Supplementary

Synthesis of 14-Substituted-14H-Dibenzo[*a,j*]Xanthene Derivatives in Presence of Effective Synergetic Catalytic System Bleaching Earth Clay and PEG-600

Sandeep T. Atkore [1,*], Giribala M. Bondle [2], Pranita V. Raithak [3], Vinod T. Kamble [4], Ravi Varala [5], Mufsir Kuniyil [6], Mohammad Rafe Hatshan [6], Baji Shaik [7], Syed Farooq Adil [6,*] and Mohammed Althaf Hussain [8]

[1] Department of Biochemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad 431004, Maharashtra, India

[2] Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad 431004, Maharashtra, India; giribalamb@gmail.com

[3] Department of Botany, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad 431004, Maharashtra, India; pvraithak@yahoo.com

[4] Department of Chemistry, Government Institute of Science, Mumbai 400032, Maharashtra, India; vtkd@rediffmail.com

[5] Scrips Pharma, Mallapur, Hyderabad 50076, Telangana, India; ravivarala@gmail.com

[6] Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia; mkuniyil@ksu.edu.sa (M.K.); mhatshan@ksu.edu.sa (M.R.H.)

[7] Department of Advanced Materials Engineering for Information & Electronics, Kyung Hee University, 1732 Deogyeong-daero, Giheung-gu, Yongin-si 446-701, Gyeonggi-do, Korea; shaikbaji2@khu.ac.kr

[8] Research Institute for the Creation of Functional and Structural Materials, Fukuoka University, 8-19-1 Nanakuma, Jonan-ku, Fukuoka 814-0180, Japan; altaf.mh7@gmail.com

* Correspondence: statkore0@gmail.com (S.T.A.); sfadil@ksu.edu.sa (S.F.A.)

1. Antibacterial Activity

The antibacterial activities of the synthesized compounds were determined by the agar well diffusion method. The compounds were evaluated for antibacterial activity against *Staphylococcus aureus* (MTCC 96) and *Pseudomonas aeruginosa* (Wild). The culture strains of bacteria were maintained on a nutrient agar slant at 37±0.5 °C for 24 h. The antibacterial activity was evaluated using nutrient agar plates seeded separately with 0.1 mL of each bacterial culture strain suspension prepared in sterile saline (0.85%) of 105 CFU/mL dilutions. Wells of 6 mm diameter were filled with 0.1 mL of compound solution at a fixed concentration of 25 μg/mL, separately for each bacterial strain. All the plates were incubated at 37±0.5 °C for 24 h. The zone of inhibition of compounds in mm were noted. The results of in vitro antibacterial activities of compounds (3a–j) against bacterial strains are summarized in Table S1.

Table S1. Antibacterial activity of synthesized 14-substituted 14*H*-benzo[*a,j*] xanthene derivatives.

		Name of the test organism	
Entry	**Product**	*Staphylococcus aureus* (MTCC 96)	*Pseudomonas aeruginosa* (Wild)
		Zone of inhibition (mm) of Std. drugs (25 ◎g)	
3a	4-chlorophenyl	1.50	1.20
3b	4-nitrophenyl	1.70	1.40
3c	3-nitrophenyl	1.90	2.00
3d	3-flurophenyl	4.25	5.70
3e	2,4-dichlorophenyl	1.01	1.20
3f	phenyl	2.03	2.70
3g	4-methoxyphenyl	1.80	2.20
3h	4-methylphenyl	3.01	4.60
3i	4-dimethylaminophenyl	4.00	3.09
3j	ethyl	3.80	3.92
Control	*Streptomycin*	34.5	19.5
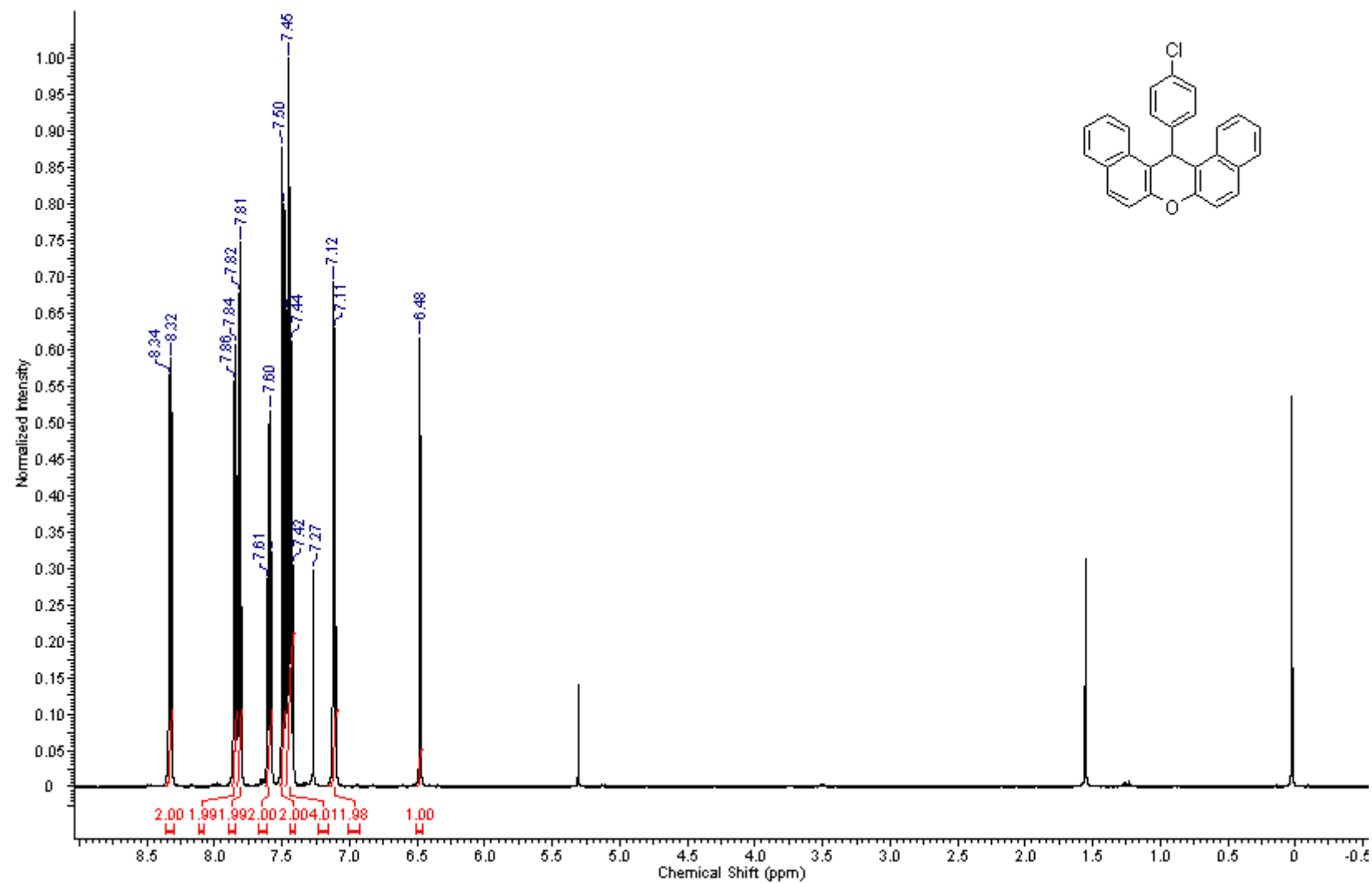
Figure S1. ¹H NMR of compound 14-(4-Chlorophenyl)-14*H*-dibenzo[*a,j*]xanthene 3a.

Figure S2. ^{13}C NMR of compound 14-(4-Chlorophenyl)-14*H*-dibenzo[*a,j*]xanthene 3a.

Figure S3. MS of compound 14-(4-Chlorophenyl)-14*H*-dibenzo[*a,j*]xanthene 3a.
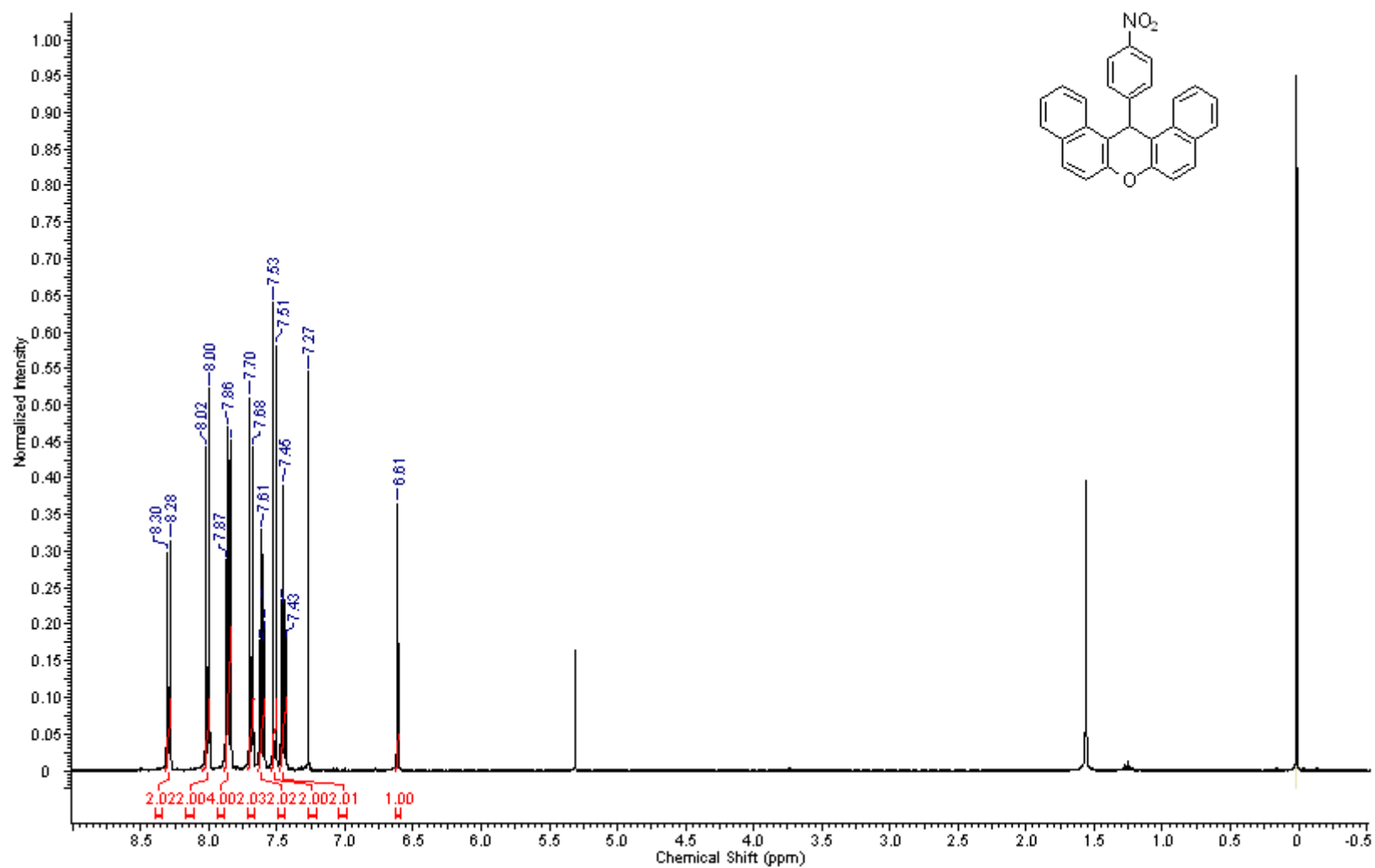
Figure S4. ^{1}H NMR of compound 14-(4-Nitrophenyl)-14*H*-dibenzo[*a,j*]xanthene 3b.

Figure S5. ^{13}C NMR of compound 14-(4-Nitrophenyl)-14*H*-dibenzo[*a,j*]xanthene 3b.

Figure S6. MS of compound 14-(4-Nitrophenyl)-14*H*-dibenzo[*a,j*]xanthene 3b.
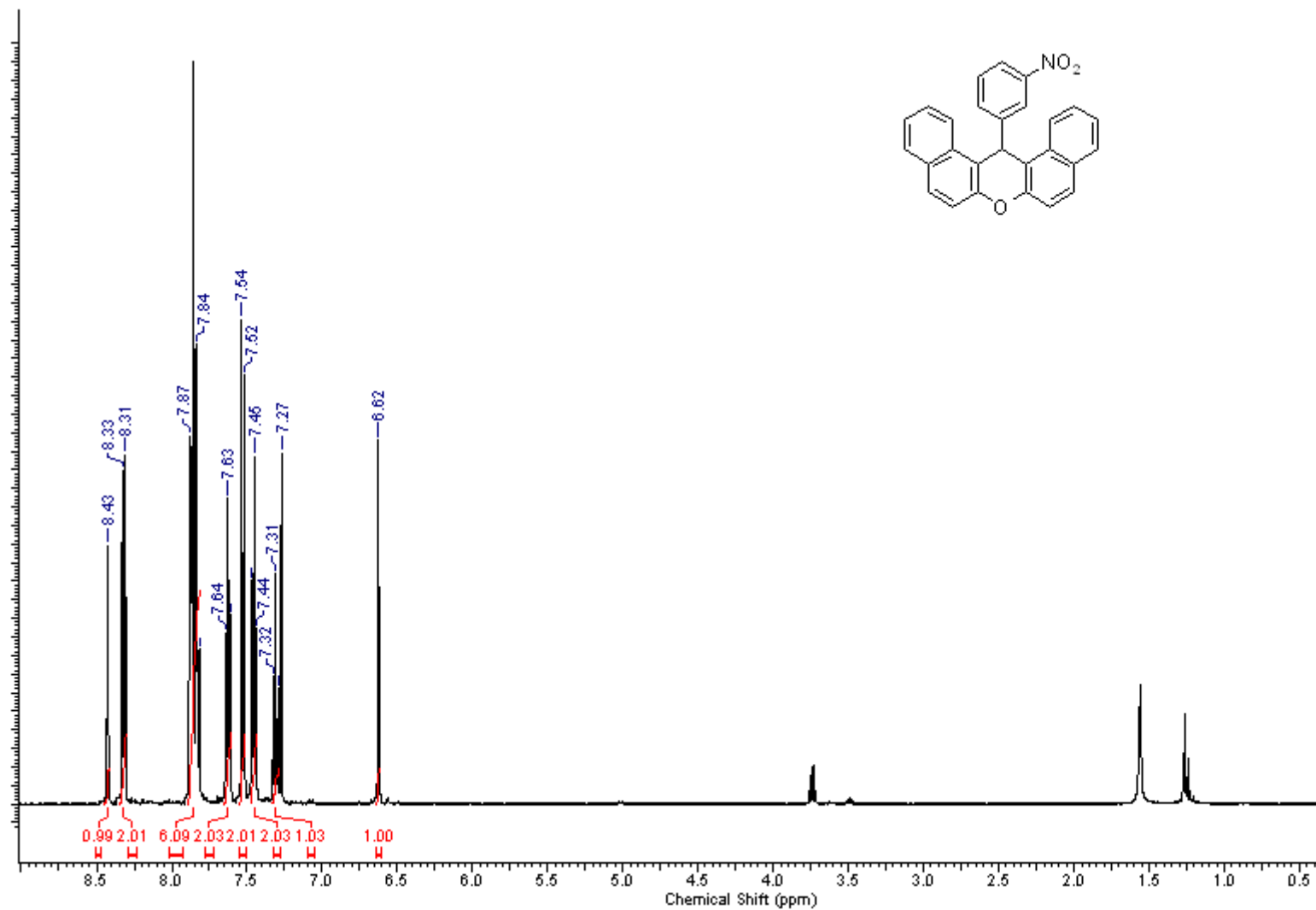
Figure S7. ¹H NMR of compound 14-(3-Nitrophenyl)-14*H*-dibenzo[*a,j*]xanthene 3c.
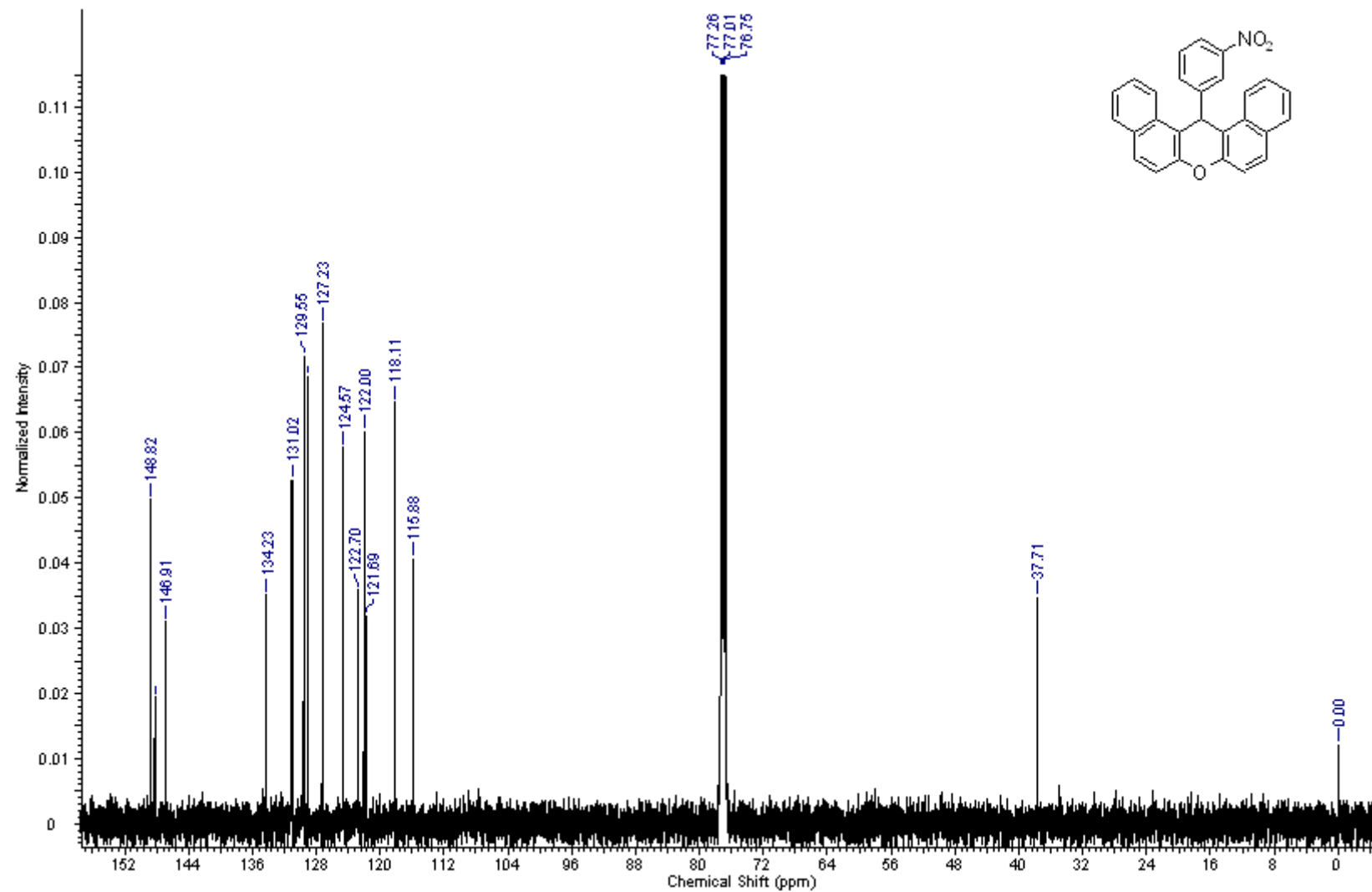
Figure S8. ^{13}C NMR of compound 14-(3-Nitrophenyl)-14*H*-dibenzo[*a,j*]xanthene 3c.
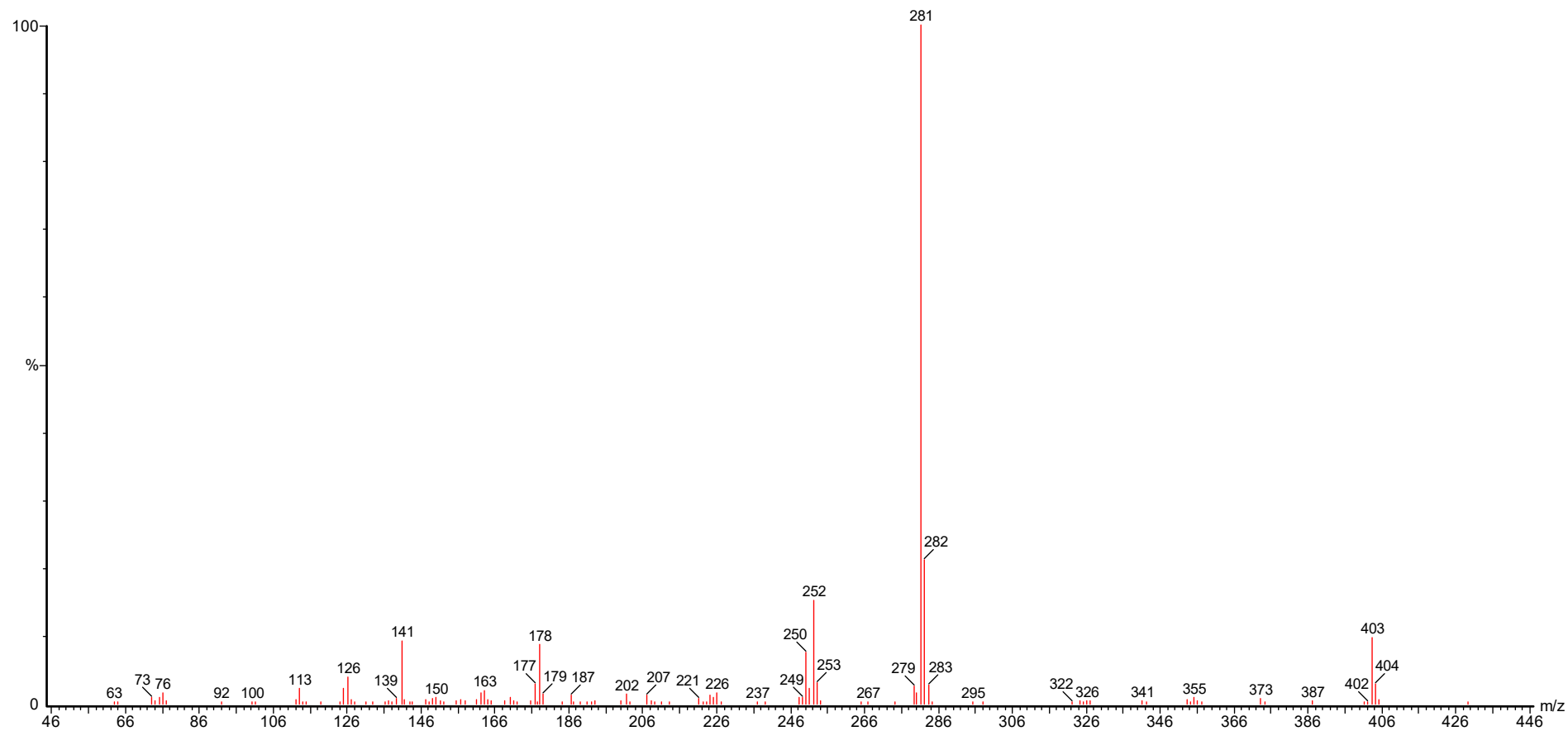
Figure S9. MS of compound 14-(3-Nitrophenyl)-14*H*-dibenzo[*a,j*]xanthene 3c.

Figure S10. ^{1}H NMR of compound 14-(3-Fluorophenyl)-14*H*-dibenzo[*a,j*]xanthene 3d.
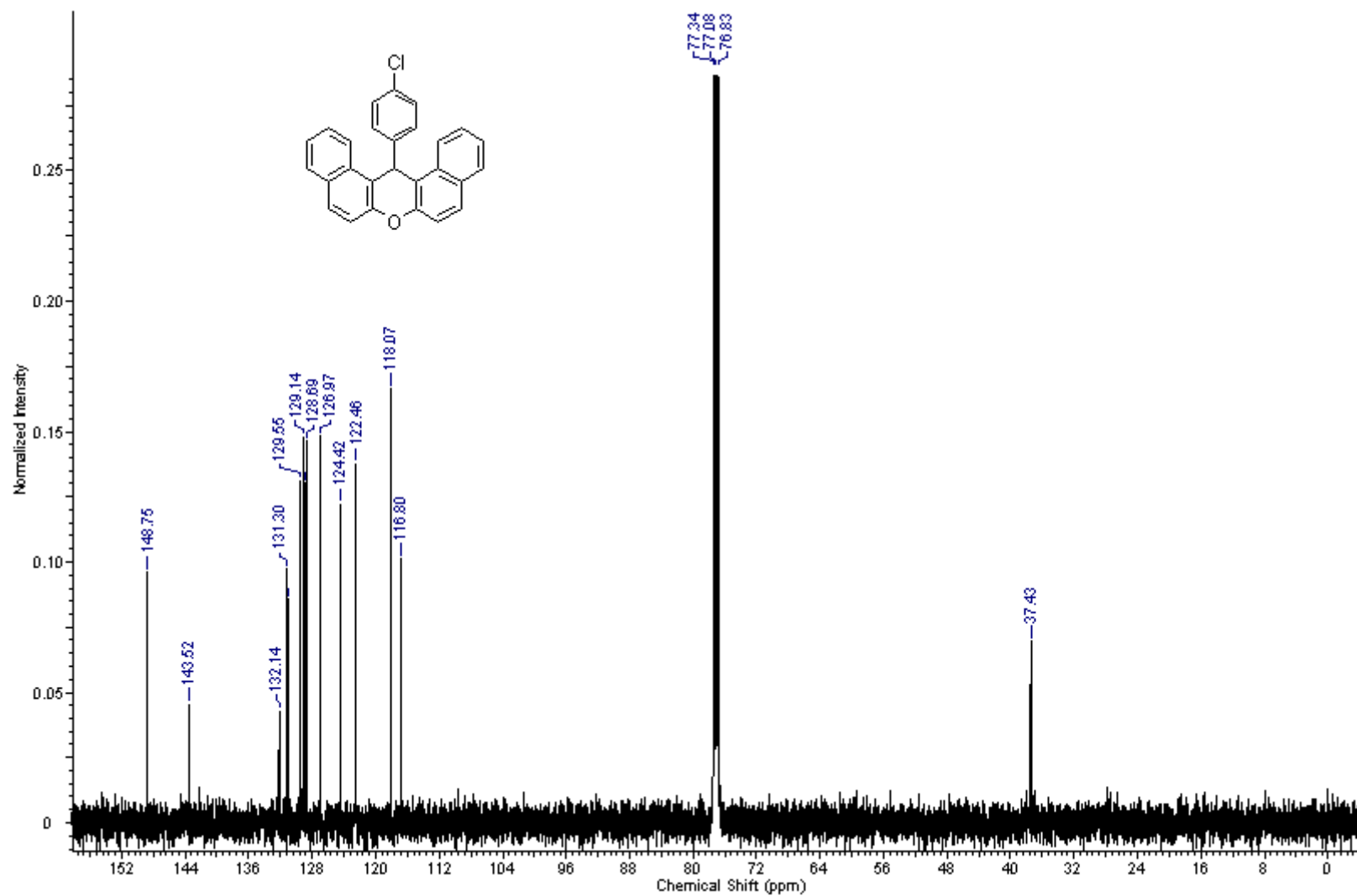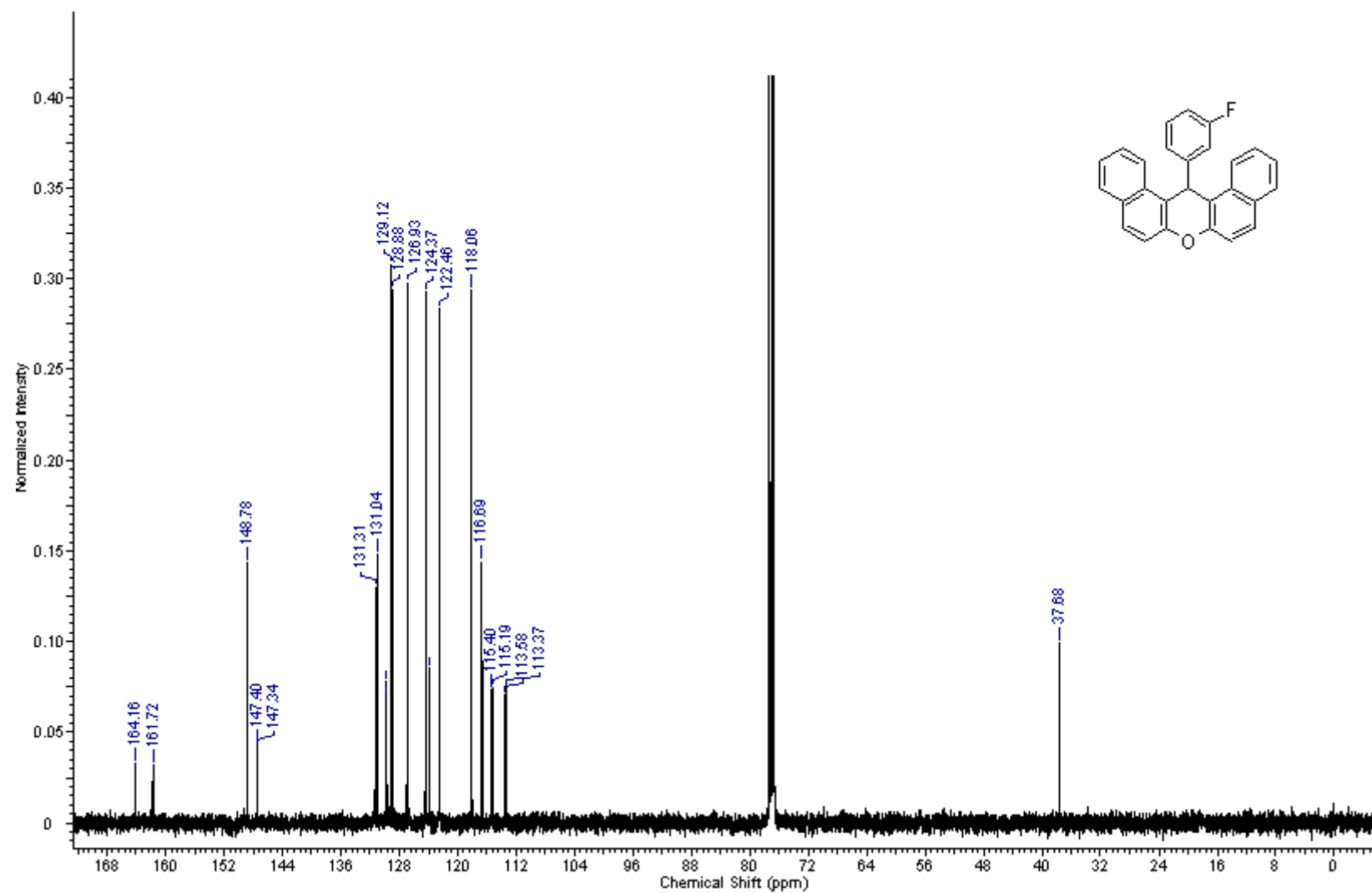
Figure S11. ^{13}C NMR of compound 14-(3-Fluorophenyl)-14*H*-dibenzo[*a,j*]xanthene 3d.
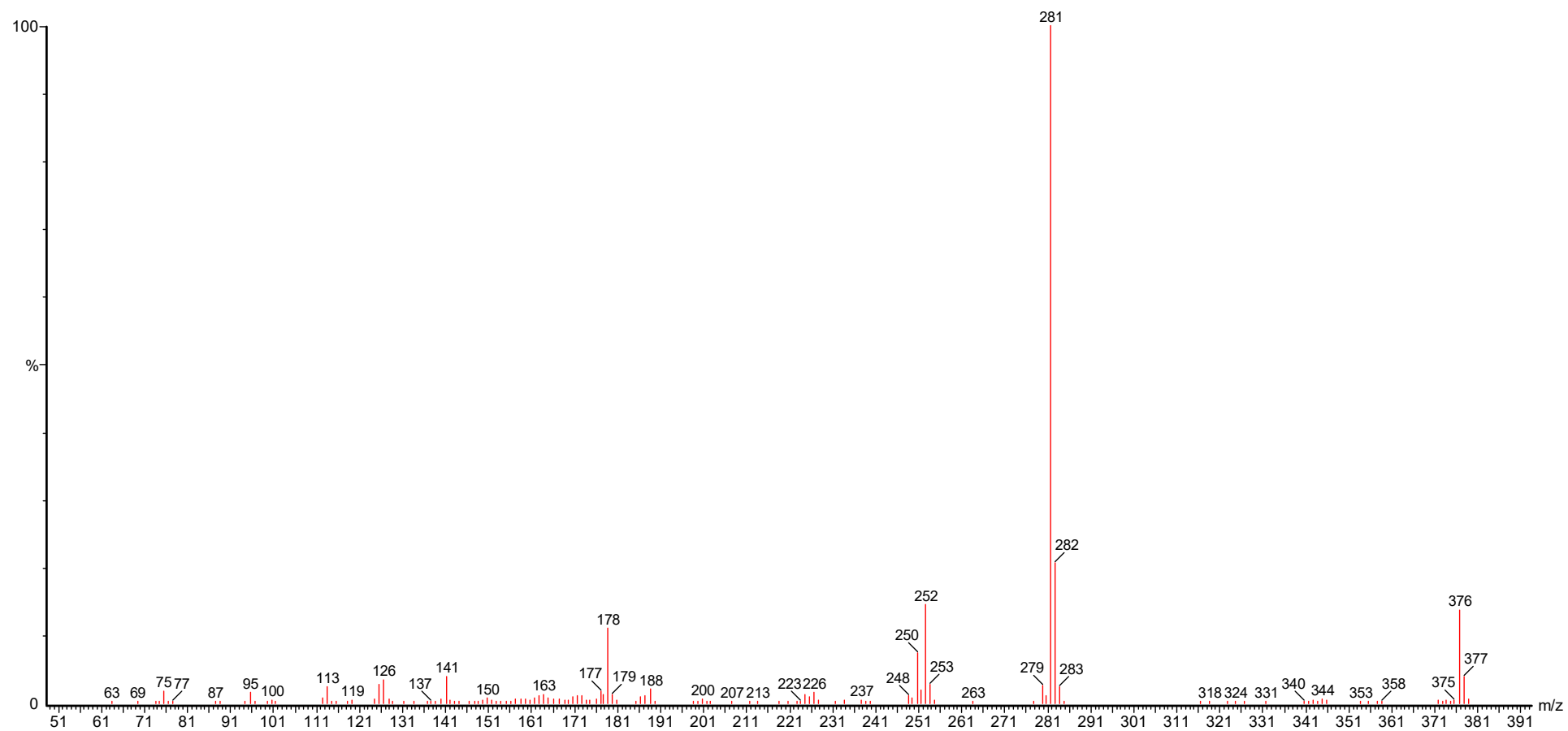
Figure S12. MS of compound 14-(3-Fluorophenyl)-14*H*-dibenzo[*a,j*]xanthene 3d.
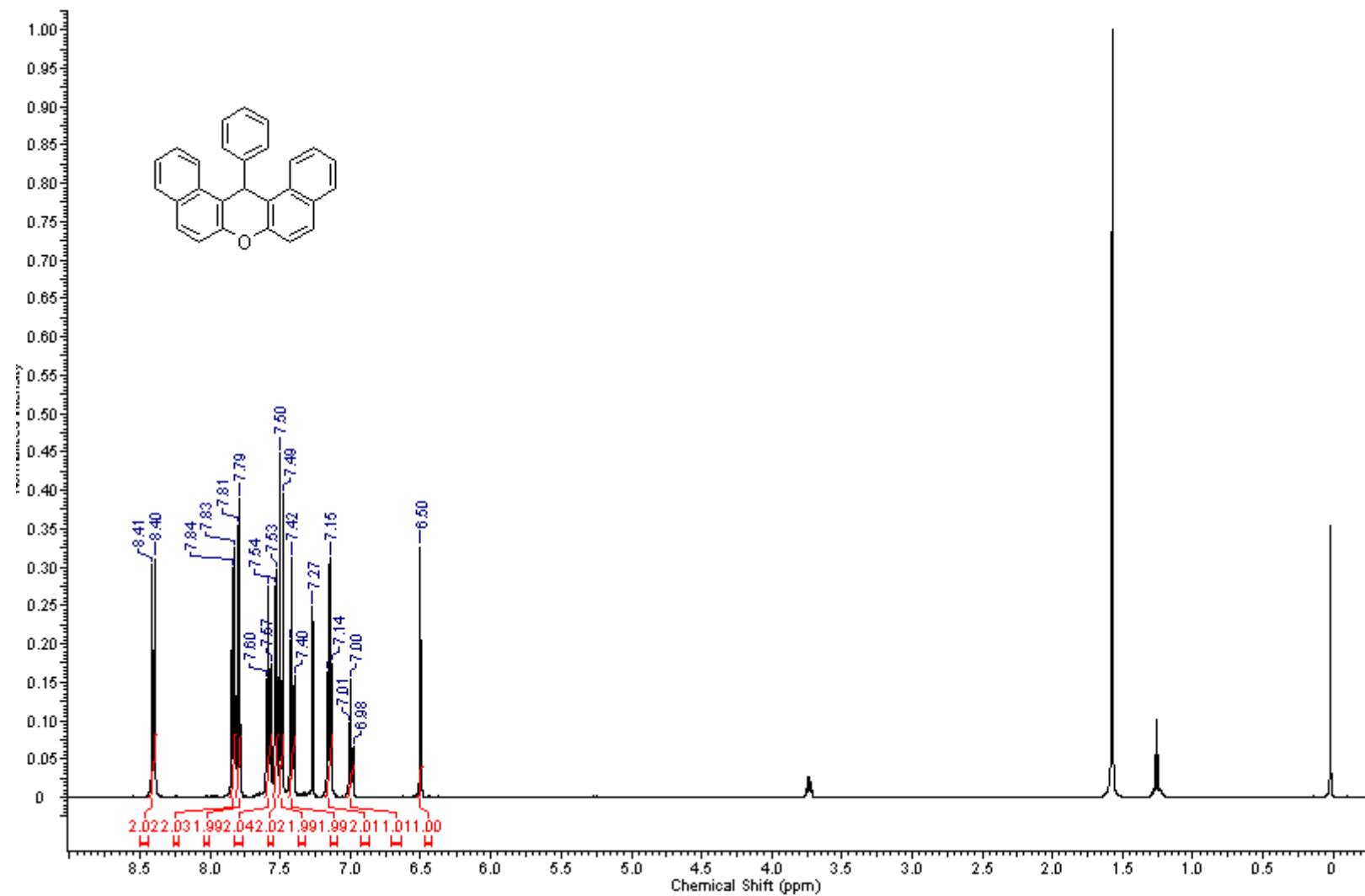
Figure S13. ¹H NMR of compound 14-Phenyl-14*H*-dibenzo[*a,j*]xanthene 3f.
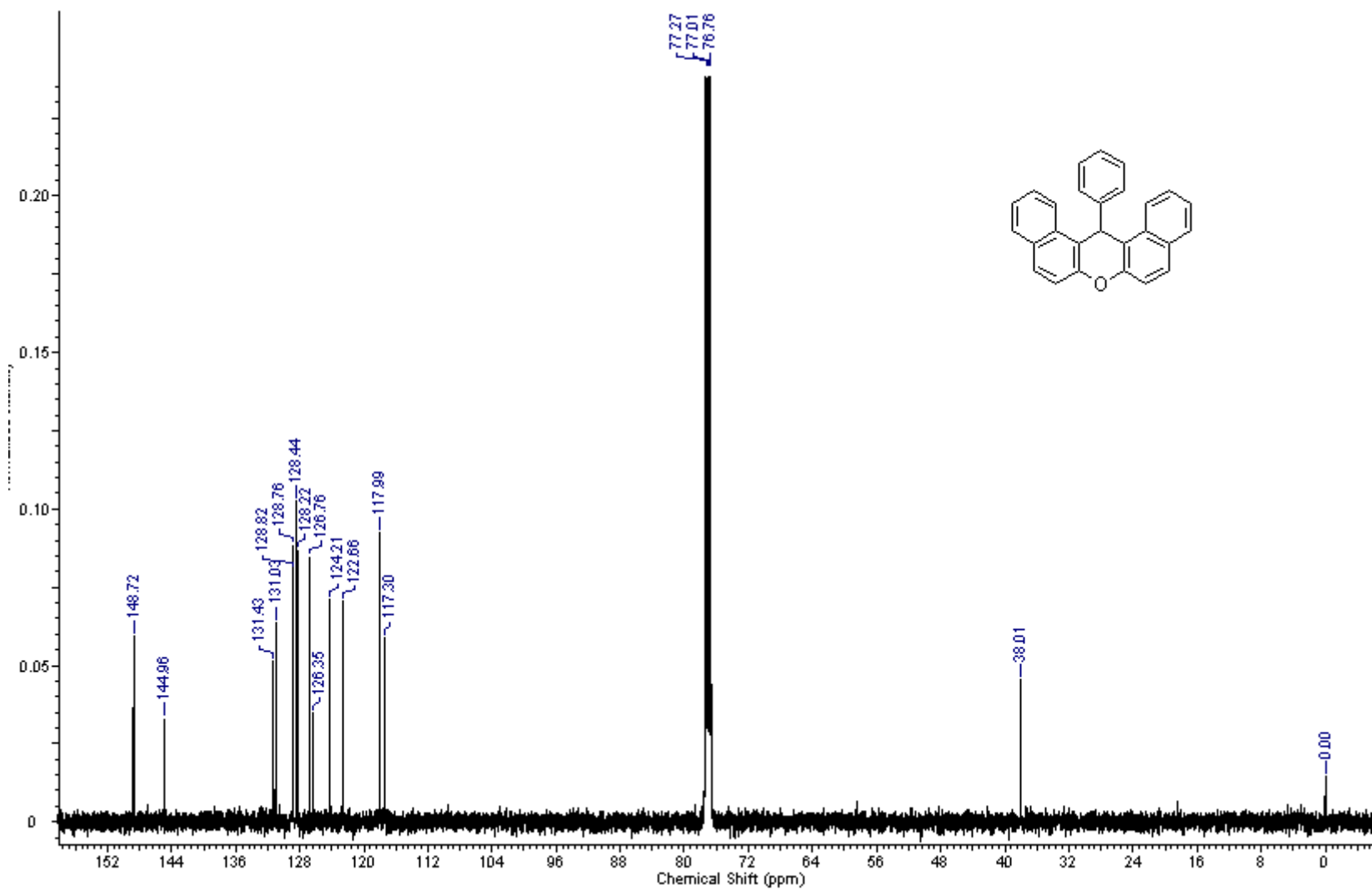
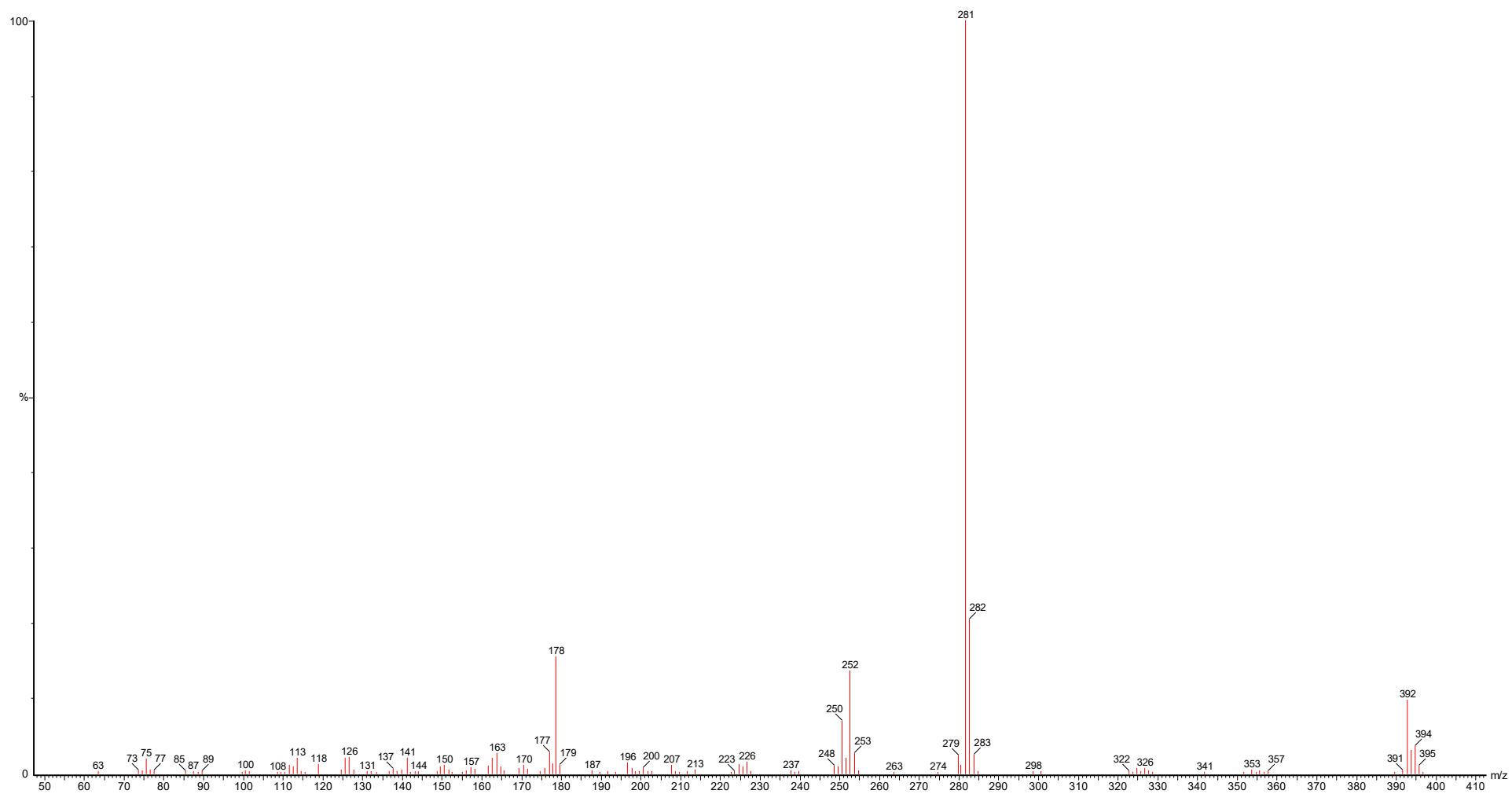**Figure S14.** ^{13}C NMR of compound 14-Phenyl-14*H*-dibenzo[*a,j*]xanthene 3f.
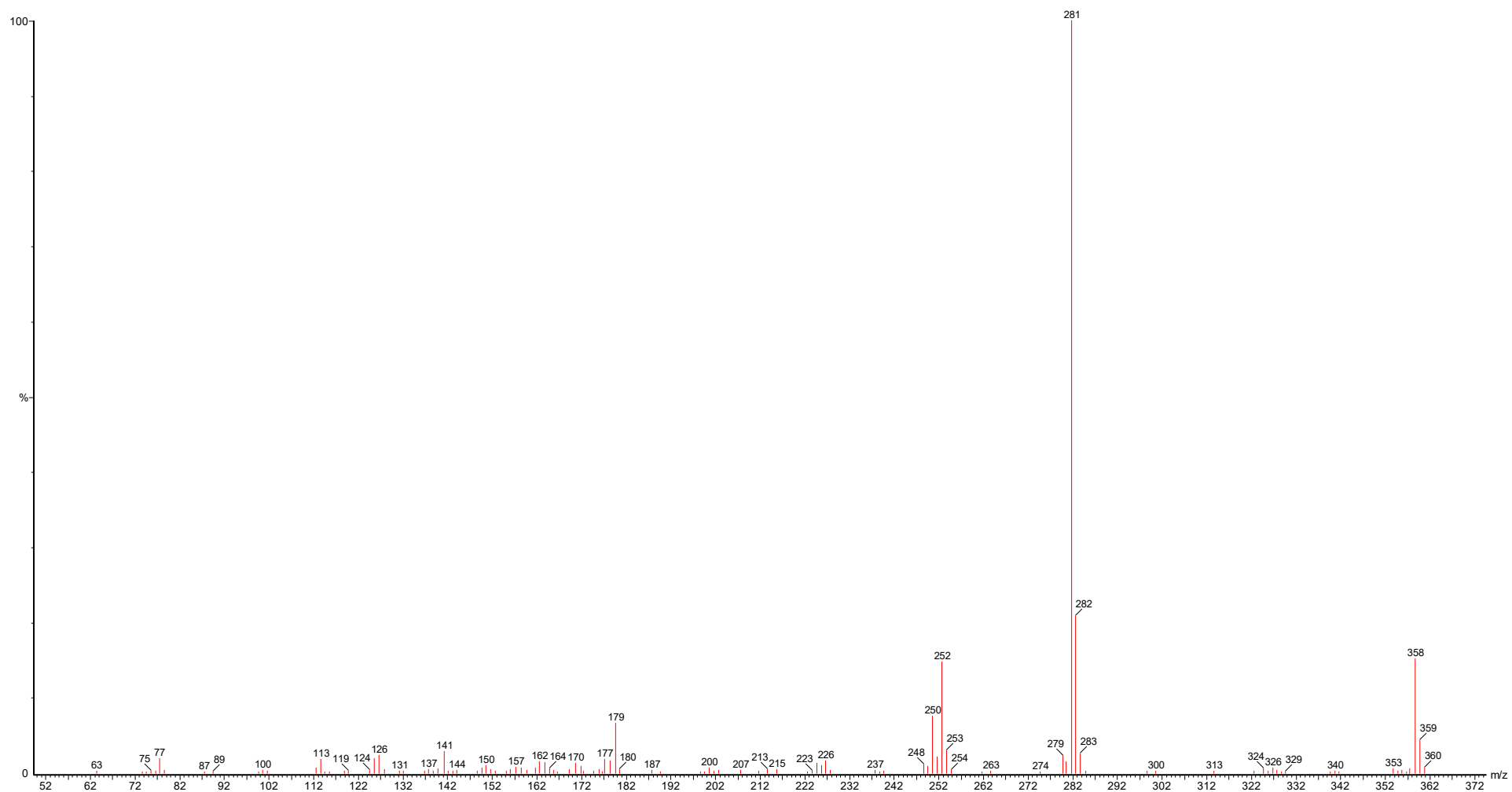
Figure S15. MS of compound 14-Phenyl-14*H*-dibenzo[*a,j*]xanthene 3f.
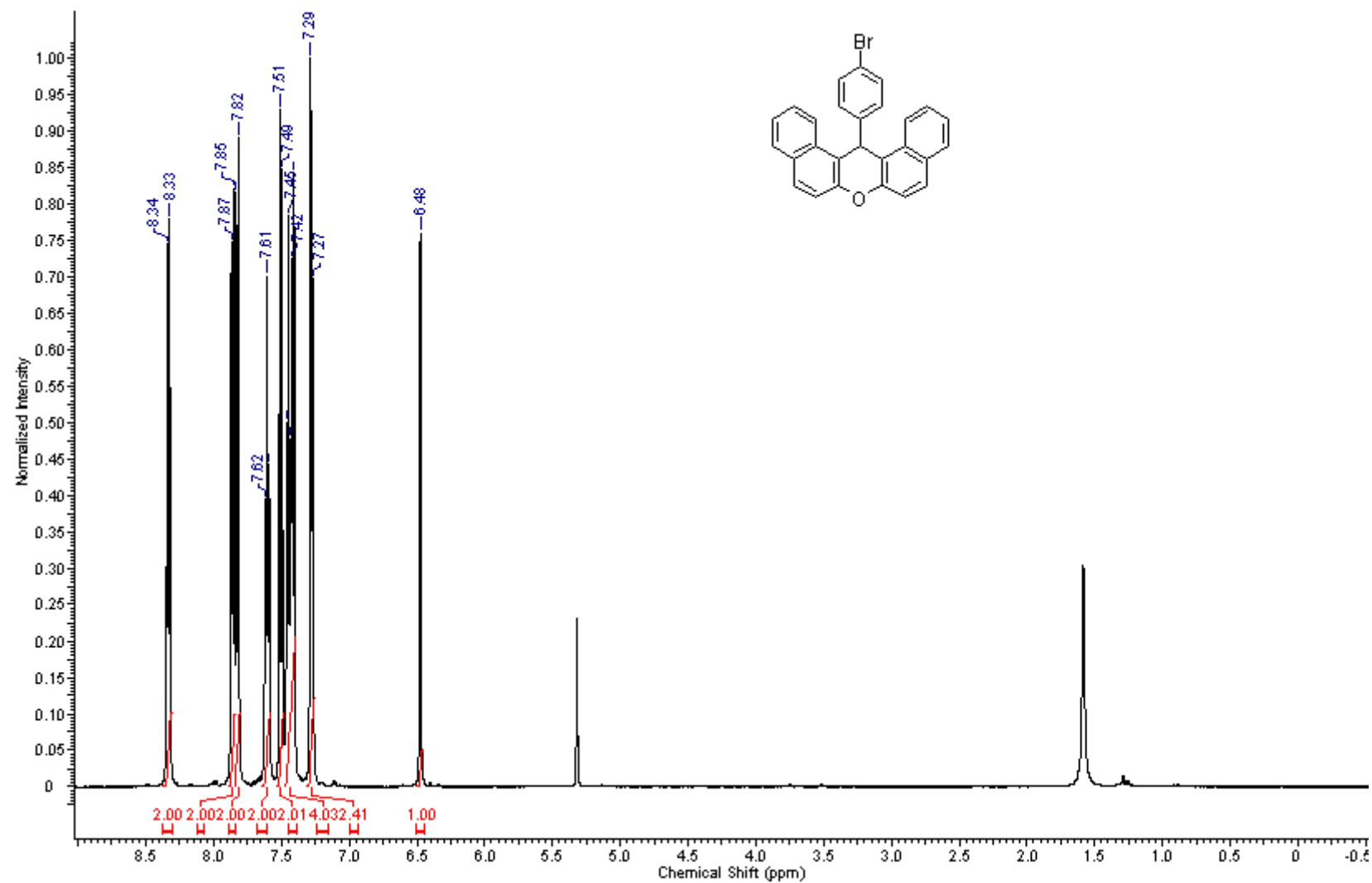
Figure S16. ^{1}H NMR of compound 14-(4-Bromophenyl)-14*H*-dibenzo[*a,j*]xanthene 3g.
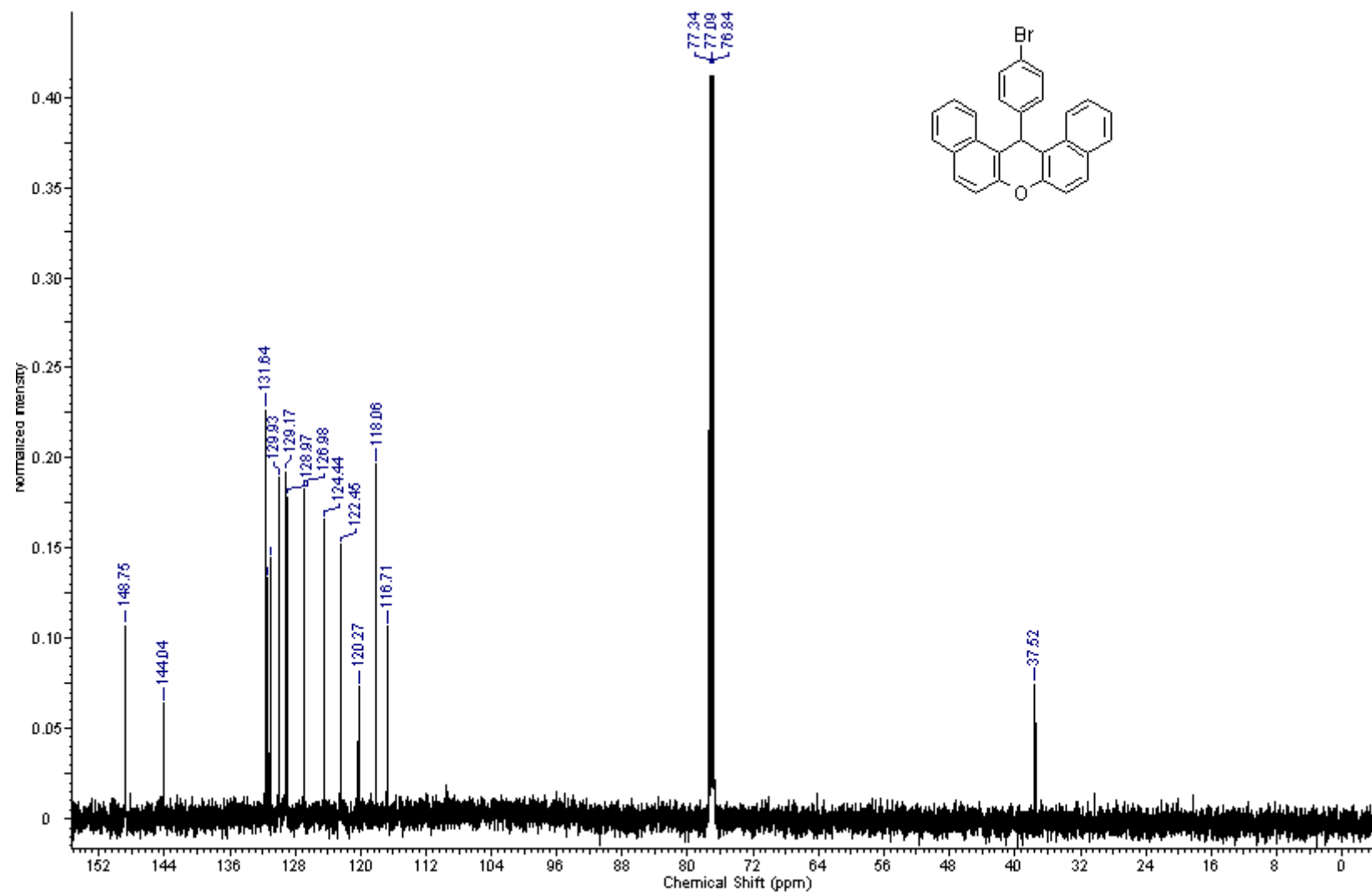
Figure S17. ^{13}C NMR of compound 14-(4-Bromophenyl)-14*H*-dibenzo[*a,j*]xanthene 3g.
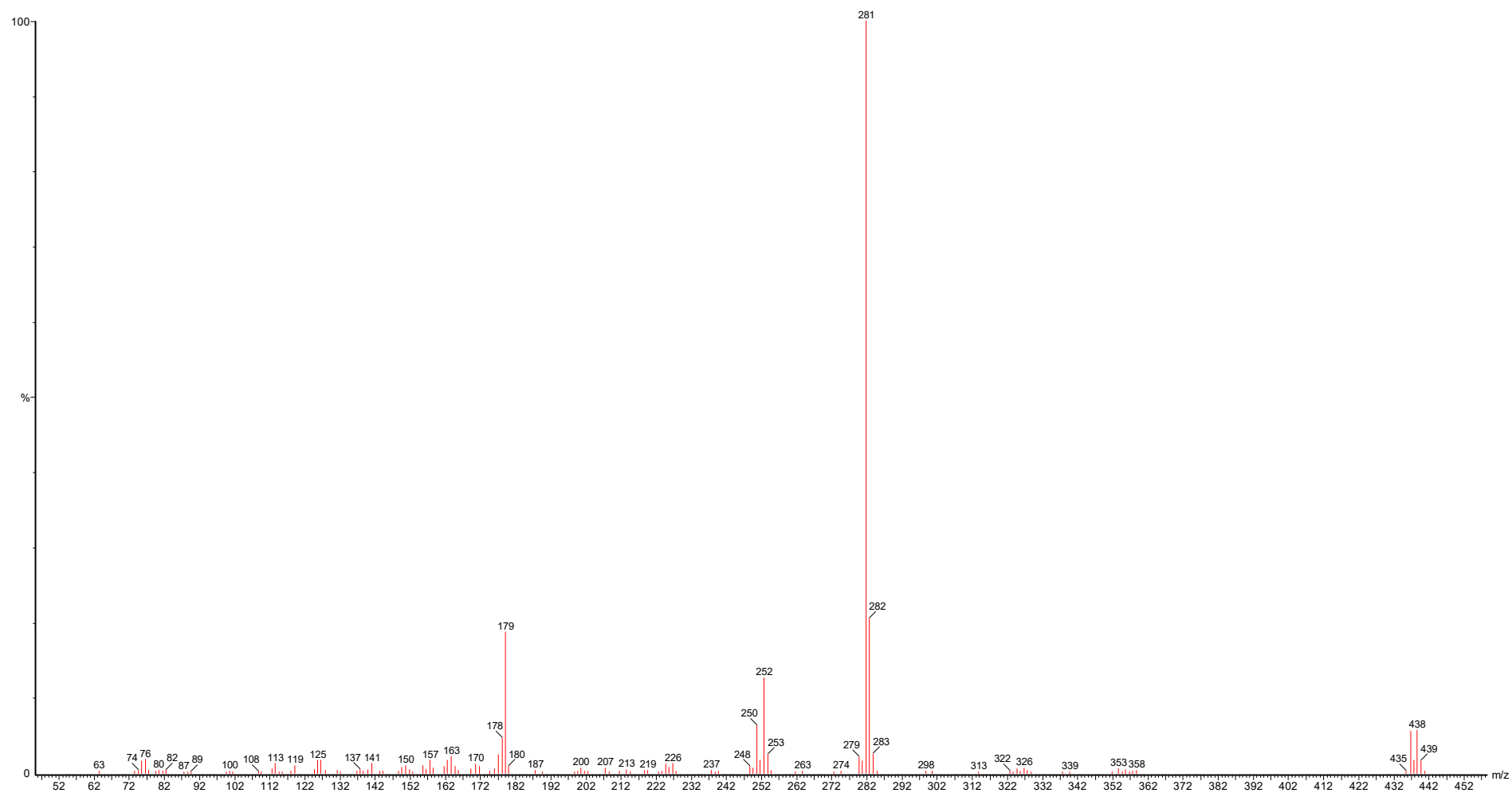
Figure S18. MS of compound 14-(4-Bromophenyl)-14*H*-dibenzo[*a,j*]xanthene 3g.
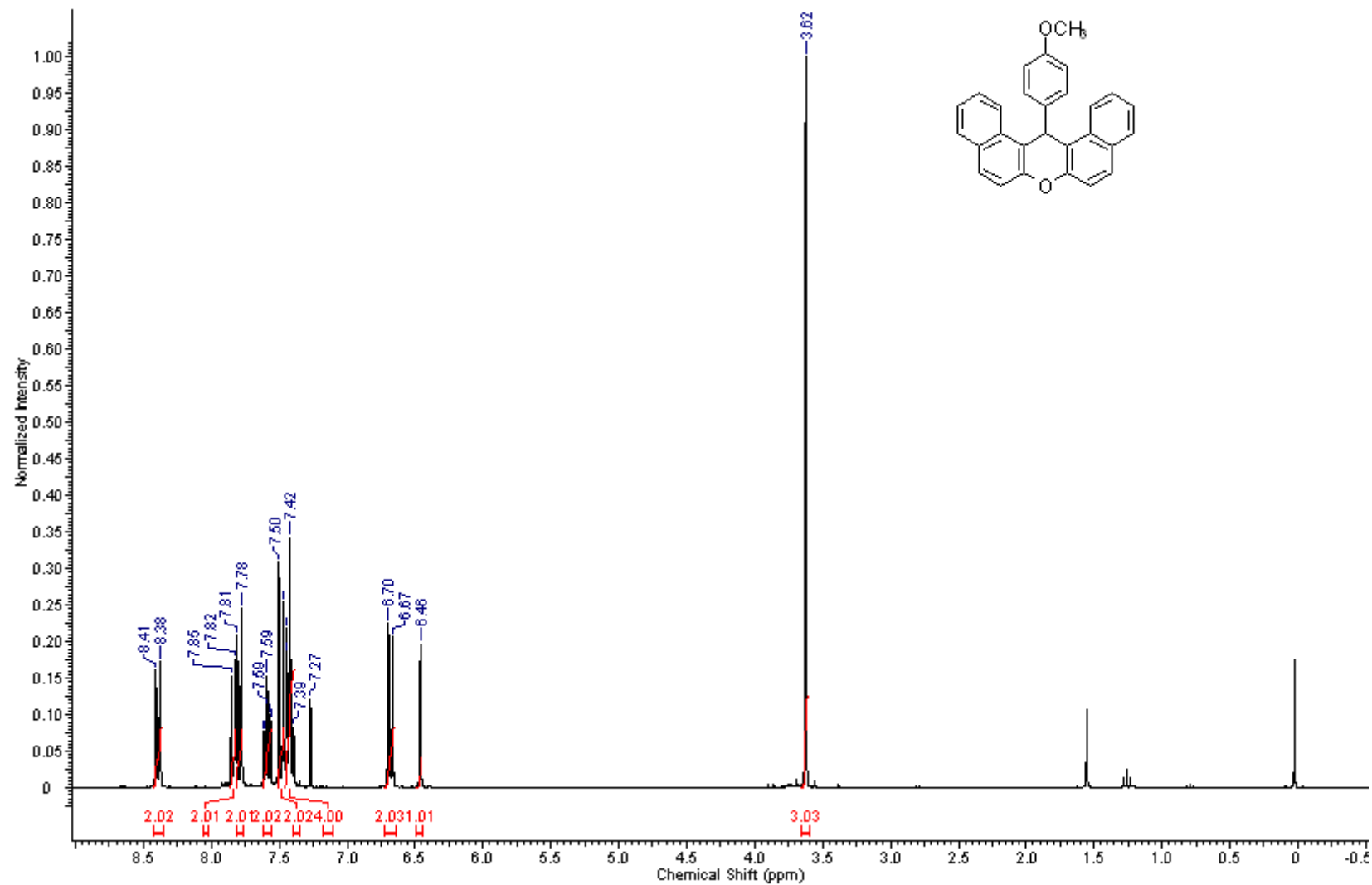
Figure S19. ¹H NMR of compound 14-(4-Methoxyphenyl)-14*H*-dibenzo[*a,j*]xanthene 3h.
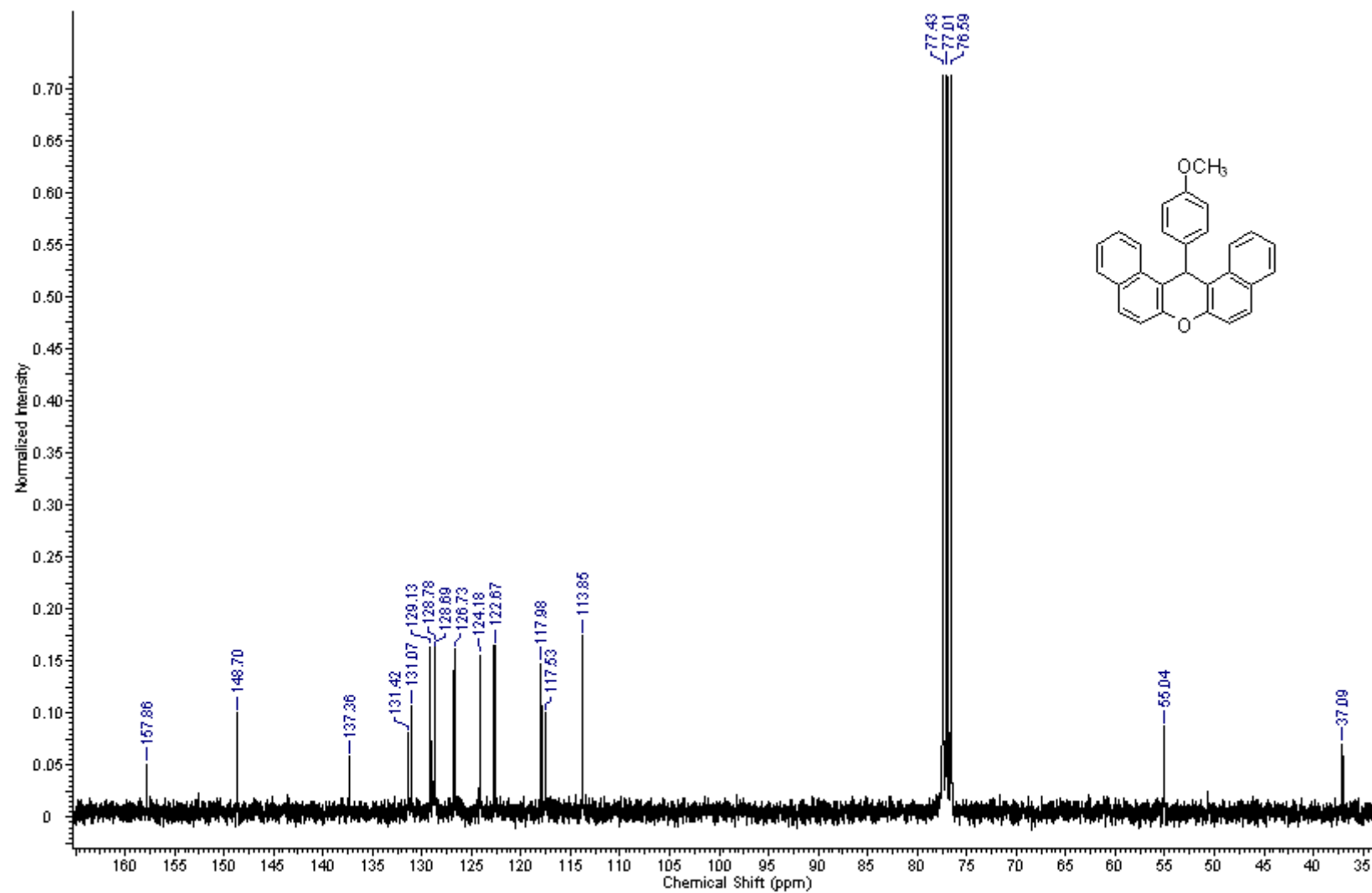
Figure S20. ^{13}C NMR of compound 14-(4-Methoxyphenyl)-14*H*-dibenzo[*a,j*]xanthene 3h.
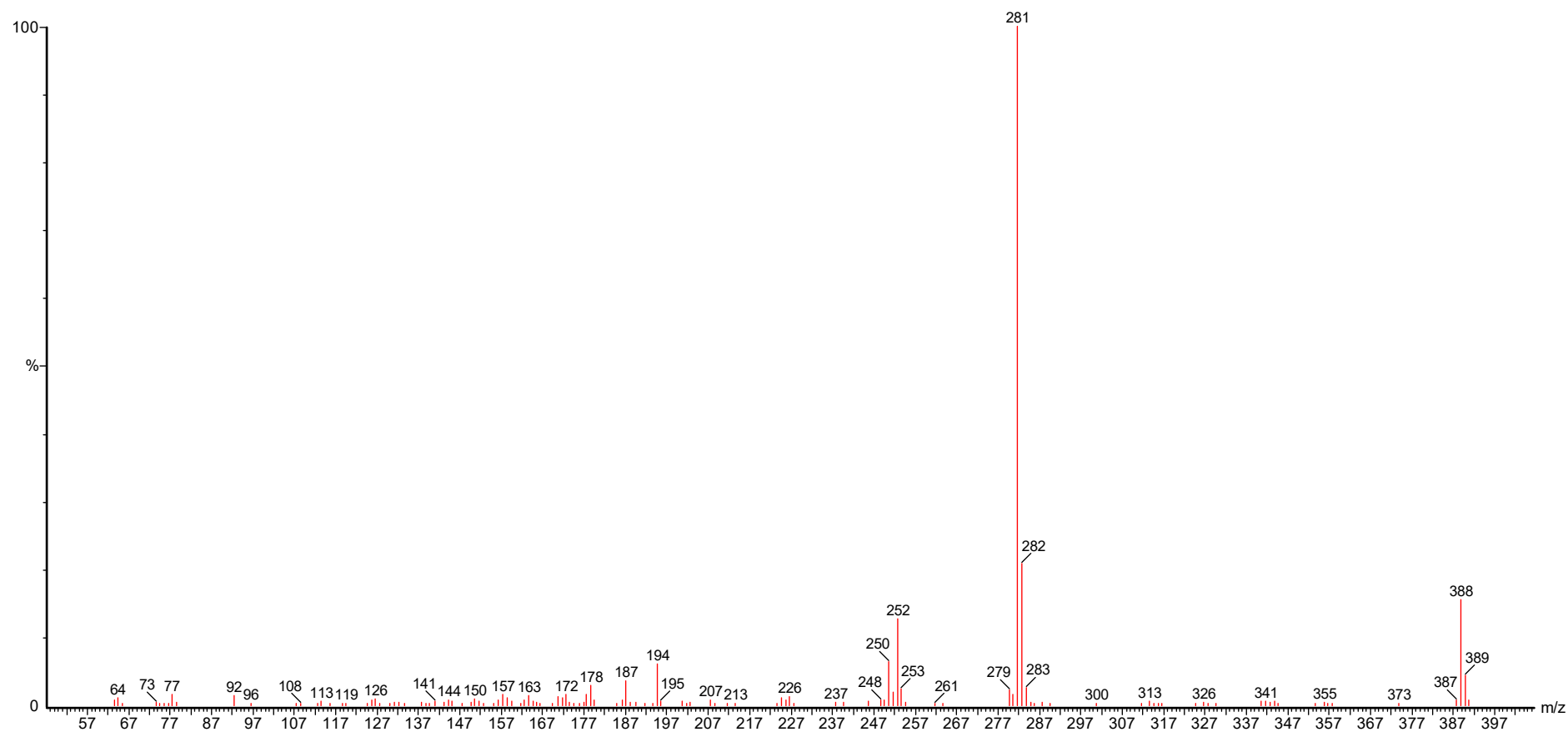
**Figure S21.** MS of compound 14-(4-Methoxyphenyl)-14*H*-dibenzo[*a,j*]xanthene 3h.
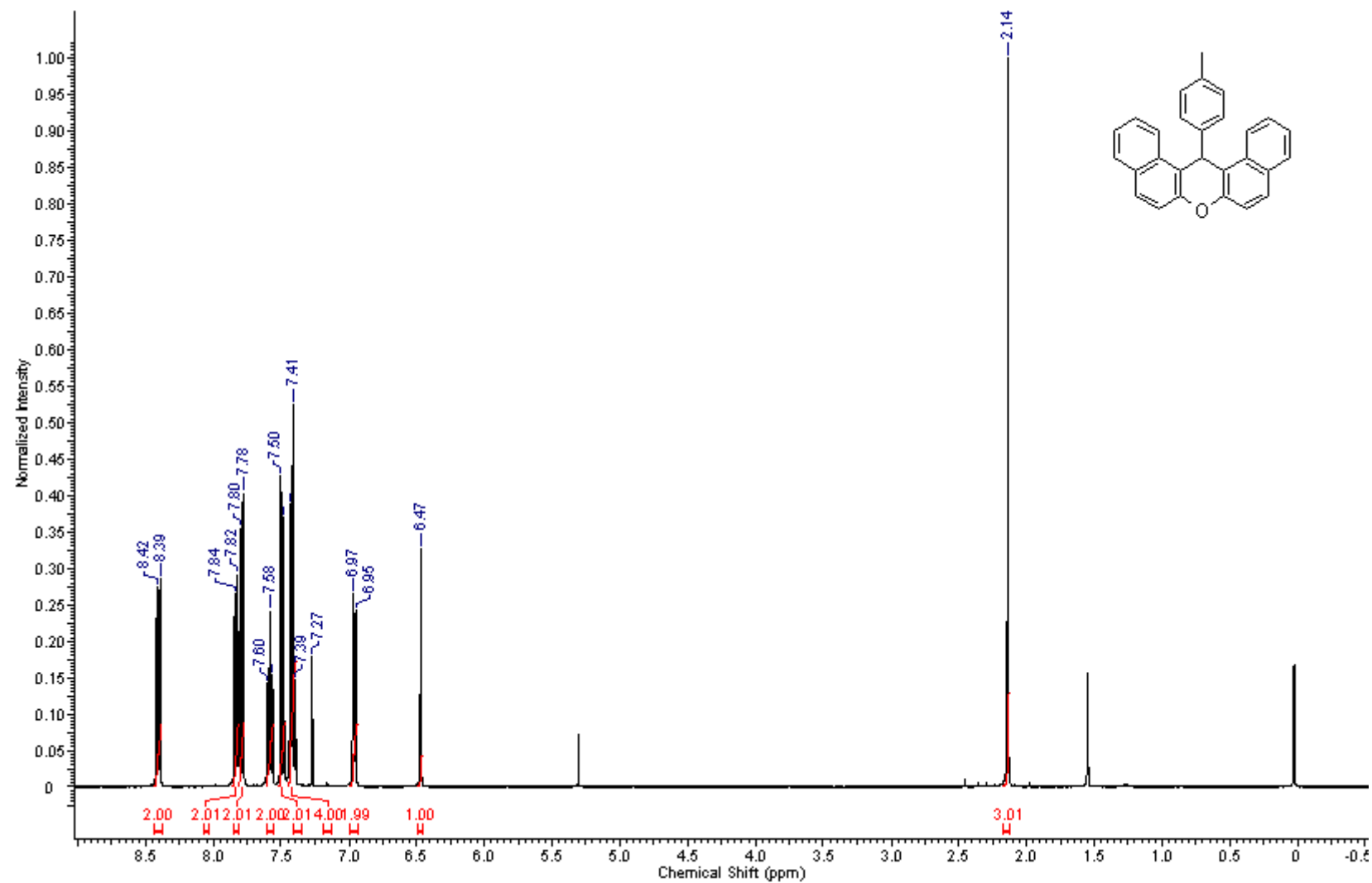
Figure S22. ¹H NMR of compound 14-(4-Methylphenyl)-14*H*-dibenzo[*a,j*]xanthene 3i.
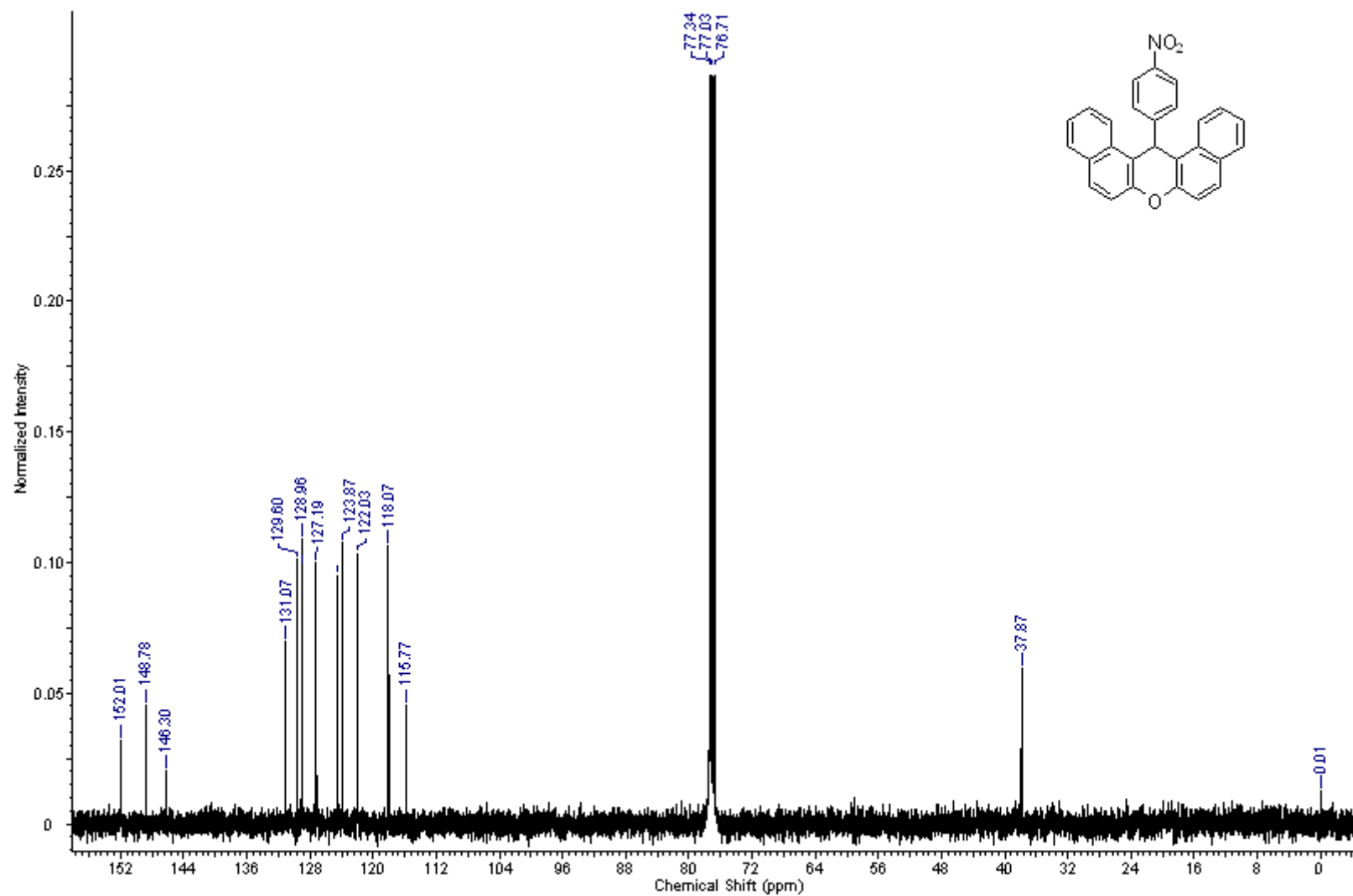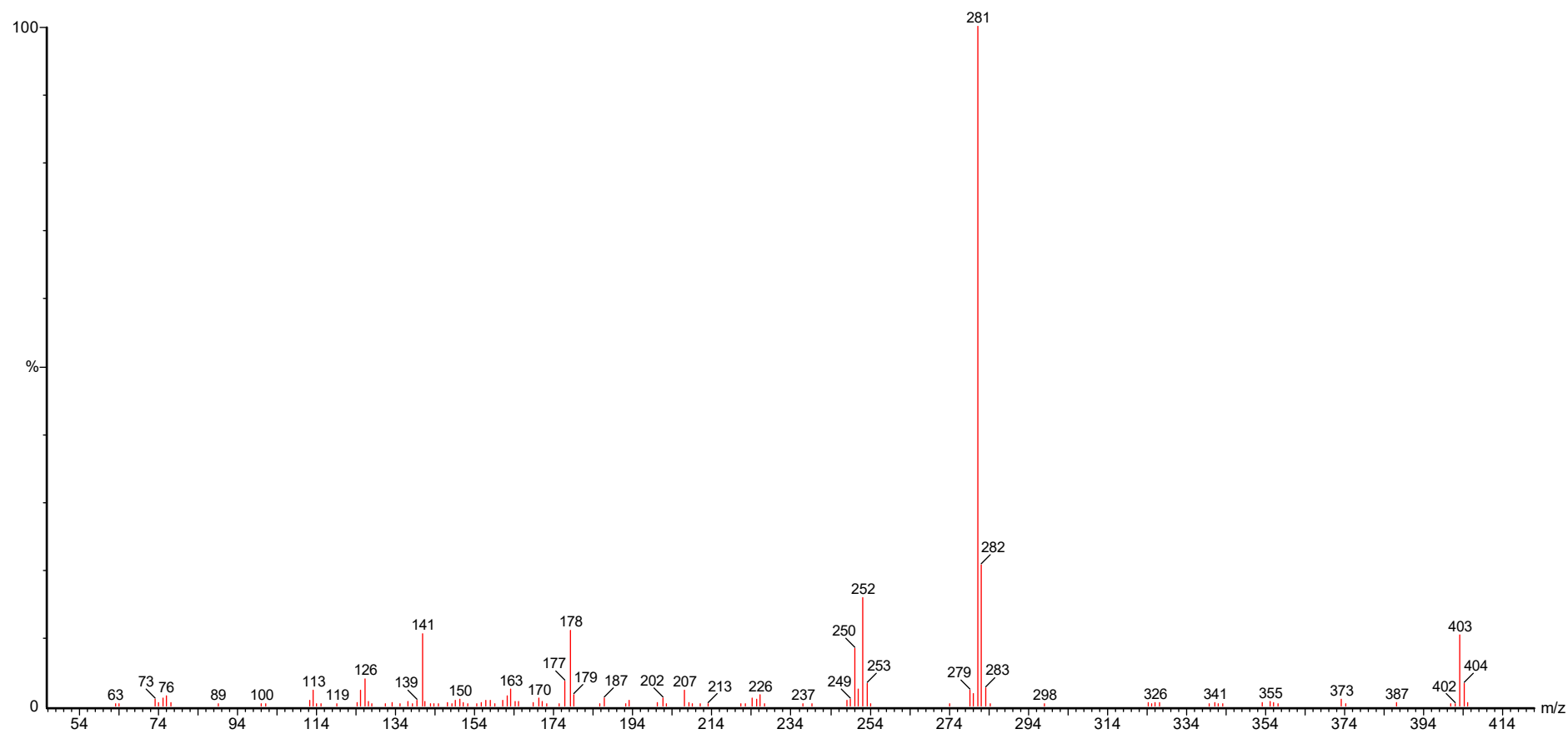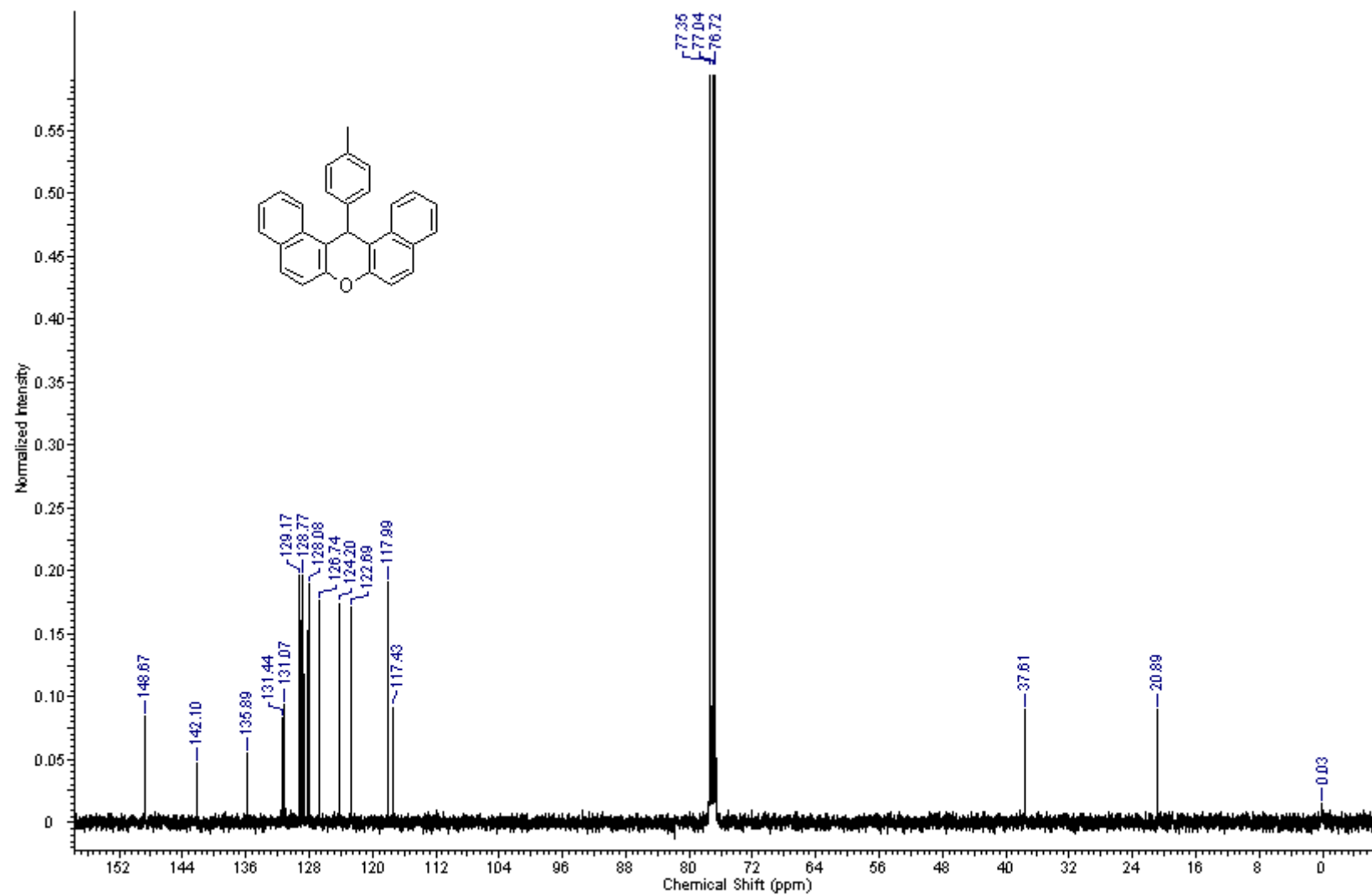
Figure S23. ^{13}C NMR of compound 14-(4-Methylphenyl)-14*H*-dibenzo[*a,j*]xanthene 3i.
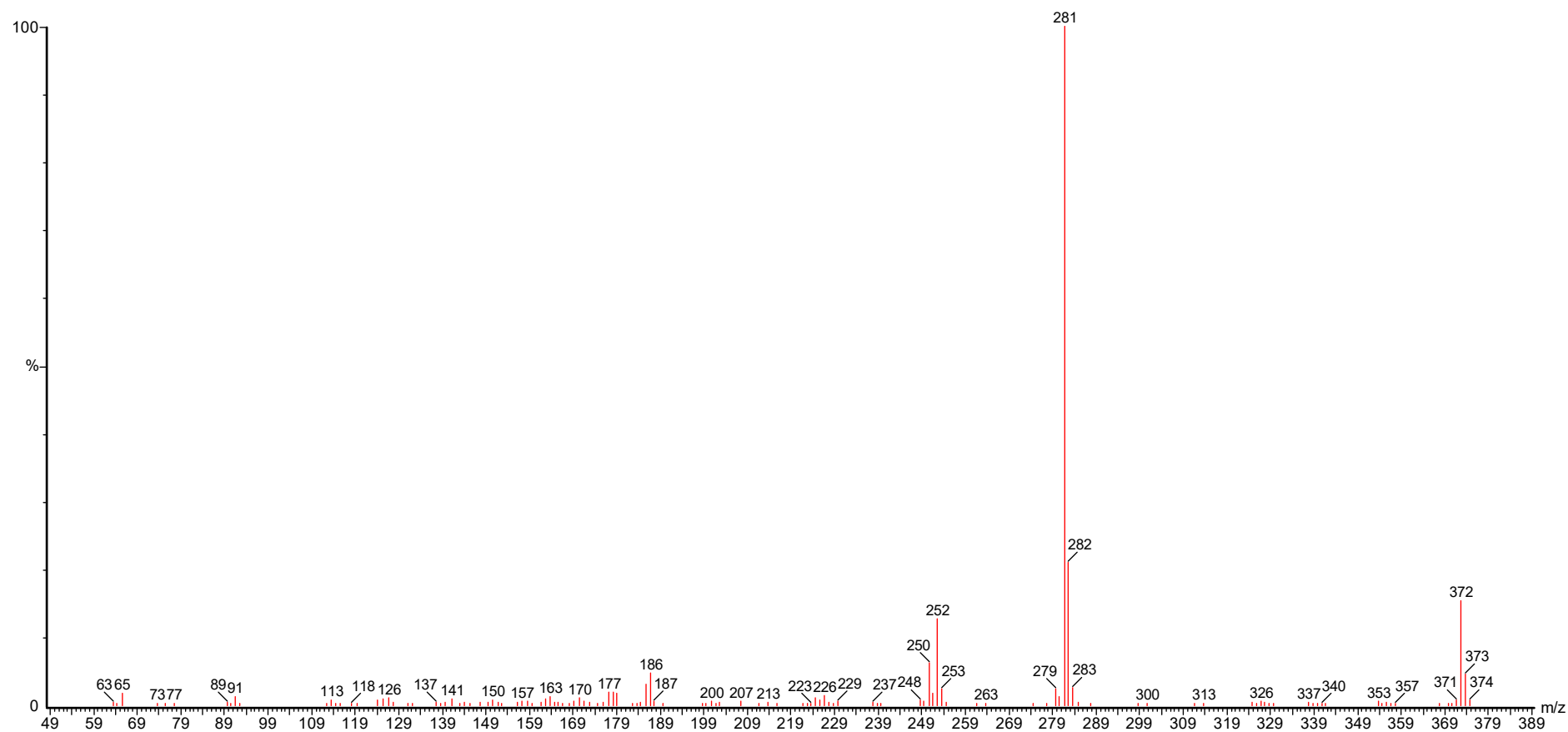
Figure S24. MS of compound 14-(4-Methylphenyl)-14*H*-dibenzo[*a,j*]xanthene 3i.
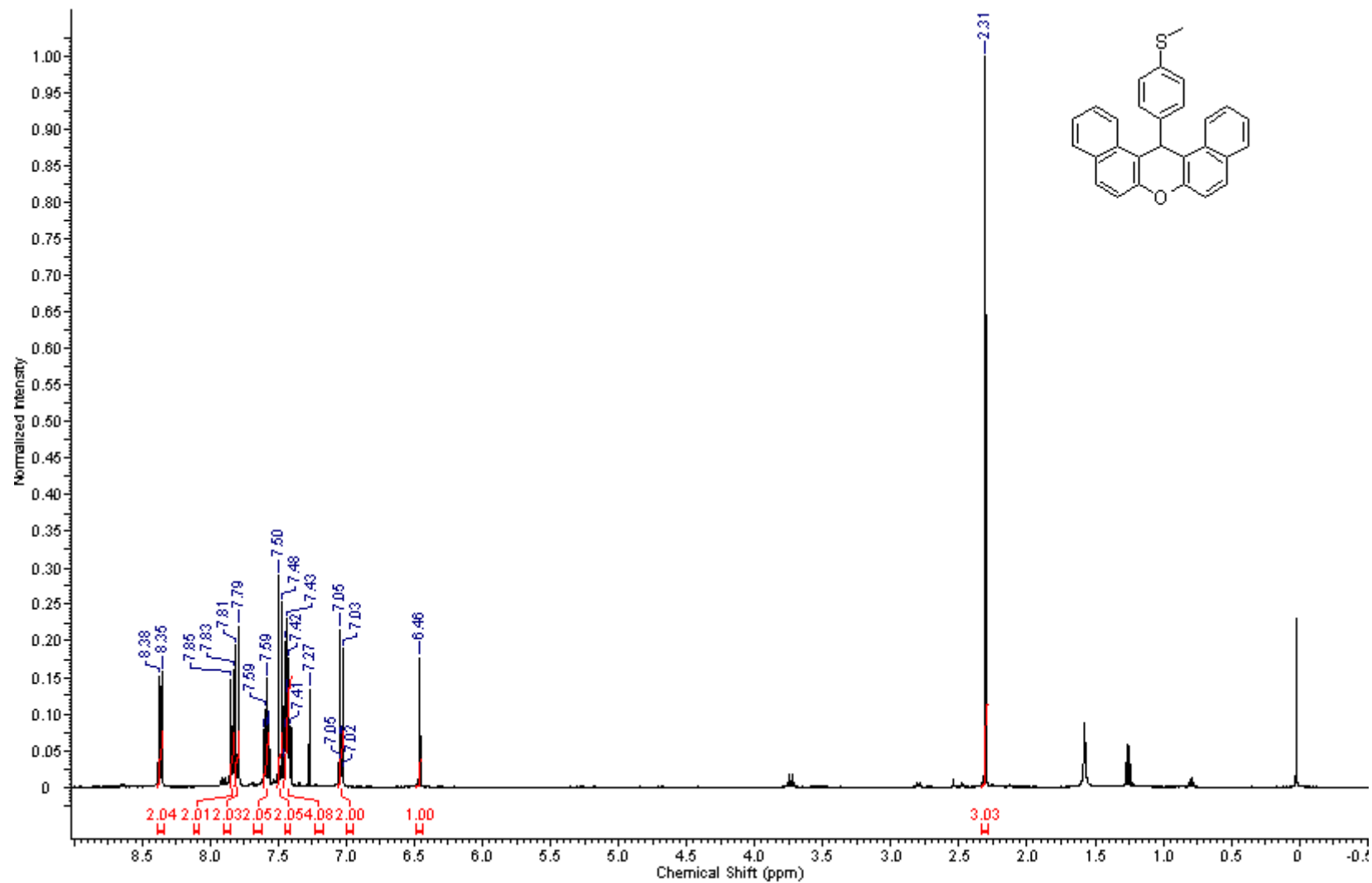
Figure S25. ^1H NMR of compound 14-(4-Methylthiophenyl)-14H-dibenzo[a,j]xanthene 3k.
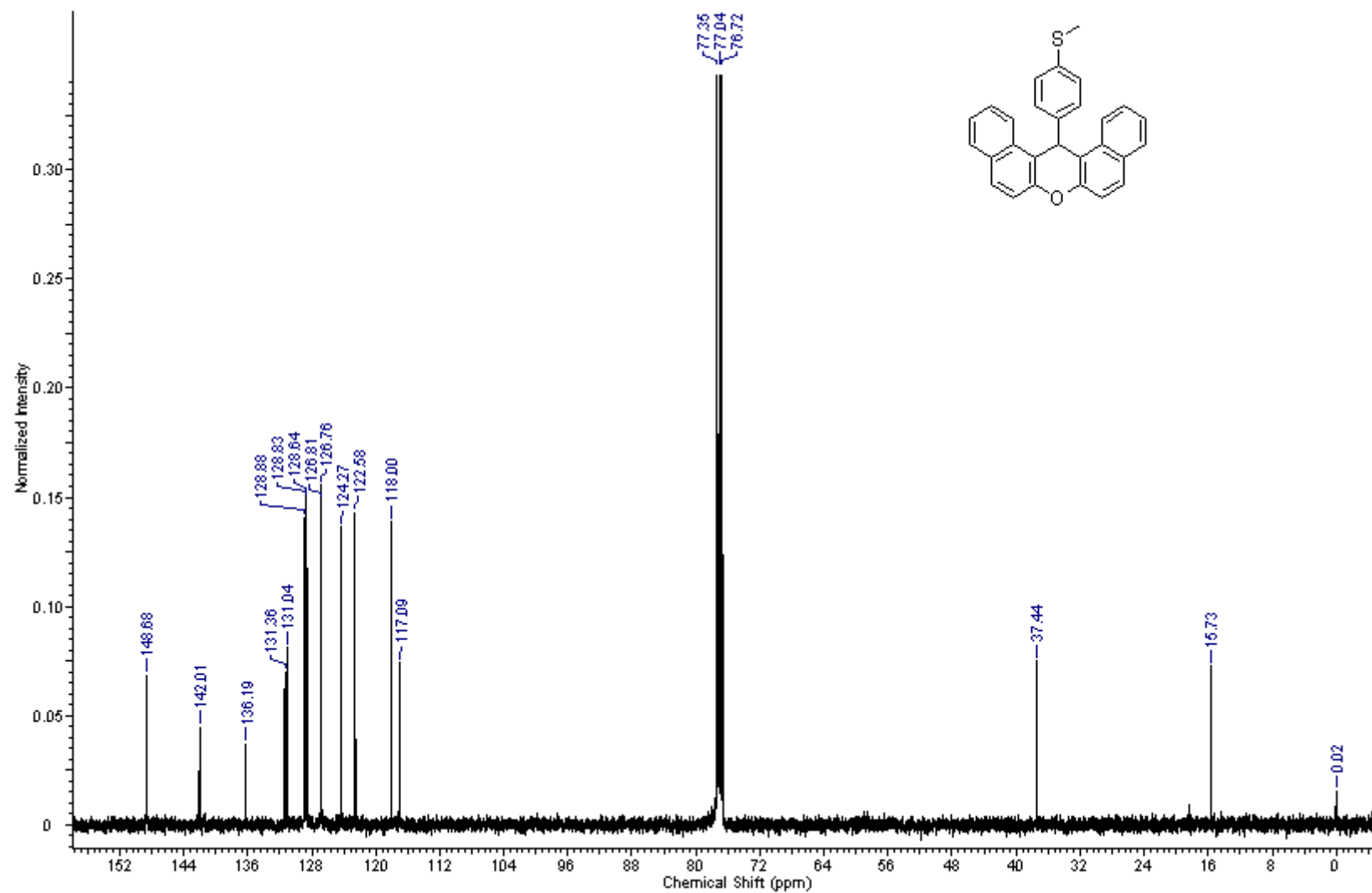
Figure S26. ^{13}C NMR of compound 14-(4-Methylthiophenyl)-14*H*-dibenzo[*a,j*]xanthene 3k.
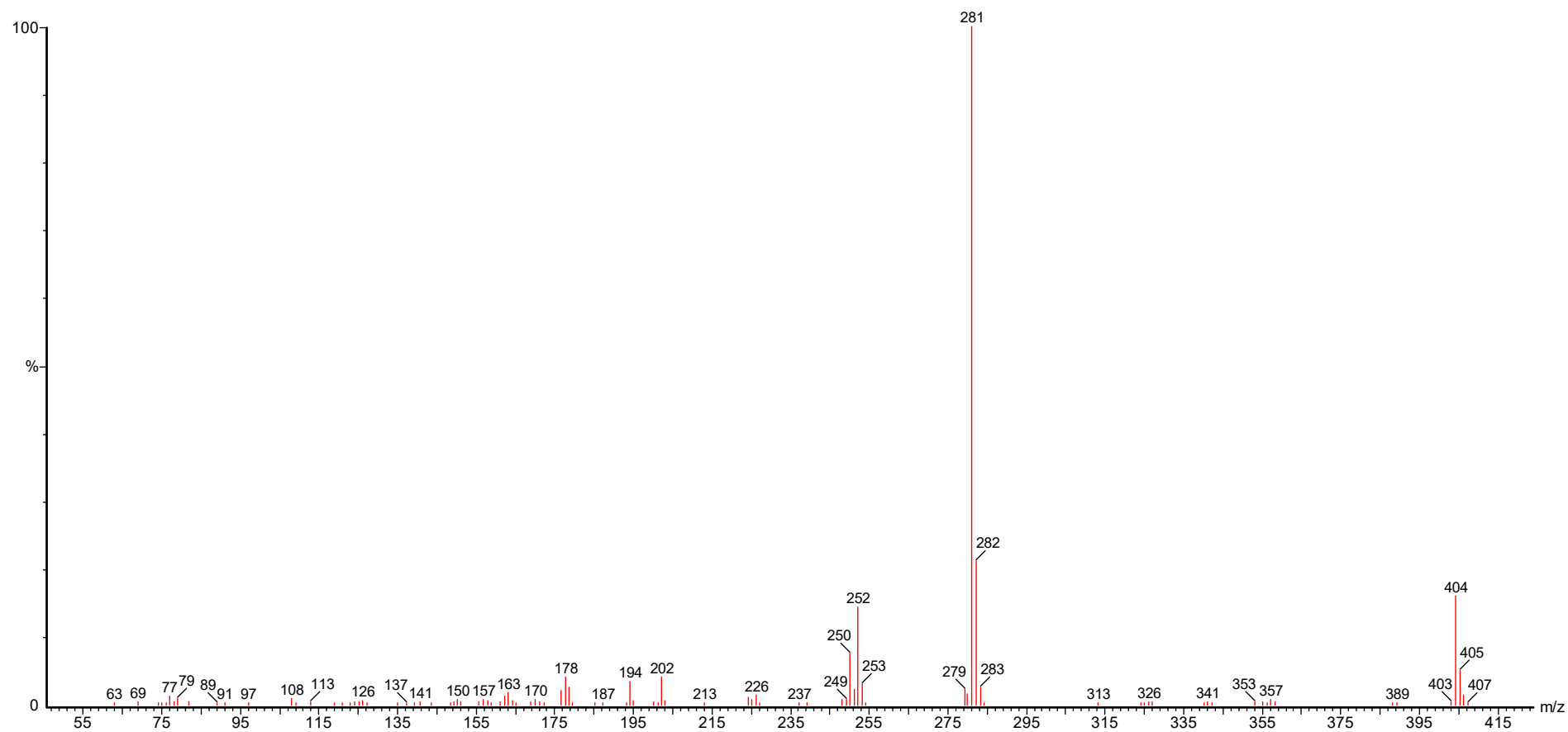
Figure S27. MS of compound 14-(4-Methylthiophenyl)-14*H*-dibenzo[*a,j*]xanthene 3k.
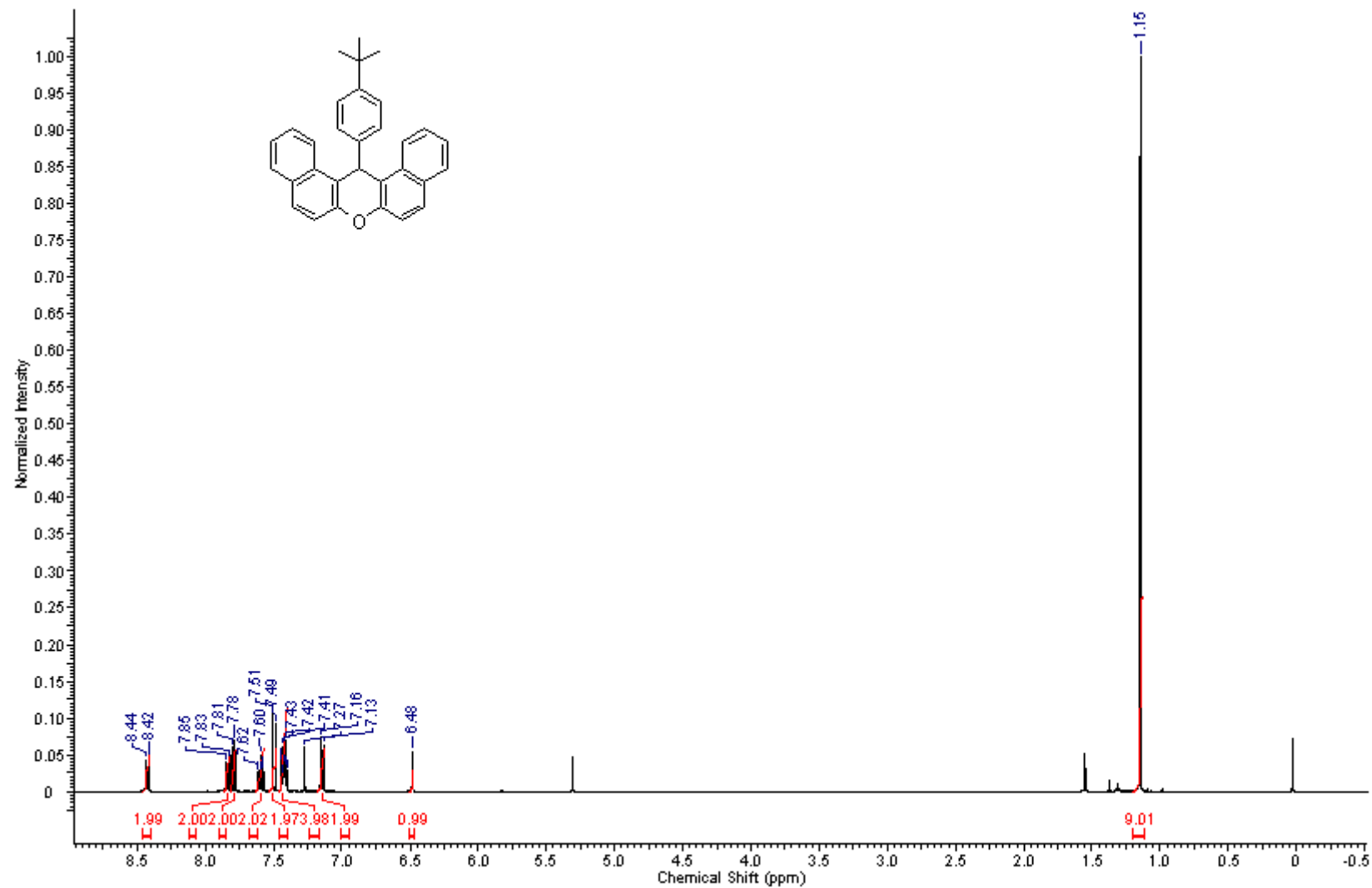
Figure S28. ¹H NMR of compound 14-(4-*t*-Butylphenyl)-14*H*-dibenzo[*a,j*]xanthene 3l.
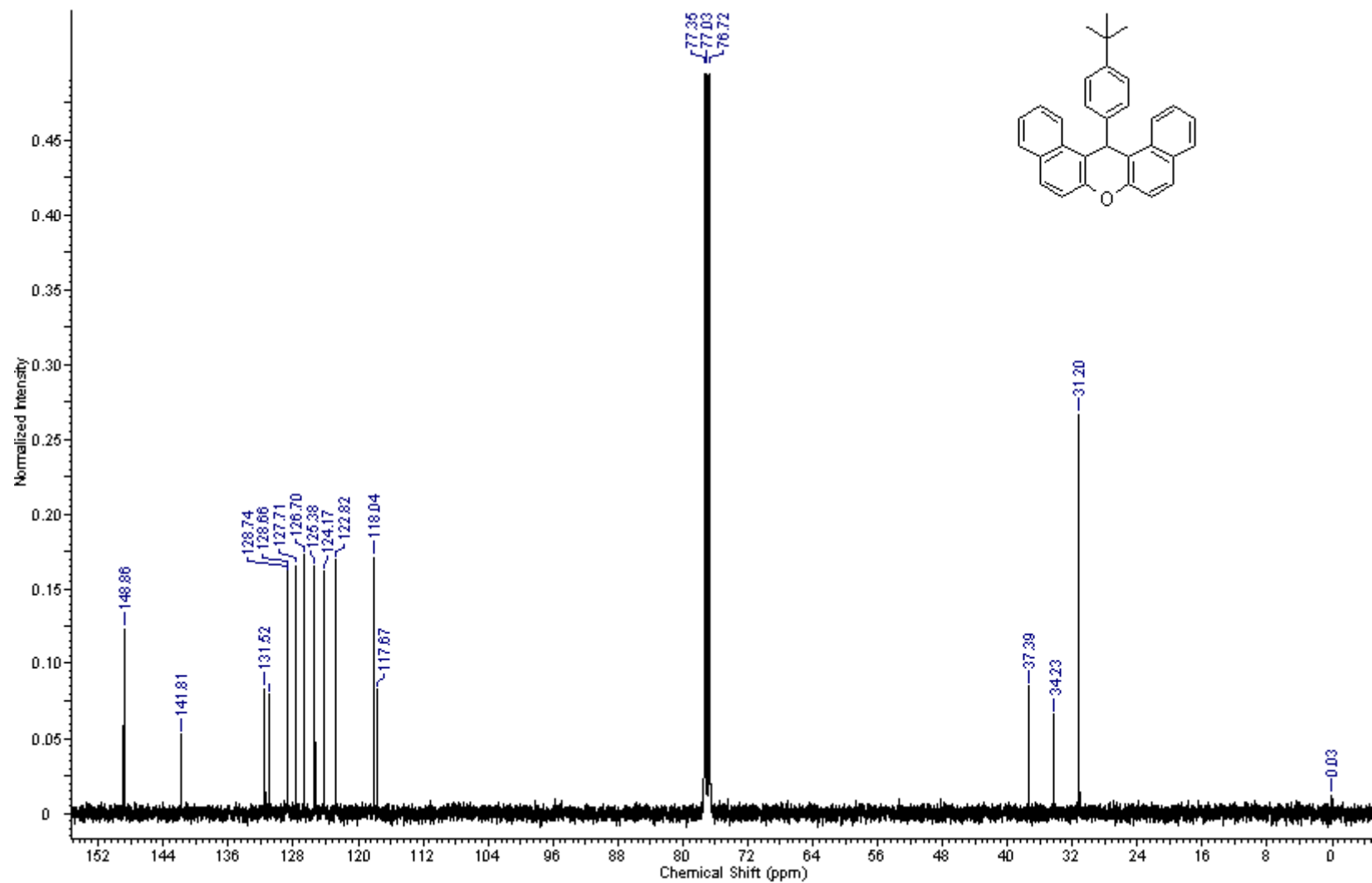
Figure S29. ^{13}C NMR of compound 14-(4-*t*-Butylphenyl)-14*H*-dibenzo[*a,j*]xanthene 3l.
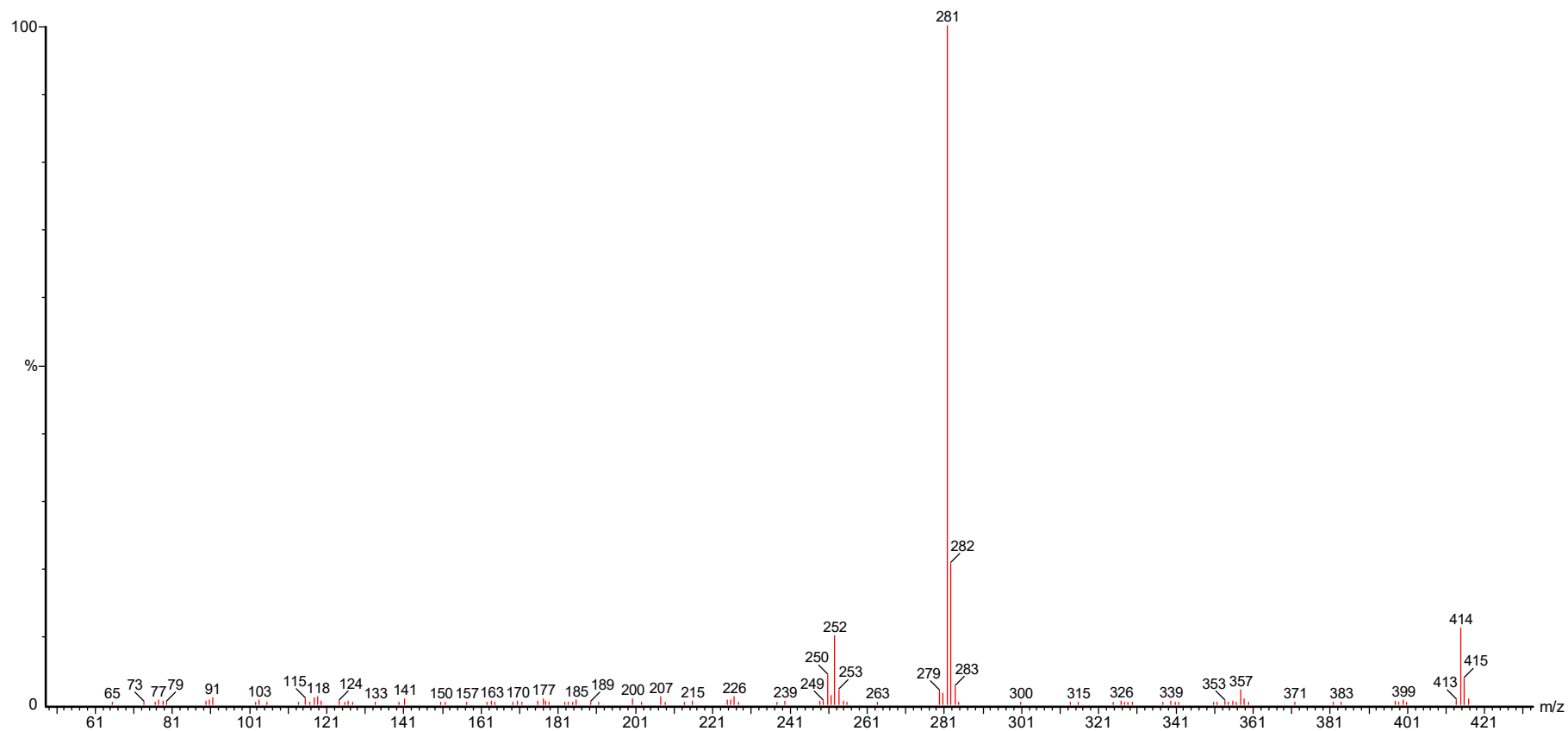
Figure S30. MS of compound 14-(4-*t*-Butylphenyl)-14*H*-dibenzo[*a,j*]xanthene 3l.

Table S2. DFT reaction mechanism study for the transformation of the aldehyde and 2-naphthol to xanthene derivatives.

Contents	Title	Page No.
Figure 1	Transition state structures of the 3b molecule transformation to the xanthene derivative optimized at M06-2X/6-31G(d,p) level of theory. The key bond distances in Å and the total energies (TE) in Hartrees are given for all five figures.	2
Figure 2	Transition state structures of the 3j molecule transformation to the xanthene derivative optimized at M06-2X/6-31G(d,p) level of theory. The key bond distances in Å and the total energies (TE) in Hartrees are given for all five figures.	3
Table 1	Geometry coordinates of the reactants, products and transition states of the 3b and 3j compounds are given.	4
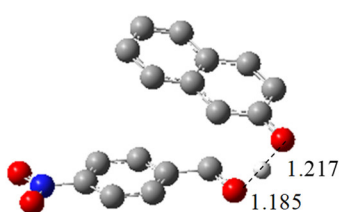
3b (1_2); TE = -1010.76167   **3b** (2_3); TE = -1010.69652   **3b** (3_4); TE = -1395.29544
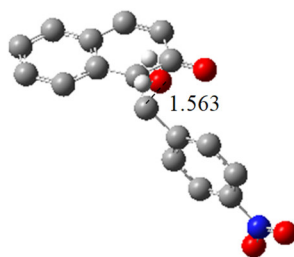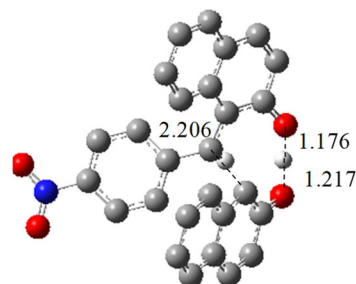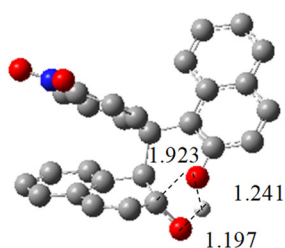
3b (4_5); TE = -1395.27816   **3b** (5_6); TE = -1395.25336
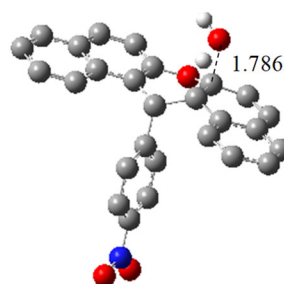
Figure S31. Transition state structures of the 3b molecule transformation to the xanthene derivatives optimized at the M06-2X/6-31G(d,p) level of theory. The key bond distances in Å and the total energies (TE) in Hartrees are given for all five figures.
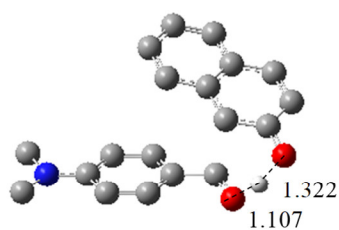
3j (1_2); TE = -940.25118   **3j** (2_3); TE = -940.18192   **3j** (3 4); TE = -1324.78407

1.554

2.290

1.322   1.361
1.107   1.078
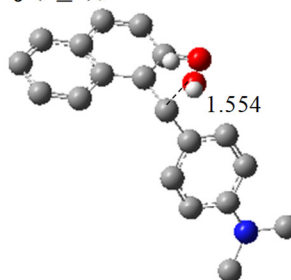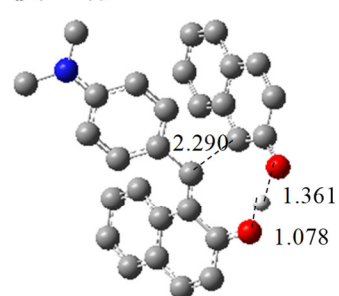
3j (4_5); TE = -1324.76124   **3j** (5_6); TE = -1324.73569

1.807

1.922

1.238

1.196
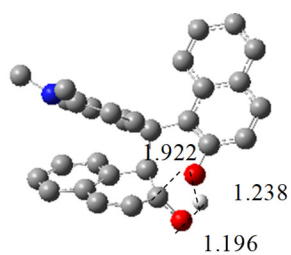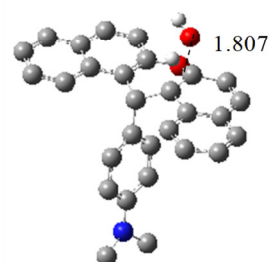
Figure S32. Transition state structures of the 3j molecule transformation to the xanthene derivatives optimized at the M06-2X/6-31G(d,p) level of theory. The key bond distances in Å and the total energies (TE) in Hartrees are given for all five figures.

Table S3. Geometry coordinates of the reactants, products and transition states of the 3b and 3j compounds are given.

3b:

1	6	0	0.476467	1.280027	0.000059
2	6	0	-0.910098	1.377597	-0.000007
3	6	0	-1.692643	0.223228	-0.000046
4	6	0	-1.099326	-1.042172	-0.000019
5	6	0	0.282458	-1.157441	0.000043
6	6	0	1.037437	0.010773	0.000081
7	1	0	1.120736	2.149748	0.000092
8	1	0	-1.740619	-1.917233	-0.000052
9	1	0	0.784905	-2.116354	0.000063
10	6	0	-3.177355	0.336992	-0.000131
11	8	0	-3.917605	-0.615488	0.000060
12	1	0	-3.571377	1.373990	0.000054
13	1	0	-1.387188	2.353760	-0.000028
14	7	0	2.509214	-0.104252	0.000151
15	8	0	2.982362	-1.224264	-0.000103
16	8	0	3.151168	0.928730	-0.000090

2-Naphthol:

1	6	0	-1.306973	1.455500	-0.980556
2	6	0	0.065677	1.473321	-0.944928
3	6	0	0.763353	2.704154	-0.895367
4	6	0	0.032741	3.926382	-0.882629
5	6	0	-1.383741	3.869435	-0.920139
6	6	0	-2.041116	2.668911	-0.967891
7	1	0	2.742295	1.829558	-0.867322
8	1	0	0.608033	0.533522	-0.955010
9	6	0	2.183452	2.761019	-0.857587
10	6	0	0.737538	5.157542	-0.832863
11	1	0	-1.947317	4.798163	-0.910372
12	1	0	-3.127771	2.636305	-0.996351
13	6	0	2.107003	5.180101	-0.797250
14	6	0	2.836002	3.964879	-0.809964
15	1	0	0.168088	6.083123	-0.823520
16	1	0	2.637972	6.125426	-0.759124
17	1	0	3.920649	3.992101	-0.781550
18	8	0	-1.937291	0.250071	-1.027846
19	1	0	-2.890571	0.386673	-1.047760

3b (2):

1	6	0	1.355083	1.790522	1.152620
2	6	0	1.968740	1.217406	-0.113914
3	6	0	2.333789	-0.241465	-0.060241
4	6	0	1.868841	-1.053570	0.986871

5	6	0	1.125722	-0.453517	2.091972
6	6	0	0.894524	0.866620	2.192789
7	1	0	3.455434	-0.188091	-1.890281
8	6	0	3.081684	-0.816672	-1.085603
9	6	0	2.138422	-2.426562	0.973604
10	1	0	0.769522	-1.126163	2.869011
11	1	0	0.363865	1.305285	3.030429
12	6	0	2.869192	-2.992888	-0.062211
13	6	0	3.349688	-2.182958	-1.090359
14	1	0	1.768959	-3.046020	1.786077
15	1	0	3.071686	-4.058387	-0.066485
16	1	0	3.933348	-2.615441	-1.896239
17	8	0	1.172944	2.999186	1.238675
18	6	0	0.939896	1.513410	-1.272046
19	8	0	0.848226	2.888392	-1.500514
20	1	0	0.931086	3.340883	-0.643718
21	1	0	2.847745	1.822797	-0.362772
22	6	0	-0.405671	0.870288	-0.969201
23	6	0	-1.443277	1.638239	-0.436353
24	6	0	-0.598510	-0.499611	-1.177136
25	6	0	-2.651408	1.048771	-0.085661
26	1	0	-1.300288	2.704784	-0.304874
27	6	0	-1.798780	-1.105906	-0.831411
28	6	0	-2.801221	-0.316458	-0.284025
29	1	0	-3.470175	1.621285	0.331724
30	1	0	-1.972718	-2.164042	-0.980358
31	1	0	1.349312	1.055773	-2.180402
32	1	0	0.198041	-1.098623	-1.609800
33	7	0	-4.073472	-0.951438	0.091370
34	8	0	-4.177991	-2.151772	-0.085872
35	8	0	-4.942154	-0.239290	0.560203

3b (3):

1	6	0	-2.304297	2.203621	-1.760401
2	6	0	-0.892182	2.484001	-1.335877
3	6	0	-0.671355	3.609992	-0.399561
4	6	0	-1.756052	4.106079	0.352745
5	6	0	-3.092053	3.565776	0.130186
6	6	0	-3.357164	2.683193	-0.845009
7	1	0	1.414511	3.887775	-0.856594
8	6	0	0.583462	4.205817	-0.235294
9	6	0	-1.551639	5.132525	1.279756
10	1	0	-3.893344	3.941088	0.762512
11	1	0	-4.359580	2.326421	-1.054249
12	6	0	-0.292892	5.690023	1.455361
13	6	0	0.773921	5.229773	0.685084
14	1	0	-2.397218	5.495307	1.857449

15	1	0	-0.145154	6.489288	2.173508
16	1	0	1.755730	5.678905	0.791880
17	8	0	-2.597894	1.580614	-2.766639
18	6	0	0.128740	1.633586	-1.602586
19	1	0	1.041878	1.815220	-1.036402
20	6	0	0.224401	0.429724	-2.442407
21	6	0	1.001386	-0.628060	-1.936602
22	6	0	-0.324324	0.312179	-3.727797
23	6	0	1.183006	-1.796858	-2.657169
24	6	0	-0.133454	-0.846299	-4.470655
25	1	0	-0.898399	1.128744	-4.139052
26	6	0	0.605370	-1.881131	-3.917483
27	1	0	1.761656	-2.627662	-2.274340
28	1	0	-0.545361	-0.957060	-5.465647
29	1	0	1.455423	-0.530789	-0.954961
30	7	0	0.802804	-3.110678	-4.702093
31	8	0	0.298946	-3.159324	-5.808540
32	8	0	1.458889	-4.001629	-4.193960

3b (4):

1	8	0	0.101966	0.157360	2.632750
2	6	0	-0.377557	-0.105719	-0.152083
3	6	0	1.069533	-0.583601	-0.207777
4	6	0	2.139799	0.214272	0.204555
5	6	0	1.346491	-1.827724	-0.791589
6	6	0	3.454894	-0.212378	0.049367
7	1	0	1.966485	1.188991	0.648668
8	6	0	2.648317	-2.270518	-0.956590
9	6	0	3.684617	-1.448881	-0.529674
10	1	0	4.293174	0.394803	0.366476
11	1	0	2.875000	-3.231132	-1.401352
12	6	0	-1.192996	-2.211881	1.085205
13	6	0	-2.167878	-3.230763	1.276761
14	6	0	-1.425957	-1.153012	0.221710
15	6	0	-3.379968	-3.161513	0.662423
16	6	0	-2.722355	-1.047189	-0.396135
17	6	0	-3.701575	-2.058976	-0.174839
18	6	0	-0.044057	3.631129	2.067959
19	6	0	0.028445	3.677387	0.610666
20	6	0	-0.135878	2.482997	2.759231
21	6	0	0.323174	4.883657	-0.031885
22	6	0	-0.148819	2.496384	-0.139714
23	6	0	-0.158683	1.196424	2.049379
24	6	0	0.461909	4.935875	-1.411940
25	1	0	0.452684	5.780773	0.567117
26	6	0	0.002654	2.564168	-1.523972
27	6	0	-0.587153	1.232650	0.588580

28	6	0	0.309642	3.769166	-2.153970
29	1	0	0.695210	5.873794	-1.903737
30	1	0	-0.099306	1.675976	-2.137373
31	1	0	0.431565	3.789662	-3.231823
32	1	0	0.040476	4.577777	2.596973
33	1	0	-0.094927	2.444756	3.841974
34	1	0	-0.602742	0.100893	-1.201854
35	6	0	-3.096559	0.040540	-1.237367
36	6	0	-4.342155	0.109266	-1.814346
37	1	0	-2.403567	0.853501	-1.430599
38	6	0	-5.297984	-0.903797	-1.594820
39	1	0	-4.591469	0.956827	-2.444907
40	6	0	-4.974149	-1.964600	-0.788054
41	1	0	-6.276709	-0.839668	-2.057819
42	1	0	-5.693896	-2.757089	-0.601192
43	1	0	-1.902166	-4.043886	1.943090
44	1	0	-4.123714	-3.938227	0.815952
45	8	0	-0.045946	-2.396667	1.770227
46	1	0	0.315891	-1.522889	2.004403
47	1	0	-1.682328	1.347417	0.694313
48	1	0	0.521030	-2.458633	-1.106522
49	7	0	5.070815	-1.904814	-0.701566
50	8	0	5.245610	-2.992776	-1.219162
51	8	0	5.959504	-1.165432	-0.318478

3b (5):

1	8	0	1.098836	-1.282713	-2.094655
2	6	0	0.578170	-0.494788	0.537965
3	6	0	-0.387636	0.652089	0.275064
4	6	0	-1.448351	0.874293	1.161192
5	6	0	-0.261077	1.473070	-0.850089
6	6	0	-2.380923	1.875440	0.924097
7	6	0	-1.180247	2.482631	-1.102127
8	1	0	0.563225	1.317539	-1.538151
9	6	0	-2.228894	2.659881	-0.210413
10	1	0	-3.210874	2.057491	1.594961
11	1	0	-1.100903	3.126878	-1.968609
12	6	0	0.031223	-1.998220	-1.463409
13	6	0	-1.239822	-1.472503	-2.086916
14	6	0	0.049702	-1.879928	0.060701
15	6	0	-2.396109	-1.500176	-1.422209
16	6	0	-1.289031	-2.217900	0.673761
17	6	0	-2.475711	-1.978095	-0.037771
18	6	0	4.435416	-0.098011	-1.365736
19	6	0	4.286341	0.436875	-0.057600
20	6	0	3.383255	-0.687344	-2.008297
21	6	0	5.366011	1.072075	0.606725

22	6	0	3.021346	0.345519	0.591837
23	6	0	2.131634	-0.778755	-1.353766
24	6	0	5.204385	1.614191	1.855323
25	1	0	6.325920	1.125606	0.100333
26	6	0	2.881397	0.931748	1.878826
27	6	0	1.940482	-0.300437	-0.078417
28	6	0	3.943227	1.548617	2.491112
29	1	0	6.035733	2.101028	2.353912
30	1	0	1.916142	0.913992	2.374316
31	1	0	3.813525	1.995907	3.471337
32	1	0	5.403455	-0.024472	-1.852862
33	1	0	3.469740	-1.090765	-3.010815
34	1	0	0.683287	-0.592049	1.623833
35	6	0	-1.359350	-2.672734	1.987337
36	6	0	-2.590933	-2.881318	2.604761
37	1	0	-0.438189	-2.863960	2.533148
38	6	0	-3.768238	-2.630613	1.904194
39	1	0	-2.630080	-3.239762	3.628117
40	6	0	-3.707120	-2.183701	0.589001
41	1	0	-4.730518	-2.787239	2.380108
42	1	0	-4.621426	-1.989550	0.035023
43	1	0	-1.162311	-1.108043	-3.107362
44	1	0	-3.315124	-1.163575	-1.894840
45	8	0	0.198135	-3.361733	-1.730970
46	1	0	0.058463	-3.499690	-2.676642
47	1	0	0.788172	-2.615427	0.399578
48	1	0	-1.554658	0.243058	2.039123
49	7	0	-3.211103	3.721424	-0.473186
50	8	0	-3.057784	4.396659	-1.474868
51	8	0	-4.120527	3.859240	0.325109

3b (6):

1	8	0	-0.000160	-2.298183	-1.849204
2	6	0	-0.000053	-0.631992	0.503191
3	6	0	0.000050	0.857651	0.158654
4	6	0	0.000185	1.840164	1.149624
5	6	0	0.000031	1.245999	-1.185371
6	6	0	0.000287	3.190576	0.818689
7	6	0	0.000132	2.586770	-1.538483
8	1	0	-0.000067	0.484395	-1.960691
9	6	0	0.000258	3.536239	-0.523535
10	1	0	0.000390	3.968565	1.571588
11	1	0	0.000115	2.910059	-2.571753
12	6	0	-1.175135	-2.054655	-1.189248
13	6	0	-2.314580	-2.645734	-1.787695
14	6	0	-1.246237	-1.303417	-0.042769
15	6	0	-3.537652	-2.479595	-1.209246

16	6	0	-2.526169	-1.126939	0.574978
17	6	0	-3.678090	-1.723983	-0.012519
18	6	0	3.537307	-2.480056	-1.209234
19	6	0	3.677842	-1.724445	-0.012518
20	6	0	2.314215	-2.646042	-1.787684
21	6	0	4.944294	-1.554359	0.598815
22	6	0	2.525997	-1.127247	0.574973
23	6	0	1.174845	-2.054813	-1.189243
24	6	0	5.079807	-0.819904	1.749075
25	1	0	5.809201	-2.020103	0.134539
26	6	0	2.701926	-0.369106	1.762379
27	6	0	1.246041	-1.303579	-0.042767
28	6	0	3.942132	-0.222166	2.333442
29	1	0	6.053956	-0.694535	2.209401
30	1	0	1.847315	0.108087	2.226912
31	1	0	4.049641	0.361899	3.241697
32	1	0	4.421306	-2.927738	-1.653556
33	1	0	2.172999	-3.224284	-2.693750
34	1	0	-0.000057	-0.729678	1.595280
35	6	0	-2.702001	-0.368807	1.762405
36	6	0	-3.942187	-0.221724	2.333474
37	1	0	-1.847329	0.108262	2.226952
38	6	0	-5.079939	-0.819302	1.749094
39	1	0	-4.049621	0.362332	3.241743
40	6	0	-4.944520	-1.553750	0.598819
41	1	0	-6.054071	-0.693821	2.209425
42	1	0	-5.809486	-2.019378	0.134536
43	1	0	-2.173438	-3.223989	-2.693764
44	1	0	-4.421708	-2.927162	-1.653572
45	1	0	0.000211	1.551390	2.197678
46	7	0	0.000368	4.961015	-0.885809
47	8	0	0.000324	5.240592	-2.070519
48	8	0	0.000507	5.773077	0.021499

H2O:

1	8	0	-0.796312	0.972645	0.000000
2	1	0	0.164426	1.014868	0.000000
3	1	0	-1.077212	1.892371	0.000000

3b (1_2):

1	6	0	0.985102	1.869749	-0.236207
2	6	0	1.606267	0.750230	-0.867193
3	6	0	2.213372	-0.286855	-0.064453
4	6	0	2.006231	-0.285074	1.335125
5	6	0	1.298795	0.819990	1.931029
6	6	0	0.812675	1.851836	1.196353

7	1	0	3.128893	-1.327440	-1.715023
8	6	0	2.965468	-1.327327	-0.640195
9	6	0	2.530570	-1.331401	2.117736
10	1	0	1.164099	0.811785	3.010094
11	1	0	0.286079	2.686625	1.644709
12	6	0	3.253255	-2.351591	1.532009
13	6	0	3.477147	-2.342919	0.145647
14	1	0	2.363390	-1.320267	3.191312
15	1	0	3.655075	-3.154601	2.140437
16	1	0	4.052736	-3.140627	-0.312626
17	8	0	0.438338	2.786234	-0.949984
18	6	0	-0.234346	0.148737	-1.625977
19	8	0	-0.597679	1.171077	-2.321358
20	1	0	-0.179076	2.132965	-1.770125
21	1	0	1.978900	0.901920	-1.876111
22	1	0	-0.709865	-0.033793	-0.650800
23	6	0	0.184811	-1.079869	-2.345100
24	6	0	0.235967	-2.300521	-1.668088
25	6	0	0.531481	-1.007948	-3.698457
26	6	0	0.637309	-3.453147	-2.331879
27	6	0	0.940669	-2.148670	-4.372372
28	1	0	0.462951	-0.050493	-4.203425
29	6	0	0.985517	-3.349464	-3.670914
30	1	0	0.691381	-4.414328	-1.836882
31	1	0	1.217146	-2.132406	-5.419054
32	1	0	-0.024811	-2.344390	-0.614222
33	7	0	1.420947	-4.564064	-4.380119
34	8	0	1.721786	-4.451643	-5.553747
35	8	0	1.455771	-5.602695	-3.746352

3b (2_3):

1	6	0	-1.106860	2.226309	0.896314
2	6	0	-1.221634	0.775702	1.081093
3	6	0	-2.217478	-0.015379	0.363056
4	6	0	-3.186205	0.672127	-0.411421
5	6	0	-3.120161	2.115692	-0.513483
6	6	0	-2.165014	2.849340	0.089179
7	1	0	-1.588873	-1.999734	0.987562
8	6	0	-2.305440	-1.420536	0.412221
9	6	0	-4.188407	-0.041585	-1.085729
10	1	0	-3.880976	2.604530	-1.118539
11	1	0	-2.113589	3.928095	-0.013671
12	6	0	-4.254739	-1.420953	-1.020478
13	6	0	-3.298849	-2.107615	-0.265353
14	1	0	-4.916308	0.515404	-1.670051
15	1	0	-5.032282	-1.962605	-1.547460
16	1	0	-3.331598	-3.191060	-0.205830

17	8	0	-0.216285	2.891097	1.430213
18	6	0	-0.075903	0.138322	1.787810
19	1	0	-1.423331	0.836293	2.633845
20	8	0	-0.534611	0.462313	3.246660
21	1	0	-0.736812	-0.342663	3.753597
22	6	0	1.325510	0.643974	1.584681
23	6	0	2.157570	1.014821	2.639081
24	6	0	1.811450	0.640091	0.274882
25	6	0	3.472343	1.386142	2.391661
26	1	0	1.769384	1.043526	3.649979
27	6	0	3.123157	1.006279	0.013817
28	1	0	1.150346	0.365315	-0.541625
29	6	0	3.931023	1.370230	1.082647
30	1	0	4.140671	1.689673	3.187366
31	1	0	3.526120	1.020034	-0.990821
32	1	0	-0.087874	-0.950669	1.718603
33	7	0	5.324728	1.753923	0.817154
34	8	0	5.703625	1.733658	-0.339601
35	8	0	6.015083	2.063708	1.770992

3b (3_4):

1	6	0	-0.310648	-0.731985	-0.732131
2	6	0	1.105058	-0.783217	-0.638588
3	6	0	1.749407	-1.612984	-1.611840
4	6	0	3.168936	-1.472039	-1.807527
5	1	0	3.606575	-2.024760	-2.630894
6	8	0	1.136191	-2.471152	-2.348829
7	1	0	-0.683851	-1.160239	-1.658315
8	6	0	-1.627478	-3.142883	-0.858536
9	6	0	-0.925046	-2.600736	0.265253
10	1	0	0.134067	-2.817249	0.318945
11	8	0	-1.058449	-3.346504	-1.986631
12	1	0	0.066680	-2.897901	-2.108799
13	6	0	1.923693	-0.131430	0.370411
14	6	0	3.328150	-0.069376	0.180558
15	6	0	3.910916	-0.718753	-0.960644
16	1	0	4.985301	-0.634750	-1.103211
17	6	0	1.400720	0.403418	1.569696
18	1	0	0.339785	0.319628	1.776495
19	6	0	4.143888	0.575033	1.131499
20	1	0	5.214743	0.618482	0.952293
21	6	0	-1.166073	0.404172	-0.290302
22	6	0	-0.650076	1.708719	-0.235842
23	6	0	-2.538475	0.213012	-0.091875
24	6	0	-1.472355	2.786741	0.056842
25	6	0	-3.373215	1.279027	0.214224
26	1	0	-2.957881	-0.780325	-0.188191

27	6	0	-2.819407	2.547792	0.292350
28	1	0	-1.091677	3.799227	0.101228
29	1	0	-4.433843	1.144243	0.383958
30	6	0	-1.615776	-2.421627	1.522847
31	6	0	-3.045251	-3.390979	-0.737401
32	1	0	-3.555060	-3.779891	-1.611721
33	6	0	-3.009276	-2.660217	1.601264
34	6	0	-3.689398	-3.164778	0.436538
35	1	0	-4.755037	-3.366084	0.516795
36	6	0	2.220967	1.013494	2.497887
37	1	0	1.788460	1.408818	3.411458
38	6	0	3.603405	1.119740	2.275888
39	1	0	4.238903	1.607327	3.007008
40	6	0	-3.690579	-2.436298	2.813067
41	6	0	-3.009778	-2.001677	3.931481
42	6	0	-0.935942	-2.007804	2.684830
43	6	0	-1.621116	-1.796924	3.865395
44	1	0	0.139010	-1.854462	2.638646
45	1	0	-1.081825	-1.475174	4.750533
46	1	0	-3.540277	-1.828867	4.861508
47	1	0	-4.761286	-2.617102	2.854972
48	1	0	0.401335	1.879216	-0.434987
49	7	0	-3.694578	3.684905	0.617322
50	8	0	-4.872961	3.449713	0.811324
51	8	0	-3.184585	4.788618	0.672957

3b (4_5):

1	8	0	0.474372	-3.537516	-0.425002
2	6	0	-0.398224	-0.126104	0.413382
3	6	0	-2.012912	-1.634776	-0.750437
4	6	0	-3.308302	-2.165993	-0.982896
5	6	0	-1.808673	-0.578701	0.113241
6	6	0	-4.390513	-1.604940	-0.368284
7	6	0	-2.940920	0.057131	0.713098
8	6	0	-4.242646	-0.475088	0.480389
9	6	0	2.734364	-1.076645	-1.214664
10	6	0	2.930866	-0.607121	0.160604
11	6	0	1.687708	-1.835399	-1.569704
12	6	0	4.114751	0.026264	0.545248
13	6	0	1.914577	-0.810671	1.108191
14	6	0	0.738656	-2.269117	-0.529440
15	6	0	4.296185	0.447570	1.858064
16	1	0	4.894784	0.186644	-0.193664
17	6	0	2.106004	-0.394892	2.421495
18	6	0	0.571110	-1.349181	0.659804
19	6	0	3.293653	0.229480	2.799955
20	1	0	5.219276	0.938057	2.147742
21	1	0	1.318695	-0.559208	3.153313

22	1	0	3.435069	0.542692	3.829044
23	1	0	3.506113	-0.835617	-1.941429
24	1	0	1.577315	-2.267344	-2.557754
25	6	0	-2.835262	1.220657	1.524333
26	6	0	-3.946559	1.796142	2.087919
27	1	0	-1.867617	1.686505	1.677847
28	6	0	-5.230803	1.245620	1.878271
29	1	0	-3.838715	2.689277	2.694997
30	6	0	-5.369448	0.135940	1.085750
31	1	0	-6.099585	1.708279	2.334105
32	1	0	-6.350631	-0.292819	0.900642
33	1	0	-3.404636	-3.009422	-1.658105
34	1	0	-5.386204	-2.005669	-0.535988
35	8	0	-0.962517	-2.173582	-1.420151
36	1	0	0.115780	-1.948768	1.454044
37	1	0	-0.404869	0.357944	1.394114
38	1	0	-0.531912	-3.263238	-1.012561
39	6	0	0.134181	0.901179	-0.575617
40	6	0	0.984292	1.916054	-0.121207
41	6	0	-0.200852	0.855228	-1.933548
42	6	0	1.511886	2.856474	-0.996480
43	6	0	0.314766	1.787445	-2.824092
44	1	0	-0.859720	0.075253	-2.299039
45	6	0	1.166601	2.769434	-2.337118
46	1	0	2.174030	3.645144	-0.662509
47	1	0	0.071153	1.766795	-3.878817
48	1	0	1.250404	1.960343	0.931721
49	7	0	1.721584	3.756421	-3.275259
50	8	0	2.467903	4.606120	-2.823293
51	8	0	1.404482	3.661451	-4.446760
3b (5_6):					
1	8	0	-0.607101	7.729447	-5.026196
2	6	0	1.795654	7.787349	-6.568062
3	6	0	2.892402	8.240414	-5.607352
4	6	0	2.592710	8.459072	-4.257502
5	6	0	4.202475	8.427677	-6.049753
6	6	0	3.575724	8.863950	-3.367906
7	6	0	5.204542	8.832750	-5.174853
8	1	0	4.449636	8.246784	-7.092603
9	6	0	4.867858	9.045572	-3.847616
10	1	0	3.366385	9.039866	-2.320345
11	1	0	6.227092	8.981294	-5.498132
12	6	0	-0.043971	6.520964	-5.324757
13	6	0	-0.268245	5.541487	-4.273878
14	6	0	1.172196	6.453955	-6.153848
15	6	0	0.564322	4.492130	-4.150420
16	6	0	2.059927	5.307866	-5.937076

17	6	0	1.729230	4.312082	-4.988658
18	6	0	-1.301386	10.830367	-6.741921
19	6	0	-0.156330	10.987470	-7.568024
20	6	0	-1.424966	9.744457	-5.923406
21	6	0	-0.017725	12.116952	-8.413971
22	6	0	0.872063	10.000867	-7.537348
23	6	0	-0.399881	8.772062	-5.909564
24	6	0	1.096220	12.279075	-9.195512
25	1	0	-0.814943	12.854924	-8.425883
26	6	0	2.016566	10.204389	-8.353721
27	6	0	0.727171	8.858492	-6.687627
28	6	0	2.124589	11.310742	-9.158390
29	1	0	1.194664	13.147868	-9.837458
30	1	0	2.825066	9.483221	-8.334578
31	1	0	3.010160	11.445677	-9.770730
32	1	0	-2.076776	11.590041	-6.769412
33	1	0	-2.282939	9.597884	-5.276799
34	1	0	2.255474	7.654496	-7.552822
35	6	0	3.245433	5.141654	-6.676116
36	6	0	4.050909	4.030011	-6.500211
37	1	0	3.530619	5.889731	-7.408969
38	6	0	3.708875	3.039523	-5.571719
39	1	0	4.956398	3.927924	-7.090141
40	6	0	2.557284	3.189721	-4.823715
41	1	0	4.342895	2.169968	-5.438444
42	1	0	2.277788	2.439559	-4.088492
43	1	0	-1.120514	5.700239	-3.623420
44	1	0	0.382802	3.752161	-3.375022
45	8	0	-1.052210	5.941657	-6.679986
46	1	0	-1.700862	6.593123	-6.995406
47	1	0	0.140413	6.099528	-7.021870
48	1	0	1.577842	8.303904	-3.901390
49	7	0	5.917014	9.475254	-2.912671
50	8	0	7.041107	9.625436	-3.356427
51	8	0	5.597878	9.655819	-1.751643

3j:

1	6	0	0.756719	0.052407	0.599998
2	6	0	2.132217	0.205941	0.600283
3	6	0	2.751696	1.188140	-0.173774
4	6	0	1.953475	2.026352	-0.960260
5	6	0	0.580121	1.890700	-0.975493
6	6	0	-0.055684	0.895565	-0.192082
7	1	0	0.310265	-0.720091	1.212717
8	1	0	2.442768	2.788024	-1.559789
9	1	0	-0.009299	2.555015	-1.594611
10	6	0	4.213597	1.340192	-0.163851

11	8	0	4.825634	2.165857	-0.805997
12	1	0	4.750445	0.623054	0.495404
13	1	0	2.742049	-0.451815	1.216004
14	7	0	-1.419876	0.755783	-0.202846
15	6	0	-2.046539	-0.266896	0.607241
16	1	0	-3.125931	-0.221585	0.467676
17	1	0	-1.707695	-1.271041	0.323383
18	1	0	-1.834092	-0.123691	1.674045
19	6	0	-2.231217	1.631588	-1.022015
20	1	0	-3.280197	1.365808	-0.896911
21	1	0	-2.109121	2.682938	-0.733736
22	1	0	-1.980216	1.537406	-2.085686

3j (2):

1	6	0	0.043952	1.426524	-1.534677
2	6	0	0.024900	0.076788	-0.842124
3	6	0	1.229152	-0.237942	0.001924
4	6	0	2.142043	0.771340	0.347746
5	6	0	1.984593	2.110235	-0.214475
6	6	0	1.027800	2.425408	-1.102905
7	1	0	0.716241	-2.308809	0.233728
8	6	0	1.415464	-1.522819	0.508448
9	6	0	3.206103	0.481428	1.208650
10	1	0	2.700976	2.865111	0.102053
11	1	0	0.932607	3.415856	-1.533712
12	6	0	3.373560	-0.798518	1.719754
13	6	0	2.478764	-1.805679	1.361267
14	1	0	3.902917	1.272346	1.472345
15	1	0	4.200259	-1.014560	2.388023
16	1	0	2.608914	-2.811767	1.746340
17	8	0	-0.813009	1.691530	-2.369596
18	6	0	-1.298458	0.050309	0.020997
19	8	0	-2.414574	0.026970	-0.824263
20	1	0	-2.228533	0.612555	-1.576758
21	1	0	-0.119502	-0.693801	-1.607882
22	6	0	-1.320241	1.196139	1.016343
23	6	0	-2.015958	2.371838	0.741329
24	6	0	-0.602678	1.130444	2.210796
25	6	0	-1.980573	3.455194	1.608685
26	1	0	-2.610537	2.436796	-0.164522
27	6	0	-0.554009	2.204629	3.088967
28	6	0	-1.230461	3.405380	2.799123
29	1	0	-2.549668	4.340689	1.355212
30	1	0	0.008087	2.098226	4.008249
31	1	0	-1.288659	-0.899692	0.568986
32	1	0	-0.067018	0.219053	2.468441
33	7	0	-1.160596	4.497417	3.655837

34	6	0	-0.642984	4.289022	4.991747
35	1	0	0.405667	3.977524	4.956880
36	1	0	-0.686670	5.230326	5.540345
37	1	0	-1.206410	3.529411	5.554660
38	6	0	-2.098543	5.583319	3.461244
39	1	0	-3.148052	5.258030	3.523479
40	1	0	-1.924945	6.343061	4.223882
41	1	0	-1.946002	6.055372	2.485922

3j (3):

1	6	0	-2.382700	2.152131	-1.481010
2	6	0	-1.020230	2.678540	-1.195044
3	6	0	-0.896854	3.753133	-0.186071
4	6	0	-1.962537	4.007115	0.704929
5	6	0	-3.202841	3.261296	0.562926
6	6	0	-3.406141	2.402457	-0.448050
7	1	0	1.048633	4.443638	-0.807704
8	6	0	0.247665	4.557369	-0.084755
9	6	0	-1.836579	4.989852	1.693635
10	1	0	-3.989222	3.452495	1.289813
11	1	0	-4.347243	1.882278	-0.590424
12	6	0	-0.679619	5.745191	1.803463
13	6	0	0.360520	5.530986	0.898527
14	1	0	-2.668269	5.158074	2.372628
15	1	0	-0.592632	6.507237	2.570486
16	1	0	1.258761	6.137954	0.949402
17	8	0	-2.676891	1.496125	-2.471910
18	6	0	0.121761	2.082871	-1.653402
19	1	0	1.020152	2.419772	-1.136017
20	6	0	0.436691	1.034517	-2.607745
21	6	0	1.670909	0.377984	-2.421448
22	6	0	-0.313345	0.657344	-3.738702
23	6	0	2.111172	-0.630968	-3.252048
24	6	0	0.123471	-0.337913	-4.592885
25	1	0	-1.243910	1.162997	-3.945717
26	6	0	1.334456	-1.027895	-4.365036
27	1	0	3.062572	-1.105066	-3.046763
28	1	0	-0.485224	-0.578069	-5.455443
29	1	0	2.297078	0.667827	-1.581096
30	7	0	1.750579	-2.033469	-5.199033
31	6	0	0.969294	-2.366126	-6.371912
32	1	0	1.444523	-3.196511	-6.893055
33	1	0	-0.045832	-2.674189	-6.097046
34	1	0	0.893108	-1.520440	-7.067752
35	6	0	3.035889	-2.663149	-4.983913
36	1	0	3.086620	-3.135772	-3.996067
37	1	0	3.183880	-3.438034	-5.735277

38	1	0	3.863175	-1.945567	-5.062498

3j (4):

1	8	0	-0.466950	8.321892	-4.412955
2	6	0	1.927457	7.732782	-5.834328
3	6	0	2.620268	8.505510	-4.717490
4	6	0	2.329504	9.831214	-4.402307
5	6	0	3.677573	7.907343	-4.024289
6	6	0	3.043476	10.530804	-3.434308
7	1	0	1.534636	10.361497	-4.919936
8	6	0	4.400275	8.585044	-3.057762
9	6	0	4.090782	9.919808	-2.725308
10	1	0	2.772747	11.560501	-3.238304
11	1	0	5.206480	8.066387	-2.554414
12	6	0	1.282494	5.771732	-4.287488
13	6	0	1.116583	4.374442	-4.069880
14	6	0	1.590043	6.268686	-5.545237
15	6	0	1.197757	3.490109	-5.100267
16	6	0	1.637605	5.342817	-6.647506
17	6	0	1.440951	3.948524	-6.423028
18	6	0	-1.211469	10.489408	-7.090182
19	6	0	0.087726	10.560444	-7.753314
20	6	0	-1.455419	9.674323	-6.051223
21	6	0	0.339426	11.572266	-8.684768
22	6	0	1.101211	9.641889	-7.409666
23	6	0	-0.389959	8.801244	-5.530418
24	6	0	1.591489	11.700668	-9.269936
25	1	0	-0.458285	12.265736	-8.936804
26	6	0	2.357417	9.793469	-7.994898
27	6	0	0.748243	8.482072	-6.489365
28	6	0	2.602184	10.813965	-8.912124
29	1	0	1.781481	12.490061	-9.989049
30	1	0	3.172661	9.130567	-7.728172
31	1	0	3.592070	10.913969	-9.345075
32	1	0	-1.979397	11.179923	-7.432156
33	1	0	-2.388577	9.690862	-5.499144
34	1	0	2.690828	7.655102	-6.613155
35	6	0	1.873916	5.749274	-7.993709
36	6	0	1.913810	4.842159	-9.025435
37	1	0	2.017388	6.797494	-8.235818
38	6	0	1.724438	3.465380	-8.786814
39	1	0	2.091605	5.193541	-10.037047
40	6	0	1.493268	3.036698	-7.504732
41	1	0	1.759686	2.758735	-9.609053
42	1	0	1.342509	1.981253	-7.293276
43	1	0	0.906551	4.060034	-3.053452
44	1	0	1.062972	2.425688	-4.929512

45	8	0	1.146124	6.520817	-3.176370
46	1	0	0.858338	7.412501	-3.435477
47	1	0	0.255988	7.749692	-7.156983
48	1	0	3.933445	6.873701	-4.243629
49	7	0	4.787110	10.595937	-1.733415
50	6	0	4.608360	12.027503	-1.621628
51	1	0	3.570196	12.269044	-1.372588
52	1	0	5.235739	12.402355	-0.812520
53	1	0	4.871535	12.563939	-2.546053
54	6	0	6.024906	10.024502	-1.246384
55	1	0	5.842794	9.060648	-0.761020
56	1	0	6.766890	9.870972	-2.044446
57	1	0	6.453955	10.692158	-0.498792

3j (5):

1	8	0	-0.470358	7.332078	-5.104838
2	6	0	1.763383	8.077754	-6.645477
3	6	0	2.754280	8.472431	-5.560929
4	6	0	4.116653	8.216201	-5.724760
5	6	0	2.352303	9.051441	-4.357033
6	6	0	5.041617	8.506830	-4.731091
7	6	0	3.261954	9.353525	-3.353337
8	1	0	1.300359	9.266627	-4.190563
9	6	0	4.635658	9.093740	-3.517973
10	1	0	6.084436	8.276611	-4.909846
11	1	0	2.893325	9.797039	-2.436870
12	6	0	0.421150	6.262089	-5.432882
13	6	0	1.178682	5.942693	-4.165779
14	6	0	1.333985	6.581867	-6.614474
15	6	0	2.388883	5.384304	-4.212304
16	6	0	2.525731	5.655608	-6.669816
17	6	0	3.063349	5.120666	-5.487779
18	6	0	-1.955148	10.282703	-6.568793
19	6	0	-0.875699	10.828445	-7.314744
20	6	0	-1.806448	9.117020	-5.871872
21	6	0	-1.008610	12.050846	-8.020928
22	6	0	0.370320	10.138227	-7.338836
23	6	0	-0.566074	8.434582	-5.907447
24	6	0	0.049572	12.586185	-8.708696
25	1	0	-1.968982	12.559123	-7.999795
26	6	0	1.453672	10.728683	-8.044447
27	6	0	0.500886	8.902605	-6.638004
28	6	0	1.296145	11.918701	-8.709148
29	1	0	-0.061458	13.523740	-9.243306
30	1	0	2.425317	10.245906	-8.030966
31	1	0	2.138084	12.356621	-9.235796
32	1	0	-2.903033	10.813158	-6.555446

33	1	0	-2.610781	8.688006	-5.284821
34	1	0	2.262832	8.203158	-7.613106
35	6	0	3.162190	5.407888	-7.882297
36	6	0	4.326847	4.644778	-7.934964
37	1	0	2.740830	5.820963	-8.795928
38	6	0	4.866743	4.123800	-6.761861
39	1	0	4.809212	4.457368	-8.888785
40	6	0	4.234116	4.361398	-5.546672
41	1	0	5.775057	3.531080	-6.794982
42	1	0	4.647707	3.956211	-4.627038
43	1	0	0.672590	6.163085	-3.230206
44	1	0	2.912068	5.115616	-3.298311
45	8	0	-0.351752	5.166675	-5.842222
46	1	0	-0.851991	4.856276	-5.076738
47	1	0	0.719062	6.418249	-7.507359
48	1	0	4.467004	7.756242	-6.646418
49	7	0	5.556184	9.418144	-2.528802
50	6	0	5.058837	9.745043	-1.209149
51	1	0	4.450841	8.939262	-0.770238
52	1	0	5.904420	9.940447	-0.549048
53	1	0	4.448408	10.652828	-1.239041
54	6	0	6.892441	8.870786	-2.629426
55	1	0	7.473990	9.191244	-1.764560
56	1	0	6.901497	7.770793	-2.669589
57	1	0	7.398858	9.246810	-3.523815

3j (6):

1	8	0	-0.565152	7.244277	-5.006772
2	6	0	1.875081	7.934037	-6.386568
3	6	0	2.905255	8.604489	-5.479845
4	6	0	4.148706	9.017191	-5.940365
5	6	0	2.605889	8.825660	-4.131272
6	6	0	5.079509	9.619443	-5.094586
7	6	0	3.513989	9.432151	-3.282917
8	1	0	1.633566	8.526226	-3.745560
9	6	0	4.780056	9.840164	-3.744861
10	1	0	6.043153	9.903307	-5.499140
11	1	0	3.230044	9.621666	-2.253782
12	6	0	0.391585	6.287023	-5.217040
13	6	0	0.073434	5.017383	-4.675418
14	6	0	1.557208	6.532373	-5.898885
15	6	0	0.942767	3.980321	-4.838812
16	6	0	2.475746	5.447884	-6.076469
17	6	0	2.161845	4.162870	-5.548097
18	6	0	-1.764301	10.309890	-6.462970
19	6	0	-0.652124	10.744348	-7.235484
20	6	0	-1.697526	9.157631	-5.737903

21	6	0	-0.715532	11.935015	-8.000558
22	6	0	0.543317	9.969966	-7.234231
23	6	0	-0.507378	8.389667	-5.756011
24	6	0	0.359756	12.357167	-8.739605
25	1	0	-1.638482	12.508464	-7.988631
26	6	0	1.640952	10.440183	-8.002706
27	6	0	0.605070	8.760804	-6.469084
28	6	0	1.550075	11.597769	-8.735693
29	1	0	0.301495	13.270557	-9.322114
30	1	0	2.570959	9.884885	-8.002710
31	1	0	2.403767	11.935369	-9.314583
32	1	0	-2.670145	10.908993	-6.463803
33	1	0	-2.530327	8.793659	-5.146690
34	1	0	2.305019	7.860747	-7.393331
35	6	0	3.707993	5.600634	-6.765551
36	6	0	4.565456	4.540831	-6.929803
37	1	0	3.983942	6.571252	-7.159220
38	6	0	4.245622	3.267389	-6.410487
39	1	0	5.501035	4.684087	-7.460896
40	6	0	3.067072	3.088749	-5.732475
41	1	0	4.932306	2.438565	-6.546510
42	1	0	2.805673	2.116561	-5.323368
43	1	0	-0.868249	4.909072	-4.149032
44	1	0	0.713028	2.999255	-4.433552
45	1	0	4.417312	8.861444	-6.984027
46	7	0	5.673517	10.485910	-2.871178
47	6	0	6.906939	10.979561	-3.446179
48	1	0	7.428877	11.575023	-2.693541
49	1	0	7.585302	10.174545	-3.777138
50	1	0	6.690613	11.625901	-4.299729
51	6	0	5.887107	9.864275	-1.572348
52	1	0	6.380887	10.581063	-0.911093
53	1	0	4.941424	9.583629	-1.111785
54	1	0	6.516983	8.962935	-1.642503

3j (1_2):

1	6	0	0.907975	2.054017	0.164870
2	6	0	1.539575	1.111323	-0.698752
3	6	0	2.282249	0.003507	-0.157410
4	6	0	2.242902	-0.243360	1.236454
5	6	0	1.545631	0.690234	2.084110
6	6	0	0.910695	1.780656	1.588019
7	1	0	3.012542	-0.708220	-2.056141
8	6	0	2.995304	-0.887111	-0.983976
9	6	0	2.905981	-1.367456	1.764048
10	1	0	1.539598	0.496370	3.154420
11	1	0	0.386767	2.484278	2.225690

12	6	0	3.595325	-2.230836	0.936101
13	6	0	3.640164	-1.983933	-0.446117
14	1	0	2.868932	-1.543733	2.835901
15	1	0	4.103855	-3.095069	1.350264
16	1	0	4.180081	-2.663603	-1.098047
17	8	0	0.217309	3.018051	-0.311819
18	6	0	-0.373338	0.437920	-1.373694
19	8	0	-0.851228	1.544160	-1.858337
20	1	0	-0.503005	2.377380	-1.217191
21	1	0	1.752784	1.431379	-1.713974
22	1	0	-0.695013	0.116565	-0.374353
23	6	0	-0.004698	-0.633774	-2.296627
24	6	0	0.208068	-1.934665	-1.830842
25	6	0	0.169043	-0.376571	-3.661927
26	6	0	0.568169	-2.956340	-2.692753
27	6	0	0.536725	-1.382417	-4.534669
28	1	0	0.001168	0.632200	-4.025781
29	6	0	0.740808	-2.705137	-4.071530
30	1	0	0.726227	-3.948983	-2.291328
31	1	0	0.659728	-1.147328	-5.584297
32	1	0	0.102675	-2.146503	-0.769191
33	7	0	1.094769	-3.710515	-4.937263
34	6	0	1.326420	-3.412018	-6.334564
35	1	0	1.596764	-4.330113	-6.855005
36	1	0	0.426359	-3.005950	-6.811019
37	1	0	2.140761	-2.688261	-6.470016
38	6	0	1.362873	-5.037246	-4.425721
39	1	0	1.629018	-5.692631	-5.254222
40	1	0	2.192217	-5.038662	-3.705959
41	1	0	0.480969	-5.459641	-3.929599

3j (2_3):

1	6	0	-1.413824	2.106024	1.629494
2	6	0	-1.310453	0.687306	1.290791
3	6	0	-2.210531	0.076268	0.316444
4	6	0	-3.321015	0.830135	-0.146926
5	6	0	-3.477582	2.200758	0.288153
6	6	0	-2.597981	2.804376	1.109064
7	1	0	-1.226374	-1.851284	0.093313
8	6	0	-2.071921	-1.233281	-0.190542
9	6	0	-4.243624	0.264239	-1.039954
10	1	0	-4.338783	2.748120	-0.089861
11	1	0	-2.704247	3.841621	1.409555
12	6	0	-4.093970	-1.028562	-1.504692
13	6	0	-2.989942	-1.772038	-1.075822
14	1	0	-5.083054	0.871938	-1.368534
15	1	0	-4.811642	-1.455477	-2.196563

16	1	0	-2.843016	-2.783608	-1.441983
17	8	0	-0.617479	2.682476	2.378792
18	6	0	-0.056758	-0.025219	1.728085
19	1	0	-1.423587	0.261105	2.773676
20	8	0	-0.422110	-0.069870	3.237781
21	1	0	-0.384849	-0.967433	3.607366
22	6	0	1.339195	0.476634	1.531181
23	6	0	1.950080	1.464148	2.307487
24	6	0	2.082192	-0.105159	0.502918
25	6	0	3.253612	1.858773	2.052693
26	1	0	1.386922	1.930141	3.104934
27	6	0	3.379190	0.296607	0.221552
28	1	0	1.636222	-0.890154	-0.105012
29	6	0	3.996231	1.303281	0.989869
30	1	0	3.692578	2.619686	2.685456
31	1	0	3.910906	-0.183993	-0.589623
32	1	0	-0.096106	-1.064105	1.400845
33	7	0	5.281438	1.729211	0.713402
34	6	0	6.075797	0.989969	-0.243099
35	1	0	7.055806	1.458968	-0.330660
36	1	0	6.218047	-0.061334	0.047794
37	1	0	5.609701	1.008183	-1.234006
38	6	0	5.951309	2.602460	1.653352
39	1	0	6.951581	2.824392	1.281399
40	1	0	5.415685	3.552079	1.753438
41	1	0	6.043271	2.155057	2.653734

3j (3_4):

1	6	0	-0.314595	-0.740199	-0.748355
2	6	0	1.112721	-0.804922	-0.690063
3	6	0	1.745303	-1.607087	-1.679908
4	6	0	3.151542	-1.450735	-1.912422
5	1	0	3.570896	-1.990374	-2.753901
6	8	0	1.135299	-2.473342	-2.438483
7	1	0	-0.727524	-1.263481	-1.603978
8	6	0	-1.589140	-3.208836	-0.735293
9	6	0	-0.906175	-2.638900	0.386649
10	1	0	0.163036	-2.798682	0.450586
11	8	0	-1.019977	-3.440494	-1.849017
12	1	0	0.194943	-2.885447	-2.109424
13	6	0	1.953211	-0.156452	0.302119
14	6	0	3.353637	-0.079666	0.085343
15	6	0	3.913353	-0.699647	-1.077777
16	1	0	4.982380	-0.603986	-1.249591
17	6	0	1.454074	0.342291	1.529167
18	1	0	0.396981	0.250574	1.750000
19	6	0	4.186592	0.548463	1.036020

20	1	0	5.252824	0.604412	0.833562
21	6	0	-1.161312	0.373125	-0.312210
22	6	0	-0.679293	1.677973	-0.113367
23	6	0	-2.552563	0.192546	-0.246032
24	6	0	-1.527015	2.729788	0.177134
25	6	0	-3.413657	1.225713	0.066870
26	1	0	-2.963478	-0.793076	-0.440145
27	6	0	-2.920164	2.528036	0.304097
28	1	0	-1.103972	3.719405	0.293950
29	1	0	-4.475170	1.020689	0.122743
30	6	0	-1.614678	-2.374438	1.610213
31	6	0	-3.017463	-3.439064	-0.614349
32	1	0	-3.515515	-3.870241	-1.476106
33	6	0	-3.018476	-2.561315	1.668573
34	6	0	-3.685175	-3.124239	0.523414
35	1	0	-4.756799	-3.298242	0.592266
36	6	0	2.290007	0.929430	2.455213
37	1	0	1.875303	1.293070	3.390180
38	6	0	3.668462	1.054726	2.205519
39	1	0	4.316232	1.526414	2.936605
40	6	0	-3.719246	-2.242589	2.847404
41	6	0	-3.053455	-1.764342	3.956730
42	6	0	-0.951919	-1.915134	2.768233
43	6	0	-1.656450	-1.611646	3.915418
44	1	0	0.128851	-1.803950	2.743356
45	1	0	-1.127070	-1.258118	4.794724
46	1	0	-3.600496	-1.520178	4.861144
47	1	0	-4.796213	-2.388585	2.871691
48	1	0	0.379703	1.881784	-0.223640
49	7	0	-3.761976	3.560186	0.632015
50	6	0	-3.234799	4.900669	0.776615
51	1	0	-2.469716	4.940886	1.560004
52	1	0	-2.789819	5.272797	-0.155897
53	1	0	-4.043191	5.572870	1.062256
54	6	0	-5.193568	3.343977	0.641512
55	1	0	-5.692020	4.269960	0.926193
56	1	0	-5.570286	3.037816	-0.343333
57	1	0	-5.471853	2.572839	1.368796

3j (4_5):

1	8	0	0.478410	-3.452457	-0.693336
2	6	0	-0.482668	-0.167529	0.510457
3	6	0	-2.074051	-1.600002	-0.780127
4	6	0	-3.358974	-2.140406	-1.048668
5	6	0	-1.883641	-0.631174	0.183295
6	6	0	-4.447601	-1.675468	-0.368331
7	6	0	-3.025404	-0.088960	0.852205

8	6	0	-4.316537	-0.631388	0.585914
9	6	0	2.636630	-0.837780	-1.244323
10	6	0	2.842515	-0.515542	0.171192
11	6	0	1.612499	-1.593692	-1.663471
12	6	0	4.012029	0.110212	0.607381
13	6	0	1.851216	-0.859844	1.104352
14	6	0	0.697059	-2.169445	-0.663172
15	6	0	4.205100	0.386544	1.956507
16	1	0	4.771491	0.380300	-0.121094
17	6	0	2.053914	-0.587117	2.452882
18	6	0	0.518813	-1.388632	0.617485
19	6	0	3.227659	0.030175	2.882328
20	1	0	5.117643	0.871893	2.286181
21	1	0	1.284812	-0.857694	3.172336
22	1	0	3.377667	0.230591	3.938144
23	1	0	3.383580	-0.486763	-1.951846
24	1	0	1.496967	-1.918192	-2.691164
25	6	0	-2.937332	0.995044	1.769380
26	6	0	-4.053589	1.481758	2.402106
27	1	0	-1.979203	1.471718	1.946525
28	6	0	-5.326168	0.916802	2.159666
29	1	0	-3.959671	2.315840	3.090324
30	6	0	-5.448713	-0.113968	1.264589
31	1	0	-6.199197	1.307859	2.671399
32	1	0	-6.421304	-0.550318	1.052795
33	1	0	-3.442292	-2.915179	-1.803481
34	1	0	-5.434455	-2.086448	-0.562203
35	8	0	-1.021601	-2.042684	-1.513655
36	1	0	0.093528	-2.083204	1.348805
37	1	0	-0.489426	0.203375	1.540020
38	1	0	-0.550431	-3.151009	-1.224659
39	6	0	-0.000616	0.973778	-0.368379
40	6	0	0.826571	1.967339	0.158208
41	6	0	-0.347787	1.078926	-1.716885
42	6	0	1.309923	3.010698	-0.620046
43	6	0	0.124156	2.114316	-2.510560
44	1	0	-0.998135	0.332811	-2.163256
45	6	0	0.979926	3.101937	-1.985067
46	1	0	1.941022	3.756677	-0.153686
47	1	0	-0.183924	2.151645	-3.547878
48	1	0	1.112897	1.923066	1.207472
49	7	0	1.479976	4.123207	-2.783096
50	6	0	0.873777	4.339099	-4.080867
51	1	0	-0.206409	4.539406	-4.019248
52	1	0	1.357933	5.189622	-4.561552
53	1	0	1.021875	3.468299	-4.726698
54	6	0	2.096271	5.261044	-2.133262

55	1	0	2.992347	4.954705	-1.584742
56	1	0	2.406713	5.978894	-2.892982
57	1	0	1.420249	5.767599	-1.427884

3j (5_6):

1	8	0	-0.480712	7.273487	-4.991108
2	6	0	1.816779	7.957089	-6.549681
3	6	0	2.857589	8.490690	-5.571642
4	6	0	4.091347	8.968842	-6.002060
5	6	0	2.609833	8.497372	-4.197624
6	6	0	5.045930	9.447438	-5.111478
7	6	0	3.545983	8.970797	-3.292349
8	1	0	1.663736	8.112495	-3.822402
9	6	0	4.788961	9.472826	-3.729799
10	1	0	5.993894	9.795508	-5.501863
11	1	0	3.306535	8.945318	-2.236708
12	6	0	0.276638	6.236580	-5.449560
13	6	0	0.255117	5.098740	-4.546533
14	6	0	1.451331	6.491555	-6.297411
15	6	0	1.253292	4.197326	-4.584754
16	6	0	2.528192	5.499827	-6.248634
17	6	0	2.401899	4.337758	-5.451800
18	6	0	-1.788198	10.376537	-6.296719
19	6	0	-0.723260	10.837119	-7.116487
20	6	0	-1.679177	9.198325	-5.615256
21	6	0	-0.824490	12.062354	-7.823371
22	6	0	0.467421	10.060957	-7.221632
23	6	0	-0.495684	8.436305	-5.739164
24	6	0	0.211009	12.516696	-8.597525
25	1	0	-1.742861	12.636235	-7.734470
26	6	0	1.525960	10.567340	-8.022519
27	6	0	0.566765	8.818010	-6.519009
28	6	0	1.400393	11.759263	-8.690739
29	1	0	0.124704	13.456257	-9.133058
30	1	0	2.454332	10.013403	-8.093437
31	1	0	2.224297	12.127010	-9.293755
32	1	0	-2.689414	10.977401	-6.218978
33	1	0	-2.470509	8.820151	-4.977520
34	1	0	2.245708	8.024538	-7.555634
35	6	0	3.702156	5.647271	-7.010253
36	6	0	4.687538	4.676105	-7.004645
37	1	0	3.836900	6.534604	-7.619695
38	6	0	4.546626	3.517843	-6.230121
39	1	0	5.579224	4.817125	-7.607689
40	6	0	3.411637	3.361145	-5.458950
41	1	0	5.321341	2.758829	-6.231231
42	1	0	3.285557	2.477233	-4.838787

43	1	0	-0.588948	5.018940	-3.871360
44	1	0	1.223574	3.335086	-3.923141
45	8	0	-0.673307	5.661388	-6.874836
46	1	0	-1.421149	6.239145	-7.100385
47	1	0	0.484187	6.072486	-7.185605
48	1	0	4.330709	8.958378	-7.064173
49	7	0	5.719604	9.976631	-2.829298
50	6	0	7.071626	10.199422	-3.296141
51	1	0	7.678119	10.565283	-2.467193
52	1	0	7.540190	9.288111	-3.697906
53	1	0	7.089130	10.964376	-4.078718
54	6	0	5.531640	9.699727	-1.420326
55	1	0	6.360350	10.133638	-0.860141
56	1	0	4.610055	10.162598	-1.054338
57	1	0	5.485359	8.622730	-1.199122