

Supplementary Information

Probing the helical integrity of multivincinal all-*syn*-fluoro alkanes.

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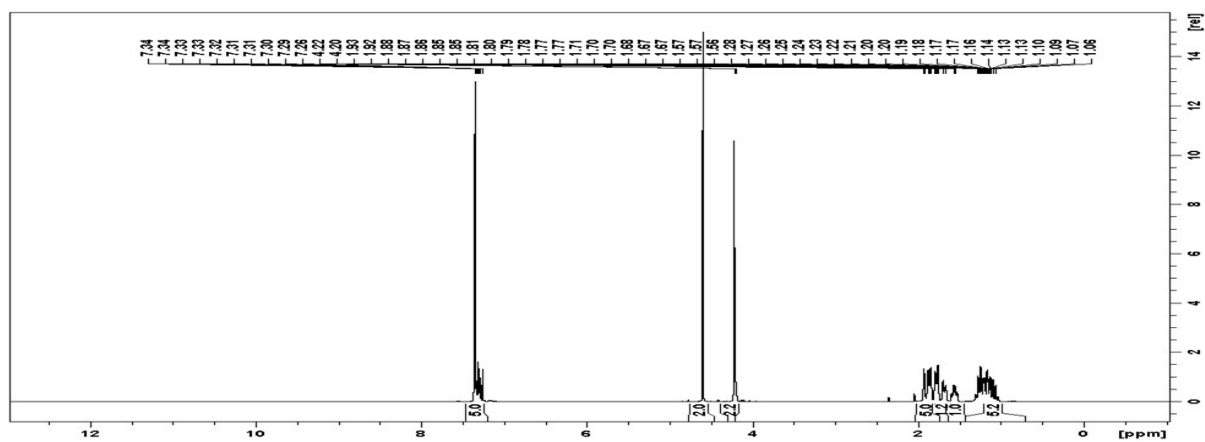
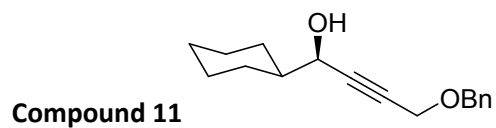
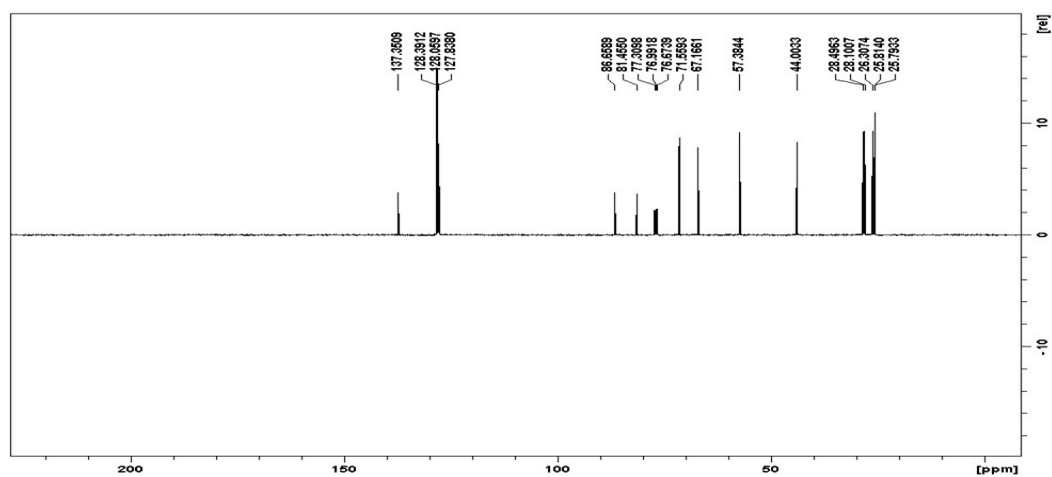
^b. *Department of Chemistry, Faculty of Science, An Najah National University, Nablus, Palestine.*

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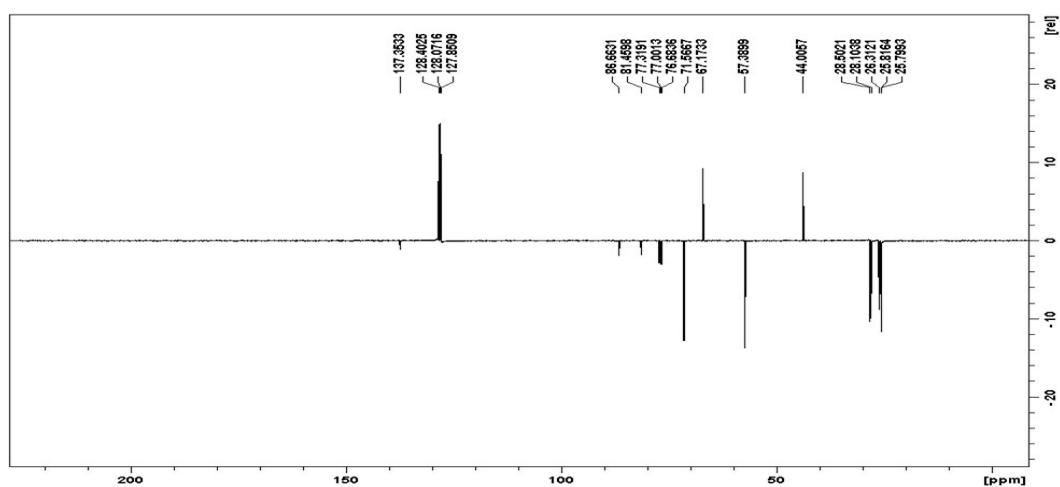
Images of selected NMR Spectra of synthetic intermediates and compound **9**

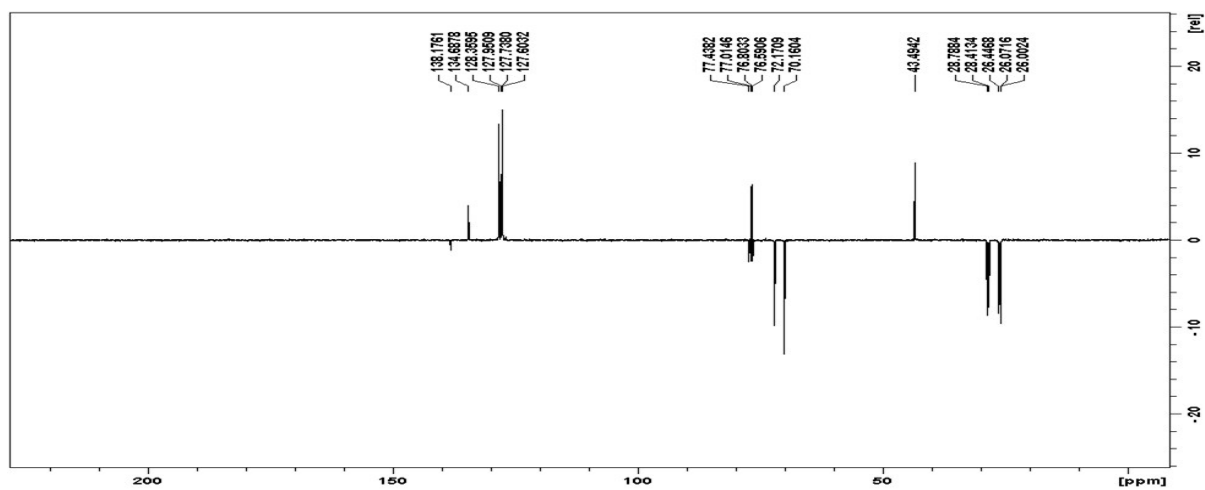
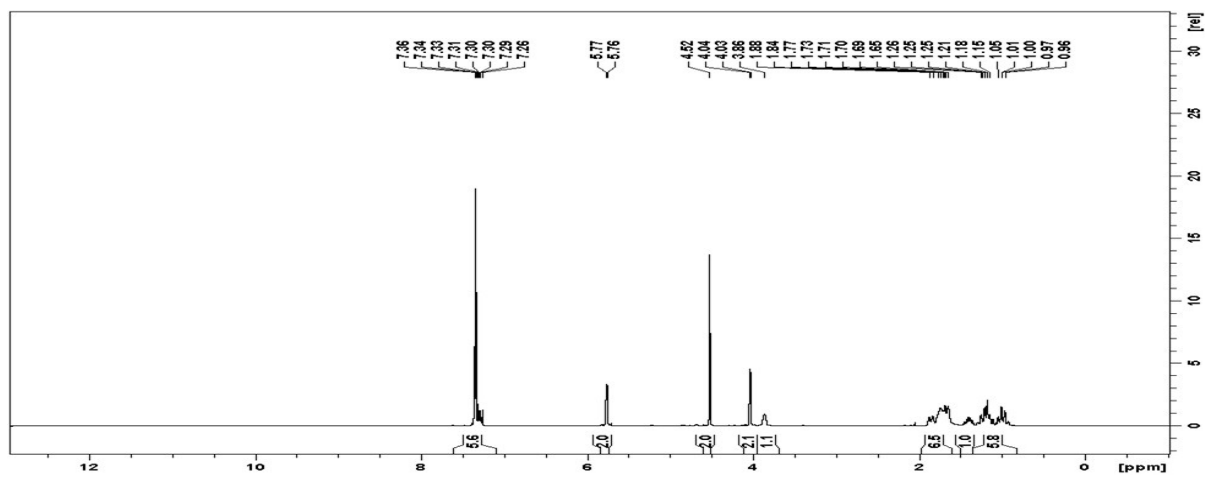
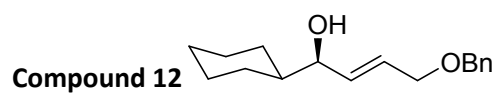
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Details of DFT Computations and coordinates for optimised structures for conformers **9a** - **9d**

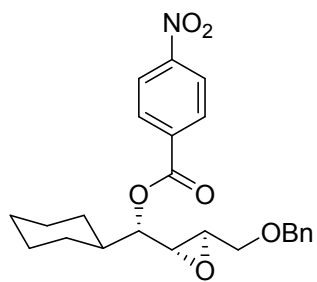
¹H-NMR 11

¹³C-NMR 11

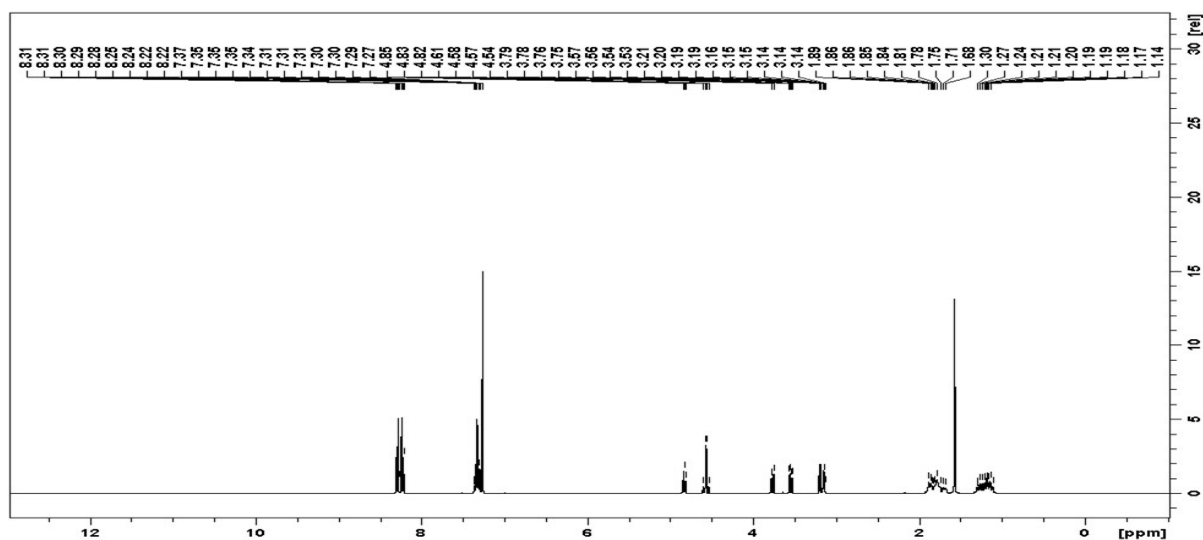
 ^{13}C -NMR DEPT



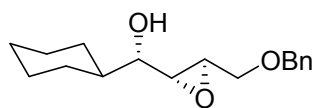




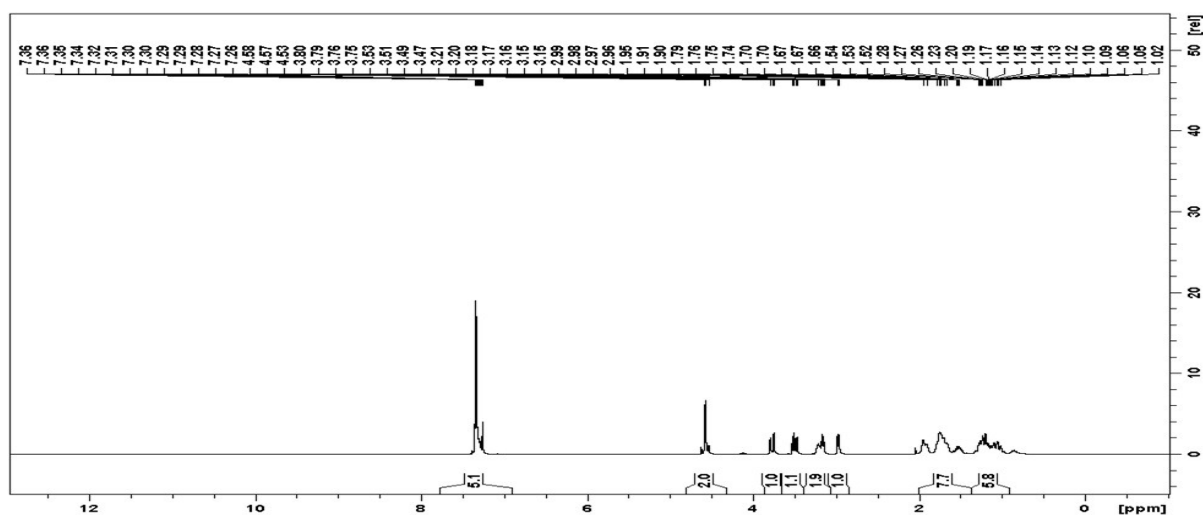
Compound 14



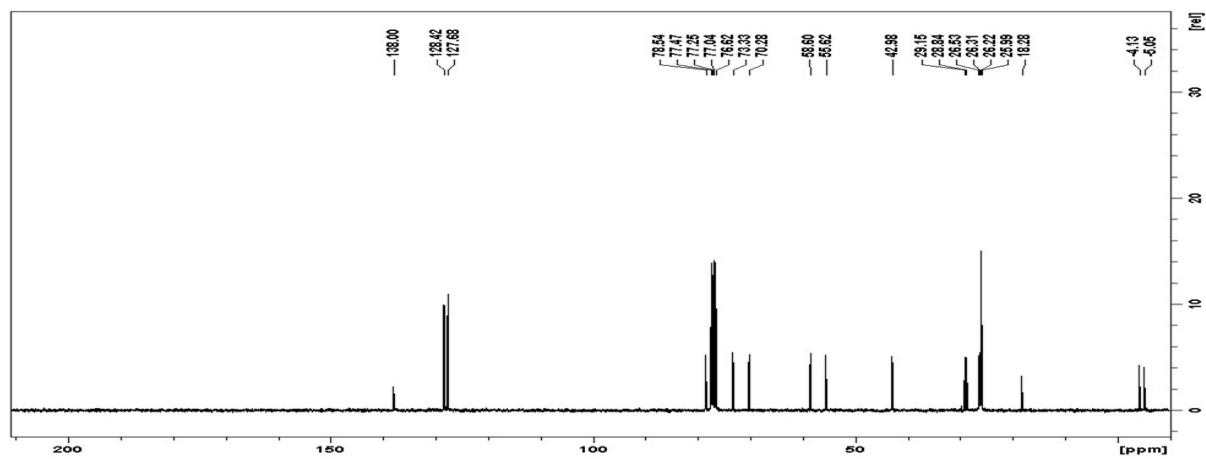
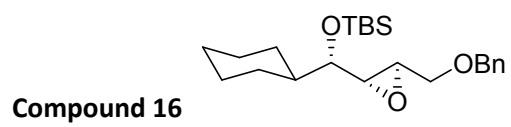
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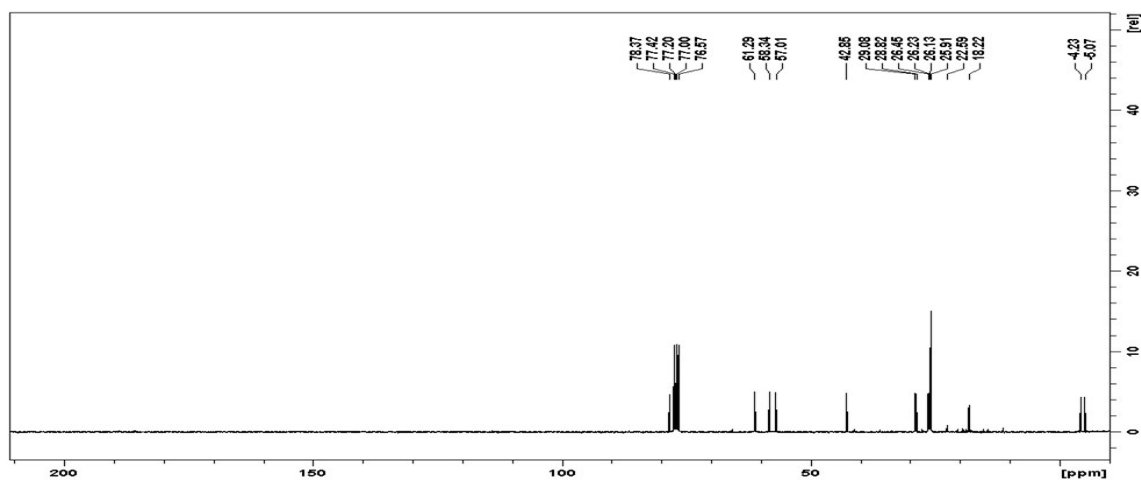
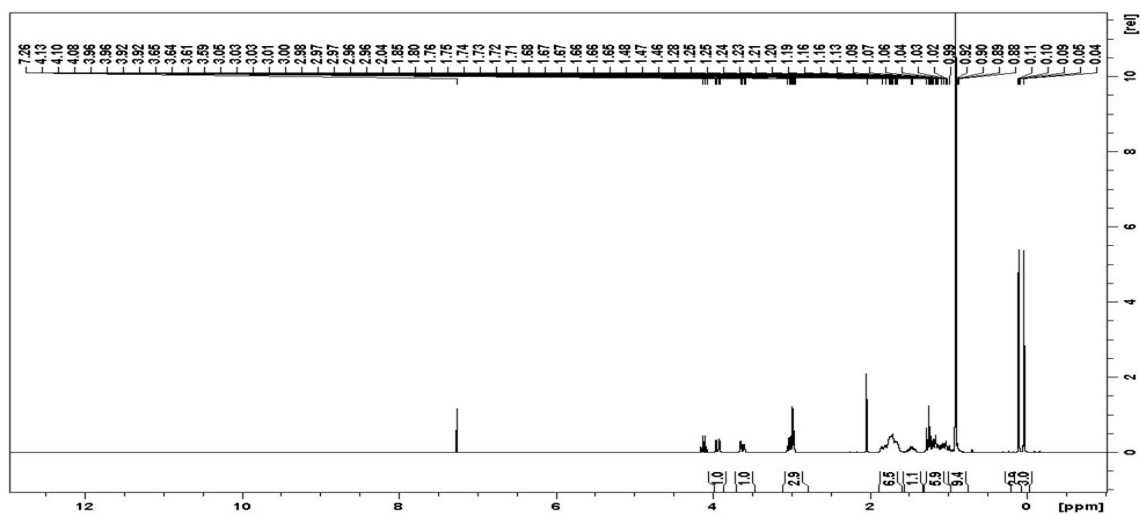
Compound 15

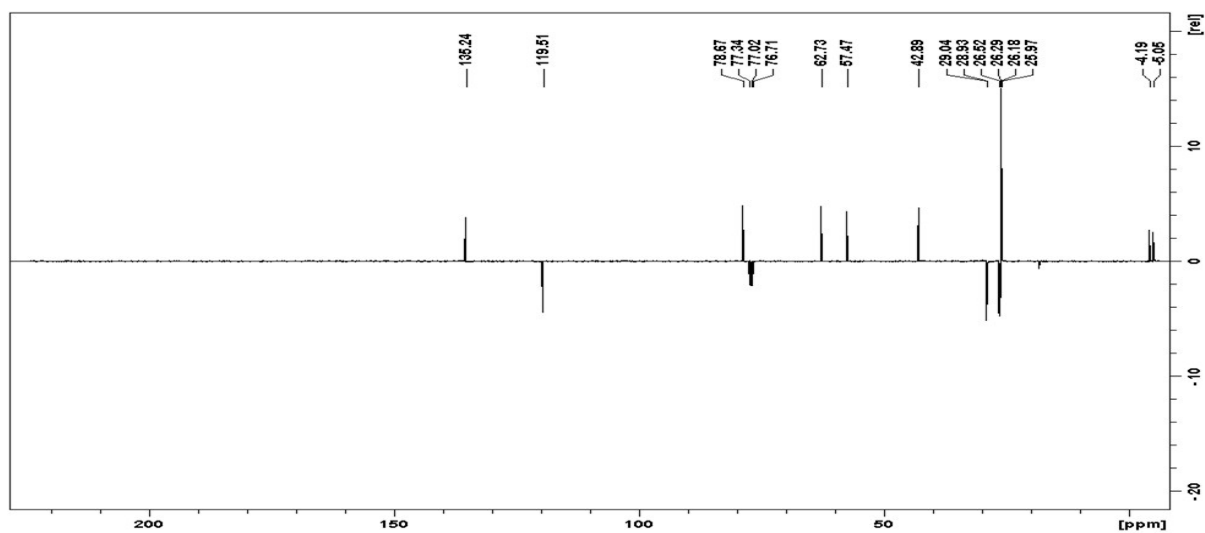
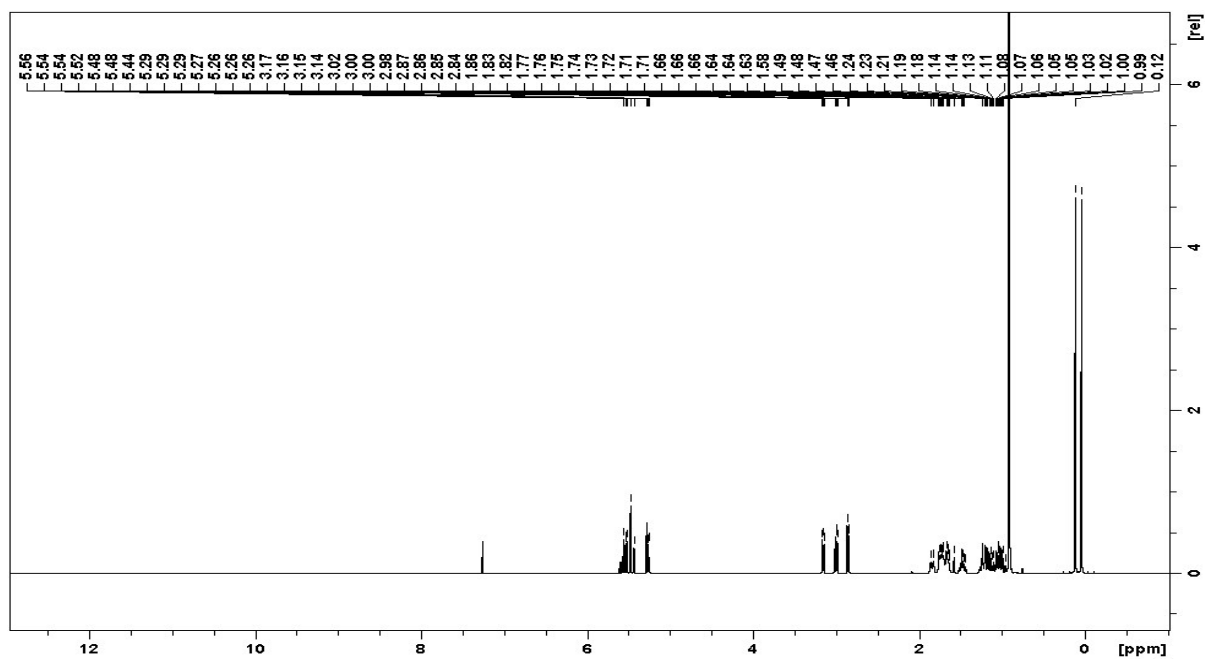
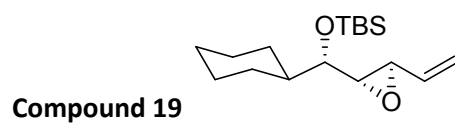


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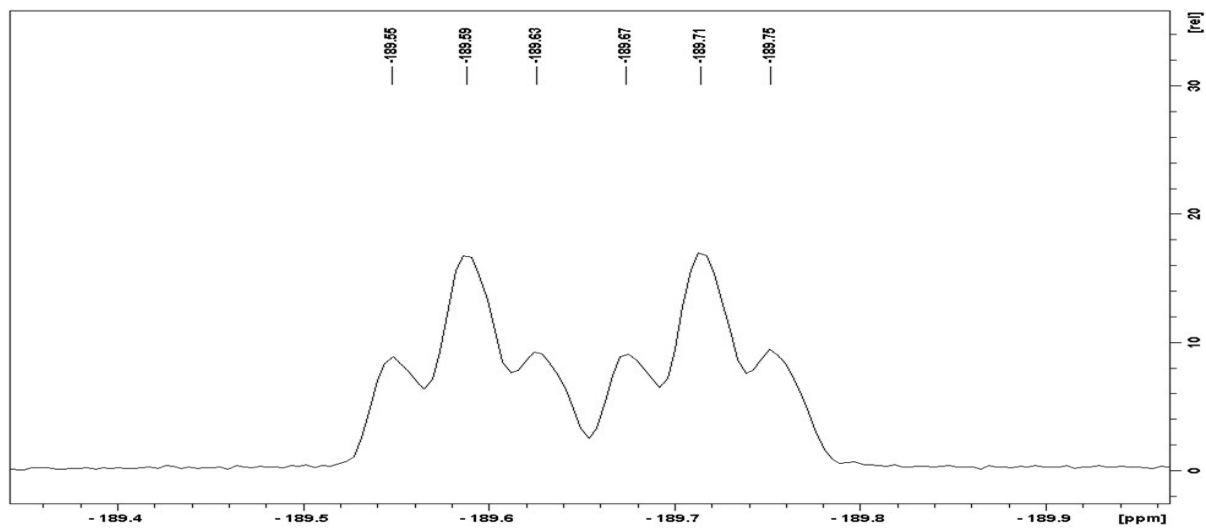


¹H-NMR 16

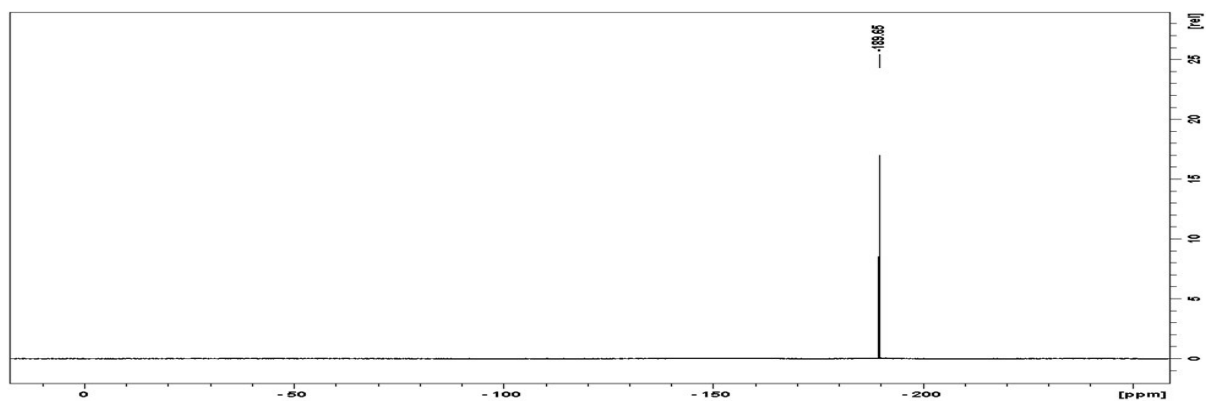




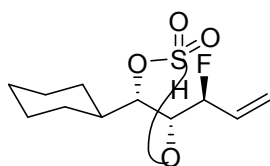




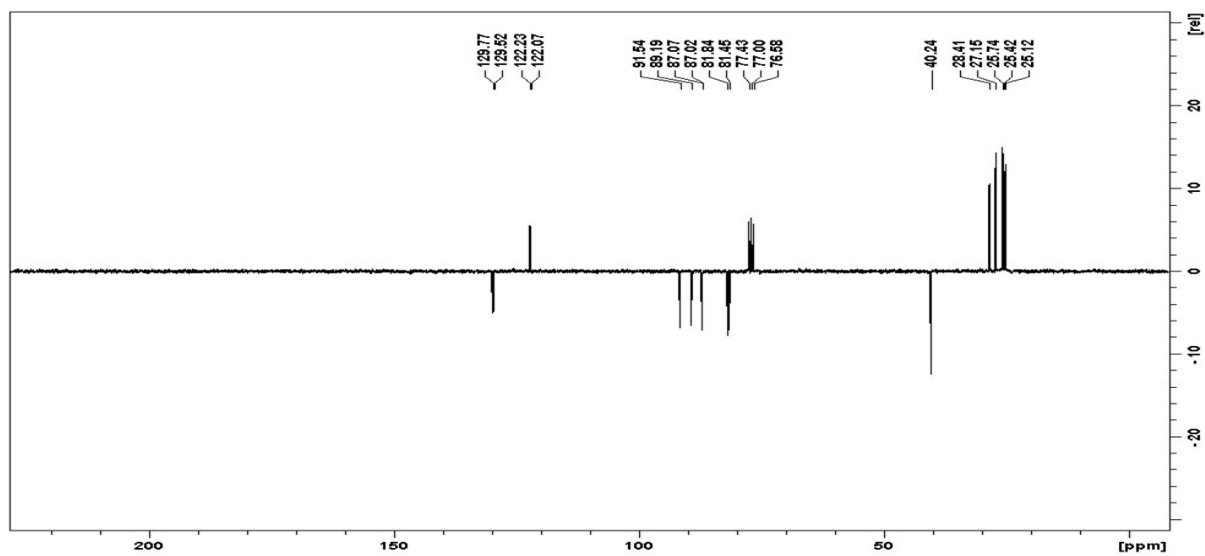
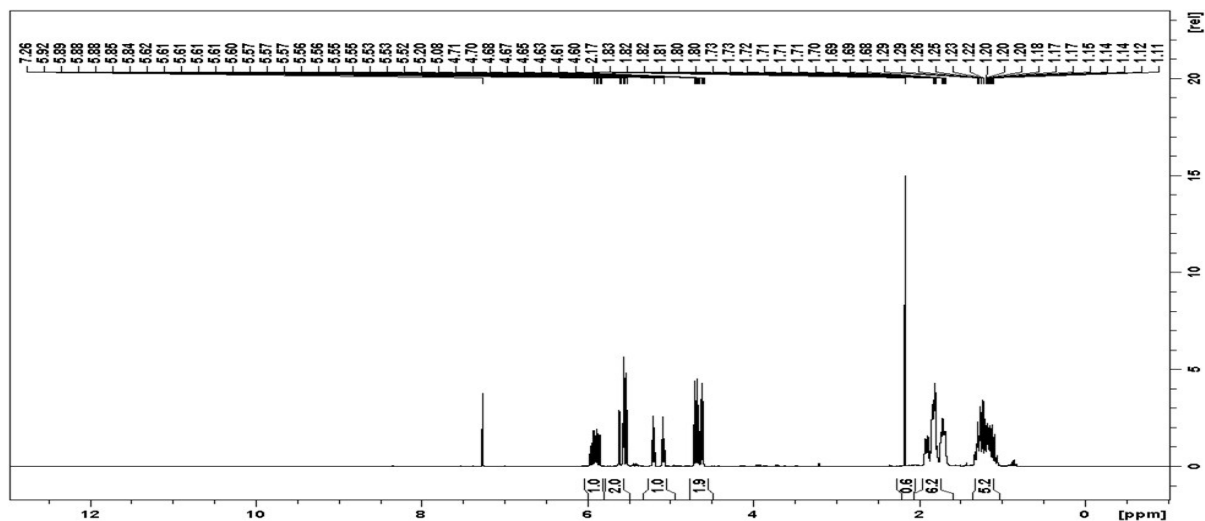
^{19}F -NMR 20

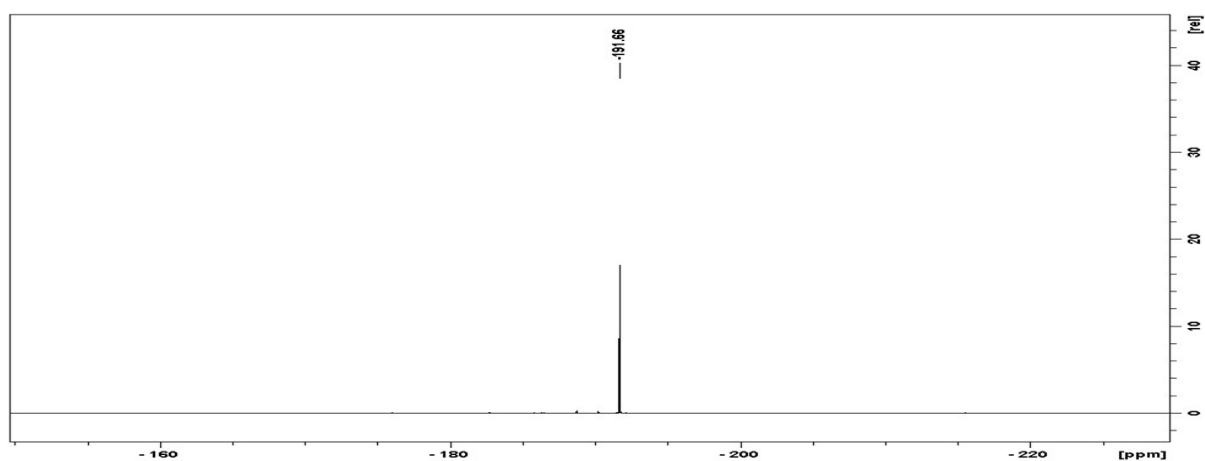


$^{19}\text{F}\{^1\text{H}\}$ -NMR 20

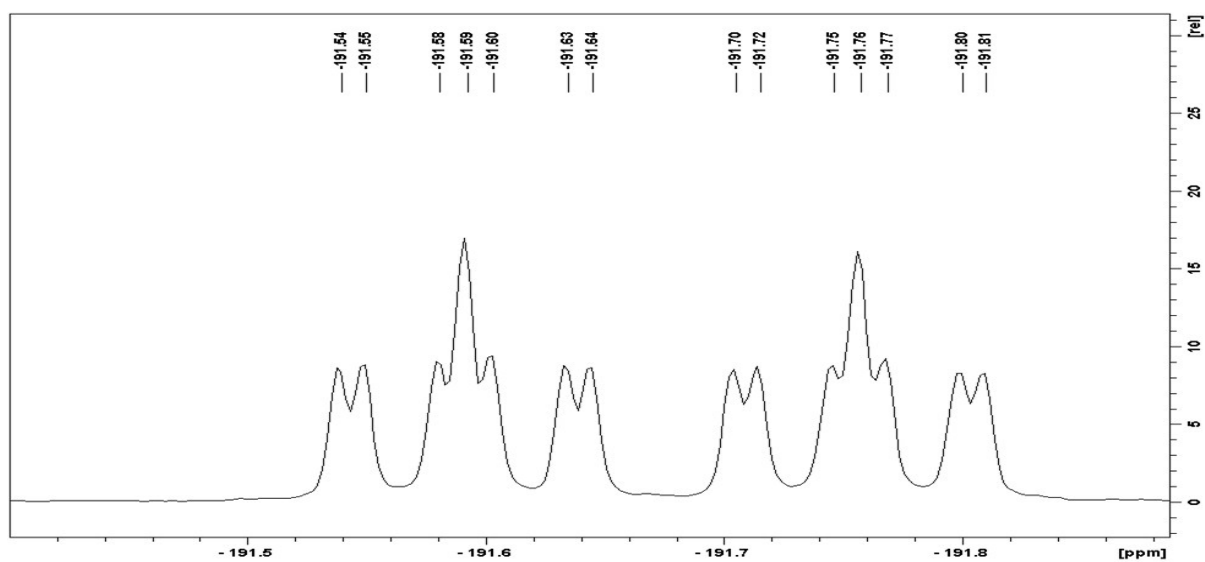


Compound 21

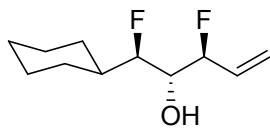




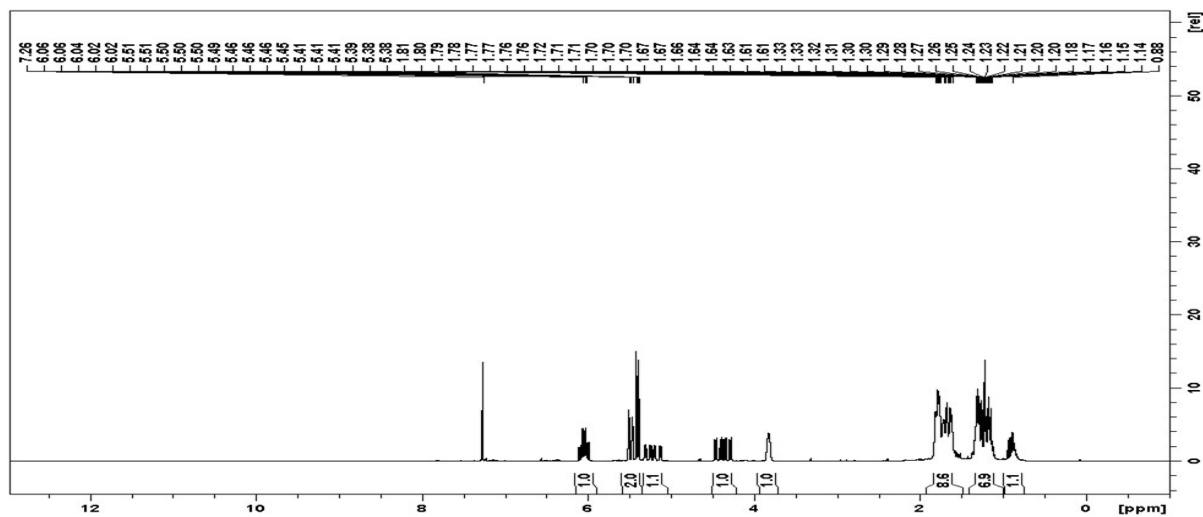
¹⁹F{¹H}-NMR 21



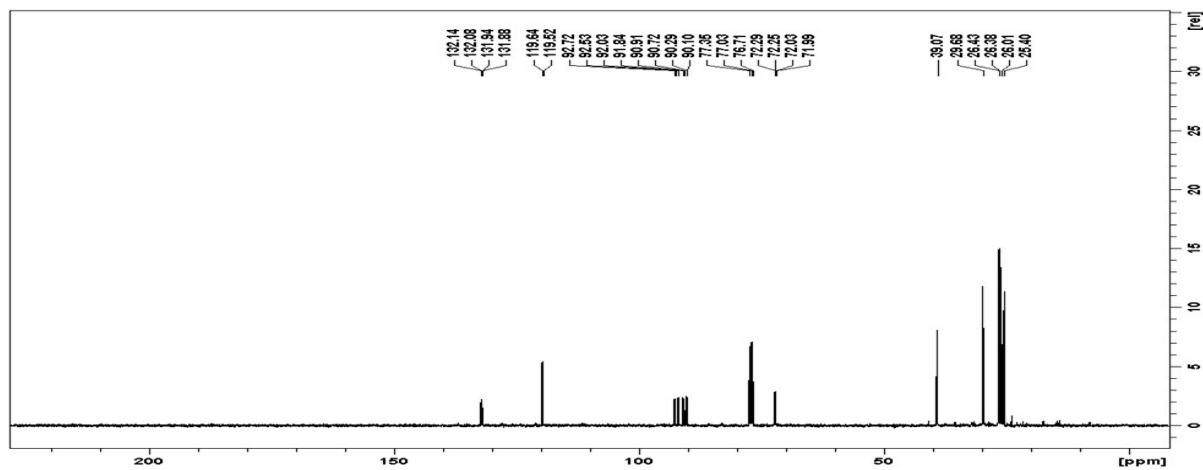
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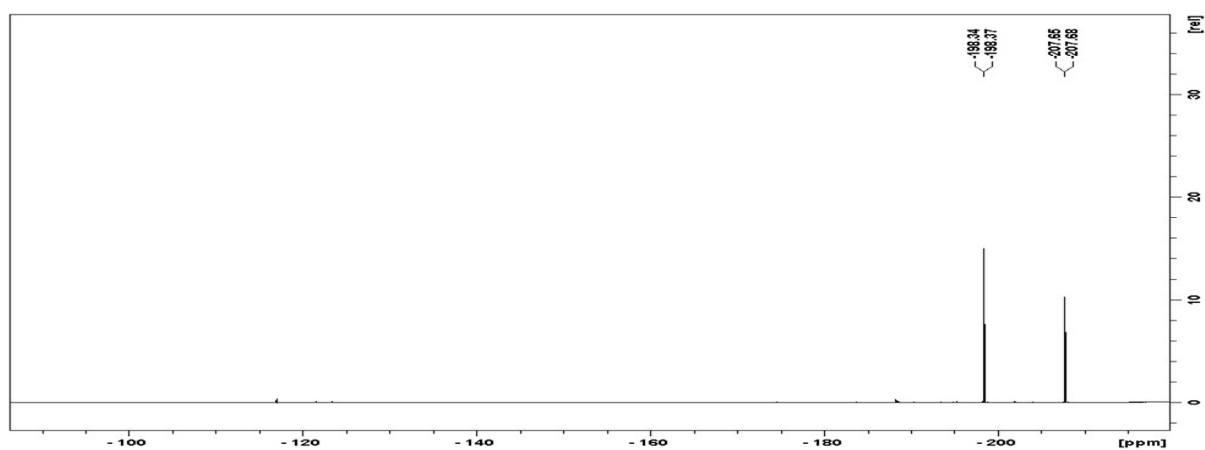
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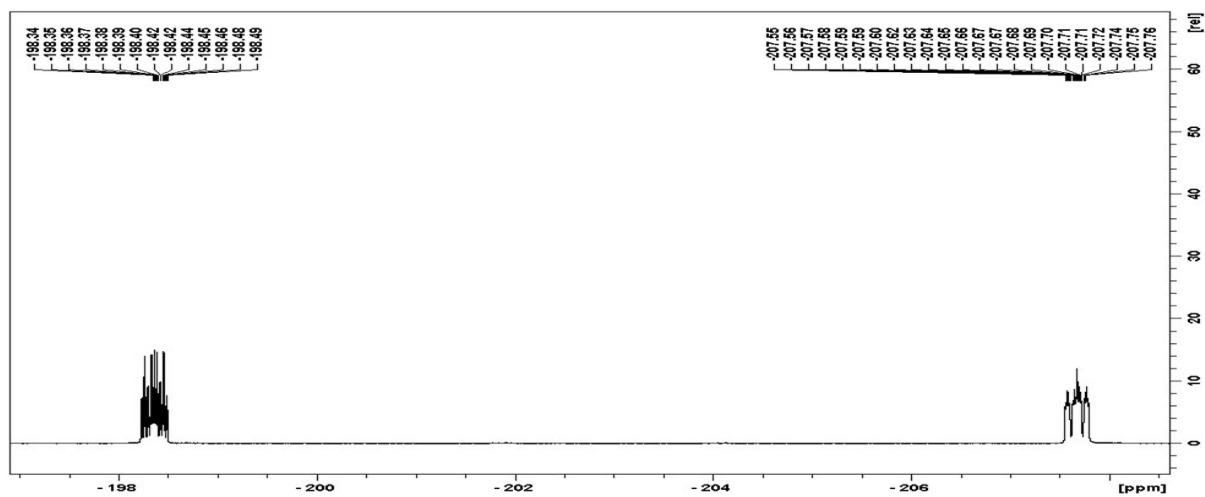
¹H-NMR 22



¹³C-NMR 22

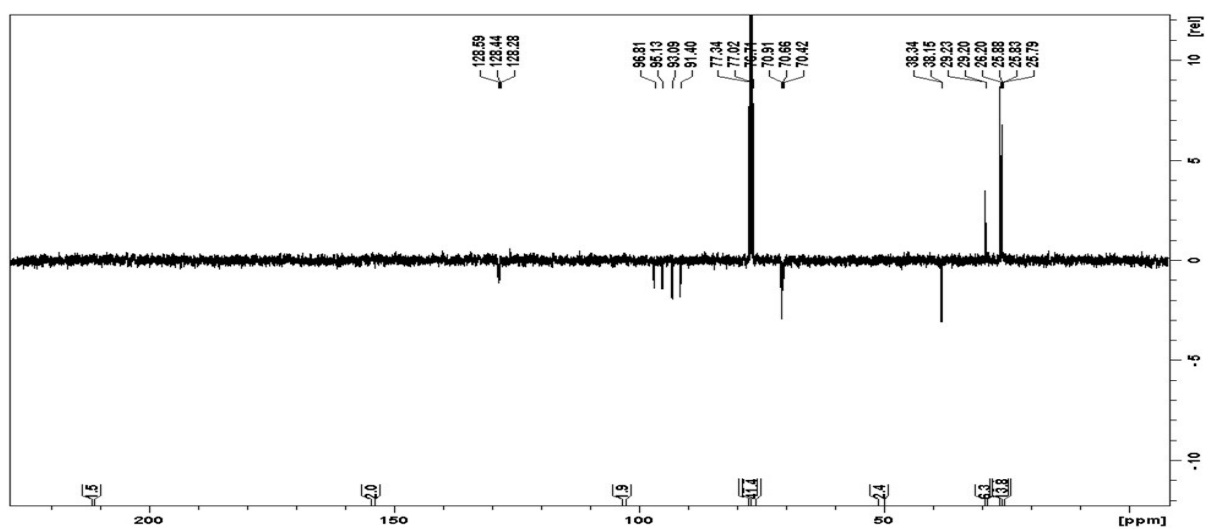
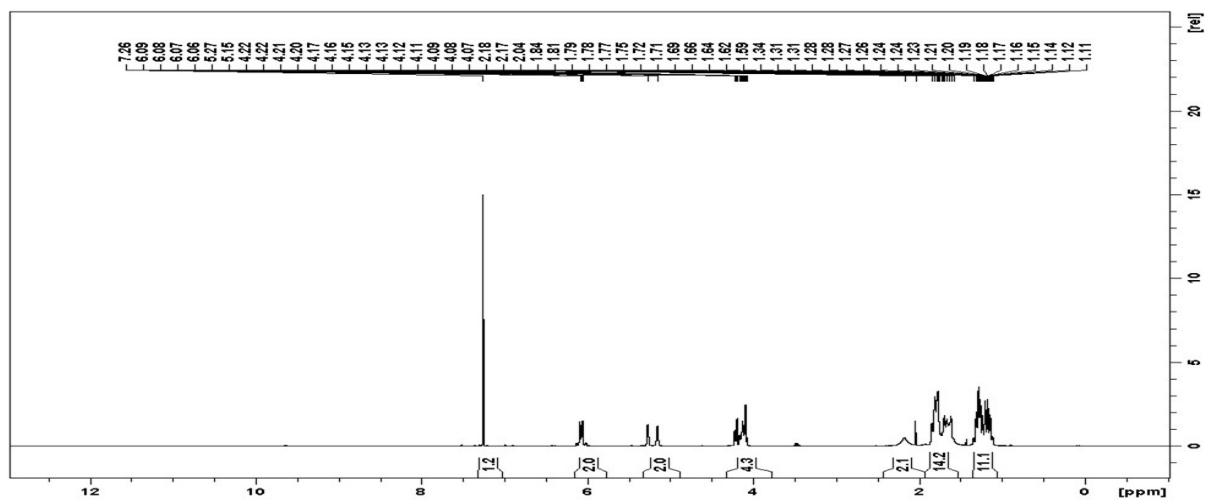
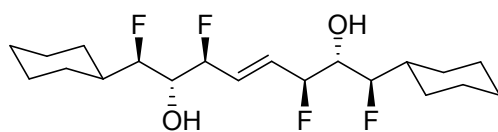


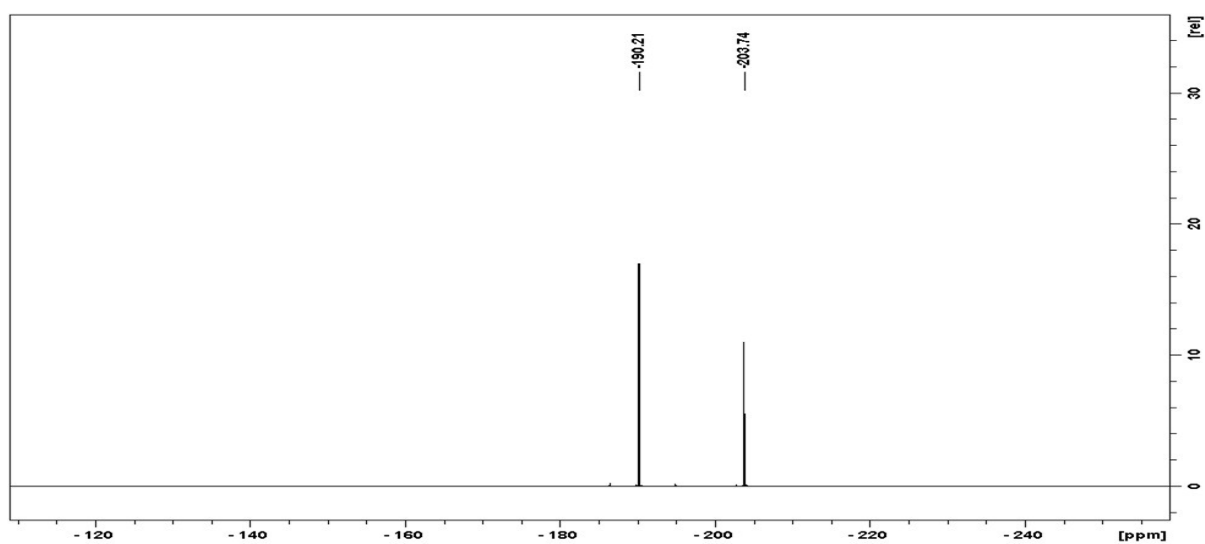
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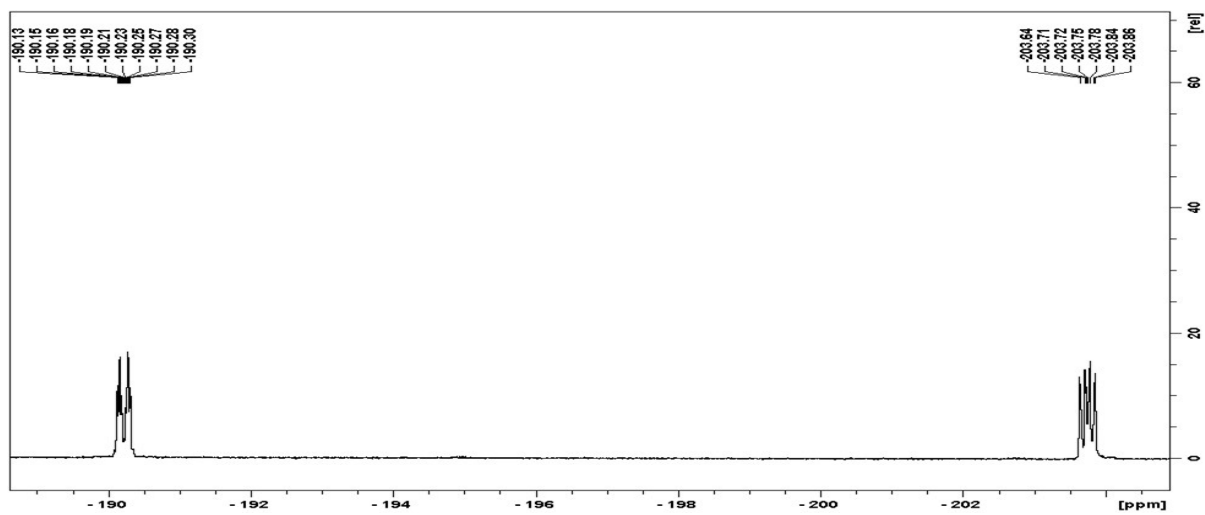
$^{19}\text{F}\{^1\text{H}\}$ -NMR 22

Compound 23



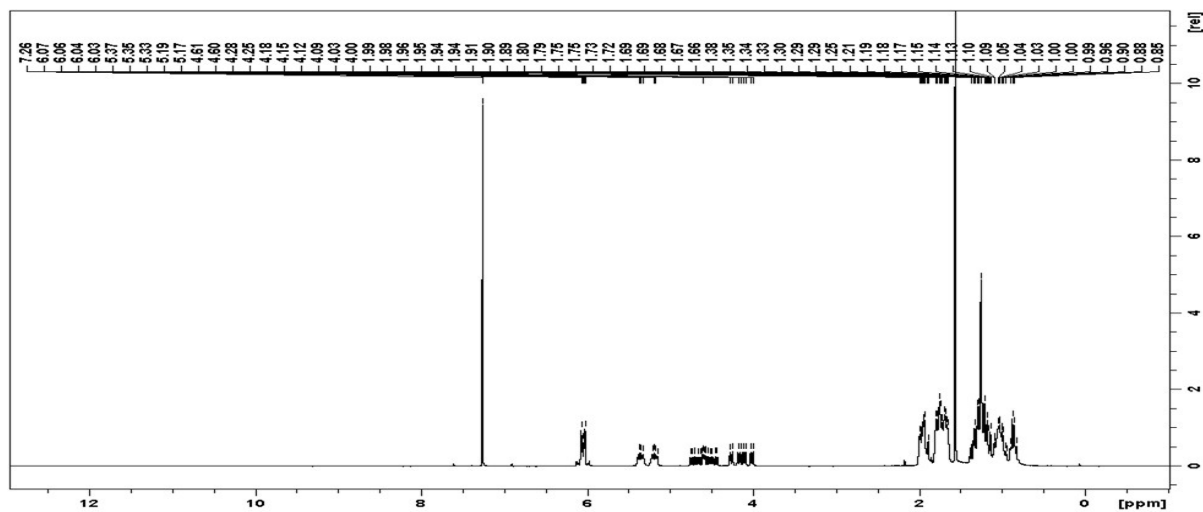
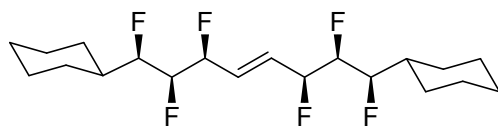


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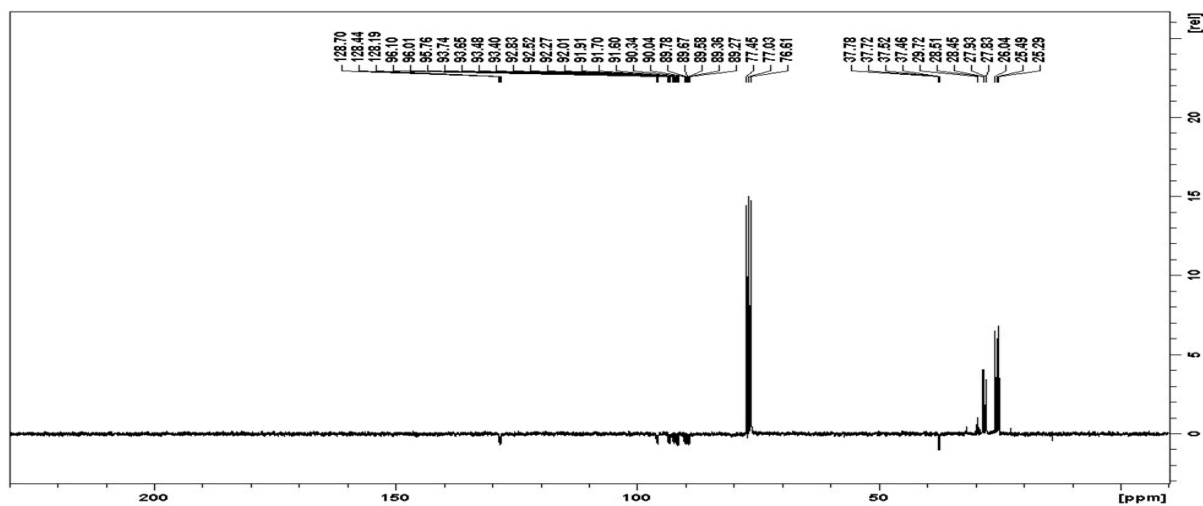


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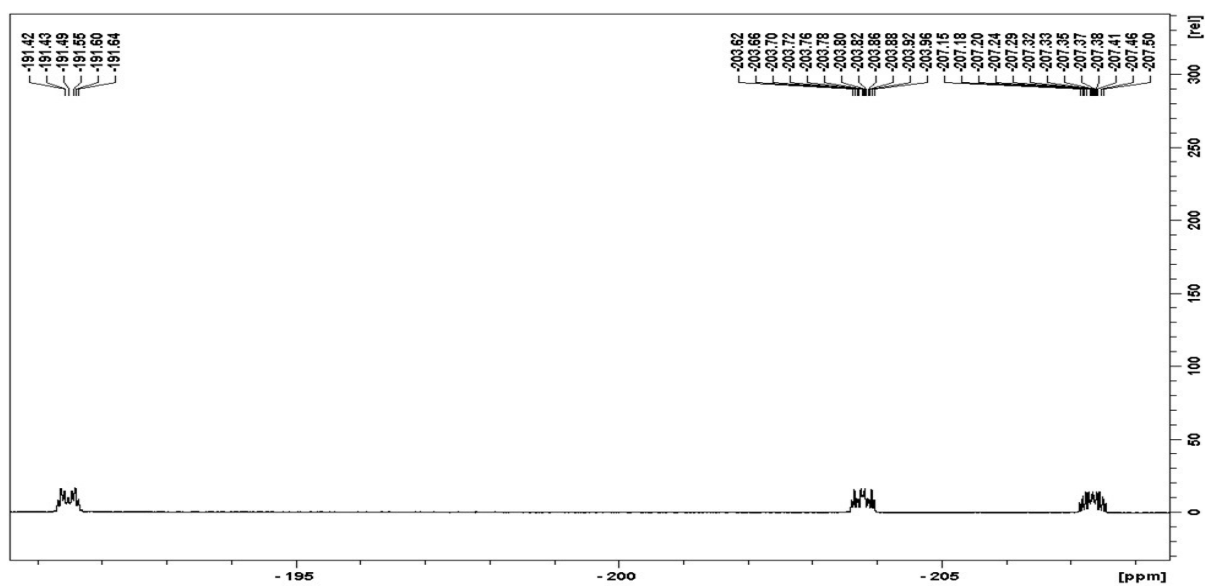
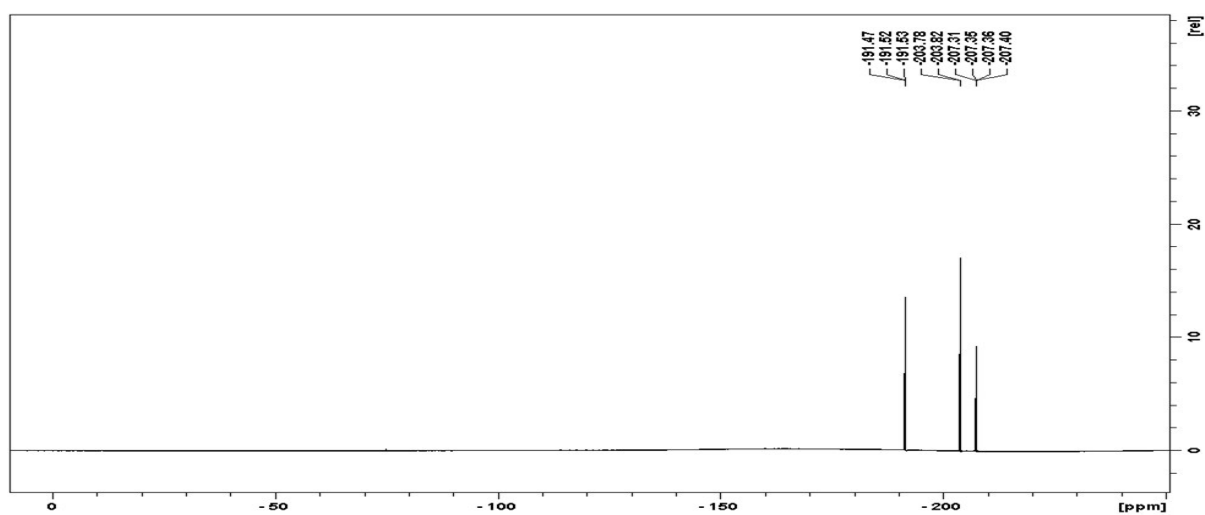
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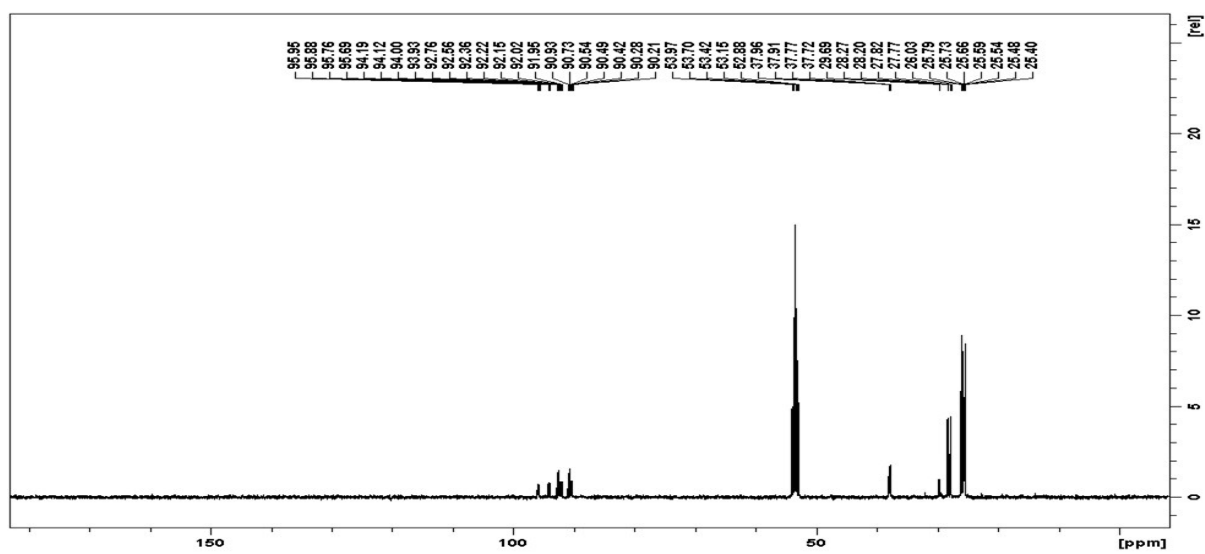
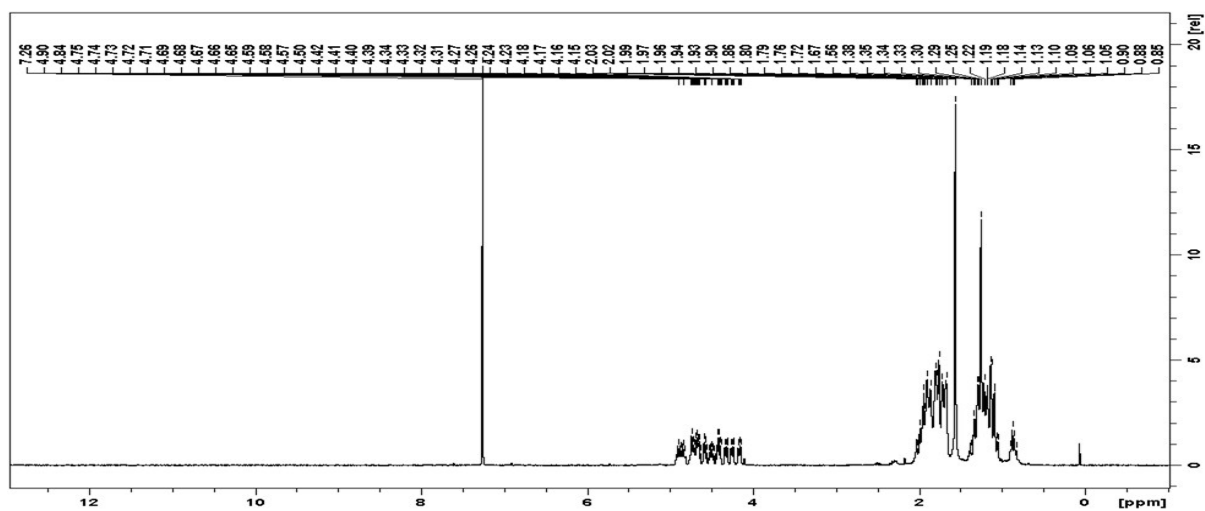
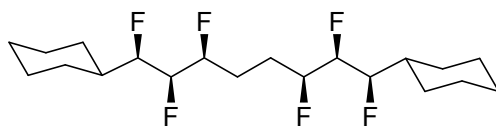
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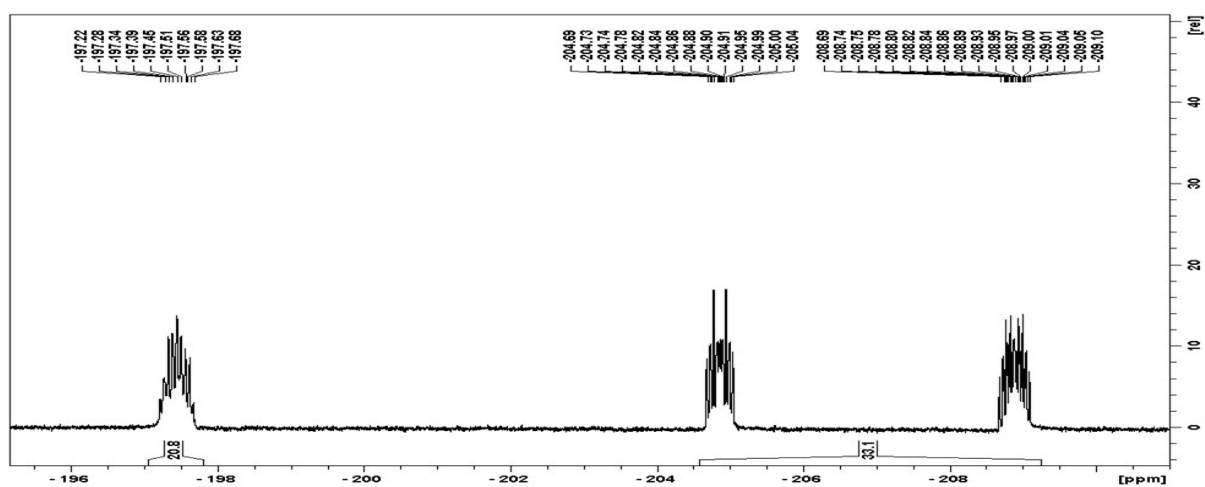
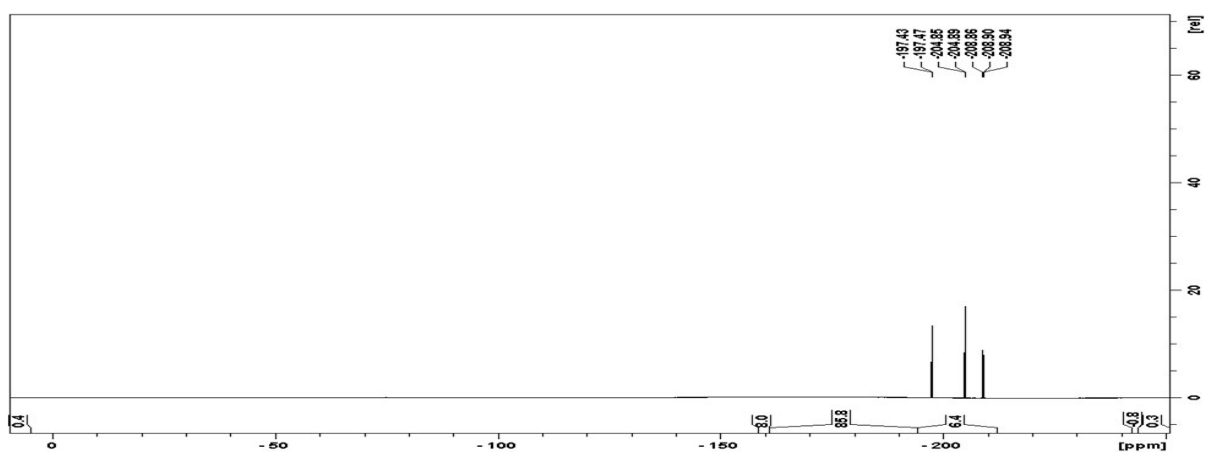
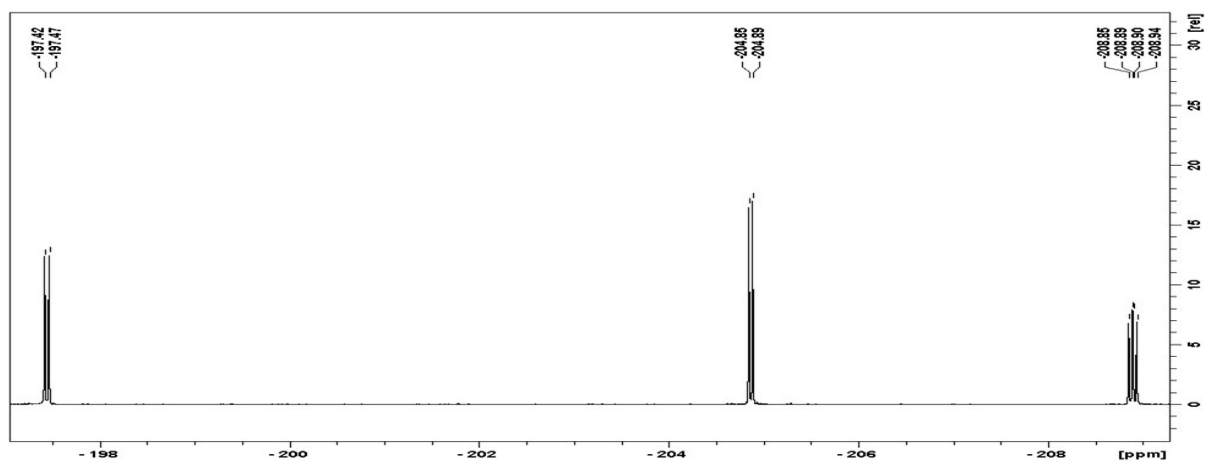


¹³C-NMR 25



Compound 9





DFT Computations

Full Gaussian reference: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J.; Peralta, J. A. J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian 09, Rev. A.02, Wallingford CT, **2009**.

Optimised Coordinates, B3LYP-D3/CPCM(CH₂Cl₂)/6-311+G level, xyz coordinates in Å**

9 conformer a

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F -4.2845769459 1.0361143551 27.7201586621
F 1.4936980609 2.7711267197 23.5306298741
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C 0.2666871681 3.4349094024 23.3173322336
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9 Conformer b

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9 Conformer c

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 H 5.5222265373 0.5916803839 2.95345935
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 C 5.6142588602 -1.4104840105 0.1058013427
 H 5.4691499505 -0.6223720397 -0.6451275514
 H 5.0480190795 -2.2805350862 -0.23288841
 C -5.4527876169 0.9313927084 -1.041351037
 H -5.1592882654 0.4467673121 -0.106647908
 H -5.0353143676 0.330001044 -1.8594636753
 C 7.3724509431 -0.0543124041 2.0487604027
 H 7.9278079949 0.8275607845 2.3814549929
 H 7.522217288 -0.8276846271 2.8122176796
 C -7.4706275898 1.6534285706 -2.4051562659
 H -8.5644063426 1.6765998587 -2.4280450186
 H -7.1470784483 1.0905973644 -3.2899631744
 C -5.3749097953 3.0703713006 -2.3874123482
 H -4.9637411533 2.5531250476 -3.2647246501
 H -4.9912495619 4.0922309565 -2.4124595374
 C 7.9185407067 -0.5574248027 0.7083821731
 H 8.9735559981 -0.8296737126 0.8090376792
 H 7.8694298059 0.2534875 -0.029390682
 C -6.9834242802 0.9351377912 -1.1433988251
 H -7.3536980726 -0.0941127337 -1.1219229375
 H -7.3971609841 1.4374545091 -0.2602736096
 C -6.9041699024 3.0746476427 -2.476855442
 H -7.3127210485 3.6693517562 -1.6502571888
 H -7.2188106719 3.5657634967 -3.4026015287
 C 7.104754738 -1.7508843415 0.1993656339
 H 7.238865845 -2.5989043722 0.8824951623
 H 7.4722935916 -2.0744375489 -0.7790596704
 H -0.8230619855 1.3140587643 -0.7360538375

9 Conformer d

F 2.7018613574 -0.3056527678 5.1833640733
 F 0.6641863917 0.9920915807 3.8955678779
 F -0.7409054004 2.9478661399 -0.0825665502
 F 3.1789850918 1.7267368711 3.086780467
 F -3.2645072019 2.6656791132 0.9517724074
 F -2.7569123588 3.1319448022 -1.9255287218
 C 1.2402200967 0.3758185425 2.7646750039
 H 0.9059775873 -0.6661632054 2.77420113
 C -1.2798229304 1.6564613072 0.0973429688
 C -2.8010205114 1.7204095299 0.015937163
 H -3.1818922942 0.7463732725 0.3346859506

C 2.7597674464 0.3966883426 2.8883627735
 H 3.1658061747 0.0772036252 1.9247898373
 C 3.3634726386 -0.5095490512 3.9478275315
 H 3.1413088963 -1.5415593712 3.654899131
 C 0.7419927046 1.0880433022 1.5179005981
 H 1.1337046235 2.1070871327 1.5055518518
 H 1.1624738938 0.5670381741 0.6509049015
 C -0.784723738 1.1050160573 1.4242664742
 H -1.2077575494 1.6958363861 2.2391374971
 H -1.1752502673 0.0864286581 1.5237705035
 C 4.8624114275 -0.3318764582 4.1706839793
 H 5.0130607511 0.6869944856 4.5460086942
 C -3.3925791728 2.0023505771 -1.3547412647
 H -3.1338452512 1.1547407394 -1.9988091168
 C -4.8996065885 2.240415112 -1.3703516927
 H -5.0877398481 3.1481291713 -0.7852680029
 C 5.6647505508 -0.4872367762 2.865594855
 H 5.3531075571 0.260172695 2.1316289285
 H 5.4576079929 -1.4729333464 2.428695438
 C 5.367171742 -1.3240354608 5.232666213
 H 5.1577397674 -2.3454921436 4.8878966008
 H 4.8148389066 -1.1827961278 6.1638794622
 C -5.676347903 1.0801020541 -0.721129812
 H -5.3767813717 0.9533886236 0.3222549944
 H -5.4318329082 0.1449440759 -1.2417821344
 C 7.1719378596 -0.3477593376 3.114302499
 H 7.7131571091 -0.4966569709 2.1752496801
 H 7.3840213208 0.6776618745 3.4412938151
 C -7.6734650717 1.5613037684 -2.2156200973
 H -8.7477863322 1.7691762152 -2.2219804865
 H -7.5236300851 0.6503272693 -2.8089596454
 C -5.3896422983 2.4757729823 -2.8096016371
 H -5.1431560389 1.5927279853 -3.4142318131
 H -4.8565086651 3.3213319343 -3.2488929002
 C 7.6688768218 -1.3286800366 4.1805033722
 H 8.7361688032 -1.1752635211 4.3669672528
 H 7.5567324422 -2.3549106218 3.8081393715
 C -7.1908302902 1.3155753362 -0.7829235968
 H -7.7124966971 0.4594982583 -0.3448537683
 H -7.4398138222 2.186729378 -0.1644664725
 C -6.9016519681 2.7161807004 -2.861809408
 H -7.13714857 3.6491131528 -2.3344571712
 H -7.2186701432 2.8540047178 -3.8999377061
 C 6.8715851972 -1.1740146675 5.4795035715
 H 7.069680108 -0.1845889301 5.9104526501
 H 7.2002414401 -1.9100017849 6.2194457197
 H -0.9134651632 1.0478014449 -0.7350331008

26 conformer a

F -1.8980251838 3.0080019371 29.0371064397
 F -3.2312010911 1.2882977524 25.535641403
 F 0.2478896292 2.9459351301 25.615735533
 F -3.6488437569 0.8027444266 28.2170534237
 F 1.340668842 1.9983282921 23.2688149319

F -1.2878701778 1.6562609227 22.0139059662
 C -2.6955001901 2.1306824 26.5305048607
 H -1.738442077 1.7033530922 26.831016876
 C -0.5519419762 2.6642368534 24.4900108563
 C 0.2895843811 2.9324911151 23.2501378776
 H 0.7408478026 3.9220700545 23.3252614193
 C -3.6560202559 2.1150226189 27.7114230752
 H -4.66787947 2.3154579225 27.3585559209
 C -3.3001118398 3.0996036168 28.8128079356
 H -3.4810099582 4.1114743487 28.4400276057
 C -2.4656416315 3.5119338457 25.9424888707
 H -1.8503392135 4.0976085511 26.6259098954
 C -1.822744221 3.4926628384 24.5622989697
 H -2.5386625482 3.1205717133 23.8290286278
 C -4.0323088697 2.8873906632 30.1306638422
 H -3.7669325565 1.8895201895 30.4970811503
 C -0.4795850545 2.8251651419 21.9440067141
 H -1.1727215385 3.6686713868 21.8837515522
 C 0.3816891817 2.7633710244 20.6901011827
 H 1.008287401 1.8677677743 20.7656076014
 C -5.5591256422 2.9442419348 29.9370314032
 H -5.8893091025 2.159760846 29.2515099377
 H -5.8286694288 3.904963243 29.4796944562
 C -3.5783454138 3.9314439726 31.1655314187
 H -3.775408855 4.934332156 30.7641660396
 H -2.4998353895 3.8562580221 31.3189866219
 C 1.3022733408 3.9934238012 20.5833770489
 H 1.978604983 4.0431078192 21.4403941862
 H 0.6901519457 4.9042929726 20.6038979837
 C -6.2979505666 2.7910266708 31.2722050276
 H -7.3758882119 2.8720168685 31.1045739547
 H -6.1147806796 1.7839549298 31.6665342031
 C 1.2392118492 3.8338295369 18.0496846697
 H 1.856762743 3.7728774649 17.148490805
 H 0.6218954801 4.735670617 17.950344671
 C -0.5067988172 2.6417173667 19.4399529968
 H -1.1876802062 3.5025216306 19.4063460007
 H -1.1283510169 1.7468780171 19.5128965135
 C -5.8366905921 3.8269051073 32.3019643136
 H -6.349769877 3.66608269 33.254917849
 H -6.1168314533 4.8301769737 31.9566645395
 C 2.1273050751 3.9636350506 19.2909139063
 H 2.7417576697 4.8665264911 19.2289122185
 H 2.8191245163 3.1132874453 19.3300931501
 C 0.3268490675 2.6078265684 18.1551472322
 H 0.9399267635 1.6979979744 18.1462568563
 H -0.3361110738 2.5484084609 17.286897681
 C -4.3184431337 3.7667423788 32.4966858194
 H -4.0482873893 2.801651566 32.9431687127
 H -3.9917316075 4.539942526 33.1983446065
 H -0.8089975888 1.6056260405 24.5363102678
 F -3.6976558307 4.1792933292 25.8142584229
 F -1.5338404846 4.8273037066 24.2232721246

26 conformer b

F -3.0840583312 -1.4295285554 -0.3934046456
F -0.8488963881 1.9652009186 -1.0723697787
F 0.6708196255 0.0328865517 3.1847526887
F -3.3059580935 1.0698162788 -1.9134055296
F 3.2833243367 -0.8162236672 3.1784690516
F 3.3165687188 -1.1802957165 0.2676765843
C -1.3955318208 0.7715641452 -0.5744368307
H -1.1118853092 -0.0221271157 -1.2681814898
C 1.3468408841 -0.2255404336 1.9815374113
C 2.8186622973 0.0938734463 2.2108641047
H 2.9077186515 1.091014941 2.6430737678
C -2.9102852799 0.9339654564 -0.5697409466
H -3.1711442216 1.8649193458 -0.0654544687
C -3.6614641848 -0.216527108 0.0780149268
H -3.4688981114 -0.1888554632 1.1540149442
C -0.8089023305 0.4546151063 0.7925829849
H -1.0942940674 -0.568366137 1.0485635514
C 0.7179812891 0.5653469433 0.8447143252
H 1.1284809429 0.1842743139 -0.0932296031
C -5.1607200047 -0.2425514337 -0.1861298811
H -5.3021992906 -0.3345811917 -1.2686946804
C 3.6800082895 0.0079881363 0.9625863796
H 3.4110581526 0.8375511625 0.3029543059
C 5.1822343481 0.0006787991 1.2105403932
H 5.4104273538 -0.8804543658 1.8204294891
C -5.8329927015 1.0613881181 0.2827891643
H -5.4203363254 1.9194628893 -0.2536001702
H -5.6182959136 1.2150093817 1.3480989612
C -5.8020982926 -1.4607167915 0.500344904
H -5.5958156463 -1.4080967624 1.5775190753
H -5.3410932362 -2.3795973896 0.13227484
C 5.6264747244 1.2558830339 1.984624892
H 5.1334749395 1.2994811921 2.9589664834
H 5.3183753776 2.1504921822 1.4284518684
C -7.3515098467 1.0154924558 0.0713305426
H -7.8008573213 1.9390031701 0.4478698654
H -7.5598199177 0.979014533 -1.0050406942
C 7.8994917607 1.1588154093 0.8571389242
H 8.9788037227 1.1360895927 1.0355374271
H 7.6982909202 2.0468406687 0.2446581834
C 5.9421828307 -0.1118373933 -0.1222607781
H 5.6560352172 0.7318439096 -0.7640917519
H 5.6443267652 -1.0239328759 -0.6435154063
C -7.9846242757 -0.2038203023 0.7486028634
H -9.0593160204 -0.2329457868 0.5450195632
H -7.8705995942 -0.1134920424 1.8362804238
C 7.1468968297 1.2804000375 2.1856995364
H 7.4319913704 2.2002542931 2.7045023005
H 7.4326773973 0.4474491783 2.8397798845
C 7.4592115063 -0.0923313759 0.0908041644
H 7.7560132302 -0.9857775612 0.6542739521
H 7.968279827 -0.1472133713 -0.8760140117
C -7.3173817782 -1.4998083107 0.2777669432
H -7.5215995719 -1.6454053568 -0.7903773096

H -7.744808404 -2.3611691712 0.7995560958
H 1.2288060246 -1.290466493 1.7725324359
F -1.3709631529 1.3051914303 1.7520598425
F 1.0842341888 1.9122732916 0.9525871103