

Supplementary information for:

Phosphine Oxide Indenoquinoline Derivatives: Synthesis and Biological Evaluation as Topoisomerase I Inhibitors and Antiproliferative agents.

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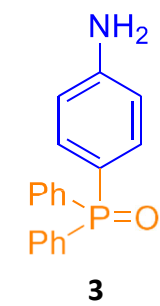
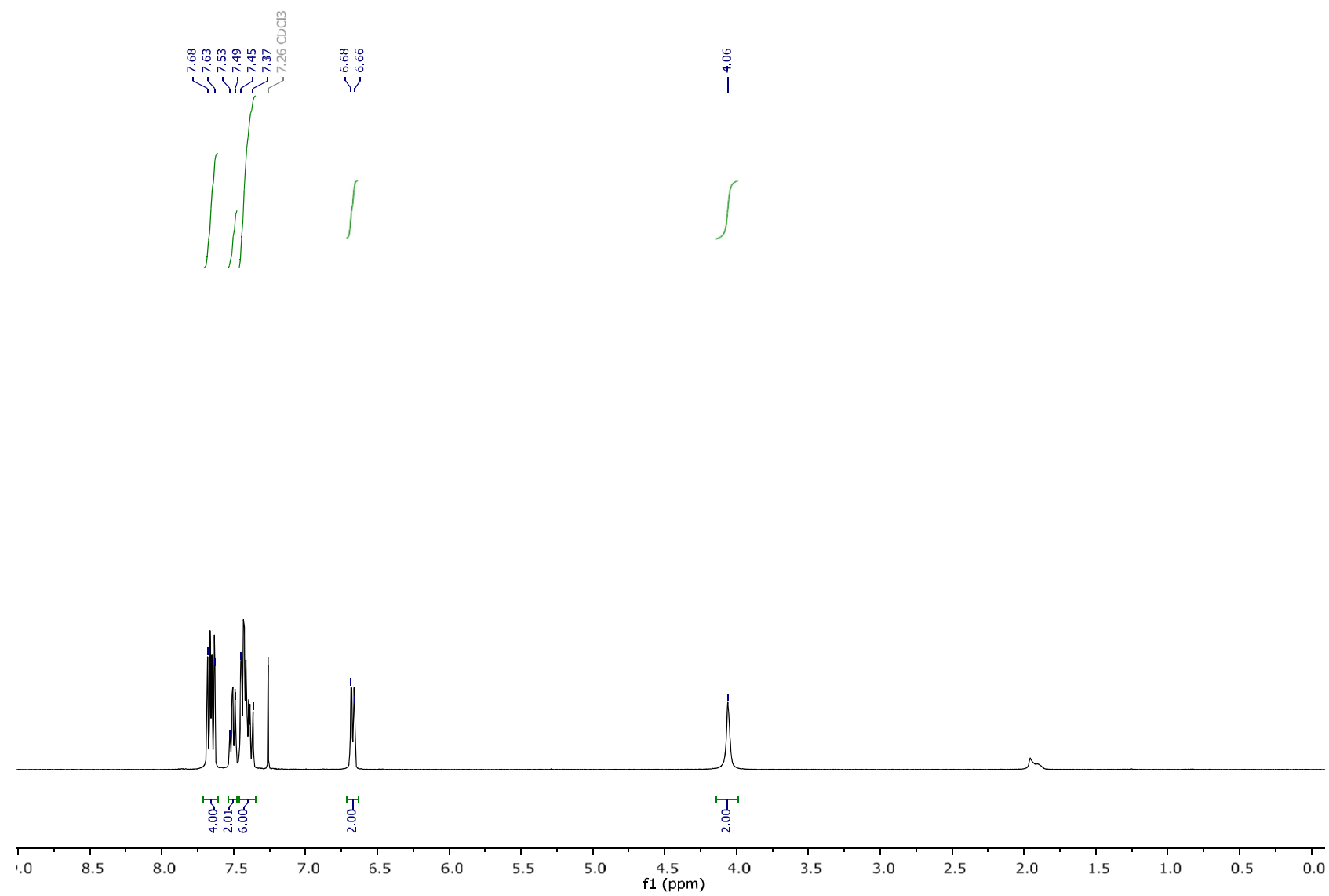
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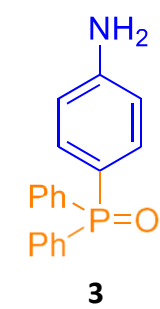
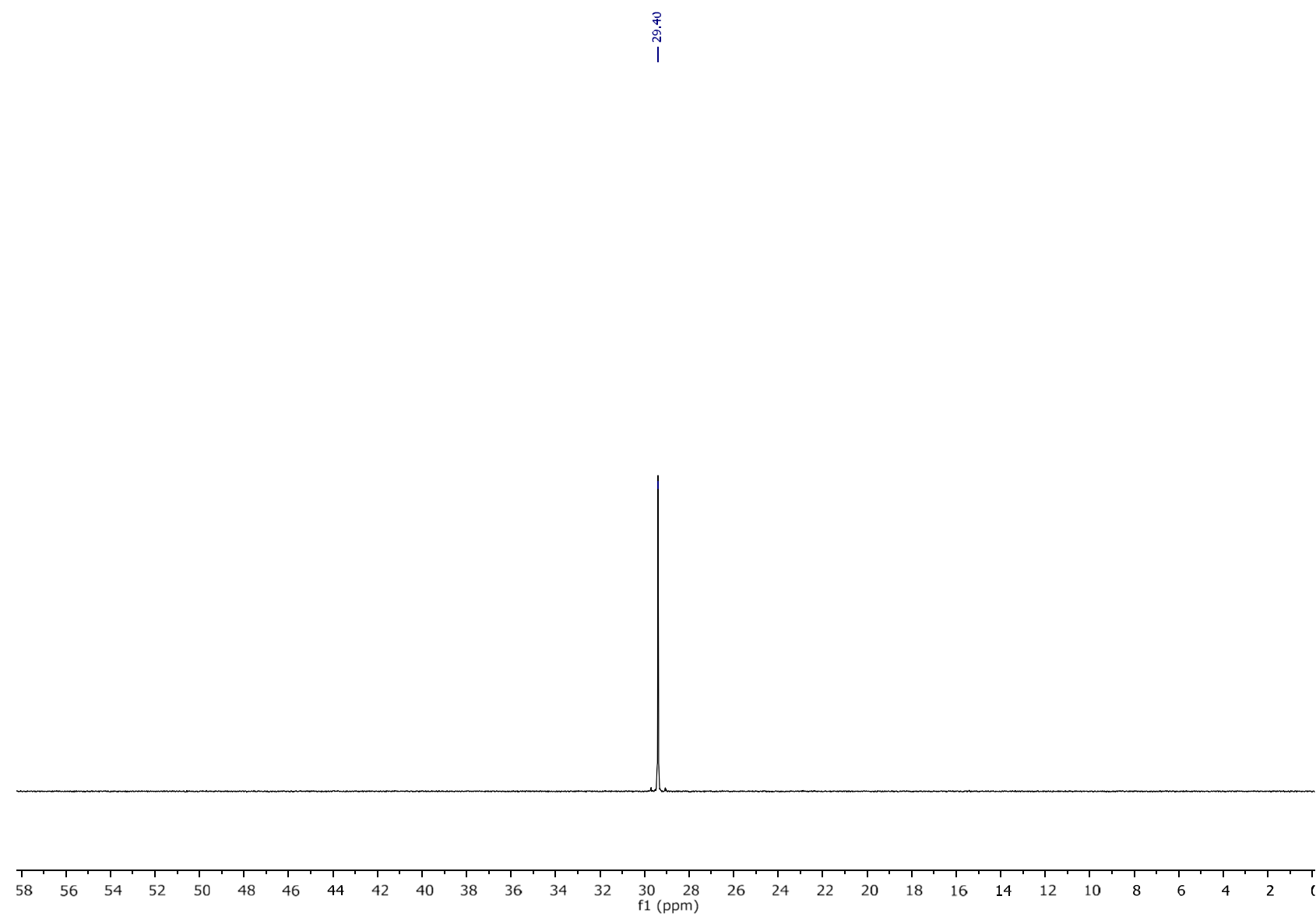
Table S1. Results of the ADME predictive study for diphenylphosphine oxide derivatives.

Entry	Comp.	Log S (mol/L)	Caco-2 Perm. (Log Paap in 10 ⁻⁶ cm/s)	Int. Abs. (% abs)	VDss (L/Kg)	Fract. Unb. (Fu.)	BBB Permeability (Log BB)	PGP subs.	PGP I inhib.	PGP II inhib.	CYP1A2 Inhib.	CYP2C19 Inhib.	CYP2C9 Inhib.	CYP2D6 inhib.	CYP3A4 Inhib.	Total Clearance numeric (Log mL/min/Kg)
1	CPT	-3.01	1.305	99.865	0.448	0.126	no	yes	yes	no	yes	no	yes	no	no	0.629
2	6a	-4.821	0.911	100	-0.9	0.321	yes	yes	yes	yes	yes	no	no	no	no	-0.506
3	6b	-4.676	0.911	100	-0.994	0.315	yes	yes	yes	yes	yes	no	no	no	no	-0.584
4	6c	-4.65	0.946	100	-1.049	0.325	yes	yes	yes	yes	yes	no	no	no	no	-0.652
5	6d	-4.607	0.948	100	-1.059	0.326	yes	yes	yes	yes	yes	no	no	no	no	-0.646
6	6e	-4.114	0.962	100	-1.204	0.338	yes	yes	yes	yes	yes	no	no	no	no	-0.692
7	6f	-4.092	0.992	100	-1.199	0.346	yes	yes	yes	yes	yes	no	no	no	no	-0.555
8	6g	-3.6	0.876	100	-0.489	0.362	yes	yes	yes	yes	yes	no	no	no	no	-0.542
9	6k	-4.049	-0.029	100	-0.853	0.329	yes	yes	yes	yes	yes	no	no	no	no	-0.485
10	7a	-4.376	0.897	100	-0.427	0.371	yes	yes	yes	yes	no	no	no	no	no	-0.106
11	7b	-4.353	0.899	100	-0.487	0.37	yes	yes	yes	yes	no	no	no	no	no	-0.179
12	7c	-3.964	0.933	100	-0.476	0.373	yes	no	yes	yes	yes	no	no	no	no	-0.361
13	7d	-3.898	0.943	100	-0.483	0.373	yes	no	no	yes	yes	no	no	no	no	-0.239
14	7f	-3.444	0.989	100	-0.521	0.38	yes	no	yes	yes	yes	no	no	no	no	-0.262
15	7g	-3.189	0.853	100	-0.172	0.38	yes	no	yes	yes	no	no	no	no	no	-0.138
16	7h	-3.98	0.857	100	-0.507	0.372	no	no	yes	yes	yes	no	no	no	no	-0.181
17	7i	-3.948	0.906	100	-0.522	0.372	no	no	no	yes	yes	no	no	no	no	-0.057
18	7j	-4.418	0.884	100	-0.456	0.37	yes	yes	yes	yes	no	no	no	no	no	-0.253
19	8a	-4.040	0.939	100	-0.570	0.372	no	no	yes	yes	yes	no	no	no	no	0.105
20	8b	-3.995	0.941	100	-0.633	0.372	no	no	yes	yes	yes	no	no	no	no	0.028
21	8d	-3.481	0.988	100	-0.614	0.378	no	no	yes	yes	yes	no	no	no	no	-0.03
22	8e	-3.163	1.004	100	-0.637	0.385	no	no	yes	yes	no	no	no	no	no	-0.133
23	8g	-3.155	0.899	100	-0.263	0.379	no	no	yes	yes	no	no	no	no	no	0.067

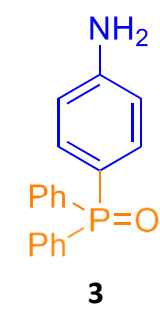
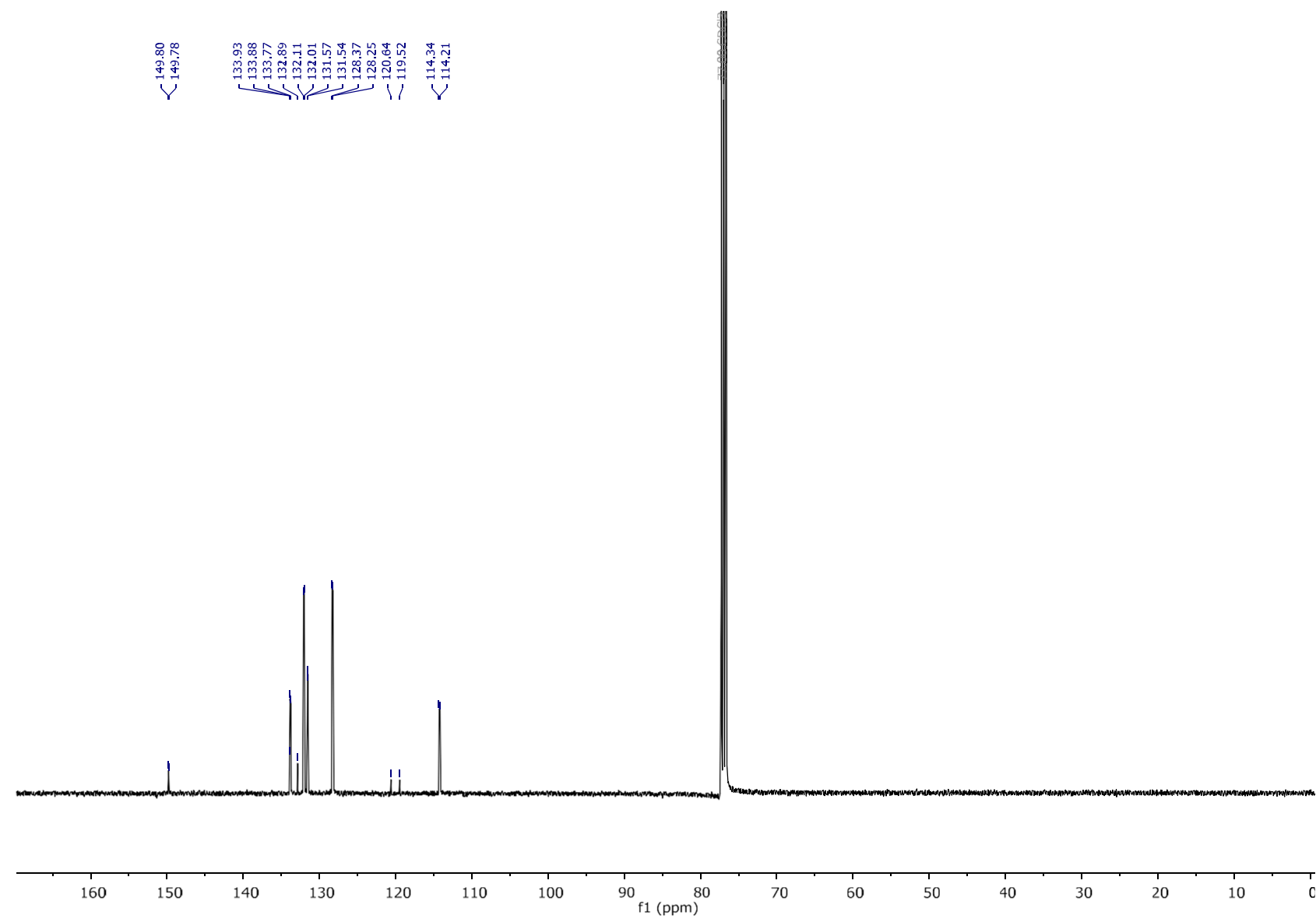
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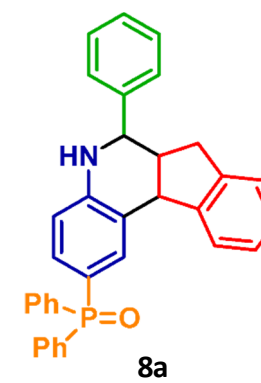
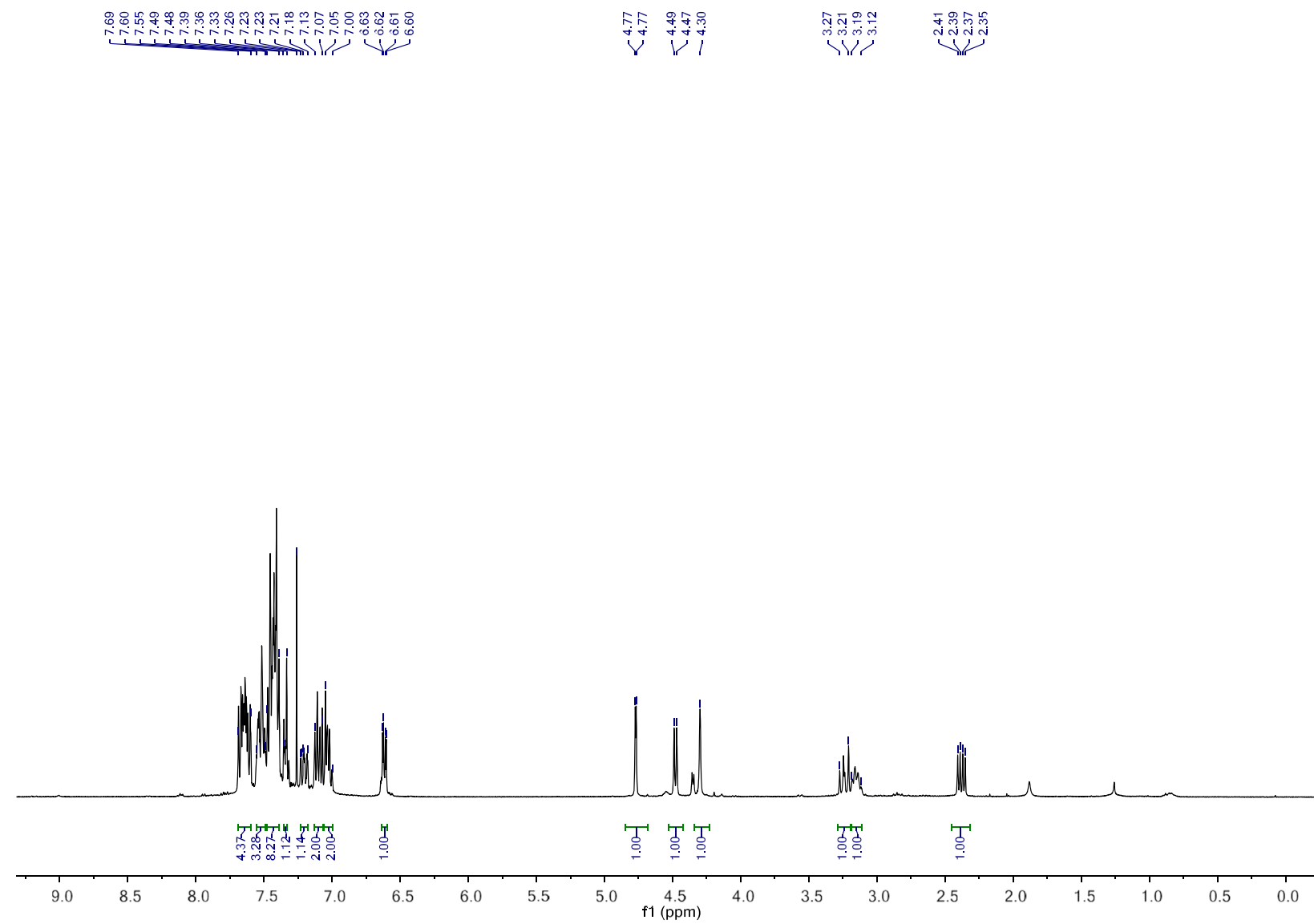
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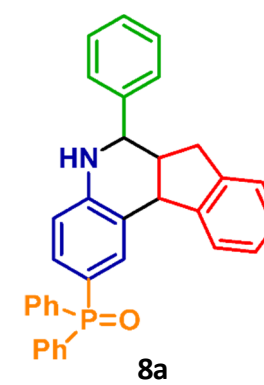
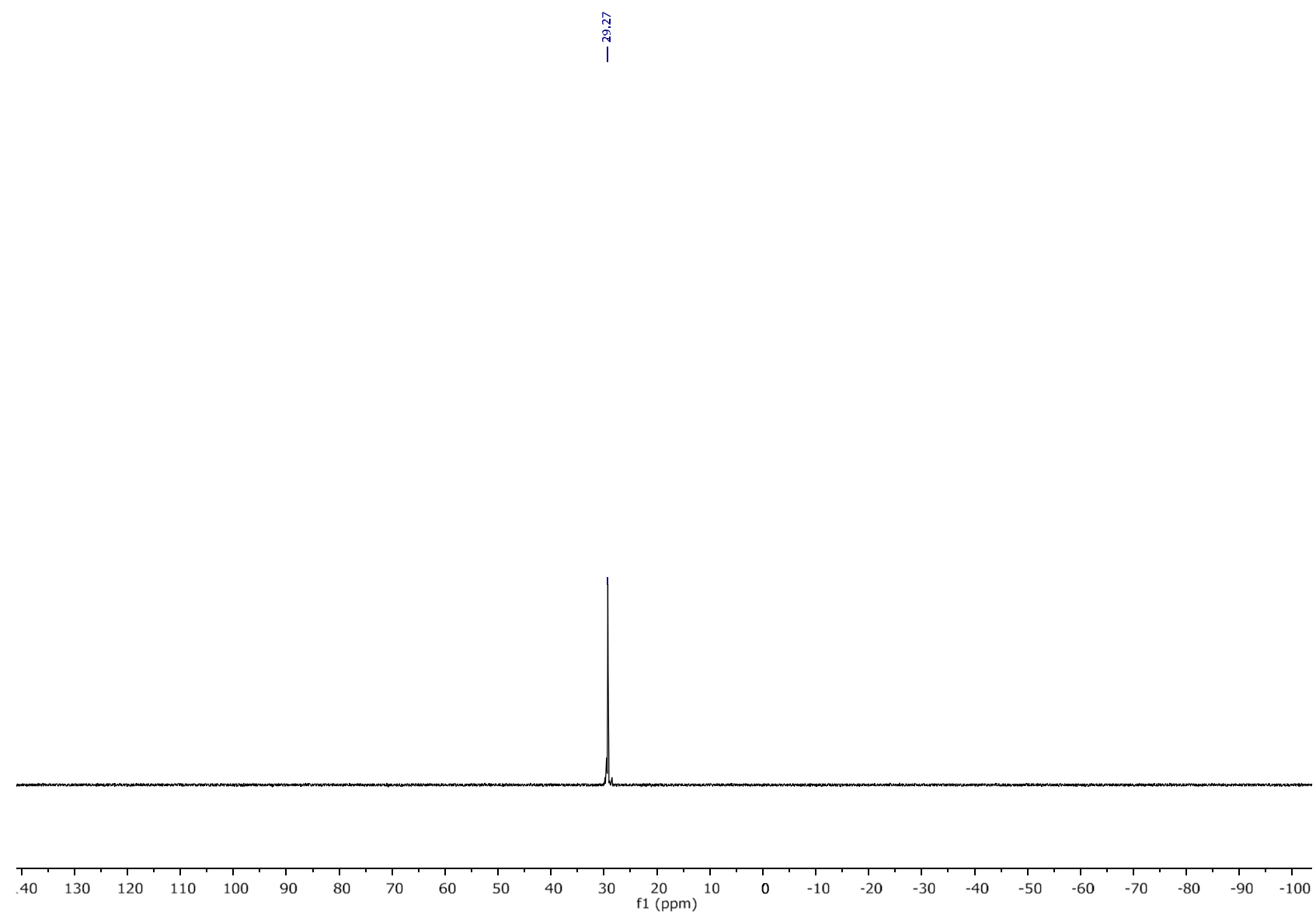
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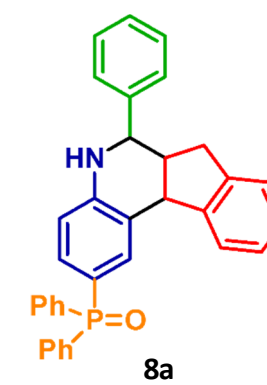
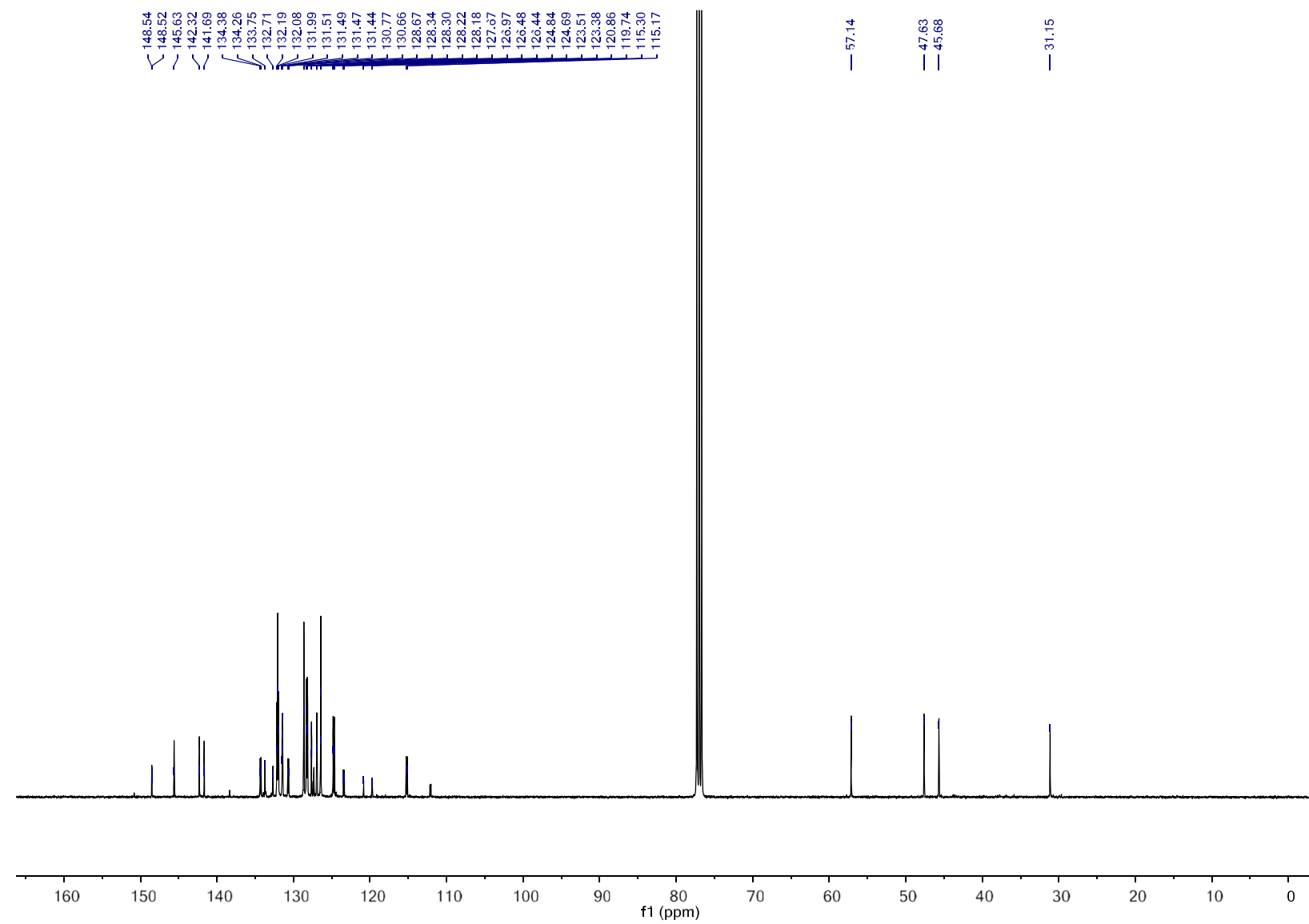
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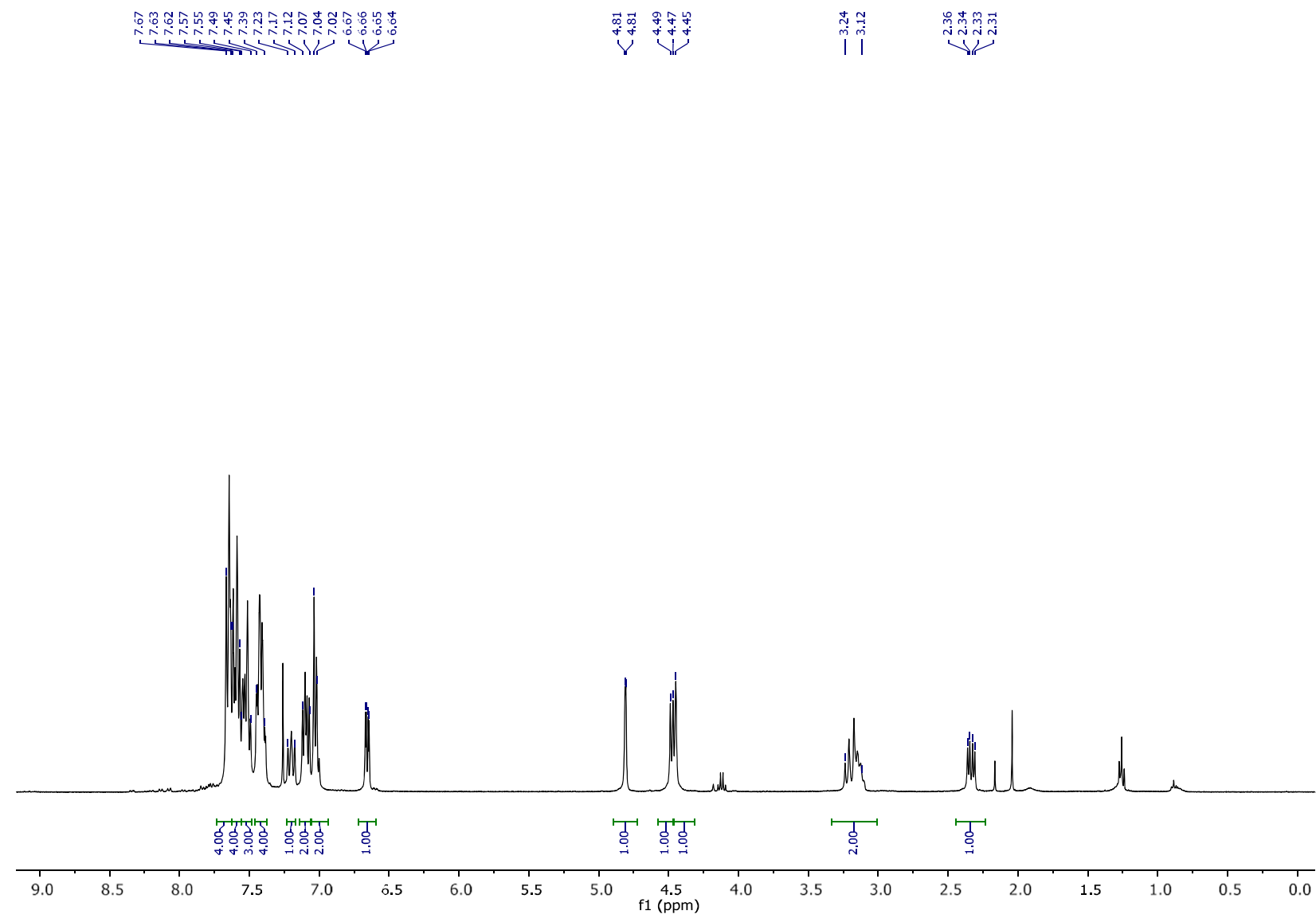
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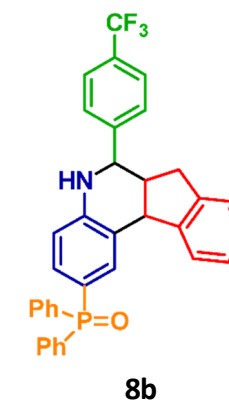
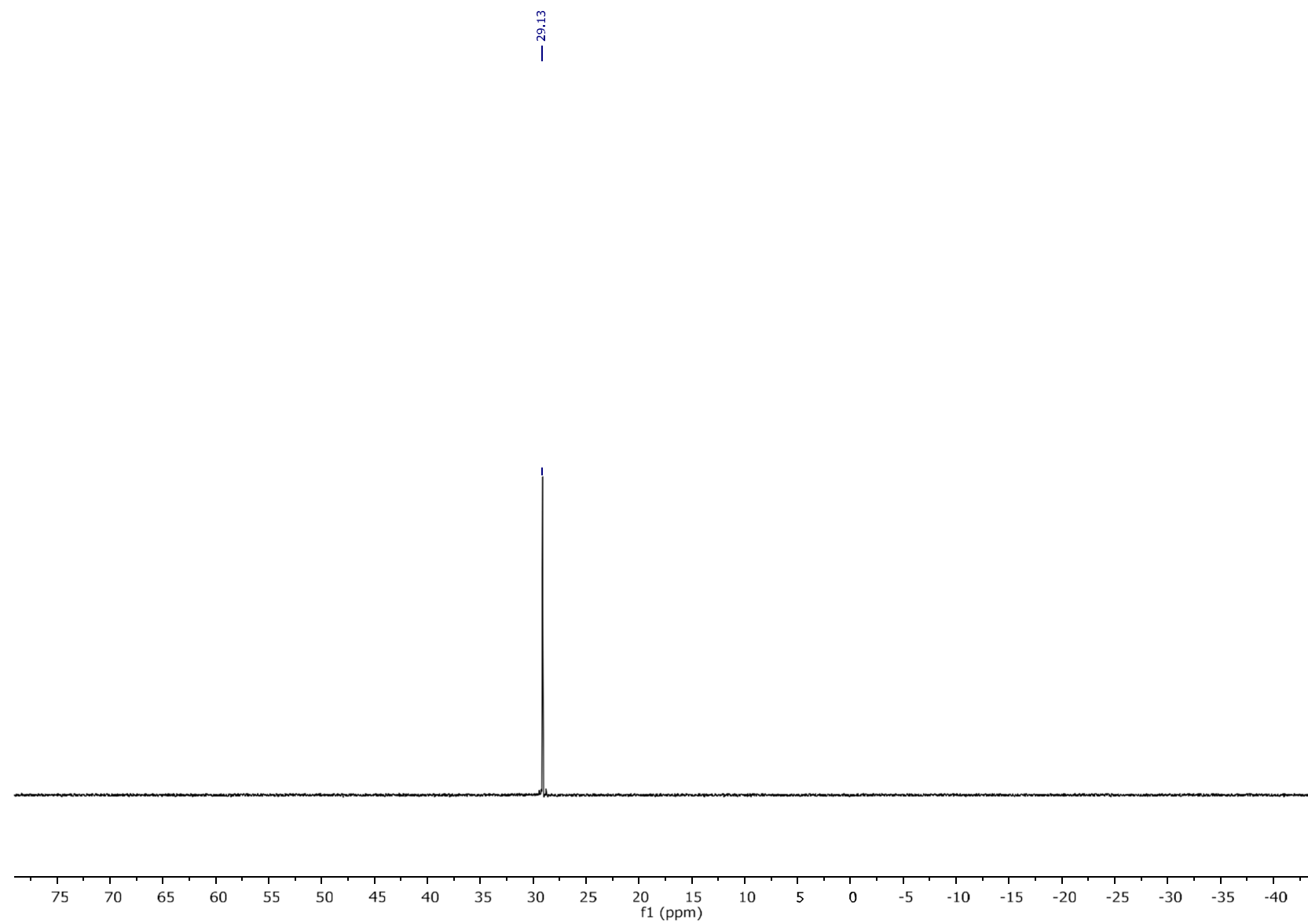
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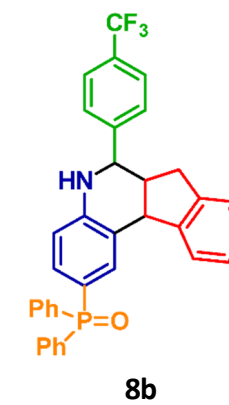
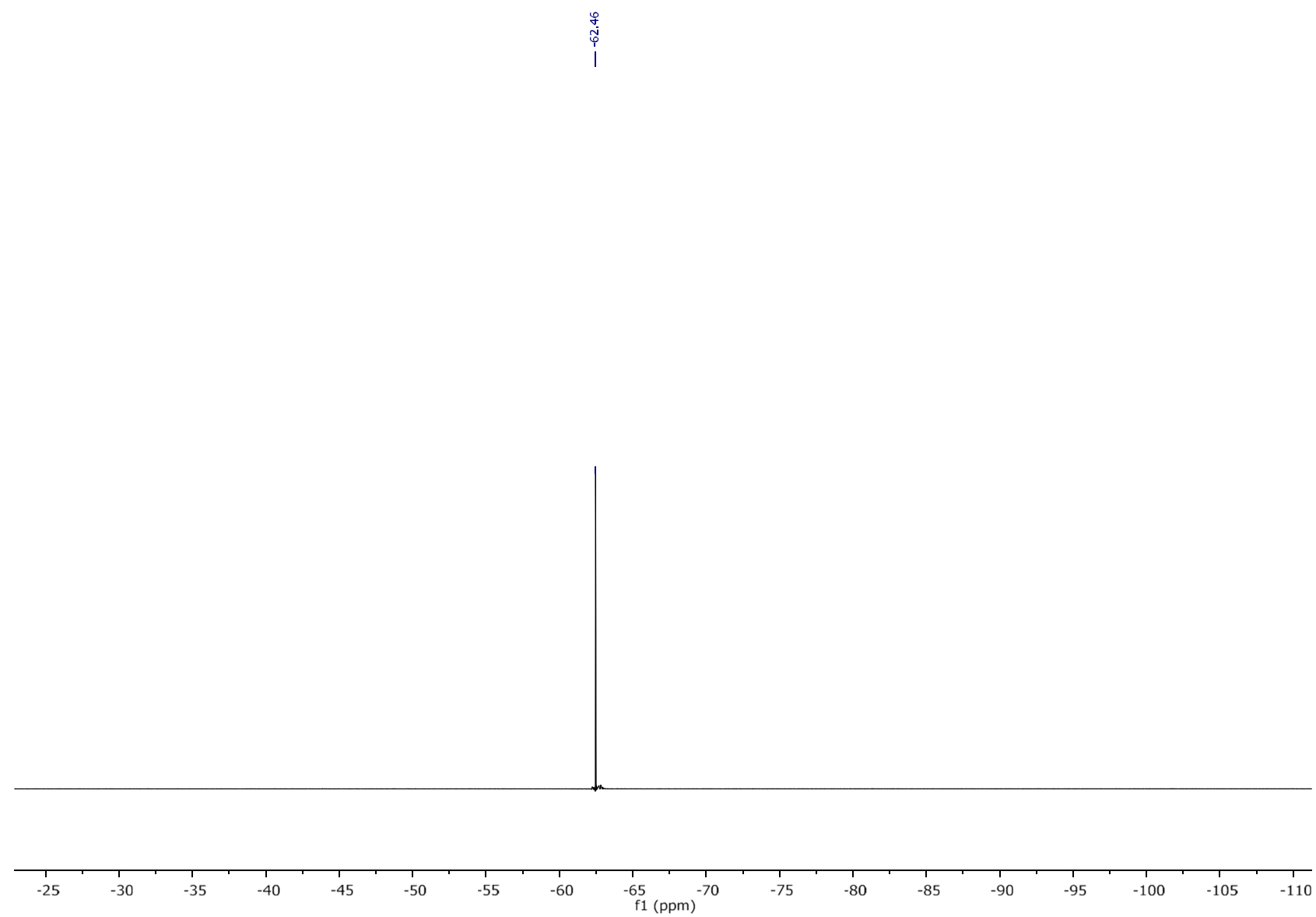
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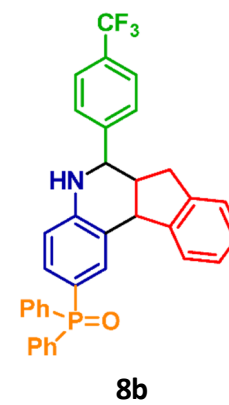
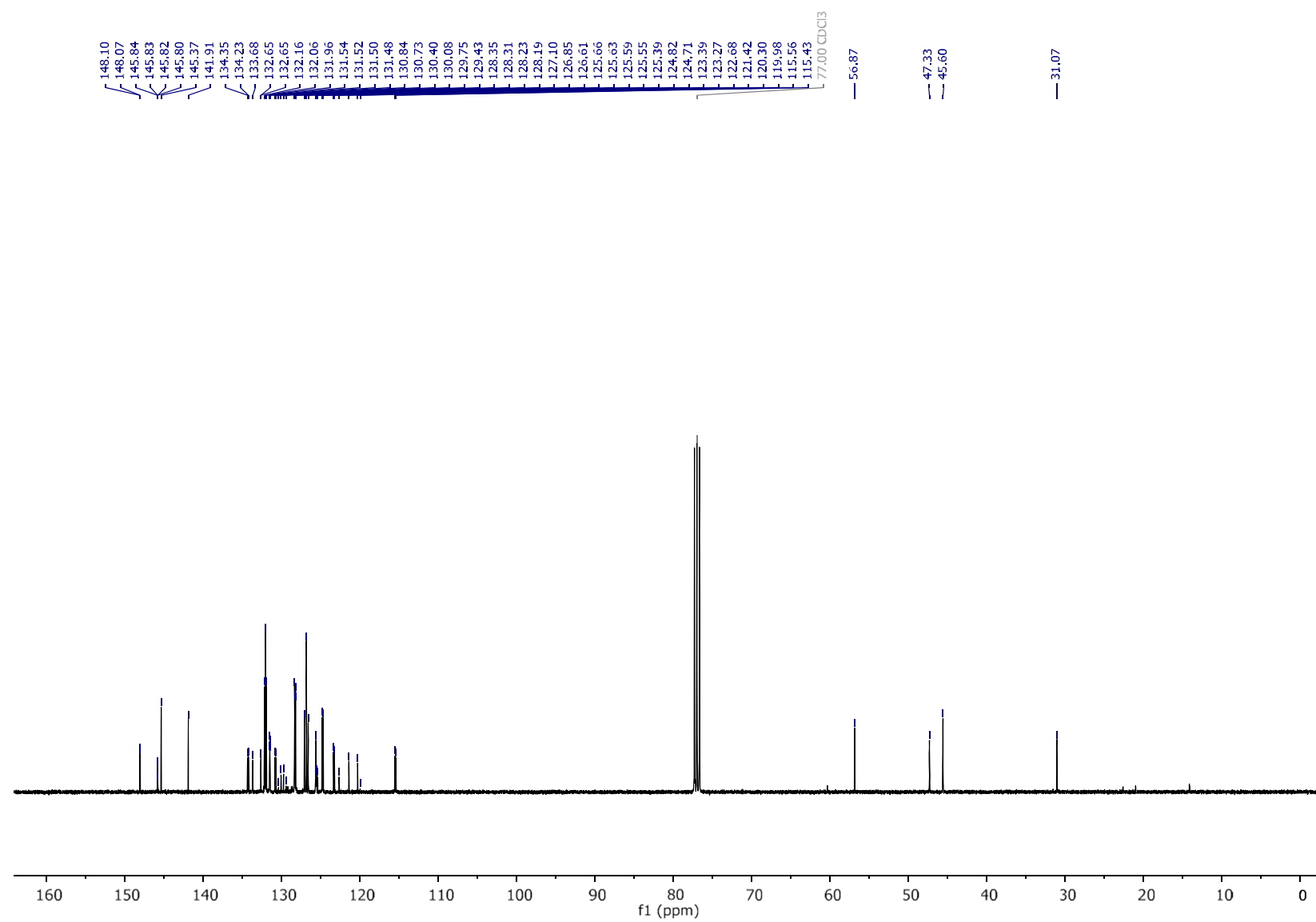
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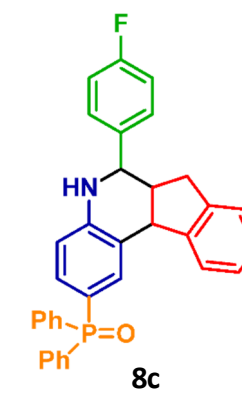
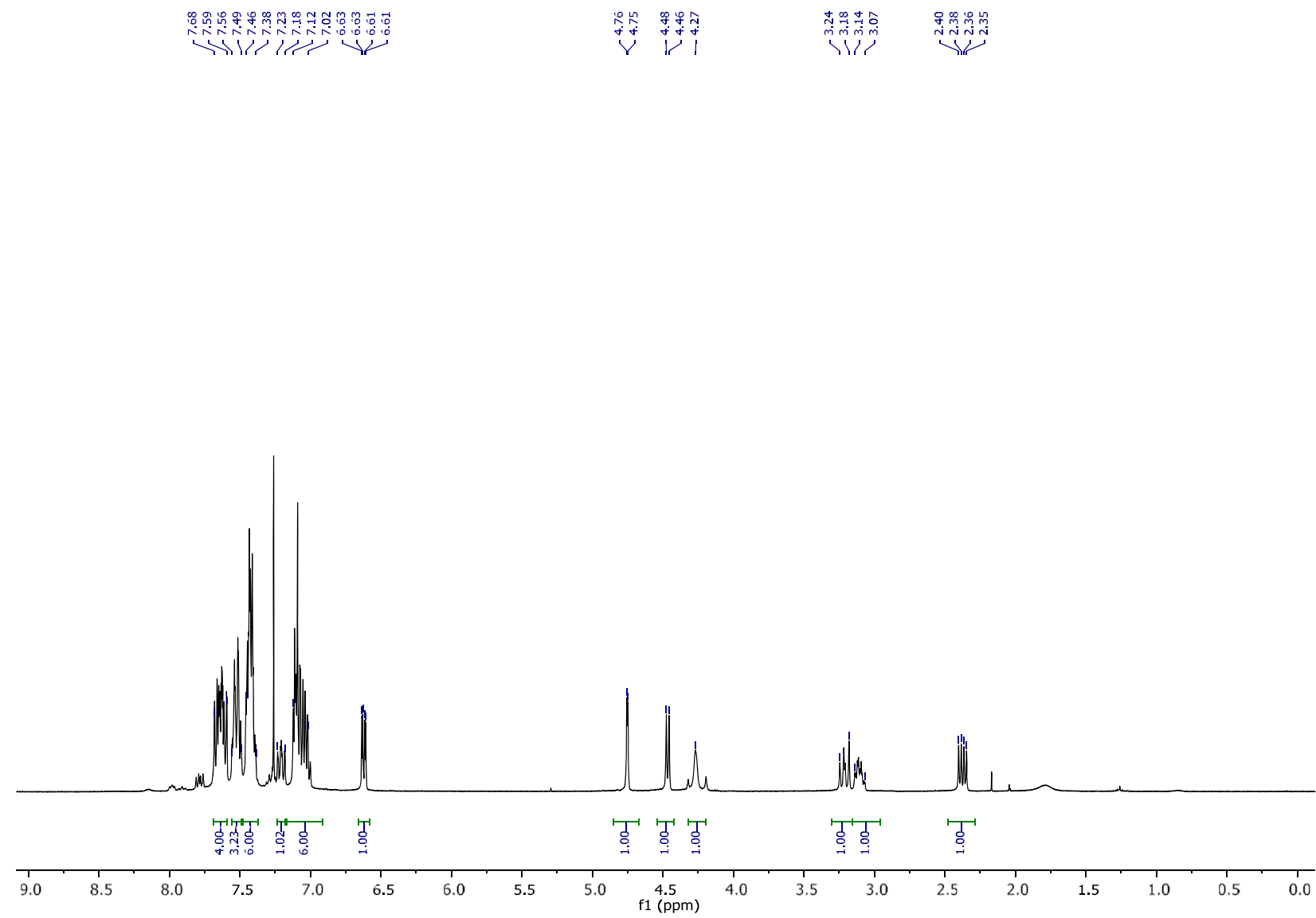
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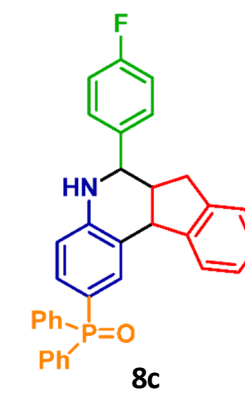
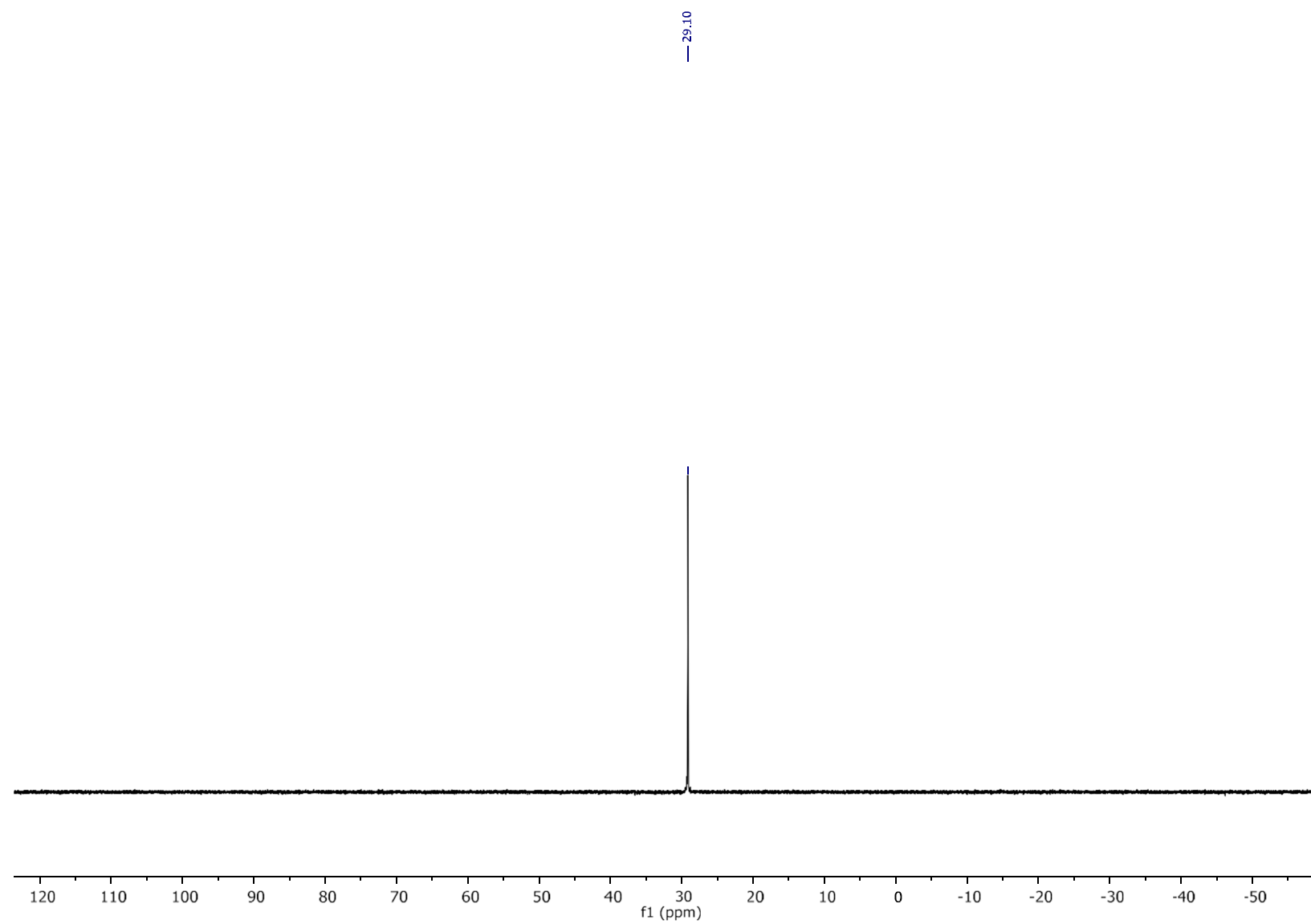
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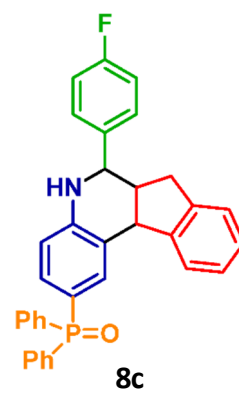
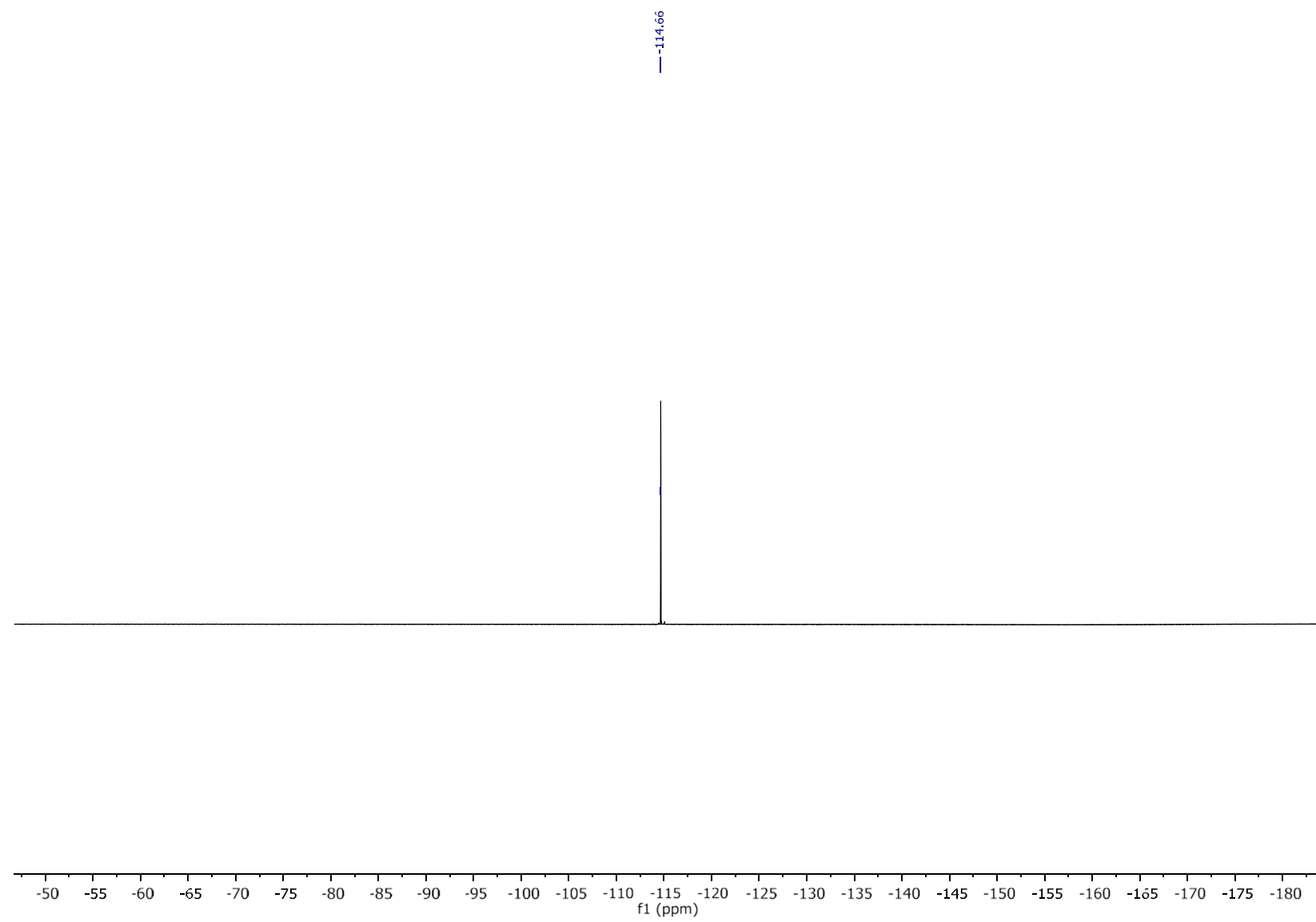
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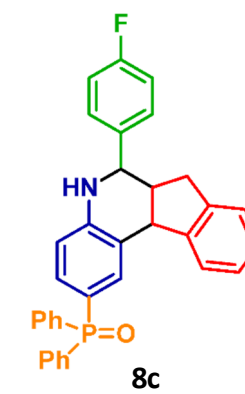
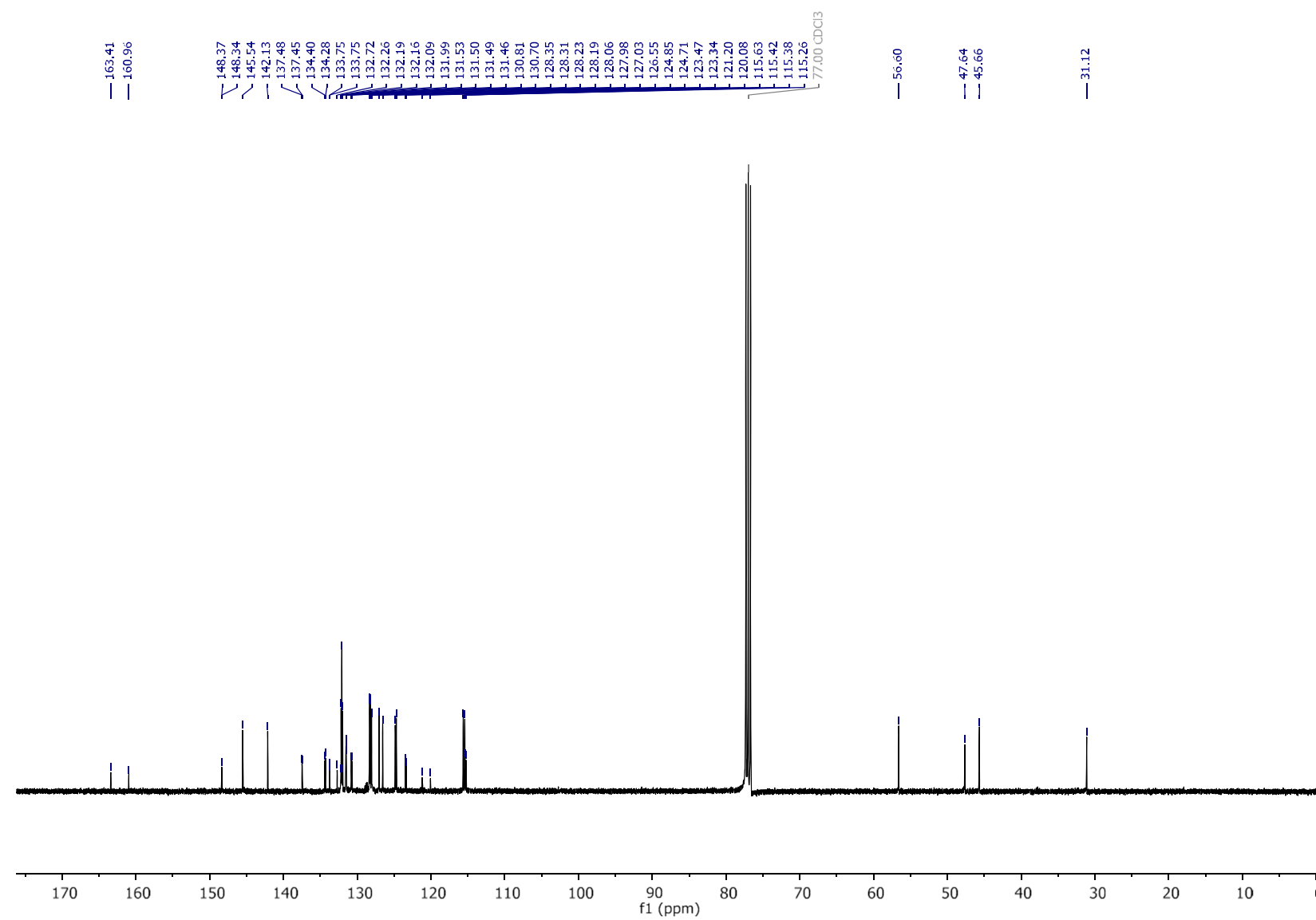
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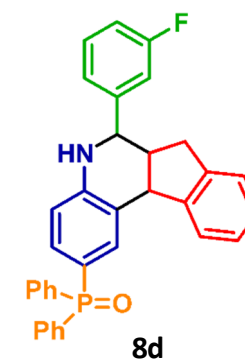
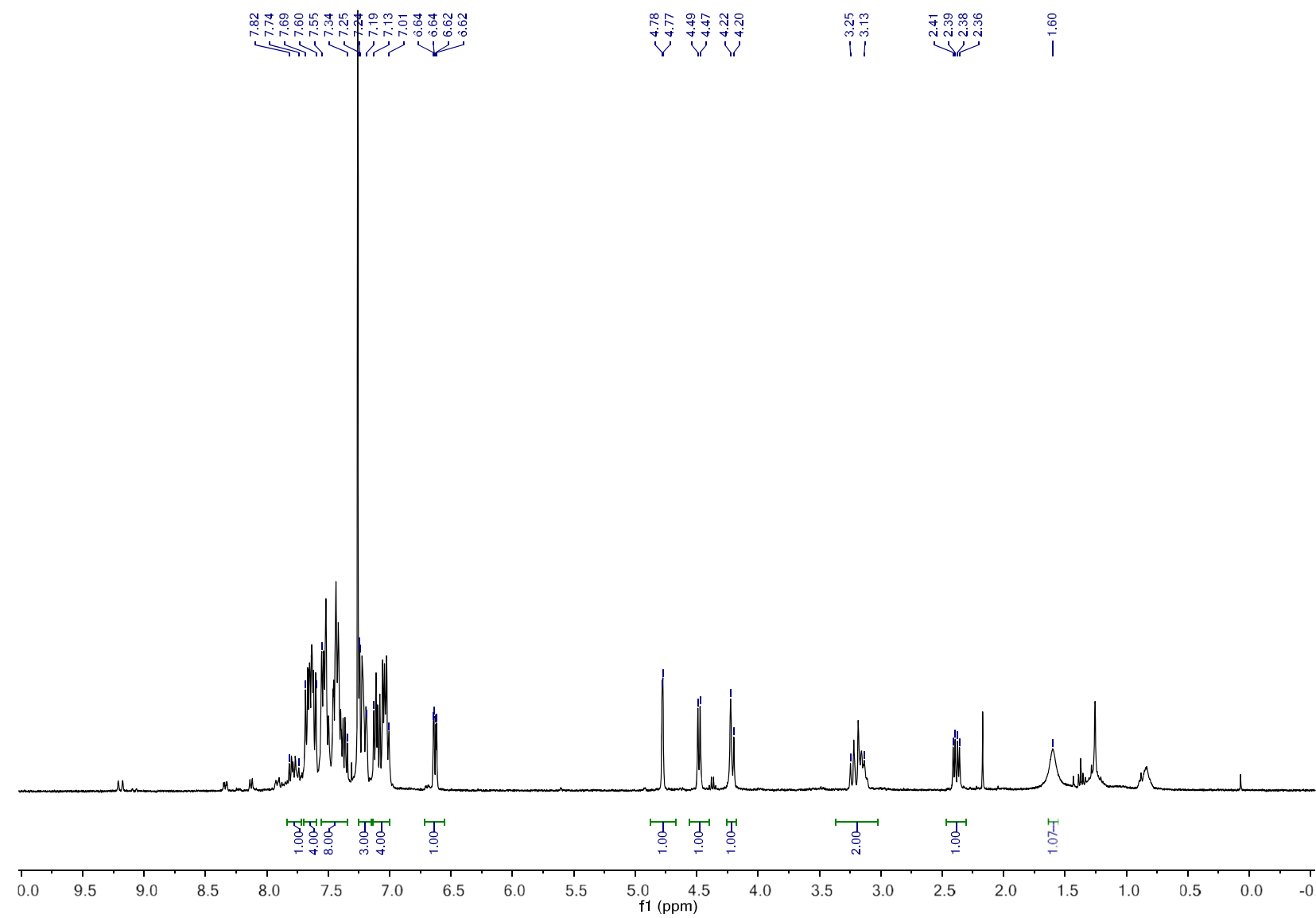
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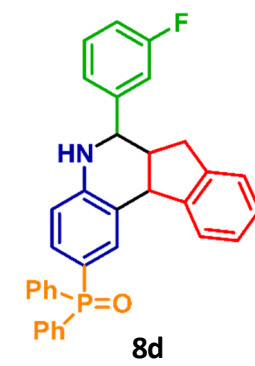
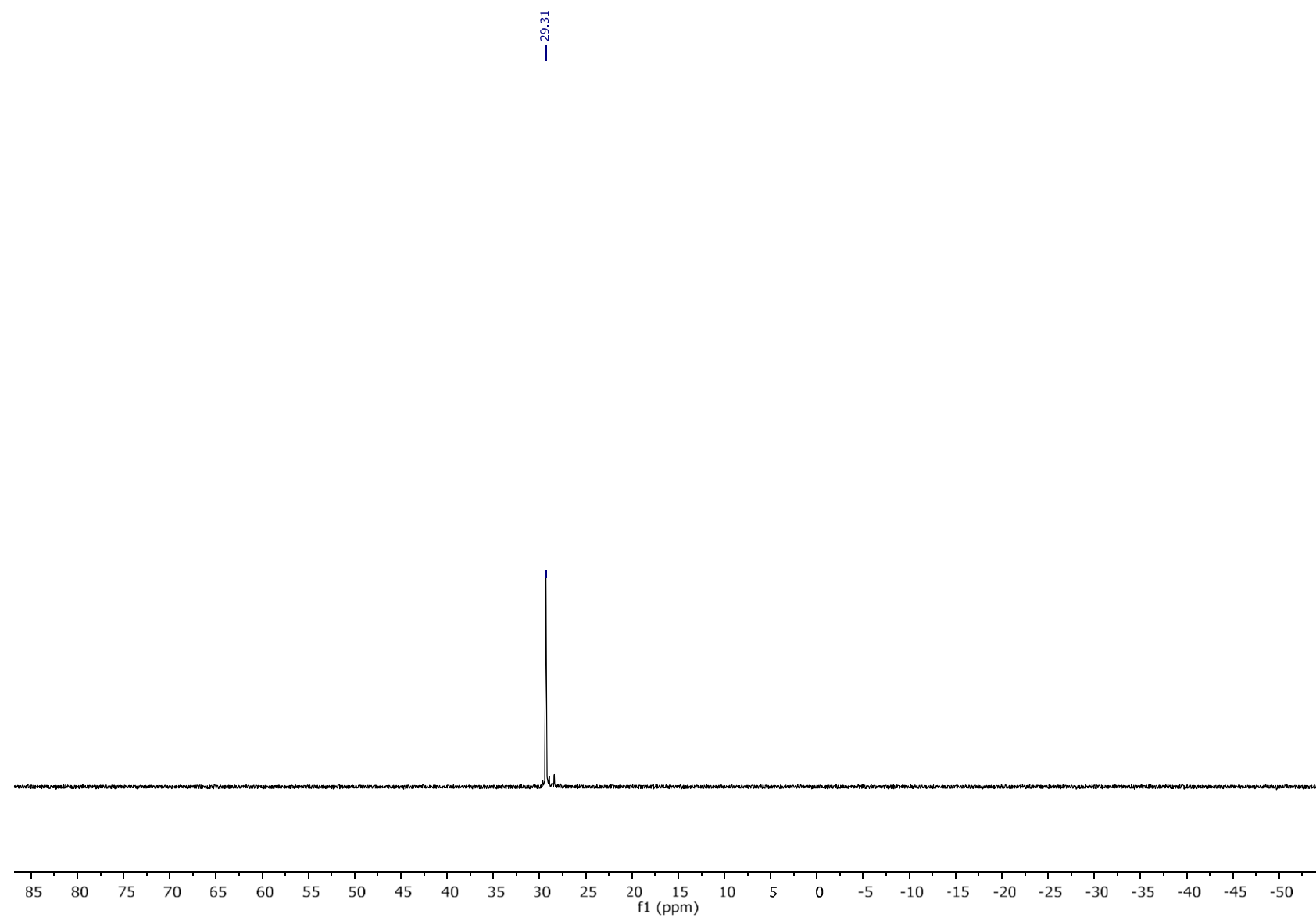
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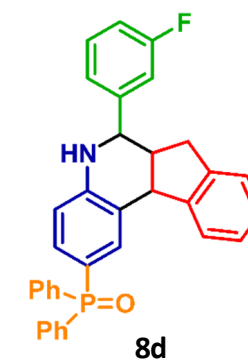
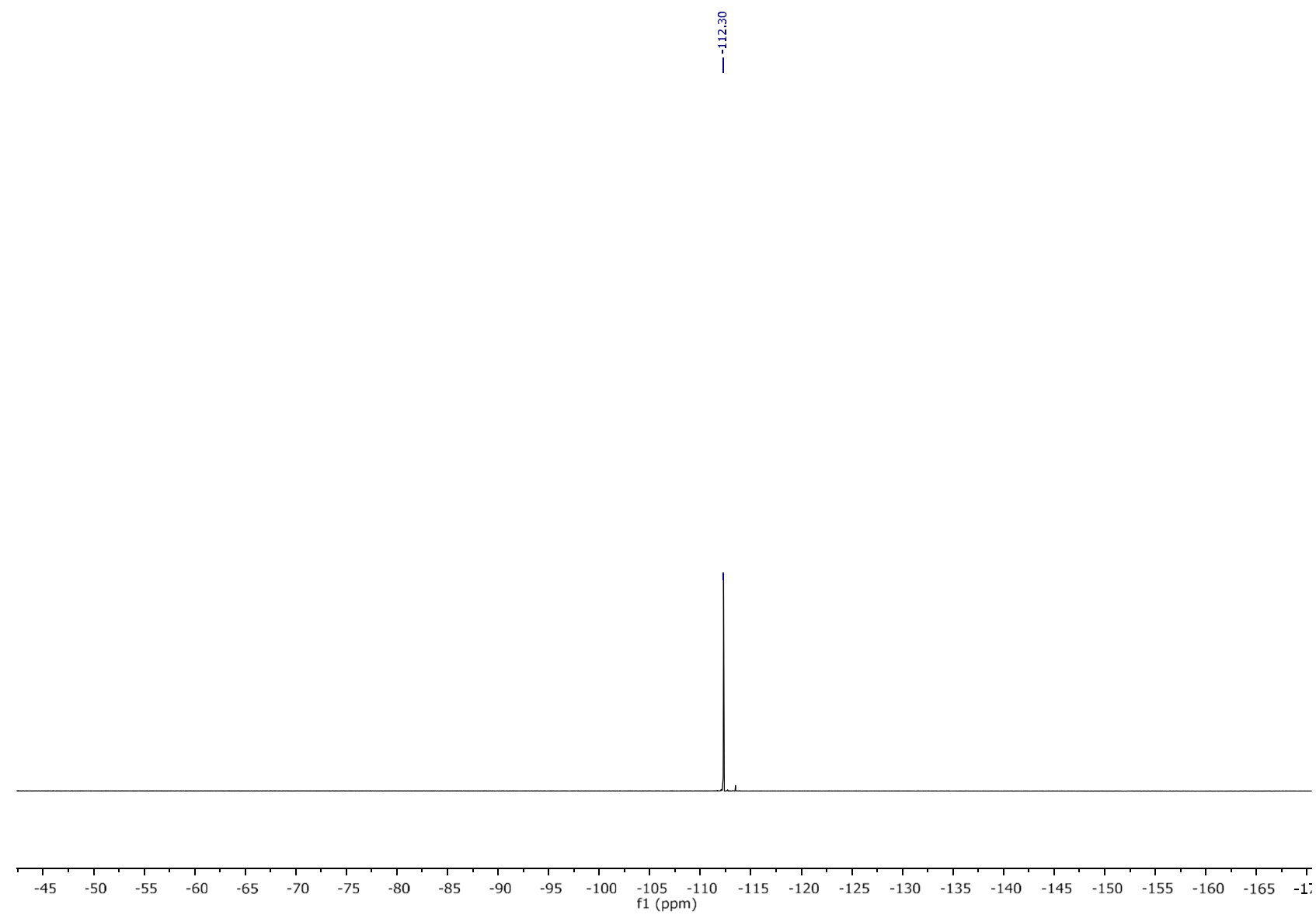
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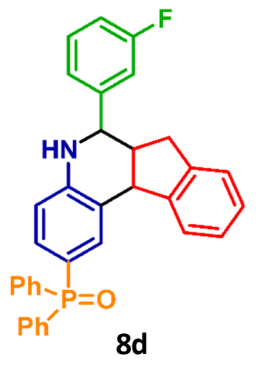
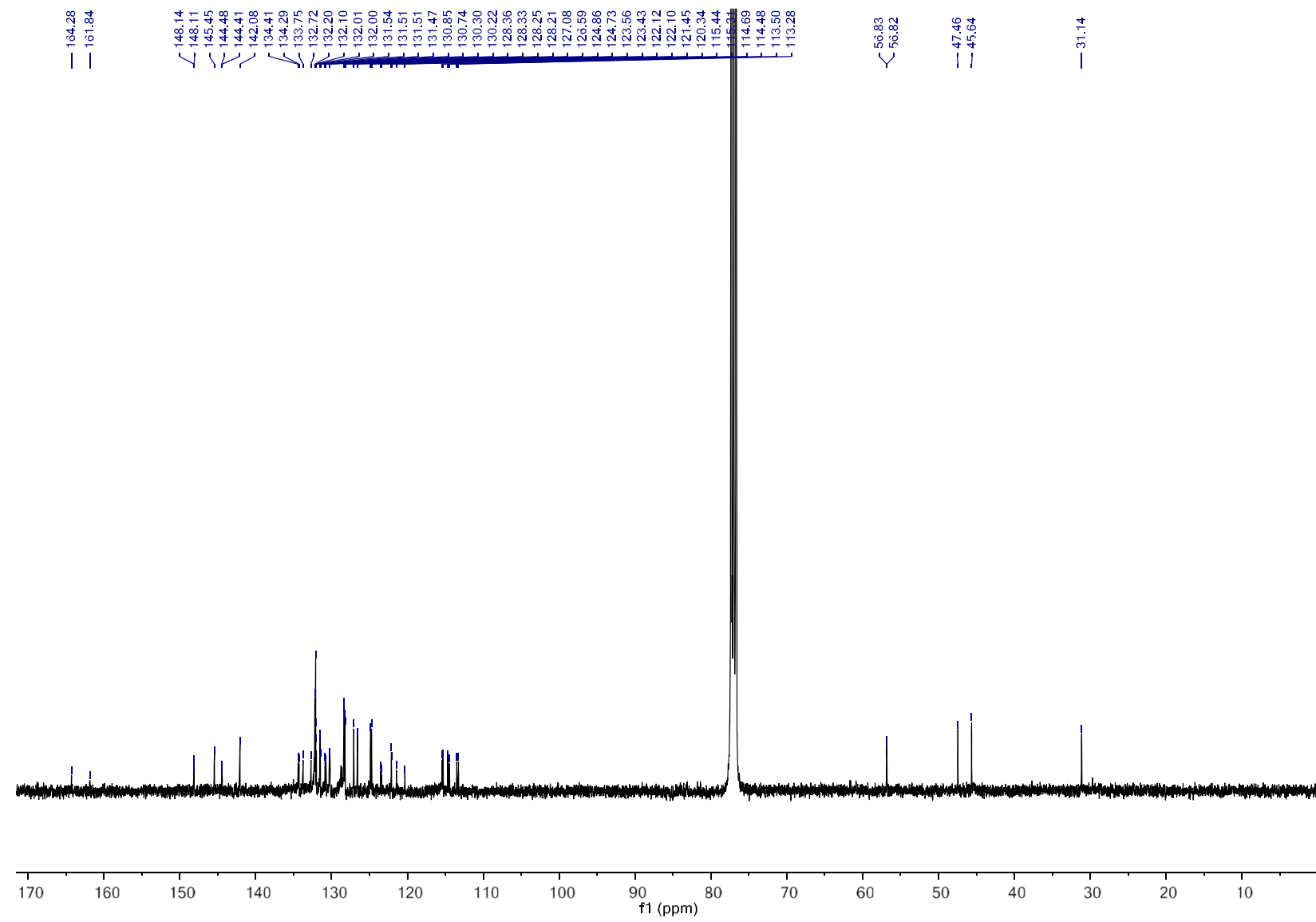
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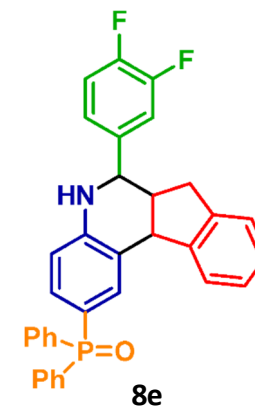
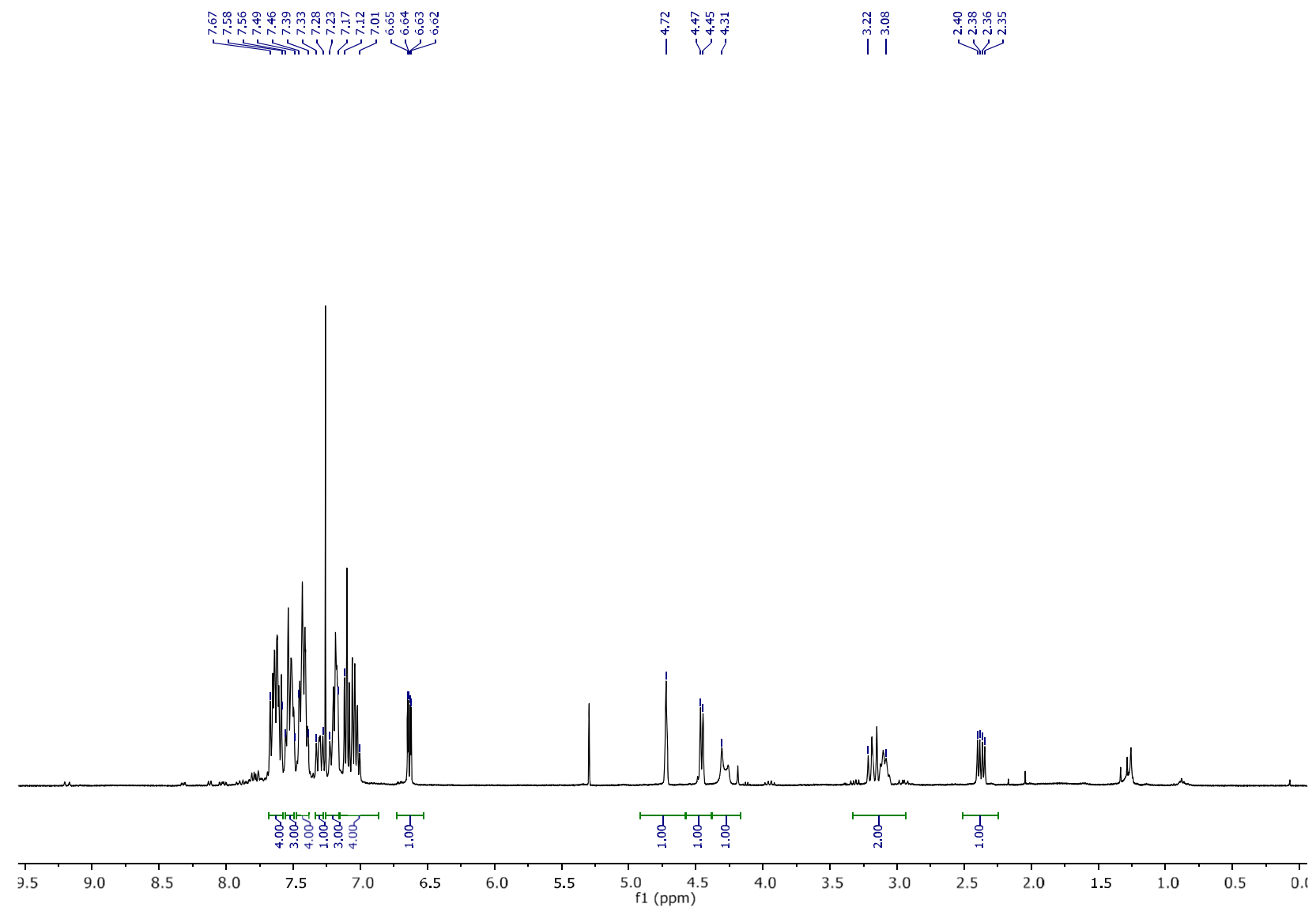
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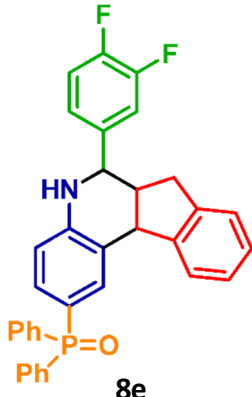
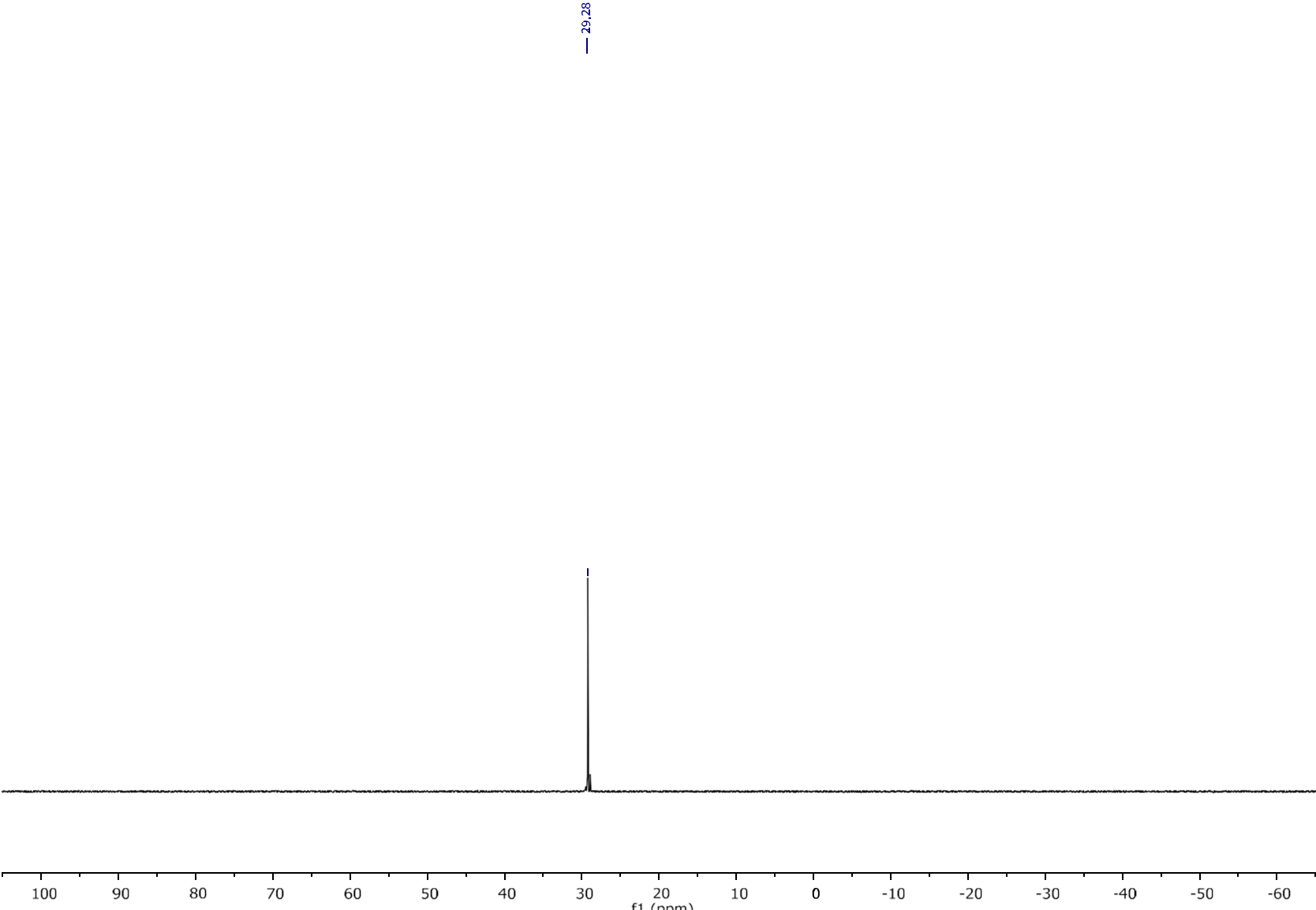


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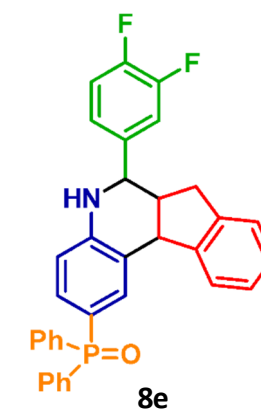
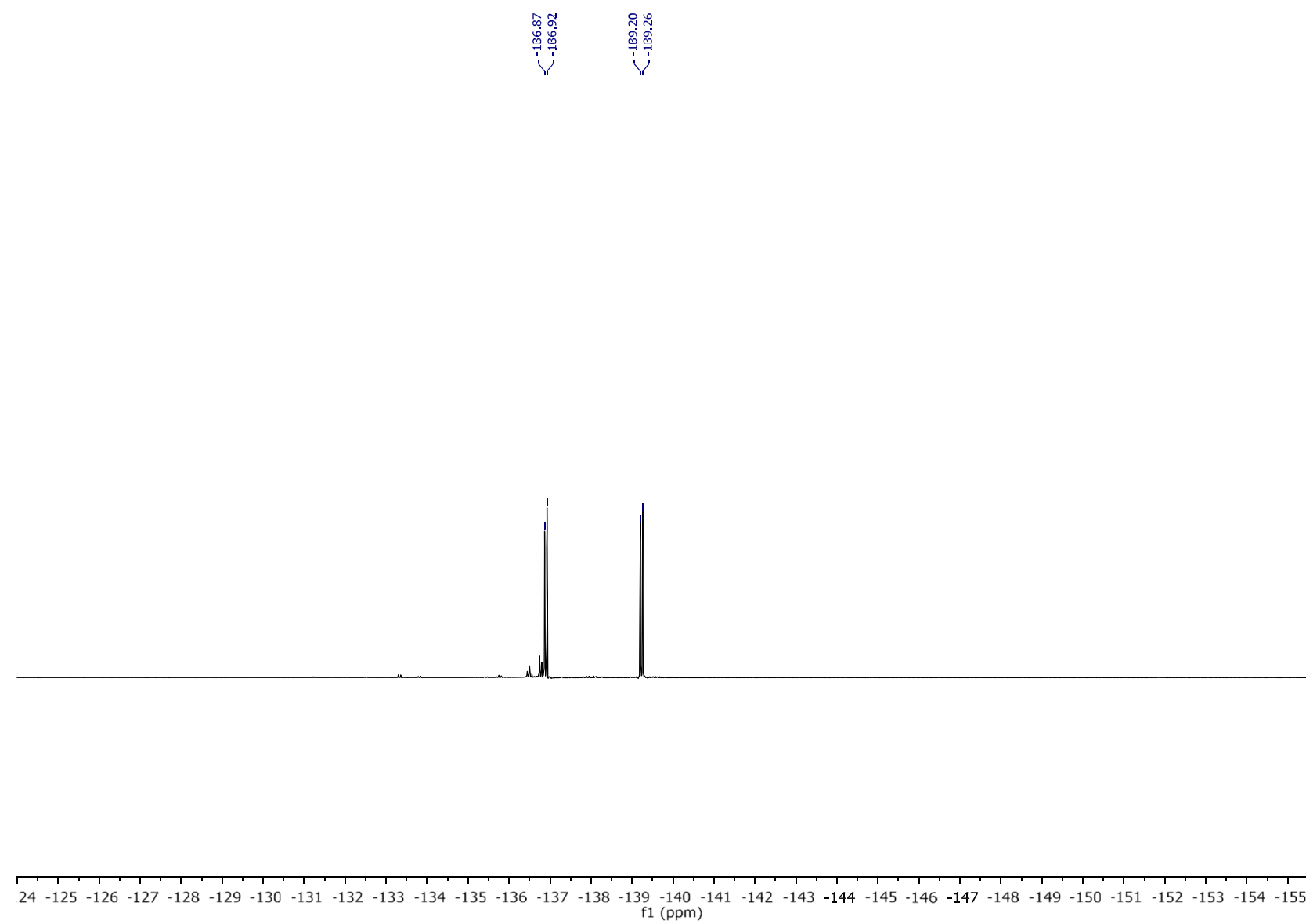


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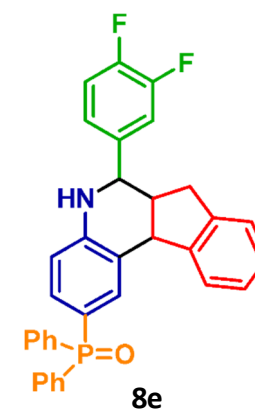
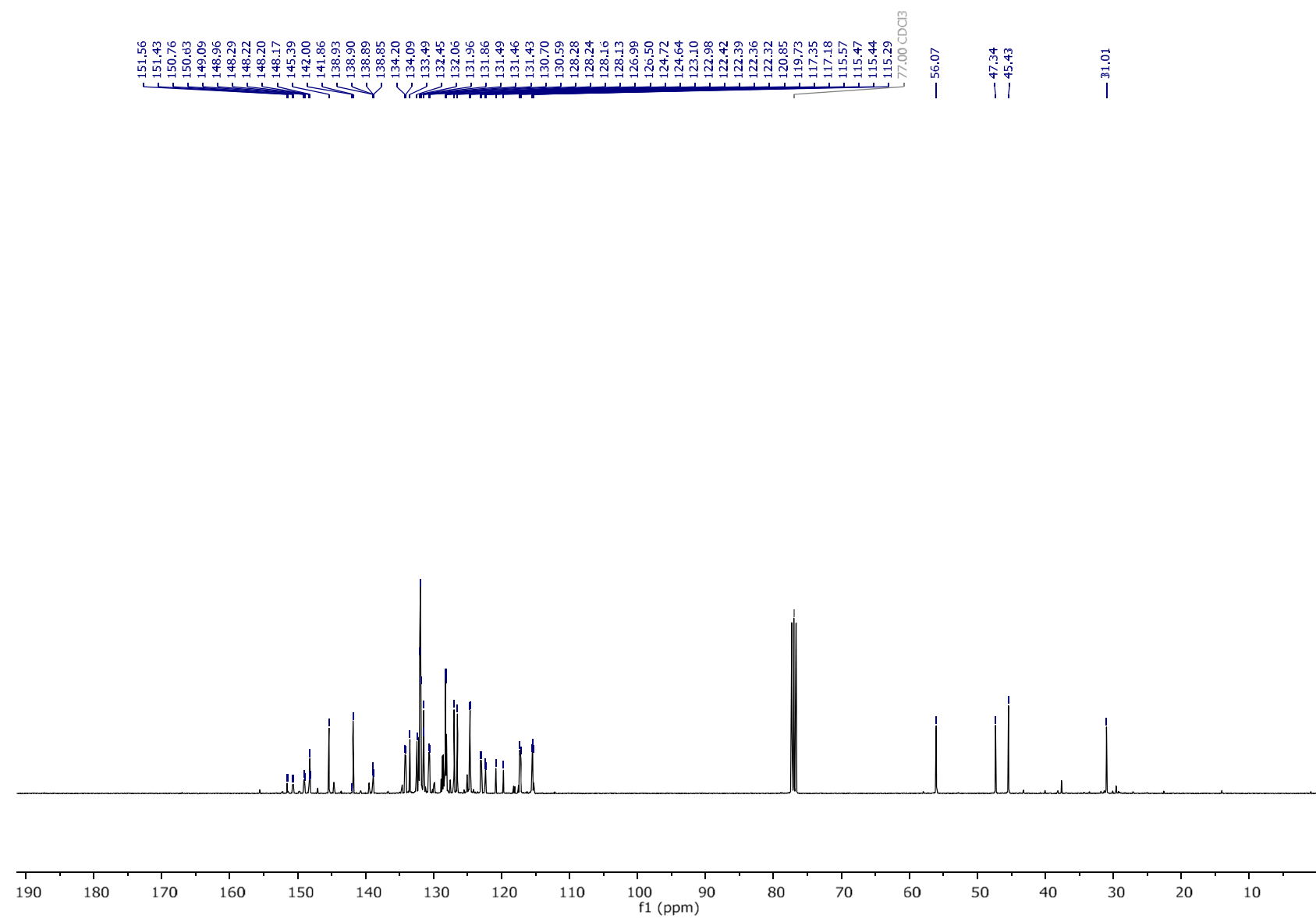


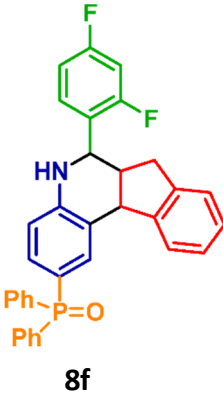
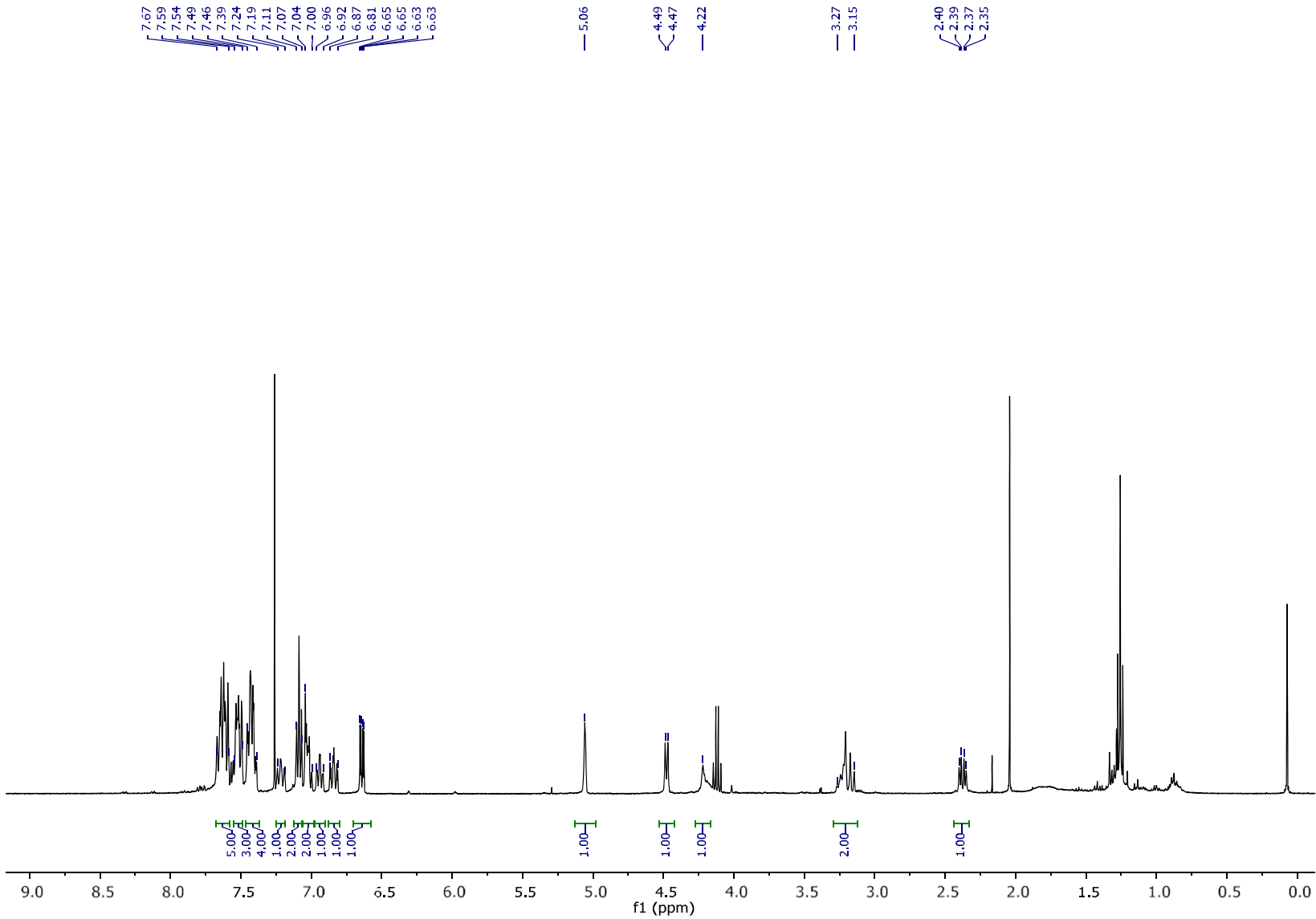
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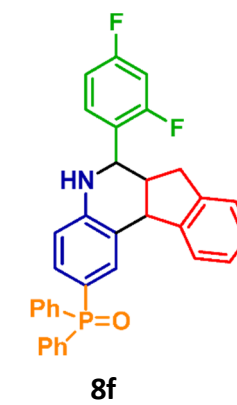
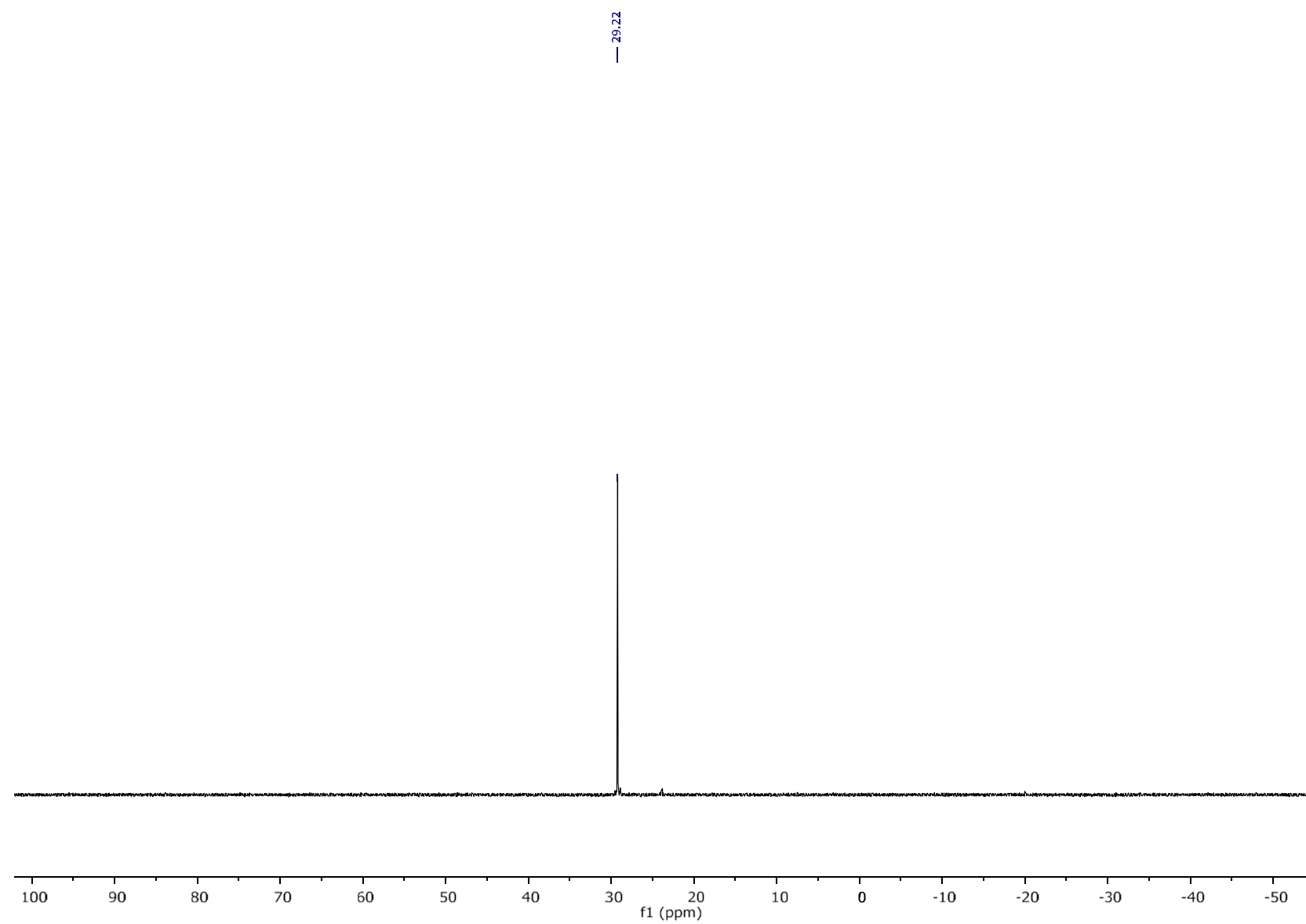


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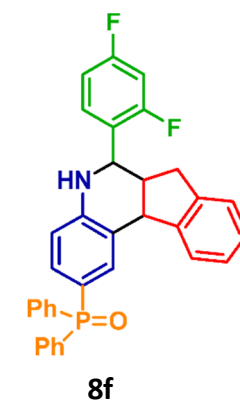
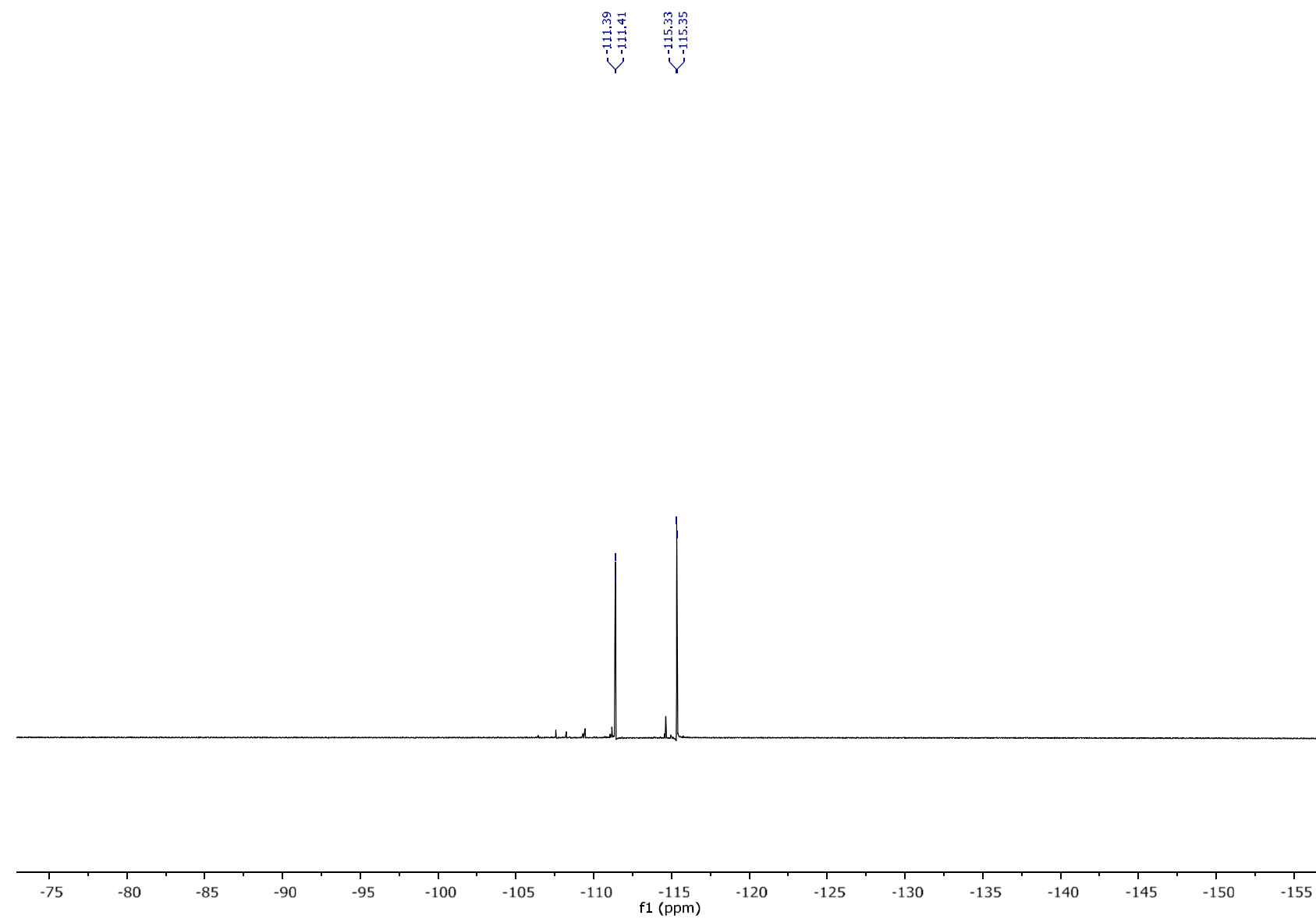


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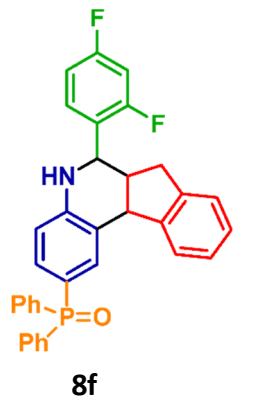
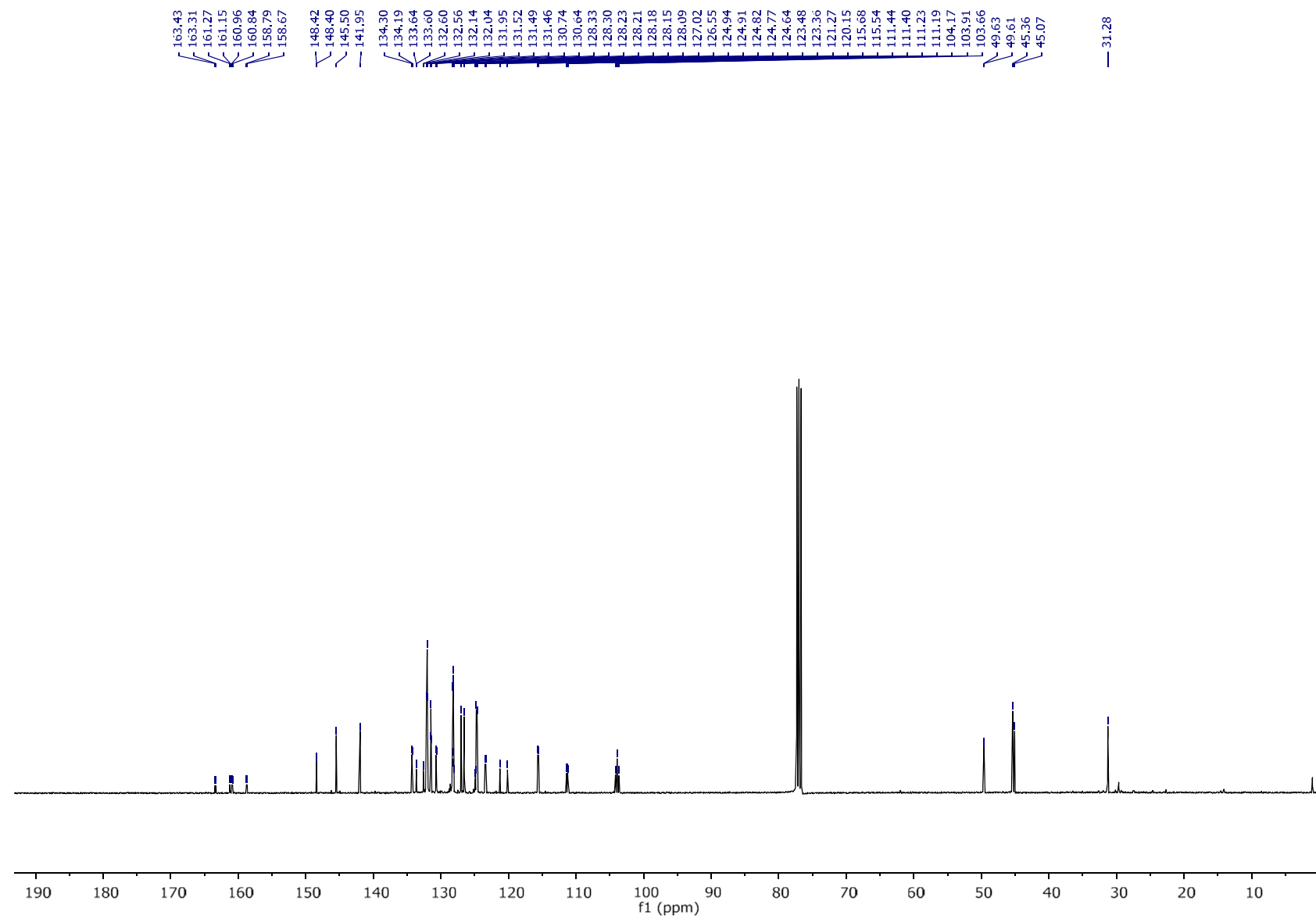
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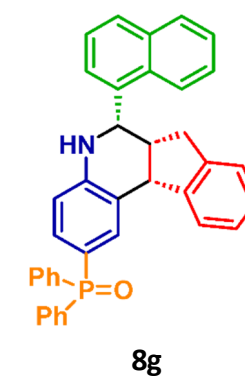
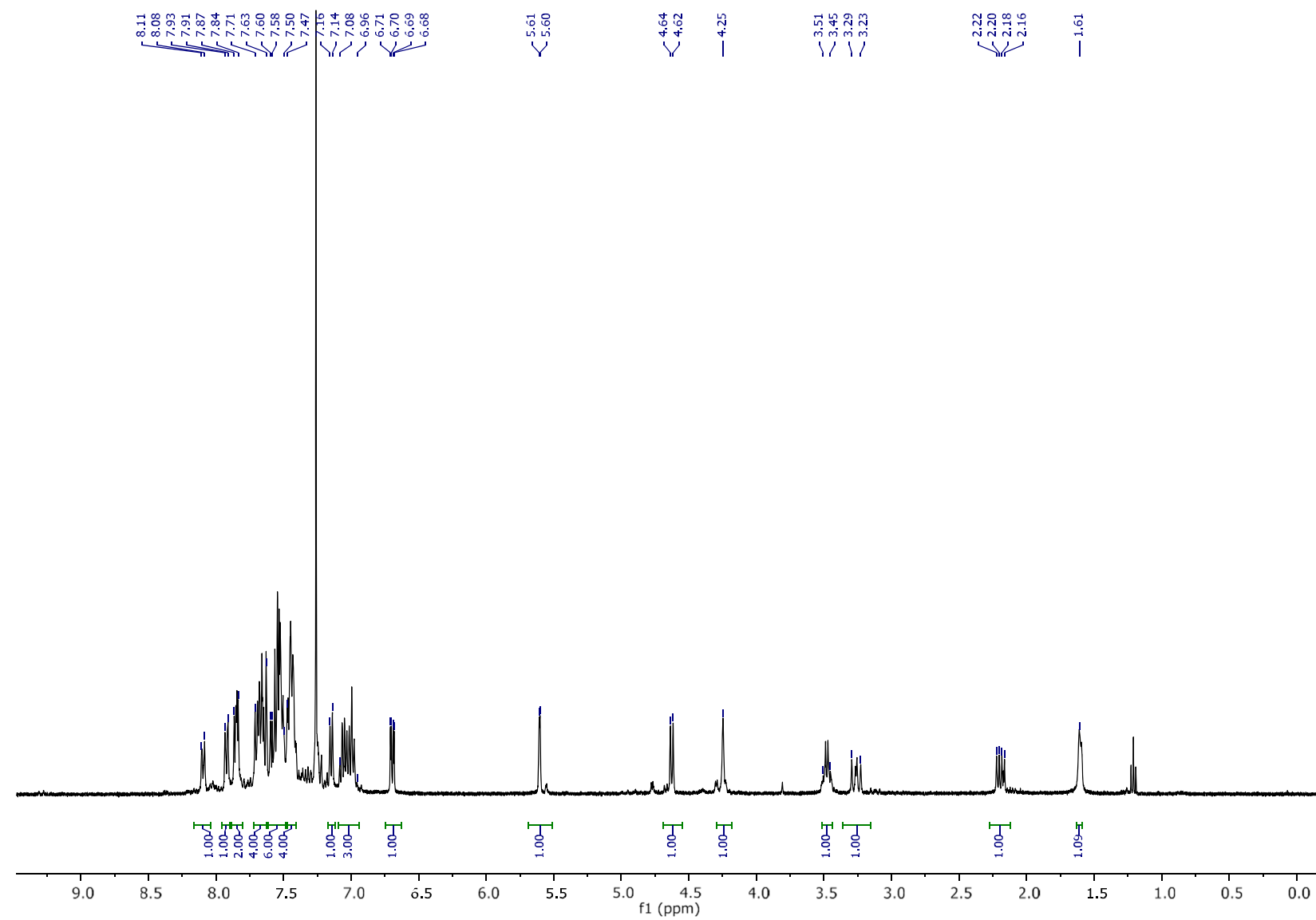
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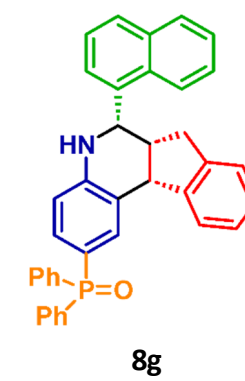
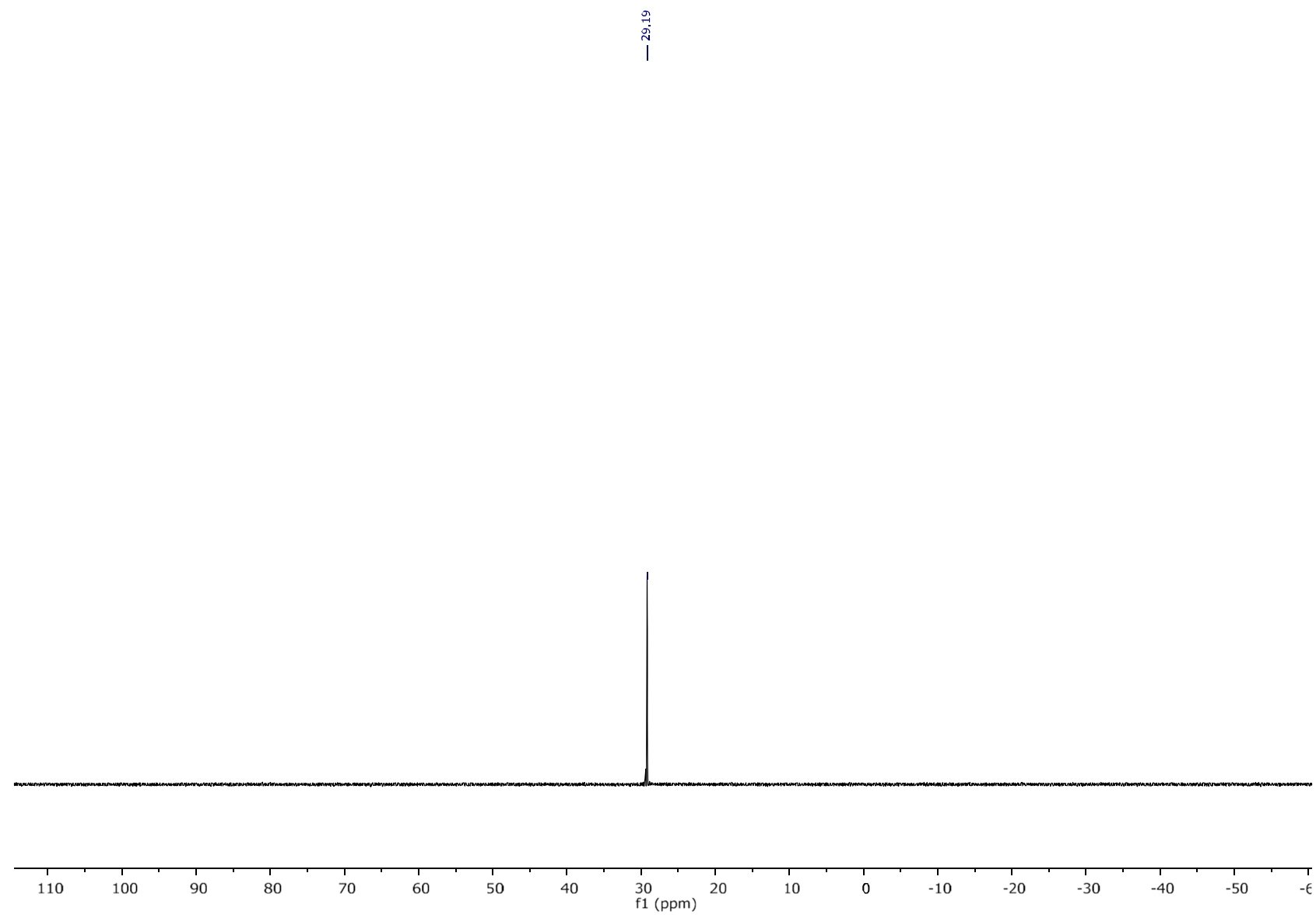
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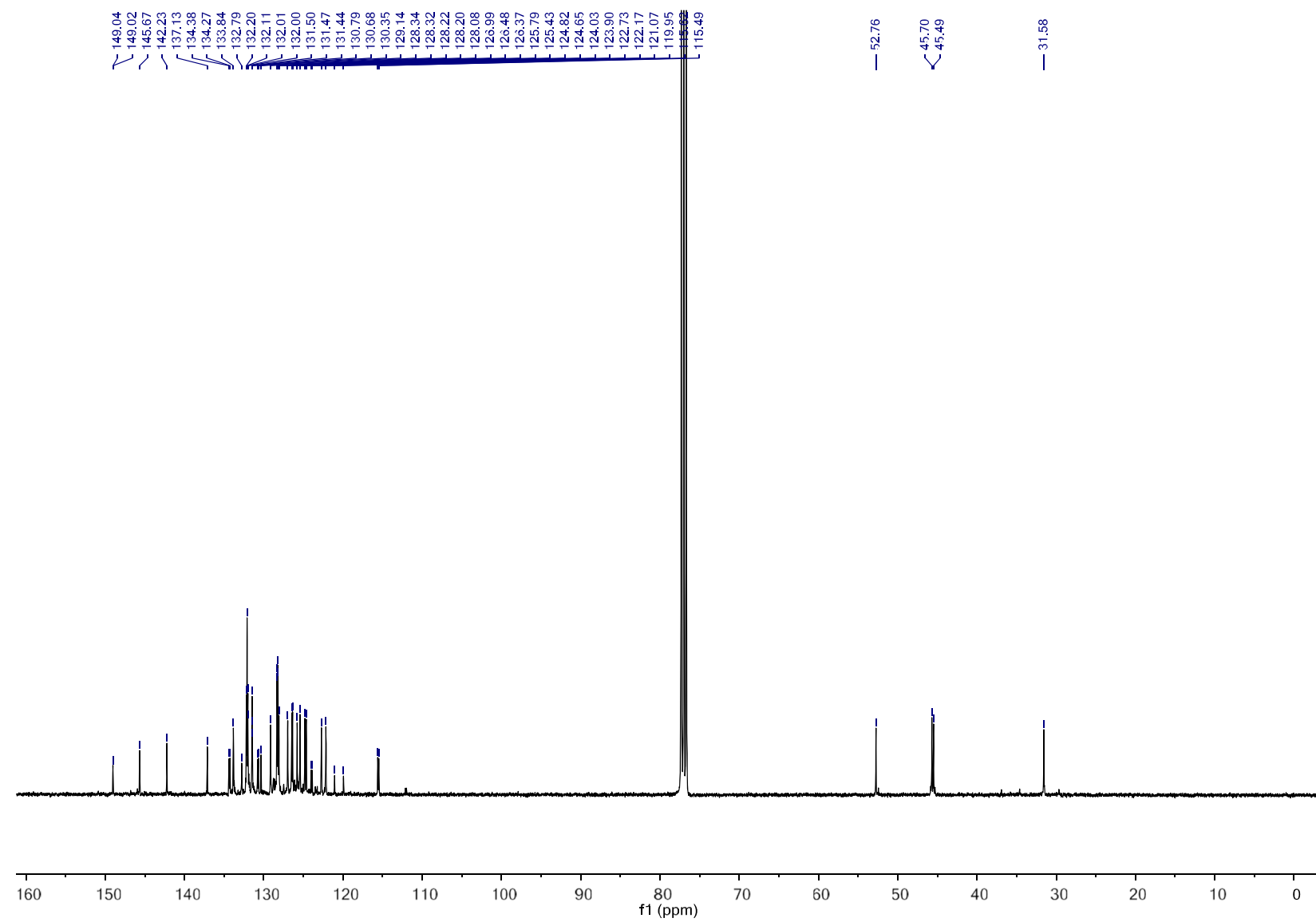
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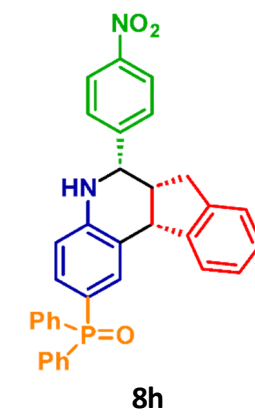
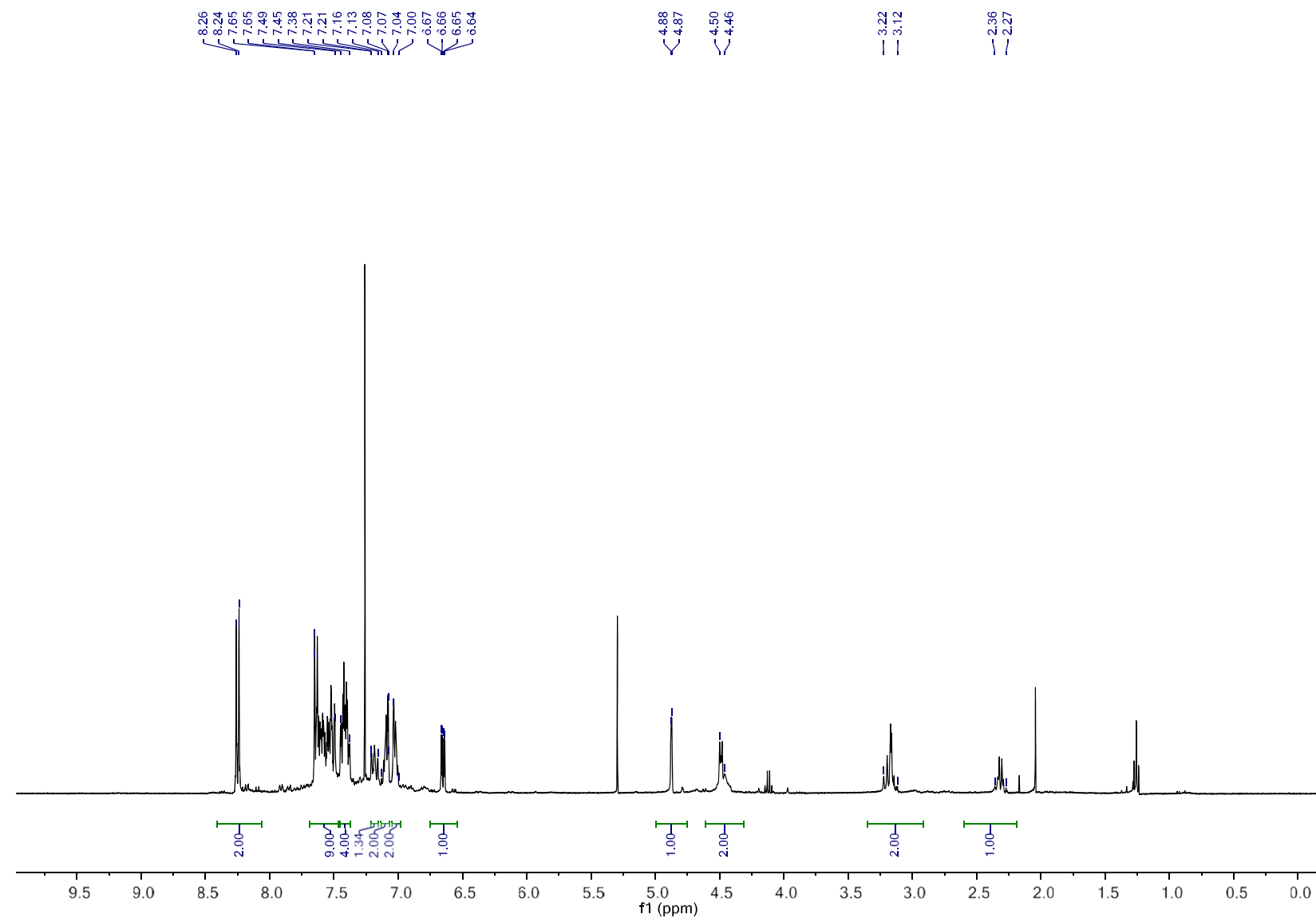
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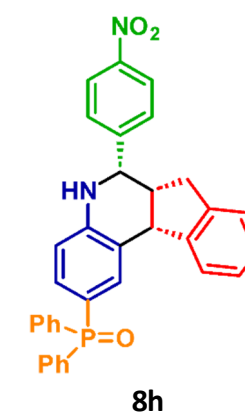
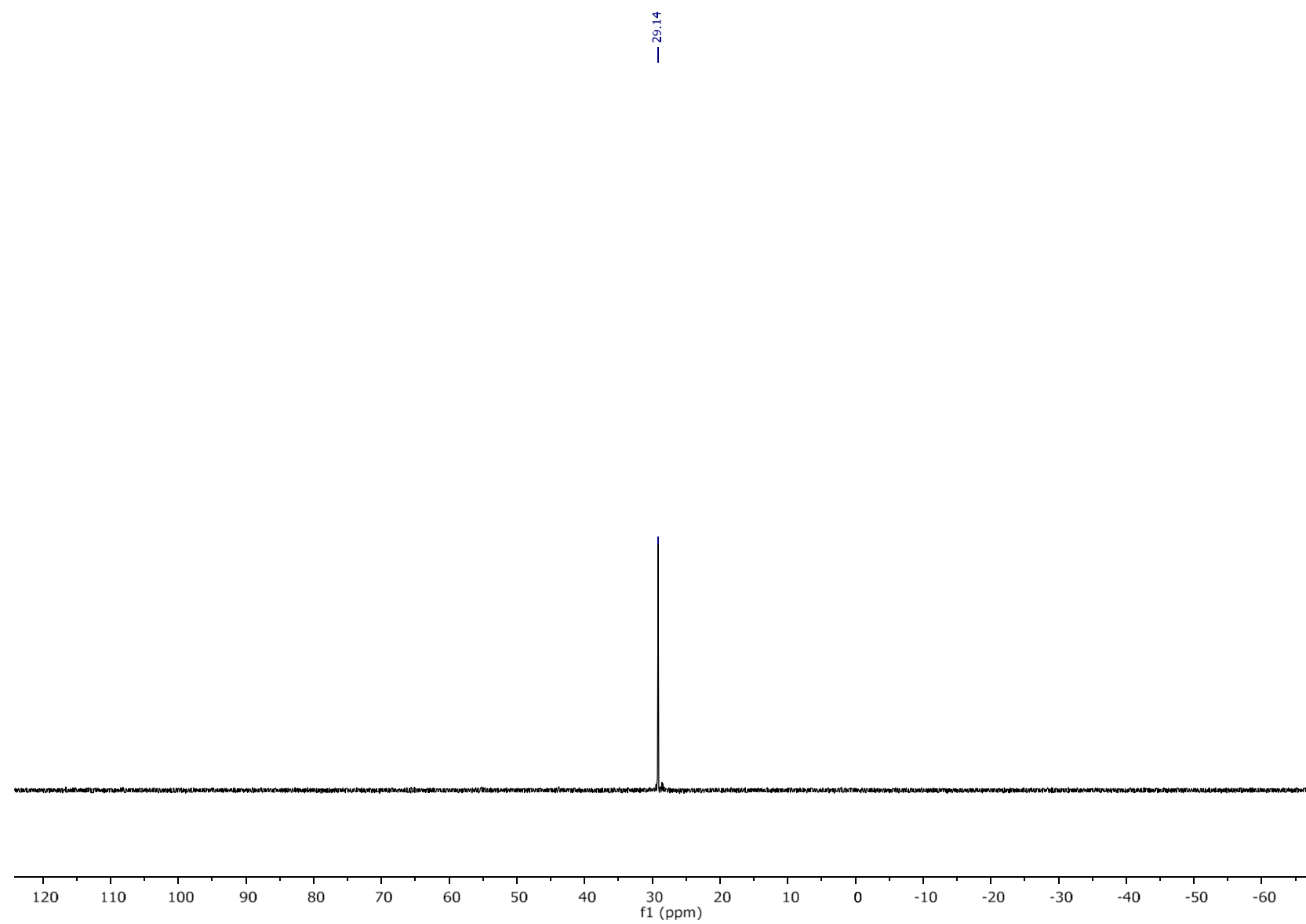
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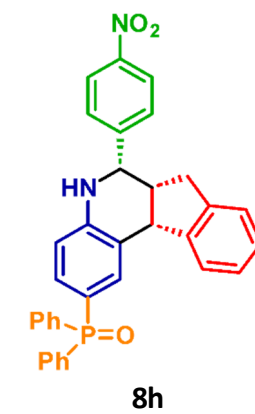
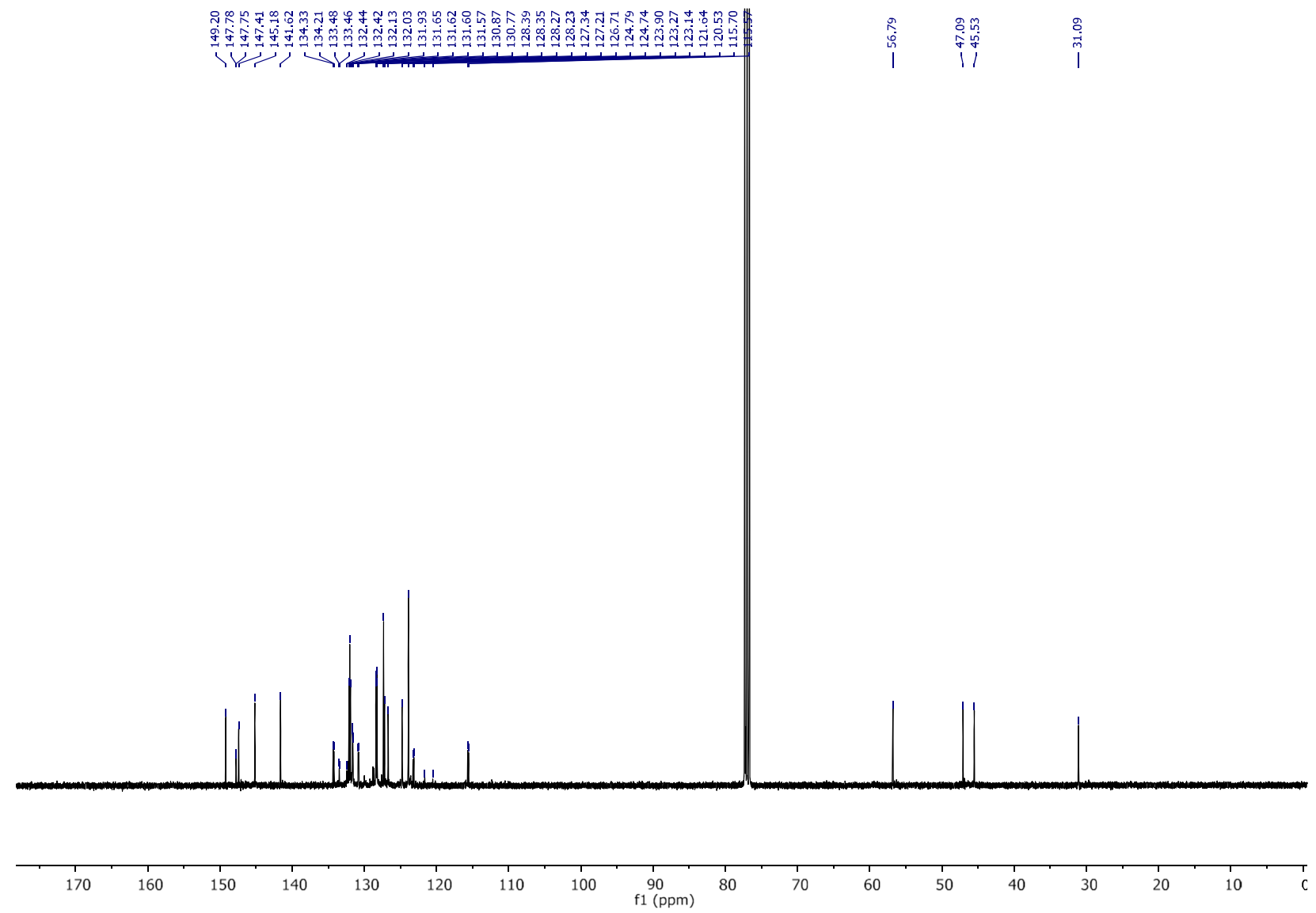
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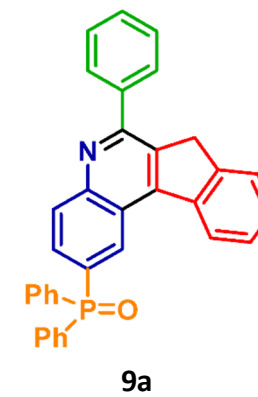
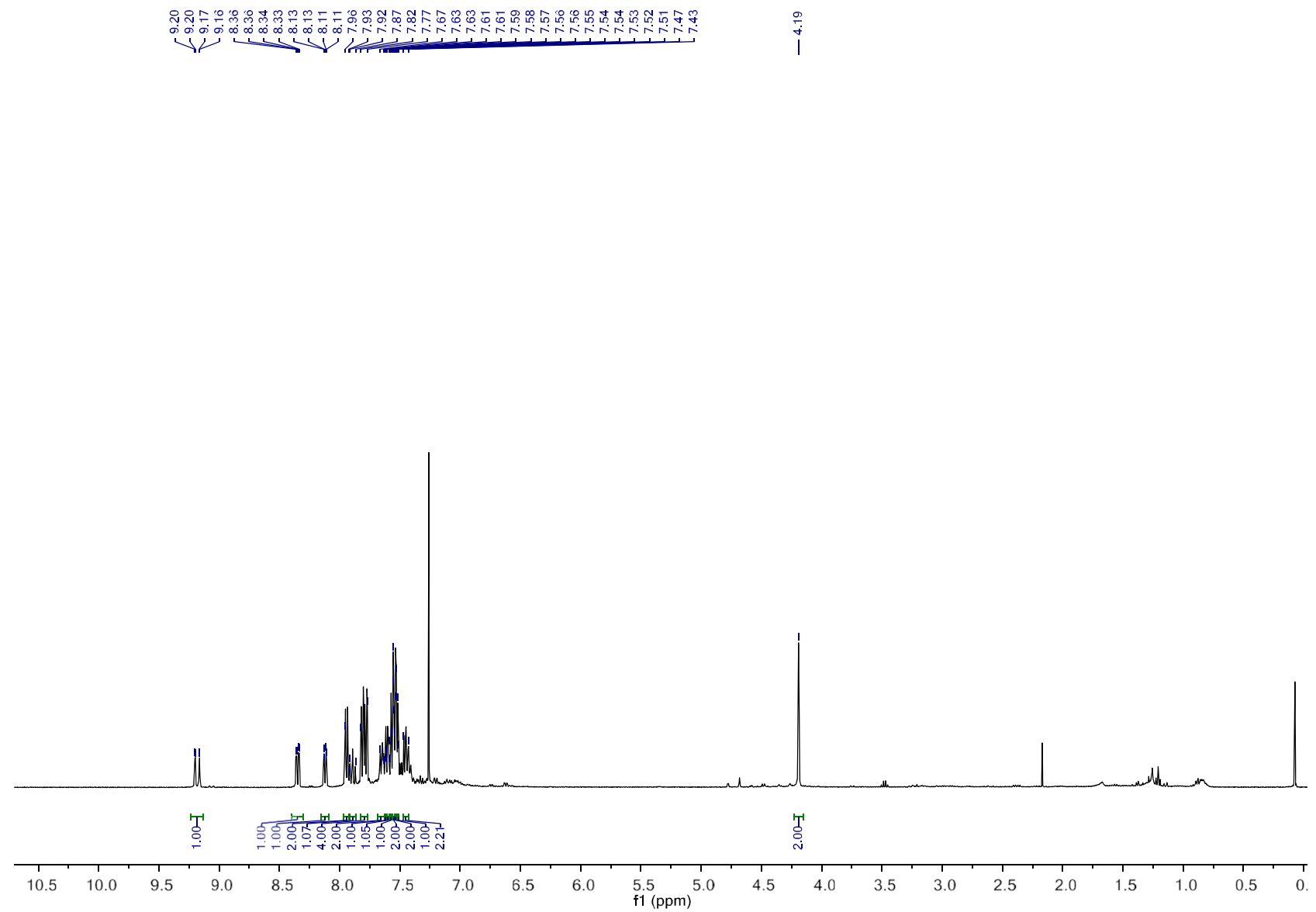
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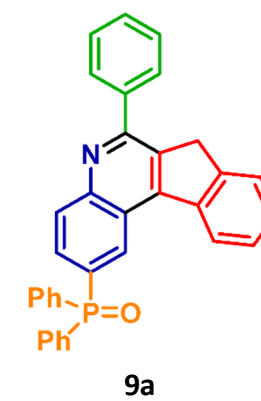
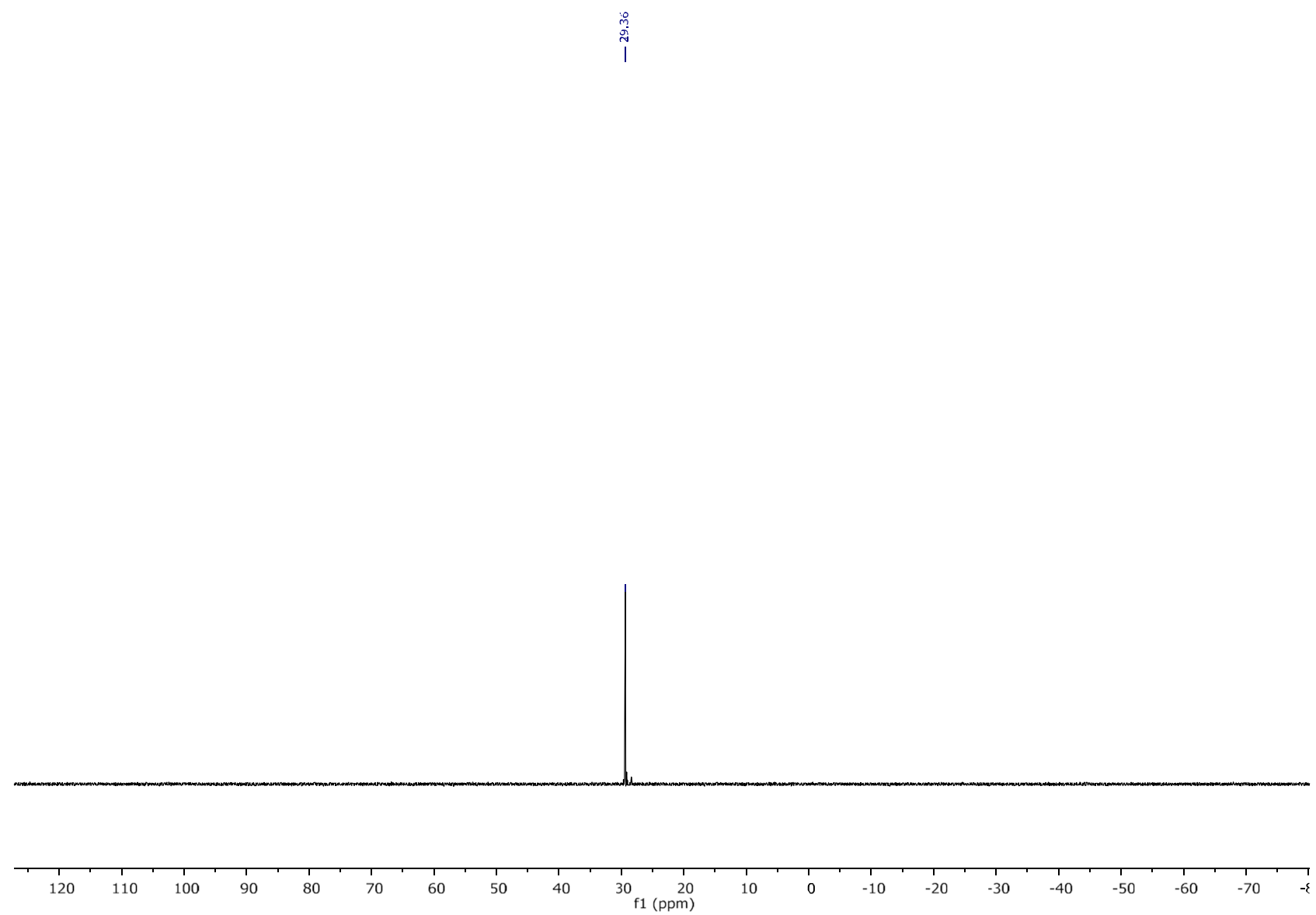
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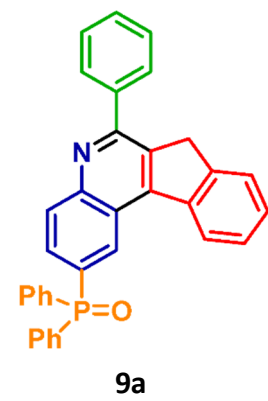
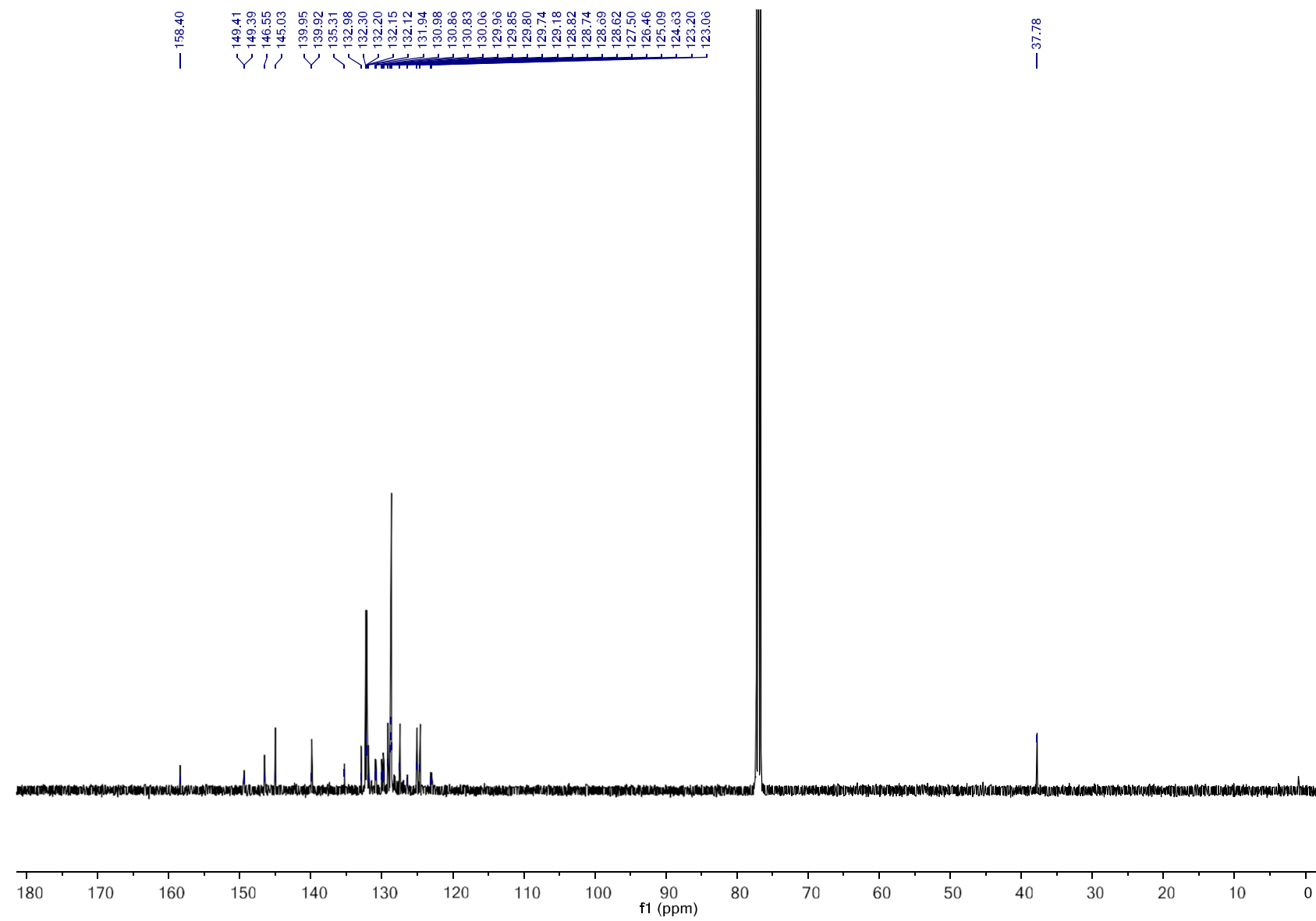
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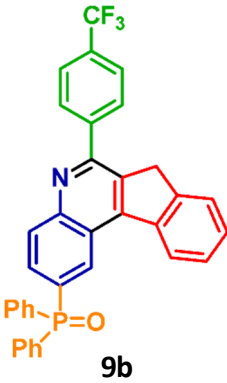
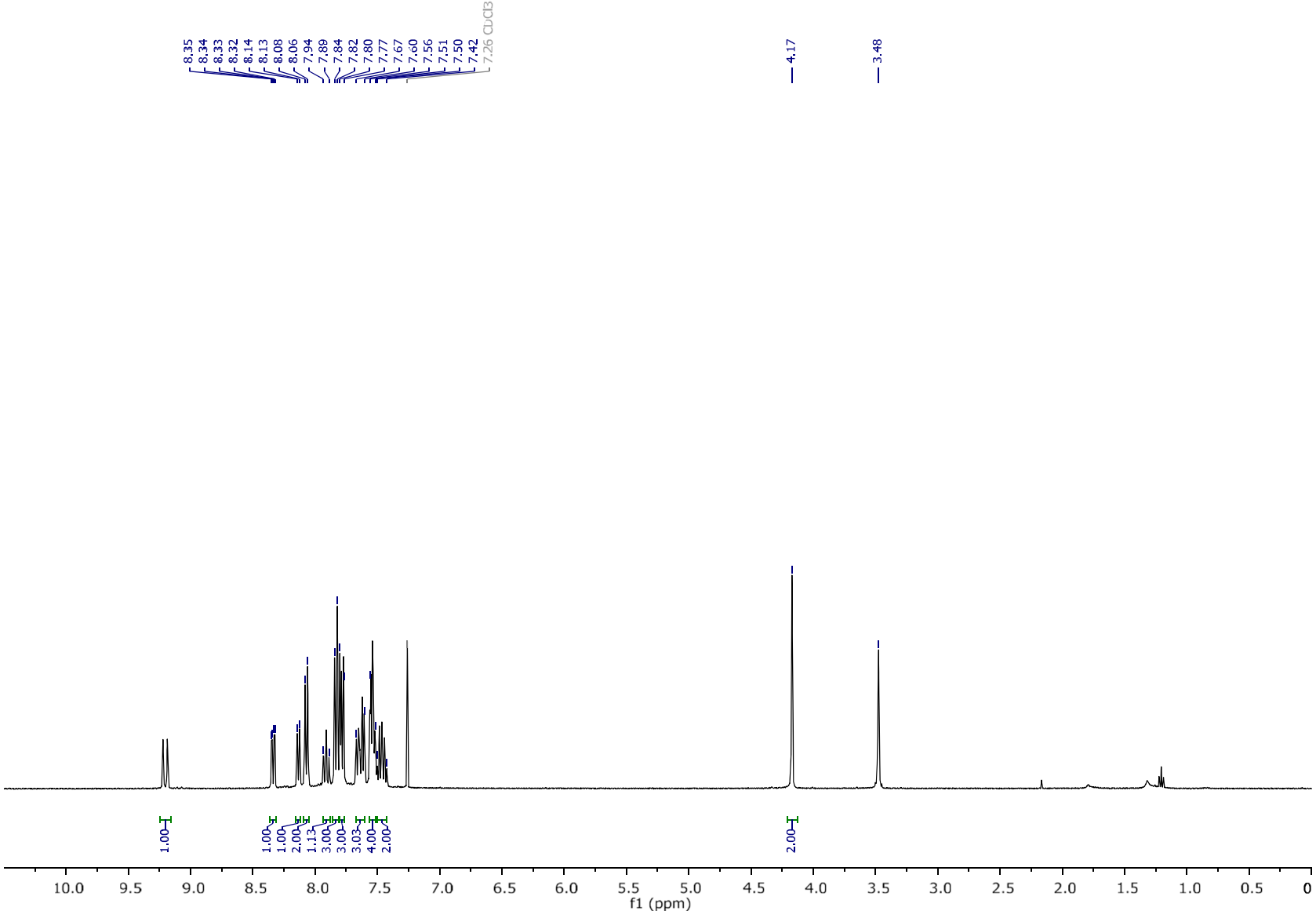


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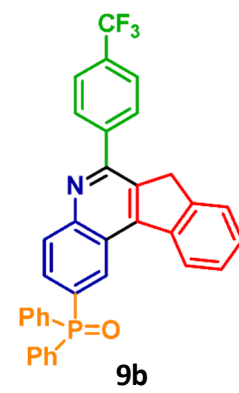
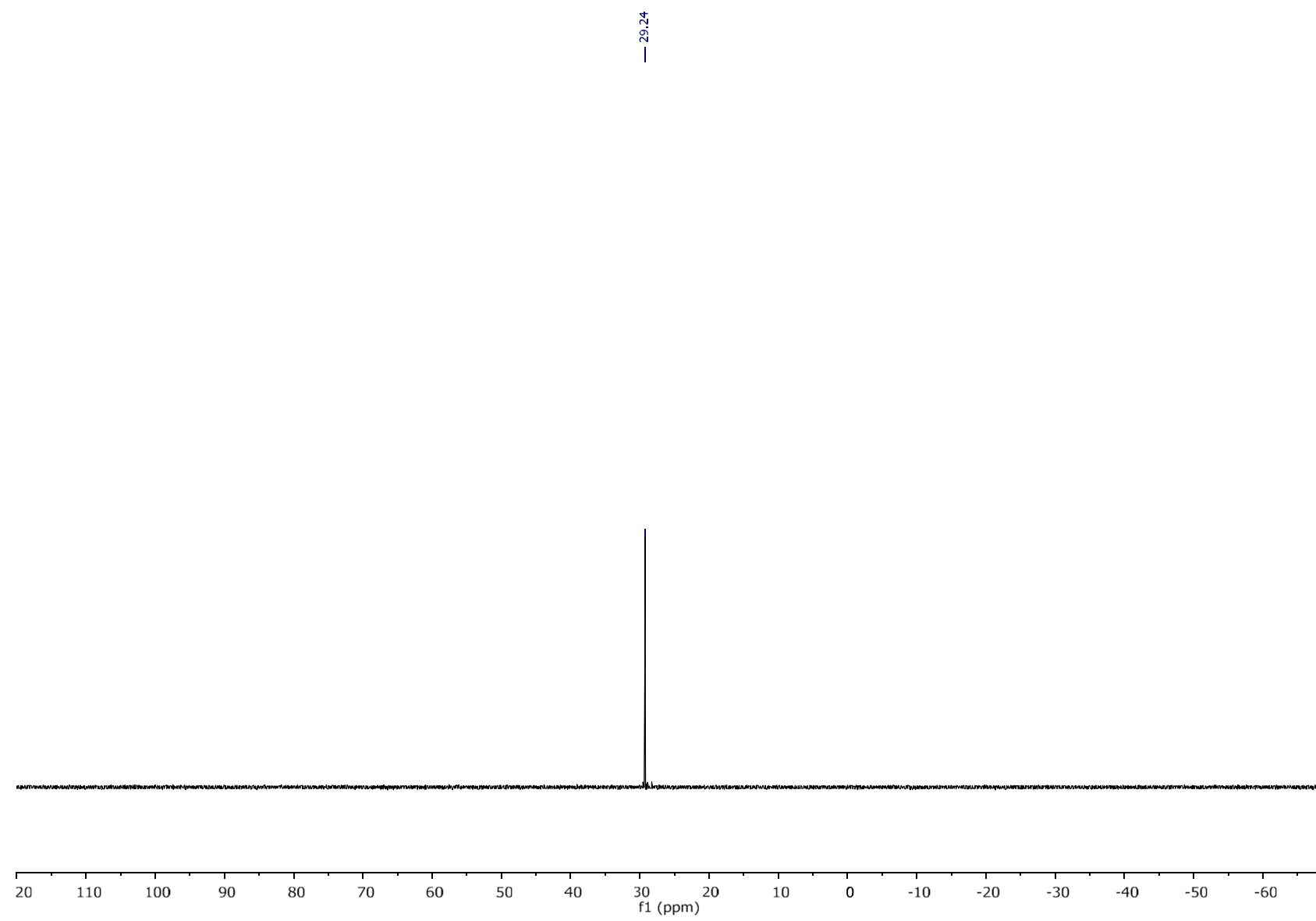


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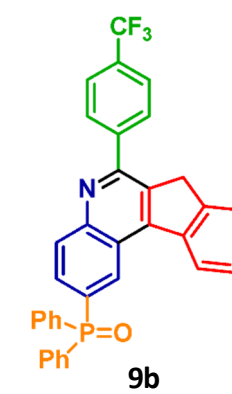
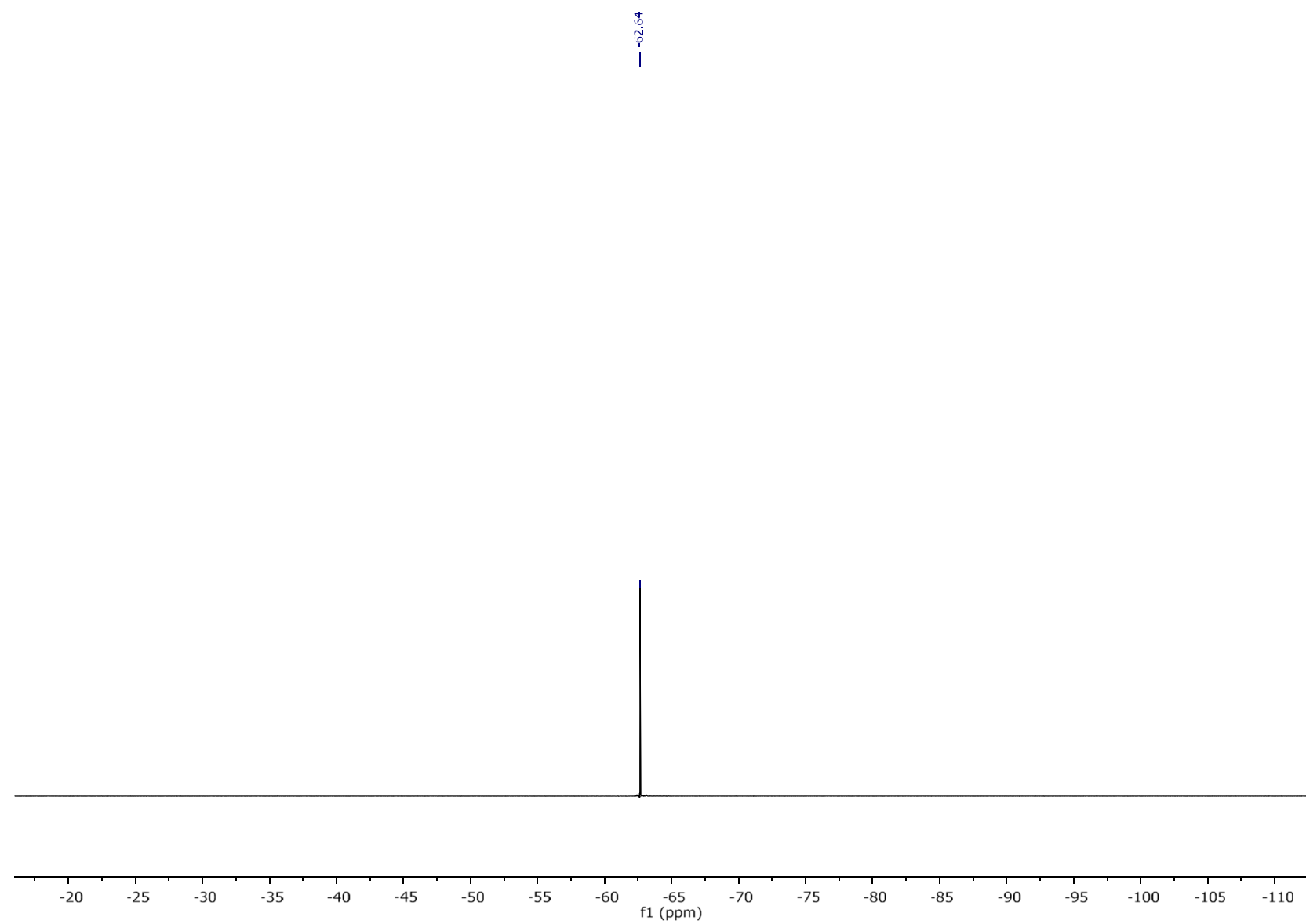


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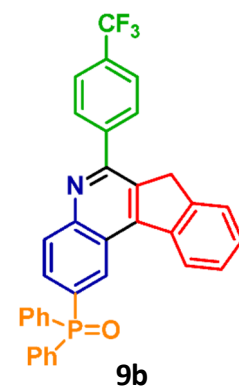
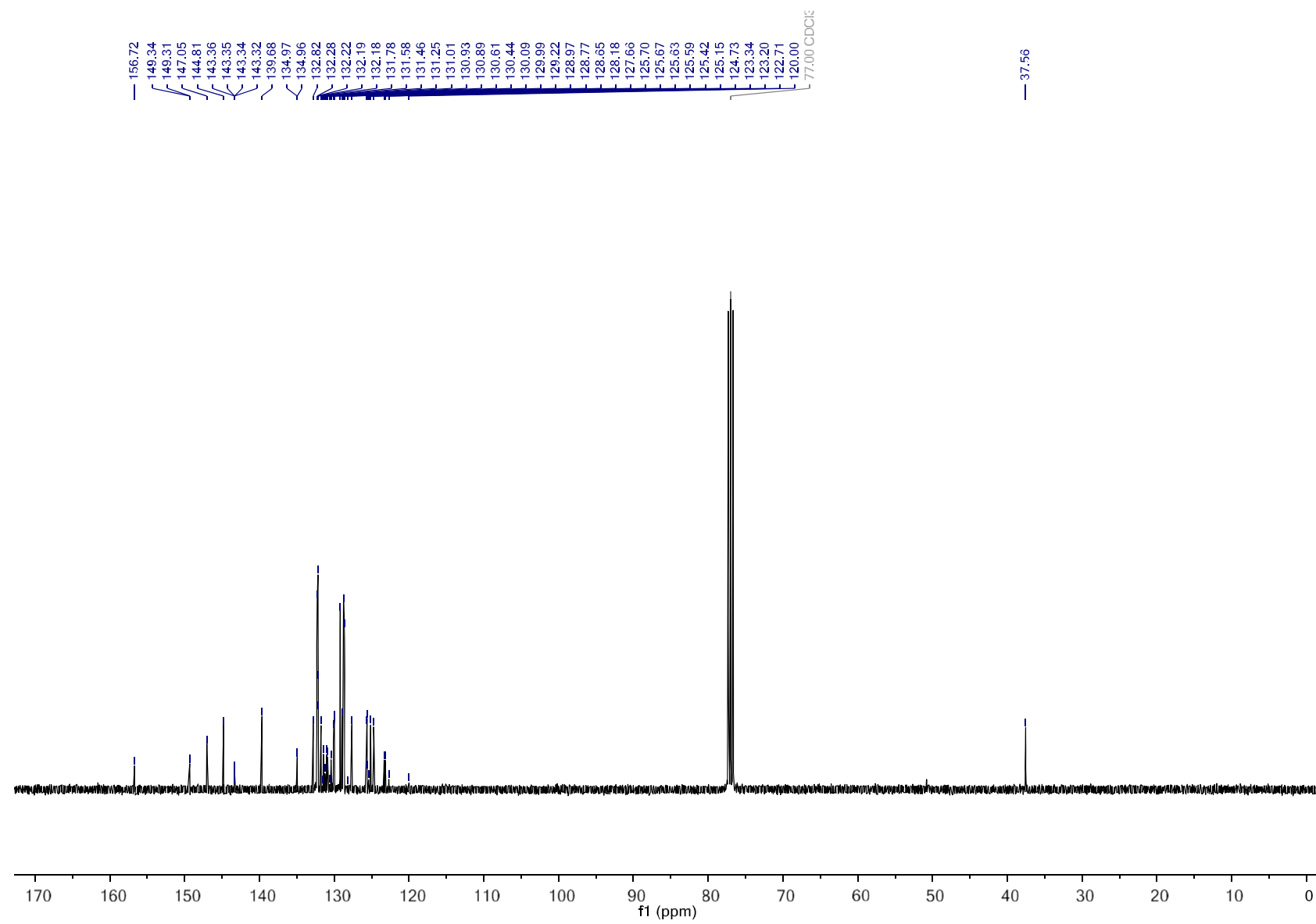
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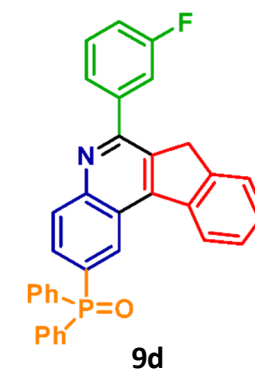
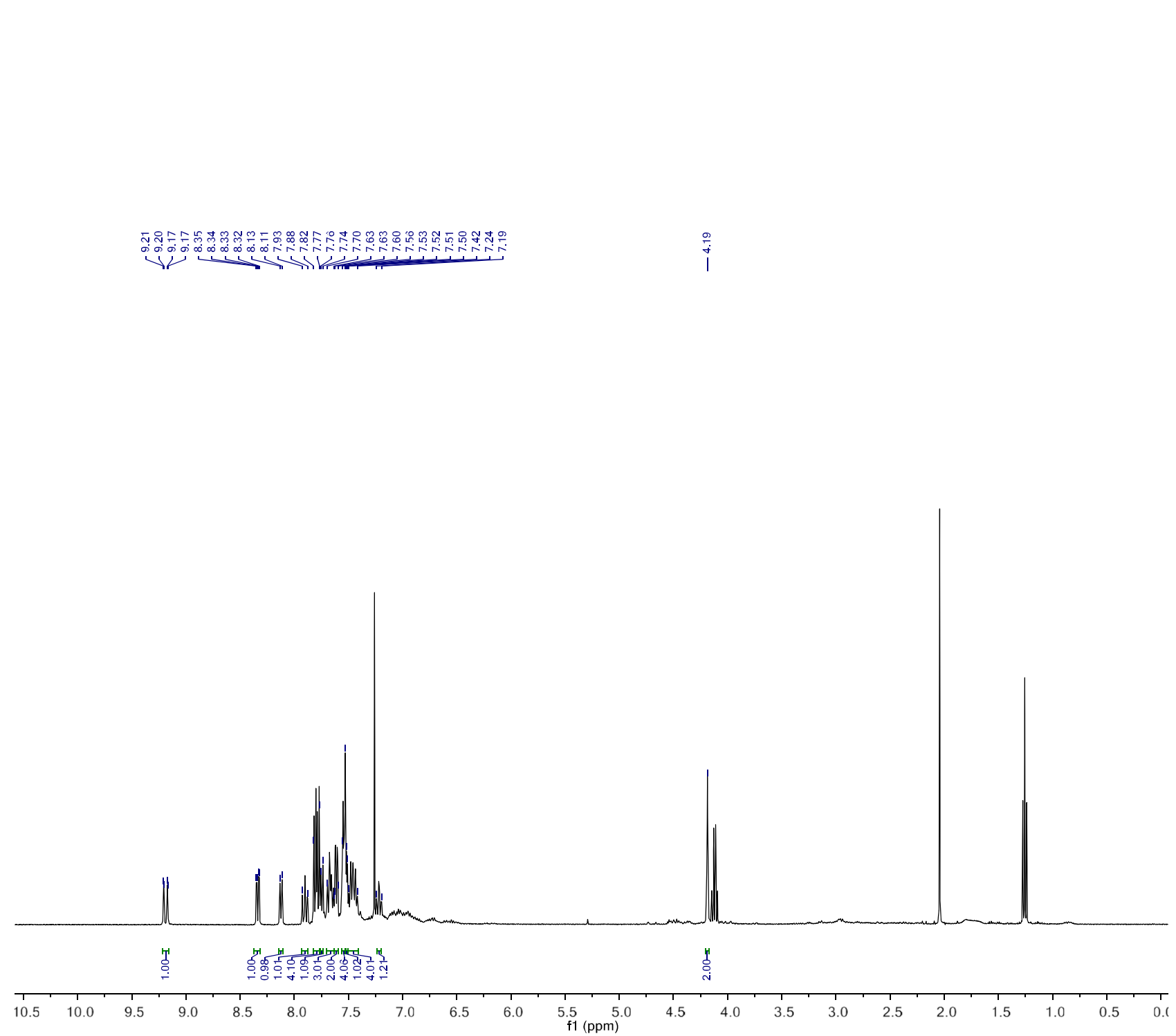
^{19}F -RMN



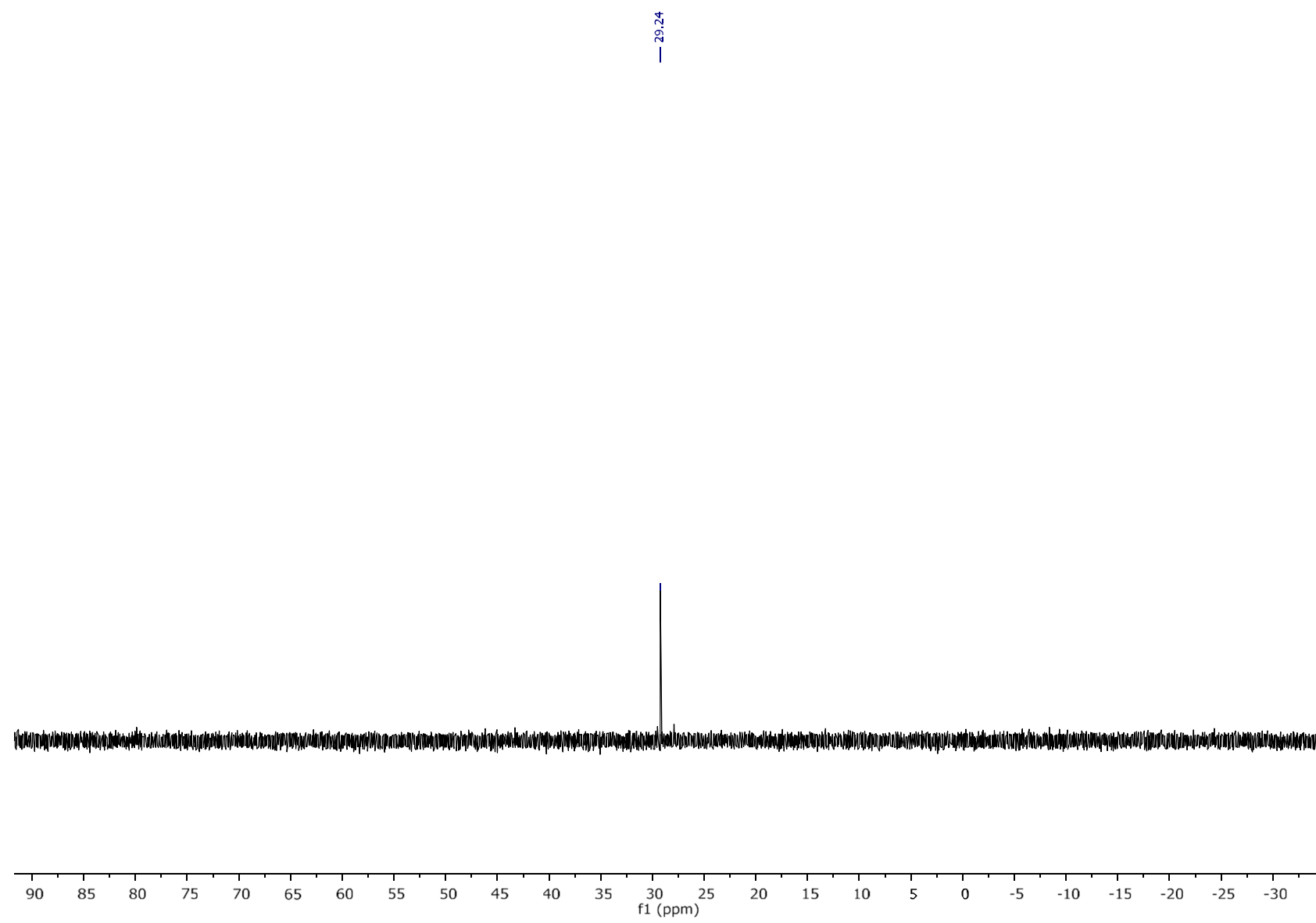
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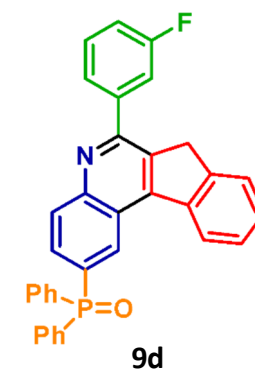
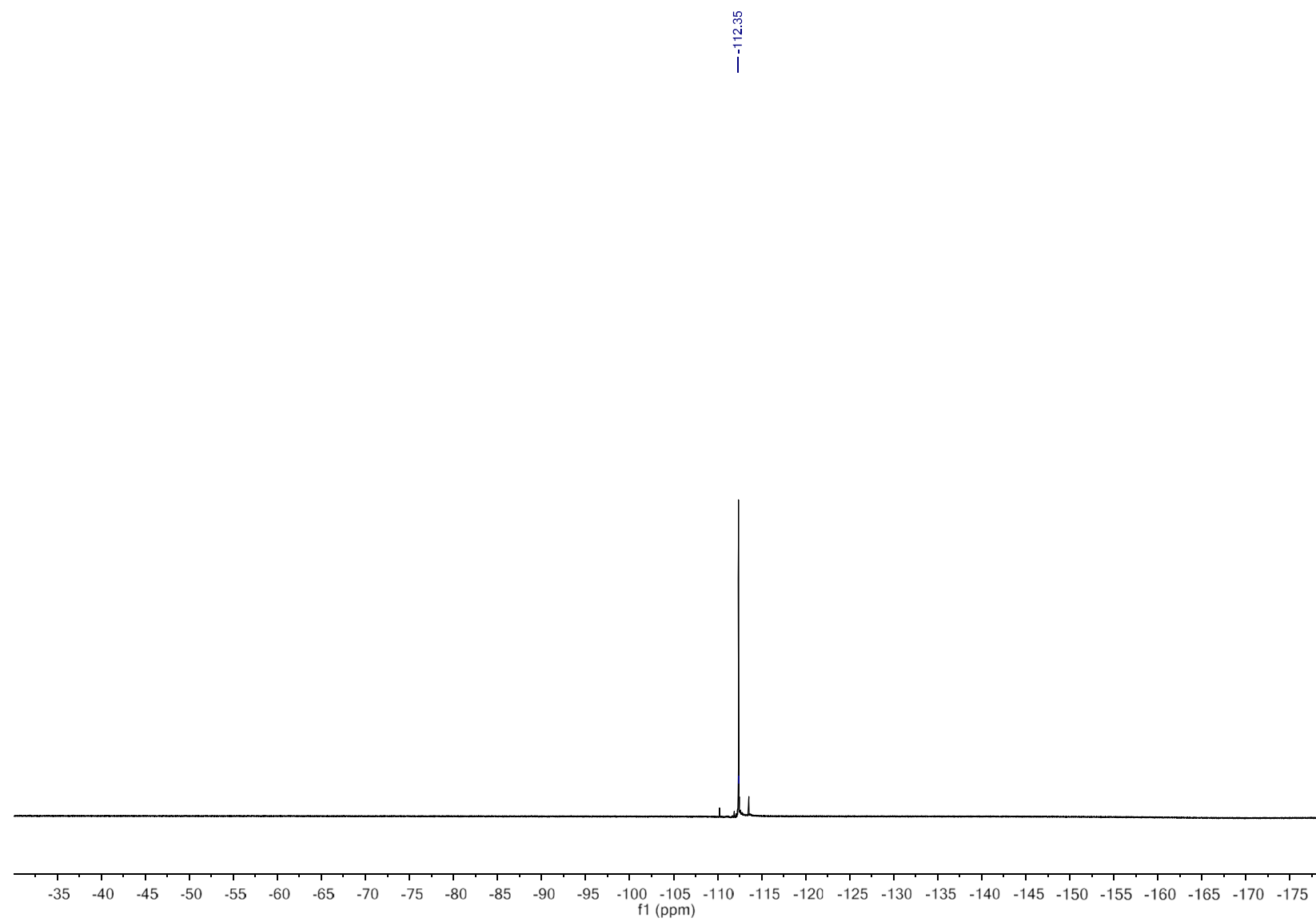
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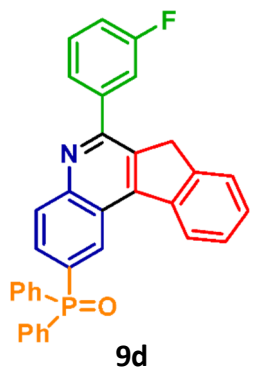
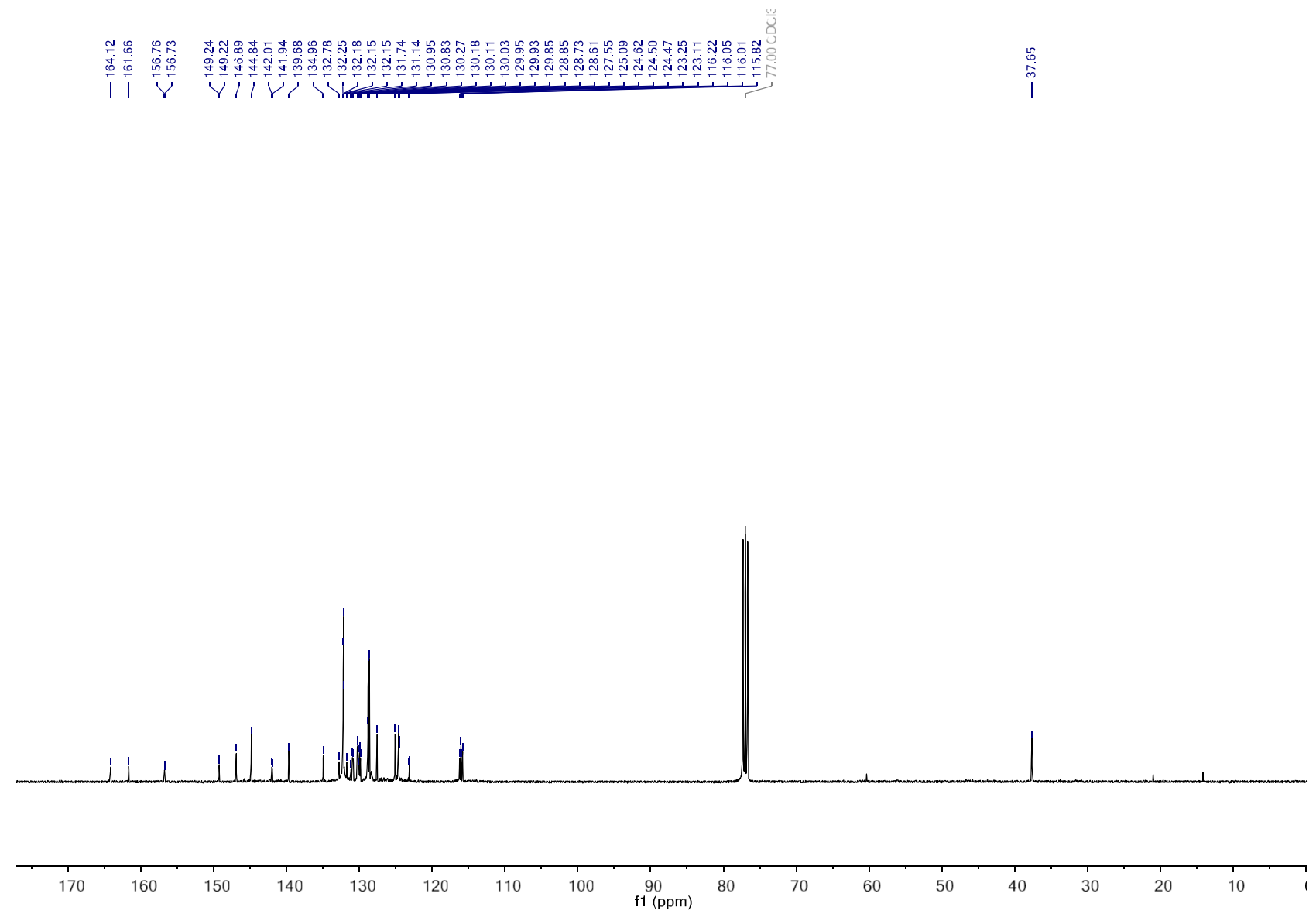
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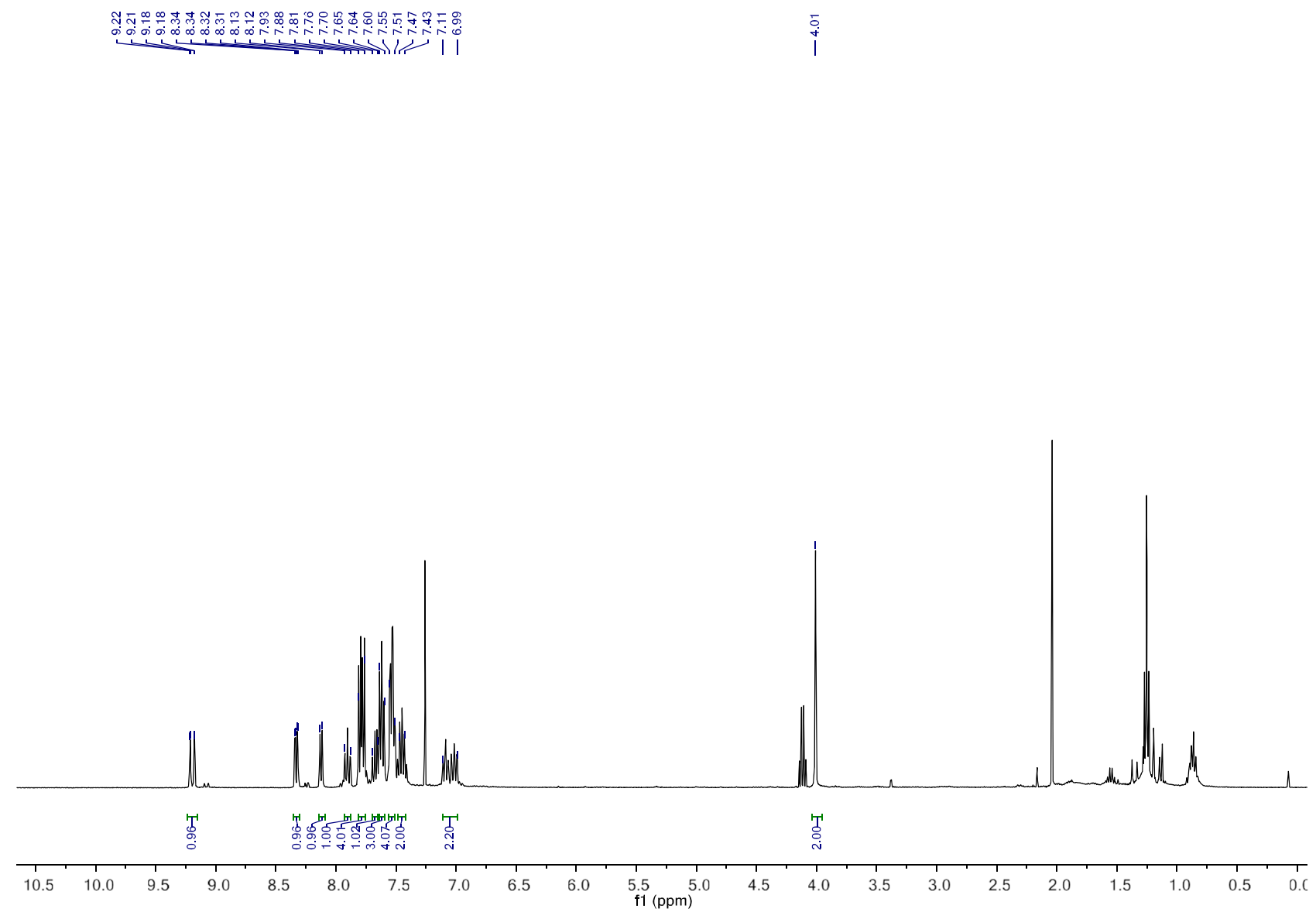
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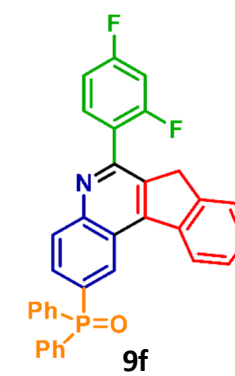
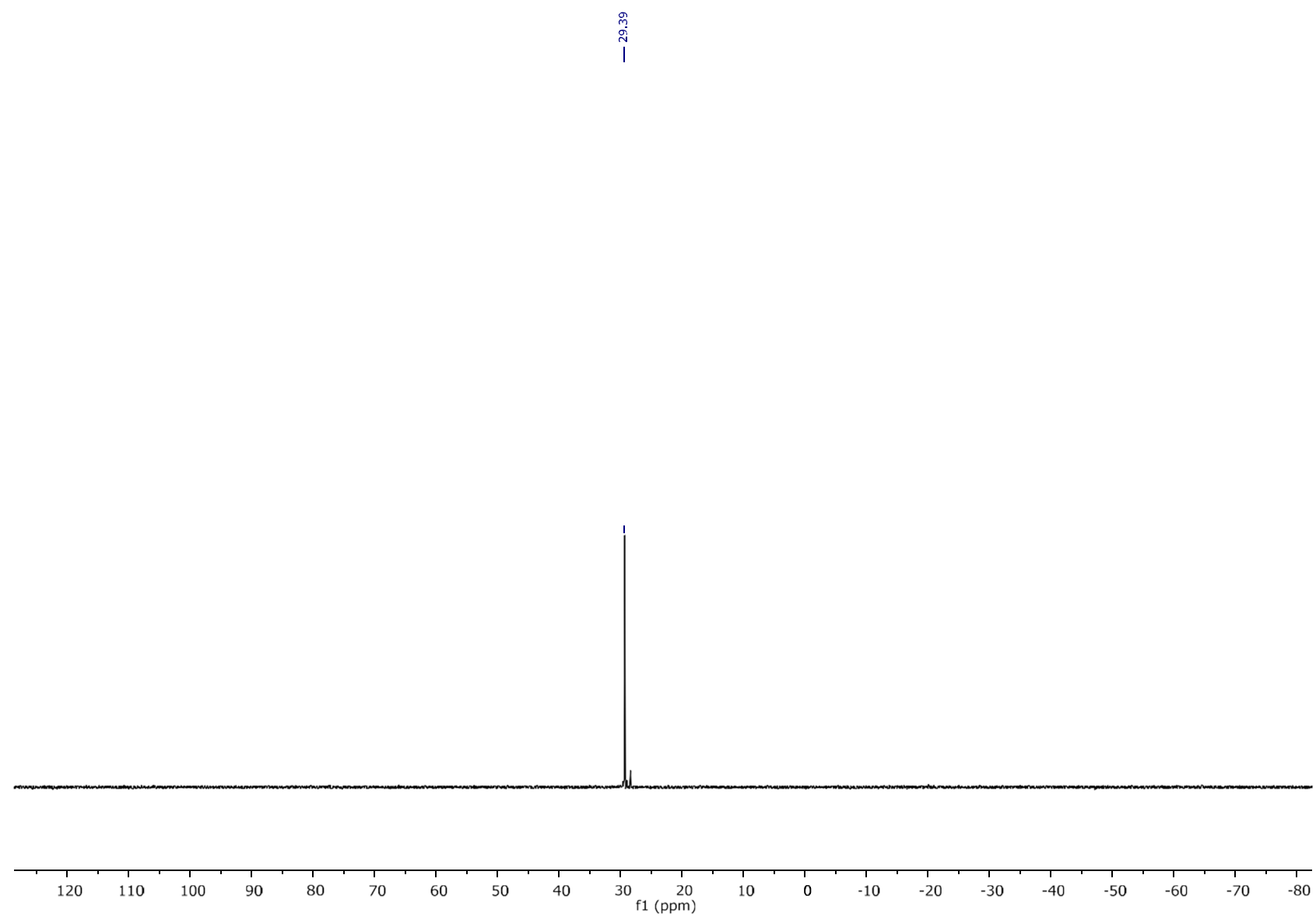
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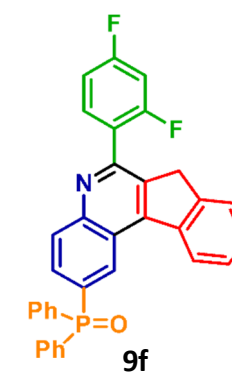
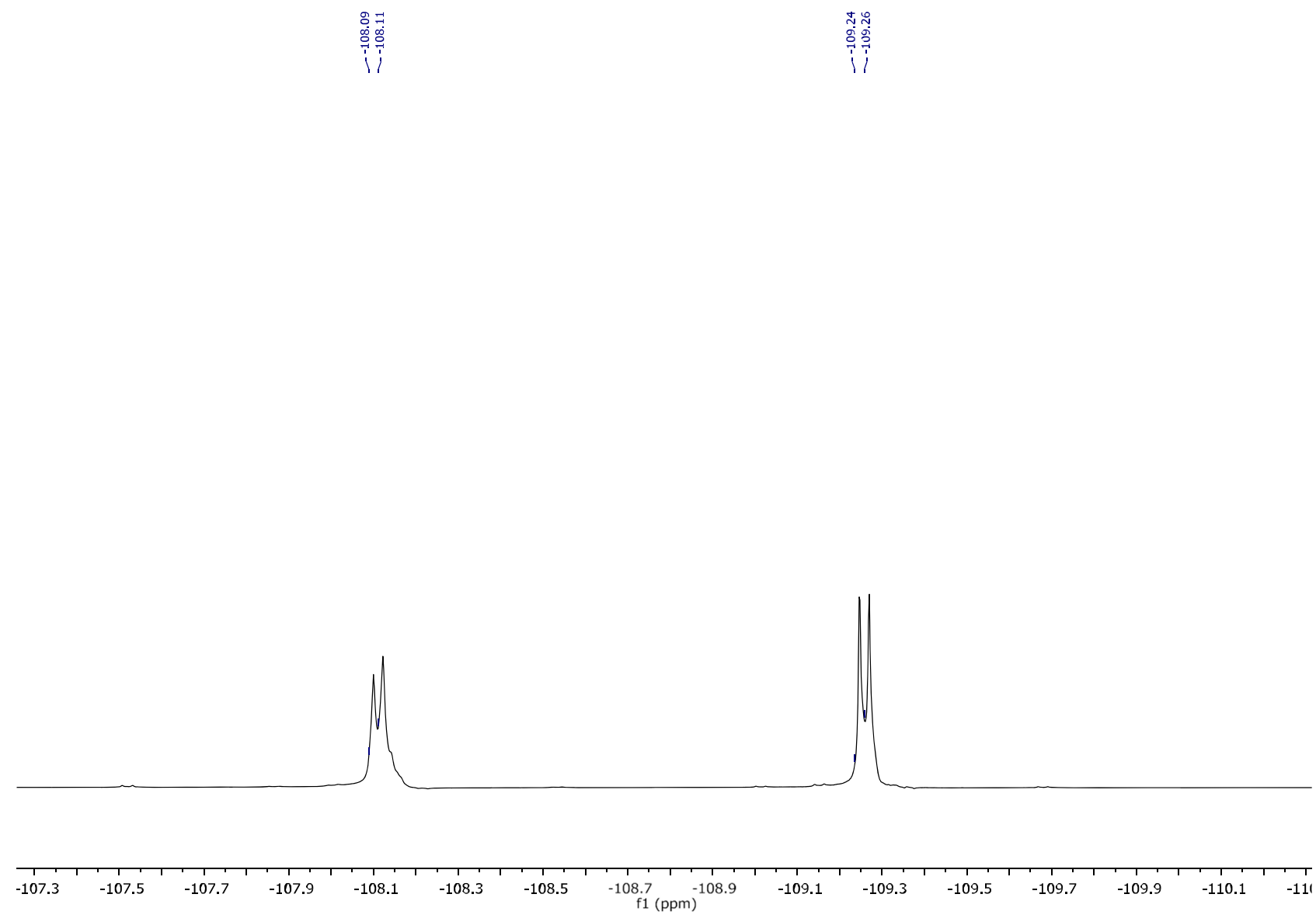
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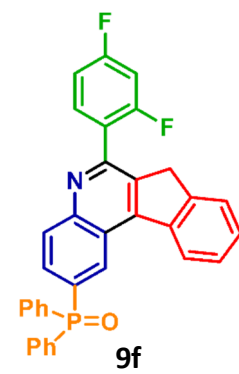
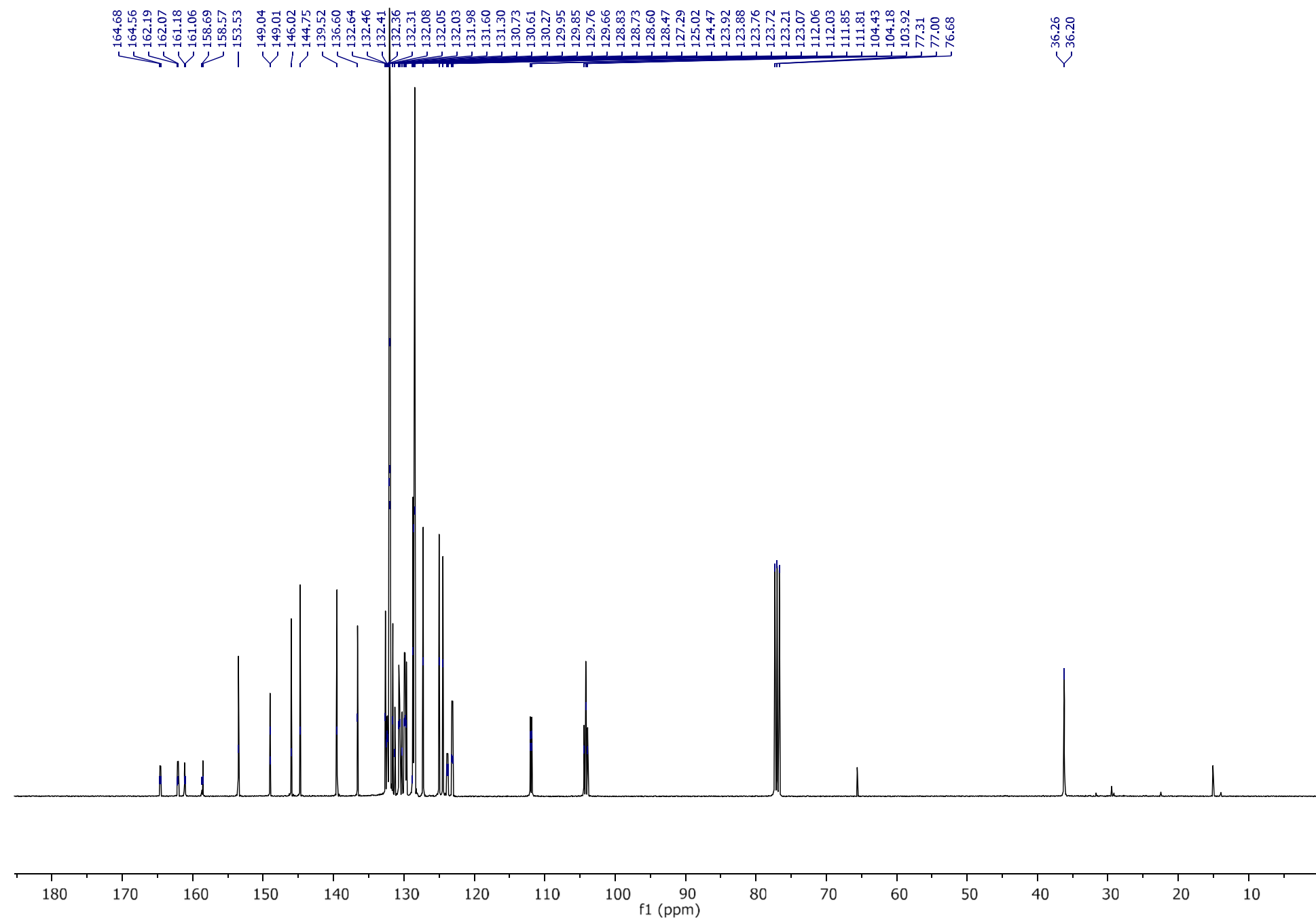
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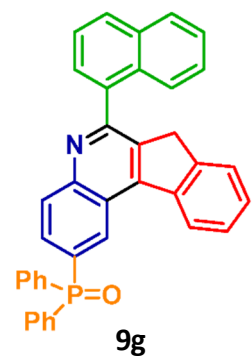
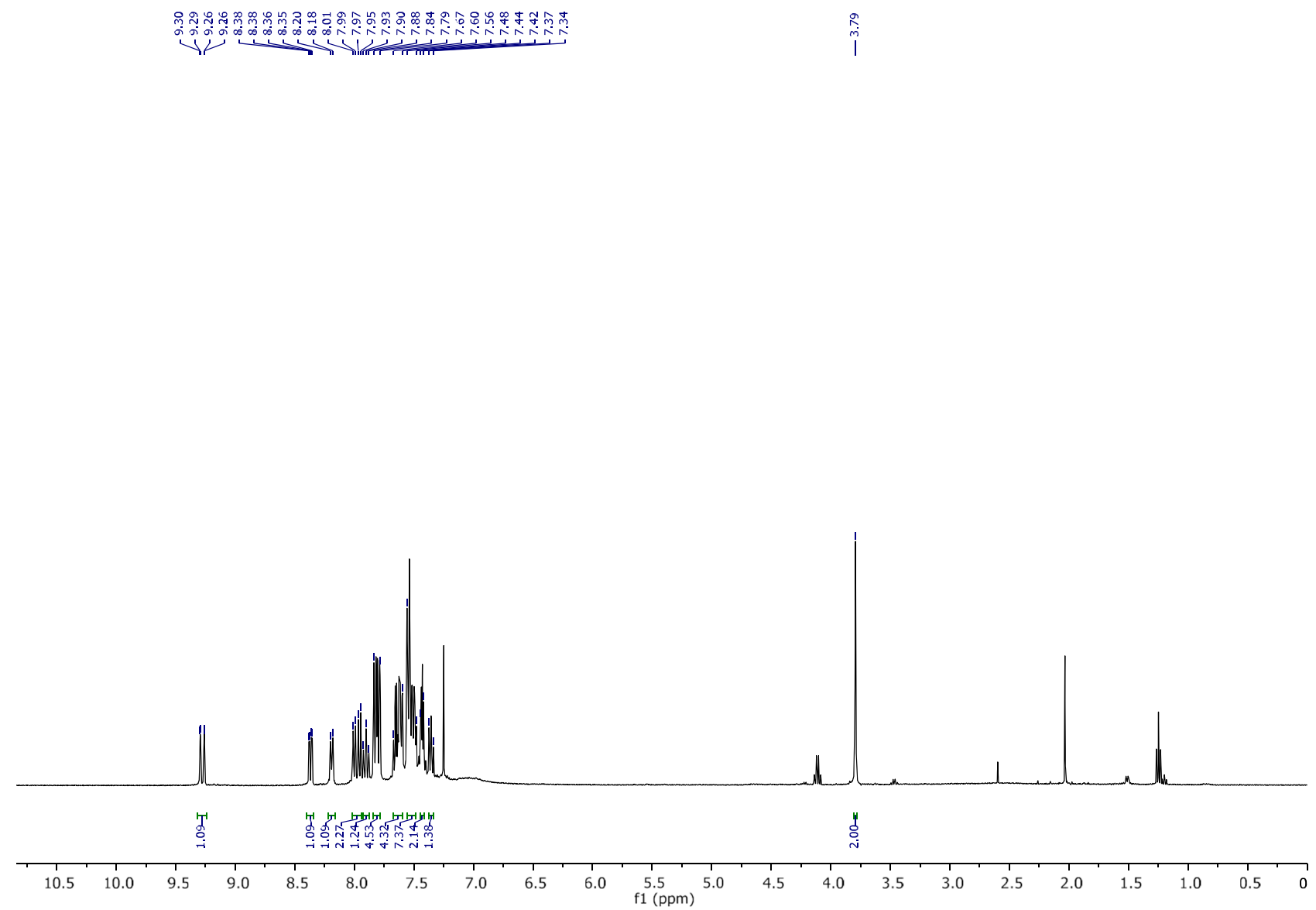
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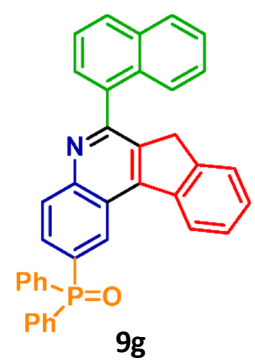
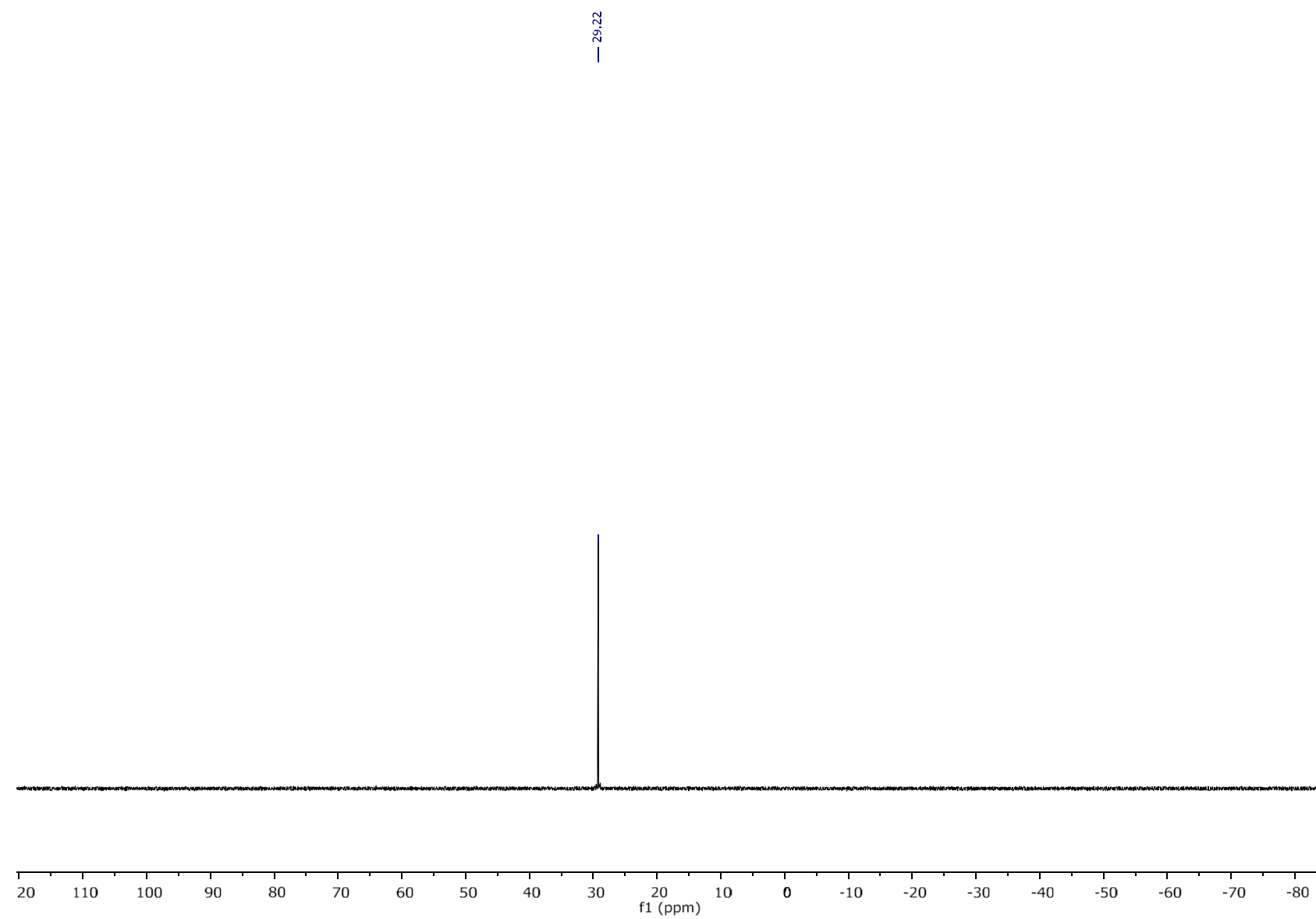
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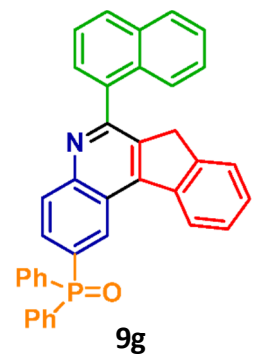
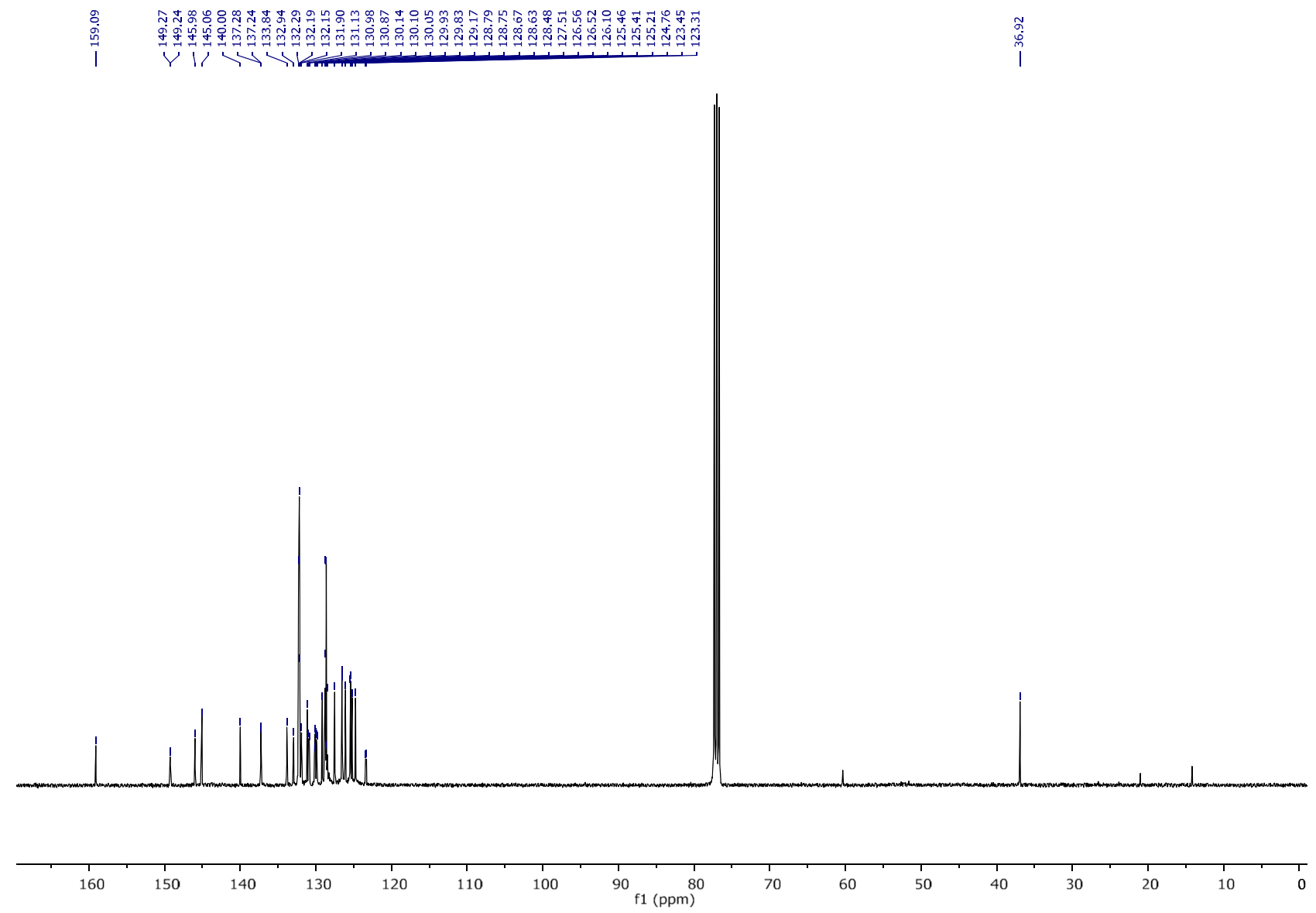
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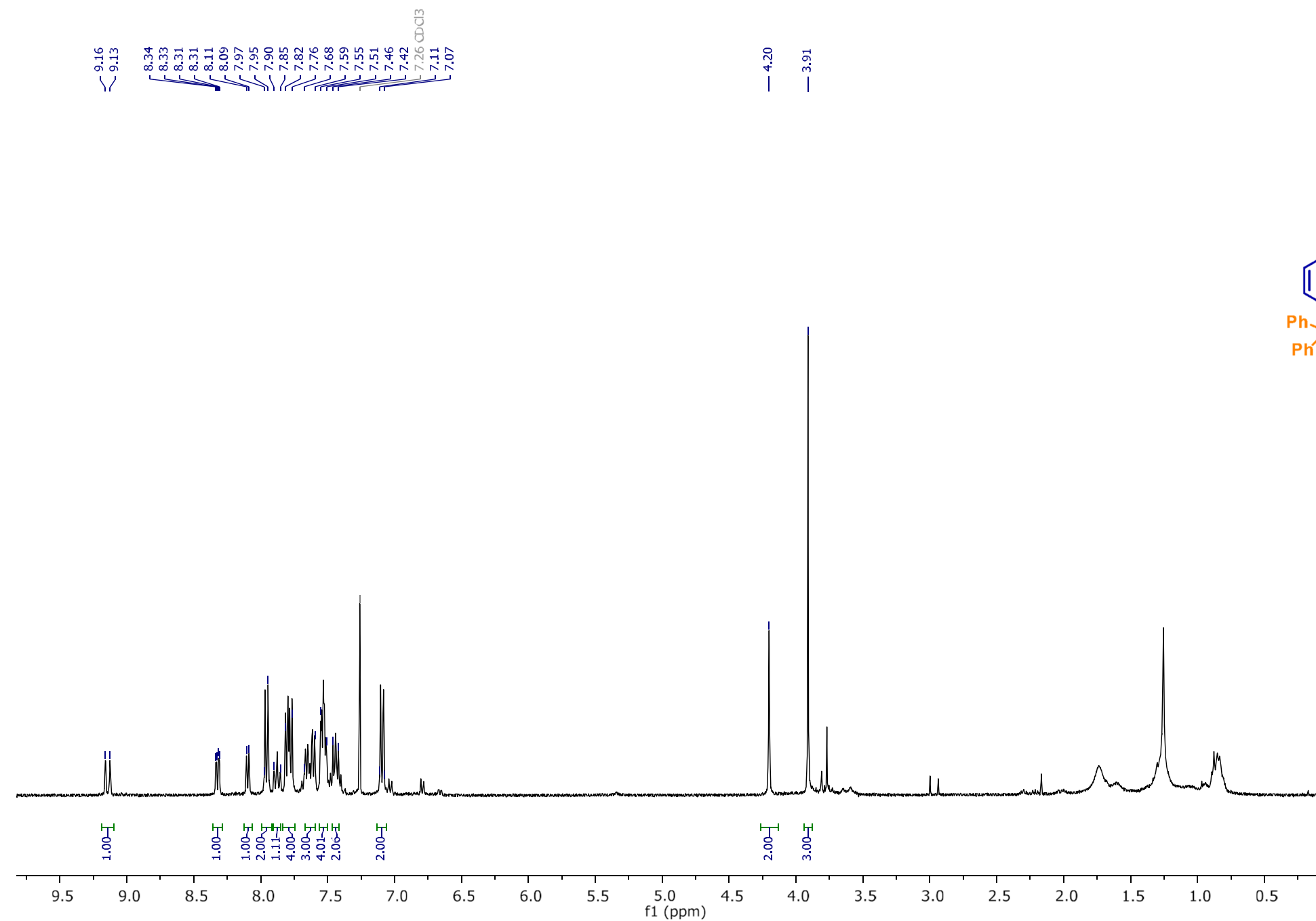
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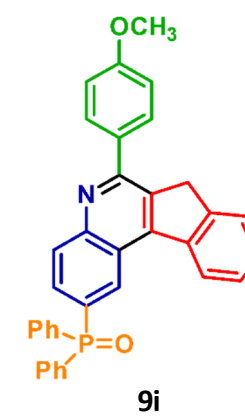
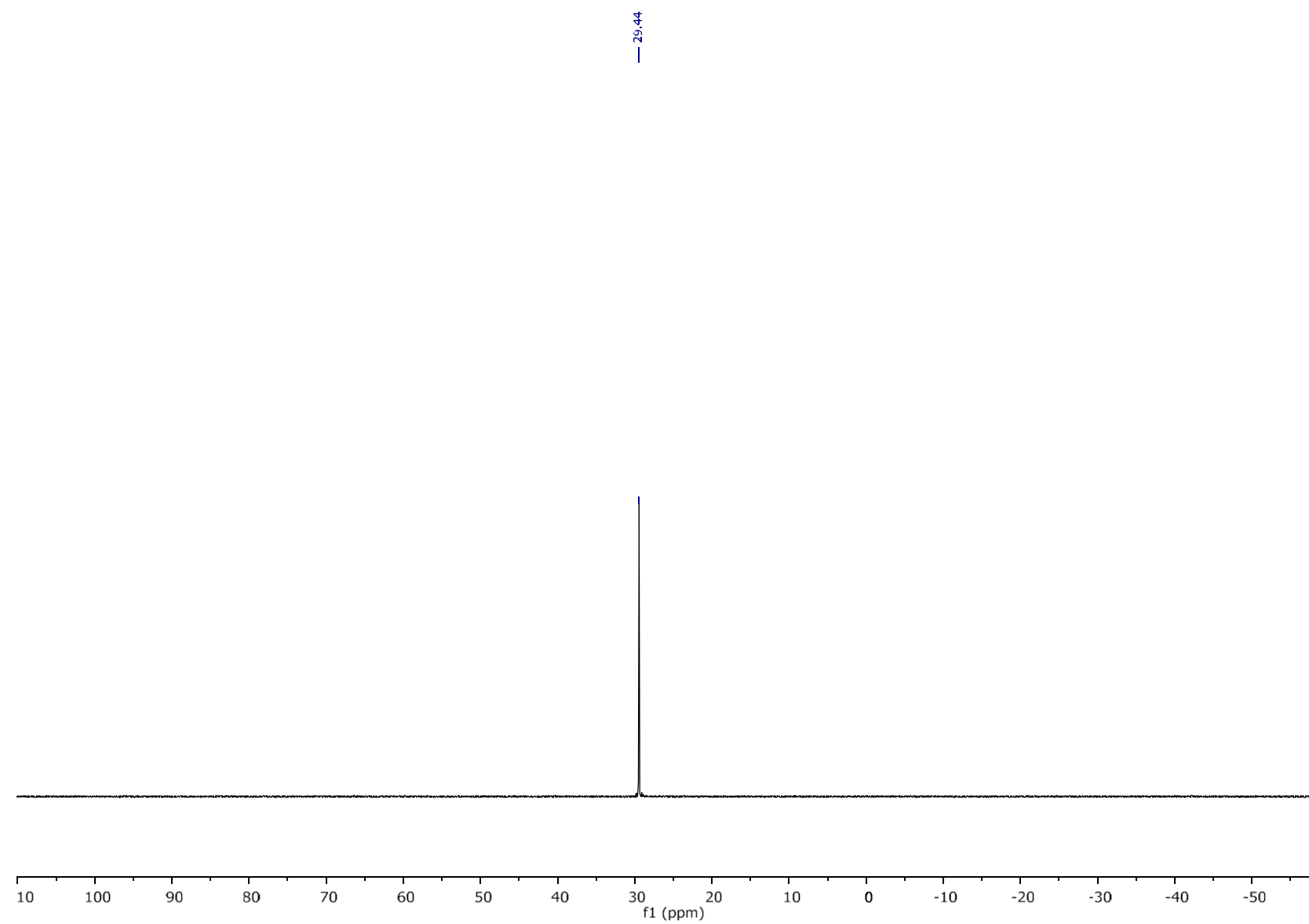
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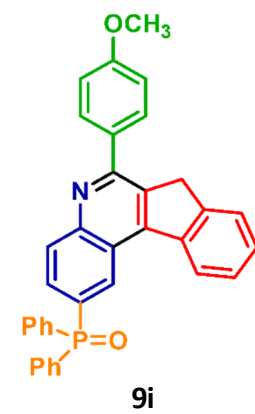
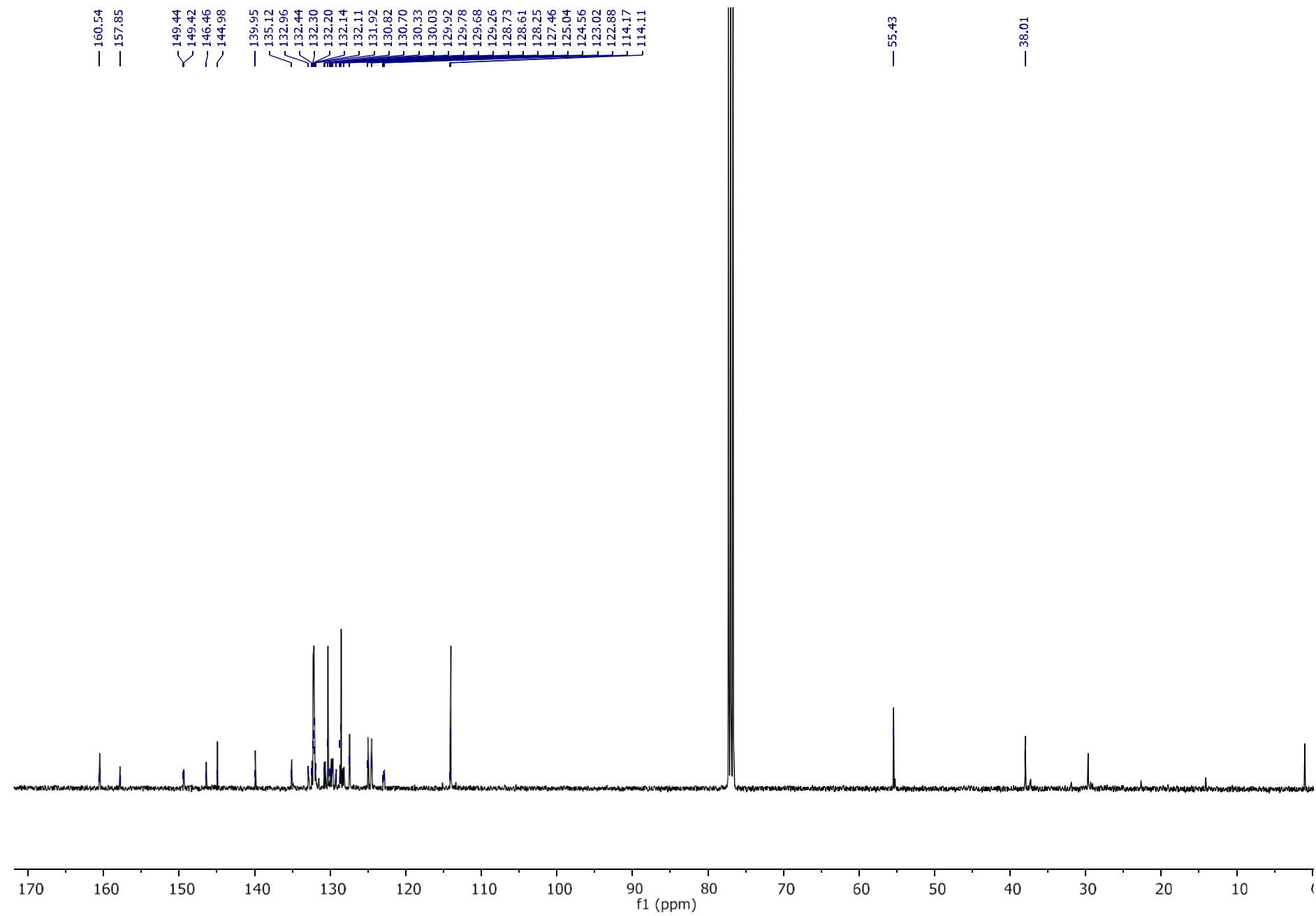
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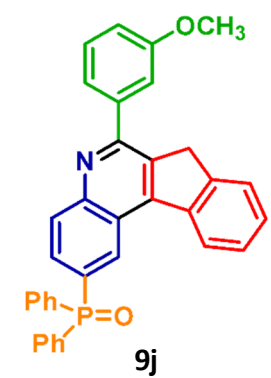
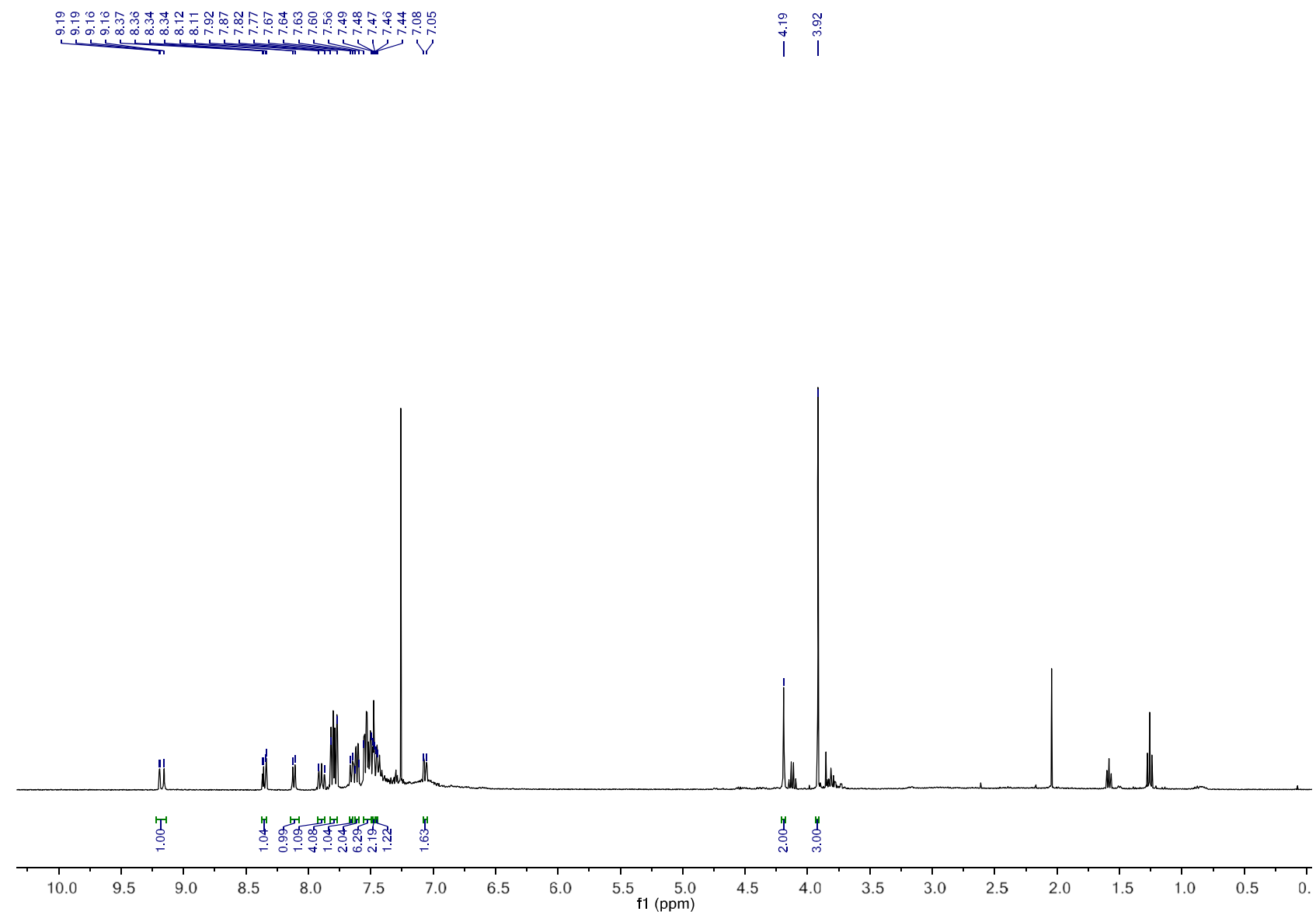
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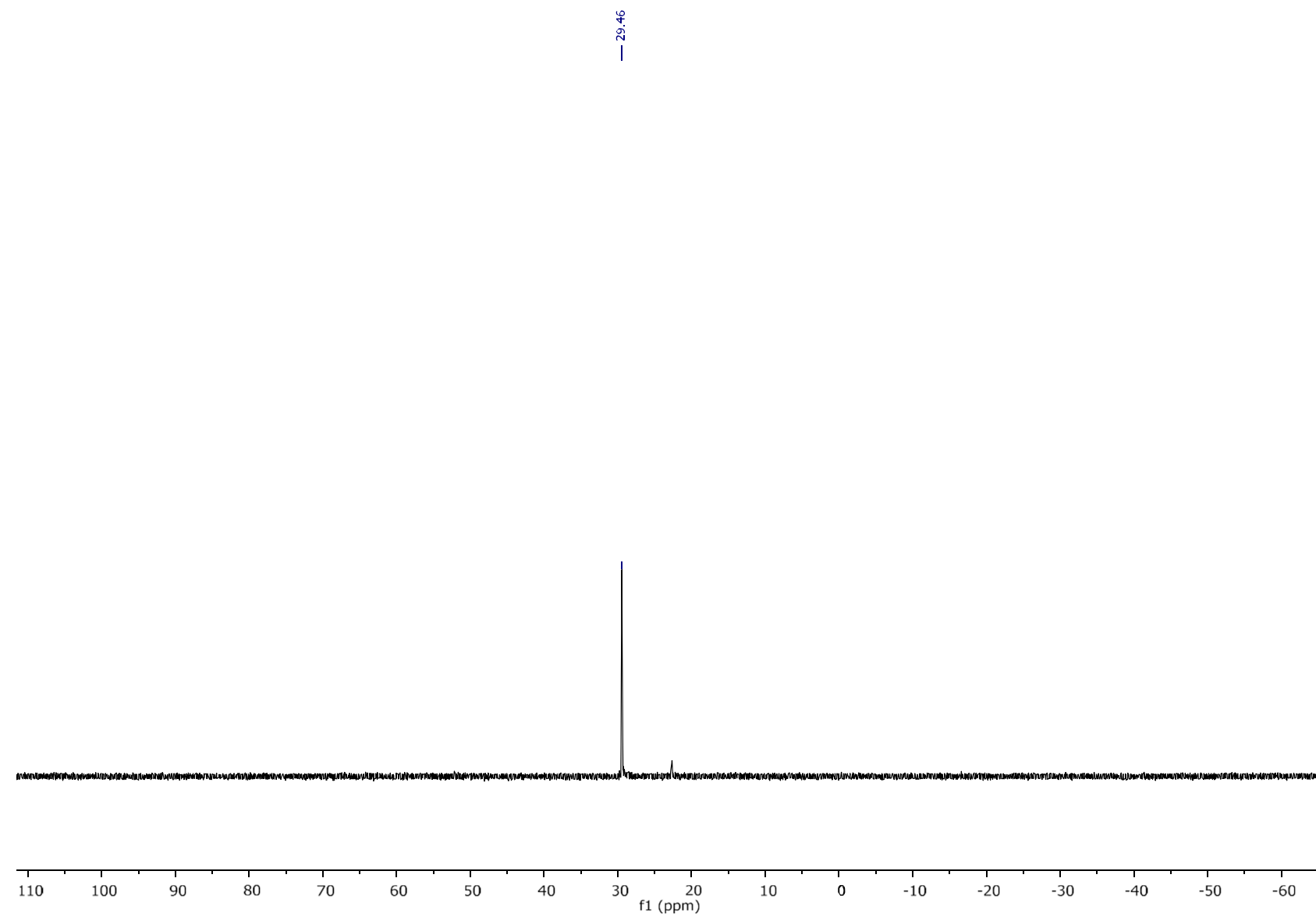
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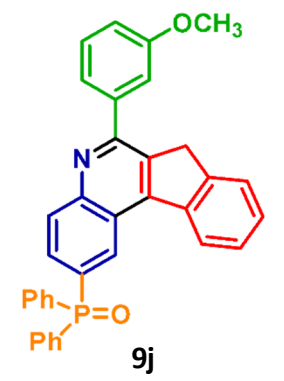
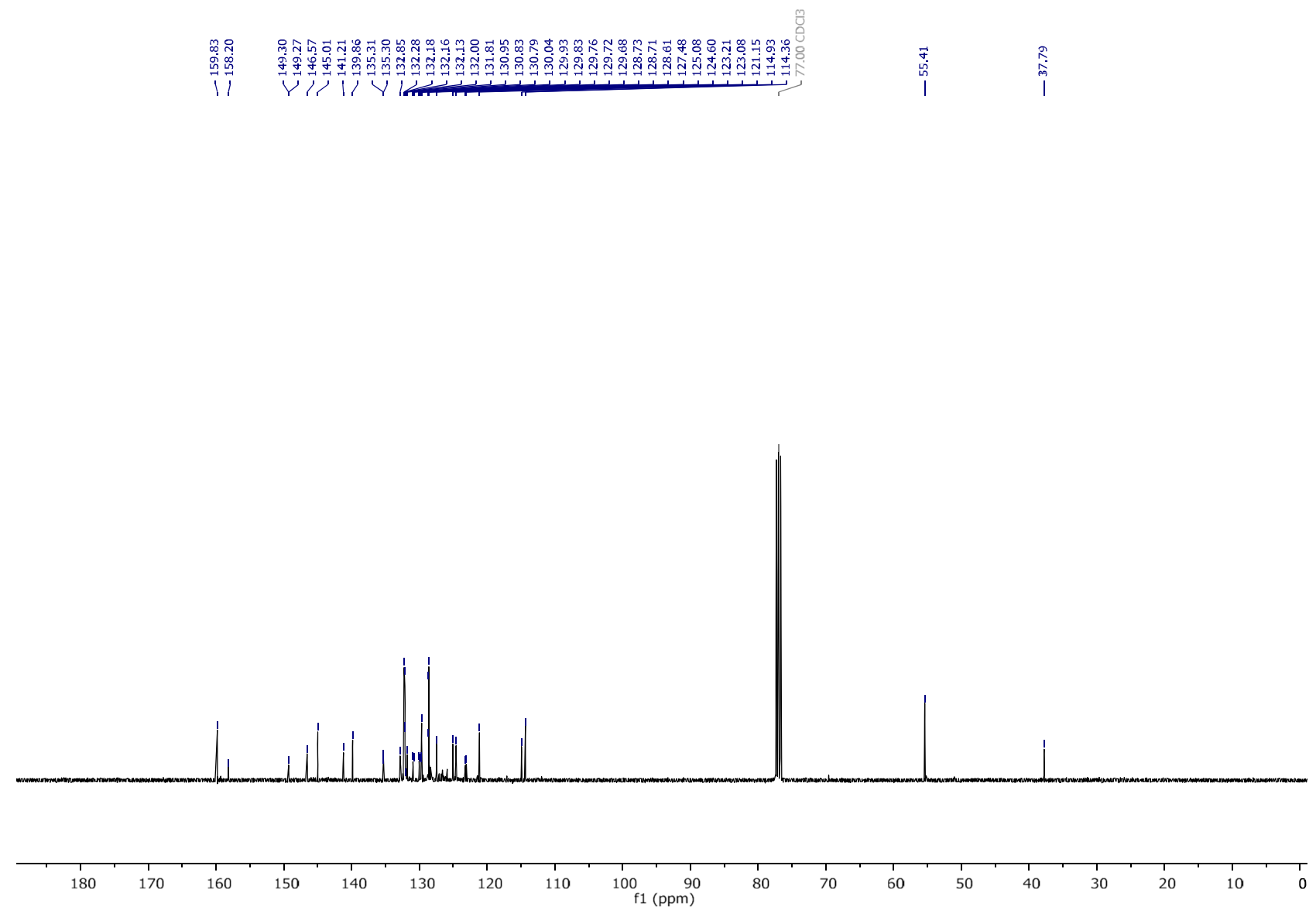
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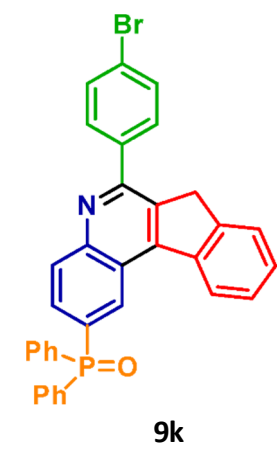
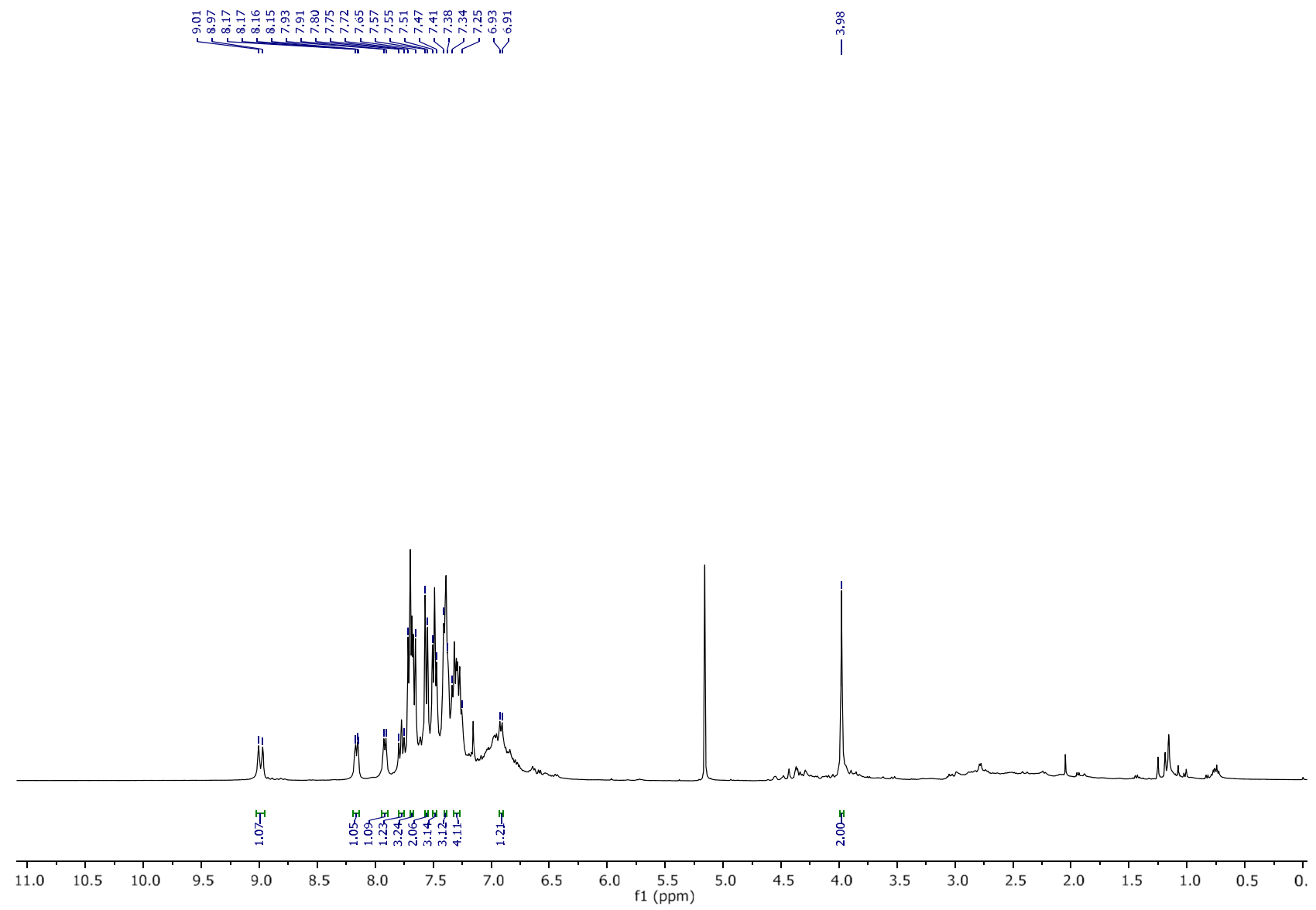
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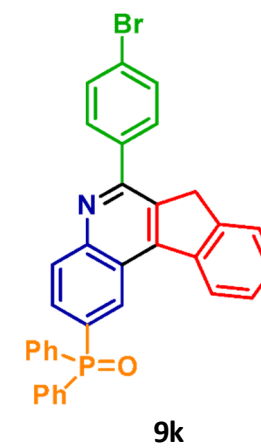
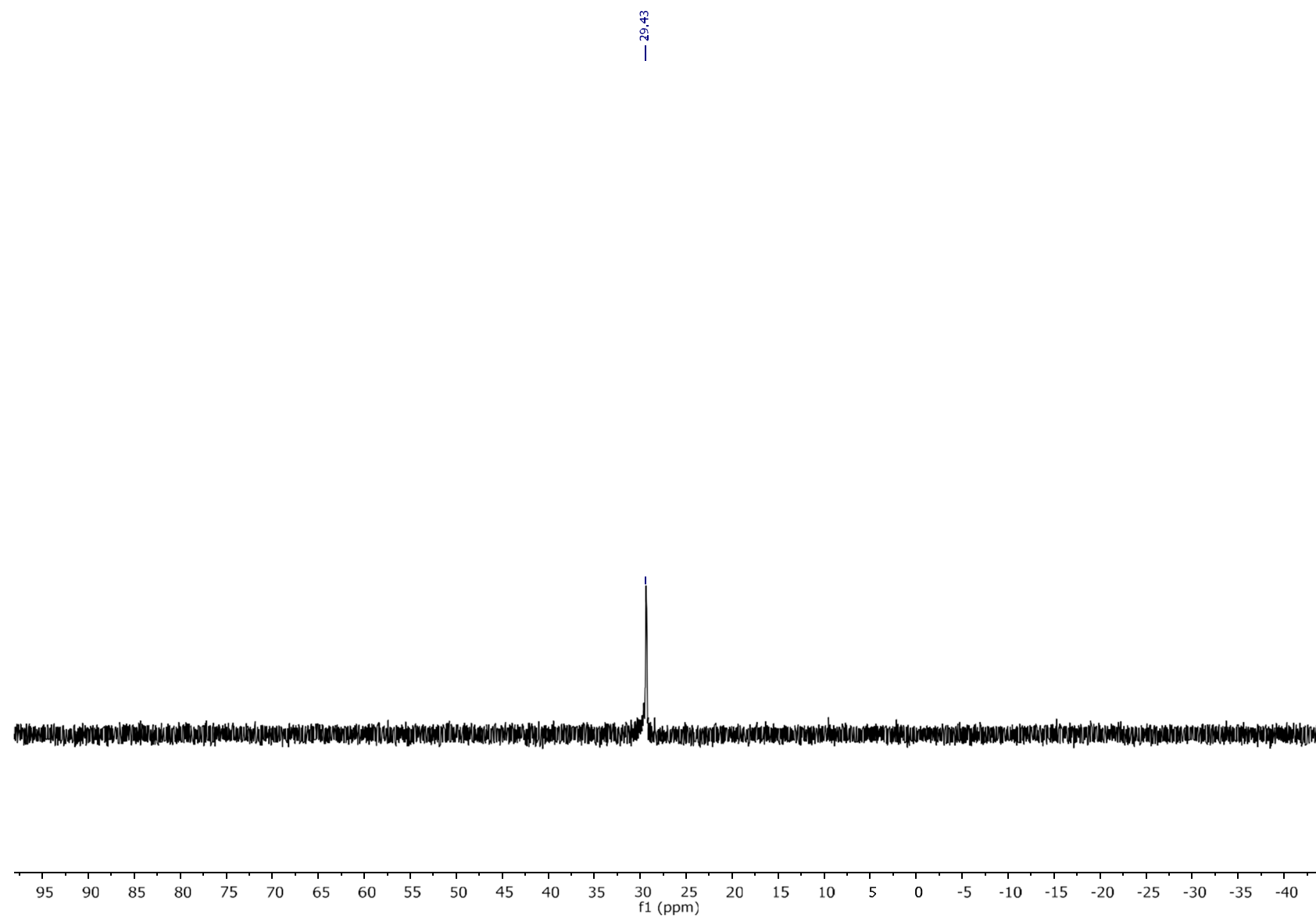
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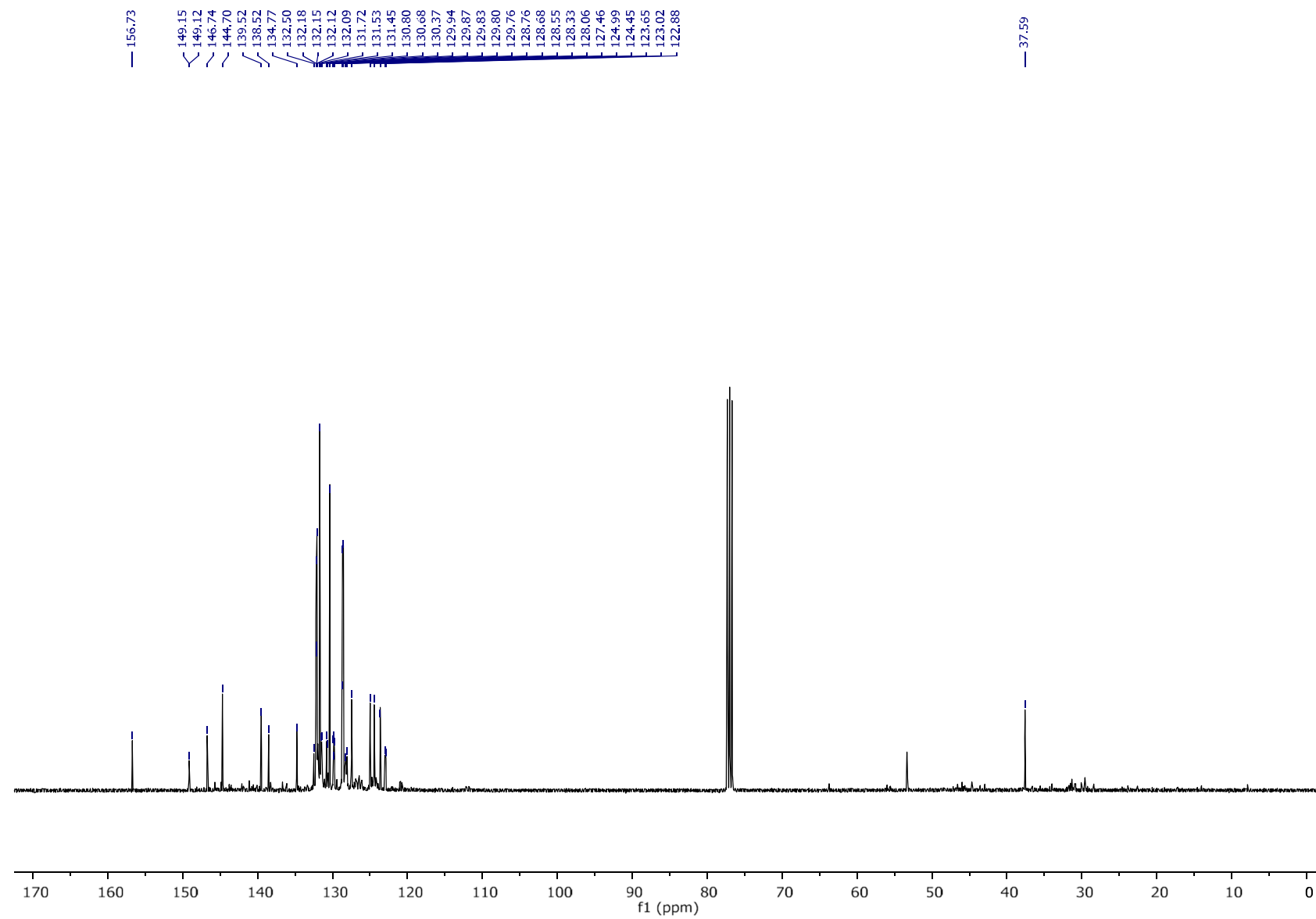
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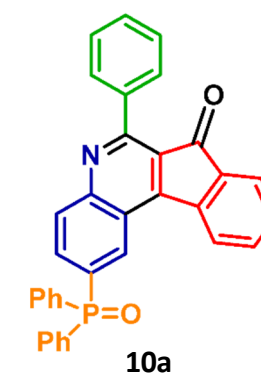
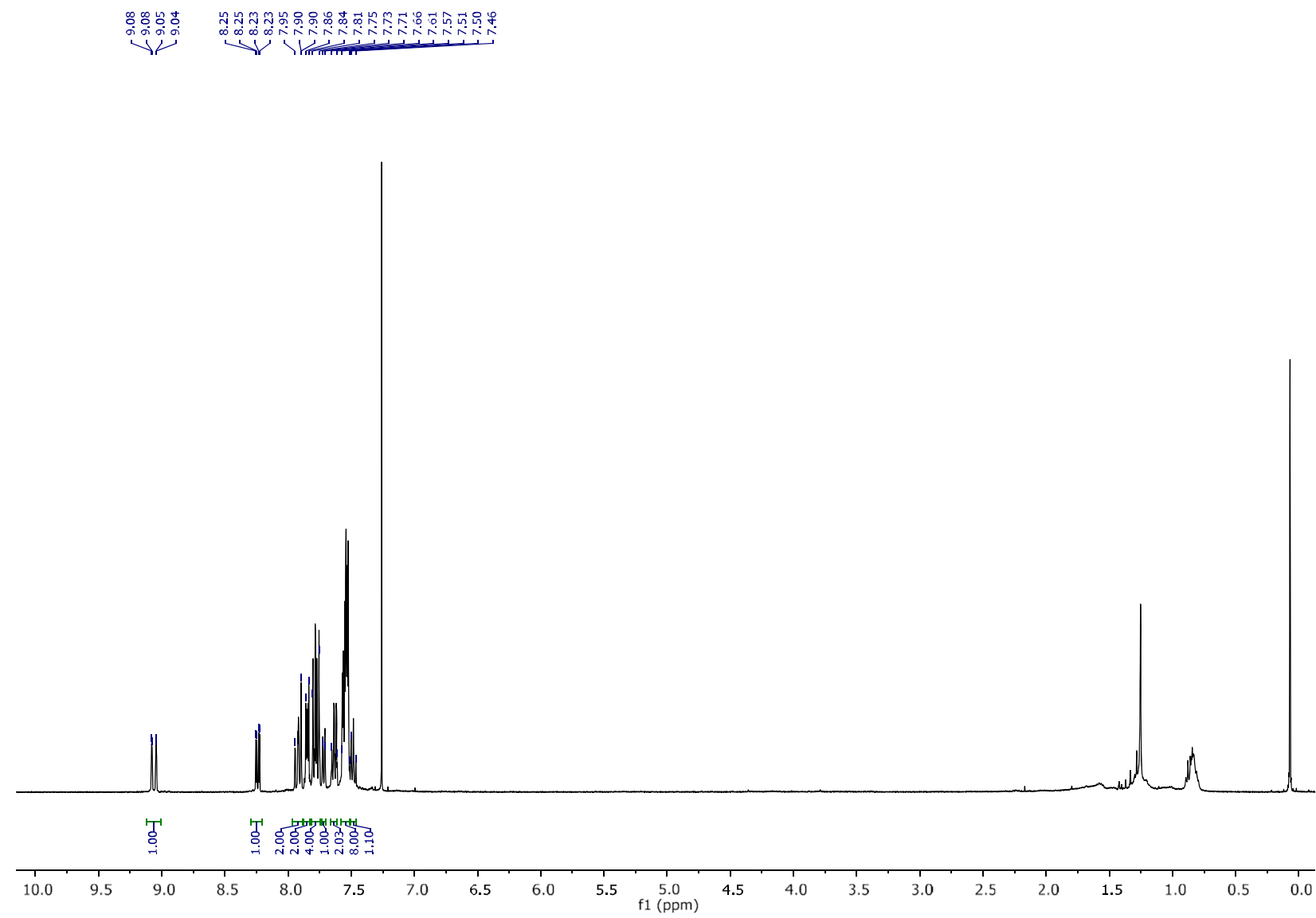
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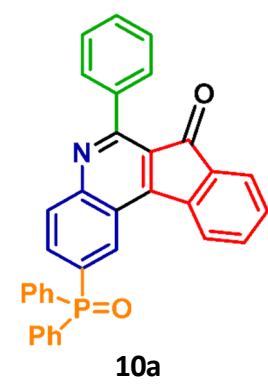
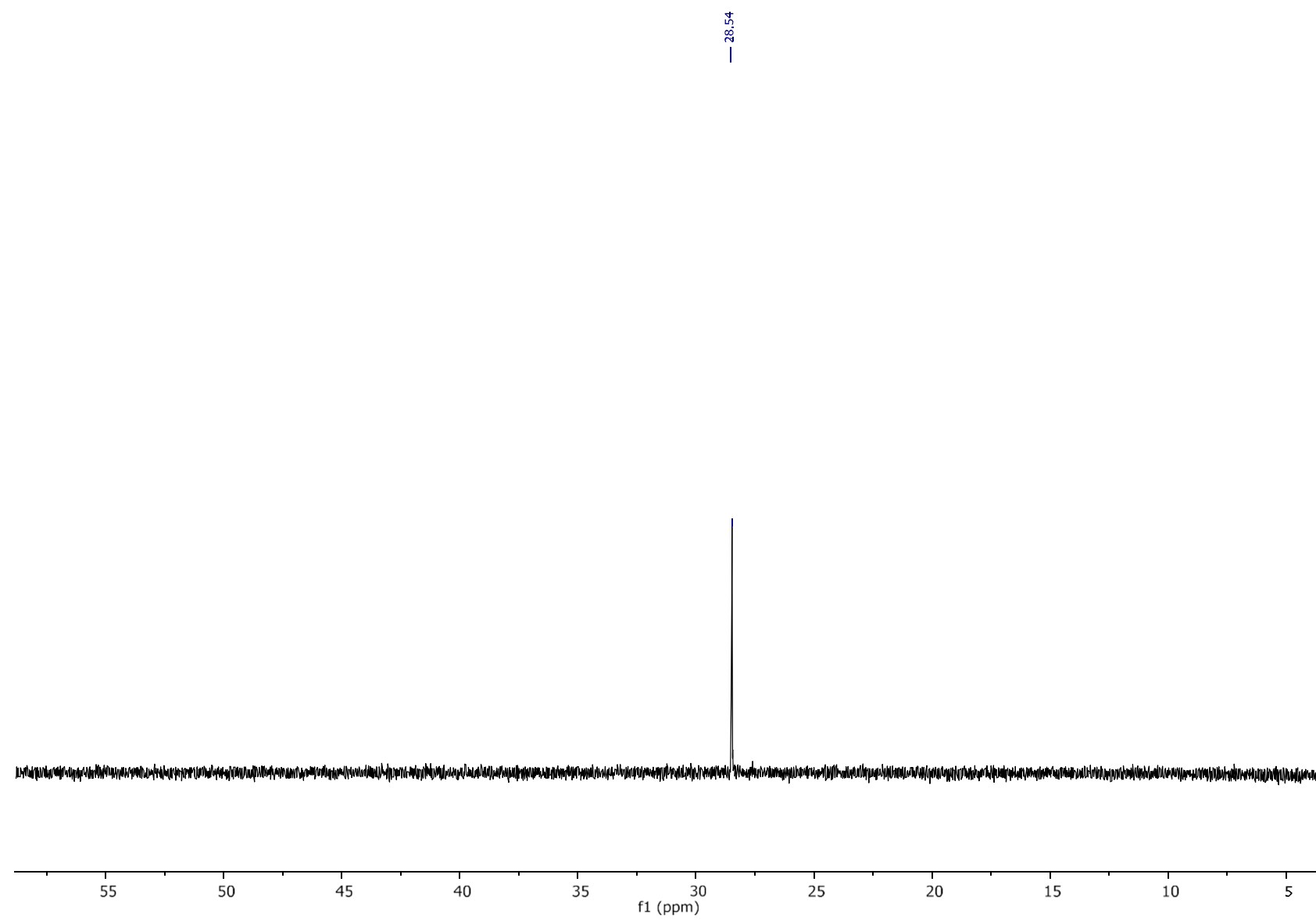
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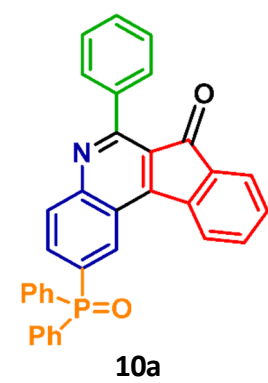
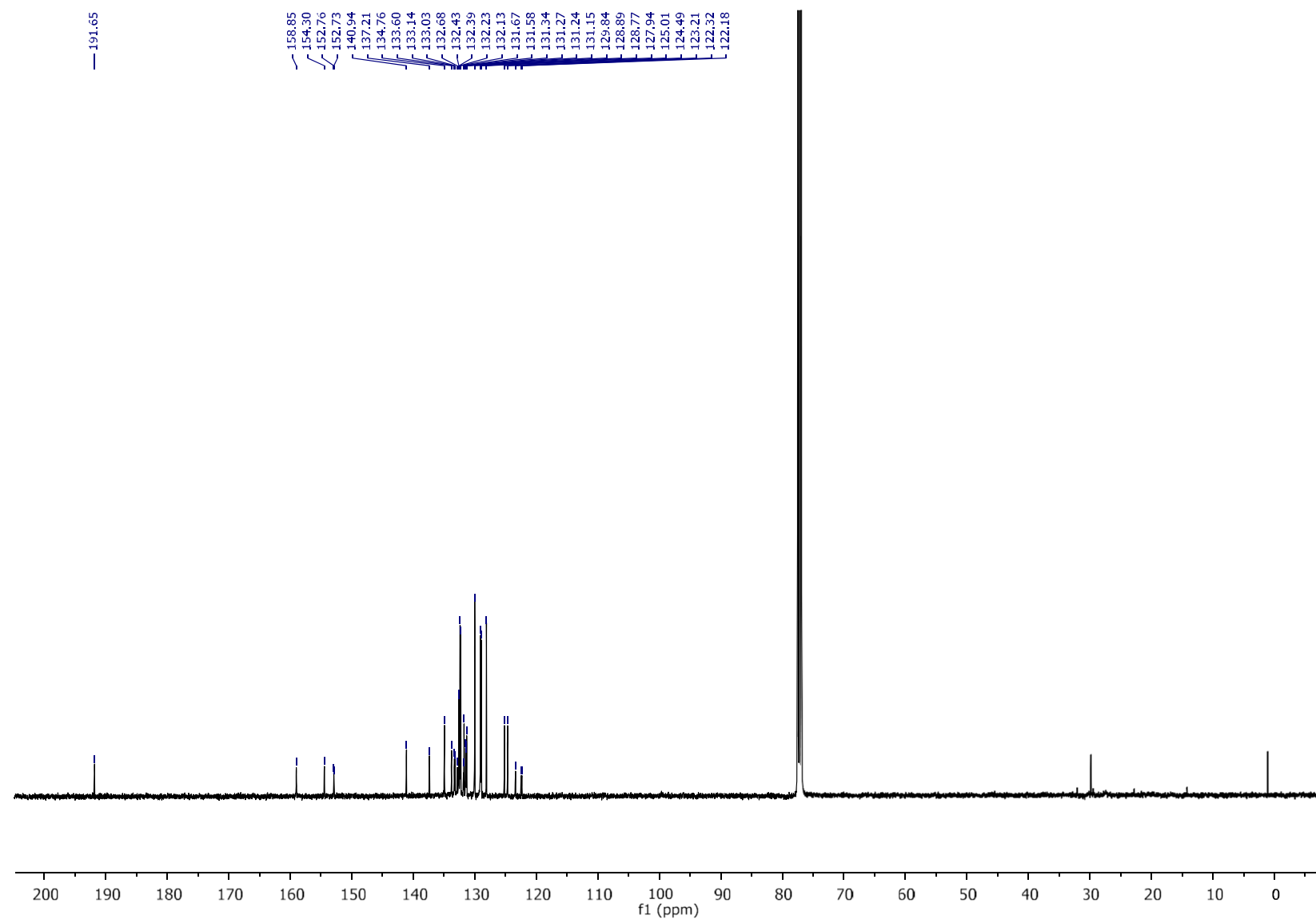
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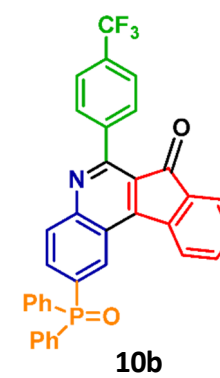
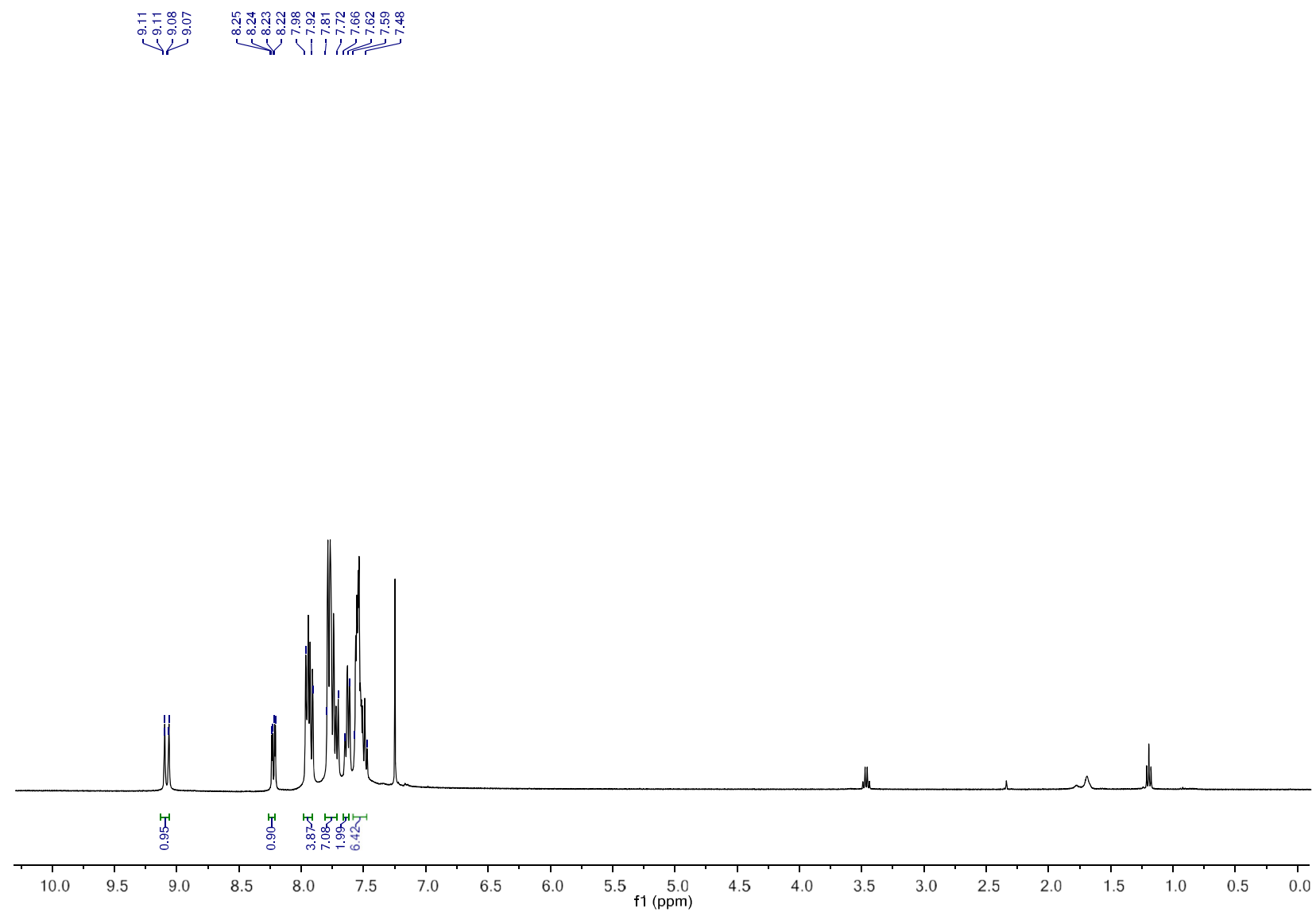
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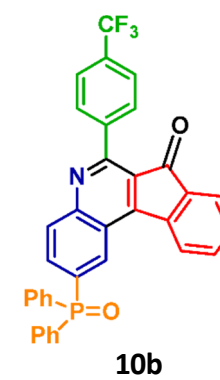
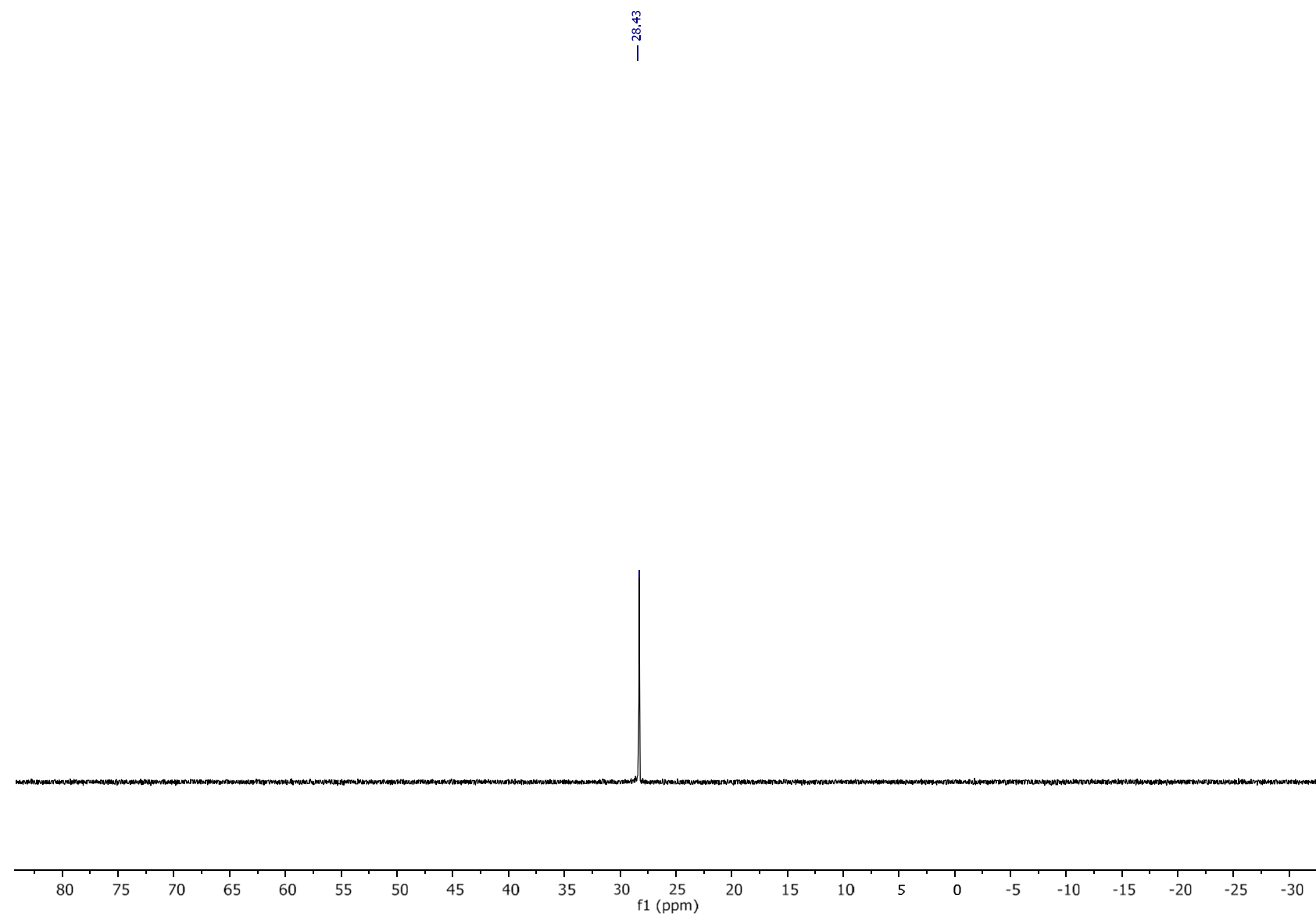
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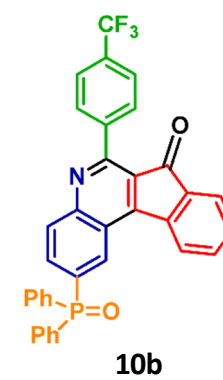
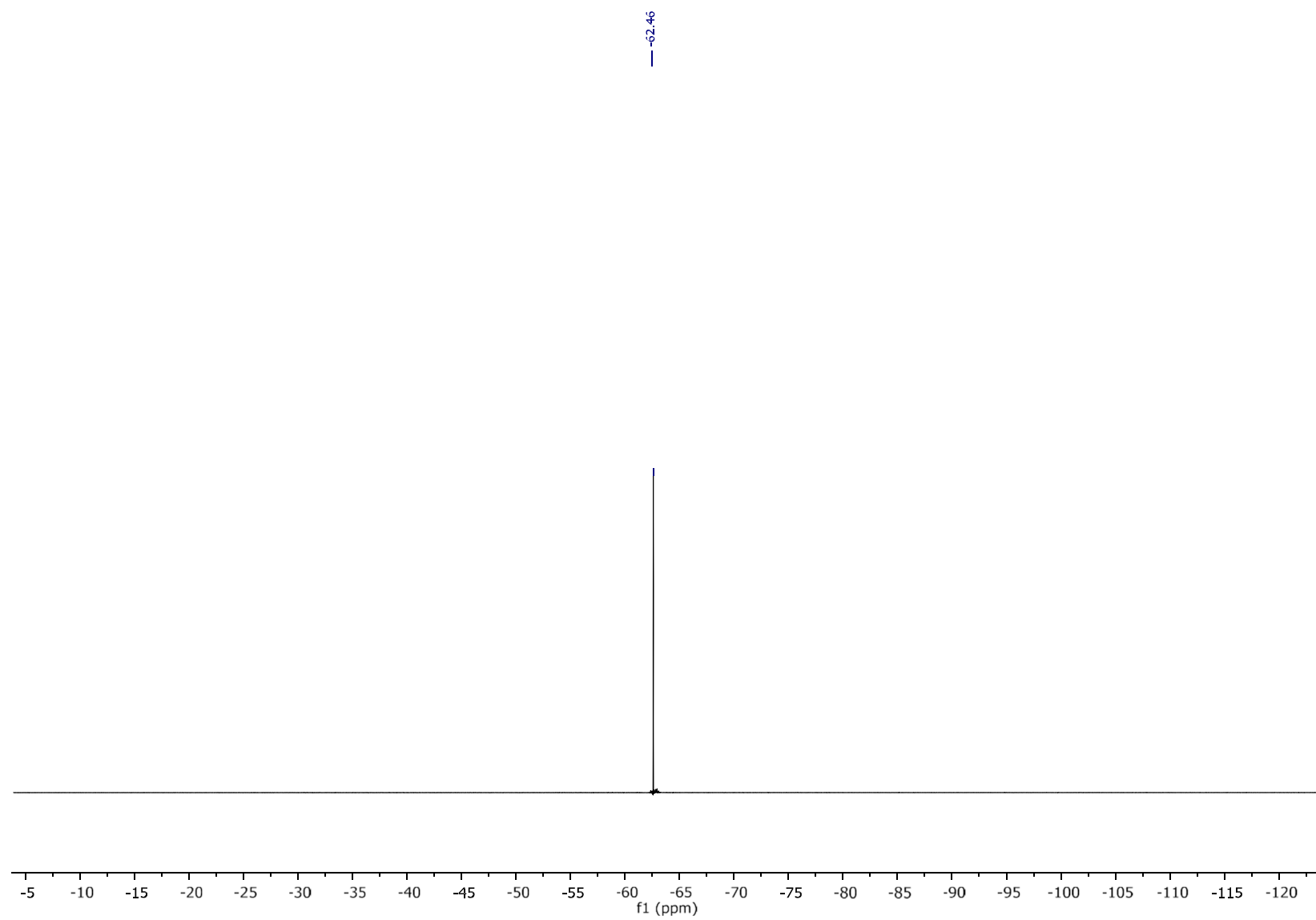
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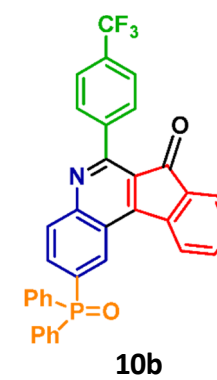
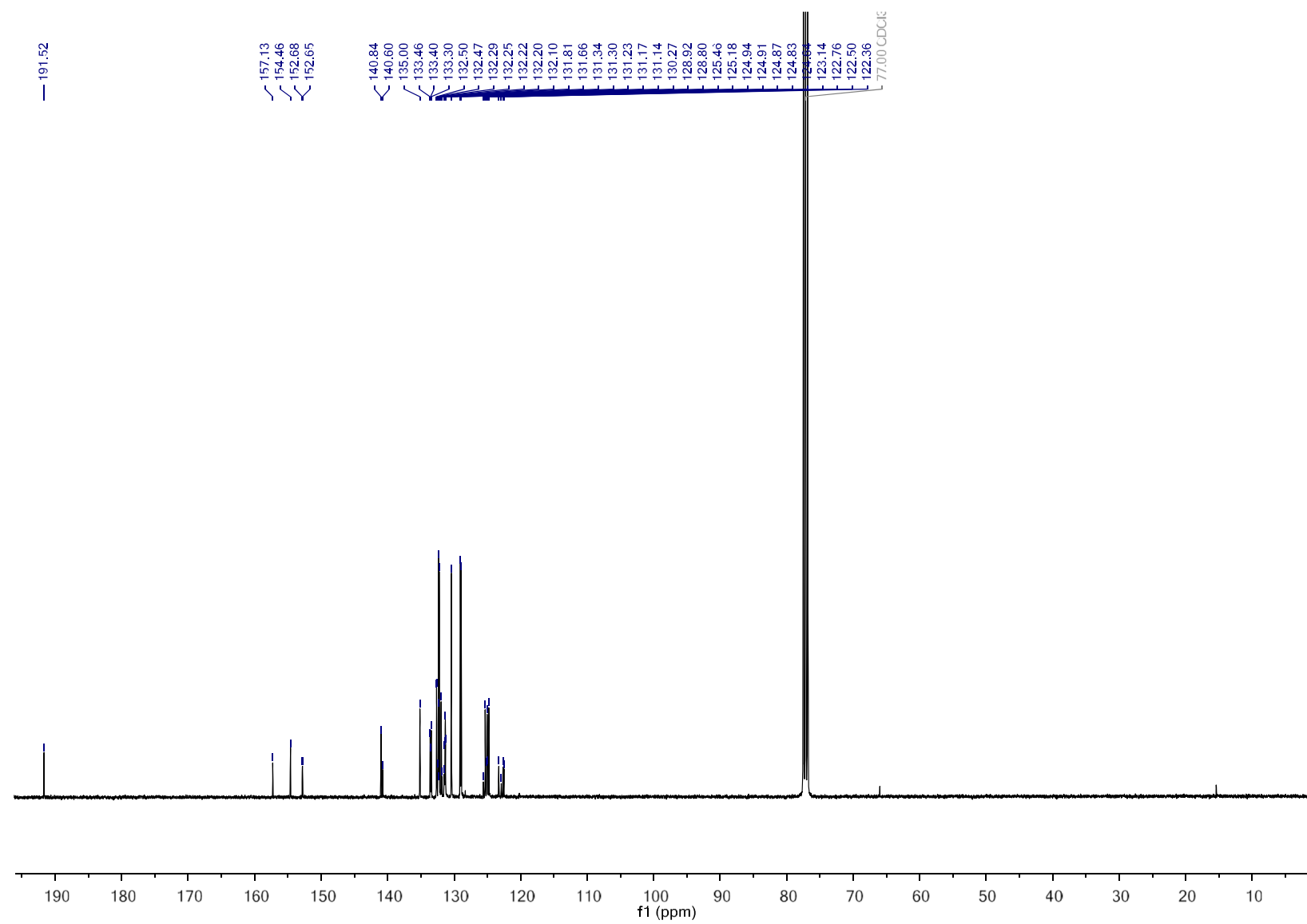
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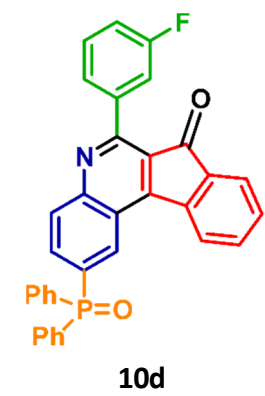
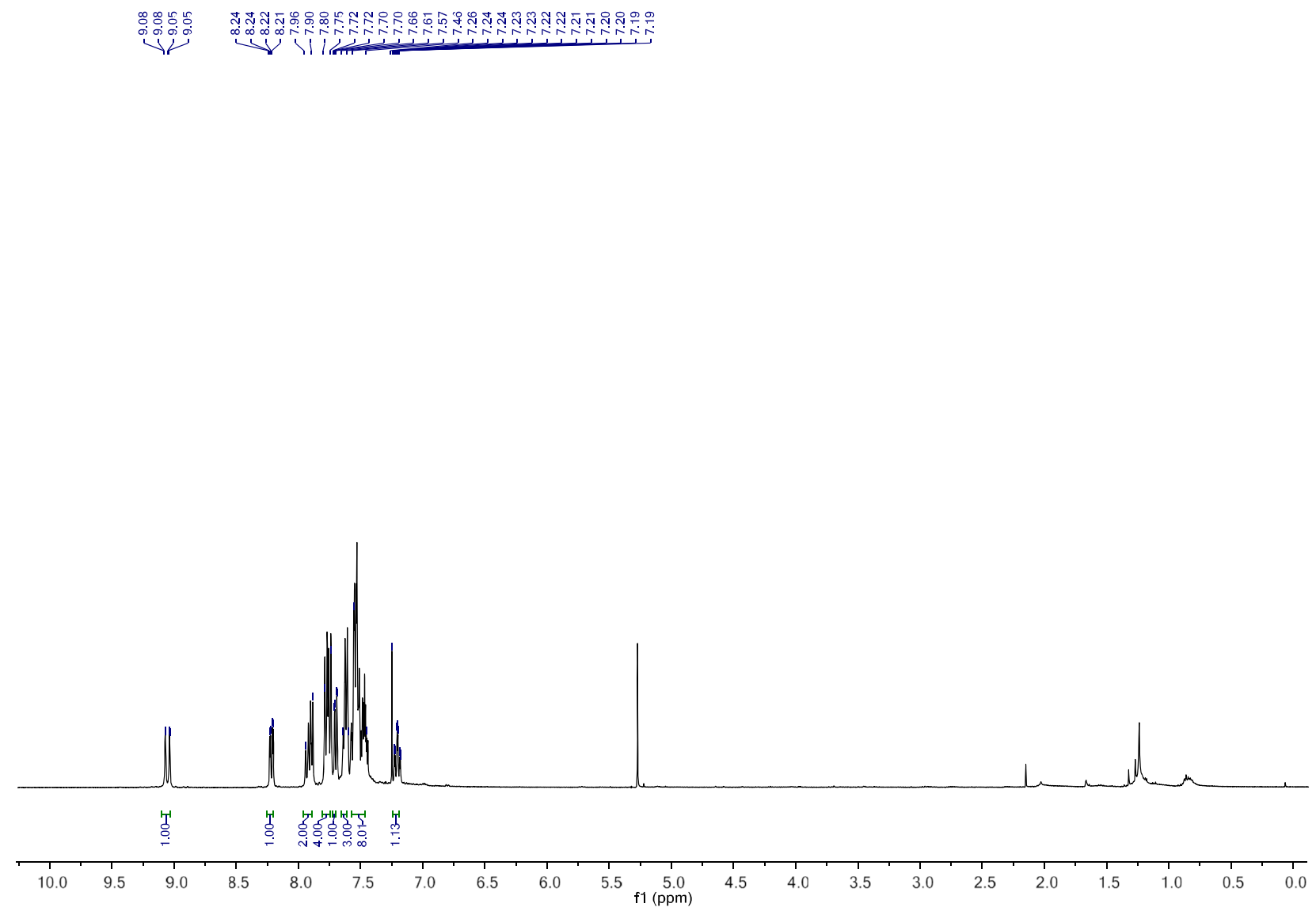
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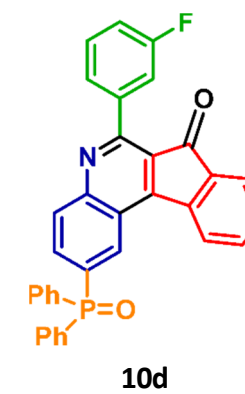
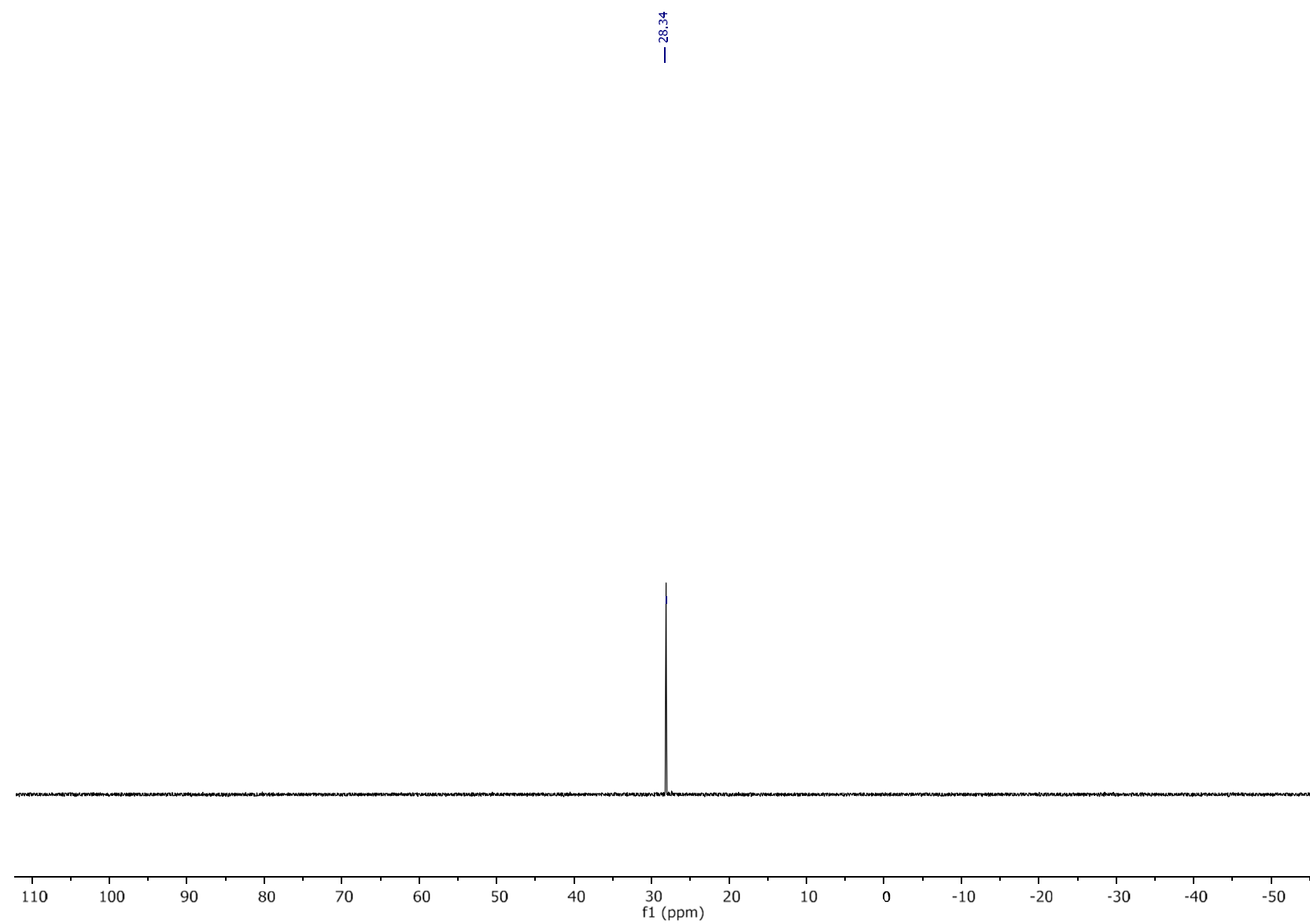
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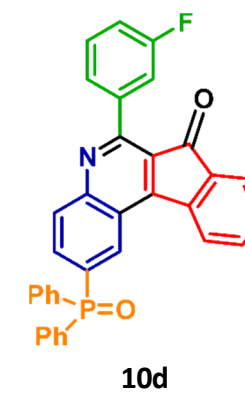
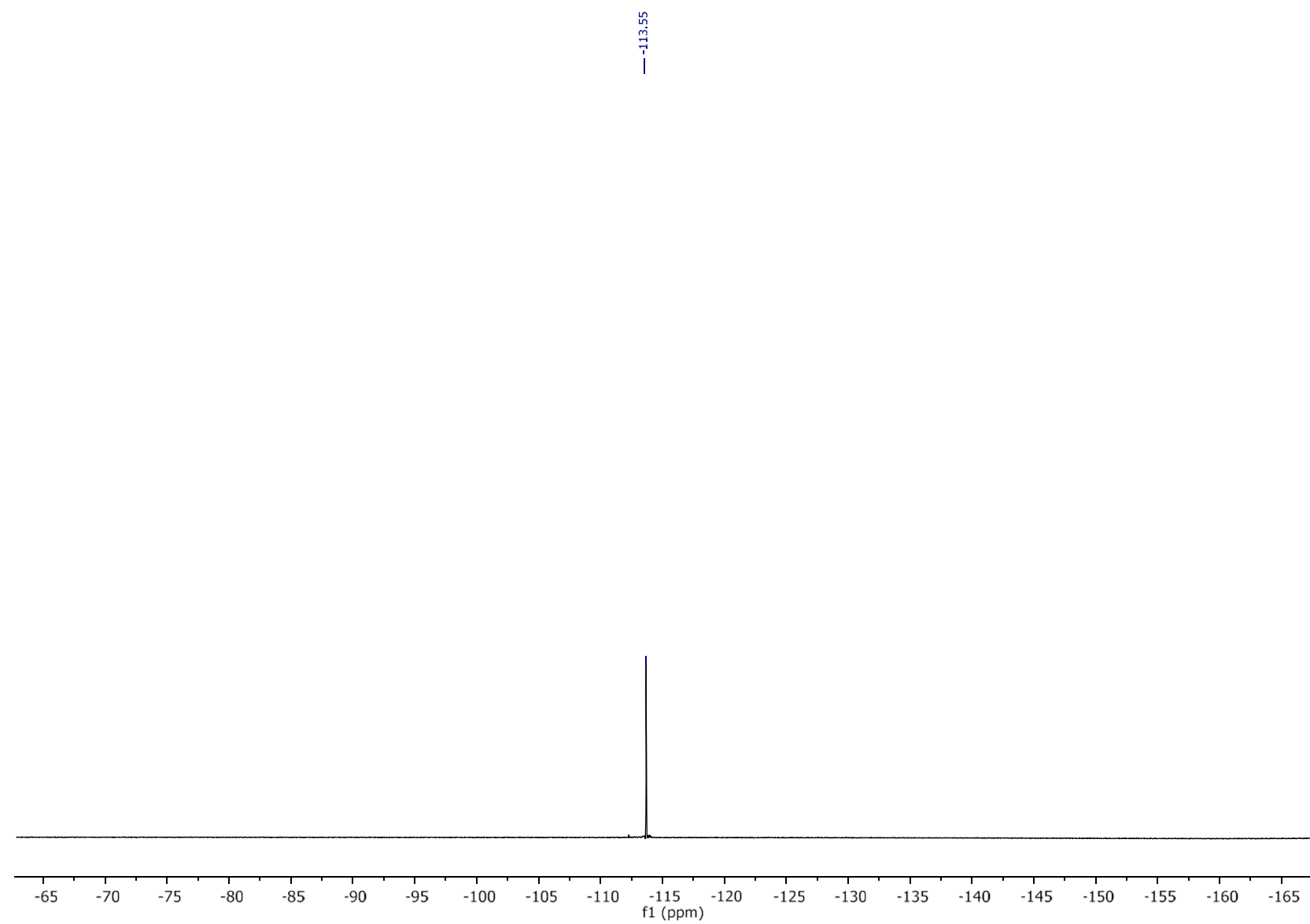
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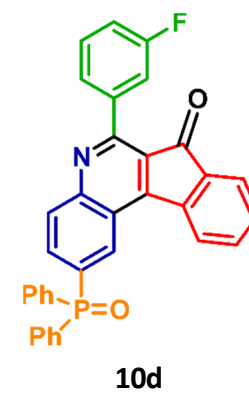
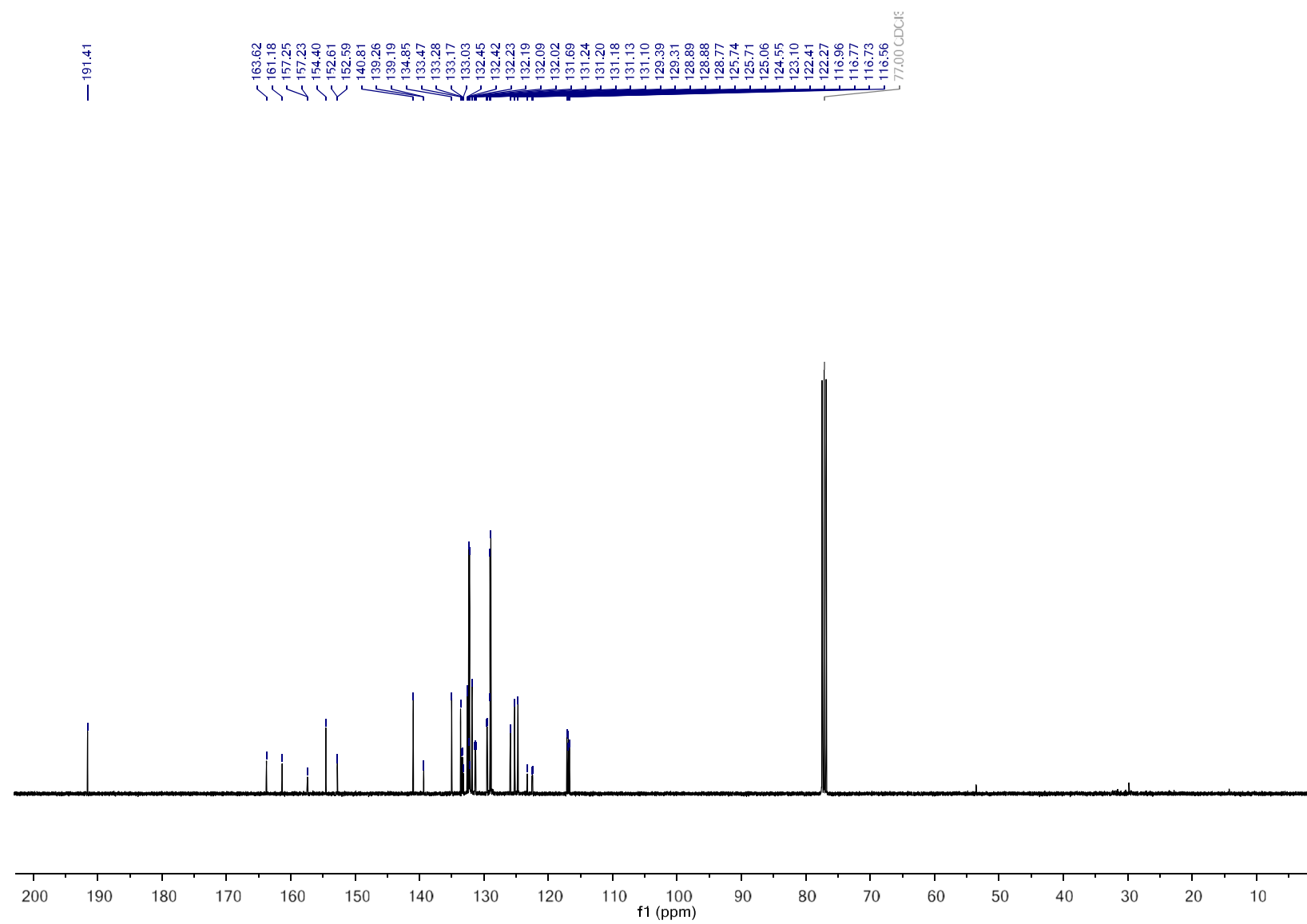
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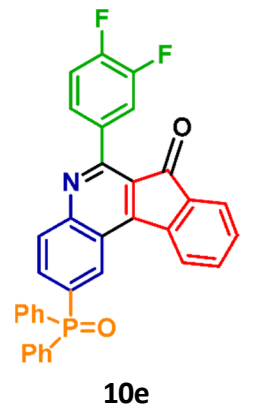
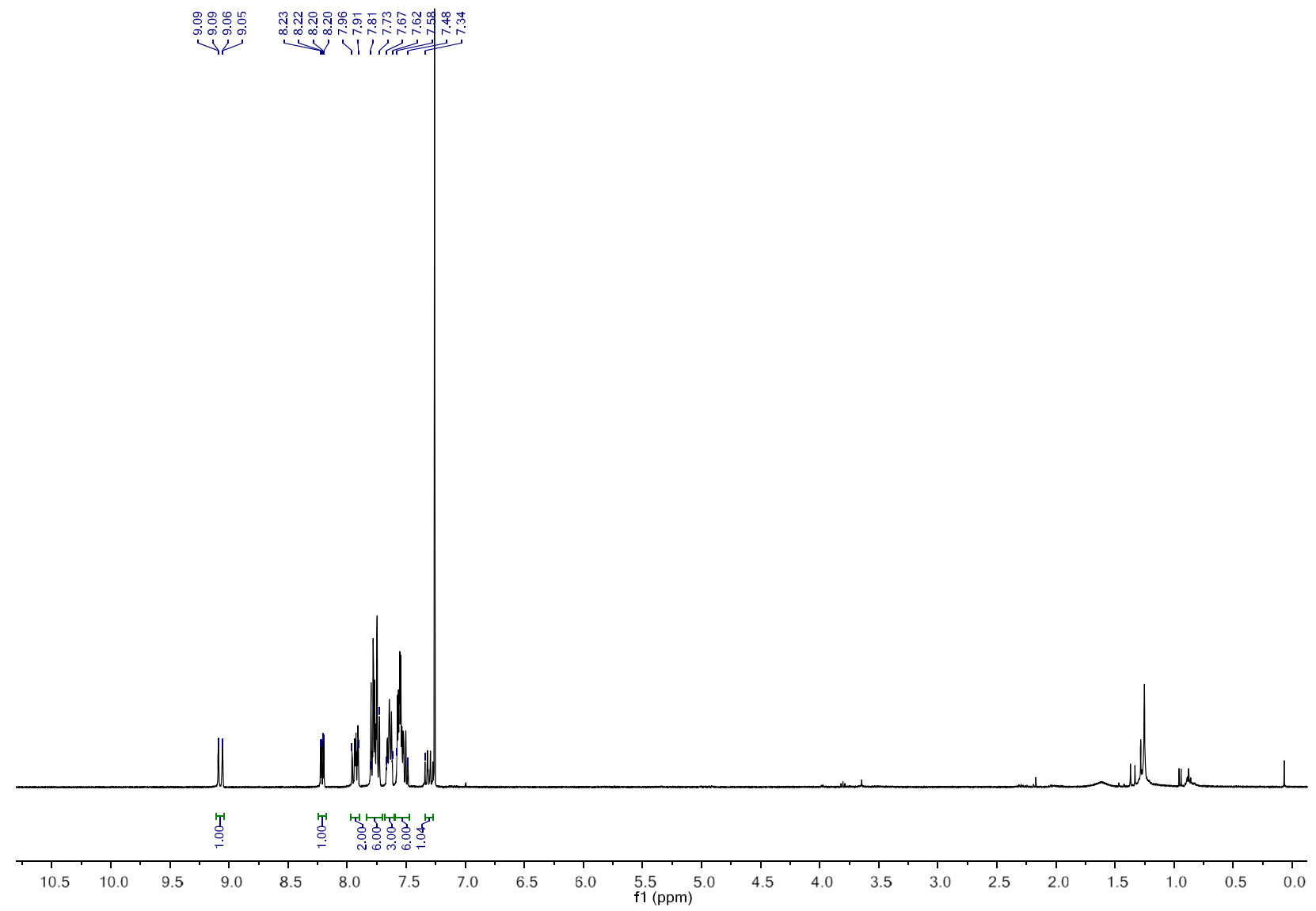
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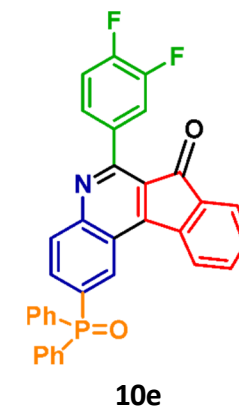
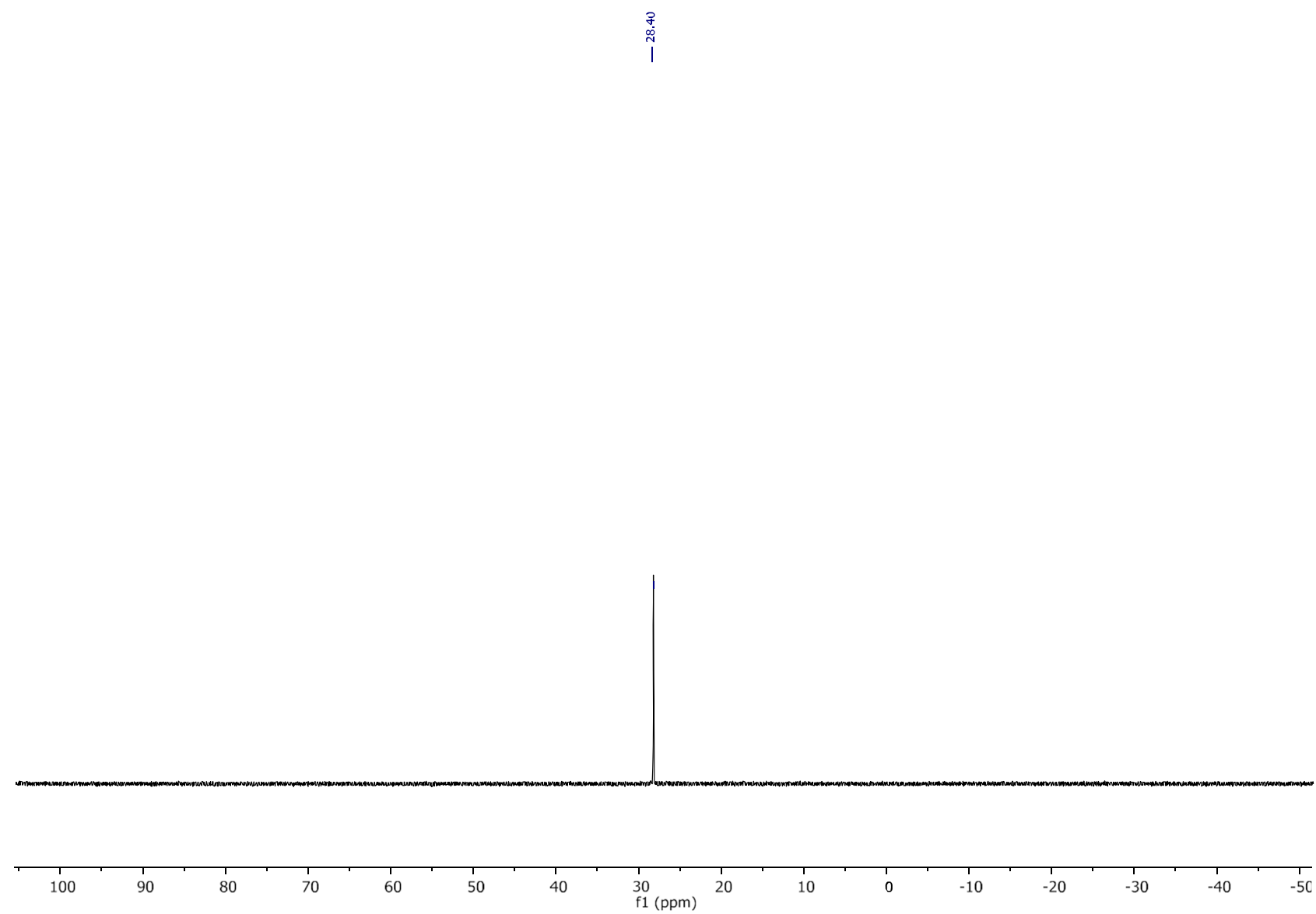
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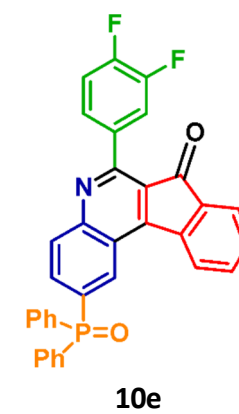
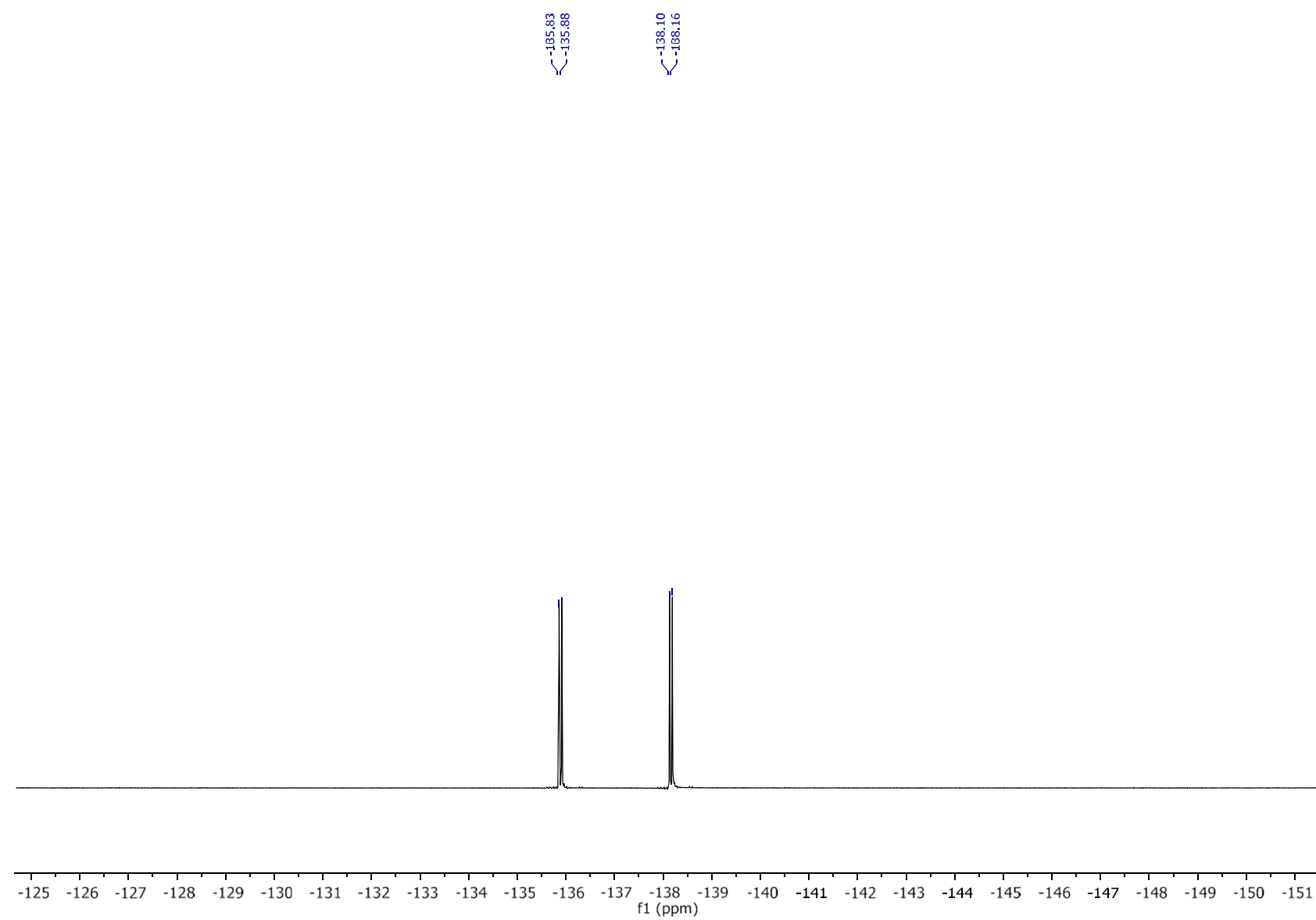
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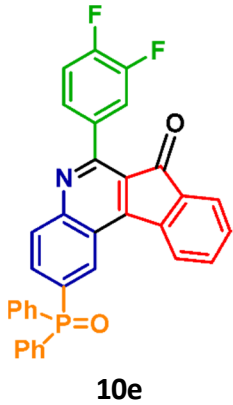
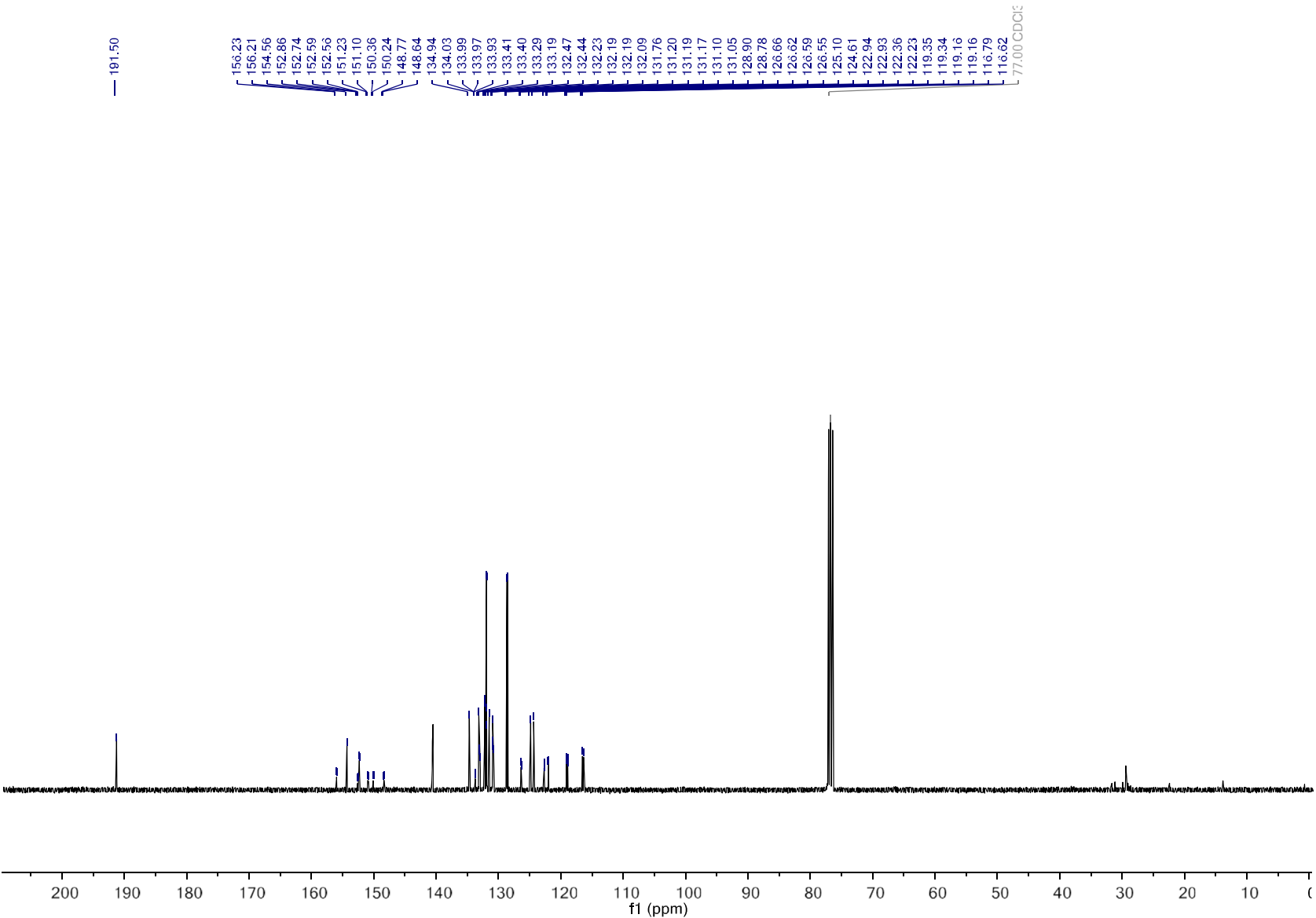
³¹P-RMN



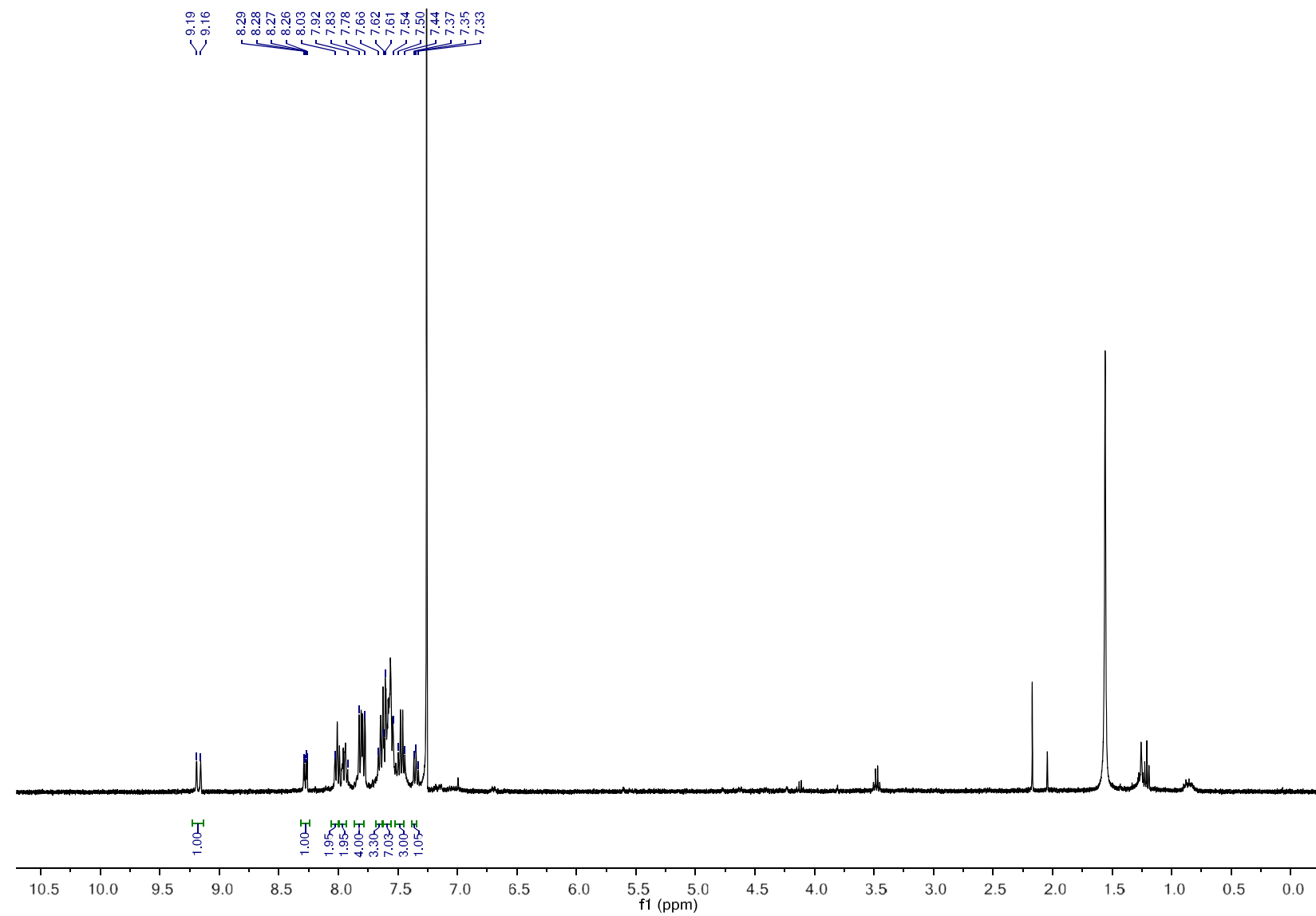
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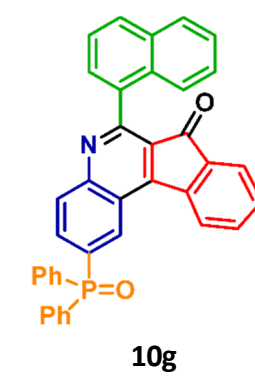
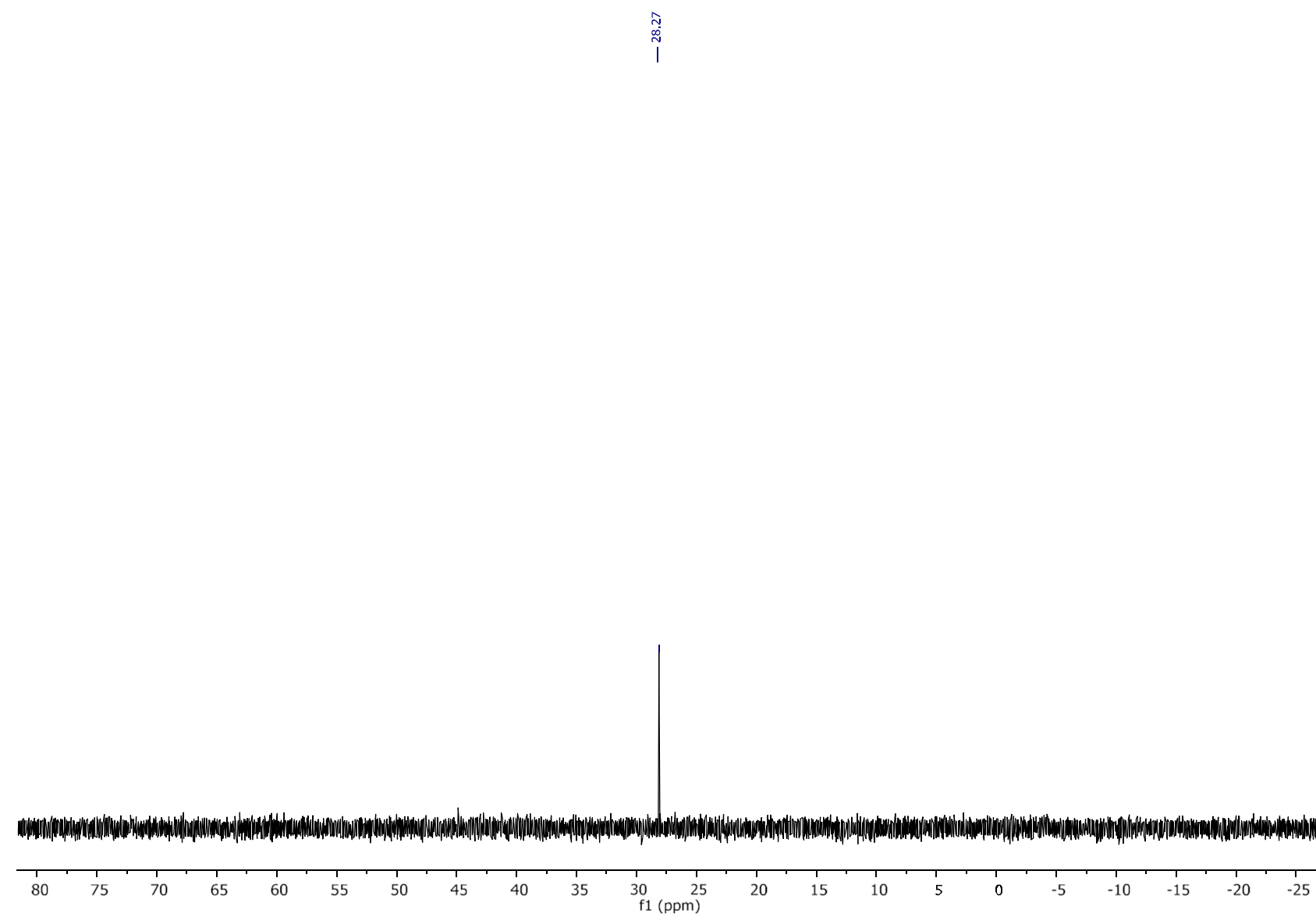
¹³C-RMN



¹H-RMN



^{31}P -RMN



¹³C-RMN

