

Novel benzothiazole based sulfonylureas/sulfonylthioureas: design, synthesis and evaluation of their antidiabetic potential

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Yakub Ali^a, Abhijeet Dhulap^b, Parwez Alam^c, M. A. Q. Pasha^c

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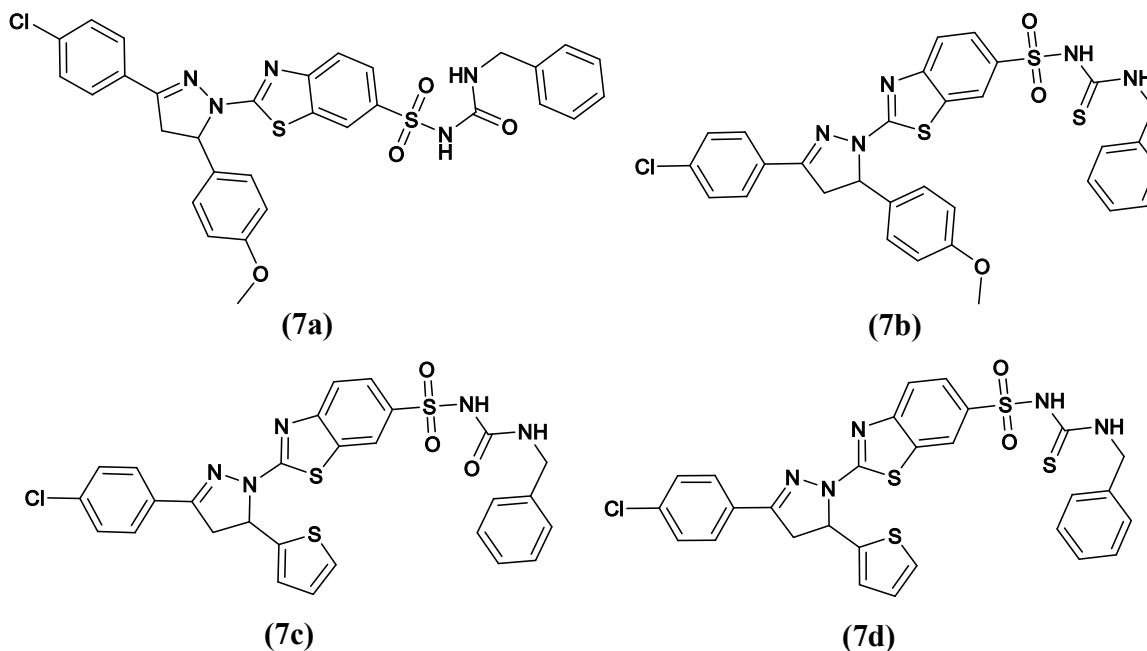
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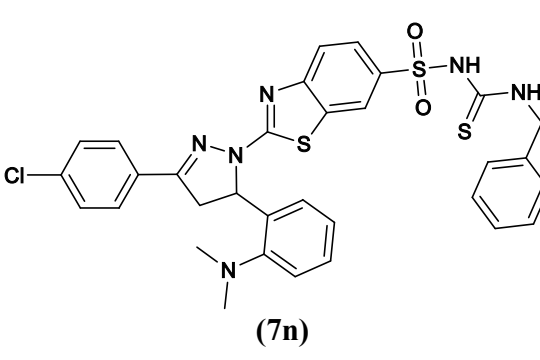
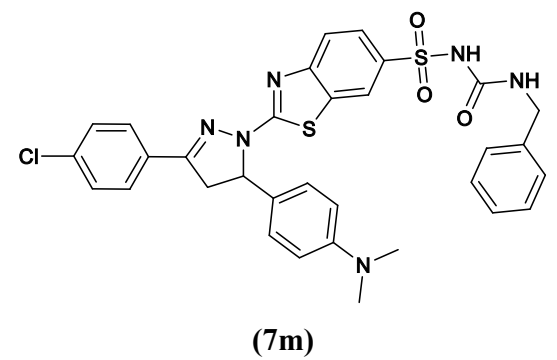
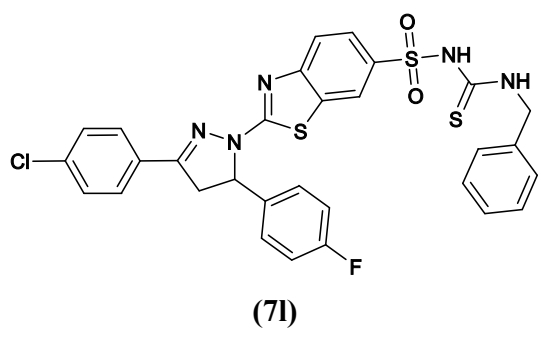
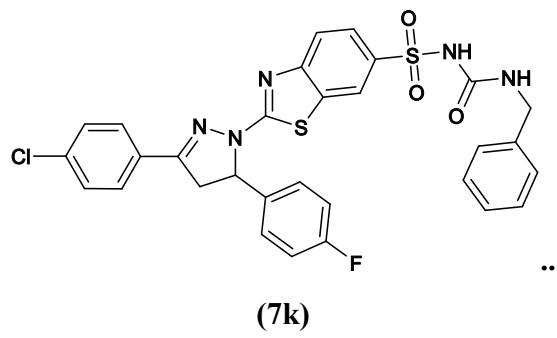
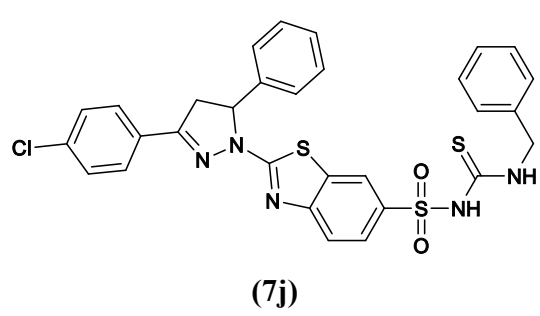
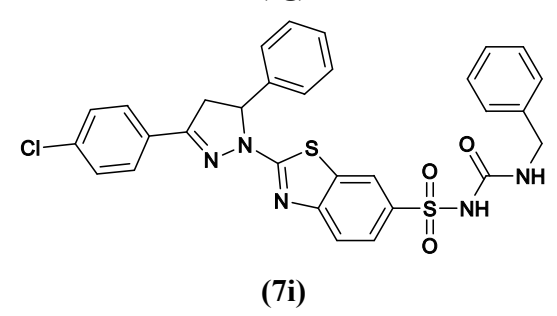
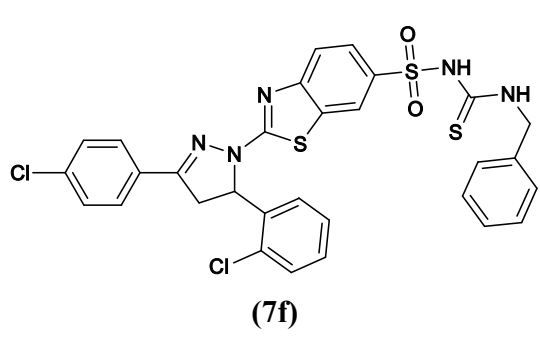
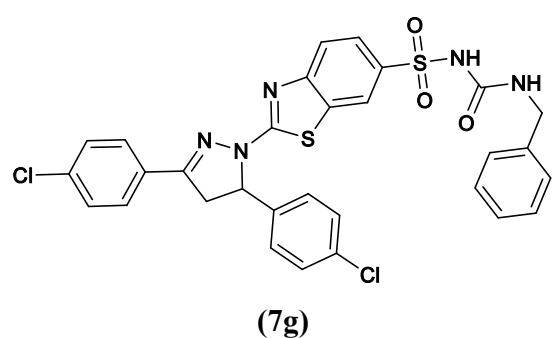
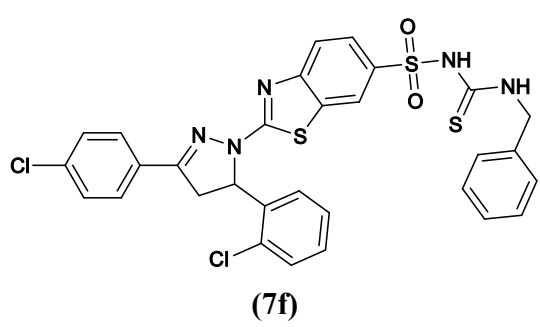
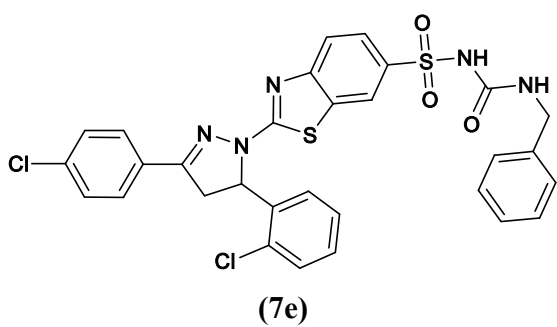
^cFunctional Genomics Unit, CSIR-Institute of Genomics & Integrative Biology, Delhi, India.

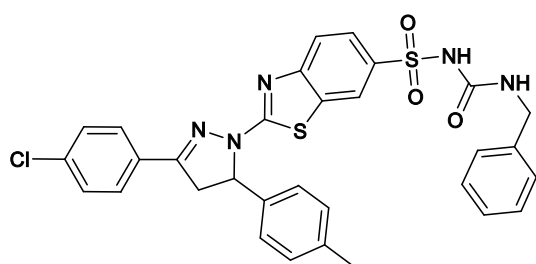
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Supplementary Data

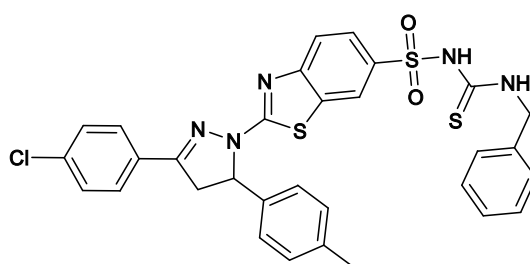
Fig S1: Structure of each compound indicating different substitutions



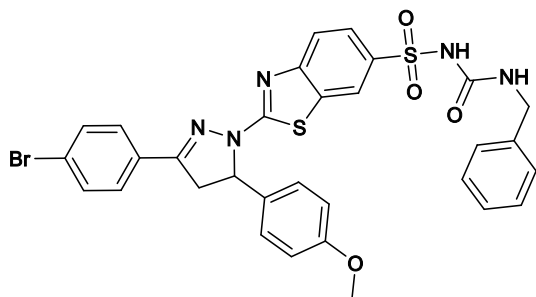




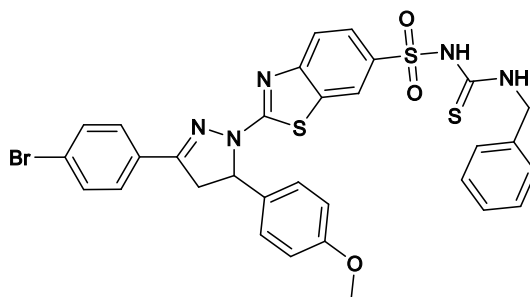
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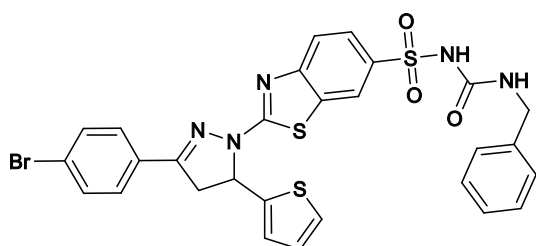
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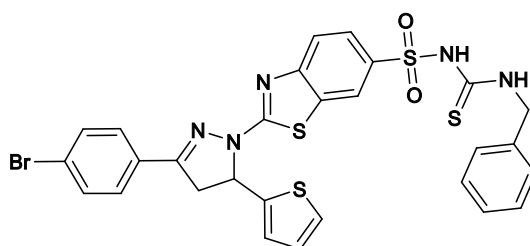
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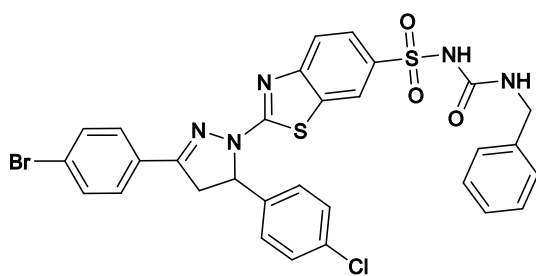
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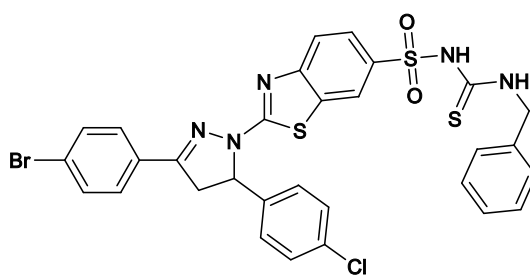
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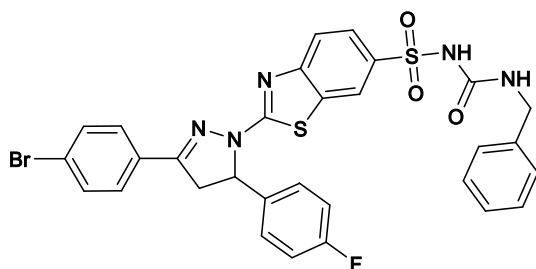
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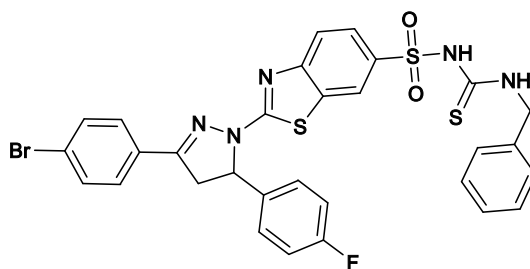
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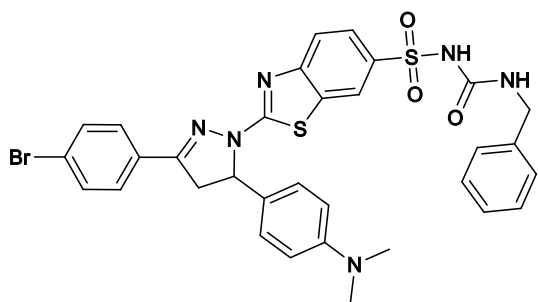
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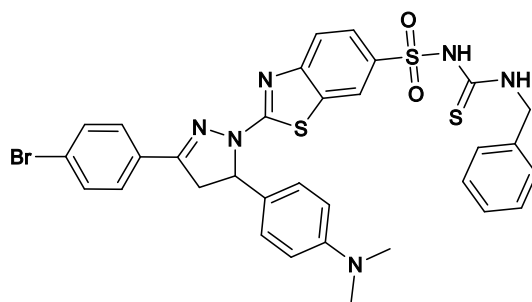
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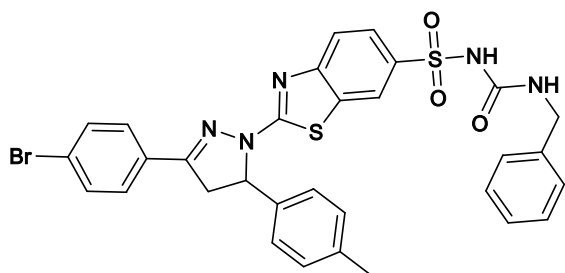
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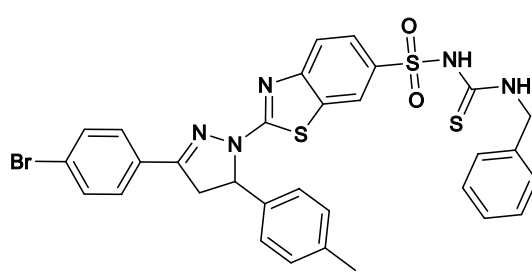
(8i)



(8j)



(8k)



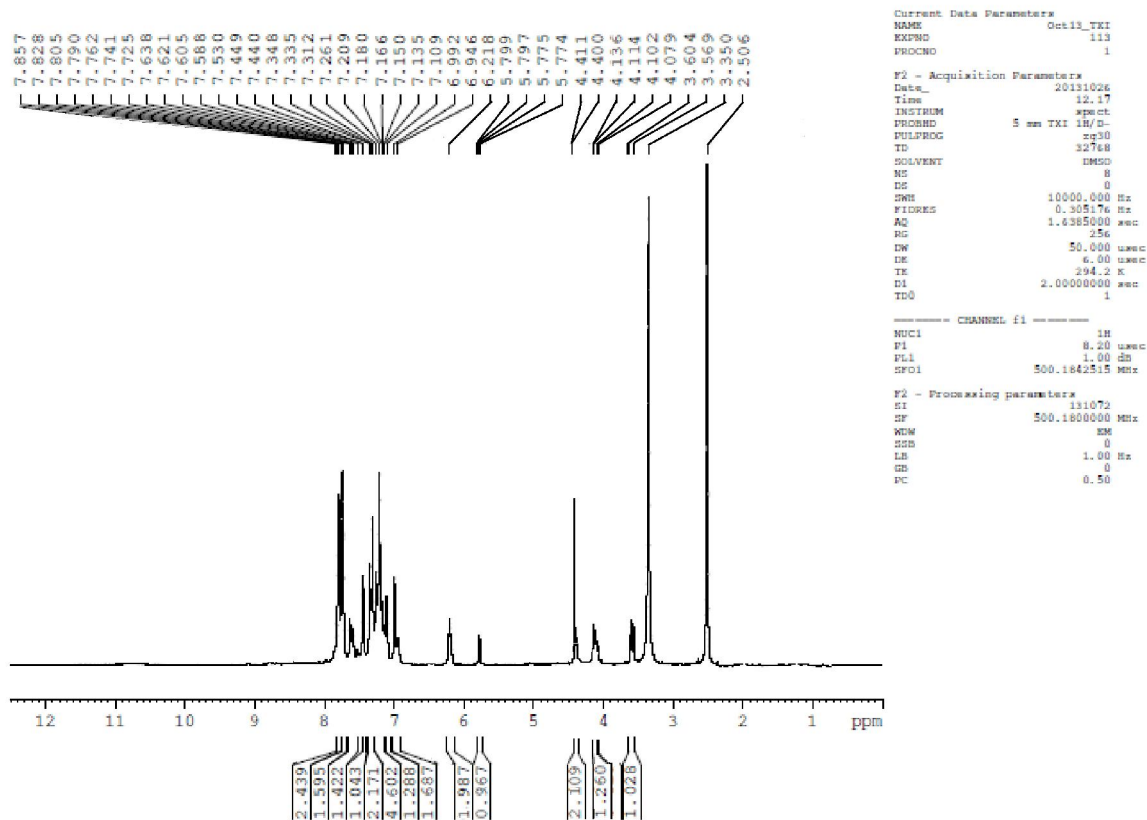
(8l)

Table S1: Dock Scores of all the ligand in 3CS8 protein site.

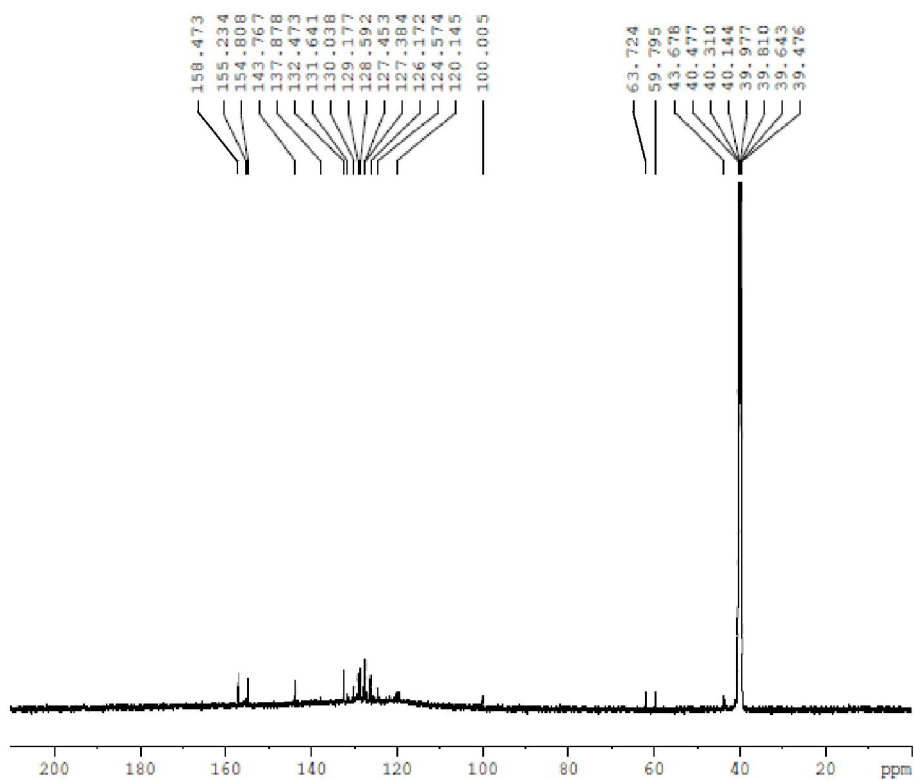
Ligand	Glide Score	Dock Score
7k	-10.06	-10.06
8h	-10.03	-9.99
8g	-9.93	-9.93
7j	-9.81	-9.77
7i	-9.62	-9.62
7l	-9.47	-9.43
7c	-9.14	-9.14
7d	-9.1	-9.07
8d	-8.99	-8.99
7a	-8.82	-8.82
8c	-8.85	-8.82
7m	-8.32	-8.31
7f	-7.83	-7.79
8f	-7.3	-7.26
7n	-9.13	-6.51
7o	-6.31	-6.31
8j	-8.89	-6.27
7b	-5.81	-5.77
Rosiglitazone	-5.72	-5.72
8k	-5.63	-5.62
8l	-5.5	-5.47
8b	-5.42	-5.39
7e	-5.13	-5.13
8a	-4.87	-4.87
7p	-6.5	-4.83
7g	-4.31	-4.31
8e	-3.54	-3.54
7h	-3.18	-3.15
8i	-2.75	-0.17

Compound 7k

¹H-NMR



¹³C-NMR



Current Data Parameters
NAME Oct13_TX1
EXPNO 114
PROCNO 1

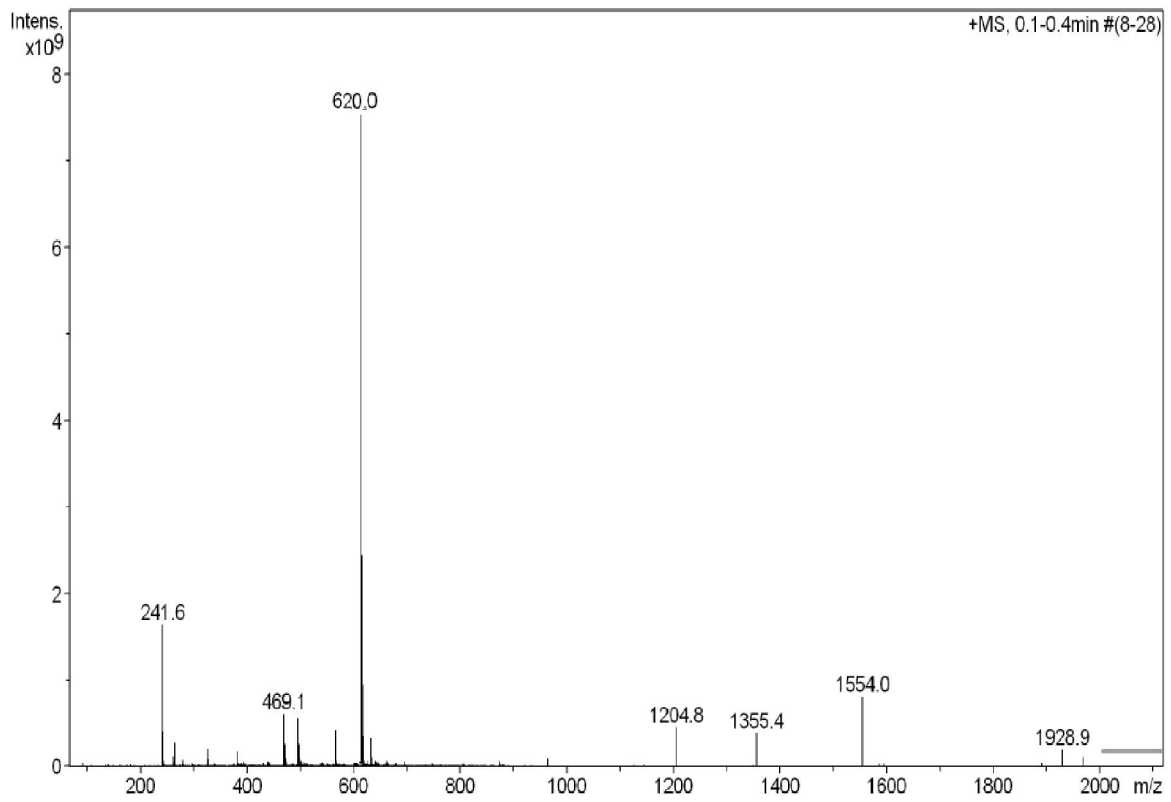
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Date_ 20131026
Time 12.58
INSTRUM spect
PROBHD 5 mm TXI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4494
DS 4
SWH 30010.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 32768
DW 16.650 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 11.40 usec
PL1 -4.00 dB
SFO1 125.7629381 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 21.30 dB
PL13 21.30 dB
SFO2 500.1620007 MHz

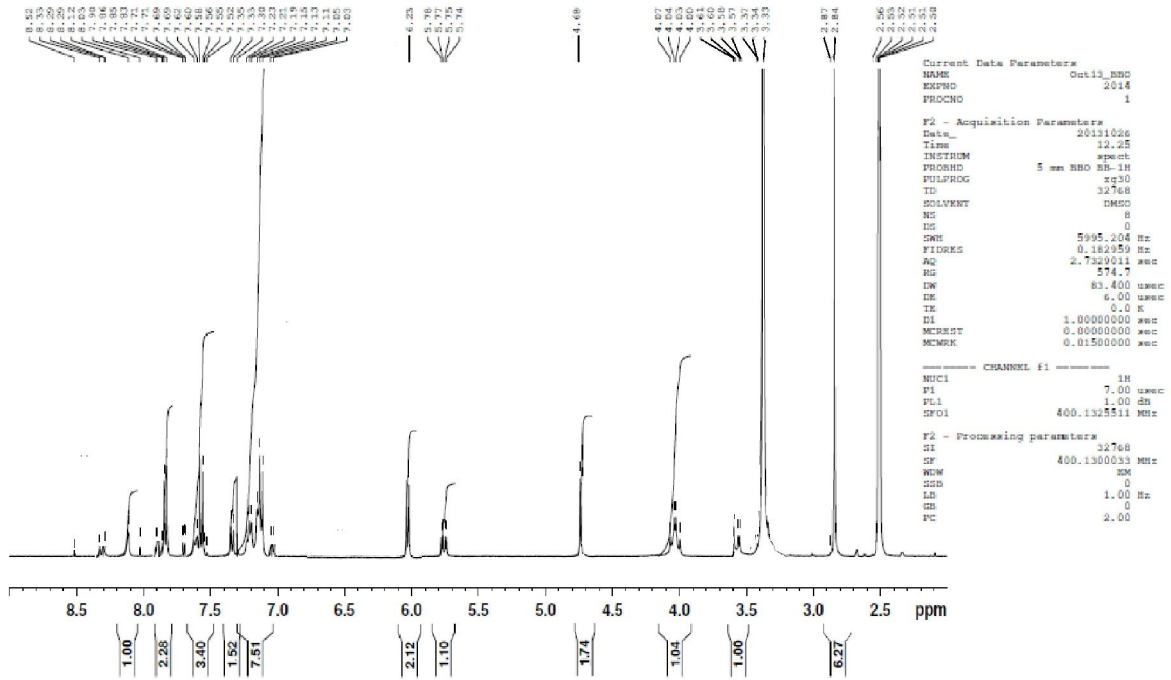
F2 - Processing parameters
SI 32768
SF 125.7703610 MHz
WM EM
SS 0
LB 3.00 Hz
GB 0
PC 3.00

Mass Spectrum



Compound 7m

¹H-NMR



¹³C-NMR

