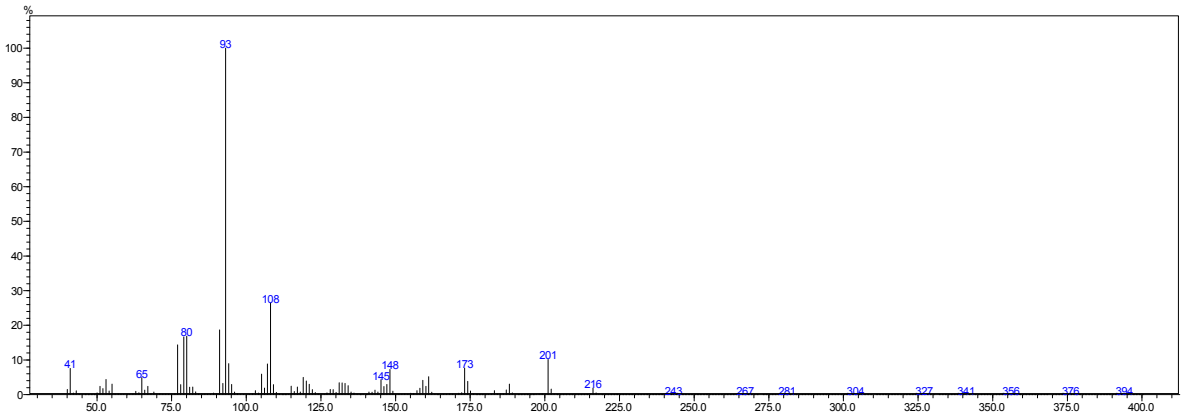
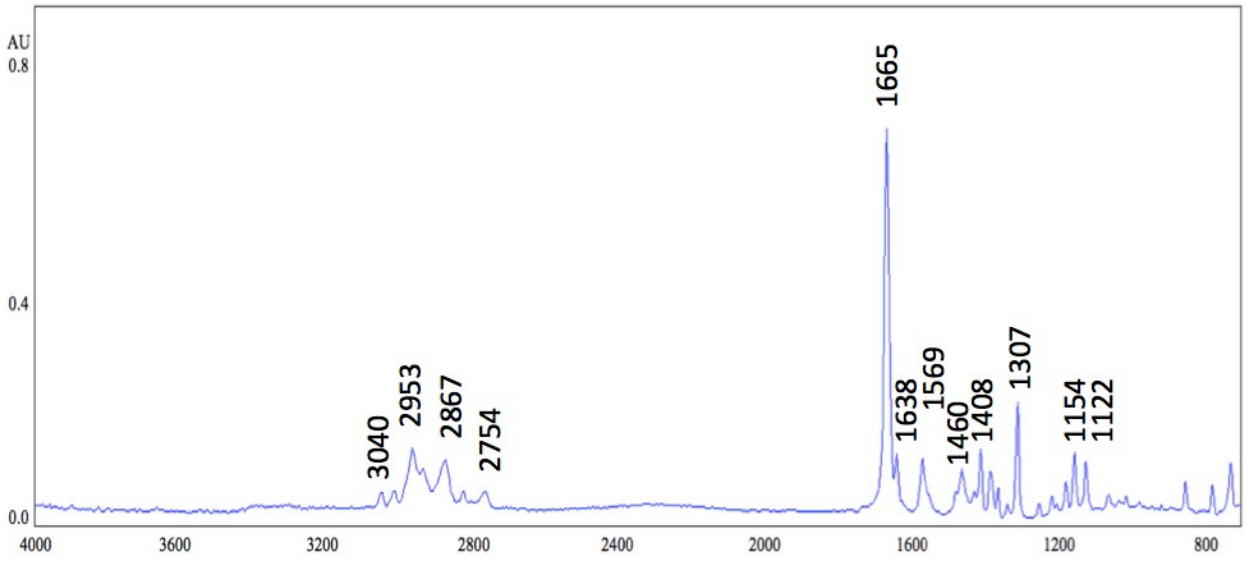
Electronic Supplementary Material (ESI) for Faraday Discussions.

Electronic Supplementary Material

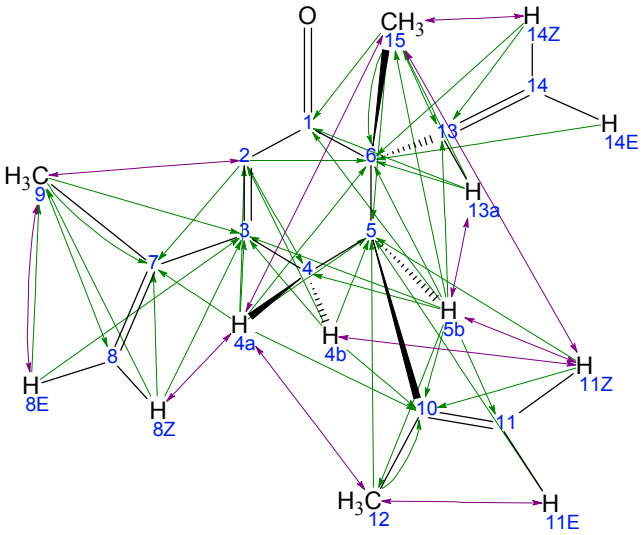
Electron impact GC-MS spectrum of the isolated component



Condensed phase GC-FTIR spectrum of the isolated component



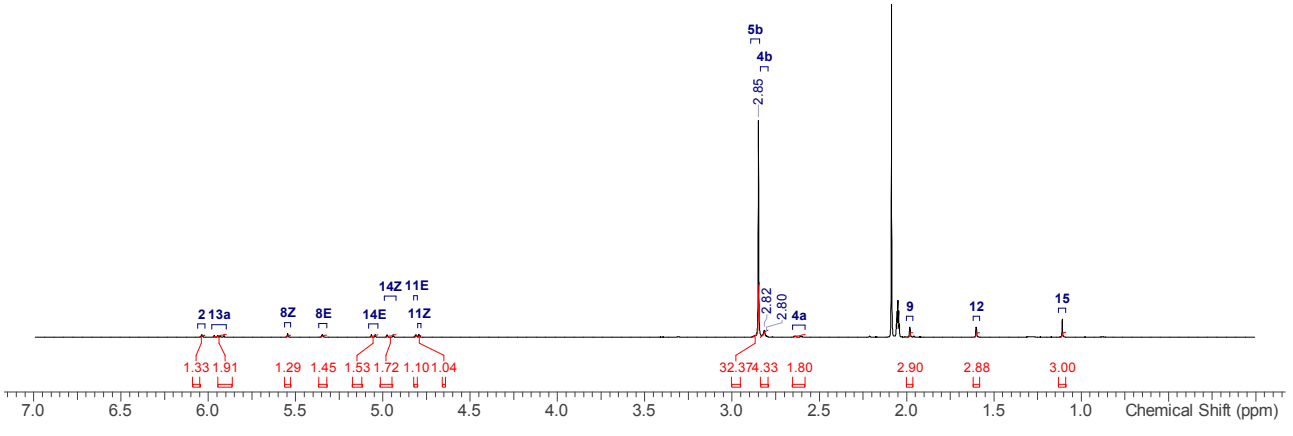
Comprehensive NMR tables and structure with assignment



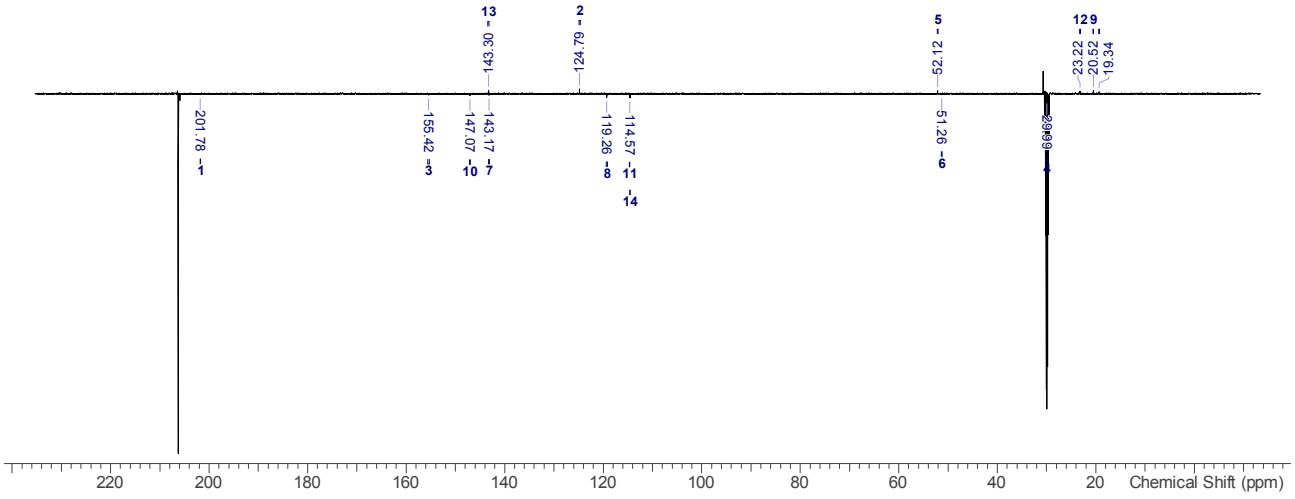
#	Atom#	C Label	C Shift	XHn	H Label	H Shift	C Calc Shift	H Calc Shift	H Multiplicity	NOESY	H HMBC	C HMBC
1	15	C 15	19.339	CH3	H 15	1.109	19.723	1.190	s	4a, 11Z, 14Z	5b, 13a	6, 5, 13, 1
2	9	C 9	20.515	CH3	H 9	1.981	21.862	1.951	s	8E, 2	8E, 8Z	8, 7, 3
3	12	C 12	23.220	CH3	H 12	1.601	22.354	1.707	d (0.64)	4a, 11E	5b	5, 10
4	4a	C 4	29.988	CH2	H 4a	2.622	32.643	2.768	br dd (17.90, 3.84)	15, 12, 8Z	5b, 2	6, 5, 2, 7, 10, 3
5	4b	C 4	29.988	CH2	H 4b	2.828	32.643	2.794	m	11Z	5b, 2	5, 2, 10, 3
6	6	C 6	51.256	C			51.794				15, 4a, 5b, 14Z, 14E, 13a, 2	
7	5b	C 5	52.125	CH	H 5b	2.867	51.084	2.801	s	11Z, 13a	15, 12, 4a, 4b, 11Z, 11E	15, 12, 4, 6, 11, 13, 10, 3, 1
8	14E	C14	114.570	CH2	H 14E	5.055	114.943	5.194	dd (10.66, 0.85)			6
9	14Z	C14	114.570	CH2	H 14Z	4.947	114.943	5.162	br dd (17.69, 0.85)	15		6, 13
10	11E	C11	114.634	CH2	H 11E	4.810	113.276	4.859	br d (1.49)	12	5b	5
11	11Z	C11	114.634	CH2	H 11Z	4.794	113.276	4.837	d (0.64)	15, 4b, 5b	5b	5, 10
12	8Z	C8	119.262	CH2	H 8Z	5.545	122.301	5.341	s	4a, 8E	9	9, 7, 3
13	8E	C8	119.262	CH2	H 8E	5.346	122.301	5.234	s	9, 8Z	9	9, 3
14	2	C 2	124.794	CH	H 2	6.037	119.329	5.978	s	9	4a, 4b	4, 6, 7
15	7	C 7	143.174	C			142.886				9, 4a, 8Z, 2	
16	13a	C 13	143.303	CH	H 13	5.938	140.341	5.961	dd (17.48, 10.66)	5b	15, 5b, 14Z	15, 6, 1
17	10	C 10	147.067	C			144.817				12, 4a, 4b, 5b, 11Z	
18	3	C 3	155.417	C			155.658				9, 4a, 4b, 5b, 8E, 8Z	
19	1	C 1	201.780	C			202.192				15, 5b, 13a	

1H-NMR data

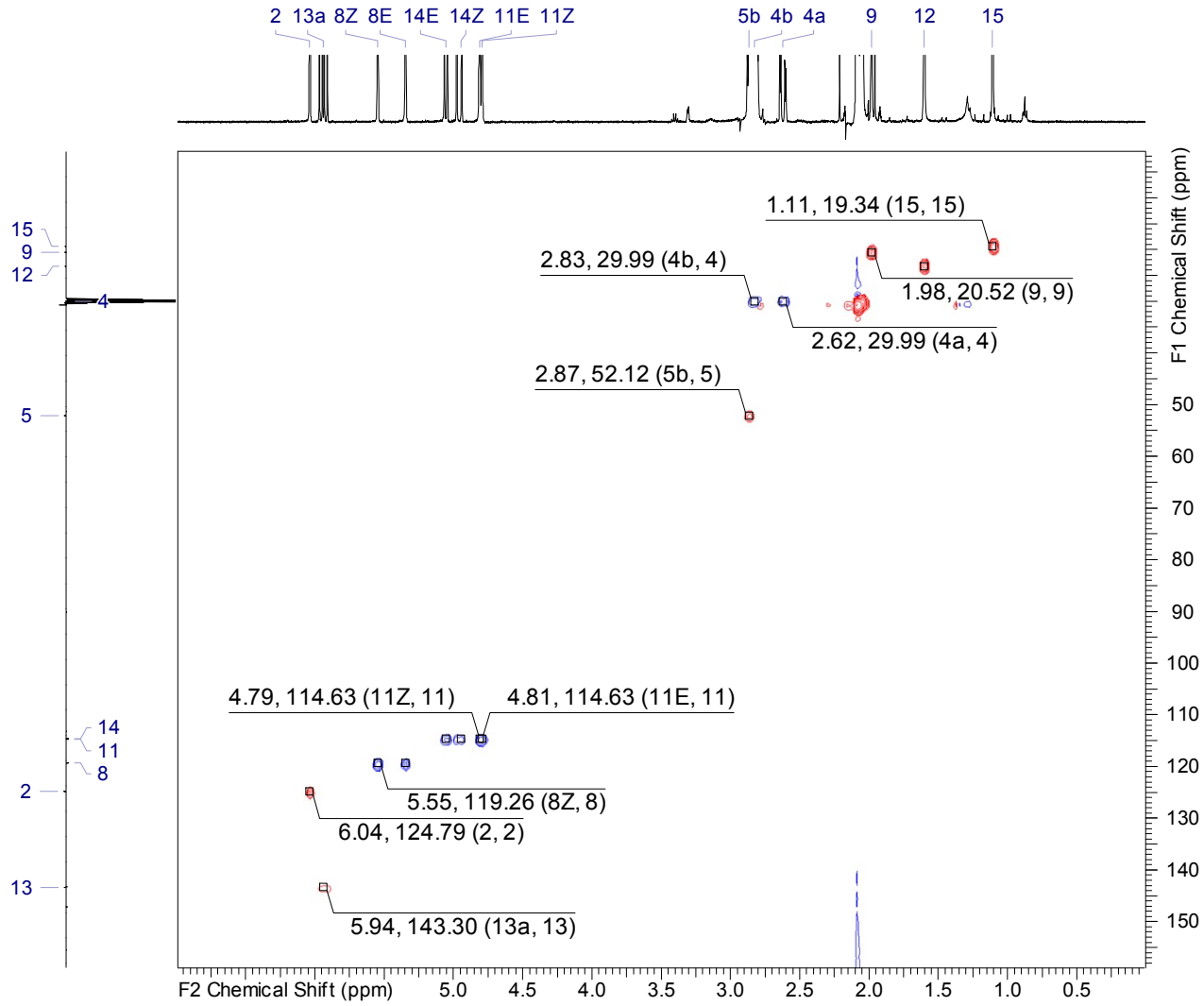
^{1}H NMR (500 MHz, Solvent) δ ppm 1.11 (s, 3 H) 1.60 (d, *J*=0.64 Hz, 3 H) 1.98 (s, 3 H) 2.62 (br dd, *J*=17.90, 3.84 Hz, 2 H) 2.79 - 2.84 (m, 4 H) 2.85 (s, 32 H) 4.79 (d, *J*=0.64 Hz, 1 H) 4.81 (br d, *J*=1.49 Hz, 1 H) 4.96 (br dd, *J*=17.69, 0.85 Hz, 2 H) 5.05 (dd, *J*=10.66, 0.85 Hz, 2 H) 5.35 (s, 1 H) 5.55 (s, 1 H) 5.94 (dd, *J*=17.48, 10.66 Hz, 2 H) 6.04 (s, 1 H)



13C NMR spectrum

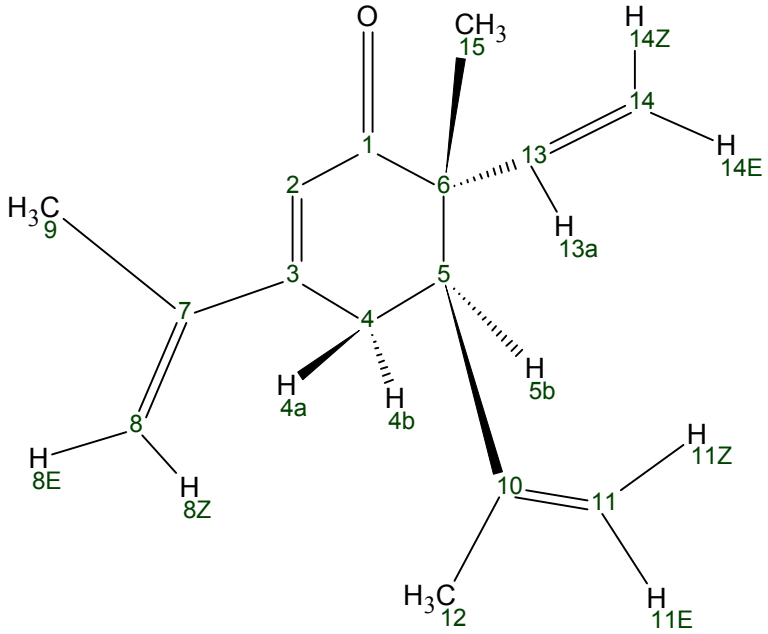


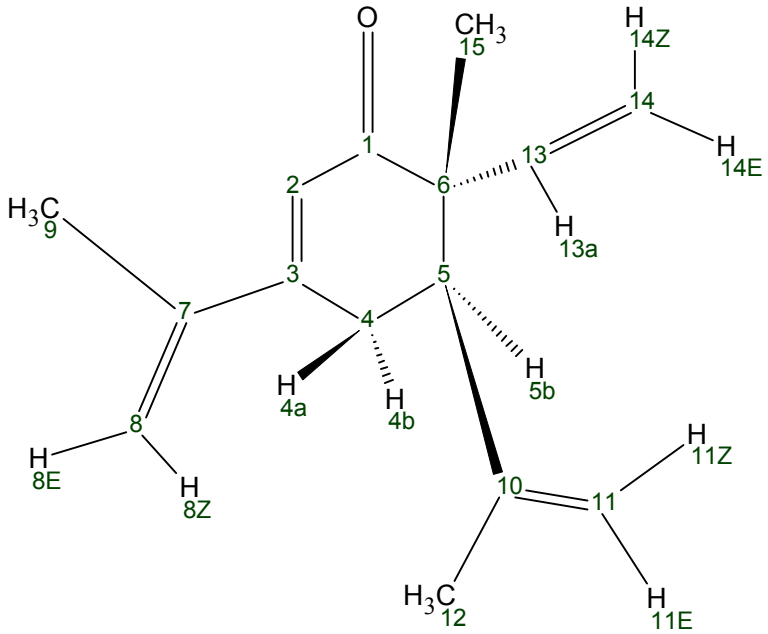
13C-1H HSQC Spectrum

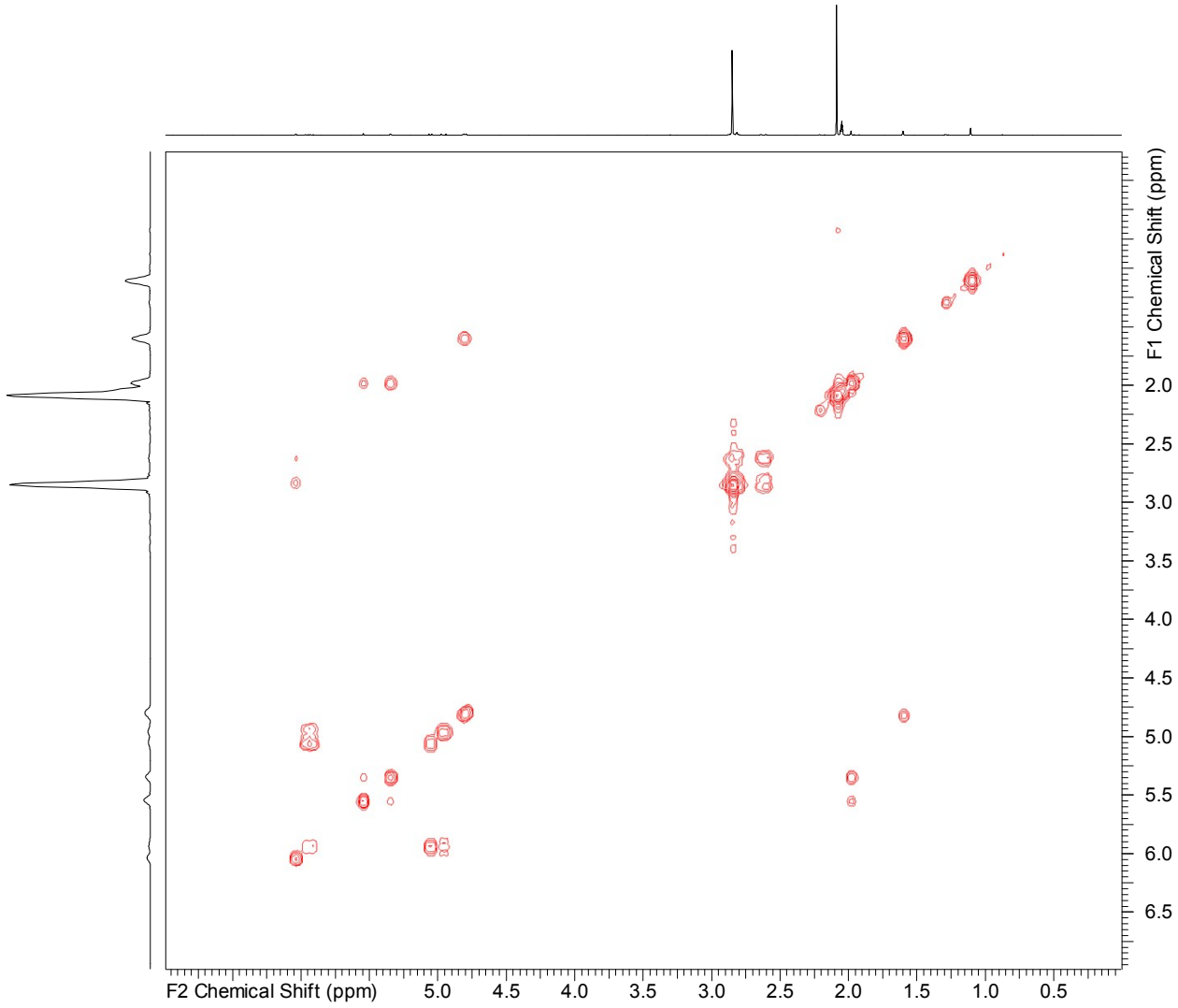


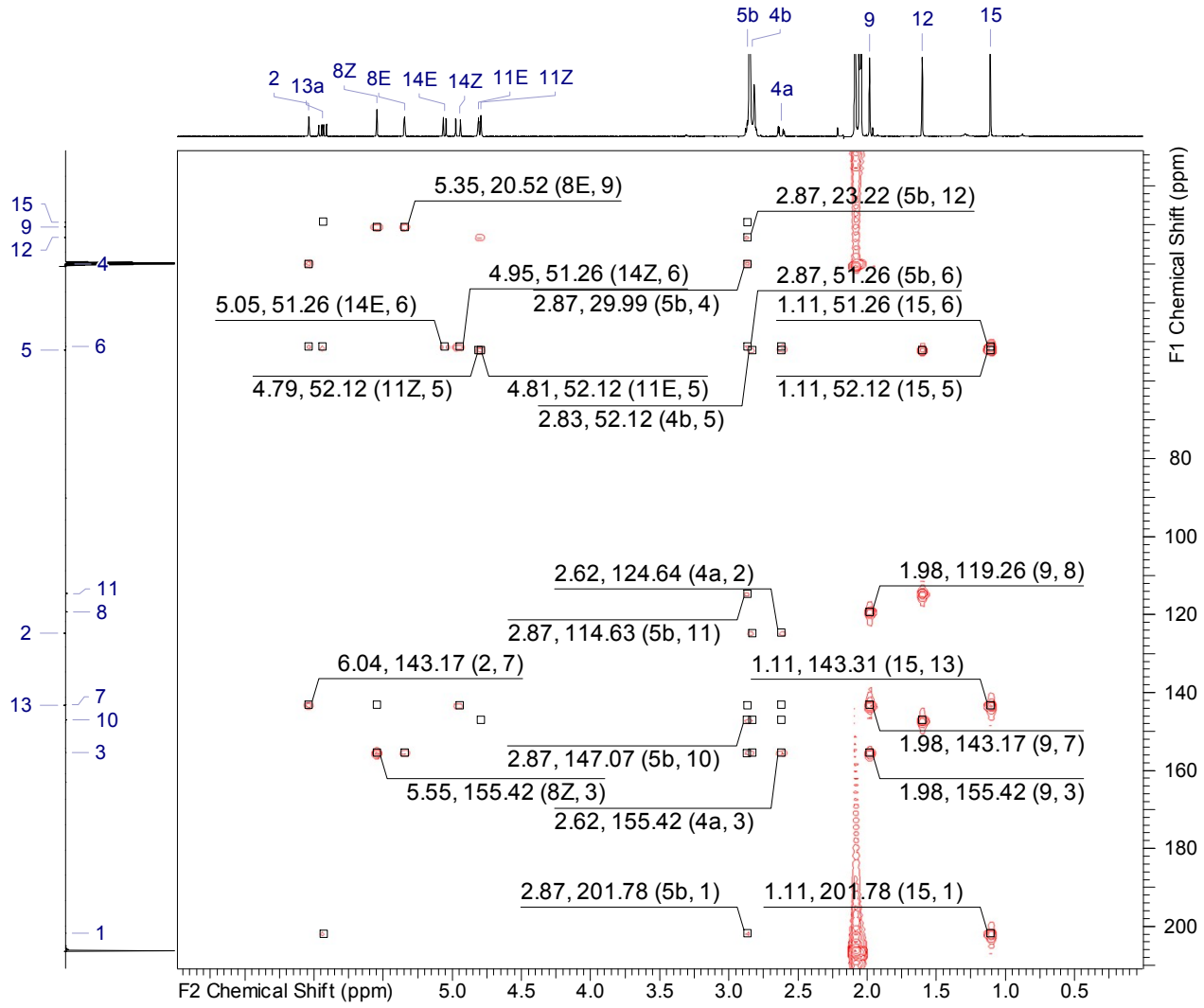
Assignment of the HSQC spots

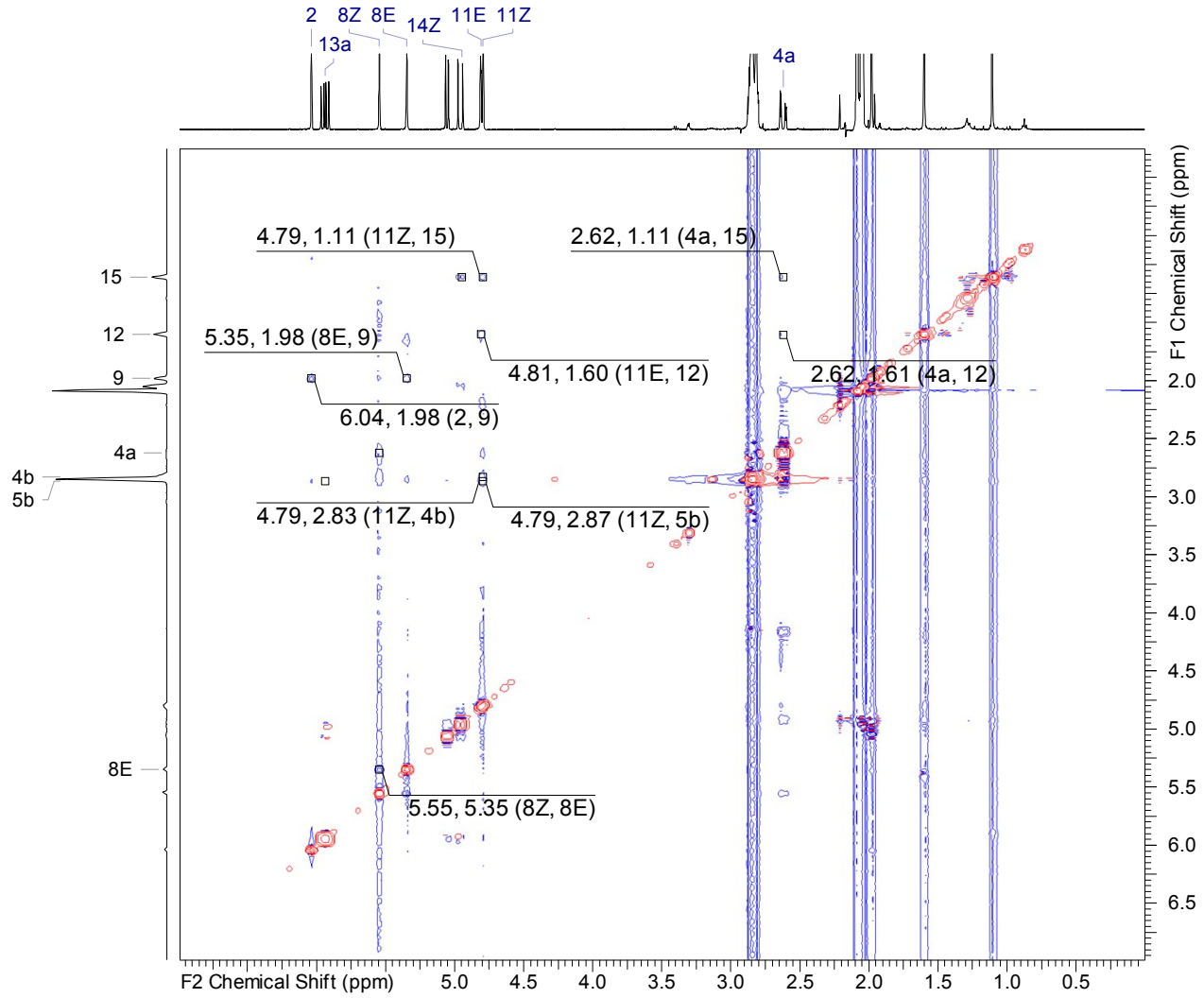
No.	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	2	2	6.04	124.79
2	4a	4	2.62	29.99
3	4b	4	2.83	29.99
4	5b	5	2.87	52.12
5	8E	8	5.35	119.26
6	8Z	8	5.55	119.26
7	9	9	1.98	20.52
8	11E	11	4.81	114.63
9	11Z	11	4.79	114.63
10	12	12	1.60	23.30
11	13a	13	5.94	143.30
12	14E	14	5.05	114.57
13	14Z	14	4.95	114.57
14	15	15	1.11	19.34

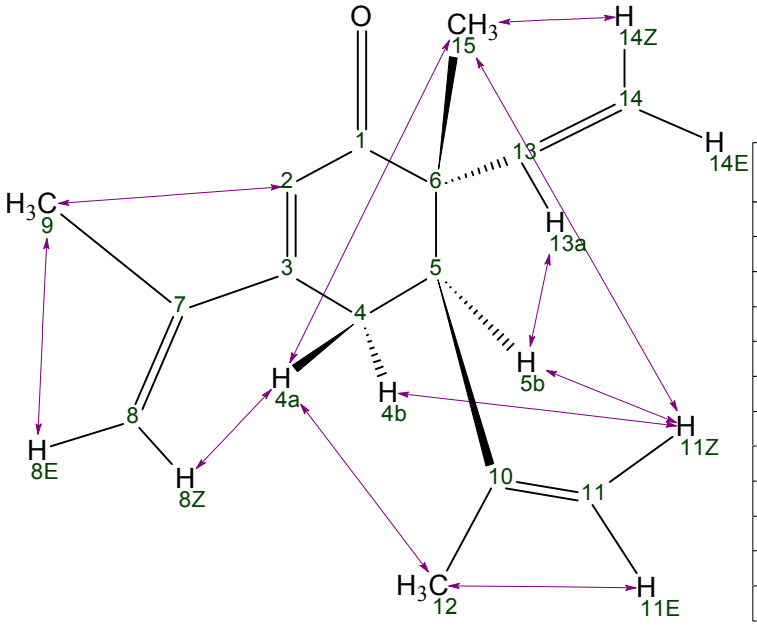

O
CH3
15
H
14Z
14
H
14E
1
13
2
6
H
13a
H3C
9
3
5
7
4
H
5b
H
4a
H
4b
8
H
11Z
H
8E
H
8Z
10
11
H3C
12
H
11E


O
CH3
15
H
14Z
14
H
14E
1
13
2
6
H
13a
H3C
9
3
5
7
4
H
5b
H
4a
H
4b
8
H
11Z
H
8E
H
8Z
10
11
H3C
12
H
11E

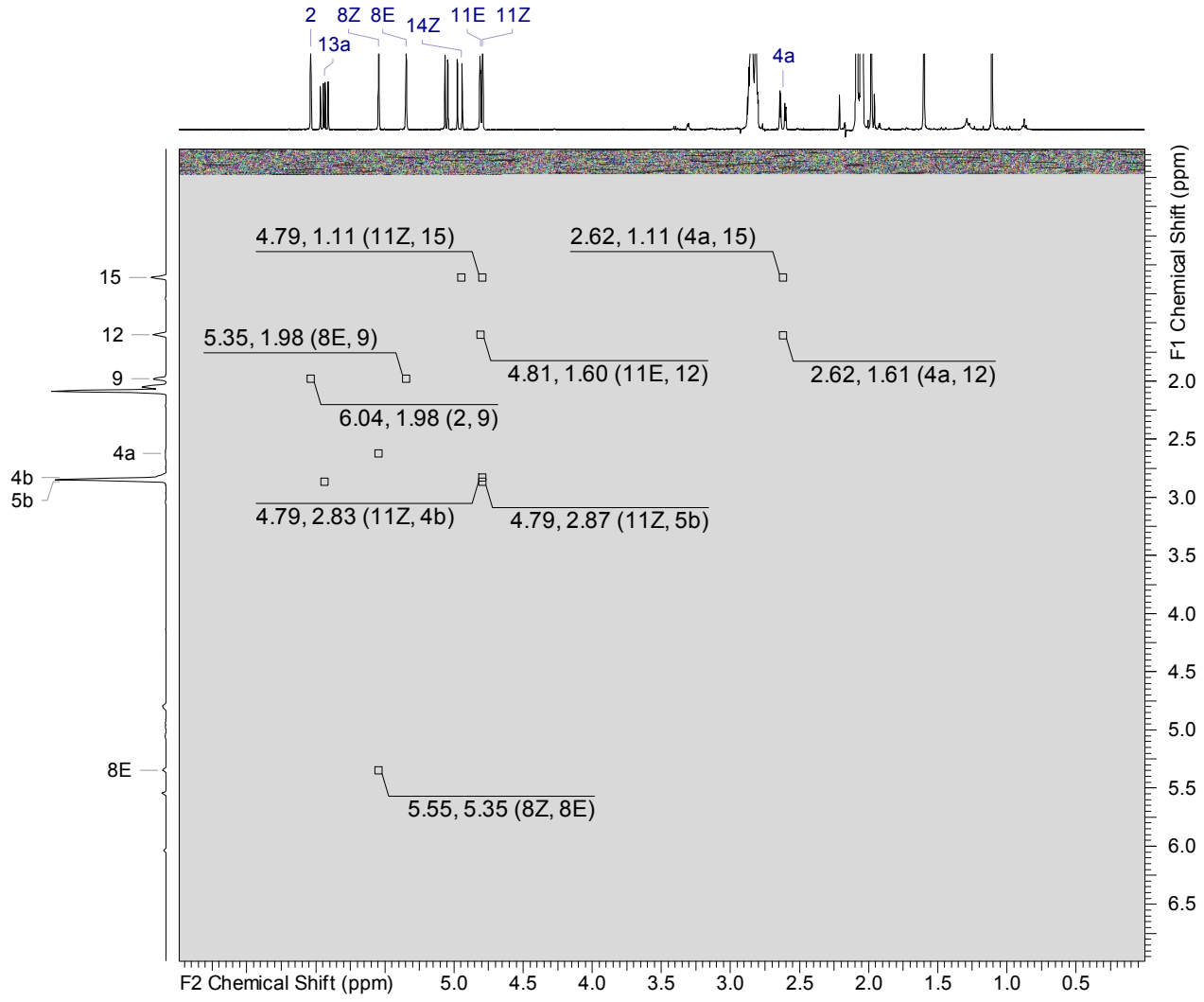

F1 Chemical Shift (ppm)
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
F2 Chemical Shift (ppm)
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

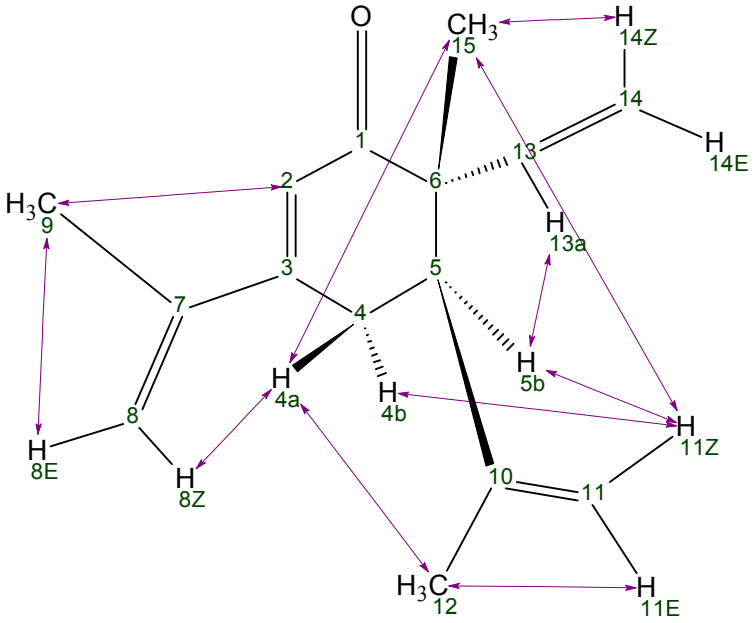

2
13a
8Z
8E
14E
14Z
11E
11Z
5b
4b
4a
9
12
15
5.35, 20.52 (8E, 9)
2.87, 23.22 (5b, 12)
4.95, 51.26 (14Z, 6)
2.87, 29.99 (5b, 4)
2.87, 51.26 (5b, 6)
5.05, 51.26 (14E, 6)
1.11, 51.26 (15, 6)
4.79, 52.12 (11Z, 5)
4.81, 52.12 (11E, 5)
1.11, 52.12 (15, 5)
2.83, 52.12 (4b, 5)
2.62, 124.64 (4a, 2)
1.98, 119.26 (9, 8)
2.87, 114.63 (5b, 11)
6.04, 143.17 (2, 7)
1.11, 143.31 (15, 13)
1.98, 143.17 (9, 7)
2.87, 147.07 (5b, 10)
5.55, 155.42 (8Z, 3)
1.98, 155.42 (9, 3)
2.62, 155.42 (4a, 3)
2.87, 201.78 (5b, 1)
1.11, 201.78 (15, 1)
F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)





No.	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	8Z	4a	5.55	2.62
2	11Z	4b	4.79	2.83
3	11Z	5b	4.79	2.87
4	13a	5b	5.94	2.87
5	8Z	8E	5.55	5.35
6	2	9	6.04	1.98
7	8E	9	5.35	1.98
8	4a	12	2.62	1.61
9	11E	12	4.81	1.60
10	4a	15	2.62	1.11
11	11Z	15	4.79	1.11
12	14Z	15	4.95	1.11


2
8Z
8E
14Z
11E
11Z
13a
4a
4.79, 1.11 (11Z, 15)
2.62, 1.11 (4a, 15)
5.35, 1.98 (8E, 9)
4.81, 1.60 (11E, 12)
2.62, 1.61 (4a, 12)
6.04, 1.98 (2, 9)
4.79, 2.83 (11Z, 4b)
4.79, 2.87 (11Z, 5b)
5.55, 5.35 (8Z, 8E)
15
12
9
4a
4b
5b
8E
F1 Chemical Shift (ppm)
F2 Chemical Shift (ppm)


O
CH3
15
H
14Z
14
H
14E
1
13
6
2
H3C
9
H
13a
3
5
7
4
H
5b
H
4a
H
4b
8
H
11Z
H
8E
H
8Z
10
11
H3C
12
H
11E