Supporting Information

DMAP and PivOH-Promoted Amination/Allenization Reaction

Bo-Sheng Zhang,[ab]‡ Yuke Li,[c]‡ Xue-Ya Gou,[b] Zhe Zhang,[b] Yang An,[b] Xin-Gang Wang,[b] and Yong-Min Liang*[b]

[a]College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu 730070, China
[b]State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, China
[c]Department of Chemistry and Centre for Scientific Modeling and Computation, Chinese University of Hong Kong, Shatin, Hong Kong, China

E-mail: liangym@lzu.edu.cn

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1. General Methods

General Procedures. Unless otherwise noted, reactions were performed under an argon atmosphere. Plastic syringes were used to transfer air- and moisture-sensitive reagents. Solvent was freshly distilled/degassed prior to use unless otherwise noted. Analytical TLC was performed with silica gel GF254 plates. For column chromatography, a 200-300 mesh silica gel was employed. Organic solutions were concentrated under reduced pressure using a rotary evaporator. Room temperature (r.t.) is 23-25°C.

Materials. Commercial reagents were purchased from Acros, Accela, Adamas, Alfa, Ark, Aladdin, or TCI, and used as received with the following exceptions. Toluene was dried over calcium hydride. Other commercially available reagents and solvents were used without further purification.

Instrumentation. Deuterated solvents were purchased from Cambridge Isotope Laboratories. ^{1}H NMR spectra were recorded on Bruker AVANCE III 400, Agilent Mercury plus 300 BB and INOVA instruments with 400, 300 and 600 MHz frequencies, and ^{13}C NMR spectra were recorded on Bruker AVANCE III 400 and Agilent Mercury plus 300 BB instruments with 101 and 75 MHz frequencies. ^{19}F NMR spectra were recorded on a Bruker AVANCE III 400 spectrometer with a ^{19}F operating frequency of 376 MHz. Chemical shifts (δ) were reported in ppm relative to the residual solvent signal ($CDCl_3$ δ = 7.26 for ^{1}H NMR and δ = 77.0 for ^{13}C NMR). Chemical shifts (ppm) were recorded with tetramethylsilane (TMS) as the internal reference standard. Multiplicities are given as s (singlet), d (doublet), t (triplet), dd (doublet of doublets), td (triplet of doublets) or m (multiplet). HRMS was obtained using a Q-TOF instrument equipped with an ESI source. Data collection for crystal structure was performed at room temperature using Mo Kα radiation on a Bruker APEXII diffractometer.

2. Control experiment for triphenylphosphine, L_{N9}, PivOH, Cs_2CO_3[a]

entry	PPh_3	L_{N9}	PivOH	Cs_2CO_3	Yield (%)
1	√	X	X	√	33
2	X	X	X	√	<5
3	√	√	X	√	60(49[b])
4	X	√	X	√	48
5	√	√	X	X	0
6	√	X	√	√	57
7	X	X	√	√	56
8	√	√	√	√	**70**
9	X	√	√	√	56

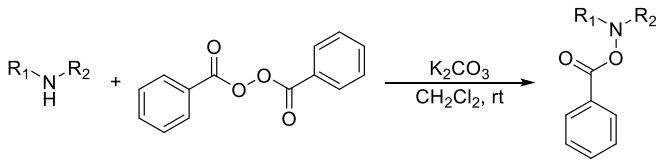
[a] Reaction conditions: substrate **1** (0.2 mmol), **2a** (0.4 mmol, 2.0 equiv.), **3** (0.6 mmol, 3.0 equiv.), $Pd(OAc)_2$ (10 mol%), PPh_3 (20 mol%), norbornene (0.4 mmol, 2.0 equiv.), L_{N9} (0.4 mmol, 2.0 equiv.), PivOH (40 mol%), Cs_2CO_3 (0.8 mmol, 4.0 equiv.), toluene (3.0 mL), 140 °C, 24 h. Isolated yields. [b] L_{N9} (0.04 mmol, 0.2 equiv.).

3. General Procedure

In a 20 mL tube, **1** (0.2 mmol), **2** (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (10 mol%), PPh_3 (20 mol%), Cs_2CO_3 (0.8 mmol, 4.0 equiv.) and 4-dimethylaminopyridine (L_{N9}, 0.4 mmol, 2.0 equiv.) were added and charged with argon more than three times (The tube was sealed with tipping plug). Alkyne **3** (0.6 mmol, 3.0 equiv.), norbornene (0.4 mmol, 2.0 equiv.) and pivalic acid (40 mol%) were dissolved in 3 mL toluene, and the mixture was injected into the tube via plastic syringes. Then the white medical adhesive tape was used to reinforce the tipping plug. The resulting light-yellow suspension was stirred vigorously at room temperature for 15 minutes before being placed in a pre-heated oil bath at 140 °C stirring at 900~1200 rpm for 24 h. After the reaction was completed, the residue was purified with chromatography column on silica gel or preparative TLC (PTLC) (Petroleum ether/EtOAc = 10:1-100:1).

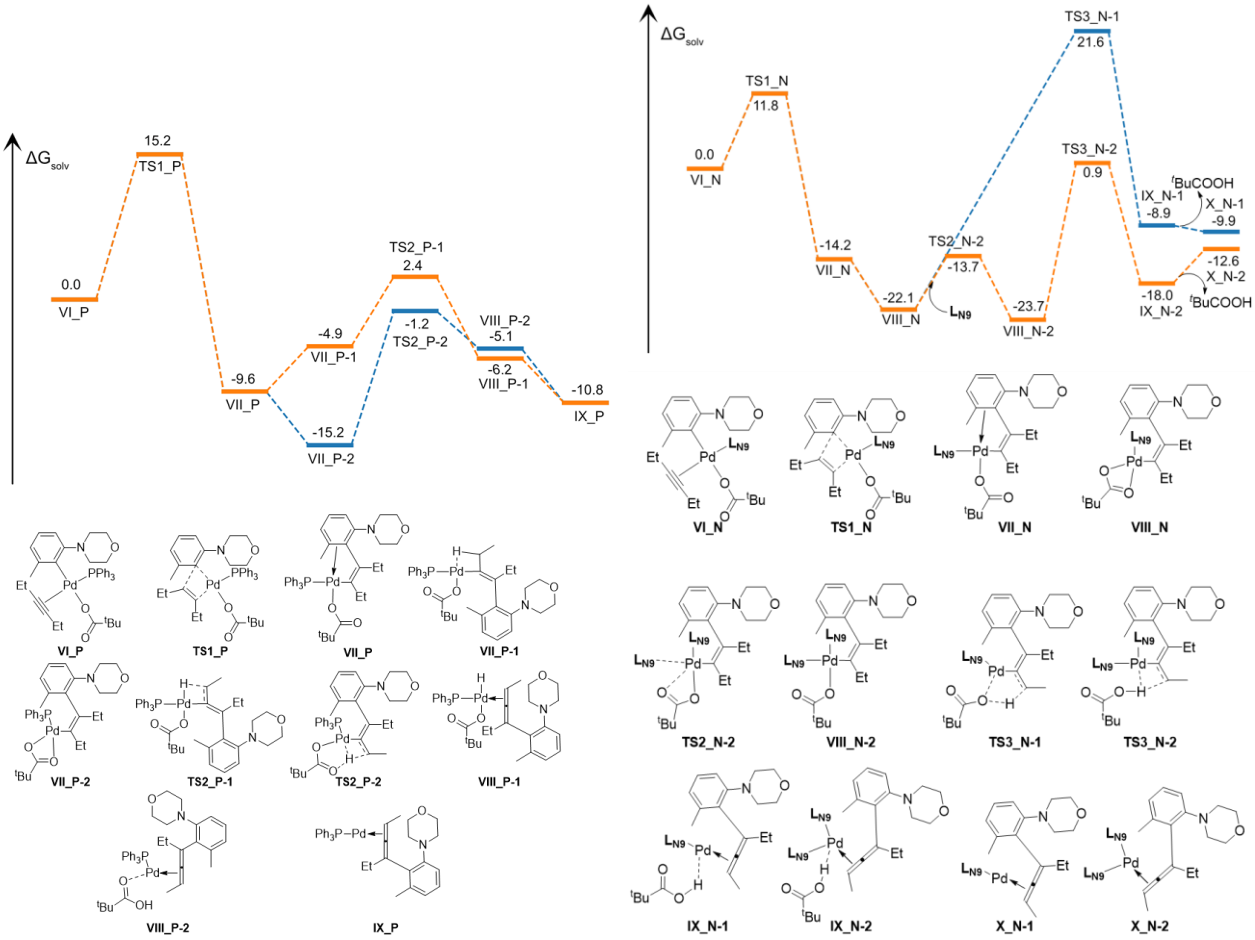
4. Preparation of Substrates

N-benzoyloxyamines (2)



O-Benzoyl hydroxylamines were prepared by literature procedure.[1-3]

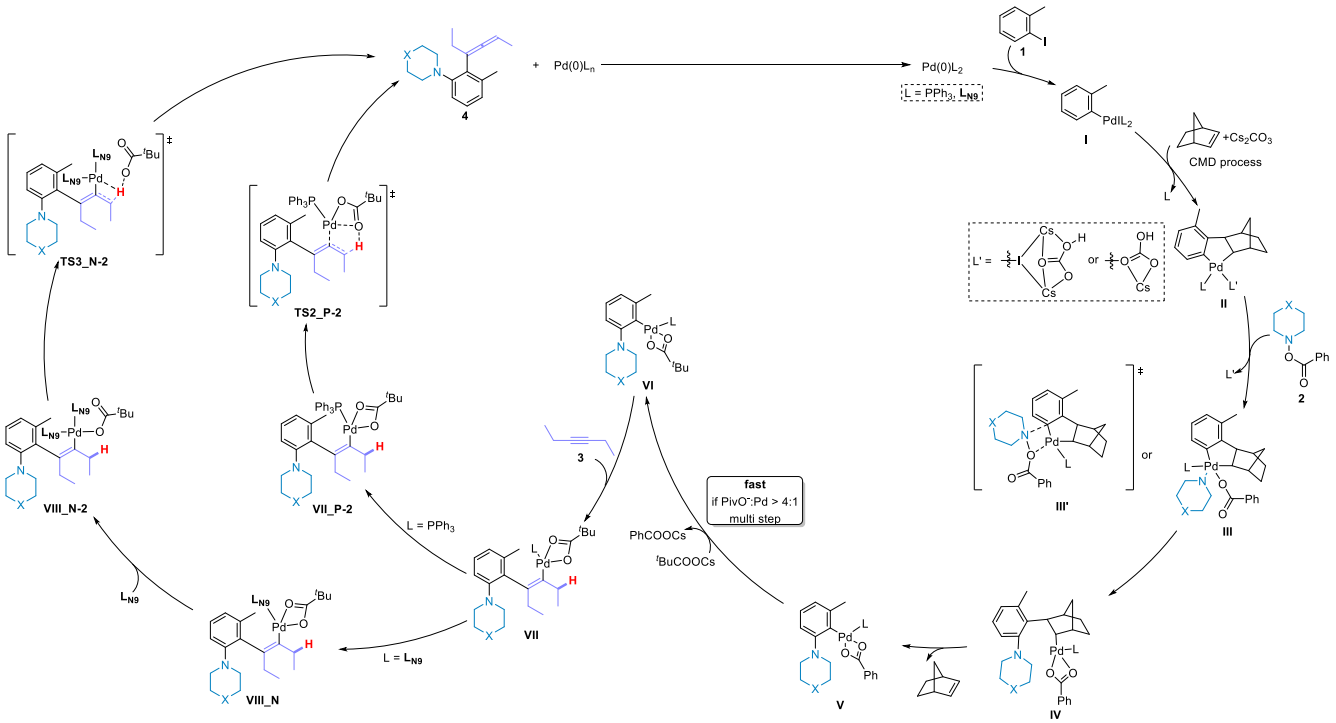
5. Density Functional Theory (DFT) Calculations and Possible Catalytic Cycle



Scheme S1. Computed Free Energy Surface (PPh_3 and L_{N9}).

Based on density functional theory (DFT) calculations, we first studied the dienenylation process when the ligand was triphenylphosphine. The results show that the energy barrier of the migration and insertion process between palladium and alkyne is very low (15.2 kcal/mol). At this time, there are two mechanism pathways. One is that palladium is coordinated with *β*-hydrogen, and then the target product is obtained via the *β*-hydrogen elimination process. The other is that the carbonyl group of carboxylic acid has a bidentate coordination with palladium, and the C(sp^3)-H-activated diene reaction is realized by the CMD process (Figure 1). The energy barrier of *β*-hydrogen elimination is 2.0 kcal/mol, which is lower than that of the CMD process, but the coordination of the carboxylic carbonyl and palladium will first release a Gibbs free energy of 5.6 kcal/mol before the CMD process. Therefore, the reaction mechanism should favor the CMD process.

When 4-dimethylaminopyridine (**L_{N9}**) was used as the ligand, the energy barrier of migration and insertion reaction between palladium and alkyne was lower, only 11.8 kcal/mol. After the migration insertion reaction, we did not find the transition state of the CMD process similar to **TS2_P-2**. After significant effort, we found another transition state **TS3_P-1**, but its energy barrier is as high as 43.7 kcal/mol, indicating that the process is impossible. Because the reaction system needs the addition of equivalent **L_{N9}** to promote the reaction, we speculate that DMAP and palladium may form a double coordination intermediate **VIII_N-2** in this process. Then, the intermediate **VIII_N-2** undergoes the *β*-hydrogen elimination process (**TS3_N-2**, Figure 1). The energy barrier of this process is only 24.6 kcal/mol, so it can be carried out very quickly at 140 °C.



Scheme S2. Possible Catalytic Cycle

6. Computational Details

All the calculations were performed using the Gaussian 09 programs[4]. All of the structures were fully optimized with the B3LYP[5-6] method and Ahlrichs' split-valence def2-SVP basis set[7] in toluene solvent employing the Polarizable Continuum Model (PCM).[8] the temperature is 413.15K. Grimmes's DFT-D3 dispersion correction was used to describe the van der waals interaction.[9] Vibrational frequency calculations were performed to ensure that a transition state has only one imaginary frequency and a local minimum has no imaginary frequency. Transition states connecting relevant minima were further examined by running intrinsic reaction coordinate (IRC) calculations.

Cartesian Coordinates

^{t}BuCOOH

H	4.72343	2.89929	0.15322
O	4.54106	0.21927	-1.20749
C	5.02263	1.22628	-0.75821
O	4.21706	2.13984	-0.16848
C	6.52342	1.57252	-0.80581
C	7.27264	0.41348	-1.47489
H	6.89847	0.23964	-2.49402
H	8.34870	0.64076	-1.52824
H	7.13860	-0.52013	-0.90943
C	6.71269	2.86688	-1.62670
H	6.20585	3.73283	-1.17022
H	7.78411	3.11290	-1.69295
H	6.32425	2.74902	-2.65021
C	7.04630	1.77659	0.63265
H	6.56337	2.62662	1.14246
H	6.88425	0.87713	1.24667
H	8.12735	1.98497	0.60946

L_{N9}

C	-0.99074	7.56553	0.81705
C	-1.23738	8.89428	1.15336
C	-2.35677	9.21299	1.96586
C	-3.15149	8.10896	2.37197
C	-2.79811	6.82439	1.96696
N	-1.74022	6.52558	1.20271
H	-0.12133	7.33419	0.18840
H	-0.56149	9.66413	0.78338
H	-4.03508	8.23924	2.99555
H	-3.42083	5.98042	2.29019
N	-2.65070	10.50031	2.33405
C	-1.81085	11.59474	1.88219
H	-2.19615	12.54078	2.28216
H	-0.76750	11.48275	2.22792
H	-1.79275	11.67541	0.78002
C	-3.81658	10.77212	3.15514
H	-3.88496	11.84978	3.34824
H	-4.75352	10.45672	2.66106
H	-3.76185	10.25718	4.13108

VI_N

Pd	-0.78192	1.40194	0.09508
O	0.81797	0.07727	0.63253
C	1.64928	-0.18924	-0.31964
O	1.47934	0.09348	-1.50974
C	2.94945	-0.89614	0.14780
C	3.78941	-1.31275	-1.06558
H	4.72757	-1.79252	-0.73958
H	3.23841	-2.02218	-1.70197
H	4.03599	-0.44105	-1.68867
C	3.73391	0.11091	1.01245
H	3.97532	1.01826	0.43449
H	3.14414	0.41417	1.89005
H	4.68148	-0.33179	1.36302
C	2.58439	-2.13123	0.99071
H	1.97755	-1.84393	1.86132
H	2.00609	-2.85771	0.39515
H	3.49543	-2.63959	1.34922
C	0.71059	2.91345	0.65939
C	0.63952	2.96848	-0.57604
C	0.86358	3.29649	-1.99093
H	1.13058	2.36285	-2.51053
H	-0.08089	3.65668	-2.42973
C	1.97075	4.34709	-2.15900
H	2.92267	3.98506	-1.74035
H	2.12741	4.56654	-3.22653
H	1.70864	5.28727	-1.64871
C	1.14427	3.02291	2.05832
H	1.20360	2.00503	2.47736
H	0.36551	3.55386	2.62426
C	2.49836	3.73465	2.18707
H	2.78889	3.81163	3.24646
H	3.28419	3.17866	1.65358
H	2.45391	4.75184	1.76739
C	-1.69430	-1.46426	0.35323
C	-2.48762	-2.59768	0.36861
C	-3.89267	-2.49182	0.18219
C	-4.38499	-1.17007	-0.00067
C	-3.51185	-0.09767	-0.00088
N	-2.17741	-0.21636	0.16698
H	-0.61627	-1.53174	0.50488
H	-2.00052	-3.55829	0.52454
H	-5.44413	-0.96647	-0.14587
H	-3.89138	0.91455	-0.14634
N	-4.71108	-3.57931	0.17982
C	-4.15425	-4.91154	0.36224
H	-4.96172	-5.65223	0.32486
H	-3.42666	-5.16161	-0.42924
H	-3.64614	-5.01145	1.33705
C	-6.14307	-3.41465	-0.01911

H	-6.63097	-4.39597	0.01356
H	-6.59454	-2.78511	0.76716
H	-6.36963	-2.95487	-0.99685
C	-2.20932	2.71515	-0.43451
C	-2.73543	3.68169	0.45995
C	-3.62256	4.66082	-0.03037
C	-3.99360	4.67926	-1.37611
C	-3.51164	3.70228	-2.24414
C	-2.62562	2.71062	-1.78437
H	-3.81459	3.70609	-3.29558
H	-4.67435	5.45355	-1.74064
H	-4.03932	5.41340	0.63940
C	-2.16373	1.63844	-2.75086
H	-1.10497	1.37431	-2.61613
H	-2.73396	0.70614	-2.59518
H	-2.31520	1.94736	-3.79640
C	-2.58273	4.87718	2.60994
C	-2.87524	2.49621	2.58798
C	-1.94745	4.75018	3.99273
H	-3.66322	5.09982	2.75423
H	-2.13278	5.72806	2.07506
C	-2.24132	2.43131	3.97113
H	-3.98135	2.55431	2.69760
H	-2.63919	1.57385	2.04324
H	-2.18027	5.64152	4.59542
H	-0.84480	4.68447	3.89336
H	-2.69475	1.61732	4.55735
H	-1.15807	2.22051	3.86877
N	-2.37451	3.65564	1.84219
O	-2.44621	3.63038	4.69752

TS1_N

Pd	0.17470	-0.81772	0.01019
O	-1.48315	-1.80864	0.86452
C	-2.35937	-2.23049	0.01565
O	-2.27298	-2.11974	-1.21128
C	-3.57888	-2.93911	0.66355
C	-4.58450	-3.34831	-0.41930
H	-5.44756	-3.86628	0.03175
H	-4.95222	-2.46854	-0.96841
H	-4.11776	-4.01822	-1.15622
C	-3.06433	-4.18670	1.40728
H	-2.55636	-4.87699	0.71393
H	-2.34752	-3.90266	2.19163
H	-3.90088	-4.73152	1.87658
C	-4.24147	-1.97433	1.66475
H	-3.53486	-1.68999	2.45823
H	-4.58012	-1.05383	1.16074
H	-5.12090	-2.44689	2.13395
C	1.32921	-2.47855	0.15602
C	2.33396	-1.72661	-0.05251

C	3.81117	-1.58107	0.01918
H	4.05400	-0.71818	0.65556
H	4.15249	-2.47936	0.56612
C	4.54142	-1.48162	-1.32391
H	4.28598	-0.55320	-1.85253
H	5.63056	-1.49259	-1.15877
H	4.28583	-2.32896	-1.97920
C	0.84683	-3.85711	0.43092
H	0.09156	-3.81034	1.22947
H	1.69539	-4.45855	0.80437
C	0.23028	-4.52100	-0.81000
H	-0.15388	-5.52161	-0.55545
H	-0.59913	-3.91514	-1.20152
H	0.97952	-4.63590	-1.60952
C	-2.09186	1.12508	0.72187
C	-2.95361	2.20895	0.70671
C	-2.79761	3.22825	-0.27133
C	-1.72323	3.04184	-1.18203
C	-0.91129	1.92390	-1.07832
N	-1.07500	0.96542	-0.14777
H	-2.22163	0.32519	1.45272
H	-3.74505	2.24523	1.45304
H	-1.51199	3.75732	-1.97444
H	-0.08567	1.78723	-1.77875
N	-3.62523	4.31070	-0.33265
C	-4.71412	4.44984	0.62083
H	-5.26428	5.37552	0.41396
H	-5.42718	3.60931	0.55468
H	-4.34403	4.50094	1.65984
C	-3.43234	5.31785	-1.36348
H	-4.19395	6.09959	-1.25691
H	-2.44072	5.79766	-1.28698
H	-3.52536	4.88940	-2.37688
C	1.73065	0.09969	-0.99721
C	2.47515	1.19728	-0.46971
C	3.03805	2.12434	-1.36997
C	2.90730	1.95954	-2.74895
C	2.21396	0.86457	-3.26213
C	1.62731	-0.07903	-2.40164
H	2.12496	0.73052	-4.34337
H	3.35195	2.69438	-3.42541
H	3.57506	2.99430	-0.99143
C	0.90061	-1.26150	-3.00398
H	1.32271	-2.20791	-2.63061
H	-0.16681	-1.27826	-2.73220
H	0.98373	-1.25570	-4.10096
C	3.87784	2.11348	1.33966
C	1.61924	1.46617	1.86151
C	4.26778	1.73200	2.76780
H	3.66945	3.20491	1.30680
H	4.73042	1.91289	0.67315

C	2.07736	1.11181	3.26843
H	1.23045	2.50751	1.84945
H	0.80001	0.79588	1.57383
H	5.08662	2.37834	3.11995
H	4.62628	0.68104	2.77598
H	1.27011	1.30584	3.99100
H	2.32821	0.03145	3.30505
N	2.72669	1.32601	0.91583
O	3.19219	1.88982	3.66838

VII_N

Pd	-0.90340	-1.16849	-0.76492
O	-0.48048	0.52201	0.35158
C	0.02241	1.53313	-0.28010
O	0.21488	1.59649	-1.49396
C	0.35937	2.73092	0.64868
C	1.00924	3.85403	-0.16869
H	1.23510	4.71872	0.47768
H	1.94534	3.51121	-0.63456
H	0.34381	4.18421	-0.97957
C	-0.95560	3.22865	1.27992
H	-1.67364	3.53661	0.50229
H	-1.42523	2.43609	1.88088
H	-0.76631	4.09818	1.93176
C	1.32075	2.25302	1.75251
H	0.85526	1.46302	2.35960
H	2.25008	1.84793	1.31886
H	1.59234	3.09043	2.41721
C	-2.85832	-0.83153	-0.78946
C	-3.34929	-2.00368	-1.20856
C	-4.78378	-2.43318	-1.41835
H	-5.41890	-1.53446	-1.48836
H	-4.85683	-2.94183	-2.39714
C	-5.34051	-3.36654	-0.33211
H	-5.34196	-2.86664	0.64921
H	-6.37632	-3.66503	-0.56269
H	-4.72963	-4.27666	-0.23886
C	-3.53192	0.44410	-0.39817
H	-3.09963	0.79678	0.55286
H	-4.60750	0.26026	-0.21696
C	-3.36180	1.54461	-1.45737
H	-3.81717	2.49016	-1.12026
H	-2.29694	1.72606	-1.66461
H	-3.84391	1.25328	-2.40495
C	1.92874	-2.30602	-1.61489
C	3.27451	-2.62588	-1.52054
C	3.99294	-2.32192	-0.33302
C	3.24317	-1.68198	0.69103
C	1.90067	-1.40223	0.49259
N	1.22990	-1.71082	-0.63331
H	1.37430	-2.53668	-2.52633

H	3.75277	-3.10225	-2.37430
H	3.69607	-1.39258	1.63742
H	1.32509	-0.88470	1.26295
N	5.31714	-2.61912	-0.18646
C	6.01122	-2.26368	1.04072
H	7.05871	-2.58097	0.97252
H	5.99742	-1.17395	1.21948
H	5.56435	-2.75775	1.92130
C	6.04415	-3.25962	-1.26997
H	7.08524	-3.42103	-0.96560
H	5.61120	-4.24213	-1.52808
H	6.04995	-2.64025	-2.18441
C	-2.18998	-2.91522	-1.59820
C	-1.71718	-4.02583	-0.79386
C	-0.75856	-4.89433	-1.37564
C	-0.32056	-4.73059	-2.68266
C	-0.78554	-3.67996	-3.47371
C	-1.71037	-2.77115	-2.94851
H	-0.43509	-3.56469	-4.50149
H	0.41907	-5.42886	-3.08412
H	-0.33166	-5.70614	-0.79183
C	-2.27732	-1.70493	-3.86328
H	-3.37157	-1.79933	-3.94559
H	-2.07708	-0.69088	-3.49335
H	-1.84870	-1.79671	-4.87135
C	-2.46451	-3.29144	1.50804
C	-1.89591	-5.57620	1.13853
C	-1.24684	-3.17328	2.42581
H	-3.33947	-3.61016	2.09899
H	-2.70007	-2.32589	1.05972
C	-0.68723	-5.42841	2.06745
H	-2.76928	-5.84950	1.75570
H	-1.75510	-6.38272	0.40848
H	-1.44940	-2.46196	3.24106
H	-0.38720	-2.79021	1.83867
H	-0.50264	-6.36402	2.61848
H	0.21808	-5.19076	1.47138
N	-2.21172	-4.30856	0.47748
O	-0.92176	-4.41678	3.02926

VIII_N

Pd	0.63493	0.83364	0.68857
C	-0.72522	2.22241	0.27394
C	-0.28850	3.03248	-0.92974
H	-0.66375	4.06740	-0.84919
H	0.81050	3.11783	-0.93409
C	-1.84554	2.46812	0.98628
C	-2.77858	3.63793	0.66902
H	-3.81157	3.31234	0.86141
H	-2.73819	3.89049	-0.40187
C	-2.47096	4.88705	1.50580

H	-3.18174	5.70091	1.28480
H	-2.53978	4.66556	2.58307
H	-1.45301	5.25918	1.30609
C	-0.75660	2.42225	-2.25879
H	-0.35054	1.40632	-2.38792
H	-1.85598	2.34859	-2.29673
H	-0.42550	3.02775	-3.11823
O	2.77830	0.07246	1.26622
C	3.07610	1.29244	1.33502
O	2.19572	2.18578	1.07248
C	4.47782	1.72695	1.77888
C	4.57929	1.42037	3.28914
H	4.41890	0.34875	3.48040
H	5.57712	1.69827	3.66638
H	3.82743	1.98977	3.85924
C	5.51994	0.89543	1.00909
H	5.46431	1.09494	-0.07344
H	6.53668	1.14918	1.35084
H	5.35236	-0.17953	1.16654
C	4.69225	3.22578	1.52805
H	4.60212	3.46633	0.45752
H	3.94652	3.82756	2.06681
H	5.69748	3.52580	1.86637
C	-0.79765	-1.32718	-0.81318
C	-1.53797	-2.47482	-1.03031
C	-2.17660	-3.12632	0.06108
C	-1.97479	-2.52948	1.33412
C	-1.21743	-1.37794	1.45203
N	-0.63014	-0.76512	0.40239
H	-0.31616	-0.82212	-1.65196
H	-1.61917	-2.84774	-2.04912
H	-2.42015	-2.93696	2.23878
H	-1.08183	-0.91163	2.42846
N	-2.94142	-4.24007	-0.10633
C	-3.14107	-4.79587	-1.43617
H	-3.78589	-5.67989	-1.36815
H	-3.62760	-4.07165	-2.11284
H	-2.18709	-5.10691	-1.89609
C	-3.59302	-4.85466	1.04041
H	-4.15636	-5.73528	0.71013
H	-2.86020	-5.18442	1.79687
H	-4.30009	-4.16126	1.52884
C	-2.25248	1.65516	2.17887
C	-3.44719	0.87545	2.14410
C	-3.81805	0.12537	3.27519
C	-3.03808	0.14466	4.43087
C	-1.88781	0.92900	4.48007
C	-1.49051	1.69877	3.37257
H	-1.29312	0.96728	5.39674
H	-3.33604	-0.45065	5.29846
H	-4.71144	-0.49901	3.24579

C	-0.27167	2.58366	3.51240
H	-0.38876	3.52708	2.96294
H	-0.07914	2.81251	4.57150
H	0.63041	2.10854	3.09670
C	-3.74171	0.34243	-0.25914
C	-5.68223	0.54580	1.14467
C	-4.56930	0.84035	-1.43480
H	-3.76785	-0.76684	-0.24543
H	-2.70169	0.65546	-0.38436
C	-6.45837	1.04301	-0.07501
H	-5.84479	-0.55101	1.24230
H	-6.08306	1.02733	2.04967
H	-4.22742	0.36785	-2.36867
H	-4.44396	1.93837	-1.53245
H	-7.51154	0.72833	-0.00947
H	-6.42525	2.15209	-0.09591
N	-4.27435	0.87774	0.99313
O	-5.93997	0.51333	-1.27966

TS2_N-2

C	-2.87722	2.75759	-0.30061
C	-4.18474	2.50964	0.10334
C	-4.42146	1.80446	1.30908
C	-3.26494	1.42972	2.03988
C	-2.00850	1.75122	1.53960
N	-1.78616	2.39712	0.38697
H	-2.70604	3.26625	-1.25507
H	-5.00068	2.83032	-0.54187
H	-3.33040	0.87985	2.97720
H	-1.12403	1.44561	2.10780
N	-5.68678	1.48559	1.73487
C	-6.83919	1.87402	0.94183
H	-7.75692	1.54758	1.44645
H	-6.89662	2.96922	0.81088
H	-6.82266	1.41332	-0.06200
C	-5.86812	0.71317	2.95033
H	-6.93833	0.53909	3.11651
H	-5.37073	-0.27161	2.88872
H	-5.46907	1.23893	3.83643
Pd	-0.57134	-0.28733	-0.92512
C	0.47439	-1.95707	-0.63975
C	0.27610	-2.90128	-1.80573
H	0.53747	-3.92998	-1.50517
H	-0.79379	-2.92776	-2.06543
C	1.23458	-2.22744	0.44184
C	1.96092	-3.56413	0.61660
H	2.90714	-3.37143	1.14293
H	2.24257	-3.98669	-0.36048
C	1.13516	-4.58894	1.40508
H	1.69607	-5.52757	1.54961
H	0.87260	-4.19806	2.40124

H	0.19480	-4.82953	0.88318
C	1.09465	-2.51720	-3.04715
H	0.78299	-1.53430	-3.43527
H	2.17099	-2.46167	-2.81316
H	0.95965	-3.25380	-3.85586
O	-2.90075	0.36870	-2.11115
C	-3.17431	-0.71416	-1.57265
O	-2.30798	-1.40289	-0.90948
C	-4.58478	-1.33267	-1.65676
C	-5.10478	-1.56981	-0.22556
H	-5.18737	-0.62158	0.32570
H	-6.10349	-2.03736	-0.25436
H	-4.42366	-2.22940	0.33116
C	-5.52532	-0.38749	-2.41400
H	-5.16855	-0.21162	-3.43955
H	-6.54063	-0.81491	-2.46375
H	-5.57781	0.59175	-1.91594
C	-4.47184	-2.68044	-2.39657
H	-4.07976	-2.53991	-3.41727
H	-3.79516	-3.36195	-1.86068
H	-5.46223	-3.15916	-2.47596
C	1.71589	1.25656	-2.09575
C	2.71155	2.21233	-2.19122
C	3.08941	2.96063	-1.04231
C	2.37514	2.66062	0.14743
C	1.39201	1.68796	0.14319
N	1.05428	0.97928	-0.95353
H	1.43484	0.67170	-2.97298
H	3.19083	2.36056	-3.15660
H	2.58336	3.16611	1.08765
H	0.85790	1.45085	1.06073
N	4.08223	3.89315	-1.07837
C	4.80106	4.14563	-2.31723
H	5.55574	4.92300	-2.14886
H	5.32023	3.24134	-2.68094
H	4.12561	4.49665	-3.11660
C	4.45024	4.61100	0.13213
H	5.25987	5.31511	-0.09368
H	3.60166	5.18853	0.53783
H	4.80484	3.92567	0.92224
C	1.40031	-1.28534	1.59535
C	2.68069	-0.72506	1.88828
C	2.81953	0.14563	2.98512
C	1.73012	0.44347	3.80248
C	0.48971	-0.13549	3.54475
C	0.30981	-1.00564	2.45455
H	-0.35545	0.07085	4.20711
H	1.85449	1.12500	4.64847
H	3.78324	0.61129	3.19189
C	-1.04860	-1.63875	2.25838
H	-0.97187	-2.65761	1.85803

H	-1.59877	-1.67256	3.21128
H	-1.65855	-1.07616	1.53600
C	3.84022	-0.72317	-0.30947
C	5.13569	-0.92790	1.70428
C	4.87817	-1.56635	-1.03512
H	4.09571	0.34837	-0.43964
H	2.85514	-0.89167	-0.75173
C	6.14164	-1.76944	0.91831
H	5.48327	0.12942	1.70353
H	5.11471	-1.27490	2.74858
H	4.96137	-1.24515	-2.08502
H	4.56535	-2.63058	-1.01864
H	7.15843	-1.60847	1.30924
H	5.88612	-2.84265	1.03974
N	3.81468	-1.06755	1.11192
O	6.16254	-1.42203	-0.45224

TS3_N-2

C	-2.55033	1.54136	-0.73184
C	-3.78584	2.02767	-1.12808
C	-4.88127	1.98178	-0.22591
C	-4.59481	1.46922	1.06654
C	-3.32254	1.00070	1.35488
N	-2.30218	1.01987	0.48106
H	-1.71053	1.55399	-1.43106
H	-3.89358	2.40659	-2.14239
H	-5.35965	1.39797	1.83693
H	-3.11545	0.55734	2.33050
N	-6.13823	2.37965	-0.58646
C	-6.39617	2.82687	-1.94509
H	-7.45315	3.10212	-2.04434
H	-5.79215	3.71384	-2.20357
H	-6.17696	2.03806	-2.68713
C	-7.24313	2.22258	0.34507
H	-8.16925	2.57570	-0.12437
H	-7.38838	1.16649	0.63540
H	-7.08762	2.81026	1.26641
Pd	-0.41446	-0.13878	0.81376
C	0.92465	-1.44574	1.34816
C	-0.27560	-2.22287	1.60597
H	-0.49736	-2.36443	2.67746
H	-1.52115	-1.69163	1.26779
C	2.25334	-1.59624	1.39133
C	2.90989	-2.85850	1.93723
H	3.53503	-3.29010	1.13677
H	2.13322	-3.60258	2.17033
C	3.77494	-2.62055	3.18188
H	4.28190	-3.54900	3.49262
H	4.55208	-1.86312	2.98963
H	3.16533	-2.27023	4.03067
C	-0.44260	-3.51665	0.79490

H	-0.43126	-3.29914	-0.28137
H	0.36912	-4.22571	1.02452
H	-1.40528	-3.99434	1.02325
O	-2.91361	-1.94352	1.12045
C	-3.24121	-1.97396	-0.12132
O	-2.47788	-1.74729	-1.06971
C	-4.71128	-2.39133	-0.42754
C	-4.65067	-3.87172	-0.85752
H	-4.25877	-4.50210	-0.04240
H	-5.65507	-4.24396	-1.12329
H	-3.99078	-3.99212	-1.73057
C	-5.61244	-2.24049	0.80472
H	-5.65393	-1.18990	1.13179
H	-6.63961	-2.57318	0.57482
H	-5.22896	-2.83277	1.64729
C	-5.25301	-1.54030	-1.58740
H	-5.35063	-0.48503	-1.28898
H	-4.56660	-1.58289	-2.44445
H	-6.24717	-1.89991	-1.90389
C	1.43249	1.53553	-0.95325
C	2.25236	2.57605	-1.34747
C	2.32127	3.75876	-0.56573
C	1.44952	3.80668	0.55478
C	0.65401	2.71366	0.85671
N	0.64907	1.57367	0.14242
H	1.41078	0.61270	-1.53170
H	2.86429	2.43748	-2.23539
H	1.39693	4.67748	1.20540
H	-0.00929	2.74323	1.72403
N	3.17557	4.77842	-0.86785
C	4.06926	4.66359	-2.00960
H	4.70453	5.55561	-2.06676
H	4.72638	3.78151	-1.92135
H	3.51346	4.58124	-2.96033
C	3.21538	5.96631	-0.03166
H	3.96583	6.66372	-0.42259
H	2.24316	6.48977	-0.01533
H	3.48775	5.72370	1.01089
C	3.19331	-0.54530	0.87732
C	3.89346	-0.77143	-0.33844
C	4.86913	0.14965	-0.76118
C	5.13542	1.29184	-0.00643
C	4.42249	1.53544	1.16667
C	3.45525	0.62594	1.62327
H	4.62206	2.43940	1.74830
H	5.89506	2.00260	-0.34415
H	5.41020	-0.01772	-1.69345
C	2.73186	0.89492	2.92056
H	1.64261	0.89992	2.77344
H	2.94075	0.10876	3.66255
H	3.03307	1.86251	3.34821

C	2.31376	-2.01657	-1.76472
C	4.66673	-2.48715	-1.93639
C	2.02139	-3.45894	-2.15596
H	2.31372	-1.38801	-2.68348
H	1.52076	-1.65497	-1.09987
C	4.30995	-3.92418	-2.31565
H	4.80551	-1.90153	-2.87272
H	5.62125	-2.47652	-1.38757
H	1.08938	-3.51750	-2.73802
H	1.89647	-4.06311	-1.23519
H	5.05910	-4.33263	-3.01192
H	4.30736	-4.54828	-1.39773
N	3.61421	-1.93841	-1.09520
O	3.05624	-3.99642	-2.96417

IX_N-2

C	-2.85285	1.83819	0.55758
C	-4.15368	2.00438	0.10634
C	-5.21513	1.30822	0.74053
C	-4.84823	0.51166	1.85778
C	-3.51475	0.41237	2.22252
N	-2.50917	1.04359	1.58705
H	-2.02797	2.34558	0.05403
H	-4.32401	2.65129	-0.75213
H	-5.58518	-0.05299	2.42577
H	-3.22492	-0.22761	3.05984
N	-6.50338	1.37740	0.28767
C	-6.81208	2.14839	-0.90508
H	-7.88584	2.07941	-1.11711
H	-6.56077	3.21572	-0.77877
H	-6.26506	1.77365	-1.78943
C	-7.54389	0.59504	0.93395
H	-8.50269	0.77937	0.43453
H	-7.33502	-0.48884	0.88274
H	-7.65968	0.86902	1.99688
Pd	-0.39754	0.27756	1.78227
C	1.03853	-1.03300	2.19192
C	-0.10962	-1.48892	2.88462
H	-0.15838	-1.25285	3.96102
H	-1.46731	-1.01287	0.36423
C	2.29267	-1.32801	1.83282
C	2.99423	-2.58697	2.32803
H	3.36760	-3.13874	1.44723
H	2.25149	-3.23757	2.81813
C	4.16209	-2.32280	3.28754
H	4.67553	-3.26039	3.55937
H	4.90856	-1.65308	2.82981
H	3.81106	-1.84828	4.21844
C	-0.83358	-2.77788	2.52651
H	-0.73538	-3.01834	1.45842
H	-0.42226	-3.63184	3.09807

H	-1.91129	-2.72201	2.75475
O	-2.12623	-1.55370	-0.16395
C	-2.32794	-0.99933	-1.35915
O	-1.68076	-0.06111	-1.77596
C	-3.45248	-1.68542	-2.14841
C	-3.02757	-3.14105	-2.43589
H	-2.85994	-3.69660	-1.50170
H	-3.81735	-3.65426	-3.00759
H	-2.10145	-3.17743	-3.03125
C	-4.74390	-1.67742	-1.30525
H	-5.07141	-0.64990	-1.08894
H	-5.55112	-2.18500	-1.85752
H	-4.59640	-2.19382	-0.34635
C	-3.67444	-0.92589	-3.46225
H	-3.96693	0.11723	-3.26765
H	-2.75719	-0.90424	-4.06861
H	-4.47182	-1.41035	-4.04764
C	0.78860	1.74855	-0.72826
C	1.73281	2.49604	-1.41164
C	2.39420	3.56758	-0.75989
C	1.96076	3.84460	0.56301
C	1.00211	3.03541	1.15414
N	0.42844	1.98130	0.54926
H	0.28234	0.91758	-1.22074
H	1.97384	2.20983	-2.43308
H	2.38187	4.66208	1.14543
H	0.68893	3.23020	2.18406
N	3.39169	4.28019	-1.36543
C	3.79005	3.95792	-2.72493
H	4.60841	4.62042	-3.03240
H	4.14360	2.91597	-2.80915
H	2.95824	4.09389	-3.43868
C	4.08931	5.31980	-0.63120
H	4.88030	5.74512	-1.26088
H	3.41436	6.14280	-0.33474
H	4.56156	4.92350	0.28572
C	3.10515	-0.44849	0.92553
C	3.38357	-0.86350	-0.40418
C	4.29005	-0.13148	-1.19158
C	4.89646	1.01699	-0.68183
C	4.57994	1.46147	0.60053
C	3.68854	0.74287	1.41356
H	5.03654	2.37659	0.98732
H	5.60552	1.57789	-1.29712
H	4.50857	-0.44971	-2.21209
C	3.38833	1.23026	2.80996
H	2.30443	1.33170	2.96315
H	3.74190	0.51346	3.56738
H	3.86598	2.20239	3.00309
C	1.30152	-1.94319	-1.12783
C	3.39043	-2.78348	-1.96441

C	0.72373	-3.34688	-1.21687
H	1.08104	-1.39956	-2.07226
H	0.82601	-1.39530	-0.30751
C	2.75422	-4.17235	-2.04367
H	3.28715	-2.29125	-2.95772
H	4.46559	-2.88378	-1.74815
H	-0.34791	-3.31030	-1.45333
H	0.84639	-3.84995	-0.23621
H	3.17204	-4.73674	-2.89223
H	2.98295	-4.72452	-1.10828
N	2.74592	-2.02512	-0.90577
O	1.35543	-4.10055	-2.24126

X_N-2

C	-2.97916	1.72857	0.35684
C	-4.27801	2.19178	0.20066
C	-5.33762	1.58335	0.92466
C	-4.95961	0.51091	1.77608
C	-3.62821	0.12901	1.85713
N	-2.63063	0.71455	1.16838
H	-2.16047	2.19337	-0.19839
H	-4.45392	3.02129	-0.48215
H	-5.69033	-0.02957	2.37533
H	-3.33645	-0.69703	2.51091
N	-6.63413	2.00146	0.81040
C	-6.96719	3.10338	-0.07610
H	-8.04721	3.29024	-0.03745
H	-6.45171	4.03593	0.21536
H	-6.69936	2.88266	-1.12471
C	-7.67980	1.34709	1.57852
H	-8.64460	1.82065	1.36012
H	-7.76451	0.27480	1.32749
H	-7.50180	1.42694	2.66568
Pd	-0.51971	-0.03546	1.37443
C	0.94278	-1.24547	1.94228
C	-0.24931	-1.78426	2.49139
H	-0.42609	-1.61491	3.56699
C	2.25440	-1.45016	1.77103
C	2.97506	-2.64057	2.39082
H	3.51073	-3.17998	1.59030
H	2.22234	-3.33706	2.79540
C	3.97111	-2.25679	3.49355
H	4.51720	-3.13941	3.86749
H	4.71656	-1.53550	3.11965
H	3.45533	-1.79107	4.34939
C	-0.86001	-3.08072	1.97784
H	-0.65233	-3.22587	0.90635
H	-0.45329	-3.95992	2.51547
H	-1.95575	-3.09900	2.10857
C	0.93655	1.38675	-1.01691
C	1.85176	2.22685	-1.62761

C	2.19787	3.45727	-1.01228
C	1.49598	3.76635	0.18183
C	0.58688	2.85507	0.69999
N	0.30779	1.66541	0.14055
H	0.70579	0.42008	-1.46939
H	2.32631	1.89332	-2.54763
H	1.66550	4.69524	0.72351
H	0.06127	3.08332	1.63200
N	3.15312	4.28541	-1.53269
C	3.82043	3.93364	-2.77459
H	4.55856	4.70580	-3.02375
H	4.34954	2.96903	-2.69211
H	3.10867	3.86047	-3.61632
C	3.51123	5.50799	-0.83662
H	4.32395	6.01089	-1.37478
H	2.66246	6.21259	-0.77016
H	3.86144	5.30325	0.19074
C	3.10561	-0.52011	0.95602
C	3.62411	-0.94981	-0.29525
C	4.54545	-0.14425	-0.98817
C	4.93201	1.09055	-0.46623
C	4.38177	1.54284	0.73196
C	3.47301	0.75157	1.45320
H	4.66744	2.52189	1.12648
H	5.65515	1.70874	-1.00571
H	4.94956	-0.47504	-1.94621
C	2.91963	1.25462	2.76378
H	1.82171	1.31372	2.72343
H	3.16013	0.56642	3.58881
H	3.32187	2.24889	3.00948
C	1.81712	-2.30057	-1.26237
C	4.09634	-2.91656	-1.71711
C	1.42108	-3.76578	-1.38236
H	1.69346	-1.81132	-2.25532
H	1.15595	-1.79769	-0.54563
C	3.64108	-4.37256	-1.81850
H	4.10321	-2.47905	-2.74119
H	5.12561	-2.87818	-1.32760
H	0.40798	-3.85914	-1.80314
H	1.42439	-4.22306	-0.37200
H	4.25543	-4.91600	-2.55359
H	3.76675	-4.85839	-0.82849
N	3.20723	-2.20110	-0.81811
O	2.29709	-4.47137	-2.24779

TS3_N-1

Pd	-1.13794	1.22634	-0.38645
C	-1.22362	-0.80356	-0.90235
C	-2.25421	-0.93236	-1.84471
H	-2.87339	-1.83705	-1.73735
H	-3.25107	0.17492	-1.08385

C	-0.47052	-1.69903	-0.21514
C	-0.38015	-3.12870	-0.74953
H	0.64311	-3.50766	-0.60614
H	-0.57738	-3.12889	-1.83336
C	-1.37218	-4.06485	-0.04393
H	-1.27298	-5.10207	-0.40688
H	-1.19968	-4.07076	1.04475
H	-2.41345	-3.74568	-0.21437
C	-2.16579	-0.36789	-3.25227
H	-1.64680	0.60512	-3.26001
H	-1.60631	-1.03746	-3.93569
H	-3.16226	-0.21216	-3.70076
O	-4.29802	2.25103	1.07713
C	-4.39384	1.37179	0.25405
O	-3.36264	1.10136	-0.56739
C	-5.63697	0.48686	0.06322
C	-5.29645	-0.92913	0.57800
H	-5.01820	-0.90684	1.64259
H	-6.17449	-1.58447	0.46487
H	-4.46431	-1.37786	0.01577
C	-6.79166	1.07912	0.88174
H	-7.04395	2.09215	0.53353
H	-7.68603	0.44393	0.78452
H	-6.52376	1.15088	1.94550
C	-6.01637	0.42556	-1.42984
H	-6.21413	1.43134	-1.83308
H	-5.22285	-0.03661	-2.03612
H	-6.92927	-0.17789	-1.55514
C	1.60266	2.15779	-1.25527
C	2.94030	2.50784	-1.19585
C	3.65457	2.38038	0.02732
C	2.89777	1.90339	1.12950
C	1.56095	1.58031	0.97076
N	0.89772	1.69386	-0.20003
H	1.06083	2.24262	-2.19948
H	3.41929	2.86545	-2.10518
H	3.34053	1.75294	2.11152
H	0.99386	1.19510	1.81871
N	4.97975	2.68176	0.13043
C	5.72141	3.12030	-1.04142
H	6.76572	3.30571	-0.76353
H	5.71244	2.35802	-1.84045
H	5.31104	4.05667	-1.45768
C	5.66899	2.50208	1.39850
H	6.71651	2.80764	1.29071
H	5.21807	3.11593	2.19712
H	5.65293	1.44807	1.72870
C	0.21154	-1.44870	1.08857
C	1.62285	-1.63380	1.22363
C	2.23010	-1.44103	2.47918
C	1.47622	-1.06978	3.59095

C	0.09878	-0.89628	3.46917
C	-0.54384	-1.09388	2.23611
H	-0.49724	-0.62658	4.34513
H	1.96794	-0.91629	4.55555
H	3.30951	-1.55006	2.58429
C	-2.04760	-0.95942	2.17827
H	-2.49398	-1.71850	1.52235
H	-2.49019	-1.05414	3.18120
H	-2.34585	0.02029	1.77244
C	2.45211	-1.14264	-1.05583
C	3.70452	-2.63797	0.35201
C	2.95086	-1.90889	-2.27209
H	3.13842	-0.29246	-0.86704
H	1.45475	-0.73724	-1.25552
C	4.16963	-3.36275	-0.91122
H	4.47710	-1.88764	0.63386
H	3.62621	-3.36564	1.17421
H	3.07147	-1.22645	-3.12759
H	2.21206	-2.68836	-2.54787
H	5.18518	-3.76310	-0.76593
H	3.48457	-4.21268	-1.11169
N	2.40951	-2.02184	0.11382
O	4.21841	-2.49726	-2.02784

IX_N-1

Pd	-2.02395	-0.36896	0.93368
C	-1.34113	-2.22820	0.57031
C	-2.71413	-2.32209	0.36125
H	-3.31212	-2.74105	1.18605
H	-2.16342	0.26421	-1.16878
C	-0.11103	-2.74013	0.58363
C	0.11667	-4.20492	0.22508
H	0.88044	-4.23473	-0.57002
H	-0.81027	-4.61615	-0.20624
C	0.57163	-5.06991	1.40685
H	0.79953	-6.09727	1.07857
H	1.47997	-4.65733	1.87495
H	-0.21019	-5.12953	2.18135
C	-3.33133	-2.50610	-1.01602
H	-2.73102	-2.02475	-1.80109
H	-3.40443	-3.58244	-1.25862
H	-4.34994	-2.09115	-1.06348
O	-2.56511	1.36820	-3.99966
C	-2.75636	1.22151	-2.81700
O	-1.93232	0.41226	-2.12419
C	-3.87603	1.93344	-2.03414
C	-3.22869	2.89789	-1.01685
H	-2.57526	3.62674	-1.52211
H	-4.01601	3.45725	-0.48668
H	-2.63098	2.36905	-0.26013
C	-4.73502	2.72640	-3.02915

H	-5.19117	2.06017	-3.77623
H	-5.53909	3.25420	-2.49277
H	-4.12942	3.46643	-3.57170
C	-4.74991	0.89813	-1.29842
H	-5.19356	0.17694	-2.00233
H	-4.17962	0.32941	-0.54376
H	-5.56993	1.41248	-0.77311
C	0.12553	1.67308	0.40313
C	1.41293	2.11510	0.64107
C	1.88324	2.23655	1.97565
C	0.92355	1.97734	2.99157
C	-0.34331	1.54101	2.64592
N	-0.75452	1.34728	1.37552
H	-0.21529	1.54310	-0.62585
H	2.05293	2.31942	-0.21434
H	1.16678	2.07493	4.04762
H	-1.06566	1.30110	3.43049
N	3.17334	2.56718	2.25963
C	4.12555	2.76855	1.17815
H	5.11478	2.98317	1.59960
H	4.21007	1.86956	0.54390
H	3.83918	3.61902	0.53571
C	3.62651	2.60655	3.63993
H	4.69085	2.86868	3.66748
H	3.07824	3.36132	4.22964
H	3.50171	1.62726	4.13515
C	1.11108	-1.95998	0.97718
C	2.09184	-1.63892	0.00072
C	3.31327	-1.06761	0.40053
C	3.55743	-0.79400	1.74626
C	2.57952	-1.06659	2.70035
C	1.35479	-1.64904	2.33465
H	2.76767	-0.84132	3.75346
H	4.50997	-0.35033	2.04845
H	4.07015	-0.82275	-0.34576
C	0.33383	-1.95798	3.40251
H	0.02297	-3.01273	3.37171
H	0.73039	-1.74178	4.40544
H	-0.58153	-1.36335	3.25439
C	0.80983	-1.05035	-1.99118
C	2.93439	-2.14467	-2.26394
C	0.34878	-1.65337	-3.30933
H	1.23274	-0.03987	-2.18354
H	-0.04727	-0.93183	-1.32414
C	2.40586	-2.74690	-3.56588
H	3.47939	-1.20641	-2.51089
H	3.64943	-2.83858	-1.79461
H	-0.32629	-0.95470	-3.82345
H	-0.20381	-2.59362	-3.10341
H	3.22806	-2.87665	-4.28714
H	1.96948	-3.74466	-3.34937

N	1.81714	-1.90880	-1.36248
O	1.44579	-1.90862	-4.17472

X_N-1

Pd	0.65966	0.68397	-1.21567
C	-1.00552	1.70689	-0.78385
C	0.02177	2.45750	-0.21679
H	0.18515	2.34920	0.86693
C	-2.28488	1.50393	-1.09908
C	-3.34945	2.52967	-0.72387
H	-3.78023	2.92789	-1.66291
H	-2.85033	3.37830	-0.22807
C	-4.49741	2.02131	0.15435
H	-5.22761	2.82752	0.33643
H	-5.02712	1.18336	-0.32339
H	-4.12518	1.66278	1.12495
C	0.50277	3.77719	-0.79796
H	0.30784	3.83595	-1.87932
H	-0.01521	4.62831	-0.31602
H	1.58389	3.92168	-0.63874
C	0.37296	-2.25839	-1.81242
C	-0.37602	-3.20030	-2.49571
C	-0.63743	-3.02326	-3.88053
C	-0.00746	-1.90367	-4.48726
C	0.71876	-1.01896	-3.71008
N	0.89545	-1.15041	-2.37808
H	0.54068	-2.37772	-0.73960
H	-0.78017	-4.04295	-1.93863
H	-0.11607	-1.69168	-5.54882
H	1.16312	-0.13317	-4.17094
N	-1.44857	-3.86714	-4.57857
C	-1.72371	-3.61436	-5.98315
H	-2.39407	-4.39159	-6.36902
H	-2.21181	-2.63509	-6.13144
H	-0.80131	-3.63404	-6.58847
C	-2.14369	-4.94075	-3.88723
H	-2.78396	-5.47734	-4.59758
H	-1.43956	-5.66970	-3.44997
H	-2.78291	-4.55035	-3.07608
C	-2.72623	0.35533	-1.96375
C	-3.30182	-0.81279	-1.40231
C	-3.85053	-1.79403	-2.24872
C	-3.80781	-1.63895	-3.63381
C	-3.19266	-0.51789	-4.18896
C	-2.64567	0.48197	-3.36963
H	-3.14206	-0.40436	-5.27541
H	-4.23927	-2.40659	-4.28185
H	-4.30294	-2.68956	-1.82034
C	-1.97010	1.67977	-3.99040
H	-2.39538	2.62714	-3.62407
H	-0.90191	1.69619	-3.71848

H	-2.05474	1.66452	-5.08718
C	-4.41589	-1.73176	0.59536
C	-2.05173	-1.29453	0.64592
C	-4.45455	-1.48358	2.10310
H	-4.30182	-2.82643	0.42827
H	-5.37041	-1.41981	0.14295
C	-2.15178	-1.06701	2.14754
H	-1.78739	-2.35918	0.45739
H	-1.25100	-0.67058	0.22608
H	-5.22449	-2.11484	2.57356
H	-4.71143	-0.42122	2.28986
H	-1.22906	-1.39710	2.64912
H	-2.28728	0.01662	2.34090
N	-3.32644	-0.96725	0.00863
O	-3.22097	-1.80717	2.71516

VI_P

Pd	-0.90967	2.15285	0.88019
O	0.69430	0.75451	0.72939
C	0.74924	0.09258	-0.37257
O	-0.03487	0.23074	-1.32151
C	1.86396	-0.98327	-0.40979
C	1.98228	-1.57585	-1.81895
H	2.75390	-2.36351	-1.84107
H	1.02541	-2.00951	-2.14343
H	2.25597	-0.80142	-2.55241
C	3.20167	-0.35800	0.02228
H	3.50990	0.43967	-0.67438
H	3.11779	0.07630	1.02865
H	3.99893	-1.12014	0.03322
C	1.45798	-2.08012	0.59686
H	1.38678	-1.67245	1.61532
H	0.47719	-2.51096	0.33585
H	2.19932	-2.89696	0.59626
C	0.81108	3.47130	-0.07499
C	-0.09774	3.60089	-0.89163
C	-0.96259	3.93723	-2.02793
H	-1.20553	3.00926	-2.56998
H	-1.91619	4.33447	-1.64662
C	-0.29890	4.95167	-2.97156
H	0.64259	4.55461	-3.38144
H	-0.97084	5.18036	-3.81317
H	-0.07338	5.89225	-2.44541
C	2.07152	3.43520	0.68273
H	2.63302	2.54494	0.36137
H	1.85874	3.27048	1.74917
C	2.89882	4.71411	0.49358
H	3.84043	4.64369	1.05964
H	3.14580	4.87291	-0.56742
H	2.34935	5.60005	0.84841
C	-2.49956	3.39554	1.00812

C	-2.61998	4.37393	2.02415
C	-3.76172	5.19141	2.07782
C	-4.79465	5.03167	1.15203
C	-4.68963	4.05487	0.16378
C	-3.55310	3.22800	0.08254
H	-5.50511	3.91247	-0.55236
H	-5.68179	5.66856	1.20668
H	-3.84785	5.95262	2.85534
C	-3.54785	2.11710	-0.94853
H	-2.54489	1.70028	-1.11500
H	-4.18492	1.28111	-0.61429
H	-3.94654	2.46465	-1.91468
C	-0.41707	5.23950	2.68169
C	-2.04807	4.80655	4.38351
C	0.68269	4.95764	3.70071
H	-0.63030	6.33243	2.67512
H	-0.08578	4.96327	1.67351
C	-0.91045	4.50624	5.35432
H	-2.31745	5.88040	4.49390
H	-2.93015	4.20598	4.64101
H	1.56693	5.58323	3.50319
H	0.98273	3.89230	3.61917
H	-1.18977	4.79507	6.37934
H	-0.70229	3.41732	5.34069
N	-1.61318	4.47978	3.03209
O	0.25773	5.23716	5.02080
P	-1.95357	0.73627	2.37009
C	-0.66522	-0.20342	3.28817
C	-0.82799	-1.55662	3.61862
C	0.50871	0.46356	3.67485
C	0.16853	-2.23082	4.33183
H	-1.72702	-2.09457	3.31249
C	1.49807	-0.20921	4.39292
H	0.65535	1.50735	3.39333
C	1.33101	-1.55961	4.72100
H	0.03600	-3.28742	4.57718
H	2.40913	0.31887	4.68476
H	2.11131	-2.08978	5.27288
C	-2.98327	-0.55643	1.55970
C	-4.07725	-1.14823	2.21563
C	-2.62258	-1.00320	0.27648
C	-4.80122	-2.17024	1.59486
H	-4.36948	-0.81425	3.21278
C	-3.34861	-2.02909	-0.33484
H	-1.78701	-0.55031	-0.26265
C	-4.43797	-2.61356	0.31919
H	-5.65194	-2.62075	2.11244
H	-3.06076	-2.36480	-1.33411
H	-5.00627	-3.41166	-0.16545
C	-3.04611	1.39940	3.69496
C	-2.68872	1.31811	5.05035

C	-4.27761	1.98237	3.34575
C	-3.54868	1.80818	6.03899
H	-1.73905	0.86813	5.34287
C	-5.13533	2.46398	4.33591
H	-4.57076	2.06685	2.29855
C	-4.77446	2.37906	5.68549
H	-3.25597	1.73981	7.08961
H	-6.08588	2.91811	4.04671
H	-5.44612	2.76042	6.45864

VII_P

Pd	-0.19184	1.46762	0.88124
O	0.01862	3.35660	1.73486
C	-0.51104	4.34779	1.10271
O	-1.20786	4.25665	0.08634
C	-0.16244	5.74510	1.67413
C	0.95292	6.30494	0.76521
H	1.23443	7.32142	1.08745
H	1.85208	5.67100	0.80791
H	0.61452	6.35212	-0.28131
C	-1.41040	6.63816	1.58751
H	-1.78582	6.67790	0.55550
H	-2.22002	6.24680	2.22532
H	-1.17451	7.66143	1.92345
C	0.33722	5.66198	3.12264
H	-0.42694	5.21795	3.78014
H	1.24174	5.04239	3.19240
H	0.57182	6.67113	3.50097
C	-1.96261	1.17592	1.80644
C	-2.42405	0.05370	1.24602
C	-3.73694	-0.65705	1.48424
H	-4.35765	-0.05460	2.16653
H	-4.27754	-0.70216	0.52258
C	-3.56657	-2.07706	2.04030
H	-3.08328	-2.06240	3.03037
H	-4.54056	-2.58200	2.14384
H	-2.94041	-2.69248	1.37367
C	-2.61103	2.09311	2.80021
H	-1.83882	2.68432	3.31553
H	-3.11079	1.47946	3.57336
C	-3.63385	3.04433	2.15757
H	-4.05320	3.73611	2.90666
H	-3.16465	3.63787	1.36074
H	-4.46838	2.47915	1.71223
C	-1.43837	-0.54183	0.25748
C	-1.73896	-0.49261	-1.15289
C	-0.96709	-1.24646	-2.04343
C	0.11087	-2.00971	-1.57868
C	0.44248	-2.02891	-0.23291
C	-0.32798	-1.31875	0.70994
H	1.30417	-2.60639	0.10928

H	0.71565	-2.57411	-2.29236
H	-1.18576	-1.22409	-3.11108
C	-0.00642	-1.54351	2.17326
H	1.03773	-1.26059	2.38189
H	-0.65818	-0.97300	2.84334
H	-0.10694	-2.61450	2.41525
C	-2.76168	1.72606	-1.52554
C	-3.51535	-0.15494	-2.82084
C	-4.15352	2.32719	-1.62507
H	-2.14344	2.10100	-2.36817
H	-2.28241	2.05874	-0.60005
C	-4.89824	0.49580	-2.87636
H	-2.94684	0.14375	-3.72797
H	-3.62443	-1.25034	-2.83186
H	-4.08662	3.42445	-1.66065
H	-4.74070	2.04053	-0.72928
H	-5.39647	0.24482	-3.82577
H	-5.51463	0.09875	-2.04254
N	-2.84313	0.25923	-1.59471
O	-4.81973	1.90377	-2.80527
P	1.97322	1.76060	-0.26957
C	3.00219	0.24500	-0.50491
C	3.74233	-0.26983	0.57427
C	2.95397	-0.49143	-1.70049
C	4.42208	-1.48487	0.45616
H	3.79646	0.28065	1.51581
C	3.64706	-1.69911	-1.82147
H	2.36174	-0.13120	-2.54283
C	4.38072	-2.20298	-0.74403
H	4.99326	-1.86801	1.30564
H	3.60230	-2.25351	-2.76251
H	4.91840	-3.14977	-0.83776
C	3.05558	2.86587	0.74086
C	3.93127	3.80879	0.17985
C	2.96342	2.77122	2.14041
C	4.70703	4.63141	1.00269
H	4.00301	3.92044	-0.90304
C	3.74849	3.58478	2.96051
H	2.25208	2.07686	2.59216
C	4.62089	4.51944	2.39355
H	5.37753	5.36726	0.55161
H	3.66247	3.50120	4.04667
H	5.22412	5.16690	3.03499
C	1.90562	2.55853	-1.92510
C	2.97241	2.51586	-2.84263
C	0.74328	3.27636	-2.25558
C	2.87193	3.16994	-4.07271
H	3.88444	1.96670	-2.59896
C	0.65131	3.93430	-3.48705
H	-0.08313	3.34880	-1.54404
C	1.70955	3.87925	-4.39811

H	3.70537	3.12756	-4.77869
H	-0.25685	4.49189	-3.72921
H	1.63252	4.38996	-5.36155

VII_P-2

Pd	1.03500	1.60142	-0.88267
C	-0.92470	1.94256	-1.06951
C	-1.19207	3.38319	-0.68312
H	-2.24062	3.49534	-0.36189
H	-0.58908	3.62523	0.20964
C	-1.86948	0.98063	-1.15990
C	-3.34294	1.26587	-0.84729
H	-3.96317	0.59220	-1.45503
H	-3.61985	2.28663	-1.15389
C	-3.66467	1.06404	0.63925
H	-4.73415	1.23933	0.84313
H	-3.42518	0.03659	0.95664
H	-3.07723	1.75013	1.27040
C	-0.89808	4.41575	-1.77791
H	0.16496	4.39427	-2.06643
H	-1.50291	4.22379	-2.67898
H	-1.12818	5.43451	-1.42695
O	2.94496	1.31312	0.32413
C	2.28932	1.58814	1.37268
O	1.05628	1.88888	1.29119
C	2.94880	1.53628	2.75428
C	2.26255	0.40357	3.54713
H	2.40605	-0.56991	3.05084
H	2.69137	0.33655	4.56024
H	1.18163	0.58718	3.63450
C	4.45226	1.26114	2.62250
H	4.94936	2.04885	2.03625
H	4.91833	1.22387	3.62052
H	4.63731	0.30386	2.11393
C	2.70812	2.88556	3.45919
H	3.17805	3.71227	2.90180
H	1.63236	3.09668	3.54263
H	3.14299	2.86675	4.47166
C	-1.59966	-0.46682	-1.46564
C	-2.13188	-1.05044	-2.66241
C	-1.89192	-2.40994	-2.93461
C	-1.20842	-3.21459	-2.02217
C	-0.76024	-2.67230	-0.82427
C	-0.95090	-1.30863	-0.52999
H	-0.25299	-3.30556	-0.09140
H	-1.03715	-4.27020	-2.25058
H	-2.24375	-2.84663	-3.86928
C	-0.48417	-0.83503	0.82779
H	0.61612	-0.81518	0.87927
H	-0.83635	0.16962	1.07970
H	-0.82826	-1.53478	1.60670

C	-2.46211	0.90072	-4.17572
C	-3.90308	-1.01005	-4.38602
C	-3.61871	1.79543	-4.59583
H	-1.88505	0.62548	-5.07770
H	-1.79664	1.44318	-3.49995
C	-5.02251	-0.05836	-4.81101
H	-3.40804	-1.40805	-5.29911
H	-4.34435	-1.85956	-3.84323
H	-3.24041	2.65797	-5.16442
H	-4.14705	2.16957	-3.69529
H	-5.68932	-0.55748	-5.53130
H	-5.61890	0.21684	-3.91610
N	-2.96676	-0.30514	-3.52338
O	-4.52151	1.10289	-5.44222
P	1.79026	1.39346	-3.02676
C	2.59560	-0.25675	-3.14502
C	3.93924	-0.42003	-3.51585
C	1.81743	-1.38678	-2.84065
C	4.49333	-1.70234	-3.58589
H	4.55783	0.44909	-3.74621
C	2.37332	-2.66447	-2.92130
H	0.77675	-1.26960	-2.53808
C	3.71314	-2.82499	-3.29207
H	5.54198	-1.82188	-3.86972
H	1.75306	-3.53083	-2.68116
H	4.15122	-3.82495	-3.34619
C	3.17527	2.59403	-3.30074
C	3.93092	3.04467	-2.20290
C	3.52769	3.01894	-4.59430
C	5.00847	3.91282	-2.40067
H	3.69296	2.70341	-1.19393
C	4.60564	3.88827	-4.78426
H	2.96461	2.67244	-5.46206
C	5.34690	4.34016	-3.68833
H	5.58649	4.25536	-1.53870
H	4.86546	4.21204	-5.79533
H	6.18782	5.02214	-3.83824
C	0.85003	1.55018	-4.60127
C	0.83551	0.53492	-5.56952
C	0.20966	2.77014	-4.87887
C	0.19039	0.73934	-6.79489
H	1.33024	-0.41825	-5.37812
C	-0.43088	2.97131	-6.10180
H	0.22304	3.57237	-4.14112
C	-0.44240	1.95508	-7.06505
H	0.18357	-0.06021	-7.53959
H	-0.92273	3.92580	-6.30452
H	-0.94861	2.11090	-8.02064

VII_P-1

Pd	0.18961	0.35729	-0.93930

C	-1.51879	0.89115	-1.78505
C	-0.64887	1.76914	-2.59223
H	0.44643	1.70704	-2.14088
C	-2.83178	0.68915	-1.68328
C	-3.81218	1.45233	-2.57298
H	-4.33578	0.71268	-3.20633
H	-3.25231	2.10585	-3.26037
C	-4.86036	2.28768	-1.82948
H	-5.52650	2.78930	-2.55036
H	-5.48247	1.66076	-1.17374
H	-4.38356	3.05272	-1.20024
C	-0.49640	1.42492	-4.07845
H	-0.26769	0.35732	-4.20691
H	-1.43835	1.63599	-4.60667
H	0.30407	2.01666	-4.54918
H	-0.84391	2.84153	-2.41908
O	-0.46701	-1.05448	0.41202
C	-0.39899	-2.29120	0.05276
O	-0.06384	-2.68470	-1.06936
C	-0.68614	-3.30808	1.18519
C	-1.41508	-4.52417	0.59390
C	0.69550	-3.73609	1.72570
C	-1.51656	-2.67824	2.31212
H	-0.84093	-4.94818	-0.24172
H	-1.55211	-5.30062	1.36474
H	-2.40725	-4.23709	0.21432
H	1.24073	-2.87703	2.14385
H	0.57559	-4.48658	2.52492
H	1.31002	-4.17798	0.92559
H	-0.98172	-1.83467	2.77054
H	-2.47633	-2.30105	1.93104
H	-1.72242	-3.42863	3.09412
C	-3.45807	-0.35996	-0.81100
C	-3.99093	-0.02513	0.45635
C	-4.77778	-0.96114	1.14804
C	-5.00619	-2.22545	0.60456
C	-4.42429	-2.57730	-0.61349
C	-3.64396	-1.65872	-1.33357
H	-4.58333	-3.57799	-1.02371
H	-5.61921	-2.94953	1.14779
H	-5.19641	-0.70596	2.12253
C	-3.00028	-2.06536	-2.63698
H	-3.21700	-1.35251	-3.44801
H	-1.90623	-2.10279	-2.51389
H	-3.34342	-3.06095	-2.95458
C	-4.70696	1.87416	1.86151
C	-2.36816	1.41102	1.57025
C	-4.35139	3.34744	2.06200
H	-4.76027	1.39067	2.86199
H	-5.70039	1.79065	1.39354
C	-2.07038	2.88776	1.77990

H	-2.29226	0.87855	2.54409
H	-1.62745	0.96153	0.90093
H	-5.05068	3.81722	2.77097
H	-4.43207	3.87554	1.08979
H	-1.10011	3.01919	2.28426
H	-2.02232	3.39064	0.79128
N	-3.70818	1.25714	1.00191
O	-3.05092	3.50374	2.59855
P	2.45331	0.21846	-0.06988
C	2.48497	-0.30471	1.69159
C	1.43248	0.11826	2.52170
C	3.49655	-1.11846	2.22495
C	1.39874	-0.25878	3.86527
H	0.62258	0.72254	2.10998
C	3.45599	-1.50055	3.56972
H	4.31313	-1.46697	1.58939
C	2.40877	-1.07209	4.39119
H	0.57109	0.06977	4.49850
H	4.24332	-2.14180	3.97369
H	2.37420	-1.37907	5.43953
C	3.61810	-0.92166	-0.92011
C	4.99389	-0.65218	-1.02133
C	3.10028	-2.11394	-1.45772
C	5.84399	-1.56719	-1.64905
H	5.40373	0.27368	-0.61123
C	3.95960	-3.02630	-2.07833
H	2.02964	-2.33333	-1.39370
C	5.32855	-2.75626	-2.17653
H	6.91258	-1.35005	-1.72542
H	3.55068	-3.95143	-2.49235
H	5.99474	-3.47028	-2.66782
C	3.33255	1.83785	-0.08410
C	3.39100	2.54008	-1.30188
C	3.92395	2.40012	1.05721
C	4.03835	3.77413	-1.37876
H	2.93533	2.11275	-2.20021
C	4.56274	3.64335	0.98020
H	3.88823	1.86816	2.01005
C	4.62370	4.33088	-0.23475
H	4.08282	4.30610	-2.33246
H	5.01706	4.07296	1.87664
H	5.12459	5.30047	-0.29220

VIII_P-2

Pd	-2.15626	-1.60792	-0.24484
C	-3.95358	-0.81933	-0.97139
C	-3.15815	0.25963	-0.64802
H	-3.33168	0.73844	0.32880
H	1.01707	0.59290	1.08530
C	-5.07040	-1.38278	-1.42341
C	-6.26271	-0.56644	-1.91063

H	-7.14971	-0.91061	-1.35098
H	-6.45150	-0.84787	-2.96395
C	-6.12696	0.94846	-1.79444
H	-7.04320	1.44908	-2.14644
H	-5.95001	1.25347	-0.75117
H	-5.28294	1.32461	-2.39258
C	-2.40547	1.10628	-1.65793
H	-2.26110	0.56592	-2.60482
H	-2.96502	2.03553	-1.87448
H	-1.41384	1.39448	-1.27519
O	0.65090	-0.88980	-1.50621
C	1.19801	-0.30456	-0.60474
O	0.45815	0.16918	0.41705
C	2.70885	-0.00425	-0.59735
C	3.43848	-1.22405	-1.18457
H	3.04827	-1.46418	-2.18294
H	4.51582	-1.01200	-1.26761
H	3.30533	-2.10905	-0.54520
C	2.90104	1.22503	-1.51429
H	2.36493	2.10541	-1.12455
H	3.97108	1.47760	-1.58111
H	2.52755	1.01474	-2.52746
C	3.24505	0.29863	0.81226
H	2.80890	1.21834	1.24206
H	3.06732	-0.54126	1.50054
H	4.33115	0.47068	0.76675
C	-5.25551	-2.86782	-1.50317
C	-6.18210	-3.51055	-0.63485
C	-6.46588	-4.87735	-0.82896
C	-5.81471	-5.60289	-1.82527
C	-4.86858	-4.98303	-2.64123
C	-4.59089	-3.61386	-2.50253
H	-4.34190	-5.55847	-3.40583
H	-6.03082	-6.66779	-1.94735
H	-7.17143	-5.38482	-0.16990
C	-3.61719	-2.94920	-3.44394
H	-4.09049	-2.10997	-3.97954
H	-2.76385	-2.52807	-2.89226
H	-3.22737	-3.66417	-4.18232
C	-6.01870	-2.11078	1.42741
C	-8.14953	-3.10560	0.84878
C	-6.07151	-2.89940	2.73688
H	-6.41803	-1.09332	1.60057
H	-4.97590	-2.00658	1.10375
C	-8.13492	-3.86508	2.17828
H	-8.70450	-2.16113	1.01209
H	-8.68733	-3.67111	0.07421
H	-5.58049	-2.33433	3.54495
H	-5.52999	-3.85836	2.61014
H	-9.15853	-3.99309	2.56540
H	-7.69116	-4.87343	2.03886

N	-6.81043	-2.77051	0.38739
O	-7.40715	-3.14307	3.15466
P	-1.17025	-3.71815	-0.05124
C	-0.92454	-4.55921	-1.67790
C	-1.46671	-5.81744	-1.97785
C	-0.22365	-3.85758	-2.67773
C	-1.31173	-6.36694	-3.25599
H	-2.02470	-6.37030	-1.22071
C	-0.05958	-4.41679	-3.94594
H	0.18367	-2.86760	-2.46203
C	-0.60777	-5.67129	-4.24193
H	-1.74727	-7.34467	-3.47846
H	0.48801	-3.86285	-4.71301
H	-0.48877	-6.10185	-5.23966
C	-2.00311	-5.01407	0.96672
C	-1.31279	-5.92299	1.78583
C	-3.40225	-5.09682	0.88073
C	-2.01377	-6.89432	2.50794
H	-0.22489	-5.87673	1.86449
C	-4.09771	-6.08120	1.58711
H	-3.94486	-4.39230	0.24937
C	-3.40649	-6.97867	2.40791
H	-1.46691	-7.59148	3.14834
H	-5.18398	-6.14028	1.49231
H	-3.95185	-7.74164	2.96948
C	0.52901	-3.68915	0.67929
C	1.59153	-4.47788	0.21065
C	0.73434	-2.86724	1.80126
C	2.83215	-4.45143	0.85727
H	1.45070	-5.11875	-0.66211
C	1.96895	-2.85347	2.45568
H	-0.08349	-2.23756	2.16239
C	3.02291	-3.64462	1.98341
H	3.65201	-5.06817	0.48018
H	2.11034	-2.22095	3.33605
H	3.99122	-3.62873	2.48997

VIII_P-1

Pd	0.10368	-0.20656	-1.35840
C	-2.00829	0.24460	-1.94498
C	-1.39296	-0.18518	-3.07438
H	0.47165	1.23834	-1.72609
C	-2.99308	0.56299	-1.12163
C	-4.37443	0.82505	-1.72412
H	-5.06283	0.07572	-1.29296
H	-4.33094	0.62764	-2.80712
C	-4.94695	2.22263	-1.47334
H	-5.94889	2.30519	-1.92521
H	-5.03719	2.43149	-0.39772
H	-4.30182	2.99991	-1.90733
C	-1.60015	-1.56452	-3.65930

H	-2.10401	-2.22566	-2.94314
H	-2.21811	-1.48035	-4.57025
H	-0.64029	-2.02659	-3.93126
H	-0.89820	0.55181	-3.72090
O	-0.35526	-2.22504	-0.81894
C	0.32823	-3.14185	-1.40400
O	1.15458	-2.93560	-2.30486
C	0.02258	-4.58728	-0.93510
C	-1.29051	-5.01711	-1.62154
C	1.16498	-5.52003	-1.35879
C	-0.15036	-4.62111	0.59232
H	-1.19489	-4.97419	-2.71863
H	-1.55078	-6.05199	-1.34223
H	-2.12397	-4.36295	-1.32324
H	2.11160	-5.22186	-0.88063
H	0.94258	-6.55963	-1.06595
H	1.31891	-5.48134	-2.44611
H	0.75735	-4.26429	1.10341
H	-0.97916	-3.97552	0.91202
H	-0.35325	-5.65090	0.93213
C	-2.91203	0.51891	0.37813
C	-2.72475	1.69118	1.15095
C	-2.77843	1.60720	2.55385
C	-3.03342	0.38943	3.18260
C	-3.22855	-0.76123	2.41970
C	-3.16696	-0.71784	1.01810
H	-3.43618	-1.71482	2.91200
H	-3.07613	0.33785	4.27383
H	-2.61594	2.50263	3.15463
C	-3.35828	-1.98388	0.22133
H	-4.10431	-1.86383	-0.57913
H	-2.40546	-2.26615	-0.25227
H	-3.68464	-2.81068	0.86891
C	-3.04405	4.12969	1.14673
C	-1.15052	3.17697	0.02112
C	-2.99308	5.29884	0.16415
H	-2.45976	4.41673	2.04831
H	-4.08378	3.94806	1.46138
C	-1.13645	4.37218	-0.91922
H	-0.47009	3.37527	0.87355
H	-0.77738	2.29011	-0.50227
H	-3.32822	6.22464	0.65707
H	-3.67213	5.09125	-0.68789
H	-0.10316	4.61413	-1.20935
H	-1.71142	4.12302	-1.83491
N	-2.51229	2.93641	0.50038
O	-1.67631	5.52809	-0.29919
P	1.83151	-0.00574	0.18907
C	1.57621	-1.15791	1.59189
C	0.28670	-1.24243	2.14371
C	2.60834	-1.95128	2.11501

C	0.04215	-2.08915	3.22454
H	-0.53158	-0.65472	1.72445
C	2.35315	-2.81045	3.18927
H	3.61101	-1.90491	1.68575
C	1.07370	-2.87603	3.74882
H	-0.96458	-2.14231	3.64388
H	3.15984	-3.43041	3.58823
H	0.87722	-3.54915	4.58717
C	3.53097	-0.33705	-0.41672
C	4.64687	0.30587	0.14745
C	3.71290	-1.29987	-1.42445
C	5.93382	-0.00958	-0.29577
H	4.51358	1.05383	0.93199
C	5.00584	-1.61114	-1.85769
H	2.85057	-1.81671	-1.85817
C	6.11499	-0.96818	-1.29903
H	6.79727	0.49534	0.14483
H	5.14210	-2.36163	-2.64035
H	7.12263	-1.21220	-1.64559
C	1.93551	1.66863	0.94800
C	2.24945	2.75305	0.10945
C	1.67653	1.90424	2.30522
C	2.31081	4.04806	0.62244
H	2.43784	2.58320	-0.95390
C	1.72182	3.20860	2.81322
H	1.43060	1.07640	2.97201
C	2.03921	4.28083	1.97699
H	2.55582	4.88276	-0.03882
H	1.50667	3.38167	3.87055
H	2.06954	5.29814	2.37438

TS1_P

Pd	0.15316	0.82873	0.27800
O	-1.52195	1.77953	-0.57744
C	-2.45727	2.16496	0.21500
O	-2.44317	2.03382	1.44646
C	-3.69964	2.79587	-0.46434
C	-4.14280	4.01715	0.35800
H	-5.07257	4.44452	-0.05306
H	-4.31206	3.73369	1.40615
H	-3.37097	4.80482	0.34157
C	-3.41132	3.20734	-1.91380
H	-2.59996	3.95085	-1.96142
H	-3.10671	2.33998	-2.51456
H	-4.31184	3.65222	-2.36998
C	-4.80012	1.71464	-0.43383
H	-4.49855	0.82759	-1.01140
H	-5.00154	1.39832	0.60115
H	-5.73588	2.10443	-0.86872
C	1.05896	2.66797	0.62419
C	2.13654	2.10357	0.99548

C	3.55906	2.22805	1.41967
H	3.71213	1.64301	2.34008
H	4.19141	1.76059	0.64960
C	3.99539	3.68047	1.63550
H	3.39640	4.16944	2.41811
H	5.05051	3.70275	1.95039
H	3.90217	4.27287	0.71401
C	0.30456	3.92913	0.38576
H	-0.54868	3.93218	1.08400
H	-0.15636	3.86585	-0.61177
C	1.11293	5.22188	0.52429
H	0.46392	6.08980	0.32660
H	1.52860	5.33449	1.53642
H	1.94816	5.25439	-0.19223
C	1.91650	0.03811	1.12637
C	2.98284	-0.52087	0.35056
C	3.86712	-1.43034	0.96504
C	3.72239	-1.77645	2.30584
C	2.69545	-1.22044	3.07158
C	1.79828	-0.30527	2.50183
H	2.59227	-1.48846	4.12631
H	4.41610	-2.49127	2.75667
H	4.66151	-1.89438	0.38115
C	0.73182	0.30851	3.37700
H	0.60539	1.38173	3.16976
H	-0.24741	-0.15928	3.19526
H	0.97188	0.17924	4.44294
C	4.56240	-0.26842	-1.53384
C	2.20617	-0.18859	-2.00285
C	4.77115	0.73850	-2.66658
H	4.70933	-1.29651	-1.92866
H	5.32618	-0.09025	-0.76236
C	2.48113	0.81675	-3.10940
H	2.18266	-1.21341	-2.42635
H	1.22070	0.01852	-1.56336
H	5.74038	0.55878	-3.15711
H	4.78194	1.76184	-2.23576
H	1.75777	0.68885	-3.92929
H	2.37388	1.84319	-2.70156
N	3.23198	-0.09346	-0.96565
O	3.77419	0.63590	-3.66110
P	-0.93746	-1.29134	-0.03494
C	-2.27945	-1.21969	-1.29169
C	-3.48479	-1.92295	-1.14249
C	-2.07173	-0.45144	-2.44984
C	-4.46476	-1.86123	-2.13830
H	-3.66602	-2.51658	-0.24447
C	-3.04665	-0.40201	-3.44817
H	-1.15248	0.12510	-2.56149
C	-4.24716	-1.10384	-3.29299
H	-5.40317	-2.40584	-2.00757

H	-2.87502	0.20136	-4.34282
H	-5.01576	-1.05315	-4.06832
C	-1.77164	-1.96699	1.46011
C	-1.77028	-3.33383	1.78424
C	-2.48058	-1.06296	2.27267
C	-2.45719	-3.78960	2.91404
H	-1.23533	-4.04958	1.15773
C	-3.17170	-1.52852	3.39470
H	-2.49169	0.00554	2.03373
C	-3.15834	-2.88880	3.72154
H	-2.44537	-4.85453	3.16027
H	-3.71816	-0.81788	4.01985
H	-3.69409	-3.24713	4.60447
C	0.14447	-2.65524	-0.63212
C	0.06772	-3.15447	-1.94344
C	1.14813	-3.14070	0.22391
C	0.97988	-4.11569	-2.38888
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H	1.23287	-2.76016	1.24316
C	1.97254	-4.59716	-1.52944
H	0.90973	-4.49210	-3.41258
H	2.82530	-4.47045	0.45806
H	2.68436	-5.34934	-1.87890

TS2_P-2

Pd	0.90921	-0.90638	-0.46667
C	-0.72487	-1.85841	-1.01677
C	0.24378	-2.94415	-0.94382
H	0.42323	-3.42123	-1.92249
H	1.65707	-2.67884	-0.86078
C	-2.02156	-1.73273	-1.30411
C	-2.85837	-2.96252	-1.65800
H	-3.77191	-2.93941	-1.04068
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C	-3.24332	-3.03667	-3.14128
H	-3.89813	-3.90220	-3.33458
H	-3.78108	-2.12994	-3.46086
H	-2.35040	-3.14129	-3.77893
C	0.12343	-3.95697	0.20093
H	-0.08296	-3.44670	1.15386
H	-0.70104	-4.66550	0.01543
H	1.05297	-4.53532	0.31781
O	3.05370	-0.92388	0.08297
C	3.60287	-1.99544	-0.27884
O	2.97277	-2.97120	-0.80288
C	5.12757	-2.13678	-0.13559
C	5.70812	-2.12707	-1.56636
H	5.47368	-1.17959	-2.07854
H	6.80452	-2.23271	-1.53017
H	5.29485	-2.95418	-2.16228

C	5.70317	-0.96599	0.67280
H	5.28425	-0.94273	1.69034
H	6.79798	-1.06602	0.75099
H	5.46837	-0.00213	0.19851
C	5.44634	-3.47822	0.54925
H	5.02724	-3.51144	1.56808
H	5.02568	-4.31859	-0.02111
H	6.53720	-3.61463	0.62643
C	-2.78407	-0.44746	-1.39488
C	-3.80568	-0.18789	-0.44409
C	-4.76087	0.80941	-0.70202
C	-4.67704	1.56979	-1.86932
C	-3.61305	1.38751	-2.75092
C	-2.65159	0.39005	-2.52420
H	-3.52392	2.02383	-3.63492
H	-5.42596	2.34082	-2.06944
H	-5.56170	1.00316	0.01274
C	-1.51028	0.20947	-3.49532
H	-0.54748	0.41106	-2.99911
H	-1.45466	-0.82266	-3.87235
H	-1.60736	0.89148	-4.35244
C	-2.72314	-0.77413	1.66843
C	-5.09639	-1.11699	1.44767
C	-2.67178	-1.92563	2.66178
H	-2.84869	0.17820	2.22944
H	-1.77594	-0.72081	1.12012
C	-4.97808	-2.27053	2.44344
H	-5.37297	-0.19467	2.00516
H	-5.90296	-1.33183	0.72953
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C	-0.02303	3.39575	-1.56268
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C	-0.90113	4.34438	-2.09551
H	0.99056	3.32297	-1.96119
C	-2.60860	3.64198	-0.53715
H	-2.09731	2.01576	0.77287
C	-2.19022	4.48096	-1.57404
H	-0.56678	4.98913	-2.91231
H	-3.62059	3.72343	-0.13731
H	-2.87139	5.23245	-1.98107
C	2.37459	2.12721	-0.00057
C	3.11560	1.81104	-1.15204
C	2.91641	3.02053	0.93512
C	4.36690	2.39032	-1.37170

H	2.72036	1.08788	-1.86938
C	4.17504	3.59115	0.71950
H	2.36692	3.26798	1.84493
C	4.90148	3.28026	-0.43385
H	4.93274	2.13293	-2.27063
H	4.58991	4.27920	1.46050
H	5.88648	3.72448	-0.59833
C	0.38255	1.39256	2.02508
C	-0.04541	2.56266	2.67735
C	0.57187	0.22351	2.78217
C	-0.28995	2.55655	4.05332
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H	0.90332	-0.69245	2.28557
C	-0.10697	1.38543	4.79623
H	-0.62856	3.47136	4.54613
H	0.47643	-0.69842	4.73164
H	-0.30613	1.38114	5.87077

TS2_P-1

Pd	0.21994	0.41475	-0.99184
C	-1.64064	0.77407	-1.90787
C	-0.75641	1.48495	-2.71120
H	0.84113	1.54891	-1.84477
C	-2.91951	0.48205	-1.69982
C	-3.96227	1.07580	-2.65152
H	-4.57914	0.24920	-3.04586
H	-3.44864	1.52657	-3.51599
C	-4.88612	2.11272	-2.00269
H	-5.61279	2.49182	-2.73960
H	-5.44894	1.67555	-1.16474
H	-4.31081	2.96359	-1.60886
C	-0.32192	0.98218	-4.07399
H	-0.28500	-0.11522	-4.10283
H	-1.06345	1.32319	-4.81784
H	0.66075	1.38004	-4.36680
H	-0.71447	2.57461	-2.57828
O	-0.49611	-1.08111	0.32266
C	-0.37708	-2.29740	-0.07379
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C	-0.66962	-3.38254	0.99309
C	-1.41145	-4.55328	0.32934
C	0.70786	-3.86272	1.49859
C	-1.48891	-2.81890	2.16126
H	-0.84536	-4.92415	-0.53653
H	-1.54925	-5.37770	1.04863
H	-2.40468	-4.23774	-0.02284
H	1.26483	-3.04085	1.97185
H	0.58309	-4.66427	2.24609
H	1.31347	-4.25520	0.66678
H	-0.94476	-2.01041	2.66787

H	-2.44616	-2.41007	1.81058
H	-1.69809	-3.61414	2.89714
C	-3.49814	-0.41946	-0.65131
C	-3.92420	0.10483	0.59129
C	-4.70775	-0.68664	1.44737
C	-5.04864	-1.98926	1.08428
C	-4.57902	-2.52433	-0.11589
C	-3.79910	-1.75623	-0.99417
H	-4.82618	-3.55456	-0.38487
H	-5.66171	-2.59929	1.75290
H	-5.04160	-0.28293	2.40443
C	-3.28175	-2.35629	-2.27933
H	-3.56055	-1.75502	-3.15893
H	-2.18201	-2.40892	-2.25848
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C	-4.48270	2.22996	1.72440
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H	-4.51233	1.91603	2.79137
H	-5.49973	2.12743	1.31471
C	-1.80321	3.06868	1.37971
H	-2.09389	1.22487	2.46885
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O	-2.71556	3.86180	2.12178
P	2.37249	0.30622	-0.01633
C	2.37231	-0.39001	1.68144
C	1.29755	-0.07751	2.53025
C	3.41518	-1.20080	2.15598
C	1.27465	-0.55969	3.84013
H	0.46481	0.51998	2.15910
C	3.38469	-1.68765	3.46635
H	4.24928	-1.46134	1.50158
C	2.31640	-1.36715	4.30979
H	0.43069	-0.31743	4.49029
H	4.19649	-2.32470	3.82585
H	2.29040	-1.75444	5.33140
C	3.57763	-0.71680	-0.95222
C	4.94312	-0.39037	-1.01418
C	3.10636	-1.87785	-1.59093
C	5.83069	-1.21941	-1.70644
H	5.31642	0.51162	-0.52434
C	4.00338	-2.70303	-2.27621
H	2.04409	-2.14198	-1.55144
C	5.36245	-2.37700	-2.33720
H	6.89124	-0.95893	-1.75233
H	3.63186	-3.60496	-2.76906

H	6.05781	-3.02345	-2.87900
C	3.21281	1.93695	0.16835
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H	2.95245	2.41793	-1.93144
C	4.35391	3.63293	1.48332
H	3.63019	1.76541	2.28883
C	4.49042	4.43486	0.34793
H	4.09253	4.61094	-1.77444
H	4.74135	3.97445	2.44646
H	4.98429	5.40720	0.41830

IX_P

Pd	-2.21653	-1.67265	-0.21579
C	-3.96397	-0.76858	-0.95996
C	-3.13793	0.26716	-0.60143
H	-3.29041	0.71912	0.39104
C	-5.08033	-1.32767	-1.41308
C	-6.27765	-0.49899	-1.86428
H	-7.15487	-0.85371	-1.29611
H	-6.48315	-0.76071	-2.91927
C	-6.13288	1.01256	-1.71988
H	-7.04926	1.52432	-2.05425
H	-5.94595	1.29676	-0.67254
H	-5.29207	1.39580	-2.31871
C	-2.35444	1.11098	-1.58953
H	-2.23713	0.59461	-2.55352
H	-2.88203	2.06465	-1.77639
H	-1.35182	1.36248	-1.20755
C	-5.25840	-2.81086	-1.54075
C	-6.16894	-3.48910	-0.68320
C	-6.46455	-4.84375	-0.93861
C	-5.83538	-5.52436	-1.97985
C	-4.90002	-4.87160	-2.78349
C	-4.61711	-3.51061	-2.58765
H	-4.39140	-5.41396	-3.58409
H	-6.05911	-6.58132	-2.14755
H	-7.16125	-5.37866	-0.29229
C	-3.66873	-2.79915	-3.52050
H	-4.15618	-1.93491	-4.00068
H	-2.80059	-2.40642	-2.97099
H	-3.29988	-3.47495	-4.30498
C	-5.95389	-2.19306	1.43803
C	-8.10240	-3.14966	0.85879
C	-5.97865	-3.05094	2.70428
H	-6.34355	-1.18471	1.67343
H	-4.91790	-2.07907	1.09683
C	-8.05800	-3.97879	2.14541
H	-8.64771	-2.21303	1.08518
H	-8.66184	-3.67067	0.06850

H	-5.46495	-2.53148	3.52861
H	-5.44594	-4.00368	2.51229
H	-9.07269	-4.12547	2.54885
H	-7.62002	-4.97847	1.94210
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C	-0.96120	-4.61039	-1.64153
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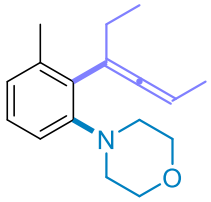
C	-0.40971	-3.85093	-2.68850
C	-1.13303	-6.50703	-3.15150
H	-1.75426	-6.55007	-1.08606
C	-0.21035	-4.41737	-3.94797
H	-0.15135	-2.80231	-2.51533
C	-0.57720	-5.74783	-4.18485
H	-1.42473	-7.54539	-3.32913
H	0.21907	-3.81471	-4.75230
H	-0.43334	-6.18885	-5.17453
C	-2.05658	-5.02516	1.01100
C	-1.44059	-5.72548	2.05978
C	-3.41048	-5.26984	0.72282
C	-2.17017	-6.65820	2.80606
H	-0.39056	-5.54631	2.29890
C	-4.12892	-6.21476	1.45682
H	-3.90129	-4.72296	-0.08288
C	-3.51227	-6.90852	2.50492
H	-1.68297	-7.19419	3.62480
H	-5.17629	-6.39901	1.20792
H	-4.07799	-7.64025	3.08732
C	0.51208	-3.72871	0.68292
C	1.50232	-4.65450	0.31424
C	0.81452	-2.74708	1.64207
C	2.77083	-4.59966	0.89903
H	1.28262	-5.41948	-0.43410
C	2.08147	-2.69817	2.23077
H	0.05106	-2.01641	1.92605
C	3.06208	-3.62381	1.85876
H	3.53547	-5.32281	0.60371
H	2.30511	-1.93071	2.97608
H	4.05531	-3.58216	2.31318

7. Characterization Data



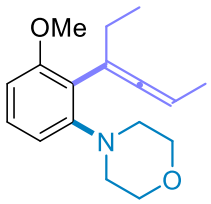
4-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)morpholine (4a)

35.8 mg, yield: 70%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.13 (t, *J* = 7.8 Hz, 1H), 6.99 – 6.88 (m, 2H), 5.21 – 5.06 (m, 1H), 3.80 (t, *J* = 4.6 Hz, 4H), 3.19 – 2.78 (m, 4H), 2.29 (s, 5H), 1.65 (d, *J* = 6.9 Hz, 3H), 1.06 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.79, 150.40, 137.46, 134.43, 127.36, 125.54, 117.11, 104.77, 86.07, 67.61, 52.88, 25.78, 20.45, 13.80, 12.49.

HRMS (ESI) Calcd for $C_{17}H_{23}NO$ $[M+H]^+$ 258.1852, found 258.1856.



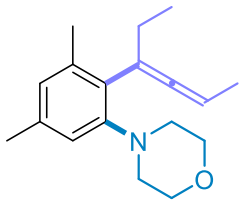
4-(2-(hexa-3,4-dien-3-yl)-3-methoxyphenyl)morpholine (4b)

18.8 mg, yield: 34%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.18 (t, *J* = 8.2 Hz, 1H), 6.68 (t, *J* = 7.4 Hz, 2H), 5.16 (qt, *J* = 6.8, 3.4 Hz, 1H), 3.85 – 3.74 (m, 7H), 3.09 – 2.91 (m, 4H), 2.39 – 2.23 (m, 2H), 1.67 (d, *J* = 6.9 Hz, 3H), 1.04 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.63, 157.63, 151.56, 128.07, 123.33, 111.96, 106.86, 101.00, 85.88, 67.53, 56.02, 52.56, 25.43, 14.11, 12.44.

HRMS (ESI) Calcd for $C_{17}H_{23}NO_2$ $[M+H]^+$ 274.1802, found 274.1811.



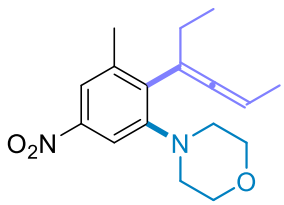
4-(2-(hexa-3,4-dien-3-yl)-3,5-dimethylphenyl)morpholine (4c)

41.3 mg, yield: 76%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.79 (s, 1H), 6.73 (s, 1H), 5.11 (qt, *J* = 6.8, 3.4 Hz, 1H), 3.79 (t, *J* = 4.5 Hz, 4H), 2.97 (s, 4H), 2.31 – 2.21 (m, 8H), 1.64 (d, *J* = 6.9 Hz, 3H), 1.05 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.93, 150.29, 137.20, 137.01, 131.36, 126.28, 117.83, 104.65, 85.82, 67.61, 52.85, 25.79, 21.19, 20.36, 13.81, 12.49.

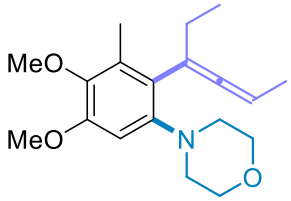
HRMS (ESI) Calcd for $C_{18}H_{25}NO$ $[M+H]^+$ 272.2009, found 272.2002.



4-(2-(hexa-3,4-dien-3-yl)-3-methyl-5-nitrophenyl)morpholine (4d)

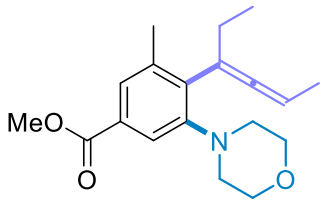
12.2 mg, yield: 20%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 1.9 Hz, 1H), 7.73 (d, *J* = 2.1 Hz, 1H), 5.29 – 5.19 (m, 1H), 3.83 (t, *J* = 4.5 Hz, 4H), 3.04 (s, 4H), 2.40 – 2.23 (m, 5H), 1.68 (d, *J* = 6.9 Hz, 3H), 1.05 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.69, 151.20, 147.09, 141.05, 139.13, 120.11, 112.19, 103.93, 87.54, 67.25, 52.49, 25.17, 20.83, 13.52, 12.39.
HRMS (ESI) Calcd for $C_{17}H_{22}N_2O_3$ $[M+H]^+$ 303.1703, found 303.1693.



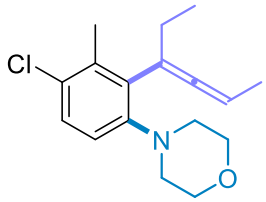
4-(2-(hexa-3,4-dien-3-yl)-4,5-dimethoxy-3-methylphenyl)morpholine (4e)

38.6 mg, yield: 61%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.54 (s, 1H), 5.22 – 4.98 (m, 1H), 3.85 (s, 3H), 3.79 (t, *J* = 4.4 Hz, 4H), 3.76 (s, 3H), 2.96 (s, 4H), 2.32 – 2.14 (m, 5H), 1.65 (d, *J* = 6.7 Hz, 3H), 1.05 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.18, 151.67, 146.37, 143.74, 131.23, 127.96, 104.46, 102.14, 85.74, 67.59, 60.13, 55.70, 53.08, 26.33, 13.90, 13.14, 12.43.
HRMS (ESI) Calcd for $C_{19}H_{27}NO_3$ $[M+H]^+$ 318.2064, found 318.2054.



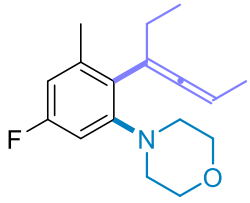
methyl 4-(hexa-3,4-dien-3-yl)-3-methyl-5-morpholinobenzoate (4f)

40.5 mg, yield: 64%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 – 7.62 (m, 1H), 7.60 – 7.54 (m, 1H), 5.24 – 5.13 (m, 1H), 3.90 (s, 3H), 3.81 (t, *J* = 4.5 Hz, 4H), 3.02 (s, 4H), 2.32 (s, 5H), 1.66 (d, *J* = 6.9 Hz, 3H), 1.05 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.55, 167.09, 150.46, 139.27, 137.79, 128.97, 126.66, 118.24, 104.39, 86.76, 67.44, 52.71, 51.98, 25.44, 20.51, 13.65, 12.39.
HRMS (ESI) Calcd for $C_{19}H_{25}NO_3$ $[M+H]^+$ 316.1907, found 316.1900.



4-(4-chloro-2-(hexa-3,4-dien-3-yl)-3-methylphenyl)morpholine (4g)

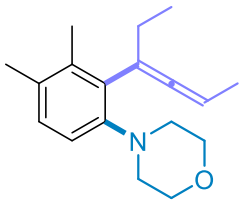
23.4 mg, yield: 40%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.23 (d, *J* = 8.5 Hz, 1H), 6.87 (d, *J* = 8.6 Hz, 1H), 5.20 – 5.10 (m, 1H), 3.79 (s, 4H), 3.20 (s, 2H), 2.70 (s, 2H), 2.41 – 2.19 (m, 5H), 1.73 – 1.61 (m, 3H), 1.06 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.79, 149.14, 136.72, 130.08, 128.06, 118.44, 104.83, 86.65, 67.53, 52.95, 26.10, 17.46, 13.74, 12.38.
HRMS (ESI) Calcd for $C_{17}H_{22}ClNO$ $[M+H]^+$ 292.1463, found 292.1457.



4-(5-fluoro-2-(hexa-3,4-dien-3-yl)-3-methylphenyl)morpholine (4h)

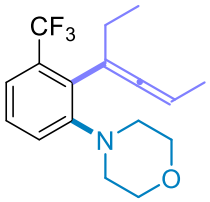
34.5 mg, yield: 63%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.70 – 6.57 (m, 2H), 5.22 – 5.05 (m, 1H), 3.80 (t, *J* = 4.4 Hz, 4H), 2.97 (s, 4H), 2.27 (s, 5H), 1.65 (d, *J* = 6.7 Hz, 3H), 1.03 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.18, 161.94 (d, *J* = 244.8 Hz), 151.85 (d, *J* = 8.2 Hz), 139.15 (d, *J* = 9.5 Hz), 129.73 (d, *J* = 3.2 Hz), 111.64 (d, *J* = 20.8 Hz), 104.34 (d, *J* = 21.9 Hz), 104.16, 86.10, 67.40, 52.61, 25.69, 20.67, 13.70, 12.45.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -115.13.
HRMS (ESI) Calcd for $C_{17}H_{22}FNO$ $[M+H]^+$ 276.1758, found 276.1750.



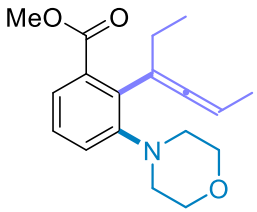
4-(2-(hexa-3,4-dien-3-yl)-3,4-dimethylphenyl)morpholine (4i)

38.6 mg, yield: 71%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.04 (d, *J* = 8.1 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 5.12 (s, 1H), 3.79 (s, 4H), 3.19 (s, 2H), 2.69 (s, 2H), 2.36 – 2.08 (m, 8H), 1.64 (s, 3H), 1.07 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.68, 148.55, 135.20, 132.57, 128.84, 117.14, 105.15, 85.99, 67.70, 53.15, 26.39, 20.40, 16.59, 13.84, 12.43.
HRMS (ESI) Calcd for $C_{18}H_{25}NO$ $[M+H]^+$ 272.2009, found 272.2003.



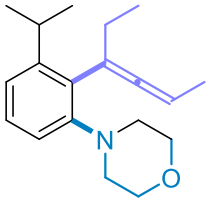
4-(2-(hexa-3,4-dien-3-yl)-3-(trifluoromethyl)phenyl)morpholine (4j) (d.r. = 56:44)

34.2 mg, yield: 55%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 (d, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.27 (t, *J* = 8.8 Hz, 1H), 5.35 – 5.07 (m, 1H), 3.90 – 3.73 (m, 4H), 3.35 – 3.19 (m, 2H), 2.78 – 2.66 (m, 2H), 2.48 – 2.38 (m, 1H), 2.19 – 2.07 (m, 1H), 1.73 – 1.57 (m, 3H), 1.15 – 1.06 (m, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.10, 202.72, 151.71, 135.35, 134.93, 132.28, 132.18, 130.54 – 129.30 (m), 128.11, 127.83, 125.45, 125.43, 123.88, 123.72, 122.71, 121.73 (q, *J* = 5.4 Hz), 121.43 (q, *J* = 5.6 Hz), 119.98, 103.21, 102.96, 87.81, 87.50, 67.48, 53.06 (d, *J* = 4.8 Hz), 26.19, 26.06, 13.70, 12.15, 12.08.
HRMS (ESI) Calcd for $C_{17}H_{20}F_3NO$ $[M+H]^+$ 312.1570, found 312.1563.



methyl 2-(hexa-3,4-dien-3-yl)-3-morpholinobenzoate (4k)

32.5 mg, yield: 54%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.26 (m, 2H), 7.20 – 7.14 (m, 1H), 5.21 – 5.10 (m, 1H), 3.85 (s, 3H), 3.83 – 3.77 (m, 4H), 2.99 (s, 4H), 2.51 – 2.39 (m, 2H), 1.61 (d, *J* = 6.9 Hz, 3H), 1.09 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.61, 169.34, 150.63, 134.38, 134.03, 127.74, 123.77, 122.34, 105.73, 86.98, 67.42, 52.56, 51.96, 25.31, 13.96, 12.25.
HRMS (ESI) Calcd for $C_{18}H_{23}NO_3$ $[M+H]^+$ 302.1751, found 302.1744.



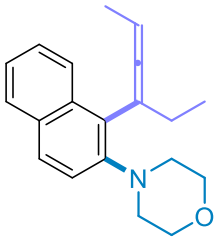
4-(2-(hexa-3,4-dien-3-yl)-3-isopropylphenyl)morpholine (4l) (d.r. = 56:44)

34.7 mg, yield: 61%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 – 7.17 (m, 1H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.93 (s, 1H), 5.36 – 4.74 (m, 1H), 3.99 – 3.59 (m, 4H), 3.37 – 2.65 (m, 5H), 2.52 – 2.09 (m, 2H), 1.83 – 1.48 (m, 3H), 1.30 – 0.99 (m, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.74, 202.57, 150.30, 148.16, 147.90, 134.00, 131.74, 127.72, 127.46, 121.36, 121.06, 119.47, 117.38, 117.22, 115.73, 104.31, 86.07, 85.84, 67.69, 67.01, 53.19, 29.98, 26.89, 24.98, 24.54, 23.92, 23.76, 14.45, 14.30, 14.03, 13.55, 12.46.

HRMS (ESI) Calcd for $C_{19}H_{27}NO$ $[M+H]^+$ 286.2165, found 286.2156.



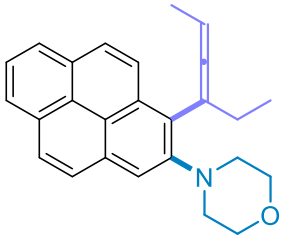
4-(1-(hexa-3,4-dien-3-yl)naphthalen-2-yl)morpholine (4m)

34.2 mg, yield: 58%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 7.77 (dd, *J* = 8.4, 3.0 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 8.3 Hz, 2H), 5.23 (s, 1H), 3.86 (s, 4H), 3.10 (d, *J* = 165.3 Hz, 4H), 2.38 (s, 2H), 1.68 (s, 3H), 1.13 (td, *J* = 7.3, 1.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.50, 146.82, 132.66, 131.02, 130.86, 128.23, 127.90, 126.02, 125.30, 124.44, 119.70, 103.47, 86.39, 67.69, 52.81, 26.52, 14.03, 12.54.

HRMS (ESI) Calcd for $C_{20}H_{23}NO$ $[M+H]^+$ 294.1852, found 294.1840.



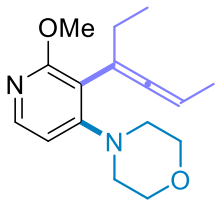
4-(1-(hexa-3,4-dien-3-yl)pyren-2-yl)morpholine (4n)

49.1 mg, yield: 67%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.52 – 8.21 (m, 1H), 8.09 (d, *J* = 7.6 Hz, 2H), 8.04 – 7.95 (m, 3H), 7.93 – 7.86 (m, 2H), 5.55 – 5.04 (m, 1H), 3.92 (s, 4H), 3.55 (s, 2H), 3.09 – 2.82 (m, 2H), 2.70 – 2.34 (m, 2H), 1.87 – 1.60 (m, 3H), 1.23 – 1.08 (m, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.89, 148.28, 131.14, 130.75, 130.46, 130.07, 127.58, 127.34, 126.91, 125.29, 125.16, 124.98, 124.75, 122.04, 116.45, 104.13, 86.40, 67.75, 53.45, 26.95, 13.96, 12.64.

HRMS (ESI) Calcd for $C_{26}H_{25}NO$ $[M+H]^+$ 368.2009, found 368.2003.

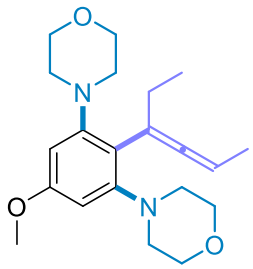


4-(3-(hexa-3,4-dien-3-yl)-2-methoxypyridin-4-yl)morpholine (4o)

23.6 mg, yield: 43%. Colorless liquid.

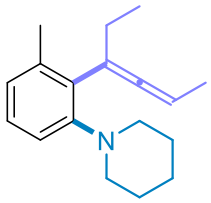
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 5.8 Hz, 1H), 6.49 (d, *J* = 5.8 Hz, 1H), 5.27 – 5.15 (m, 1H), 3.90 (s, 3H), 3.85 – 3.69 (m, 4H), 3.23 – 3.07 (m, 4H), 2.35 – 2.24 (m, 2H), 1.70 (d, *J* = 7.0 Hz, 3H), 1.03 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.90, 162.58, 157.49, 145.52, 112.53, 107.38, 100.29, 86.62, 67.01, 53.69, 50.45, 24.04, 13.76, 12.21.
HRMS (ESI) Calcd for $C_{16}H_{22}N_2O_2$ $[M+H]^+$ 275.1754, found 275.1748.



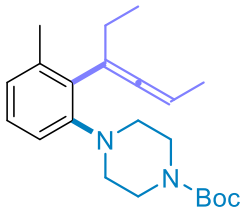
4,4'-(2-(hexa-3,4-dien-3-yl)-5-methoxy-1,3-phenylene)dimorpholine (4p)

12.3 mg, yield: 17%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.39 (s, 2H), 5.14 – 5.00 (m, 1H), 3.79 (d, *J* = 5.9 Hz, 11H), 2.95 (s, 8H), 2.34 (dtt, *J* = 14.9, 7.4, 3.7 Hz, 1H), 2.25 – 2.14 (m, 1H), 1.62 (d, *J* = 6.9 Hz, 3H), 1.04 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.87, 159.65, 152.72, 123.35, 103.64, 101.17, 85.77, 67.55, 55.17, 53.04, 26.65, 13.94, 12.54.
HRMS (ESI) Calcd for $C_{21}H_{30}N_2O_3$ $[M+H]^+$ 359.2329, found 359.2321.



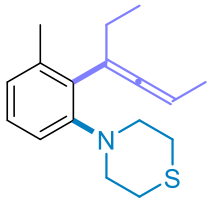
1-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperidine (4q)

27.7 mg, yield: 54%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.10 (t, *J* = 7.7 Hz, 1H), 6.90 (d, *J* = 7.8 Hz, 2H), 5.21 – 5.05 (m, 1H), 2.87 (s, 4H), 2.28 (s, 5H), 1.66 (d, *J* = 6.9 Hz, 7H), 1.56 – 1.50 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.83, 152.19, 137.12, 134.62, 127.14, 124.81, 117.35, 105.04, 85.80, 54.06, 26.81, 25.69, 24.50, 20.47, 13.84, 12.51.
HRMS (ESI) Calcd for $C_{18}H_{25}N$ $[M+H]^+$ 256.2060, found 256.2054.



tert-butyl 4-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperazine-1-carboxylate (4r)

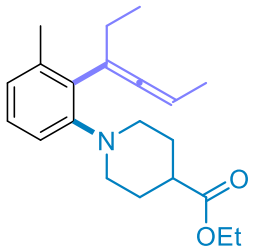
49.6 mg, yield: 70%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.12 (t, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 7.4 Hz, 1H), 6.88 (d, *J* = 7.9 Hz, 1H), 5.22 – 5.10 (m, 1H), 3.51 (s, 4H), 2.94 (s, 4H), 2.29 (s, 5H), 1.66 (d, *J* = 6.9 Hz, 3H), 1.48 (s, 9H), 1.05 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.68, 154.89, 150.45, 137.40, 134.59, 127.30, 125.61, 117.26, 104.68, 86.12, 79.58, 52.40, 44.76, 28.41, 25.83, 20.38, 13.84, 12.47.
HRMS (ESI) Calcd for $C_{22}H_{32}N_2O_2$ $[M+H]^+$ 357.2537, found 357.2532.



4-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)thiomorpholine (4s)

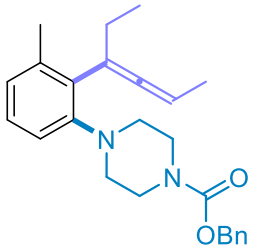
27.9 mg, yield: 51%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.12 (t, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 7.1 Hz, 1H), 6.90 (d, *J* = 7.9 Hz, 1H), 5.21 – 5.08 (m, 1H), 3.19 (s, 4H), 2.80 – 2.69 (m, 4H), 2.28 (s, 5H), 1.66 (d, *J* = 6.9 Hz, 3H), 1.06 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.62, 151.81, 137.39, 134.95, 127.32, 125.66, 118.06, 104.55, 86.07, 55.07, 28.62, 26.01, 20.35, 13.94, 12.47.
HRMS (ESI) Calcd for $C_{17}H_{23}NS$ $[M+H]^+$ 274.1624, found 274.1619.



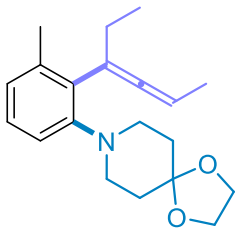
ethyl 1-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperidine-4-carboxylate (4t)

40.1 mg, yield: 61%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.10 (t, *J* = 7.7 Hz, 1H), 6.96 – 6.87 (m, 2H), 5.21 – 5.08 (m, 1H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.25 (s, 2H), 2.65 (s, 2H), 2.28 (s, 6H), 2.01 – 1.92 (m, 2H), 1.88 – 1.78 (m, 2H), 1.66 (d, *J* = 6.9 Hz, 3H), 1.27 (t, *J* = 7.1 Hz, 3H), 1.05 (d, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.71, 175.34, 151.27, 137.27, 134.64, 127.16, 125.22, 117.28, 104.82, 85.88, 60.28, 41.21, 29.12, 29.05, 25.82, 20.42, 14.21, 13.86, 12.52.
HRMS (ESI) Calcd for $C_{21}H_{29}NO_2$ $[M+H]^+$ 328.2271, found 328.2263.



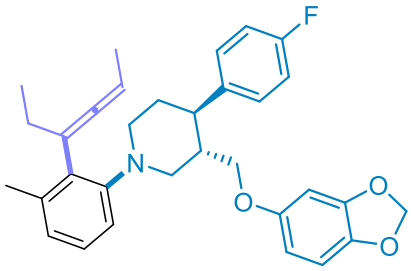
benzyl 4-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperazine-1-carboxylate (4u)

48.9 mg, yield: 63%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.30 (m, 5H), 7.12 (t, *J* = 7.7 Hz, 1H), 6.96 (d, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 7.9 Hz, 1H), 5.20 – 5.05 (m, 3H), 3.60 (s, 4H), 2.94 (s, 4H), 2.28 (s, 5H), 1.65 (d, *J* = 6.2 Hz, 3H), 1.04 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.62, 155.32, 150.25, 137.44, 136.66, 134.54, 128.44, 127.97, 127.90, 127.32, 125.71, 117.23, 104.60, 86.17, 67.09, 52.31, 44.49, 25.84, 20.37, 13.86, 12.47.
HRMS (ESI) Calcd for $C_{25}H_{30}N_2O_2$ $[M+H]^+$ 391.2380, found 391.2372.



8-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)-1,4-dioxa-8-azaspiro[4.5]decane (4v)

36.1 mg, yield: 58%. Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.10 (t, *J* = 7.7 Hz, 1H), 7.00 – 6.86 (m, 2H), 5.28 – 4.98 (m, 1H), 3.99 (s, 4H), 3.03 (s, 4H), 2.28 (s, 5H), 1.84 (t, *J* = 5.1 Hz, 4H), 1.65 (d, *J* = 6.8 Hz, 3H), 1.05 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.60, 151.00, 137.19, 134.59, 127.18, 125.20, 117.51, 107.27, 104.92, 85.95, 64.21, 50.88, 35.79, 25.79, 20.39, 13.83, 12.53.
HRMS (ESI) Calcd for $C_{20}H_{27}NO_2$ $[M+H]^+$ 314.2115, found 314.2106.



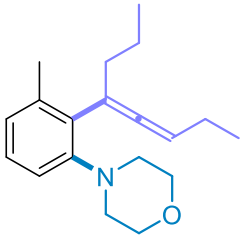
(3S,4R)-3-((benzo[d][1,3]dioxol-5-yloxy)methyl)-4-(4-fluorophenyl)-1-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperidine (4w) (d.r. = 1:1)

58.5 mg, yield: 59%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 – 7.11 (m, 3H), 7.07 – 6.91 (m, 4H), 6.61 (d, *J* = 8.4 Hz, 1H), 6.33 (s, 1H), 6.12 (d, *J* = 8.4 Hz, 1H), 5.86 (s, 2H), 5.35 – 5.04 (m, 1H), 3.83 – 3.18 (m, 4H), 2.96 – 2.19 (m, 9H), 1.89 (s, 2H), 1.77 – 1.56 (m, 3H), 1.13 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.78, 161.47 (d, *J* = 244.3 Hz), 154.43, 151.29 (d, *J* = 10.2 Hz), 148.06, 141.45 (d, *J* = 1.8 Hz), 140.36 – 139.60 (m), 137.28, 134.69, 128.79 (dd, *J* = 7.7, 3.4 Hz), 127.26, 125.33 (d, *J* = 12.5 Hz), 117.56 (d, *J* = 27.8 Hz), 115.37 (dd, *J* = 21.0, 4.2 Hz), 107.77 (d, *J* = 1.5 Hz), 105.41 (d, *J* = 5.5 Hz), 104.74, 101.00, 97.85 (d, *J* = 6.5 Hz), 86.08 (d, *J* = 9.5 Hz), 69.63, 60.37, 44.25, 44.09, 42.88, 42.80, 35.43, 35.21, 25.98, 25.91, 21.02, 20.55, 20.42, 14.17, 13.86, 12.69.

HRMS (ESI) Calcd for $C_{32}H_{34}FNO_3$ $[M+H]^+$ 500.2595, found 500.2585.



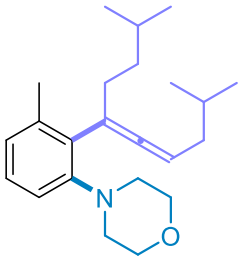
4-(3-methyl-2-(octa-4,5-dien-4-yl)phenyl)morpholine (4aa)

38.8 mg, yield: 68%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.13 (t, *J* = 7.7 Hz, 1H), 7.00 – 6.87 (m, 2H), 5.13 (s, 1H), 3.80 (s, 4H), 2.99 (s, 4H), 2.29 (s, 5H), 2.02 (s, 2H), 1.49 (h, *J* = 7.3 Hz, 2H), 1.12 – 0.88 (m, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 201.61, 150.45, 137.55, 134.54, 127.31, 125.62, 117.18, 103.83, 92.97, 67.55, 52.91, 35.11, 22.19, 21.19, 20.51, 14.40, 14.26.

HRMS (ESI) Calcd for $C_{19}H_{27}NO$ $[M+H]^+$ 286.2165, found 286.2158.



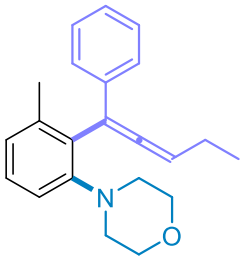
4-(2-(2,9-dimethyldeca-5,6-dien-5-yl)-3-methylphenyl)morpholine (4ab)

37.7 mg, yield: 55%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.13 (t, *J* = 7.7 Hz, 1H), 7.01 – 6.83 (m, 2H), 5.07 (s, 1H), 3.80 (s, 4H), 3.00 (d, *J* = 208.8 Hz, 4H), 2.29 (s, 5H), 1.89 (s, 2H), 1.68 – 1.55 (m, 2H), 1.36 (q, *J* = 7.5 Hz, 2H), 1.00 – 0.80 (m, 12H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 202.54, 150.34, 137.41, 134.46, 127.28, 125.52, 117.01, 103.14, 89.85, 67.57, 52.86, 38.04, 37.19, 30.56, 28.85, 27.86, 22.68, 22.37, 22.25, 20.55.

HRMS (ESI) Calcd for $C_{23}H_{35}NO$ $[M+H]^+$ 342.2791, found 342.2782.



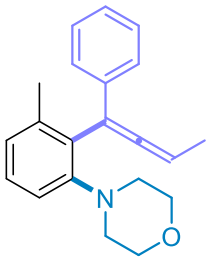
4-(3-methyl-2-(1-phenylpenta-1,2-dien-1-yl)phenyl)morpholine (4ac)

18.1 mg, yield: 28%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26 – 7.20 (m, 3H), 7.15 (t, *J* = 6.8 Hz, 3H), 7.02 (d, *J* = 7.5 Hz, 1H), 6.95 (d, *J* = 7.9 Hz, 1H), 5.77 – 5.39 (m, 1H), 3.46 (s, 4H), 2.88 (s, 4H), 2.28 – 2.15 (m, 5H), 1.12 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.76, 151.25, 131.74, 129.31, 128.08, 128.01, 126.71, 126.17, 125.84, 125.51, 124.79, 117.56, 95.39, 67.15, 52.22, 22.05, 20.62, 14.24.

HRMS (ESI) Calcd for $C_{22}H_{25}NO$ $[M+H]^+$ 320.2009, found 320.2003.



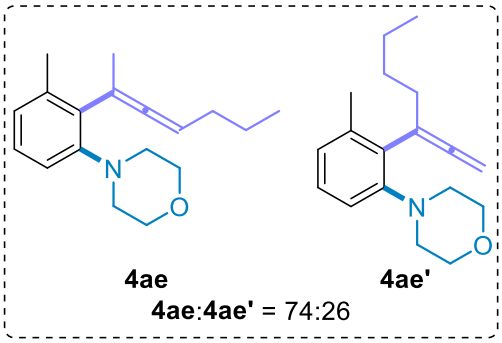
4-(3-methyl-2-(1-phenylbuta-1,2-dien-1-yl)phenyl)morpholine (4ad)

21.8 mg, yield: 36%. Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26 – 7.20 (m, 3H), 7.18 – 7.08 (m, 3H), 7.03 (d, *J* = 7.5 Hz, 1H), 6.95 (d, *J* = 7.9 Hz, 1H), 5.53 (d, *J* = 6.6 Hz, 1H), 3.44 (s, 4H), 3.21 – 2.58 (m, 4H), 2.27 (s, 3H), 1.80 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 204.95, 151.15, 137.48, 131.71, 128.11, 127.99, 126.18, 125.94, 125.51, 117.56, 88.06, 67.16, 52.22, 20.63, 13.48.

HRMS (ESI) Calcd for $C_{21}H_{23}NO$ $[M+H]^+$ 306.1852, found 306.1846.



4-(2-(hepta-2,3-dien-2-yl)-3-methylphenyl)morpholine (4ae) and 4-(2-(hepta-1,2-dien-3-yl)-3-methylphenyl)morpholine (4ae') (4ae:4ae' = 74:26)

21.5 mg, yield: 40%. Colorless liquid.

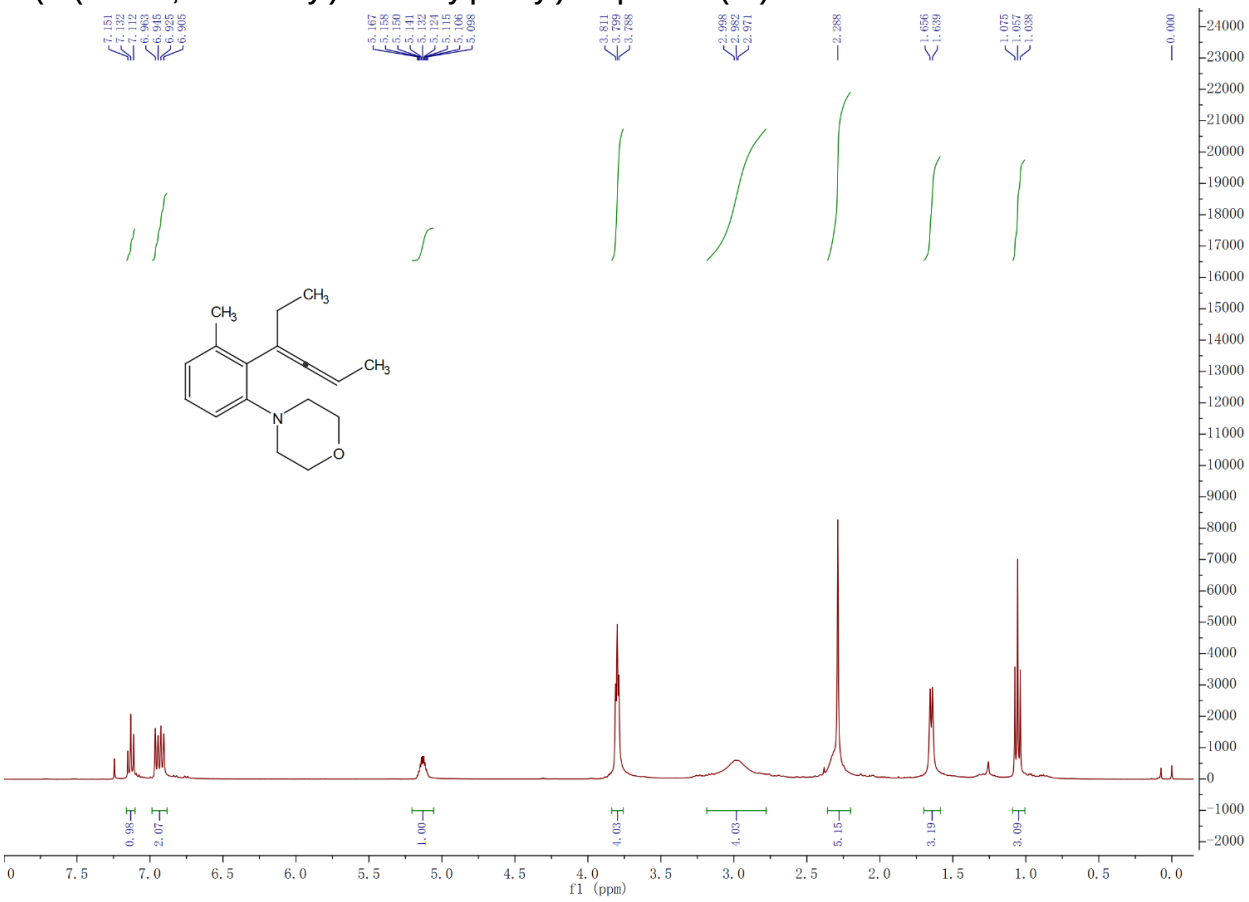
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.17 – 7.11 (m, 1H), 6.98 – 6.89 (m, 2H), 5.10 – 4.92 (m, 0.74H), 4.69 (s, 0.51H), 3.87 – 3.76 (m, 4H), 3.02 (s, 4H), 2.33 – 2.26 (m, 3.33H), 2.05 – 1.93 (m, 3.71H), 1.50 – 1.32 (m, 3H), 0.92 (t, *J* = 7.3 Hz, 3H).

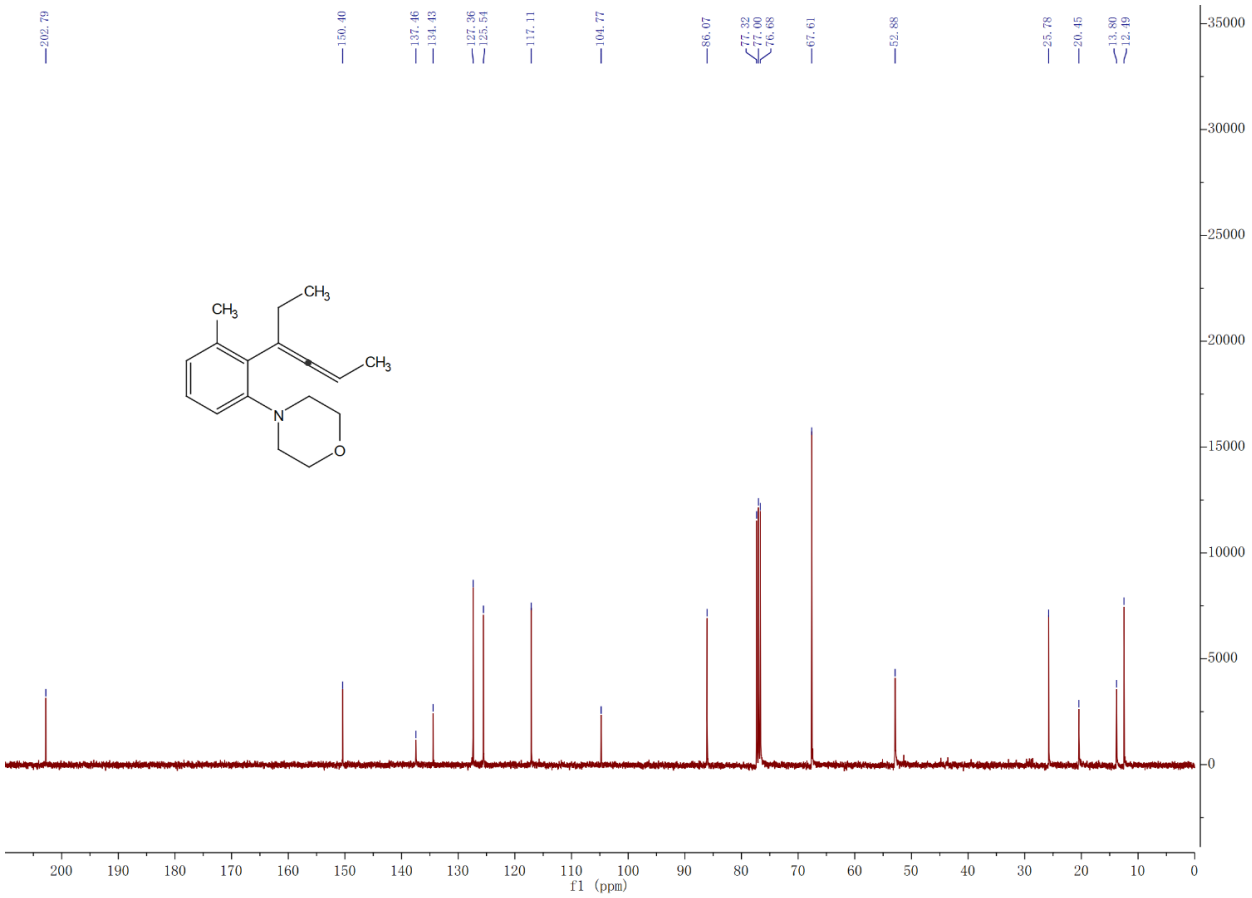
^{13}C NMR (101 MHz, Chloroform-*d*) δ 206.50, 202.96, 150.39, 150.33, 137.72, 137.27, 134.61, 127.58, 127.36, 125.58, 125.50, 117.15, 117.02, 103.27, 98.23, 89.19, 74.64, 67.59, 52.87, 31.73, 30.75, 30.01, 22.90, 22.71, 20.45, 20.29, 19.92, 14.07, 13.65.

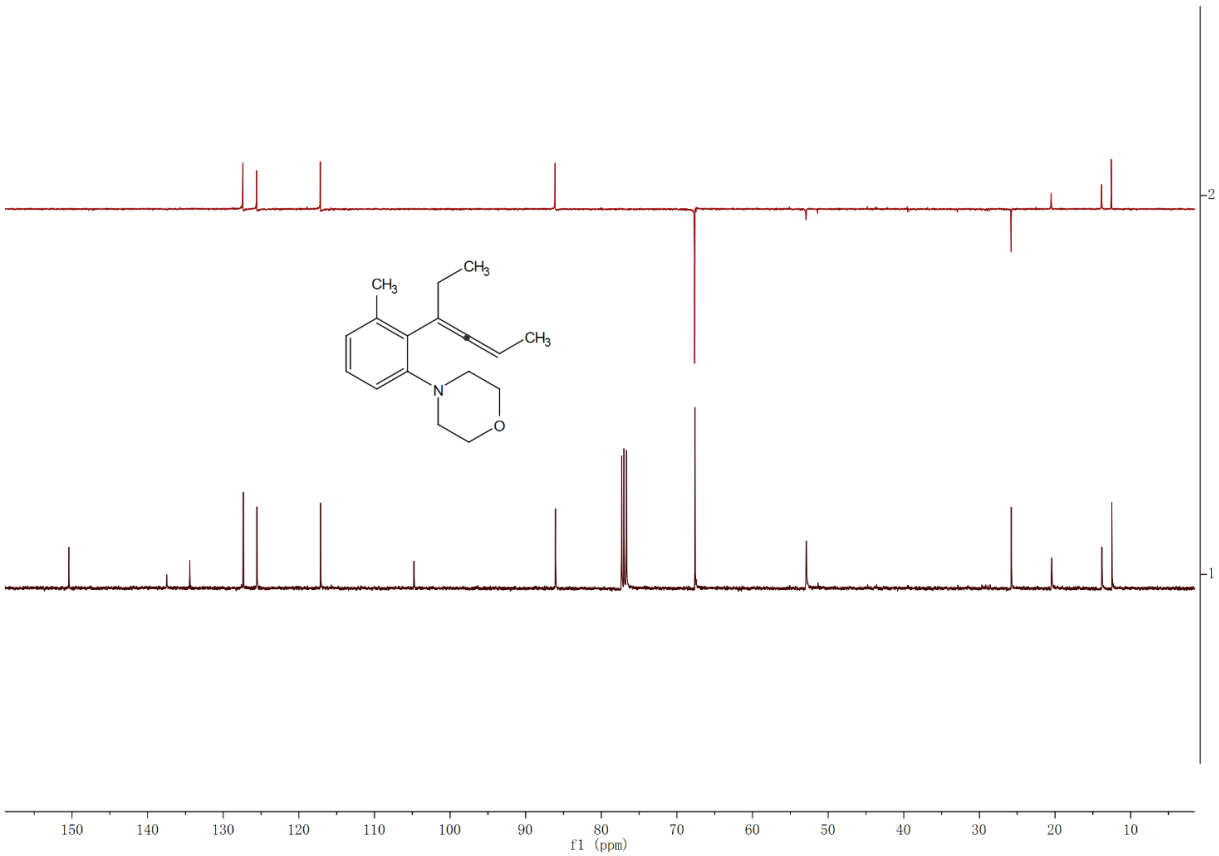
HRMS (ESI) Calcd for $C_{18}H_{25}NO$ $[M+H]^+$ 272.2009, found 272.2003.

8. NMR Spectroscopic Data

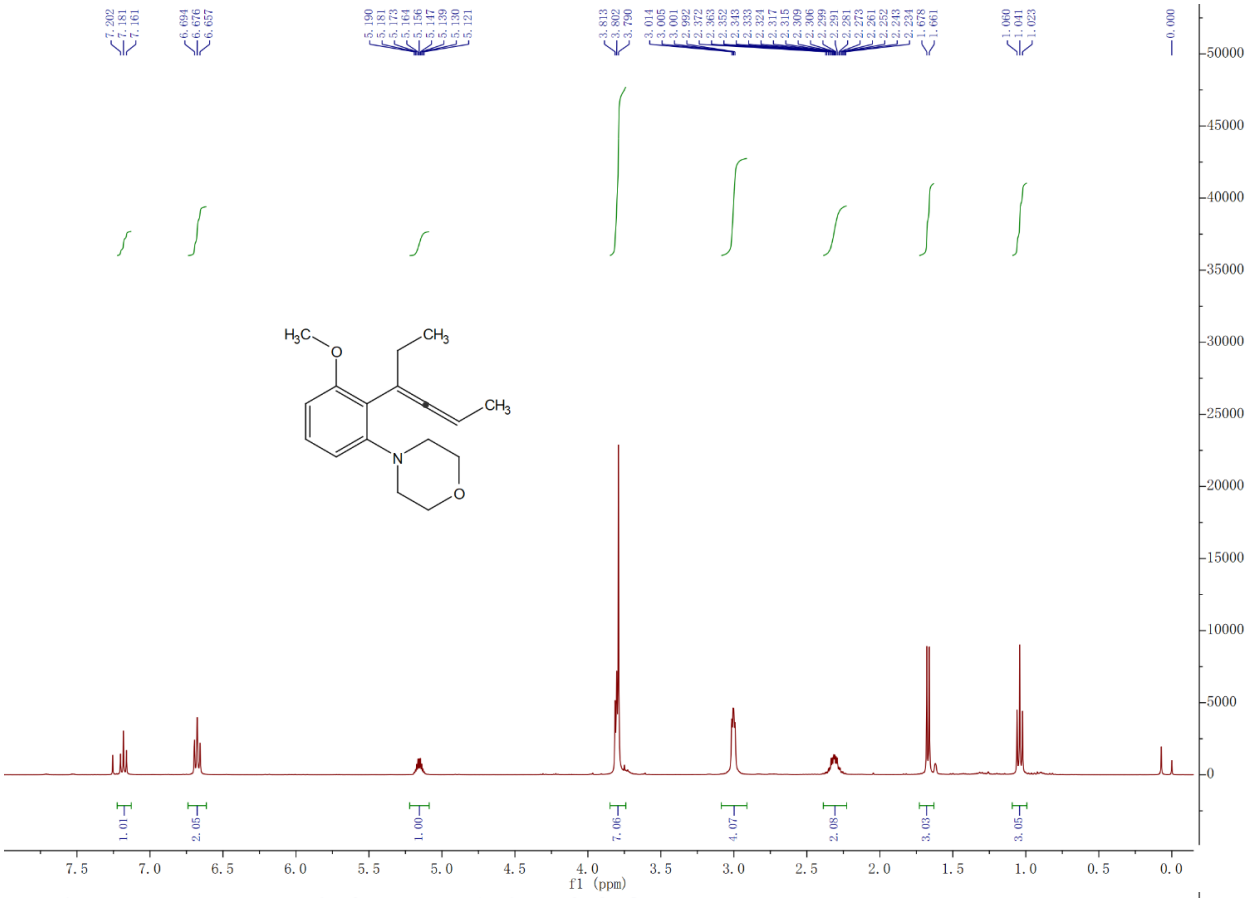
4-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)morpholine (4a)

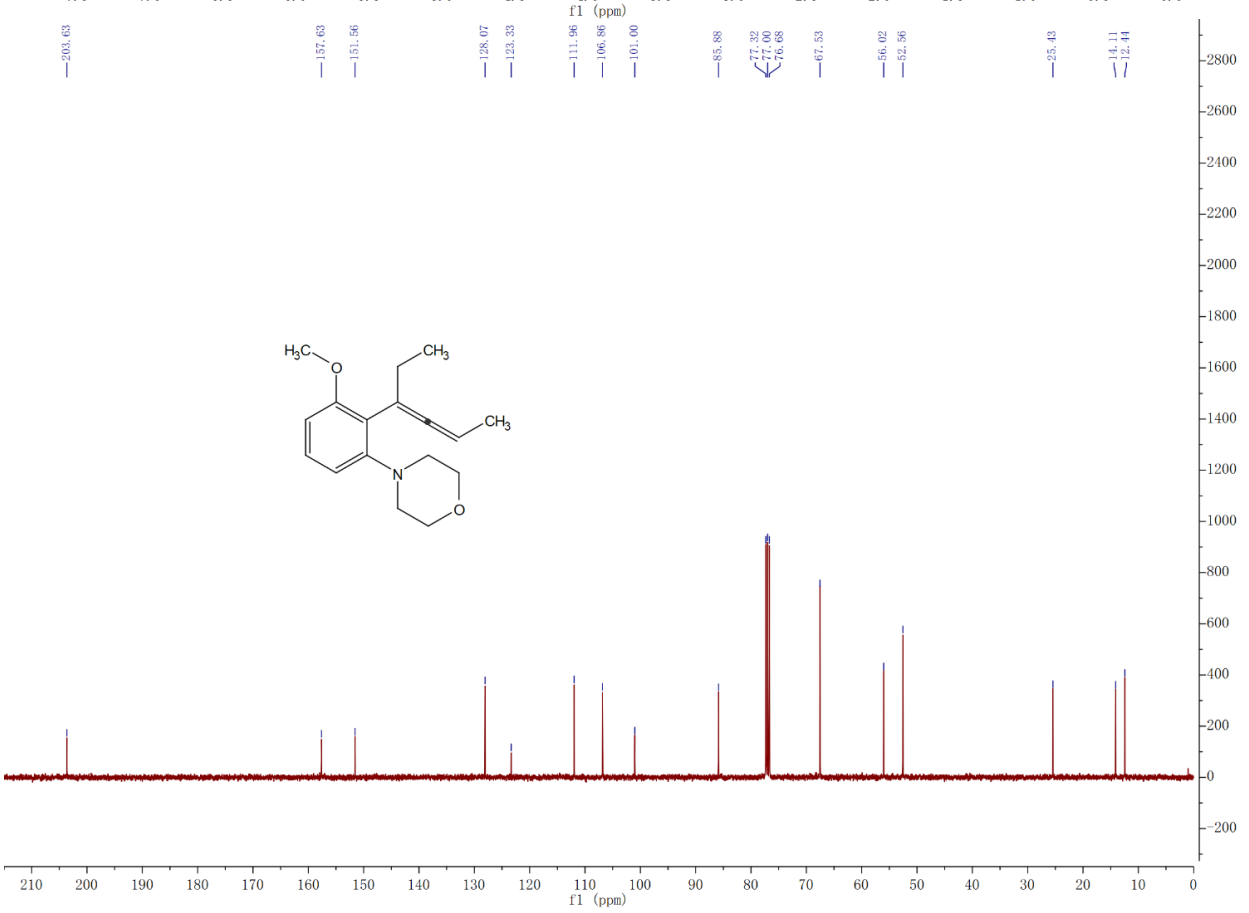



202.79
150.40
137.46
134.43
127.36
125.54
117.11
104.77
86.07
77.32
77.00
76.68
67.61
52.88
25.78
20.45
13.80
12.49
CH3
CH3
CH3
N
O
35000
30000
25000
20000
15000
10000
5000
0
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

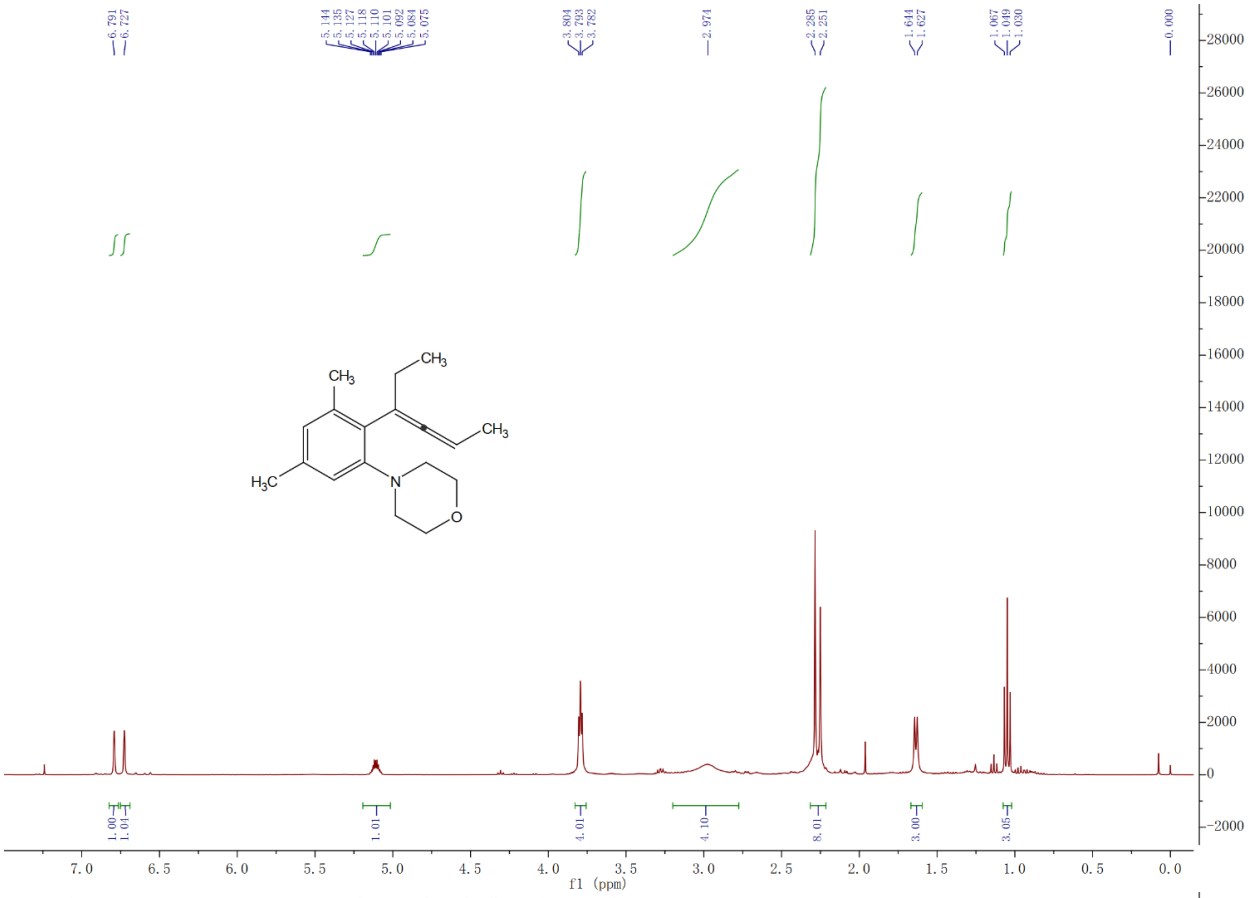

CH3
CH3
CH3
N
O
2
1
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

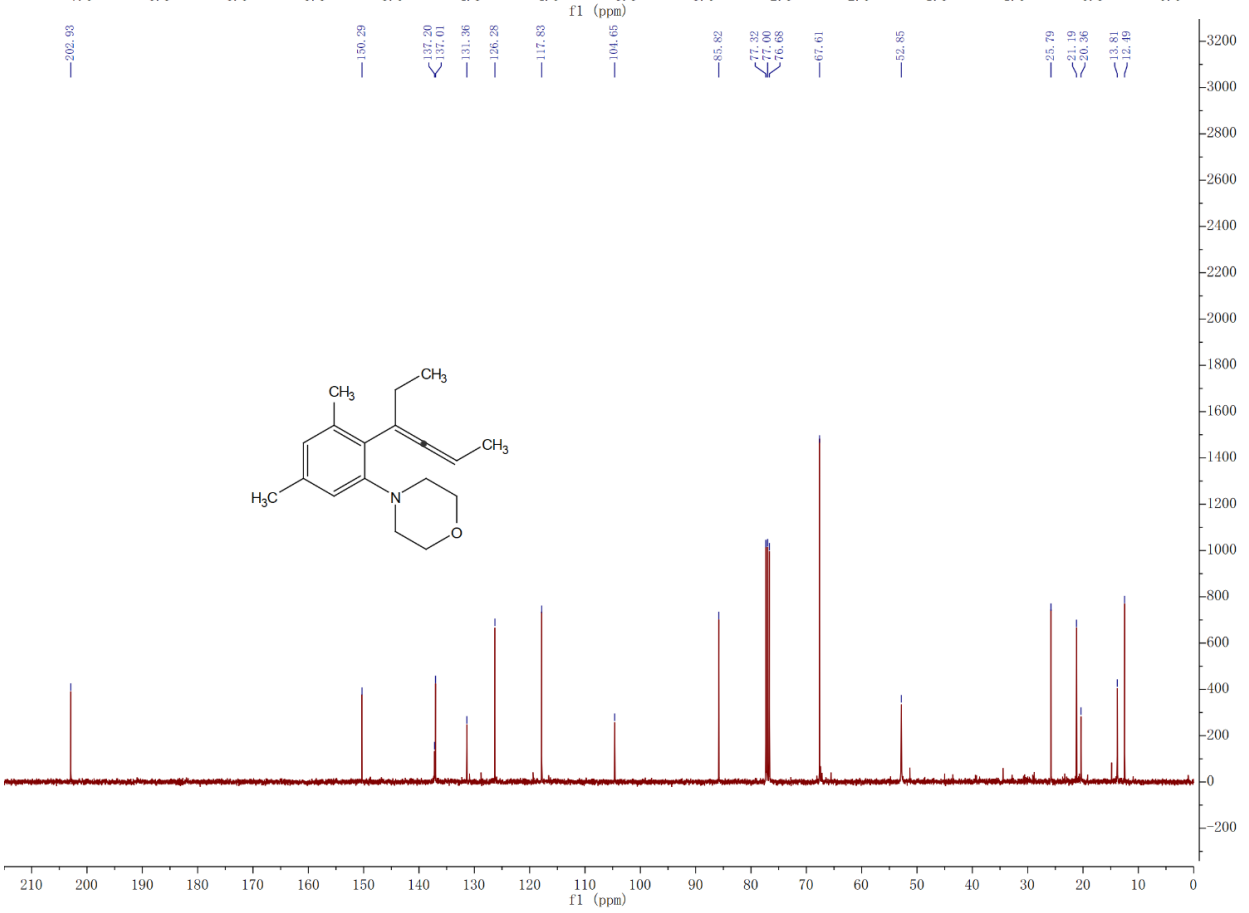
4-(2-(hexa-3,4-dien-3-yl)-3-methoxyphenyl)morpholine (4b)



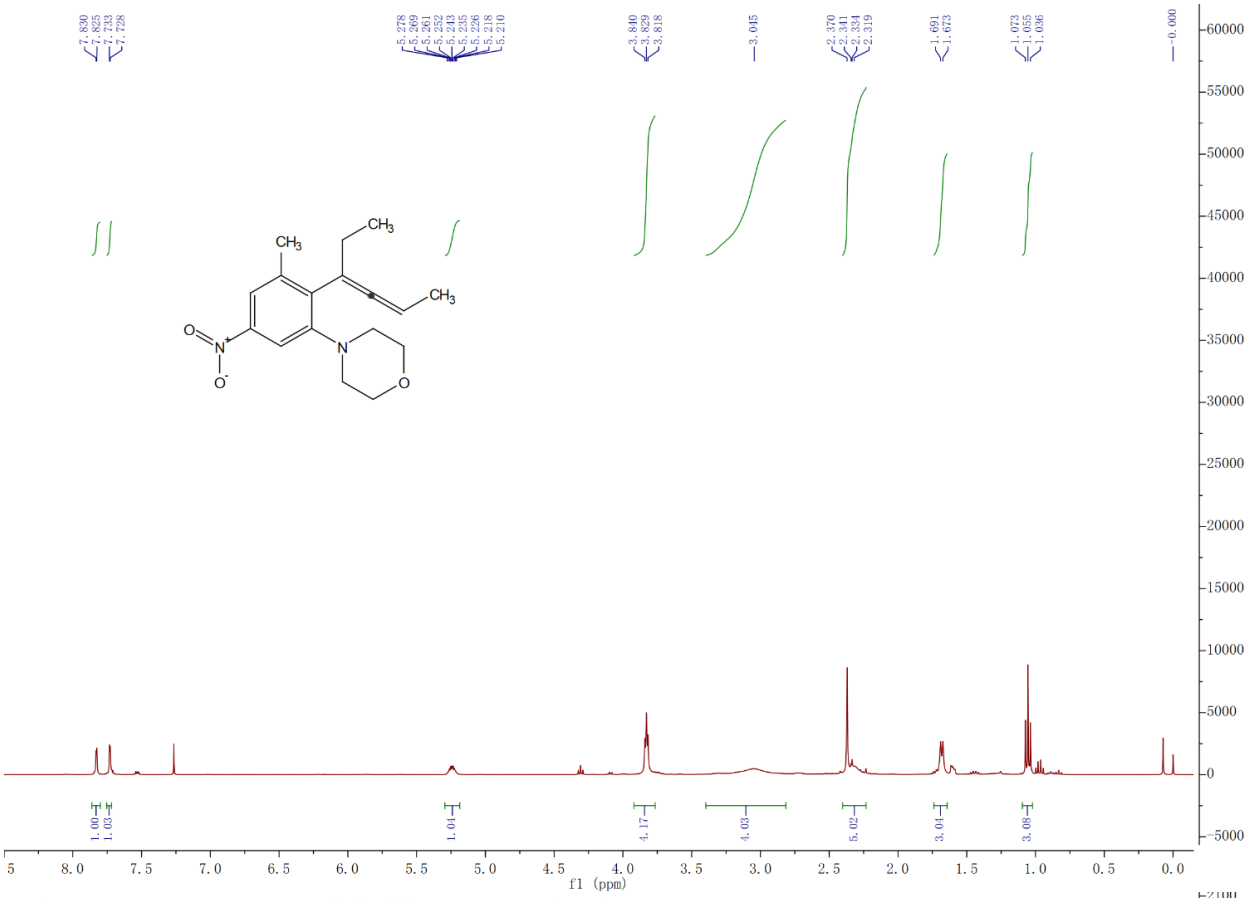


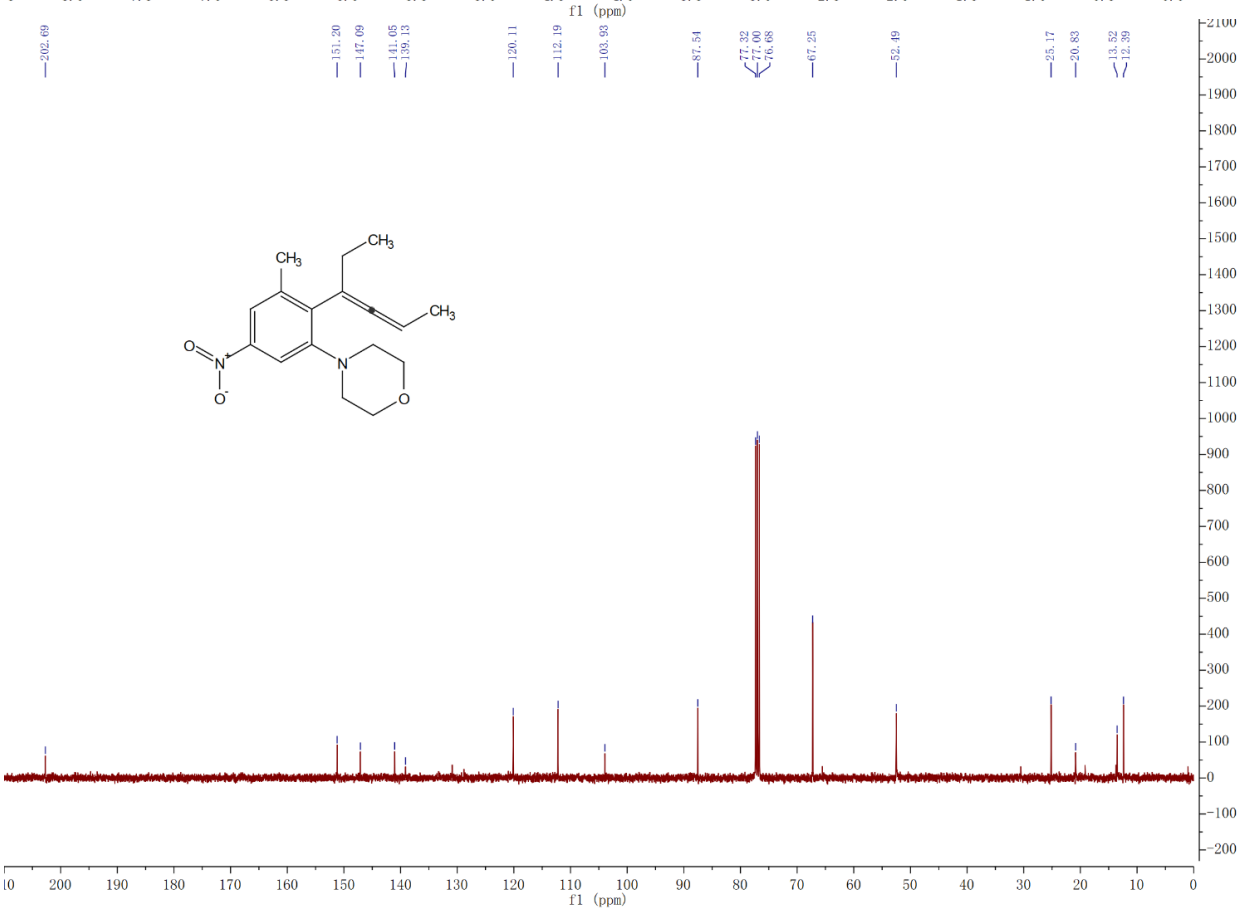
4-(2-(hexa-3,4-dien-3-yl)-3,5-dimethylphenyl)morpholine (4c)



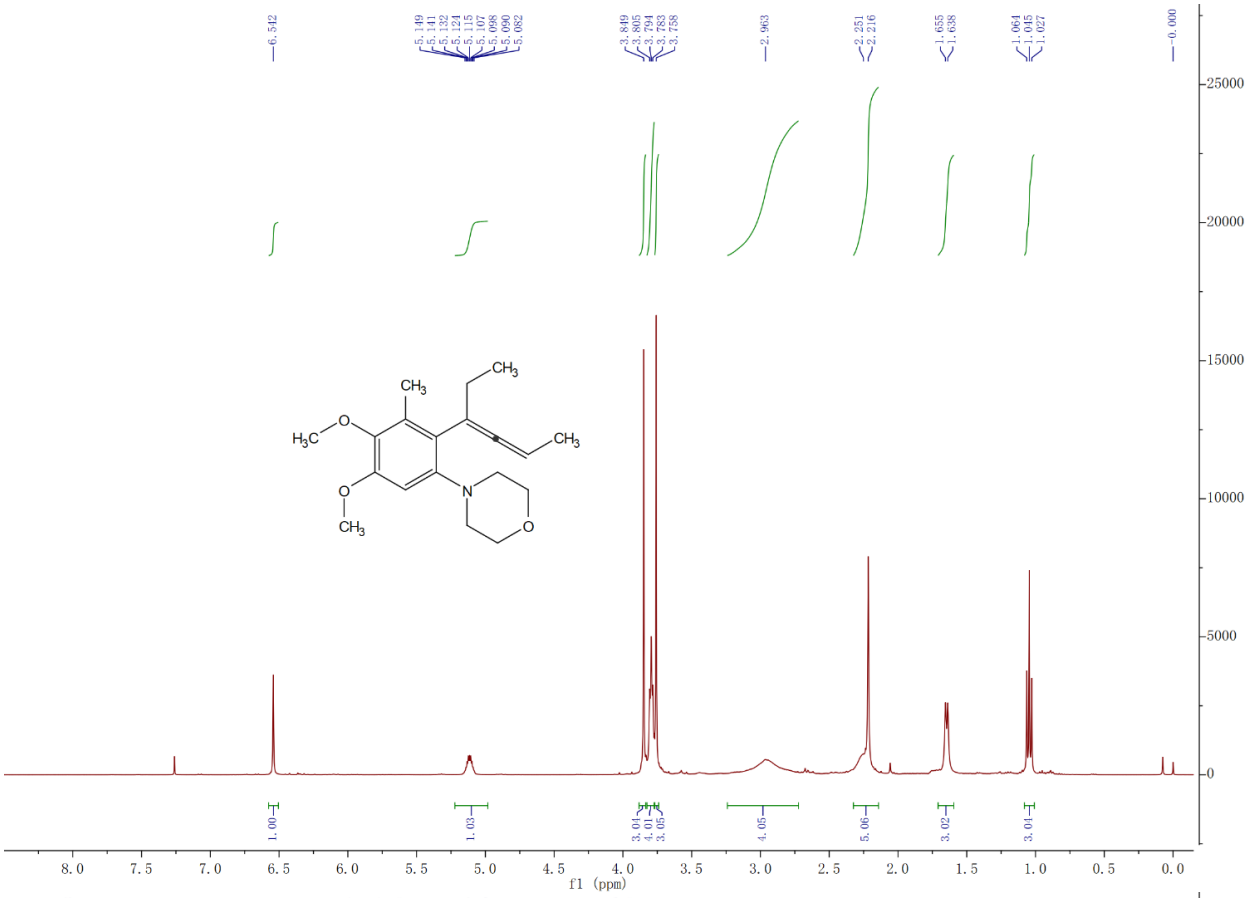


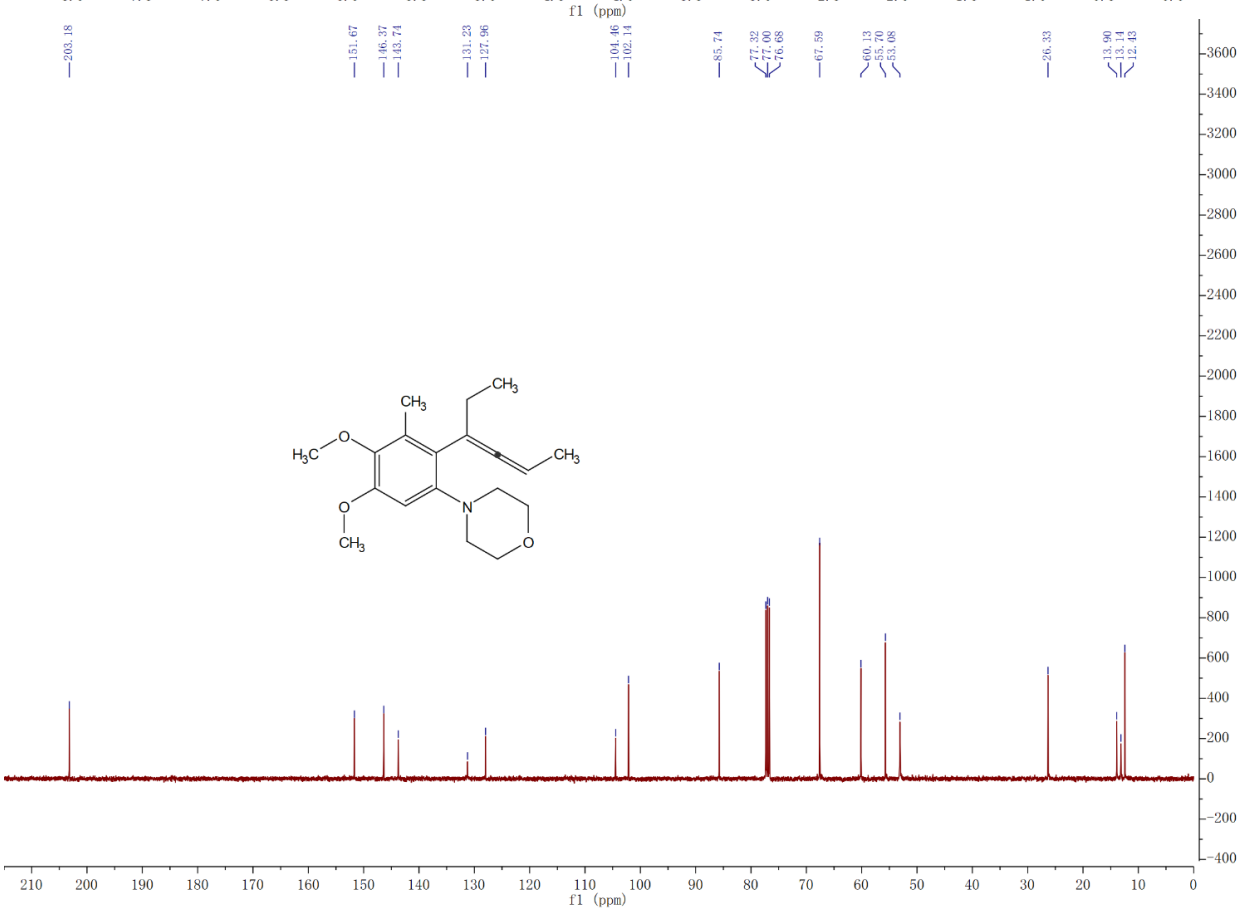
4-(2-(hexa-3,4-dien-3-yl)-3-methyl-5-nitrophenyl)morpholine (4d)



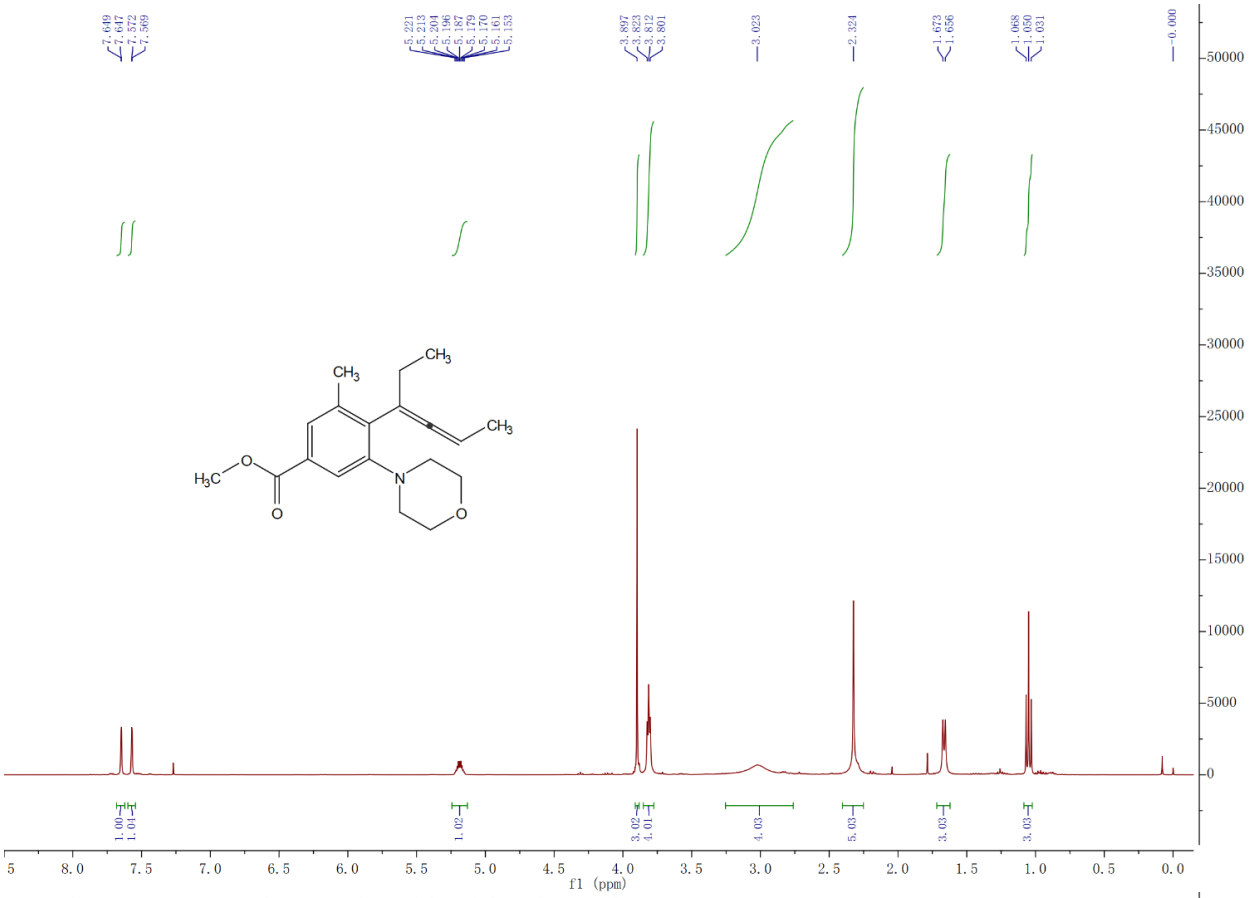


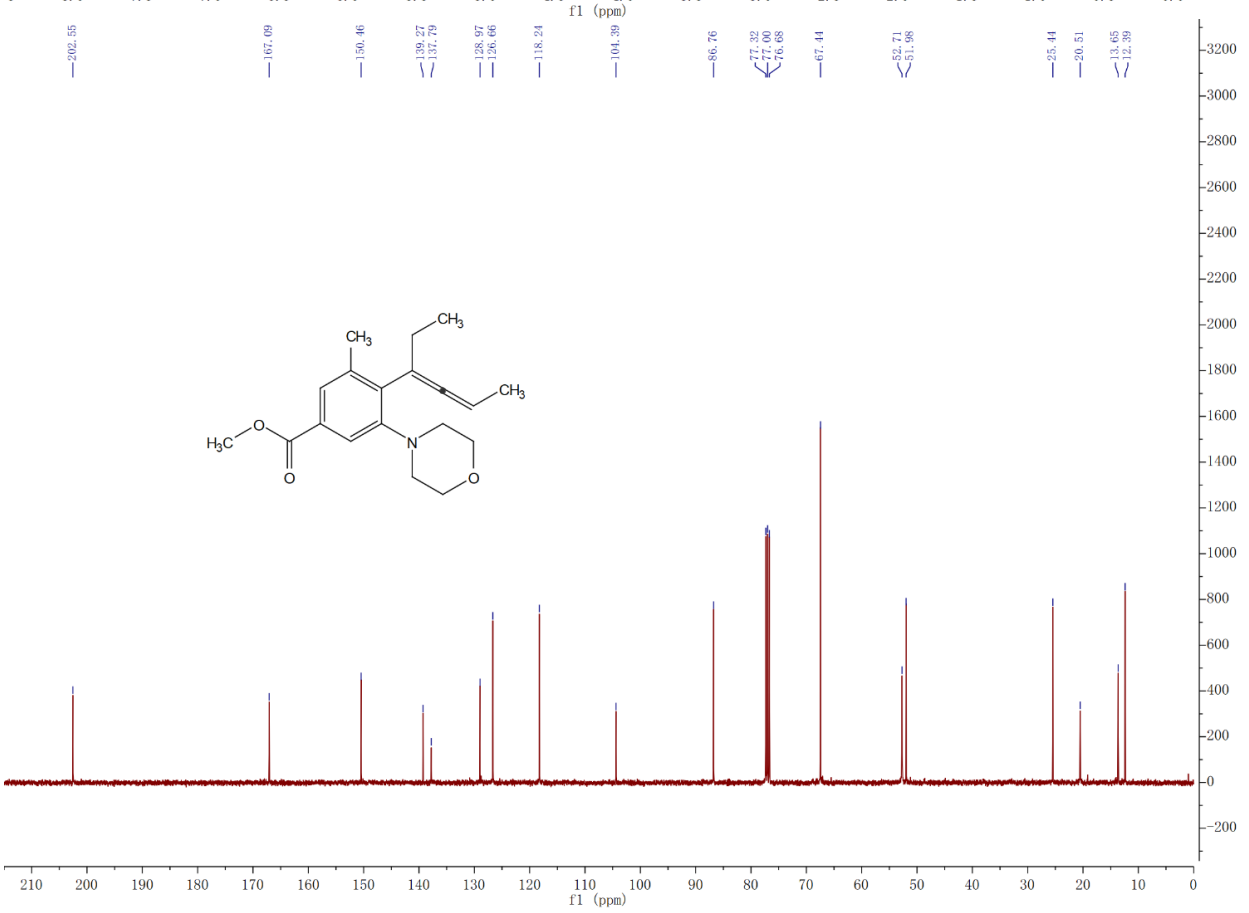
4-(2-(hexa-3,4-dien-3-yl)-4,5-dimethoxy-3-methylphenyl)morpholine (4e)



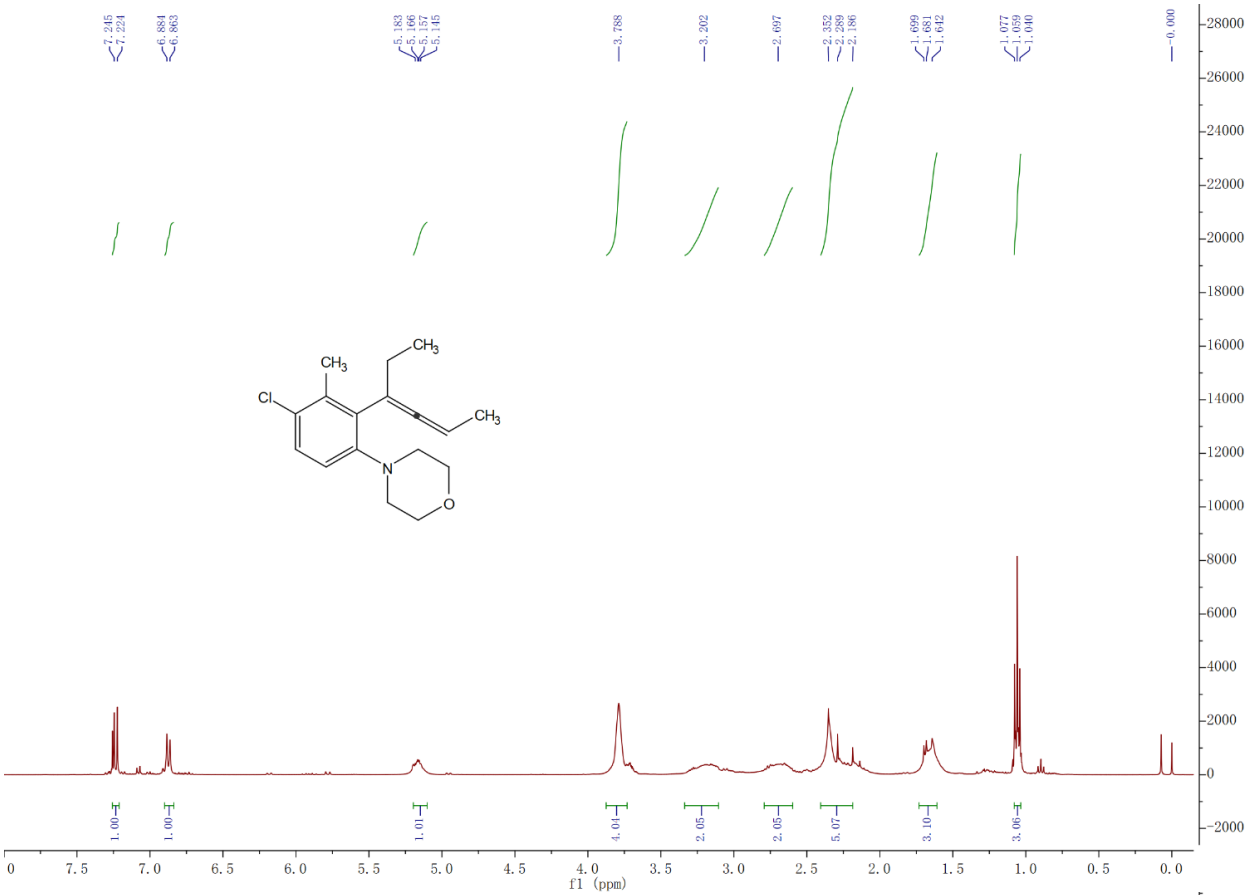


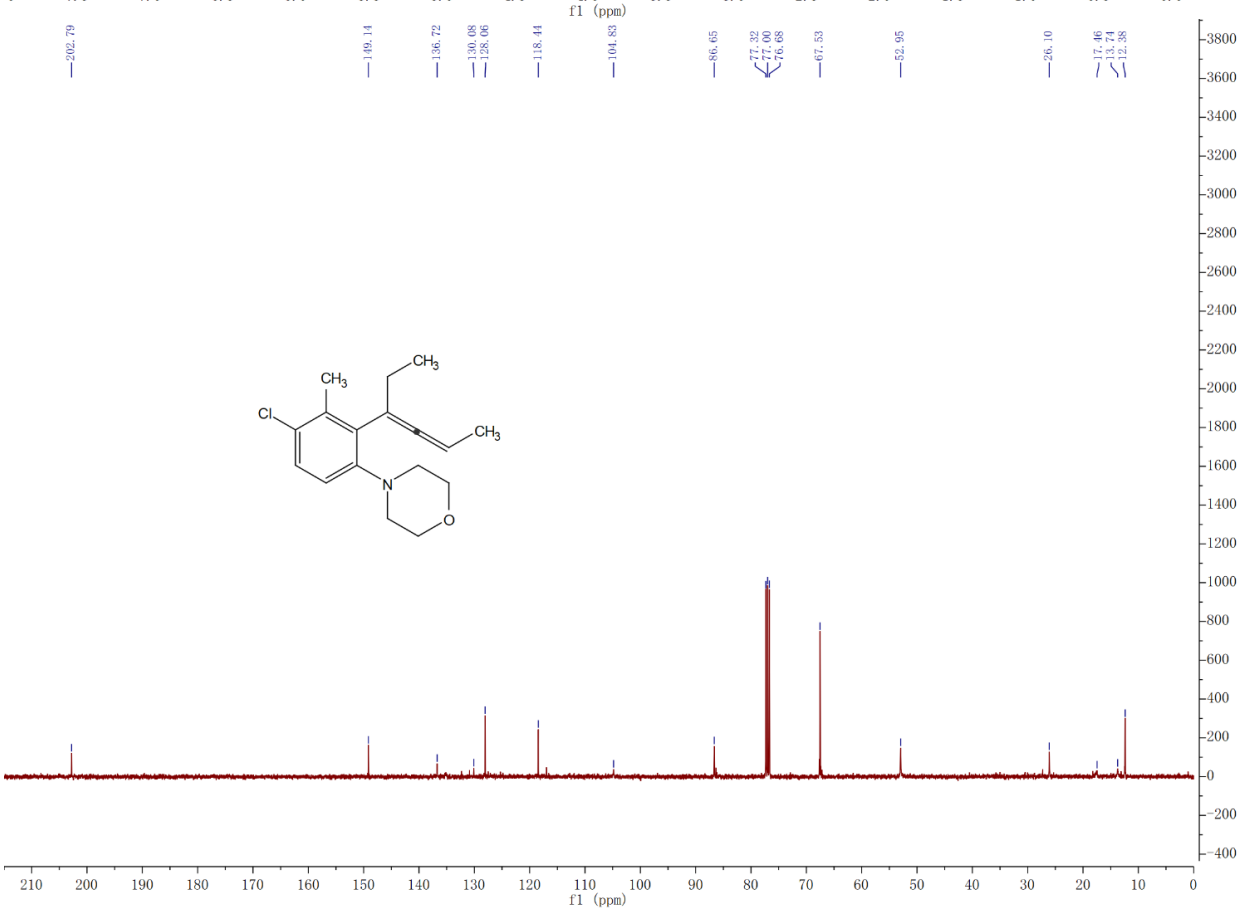
methyl 4-(hexa-3,4-dien-3-yl)-3-methyl-5-morpholinobenzoate (4f)



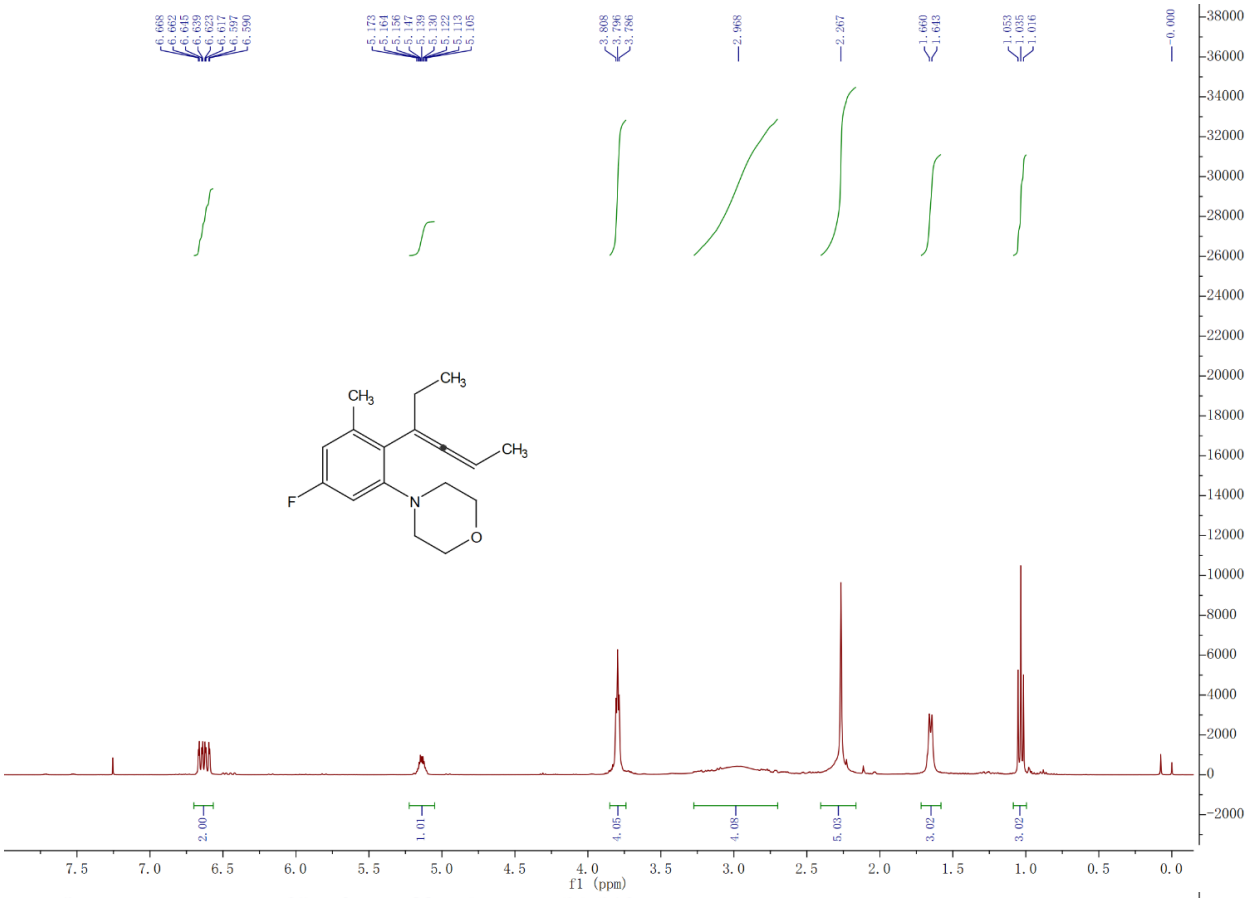


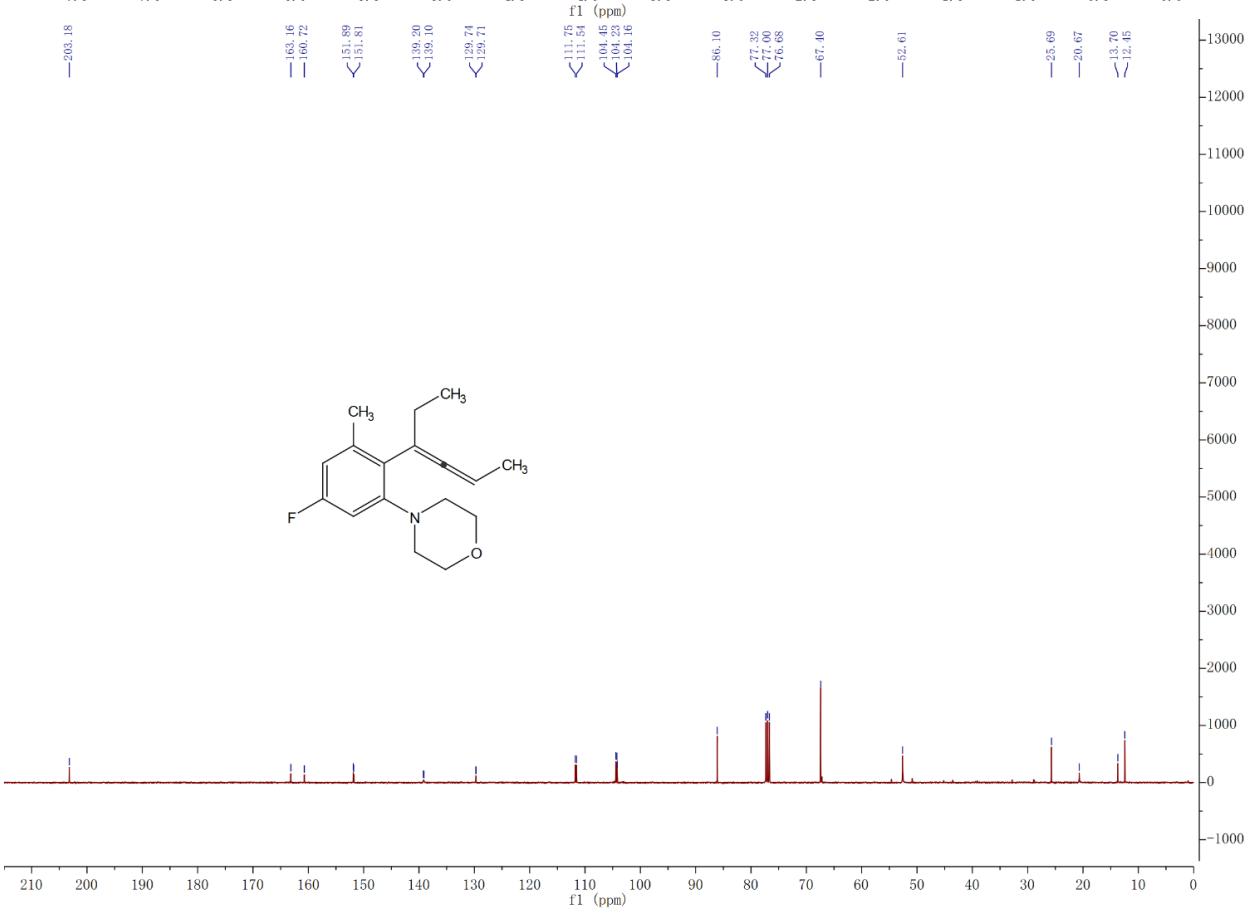
4-(4-chloro-2-(hexa-3,4-dien-3-yl)-3-methylphenyl)morpholine (4g)

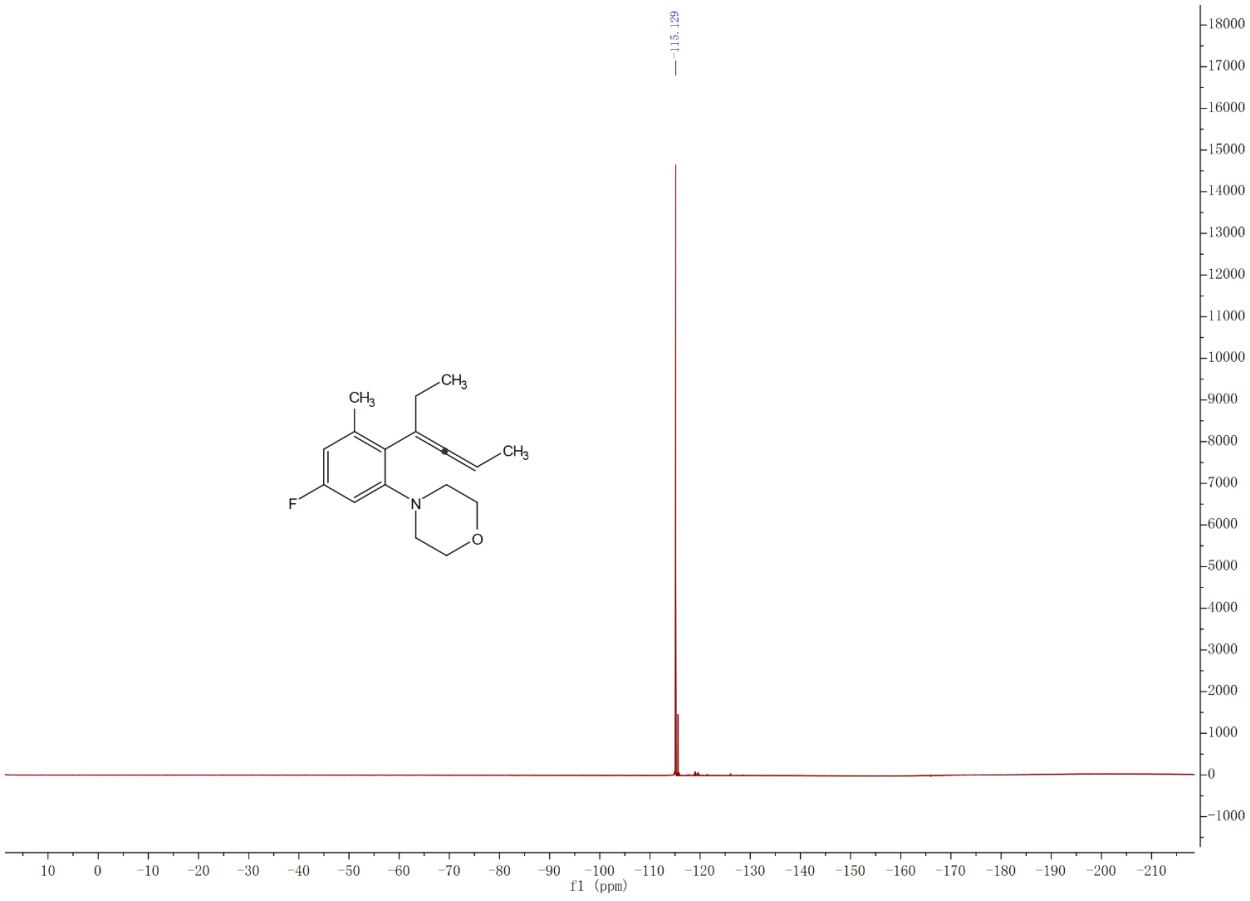




4-(5-fluoro-2-(hexa-3,4-dien-3-yl)-3-methylphenyl)morpholine (4h)






-115.129
CH3
CH3
CH3
F
N
O
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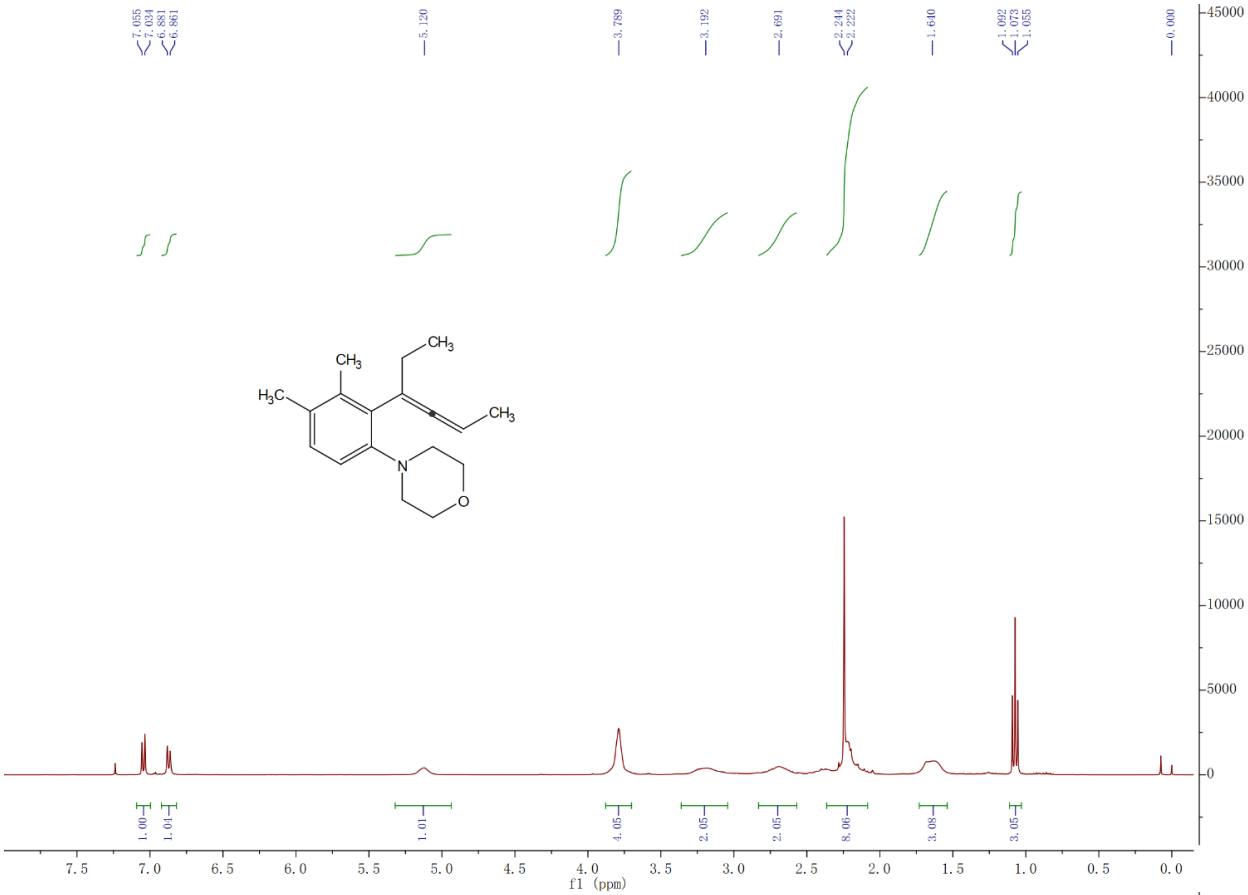
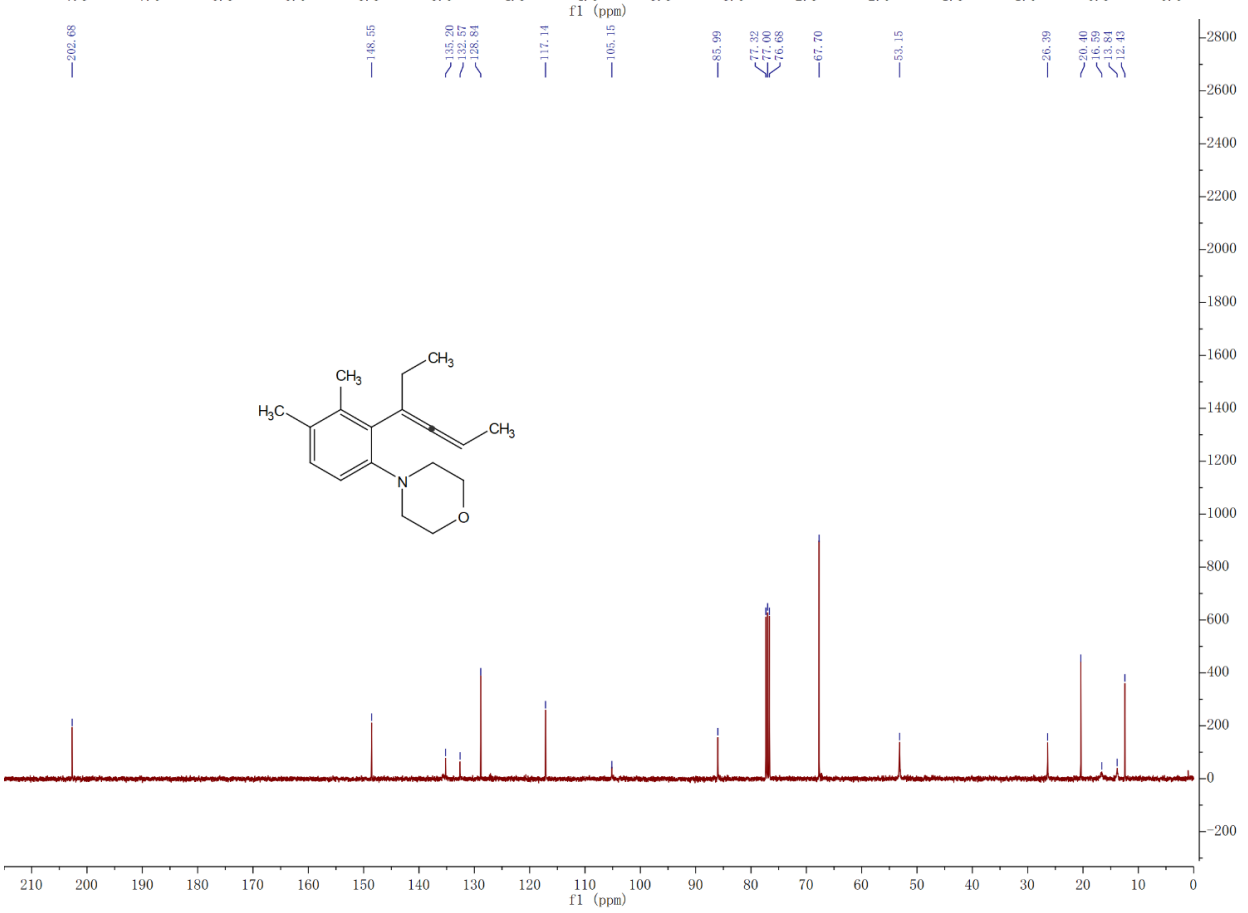
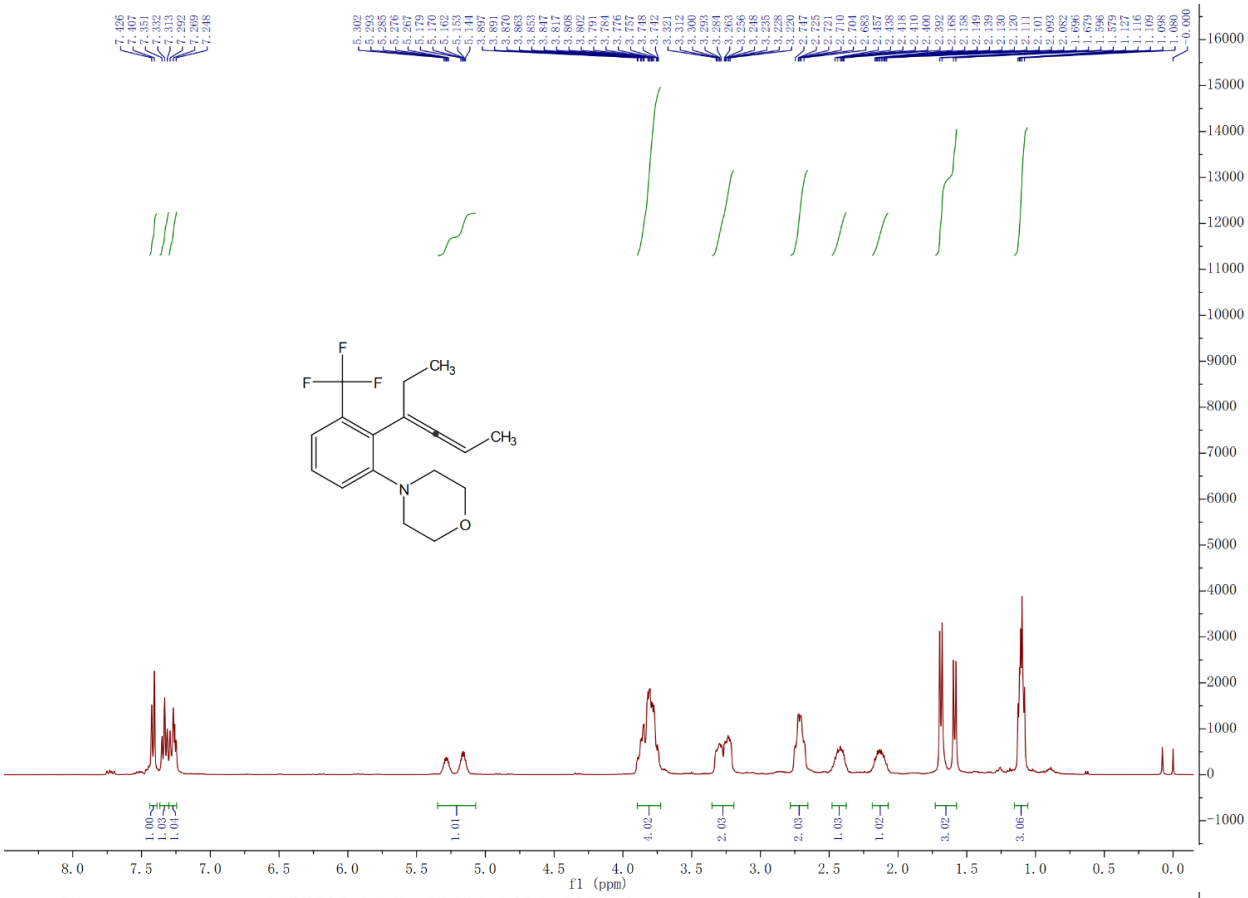
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

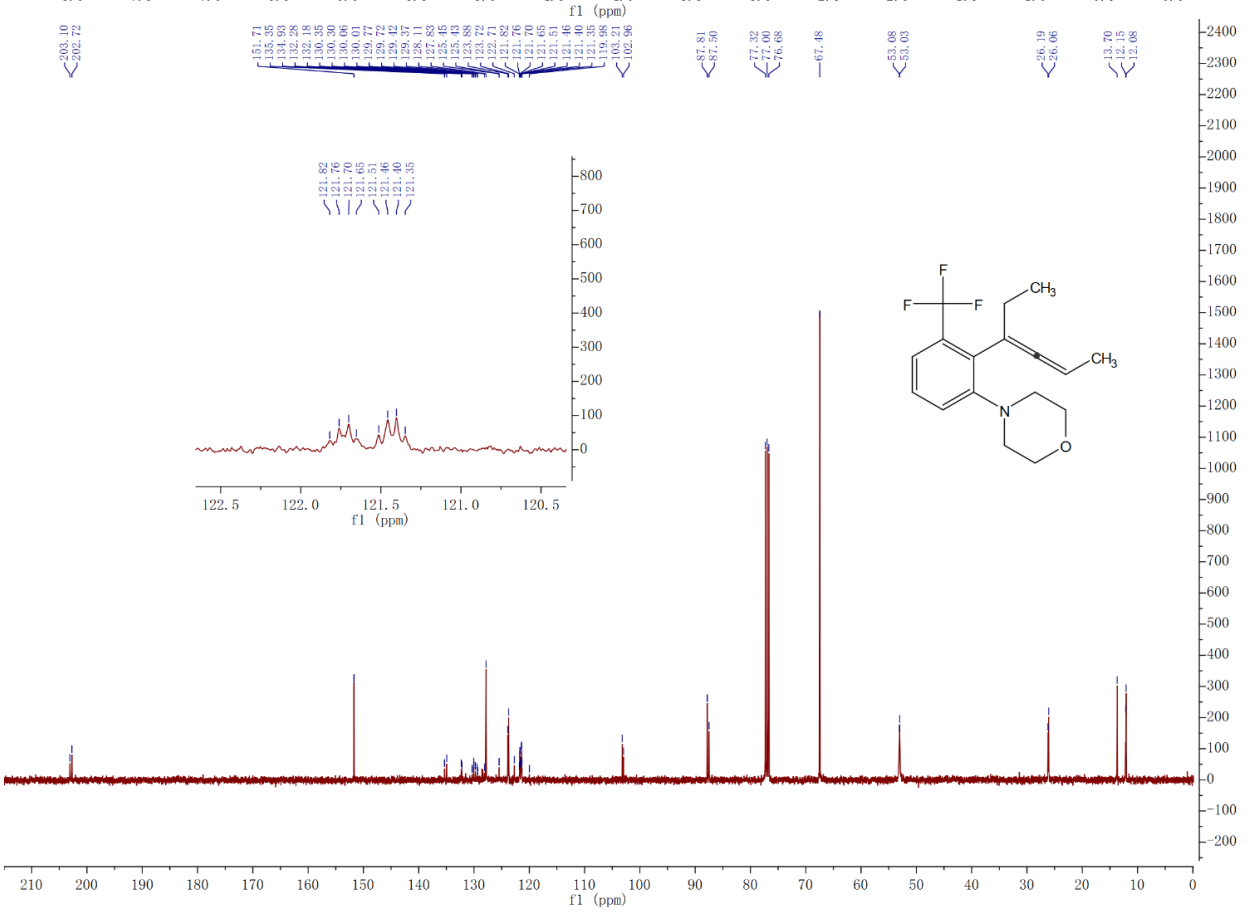
4-(2-(hexa-3,4-dien-3-yl)-3,4-dimethylphenyl)morpholine (4i)



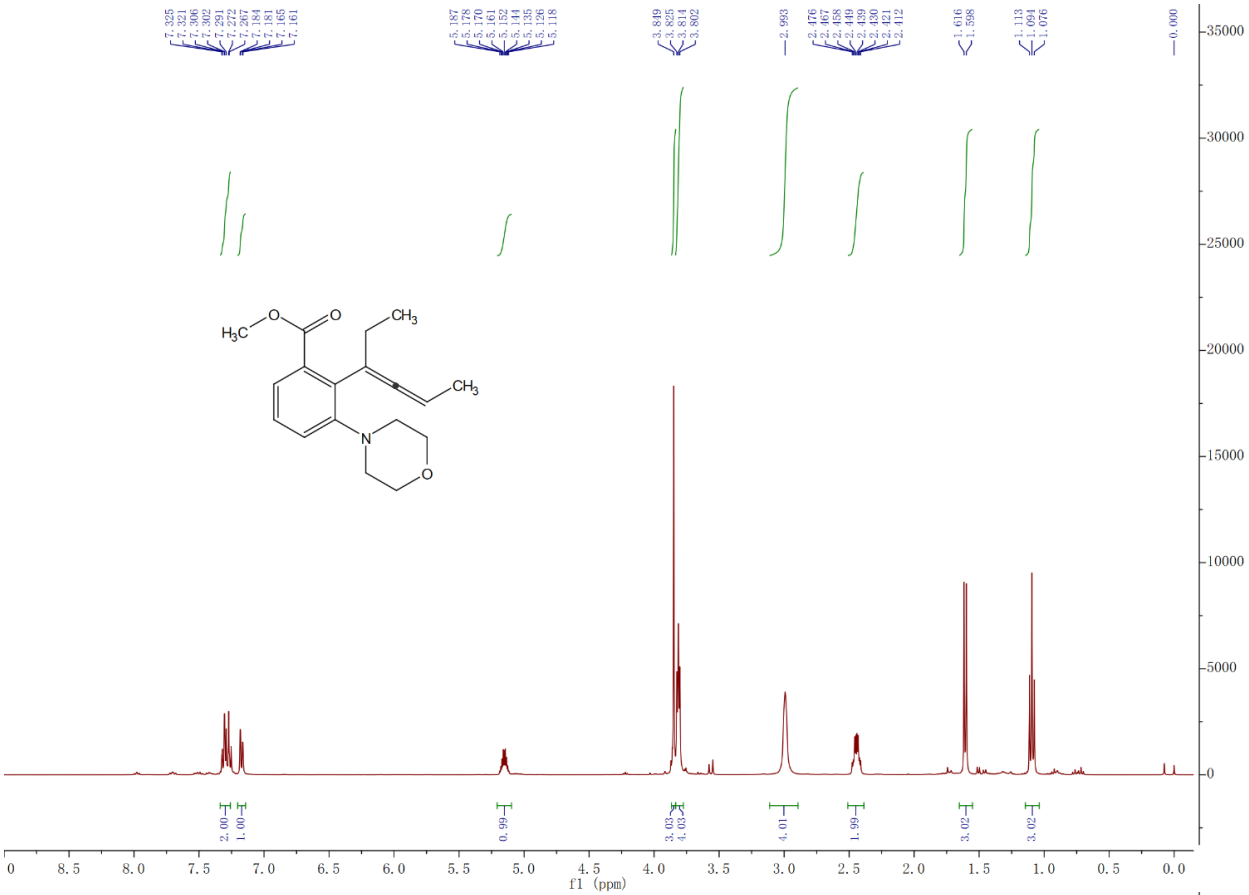


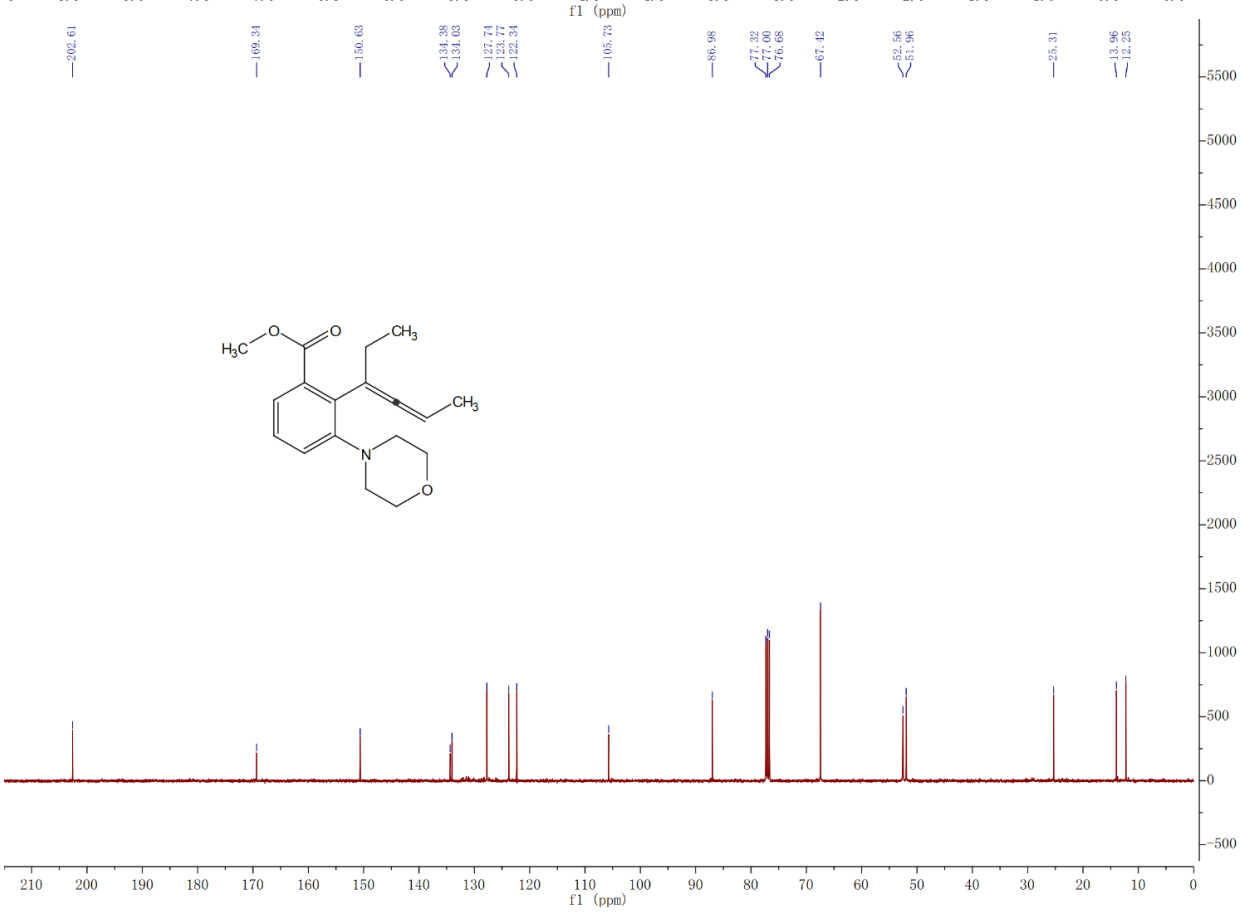
4-(2-(hexa-3,4-dien-3-yl)-3-(trifluoromethyl)phenyl)morpholine (4j) (d.r. = 56:44)



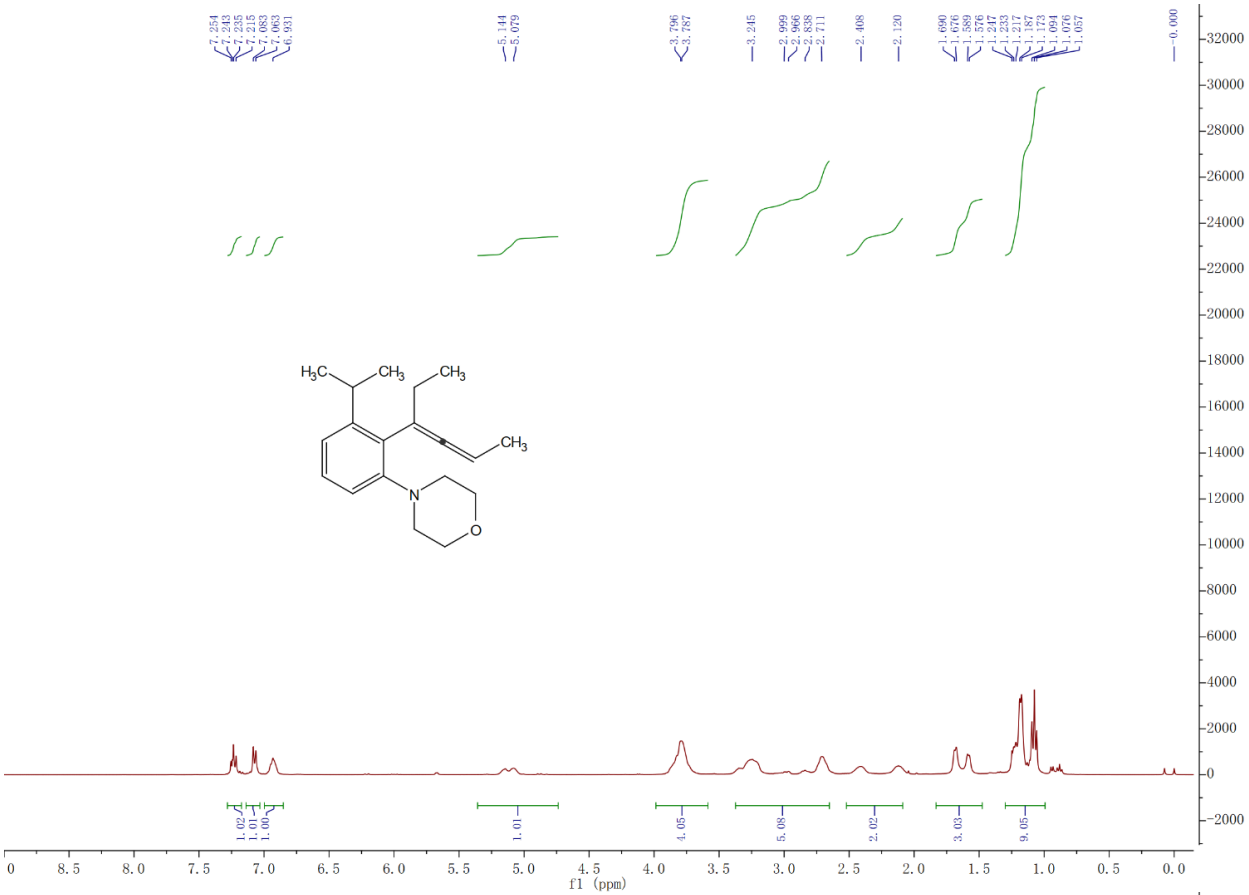


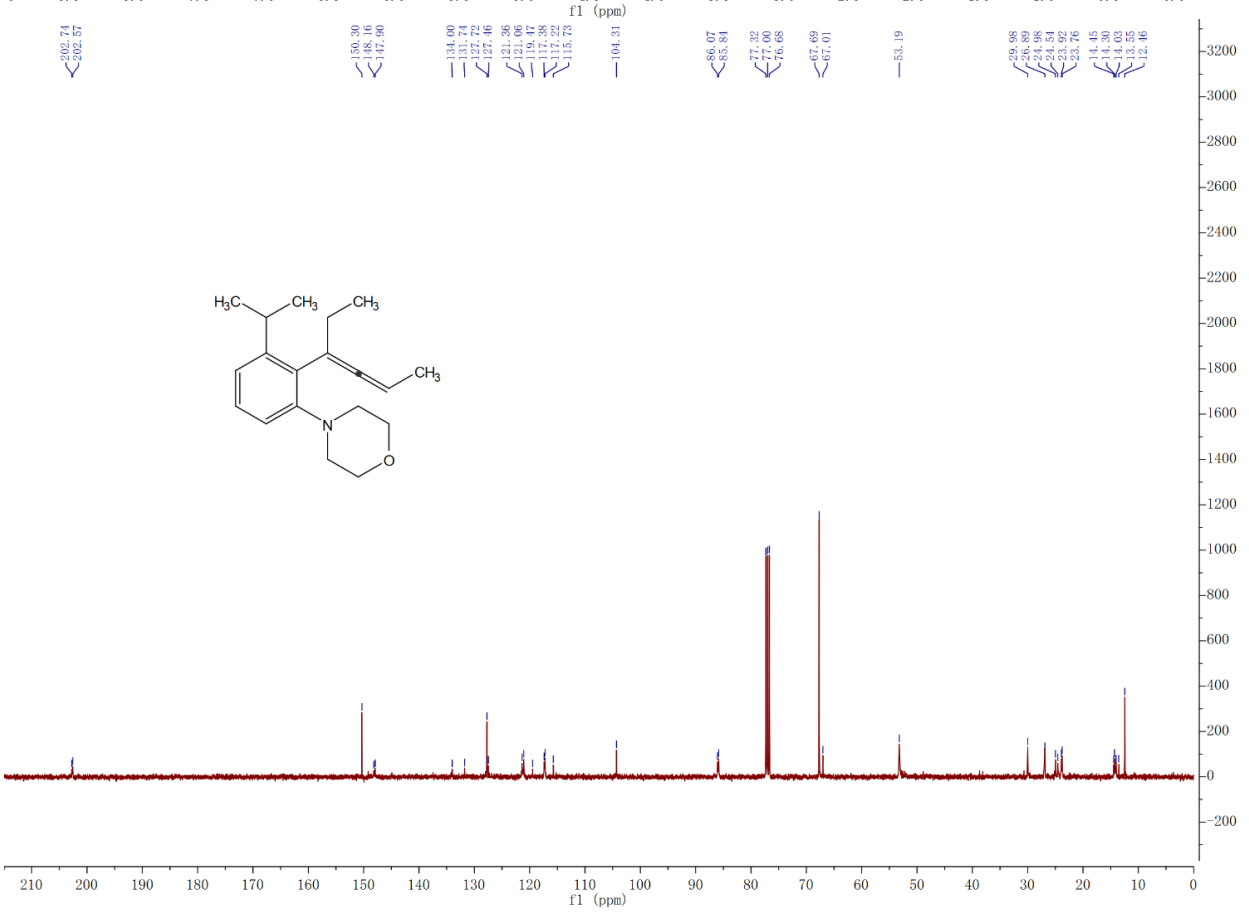
methyl 2-(hexa-3,4-dien-3-yl)-3-morpholinobenzoate (4k)



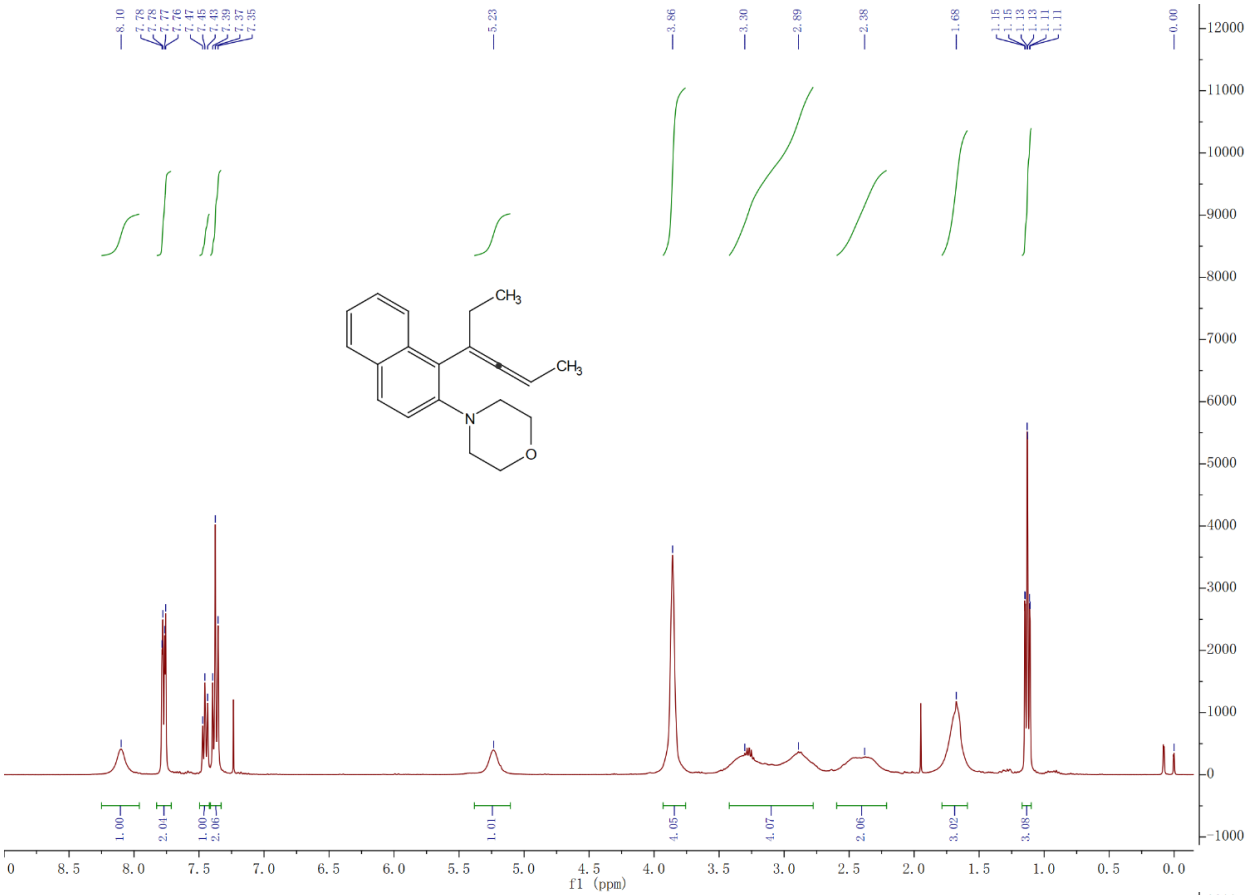


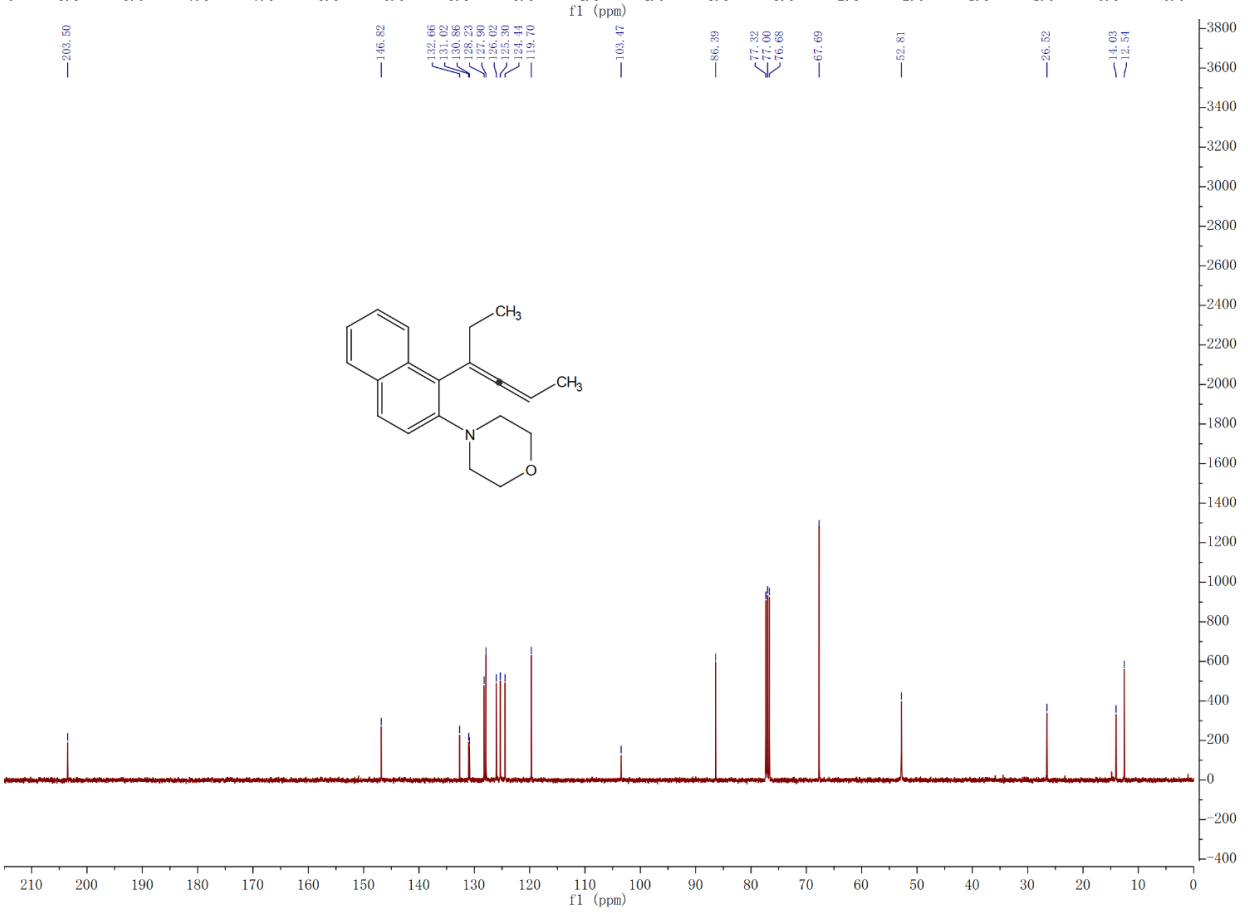
4-(2-(hexa-3,4-dien-3-yl)-3-isopropylphenyl)morpholine (4l)



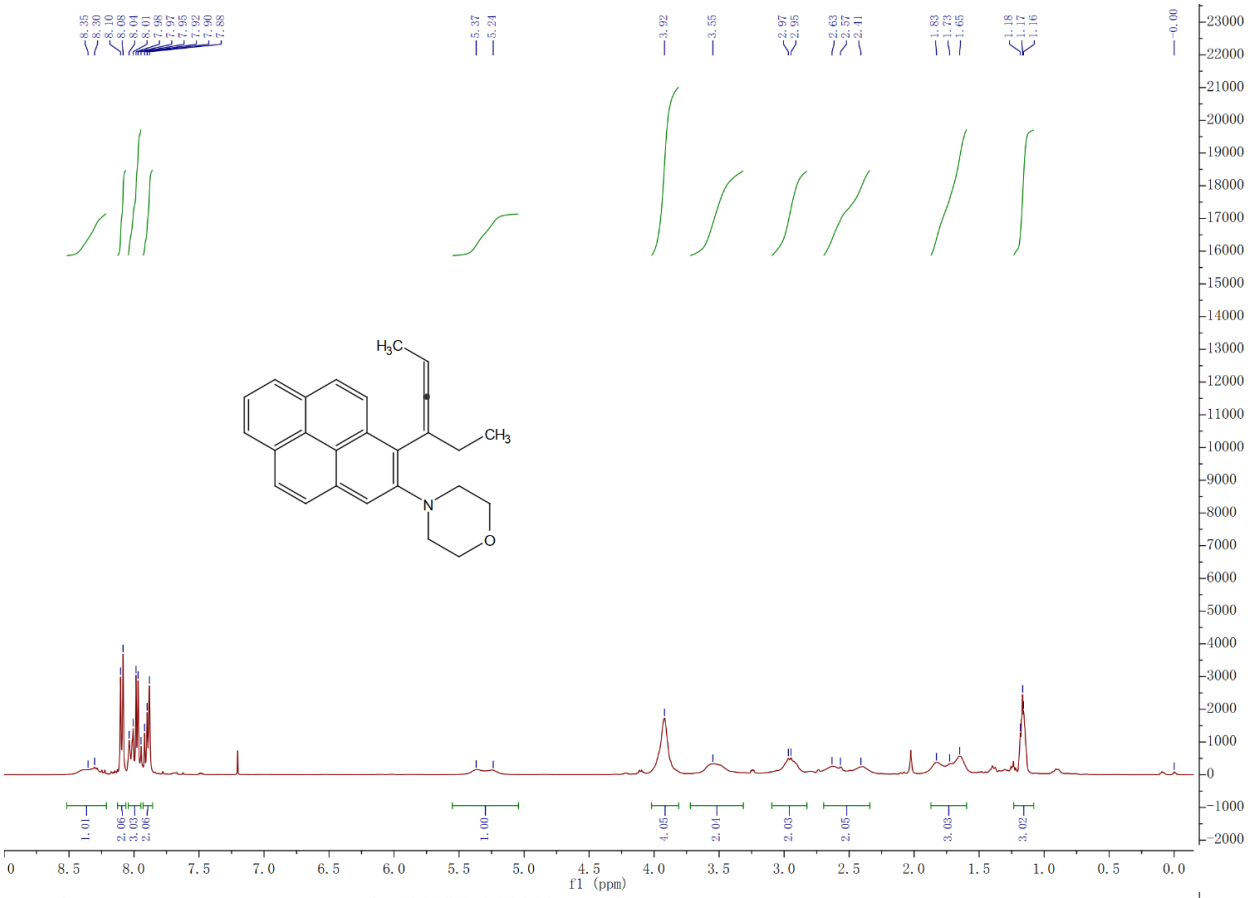


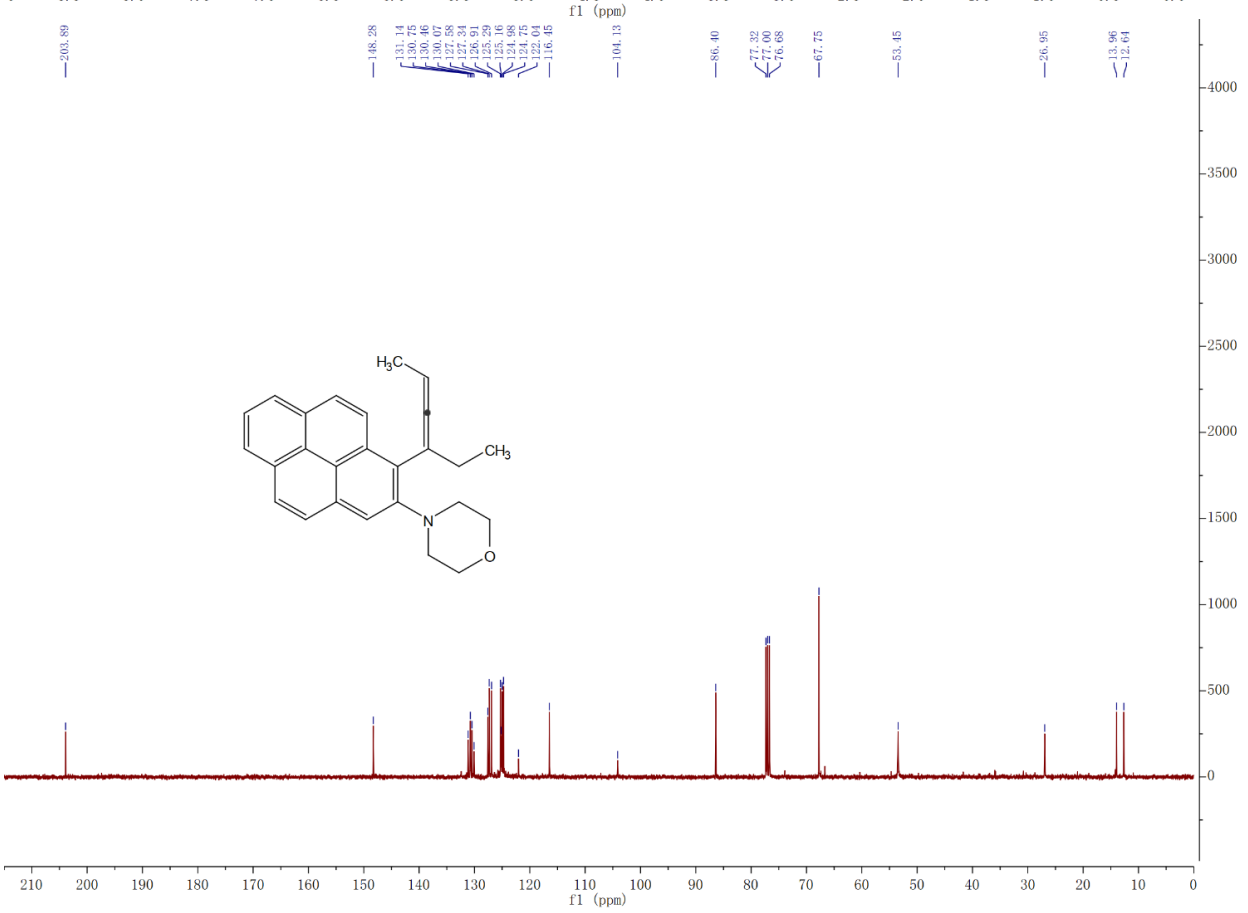
4-(1-(hexa-3,4-dien-3-yl)naphthalen-2-yl)morpholine (4m)



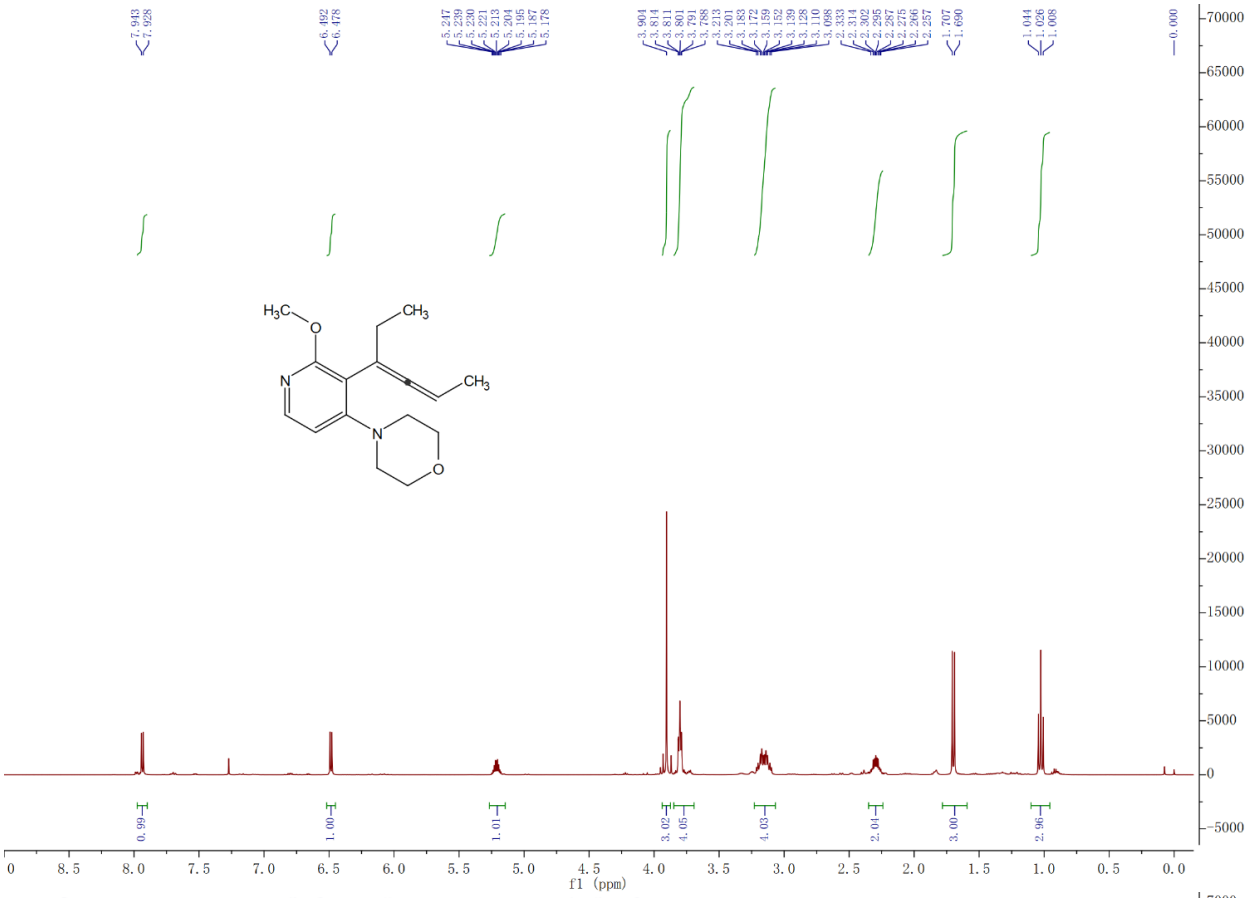


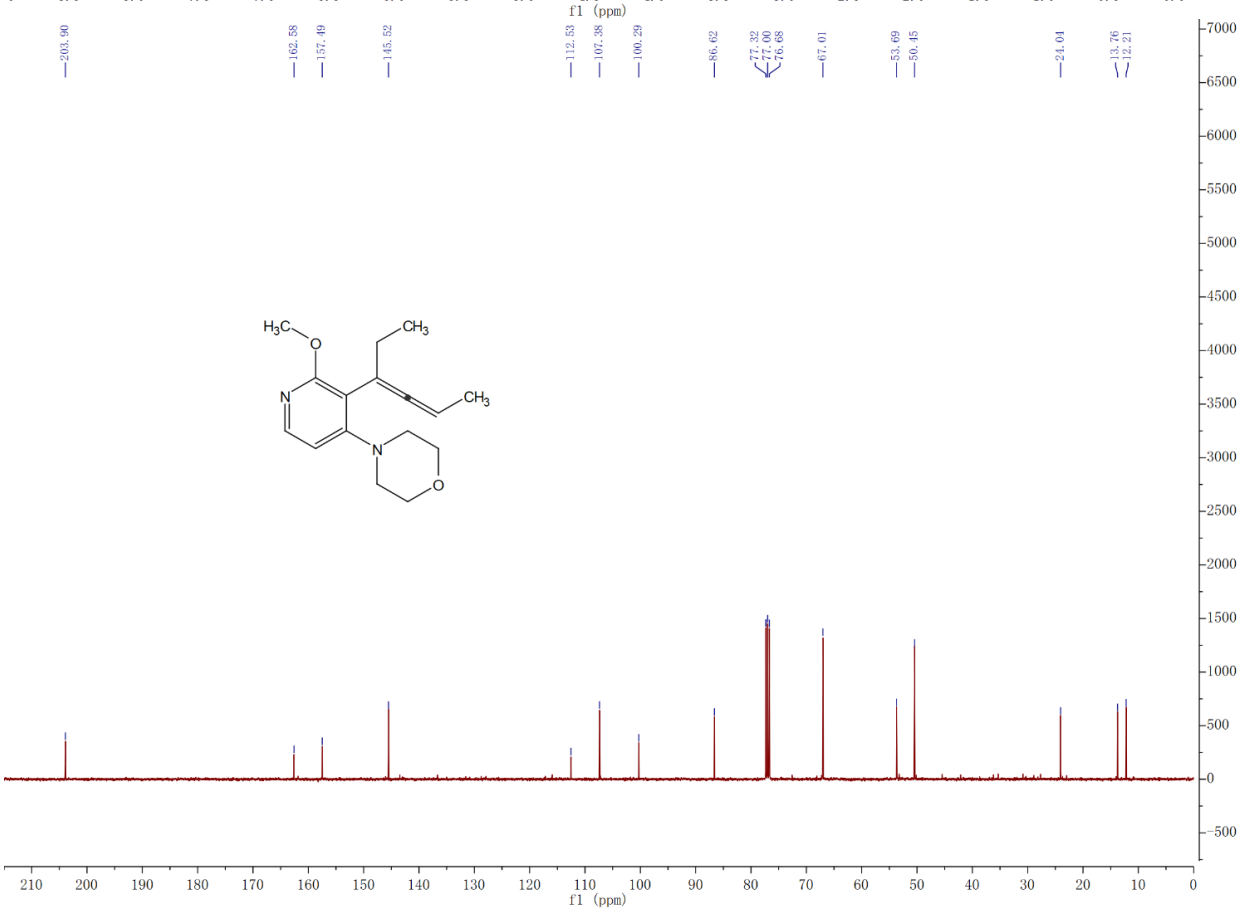
4-(1-(hexa-3,4-dien-3-yl)pyren-2-yl)morpholine (4n)



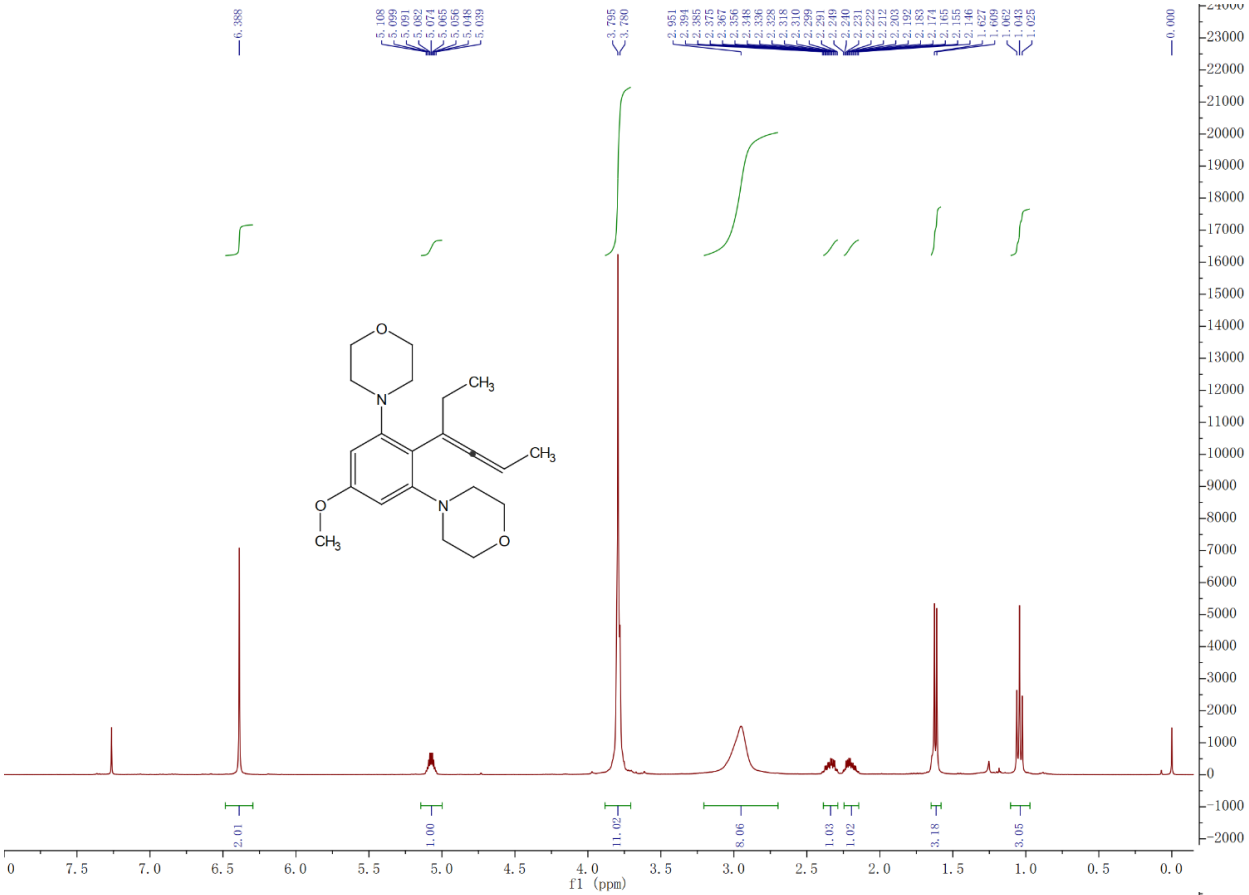


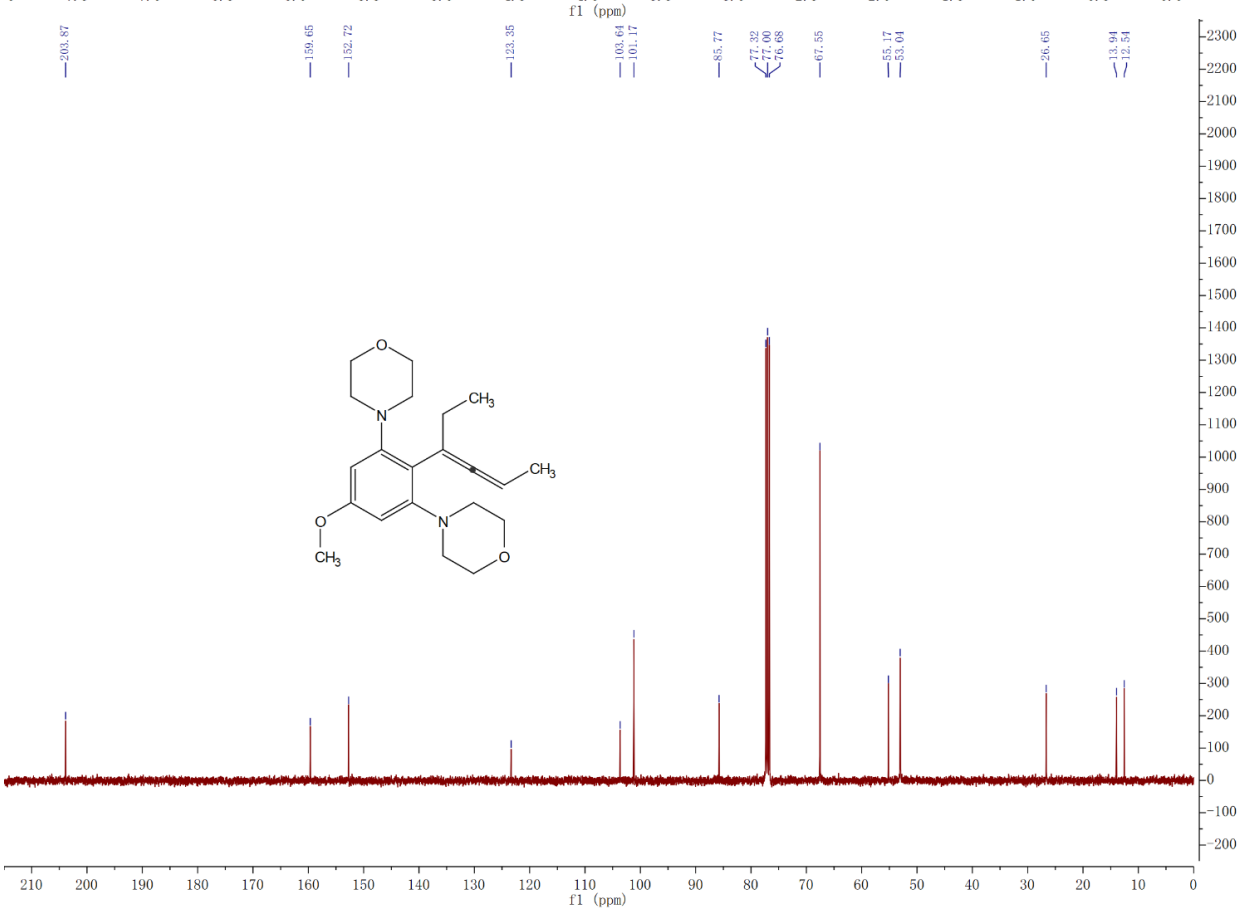
4-(3-(hexa-3,4-dien-3-yl)-2-methoxypyridin-4-yl)morpholine (4o)



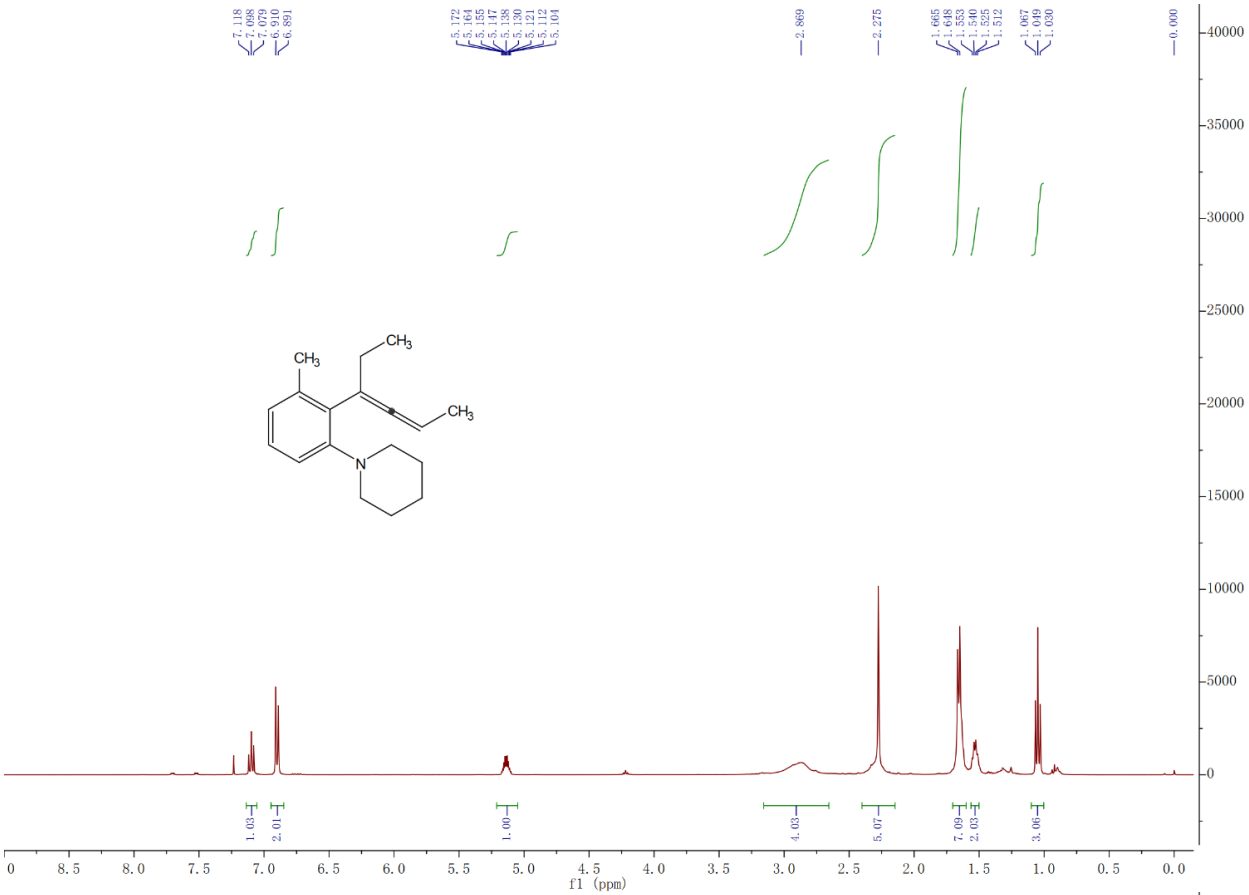


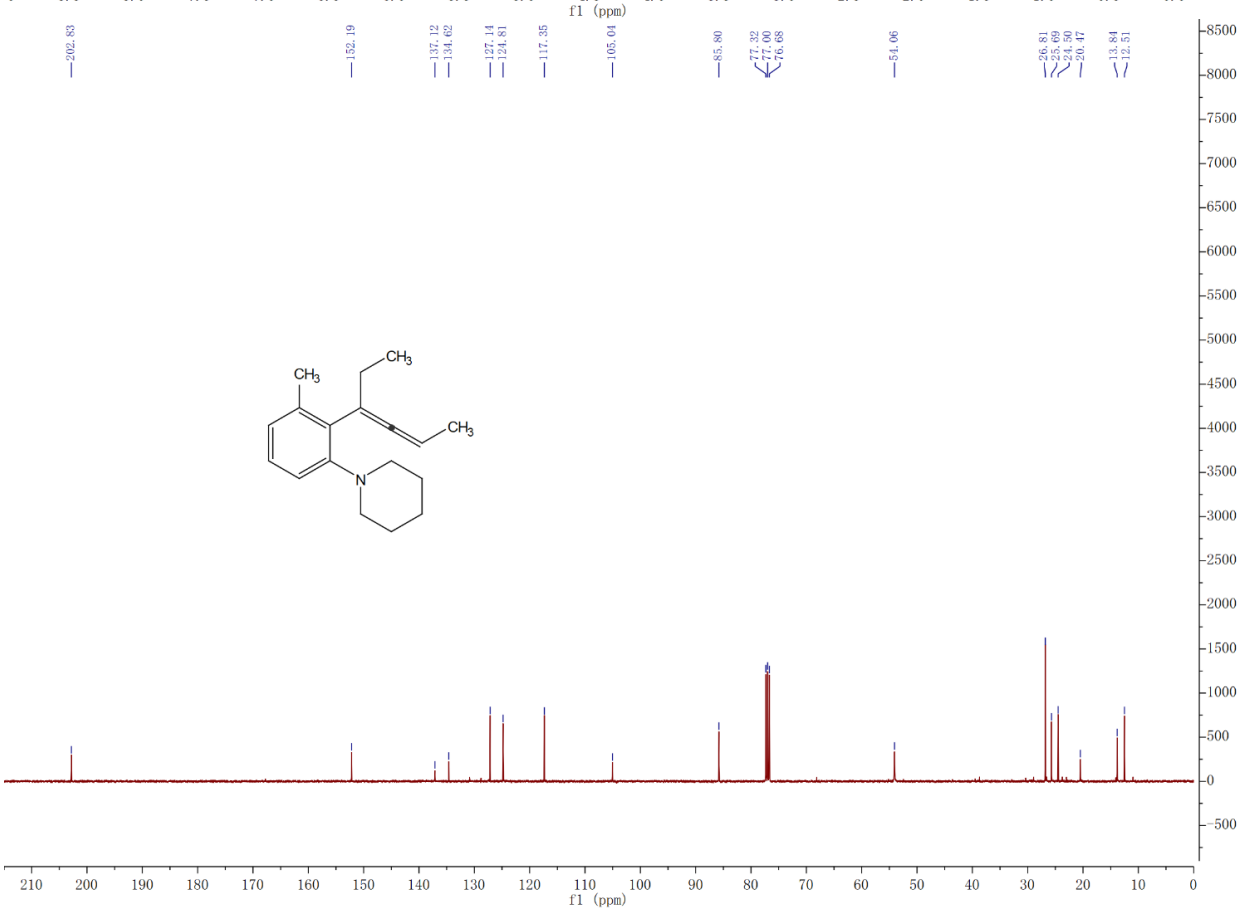
4,4'-(2-(hexa-3,4-dien-3-yl)-5-methoxy-1,3-phenylene)dimorpholine (4p)



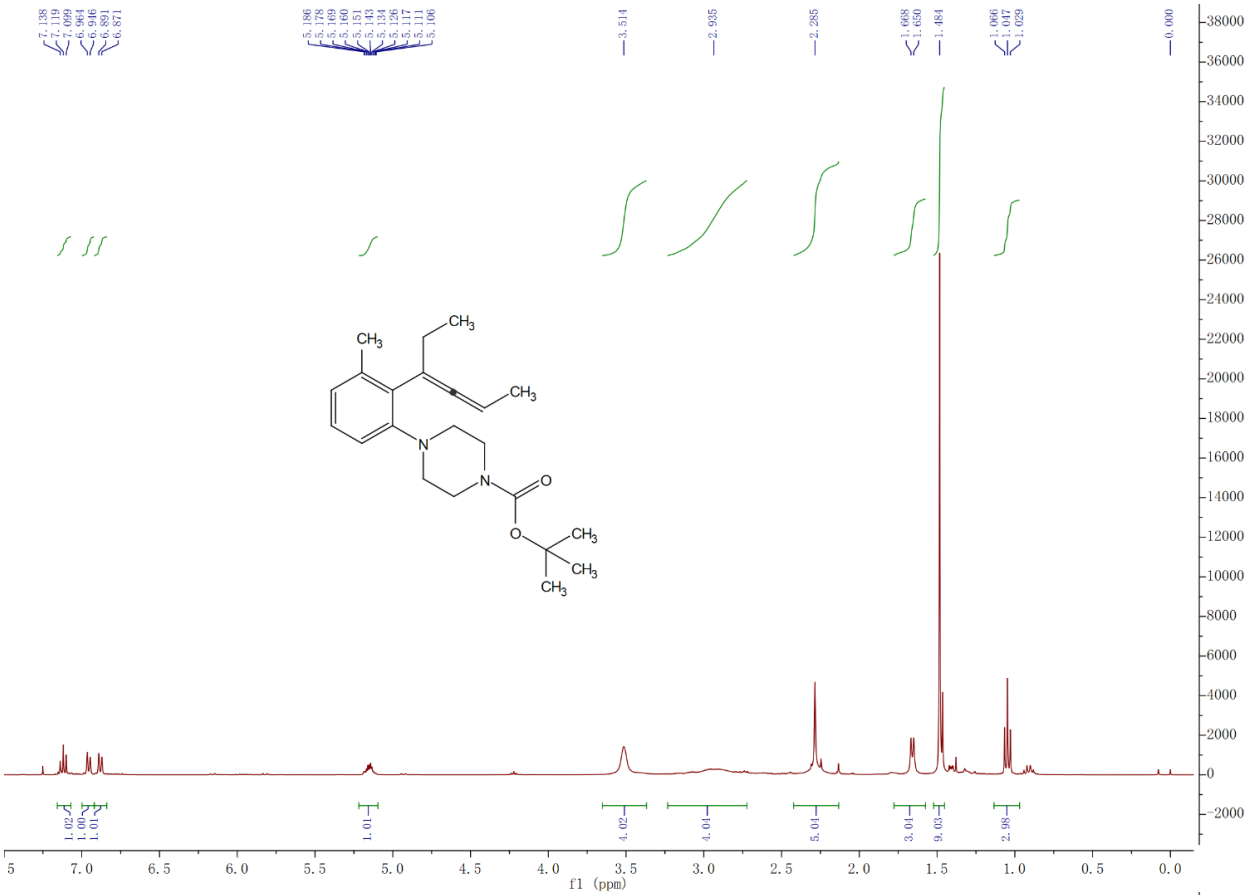


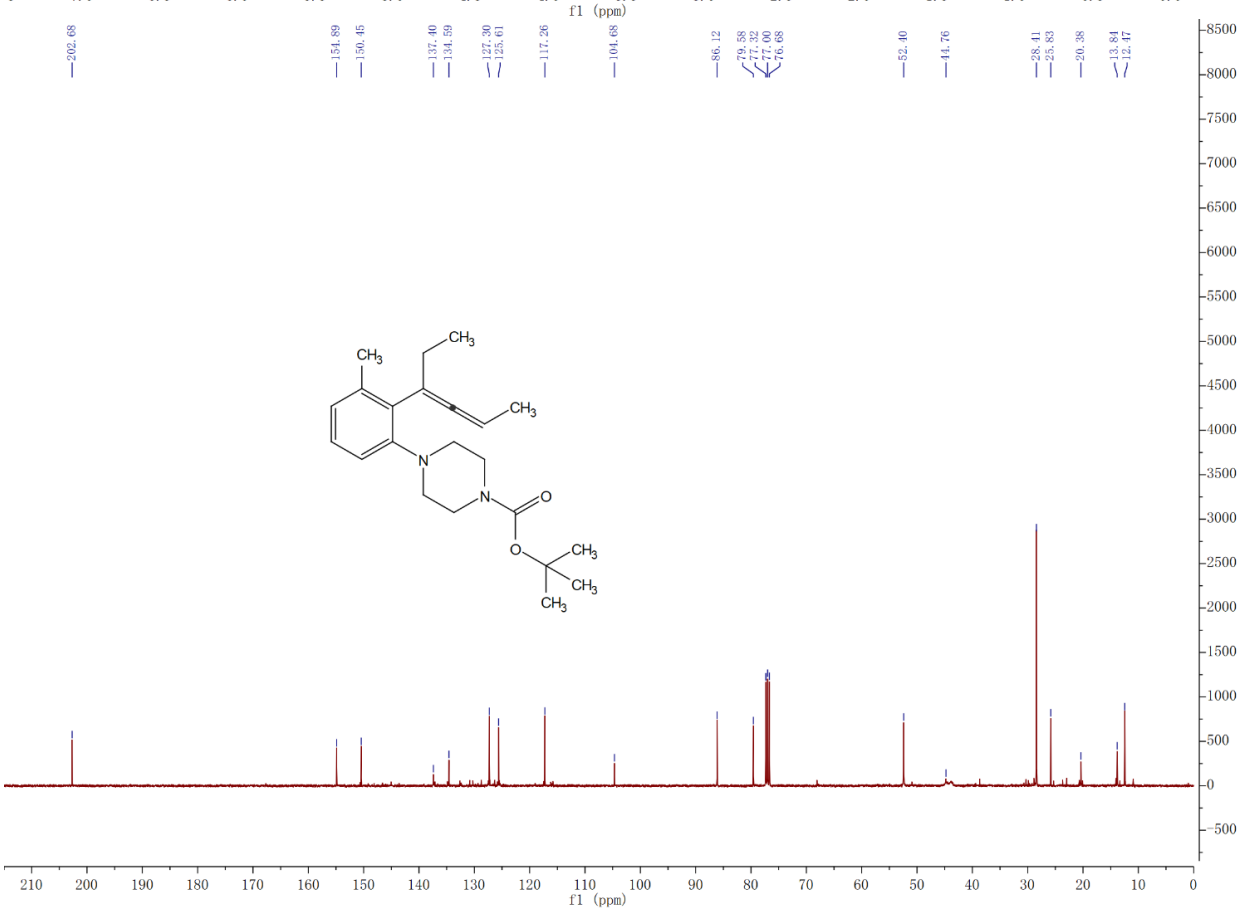
1-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperidine (4q)



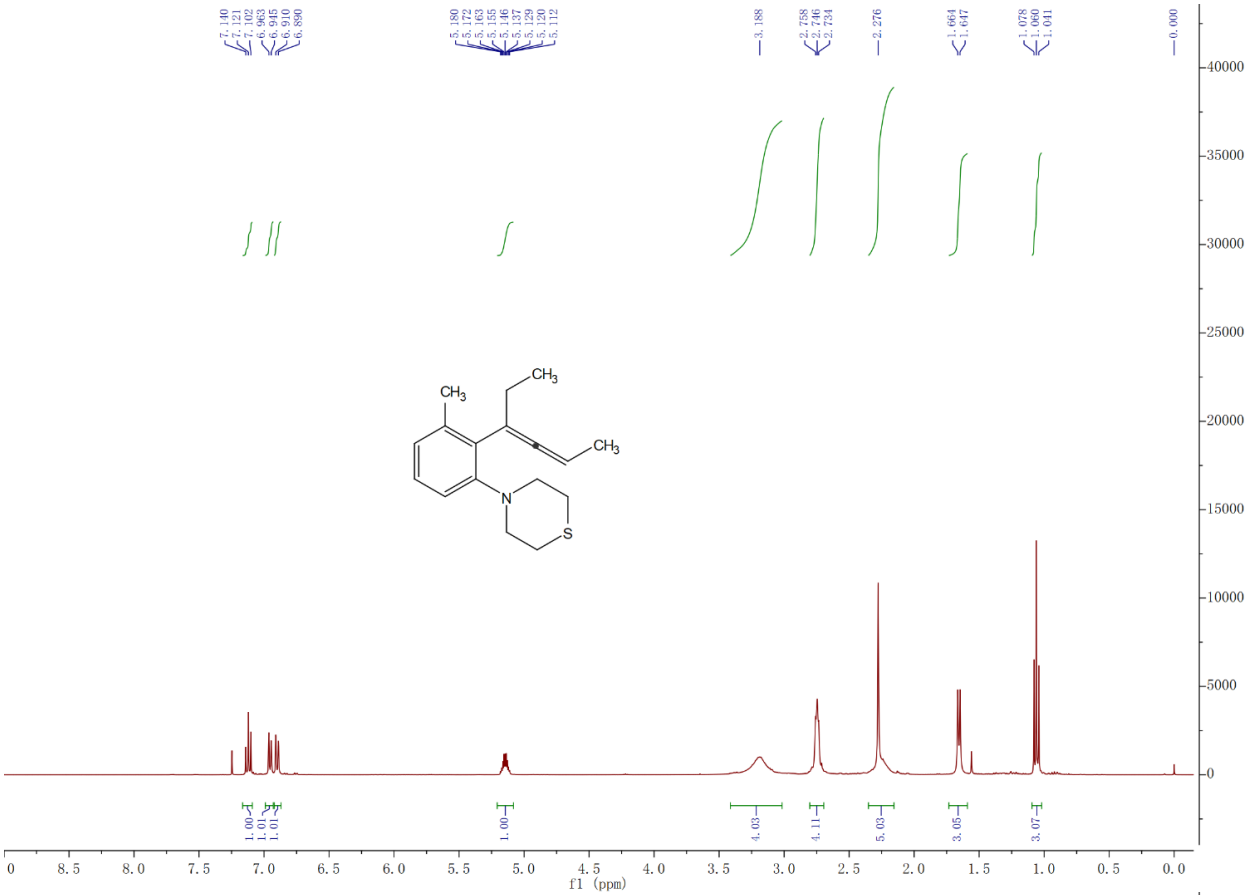


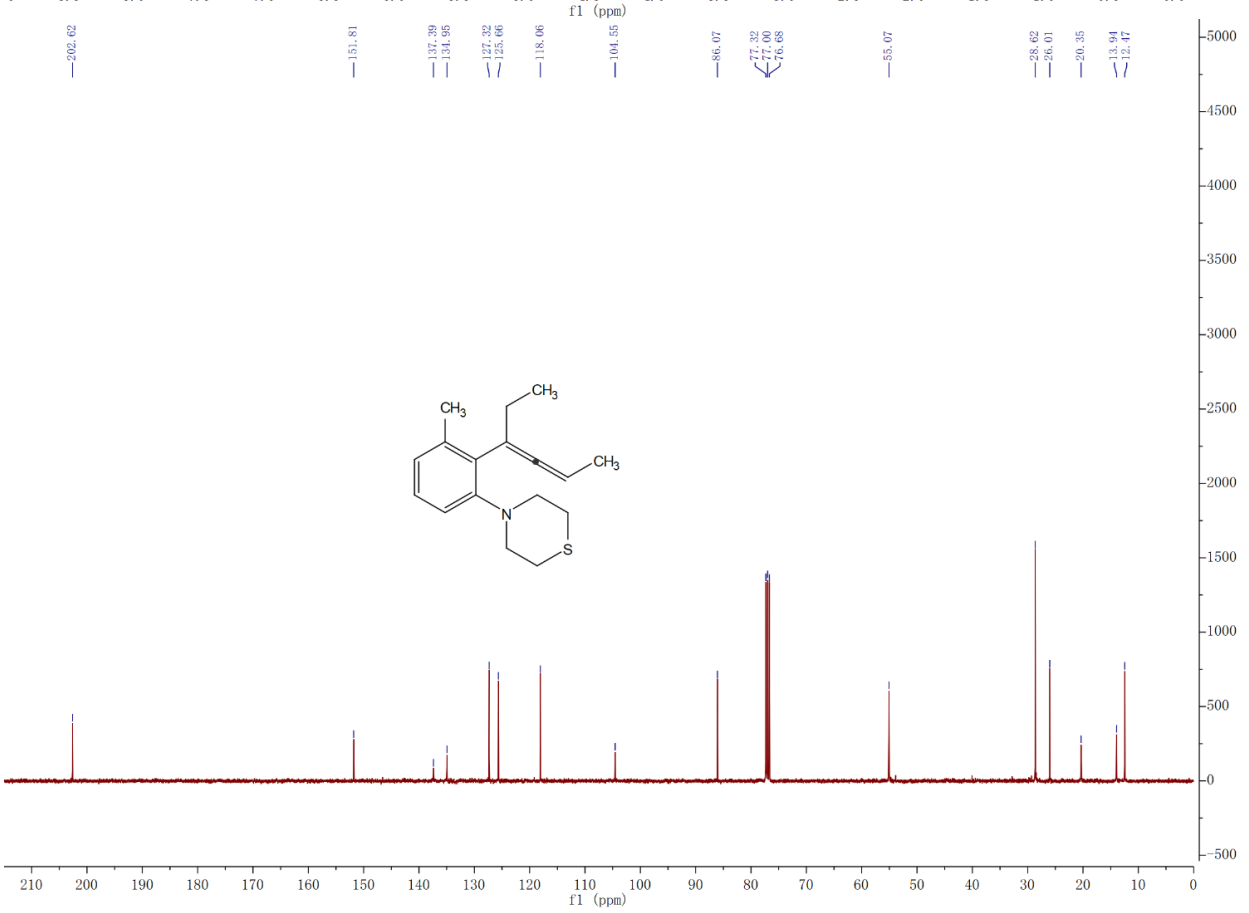
tert-butyl 4-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperazine-1-carboxylate (4r)



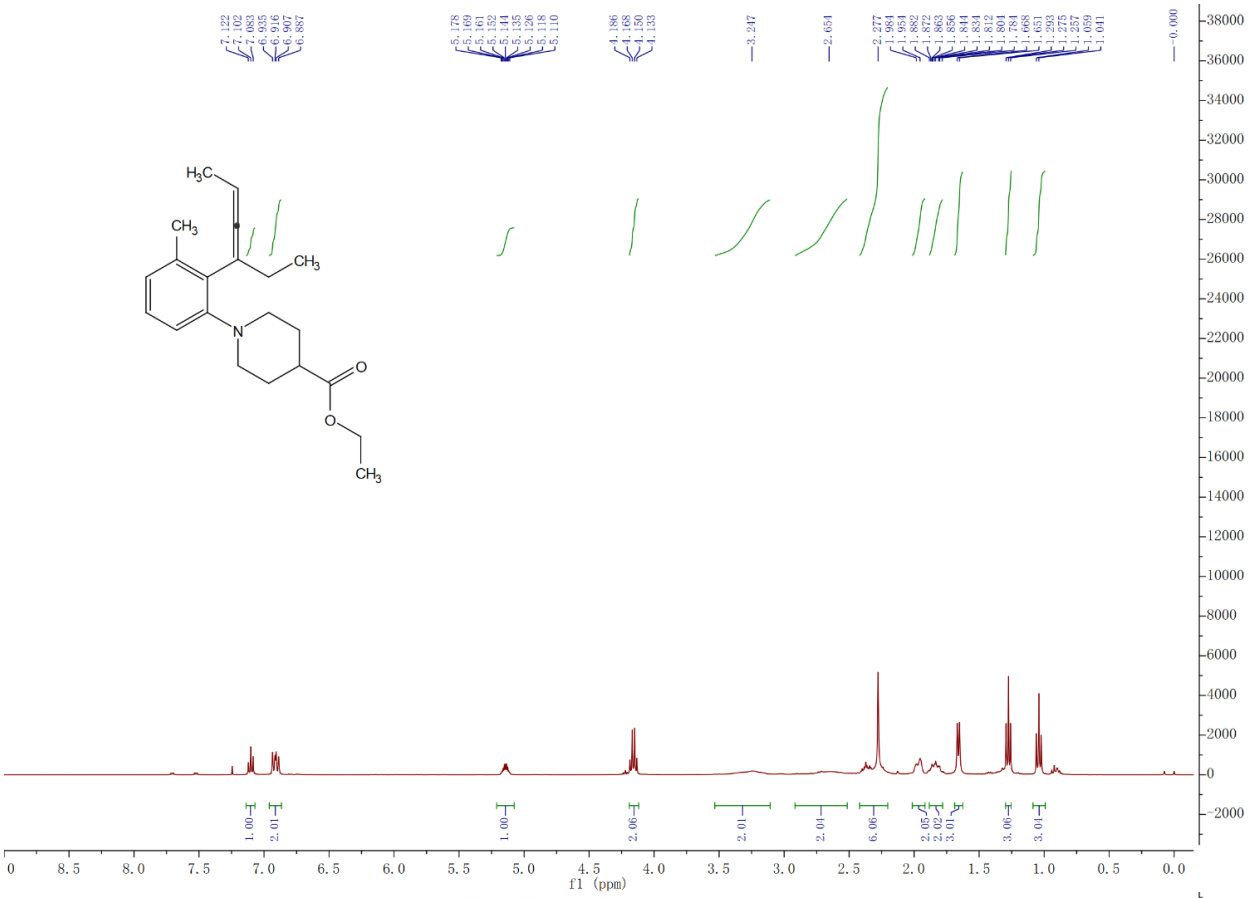


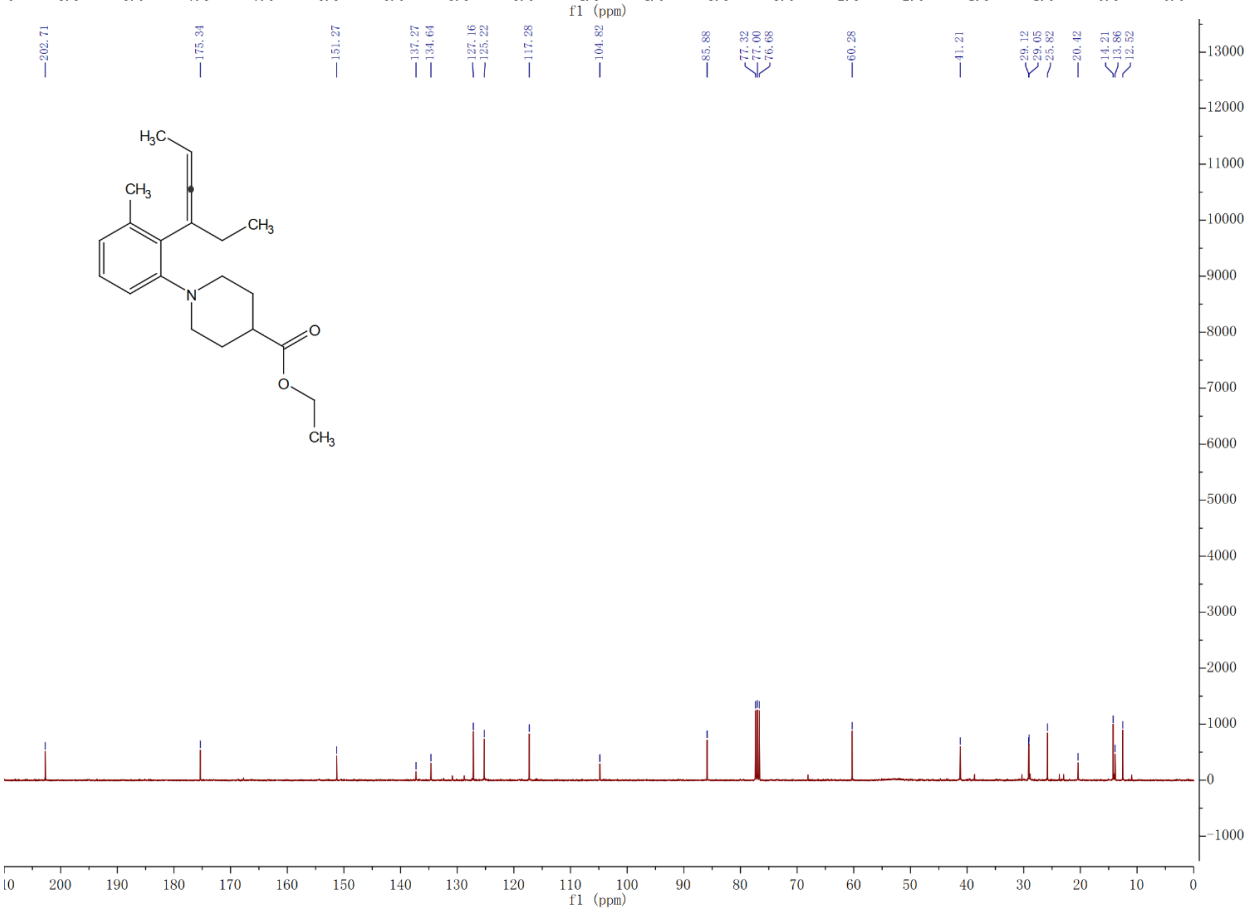
4-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)thiomorpholine (4s)



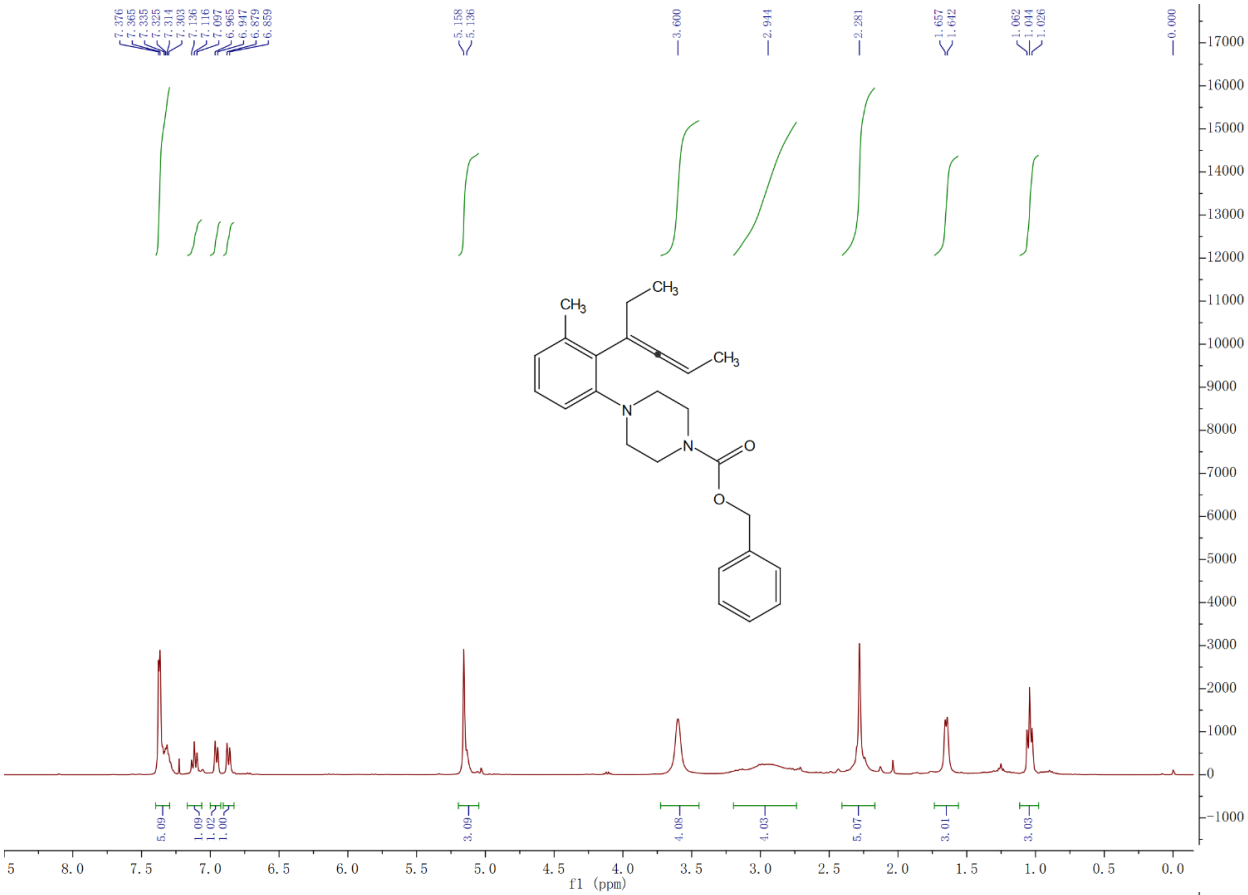


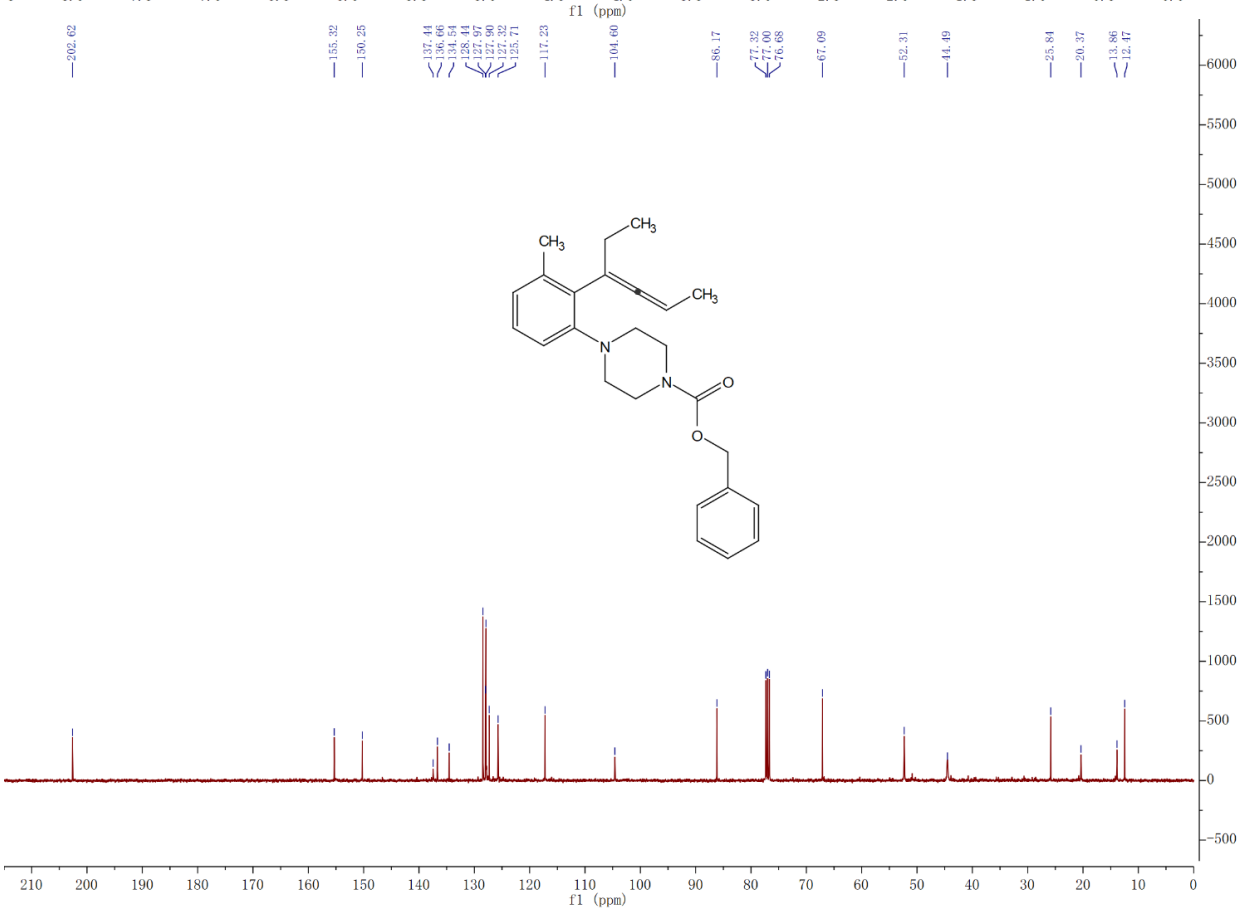
ethyl 1-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperidine-4-carboxylate (4t)



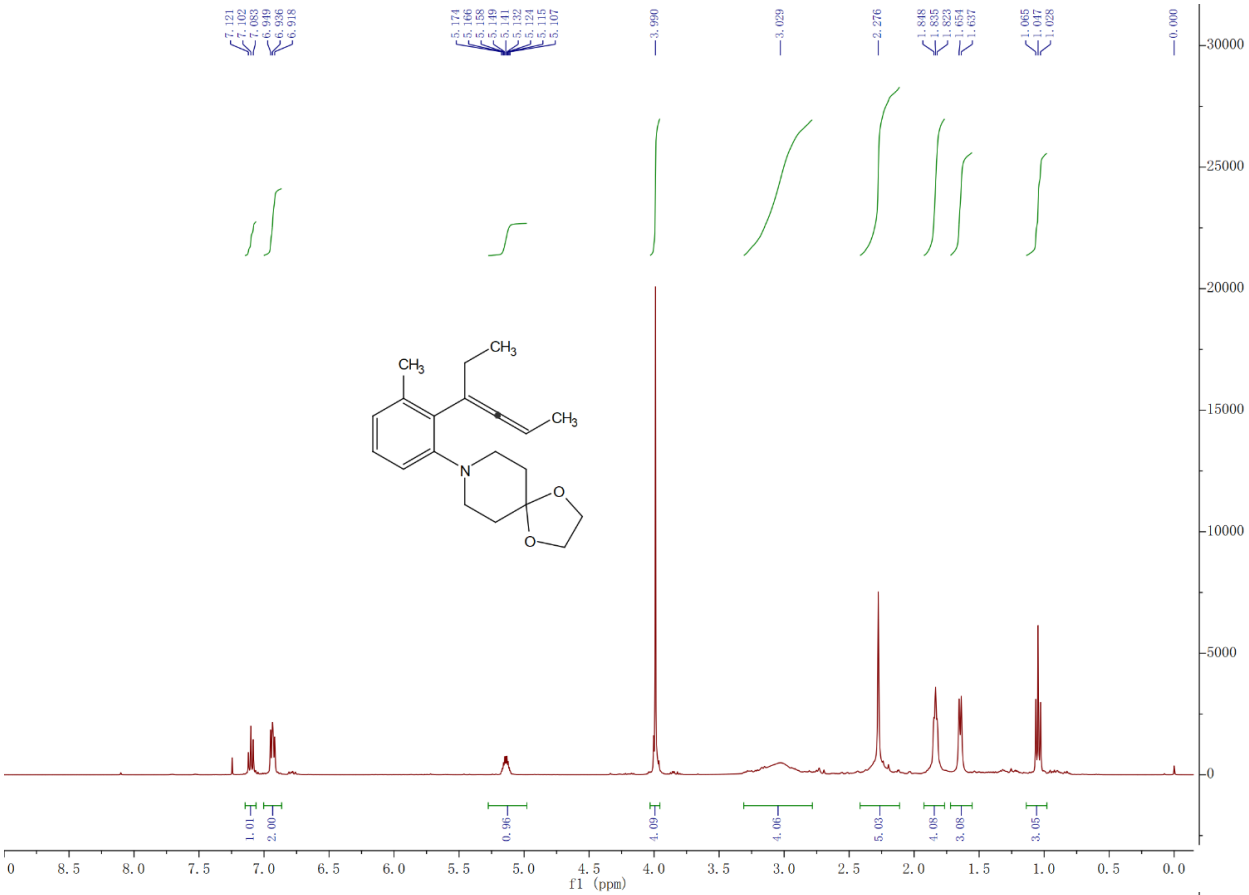


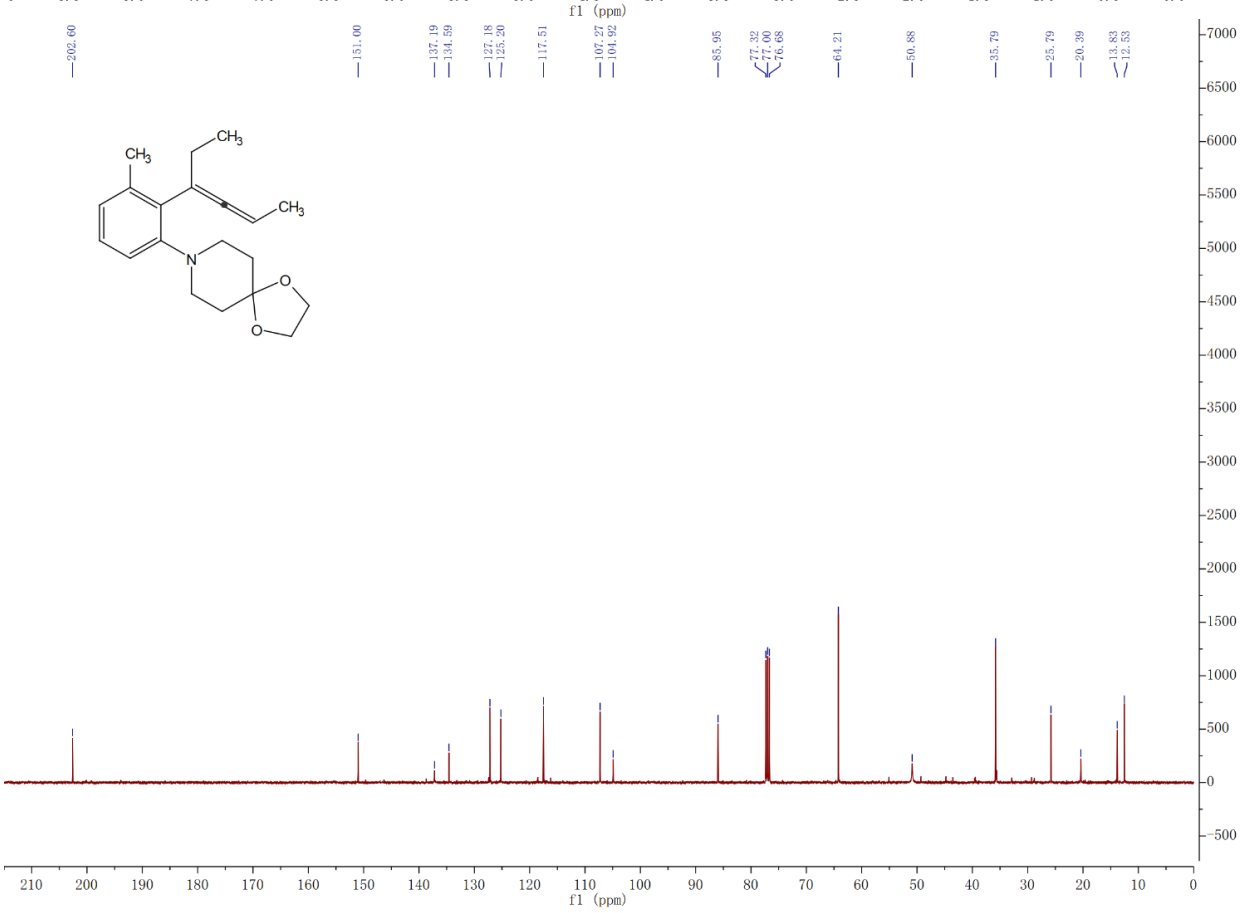
benzyl 4-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperazine-1-carboxylate (4u)



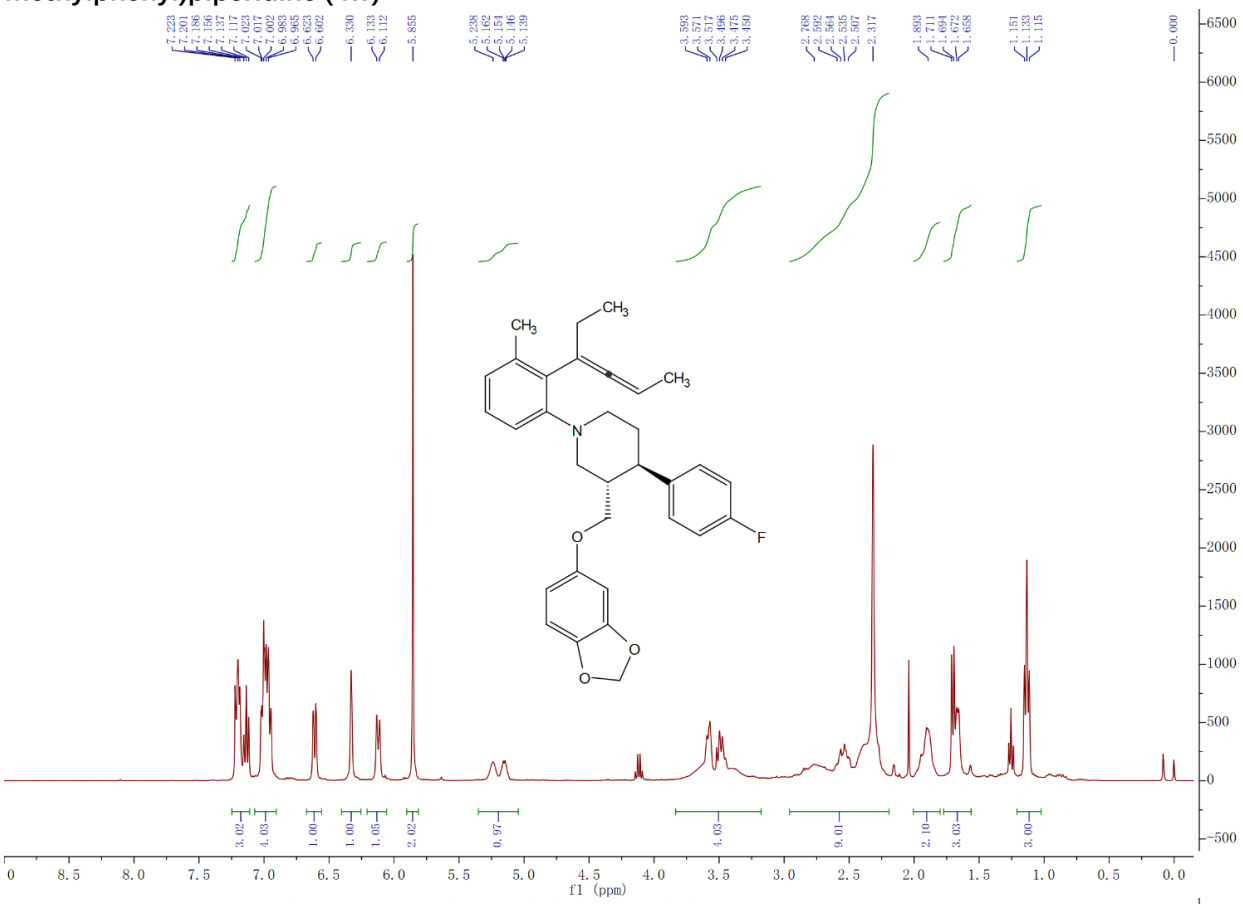


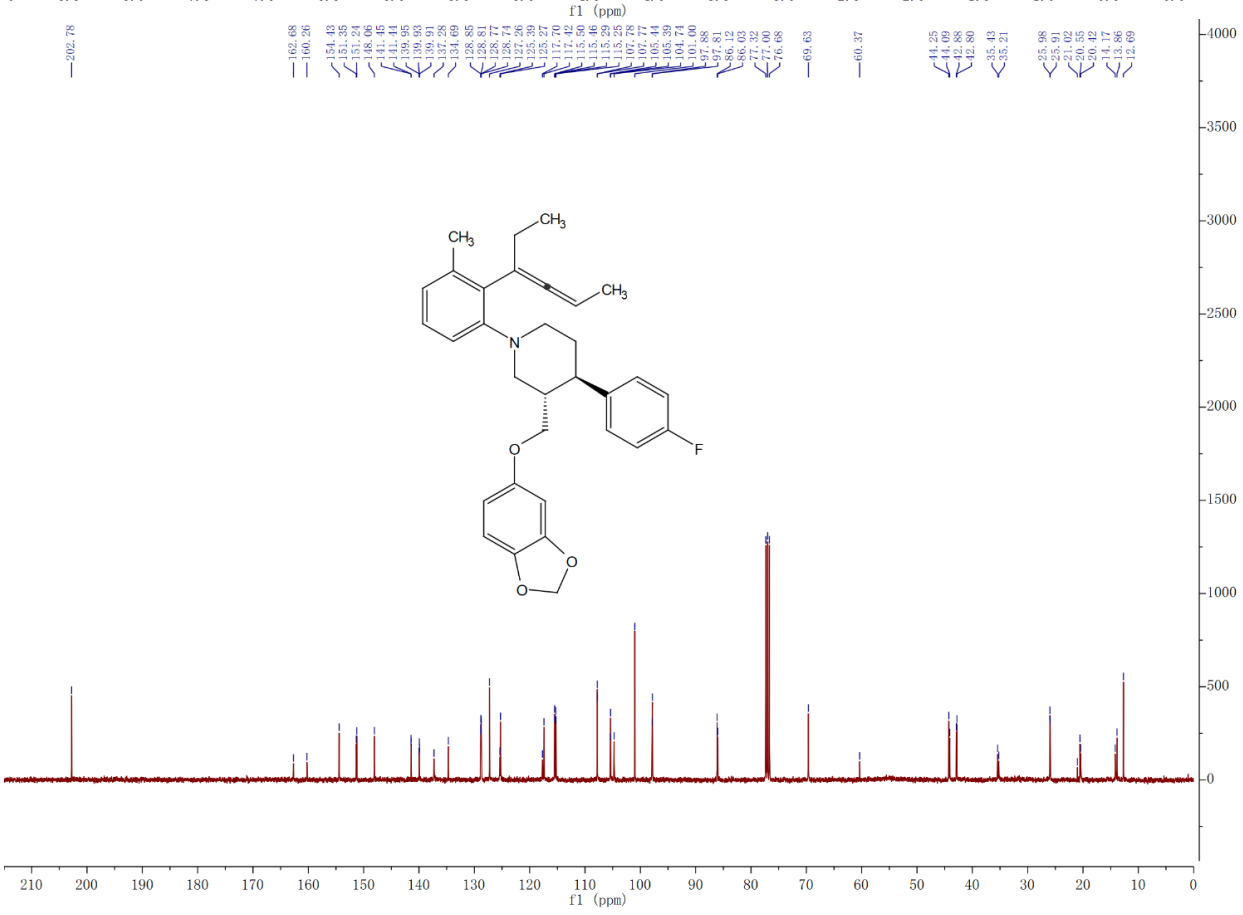
8-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)-1,4-dioxa-8-azaspiro[4.5]decane (5v)





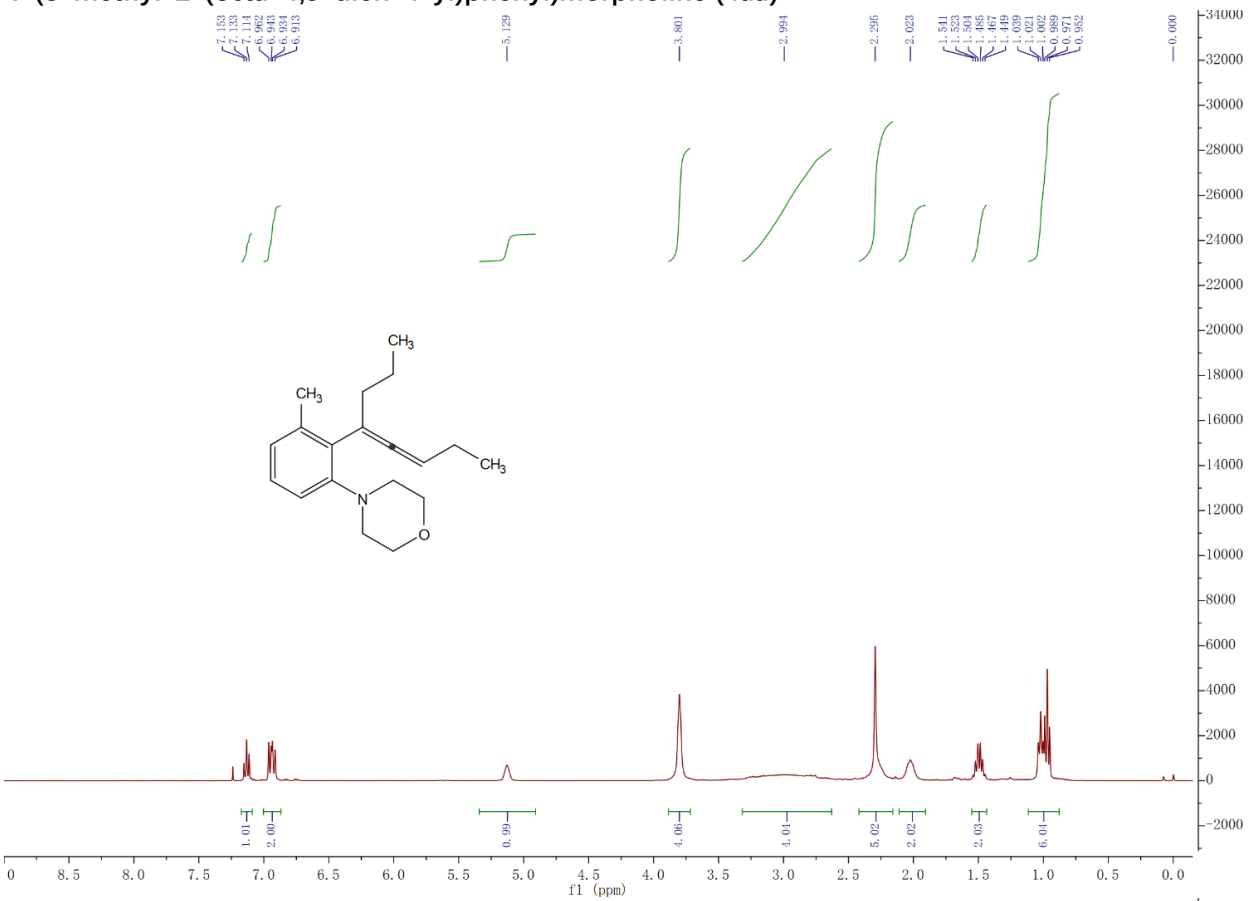
(3S,4R)-3-((benzo[d][1,3]dioxol-5-yloxy)methyl)-4-(4-fluorophenyl)-1-(2-(hexa-3,4-dien-3-yl)-3-methylphenyl)piperidine (4w)

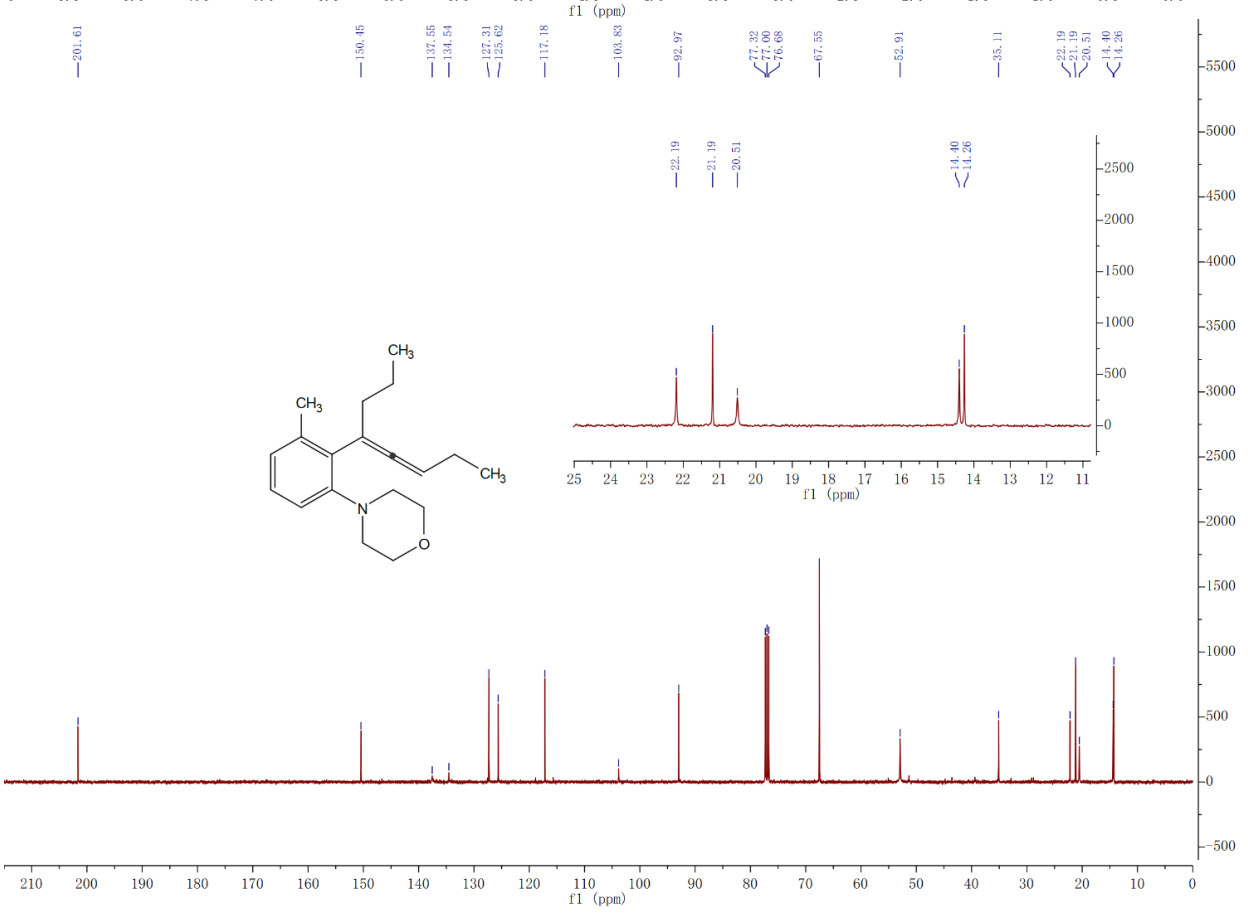




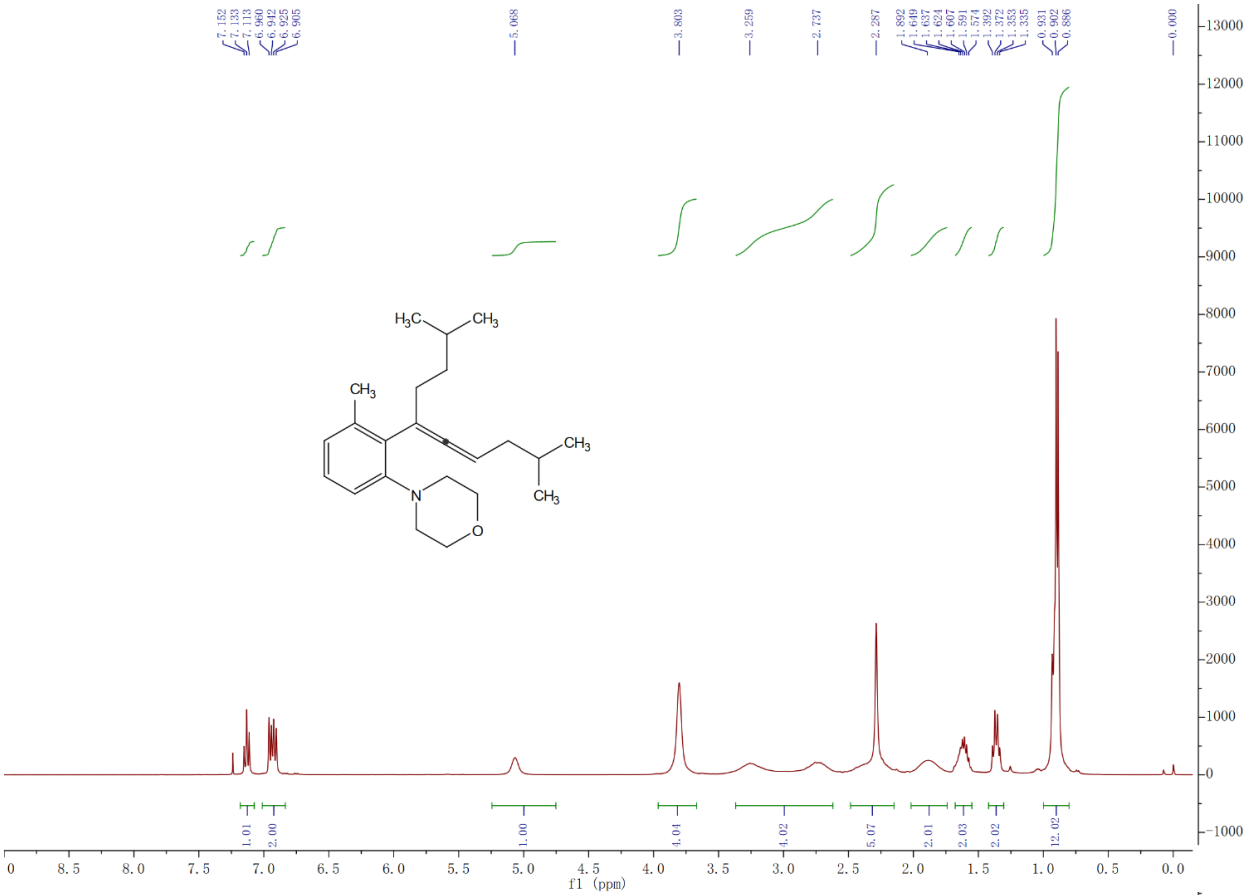

-116.449
-116.504
CH3
CH3
CH3
N
O
F
O
O
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

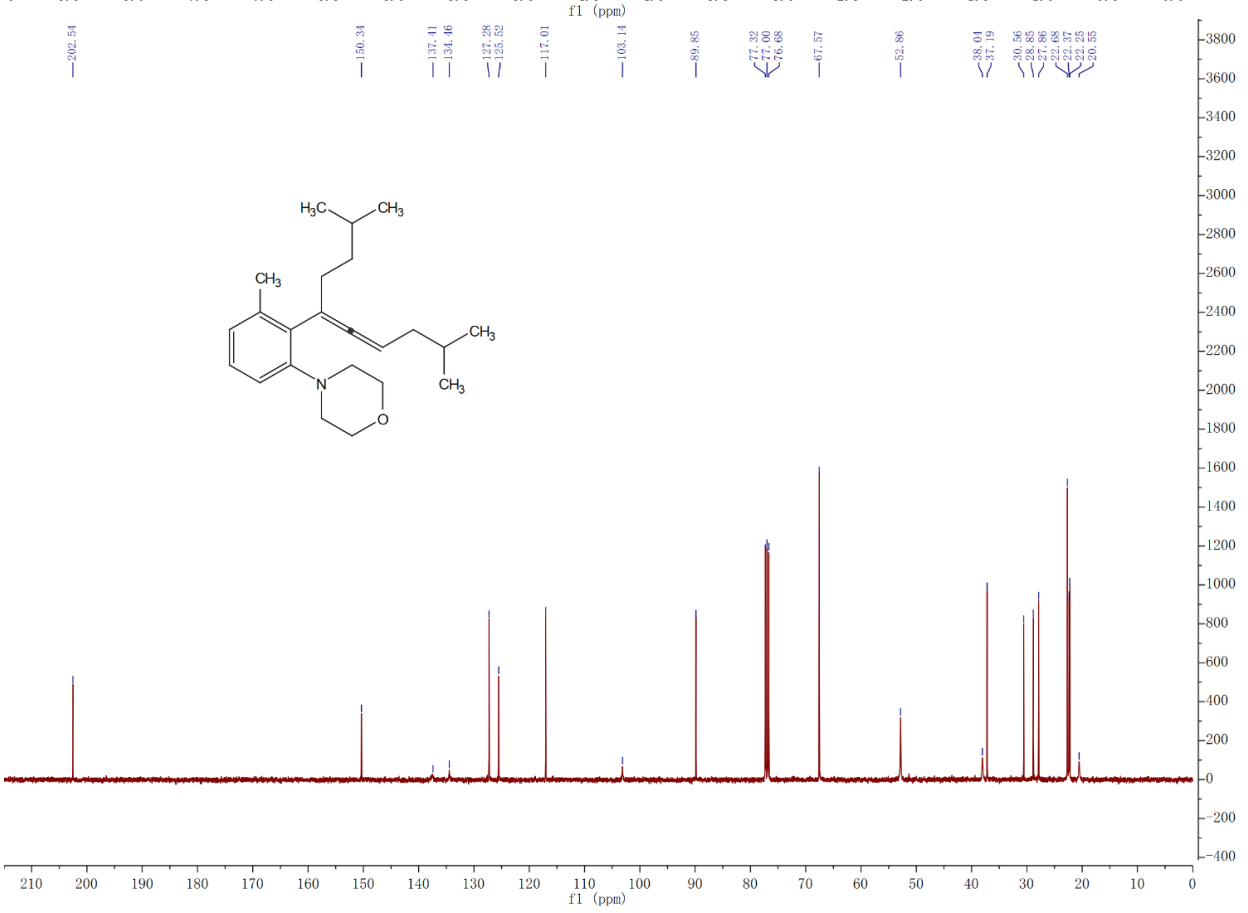
4-(3-methyl-2-(octa-4,5-dien-4-yl)phenyl)morpholine (4aa)



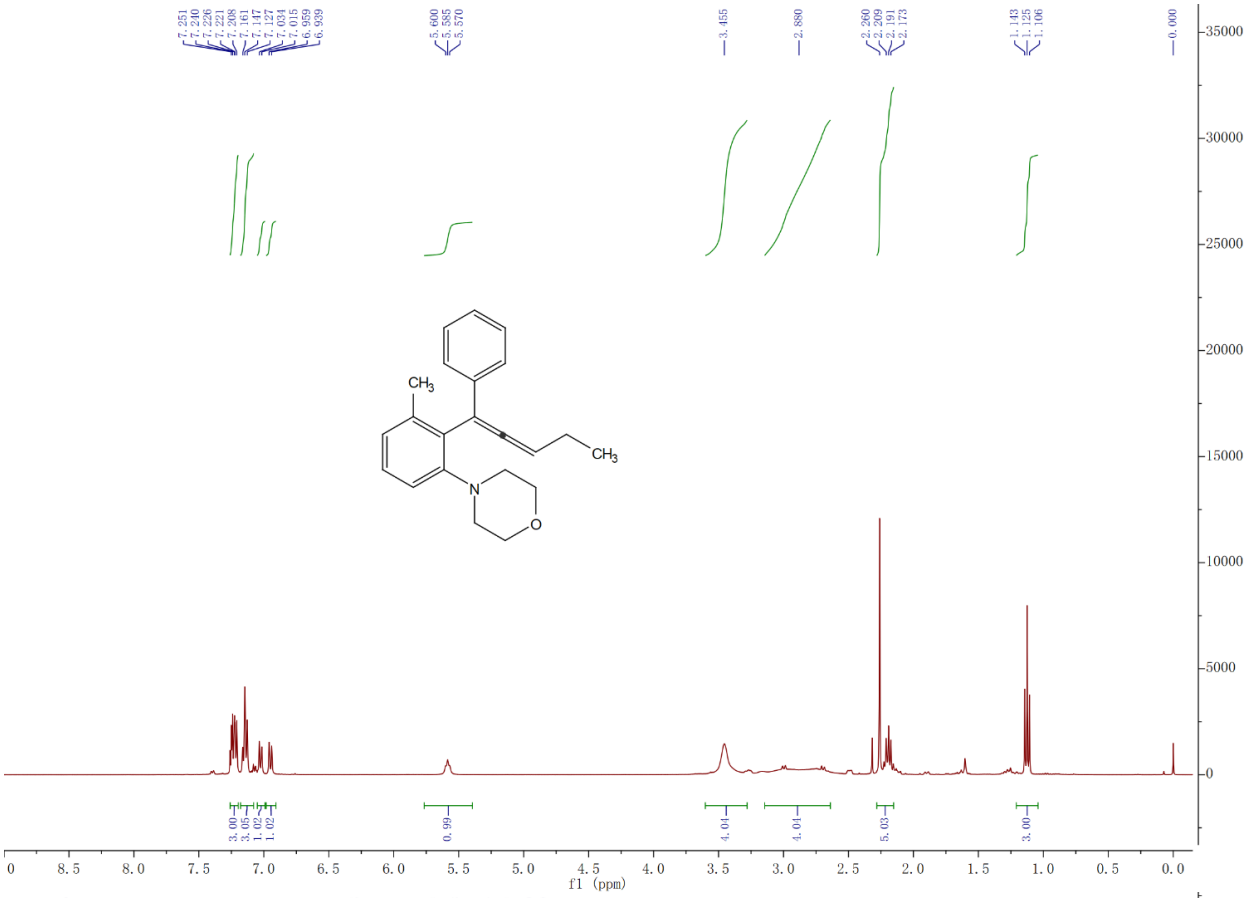


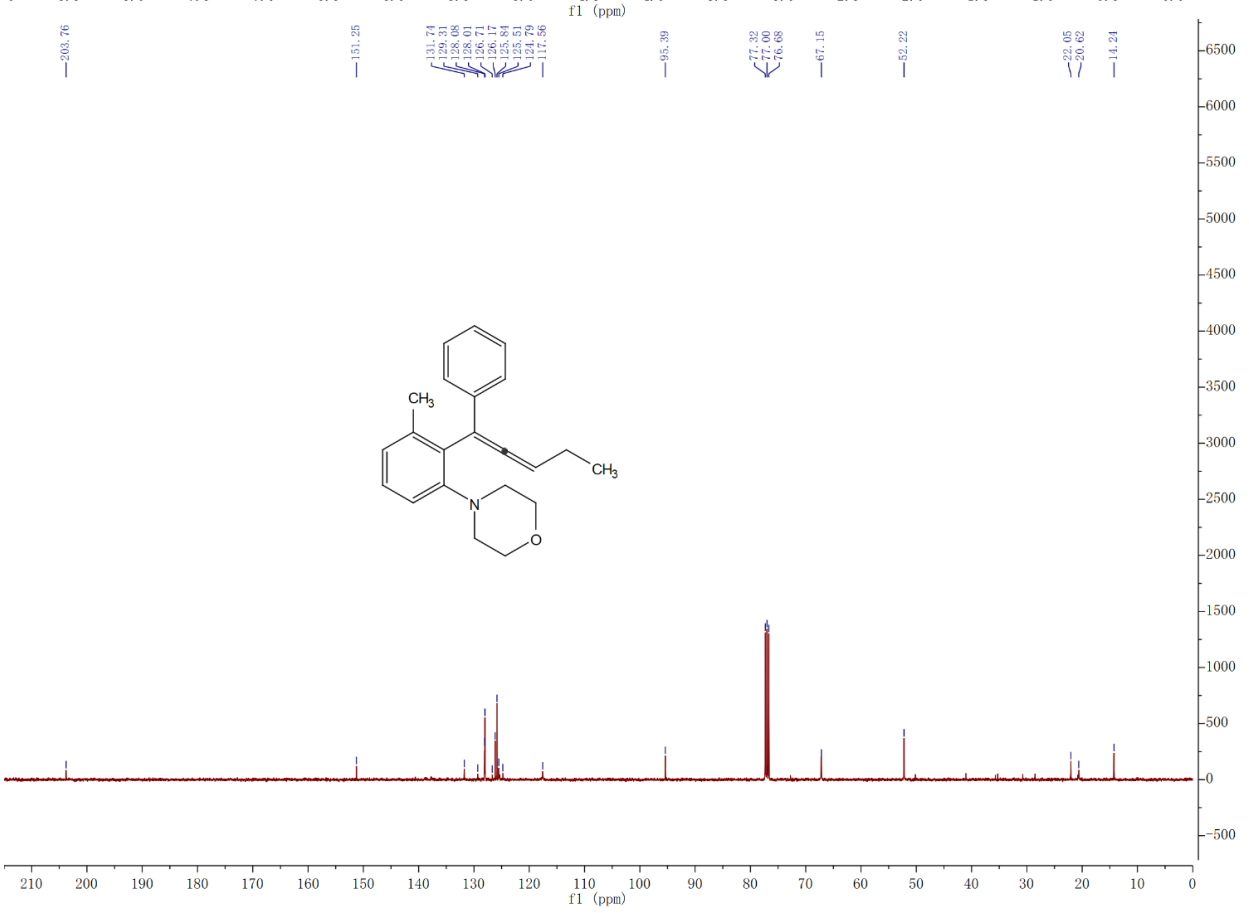
4-(2-(2,9-dimethyldeca-5,6-dien-5-yl)-3-methylphenyl)morpholine (4ab)



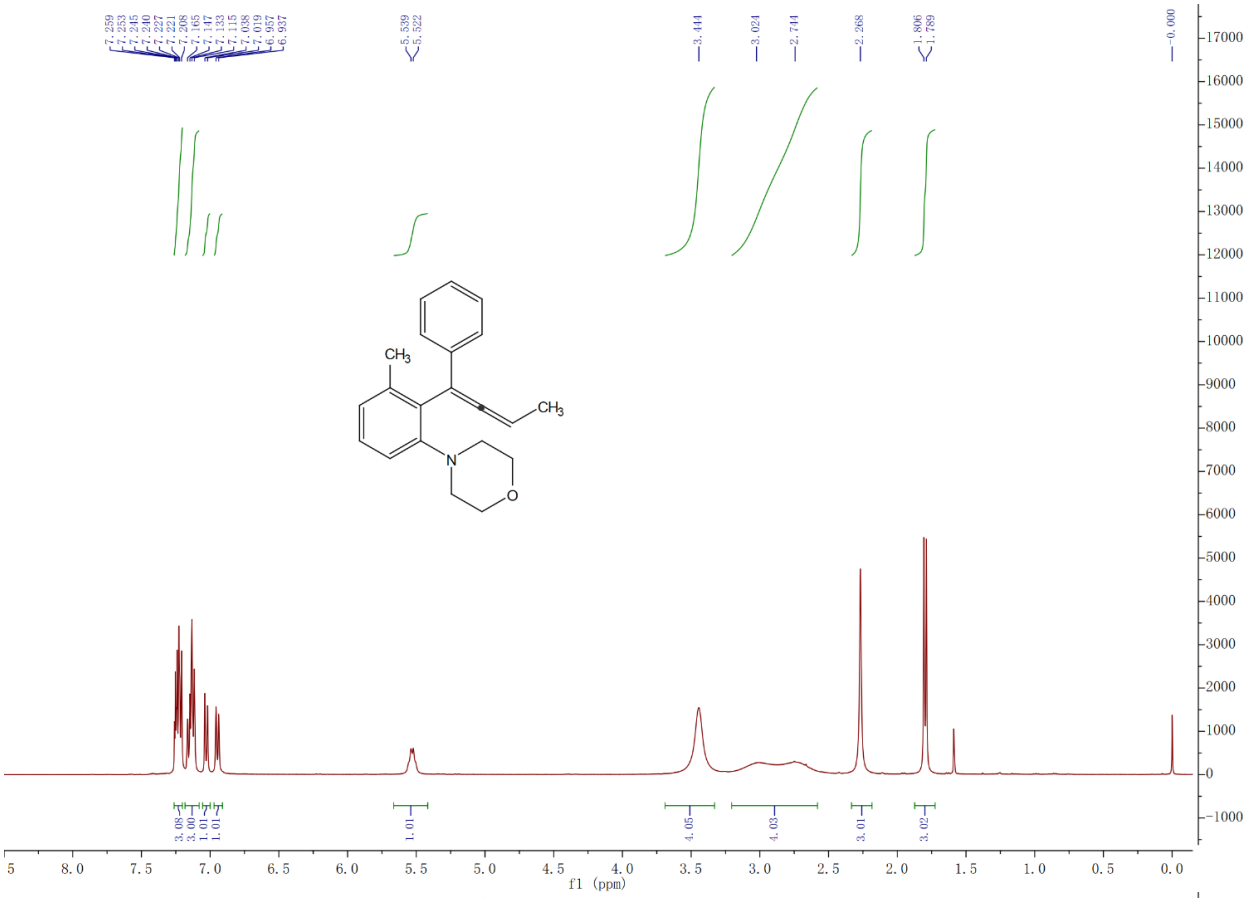


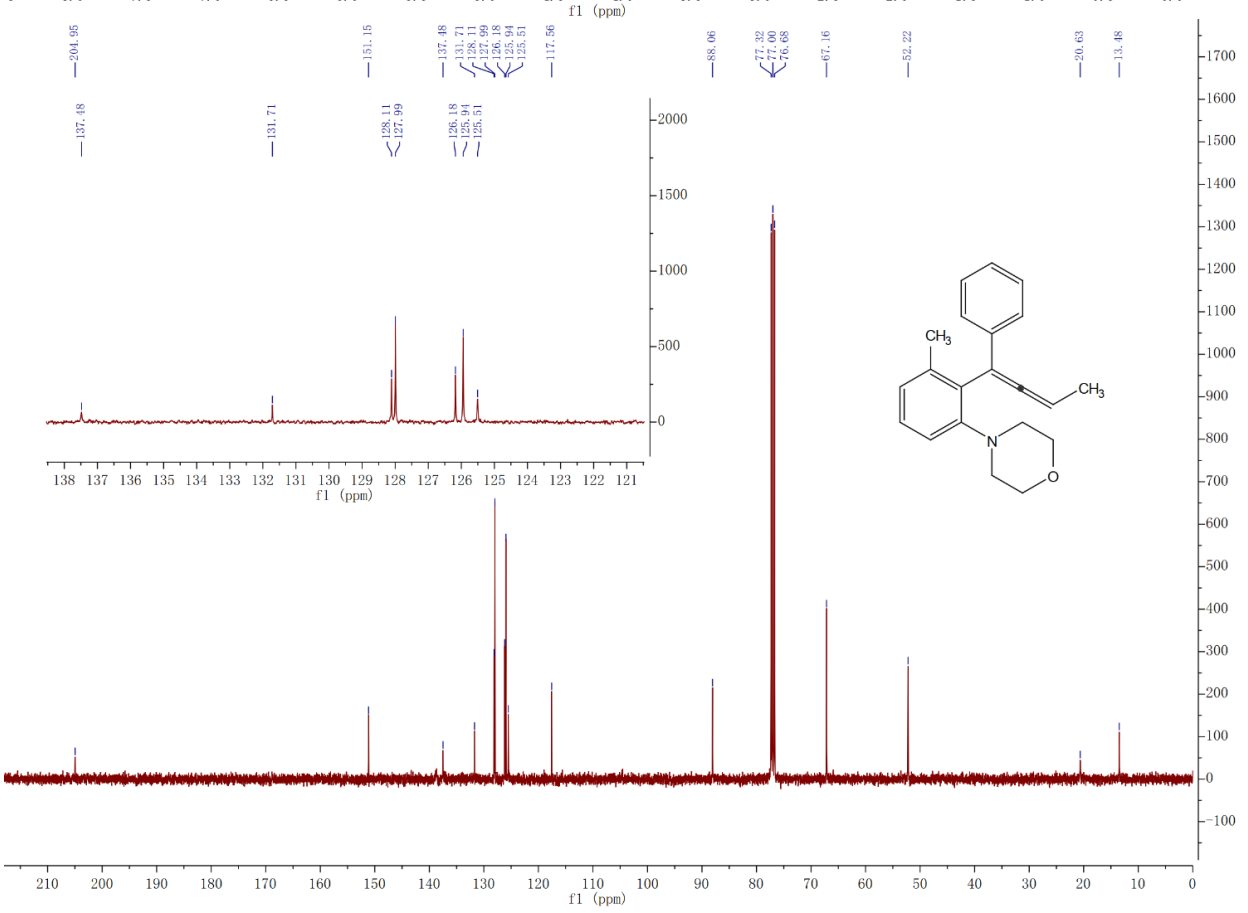
4-(3-methyl-2-(1-phenylpenta-1,2-dien-1-yl)phenyl)morpholine (4ac)



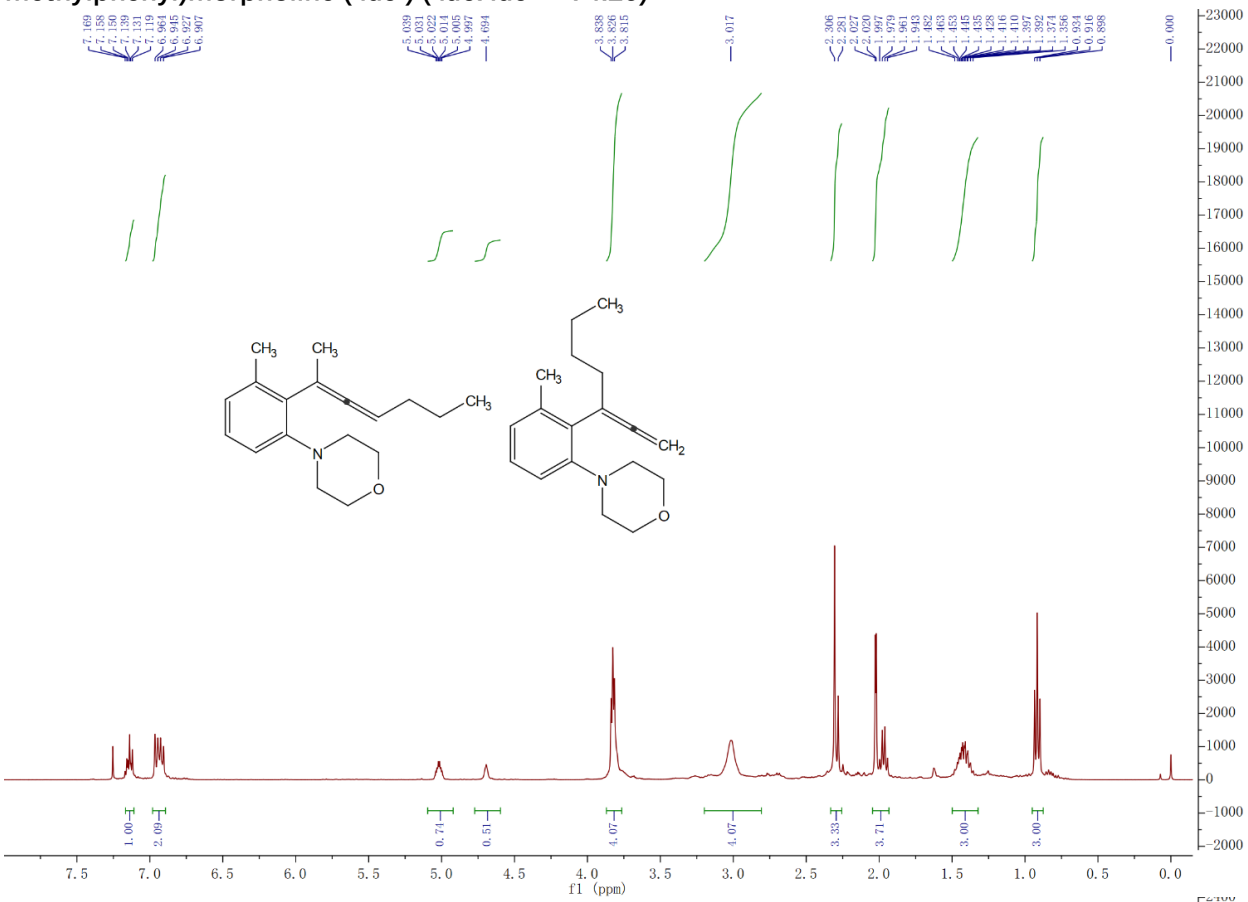


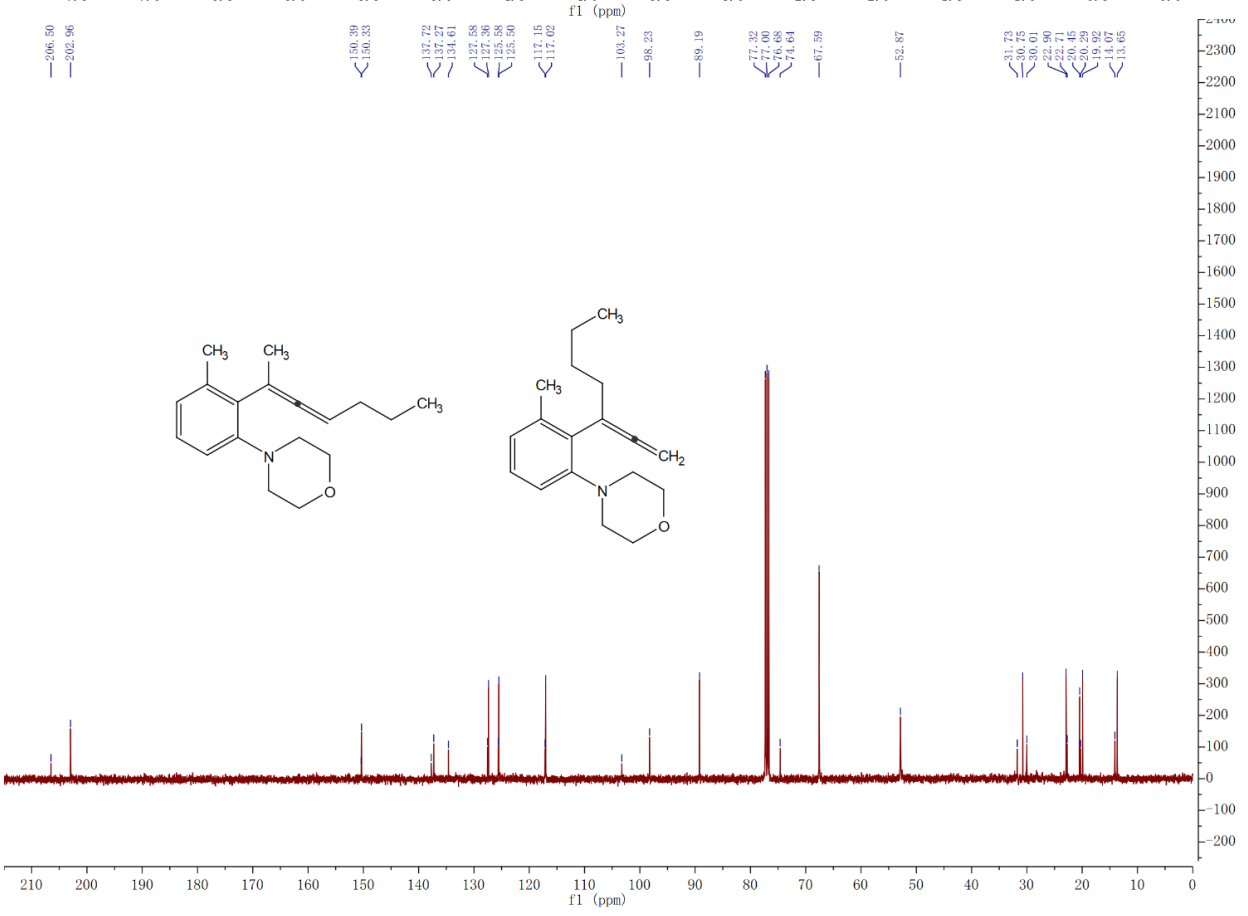
4-(3-methyl-2-(1-phenylbuta-1,2-dien-1-yl)phenyl)morpholine (4ad)





4-(2-(hepta-2,3-dien-2-yl)-3-methylphenyl)morpholine (4ae) and 4-(2-(hepta-1,2-dien-3-yl)-3-methylphenyl)morpholine (4ae') (4ae:4ae' = 74:26)





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