

Supporting Information *for*

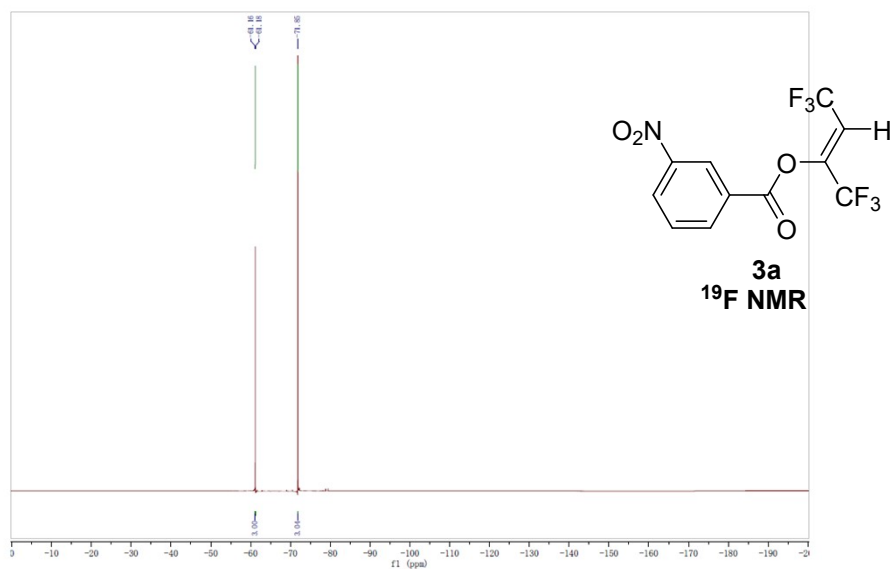
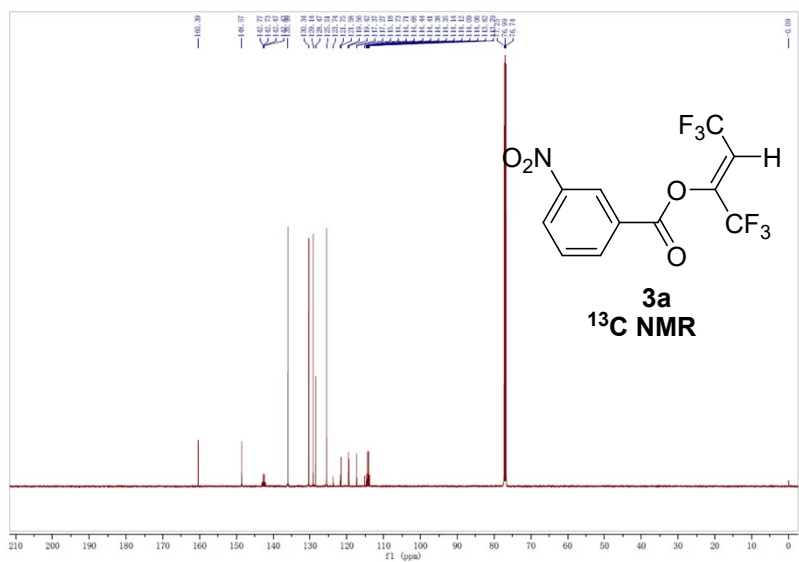
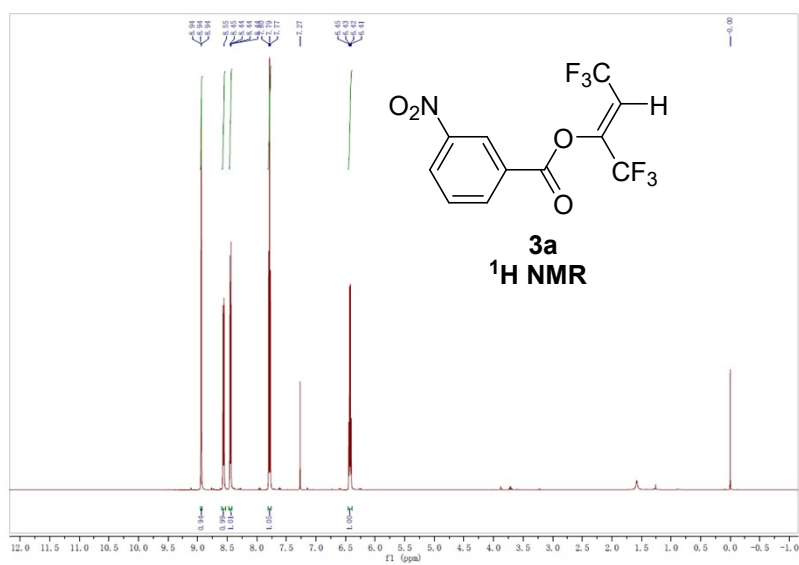
**Metal-free catalytic hydrocarboxylation of
hexafluorobut-2-yne**

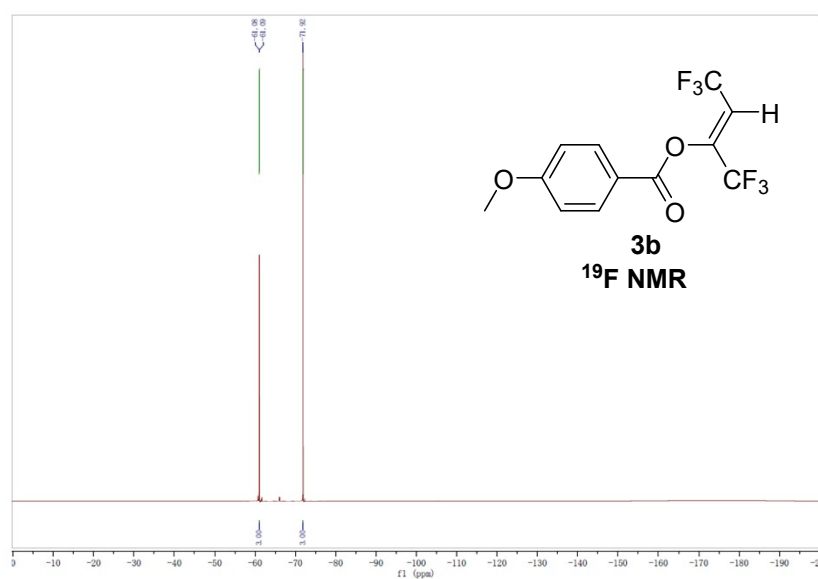
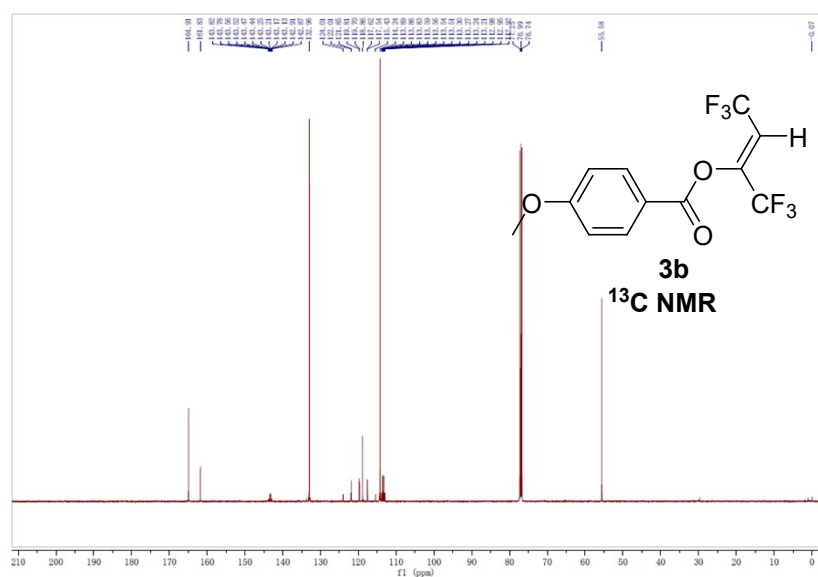
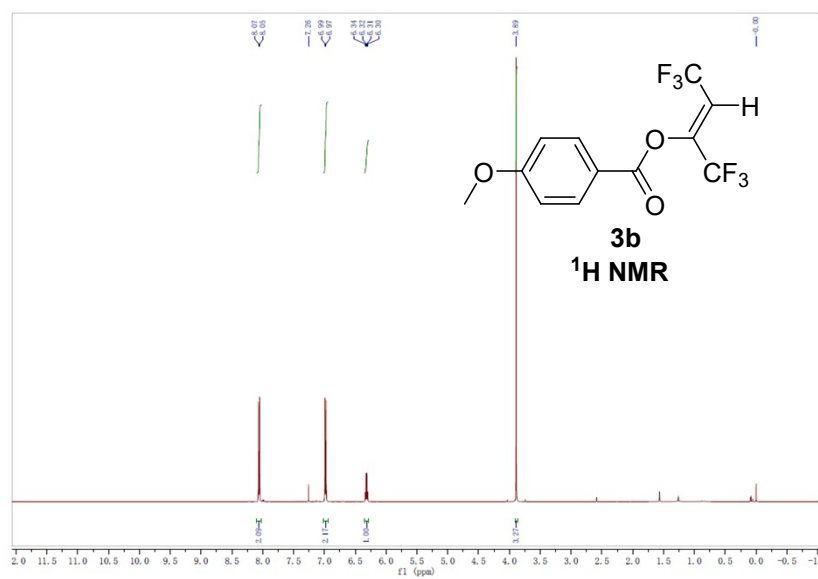
Ji-jun Zeng, Bo Zhao, Xiao-bo Tang, Sheng Han, Zhi-qiang Yang, Ze-Peng Liu, Wei
Zhang* and Jian Lu*

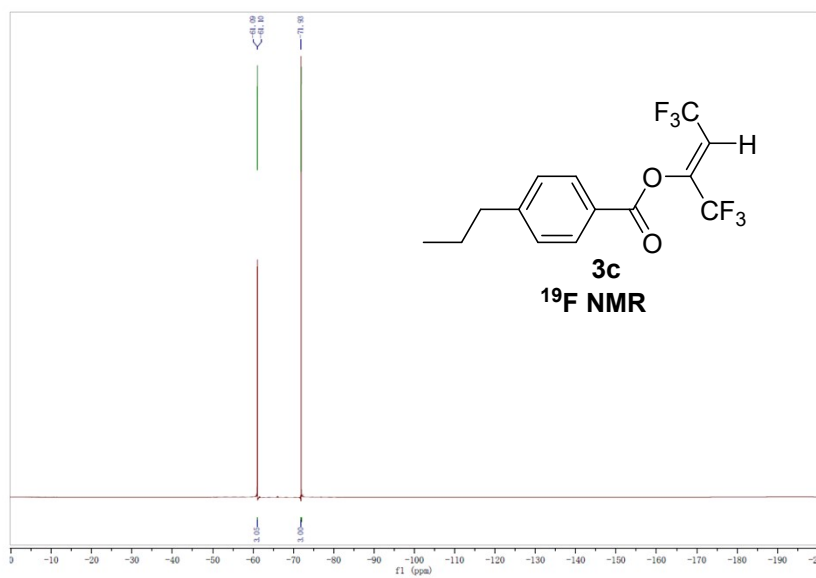
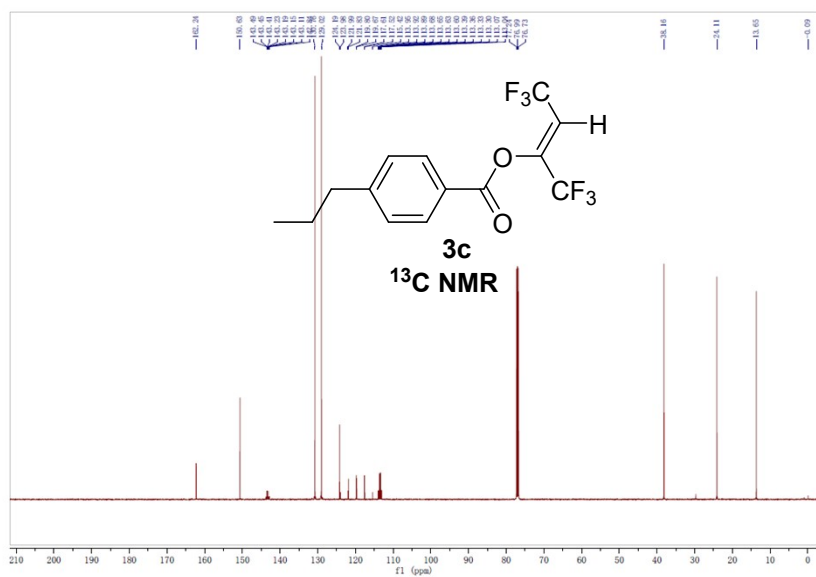
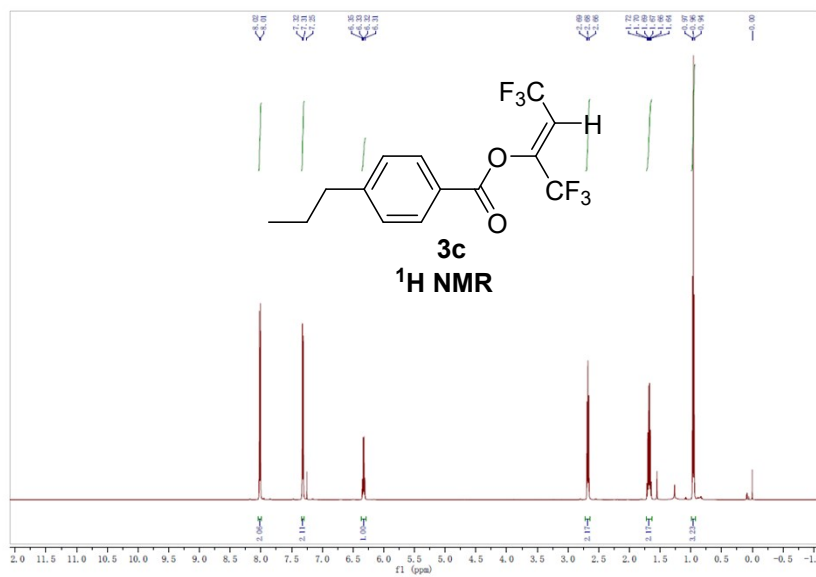
State Key Laboratory of Fluorine & Nitrogen Chemicals, Xi'an Modern Chemistry Research Institute,
Xi'an, 710065, China.

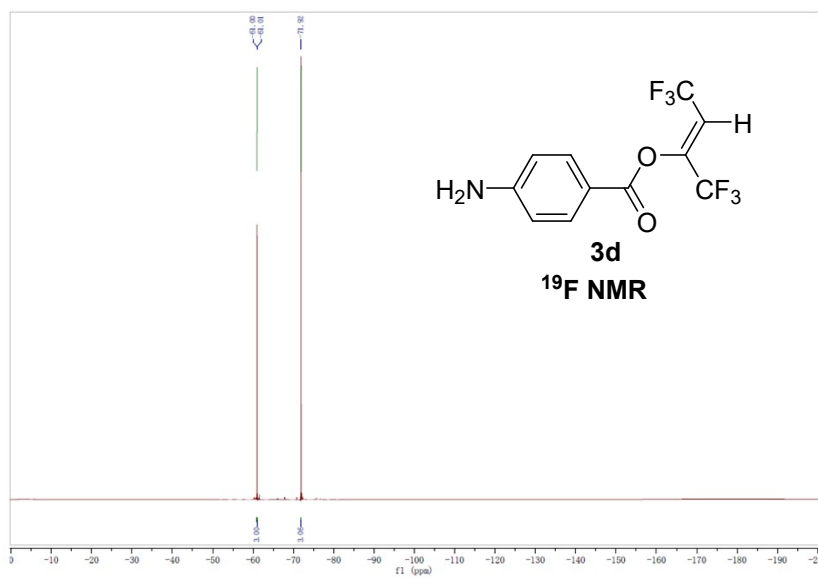
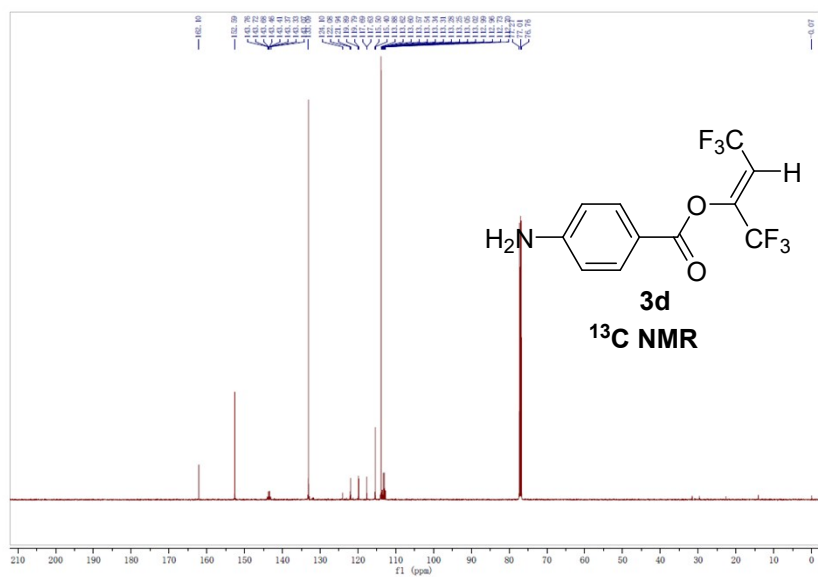
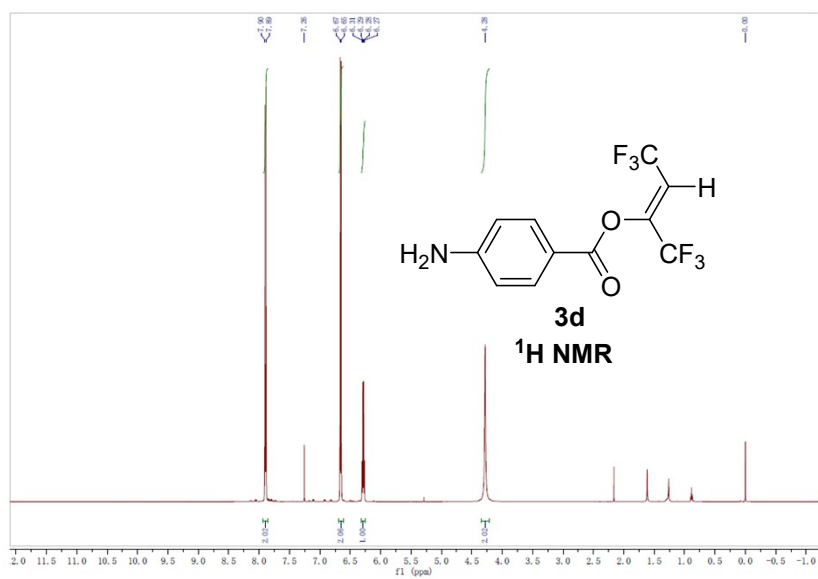
1. NMR spectra of products.....	S1
2. Cartesian coordinates and the initial, transition and final structure energies of R1- R3 obtained via DFT calculations.....	S22

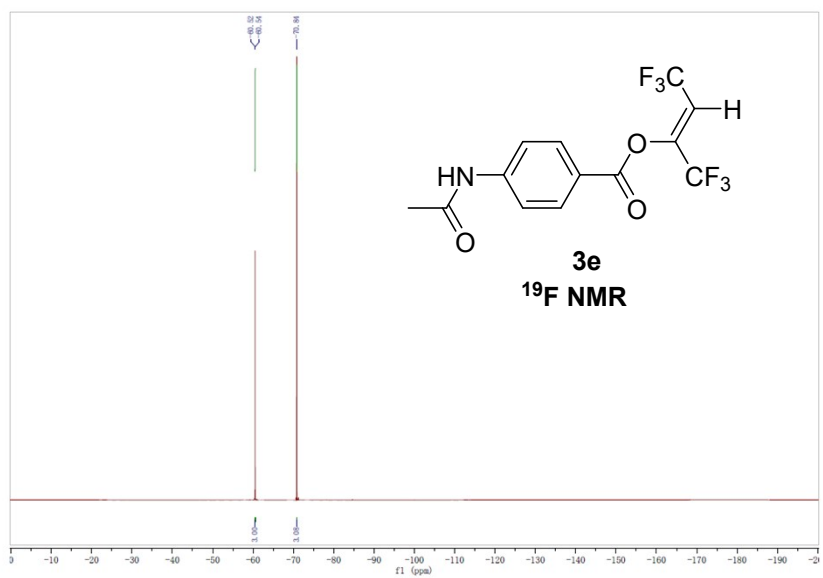
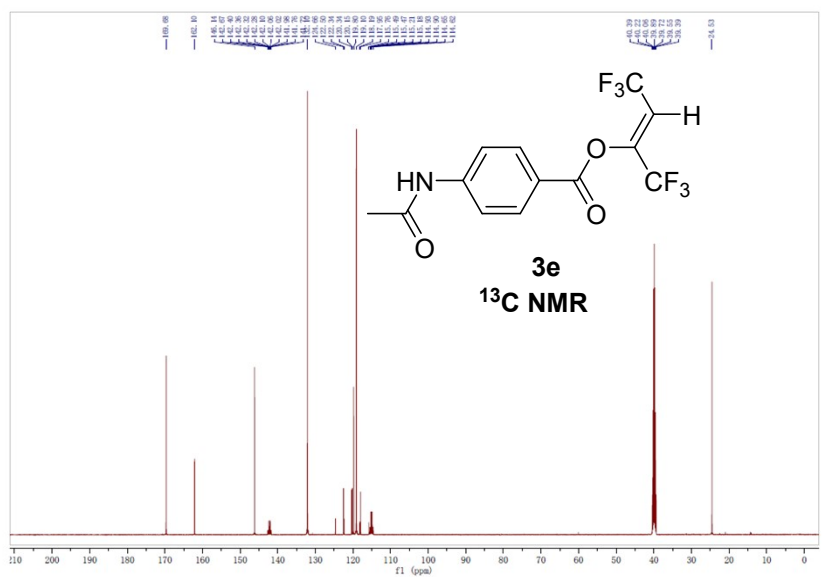
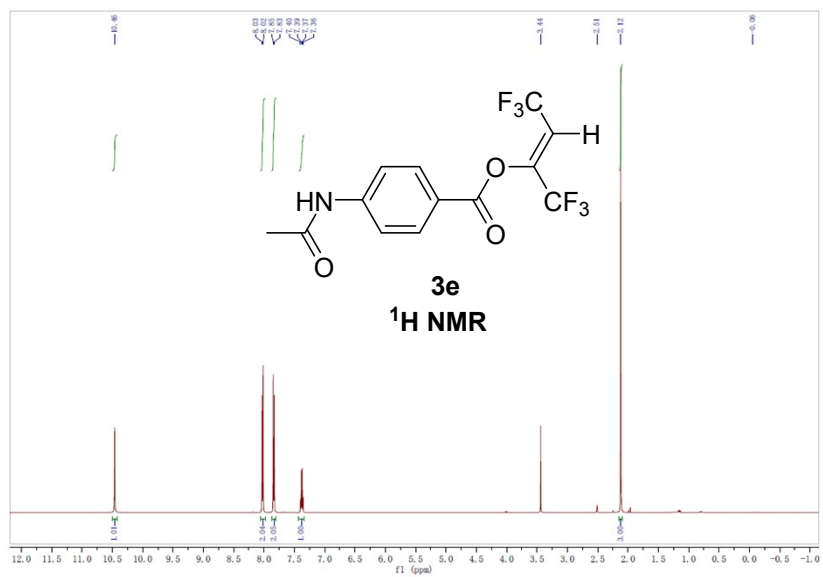
1. NMR spectra of products

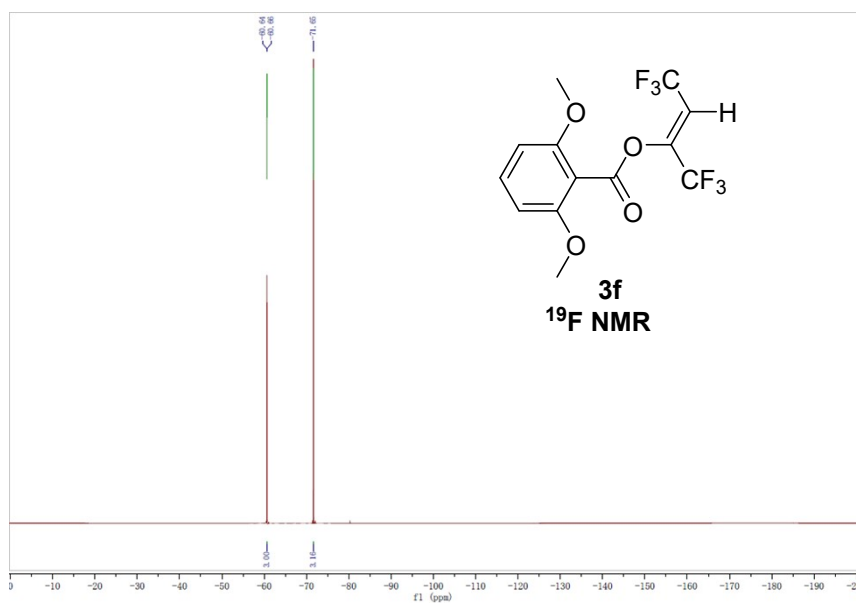
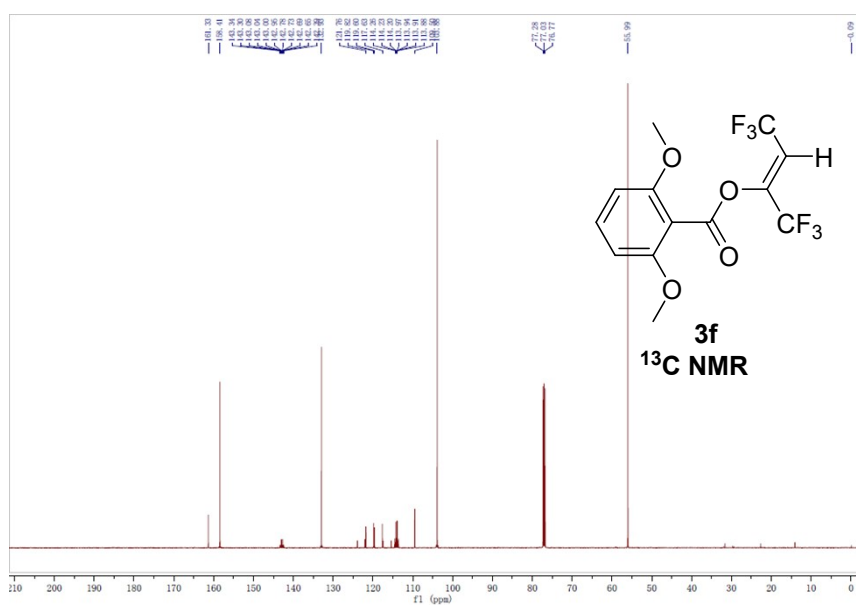
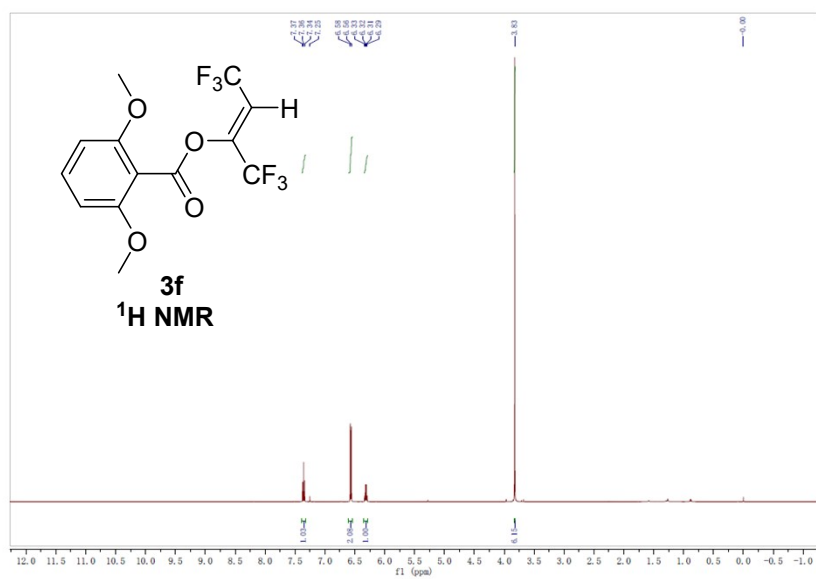


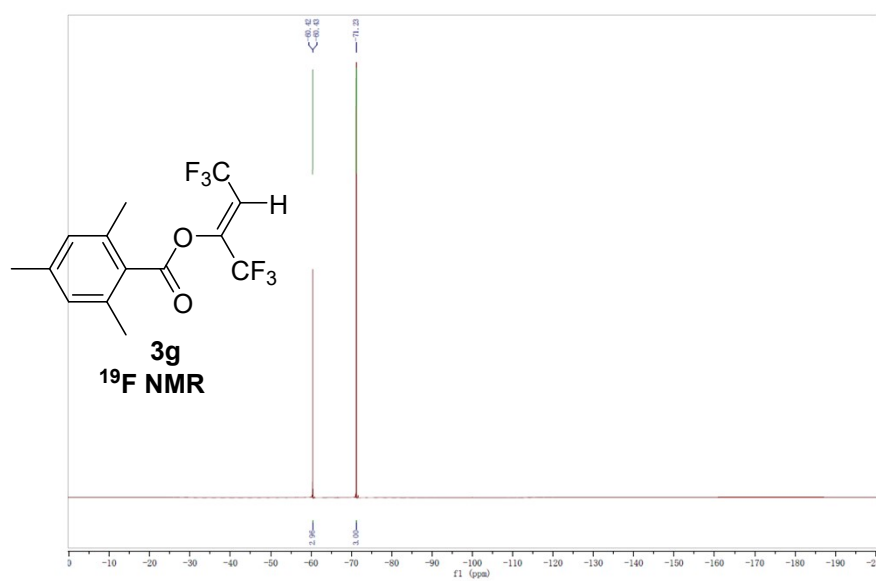
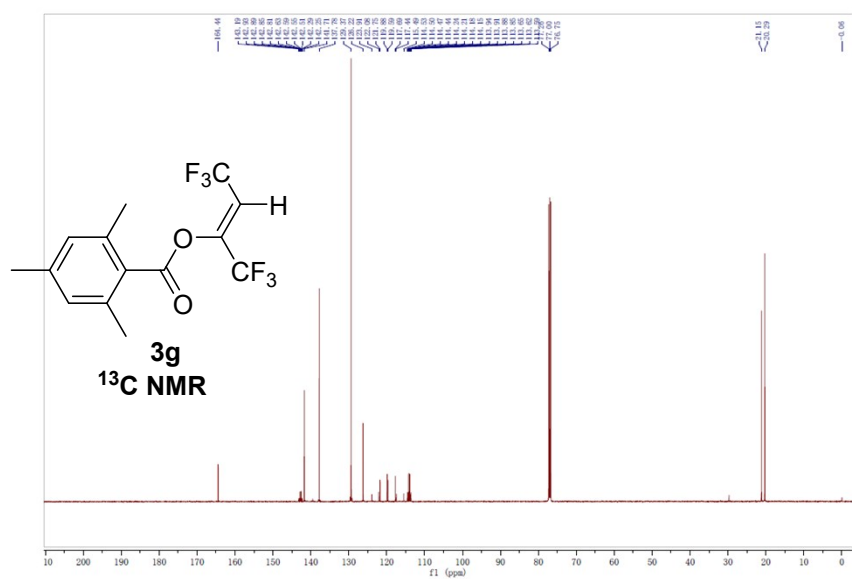
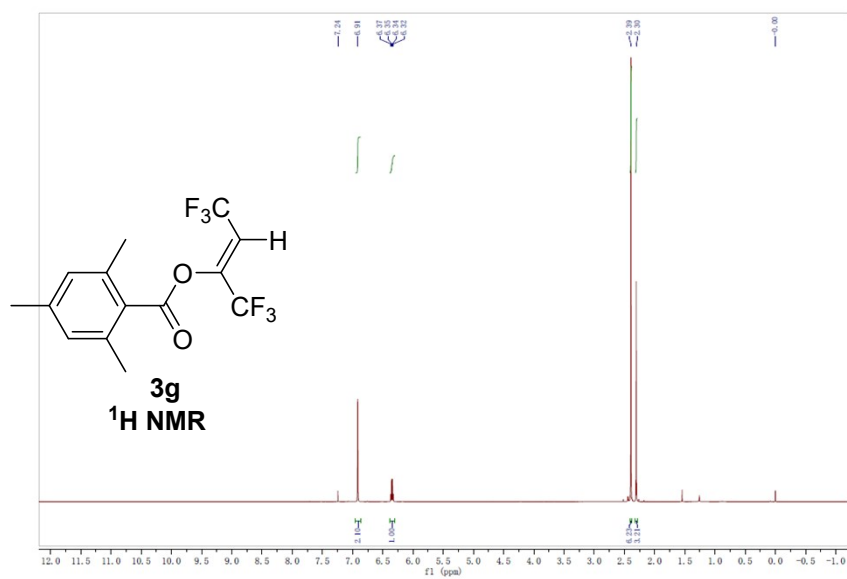


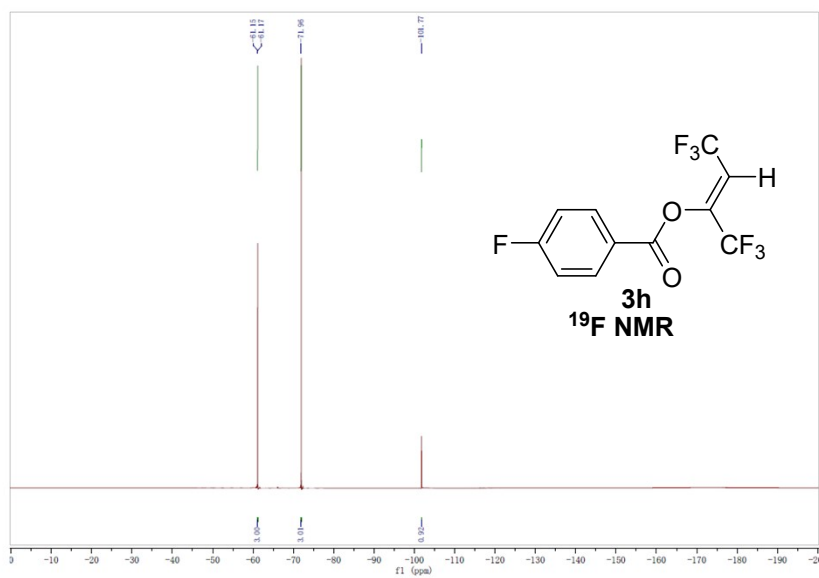
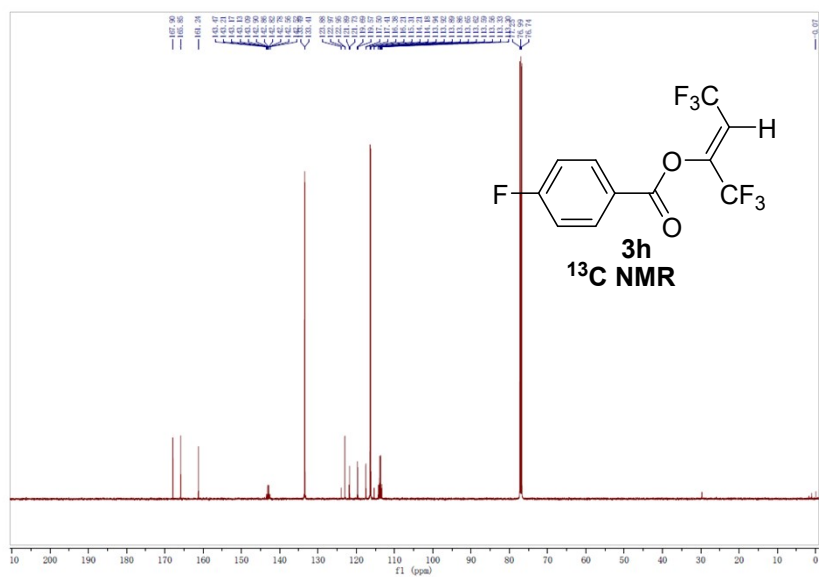
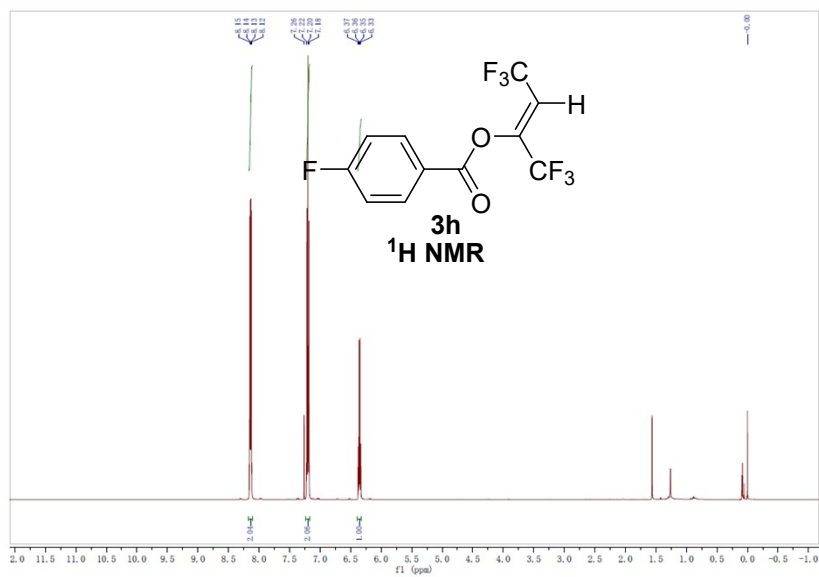


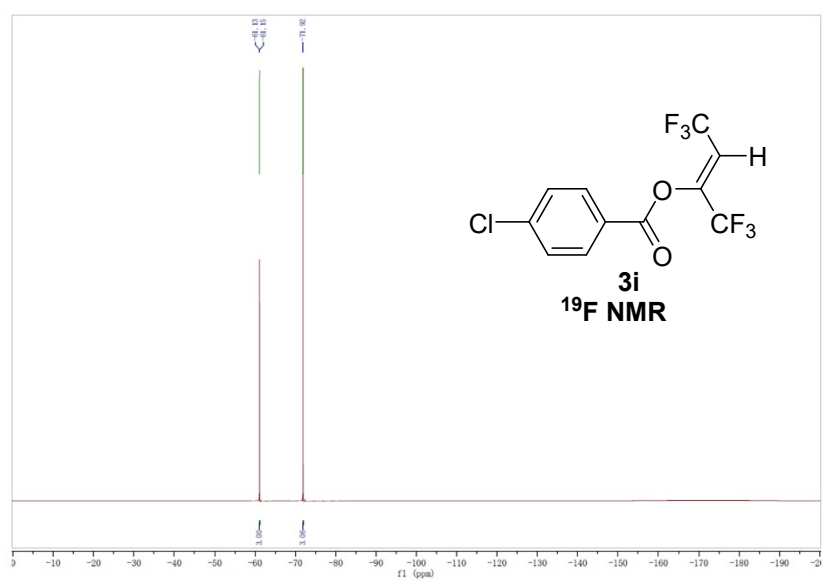
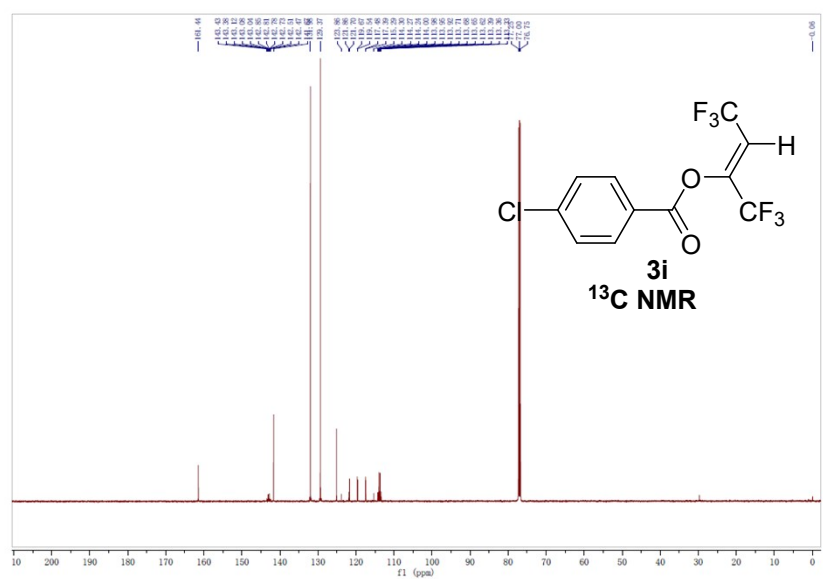
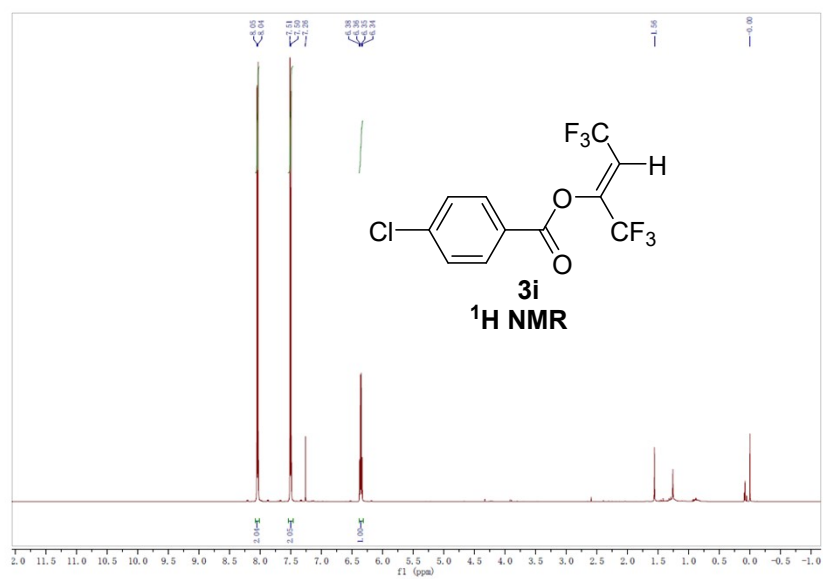


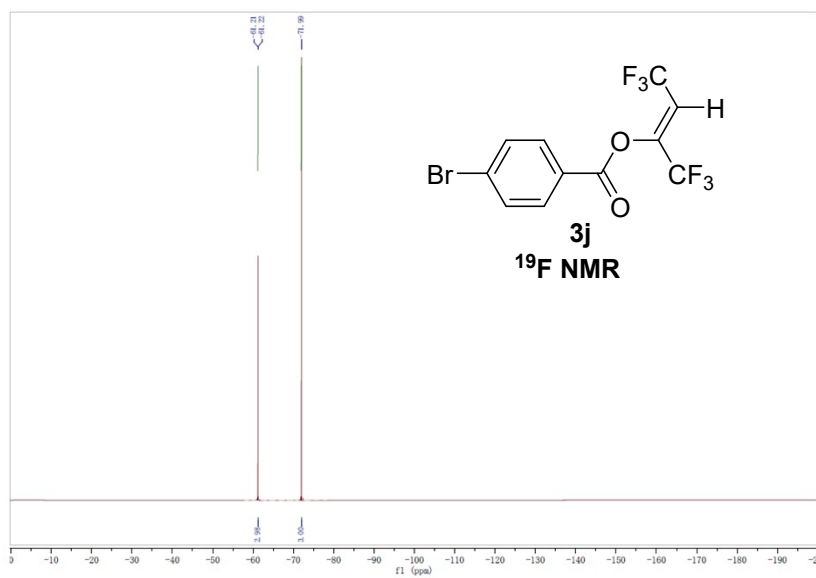
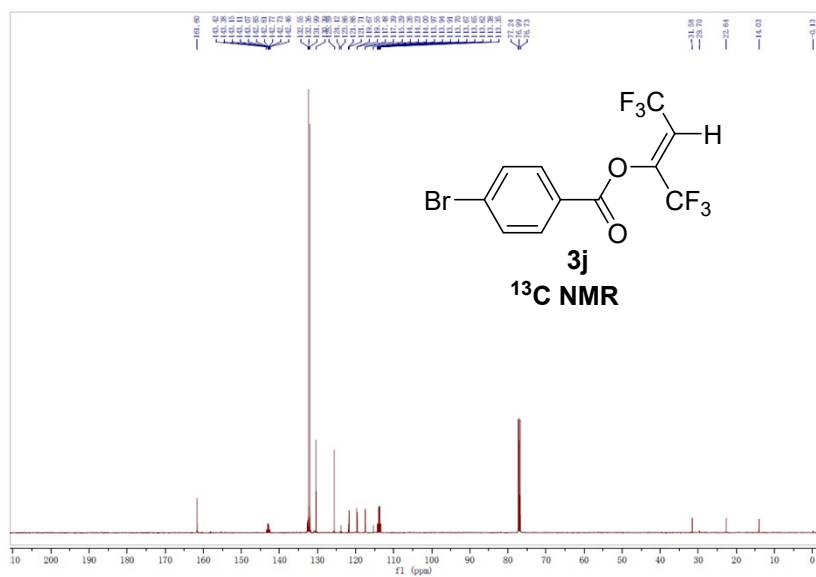
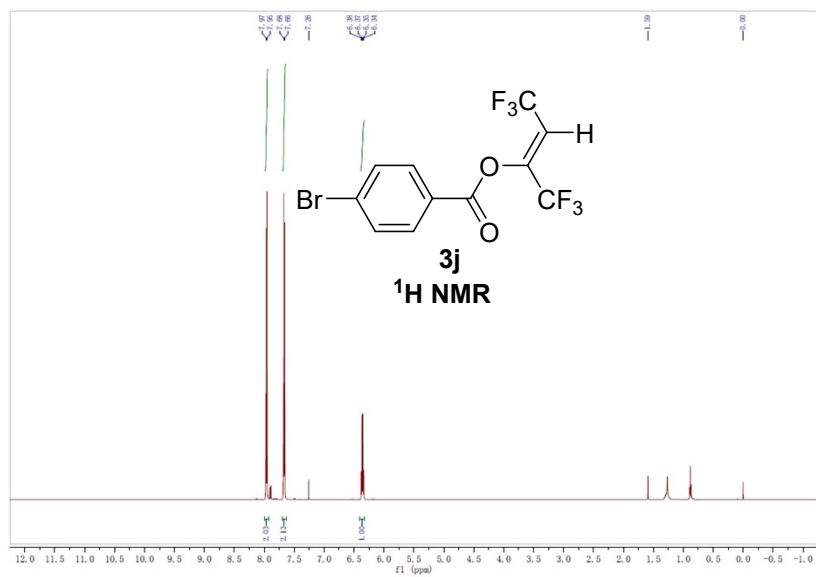


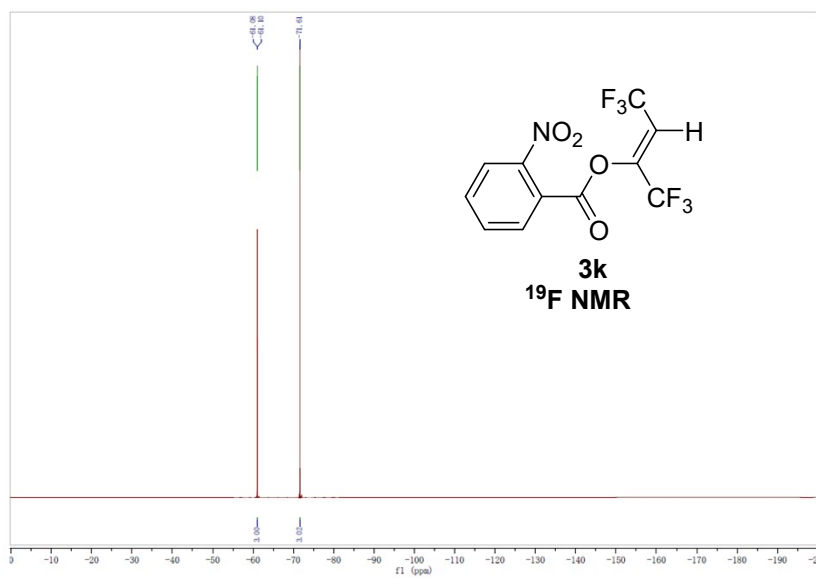
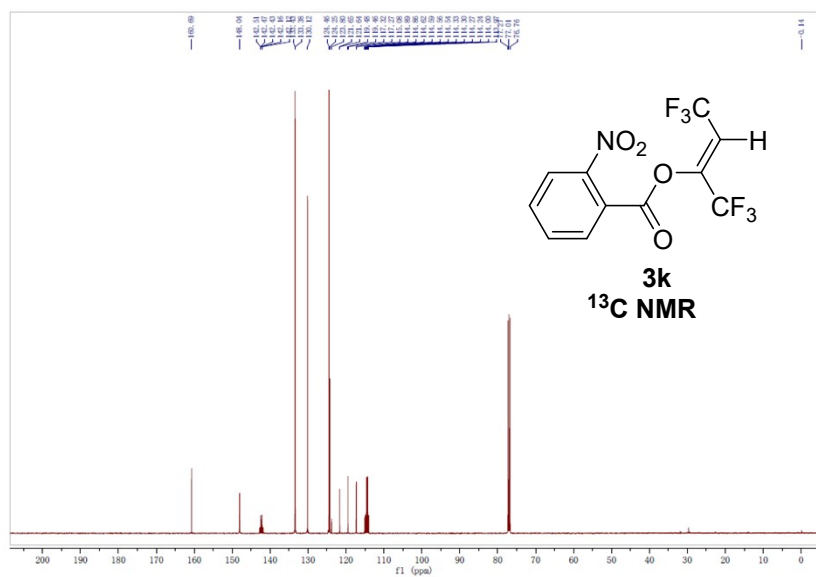
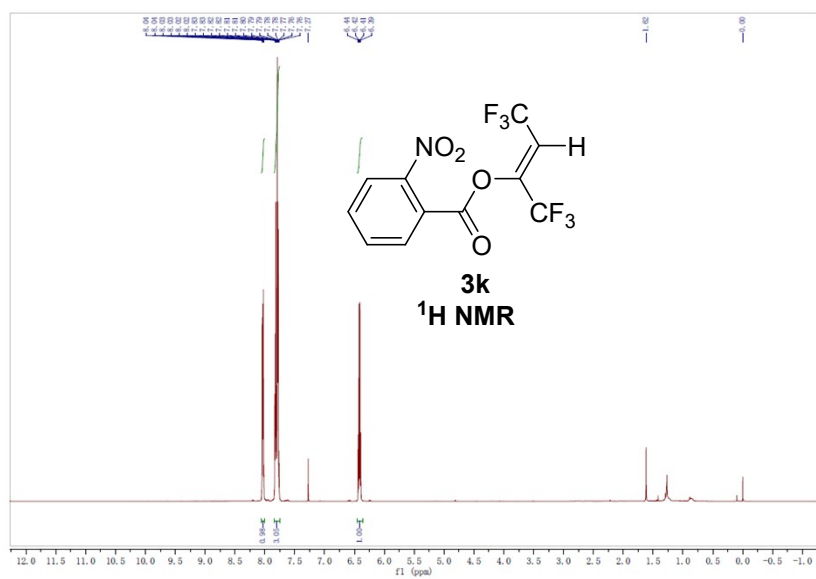


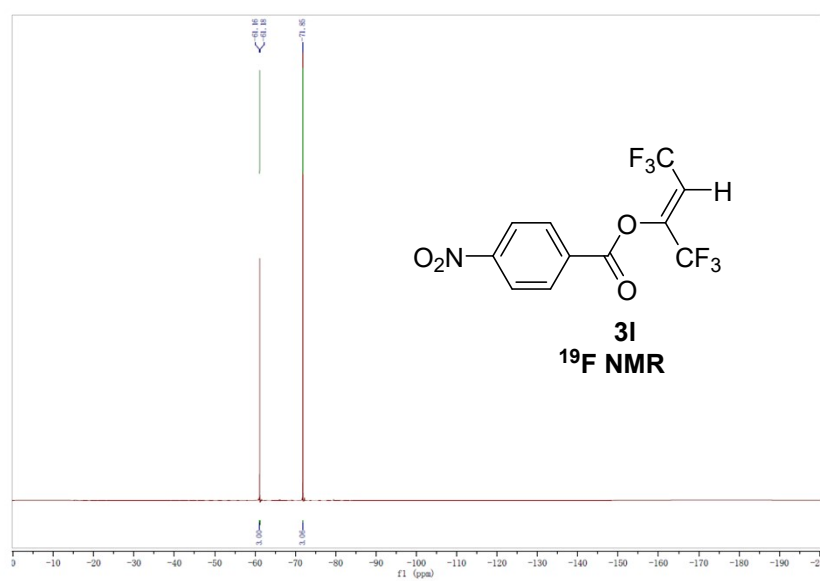
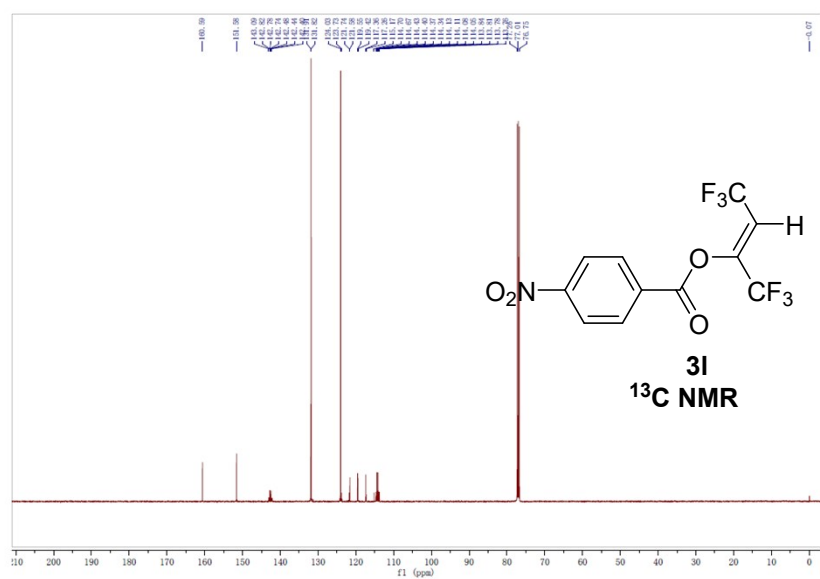
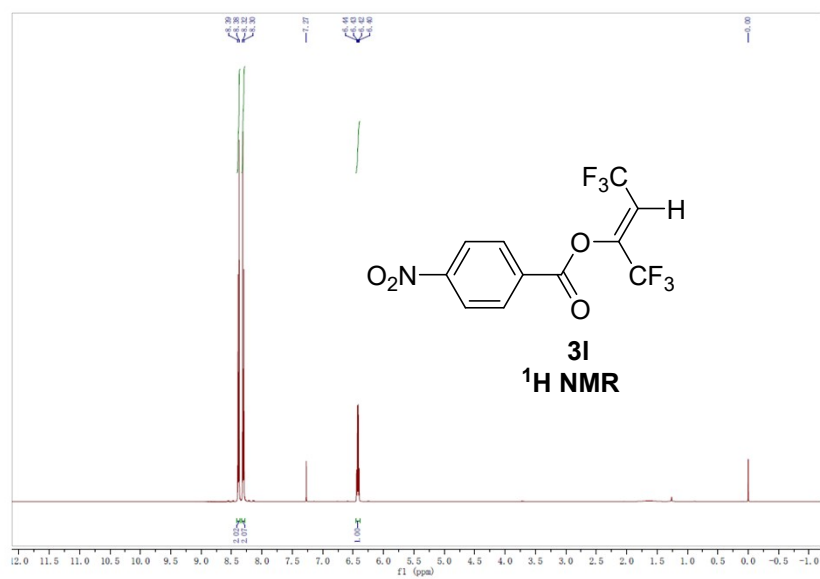


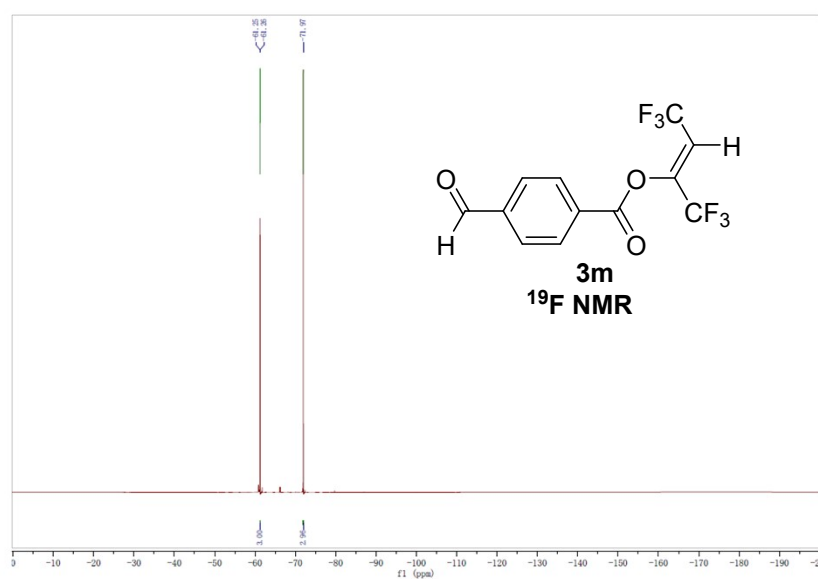
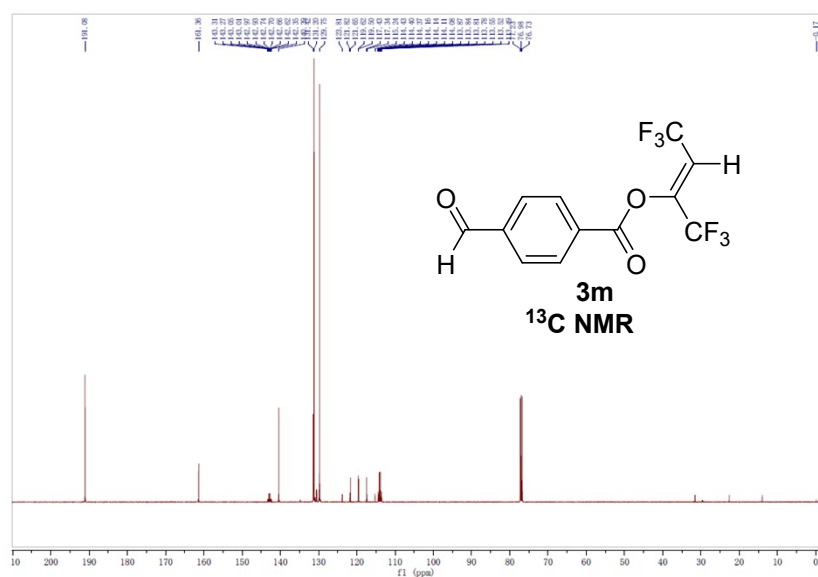
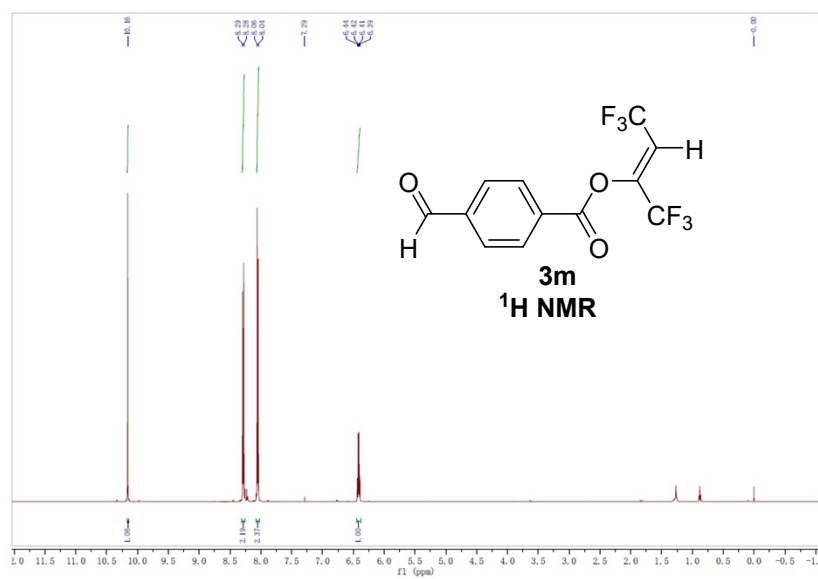


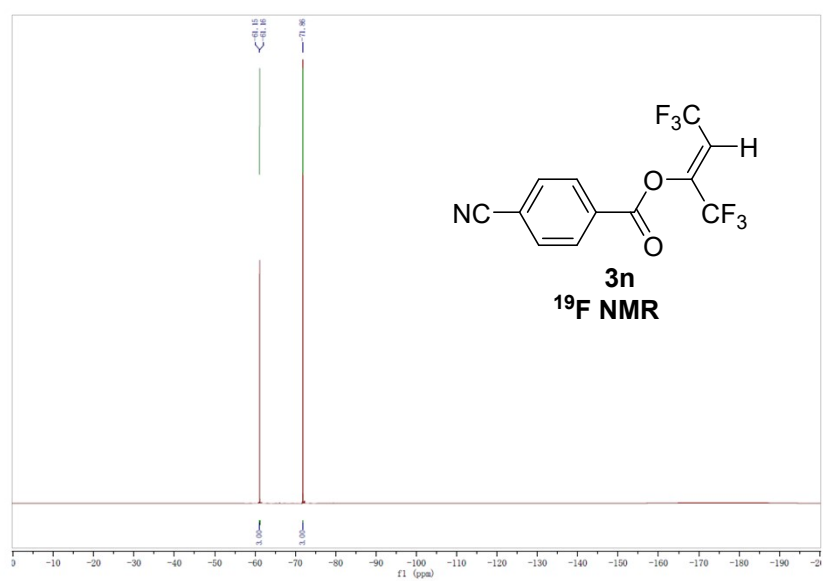
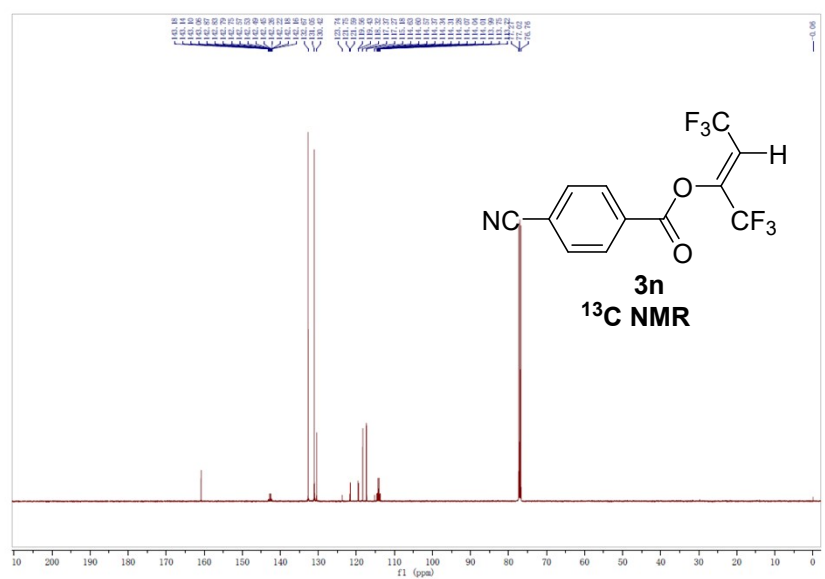
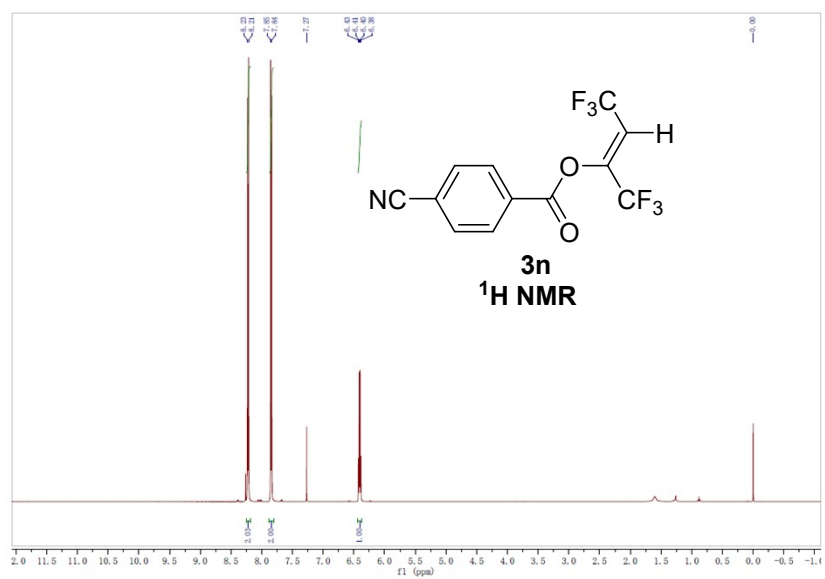


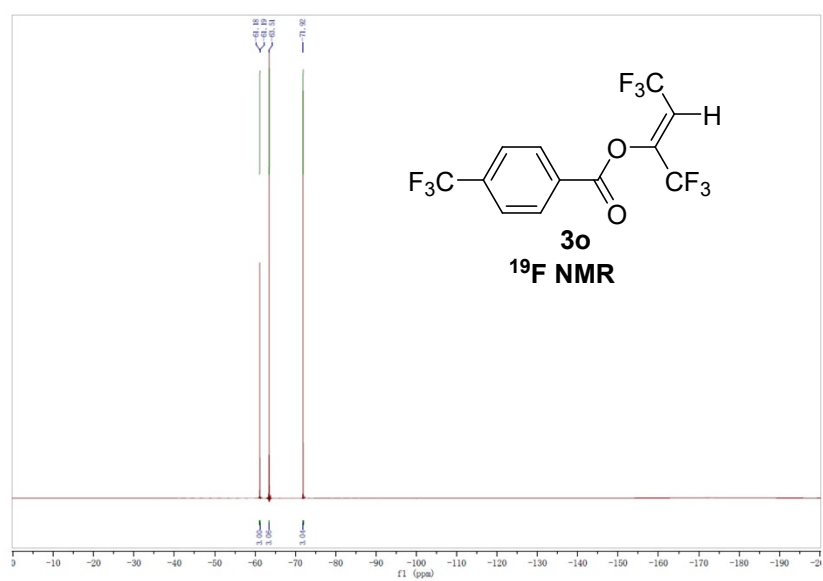
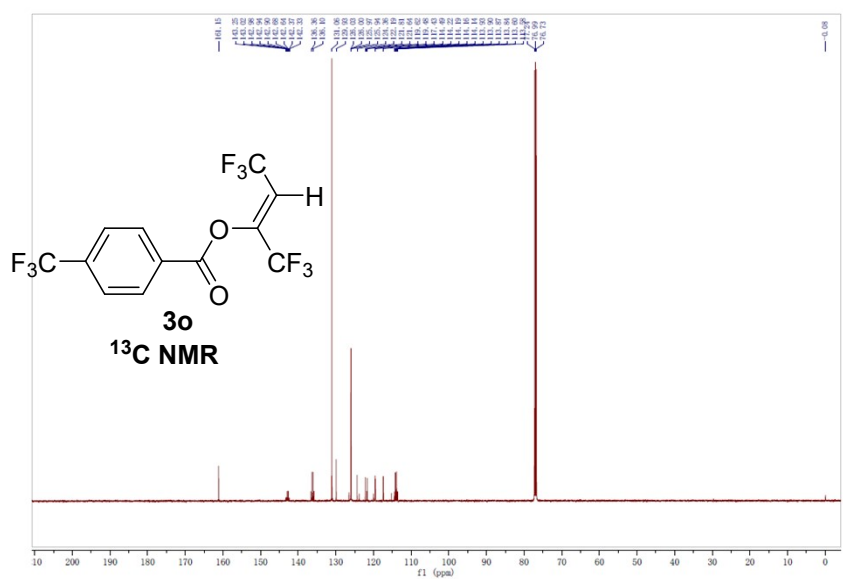
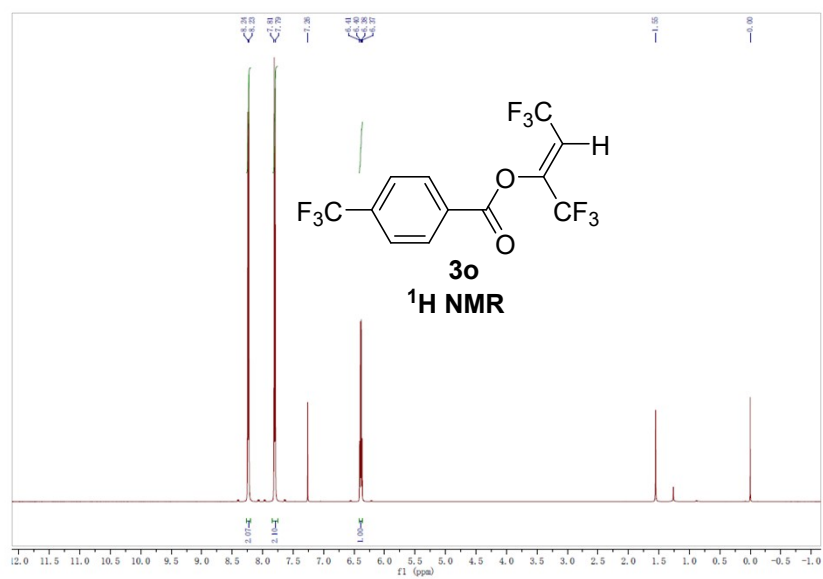


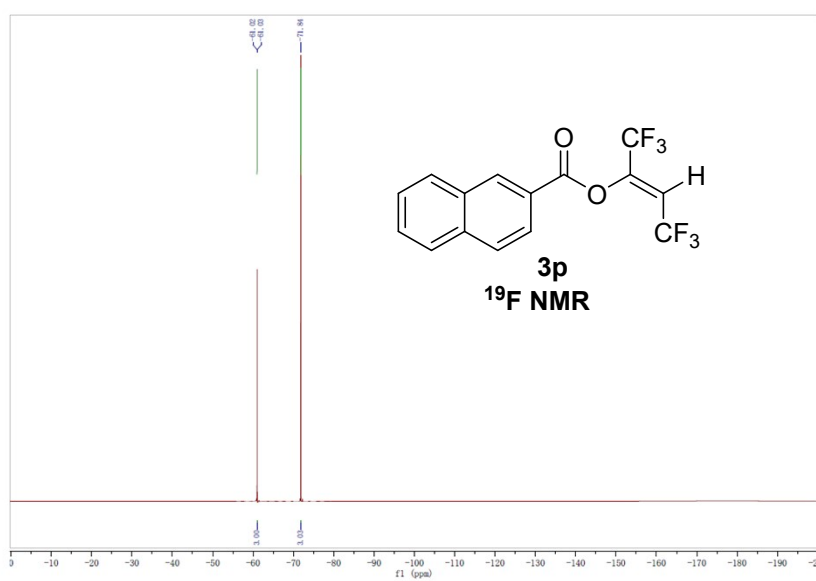
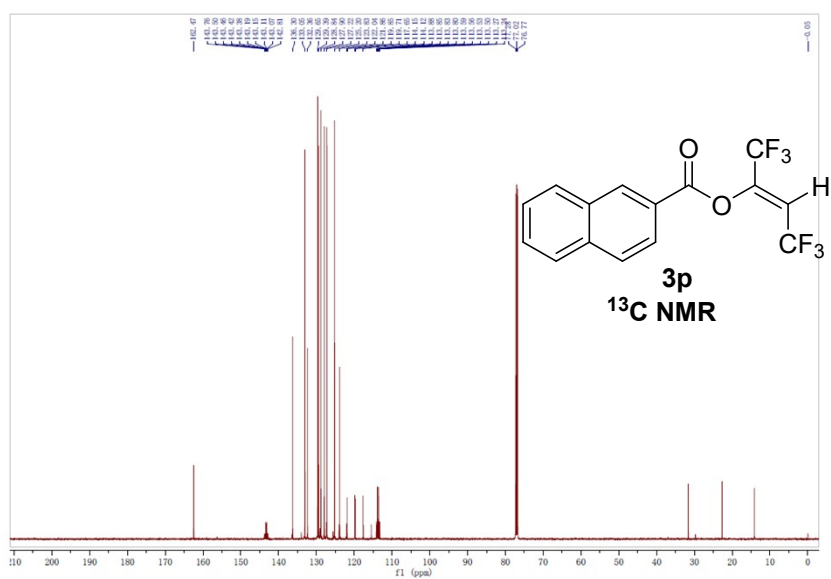
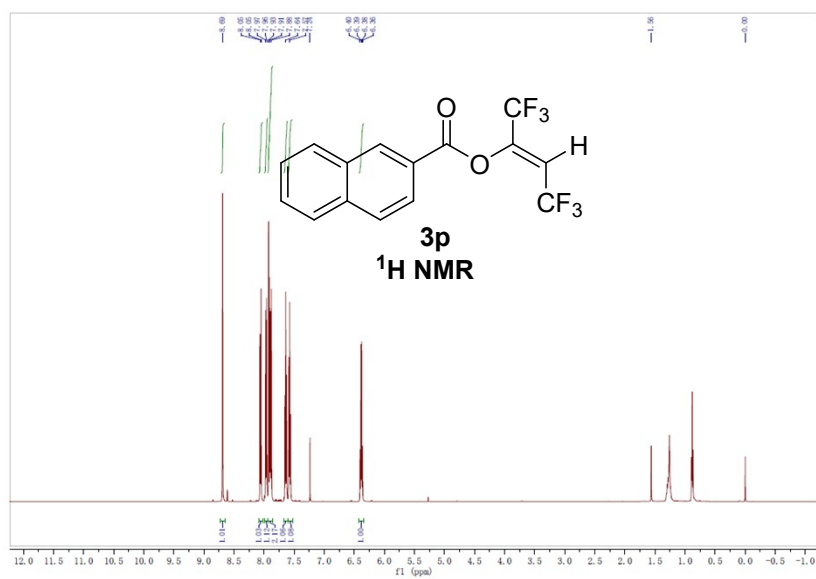


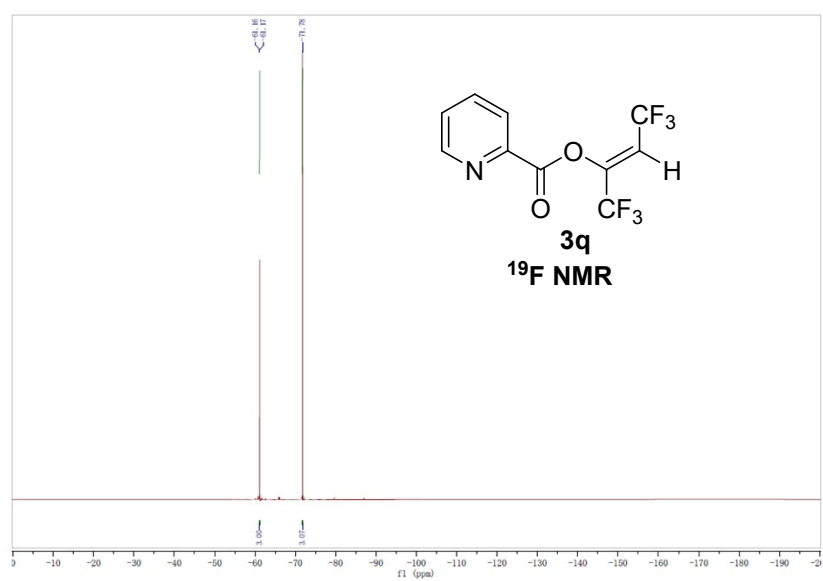
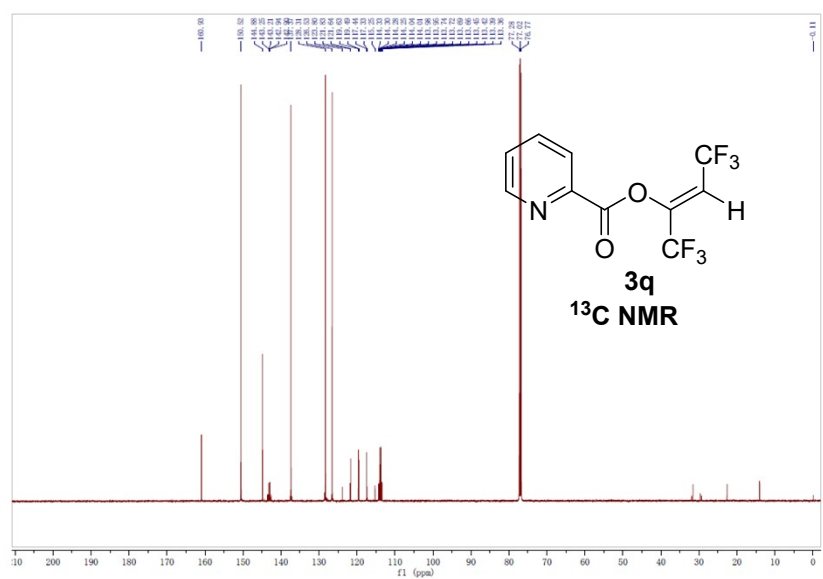
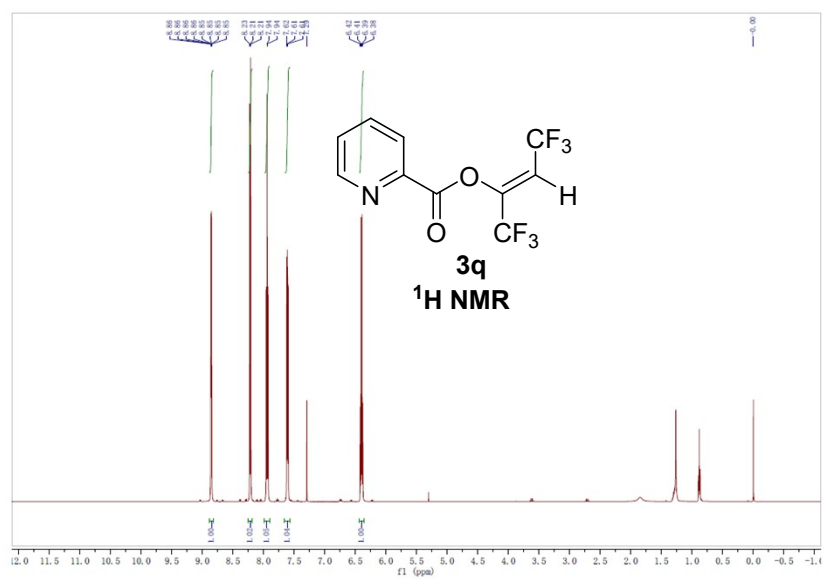


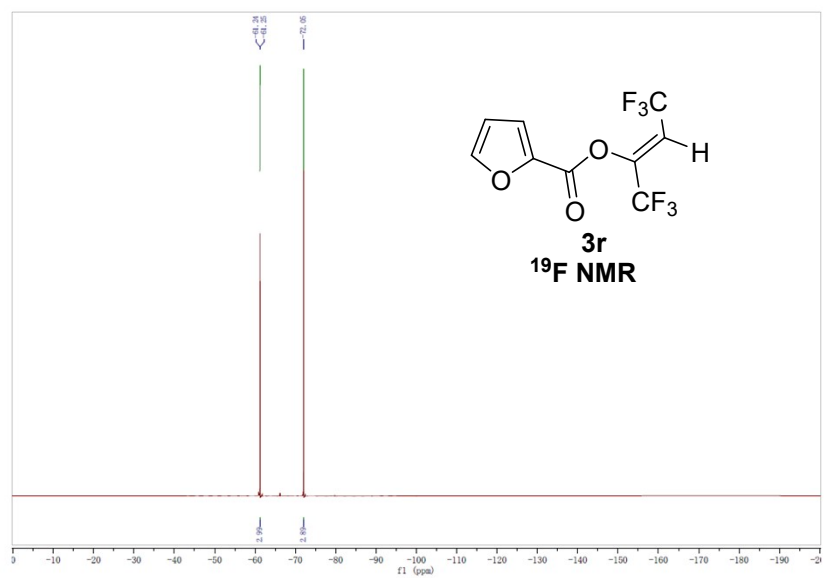
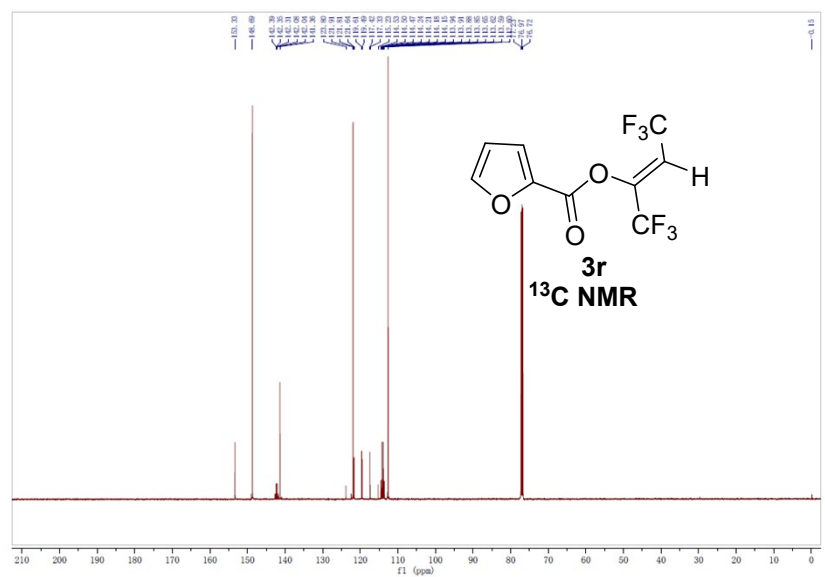
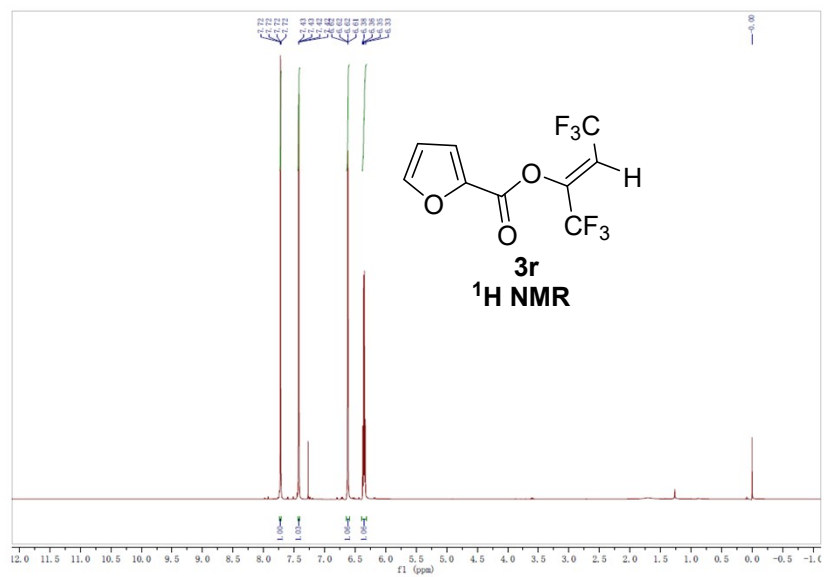


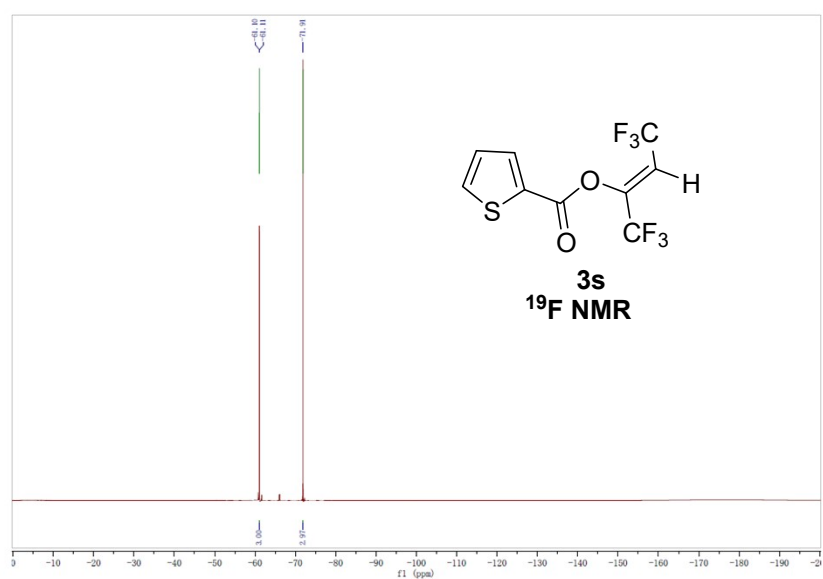
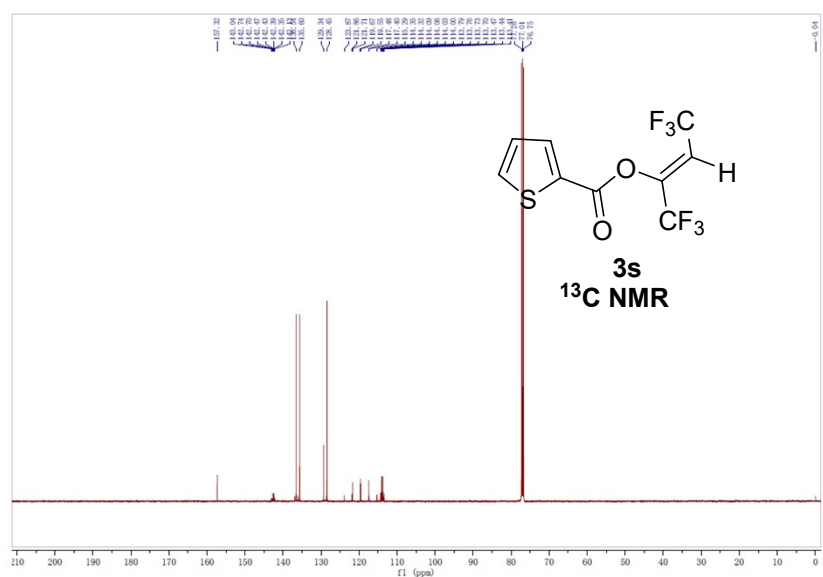
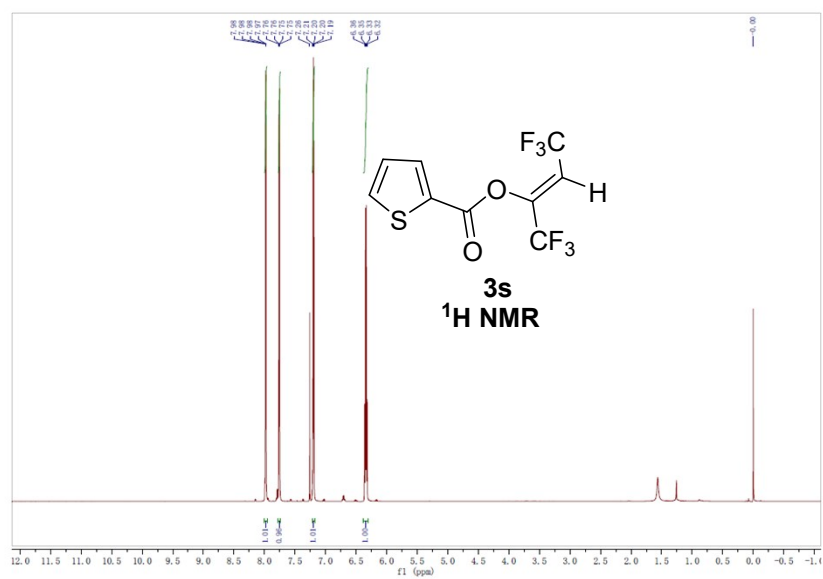


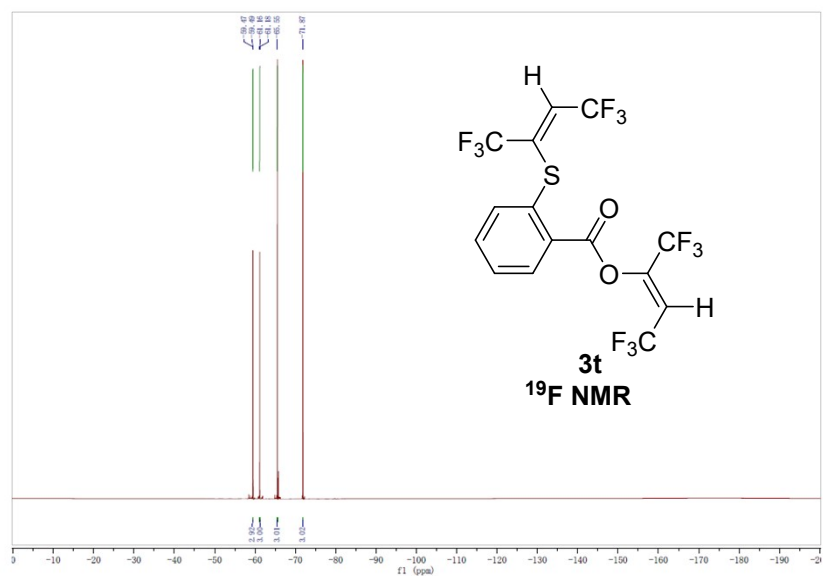
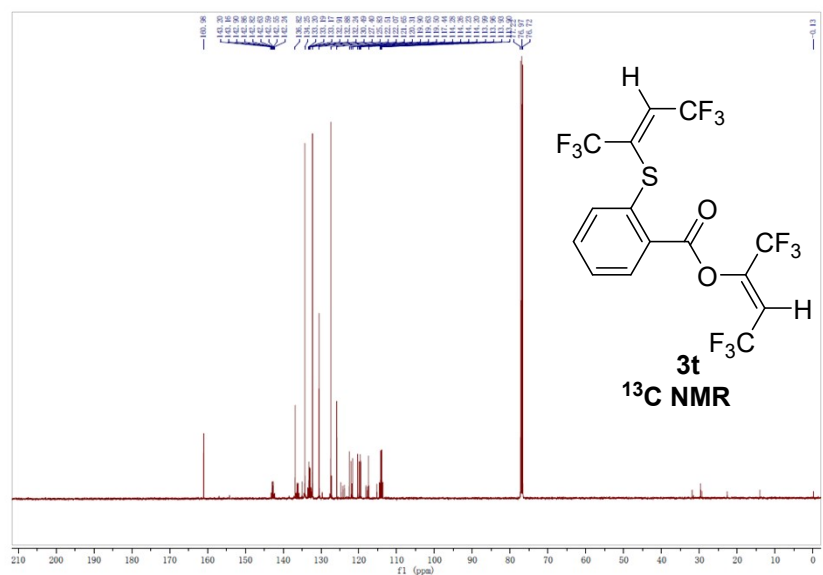
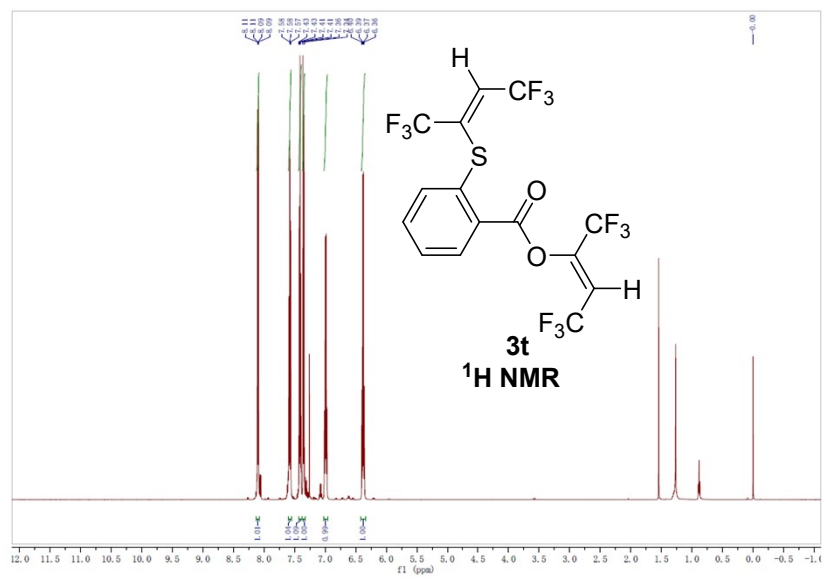


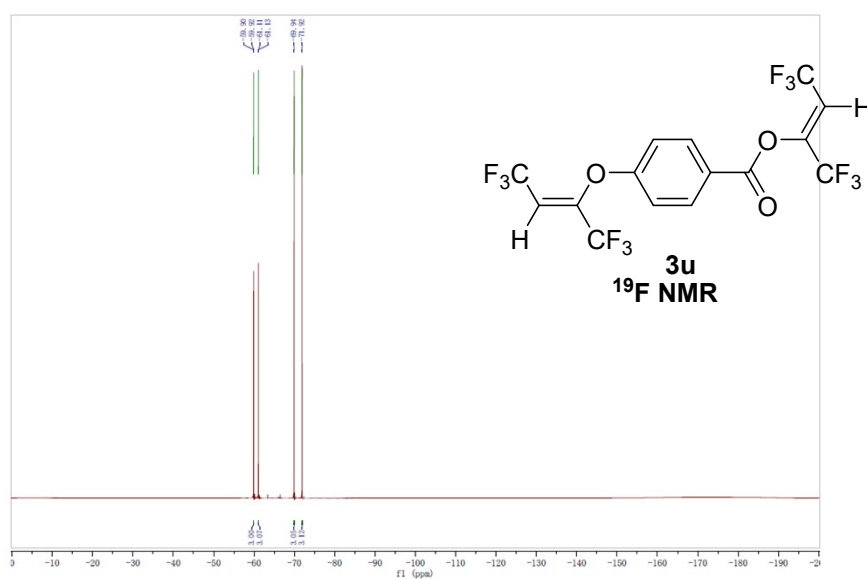
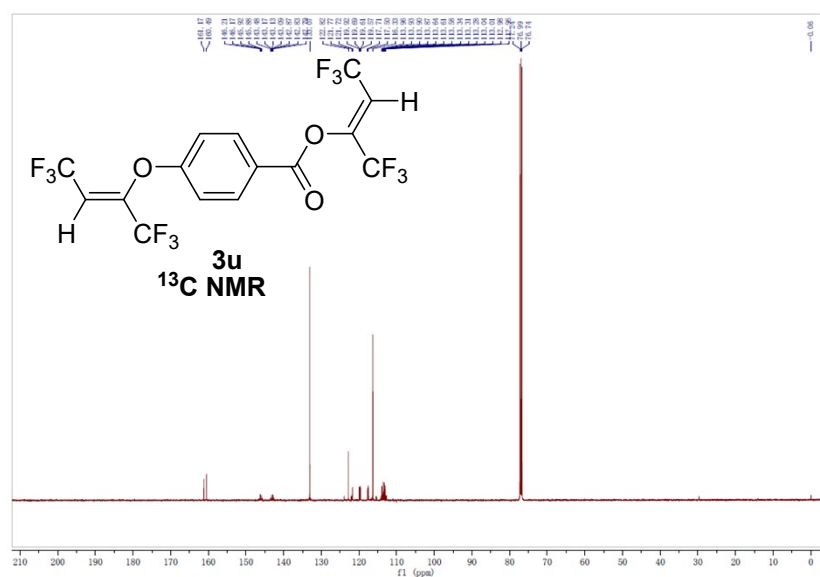
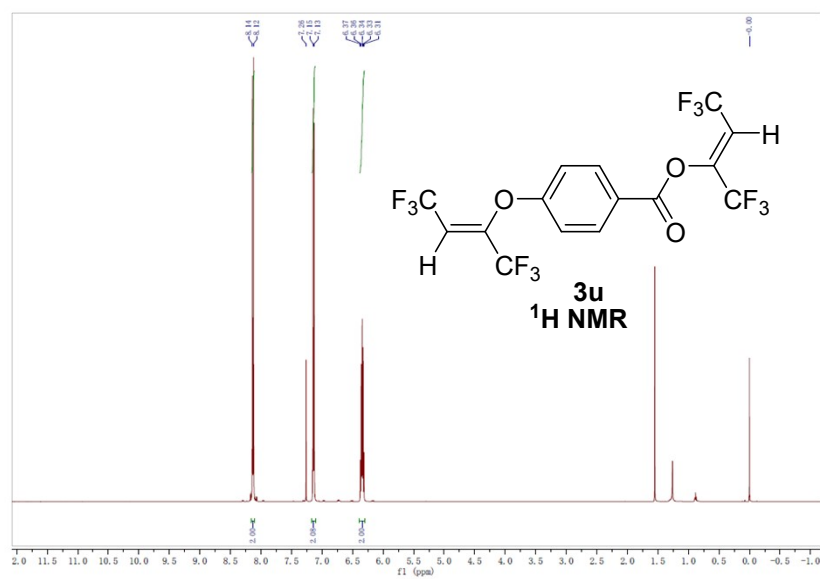










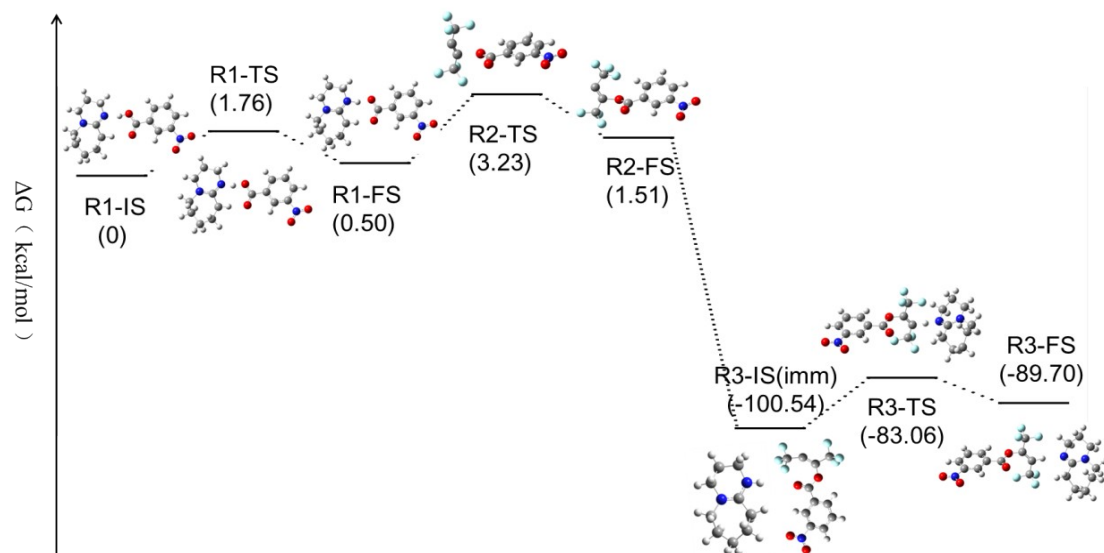


2. Cartesian coordinates and the initial, transition and final structure energies of R1-R3 obtained via DFT calculations.

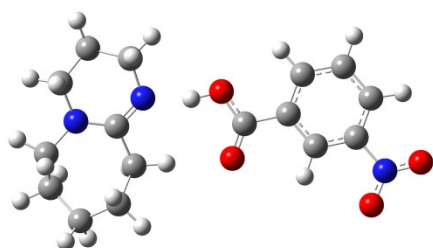
All of the calculations were performed with Gaussian09 package.¹ Geometry optimization of all the minima and transition states involved was carried out at the B3LYP level^{2, 3} with the 6-31G(d) basis set for C, H, O, N, F. Default convergence criteria were used. The vibrational frequency calculations were conducted at the same level of theory as geometry optimization to confirm whether each optimized structure is an energy minimum or a saddle point. For transition state, intrinsic reaction coordinate (IRC) analysis⁴ was performed to verify that it connects the right reactants and products. The solvent effects were considered using the PCM model^{5,6} with the as-phase-optimized structures as the initial geometries.

R1			
	IS	TS	FS
G (hartree)	-1087.104495	-1087.101694	-1087.103697
H (hartree)	-1087.026811	-1087.025248	-1087.028181
Ea (kcal/mol)	-	1.76	0.50
ΔH (kcal/mol)	-	0.98	-0.86
R2			
	IS	TS	FS
G (hartree)	-1376.067203	-1376.062857	-1376.0656
H (hartree)	-1375.989165	-1375.988223	-1375.994503
Ea (kcal/mol)	-	2.73	1.01
ΔH (kcal/mol)	-	0.59	-3.07
R3			
	IS(imm)	TS	FS
G (hartree)	-1838.338056	-1838.472814	-1838.50037
H (hartree)	-1838.219259	-1838.37975	-1838.396849

E_a (kcal/mol)	-	17.49	10.84
ΔH (kcal/mol)	-	0.20	0.11



R1-IS:

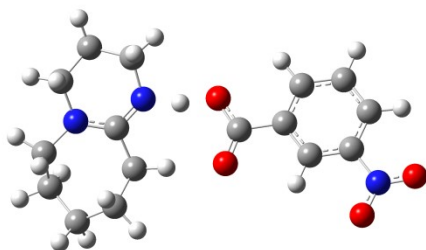


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C	0.36995300	-0.72079400	-0.13643100
C	-2.09835000	-1.18899000	0.53080100
C	-0.84225800	1.47462200	0.27234200
C	-2.95849200	0.00421200	0.08325800
C	-2.12872000	1.15904300	-0.50187100
H	-1.23120000	-1.30391300	-1.45899700
H	-1.03884500	1.43507600	1.35897300
H	-1.70748500	-1.01644000	1.54222600
H	-3.54872900	0.36782900	0.93491700

H	-0.63048300	-2.53014800	-0.35349500
H	-2.73073400	-2.08185600	0.60533400
H	-0.56433400	2.51232000	0.05558700
H	-3.68327400	-0.32442600	-0.67332700
H	-2.74448300	2.06714200	-0.51944000
H	-1.85834800	0.95544900	-1.54469500
N	0.34275700	0.67804700	-0.07708200
N	1.42163000	-1.45903100	-0.03946700
C	2.72389200	-0.84740100	0.18562600
H	3.47819000	-1.45522100	-0.33057800
C	2.79618800	0.60592800	-0.28287700
C	1.59376300	1.35788500	0.27515900
H	2.96782600	-0.91105100	1.25798900
H	3.72517800	1.09066500	0.04080400
H	2.76841300	0.64253200	-1.37911800
H	1.55098400	2.37556700	-0.13303100
H	1.68708400	1.45717700	1.37099200
C	5.06154328	-1.80978307	-5.30444157
C	4.12574276	-1.86246545	-4.26700043
C	3.76148346	-3.08030299	-3.68156143
C	4.35049862	-4.25844852	-4.15067255
C	5.28337981	-4.19209736	-5.18439193
C	5.65349174	-2.97918628	-5.77579737
H	5.33246491	-0.85488857	-5.74946264
H	3.64628726	-0.96922726	-3.87756000
H	4.06322635	-5.19986578	-3.69687512
H	6.38154500	-2.97641985	-6.57715407
N	5.90224048	-5.42453350	-5.67777799
O	5.59720669	-6.48872629	-5.13503070
O	6.74549632	-5.33220552	-6.58007998

C	2.71552716	-3.12821100	-2.53304842
O	2.27241454	-2.00477380	-2.16849424
O	2.43426946	-4.27194392	-2.10117663
H	1.52293036	-1.95540974	-1.57063417

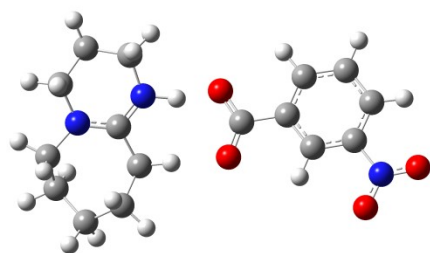
R1-TS:



C	-2.35553400	1.15677400	0.48196600
C	-2.96337000	-0.16044500	0.03139200
C	-2.88067700	2.42409400	-0.21462200
C	-5.29633100	0.78396300	-0.24653000
C	-4.15589100	2.99054600	0.42475500
C	-5.15790600	1.88996500	0.80555100
H	-2.48294700	1.24222900	1.57041800
H	-5.31312400	1.21792300	-1.25793900
H	-3.04946100	2.20975600	-1.27792700
H	-4.62853300	3.70003200	-0.26683600
H	-1.27999100	1.07334300	0.29409800
H	-2.08718900	3.17856000	-0.19054200
H	-6.26516700	0.29548000	-0.10627800
H	-3.89934000	3.56248200	1.32556200
H	-6.14991600	2.33354700	0.95466700
H	-4.88712300	1.42637700	1.76165500
N	-4.30385000	-0.30978700	-0.18483300
N	-2.11546200	-1.14828400	-0.10174200
C	-2.50887900	-2.49748900	-0.49600400

H	-1.84141200	-3.19596100	0.01890900
C	-3.96994400	-2.76164000	-0.15841900
C	-4.81015500	-1.60141500	-0.68132300
H	-2.33104600	-2.62451200	-1.57318200
H	-4.31491400	-3.70026600	-0.60467200
H	-4.09492700	-2.84343100	0.92780600
H	-5.84740200	-1.70228900	-0.34661500
H	-4.82270500	-1.60006000	-1.78172300
C	4.41429200	-2.10226200	0.65617700
C	3.04346500	-1.85096700	0.55663800
C	2.57539300	-0.58940100	0.16811000
C	3.49058800	0.42532400	-0.12302500
C	4.85149400	0.15426600	-0.01958400
C	5.33463300	-1.09726100	0.36713000
H	4.76835900	-3.08343600	0.95950400
H	2.31650200	-2.62457300	0.77855800
H	3.13368800	1.40209600	-0.42330700
H	6.40322800	-1.25974700	0.43375500
N	5.81884600	1.22000400	-0.32693300
O	5.37751600	2.31689200	-0.66706500
O	7.01764200	0.95196300	-0.22600800
C	1.09436200	-0.29410200	0.05540400
O	0.32107900	-1.29410800	0.33986300
O	0.72722600	0.83938600	-0.28162200
H	-0.90425900	-1.07384800	0.13161500

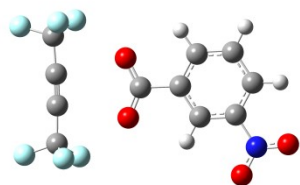
R1-FS:



C	-0.92105400	-1.48014000	-0.41905800
C	0.36995300	-0.72079400	-0.13643100
C	-2.09835000	-1.18899000	0.53080100
C	-0.84225800	1.47462200	0.27234200
C	-2.95849200	0.00421200	0.08325800
C	-2.12872000	1.15904300	-0.50187100
H	-1.23120000	-1.30391300	-1.45899700
H	-1.03884500	1.43507600	1.35897300
H	-1.70748500	-1.01644000	1.54222600
H	-3.54872900	0.36782900	0.93491700
H	-0.63048300	-2.53014800	-0.35349500
H	-2.73073400	-2.08185600	0.60533400
H	-0.56433400	2.51232000	0.05558700
H	-3.68327400	-0.32442600	-0.67332700
H	-2.74448300	2.06714200	-0.51944000
H	-1.85834800	0.95544900	-1.54469500
N	0.34275700	0.67804700	-0.07708200
N	1.42163000	-1.45903100	-0.03946700
C	2.72389200	-0.84740100	0.18562600
H	3.47819000	-1.45522100	-0.33057800
C	2.79618800	0.60592800	-0.28287700
C	1.59376300	1.35788500	0.27515900
H	2.96782600	-0.91105100	1.25798900
H	3.72517800	1.09066500	0.04080400
H	2.76841300	0.64253200	-1.37911800

H	1.55098400	2.37556700	-0.13303100
H	1.68708400	1.45717700	1.37099200
C	4.74818165	-3.06262624	-5.11486873
C	3.81238113	-3.11530862	-4.07742759
C	3.44812183	-4.33314616	-3.49198859
C	4.03713699	-5.51129169	-3.96109971
C	4.97001818	-5.44494053	-4.99481909
C	5.34013011	-4.23202945	-5.58622453
H	5.01910328	-2.10773174	-5.55988980
H	3.33292563	-2.22207043	-3.68798716
H	3.74986472	-6.45270895	-3.50730228
H	6.06818337	-4.22926302	-6.38758123
N	5.58887885	-6.67737667	-5.48820515
O	5.28384506	-7.74156946	-4.94545786
-O	6.43213469	-6.58504869	-6.39050714
C	2.40216553	-4.38105417	-2.34347558
O	1.95905291	-3.25761697	-1.97892140
O	2.12090783	-5.52478709	-1.91160379
H	1.34345753	-2.45280473	-0.11885742

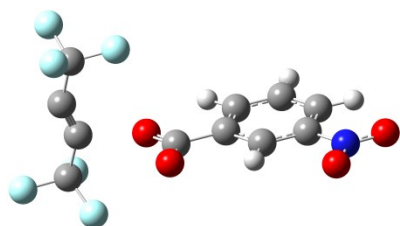
R2-IS:



C	-2.63283639	2.36578467	-1.03084825
C	-1.37021239	1.77912167	-0.95859325
C	-1.16005439	0.64389067	-0.16277525

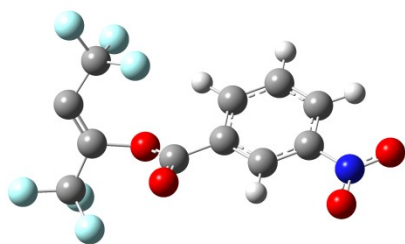
C	-2.21906539	0.09233167	0.56491375
C	-3.46899539	0.69648567	0.47498275
C	-3.69789939	1.82561367	-0.31069025
H	-2.79062239	3.24496767	-1.64762325
H	-0.52982739	2.18482867	-1.51186425
H	-2.08280739	-0.78249333	1.18656875
H	-4.69083539	2.25677967	-0.34566925
N	-4.59192739	0.12175867	1.23853675
O	-4.36458039	-0.87402733	1.92267975
O	-5.68602839	0.67563467	1.14256075
C	0.21025561	0.05804267	-0.12387325
O	1.15766461	0.49757567	-0.74726925
O	0.29929861	-1.02173333	0.67922775
C	3.30148000	0.71750300	0.32077300
C	3.41325100	-0.44933300	0.11855700
C	3.51682100	-1.88293200	-0.15228400
C	3.12523900	2.15714800	0.55454300
F	1.82987400	2.44709800	0.75813500
F	4.58896000	-2.41904400	0.44740200
F	2.42122600	-2.53898500	0.33009100
F	3.59177900	-2.13294500	-1.46374600
F	3.81861100	2.55152200	1.63697300
F	3.55657200	2.86645100	-0.50070200

R2-TS:



C	-3.06738200	-0.47647700	2.24089300
C	-1.77895400	-0.55303100	1.70176600
C	-1.55492500	-0.33151000	0.33779900
C	-2.63925100	-0.03241100	-0.49061700
C	-3.91738300	0.03598000	0.06156800
C	-4.15404800	-0.18104500	1.42266900
H	-3.22669000	-0.64839400	3.30270800
H	-0.91849300	-0.78495400	2.32070700
H	-2.46129900	0.14112400	-1.54466500
H	-5.16448300	-0.11562100	1.80652200
N	-5.06098700	0.34525700	-0.80381300
O	-4.85278400	0.52883100	-2.00388300
O	-6.18226400	0.40609700	-0.28538800
C	-0.14541600	-0.41520200	-0.26839000
O	0.75190800	-0.74736900	0.58548000
O	-0.02659600	-0.16724800	-1.47409800
C	2.70112800	-0.42893100	-0.07378100
C	3.19935200	0.70167200	-0.09435400
C	2.99604800	2.12263700	0.10891200
C	2.94802000	-1.87269600	-0.24197800
F	2.14269700	-2.45692100	-1.14382900
F	3.43133500	2.85657600	-0.95103900
F	1.70484600	2.48886900	0.31161000
F	3.68982300	2.56695500	1.19537500
F	4.22534300	-2.07666000	-0.67002200
F	2.82291400	-2.55496900	0.91764000

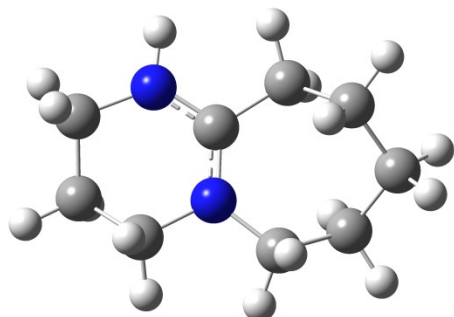
R2-FS:



C	-2.48279800	1.56165400	1.47270100
C	-1.26668100	1.02782900	1.03851900
C	-1.24767500	-0.04606100	0.13698000
C	-2.44943100	-0.57410300	-0.34000800
C	-3.64907100	-0.03680300	0.12078900
C	-3.68850900	1.02789700	1.02449400
H	-2.49046800	2.40061700	2.16291900
H	-0.32136700	1.44729200	1.36437300
H	-2.43777300	-1.38395200	-1.05856900
H	-4.64573600	1.41613000	1.34943100
N	-4.91742700	-0.59818500	-0.35972500
O	-4.87267300	-1.54259100	-1.14866200
O	-5.96610700	-0.09420900	0.05431000
C	0.04998800	-0.62283400	-0.36721400
O	1.03371800	-0.37672100	0.49939400
O	0.12358600	-1.22560200	-1.41992500
C	2.45830200	-0.35700700	0.03651500
C	3.10441700	0.70890900	-0.37688000
C	2.37619200	1.97782000	-0.47725700
C	3.04184300	-1.69702900	0.34752700
F	2.35399700	-2.72884000	-0.21244800
F	3.06085000	2.95077700	-1.15681300
F	1.14986900	1.94281800	-1.12235100
F	2.11490000	2.53535200	0.75672400
F	4.32055000	-1.81346100	-0.05590200

F	3.03202000	-1.95347100	1.69323400
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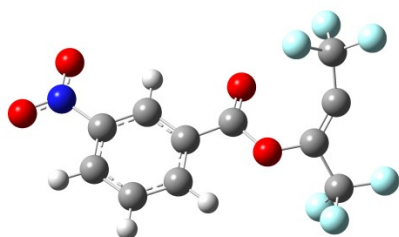
R3-IS-DBU:



C	-0.41753655	0.83507306	0.00000000
C	0.03595245	2.19302506	0.48094200
C	0.29440845	0.33647706	-1.27301400
C	2.47417445	1.81136706	0.11613200
C	1.62548745	-0.37630194	-0.97555400
C	2.43009145	0.27957606	0.16054500
H	-0.27869055	0.13268306	0.82951400
H	2.61266145	2.16972906	-0.91346900
H	0.45640545	1.18180606	-1.95387000
H	2.23036445	-0.40587894	-1.88991200
H	-1.49973955	0.89220206	-0.14455100
H	-0.38044855	-0.34357994	-1.80184300
H	3.34369845	2.15241406	0.68422800
H	1.43070545	-1.42003194	-0.70169200
H	3.46549345	-0.07690894	0.12154000
H	2.04598445	-0.02815994	1.14007000
N	1.31594045	2.51680506	0.72085800
N	-0.92985355	3.04808706	0.74649000
C	-0.81208155	4.36157606	1.36593700
H	-1.67483255	4.44975606	2.02779300

C	0.51397445	4.40752406	2.11341700
C	1.63180045	3.87537306	1.21901600
H	-0.87563655	5.13596406	0.59158500
H	0.74369145	5.42819106	2.43180300
H	0.44426545	3.78329806	3.01042200
H	2.56504945	3.79728706	1.78356800
H	1.81515145	4.54201006	0.36518800

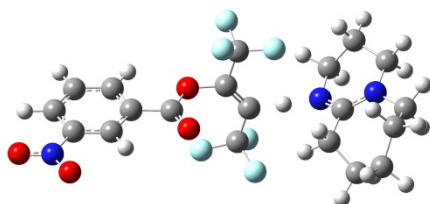
R3-IS-ArCOOC4F6:



C	-5.03906100	1.76322600	0.81811600
C	-3.64798200	1.64813400	0.80305400
C	-3.04139400	0.47460300	0.33371900
C	-3.83142000	-0.58386000	-0.12162700
C	-5.21395700	-0.44663900	-0.09373500
C	-5.83721600	0.71275000	0.36942700
H	-5.50362100	2.67513200	1.18016100
H	-3.02280100	2.46279500	1.14960700
H	-3.37009000	-1.49095700	-0.48980400
H	-6.91848300	0.77292700	0.37039200
N	-6.04945500	-1.56206000	-0.57007500
O	-5.47764400	-2.57394200	-0.97185500
O	-7.27115000	-1.41391400	-0.53655000
C	-1.55522400	0.30430400	0.29383000
O	-0.91746100	1.36014300	0.81656800
O	-1.01949900	-0.68966000	-0.16605300
C	0.54378500	1.36193700	0.77214700

C	1.32513500	1.80617600	-0.19529500
C	0.75015000	2.30498700	-1.44859200
C	1.00345000	0.88446000	2.12095700
F	0.36982500	-0.26352100	2.50548100
F	1.34796600	1.65815700	-2.55206100
F	-0.58753900	2.15690100	-1.71784200
F	1.00948300	3.62131600	-1.62781400
F	2.32783300	0.60459600	2.15695900
F	0.76511300	1.78400800	3.10269500

R3-TS:

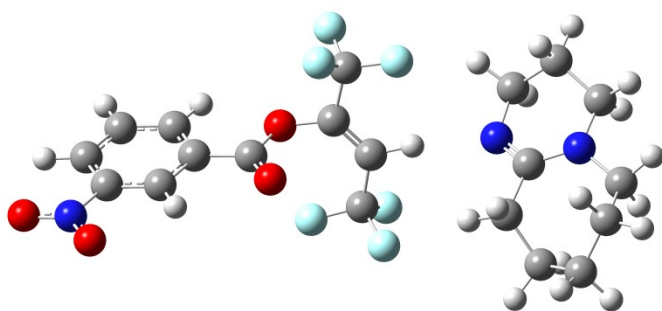


C	-5.67053200	-1.72690800	0.29748500
C	-4.28940600	-1.54167400	0.21416200
C	-3.76574000	-0.28613700	-0.12622200
C	-4.62760100	0.78477500	-0.38402400
C	-5.99788500	0.57329400	-0.29515000
C	-6.53917400	-0.66753000	0.04262900
H	-6.07198200	-2.70015300	0.56223800
H	-3.61258500	-2.36459300	0.41242000
H	-4.23050200	1.75711000	-0.64641800
H	-7.61468600	-0.78162000	0.09942900
N	-6.91206800	1.69742100	-0.56695500
O	-6.41212100	2.77902900	-0.86797300
O	-8.12014300	1.48132300	-0.47570500
C	-2.30063200	-0.02416700	-0.22922600

O	-1.57353400	-1.15417600	0.03502600
O	-1.81218600	1.04366400	-0.50818600
C	-0.17320900	-1.06430300	-0.03760500
C	0.64945700	-0.65008000	0.91760400
C	0.19003500	-0.13535400	2.23825000
C	0.28793900	-1.62082500	-1.36144900
F	-0.36014600	-1.03834100	-2.39207600
F	0.69539600	1.11182100	2.45083800
F	-1.14678800	-0.03960600	2.43591100
F	0.67007000	-0.92177000	3.23368100
F	1.61099800	-1.44593900	-1.56100900
F	0.04166500	-2.94936600	-1.44532300
C	3.29731700	1.66571700	0.16563200
C	3.96029000	0.29506400	0.15132900
C	4.18600600	2.83445800	0.63100400
C	6.13770400	1.16707800	-0.81134900
C	5.00365100	3.46348400	-0.50742000
C	5.56443500	2.41949600	-1.48590500
H	2.88951500	1.87618100	-0.83231000
H	6.72516400	1.44895900	0.07729700
H	4.85224300	2.48550100	1.43086800
H	5.82657900	4.05221000	-0.08180300
H	2.44207200	1.57289500	0.83490000
H	3.54918400	3.59971500	1.08846200
H	6.84161800	0.69728500	-1.50529000
H	4.37727200	4.16920600	-1.06759700
H	6.36647000	2.87564400	-2.07900600
H	4.79829200	2.10530700	-2.20439600
N	5.17371500	0.10491500	-0.46488200
N	3.26831900	-0.65507900	0.71245400

C	3.75719600	-2.02843100	0.74682200
H	2.88110500	-2.68848700	0.73171200
C	4.68893500	-2.32217700	-0.42384200
C	5.76453700	-1.24329000	-0.47175000
H	4.26972000	-2.20626300	1.70320000
H	5.15824300	-3.30731500	-0.32643300
H	4.11318400	-2.31479300	-1.35595600
H	6.36057900	-1.33918800	-1.38633000
H	6.45681700	-1.35397200	0.37787100
H	1.91512500	-0.61928700	0.81346500

R3-FS:



C	-5.96966300	1.33527400	-1.03788300
C	-4.59459500	1.25884000	-0.81219900
C	-4.06809200	0.23124200	-0.01566300
C	-4.92003500	-0.72023000	0.55576000
C	-6.28432100	-0.61988100	0.31513800
C	-6.82857000	0.39356900	-0.47414100
H	-6.37400800	2.13154700	-1.65483700
H	-3.92674200	1.99189300	-1.24941300
H	-4.52196400	-1.51676000	1.17163000
H	-7.89958900	0.42830300	-0.63144700
N	-7.18945600	-1.61843100	0.91469100
O	-6.68543400	-2.50081300	1.60521800

O	-8.39220700	-1.50250500	0.68417600
C	-2.61298000	0.09411400	0.26363100
O	-1.89001600	1.08764400	-0.36815400
O	-2.10883200	-0.76113700	0.94487400
C	-0.52144100	1.13315100	-0.16241600
C	0.39136400	0.40706300	-0.79886800
C	0.11961300	-0.64512800	-1.82841400
C	-0.17252300	2.20183600	0.84730500
F	-0.80309900	1.97127000	2.01605300
F	0.67657100	-1.81971700	-1.45175400
F	-1.18674100	-0.88013600	-2.06509300
F	0.68317800	-0.29703800	-3.00494200
F	1.14717200	2.26516000	1.08747200
F	-0.57475000	3.41411600	0.40957100
C	3.86324300	-1.60847200	0.22762900
C	4.43538300	-0.20771300	0.04149400
C	4.69881500	-2.76656900	-0.35123500
C	6.80198300	-0.94691000	0.60450400
C	5.75178200	-3.30393300	0.62980700
C	6.44515200	-2.18931300	1.43028800
H	3.67516700	-1.78494700	1.29622500
H	7.20589100	-1.24938400	-0.37728100
H	5.18036900	-2.43328000	-1.27986500
H	6.50201300	-3.88451800	0.07702100
H	2.88743200	-1.58105300	-0.25773000
H	4.02485900	-3.58077500	-0.64195000
H	7.61652400	-0.42341300	1.11659200
H	5.28064500	-4.00217700	1.33384600
H	7.37207900	-2.58320500	1.86544600
H	5.82411600	-1.87160000	2.27615600

N	5.74086300	0.05990500	0.44328500
N	3.60777300	0.66336100	-0.43771400
C	4.03045600	2.04615600	-0.63116800
H	3.15818000	2.69124600	-0.47531200
C	5.16890700	2.45359000	0.30089900
C	6.27245600	1.40761000	0.20629900
H	4.33305000	2.18514000	-1.68089300
H	5.56698500	3.44207500	0.04355700
H	4.80026800	2.50263600	1.33288200
H	7.04947600	1.59870400	0.95652800
H	6.76115500	1.46078700	-0.78138600
H	1.45917100	0.55076200	-0.59688500

Notes and references

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