Electronic Supplementary Material (ESI) for RSC Advances.

THE SUPPORTING INFORMATION

Table S1 *In silico* ADMET profile of the most active compounds, ciprofloxacin, fluconazole, and paclitaxel

Parameter	1d	2d	3s	4b	4k	Cipro	Flu	PTX
Absorption								
Caco-2 permeability	-4.893	-4.820	-4.685	-4.655	-4.721	-5.269	-4.950	-5.461
MDCK permeability	$9.0x10^{-6}$	$8.6x10^{-5}$	$11.0x10^{-5}$	$8.8x10^{-5}$	$2.8x10^{-5}$	$3.0x10^{-6}$	$2.8x10^{-5}$	$5.4x10^{-5}$
Pgp-inhibitor	--	---	+++	+++	+++	---	---	+++
Pgp-substrate	---	---	++	---	---	+++	---	+++
HIA	+++	+++	+++	+++	+++	+++	+++	+++
$F_{20\%}$	+++	+++	+	+++	+++	+++	+++	---
$F_{30\%}$	---	+++	+++	++	+++	+++	+++	---
Distribution								
PPB (%)	99.953	100.185	99.428	100.069	98.764	37.456	61.763	94.571
VD (L/kg)	1.485	0.460	1.171	0.324	0.385	2.324	0.835	0.907
BBB penetration	---	-	++	+	--	---	+++	--
Fu (%)	1.174	0.672	1.322	0.638	1.170	78.856	51.002	6.779
Log Kp (cm/s)	-4.54	-4.86	-4.64	-4.92	-5.03	-9.090	-7.920	
Metabolism								
CYP1A2 inhibitor	+++	+++	+++	+++	++	--	-	---
CYP1A2 substrate	--	--	-	--	--	--	-	---
CYP2C19 inhibitor	++	+++	++	+++	++	---	+	---
CYP2C19 substrate	---	---	---	---	---	--	---	---
CYP2C9 inhibitor	+	++	++	+++	++	---	--	++

CYP2C9 substrate	++	++	+	++	++	---	+	---
CYP2D6 inhibitor	++	++	+++	++	++	---	-	---
CYP2D6 substrate	-	-	++	++	++	--	--	---
CYP3A4 inhibitor	--	+	+	++	+	---	-	++
CYP3A4 substrate	-	--	--	--	-	--	--	+
Excretion								
CL (mL/min/kg)	4.885	3.983	7.914	4.476	6.550	3.214	5.960	3.416
$T_{1/2}$	0.125	0.170	0.082	0.066	0.056	0.056	0.228	0.028
Toxicity								
hERG blockers	--	-	++	--	+++	--	---	--
H-HT	--	--	---	---	---	+++	+++	+++
DILI	++	++	-	-	+	+++	+++	+++
AMES toxicity	-	+++	+++	+++	+++	--	++	---
Rat oral acute toxicity	--	--	--	---	---	--	+++	-
FDAMDD	++	++	++	++	++	++	++	++
Skin sensitization	--	-	---	-	-	+	+++	---
Carcinogenicity	-	+	++	+	++	-	+++	---
Eye corrosion	---	---	---	---	---	---	---	---
Eye irritation	+++	+++	+++	+++	+++	---	--	---
Respiratory toxicity	--	+++	++	++	++	++	++	+++
Tox21 Pathway								
NR-AR	+	+	--	-	-	++	---	--
NR-AR-LBD	---	+	--	++	+	---	---	+++
NR-AhR	++	+++	+	+++	++	--	+	---

NR-Aromatase	++	++	++	+	++	---	+++	++
NR-ER	++	++	++	++	++	-	---	+
NR-ER-LBD	-	-	-	+	+	---	---	+
NR-PPAR-gamma	---	---	---	---	---	---	---	+++
SR-ARE	++	+++	+++	+++	+++	-	--	++
SR-ATAD5	+++	++	+	+	-	---	---	+++
SR-HSE	+	-	---	-	--	---	---	-
SR-MMP	++	++	++	++	+++	---	--	+++
SR-p53	++	+++	++	+++	+++	---	---	+++
Toxicophore Rules								
Acute Toxicity Rule	0 alert	0 alert	0 alert	0 alert	0 alert	1 alert	0 alert	0 alert
Genotoxic Carcinogenicity Rule	0 alerts	5 alert	4 alert	5 alerts	9 alerts	1 alert	0 alert	1 alert
NonGenotoxic Carcinogenicity Rule	1 alert	0 alert	1 alert	0 alert	1 alert	1 alert	0 alert	0 alert
Skin Sensitization Rule	1 alert	1 alert	1 alert	1 alert	1 alert	0 alert	0 alert	6 alerts
Aquatic Toxicity Rule	1 alert	1 alert	1 alert	1 alert	1 alert	1 alert	1 alert	2 alerts
NonBiodegradable Rule	1 alert	3 alert	2 alert	3 alerts	3 alerts	2 alerts	1 alert	2 alerts
SureChEMBL Rule	0 alert	0 alert	0 alert	0 alert	0 alert	0 alert	0 alert	0 alert
FAF-Drugs4 Rule	2 alerts	4 alerts	2 alerts	5 alerts	4 alerts	1 alert	1 alert	1 alert

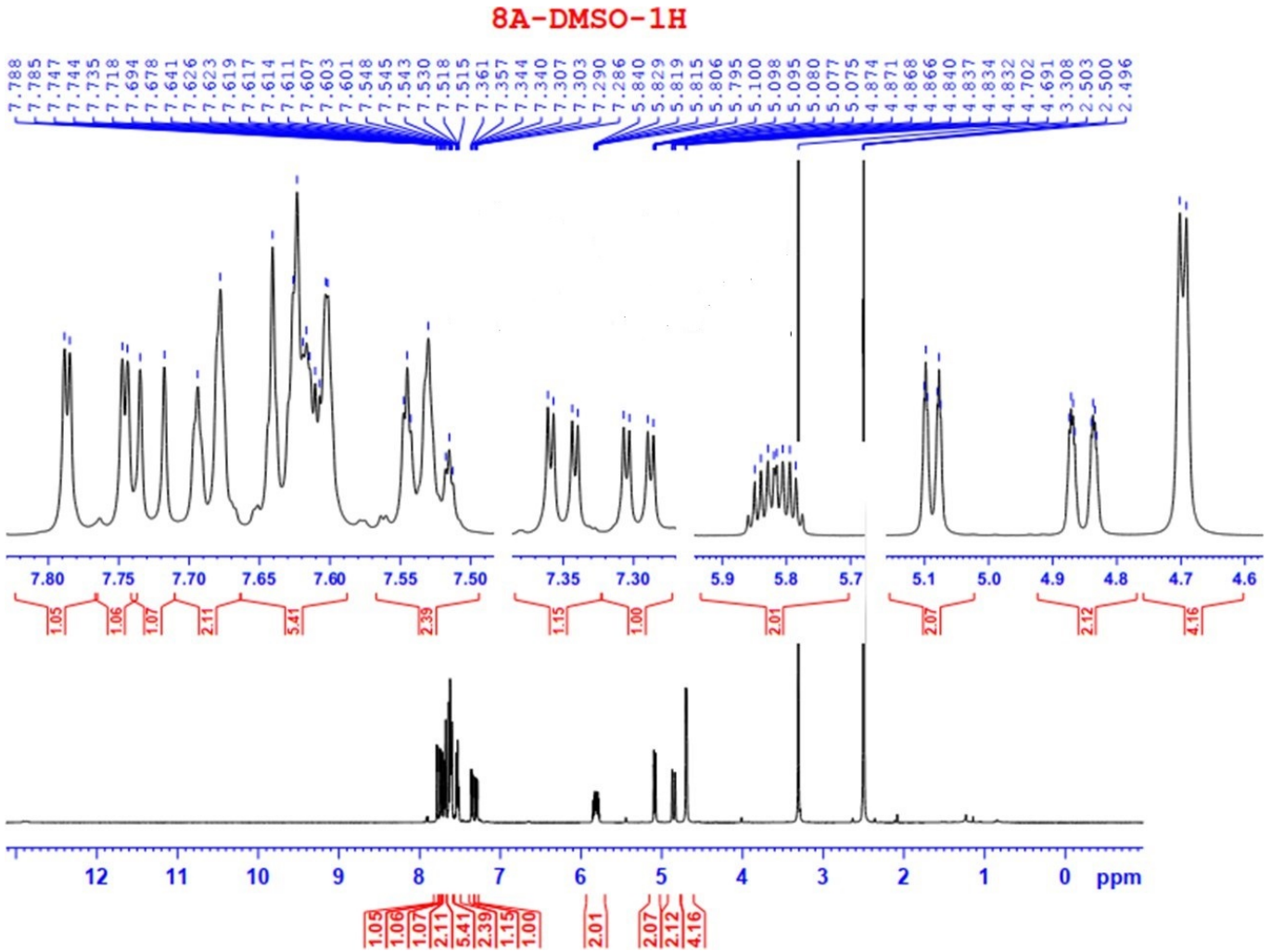
Cipro *- ciprofloxacin,* ***Flu*** *- fluconazole,* ***PTX*** *- paclitaxel,* ***Caco-2 permeability*** *(optimal: higher than -5.15 Log unit),* ***MDCK permeability*** *(low permeability: <2x10^{-6} cm/s, medium permeability: 2-20x10^{-6} cm/s, high passive permeability: > 20x10^{-6} cm/s),* ***Pgp*** *- P-glycoprotein,* ***HIA*** *- human intestinal absorption (-: <30%, +: ≥30%),* ***F*** *- bioavailability (-: <percent value, +: ≥percent value),* ***PPB*** *- plasma protein binding (optimal: <90%),* ***VD*** *- volume distribution (optimal: 0.04-20 L/kg),* ***BBB*** *- blood-brain barrier,* ***Fu*** *- the fraction unbound in plasms (low: <5%, middle: 5-20%, high: >20%),* ***Log Kp*** *(skin permeation),* ***CL*** *- clearance (low: <5 mL/min/kg, moderate: 5-15 mL/min/kg, high: >15 mL/min/kg),* ***T$_{1/2}$*** *(category 1: long half-life (>3 h), category 0: short half-life (<3 h)),* ***H-HT*** *- human hepatotoxicity,* ***DILI*** *- drug-induced liver injury,* ***FDAMDD*** *- maximum*

recommended daily dose, ***AR*** *- androgen receptor,* ***AR-LBD*** *- androgen receptor ligand-binding domain,* ***AhR*** *- aryl hydrocarbon receptor,* ***ER*** *- estrogen receptor,* ***ER-LBD*** *- estrogen receptor ligand-binding domain,* ***PPAR-gamma*** *- peroxisome proliferator-activated receptor gamma,* ***ARE*** *- antioxidant response element,* ***ATAD5*** *- ATPase family AAA domain-containing protein 5,* ***HSE*** *- heat shock factor response element,* ***MMP*** *- mitochondrial membrane potential.*

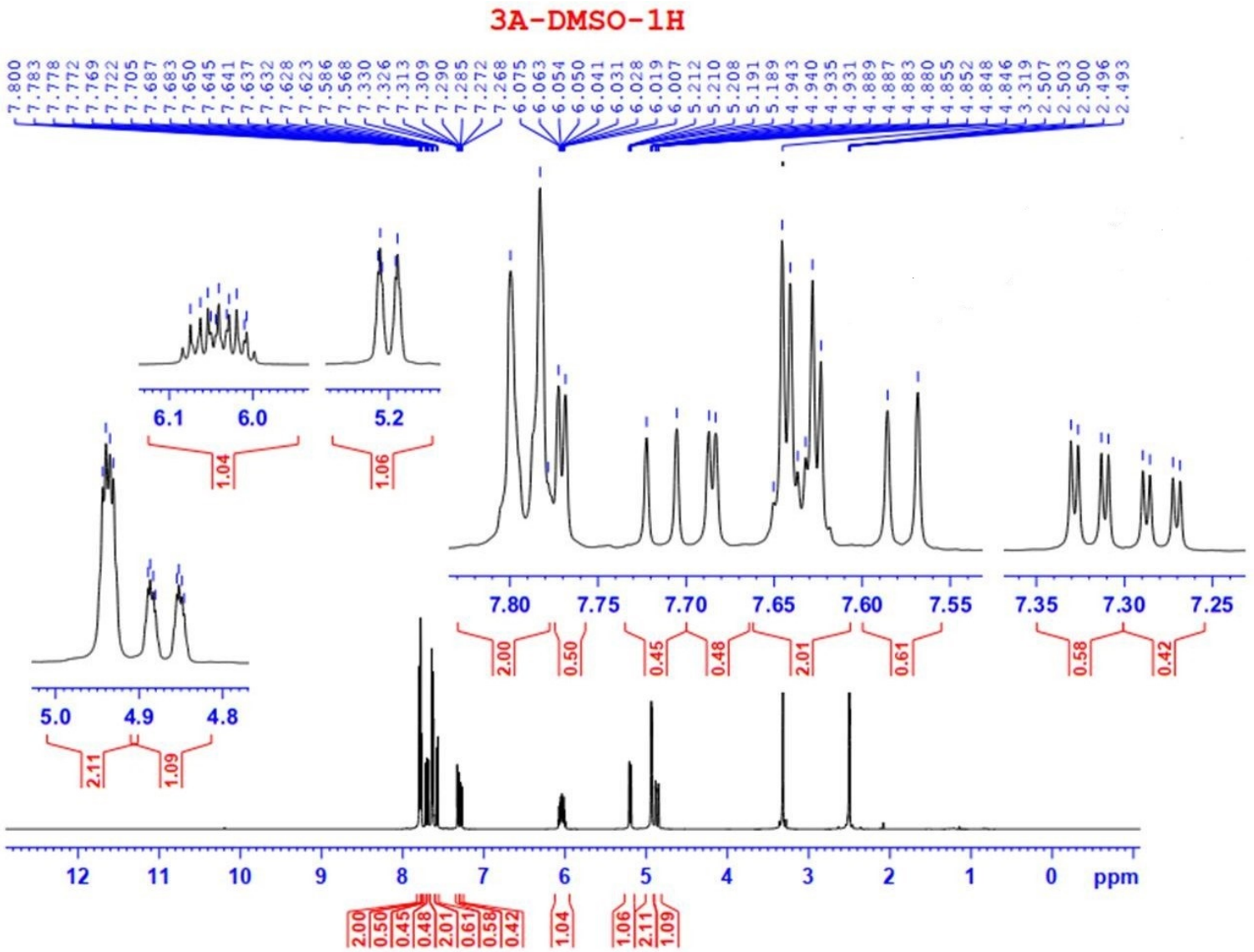
The output value is the probability of being inhibitor/substrate/active/positive/high-toxicity/sensitizer/carcinogens/corrosives/irritants (category 1) or non-inhibitor/non-substrate/inactive/negative/low-toxicity/non-sensitizer/non-carcinogens/noncorrosives/nonirritants (category 0). For the classification endpoints, the prediction probability values are transformed into six symbols: 0-0.1(---), 0.1-0.3(--), 0.3-0.5(-), 0.5-0.7(+), 0.7-0.9(++), and 0.9-1.0(+++).

1H NMR SPECTRA

Compound 3a



Compound 3b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7.722
7.705
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7.645
7.641
7.637
7.632
7.628
7.623
7.586
7.568
7.330
7.326
7.313
7.309
7.290
7.285
7.272
7.268
6.075
6.063
6.054
6.050
6.041
6.031
6.028
6.019
6.007
5.212
5.210
5.208
5.191
5.189
4.943
4.940
4.935
4.931
4.889
4.887
4.883
4.880
4.855
4.852
4.848
4.846
3.319
2.507
2.503
2.500
2.496
2.493
6.1
6.0
5.2
1.04
1.06
5.0
4.9
4.8
2.11
1.09
7.80
7.75
7.70
7.65
7.60
7.55
7.35
7.30
7.25
2.00
0.50
0.45
0.48
2.01
0.61
0.58
0.42
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
0.50
0.45
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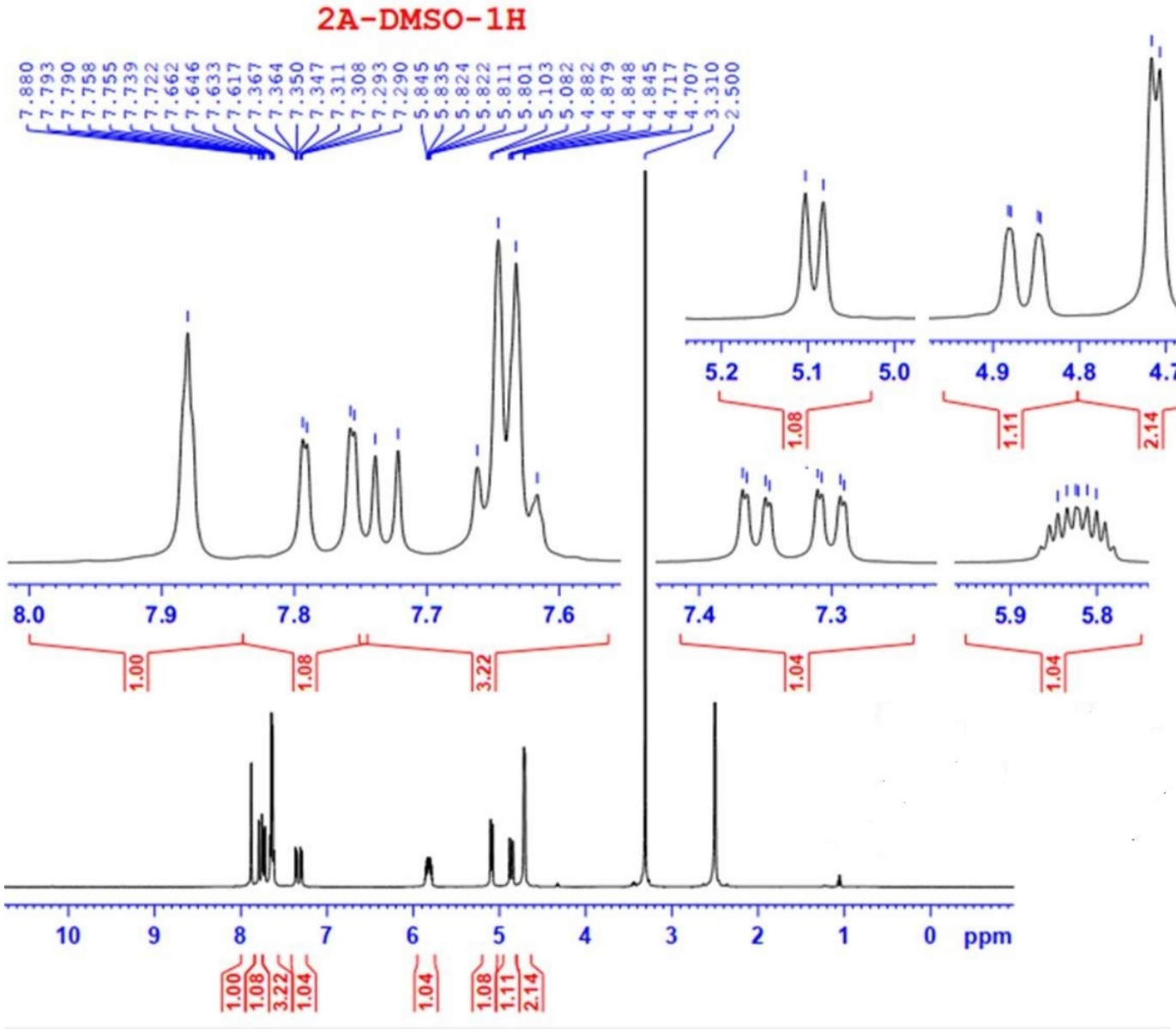
2.01
0.61
0.58
0.42
1.04
1.06
2.11
1.09

Compound 3c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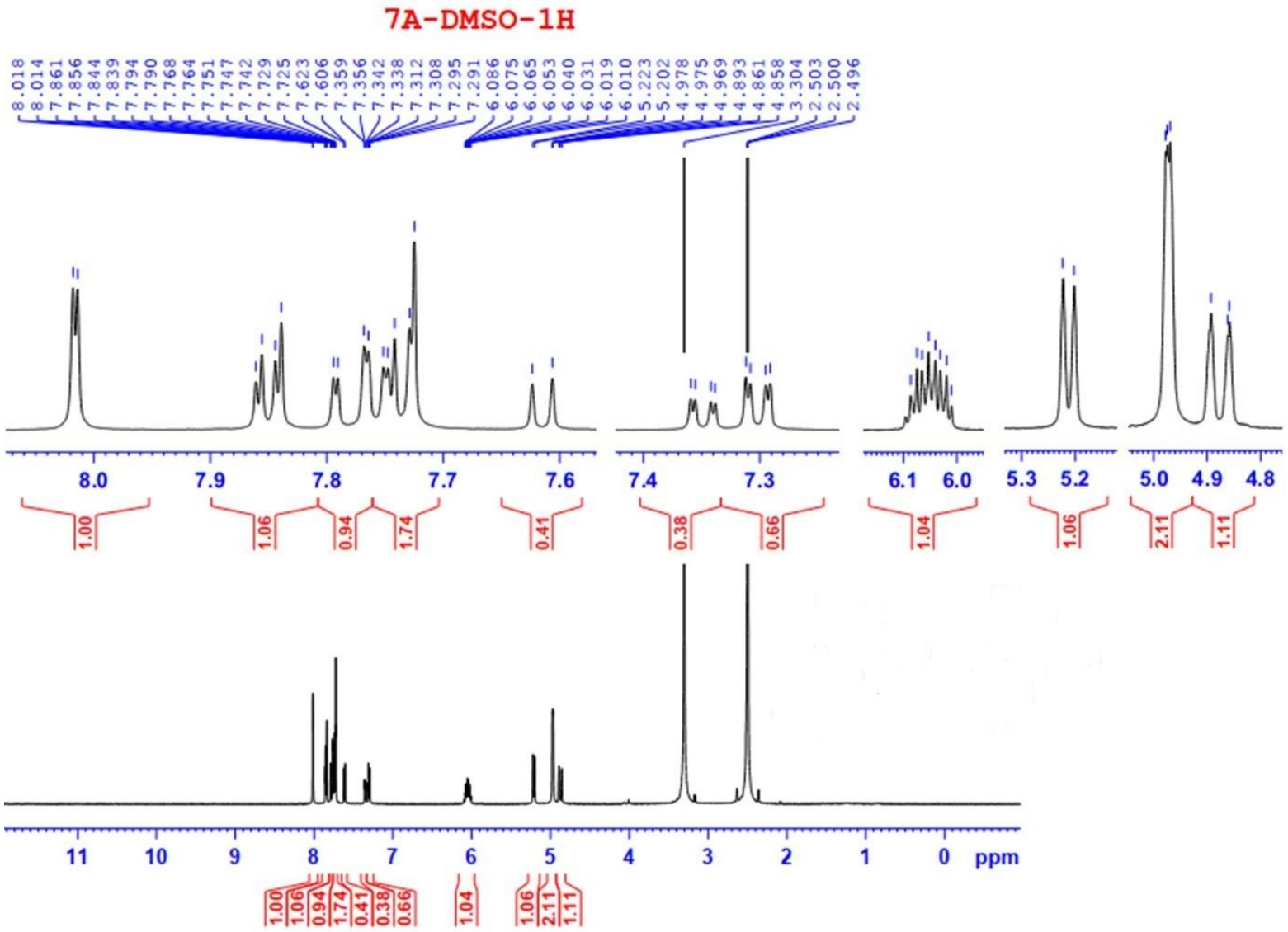
7.790
7.758
7.755
7.739
7.722
7.662
7.646
7.633
7.617
7.367
7.364
7.350
7.347
7.311
7.308
7.293
7.290
5.845
5.835
5.824
5.822
5.811
5.801
5.103
5.082
4.882
4.879
4.848
4.845
4.717
4.707
3.310
2.500
8.0
7.9
7.8
7.7
7.6
7.4
7.3
5.9
5.8
5.2
5.1
5.0
4.9
4.8
4.7
1.00
1.08
3.22
1.04
1.04
1.08
1.11
2.14
10
9
8
7
6
5
4
3
2
1
0
ppm

Compound 3d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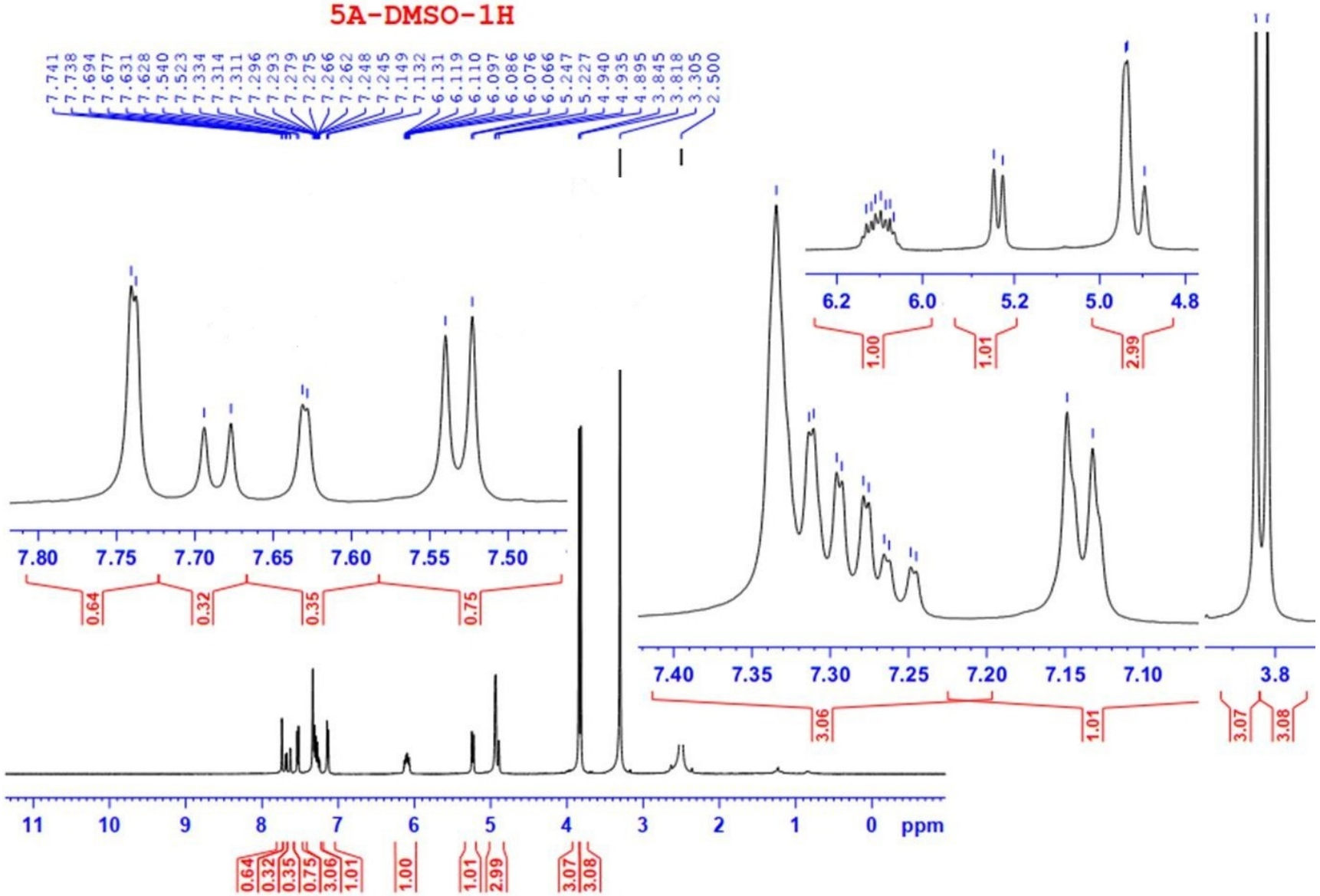
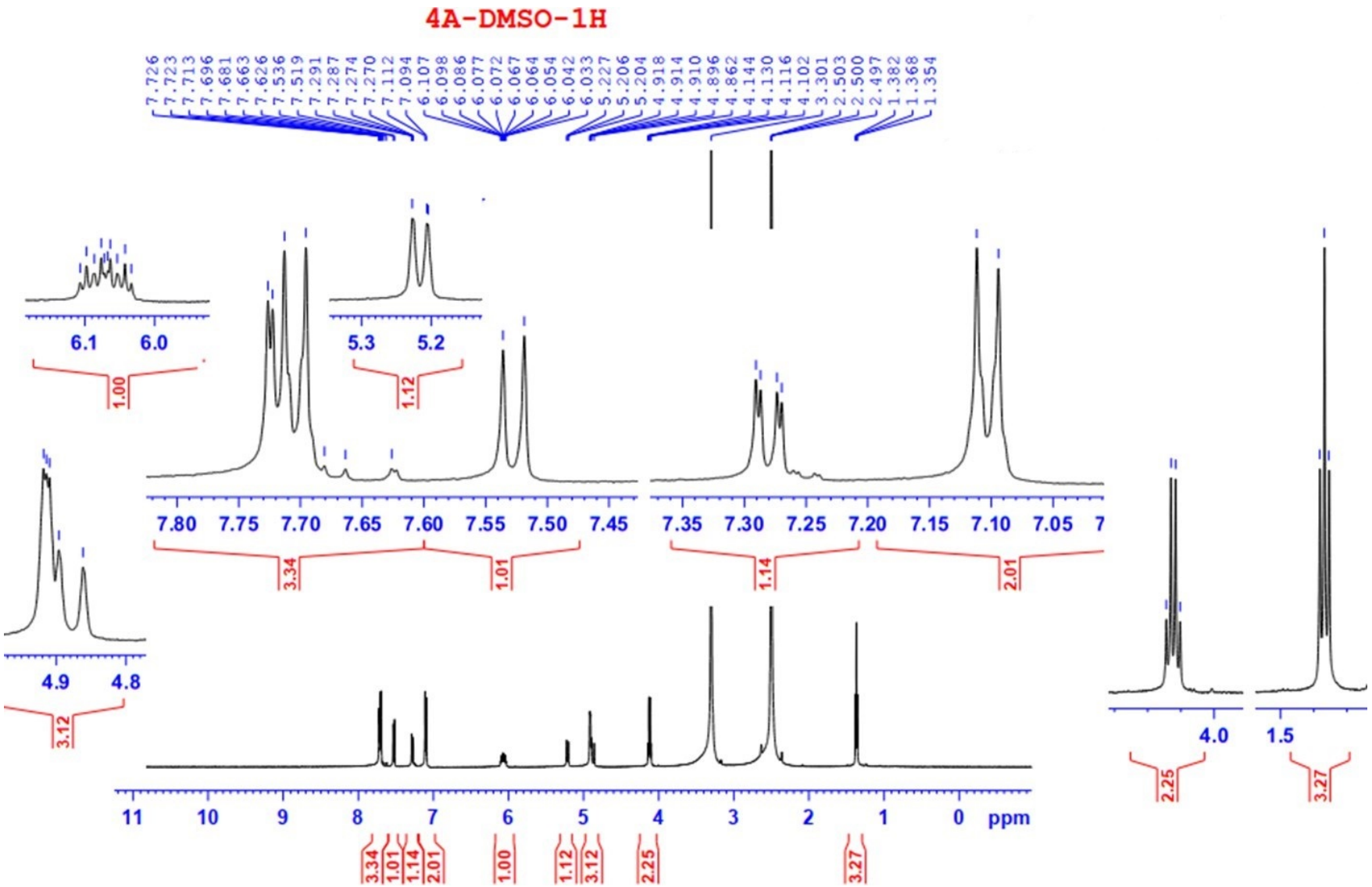
7.839
7.794
7.790
7.768
7.764
7.751
7.747
7.742
7.729
7.725
7.623
7.606
7.359
7.356
7.342
7.338
7.312
7.308
7.295
7.291
6.086
6.075
6.065
6.053
6.040
6.031
6.019
6.010
5.223
5.202
4.978
4.975
4.969
4.893
4.861
4.858
3.304
2.503
2.500
2.496
8.0
7.9
7.8
7.7
7.6
7.4
7.3
6.1
6.0
5.3
5.2
5.0
4.9
4.8
1.00
1.06
0.94
1.74
0.41
0.38
0.66
1.04
1.06
2.11
1.11
11
10
9
8
7
6
5
4
3
2
1
0
ppm

Compound 3e


5A-DMSO-1H
7.741
7.738
7.694
7.677
7.631
7.628
7.540
7.523
7.334
7.314
7.311
7.296
7.293
7.279
7.275
7.266
7.262
7.248
7.245
7.149
7.132
6.131
6.119
6.110
6.097
6.086
6.076
6.066
5.247
4.940
4.935
4.895
3.845
3.818
3.305
2.500
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.64 0.32 0.35 0.75 3.06 1.01 1.00 1.01 2.99 3.07 3.08
7.80 7.75 7.70 7.65 7.60 7.55 7.50
0.64 0.32 0.35 0.75
6.2 6.0 5.2 5.0 4.8
1.00 1.01 2.99
7.40 7.35 7.30 7.25 7.20 7.15 7.10
3.06 1.01
3.8
3.07 3.08

Compound 3f


4A-DMSO-1H
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7.723
7.713
7.696
7.681
7.663
7.626
7.536
7.519
7.291
7.287
7.274
7.270
7.112
7.094
6.107
6.098
6.086
6.077
6.072
6.067
6.064
6.054
6.042
6.033
5.227
5.206
5.204
4.918
4.914
4.910
4.896
4.862
4.144
4.130
4.116
4.102
3.301
2.503
2.500
2.497
1.382
1.368
1.354
6.1
6.0
1.00
5.3
5.2
1.12
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
3.34
1.01
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7
1.14
2.01
4.9
4.8
3.12
4.0
1.5
2.25
3.27
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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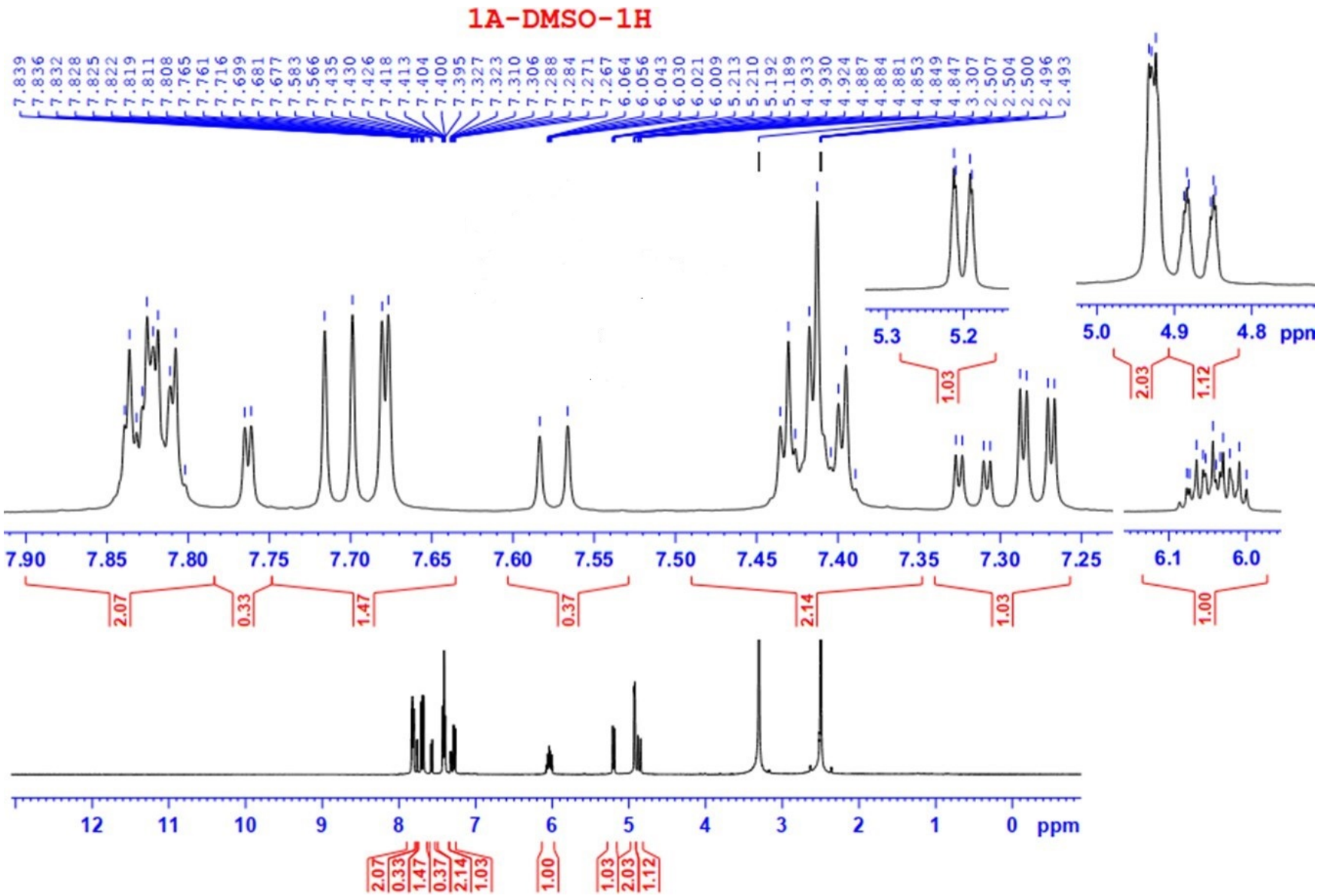
1.01
1.14
2.01
1.00
1.12
3.12
2.25
3.27

Compound 3g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7.836
7.832
7.828
7.825
7.822
7.819
7.811
7.808
7.765
7.761
7.716
7.699
7.681
7.677
7.583
7.566
7.435
7.430
7.426
7.418
7.413
7.404
7.400
7.395
7.327
7.323
7.310
7.306
7.288
7.284
7.271
7.267
6.064
6.056
6.043
6.030
6.021
6.009
5.213
5.210
5.192
5.189
4.933
4.930
4.924
4.887
4.884
4.881
4.853
4.849
4.847
3.307
2.507
2.504
2.500
2.496
2.493
5.3
5.2
1.03
5.0
4.9
4.8
ppm
2.03
1.12
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
2.07
0.33
1.47
0.37
2.14
1.03
6.1
6.0
1.00
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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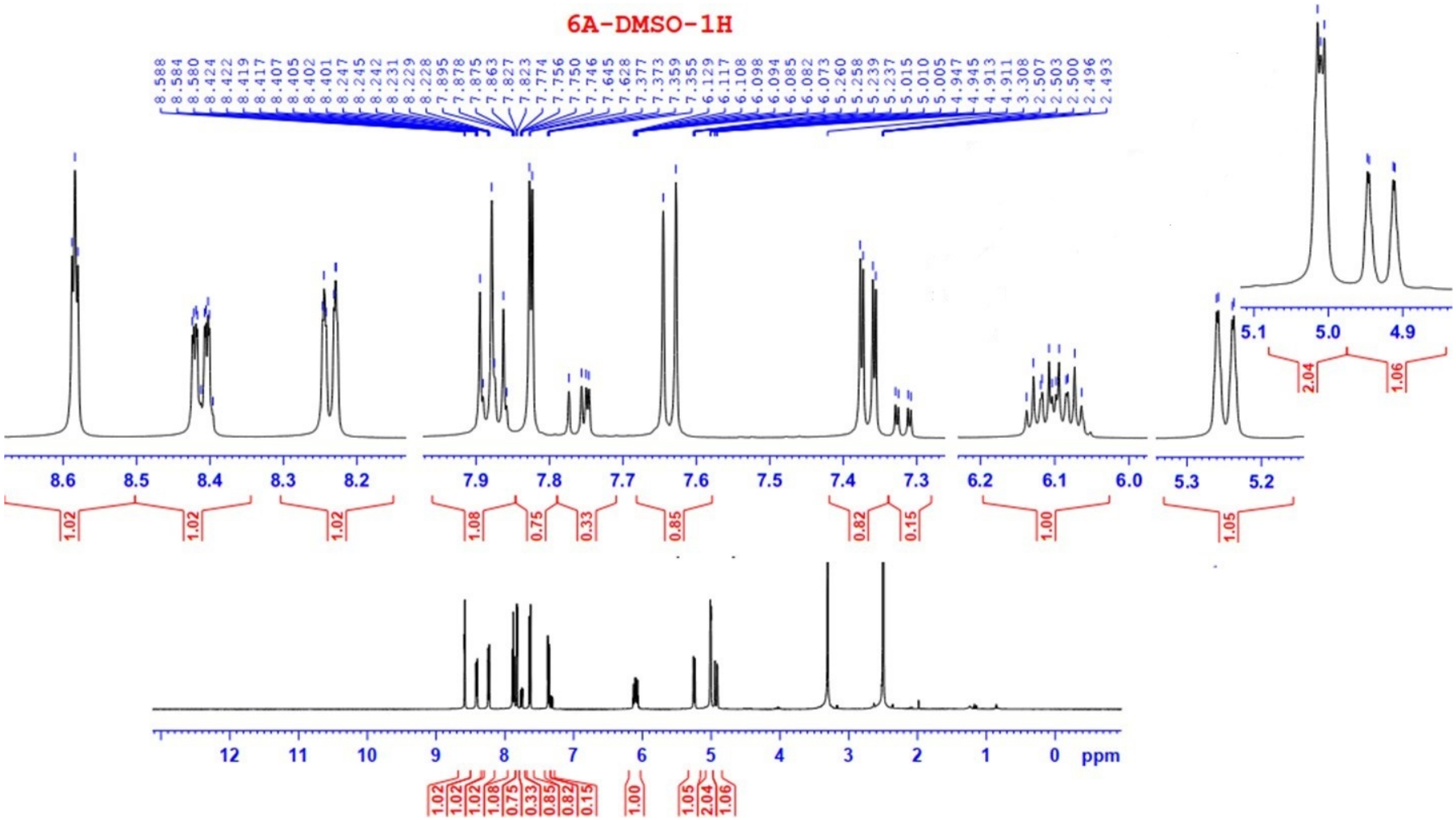
1.47
0.37
2.14
1.03
1.00
1.03
2.03
1.12

Compound 3h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8.580
8.424
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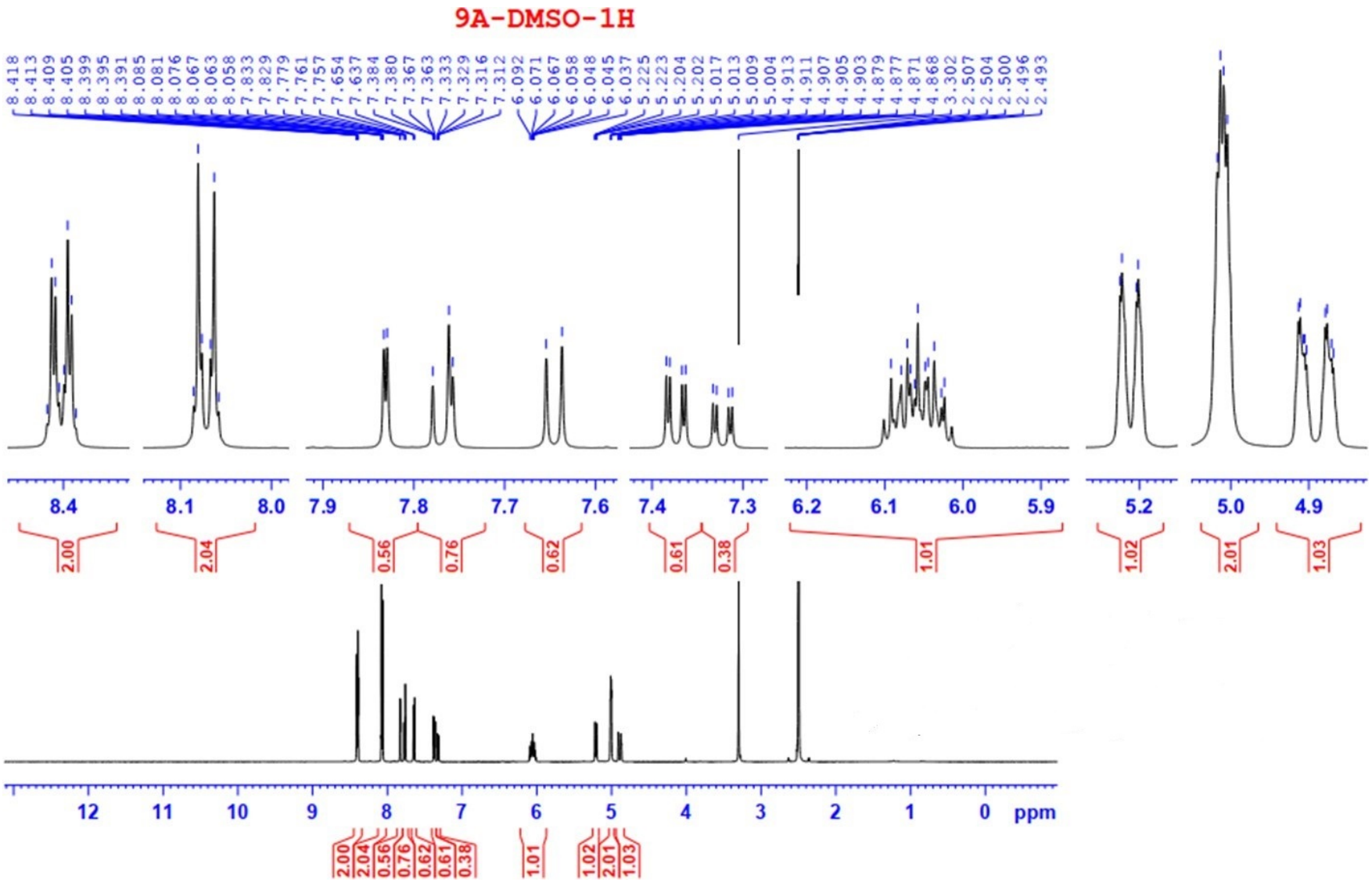
8.419
8.417
8.407
8.405
8.402
8.401
8.247
8.245
8.242
8.231
8.229
8.228
7.895
7.878
7.875
7.863
7.827
7.823
7.774
7.756
7.750
7.746
7.645
7.628
7.377
7.373
7.359
7.355
6.129
6.117
6.108
6.098
6.094
6.085
6.082
6.073
5.260
5.258
5.239
5.237
5.015
5.010
5.005
4.947
4.945
4.913
4.911
3.308
2.507
2.503
2.500
2.496
2.493
8.6
8.5
8.4
8.3
8.2
7.9
7.8
7.7
7.6
7.5
7.4
7.3
6.2
6.1
6.0
5.3
5.2
5.1
5.0
4.9
1.02
1.02
1.02
1.08
0.75
0.33
0.85
0.82
0.15
1.00
1.05
2.04
1.06
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

Compound 3i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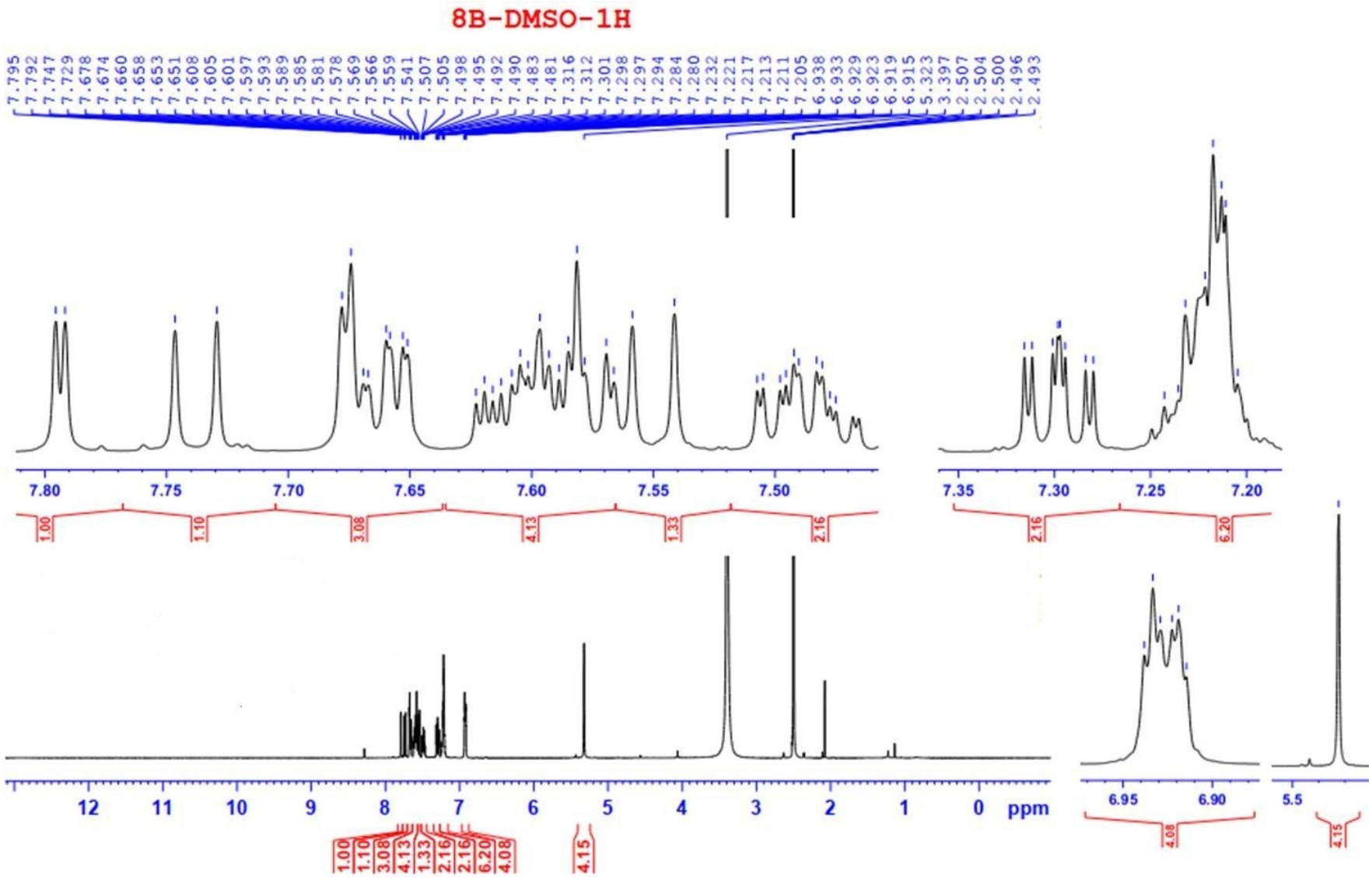
8.409
8.405
8.399
8.395
8.391
8.085
8.081
8.076
8.067
8.063
8.058
7.833
7.829
7.779
7.761
7.757
7.654
7.637
7.384
7.380
7.367
7.363
7.333
7.329
7.316
7.312
6.092
6.071
6.067
6.058
6.048
6.045
6.037
5.225
5.223
5.204
5.202
5.017
5.013
5.009
5.004
4.913
4.911
4.907
4.905
4.903
4.879
4.877
4.871
4.868
3.302
2.507
2.504
2.500
2.496
2.493
8.4
8.1
8.0
7.9
7.8
7.7
7.6
7.4
7.3
6.2
6.1
6.0
5.9
5.2
5.0
4.9
2.00
2.04
0.56
0.76
0.62
0.61
0.38
1.01
1.02
2.01
1.03
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

Compound 3j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7.729
7.678
7.674
7.660
7.658
7.653
7.651
7.608
7.605
7.601
7.597
7.593
7.589
7.585
7.581
7.578
7.569
7.566
7.559
7.541
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7.505
7.498
7.495
7.492
7.490
7.483
7.481
7.316
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7.297
7.294
7.284
7.280
7.232
7.221
7.217
7.213
7.211
7.205
6.938
6.933
6.929
6.923
6.919
6.915
5.323
3.397
2.507
2.504
2.500
2.496
2.493
7.80
7.75
7.70
7.65
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7.50
7.35
7.30
7.25
7.20
6.95
6.90
5.5
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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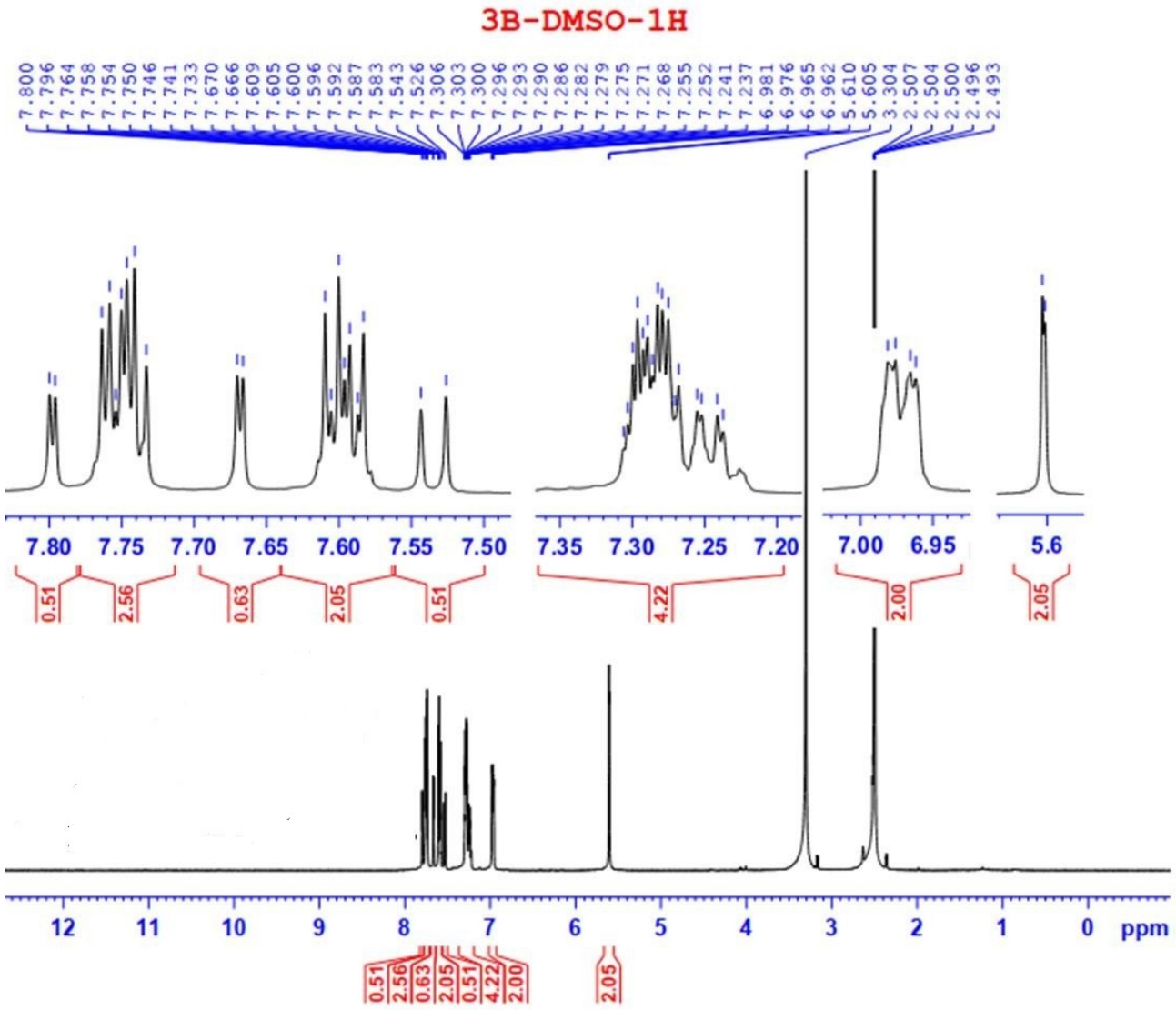
3.08
4.13
1.33
2.16
2.16
6.20
4.08
4.15

Compound 3k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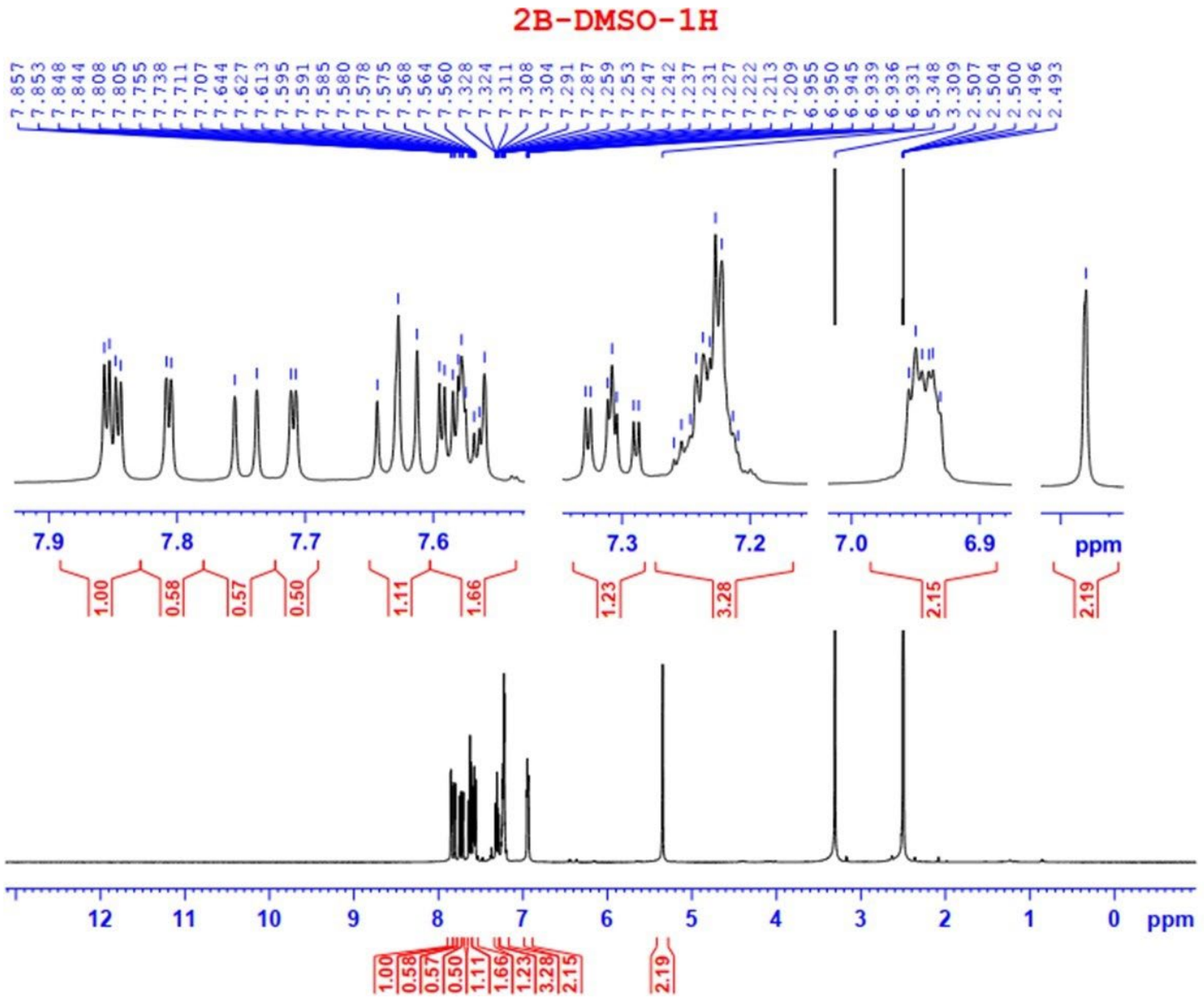
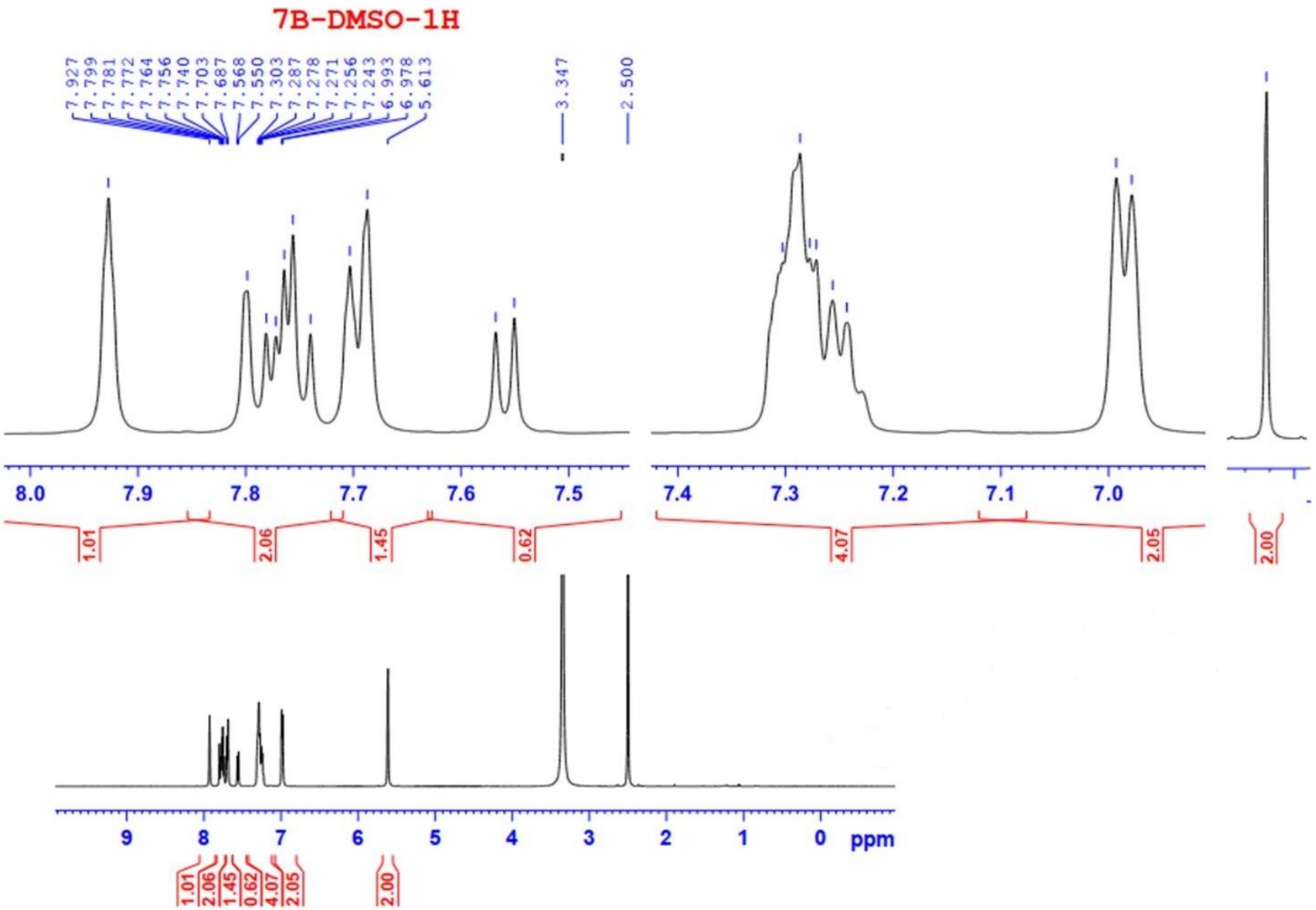
7.796
7.764
7.758
7.754
7.750
7.746
7.741
7.733
7.670
7.666
7.609
7.605
7.600
7.596
7.592
7.587
7.583
7.543
7.526
7.306
7.303
7.300
7.296
7.293
7.290
7.286
7.282
7.279
7.275
7.271
7.268
7.255
7.252
7.241
7.237
6.981
6.976
6.965
6.962
5.610
5.605
3.304
2.507
2.504
2.500
2.496
2.493
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.35
7.30
7.25
7.20
7.00
6.95
5.6
0.51
2.56
0.63
2.05
0.51
4.22
2.00
2.05
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.51
2.56
0.63
2.05
0.51
4.22
2.00
2.05

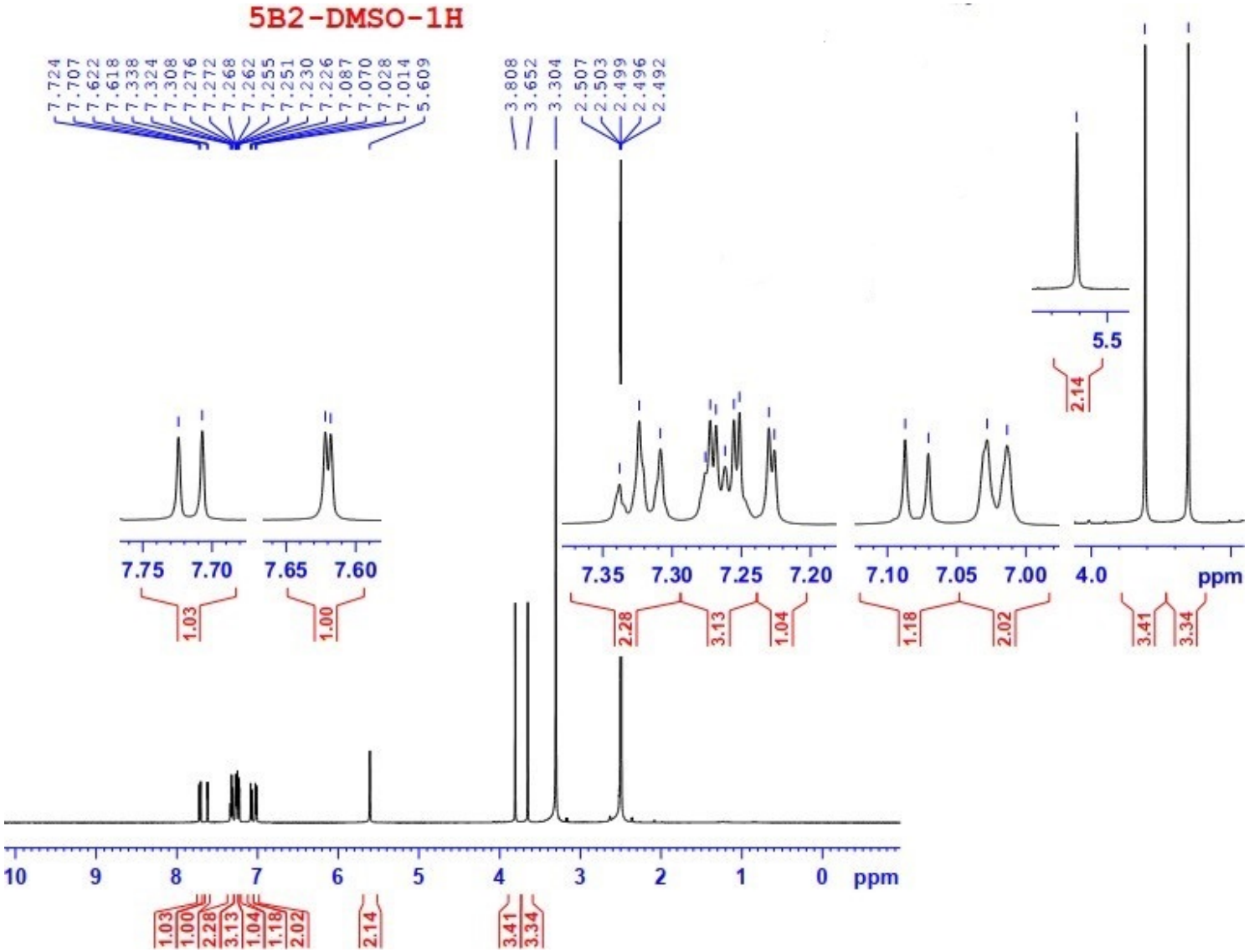
Compound 3l


2B-DMSO-1H
7.857
7.853
7.848
7.844
7.808
7.805
7.755
7.738
7.711
7.707
7.644
7.627
7.613
7.595
7.591
7.585
7.580
7.578
7.575
7.568
7.564
7.560
7.328
7.324
7.311
7.308
7.304
7.291
7.287
7.259
7.253
7.247
7.242
7.237
7.231
7.227
7.222
7.213
7.209
6.955
6.950
6.945
6.939
6.936
6.931
5.348
3.309
2.507
2.504
2.500
2.496
2.493
7.9
7.8
7.7
7.6
7.3
7.2
7.0
6.9
ppm
1.00
0.58
0.57
0.50
1.11
1.66
1.23
3.28
2.15
2.19
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.58
0.57
0.50
1.11
1.66
1.23
3.28
2.15
2.19

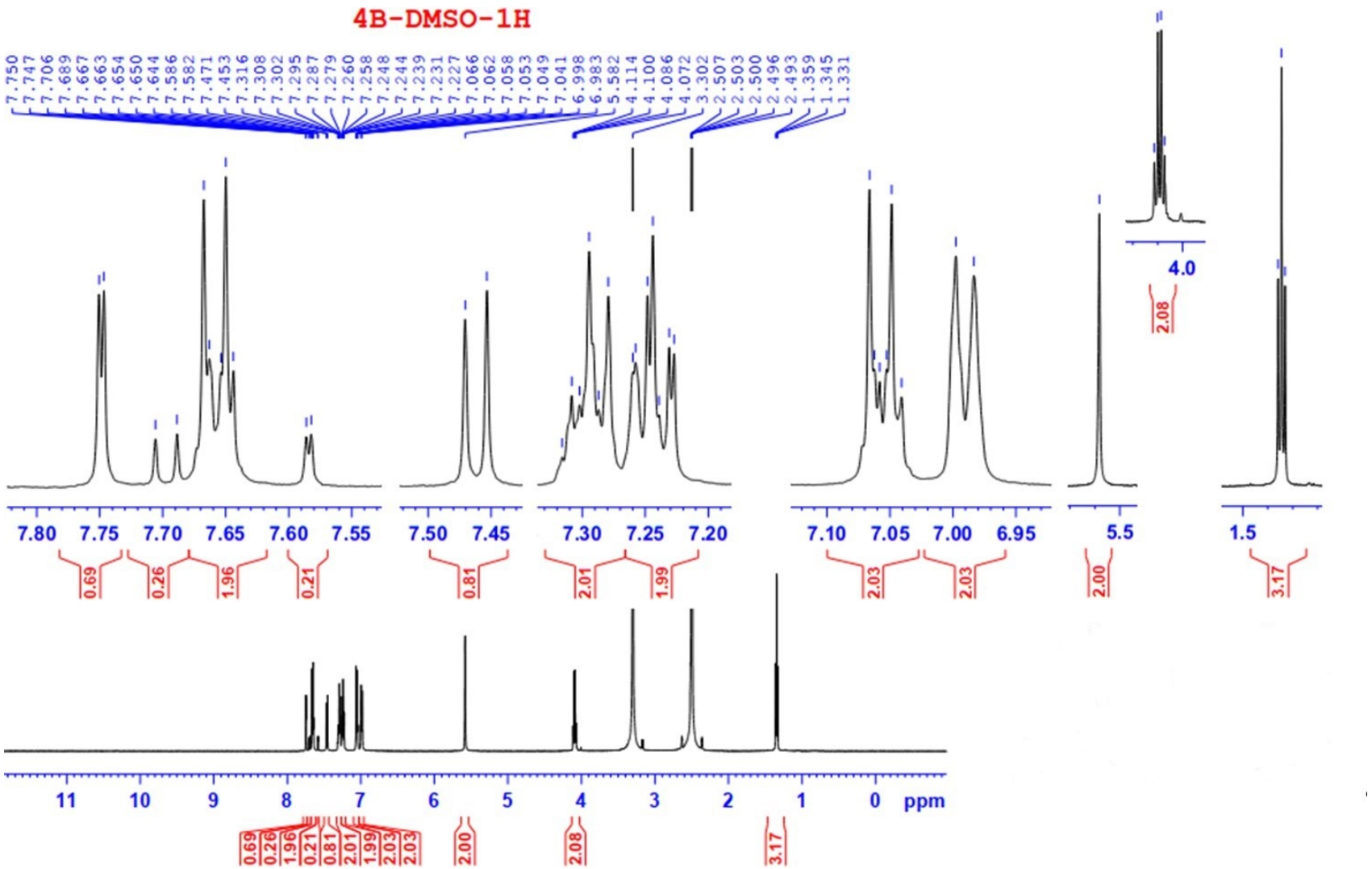
Compound 3m


7B-DMSO-1H
7.927
7.799
7.781
7.772
7.764
7.756
7.740
7.703
7.687
7.568
7.550
7.303
7.287
7.278
7.271
7.256
7.243
6.993
6.978
5.613
3.347
2.500
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
1.01
2.06
1.45
0.62
4.07
2.05
2.00
9
8
7
6
5
4
3
2
1
0
ppm

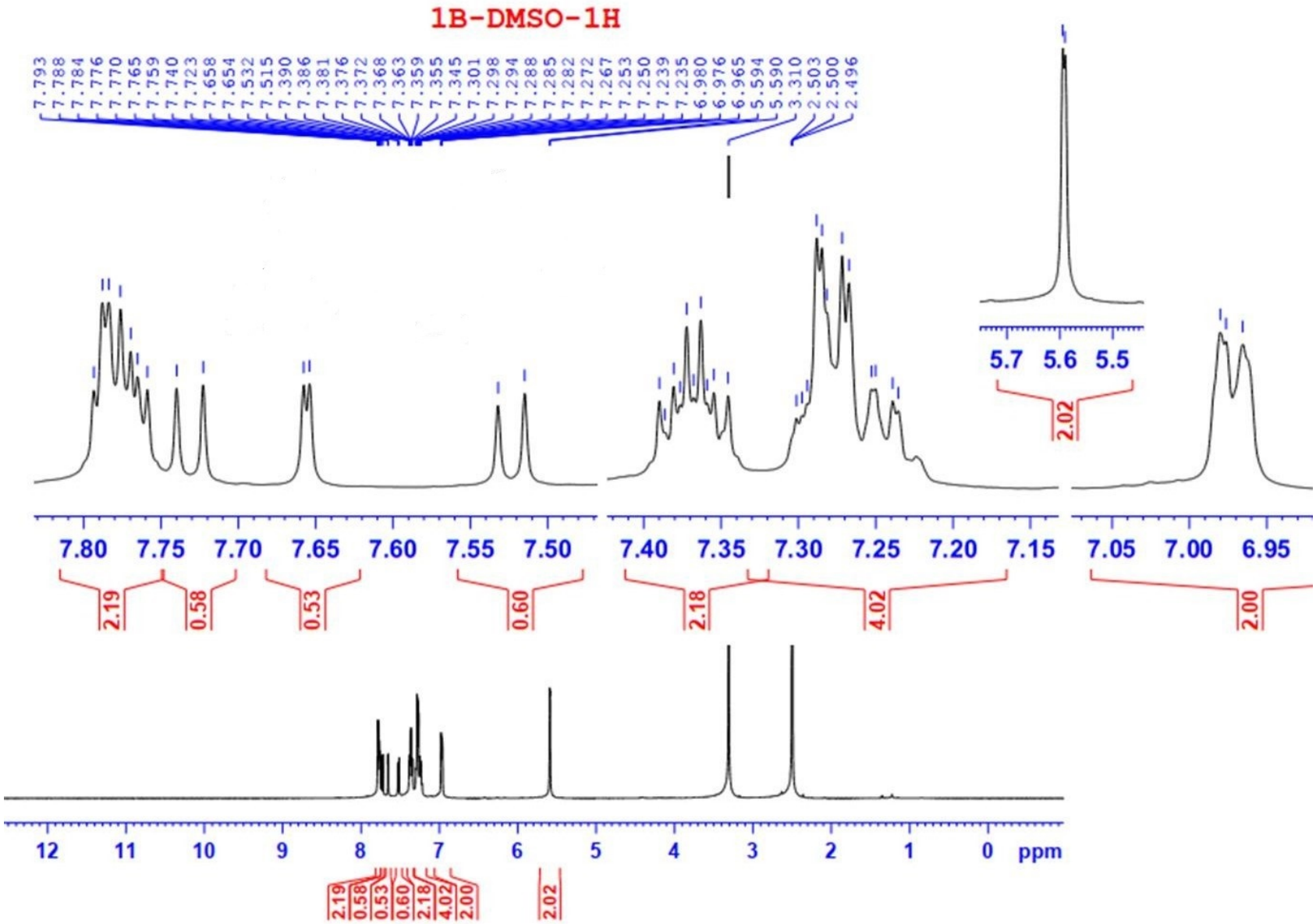
Compound 3n


5B2-DMSO-1H
7.724
7.707
7.622
7.618
7.338
7.324
7.308
7.276
7.272
7.268
7.262
7.255
7.251
7.230
7.226
7.087
7.070
7.028
7.014
5.609
3.808
3.652
3.304
2.507
2.503
2.499
2.496
2.492
7.75
7.70
7.65
7.60
7.35
7.30
7.25
7.20
7.10
7.05
7.00
5.5
4.0
ppm
1.03
1.00
2.28
3.13
1.04
1.18
2.02
2.14
3.41
3.34
10
9
8
7
6
5
4
3
2
1
0
ppm

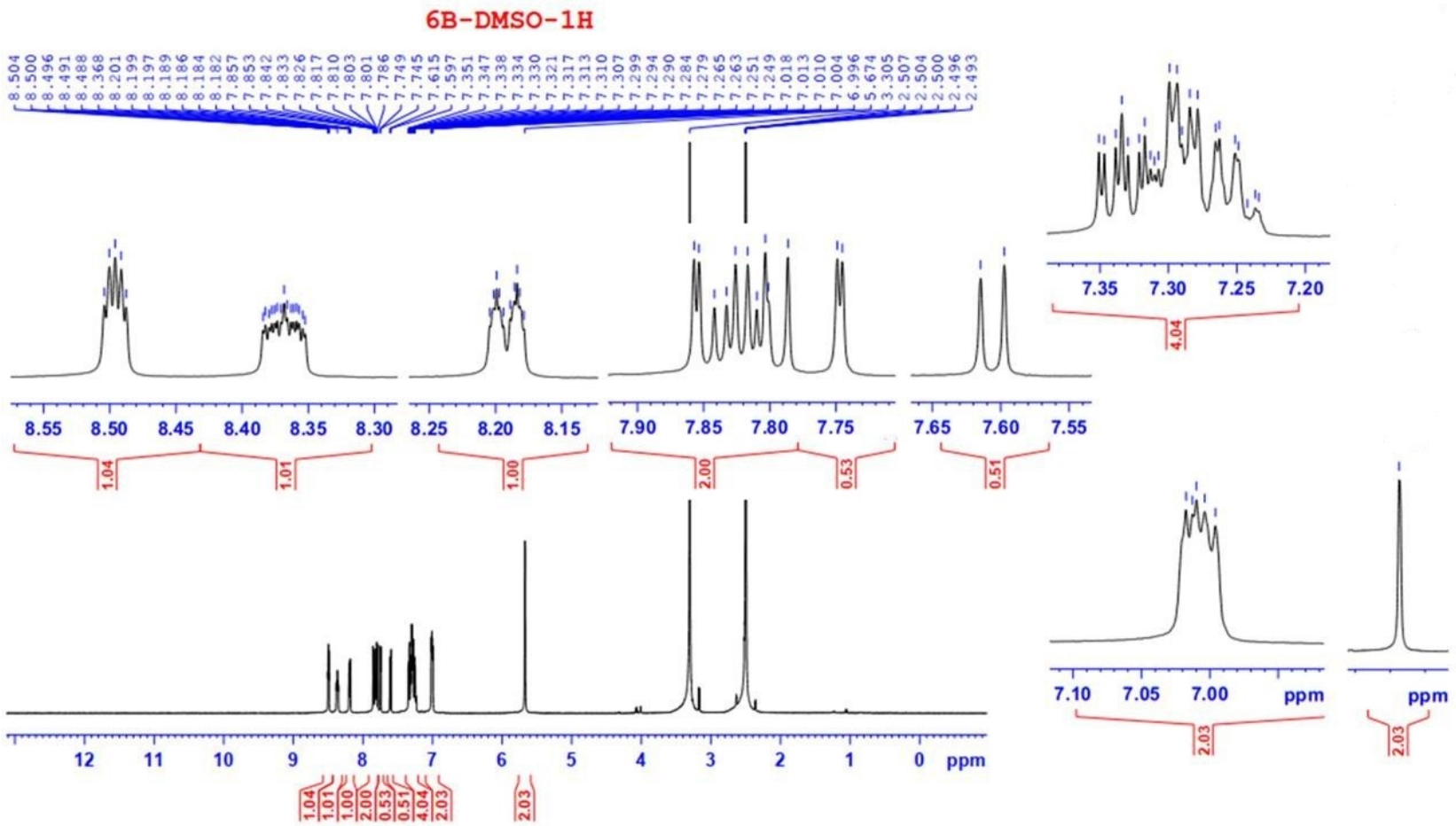
Compound 3o


4B-DMSO-1H
7.750
7.747
7.706
7.689
7.667
7.663
7.654
7.650
7.644
7.586
7.582
7.471
7.453
7.316
7.308
7.302
7.295
7.287
7.279
7.260
7.258
7.248
7.244
7.239
7.231
7.227
7.066
7.062
7.058
7.053
7.049
7.041
6.998
6.983
5.582
4.114
4.100
4.086
4.072
3.302
2.507
2.503
2.500
2.496
2.493
1.359
1.345
1.331
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.30
7.25
7.20
7.10
7.05
7.00
6.95
5.5
4.0
1.5
0.69
0.26
1.96
0.21
0.81
2.01
1.99
2.03
2.03
2.00
2.08
3.17
11
10
9
8
7
6
5
4
3
2
1
0
ppm

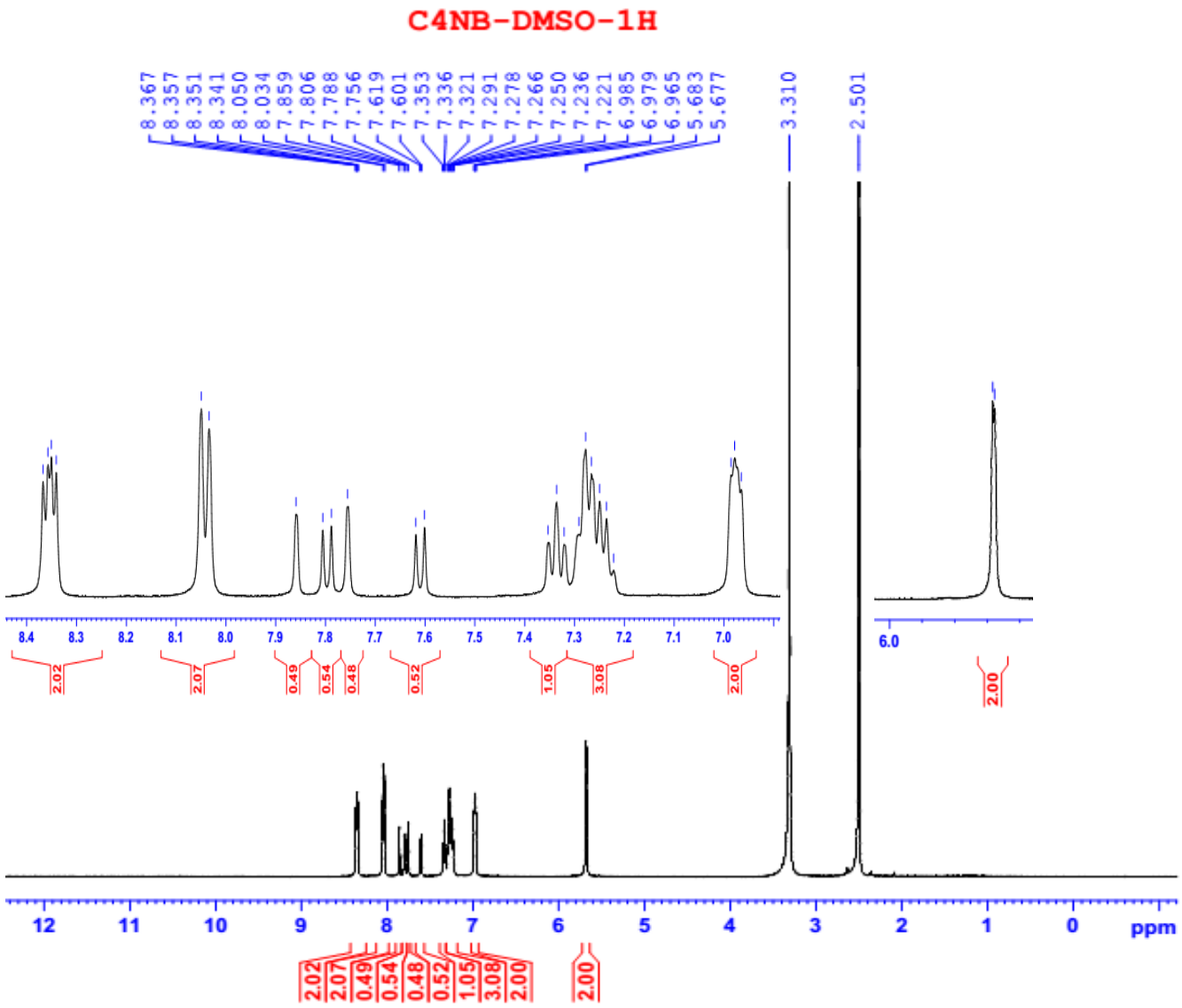
Compound 3p


1B-DMSO-1H
7.793
7.788
7.784
7.776
7.770
7.765
7.759
7.740
7.723
7.658
7.654
7.532
7.515
7.390
7.386
7.381
7.376
7.372
7.368
7.363
7.359
7.355
7.345
7.301
7.298
7.294
7.288
7.285
7.282
7.272
7.267
7.253
7.250
7.239
7.235
6.980
6.976
6.965
5.594
5.590
3.310
2.503
2.500
2.496
5.7 5.6 5.5
2.02
7.80 7.75 7.70 7.65 7.60 7.55 7.50
7.40 7.35 7.30 7.25 7.20 7.15
7.05 7.00 6.95
2.19 0.58 0.53 0.60 2.18 4.02 2.00
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.19 0.58 0.53 0.60 2.18 4.02 2.00 2.02

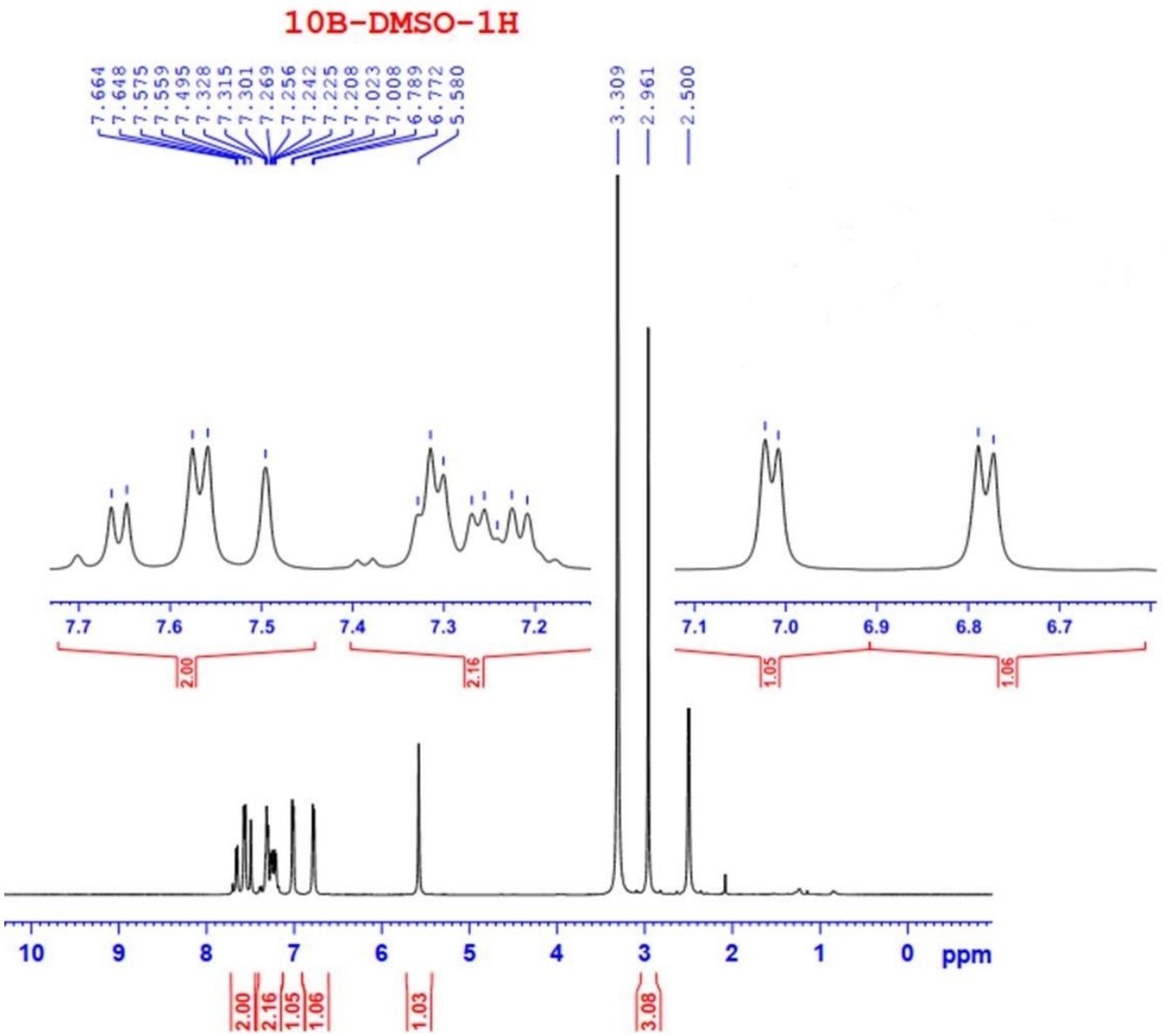
Compound 3q


6B-DMSO-1H
8.504
8.500
8.496
8.491
8.488
8.368
8.201
8.199
8.197
8.189
8.186
8.184
8.182
7.857
7.853
7.842
7.833
7.826
7.817
7.810
7.803
7.801
7.786
7.749
7.745
7.615
7.597
7.351
7.347
7.338
7.334
7.330
7.321
7.317
7.313
7.310
7.307
7.299
7.294
7.290
7.284
7.279
7.265
7.263
7.251
7.249
7.018
7.013
7.010
7.004
6.996
5.674
3.305
2.507
2.504
2.500
2.496
2.493
8.55 8.50 8.45 8.40 8.35 8.30 8.25 8.20 8.15 7.90 7.85 7.80 7.75 7.65 7.60 7.55
1.04 1.01 1.00 2.00 0.53 0.51
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.04 1.01 1.00 2.00 0.53 0.51 4.04 2.03
2.03
7.35 7.30 7.25 7.20
4.04
7.10 7.05 7.00 ppm
2.03
ppm
2.03

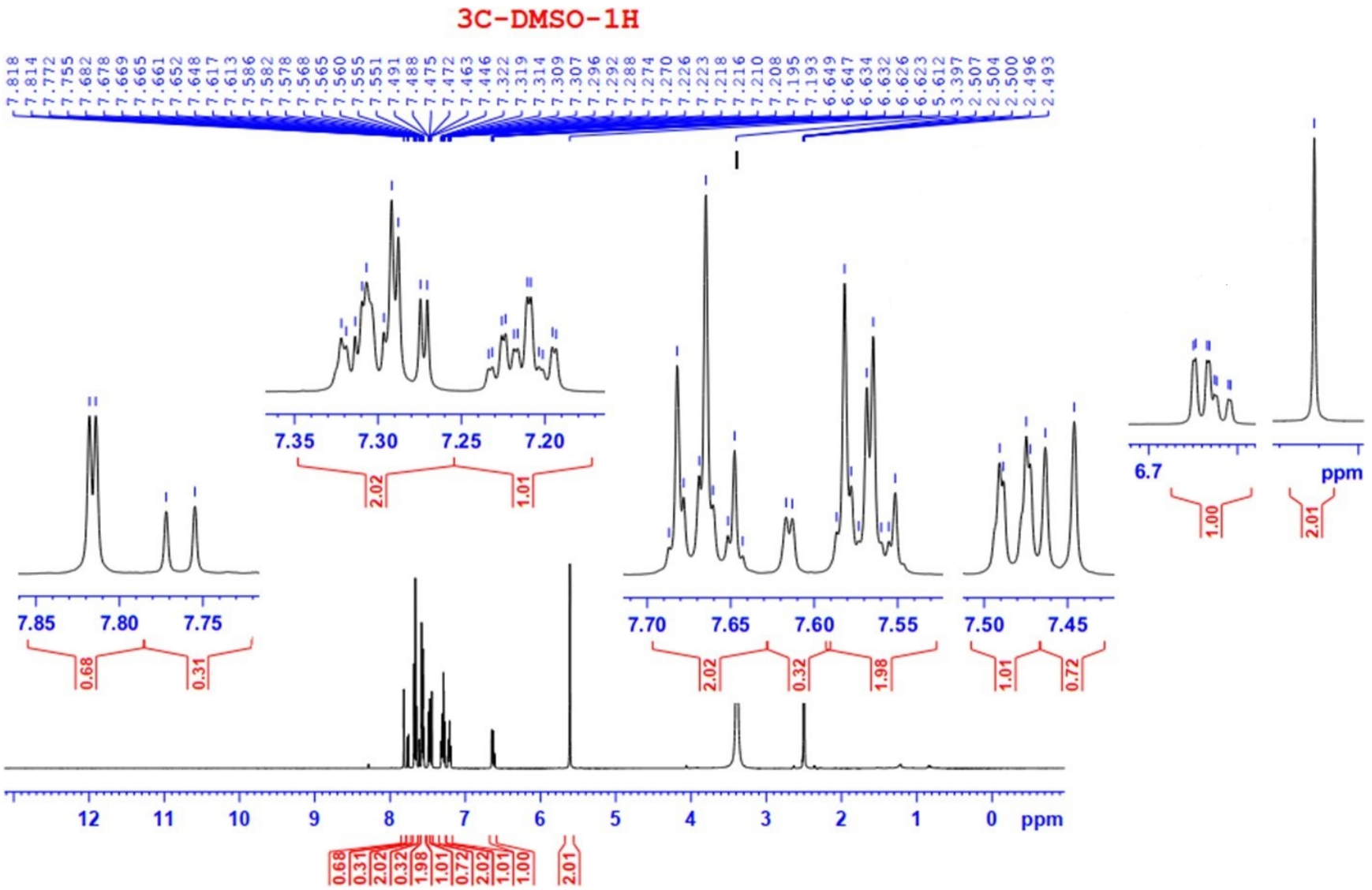
Compound 3r


C4NB-DMSO-1H
8.367
8.357
8.351
8.341
8.050
8.034
7.859
7.806
7.788
7.756
7.619
7.601
7.353
7.336
7.321
7.291
7.278
7.266
7.250
7.236
7.221
6.985
6.979
6.965
5.683
5.677
3.310
2.501
ppm

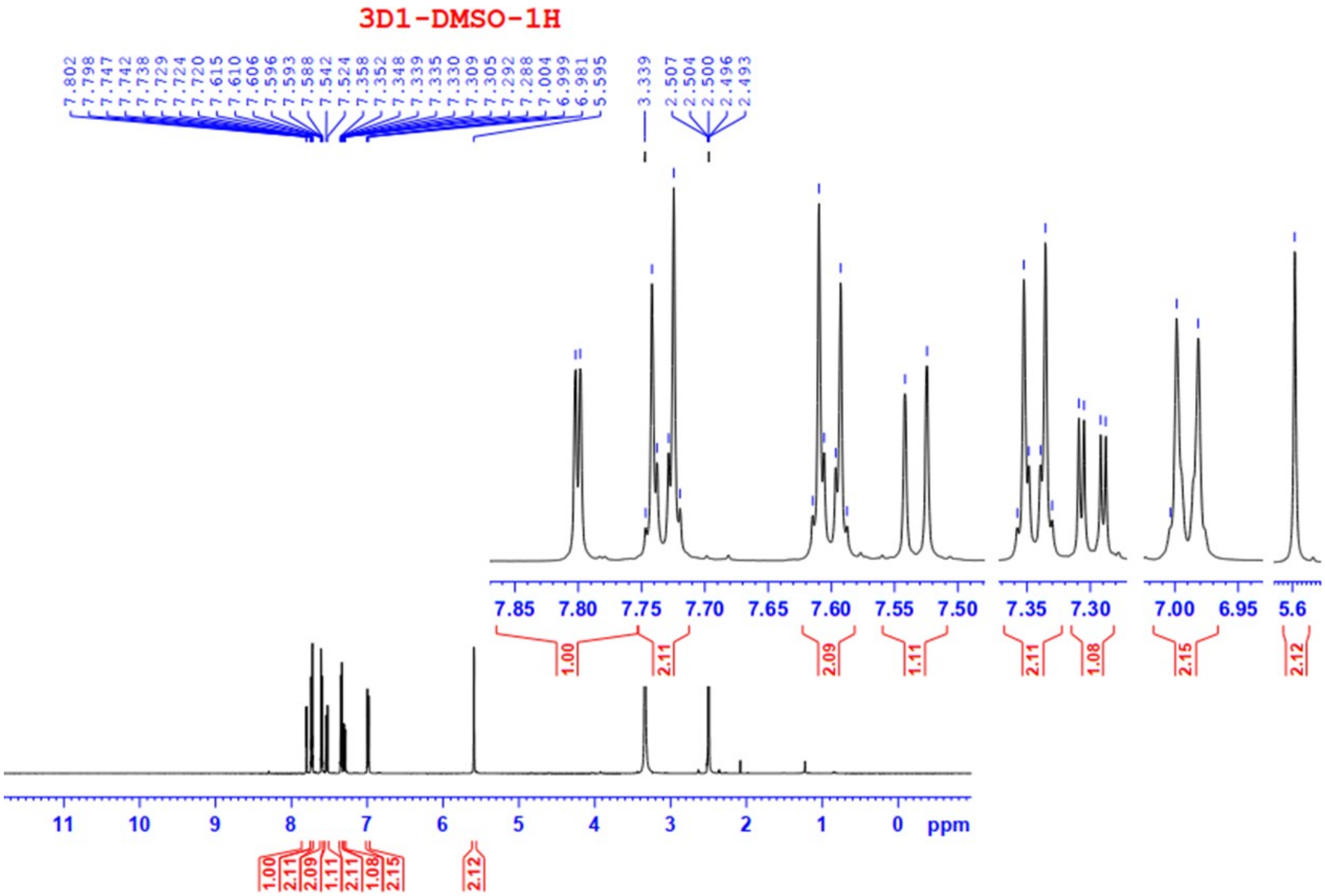
Compound 3s


10B-DMSO-1H
7.664
7.648
7.575
7.559
7.495
7.328
7.315
7.301
7.269
7.256
7.242
7.225
7.208
7.023
7.008
6.789
6.772
5.580
3.309
2.961
2.500
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
2.00
2.16
1.05
1.06
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.16
1.05
1.06
1.03
3.08

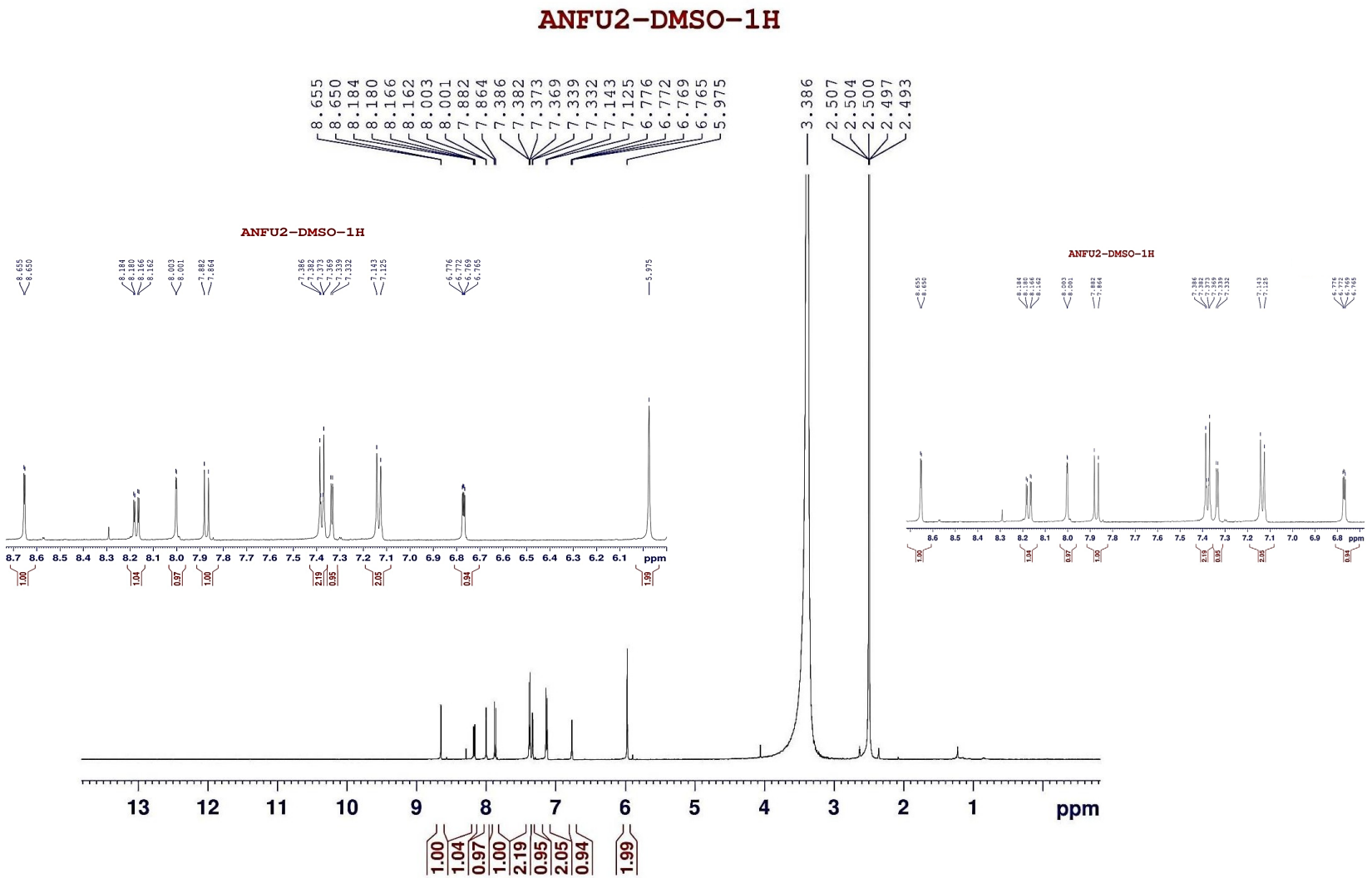
Compound 3t


3C-DMSO-1H
7.818
7.814
7.772
7.755
7.682
7.678
7.669
7.665
7.661
7.652
7.648
7.617
7.613
7.586
7.582
7.578
7.568
7.565
7.560
7.555
7.551
7.491
7.488
7.475
7.472
7.463
7.446
7.322
7.319
7.314
7.309
7.307
7.296
7.292
7.288
7.274
7.270
7.226
7.223
7.218
7.216
7.210
7.208
7.195
7.193
6.649
6.647
6.634
6.632
6.626
6.623
5.612
3.397
2.507
2.504
2.500
2.496
2.493
7.35
7.30
7.25
7.20
2.02
1.01
7.85
7.80
7.75
0.68
0.31
7.70
7.65
7.60
7.55
2.02
0.32
1.98
7.50
7.45
1.01
0.72
6.7
1.00
2.01
ppm
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.68
0.31
2.02
0.32
1.98
1.01
0.72
2.02
1.01
1.00
2.01

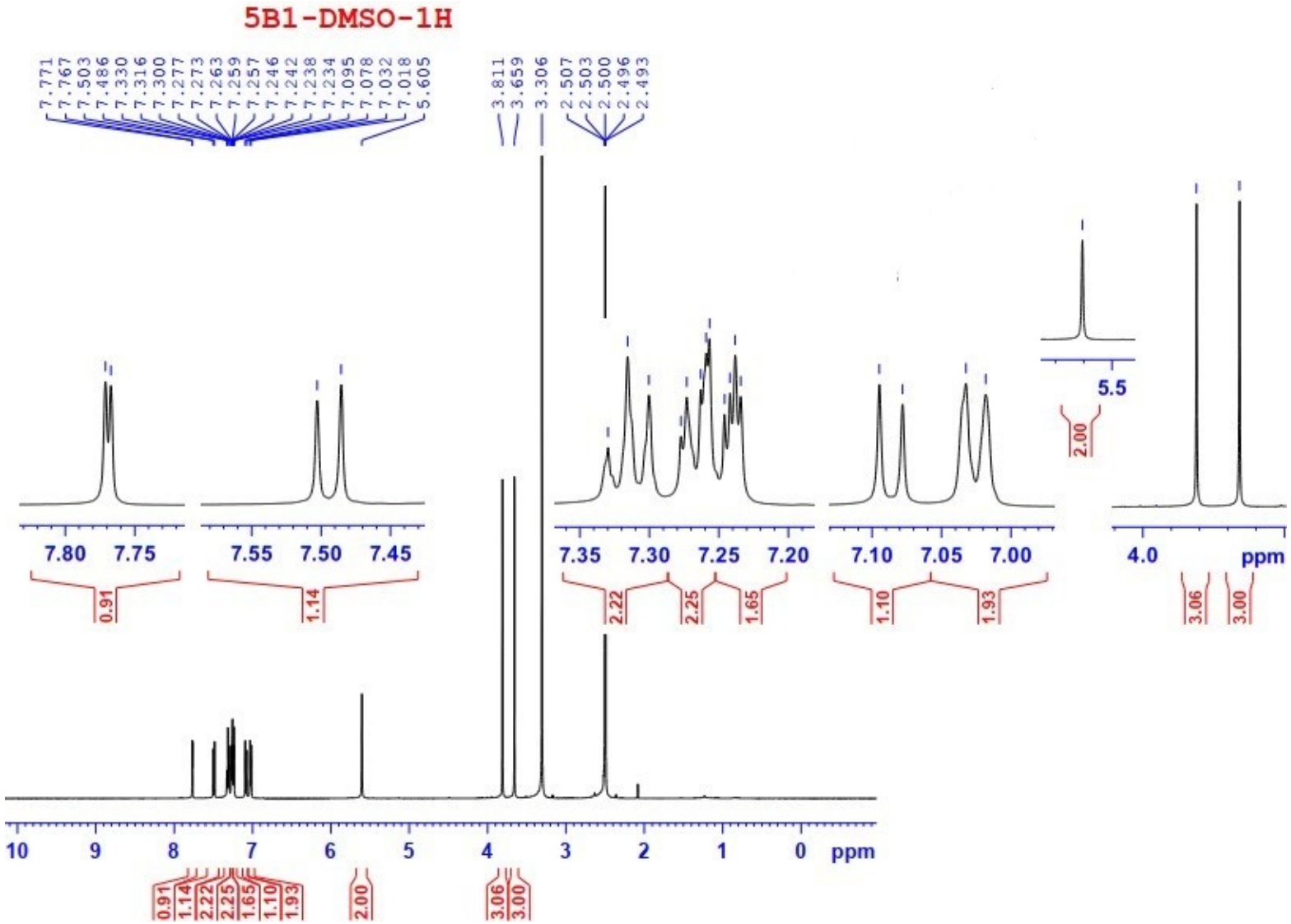
Compound 3u


3D1-DMSO-1H
7.802
7.798
7.747
7.742
7.738
7.729
7.724
7.720
7.615
7.610
7.606
7.596
7.593
7.588
7.542
7.524
7.358
7.352
7.348
7.339
7.335
7.330
7.309
7.305
7.292
7.288
7.004
6.999
6.981
5.595
3.339
2.507
2.504
2.500
2.496
2.493
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.35
7.30
7.00
6.95
5.6
1.00
2.11
2.09
1.11
2.11
1.08
2.15
2.12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

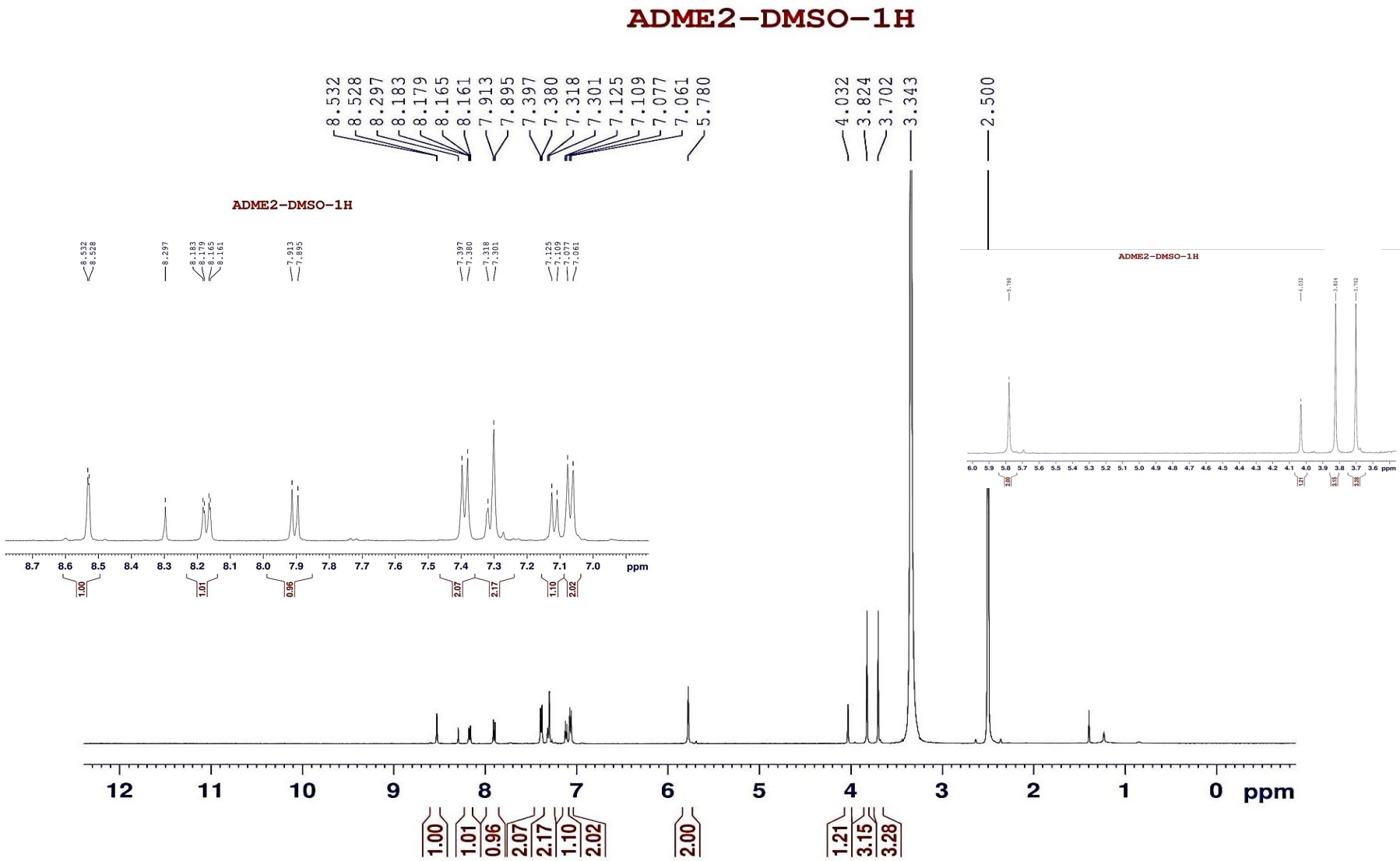
Compound 3v


ANFU2-DMSO-1H
8.655
8.650
8.184
8.180
8.166
8.162
8.003
8.001
7.882
7.864
7.386
7.382
7.373
7.369
7.339
7.332
7.143
7.125
6.776
6.772
6.769
6.765
5.975
3.386
2.507
2.504
2.500
2.497
2.493
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.04 0.97 1.00 2.19 0.95 2.05 0.94 1.99

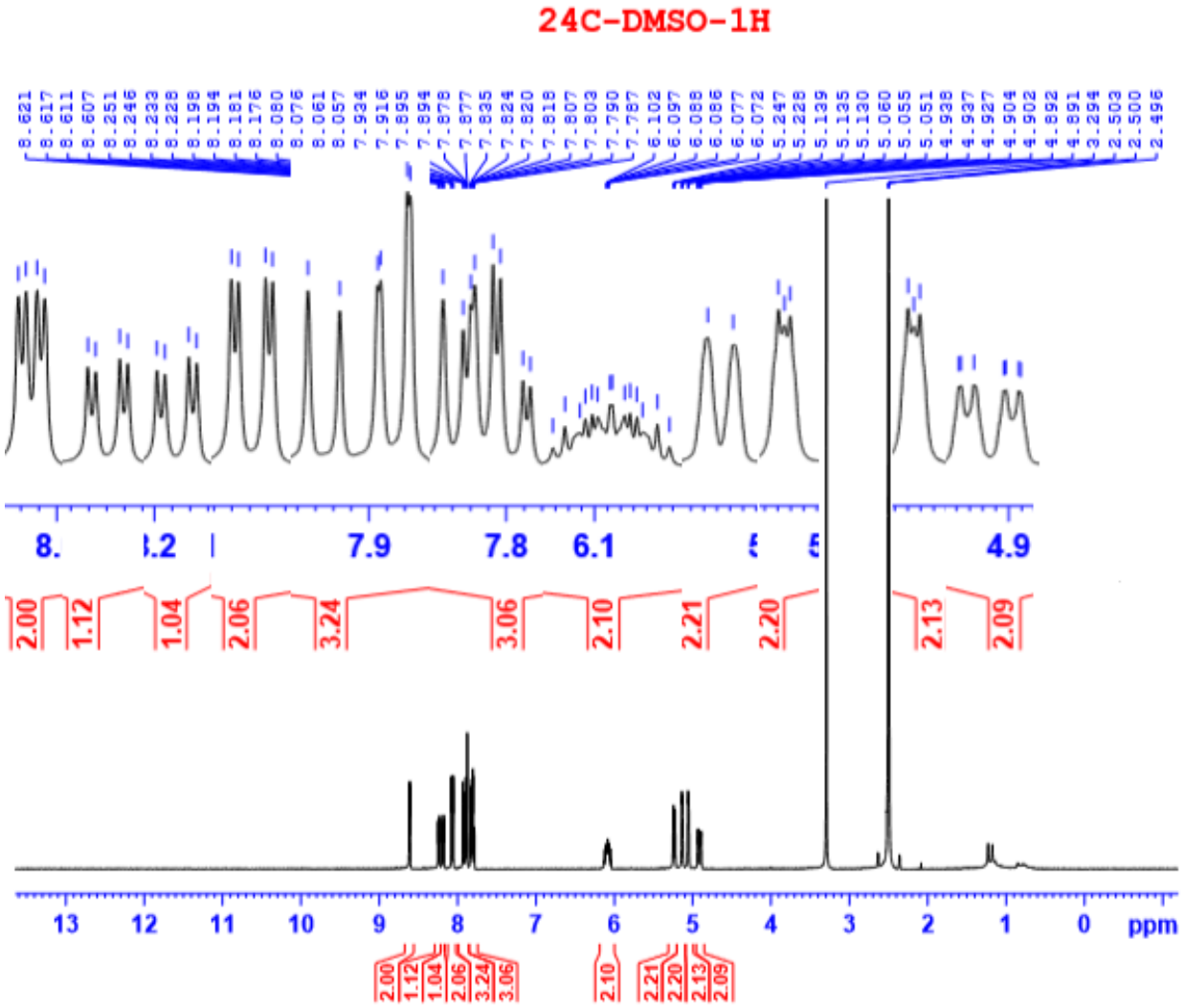
Compound 3w


5B1-DMSO-1H
7.771
7.767
7.503
7.486
7.330
7.316
7.300
7.277
7.273
7.263
7.259
7.257
7.246
7.242
7.238
7.234
7.095
7.078
7.032
7.018
5.605
3.811
3.659
3.306
2.507
2.503
2.500
2.496
2.493
7.80
7.75
7.55
7.50
7.45
7.35
7.30
7.25
7.20
7.10
7.05
7.00
5.5
4.0
ppm
10
9
8
7
6
5
4
3
2
1
0
ppm
0.91
1.14
2.22
2.25
1.65
1.10
1.93
2.00
3.06
3.00

Compound 3x

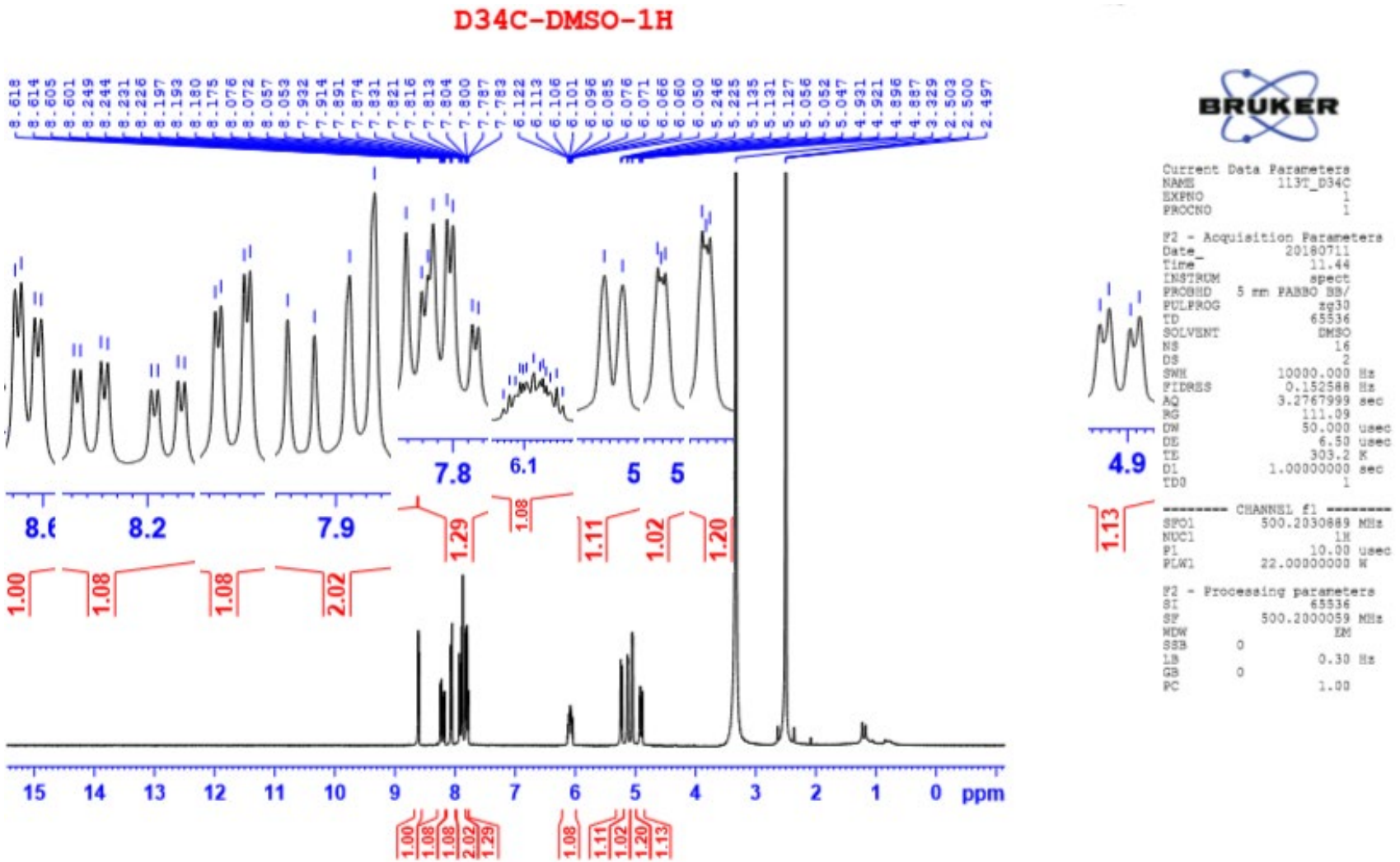

ADME2-DMSO-1H
8.532
8.528
8.297
8.183
8.179
8.165
8.161
7.913
7.895
7.397
7.380
7.318
7.301
7.125
7.109
7.077
7.061
5.780
4.032
3.824
3.702
3.343
2.500
ppm
1.00
1.01
0.96
2.07
2.17
1.10
2.02
2.00
1.21
3.15
3.28

Compound 4a




```
Current Data Parameters
NAME                  1137_24C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180627
Time                     11.19
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                  DMSO
NS                         16
DS                          2
SWH                 10000.000 Hz
FIDRES                  0.152588 Hz
AQ                  3.2767999 sec
RG                       175.34
DW                       50.000 usec
DE                        6.50 usec
TE                       304.0 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                500.2030889 MHz
NUC1                        1H
P1                       10.00 usec
PLW1                22.00000000 W

F2 - Processing parameters
SI                      65536
SF                  500.2000053 MHz
WDW                        EM
SSB                 0
LB                       0.30 Hz
GB                  0
PC                       1.00
```

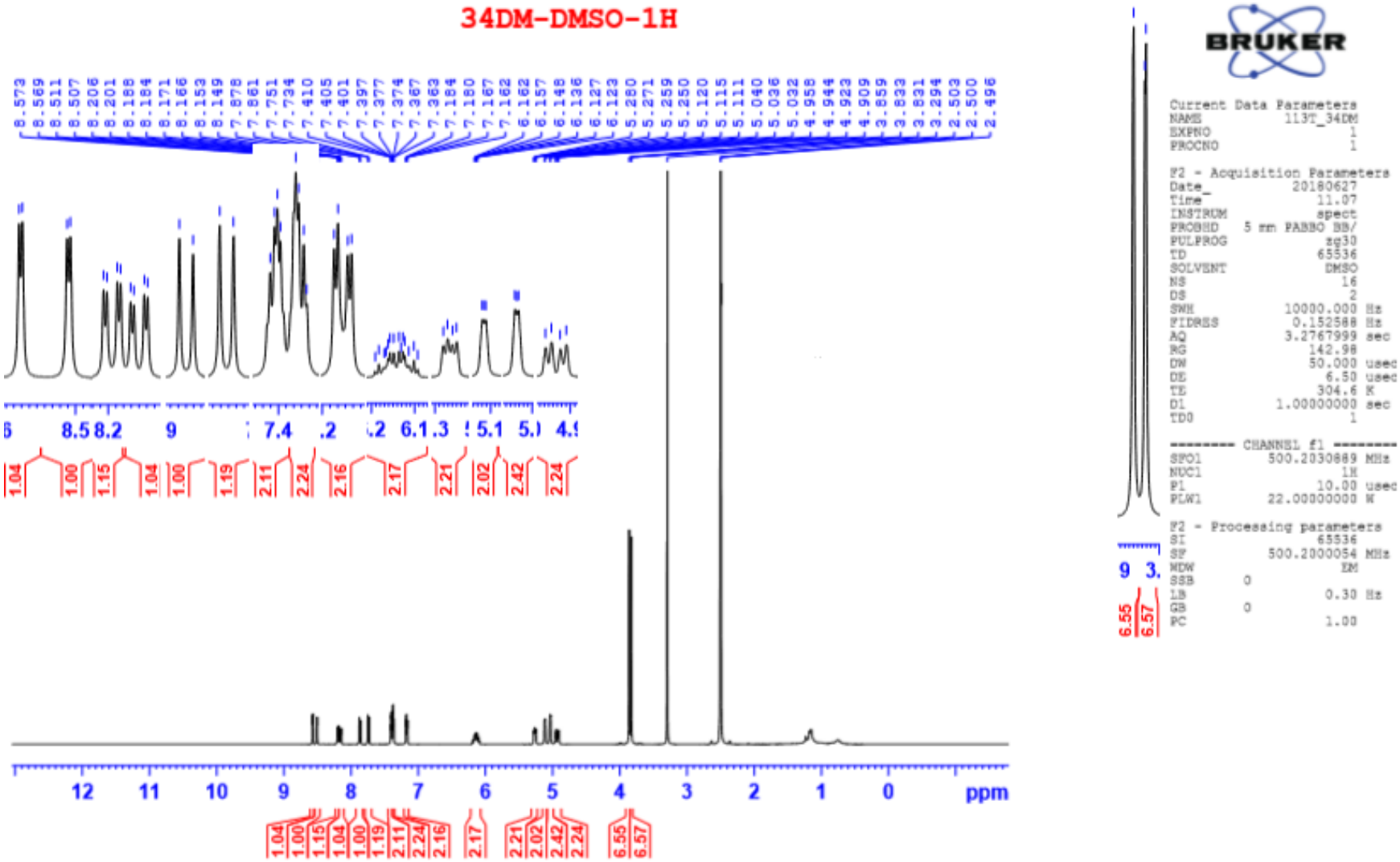
Compound 4b



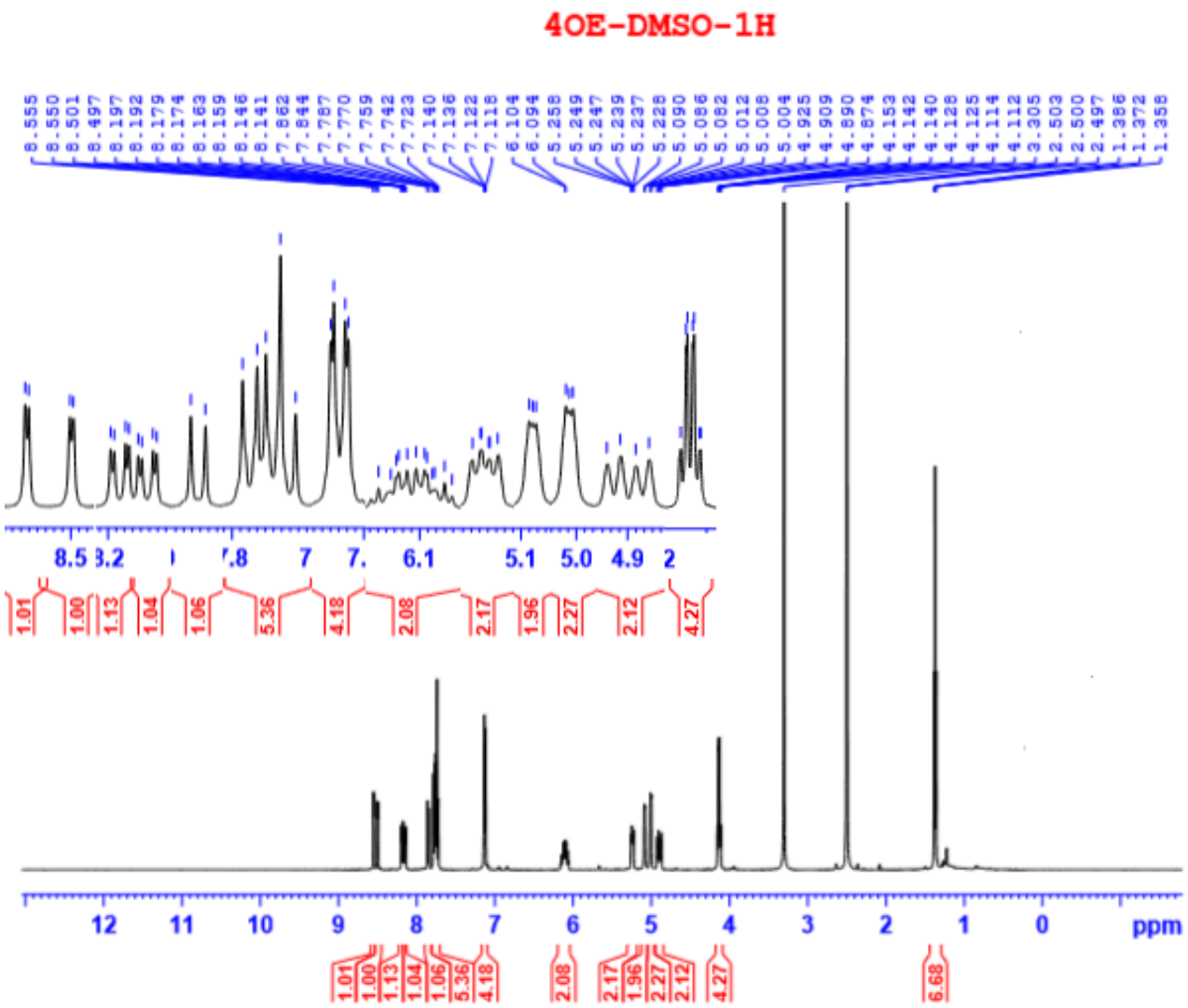
BRUKER

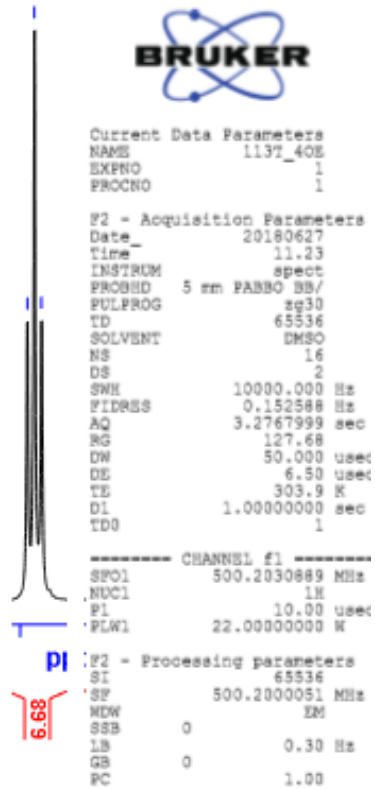
```
Current Data Parameters
NAME                  113T_D34C
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20180711
Time                      11.44
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                   DMSO
NS                           16
DS                            2
SWH                   10000.000 Hz
FIDRES                0.152588 Hz
AQ                    3.2767999 sec
RG                       111.09
DW                       50.000 usec
DE                         6.50 usec
TE                        303.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                500.2030689 MHz
NUC1                        1H
P1                        10.00 usec
PLW1                22.00000000 W

F2 - Processing parameters
SI                        65536
SF                  500.2000059 MHz
WDW                          EM
SSB                       0
LB                        0.30 Hz
GB                        0
PC                        1.00
```

Compound 4c

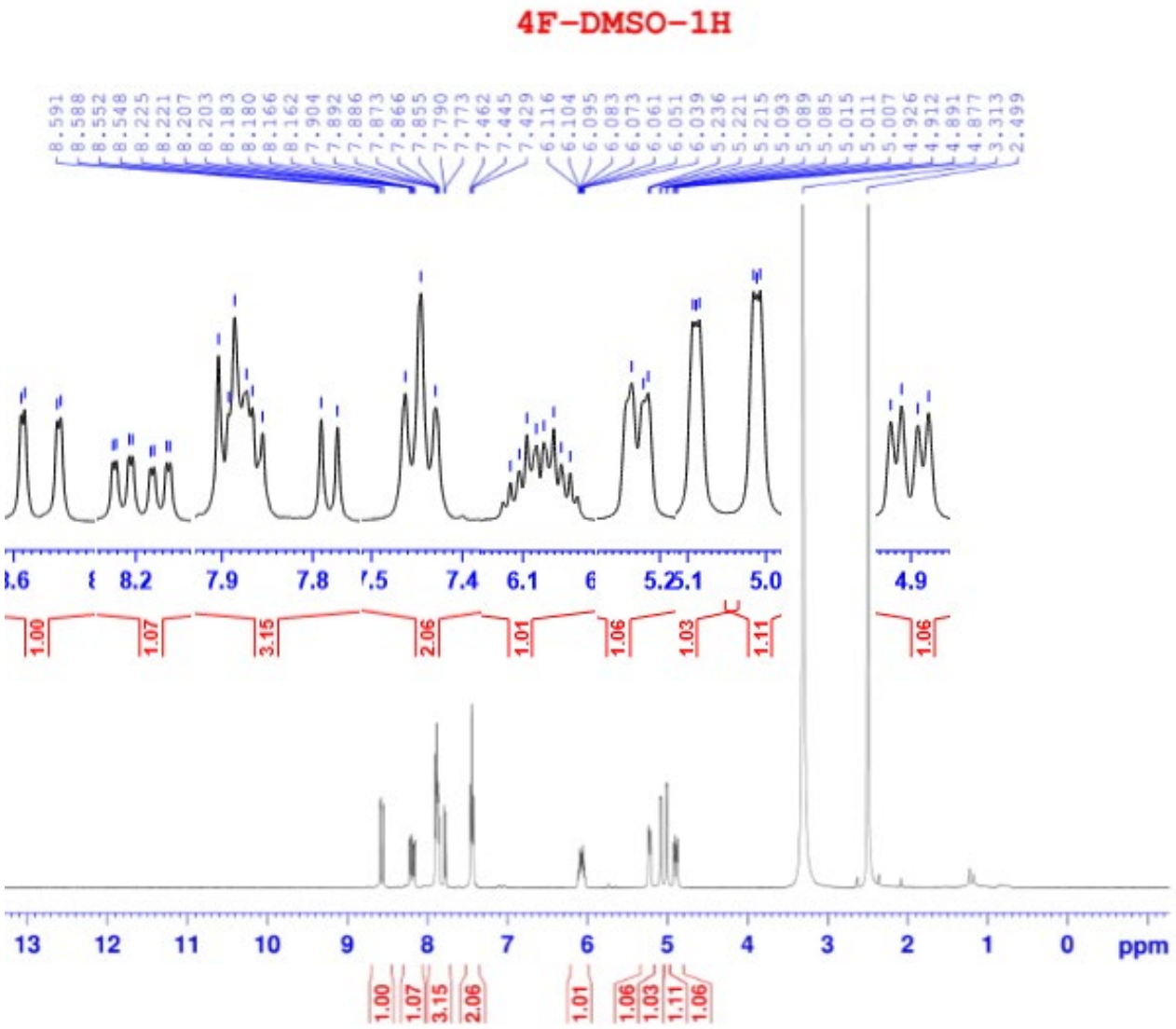

34DM-DMSO-1H
BRUKER
Current Data Parameters
NAME 113T_34DM
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180627
Time 11.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 142.98
DW 50.000 usec
DE 6.50 usec
TE 304.6 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 500.2030889 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.00000000 W
F2 - Processing parameters
SI 65536
SF 500.2000054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

Compound 4d


4OE-DMSO-1H
8.555 8.550 8.501 8.497 8.197 8.192 8.179 8.174 8.163 8.159 8.146 8.141 7.862 7.844 7.787 7.770 7.759 7.742 7.723 7.140 7.136 7.122 7.118 6.104 6.094 5.258 5.249 5.247 5.239 5.237 5.228 5.090 5.086 5.082 5.012 5.008 5.004 4.925 4.909 4.890 4.874 4.153 4.142 4.140 4.128 4.125 4.114 4.112 3.305 2.503 2.500 2.497 1.386 1.372 1.358
8.5 8.2 7.8 7 7. 6.1 5.1 5.0 4.9 2
1.01 1.00 1.13 1.04 1.06 5.36 4.18 2.08 2.17 1.96 2.27 2.12 4.27
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.01 1.00 1.13 1.04 1.06 5.36 4.18 2.08 2.17 1.96 2.27 2.12 4.27 6.68


BRUKER
Current Data Parameters
NAME 1137_4OE
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180627
Time 11.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 127.68
DW 50.000 usec
DE 6.50 usec
TE 303.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.2030889 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.00000000 W
F2 - Processing parameters
SI 65536
SF 500.2000051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
pl
6.68

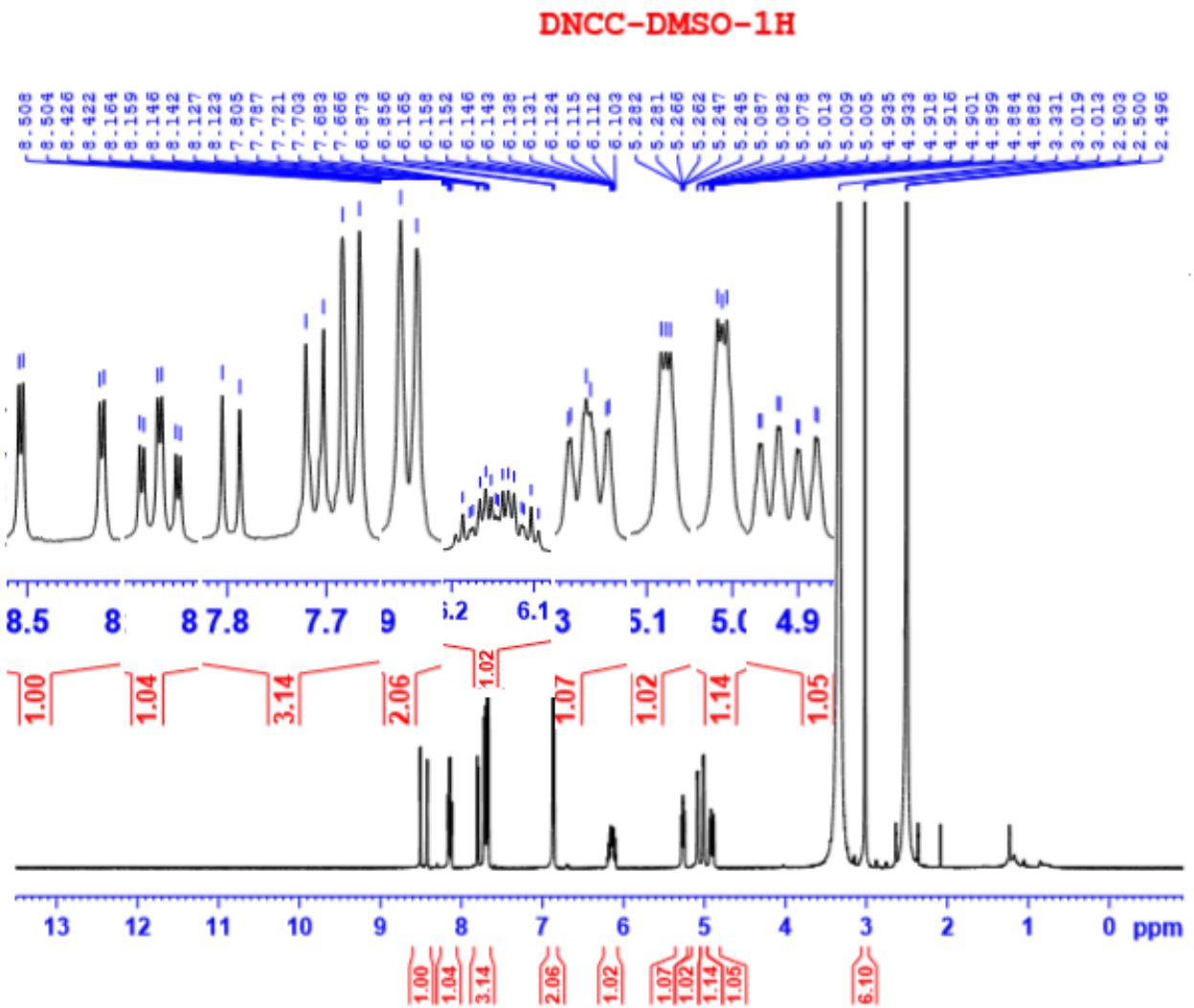
Compound 4e



BRUKER

```
Current Data Parameters
NAME                  113T_4F
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20180627
Time                  10.39
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ             3.2767999 sec
RG                   97.76
DW                 50.000 usec
DE                  6.50 usec
TE                 309.7 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          500.2030889 MHz
NUC1                    1H
P1                  10.00 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                   65536
SF            500.2000053 MHz
WDW                     EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

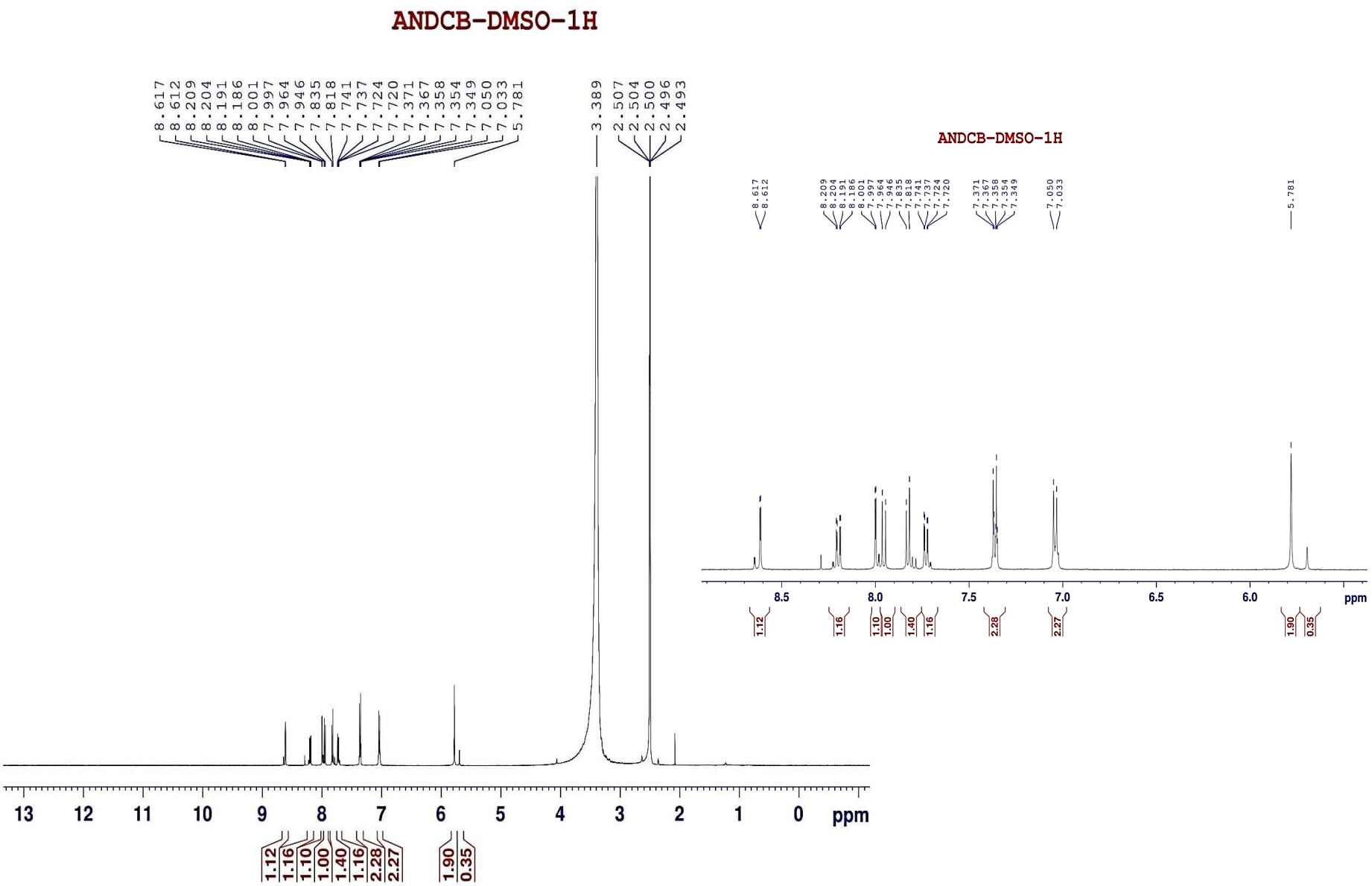
Compound 4f



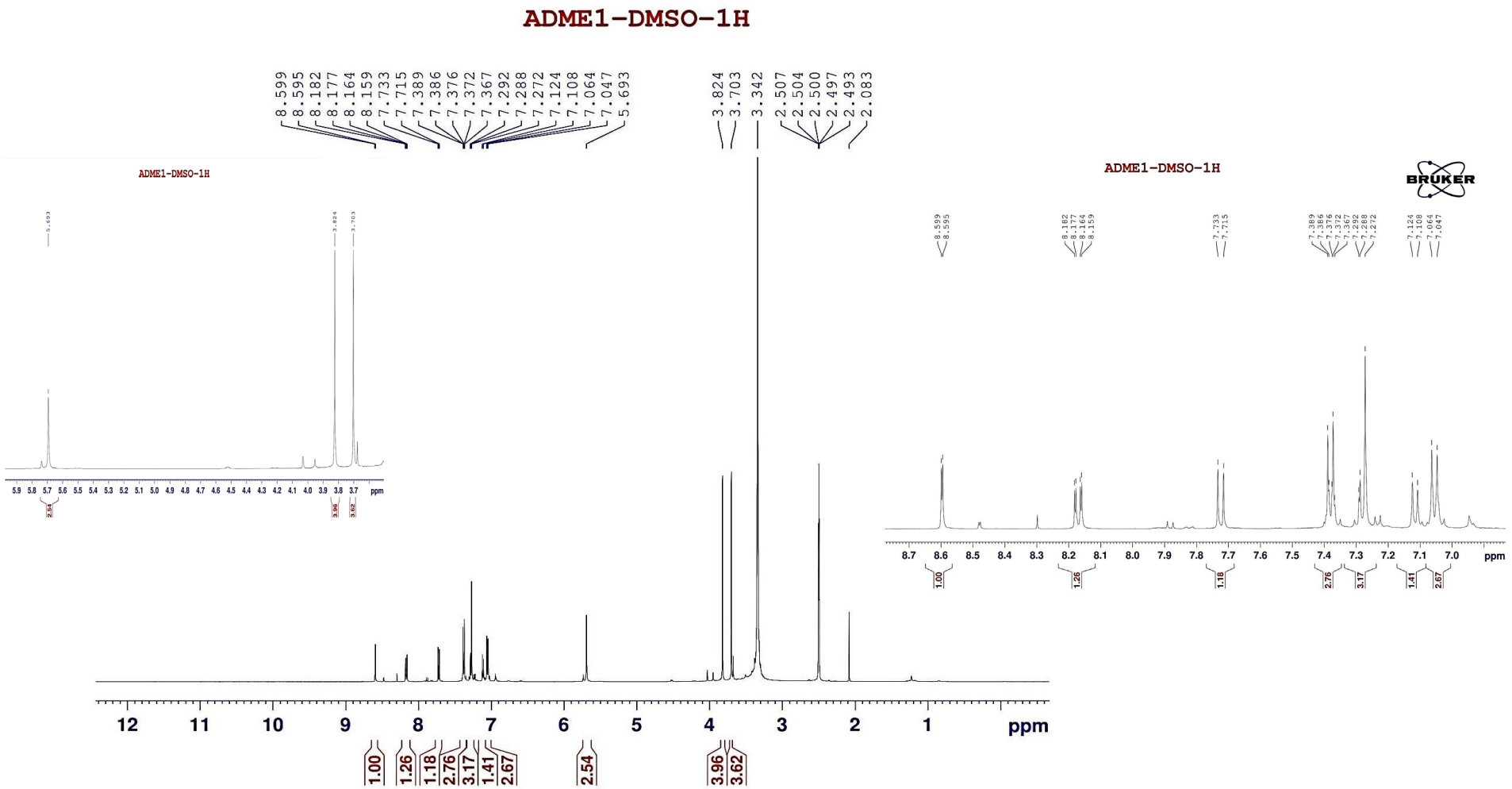
BRUKER

```
Current Data Parameters
NAME                  113T_DNCC
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20180711
Time                      11.48
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                  10000.000 Hz
FIDRES                0.152588 Hz
AQ                    3.2767999 sec
RG                       111.09
DW                       50.000 usec
DE                         6.50 usec
TE                        303.3 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                500.2030889 MHz
NUC1                        1H
P1                       10.00 usec
PLW1                22.00000000 W

F2 - Processing parameters
SI                        65536
SF                  500.2000054 MHz
WDW                          EM
SSB                 0
LB                        0.30 Hz
GB                  0
PC                        1.00
```

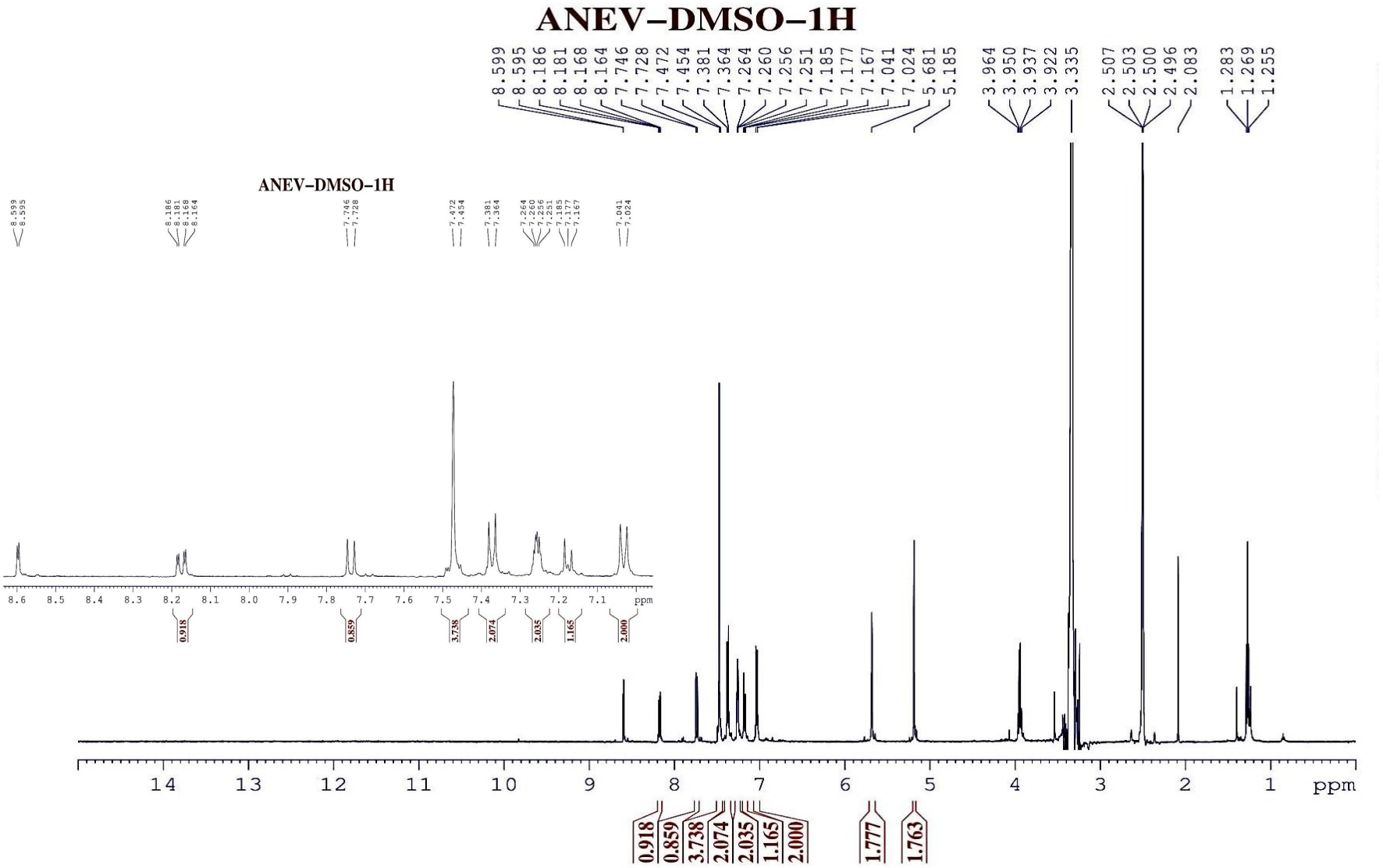
Compound 4g


ANDCB-DMSO-1H
8.617
8.612
8.209
8.204
8.191
8.186
8.001
7.997
7.964
7.946
7.835
7.818
7.741
7.737
7.724
7.720
7.371
7.367
7.358
7.354
7.349
7.050
7.033
5.781
3.389
2.507
2.504
2.500
2.496
2.493
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.12 1.16 1.10 1.00 1.40 1.16 2.28 2.27 1.90 0.35
ANDCB-DMSO-1H
8.5 8.0 7.5 7.0 6.5 6.0 ppm
1.12 1.16 1.10 1.00 1.40 1.16 2.28 2.27 1.90 0.35

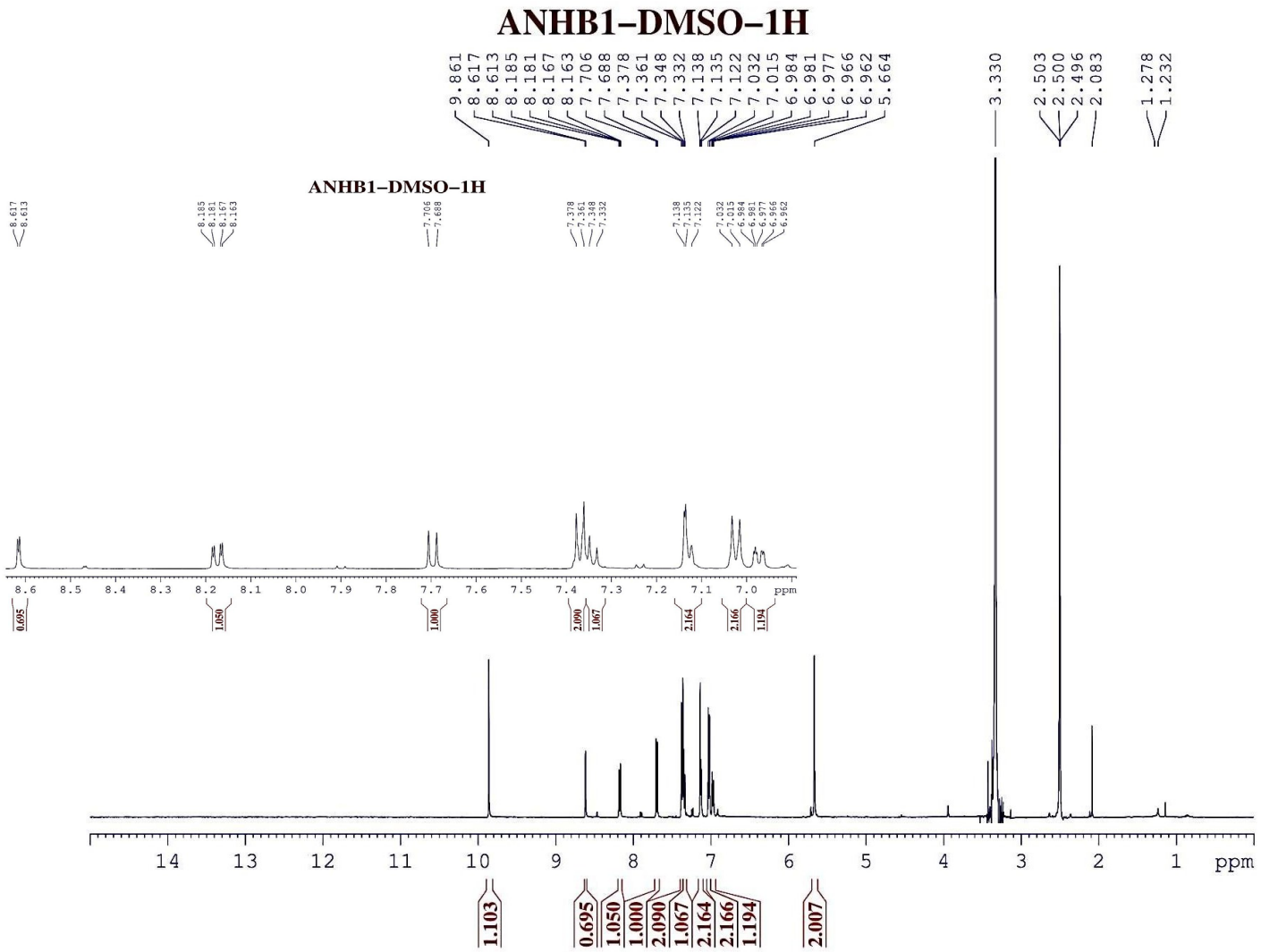
Compound 4h


ADME1-DMSO-1H
8.599
8.595
8.182
8.177
8.164
8.159
7.733
7.715
7.389
7.386
7.376
7.372
7.367
7.292
7.288
7.272
7.124
7.108
7.064
7.047
5.693
3.824
3.703
3.342
2.507
2.504
2.500
2.497
2.493
2.083
ppm
1.00
1.26
1.18
2.76
3.17
1.41
2.67
2.54
3.96
3.62
BRUKER

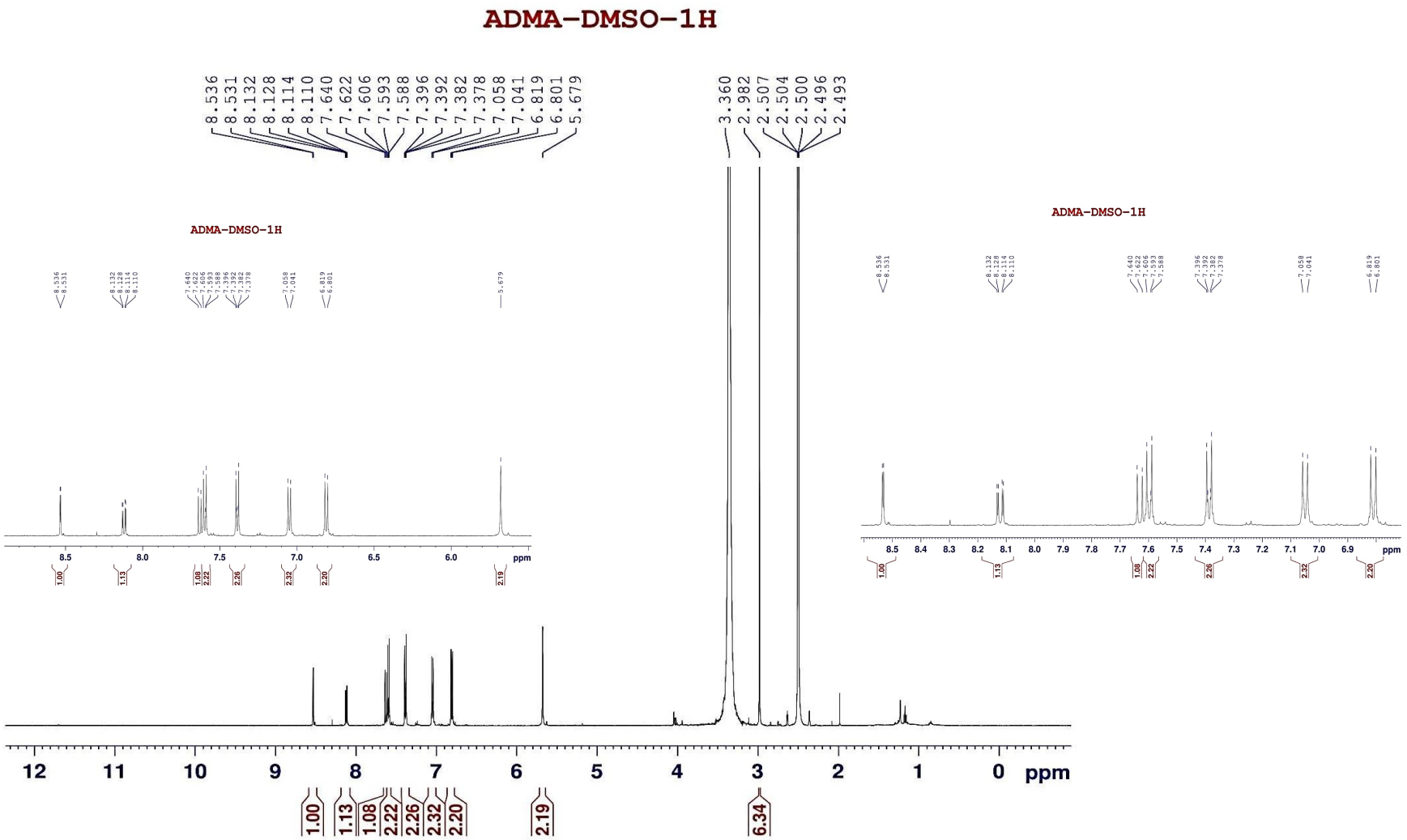
Compound 4i


ANEV–DMSO–1H
8.599
8.595
8.186
8.181
8.168
8.164
7.746
7.728
7.472
7.454
7.381
7.364
7.264
7.260
7.256
7.251
7.185
7.177
7.167
7.041
7.024
5.681
5.185
3.964
3.950
3.937
3.922
3.335
2.507
2.503
2.500
2.496
2.083
1.283
1.269
1.255
ANEV–DMSO–1H
ppm
0.918
0.859
3.738
2.074
2.035
1.165
2.000
1.777
1.763

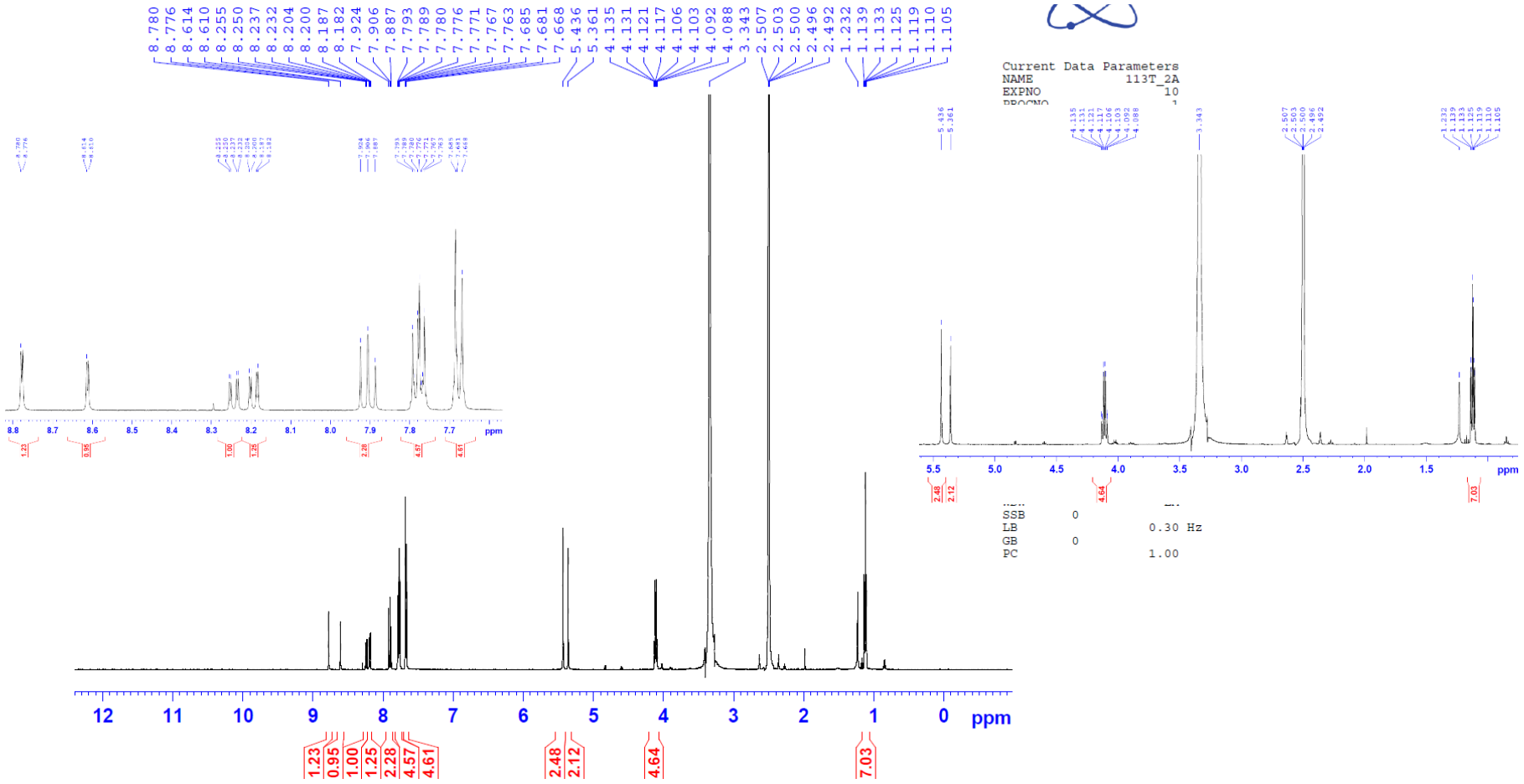
Compound 4j


ANHB1–DMSO–1H
9.861
8.617
8.613
8.185
8.181
8.167
8.163
7.706
7.688
7.378
7.361
7.348
7.332
7.138
7.135
7.122
7.032
7.015
6.984
6.981
6.977
6.966
6.962
5.664
3.330
2.503
2.500
2.496
2.083
1.278
1.232
ANHB1–DMSO–1H
ppm
1.103
0.695
1.050
1.000
2.090
1.067
2.164
2.166
1.194
2.007

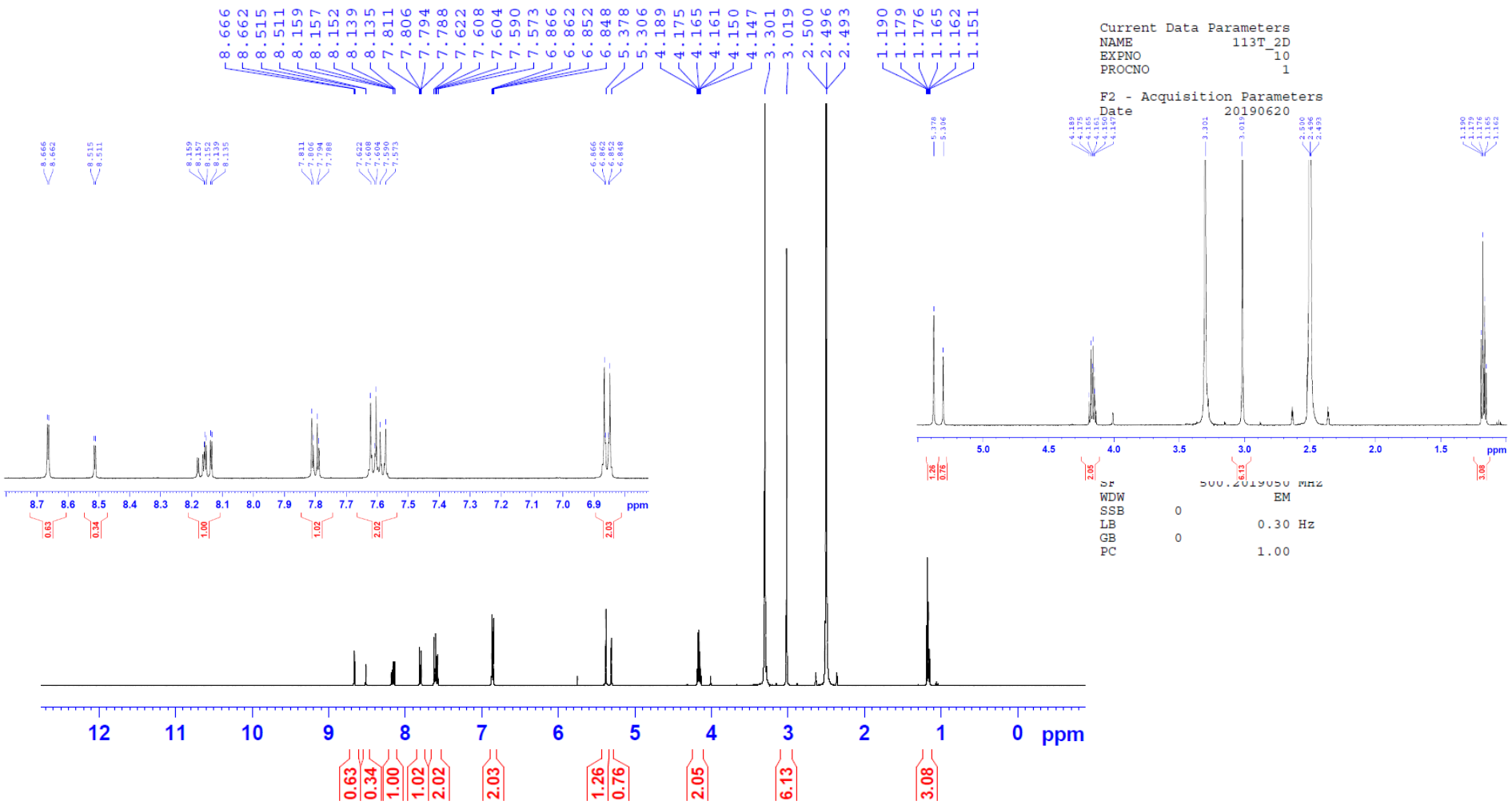
Compound 4k


ADMA-DMSO-1H
8.536
8.531
8.132
8.128
8.114
8.110
7.640
7.622
7.606
7.593
7.588
7.396
7.392
7.382
7.378
7.058
7.041
6.819
6.801
5.679
3.360
2.982
2.507
2.504
2.500
2.496
2.493
ADMA-DMSO-1H
ADMA-DMSO-1H
ppm
1.00
1.13
1.08
2.22
2.26
2.32
2.20
2.19
6.34

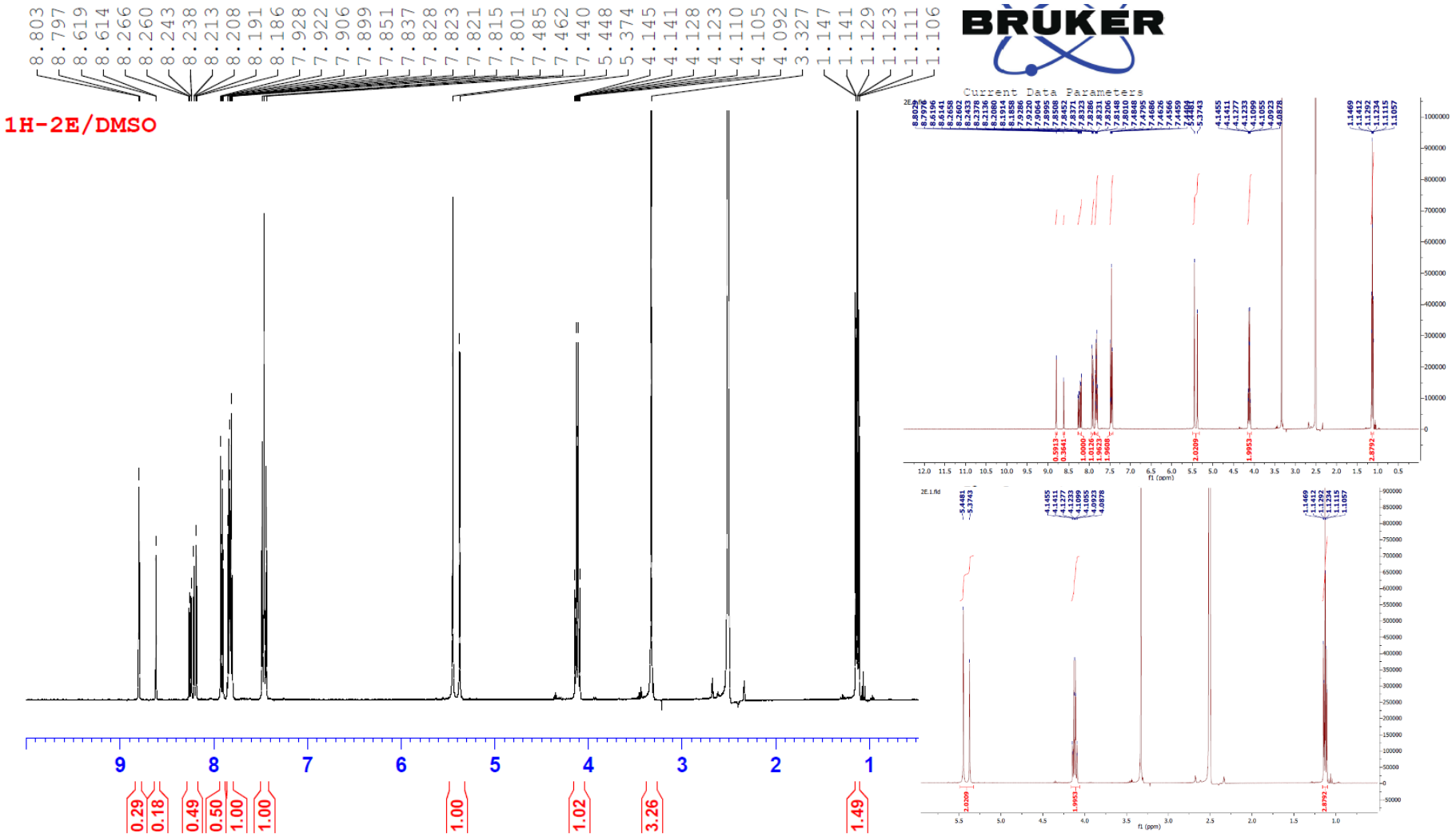
Compound 4l


8.780
8.776
8.614
8.610
8.255
8.250
8.237
8.232
8.204
8.200
8.187
8.182
7.924
7.906
7.887
7.793
7.789
7.780
7.776
7.771
7.767
7.763
7.685
7.681
7.668
5.436
5.361
4.135
4.131
4.121
4.117
4.106
4.103
4.092
4.088
3.343
2.507
2.503
2.500
2.496
2.492
1.232
1.139
1.133
1.125
1.119
1.110
1.105
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.23 0.95 1.00 1.25 2.28 4.57 4.61 2.48 2.12 4.64 7.03
Current Data Parameters
NAME 113T_2A
EXPNO 10
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

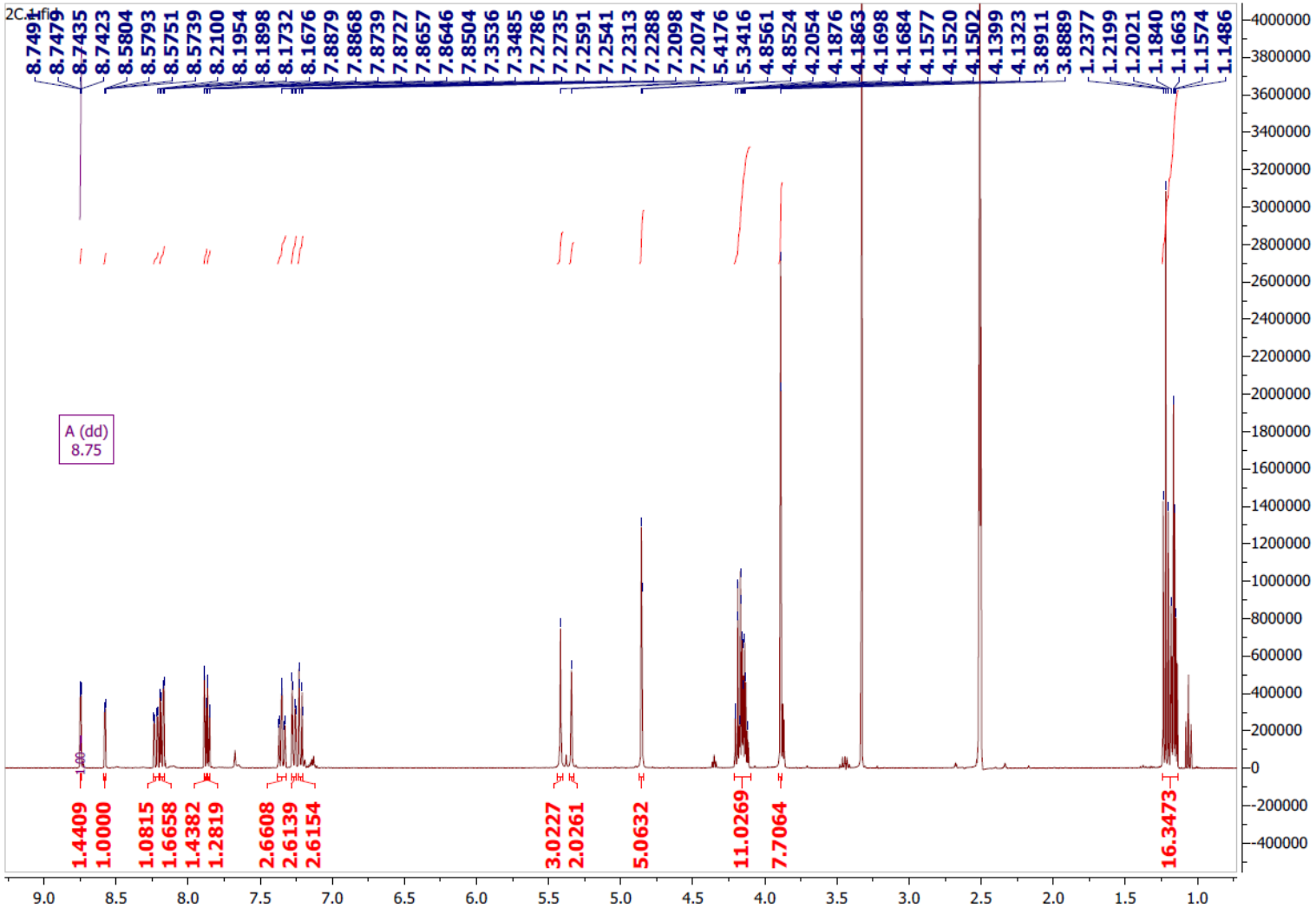
Compound 4m

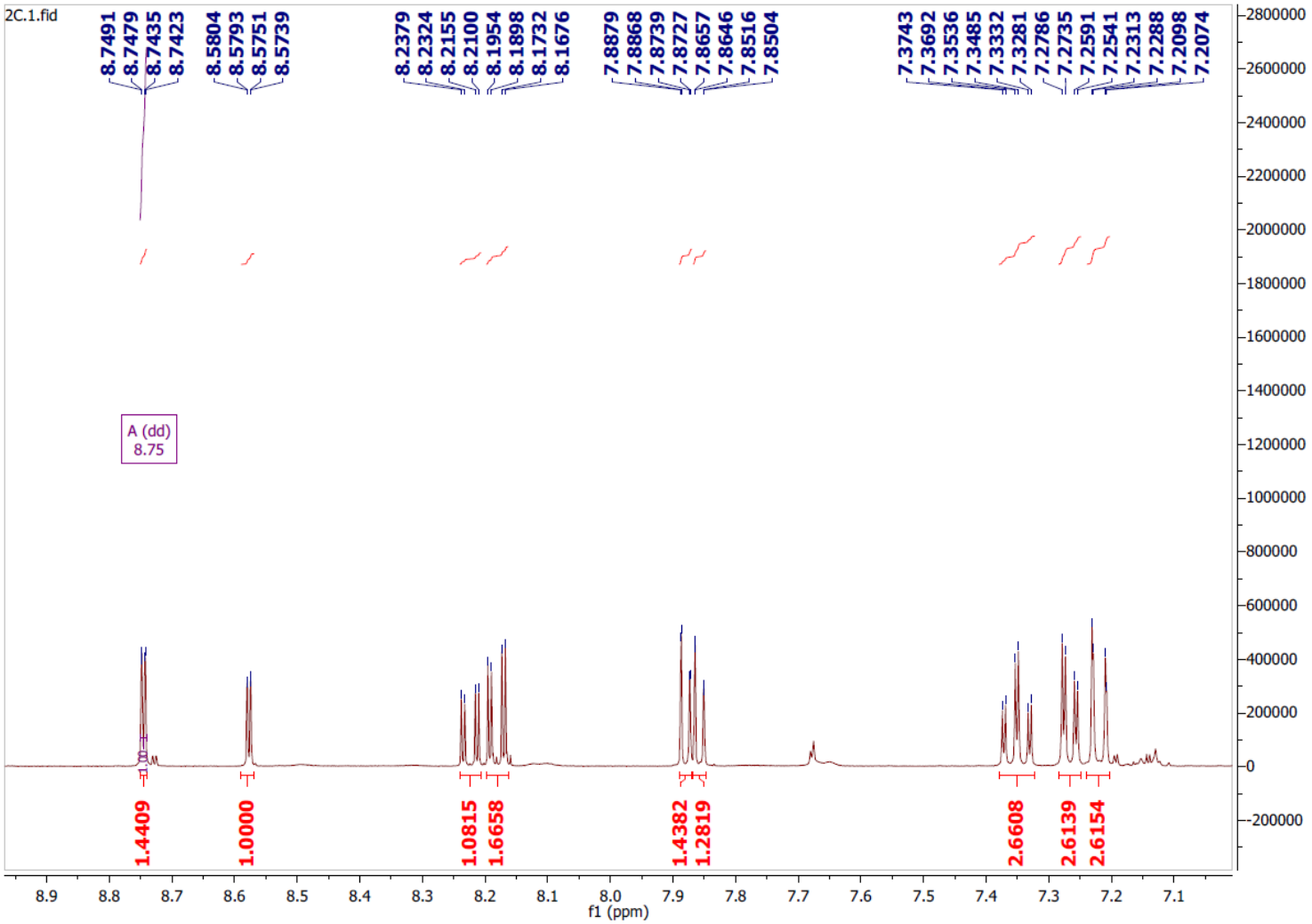

8.666
8.662
8.515
8.511
8.159
8.157
8.152
8.139
8.135
7.811
7.806
7.794
7.788
7.622
7.608
7.604
7.590
7.573
6.866
6.862
6.852
6.848
5.378
5.306
4.189
4.175
4.165
4.161
4.150
4.147
3.301
3.019
2.500
2.496
2.493
1.190
1.179
1.176
1.165
1.162
1.151
ppm
0.63
0.34
1.00
1.02
2.02
2.03
1.26
0.76
2.05
6.13
3.08
Current Data Parameters
NAME 113T_2D
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date 20190620
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

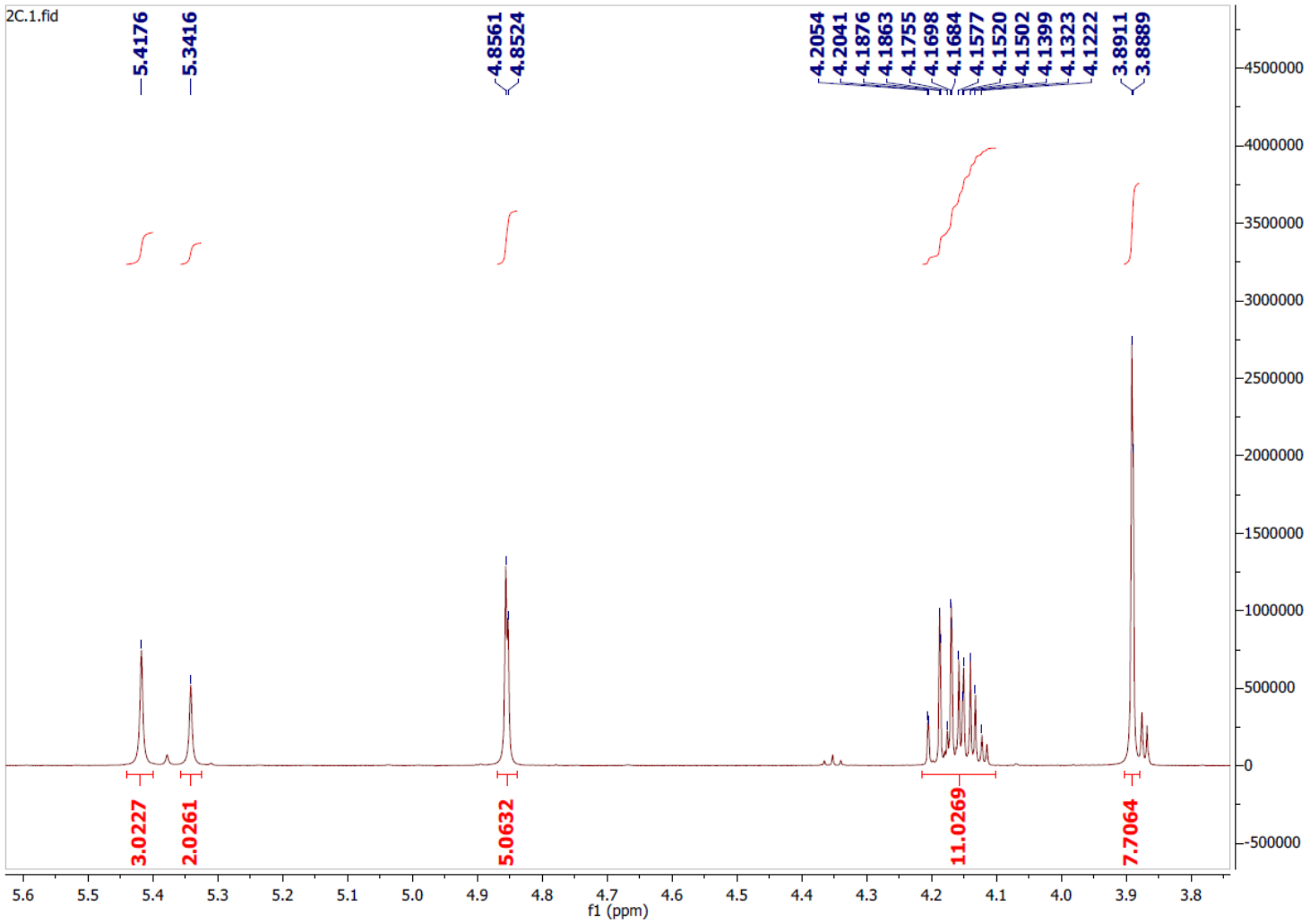
Compound 4n


8.803
8.797
8.619
8.614
8.266
8.260
8.243
8.238
8.213
8.208
8.191
8.186
7.928
7.922
7.906
7.899
7.851
7.837
7.828
7.823
7.821
7.815
7.801
7.485
7.462
7.440
5.448
5.374
4.145
4.141
4.128
4.123
4.110
4.105
4.092
3.327
1.147
1.141
1.129
1.123
1.111
1.106
1H-2E/DMSO
BRUKER
Current Data Parameters
9
8
7
6
5
4
3
2
1
0.29
0.18
0.49
0.50
1.00
1.00
1.00
1.02
3.26
1.49
f1 (ppm)

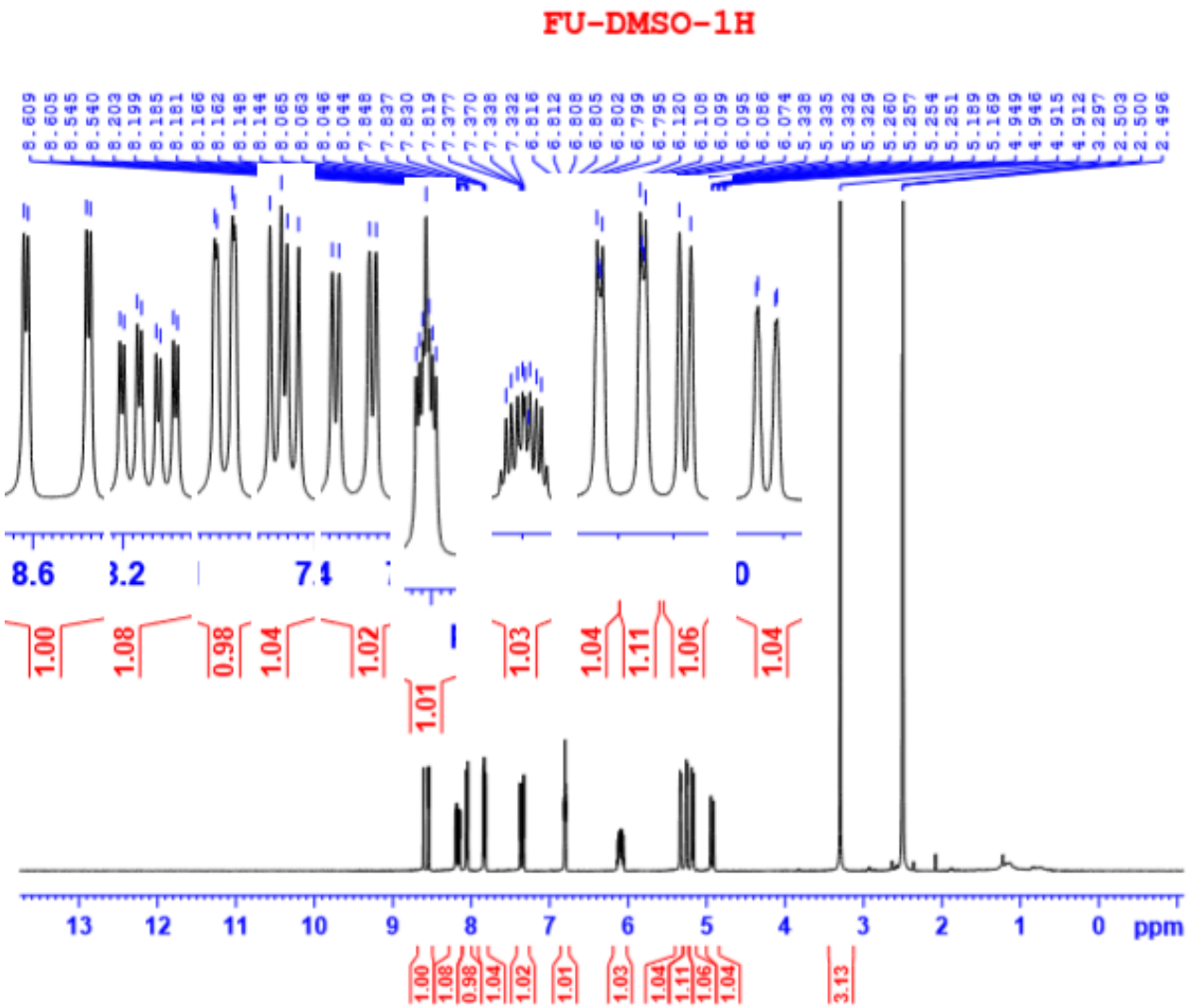
Compound 4o


2C.1.fid
8.7491
8.7479
8.7435
8.7423
8.5804
8.5793
8.5751
8.5739
8.2100
8.1954
8.1898
8.1732
8.1676
7.8879
7.8868
7.8739
7.8727
7.8657
7.8646
7.8504
7.3536
7.3485
7.2786
7.2735
7.2591
7.2541
7.2313
7.2288
7.2098
7.2074
5.4176
5.3416
4.8561
4.8524
4.2054
4.1876
4.1863
4.1698
4.1684
4.1577
4.1520
4.1502
4.1399
4.1323
3.8911
3.8889
1.2377
1.2199
1.2021
1.1840
1.1663
1.1574
1.1486
A (dd)
8.75
1.4409
1.0000
1.0815
1.6658
1.4382
1.2819
2.6608
2.6139
2.6154
3.0227
2.0261
5.0632
11.0269
7.7064
16.3473
4000000
3800000
3600000
3400000
3200000
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
-200000
-400000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0


2C.1.fid
8.7491
8.7479
8.7435
8.7423
8.5804
8.5793
8.5751
8.5739
8.2379
8.2324
8.2155
8.2100
8.1954
8.1898
8.1732
8.1676
7.8879
7.8868
7.8739
7.8727
7.8657
7.8646
7.8516
7.8504
7.3743
7.3692
7.3536
7.3485
7.3332
7.3281
7.2786
7.2735
7.2591
7.2541
7.2313
7.2288
7.2098
7.2074
A (dd)
8.75
1.4409
1.0000
1.0815
1.6658
1.4382
1.2819
2.6608
2.6139
2.6154
f1 (ppm)

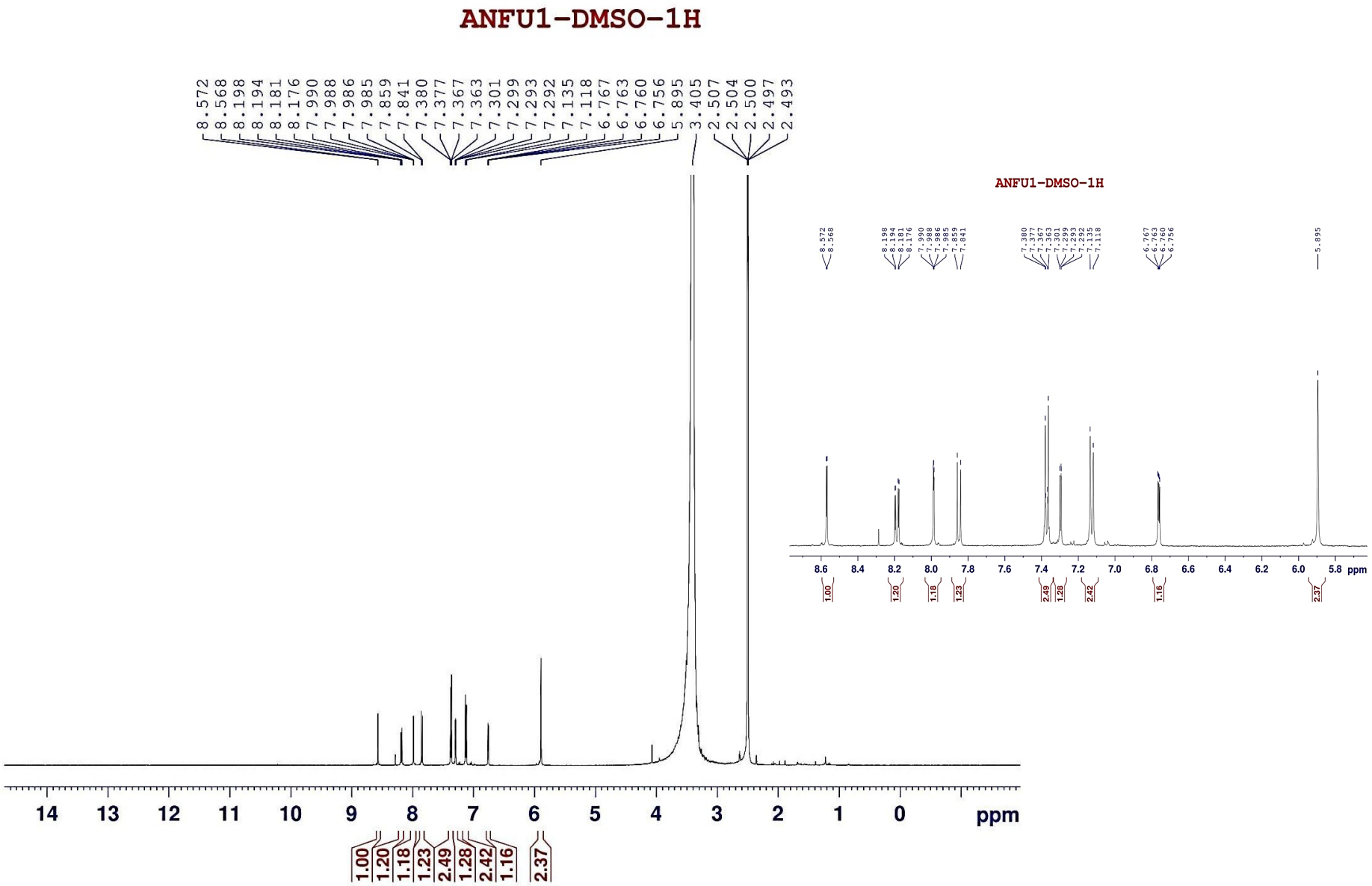

2C.1.fid
5.4176
5.3416
4.8561
4.8524
4.2054
4.2041
4.1876
4.1863
4.1755
4.1698
4.1684
4.1577
4.1520
4.1502
4.1399
4.1323
4.1222
3.8911
3.8889
3.0227
2.0261
5.0632
11.0269
7.7064
f1 (ppm)

Compound 4p

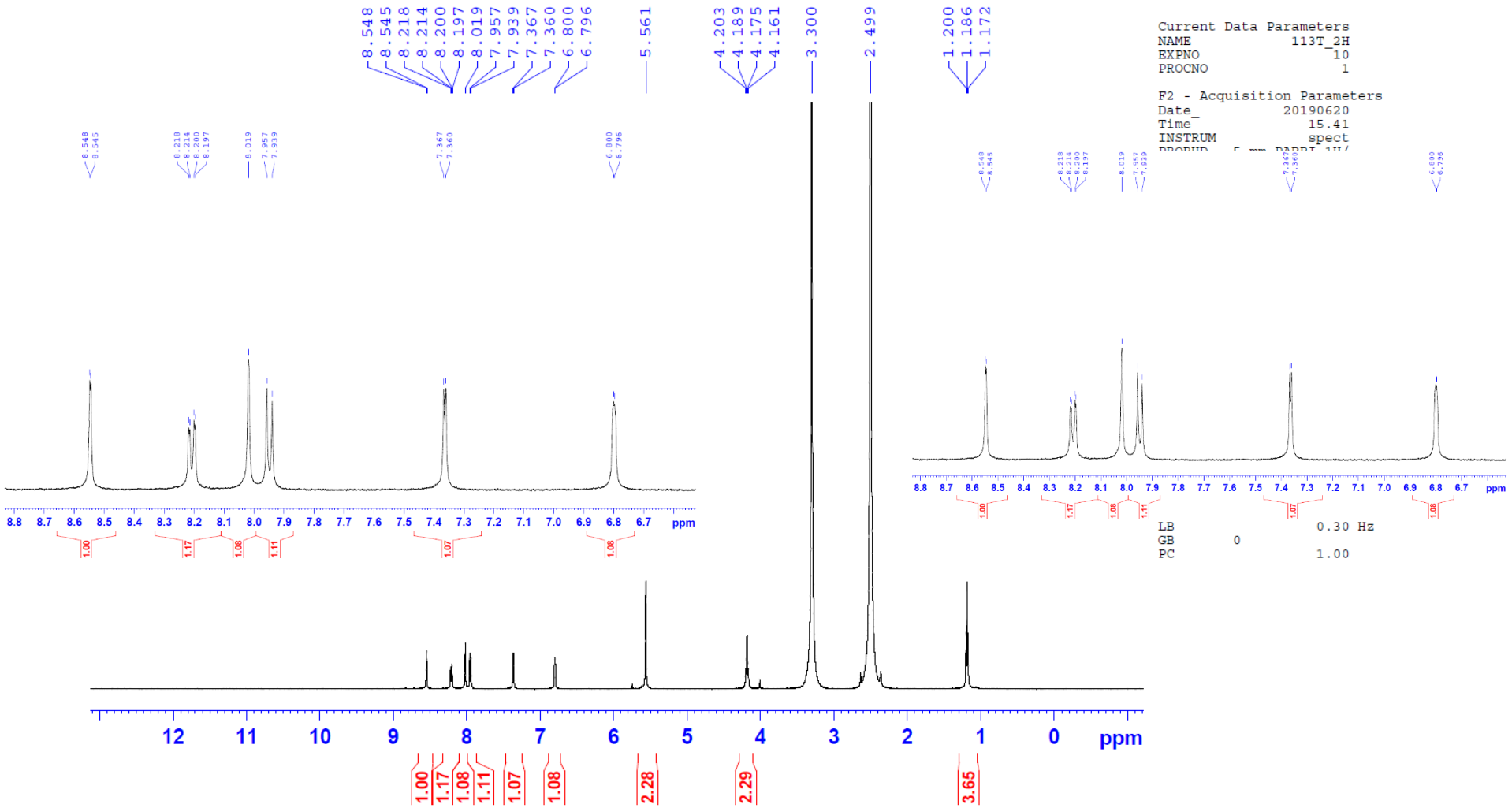



```
Current Data Parameters
NAME                  1137_FU
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20180627
Time                  11.15
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                3.2767999 sec
RG                   142.98
DW                   50.000 usec
DE                     6.50 usec
TE                   304.2 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             500.2030889 MHz
NUC1                      1H
P1                     10.00 usec
PLW1            22.00000000 W

F2 - Processing parameters
SI                    65536
SF               500.2000053 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

Compound 4q

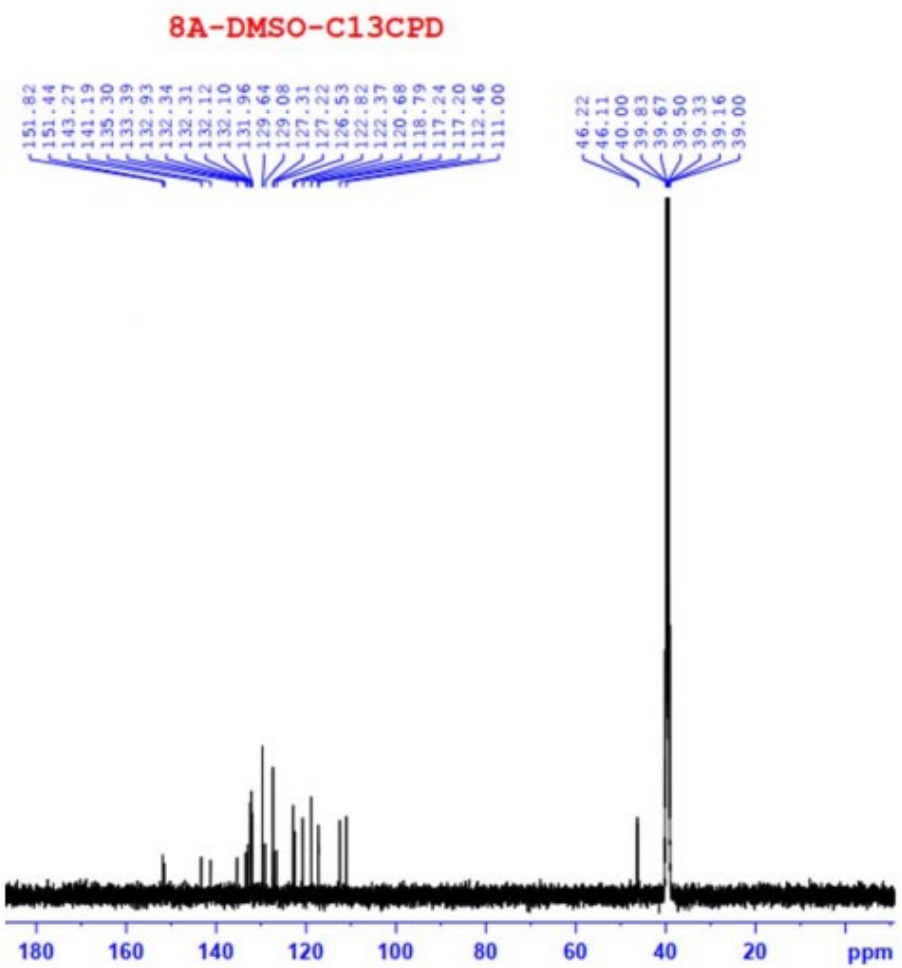

ANFU1-DMSO-1H
8.572
8.568
8.198
8.194
8.181
8.176
7.990
7.988
7.986
7.985
7.859
7.841
7.380
7.377
7.367
7.363
7.301
7.299
7.293
7.292
7.135
7.118
6.767
6.763
6.760
6.756
5.895
3.405
2.507
2.504
2.500
2.497
2.493
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.20 1.18 1.23 2.49 1.28 2.42 1.16 2.37
ANFU1-DMSO-1H
8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 ppm
1.00 1.20 1.18 1.23 2.49 1.28 2.42 1.16 2.37

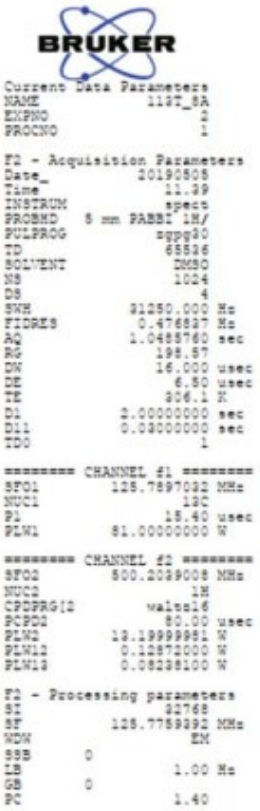
Compound 4r


8.548
8.545
8.218
8.214
8.200
8.197
8.019
7.957
7.939
7.367
7.360
6.800
6.796
5.561
4.203
4.189
4.175
4.161
3.300
2.499
1.200
1.186
1.172
Current Data Parameters
NAME 113T_2H
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190620
Time 15.41
INSTRUM spect
LB 0.30 Hz
GB 0
PC 1.00
ppm
1.00
1.17
1.08
1.11
1.07
1.08
2.28
2.29
3.65

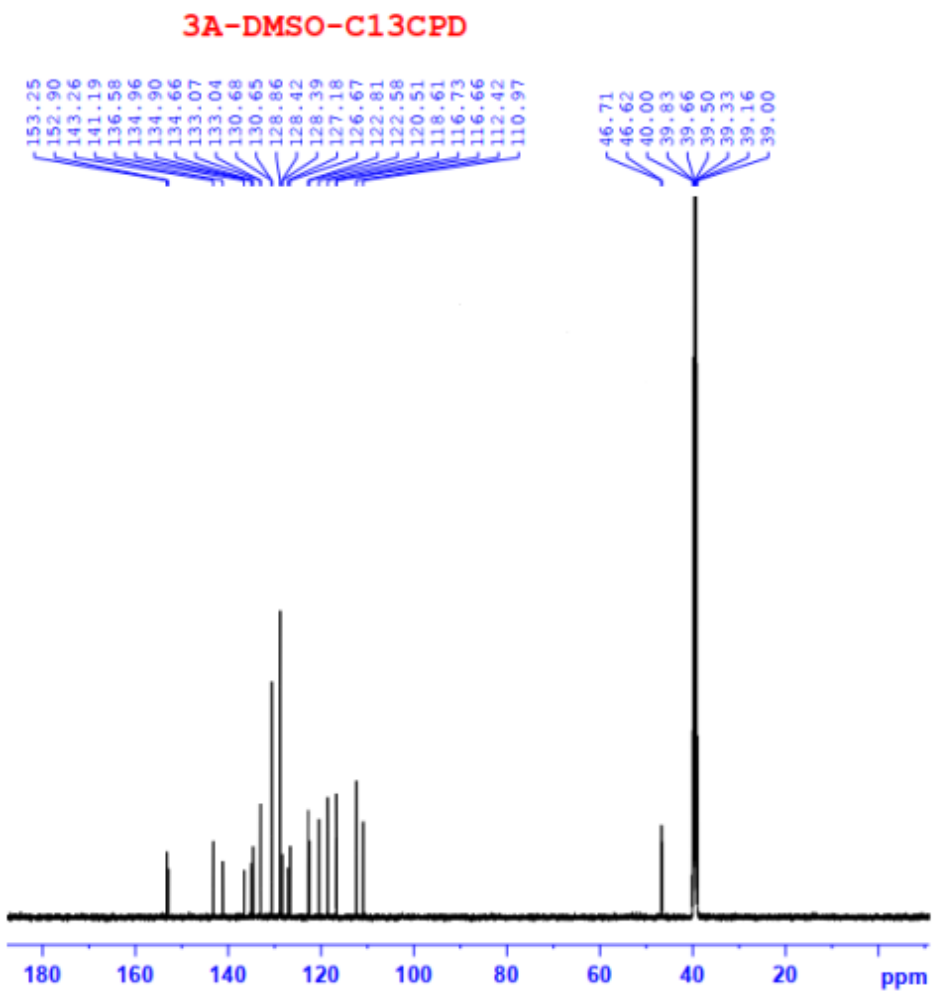
13C NMR SPECTRA

Compound 3a





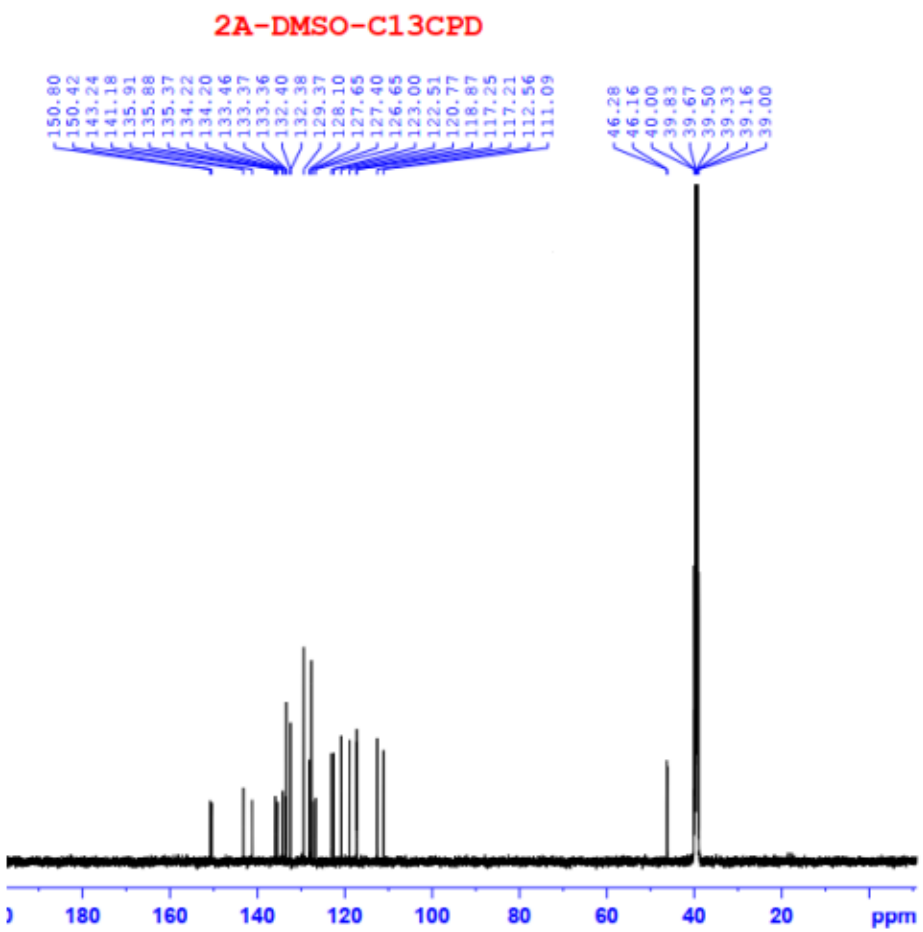
Compound 3b



BRUKER

```
Current Data Parameters
NAME                  113T_3A
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190307
Time                    17.19
INSTRUM                 spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                      65536
SOLVENT                 DMSO
NS                        512
DS                          4
SWH                 31250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0485760 sec
RG                     198.57
DW                     16.000 usec
DE                      6.50 usec
TE                     303.1 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               125.7692253 MHz
NUC1                       13C
P1                       10.00 usec
PLW1               88.00000000 W

======== CHANNEL f2 ========
SFO2               500.2020008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               22.00000000 W
PLW12               0.84875000 W
PLW13               0.22000000 W

F2 - Processing parameters
SI                        32768
SF                 125.7753900 MHz
WDW                          EM
SSB                 0
LB                       1.00 Hz
GB                  0
PC                       1.40
```

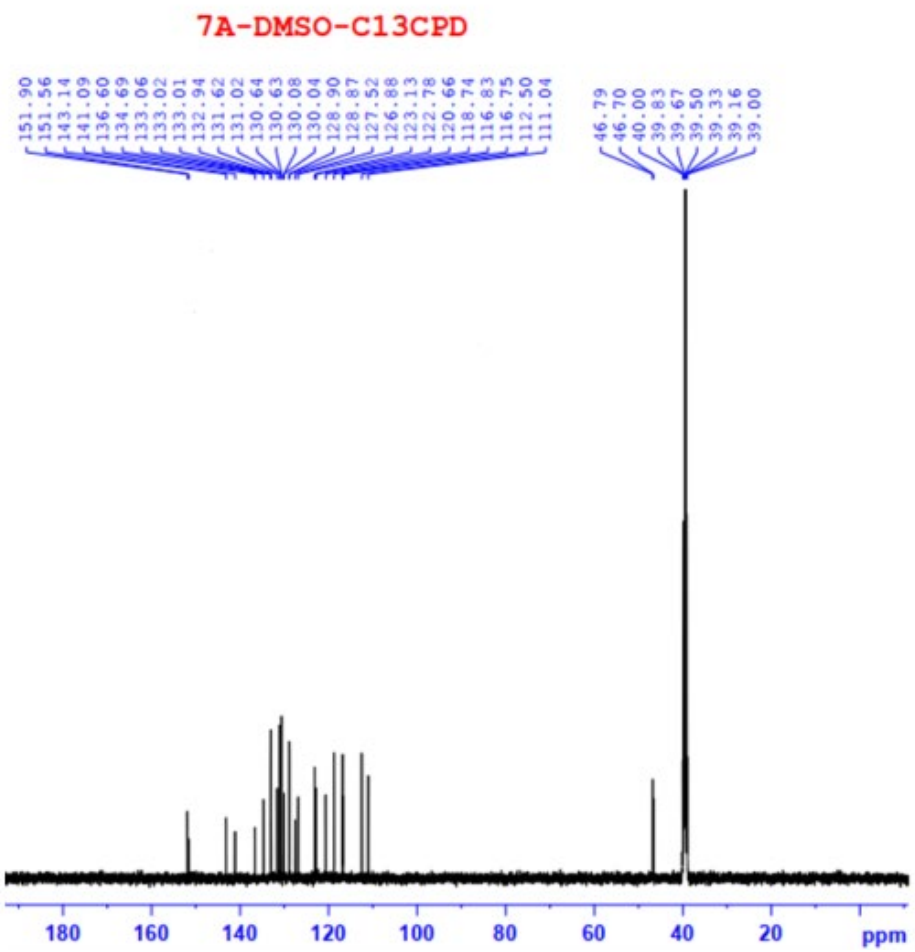
Compound 3c

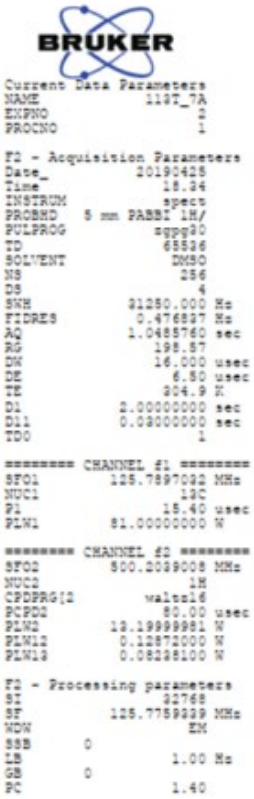


BRUKER

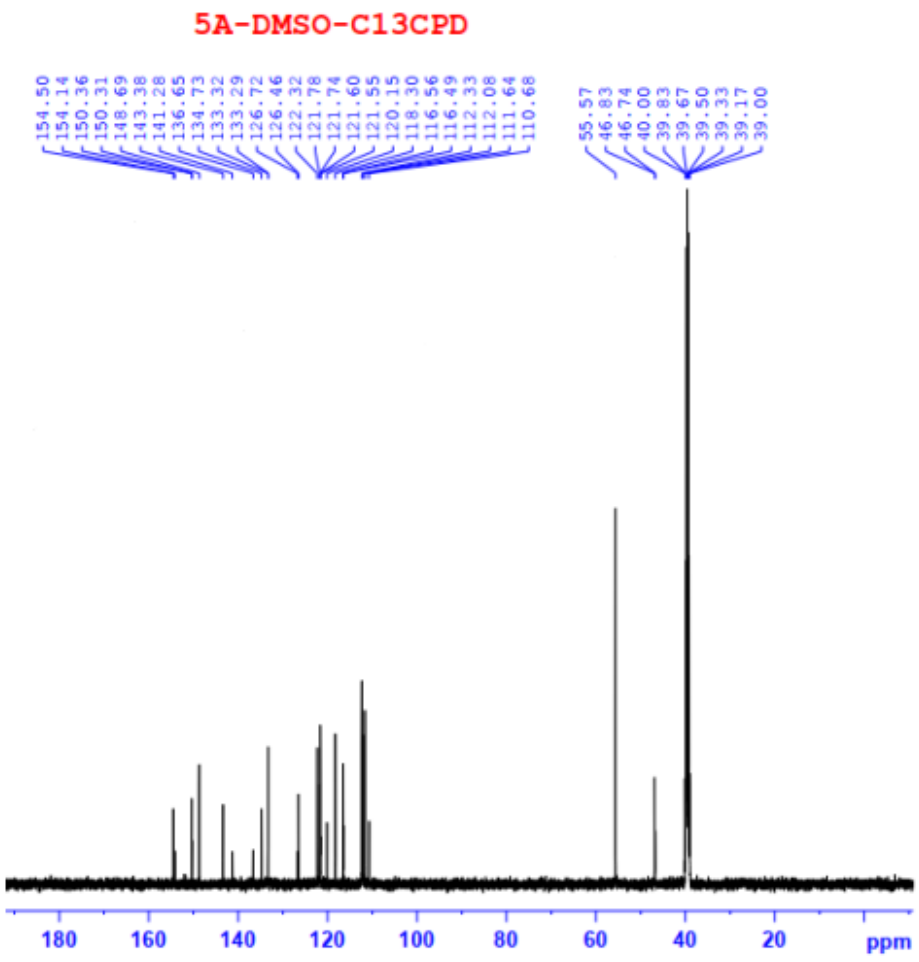
```
Current Data Parameters
NAME                  1137_2A
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190307
Time                   16.38
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                      65536
SOLVENT                 DMSO
NS                       1024
DS                          4
SWH                31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                    198.57
DW                   16.000 usec
DE                    6.50 usec
TE                   303.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               125.7892253 MHz
NUC1                       13C
P1                       10.00 usec
PLW1               88.00000000 W

======== CHANNEL f2 ========
SFO2               500.2020008 MHz
NUC2                       1H
CPDPRG[2               waltz16
PCPD2                    80.00 usec
PLW2               22.00000000 W
PLW12               0.34375000 W
PLW13               0.22000000 W

F2 - Processing parameters
SI                        32768
SF                 125.7754592 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

Compound 3d


7A-DMSO-C13CPD
151.90
151.56
143.14
141.09
136.60
134.69
133.06
133.02
133.01
132.94
131.62
131.02
130.64
130.63
130.08
130.04
128.90
128.87
127.52
126.88
123.13
122.78
120.66
118.74
116.83
116.75
112.50
111.04
46.79
46.70
40.00
39.83
39.67
39.50
39.33
39.16
39.00
180
160
140
120
100
80
60
40
20
ppm


BRUKER
Current Data Parameters
NAME 1197_7A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190425
Time 18.34
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 198.57
DW 16.000 usec
DE 6.50 usec
TE 304.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7897032 MHz
NUC1 13C
P1 15.40 usec
PLW1 61.00000000 W
======== CHANNEL f2 ========
SFO2 500.2039008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.19999981 W
PLW12 0.12872000 W
PLW13 0.08228100 W
F2 - Processing parameters
SI 32768
SF 125.7759939 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

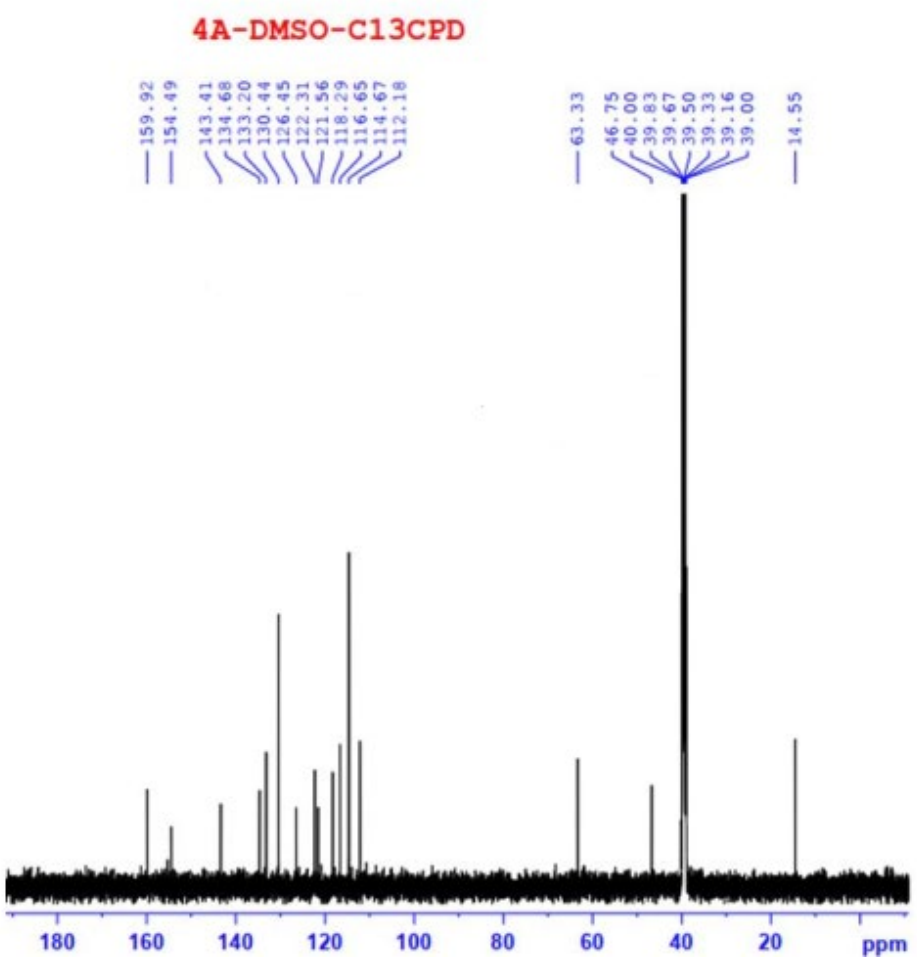
Compound 3e



BRUKER

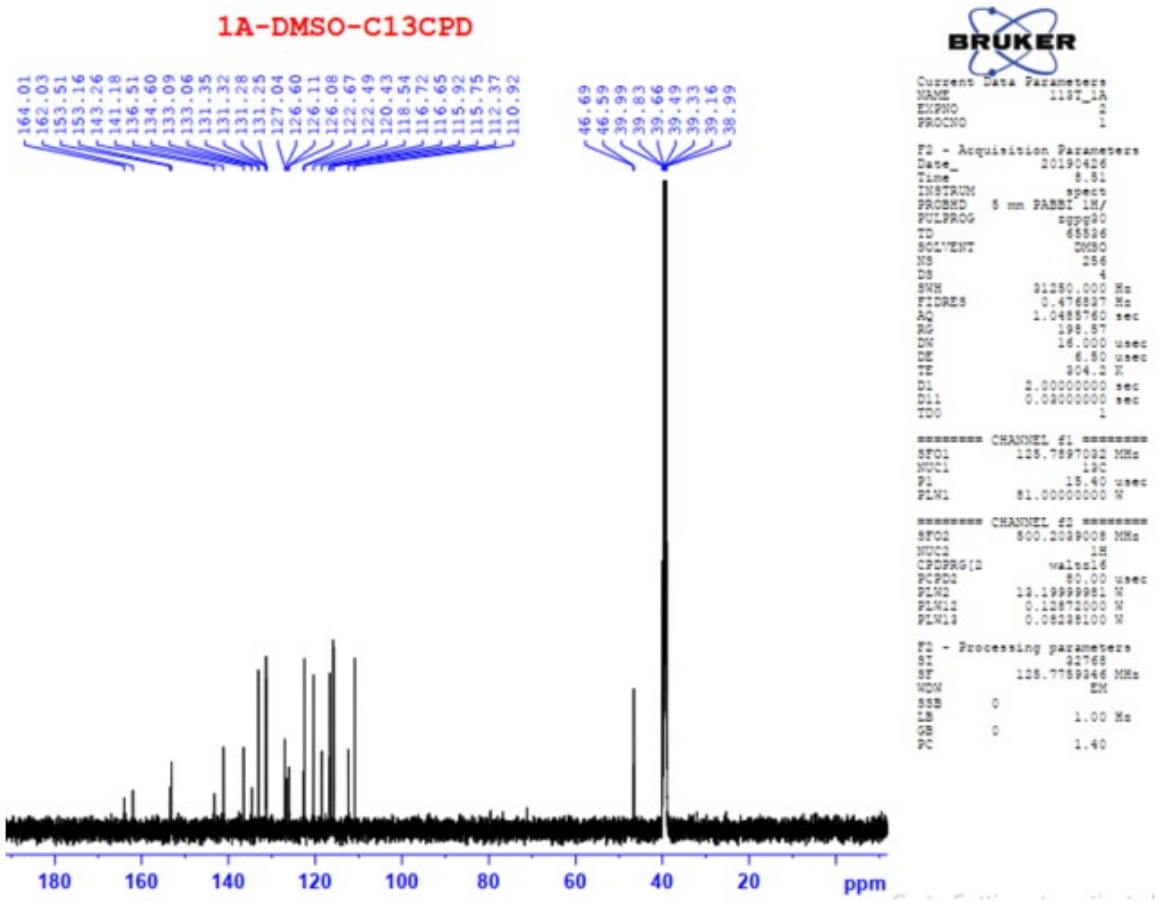
```
Current Data Parameters
NAME                  1137_5A
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190426
Time                   11.59
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG             zgpg30
TD                     65536
SOLVENT                DMSO
NS                       256
DS                         4
SWH              31250.000 Hz
FIDRES           0.476837 Hz
AQ               1.0485760 sec
RG                     198.57
DW                   16.000 usec
DE                     6.50 usec
TE                   304.6 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           125.7897032 MHz
NUC1                    13C
P1                    15.40 usec
PLW1           81.00000000 W

======== CHANNEL f2 ========
SFO2           500.2099008 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                 80.00 usec
PLW2           19.19999981 W
PLW12           0.12871000 W
PLW13           0.08288100 W

F2 - Processing parameters
SI                     32768
SF             125.7759923 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

Compound 3f

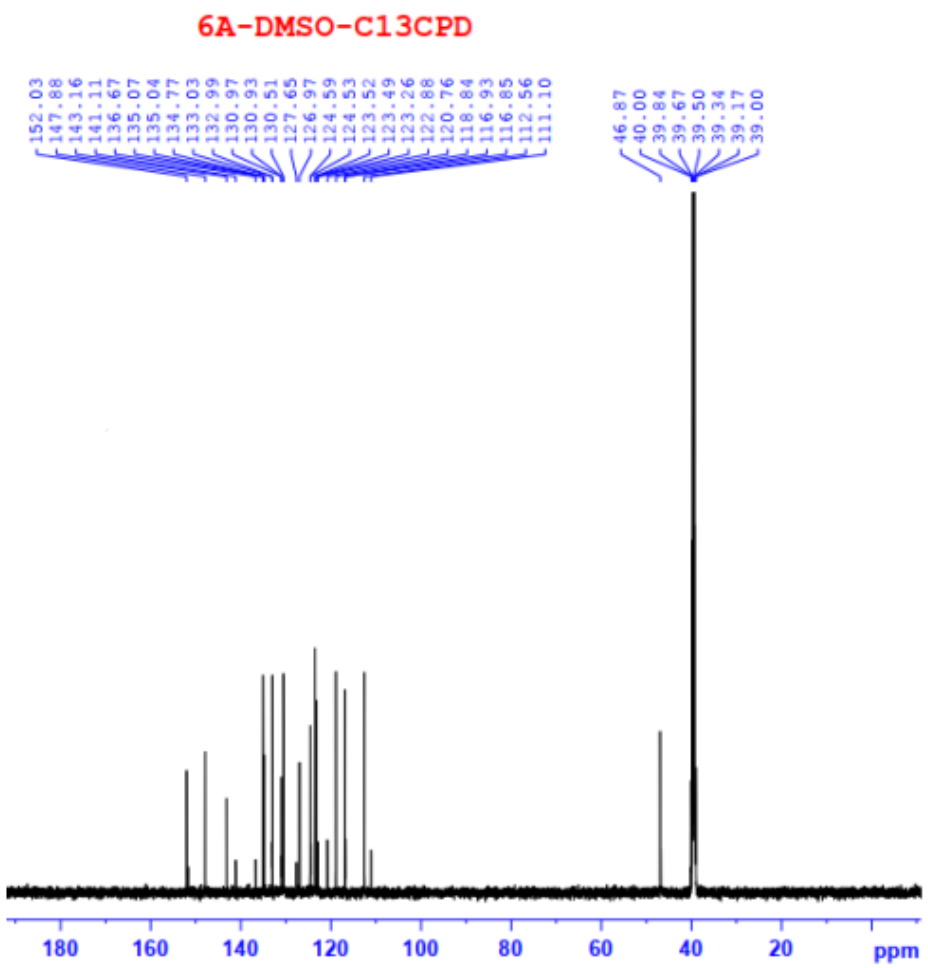



```
Current Data Parameters
NAME                  1197_4A
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190426
Time                    8.26
INSTRUM                 spect
PROBHD   5 mm PABBI 1H/
PULPROG                 zgpg30
TD                      65536
SOLVENT                 DMSO
NS                        256
DS                          4
SWH               31250.000 Hz
FIDRES                0.476837 Hz
AQ                1.0485760 sec
RG                      198.57
DW                     16.000 usec
DE                      6.50 usec
TE                     304.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             125.7897032 MHz
NUC1                      13C
P1                      15.40 usec
PLW1             81.00000000 W

======== CHANNEL f2 ========
SFO2             500.2039008 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                   80.00 usec
PLW2             19.19999981 W
PLW12             0.12873000 W
PLW13             0.08298100 W

F2 - Processing parameters
SI                        32768
SF               125.7759291 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

Compound 3g


1A-DMSO-C13CPD
164.01
162.03
153.51
153.16
143.26
141.18
136.51
134.60
133.09
133.06
131.35
131.32
131.28
131.25
127.04
126.60
126.11
126.08
122.67
122.49
120.43
118.54
116.72
116.65
115.92
115.75
112.37
110.92
46.69
46.59
39.99
39.83
39.66
39.49
39.33
39.16
38.99
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME 1197_1A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190426
Time 8.51
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 198.57
DW 16.000 usec
DE 6.50 usec
TE 304.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7897032 MHz
NUC1 13C
P1 15.40 usec
PLW1 81.00000000 W
======== CHANNEL f2 ========
SFO2 500.2039008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 19.19999981 W
PLW12 0.12871000 W
PLW13 0.08238100 W
F2 - Processing parameters
SI 32768
SF 125.7759346 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

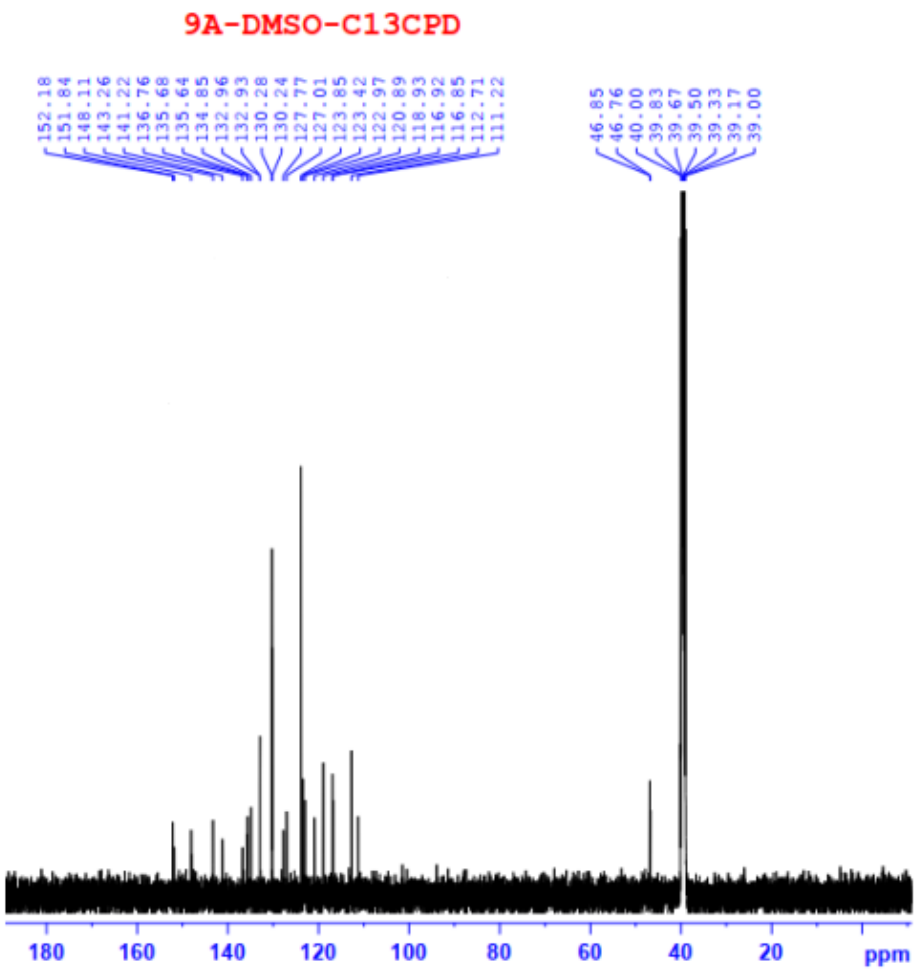
Compound 3h



BRUKER

```
Current Data Parameters
NAME                  1197_6A
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190425
Time                   18.00
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG                zgpg30
TD                     65536
SOLVENT                DMSO
NS                       256
DS                         4
SWH                31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                    198.57
DW                   16.000 usec
DE                    6.50 usec
TE                   304.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             125.7897092 MHz
NUC1                     13C
P1                     15.40 usec
PLW1             61.00000000 W

======== CHANNEL f2 ========
SFO2             500.2039008 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2             13.19999981 W
PLW12             0.12872000 W
PLW13             0.08238100 W

F2 - Processing parameters
SI                       32768
SF                 125.7759827 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

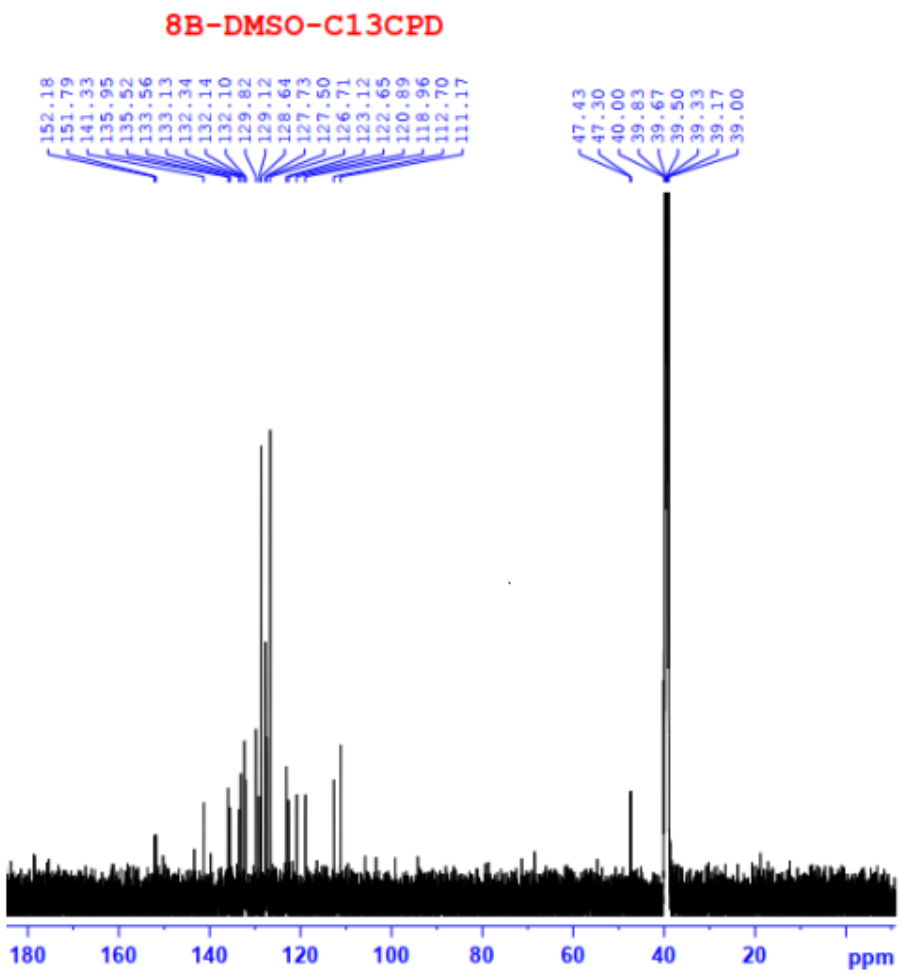
Compound 3i



BRUKER

```
Current Data Parameters
NAME                  113T_9A
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190505
Time                    9.00
INSTRUM                 spect
PROBHD    5 mm PABBI 1H/
PULPROG                 zgpg30
TD                      65536
SOLVENT                 DMSO
NS                      2048
DS                         4
SWH                31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                    198.67
DW                    16.000 usec
DE                     6.50 usec
TE                    303.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               125.7897032 MHz
NUC1                      13C
P1                      15.40 usec
PLW1               61.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                   80.00 usec
PLW2               13.19999981 W
PLW12               0.12872000 W
PLW13               0.08238100 W

F2 - Processing parameters
SI                        32768
SF                 125.7759361 MHz
WDW                          EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

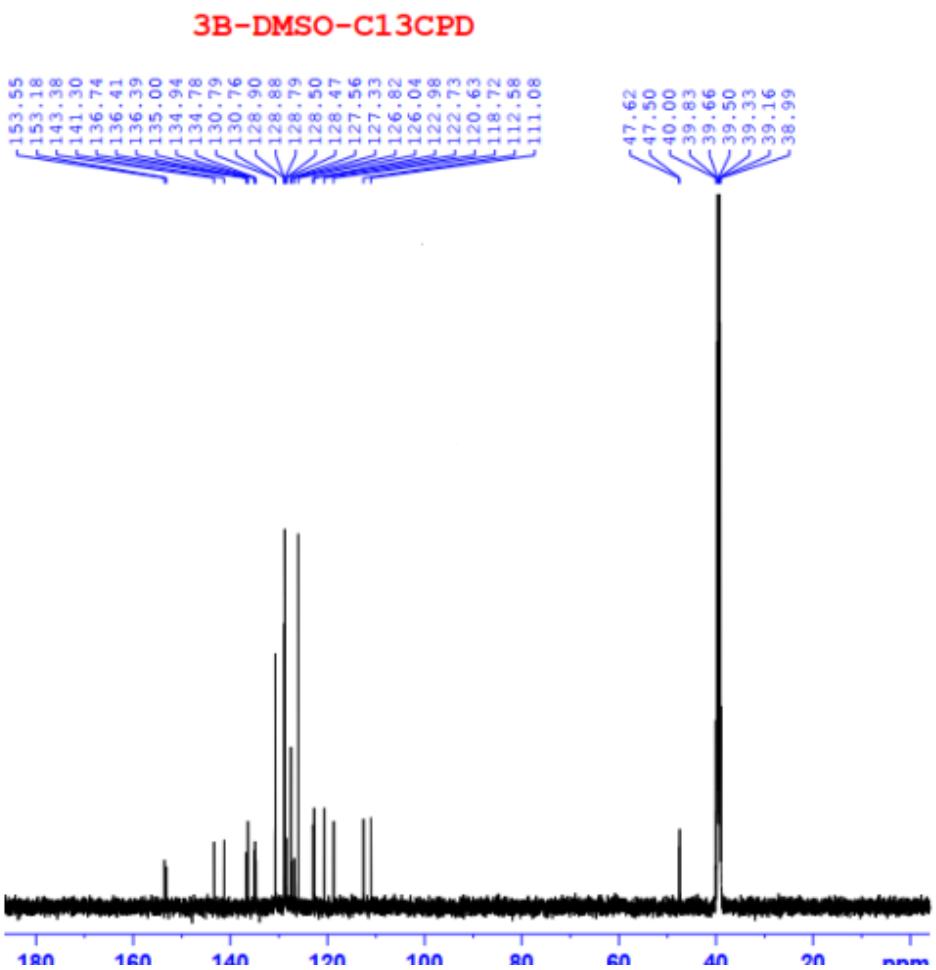
Compound 3j



BRUKER

```
Current Data Parameters
NAME                  1137_8B
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190508
Time                    8.38
INSTRUM                 spect
PROBHD    5 mm PABBI 1H/
PULPROG                 zgpg30
TD                      65536
SOLVENT                   DMSO
NS                        2048
DS                           4
SWH                31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                      198.57
DW                      16.000 usec
DE                       6.50 usec
TE                      303.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               125.7897032 MHz
NUC1                       13C
P1                       15.40 usec
PLW1               81.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               13.19999981 W
PLW12               0.12872000 W
PLW13               0.08238100 W

F2 - Processing parameters
SI                       32768
SF                 125.7759235 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

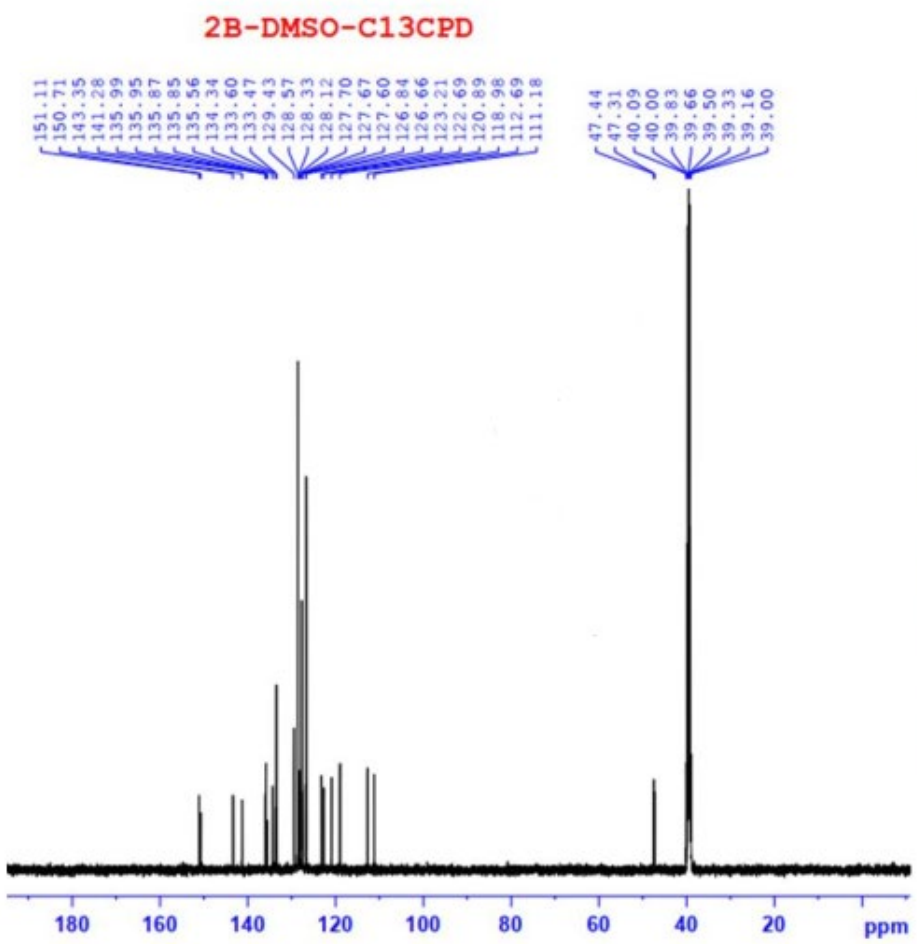
Compound 3k



BRUKER

```
Current Data Parameters
NAME                  1197_3B
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190428
Time                    19.07
INSTRUM                 spect
PROBHD    5 mm PABBI 1H/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  DMSO
NS                        256
DS                          4
SWH                 31250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0485760 sec
RG                     198.97
DW                     16.000 usec
DE                       6.50 usec
TE                      304.7 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               125.7897032 MHz
NUC1                      13C
P1                      15.40 usec
PLW1               81.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   80.00 usec
PLW2               13.19999981 W
PLW12               0.12872000 W
PLW13               0.08228100 W

F2 - Processing parameters
SI                        32768
SF                 125.7759342 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

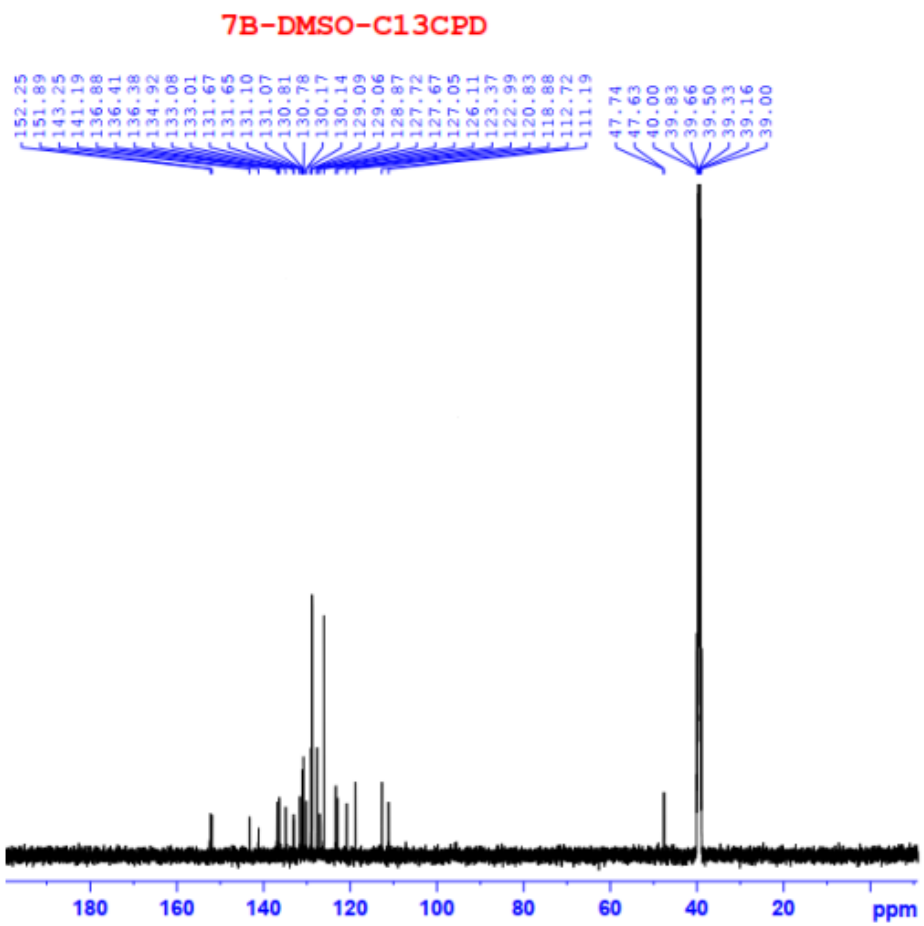
Compound 3l



BRUKER

```
Current Data Parameters
NAME                  1197_2B
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190425
Time                   18.50
INSTRUM                spect
PROBHD   5 mm PABBI 1H/
PULPROG                zgpg30
TD                      65536
SOLVENT                 DMSO
NS                        256
DS                          4
SWH                91250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0488760 sec
RG                     198.87
DW                     16.000 usec
DE                      6.50 usec
TE                     304.8 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               125.7897032 MHz
NUC1                       13C
P1                       15.40 usec
PLW1               81.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               13.19999981 W
PLW12               0.12872000 W
PLW13               0.08228100 W

F2 - Processing parameters
SI                        32768
SF                 125.7759308 MHz
WDW                          EM
SSB                 0
LB                       1.00 Hz
GB                  0
PC                       1.40
```

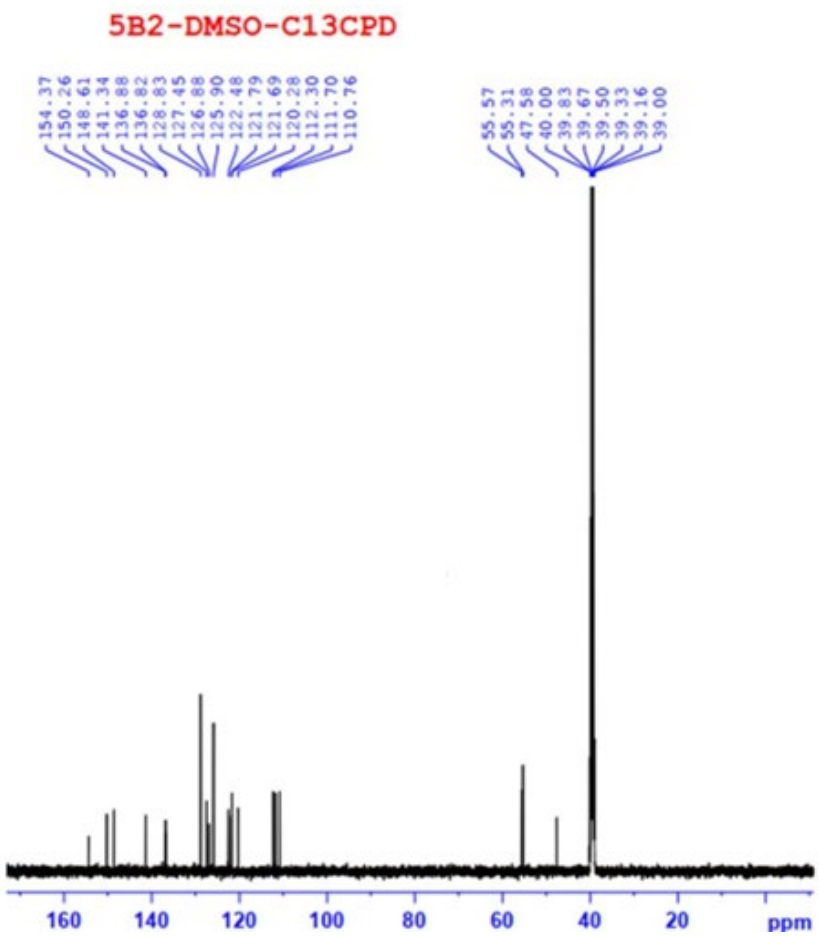
Compound 3m

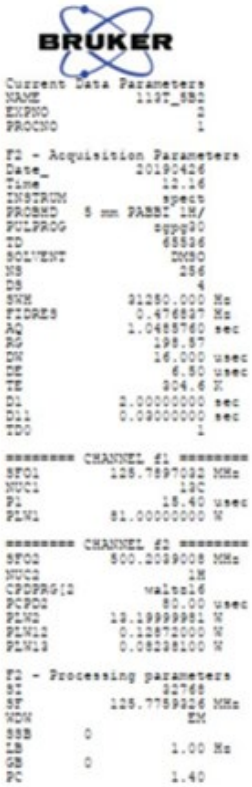


BRUKER

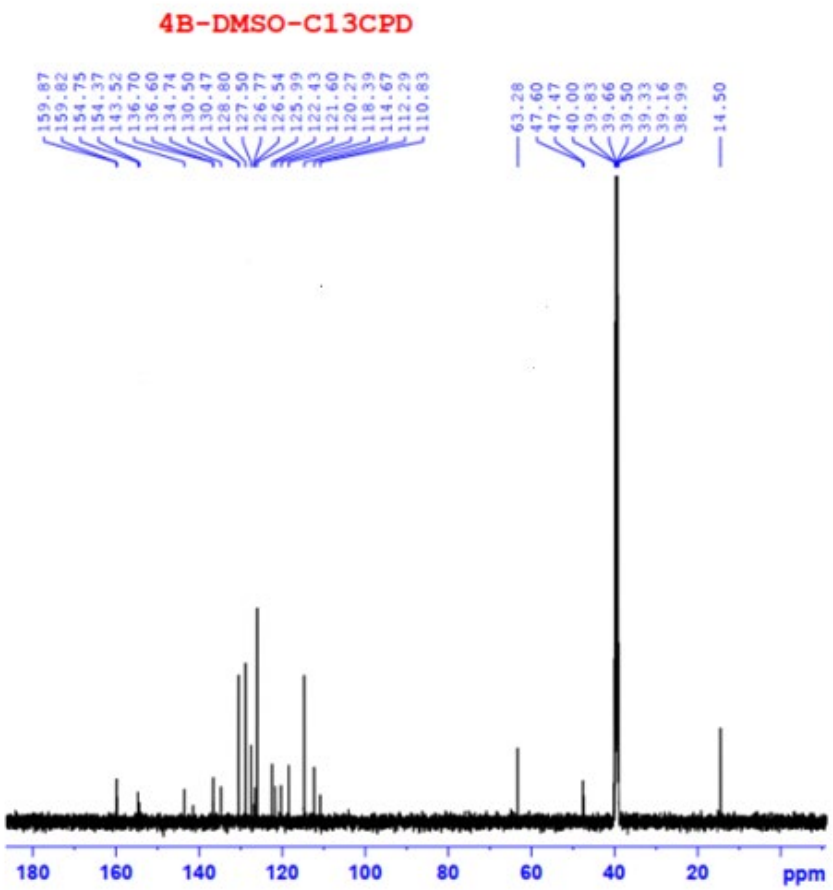
```
Current Data Parameters
NAME                  1137_7B
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190518
Time                   20.38
INSTRUM                spect
PROBHD    5 mm PABBI 1H/
PULPROG              qqpg30
TD                    65536
SOLVENT                DMSO
NS                       512
DS                         4
SWH               31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                    198.87
DW                    16.000 usec
DE                     6.50 usec
TE                    308.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             125.7897032 MHz
NUC1                    13C
P1                    13.40 usec
PLW1             81.00000000 W

======== CHANNEL f2 ========
SFO2             500.2039008 MHz
NUC2                    1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2             18.19999981 W
PLW12             0.12872000 W
PLW13             0.08238100 W

F2 - Processing parameters
SI                      32768
SF               125.7759283 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

Compound 3n


5B2-DMSO-C13CPD
154.37
150.26
148.61
141.34
136.88
136.82
128.83
127.45
126.88
125.90
122.48
121.79
121.69
120.28
112.30
111.70
110.76
55.57
55.31
47.58
40.00
39.83
39.67
39.50
39.33
39.16
39.00
160
140
120
100
80
60
40
20
ppm


BRUKER
Current Data Parameters
NAME 1197_5B2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190426
Time 12.16
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 198.57
DW 16.000 usec
DE 6.50 usec
TE 304.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7897092 MHz
NUC1 13C
P1 15.40 usec
PLW1 81.00000000 W
======== CHANNEL f2 ========
SFO2 500.2089008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 18.19999981 W
PLW11 0.12872000 W
PLW12 0.08238100 W
F2 - Processing parameters
SI 32768
SF 125.7759326 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

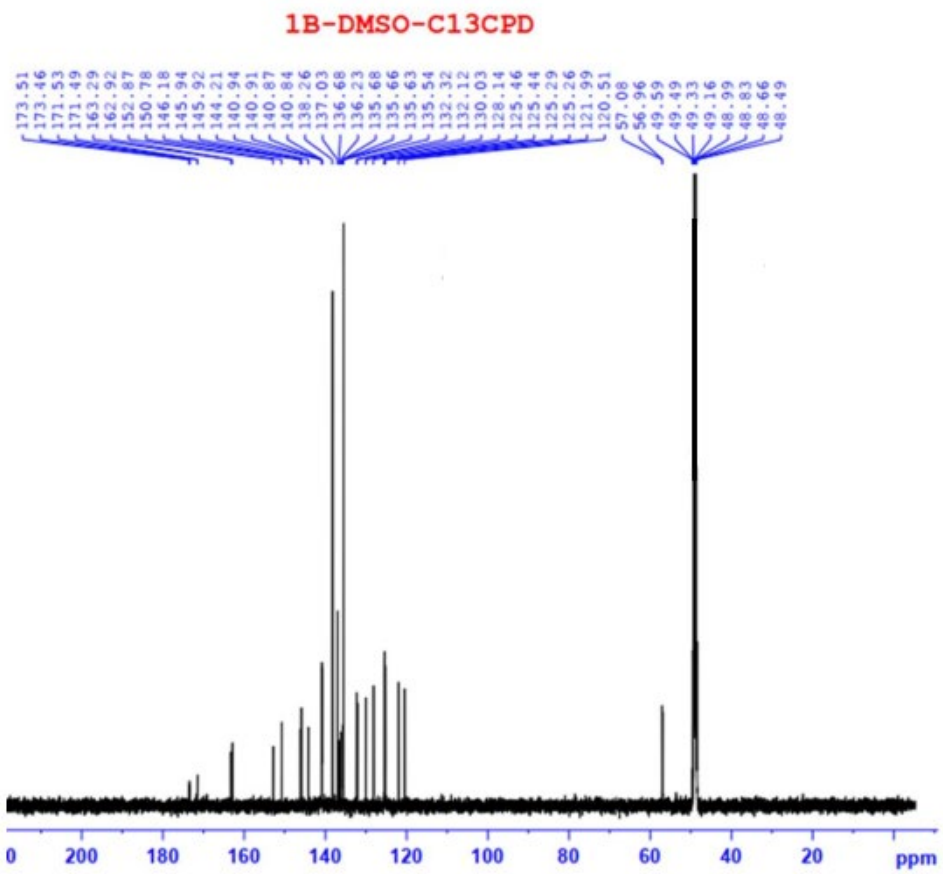
Compound 3o



BRUKER

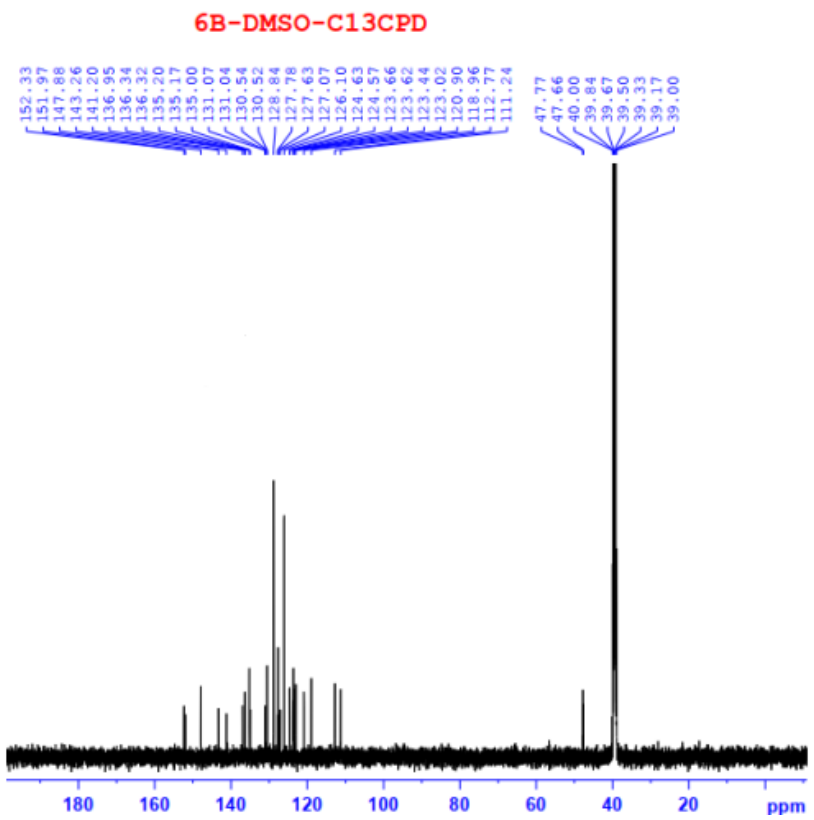
```
Current Data Parameters
NAME                  1197_4B
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190426
Time                    9.24
INSTRUM                 spect
PROBHD    5 mm PABBI 1H/
PULPROG                 zgpg30
TD                      65536
SOLVENT                 DMSO
NS                        256
DS                          4
SWH                31280.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0488760 sec
RG                     198.87
DW                     16.000 usec
DE                      6.50 usec
TE                     304.2 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               125.7897035 MHz
NUC1                       13C
P1                       18.40 usec
PLW1               81.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               13.19999981 W
PLW12               0.12872000 W
PLW13               0.06238100 W

F2 - Processing parameters
SI                        32768
SF                 125.7759330 MHz
WDW                          EM
SSB                 0
LB                       1.00 Hz
GB                  0
PC                       1.40
```

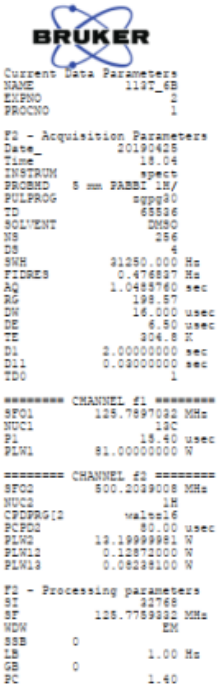
Compound 3p



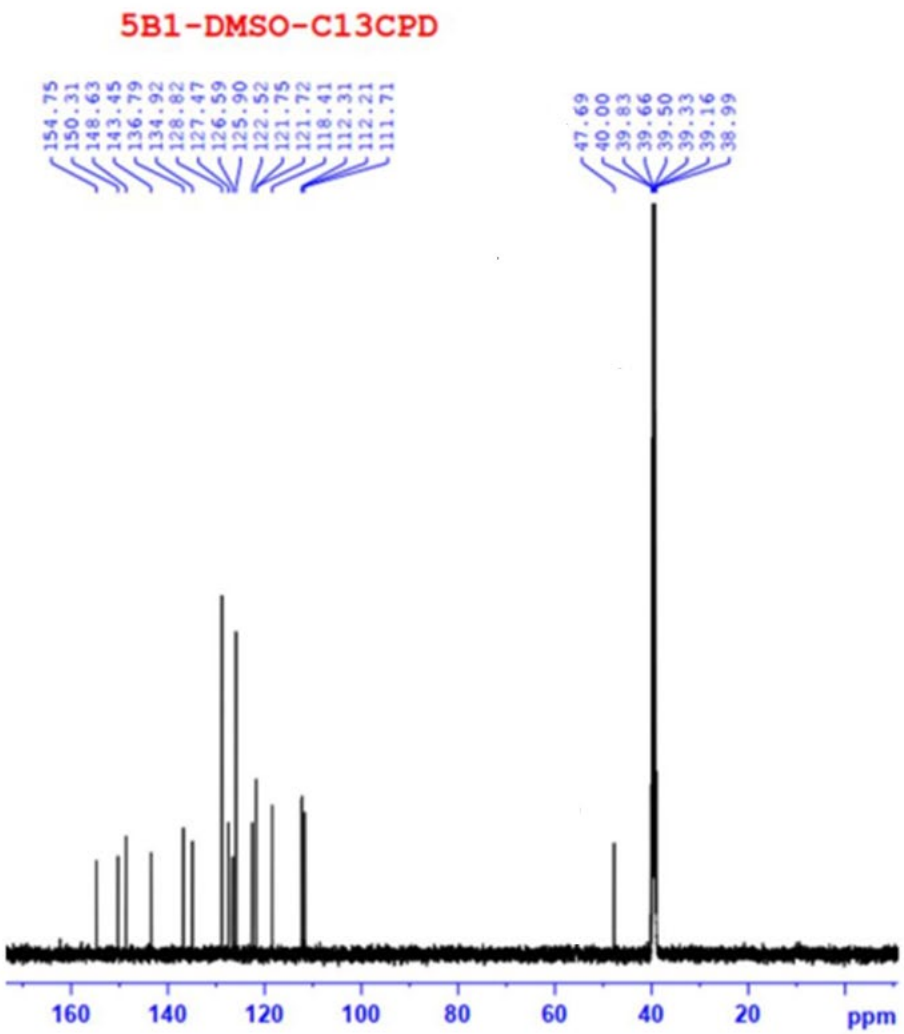

```
Current Data Parameters
NAME                  1197_1B
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190426
Time                   9.08
INSTRUM                spect
PROBHD     5 mm PABBI 1H/
PULPROG             zgpg30
TD                     65536
SOLVENT                DMSO
NS                       256
DS                         4
SWH               31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.04857600 sec
RG                    198.57
DW                    16.000 usec
DE                     6.50 usec
TE                    304.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             125.7897032 MHz
NUC1                    13C
P1                    15.40 usec
PLW1             81.00000000 W

======== CHANNEL f2 ========
SFO2             500.2099008 MHz
NUC2                    1H
CPDPRG[2          waltz16
PCPD2                 80.00 usec
PLW2             18.19999981 W
PLW12             0.12872000 W
PLW13             0.08238100 W

F2 - Processing parameters
SI                     32768
SF               125.7747406 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

Compound 3q


6B-DMSO-C13CPD
152.33
151.97
147.88
143.26
141.20
136.95
136.34
136.32
135.20
135.17
135.00
131.07
131.04
130.54
130.52
128.84
127.78
127.63
127.07
126.10
124.63
124.57
123.66
123.62
123.44
123.02
120.90
118.96
112.77
111.24
47.77
47.66
40.00
39.84
39.67
39.50
39.33
39.17
39.00
180
160
140
120
100
80
60
40
20
ppm


BRUKER
Current Data Parameters
NAME 1197_6B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190425
Time 18.04
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 198.57
DW 16.000 usec
DE 6.50 usec
TE 304.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7897032 MHz
NUC1 13C
P1 10.40 usec
PLW1 61.00000000 W
======== CHANNEL f2 ========
SFO2 500.2039008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 13.19999981 W
PLW12 0.12872000 W
PLW13 0.08238100 W
F2 - Processing parameters
SI 32768
SF 125.7758232 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

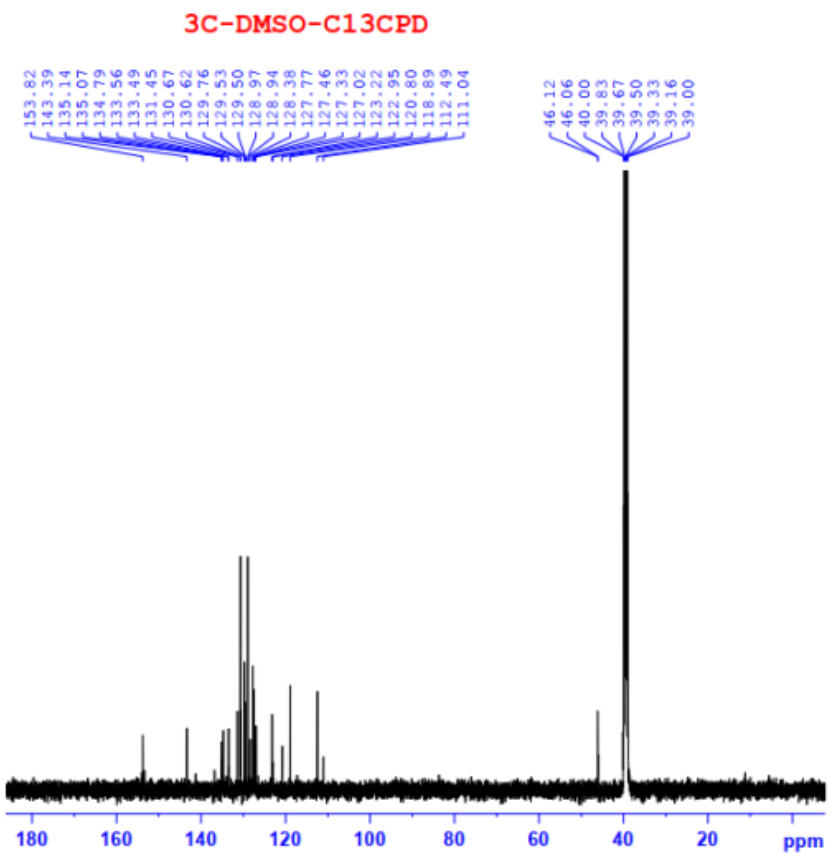
Compound 3s



BRUKER

```
Current Data Parameters
NAME                  1197_5B1
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190426
Time                    8.18
INSTRUM                 spect
PROBHD    5 mm PABBI 1H/
PULPROG                 zgpg30
TD                      65536
SOLVENT                 DMSO
NS                        256
DS                          4
SWH                31250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0485760 sec
RG                     198.57
DW                     16.000 usec
DE                      6.50 usec
TE                     304.2 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               125.7897032 MHz
NUC1                       13C
P1                       15.40 usec
PLW1               61.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               19.19999981 W
PLW12               0.12872000 W
PLW13               0.08288100 W

F2 - Processing parameters
SI                       32768
SF                 125.7759325 MHz
WDW                        EM
SSB                 0
LB                       1.00 Hz
GB                  0
PC                       1.40
```

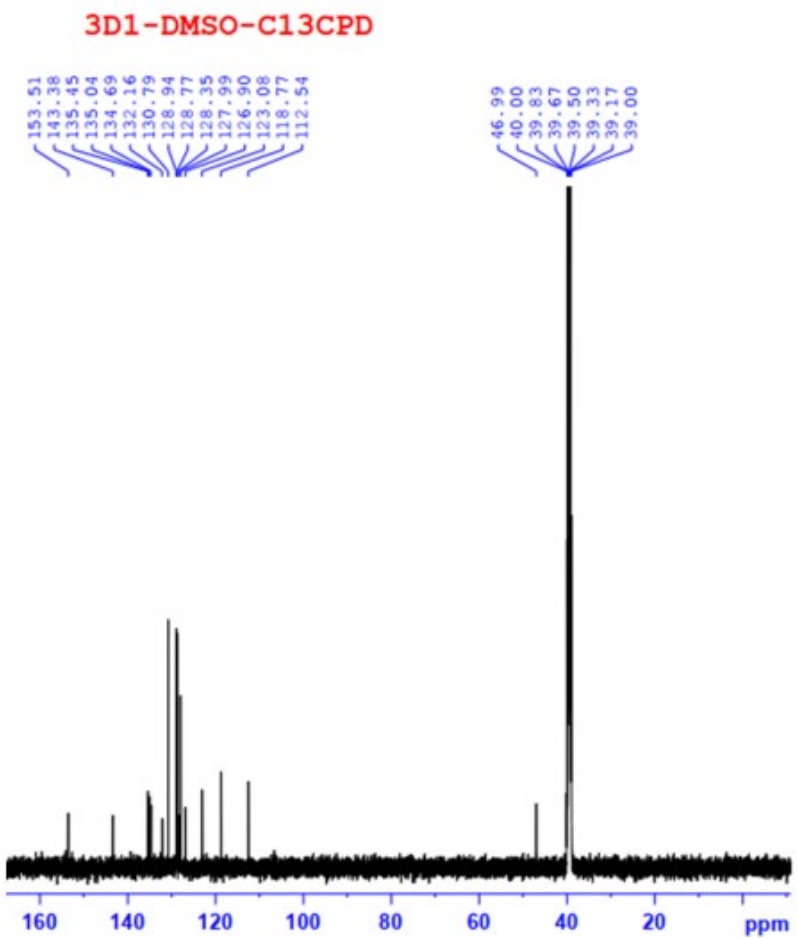
Compound 3t



BRUKER

```
Current Data Parameters
NAME                  119T_9C
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20190508
Time                    0.19
INSTRUM                 spect
PROBHD   5 mm PABBI 1H/
PULPROG                 zgpg30
TD                      65536
SOLVENT                 DMSO
NS                        512
DS                          4
SWH                31250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0485760 sec
RG                      198.57
DW                      16.000 usec
DE                       6.50 usec
TE                      303.5 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               125.7897032 MHz
NUC1                       13C
P1                       15.40 usec
PLW1               81.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               13.19999981 W
PLW12               0.12872000 W
PLW13               0.08228100 W

F2 - Processing parameters
SI                        32768
SF                 125.7789260 MHz
WDW                          EM
SSB                 0
LB                        1.00 Hz
GB                  0
PC                        1.40
```

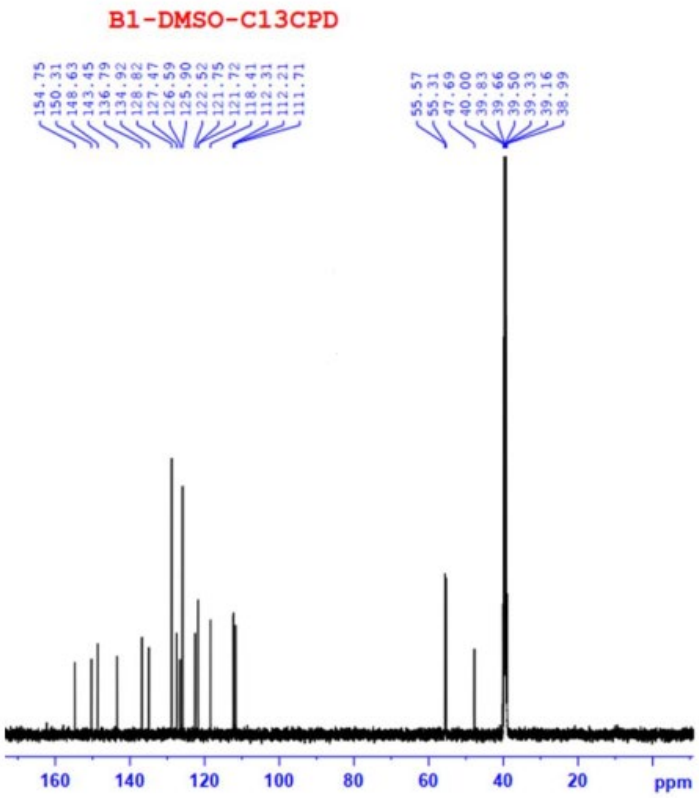
Compound 3w



BRUKER

```
Current Data Parameters
NAME                  1197_3D1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190426
Time                    8.01
INSTRUM                 spect
PROBHD   5 mm PABBI 1H/
PULPROG                 zgpg30
TD                      65536
SOLVENT                 DMSO
NS                        512
DS                          4
SWH                 31250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0485760 sec
RG                     198.57
DW                     16.000 usec
DE                      6.50 usec
TE                     304.3 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               125.7897032 MHz
NUC1                       13C
P1                       15.40 usec
PLW1               81.00000000 W

======== CHANNEL f2 ========
SFO2               500.2099008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               13.19999981 W
PLW12               0.12872000 W
PLW13               0.08298100 W

F2 - Processing parameters
SI                       32768
SF                 125.7759948 MHz
WDW                         EM
SSB                  0
LB                       1.00 Hz
GB                   0
PC                       1.40
```

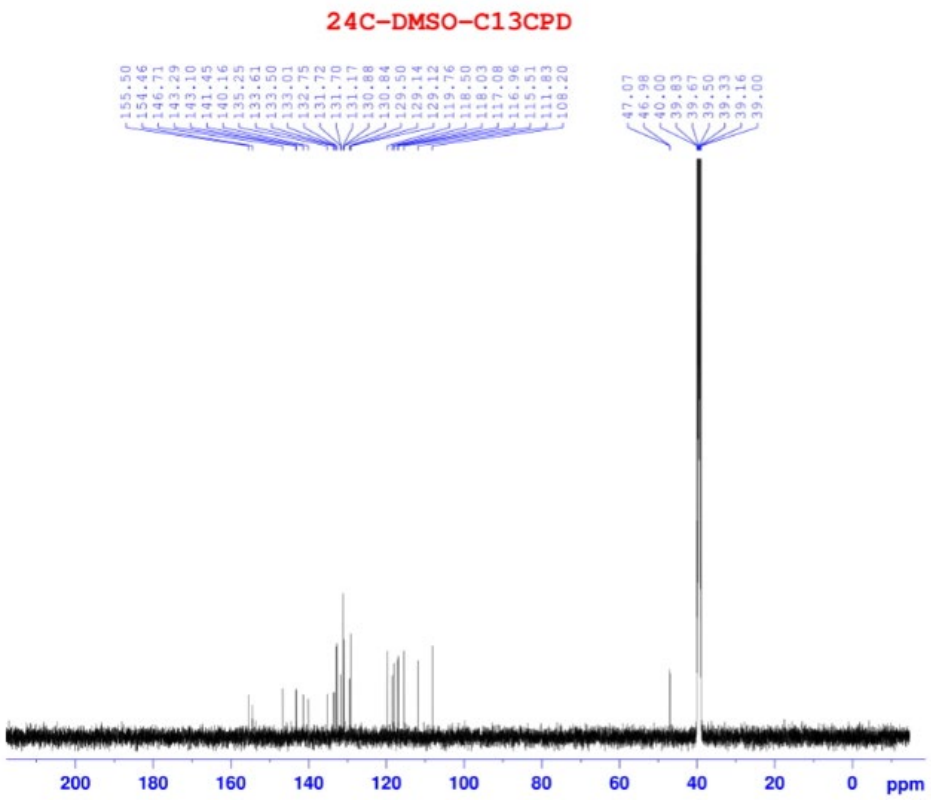
Compound 3x



BRUKER

```
Current Data Parameters
NAME                  1197_SB1
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190426
Time                    8.18
INSTRUM                 spect
PROBHD     5 mm PABBI 1H/
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                         256
DS                           4
SWH               31250.000 Hz
FIDRES                0.476837 Hz
AQ                    1.0485760 sec
RG                       198.57
DW                      16.000 usec
DE                       6.50 usec
TE                      304.2 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SF01              125.7897032 MHz
NUC1                      13C
P1                      15.40 usec
PLW1             81.00000000 W

======== CHANNEL f2 ========
SF02              500.2039008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2             19.19999981 W
PLW12             0.12872000 W
PLW13             0.08298100 W

F2 - Processing parameters
SI                       32768
SF                125.7750325 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

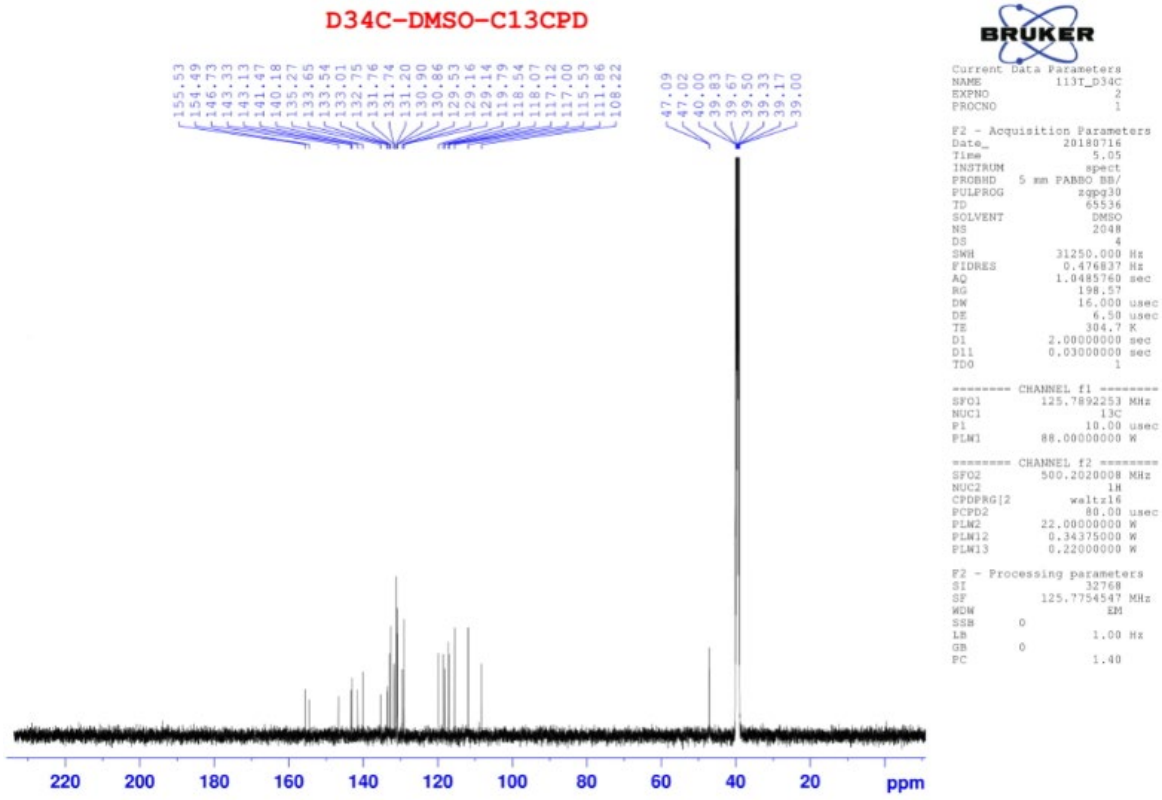
Compound 4a



BRUKER

```
Current Data Parameters
NAME                  113T_24C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20180705
Time                    3.55
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    3072
DS                       4
SWH                31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                   198.57
DW                  16.000 usec
DE                   6.50 usec
TE                  303.5 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1             125.7892253 MHz
NUC1                    13C
P1                   10.00 usec
PLW1            88.00000000 W

======== CHANNEL f2 ========
SFO2             500.2020008 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                80.00 usec
PLW2            22.00000000 W
PLW12            0.34375000 W
PLW13            0.22000000 W

F2 - Processing parameters
SI                      32768
SF               125.7754583 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

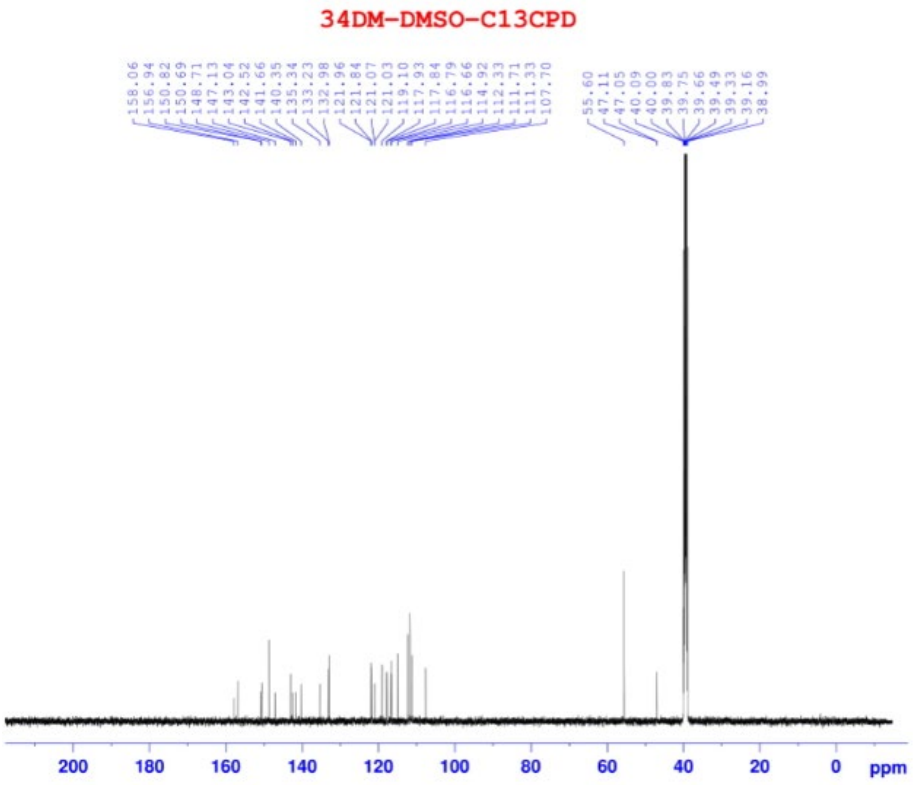
Compound 4b



BRUKER

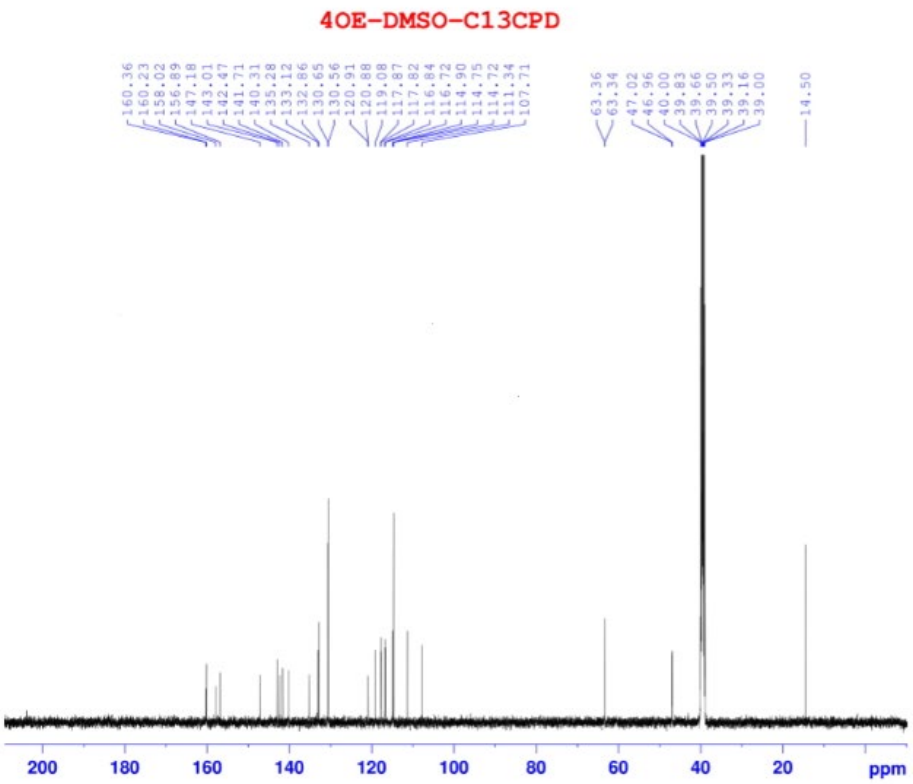
```
Current Data Parameters
NAME                  113T_D34C
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20180716
Time                     5.05
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                        2048
DS                           4
SWH                 31250.000 Hz
FIDRES                0.476837 Hz
AQ                    1.0485760 sec
RG                       198.57
DW                       16.000 usec
DE                        6.50 usec
TE                       304.7 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                125.7892253 MHz
NUC1                        13C
P1                        10.00 usec
PLW1                88.00000000 W

======== CHANNEL f2 ========
SFO2                500.2020008 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                22.00000000 W
PLW12                0.34375000 W
PLW13                0.22000000 W

F2 - Processing parameters
SI                        32768
SF                  125.7754547 MHz
WDW                          EM
SSB                  0
LB                        1.00 Hz
GB                   0
PC                        1.40
```

Compound 4c




```
Current Data Parameters
NAME                  113T_34DM
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20180705
Time                    9.21
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                        2048
DS                           4
SWH                 31250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0485760 sec
RG                      198.57
DW                      16.000 usec
DE                        6.50 usec
TE                       304.1 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1             125.7892253 MHz
NUC1                       13C
P1                       10.00 usec
PLW1             88.00000000 W

======== CHANNEL f2 ========
SFO2             500.2020008 MHz
NUC2                       1H
CPDPRG[2               waltz16
PCPD2                    80.00 usec
PLW2             22.00000000 W
PLW12             0.34375000 W
PLW13             0.22000000 W

F2 - Processing parameters
SI                        32768
SF               125.7754579 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

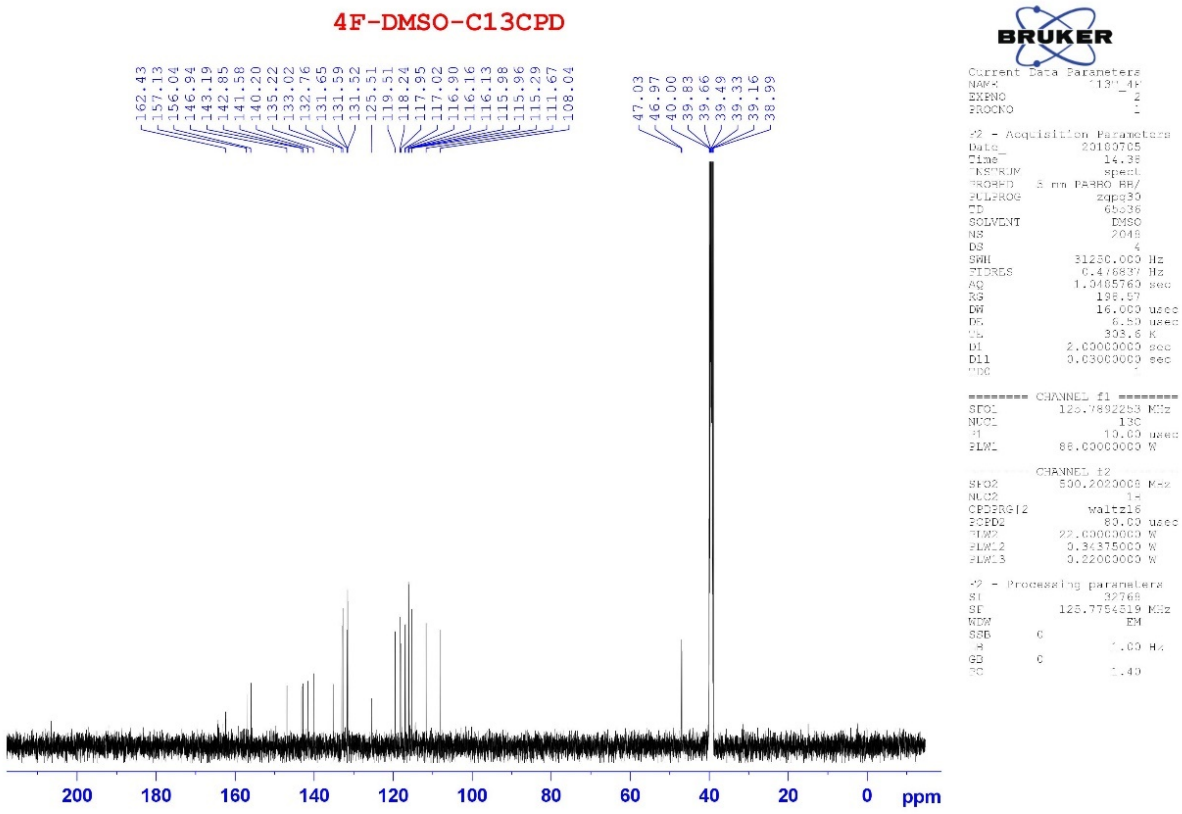
Compound 4d



BRUKER

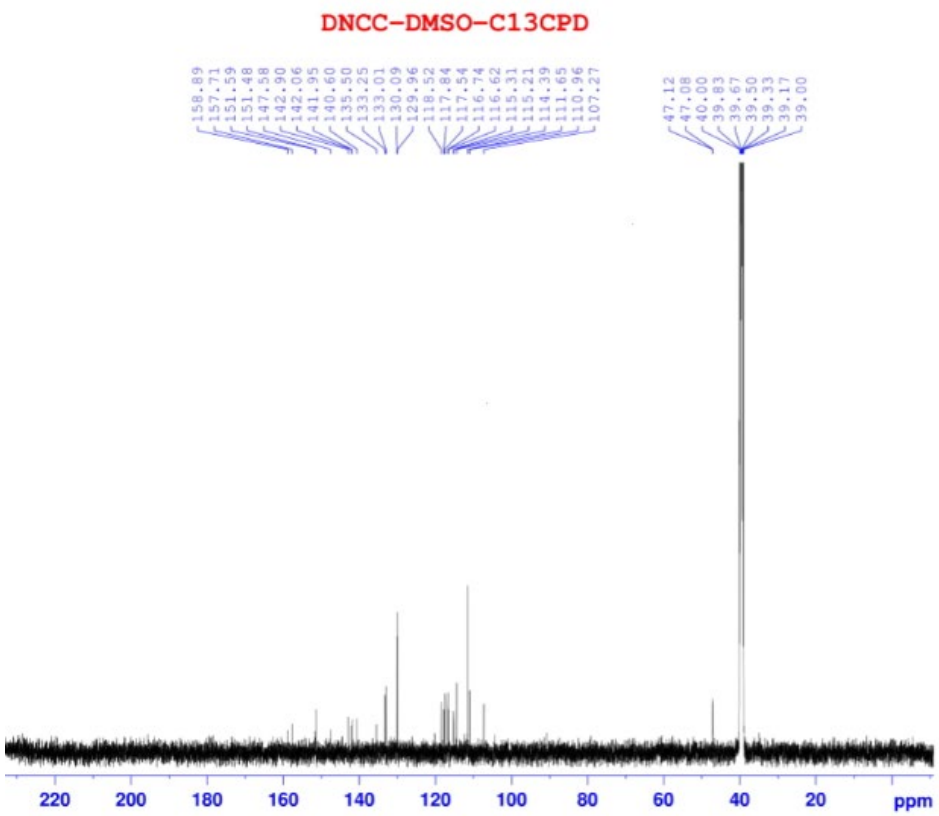
```
Current Data Parameters
NAME                  113T_4OE
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20180705
Time                   11.41
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     2048
DS                        4
SWH                31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                    198.57
DW                    16.000 usec
DE                     6.50 usec
TE                    303.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             125.7892253 MHz
NUC1                      13C
P1                      10.00 usec
PLW1             88.00000000 W

======== CHANNEL f2 ========
SFO2             500.2020008 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                   80.00 usec
PLW2             22.00000000 W
PLW12             0.34375000 W
PLW13             0.22000000 W

F2 - Processing parameters
SI                       32768
SF                 125.7754572 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

Compound 4e


4F-DMSO-C13CPD
162.43
157.13
156.04
146.84
143.19
142.85
141.58
140.20
135.22
133.02
132.76
131.65
131.59
131.52
125.51
119.51
118.24
117.95
117.02
116.90
116.16
116.13
115.98
115.96
115.29
111.67
108.04
47.03
46.97
40.00
39.83
39.66
39.49
39.33
39.16
38.99
200
180
160
140
120
100
80
60
40
20
0
ppm

BRUKER
Current Data Parameters
NAME 4F_4E
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180705
Time 14.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 198.57
DW 16.000 usec
DE 6.50 usec
TE 303.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.7892253 MHz
NUC1 13C
P1 10.00 usec
PLW1 88.00000000 W
CHANNEL f2
SFO2 500.2023008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 22.00000000 W
PLW12 0.34375000 W
PLW13 0.22000000 W
F2 - Processing parameters
SI 32768
SF 125.7754319 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

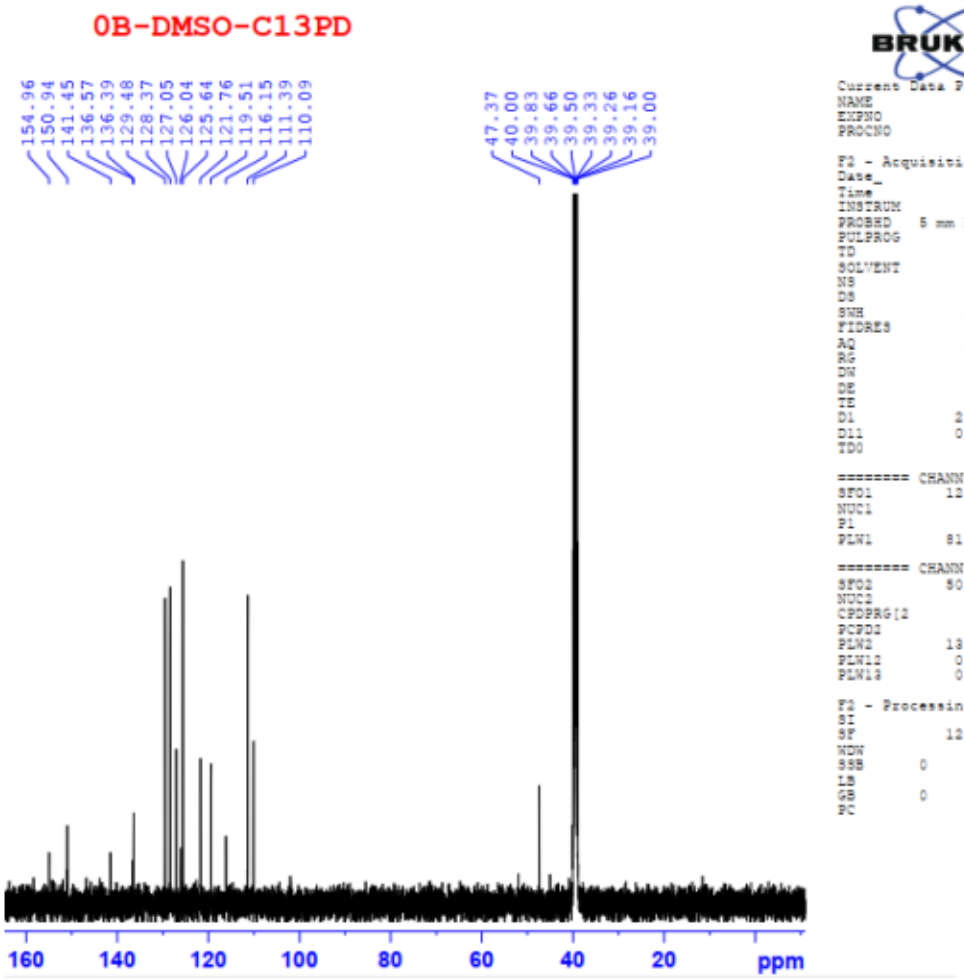
Compound 4f



BRUKER

```
Current Data Parameters
NAME                  113T_DNCC
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20180716
Time                      3.15
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       2048
DS                          4
SWH                 31250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0485760 sec
RG                     198.57
DW                   16.000 usec
DE                    6.50 usec
TE                    304.7 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1             125.7892253 MHz
NUC1                      13C
P1                      10.00 usec
PLW1             88.00000000 W

======== CHANNEL f2 ========
SFO2             500.2020008 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                   80.00 usec
PLW2             22.00000000 W
PLW12             0.34375000 W
PLW13             0.22000000 W

F2 - Processing parameters
SI                        32768
SF               125.7754541 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.00
```

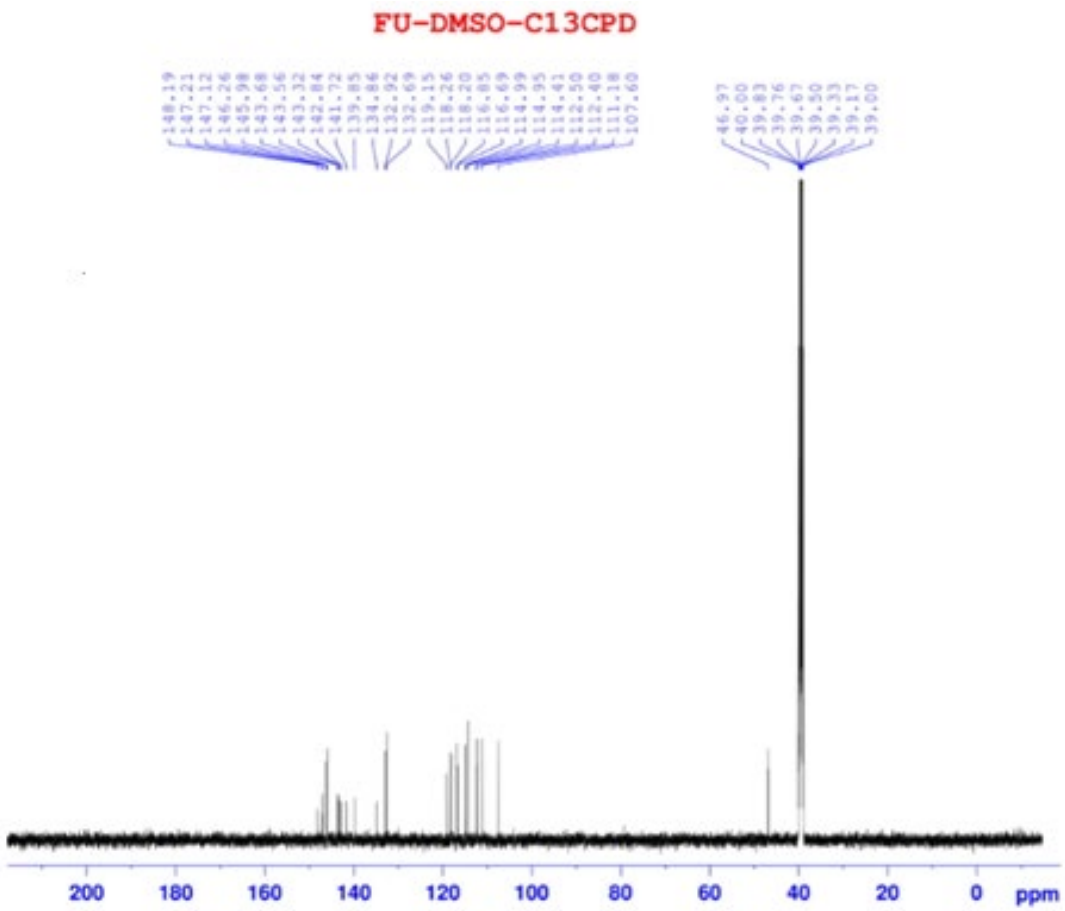
Compound 4k



BRUKER

```
Current Data Parameters
NAME                  1187_10B
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20190819
Time                    12.30
INSTRUM                 spect
PROBHD    5 mm PABBI 1H/
PULPROG                 zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       2048
DS                          4
SWH                 31250.000 Hz
FIDRES              0.476837 Hz
AQ                  1.0485760 sec
RG                      196.57
DW                      16.000 usec
DE                       6.50 usec
TE                      353.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               125.7897031 MHz
NUC1                       13C
P1                       15.40 usec
PLW1               81.00000000 W

======== CHANNEL f2 ========
SFO2               500.2039008 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2               18.19999981 W
PLW12               0.12872000 W
PLW13               0.06238100 W

F2 - Processing parameters
SI                       32768
SF                 125.7758779 MHz
WDW                         EM
SSB                 0
LB                       1.00 Hz
GB                  0
PC                       1.40
```

Compound 4p

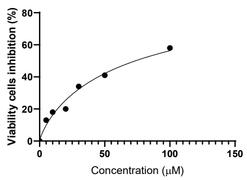
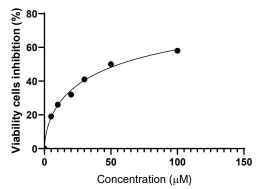
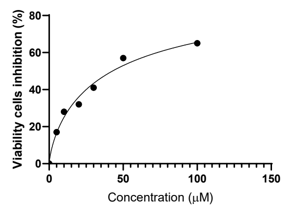
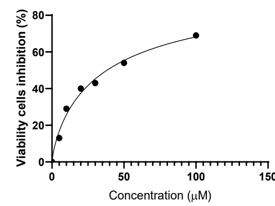
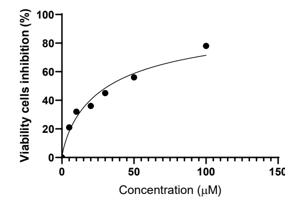
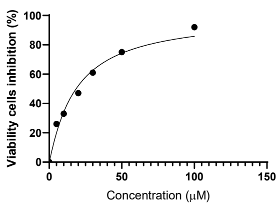
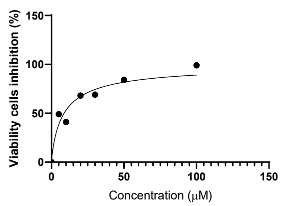
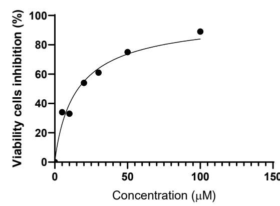
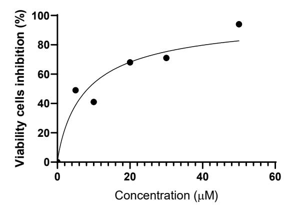
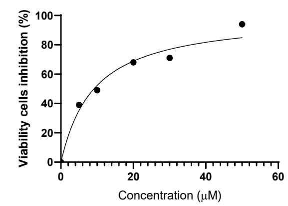
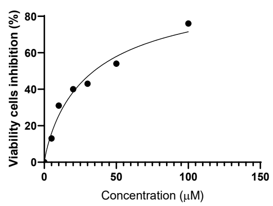
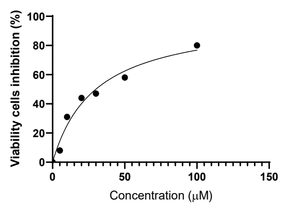
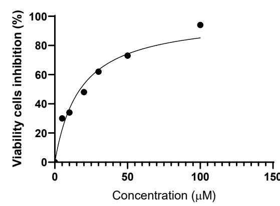
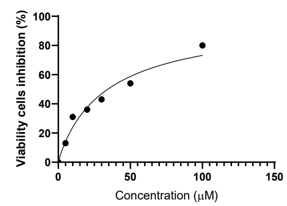
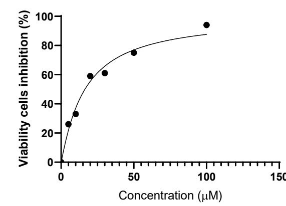


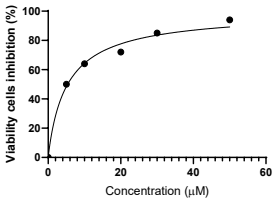
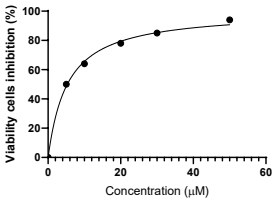
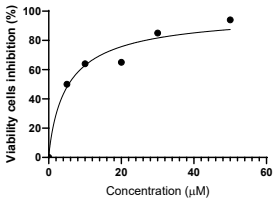
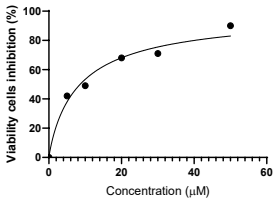
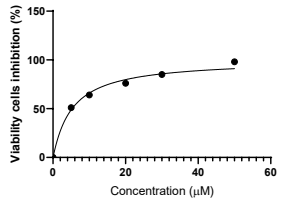
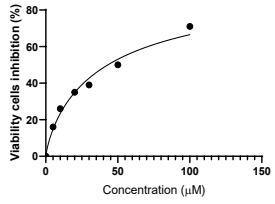
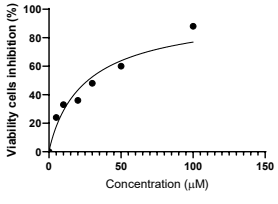
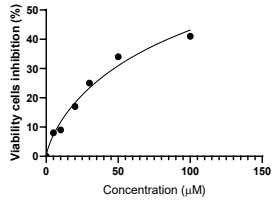
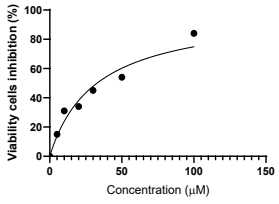
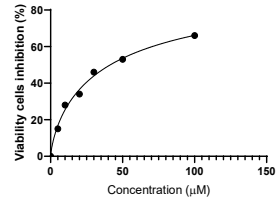
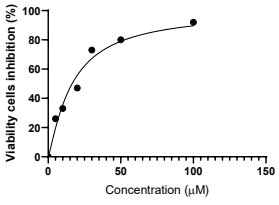
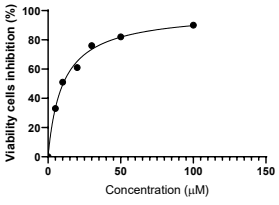
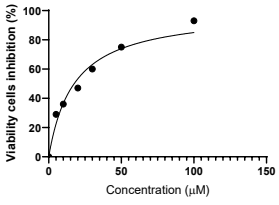
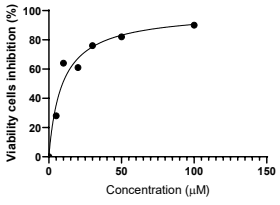
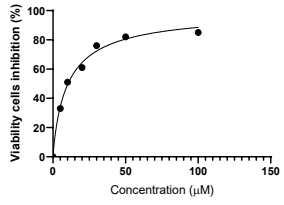
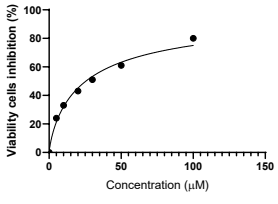
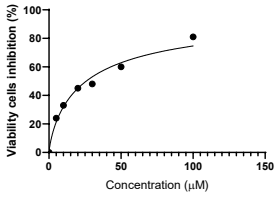
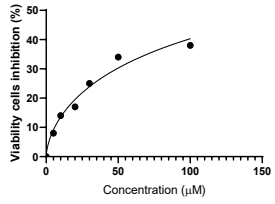
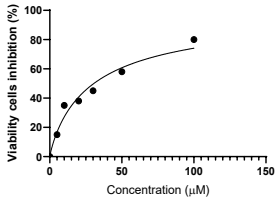
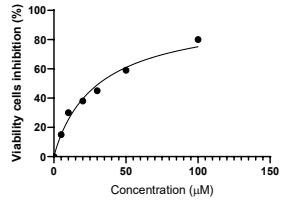
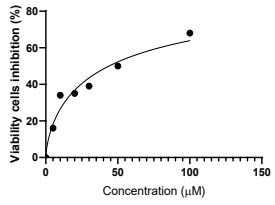
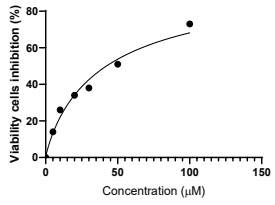
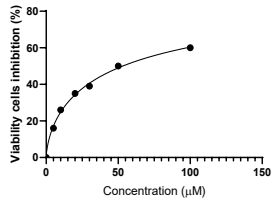
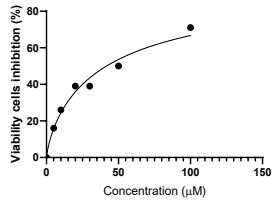
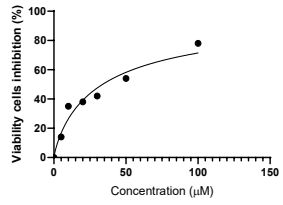
BRUKER

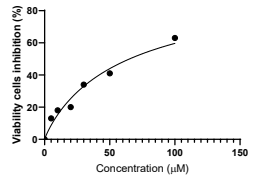
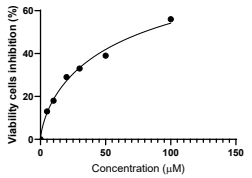
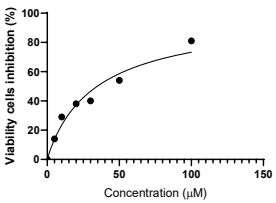
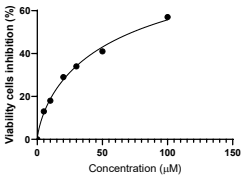
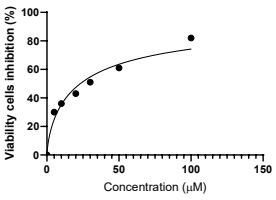
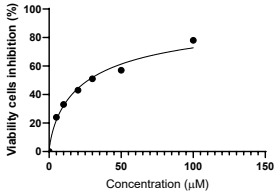
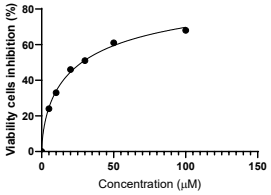
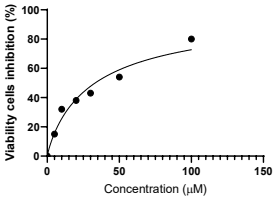
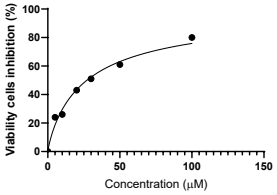
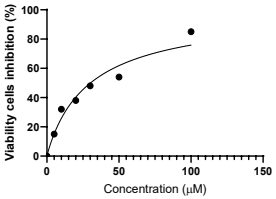
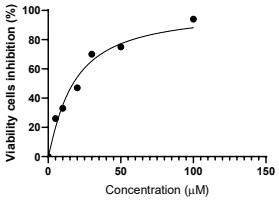
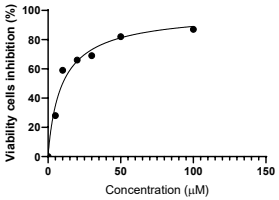
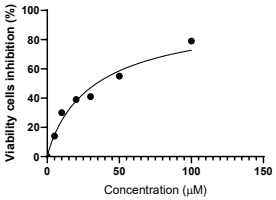
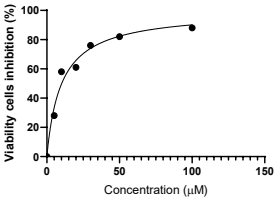
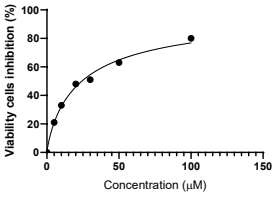
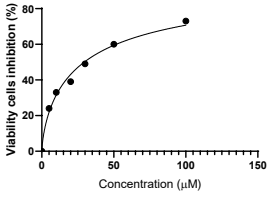
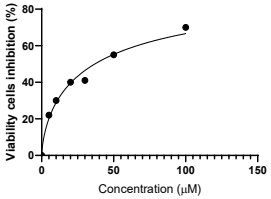
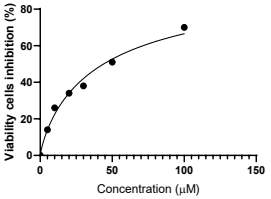
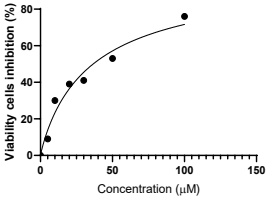
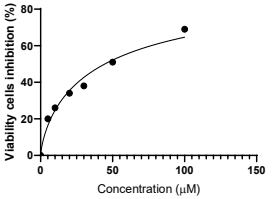
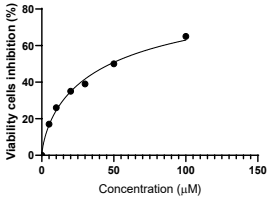
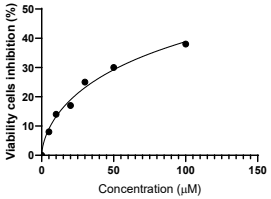
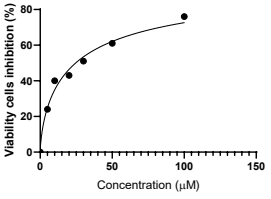
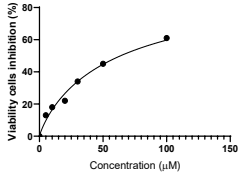
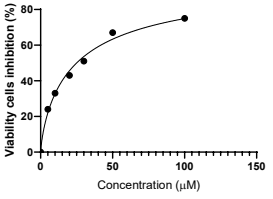
```
Current Data Parameters
NAME                  1137_FU
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20180705
Time                    7.32
INSTRUM                 spect
PROBHD     5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                DMSO
NS                      2048
DS                         4
SWH                31250.000 Hz
FIDRES             0.476837 Hz
AQ                 1.0485760 sec
RG                    198.57
DW                    16.000 usec
DE                     6.50 usec
TE                    304.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            125.7892253 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           88.00000000 W

======== CHANNEL f2 ========
SFO2            500.2020008 MHz
NUC2                    1H
CPDPRG[2          waltz16
PCPD2                 80.00 usec
PLW2           22.00000000 W
PLW12           0.34375000 W
PLW13           0.22000000 W

F2 - Processing parameters
SI                     32768
SF              125.7754572 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

THE CONCENTRATION-RESPONSE CURVES FOR IC_{50} VALUES

(ANTICANCER ACTIVITY)

Compound	HepG2	MDA-MB-231	MCF7	C26	RMS
1a					
	R^2 = 0.9777	R^2 = 0.9951	R^2 = 0.9843	R^2 = 0.9887	R^2 = 0.9711
1b					
	R^2 = 0.9818	R^2 = 0.9381	R^2 = 0.9729	R^2 = 0.9202	R^2 = 0.9723
1c					
	R^2 = 0.9760	R^2 = 0.9722	R^2 = 0.9694	R^2 = 0.9669	R^2 = 0.9812

1d					
	$R^2 = 0.9894$	$R^2 = 0.9970$	$R^2 = 0.9685$	$R^2 = 0.9785$	$R^2 = 0.9879$
1e					
	$R^2 = 0.9838$	$R^2 = 0.9425$	$R^2 = 0.9805$	$R^2 = 0.9552$	$R^2 = 0.9932$
1f					
	$R^2 = 0.9745$	$R^2 = 0.9953$	$R^2 = 0.9721$	$R^2 = 0.9594$	$R^2 = 0.9921$
1g					
	$R^2 = 0.9881$	$R^2 = 0.9798$	$R^2 = 0.9751$	$R^2 = 0.9674$	$R^2 = 0.9840$
1h					
	$R^2 = 0.9633$	$R^2 = 0.9801$	$R^2 = 0.9971$	$R^2 = 0.9799$	$R^2 = 0.9554$

1i					
	$R^2 = 0.9710$	$R^2 = 0.9922$	$R^2 = 0.9629$	$R^2 = 0.9960$	$R^2 = 0.9681$
1j					
	$R^2 = 0.9857$	$R^2 = 0.9974$	$R^2 = 0.9647$	$R^2 = 0.9845$	$R^2 = 0.9580$
1k					
	$R^2 = 0.9750$	$R^2 = 0.9746$	$R^2 = 0.9554$	$R^2 = 0.9781$	$R^2 = 0.9928$
1l					
	$R^2 = 0.9910$	$R^2 = 0.9849$	$R^2 = 0.9864$	$R^2 = 0.9671$	$R^2 = 0.9798$
1m					

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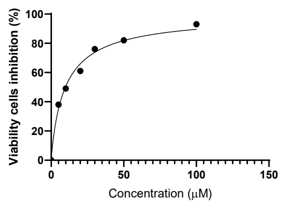
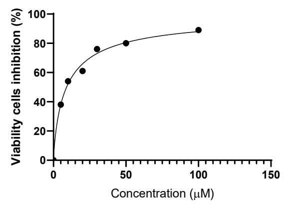
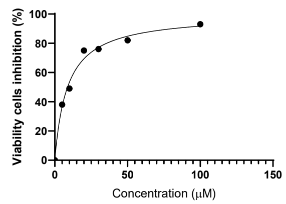
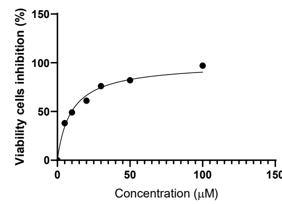
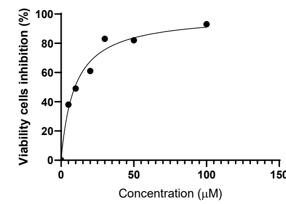
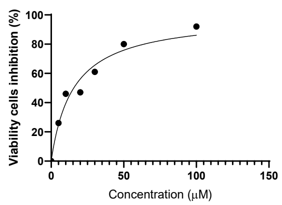
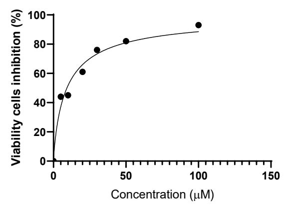
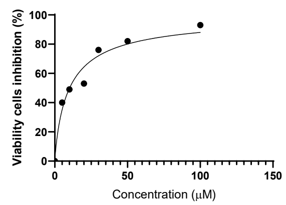
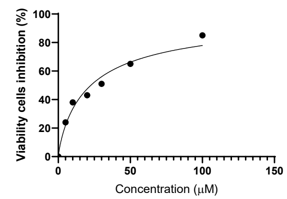
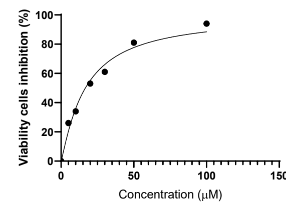
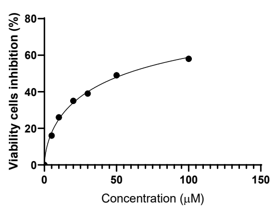
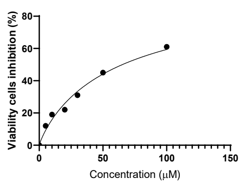
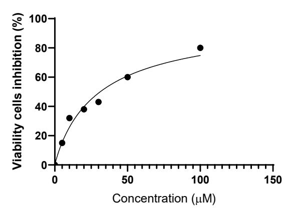
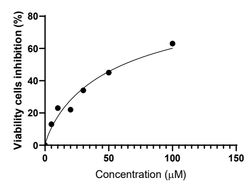
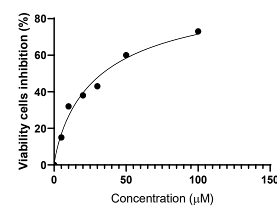
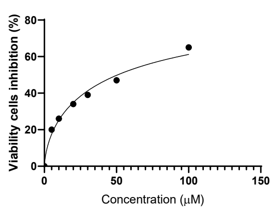
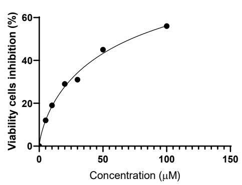
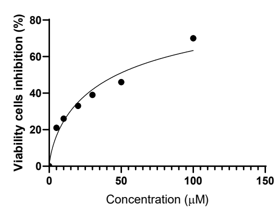
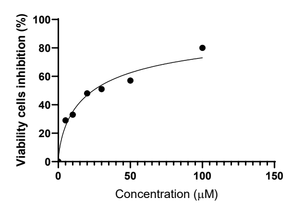
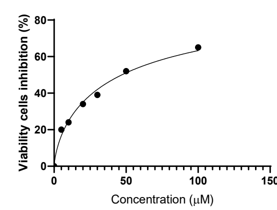
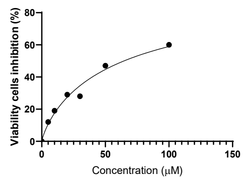
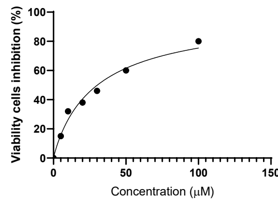
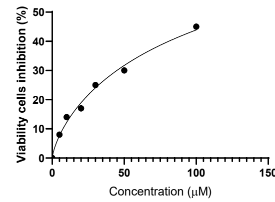
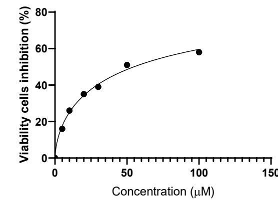
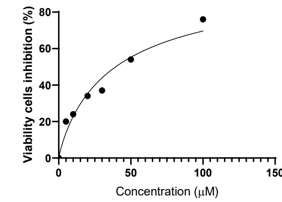
1n					
	$R^2 = 0.9912$	$R^2 = 0.9932$	$R^2 = 0.9898$	$R^2 = 0.9852$	$R^2 = 0.9809$
1o					
	$R^2 = 0.9657$	$R^2 = 0.9752$	$R^2 = 0.9663$	$R^2 = 0.9731$	$R^2 = 0.9829$
1p					
	$R^2 = 0.9968$	$R^2 = 0.9836$	$R^2 = 0.9748$	$R^2 = 0.9701$	$R^2 = 0.9836$
1q					
	$R^2 = 0.9862$	$R^2 = 0.9931$	$R^2 = 0.9630$	$R^2 = 0.9713$	$R^2 = 0.9906$

2a					
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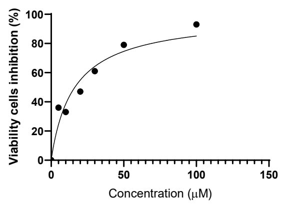
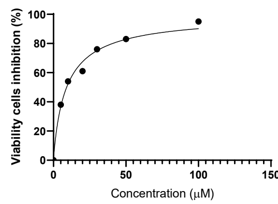
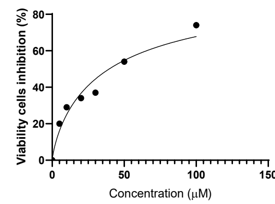
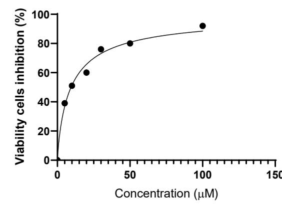
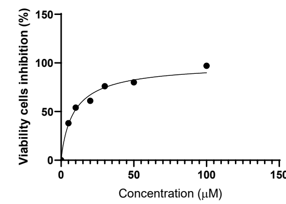
2b					
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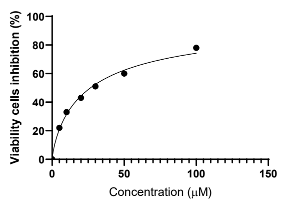
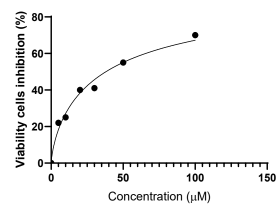
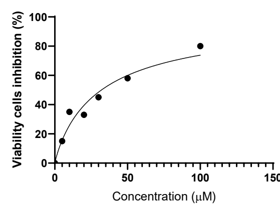
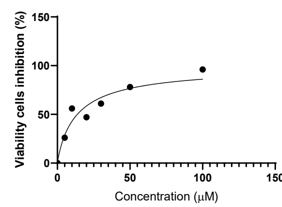
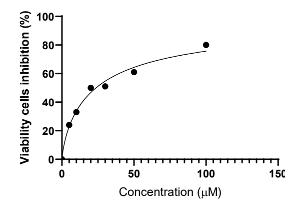
2c					
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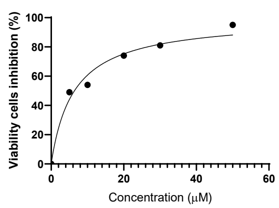
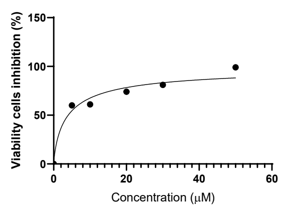
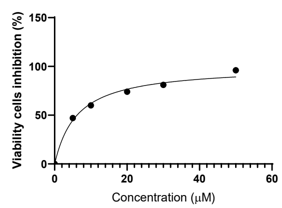
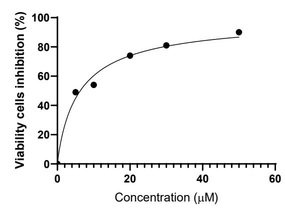
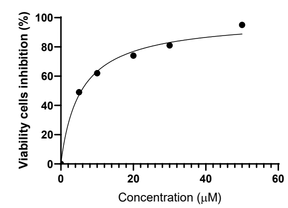
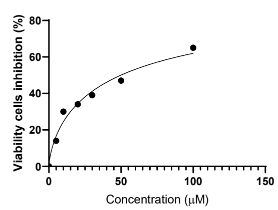
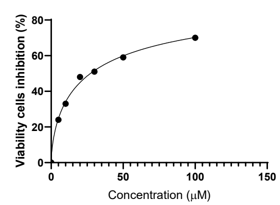
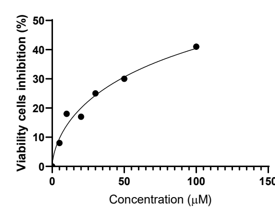
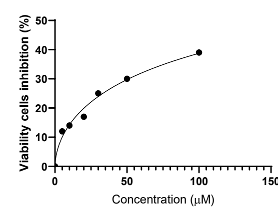
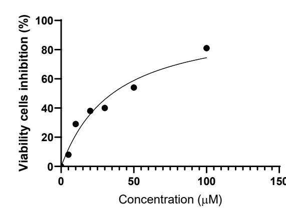
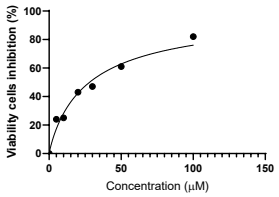
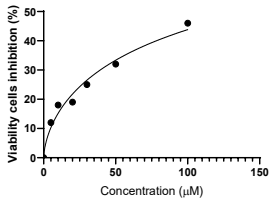
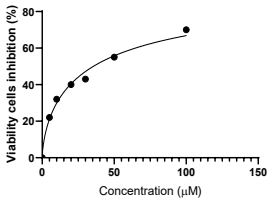
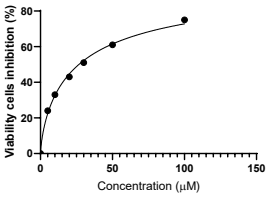
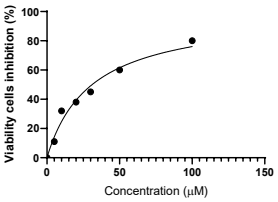
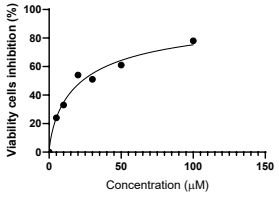
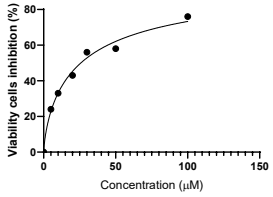
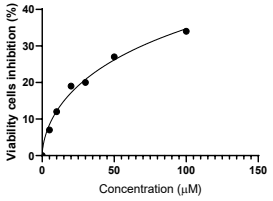
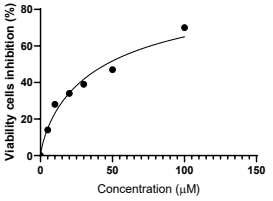
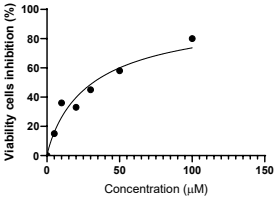
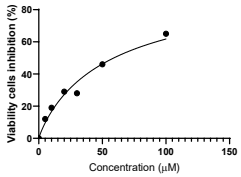
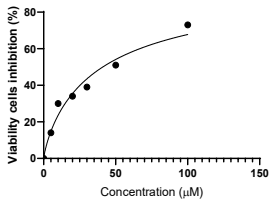
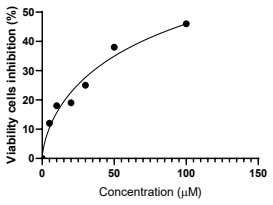
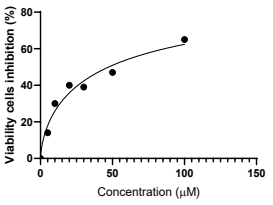
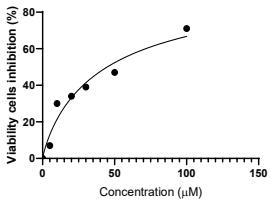
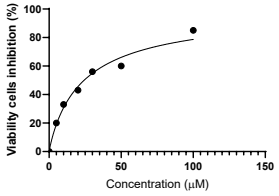
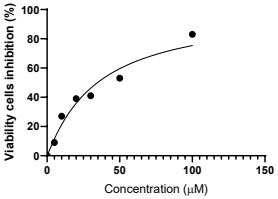
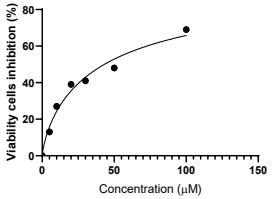
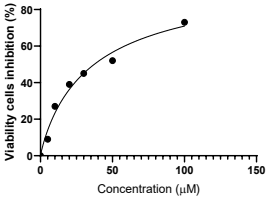
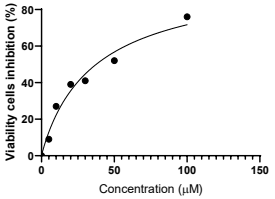
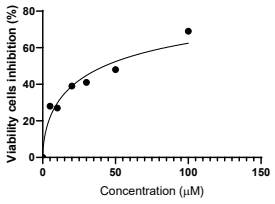
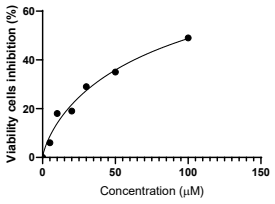
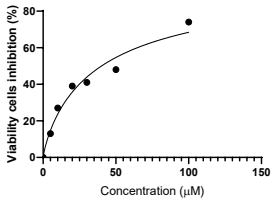
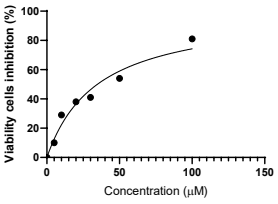
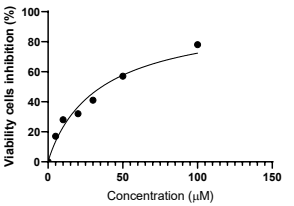
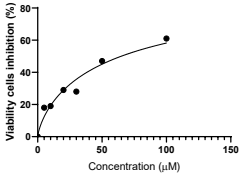
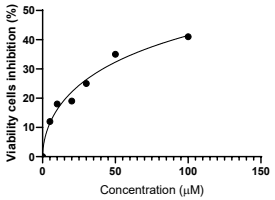
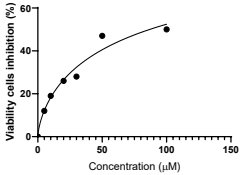
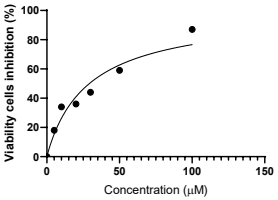
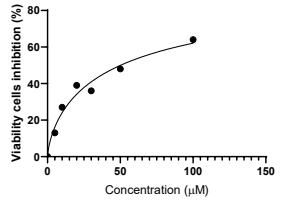
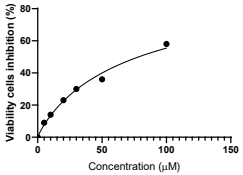
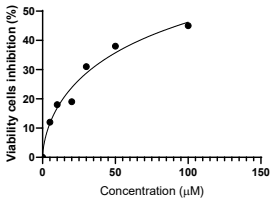
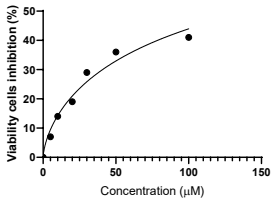
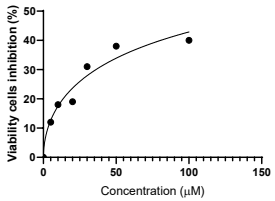
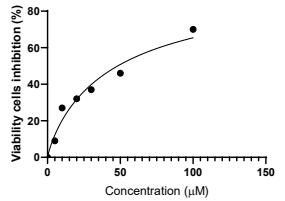
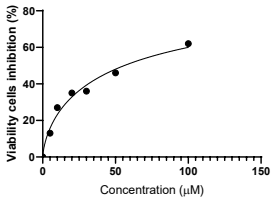
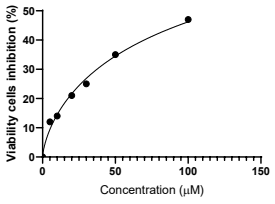
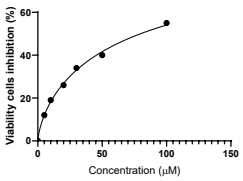
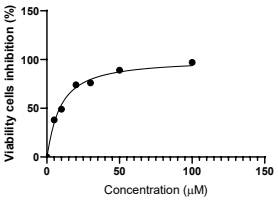
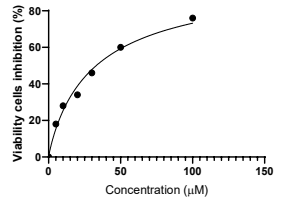
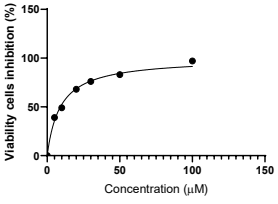
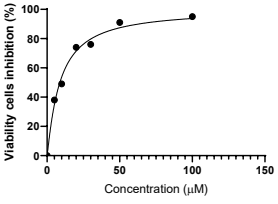
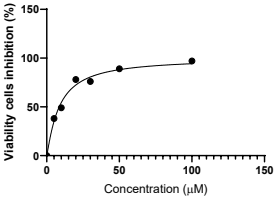
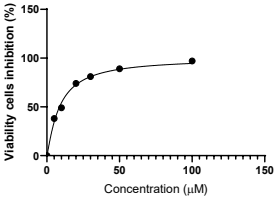
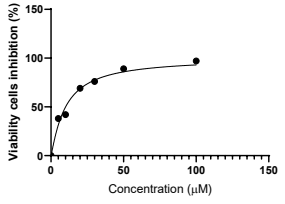
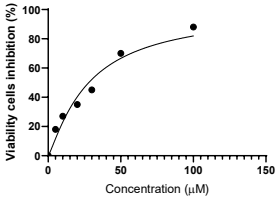
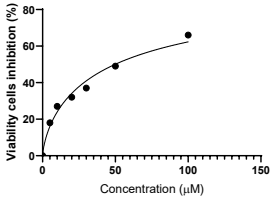
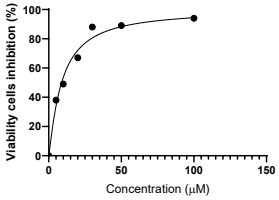
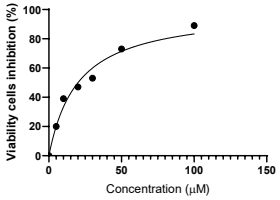
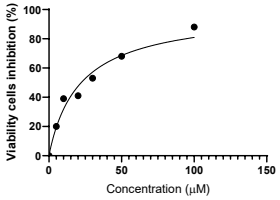
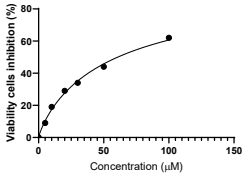
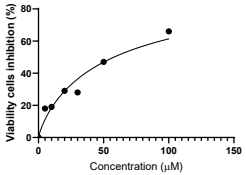
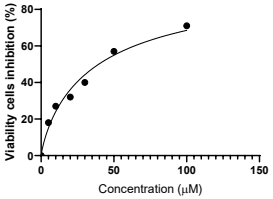
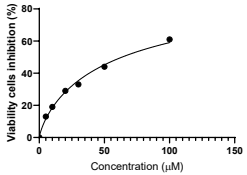
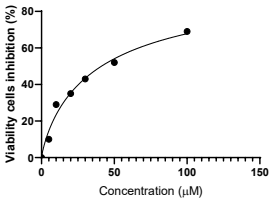
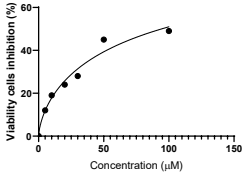
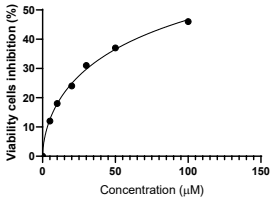
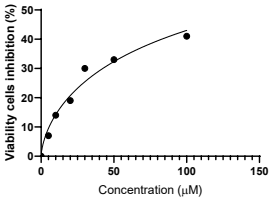
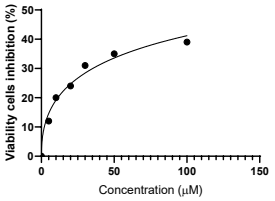
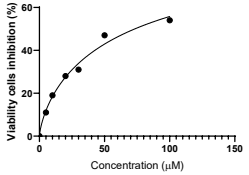
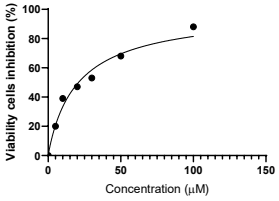
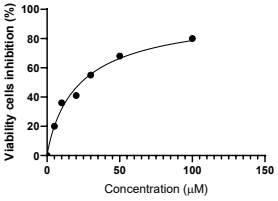
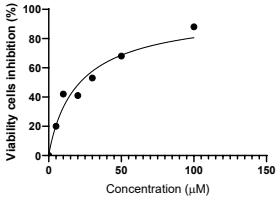
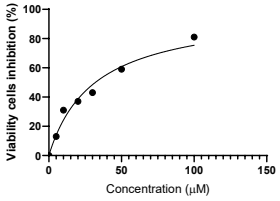
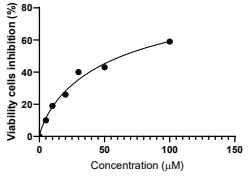
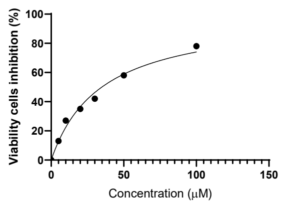
2d					
	R^2 = 0.9787	R^2 = 0.9628	R^2 = 0.9883	R^2 = 0.9870	R^2 = 0.9900
2e					

	$R^2 = 0.9776$	$R^2 = 0.9964$	$R^2 = 0.9744$	$R^2 = 0.9861$	$R^2 = 0.9608$
2f					
	$R^2 = 0.9735$	$R^2 = 0.9786$	$R^2 = 0.9890$	$R^2 = 0.9967$	$R^2 = 0.9775$
2g					
	$R^2 = 0.9798$	$R^2 = 0.9892$	$R^2 = 0.9911$	$R^2 = 0.9740$	$R^2 = 0.9522$
2h					
	$R^2 = 0.9732$	$R^2 = 0.9702$	$R^2 = 0.9738$	$R^2 = 0.9699$	$R^2 = 0.9527$
2i					
	$R^2 = 0.9805$	$R^2 = 0.9617$	$R^2 = 0.9792$	$R^2 = 0.9814$	$R^2 = 0.9736$

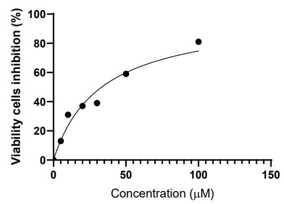
2j					
	$R^2 = 0.9550$	$R^2 = 0.9802$	$R^2 = 0.9690$	$R^2 = 0.9653$	$R^2 = 0.9718$
2k					
	$R^2 = 0.9575$	$R^2 = 0.9801$	$R^2 = 0.9652$	$R^2 = 0.9456$	$R^2 = 0.9731$
2l					
	$R^2 = 0.9890$	$R^2 = 0.9751$	$R^2 = 0.9726$	$R^2 = 0.9550$	$R^2 = 0.9667$
2m					
	$R^2 = 0.9818$	$R^2 = 0.9919$	$R^2 = 0.9971$	$R^2 = 0.9906$	$R^2 = 0.9874$
2n					

	$R^2 = 0.9913$	$R^2 = 0.9903$	$R^2 = 0.9859$	$R^2 = 0.9933$	$R^2 = 0.9806$
2o					
	$R^2 = 0.9663$	$R^2 = 0.9821$	$R^2 = 0.9831$	$R^2 = 0.9772$	$R^2 = 0.9862$
2p					
	$R^2 = 0.9952$	$R^2 = 0.9493$	$R^2 = 0.9814$	$R^2 = 0.9943$	$R^2 = 0.9827$
2q					
	$R^2 = 0.9713$	$R^2 = 0.9977$	$R^2 = 0.9738$	$R^2 = 0.9810$	$R^2 = 0.9865$
3a					
	$R^2 = 0.9450$	$R^2 = 0.9885$	$R^2 = 0.9585$	$R^2 = 0.9743$	$R^2 = 0.9865$

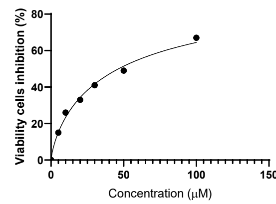
3b



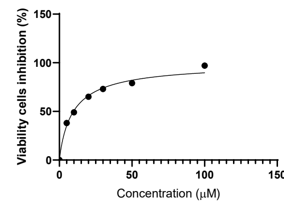
R^2 = 0.9861



R^2 = 0.9615



R^2 = 0.9927



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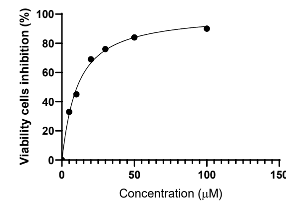
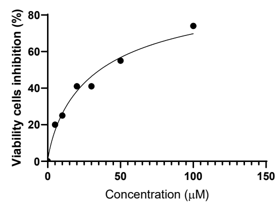


R^2 = 0.9958

3c



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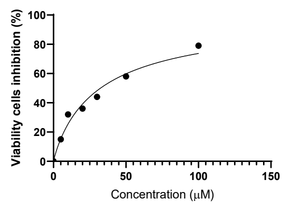

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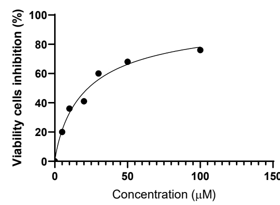
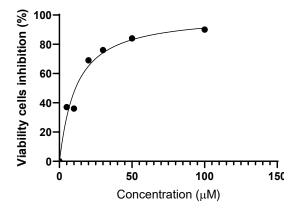


R^2 = 0.9834



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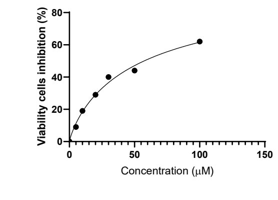
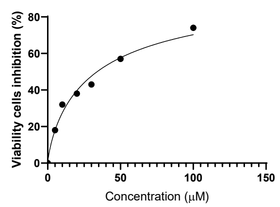
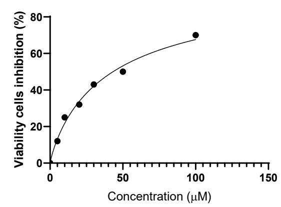


R^2 = 0.9905

3d



R^2 = 0.9836



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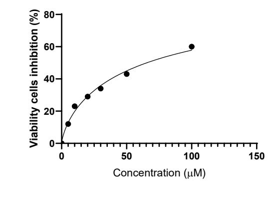
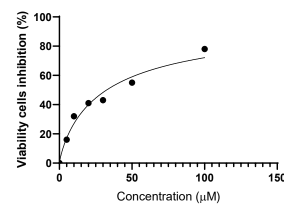


R^2 = 0.9901



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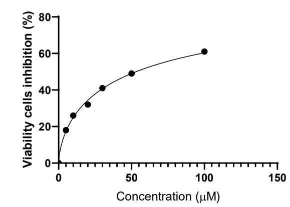
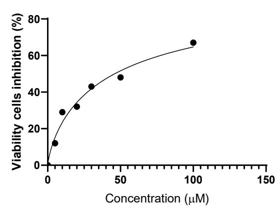


R^2 = 0.9968

3e



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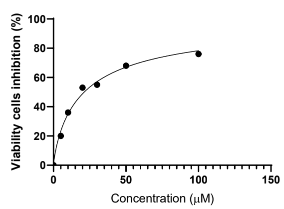

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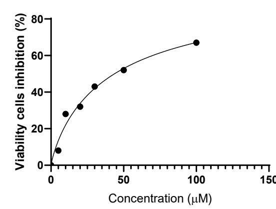

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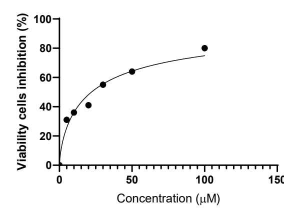

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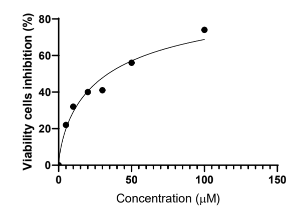
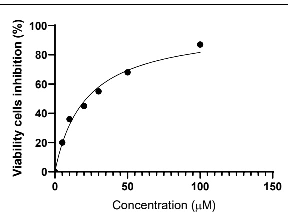
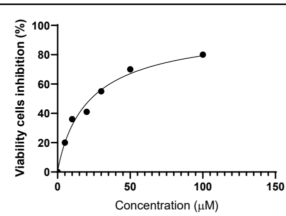
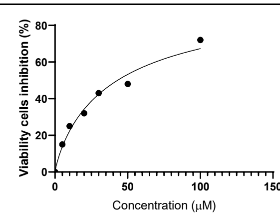


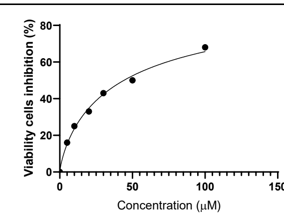
R^2 = 0.9740

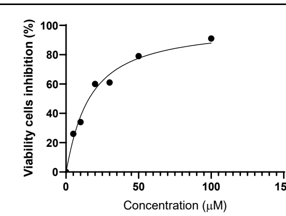
3f











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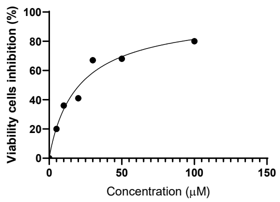
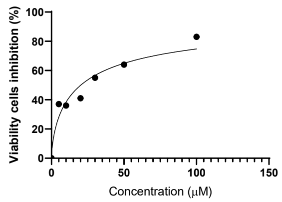
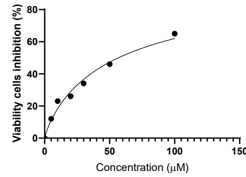
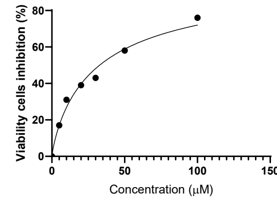
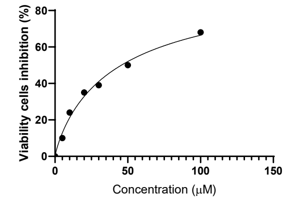
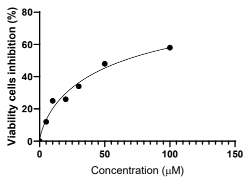
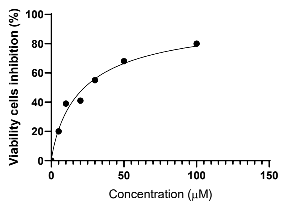
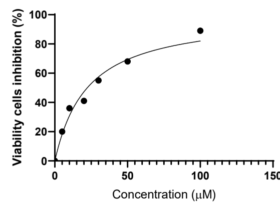
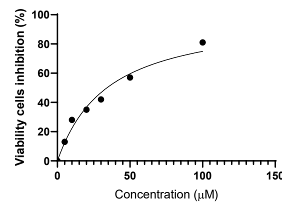
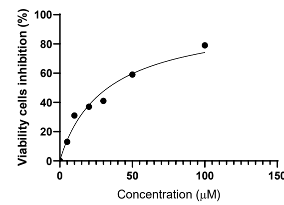
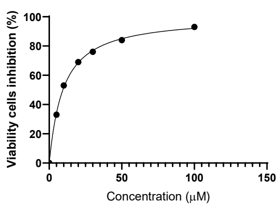
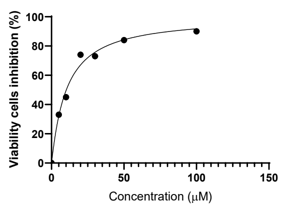
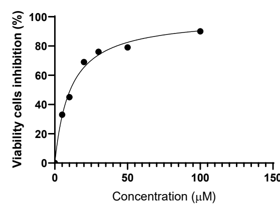
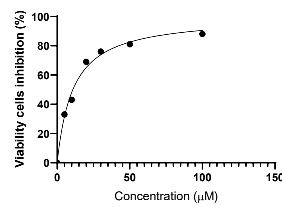
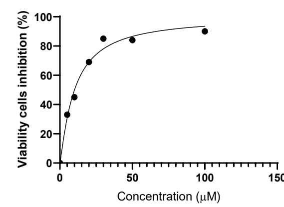
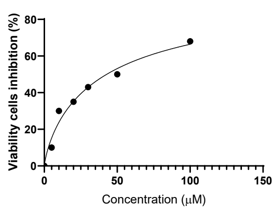
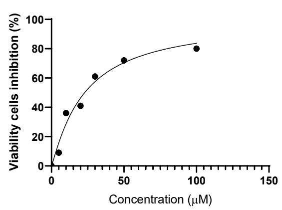
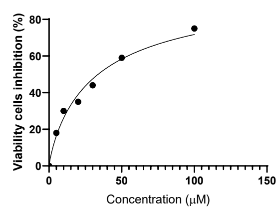
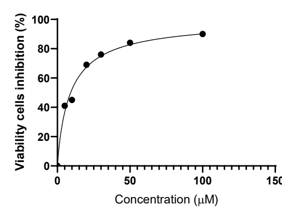
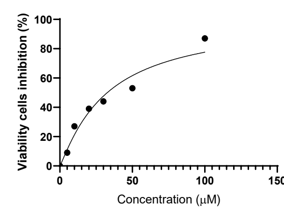
3g					
	R^2 = 0.9702	R^2 = 0.9421	R^2 = 0.9823	R^2 = 0.9839	R^2 = 0.9904
3h					
	R^2 = 0.9789	R^2 = 0.9816	R^2 = 0.9761	R^2 = 0.9767	R^2 = 0.9724
3i					
	R^2 = 0.9990	R^2 = 0.9874	R^2 = 0.9928	R^2 = 0.9907	R^2 = 0.9858
3j					
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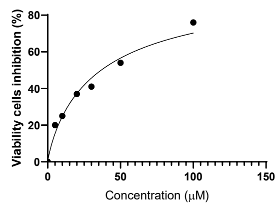
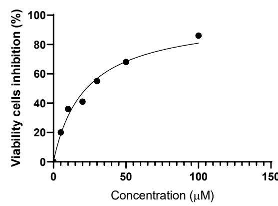
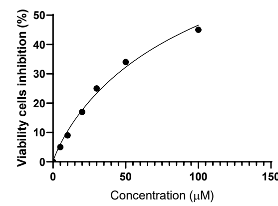
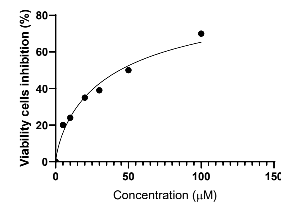
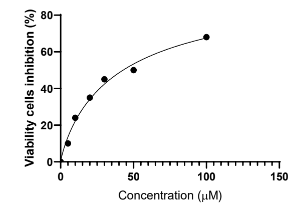
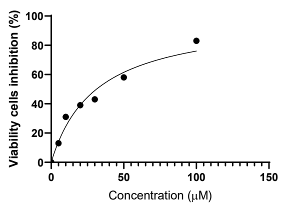
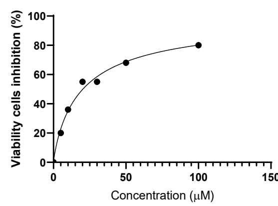
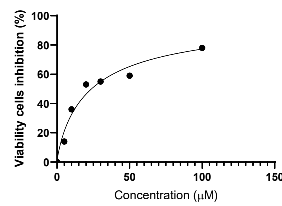
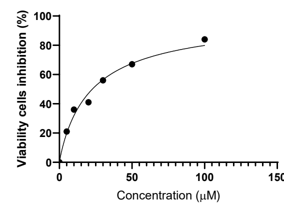
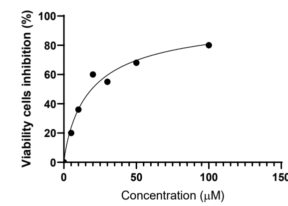
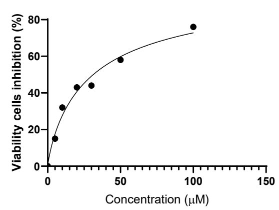
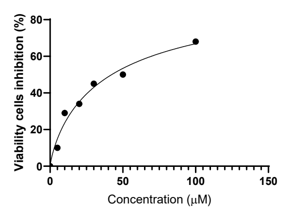
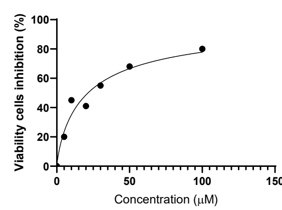
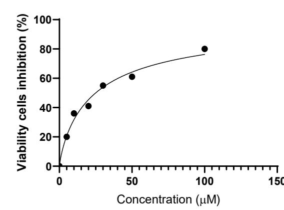
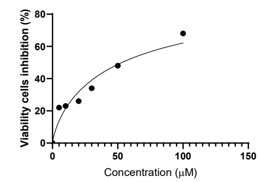
3k					
	R^2 = 0.9769	R^2 = 0.9820	R^2 = 0.9926	R^2 = 0.9803	R^2 = 0.9896
3l					
	R^2 = 0.9919	R^2 = 0.9895	R^2 = 0.9671	R^2 = 0.9847	R^2 = 0.9748
3m					
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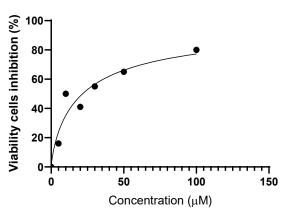
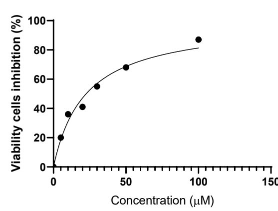
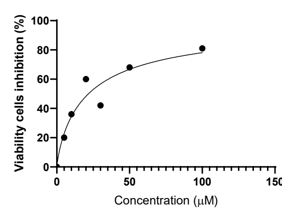
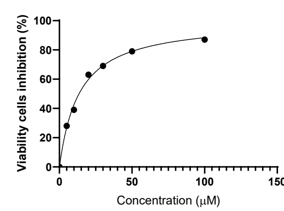
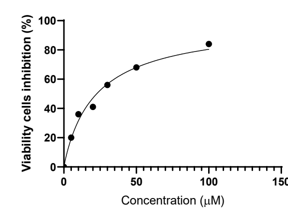
3n					
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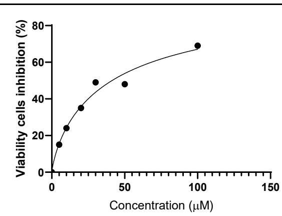
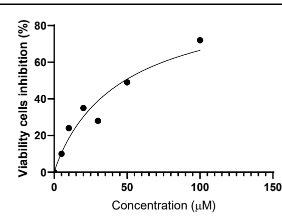
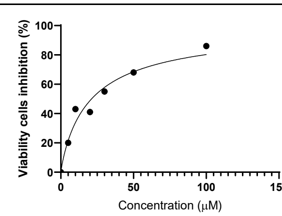
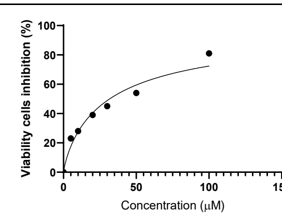
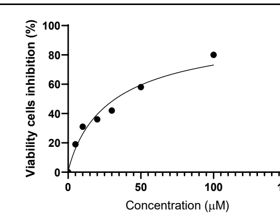
3o					

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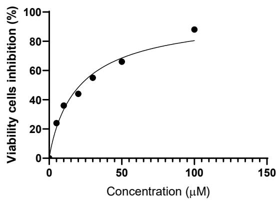
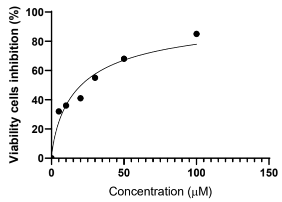
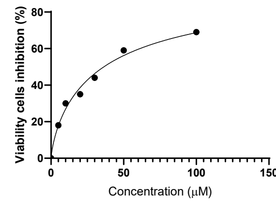
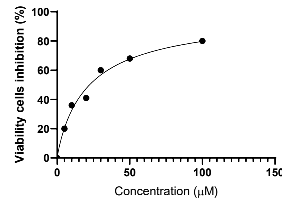
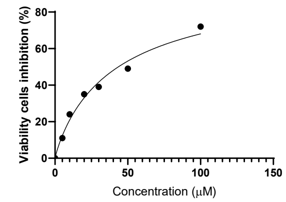
3p					
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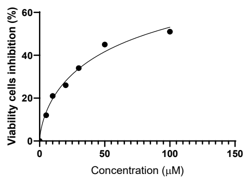
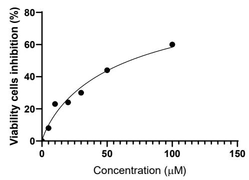
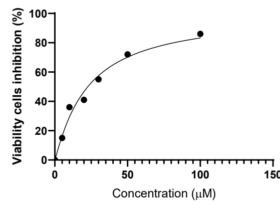
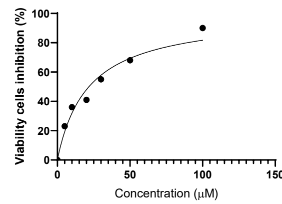
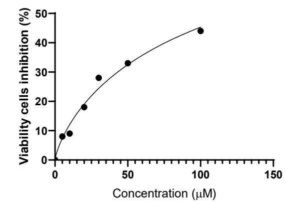
3q					
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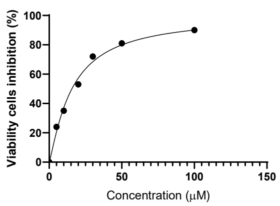
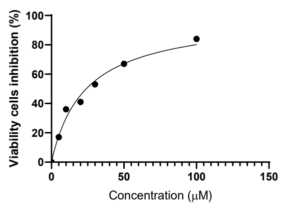
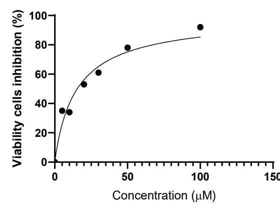
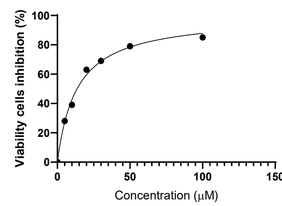
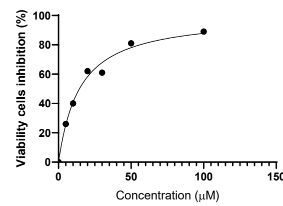
3r					
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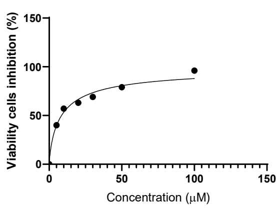
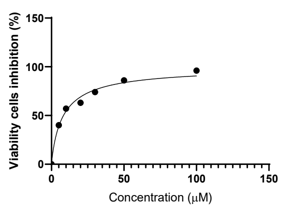
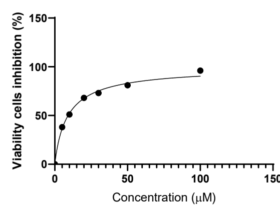
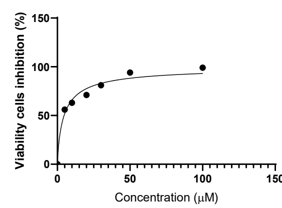
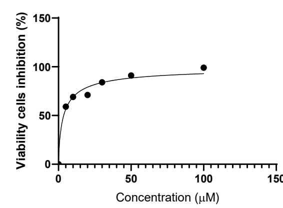
3s					
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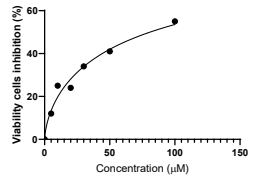
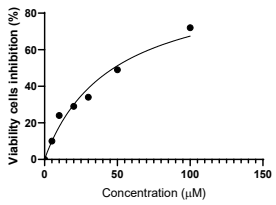
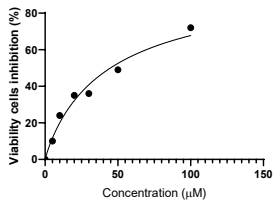
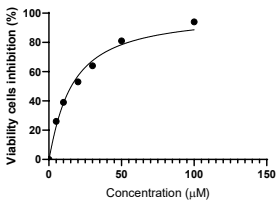
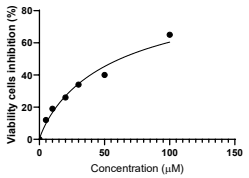
3t					
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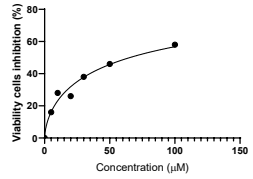
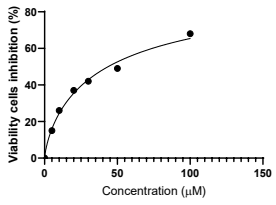
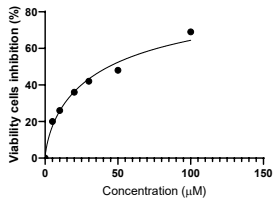
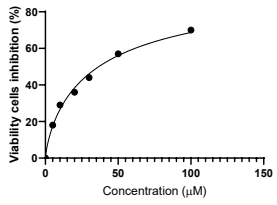
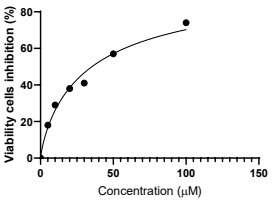
3u					
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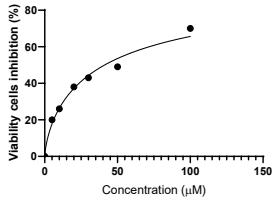
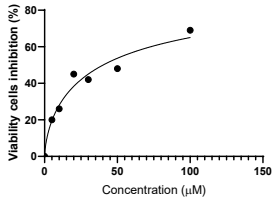
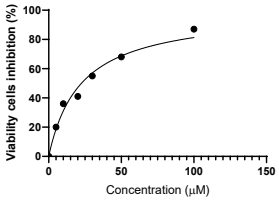
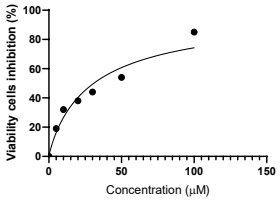
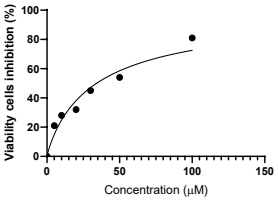
3v					
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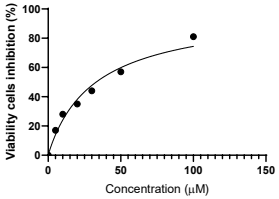
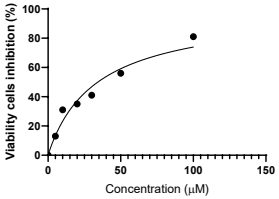
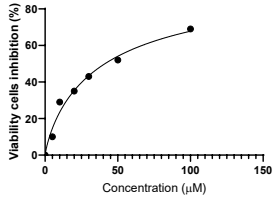
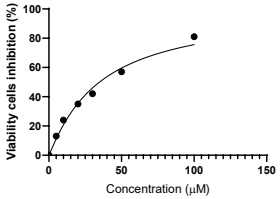
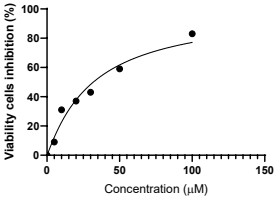
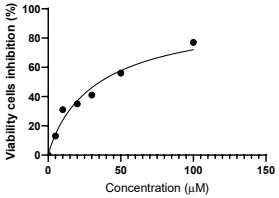
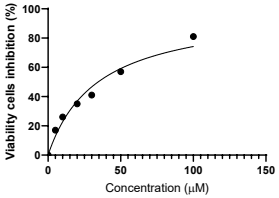
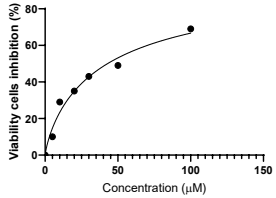
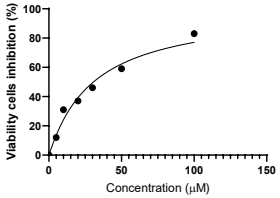
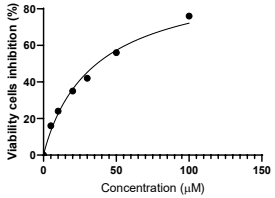
3w					
	$R^2 = 0.9764$	$R^2 = 0.9630$	$R^2 = 0.9827$	$R^2 = 0.9852$	$R^2 = 0.9682$
3x					

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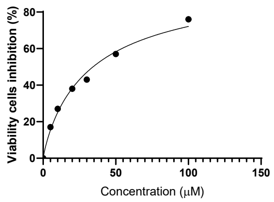
<td> 
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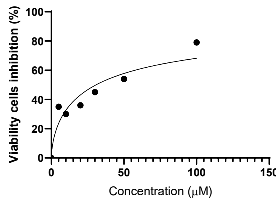
<td> 
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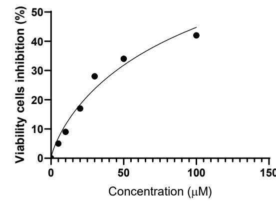
<td> 
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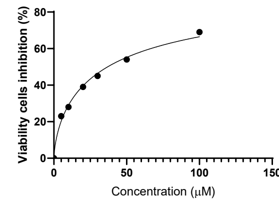
<td> 
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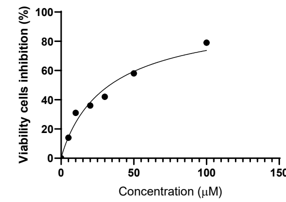
<td> 
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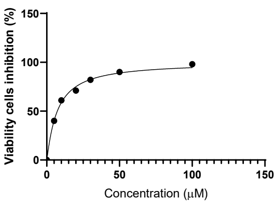
<td> 
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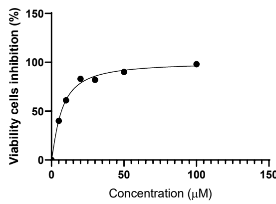
<td> 
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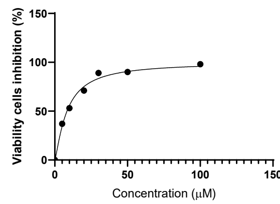
<td> 
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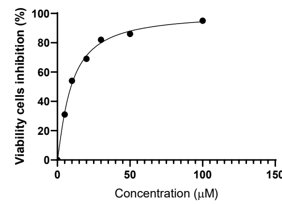
<td> 
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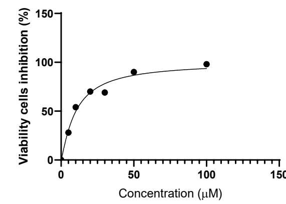
<td> 
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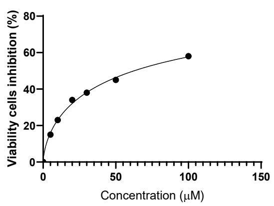
<td> 
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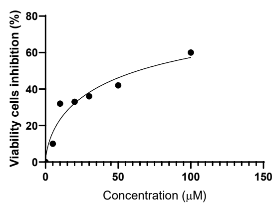
<td> 
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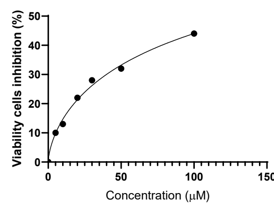
<td> 
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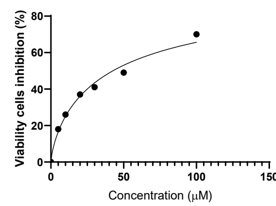
<td> 
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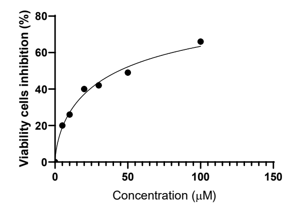
<td> 
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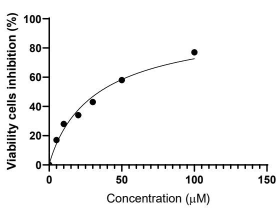
<td> 
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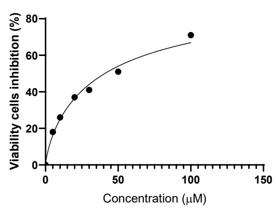
<td> 
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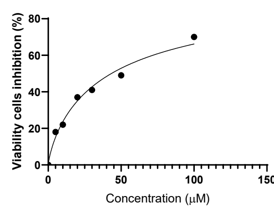
<td> 
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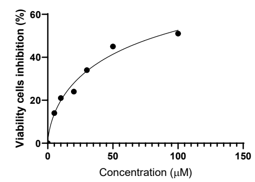
<td> 
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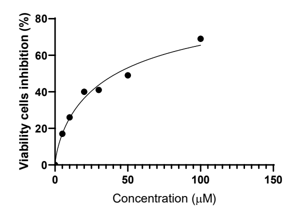
<td> 
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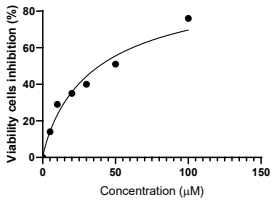
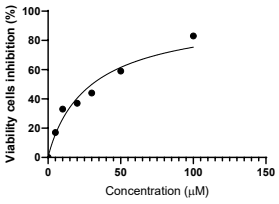
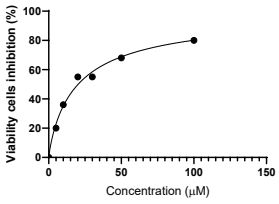
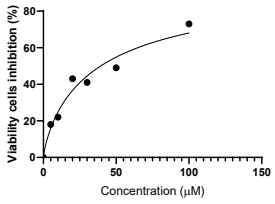
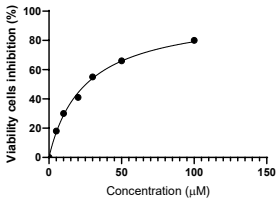
4e					
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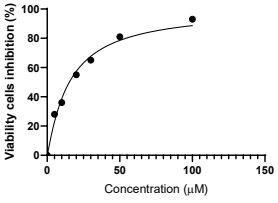
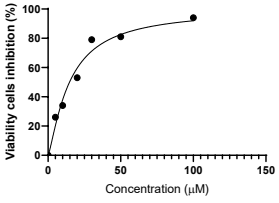
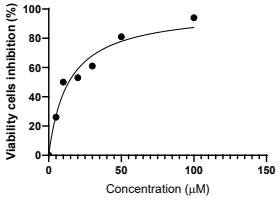
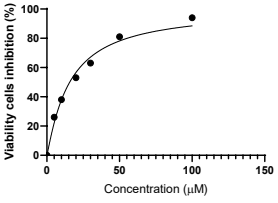
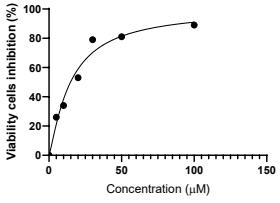
4f					
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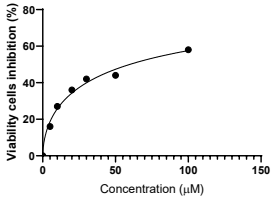
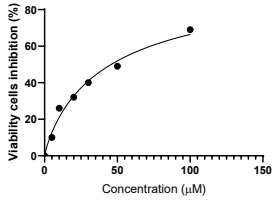
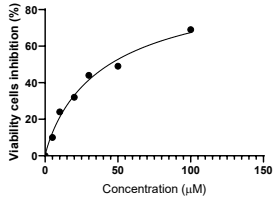
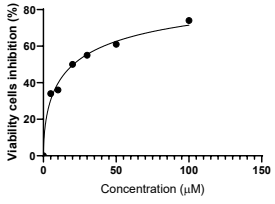
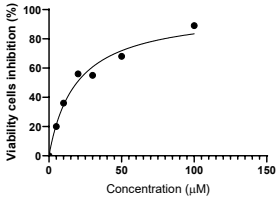
4g					
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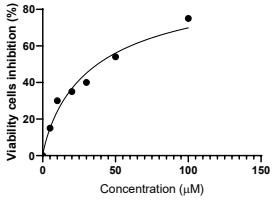
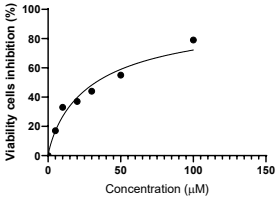
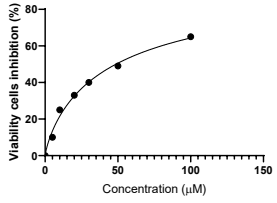
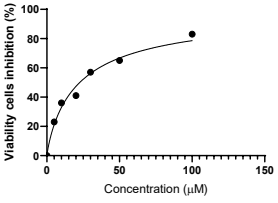
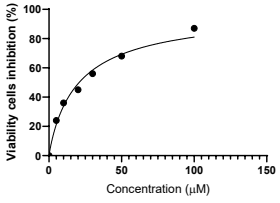
4h					
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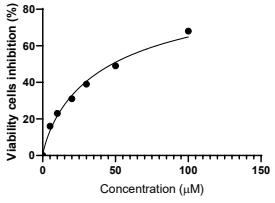
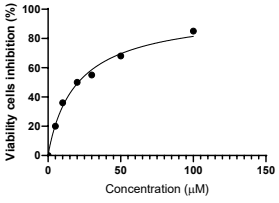
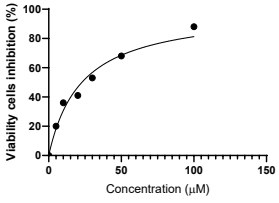
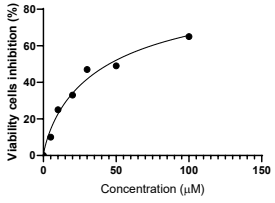
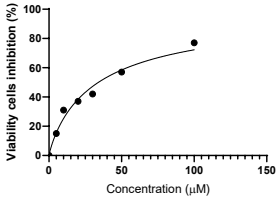
4i					
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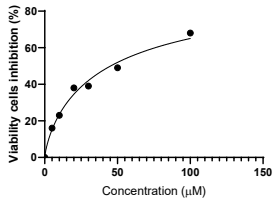
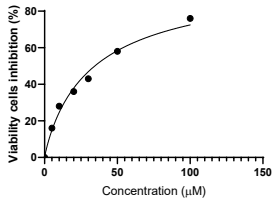
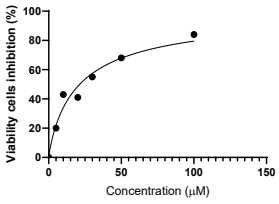
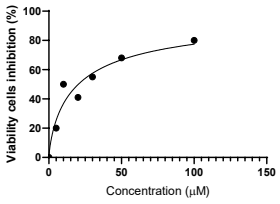
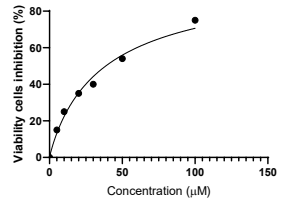
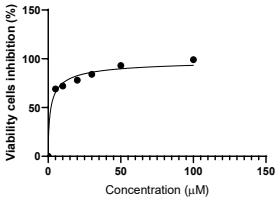
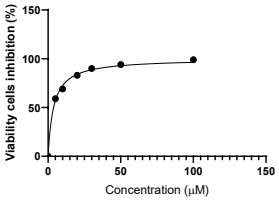
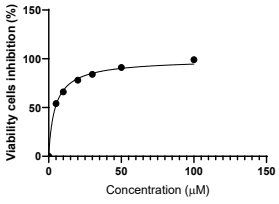
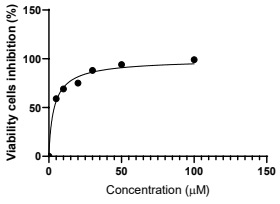
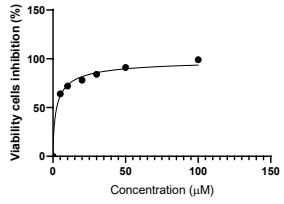
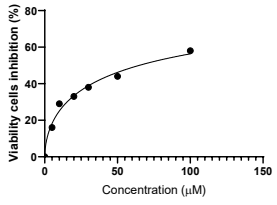
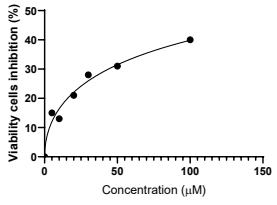
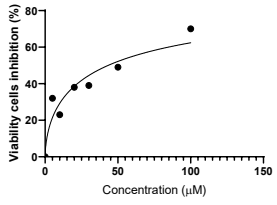
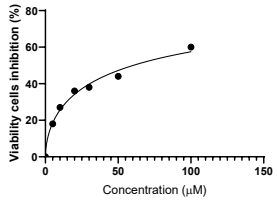
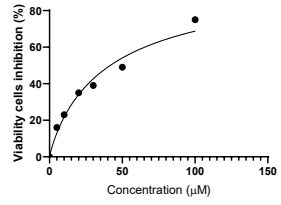
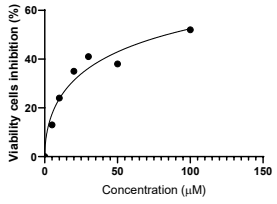
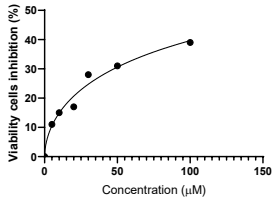
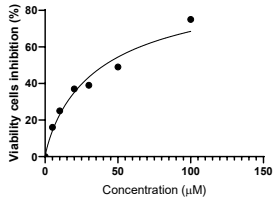
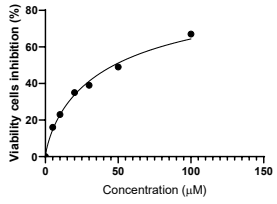
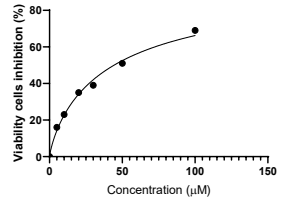
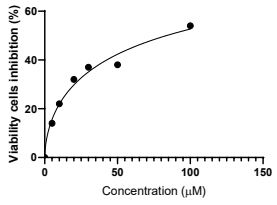
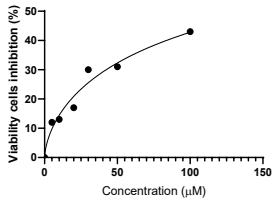
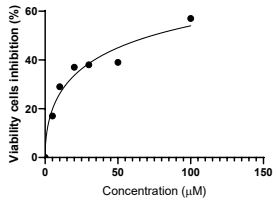
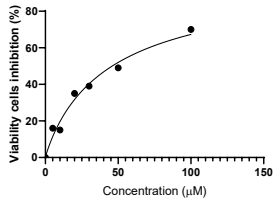
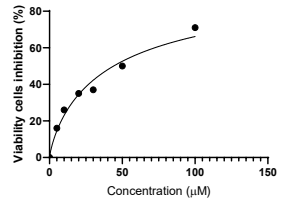
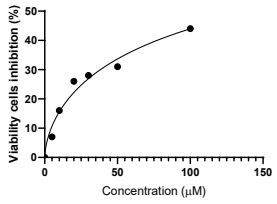
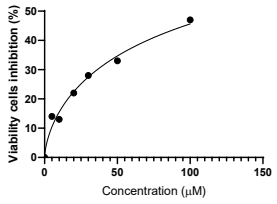
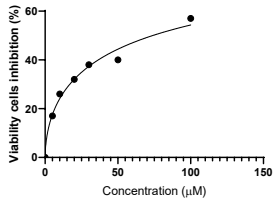
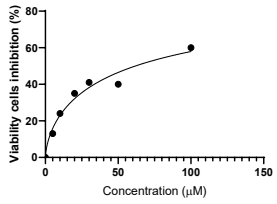
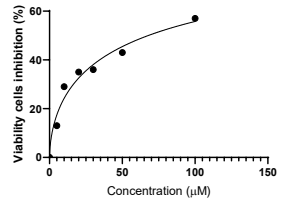
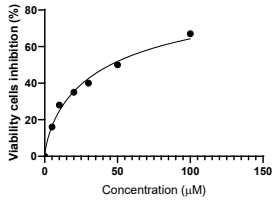
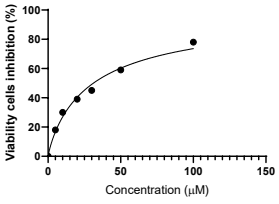
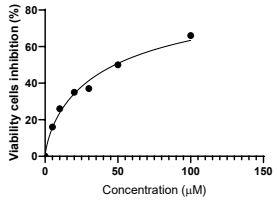
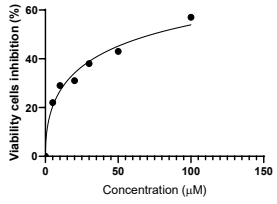
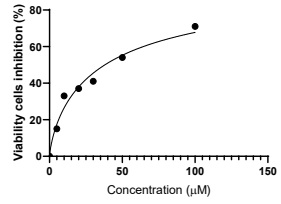
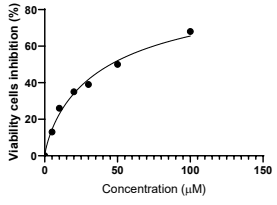
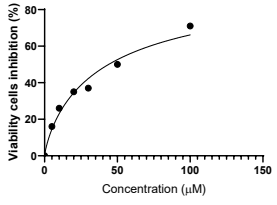
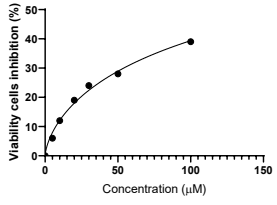
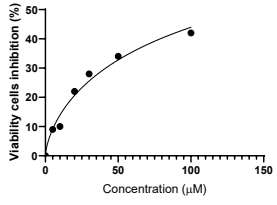
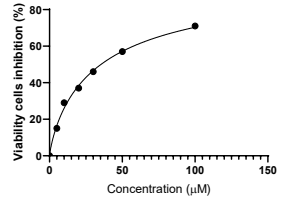
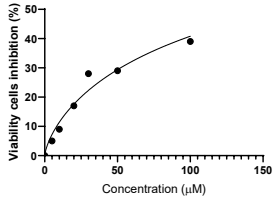
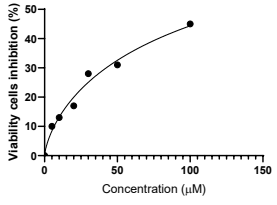
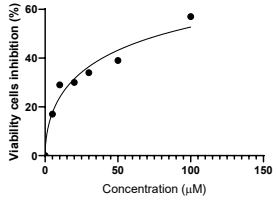
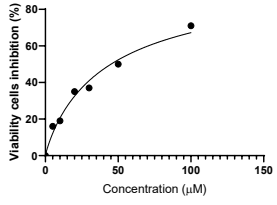
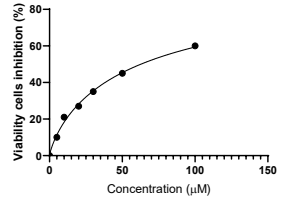
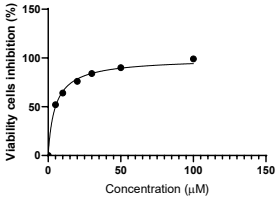
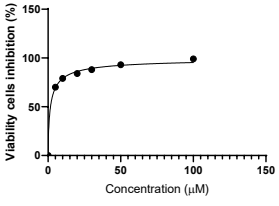
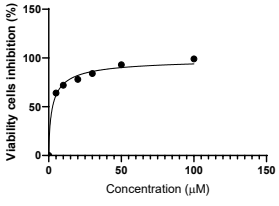
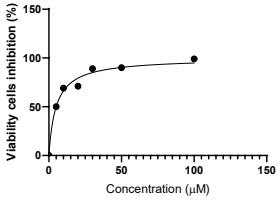
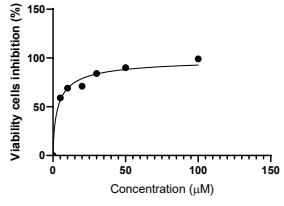
4j					
	$R^2 = 0.9869$	$R^2 = 0.9885$	$R^2 = 0.9650$	$R^2 = 0.9348$	$R^2 = 0.9863$
4k					
	$R^2 = 0.9860$	$R^2 = 0.9961$	$R^2 = 0.9955$	$R^2 = 0.9880$	$R^2 = 0.9917$
4l					
	$R^2 = 0.9864$	$R^2 = 0.9750$	$R^2 = 0.9111$	$R^2 = 0.9885$	$R^2 = 0.9743$
4m					
	$R^2 = 0.9573$	$R^2 = 0.9766$	$R^2 = 0.9705$	$R^2 = 0.9932$	$R^2 = 0.9925$
4n					
	$R^2 = 0.9832$	$R^2 = 0.9653$	$R^2 = 0.9636$	$R^2 = 0.9787$	$R^2 = 0.9781$

4o					
	$R^2 = 0.9733$	$R^2 = 0.9827$	$R^2 = 0.9843$	$R^2 = 0.9698$	$R^2 = 0.9718$
4p					
	$R^2 = 0.9902$	$R^2 = 0.9871$	$R^2 = 0.9885$	$R^2 = 0.9831$	$R^2 = 0.9753$
4q					
	$R^2 = 0.9899$	$R^2 = 0.9781$	$R^2 = 0.9923$	$R^2 = 0.9792$	$R^2 = 0.9960$
4r					
	$R^2 = 0.9619$	$R^2 = 0.9832$	$R^2 = 0.9624$	$R^2 = 0.9823$	$R^2 = 0.9955$
PTX					
	$R^2 = 0.9946$	$R^2 = 0.9969$	$R^2 = 0.9906$	$R^2 = 0.9838$	$R^2 = 0.9827$

COMPUTATIONAL DATA in Supplementary Information

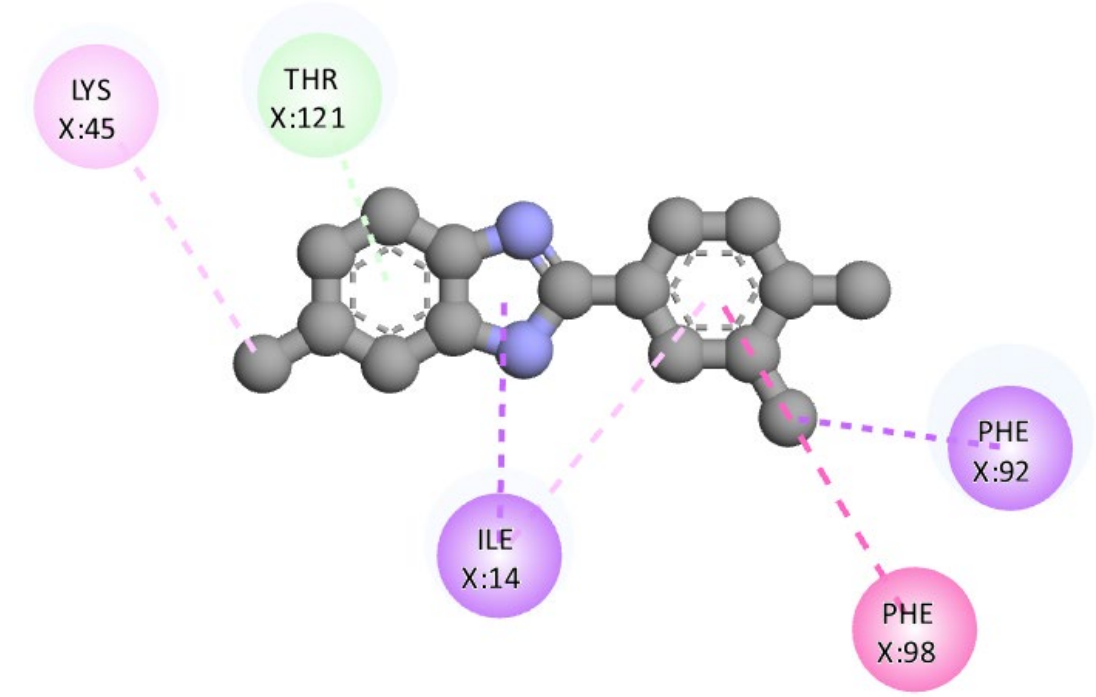
1. Dihydrofolate Reductase – Bacteria (PDB: 3FYV)

Grid box volume – Autodock Vina

```
receptor = 3fyvDHFRB.pdbqt
ligand = ligand.pdbqt

out = out.pdbqt

center_x = 23.972
center_y = 17.083
center_z = 41.528

size_x = 30
size_y = 35
size_z = 30

energy_range = 4
exhaustiveness = 8
```

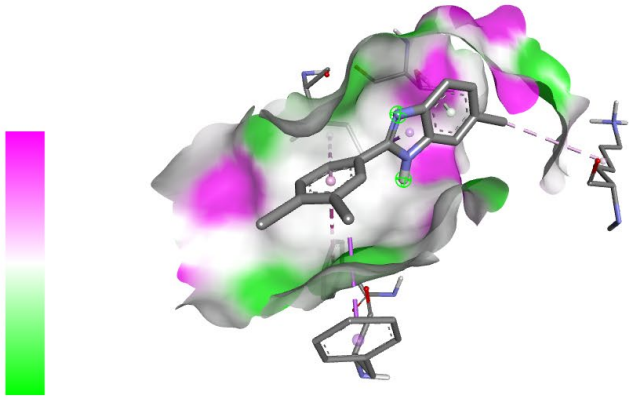
1.1. Compound 1d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -263030504
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.6      0.000      0.000
   2         -8.2      1.607      6.931
   3         -8.1      1.868      2.433
   4         -7.9      1.176      1.865
   5         -7.9      2.500      3.231
   6         -7.9      2.138      6.922
   7         -7.8      2.893      3.788
   8         -7.8      2.519      3.071
   9         -7.7      1.054      1.219
Writing output ... done.
```



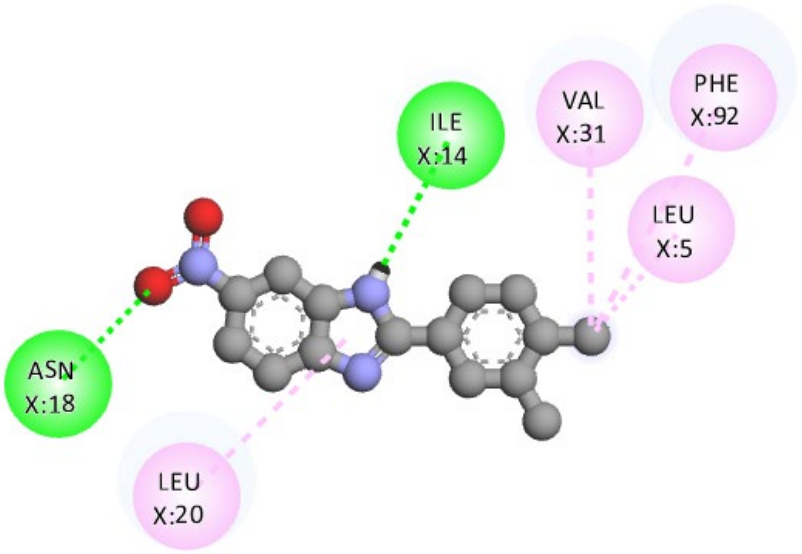
Interactions

- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl



1.2. Compound 2d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 747936400
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.9      0.000      0.000
   2         -8.6      5.202      7.359
   3         -8.4      1.587      2.370
   4         -8.4      2.604      3.753
   5         -8.1      1.712      2.368
   6         -7.8      2.563      3.831
   7         -7.7      5.403      7.326
   8         -7.6      2.914      3.991
   9         -7.5      4.329      6.302
Writing output ... done.
```

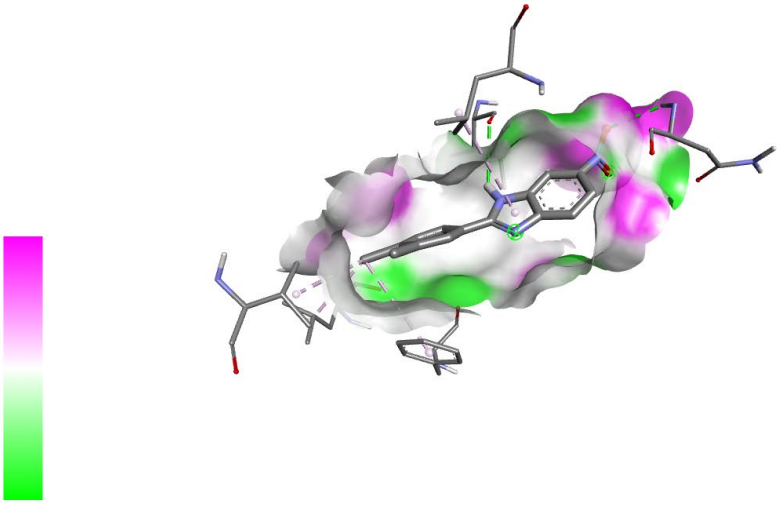


Interactions

Conventional Hydrogen Bond

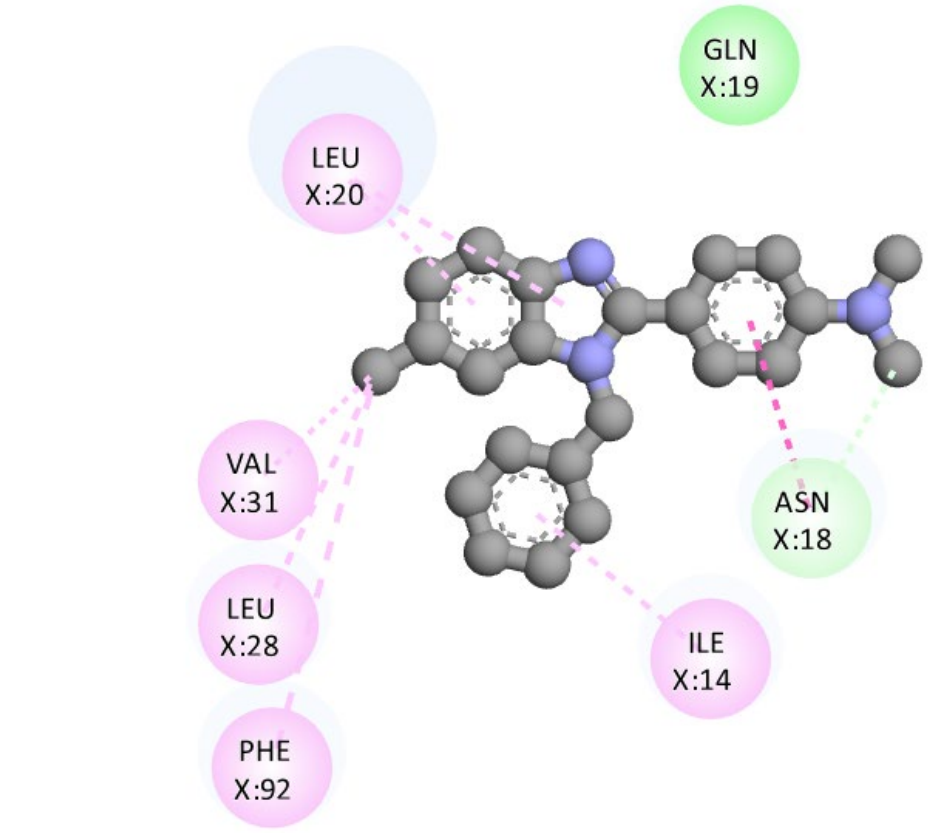
Pi-Alkyl

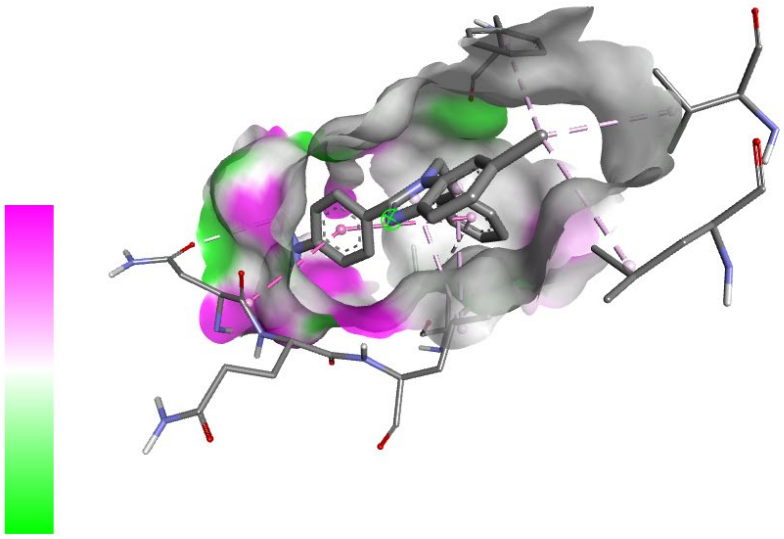
Alkyl



1.3. Compound 3s

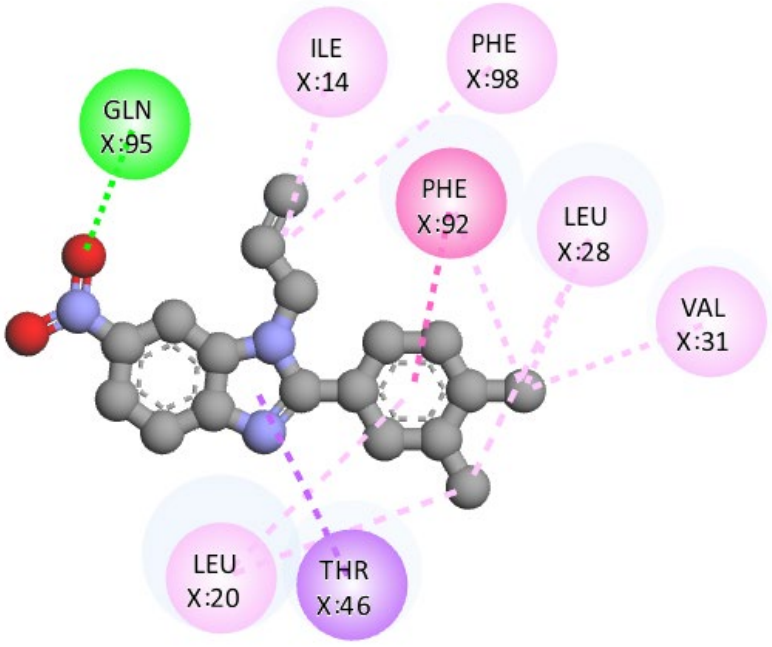
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 5130864
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.2      0.000      0.000
   2         -8.9      3.035      6.464
   3         -8.6      3.237      7.180
   4         -8.5      1.839      2.883
   5         -8.5      1.492      2.223
   6         -8.3      3.051      7.556
   7         -8.1      1.753      4.082
   8         -8.1      1.889      4.167
   9         -8.1      2.962      6.188
Writing output ... done.
```


GLN
X:19
LEU
X:20
VAL
X:31
LEU
X:28
PHE
X:92
ILE
X:14
ASN
X:18
Interactions
van der Waals
Carbon Hydrogen Bond
Amide-Pi Stacked
Alkyl
Pi-Alkyl



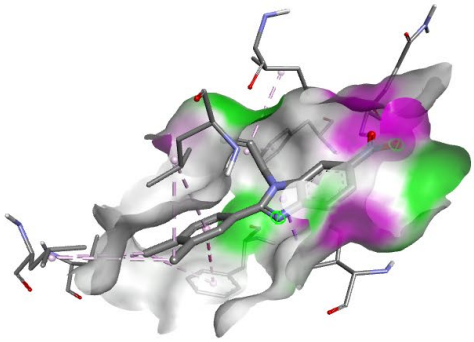
1.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1301333348
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.2      0.000      0.000
   2         -8.9      5.034      7.433
   3         -8.5      1.970      3.156
   4         -8.4      4.722      6.904
   5         -8.4      1.170      1.630
   6         -8.3      1.667      3.208
   7         -8.2      1.929      3.168
   8         -8.2      1.921      3.428
   9         -7.8      2.440      4.093
Writing output ... done.
```



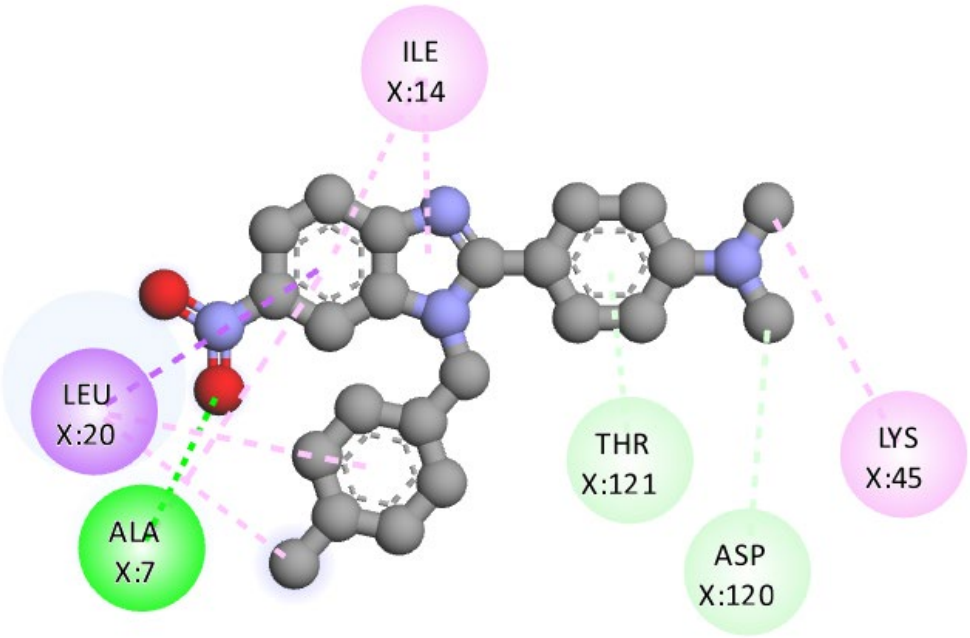
Interactions

- Conventional Hydrogen Bond
- Alkyl
- Pi-Sigma
- Pi-Alkyl
- Pi-Pi Stacked



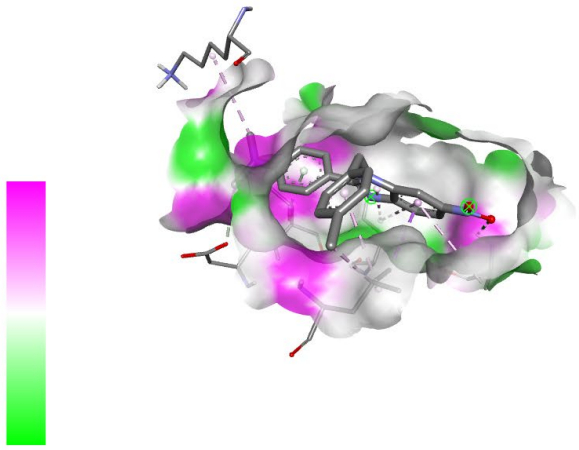
1.5. Compound 4k

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -70295152
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.4      0.000      0.000
   2         -9.3      4.240      8.642
   3         -9.1      3.214      5.404
   4         -9.0      3.160      6.906
   5         -8.8      3.328      6.857
   6         -8.6      3.783      7.838
   7         -8.5      3.794      7.588
   8         -8.3      6.298      8.877
   9         -8.3      6.358      8.899
Writing output ... done.
```



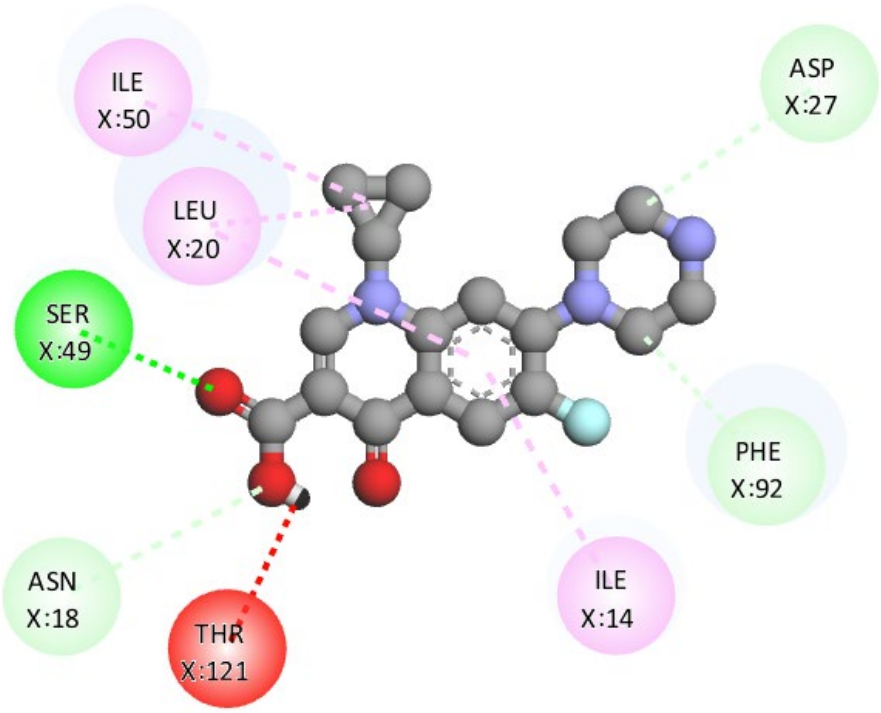
Interactions

Conventional Hydrogen Bond	Pi-Sigma
Carbon Hydrogen Bond	Alkyl
Pi-Donor Hydrogen Bond	Pi-Alkyl



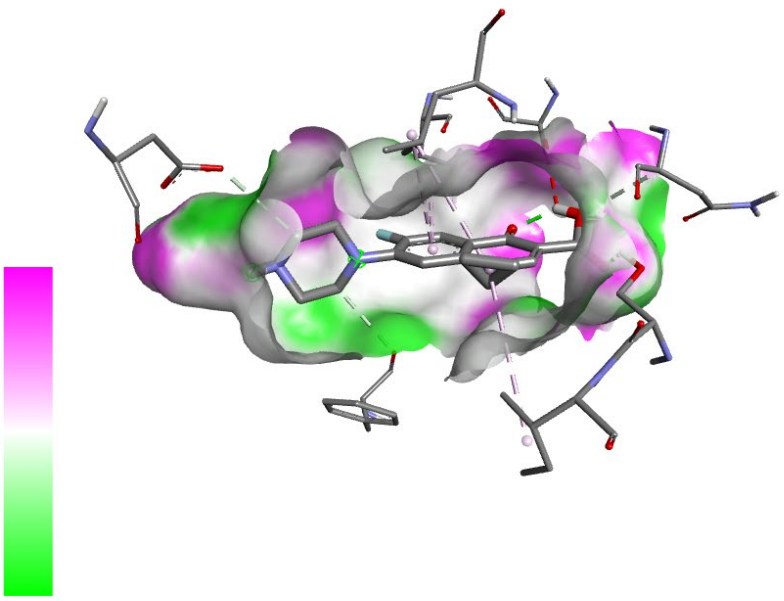
1.6. Compound Cipro

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -215246968
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.1      0.000      0.000
   2         -8.7      3.423      6.648
   3         -8.6      3.981      7.327
   4         -8.4      3.575      6.566
   5         -8.1      2.874      4.619
   6         -8.0      4.052      5.964
   7         -7.8      4.025      7.178
   8         -7.7      8.845     12.410
   9         -7.6      3.533      6.043
Writing output ... done.
```



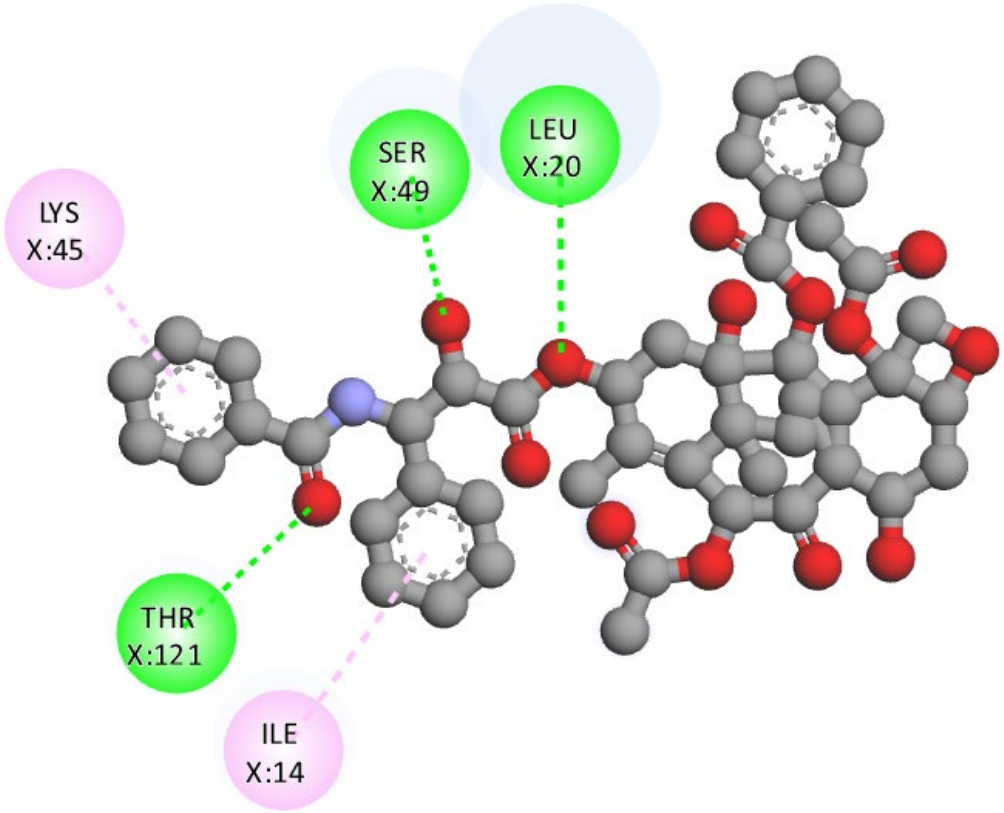
Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Donor-Donor
- Alkyl
- Pi-Alkyl



1.7. Compound PTX

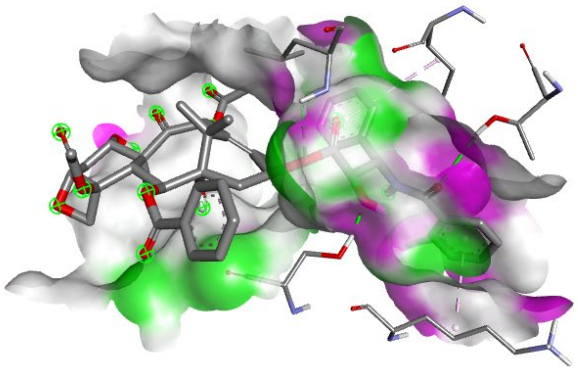
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -2051321328
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -10.0      0.000      0.000
   2         -8.1      1.596      5.444
   3         -8.1      0.944      3.622
   4         -8.0     10.018     18.422
   5         -7.6     10.188     17.799
   6         -7.5      8.739     18.280
   7         -7.3      2.112      5.745
   8         -7.2     10.636     19.300
   9         -7.1      2.459      7.199
Writing output ... done.
```



Interactions

Conventional Hydrogen Bond

Pi-Alkyl



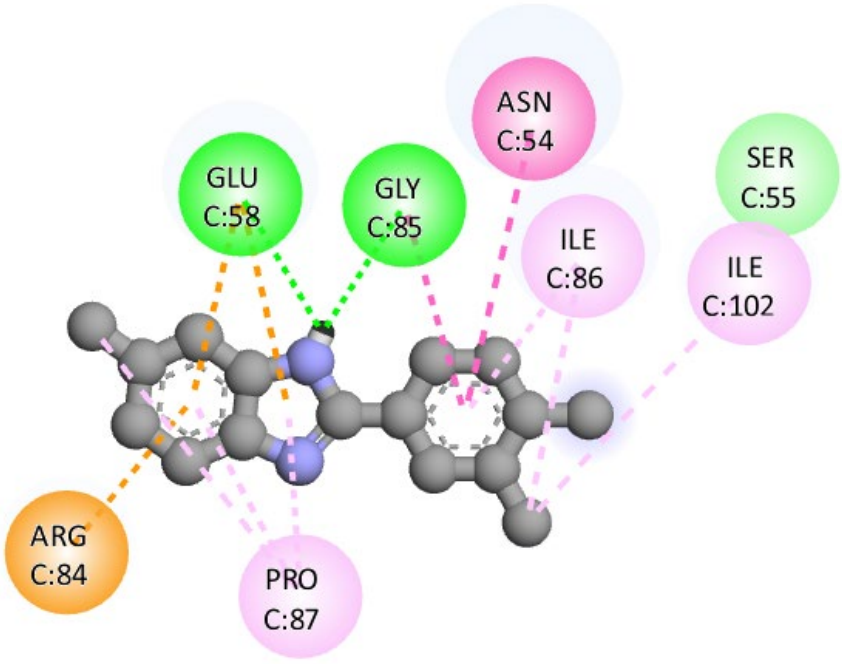
2. Gyrase B (PDB: 4URM)

Grid box volume – Autodock Vina

```
receptor = 4urmGyrB.pdbqt
ligand = ligand.pdbqt

out = out.pdbqt

center_x = 23.9228
center_y = 7.94566
center_z = 90.4085

size_x = 30
size_y = 30
size_z = 30

energy_range = 4
exhaustiveness = 8
```

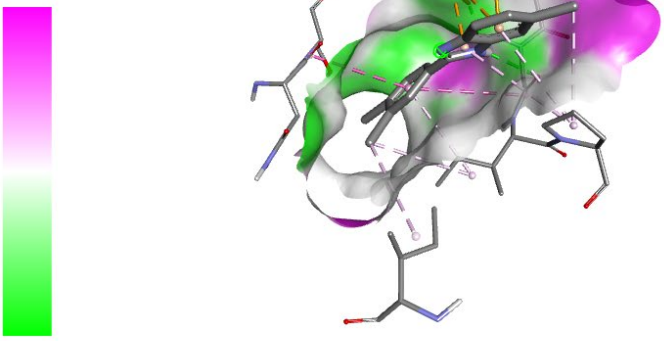
2.1. Compound 1d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1089847928
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.4      0.000      0.000
   2         -7.3      3.005      7.402
   3         -7.3      2.347      2.827
   4         -7.1      2.833      7.108
   5         -6.8      1.578      2.330
   6         -6.6      1.216      6.697
   7         -6.6      2.954      6.927
   8         -6.3      3.078      3.788
   9         -6.1      4.113      6.985
Writing output ... done.
```



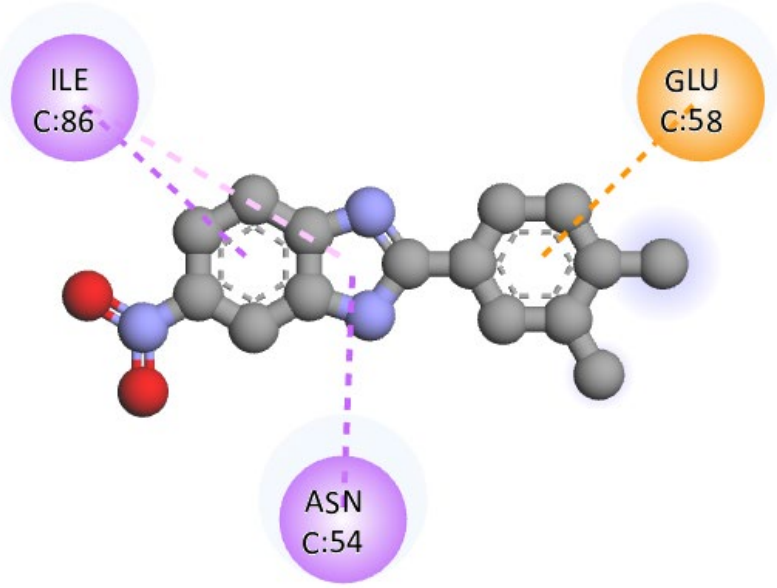
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Anion
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



2.2. Compound 2d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 2056033640
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.7      0.000      0.000
   2         -7.6      0.967      1.764
   3         -7.5      5.220      7.566
   4         -7.4      1.640      1.933
   5         -7.1      5.342      7.520
   6         -7.0      6.024      8.189
   7         -7.0      5.472      7.790
   8         -6.9      3.057      4.384
   9         -6.6      2.525      3.339
Writing output ... done.
```

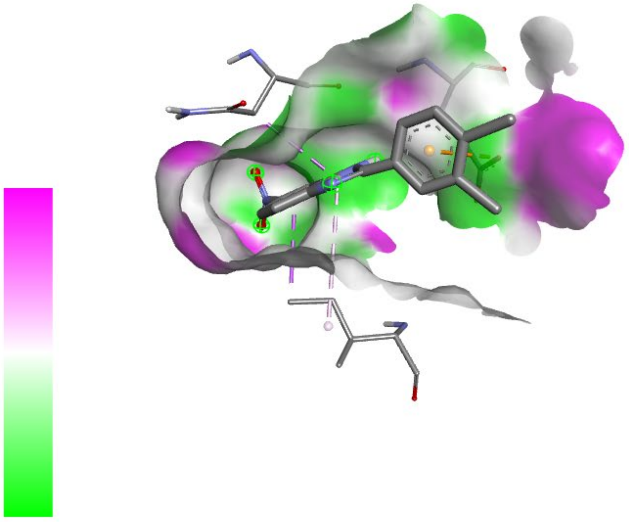


Interactions

Pi-Anion

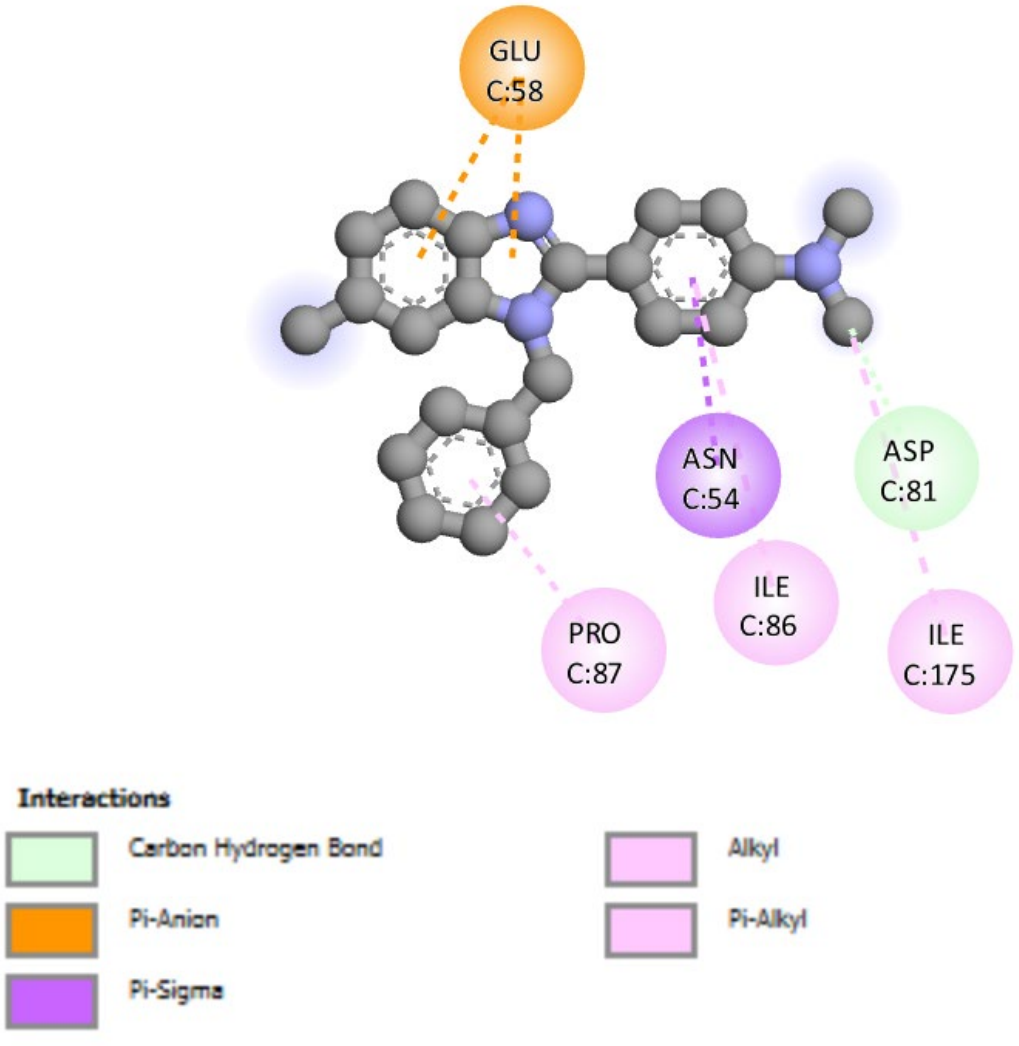
Pi-Sigma

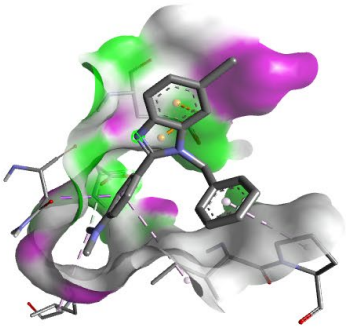
Pi-Alkyl



2.3. Compound 3s

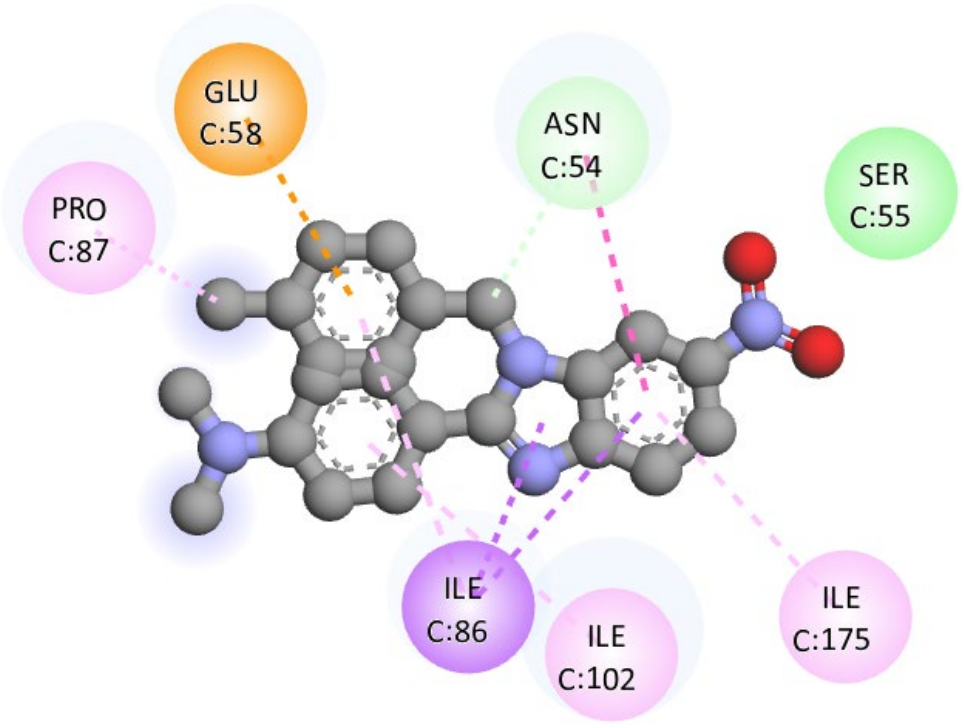
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1999731128
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.7      0.000      0.000
   2         -7.6      3.401      6.814
   3         -7.6      2.838      6.537
   4         -7.3      1.341      2.135
   5         -6.3      3.091      6.575
   6         -6.3      3.173      6.949
   7         -6.3      2.183      4.424
   8         -6.2      4.086      6.678
   9         -6.2     13.111     14.820
Writing output ... done.
```


GLU
C:58
ASN
C:54
ASP
C:81
ILE
C:86
PRO
C:87
ILE
C:175
Interactions
Carbon Hydrogen Bond
Pi-Anion
Pi-Sigma
Alkyl
Pi-Alkyl



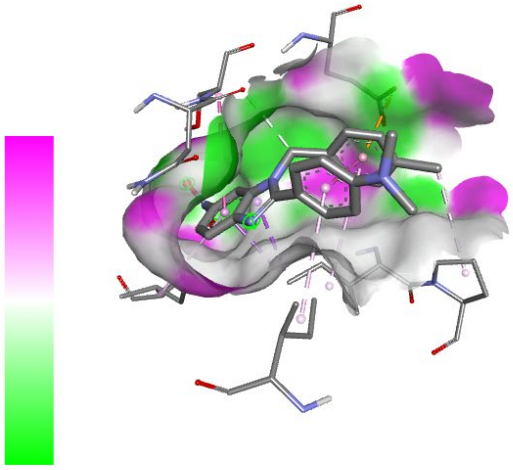
2.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1394259368
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.6      0.000      0.000
   2         -7.3      5.758      7.960
   3         -7.2      5.841      8.151
   4         -7.0      5.275      7.606
   5         -7.0      2.634      4.006
   6         -6.8      2.976      4.087
   7         -6.7      2.656      4.293
   8         -6.2      3.458      5.121
   9         -6.0      5.836      8.230
Writing output ... done.
```



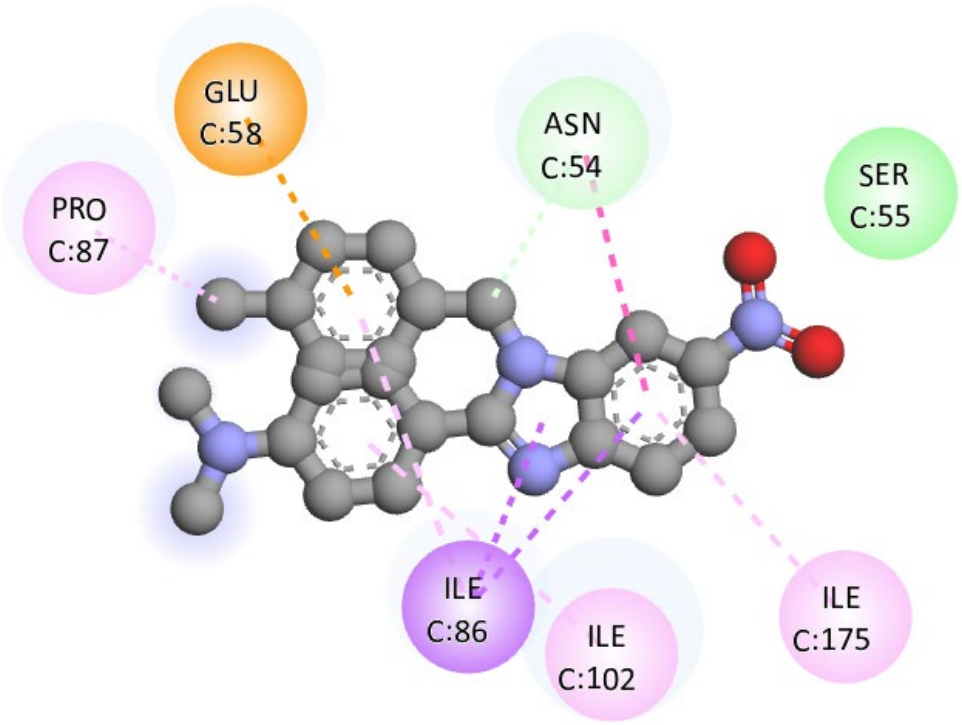
Interactions

- van der Waals
- Carbon Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



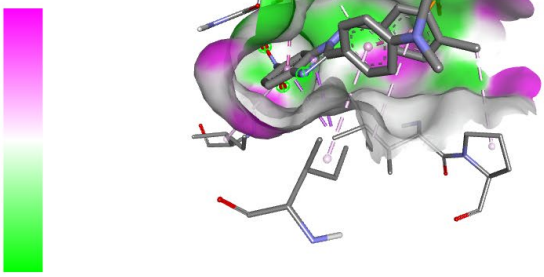
2.5. Compound 4k

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -2026544880
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.1      0.000      0.000
   2         -7.8      2.708      4.370
   3         -7.5      4.618      7.666
   4         -7.4      4.700      7.804
   5         -7.2      4.329      7.686
   6         -6.9      4.432      7.808
   7         -6.6      2.570      3.882
   8         -6.4     12.468     13.994
   9         -6.3      2.923      4.477
Writing output ... done.
```



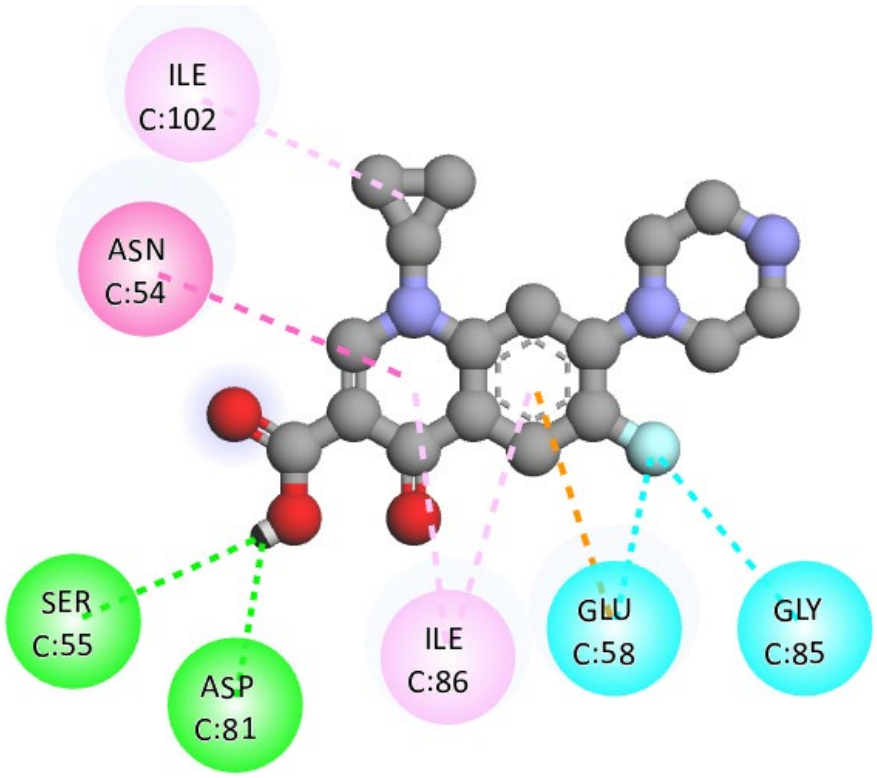
Interactions

- van der Waals
- Carbon Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



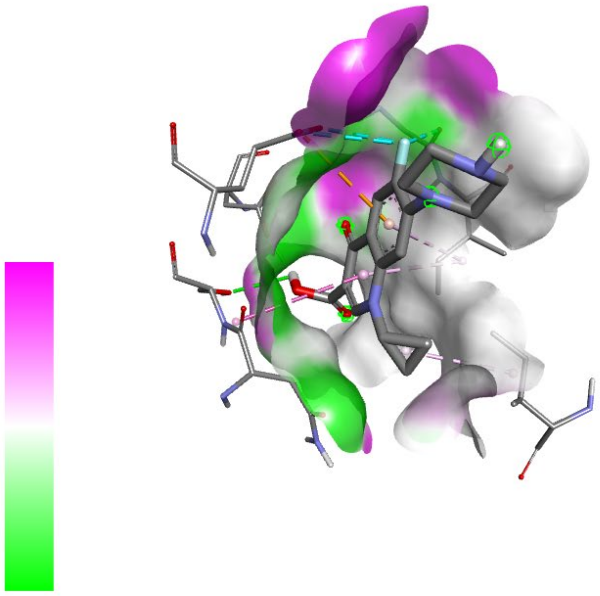
2.6. Compound Cipro

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -260904248
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.3      0.000      0.000
   2         -6.9      2.891      4.494
   3         -6.8      3.615      6.726
   4         -6.8      2.343      3.878
   5         -6.3      3.850      7.243
   6         -6.3      4.582      7.334
   7         -6.1      4.079      7.491
   8         -6.1      5.292      8.112
   9         -5.9      4.651      7.100
Writing output ... done.
```



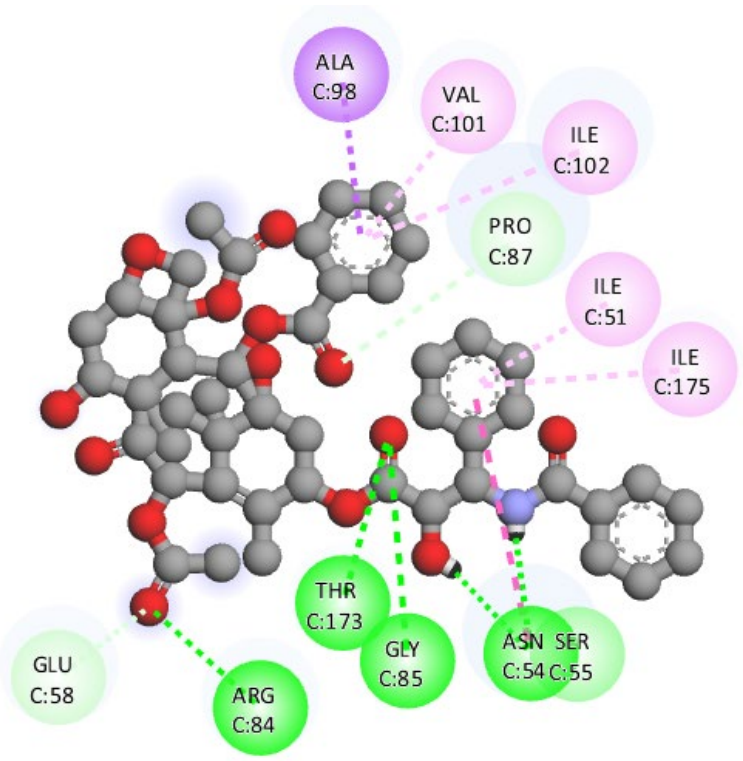
Interactions

- Conventional Hydrogen Bond
- Halogen (Fluorine)
- Pi-Anion
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



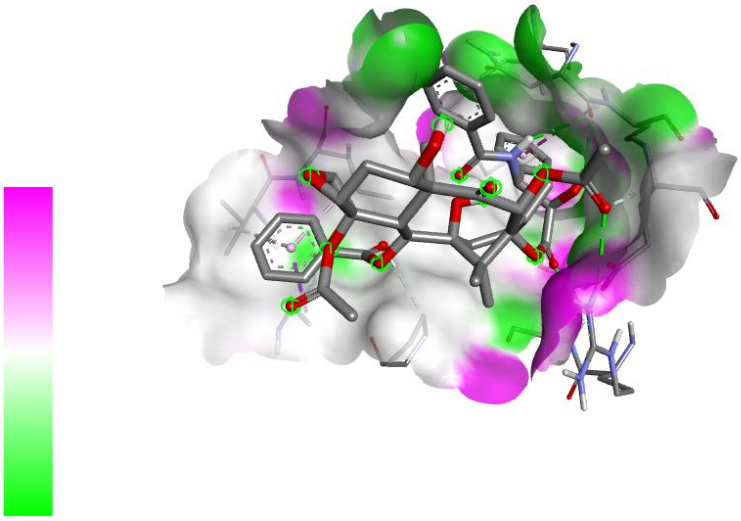
2.7. Compound PTX

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 934984084
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.8      0.000      0.000
   2         -7.6      2.335      4.921
   3         -7.5      2.945      8.770
   4         -7.4      3.629      9.582
   5         -7.4      3.099      6.925
   6         -7.3      2.977      7.101
   7         -7.3      4.177     10.014
   8         -7.3      3.805      7.256
   9         -7.2      2.564      5.400
Writing output ... done.
```



Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Sigma
- Amide-Pi Stacked
- Pi-Alkyl



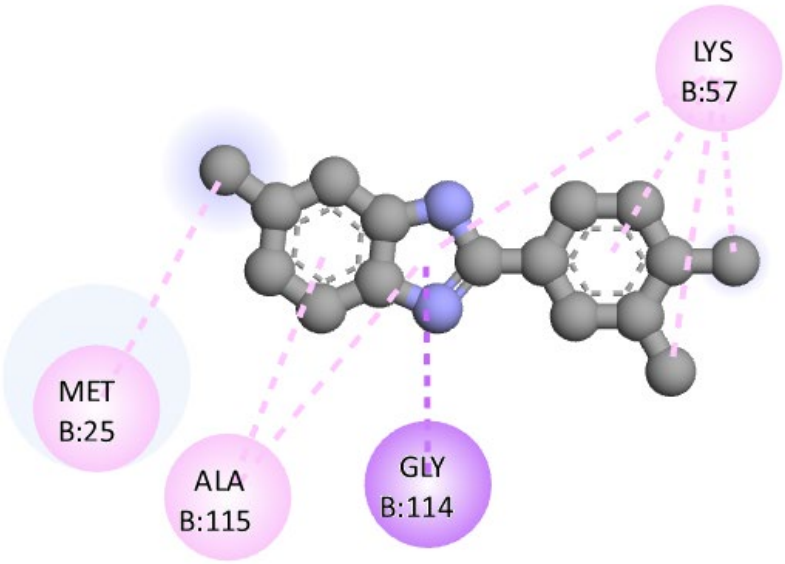
3. Dihydrofolate Reductase - Fungi (PDB: 4HOF)

Grid box volume – Autodock Vina

```
receptor = 4hofDHFRF.pdbqt
ligand = ligand.pdbqt

out = out.pdbqt

center_x = 11.44
center_y = -32.6283
center_z = 17.3865

size_x = 30
size_y = 30
size_z = 30

energy_range = 4

exhaustiveness = 8
```

3.1. Compound 1d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1088034812
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.7      0.000      0.000
   2         -7.5      3.816      5.519
   3         -7.5     11.587     12.965
   4         -7.4      3.840      8.177
   5         -7.3     10.822     13.066
   6         -7.3      4.128      5.821
   7         -7.2      4.146      6.107
   8         -7.0      3.393      7.813
   9         -7.0     11.930     14.135
Writing output ... done.
```

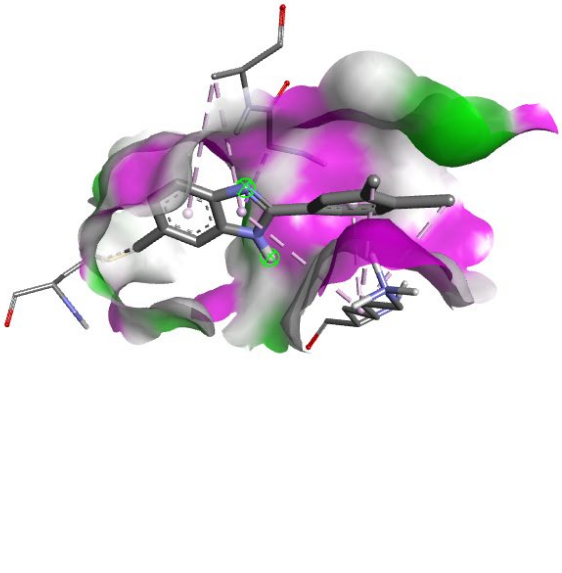


Interactions

Pi-Sigma

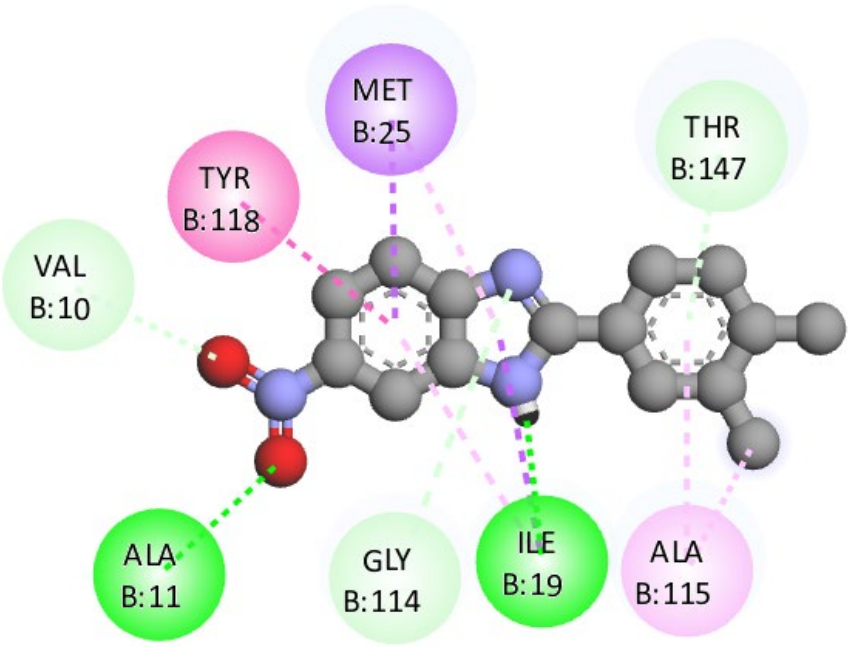
Pi-Alkyl

Alkyl



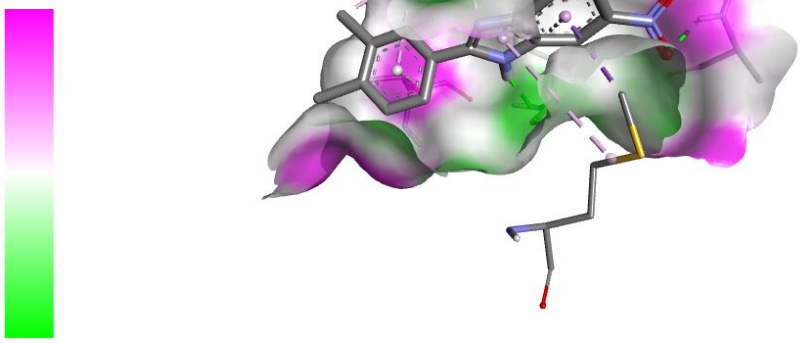
3.2. Compound 2d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 704858144
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.4      0.000      0.000
   2         -8.1      9.183     10.969
   3         -8.0      5.153      7.495
   4         -8.0      1.604      2.344
   5         -7.7      8.695     10.156
   6         -7.6      6.851      8.750
   7         -7.5      3.945      4.880
   8         -7.4      8.625     10.773
   9         -7.3      3.736      4.817
Writing output ... done.
```



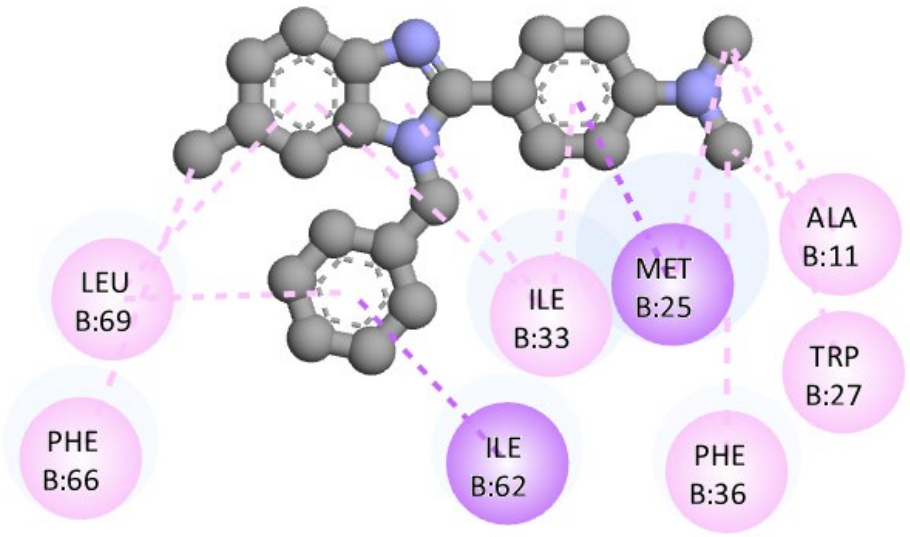
Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl



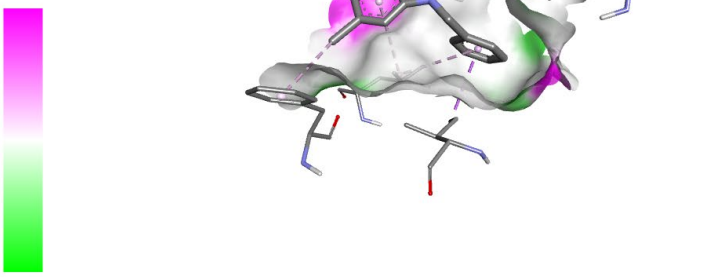
3.3. Compound 3s

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1977351540
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.4      0.000      0.000
   2         -8.1      2.707      4.651
   3         -8.0     11.550     14.767
   4         -8.0      1.965      2.777
   5         -7.8      2.013      3.949
   6         -7.7      3.706      6.036
   7         -7.7      2.939      4.856
   8         -7.5     11.765     14.733
   9         -7.0      3.739      6.643
Writing output ... done.
```



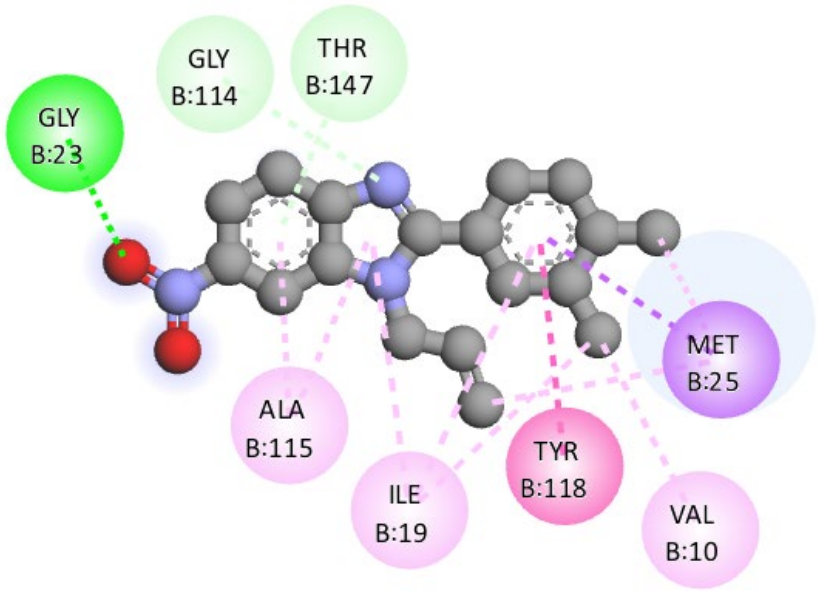
Interactions

- Pi-Sigma
- Pi-Sulfur
- Alkyl
- Pi-Alkyl



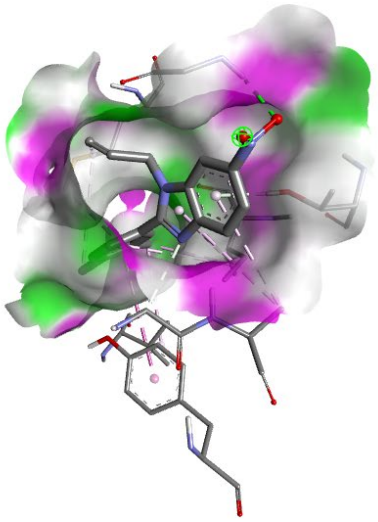
3.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1619326992
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.7      0.000      0.000
   2         -7.7      8.822     10.863
   3         -7.5      9.125     10.949
   4         -7.2      9.856     11.960
   5         -7.2      9.068     10.650
   6         -7.0     10.381     12.862
   7         -6.8      4.970      7.567
   8         -6.7      3.759      5.245
   9         -6.7     10.118     12.266
Writing output ... done.
```



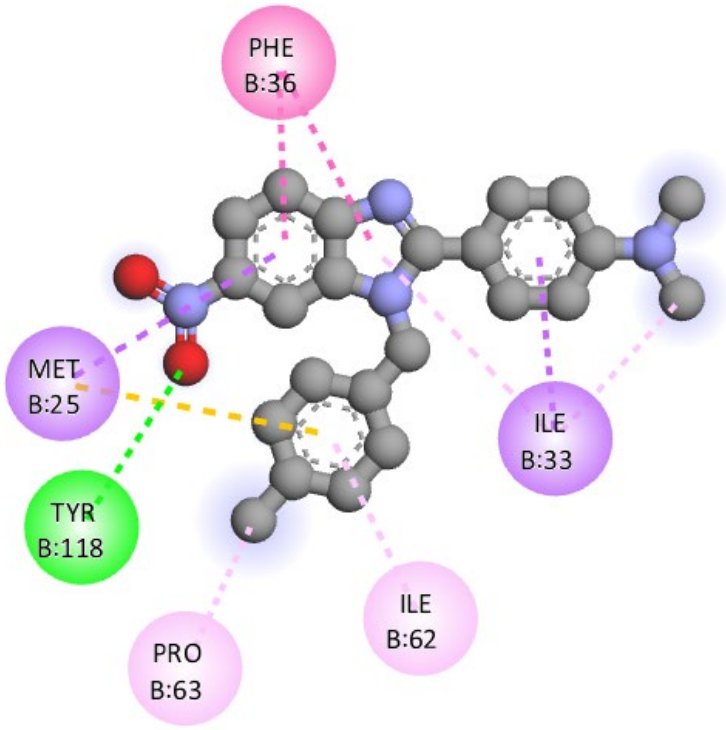
Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl



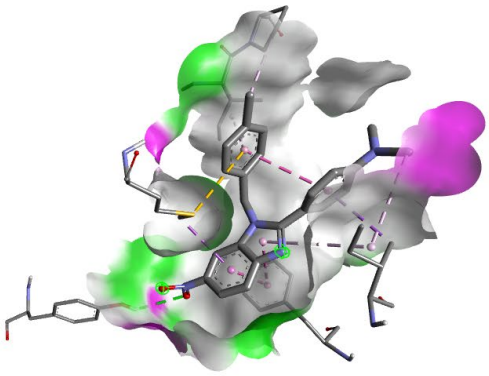
3.5. Compound 4k

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 817433168
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.2      0.000      0.000
   2         -8.1      4.020      6.603
   3         -7.6     12.333     14.551
   4         -7.6      3.905      7.122
   5         -7.3     12.382     15.322
   6         -7.2     12.440     15.297
   7         -7.1     15.866     17.991
   8         -6.6     14.639     17.928
   9         -6.6     13.676     16.414
Writing output ... done.
```



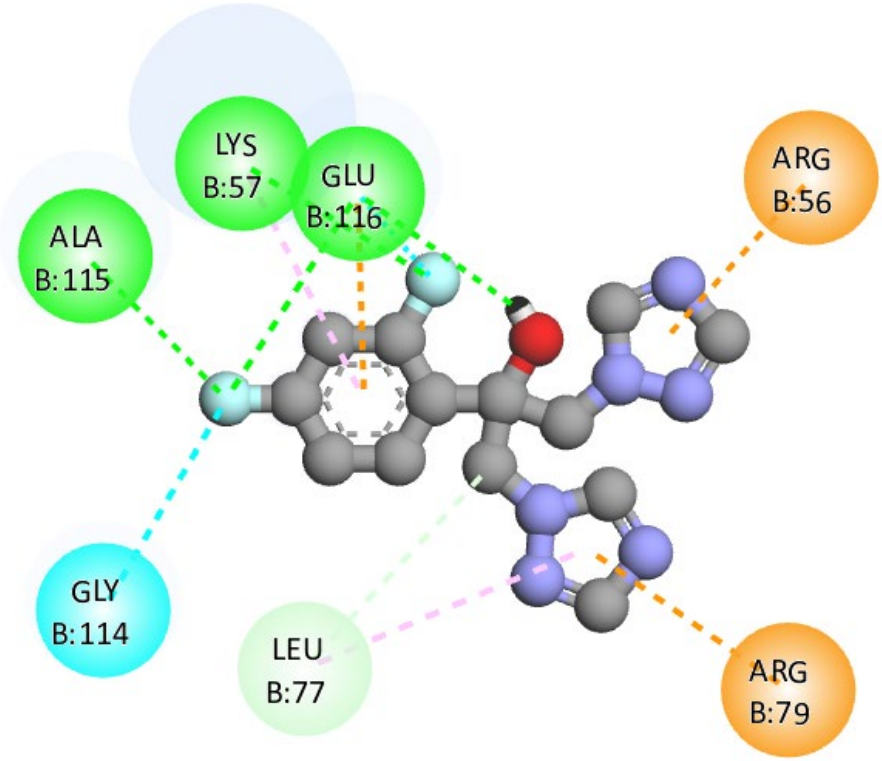
Interactions

- Conventional Hydrogen Bond
- Pi-Sigma
- Pi-Sulfur
- Pi-Pi Stacked
- Alkyl
- Pi-Alkyl



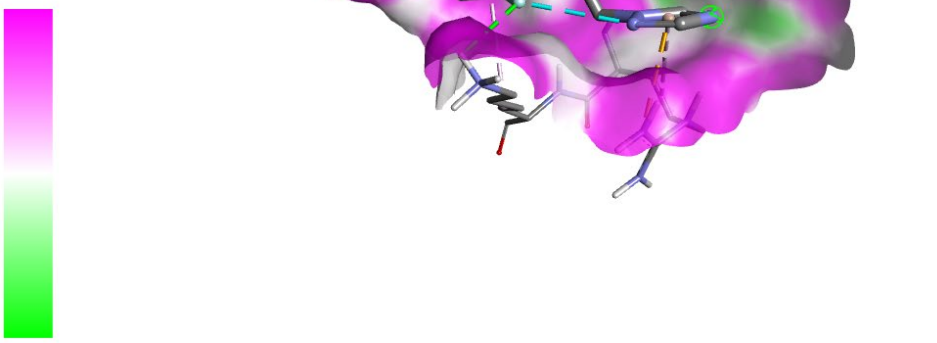
3.6. Compound Flu

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1446104232
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.0      0.000      0.000
   2         -6.9      0.967      3.654
   3         -6.6      6.812      8.965
   4         -6.5     15.477     17.482
   5         -6.3      6.744      9.198
   6         -6.3      6.201      8.334
   7         -6.3      6.133      8.712
   8         -6.2     16.145     17.921
   9         -6.2      5.952      8.003
Writing output ... done.
```



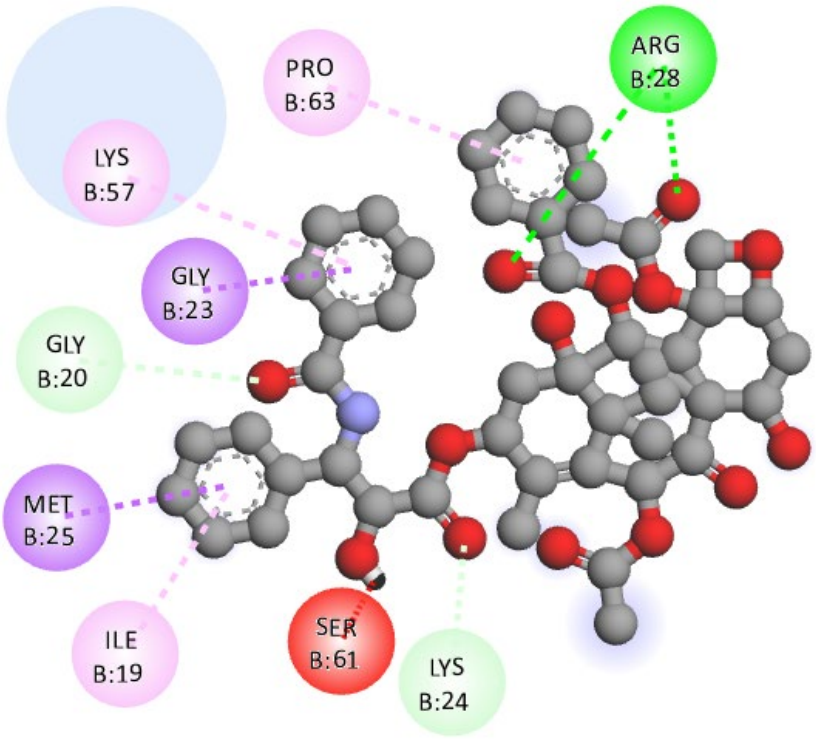
Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Halogen (Fluorine)
- Pi-Cation
- Pi-Anion
- Pi-Alkyl



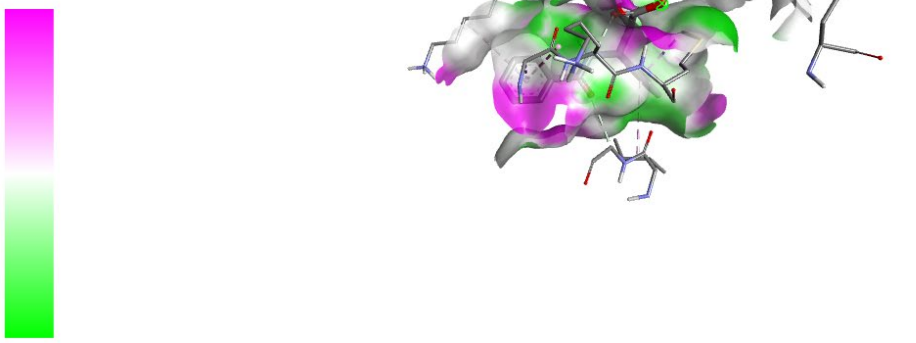
3.7. Compound PTX

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1298481664
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.5      0.000      0.000
   2         -8.4     11.499     19.266
   3         -8.3     14.515     22.467
   4         -8.1     11.057     19.824
   5         -7.9      9.306     14.573
   6         -7.7     11.349     17.544
   7         -7.7     10.169     14.970
   8         -7.5      9.634     17.562
   9         -7.5     14.073     22.233
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Donor-Donor
- Pi-Sigma
- Amide-Pi Stacked
- Pi-Alkyl



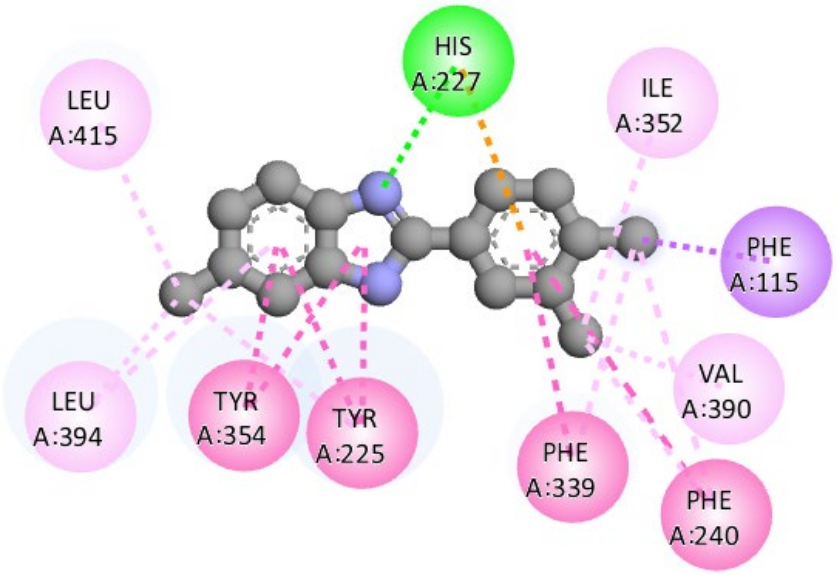
4. *N*-myristoyl Transferase (PDB: 1IYL)

Grid box volume – Autodock Vina

```
receptor = 1iylNMTF.pdbqt
ligand = ligand.pdbqt

out = out.pdbqt

center_x = 12.6146
center_y = 47.7652
center_z = -0.440754

size_x = 25
size_y = 25
size_z = 25

energy_range = 4
exhaustiveness = 8
```

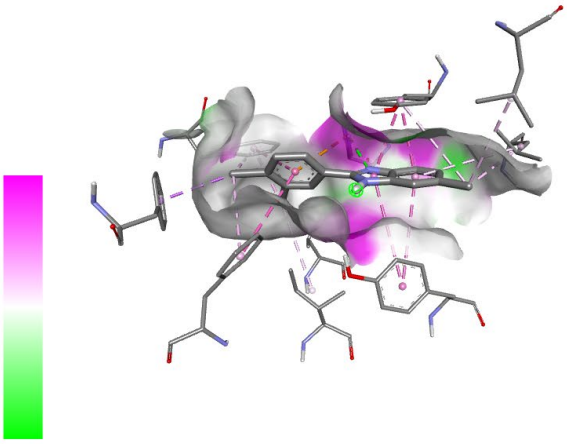
4.1. Compound 1d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1767034448
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -10.1      0.000      0.000
   2         -9.4      1.023      1.777
   3         -9.4      1.309      6.723
   4         -9.1      1.230      6.804
   5         -8.6      4.123      6.304
   6         -8.2      2.222      7.256
   7         -8.0      1.620      7.250
   8         -7.9      4.043      7.410
   9         -7.9      2.519      7.563
Writing output ... done.
```



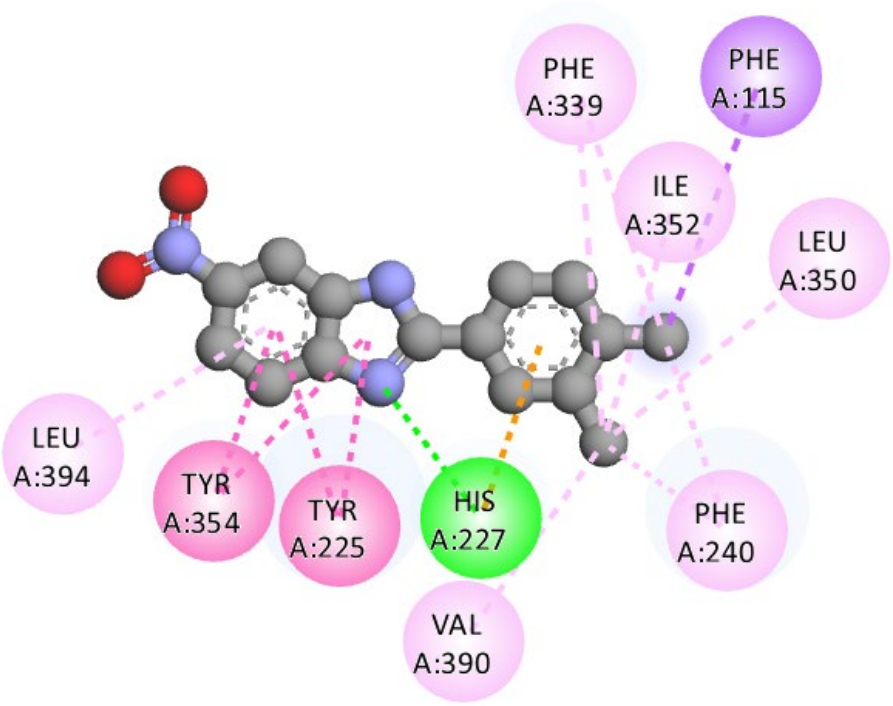
Interactions

- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Sigma
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl



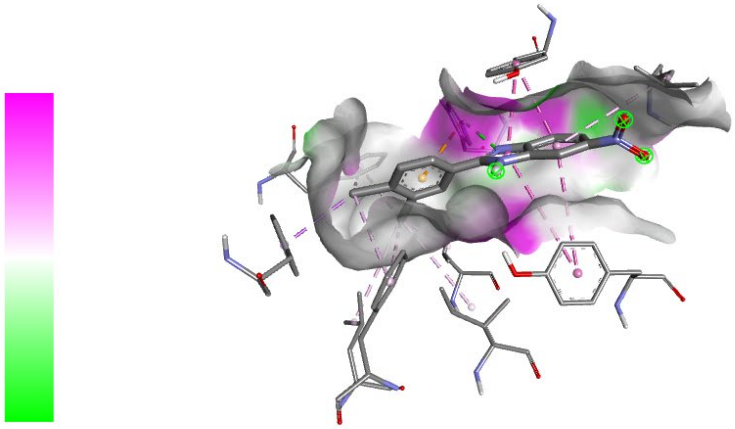
4.2. Compound 2d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 2050863144
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -10.1      0.000      0.000
   2         -8.8      1.645      2.214
   3         -8.6      5.139      6.787
   4         -8.6      5.302      7.524
   5         -8.5      4.511      6.378
   6         -8.5      5.315      7.747
   7         -8.2      5.188      7.562
   8         -8.0      5.233      7.579
   9         -7.8      4.789      6.348
Writing output ... done.
```



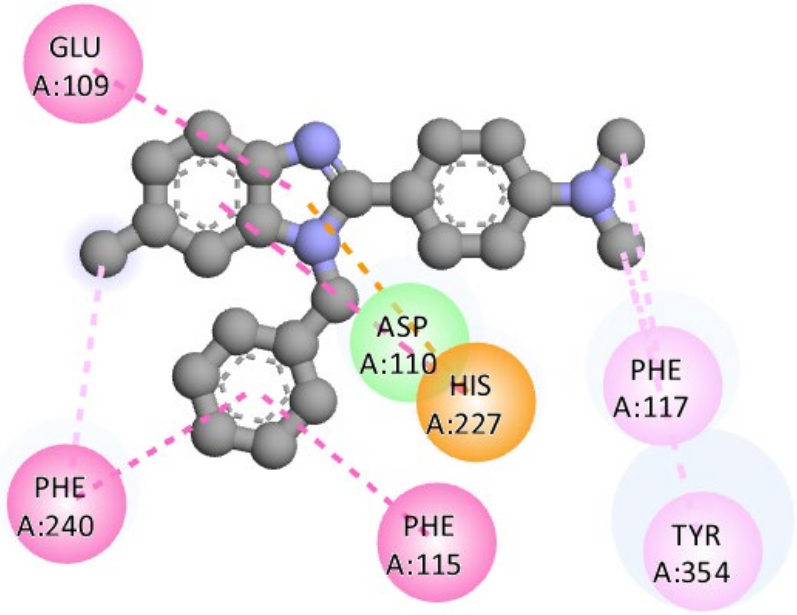
Interactions

- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Sigma
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl



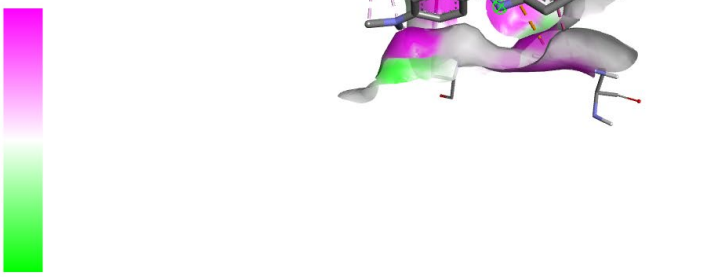
4.3. Compound 3s

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -340508208
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.6      0.000      0.000
   2         -9.5      2.659      6.568
   3         -9.3      2.722      4.910
   4         -9.1      3.504      7.534
   5         -8.9      7.666      9.685
   6         -8.6      1.818      2.549
   7         -8.6      5.244      8.644
   8         -8.5      3.660      7.901
   9         -8.5      4.216      8.579
Writing output ... done.
```



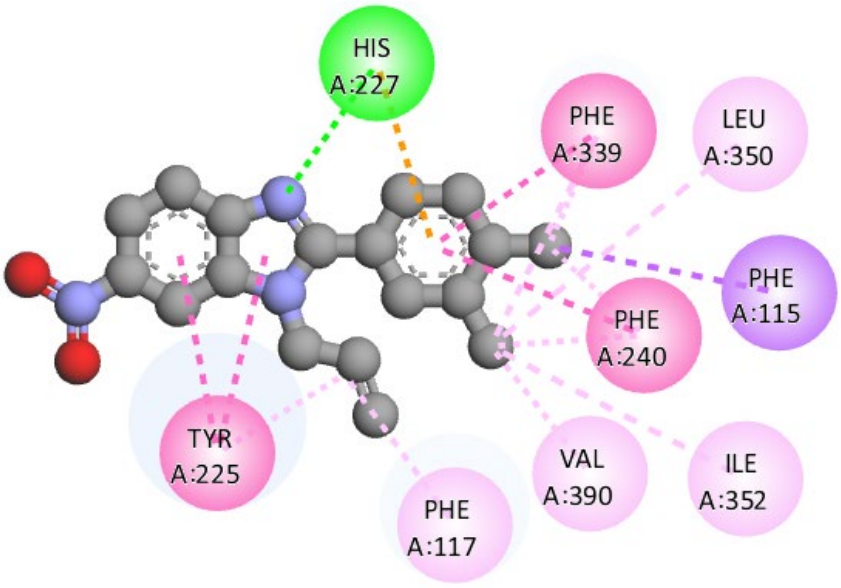
Interactions

- van der Waals
- Pi-Cation
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Amide-Pi Stacked
- Pi-Alkyl



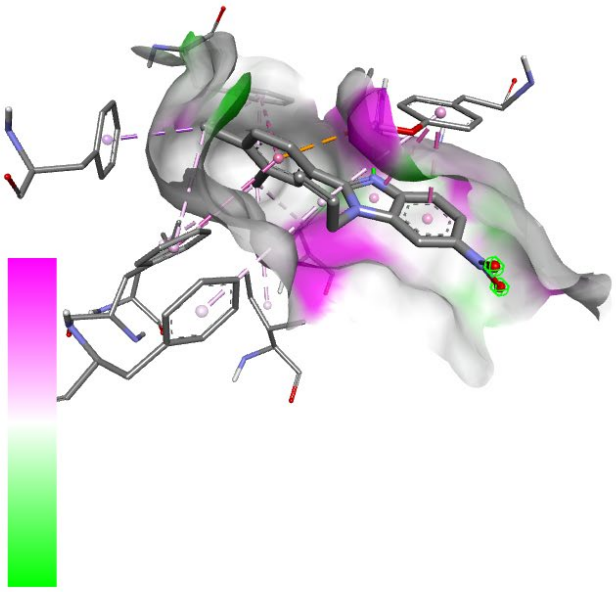
4.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -512187988
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.9      0.000      0.000
   2         -8.6      4.939      7.033
   3         -8.4      4.479      6.800
   4         -8.3      1.971      2.712
   5         -8.3      4.364      5.710
   6         -8.1      3.785      5.001
   7         -8.0      4.703      6.653
   8         -8.0      5.801      8.024
   9         -8.0      4.510      6.027
Writing output ... done.
```



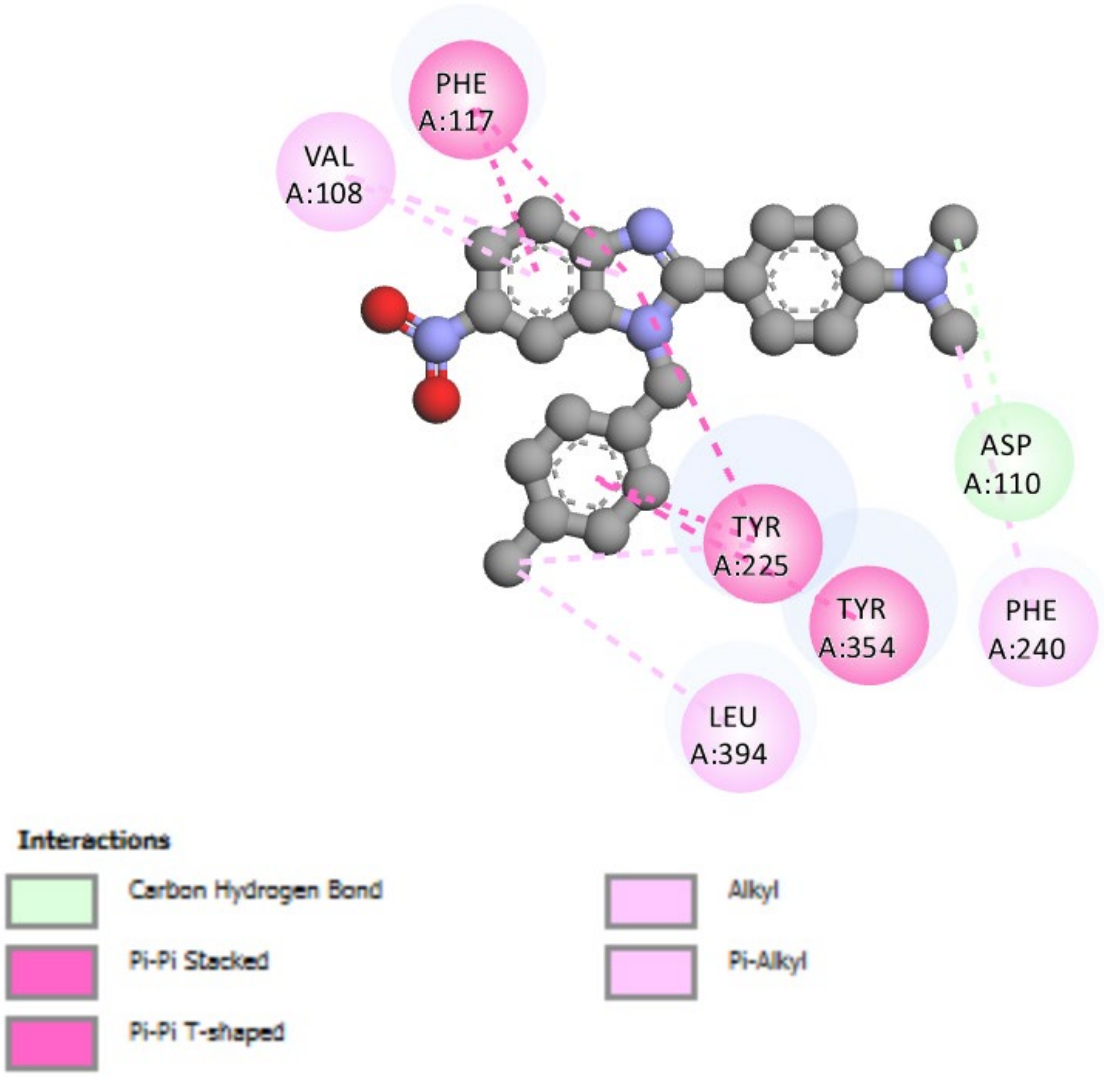
Interactions

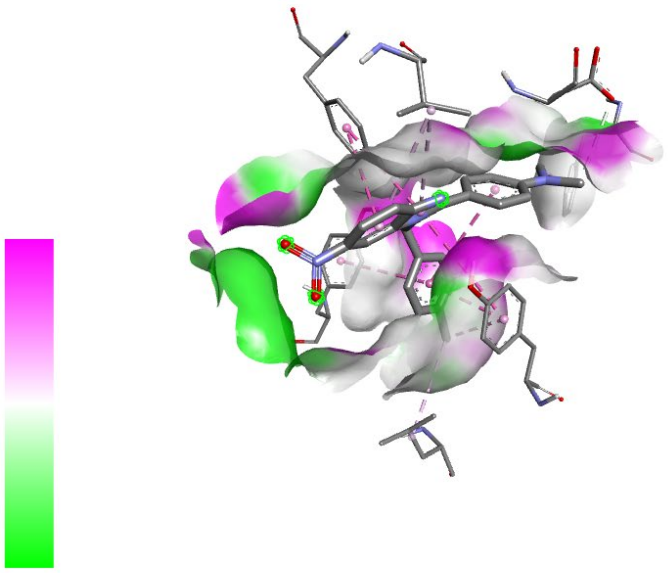
- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Sigma
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl



4.5. Compound 4k

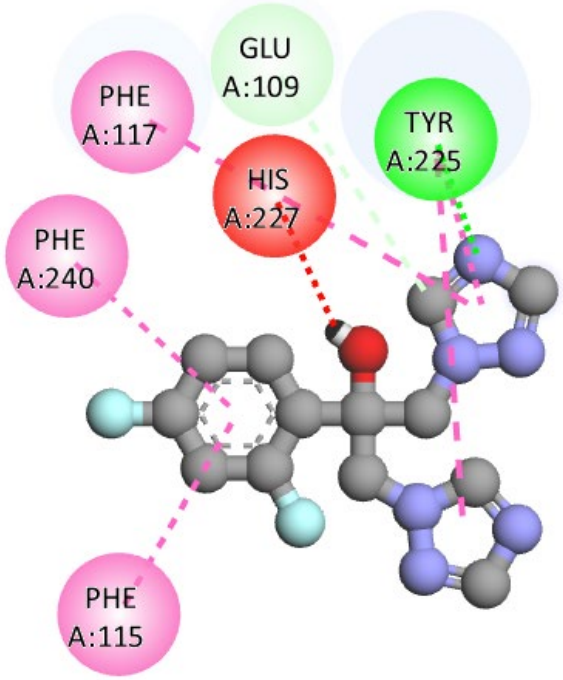
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1607913660
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.9      0.000      0.000
   2         -9.6      3.411      5.568
   3         -9.6      5.043      8.727
   4         -9.5      4.965      8.316
   5         -9.3      3.735      6.602
   6         -9.0      3.039      5.013
   7         -8.9      3.906      5.786
   8         -8.9      3.998      7.333
   9         -8.9      2.262      3.264
Writing output ... done.
```


PHE
A:117
VAL
A:108
ASP
A:110
TYR
A:225
TYR
A:354
PHE
A:240
LEU
A:394
Interactions
Carbon Hydrogen Bond
Pi-Pi Stacked
Pi-Pi T-shaped
Alkyl
Pi-Alkyl



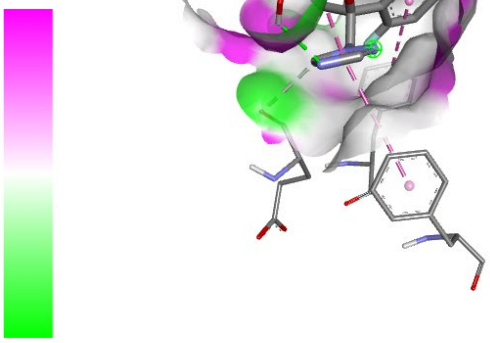
4.6. Compound Flu

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1075688508
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.9      0.000      0.000
   2         -7.8      2.200      2.868
   3         -7.8      1.126      3.929
   4         -7.3      5.388      7.088
   5         -7.3      6.029      8.223
   6         -7.1      6.700      8.796
   7         -7.1      7.616      9.573
   8         -7.1      5.968      7.483
   9         -7.0      5.800      8.368
Writing output ... done.
```



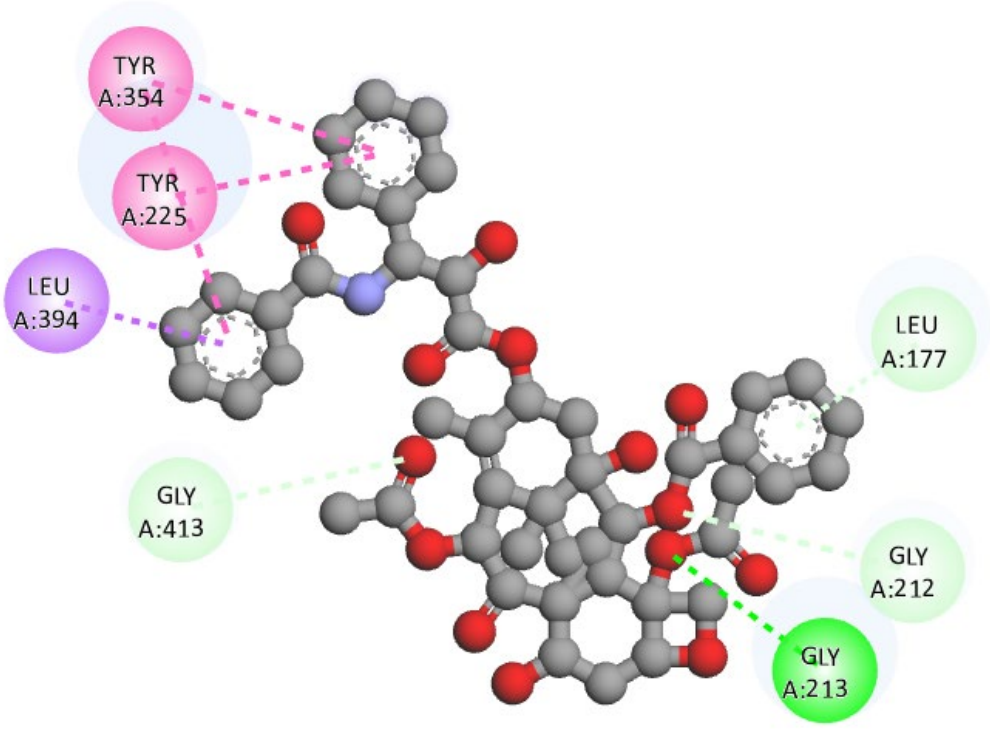
Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Donor-Donor
- Pi-Pi Stacked
- Pi-Pi T-shaped



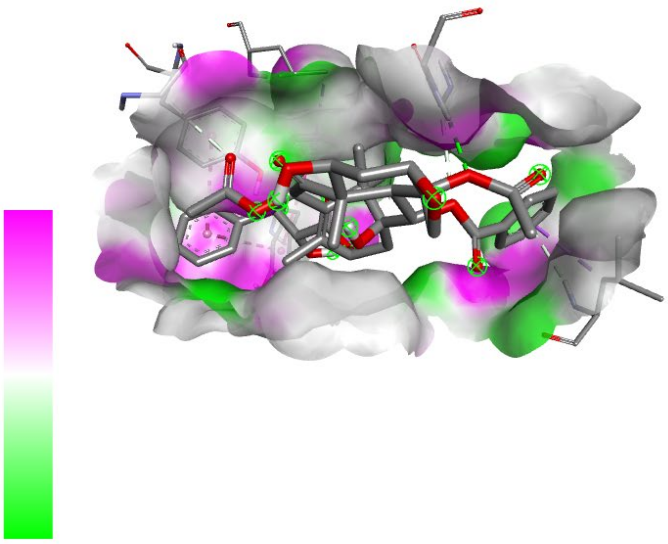
4.7. Compound PTX

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1697931708
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -11.4      0.000      0.000
   2        -10.8      1.142      3.784
   3        -10.0      3.254      7.148
   4         -9.7      1.651      4.239
   5         -9.5      3.229     10.323
   6         -9.4      3.191      7.252
   7         -9.3      3.160      9.844
   8         -9.3      2.344      3.916
   9         -8.5      3.061      9.289
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Pi-Pi Stacked
- Pi-Pi T-shaped



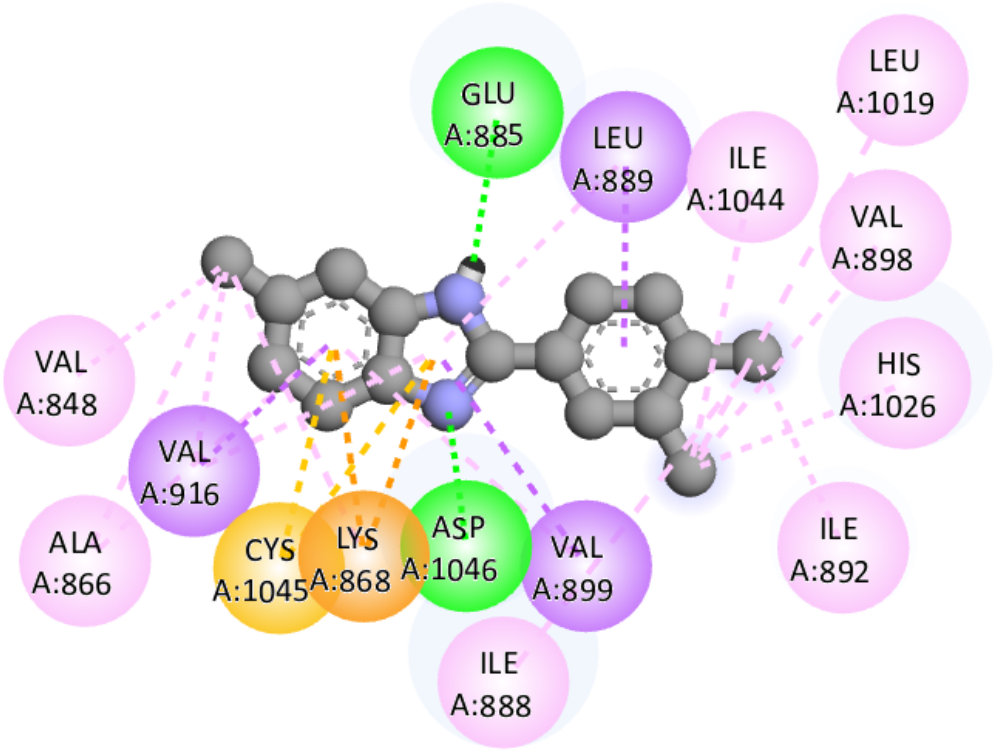
5. Vascular endothelial growth factor receptor 2 (PDB: 5EW3)

Grid box volume – Autodock Vina

```
receptor = 5ew3VEGFR2.pdbqt
ligand = ligand.pdbqt

out = out.pdbqt

center_x = 18.728
center_y = 9.165
center_z = 12.278

size_x = 36
size_y = 34
size_z = 34

energy_range = 4
exhaustiveness = 8
```

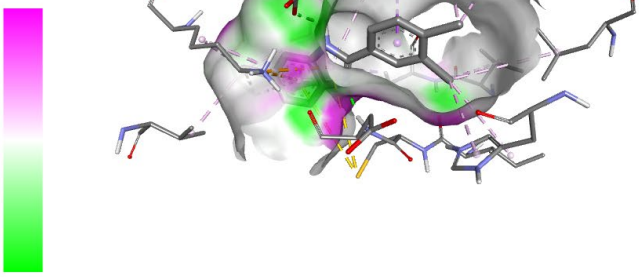
5.1. Compound 1d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 357772200
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.7      0.000      0.000
   2         -9.0      1.247      6.694
   3         -8.3      1.160      2.302
   4         -7.3      5.278      6.957
   5         -7.2      4.825      7.140
   6         -7.2     11.725     13.274
   7         -7.2     15.924     16.716
   8         -7.2      5.743      8.042
   9         -7.1      4.661      6.902
Writing output ... done.
```



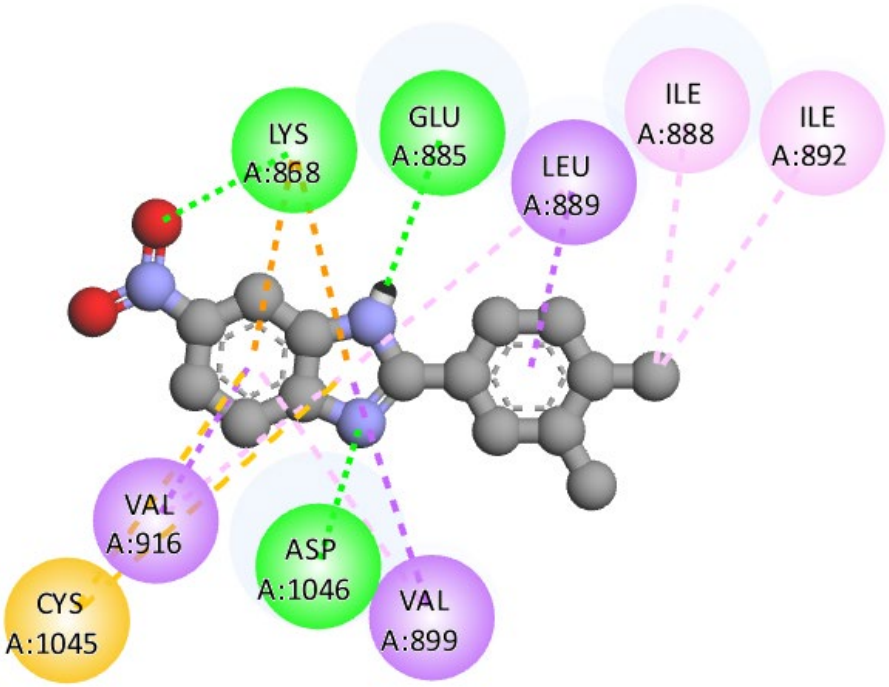
Interactions

- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Sigma
- Pi-Sulfur
- Alkyl
- Pi-Alkyl



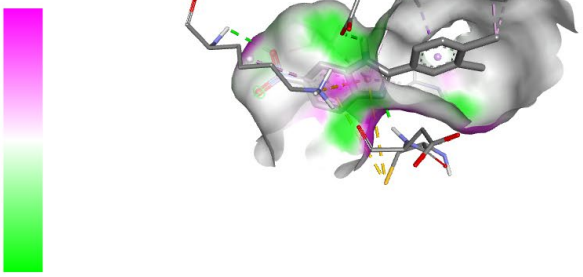
5.2. Compound 2d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1649512408
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.1      0.000      0.000
   2         -8.3      5.312      7.203
   3         -7.4      4.190      5.996
   4         -7.4      6.482      8.080
   5         -7.3      7.366      9.813
   6         -7.2     16.091     17.426
   7         -7.2      5.729      7.440
   8         -7.1      7.025      8.573
   9         -7.0      6.298      8.069
Writing output ... done.
```



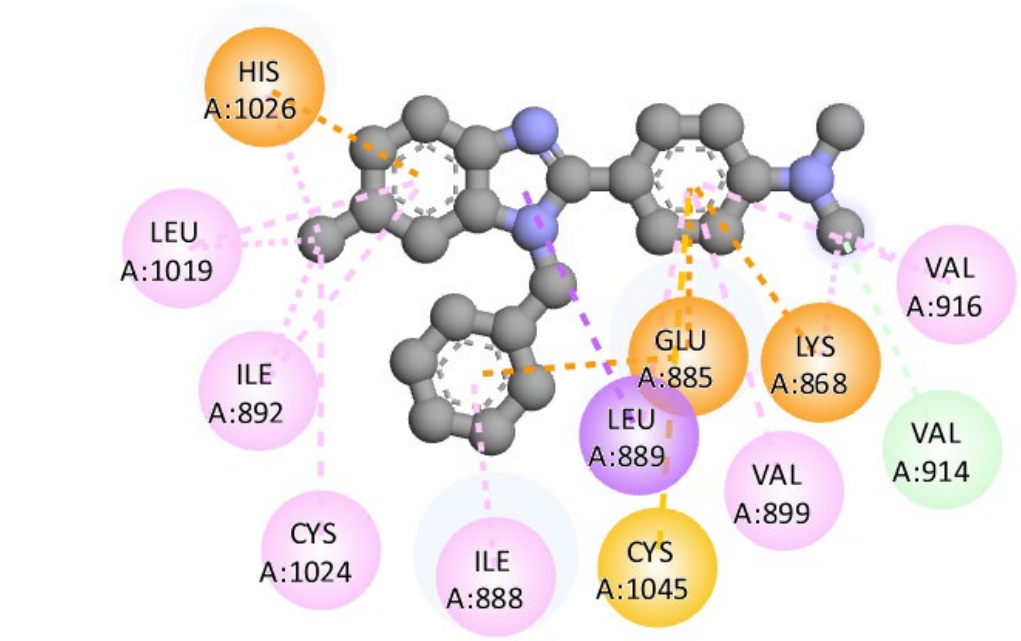
Interactions

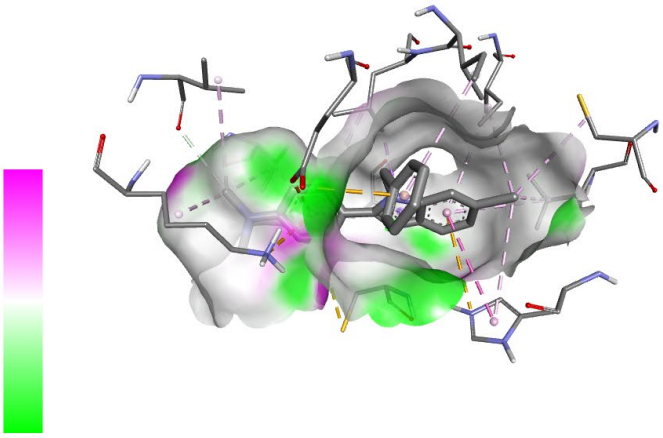
- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Sigma
- Pi-Sulfur
- Alkyl
- Pi-Alkyl



5.3. Compound 3s

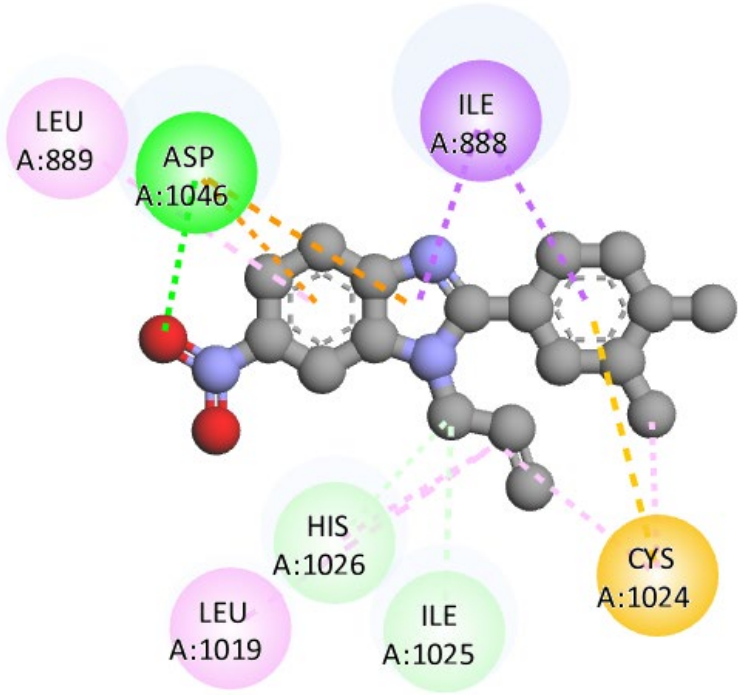
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -446671040
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.4      0.000      0.000
   2         -9.0      3.452      6.212
   3         -8.2      4.088      7.349
   4         -8.1      4.996      7.908
   5         -8.1      4.407      7.814
   6         -7.9      4.291      7.752
   7         -7.8      3.501      8.346
   8         -7.6      3.936      6.892
   9         -7.4      4.782      8.257
Writing output ... done.
```


HIS
A:1026
LEU
A:1019
ILE
A:892
CYS
A:1024
ILE
A:888
CYS
A:1045
LEU
A:889
GLU
A:885
LYS
A:868
VAL
A:916
VAL
A:914
VAL
A:899
Interactions
Carbon Hydrogen Bond
Pi-Cation
Pi-Anion
Pi-Sigma
Pi-Sulfur
Pi-Pi T-shaped
Alkyl
Pi-Alkyl



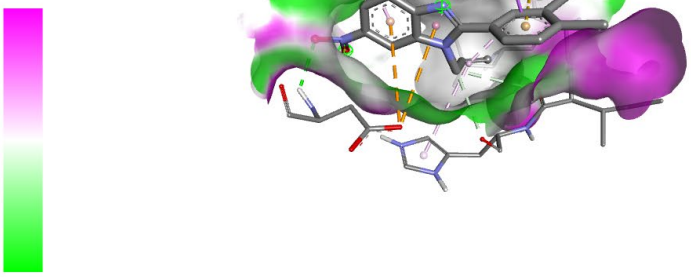
5.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 814937824
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.5      0.000      0.000
   2         -7.5      3.546      4.475
   3         -6.9      3.800      4.606
   4         -6.8      4.950      7.371
   5         -6.7      5.094      7.015
   6         -6.5     12.937     14.478
   7         -6.5      3.159      4.221
   8         -6.5      4.827      7.037
   9         -6.4      4.947      6.914
Writing output ... done.
```



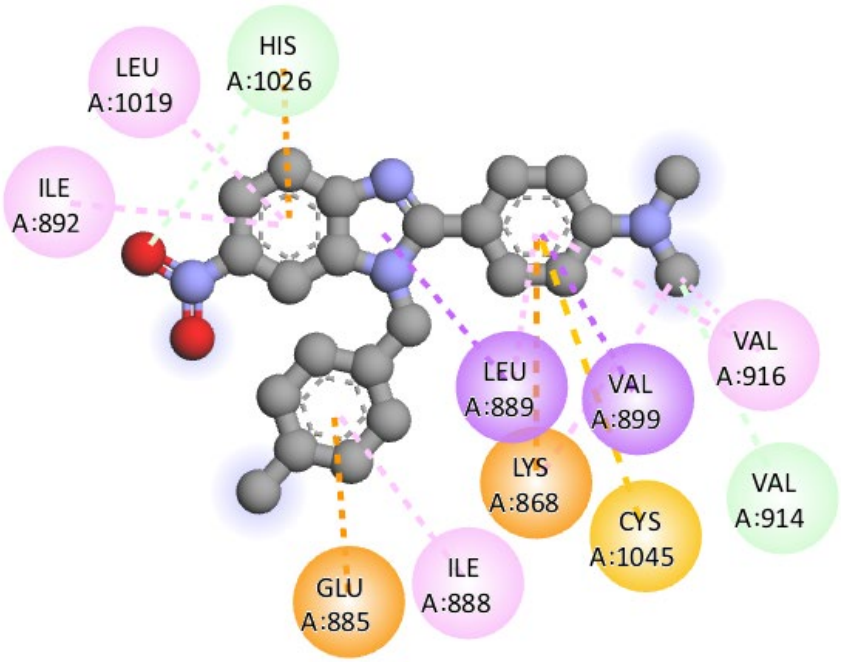
Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Pi-Sulfur
- Alkyl
- Pi-Alkyl



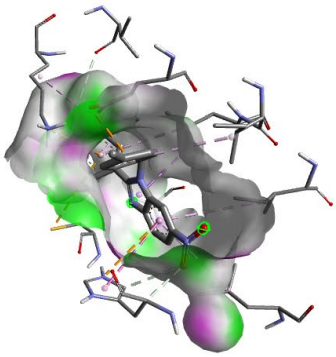
5.5. Compound 4k

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1112742280
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.7      0.000      0.000
   2         -9.2      3.687      6.656
   3         -9.1      3.824      7.907
   4         -8.6      4.792      7.721
   5         -8.5      4.793      7.686
   6         -8.1      4.185      7.049
   7         -8.0      7.063     10.436
   8         -7.7     11.875     13.393
   9         -7.6     12.848     15.720
Writing output ... done.
```



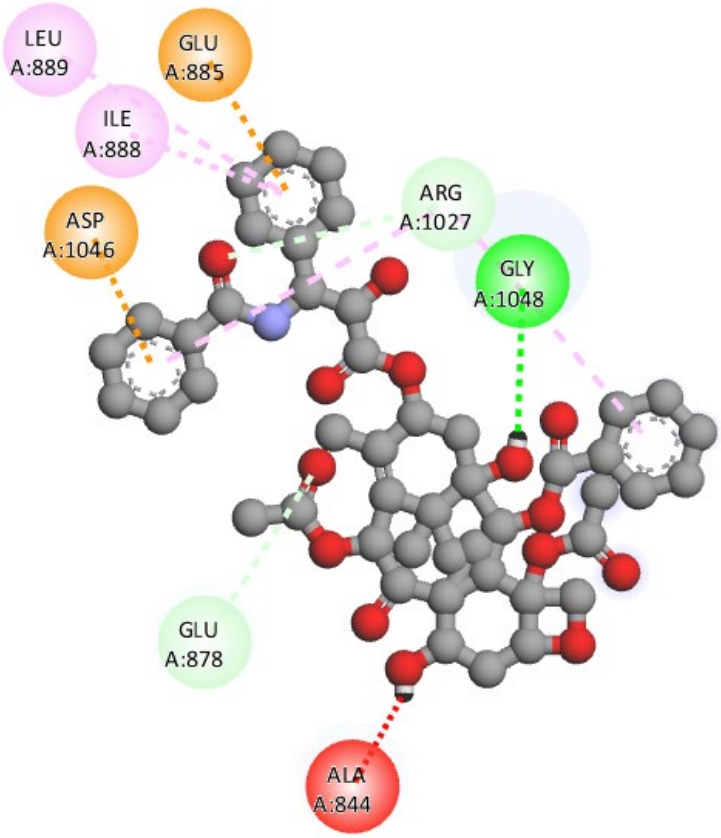
Interactions

- Carbon Hydrogen Bond
- Pi-Cation
- Pi-Anion
- Pi-Sigma
- Pi-Sulfur
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl



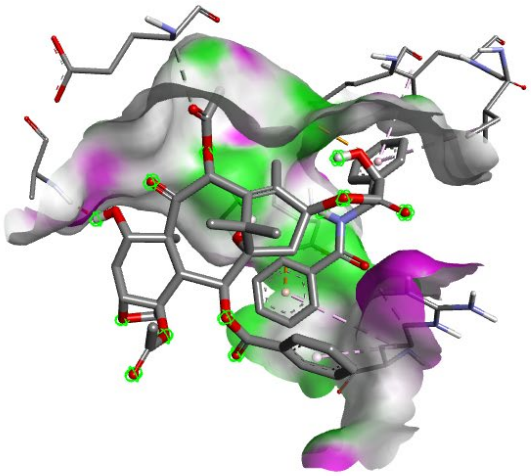
5.6. Compound PTX

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 830497308
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.8      0.000      0.000
   2         -7.6      1.432      3.556
   3         -7.3      2.745      4.845
   4         -7.3      3.505      7.224
   5         -7.1      2.472      4.817
   6         -7.0      3.374      7.920
   7         -6.8      5.740      9.612
   8         -6.7      3.257      6.261
   9         -6.7      8.865     12.688
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Donor-Donor
- Pi-Anion
- Pi-Alkyl



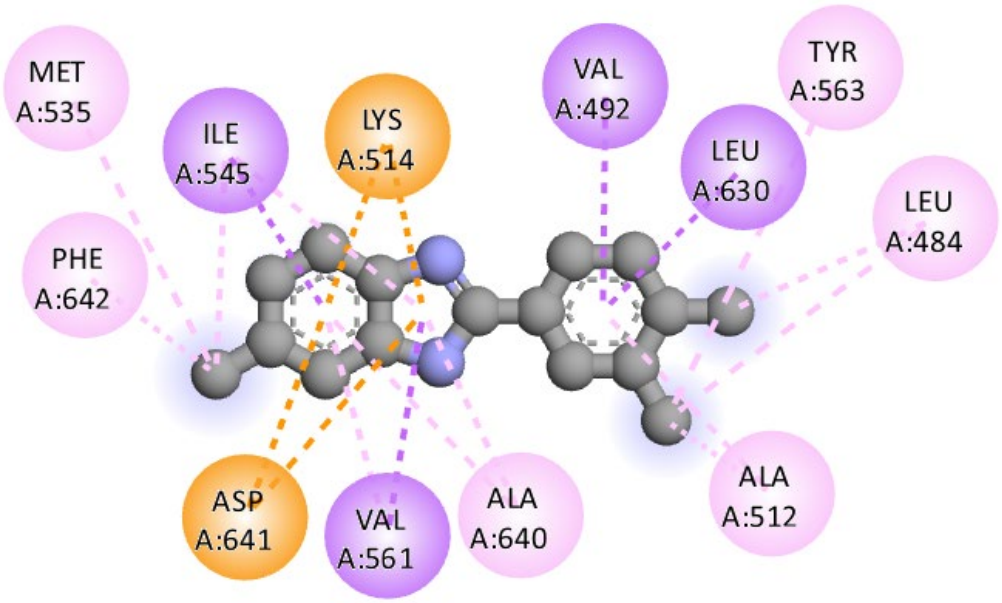
6. Fibroblast growth factor receptor 1 (PDB: 5A46)

Grid box volume – Autodock Vina

```
receptor = 5a46FGFR1.pdbqt
ligand = ligand.pdbqt

out = out.pdbqt

center_x = 85.27
center_y = 1.20
center_z = 8.409

size_x = 52
size_y = 42
size_z = 48

energy_range = 4
exhaustiveness = 8
```

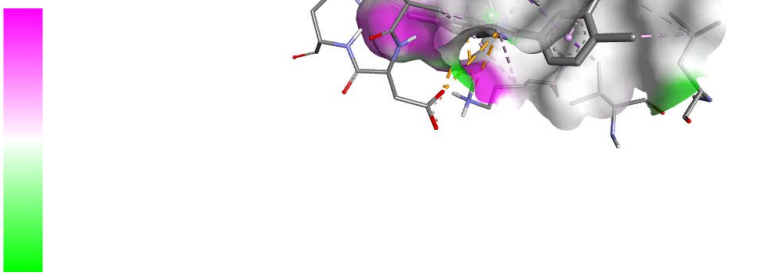
6.1. Compound 1d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 41367724
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.3      0.000      0.000
   2         -7.6      4.861      9.436
   3         -7.5      3.348      7.863
   4         -7.2      3.750      5.296
   5         -7.1      4.715      7.049
   6         -6.7     23.537     25.733
   7         -6.6     26.071     27.622
   8         -6.6      3.732      5.449
   9         -6.5     26.198     26.869
Writing output ... done.
```



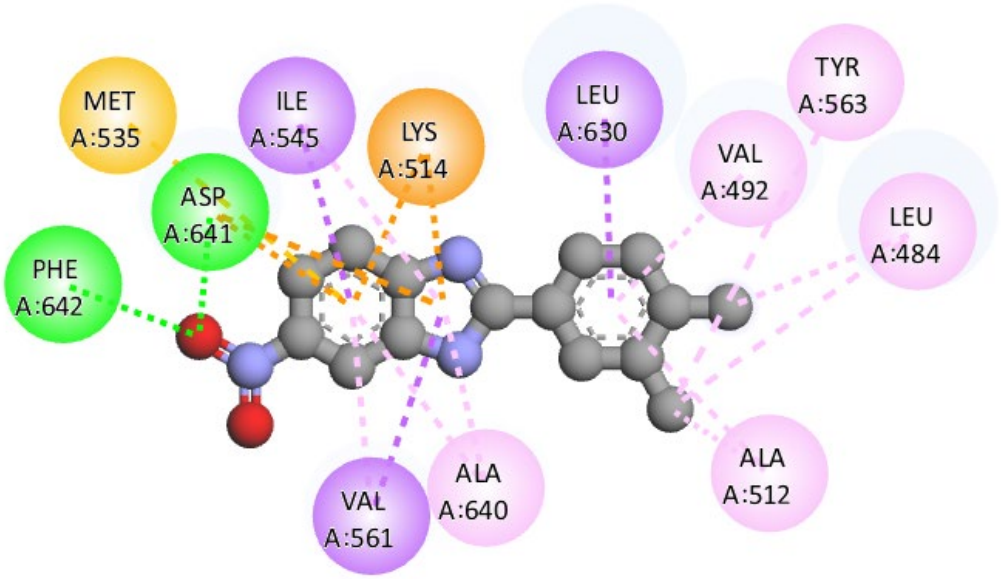
Interactions

- Pi-Cation
- Pi-Anion
- Pi-Sigma
- Alkyl
- Pi-Alkyl



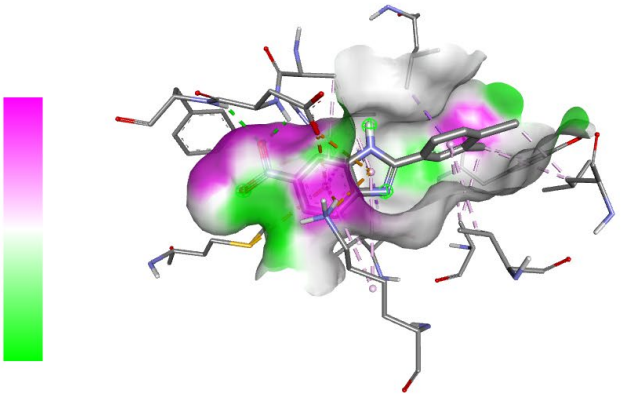
6.2. Compound 2d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -611865088
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.1      0.000      0.000
   2         -8.0      6.684      9.254
   3         -7.9      3.659      5.226
   4         -7.8      3.632      5.394
   5         -7.3     25.932     26.790
   6         -7.2     25.920     27.152
   7         -7.2      6.715      9.362
   8         -7.0      7.760     10.694
   9         -6.9      2.499      3.464
Writing output ... done.
```



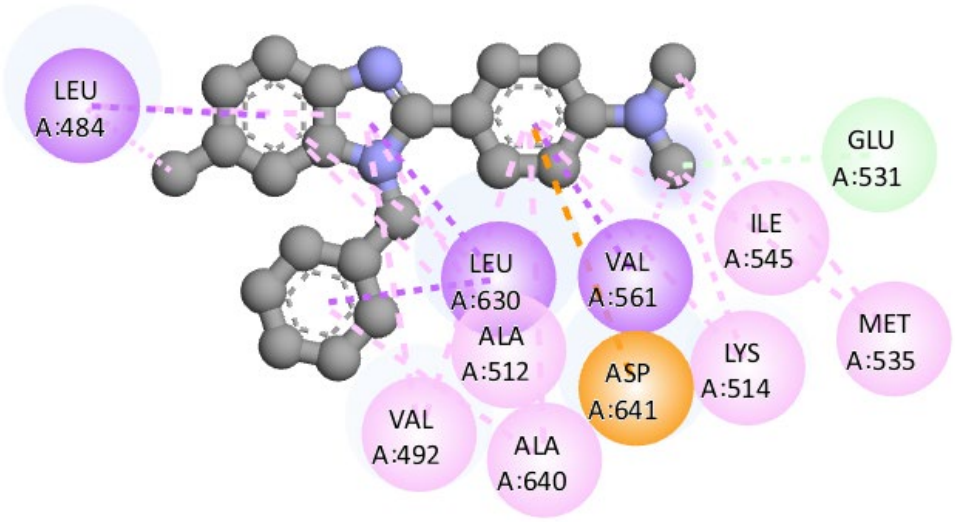
Interactions

- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Anion
- Pi-Sigma
- Pi-Sulfur
- Alkyl
- Pi-Alkyl



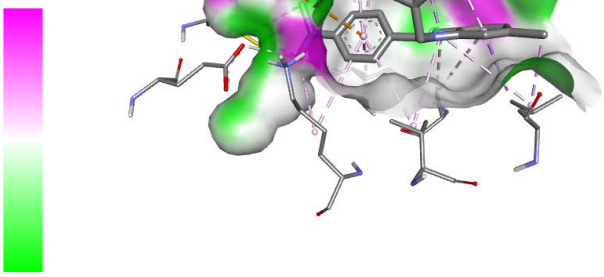
6.3. Compound 3s

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1229292912
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.6      0.000      0.000
   2         -8.6      1.668      2.494
   3         -7.7      1.826      4.264
   4         -7.2      3.430      7.869
   5         -7.2      1.965      2.924
   6         -7.1      3.357      5.590
   7         -7.1     24.882     26.990
   8         -7.0     25.811     28.059
   9         -7.0      2.883      5.882
Writing output ... done.
```



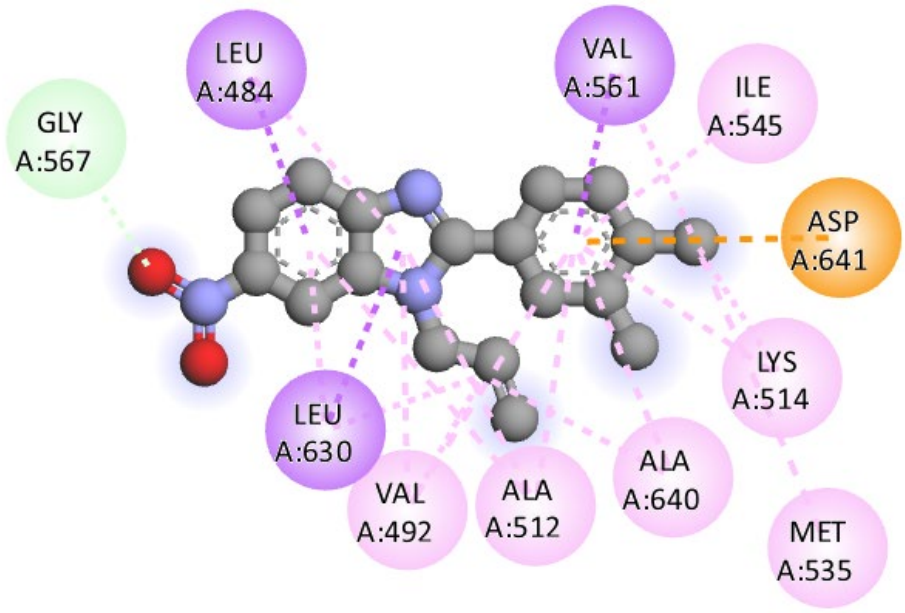
Interactions

- Carbon Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Alkyl
- Pi-Alkyl



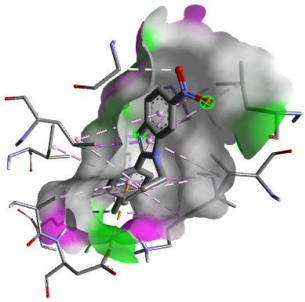
6.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1514471776
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.0      0.000      0.000
   2         -7.2      4.902      6.985
   3         -7.1     25.175     26.689
   4         -7.1      4.990      7.272
   5         -6.9      5.220      7.485
   6         -6.8      5.407      7.802
   7         -6.7     22.683     24.504
   8         -6.7      3.435      5.041
   9         -6.7     25.363     27.466
Writing output ... done.
```



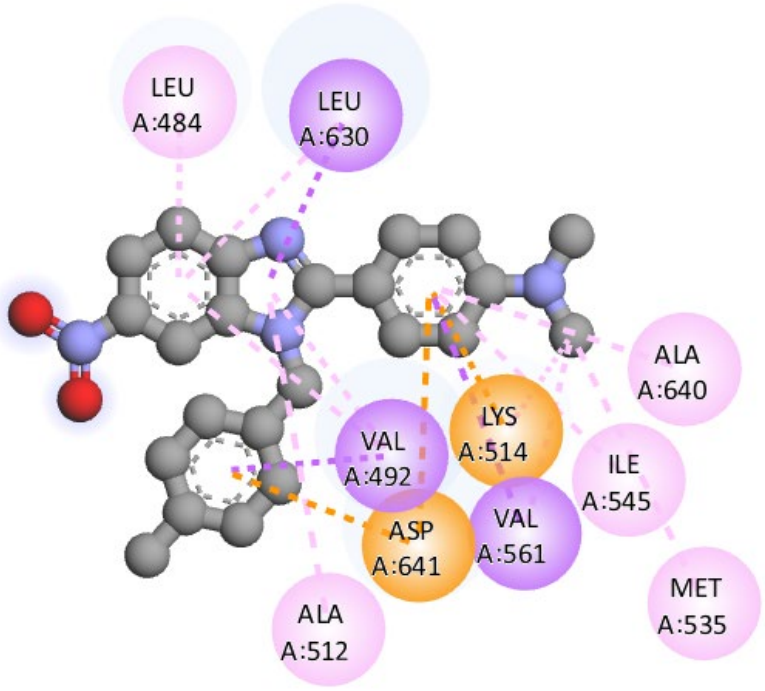
Interactions

- Carbon Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Alkyl
- Pi-Alkyl



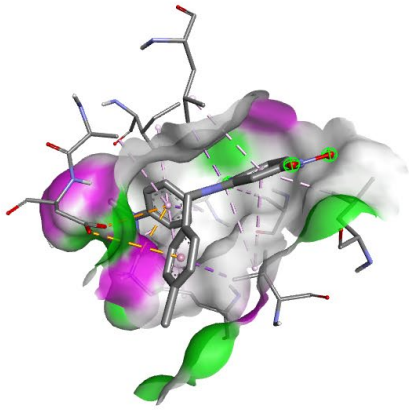
6.5. Compound 4k

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1139121352
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.5      0.000      0.000
   2         -8.1      3.900      5.823
   3         -7.7      2.280      2.755
   4         -7.7     25.341     27.273
   5         -7.6     24.782     27.193
   6         -7.5     25.390     28.124
   7         -7.5     25.655     28.153
   8         -7.4     26.154     28.429
   9         -7.3      4.054      6.422
Writing output ... done.
```



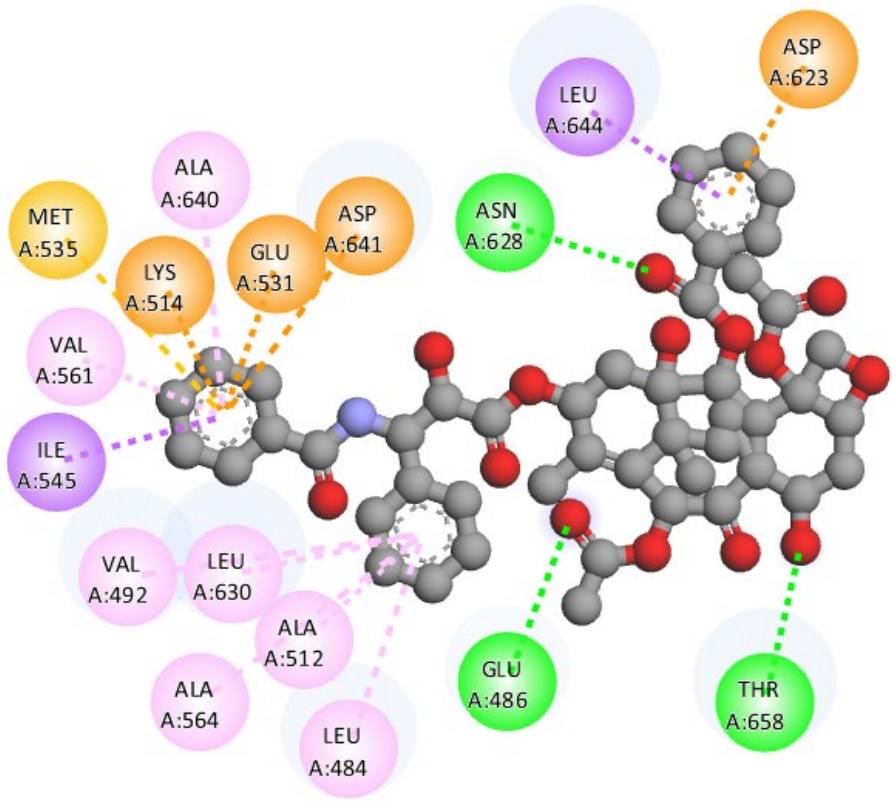
Interactions

- Pi-Cation
- Pi-Anion
- Pi-Sigma
- Alkyl
- Pi-Alkyl



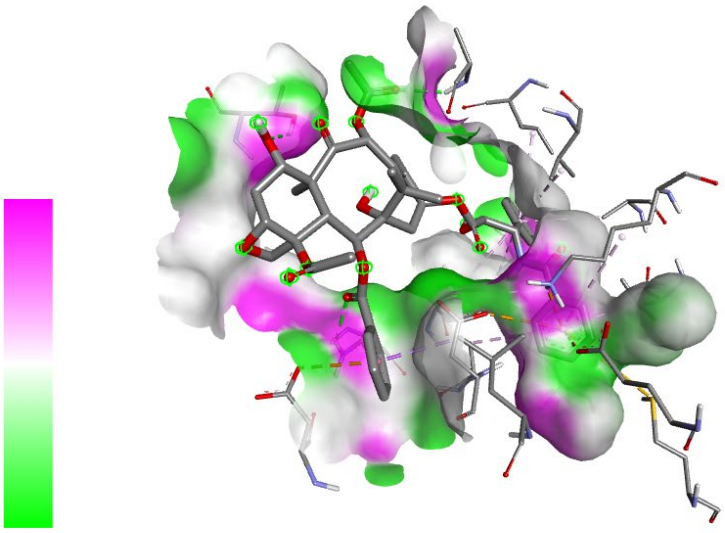
6.6. Compound PTX

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 156777752
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -10.5      0.000      0.000
   2         -9.8      2.913      4.940
   3         -9.5      1.946      4.442
   4         -9.4      3.558     10.426
   5         -9.4      2.684      4.388
   6         -9.3      3.141      5.010
   7         -9.2      4.014      9.926
   8         -9.2      3.942      9.070
   9         -9.1      3.016      6.438
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Pi-Sigma
- Pi-Cation
- Pi-Sulfur
- Pi-Anion
- Pi-Alkyl



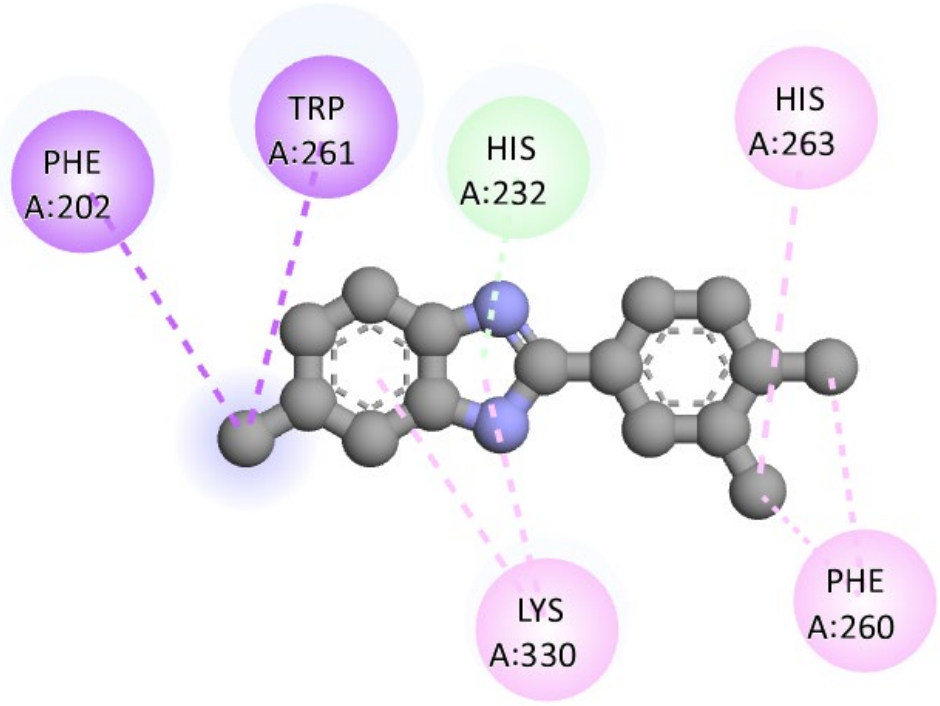
7. Histone deacetylase 6 (PDB: 5EEF)

Grid box volume – Autodock Vina

```
receptor = 5eefHDAC6.pdbqt
ligand = ligand.pdbqt

out = out.pdbqt

center_x = -18.649
center_y = -42.547
center_z = -12.834

size_x = 30
size_y = 42
size_z = 30

energy_range = 4
exhaustiveness = 8
```

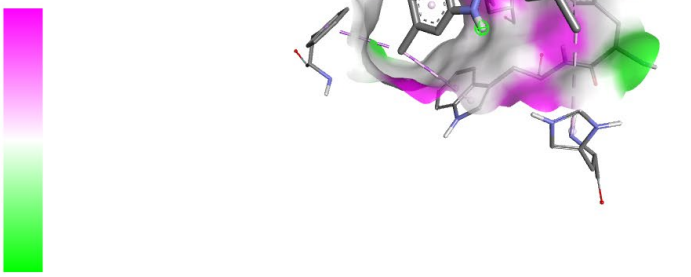
7.1. Compound 1d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1674649056
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.4      0.000      0.000
   2         -7.1      1.181      6.764
   3         -7.1      0.958      1.781
   4         -6.9      2.769      3.886
   5         -6.9      1.780      2.415
   6         -6.8     13.849     16.312
   7         -6.7      2.160      2.556
   8         -6.6      1.405      2.213
   9         -6.6      4.191      6.987
Writing output ... done.
```



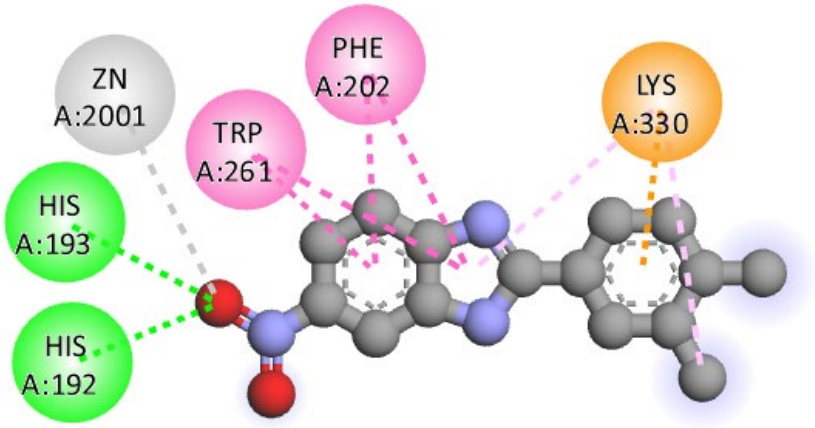
Interactions

- Pi-Donor Hydrogen Bond
- Pi-Pi T-shaped
- Pi-Sigma
- Pi-Alkyl



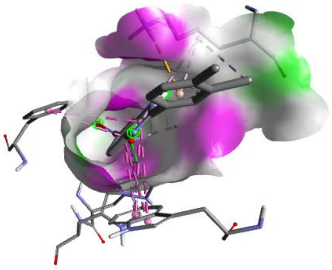
7.2. Compound 2d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -44090860
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.2      0.000      0.000
   2         -8.1      0.702      1.564
   3         -8.0      1.686      1.930
   4         -7.4      3.010      3.648
   5         -7.2      3.153      3.784
   6         -7.1      5.579      7.837
   7         -7.1      3.337      4.433
   8         -6.9     13.935     15.213
   9         -6.7     14.524     15.626
Writing output ... done.
```



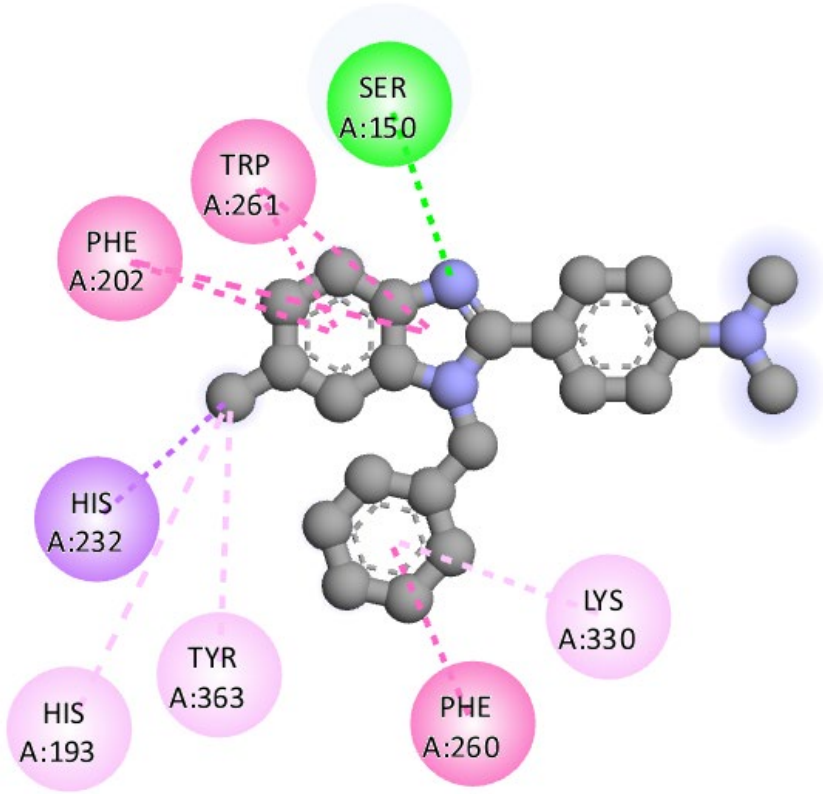
Interactions

- Conventional Hydrogen Bond
- Metal-Acceptor
- Pi-Cation
- Pi-Pi Stacked
- Alkyl
- Pi-Alkyl



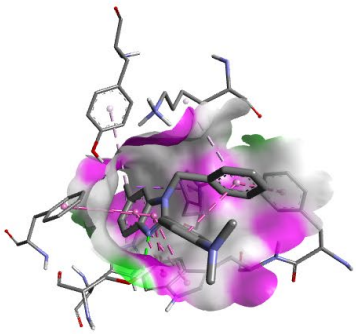
7.3. Compound 3s

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1911046216
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.6      0.000      0.000
   2         -7.0      2.977      5.814
   3         -7.0      3.317      5.592
   4         -6.9      3.187      5.676
   5         -6.9      2.803      5.544
   6         -6.6      2.871      4.163
   7         -6.6      1.436      2.090
   8         -6.3     11.991     14.459
   9         -6.3     11.026     13.287
Writing output ... done.
```



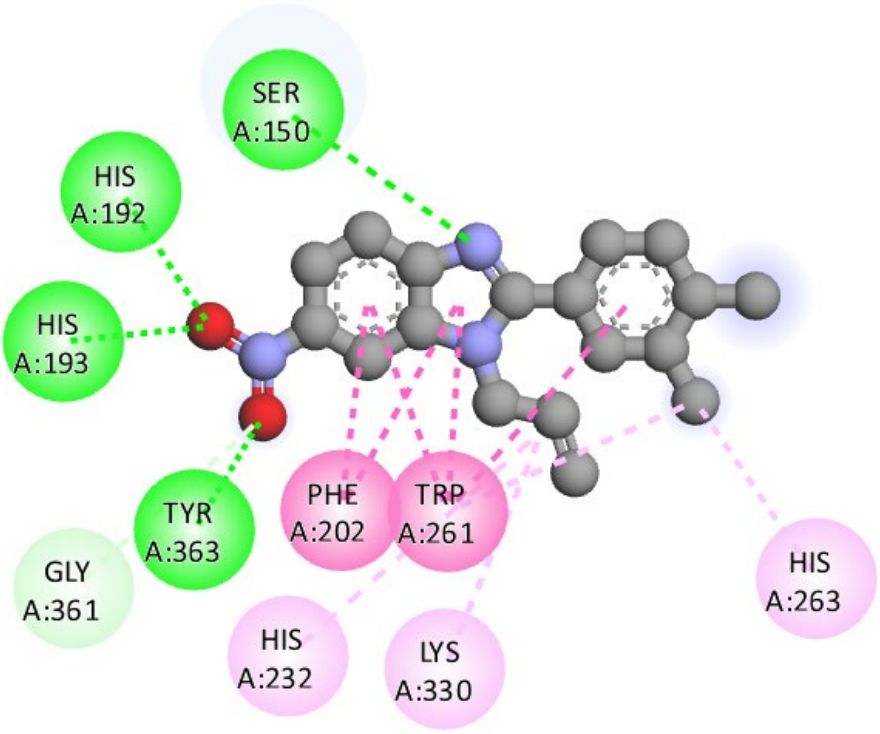
Interactions

- Conventional Hydrogen Bond
- Pi-Pi Stacked
- Pi-Sigma
- Pi-Alkyl



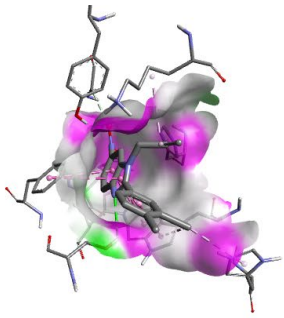
7.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 924438784
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.9      0.000      0.000
   2         -7.7      1.586      2.485
   3         -7.0      5.247      7.428
   4         -7.0      1.988      2.836
   5         -6.5     12.783     14.597
   6         -6.2      4.781      6.844
   7         -6.2      5.827      7.962
   8         -6.2      4.422      6.417
   9         -6.1     10.367     12.309
Writing output ... done.
```



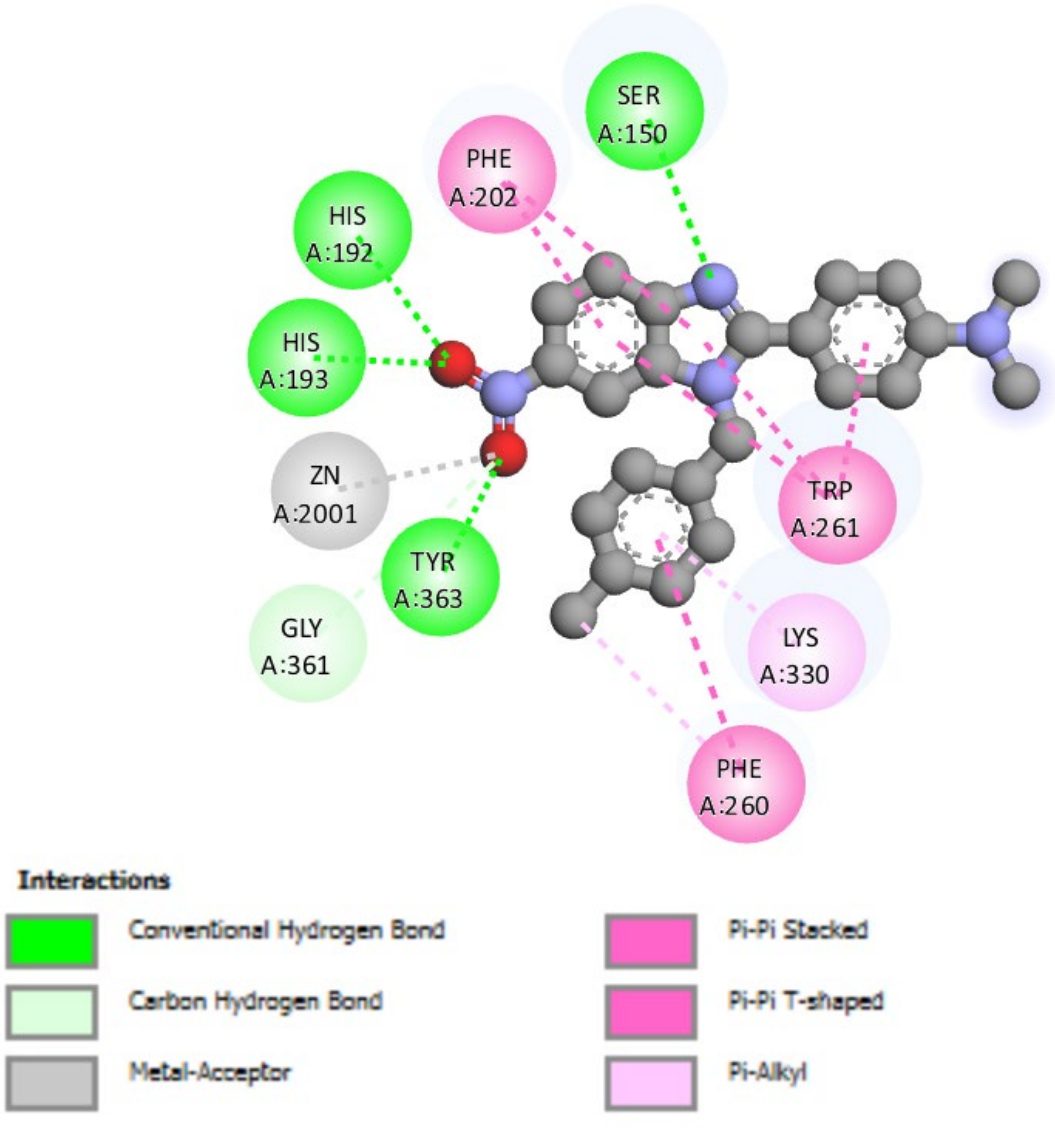
Interactions

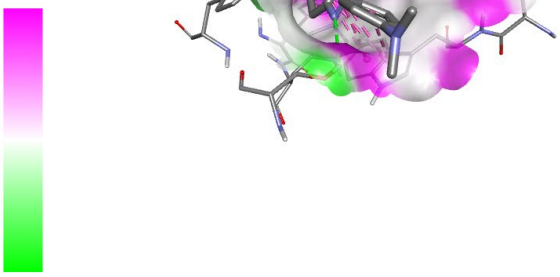
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl



7.5. Compound 4k

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1168086400
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.9      0.000      0.000
   2         -8.4      1.263      1.696
   3         -7.7      2.984      4.269
   4         -7.4      4.045      6.254
   5         -7.2      4.236      6.264
   6         -7.0     12.463     14.806
   7         -6.9      4.631      7.618
   8         -6.9      2.068      2.984
   9         -6.7      3.937      6.194
Writing output ... done.
```


SER
A:150
PHE
A:202
HIS
A:192
HIS
A:193
ZN
A:2001
TYR
A:363
GLY
A:361
TRP
A:261
LYS
A:330
PHE
A:260
Interactions
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Metal-Acceptor
Pi-Pi Stacked
Pi-Pi T-shaped
Pi-Alkyl



7.6. Compound PTX

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
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#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1815704864
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.8      0.000      0.000
   2         -8.6      1.433      3.830
   3         -8.6      2.045      4.464
   4         -8.2      3.041     10.618
   5         -8.2      1.686      2.402
   6         -8.1      2.727     10.379
   7         -8.0      2.358      4.290
   8         -7.9      2.207      4.677
   9         -7.8      2.552      9.861
Writing output ... done.
```

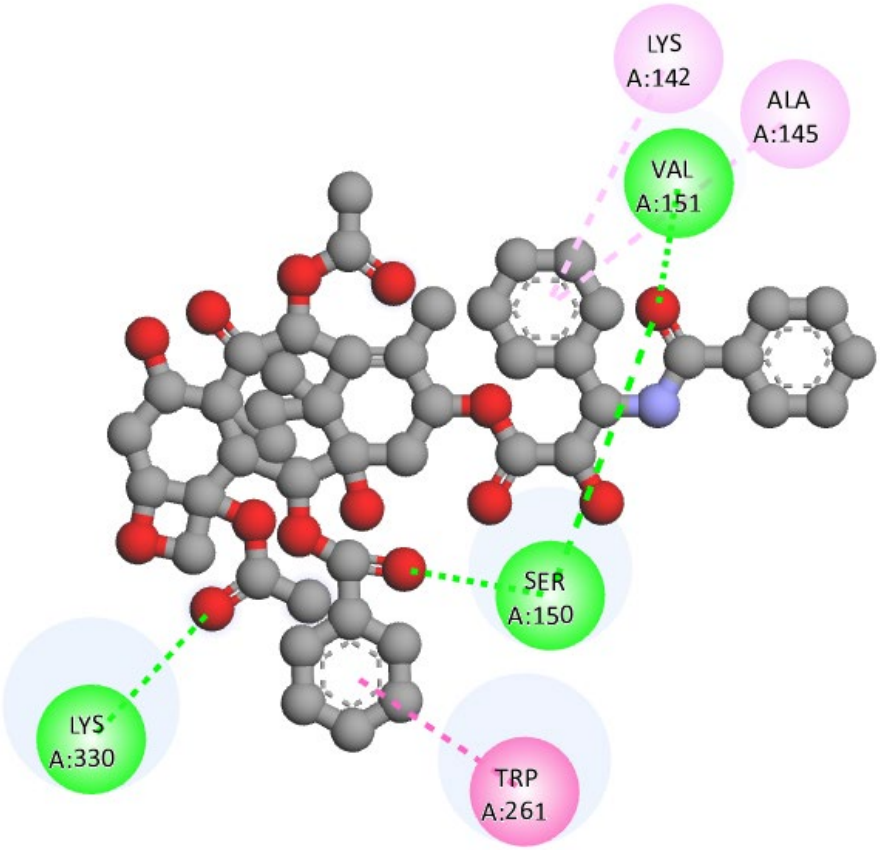

Interactions

Conventional Hydrogen Bond

Pi-Alkyl

Pi-Pi Stacked