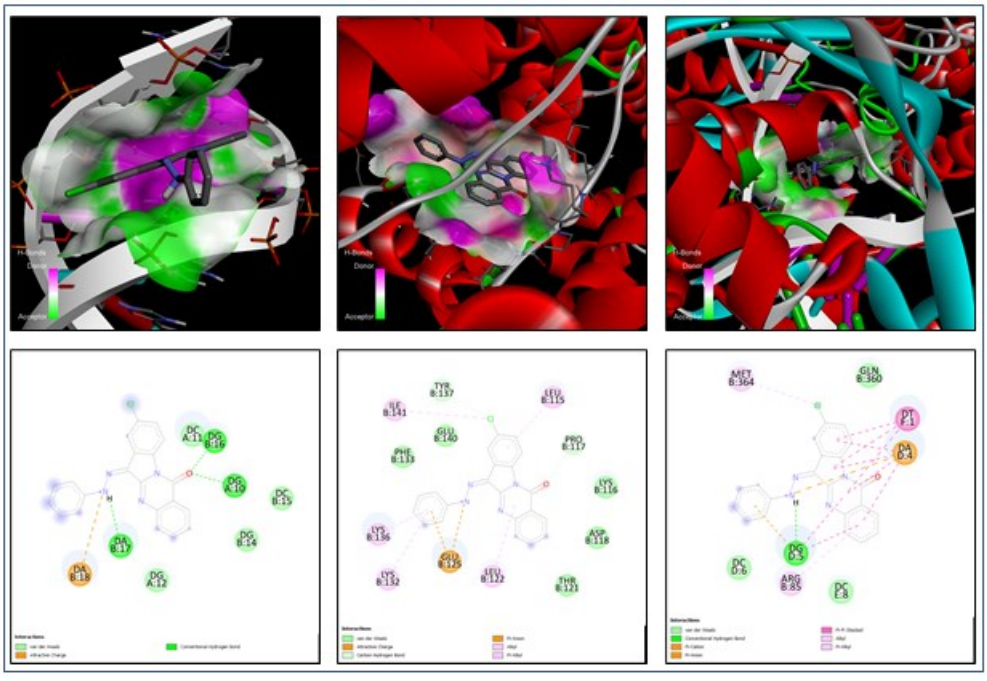
	Atom	Charge		Atom	Charge
1	C	-0.30514	23	N	-0.28821
2	C	0.21142	25	C	0.32456
3	C	0.305457	26	C	-0.20138
4	C	-0.30112	27	C	-0.20532
5	C	-0.16423	28	C	-0.12984
6	C	-0.20089	29	C	-0.23155
10	N	-0.23322	30	C	-0.16016
11	C	0.149261	34	Re	0.305236
12	N	-0.31386	35	Cl	0.040445
13	C	0.095077	36	C	0.033763
14	C	0.014461	37	C	0.10727
15	O	-0.19675	38	C	-0.01622
16	C	-0.05397	39	O	-0.03919
17	C	0.033293	40	O	-0.05571
18	C	0.006827	41	O	-0.04406
19	C	0.069736	42	Cl	-0.03622
20	C	-0.09769	43	Cl	-0.01712
21	C	0.016991	44	Cl	-0.02645
22	N	-0.299			

ESI 3: Docking image for DNA, BSA, and TOPO II of the ligands L^1–L^6 and metal complexes C^1–C^6

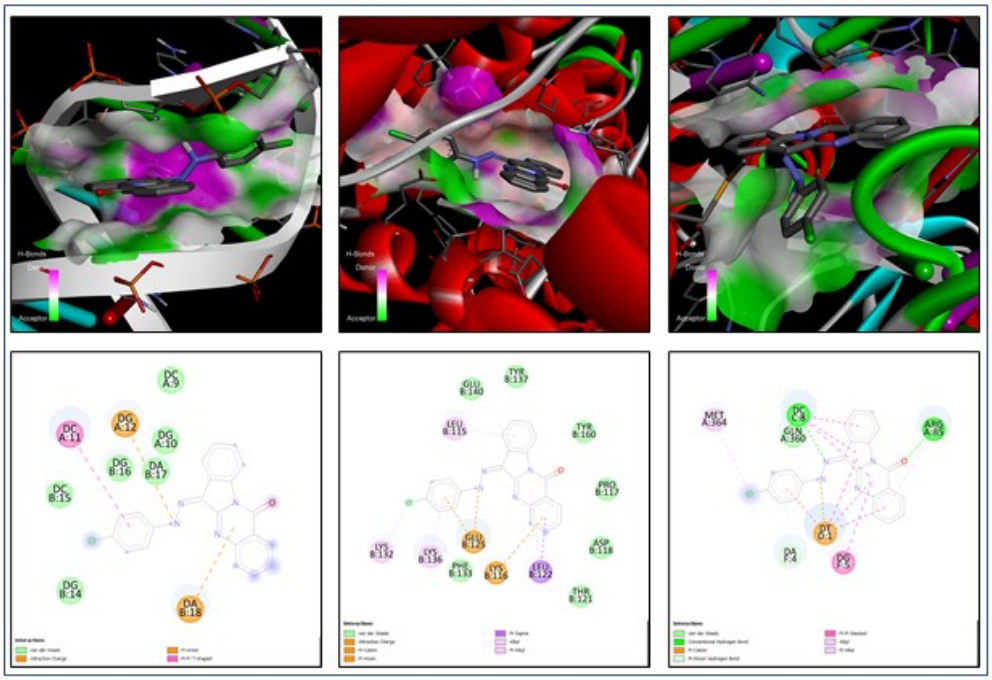
L^1



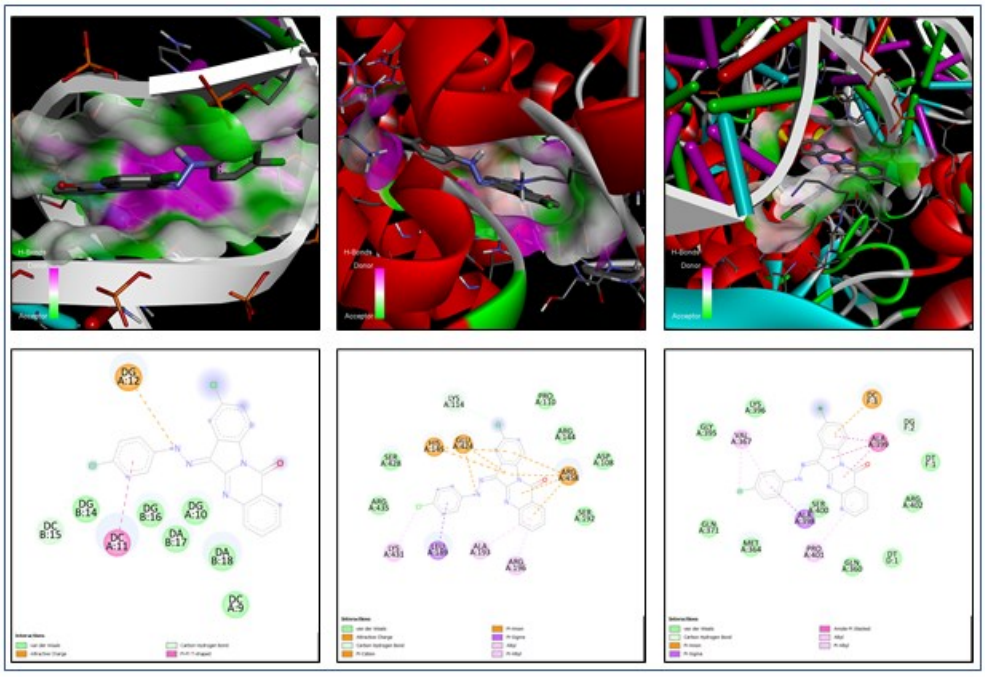
L^2



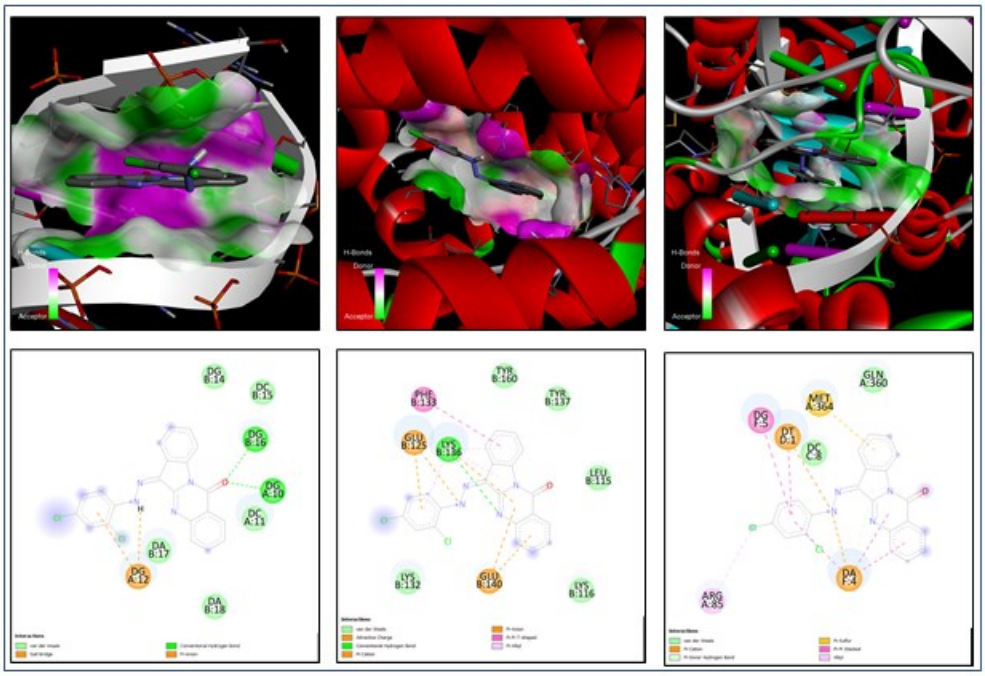
L^3



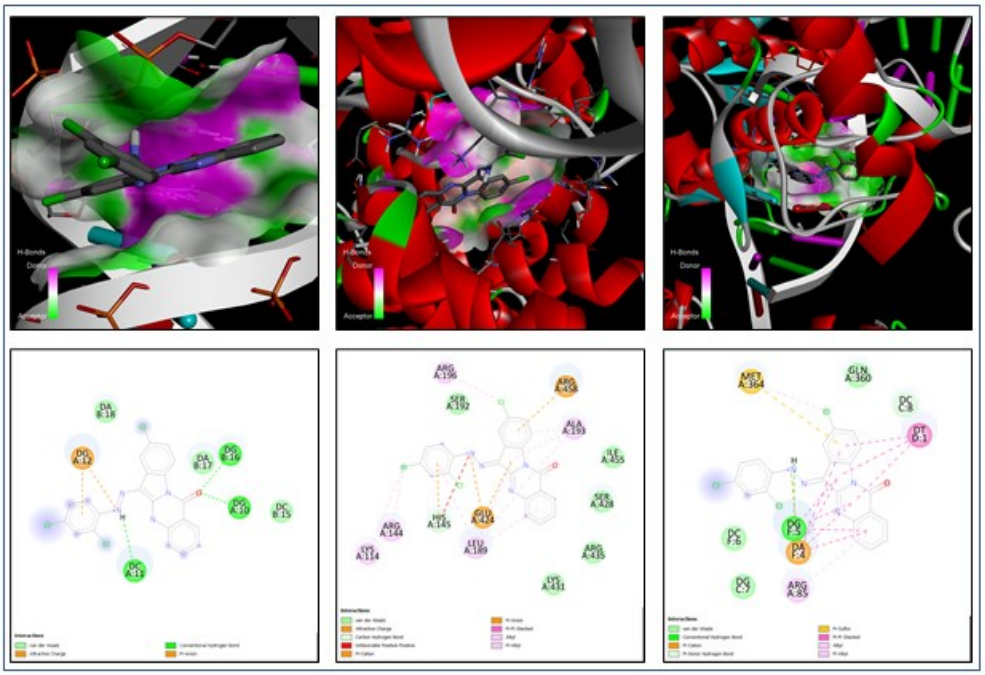
L^4



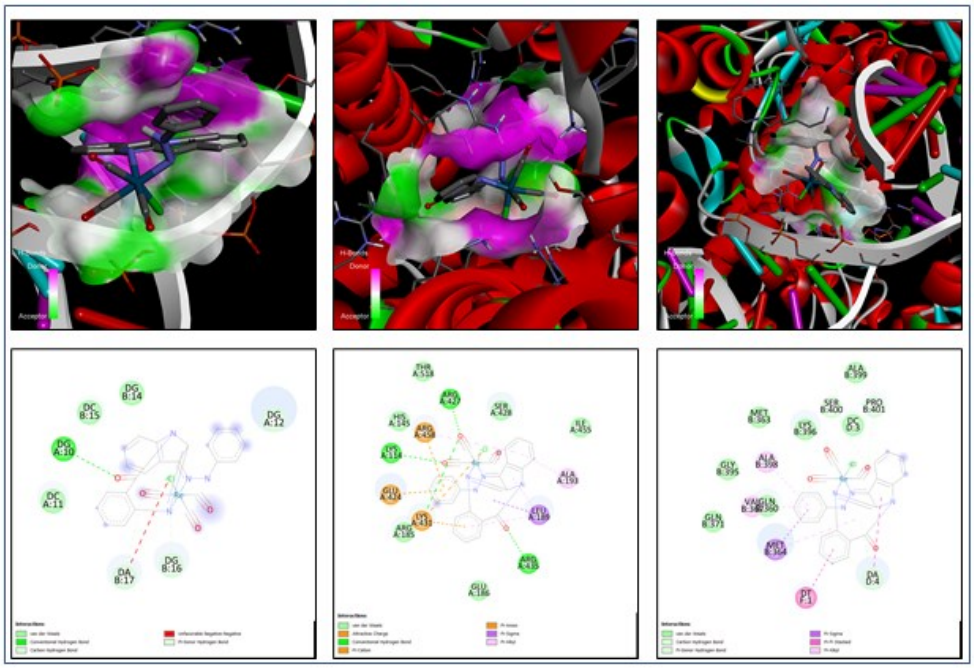
L[5]



L[6]



C[1]



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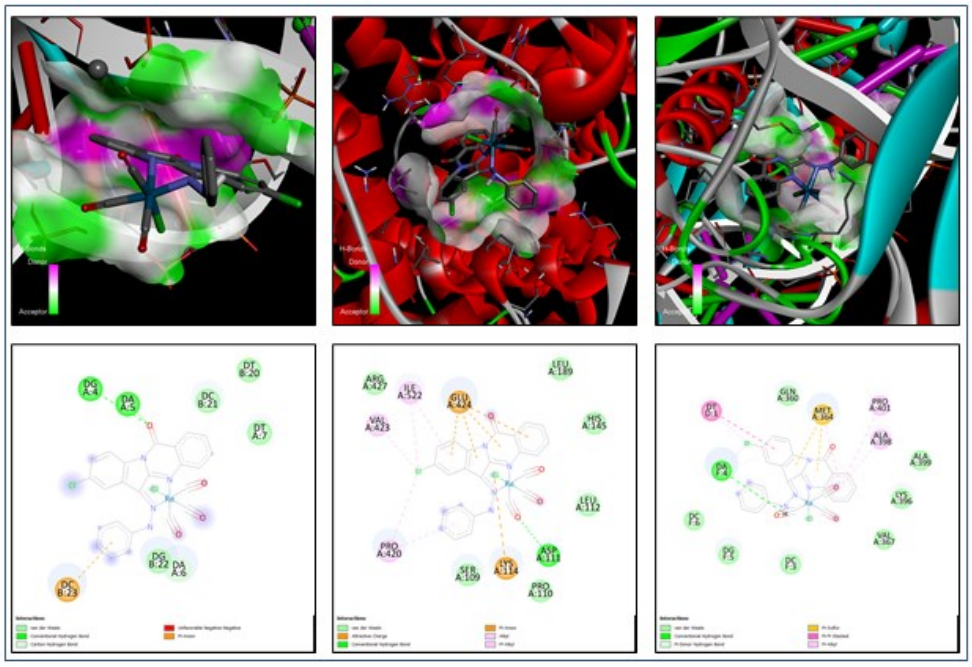

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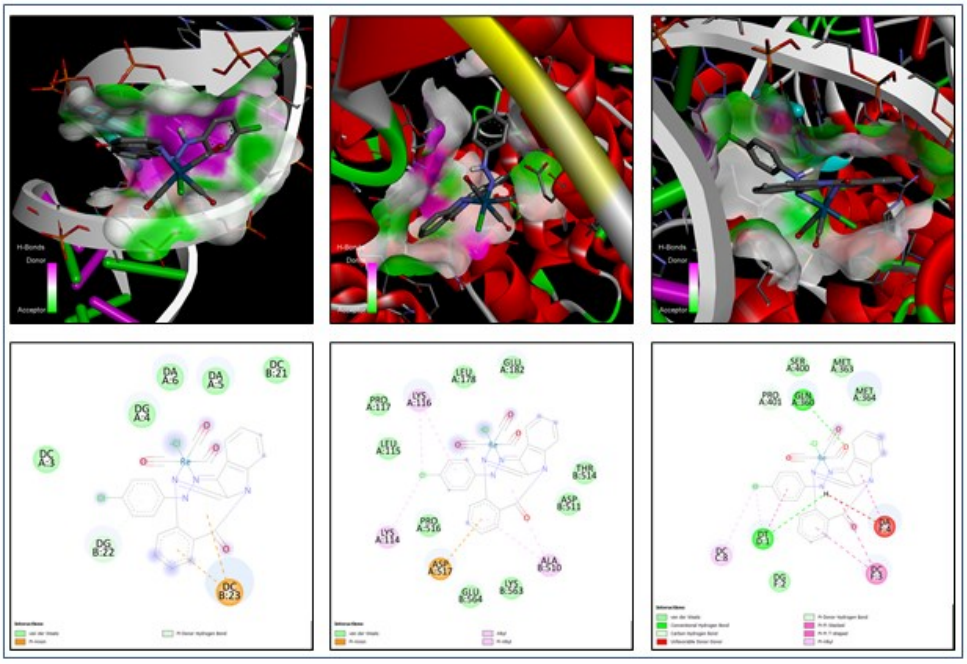
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Donor
Acceptor
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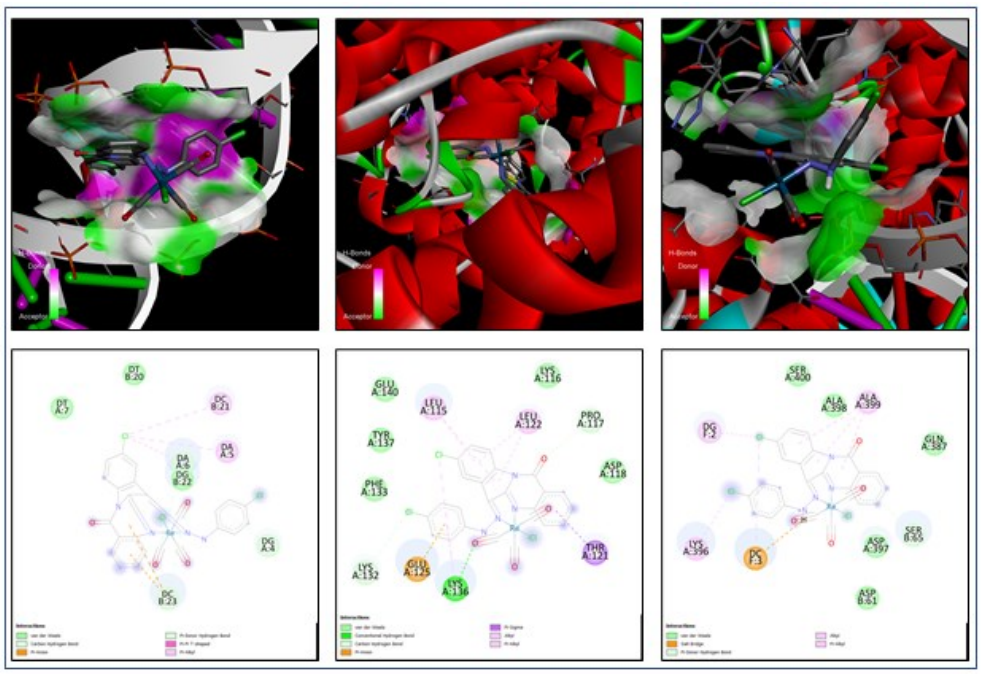
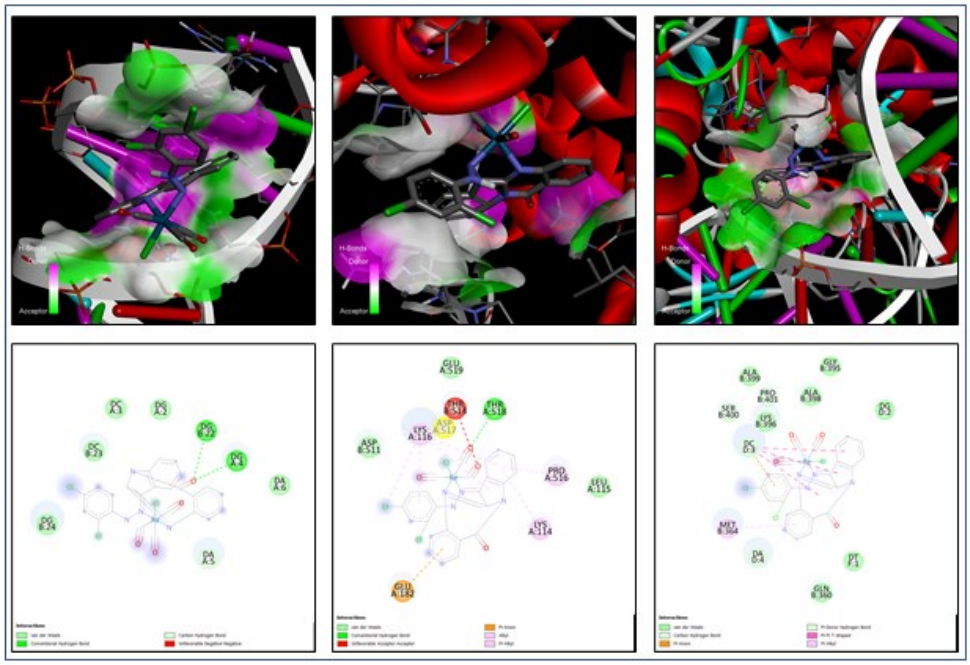
DA A:5
DC B:21
DG A:4
DC A:3
DG B:22
DC B:23
GLU A:182
LEU A:178
PRO A:117
LYS A:116
LEU A:115
THR B:514
ASP B:511
PRO A:516
LYS A:114
ASP A:517
ALA B:510
GLU B:564
LYS B:563
SER A:400
MET A:363
PRO A:401
GLN A:360
MET A:364
DT A:1
DA A:2
DC A:8
DG A:7
DC A:3

C[4]


H-Bonds
Donor
Acceptor
DT B:20
DT A:7
DC B:21
DA A:5
DA A:6
DG B:22
DG A:4
DC B:23
GLU A:140
LEU A:115
LYS A:116
LEU A:122
PRO A:117
TYR A:137
ASP A:118
PHE A:133
LYS A:132
GLU A:125
LYS A:136
THR A:121
SER A:400
ALA A:398
ALA A:399
DG P:2
GLN A:387
LYS A:396
DC P:3
ASP A:397
SER B:65
ASP B:61

C[5]



C[6]