Supplementary information

Fused Alq$_3$ derivatives: syntheses and photophysical characteristics

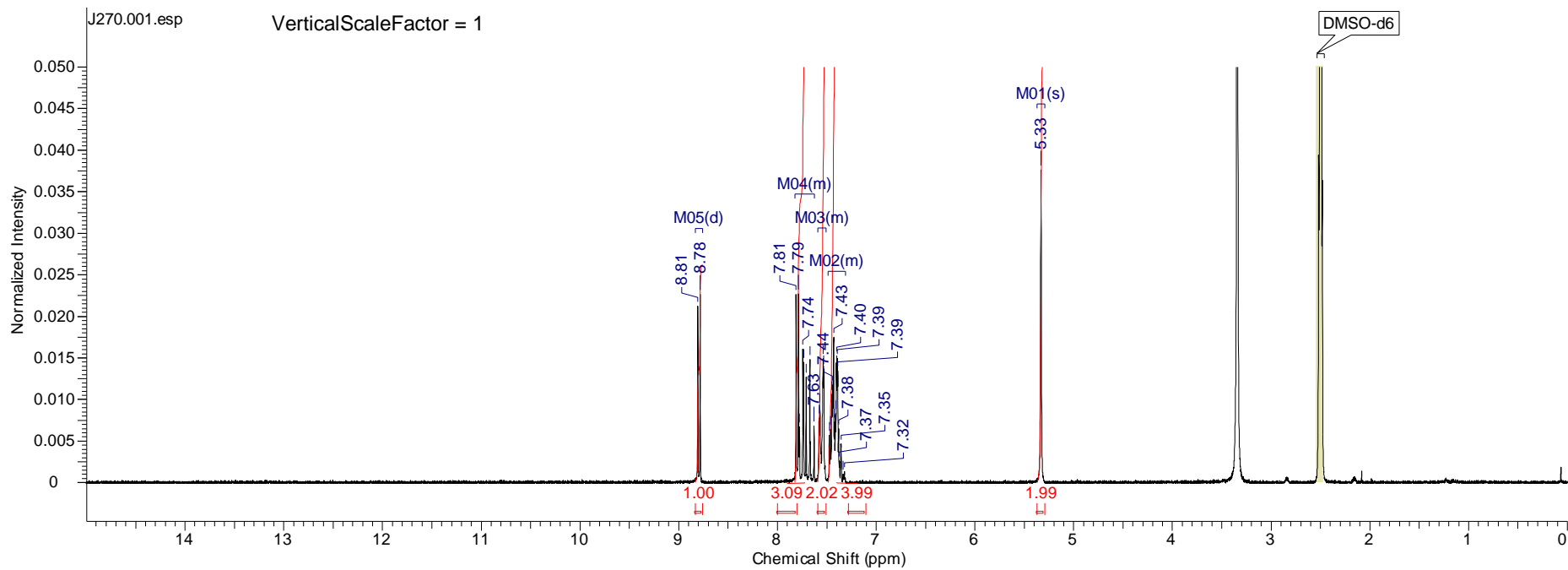Juha P. Heiskanen,[a,*] Antti E. Tolkki,[a] Helge J. Lemmetyinen,[a] Osmo E. O. Hormi[b]

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*juha.heiskanen@tut.fi

^{1}H NMR spectrum of 8-(benzyloxy)-4-chloroquinoline (**2**)

J270.001.esp

VerticalScaleFactor = 1

DMSO-d6

M01(s)

5.33

M04(m)

M05(d)

M03(m)

8.81
8.78

7.81
7.79

M02(m)

7.74

7.63

7.44

7.43

7.40
7.39

7.39

7.38

7.37
7.35

7.32

Normalized Intensity

0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0

14   13   12   11   10   9   8   7   6   5   4   3   2   1   0

Chemical Shift (ppm)

1.00   3.09 2.02 3.99   1.99

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	5.33	2	s	-	M01	[5.29 .. 5.37]
2	7.40	4	m	-	M02	[7.31 .. 7.49]
3	7.55	2	m	-	M03	[7.51 .. 7.59]
4	7.73	3	m	-	M04	[7.62 .. 7.82]
5	8.79	1	d	4.70	M05	[8.76 .. 8.83]

2

^{13}C NMR spectrum of 8-(benzyloxy)-4-chloroquinoline (**2**)
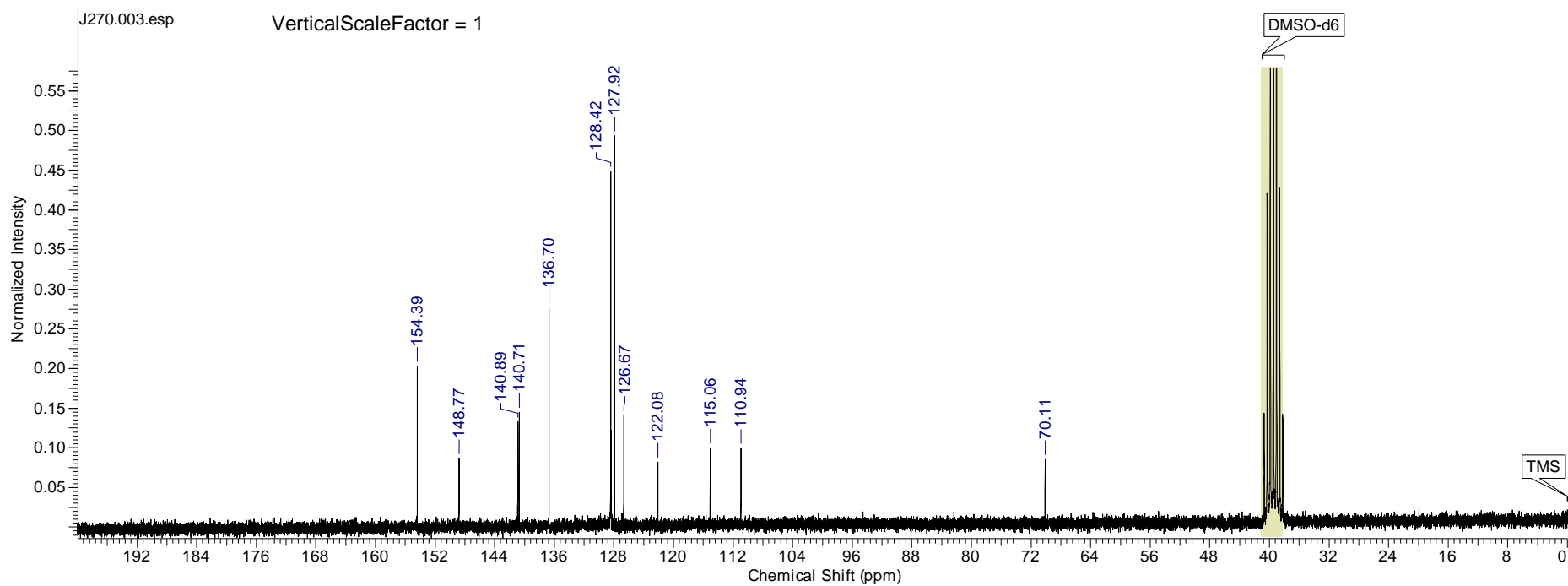
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	70.11	3528.2	0.0854	4	122.08	6143.5	0.0822	7	128.36	6459.3	0.1224	10	140.71	7080.7	0.1447	13	154.39	7769.5	0.2031
2	110.94	5583.0	0.0994	5	126.67	6374.2	0.1411	8	128.42	6462.2	0.4486	11	140.89	7090.2	0.1323				
3	115.06	5789.9	0.0999	6	127.92	6437.3	0.4936	9	136.70	6878.9	0.2765	12	148.77	7486.7	0.0868				

HRMS of 8-(benzyloxy)-4-chloroquinoline (**2**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa / DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Odd and Even Electron Ions

116 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)
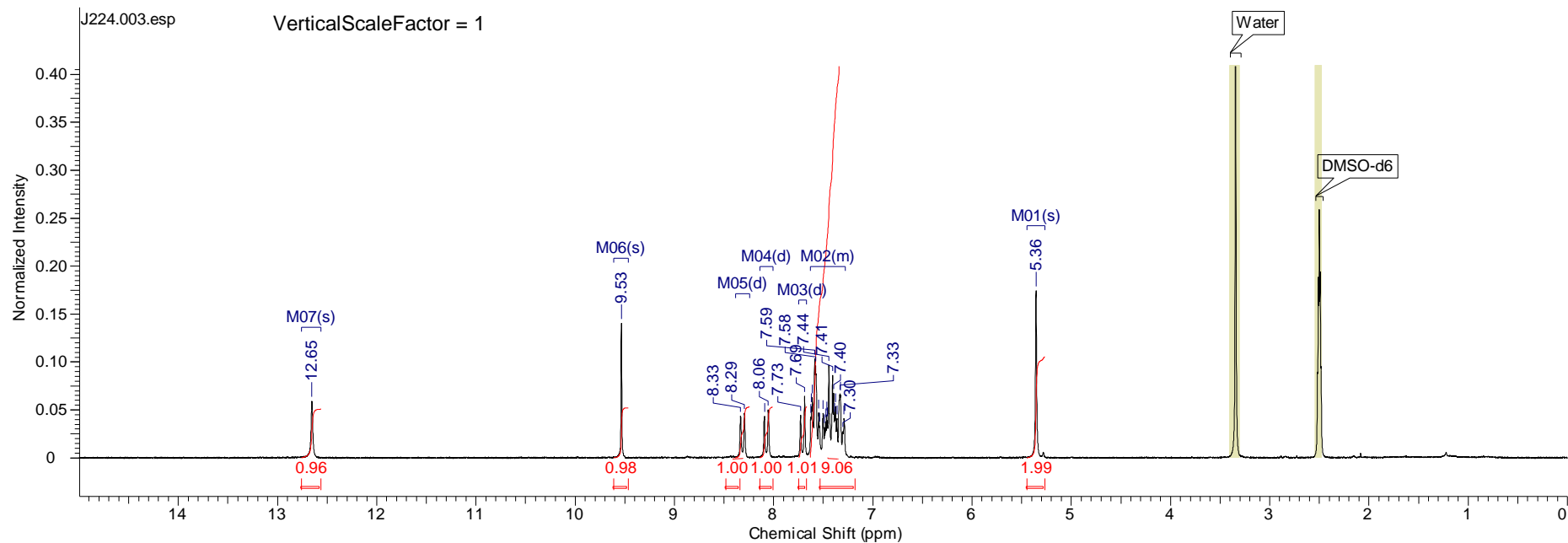
Minimum:				-0.5	
Maximum:		5.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
270.0679	270.0681	-0.1	-0.5	15.0	C19 H10 O2
	270.0686	**-0.6**	**-2.4**	**10.5**	**C16 H13 N O Cl**
	270.0662	1.8	6.6	7.5	C14 H14 N O Na Cl
	270.0657	2.3	8.4	12.0	C17 H11 O2 Na

J217

LCT-24456 168 (3.366) AM (Cen,2, 70.00, Ar,5000.0,556.28); Sm (SG, 1x2.00); Sb (1,40.00)
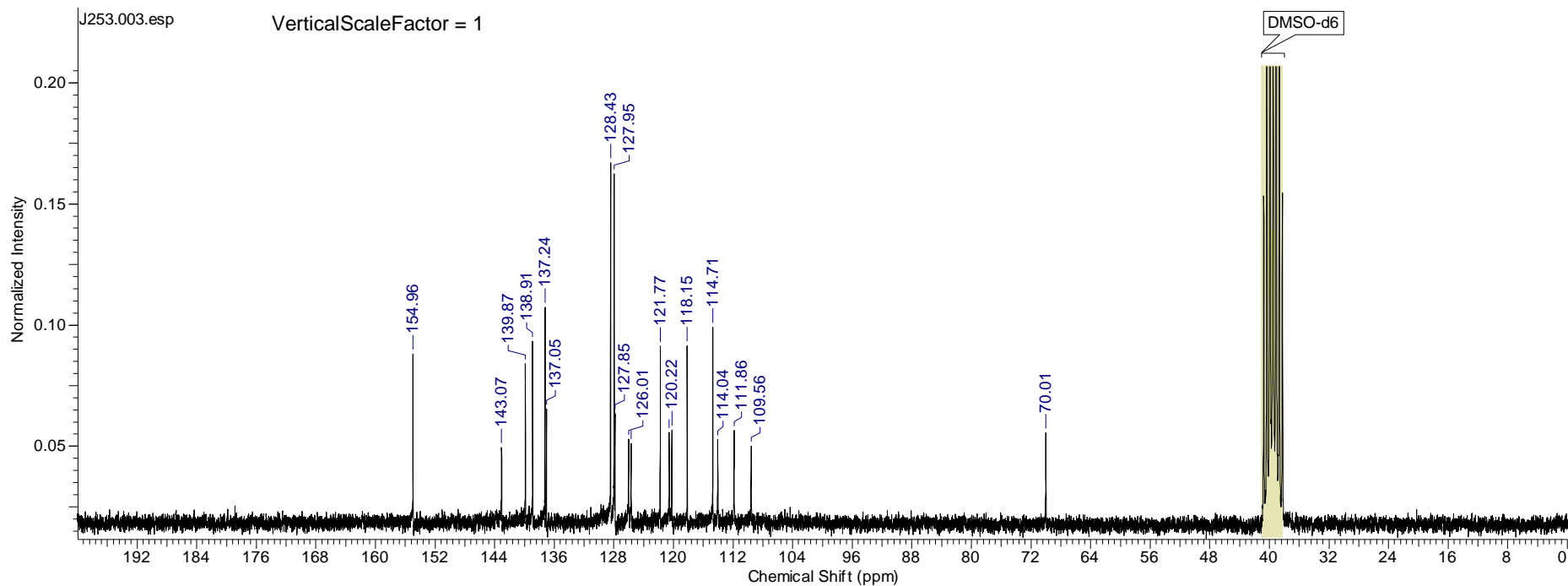

4
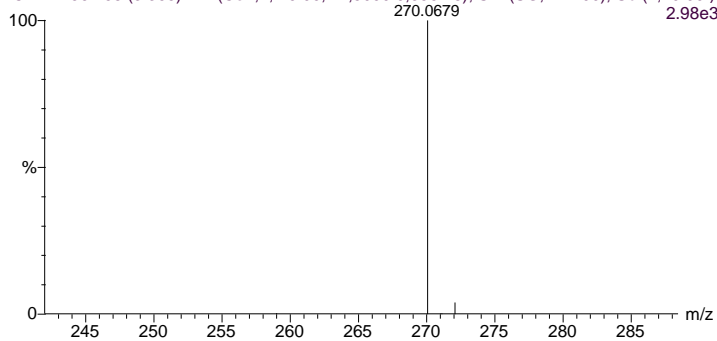
^{1}H NMR spectrum of 4-benzyloxy-11*H*-indol[3,2-*c*]quinoline (**3**)

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	Connections	(ppm)
1	5.36	2	s	-	M01	-	[5.26 .. 5.45]
2	7.46	10	m	-	M02	-	[7.28 .. 7.63]
3	7.71	1	d	8.02	M03	M05	[7.67 .. 7.75]
4	8.07	1	d	7.24	M04	-	[8.01 .. 8.14]
5	8.31	1	d	7.83	M05	M03	[8.24 .. 8.38]
6	9.53	1	s	-	M06	-	[9.46 .. 9.61]
7	12.65	1	s	-	M07	-	[12.56 .. 12.76]

^{13}C NMR spectrum of 4-benzyloxy-11H-indol[3,2-c]quinoline (**3**)

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	70.01	3523.3	0.0555	5	114.71	5772.5	0.0991	9	121.77	6127.9	0.0913	13	127.95	6439.0	0.1624	17	138.91	6990.3	0.0932
2	109.56	5513.5	0.0500	6	118.15	5945.6	0.0914	10	125.68	6324.5	0.0511	14	128.43	6463.2	0.1671	18	139.87	7038.7	0.0840
3	111.86	5629.1	0.0565	7	120.22	6049.8	0.0567	11	126.01	6341.0	0.0530	15	137.05	6896.7	0.0653	19	143.07	7199.7	0.0495
4	114.04	5738.8	0.0526	8	120.57	6067.4	0.0558	12	127.85	6433.8	0.0634	16	137.24	6906.3	0.1074	20	154.96	7798.0	0.0880

HRMS of 4-benzyloxy-11*H*-indol[3,2-*c*]quinoline (**3**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa   /   DBE: min = -0.5, max = 100.0
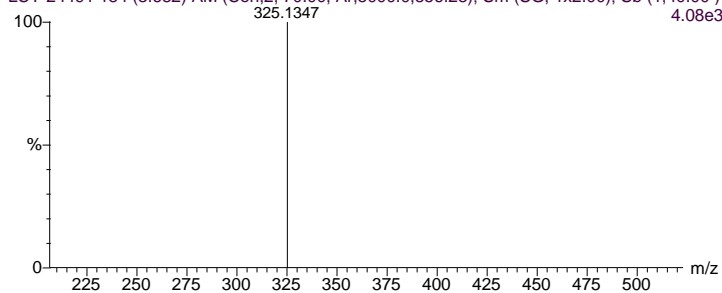
Monoisotopic Mass, Odd and Even Electron Ions

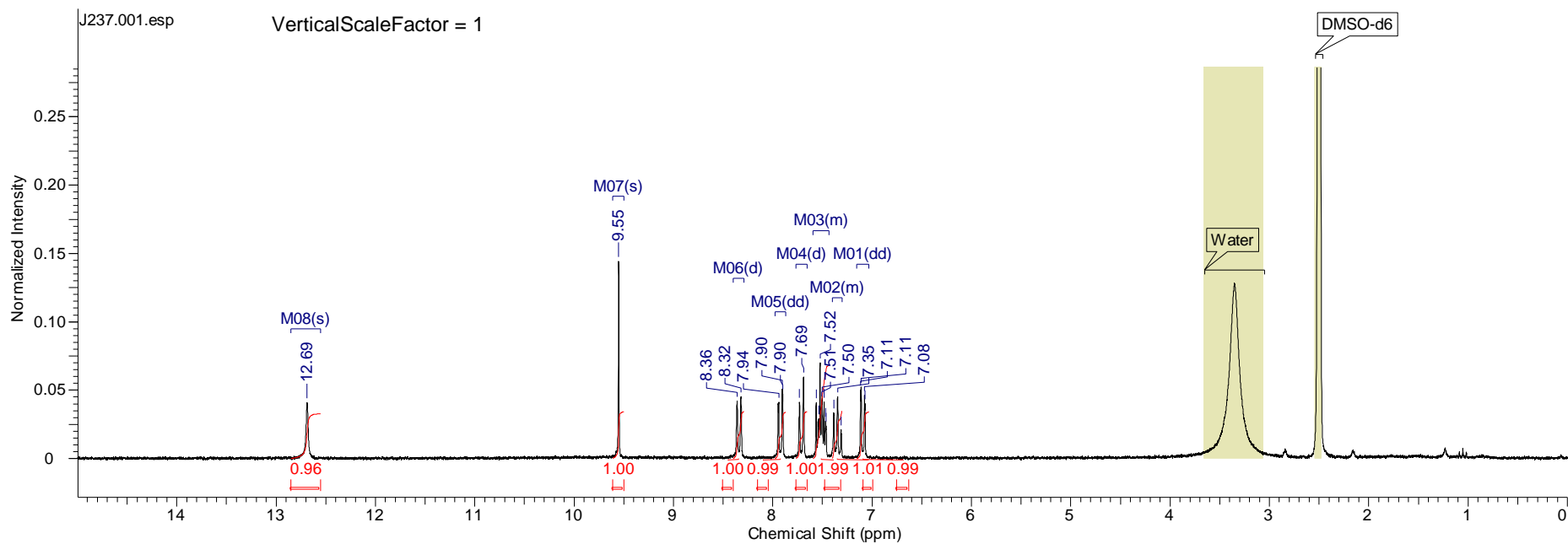74 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Minimum: -0.5

Maximum: 5.0   10.0   100.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
325.1347	**325.1341**	**0.6**	**1.9**	**15.5**	**C22 H17 N2 O**
	325.1317	3.0	9.3	12.5	C20 H18 N2 O Na

J222

LCT-24491 184 (3.682) AM (Cen,2, 70.00, Ar,5000.0,556.28); Sm (SG, 1x2.00); Sb (1,40.00)
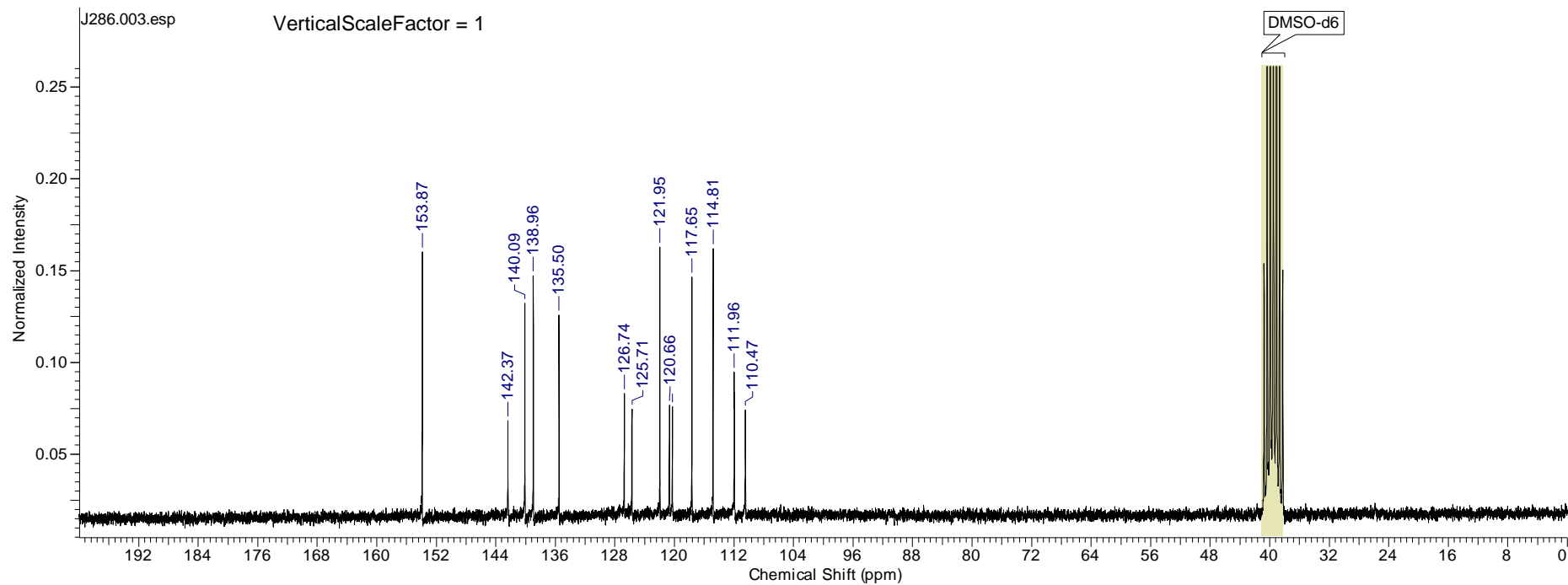
^{1}H NMR spectrum of 11H-indolo[3,2-c]quinolin-4-ol (**4**)

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	Connections	(ppm)
1	7.09	1	dd	7.73, 1.08	M01	M04, M05	[7.03 .. 7.15]
2	7.35	1	m	-	M02	-	[7.30 .. 7.40]
3	7.51	2	m	-	M03	-	[7.43 .. 7.59]
4	7.71	1	d	8.02	M04	M01	[7.66 .. 7.77]
5	7.92	1	dd	8.22, 1.17	M05	M06, M01	[7.87 .. 7.98]
6	8.34	1	d	7.83	M06	M05	[8.29 .. 8.40]
7	9.55	1	s	-	M07	-	[9.50 .. 9.61]
8	12.69	1	s	-	M08	-	[12.55 .. 12.85]

^{13}C NMR spectrum of 11H-indolo[3,2-c]quinolin-4-ol (**4**)

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	110.47	5559.4	0.0741	4	114.81	5777.6	0.1621	7	120.66	6071.8	0.0768	10	126.74	6377.7	0.0832	13	140.09	7049.7	0.1323
2	111.93	5632.8	0.0835	5	117.65	5920.3	0.1466	8	121.95	6136.7	0.1628	11	135.50	6818.6	0.1258	14	142.37	7164.5	0.0684
3	111.96	5634.2	0.0946	6	120.26	6052.0	0.0760	9	125.71	6326.0	0.0748	12	138.96	6992.8	0.1472	15	153.87	7743.3	0.1603

HRMS of 11*H*-indolo[3,2-*c*]quinolin-4-ol (**4**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

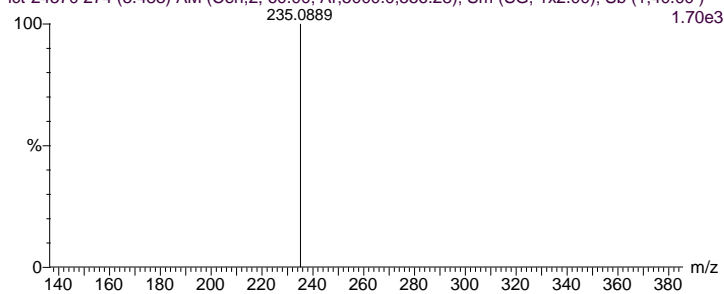Tolerance = 5.0 mDa   /   DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Even Electron Ions

53 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
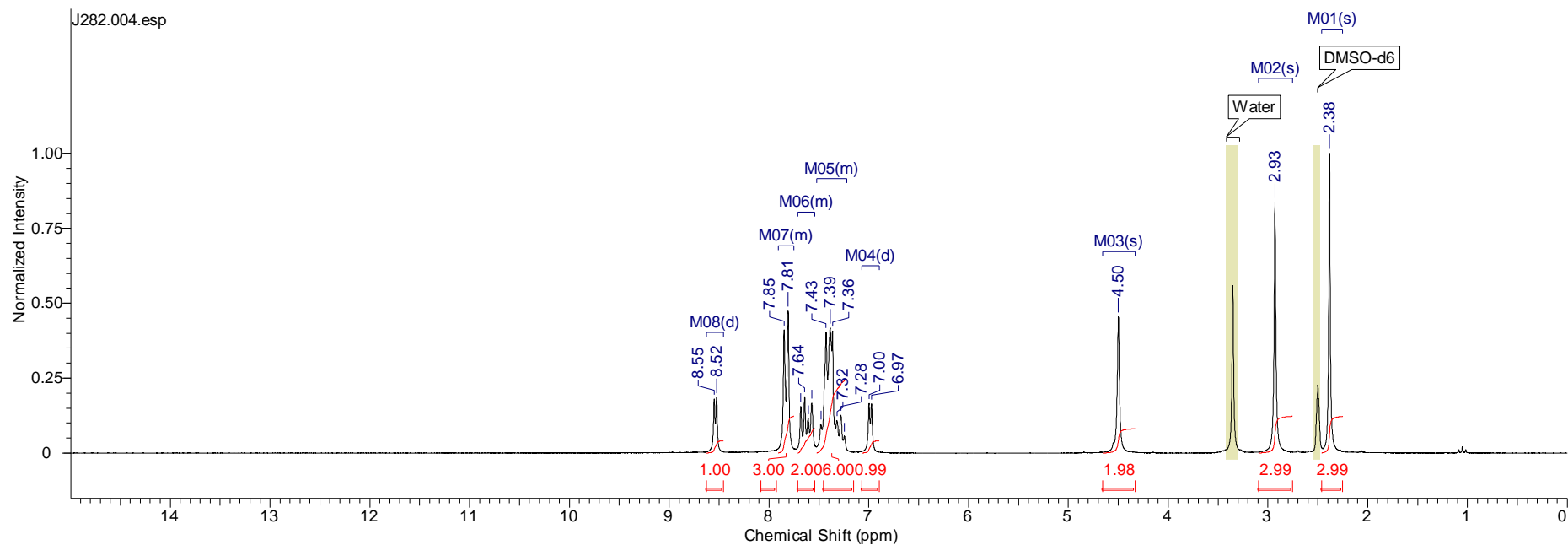
Minimum:				-0.5	
Maximum:		5.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
235.0889	**235.0871**	**1.7**	**7.4**	**11.5**	**C15 H11 N2 O**

J226
lct-24570 274 (5.483) AM (Cen,2, 60.00, Ar,5000.0,556.28); Sm (SG, 1x2.00); Sb (1,40.00)

^{1}H NMR spectrum of 4-((2-bromobenzyl)(methyl)amino)quinolin-8-yl 4-methylbenzenesulfonate (**5**)

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	Connections	(ppm)
1	2.38	3	s	-	M01	-	[2.25 .. 2.46]
2	2.93	3	s	-	M02	-	[2.75 .. 3.10]
3	4.50	2	s	-	M03	-	[4.33 .. 4.66]
4	6.98	1	d	5.09	M04	M08	[6.90 .. 7.07]
5	7.36	6	m	-	M05	-	[7.22 .. 7.52]
6	7.63	2	m	-	M06	-	[7.54 .. 7.71]
7	7.83	3	m	-	M07	-	[7.75 .. 7.91]
8	8.54	1	d	4.89	M08	M04	[8.46 .. 8.63]

¹³C NMR spectrum of 4-((2-bromobenzyl)(methyl)amino)quinolin-8-yl 4-methylbenzenesulfonate (**5**)
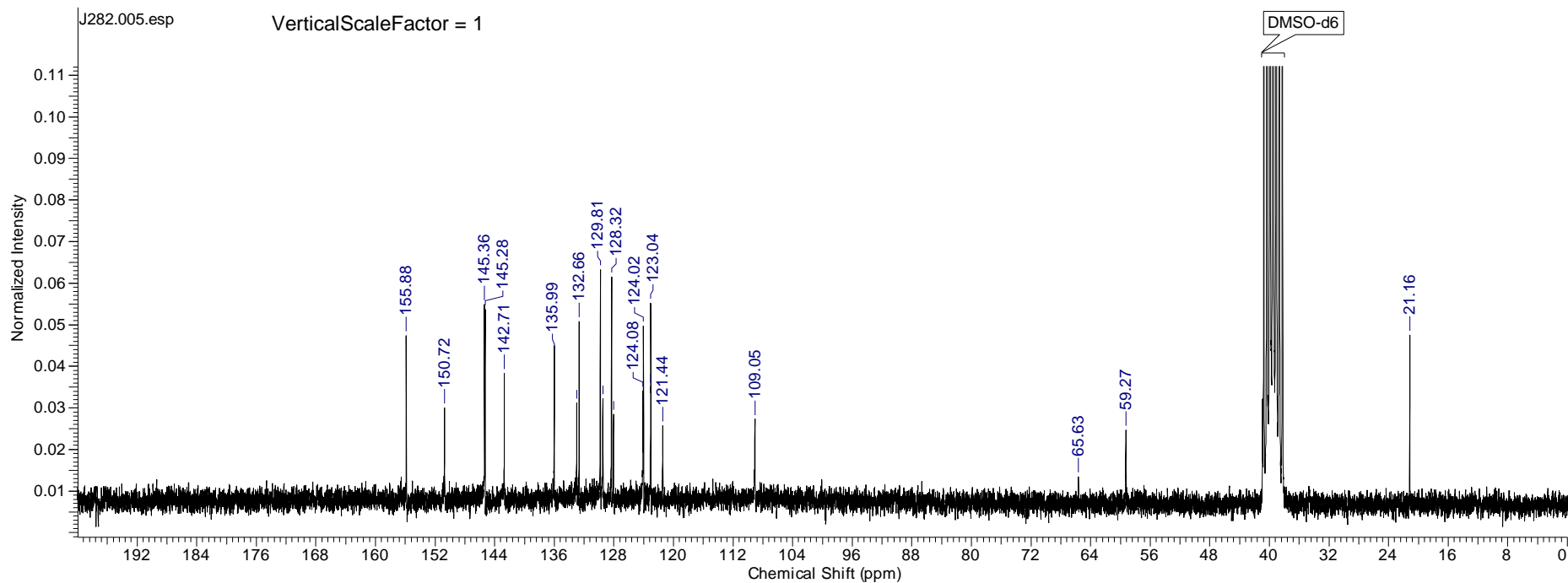
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.16	1064.7	0.0475	6	123.04	6191.8	0.0552	11	128.32	6457.3	0.0615	16	132.98	6692.1	0.0312	21	150.72	7584.9	0.0300
2	59.27	2982.6	0.0247	7	123.07	6193.2	0.0350	12	129.45	6514.2	0.0303	17	135.99	6843.6	0.0434	22	155.88	7844.2	0.0474
3	65.63	3302.5	0.0134	8	124.02	6240.9	0.0497	13	129.49	6516.4	0.0323	18	142.71	7181.7	0.0383				
4	109.05	5487.9	0.0272	9	124.08	6244.2	0.0341	14	129.81	6532.5	0.0632	19	145.28	7310.9	0.0536				
5	121.44	6111.1	0.0257	10	128.06	6444.1	0.0285	15	132.66	6675.6	0.0507	20	145.36	7314.9	0.0549				

HRMS of 4-((2-bromobenzyl)(methyl)amino)quinolin-8-yl 4-methylbenzenesulfonate (**5**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa / DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Even Electron Ions

822 formula(e) evaluated with 11 results within limits (up to 50 closest results for each mass)

Minimum:				-0.5	
Maximum:		5.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
497.0531	**497.0535**	**-0.3**	**-0.6**	**14.5**	**C24 H22 N2 O3 S Br**
	497.0528	0.3	0.7	5.5	C16 H26 N4 O5 S2 Br
	497.0541	-1.0	-2.0	23.5	C32 H18 O Br
	497.0560	-2.8	-5.7	10.5	C20 H22 N2 O8 Br
	497.0503	2.8	5.7	9.5	C20 H26 N4 S3 Br
	497.0562	-3.0	-6.1	0.5	C13 H30 N4 O5 S3 Br
	497.0501	3.1	6.1	19.5	C27 H18 N2 O3 Br
	497.0568	-3.7	-7.4	9.5	C21 H26 N2 O3 S2 Br
	497.0494	3.7	7.4	10.5	C19 H22 N4 O5 S Br
	497.0490	4.2	8.4	4.5	C19 H30 O4 S3 Br
	497.0575	-4.3	-8.7	18.5	C29 H22 O S Br

J264
Ict-24913 361 (7.226) AM (Cen,2, 80.00, Ar,5000.0,609.28); Sm (SG, 1x2.00); Sb (4,40.00); S
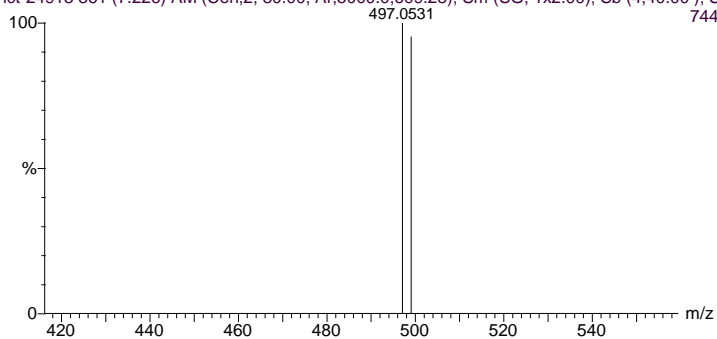

13

^{1}H NMR spectrum of 5-methyl-5,6-dihydrodibenzo[*c*,*h*][1,6]naphthyridin-1-yl 4-methylbenzenesulfonate (**6**)
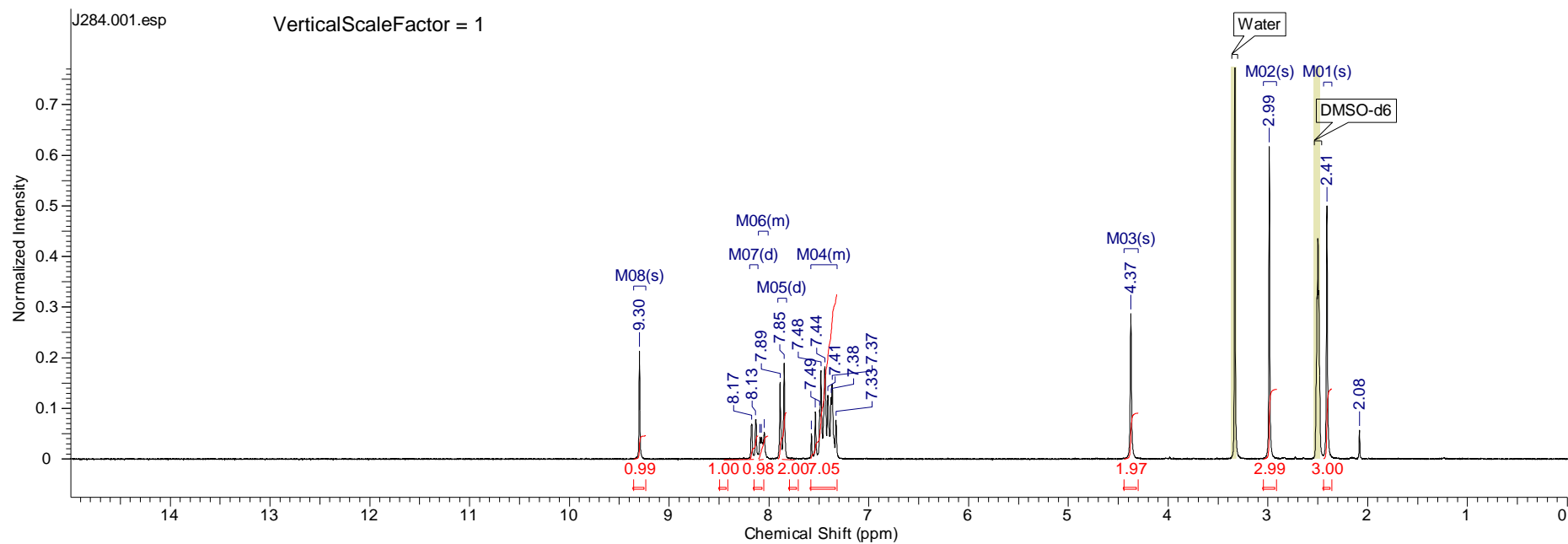
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	2.41	3	s	-	M01	[2.36 .. 2.44]
2	2.99	3	s	-	M02	[2.91 .. 3.05]
3	4.37	2	s	-	M03	[4.30 .. 4.44]
4	7.44	7	m	-	M04	[7.32 .. 7.58]
5	7.87	2	d	8.22	M05	[7.83 .. 7.91]
6	8.07	1	m	-	M06	[8.01 .. 8.11]
7	8.15	1	d	7.63	M07	[8.11 .. 8.20]
8	9.30	1	s	-	M08	[9.24 .. 9.35]

^{13}C NMR spectrum of 5-methyl-5,6-dihydrodibenzo[*c*,*h*][1,6]naphthyridin-1-yl 4-methylbenzenesulfonate (**6**)
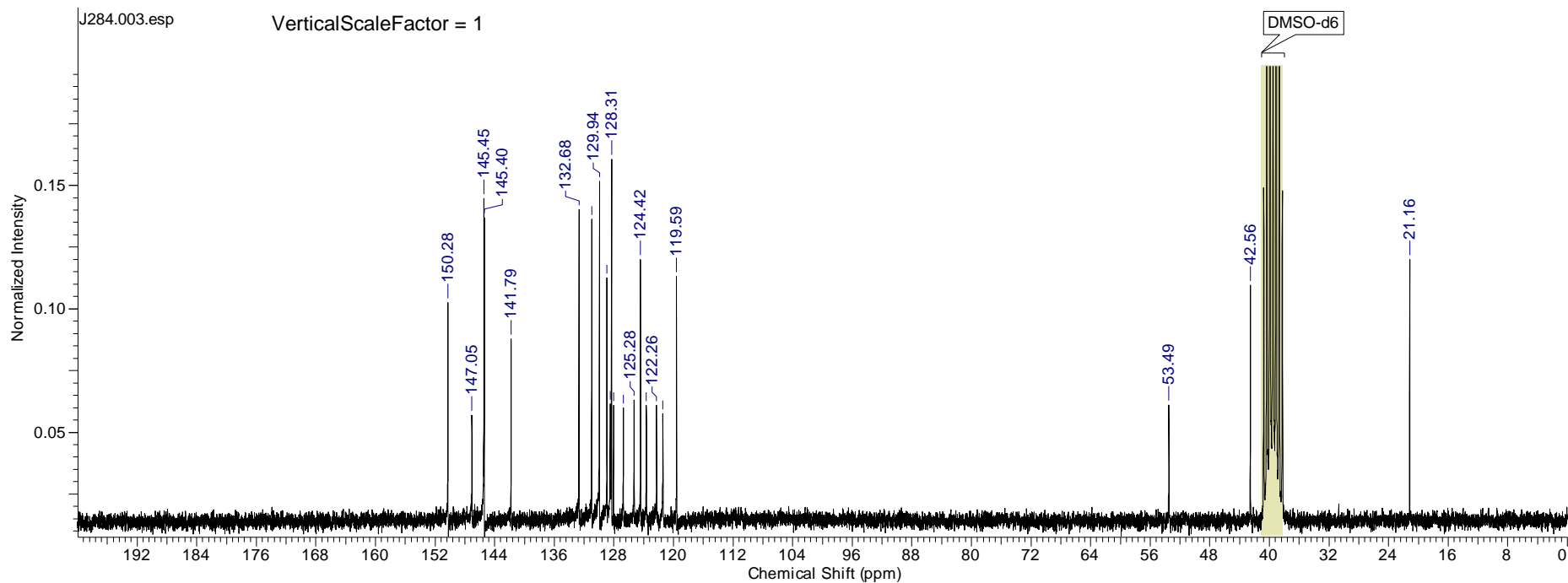
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.16	1065.0	0.1200	6	122.26	6152.5	0.0609	11	128.03	6443.0	0.0609	16	130.98	6591.2	0.1362	21	147.05	7400.0	0.0570
2	42.56	2141.6	0.1097	7	123.62	6221.1	0.0608	12	128.31	6456.9	0.1606	17	132.68	6677.0	0.1401	22	150.28	7562.5	0.1026
3	53.49	2691.8	0.0611	8	124.42	6261.1	0.1200	13	128.49	6466.1	0.0615	18	141.79	7135.2	0.0878				
4	119.59	6017.9	0.1131	9	125.28	6304.4	0.0630	14	128.93	6488.1	0.1126	19	145.40	7316.7	0.1369				
5	121.43	6110.7	0.0576	10	126.72	6377.0	0.0599	15	129.94	6539.1	0.1516	20	145.45	7319.7	0.1447				

HRMS of 5-methyl-5,6-dihydrodibenzo[*c*,*h*][1,6]naphthyridin-1-yl 4-methylbenzenesulfonate (**6**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa / DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Odd and Even Electron Ions

338 formula(e) evaluated with 11 results within limits (up to 50 closest results for each mass)
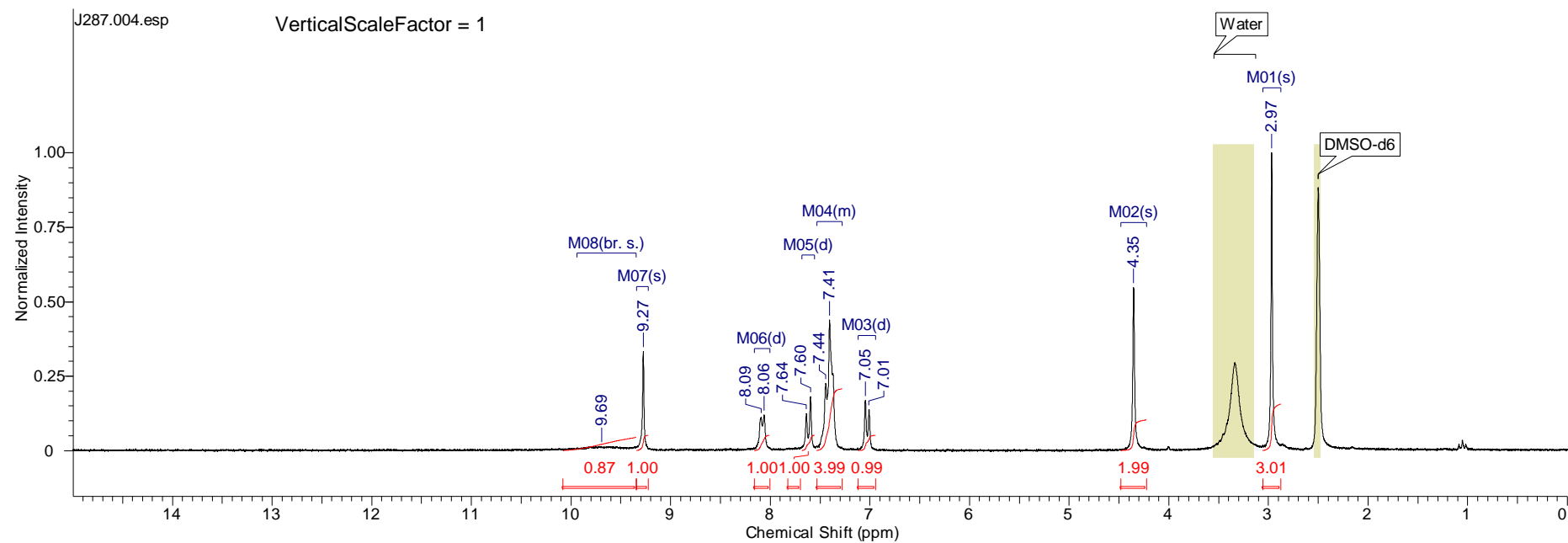
Minimum:				-0.5		
Maximum:		5.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Formula	
439.1104	439.1109	-0.5	-1.1	28.0	C32 H13 N3	
	439.1099	0.6	1.3	24.5	C32 H16 O Na	
	439.1116	-1.2	-2.7	18.5	C26 H19 N2 O3 S	
	439.1092	**1.2**	**2.8**	**15.5**	**C24 H20 N2 O3 Na S**	
	439.1119	-1.5	-3.4	20.0	C27 H18 N3 Na S	
	439.1123	-1.8	-4.2	27.5	C34 H15 O	
	439.1085	1.9	4.3	25.0	C30 H14 N3 Na	
	439.1083	2.2	5.0	23.5	C29 H15 N2 O3	
	439.1133	-2.8	-6.4	19.5	C29 H20 O Na S	
	439.1143	-3.9	-8.8	23.0	C29 H17 N3 S	
	439.1059	4.6	10.4	20.5	C27 H16 N2 O3 Na	

J273

LCT-24948 289 (5.786) AM (Cen,2, 75.00, Ar,5000.0,609.28); Sm (SG, 1x2.00); Sb (4,40.00)

439.1104   652

440.1503

16
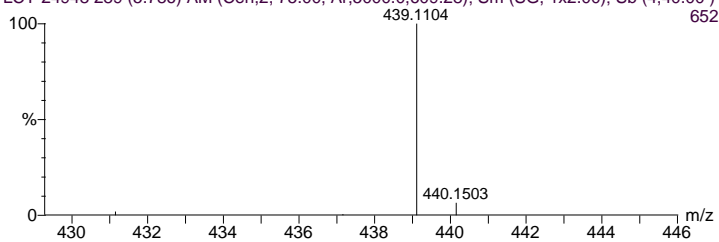
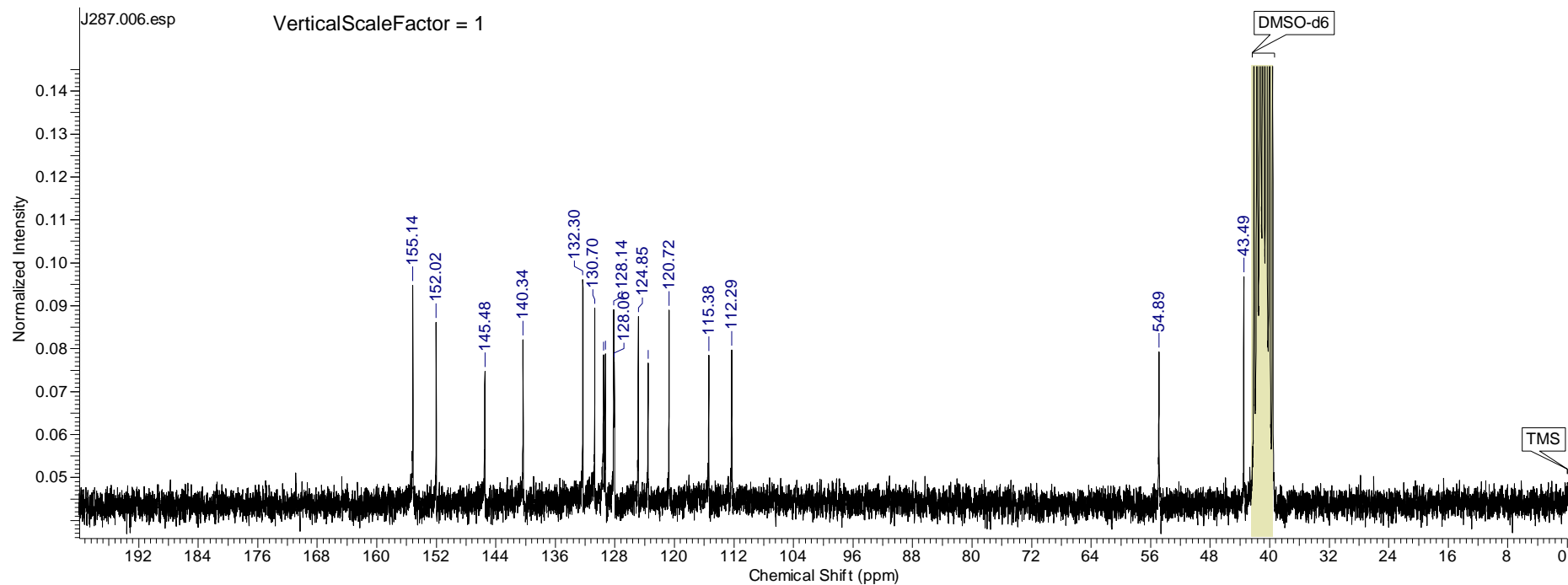^{1}H NMR spectrum of 5-methyl-5,6-dihydrodibenzo[*c*,*h*][1,6]naphthyridin-1-ol (**7**)

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	2.97	3	s	-	M01	[2.88 .. 3.05]
2	4.35	2	s	-	M02	[4.22 .. 4.48]
3	7.03	1	d	7.43	M03	[6.94 .. 7.12]
4	7.42	4	m	-	M04	[7.28 .. 7.53]
5	7.62	1	d	8.22	M05	[7.56 .. 7.68]
6	8.08	1	d	6.06	M06	[8.01 .. 8.16]
7	9.27	1	s	-	M07	[9.22 .. 9.34]
8	9.69	1	br. s.	-	M08	[9.34 .. 9.94]

^{13}C NMR spectrum of 5-methyl-5,6-dihydrodibenzo[*c*,*h*][1,6]naphthyridin-1-ol (**7**)

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	43.49	2188.3	0.0968	5	120.72	6074.9	0.0889	9	128.14	6448.3	0.0891	13	132.30	6657.7	0.0961	17	155.14	7807.3	0.0947
2	54.89	2762.0	0.0792	6	123.54	6216.9	0.0767	10	129.28	6505.9	0.0788	14	140.34	7062.3	0.0821				
3	112.29	5650.9	0.0797	7	124.85	6282.9	0.0875	11	129.52	6517.6	0.0786	15	145.48	7320.9	0.0748				
4	115.38	5806.0	0.0785	8	128.06	6444.3	0.0769	12	130.70	6577.4	0.0894	16	152.02	7649.9	0.0862				

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HRMS of 5-methyl-5,6-dihydrodibenzo[*c*,*h*][1,6]naphthyridin-1-ol (**7**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa   /   DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Odd and Even Electron Ions

64 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
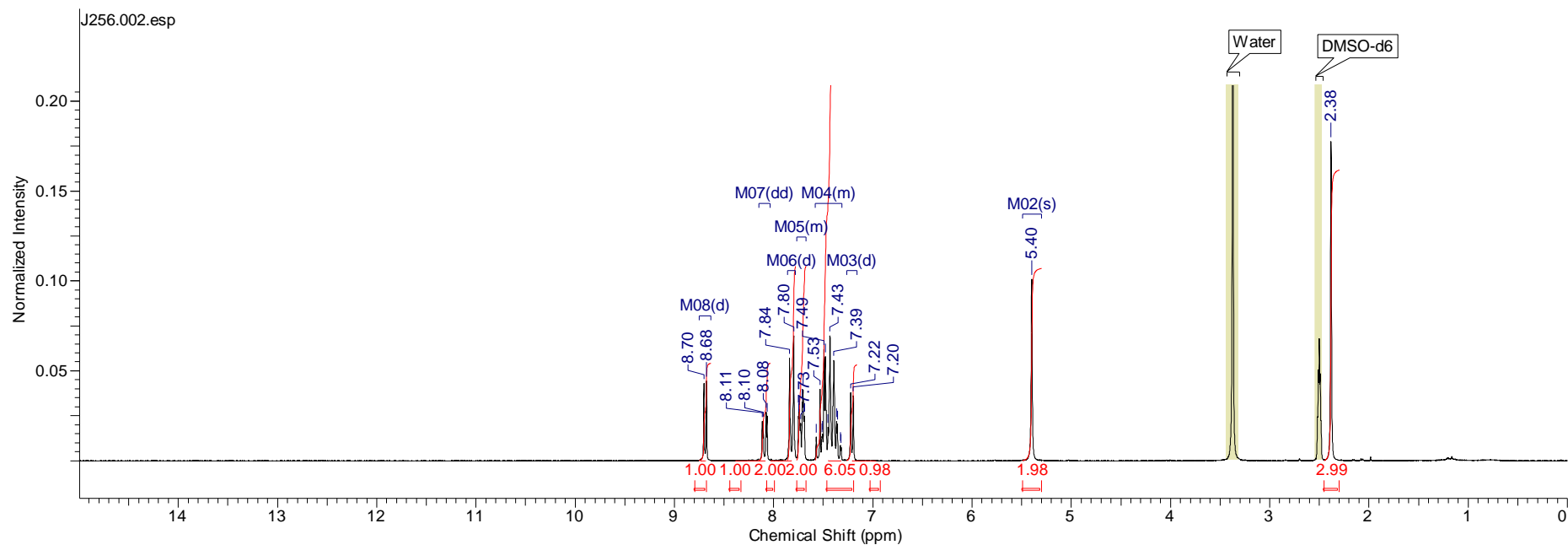
Minimum:				-0.5	
Maximum:		5.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
263.1181	**263.1184**	**-0.3**	**-1.3**	**11.5**	**C17 H15 N2 O**
	263.1160	2.1	7.9	8.5	C15 H16 N2 O Na

J280
LCT-24998 14 (0.281) AM (Cen,2, 90.00, Ar,5000.0,609.28); Sm (SG, 1x2.00); Sb (4,40.00)
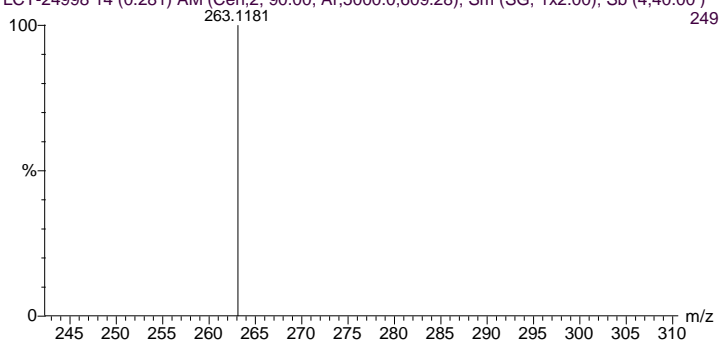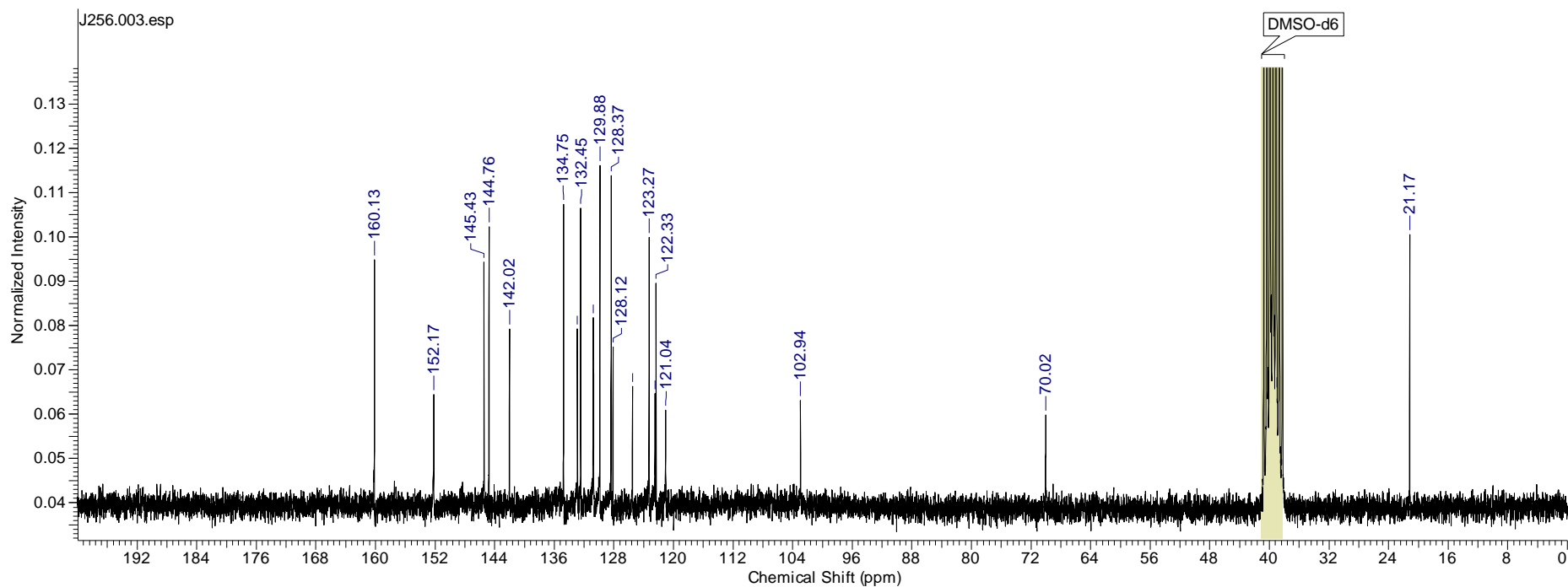
^{1}H NMR spectrum of 4-(2-bromobenzyloxy)quinolin-8-yl 4-methylbenzenesulfonate (**9**)

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	Connections	(ppm)
1	2.38	3	s	-	M01	-	[2.30 .. 2.45]
2	5.40	2	s	-	M02	-	[5.30 .. 5.49]
3	7.21	1	d	5.28	M03	M08	[7.16 .. 7.26]
4	7.44	6	m	-	M04	-	[7.31 .. 7.58]
5	7.72	2	m	-	M05	-	[7.67 .. 7.77]
6	7.82	2	d	8.22	M06	-	[7.78 .. 7.86]
7	8.09	1	dd	7.73, 2.05	M07	-	[8.04 .. 8.15]
8	8.69	1	d	5.28	M08	M03	[8.63 .. 8.75]

^{13}C NMR spectrum of 4-(2-bromobenzyloxy)quinolin-8-yl 4-methylbenzenesulfonate (**9**)

No.	(ppm)	(Hz)	Height
1	21.17	1065.4	0.1005
2	70.02	3523.7	0.0598
3	102.94	5180.1	0.0631
4	121.04	6090.9	0.0609
5	122.33	6155.8	0.0895

No.	(ppm)	(Hz)	Height
6	122.48	6163.5	0.0646
7	123.27	6203.5	0.0999
8	125.50	6315.7	0.0662
9	128.12	6447.4	0.0752
10	128.37	6459.9	0.1138

No.	(ppm)	(Hz)	Height
11	129.88	6535.8	0.1162
12	130.70	6577.3	0.0693
13	130.77	6580.9	0.0817
14	132.45	6665.3	0.1065
15	132.90	6688.0	0.0793

No.	(ppm)	(Hz)	Height
16	134.75	6780.8	0.1074
17	142.02	7146.9	0.0793
18	144.76	7284.8	0.1023
19	145.43	7318.6	0.0943
20	152.17	7657.5	0.0645

No.	(ppm)	(Hz)	Height
21	160.13	8058.4	0.0948

21

HRMS of 4-(2-bromobenzyloxy)quinolin-8-yl 4-methylbenzenesulfonate (**9**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results) - displaying only valid results

Tolerance = 3.0 mDa   /   DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Even Electron Ions

387 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)
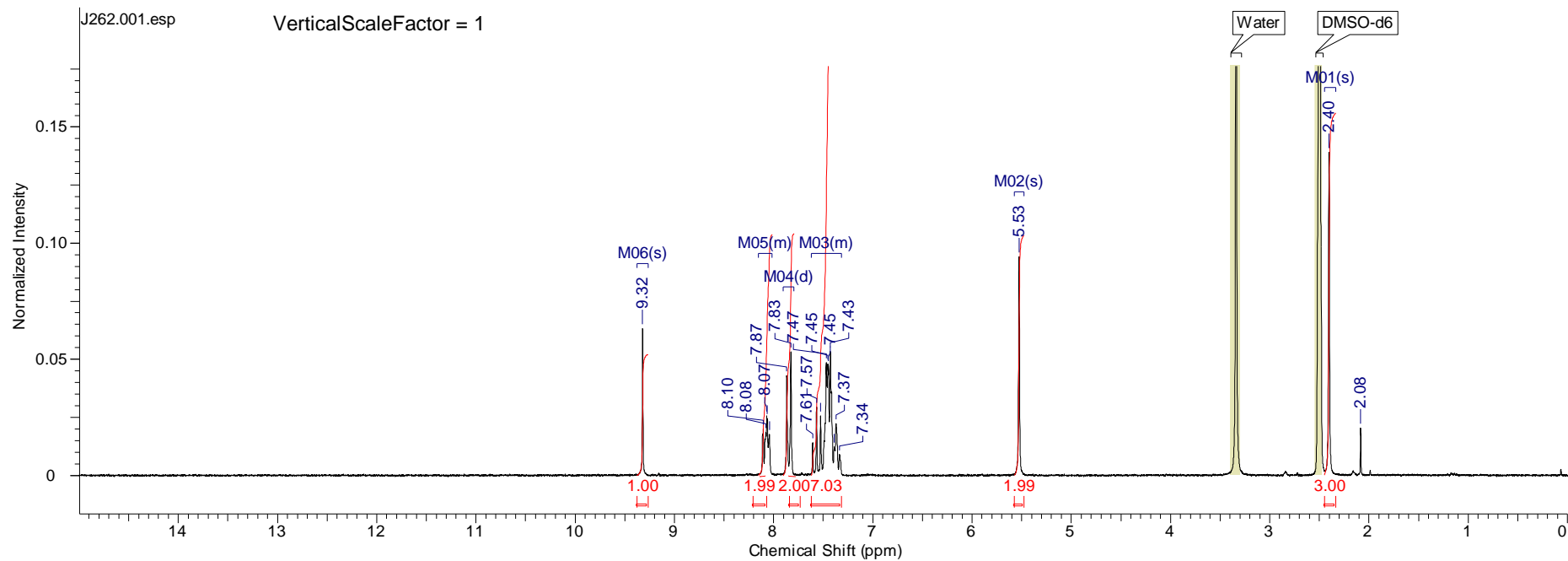
Minimum:				-0.5	
Maximum:		3.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
484.0208	484.0216	-0.8	-1.6	11.5	C15 H15 N7 O7 Br
	484.0218	**-1.0**	**-2.0**	**14.5**	**C23 H19 N O4 S Br**
	484.0191	1.7	3.5	15.5	C19 H15 N7 O2 S Br
	484.0184	2.4	5.0	19.5	C26 H15 N O4 Br

J254

LCT-24762 24 (0.482) AM (Cen,2, 70.00, Ar,5000.0,556.28); Sm (SG, 1x2.00); Sb (4,40.00)

22
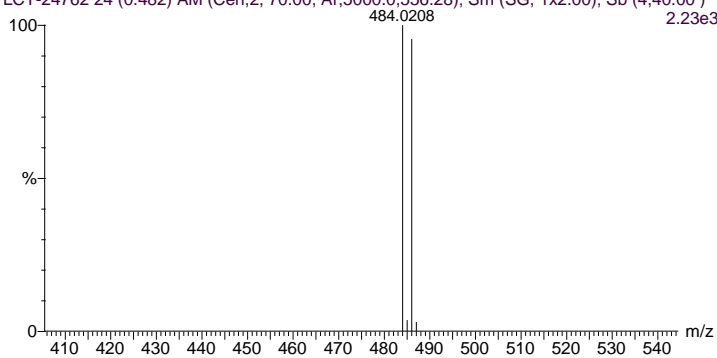
^{1}H NMR spectrum of 6*H*-isochromeno[4,3-*c*]quinolin-1-yl 4-methylbenzenesulfonate (**10**)

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	2.40	3	s	-	M01	[2.34 .. 2.45]
2	5.53	2	s	-	M02	[5.47 .. 5.58]
3	7.47	7	m	-	M03	[7.32 .. 7.62]
4	7.85	2	d	8.22	M04	[7.79 .. 7.90]
5	8.08	2	m	-	M05	[8.02 .. 8.15]
6	9.32	1	s	-	M06	[9.26 .. 9.38]

23

^{13}C NMR spectrum of 6*H*-isochromeno[4,3-*c*]quinolin-1-yl 4-methylbenzenesulfonate (**10**)
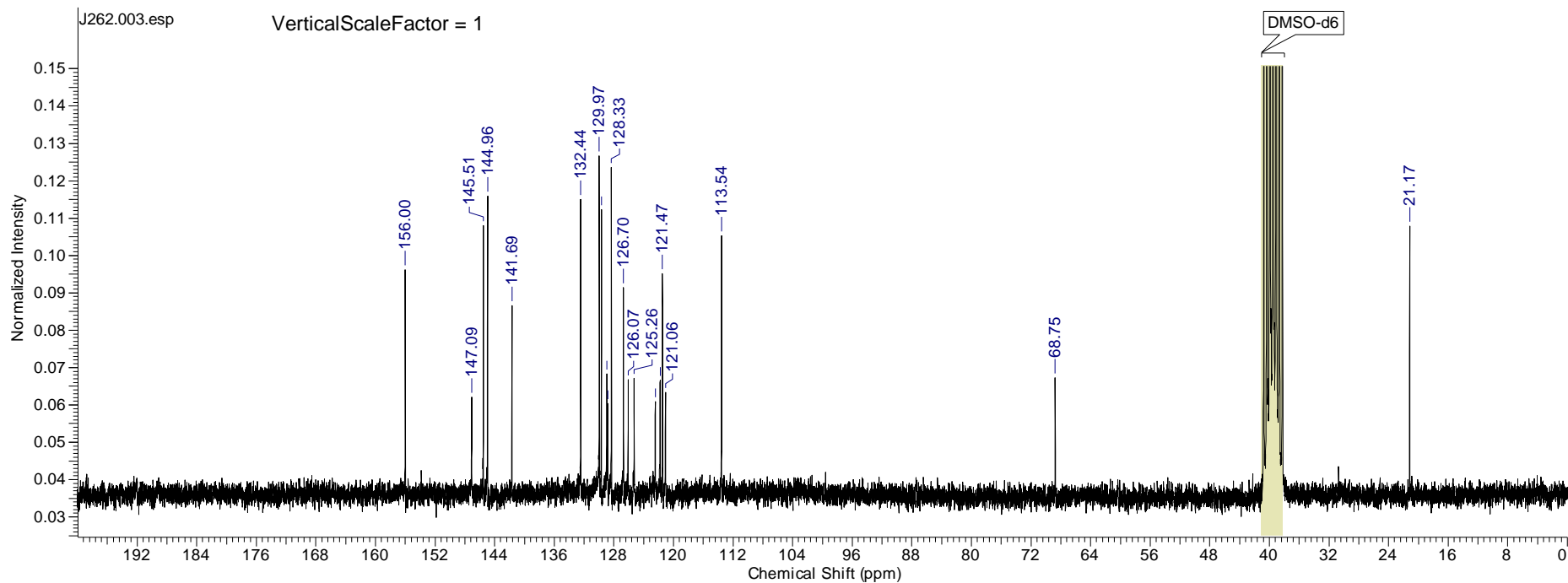
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.17	1065.4	0.1079	6	121.79	6128.7	0.0667	11	128.33	6457.7	0.1235	16	132.44	6664.9	0.1150	21	156.00	7850.4	0.0962
2	68.75	3459.8	0.0673	7	122.44	6161.3	0.0609	12	128.83	6483.0	0.0604	17	141.69	7130.4	0.0867				
3	113.54	5713.8	0.1053	8	125.26	6303.6	0.0671	13	128.94	6488.5	0.0683	18	144.96	7294.7	0.1159				
4	121.06	6092.0	0.0633	9	126.07	6344.3	0.0668	14	129.67	6525.5	0.1123	19	145.51	7322.2	0.1080				
5	121.47	6112.9	0.0951	10	126.70	6375.9	0.0913	15	129.97	6540.2	0.1267	20	147.09	7401.8	0.0621				

HRMS of 6*H*-isochromeno[4,3-*c*]quinolin-1-yl 4-methylbenzenesulfonate (**10**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa / DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Even Electron Ions

393 formula(e) evaluated with 7 results within limits (up to 50 closest results for each mass)

Minimum: -0.5

Maximum: 5.0   10.0   100.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
404.0950	404.0955	-0.4	-1.1	12.5	C15 H14 N7 O7
	404.0957	**-0.6**	**-1.5**	**15.5**	**C23 H18 N O4 S**
	404.0930	2.1	5.1	16.5	C19 H14 N7 O2 S
	404.0923	2.7	6.8	20.5	C26 H14 N O4
	404.0916	3.4	8.4	11.5	C18 H18 N3 O6 S
	404.0988	-3.8	-9.4	7.5	C12 H18 N7 O7 S
	404.0995	-4.5	-11.0	16.5	C20 H14 N5 O5

J255

lct-24826 40 (0.804) AM (Cen,2, 65.00, Ar,5000.0,556.28); Sm (SG, 1x2.00); Sb (4,40.00); Sb
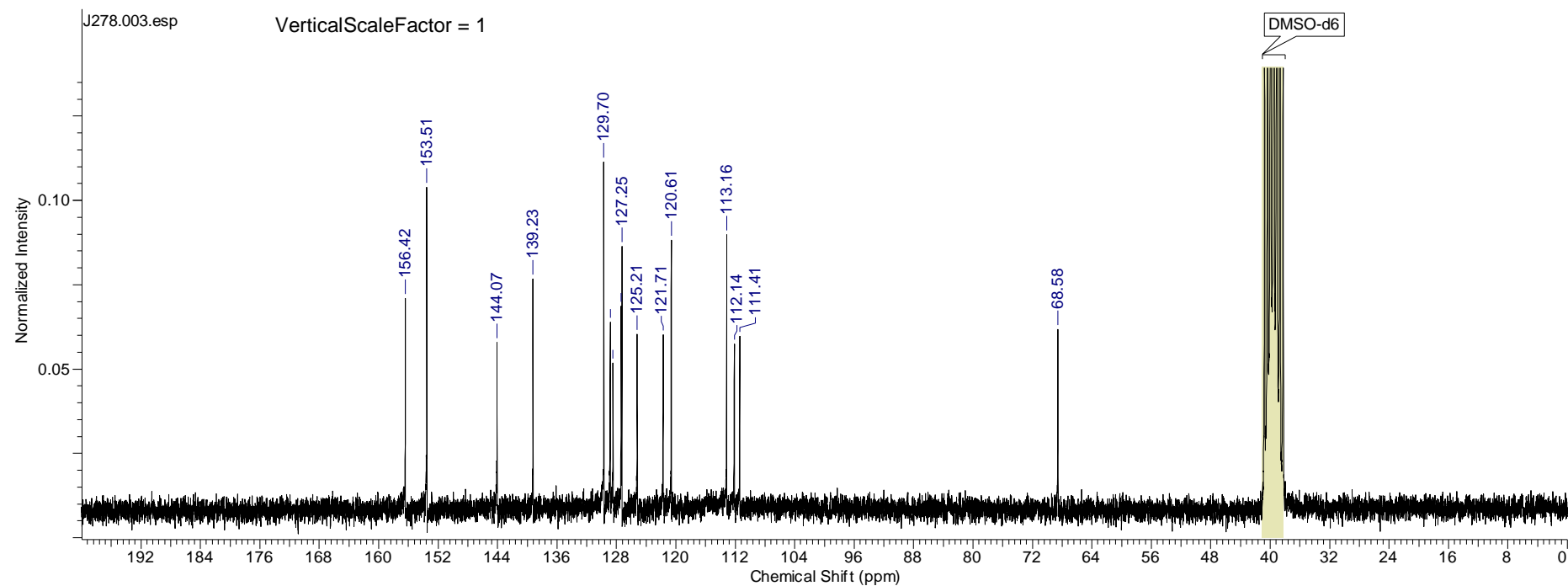

25
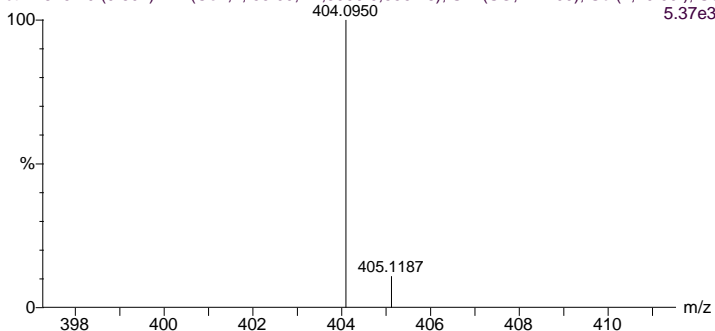
^{1}H NMR spectrum of 6*H*-isochromeno[4,3-*c*]quinolin-1-ol (**11**)
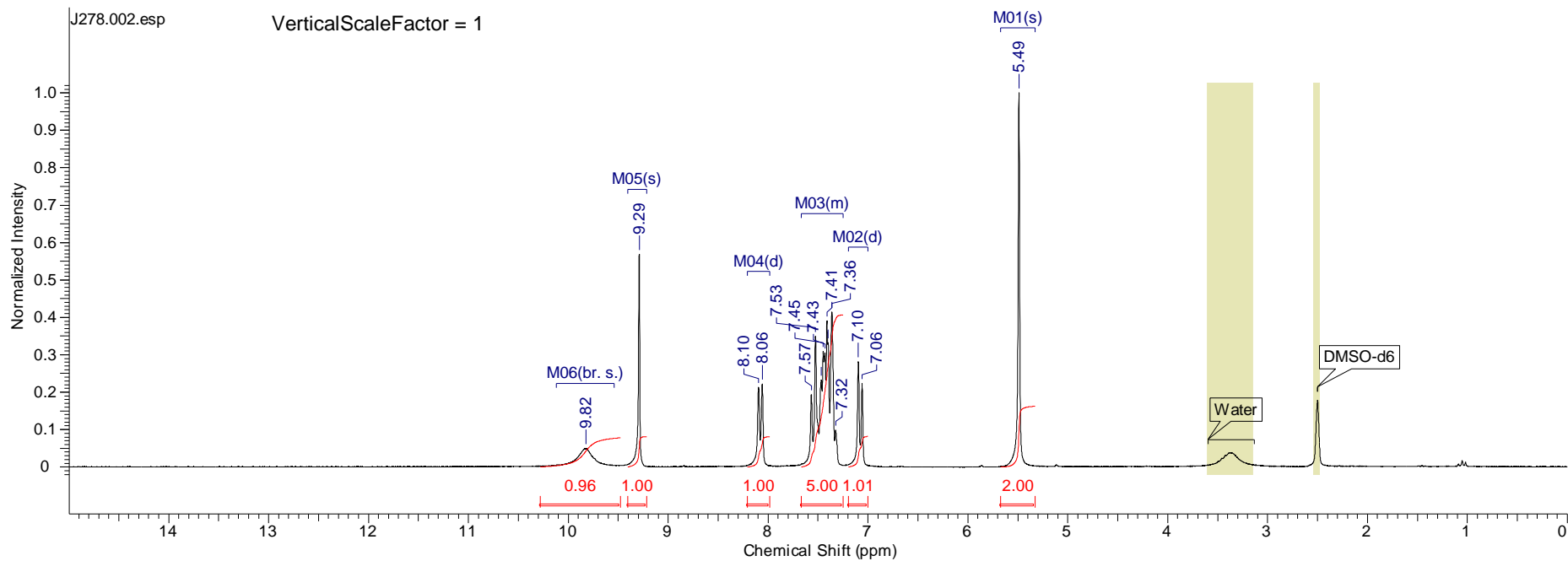
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	Connections	(ppm)
1	5.49	2	s	-	M01	-	[5.33 .. 5.67]
2	7.08	1	d	7.43	M02	M04	[7.00 .. 7.20]
3	7.44	5	m	-	M03	-	[7.25 .. 7.67]
4	8.08	1	d	7.24	M04	M02	[7.98 .. 8.21]
5	9.29	1	s	-	M05	-	[9.22 .. 9.41]
6	9.82	1	br. s.	-	M06	-	[9.54 .. 10.12]

^{13}C NMR spectrum of *6H*-isochromeno[4,3-*c*]quinolin-1-ol (**11**)

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	68.58	3451.0	0.0617	5	120.61	6069.6	0.0883	9	127.36	6408.9	0.0686	13	139.23	7006.4	0.0767
2	111.41	5606.3	0.0598	6	121.71	6124.6	0.0602	10	128.46	6464.7	0.0519	14	144.07	7250.0	0.0579
3	112.14	5643.0	0.0575	7	125.21	6300.7	0.0603	11	128.84	6483.4	0.0639	15	153.51	7725.0	0.1039
4	113.16	5694.7	0.0898	8	127.25	6403.8	0.0863	12	129.70	6526.6	0.1114	16	156.42	7871.3	0.0710

HRMS of 6*H*-isochromeno[4,3-*c*]quinolin-1-ol (**11**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa   /   DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Even Electron Ions

106 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
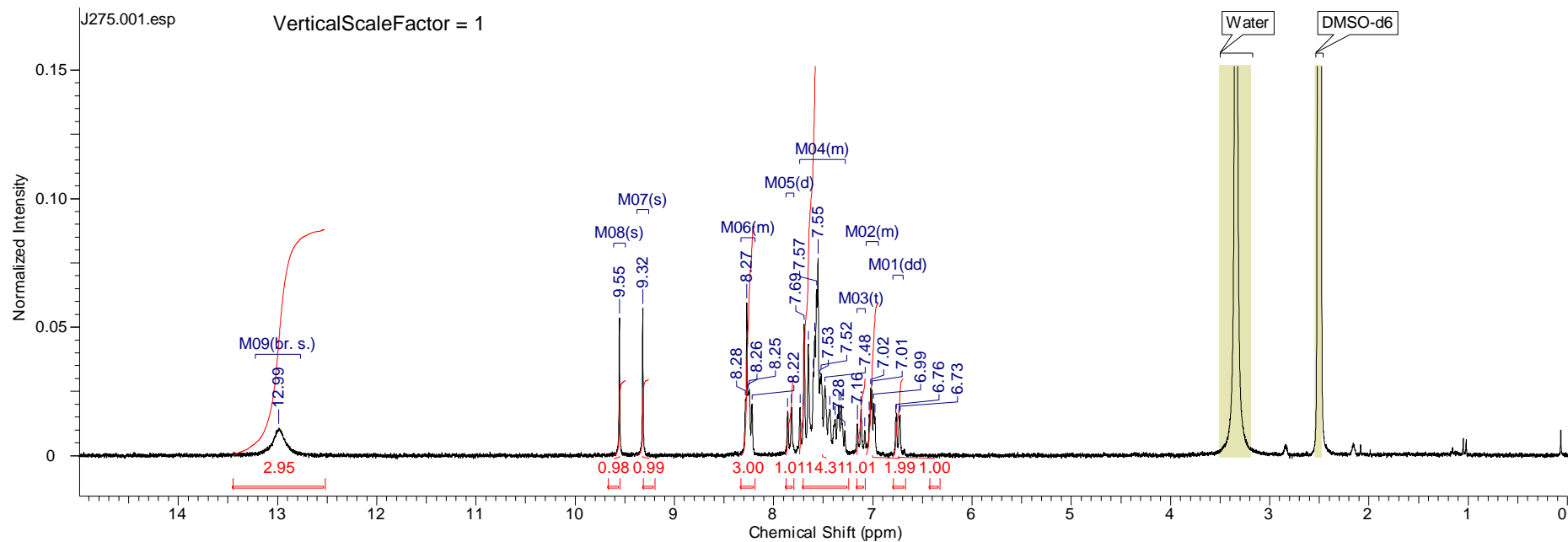
Minimum:				-0.5	
Maximum:		5.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
250.0873	**250.0868**	**0.5**	**2.1**	**11.5**	**C16 H12 N O2**
	250.0828	4.5	18.2	7.5	C11 H12 N3 O4

J259

LCT-24905 280 (5.604) AM (Cen,2, 70.00, Ar,5000.0,556.28); Sm (SG, 1x2.00); Sb (4,40.00)

^{1}H NMR of tris-(11*H*-indolo[3,2-*c*]quinolin-4-ol)aluminum (**12**)

No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	6.75	1	dd	7.14, 1.27	M01	[6.69 .. 6.80]
2	7.01	2	m	-	M02	[6.94 .. 7.06]
3	7.12	1	t	7.43	M03	[7.08 .. 7.16]
4	7.51	14	m	-	M04	[7.28 .. 7.74]
5	7.84	1	d	8.02	M05	[7.80 .. 7.87]
6	8.26	3	m	-	M06	[8.19 .. 8.33]
7	9.32	1	s	-	M07	[9.26 .. 9.38]
8	9.55	1	s	-	M08	[9.50 .. 9.61]
9	12.99	3	br. s.	-	M09	[12.77 .. 13.23]

29

HRMS of tris-(11*H*-indolo[3,2-*c*]quinolin-4-ol)aluminum (**12**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa   /   DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Odd and Even Electron Ions

616 formula(e) evaluated with 8 results within limits (up to 50 closest results for each mass)

Minimum:				-0.5	
Maximum:		5.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
749.1842	749.1850	-0.8	-1.1	46.5	C58 H26 Al
	749.1858	**-1.6**	**-2.1**	**35.5**	**C45 H27 N6 O3 Na Al**
	749.1826	1.6	2.2	43.5	C56 H27 Na Al
	749.1871	-2.9	-3.9	35.0	C47 H29 N3 O4 Na Al
	749.1810	3.2	4.3	42.5	C53 H26 N2 O2 Al
	749.1882	-4.0	-5.3	38.5	C47 H26 N6 O3 Al
	749.1885	-4.3	-5.7	40.0	C48 H25 N7 Na Al

J275

lct-25119 280 (5.604) AM (Cen,2, 60.00, Ar,5000.0,609.28); Sm (SG, 1x2.00); Sb (4,40.00); Sl
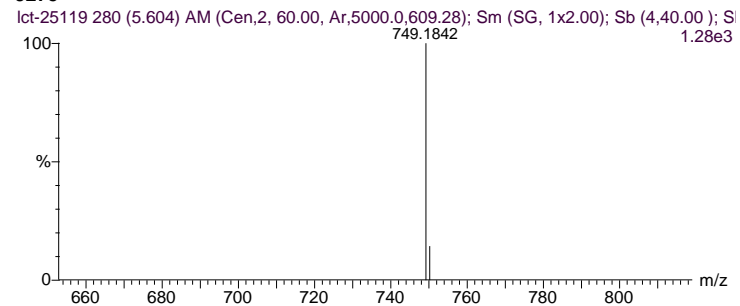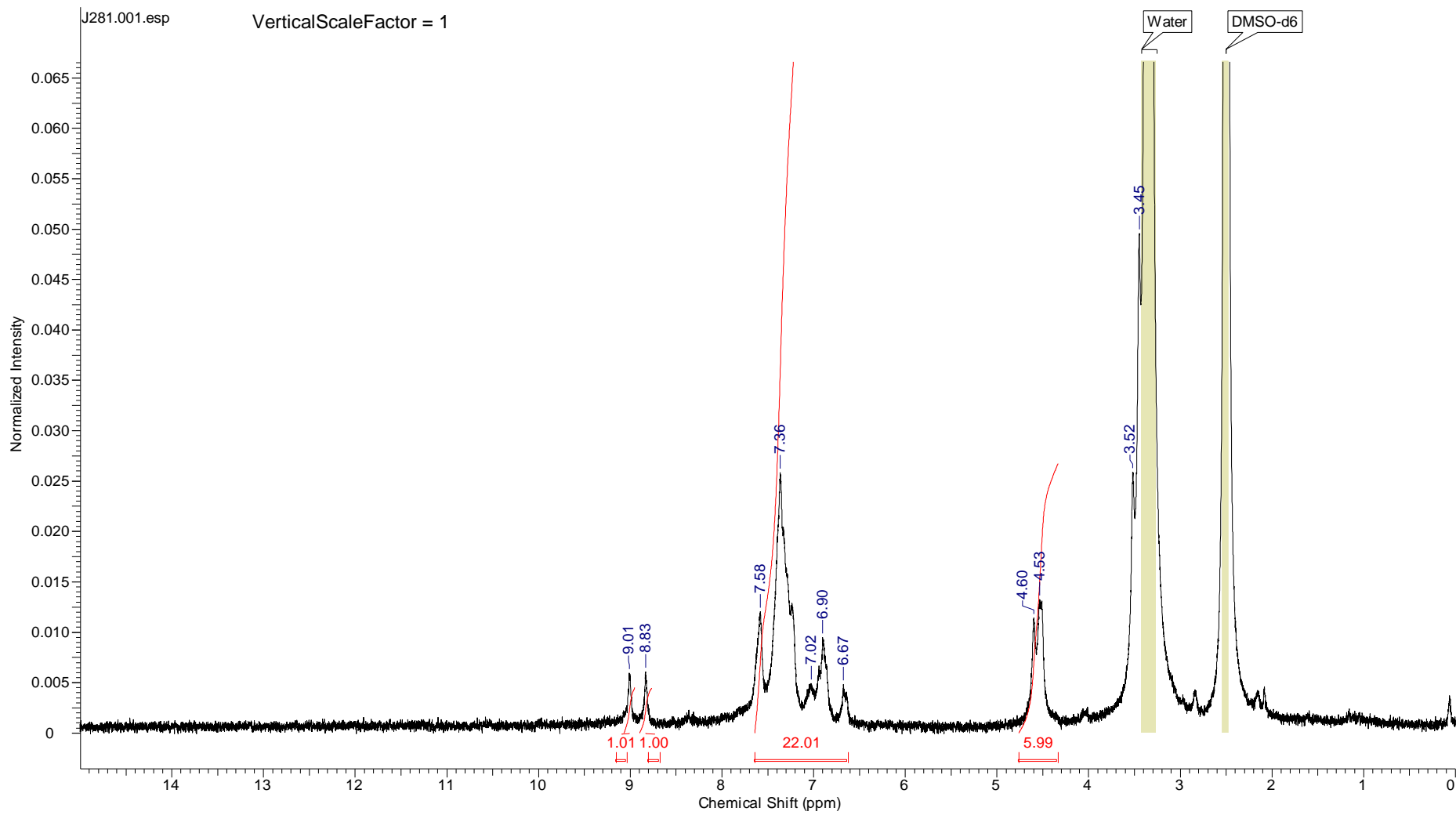
^{1}H NMR of tris-(5-methyl-5,6-dihydrodibenzo[*c*,*h*][1,6]naphthyridin-1-ol)aluminum (**13**)

Due to overlapping peaks and poor solubility of the studied compound, ^{1}H NMR spectrum was measured both in CDCl$_3$ and DMSO-d_6.

J281.001.esp

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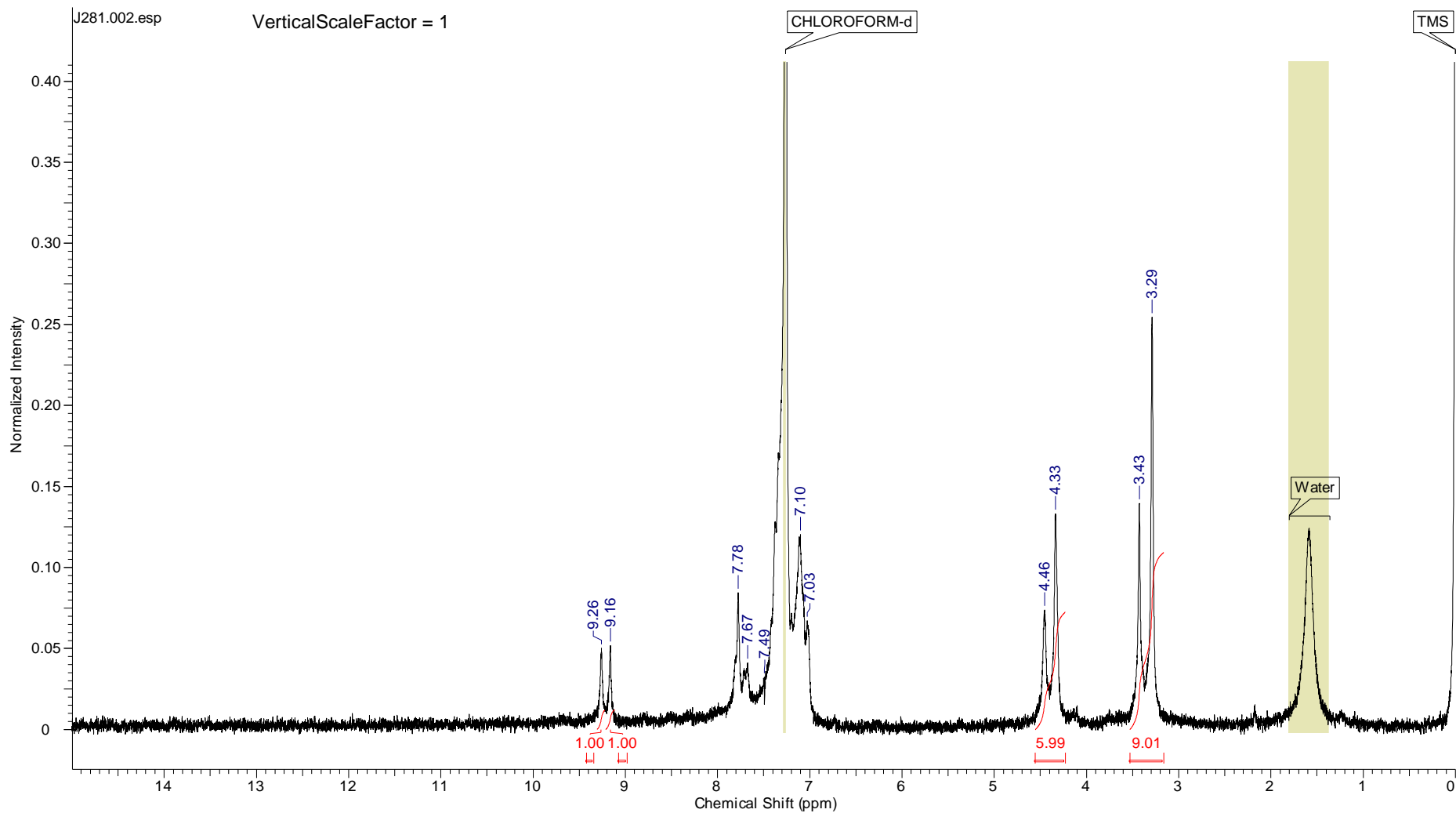
HRMS of tris-(5-methyl-5,6-dihydrodibenzo[*c,h*][1,6]naphthyridin-1-ol)aluminum (**13**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results) - displaying only valid results

Tolerance = 5.0 mDa / DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Odd and Even Electron Ions

232 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

Minimum:					-0.5			
Maximum:		5.0		10.0	100.0			
Mass	Calc. Mass	mDa		PPM	DBE	Formula		
811.2981	811.2980	0.1		0.1	37.0	C52 H39 N7 Na Al		
	811.2977	**0.4**		**0.5**	**35.5**	**C51 H40 N6 O3 Al**		
	811.3004	-2.3		-2.9	40.0	C54 H38 N7 Al		
	811.2953	2.8		3.4	32.5	C49 H41 N6 O3 Na Al		

J281

lct-25009 347 (6.944) AM (Cen,2, 80.00, Ar,5000.0,609.28); Sm (SG, 1x2.00); Sb (4,40.00); SI
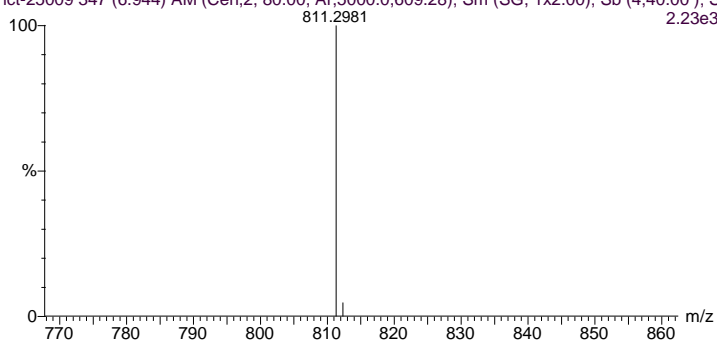
^{1}H NMR of tris-(6*H*-isochromeno[4,3-*c*]quinolin-1-ol)aluminum (**14**)
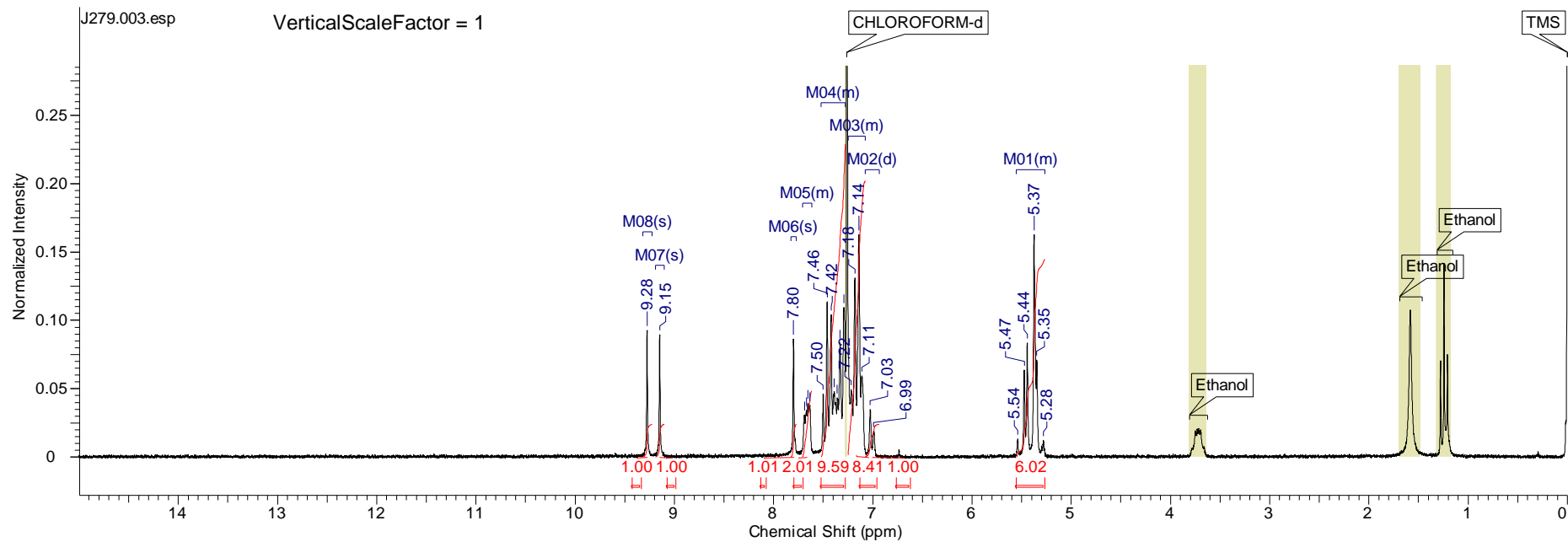
No.	Shift1 (ppm)	H's	Type	J (Hz)	Multiplet1	(ppm)
1	5.41	6	m	-	M01	[5.26 .. 5.55]
2	7.01	1	d	6.80	M02	[6.93 .. 7.08]
3	7.16	9	m	-	M03	[7.08 .. 7.25]
4	7.39	10	m	-	M04	[7.28 .. 7.52]
5	7.66	2	m	-	M05	[7.62 .. 7.71]
6	7.80	1	s	-	M06	[7.77 .. 7.82]
7	9.15	1	s	-	M07	[9.10 .. 9.19]
8	9.28	1	s	-	M08	[9.23 .. 9.32]

HRMS of tris-(6*H*-isochromeno[4,3-*c*]quinolin-1-ol)aluminum (**14**)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa   /   DBE: min = -0.5, max = 100.0

Monoisotopic Mass, Odd and Even Electron Ions

604 formula(e) evaluated with 10 results within limits (up to 50 closest results for each mass)

Minimum:				-0.5	
Maximum:		5.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
794.1868	794.1872	-0.4	-0.5	38.5	C50 H29 N3 O6 Al
	794.1861	0.7	0.8	35.0	C50 H32 O7 Na Al
	794.1875	-0.7	-0.9	40.0	C51 H28 N4 O3 Na Al
	794.1885	-1.8	-2.2	38.0	C52 H31 O7 Al
	794.1848	**2.0**	**2.5**	**35.5**	**C48 H30 N3 O6 Na Al**
	794.1888	-2.0	-2.6	39.5	C53 H30 N O4 Na Al
	794.1899	-3.1	-3.9	43.0	C53 H27 N4 O3 Al
	794.1826	4.1	5.2	47.0	C59 H27 O2 Al
	794.1912	-4.4	-5.6	42.5	C55 H29 N O4 Al
	794.1915	-4.7	-5.9	44.0	C56 H28 N2 O Na Al

J279

LCT-25010 90 (1.801) AM (Cen,2, 70.00, Ar,5000.0,995.31); Sm (SG, 2x2.00); Sb (4,40.00); S

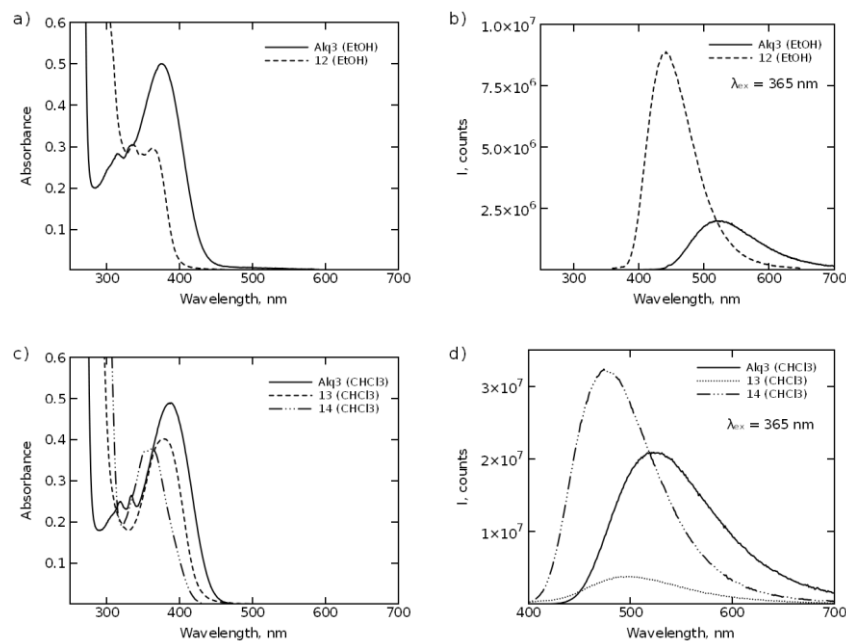35
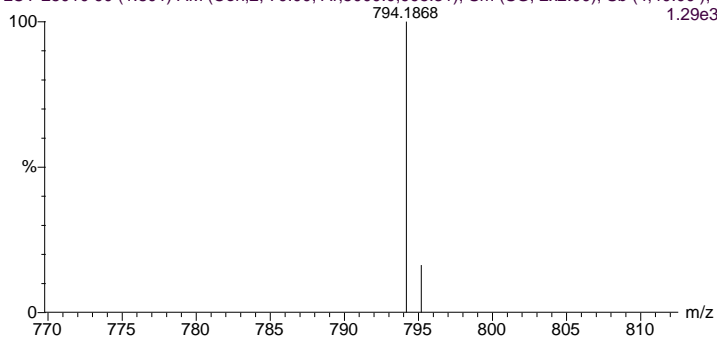
Fluorescence quantum yield determination in steady state

Figure S1. Absorption (a and c) and emission (b and d) spectra in absolute scale of the parent Alq_3, derivative **12** (in ethanol) and derivatives **13** and **14** (in chloroform) solutions. The parent Alq_3 was used as a reference both in chloroform and ethanol. Excitation wavelength was the crossing point in absorption (365 nm), in order to cancel out the effect of transmittance. Therefore, relative fluorescence quantum yield is the ratio of integrated intensity of the sample to the reference throughout the measured range.

Note: In Figure S1c, the transmittances of samples **13**, **14** and the parent Alq_3 at the excitation wavelength (365 nm) are not exactly equal. This was taken into account in the calculation and it turned out, that the contribution rising from this difference is negligible. Experiments were repeated by using solutions of lower concentration, and by using different excitation wavelengths. In each case, the results corresponded very well with the ones presented here.

Fluorescence quantum yield (Φ) in steady state was calculated by using the equation 1:

$$\frac{\Phi}{\Phi_{ref}} = \frac{\int\limits_{\lambda_1}^{\lambda_2} I(\lambda)d\lambda}{\int\limits_{\lambda_1}^{\lambda_2} I_{ref}(\lambda)d\lambda} \times \frac{(1-T_{ex,ref})}{(1-T_{ex})} \times \frac{n^2}{n_{ref}^2} \tag{1}$$

λ_1 and λ_2 are determined from the measured wavelength range. Integrals can be estimated as sums of the measured intensities throughout the spectrum (corrected according to the instruments wavelength sensitivity). By selecting the excitation wavelength in a way, that transmittance of the sample equals with the reference ($T_{ex} = T_{ex,ref}$), using the same solvent ($n = n_{ref}$) and normalizing Φ_{ref} to 1 (the parent Alq$_3$), relative fluorescence quantum yield can be obtained by comparing intensities only (equation 2).

$$\Phi = \frac{\sum\limits_{\lambda_1}^{\lambda_2} I(\lambda)}{\sum\limits_{\lambda_1}^{\lambda_2} I_{ref}(\lambda)} \tag{2}$$

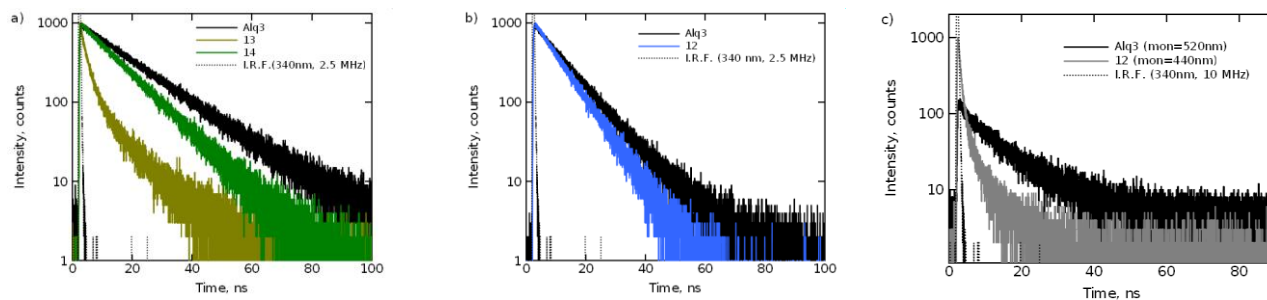Fluorescence decays obtained with TCSPC method and calculation of parameters

Figure S2. Fluorescence decays of the parent Alq_3 (λ_{mon} = 520 nm) and compounds **13** and **14** (λ_{mon} = 490 nm) in $CHCl_3$ (a), the parent Alq_3 (λ_{mon} = 520 nm) and compound **12** (λ_{mon} = 440 nm) in ethanol (b) and thin films of the parent Alq_3 and compound **12** (c).
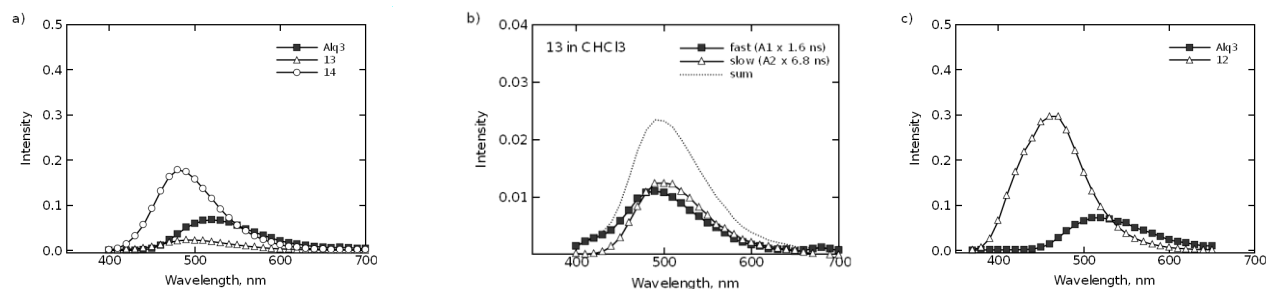

Figure S3. Decay associated spectra of the parent Alq_3 (λ_{mon} = 520 nm) and compounds **13** and **14** (λ_{mon} = 490 nm) in $CHCl_3$ (a), two components of the compound **13** in $CHCl_3$ (b), and the parent Alq_3 (λ_{mon} = 520 nm) and compound **12** (λ_{mon} = 440 nm) in ethanol (c).

Relative fluorescence quantum yield can be obtained from decay associated spectrum by comparing the sum intensities (I_{sum} , equations 4a and b) of the sample and the reference, and it should correlate with the quantum yield in steady-state (Φ).

Fluorescence decays were fitted to the well known exponential model (A = Amplitude, I = Intensity):

$$I_{1-\exp} = A_0 + A_1 e^{-\frac{t}{\tau_1}} \tag{3a}$$

$$I_{n-\exp} = \sum_{i=0}^{n} (A_i e^{-\frac{t}{\tau_i}}) \tag{3b}$$

Integrating time from zero to infinity, summing the intensities throughout the measured spectrum and by taking transmittance (T) of the excitation pulse (340 nm) into account leads to:

$$I_{sum,1-\exp} = \frac{1}{(1-T)} \sum_{\lambda_1}^{\lambda_2} A_1(\lambda)\tau_1 \tag{4a}$$

$$I_{sum,n-\exp} = \frac{1}{(1-T)} \sum_{\lambda_1}^{\lambda_2} (\sum_{i=0}^{n} A_i(\lambda)\tau_i) \tag{4b}$$

Constant A_0 was negligible and was therefore excluded from the analysis. In solution, derivative 13 revealed two-exponential decay (equation 4b, $n = 2$), while the decays of the parent Alq_3 and derivatives 12 and 14 were single exponential (equation 4a).

Radiative fluorescence rate constants (k_r) were calculated by using equation:

$$k_r = \frac{\Phi}{\tau_F} \tag{5}$$

where Φ is an absolute fluorescence quantum yield and τ_F fluorescence lifetime.

Non-radiative rate constants (k_{nr}) were calculated by using equation:

$$k_{nr} = \frac{1}{\tau_F} - k_r \tag{6}$$