

Supporting Information

From Tryptamine to Discovery Efficient Multi-Target Directed Ligands Against Cholinesterase-Associated Neurodegenerative Disorders

Junbo Wu^{1,6§}, Honghua Zhang^{2§}, Yuying Wang⁴, Gaofeng Yin⁵, Qien Li⁷, Linsheng Zhuo^{2*}, Hongjin Chen^{1*}, Zhen Wang^{2, 3*}

¹Department of Colorectal Surgery, The Affiliated Hospital, Nanjing University of Chinese Medicine, Nanjing, Jiangsu, 210029, China.

²School of Pharmaceutical Science, Hengyang Medical School, University of South China, Hengyang, Hunan, 421001, China

³The First Affiliated Hospital, Hengyang Medical School, University of South China, Hengyang, Hunan 421001, China

⁴State Key Laboratory of Applied Organic Chemistry, College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, China

⁵School of Pharmacy, Lanzhou University, Lanzhou, 730000, China

⁶Department of Colorectal Surgery, Hengyang Central Hospital, Hengyang, Hunan, 410000, China

⁷Tibetan Medical College, Qinghai University, Xining 810016, Qinghai, China

[§]Wu JB and Zhang HH contributed equally to this work.

***Correspondence:**

Zhen Wang, Linsheng Zhuo, Hongjin Chen

zhenw@lzu.edu.cn; lszhuo@mail.ccnu.edu.cn; 260789@njucm.edu.cn

Table of Contents

¹H NMR and ¹³C NMR of synthesized compounds

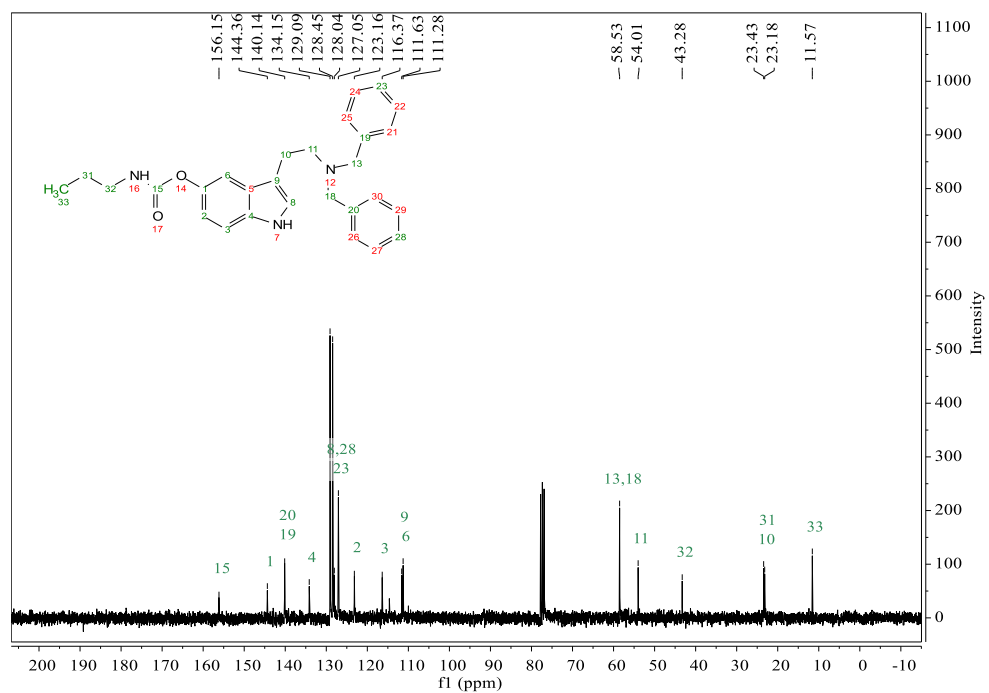
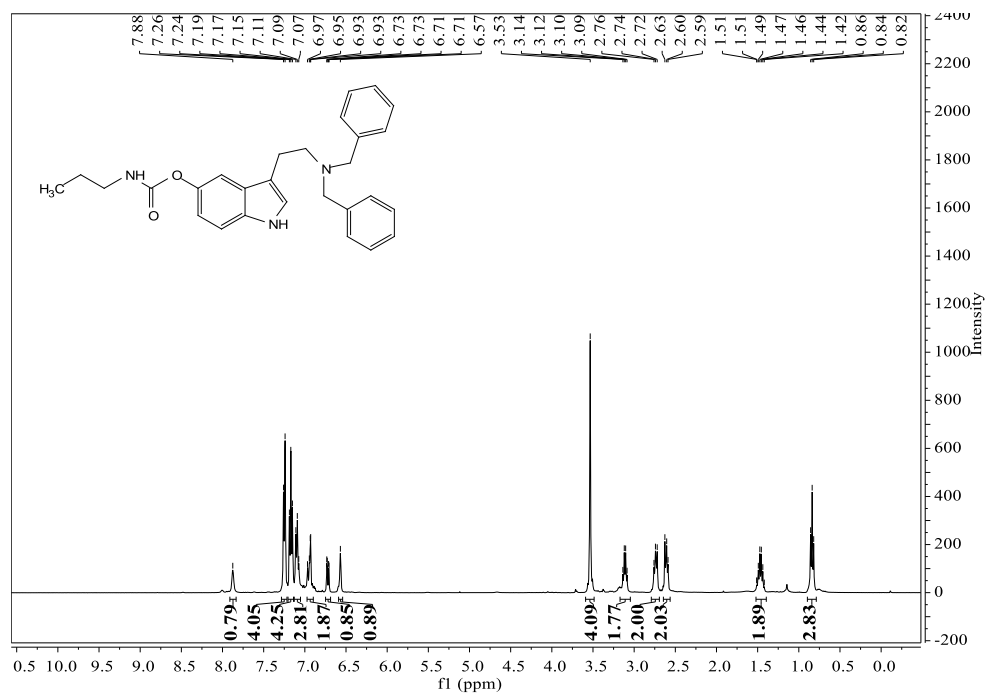
HPLC results of synthesized compounds

HRMS spectras of synthesized compounds

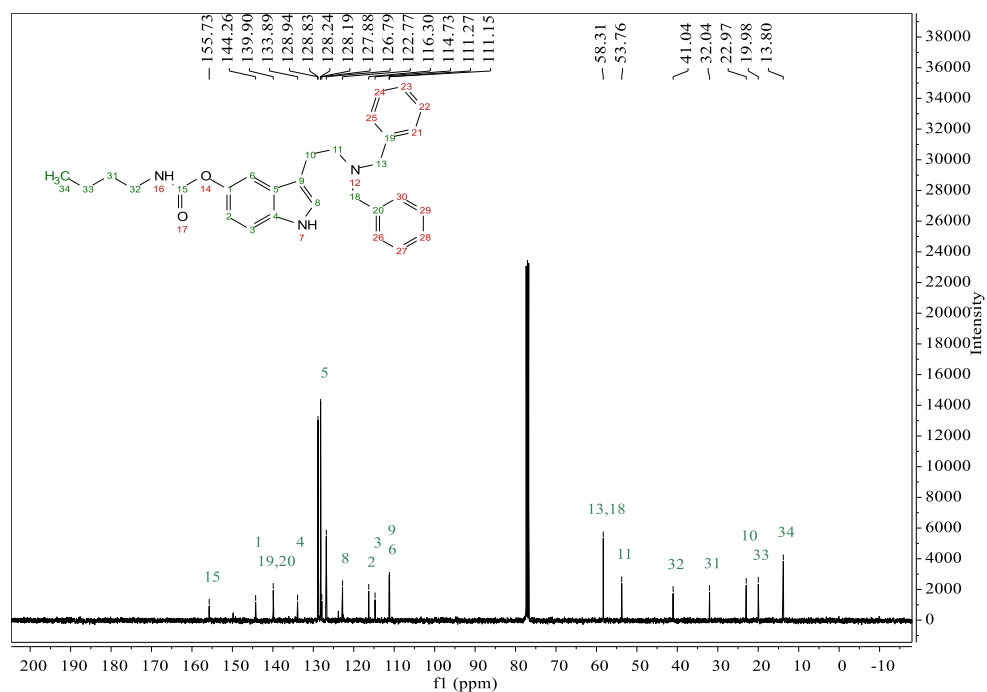
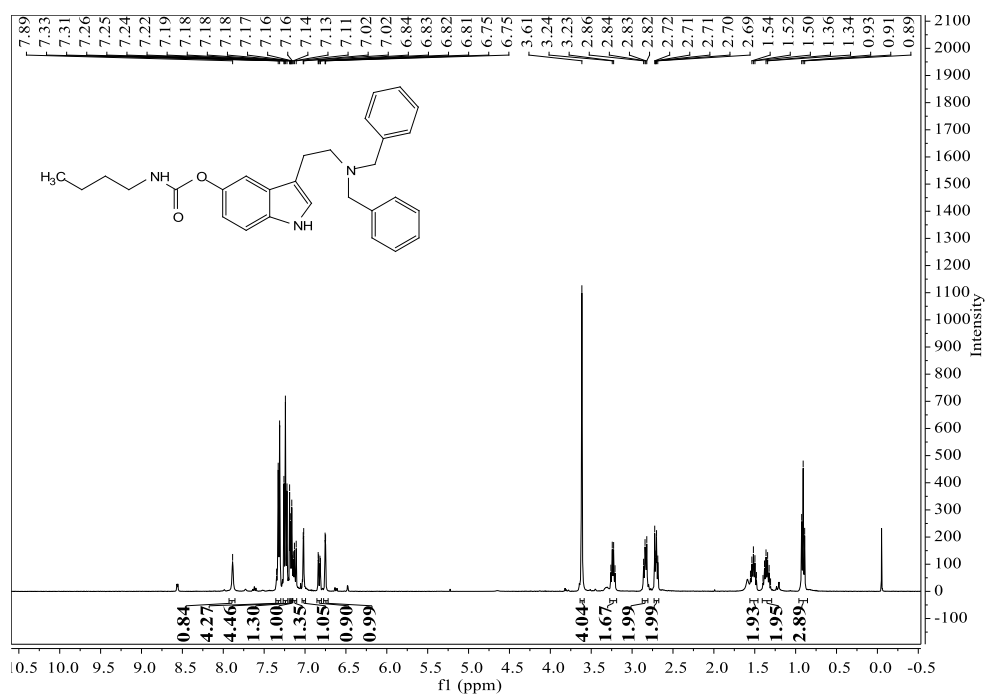
Molecular Formula Strings of synthesized compounds

¹H NMR and ¹³C NMR of synthesized compounds

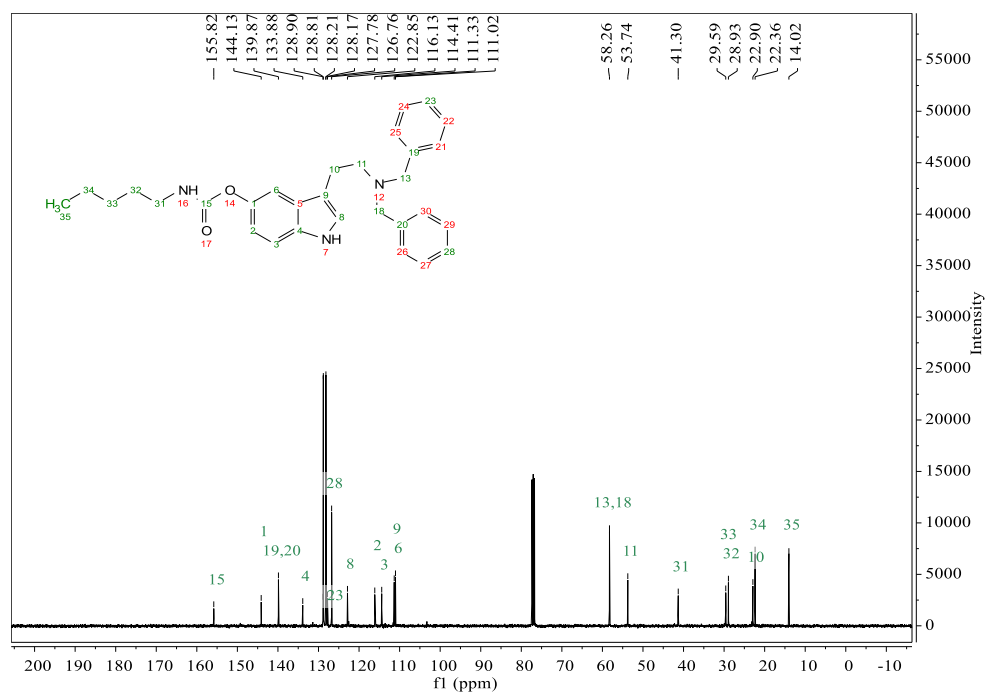
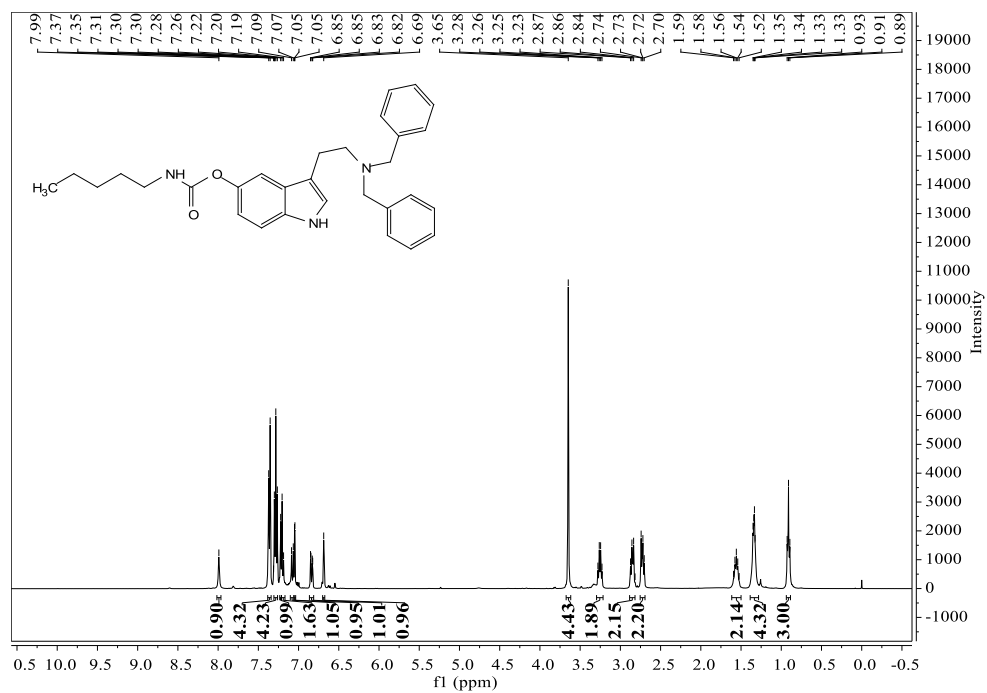
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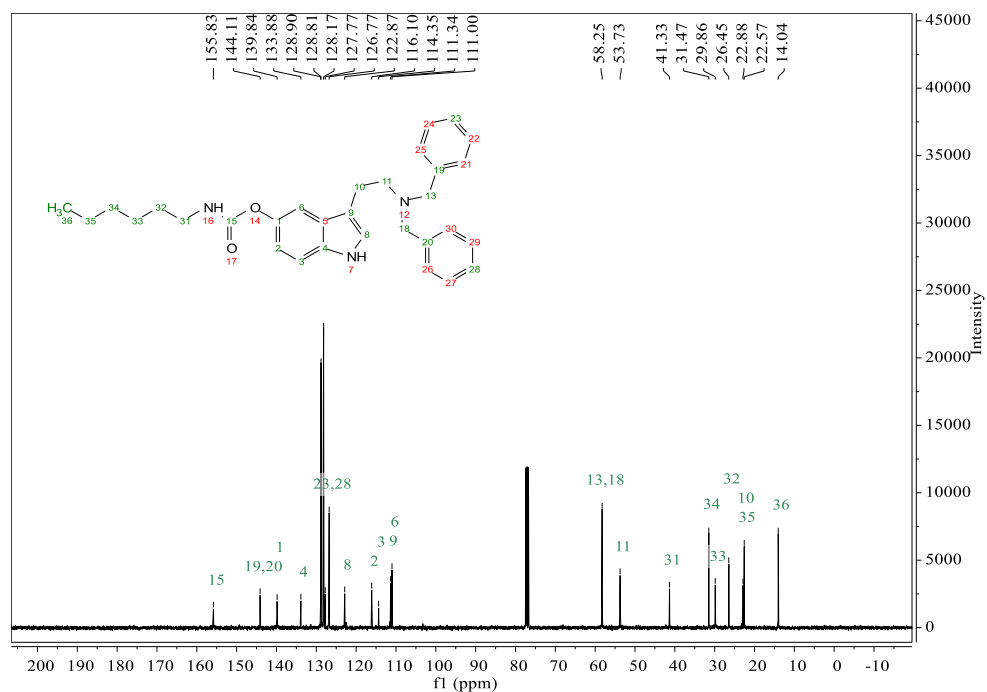
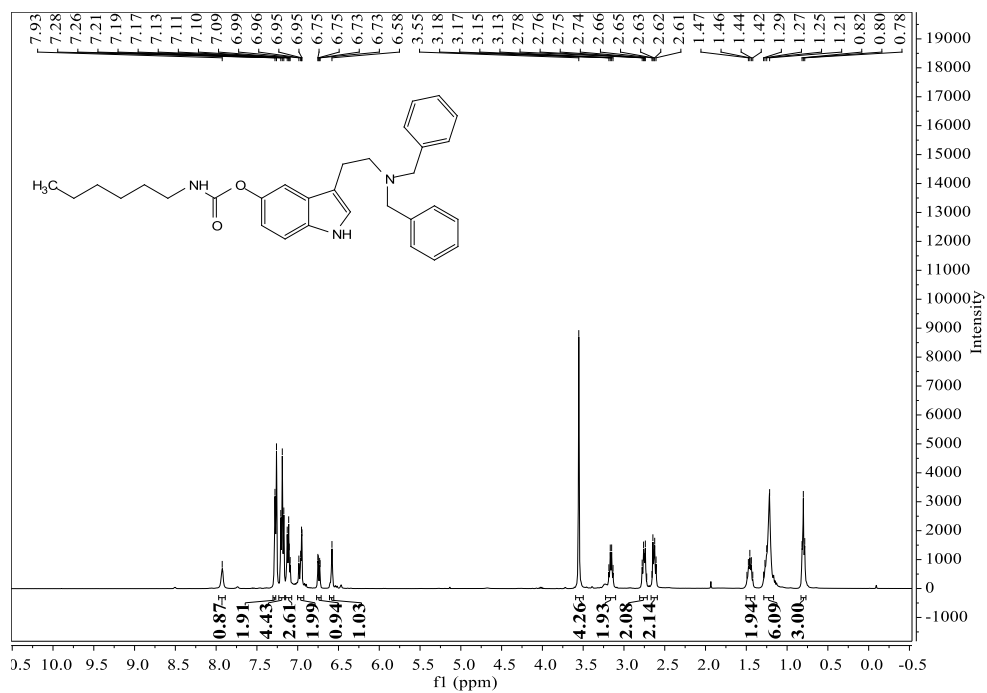
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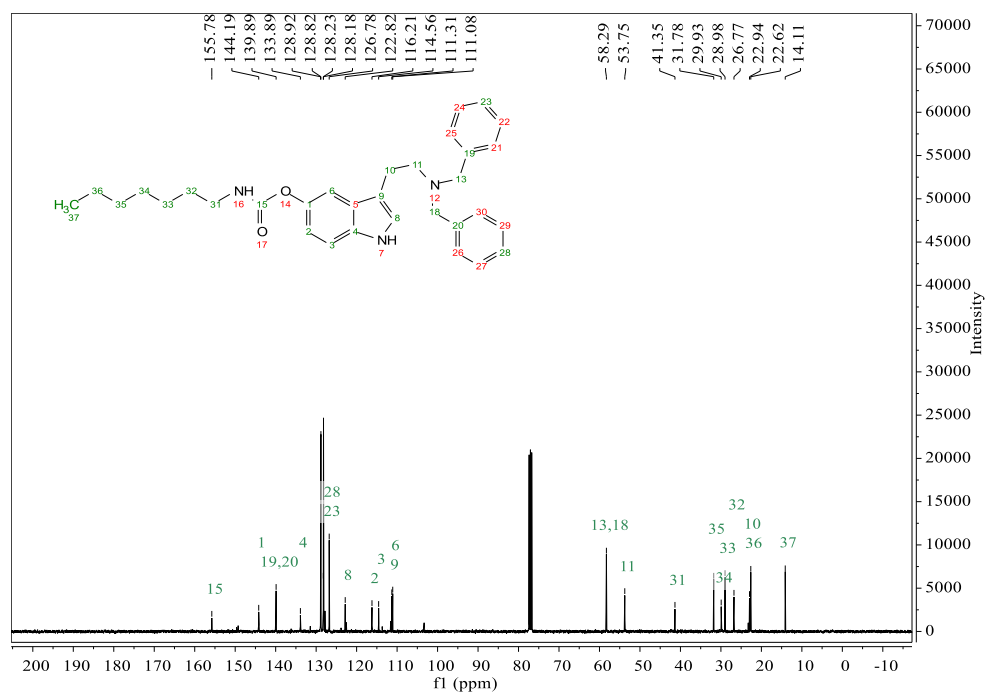
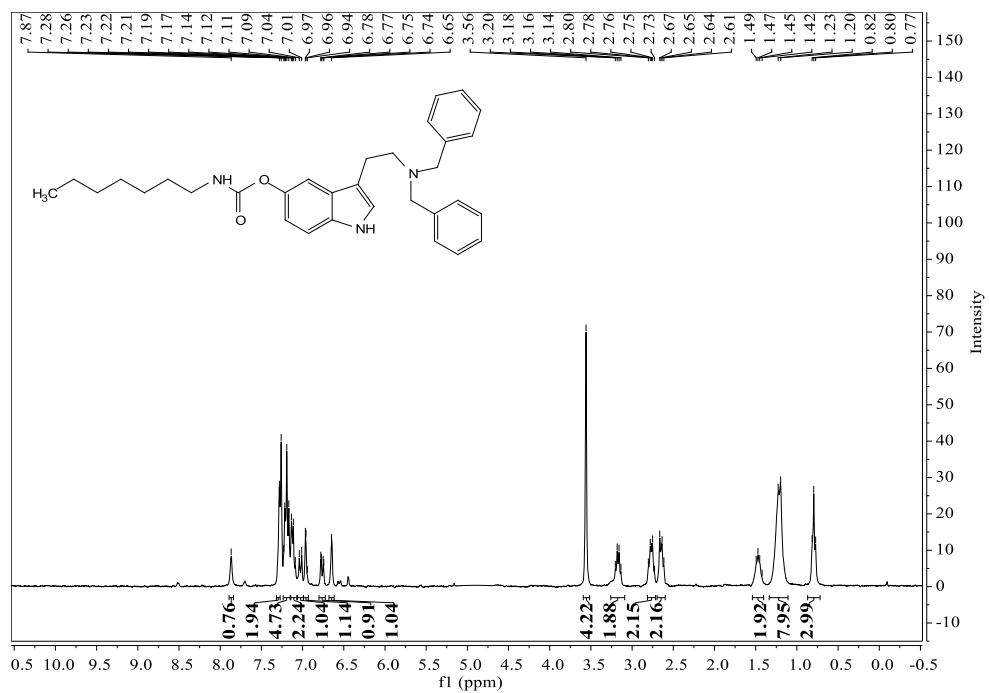
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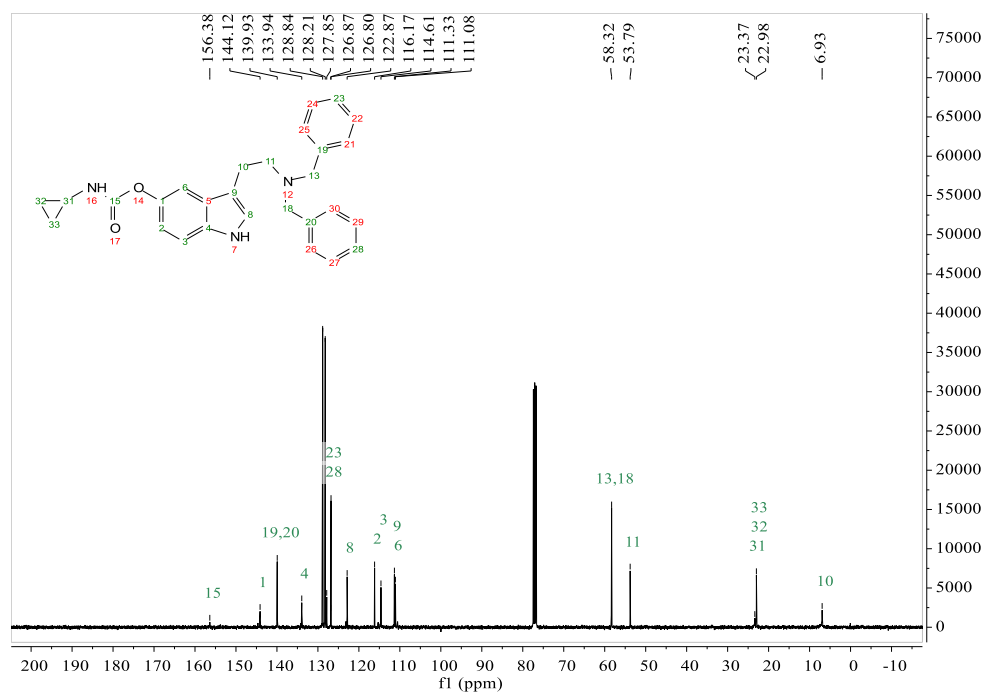
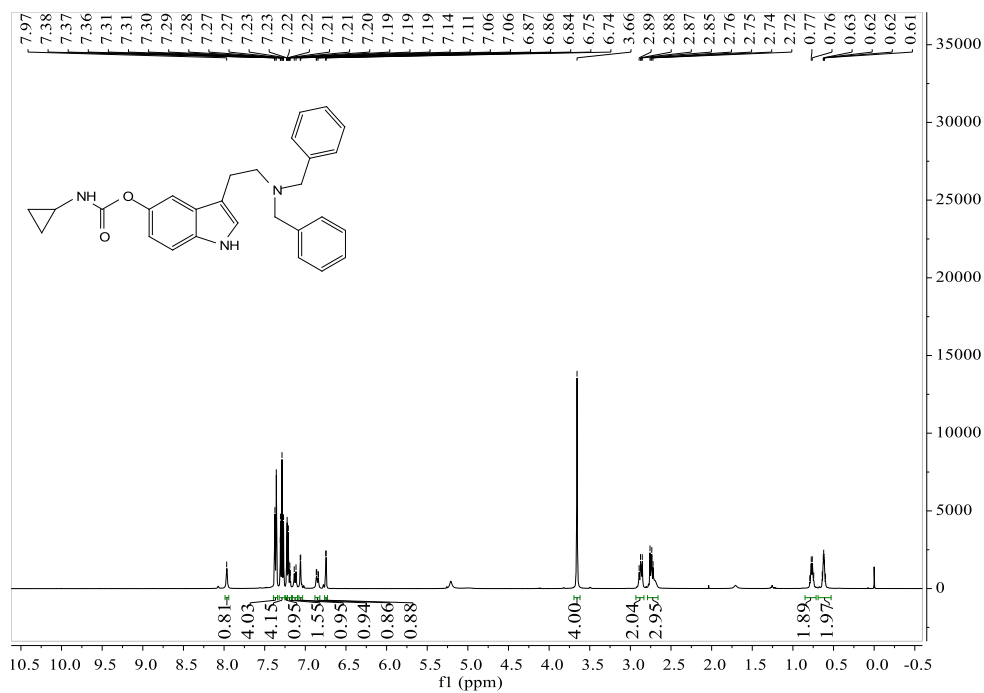
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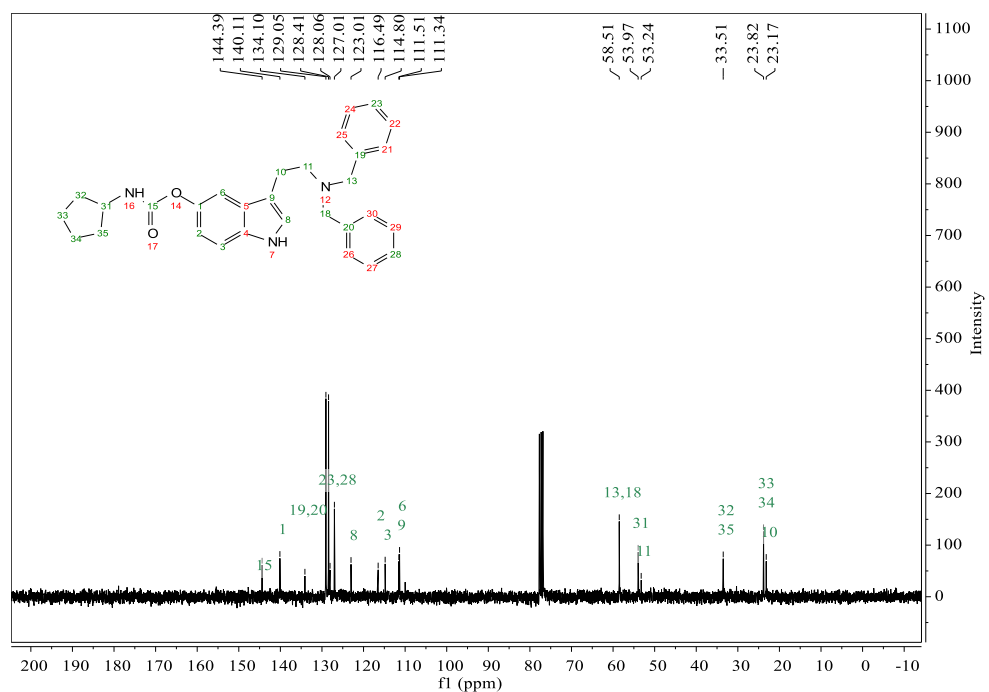
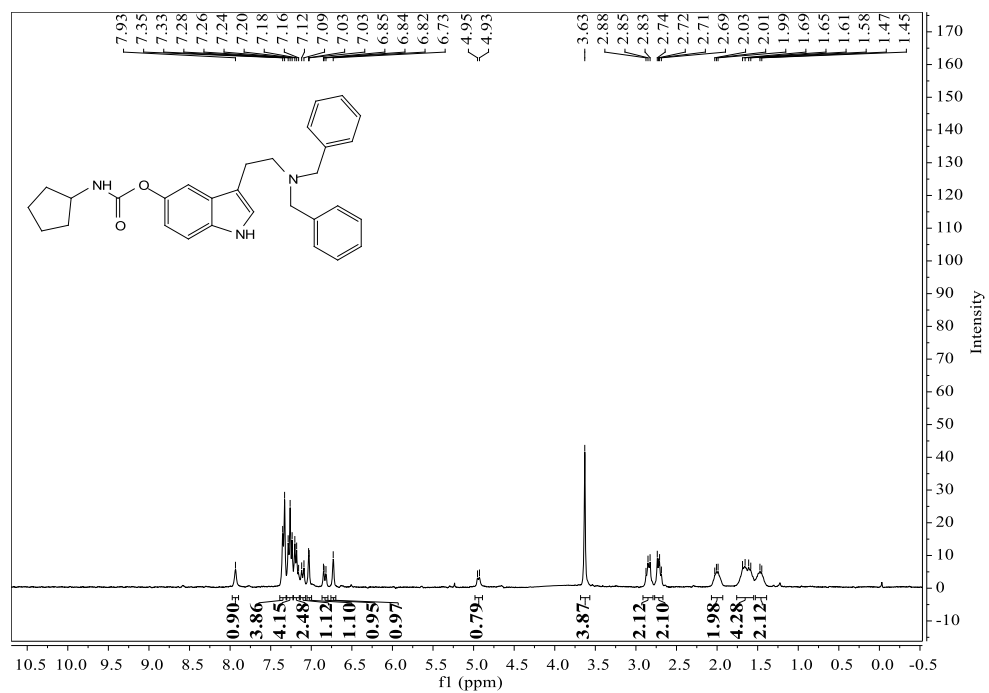
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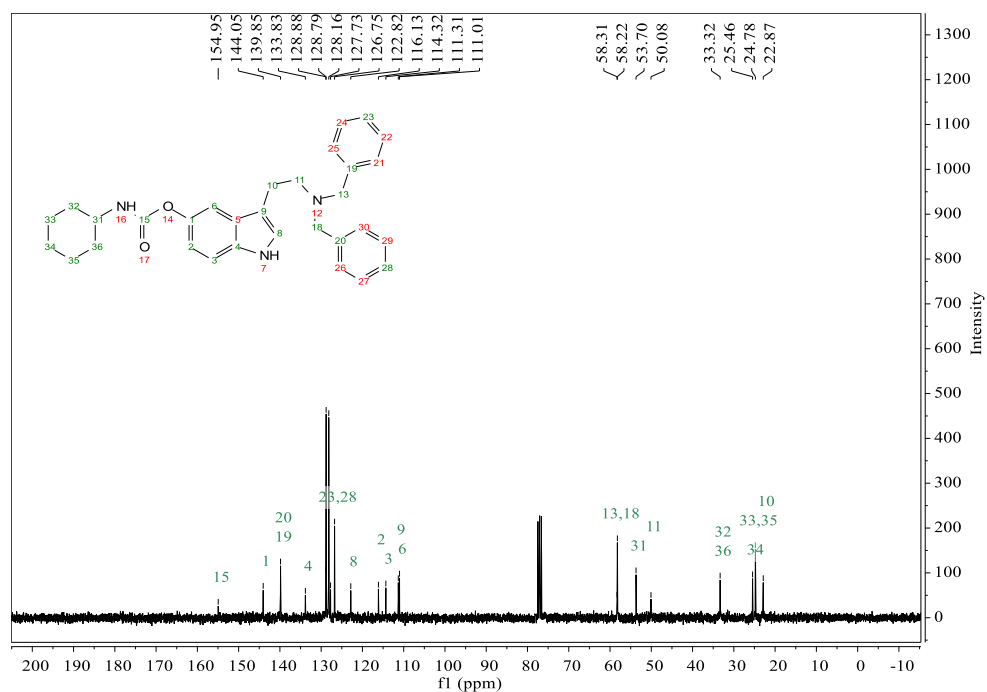
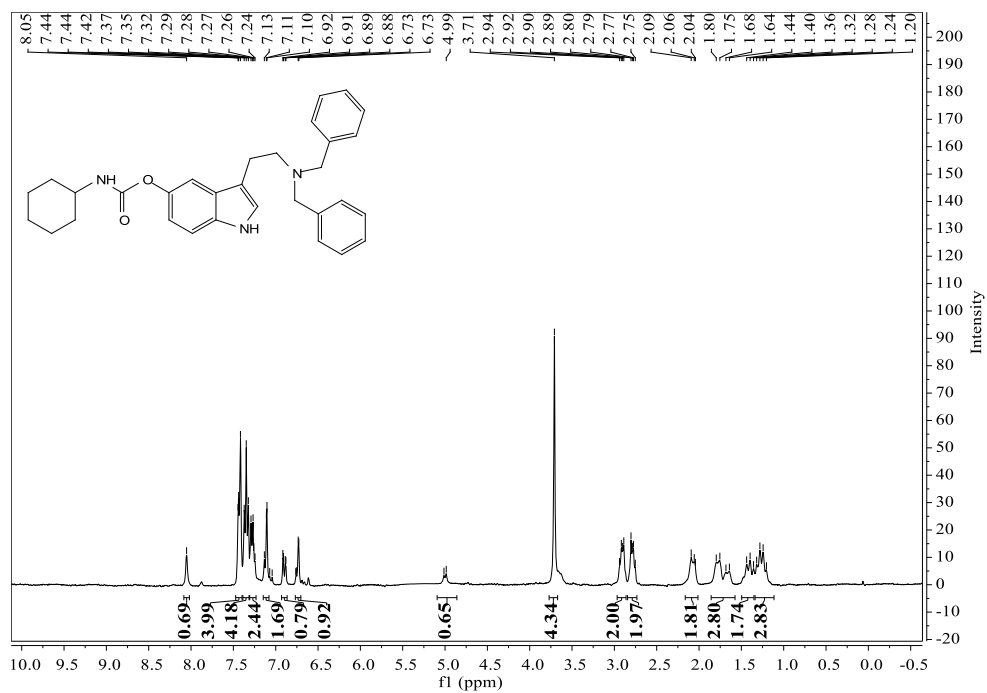
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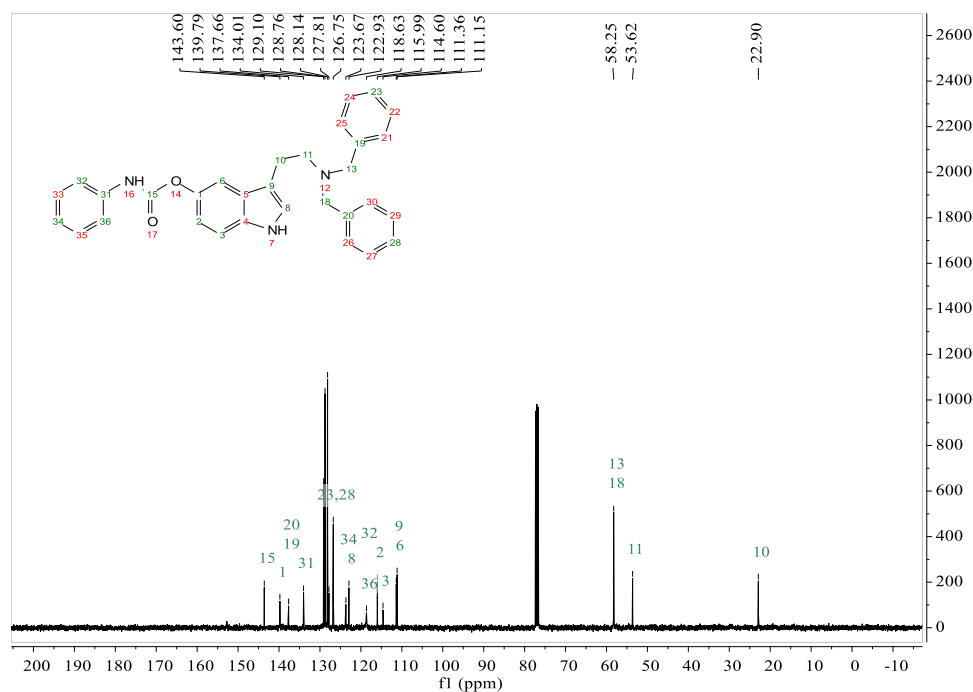
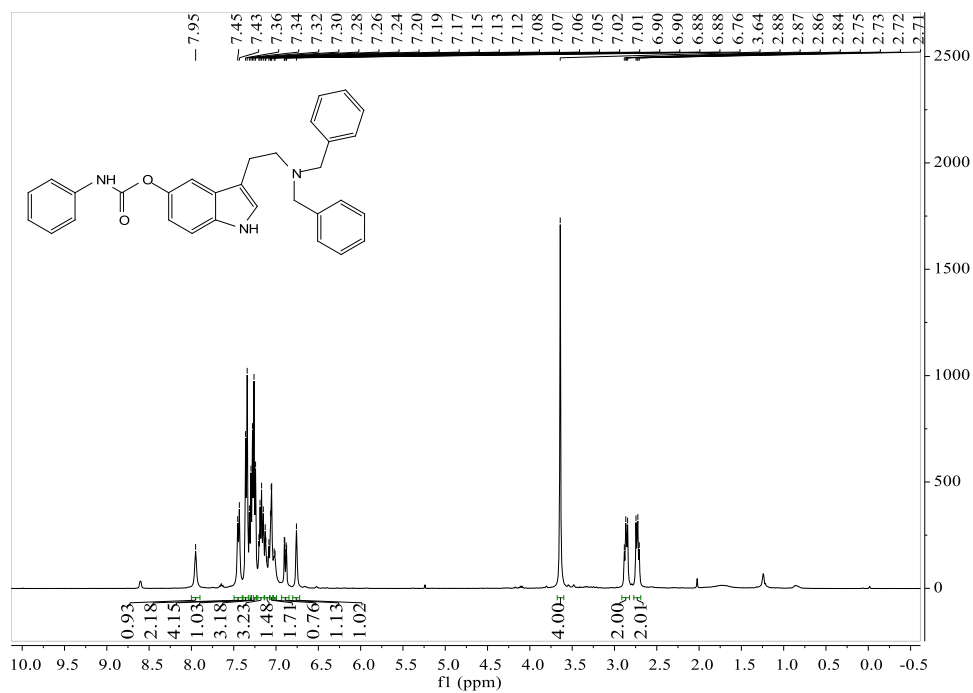
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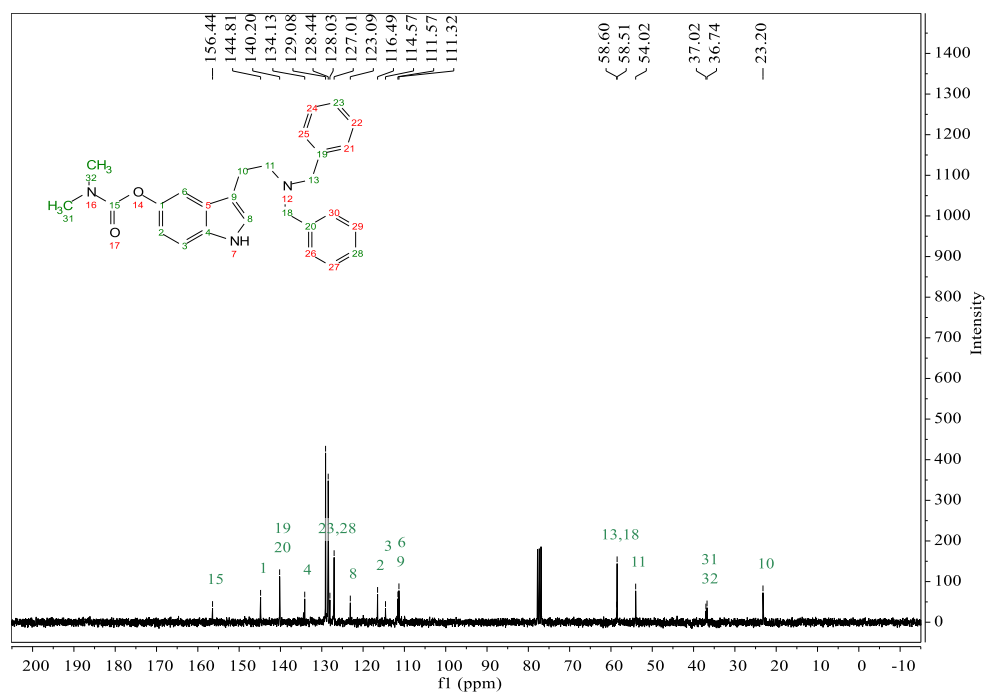
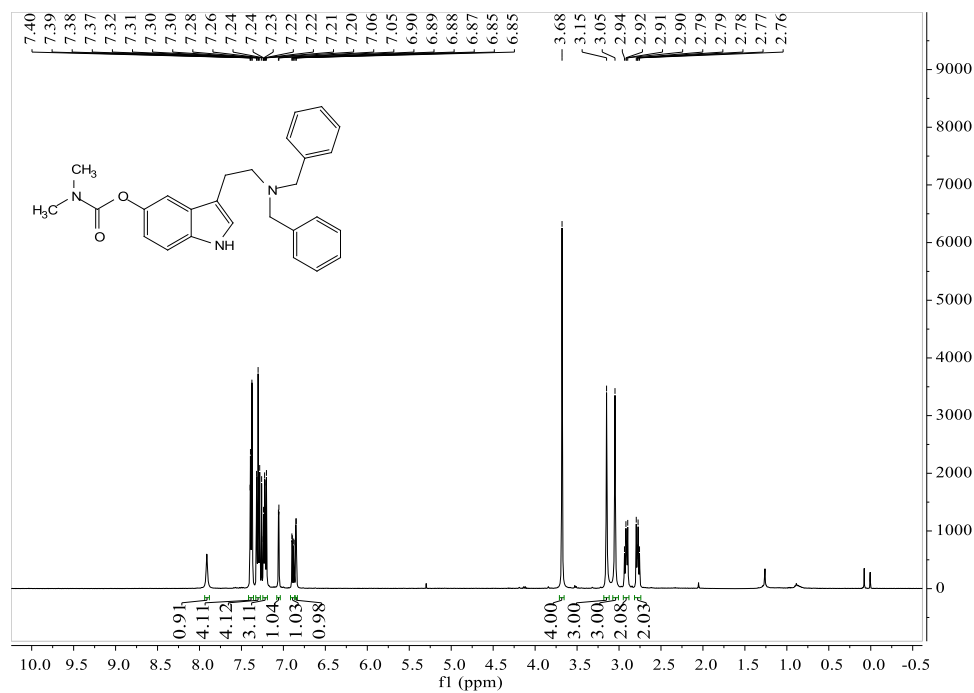
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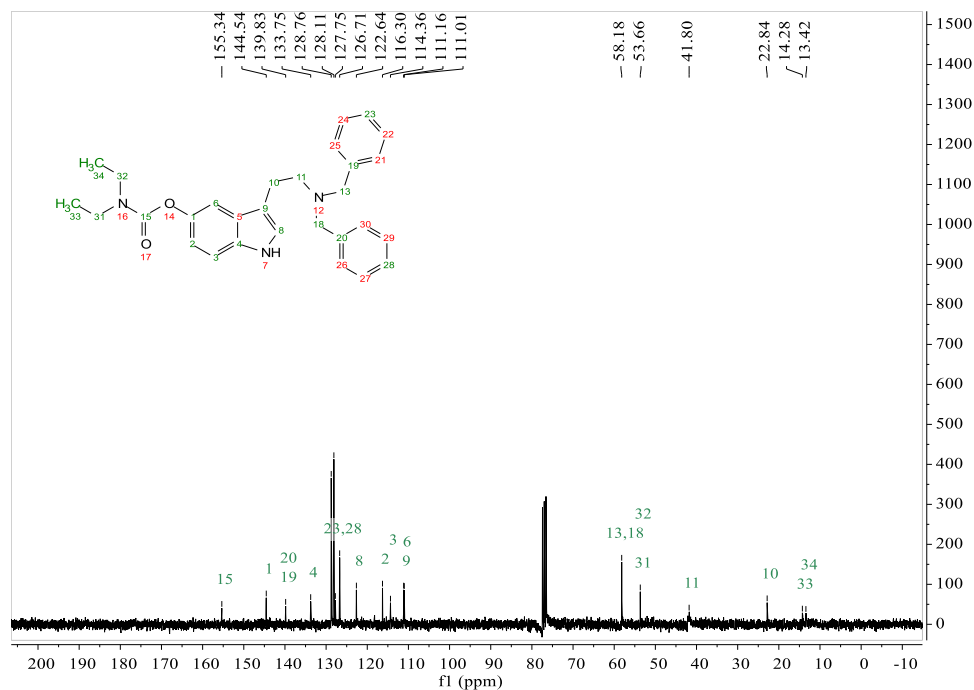
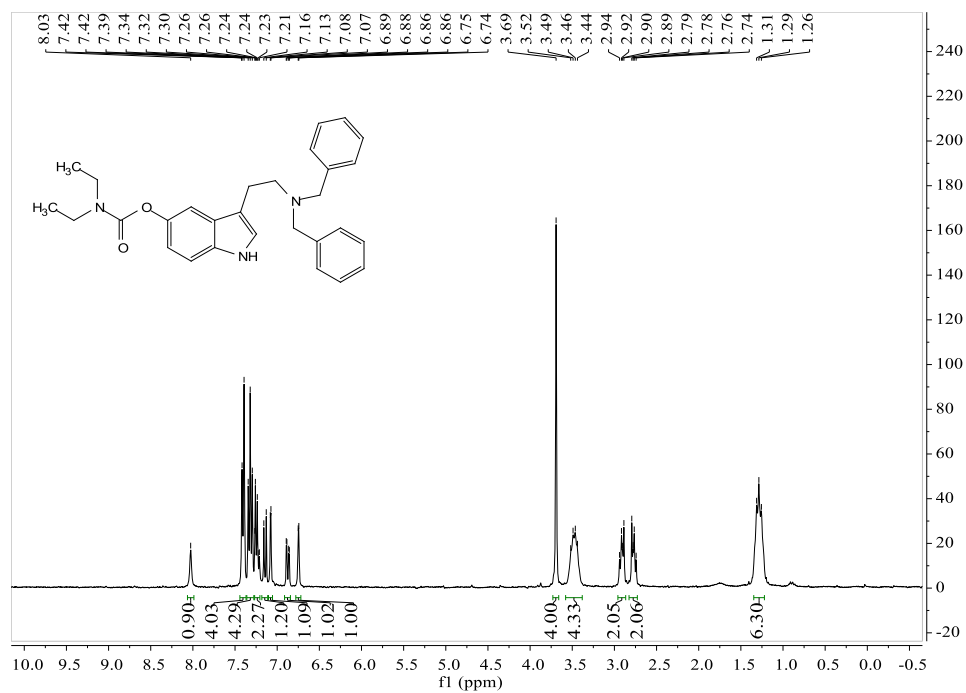
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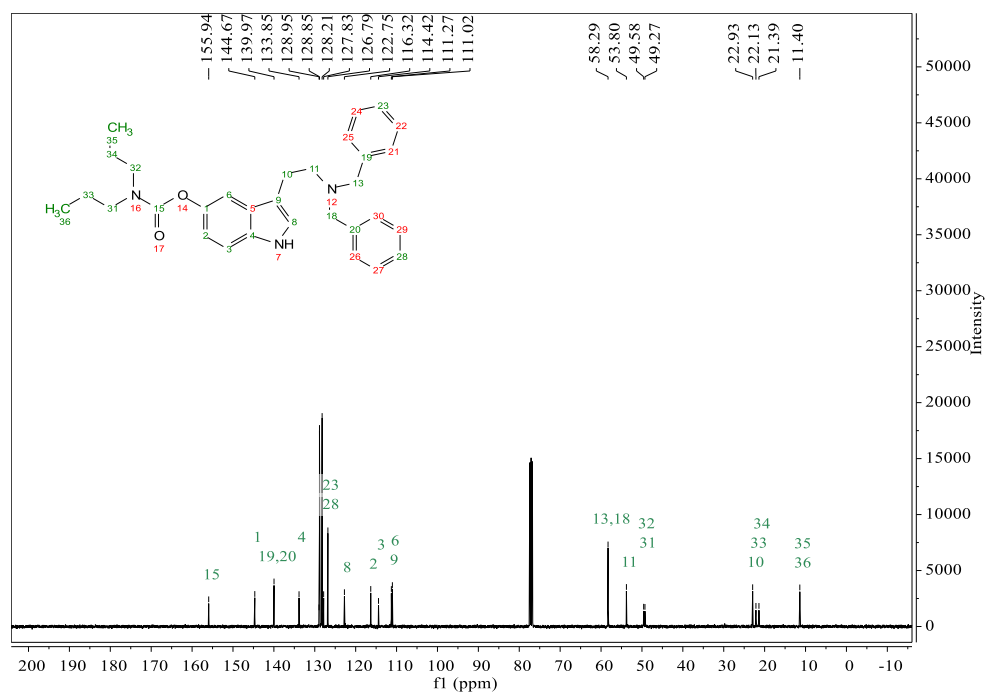
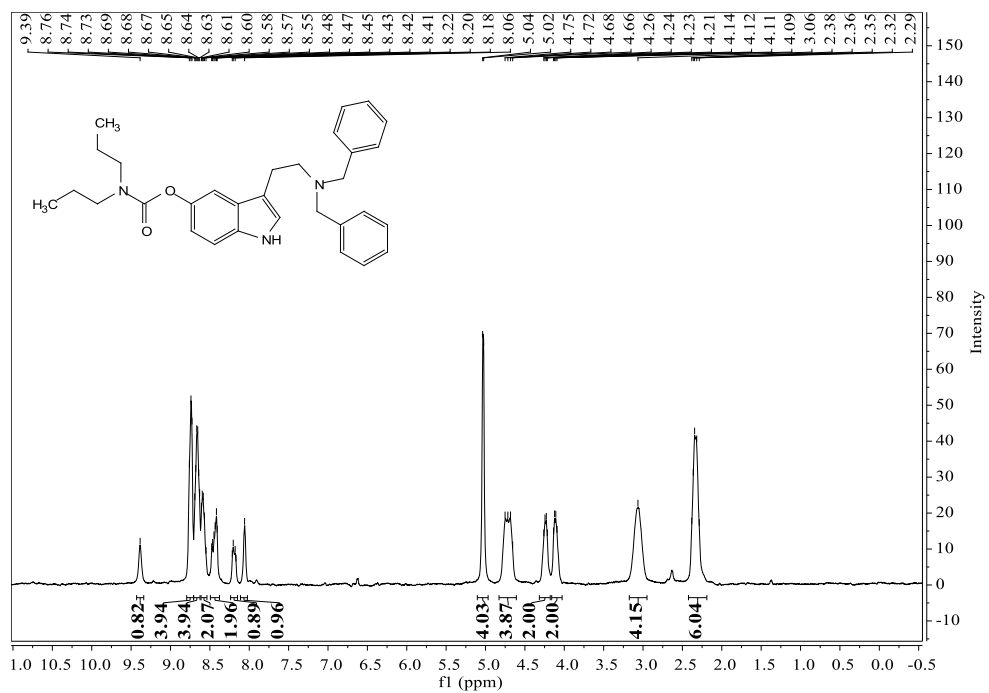
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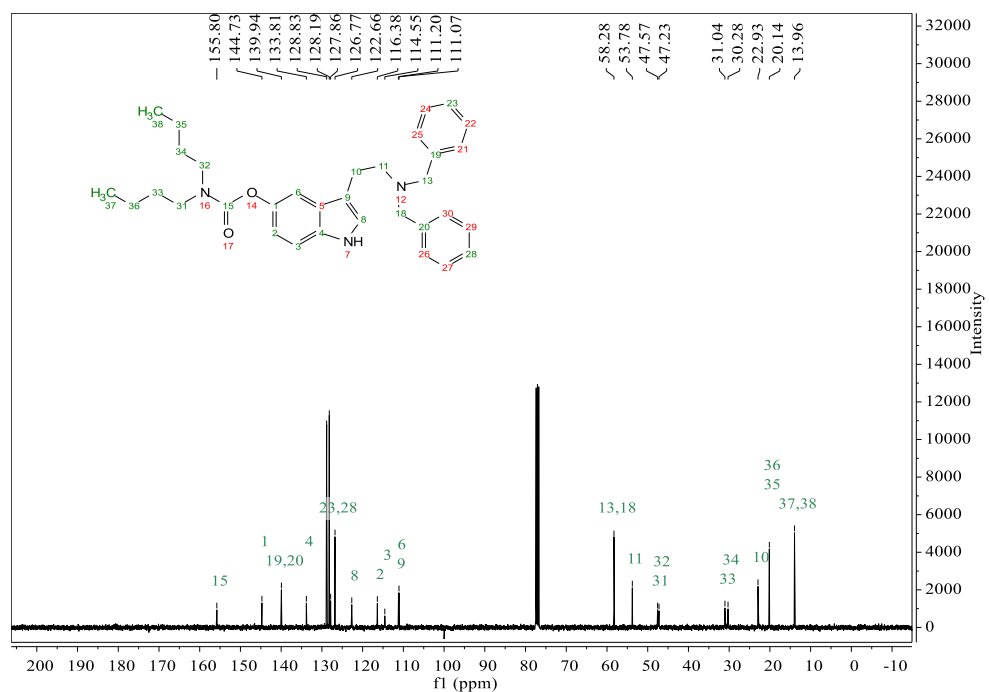
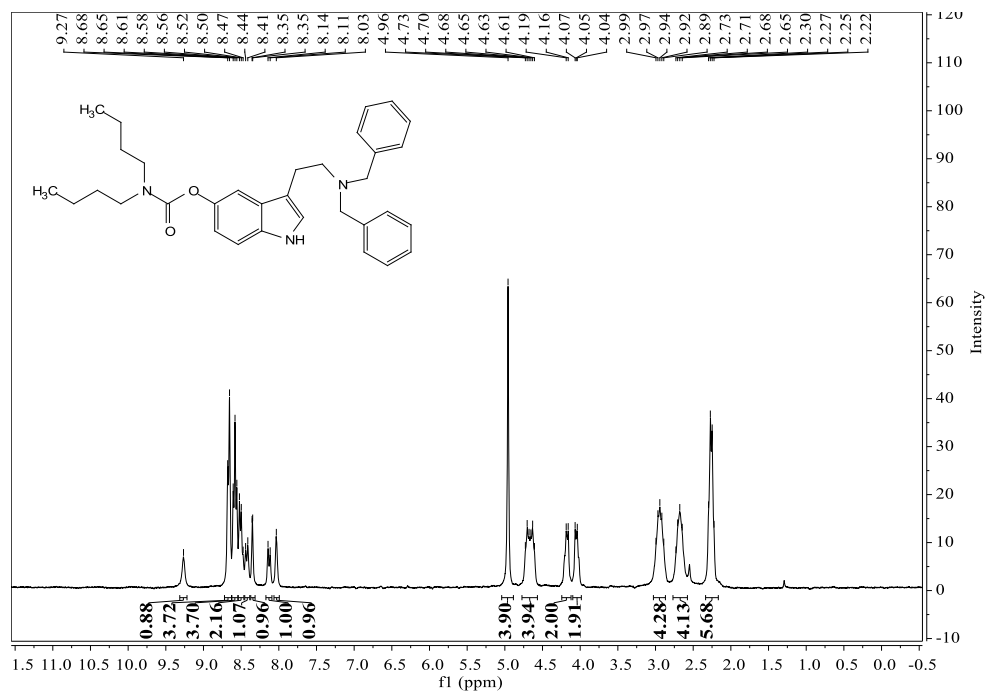
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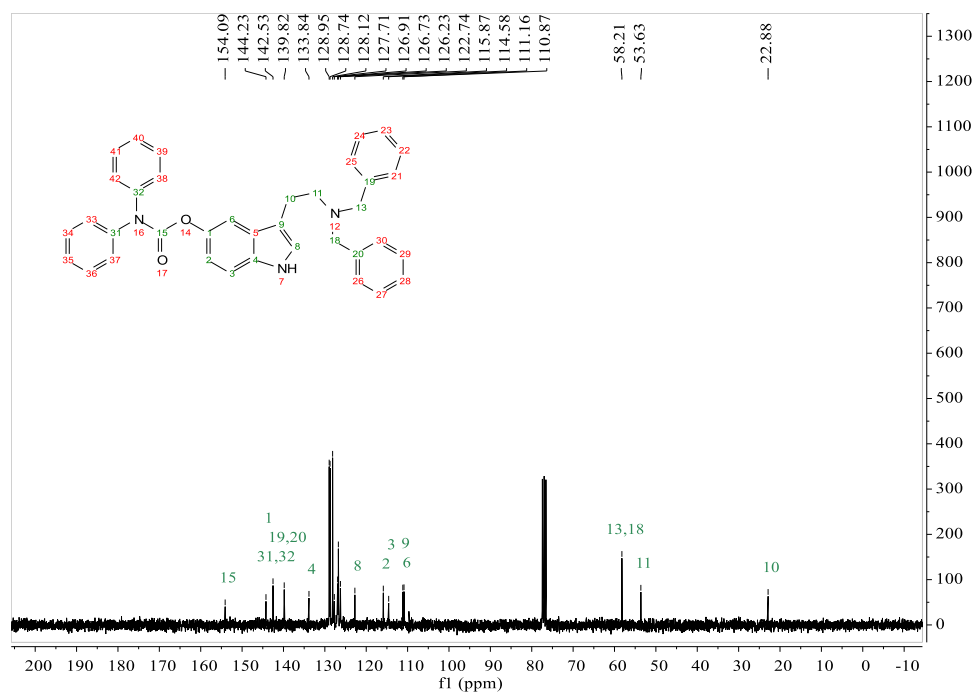
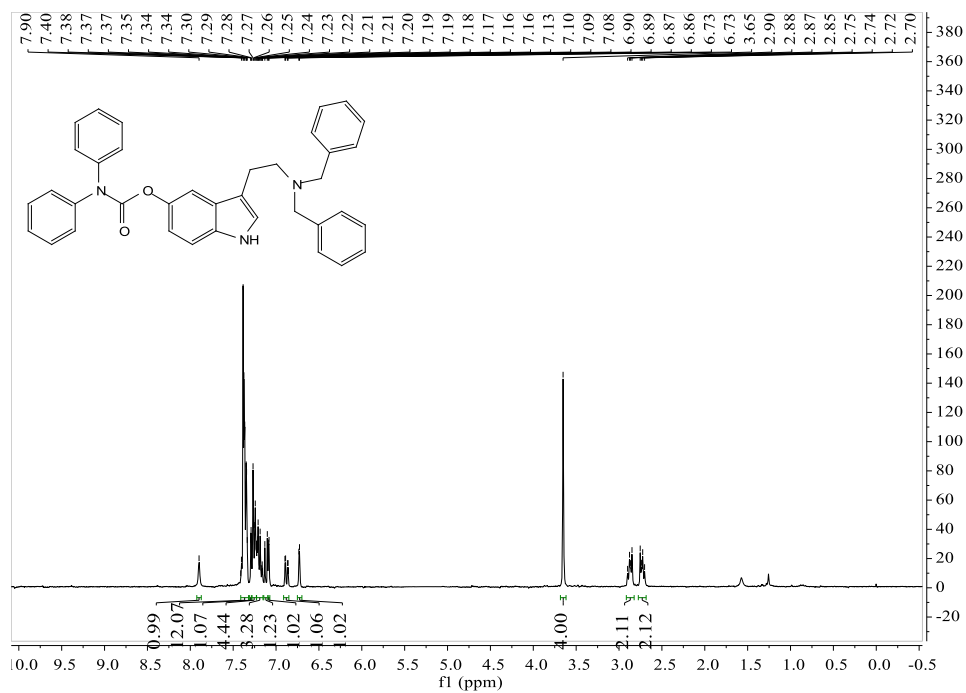
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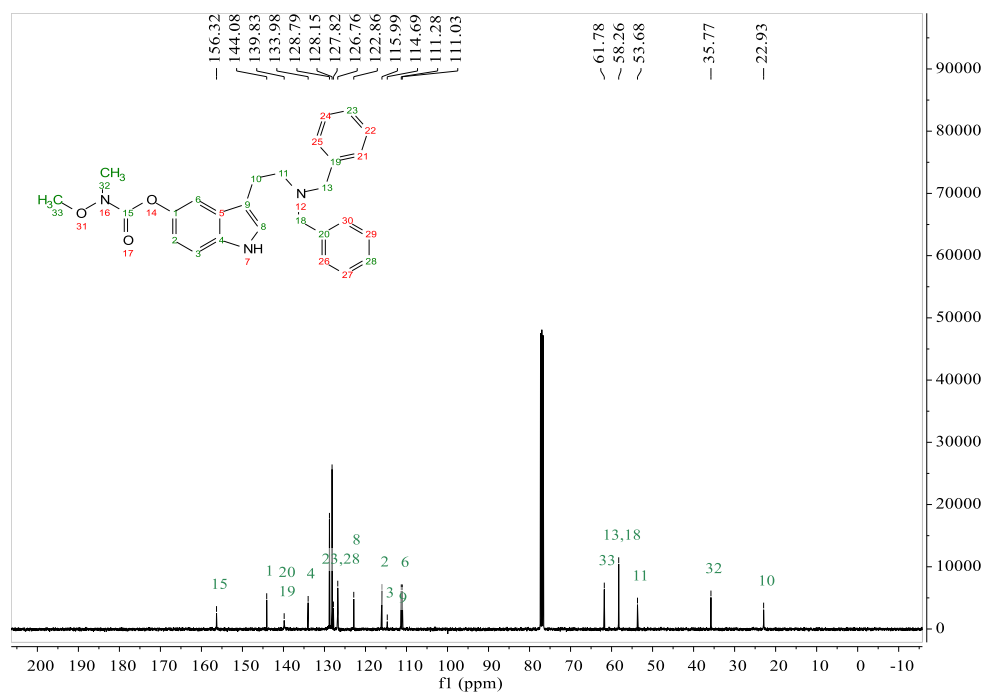
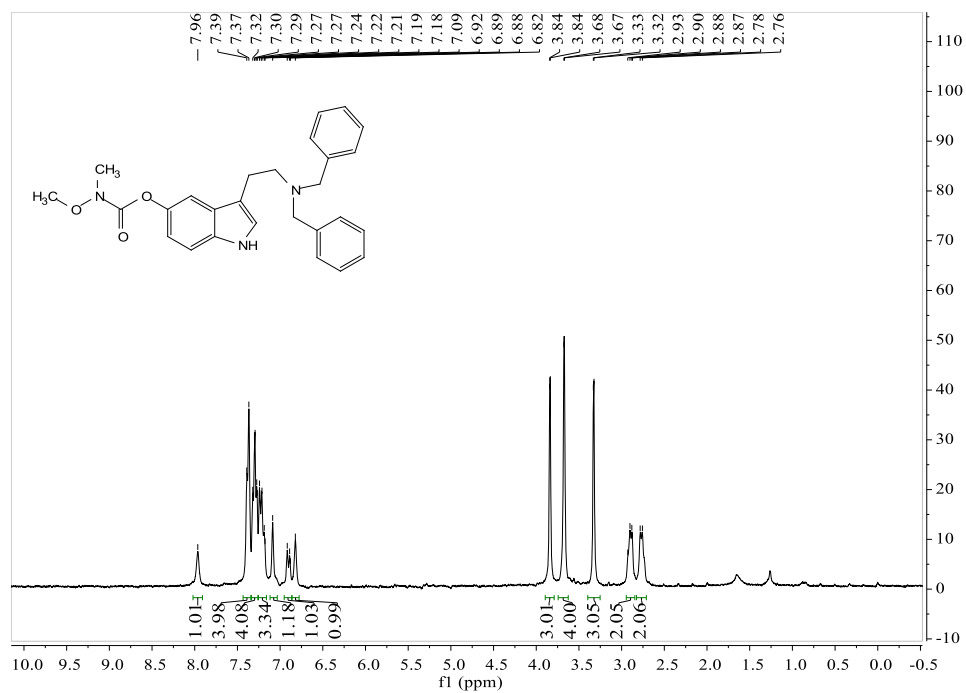
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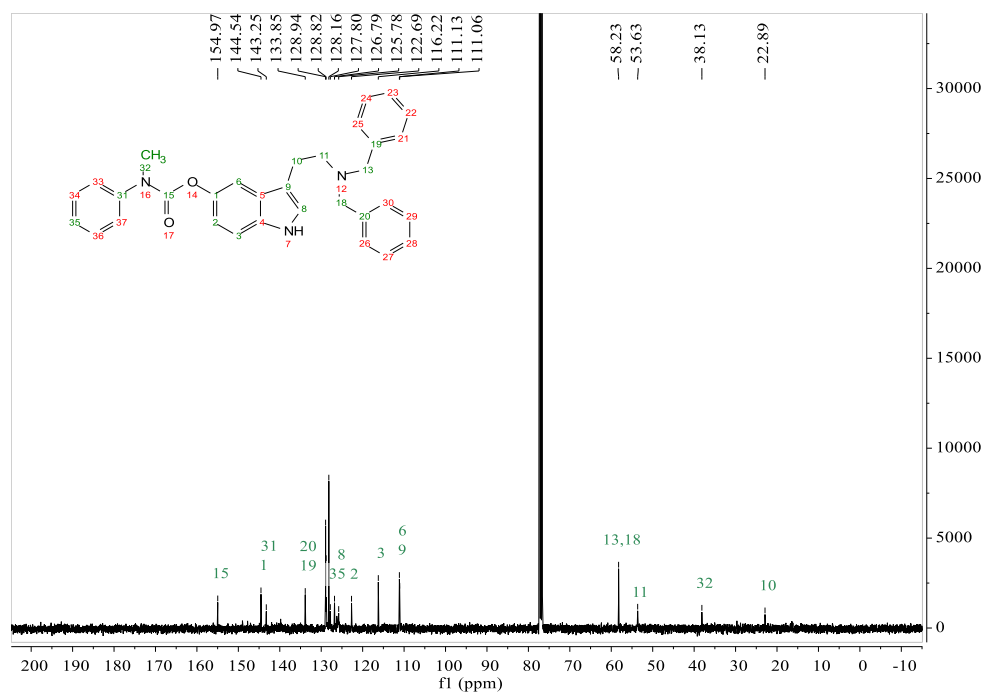
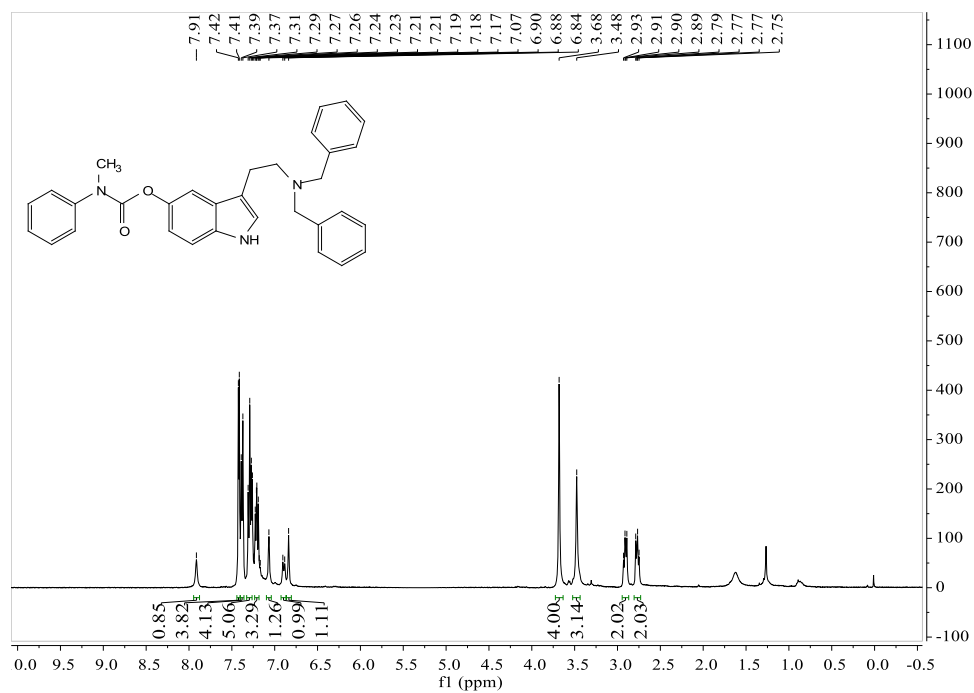
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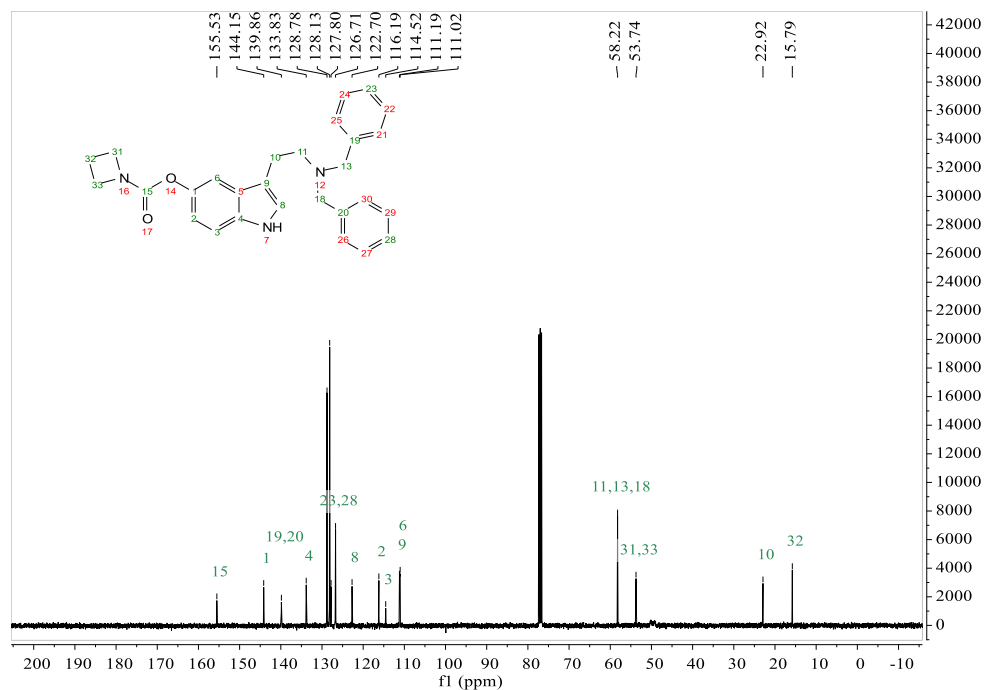
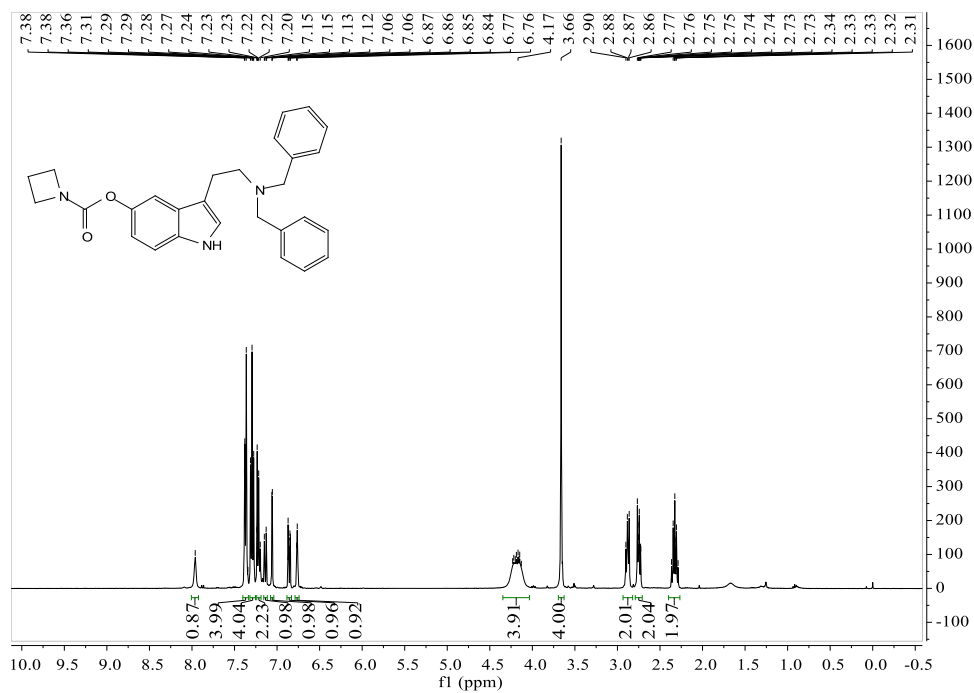
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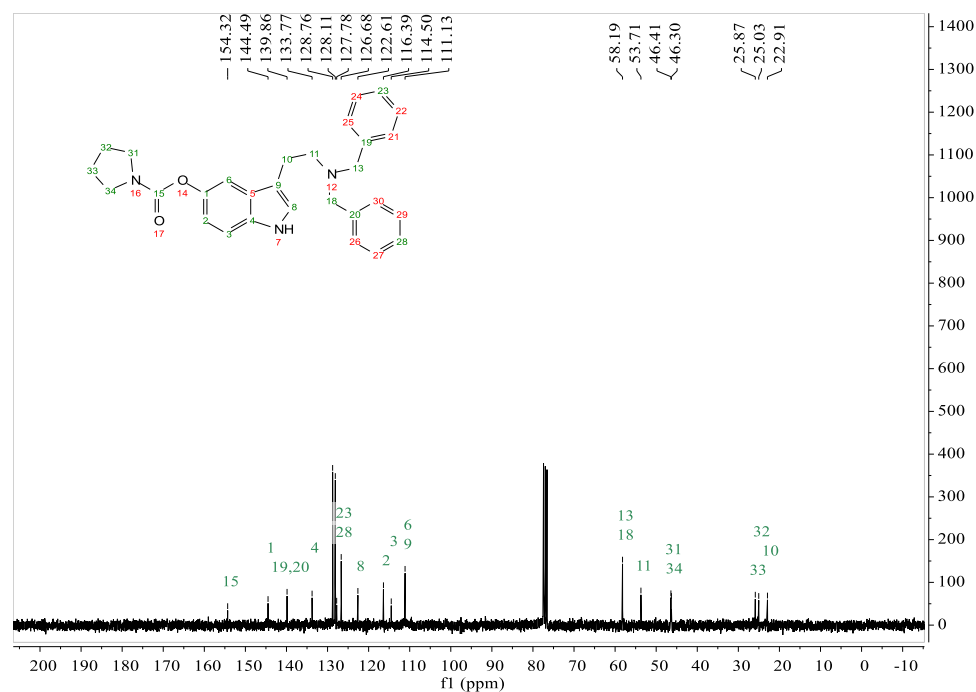
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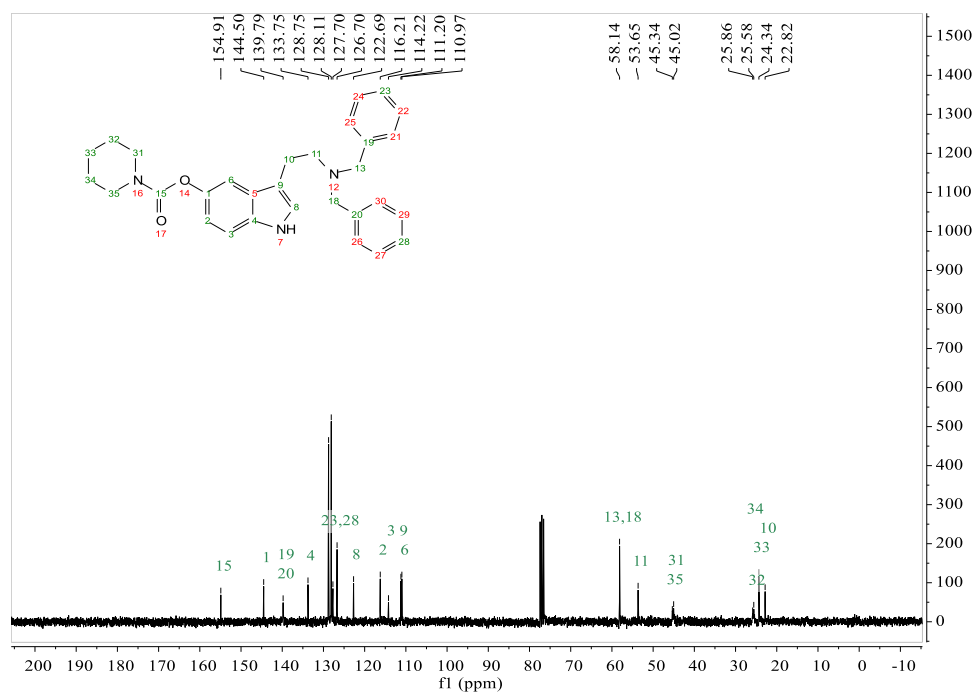
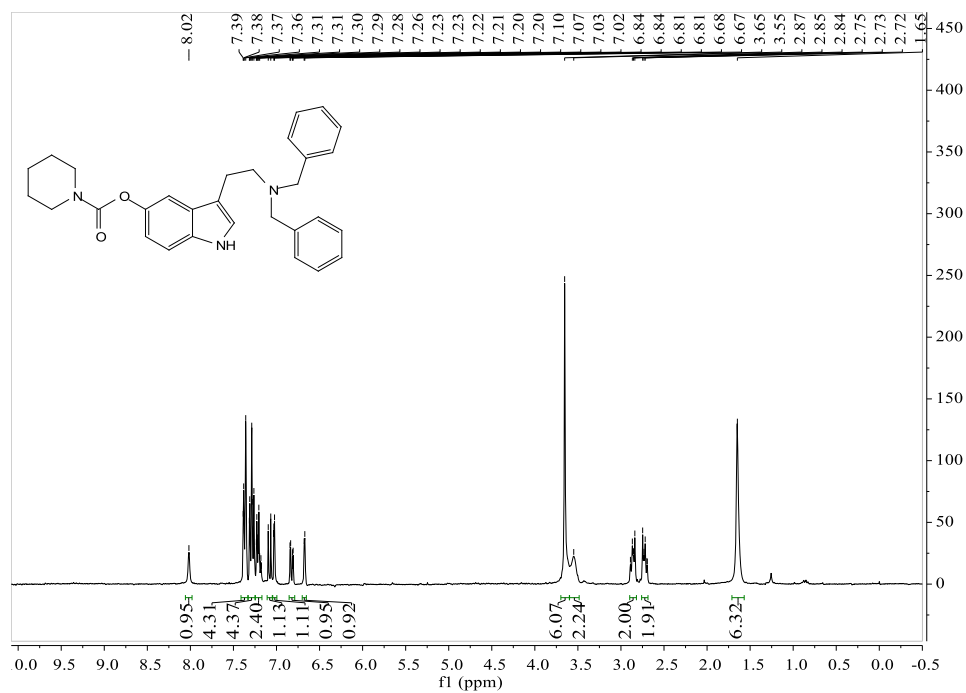
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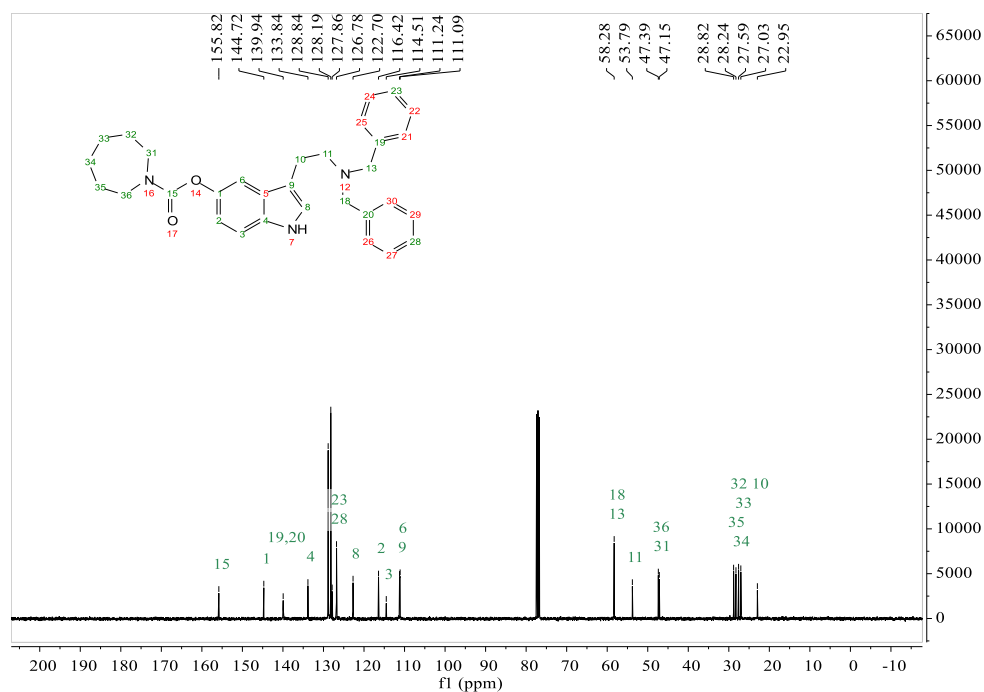
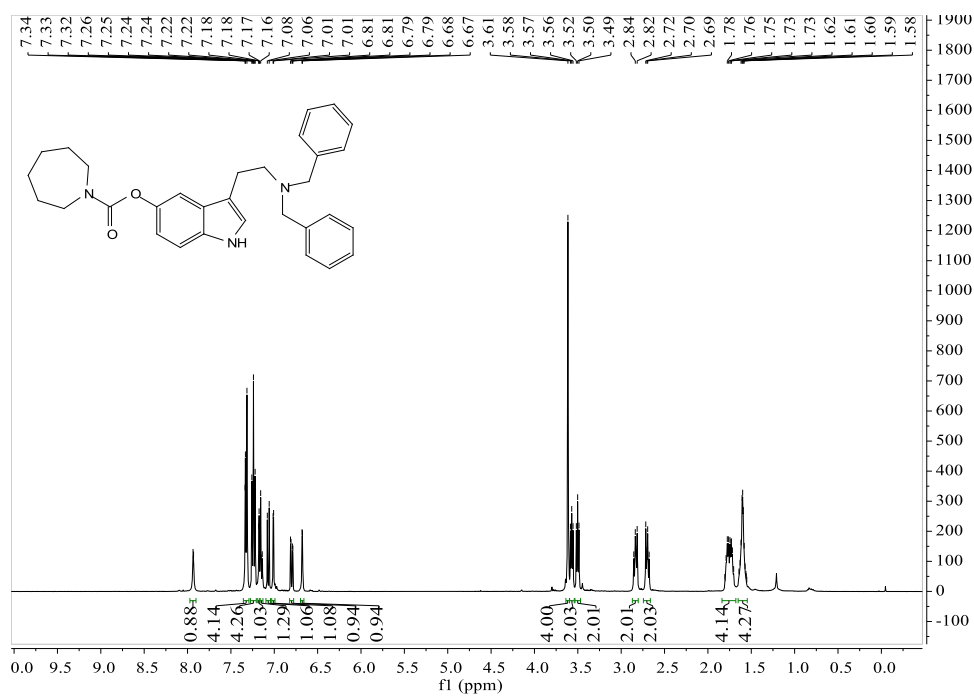
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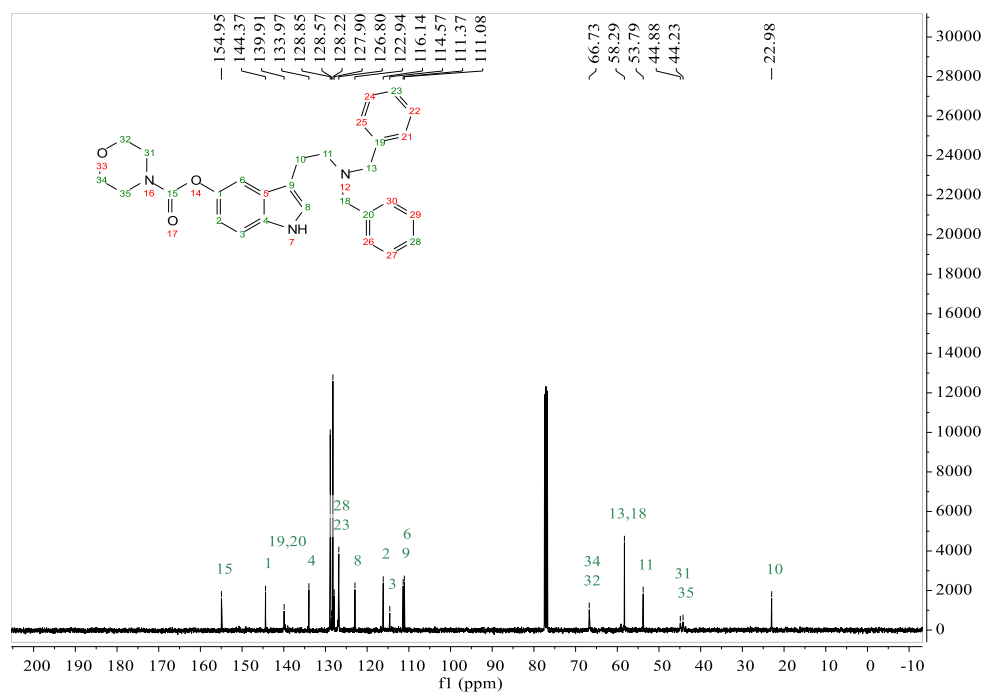
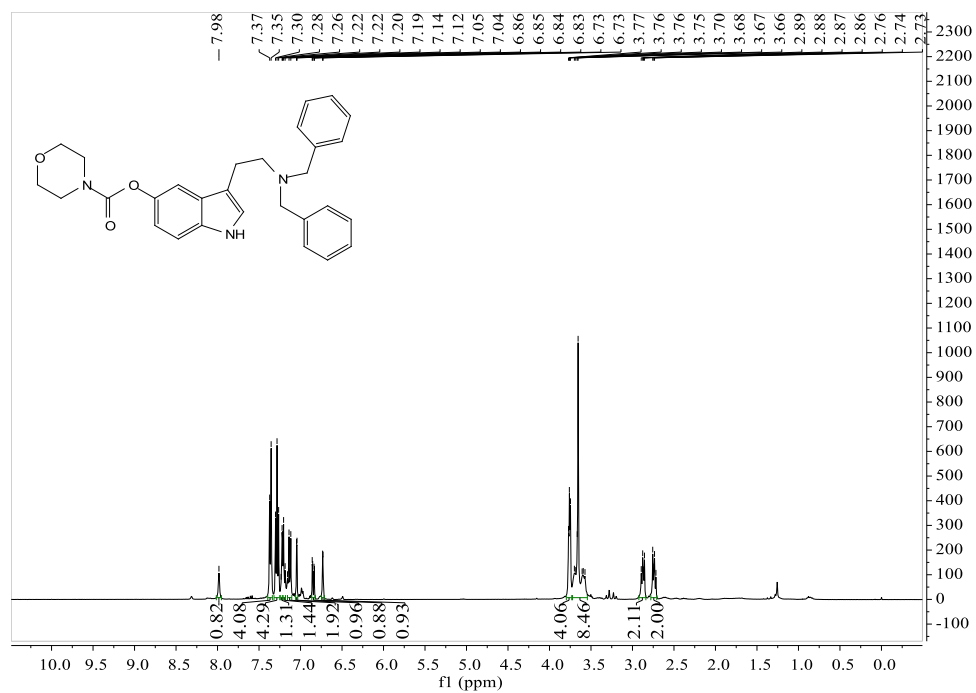
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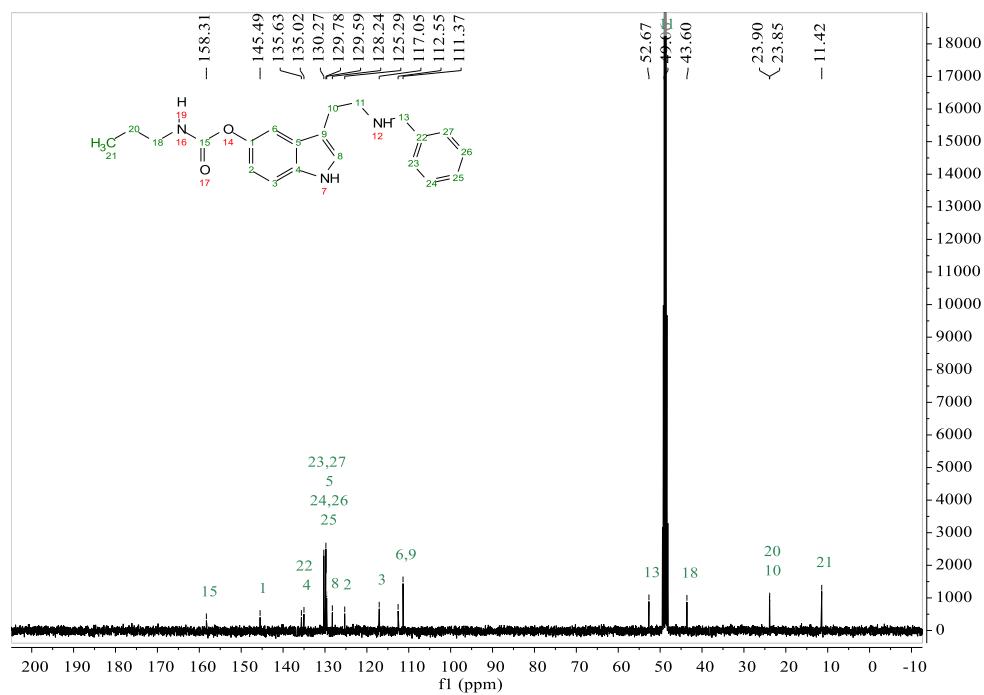
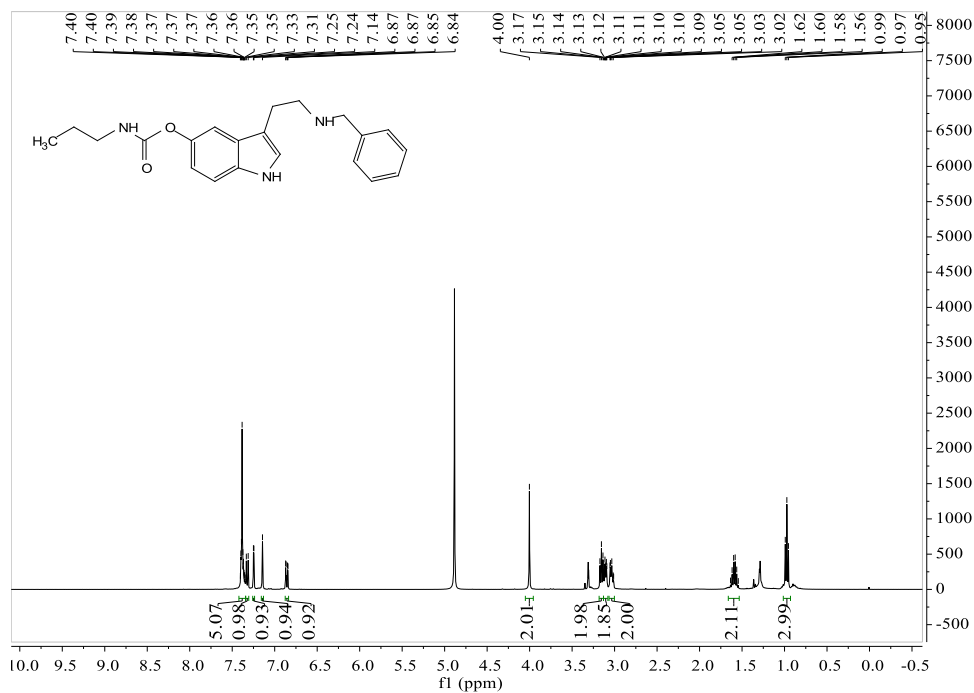
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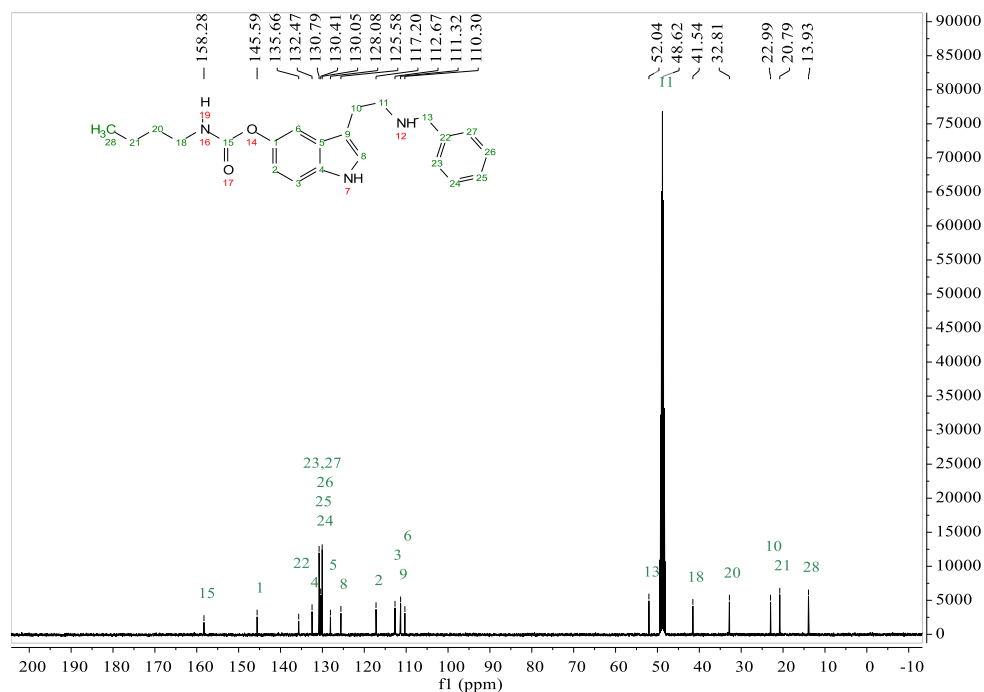
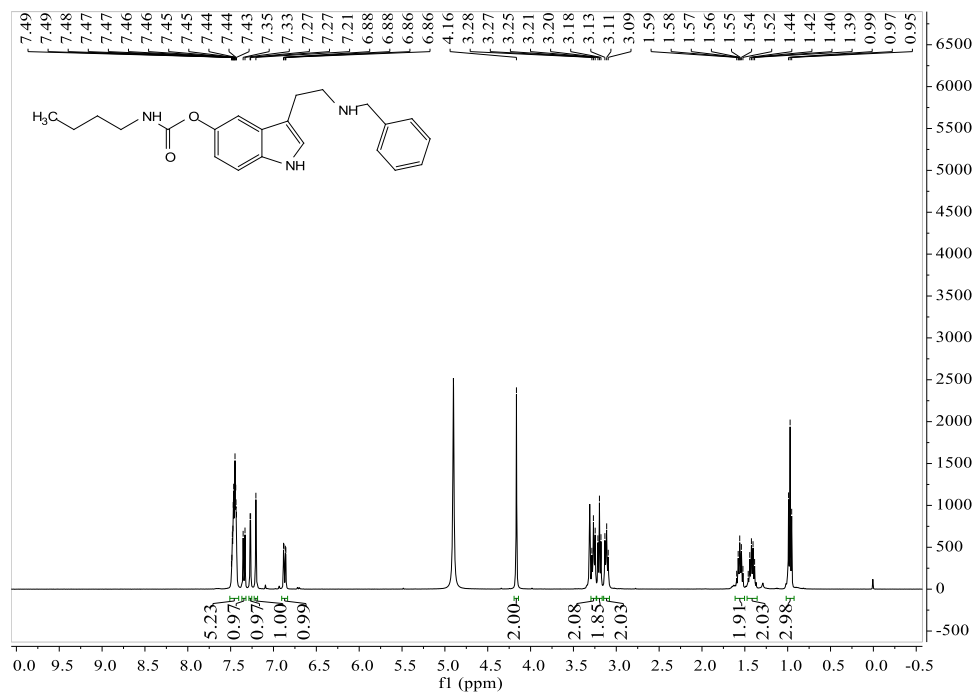
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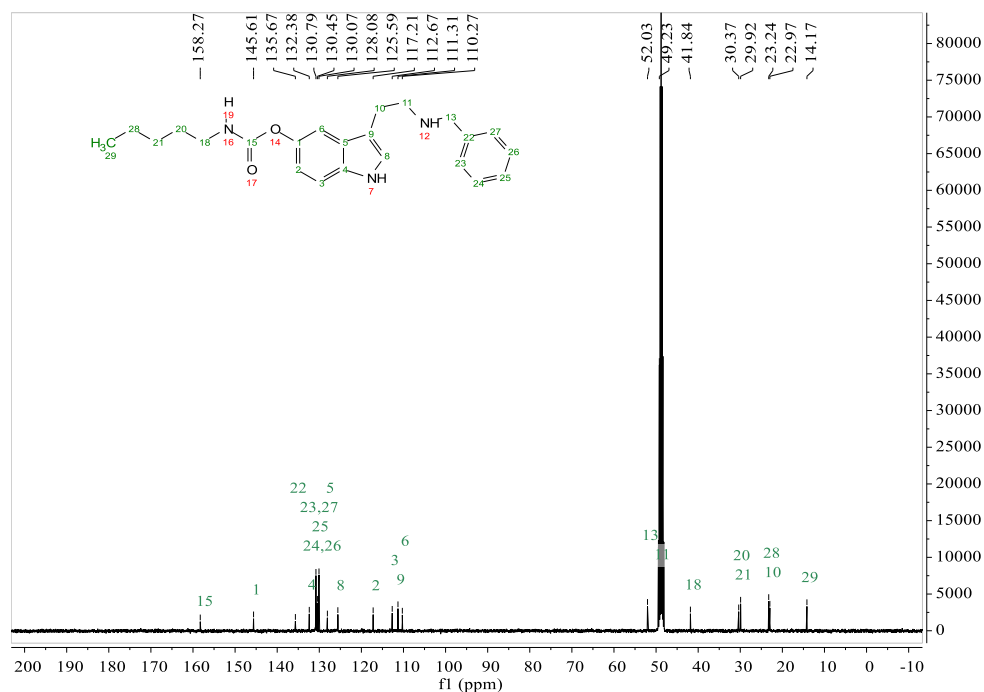
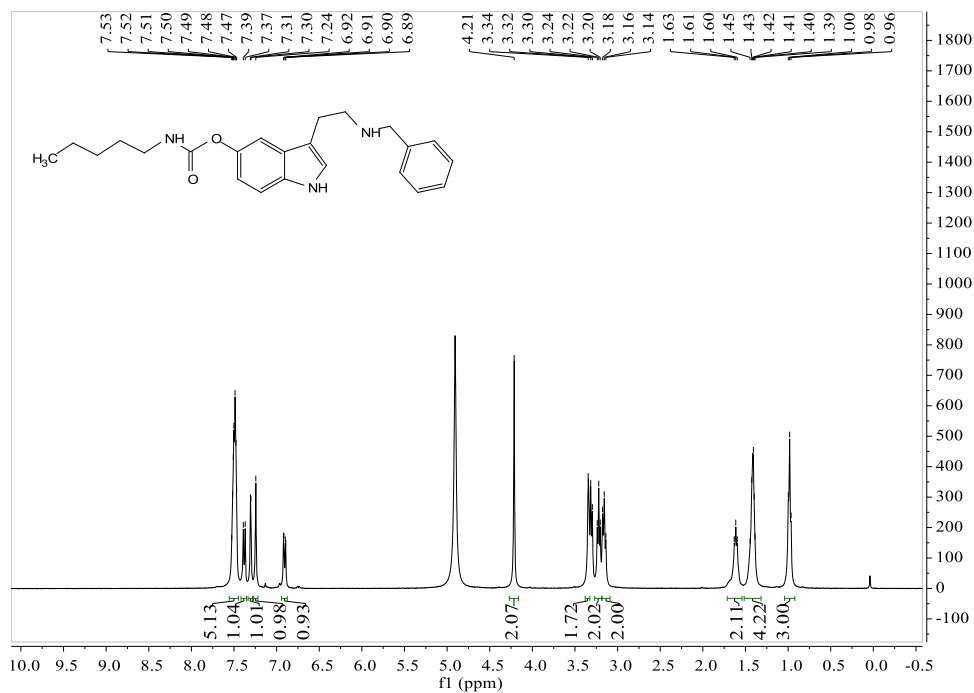
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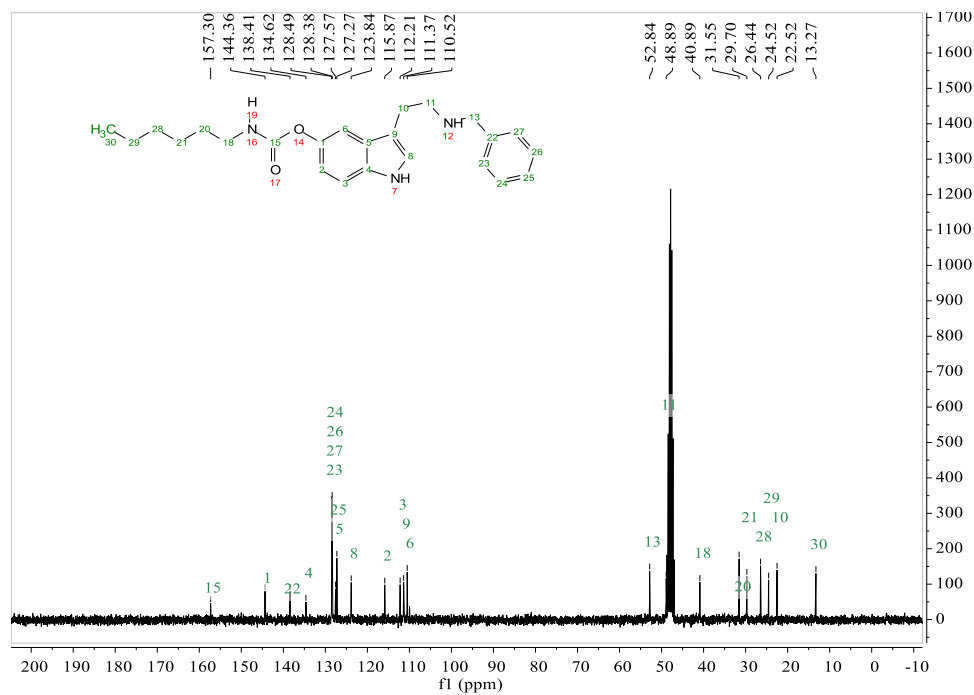
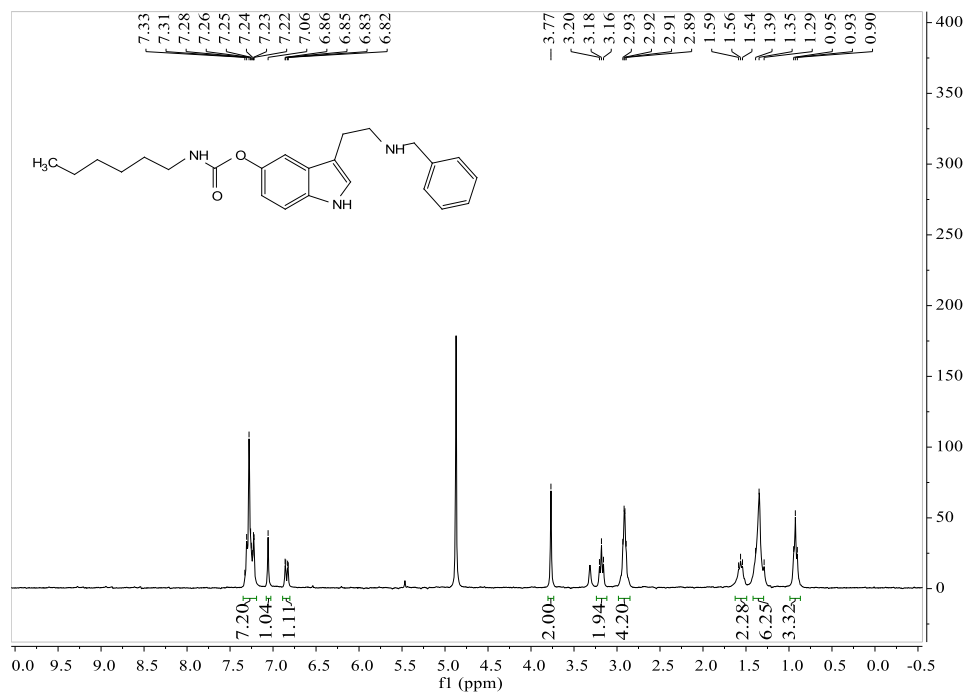
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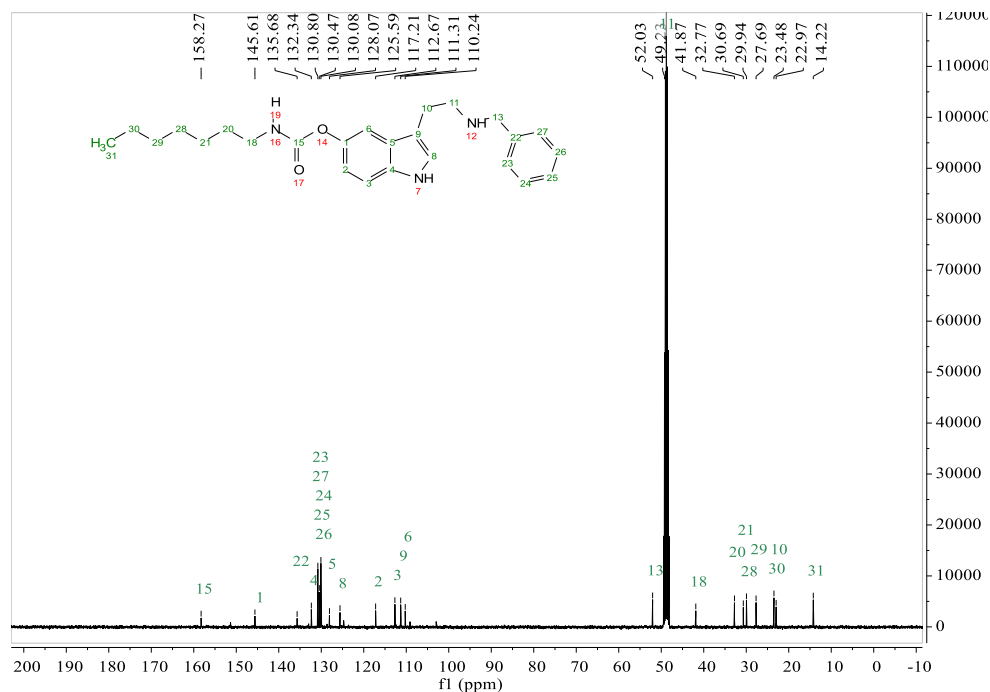
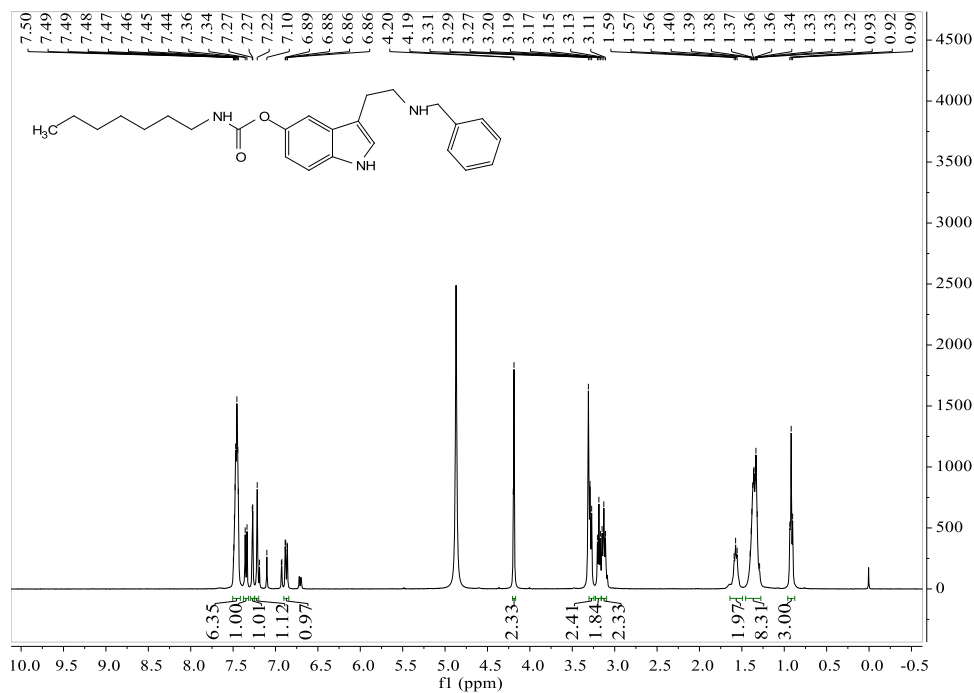
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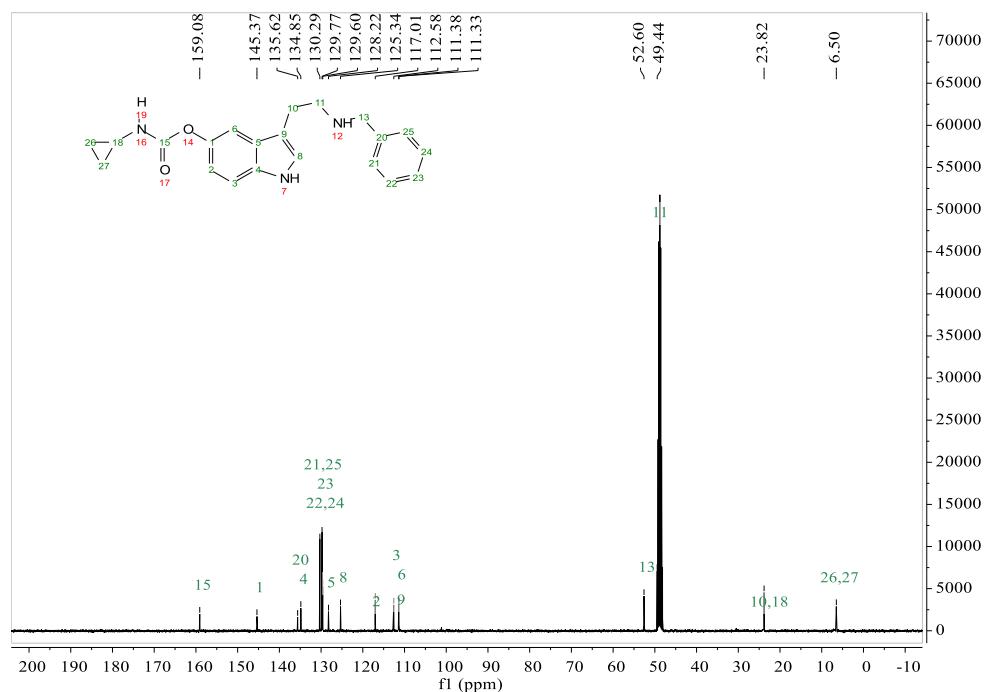
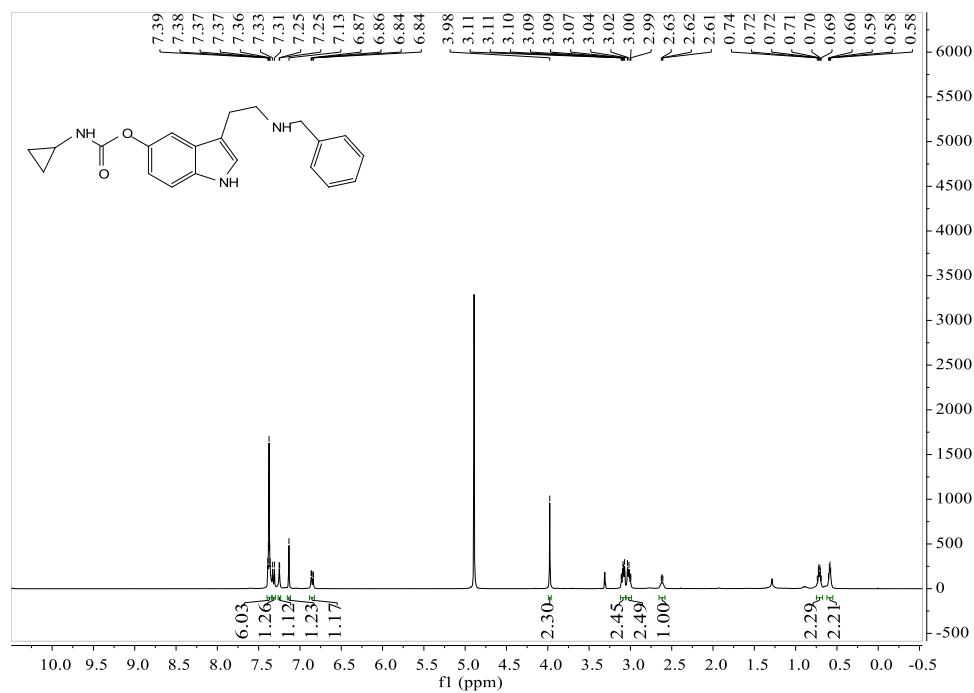
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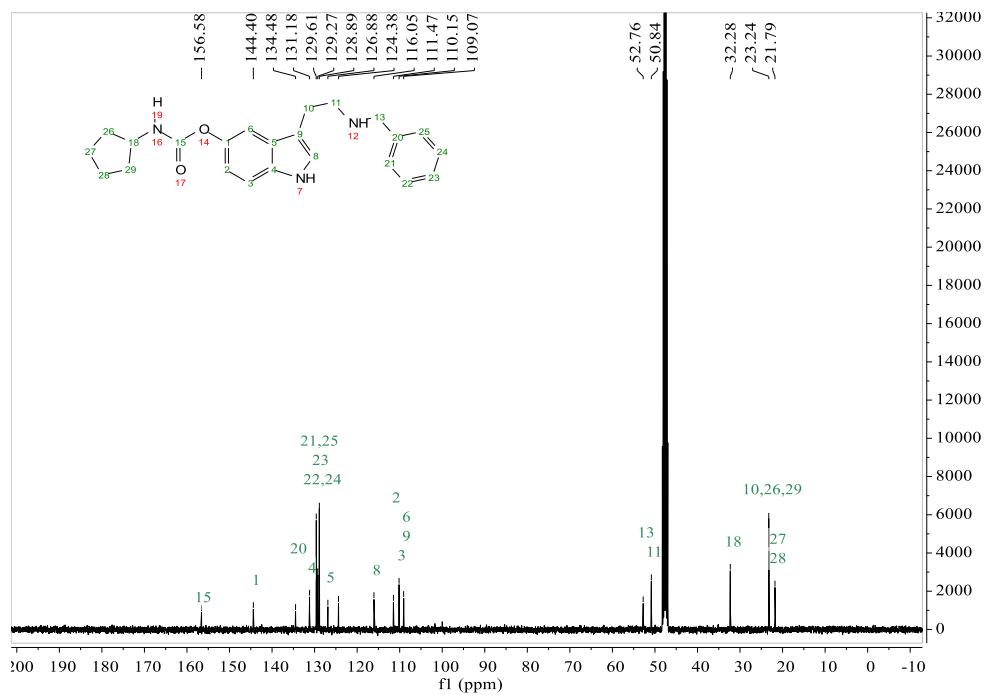
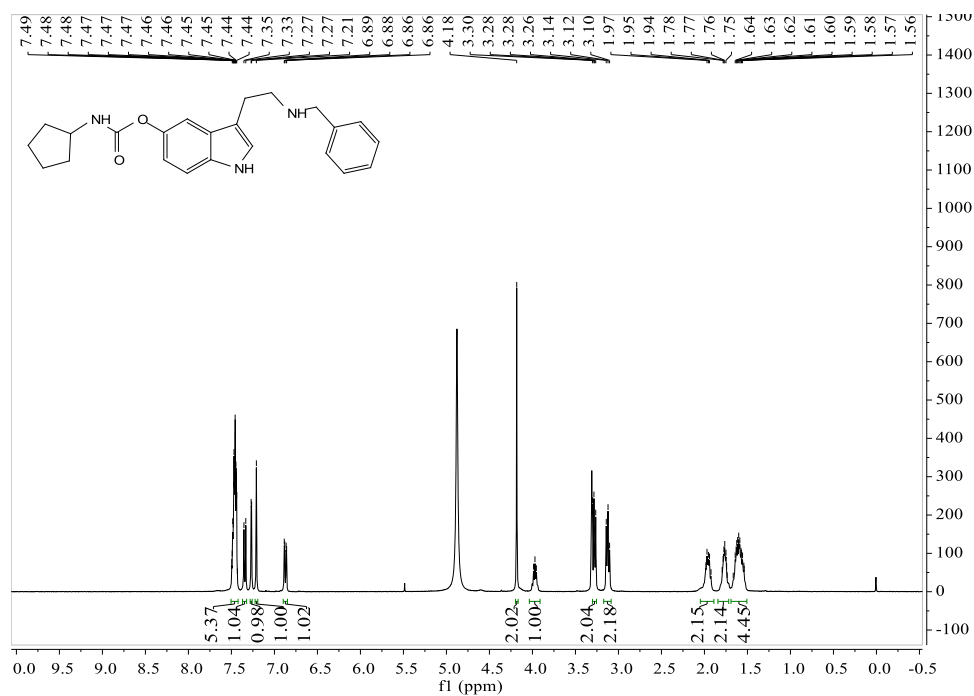
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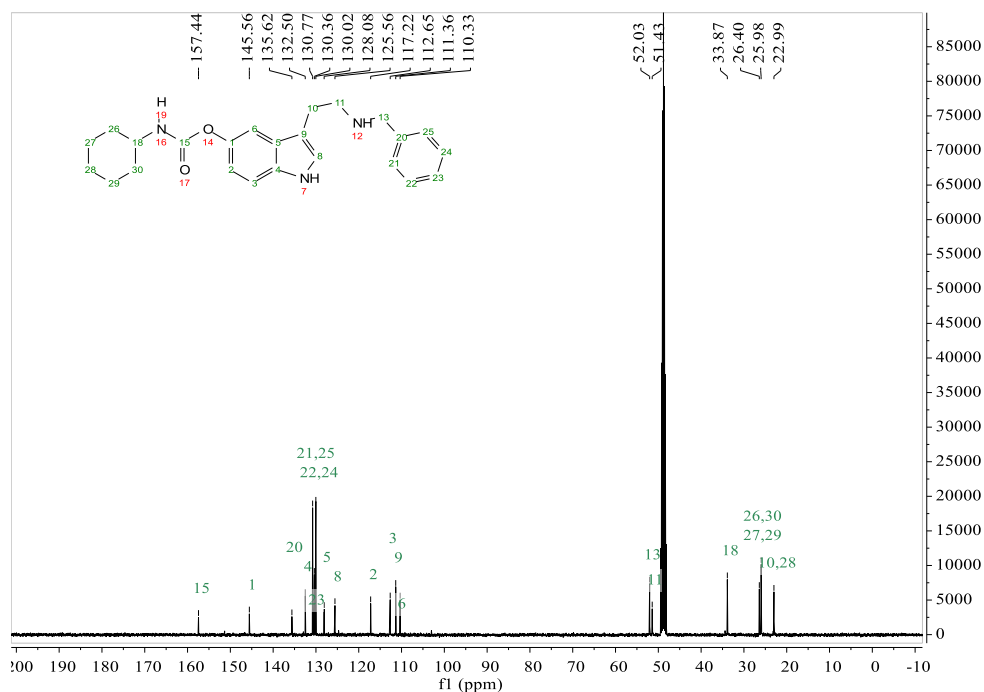
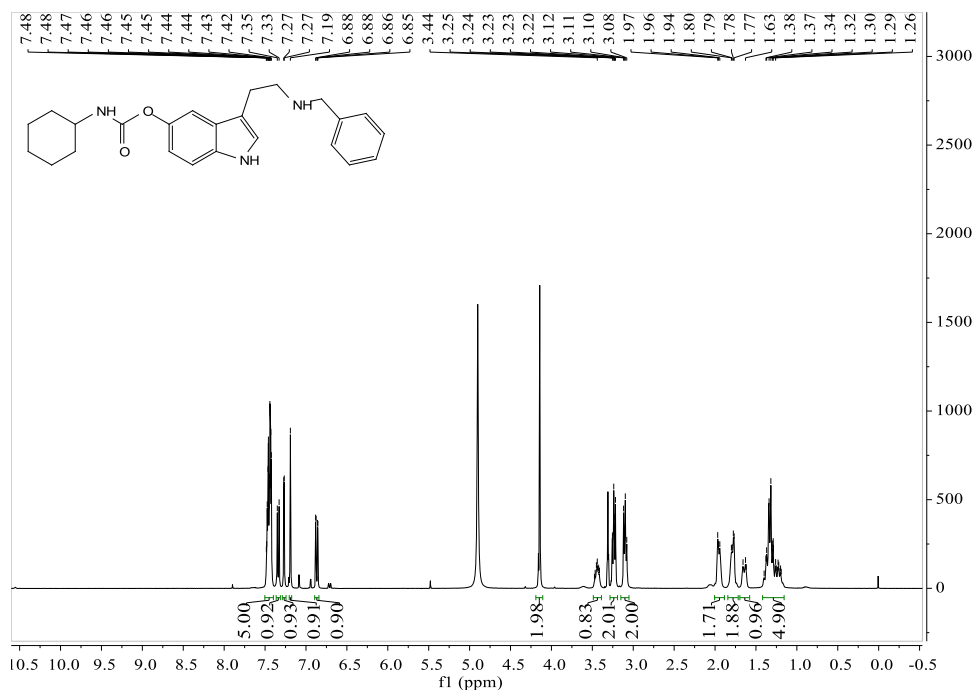
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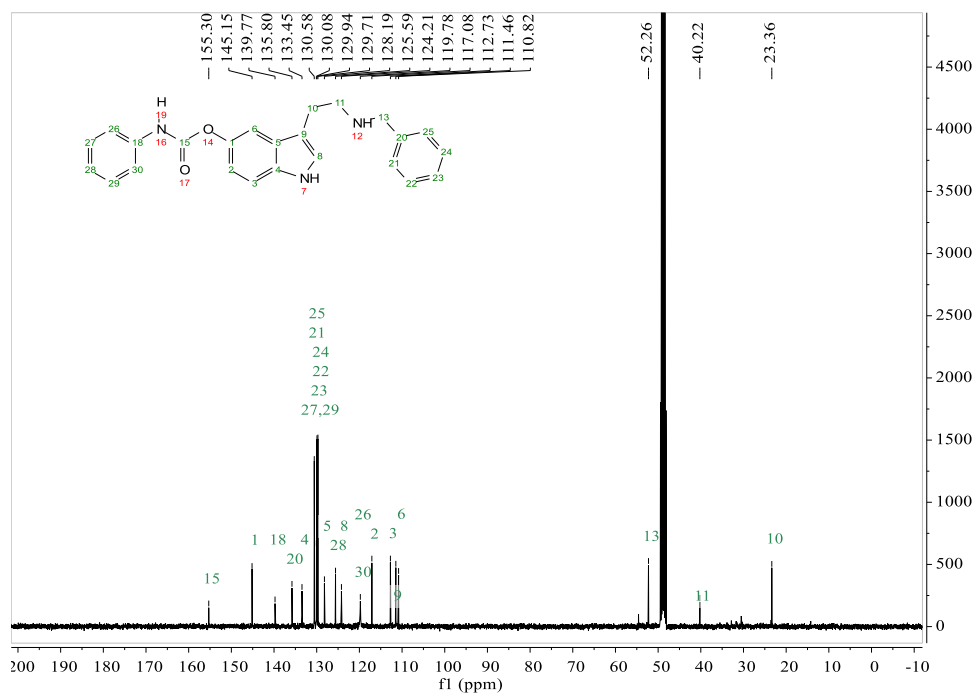
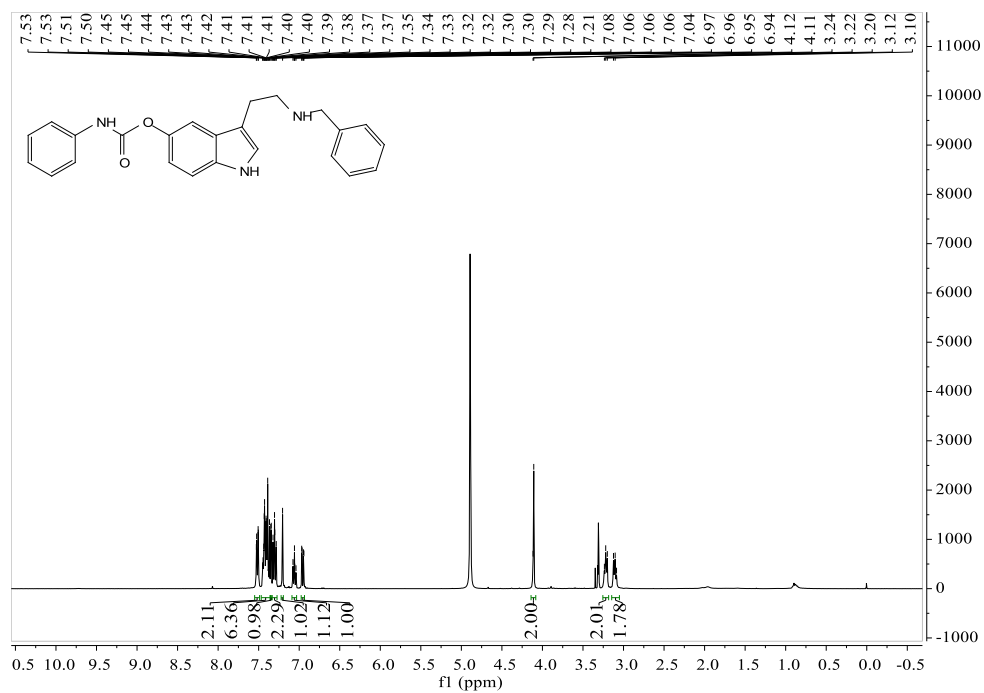
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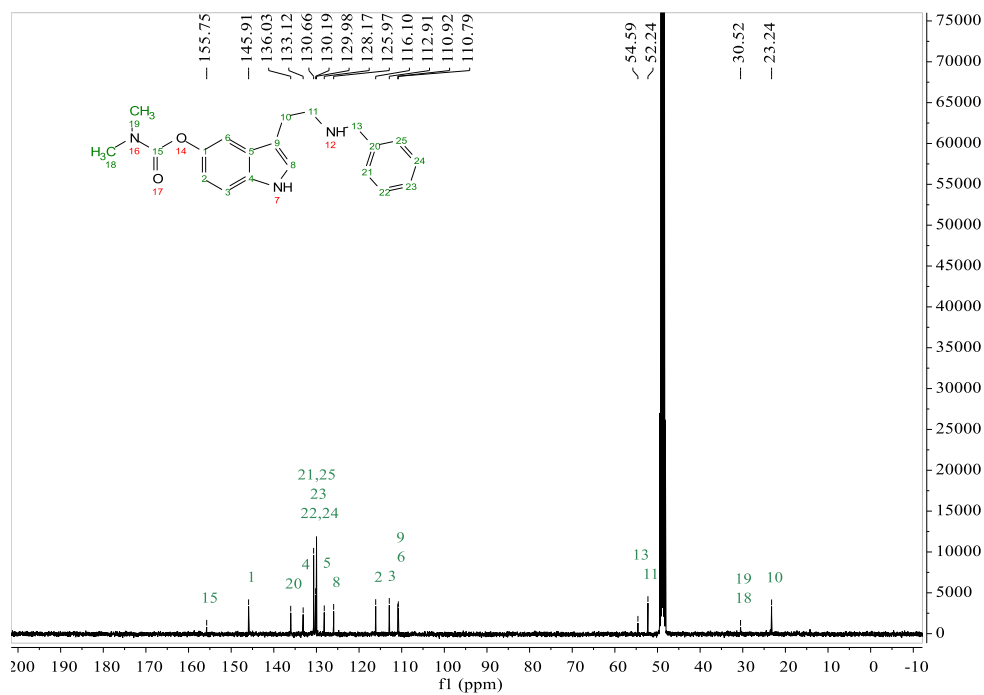
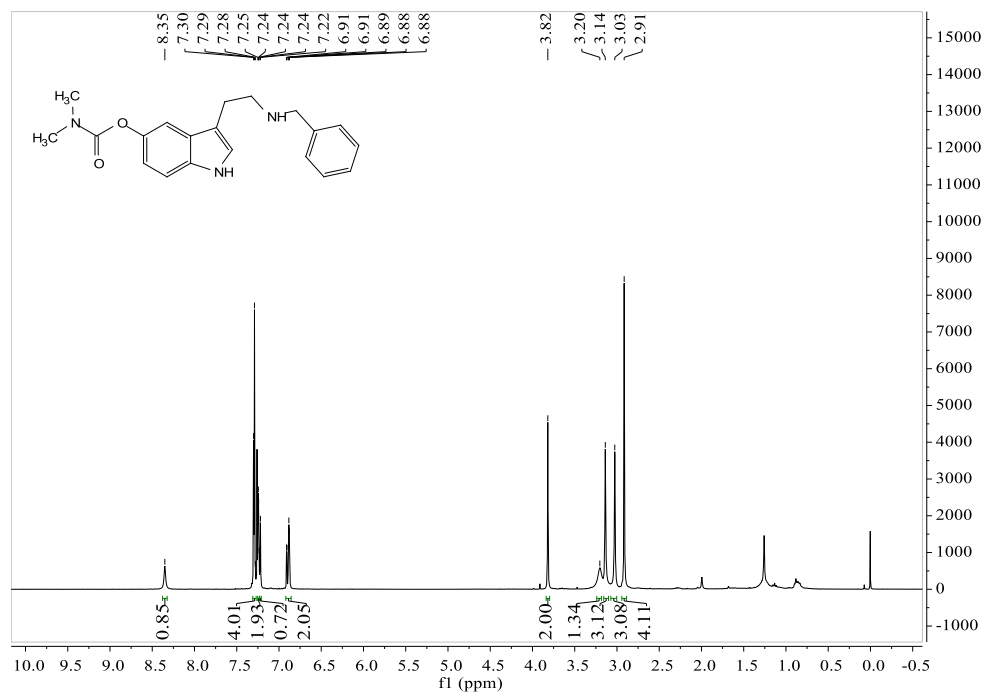
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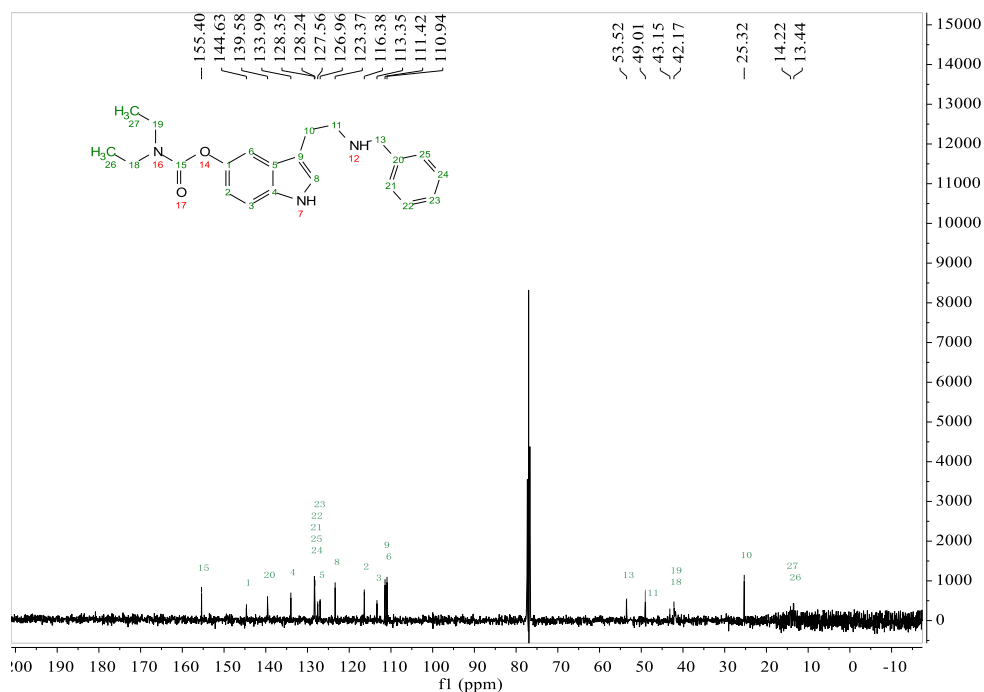
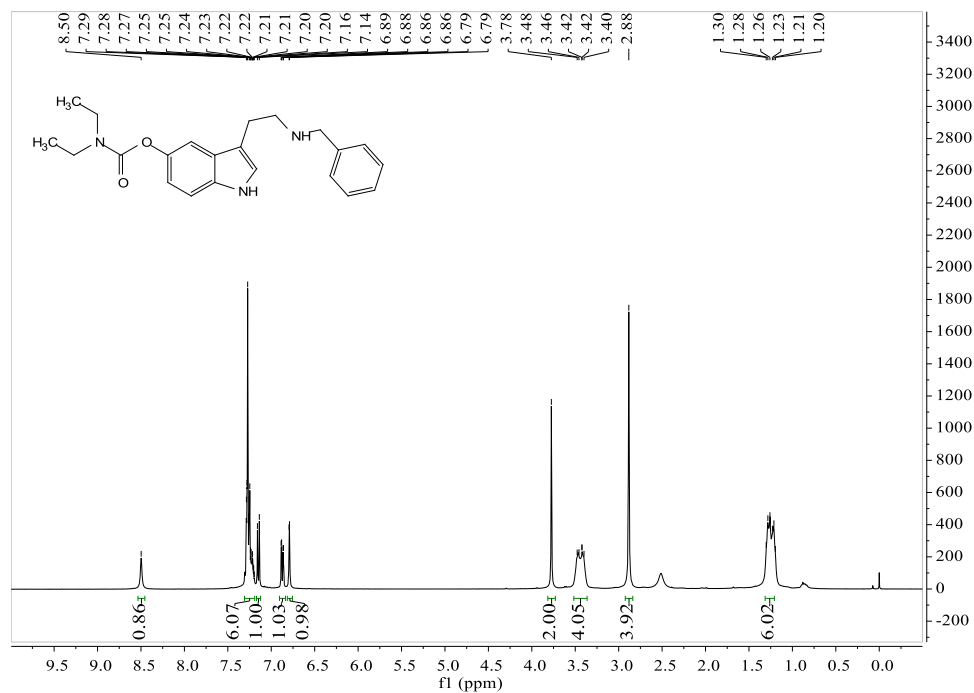
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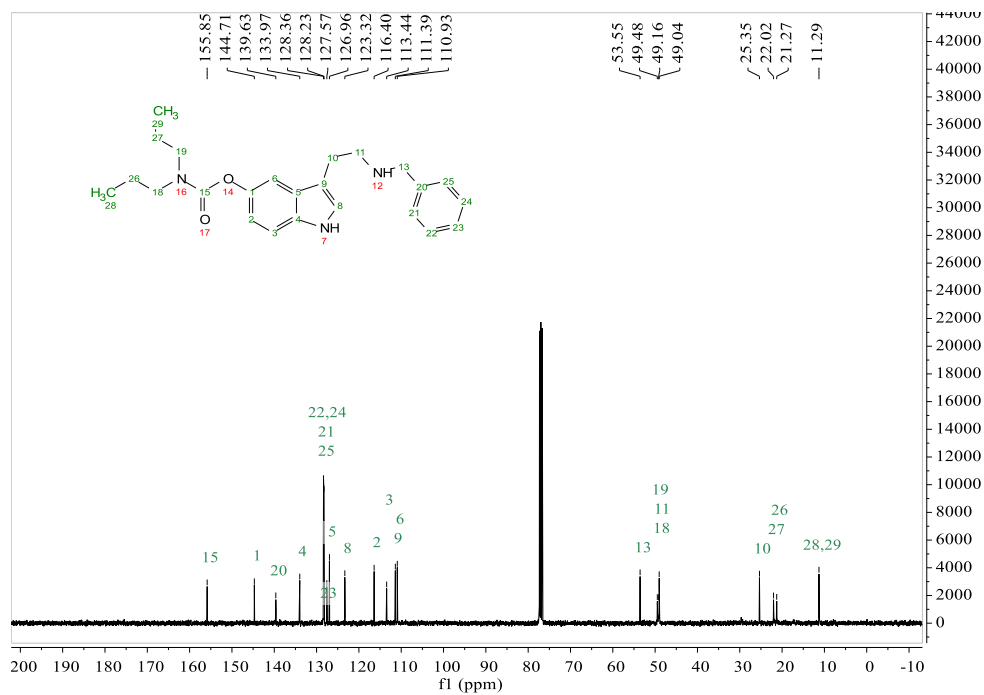
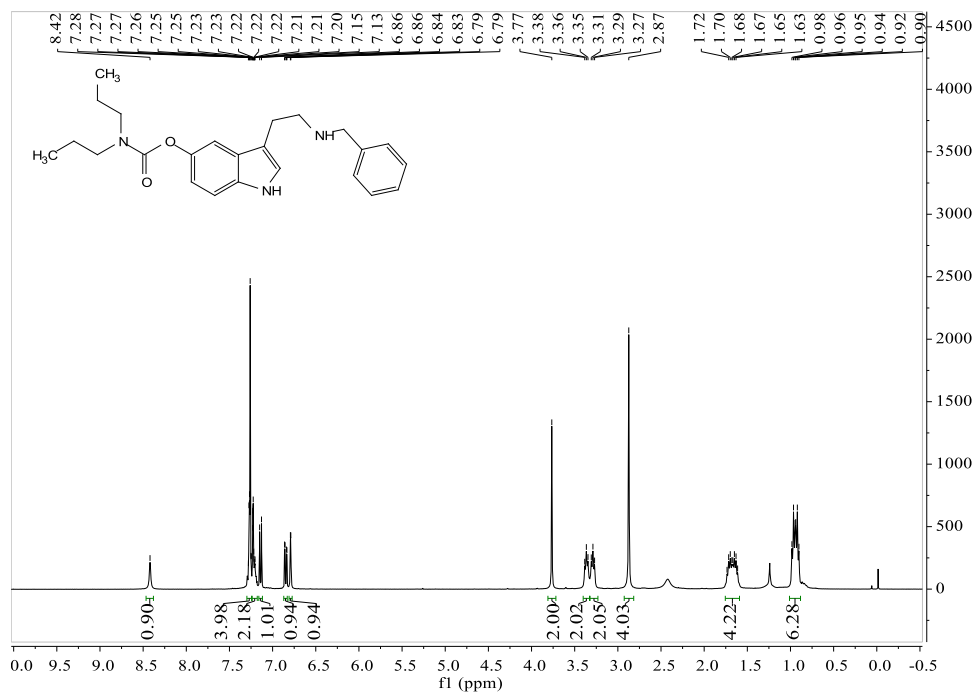
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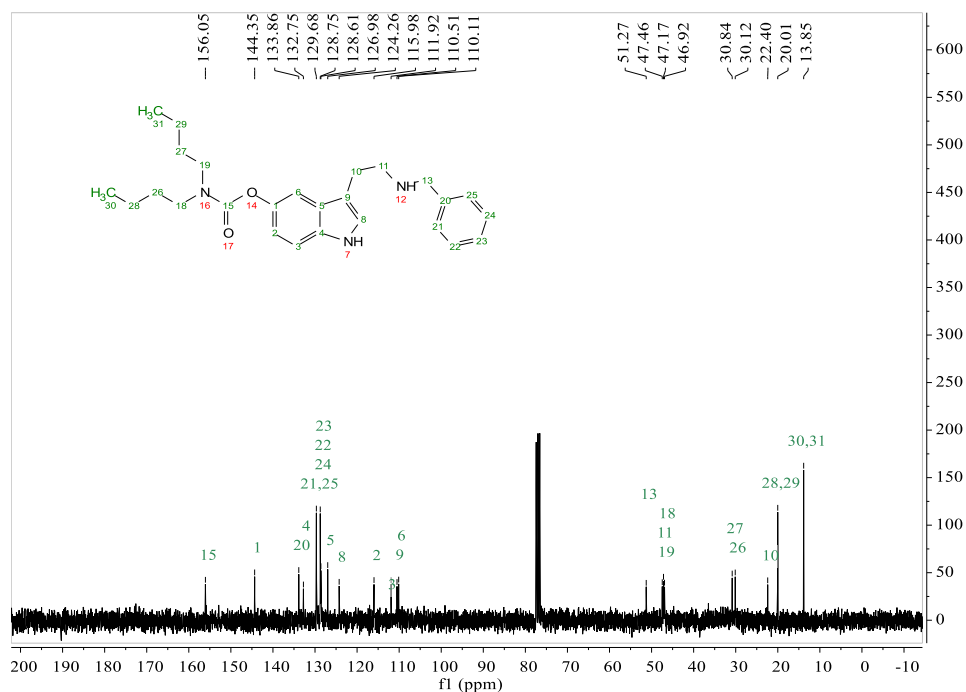
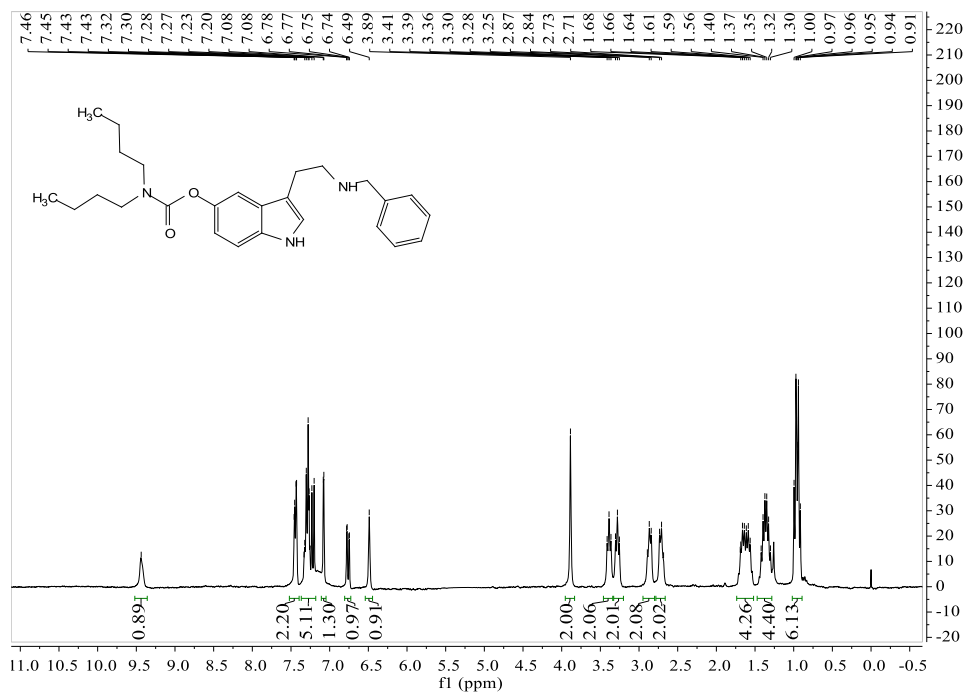
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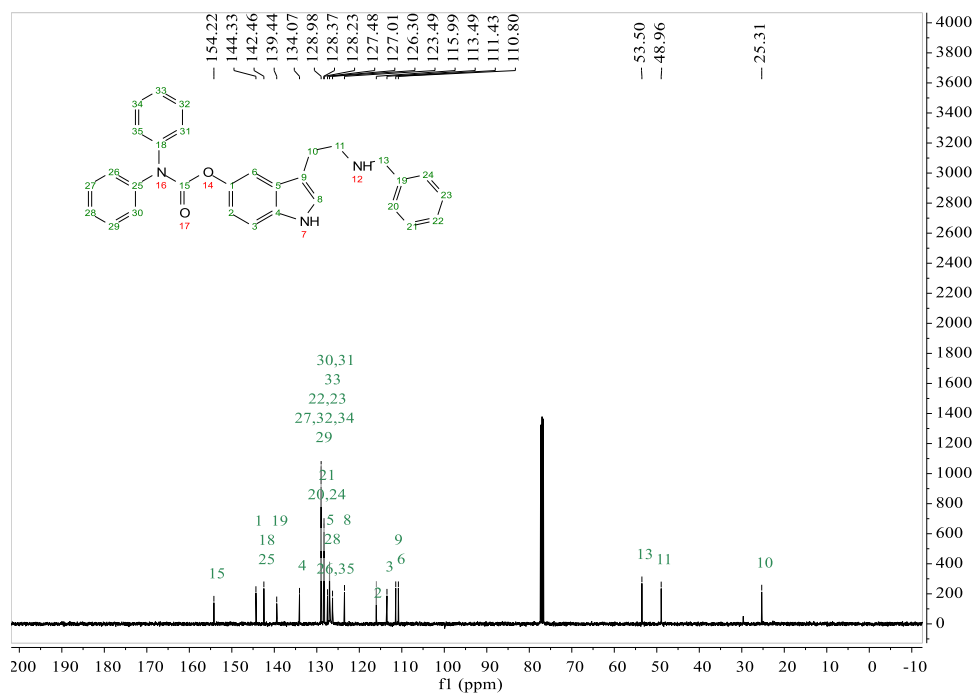
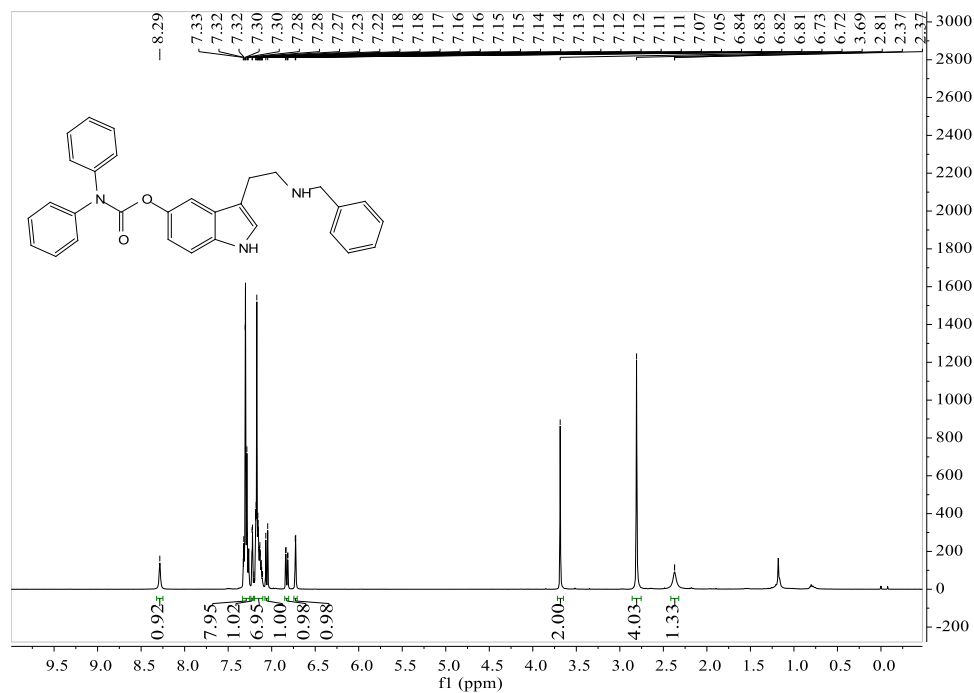
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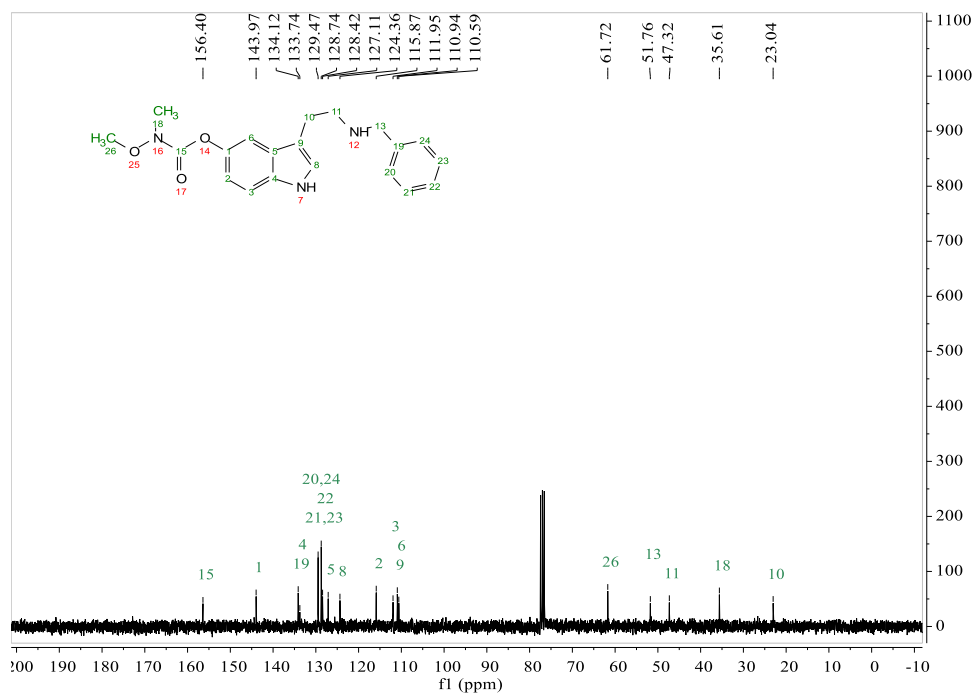
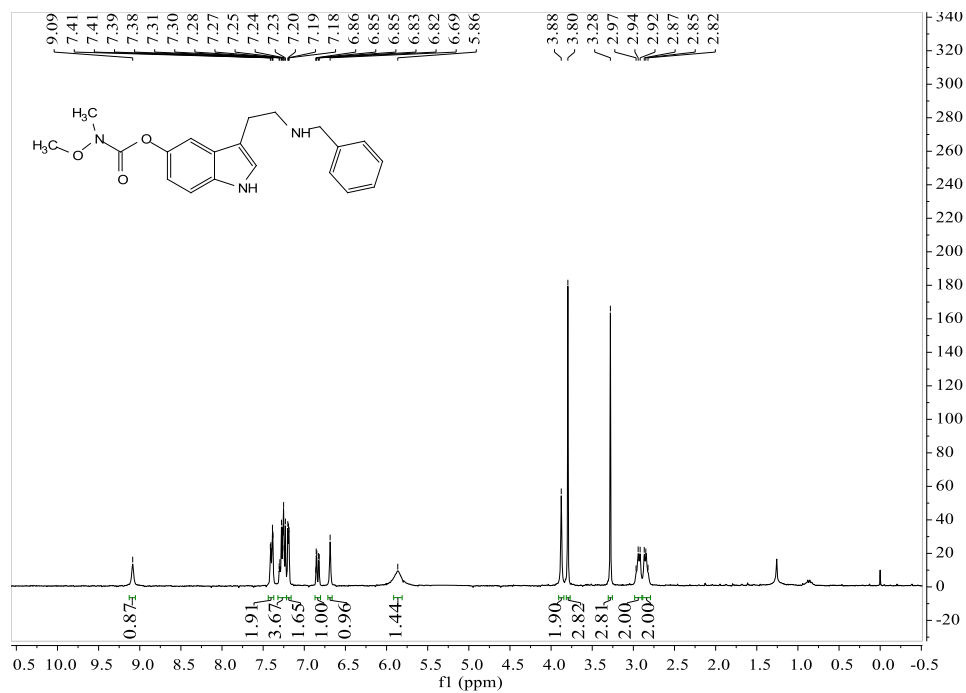
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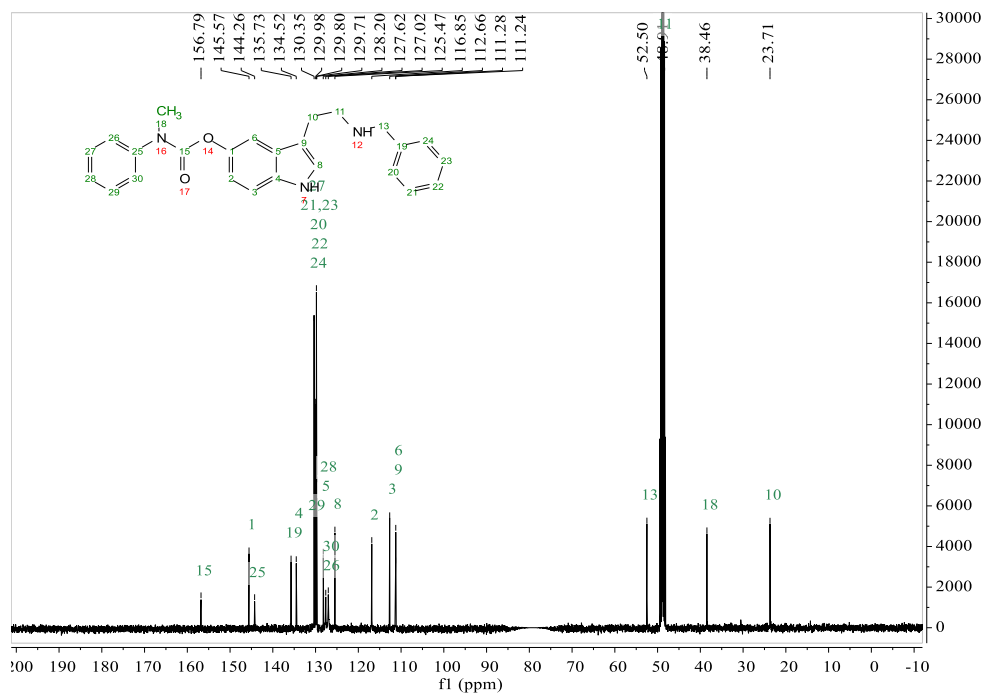
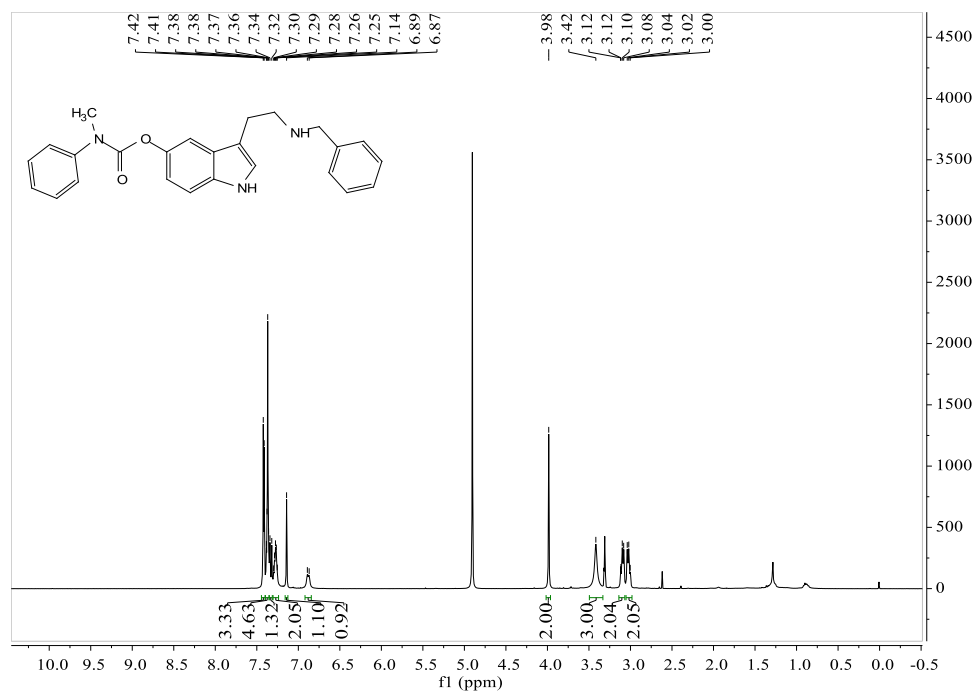
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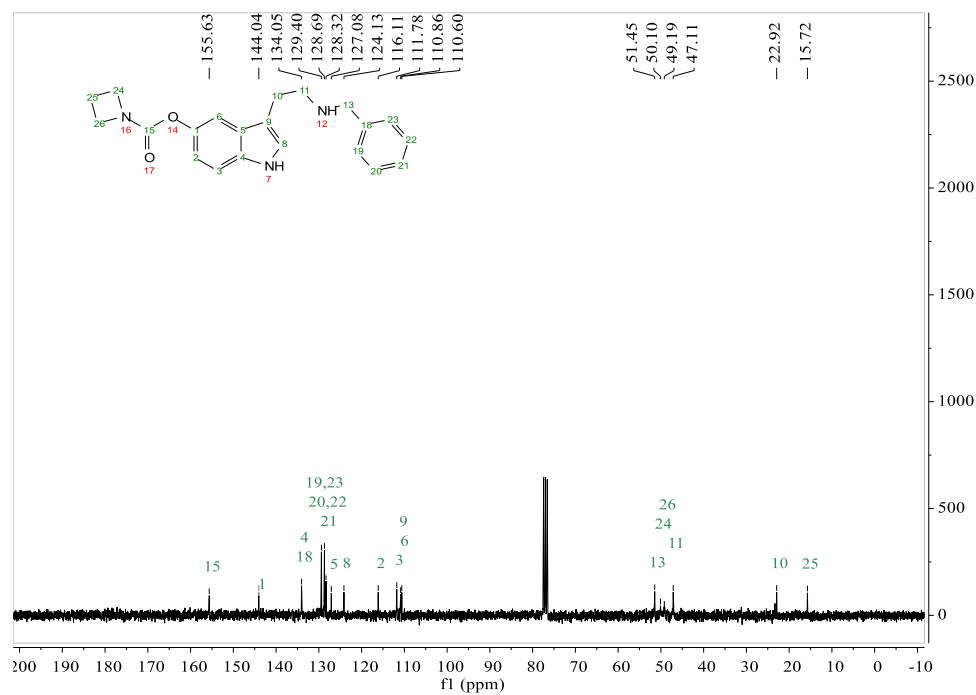
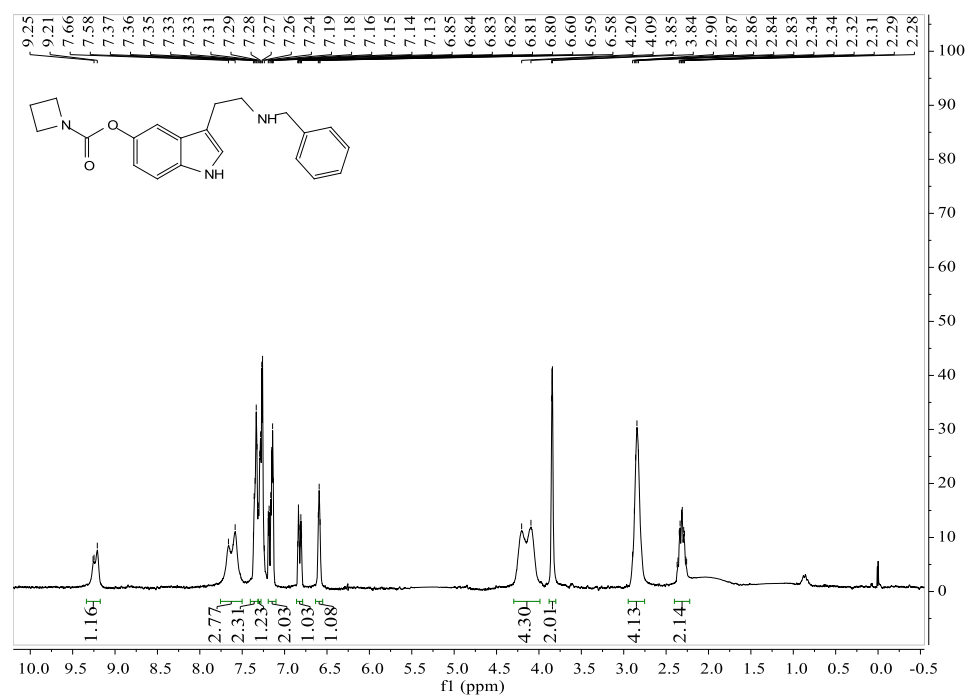
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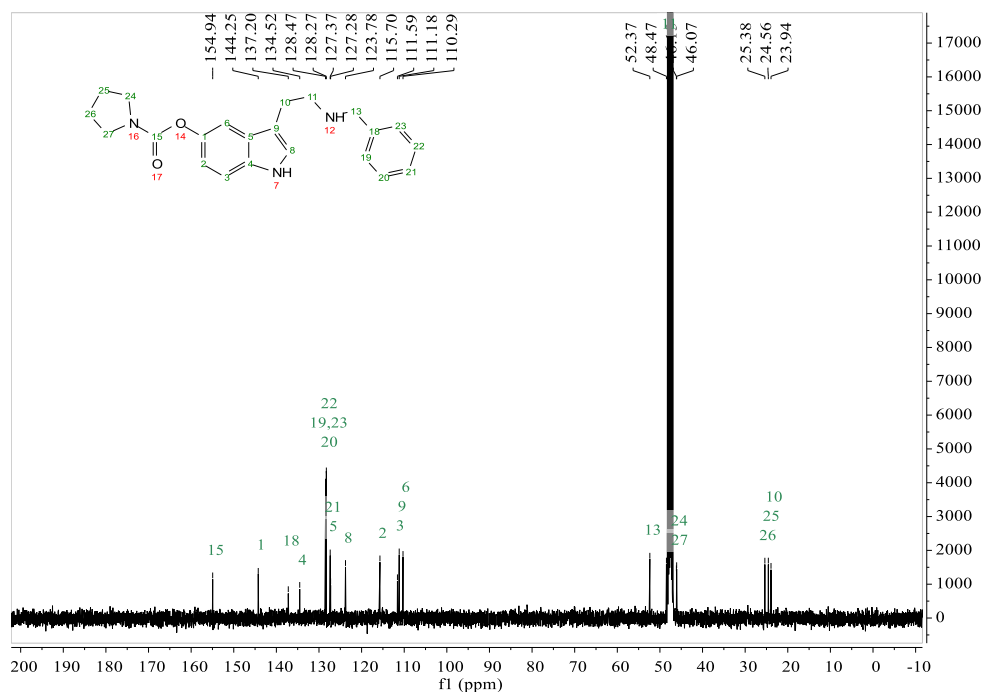
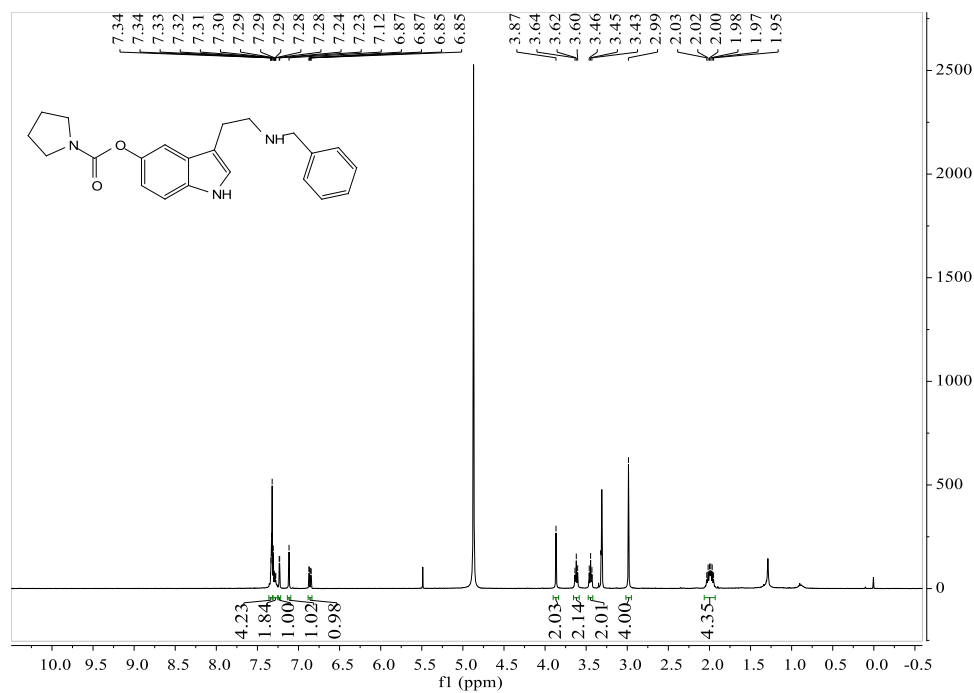
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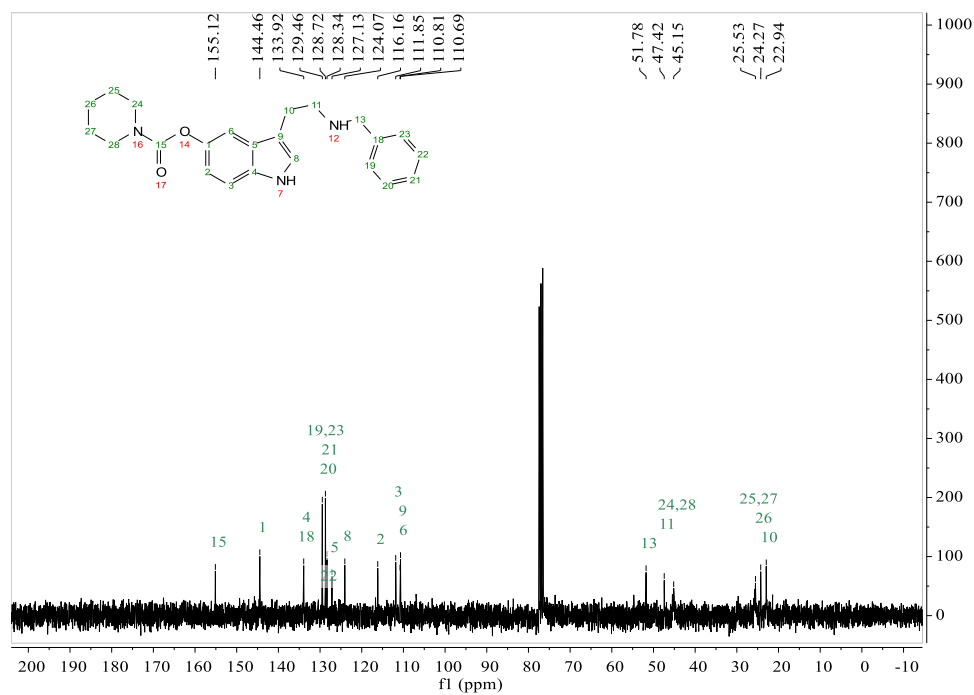
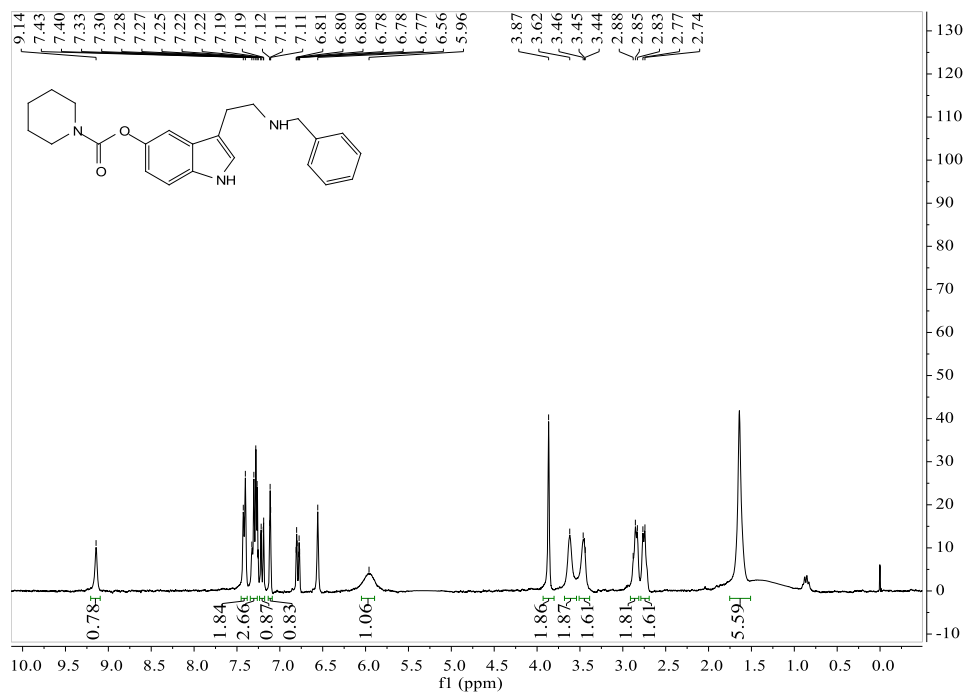
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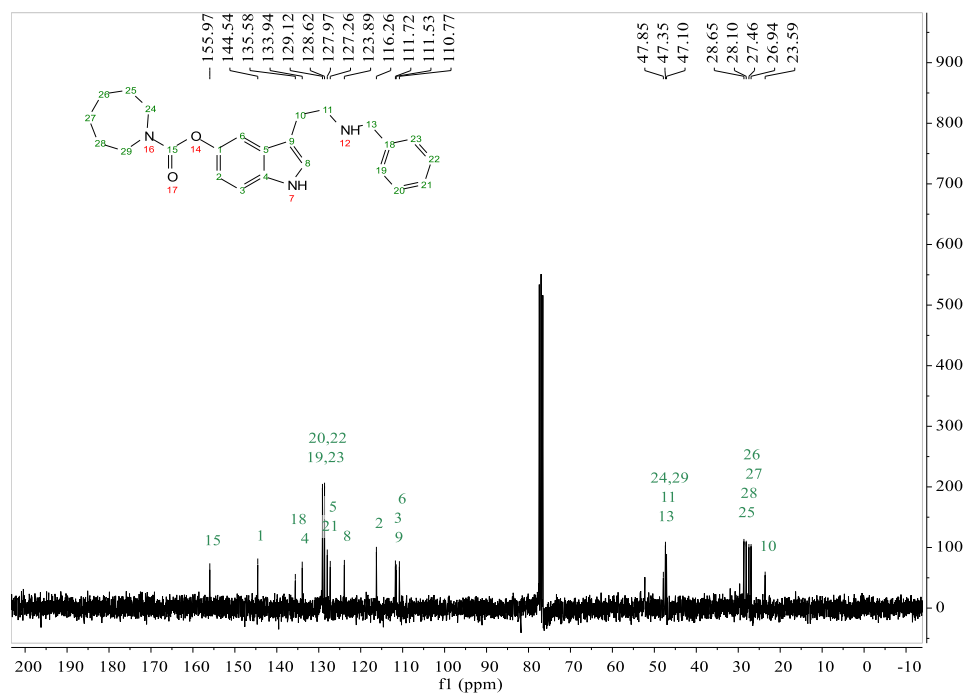
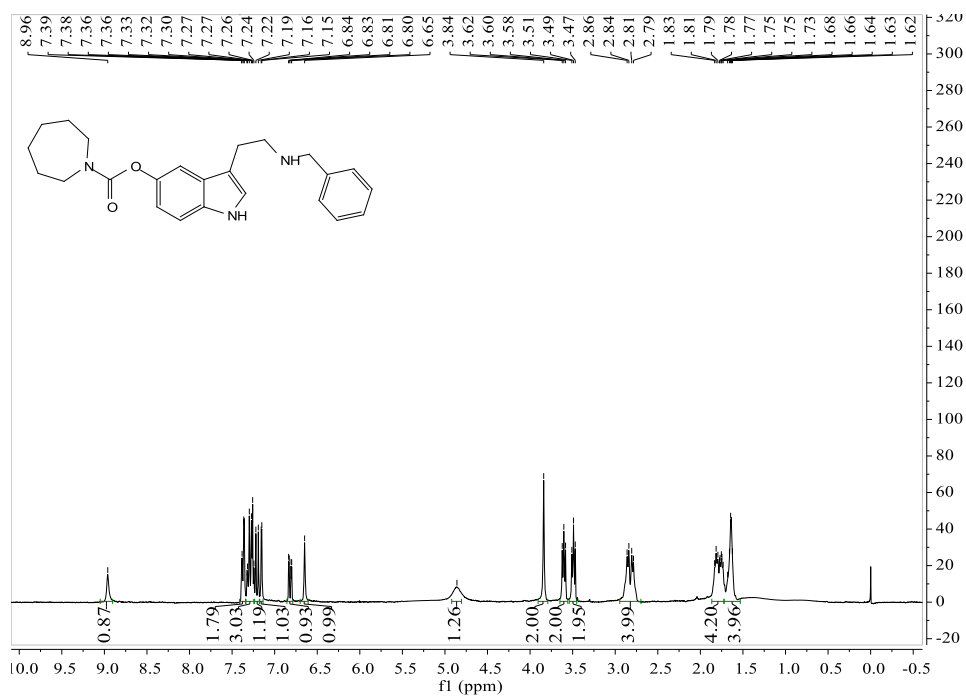
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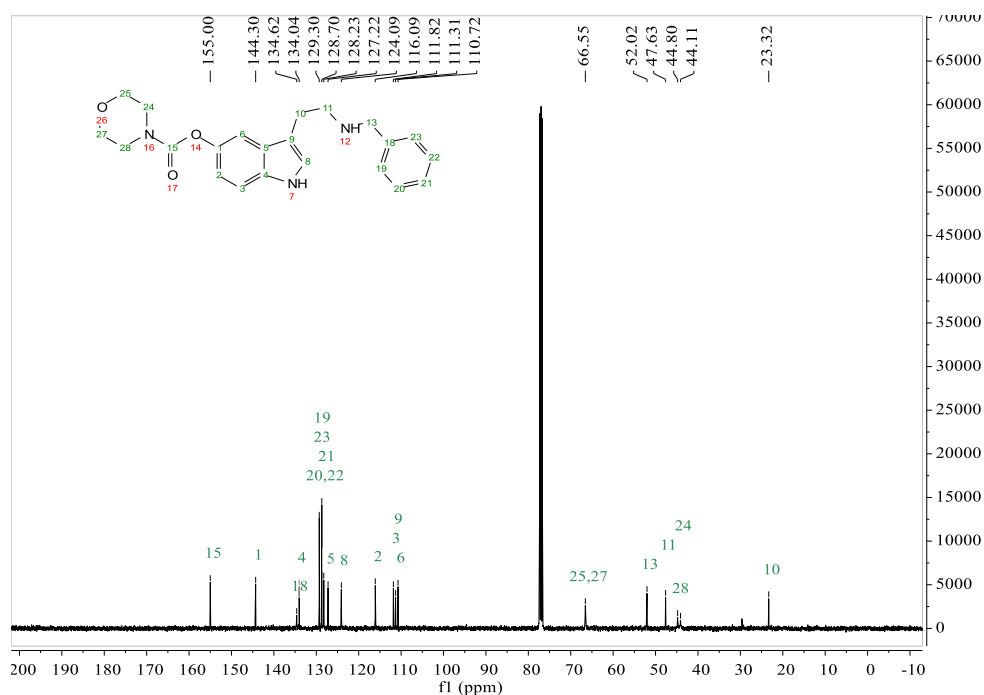
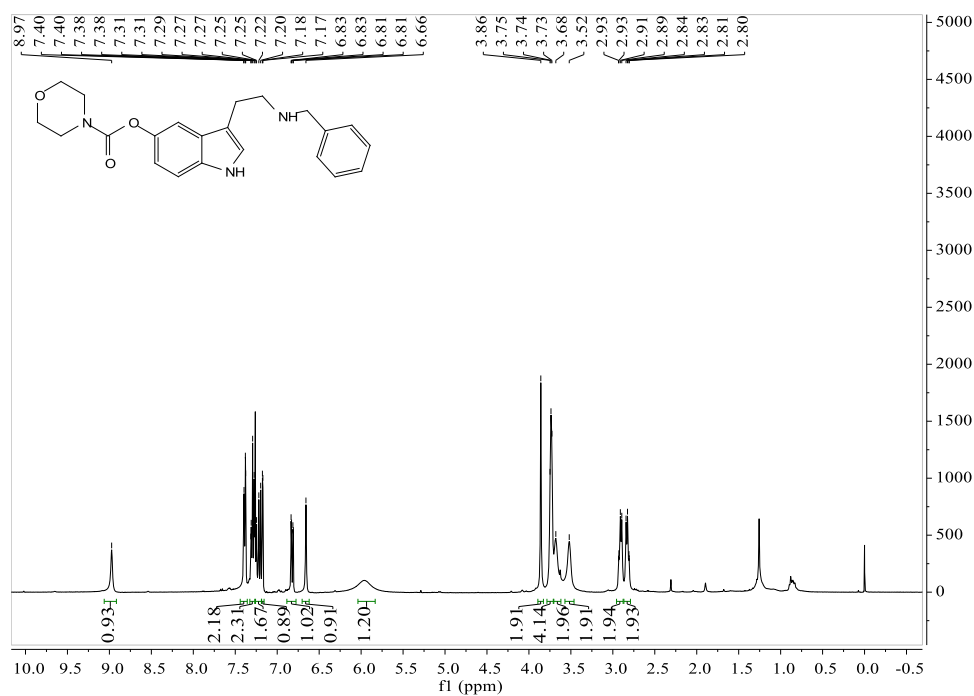
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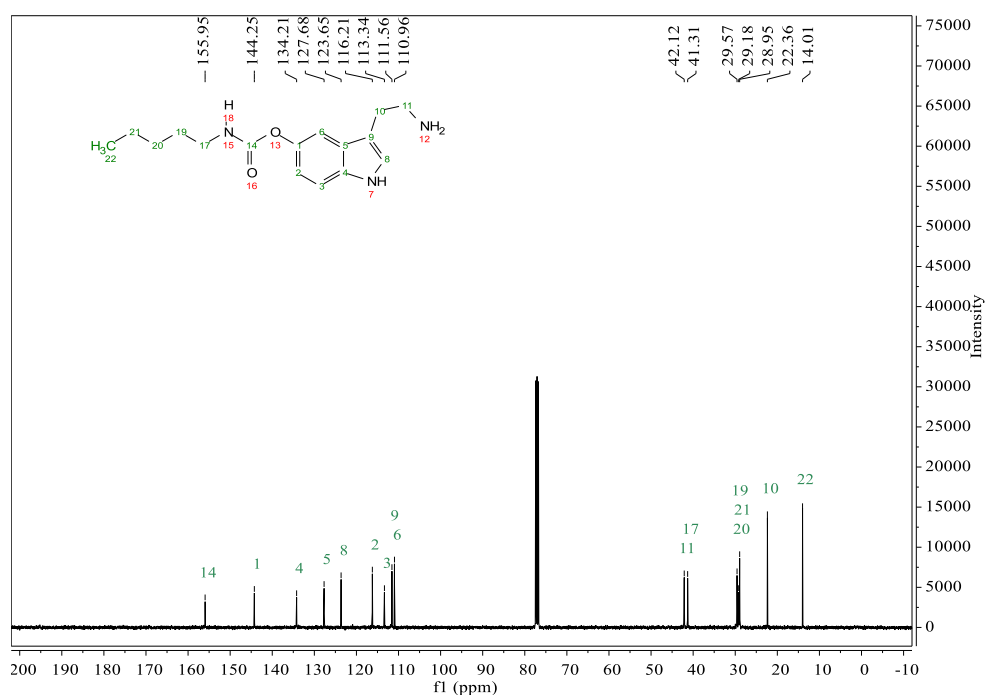
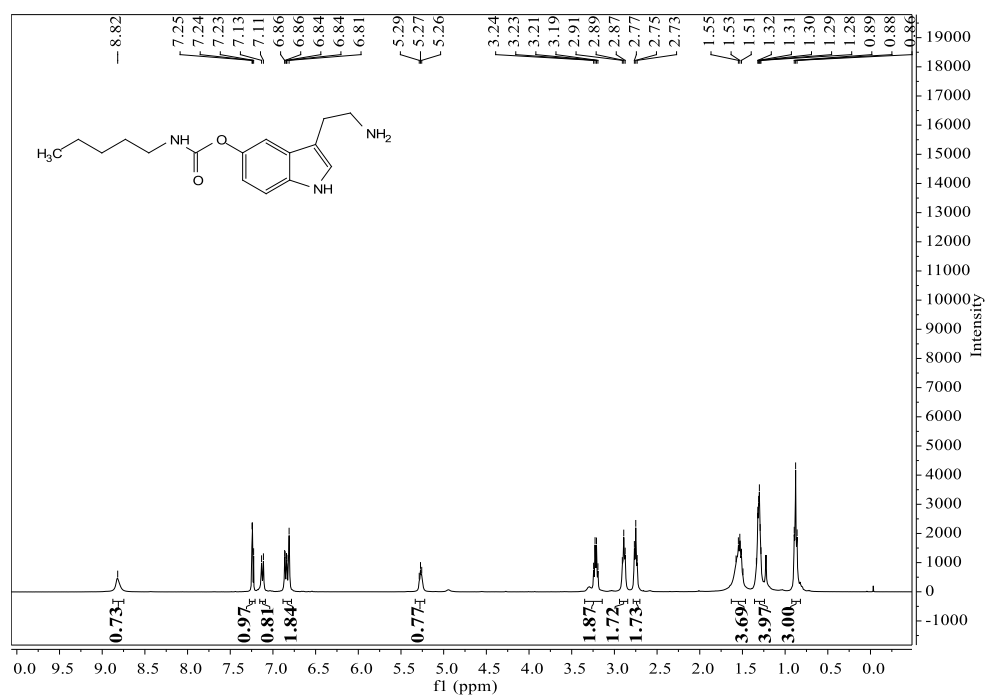
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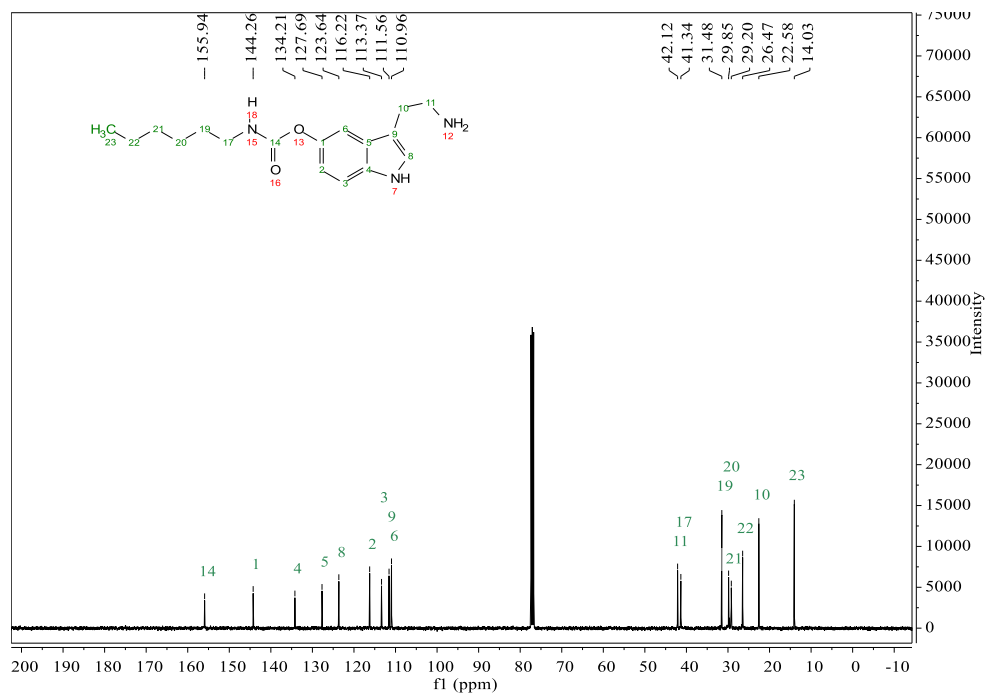
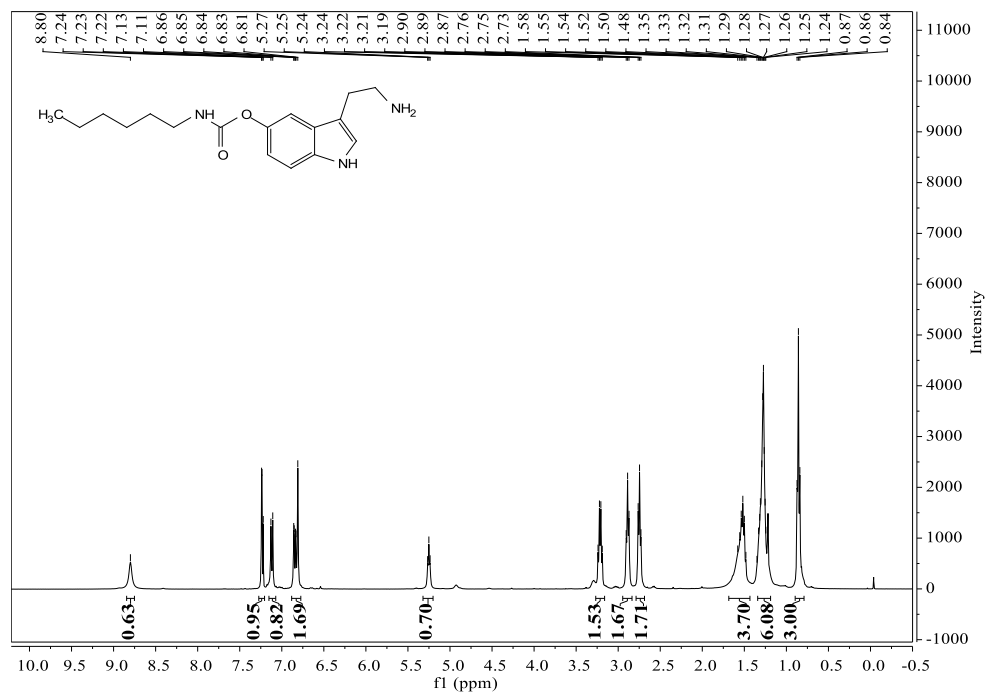
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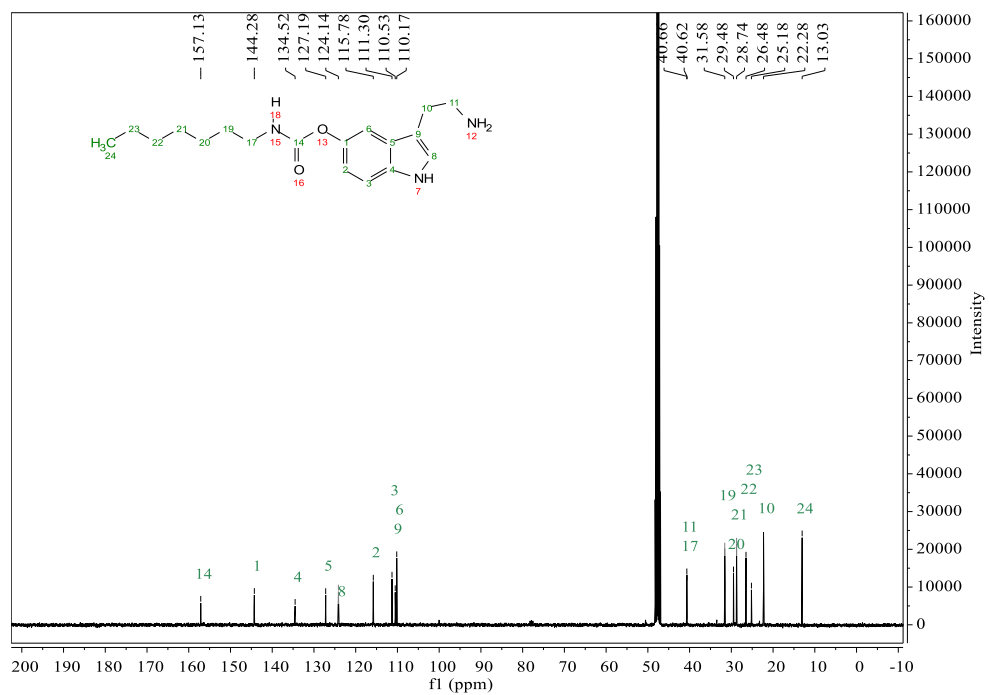
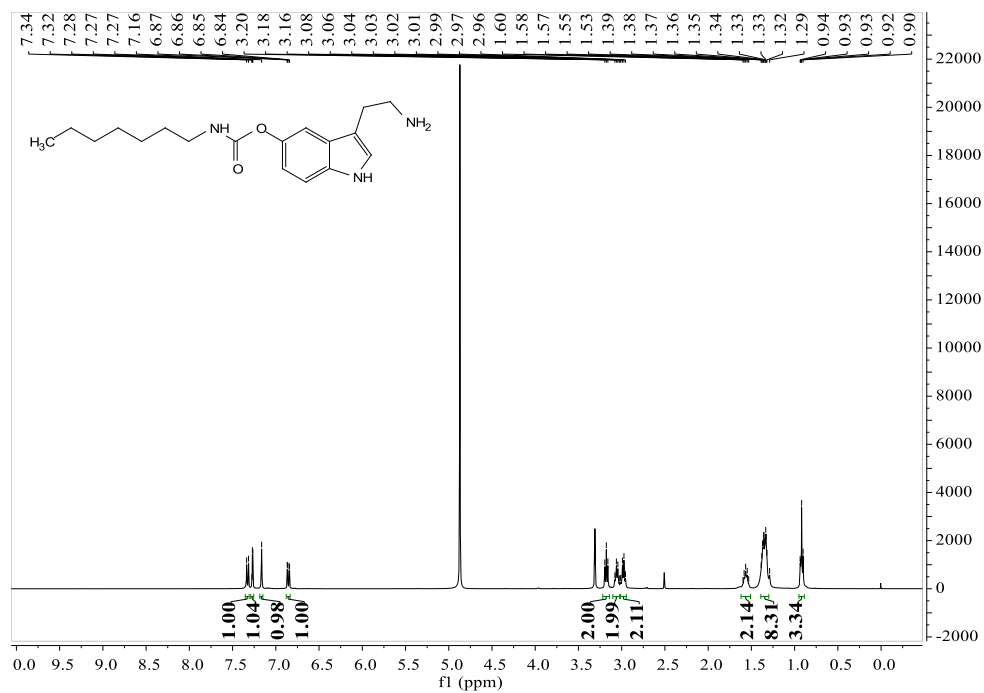
4c:



4d:

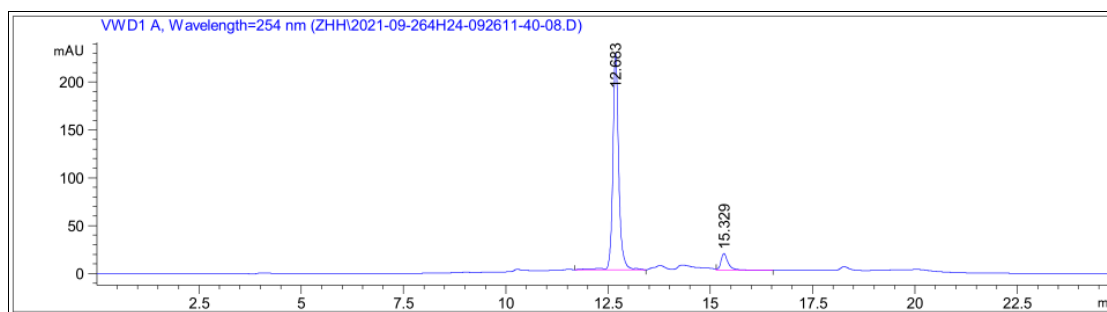


4e:



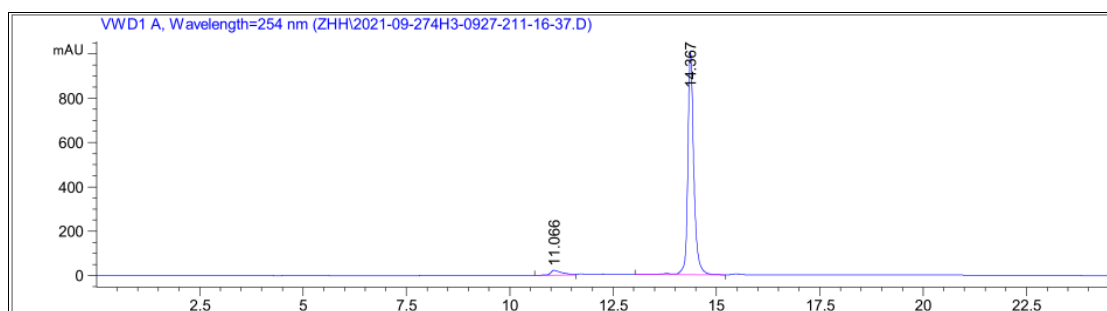
HPLC results of synthesized compounds

Compound 2a (96.11%)



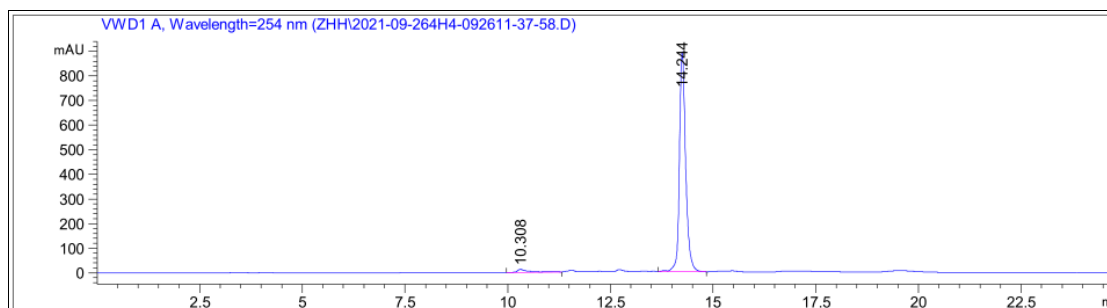
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.683	VV R	0.1489	2266.37378	226.24910	96.1103
2	15.329	MM	0.1263	91.72200	12.10147	3.8897

Compound 2b (96.18%)



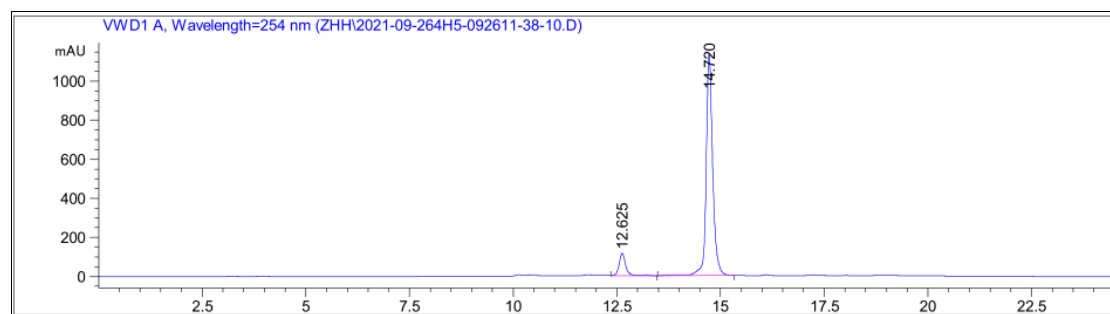
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.066	BV	0.2535	402.79239	21.40935	3.8194
2	14.367	VB R	0.1508	1.01431e4	1002.57697	96.1806

Compound 2c (97.87%)



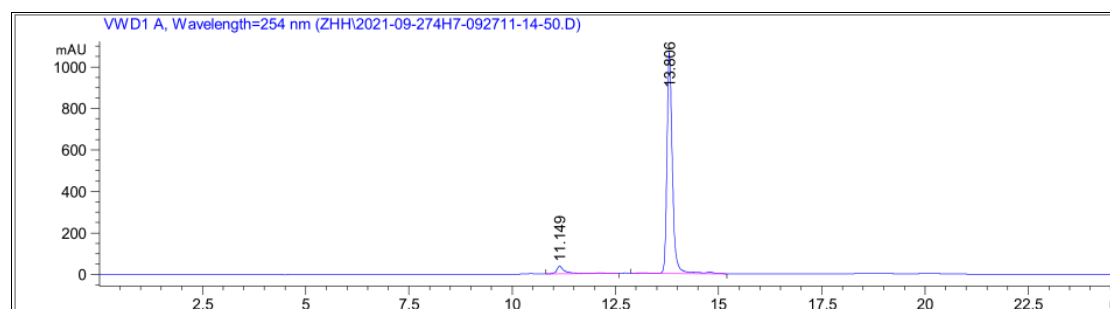
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.308	BV R	0.2387	204.70920	11.66859	2.1318
2	14.244	VB R	0.1564	9397.82422	892.25366	97.8682

Compound 2d (95.35%)



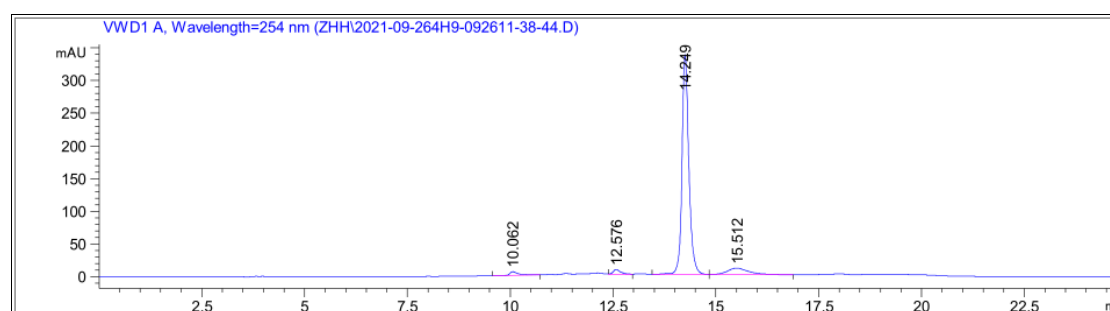
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.625	MM	0.1227	607.81915	82.54528	4.6466
2	14.720	VB R	0.1630	1.24731e4	1137.63208	95.3534

Compound 2f (97.38%)



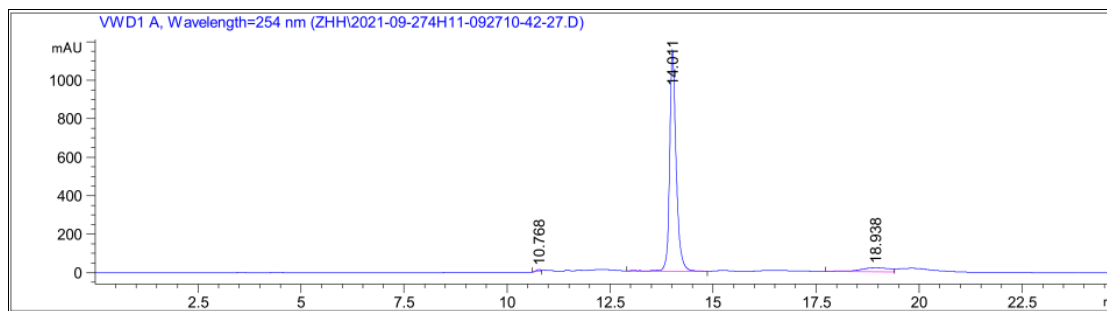
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.149	MM	0.1324	265.27377	33.40529	2.6171
2	13.806	VV R	0.1389	9871.05371	1067.05896	97.3829

Compound 2h (96.09%)



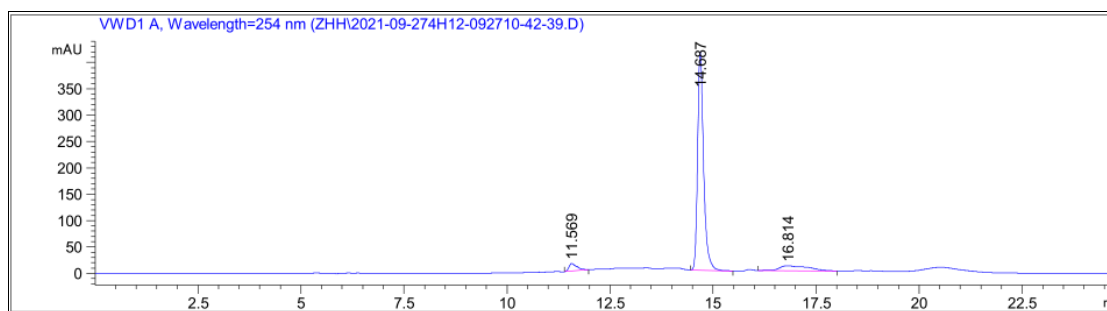
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.062	MM	0.1144	34.73880	5.06237	0.8603
2	12.576	MM	0.1205	39.93761	5.52498	0.9891
3	14.249	VV R	0.1751	3880.01563	334.99265	96.0890
4	15.512	MM	0.2606	83.24635	5.32469	2.0616

Compound 2i (95.16%)



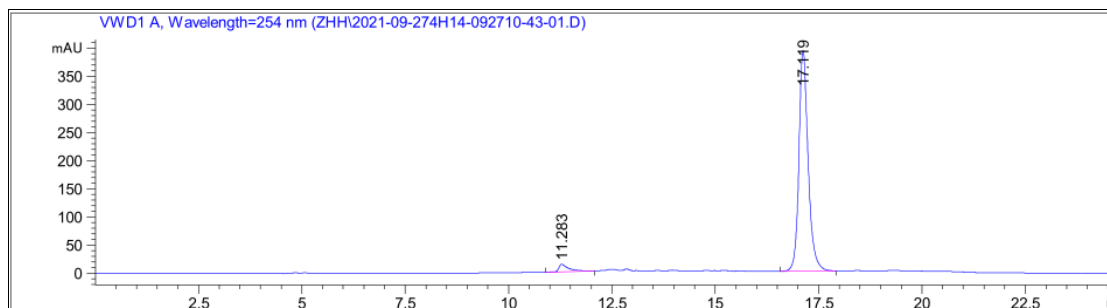
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.768	MM	0.2351	252.67273	17.90887	1.9090
2	14.011	VB R	0.1620	1.25960e4	1146.89172	95.1639
3	18.938	MM	0.5379	387.43594	12.00535	2.9271

Compound 2j (95.75%)



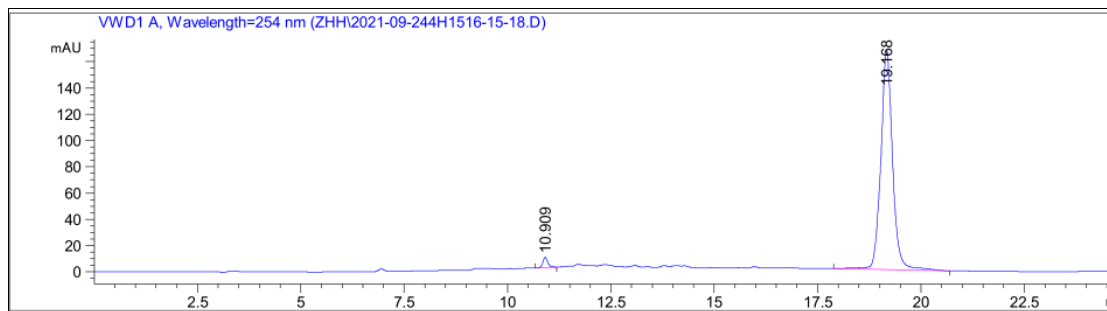
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.569	MM	0.1636	104.30507	10.62770	2.3837
2	14.687	BV R	0.1522	4189.71484	413.61844	95.7491
3	16.814	MM	0.2877	81.70151	4.73286	1.8672

Compound 2l (96.50%)



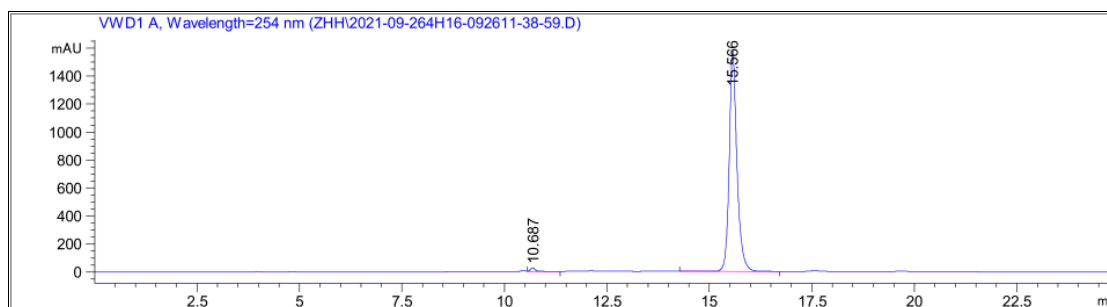
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.283	BV R	0.2345	219.64853	13.55718	3.4951
2	17.119	BB	0.1522	6064.74805	391.89551	96.5049

Compound 2m (98.08%)



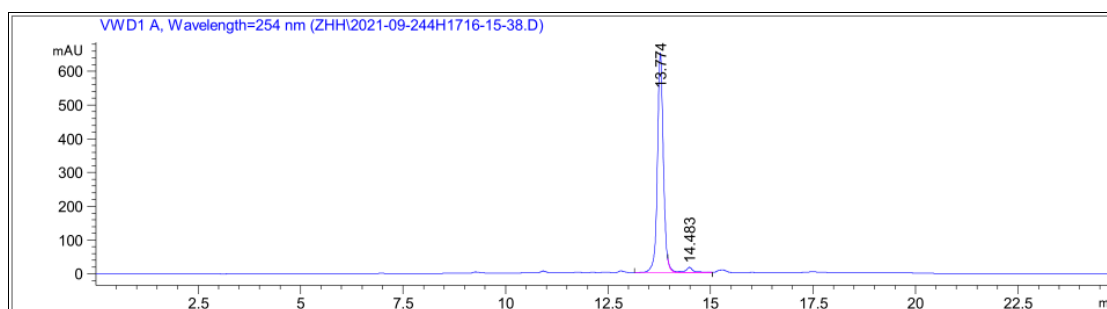
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.909	BB	0.1288	64.51392	7.77818	1.9161
2	19.168	BB	0.2929	3302.45190	166.83865	98.0839

Compound 2n (98.89%)



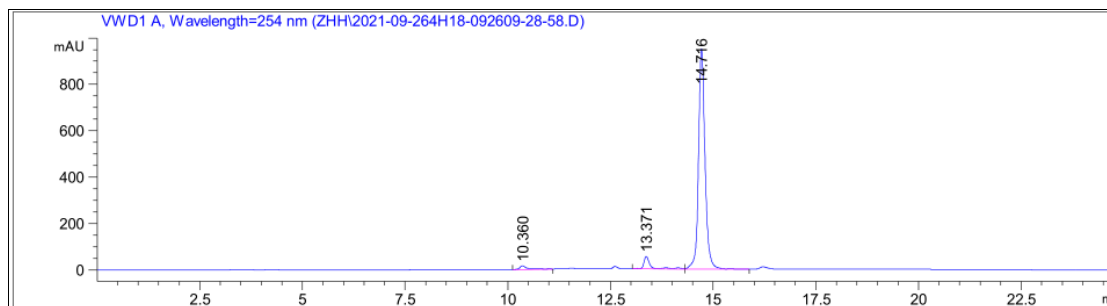
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.687	VV R	0.1319	234.16629	26.81316	1.1142
2	15.566	VB R	0.1937	2.07831e4	1575.46240	98.8858

Compound 2o (96.70%)



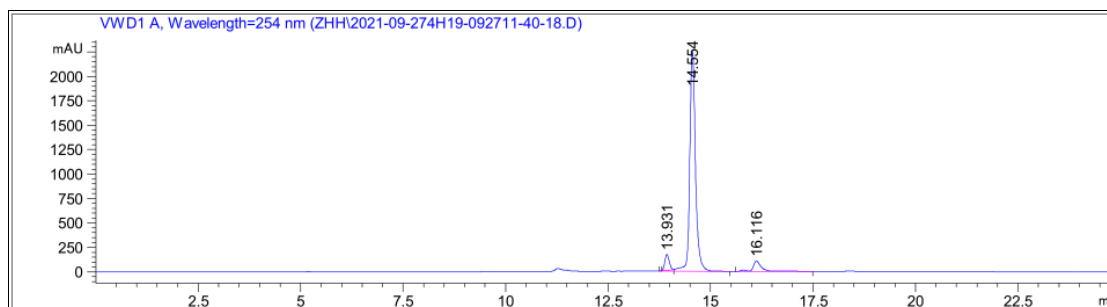
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.774	BV R	0.1523	6594.06055	650.35938	96.7037
2	14.483	VB E	0.2043	224.76872	15.22207	3.2963

Compound 2p (96.90%)



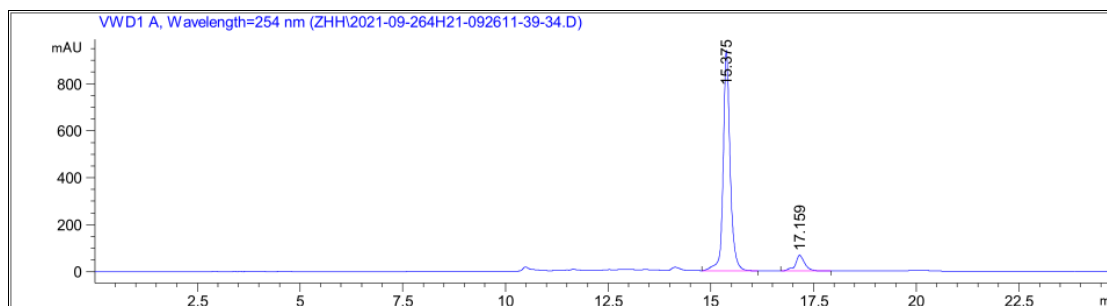
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.360	MM	0.0947	94.33377	16.60680	0.8769
2	13.371	MM	0.1025	238.92009	38.84423	2.2209
3	14.716	VV R	0.1641	1.04247e4	949.26740	96.9023

Compound 2q (95.27%)



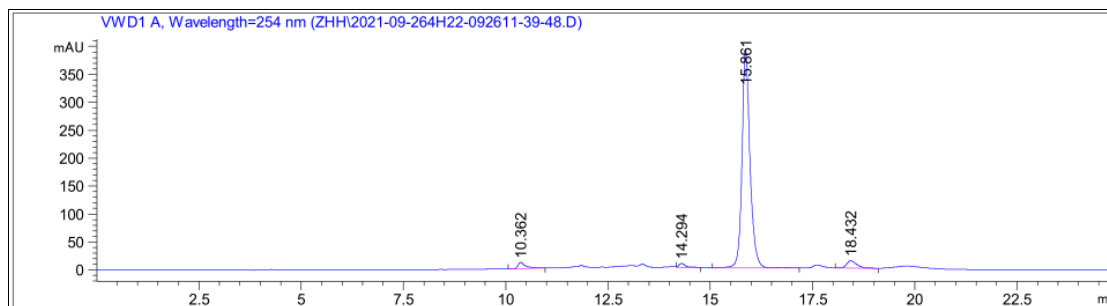
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.931	MM	0.0839	506.04095	100.47110	2.1401
2	14.554	MM	0.1658	2.25275e4	2264.38281	95.2712
3	16.116	MM	0.1241	612.12476	82.21546	2.5887

Compound 2s (96.07%)



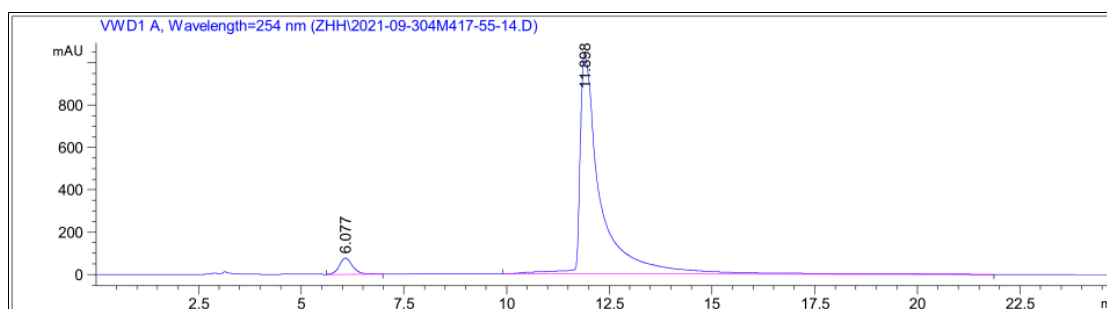
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.375	BB	0.1733	1.10653e4	940.56366	96.0703
2	17.159	MM	0.1574	452.62076	47.94029	3.9297

Compound 2t (96.25%)



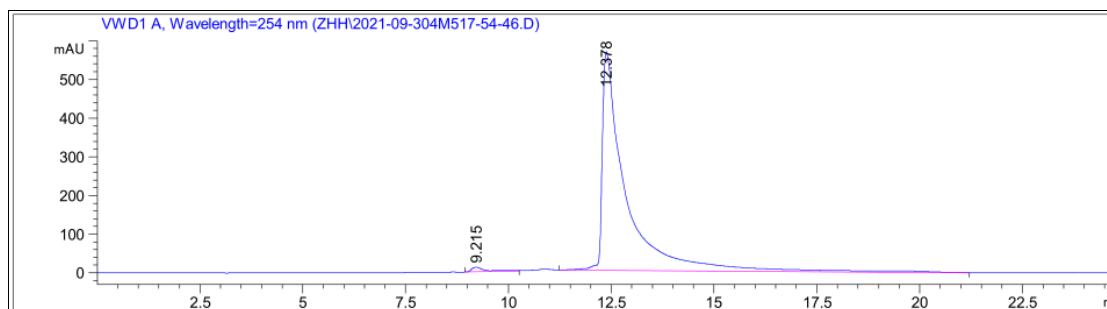
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.362	MM	0.1293	73.10896	9.42502	1.3246
2	14.301	MM	0.1101	35.05720	5.30745	0.6352
3	15.861	BV R	0.2009	5312.41699	390.04886	96.2511
4	18.432	MM	0.1655	98.75054	9.94713	1.7892

Compound 3c (95.56%)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.077	BB	0.3405	1709.30701	76.54395	4.4392
2	11.898	BB	0.4663	3.67957e4	1041.10461	95.5608

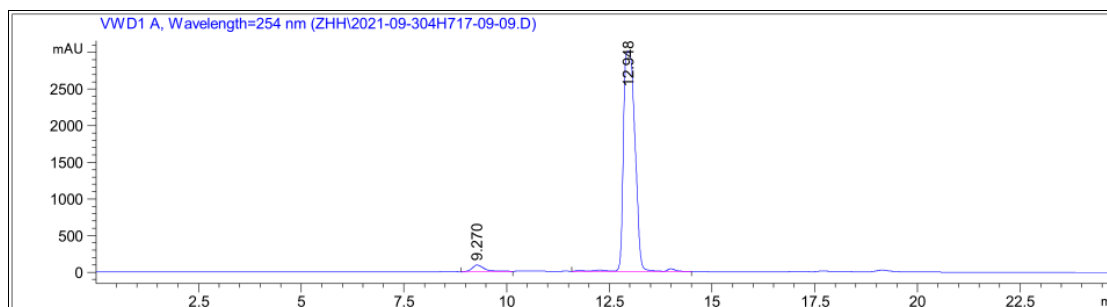
Compound 3d (98.76%)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.215	BV R	0.2957	284.24548	11.61274	1.2355

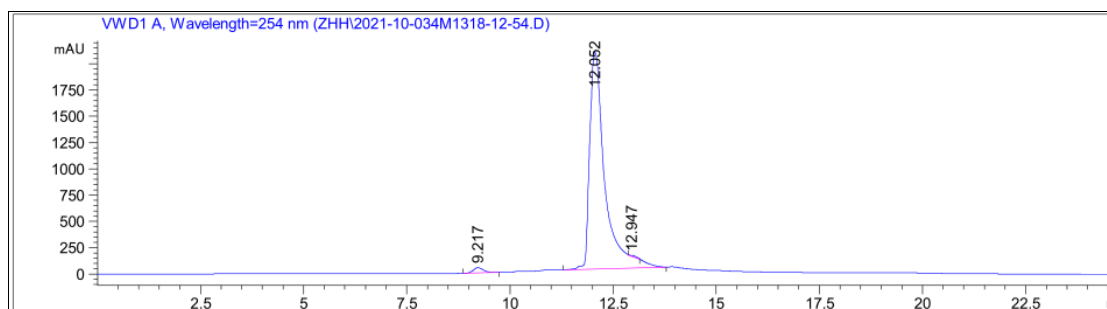
2	12.378	BB	0.5412	2.27219e4	564.98132	98.7645
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Compound 3f (96.98%)



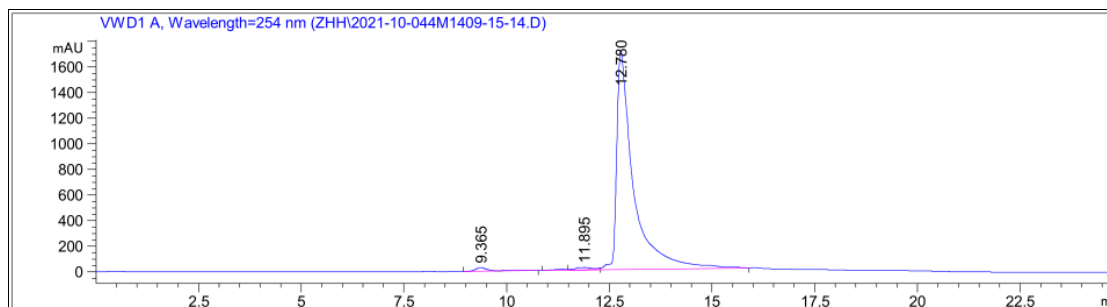
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.270	BB	0.3084	1840.30713	90.04299	3.0238
2	12.948	VV R	0.3031	5.90210e4	3003.79297	96.9762

Compound 3k (98.16%)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.217	BV R	0.2396	858.72552	51.21434	1.5880
2	12.052	BV R	0.3873	5.30844e4	2069.25586	98.1642
3	12.947	VB E	0.1833	134.00050	9.93756	0.2478

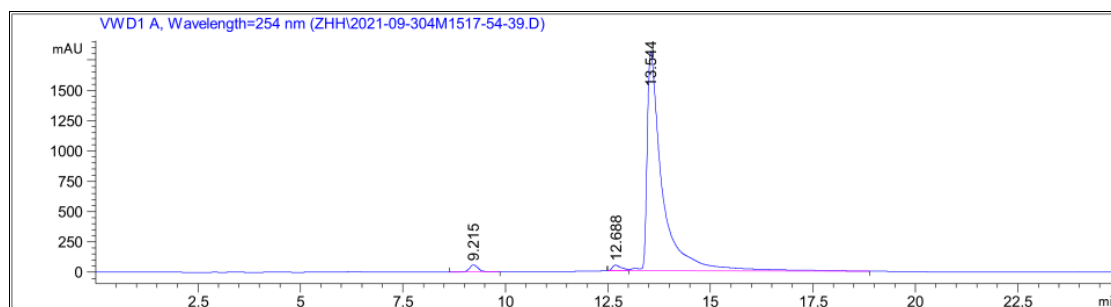
Compound 3l (97.66%)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.365	BV R	0.2910	645.30835	29.62616	1.2952

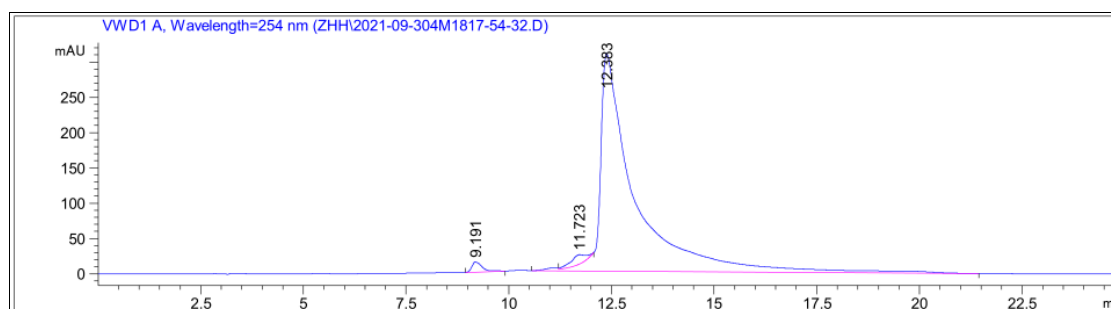
2	11.895	VV E	0.3724	520.21014	18.94187	1.0441
3	12.780	VV R	0.3831	4.86591e4	1707.44263	97.6608

Compound 3m (96.73%)



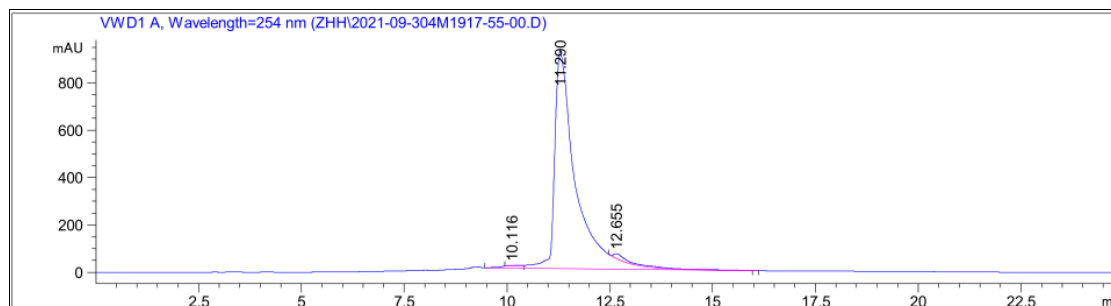
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.215	BB	0.2284	841.56879	57.61187	1.7114
2	12.688	BV E	0.2414	768.66034	46.85566	1.5632
3	13.544	VV R	0.3809	4.75629e4	1807.93433	96.7254

Compound 3p (96.85%)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.191	BV R	0.2771	250.19003	14.23428	1.3233
2	11.723	VV E	0.3591	346.15891	13.23492	1.8309
3	12.383	VB R	0.7671	1.83102e4	308.27759	96.8458

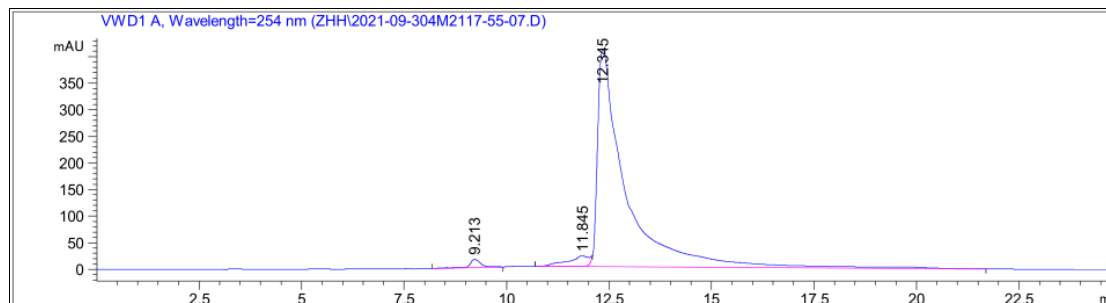
Compound 3q (97.58%)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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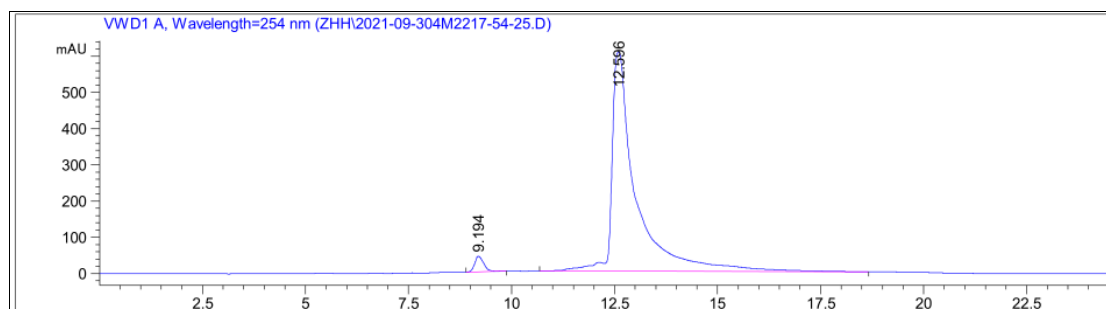
1	10.116	BV E	0.2502	29.00440	2.08663	0.0857
2	11.290	VV R	0.5232	3.30449e4	919.68774	97.5821
3	12.655	VB E	0.4915	789.79517	20.77492	2.3323

Compound 3s (95.21%)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.213	BV R	0.2795	280.43924	15.46843	1.3536
2	11.845	BV E	0.4700	712.02106	19.87464	3.4368
3	12.345	VB R	0.6499	1.97252e4	409.54944	95.2096

Compound 3t (97.42%)

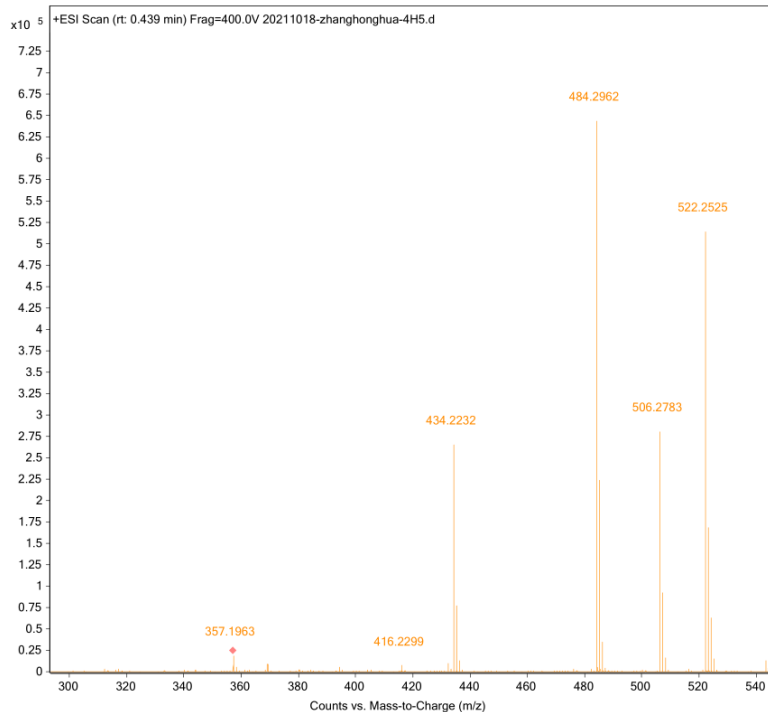


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.194	BV R	0.2420	654.82684	42.91409	2.5775
2	12.596	VB R	0.5482	2.47509e4	605.84290	97.4225

HRMS spectra of synthesized compounds

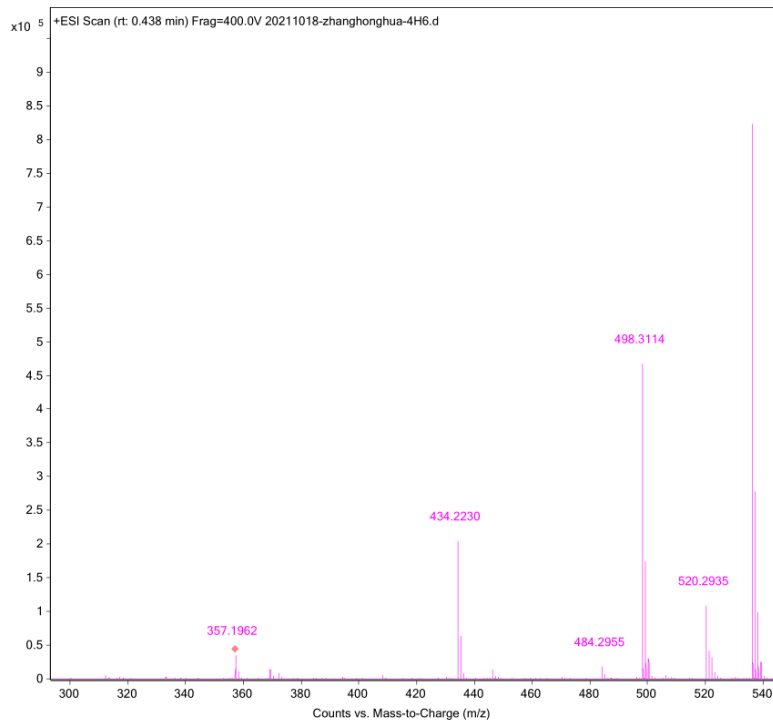
Compound 2d

Sample Name	Sample19	Position	P1-C1	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20211018-zhanghonghua-4H5.d
ACQ Method	0.750mz AB POS MSMS.m	Comment		Acquired Time	10/18/2021 5:56:39 PM (UTC+08:00)



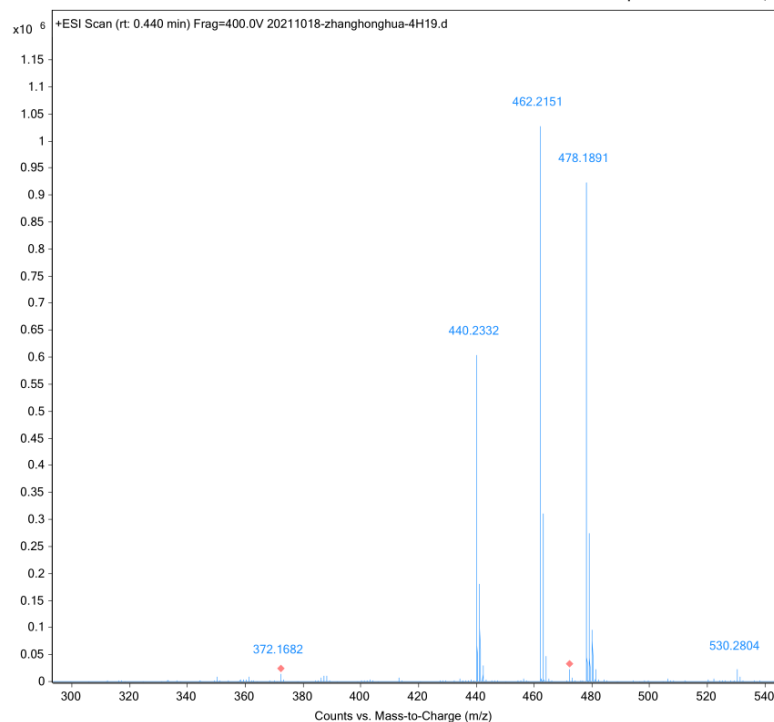
Compound 2e

Sample Name	Sample20	Position	P1-C2	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20211018-zhanghonghua-4H6.d
ACQ Method	0.750mz AB POS MSMS.m	Comment		Acquired Time	10/18/2021 5:58:13 PM (UTC+08:00)



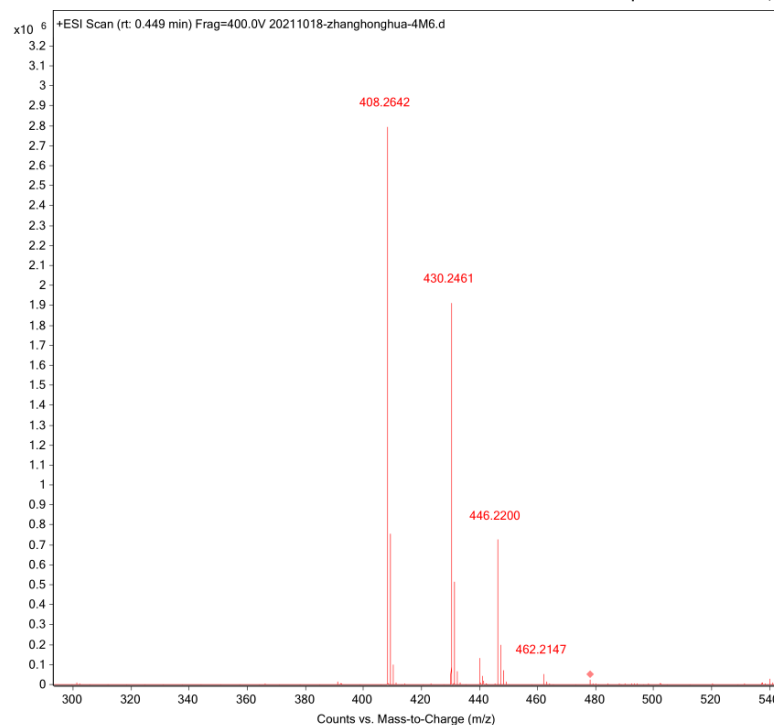
Compound 2q

Sample Name	Sample21	Position	P1-C3	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20211018-zhanghonghua-4H19.d
ACQ Method	0.750mz AB POS MSMS.m	Comment		Acquired Time	10/18/2021 5:59:47 PM (UTC+08:00)



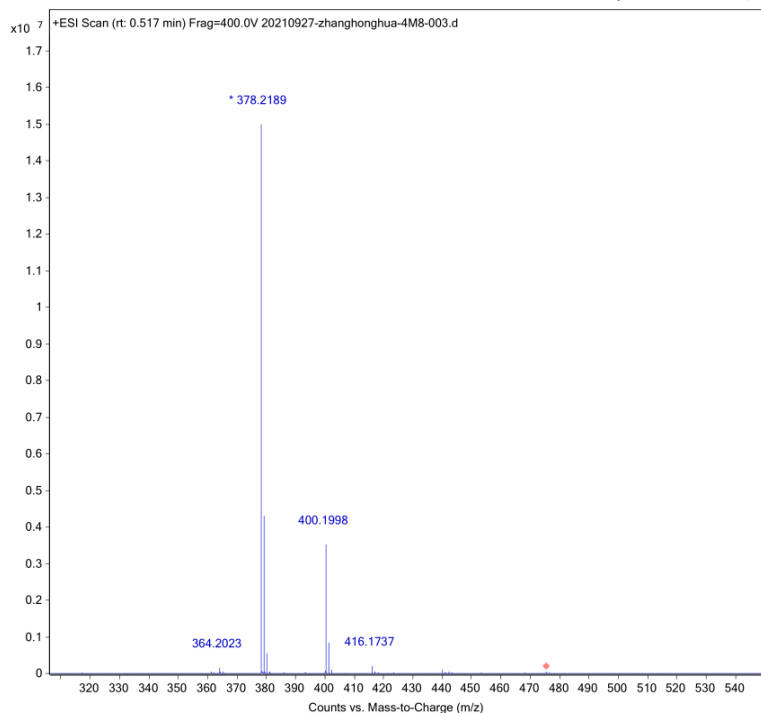
Compound 3e

Sample Name	Sample22	Position	P1-C4	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20211018-zhanghonghua-4M6.d
ACQ Method	0.750mz AB POS MSMS.m	Comment		Acquired Time	10/18/2021 6:01:21 PM (UTC+08:00)



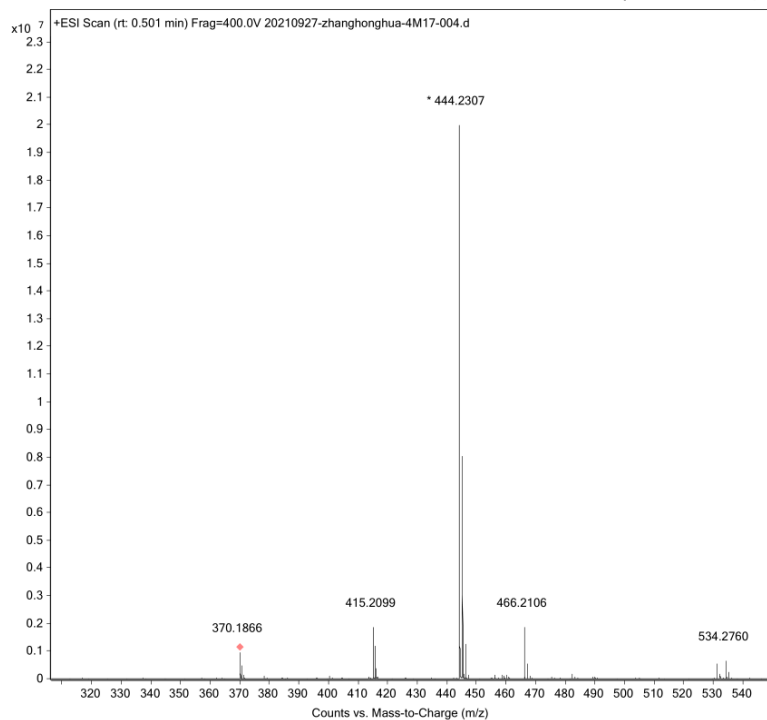
Compound 3g

Sample Name		Position	P1a2	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20210927-zhanghonghua-4M8-003.d
ACQ Method	0 750mz AB POS MSMS.m	Comment		Acquired Time	9/27/2021 10:56:41 AM (UTC+08:00)



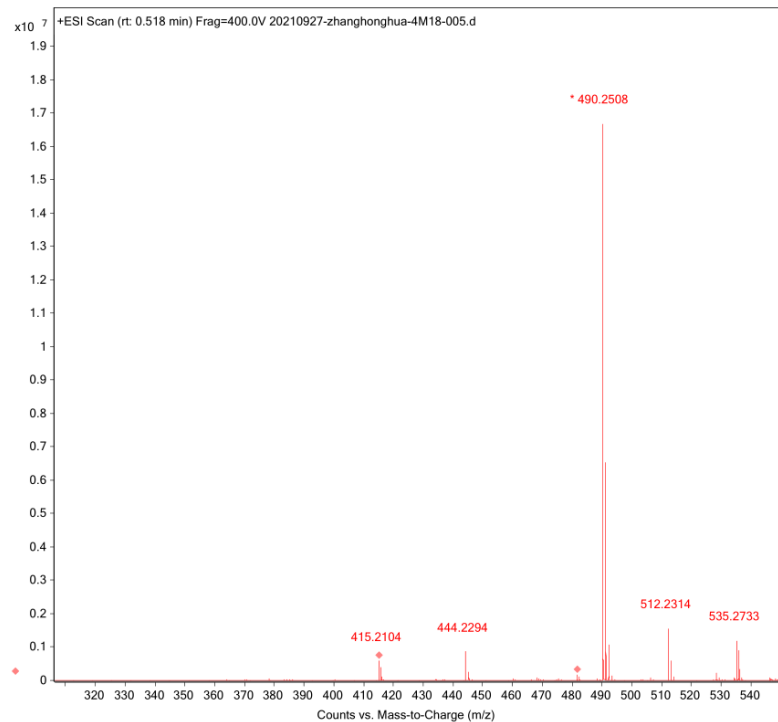
Compound 3o

Sample Name		Position	P1a3	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20210927-zhanghonghua-4M17-004.d
ACQ Method	0 750mz AB POS MSMS.m	Comment		Acquired Time	9/27/2021 10:58:26 AM (UTC+08:00)



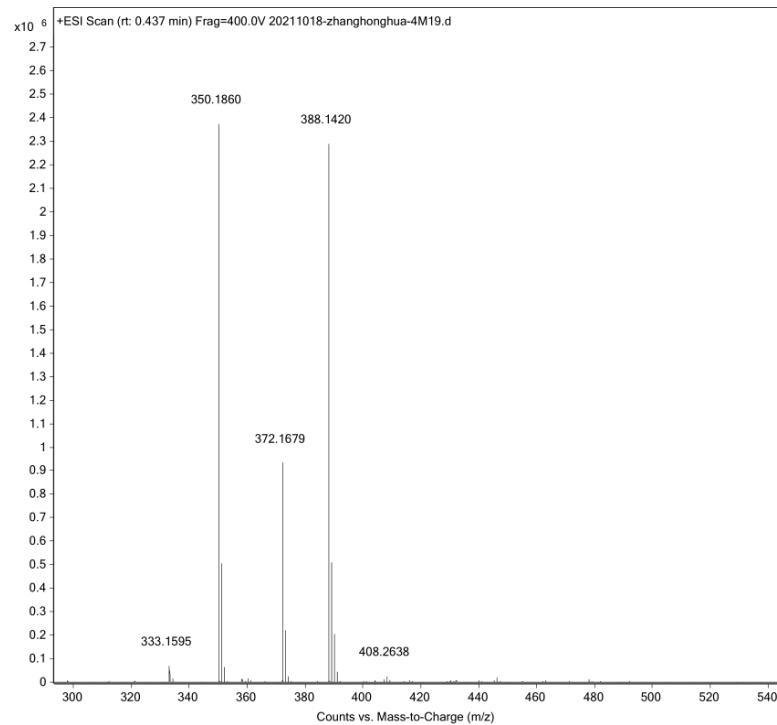
Compound 3p

Sample Name		Position	P1a4	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20210927-zhanghonghua-4M18-005.d
ACQ Method	0 750mz AB POS MSMS.m	Comment		Acquired Time	9/27/2021 11:00:18 AM (UTC+08:00)



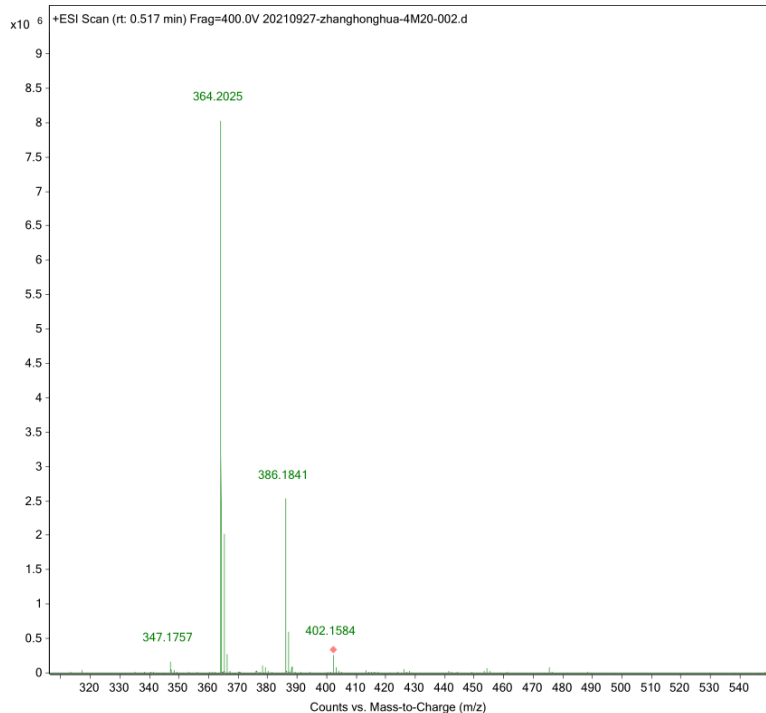
Compound 3q

Sample Name	Sample23	Position	P1-C5	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20211018-zhanghonghua-4M19.d
ACQ Method	0 750mz AB POS MSMS.m	Comment		Acquired Time	10/18/2021 6:02:54 PM (UTC+08:00)



Compound 3r

Sample Name		Position	Pia1	Instrument Name	Instrument 1
User Name		Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	20210927-zhanghonghua-4M20-002.d
ACQ Method	0 750mz AB POS MSMS.m	Comment		Acquired Time	9/27/2021 10:54:47 AM (UTC+08:00)



Molecular formula strings of synthesized compounds

Comp.	Smile String
2a	<chem>O=C(NCCC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2b	<chem>O=C(NCCCC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2c	<chem>O=C(NCCCCC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2d	<chem>O=C(NCCCCC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2e	<chem>O=C(NCCCCCCC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2f	<chem>O=C(NC1CC1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
2g	<chem>O=C(NC1CCCC1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
2h	<chem>O=C(NC1CCCCC1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
2i	<chem>O=C(NC1=CC=CC=C1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
2j	<chem>O=C(N(C)C)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2k	<chem>O=C(N(CC)CC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2l	<chem>O=C(N(CCC)CCC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2m	<chem>O=C(N(CCCC)CCCC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2n	<chem>O=C(N(C1=CC=CC=C1)C2=CC=CC=C2)OC3=CC=C(NC=C4CCN(CC5=CC=CC=C5)CC6=CC=CC=C6)C4=C3</chem>
2o	<chem>O=C(N(C)OC)OC1=CC=C(NC=C2CCN(CC3=CC=CC=C3)CC4=CC=CC=C4)C2=C1</chem>
2p	<chem>O=C(N(C)C1=CC=CC=C1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
2q	<chem>O=C(N1CCC1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>

2r	<chem>O=C(N1CCCC1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
2s	<chem>O=C(N1CCCCC1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
2t	<chem>O=C(N1CCCCC1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
2u	<chem>O=C(N1CCOCC1)OC2=CC=C(NC=C3CCN(CC4=CC=CC=C4)CC5=CC=CC=C5)C3=C2</chem>
3a	<chem>O=C(NCCCC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3b	<chem>O=C(NCCCC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3c	<chem>O=C(NCCCCC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3d	<chem>O=C(NCCCCC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3e	<chem>O=C(NCCCCC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3f	<chem>O=C(NC1CC1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3g	<chem>O=C(NC1CCCC1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3h	<chem>O=C(NC1CCCCC1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3i	<chem>O=C(NC1=CC=CC=C1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3j	<chem>O=C(N(C)C)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3k	<chem>O=C(N(CC)CC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3l	<chem>O=C(N(CCC)CCC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3m	<chem>O=C(N(CCCC)CCCC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3n	<chem>O=C(N(C1=CC=CC=C1)C2=CC=CC=C2)OC3=CC=C(NC=C4CCNCC5=CC=CC=C5)C4=C3</chem>
3o	<chem>O=C(N(C)OC)OC1=CC=C(NC=C2CCNCC3=CC=CC=C3)C2=C1</chem>
3p	<chem>O=C(N(C)C1=CC=CC=C1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3q	<chem>O=C(N1CCC1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3r	<chem>O=C(N1CCCC1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3s	<chem>O=C(N1CCCCC1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3t	<chem>O=C(N1CCCCC1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
3u	<chem>O=C(N1CCOCC1)OC2=CC=C(NC=C3CCNCC4=CC=CC=C4)C3=C2</chem>
4c	<chem>NCCCC1=CNC2=CC=C(OC(NCCCCC)=O)C=C21</chem>
4d	<chem>NCCCC1=CNC2=CC=C(OC(NCCCCC)=O)C=C21</chem>
4e	<chem>NCCCC1=CNC2=CC=C(OC(NCCCCC)=O)C=C21</chem>