SUPPORTING INFORMATION

Synthesis, In Silico and In Vitro Evaluation of Some Flavone Derivatives for Acetylcholinesterase and BACE-1 Inhibitory Activity

Thai-Son Tran [1,2], Thanh-Dao Tran [1], The-Huan Tran [2], Thanh-Tan Mai [1], Ngoc-Le Nguyen [3], Khac-Minh Thai [1,*] and Minh-Tri Le [1,4,*]

[1] Department of Medicinal Chemistry, Faculty of Pharmacy, University of Medicine and Pharmacy at Ho Chi Minh City, Ho Chi Minh City 700000, Vietnam; ttson@huemed-univ.edu.vn (T.-S.T.); tranthanhdao@uphcm.edu.vn (T.-D.T.); mthtan@ump.edu.vn (T.-T.M.)

[2] Department of Pharmaceutical Chemistry, Faculty of Pharmacy, College of Medicine and Pharmacy, Hue University, Hue City 530000, Vietnam; tthuan@hueuni.edu.vn

[3] Department of Pharmaceutics and Industrial Pharmacy, Faculty of Pharmacy, South Can Tho University, Can Tho City 640000, Vietnam; dsngocle1984@gmail.com

[4] School of Medicine, Vietnam National University Ho Chi Minh City, Ho Chi Minh City 700000, Vietnam

* Correspondence: leminhtri@ump.edu.vn (M.-T.L.); thaikhacminh@gmail.com or thaikhacminh@uphcm.edu.vn (K.-M.T.); Tel.: +84-28-3855-2225 or +84-909-680-385 (K-M.T.); +84-903-718-190 (M.-T.L.); Fax: +84-28-3822-5435 (K.-M.T.)

Table S1. Selected descriptors used for building 2D-QSAR models reported in the previous published work [1]

Code	Category	Description
BCUT_SlogP_3	Adjacency and distance matrix	A Burden's parameter using atomic contribution to logP (using the Wildman and Crippen SlogP method [2]) instead of partial charge.
BCUT_PEOE_1	Adjacency and distance matrix	A descriptor relating topological shape and partial charges
petitjean	Adjacency and distance matrix	Value of (diameter - radius) / diameter.
reactive	Physical property	An indicator of the presence of reactive groups. A non-zero value indicates that the molecule contains a reactive group. The table of reactive groups is based on the Oprea set [3] and includes metals, phospho-, N/O/S-N/O/S single bonds, thiols, acyl halides, Michael Acceptors, azides, esters, etc.
logS	Physical property	The log of the aqueous solubility (mol/L).
PEOE_VSA-0, PEOE_VSA+1, PEOE_VSA-3, PEOE_VSA-6	Partial charge	Sum of the proximate accessible *van der Waals* surface area (Å^2), v_i, calculation for each atom over all the atoms *i*, such that partial charge of atom *i* is in a specified range.
SlogP_VSA2, SlogP_VSA3, SlogP_VSA5	Subdivided surface areas	Sum of the proximate accessible *van der Waals* surface area (Å^2), v_i, calculated for each atom over all the atoms, such that partition coefficient for atom *i* is in a specified range
SMR_VSA2	Subdivided surface areas	Sum of the proximate accessible *van der Waals* surface area (Å^2), v_i, calculation for each atom over all the atoms *i*, such that molar refractivity for atom *i* is in a specified range.
a_ICM	Atom counts and bond counts	The entropy of the element distribution in the molecule (including implicit hydrogens but not lone pair pseudo-atoms)
chiral_u	Atom counts and bond counts	The number of unconstrained chiral centers.
rings	Atom counts and bond counts	The number of rings
a_Nn	Atom counts and bond counts	The number of nitrogen atoms.

Table S2. Values of selected descriptors used in the prediction of pIC_{50} of the synthesized flavone derivatives (AChE)

Compound	BCUT_SLOGP_3	reactive	PEOE_VSA+1	PEOE_VSA-3	SlogP_VSA2	SMR_VSA2	**Predicted pIC_{50}**
B1 (Baicalein)	2.52	1	48.98	0.00	0.00	0.00	**4.66**
B2	2.53	1	74.58	0.00	0.00	0.00	**4.59**
B3	2.54	1	95.95	0.00	0.00	0.00	**4.55**
B4	2.53	1	121.54	0.00	0.00	0.00	**4.44**
B5	2.54	1	157.82	0.00	0.00	0.00	**4.32**
B6	2.58	1	183.41	0.00	0.00	0.00	**4.32**
B7	2.52	1	48.98	0.00	71.59	0.00	**4.52**
B8	2.54	1	48.98	0.00	71.59	0.00	**4.56**
D1 (Diosmetin)	2.49	1	74.43	0.00	0.00	0.00	**4.50**
D2	2.49	1	100.02	0.00	0.00	0.00	**4.42**
D3	2.50	1	121.40	0.00	0.00	0.00	**4.37**
D4	2.50	1	146.99	0.00	0.00	0.00	**4.26**
D5	2.50	1	112.82	0.00	0.00	0.00	**4.39**
D6	2.51	1	144.88	0.00	0.00	0.00	**4.31**
D7	2.49	1	117.08	0.00	0.00	0.00	**4.35**
Galanthamine	2.77	0	114.49	0.00	12.94	0.00	**5.14**

Table S3. Values of selected descriptors used in the prediction of pIC_{50} of the synthesized chalcone derivatives (BACE-1)

Compound	petitjean	BCUT_PEOE_1	a_ICM	chiral_u	rings	a_nN	PEOE_VSA-0	PEOE_VSA-6	logS	SlogP_VSA3	SlogP_VSA5	**Predicted pIC_{50}**
B1 (Baicalein)	0.50	-0.72	1.46	0	3	0	0.00	25.81	-3.46	0.00	0.00	**3.66**
B2	0.45	-0.62	1.44	0	3	0	0.00	15.28	-4.29	0.00	70.77	**4.82**
B3	0.50	-0.58	1.41	0	3	0	37.50	15.28	-4.94	41.85	0.00	**5.11**
B4	0.46	-0.67	1.39	0	3	0	0.00	15.28	-5.28	41.85	0.00	**4.35**
B5	0.46	-0.66	1.36	0	3	0	0.00	10.02	-6.19	62.78	0.00	**4.60**
B6	0.47	-0.65	1.29	0	6	0	6.63	10.02	-10.00	0.00	0.00	**5.18**
B7	0.50	-0.57	1.49	0	3	0	0.00	2.50	-5.61	0.00	0.00	**4.73**
B8	0.46	-0.57	1.46	0	3	0	0.00	2.50	-6.21	0.00	0.00	**4.75**
D1 (Diosmetin)	0.45	-0.87	1.48	0	3	0	61.27	28.31	-3.51	0.00	35.38	**3.55**
D2	0.50	-0.60	1.46	0	3	0	61.27	17.78	-4.34	0.00	106.15	**5.83**
D3	0.46	-0.56	1.43	0	3	0	98.77	17.78	-4.99	41.85	35.38	**6.04**
D4	0.47	-0.66	1.42	0	3	0	61.27	17.78	-5.33	41.85	35.38	**5.24**
D5	0.50	-0.59	1.44	0	3	0	61.27	12.52	-4.75	0.00	141.54	**6.20**
D6	0.46	-0.56	1.40	0	3	0	117.52	12.52	-5.73	62.78	35.38	**6.34**
D7	0.47	-0.65	1.42	0	5	0	98.04	12.78	-8.47	0.00	35.38	**6.07**
Umibecestat	0.50	-0.56	2.09	2	3	5	74.26	9.29	-5.92	20.93	16.79	**7.67**
Quercetin	0.50	-0.63	-1.52	0	3	0	61.27	41.34	-2.77	25.39	5.24	**5.24**

Table S4. Results of re-docking (RMSD in Å)

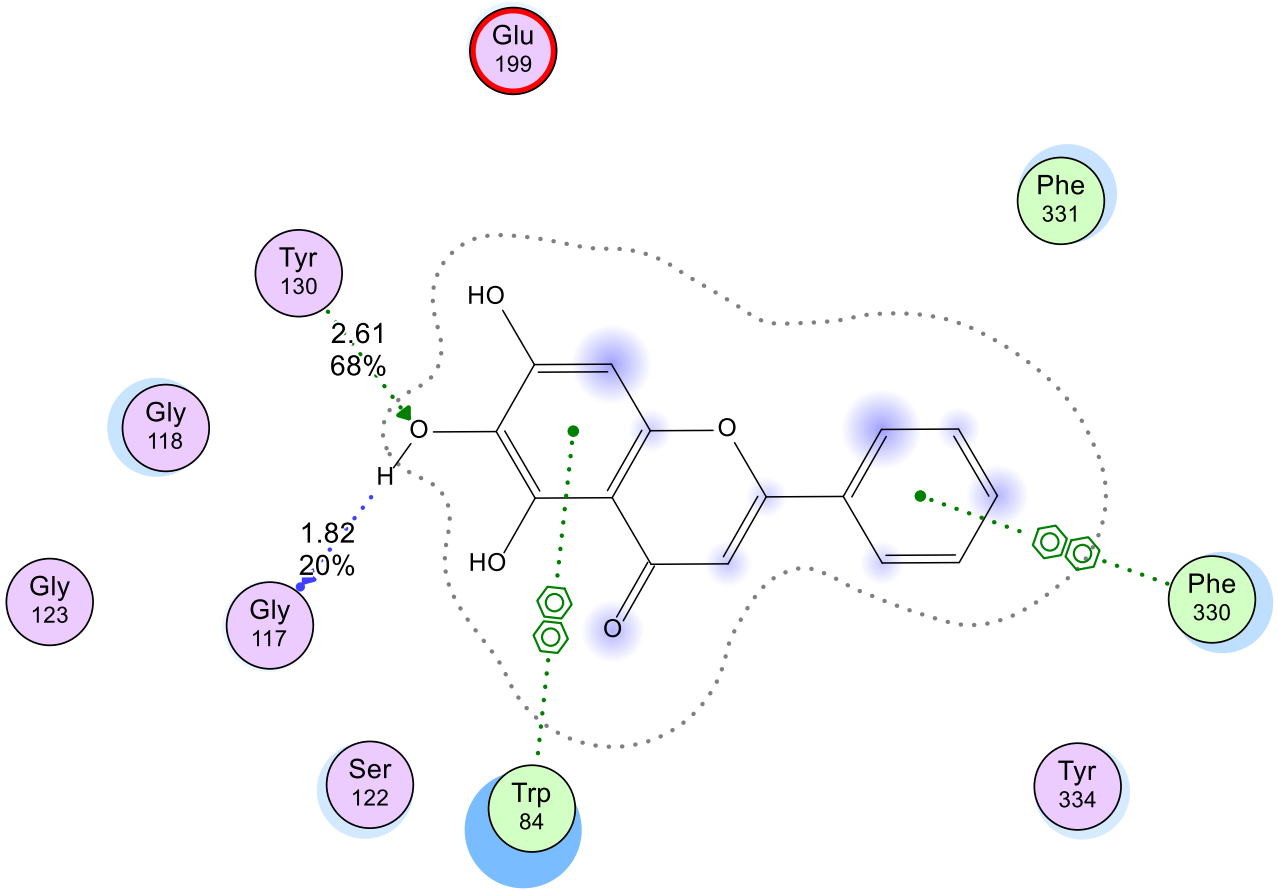
Ligand	AChE	BACE-1
	1DX6	6EQM
1	0.49	0.75
2	0.50	0.80
3	0.89	0.92

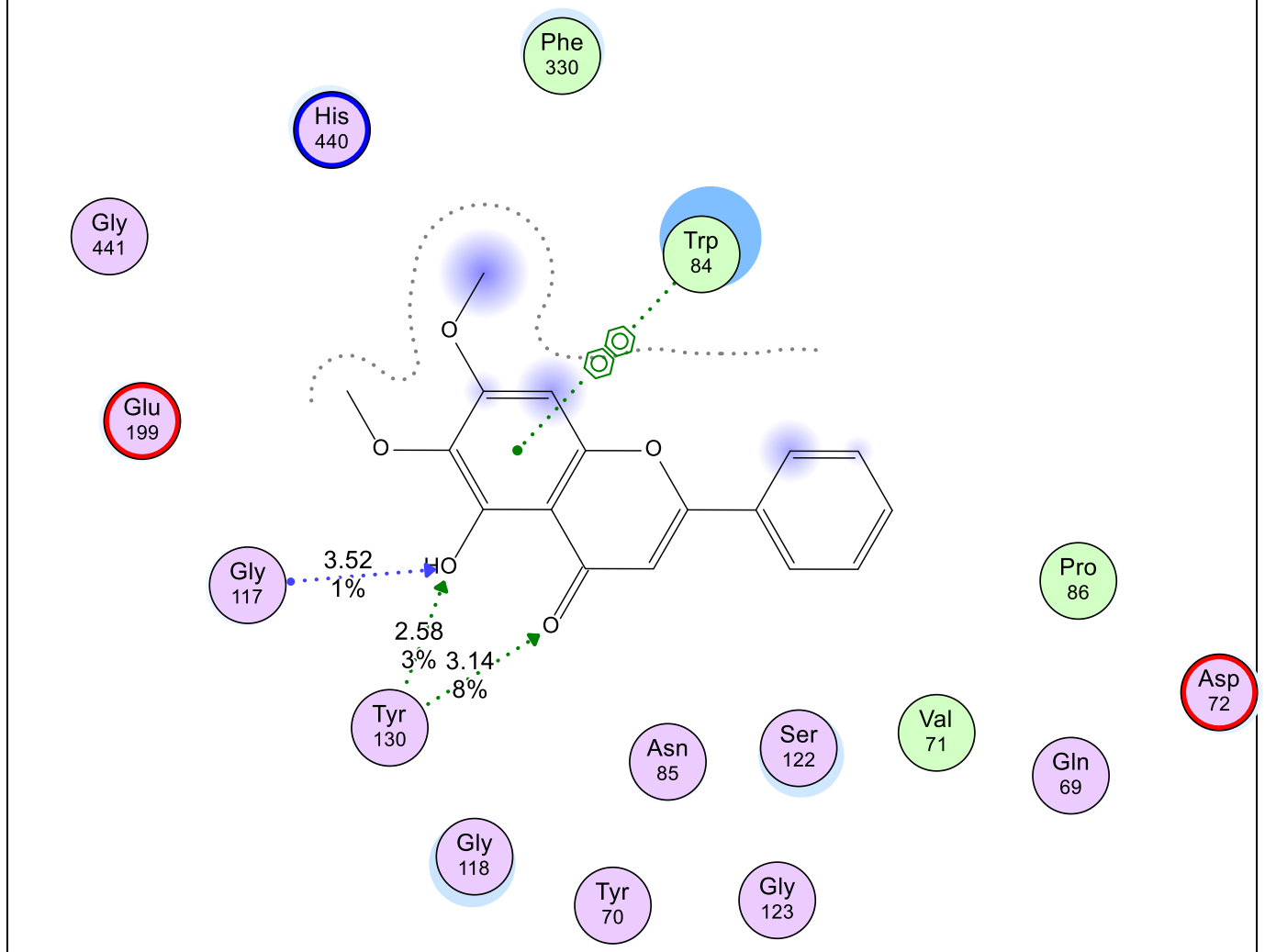
- Ligand 1: separated from the complex (native form, not prepared).

- Ligand 2: separated from the complex and re-prepared using appropriate procedure indicated in the section of Materials and Methods

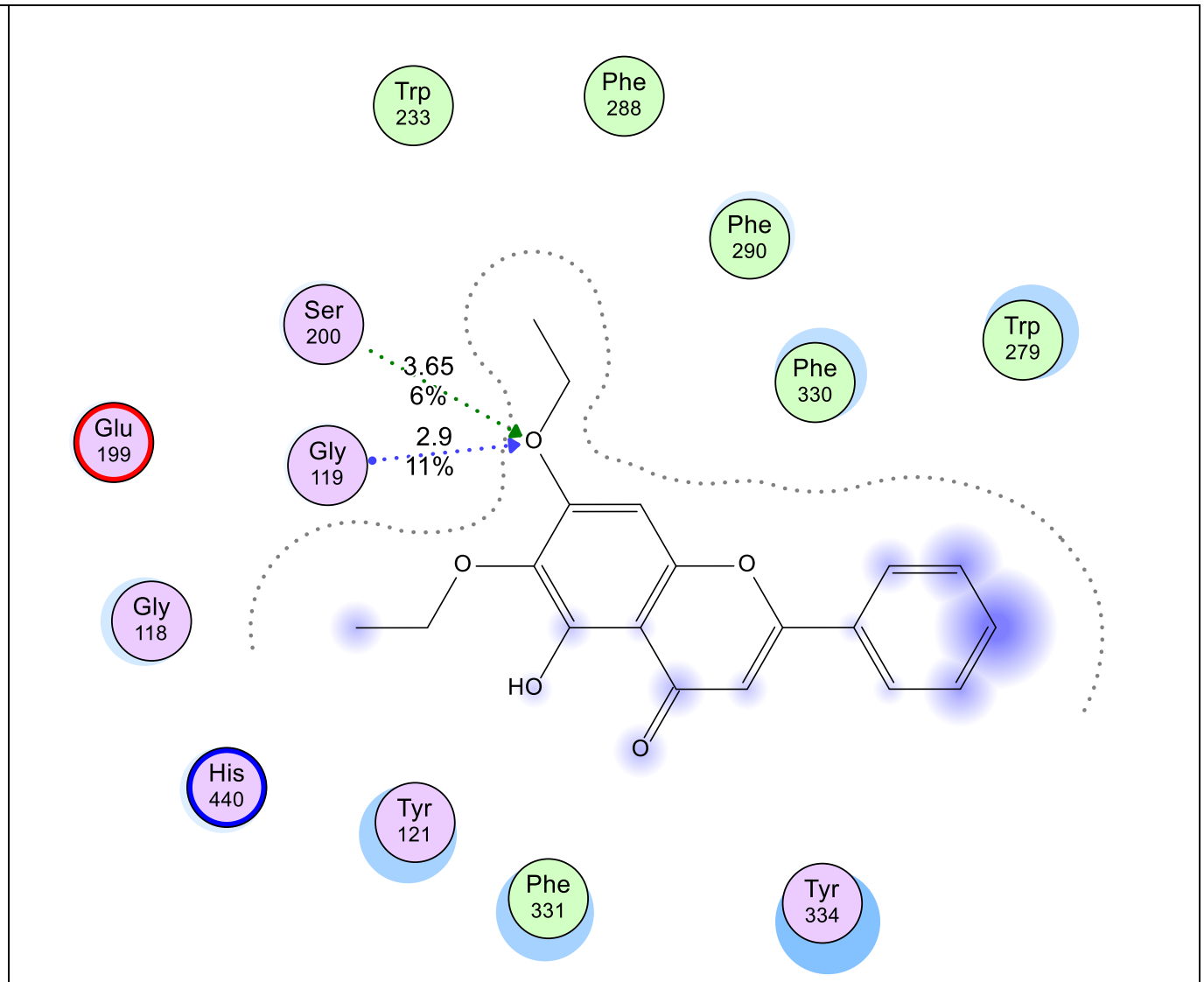
- Ligand 3: built and prepared from the beginning.

Table S5: Docking results and ligand interaction (Co-crystallized 1DX6)

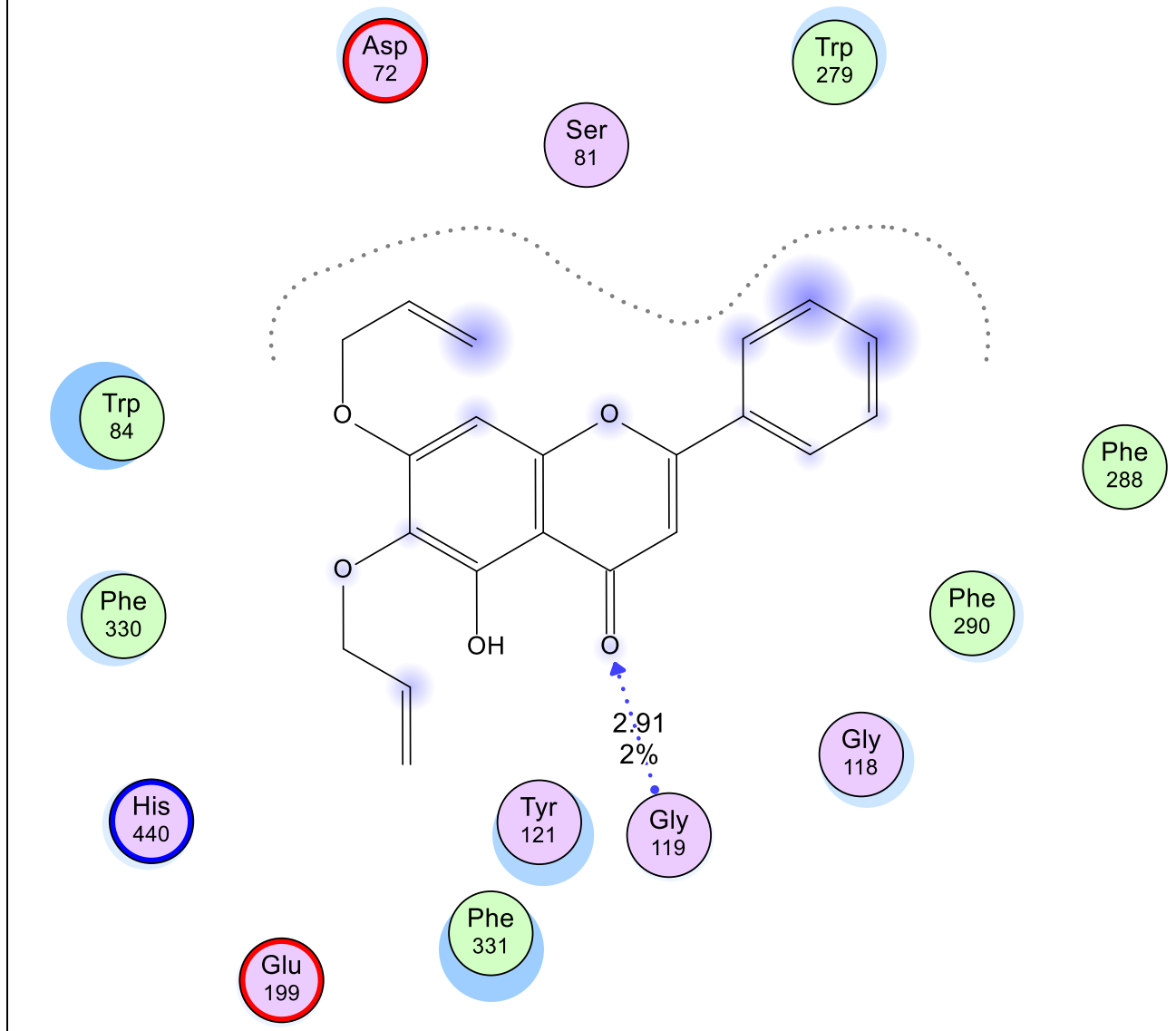
Compound	Observed pIC50	Docking score (kJ.mol^{-1})	Interactions
B1 (Baicalein)	4.43	–27.06	

B2	4.59	–17.67	

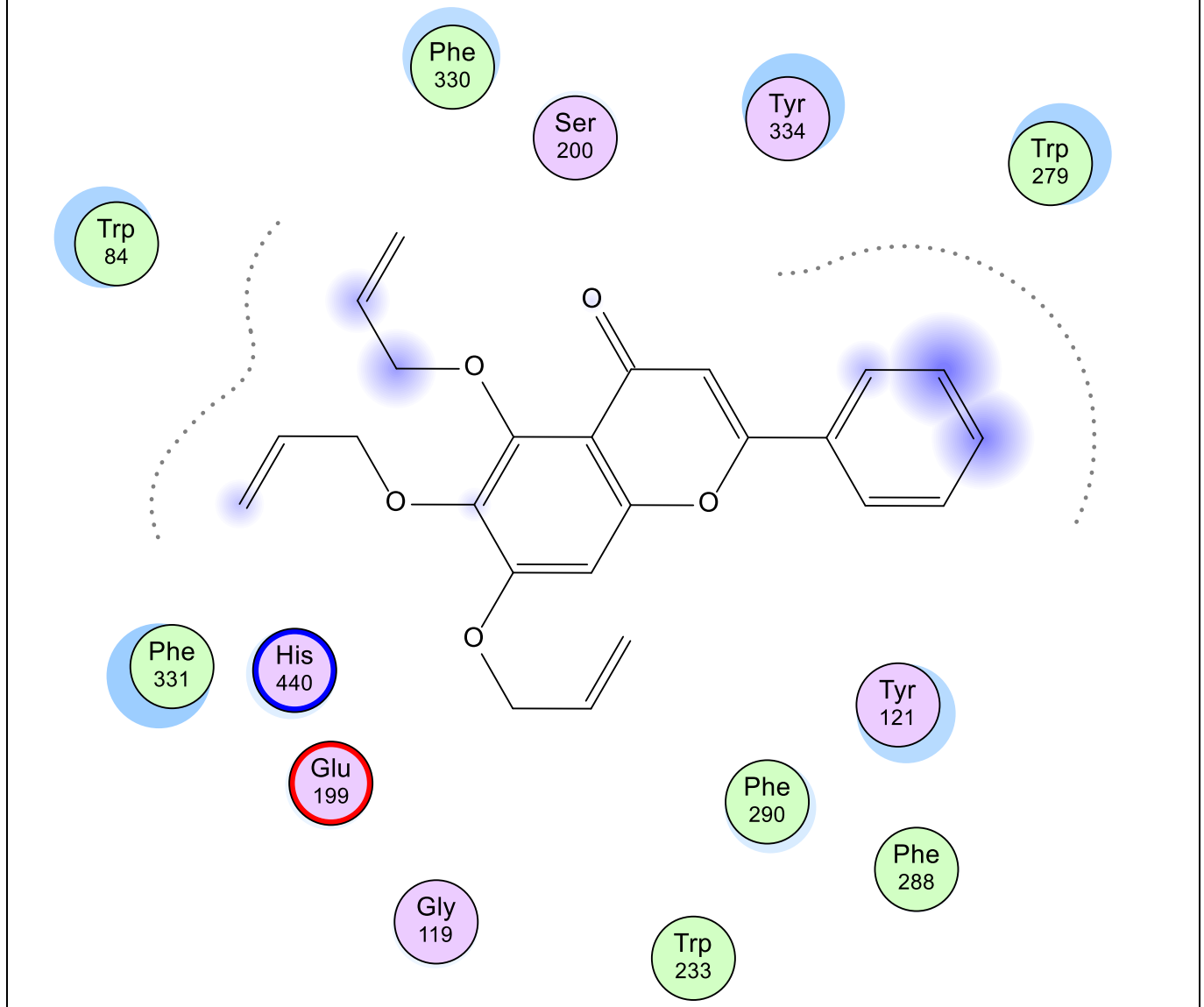
Phe
330
His
440
Gly
441
Trp
84
Glu
199
O
O
O
Gly
117
3.52
1%
HO
2.58
3%
3.14
8%
O
Pro
86
Asp
72
Tyr
130
Asn
85
Ser
122
Val
71
Gln
69
Gly
118
Tyr
70
Gly
123

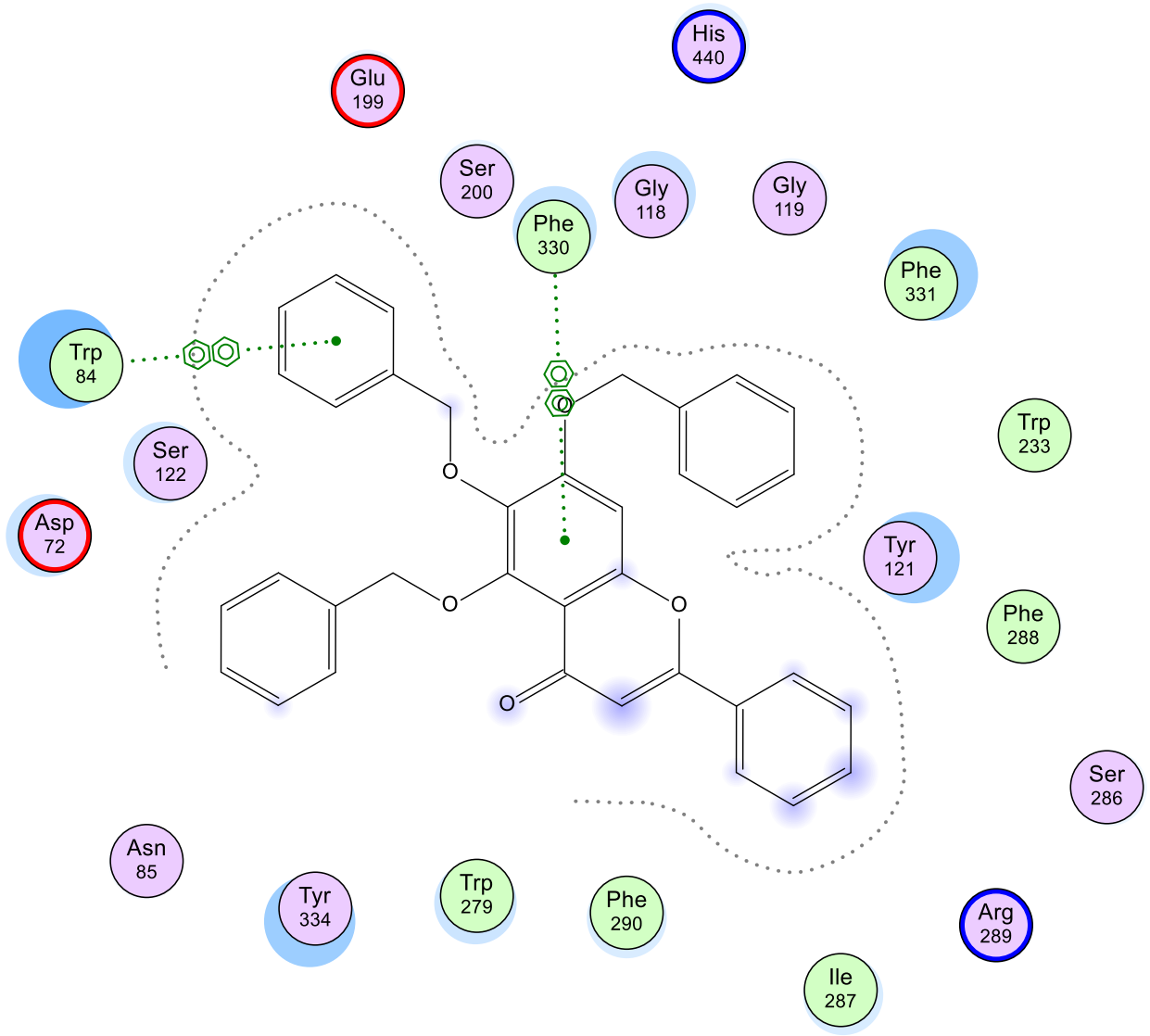
B3	4.52	–17.55	

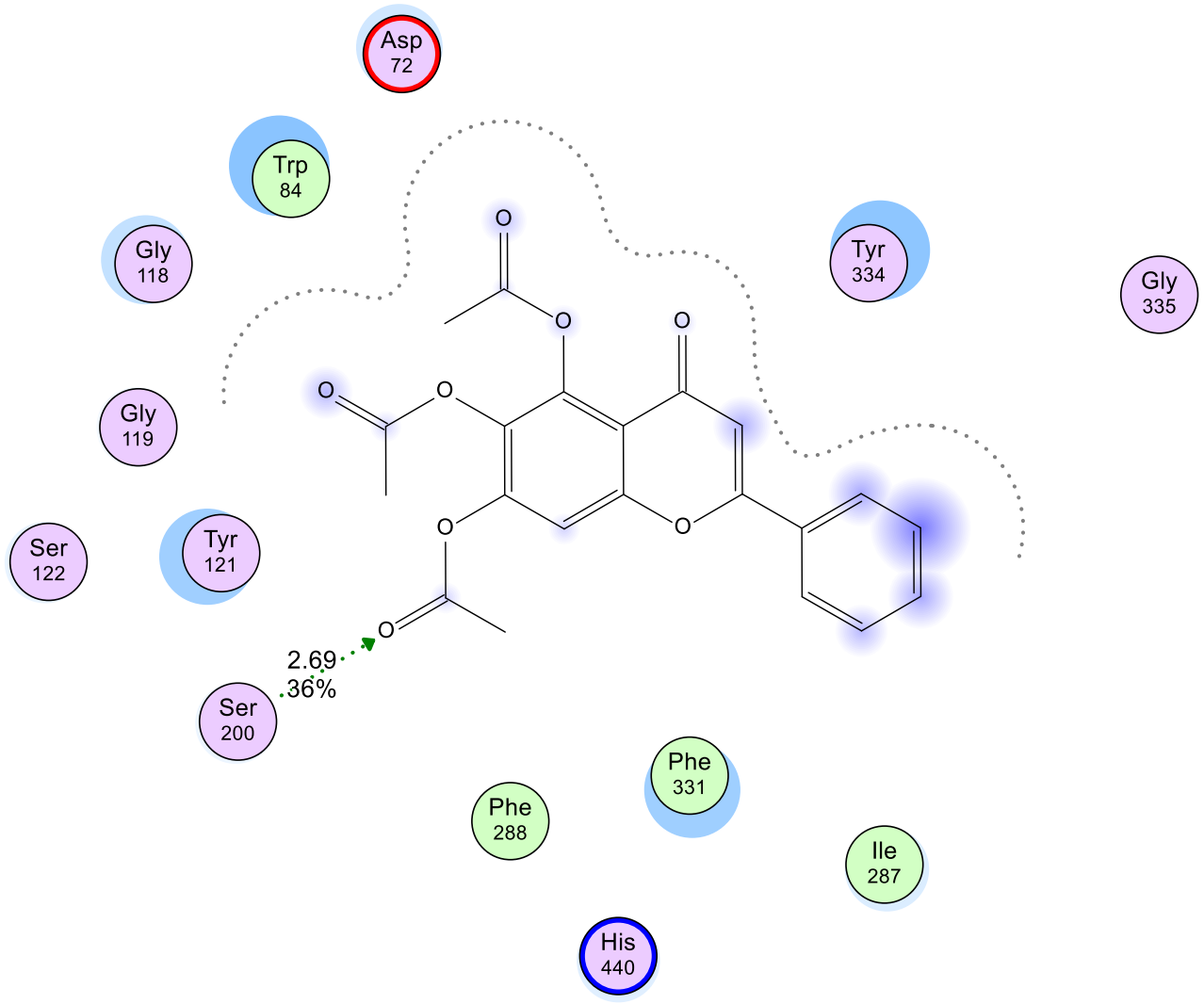
Trp
233
Phe
288
Phe
290
Ser
200
3.65
6%
Trp
279
Phe
330
Glu
199
Gly
119
2.9
11%
O
O
O
Gly
118
HO
O
His
440
Tyr
121
Phe
331
Tyr
334

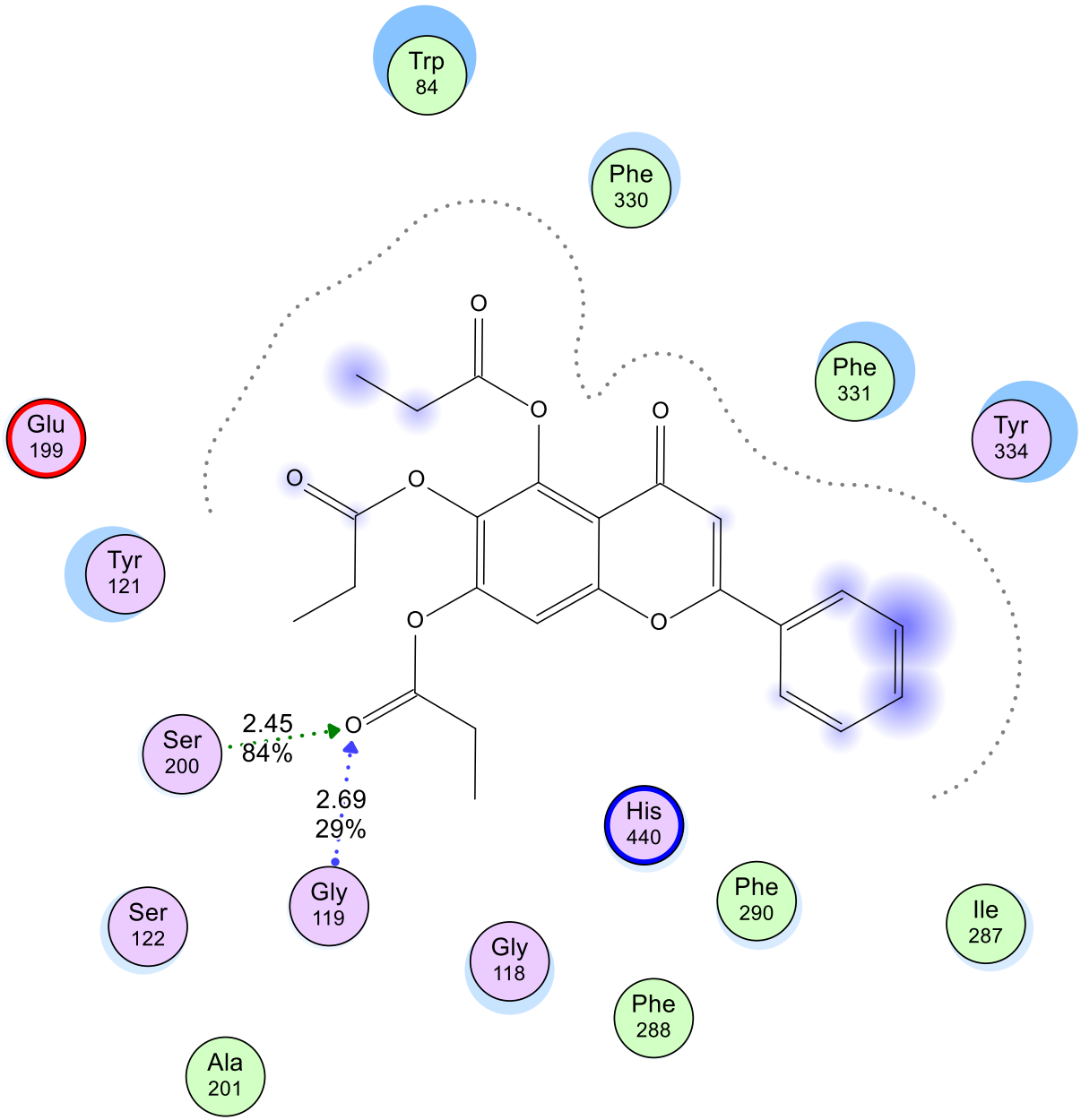
B4	4.29	–10.36	

Asp
72
Trp
279
Ser
81
Trp
84
Phe
288
Phe
330
Phe
290
OH
2.91
2%
Gly
118
His
440
Tyr
121
Gly
119
Phe
331
Glu
199

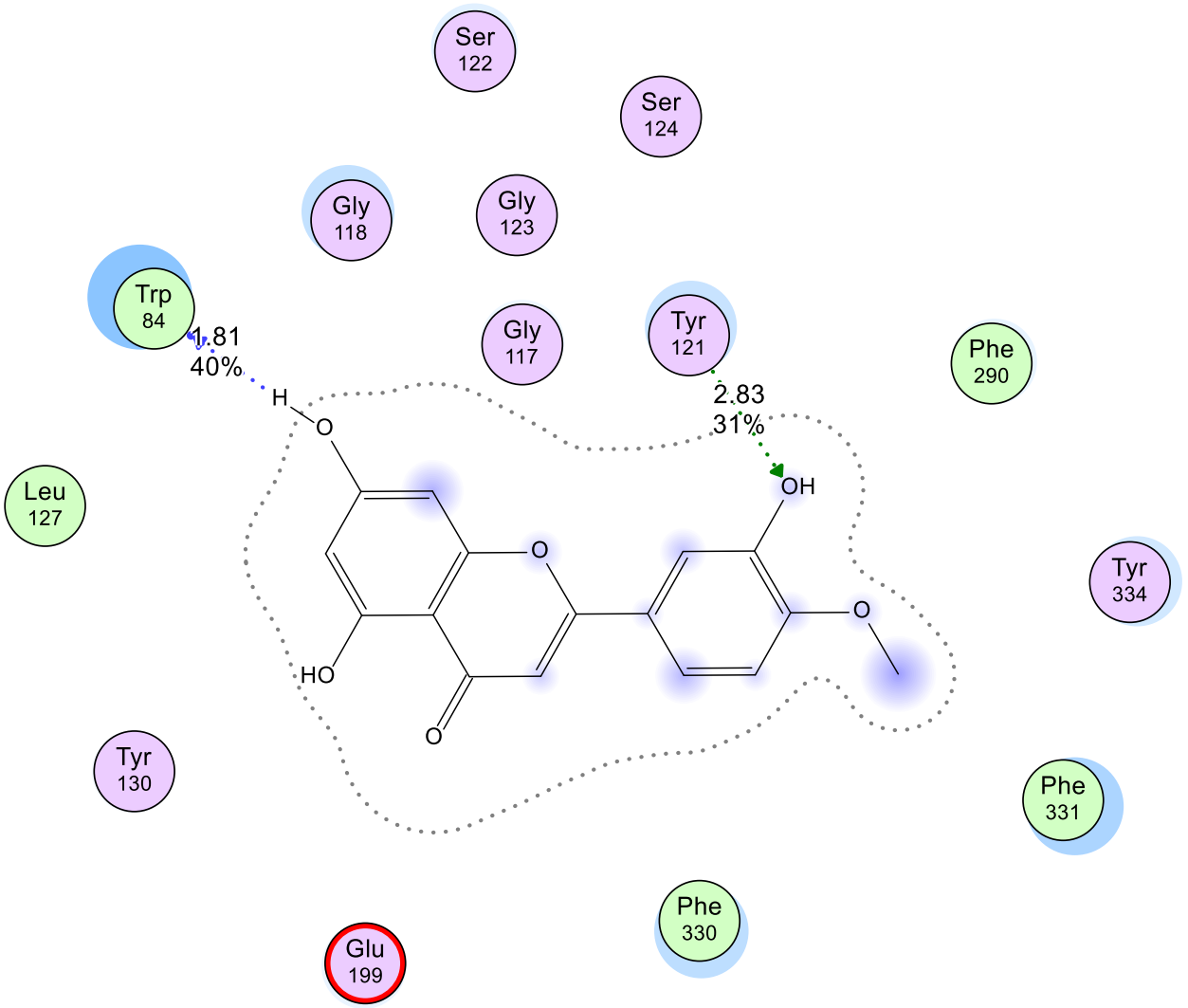
B5	3.72	–10.49	 Phe 330 Ser 200 Tyr 334 Trp 279 Trp 84 O O O O O Phe 331 His 440 Glu 199 Tyr 121 Phe 290 Phe 288 Gly 119 Trp 233

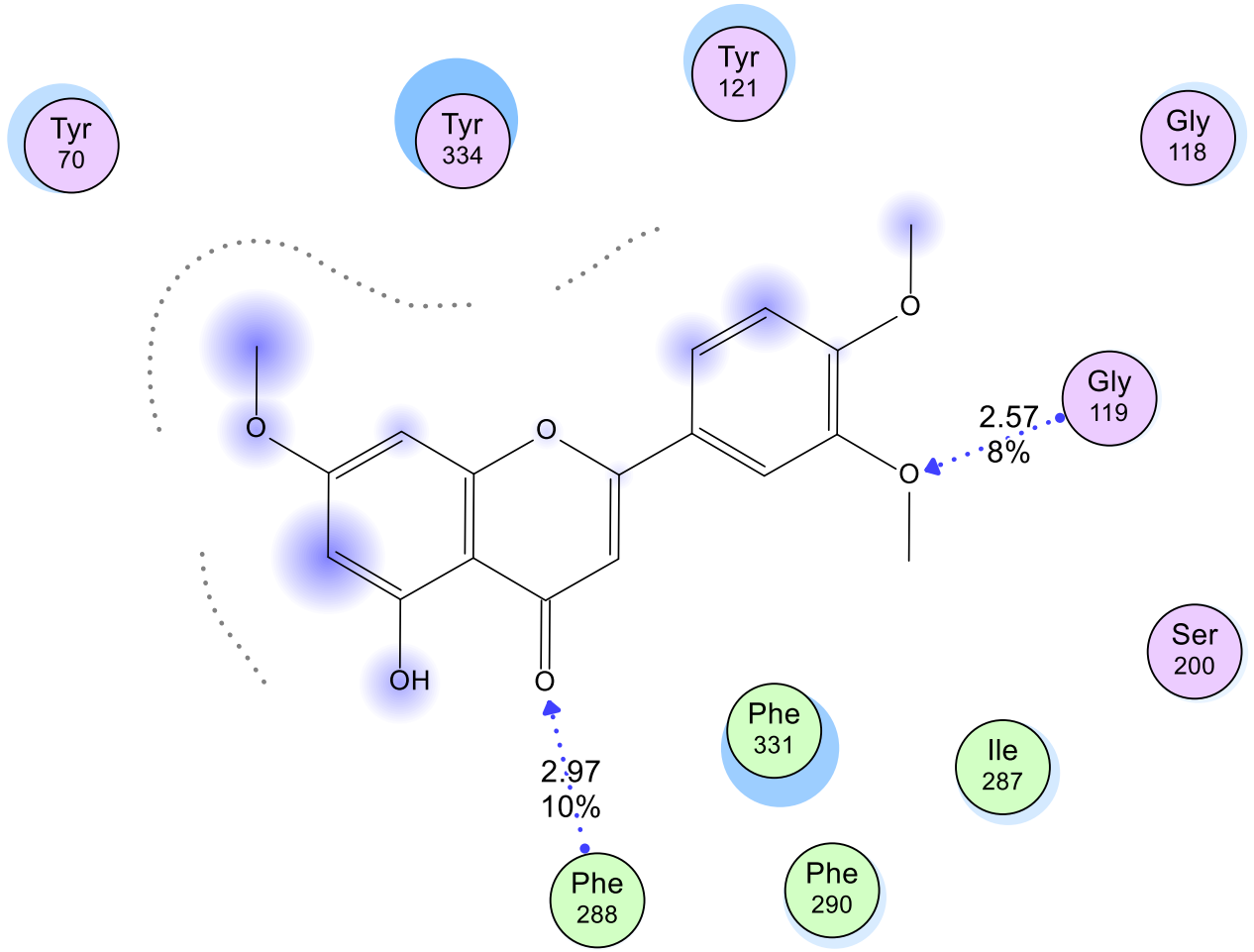
B6	4.10	–15.71	 His 440 Glu 199 Ser 200 Gly 118 Gly 119 Phe 330 Phe 331 Trp 84 Ser 122 Asp 72 Trp 233 Tyr 121 Phe 288 Ser 286 Asn 85 Tyr 334 Trp 279 Phe 290 Arg 289 Ile 287 O O O O

B7	4.29	–17.91	 Asp 72 Trp 84 Gly 118 Tyr 334 Gly 335 Gly 119 Ser 122 Tyr 121 2.69 36% Ser 200 Phe 331 Phe 288 Ile 287 His 440

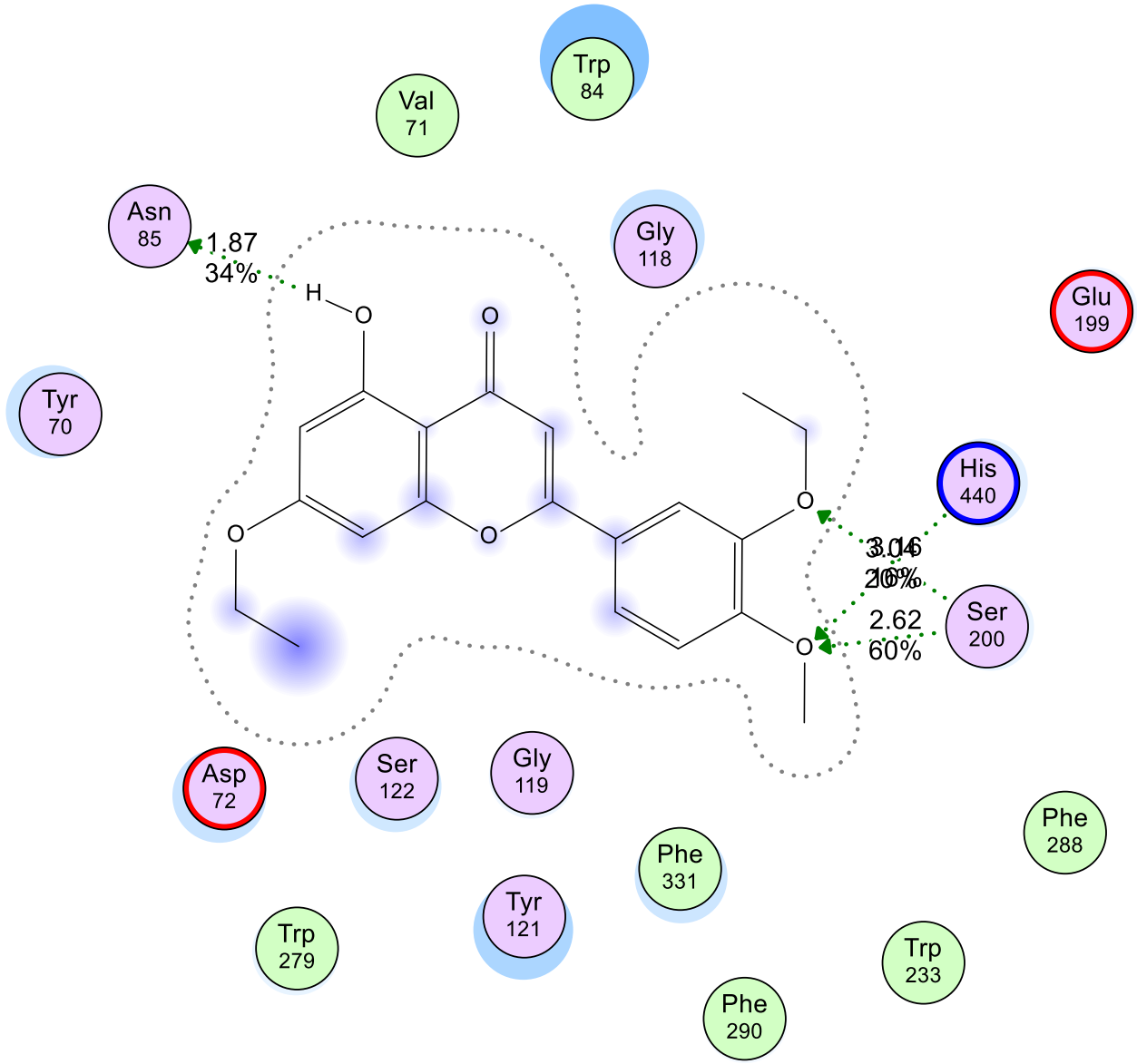
B8	4.18	–19.61	

Trp
84
Phe
330
Phe
331
Tyr
334
Glu
199
Tyr
121
O
O
O
O
O
O
O
Ser
200
2.45
84%
2.69
29%
His
440
Gly
119
Ser
122
Gly
118
Phe
290
Ile
287
Phe
288
Ala
201

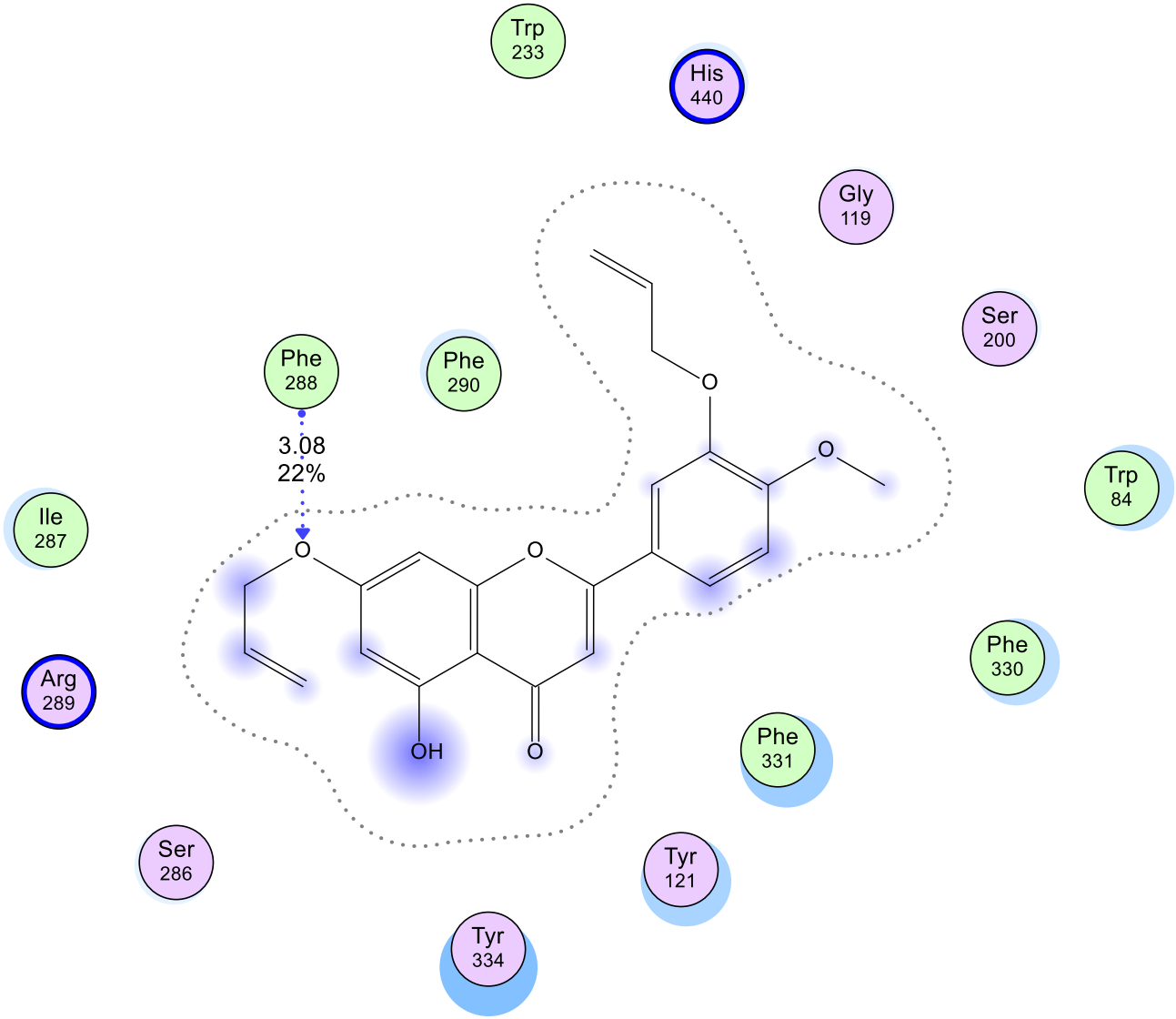
D1 (Diosmetin)	3.83	–22.86	

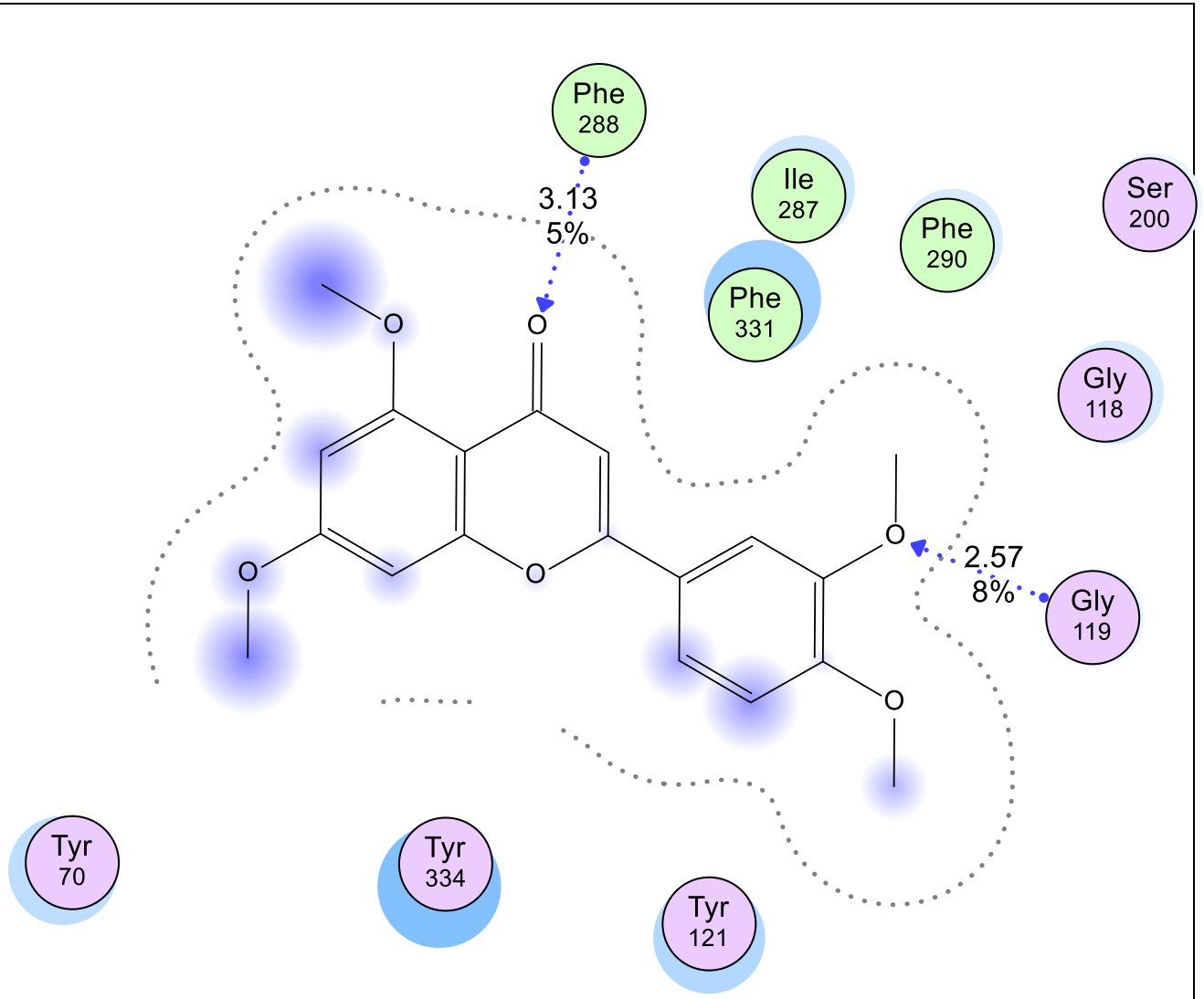
D2	4.06	–21.05	

Tyr
70
Tyr
334
Tyr
121
Gly
118
Gly
119
2.57
8%
O
O
O
O
OH
O
Ser
200
Phe
331
Ile
287
2.97
10%
Phe
288
Phe
290

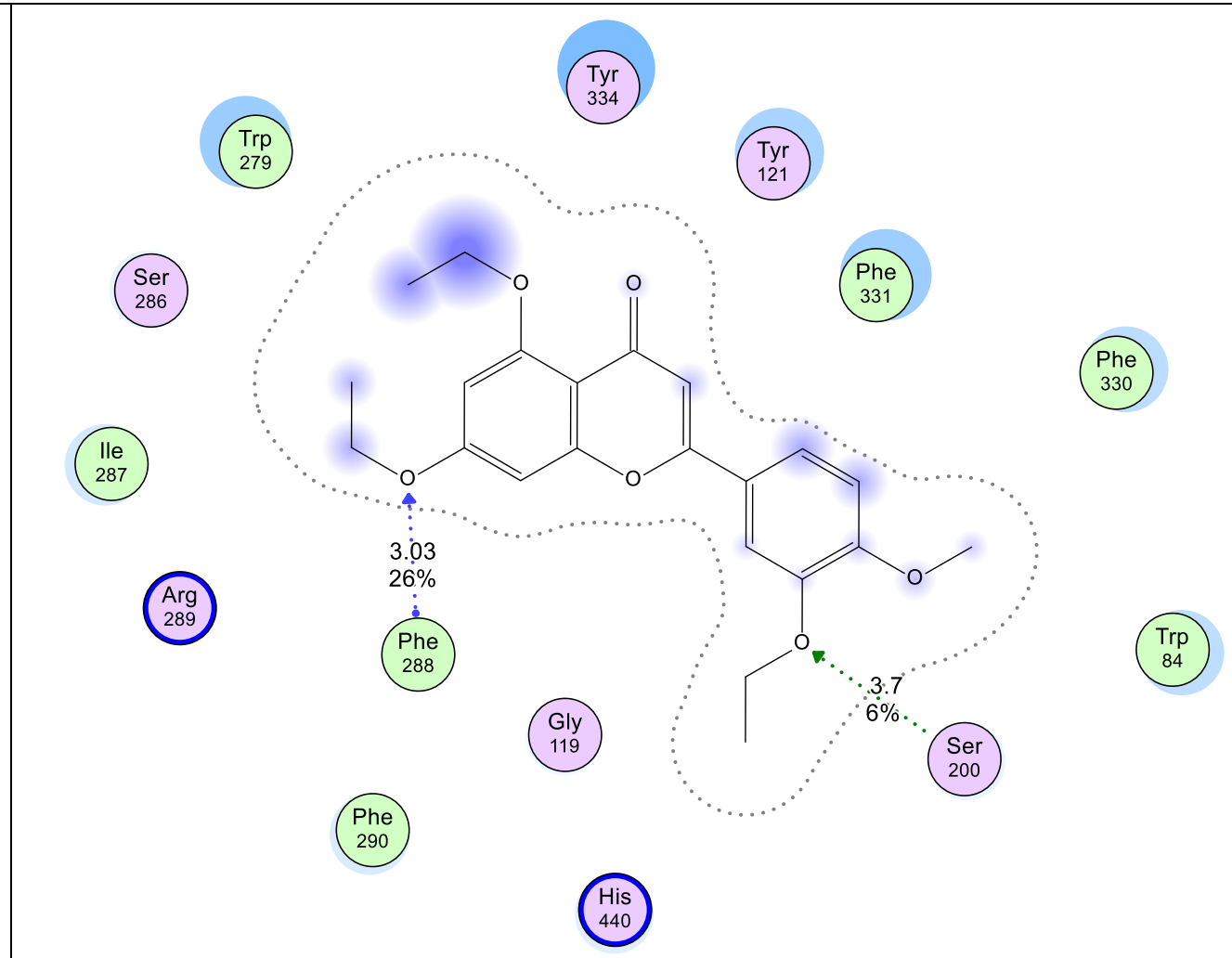
D3	3.89	–20.90	

Trp
84
Val
71
Asn
85
1.87
34%
Gly
118
Glu
199
Tyr
70
His
440
Ser
200
2.62
60%
Asp
72
Ser
122
Gly
119
Phe
288
Phe
331
Tyr
121
Trp
279
Trp
233
Phe
290

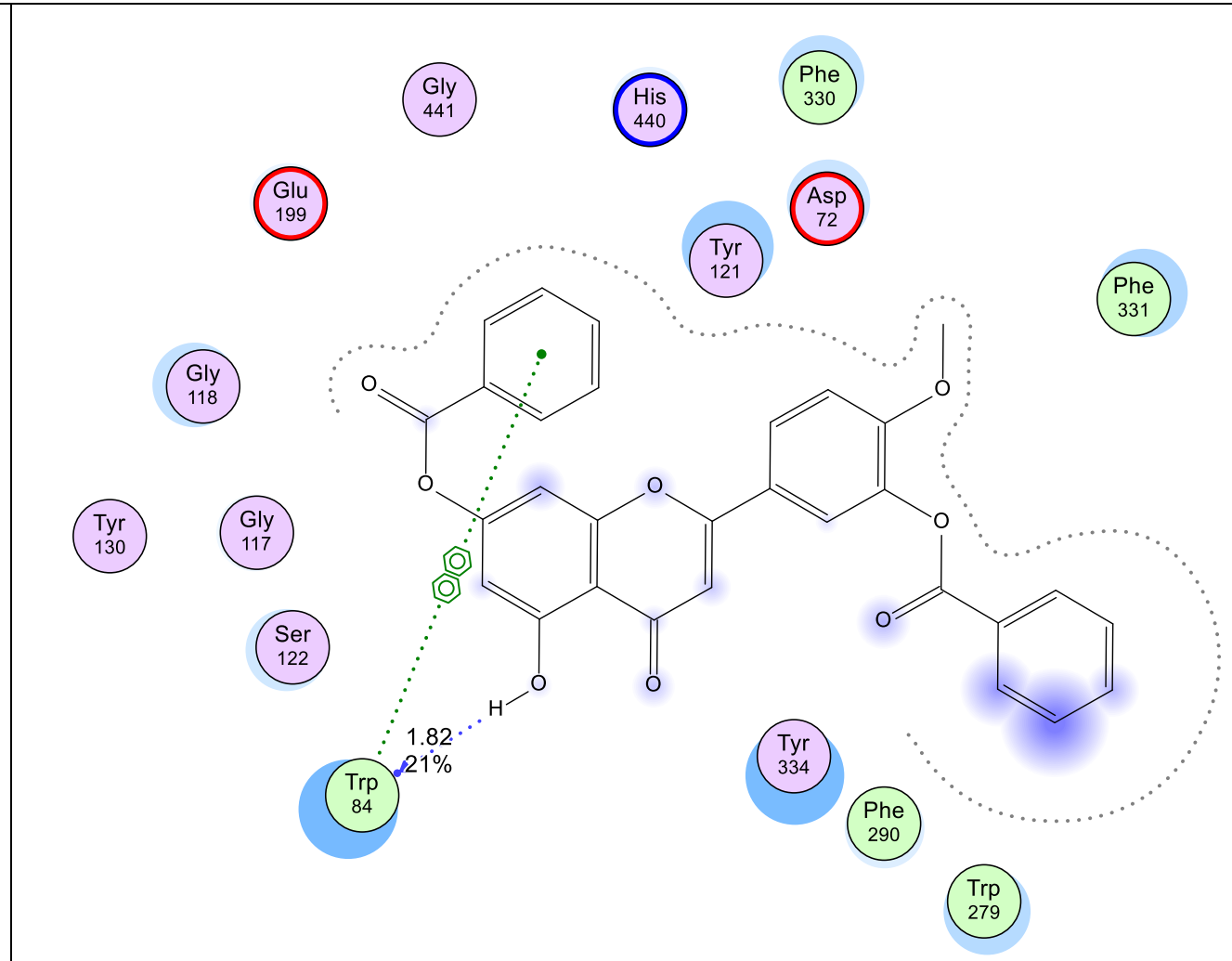
D4	3.82	–15.22	 Trp 233 His 440 Gly 119 Ser 200 Phe 288 Phe 290 3.08 22% Trp 84 Ile 287 Arg 289 Phe 330 Phe 331 Ser 286 Tyr 121 Tyr 334 O O O O OH O

D5	4.13	–21.80	

Phe
288
3.13
5%
Ile
287
Phe
290
Ser
200
Phe
331
Gly
118
O
O
O
O
O
O
2.57
8%
Gly
119
Tyr
70
Tyr
334
Tyr
121

D6	4.12	–20.39	

Tyr
334
Trp
279
Tyr
121
Ser
286
Phe
331
Phe
330
Ile
287
3.03
26%
Arg
289
Phe
288
Trp
84
3.7
6%
Gly
119
Ser
200
Phe
290
His
440

D7	3.47	–25.35	 Gly 441 His 440 Phe 330 Glu 199 Asp 72 Tyr 121 Phe 331 Gly 118 Tyr 130 Gly 117 Ser 122 1.82 21% Trp 84 Tyr 334 Phe 290 Trp 279

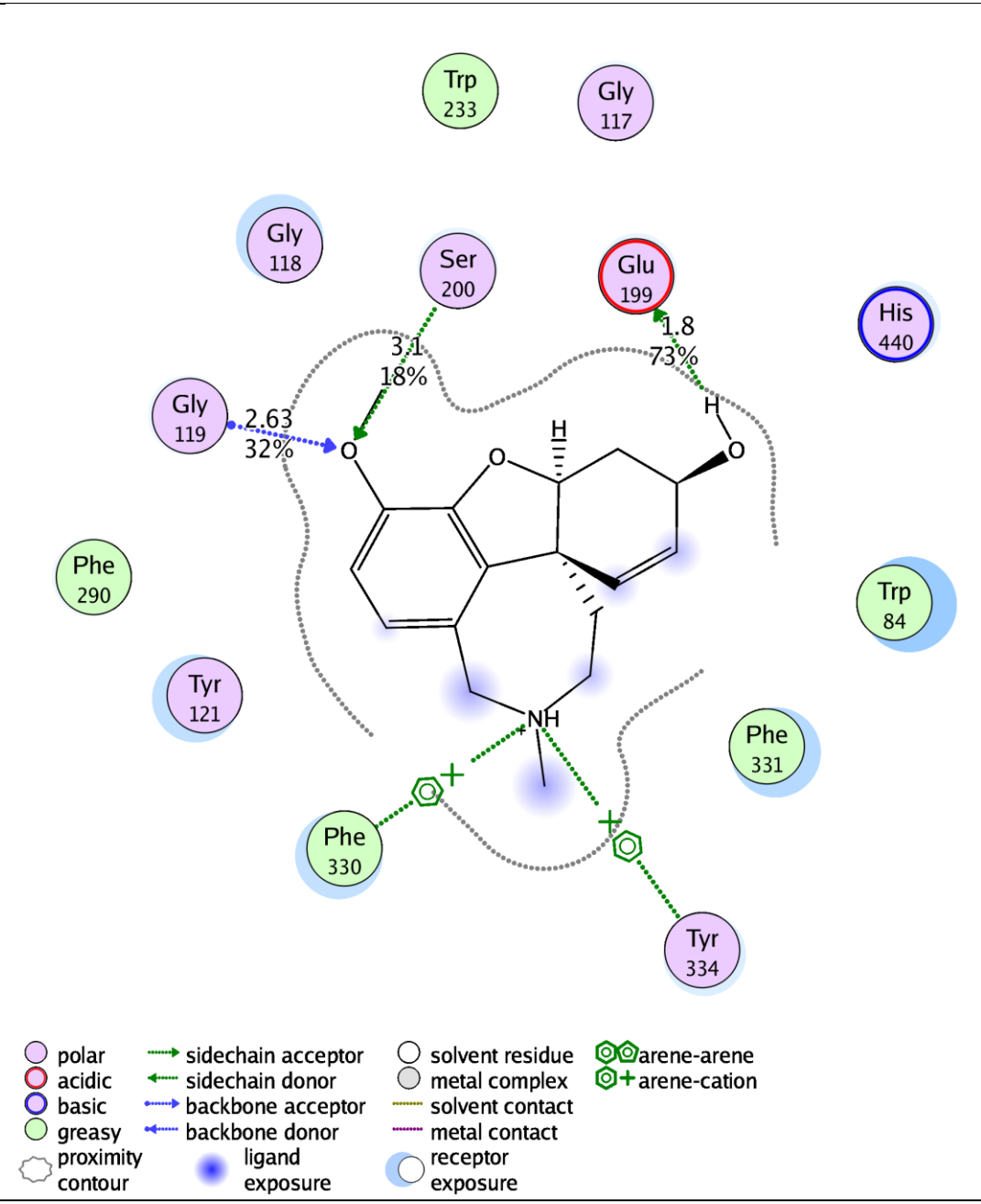
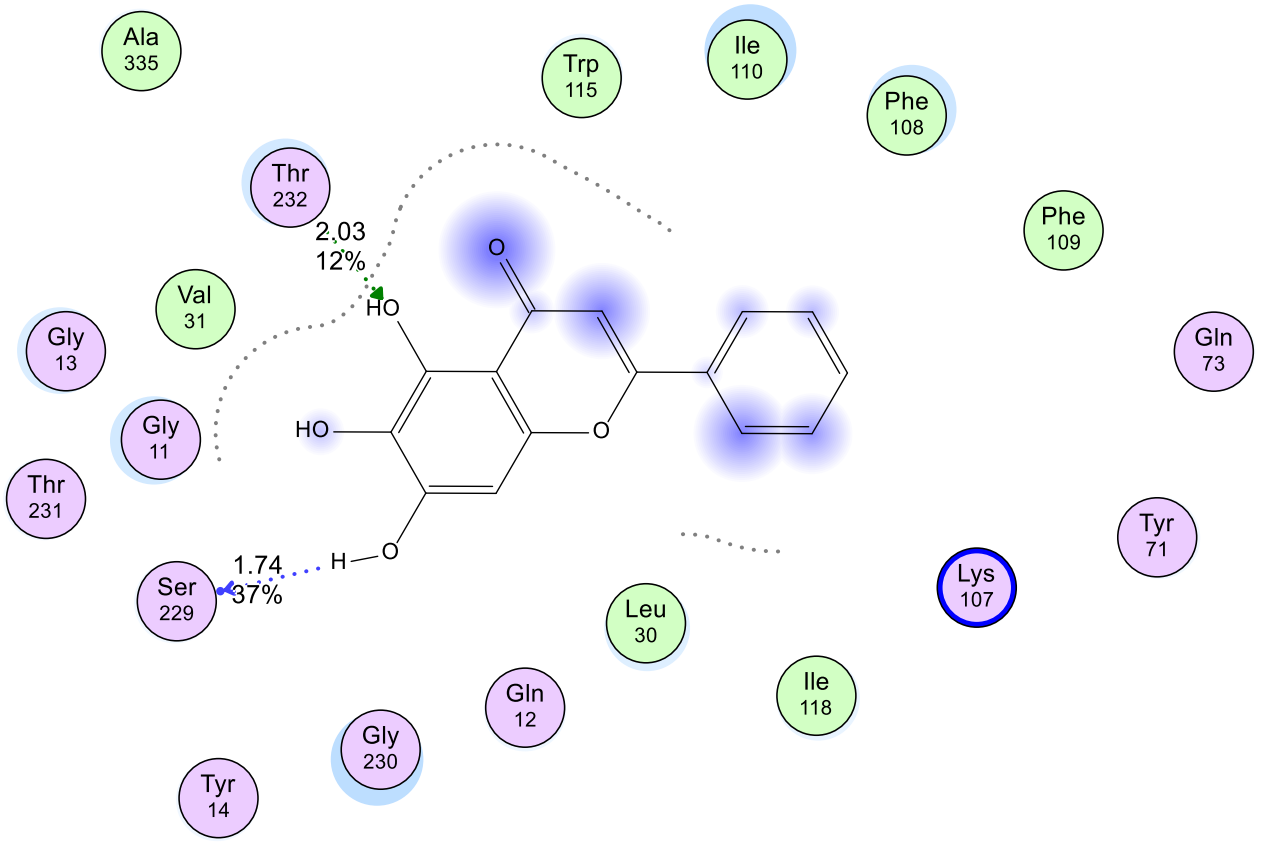
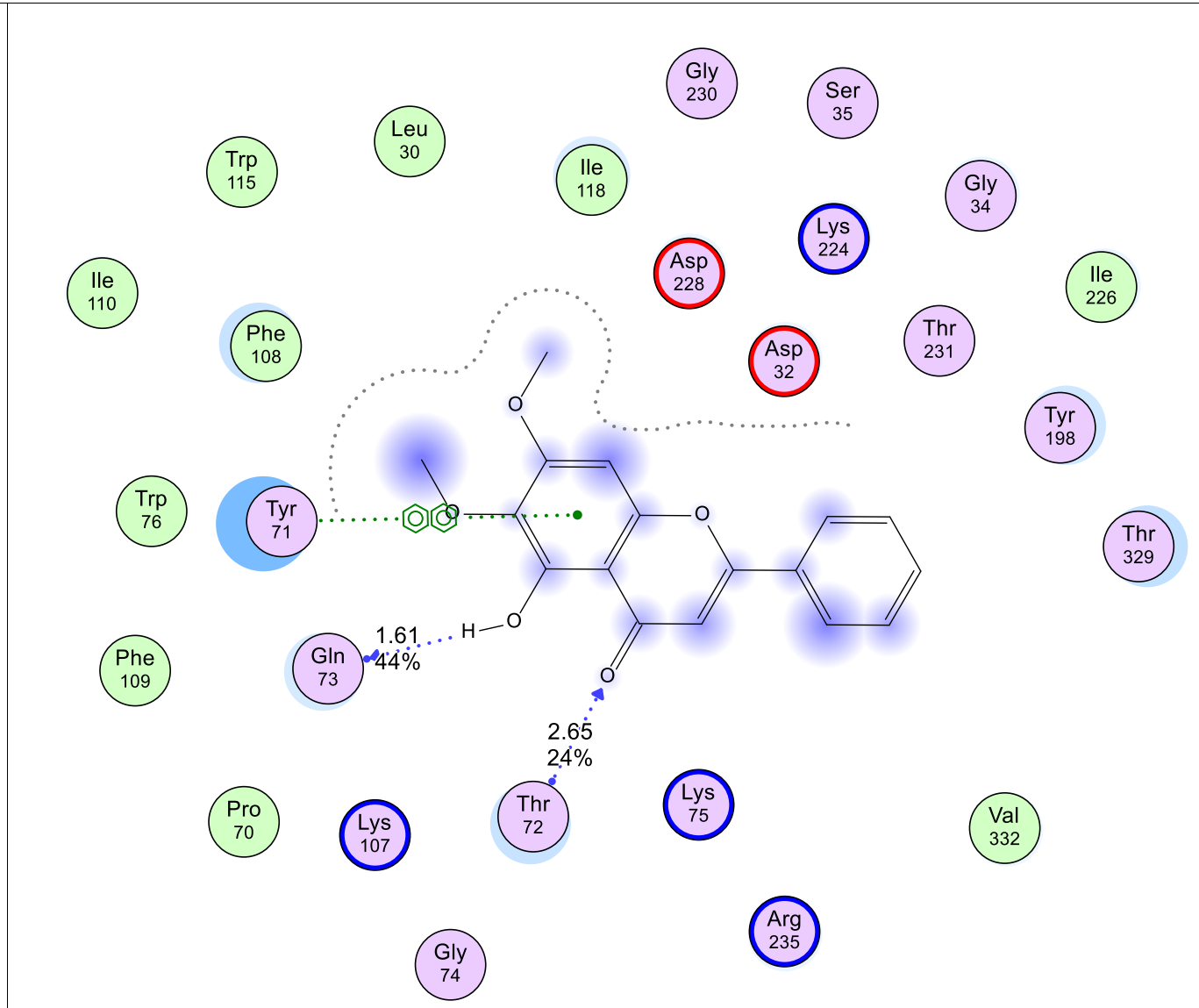
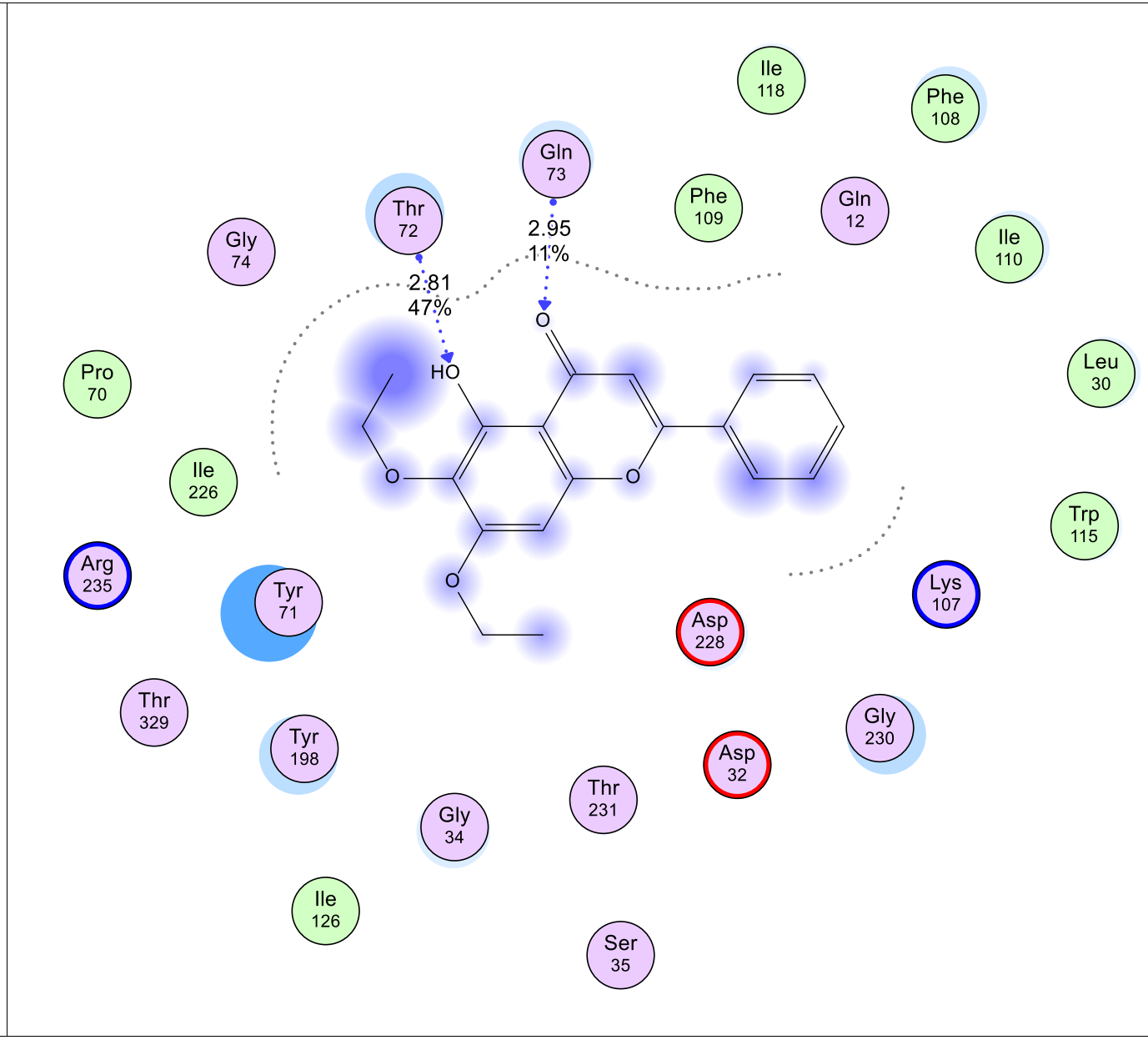
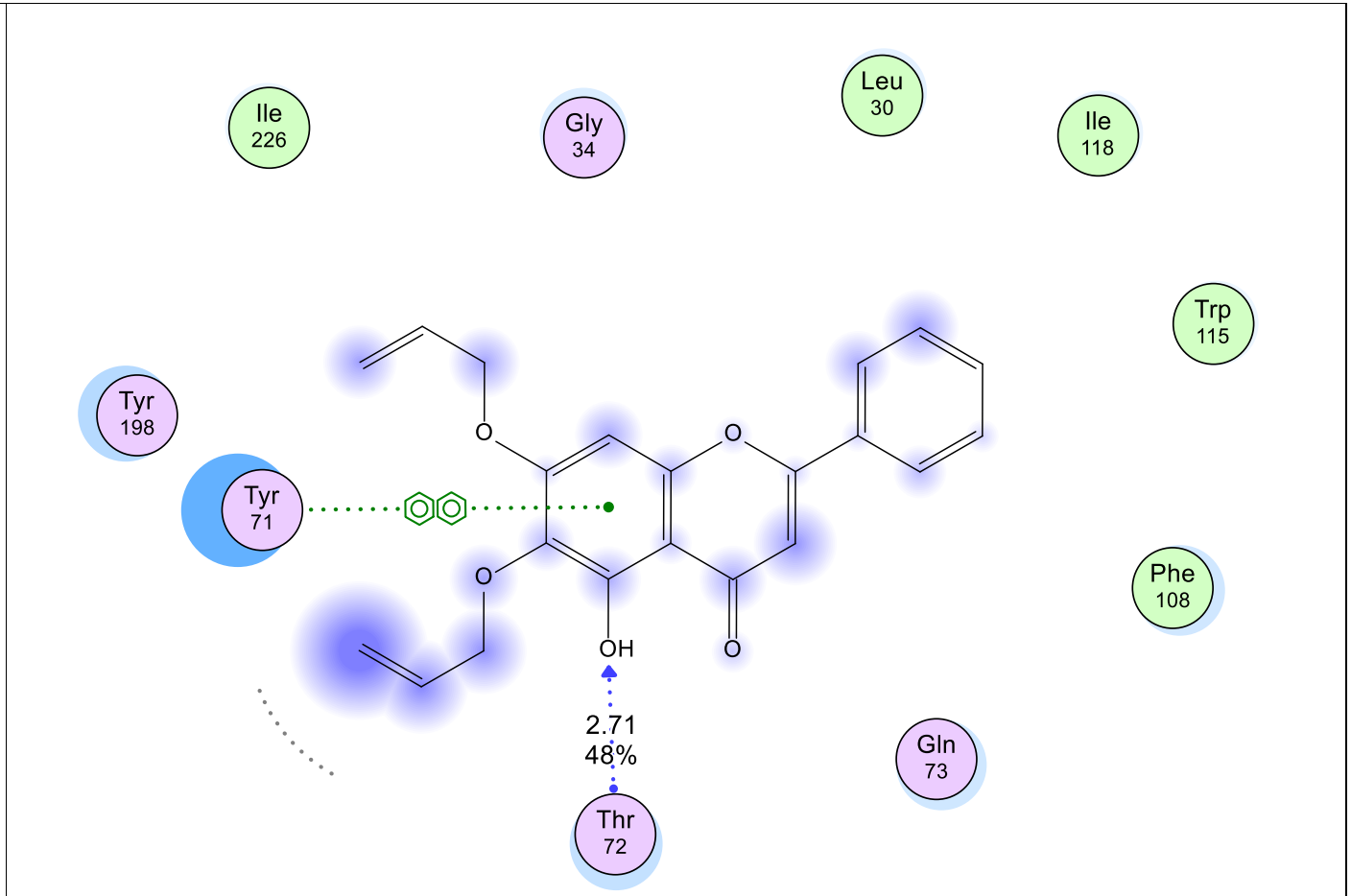
Galanthamine	5.88	–33.28	

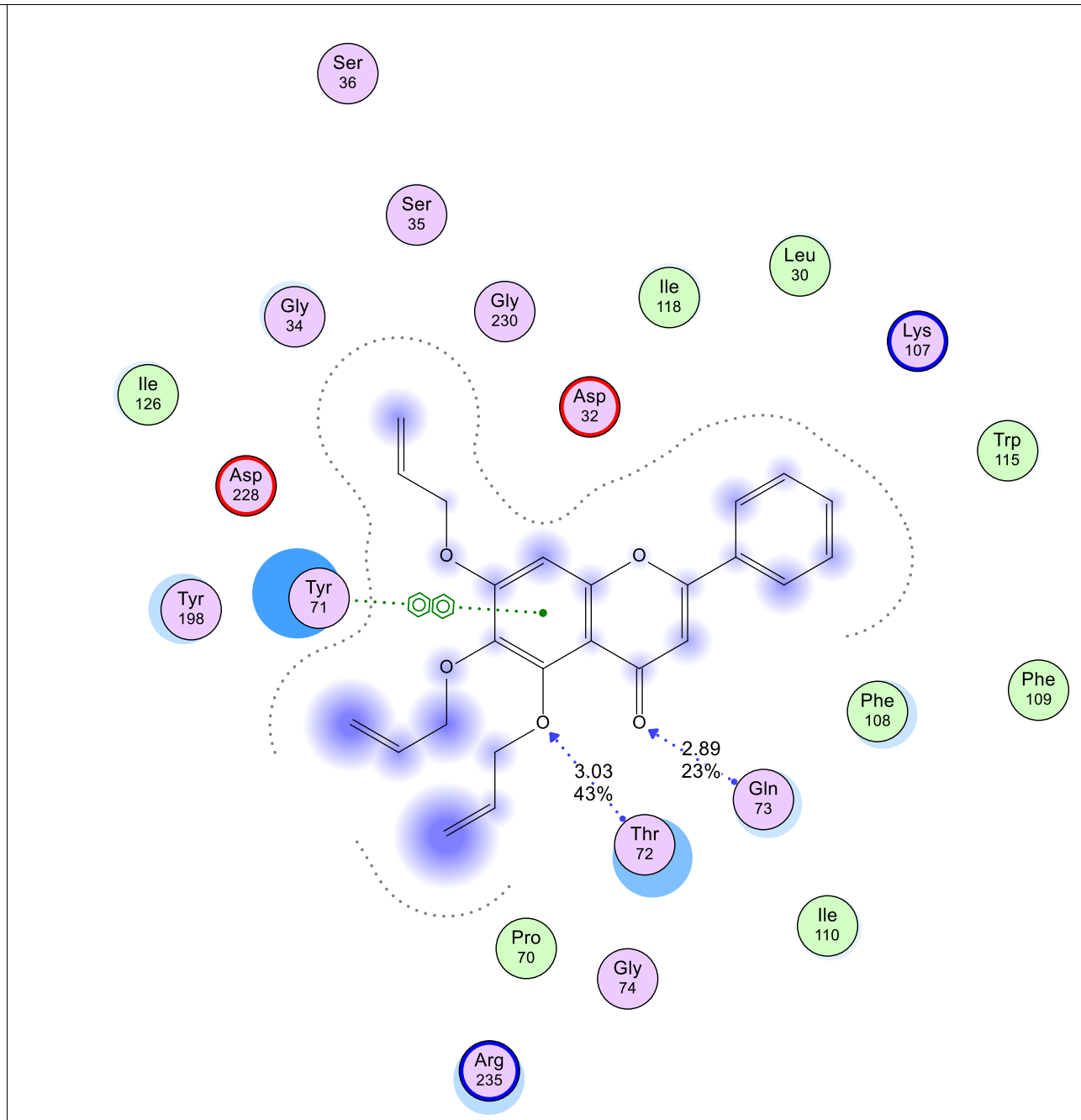
Table S6. Docking results and ligand interaction (Co-crystallized 6EQM)

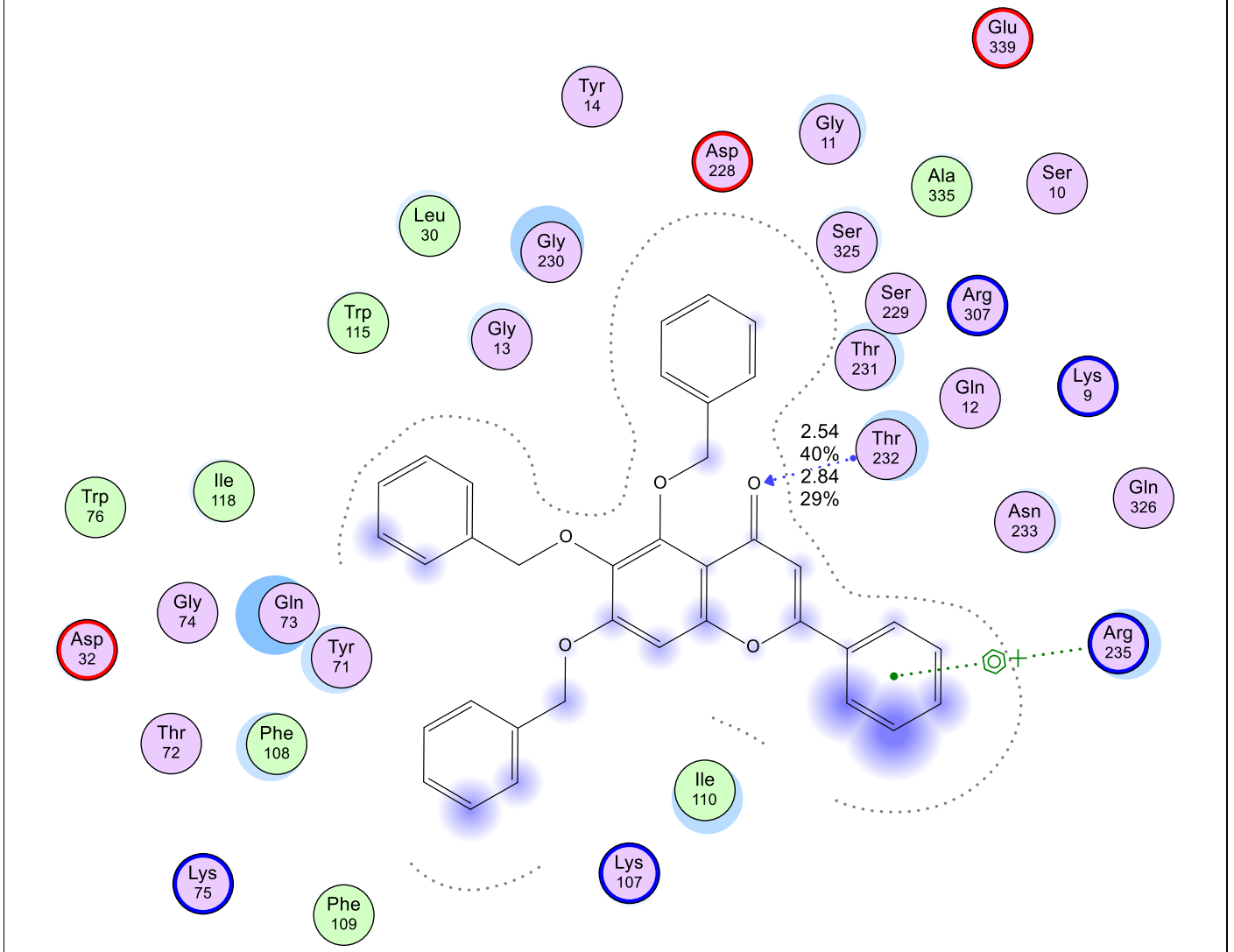
Compound	Observed pIC50	Docking score (kJ.mol^{-1})	Interactions
B1 (Baicalein)	4.16	–17.64	

B2	4.36	–16.37	 Gly 230 Ser 35 Leu 30 Trp 115 Ile 118 Gly 34 Lys 224 Asp 228 Ile 110 Ile 226 Phe 108 Thr 231 Asp 32 Tyr 198 Trp 76 Tyr 71 Thr 329 1.61 44% Phe 109 Gln 73 2.65 24% Pro 70 Lys 107 Thr 72 Lys 75 Val 332 Arg 235 Gly 74

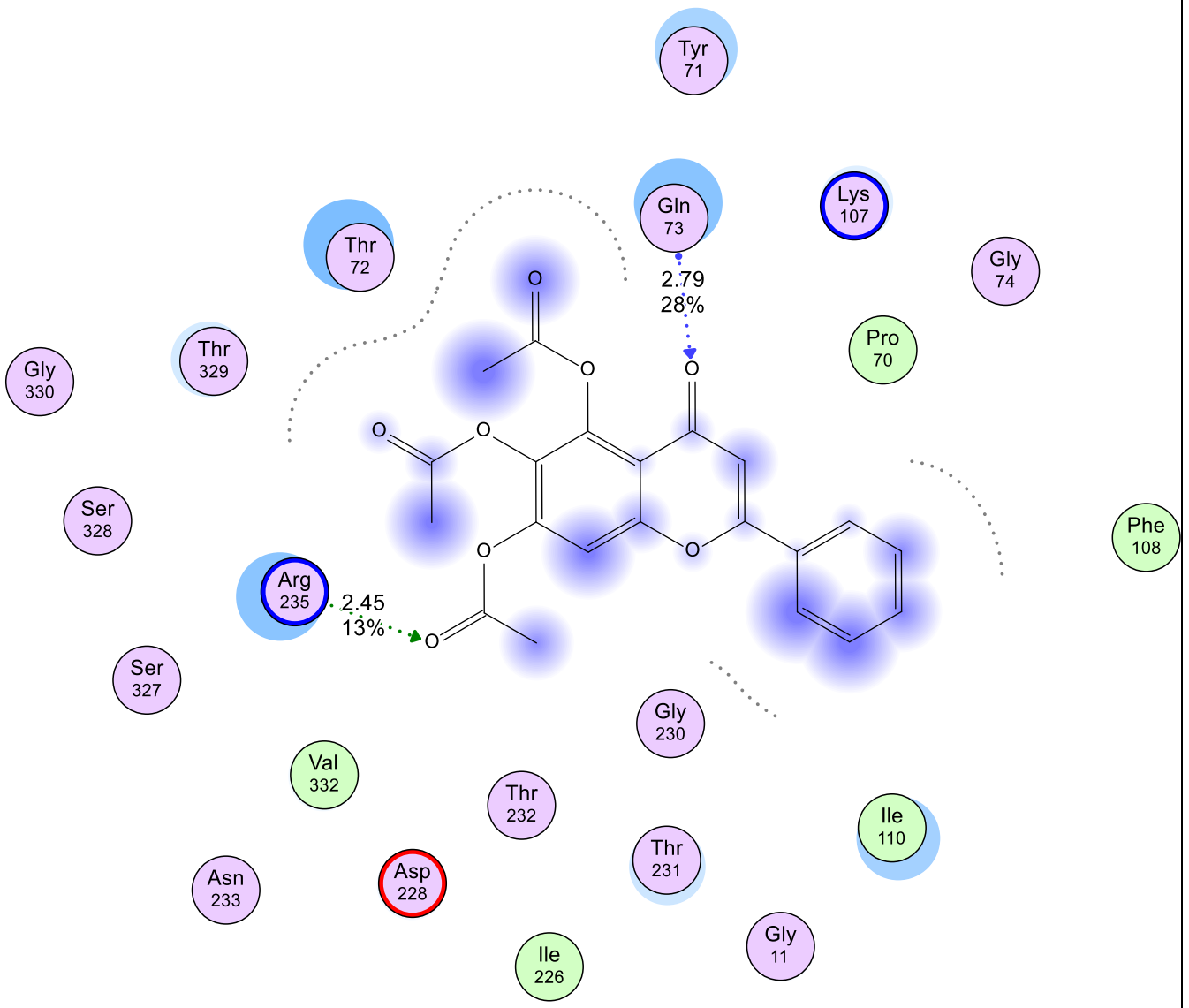
B3	5.40	–12.35	 Ile 118 Phe 108 Gln 73 Thr 72 Phe 109 Gln 12 Gly 74 2.95 11% Ile 110 2.81 47% Pro 70 Leu 30 Ile 226 Trp 115 Arg 235 Tyr 71 Lys 107 Asp 228 Thr 329 Gly 230 Tyr 198 Asp 32 Thr 231 Gly 34 Ile 126 Ser 35

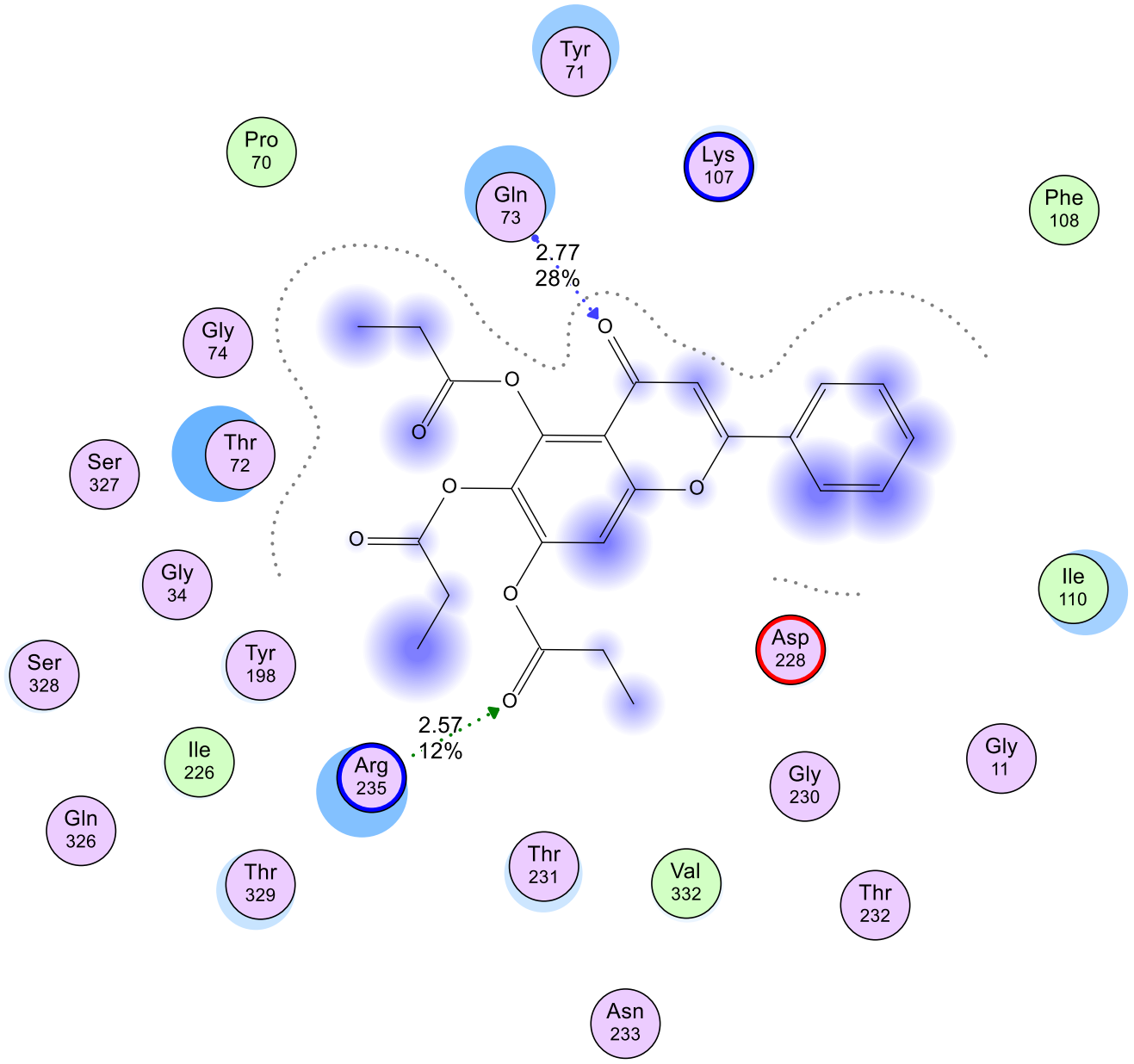
B4	4.15	–10.84	 Ile 226 Gly 34 Leu 30 Ile 118 Trp 115 Tyr 198 Tyr 71 Phe 108 Gln 73 Thr 72 O O O OH O 2.71 48%

B5	4.77	–8.29	 Ser 36 Ser 35 Leu 30 Ile 118 Gly 34 Gly 230 Lys 107 Ile 126 Asp 32 Trp 115 Asp 228 Tyr 198 Tyr 71 Phe 109 Phe 108 2.89 23% 3.03 43% Gln 73 Thr 72 Ile 110 Pro 70 Gly 74 Arg 235

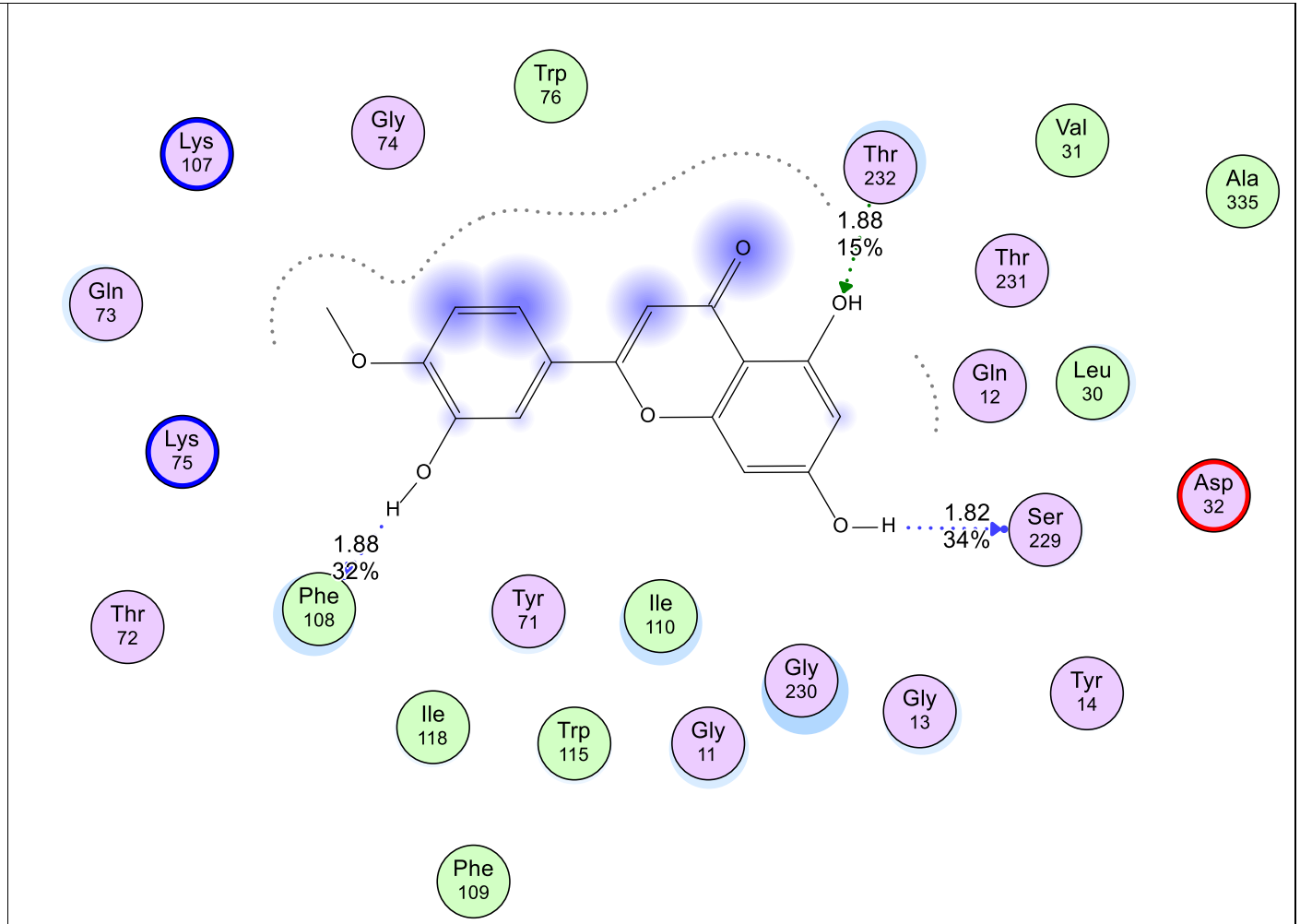
B6	4.90	–17.35	

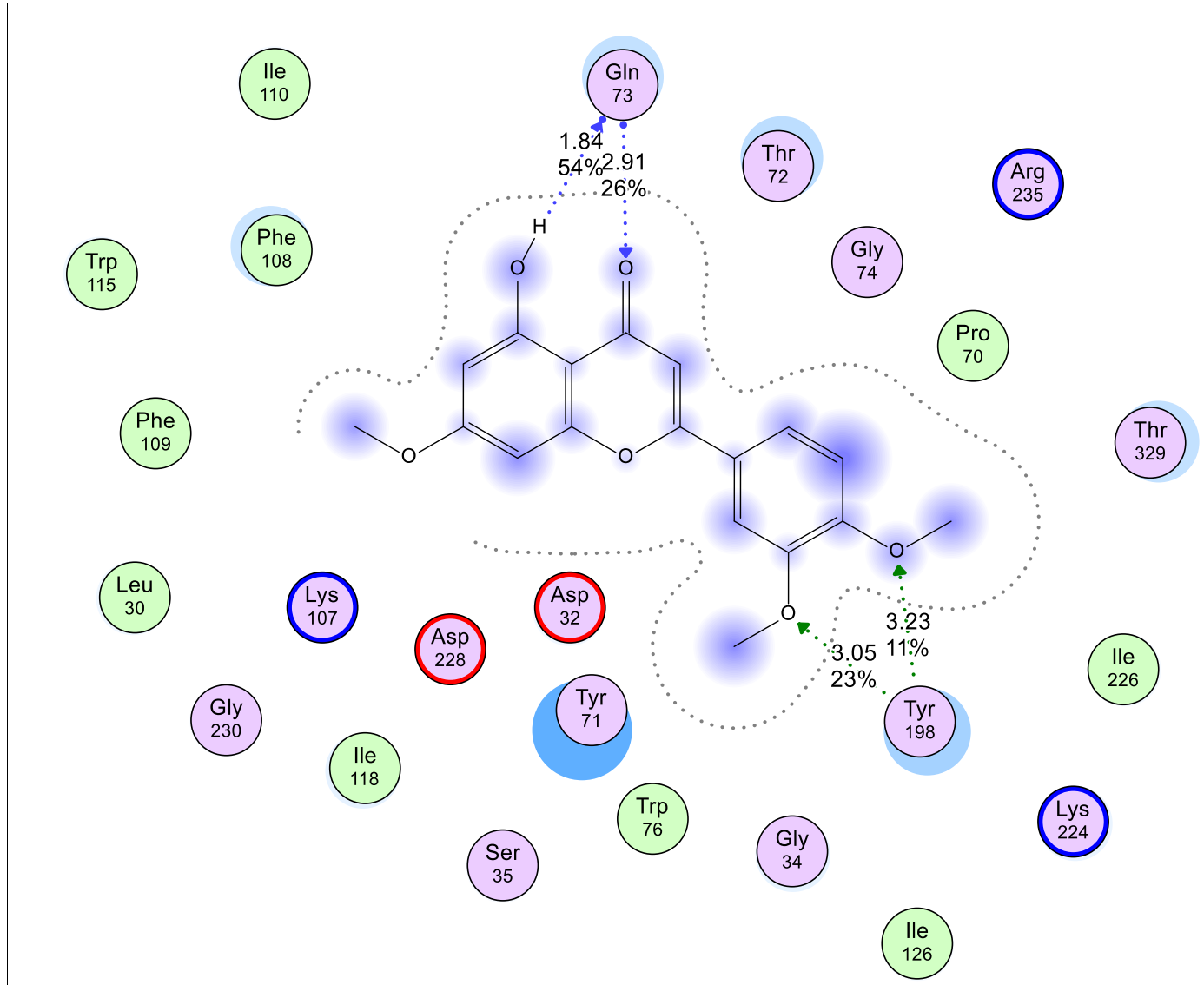
Glu 339
Tyr 14
Gly 11
Asp 228
Ala 335
Ser 10
Leu 30
Gly 230
Ser 325
Ser 229
Arg 307
Trp 115
Gly 13
Thr 231
Gln 12
Lys 9
2.54
40%
2.84
29%
Thr 232
Trp 76
Ile 118
Asn 233
Gln 326
Gly 74
Gln 73
Asp 32
Tyr 71
Arg 235
Thr 72
Phe 108
Ile 110
Lys 107
Lys 75
Phe 109

B7	4.50	–12.95	 Tyr 71 Gln 73 Lys 107 Thr 72 Gly 74 2.79 28% Thr 329 Pro 70 Gly 330 Ser 328 Phe 108 Arg 235 2.45 13% Ser 327 Gly 230 Val 332 Thr 232 Ile 110 Thr 231 Asn 233 Asp 228 Gly 11 Ile 226

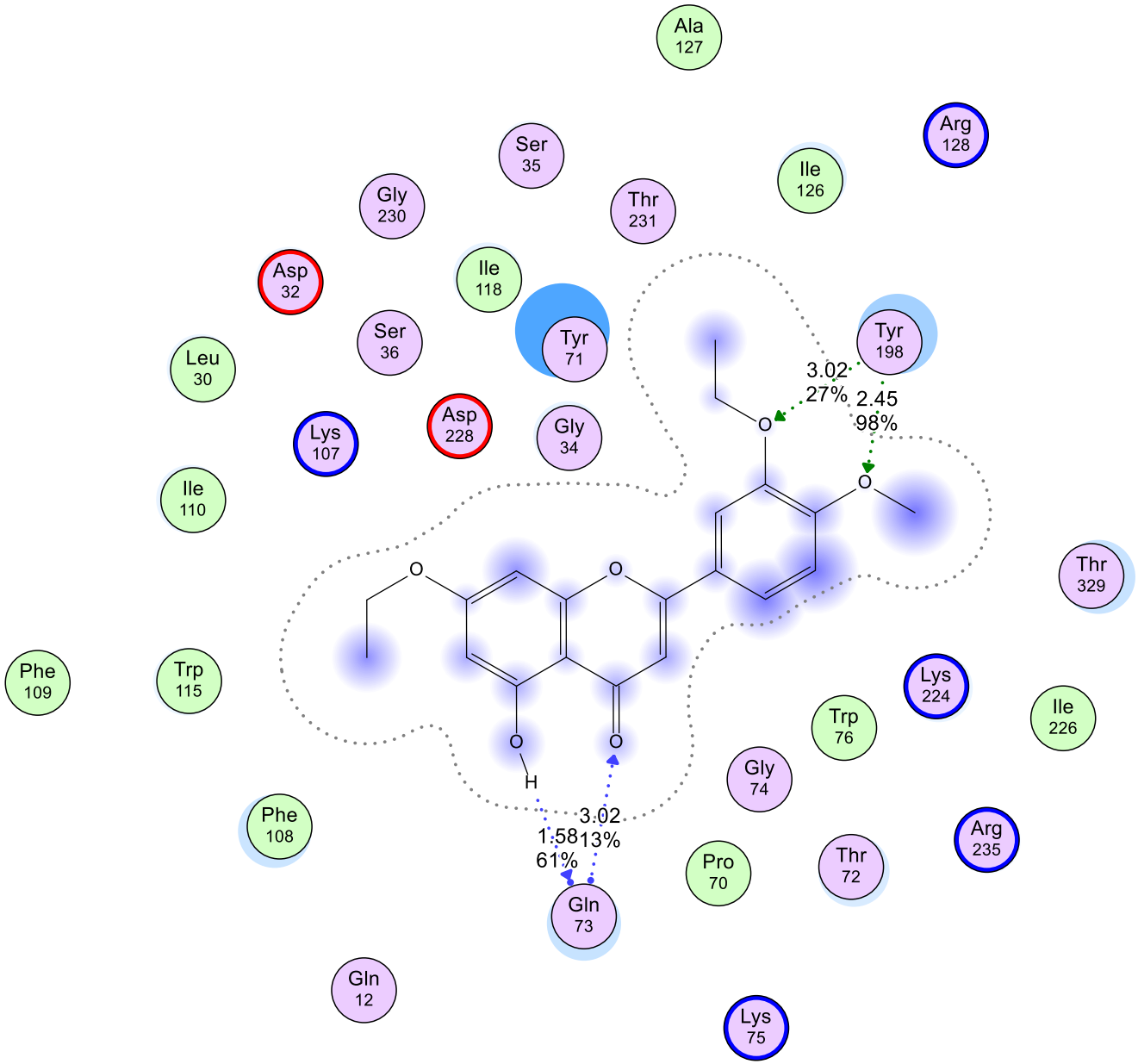
B8	4.65	–10.75	

Tyr 71
Pro 70
Lys 107
Gln 73
Phe 108
2.77
28%
Gly 74
Thr 72
Ser 327
Gly 34
Ile 110
Asp 228
Ser 328
Tyr 198
2.57
12%
Ile 226
Arg 235
Gly 11
Gly 230
Gln 326
Thr 231
Thr 329
Val 332
Thr 232
Asn 233

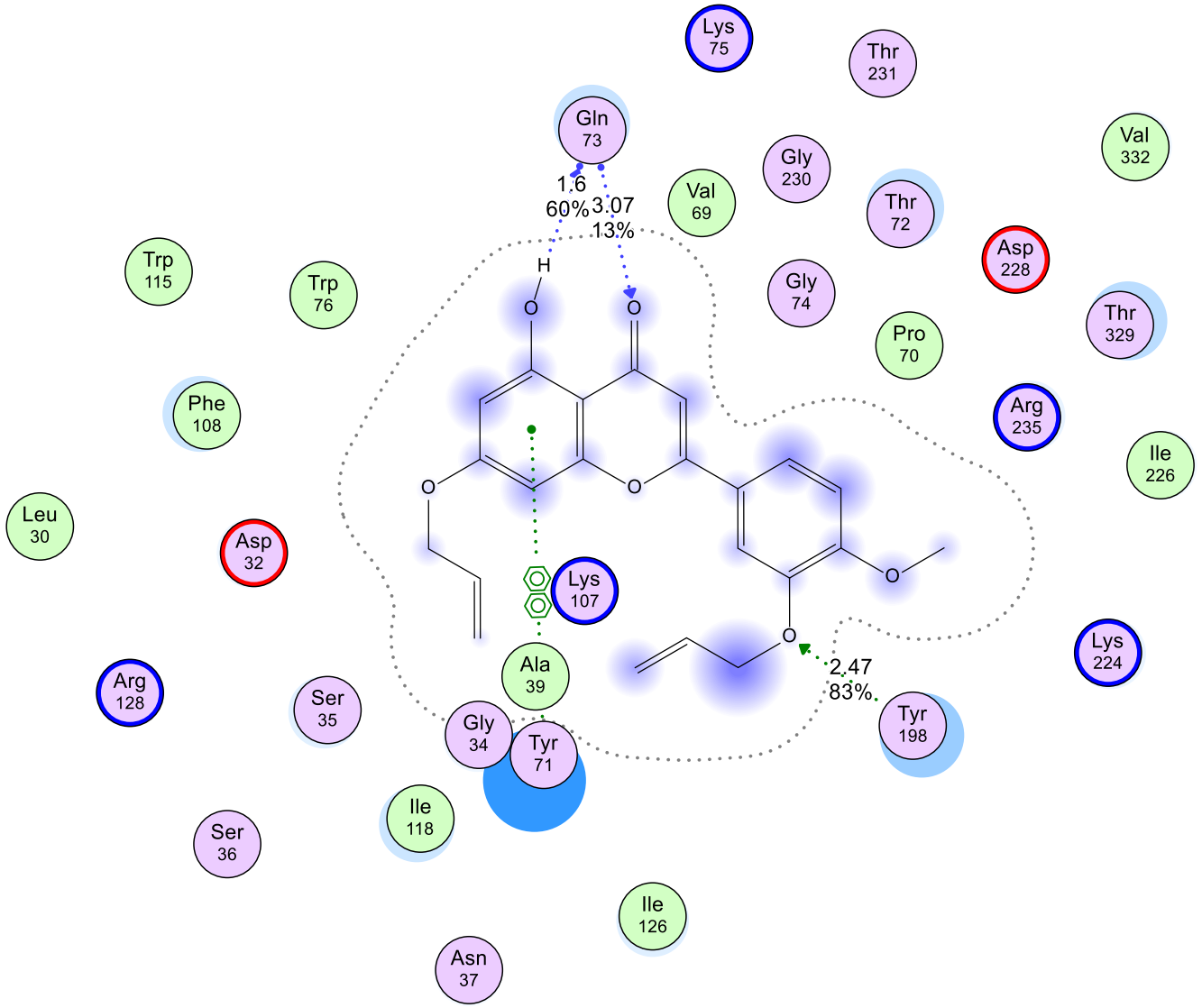
D1 (Diosmetin)	4.36	–19.32	

D2	5.67	–19.33	

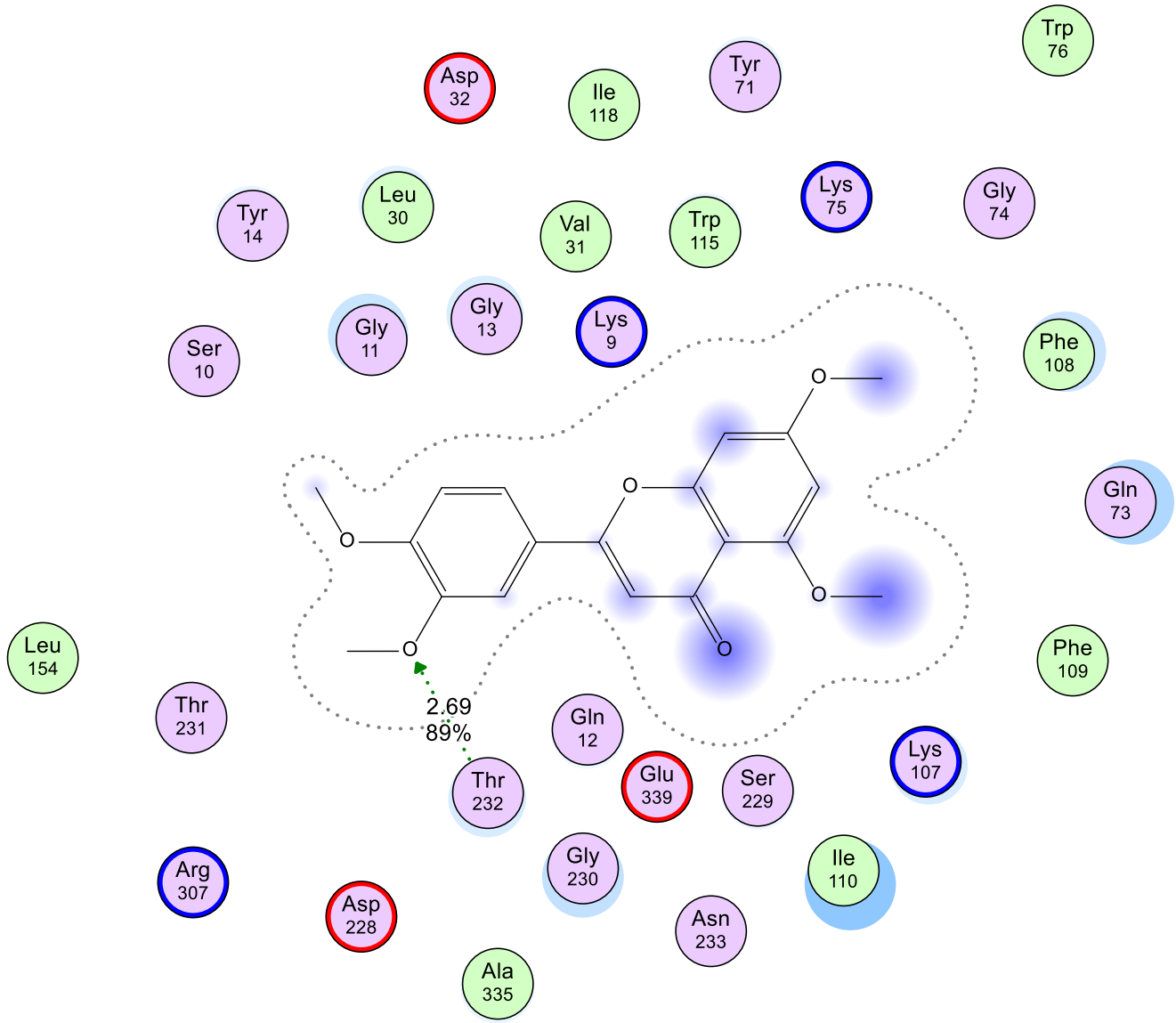
Ile 110
Gln 73
1.84 54%
2.91 26%
Thr 72
Arg 235
Phe 108
H
O
O
Gly 74
Trp 115
Pro 70
Phe 109
Thr 329
O
O
O
O
Leu 30
Lys 107
Asp 32
Asp 228
3.23 11%
3.05 23%
Ile 226
Tyr 71
Tyr 198
Gly 230
Ile 118
Trp 76
Lys 224
Gly 34
Ser 35
Ile 126

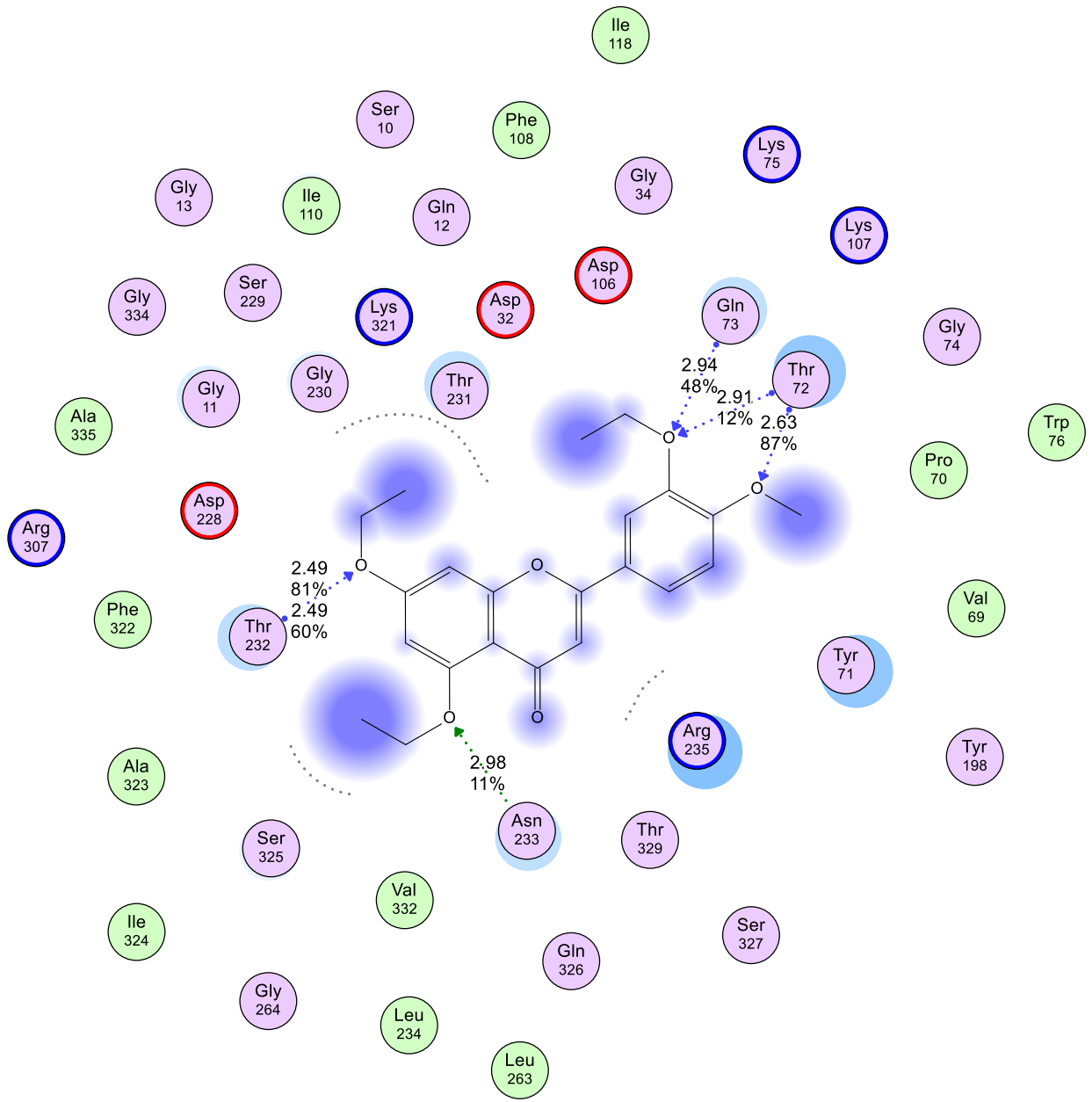
D3	5.50	–17.18	

Ala 127
Arg 128
Ser 35
Ile 126
Gly 230
Thr 231
Asp 32
Ile 118
Ser 36
Tyr 71
Tyr 198
Leu 30
3.02
27%
2.45
98%
Asp 228
Gly 34
Lys 107
Ile 110
Thr 329
Phe 109
Trp 115
Lys 224
Trp 76
Ile 226
Gly 74
Phe 108
3.02
1.58
61%
13%
Arg 235
Pro 70
Thr 72
Gln 73
Gln 12
Lys 75

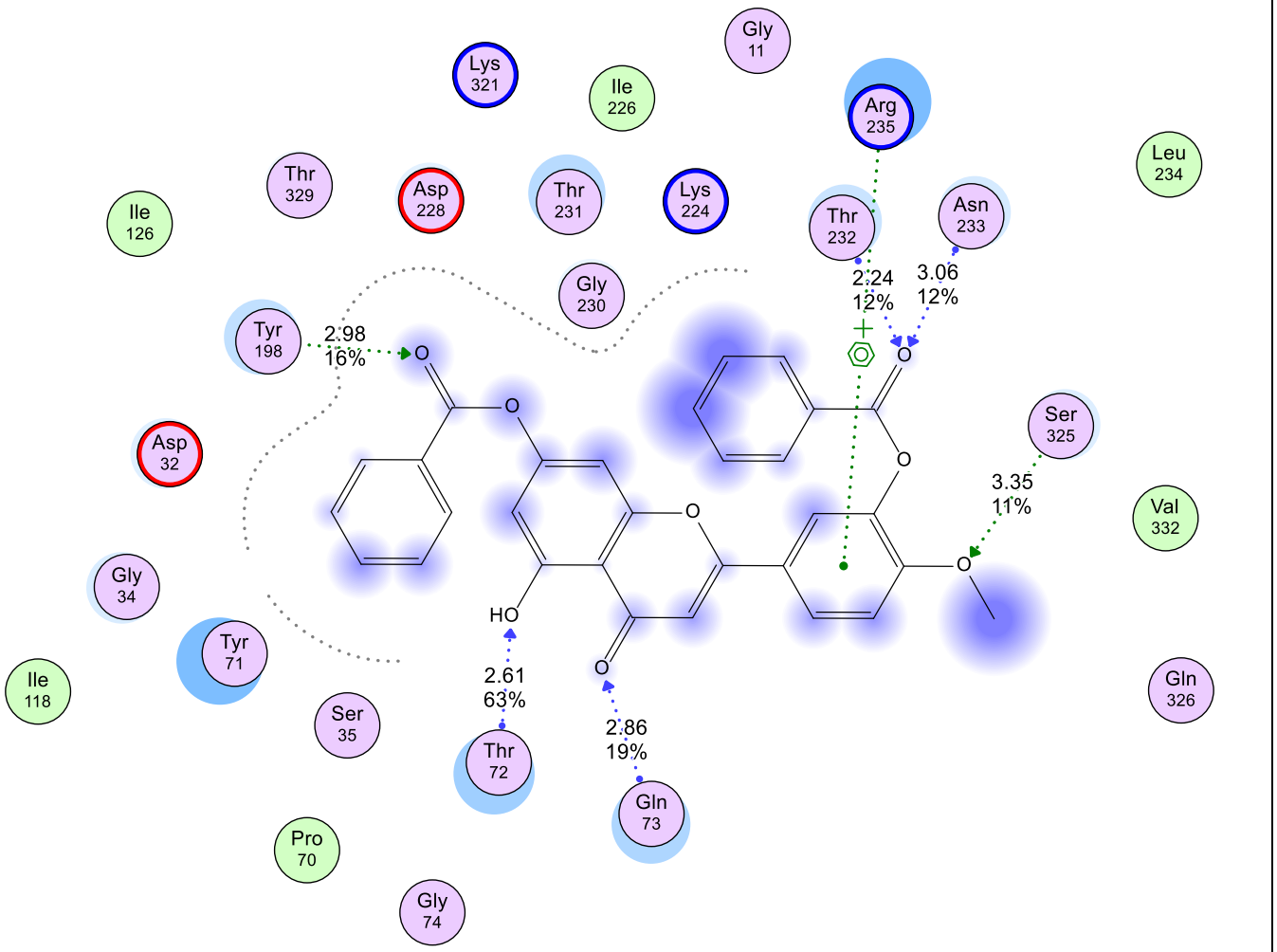
D4	5.44	–13.31	

Lys 75
Thr 231
Gln 73
Val 332
Gly 230
1.6
60%
3.07
13%
Val 69
Thr 72
Asp 228
Trp 115
Trp 76
H
O
O
Gly 74
Thr 329
Pro 70
Phe 108
Arg 235
Ile 226
Leu 30
Asp 32
O
O
O
Lys 107
O
Lys 224
Ala 39
2.47
83%
Arg 128
Ser 35
Gly 34
Tyr 198
Tyr 71
Ile 118
Ser 36
Ile 126
Asn 37

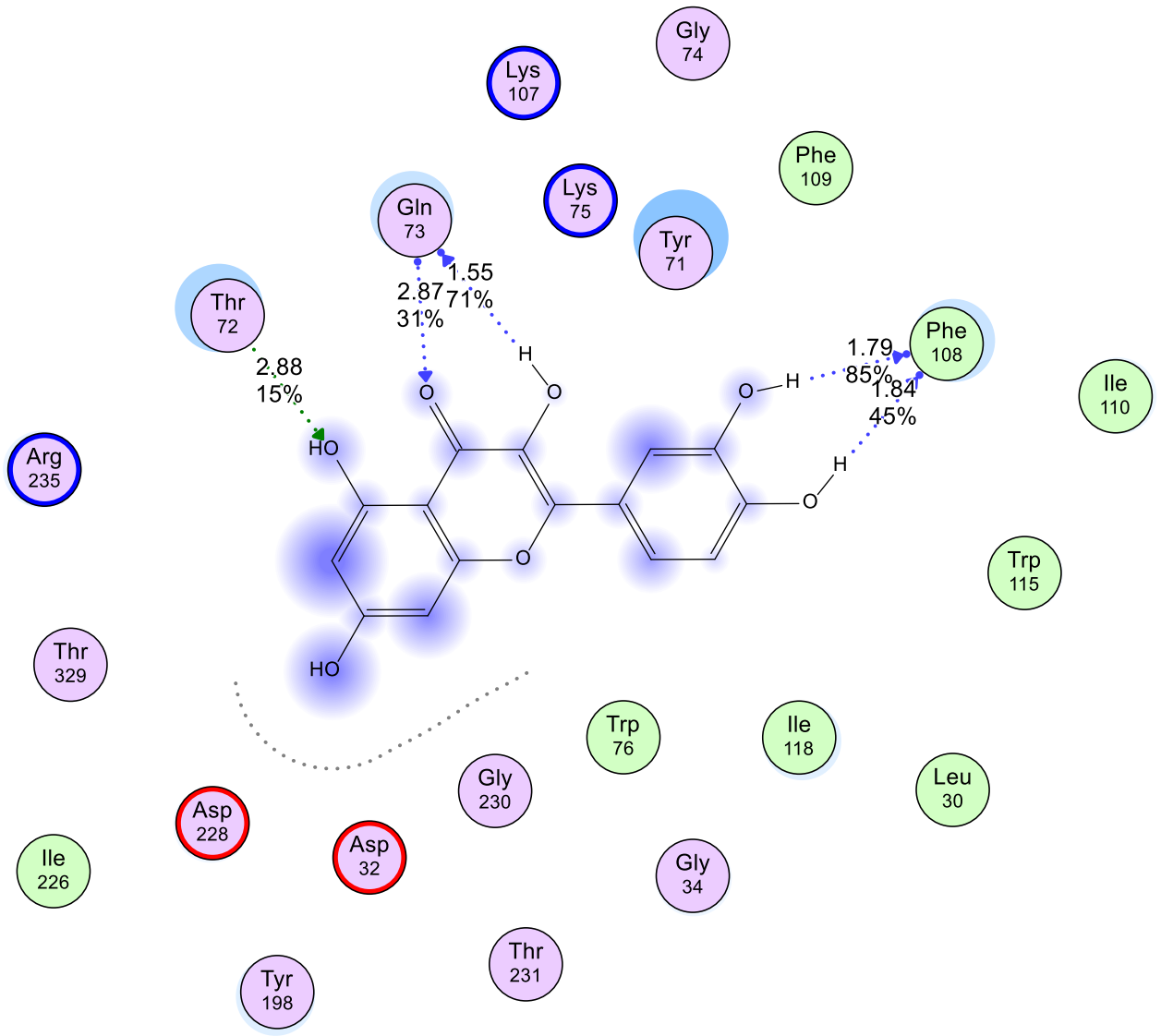
D5	5.78	–13.46	 Trp 76 Asp 32 Ile 118 Tyr 71 Lys 75 Gly 74 Leu 30 Tyr 14 Val 31 Trp 115 Gly 13 Gly 11 Lys 9 Ser 10 Phe 108 Gln 73 Leu 154 Phe 109 Thr 231 2.69 89% Gln 12 Lys 107 Thr 232 Glu 339 Ser 229 Gly 230 Ile 110 Arg 307 Asp 228 Asn 233 Ala 335

D6	5.80	–12.02	

Ile 118
Ser 10
Phe 108
Lys 75
Gly 13
Ile 110
Gln 12
Gly 34
Lys 107
Asp 106
Ser 229
Gly 334
Lys 321
Asp 32
Gln 73
Gly 74
Gly 230
Thr 231
Thr 72
Gly 11
Ala 335
2.94 48%
2.91 12%
2.63 87%
Trp 76
Pro 70
Asp 228
Arg 307
2.49 81%
2.49 60%
Val 69
Phe 322
Thr 232
Tyr 71
Arg 235
Ala 323
2.98 11%
Tyr 198
Asn 233
Thr 329
Ser 325
Val 332
Ile 324
Ser 327
Gln 326
Gly 264
Leu 234
Leu 263

D7	5.54	–22.07	

Gly 11
Lys 321
Ile 226
Arg 235
Leu 234
Thr 329
Asp 228
Thr 231
Lys 224
Thr 232
Asn 233
Ile 126
2.24 12%
3.06 12%
Gly 230
Tyr 198
2.98 16%
O
O
O
O
Ser 325
Asp 32
3.35 11%
Val 332
Gly 34
HO
Tyr 71
O
Ile 118
2.61 63%
2.86 19%
Gln 326
Ser 35
Thr 72
Gln 73
Pro 70
Gly 74

Quercetin	5.02	–22.55	

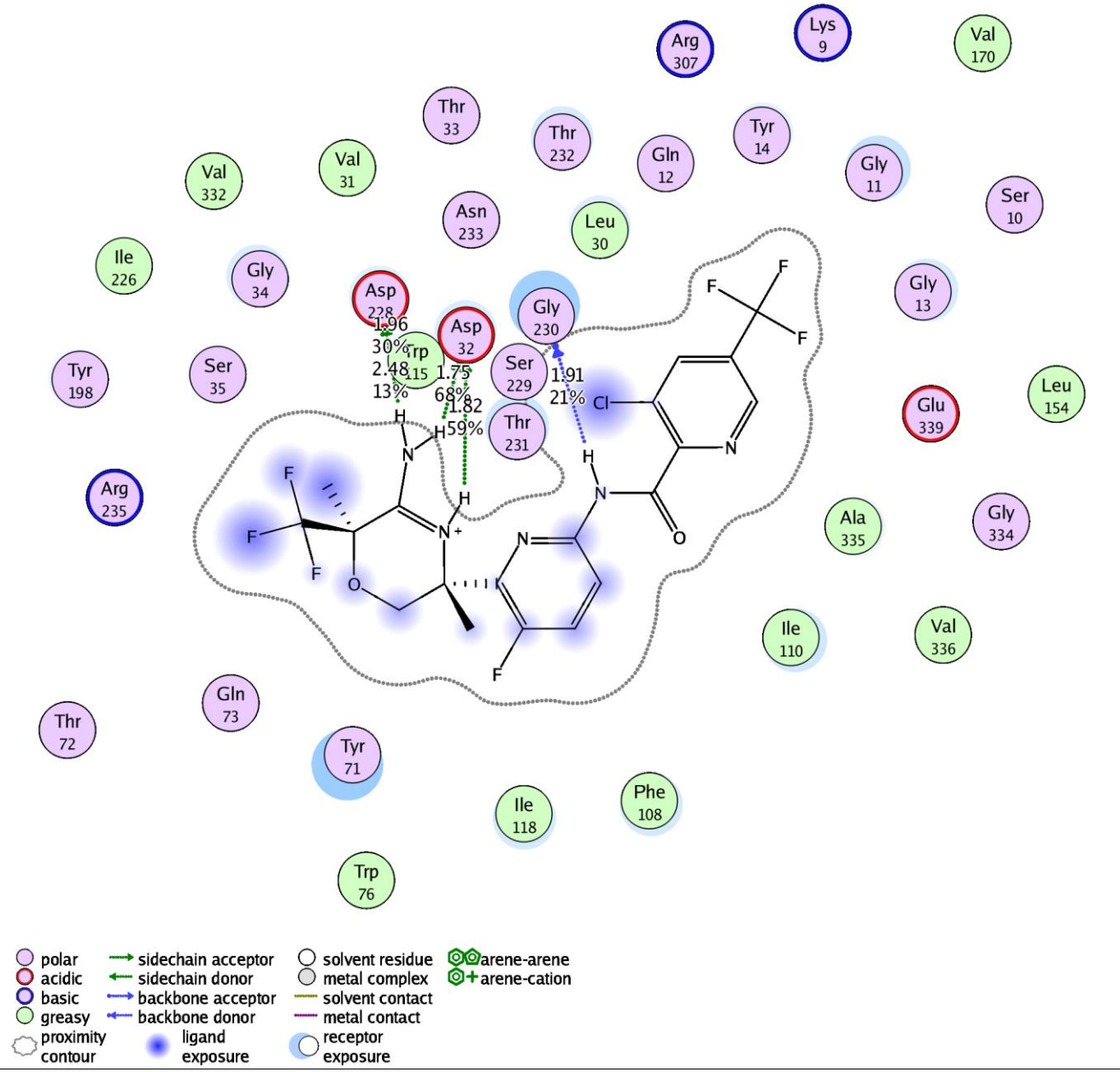
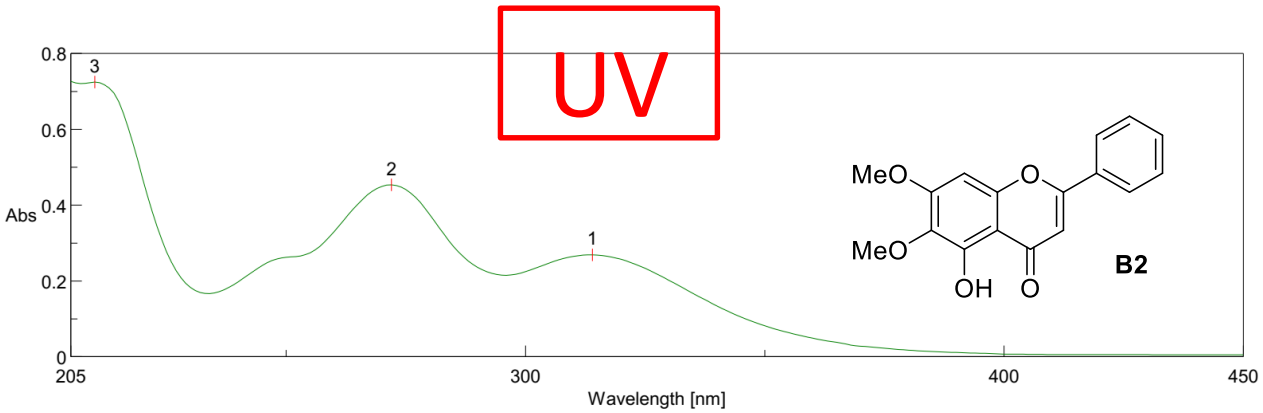
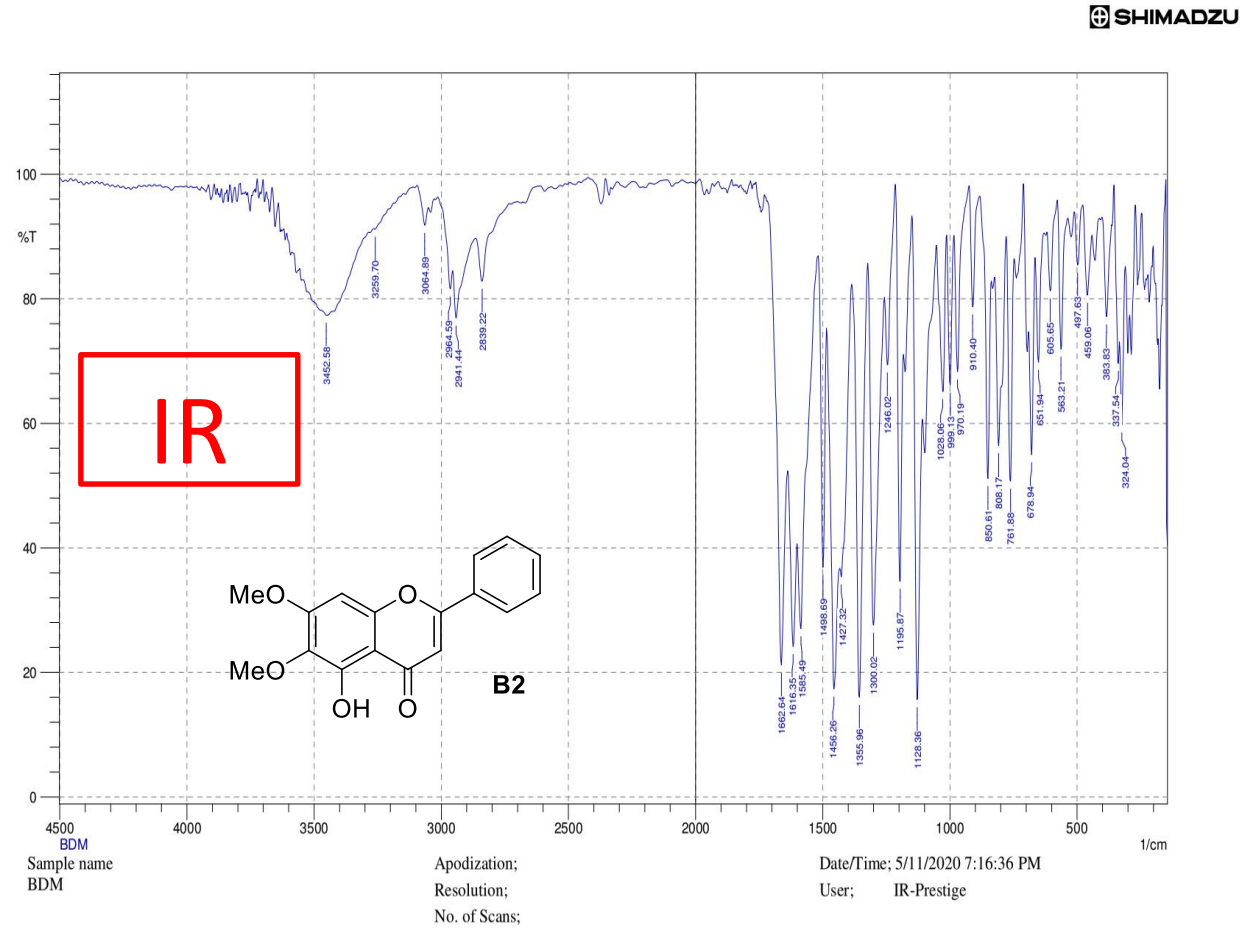
Umibecestat	7.96 [4]	–47.04	

Table S7. Spectra of synthesized flavone derivatives



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	314	0.268399	2	272	0.452919	3	210	0.724239



Sample name BDM

Apodization;
Resolution;
No. of Scans;

Date/Time; 5/11/2020 7:16:36 PM
User; IR-Prestige

MS

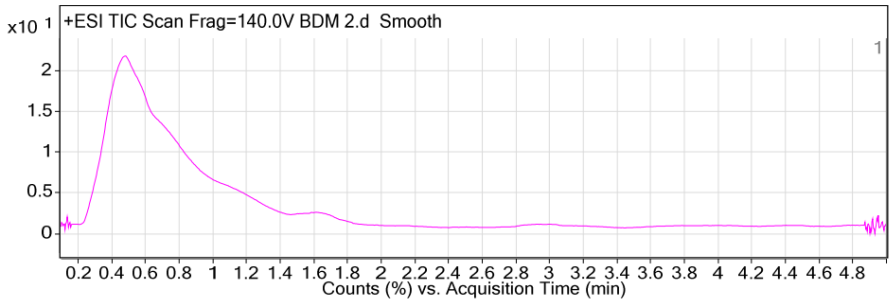
Qualitative Analysis Report

Data Filename	BDM 2.d	**Sample Name**	BDM 2
Sample Type	Sample	**Position**	P2-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 8:02:09 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

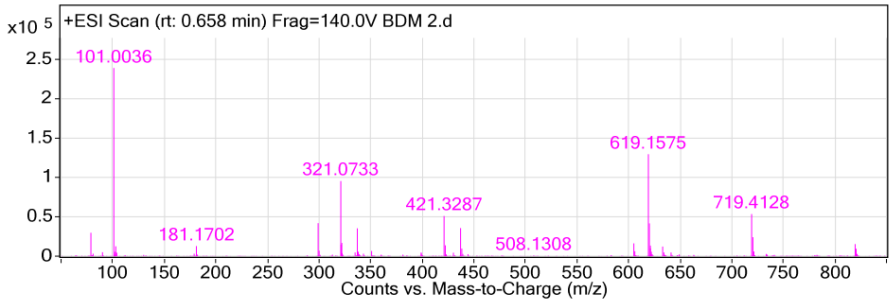
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



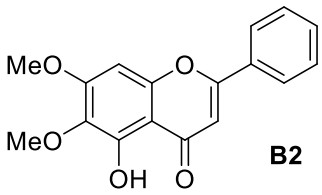
User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
140	0	ESI



Peak List

m/z	z	Abund
79.0213	1	29725.18
101.0036	1	239362.81
299.0917	1	41948.91
321.0733	1	95620.17
337.0475	1	35516.83
421.3287	1	51010.1
437.3026	1	35858.05
619.1575	1	129711.47
620.1605	1	41771.26
719.4128	1	53729.01

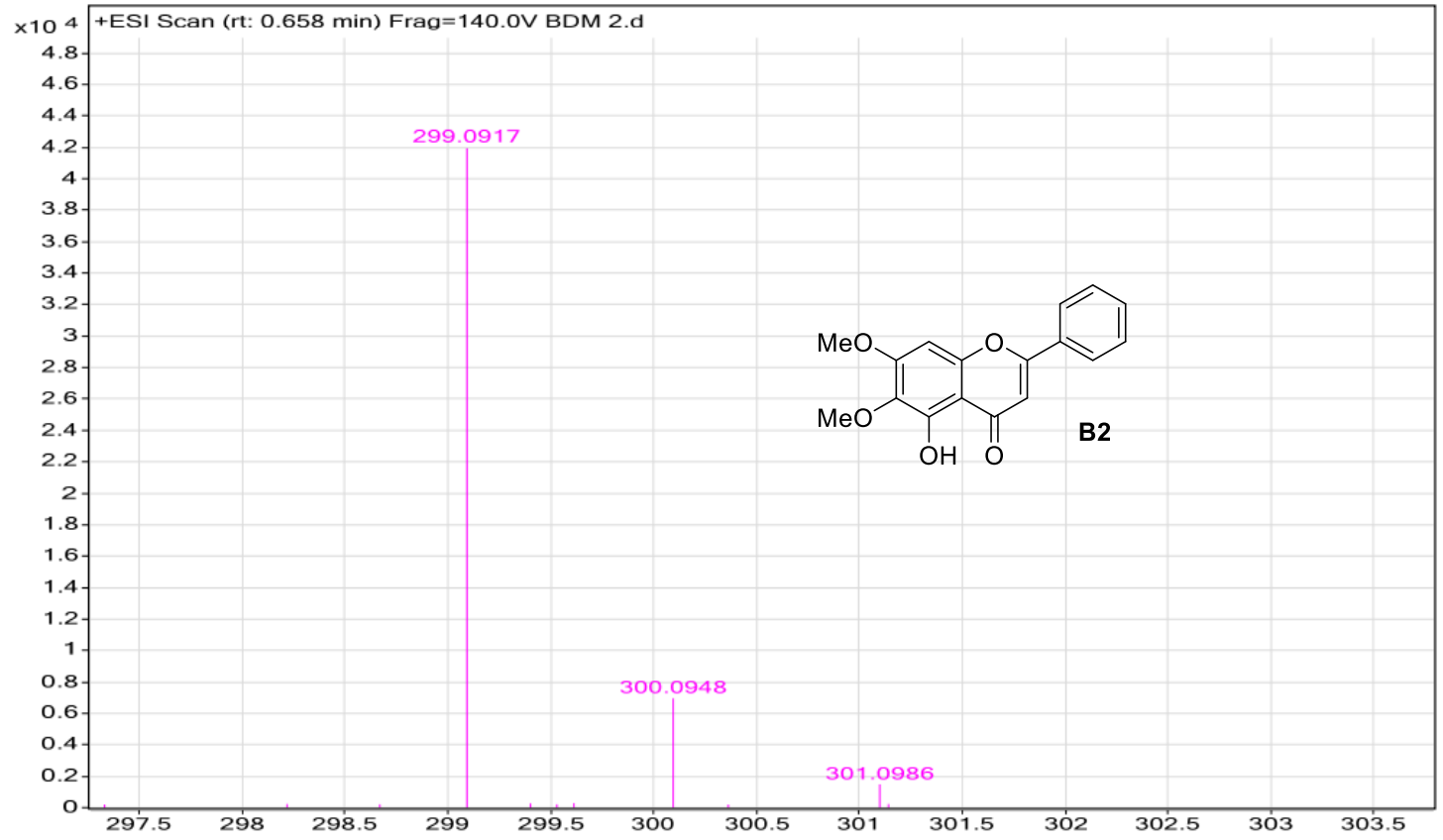


B2

--- End Of Report ---

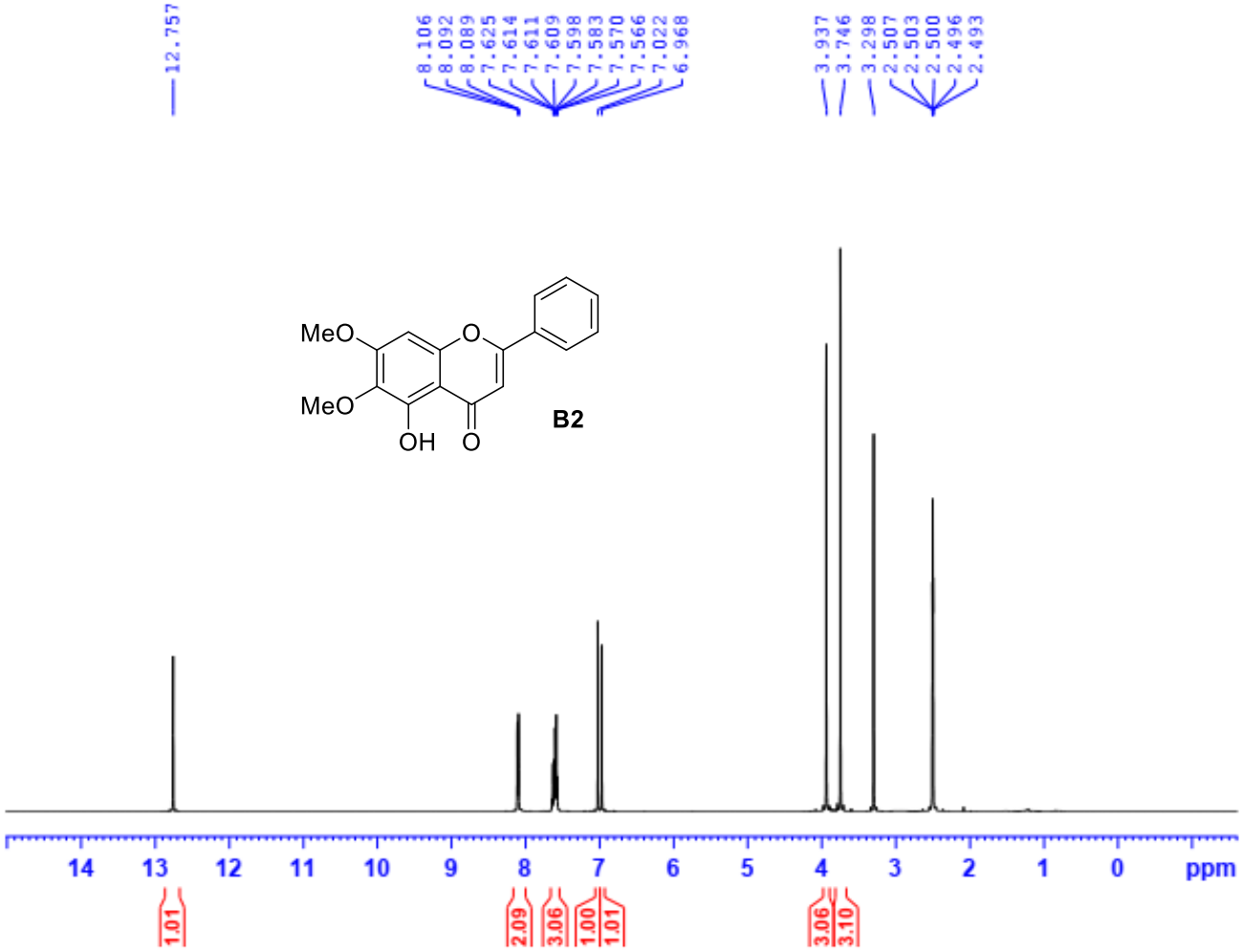
MS

Sample Name	BDM 2	**Position**	P2-C1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	BDM 2.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 8:02:09 PM



^{1}H-NMR

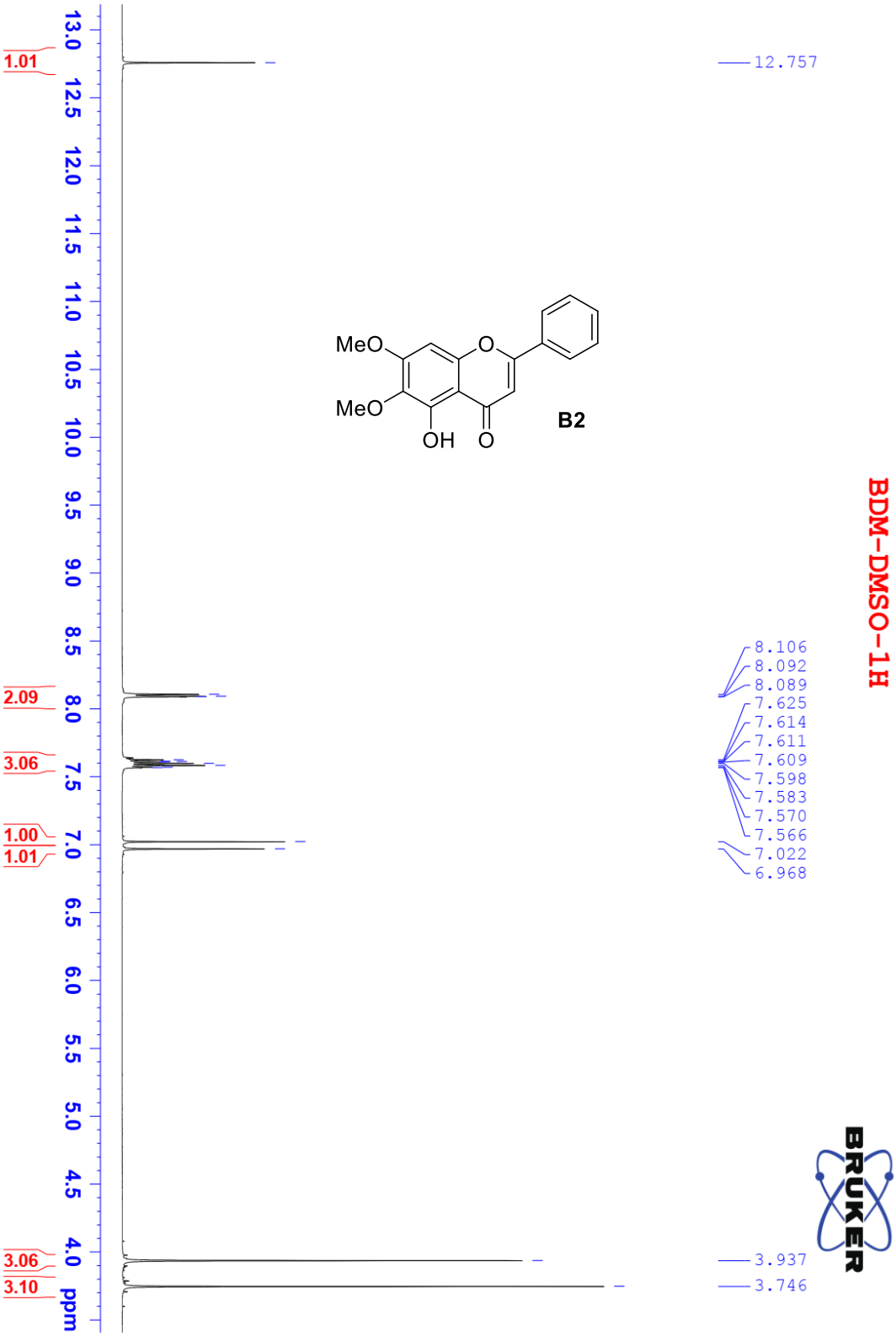
BDM-DMSO-1H



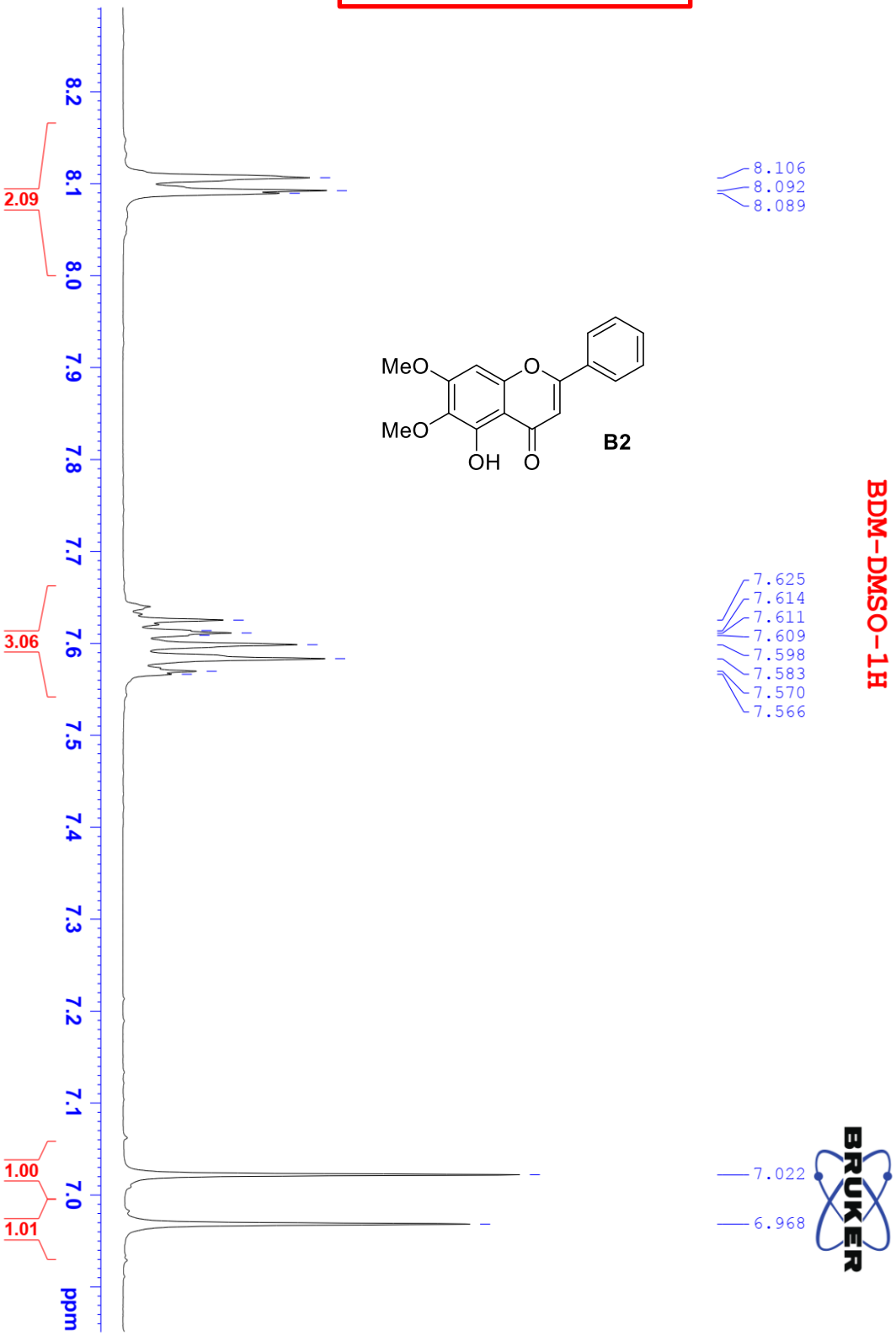
BRUKER

```
Current Data Parameters
NAME          113HUAN_BDM
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20191008
Time              12.10
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               304.6 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1920889 MHz
NUC1                1H
P1                10.20 usec
PLW1         22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.1890050 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{1}H-NMR

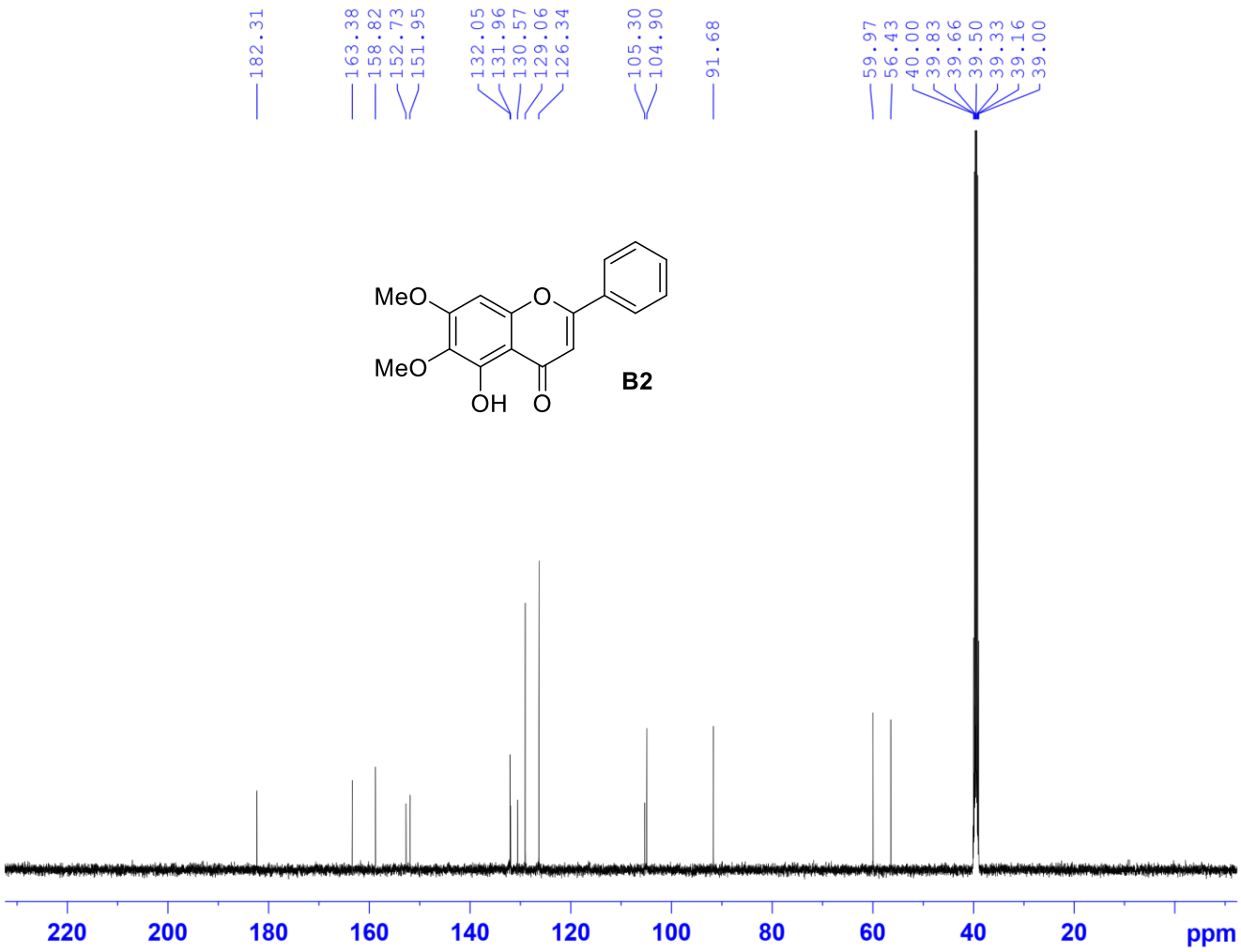

13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm
1.01
2.09
3.06
1.00
1.01
3.06
3.10
12.757
8.106
8.092
8.089
7.625
7.614
7.611
7.609
7.598
7.583
7.570
7.566
7.022
6.968
3.937
3.746
MeO
MeO
OH
O
O
B2
BDM-DMSO-1H
BRUKER

^{1}H-NMR


8.106
8.092
8.089
7.625
7.614
7.611
7.609
7.598
7.583
7.570
7.566
7.022
6.968
2.09
3.06
1.00
1.01
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
MeO
MeO
OH
O
O
B2
BDM-DMSO-1H
BRUKER

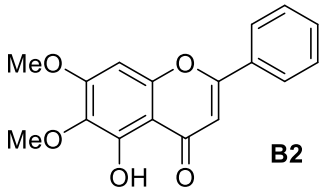
^{13}C-NMR

BDM-DMSO-C13CPD




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

F2 - Acquisition Parameters
Date_           20191008
Time               16.40
INSTRUM            spect
PROBHD   5 mm PABBO BB/
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                304.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7864591 MHz
NUC1                  13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2        500.1910008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.35764000 W
PLW13         0.17989001 W

F2 - Processing parameters
SI                 32768
SF          125.7726928 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{13}C-NMR



B2

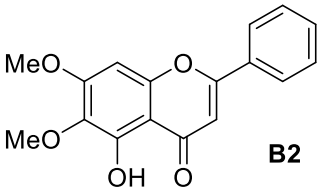
182.31
163.38
158.82
152.73
151.95
132.05
131.96
130.57
129.06
126.34
105.30
104.90
91.68
59.97
56.43

BDM-DMSO-C13CPD

BRUKER

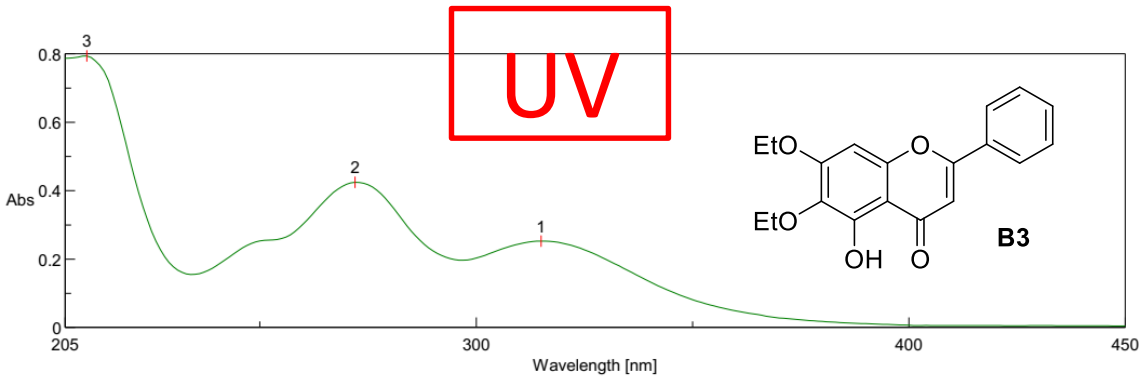
180 170 160 150 140 130 120 110 100 90 80 70 60 ppm

^{13}C-NMR


MeO
MeO
OH
O
O

B2

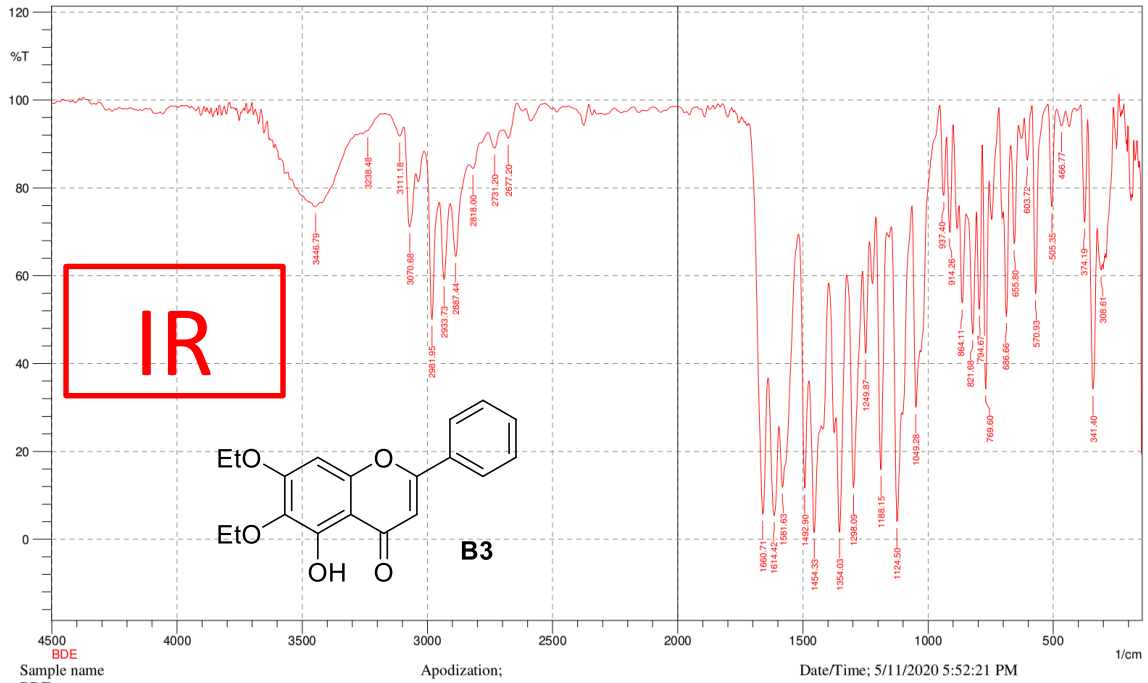
135
130
125
120
115
110
105
ppm
132.05
131.96
130.57
129.06
126.34
105.30
104.90
BDM-DMSO-C13CPD
BRUKER



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	315	0.252366	2	272	0.424071	3	210	0.793522

SHIMADZU



BDE

Sample name BDE

Apodization;
Resolution;
No. of Scans;

Date/Time; 5/11/2020 5:52:21 PM
User; IR-Prestige

MS

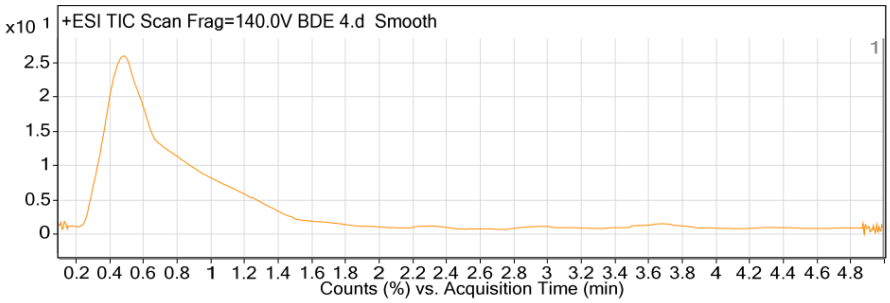
Qualitative Analysis Report

Data Filename	BDE 4.d	**Sample Name**	BDE 4
Sample Type	Sample	**Position**	P2-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 7:17:38 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

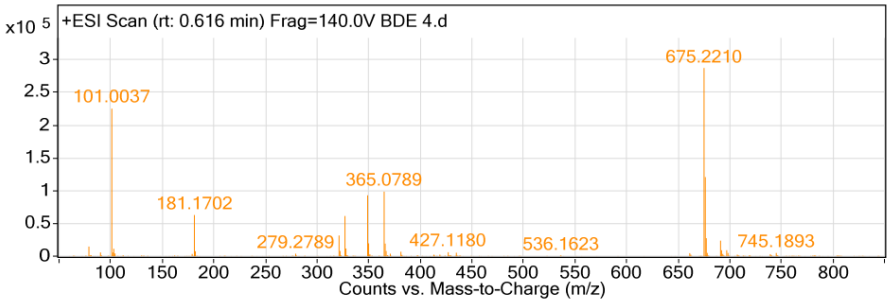
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



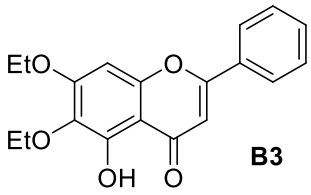
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
101.0037	1	225364.16
181.1702	1	62704.9
321.3268	1	31494.73
327.123	1	61334.02
349.105	1	92764.2
365.0789	1	98738.83
675.221	1	287090.03
676.2238	1	120780.58
677.2262	1	27656.04
691.1934	1	23767.92

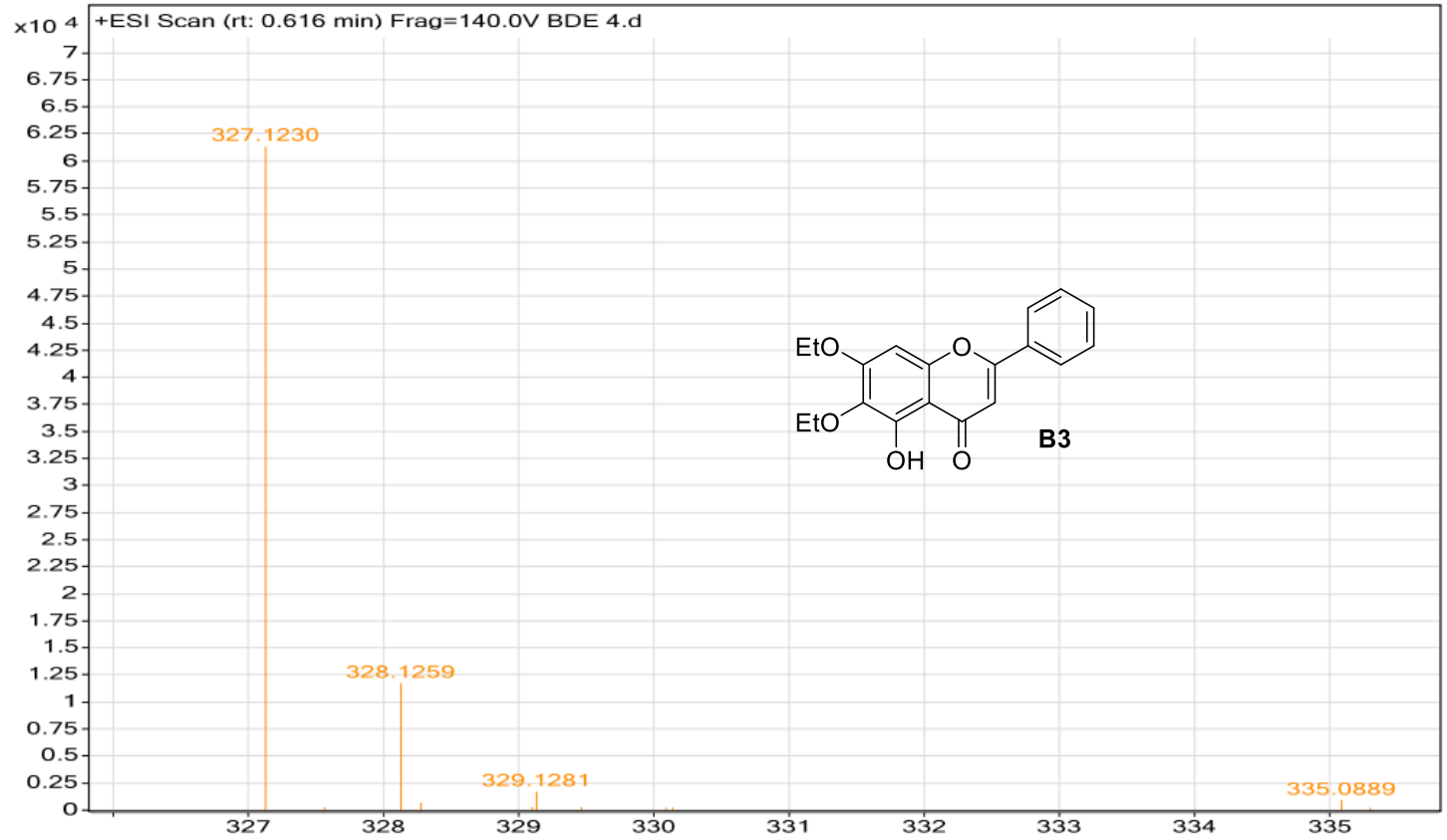


B3

--- End Of Report ---

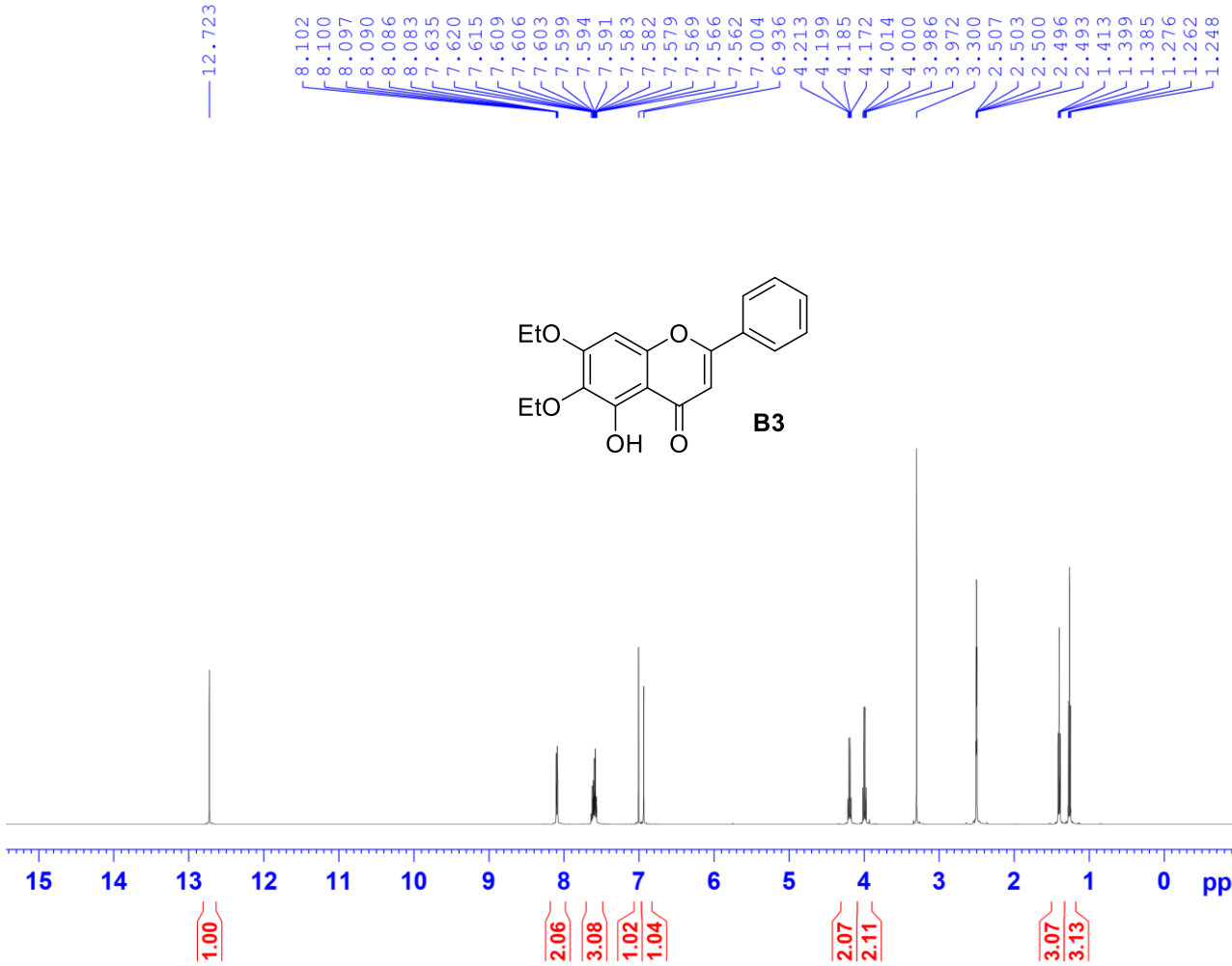
MS

Sample Name	BDE 4	**Position**	P2-B2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	BDE 4.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 7:17:38 PM



^{1}H-NMR

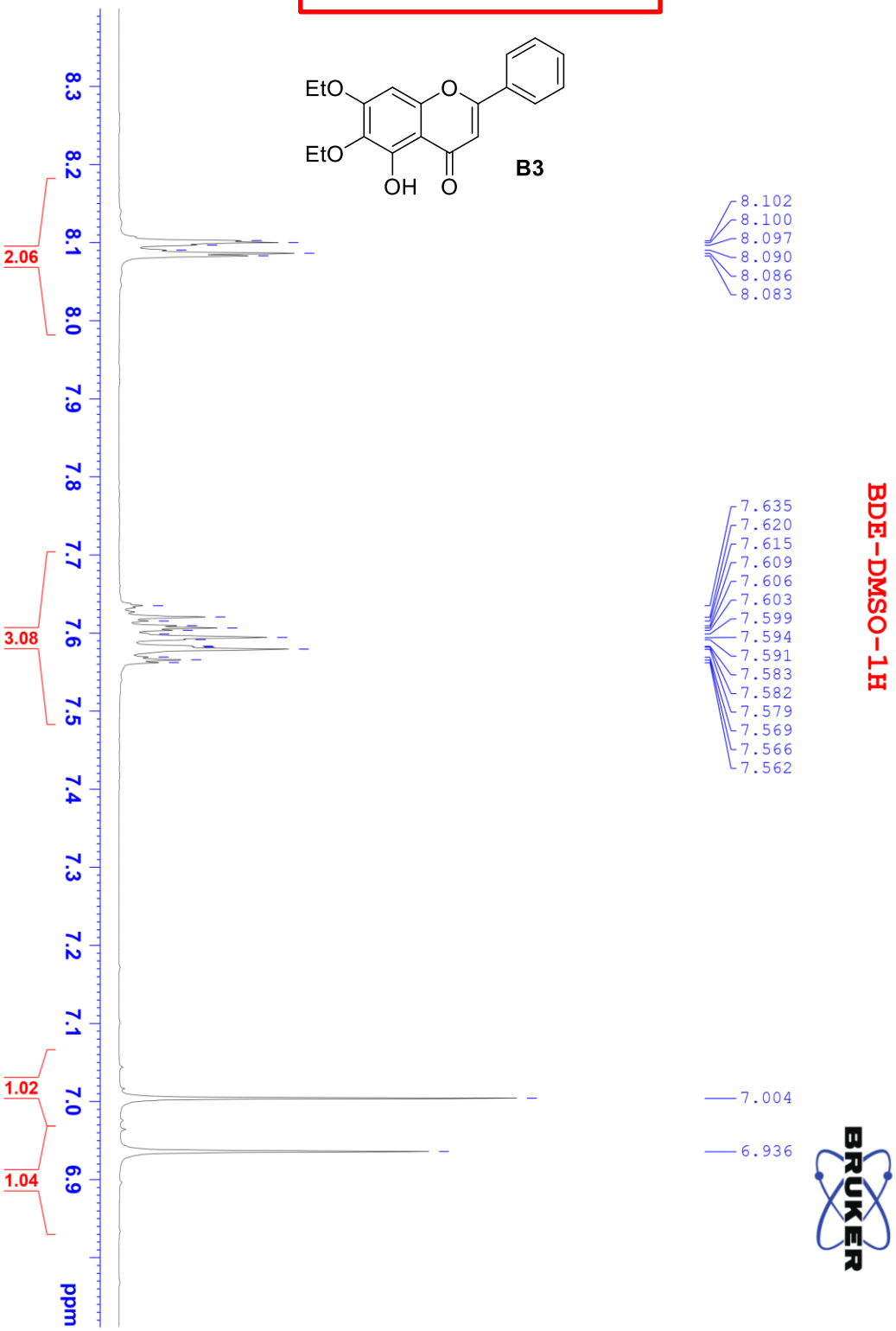
BDE-DMSO-1H



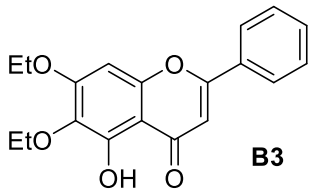
BRUKER

```
Current Data Parameters
NAME         110HUAN_BDE
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time              11.33
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                303.9 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1920889 MHz
NUC1                 1H
P1                10.20 usec
PLW1        22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.1890047 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{1}H-NMR


EtO
EtO
OH
O
O
B3
8.102
8.100
8.097
8.090
8.086
8.083
7.635
7.620
7.615
7.609
7.606
7.603
7.599
7.594
7.591
7.583
7.582
7.579
7.569
7.566
7.562
7.004
6.936
2.06
3.08
1.02
1.04
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
ppm
BDE-DMSO-1H
BRUKER

^{1}H-NMR



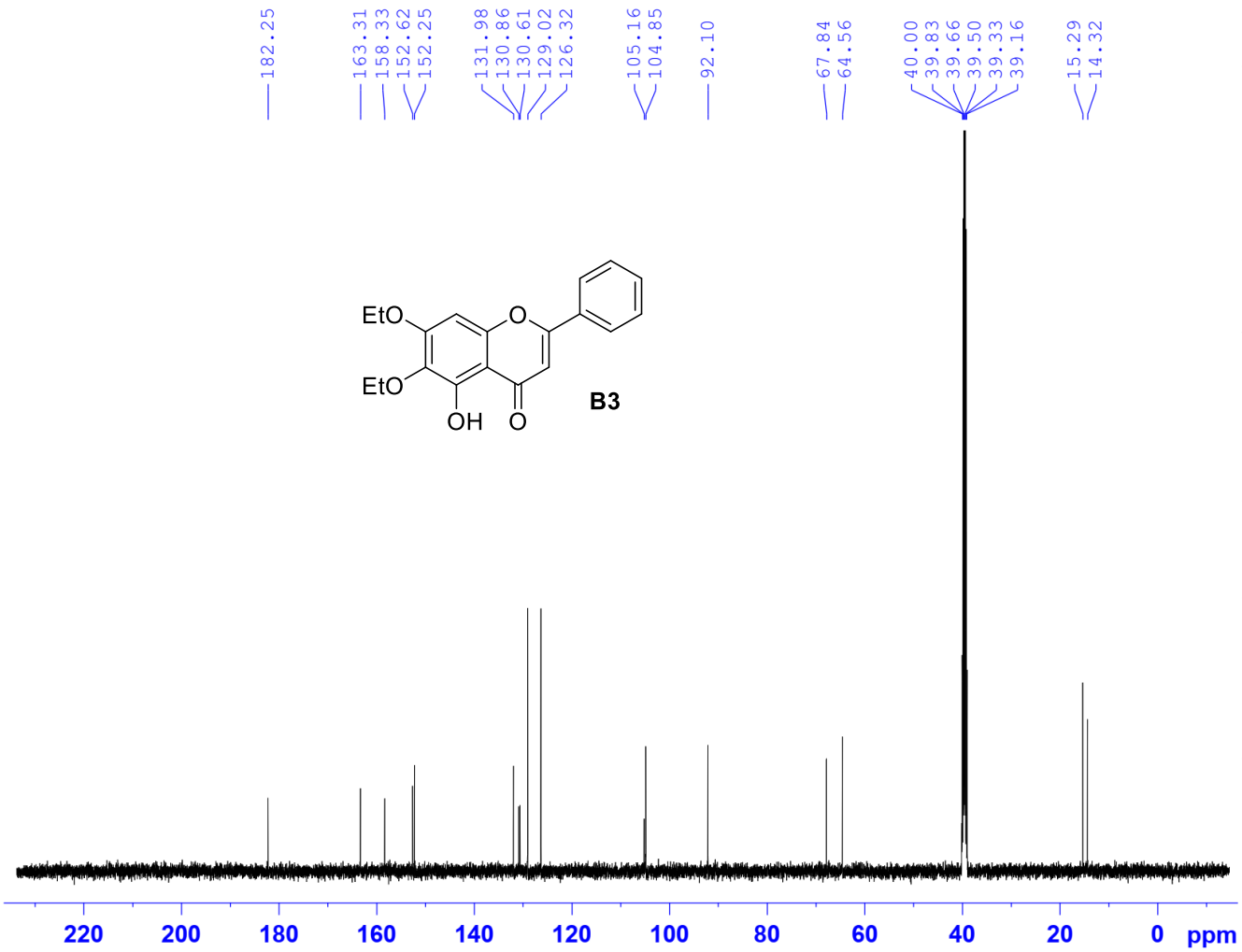
B3

BDE-DMSO-1H

BRUKER

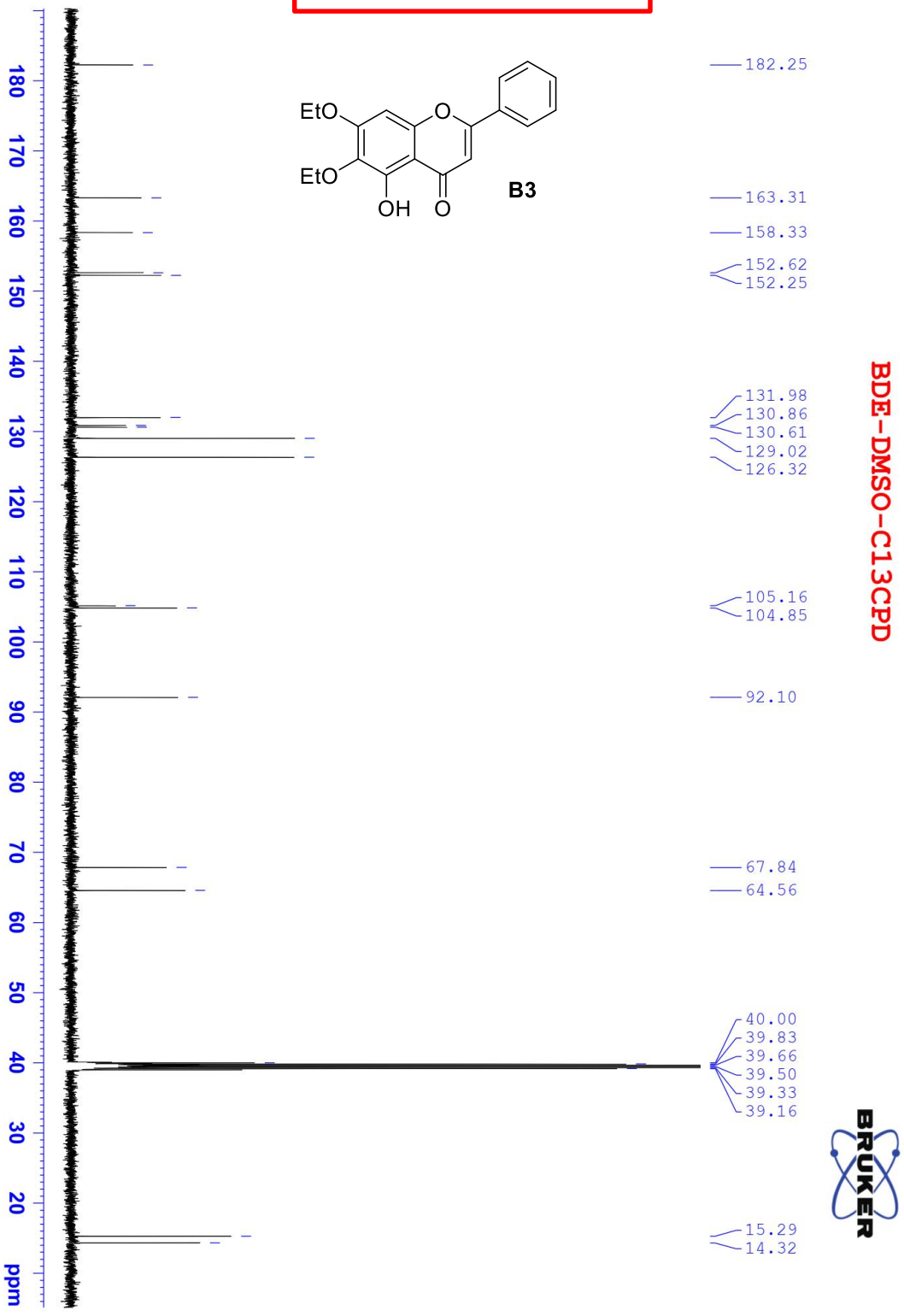
^{13}C-NMR

BDE-DMSO-C13CPD

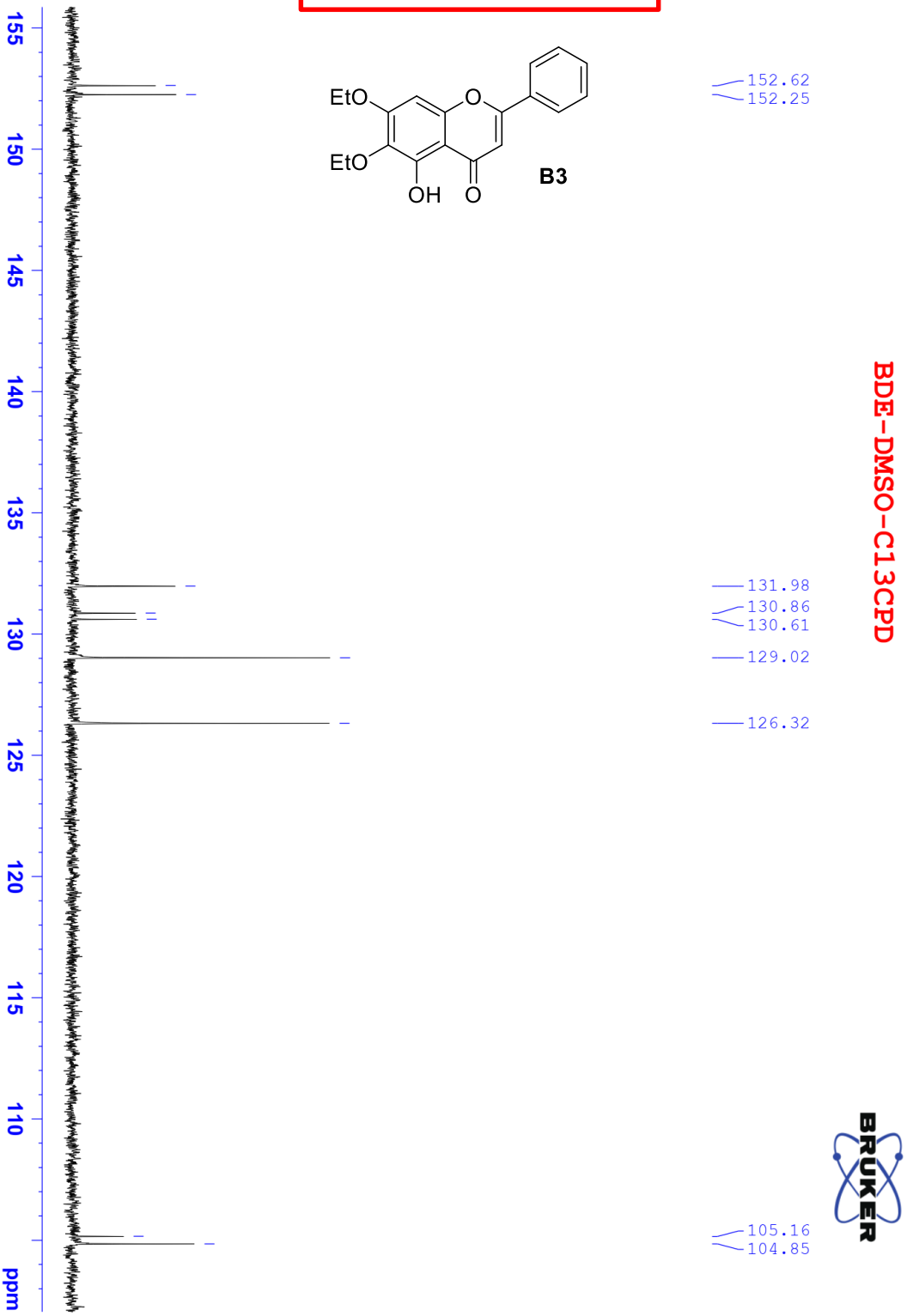


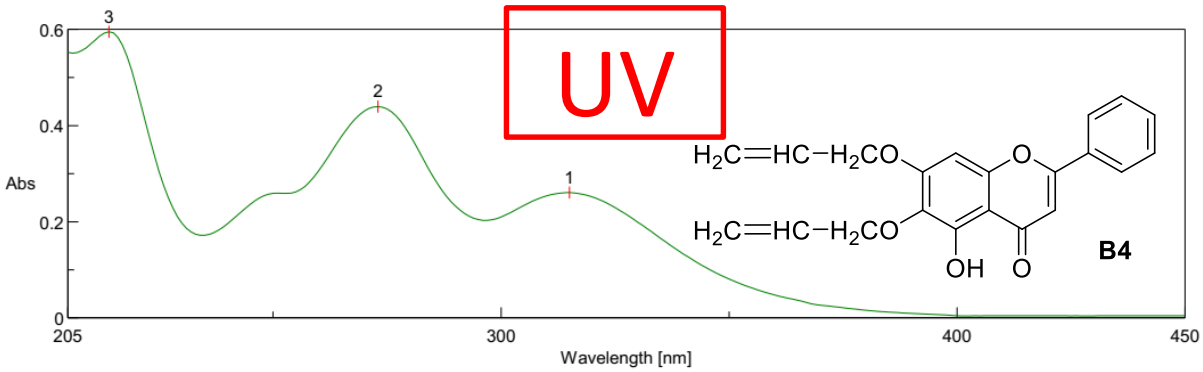

```
Current Data Parameters
NAME         110HUAN_BDE
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time               17.24
INSTRUM            spect
PROBHD   5 mm PABBO BB/
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                306.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7864591 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.1910008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.35764000 W
PLW13         0.17989001 W

F2 - Processing parameters
SI                 32768
SF           125.7726952 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

^{13}C-NMR


EtO
EtO
OH
O
O
B3
182.25
163.31
158.33
152.62
152.25
131.98
130.86
130.61
129.02
126.32
105.16
104.85
92.10
67.84
64.56
40.00
39.83
39.66
39.50
39.33
39.16
15.29
14.32
ppm
BDE-DMSO-C13CPD
BRUKER

^{13}C-NMR

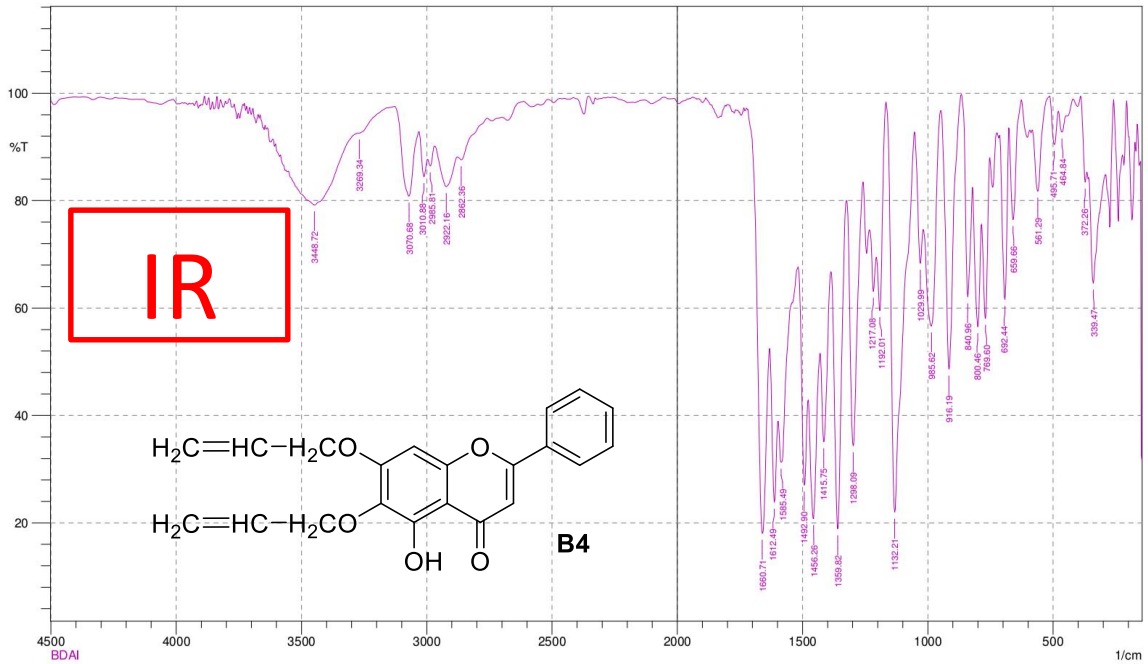

155
150
145
140
135
130
125
120
115
110
ppm
EtO
EtO
OH
O
O
B3
152.62
152.25
131.98
130.86
130.61
129.02
126.32
105.16
104.85
BDE-DMSO-C13CPD
BRUKER



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	315	0.260353	2	273	0.439249	3	214	0.594943

SHIMADZU



Sample name
BDAI

Apodization;
Resolution;
No. of Scans;

Date/Time; 5/11/2020 7:32:35 PM
User; IR-Prestige

MS

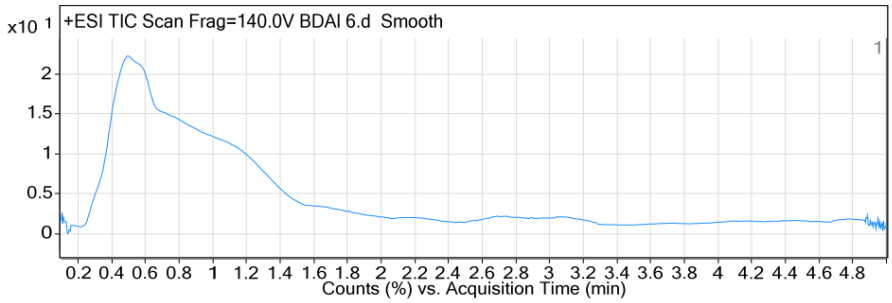
Qualitative Analysis Report

Data Filename	BDAI 6.d	**Sample Name**	BDAI 6
Sample Type	Sample	**Position**	P2-C5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 8:24:25 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

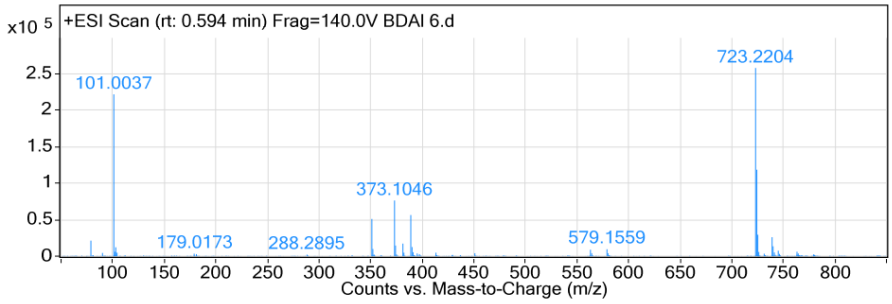
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



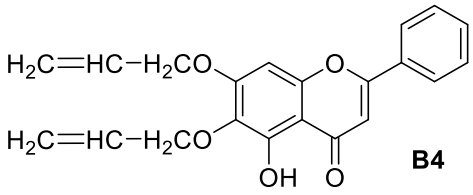
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
79.0213	1	21162.16
101.0037	1	221657.94
351.1224	1	50865.48
373.1046	1	76269.85
381.2974	1	17324.84
389.0783	1	56522.68
723.2204	1	257544.19
724.223	1	118534.92
725.2257	1	29415.95
739.193	1	26186.25

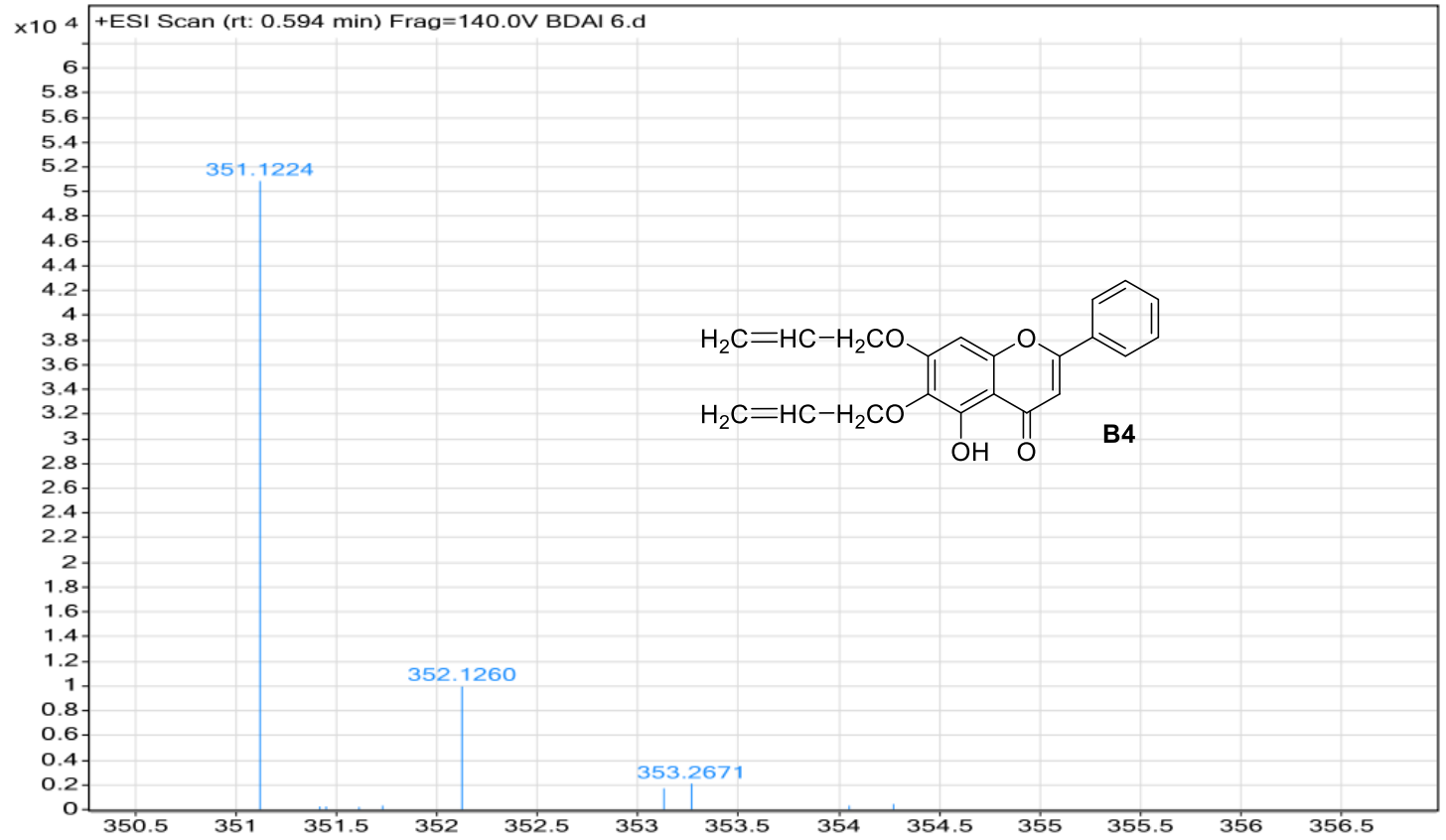


B4

--- End Of Report ---

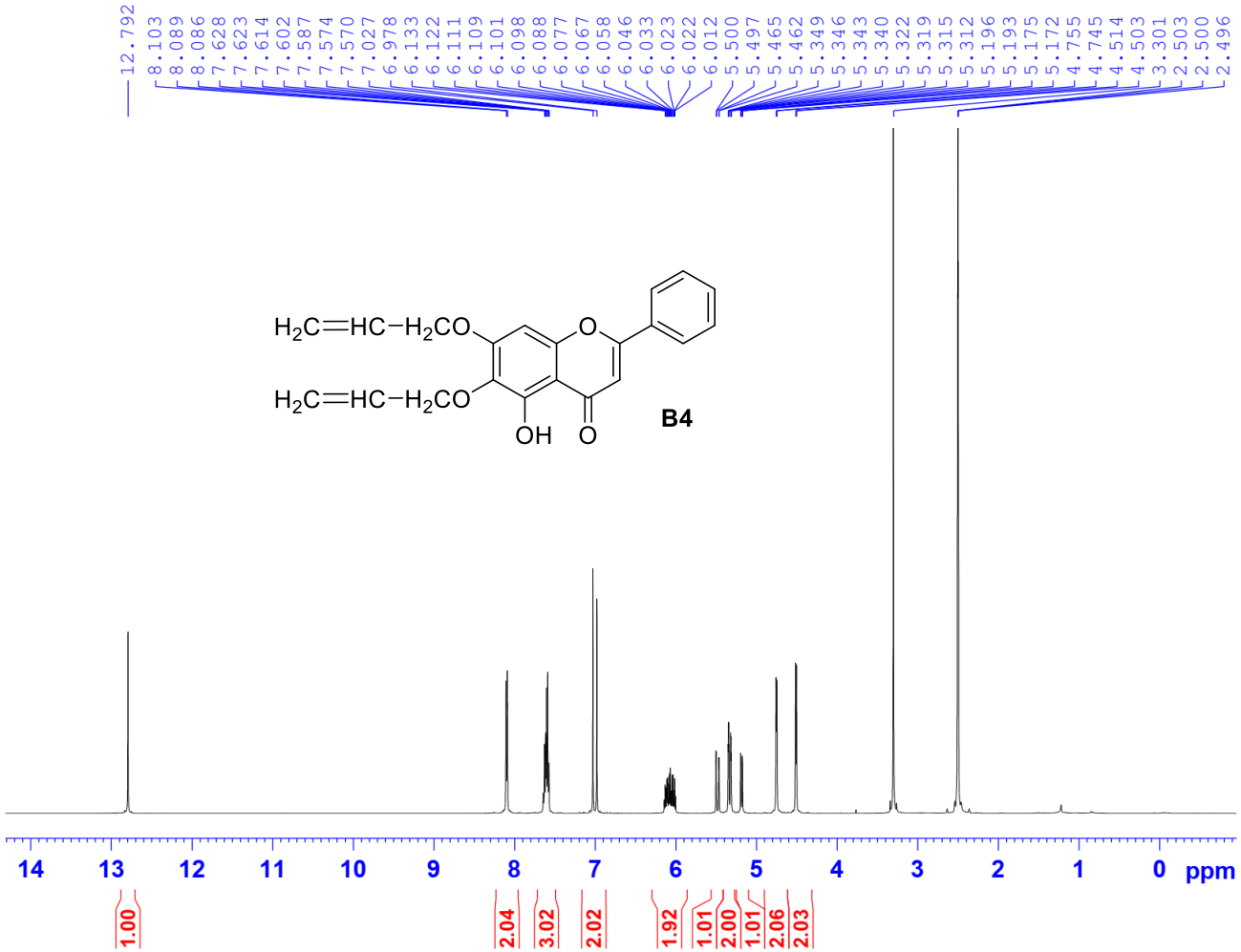
MS

Sample Name	BDAI 6	**Position**	P2-C5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	BDAI 6.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 8:24:25 PM



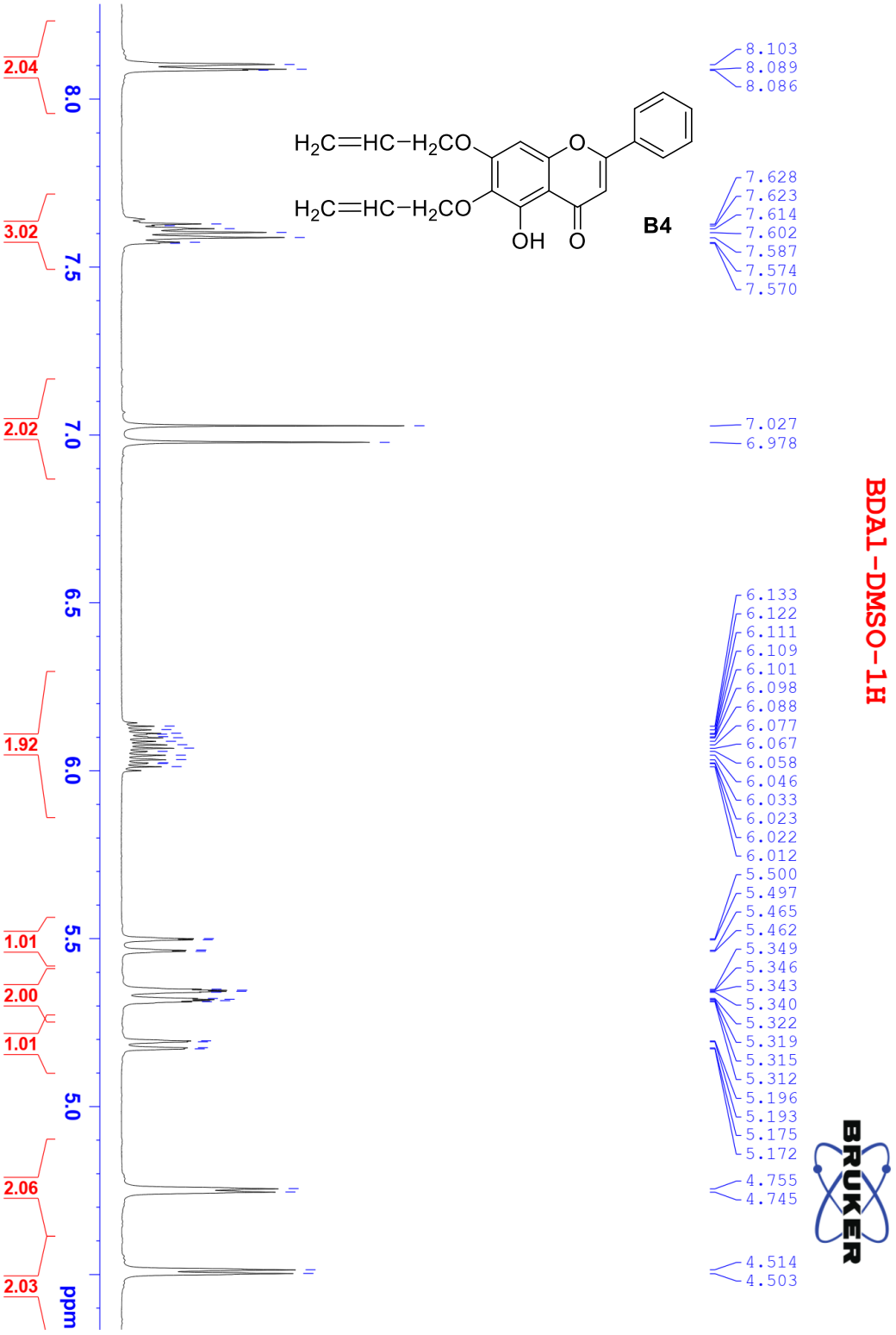
^{1}H-NMR

BDA1-DMSO-1H



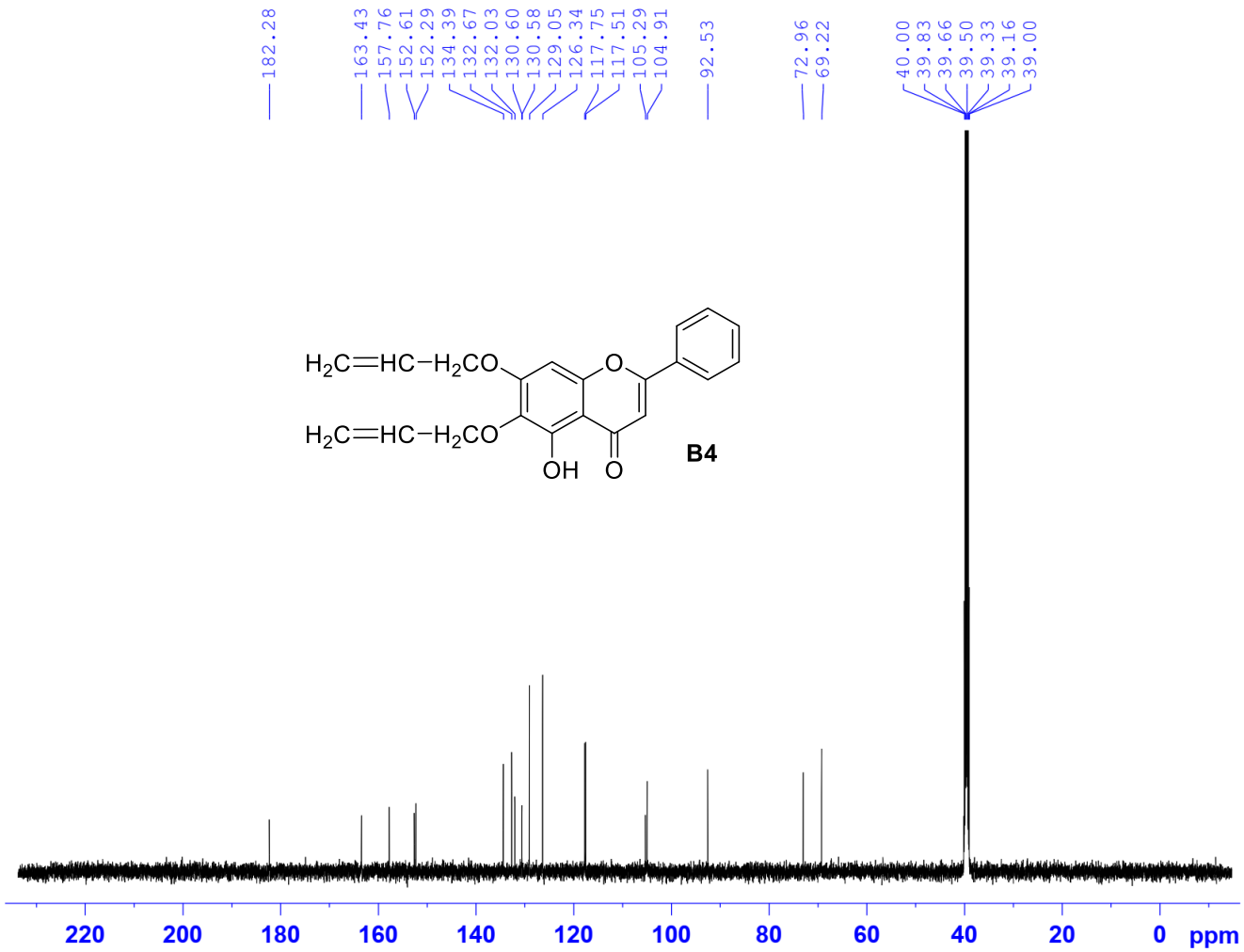

```
Current Data Parameters
NAME        110HUAN_BDA1
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time              11.29
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         500.1920889 MHz
NUC1                 1H
P1                10.20 usec
PLW1        22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.1890052 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{1}H-NMR


2.04
3.02
2.02
1.92
1.01
2.00
1.01
2.06
2.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
ppm
H2C=HC-H2CO
H2C=HC-H2CO
OH
O
O
B4
8.103
8.089
8.086
7.628
7.623
7.614
7.602
7.587
7.574
7.570
7.027
6.978
6.133
6.122
6.111
6.109
6.101
6.098
6.088
6.077
6.067
6.058
6.046
6.033
6.023
6.022
6.012
5.500
5.497
5.465
5.462
5.349
5.346
5.343
5.340
5.322
5.319
5.315
5.312
5.196
5.193
5.175
5.172
4.755
4.745
4.514
4.503
BDA1-DMSO-1H
BRUKER

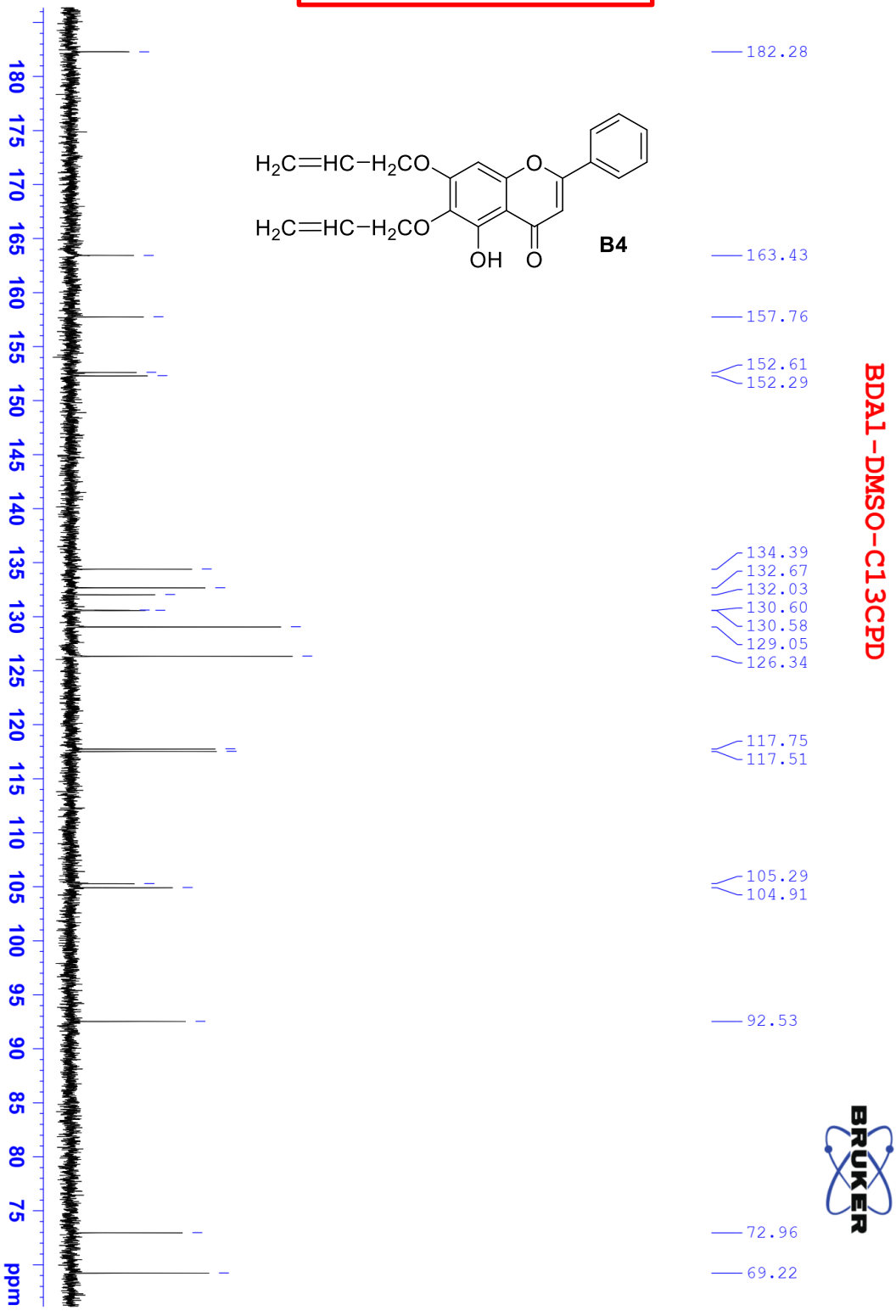
^{13}C-NMR

BDAl-DMSO-C13CPD




```
Current Data Parameters
NAME        110HUAN_BDAl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time               17.15
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                307.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7864591 MHz
NUC1                  13C
P1                 10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.1910008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.35764000 W
PLW13         0.17989001 W

F2 - Processing parameters
SI                 32768
SF           125.7726956 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

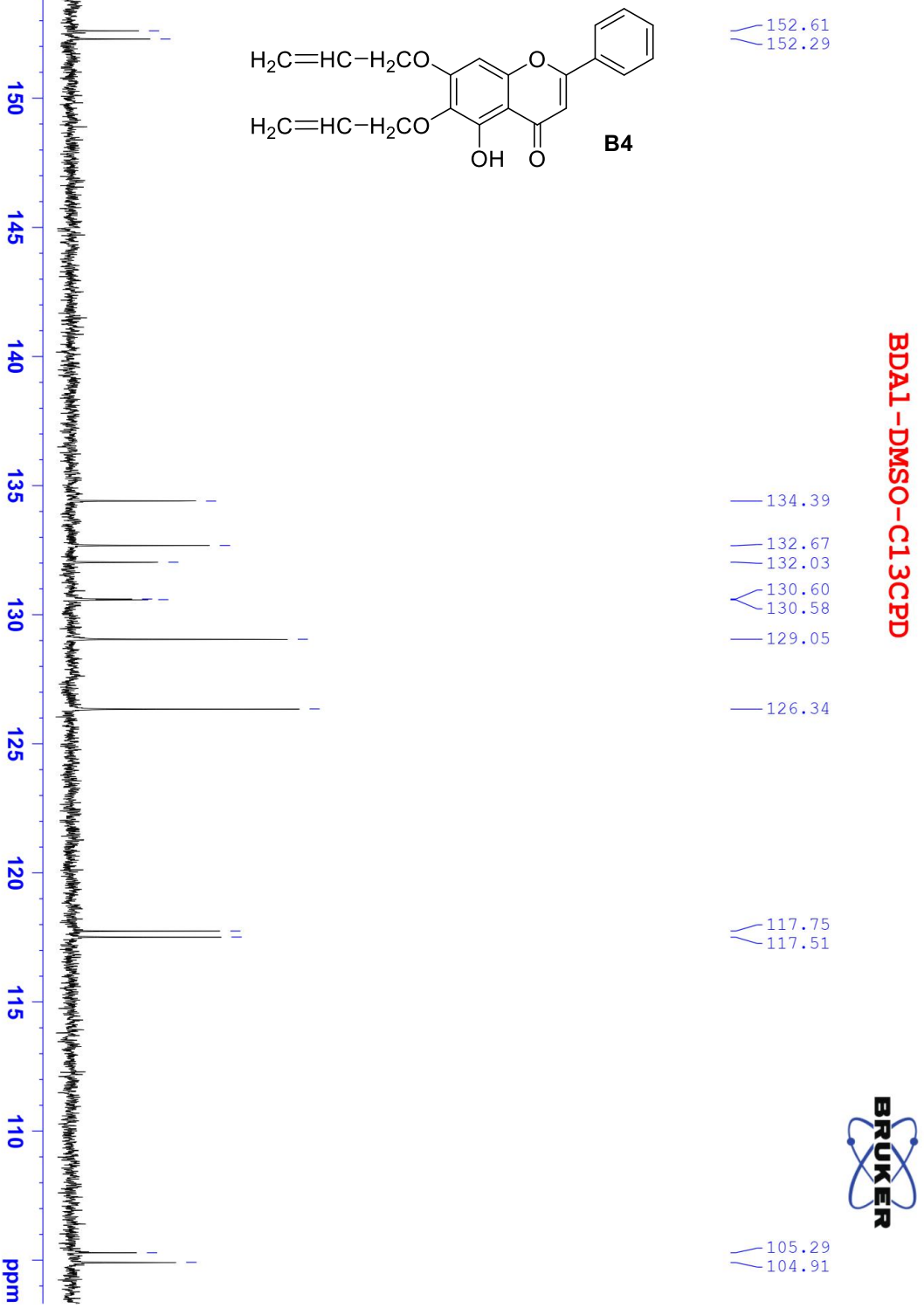
^{13}C-NMR


182.28
163.43
157.76
152.61
152.29
134.39
132.67
132.03
130.60
130.58
129.05
126.34
117.75
117.51
105.29
104.91
92.53
72.96
69.22
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75
ppm
BDA1-DMSO-C13CPD
BRUKER

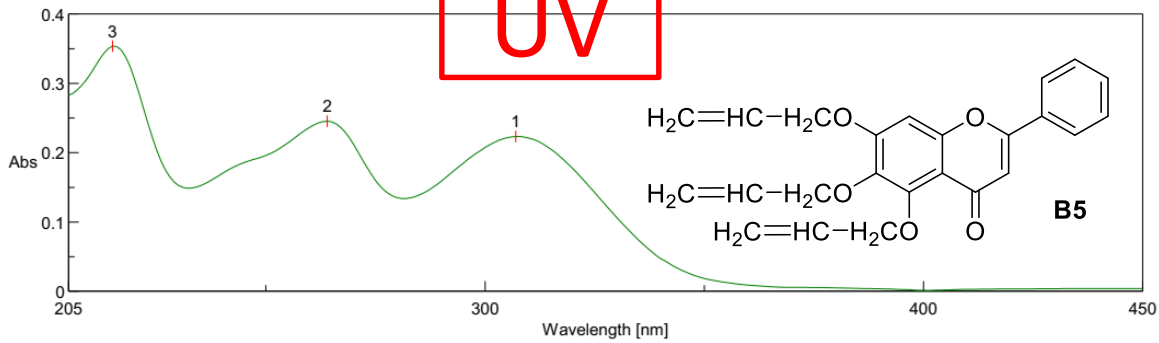
H2C=HC-H2CO
H2C=HC-H2CO
O
OH
O

B4

^{13}C-NMR


H2C=HC–H2CO
H2C=HC–H2CO
O
OH
O
B4
152.61
152.29
134.39
132.67
132.03
130.60
130.58
129.05
126.34
117.75
117.51
105.29
104.91
150
145
140
135
130
125
120
115
110
ppm
BDA1-DMSO-C13CPD
BRUKER

UV

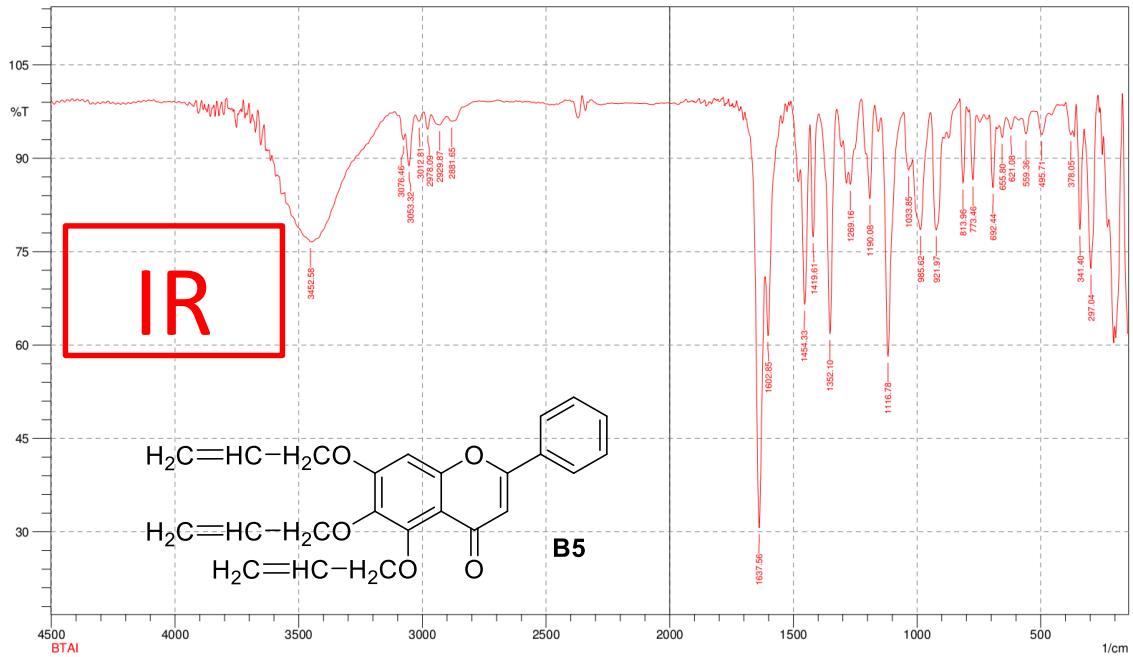


[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	307	0.223122	2	264	0.245246	3	215	0.353469

SHIMADZU

IR



BTAl

Sample name
BTAl

Apodization;
Resolution;
No. of Scans;

Date/Time; 5/8/2020 5:35:02 PM
User; IR-Prestige

MS

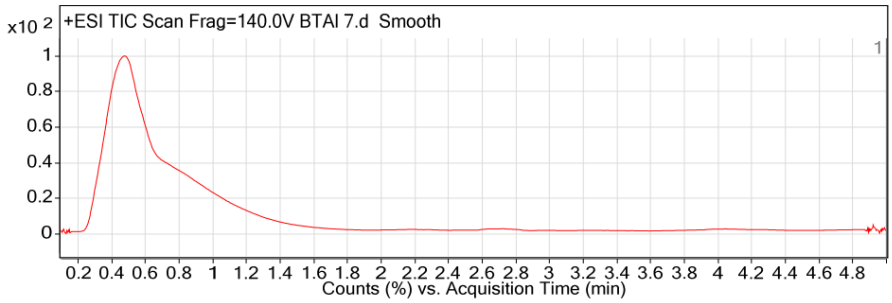
Qualitative Analysis Report

Data Filename	BTAI 7.d	**Sample Name**	BTAI 7
Sample Type	Sample	**Position**	P2-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 8:13:17 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

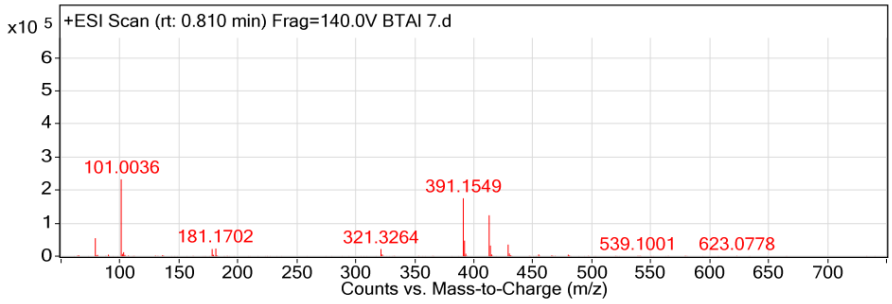
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



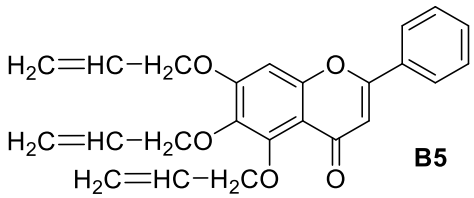
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
79.0213	1	54313.98
101.0036	1	232908.31
391.1549	1	175124.36
392.1574	1	46811.03
413.1363	1	124046.12
803.2834	1	568929.69
804.2872	1	294397.13
805.2892	1	88924.84
819.257	1	166365.66
820.2596	1	80525.21

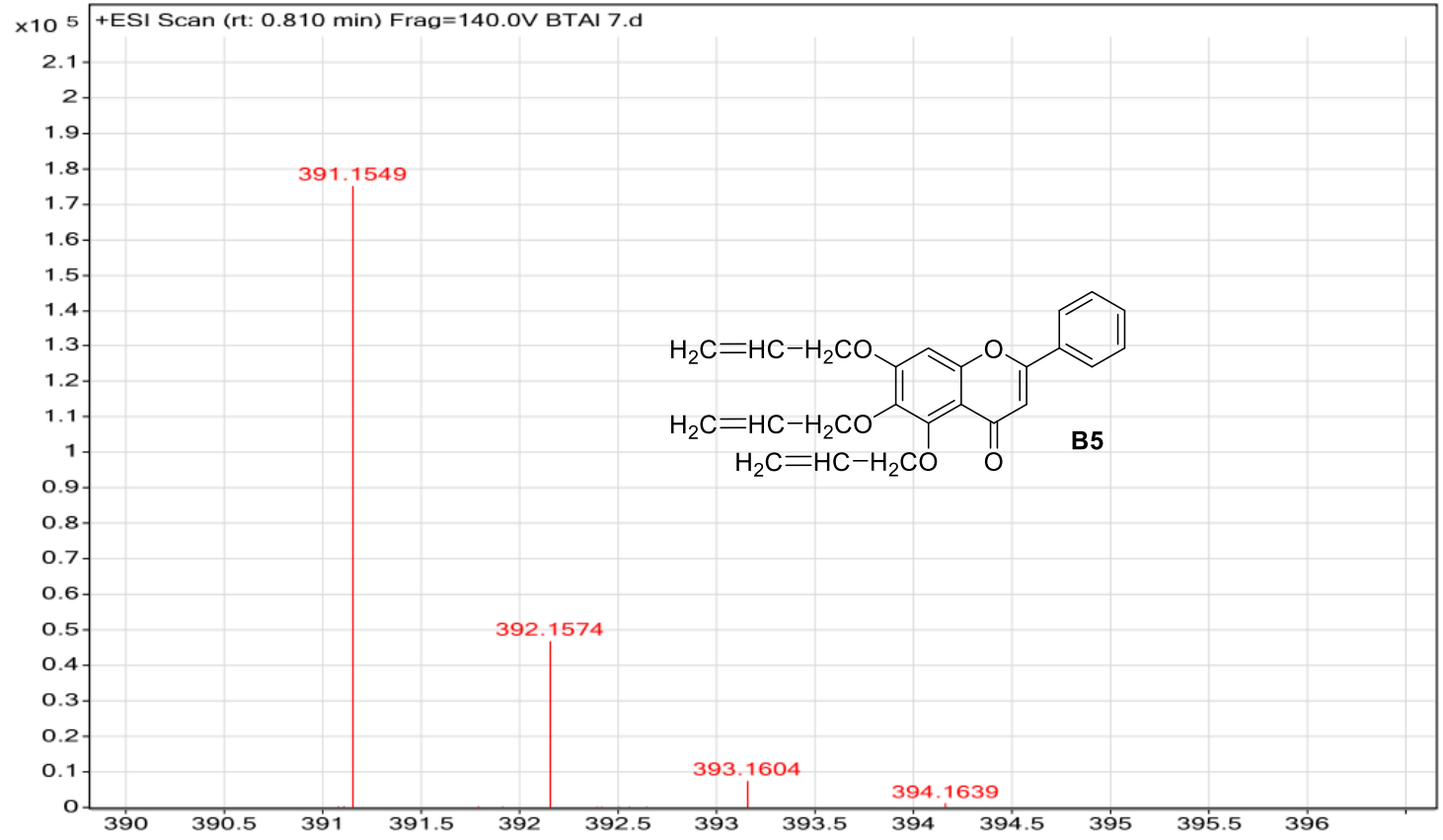


B5

--- End Of Report ---

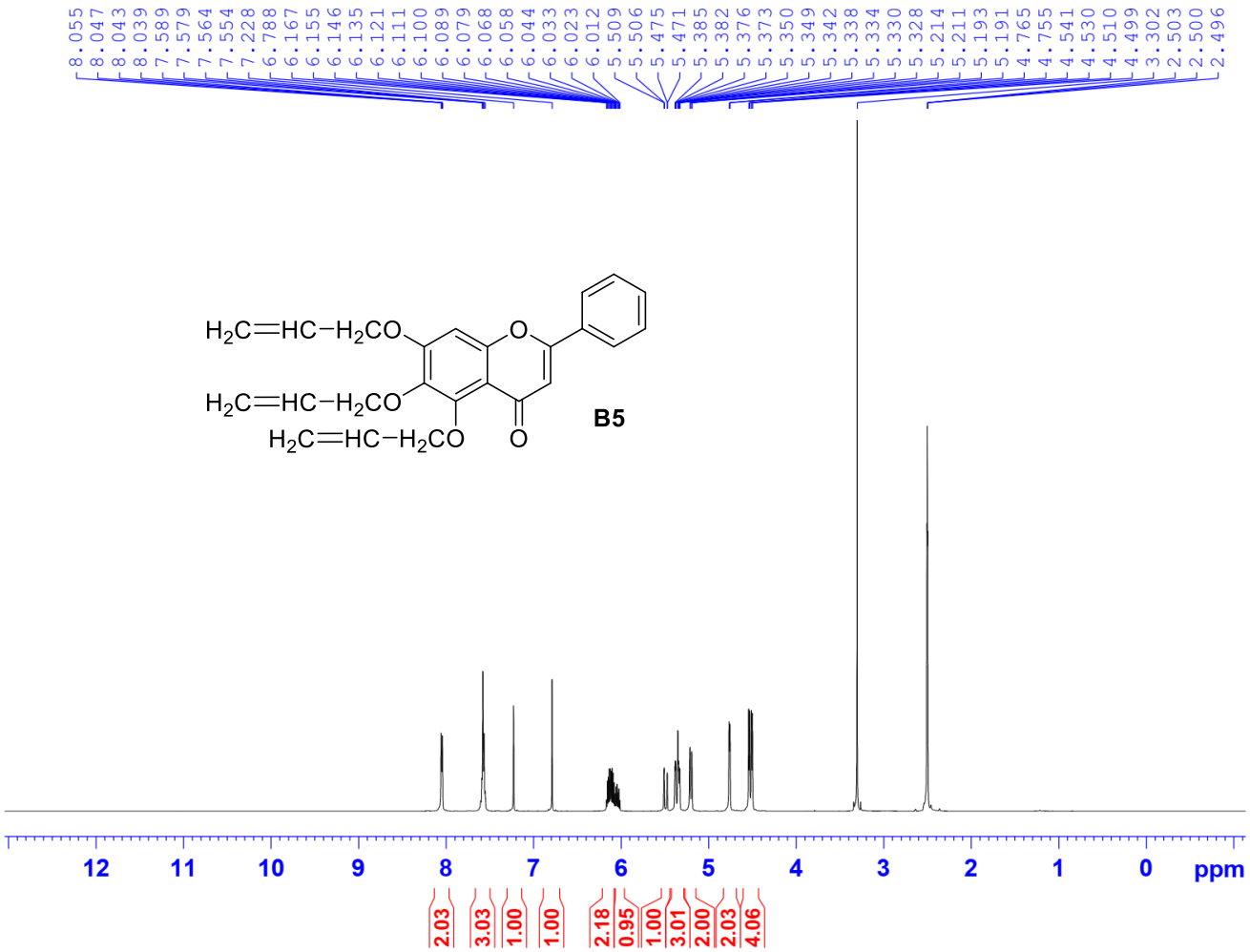
MS

Sample Name	BTAl 7	**Position**	P2-C3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	BTAl 7.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 8:13:17 PM



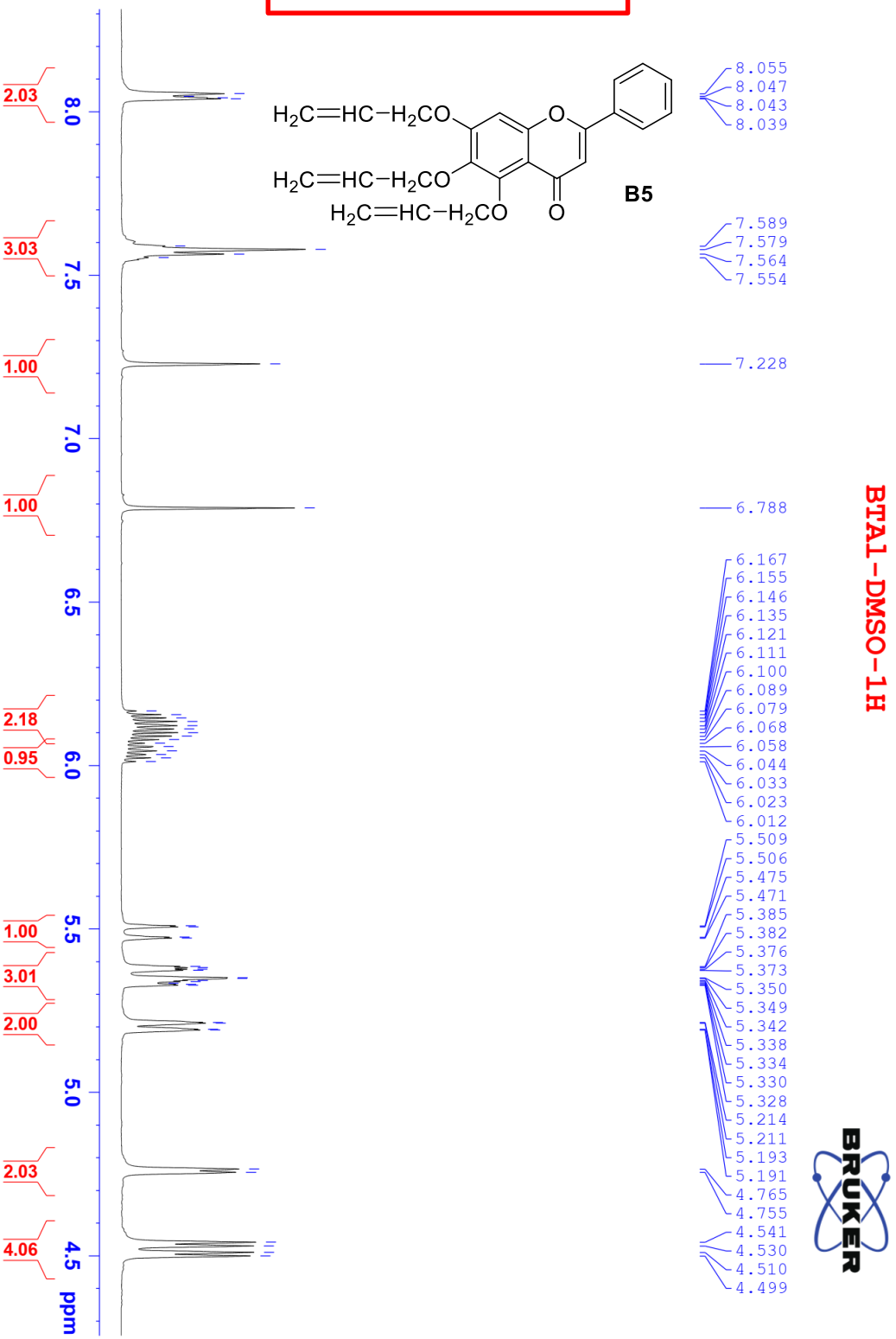
^{1}H-NMR

BTA1-DMSO-1H

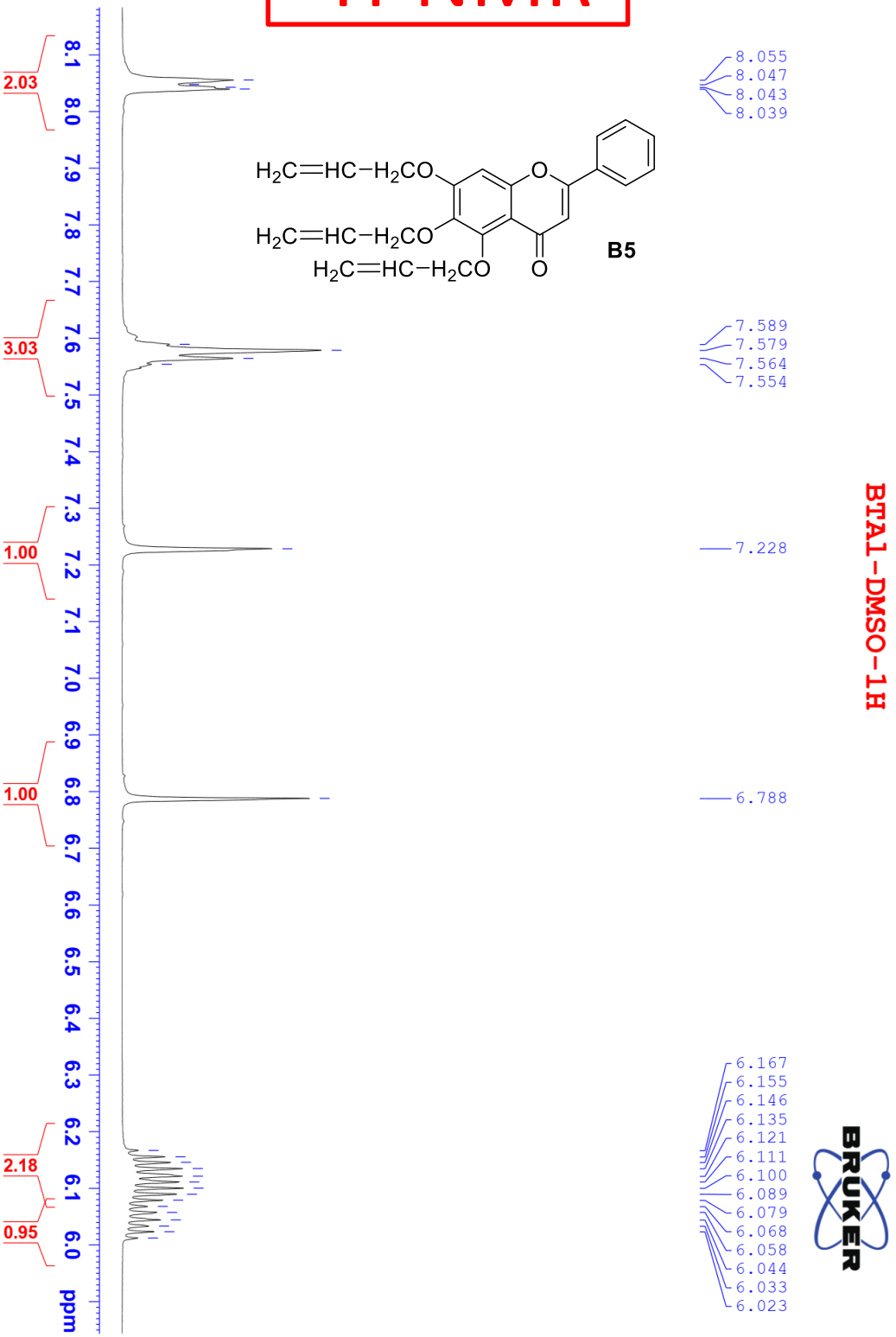



```
Current Data Parameters
NAME        110HUAN_BTA1
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time               11.18
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                 304.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.1920889 MHz
NUC1                  1H
P1                 10.20 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1890053 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H-NMR


2.03
3.03
1.00
1.00
2.18
0.95
1.00
3.01
2.00
2.03
4.06
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
ppm
H2C=HC-H2CO
H2C=HC-H2CO
H2C=HC-H2CO
O
O
B5
8.055
8.047
8.043
8.039
7.589
7.579
7.564
7.554
7.228
6.788
6.167
6.155
6.146
6.135
6.121
6.111
6.100
6.089
6.079
6.068
6.058
6.044
6.033
6.023
6.012
5.509
5.506
5.475
5.471
5.385
5.382
5.376
5.373
5.350
5.349
5.342
5.338
5.334
5.330
5.328
5.214
5.211
5.193
5.191
4.765
4.755
4.541
4.530
4.510
4.499
BTA1-DMSO-1H
BRUKER

^{1}H-NMR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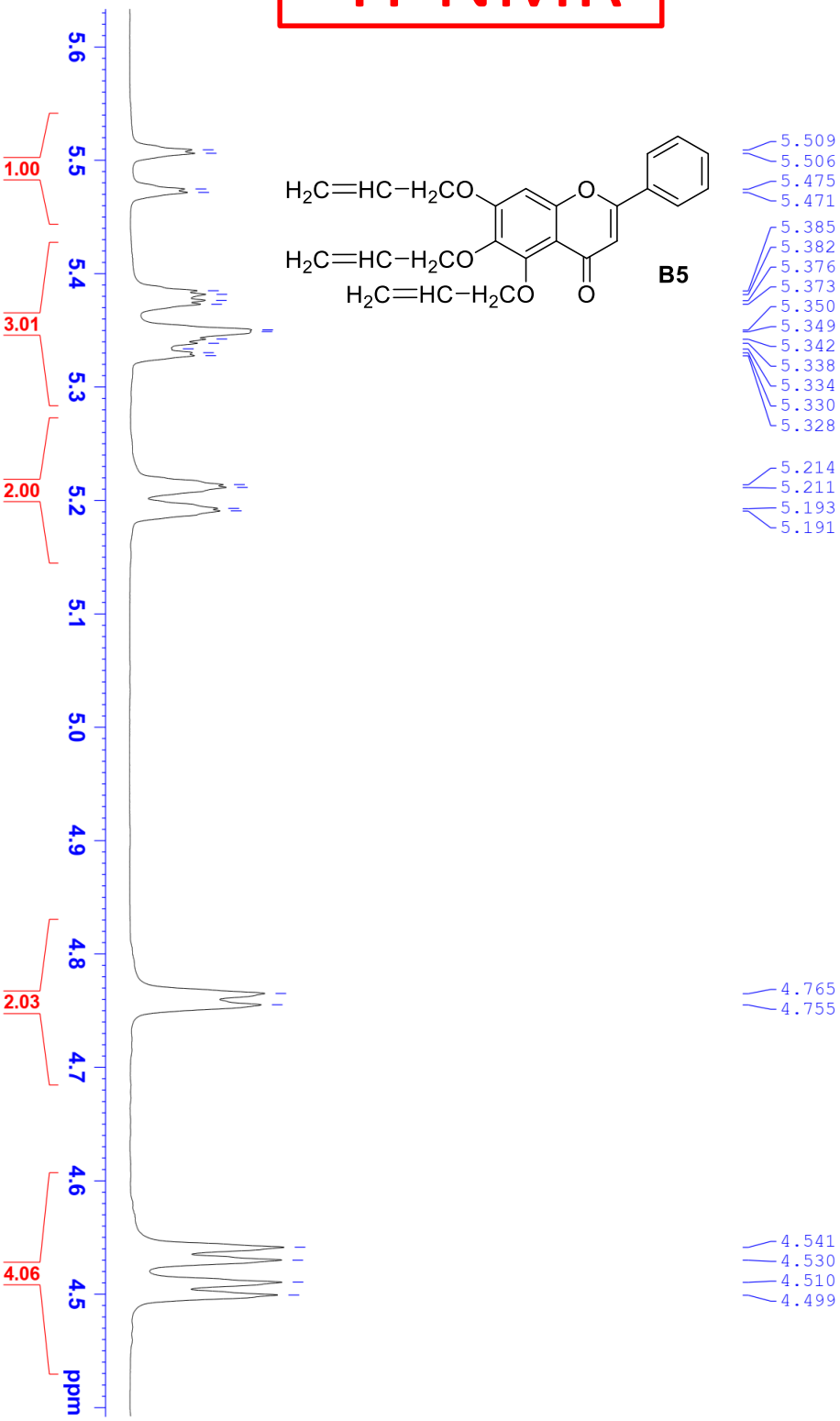
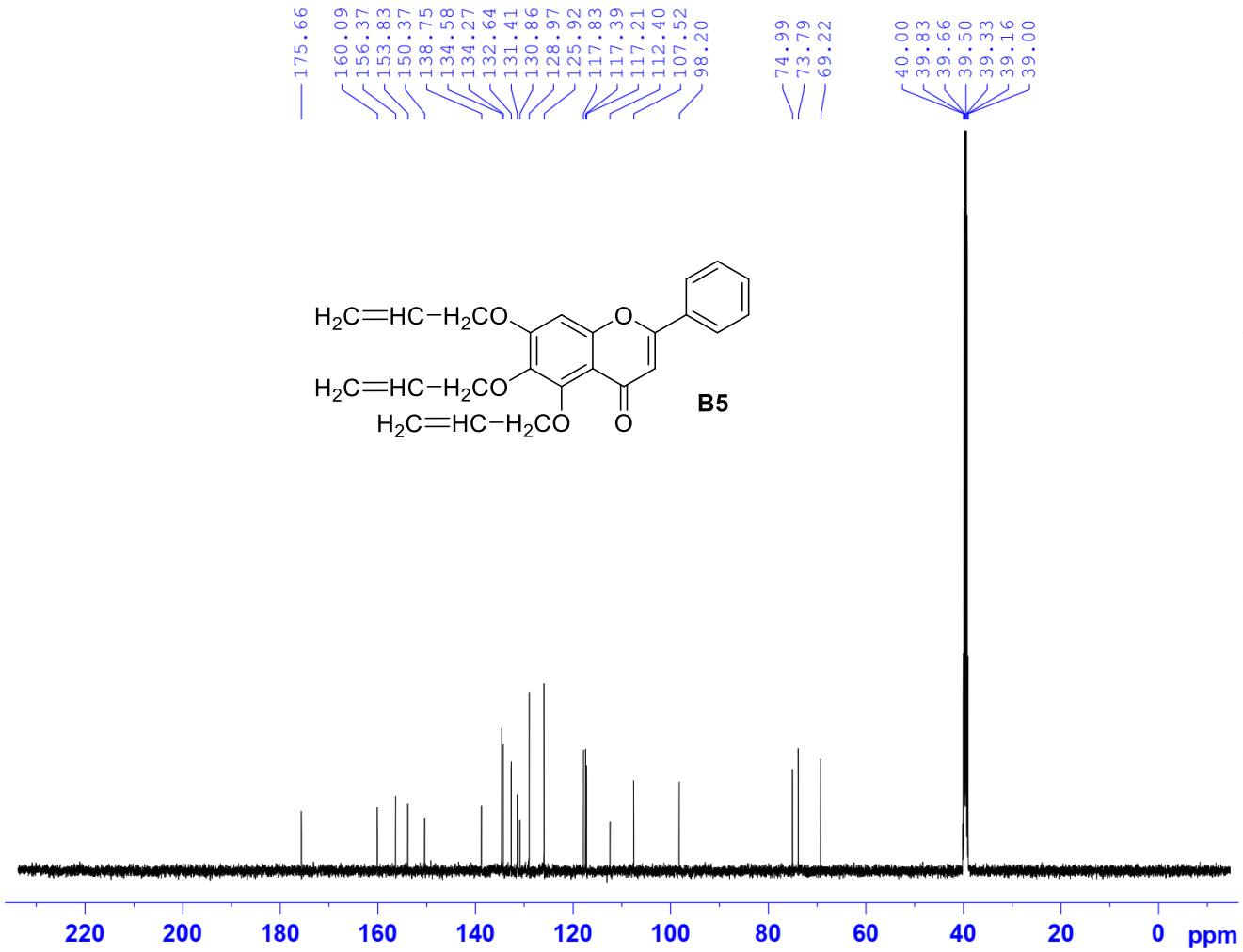
8.047
8.043
8.039
7.589
7.579
7.564
7.554
7.228
6.788
6.167
6.155
6.146
6.135
6.121
6.111
6.100
6.089
6.079
6.068
6.058
6.044
6.033
6.023
2.03
3.03
1.00
1.00
2.18
0.95
ppm
B5
BTA1-DMSO-1H
BRUKER

^{1}H-NMR


5.6
5.5
5.4
5.3
5.2
5.1
5.0
4.9
4.8
4.7
4.6
4.5
ppm
1.00
3.01
2.00
2.03
4.06
H2C=HC-H2CO
H2C=HC-H2CO
H2C=HC-H2CO
O
O
B5
5.509
5.506
5.475
5.471
5.385
5.382
5.376
5.373
5.350
5.349
5.342
5.338
5.334
5.330
5.328
5.214
5.211
5.193
5.191
4.765
4.755
4.541
4.530
4.510
4.499
BTA1-DMSO-1H
BRUKER

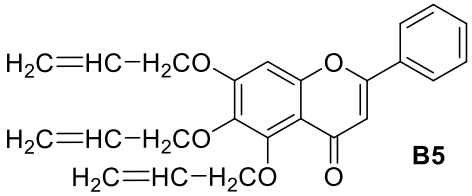
^{13}C-NMR

BTAl-DMSO-C13CPD



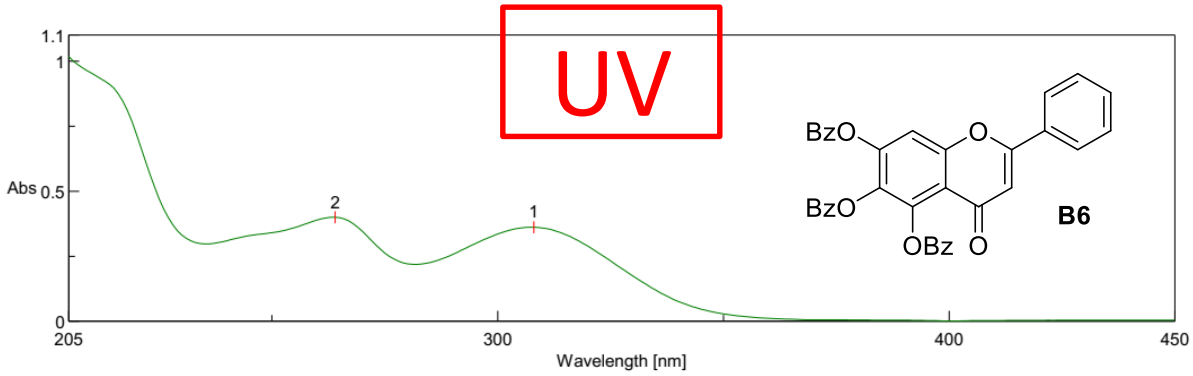

```
Current Data Parameters
NAME        110HUAN_BTAl
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time               13.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
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                305.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7864591 MHz
NUC1                  13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.1910008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.35764000 W
PLW13         0.17989001 W

F2 - Processing parameters
SI                 32768
SF           125.7726941 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{13}C-NMR


H2C=HC–H2CO
H2C=HC–H2CO
H2C=HC–H2CO
O
O

B5

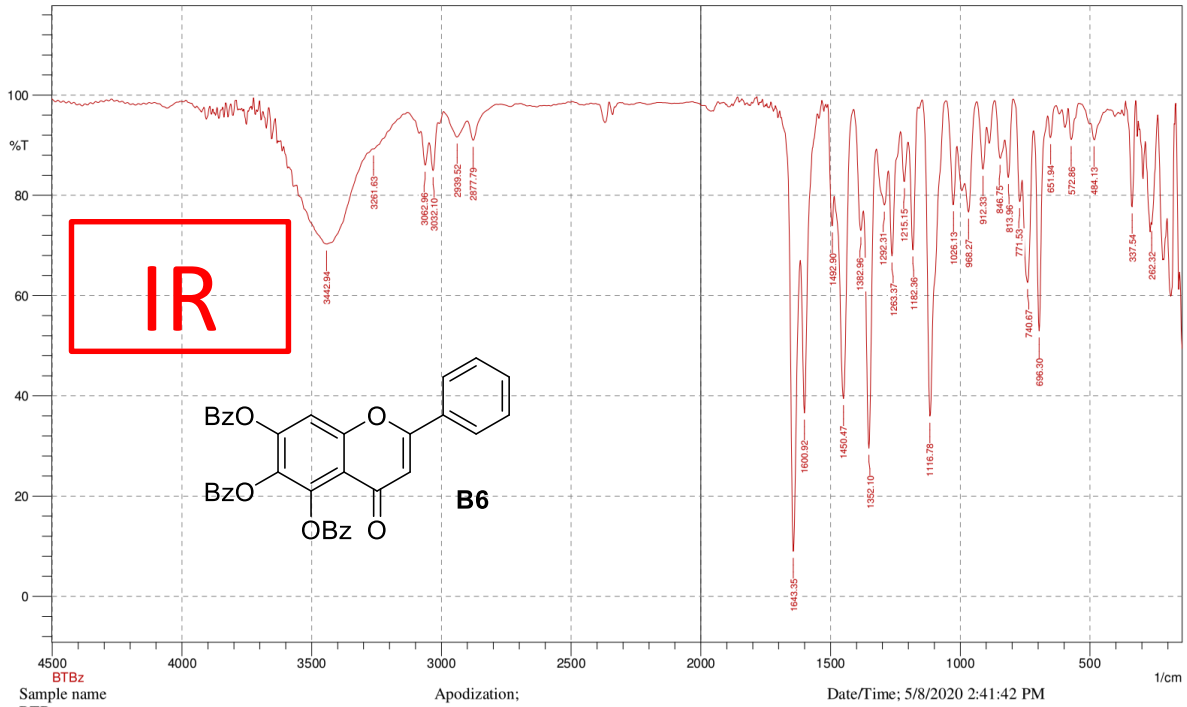
175.66
160.09
156.37
153.83
150.37
138.75
134.58
134.27
132.64
131.41
130.86
128.97
125.92
117.83
117.39
117.21
112.40
107.52
98.20
74.99
73.79
69.22
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75
ppm
BTA1-DMSO-C13CPD
BRUKER



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	308	0.361351	2	264	0.399643			

SHIMADZU



BTBz

Sample name
BTBz

Apodization;
Resolution;
No. of Scans;

Date/Time; 5/8/2020 2:41:42 PM
User; IR-Prestige

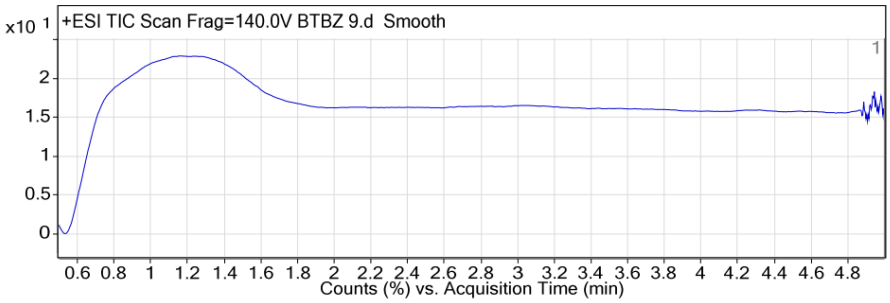
MS

Qualitative Analysis Report

Data Filename	BTBZ 9.d	**Sample Name**	BTBZ 9
Sample Type	Sample	**Position**	P2-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 8:07:43 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

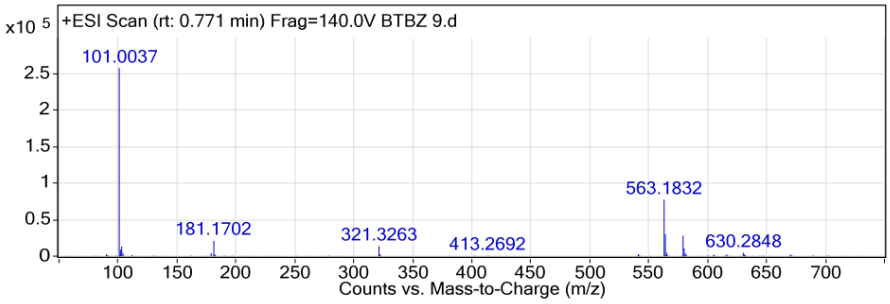
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



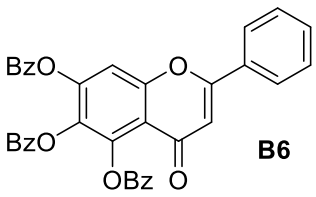
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
101.0037	1	258011.27
102.006	1	8774.61
102.9991	1	13193.66
181.1702	1	20953.3
321.3263	1	13905.09
563.1832	1	77298.47
564.1861	1	30128.7
579.1568	1	28046.29
580.1599	1	10937.76
630.2848	1	4755.01

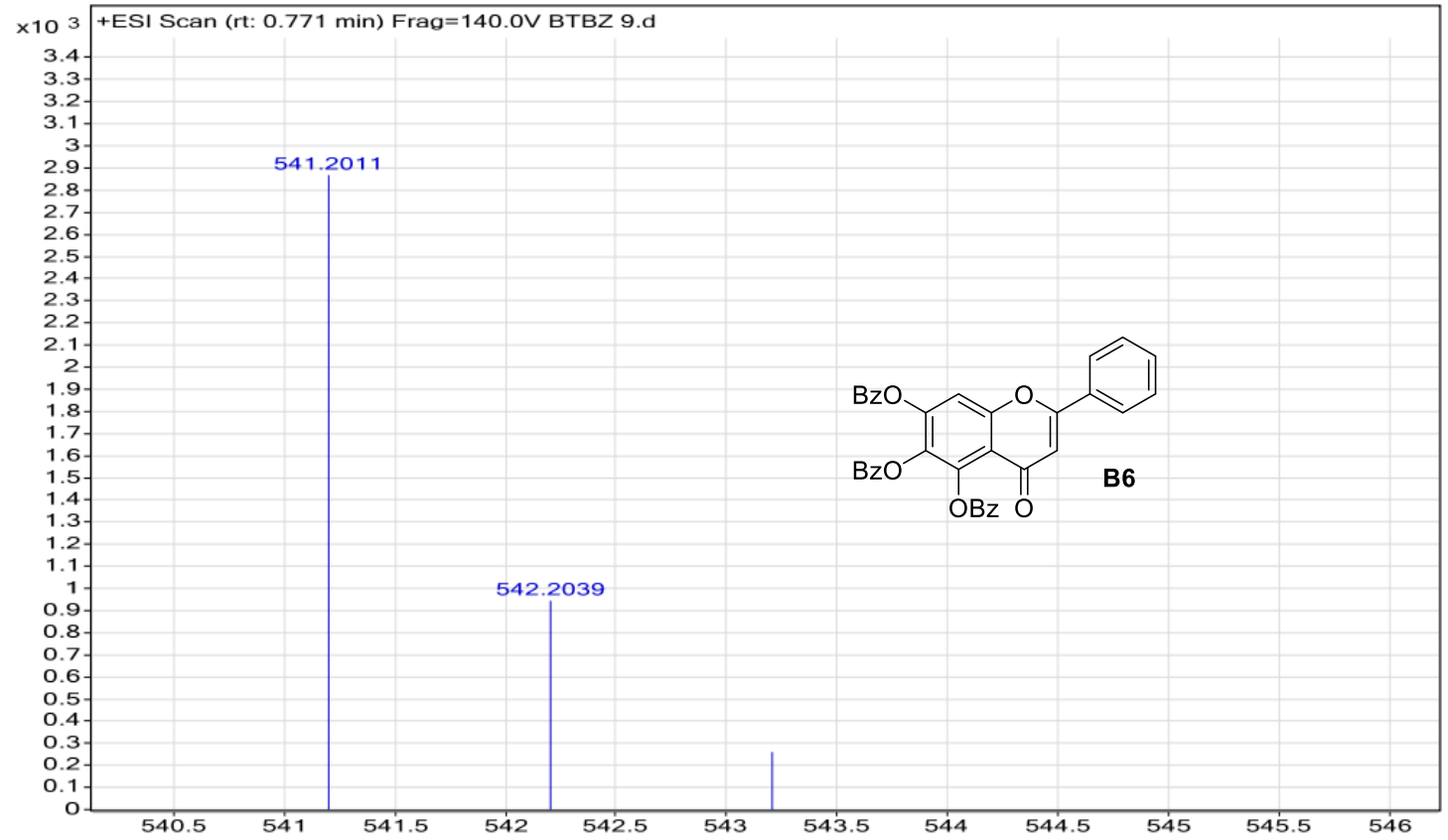


B6

--- End Of Report ---

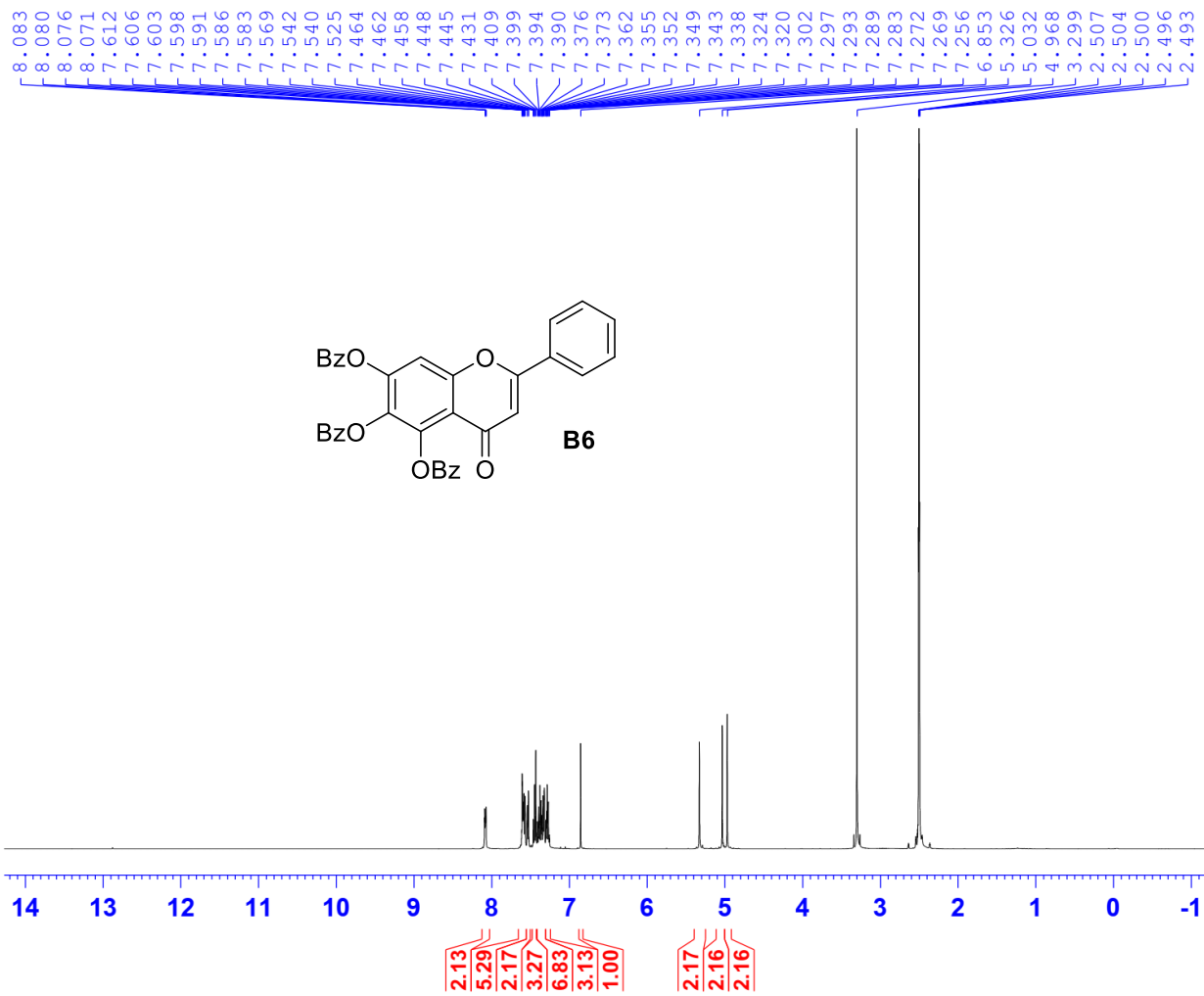
MS

Sample Name	BTBZ 9	**Position**	P2-C2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	BTBZ 9.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 8:07:43 PM



^{1}H-NMR

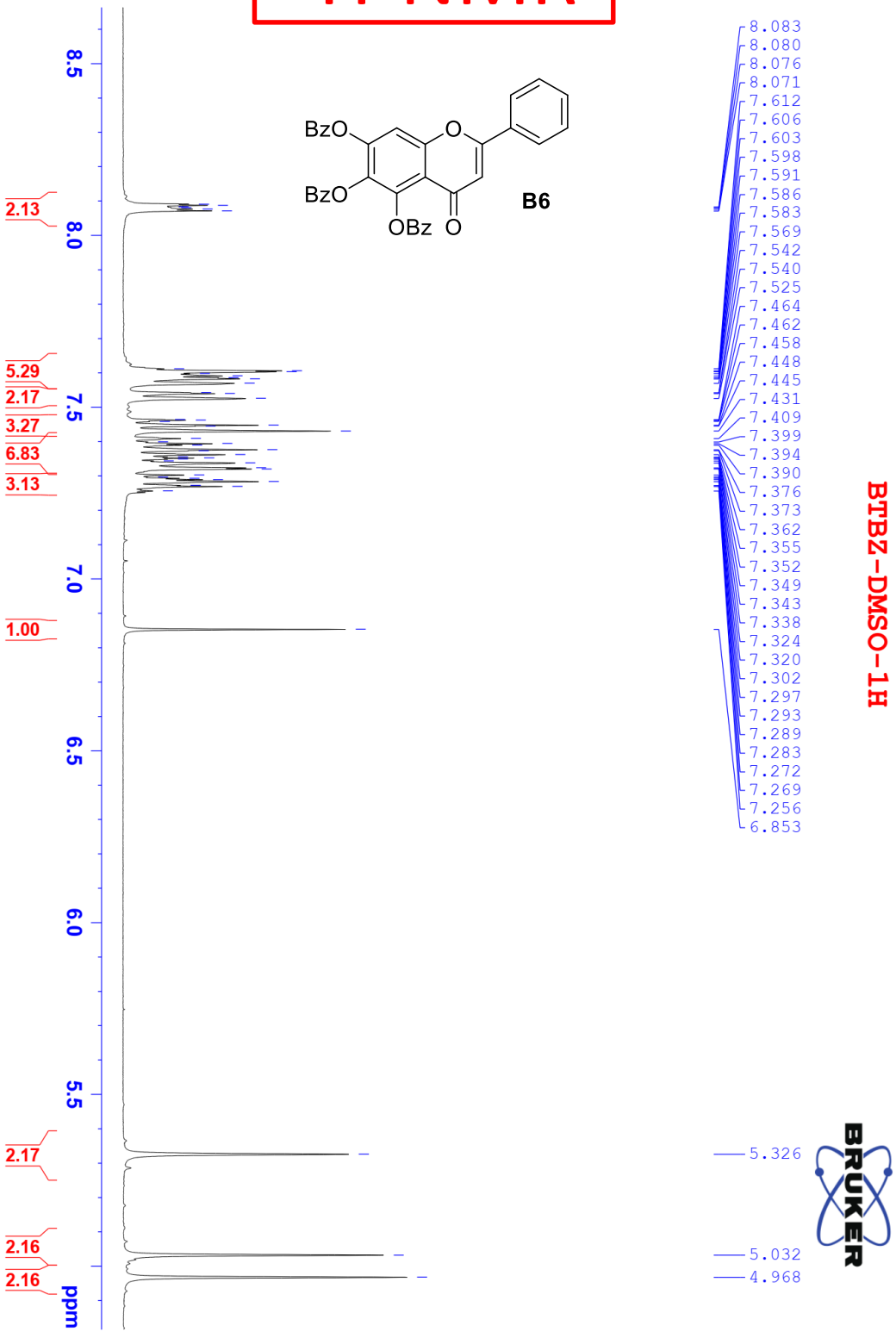
BTBZ-DMSO-1H



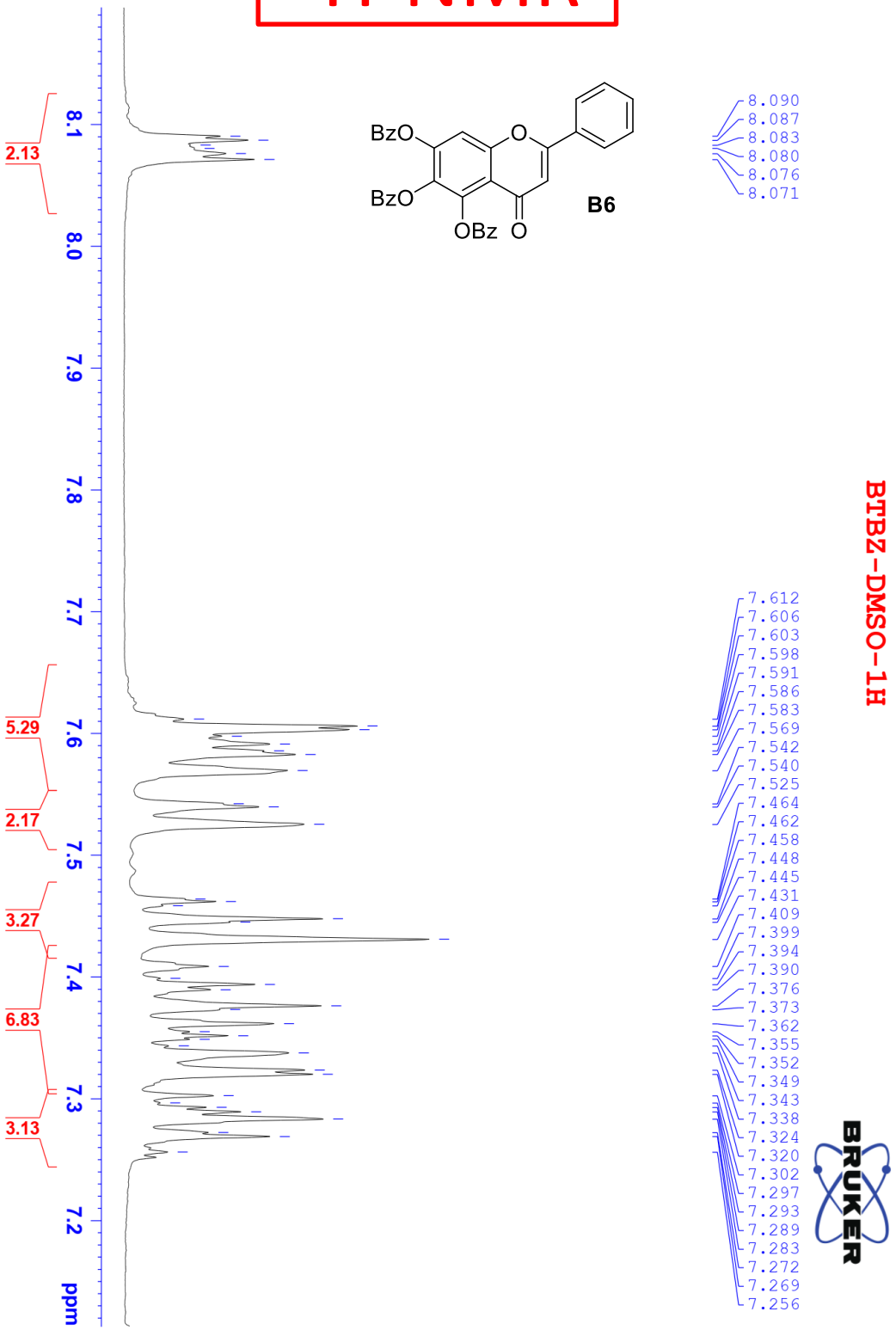
BRUKER

```
Current Data Parameters
NAME        110HUAN_BTBZ
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time              11.25
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                157.35
DW                50.000 usec
DE                 6.50 usec
TE                303.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.1920889 MHz
NUC1                  1H
P1                10.20 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                65536
SF            500.1890048 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H-NMR


BzO
BzO
OBz
O
O
B6
8.083
8.080
8.076
8.071
7.612
7.606
7.603
7.598
7.591
7.586
7.583
7.569
7.542
7.540
7.525
7.464
7.462
7.458
7.448
7.445
7.431
7.409
7.399
7.394
7.390
7.376
7.373
7.362
7.355
7.352
7.349
7.343
7.338
7.324
7.320
7.302
7.297
7.293
7.289
7.283
7.272
7.269
7.256
6.853
5.326
5.032
4.968
2.13
5.29
2.17
3.27
6.83
3.13
1.00
2.17
2.16
2.16
8.5
8.0
7.5
7.0
6.5
6.0
5.5
ppm
BTBZ-DMSO-1H
BRUKER

^{1}H-NMR


BzO
BzO
OBz
O
O
B6
8.090
8.087
8.083
8.080
8.076
8.071
7.612
7.606
7.603
7.598
7.591
7.586
7.583
7.569
7.542
7.540
7.525
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7.458
7.448
7.445
7.431
7.409
7.399
7.394
7.390
7.376
7.373
7.362
7.355
7.352
7.349
7.343
7.338
7.324
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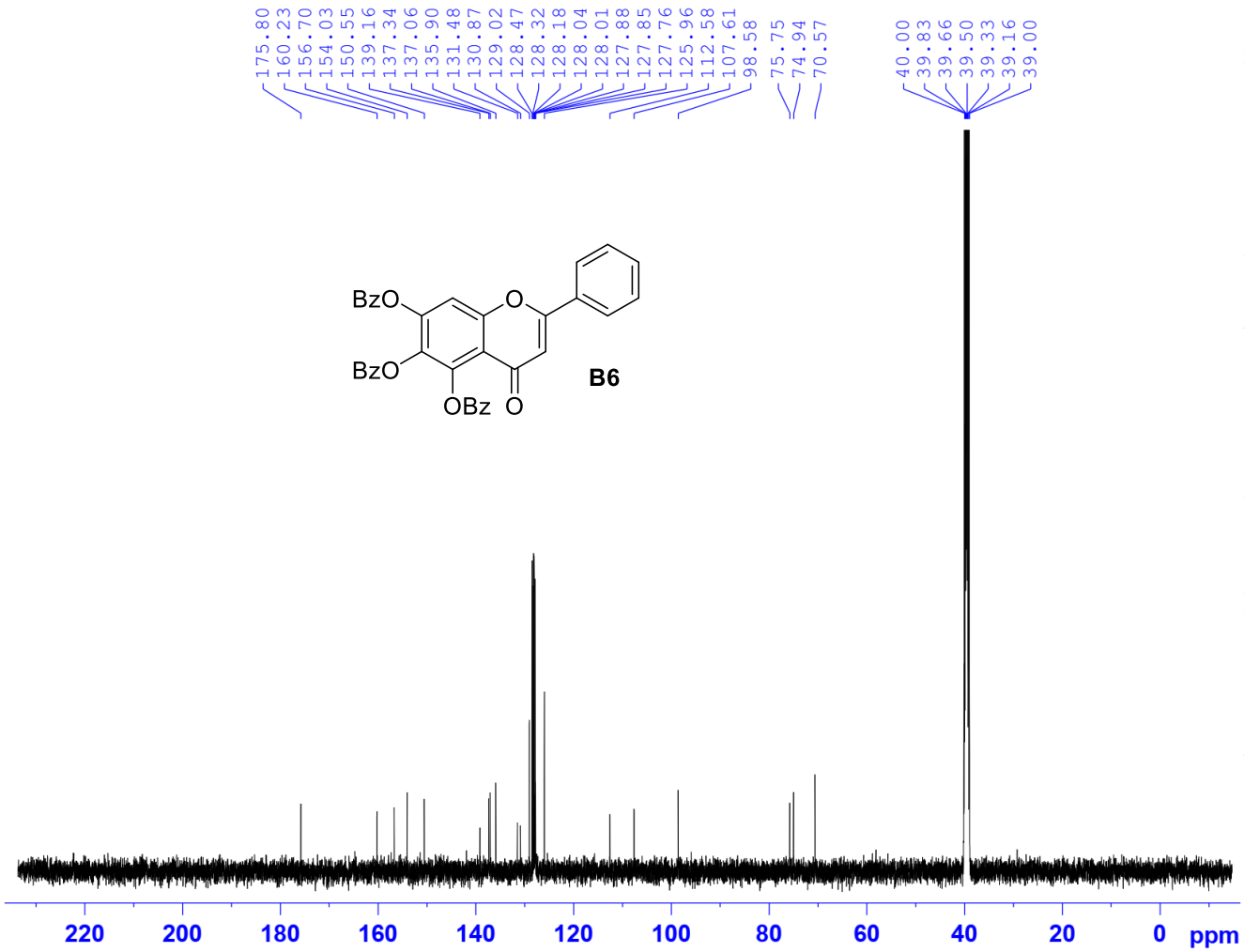
7.302
7.297
7.293
7.289
7.283
7.272
7.269
7.256
2.13
5.29
2.17
3.27
6.83
3.13
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
BTBZ-DMSO-1H
BRUKER

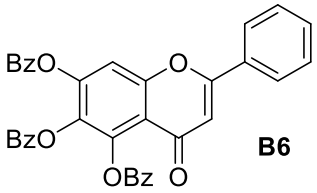
^{13}C-NMR

BTBZ-DMSO-C13CPD




```
Current Data Parameters
NAME        110HUAN_BTBZ
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191126
Time               12.04
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                305.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7864591 MHz
NUC1                  13C
P1                 10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.1910008 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.35764000 W
PLW13         0.17989001 W

F2 - Processing parameters
SI                 32768
SF           125.7726241 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{13}C-NMR

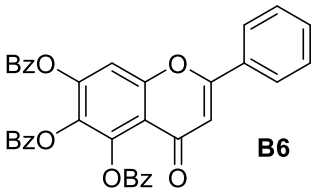


B6

BTBZ-DMSO-C13CPD

BRUKER

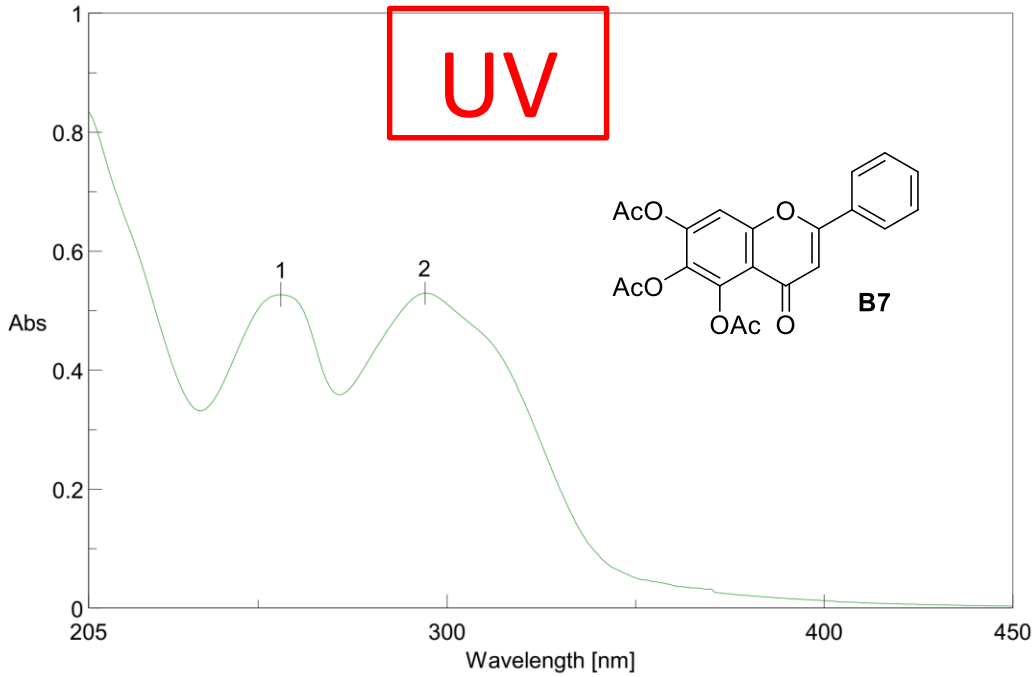
^{13}C-NMR



B6

BTBZ-DMSO-C13CPD

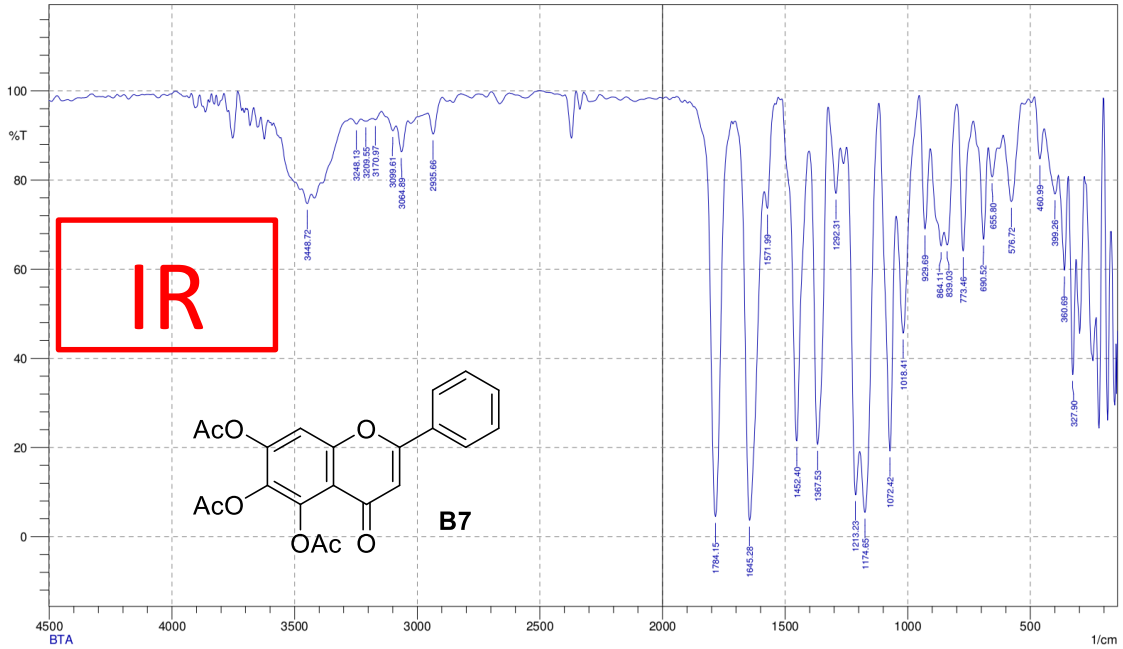
BRUKER



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	256	0.526452	2	294	0.529178

SHIMADZU



BTA

Sample name
BTA

Apodization;
Resolution;
No. of Scans;

Date/Time; 5/11/2020 2:02:26 PM
User; IR-Prestige

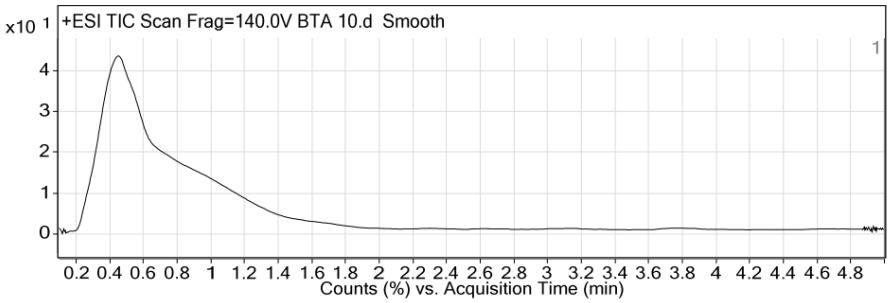
MS

Qualitative Analysis Report

Data Filename	BTA 10.d	**Sample Name**	BTA 10
Sample Type	Sample	**Position**	P2-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 7:12:04 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

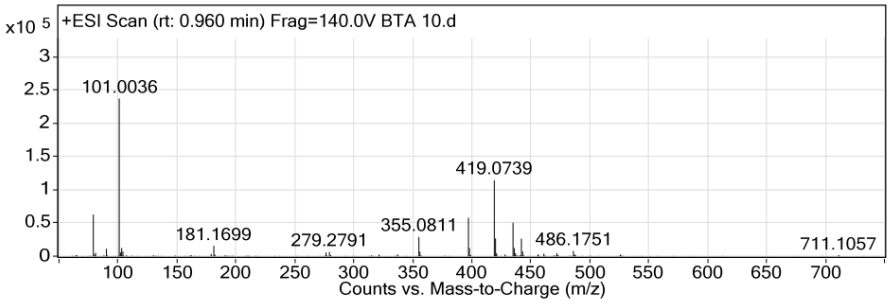
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



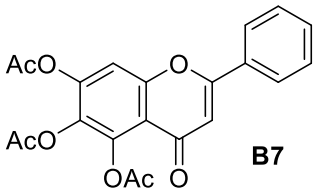
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
79.0213	1	62825.86
101.0036	1	237001.98
397.0916	1	57811.62
419.0739	1	114020.98
435.0476	1	50508.92
815.1593	1	282822.72
816.1616	1	139684.63
831.133	1	223102.61
832.1356	1	108772.73
833.1357	1	42507.65

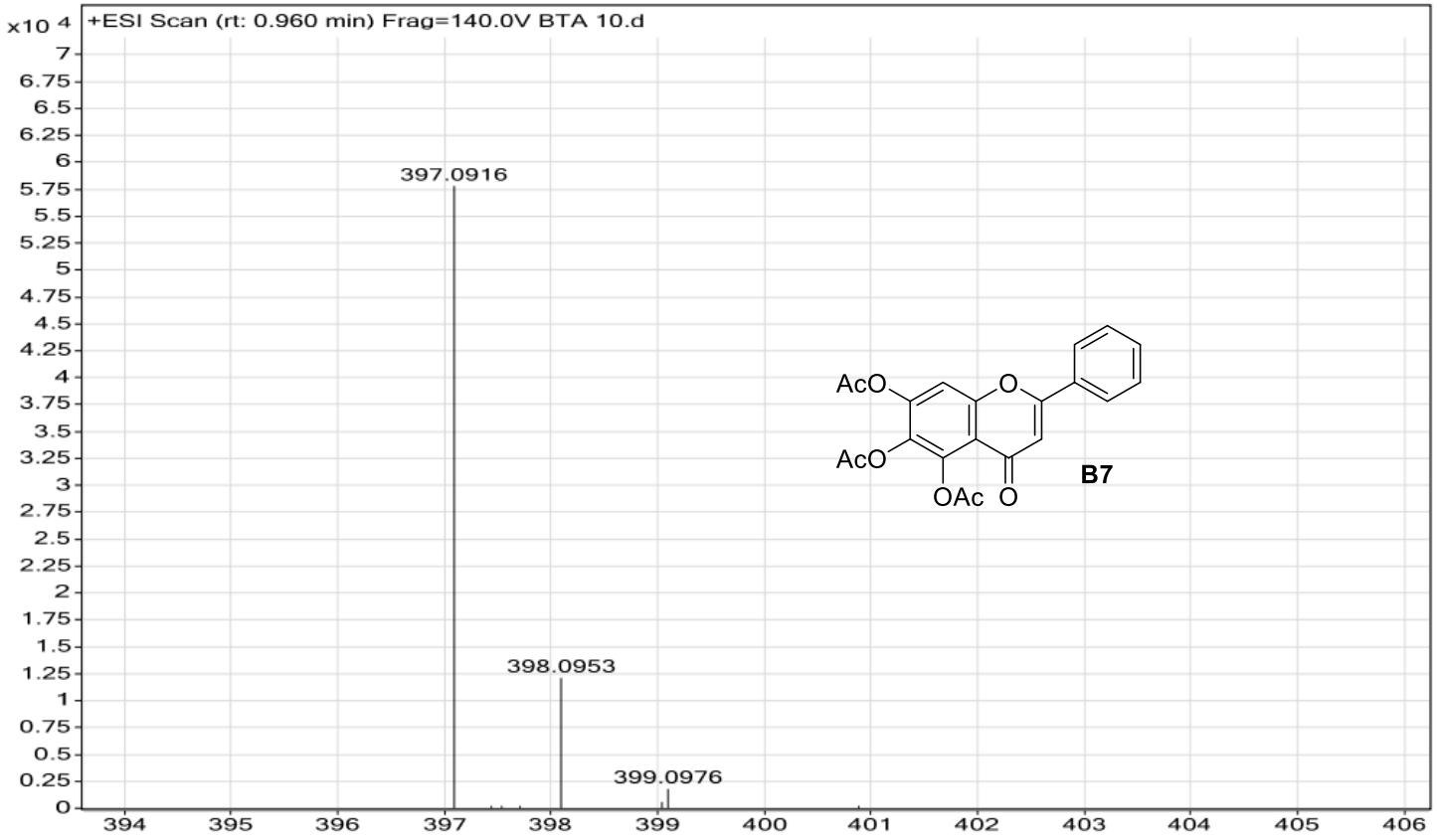


B7

--- End Of Report ---

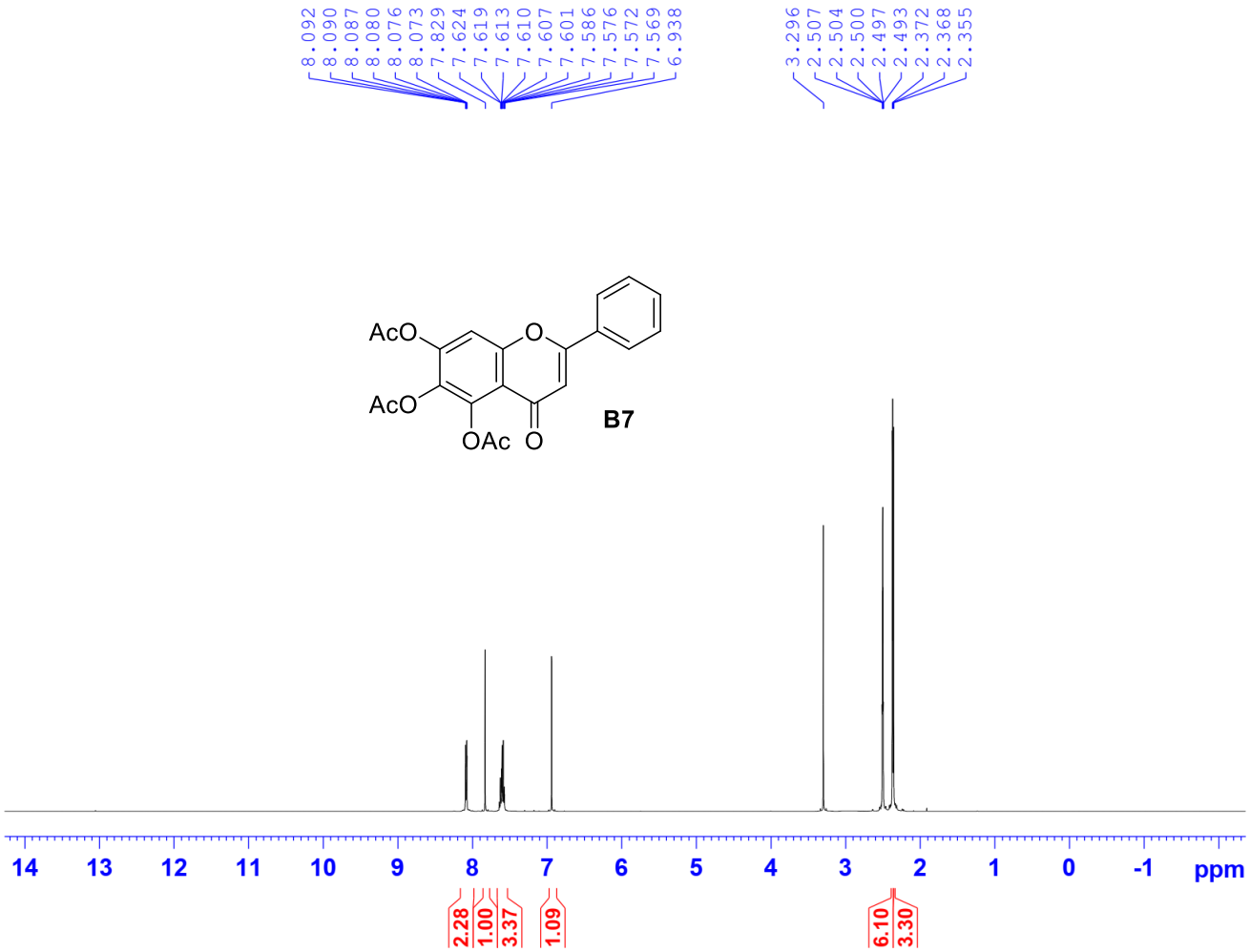
MS

Sample Name	BTA 10	**Position**	P2-B1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	BTA 10.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 7:12:04 PM



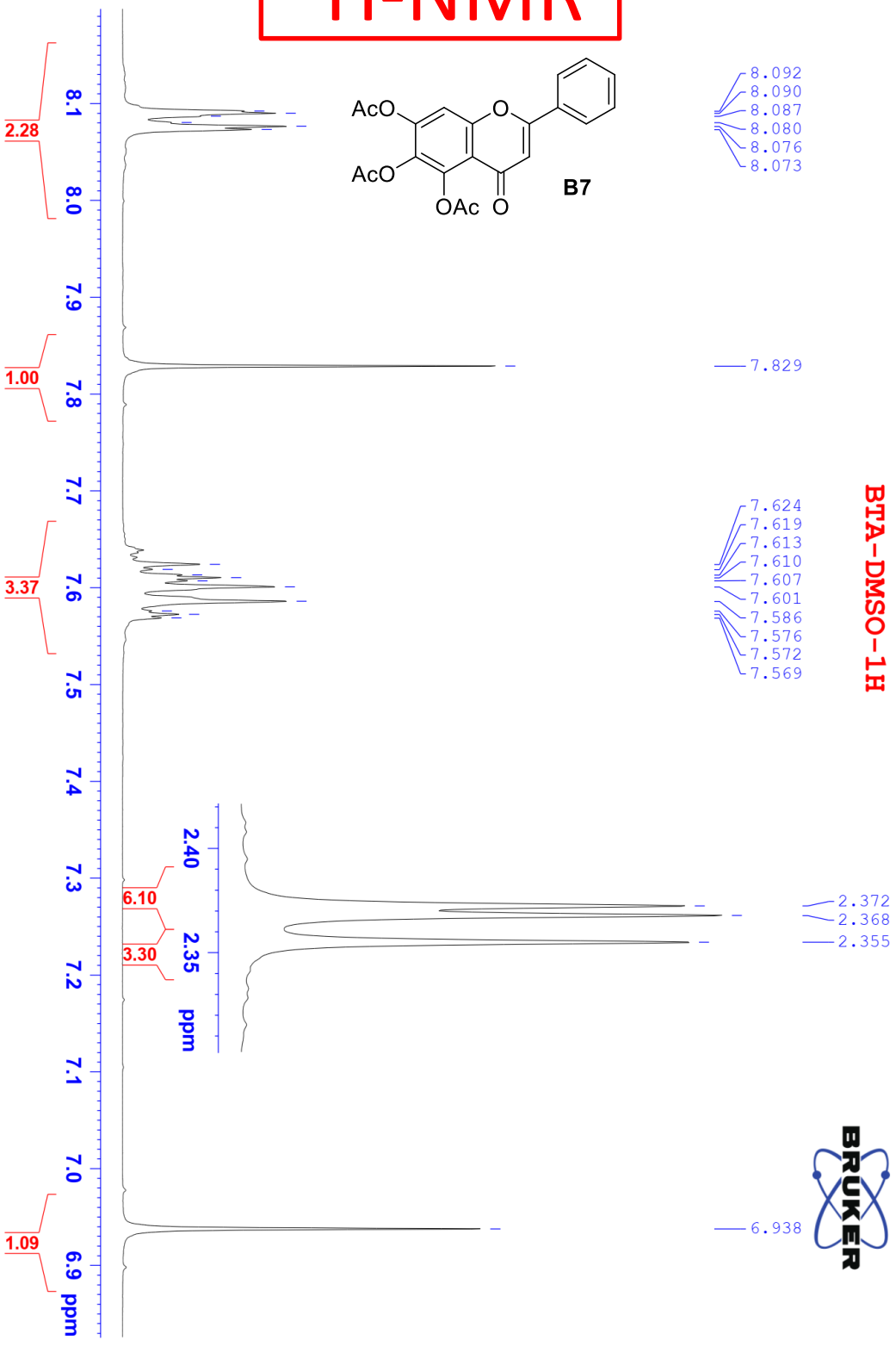
^{1}H-NMR

BTA-DMSO-1H



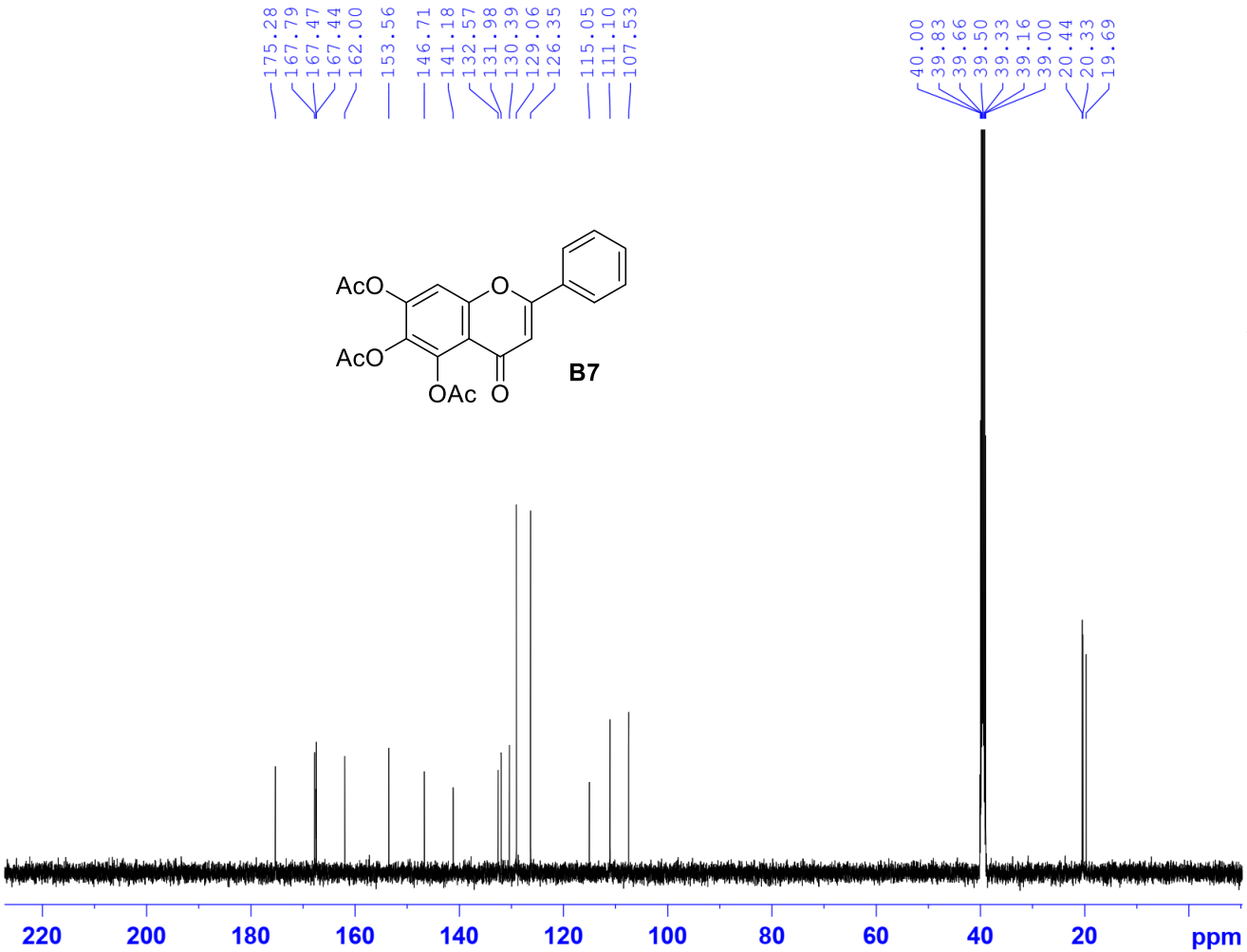

```
Current Data Parameters
NAME         113HUAN_BTA
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191008
Time              12.03
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                304.7 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1920889 MHz
NUC1                   1H
P1                10.20 usec
PLW1        22.00000000 W

F2 - Processing parameters
SI                65536
SF           500.1890048 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H-NMR


AcO
AcO
OAc
O
O
B7
8.092
8.090
8.087
8.080
8.076
8.073
7.829
7.624
7.619
7.613
7.610
7.607
7.601
7.586
7.576
7.572
7.569
2.372
2.368
2.355
6.938
2.28
1.00
3.37
6.10
3.30
1.09
2.40
2.35
ppm
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
ppm
BTA-DMSO-1H
BRUKER

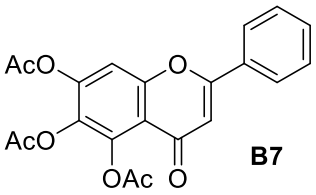
^{13}C-NMR

BTA-DMSO-C13CPD



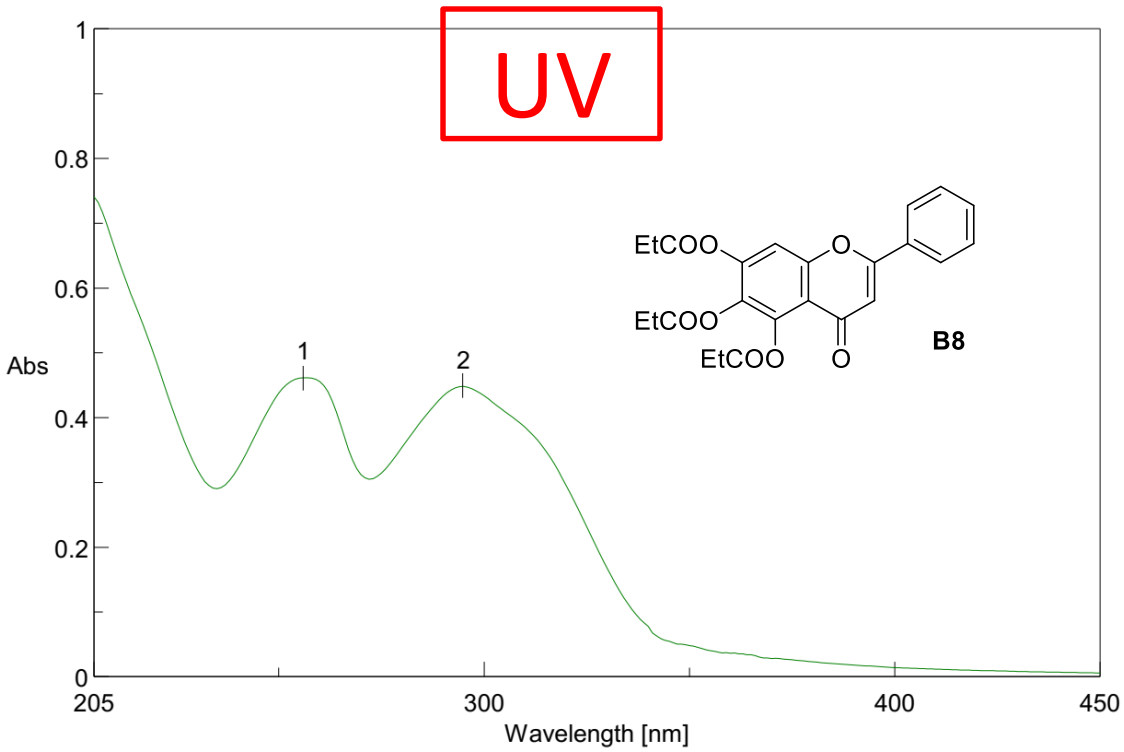

```
Current Data Parameters
NAME          113HUAN_BTA
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20191008
Time               16.14
INSTRUM            spect
PROBHD   5 mm PABBO BB/
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                304.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         125.7864591 MHz
NUC1                  13C
P1                10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.1910008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         22.00000000 W
PLW12         0.35764000 W
PLW13         0.17989001 W

F2 - Processing parameters
SI                  32768
SF           125.7726931 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{13}C-NMR


AcO
AcO
OAc
O
O

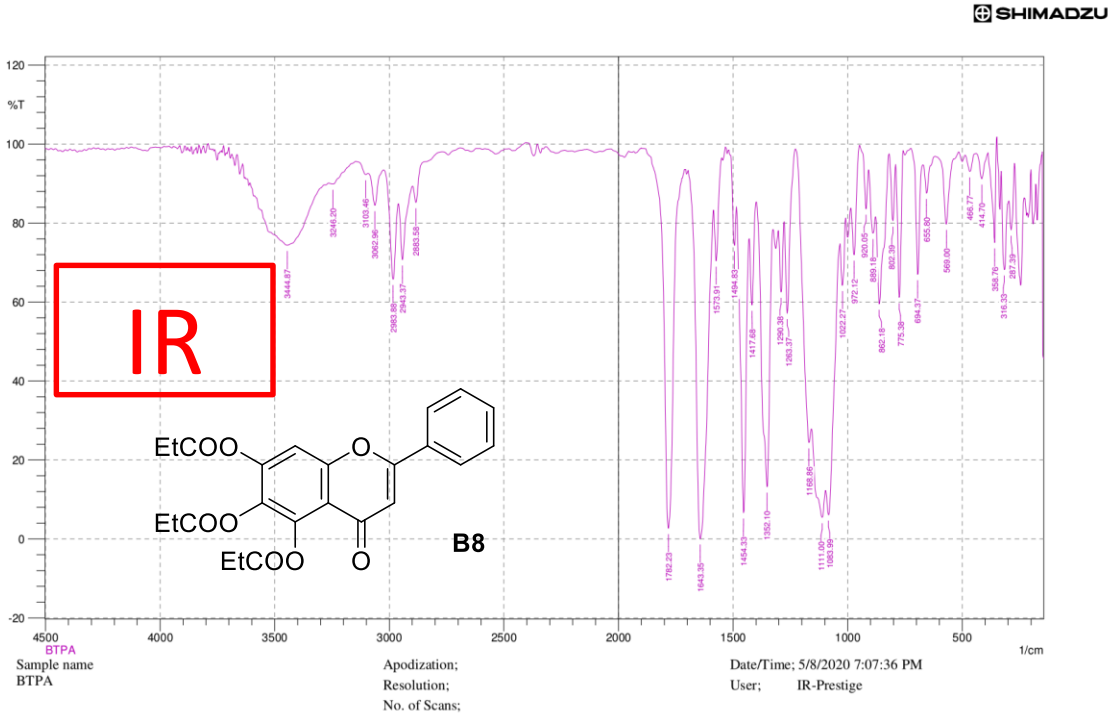
B7

175.28
167.79
167.47
167.44
162.00
153.56
146.71
141.18
132.57
131.98
130.39
129.06
126.35
115.05
111.10
107.53
20.44
20.33
19.69
ppm
ppm
BTA-DMSO-C13CPD
BRUKER



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	256	0.461275	2	295	0.447673



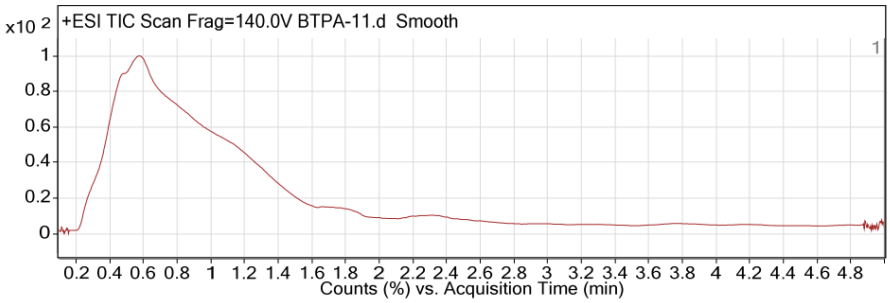
MS

Qualitative Analysis Report

Data Filename	BTPA-11.d	**Sample Name**	BTPA-11
Sample Type	Sample	**Position**	P2-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 7:39:54 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

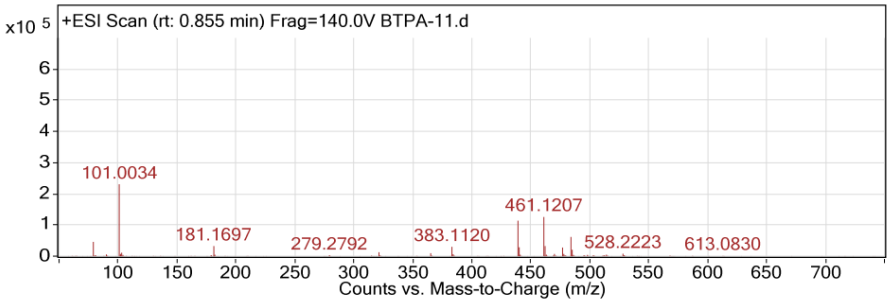
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



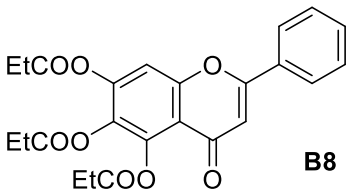
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
101.0034	1	230474.77
439.1384	1	113750.94
461.1207	1	126043.83
484.1962	1	61900.38
899.2526	1	602931.81
900.2562	1	308889.25
901.258	1	98654.03
915.2266	1	269624.84
916.2292	1	142459.03
917.2297	1	56441.81

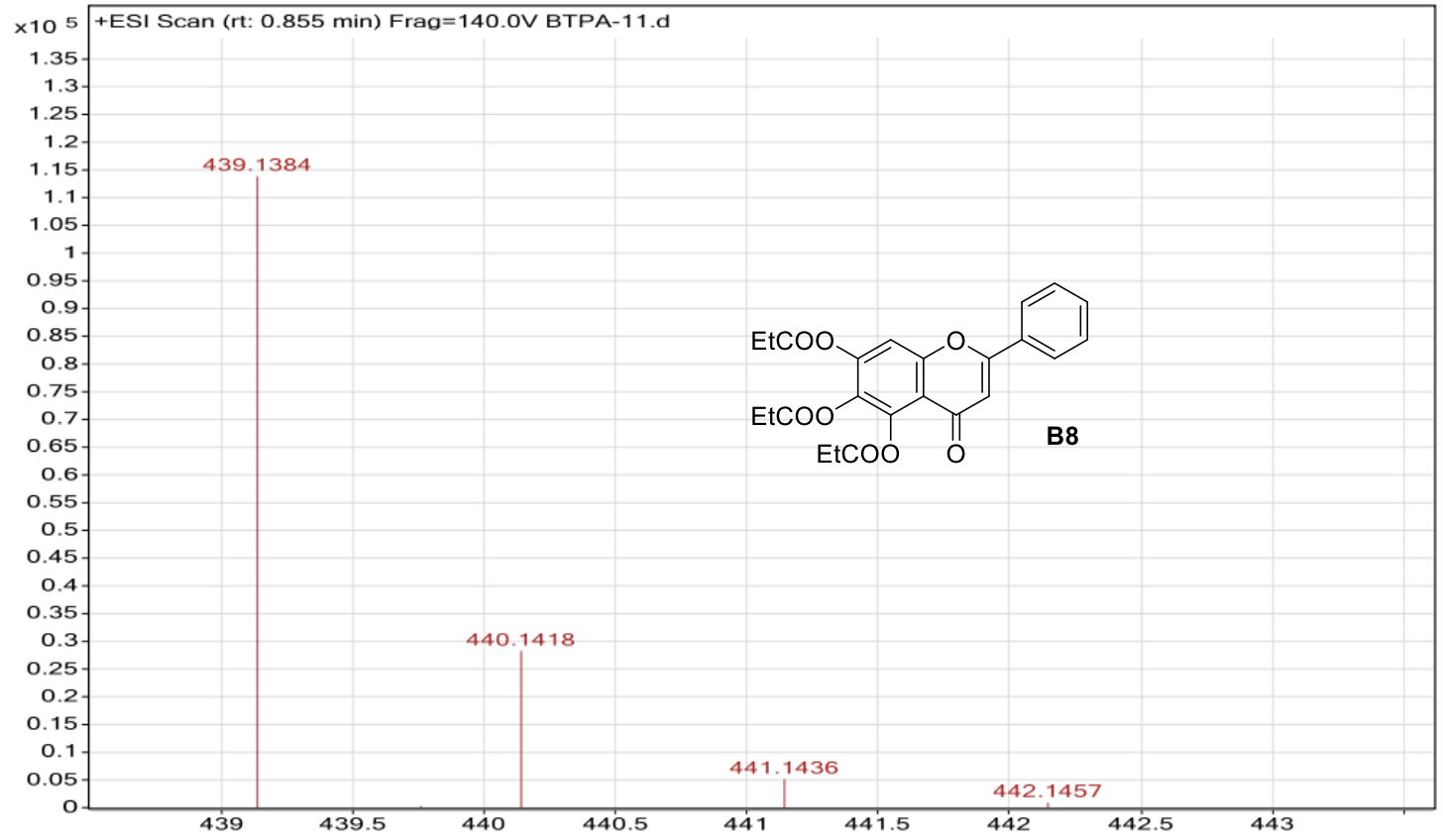


B8

--- End Of Report ---

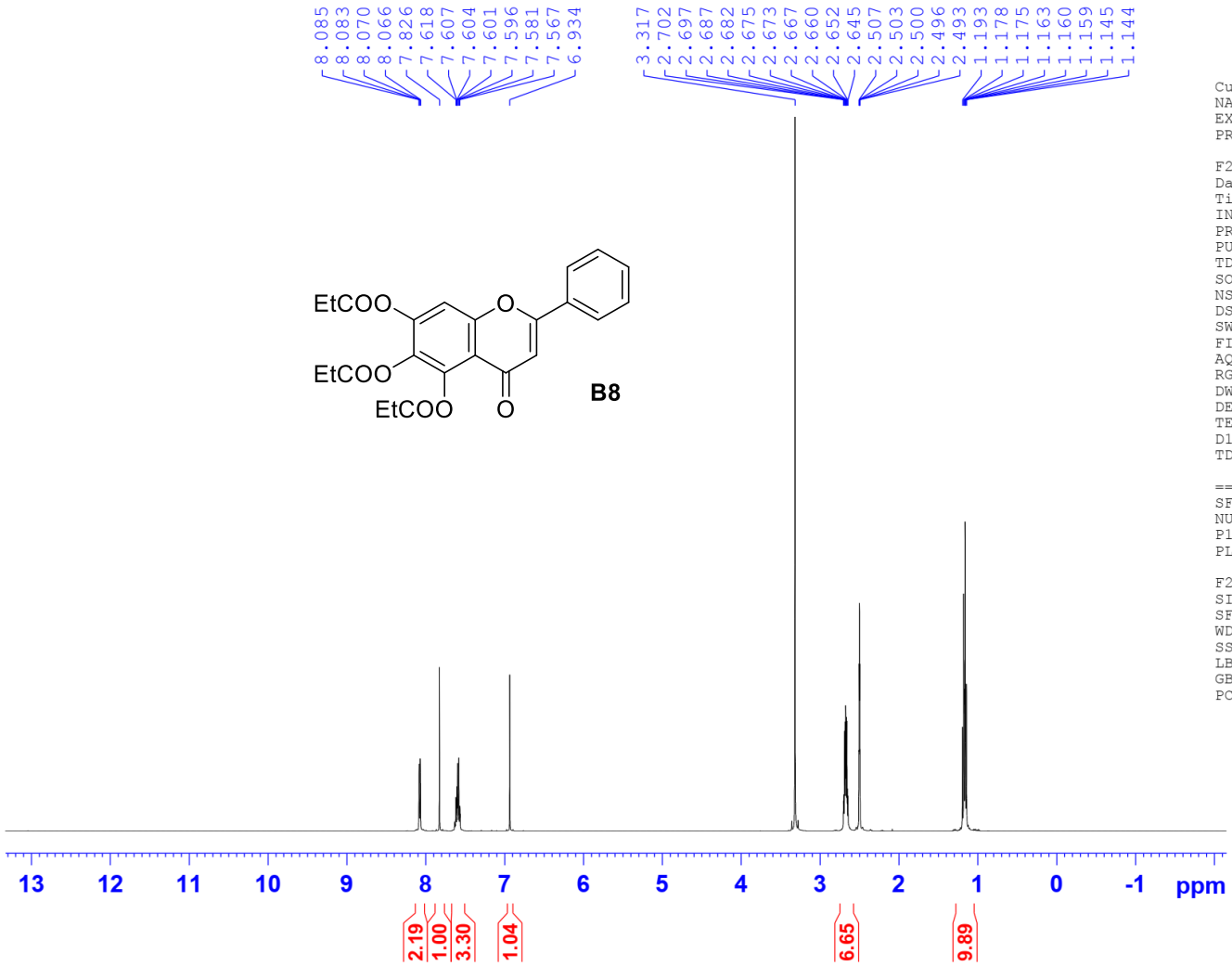
MS

Sample Name	BTPA-11	**Position**	P2-B6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	BTPA-11.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 7:39:54 PM



^{1}H-NMR

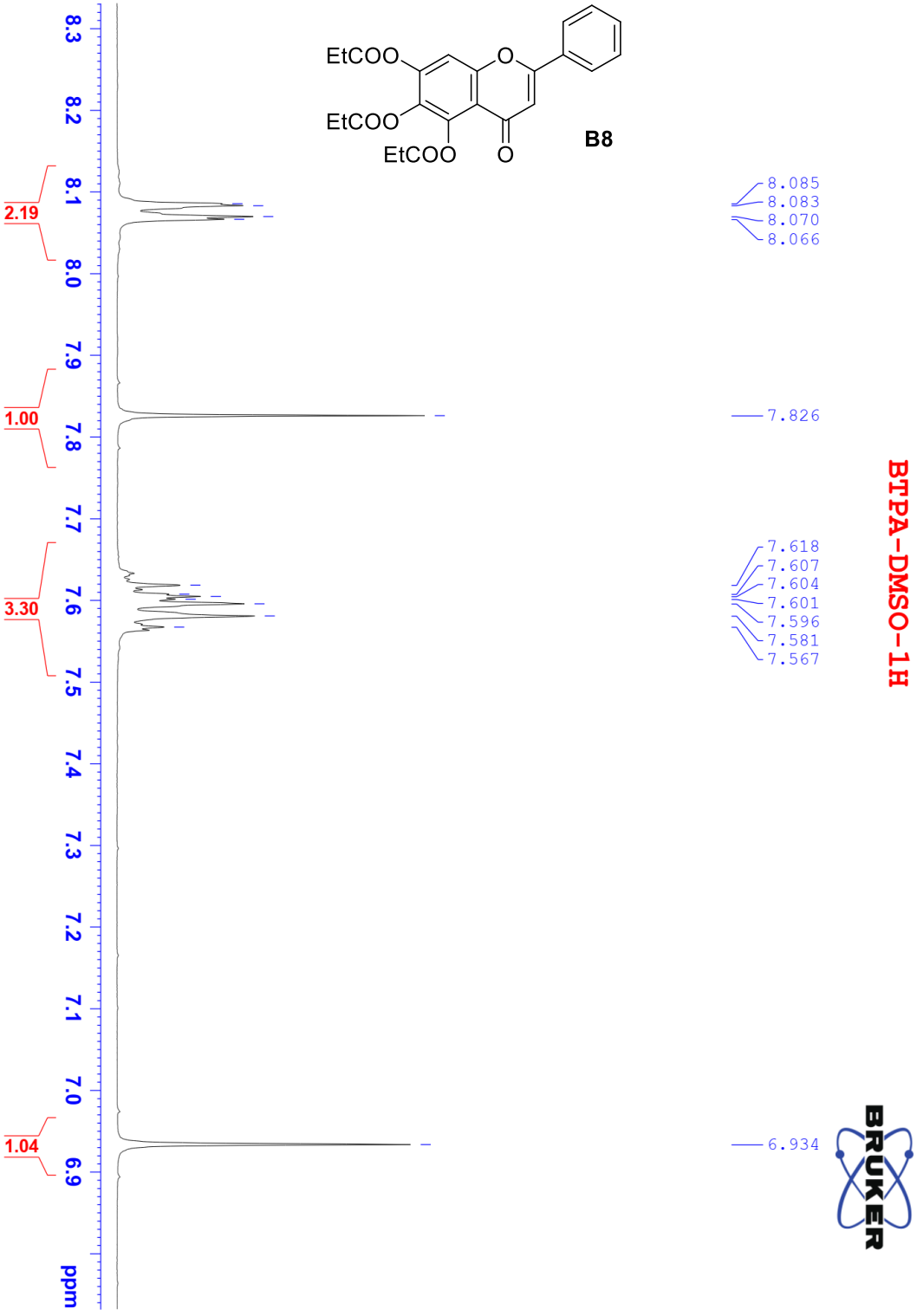
BTPA-DMSO-1H



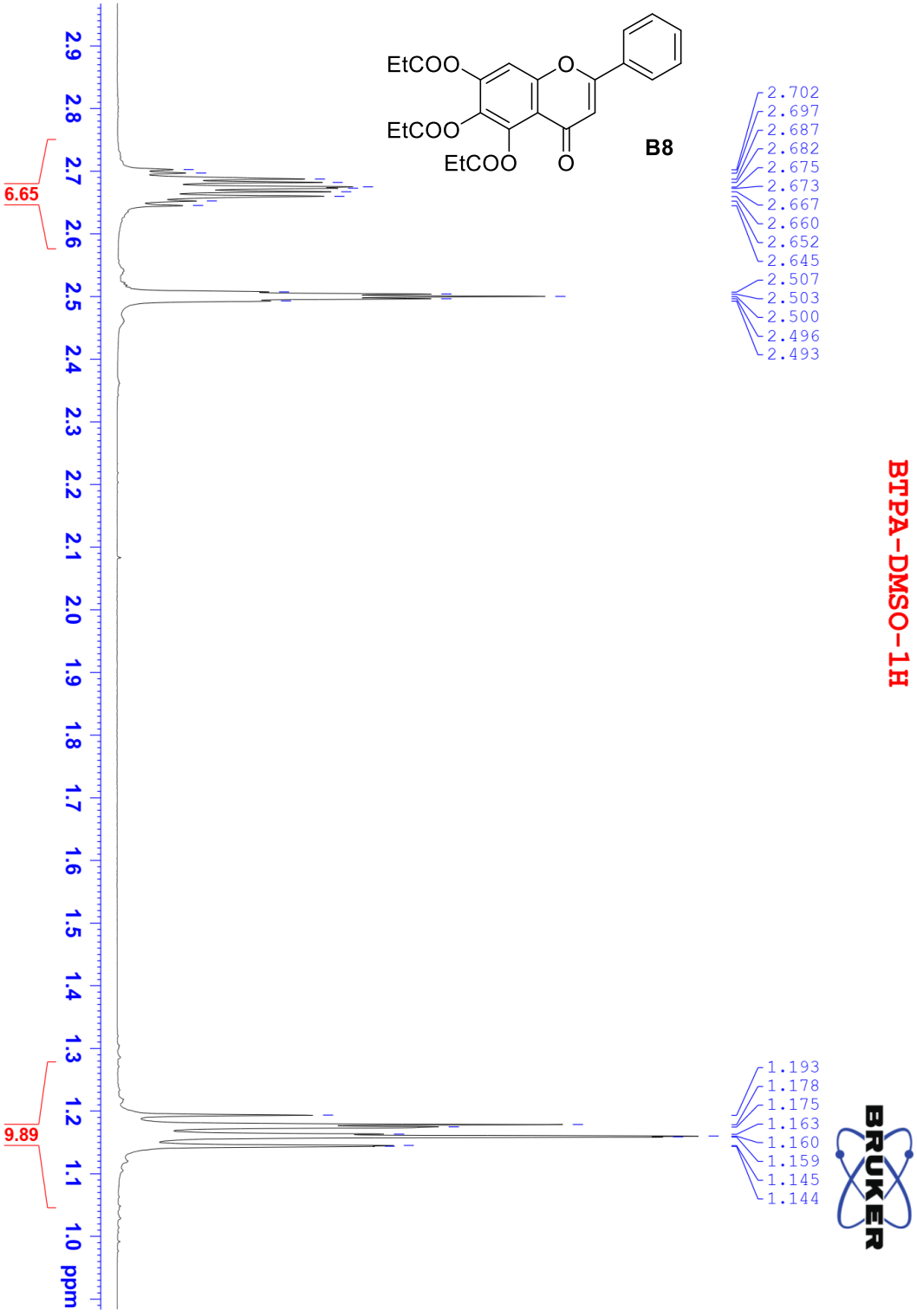
BRUKER

```
Current Data Parameters
NAME         110HUAN_BTPA
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20200109
Time               14.49
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                 89.63
DW                 50.000 usec
DE                  6.50 usec
TE                303.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.1920889 MHz
NUC1                  1H
P1                 10.20 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1890047 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

^{1}H-NMR

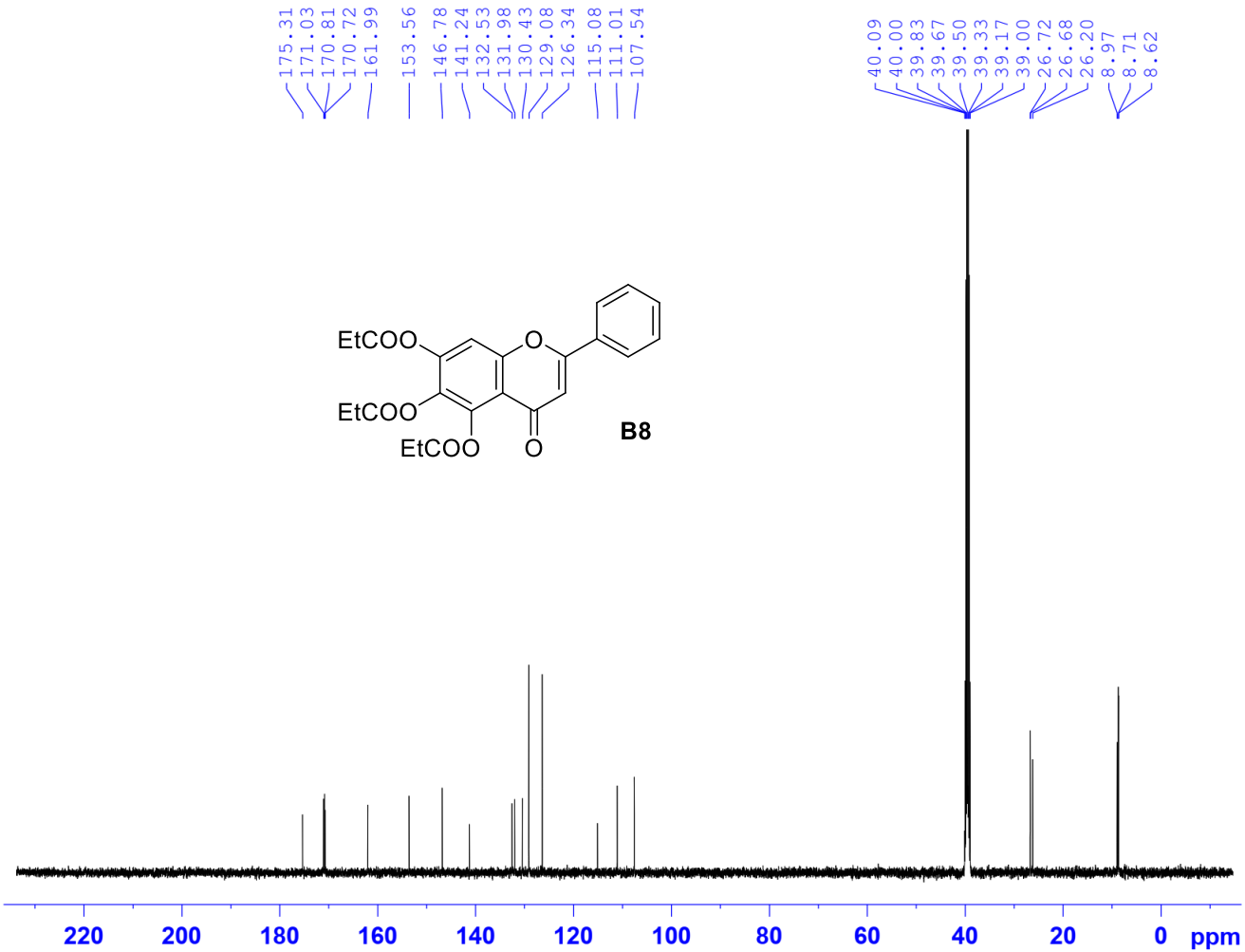

EtCOO
EtCOO
EtCOO
O
O
B8
8.085
8.083
8.070
8.066
7.826
7.618
7.607
7.604
7.601
7.596
7.581
7.567
6.934
2.19
1.00
3.30
1.04
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
ppm
BTPA-DMSO-1H
BRUKER

^{1}H-NMR


EtCOO
EtCOO
EtCOO
O
O
B8
2.702
2.697
2.687
2.682
2.675
2.673
2.667
2.660
2.652
2.645
2.507
2.503
2.500
2.496
2.493
6.65
9.89
1.193
1.178
1.175
1.163
1.160
1.159
1.145
1.144
2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 ppm
BTPA-DMSO-1H
BRUKER

^{13}C-NMR

BTPA-DMSO-C13CPD



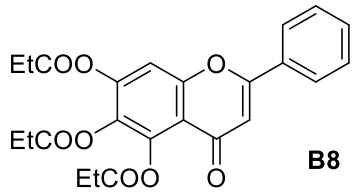

```
Current Data Parameters
NAME         110HUAN_BTPA
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20200109
Time               17.18
INSTRUM            spect
PROBHD   5 mm PABBO BB/
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                303.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         125.7864591 MHz
NUC1                  13C
P1                 10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.1910008 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         22.00000000 W
PLW12         0.35764000 W
PLW13         0.17989001 W

F2 - Processing parameters
SI                 32768
SF           125.7726903 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{13}C-NMR

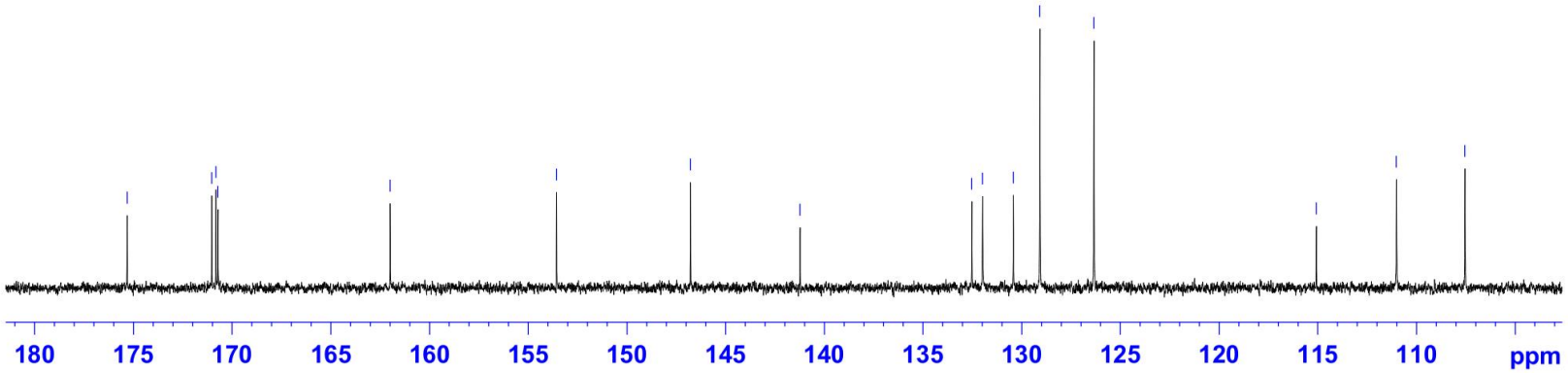
BTPA-DMSO-C13CPD

BRUKER

175.31
171.03
170.81
170.72
161.99
153.56
146.78
141.24
132.53
131.98
130.43
129.08
126.34
115.08
111.01
107.54

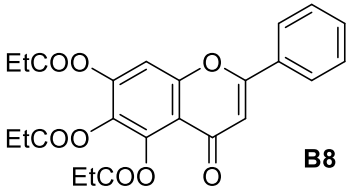


B8

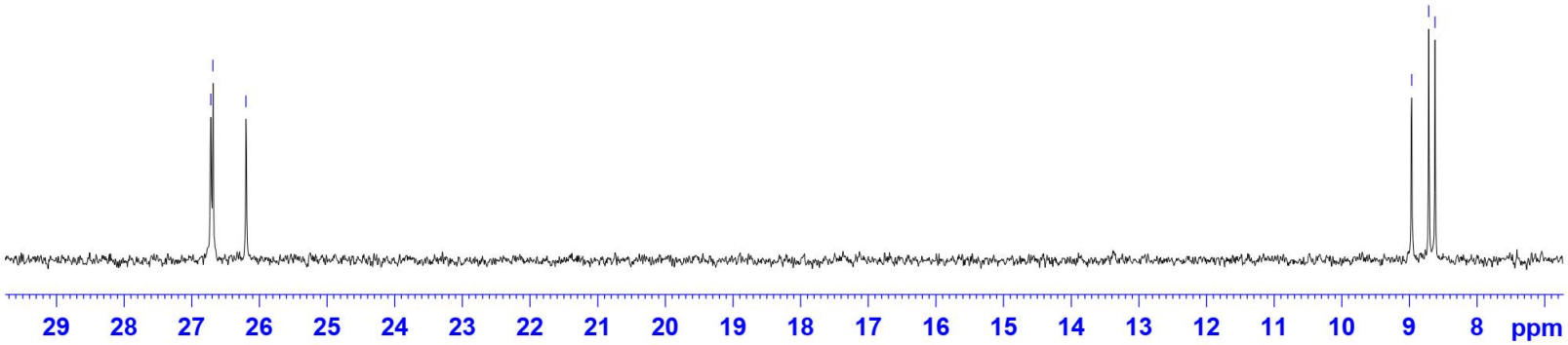


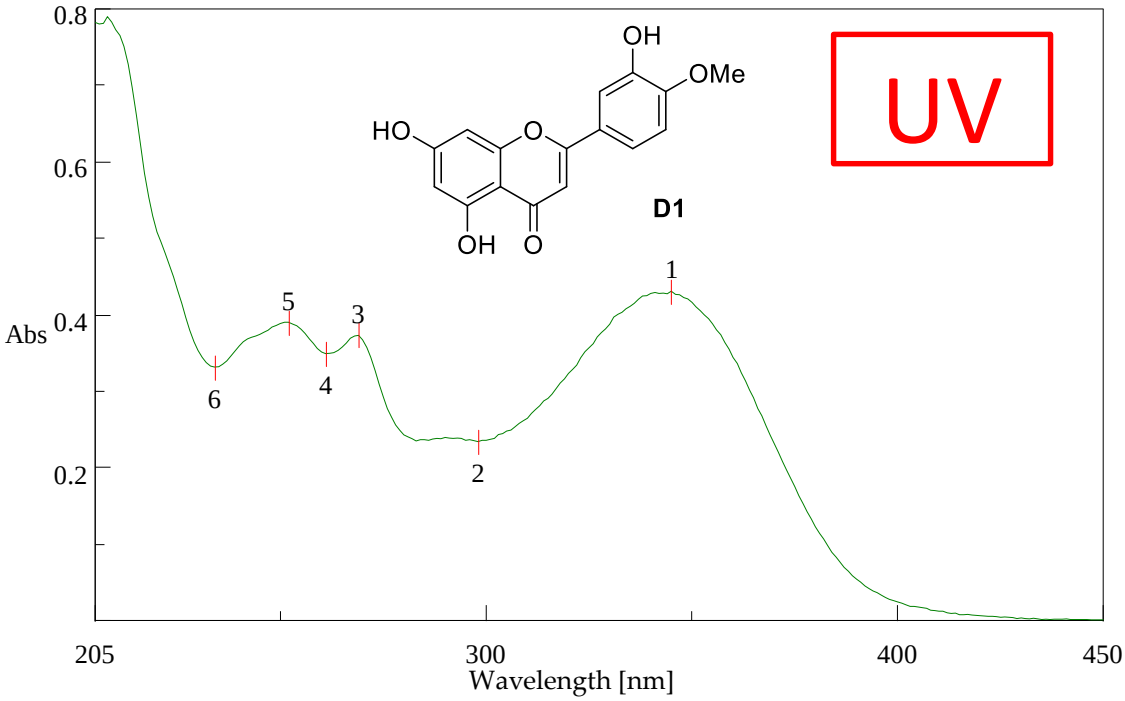
^{13}C-NMR

BTPA-DMSO-C13CPD



B8



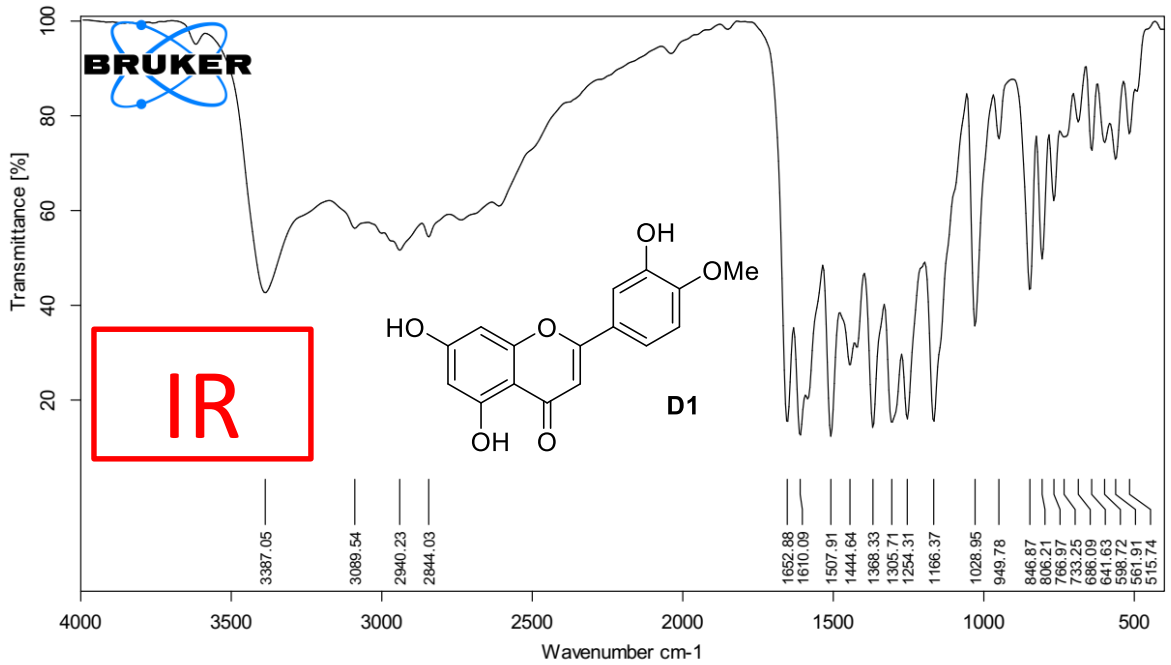


[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	345	0.43004	2	298	0.233573	3	269	0.372553
4	261	0.348546	5	252	0.389723	6	234	0.330926

VIEN CONG NGHE HOA HOC
01 Mac Dinh Chi - Q.1 - Tp HCM

Tel: 08.38296127
Fax: 08.38293889



E:\OPUS 7\2016\20160812\HD1.0	HD1	TENSOR 27 - BRUKER - GERMANY	8/12/2016

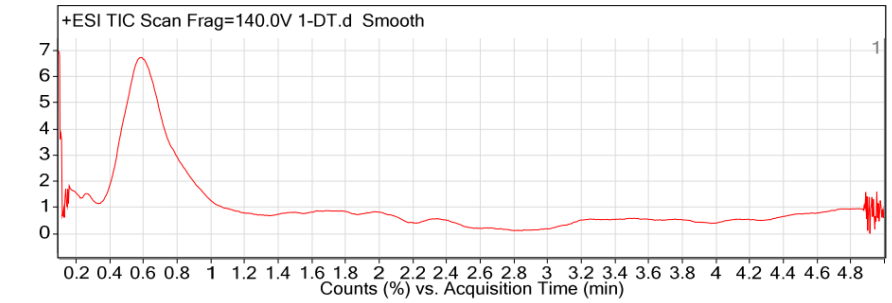
MS

Qualitative Analysis Report

Data Filename	1-DT.d	**Sample Name**	1-DT
Sample Type	Sample	**Position**	P2-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 8:29:59 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

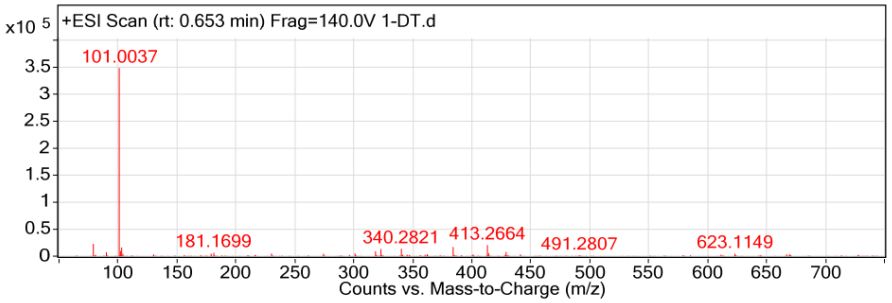
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



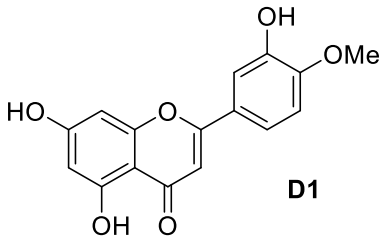
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
79.0214	1	22762.52
101.0037	1	348713.09
102.0062	1	9852.9
102.9991	1	16236.17
318.3002	1	9053.3
323.0526	1	13376.74
340.2821	1	13906.29
384.3083	1	16981.61
413.2664	1	20418.92
429.2402	1	7832.86

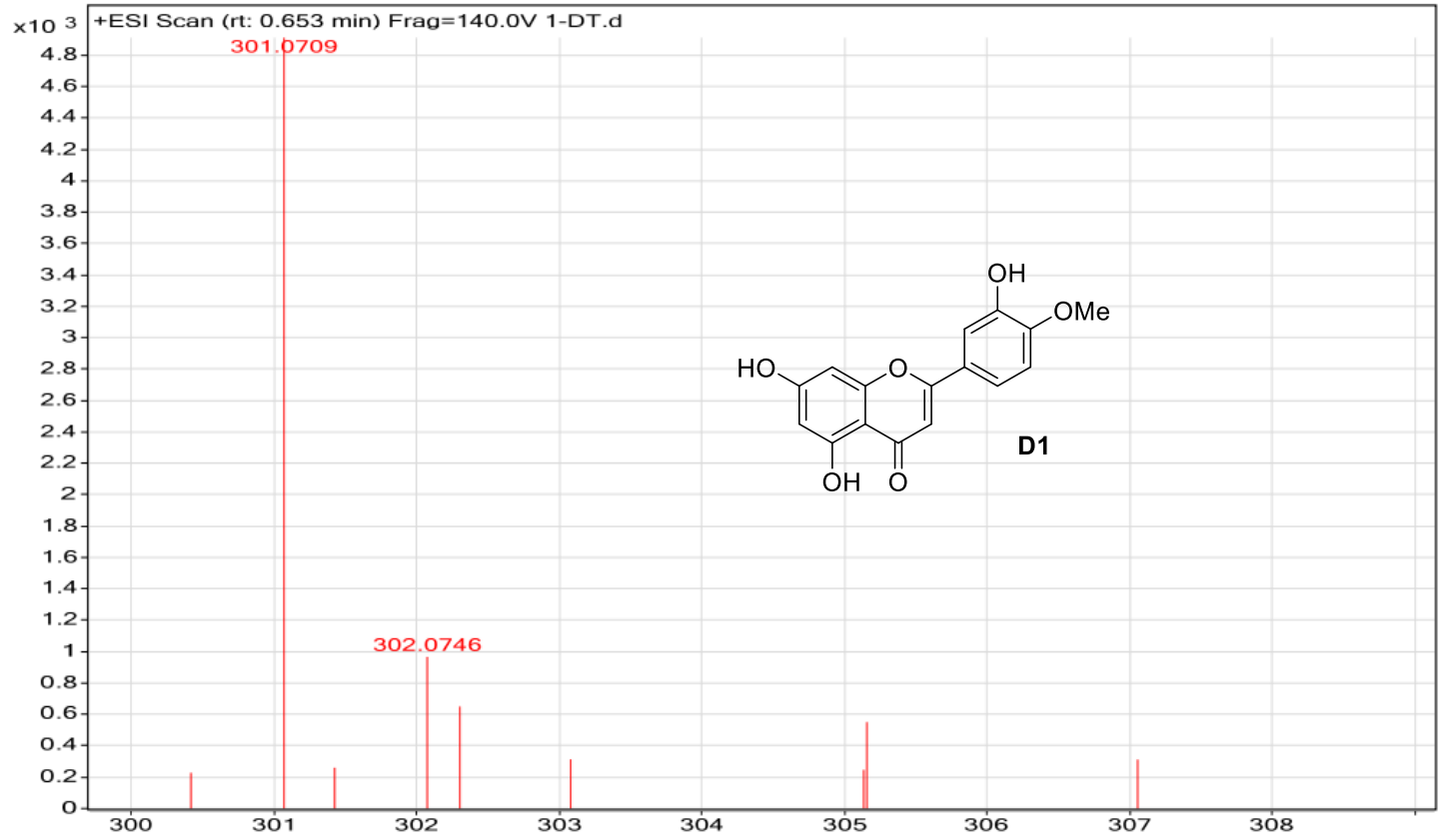


D1

--- End Of Report ---

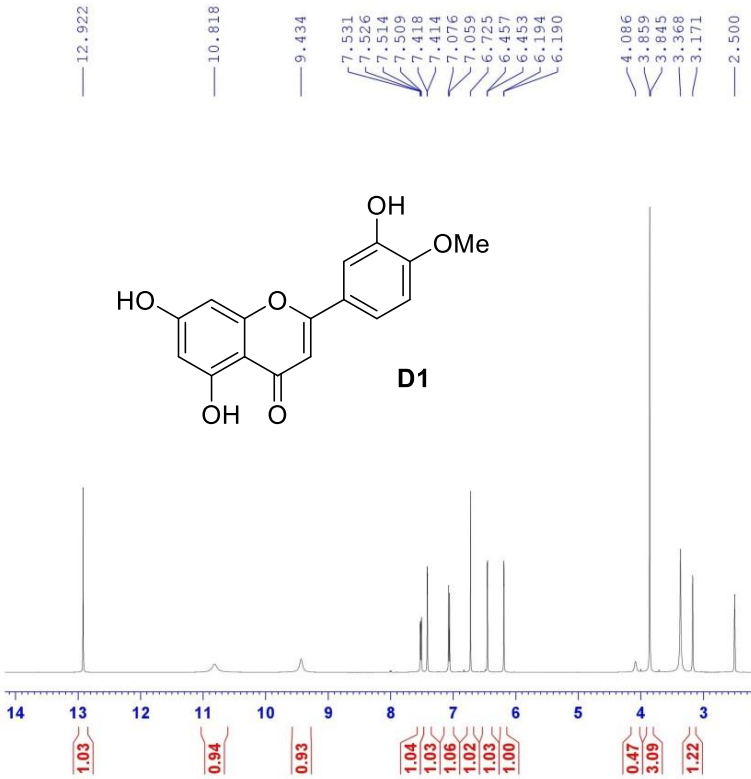
MS

Sample Name	1-DT	**Position**	P2-C6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	1-DT.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 8:29:59 PM



^{1}H-NMR

DT-DMSO-1H

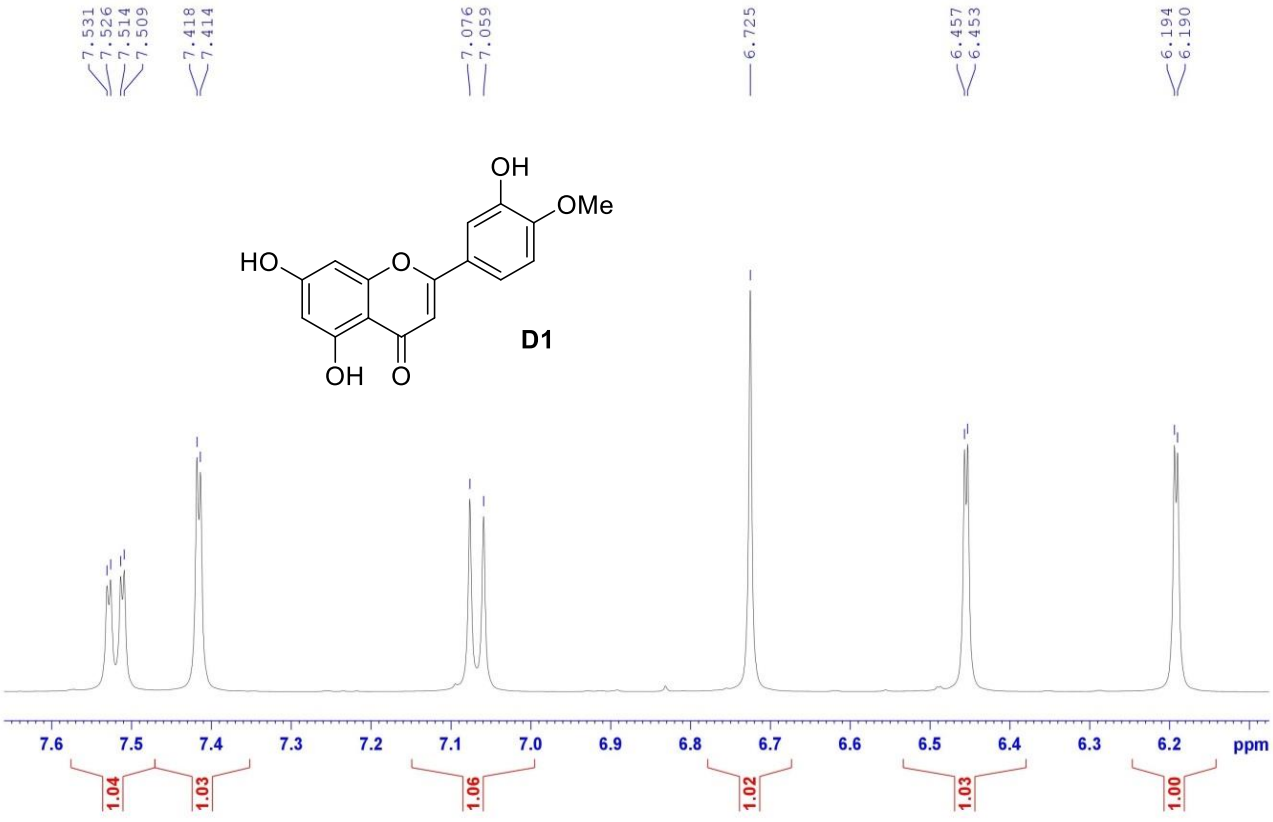


BRUKER

```
Current Data Parameters
NAME          110HUAN_HD1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190129
Time               19.55
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                 89.63
DW                50.000 usec
DE                 6.50 usec
TE                301.5 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            500.2000042 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

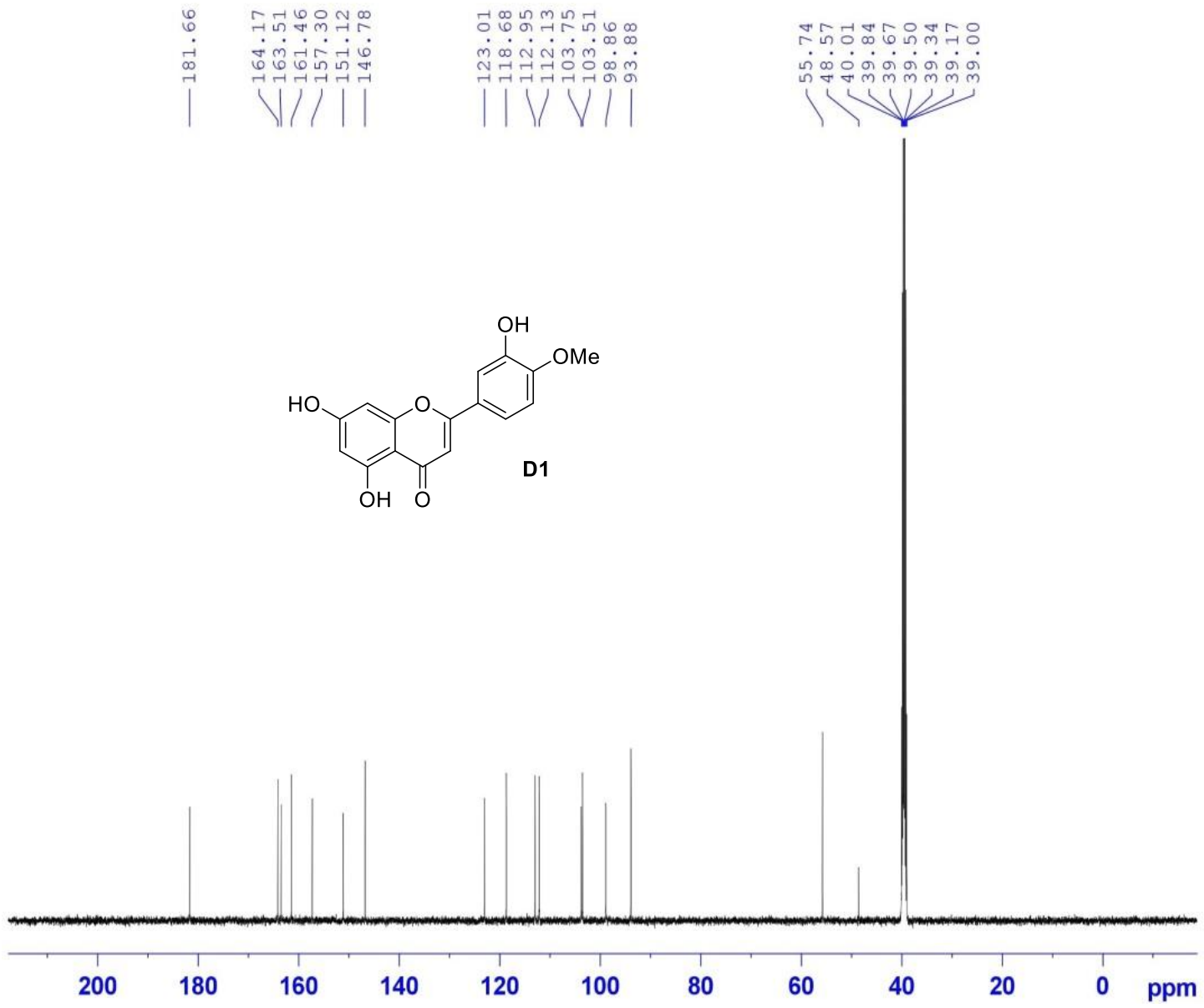
DT-DMSO-1H

BRUKER

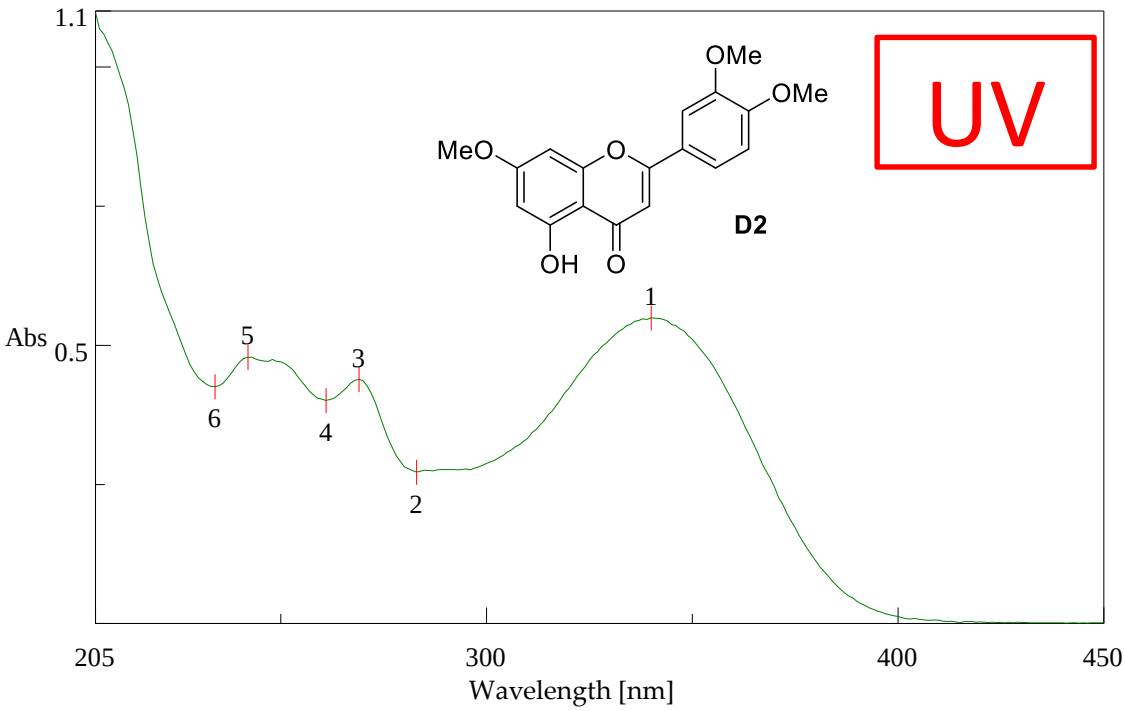


DT-DMSO-C13CPD

^{13}C-NMR

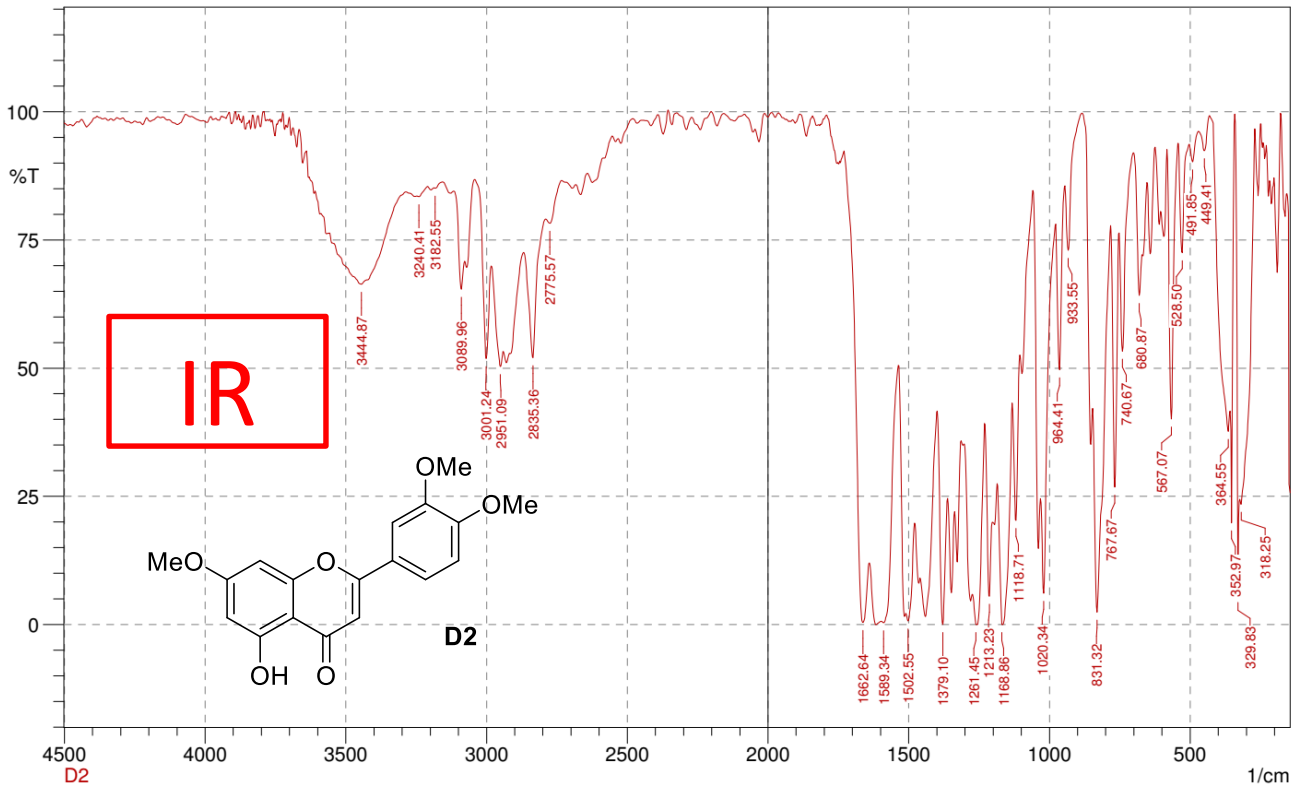



```
Current Data Parameters
NAME          110HUAN_HD1
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190129
Time                18.54
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                    512
DS                      4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                302.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         125.7879670 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           125.7754515 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	340	0.548955	2	283	0.271724	3	269	0.438749
4	261	0.400295	5	242	0.478333	6	234	0.425517



MS

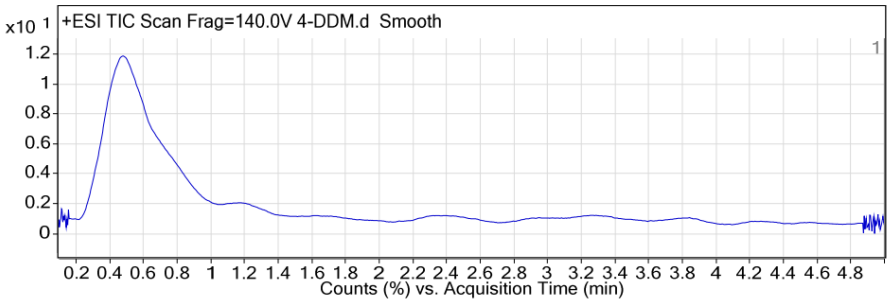
Qualitative Analysis Report

Data Filename	4-DDM.d	**Sample Name**	4-DDM
Sample Type	Sample	**Position**	P2-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 7:34:20 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

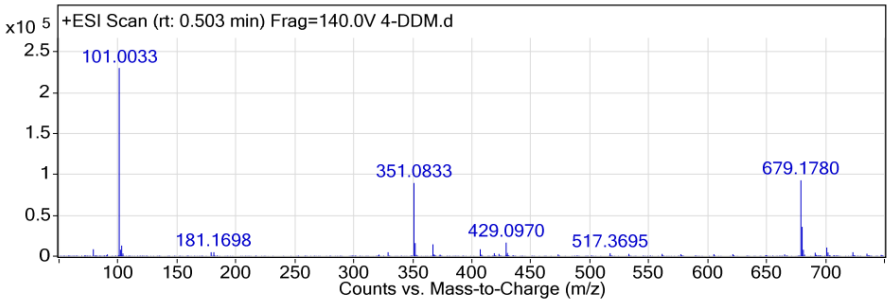
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



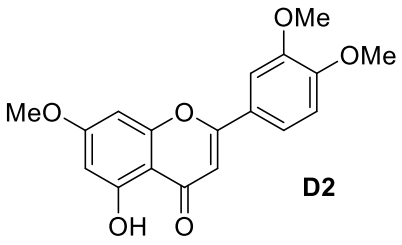
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
79.0211		8484.25
101.0033	1	230221.81
102.999	1	12995.89
351.0833	1	89560.98
352.0868	1	15988.85
367.0573	1	14627.99
429.097	1	16630.26
679.178	1	92758.16
680.1805	1	36038.07
701.1592	1	10518.93

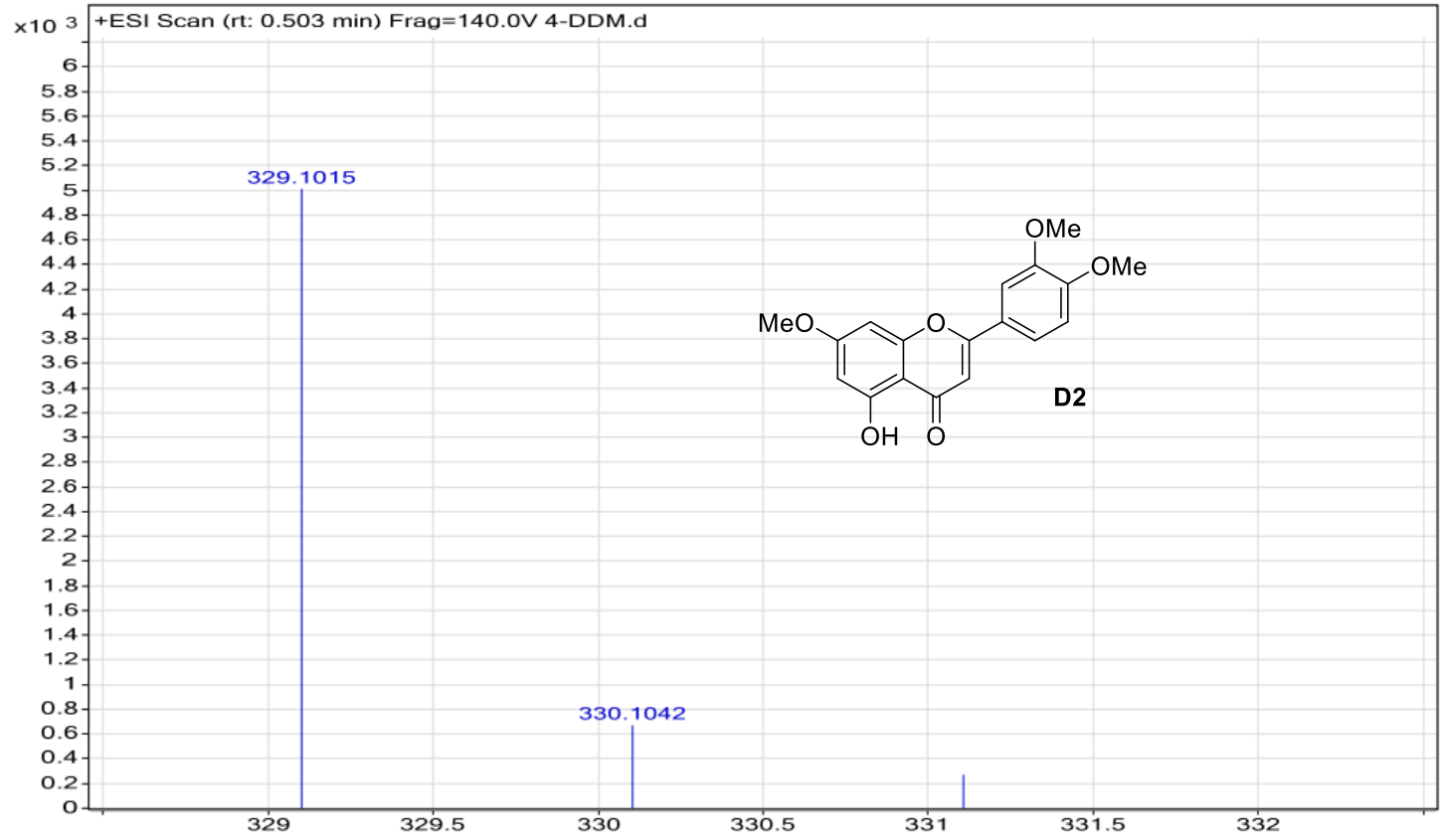


D2

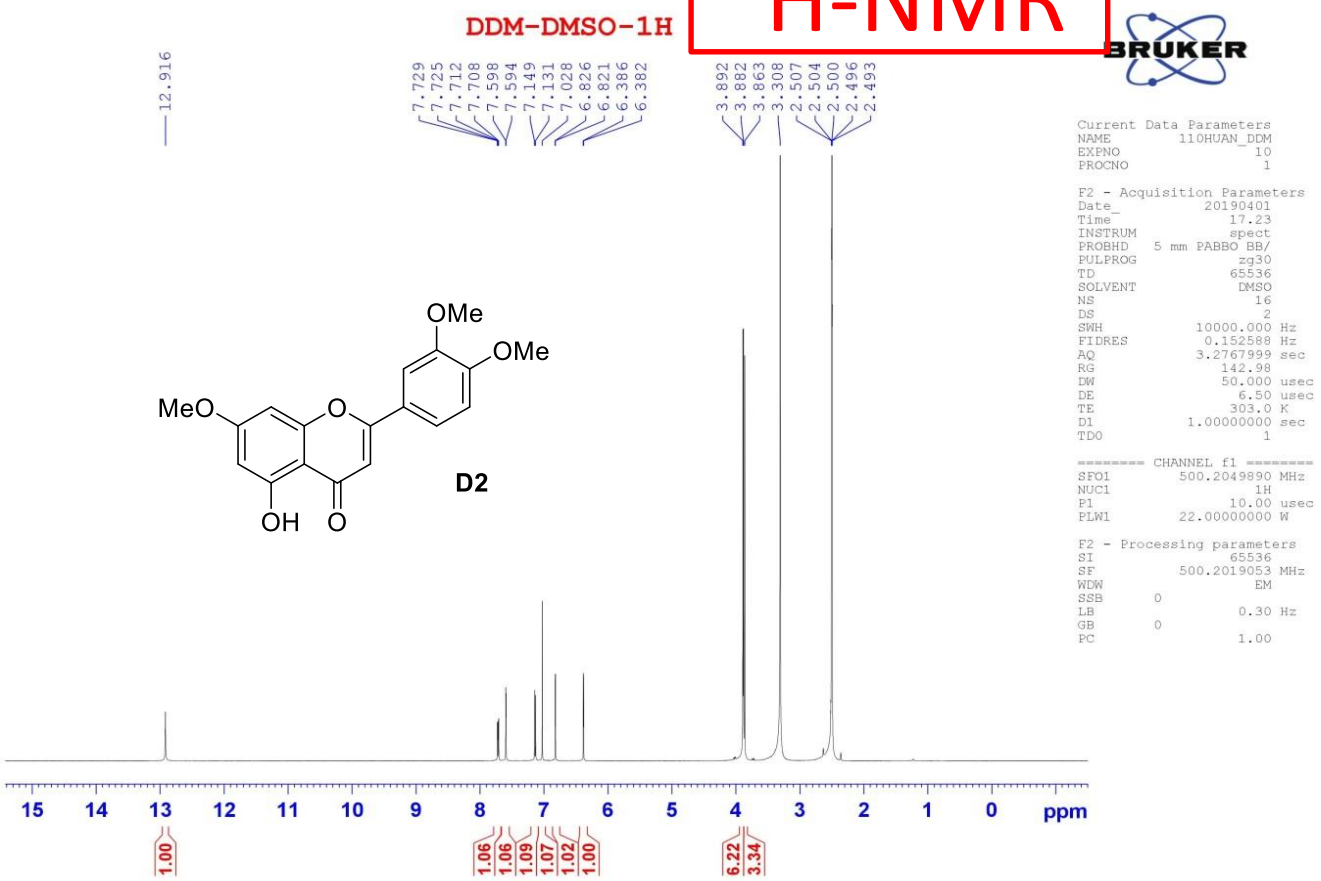
--- End Of Report ---

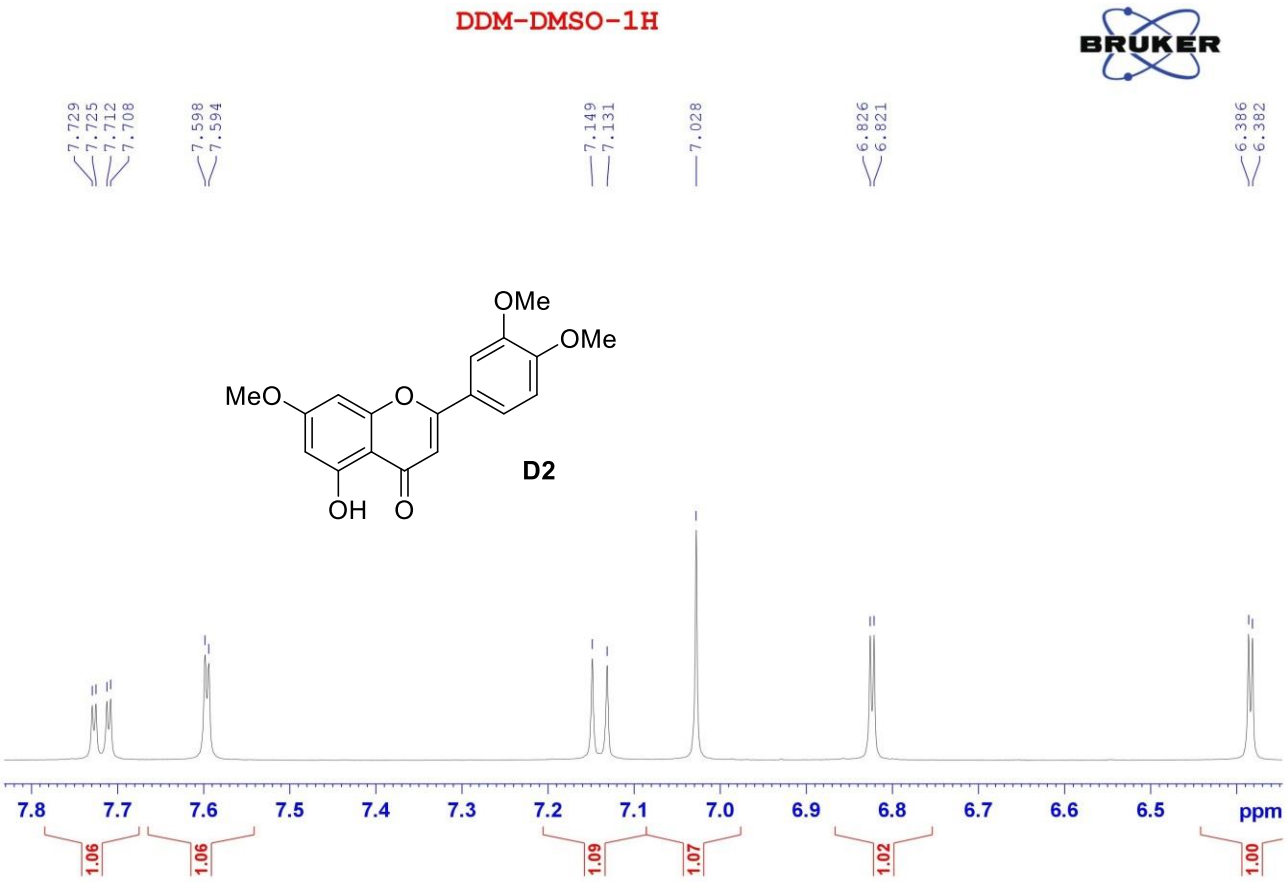
MS

Sample Name	4-DDM	**Position**	P2-B5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	4-DDM.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 7:34:20 PM



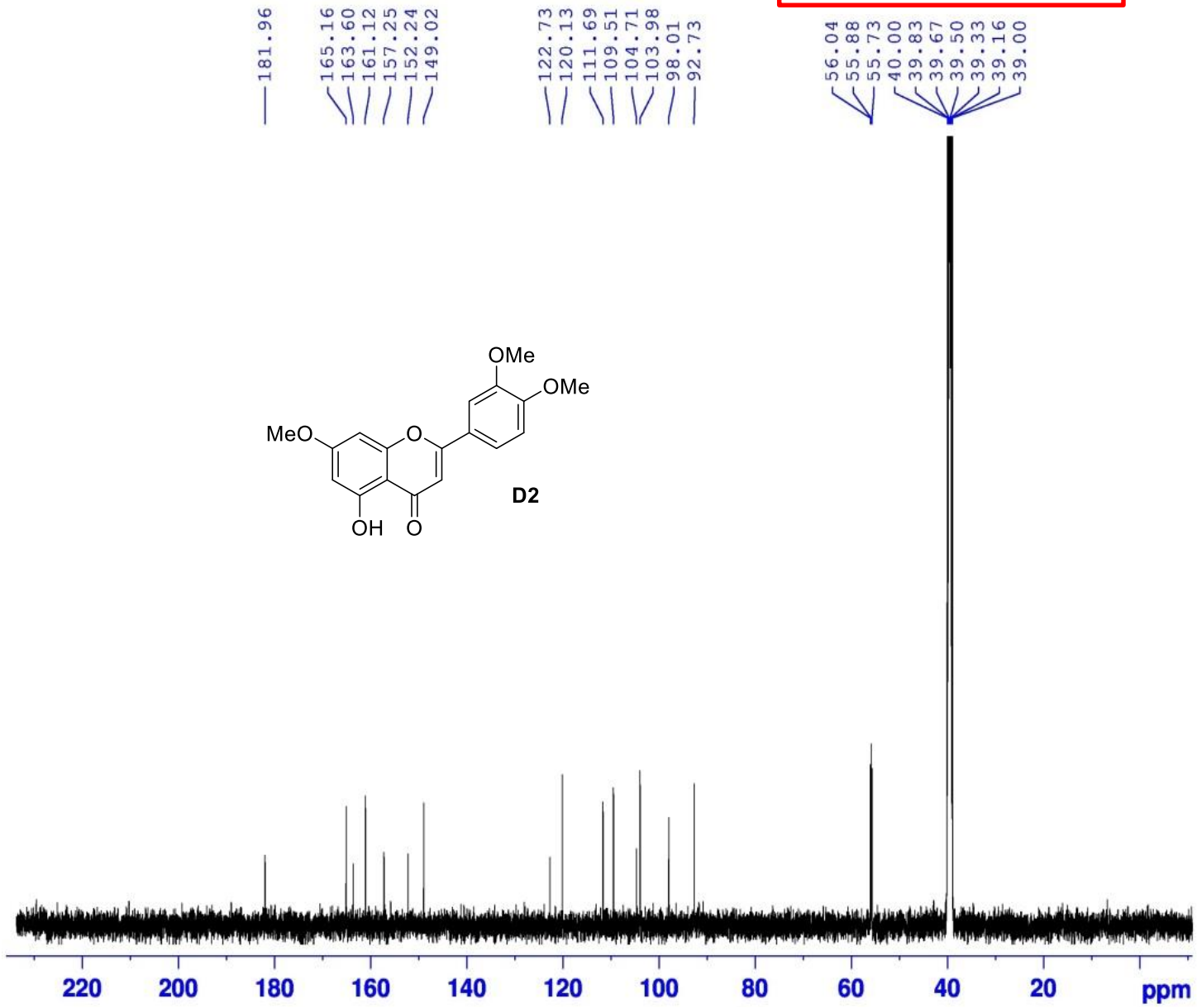
^{1}H-NMR


DDM-DMSO-1H
BRUKER
12.916
7.729
7.725
7.712
7.708
7.598
7.594
7.149
7.131
7.028
6.826
6.821
6.386
6.382
3.892
3.882
3.863
3.308
2.507
2.504
2.500
2.496
2.493
OMe
OMe
MeO
O
OH
O
D2
Current Data Parameters
NAME 110HUAN_DDM
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190401
Time 17.23
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 142.98
DW 50.000 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.2049890 MHz
NUC1 1H
P1 10.00 usec
PLW1 22.00000000 W
F2 - Processing parameters
SI 65536
SF 500.2019053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.06
1.06
1.09
1.07
1.02
1.00
6.22
3.34


DDM-DMSO-1H
BRUKER
7.729
7.725
7.712
7.708
7.598
7.594
7.149
7.131
7.028
6.826
6.821
6.386
6.382
OMe
OMe
MeO
O
OH
O
D2
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 ppm
1.06
1.06
1.09
1.07
1.02
1.00

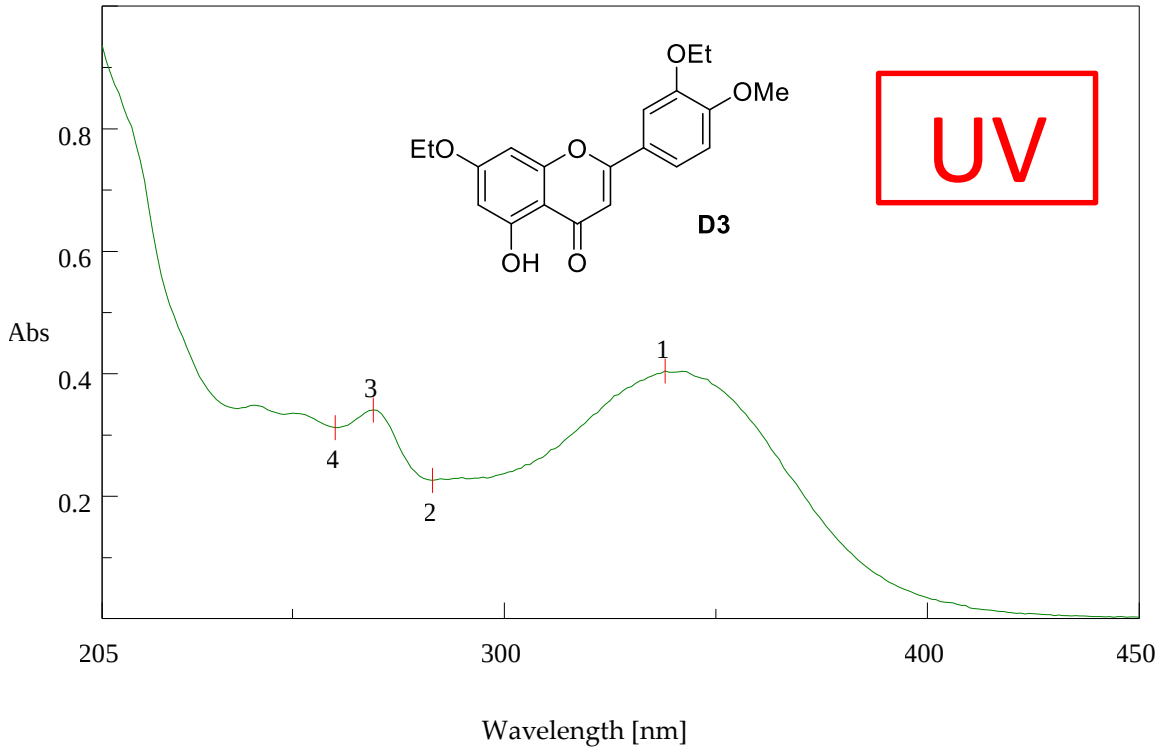
DDM-DMSO-C13CPD

^{13}C-NMR



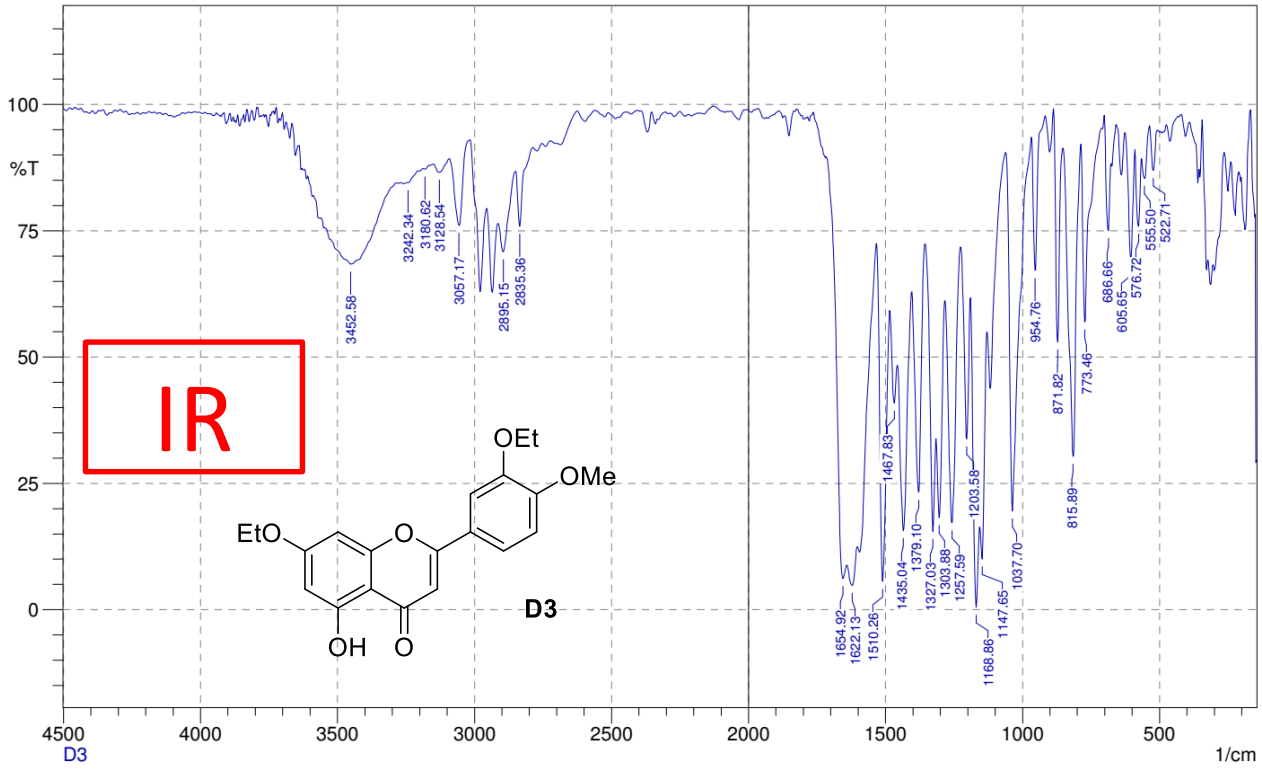
BRUKER

```
Current Data Parameters
NAME          110HUAN_DDM
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_              20190401
Time                 19.40
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                 303.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          125.7897032 MHz
NUC1                    13C
P1                  10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2          500.2039008 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            125.7759351 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	338	0.404347	2	283	0.225658	3	269	0.340507
4	260	0.311738						



MS

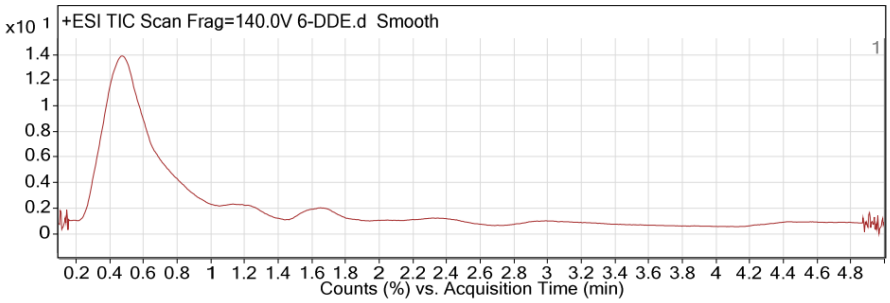
Qualitative Analysis Report

Data Filename	6-DDE.d	**Sample Name**	6-DDE
Sample Type	Sample	**Position**	P2-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 7:23:11 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

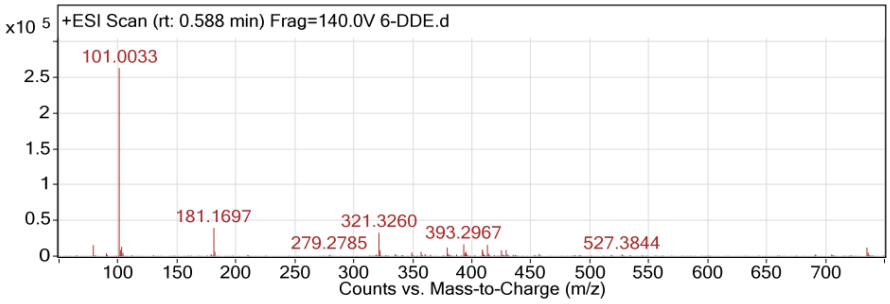
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



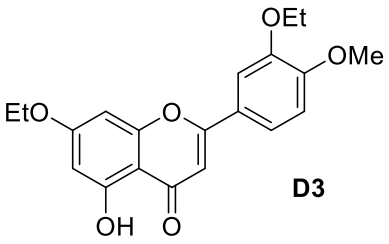
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
79.0209	1	15483.26
101.0033	1	263178.06
102.9988	1	13295.03
181.1697	1	39590.21
321.326	1	32958.98
379.1142	1	12143.51
393.2967	1	16460.94
409.1613	1	9409.05
413.2654	1	15935.65
735.2404	1	12220.2

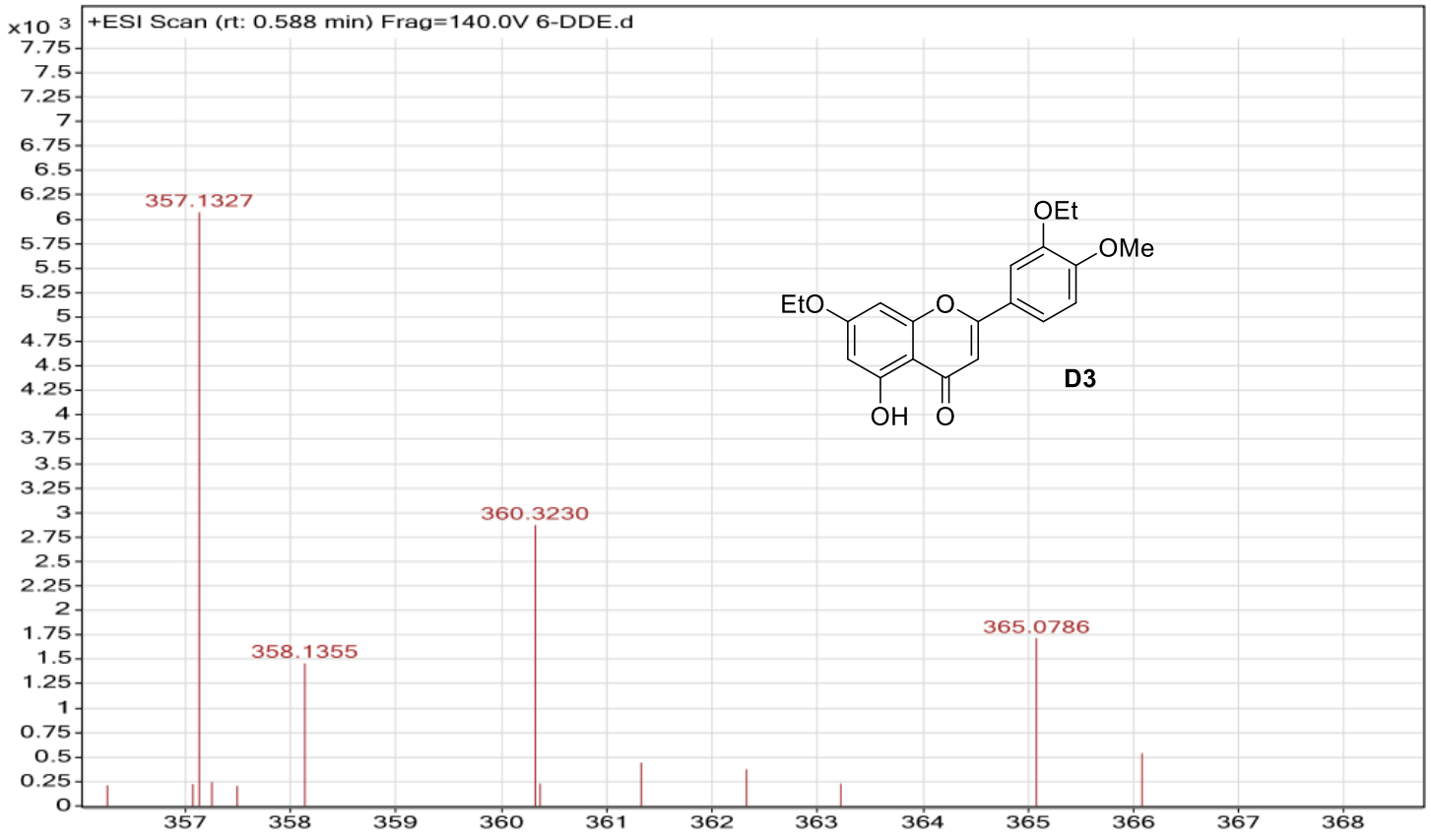


D3

--- End Of Report ---

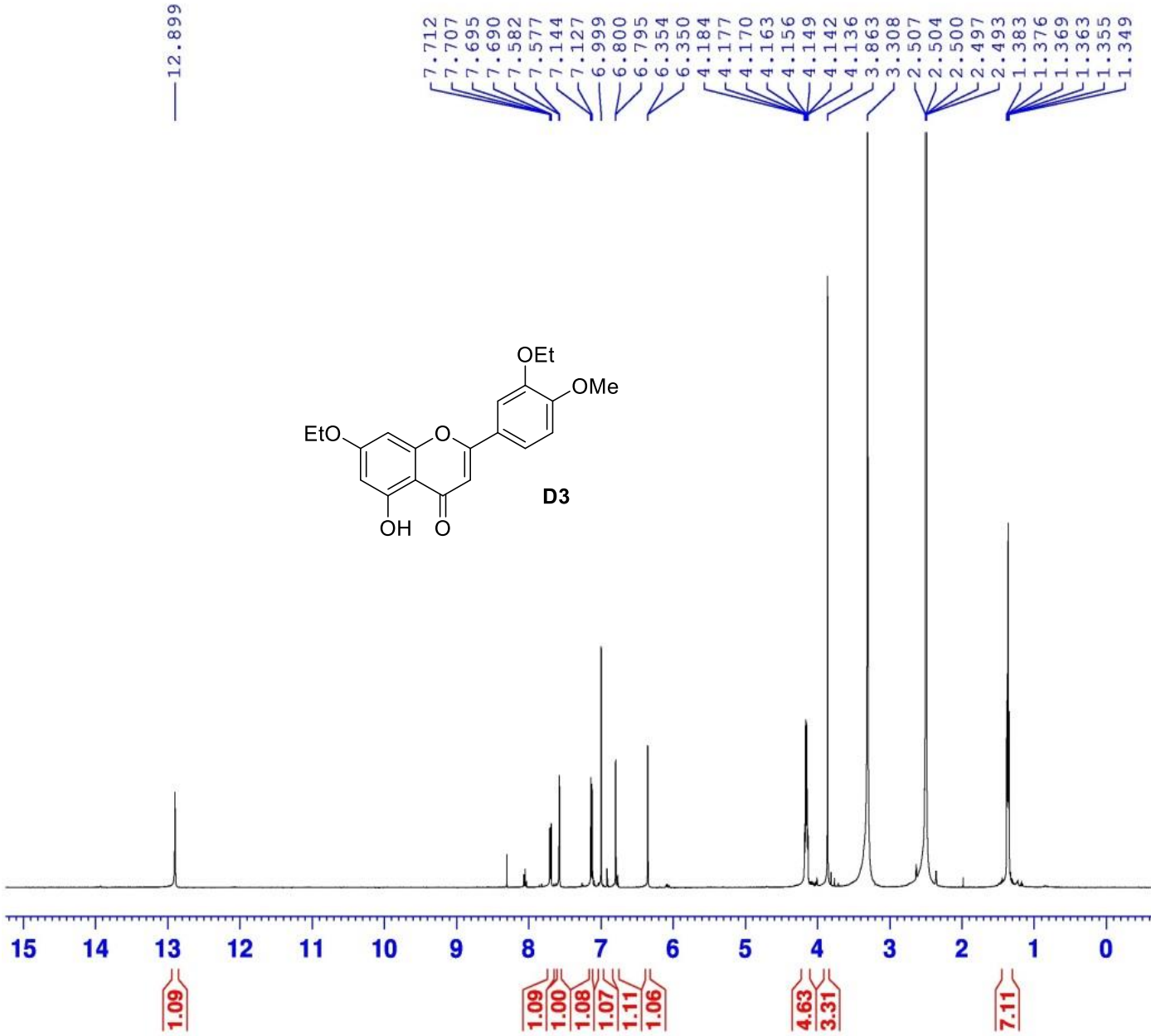
MS

Sample Name	6-DDE	**Position**	P2-B3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	6-DDE.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 7:23:11 PM



^{1}H-NMR

DDE-DMSO-1H

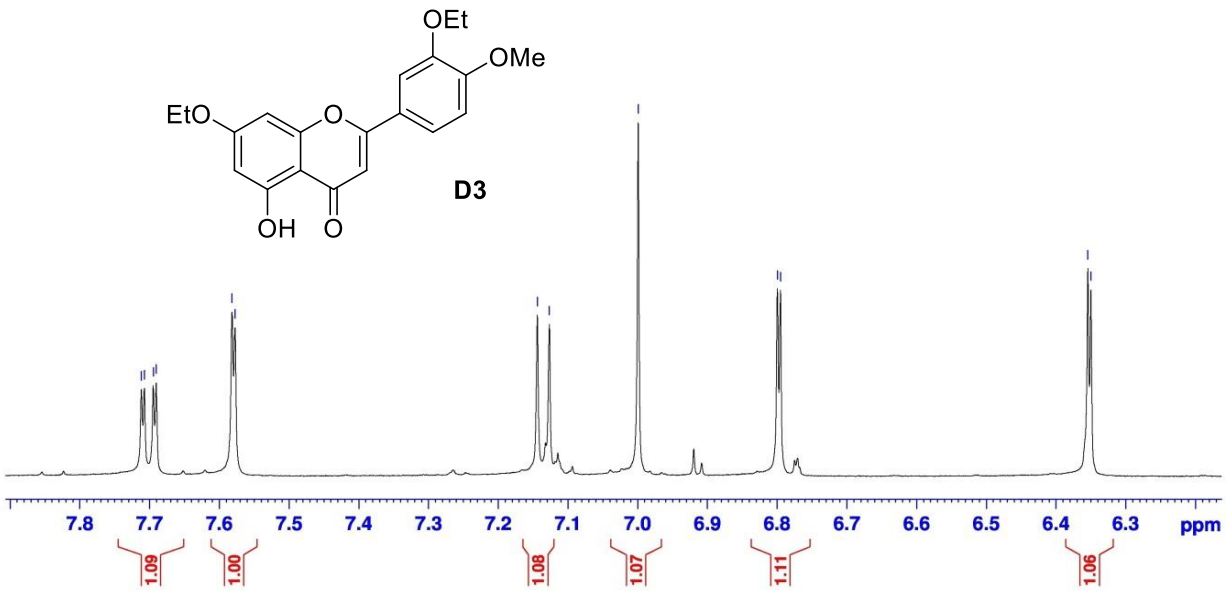


BRUKER

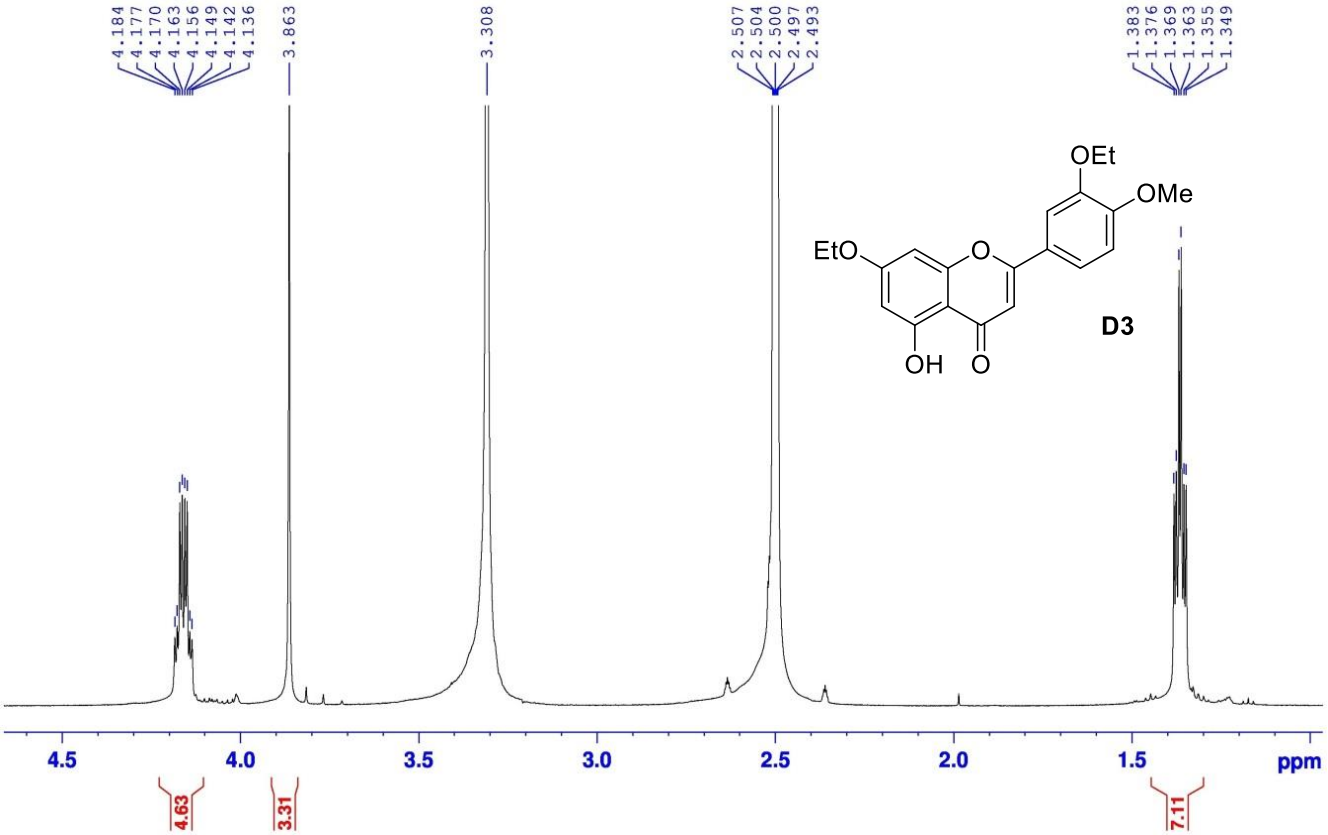
```
Current Data Parameters
NAME          110HUAN_DDE
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190401
Time                17.13
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                 303.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.2049890 MHz
NUC1                   1H
P1                 10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.2019051 MHz
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

DDE-DMSO-1H

^{1}H-NMR

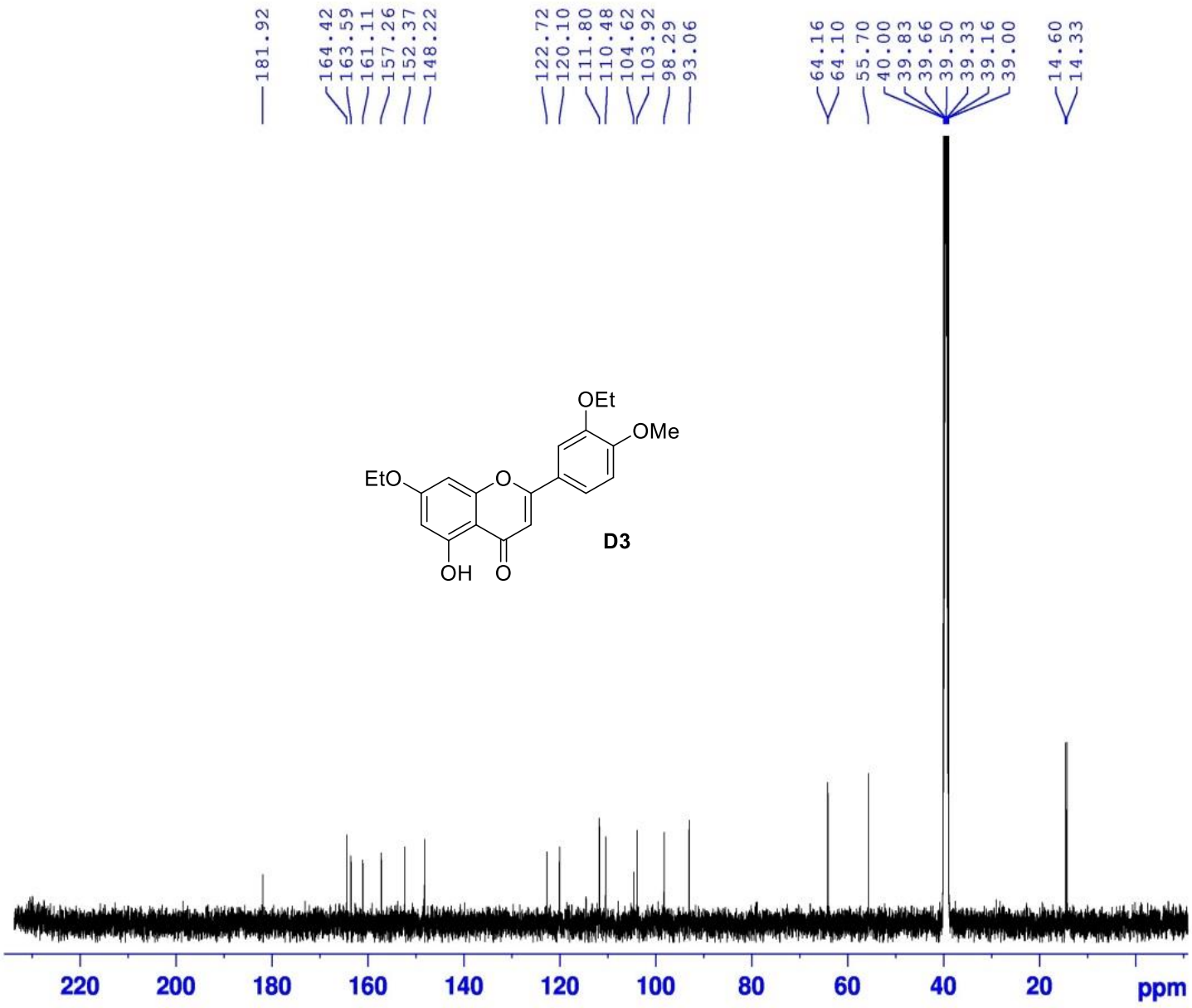


DDE-DMSO-1H



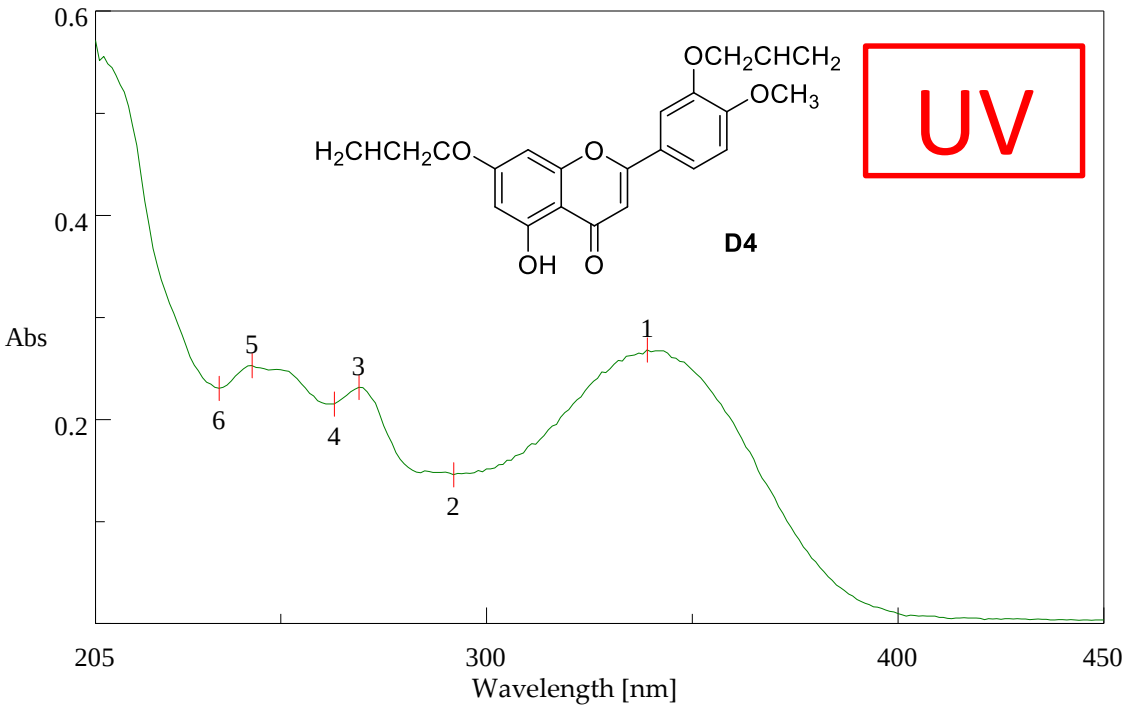
DDE-DMSO-C13CPD

^{13}C-NMR



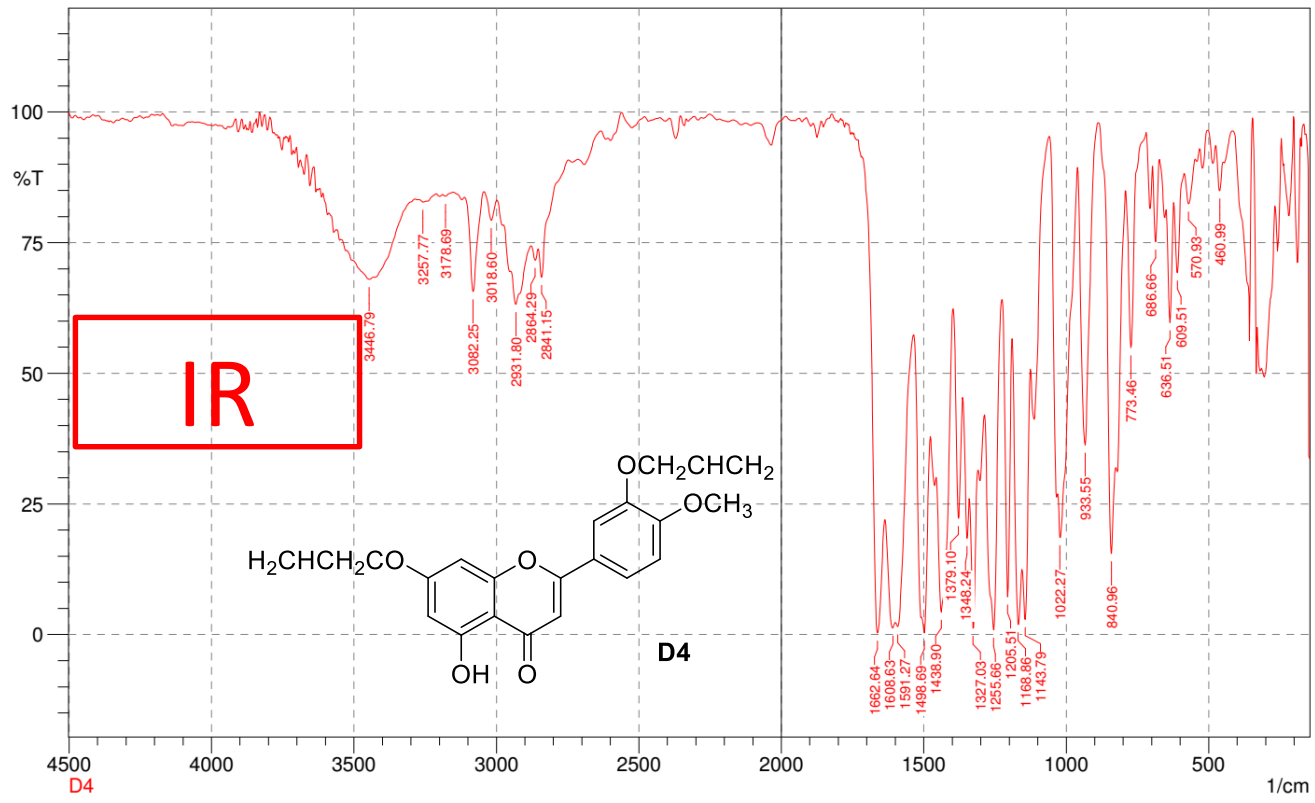
BRUKER

```
Current Data Parameters
NAME          110HUAN_DDE
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190401
Time               18.25
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               303.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7897032 MHz
NUC1               13C
P1               10.00 usec
PLW1         88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2039008 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           125.7759349 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	339	0.268015	2	292	0.145635	3	269	0.231266
4	263	0.214911	5	243	0.252528	6	235	0.230563



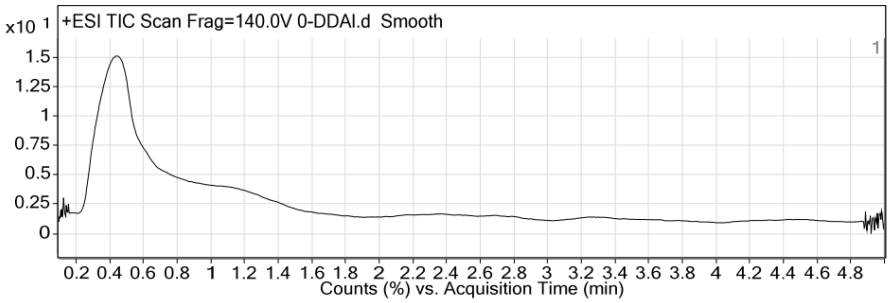
MS

Qualitative Analysis Report

Data Filename	0-DDAI.d	**Sample Name**	0-DDAI
Sample Type	Sample	**Position**	P2-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 7:06:30 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

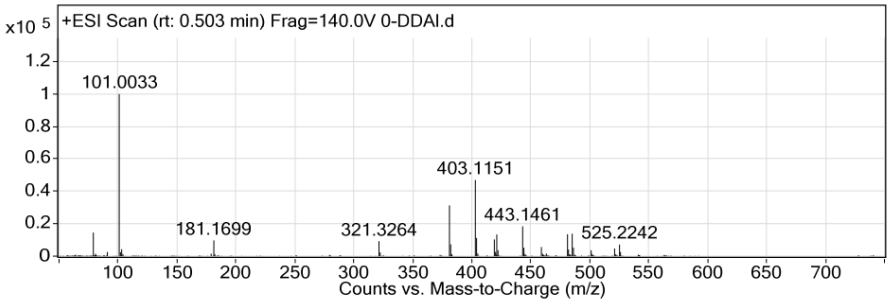
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



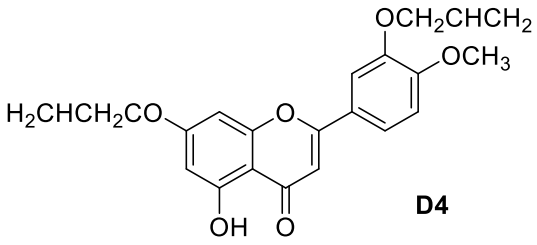
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
101.0033	1	99821.3
381.1333	1	31223.72
403.1151	1	46981.47
443.1461	1	18364.74
783.2412	1	115923.51
784.2443	1	55489.42
785.2467	1	14720.78
823.2723	1	99211.97
824.2753	1	45365.66
863.3028	1	25991.62

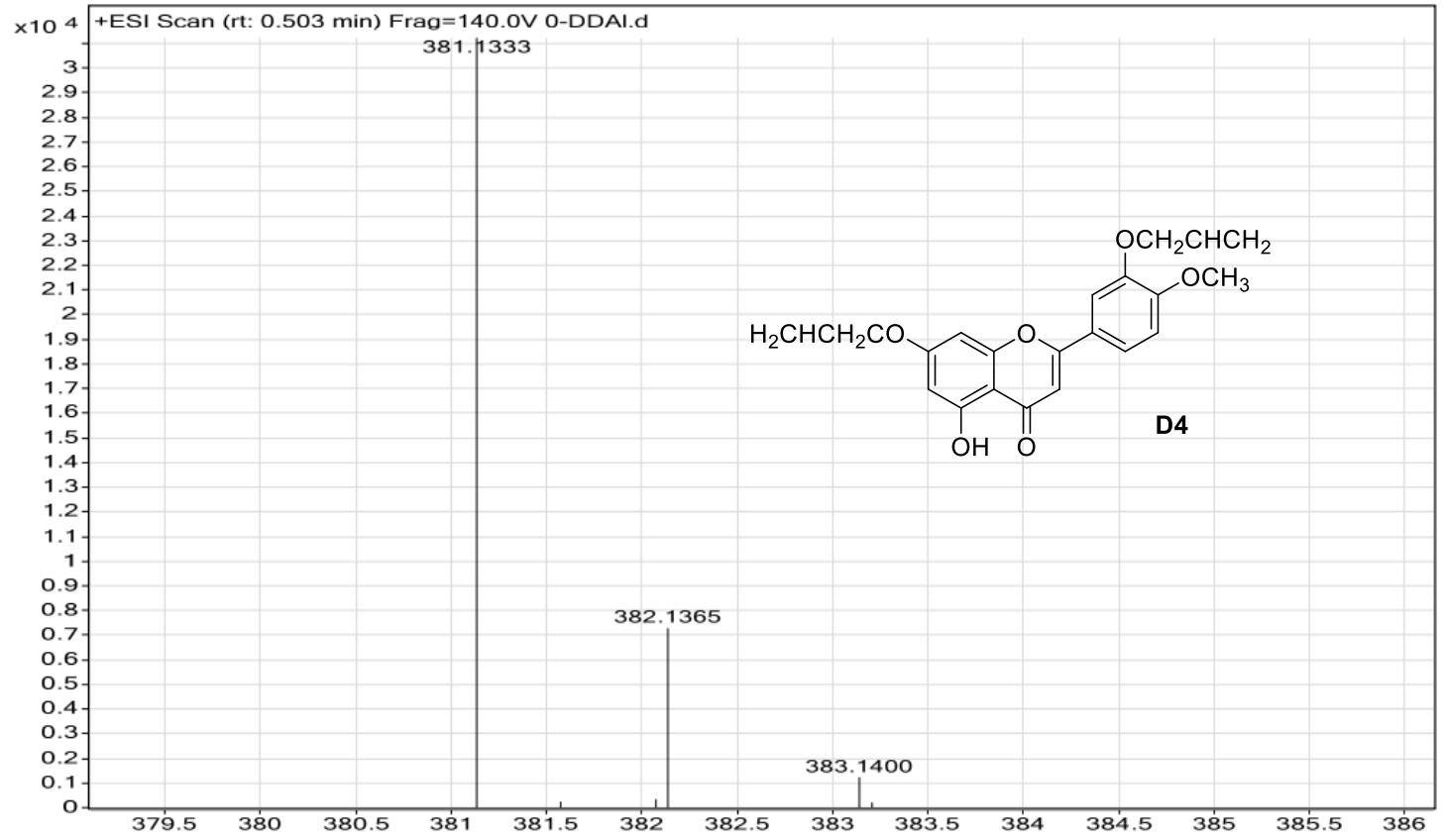


D4

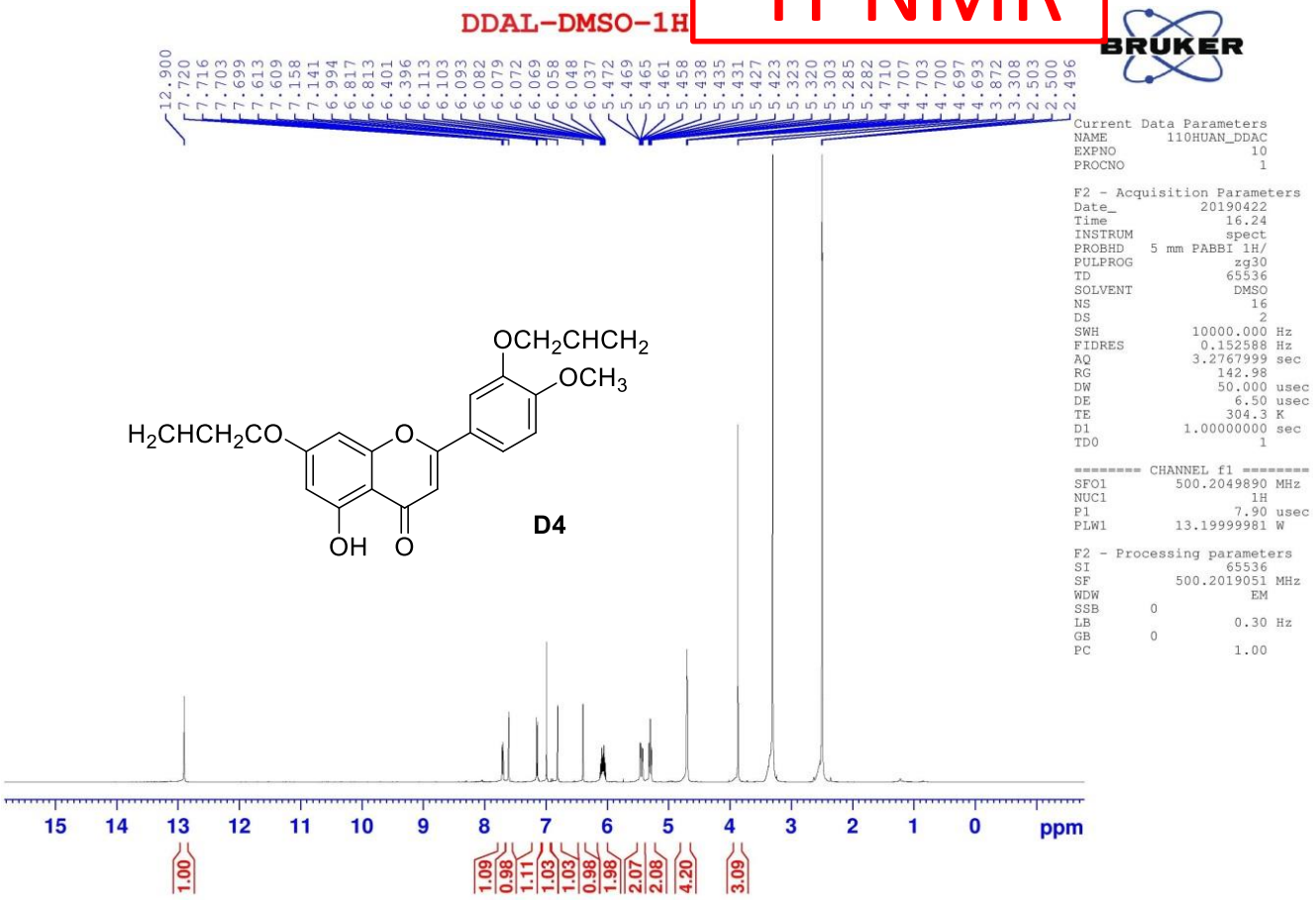
--- End Of Report ---

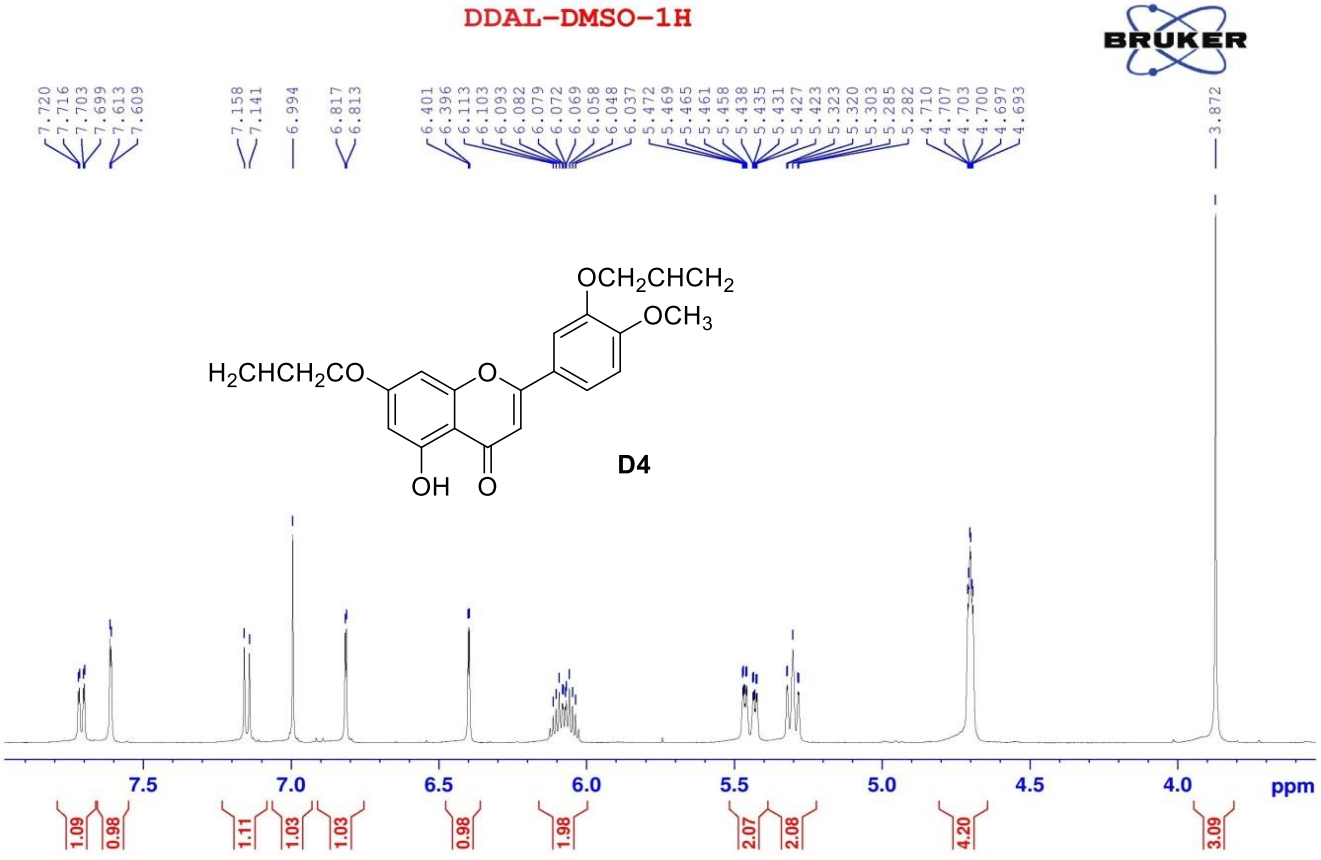
MS

Sample Name	0-DDAl	**Position**	P2-A9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	0-DDAl.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 7:06:30 PM



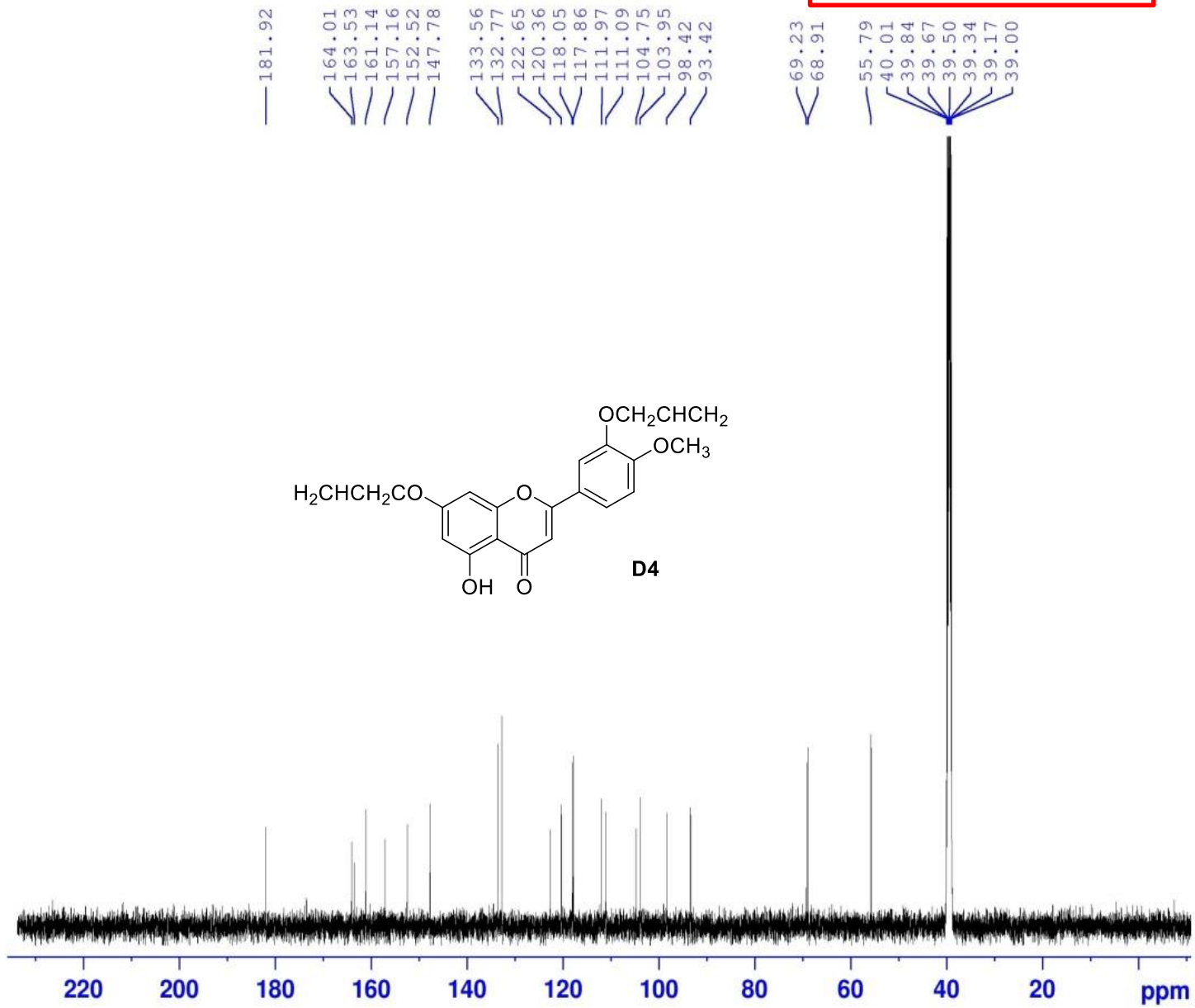
^{1}H-NMR


DDAL-DMSO-1H
BRUKER
12.900
7.720
7.716
7.703
7.699
7.613
7.609
7.158
7.141
6.994
6.817
6.813
6.401
6.396
6.113
6.103
6.093
6.082
6.079
6.072
6.069
6.058
6.048
6.037
5.472
5.469
5.465
5.461
5.458
5.438
5.435
5.431
5.427
5.423
5.323
5.320
5.303
5.285
5.282
4.710
4.707
4.703
4.700
4.697
4.693
3.872
3.308
2.503
2.500
2.496
Current Data Parameters
NAME 110HUAN_DDAC
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190422
Time 16.24
INSTRUM spect
PROBHD 5 mm PABBI 1H/
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 304.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.2049890 MHz
NUC1 1H
P1 7.90 usec
PLW1 13.19999981 W
F2 - Processing parameters
SI 65536
SF 500.2019051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OCH2CHCH2
OCH3
H2CHCH2CO
O
OH
O
D4
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.09
0.98
1.11
1.03
1.03
0.98
1.98
2.07
2.08
4.20
3.09


DDAL-DMSO-1H
BRUKER
7.720
7.716
7.703
7.699
7.613
7.609
7.158
7.141
6.994
6.817
6.813
6.401
6.396
6.113
6.103
6.093
6.082
6.079
6.072
6.069
6.058
6.048
6.037
5.472
5.469
5.465
5.461
5.458
5.438
5.435
5.431
5.427
5.423
5.323
5.320
5.303
5.285
5.282
4.710
4.707
4.703
4.700
4.697
4.693
3.872
OCH2CHCH2
OCH3
H2CHCH2CO
O
OH
O
D4
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 ppm
1.09
0.98
1.11
1.03
1.03
0.98
1.98
2.07
2.08
4.20
3.09

DDAL-DMSO-C13CPD

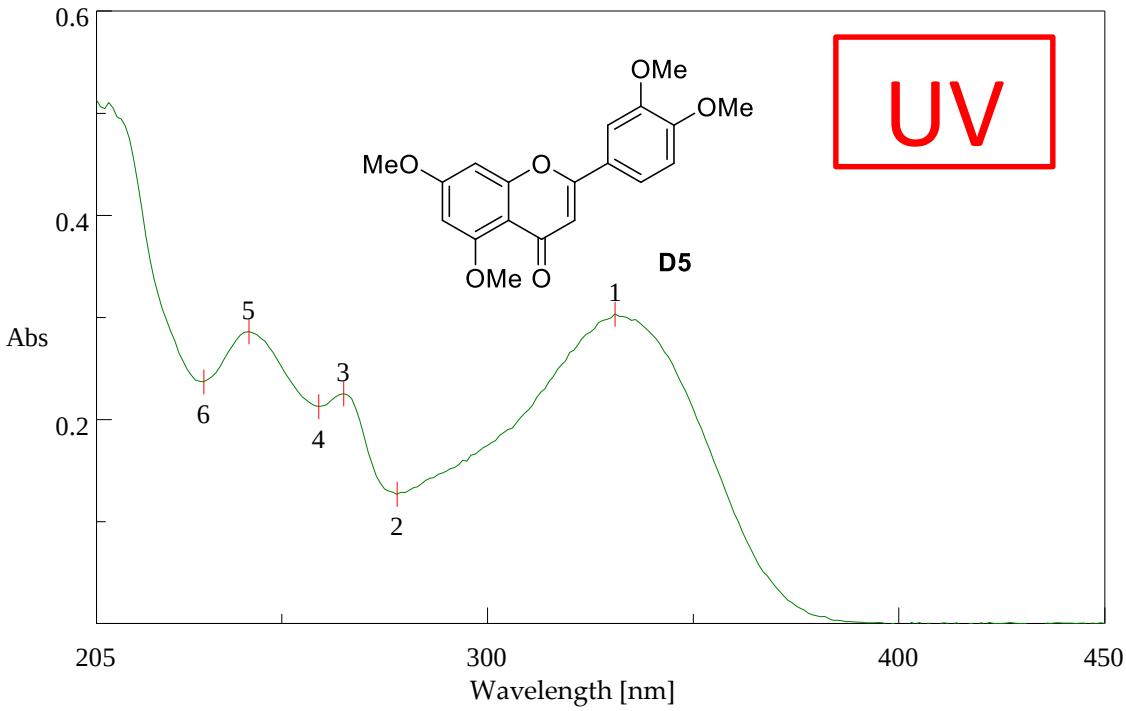
^{13}C-NMR



D4

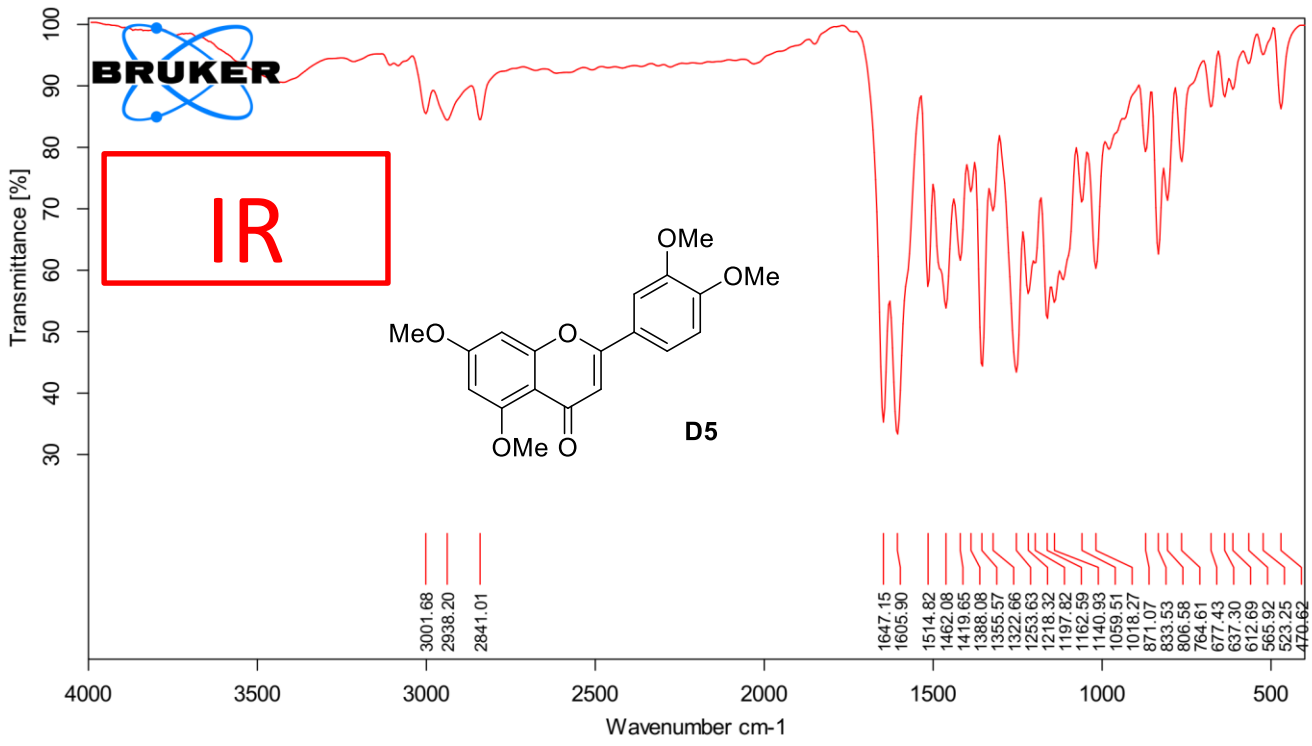
BRUKER

```
Current Data Parameters
NAME          110HUAN_DDAC
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20190422
Time                 18.15
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                 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            500.2039008 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              125.7759348 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	331	0.303043	2	278	0.12678	3	265	0.224947
4	259	0.212534	5	242	0.286019	6	231	0.236756



MS

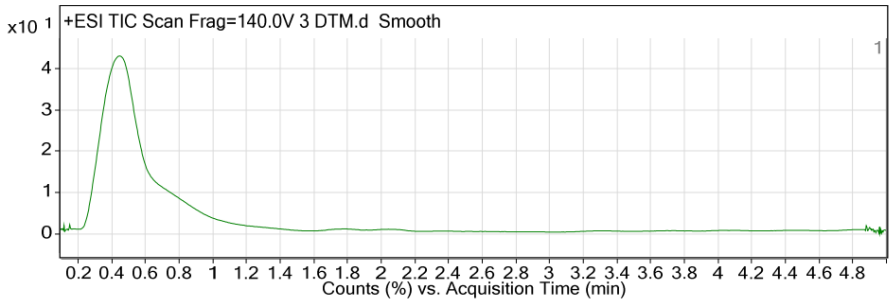
Qualitative Analysis Report

Data Filename	3 DTM.d	**Sample Name**	3 DTM
Sample Type	Sample	**Position**	P2-C4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 8:18:51 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

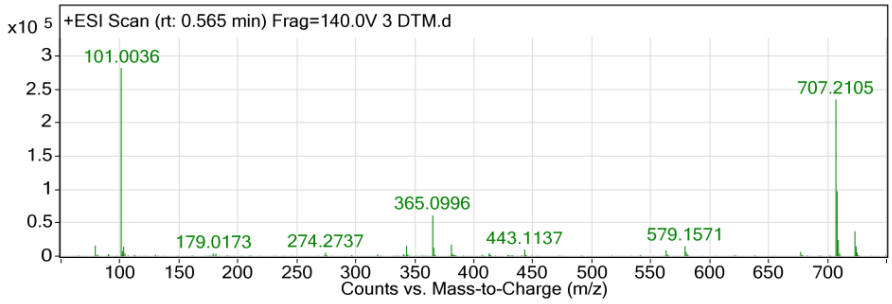
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



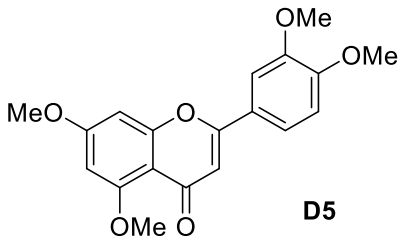
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
101.0036	1	281893.06
365.0996	1	61498.7
381.0737	1	17344.12
707.2105	1	234806.06
708.2135	1	97507.42
709.2158	1	24530
723.1833	1	37419.95
755.2456	1	17528.59
905.2926	1	62656.96
906.296	1	37812.45

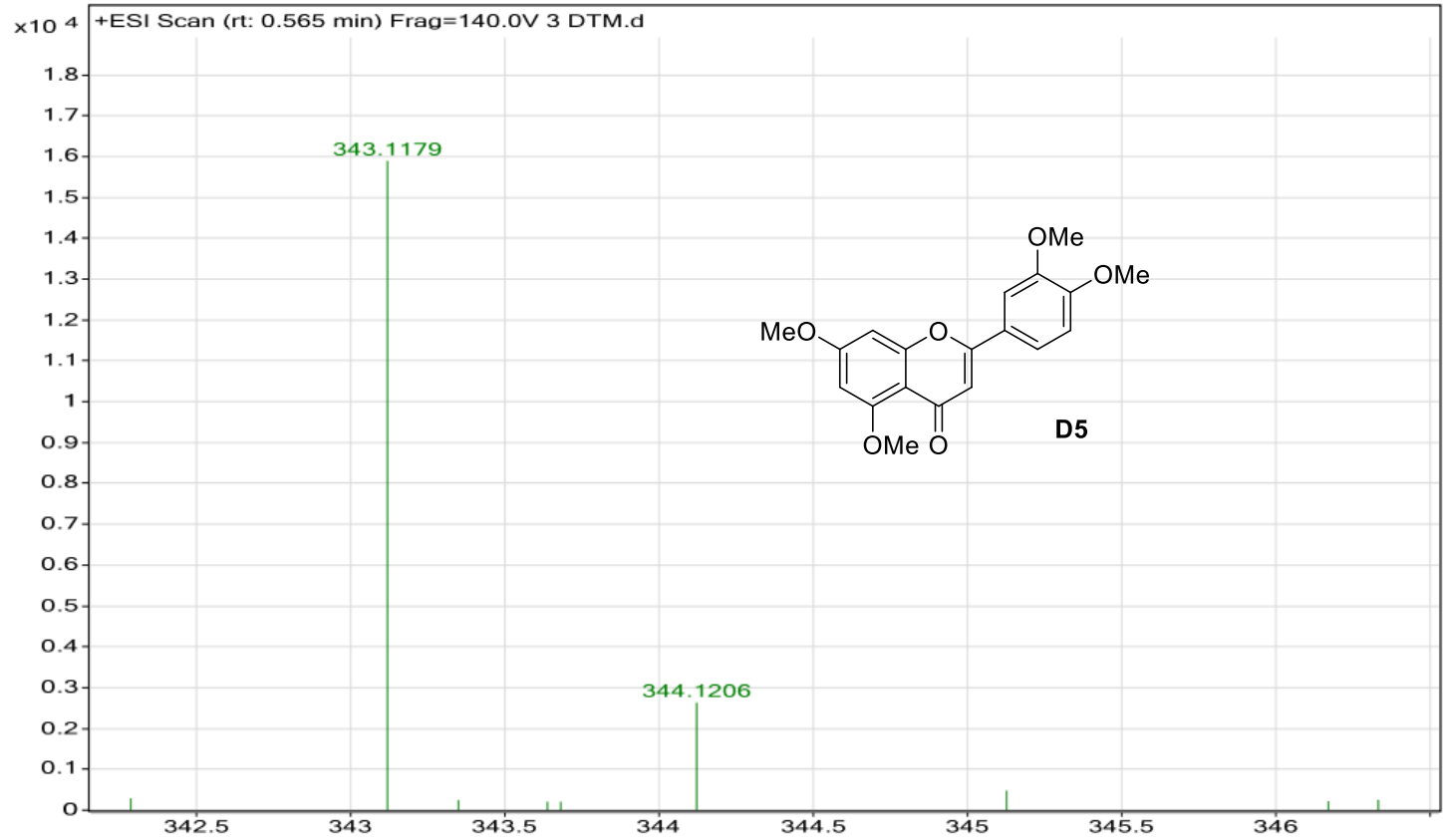


D5

--- End Of Report ---

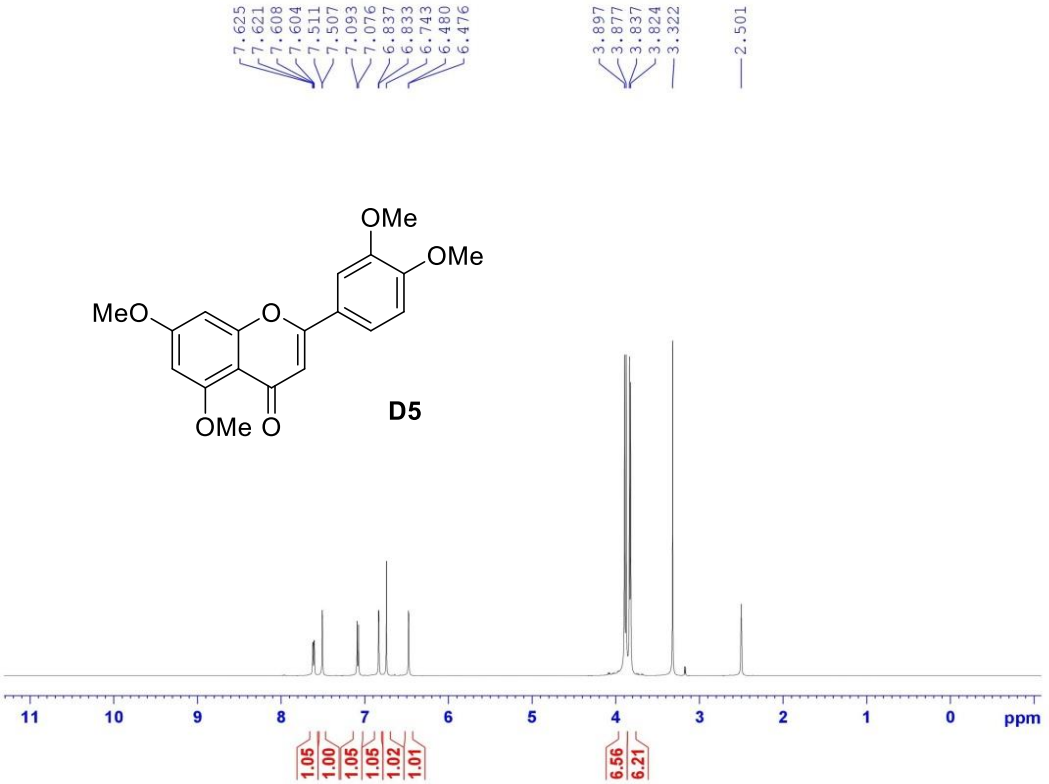
MS

Sample Name	3 DTM	**Position**	P2-C4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	3 DTM.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 8:18:51 PM



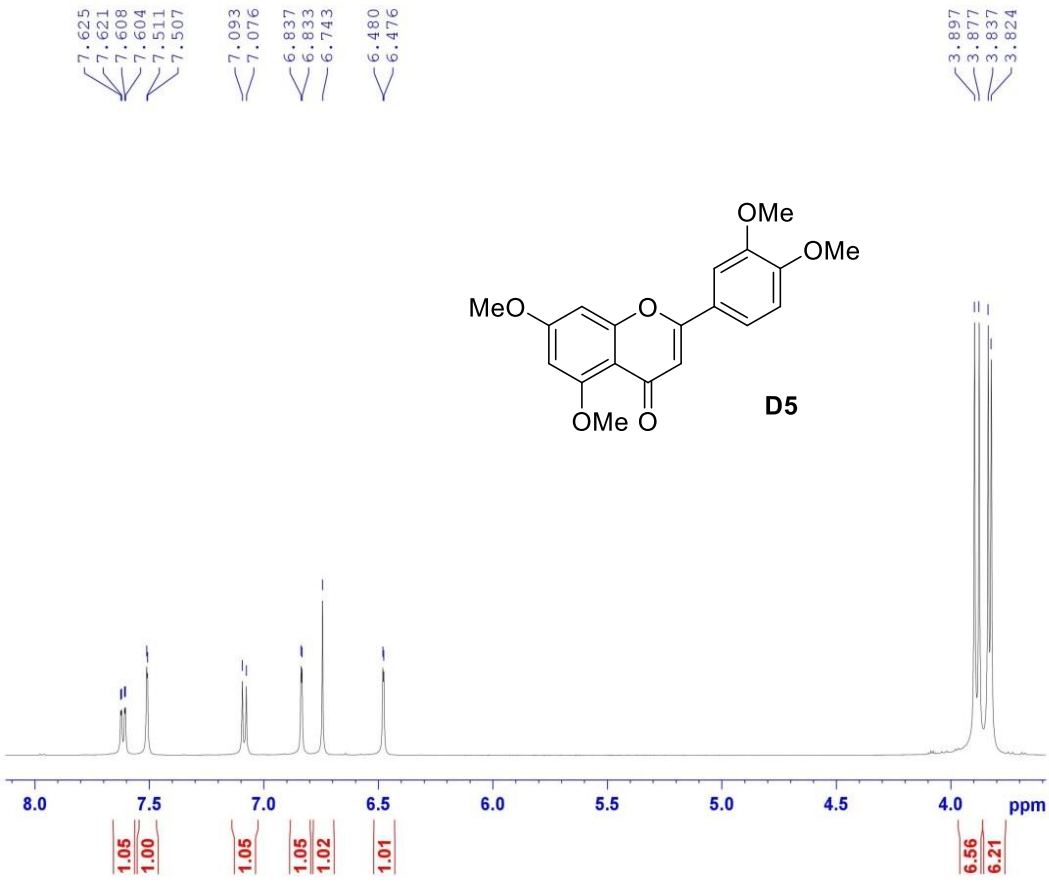
^{1}H-NMR

DTM-DMSO-1H




```
Current Data Parameters
NAME          110HUAN_HD4
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190129
Time                11.47
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                 89.63
DW                50.000 usec
DE                 6.50 usec
TE                301.6 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            500.2000036 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

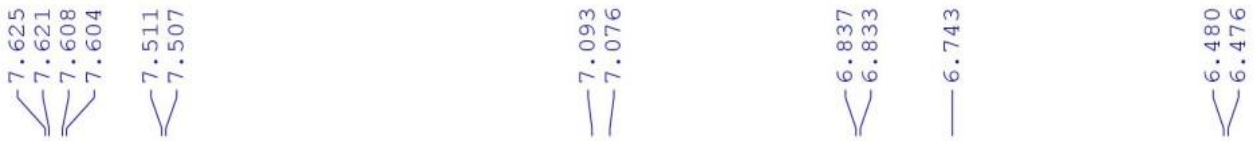
DTM-DMSO-1H

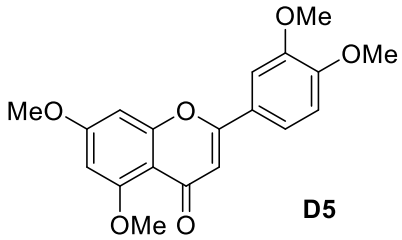



```
Current Data Parameters
NAME          110HUAN_HD4
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190129
Time                11.47
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                 89.63
DW                50.000 usec
DE                 6.50 usec
TE                301.6 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            500.2000036 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

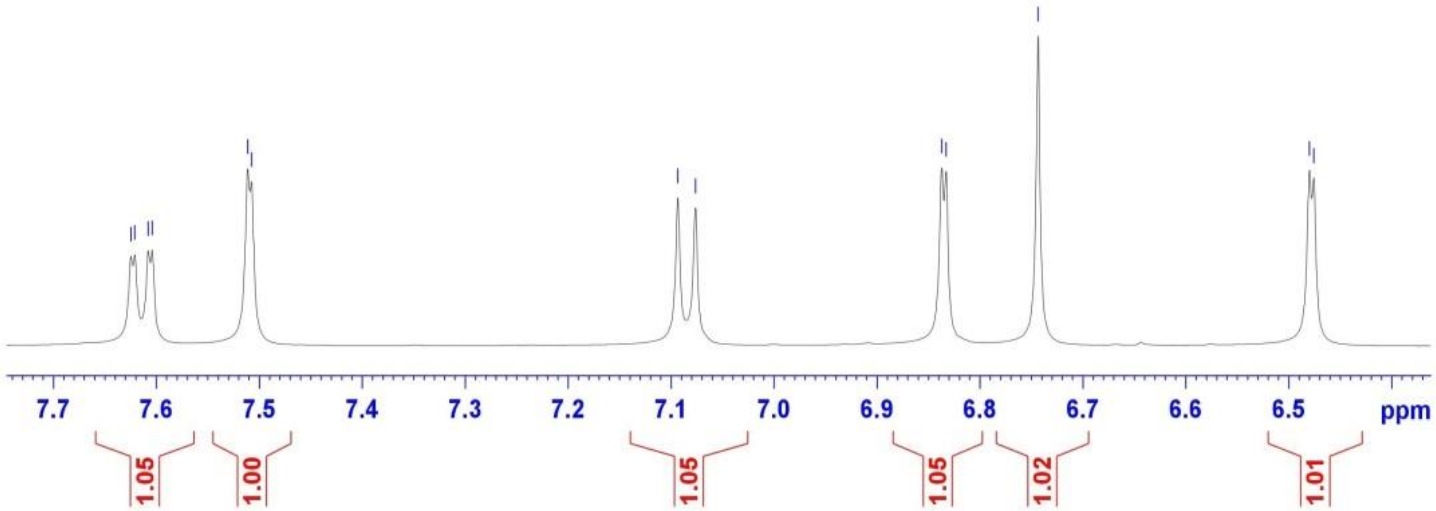
DTM-DMSO-1H

^{1}H-NMR





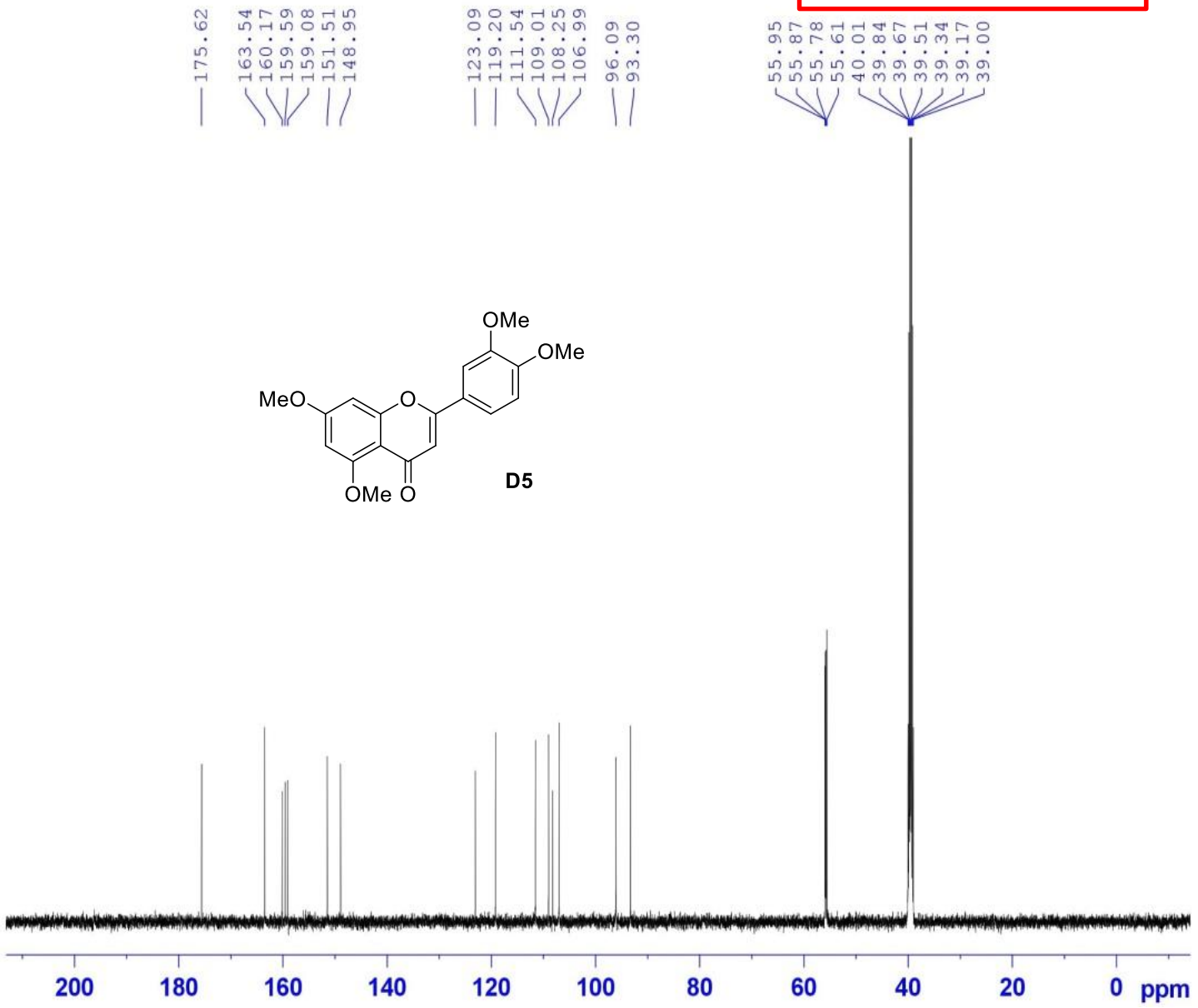
D5




```
Current Data Parameters
NAME          110HUAN_HD4
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190129
Time                11.47
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                 89.63
DW                50.000 usec
DE                 6.50 usec
TE                301.6 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            500.2000036 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

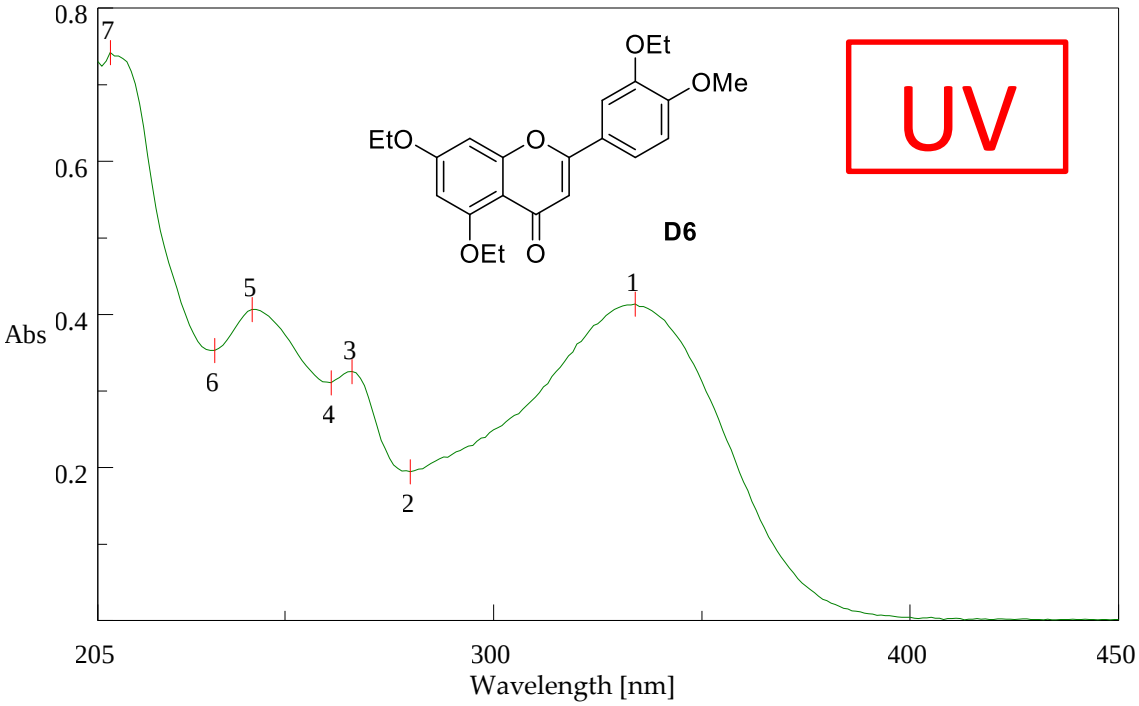
DTM-DMSO-C13CPD

^{13}C-NMR



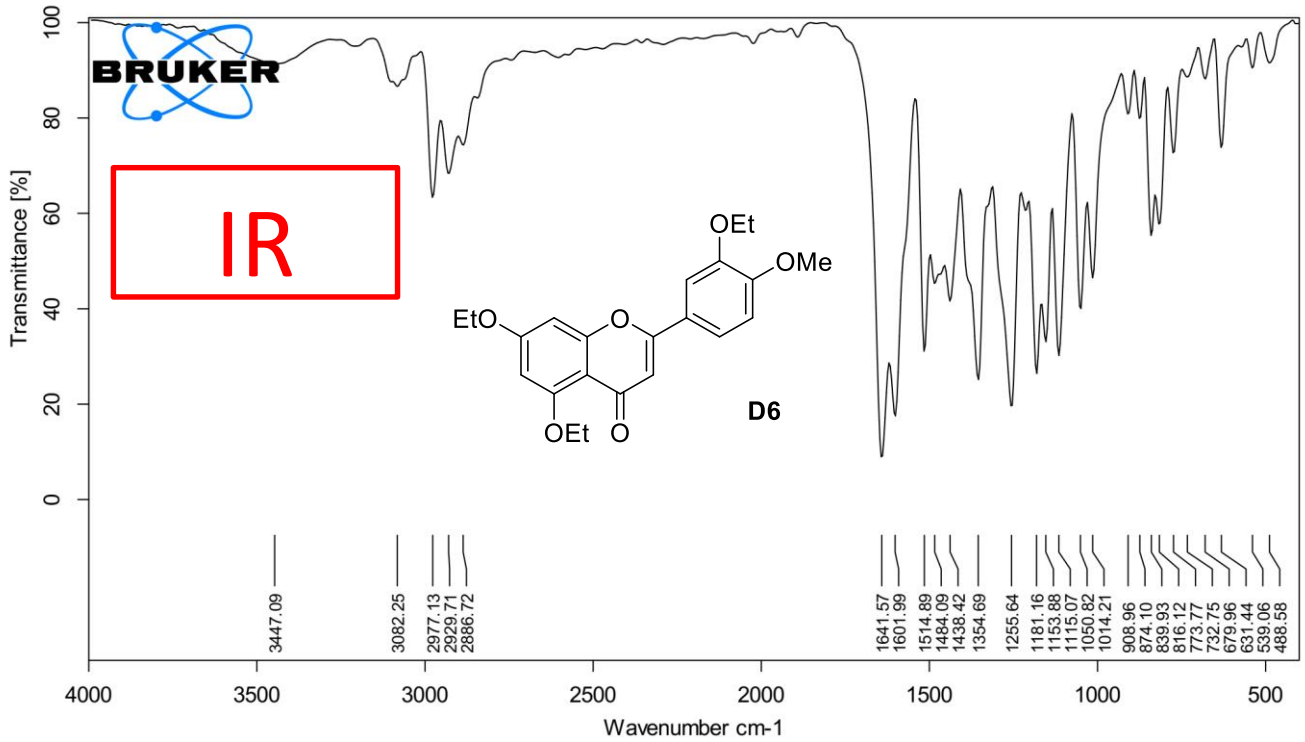
D5

```
Current Data Parameters
NAME          110HUAN_HD4
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190129
Time                17.49
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   128
DS                     4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                198.57
DW                16.800 usec
DE                 6.50 usec
TE                302.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7879670 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                 1.40
```



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	334	0.413532	2	280	0.19431	3	266	0.325215
4	261	0.310755	5	242	0.406389	6	233	0.352706
7	208	0.741798						



MS

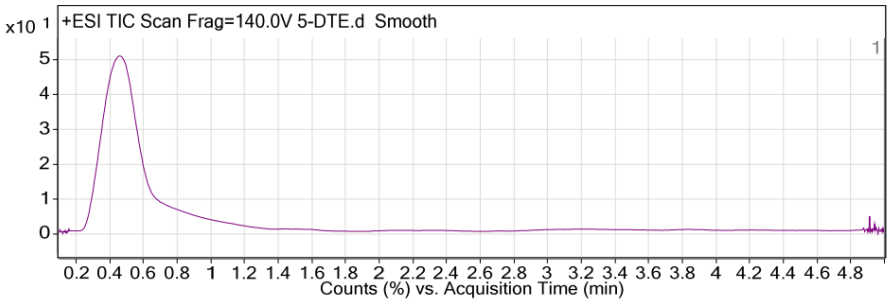
Qualitative Analysis Report

Data Filename	5-DTE.d	**Sample Name**	5-DTE
Sample Type	Sample	**Position**	P2-B4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 7:28:45 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

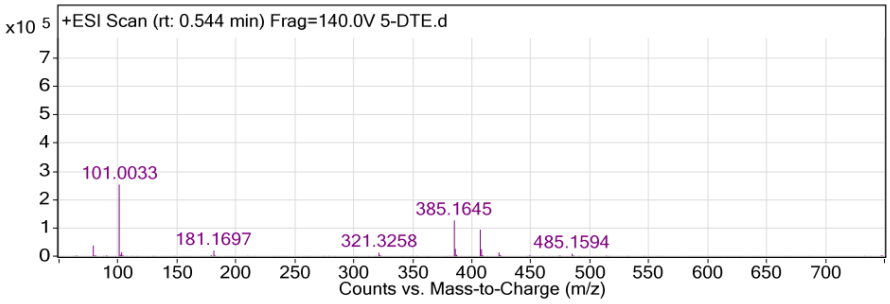
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



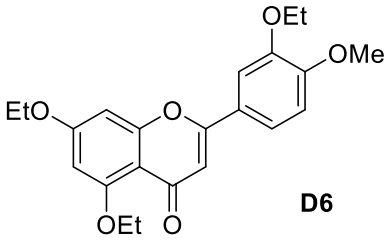
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
79.0211	1	37639.98
101.0033	1	252987.19
385.1645	1	126322.29
407.1463	1	94535.22
791.3043	1	664562.75
791.4165		43104.09
792.3076	1	319582.63
793.3099	1	90412.51
807.2774	1	135345.67
808.2803	1	61167.45

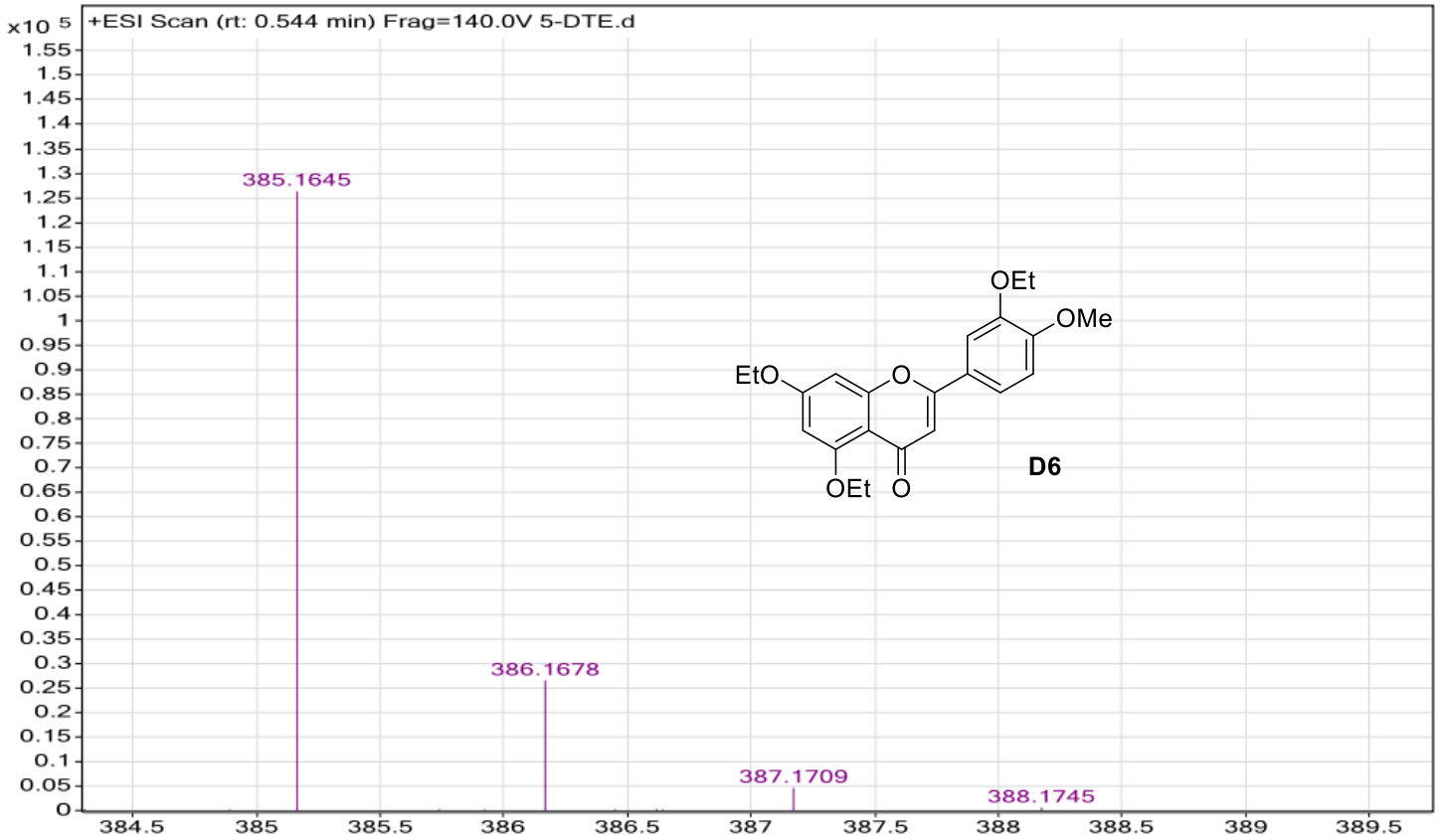


D6

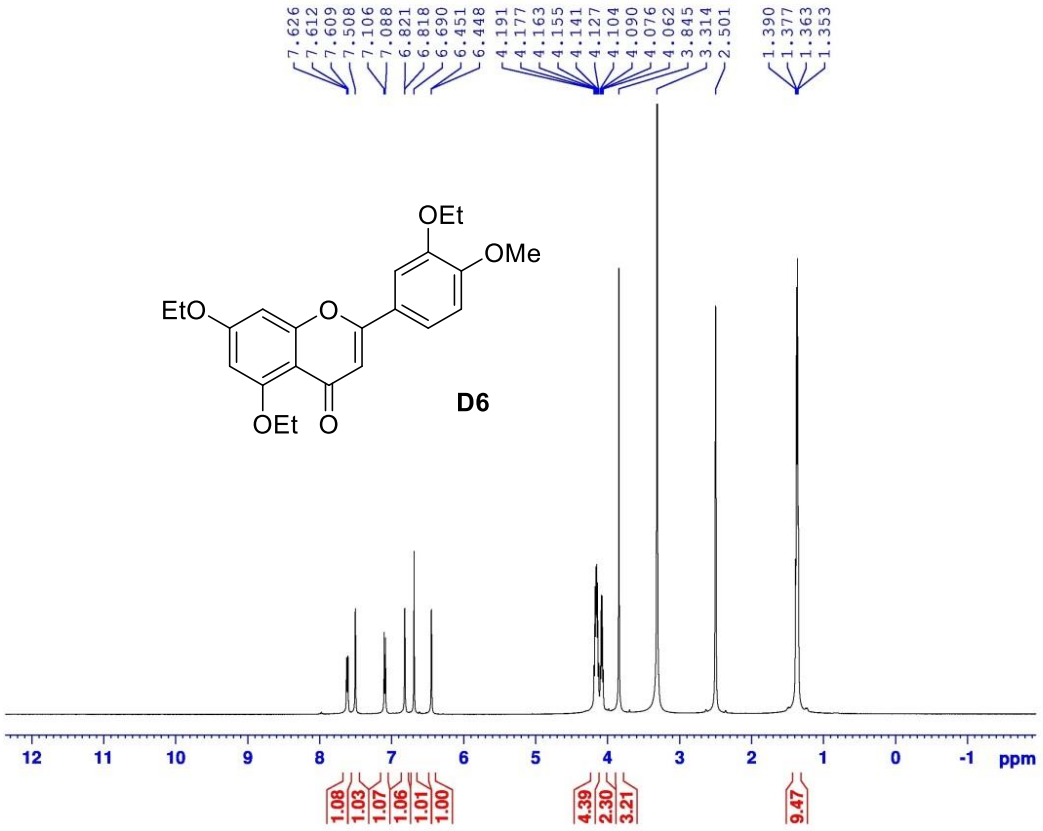
--- End Of Report ---

MS

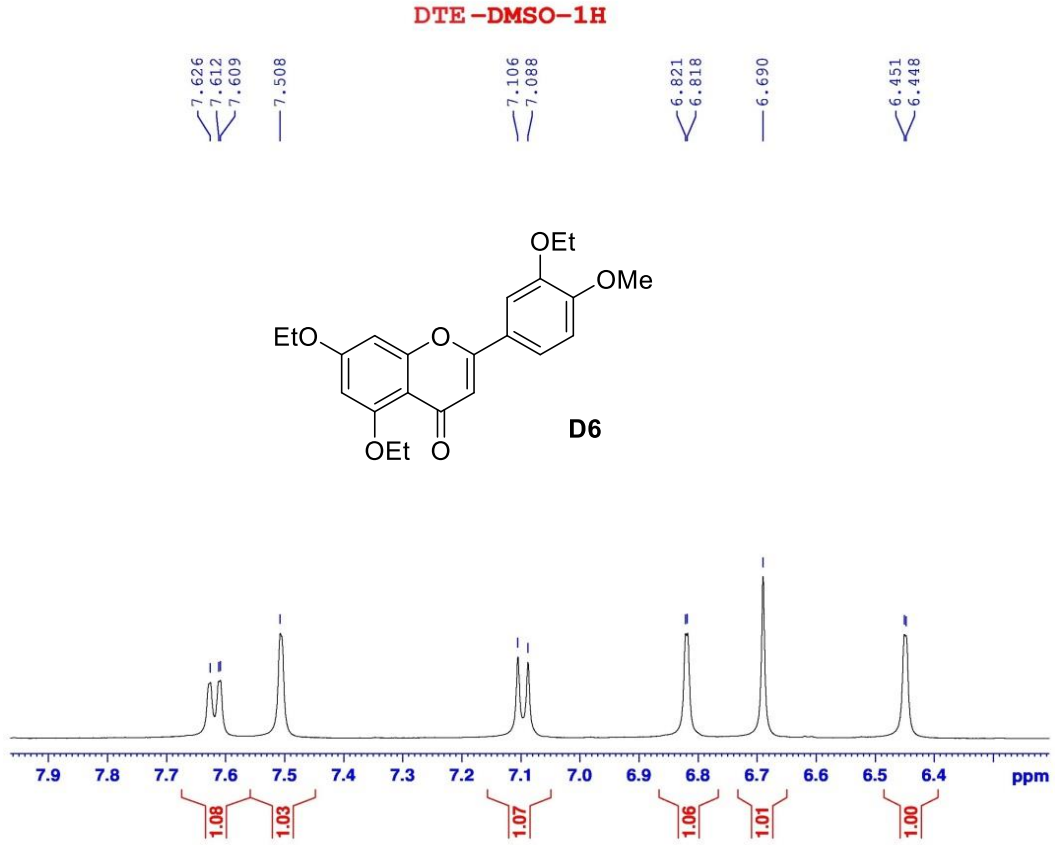
Sample Name	5-DTE	**Position**	P2-B4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	5-DTE.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 7:28:45 PM



^{1}H-NMR



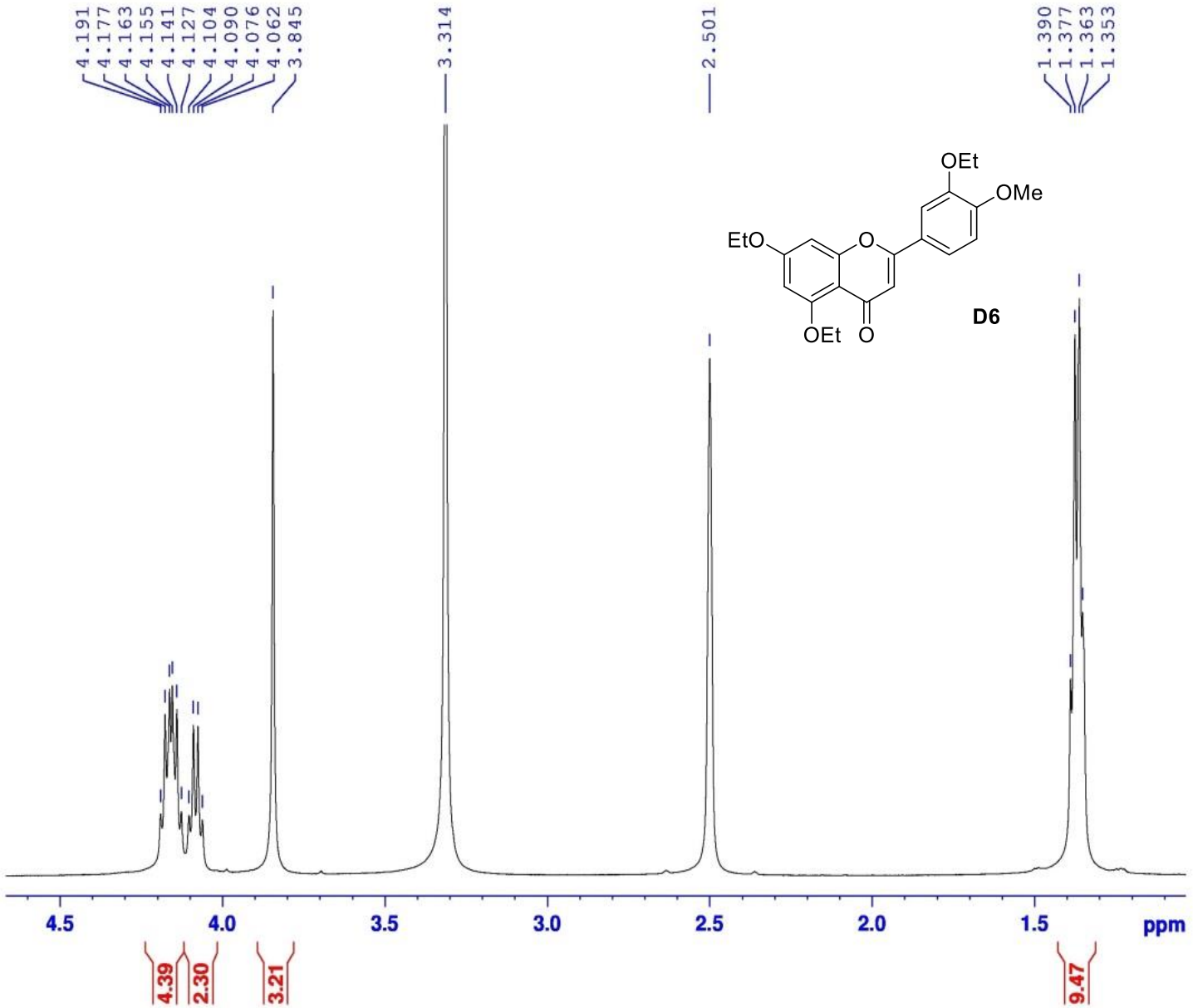

```
Current Data Parameters
NAME         110HUAN_HD5
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190129
Time               11.43
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                301.6 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            500.2000033 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME         110HUAN_HD5
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190129
Time               11.43
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                301.6 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            500.2000033 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

DTE-DMSO-1H

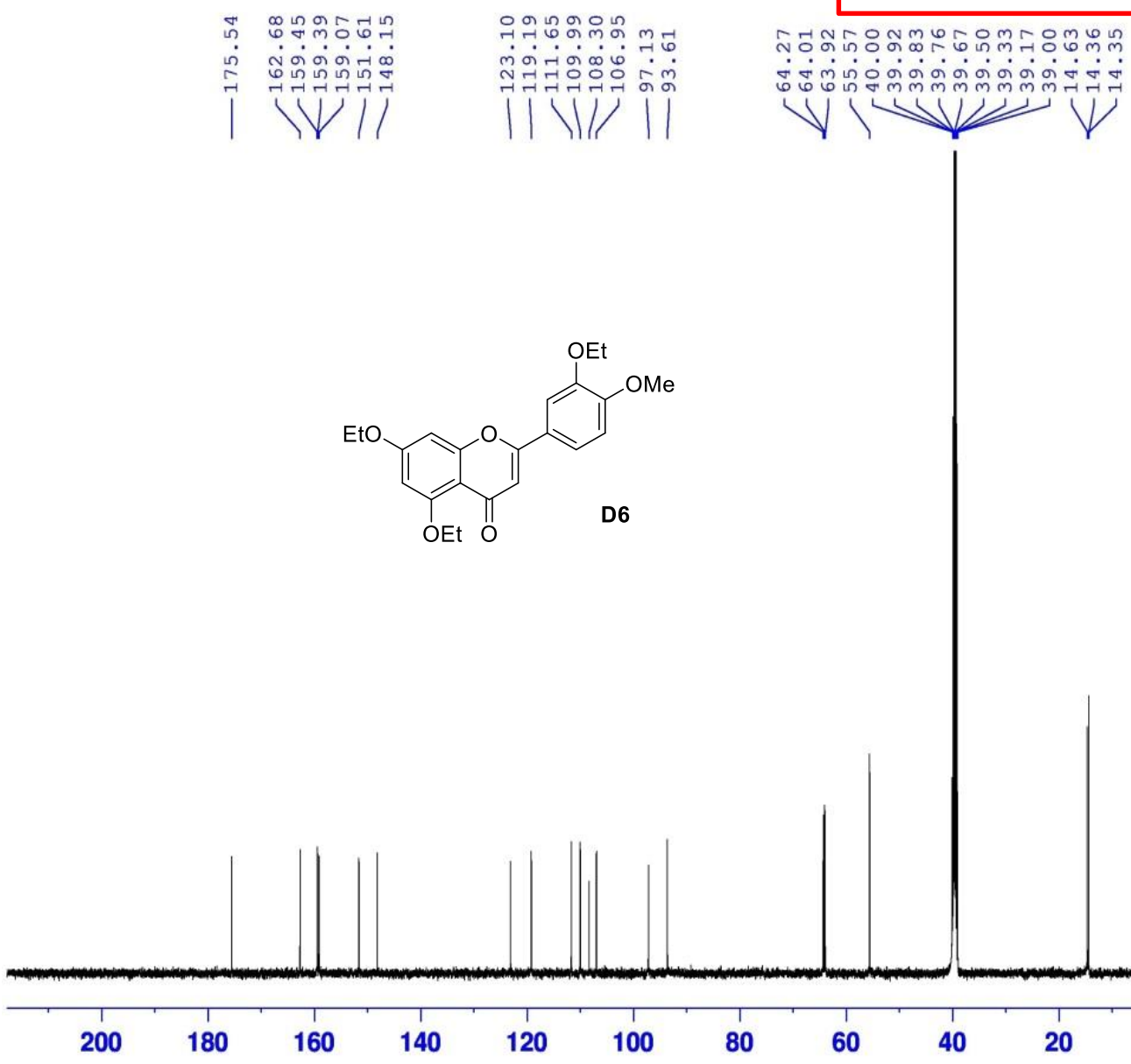
^{1}H-NMR



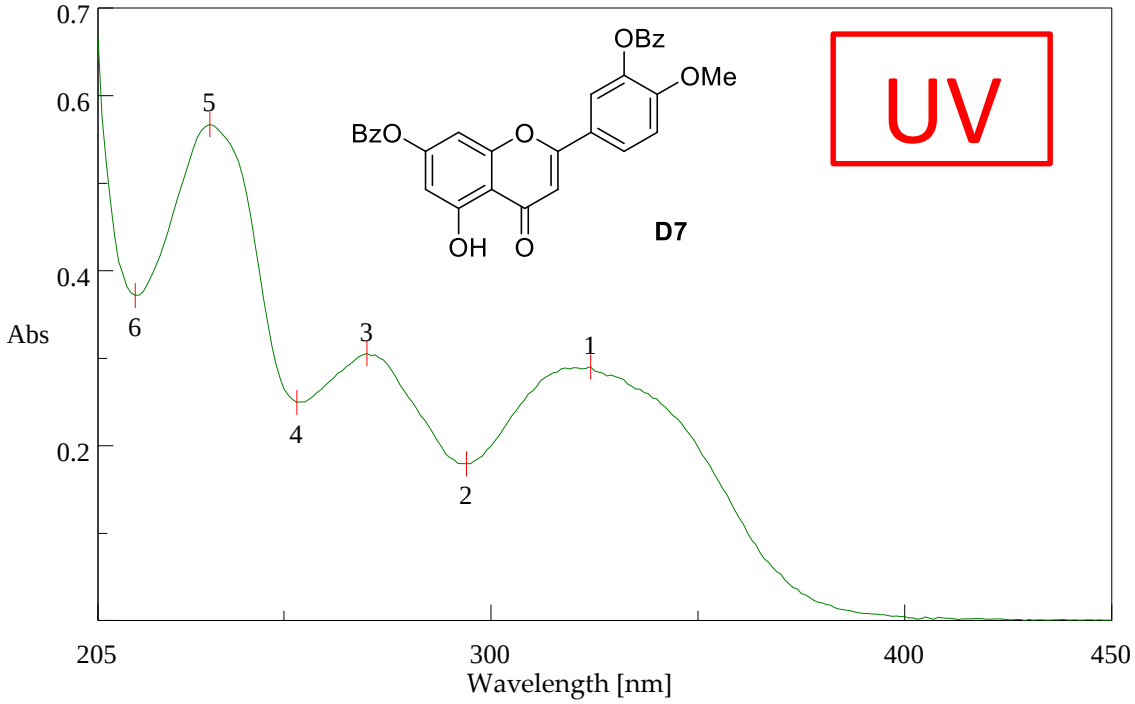

```
Current Data Parameters
NAME          110HUAN_HD5
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190129
Time               11.43
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                301.6 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            500.2000033 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

DTE-DMSO-C13CPD

^{13}C-NMR

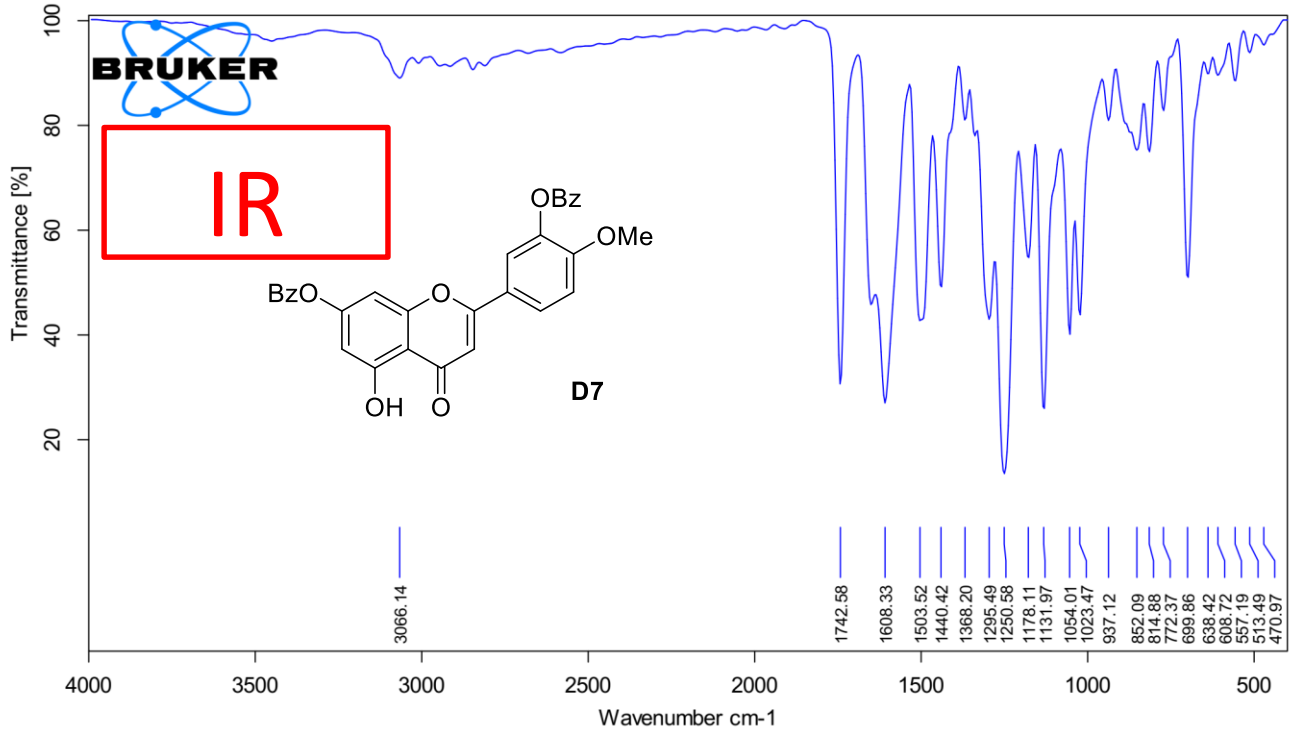



```
Current Data Parameters
NAME          110HUAN_HD5
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190129
Time                17.07
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                    256
DS                      4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                 198.57
DW                 16.800 usec
DE                  6.50 usec
TE                302.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          125.7879670 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            125.7754556 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	324	0.290155	2	294	0.179039	3	270	0.305058
4	253	0.249541	5	232	0.566944	6	214	0.371536



MS

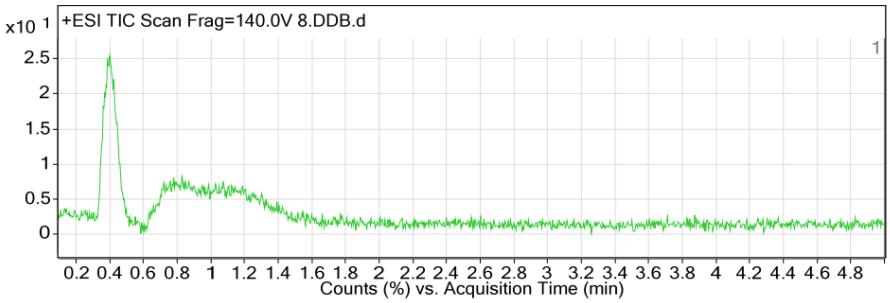
Qualitative Analysis Report

Data Filename	8.DDB.d	**Sample Name**	8.DDB
Sample Type	Sample	**Position**	P2-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Cot ngan - MSMS_Pos.m	**Acquired Time**	04/08/2020 7:45:28 PM
IRM Calibration Status	Success	**DA Method**	COTNGAN.M.m
Comment			

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

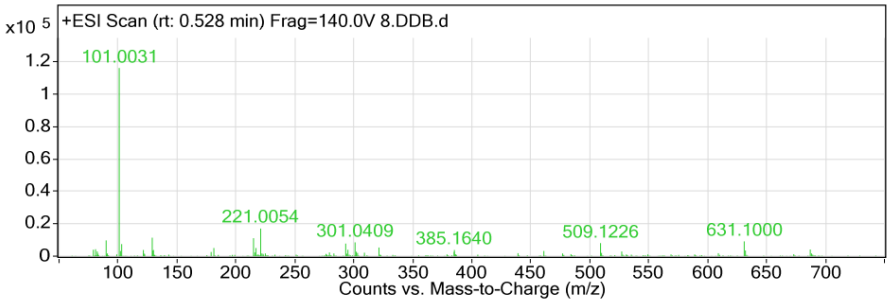
User Chromatograms

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



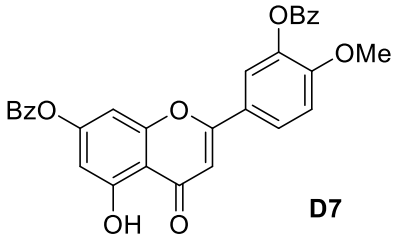
User Spectra

Fragmentor Voltage 140 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund
90.0059	2	9788.28
101.0031	1	116298.95
102.9987	1	7500.39
129.0125	2	11382.23
214.9812	1	11176.09
221.0054	1	17083.07
292.9947	1	7780.54
301.0409	1	8574.88
509.1226	1	8061.85
631.1	1	9216.2

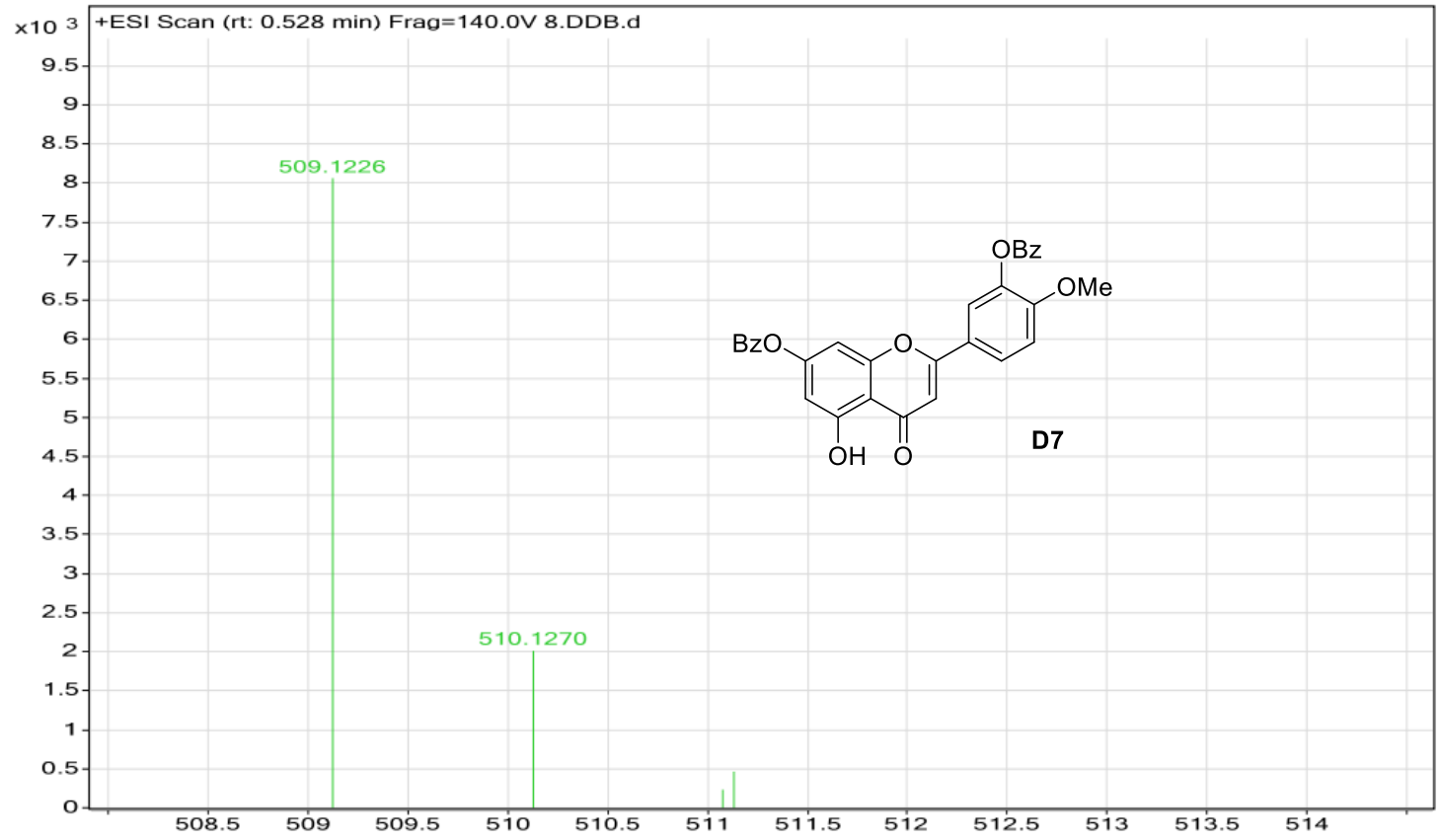


D7

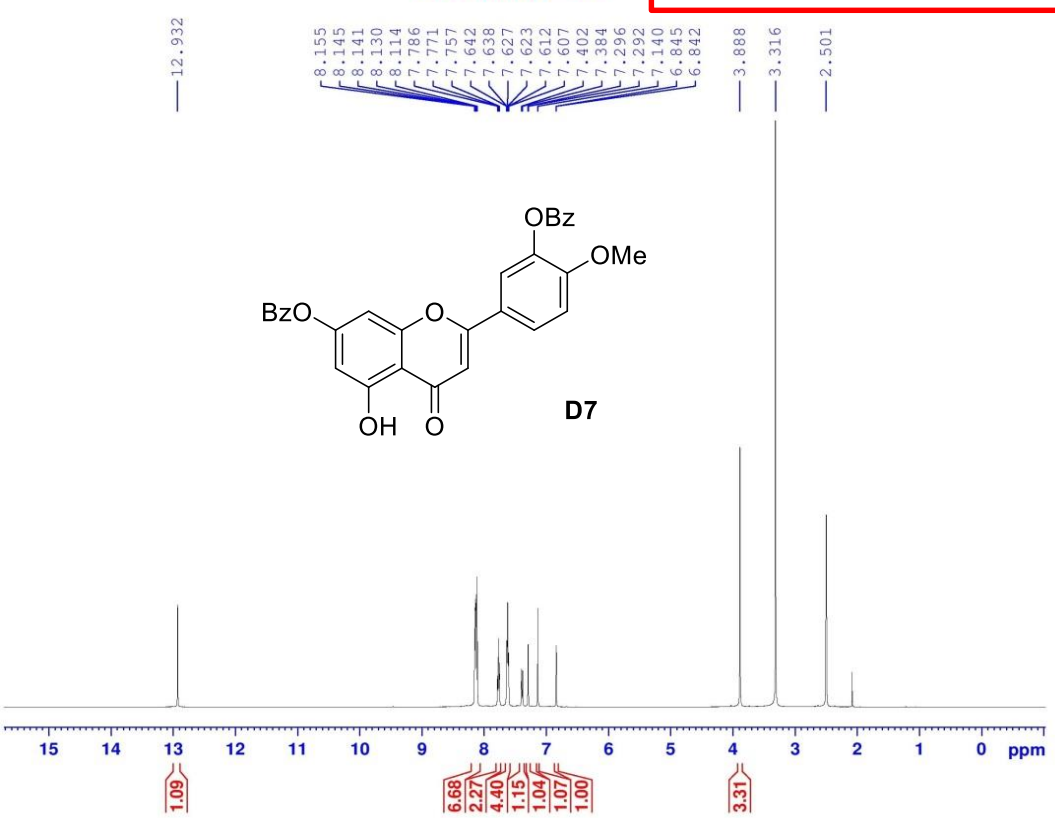
--- End Of Report ---

MS

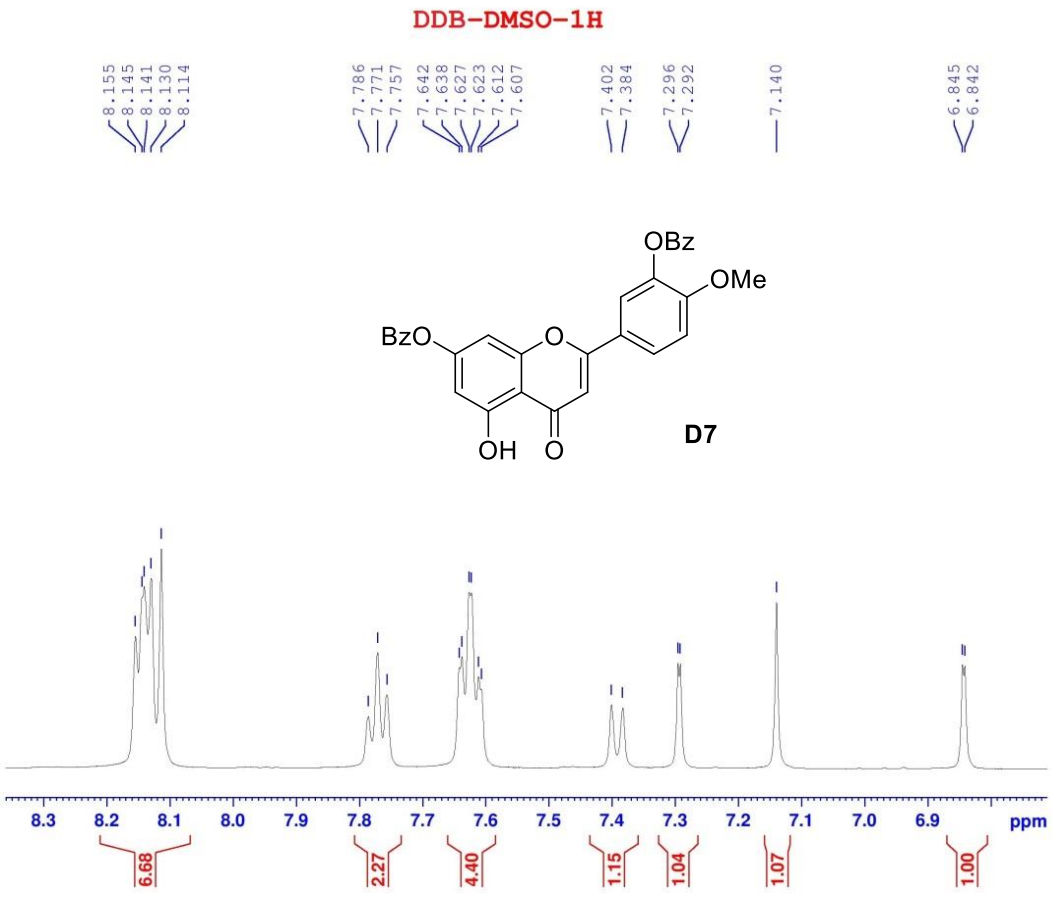
Sample Name	8.DDB	**Position**	P2-B7	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	8.DDB.d	**ACQ Method**	Cot ngan - MSMS_Pos.	**Comment**		**Acquired Time**	04/08/2020 7:45:28 PM



^{1}H-NMR



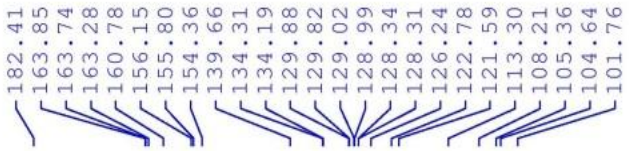

```
Current Data Parameters
NAME          110HUAN_HD3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20190129
Time                 11.51
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                   301.6 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              500.2000036 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

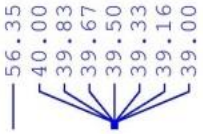


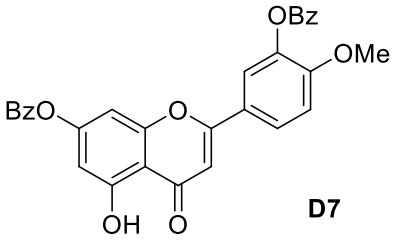

```
Current Data Parameters
NAME          110HUAN_HD3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20190129
Time                 11.51
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                   301.6 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              500.2000036 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

DDB-DMSO-C13CPD

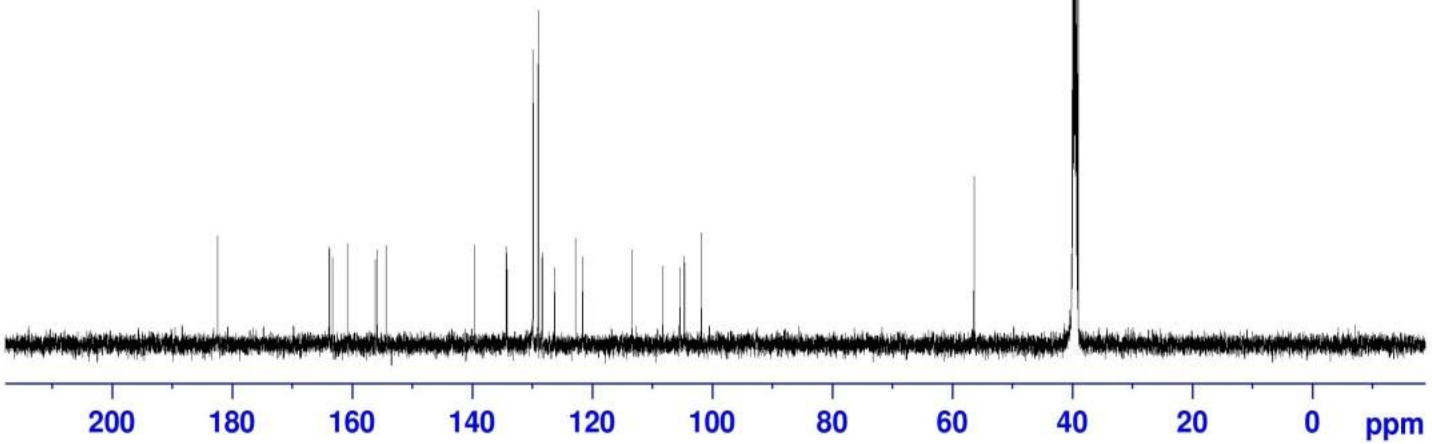
^{13}C-NMR







D7




```
Current Data Parameters
NAME          110HUAN_HD3
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190129
Time                12.35
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                     256
DS                       4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                 198.57
DW                 16.800 usec
DE                  6.50 usec
TE                 302.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1         125.7879670 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           125.7754559 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

Reference

1. Tran, T.-S.; Le, M.-T.; Tran, T.-D.; Tran, T.-H.; Thai, K.-M. Design of Curcumin and Flavonoid Derivatives with Acetylcholinesterase and Beta-Secretase Inhibitory Activities Using in Silico Approaches. *Molecules* **2020**, *25*, 3644.
2. Wildman, S.A.; Crippen, G.M. Prediction of Physicochemical Parameters by Atomic Contributions. *J Chem Inf Comput Sci* **1999**, *39*, 868-873, doi:10.1021/ci990307l.
3. Oprea, T.I. Property distribution of drug-related chemical databases. *Journal of computer-aided molecular design* **2000**, *14*, 251-264, doi:10.1023/a:1008130001697.
4. Neumann, U.; Ufer, M.; Jacobson, L.H.; Rouzade-Dominguez, M.-L.; Huledal, G.; Kolly, C.; Lüönd, R.M.; Machauer, R.; Veenstra, S.J.; Hurth, K., et al. The BACE-1 inhibitor CNP520 for prevention trials in Alzheimer's disease. *EMBO Mol Med* **2018**, *10*, e9316, doi:10.15252/emmm.201809316.