

Expedient Synthesis of Nitrovinyl Substituted Bicyclo[2.2.2]octenone Scaffolds

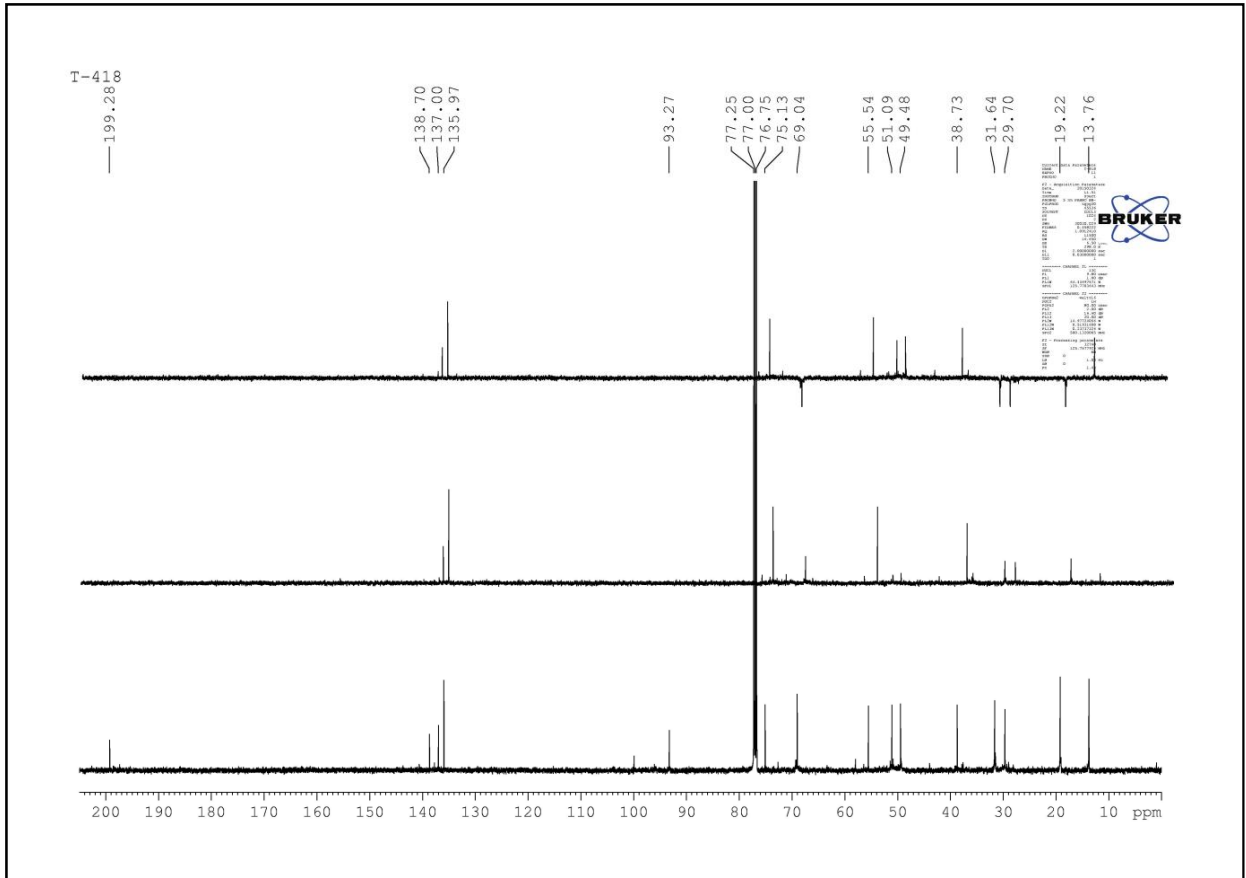
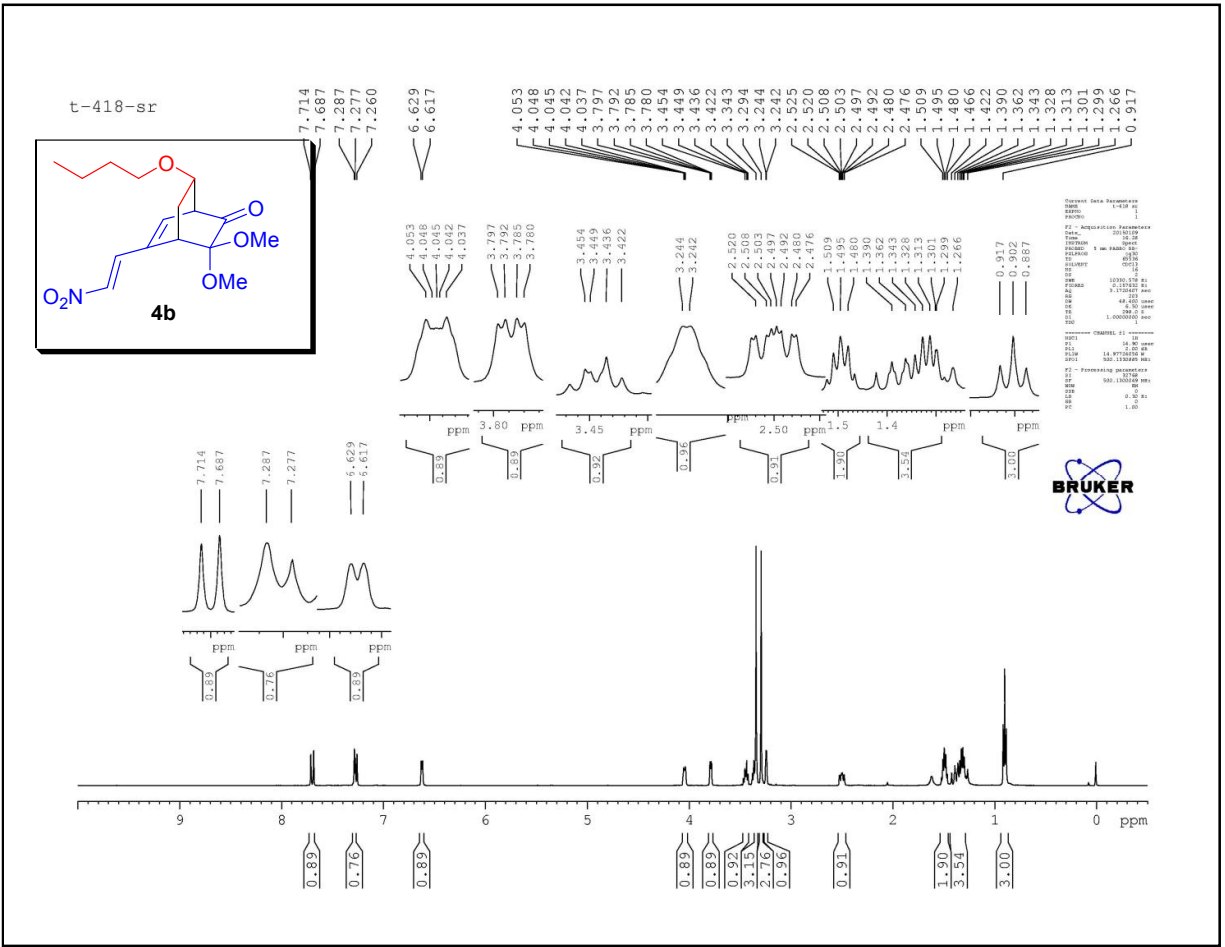
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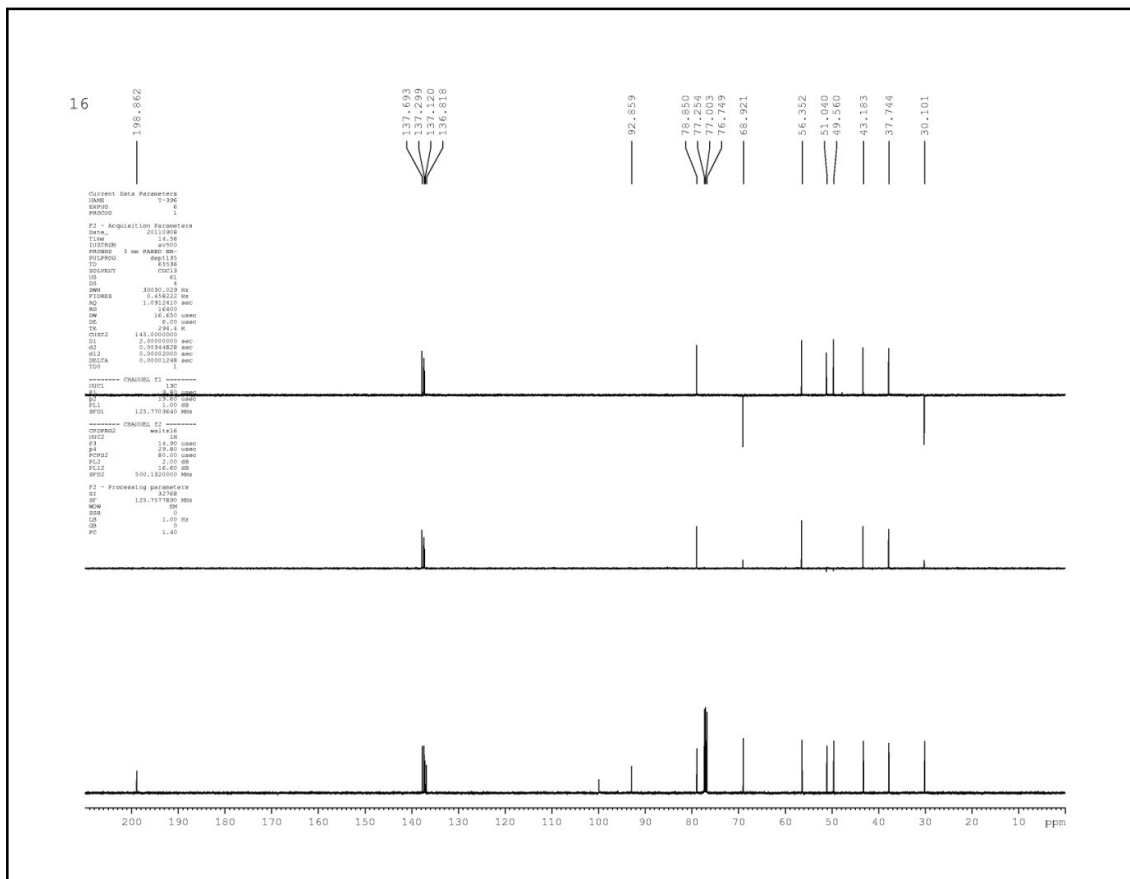
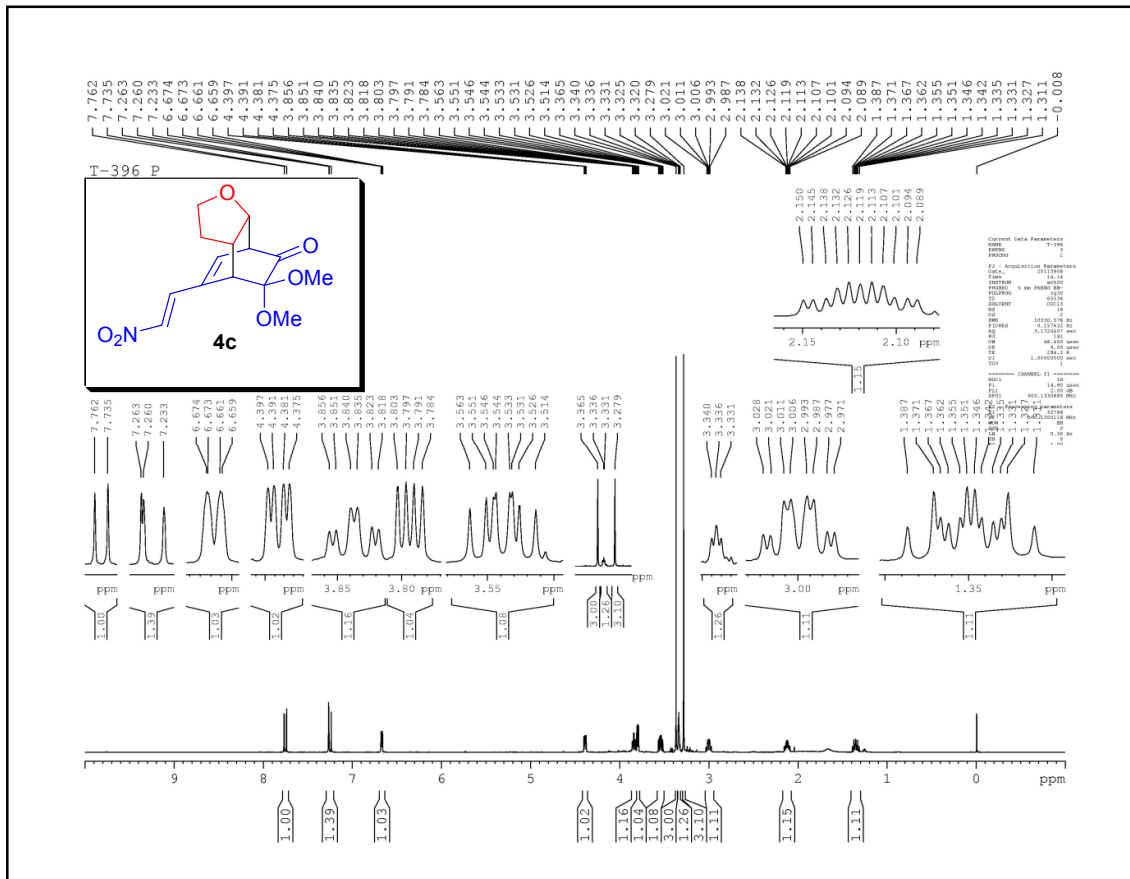
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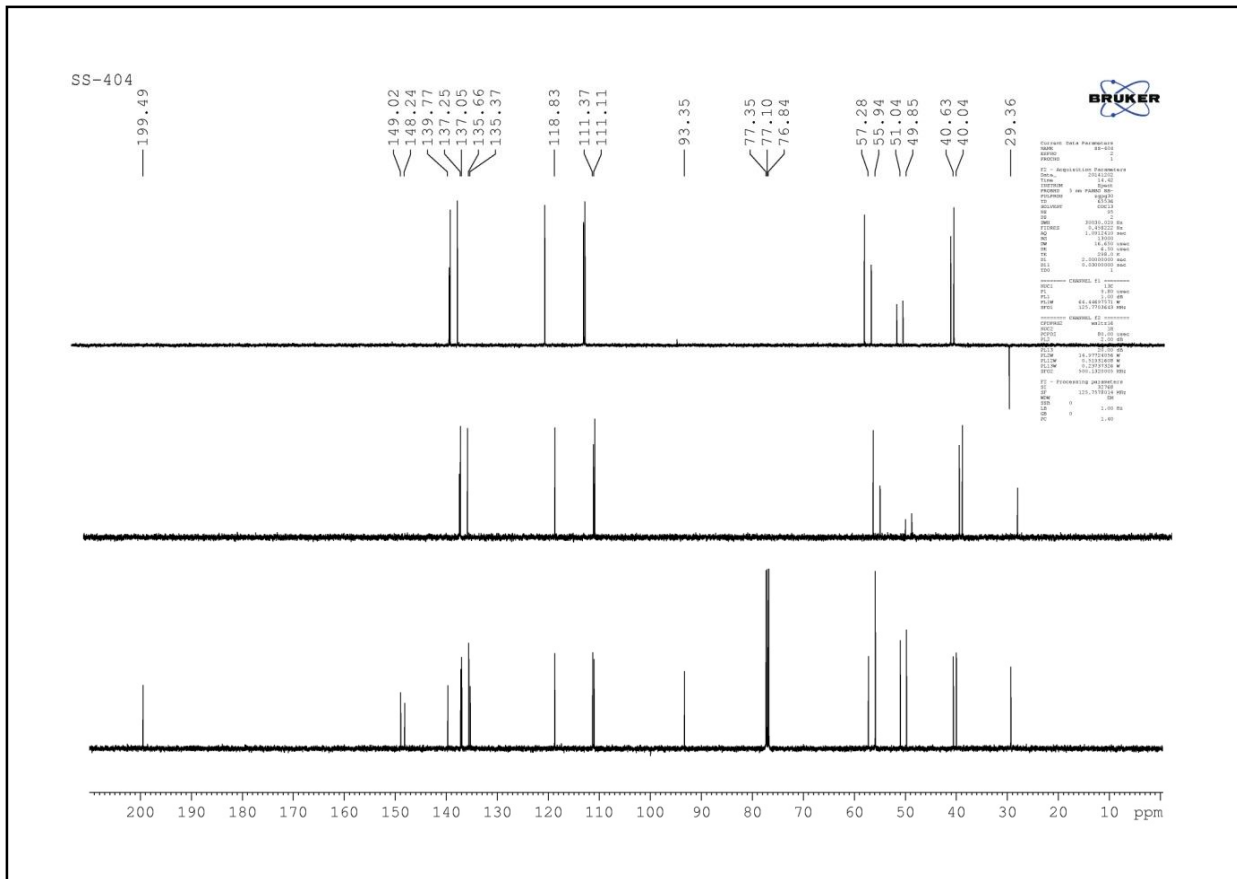
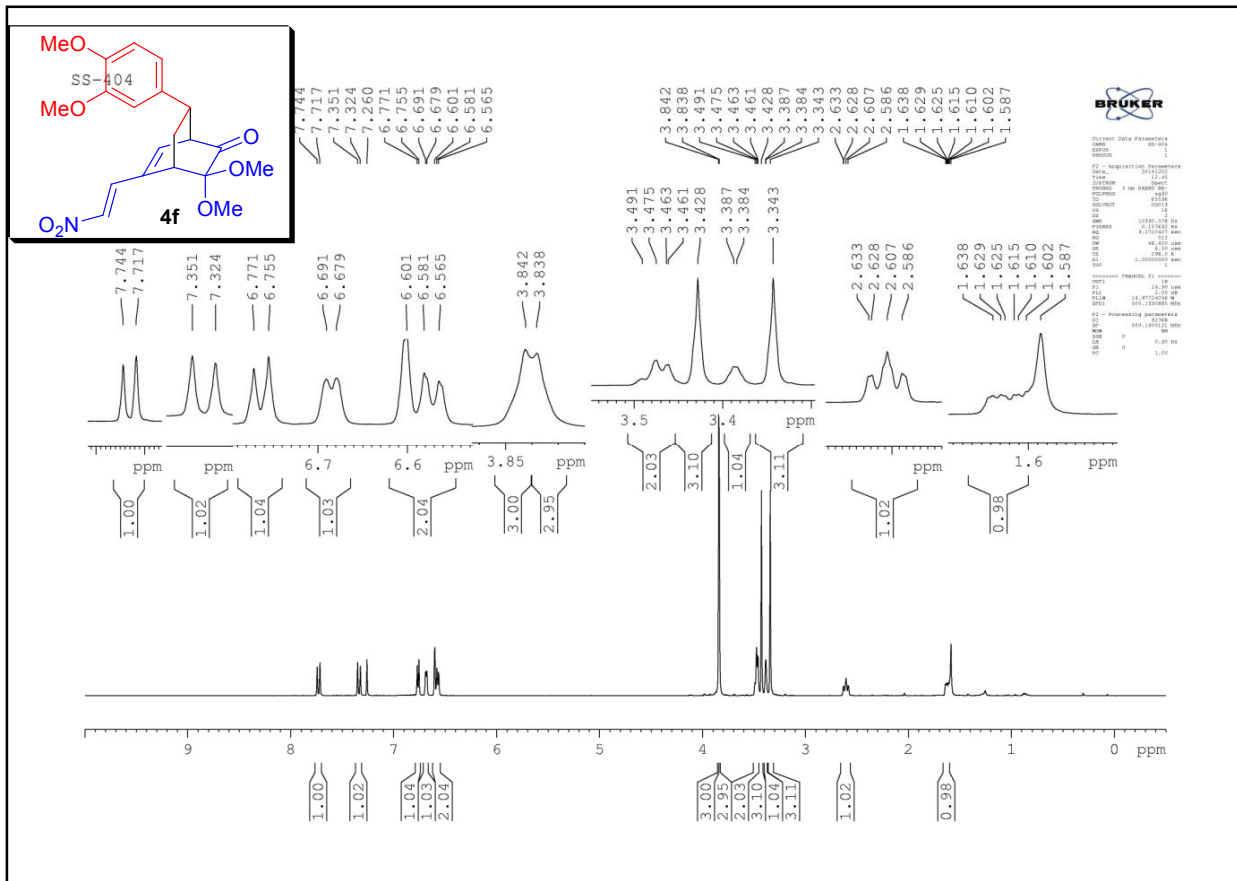
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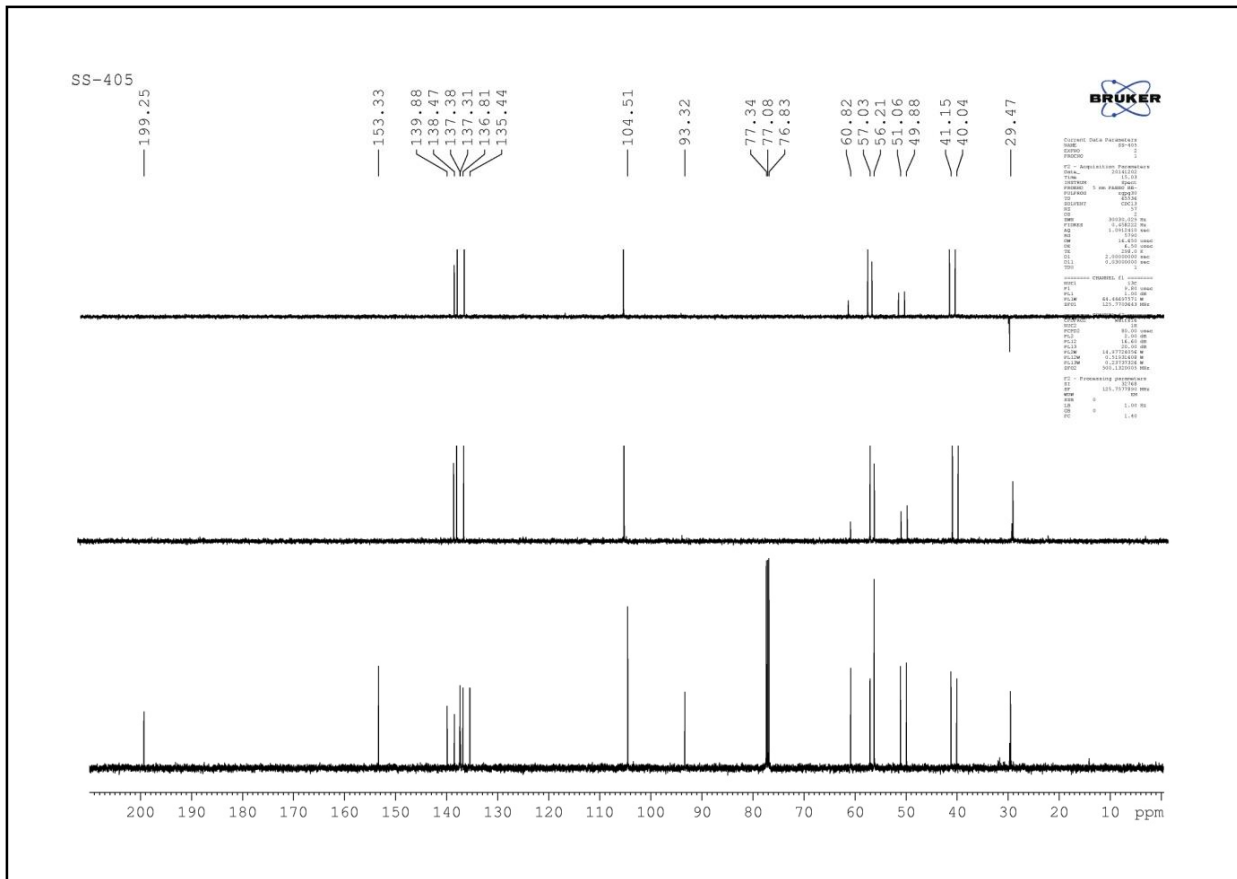
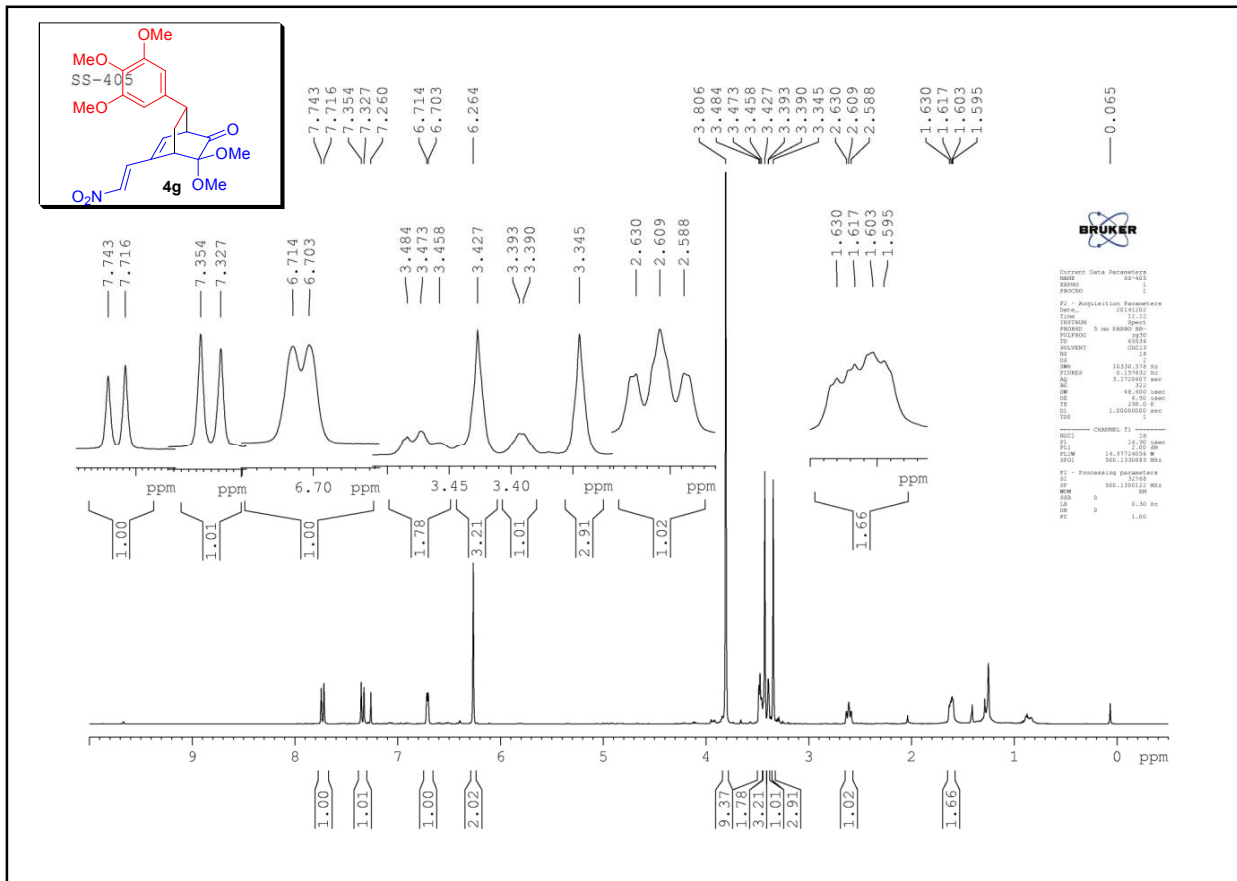
ELECTRONIC SUPPLEMENTARY INFORMATION

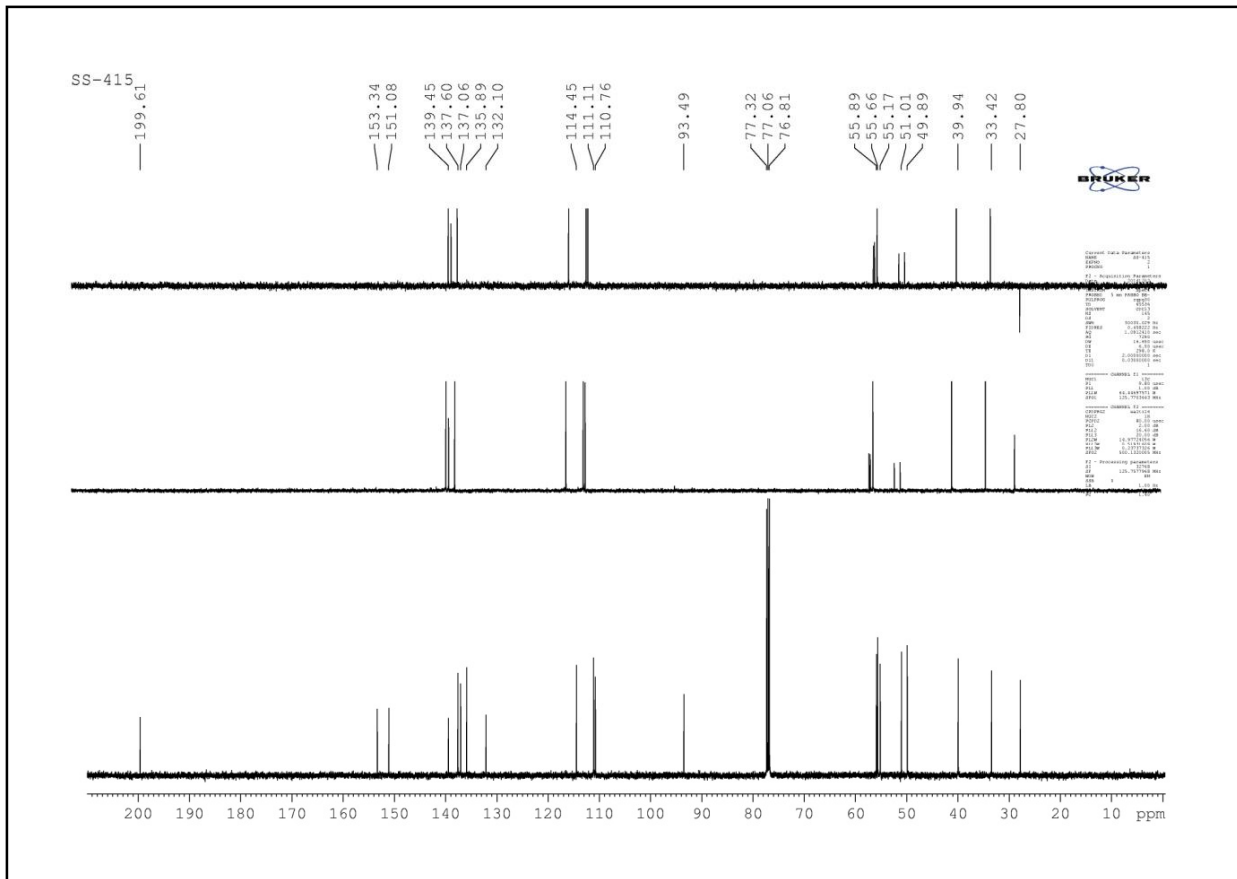
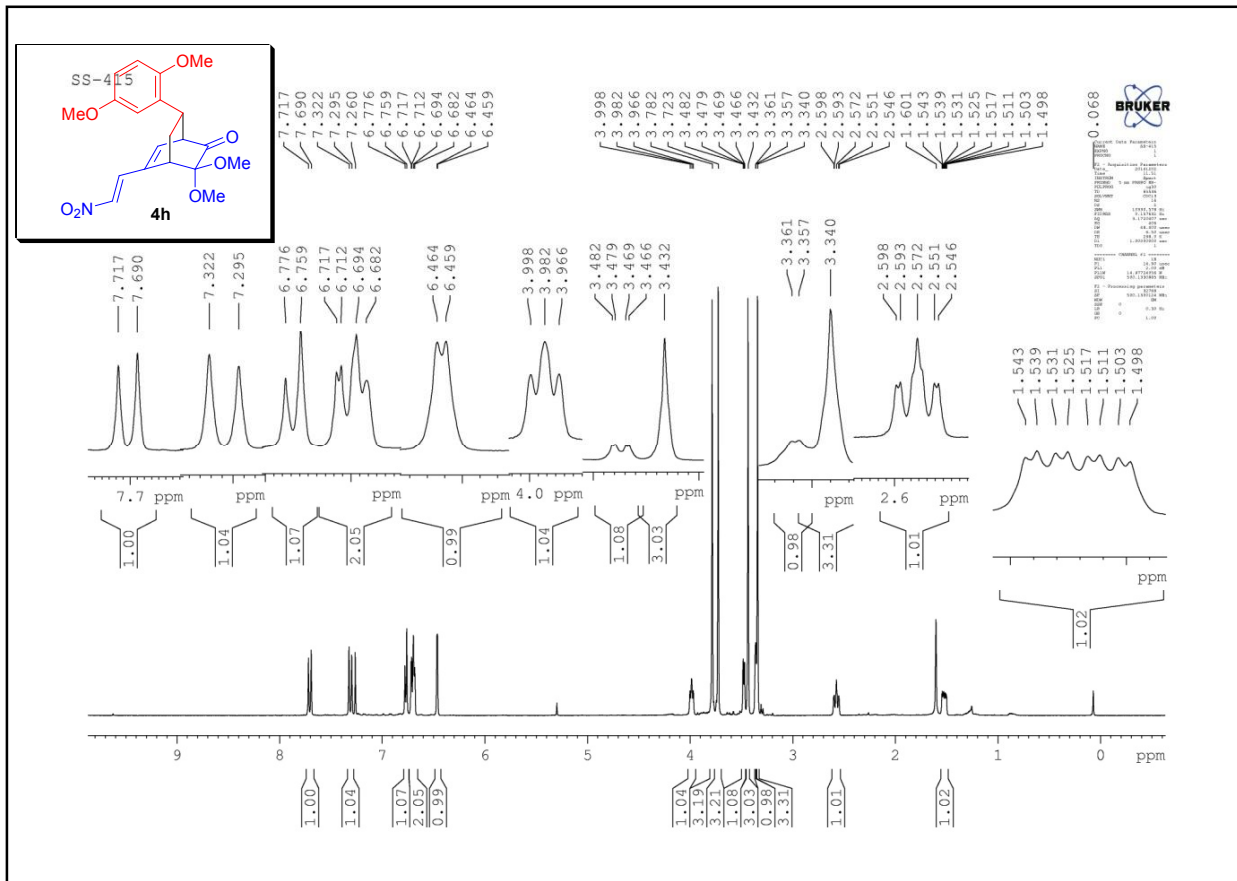
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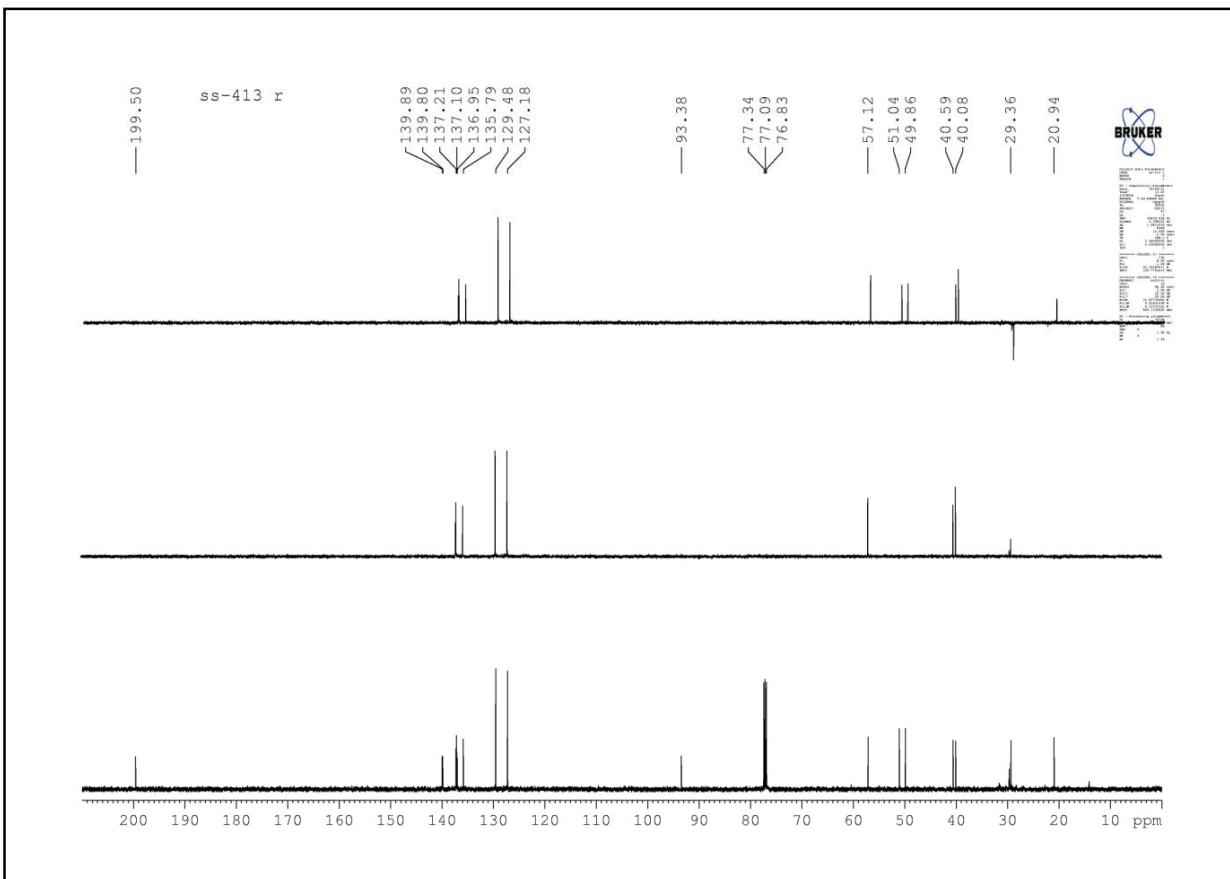
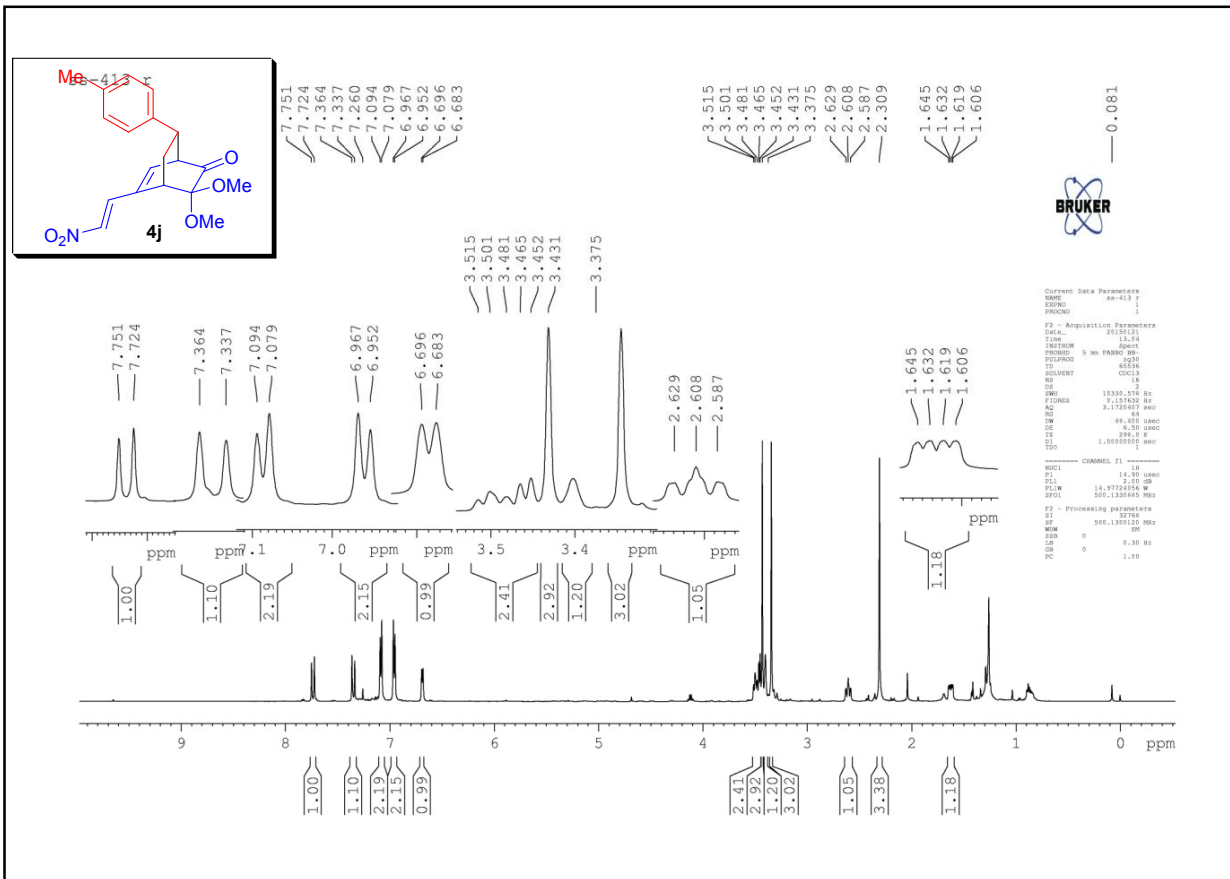


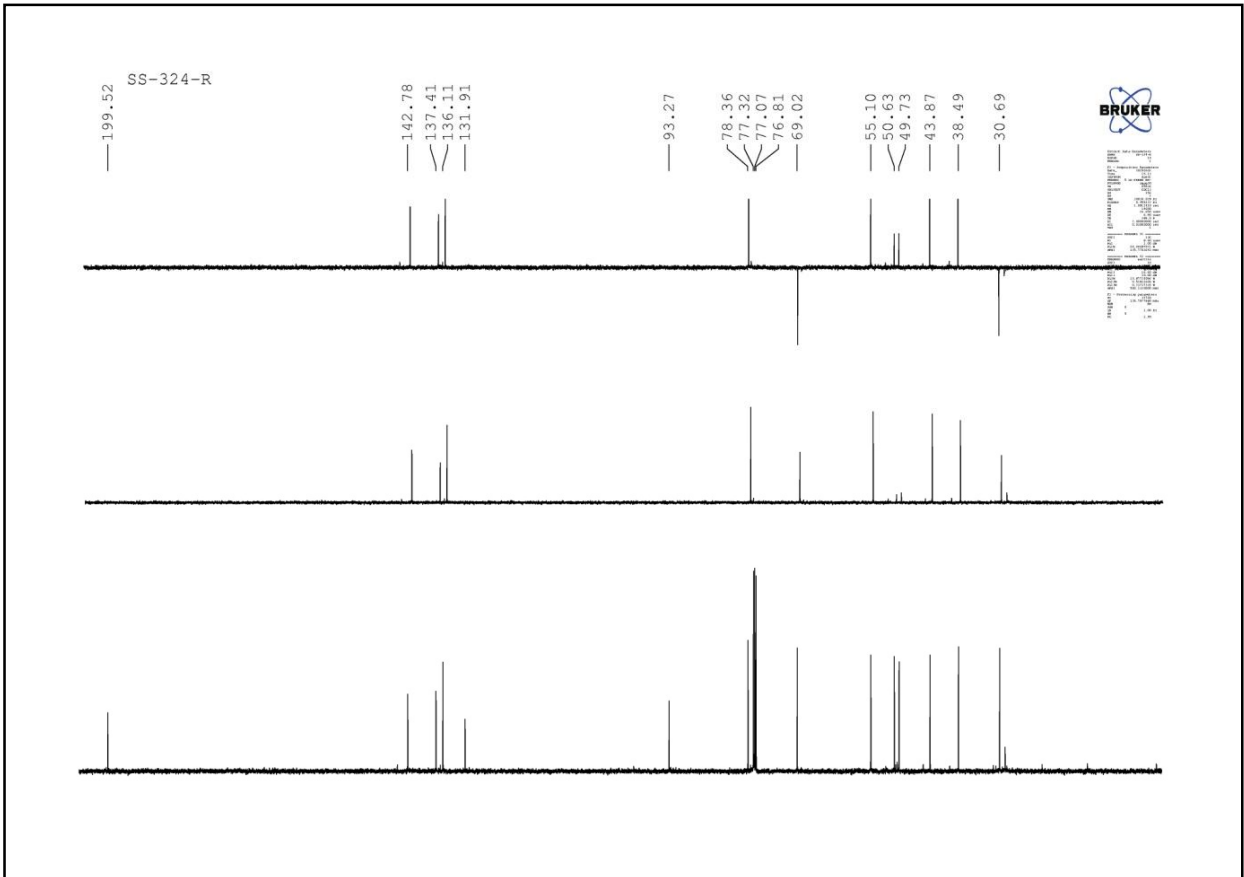


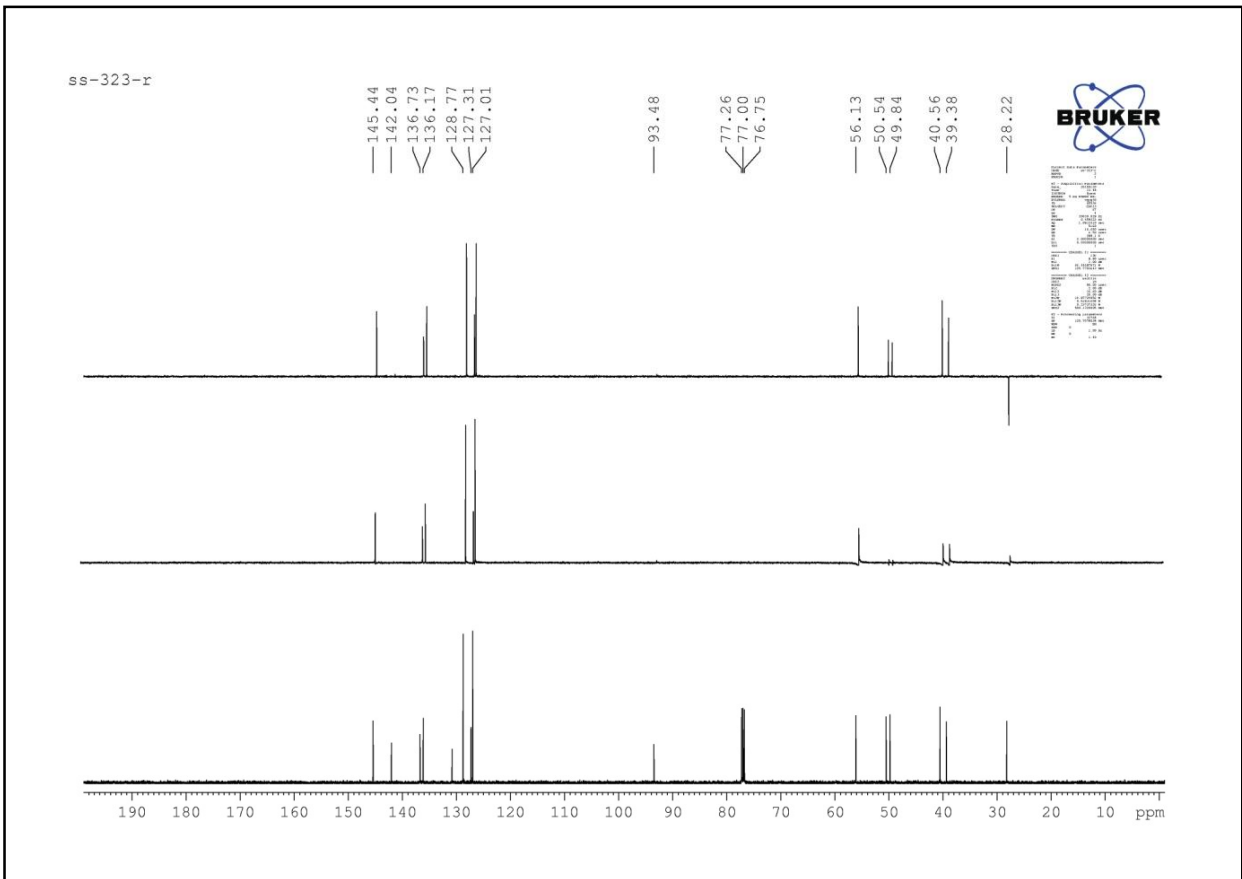
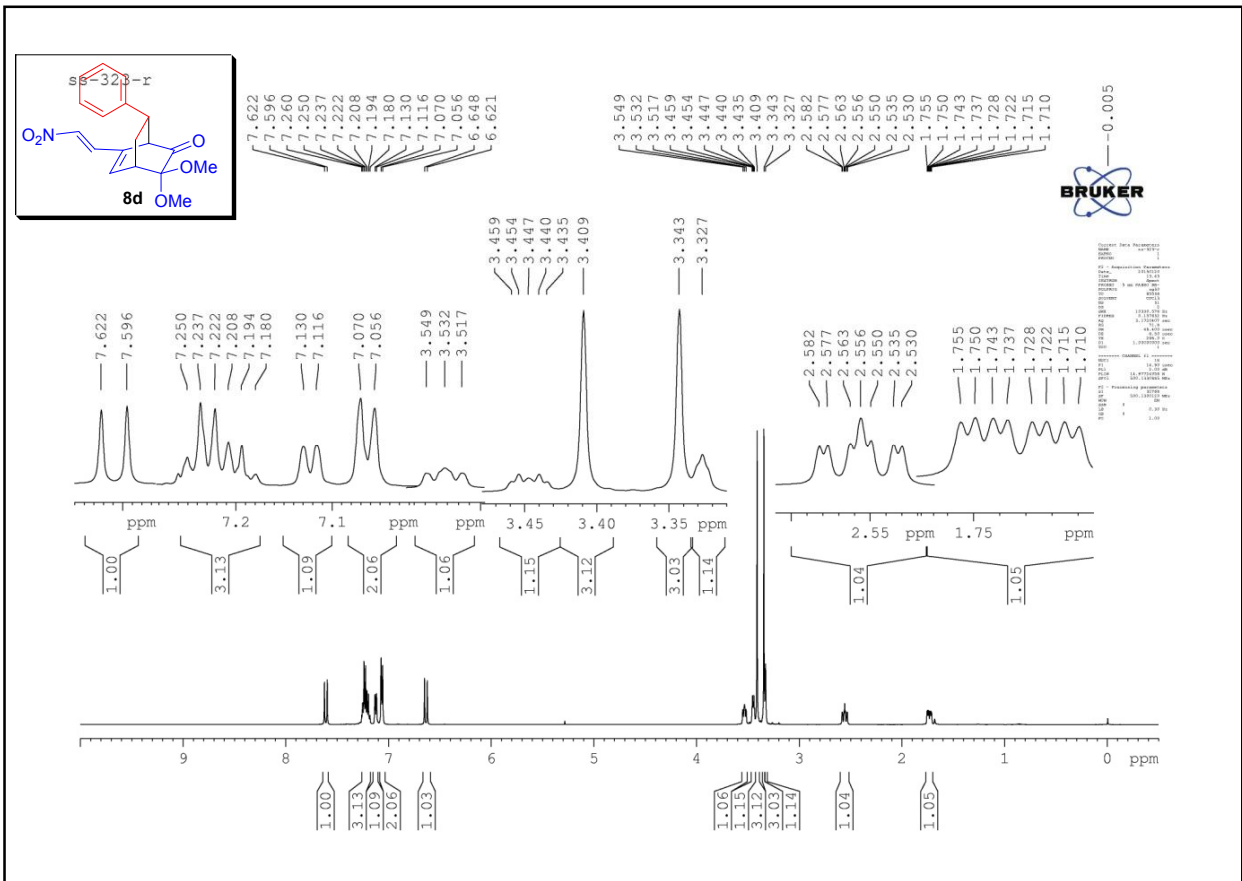


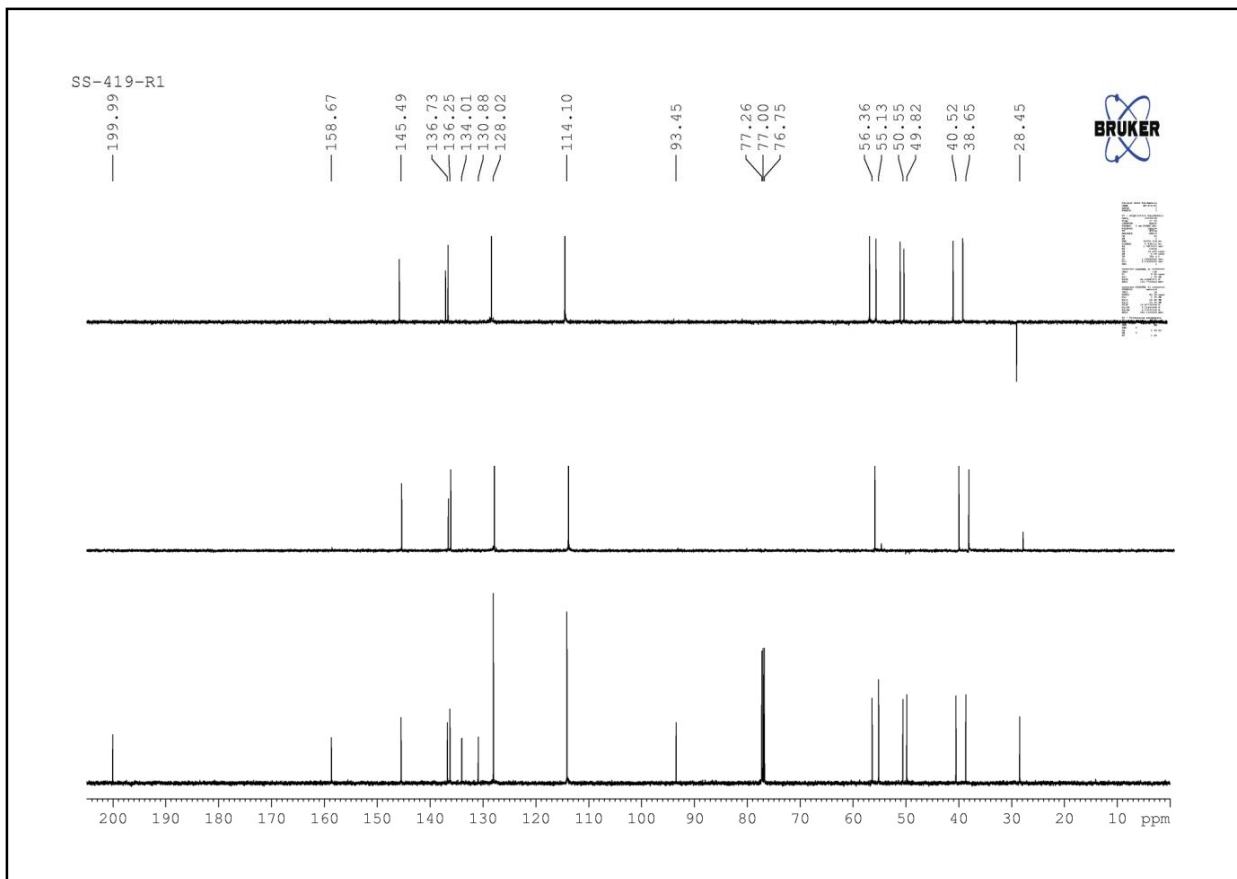
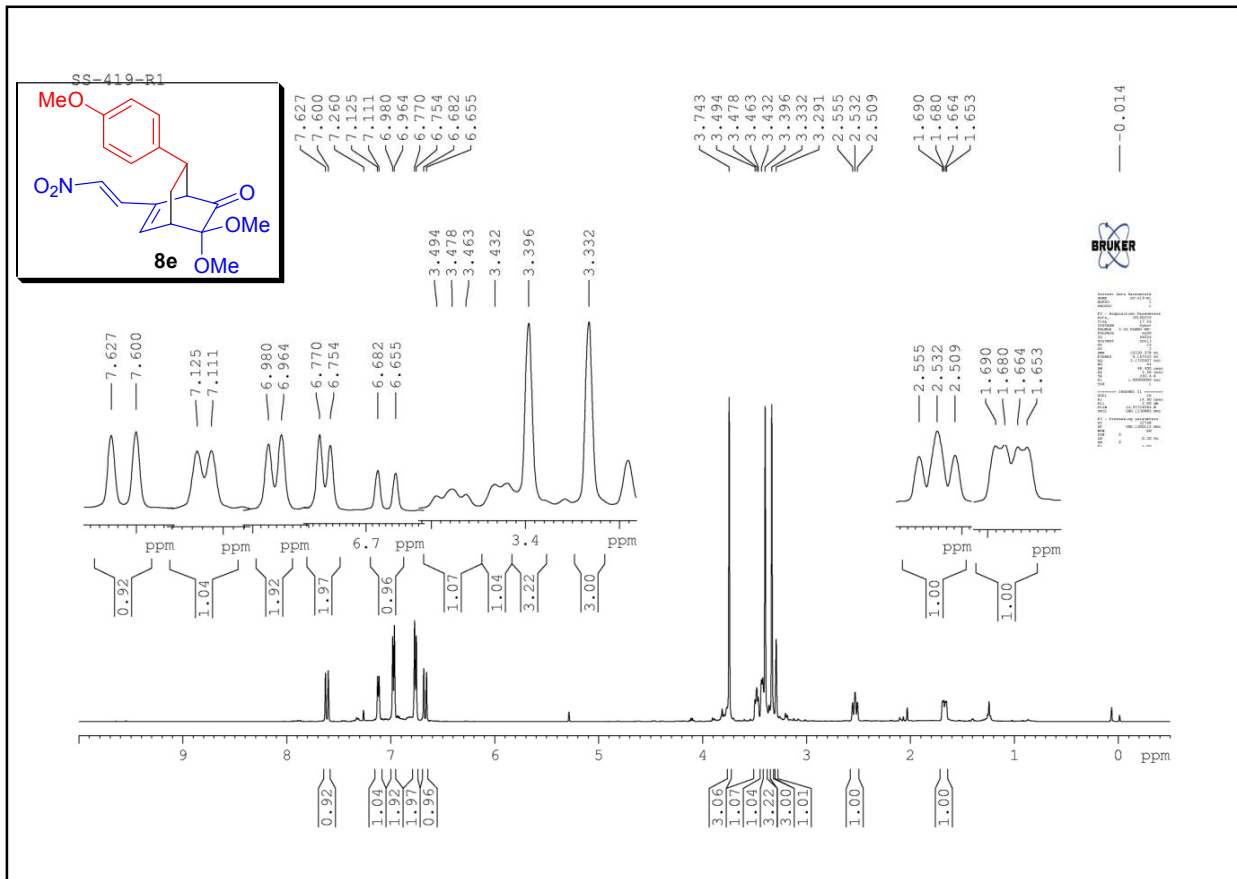


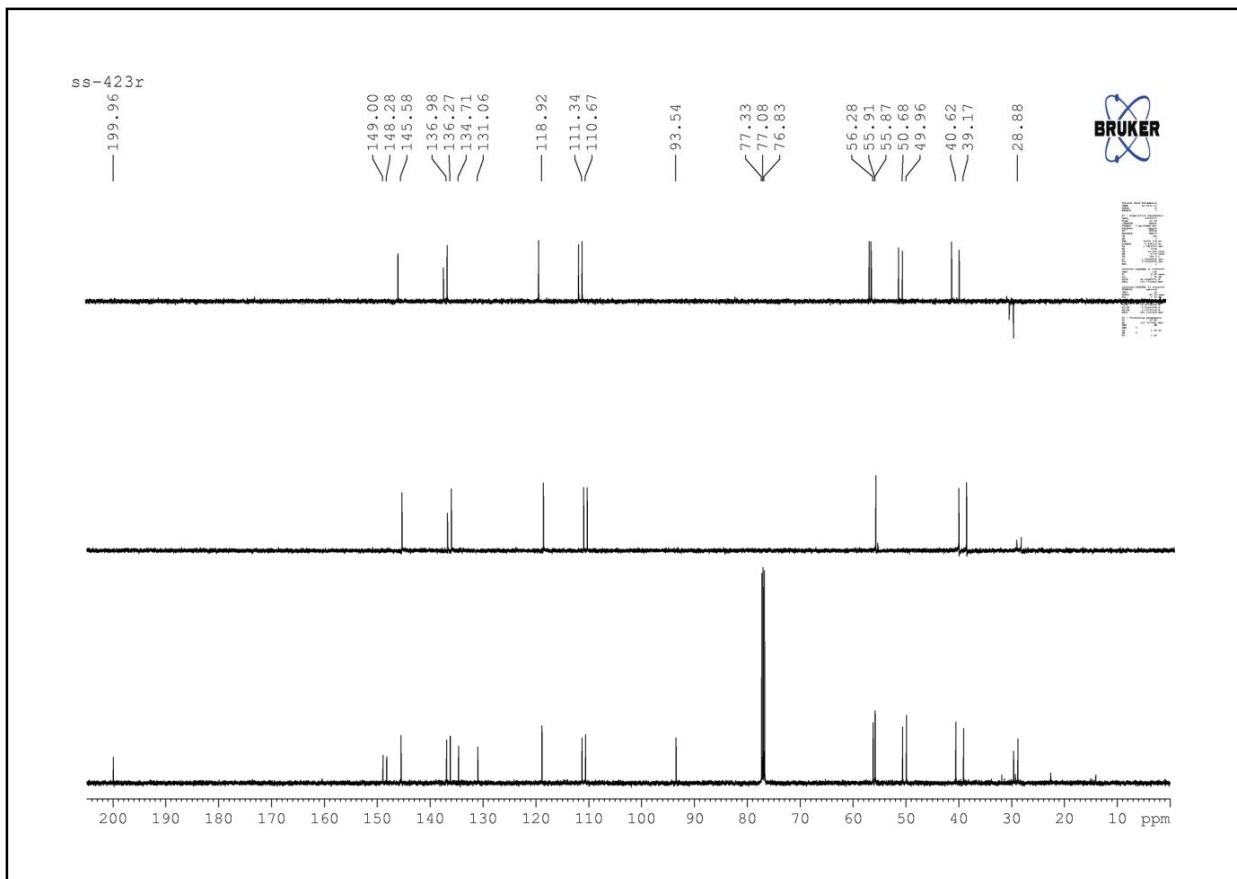
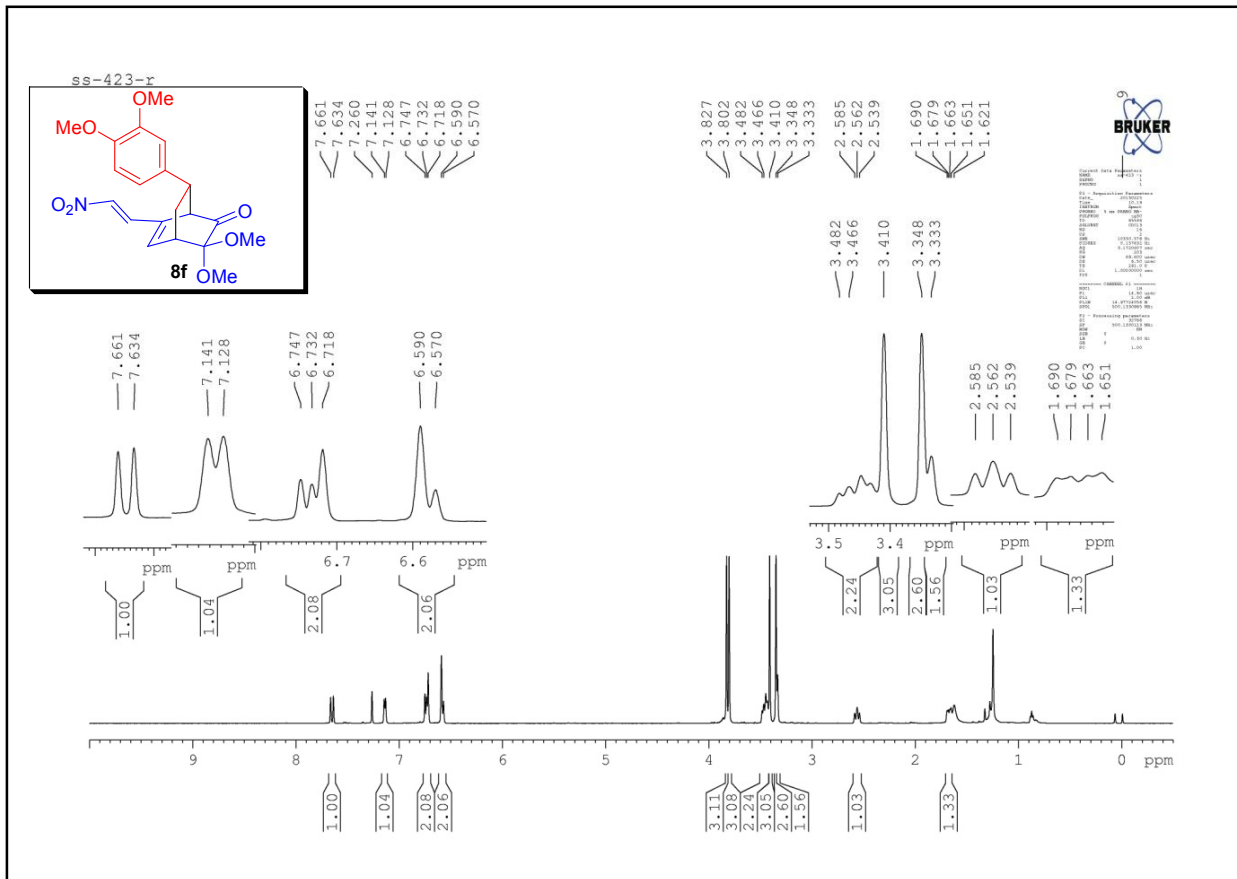


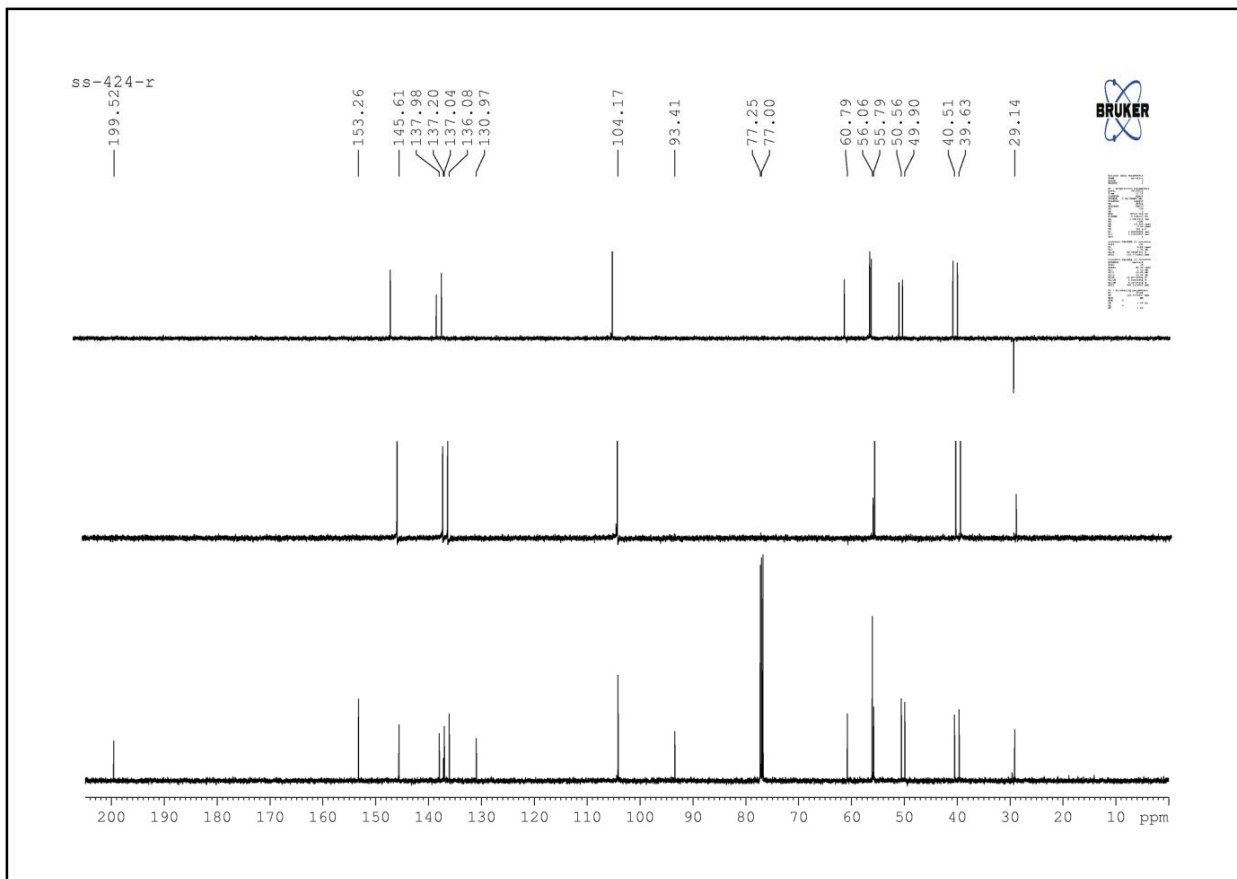
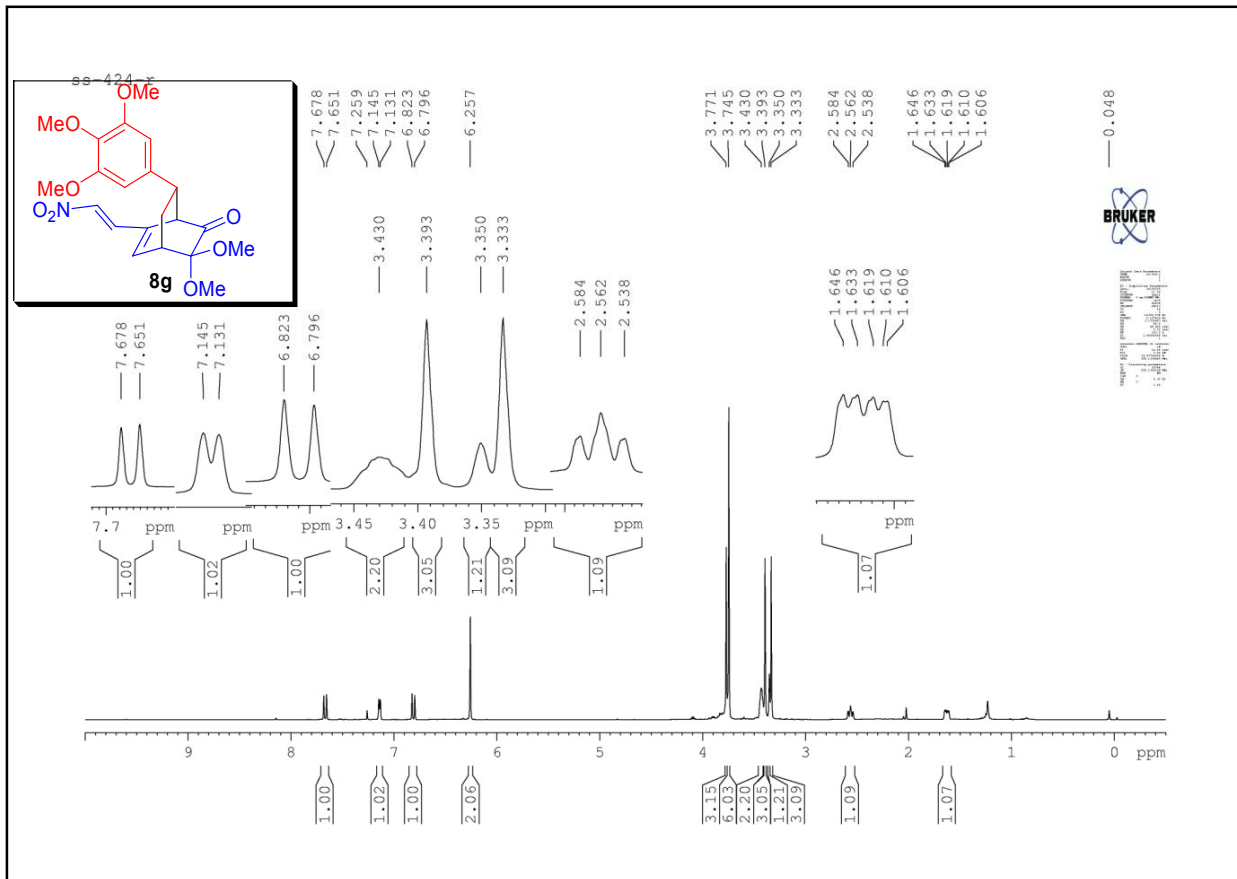


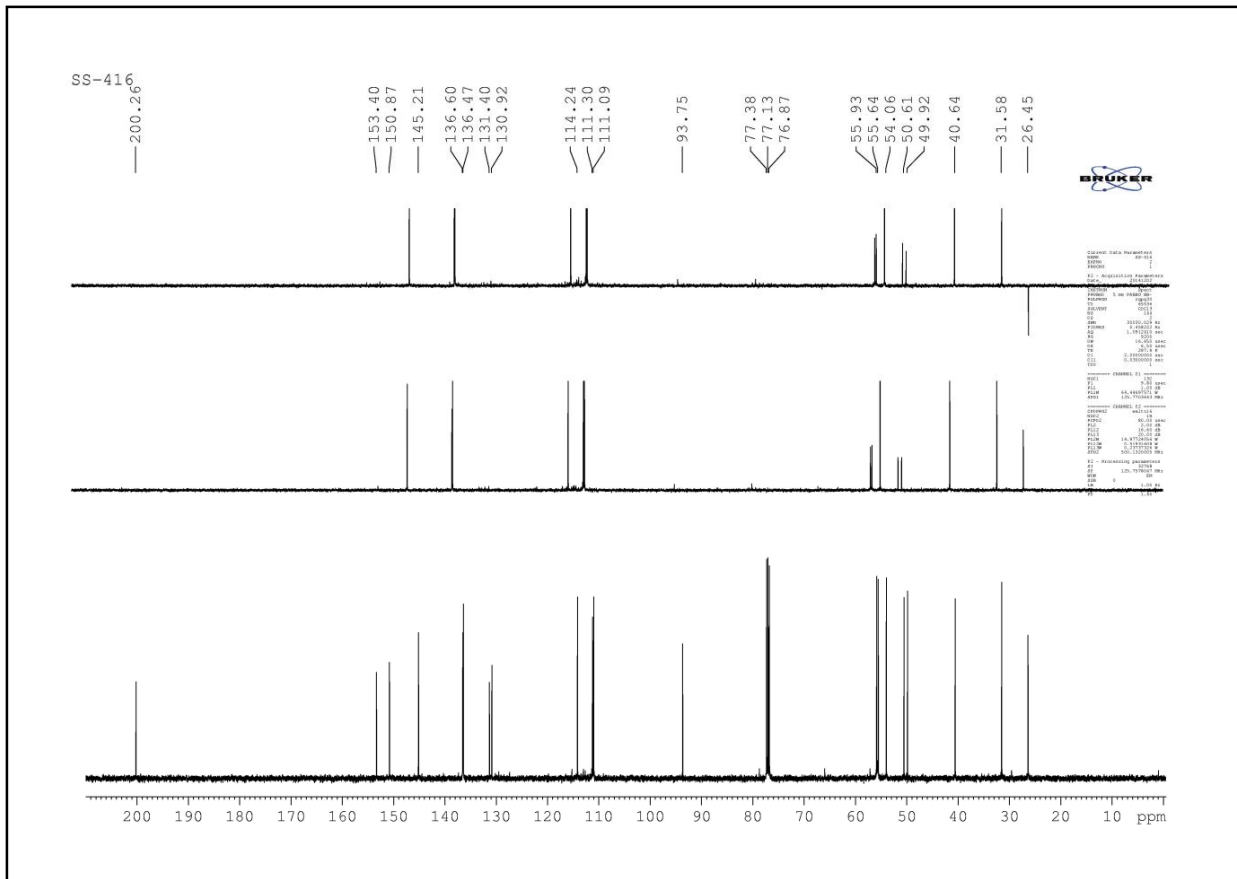
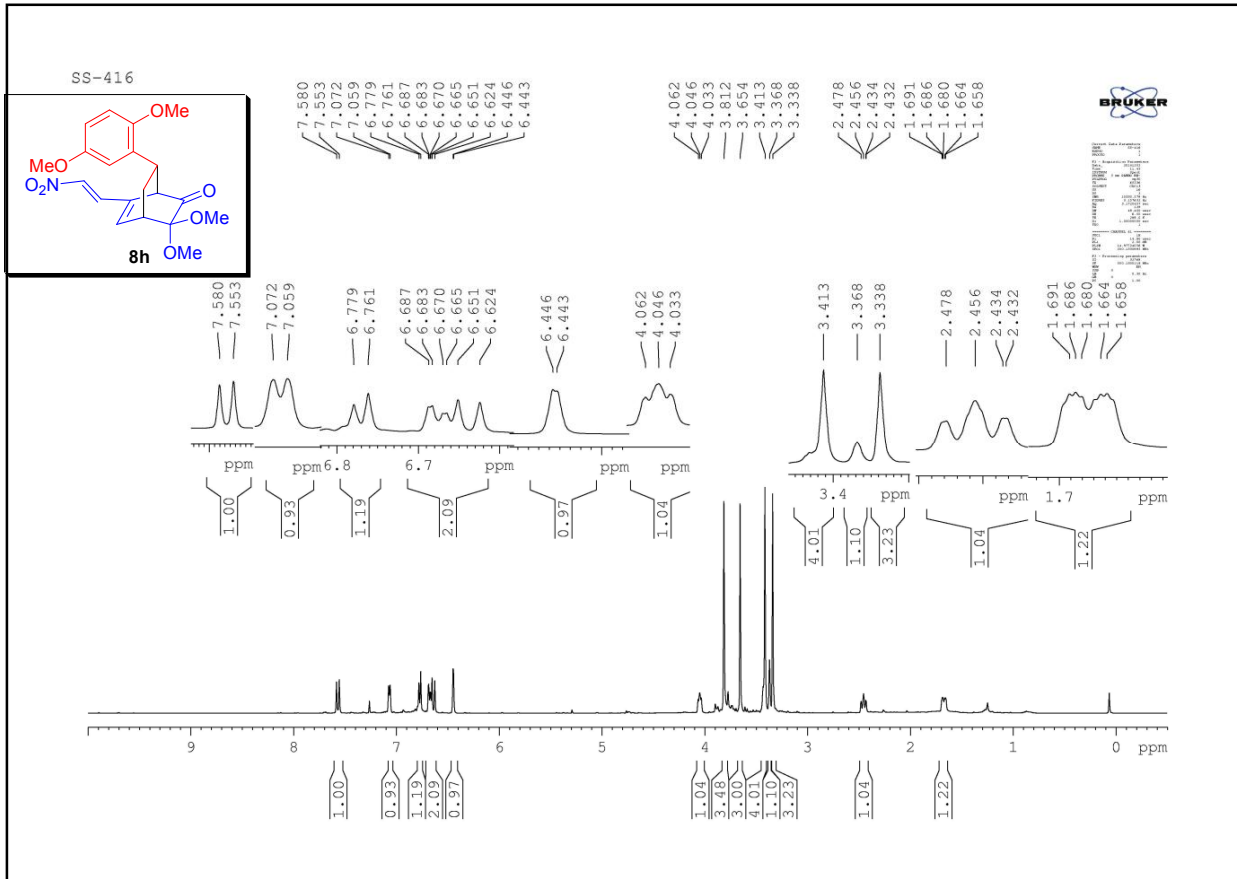


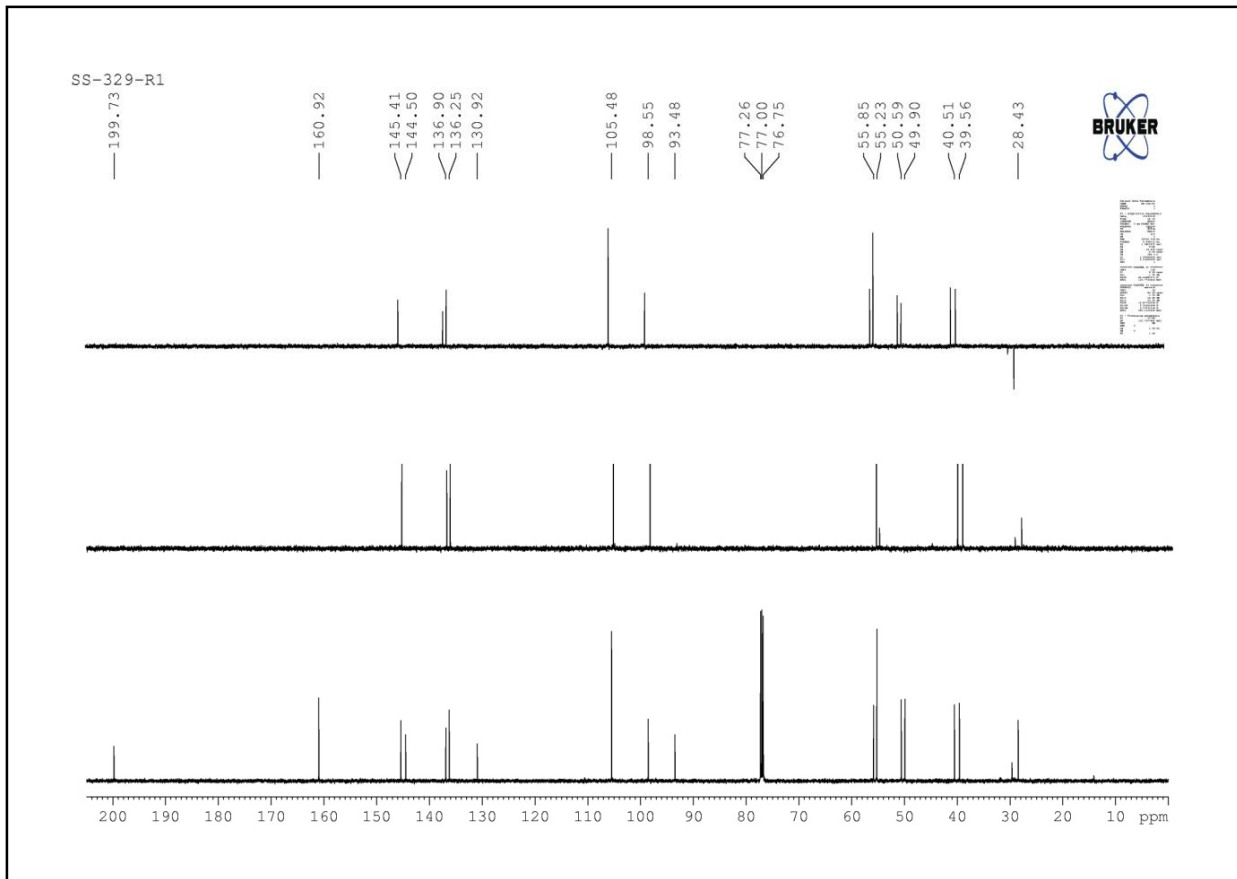
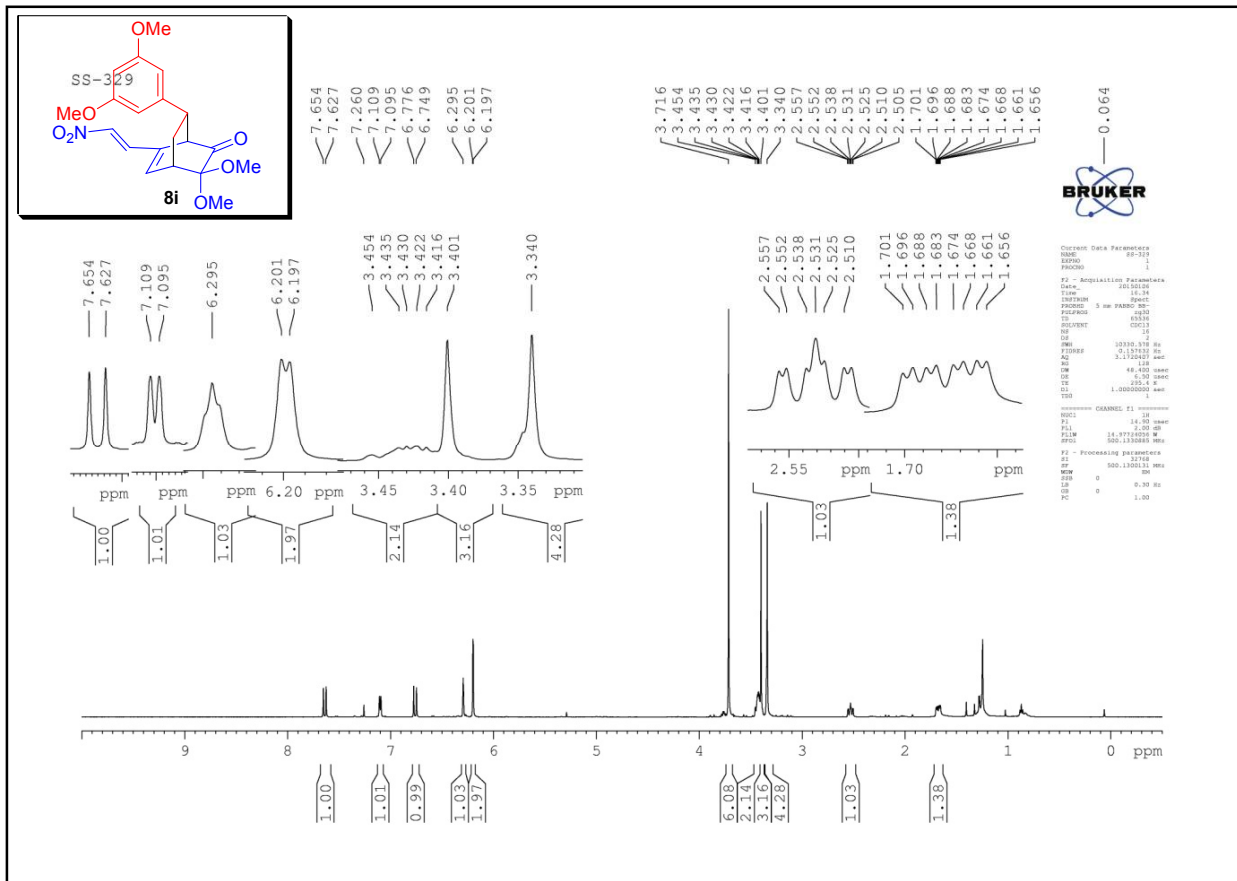


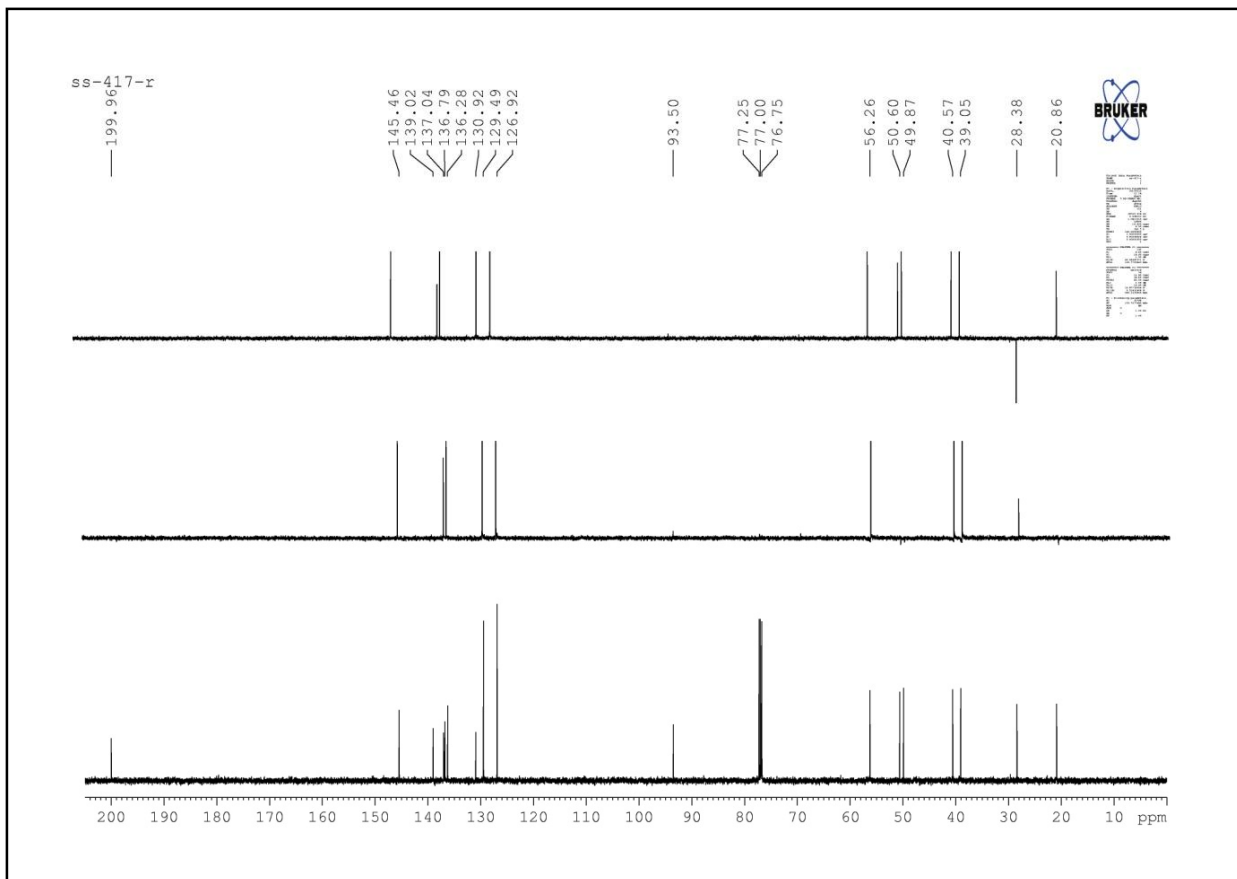
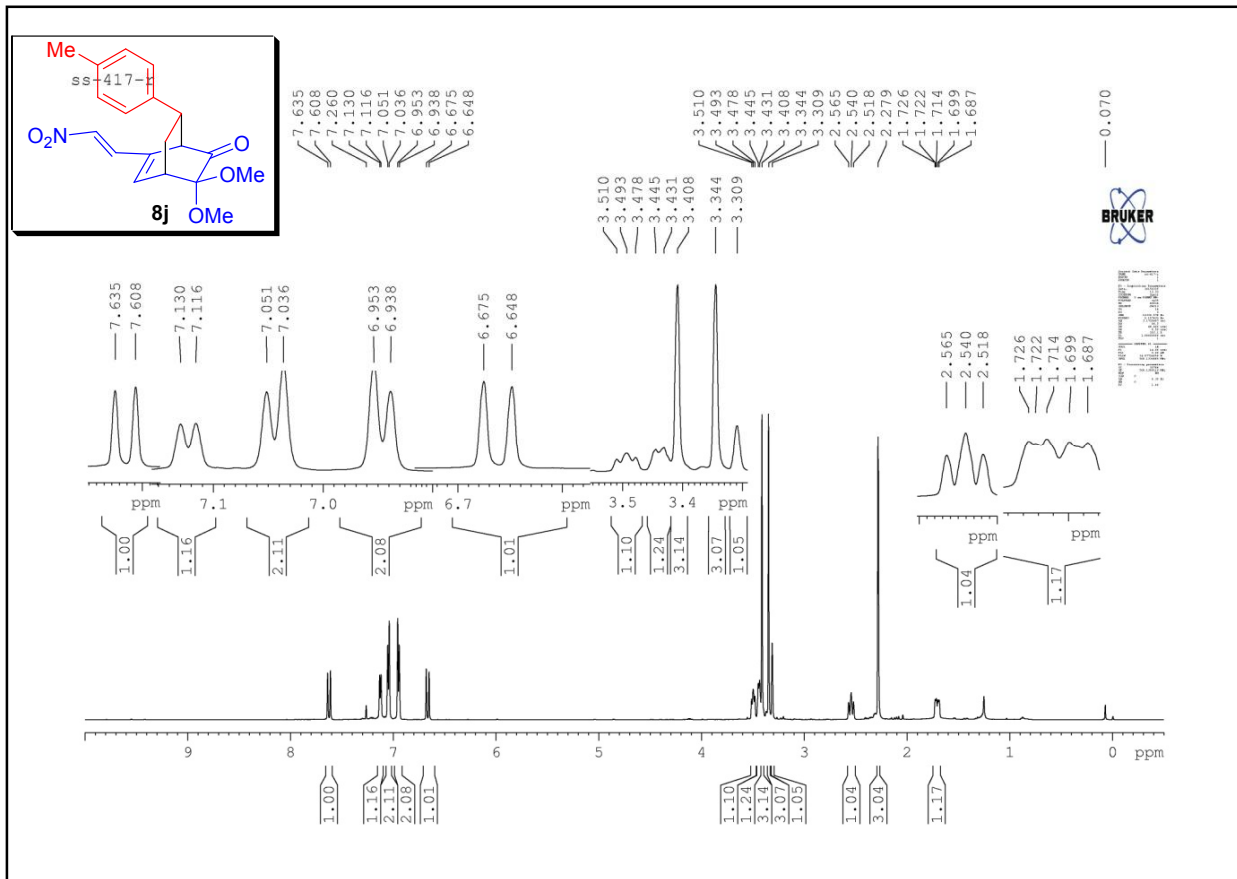




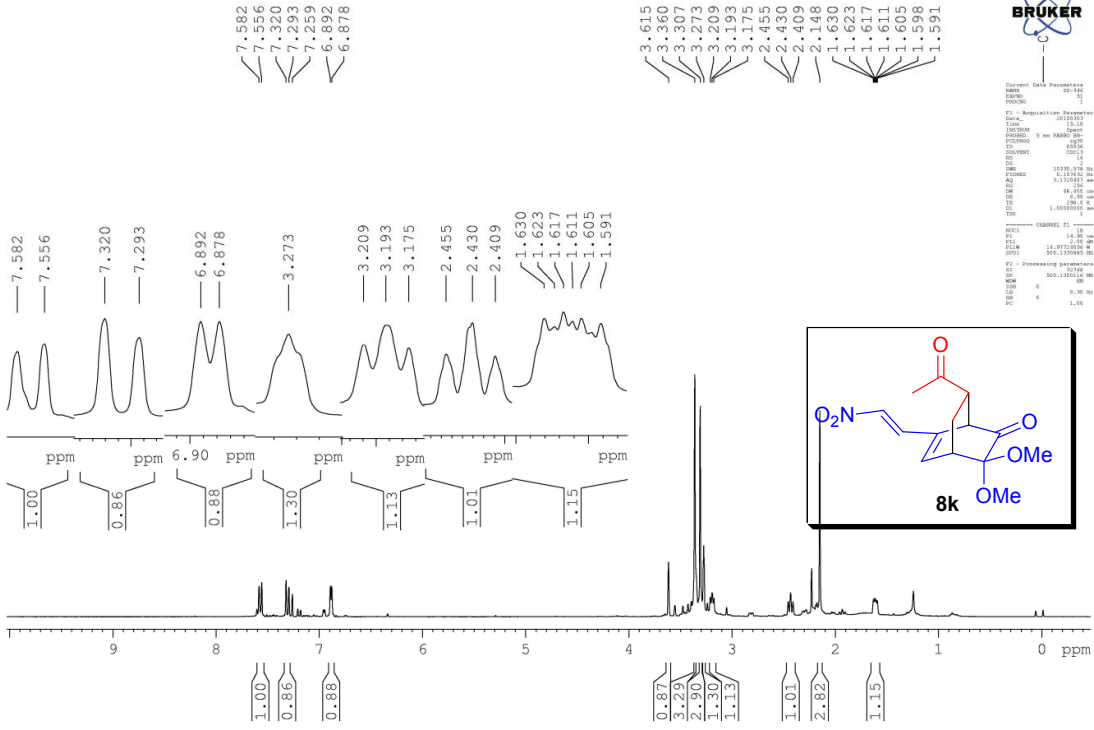




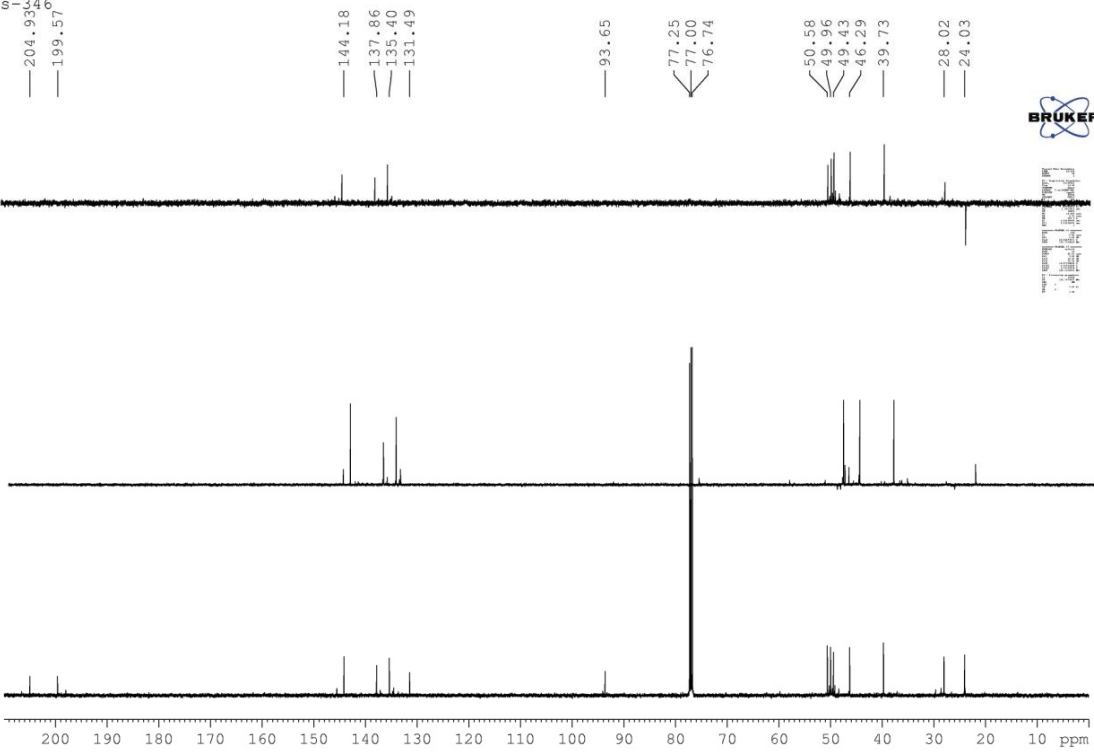


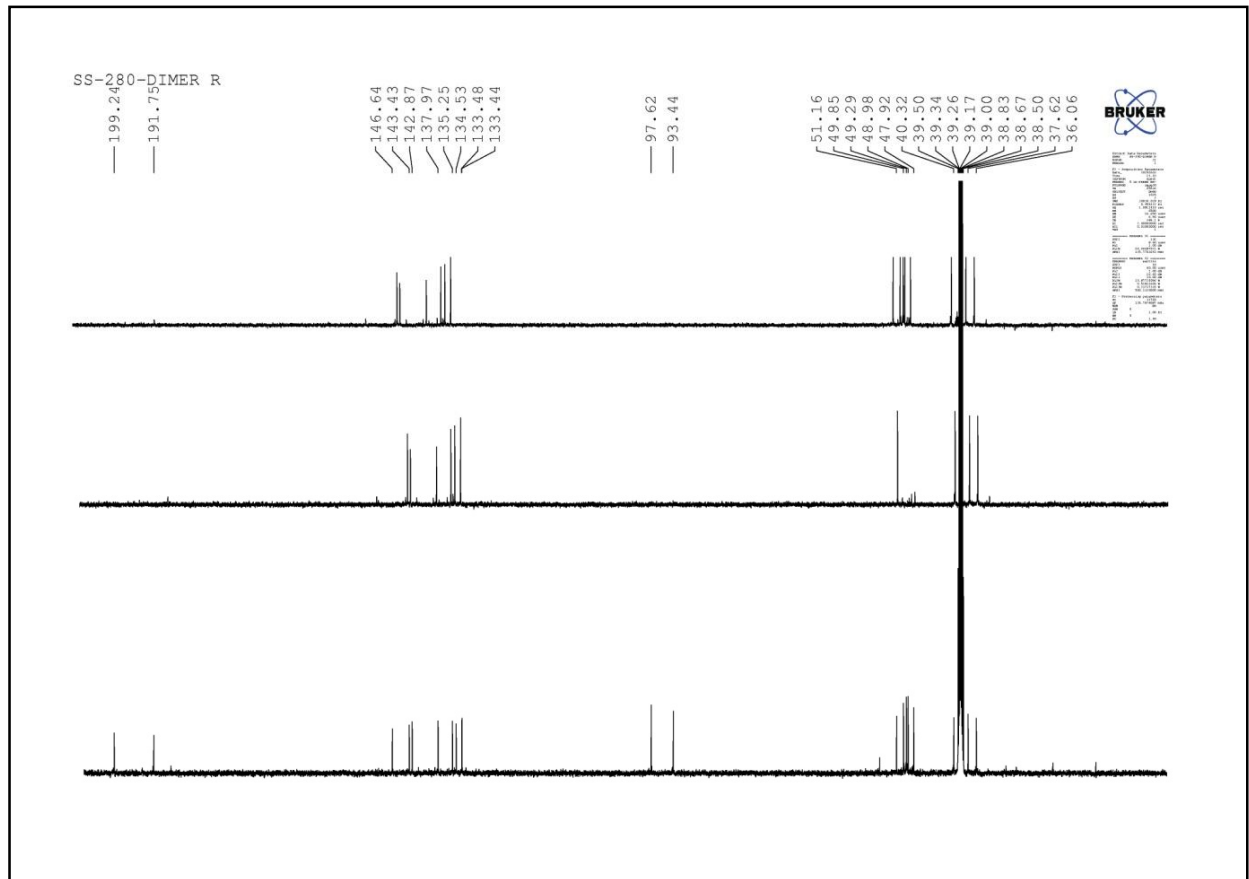
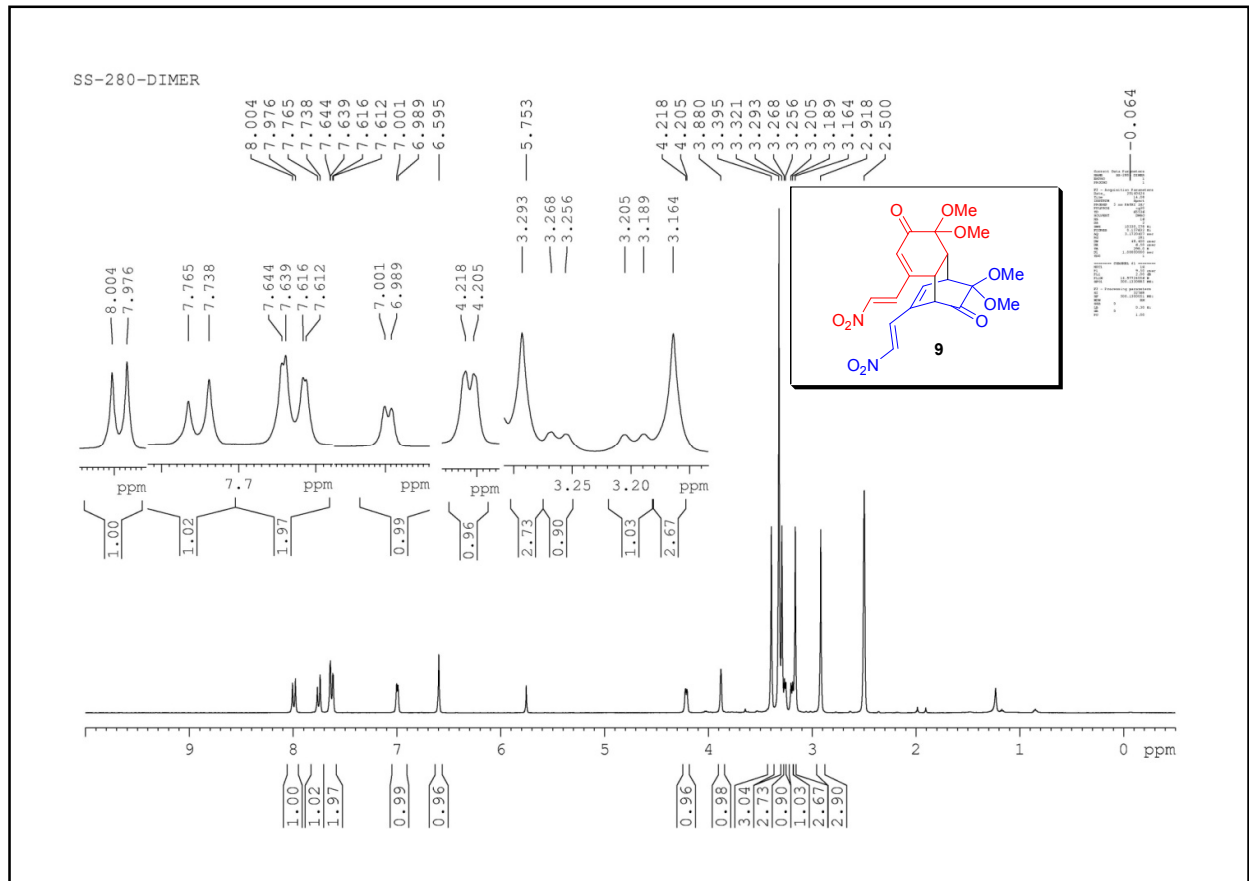


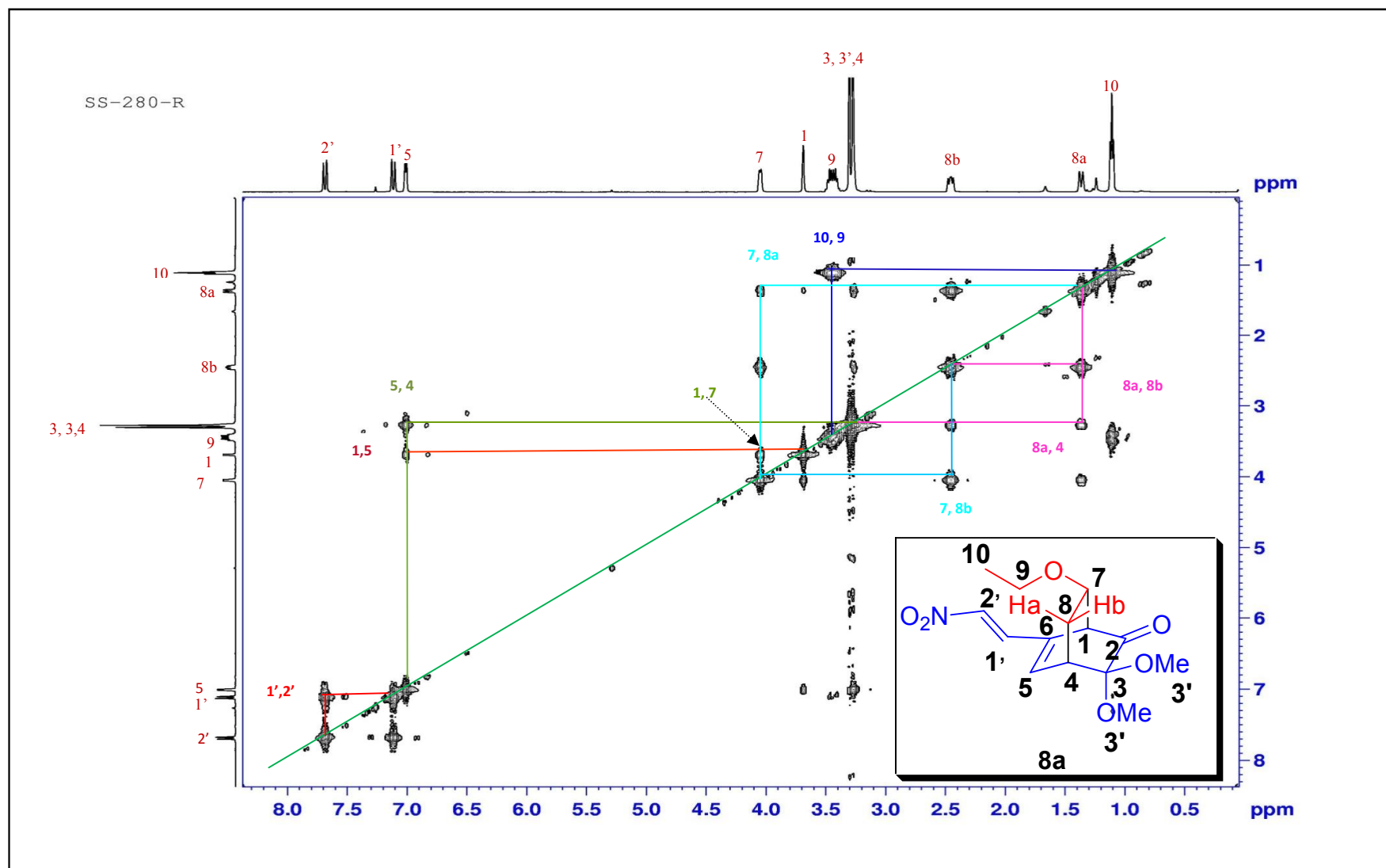
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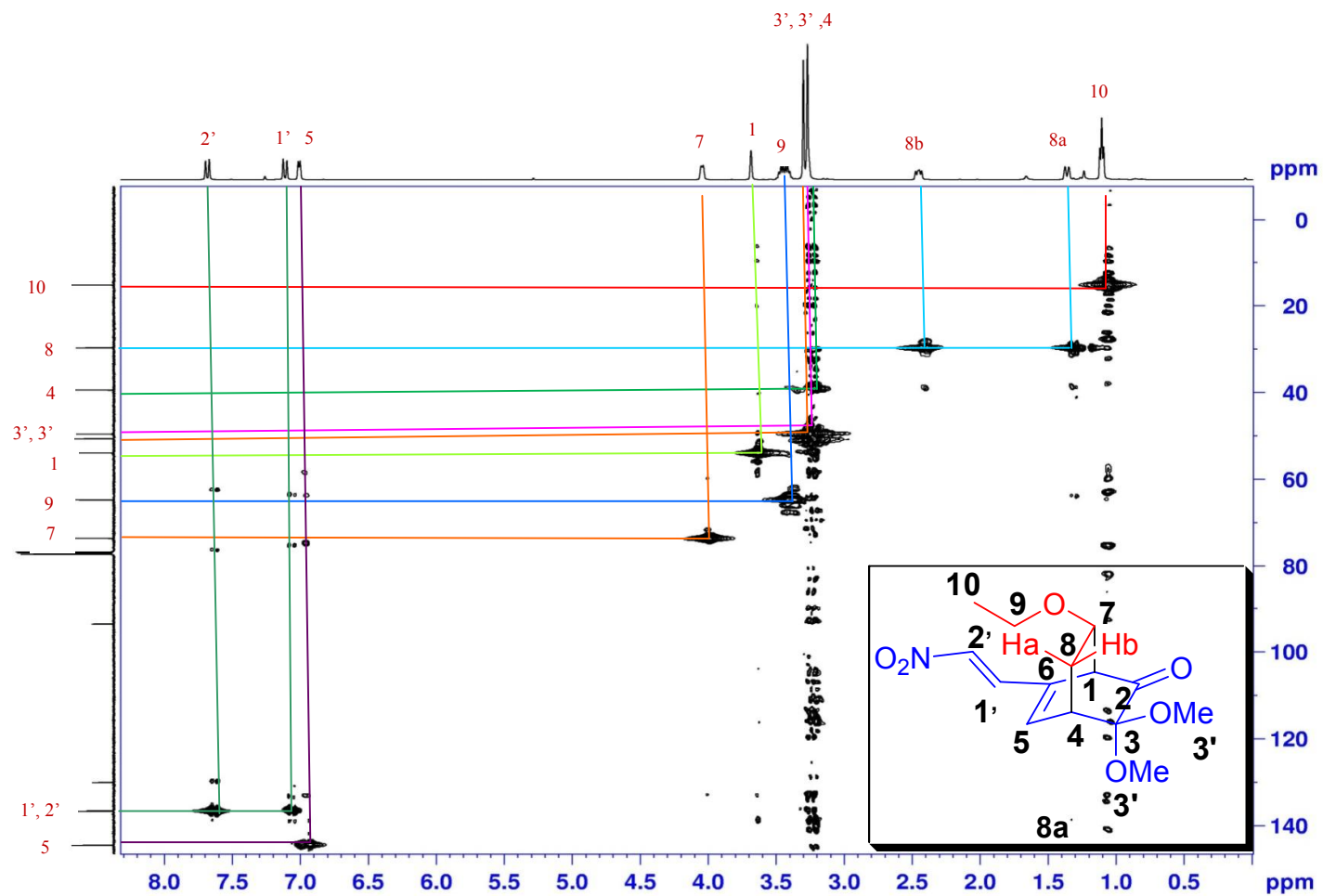






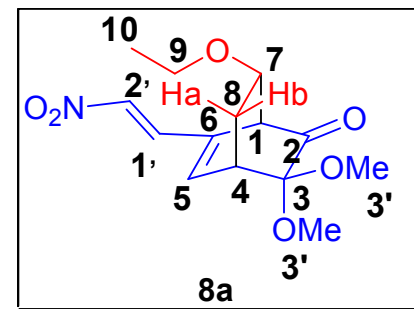
^1H - ^1H Cosy Spectrum of cycloadduct **8a**

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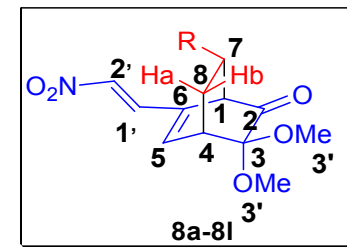
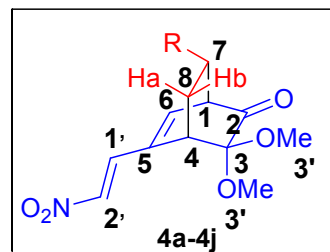
HMQC Spectrum of cycloadduct **8a**

Table SI-1: Proton–proton and proton–carbon connectivity in **8a**.



^1H - ^1H COSY	^{13}C Signals	δ (ppm)	Connectivity from HMQC
H_1 – H_5 H_1 – H_7	C_1	53.9	H_1 – C_1
–	$\text{C}_{3'}$ (OMe)	49.6, 50.7	$\text{H}_{3'}$ – $\text{C}_{3'}$
H_4 – H_5 H_4 – H_{8a}	C_4	39.4	H_4 – C_4
H_5 – H_1	C_5	144.4	H_5 – C_5
H_7 – H_1	C_7	73.60	H_7 – C_7
H_{8a} – H_{8b} H_{8a} – H_4 H_{8a} – H_7	C_8	29.7	H_{8a} – C_8 H_{8b} – C_8
H_9 – H_{10}	C_9	64.7	H_9 – C_9
H_{10} – H_9	C_{10}	15.2	H_{10} – C_{10}
$\text{H}_{1'}$ – $\text{H}_{2'}$	$\text{C}_{1'}$	136.5	$\text{H}_{1'}$ – $\text{C}_{1'}$
	$\text{C}_{2'}$	136.6	$\text{H}_{2'}$ – $\text{C}_{2'}$

Table SI-2: Selected ^1H Chemical shifts (in ppm) of Diels-Alder adducts.



S.No.	Adduct	H-1	H-4	H-6 (4a-4j)/ H-5 (8a-8l)	H-7	H-8a	H-8b	H-1'	H-2'
1	4a	3.77	3.23	6.62	4.06-4.03	1.36	2.48	7.26	7.68
2	4b	3.79	3.25-3.23	6.62	4.05-4.03	1.50-1.47	2.50	7.27	7.70
3	4c	3.79	3.34	6.67	4.39	-	3.00	7.20	7.75
4	4d	3.42-3.40	3.49	6.71	3.53	1.65	2.63	7.35	7.75
5	4e	3.45-3.43	3.39-3.37	6.68	3.50-3.45	1.60-1.56	2.64-2.56	7.33	7.73
6	4f	3.50-3.45	3.39	6.69	3.50-3.45	1.65-1.57	2.65-2.55	7.34	7.73
7	4g	3.49-3.45	3.39	6.71	3.49-3.45	1.65-1.58	2.64-2.57	7.34	7.73
8	4h	3.47	3.36	-	3.98	1.52	2.62-2.53	7.31	7.70
9	4i	3.42	3.37	6.71	3.48	1.64-1.56	2.64-2.55	7.32	7.72
10	4j	3.52-3.44	3.39	6.69	3.52-3.44	1.62	2.63-2.57	7.35	7.74
11	8a	3.68	3.28	7.01	4.06-4.02	1.37	2.46	7.11	7.69
12	8b	3.67	3.25	6.98	4.01-3.97	1.34-1.30	2.44-2.38	7.09	7.65
13	8c	3.70	3.56-3.50	6.85	4.42	-	3.40	7.16	7.66
14	8d	3.46-3.43	3.33	7.12	3.55-3.50	1.73	2.56	6.63	7.61
15	8e	3.44-3.41	3.29	7.12	3.48	1.67	2.56-2.49	6.67	7.61
16	8f	3.49-3.43	3.33	7.13	3.49-3.43	1.67	2.56	-	7.65
17	8g	3.46-3.42	3.35	7.14	3.46-3.42	1.66-1.59	2.59-2.52	6.80	7.66
18	8h	3.41	3.37	7.14	4.07-4.02	1.70-1.65	2.48-2.42	-	7.57
19	8i	3.46-3.39	3.34	7.10	3.46-3.39	1.68	2.53	6.76	7.64
20	8j	3.45-3.42	3.31	7.12	3.52-3.46	1.73-1.67	2.52-2.50	6.95	7.62

21	8k	3.27	3.21-3.16	6.89	3.62	1.64-1.58	2.46-2.41	7.31	7.57
22	8l	3.74-3.67	3.18-3.13	6.96	3.74-3.67	1.86-1.80	2.39-2.32	7.22	7.59

Table SI-3: Selected ^{13}C Chemical shifts (in ppm) of Diels-Alder adducts.

S.No.	Adduct	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-1'	C-2'
1	4a	55.4	199.2	93.1	38.5	138.6	136.9	74.8	29.6	135.9	135.9
2	4b	55.5	199.3	93.3	38.7	138.7	137.0	69.0	29.7	136.0	137.0
3	4c	56.4	198.8	92.8	37.7	137.6	137.2	78.9	30.0	136.7	137.0
4	4d	56.8	199.4	93.3	39.9	139.7	137.1	40.8	29.3	135.7	136.9
5	4e	55.2	199.5	93.3	39.9	139.7	137.1	40.2	29.3	134.8	135.7
6	4f	57.3	199.5	93.4	40.0	139.8	137.3	40.6	29.4	135.7	137.1
7	4g	56.2	199.3	93.3	40.0	139.9	136.8	41.2	29.5	135.4	137.4
8	4h	55.2	199.6	93.5	33.4	139.5	137.6	39.9	27.8	137.1	137.6
9	4i	56.7	199.3	93.3	40.0	139.7	137.2	41.0	29.3	-	-
10	4j	57.1	199.5	93.4	40.1	139.8	137.1	40.6	29.4	137.1	137.1
11	8a	53.9	199.7	93.5	39.4	144.4	130.0	73.6	29.7	136.5	136.6
12	8b	53.9	199.8	93.6	39.4	144.5	130.1	73.8	29.6	136.6	136.6
13	8c	55.1	199.5	93.3	38.5	142.8	131.9	78.4	43.9	136.1	137.4
14	8d	56.1	199.8	93.5	39.4	145.4	130.0	40.6	28.2	136.2	136.7

15	8e	56.4	200.0	93.5	38.7	145.5	130.9	40.5	28.5	136.3	136.7
16	8f	55.9	199.9	93.5	39.2	145.6	131.1	40.6	28.9	136.3	137.0
17	8g	55.8	199.5	93.4	39.6	145.6	131.0	40.5	29.1	137.0	137.2
18	8h	54.1	200.3	93.8	31.6	145.2	131.4	40.6	26.5	136.5	136.6
19	8i	55.9	199.7	93.5	39.6	145.4	130.9	40.5	28.4	136.3	136.9
20	8j	56.3	200.0	93.5	39.1	144.5	130.9	40.6	20.9	136.3	136.8
21	8k	50.0	199.6	93.7	39.7	144.2	131.5	46.3	24.0	135.4	137.9
22	8l	50.1	199.3	93.6	38.7	145.4	131.1	39.7	24.1	135.4	137.5