Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Design and Synthesis of a New Series of 3,5-Disubstituted-1,2,4-Oxadiazoles as Potential Colchicine Binding Site Inhibitors: Antiproliferative activity, Molecular docking, and SAR Studies

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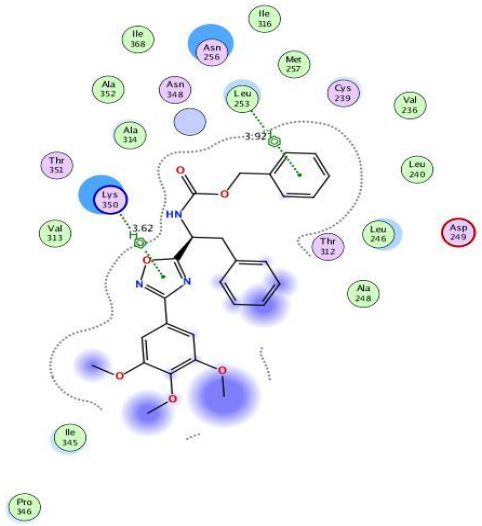
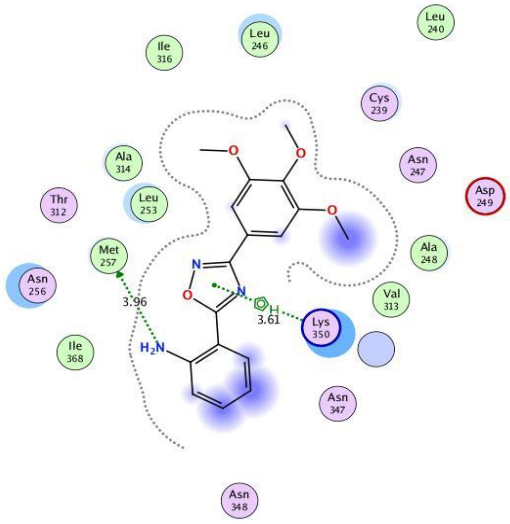
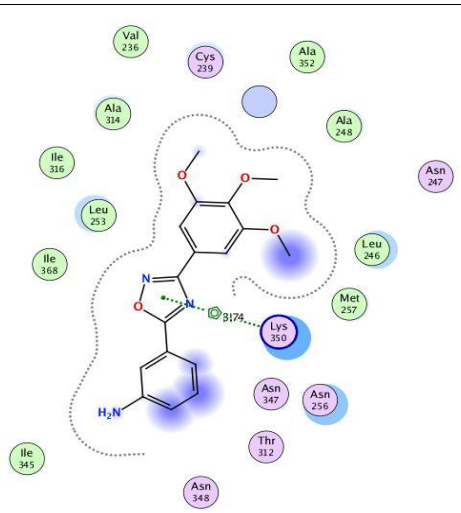
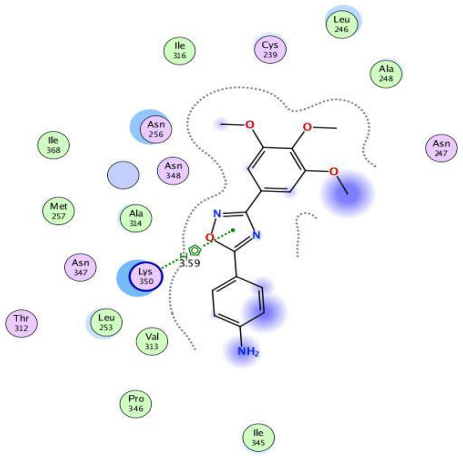
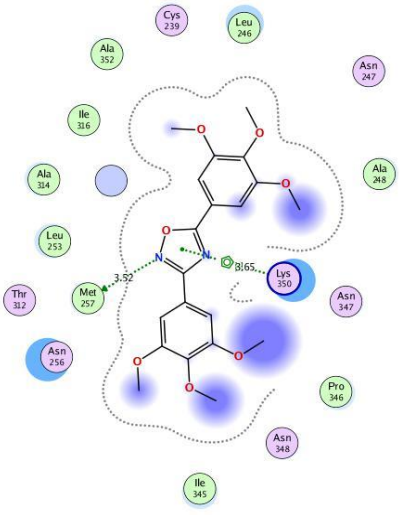
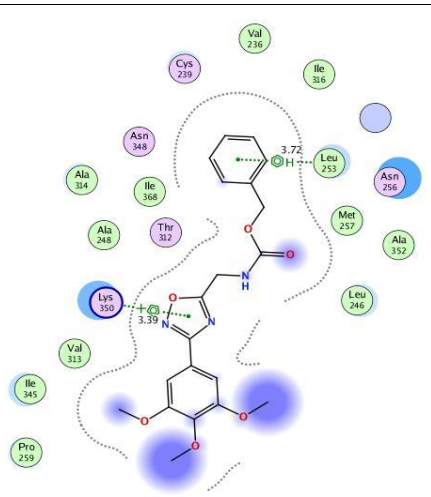
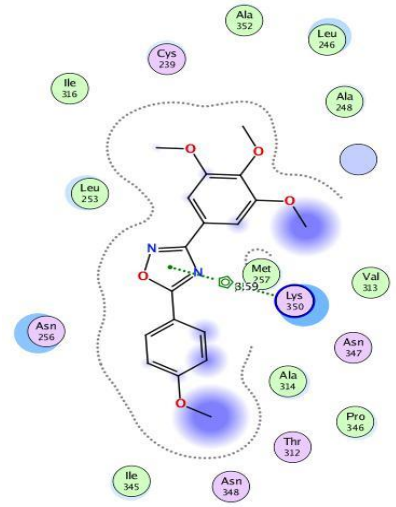
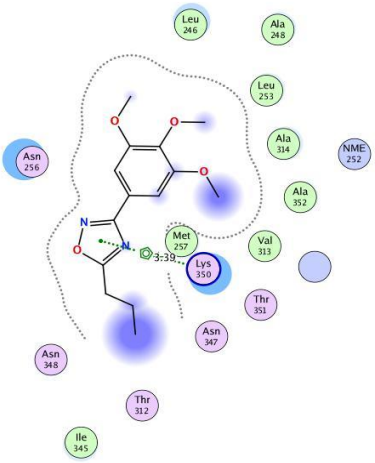
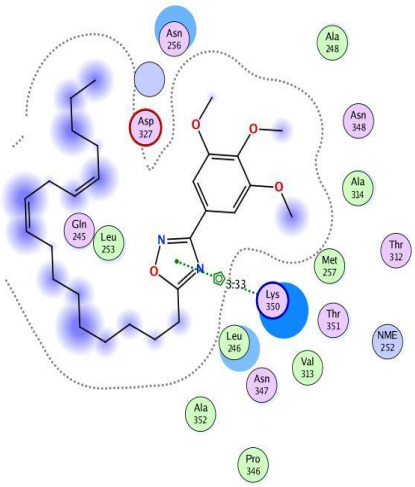
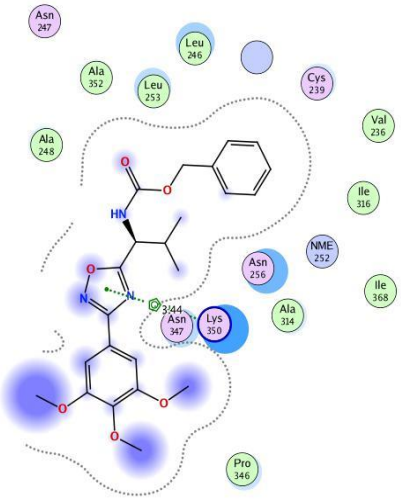
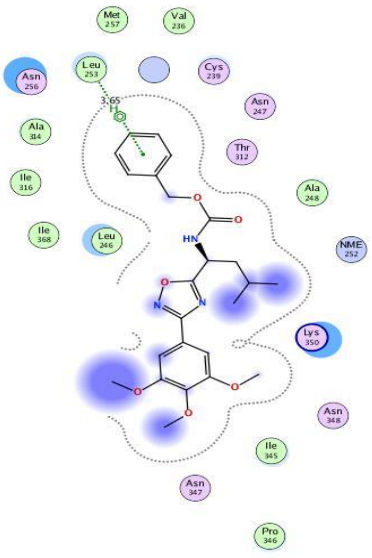
Contents:

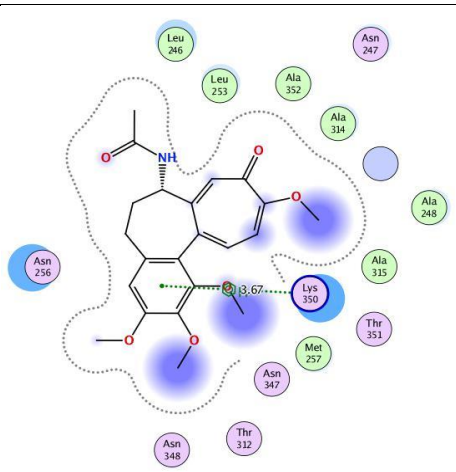
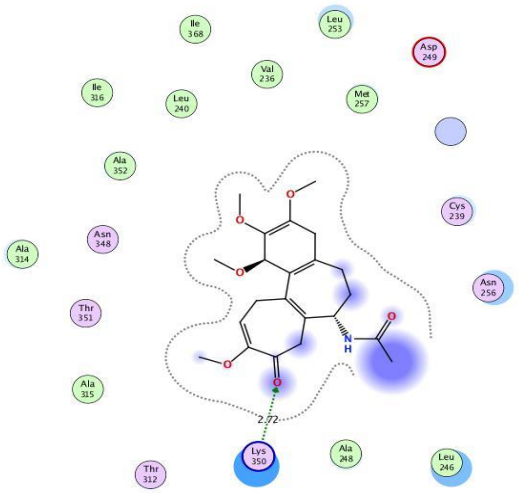
Table SI1: 2 D pictures of the binding interactions between the newly synthesized series of 3,5 disubstituted 1,2,4-oxadiazoles (**5a-5k**) into the colchicine binding site in β-tubulin compared to Col and the docked co-crystallized inhibitor.

No.	Compound	2 D binding interactions
1	**5a**	
2	5b	

3	5c	 Val 236 Cys 239 Ala 352 Ala 314 Ala 248 Ile 316 Asn 247 Leu 253 Leu 246 Ile 368 Met 257 3.74 Lys 350 Asn 347 Asn 256 H_2N Thr 312 Ile 345 Asn 348
4	5d	 Leu 246 Ile 316 Cys 239 Ala 248 Asn 256 Ile 368 Asn 247 Asn 348 Met 257 Ala 314 Asn 347 3.59 Lys 350 Thr 312 Leu 253 Val 313 NH_2 Pro 346 Ile 345
5	**5e**	 Cys 239 Leu 246 Ala 352 Asn 247 Ile 316 Ala 314 Ala 248 Leu 253 3.65 Lys 350 3.52 Thr 312 Met 257 Asn 347 Asn 256 Pro 346 Asn 348 Ile 345

6	5f	 Val 236 Cys 239 Ile 316 Asn 348 3.72 Leu 253 Asn 256 Ala 314 Ile 368 Met 257 Ala 248 Thr 312 Ala 352 Lys 350 3.39 Leu 246 Val 313 Ile 345 Pro 259
7	5g	 Ala 352 Leu 246 Cys 239 Ile 316 Ala 248 Leu 253 Met 257 3.59 Val 313 Lys 350 Asn 256 Asn 347 Ala 314 Pro 346 Thr 312 Ile 345 Asn 348
8	5h	 Leu 246 Ala 248 Leu 253 Asn 256 Ala 314 NME 252 Ala 352 Met 257 Val 313 3.39 Lys 350 Thr 351 Asn 347 Asn 348 Thr 312 Ile 345

9	5i	
10	5j	
11	5k	

12	**Col**	
13	**Docked co-crystallized inhibitor**	

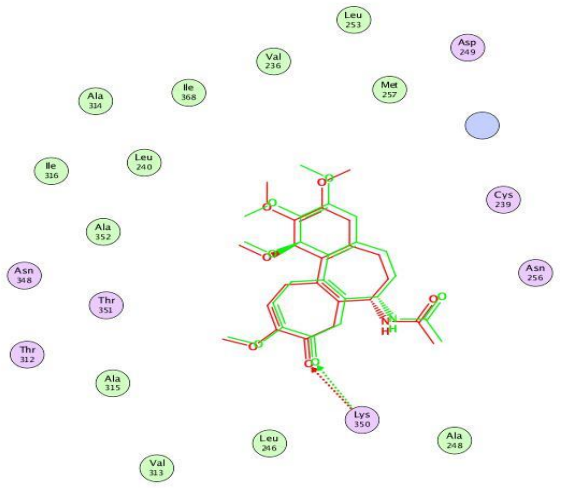
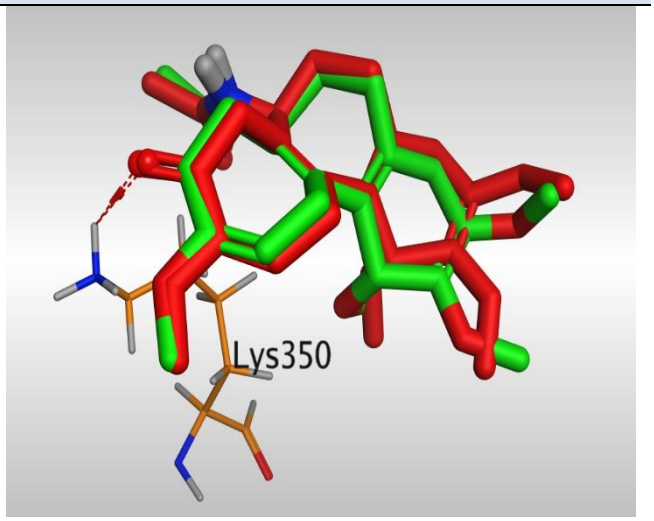
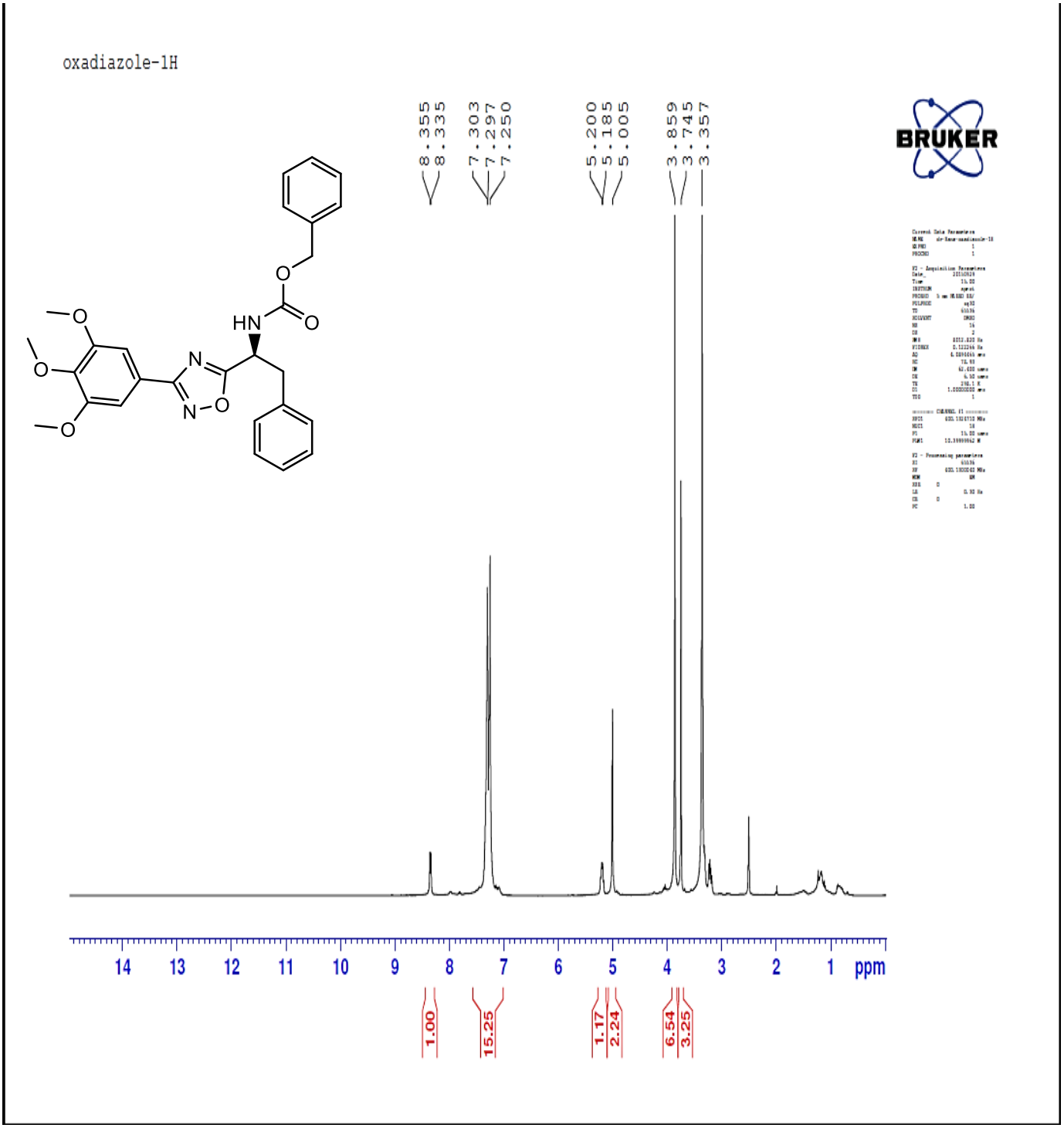
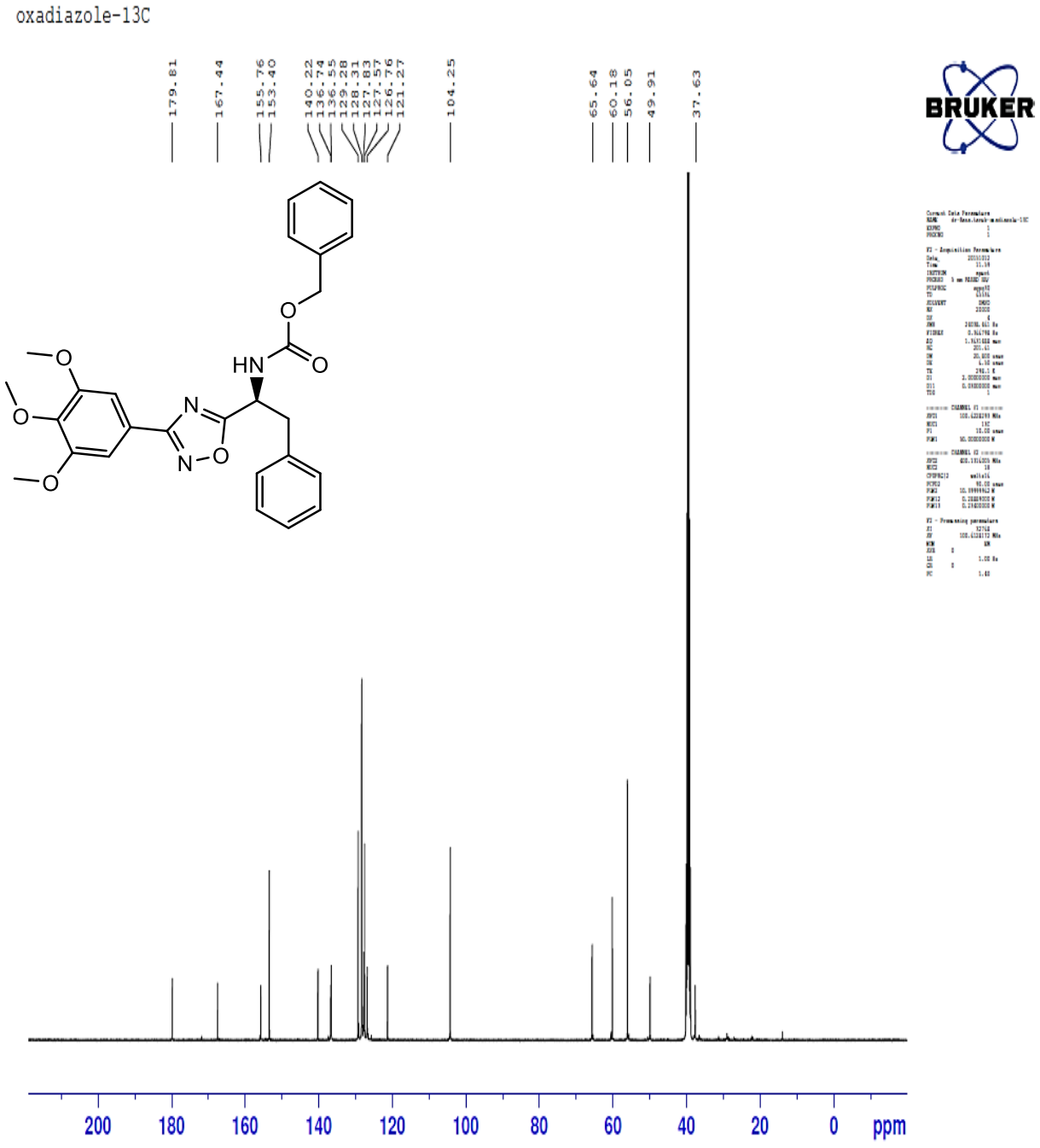
Redocked Co-crystallized Inhibitor	
2 D	**3 D**
	

Figure SI1: 2 D and 3 D representations of the redocking process between the co-crystallized inhibitor (green) and the docked one (red).

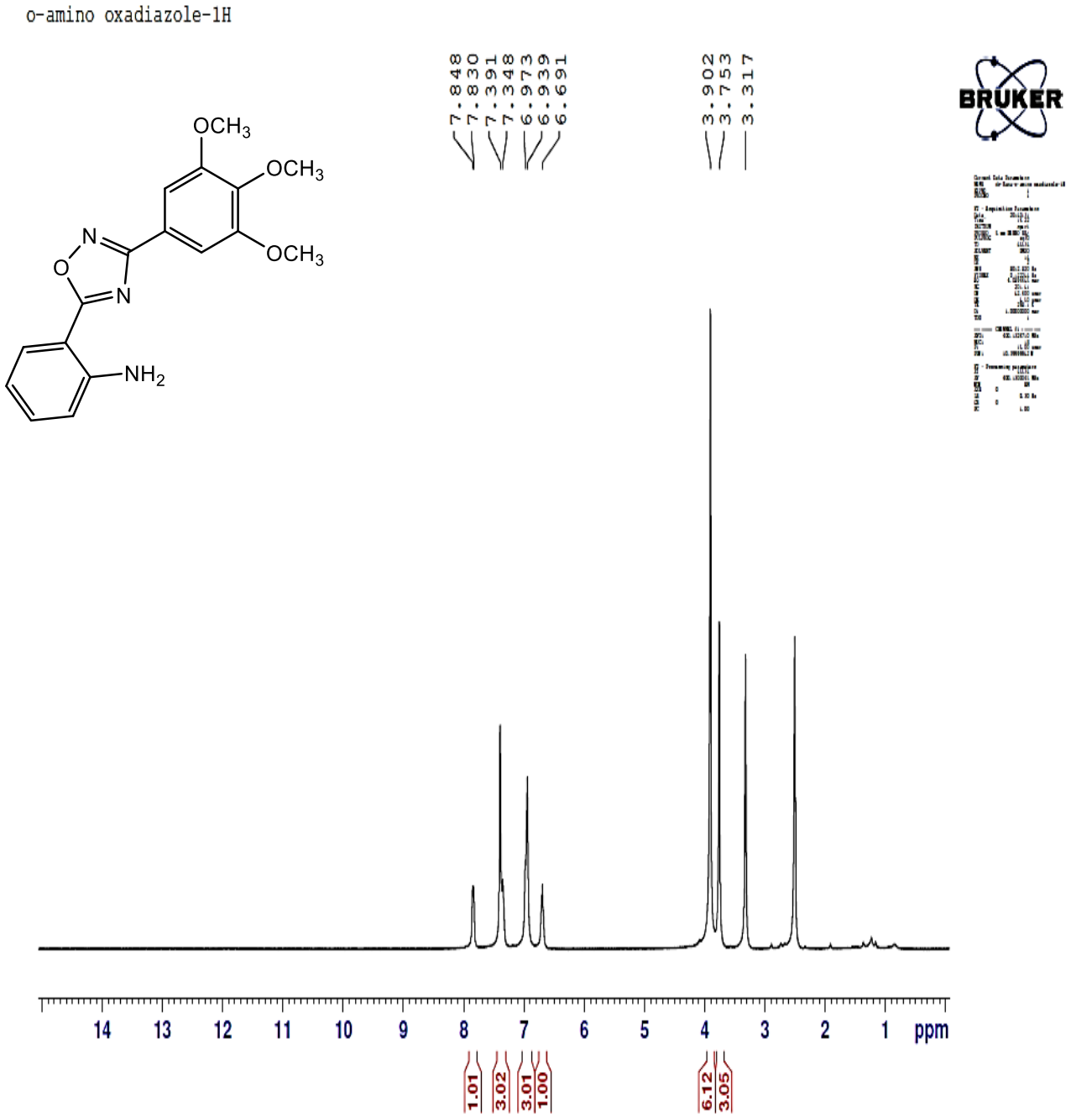
5a


oxadiazole-1H
8.355
8.335
7.303
7.297
7.250
5.200
5.185
5.005
3.859
3.745
3.357
BRUKER
HN
O
N
N-O
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
15.25
1.17
2.24
6.54
3.25

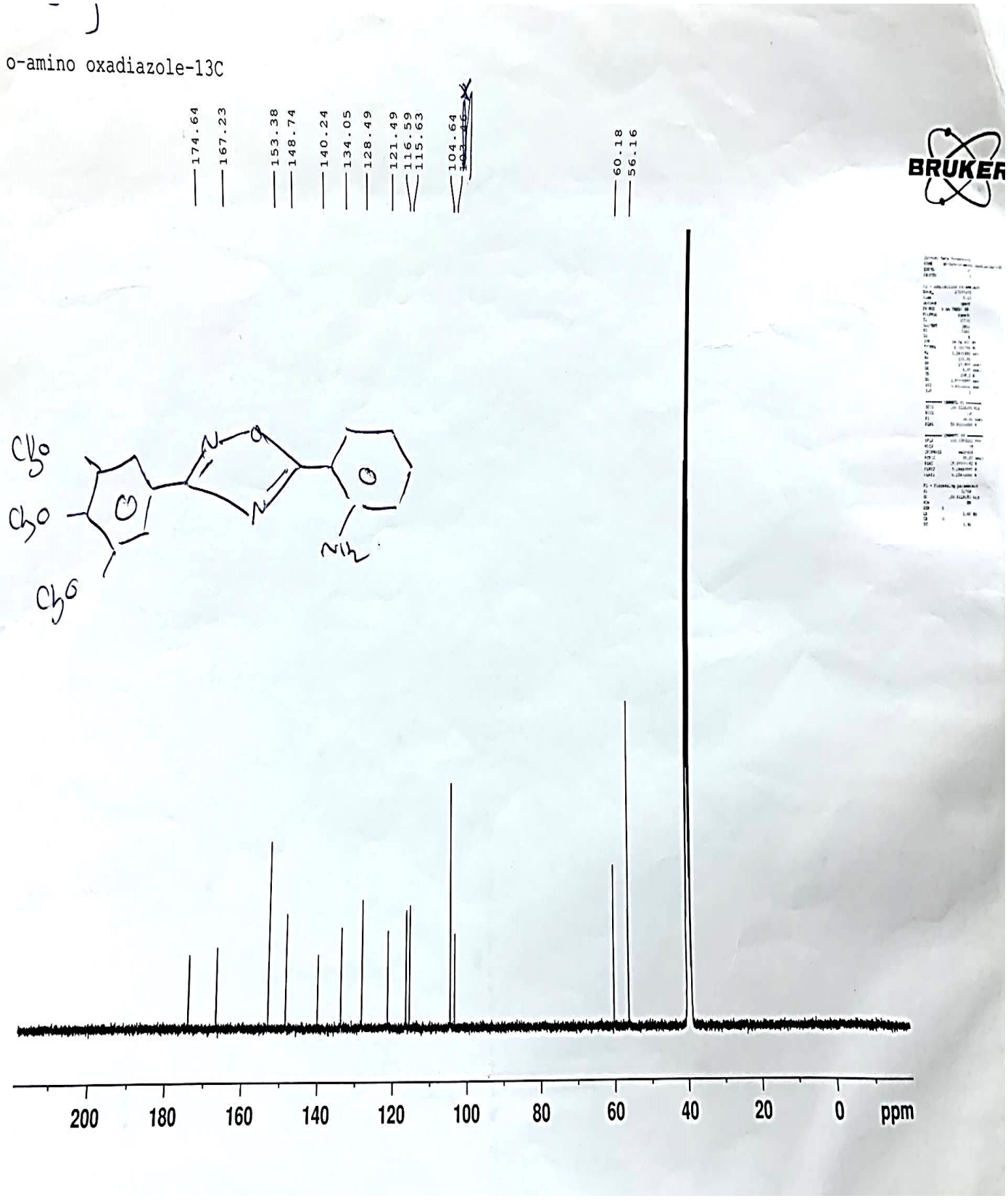
5a


oxadiazole-13C
179.81
167.44
155.76
153.40
140.22
136.74
136.55
129.28
128.31
127.57
126.76
121.27
104.25
65.64
60.18
56.05
49.91
37.63
BRUKER
HN
O
N
N-O
200
180
160
140
120
100
80
60
40
20
0
ppm

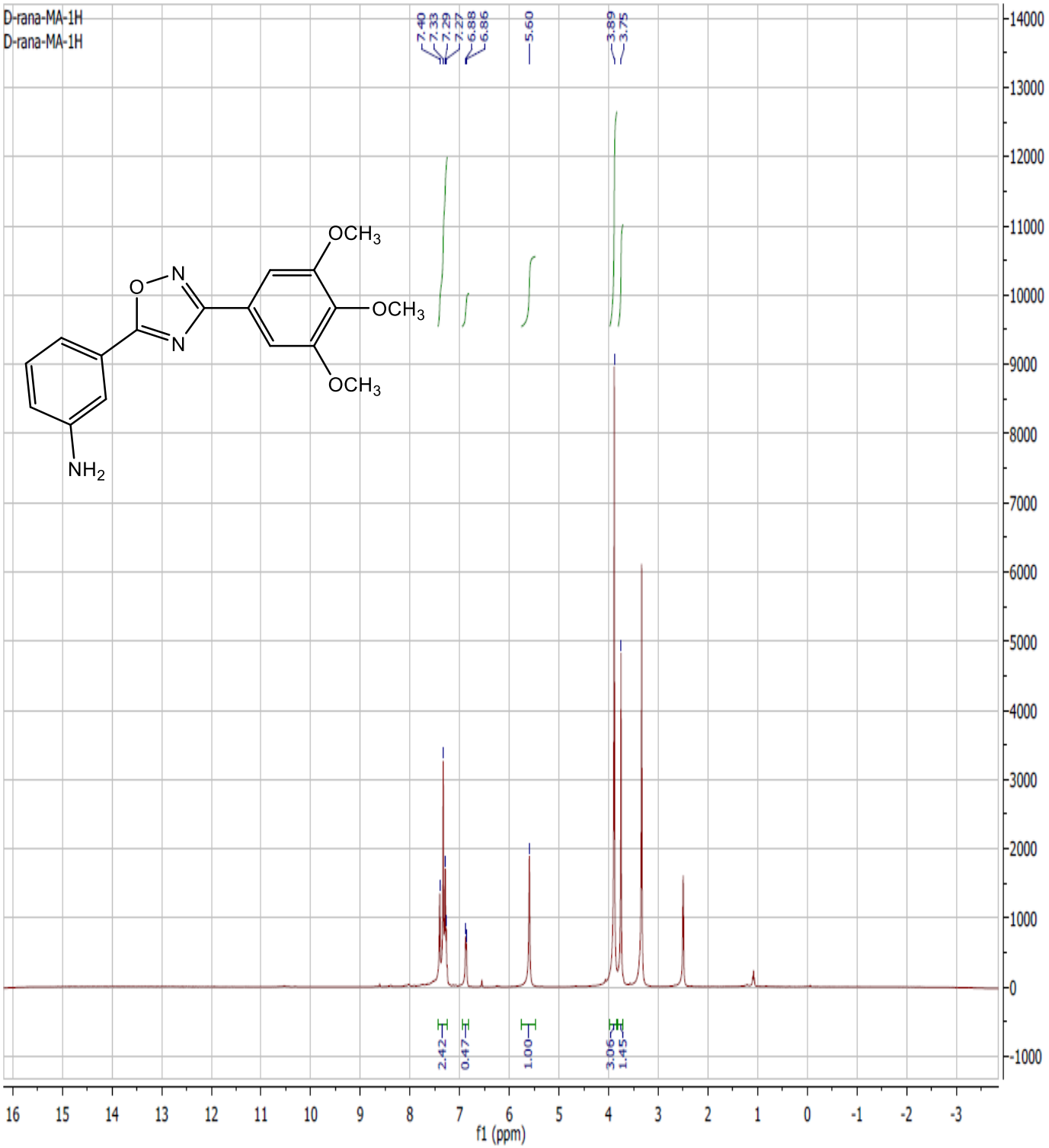
5b


o-amino oxadiazole-1H
7.848
7.830
7.391
7.348
6.973
6.939
6.691
3.902
3.753
3.317
OCH3
OCH3
OCH3
N
O
N
NH2
BRUKER
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.01
3.02
3.01
1.00
6.12
3.05

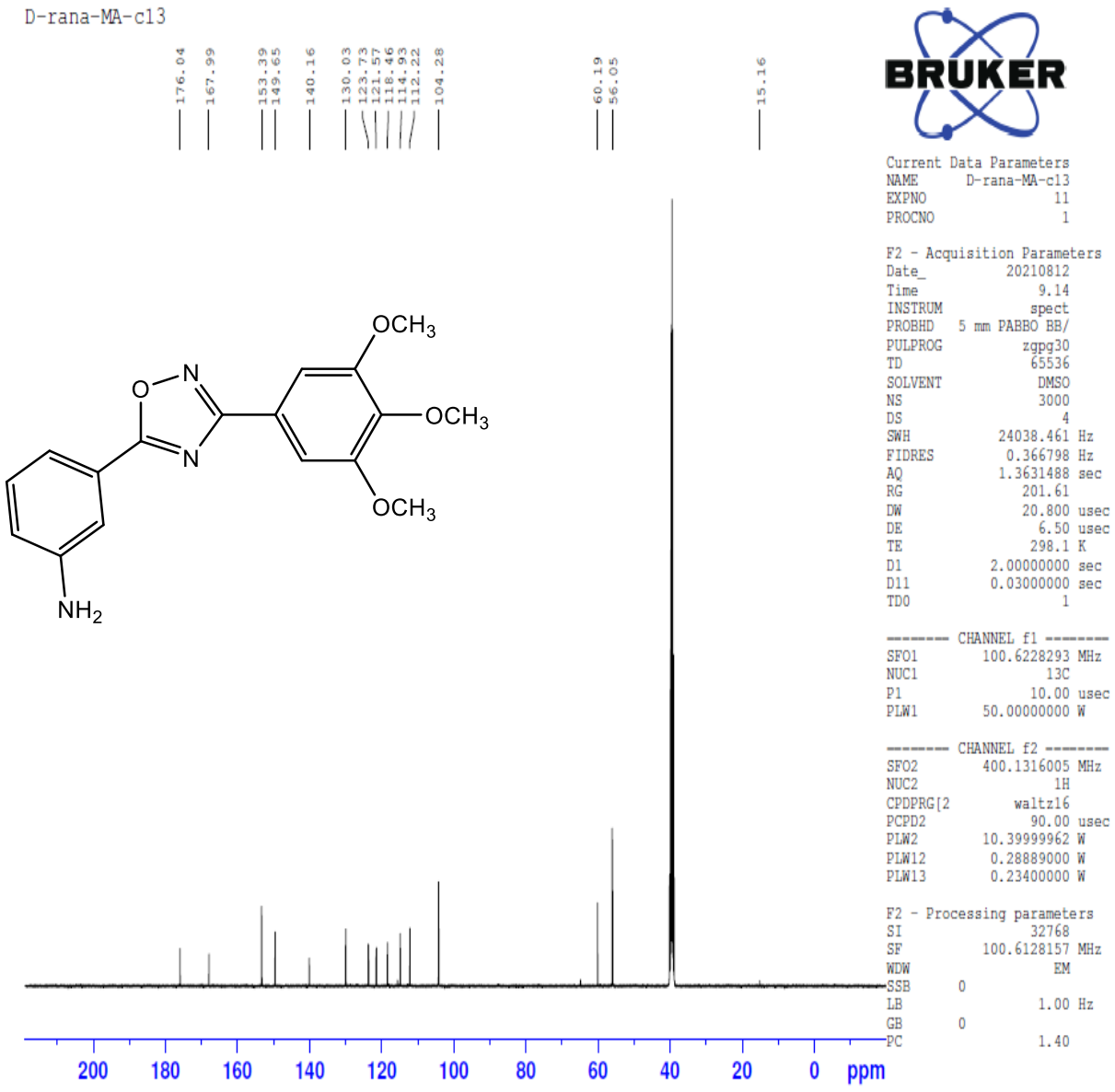
5b


o-amino oxadiazole-13C
174.64
167.23
153.38
148.74
140.24
134.05
128.49
121.49
116.59
115.63
104.64
103.46
60.18
56.16
BRUKER
200
180
160
140
120
100
80
60
40
20
0
ppm

5c


D-rana-MA-1H
D-rana-MA-1H
7.40
7.33
7.29
7.27
6.88
6.86
5.60
3.89
3.75
OCH3
OCH3
OCH3
N
O
N
NH2
2.42
0.47
1.00
3.06
1.45
f1 (ppm)

5c



BRUKER

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PROCNO               1

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Time               9.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT            DMSO
NS                 3000
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG               201.61
DW               20.800 usec
DE                6.50 usec
TE               298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1               13C
P1               10.00 usec
PLW1         50.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2         10.39999962 W
PLW12         0.28889000 W
PLW13         0.23400000 W

F2 - Processing parameters
SI                32768
SF           100.6128157 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
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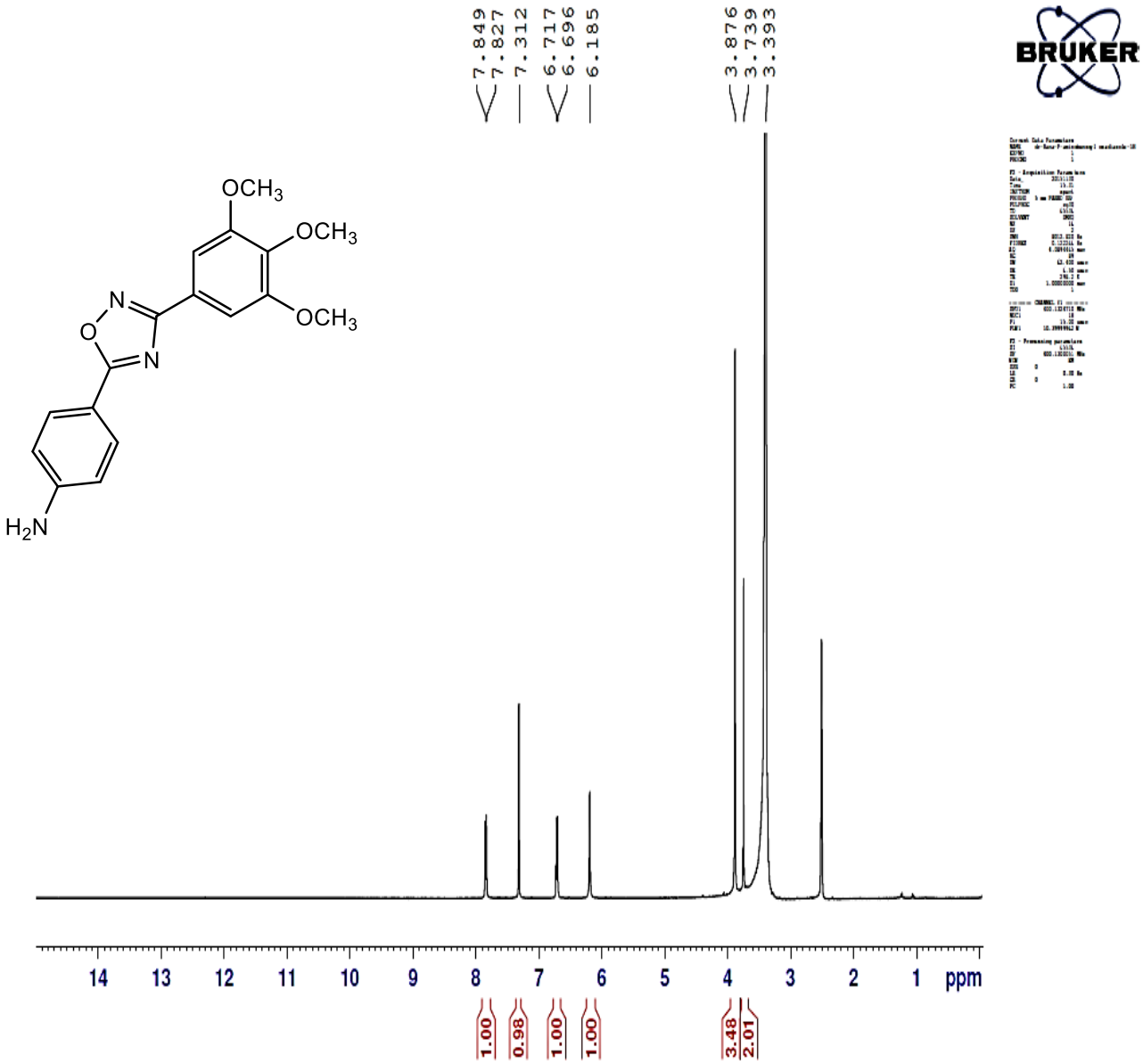
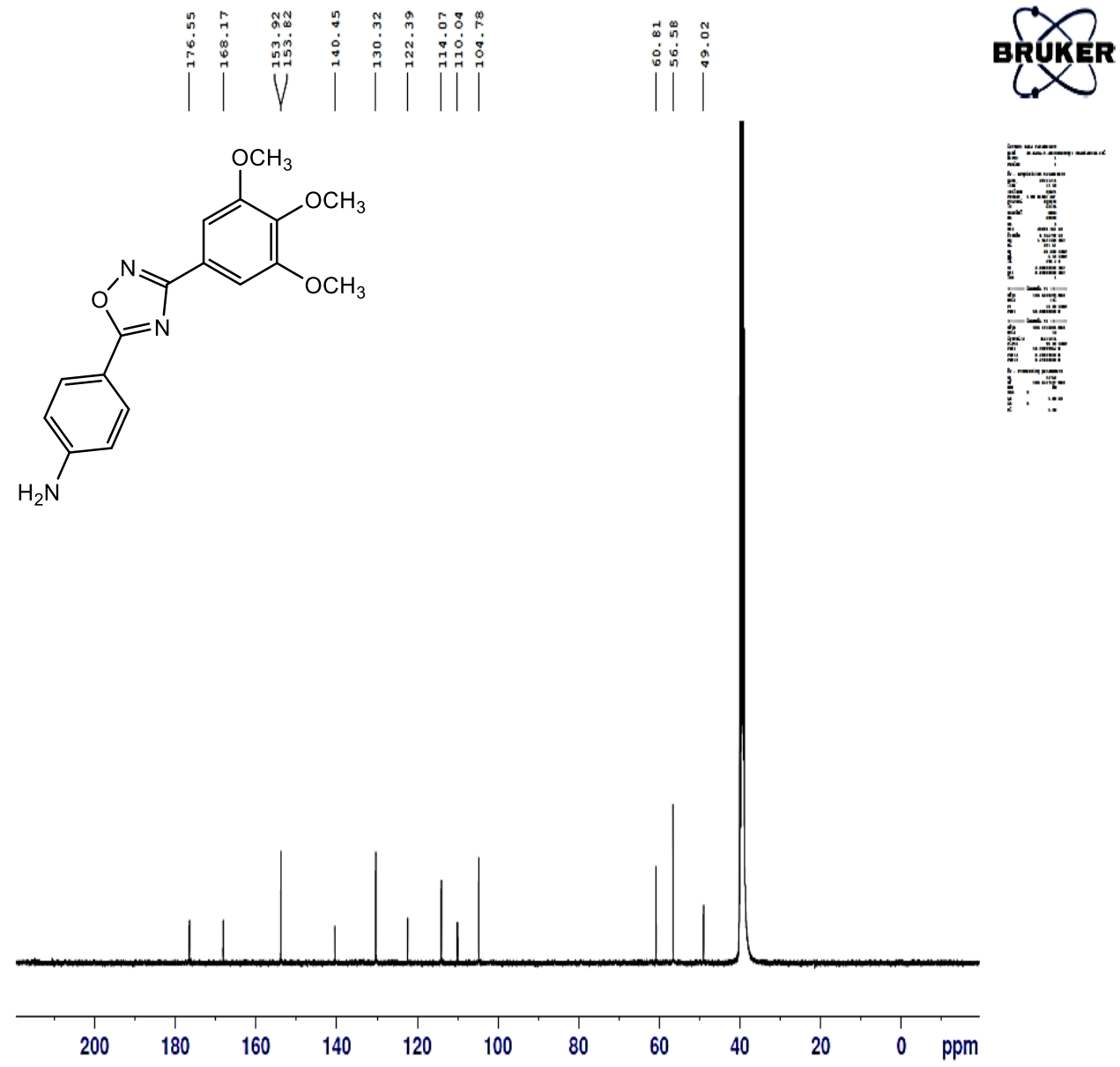
5d

P-aminobenzoyl oxadiazole-1H



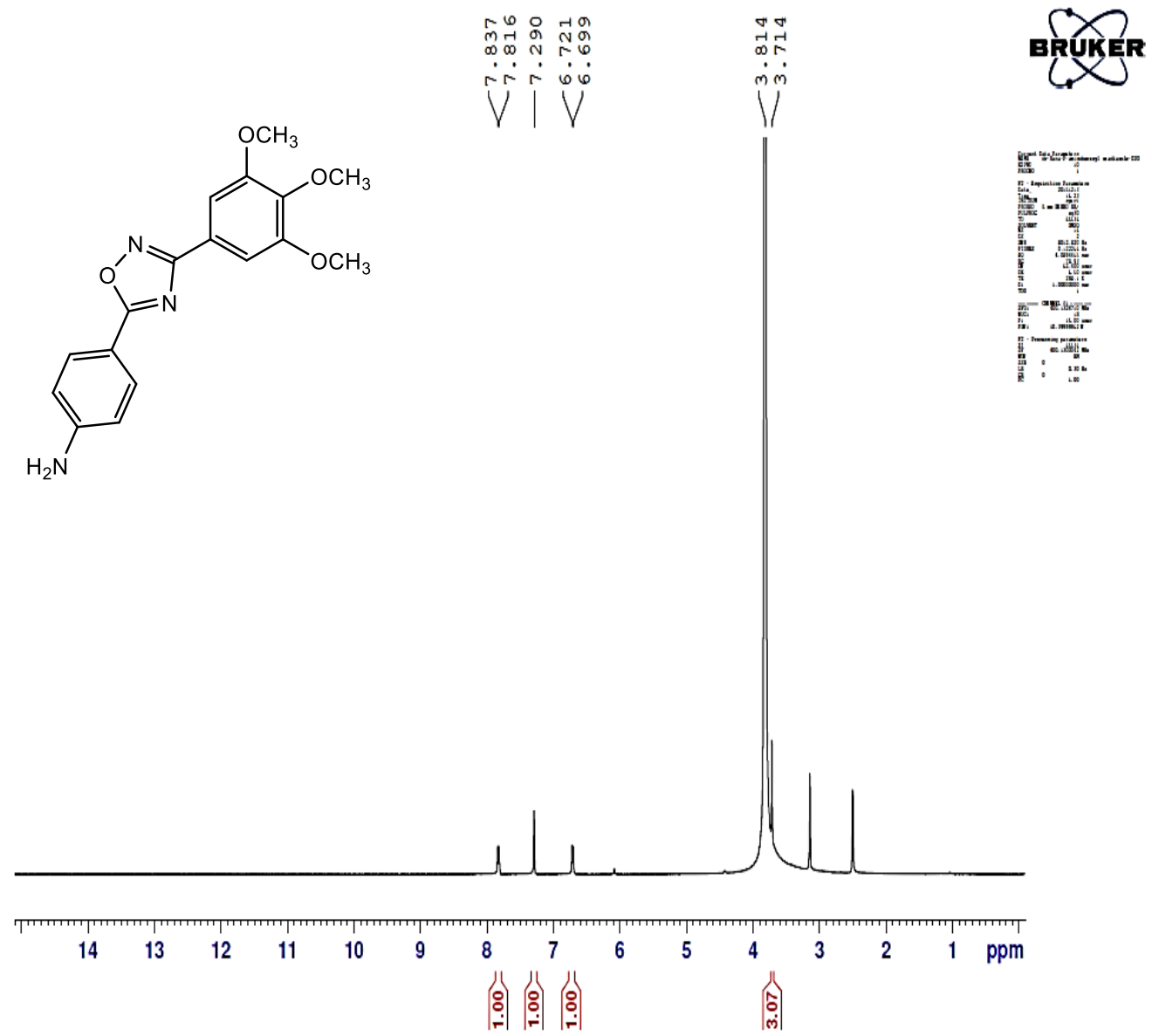
5d

P-aminobenzoyl oxadiazole-13C

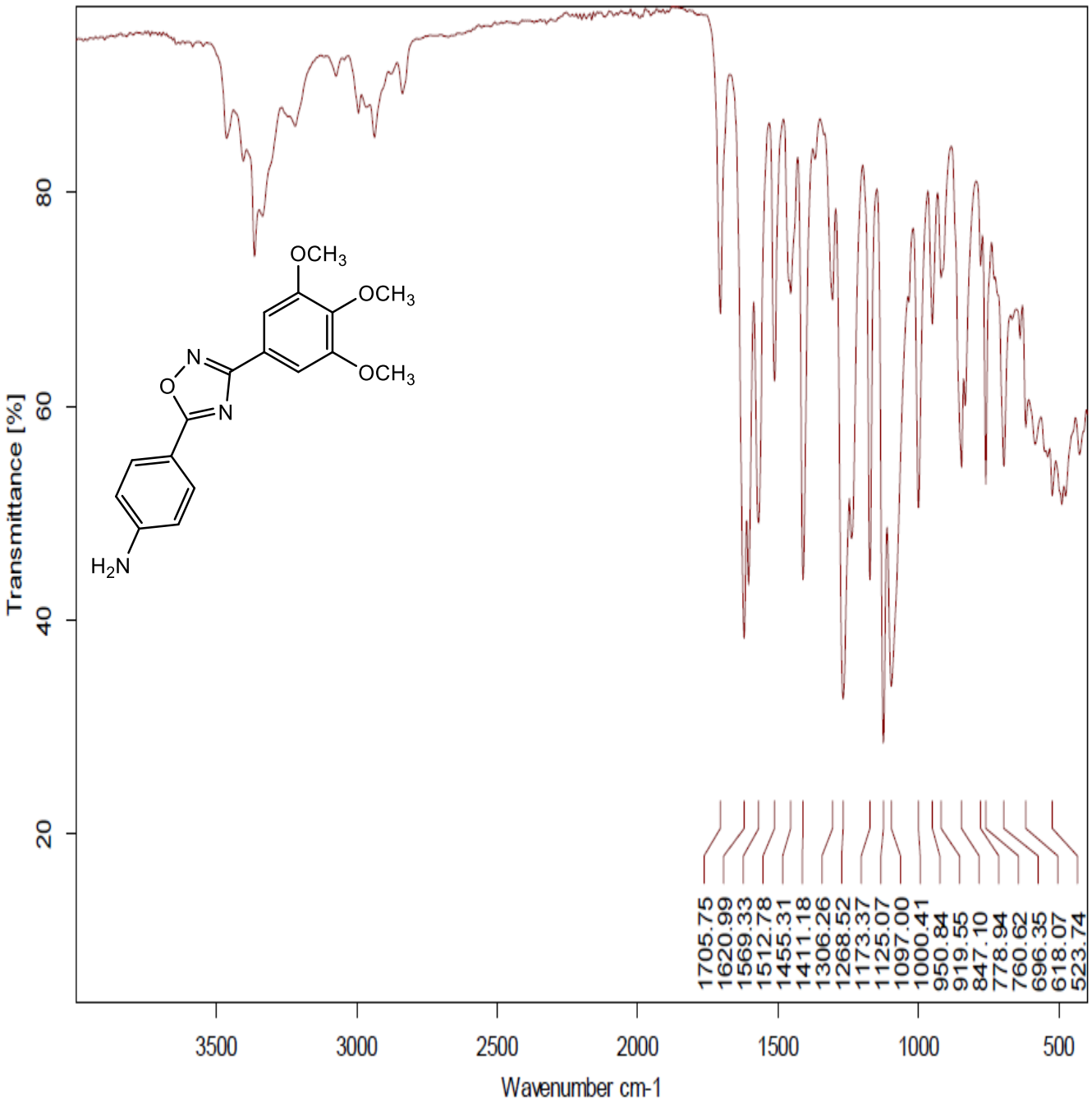


5d

P-aminobenzoyl oxadiazole-D20



5d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40
60
80
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
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OCH3
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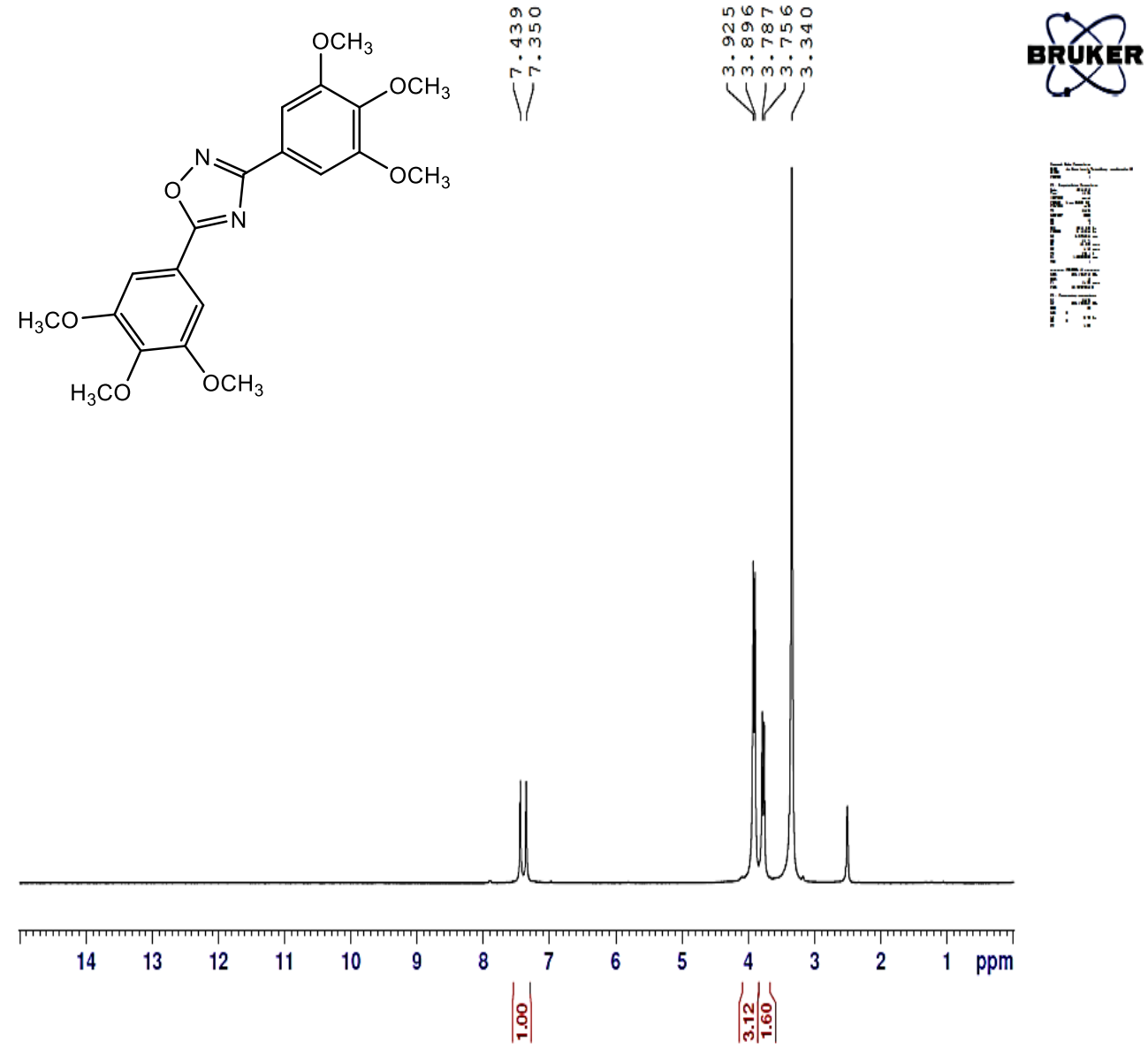
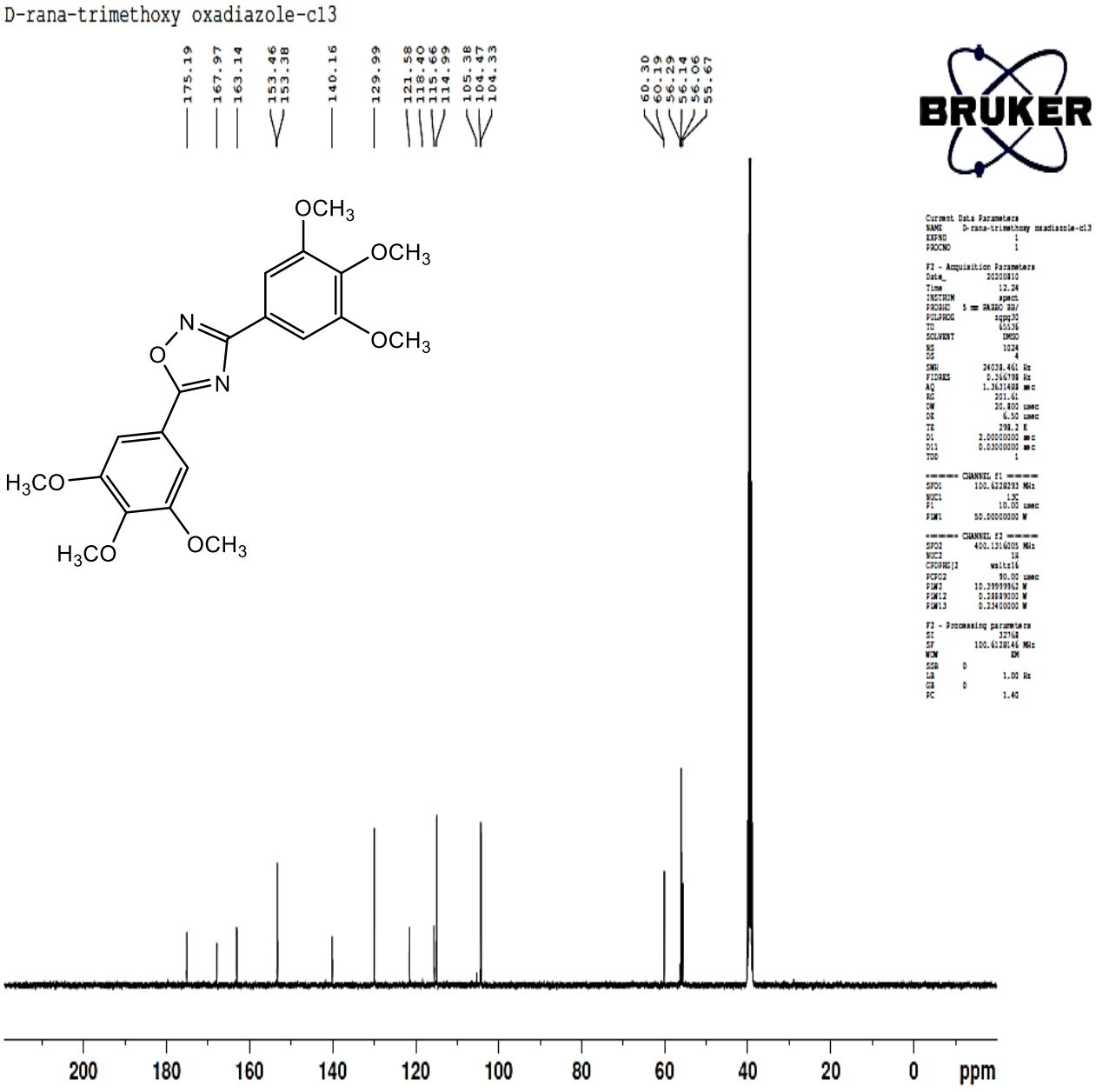
O
N
H2N
1705.75
1620.99
1569.33
1512.78
1455.31
1411.18
1306.26
1268.52
1173.37
1125.07
1097.00
1000.41
950.84
919.55
847.10
778.94
760.62
696.35
618.07
523.74

5e

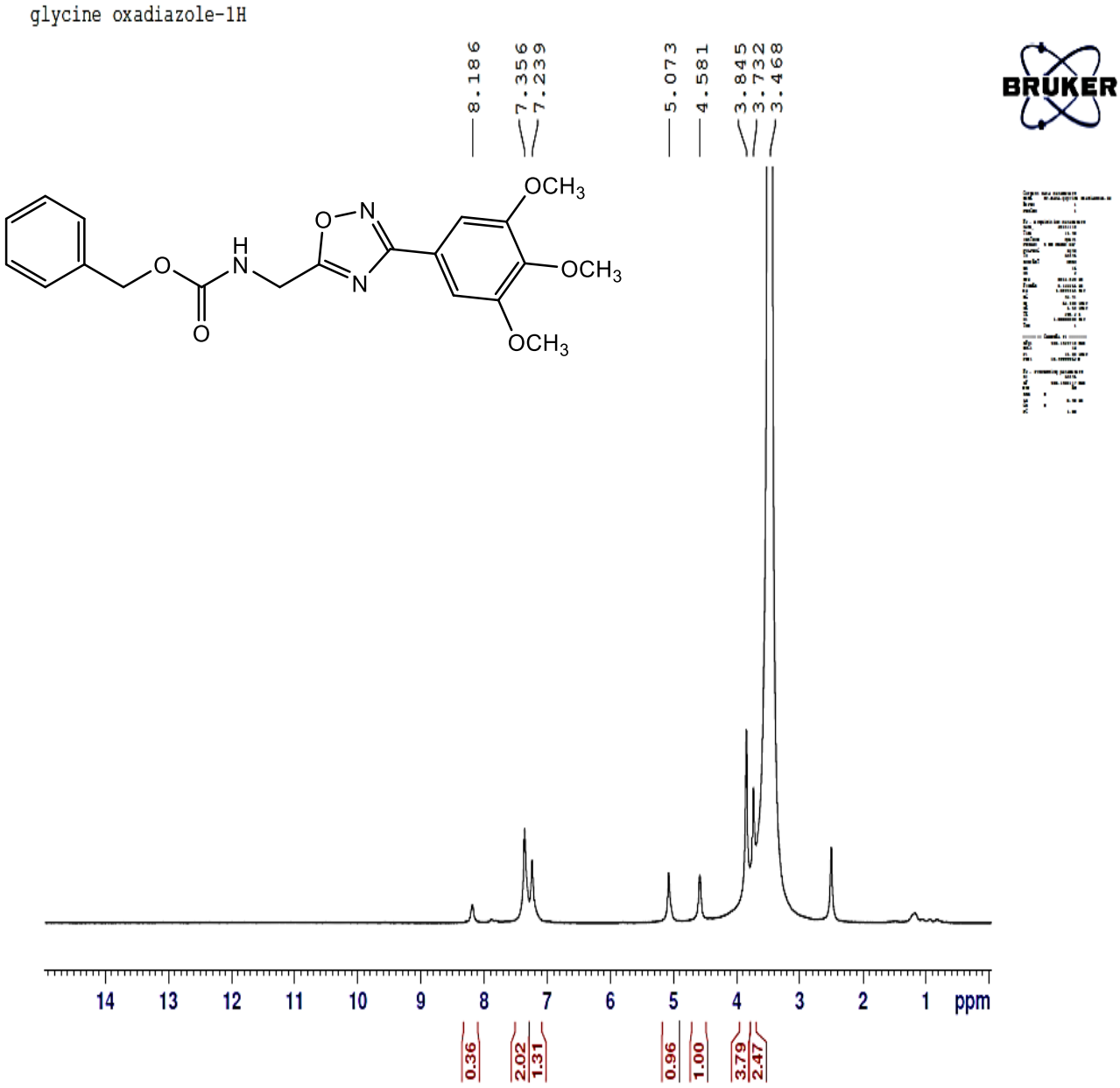
Trimethoxy oxadiazole-1H



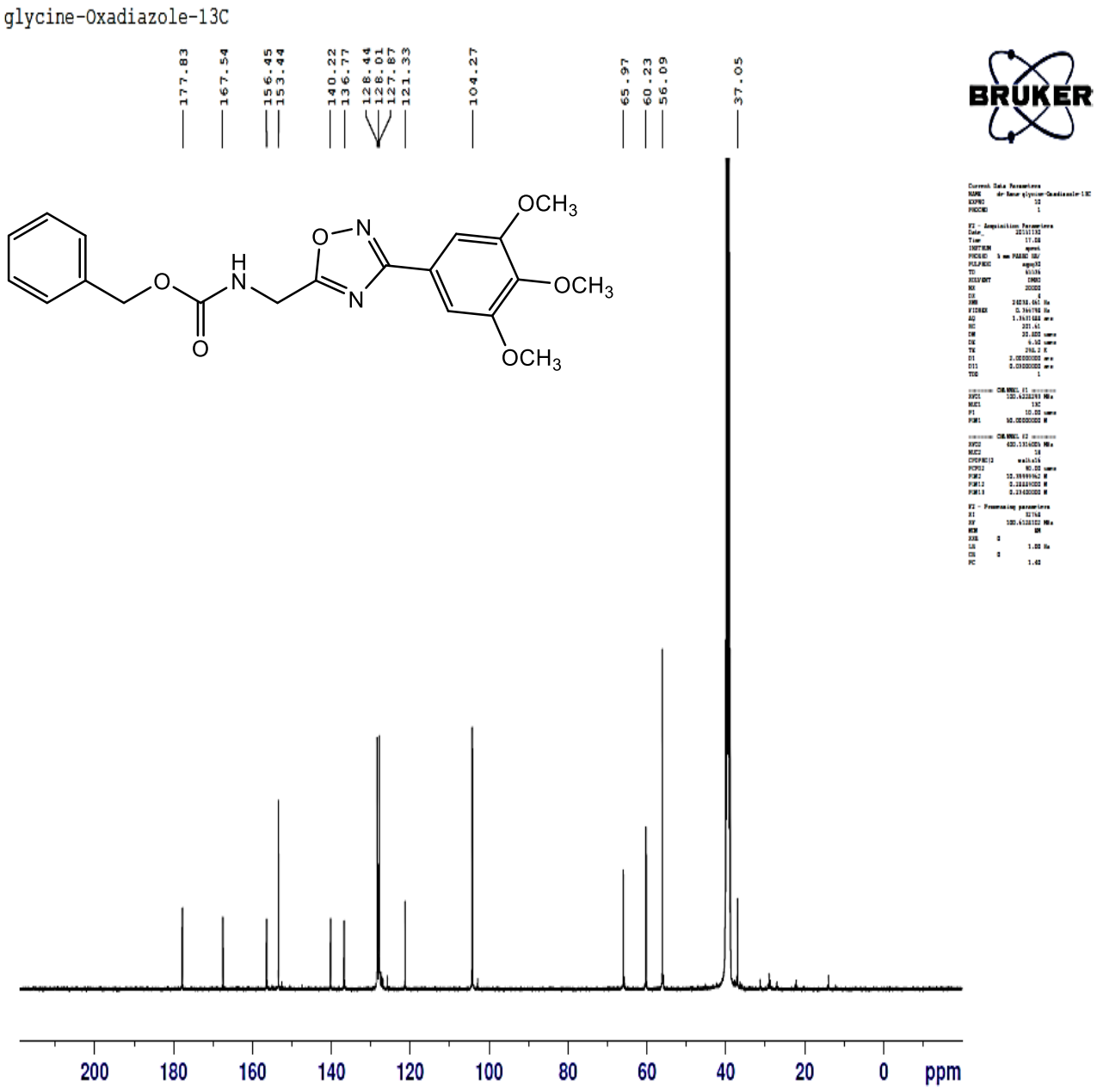
5e


D-rana-trimethoxy oxadiazole-c13
175.19
167.97
163.14
153.46
153.38
140.16
129.99
121.58
118.40
115.66
114.99
105.38
104.47
104.33
60.30
60.19
56.29
56.14
56.06
55.67
BRUKER
OCH3
OCH3
OCH3
N
O
N
H3CO
H3CO
OCH3
200
180
160
140
120
100
80
60
40
20
0
ppm

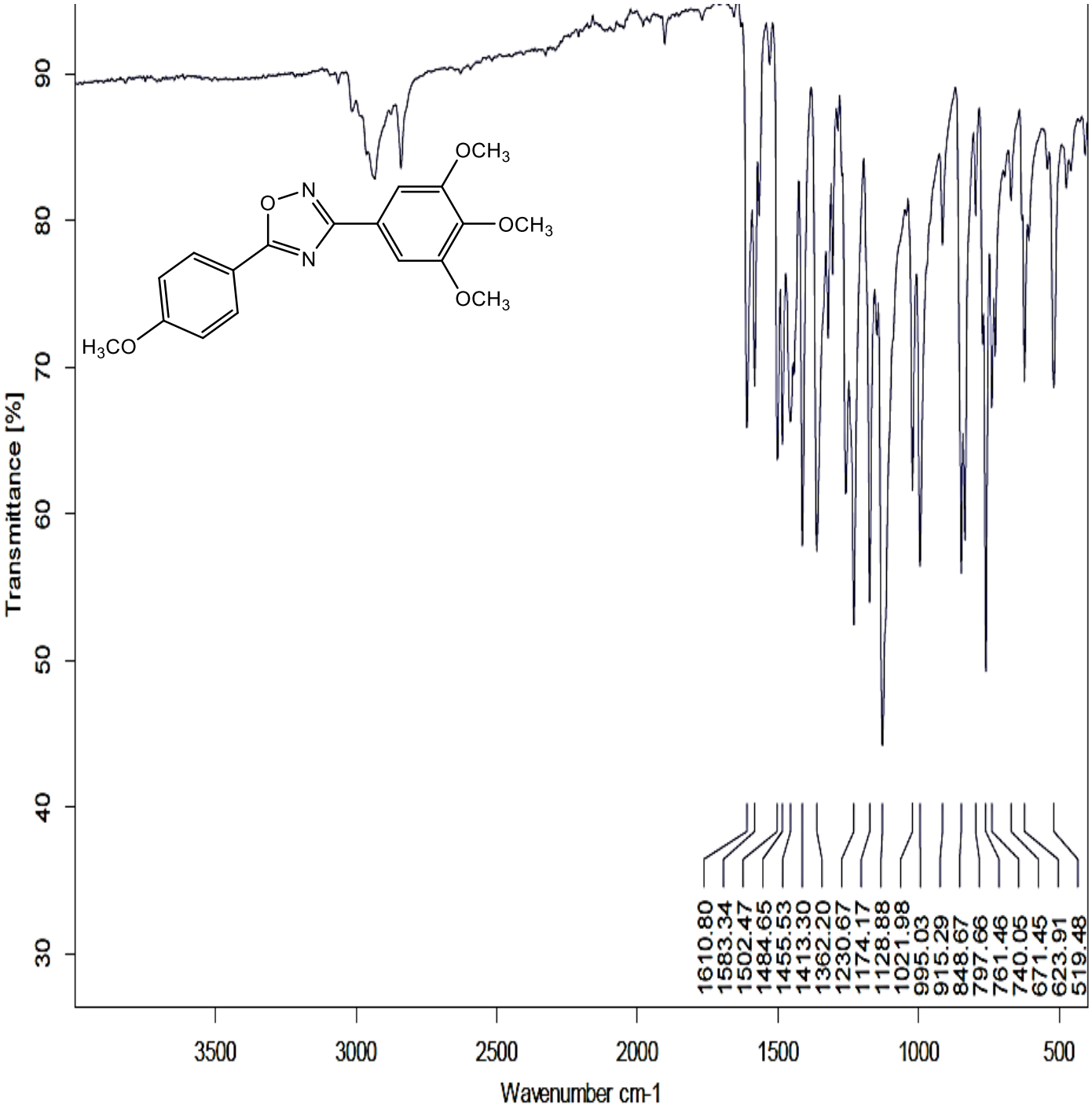
5f


glycine oxadiazole-1H
8.186
7.356
7.239
5.073
4.581
3.845
3.732
3.468
BRUKER
OCH3
OCH3
OCH3
O
N
H
O
N
O
O
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.36
2.02
1.31
0.96
1.00
3.79
2.47

5f


glycine-Oxadiazole-13C
177.83
167.54
156.45
153.44
140.22
136.77
128.44
128.01
127.87
121.33
104.27
65.97
60.23
56.09
37.05
BRUKER
OCH3
OCH3
OCH3
O
N
H
O
N
O
O
200
180
160
140
120
100
80
60
40
20
0
ppm

5g


Transmittance [%]
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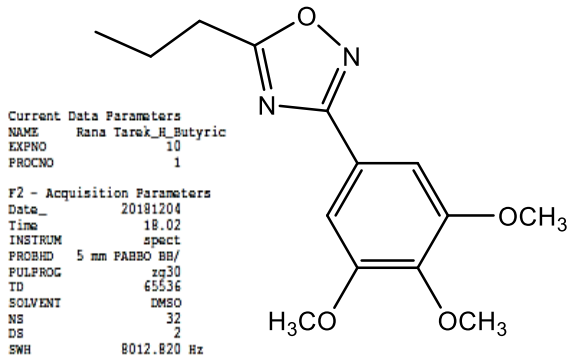
70
60
50
40
30
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
OCH3
OCH3
OCH3
N
O
N
H3CO
1610.80
1583.34
1502.47
1484.65
1455.53
1413.30
1362.20
1230.67
1174.17
1128.88
1021.98
995.03
915.29
848.67
797.66
761.46
740.05
671.45
623.91
519.48

5h

Rana Tarek_H_Butyric

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

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PROCNO                       1

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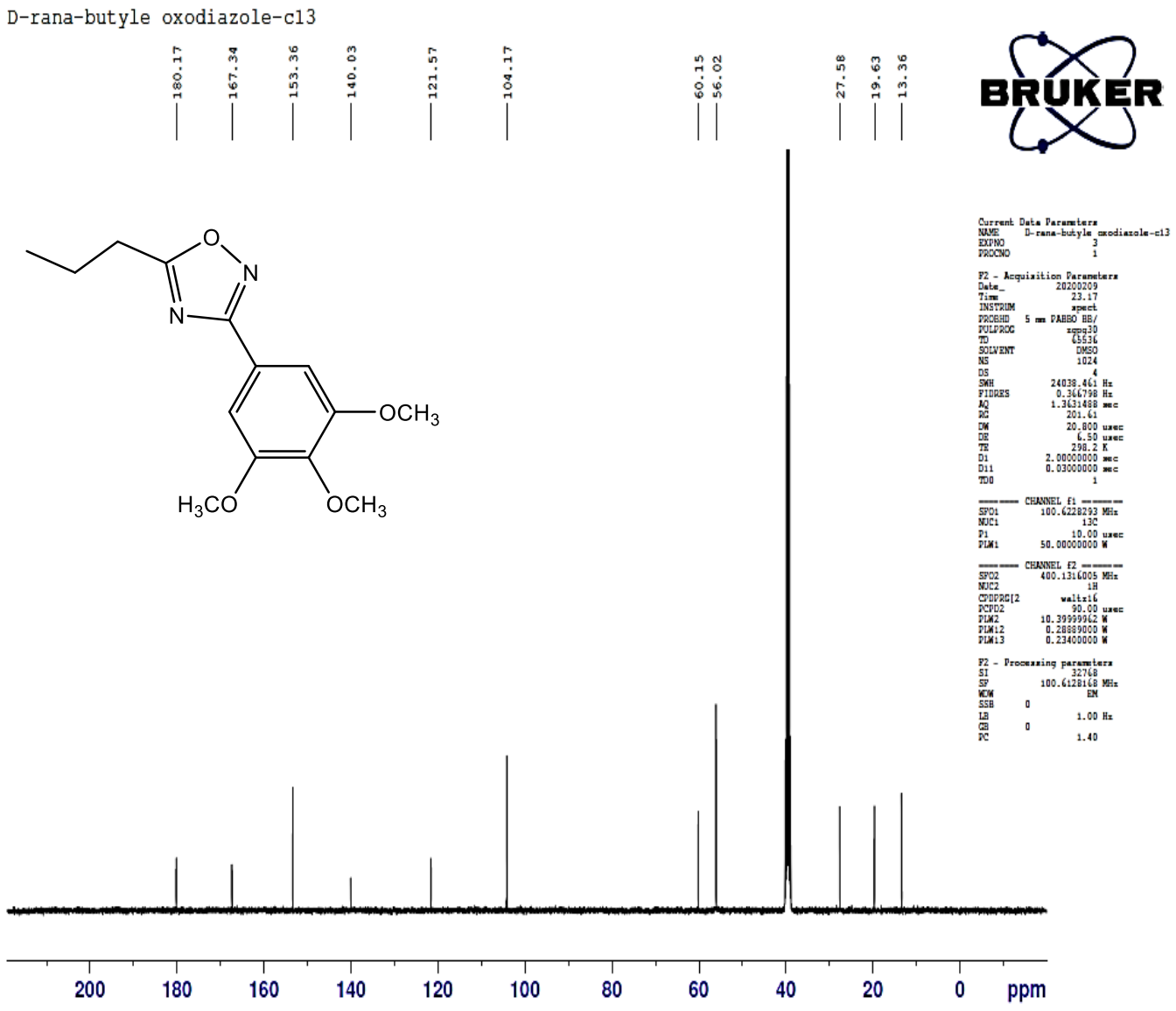
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       32
DS                        2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894465 sec
RG                    129.43
DW                    62.400 usec
DE                     6.50 usec
TE                    298.1 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1924713 MHz
NUC1                       1H
P1                      15.00 usec
PLW1             10.39999962 W

F2 - Processing parameters
SI                        65536
SF               400.1900000 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

5h



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PROCNO 1

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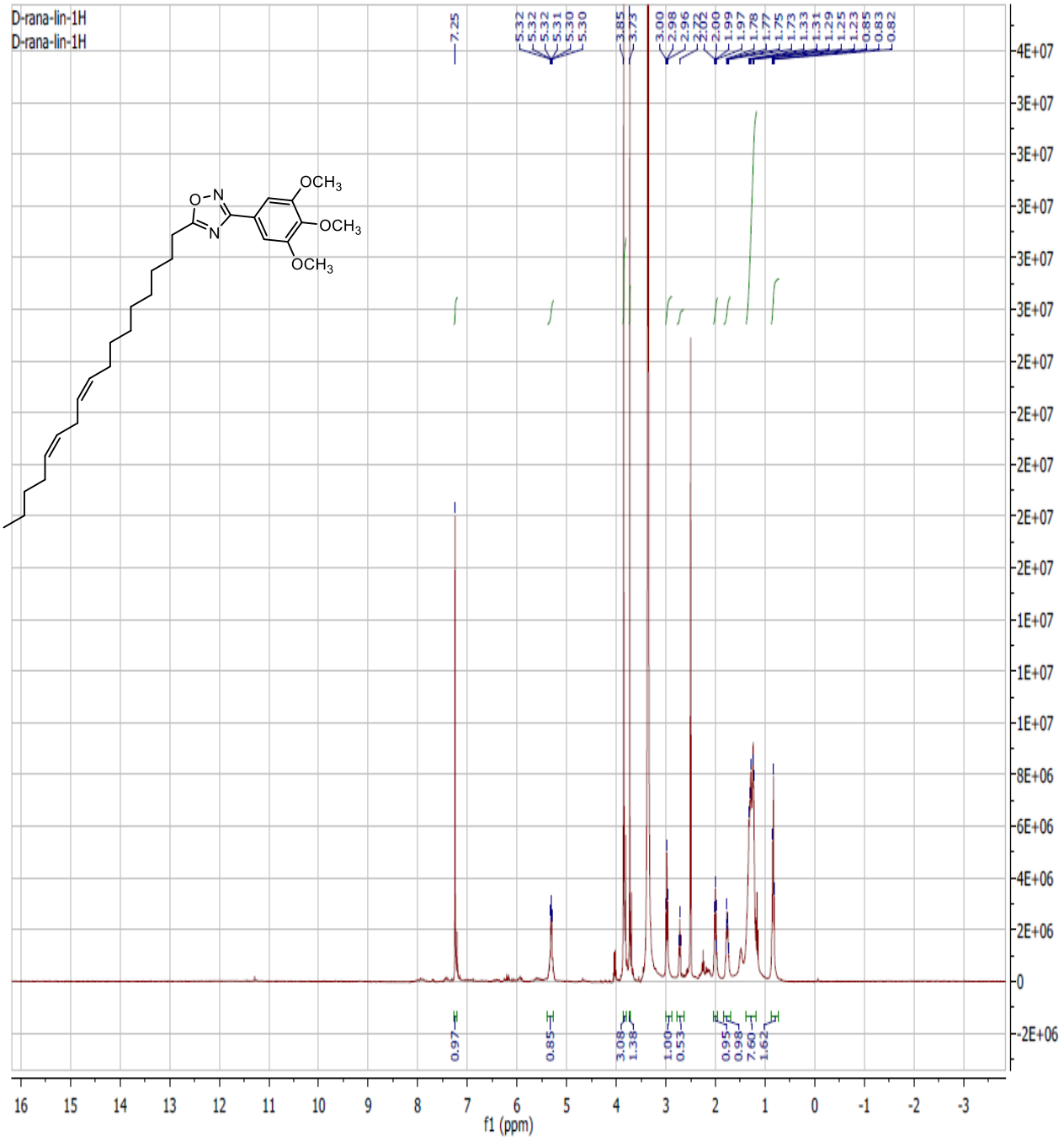
Time 23.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 201.61
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 50.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.39999962 W
PLW12 0.28889000 W
PLW13 0.23400000 W

F2 - Processing parameters
SI 32768
SF 100.6128168 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5i



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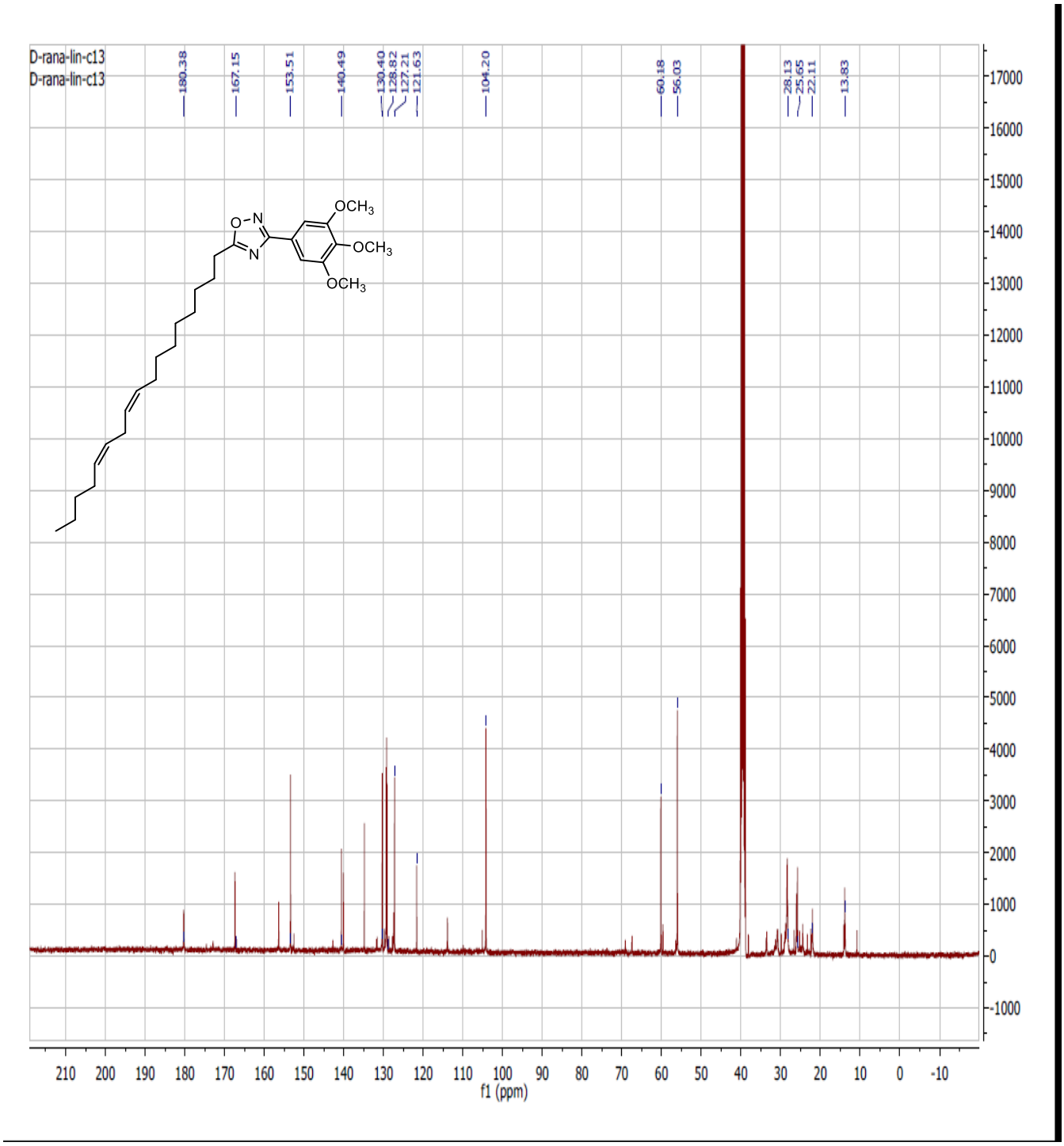
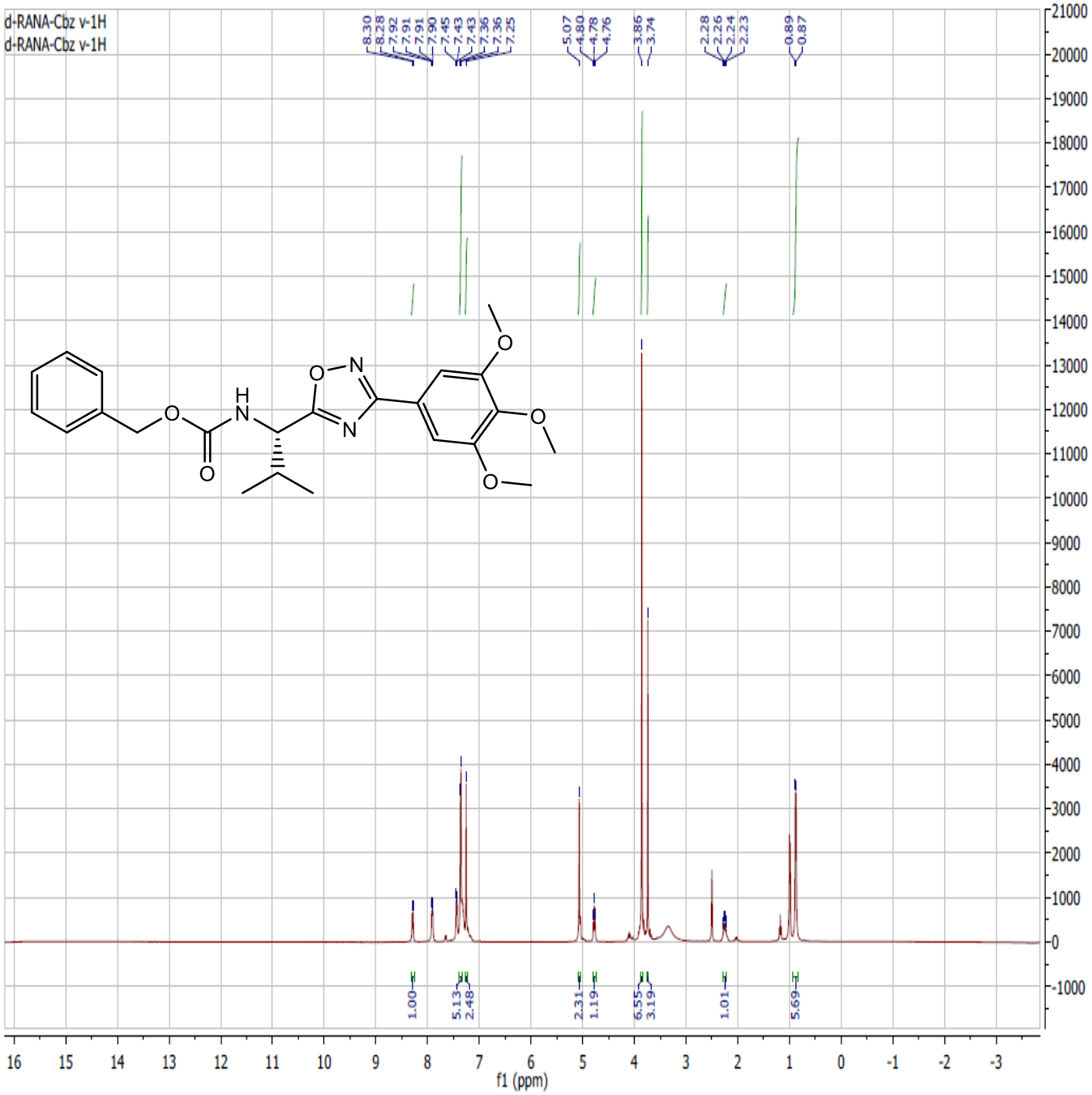
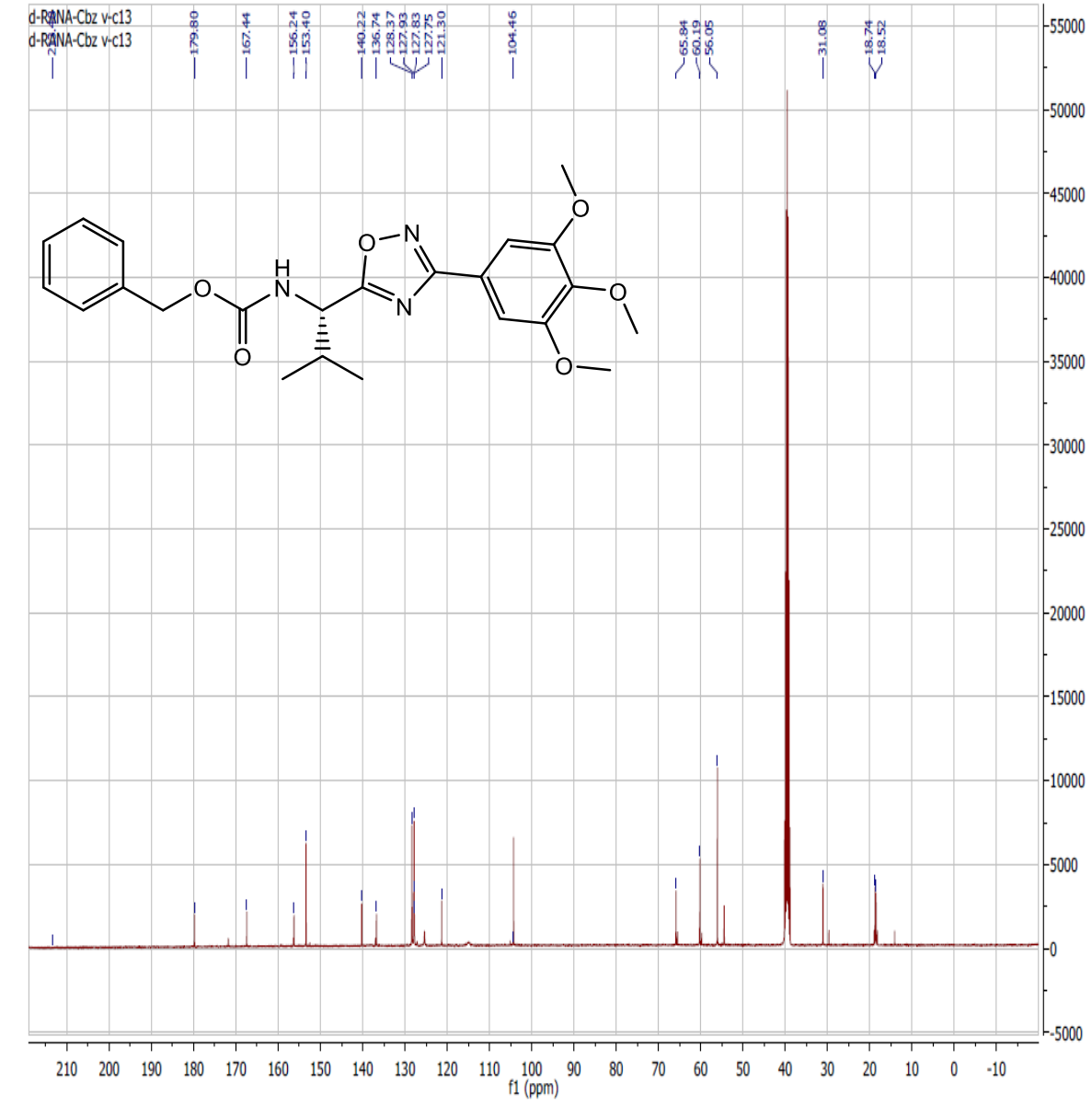

D-rana-lin-c13
D-rana-lin-c13
180.38
167.15
153.51
140.49
130.40
128.82
127.21
121.63
104.20
60.18
56.03
28.13
25.65
22.11
13.83
OCH3
OCH3
OCH3
O
N
N
f1 (ppm)

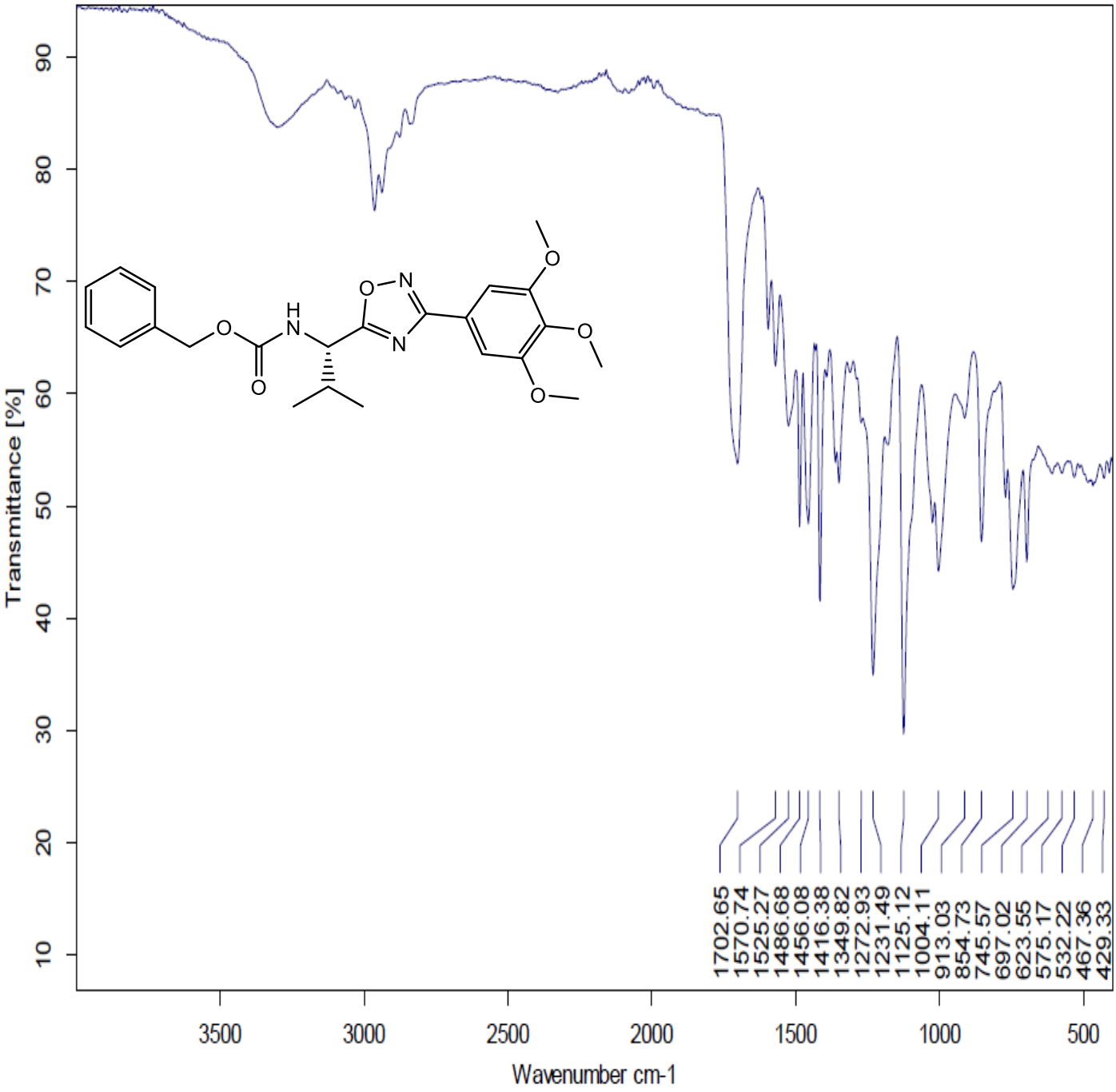
5j


d-RANA-Cbz v-1H
d-RANA-Cbz v-1H
8.30
8.28
7.92
7.91
7.91
7.90
7.45
7.43
7.43
7.36
7.36
7.25
5.07
4.80
4.78
4.76
3.86
3.74
2.28
2.26
2.24
2.23
0.89
0.87
1.00
5.13
2.48
2.31
1.19
6.55
3.19
1.01
5.69
f1 (ppm)

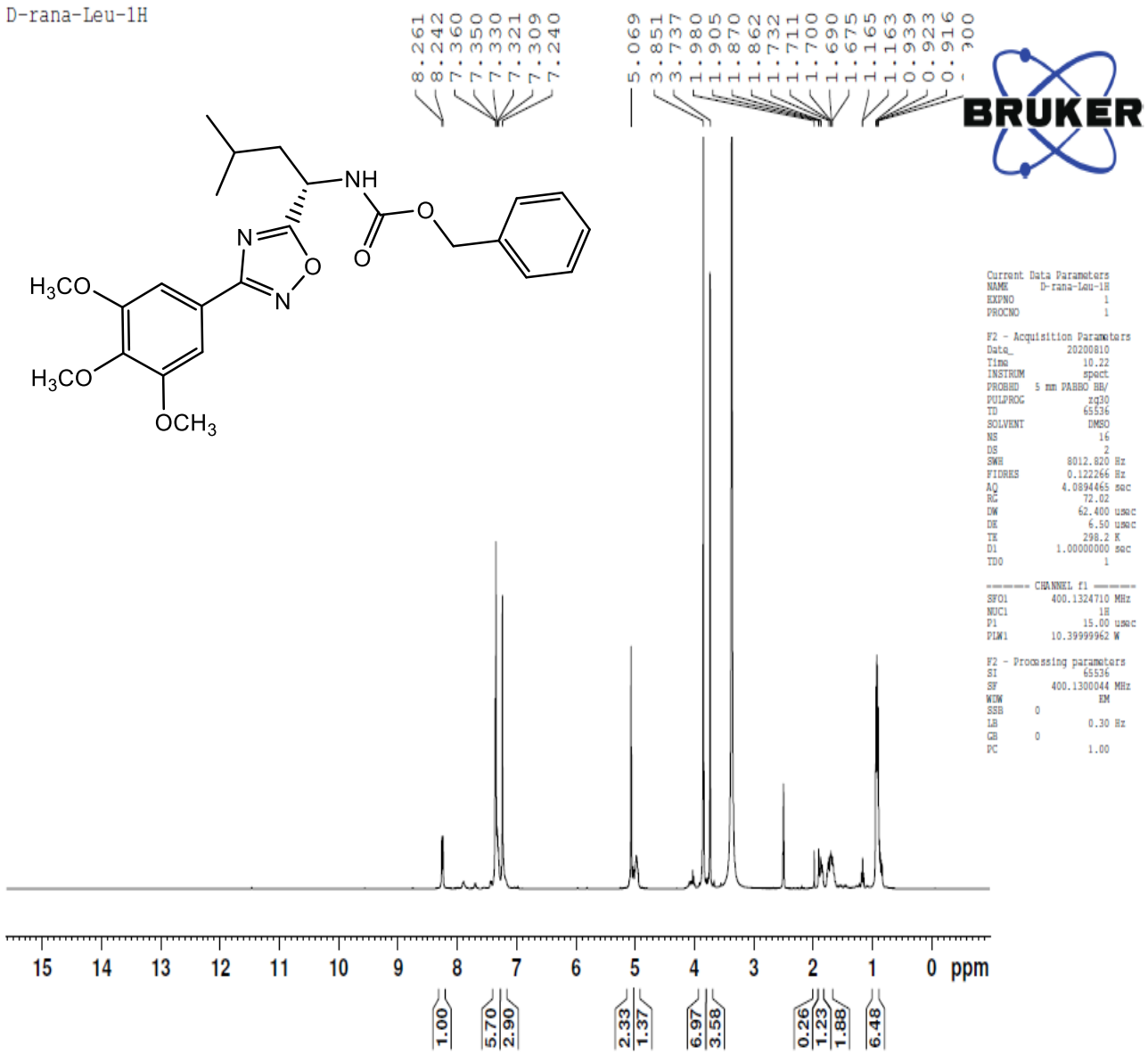
5j


d-RANA-Cbz v-c13
d-RANA-Cbz v-c13
179.80
167.44
156.24
153.40
140.22
136.74
128.37
127.93
127.83
127.75
121.30
104.46
65.84
60.19
56.05
31.08
18.74
18.52
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

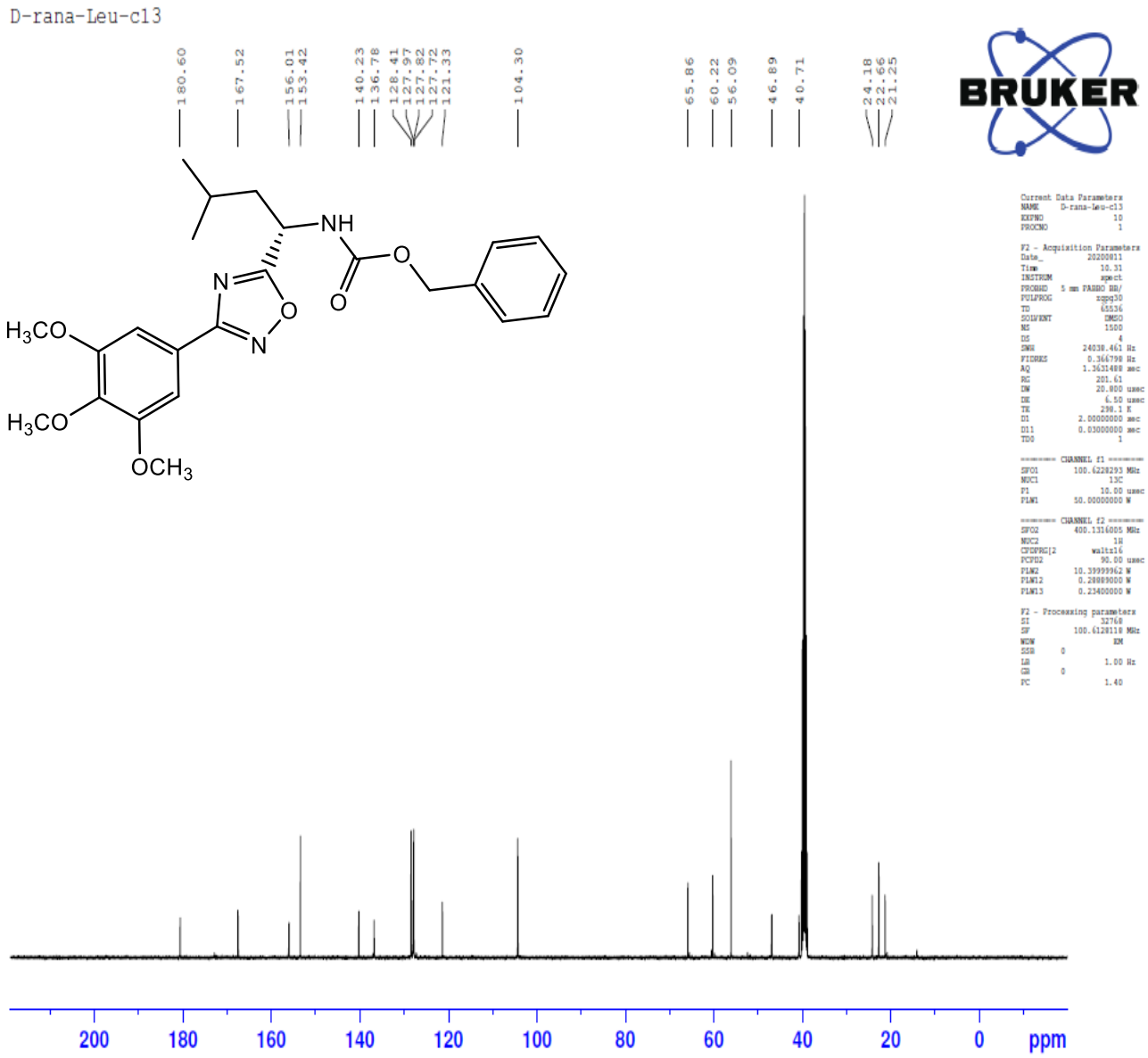
5j


Transmittance [%]
10
20
30
40
50
60
70
80
90
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
1702.65
1570.74
1525.27
1486.68
1456.08
1416.38
1349.82
1272.93
1231.49
1125.12
1004.11
913.03
854.73
745.57
697.02
623.55
575.17
532.22
467.36
429.33
O
N
H
O
O
N
O
O
O

5k


D-rana-Leu-1H
8.261
8.242
7.360
7.350
7.330
7.321
7.309
7.240
5.069
3.851
3.737
1.980
1.905
1.870
1.862
1.732
1.711
1.700
1.690
1.675
1.165
1.163
0.939
0.923
0.916
BRUKER
NH
O
O
N
O
N
H3CO
H3CO
OCH3
Current Data Parameters
NAME D-rana-Leu-1H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200810
Time 10.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 72.02
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1300044 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
5.70
2.90
2.33
1.37
6.97
3.58
0.26
1.23
1.88
6.48

5k


D-rana-Leu-c13
180.60
167.52
156.01
153.42
140.23
136.78
128.41
127.97
127.82
127.72
127.33
104.30
65.86
60.22
56.09
46.89
40.71
24.18
22.66
21.25
BRUKER
NH
O
O
N
O
N
H3CO
H3CO
OCH3
200
180
160
140
120
100
80
60
40
20
0
ppm

Elemental analysis report

جامعة الأزهر
Al-Azhar University
المركز الإقليمي للمطريات وتطبيقاتها
The Regional Center for Mycology and Biotechnology

Requester Data:

Name: Dr. Rana Tarek Diab
Authority: Faculty of Pharmacy, Zaga Zig University

Sample Data:

Nine samples had been submitted for elemental analysis.

Analysis Report:

Sample Code	C%	H%	N%	S%
5h	60.71	6.68	10.28	0
5k	63.39	6.48	9.47	0
5i	62.75	6.42	9.73	0
5f	60.39	5.52	1079	0
L	67.84	8.95	7.31	0
5i	71.32	8.95	6.17	0
5c	62.50	5.41	13.10	0
Mi	69.04	9.28	6.85	0
Ni	61.09	4.97	13.68	0

INVESTIGATOR

DIRECTOR

شارع المعهد الدائم - مدينة نصر - القاهرة
البريد الإلكتروني : rcmb@azhar.edu.eg
الموقع الإلكتروني:
صندوق بريد ١١٧٥١ مدينة نصر القاهرة
تليفون: ٢٢٦٢٠٣٧٣ (٠٢٠٢) فاكس: ٢٢٦٢٠٣٧٣ (٠٢٠٢)
http:// www.azhar.edu.eg.htm
http://www.azhar.edu.eg/pages/fungi_center.htm
Facebook: RCMB AZHAR

Requester Data:

Name: Dr. Rana Tarek Diab
Authority: Faculty of Pharmacy, Zaga Zig University

Sample Data:

Ten samples had been submitted for elemental analysis.

Analysis Report:

Sample Code	C%	H%	N%	S%
N-T-D	55.70	5.49	6.83	7.51
N-T-L	55.68	5.52	9.91	21.98
5b	62.16	5.37	13.12	0
OL	71.38	9.52	6.17	0
5d	62.19	5.40	13.08	0
Ph	65.16	5.38	9.13	0
5a	66.43	5.79	8.81	0
5g	63.38	5.43	8.40	0
S	70.71	9.85	6.13	0
5e	59.89	5.63	7.22	0

INVESTIGATOR

DIRECTOR

شارع المعهد الدائم - مدينة نصر - القاهرة
البريد الإلكتروني : rcmb@azhar.edu.eg
الموقع الإلكتروني:
صندوق بريد ١١٧٥١ مدينة نصر القاهرة
تليفون: ٢٢٦٢٠٣٧٣ (٠٢٠٢) فاكس: ٢٢٦٢٠٣٧٣ (٠٢٠٢)
http:// www.azhar.edu.eg.htm
http://www.azhar.edu.eg/pages/fungi_center.htm
Facebook: RCMB AZHAR

One dose assay graph for compounds 5a-k

5a

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-824575 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 17, 2020
Experiment ID: 2008OS33		Report Date: Sep 05, 202

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	94.78
HL-60(TB)	90.98
K-562	70.02
MOLT-4	90.11
RPMI-8226	80.69
SR	76.16
Non-Small Cell Lung Cancer	
A549/ATCC	89.54
EKVX	76.50
HOP-62	91.12
HOP-92	38.35
NCI-H226	85.05
NCI-H23	87.21
NCI-H322M	87.27
NCI-H460	93.33
NCI-H522	77.51
Colon Cancer	
COLO 205	102.32
HCC-2998	100.66
HCT-116	87.92
HCT-15	81.95
HT29	89.30
KM12	95.87
SW-620	92.62
CNS Cancer	
SF-268	86.39
SF-295	89.04
SF-539	92.48
SNB-19	91.76
SNB-75	83.95
U251	94.82
Melanoma	
LOX IMVI	83.43
MALME-3M	106.65
M14	94.12
MDA-MB-435	93.82
SK-MEL-2	93.01
SK-MEL-28	100.27
SK-MEL-5	88.26
UACC-257	103.80
UACC-62	85.26
Ovarian Cancer	
IGROV1	96.15
OVCAR-3	90.01
OVCAR-4	77.31
OVCAR-5	97.40
OVCAR-8	91.80
NCI/ADR-RES	92.15
SK-OV-3	98.96
Renal Cancer	
786-0	85.48
A498	22.18
ACHN	85.80
CAKI-1	57.56
RXF 393	88.47
SN12C	81.59
TK-10	111.90
UO-31	54.96
Prostate Cancer	
PC-3	93.25
DU-145	97.15
Breast Cancer	
MCF7	77.24
MDA-MB-231/ATCC	71.58
HS 578T	74.27
BT-549	95.88
T-47D	96.44
Mean	84.50
Delta	82.32
Range	89.72

Mean Growth Percent - Growth Percent

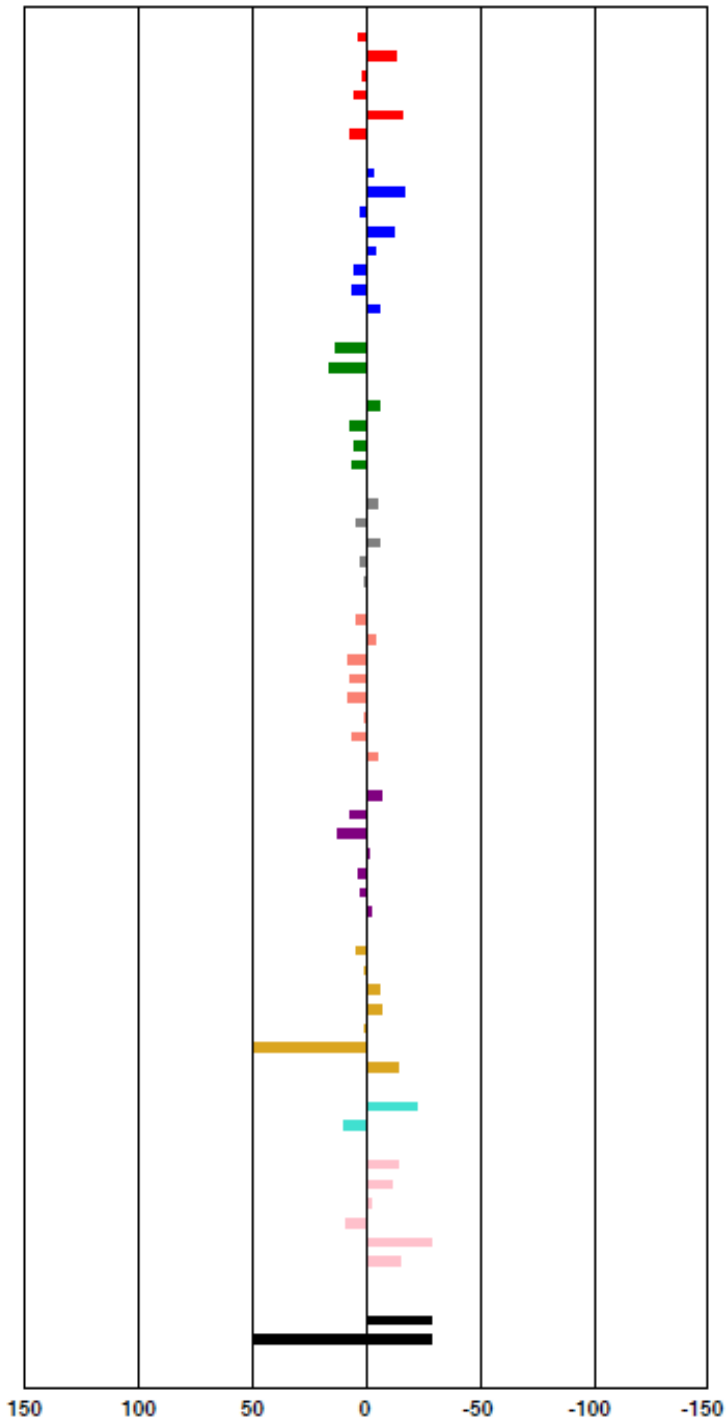
150 100 50 0 -50 -100 -150

5b

Developmental Therapeutics Program	NSC: D-826468 / 1	Conc: 1.00E-5 Molar	Test Date: Oct 26, 2020
One Dose Mean Graph	Experiment ID: 2010OS50		Report Date: Mar 07, 202

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	95.16
HL-60(TB)	79.00
K-562	93.26
MOLT-4	97.23
RPMI-8226	76.01
SR	98.92
Non-Small Cell Lung Cancer	
A549/ATCC	88.73
EKVX	75.62
HOP-62	94.68
NCI-H226	79.01
NCI-H23	88.22
NCI-H322M	96.82
NCI-H460	97.83
NCI-H522	86.22
Colon Cancer	
COLO 205	105.85
HCC-2998	107.99
HCT-116	91.89
HCT-15	86.01
HT29	99.36
KM12	96.83
SW-620	97.79
CNS Cancer	
SF-268	87.05
SF-295	96.72
SF-539	86.43
SNB-19	94.37
U251	93.12
Melanoma	
MALME-3M	96.79
M14	88.09
MDA-MB-435	100.13
SK-MEL-2	98.88
SK-MEL-28	99.65
SK-MEL-5	92.85
UACC-257	97.88
UACC-62	87.57
Ovarian Cancer	
IGROV1	85.40
OVCAR-3	99.33
OVCAR-4	104.74
OVCAR-5	99.01
OVCAR-8	95.46
NCI/ADR-RES	94.13
SK-OV-3	89.83
Renal Cancer	
786-0	99.08
ACHN	93.09
CAKI-1	89.40
RXF 393	85.37
SN12C	93.13
TK-10	141.79
UO-31	78.45
Prostate Cancer	
PC-3	89.83
DU-145	101.81
Breast Cancer	
MCF7	78.08
MDA-MB-231/ATCC	89.89
HS 578T	89.84
BT-549	100.91
T-47D	83.11
MDA-MB-468	77.37
Mean	91.93
Delta	28.82
Range	78.08

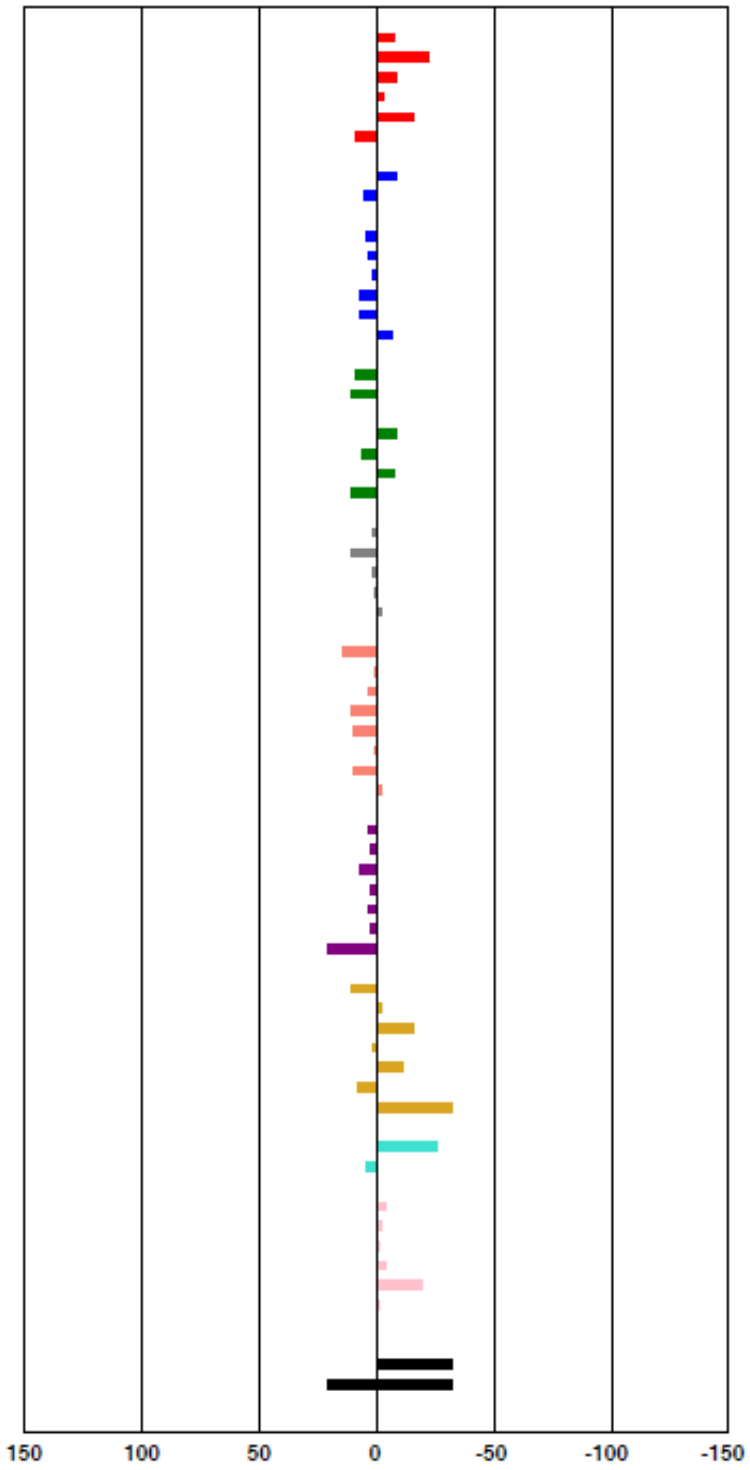
Mean Growth Percent - Growth Percent



5c

Developmental Therapeutics Program	NSC: D-820400 / 1	Conc: 1.00E-5 Molar	Test Date: Oct 26, 2020
One Dose Mean Graph	Experiment ID: 2010OS59		Report Date: Mar 07, 2021

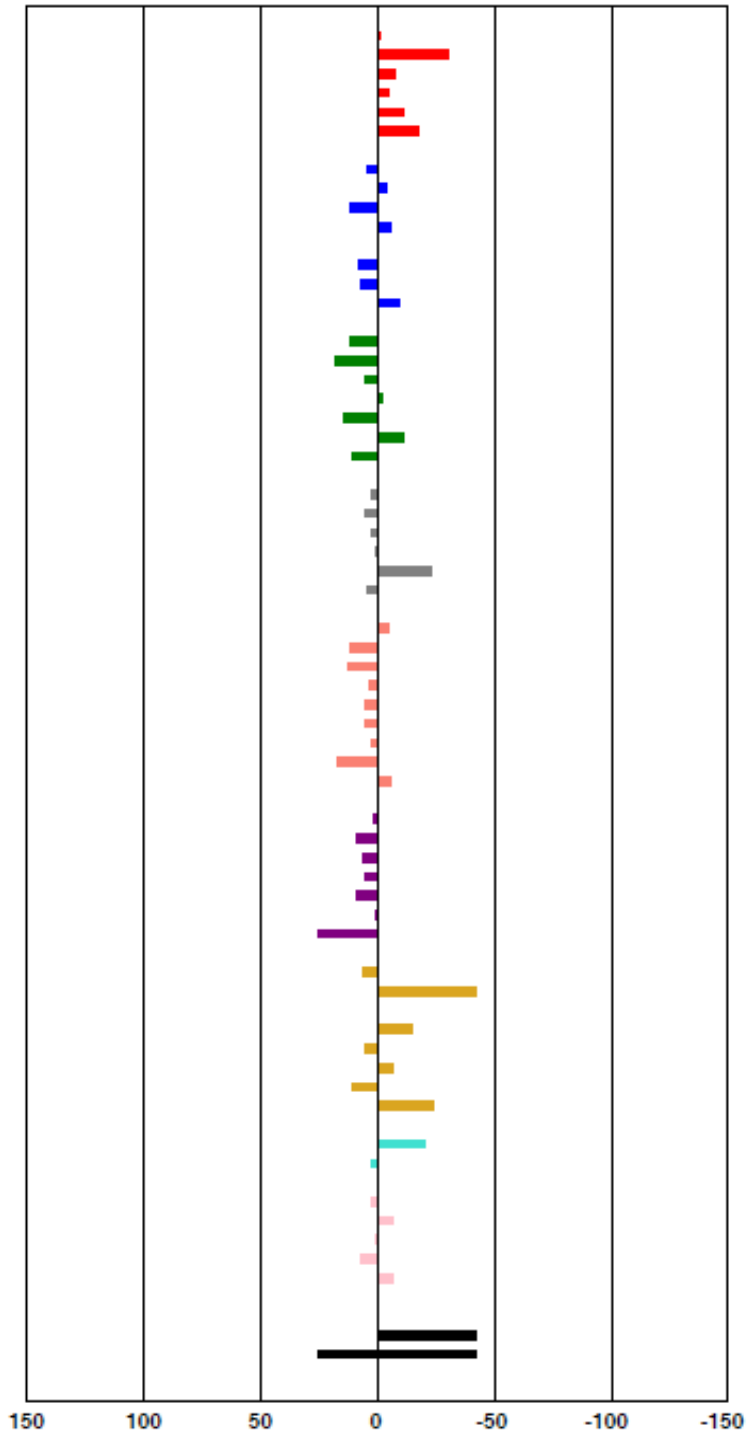
Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	84.07
HL-60(TB)	70.21
K-562	83.30
MOLT-4	88.76
RPMI-8226	75.89
SR	100.56
Non-Small Cell Lung Cancer	
A549/ATCC	83.74
EKVX	97.10
HOP-62	91.42
HOP-92	96.00
NCI-H226	95.75
NCI-H23	93.55
NCI-H322M	98.75
NCI-H460	99.27
NCI-H522	84.96
Colon Cancer	
COLO 205	101.34
HCC-2998	102.50
HCT-116	91.80
HCT-15	83.58
HT29	98.24
KM12	84.15
SW-620	102.59
CNS Cancer	
SF-268	93.26
SF-295	102.46
SF-539	94.05
SNB-19	92.85
U251	90.25
Melanoma	
MALME-3M	106.27
M14	93.14
MDA-MB-435	95.17
SK-MEL-2	102.54
SK-MEL-28	101.89
SK-MEL-5	92.81
UACC-257	102.09
UACC-62	90.27
Ovarian Cancer	
IGROV1	95.88
OVCAR-3	94.34
OVCAR-4	99.15
OVCAR-5	94.62
OVCAR-8	95.01
NCI/ADR-RES	94.84
SK-OV-3	112.39
Renal Cancer	
786-0	102.96
ACHN	99.08
CAKI-1	75.94
RXF 393	93.78
SN12C	81.30
TK-10	99.60
UO-31	59.99
Prostate Cancer	
PC-3	96.49
DU-145	99.64
Breast Cancer	
MCF7	88.56
MDA-MB-231/ATCC	99.24
HS 578T	99.86
BT-549	88.23
T-47D	72.69
MDA-MB-468	99.75
Mean	91.91
Delta	31.92
Range	52.40



5d

Developmental Therapeutics Program	NSC: D-824578 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 17, 2020
One Dose Mean Graph	Experiment ID: 2008OS33		Report Date: Sep 05, 2020

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	89.51
HL-60(TB)	90.02
K-562	83.03
MOLT-4	85.62
RPMI-8226	79.39
SR	73.07
Non-Small Cell Lung Cancer	
A549/ATCC	95.38
EKVX	87.24
HOP-62	101.99
NCI-H226	84.78
NCI-H23	99.84
NCI-H322M	99.13
NCI-H460	97.82
NCI-H522	81.34
Colon Cancer	
COLO 205	102.14
HCC-2998	108.50
HCT-116	99.14
HCT-15	88.31
HT29	104.81
KM12	79.99
SW-620	101.07
CNS Cancer	
SF-268	93.01
SF-295	95.63
SF-539	92.99
SNB-19	91.78
SNB-75	97.89
U251	95.26
Melanoma	
LOX IMVI	89.32
MALME-3M	102.17
M14	103.08
MDA-MB-435	94.51
SK-MEL-2	95.87
SK-MEL-28	99.19
SK-MEL-5	93.01
UACC-257	107.39
UACC-62	84.99
Ovarian Cancer	
IGROV1	92.42
OVCAR-3	99.28
OVCAR-4	99.81
OVCAR-5	95.81
OVCAR-8	99.77
NCI/ADR-RES	91.47
SK-OV-3	115.07
Renal Cancer	
786-0	99.58
A498	48.55
ACHN	99.42
CAKI-1	79.28
RXF 393	95.74
SN12C	83.97
TK-10	101.17
UO-31	99.81
Prostate Cancer	
PC-3	79.54
DU-145	93.34
Breast Cancer	
MCF7	93.37
MDA-MB-231/ATCC	84.29
HS 578T	91.70
BT-549	98.21
T-47D	84.32
Mean	90.63
Delta	42.08
Range	67.12



5e

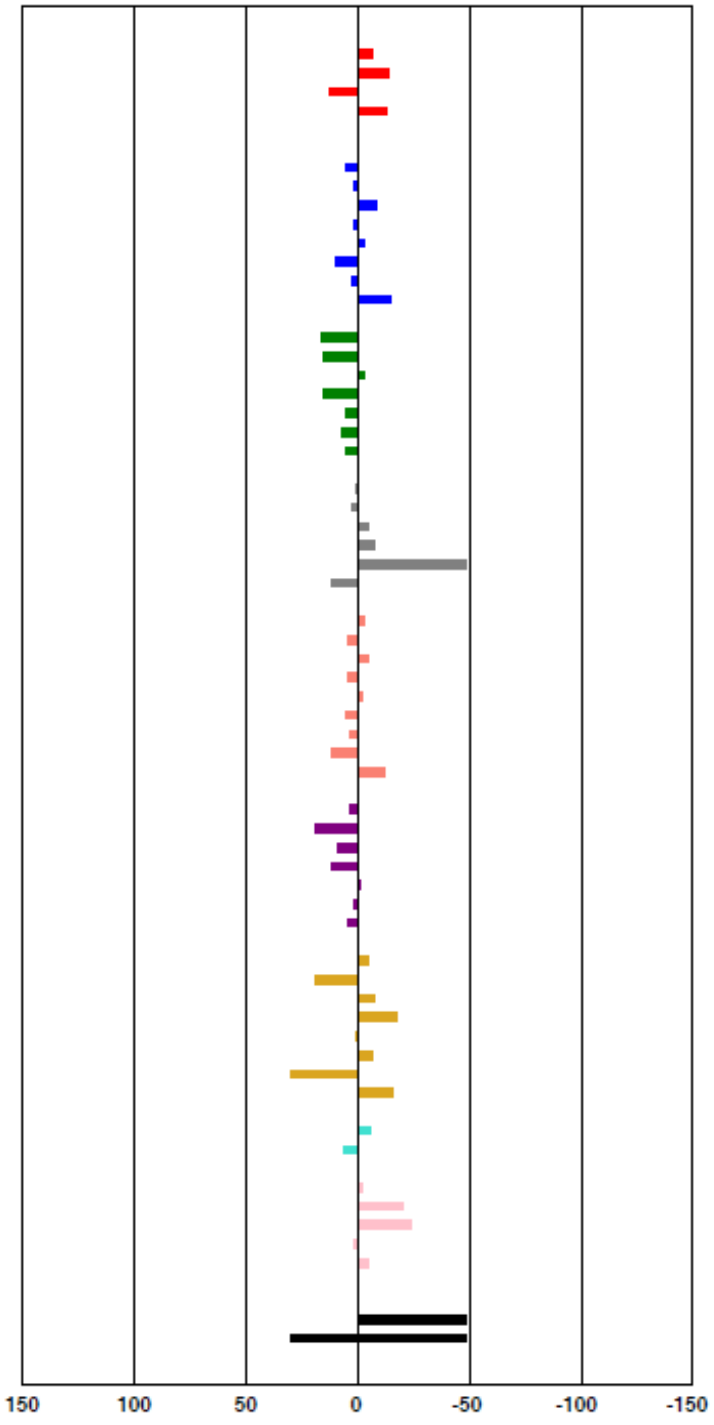
Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-824577 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 17, 2020
Experiment ID: 2008OS33		Report Date: Sep 05, 2020

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	80.83
HL-60(TB)	83.08
K-562	70.24
MOLT-4	102.58
RPMI-8226	77.21
SR	80.74
Non-Small Cell Lung Cancer	
A549/ATCC	95.62
EKVX	91.32
HOP-62	81.17
NCI-H226	91.12
NCI-H23	86.90
NCI-H322M	90.63
NCI-H460	92.28
NCI-H522	74.90
Colon Cancer	
COLO 205	100.00
HCC-2998	104.85
HCT-116	87.16
HCT-15	105.36
HT29	95.31
KM12	97.43
SW-620	94.85
CNS Cancer	
SF-268	90.85
SF-295	92.78
SF-539	85.35
SNB-19	82.60
SNB-75	41.01
U251	101.76
Melanoma	
LOX IMVI	87.16
MALME-3M	94.70
M14	85.59
MDA-MB-435	93.95
SK-MEL-2	88.26
SK-MEL-28	94.83
SK-MEL-5	93.31
UACC-257	101.91
UACC-62	77.76
Ovarian Cancer	
IGROV1	93.40
OVCAR-3	100.10
OVCAR-4	90.04
OVCAR-5	101.30
OVCAR-8	88.49
NCI/ADR-RES	91.64
SK-OV-3	94.42
Renal Cancer	
786-0	84.77
A498	100.01
ACHN	82.56
CAKI-1	72.41
RXF 393	90.36
SN12C	83.64
TK-10	110.73
UO-31	74.59
Prostate Cancer	
PC-3	84.25
DU-145	90.10
Breast Cancer	
MCF7	88.32
MDA-MB-231/ATCC	90.59
HS 578T	90.38
BT-549	91.22
T-47D	85.35
Mean	80.84
Delta	48.23
Range	78.12

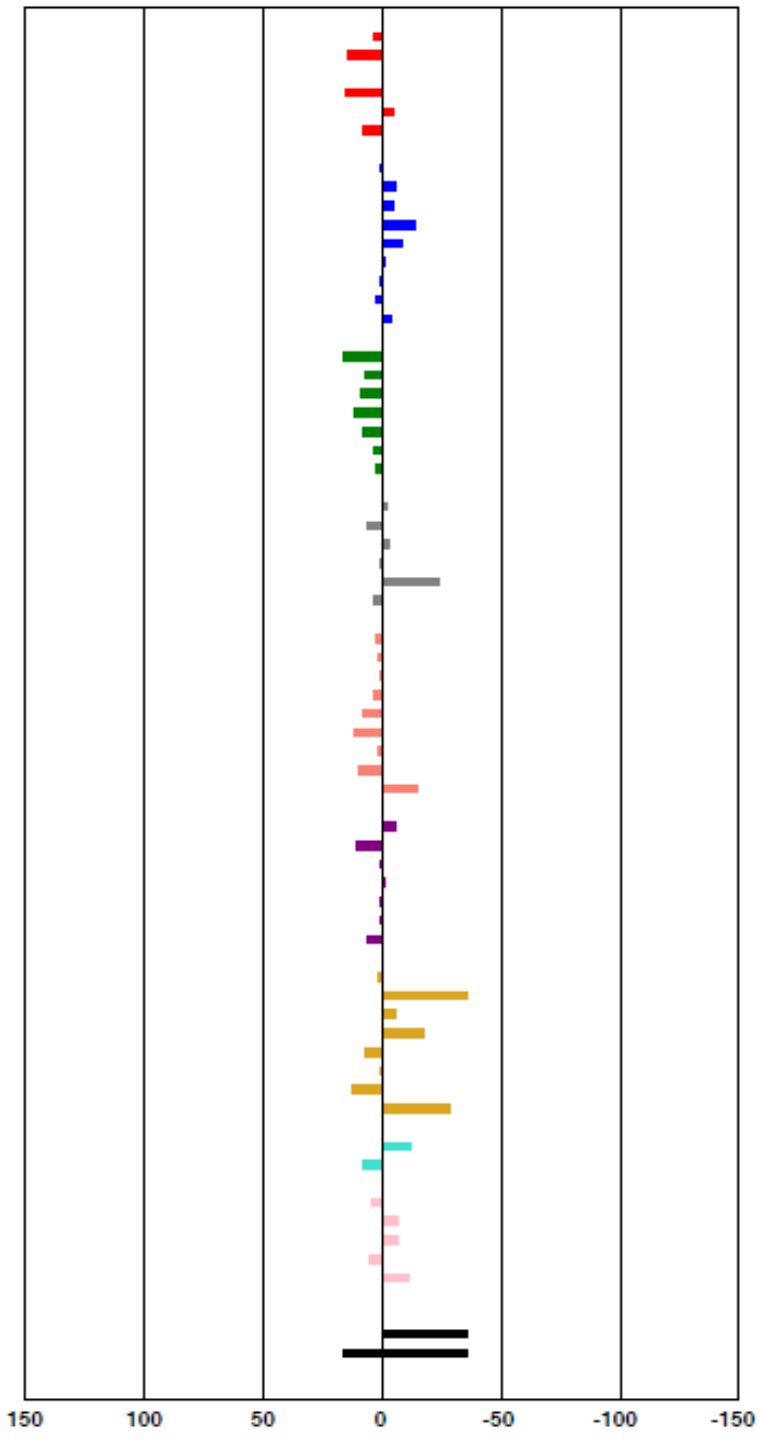
Mean Growth Percent - Growth Percent



5f

Developmental Therapeutics Program	NSC: D-824574 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 17, 2020
One Dose Mean Graph	Experiment ID: 2008OS33		Report Date: Sep 05, 2020

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	101.28
HL-60(TB)	112.42
K-562	98.12
MOLT-4	113.07
RPMI-8226	92.78
SR	100.25
Non-Small Cell Lung Cancer	
A549/ATCC	98.95
EKVX	92.00
HOP-62	92.83
HOP-92	84.14
NCI-H226	89.04
NCI-H23	96.37
NCI-H322M	98.99
NCI-H460	100.35
NCI-H522	94.23
Colon Cancer	
COLO 205	114.27
HCC-2998	104.85
HCT-116	100.98
HCT-15	100.77
HT29	100.25
KM12	101.54
SW-620	100.42
CNS Cancer	
SF-268	96.32
SF-295	104.42
SF-539	94.75
SNB-19	98.51
SNB-75	73.63
U251	101.10
Melanoma	
LOX IMVI	100.26
MALME-3M	99.51
M14	98.62
MDA-MB-435	101.20
SK-MEL-2	105.90
SK-MEL-28	100.63
SK-MEL-5	99.50
UACC-257	107.55
UACC-62	83.55
Ovarian Cancer	
IGROV1	92.62
OVCAR-3	108.72
OVCAR-4	98.53
OVCAR-5	99.81
OVCAR-8	98.99
NCI/ADR-RES	98.60
SK-OV-3	103.81
Renal Cancer	
786-0	99.21
A498	82.58
ACHN	92.37
CAKI-1	80.72
RXF 393	104.72
SN12C	98.52
TK-10	110.04
UO-31	89.13
Prostate Cancer	
PC-3	85.97
DU-145	105.04
Breast Cancer	
MCF7	102.09
MDA-MB-231/ATCC	91.01
HS 578T	91.45
BT-549	103.62
T-47D	86.92
Mean	97.83
Delta	35.25
Range	51.69



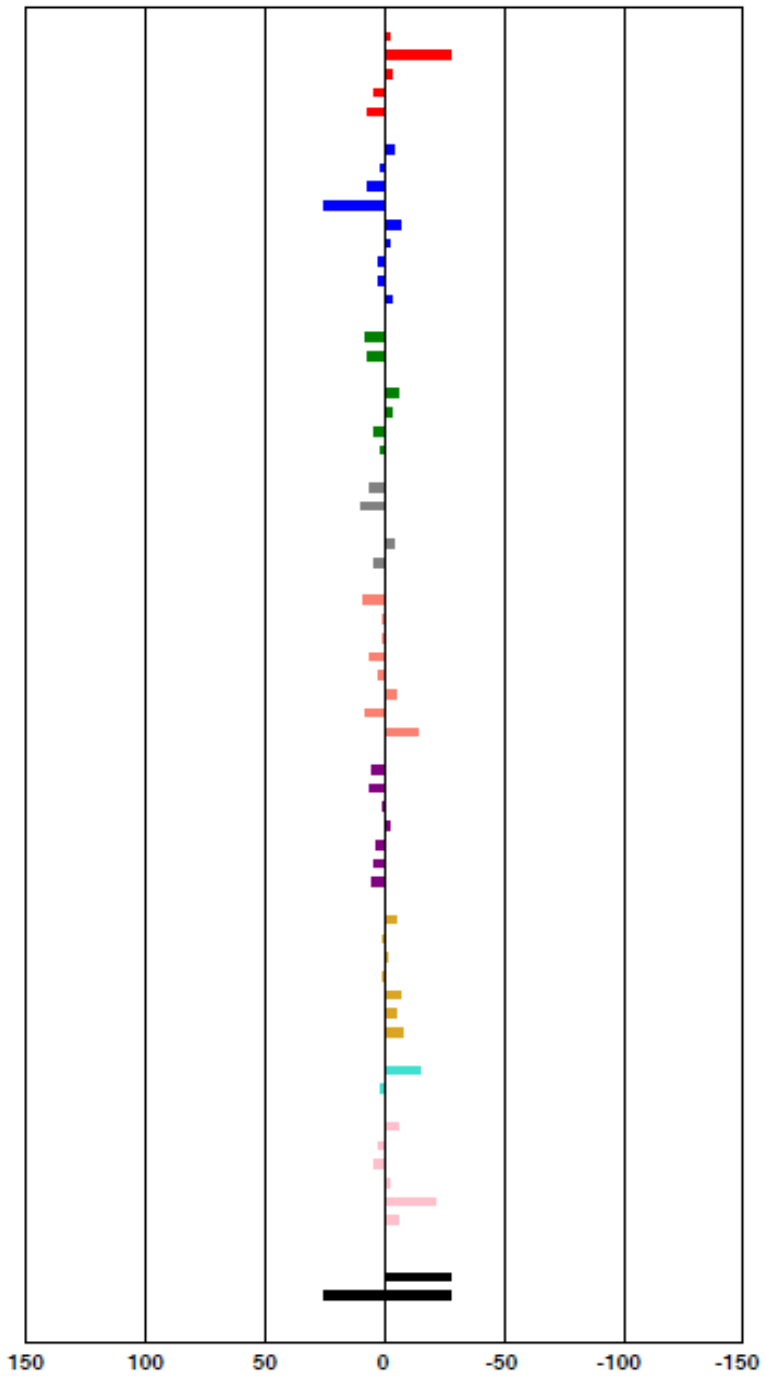
5g

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-826470 / 1	Conc: 1.00E-5 Molar	Test Date: Oct 26, 2020
Experiment ID: 2010OS50		Report Date: Mar 07, 2021

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	93.01
HL-60(TB)	97.40
K-562	92.65
MOLT-4	99.43
SR	101.99
Non-Small Cell Lung Cancer	
A549/ATCC	91.32
EKVX	96.70
HOP-62	101.91
HOP-92	120.13
NCI-H226	88.31
NCI-H23	93.62
NCI-H322M	97.30
NCI-H460	97.29
NCI-H522	91.93
Colon Cancer	
COLO 205	102.99
HCC-2998	102.57
HCT-116	94.94
HCT-15	89.57
HT29	92.42
KM12	99.22
SW-620	96.44
CNS Cancer	
SF-268	101.69
SF-295	104.82
SF-539	94.76
SNB-19	91.34
U251	99.23
Melanoma	
MALME-3M	104.00
M14	95.91
MDA-MB-435	95.57
SK-MEL-2	101.07
SK-MEL-28	97.67
SK-MEL-5	99.66
UACC-257	103.16
UACC-62	81.55
Ovarian Cancer	
IGROV1	100.24
OVCAR-3	101.24
OVCAR-4	95.63
OVCAR-5	93.54
OVCAR-8	98.77
NCI/ADR-RES	99.62
SK-OV-3	100.20
Renal Cancer	
786-0	99.12
ACHN	96.20
CAKI-1	94.34
RXF 393	95.46
SN12C	88.86
TK-10	99.77
UO-31	87.43
Prostate Cancer	
PC-3	80.74
DU-145	96.58
Breast Cancer	
MCF7	89.97
MDA-MB-231/ATCC	97.80
HS 578T	99.65
BT-549	93.14
T-47D	74.46
MDA-MB-468	89.41
Mean	95.12
Delta	27.72
Range	52.73

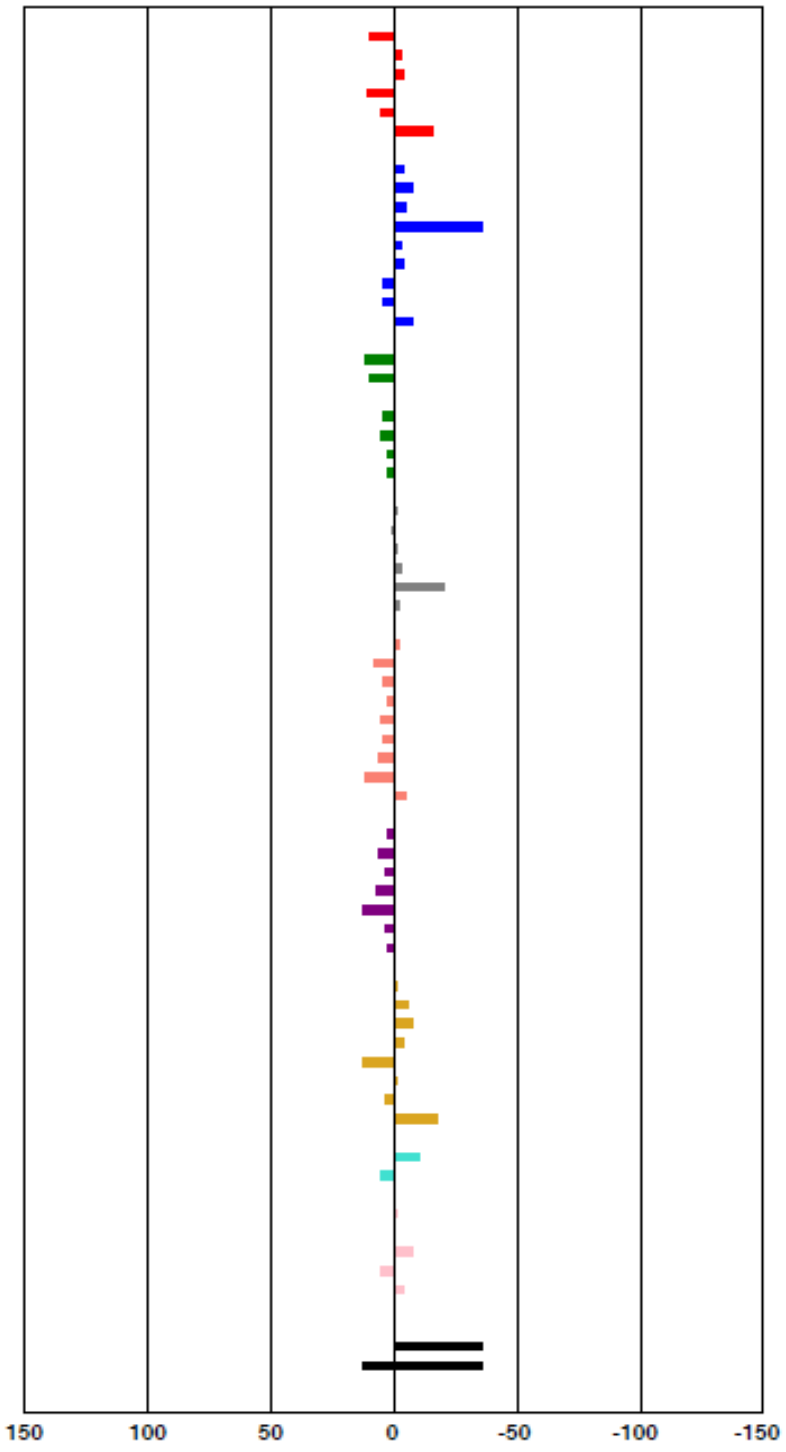


5h

Developmental Therapeutics Program	NSC: D-824572 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 17, 2020
One Dose Mean Graph	Experiment ID: 2008OS33		Report Date: Sep 05, 2020

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	107.33
HL-60(TB)	94.44
K-562	94.07
MOLT-4	108.94
RPMI-8226	103.40
SR	81.90
Non-Small Cell Lung Cancer	
A549/ATCC	94.02
EKVX	90.04
HOP-62	92.50
HOP-92	61.90
NCI-H226	94.60
NCI-H23	94.28
NCI-H322M	102.23
NCI-H460	101.87
NCI-H522	90.40
Colon Cancer	
COLO 205	109.73
HCC-2998	107.40
HCT-116	97.56
HCT-15	102.24
HT29	102.64
KM12	100.36
SW-620	100.57
CNS Cancer	
SF-268	90.40
SF-295	98.51
SF-539	96.65
SNB-19	94.06
SNB-75	77.44
U251	95.95
Melanoma	
LOX IMVI	96.16
MALME-3M	105.36
M14	102.34
MDA-MB-435	100.40
SK-MEL-2	103.12
SK-MEL-28	102.30
SK-MEL-5	104.31
UACC-257	100.15
UACC-62	93.24
Ovarian Cancer	
IGROV1	100.09
OVCAR-3	103.73
OVCAR-4	100.76
OVCAR-5	105.23
OVCAR-8	110.24
NCI/ADR-RES	101.41
SK-OV-3	100.65
Renal Cancer	
786-0	96.91
A498	91.83
ACHN	90.66
CAKI-1	94.05
RXF 393	110.10
SN12C	96.77
TK-10	101.30
UO-31	80.33
Prostate Cancer	
PC-3	87.28
DU-145	103.15
Breast Cancer	
MCF7	96.39
MDA-MB-231/ATCC	97.32
HS 578T	89.87
BT-549	102.70
T-47D	94.29
Mean	97.70
Delta	35.80
Range	48.34

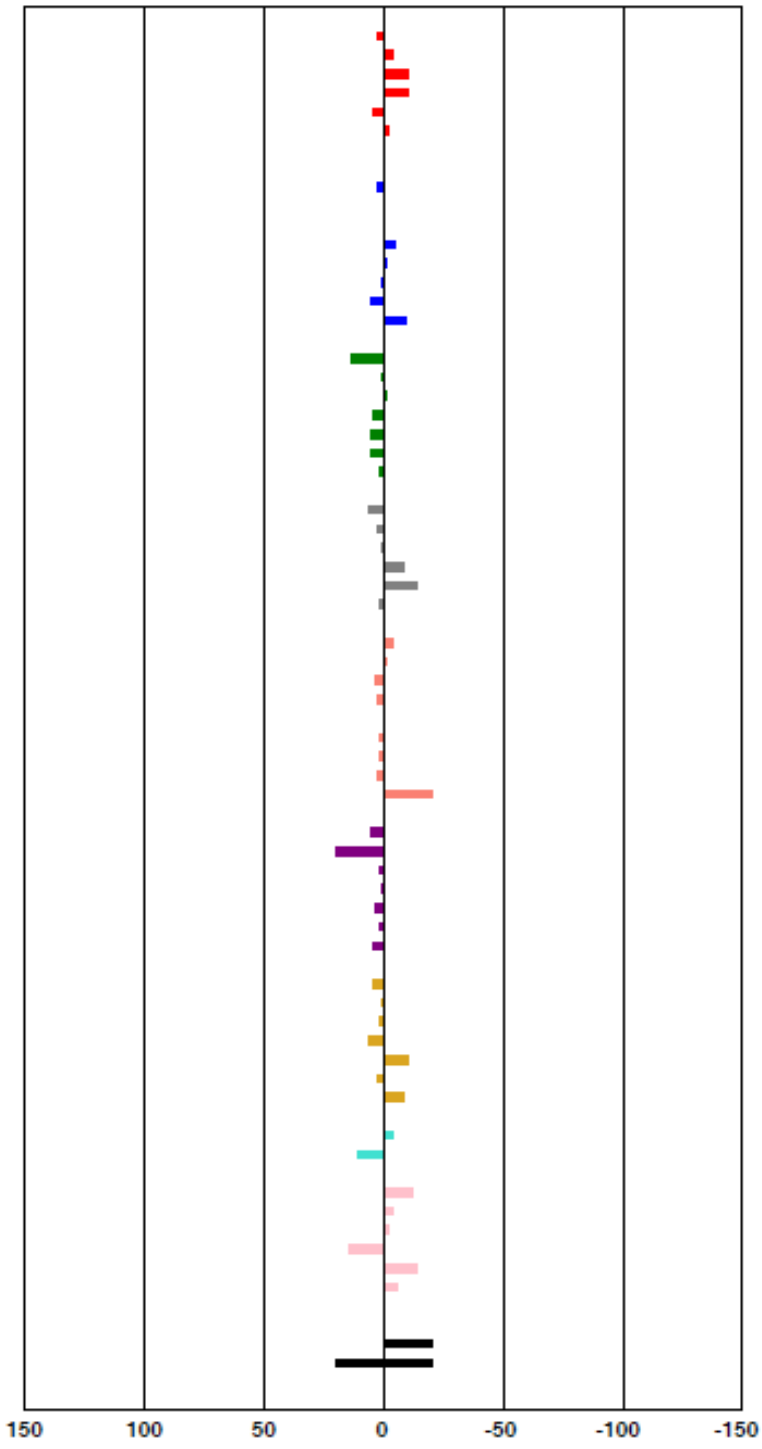
Mean Growth Percent - Growth Percent



5i

Developmental Therapeutics Program	NSC: D-820785 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 02, 2020
One Dose Mean Graph	Experiment ID: 2011OS01		Report Date: Mar 07, 2021

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	100.39
HL-60(TB)	93.85
K-562	87.40
MOLT-4	87.57
RPMI-8226	102.14
SR	95.40
Non-Small Cell Lung Cancer	
A549/ATCC	97.59
EKVX	100.30
HOP-62	97.46
HOP-92	97.02
NCI-H226	93.13
NCI-H23	90.00
NCI-H322M	98.46
NCI-H460	102.36
NCI-H522	88.33
Colon Cancer	
COLO 205	110.53
HCC-2998	98.53
HCT-116	90.33
HCT-15	101.52
HT29	102.92
KM12	102.66
SW-620	98.88
CNS Cancer	
SF-268	103.22
SF-295	99.84
SF-539	98.20
SNB-19	89.23
SNB-75	83.21
U251	99.48
Melanoma	
LOX IMVI	93.24
MALME-3M	95.89
M14	100.01
MDA-MB-435	99.58
SK-MEL-2	99.88
SK-MEL-28	99.10
SK-MEL-5	99.16
UACC-257	100.37
UACC-62	77.01
Ovarian Cancer	
IGROV1	102.69
OVCAR-3	117.38
OVCAR-4	99.31
OVCAR-5	97.75
OVCAR-8	100.00
NCI/ADR-RES	98.97
SK-OV-3	101.73
Renal Cancer	
786-0	101.89
ACHN	97.94
CAKI-1	99.18
RXF 393	103.48
SN12C	87.13
TK-10	100.18
UO-31	89.00
Prostate Cancer	
PC-3	93.29
DU-145	108.52
Breast Cancer	
MCF7	85.41
MDA-MB-231/ATCC	93.24
HS 578T	95.31
BT-549	111.36
T-47D	83.56
MDA-MB-468	92.10
Mean	97.36
Delta	10.75
Range	39.77



5j

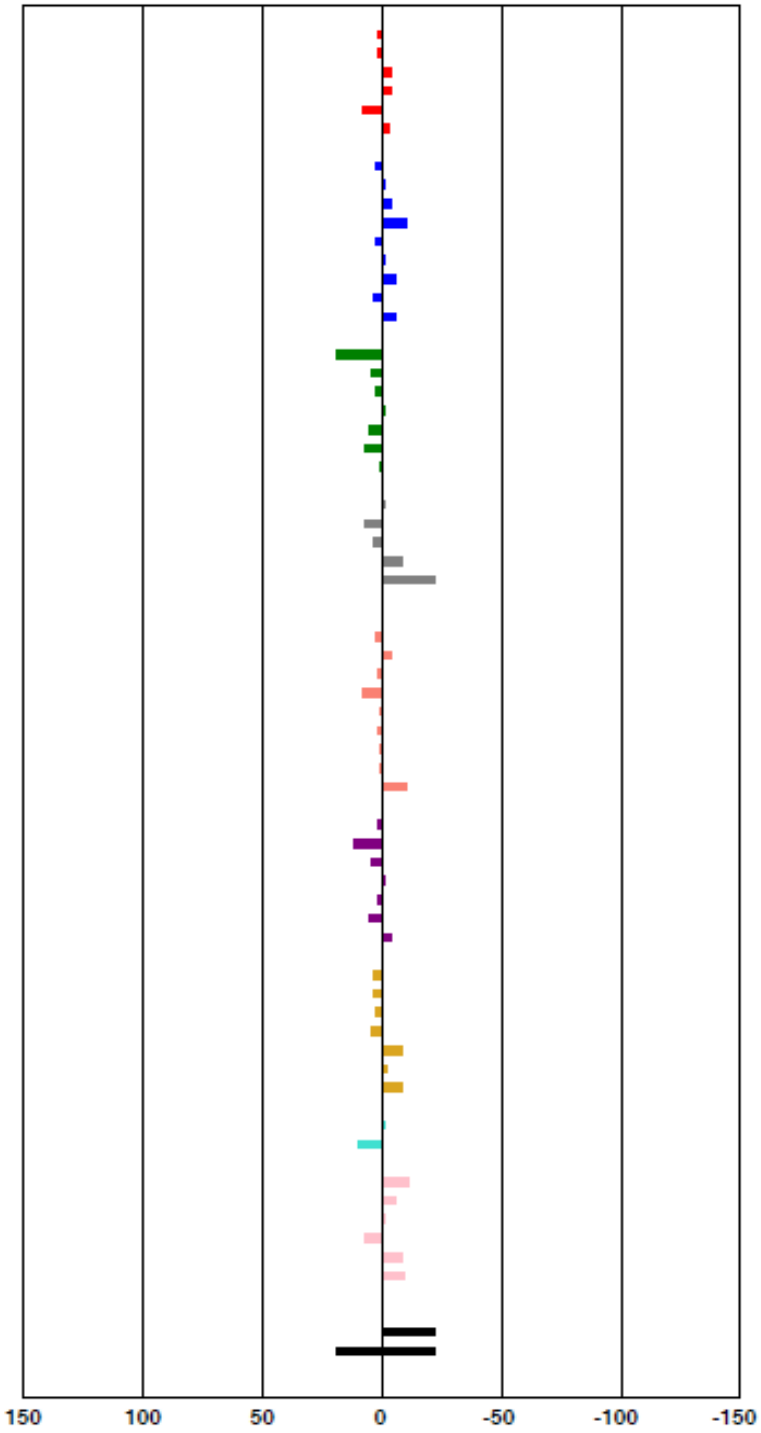
Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-826786 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 02, 2020
Experiment ID: 2011OS01		Report Date: Mar 07, 202

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	99.85
HL-60(TB)	99.99
K-562	94.36
MOLT-4	93.94
RPMI-8226	106.04
SR	94.98
Non-Small Cell Lung Cancer	
A549/ATCC	100.43
EKVX	96.93
HOP-62	94.38
HOP-92	88.33
NCI-H226	100.57
NCI-H23	96.92
NCI-H322M	92.32
NCI-H460	101.58
NCI-H522	92.14
Colon Cancer	
COLO 205	117.41
HCC-2998	102.89
HCT-116	101.07
HCT-15	97.40
HT29	103.55
KM12	104.83
SW-620	98.50
CNS Cancer	
SF-268	97.48
SF-295	105.10
SF-539	101.67
SNB-19	89.56
SNB-75	76.31
U251	98.39
Melanoma	
LOX IMVI	100.68
MALME-3M	94.42
M14	100.02
MDA-MB-435	105.89
SK-MEL-2	99.27
SK-MEL-28	100.04
SK-MEL-5	99.27
UACC-257	98.51
UACC-62	88.37
Ovarian Cancer	
IGROV1	99.47
OVCAR-3	109.83
OVCAR-4	102.47
OVCAR-5	97.31
OVCAR-8	100.22
NCI/ADR-RES	103.89
SK-OV-3	94.46
Renal Cancer	
786-0	101.44
ACHN	102.08
CAKI-1	100.41
RXF 393	102.29
SN12C	99.10
TK-10	96.11
UO-31	89.80
Prostate Cancer	
PC-3	97.03
DU-145	107.99
Breast Cancer	
MCF7	87.34
MDA-MB-231/ATCC	92.10
HS 578T	97.22
BT-549	105.43
T-47D	99.23
MDA-MB-468	88.50
Mean	98.12
Delta	21.81
Range	41.10

Mean Growth Percent - Growth Percent

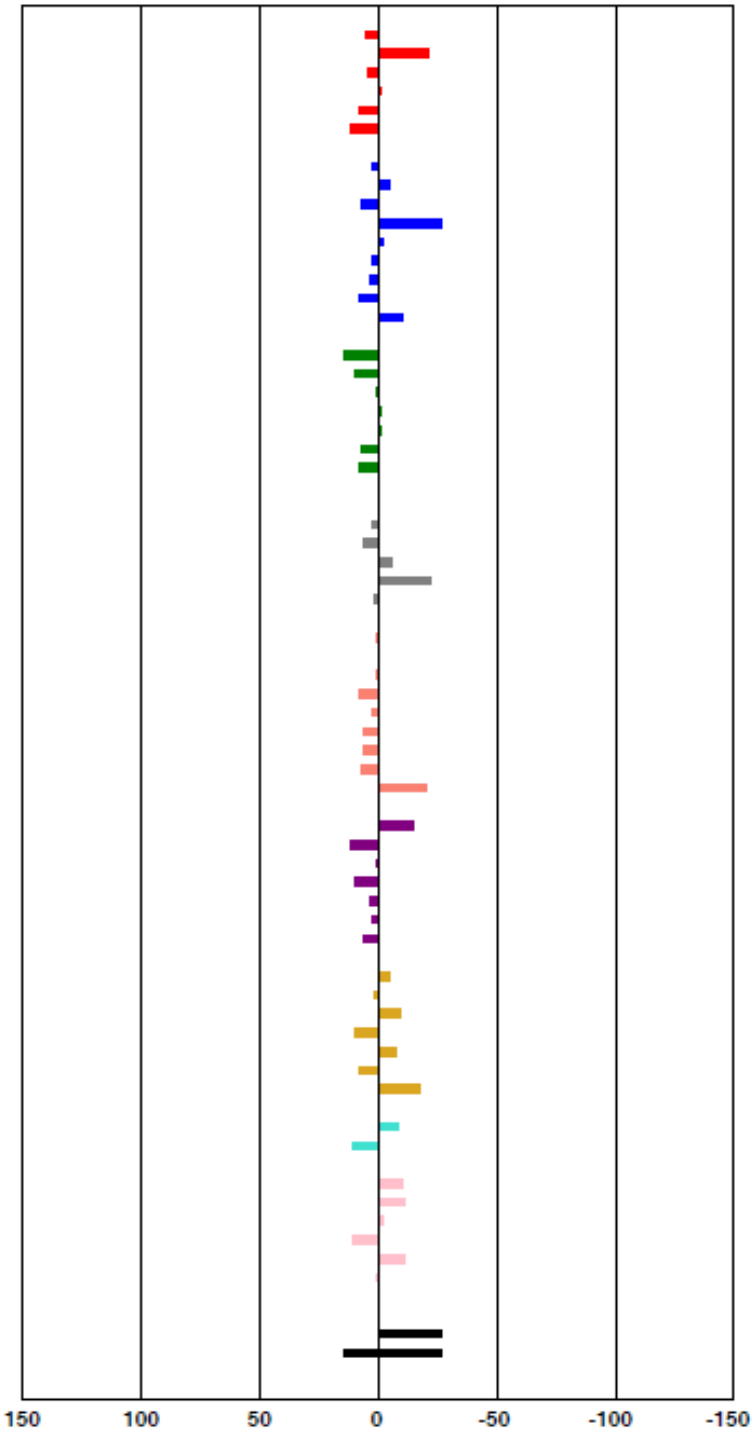


5k

Developmental Therapeutics Program	NSC: D-826787 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 02, 2020
One Dose Mean Graph	Experiment ID: 2011OS01		Report Date: Mar 07, 202

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	97.38
HL-60(TB)	70.03
K-562	96.40
MOLT-4	91.06
RPMI-8226	99.08
SR	103.76
Non-Small Cell Lung Cancer	
A549/ATCC	94.09
EKVX	86.79
HOP-62	98.70
HOP-92	85.14
NCI-H226	90.15
NCI-H23	94.79
NCI-H322M	95.88
NCI-H460	99.55
NCI-H522	81.59
Colon Cancer	
COLO 205	106.54
HCC-2998	101.48
HCT-116	92.60
HCT-15	91.33
HT29	91.03
KM12	99.16
SW-620	99.89
CNS Cancer	
SF-268	92.04
SF-295	94.54
SF-539	98.44
SNB-19	86.20
SNB-75	89.52
U251	93.97
Melanoma	
LOX IMVI	92.47
MALME-3M	92.14
M14	93.07
MDA-MB-435	99.97
SK-MEL-2	94.45
SK-MEL-28	98.01
SK-MEL-5	98.15
UACC-257	99.03
UACC-62	71.91
Ovarian Cancer	
IGROV1	77.25
OVCAR-3	103.83
OVCAR-4	92.71
OVCAR-5	101.90
OVCAR-8	95.71
NCI/ADR-RES	94.21
SK-OV-3	97.77
Renal Cancer	
786-0	87.15
ACHN	93.91
CAKI-1	82.68
RXF 393	101.95
SN12C	84.77
TK-10	99.77
UO-31	74.17
Prostate Cancer	
PC-3	83.17
DU-145	103.07
Breast Cancer	
MCF7	81.86
MDA-MB-231/ATCC	80.46
HS 578T	89.70
BT-549	102.68
T-47D	86.96
MDA-MB-468	92.46
Mean	91.93
Delta	26.79
Range	41.40

Mean Growth Percent - Growth Percent



Tubulin polymerization report

Researcher	: Dr..Rana Tarek email: r.diab@zu.edu.eg mob.
Assay	: Tubulin enzyme assay
Samples	: 2 compounds
Ref.	: ---
Date	: 09-03-2018
Reader	: Tecan-Spark reader
Kit used	: Cloud-clone corp) SEB870Hu EIA Kit For Tubulin Beta (TUBb).
Solvent	: DMSO

Lab Report

ser	Compound		Tubulin Binding	SD ±
			IC50	
	ID	M.W g/mol	uM	
1	pha	489	1.18	0.037
**	Colchicine	399	2.37	0.075