Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Synthesis of β-carboline-benzimidazole conjugates using lanthanum nitrate as a catalyst and their biological evaluation

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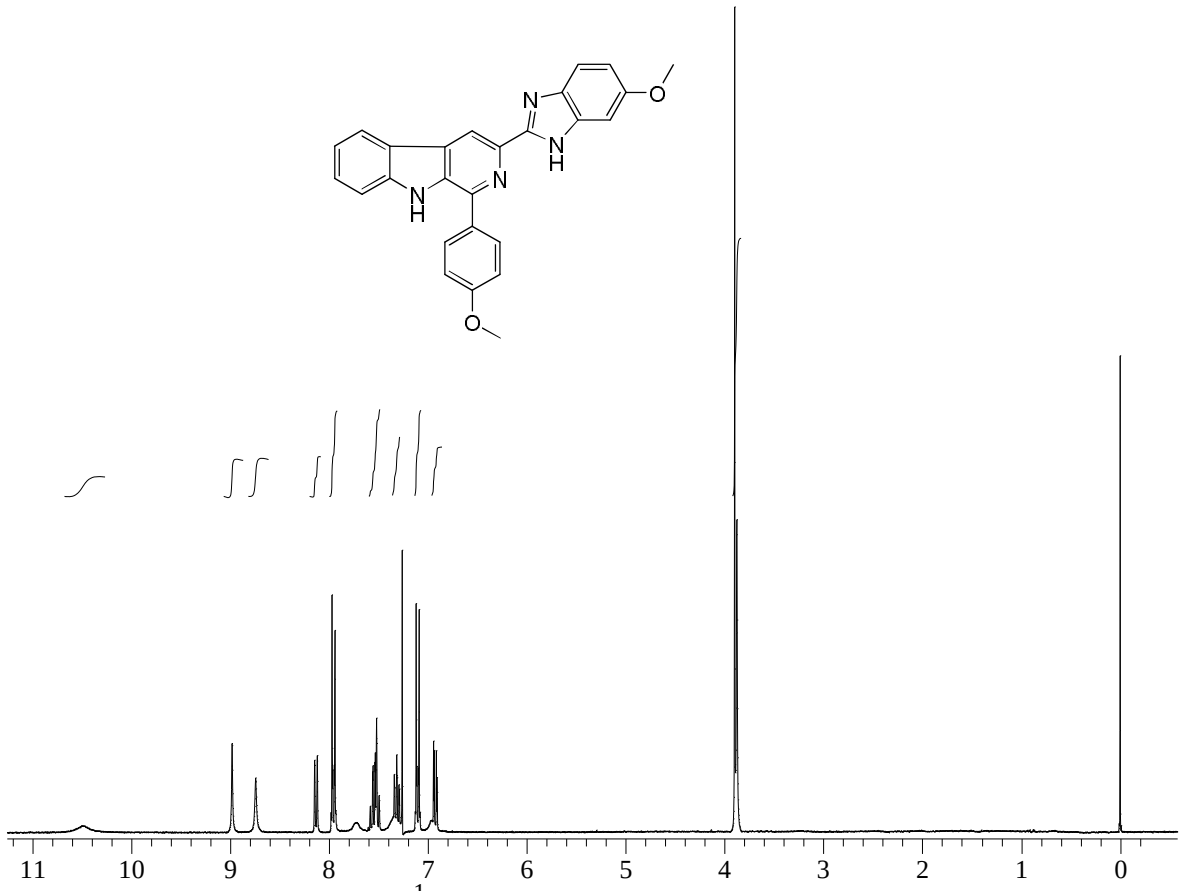
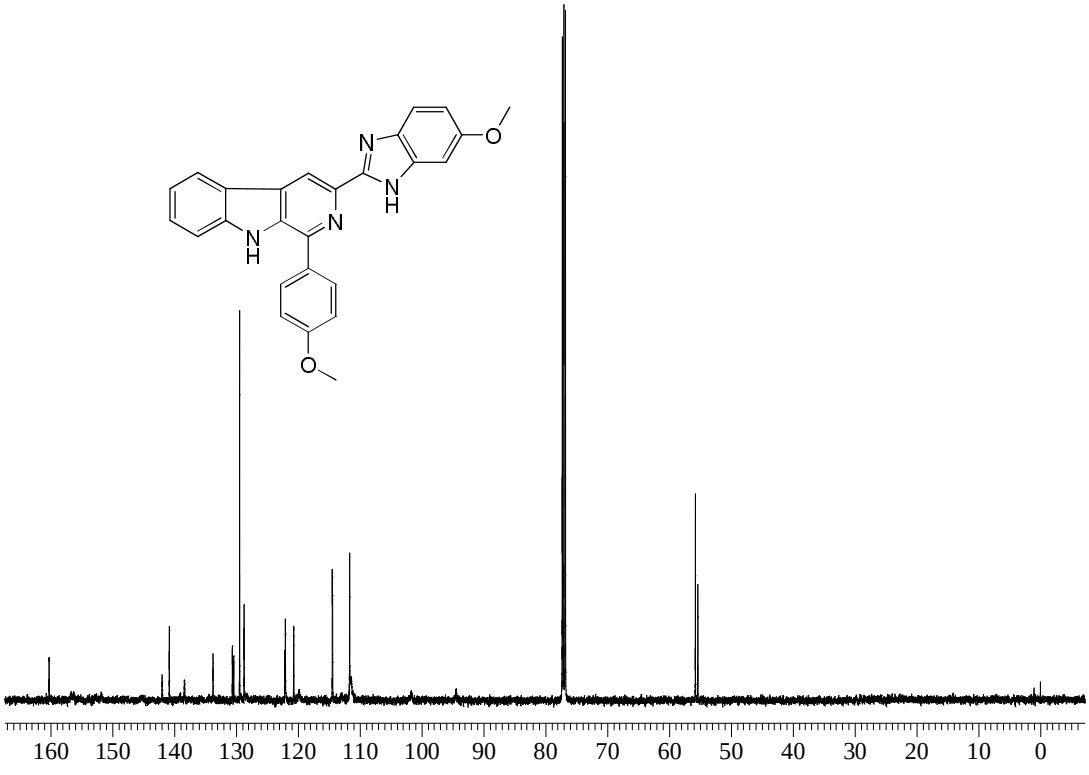
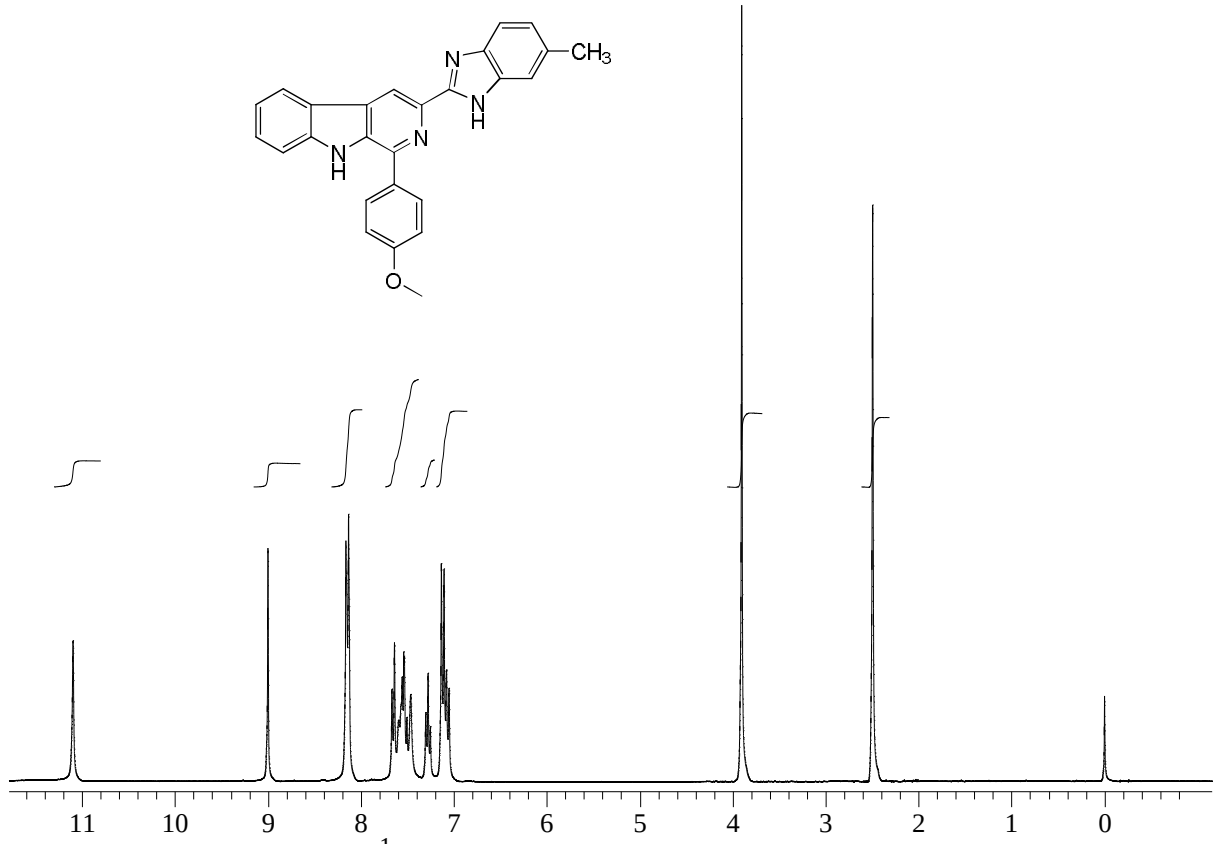
NMR spectral copies of the products



^{1}H NMR of Compound **5a**



^{13}C NMR of Compound **5a**



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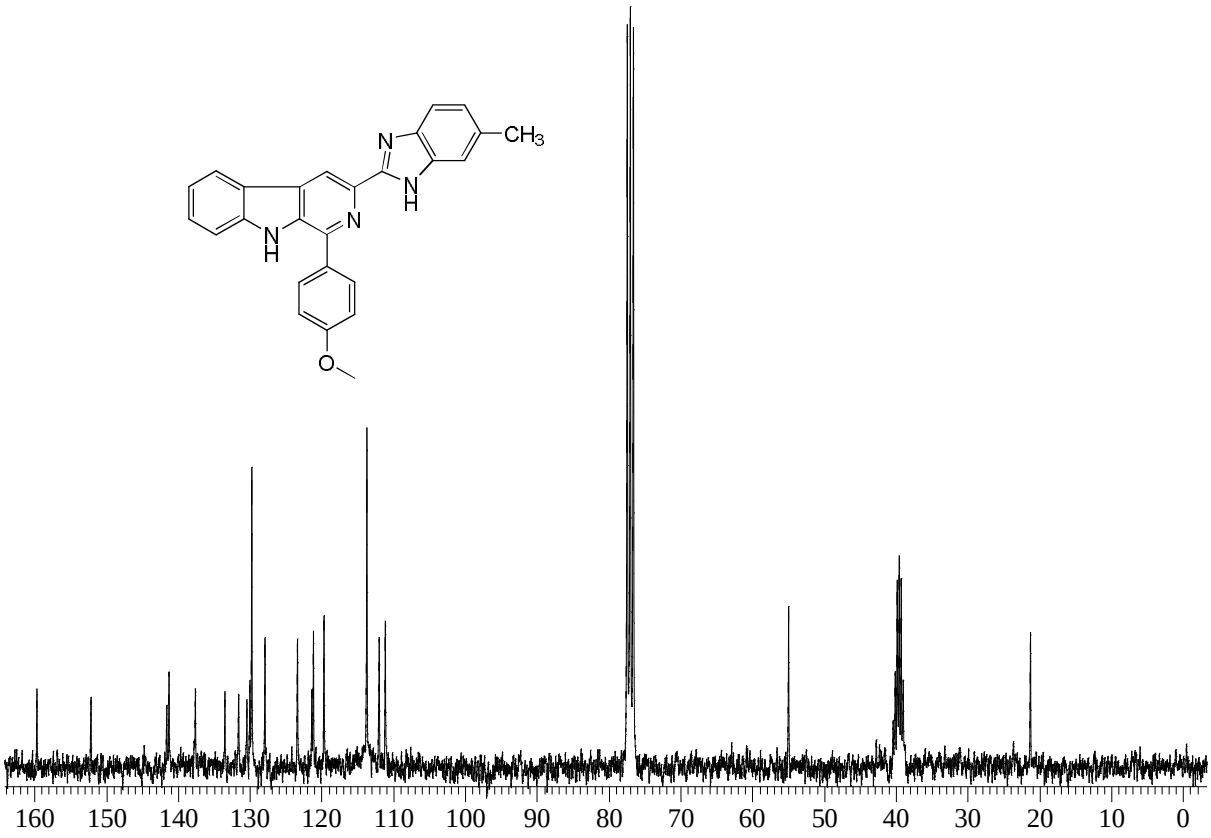

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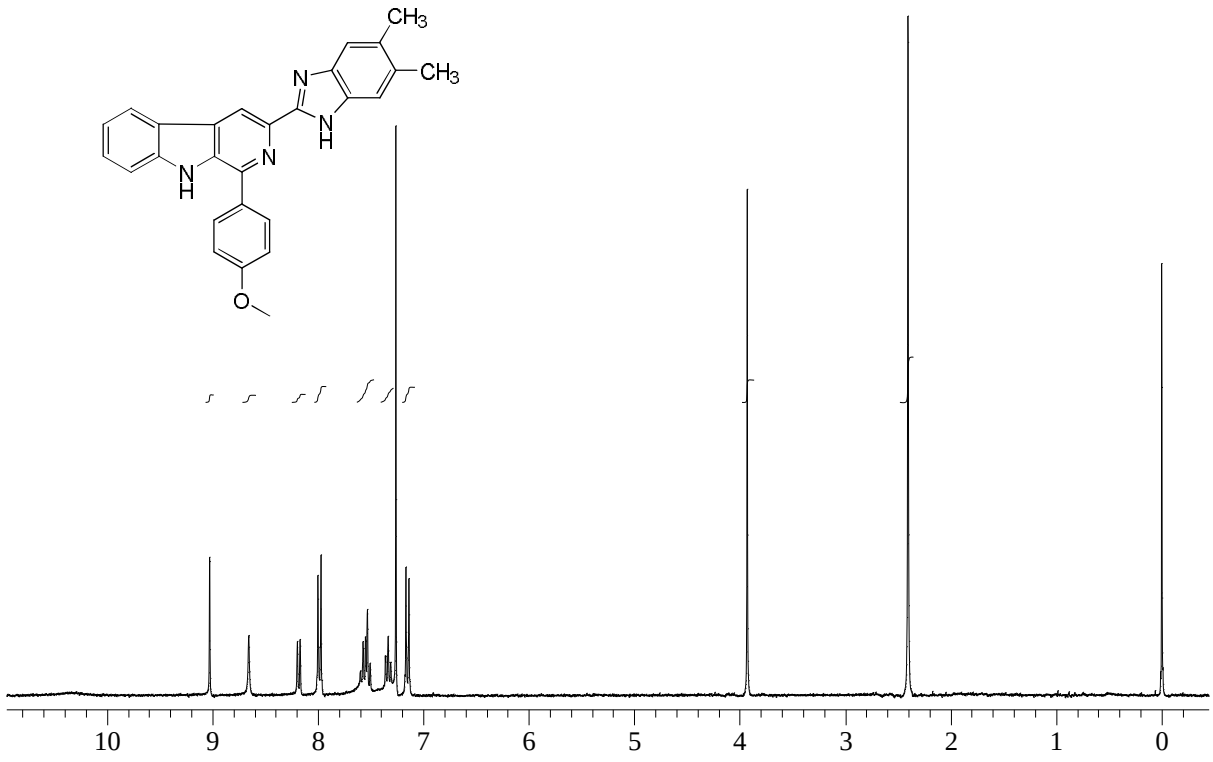

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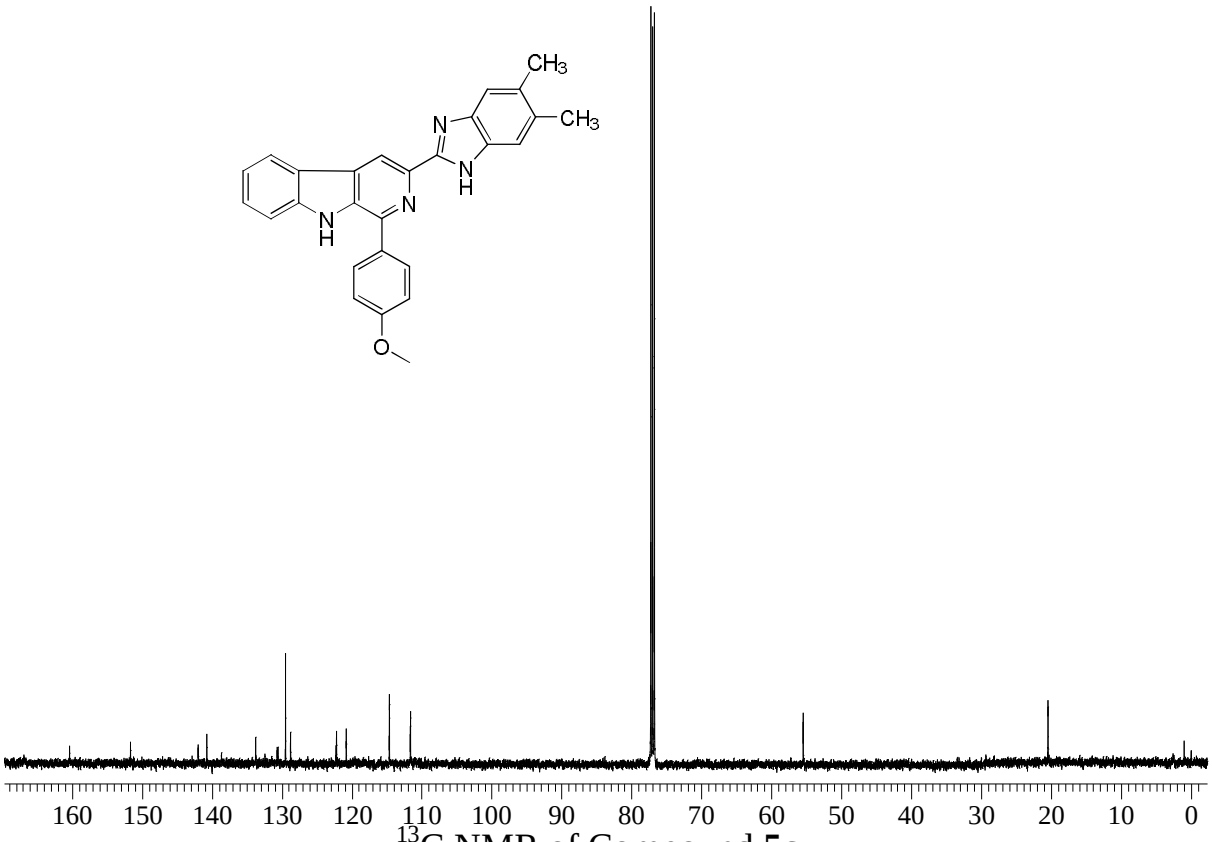
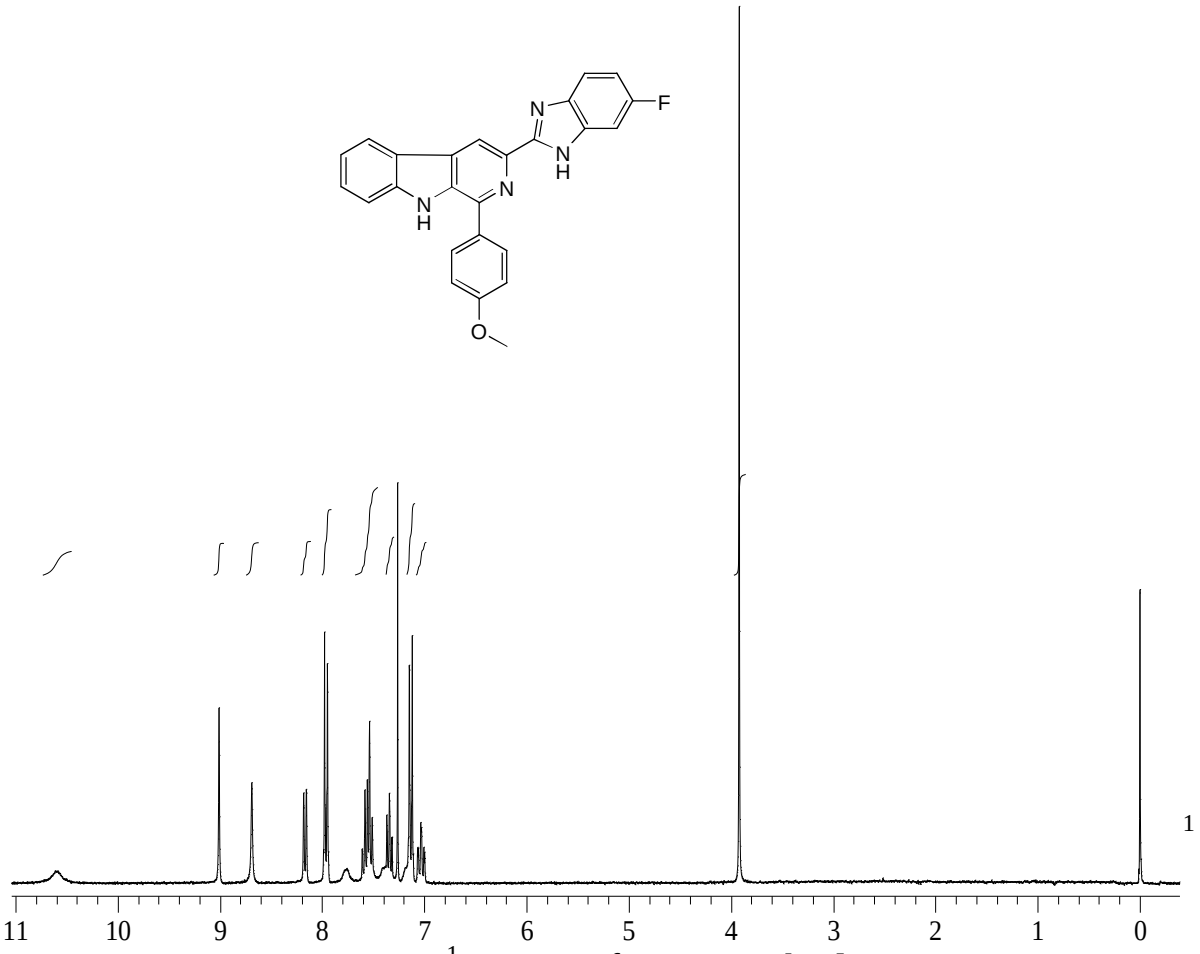


^{13}C NMR of Compound **5c**



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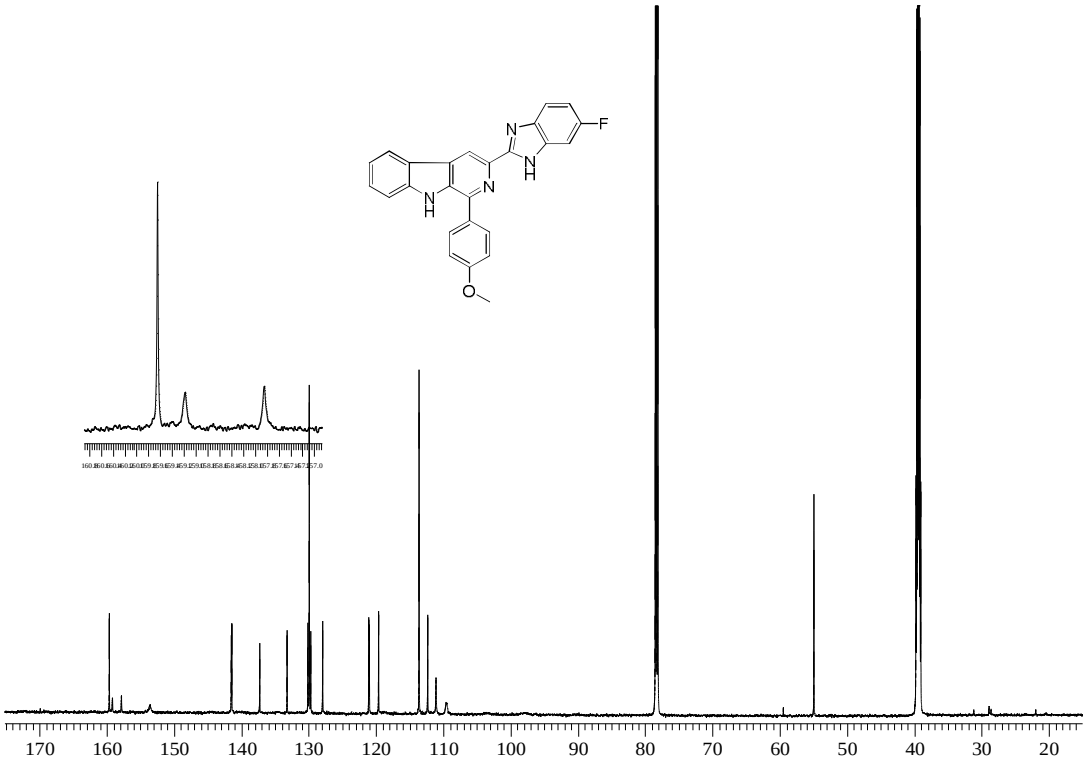

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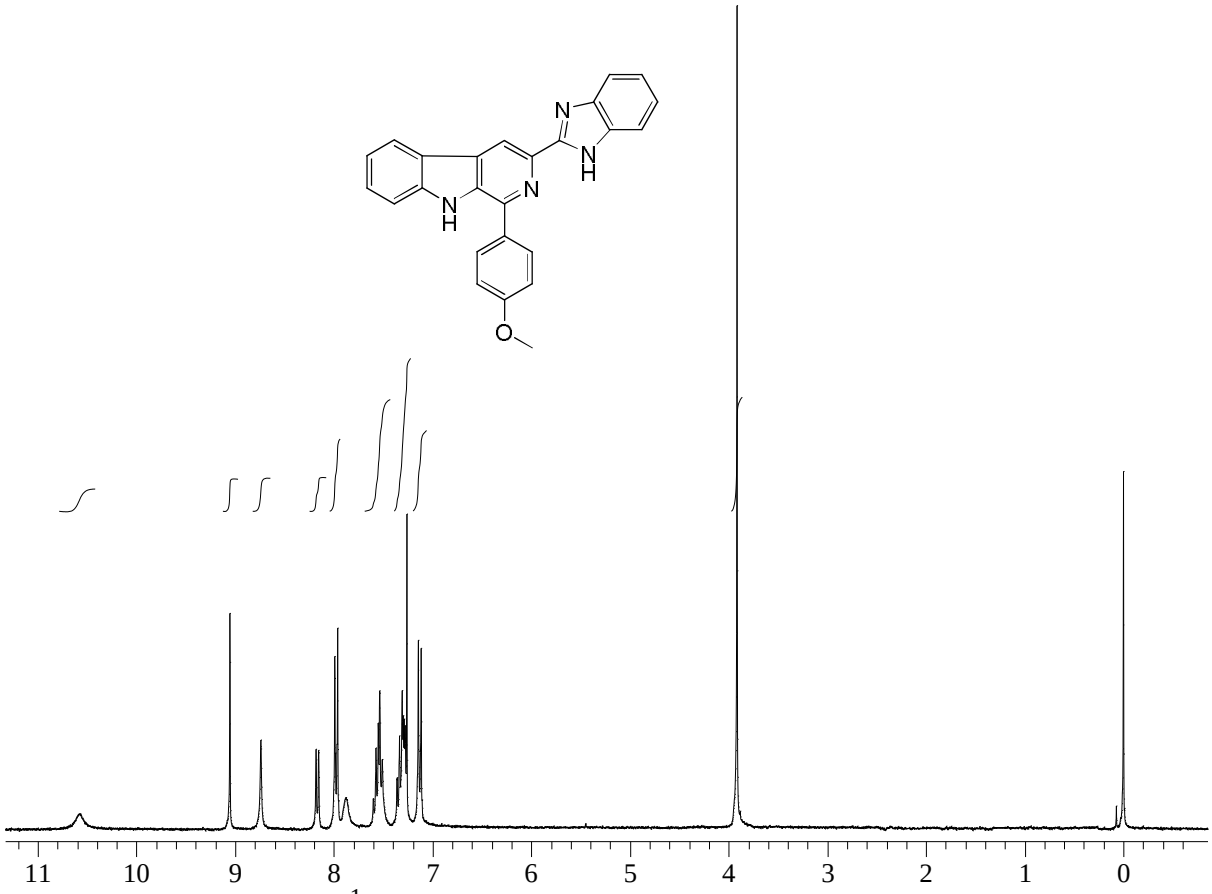

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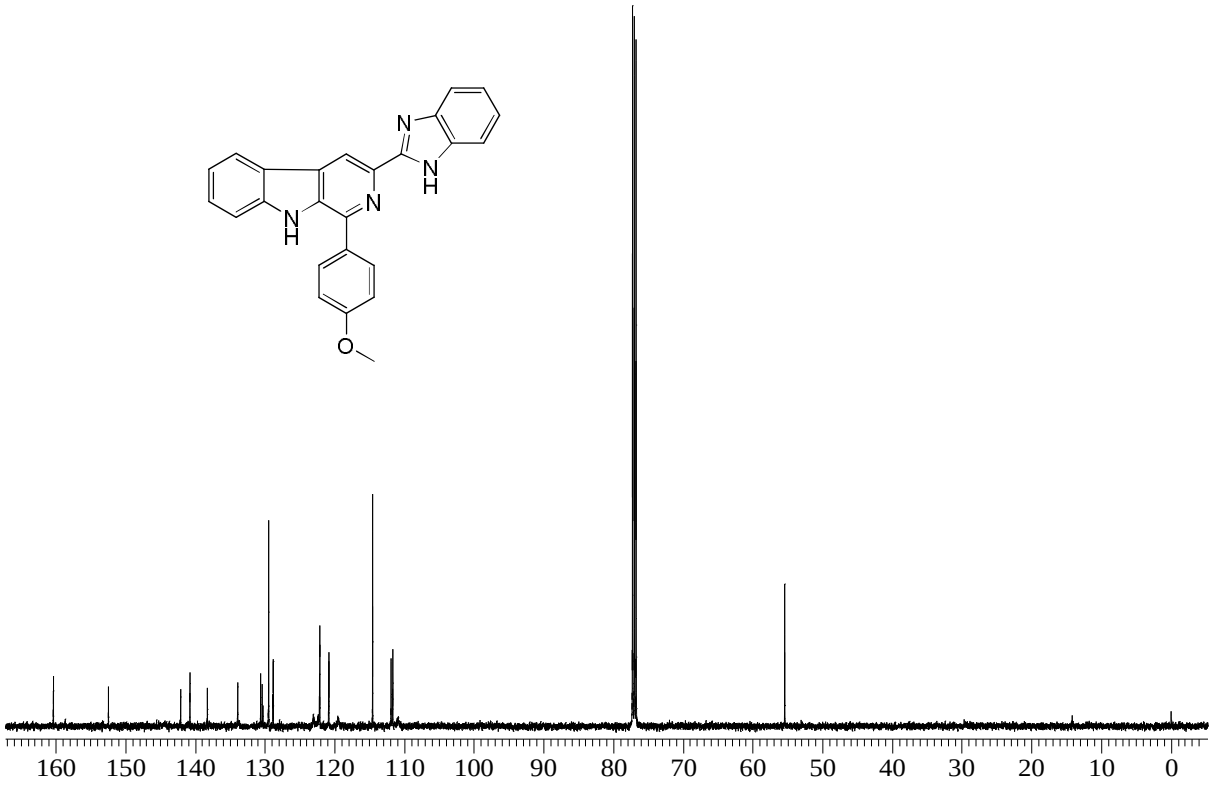

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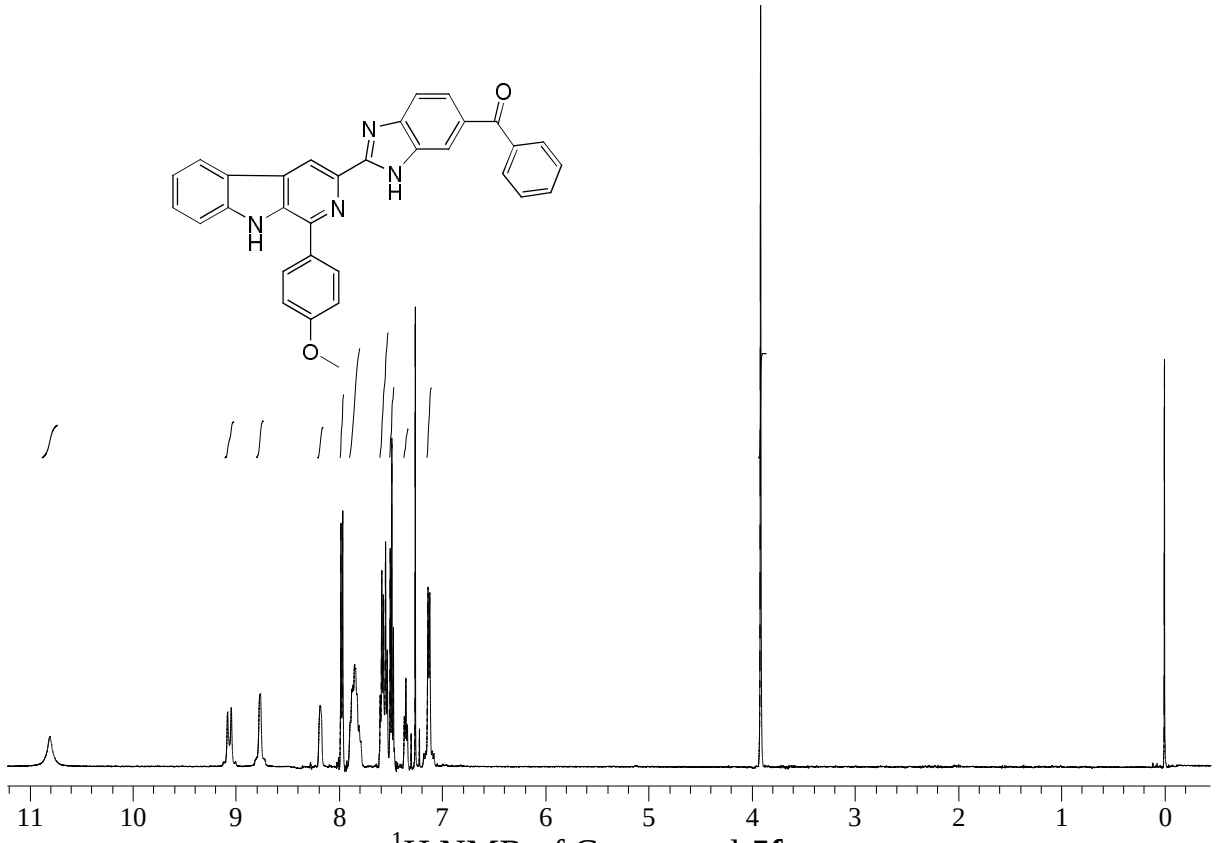

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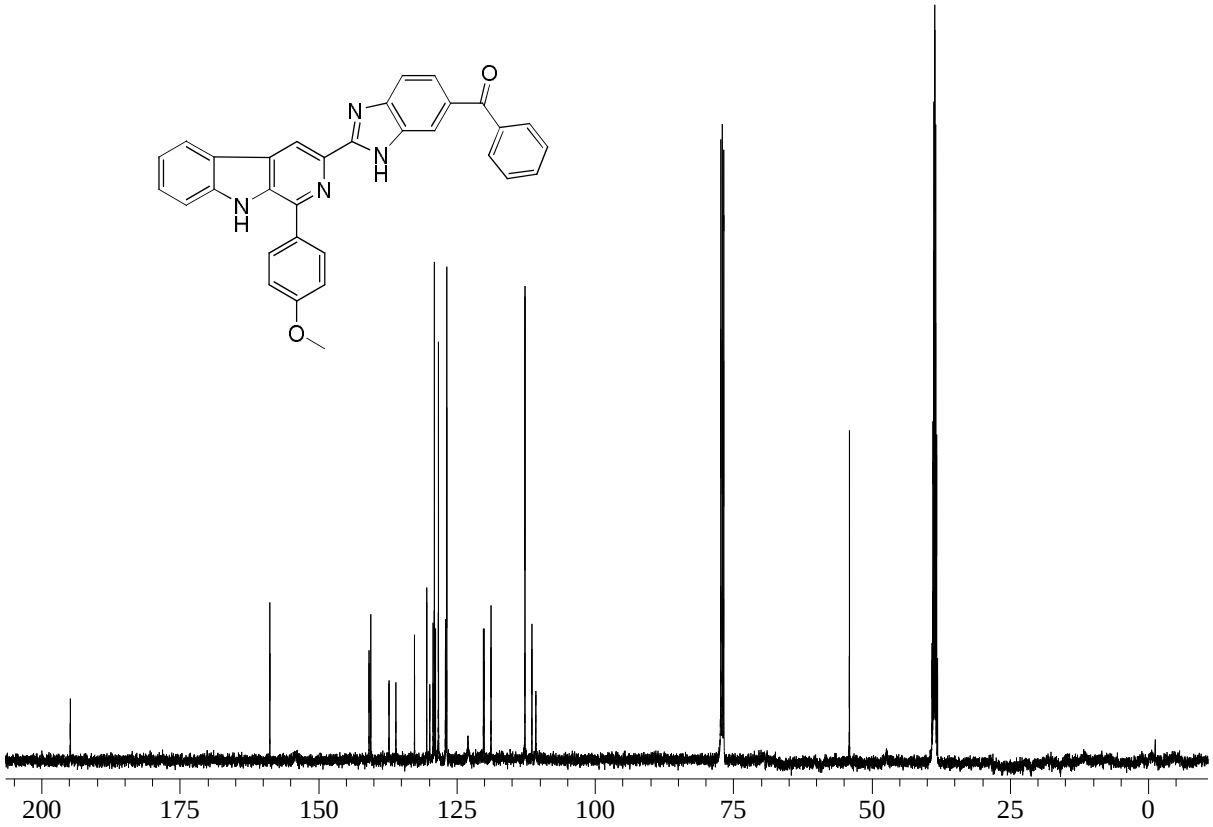

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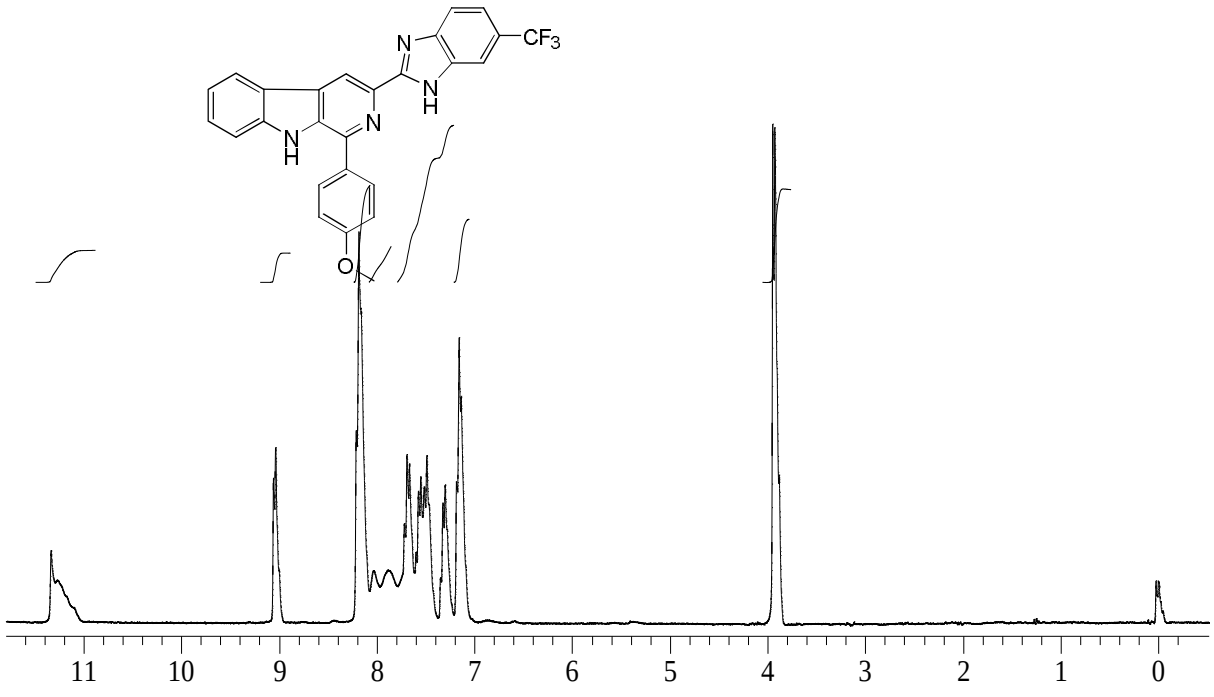

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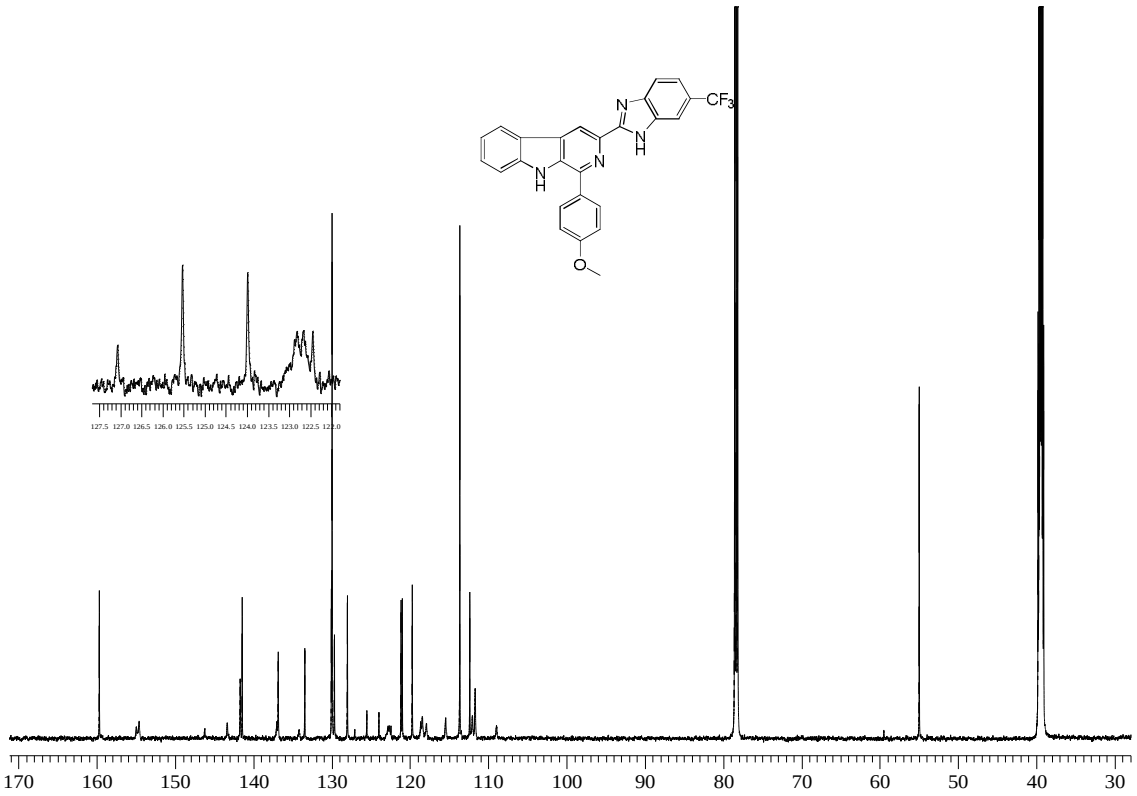

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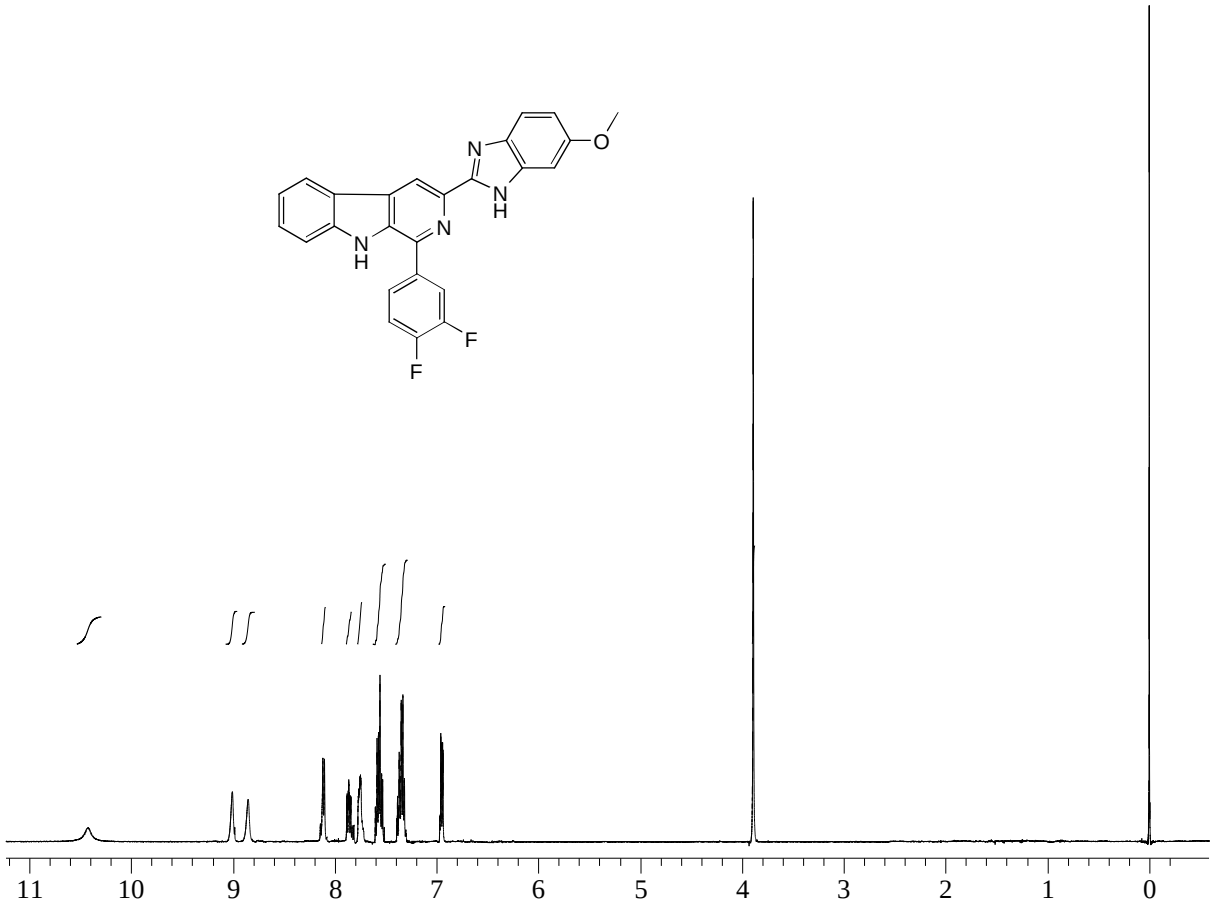
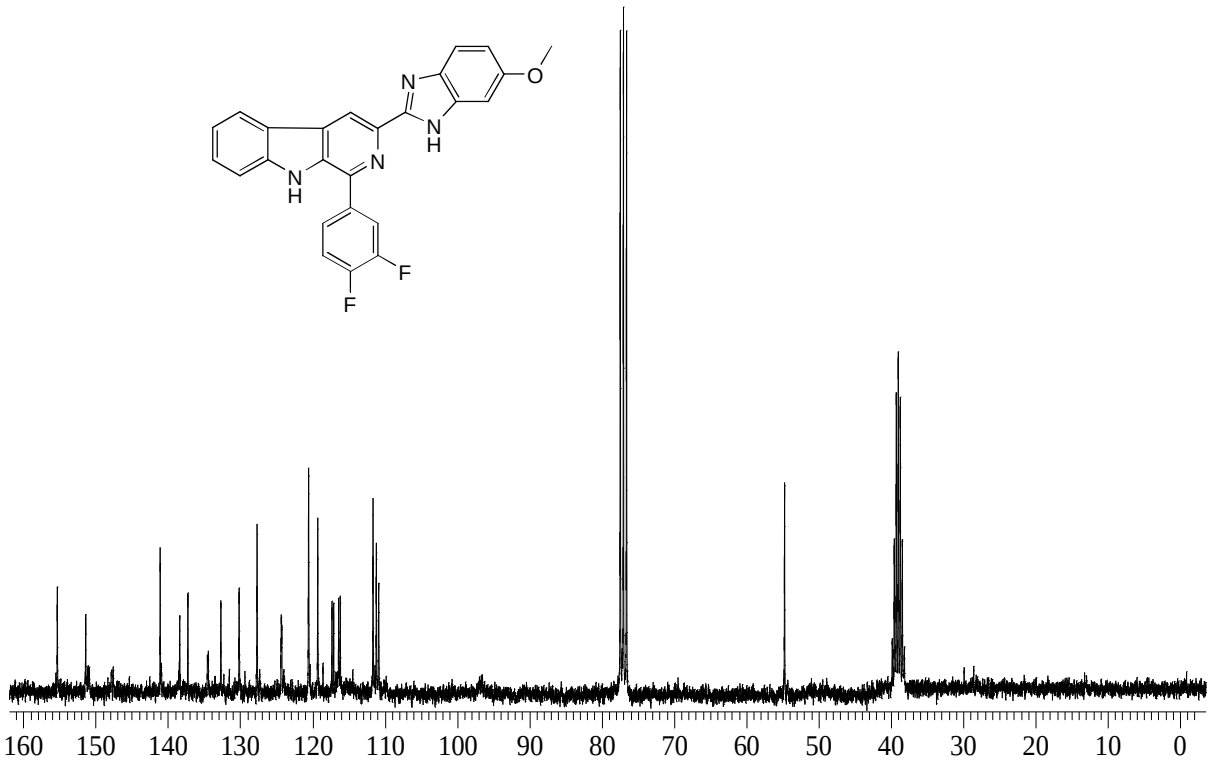


^{1}H NMR of Compound-**5h**



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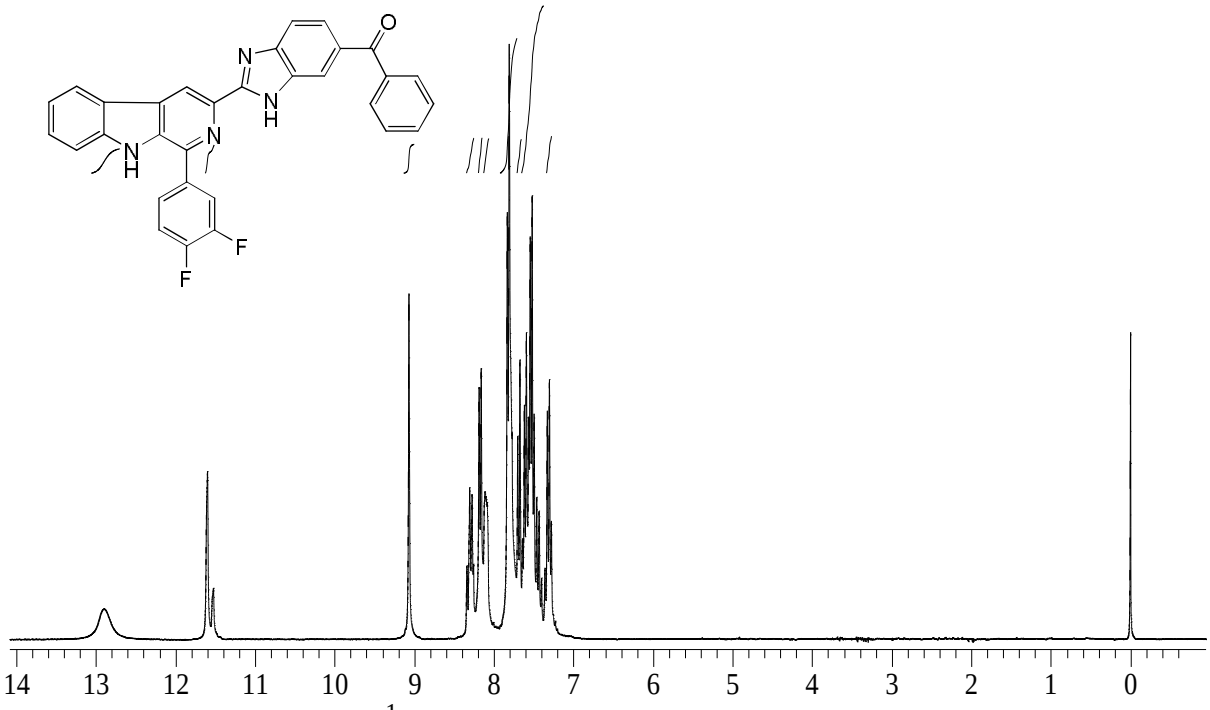

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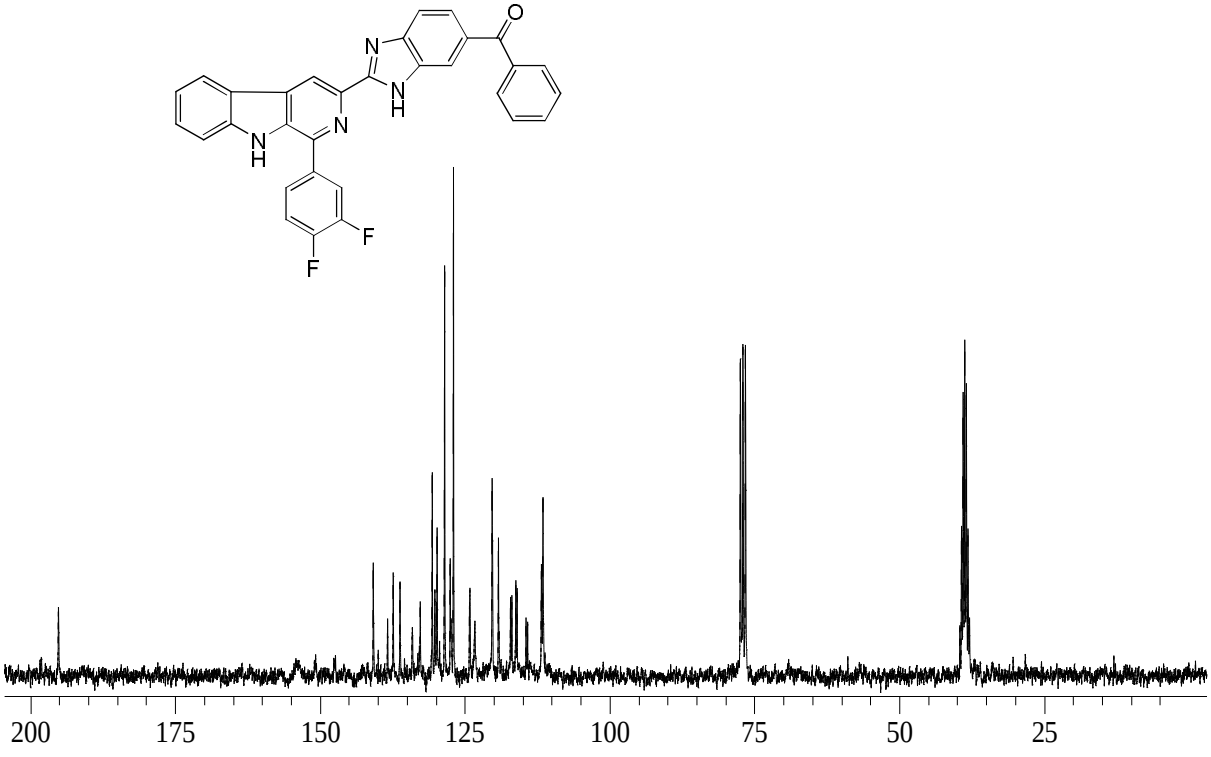

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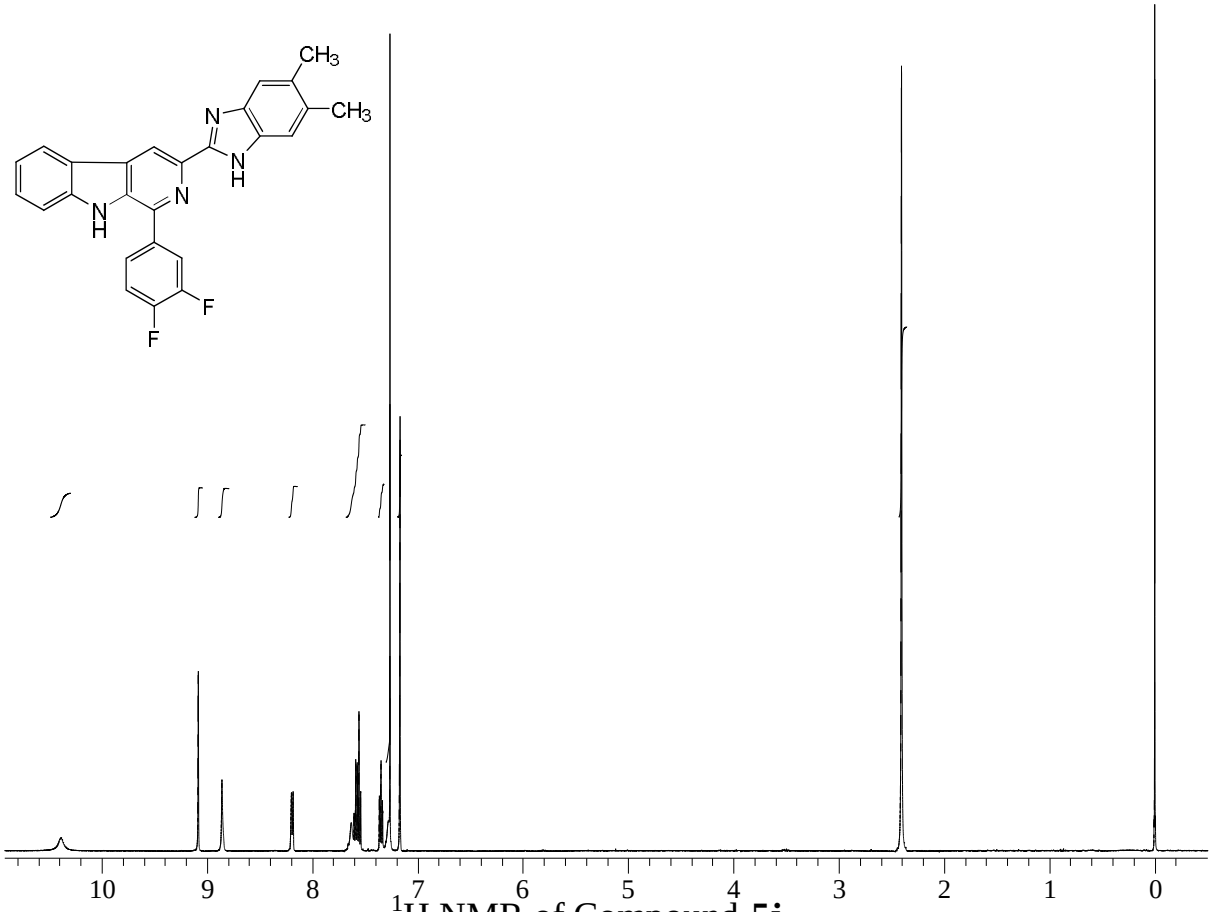

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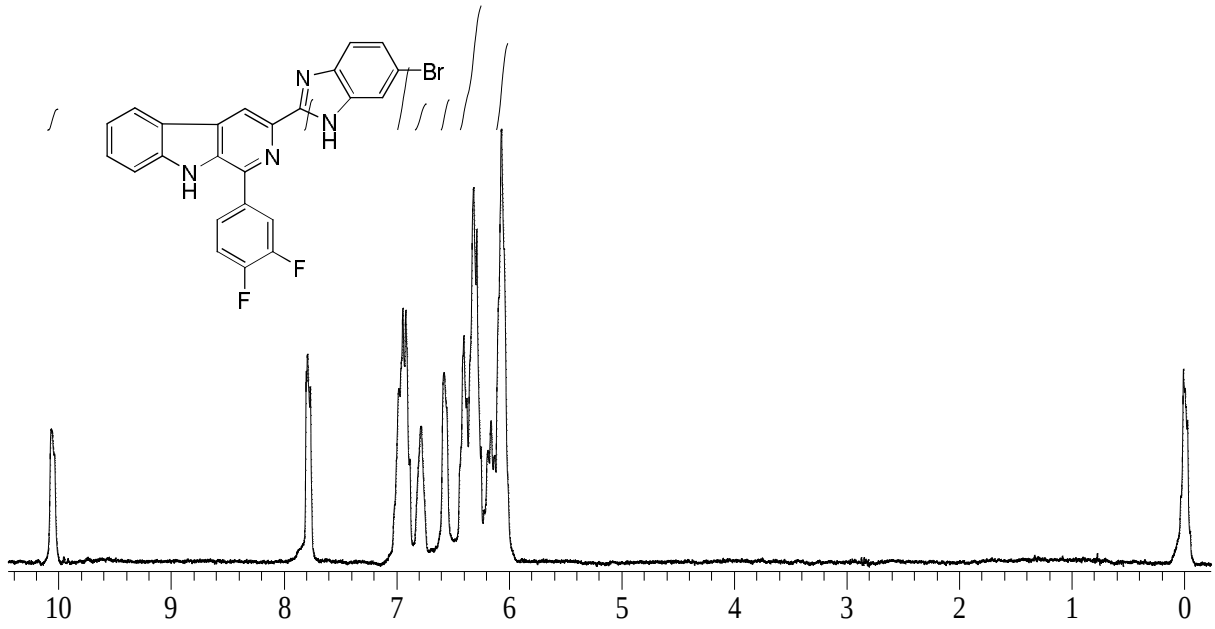

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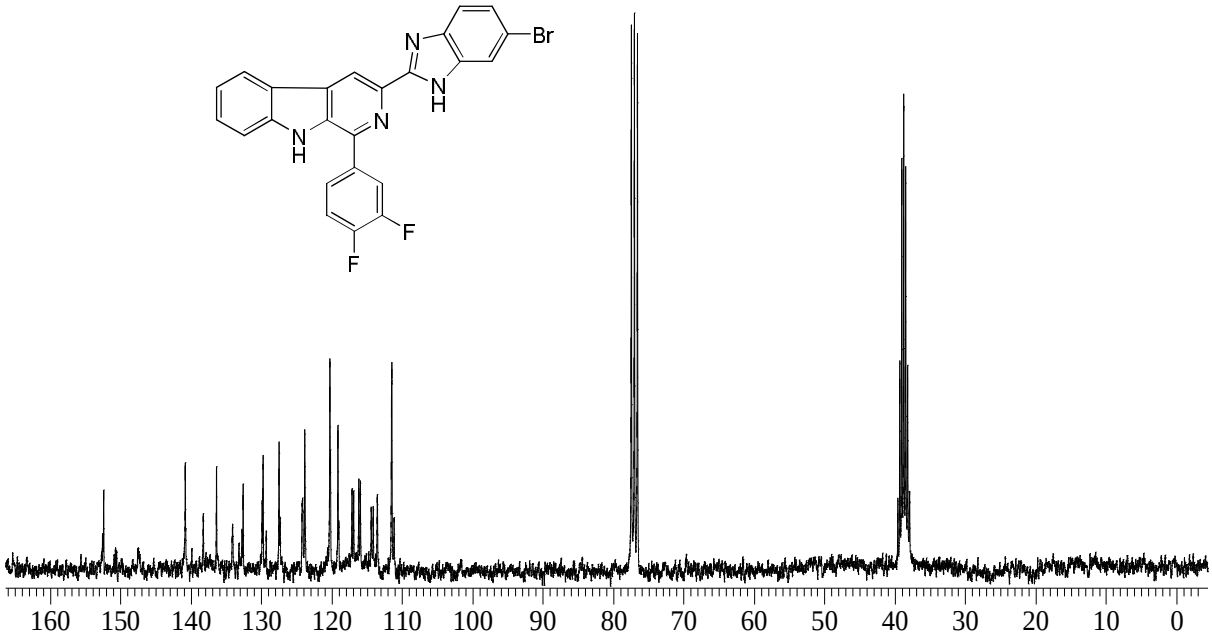

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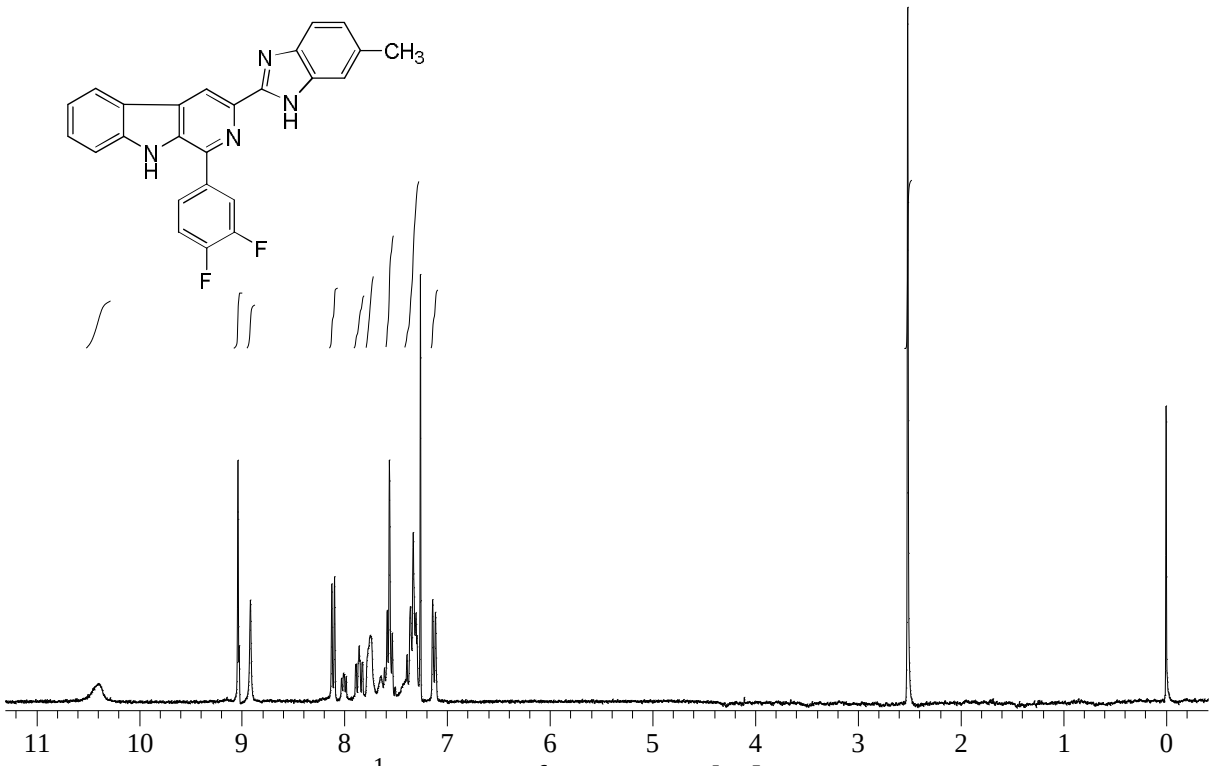

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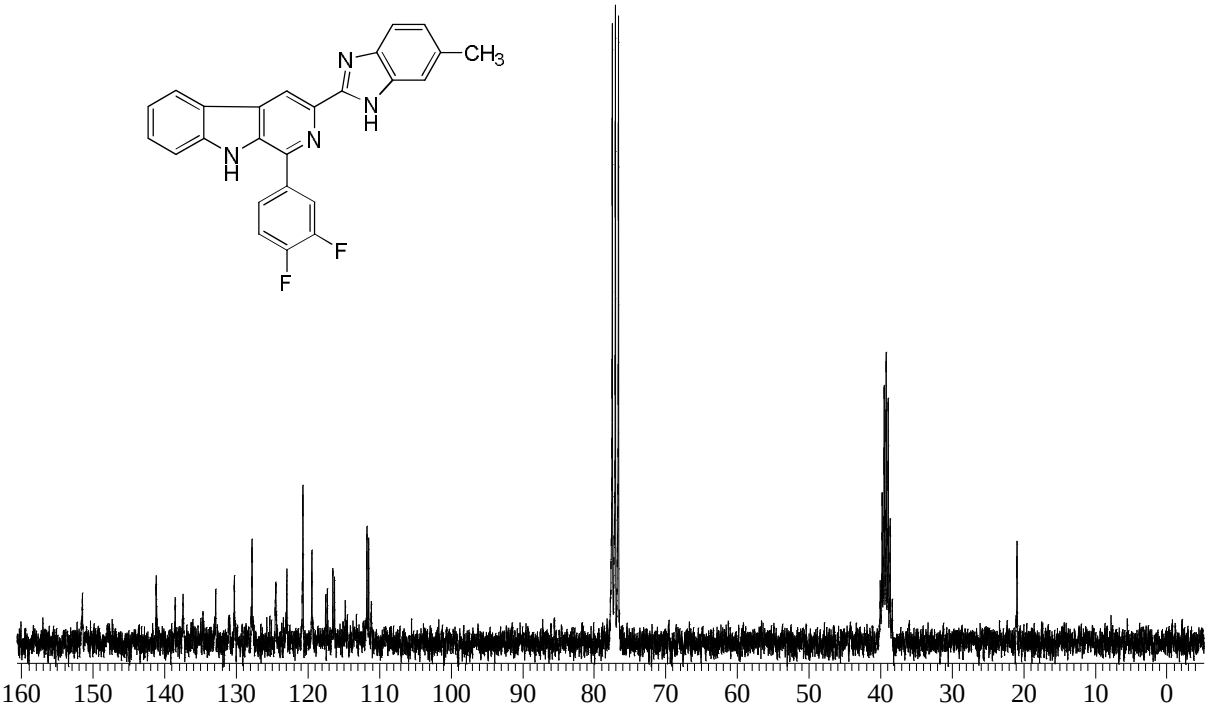

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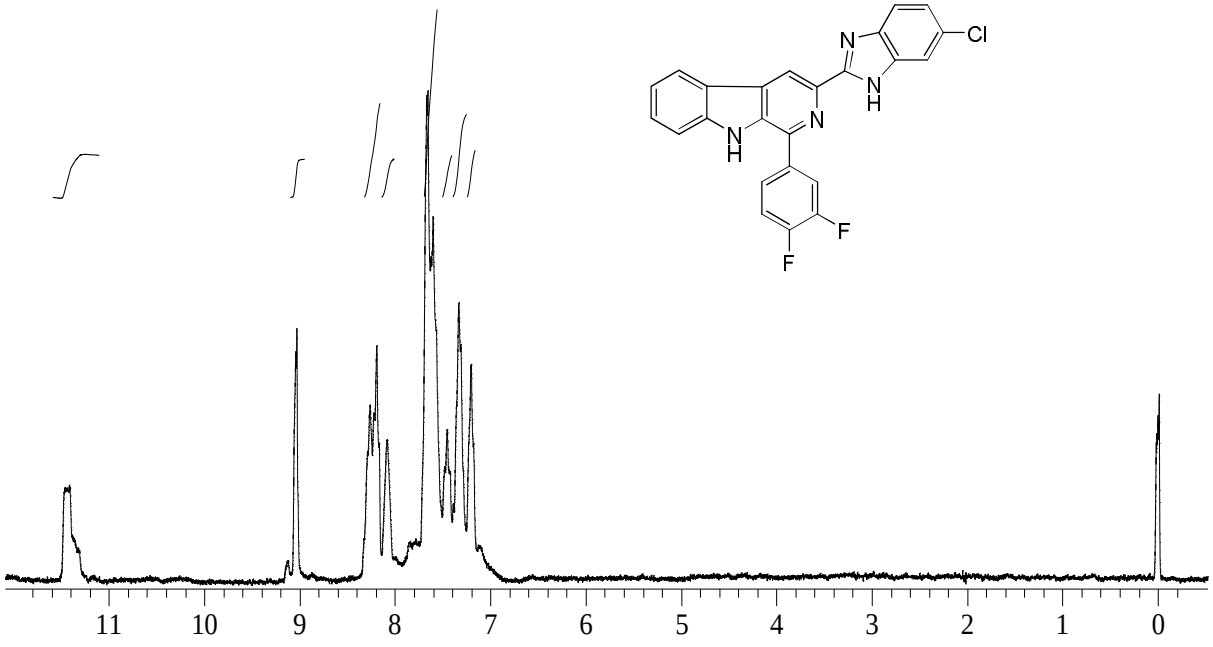

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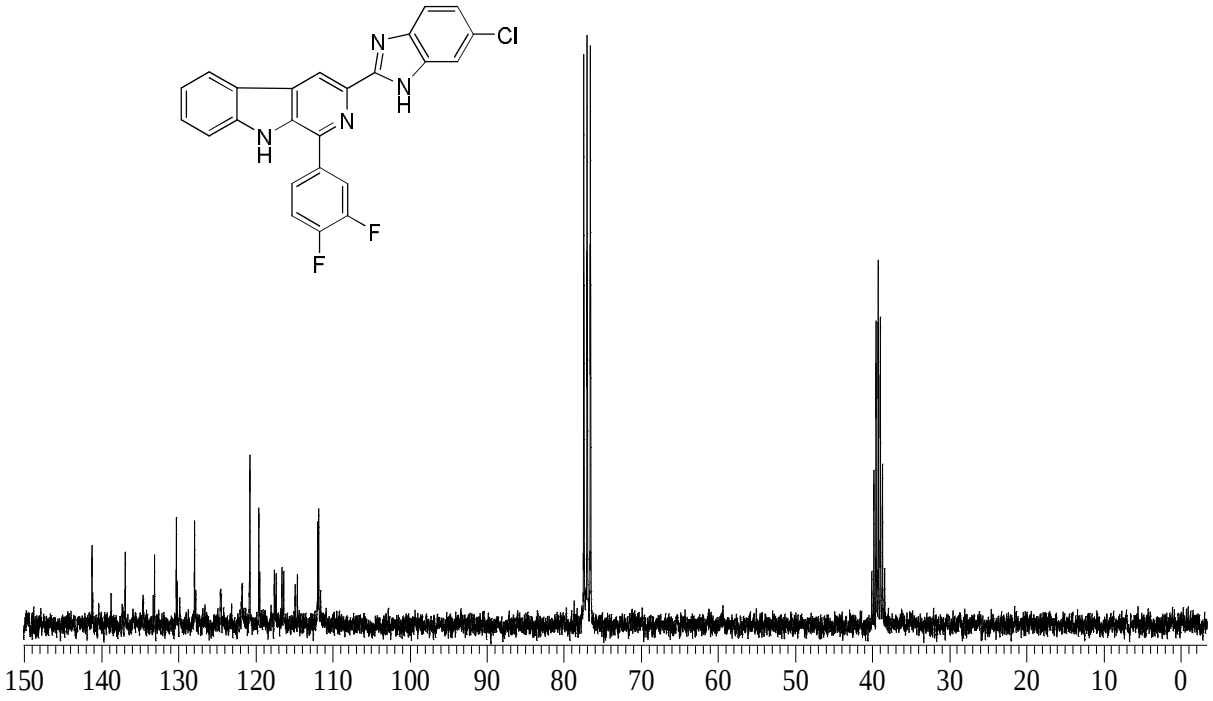

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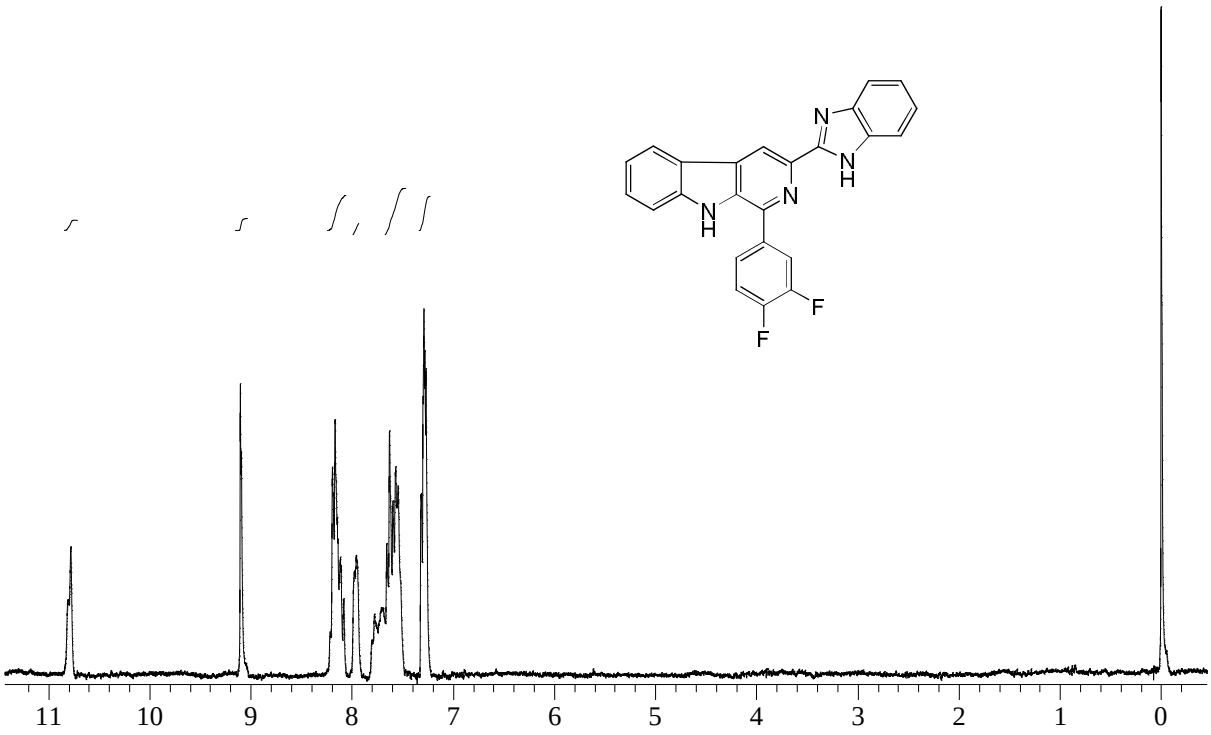

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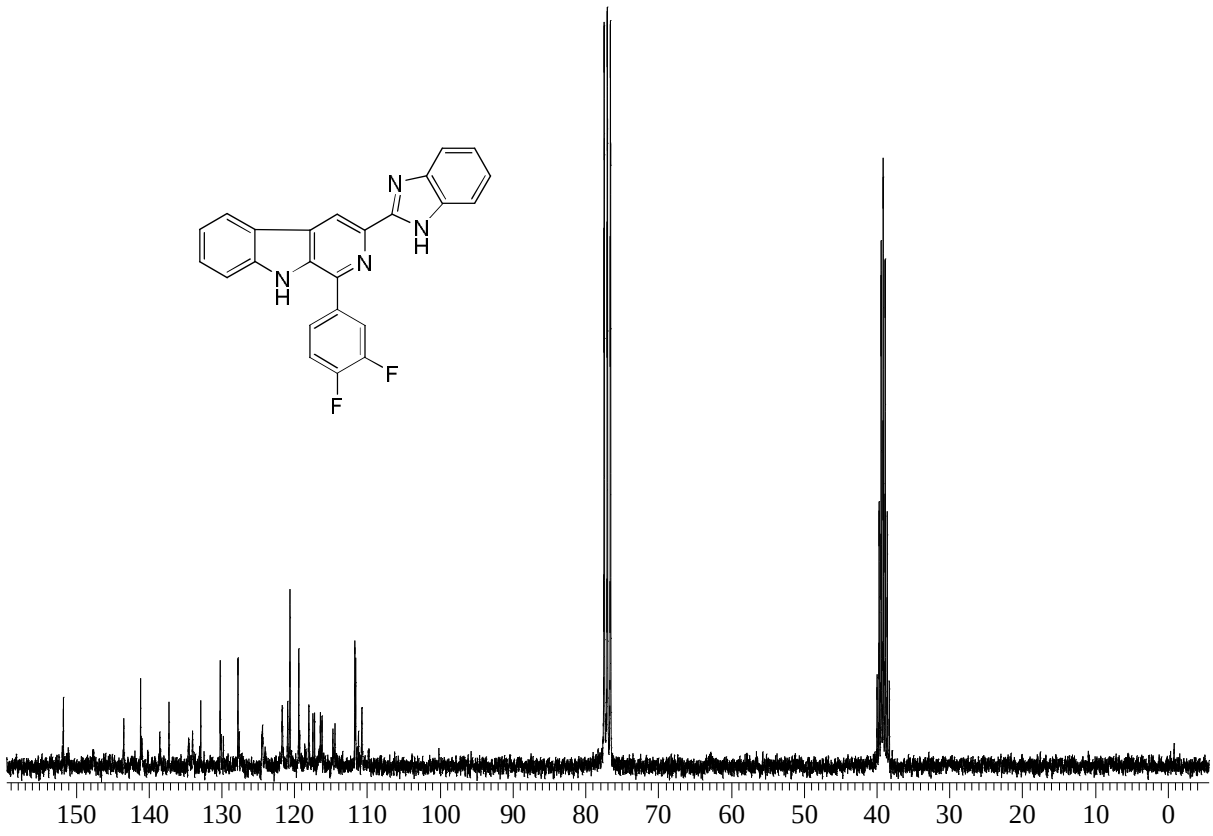

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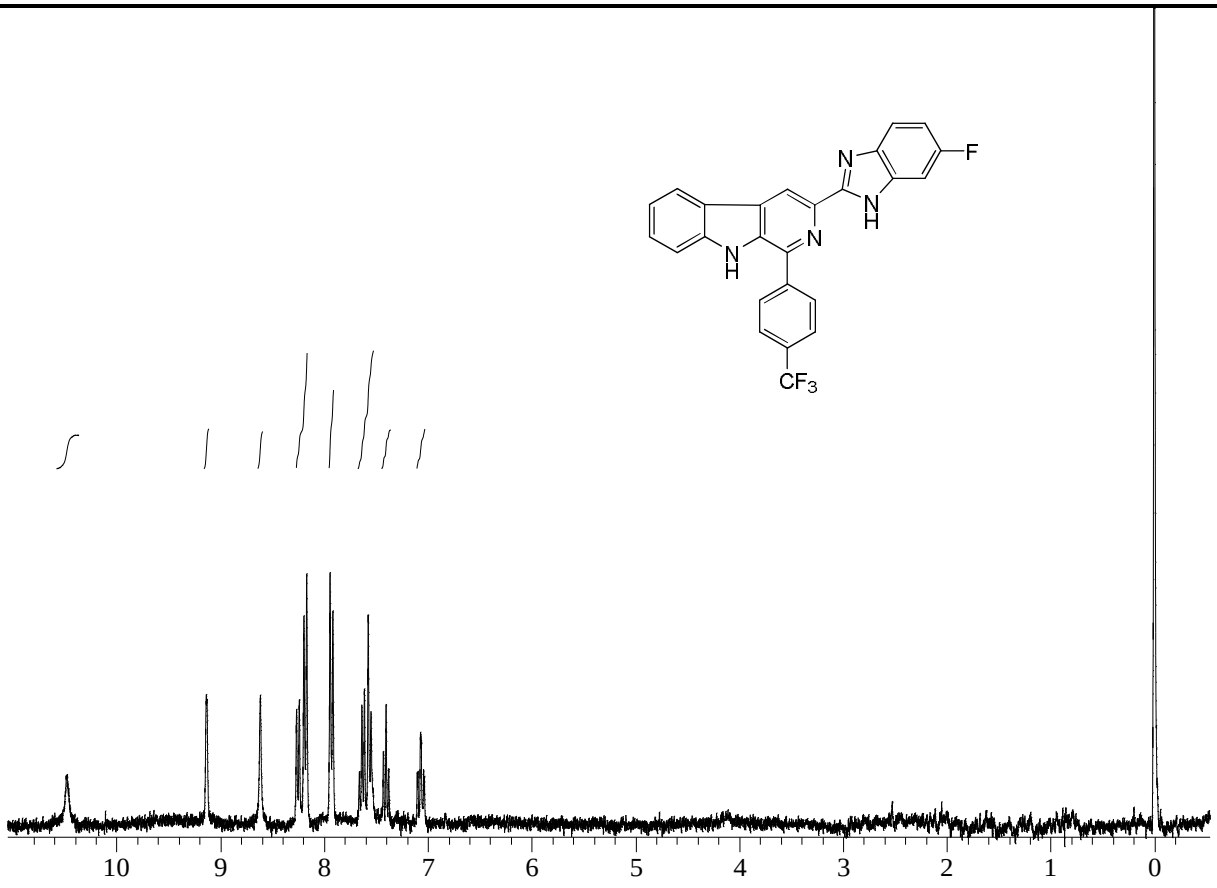

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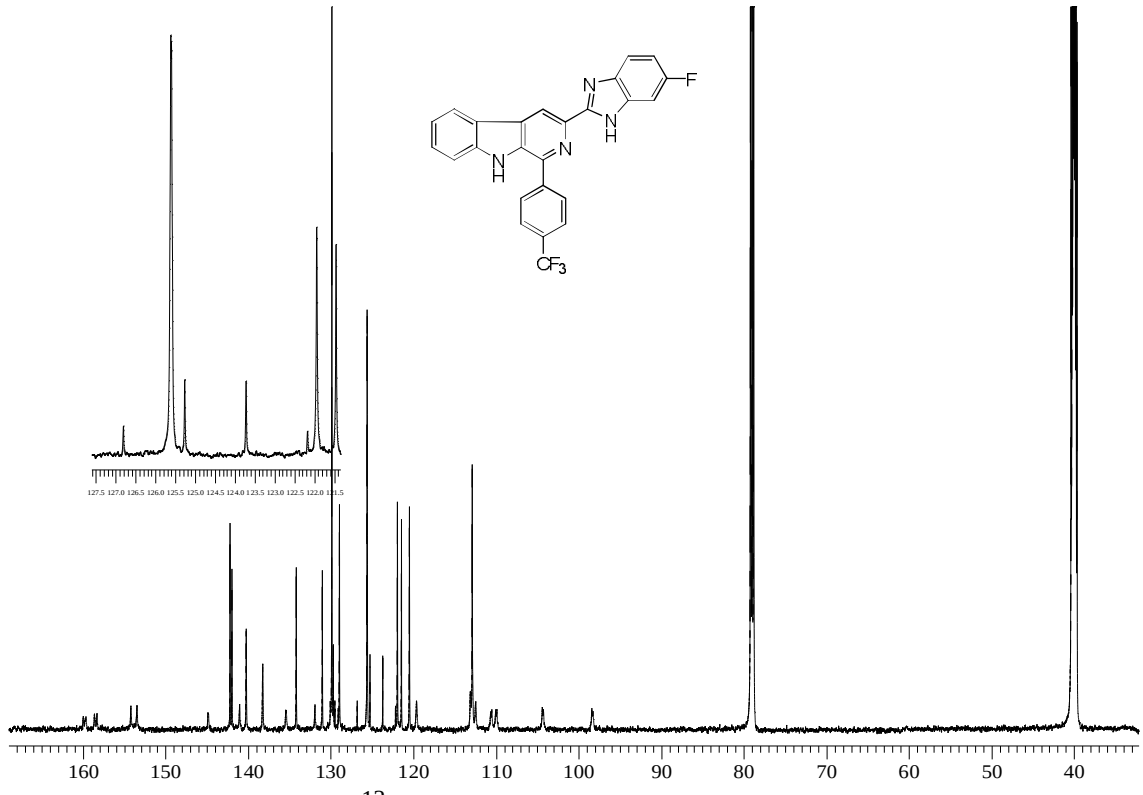

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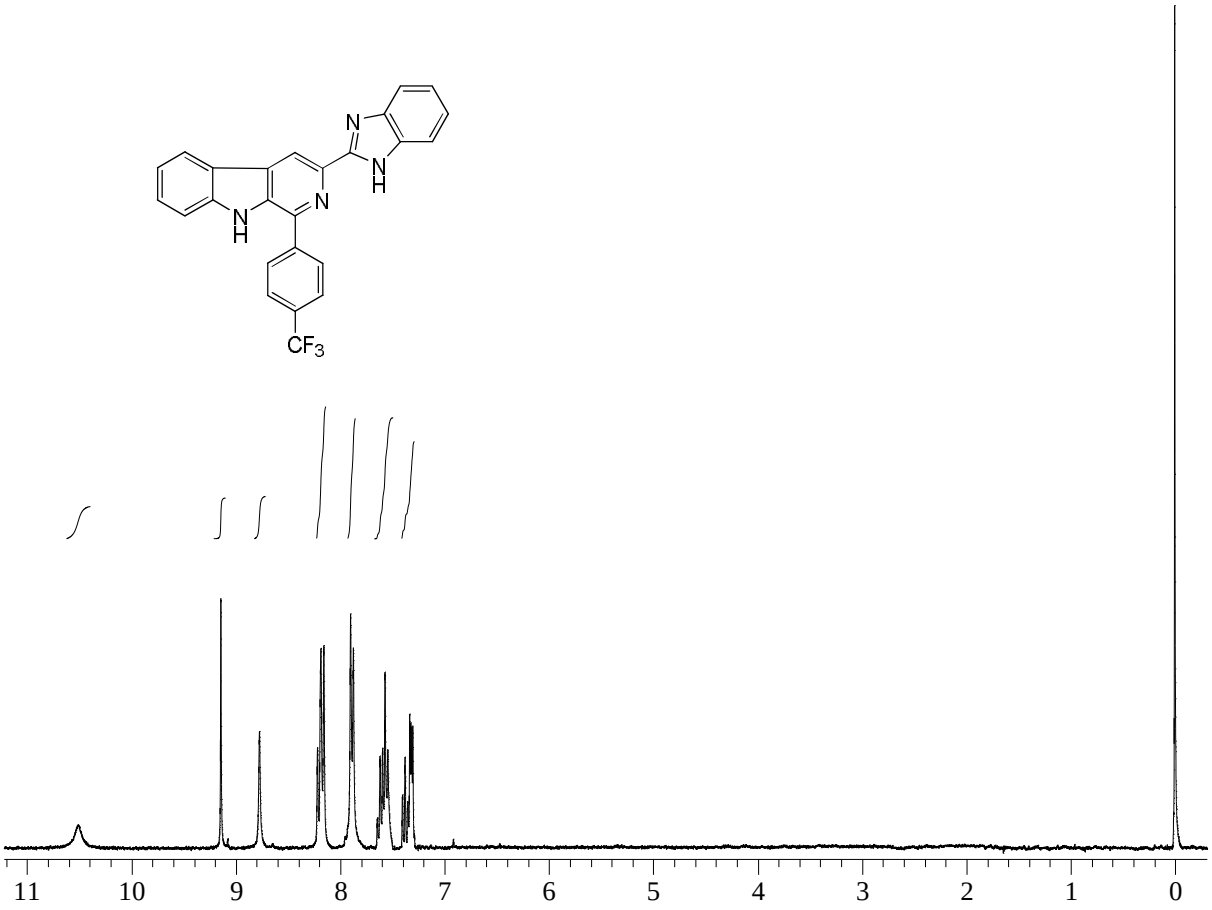

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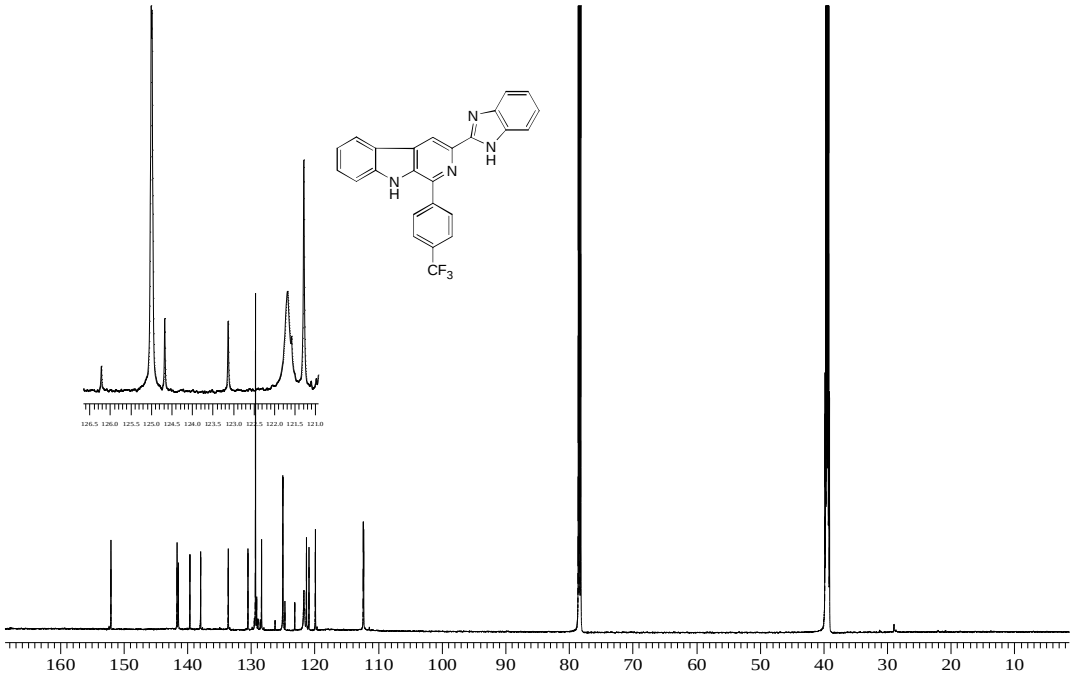

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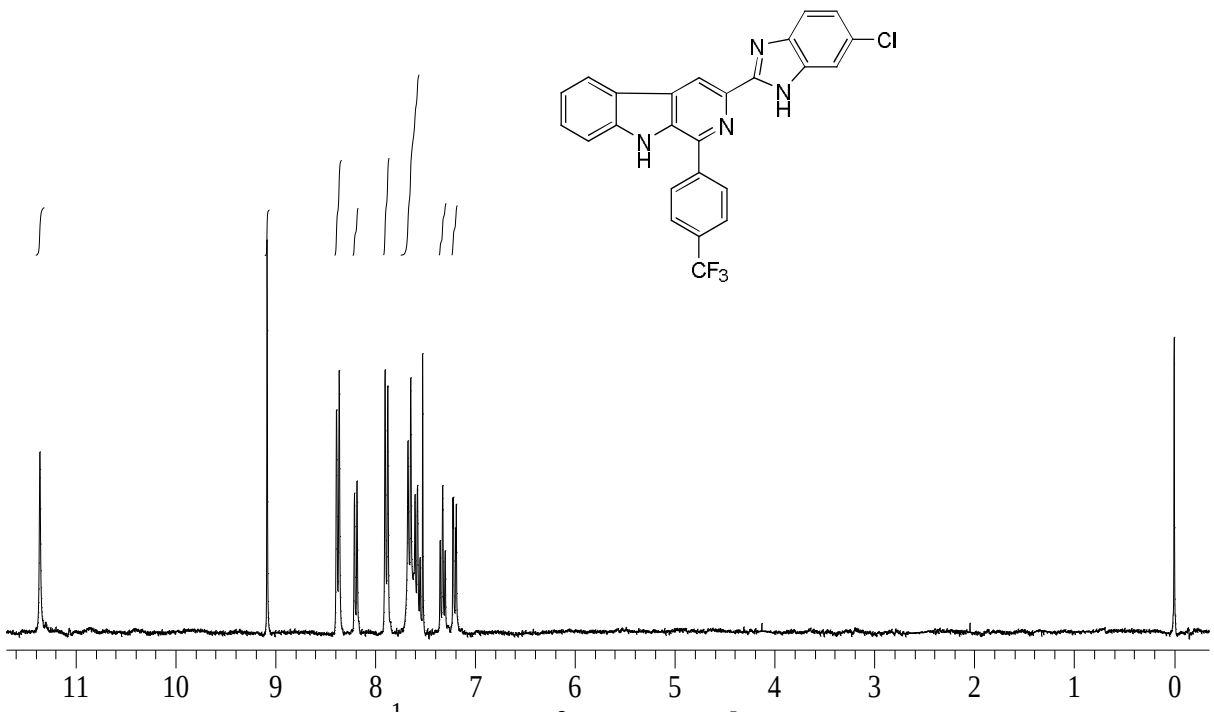

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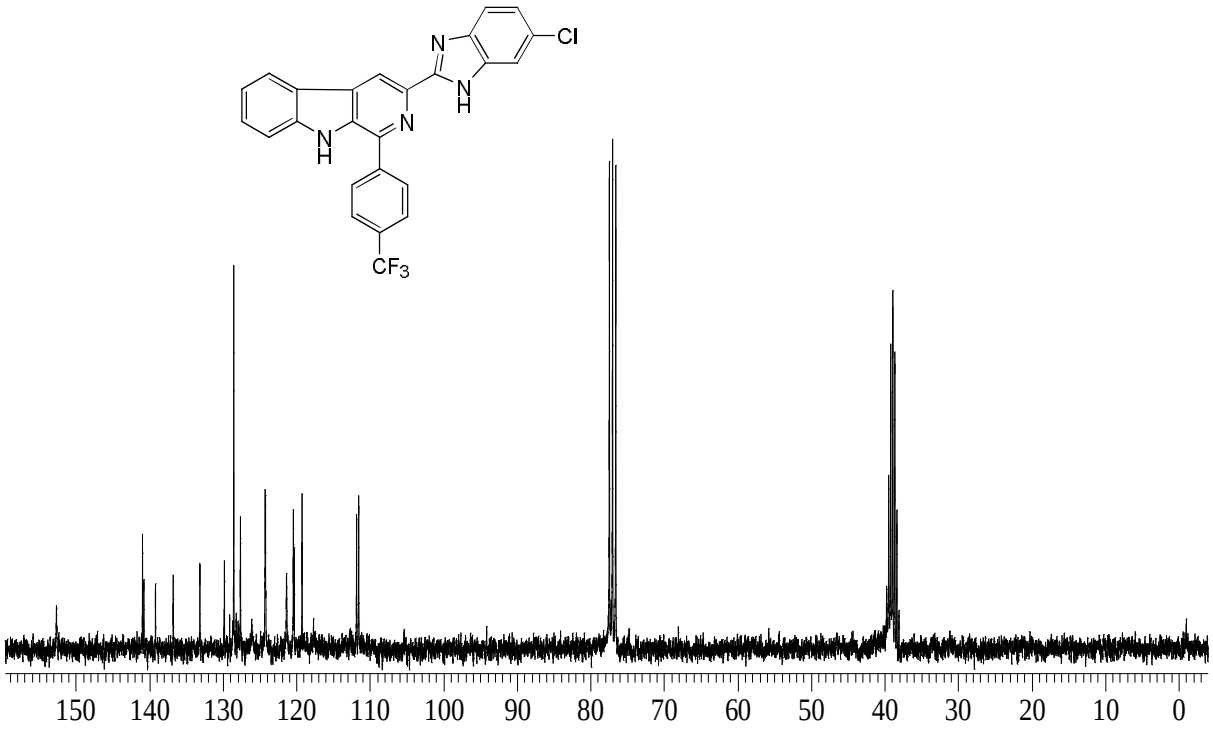

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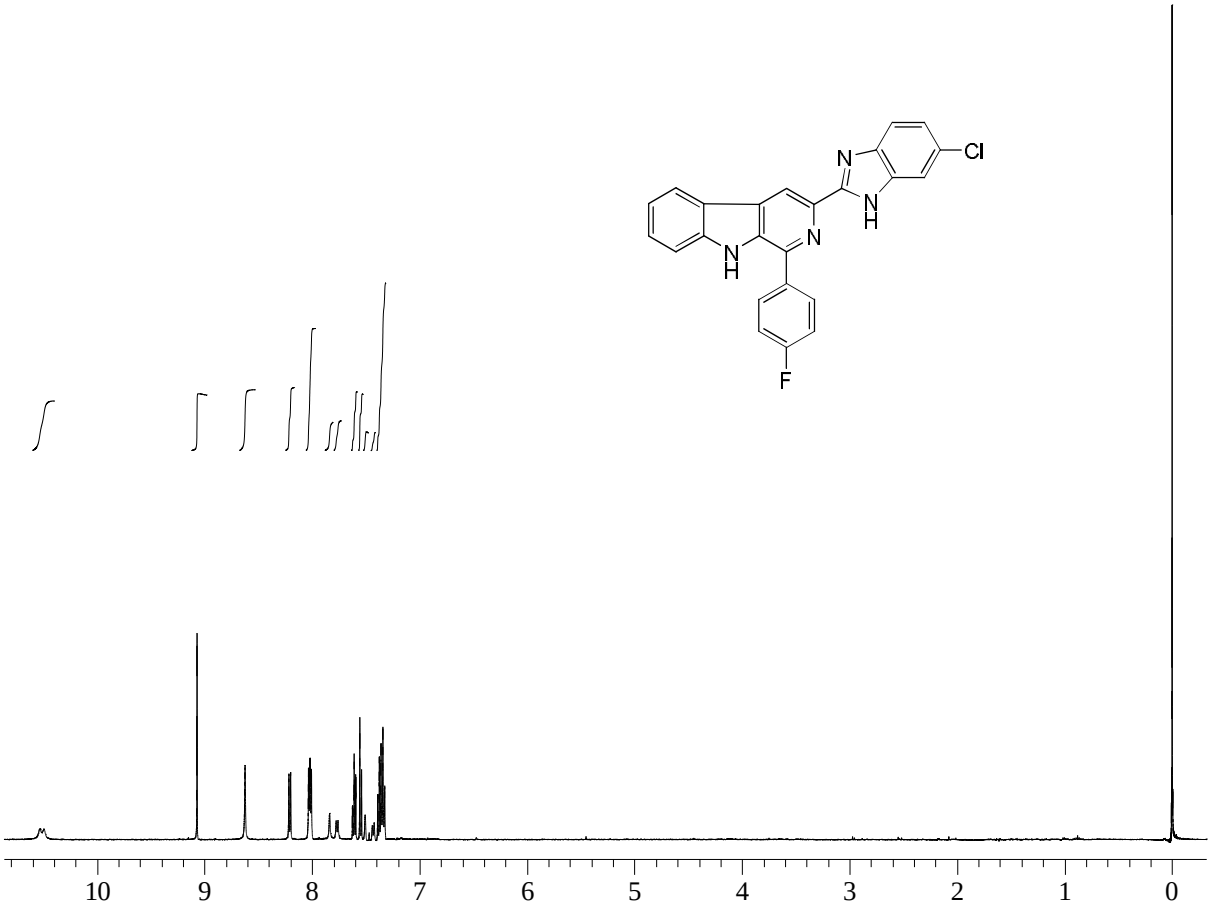

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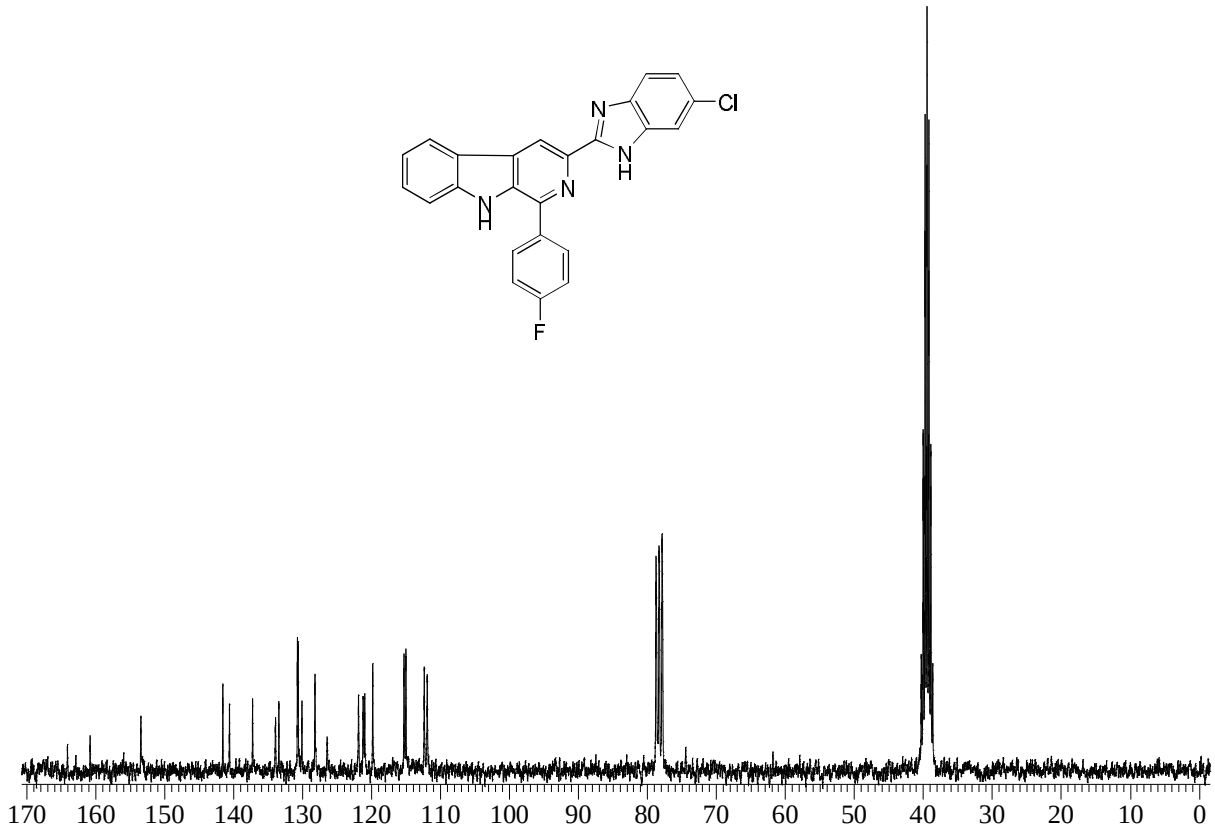

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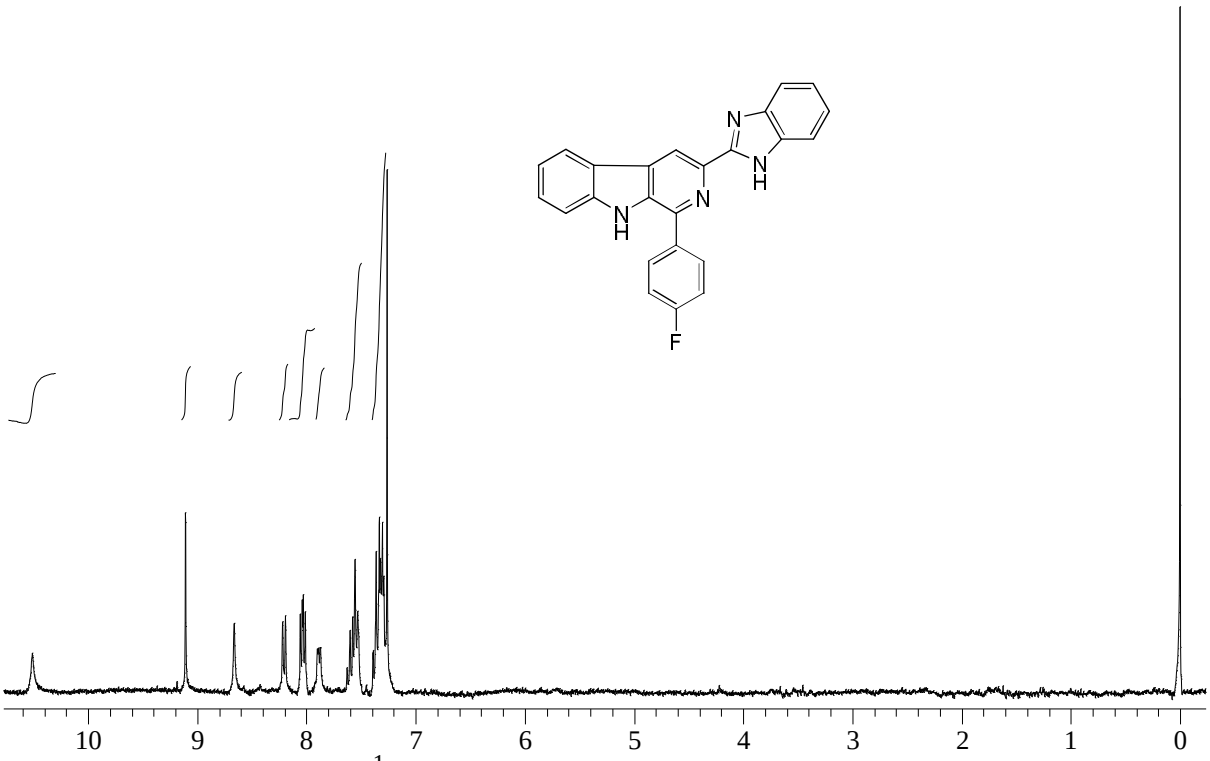

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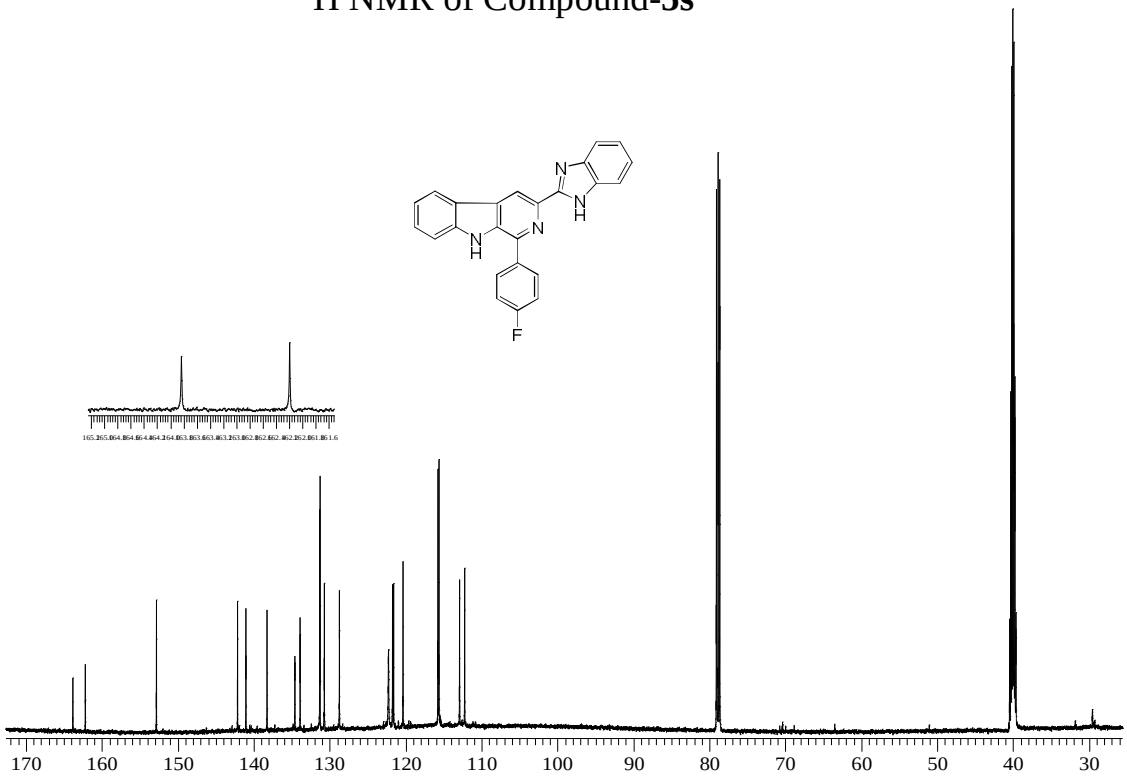

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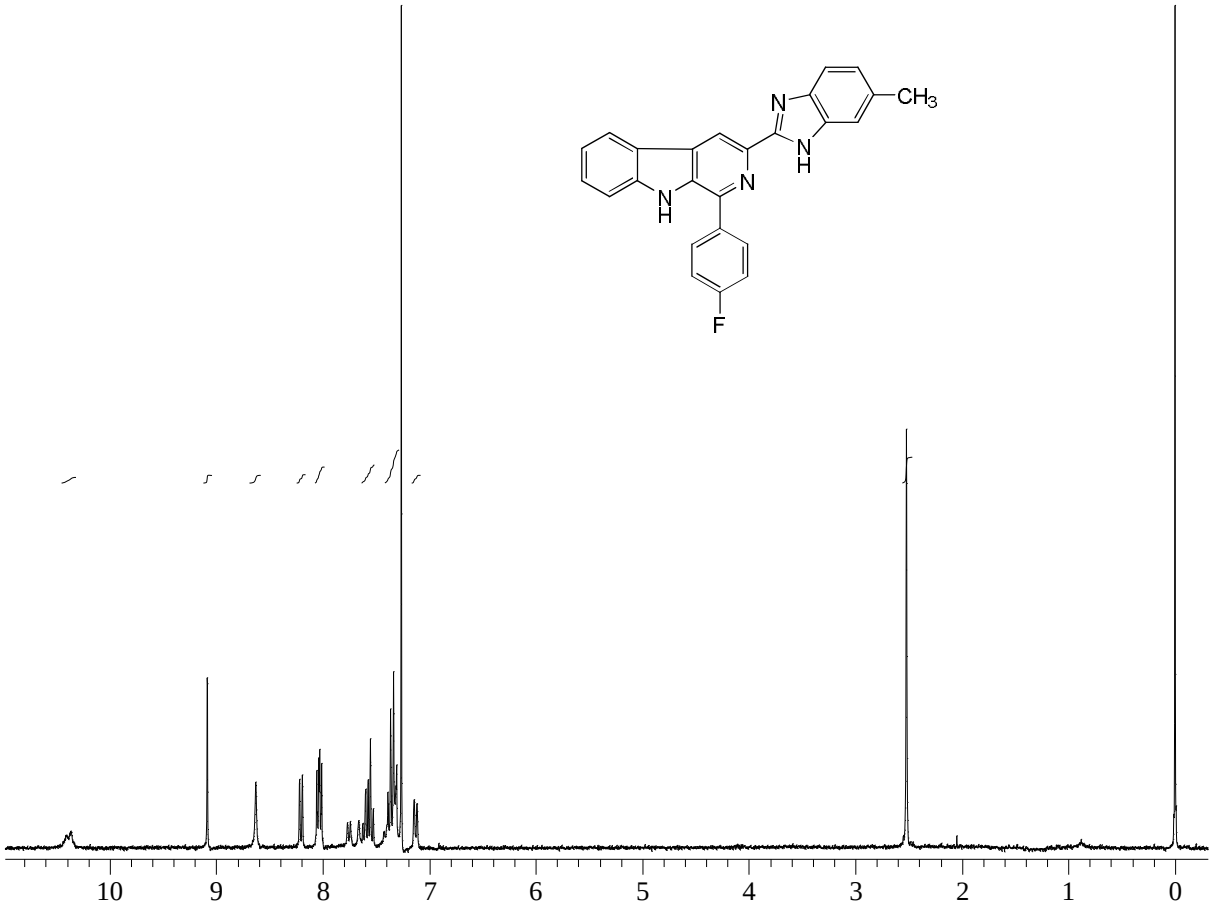

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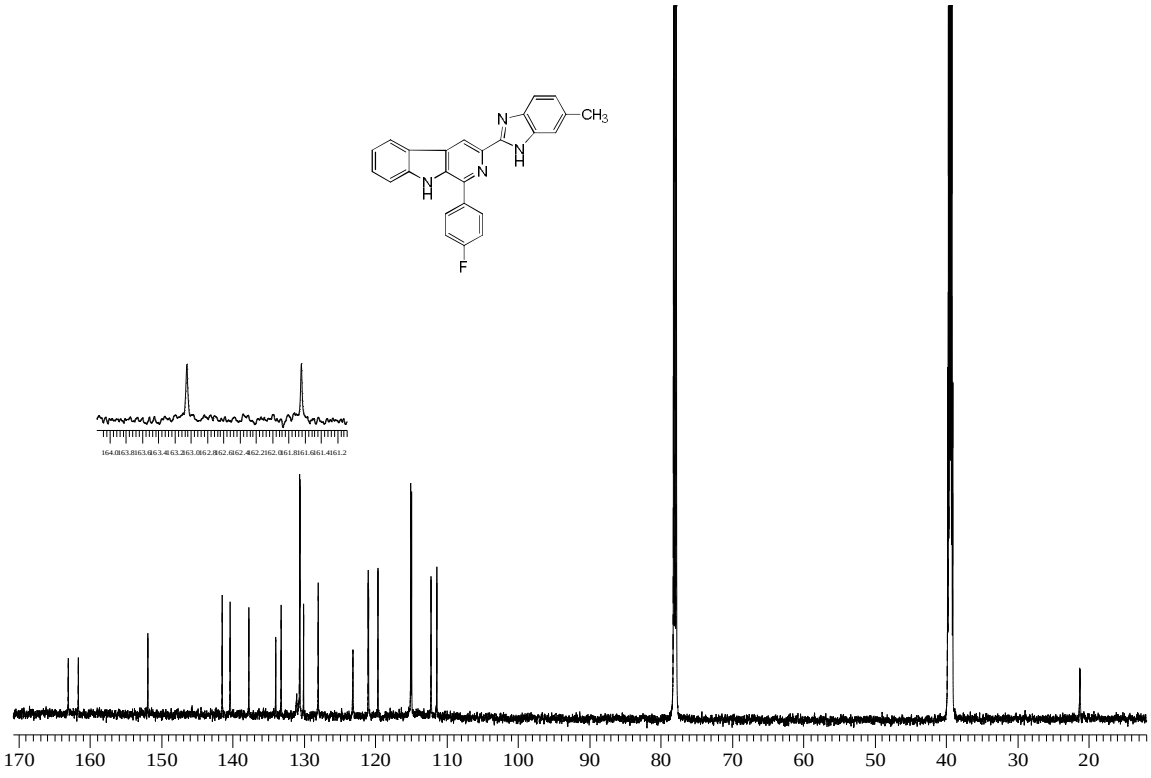

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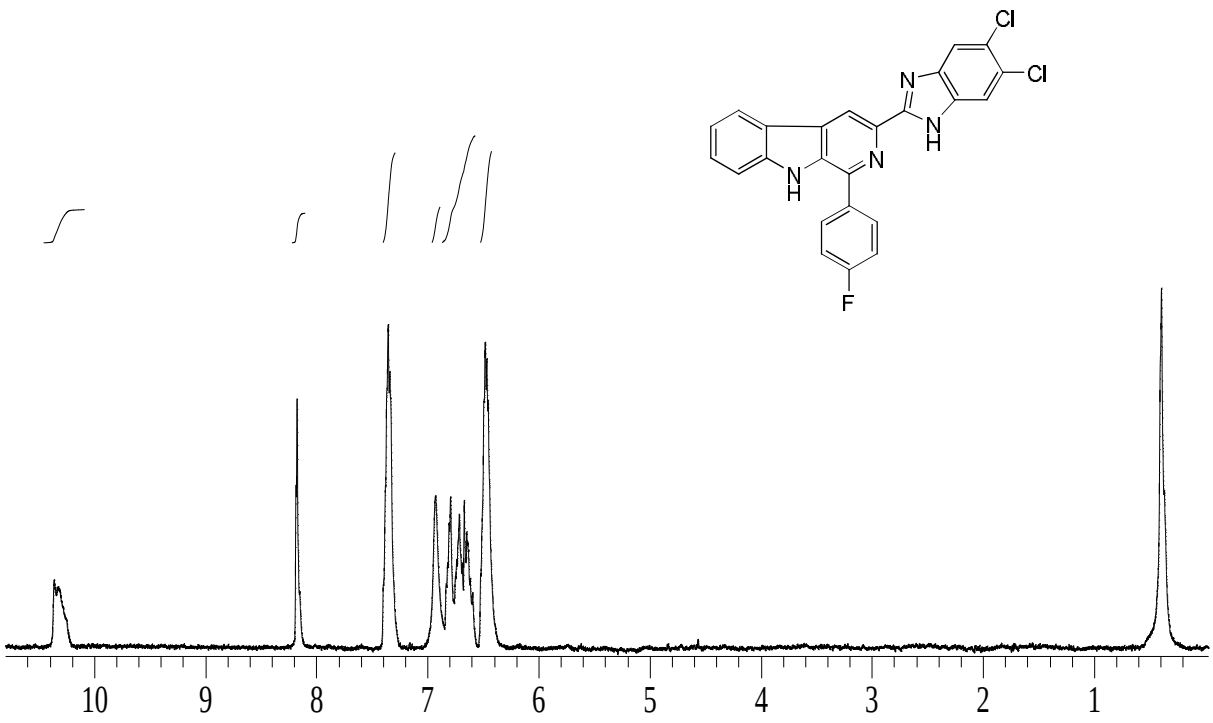

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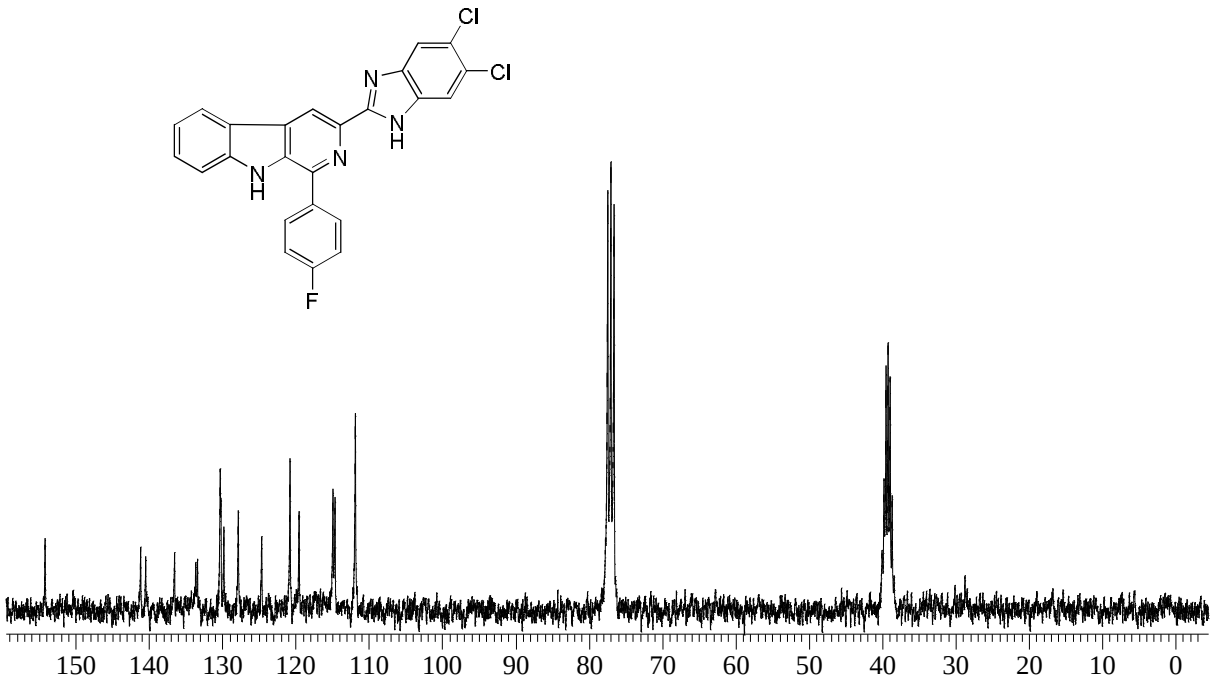

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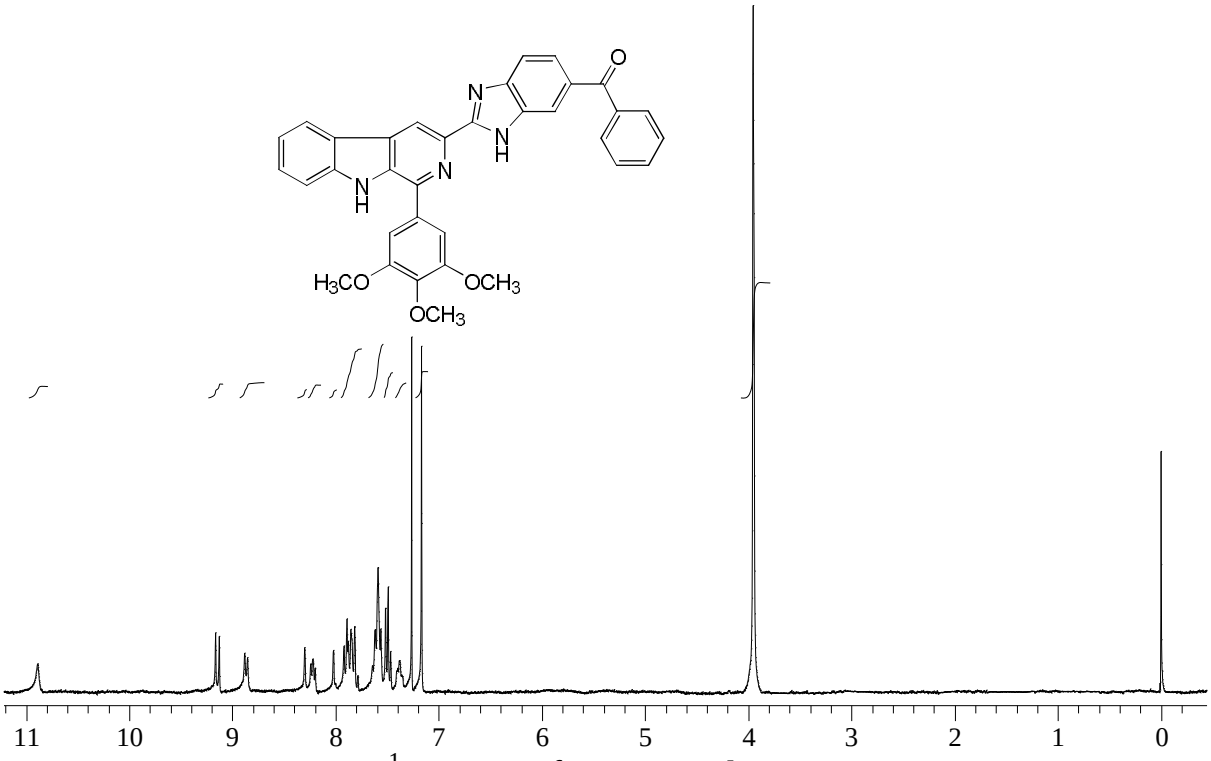

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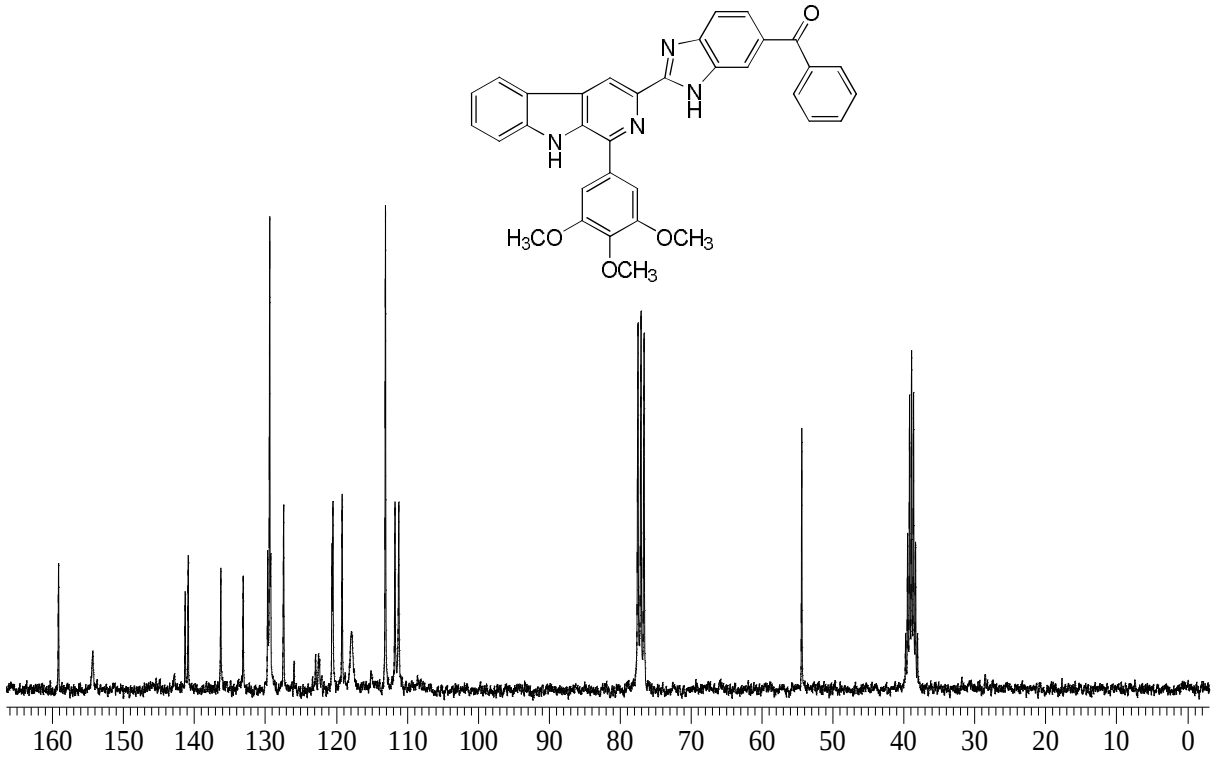

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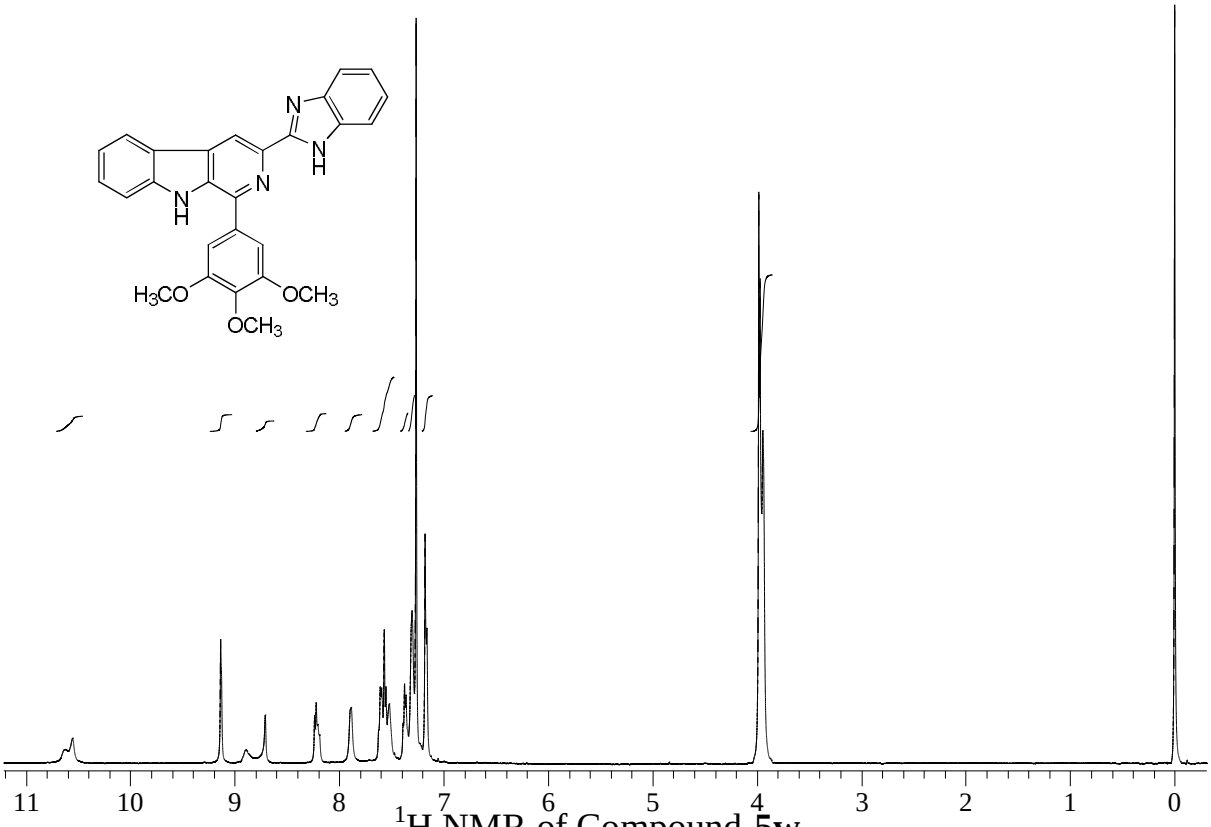

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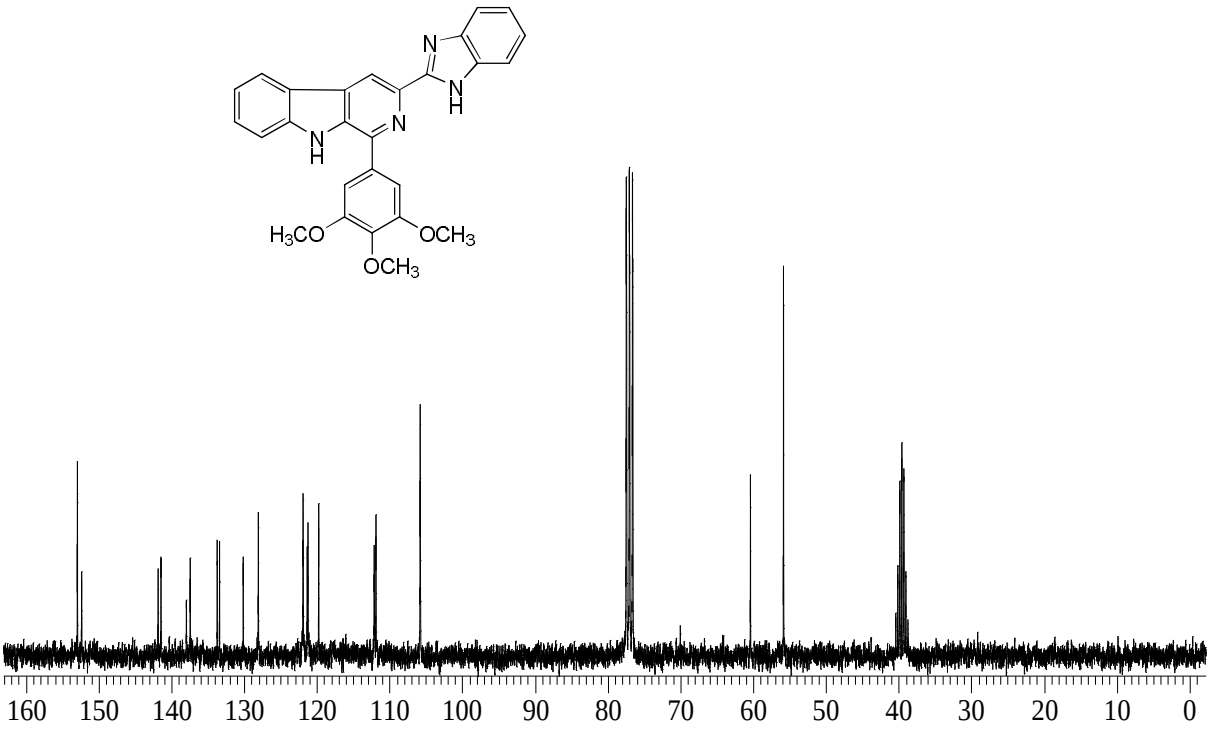

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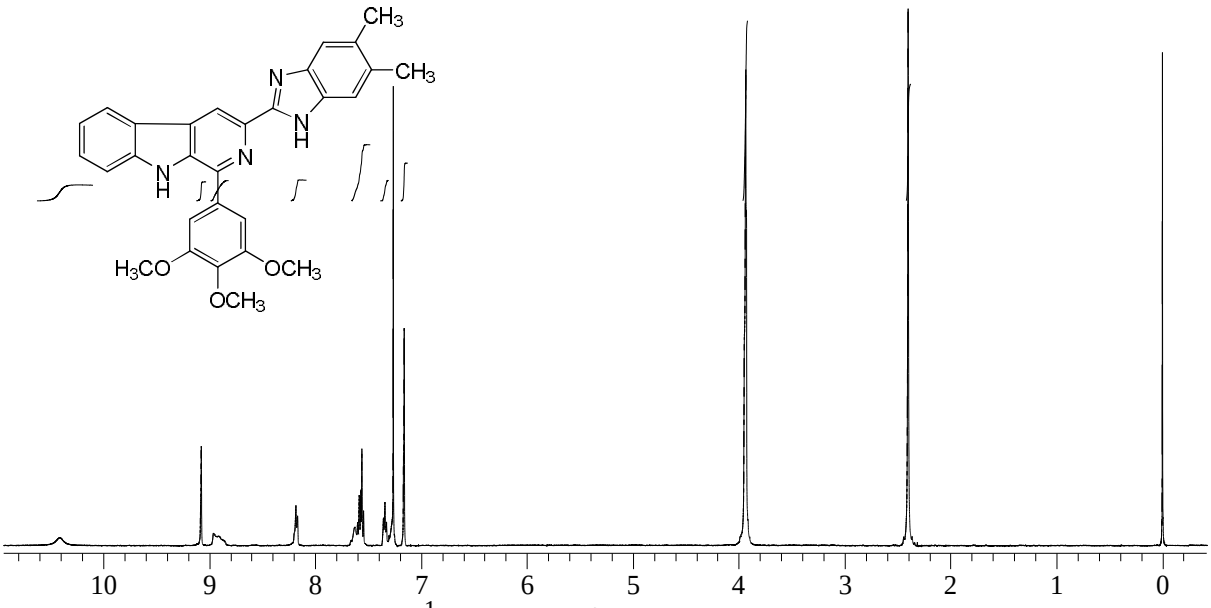

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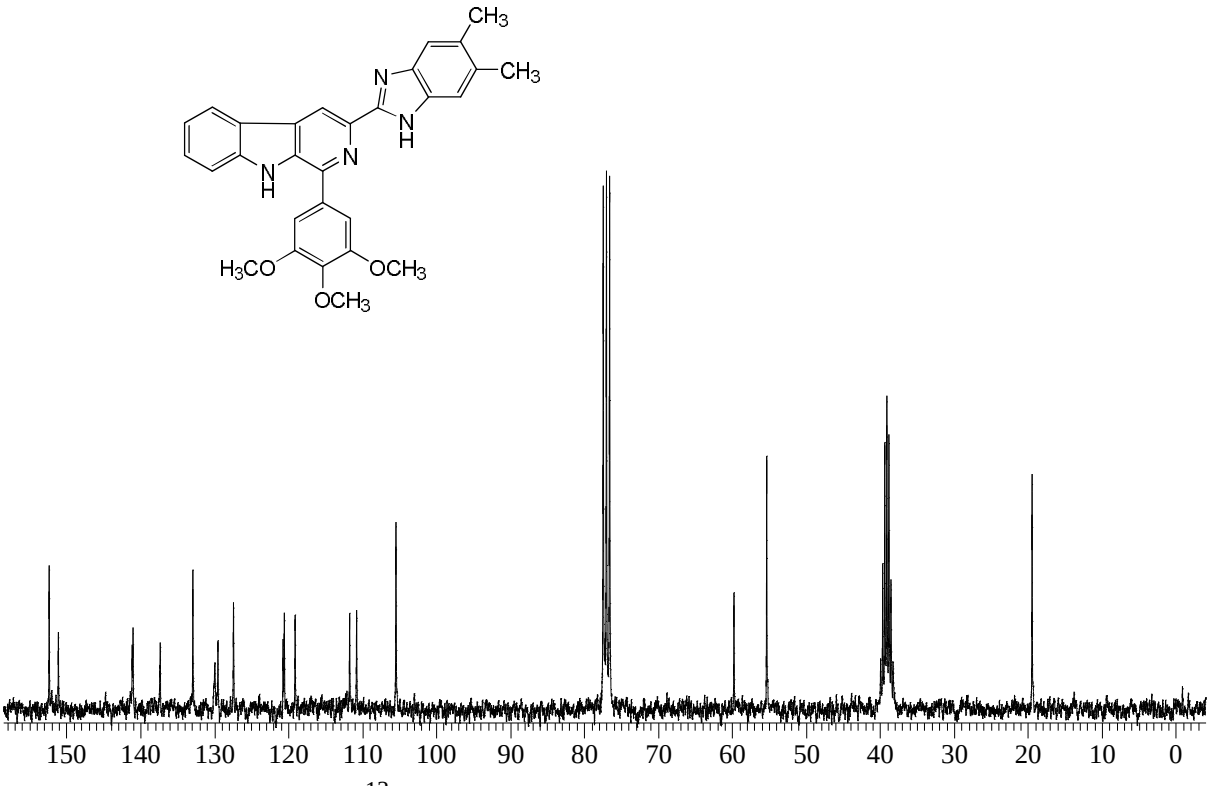

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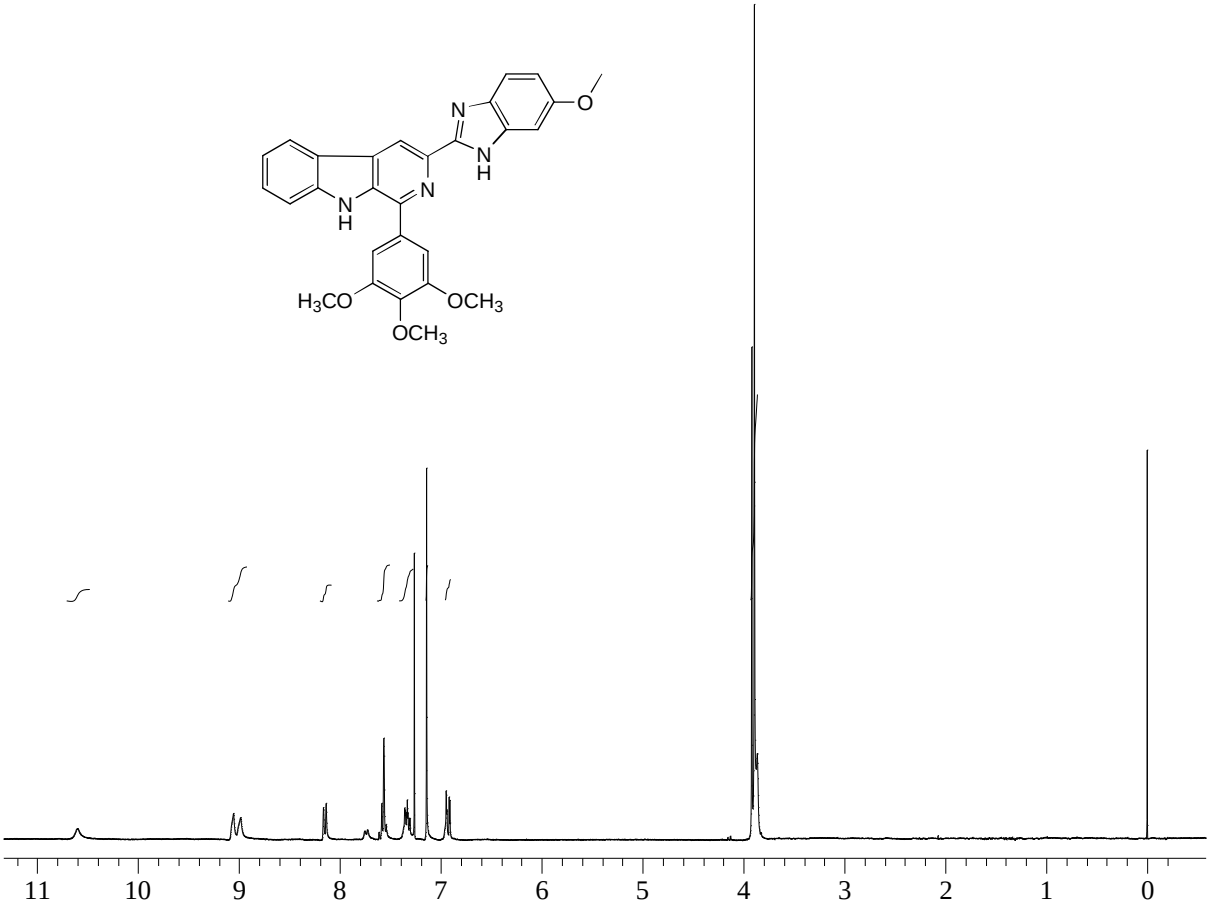

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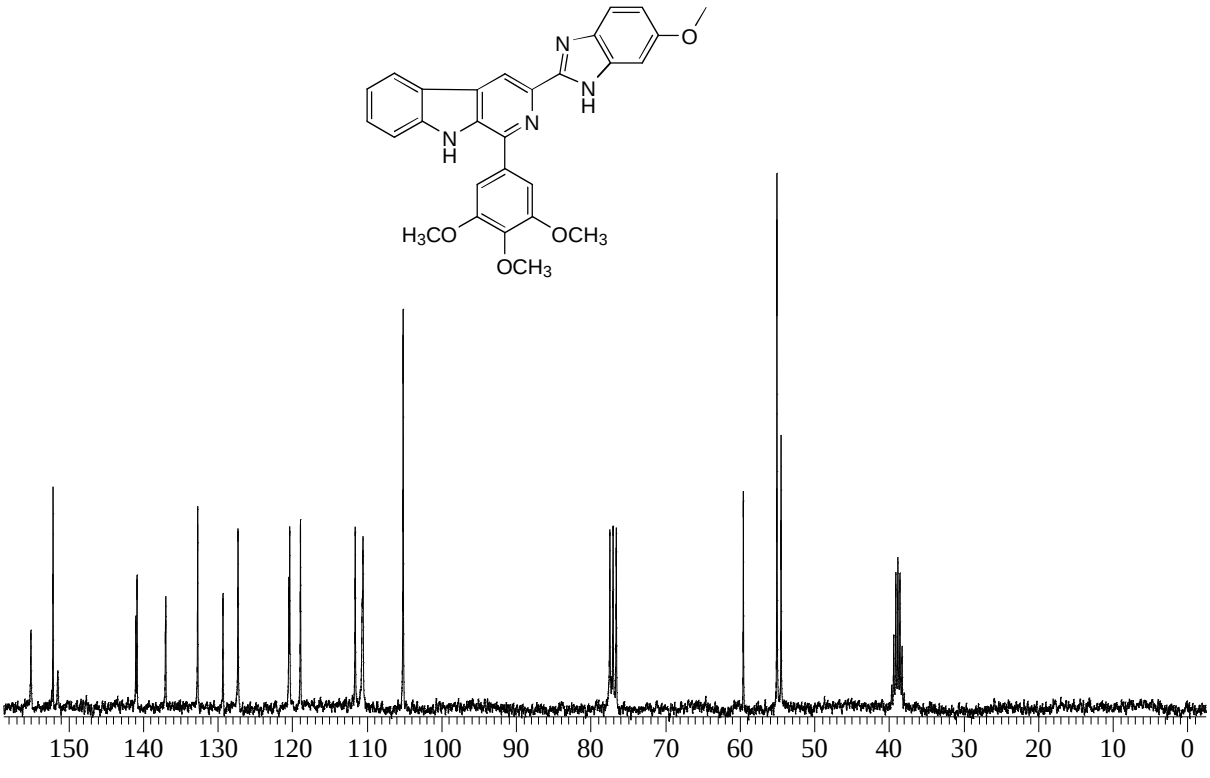

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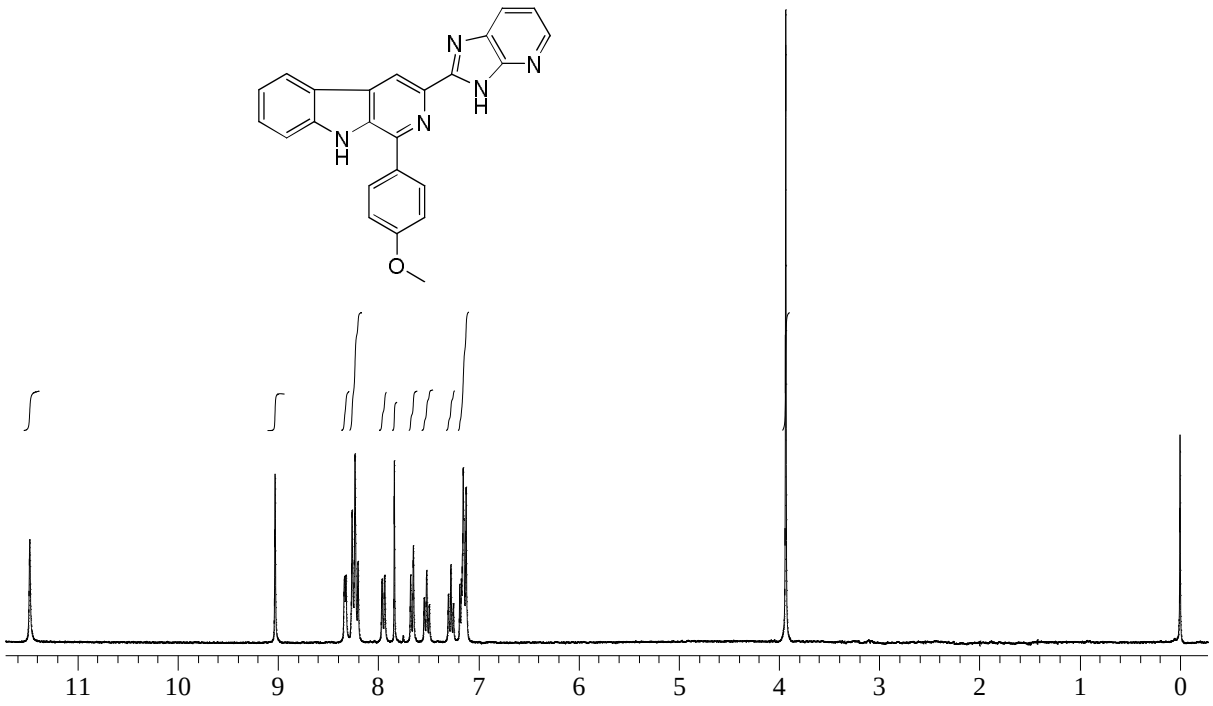
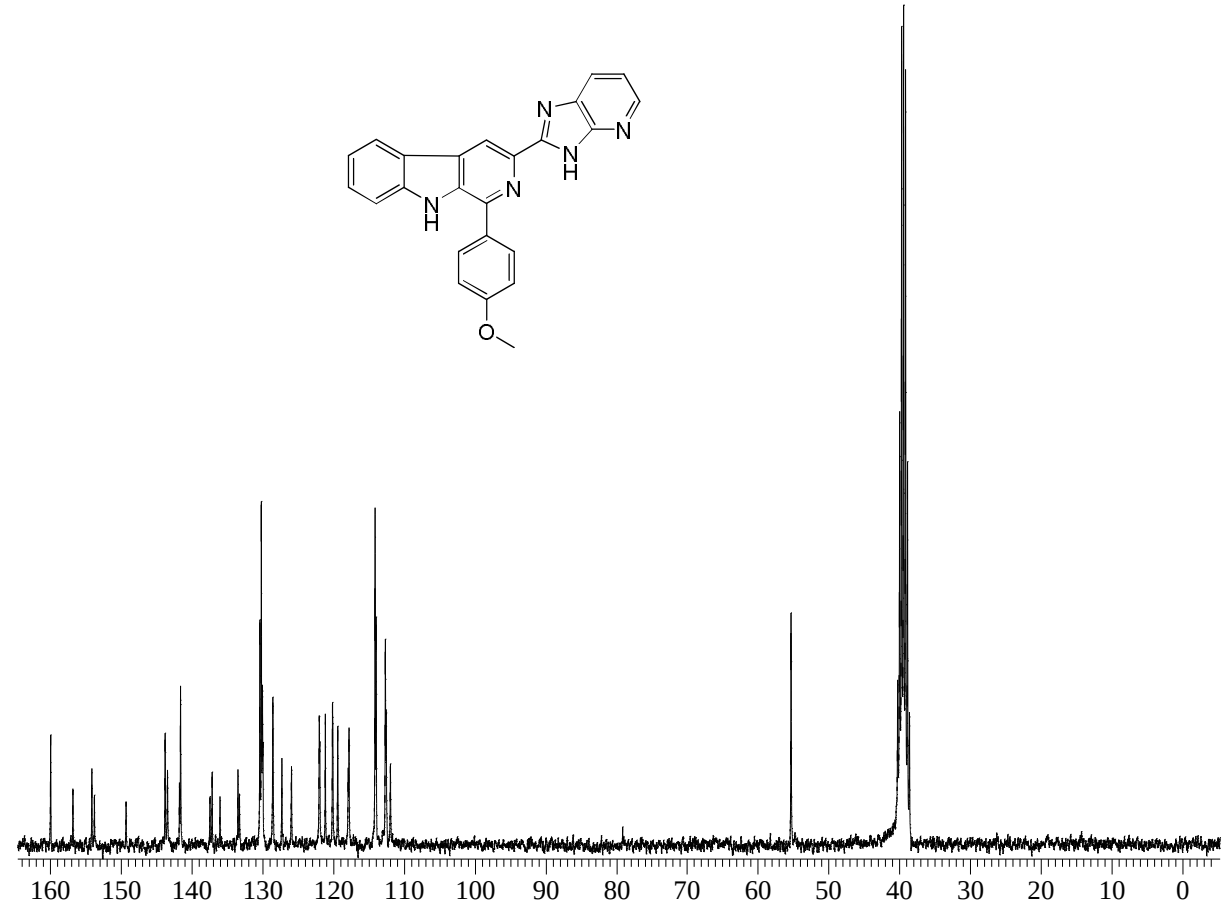


^{1}H NMR of Compound-**6a**



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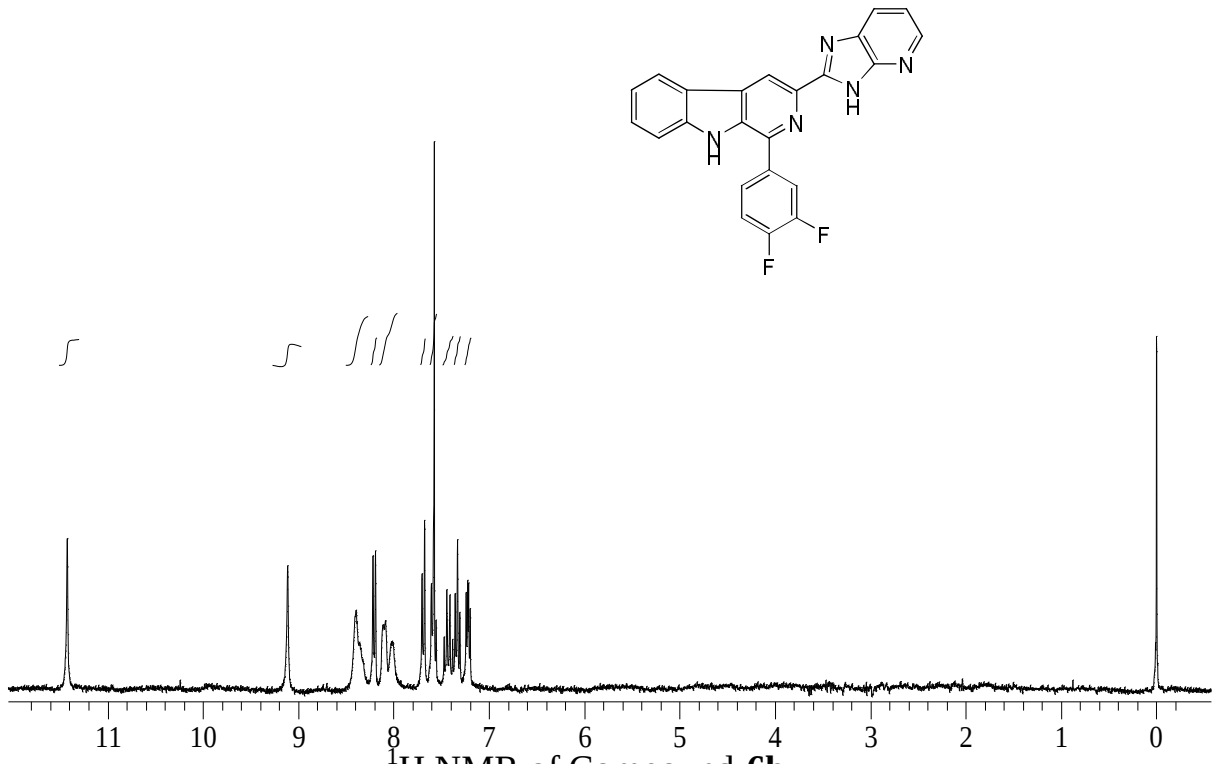

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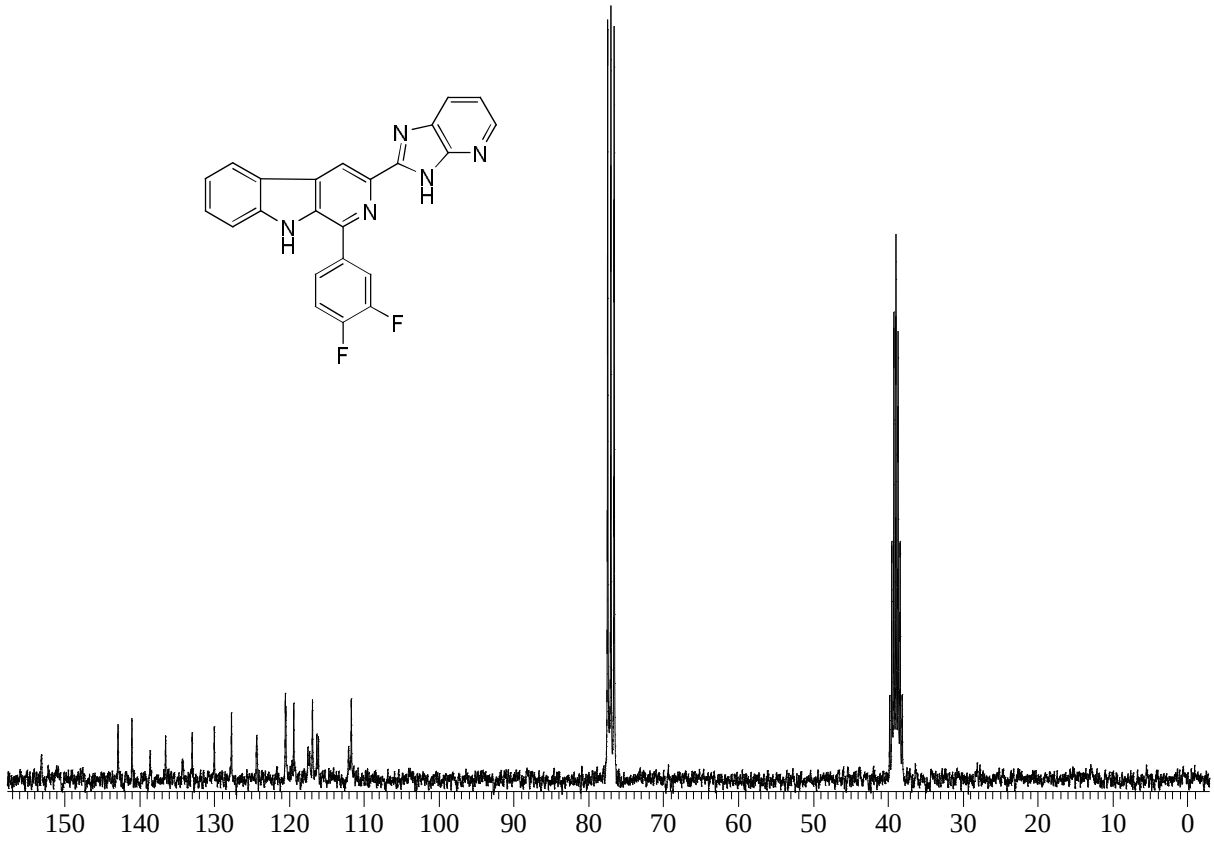

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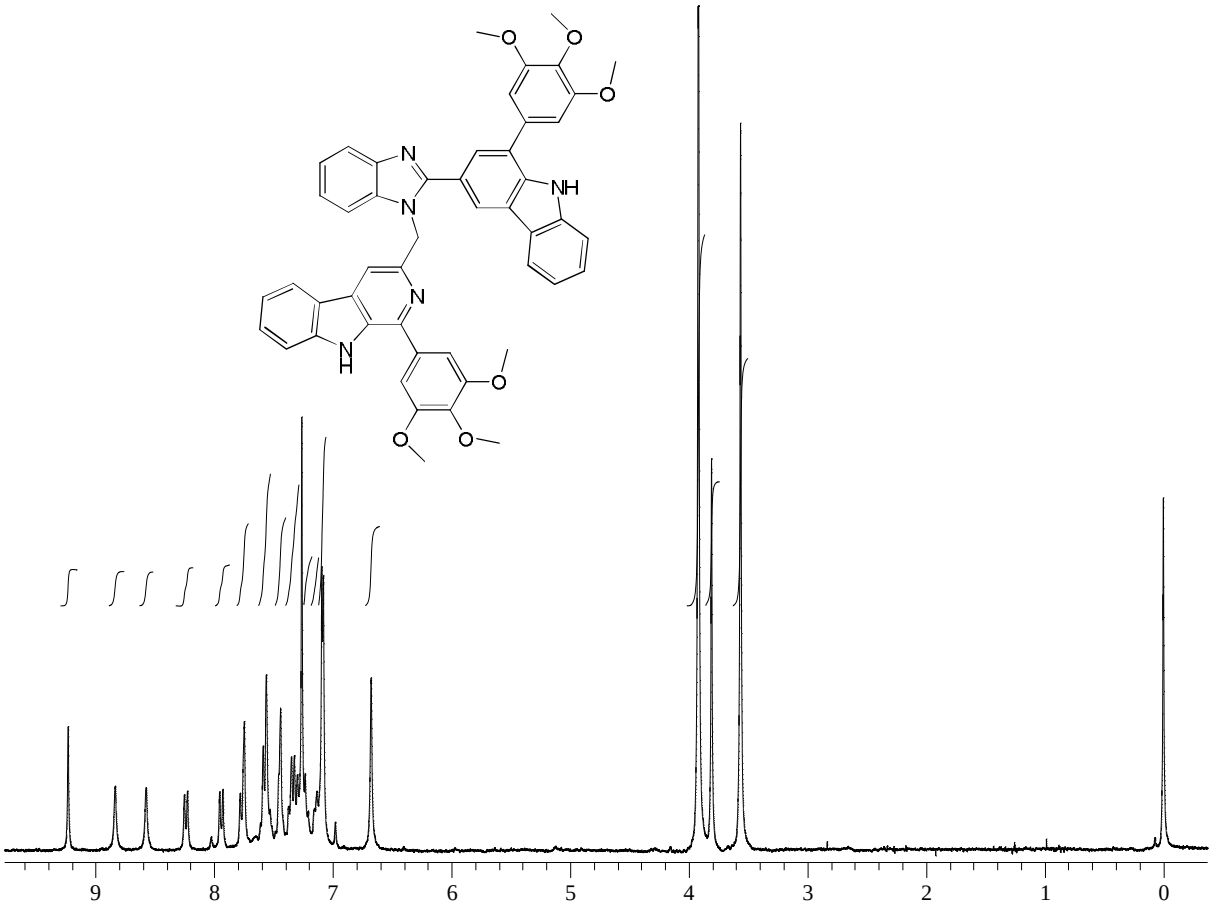
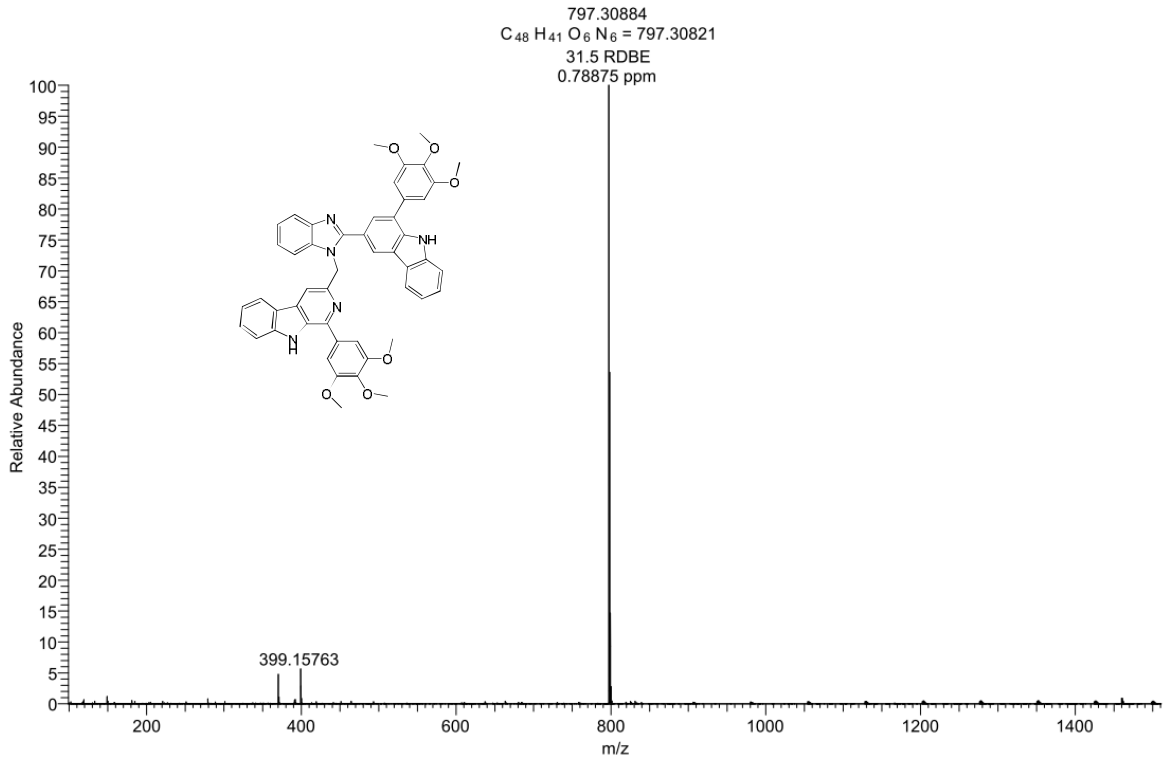


^{1}HNMR of (1-(3,4,5-trimethoxyphenyl)-3-((2-(1-(3,4,5-trimethoxyphenyl)-9H-carbazol-3-yl)-1H-benzo[d]imidazol-1-yl)methyl)-9H-pyrido[3,4-b]indole)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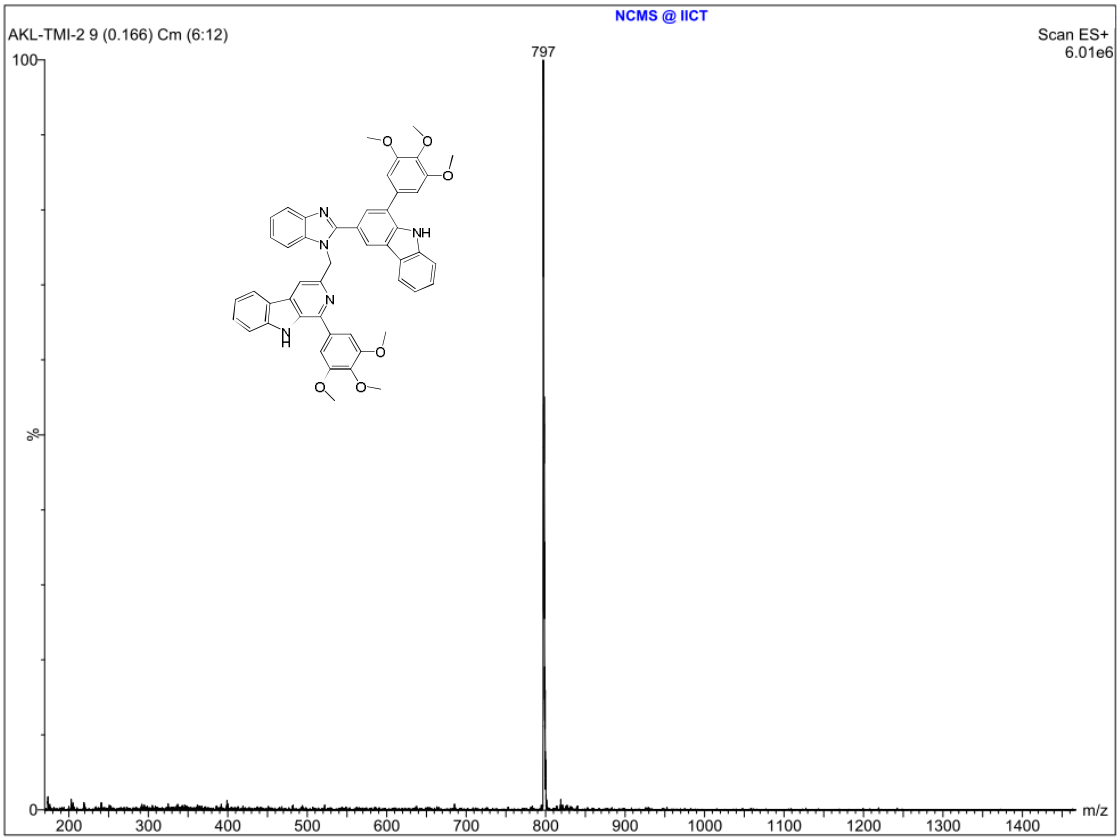
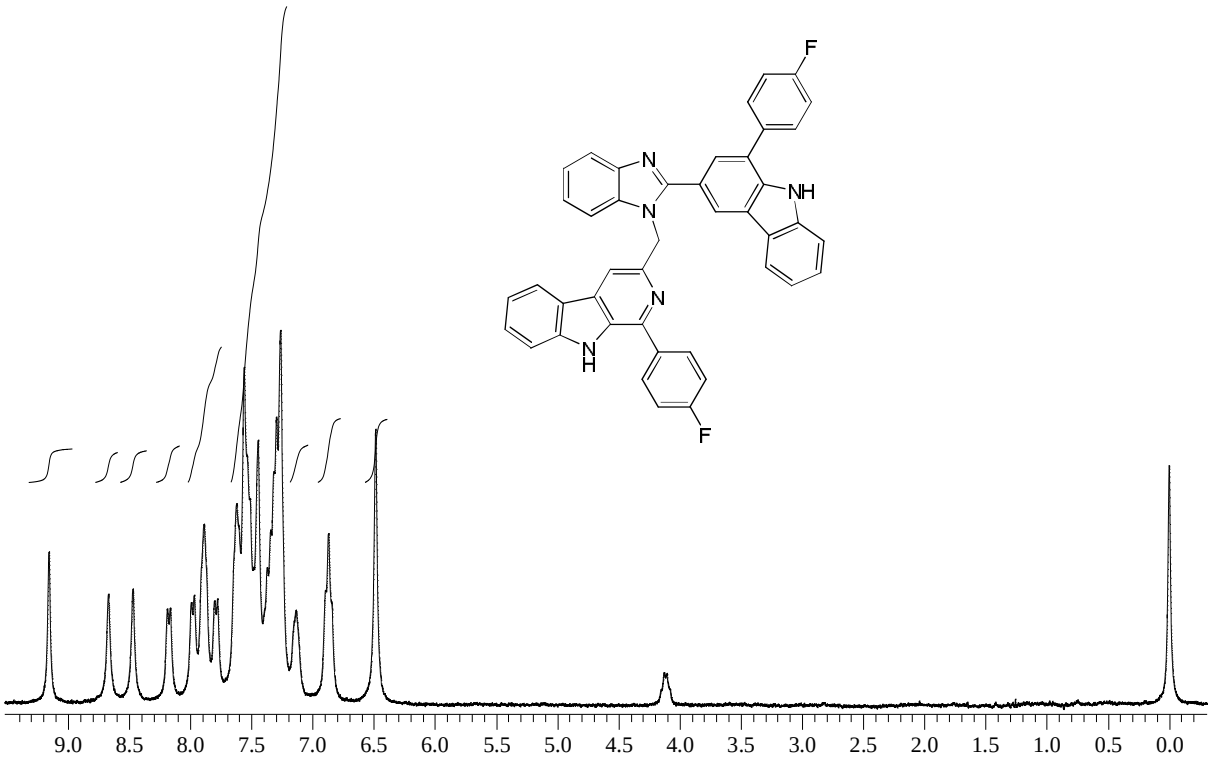
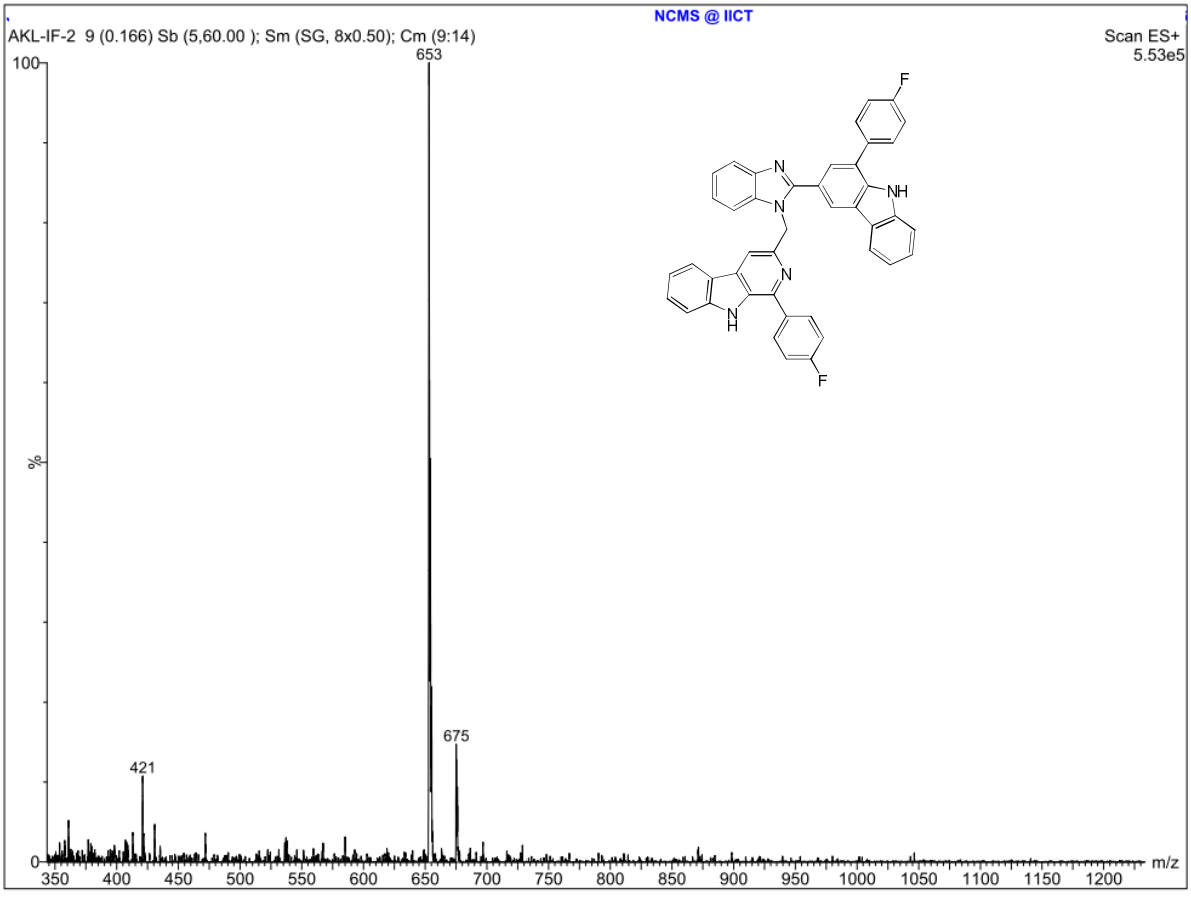
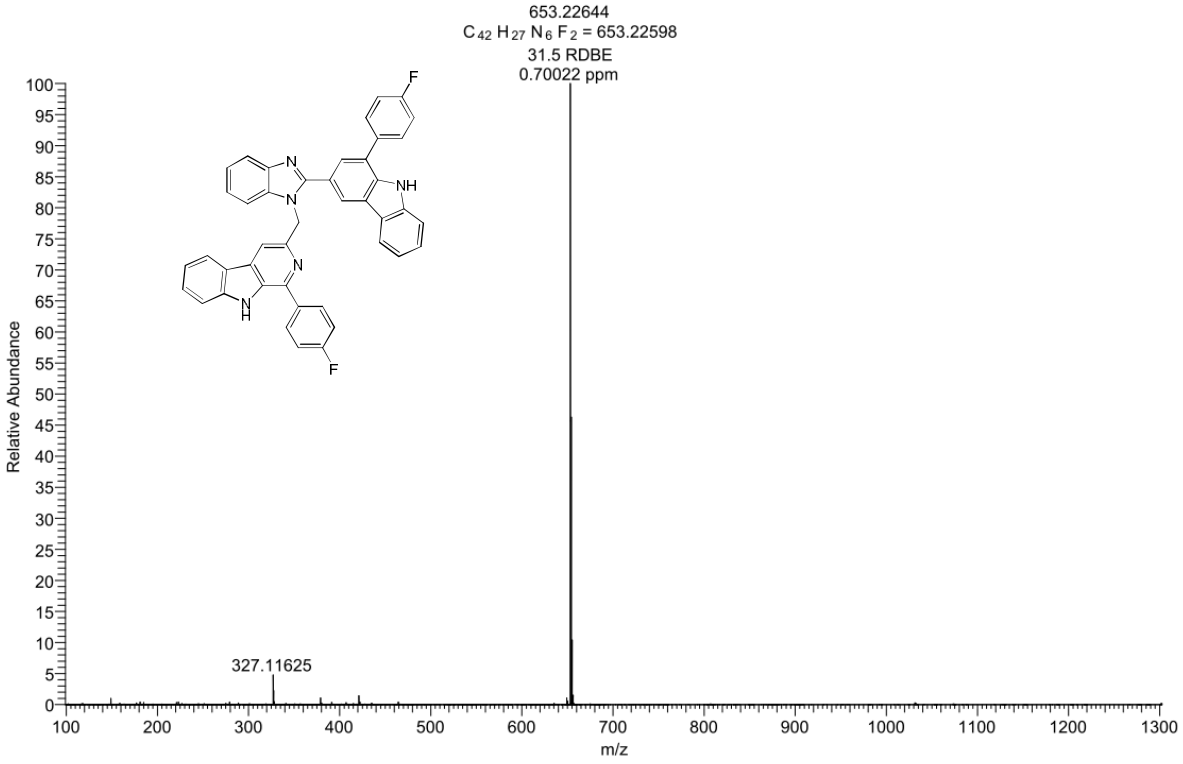
C48 H41 O6 N6 = 797.30821
31.5 RDBE
0.78875 ppm
Relative Abundance
399.15763
m/z


NCMS @ IICT
AKL-TMI-2 9 (0.166) Cm (6:12)
Scan ES+
6.01e6
797
%
m/z



1HNMR of 1-(4-fluorophenyl)-3-((2-(1-(4-fluorophenyl)-9H-carbazol-3-yl)-1H-benzo[d]imidazol-1-yl)methyl)-9H-pyrido[3,4-b]indole




653.22644
C 42 H 27 N 6 F 2 = 653.22598
31.5 RDBE
0.70022 ppm
327.11625
Relative Abundance
m/z
F
F
N
N
NH
N
H

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 765800 / 1	Experiment ID : 1207NS11	Test Type : 08	Units : Molar
Report Date : December 23, 2013	Test Date : July 23, 2012	QNS :	MC :
COMI : AKL-BCTB (114232)	Stain Reagent : SRB Dual-Pass Related	SSPL : Q80Q	

		Log10 Concentration													
	Time	Mean Optical Densities						Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.516	2.129	2.145	2.118	1.279	0.800	0.774	101	99	47	18	16	8.87E-7	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.673	2.119	2.248	2.209	1.917	1.064	0.962	109	106	86	27	20	4.08E-6	> 1.00E-4	> 1.00E-4
K-562	0.353	2.299	2.304	2.380	1.478	0.637	0.581	100	104	58	15	12	1.52E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.609	2.092	2.131	2.214	1.531	0.924	0.809	103	108	62	21	13	1.98E-6	> 1.00E-4	> 1.00E-4
RPMI-8226	0.999	2.561	2.478	2.333	1.345	0.736	0.698	95	85	22	-26	-30	3.63E-7	2.86E-6	> 1.00E-4
SR	0.194	0.751	0.781	0.742	0.752	0.310	0.299	105	98	100	21	19	4.29E-6	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.413	1.584	1.570	1.516	1.199	0.488	0.542	99	94	67	6	11	1.92E-6	> 1.00E-4	> 1.00E-4
HOP-62	0.514	1.486	1.447	1.448	1.319	0.810	0.847	96	96	83	30	34	4.24E-6	> 1.00E-4	> 1.00E-4
NCI-H226	0.746	2.167	2.090	2.045	1.879	1.220	1.261	95	91	80	33	36	4.37E-6	> 1.00E-4	> 1.00E-4
NCI-H23	1.173	3.066	3.025	3.044	2.922	1.871	1.852	98	99	92	37	36	5.80E-6	> 1.00E-4	> 1.00E-4
NCI-H322M	0.689	1.542	1.547	1.584	1.467	0.867	0.907	101	105	91	21	25	3.85E-6	> 1.00E-4	> 1.00E-4
NCI-H460	0.271	2.403	2.460	2.349	1.807	0.304	0.351	103	97	72	2	4	2.05E-6	> 1.00E-4	> 1.00E-4
NCI-H522	0.986	1.598	1.578	1.637	1.489	1.033	1.025	97	106	82	8	6	2.70E-6	> 1.00E-4	> 1.00E-4
Colon Cancer															
COLO 205	0.374	1.238	1.236	1.230	1.214	0.723	0.763	100	99	97	40	45	6.76E-6	> 1.00E-4	> 1.00E-4
HCC-2998	0.542	1.468	1.386	1.535	1.546	0.885	0.909	91	107	108	37	40	6.57E-6	> 1.00E-4	> 1.00E-4
HCT-116	0.192	2.430	2.503	2.535	1.839	0.501	0.512	103	105	74	14	14	2.48E-6	> 1.00E-4	> 1.00E-4
HCT-15	0.249	2.120	2.045	2.069	1.692	0.588	0.632	96	97	77	18	20	2.88E-6	> 1.00E-4	> 1.00E-4
HT29	0.300	1.306	1.309	1.288	1.306	0.373	0.391	100	98	100	7	9	3.46E-6	> 1.00E-4	> 1.00E-4
KM12	0.515	2.474	2.502	2.525	1.990	0.781	0.822	101	103	75	14	16	2.57E-6	> 1.00E-4	> 1.00E-4
SW-620	0.251	1.856	1.806	1.866	1.706	0.752	0.804	97	101	91	31	34	4.83E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.737	2.059	2.024	2.069	1.952	1.150	1.209	97	101	92	31	36	4.90E-6	> 1.00E-4	> 1.00E-4
SF-539	0.797	2.677	2.653	2.662	2.502	1.712	1.647	99	99	91	49	45	9.29E-6	> 1.00E-4	> 1.00E-4
SNB-19	0.753	2.284	2.179	2.202	2.074	1.020	1.114	93	95	86	17	24	3.37E-6	> 1.00E-4	> 1.00E-4
U251	0.678	2.275	2.258	2.232	2.028	0.832	0.858	99	97	85	10	11	2.89E-6	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.552	2.761	2.714	2.712	2.396	0.908	0.931	98	98	83	16	17	3.14E-6	> 1.00E-4	> 1.00E-4
MALME-3M	0.673	1.383	1.381	1.384	1.300	1.044	1.008	100	100	88	52	47	2.76E-5	> 1.00E-4	> 1.00E-4
M14	0.425	1.883	1.904	1.972	1.545	0.798	0.782	101	106	77	26	24	3.34E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.396	1.906	1.813	1.800	1.594	0.896	0.984	94	93	79	33	39	4.31E-6	> 1.00E-4	> 1.00E-4
SK-MEL-2	1.283	2.104	2.201	2.300	2.042	1.372	1.221	112	124	92	11	-5	3.31E-6	4.92E-5	> 1.00E-4
SK-MEL-28	0.449	1.171	1.205	1.204	1.126	0.781	0.810	105	105	94	46	50	1.00E-4	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.729	3.028	2.956	2.875	2.244	1.166	1.173	97	93	66	19	19	2.18E-6	> 1.00E-4	> 1.00E-4
UACC-257	0.996	1.647	1.598	1.577	1.599	1.164	1.135	92	89	93	26	21	4.34E-6	> 1.00E-4	> 1.00E-4
UACC-62	0.857	3.002	2.870	2.893	2.497	1.207	1.248	94	95	76	16	18	2.75E-6	> 1.00E-4	> 1.00E-4
Ovarian Cancer															
IGROV1	0.662	1.959	2.008	1.991	1.735	0.796	0.874	104	102	83	10	16	2.83E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.601	1.771	1.865	1.908	1.661	0.791	0.871	108	112	91	16	23	3.51E-6	> 1.00E-4	> 1.00E-4
OVCAR-4	0.644	1.172	1.177	1.189	1.163	0.948	0.955	101	103	98	58	59	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-5	0.406	1.202	1.172	1.147	1.213	0.900	0.883	96	93	101	62	60	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-8	0.564	1.924	1.905	1.885	1.253	0.701	0.741	99	97	51	10	13	1.04E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.868	2.628	2.712	2.760	1.998	1.224	1.245	105	107	64	20	21	2.10E-6	> 1.00E-4	> 1.00E-4
SK-OV-3	0.651	1.410	1.391	1.381	1.435	1.164	1.245	97	96	103	68	78	> 1.00E-4	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.732	2.625	2.619	2.669	2.468	1.281	1.294	100	102	92	29	30	4.62E-6	> 1.00E-4	> 1.00E-4
A498	1.207	1.886	1.849	1.838	1.706	1.402	1.462	95	93	73	29	38	3.34E-6	> 1.00E-4	> 1.00E-4
ACHN	0.340	1.669	1.667	1.604	1.257	0.569	0.620	100	95	69	17	21	2.33E-6	> 1.00E-4	> 1.00E-4
CAKI-1	0.946	3.034	2.911	2.886	2.925	1.732	1.883	94	93	95	38	45	6.07E-6	> 1.00E-4	> 1.00E-4
RXF 393	0.779	1.265	1.249	1.211	1.159	0.850	0.894	97	89	78	15	24	2.77E-6	> 1.00E-4	> 1.00E-4
SN12C	0.721	2.785	2.737	2.721	2.489	1.133	1.137	98	97	86	20	20	3.49E-6	> 1.00E-4	> 1.00E-4
TK-10	0.770	1.319	1.349	1.374	1.261	0.826	0.799	105	110	89	10	5	3.14E-6	> 1.00E-4	> 1.00E-4
UO-31	0.706	2.044	1.940	2.038	1.527	0.837	0.897	92	100	61	10	14	1.66E-6	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.651	1.812	1.757	1.713	1.357	0.666	0.817	95	91	61	1	14	1.52E-6	> 1.00E-4	> 1.00E-4
DU-145	0.333	1.219	1.230	1.244	0.948	0.401	0.459	101	103	69	8	14	2.06E-6	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.380	1.803	1.651	1.746	1.431	0.595	0.620	89	96	74	15	17	2.55E-6	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.625	1.441	1.448	1.492	1.325	1.011	0.961	101	106	86	47	41	8.51E-6	> 1.00E-4	> 1.00E-4
HS 578T	0.954	2.004	1.989	1.978	1.850	1.036	1.163	99	97	85	8	20	2.86E-6	> 1.00E-4	> 1.00E-4
BT-549	0.918	2.097	2.140	2.167	1.916	1.436	1.413	104	106	85	44	42	7.10E-6	> 1.00E-4	> 1.00E-4
T-47D	0.681	1.650	1.567	1.554	1.374	0.789	0.868	91	90	71	11	19	2.27E-6	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.679	1.511	1.419	1.398	1.311	0.879	0.788	89	86	76	24	13	3.16E-6	> 1.00E-4	> 1.00E-4

NCI 5 dose-data for conjugate **5a**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 764568 / 1	Experiment ID : 1206NS89	Test Type : 08	Units : Molar
Report Date : December 23, 2013	Test Date : June 11, 2012	QNS :	MC :
COMI : AKL-BCTB-8 (114840)	Stain Reagent : SRB Dual-Pass Related	SSPL : Q80Q	

		Log10 Concentration												
	Time	Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.394	1.588	1.537	1.576	1.469	0.448	0.346	96	99	90	5	-12	2.94E-6	1.87E-5	> 1.00E-4
HL-60(TB)	0.868	2.851	3.057	3.008	3.007	1.137	0.782	110	108	108	14	-10	4.11E-6	3.77E-5	> 1.00E-4
K-562	0.184	1.464	1.517	1.513	1.350	0.278	0.197	104	104	91	7	1	3.09E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.468	1.687	1.750	1.827	1.426	0.469	0.253	105	111	79	.	-46	2.31E-6	1.00E-5	> 1.00E-4
RPMI-8226	1.010	2.357	2.445	2.311	2.076	0.707	0.637	106	97	79	-30	-37	1.85E-6	5.30E-6	> 1.00E-4
SR	0.450	1.627	1.600	1.561	1.421	0.529	0.413	98	94	83	7	-8	2.68E-6	2.78E-5	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.318	1.671	1.612	1.544	1.476	0.578	0.438	96	91	86	19	9	3.43E-6	> 1.00E-4	> 1.00E-4
HOP-62	0.413	1.126	1.140	1.158	1.226	0.627	0.462	102	104	114	30	7	5.78E-6	> 1.00E-4	> 1.00E-4
HOP-92	1.472	1.870	1.759	1.741	1.789	1.355	1.396	72	67	79	-8	-5	2.17E-6	8.11E-6	> 1.00E-4
NCI-H226	0.638	1.626	1.592	1.640	1.652	0.890	0.589	96	101	103	25	-8	4.81E-6	5.87E-5	> 1.00E-4
NCI-H23	0.545	1.596	1.582	1.661	1.601	0.874	0.637	99	106	100	31	9	5.36E-6	> 1.00E-4	> 1.00E-4
NCI-H322M	0.640	1.483	1.448	1.497	1.423	0.925	0.725	96	102	93	34	10	5.32E-6	> 1.00E-4	> 1.00E-4
NCI-H460	0.253	2.412	2.427	2.350	2.145	0.437	0.290	101	97	88	9	2	2.99E-6	> 1.00E-4	> 1.00E-4
NCI-H522	0.700	1.711	1.690	1.682	1.707	0.926	0.606	98	97	100	22	-13	4.39E-6	4.21E-5	> 1.00E-4
Colon Cancer															
COLO 205	0.265	1.169	1.198	1.212	1.159	0.241	0.129	103	105	99	-9	-51	2.83E-6	8.21E-6	9.30E-5
HCC-2998	0.554	2.093	2.024	2.105	2.113	1.218	0.965	96	101	101	43	27	7.61E-6	> 1.00E-4	> 1.00E-4
HCT-116	0.198	1.714	1.793	1.790	1.708	0.341	0.186	105	105	100	9	-6	3.55E-6	4.05E-5	> 1.00E-4
HCT-15	0.260	1.607	1.554	1.514	1.387	0.489	0.297	96	93	84	17	3	3.20E-6	> 1.00E-4	> 1.00E-4
HT29	0.226	1.186	1.242	1.342	1.348	0.460	0.340	106	116	117	24	12	5.29E-6	> 1.00E-4	> 1.00E-4
KM12	0.460	2.086	2.090	2.168	2.019	0.566	0.286	100	105	96	7	-38	3.26E-6	1.40E-5	> 1.00E-4
SW-620	0.265	1.681	1.667	1.689	1.712	0.782	0.532	99	101	102	37	19	6.23E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.555	1.584	1.609	1.657	1.670	0.949	0.723	102	107	108	38	16	6.80E-6	> 1.00E-4	> 1.00E-4
SF-539	0.772	2.215	2.152	2.115	1.978	1.161	0.916	96	93	84	27	10	3.92E-6	> 1.00E-4	> 1.00E-4
SNB-19	0.494	1.554	1.515	1.444	1.473	0.952	0.817	96	90	92	43	30	7.28E-6	> 1.00E-4	> 1.00E-4
SNB-75	0.872	1.408	1.253	1.265	1.314	0.989	1.055	71	73	83	22	34	3.43E-6	> 1.00E-4	> 1.00E-4
U251	0.282	1.331	1.257	1.245	1.240	0.429	0.323	93	92	91	14	4	3.42E-6	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.294	1.914	1.904	1.978	1.881	0.398	0.232	99	104	98	6	-21	3.34E-6	1.71E-5	> 1.00E-4
MALME-3M	0.613	1.030	1.031	1.087	1.022	0.739	0.583	100	114	98	30	-5	5.10E-6	7.25E-5	> 1.00E-4
M14	0.481	1.710	1.719	1.724	1.627	0.542	0.156	101	101	93	5	-68	3.09E-6	1.17E-5	5.72E-5
MDA-MB-435	0.474	2.173	2.121	2.056	1.983	0.876	0.690	97	93	89	24	13	3.94E-6	> 1.00E-4	> 1.00E-4
SK-MEL-2	0.679	1.266	1.259	1.309	1.279	0.654	0.419	99	107	102	-4	-38	3.11E-6	9.22E-6	> 1.00E-4
SK-MEL-28	0.589	1.491	1.438	1.400	1.397	0.886	0.687	94	90	90	33	11	5.00E-6	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.626	2.757	2.707	2.711	2.515	0.848	0.038	98	98	89	10	-94	3.12E-6	1.26E-5	3.79E-5
UACC-257	0.688	1.731	1.675	1.625	1.631	0.923	0.772	95	90	90	23	8	3.94E-6	> 1.00E-4	> 1.00E-4
UACC-62	0.507	1.713	1.546	1.630	1.629	0.639	0.410	86	93	93	11	-19	3.34E-6	2.31E-5	> 1.00E-4
Ovarian Cancer															
IGROV1	0.837	1.894	1.969	2.016	1.895	0.939	0.875	107	112	100	10	4	3.58E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.607	1.700	1.812	1.837	1.804	0.633	0.443	110	113	110	2	-27	3.59E-6	1.20E-5	> 1.00E-4
OVCAR-4	0.484	1.146	1.112	1.111	1.071	0.653	0.498	95	95	89	25	2	4.09E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.510	1.312	1.272	1.240	1.243	0.845	0.637	95	91	91	42	16	6.83E-6	> 1.00E-4	> 1.00E-4
OVCAR-8	0.422	1.832	1.781	1.710	1.690	0.516	0.498	96	91	90	7	5	3.02E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.456	1.539	1.559	1.565	1.494	0.624	0.513	102	102	96	15	5	3.72E-6	> 1.00E-4	> 1.00E-4
SK-OV-3	0.614	1.283	1.310	1.343	1.368	1.105	0.906	104	109	113	73	44	6.10E-5	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.657	2.125	2.095	2.212	1.781	1.523	1.062	98	106	77	59	28	1.93E-5	> 1.00E-4	> 1.00E-4
A498	1.448	2.158	2.049	2.042	1.956	1.546	1.567	85	84	71	14	17	2.36E-6	> 1.00E-4	> 1.00E-4
ACHN	0.315	1.220	1.189	1.160	1.110	0.403	0.329	97	93	88	10	2	3.05E-6	> 1.00E-4	> 1.00E-4
CAKI-1	0.716	1.885	1.813	1.770	1.809	0.824	0.769	94	90	94	9	5	3.28E-6	> 1.00E-4	> 1.00E-4
RXF 393	0.455	0.941	0.911	0.873	0.890	0.561	0.506	94	86	89	22	10	3.82E-6	> 1.00E-4	> 1.00E-4
SN12C	0.452	1.845	1.775	1.848	1.691	0.784	0.692	95	100	89	24	17	3.96E-6	> 1.00E-4	> 1.00E-4
TK-10	0.502	1.102	1.134	1.170	1.174	0.669	0.519	105	111	112	28	3	5.45E-6	> 1.00E-4	> 1.00E-4
UO-31	0.693	1.580	1.486	1.555	1.456	0.784	0.750	89	97	86	10	6	2.99E-6	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.491	1.899	1.915	1.836	1.660	0.596	0.561	101	96	83	7	5	2.74E-6	> 1.00E-4	> 1.00E-4
DU-145	0.417	1.450	1.545	1.577	1.503	0.690	0.528	109	112	105	26	11	5.02E-6	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.554	2.400	2.214	2.127	2.064	0.855	0.524	90	85	82	16	-5	3.06E-6	5.63E-5	> 1.00E-4
MDA-MB-231/ATCC	0.486	1.428	1.404	1.489	1.405	0.870	0.749	97	107	98	41	28	6.88E-6	> 1.00E-4	> 1.00E-4
HS 578T	0.932	1.689	1.574	1.547	1.581	1.191	1.082	85	81	86	34	20	4.94E-6	> 1.00E-4	> 1.00E-4
BT-549	0.709	1.691	1.721	1.756	1.748	1.094	0.750	103	107	106	39	4	6.88E-6	> 1.00E-4	> 1.00E-4
T-47D	0.706	1.572	1.570	1.598	1.556	0.818	0.476	100	103	98	13	-33	3.67E-6	1.92E-5	> 1.00E-4
MDA-MB-468	0.612	1.172	1.164	1.092	1.065	0.662	0.530	98	86	81	9	-13	2.69E-6	2.50E-5	> 1.00E-4

NCI 5 dose-data for conjugate **5b**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 764570 / 1	Experiment ID : 1206NS89	Test Type : 08	Units : Molar
Report Date : December 23, 2013	Test Date : June 11, 2012	QNS :	MC :
COMI : BCTB-10 (115210)	Stain Reagent : SRB Dual-Pass Related	SSPL : Q80Q	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.394	1.521	1.454	1.464	1.364	0.353	0.357	94	95	86	-10	-9	2.36E-6	7.80E-6	> 1.00E-4
HL-60(TB)	0.868	2.821	2.773	2.840	2.906	0.711	0.474	98	101	104	-18	-45	2.78E-6	7.12E-6	> 1.00E-4
K-562	0.184	1.299	1.265	1.297	1.185	0.341	0.143	97	100	90	14	-22	3.35E-6	2.43E-5	> 1.00E-4
MOLT-4	0.468	1.564	1.571	1.521	1.318	0.413	0.301	101	96	78	-12	-36	2.03E-6	7.39E-6	> 1.00E-4
RPMI-8226	1.010	2.164	2.206	2.168	1.837	0.591	0.649	104	100	72	-42	-36	1.55E-6	4.29E-6	> 1.00E-4
SR	0.450	1.657	1.514	1.557	1.387	0.377	0.359	88	92	78	-16	-20	1.97E-6	6.70E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.318	1.667	1.622	1.679	1.489	0.672	0.063	97	101	87	26	-80	4.05E-6	1.76E-5	5.19E-5
HOP-62	0.413	1.082	1.041	1.055	1.101	0.783	0.080	94	96	103	55	-81	1.09E-5	2.55E-5	5.94E-5
HOP-92	1.472	1.905	1.840	1.878	1.788	1.660	0.749	85	94	73	43	-49	5.96E-6	2.94E-5	> 1.00E-4
NCI-H226	0.638	1.557	1.505	1.508	1.460	1.079	0.458	94	95	89	48	-28	8.92E-6	4.25E-5	> 1.00E-4
NCI-H23	0.545	1.655	1.568	1.561	1.598	0.989	0.267	92	91	95	40	-51	6.56E-6	2.75E-5	9.75E-5
NCI-H322M	0.640	1.439	1.387	1.377	1.371	0.893	0.457	93	92	91	32	-29	4.93E-6	3.35E-5	> 1.00E-4
NCI-H460	0.253	2.357	2.395	2.378	2.145	0.368	0.125	102	101	90	5	-51	2.97E-6	1.25E-5	9.68E-5
NCI-H522	0.700	1.831	1.705	1.655	1.674	1.268	0.387	89	84	86	50	-45	1.00E-5	3.38E-5	> 1.00E-4
Colon Cancer															
COLO 205	0.265	1.180	1.173	1.073	1.042	0.154	0.003	99	88	85	-42	-99	1.88E-6	4.66E-6	1.38E-5
HCC-2998	0.554	1.939	1.856	1.856	2.021	1.208	0.167	94	94	106	47	-70	8.96E-6	2.53E-5	6.76E-5
HCT-116	0.198	1.093	1.079	1.076	1.108	0.072	0.051	98	98	102	-64	-74	2.05E-6	4.11E-6	8.24E-6
HCT-15	0.260	1.700	1.670	1.687	1.573	0.459	0.134	98	99	91	14	-48	3.41E-6	1.67E-5	> 1.00E-4
HT29	0.226	1.259	1.290	1.320	1.336	0.300	0.101	103	106	107	7	-56	3.74E-6	1.30E-5	8.16E-5
KM12	0.460	2.033	1.966	1.891	1.774	0.645	0.043	96	91	84	12	-91	2.93E-6	1.30E-5	4.01E-5
SW-620	0.265	1.644	1.603	1.553	1.515	0.694	0.127	97	93	91	31	-52	4.82E-6	2.37E-5	9.44E-5
CNS Cancer															
SF-268	0.555	1.641	1.513	1.501	1.500	0.974	0.515	88	87	87	39	-7	5.80E-6	6.96E-5	> 1.00E-4
SF-539	0.772	2.360	2.291	2.346	2.234	1.998	0.262	96	99	92	77	-66	1.55E-5	3.46E-5	7.72E-5
SNB-19	0.494	1.600	1.545	1.598	1.478	1.016	0.521	95	100	89	47	2	8.57E-6	> 1.00E-4	> 1.00E-4
SNB-75	0.872	1.421	1.282	1.274	1.329	1.276	0.155	75	73	83	74	-82	1.42E-5	2.97E-5	6.21E-5
U251	0.282	1.395	1.373	1.326	1.275	0.288	0.088	98	94	89	1	-69	2.77E-6	1.02E-5	5.33E-5
Melanoma															
LOX IMVI	0.294	2.004	1.868	1.809	1.827	0.344	0.060	92	89	90	3	-80	2.86E-6	1.08E-5	4.37E-5
MALME-3M	0.613	1.025	0.994	0.987	1.057	0.955	0.172	92	91	108	83	-72	1.63E-5	3.43E-5	7.22E-5
M14	0.481	1.310	1.282	1.235	1.252	0.662	0.126	97	91	93	22	-74	4.02E-6	1.69E-5	5.64E-5
MDA-MB-435	0.474	1.977	1.950	1.966	1.820	0.772	0.067	98	99	90	20	-86	3.69E-6	1.54E-5	4.57E-5
SK-MEL-2	0.679	1.393	1.377	1.409	1.412	1.102	0.341	98	102	103	59	-50	1.21E-5	3.49E-5	> 1.00E-4
SK-MEL-28	0.589	1.476	1.513	1.501	1.475	1.176	0.076	104	103	100	66	-87	1.27E-5	2.70E-5	5.73E-5
SK-MEL-5	0.626	2.864	2.831	2.724	2.446	1.431	0.190	99	94	81	36	-70	4.91E-6	2.19E-5	6.52E-5
UACC-257	0.688	1.766	1.699	1.872	1.718	1.067	0.223	94	110	96	35	-68	5.68E-6	2.20E-5	6.73E-5
UACC-62	0.507	1.646	1.618	1.606	1.521	0.515	0.090	98	97	89	1	-82	2.76E-6	1.02E-5	4.08E-5
Ovarian Cancer															
IGROV1	0.837	1.854	1.872	1.878	1.811	1.111	0.646	102	102	96	27	-23	4.62E-6	3.47E-5	> 1.00E-4
OVCAR-3	0.607	1.688	1.607	1.579	1.626	0.248	0.028	92	90	94	-59	-95	1.94E-6	4.12E-6	8.72E-6
OVCAR-4	0.484	1.134	1.153	1.091	1.085	0.740	0.173	103	93	92	39	-64	6.30E-6	2.40E-5	7.28E-5
OVCAR-5	0.510	1.441	1.399	1.400	1.380	1.200	0.396	95	96	93	74	-22	1.78E-5	5.86E-5	> 1.00E-4
OVCAR-8	0.422	1.753	1.695	1.662	1.569	0.582	0.277	96	93	86	12	-34	3.08E-6	1.81E-5	> 1.00E-4
NCI/ADR-RES	0.456	1.543	1.507	1.490	1.486	0.708	0.432	97	95	95	23	-5	4.22E-6	6.48E-5	> 1.00E-4
SK-OV-3	0.614	1.270	1.236	1.250	1.298	1.229	0.033	95	97	104	94	-95	1.71E-5	3.14E-5	5.79E-5
Renal Cancer															
786-0	0.657	1.592	1.591	1.557	1.634	1.134	0.149	100	96	104	51	-77	1.02E-5	2.49E-5	6.12E-5
A498	1.448	2.181	2.134	2.071	2.054	1.813	1.211	94	85	83	50	-16	9.85E-6	5.66E-5	> 1.00E-4
ACHN	0.315	1.256	1.272	1.221	1.188	0.391	0.088	102	96	93	8	-72	3.20E-6	1.26E-5	5.30E-5
CAKI-1	0.716	1.771	1.648	1.586	1.598	0.687	0.165	88	82	84	-4	-77	2.41E-6	8.97E-6	4.26E-5
RXF 393	0.455	0.933	0.960	0.928	0.907	0.513	0.042	105	99	95	12	-91	3.46E-6	1.31E-5	4.01E-5
SN12C	0.452	1.874	1.872	1.716	1.637	0.845	0.240	100	89	83	28	-47	3.97E-6	2.35E-5	> 1.00E-4
TK-10	0.502	1.179	1.182	1.131	1.201	0.631	0.195	100	93	103	19	-61	4.29E-6	1.73E-5	7.26E-5
UO-31	0.693	1.541	1.423	1.280	1.169	0.856	0.184	86	69	56	19	-73	1.46E-6	1.61E-5	5.58E-5
Prostate Cancer															
PC-3	0.491	1.869	1.785	1.786	1.587	0.792	0.294	94	94	80	22	-40	3.25E-6	2.25E-5	> 1.00E-4
DU-145	0.417	1.478	1.478	1.436	1.420	0.653	0.121	100	96	95	22	-71	4.13E-6	1.73E-5	5.94E-5
Breast Cancer															
MCF7	0.554	2.321	2.246	2.181	2.078	0.822	0.280	96	92	86	15	-50	3.23E-6	1.71E-5	> 1.00E-4
MDA-MB-231/ATCC	0.486	1.447	1.483	1.412	1.357	0.982	0.265	104	96	91	52	-46	1.04E-5	3.40E-5	> 1.00E-4
HS 578T	0.932	1.719	1.633	1.630	1.545	1.311	0.660	89	89	78	48	-29	8.68E-6	4.19E-5	> 1.00E-4
BT-549	0.709	1.348	1.278	1.283	1.319	0.956	0.208	89	90	95	39	-71	6.30E-6	2.25E-5	6.46E-5
T-47D	0.706	1.525	1.478	1.493	1.479	0.847	0.424	94	96	94	17	-40	3.76E-6	2.00E-5	> 1.00E-4
MDA-MB-468	0.612	1.181	1.112	1.146	1.078	0.268	0.061	88	94	82	-56	-90	1.70E-6	3.92E-6	9.02E-6

NCI 5 dose-data for conjugate **5h**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 765810 / 1	Experiment ID : 1207NS11	Test Type : 08	Units : Molar
Report Date : December 23, 2013	Test Date : July 23, 2012	QNS :	MC :
COMI : BCTB-22 (117010)	Stain Reagent : SRB Dual-Pass Related	SSPL : Q80Q	

		Log10 Concentration												
	Time	Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.516	2.236	2.248	2.201	2.183	0.655	0.423	101	98	97	8	-18	3.37E-6	2.03E-5	> 1.00E-4
HL-60(TB)	0.673	2.077	2.312	2.254	2.381	0.797	0.494	117	113	122	9	-27	4.32E-6	1.78E-5	> 1.00E-4
K-562	0.353	2.256	2.361	2.449	2.224	0.459	0.339	106	110	98	6	-4	3.32E-6	3.84E-5	> 1.00E-4
MOLT-4	0.609	2.022	2.125	2.278	1.844	0.565	0.398	107	118	87	-7	-35	2.48E-6	8.37E-6	> 1.00E-4
RPMI-8226	0.999	2.573	2.516	2.446	2.164	0.835	0.673	96	92	74	-16	-33	1.84E-6	6.58E-6	> 1.00E-4
SR	0.194	0.771	0.772	0.746	0.713	0.308	0.264	100	96	90	20	12	3.71E-6	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.413	1.830	1.805	1.784	1.676	0.475	0.232	98	97	89	4	-44	2.89E-6	1.23E-5	> 1.00E-4
HOP-62	0.514	1.602	1.610	1.542	1.585	0.688	0.221	101	94	98	16	-57	3.87E-6	1.65E-5	7.99E-5
HOP-92	1.087	1.341	1.272	1.257	1.255	0.897	0.506	73	67	66	-17	-53	1.56E-6	6.18E-6	8.00E-5
NCI-H226	0.746	2.200	2.139	2.136	2.076	0.925	0.354	96	96	92	12	-53	3.34E-6	1.55E-5	9.14E-5
NCI-H23	1.173	3.069	3.020	3.069	2.940	1.486	0.771	97	100	93	16	-34	3.66E-6	2.11E-5	> 1.00E-4
NCI-H322M	0.689	1.601	1.604	1.517	1.533	0.826	0.411	100	91	93	15	-40	3.54E-6	1.86E-5	> 1.00E-4
NCI-H460	0.271	2.385	2.448	2.362	2.259	0.290	0.168	103	99	94	1	-38	2.97E-6	1.05E-5	> 1.00E-4
NCI-H522	0.986	1.944	1.888	1.878	1.778	1.063	0.355	94	93	83	8	-64	2.74E-6	1.29E-5	6.39E-5
Colon Cancer															
COLO 205	0.374	1.288	1.285	1.196	1.194	0.173	0.004	100	90	90	-54	-99	1.89E-6	4.22E-6	9.42E-6
HCC-2998	0.542	1.455	1.457	1.430	1.554	0.809	0.183	100	97	111	29	-66	5.56E-6	2.02E-5	6.75E-5
HCT-116	0.192	1.818	1.864	1.845	1.758	0.301	0.075	103	102	96	7	-61	3.29E-6	1.25E-5	6.84E-5
HCT-15	0.249	2.200	2.101	2.074	2.124	0.517	0.114	95	94	96	14	-54	3.63E-6	1.59E-5	8.67E-5
HT29	0.300	1.491	1.496	1.628	1.716	0.423	0.039	100	111	119	10	-87	4.31E-6	1.28E-5	4.17E-5
KM12	0.515	2.468	2.511	2.515	2.422	0.697	0.217	102	102	98	9	-58	3.46E-6	1.37E-5	7.61E-5
SW-620	0.251	1.913	1.907	1.844	1.837	0.585	0.123	100	96	95	20	-51	4.01E-6	1.92E-5	9.68E-5
CNS Cancer															
SF-268	0.737	2.130	2.131	2.148	2.155	0.875	0.515	100	101	102	10	-30	3.66E-6	1.77E-5	> 1.00E-4
SF-539	0.797	2.756	2.675	2.658	2.625	1.084	0.076	96	95	93	15	-90	3.55E-6	1.38E-5	4.12E-5
SNB-19	0.753	2.179	2.065	2.074	2.090	1.102	0.818	92	93	94	24	5	4.28E-6	> 1.00E-4	> 1.00E-4
U251	0.678	2.381	2.308	2.359	2.300	0.818	0.516	96	99	95	8	-24	3.31E-6	1.80E-5	> 1.00E-4
Melanoma															
LOX IMVI	0.552	2.924	2.874	2.923	2.769	0.440	0.038	98	100	93	-20	-93	2.41E-6	6.63E-6	2.56E-5
MALME-3M	0.673	1.373	1.364	1.365	1.359	0.848	0.134	99	99	98	25	-80	4.54E-6	1.73E-5	5.17E-5
M14	0.425	1.886	1.879	1.891	1.780	0.489	0.121	100	100	93	4	-72	3.05E-6	1.14E-5	5.19E-5
MDA-MB-435	0.396	1.821	1.787	1.785	1.770	0.579	0.122	98	97	96	13	-69	3.59E-6	1.43E-5	5.84E-5
SK-MEL-2	1.283	2.256	2.274	2.344	2.262	1.103	0.219	102	109	101	-14	-83	2.76E-6	7.54E-6	3.32E-5
SK-MEL-28	0.449	1.105	1.152	1.144	1.126	0.571	0.053	107	106	103	19	-88	4.25E-6	1.49E-5	4.38E-5
SK-MEL-5	0.729	3.064	2.980	2.911	2.789	1.155	0.157	96	93	88	18	-79	3.52E-6	1.54E-5	5.07E-5
UACC-257	0.996	1.882	1.840	1.835	1.823	0.794	0.243	95	95	93	-20	-76	2.41E-6	6.62E-6	3.44E-5
UACC-62	0.857	2.799	2.707	2.682	2.549	0.714	0.077	95	94	87	-17	-91	2.28E-6	6.90E-6	2.80E-5
Ovarian Cancer															
IGROV1	0.662	2.005	2.131	1.988	1.837	0.746	0.219	109	99	88	6	-67	2.89E-6	1.22E-5	5.87E-5
OVCAR-3	0.601	1.812	1.928	1.881	1.870	0.479	0.252	110	106	105	-20	-58	2.74E-6	6.87E-6	6.08E-5
OVCAR-4	0.644	1.158	1.124	1.172	1.173	0.775	0.111	93	103	103	25	-83	4.81E-6	1.72E-5	4.98E-5
OVCAR-5	0.406	1.268	1.205	1.255	1.237	0.729	0.117	93	98	96	37	-71	6.13E-6	2.21E-5	6.38E-5
OVCAR-8	0.564	2.076	2.065	2.049	1.944	0.587	0.277	99	98	91	2	-51	2.88E-6	1.07E-5	9.58E-5
NCI/ADR-RES	0.868	2.701	2.771	2.825	2.600	1.073	0.751	104	107	94	11	-14	3.42E-6	2.83E-5	> 1.00E-4
SK-OV-3	0.651	1.502	1.460	1.473	1.517	1.011	0.221	95	97	102	42	-66	7.43E-6	2.46E-5	7.11E-5
Renal Cancer															
786-0	0.732	2.680	2.694	2.732	2.693	1.389	0.075	101	103	101	34	-90	5.71E-6	1.88E-5	4.76E-5
A498	1.207	1.827	1.777	1.758	1.654	1.196	0.200	92	89	72	-1	-83	2.01E-6	9.70E-6	3.93E-5
ACHN	0.340	1.848	1.787	1.847	1.718	0.432	0.209	96	100	91	6	-39	3.06E-6	1.37E-5	> 1.00E-4
CAKI-1	0.946	3.088	2.951	2.917	2.861	1.198	0.765	94	92	89	12	-19	3.22E-6	2.40E-5	> 1.00E-4
RXF 393	0.779	1.074	1.063	0.999	0.994	0.497	0.034	96	74	73	-36	-96	1.62E-6	4.66E-6	1.71E-5
SN12C	0.721	2.646	2.497	2.525	2.411	0.906	0.612	92	94	88	10	-15	3.04E-6	2.44E-5	> 1.00E-4
TK-10	0.770	1.389	1.428	1.441	1.426	0.765	0.371	106	108	106	-1	-52	3.35E-6	9.86E-6	9.19E-5
UO-31	0.706	2.110	1.997	1.991	1.823	0.733	0.229	92	92	80	2	-68	2.40E-6	1.07E-5	5.59E-5
Prostate Cancer															
PC-3	0.651	1.966	1.926	1.850	1.713	0.553	0.153	97	91	81	-15	-77	2.09E-6	6.95E-6	3.69E-5
DU-145	0.333	1.235	1.294	1.282	1.228	0.395	0.065	107	105	99	7	-81	3.41E-6	1.20E-5	4.47E-5
Breast Cancer															
MCF7	0.380	1.754	1.702	1.722	1.652	0.515	0.248	96	98	93	10	-35	3.27E-6	1.66E-5	> 1.00E-4
MDA-MB-231/ATCC	0.625	1.446	1.412	1.443	1.306	0.717	0.173	96	100	83	11	-72	2.88E-6	1.36E-5	5.40E-5
HS 578T	0.954	2.058	2.001	1.916	1.935	1.125	0.907	95	87	89	15	-5	3.38E-6	5.70E-5	> 1.00E-4
BT-549	0.918	2.102	2.095	2.125	2.109	1.208	0.314	99	102	101	25	-66	4.62E-6	1.87E-5	6.68E-5
T-47D	0.681	1.809	1.710	1.692	1.598	0.774	0.563	91	90	81	8	-17	2.68E-6	2.09E-5	> 1.00E-4
MDA-MB-468	0.679	1.506	1.385	1.381	1.325	0.723	0.107	85	85	78	5	-84	2.43E-6	1.15E-5	4.14E-5

NCI 5 dose-data for conjugate **5r**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 765814 / 1	Experiment ID : 1207NS11	Test Type : 08	Units : Molar
Report Date : December 23, 2013	Test Date : July 23, 2012	QNS :	MC :
COMI : BCTB-24 (117680)	Stain Reagent : SRB Dual-Pass Related	SSPL : Q80Q	

Log10 Concentration

	Time	Mean Optical Densities						Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.516	2.249	2.245	2.198	1.829	0.590	0.484	100	97	76	4	-6	2.29E-6	2.56E-5	> 1.00E-4
HL-60(TB)	0.673	2.056	2.305	2.117	2.131	0.557	0.541	118	104	105	-17	-20	2.83E-6	7.23E-6	> 1.00E-4
K-562	0.353	2.167	2.318	2.348	1.944	0.408	0.361	108	110	88	3	.	2.79E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.609	1.804	2.028	2.118	1.401	0.501	0.415	119	126	66	-18	-32	1.56E-6	6.14E-6	> 1.00E-4
RPMI-8226	0.999	2.523	2.438	2.362	1.855	0.614	0.597	94	89	56	-39	-40	1.16E-6	3.92E-6	> 1.00E-4
SR	0.194	0.692	0.692	0.664	0.636	0.268	0.262	100	94	89	15	14	3.34E-6	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.413	1.584	1.544	1.544	1.377	0.365	0.327	97	97	82	-12	-21	2.21E-6	7.50E-6	> 1.00E-4
HOP-62	0.514	1.587	1.543	1.554	1.545	0.572	0.510	96	97	96	5	-1	3.22E-6	7.47E-5	> 1.00E-4
NCI-H226	0.746	2.187	2.117	2.138	2.043	0.878	0.822	95	97	90	9	5	3.12E-6	> 1.00E-4	> 1.00E-4
NCI-H23	1.173	3.118	3.048	3.102	3.033	1.179	1.091	96	99	96	.	-7	3.01E-6	1.09E-5	> 1.00E-4
NCI-H322M	0.689	1.486	1.531	1.545	1.441	0.650	0.600	106	107	94	-6	-13	2.77E-6	8.78E-6	> 1.00E-4
NCI-H460	0.271	2.359	2.388	2.286	1.978	0.203	0.226	101	96	82	-25	-17	1.98E-6	5.81E-6	> 1.00E-4
NCI-H522	0.986	1.720	1.655	1.719	1.585	0.754	0.581	91	100	82	-24	-41	2.00E-6	5.97E-6	> 1.00E-4
Colon Cancer															
COLO 205	0.374	1.329	1.337	1.312	1.292	0.199	0.128	101	98	96	-47	-66	2.10E-6	4.71E-6	1.47E-5
HCC-2998	0.542	1.472	1.506	1.581	1.510	0.627	0.473	104	112	104	9	-13	3.71E-6	2.62E-5	> 1.00E-4
HCT-116	0.192	1.598	1.678	1.728	1.516	0.176	0.152	106	109	94	-9	-21	2.69E-6	8.25E-6	> 1.00E-4
HCT-15	0.249	1.907	1.866	1.793	1.730	0.284	0.267	97	93	89	2	1	2.82E-6	> 1.00E-4	> 1.00E-4
HT29	0.300	1.331	1.402	1.424	1.318	0.286	0.248	107	109	99	-5	-18	2.96E-6	9.01E-6	> 1.00E-4
KM12	0.515	2.402	2.373	2.535	2.188	0.546	0.426	98	107	89	2	-17	2.78E-6	1.22E-5	> 1.00E-4
SW-620	0.251	1.873	1.863	1.814	1.905	0.430	0.370	99	96	102	11	7	3.73E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.737	2.053	2.043	2.087	2.006	0.809	0.760	99	103	96	5	2	3.24E-6	> 1.00E-4	> 1.00E-4
SF-539	0.797	2.630	2.521	2.499	2.495	0.774	0.648	94	93	93	-3	-19	2.80E-6	9.33E-6	> 1.00E-4
SNB-19	0.753	2.203	2.130	2.135	2.005	0.882	0.881	95	95	86	9	9	2.94E-6	> 1.00E-4	> 1.00E-4
U251	0.678	2.239	2.187	2.226	2.084	0.580	0.533	97	99	90	-15	-21	2.42E-6	7.26E-6	> 1.00E-4
Melanoma															
LOX IMVI	0.552	2.866	2.836	2.908	2.766	0.352	0.180	99	102	96	-36	-67	2.22E-6	5.31E-6	2.76E-5
MALME-3M	0.673	1.346	1.322	1.344	1.220	0.647	0.423	96	100	81	-4	-37	2.33E-6	8.99E-6	> 1.00E-4
M14	0.425	1.647	1.682	1.788	1.590	0.355	0.256	103	111	95	-16	-40	2.54E-6	7.12E-6	> 1.00E-4
MDA-MB-435	0.396	1.918	1.815	1.769	1.662	0.434	0.329	93	90	83	2	-17	2.58E-6	1.34E-5	> 1.00E-4
SK-MEL-2	1.283	2.078	2.078	2.174	2.078	0.586	0.346	100	112	100	-54	-73	2.11E-6	4.45E-6	9.37E-6
SK-MEL-28	0.449	1.156	1.161	1.124	1.133	0.512	0.463	101	95	97	9	2	3.40E-6	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.729	3.052	2.920	2.914	2.620	0.428	0.028	94	94	81	-41	-96	1.80E-6	4.61E-6	1.44E-5
UACC-257	0.996	1.626	1.565	1.574	1.565	0.575	0.439	90	92	90	-42	-56	2.01E-6	4.80E-6	3.67E-5
UACC-62	0.857	2.913	2.839	2.829	2.661	0.413	0.331	96	96	88	-52	-61	1.86E-6	4.25E-6	9.71E-6
Ovarian Cancer															
IGROV1	0.662	1.993	2.002	2.032	1.775	0.655	0.633	101	103	84	-1	-4	2.49E-6	9.70E-6	> 1.00E-4
OVCAR-3	0.601	1.763	1.826	1.838	1.757	0.345	0.373	105	106	99	-43	-38	2.23E-6	5.01E-6	> 1.00E-4
OVCAR-4	0.644	1.203	1.179	1.214	1.151	0.830	0.669	96	102	91	33	4	5.10E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.406	1.213	1.173	1.181	1.190	0.604	0.498	95	96	97	25	11	4.46E-6	> 1.00E-4	> 1.00E-4
OVCAR-8	0.564	1.936	1.887	1.891	1.549	0.479	0.448	96	97	72	-15	-21	1.78E-6	6.69E-6	> 1.00E-4
NCI/ADR-RES	0.868	2.754	2.861	2.846	2.426	1.035	0.906	106	105	83	9	2	2.77E-6	> 1.00E-4	> 1.00E-4
SK-OV-3	0.651	1.489	1.461	1.455	1.490	0.792	0.700	97	96	100	17	6	4.00E-6	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.732	2.546	2.548	2.558	2.492	0.860	0.784	100	101	97	7	3	3.33E-6	> 1.00E-4	> 1.00E-4
A498	1.207	1.806	1.742	1.675	1.627	1.196	1.106	89	78	70	-1	-8	1.92E-6	9.70E-6	> 1.00E-4
ACHN	0.340	1.666	1.668	1.622	1.526	0.384	0.345	100	97	89	3	.	2.87E-6	> 1.00E-4	> 1.00E-4
CAKI-1	0.946	3.157	3.074	3.029	2.988	1.393	1.202	96	94	92	20	12	3.87E-6	> 1.00E-4	> 1.00E-4
RXF 393	0.779	1.184	1.160	1.115	1.094	0.465	0.420	94	83	78	-40	-46	1.72E-6	4.55E-6	> 1.00E-4
SN12C	0.721	2.702	2.660	2.580	2.445	0.892	0.814	98	94	87	9	5	2.97E-6	> 1.00E-4	> 1.00E-4
TK-10	0.770	1.298	1.292	1.303	1.220	0.634	0.552	99	101	85	-18	-28	2.20E-6	6.74E-6	> 1.00E-4
UO-31	0.706	2.103	2.046	2.085	1.933	0.668	0.596	96	99	88	-5	-16	2.54E-6	8.74E-6	> 1.00E-4
Prostate Cancer															
PC-3	0.651	1.945	1.944	1.854	1.578	0.501	0.514	100	93	72	-23	-21	1.69E-6	5.71E-6	> 1.00E-4
DU-145	0.333	1.152	1.235	1.226	1.126	0.328	0.301	110	109	97	-2	-10	2.99E-6	9.65E-6	> 1.00E-4
Breast Cancer															
MCF7	0.380	1.736	1.619	1.672	1.486	0.426	0.385	91	95	82	3	.	2.53E-6	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.625	1.454	1.438	1.470	1.294	0.600	0.515	98	102	81	-4	-18	2.30E-6	8.95E-6	> 1.00E-4
HS 578T	0.954	2.001	1.965	1.970	1.893	0.971	1.043	97	97	90	2	8	2.82E-6	> 1.00E-4	> 1.00E-4
BT-549	0.918	1.849	1.884	1.898	1.865	0.907	0.818	104	105	102	-1	-11	3.18E-6	9.72E-6	> 1.00E-4
T-47D	0.681	1.752	1.738	1.661	1.545	0.741	0.699	99	92	81	6	2	2.56E-6	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.679	1.510	1.389	1.358	1.255	0.753	0.694	85	82	69	9	2	2.08E-6	> 1.00E-4	> 1.00E-4

NCI 5 dose-data for conjugate **5d**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 765815 / 1	Experiment ID : 1207NS11	Test Type : 08	Units : Molar
Report Date : December 23, 2013	Test Date : July 23, 2012	QNS :	MC :
COMI : BCTB-25 (117681)	Stain Reagent : SRB Dual-Pass Related	SSPL : Q80Q	

Log10 Concentration

	Time	Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.516	2.207	2.239	2.260	2.134	0.843	0.906	102	103	96	19	23	3.96E-6	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.673	1.969	2.040	1.966	1.983	0.951	0.839	105	100	101	21	13	4.37E-6	> 1.00E-4	> 1.00E-4
K-562	0.353	2.094	2.015	2.173	2.134	0.704	0.674	95	105	102	20	18	4.33E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.609	1.934	2.006	2.026	1.862	0.869	0.933	105	107	95	20	24	3.93E-6	> 1.00E-4	> 1.00E-4
RPMI-8226	0.999	2.648	2.549	2.530	2.280	0.945	0.869	94	93	78	-5	-13	2.15E-6	8.61E-6	> 1.00E-4
SR	0.194	0.798	0.772	0.765	0.760	0.490	0.480	96	95	94	49	47	9.50E-6	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.413	1.588	1.578	1.551	1.426	0.585	0.614	99	97	86	15	17	3.20E-6	> 1.00E-4	> 1.00E-4
HOP-62	0.514	1.561	1.566	1.579	1.518	0.893	0.850	101	102	96	36	32	5.87E-6	> 1.00E-4	> 1.00E-4
HOP-92	1.087	1.308	1.281	1.262	1.173	0.932	0.961	88	79	39	-14	-12	5.26E-7	5.38E-6	> 1.00E-4
NCI-H226	0.746	2.071	2.068	2.106	2.057	1.300	1.198	100	103	99	42	34	7.19E-6	> 1.00E-4	> 1.00E-4
NCI-H23	1.173	3.077	2.908	2.906	2.889	1.702	1.840	91	91	90	28	35	4.40E-6	> 1.00E-4	> 1.00E-4
NCI-H322M	0.689	1.468	1.417	1.442	1.443	1.099	1.067	93	97	97	53	49	4.41E-5	> 1.00E-4	> 1.00E-4
NCI-H460	0.271	2.359	2.398	2.419	2.247	0.689	0.554	102	103	95	20	14	3.96E-6	> 1.00E-4	> 1.00E-4
NCI-H522	0.986	1.609	1.522	1.528	1.526	1.107	1.040	86	87	87	19	9	3.51E-6	> 1.00E-4	> 1.00E-4
Colon Cancer															
COLO 205	0.374	1.286	1.283	1.305	1.213	0.634	0.615	100	102	92	28	26	4.58E-6	> 1.00E-4	> 1.00E-4
HCC-2998	0.542	1.489	1.406	1.456	1.476	0.943	0.921	91	97	99	42	40	7.32E-6	> 1.00E-4	> 1.00E-4
HCT-116	0.192	1.670	1.663	1.738	1.654	0.443	0.431	100	105	99	17	16	3.95E-6	> 1.00E-4	> 1.00E-4
HCT-15	0.249	2.193	2.145	2.060	2.013	0.729	0.669	98	93	91	25	22	4.14E-6	> 1.00E-4	> 1.00E-4
HT29	0.300	1.290	1.322	1.370	1.422	0.673	0.550	103	108	113	38	25	6.87E-6	> 1.00E-4	> 1.00E-4
KM12	0.515	2.442	2.455	2.420	2.379	0.783	0.777	101	99	97	14	14	3.66E-6	> 1.00E-4	> 1.00E-4
SW-620	0.251	1.908	1.888	1.876	1.840	0.949	0.861	99	98	96	42	37	7.14E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.737	2.073	1.960	1.948	1.969	1.142	1.114	92	91	92	30	28	4.81E-6	> 1.00E-4	> 1.00E-4
SF-539	0.797	2.730	2.693	2.675	2.599	1.855	1.605	98	97	93	55	42	2.31E-5	> 1.00E-4	> 1.00E-4
SNB-19	0.753	2.267	2.124	2.142	2.188	1.493	1.466	91	92	95	49	47	9.45E-6	> 1.00E-4	> 1.00E-4
U251	0.678	2.269	2.222	2.256	2.125	1.164	1.004	97	99	91	31	20	4.76E-6	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.552	2.790	2.708	2.706	2.758	1.144	0.966	96	96	99	26	18	4.72E-6	> 1.00E-4	> 1.00E-4
MALME-3M	0.673	1.351	1.329	1.313	1.277	0.859	0.927	97	94	89	27	37	4.31E-6	> 1.00E-4	> 1.00E-4
M14	0.425	1.815	1.788	1.818	1.716	0.757	0.859	98	100	93	24	31	4.18E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.396	1.907	1.865	1.831	1.655	0.759	0.796	97	95	83	24	26	3.65E-6	> 1.00E-4	> 1.00E-4
SK-MEL-2	1.283	2.051	2.044	2.082	2.109	1.310	1.289	99	104	108	4	1	3.58E-6	> 1.00E-4	> 1.00E-4
SK-MEL-28	0.449	1.146	1.141	1.145	1.108	0.738	0.669	99	100	95	41	32	6.89E-6	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.729	3.058	3.044	3.004	2.626	1.089	1.022	99	98	81	15	13	2.99E-6	> 1.00E-4	> 1.00E-4
UACC-257	0.996	1.635	1.582	1.595	1.557	1.121	1.171	92	94	88	19	27	3.57E-6	> 1.00E-4	> 1.00E-4
UACC-62	0.857	2.969	2.907	2.899	2.771	1.150	1.206	97	97	91	14	17	3.38E-6	> 1.00E-4	> 1.00E-4
Ovarian Cancer															
IGROV1	0.662	1.942	1.879	1.853	1.821	0.712	0.775	95	93	91	4	9	2.94E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.601	1.756	1.786	1.826	1.771	1.023	0.934	103	106	101	37	29	6.20E-6	> 1.00E-4	> 1.00E-4
OVCAR-4	0.644	1.229	1.186	1.206	1.147	0.965	0.923	93	96	86	55	48	4.74E-5	> 1.00E-4	> 1.00E-4
OVCAR-5	0.406	1.282	1.223	1.276	1.295	1.098	1.031	93	99	101	79	71	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-8	0.564	1.840	1.817	1.803	1.668	0.620	0.664	98	97	87	4	8	2.79E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.868	2.655	2.601	2.619	2.551	1.127	1.163	97	98	94	14	16	3.59E-6	> 1.00E-4	> 1.00E-4
SK-OV-3	0.651	1.445	1.417	1.473	1.498	1.354	1.283	97	104	107	89	80	> 1.00E-4	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.732	2.607	2.616	2.535	2.572	1.853	1.593	100	96	98	60	46	5.07E-5	> 1.00E-4	> 1.00E-4
A498	1.207	1.874	1.717	1.768	1.649	1.368	1.464	76	84	66	24	39	2.43E-6	> 1.00E-4	> 1.00E-4
ACHN	0.340	1.738	1.758	1.762	1.683	0.745	0.693	101	102	96	29	25	4.86E-6	> 1.00E-4	> 1.00E-4
CAKI-1	0.946	3.045	2.932	2.931	2.892	1.834	1.761	95	95	93	42	39	7.03E-6	> 1.00E-4	> 1.00E-4
RXF 393	0.779	1.275	1.357	1.267	1.188	0.874	0.790	116	98	82	19	2	3.25E-6	> 1.00E-4	> 1.00E-4
SN12C	0.721	2.737	2.692	2.720	2.608	1.506	1.403	98	99	94	39	34	6.27E-6	> 1.00E-4	> 1.00E-4
TK-10	0.770	1.279	1.244	1.240	1.224	0.927	0.837	93	92	89	31	13	4.70E-6	> 1.00E-4	> 1.00E-4
UO-31	0.706	1.997	1.832	1.898	1.884	0.931	0.968	87	92	91	17	20	3.62E-6	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.651	1.877	1.821	1.801	1.710	0.654	0.694	95	94	86	.	3	2.64E-6	> 1.00E-4	> 1.00E-4
DU-145	0.333	1.207	1.240	1.218	1.243	0.650	0.568	104	101	104	36	27	6.27E-6	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.380	1.671	1.658	1.607	1.606	0.660	0.587	99	95	95	22	16	4.11E-6	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.625	1.458	1.508	1.436	1.382	1.013	0.923	106	97	91	47	36	8.38E-6	> 1.00E-4	> 1.00E-4
HS 578T	0.954	2.053	1.970	1.979	1.963	1.254	1.219	92	93	92	27	24	4.44E-6	> 1.00E-4	> 1.00E-4
BT-549	0.918	1.839	1.803	1.842	1.895	1.196	1.191	96	100	106	30	30	5.48E-6	> 1.00E-4	> 1.00E-4
T-47D	0.681	1.669	1.605	1.637	1.446	0.865	0.806	93	97	77	19	13	2.92E-6	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.679	1.445	1.395	1.380	1.301	0.843	0.738	94	91	81	21	8	3.32E-6	> 1.00E-4	> 1.00E-4

NCI 5 dose-data for conjugate **5w**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 764567 / 1	Experiment ID : 1206NS89	Test Type : 08	Units : Molar
Report Date : December 23, 2013	Test Date : June 11, 2012	QNS :	MC :
COMI : BCTB-6 (114638)	Stain Reagent : SRB Dual-Pass Related	SSPL : Q80Q	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.394	1.506	1.511	1.493	1.415	0.344	0.253	100	99	92	-13	-36	2.51E-6	7.56E-6	> 1.00E-4
HL-60(TB)	0.868	2.935	3.087	3.068	3.077	0.600	0.433	107	106	107	-31	-50	2.59E-6	5.96E-6	9.86E-5
K-562	0.184	1.376	1.516	1.509	1.388	0.233	0.168	112	111	101	4	-9	3.36E-6	2.09E-5	> 1.00E-4
MOLT-4	0.468	1.595	1.648	1.707	1.515	0.366	0.266	105	110	93	-22	-43	2.37E-6	6.46E-6	> 1.00E-4
RPMI-8226	1.010	2.224	2.240	2.145	1.943	0.697	0.523	101	93	77	-31	-48	1.77E-6	5.16E-6	> 1.00E-4
SR	0.450	1.689	1.660	1.674	1.537	0.384	0.285	98	99	88	-15	-37	2.33E-6	7.17E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.318	1.646	1.604	1.575	1.524	0.613	0.411	97	95	91	22	7	3.94E-6	> 1.00E-4	> 1.00E-4
HOP-62	0.413	1.145	1.160	1.165	1.175	0.726	0.422	102	103	104	43	1	7.63E-6	> 1.00E-4	> 1.00E-4
NCI-H226	0.638	1.621	1.582	1.648	1.506	0.784	0.605	96	103	88	15	-5	3.32E-6	5.48E-5	> 1.00E-4
NCI-H23	0.545	1.627	1.605	1.653	1.588	1.113	0.488	98	102	96	52	-10	1.10E-5	6.82E-5	> 1.00E-4
NCI-H322M	0.640	1.464	1.489	1.484	1.467	1.011	0.806	103	102	100	45	20	8.11E-6	> 1.00E-4	> 1.00E-4
NCI-H460	0.253	2.457	2.491	2.456	2.230	0.619	0.346	102	100	90	17	4	3.49E-6	> 1.00E-4	> 1.00E-4
NCI-H522	0.700	1.855	1.826	1.856	1.758	0.751	0.496	97	100	92	4	-29	3.00E-6	1.35E-5	> 1.00E-4
Colon Cancer															
COLO 205	0.265	1.161	1.198	1.192	1.061	0.095	0.028	104	103	89	-64	-89	1.79E-6	3.80E-6	8.06E-6
HCC-2998	0.554	2.079	2.074	2.126	2.158	0.728	0.553	100	103	105	11	.	3.88E-6	9.48E-5	> 1.00E-4
HCT-116	0.198	1.826	1.851	1.883	1.721	0.326	0.079	102	104	94	8	-60	3.22E-6	1.30E-5	7.10E-5
HCT-15	0.260	1.637	1.556	1.487	1.428	0.309	0.259	94	89	85	4	-1	2.68E-6	7.25E-5	> 1.00E-4
HT29	0.226	1.295	1.346	1.444	1.411	0.281	0.267	105	114	111	5	4	3.76E-6	> 1.00E-4	> 1.00E-4
KM12	0.460	2.054	2.105	2.146	1.970	0.659	0.373	103	106	95	12	-19	3.50E-6	2.49E-5	> 1.00E-4
SW-620	0.265	1.640	1.608	1.607	1.667	0.853	0.425	98	98	102	43	12	7.54E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.555	1.525	1.523	1.672	1.601	1.071	0.770	100	115	108	53	22	1.27E-5	> 1.00E-4	> 1.00E-4
SF-539	0.772	2.141	2.135	2.036	1.866	0.406	0.273	100	92	80	-47	-65	1.72E-6	4.24E-6	1.41E-5
SNB-19	0.494	1.597	1.485	1.462	1.544	1.207	1.014	90	88	95	65	47	6.89E-5	> 1.00E-4	> 1.00E-4
SNB-75	0.872	1.409	1.282	1.234	1.336	0.972	0.736	76	67	86	19	-16	3.44E-6	3.50E-5	> 1.00E-4
U251	0.282	1.319	1.248	1.299	1.236	0.335	0.232	93	98	92	5	-18	3.04E-6	1.66E-5	> 1.00E-4
Melanoma															
LOX IMVI	0.294	1.834	1.859	1.864	1.759	0.336	0.144	102	102	95	3	-51	3.08E-6	1.12E-5	9.57E-5
MALME-3M	0.613	1.005	1.030	1.058	1.074	0.674	0.271	106	114	118	16	-56	4.60E-6	1.65E-5	8.30E-5
M14	0.481	1.768	1.776	1.812	1.706	0.767	0.317	101	103	95	22	-34	4.16E-6	2.48E-5	> 1.00E-4
MDA-MB-435	0.474	2.144	2.146	2.096	2.045	0.816	0.517	100	97	94	20	3	3.97E-6	> 1.00E-4	> 1.00E-4
SK-MEL-2	0.679	1.351	1.394	1.445	1.447	0.609	0.357	106	114	114	-10	-47	3.28E-6	8.25E-6	> 1.00E-4
SK-MEL-28	0.589	1.484	1.468	1.457	1.415	0.593	0.477	98	97	92	.	-19	2.89E-6	1.05E-5	> 1.00E-4
SK-MEL-5	0.626	2.833	2.818	2.731	2.473	0.864	0.023	99	95	84	11	-96	2.90E-6	1.26E-5	3.69E-5
UACC-257	0.688	1.711	1.633	1.616	1.641	0.825	0.206	92	91	93	13	-70	3.47E-6	1.44E-5	5.74E-5
UACC-62	0.507	1.702	1.558	1.606	1.547	0.414	0.229	88	92	87	-18	-55	2.25E-6	6.70E-6	7.33E-5
Ovarian Cancer															
IGROV1	0.837	1.878	2.011	2.016	1.941	1.357	0.846	113	113	106	50	1	9.99E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.607	1.626	1.696	1.731	1.691	0.279	0.180	107	110	106	-54	-70	2.25E-6	4.60E-6	9.43E-6
OVCAR-4	0.484	1.191	1.164	1.154	1.100	0.789	0.616	96	95	87	43	19	6.98E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.510	1.378	1.310	1.265	1.249	0.744	0.564	92	87	85	27	6	4.01E-6	> 1.00E-4	> 1.00E-4
OVCAR-8	0.422	1.867	1.849	1.782	1.727	0.646	0.447	99	94	90	15	2	3.46E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.456	1.468	1.499	1.624	1.449	0.844	0.507	103	115	98	38	5	6.37E-6	> 1.00E-4	> 1.00E-4
SK-OV-3	0.614	1.285	1.313	1.332	1.370	1.016	0.443	104	107	113	60	-28	1.30E-5	4.81E-5	> 1.00E-4
Renal Cancer															
786-0	0.657	2.131	2.207	2.221	2.250	0.449	0.395	105	106	108	-32	-40	2.60E-6	5.93E-6	> 1.00E-4
A498	1.448	2.097	1.998	2.025	2.050	1.881	0.874	85	89	93	67	-40	1.44E-5	4.24E-5	> 1.00E-4
ACHN	0.315	1.266	1.305	1.187	1.081	0.381	0.288	104	92	81	7	-9	2.60E-6	2.79E-5	> 1.00E-4
CAKI-1	0.716	1.895	1.725	1.698	1.599	0.844	0.674	86	83	75	11	-6	2.44E-6	4.45E-5	> 1.00E-4
RXF 393	0.455	0.935	0.933	0.948	0.868	0.152	0.129	100	103	86	-67	-72	1.72E-6	3.66E-6	7.77E-6
SN12C	0.452	1.902	1.802	1.748	1.719	0.991	0.778	93	89	87	37	22	5.54E-6	> 1.00E-4	> 1.00E-4
TK-10	0.502	1.230	1.261	1.321	1.343	0.810	0.540	104	113	115	42	5	7.85E-6	> 1.00E-4	> 1.00E-4
UO-31	0.693	1.639	1.484	1.345	1.283	0.993	0.608	84	69	62	32	-12	2.53E-6	5.25E-5	> 1.00E-4
Prostate Cancer															
PC-3	0.491	1.782	1.765	1.634	1.559	0.605	0.467	99	89	83	9	-5	2.77E-6	4.40E-5	> 1.00E-4
DU-145	0.417	1.448	1.522	1.630	1.572	0.885	0.557	107	118	112	45	14	8.53E-6	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.554	2.296	2.189	2.050	1.946	0.919	0.521	94	86	80	21	-6	3.22E-6	5.97E-5	> 1.00E-4
MDA-MB-231/ATCC	0.486	1.341	1.323	1.372	1.270	0.431	0.412	98	104	92	-11	-15	2.54E-6	7.76E-6	> 1.00E-4
HS 578T	0.932	1.697	1.599	1.542	1.531	1.205	1.063	87	80	78	36	17	4.60E-6	> 1.00E-4	> 1.00E-4
BT-549	0.709	1.704	1.759	1.753	1.737	0.641	0.420	106	105	103	-10	-41	2.96E-6	8.21E-6	> 1.00E-4
T-47D	0.706	1.528	1.548	1.607	1.610	0.619	0.376	102	110	110	-12	-47	3.09E-6	7.92E-6	> 1.00E-4
MDA-MB-468	0.612	1.195	1.106	1.136	1.132	0.355	0.384	85	90	89	-42	-37	1.99E-6	4.78E-6	> 1.00E-4

NCI 5 dose-data for conjugate **5c**

The solubility parameters (ADME) of active β-carboline-benzimidazole conjugates analyzed by using ADMET tool in Discovery Studio and the data is presented in Table. Conjugate **5r** shows good absorption level with possible solubility. In addition, we have further analyzed the cellular permeability of these molecules using Accelrys and QikProp module of Schrödinger softwares and data suggests that these conjugates are good enough to cross the cellular membrane.

Compound	[a]**Absorption level**	[a]**Solubility** (logSw)	[b]**QPPCaco**	[a]**Solubility level**
5a	1	-8.416	2739.989	0
5b	1	-8.416	2739.989	0
5c	2	-9.298	2739.989	0
5d	1	-8.67	2741.732	0
5h	1	-9.009	2727.326	0
5r	0	-7.791	2856.859	1
5w	1	-8.517	2953.542	0

Absorption level: 0-Good absorption; 1-Moderate absorption; 2-Low absorption; 3-Very low absorption.

Solubility level: 0-Extremely low; 1-No, very low but possible; 2-Yes, low; 3-Yes, good; 4-Yes, optimal; 5- No, too soluble; 6-Warning: molecules with one or more unknown AlogP98 types.

QPPCaco: Predicted apparent Caco-2 cell permeability in nm/sec. Caco-2 cells are a model for the gut blood barrier. <25 poor, >500 great.

[a] Discovery Studio citation

Accelrys Software Inc., Discovery Studio Modelling Environment, Release 4.0, San Diego: Accelrys Software Inc., 2013.

[b] Schrodinger citation

QikProp, version 3.5, Schrödinger, LLC, New York, NY, 2012