Electronic Supplementary Information

Direct synthesis of conjugated tetraenes from 1,3-enynes with 1,3-dienes

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Spectroscopic data of new compounds:

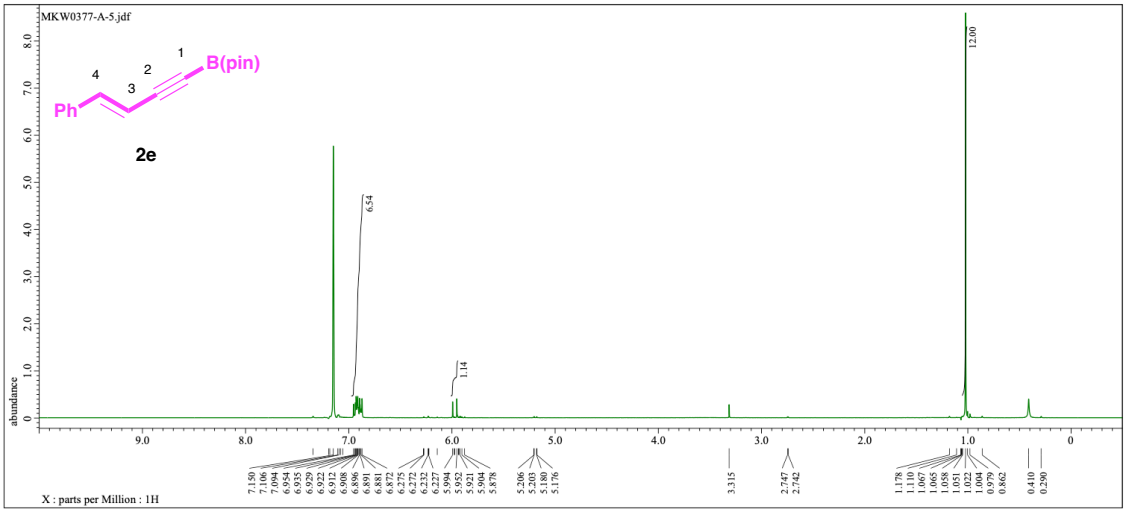

Fig.S1. ^{1}H NMR Spectrum of (*E*)-4,4,5,5-tetramethyl-2-(4-phenylbut-3-en-1-yn-1-yl)-1,3,2-dioxoborolane (**2e**) (400 MHz, C_6D_6).

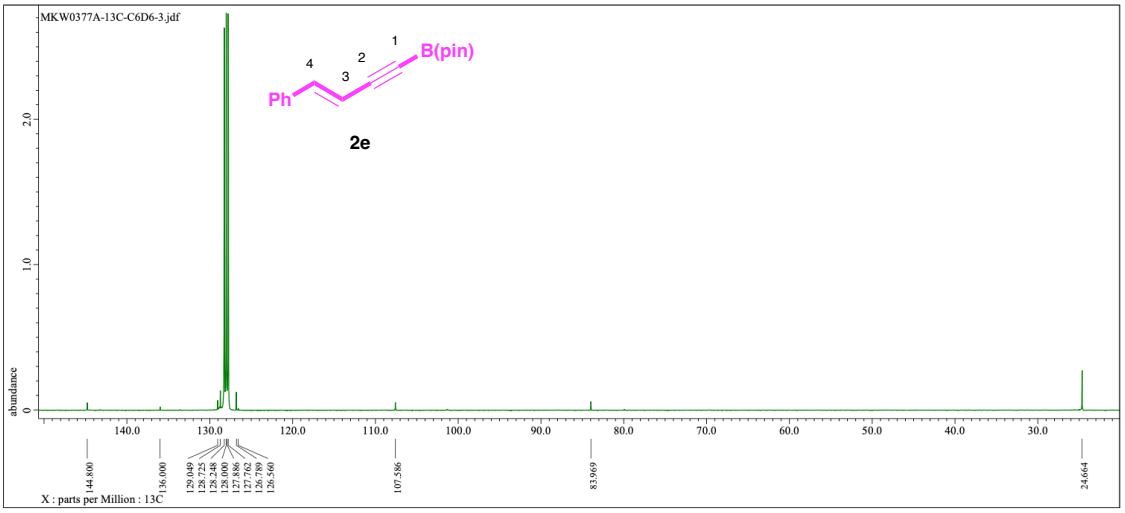

Fig.S2. ^{13}C{^{1}H} NMR Spectrum of (*E*)-4,4,5,5-tetramethyl-2-(4-phenylbut-3-en-1-yn-1-yl)-1,3,2-dioxoborolane (**2e**) (100 MHz, C_6D_6).

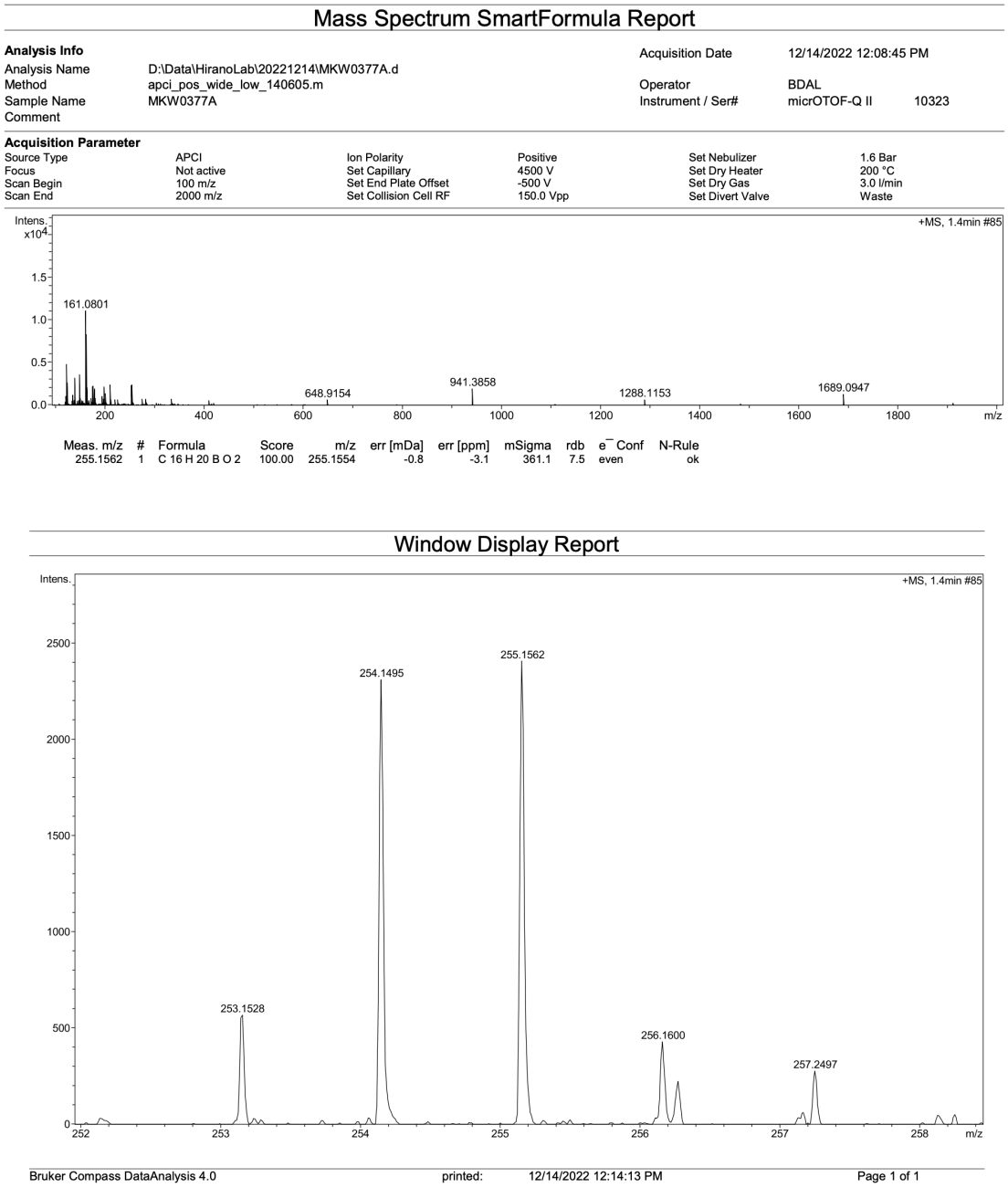

Fig.S3. HRMS Spectra of (*E*)-4,4,5,5-tetramethyl-2-(4-phenylbut-3-en-1-yn-1-yl)-1,3,2-dioxoborolane (**2e**) (APCI).

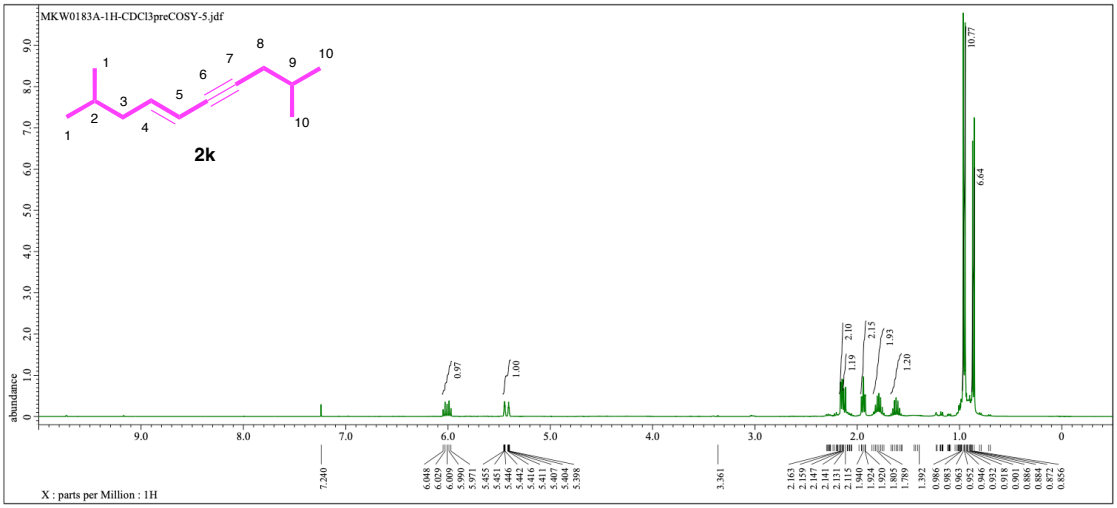

Fig.S4. ^{1}H NMR Spectrum of (*E*)-2,9-dimethyldec-4-en-6-yne (**2k**) (400 MHz, $CDCl_3$).

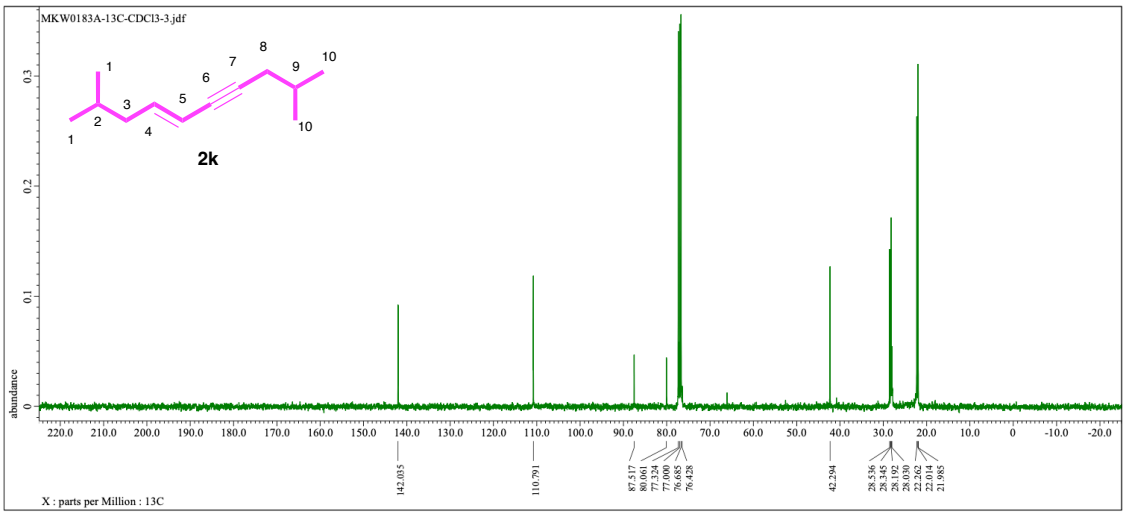

Fig.S5. $^{13}C\{^{1}H\}$ NMR Spectrum of (*E*)-2,9-dimethyldec-4-en-6-yne (**2k**) (100 MHz, $CDCl_3$).

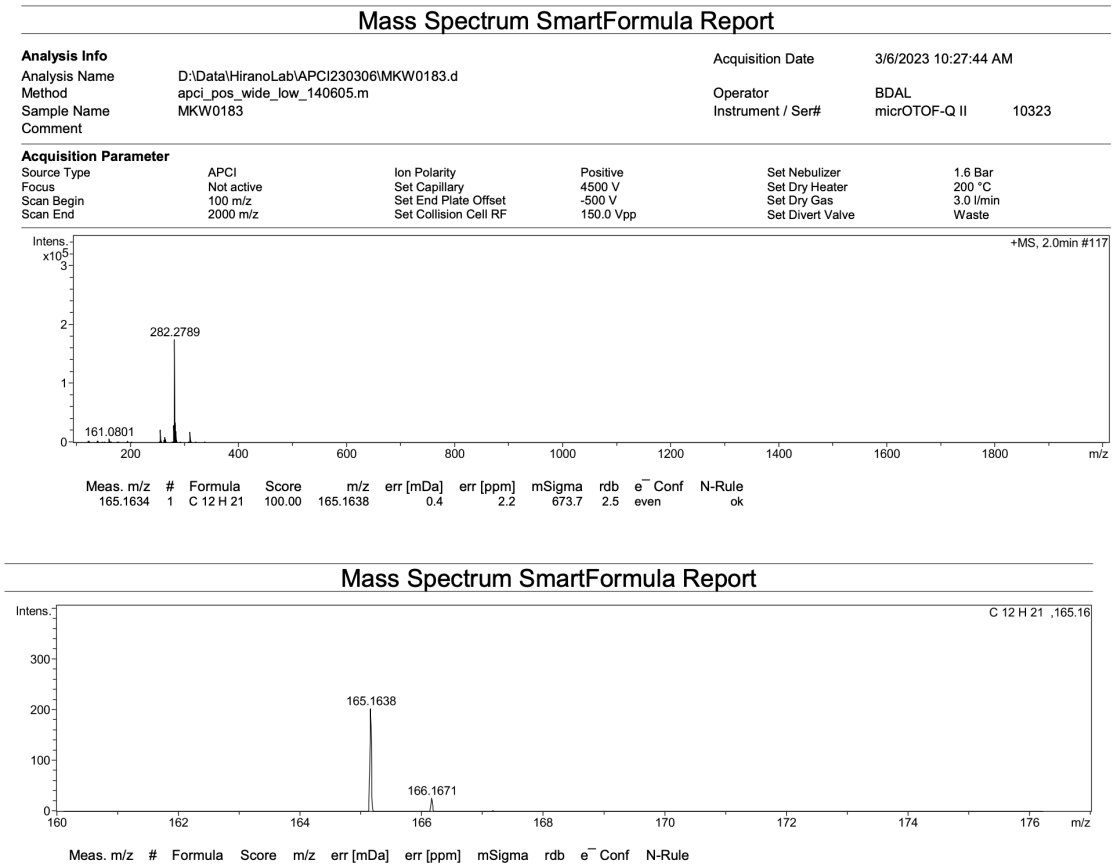

Fig.S6. HRMS Spectra of (*E*)-2,9-dimethyldec-4-en-6-yne (**2k**) (APCI).

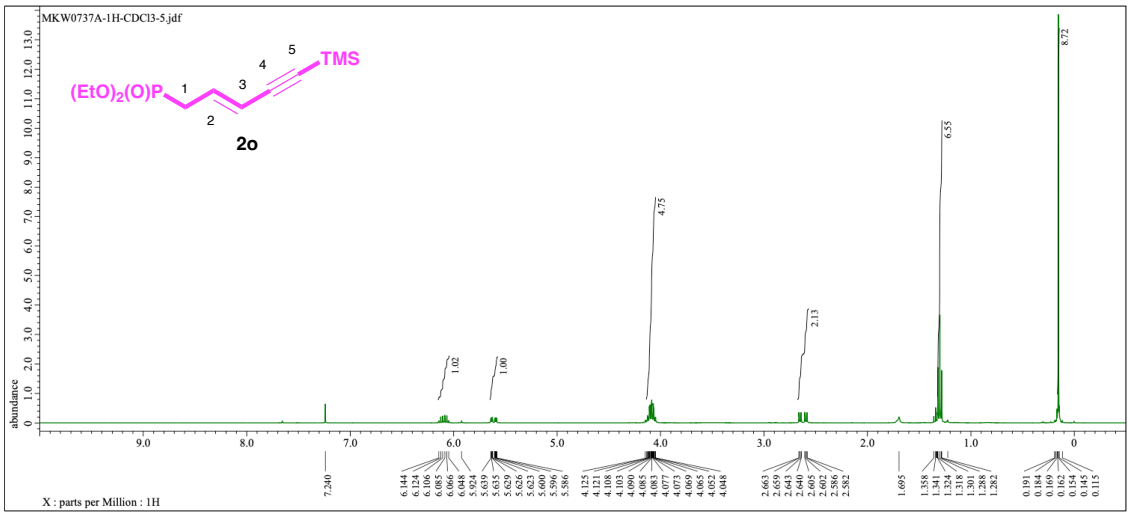

Fig.S7. ^{1}H NMR Spectrum of diethyl (*E*)-(5-(trimethylsilyl)pent-2-en-4-yn-1-yl)phosphonate (**2o**) (400 MHz, $CDCl_3$).

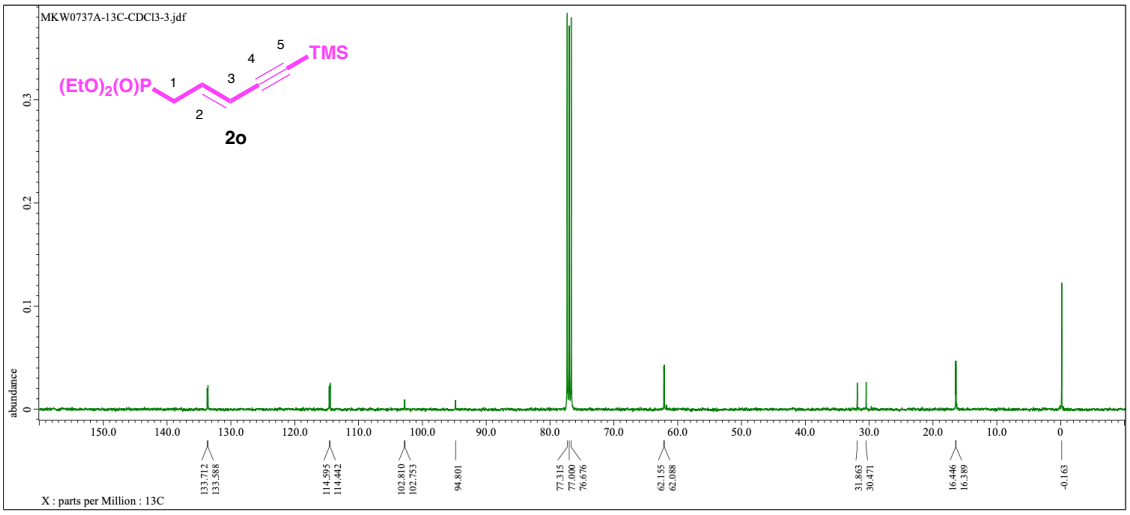

Fig.S8. $^{13}C\{^{1}H\}$ NMR Spectrum of diethyl (*E*)-(5-(trimethylsilyl)pent-2-en-4-yn-1-yl)phosphonate (**2o**) (100 MHz, $CDCl_3$).

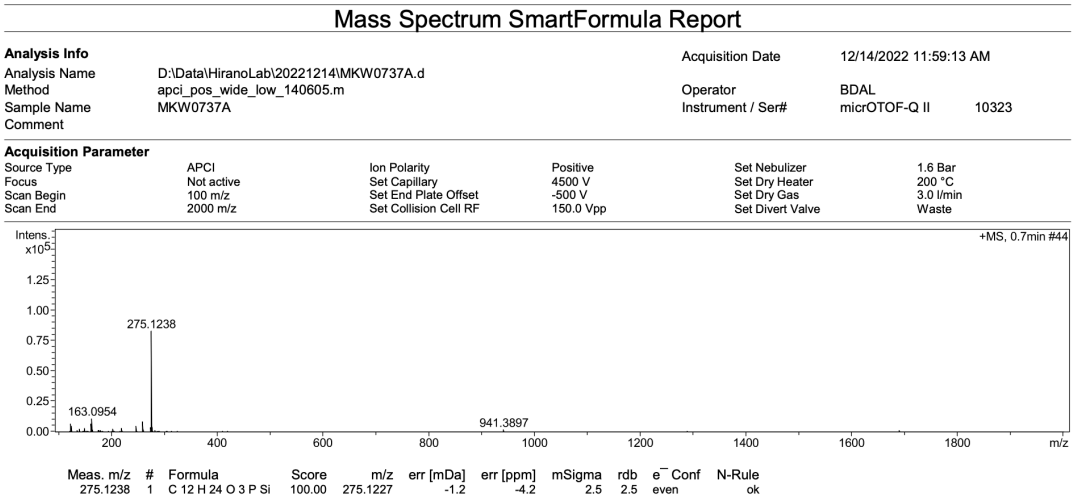

Fig.S9. HRMS Spectrum of diethyl (*E*)-(5-(trimethylsilyl)pent-2-en-4-yn-1-yl)phosphonate (**2o**) (APCI).

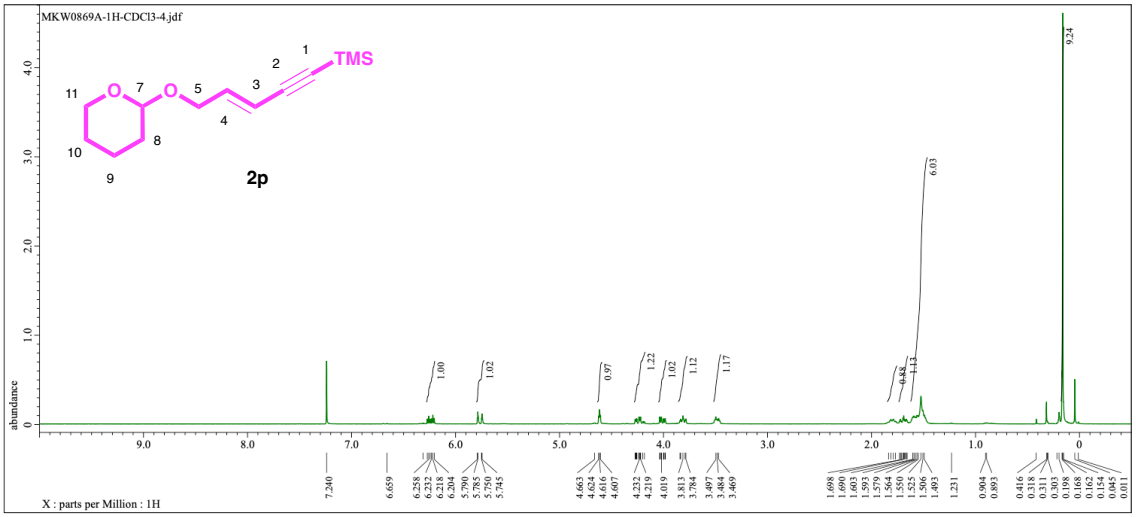

Fig.S10. ^{1}H NMR Spectrum of (*E*)-trimethyl(5-((tetrahydro-2*H*-pyran-2-yl)oxy)pent-3-en-1-yn-1-yl)silane (**2p**) (400 MHz, $CDCl_3$).

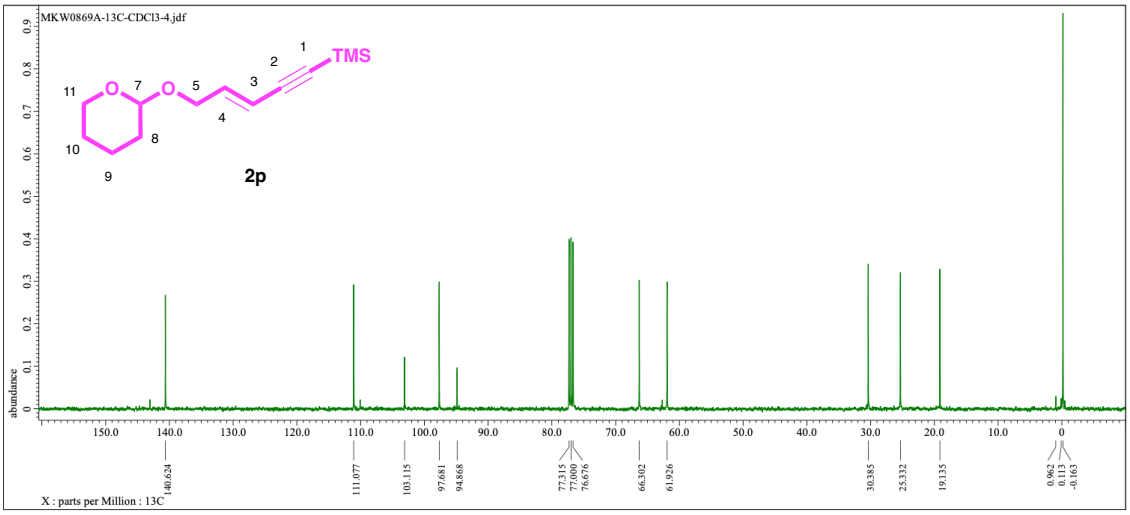

Fig.S11. $^{13}C\{^{1}H\}$ NMR Spectrum of (*E*)-trimethyl(5-((tetrahydro-2*H*-pyran-2-yl)oxy)pent-3-en-1-yn-1-yl)silane (**2p**) (100 MHz, $CDCl_3$).

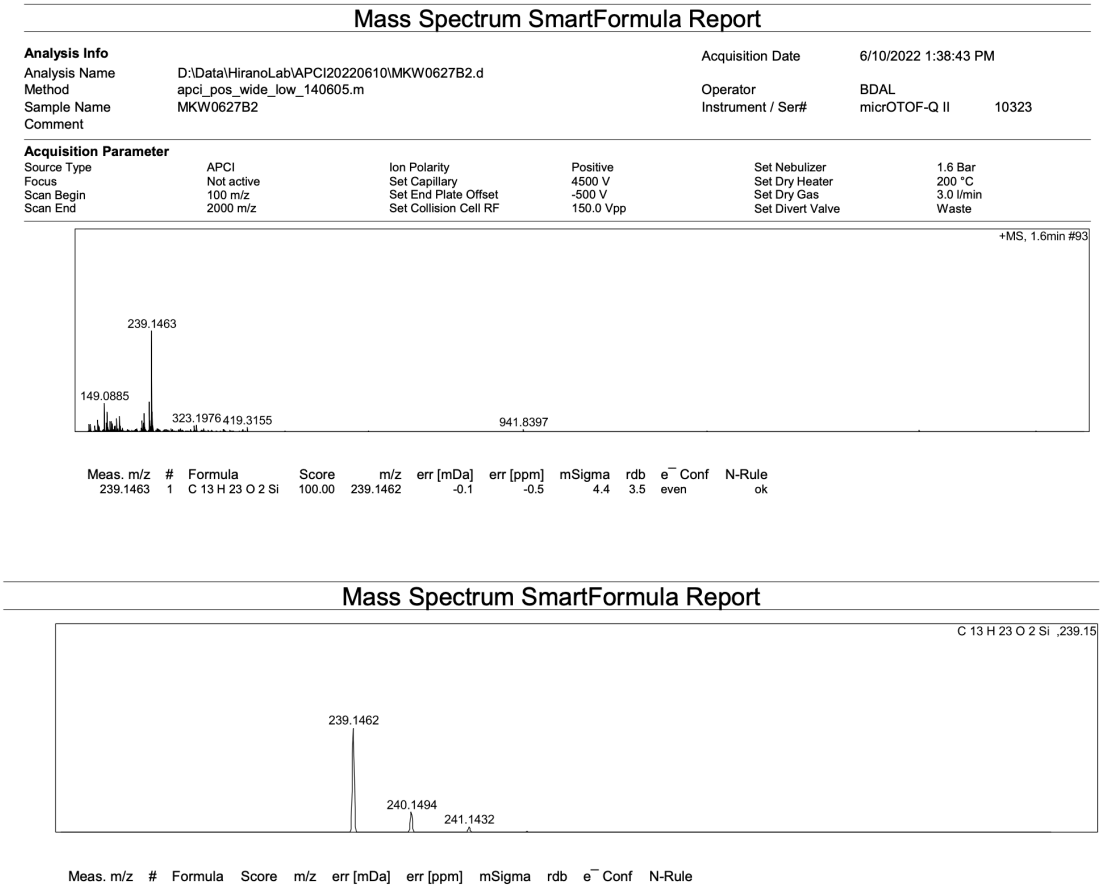

Fig.S12. HRMS Spectra of (*E*)-trimethyl(5-((tetrahydro-2*H*-pyran-2-yl)oxy)pent-3-en-1-yn-1-yl)silane (**2p**) (APCI).

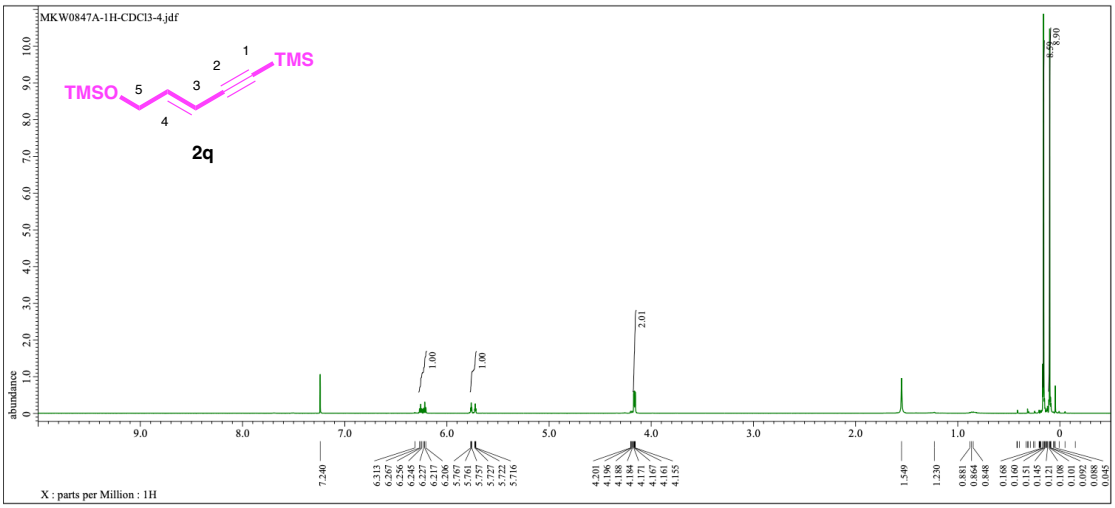

Fig.S13. ^{1}H NMR Spectrum of (*E*)-trimethyl(5-((trimethylsilyl)oxy)pent-3-en-1-yn-1-yl)silane (**2q**) (400 MHz, $CDCl_3$).

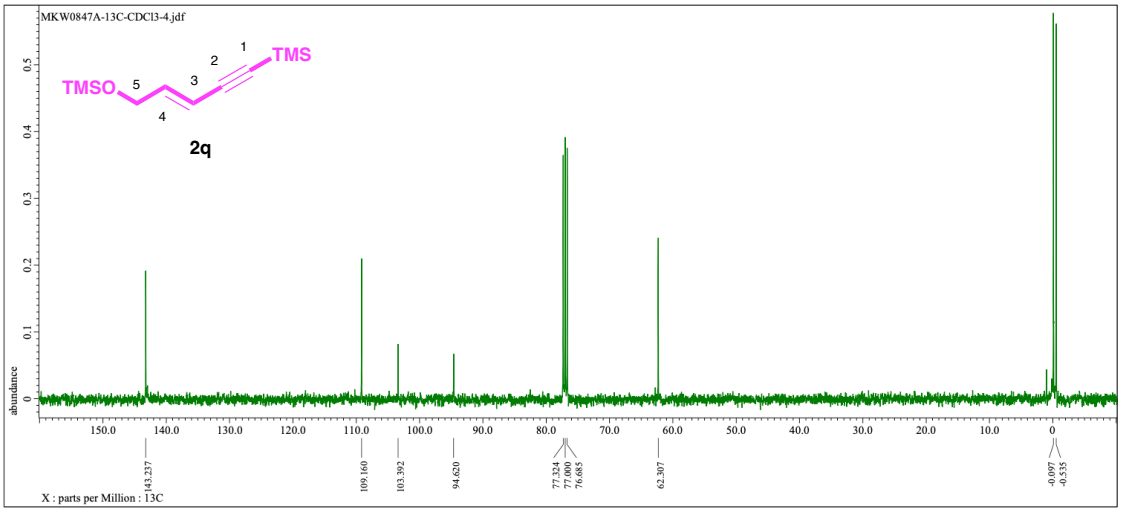

Fig.S14. ^{13}C{^{1}H} NMR Spectrum of (*E*)-trimethyl(5-((trimethylsilyl)oxy)pent-3-en-1-yn-1-yl)silane (**2q**) (100 MHz, $CDCl_3$).

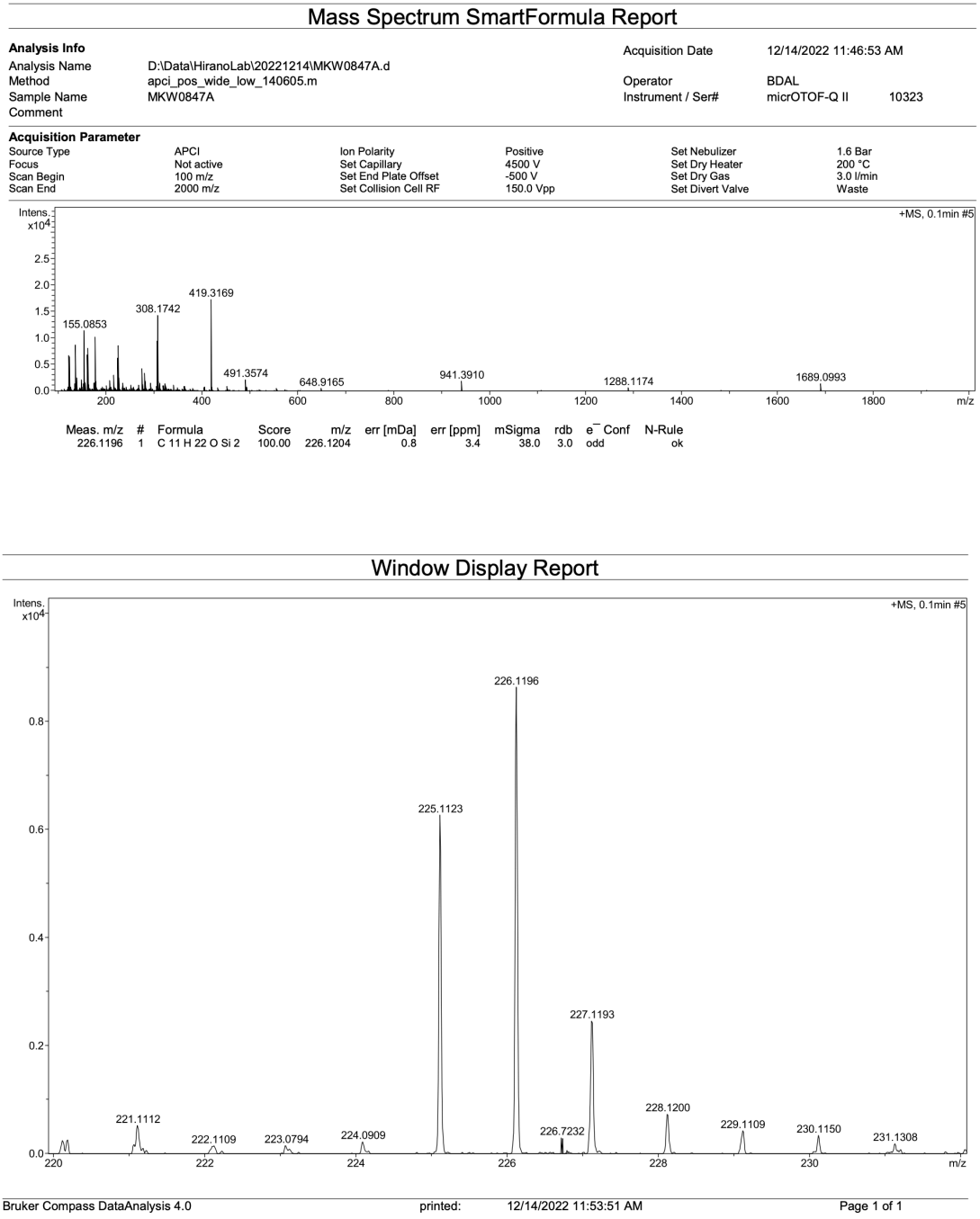

Fig.S15. HRMS Spectraof (*E*)-trimethyl(5-((trimethylsilyl)oxy)pent-3-en-1-yn-1-yl)silane (**2q**) (APCI).

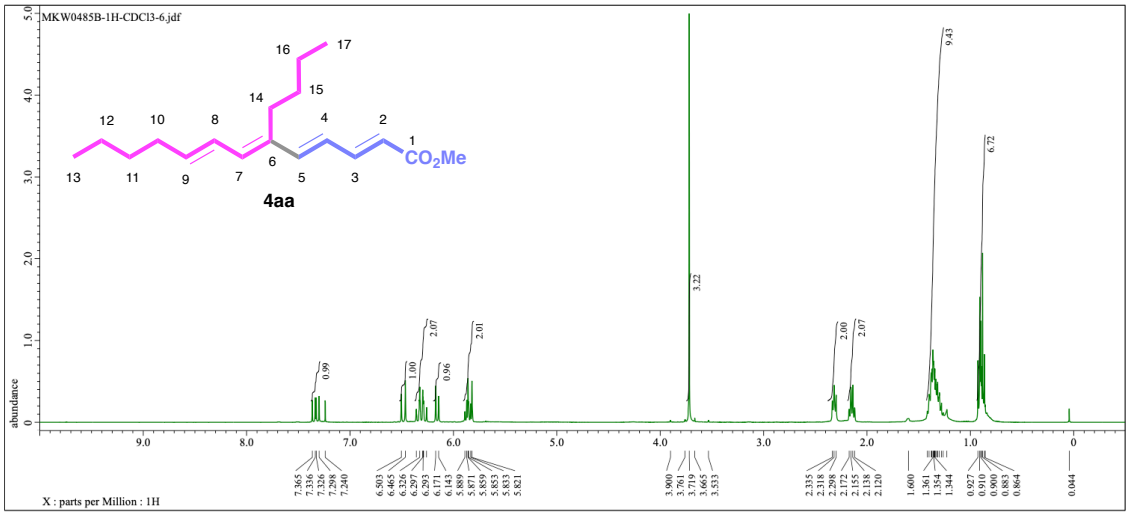

Fig.S16. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,6*E*,8*E*)-6-butyltrideca-2,4,6,7-tetraenoate (**4aa**) (400 MHz, $CDCl_3$).

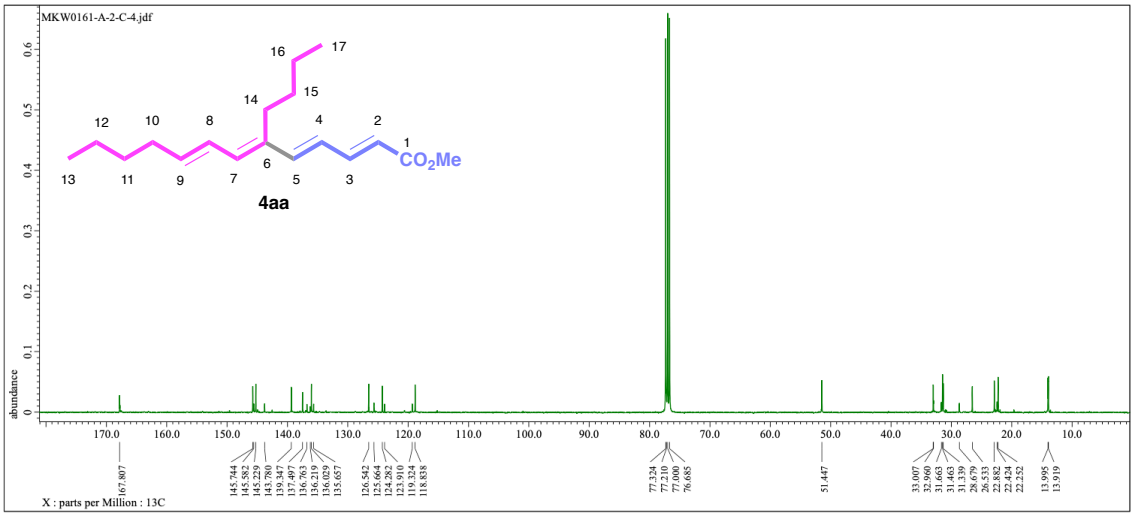

Fig.S17. ^{13}C{^{1}H} NMR Spectrum of methyl (2*E*,4*E*,6*E*,8*E*)-6-butyltrideca-2,4,6,7-tetraenoate (**4aa**) (100 MHz, $CDCl_3$).

Mass Spectrum SmartFormula Report

Analysis Info

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Comment			

Acquisition Parameter

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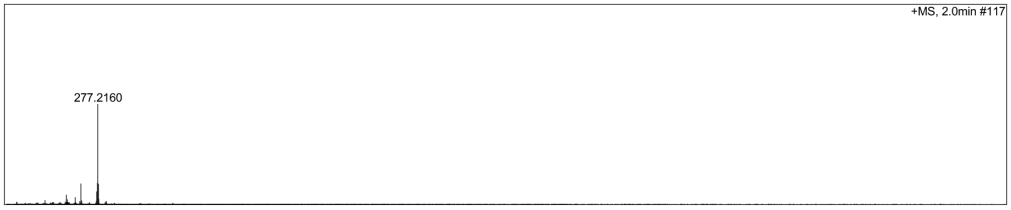

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	2	C 14 H 25 N 6	18.80	277.2135	-2.5	-8.9	26.0	5.5	even	ok
	3	C 13 H 29 N 2 O 4	3.85	277.2122	-3.8	-13.8	36.0	0.5	even	ok

Fig.S18. HRMS Spectrum of methyl (2*E*,4*E*,6*E*,8*E*)-6-butyltrideca-2,4,6,7-tetraenoate (**4aa**) (APCI).

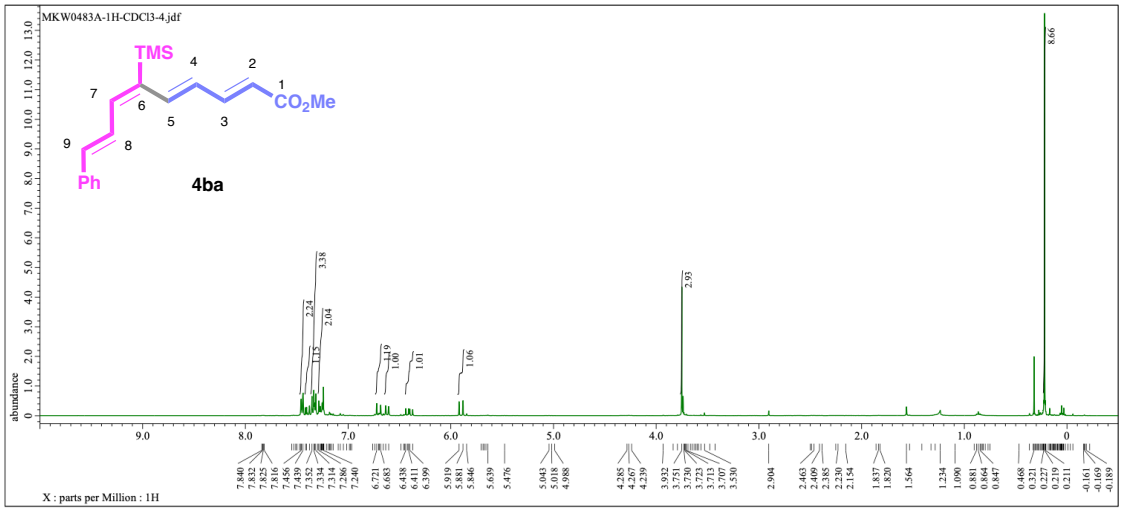


Fig.S19. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,6*E*,8*E*)-9-phenyl-6-(trimethylsilyl)nona-2,4,6,8-tetraenoate (**4ba**) (400 MHz, $CDCl_3$).

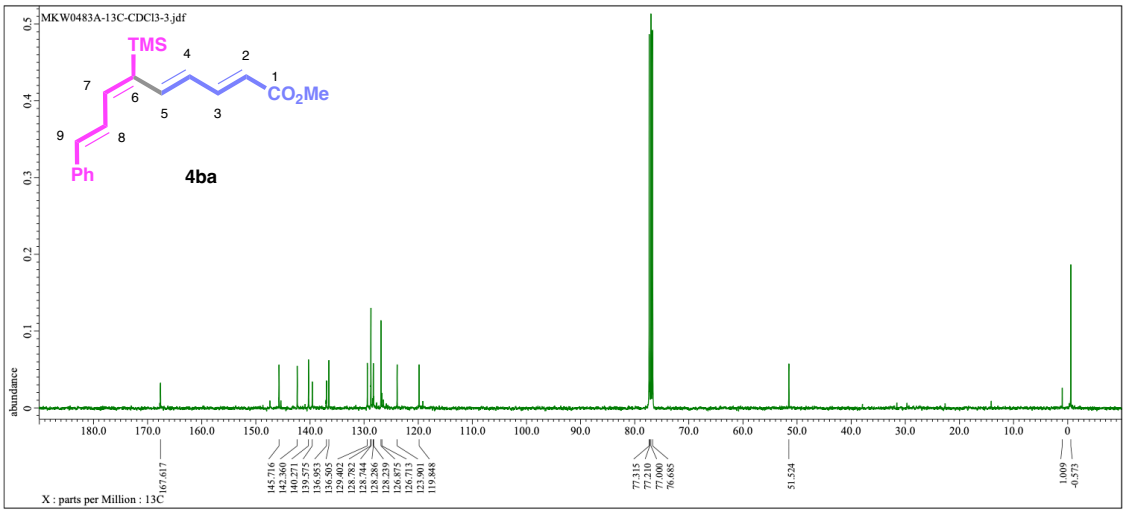


Fig.S20. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl (2*E*,4*E*,6*E*,8*E*)-9-phenyl-6-(trimethylsilyl)nona-2,4,6,8-tetraenoate (**4ba**) (100 MHz, $CDCl_3$).

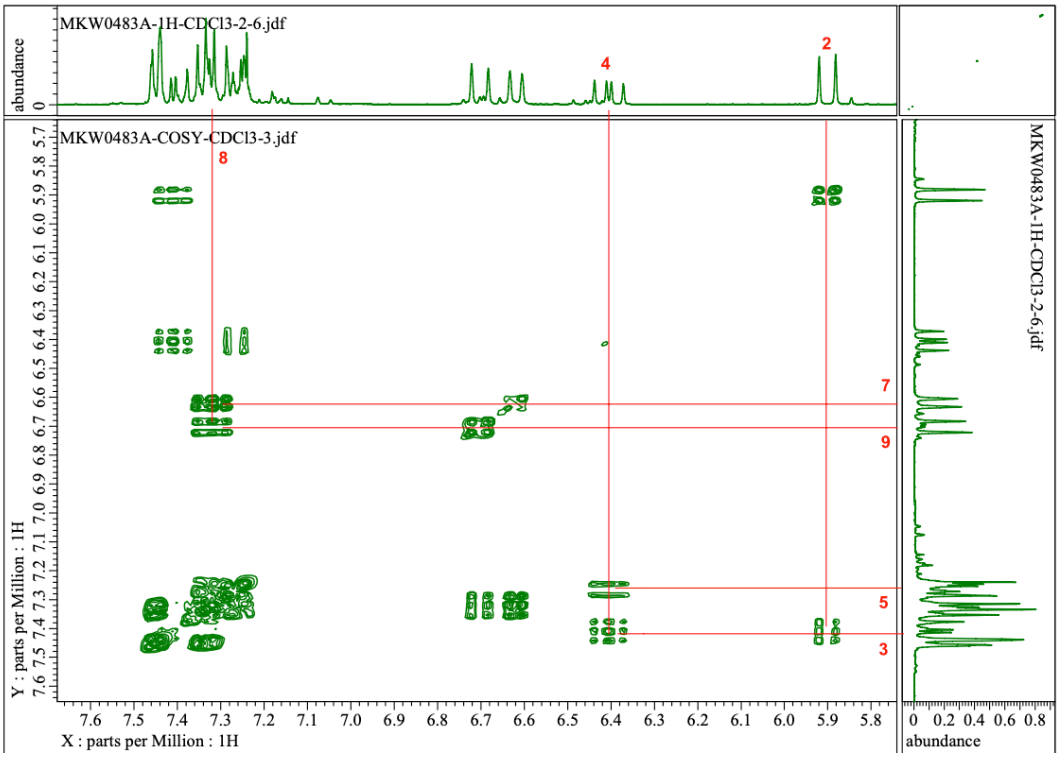


Fig.S21. ^{1}H-^{1}H COSY of methyl (2*E*,4*E*,6*E*,8*E*)-9-phenyl-6-(trimethylsilyl)nona-2,4,6,8-tetraenoate (**4ba**) (400 MHz, $CDCl_3$).

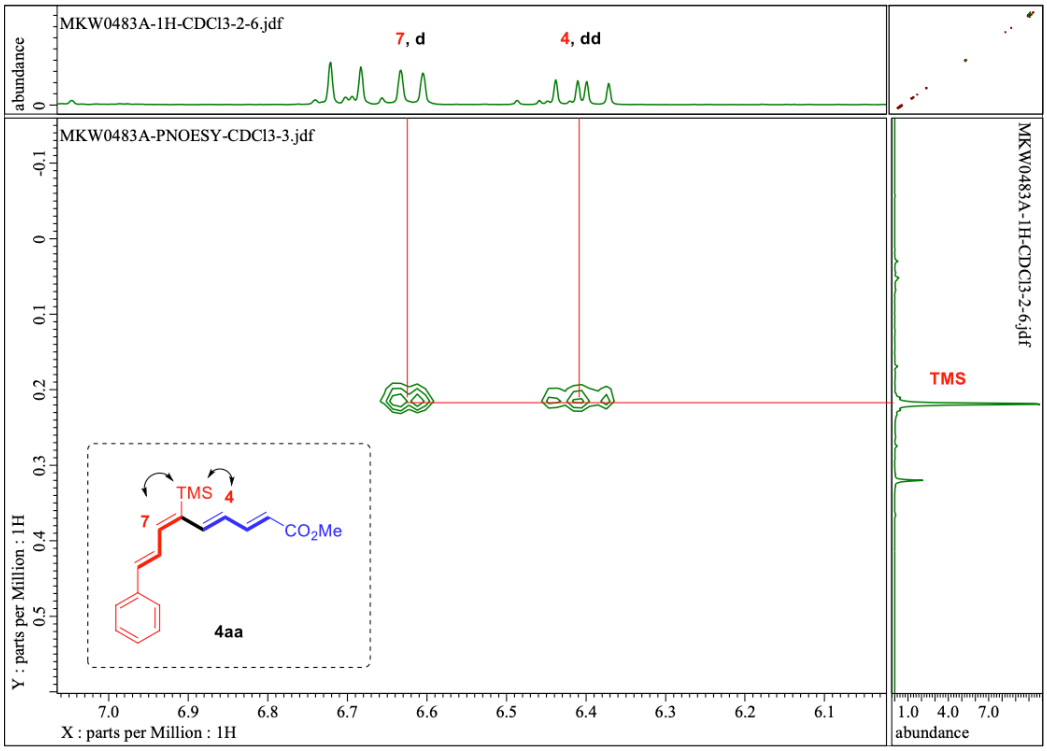


Fig.S22. *p*NOESY of methyl (2*E*,4*E*,6*E*,8*E*)-9-phenyl-6-(trimethylsilyl)nona-2,4,6,8-tetraenoate (**4ba**) (400 MHz, $CDCl_3$).

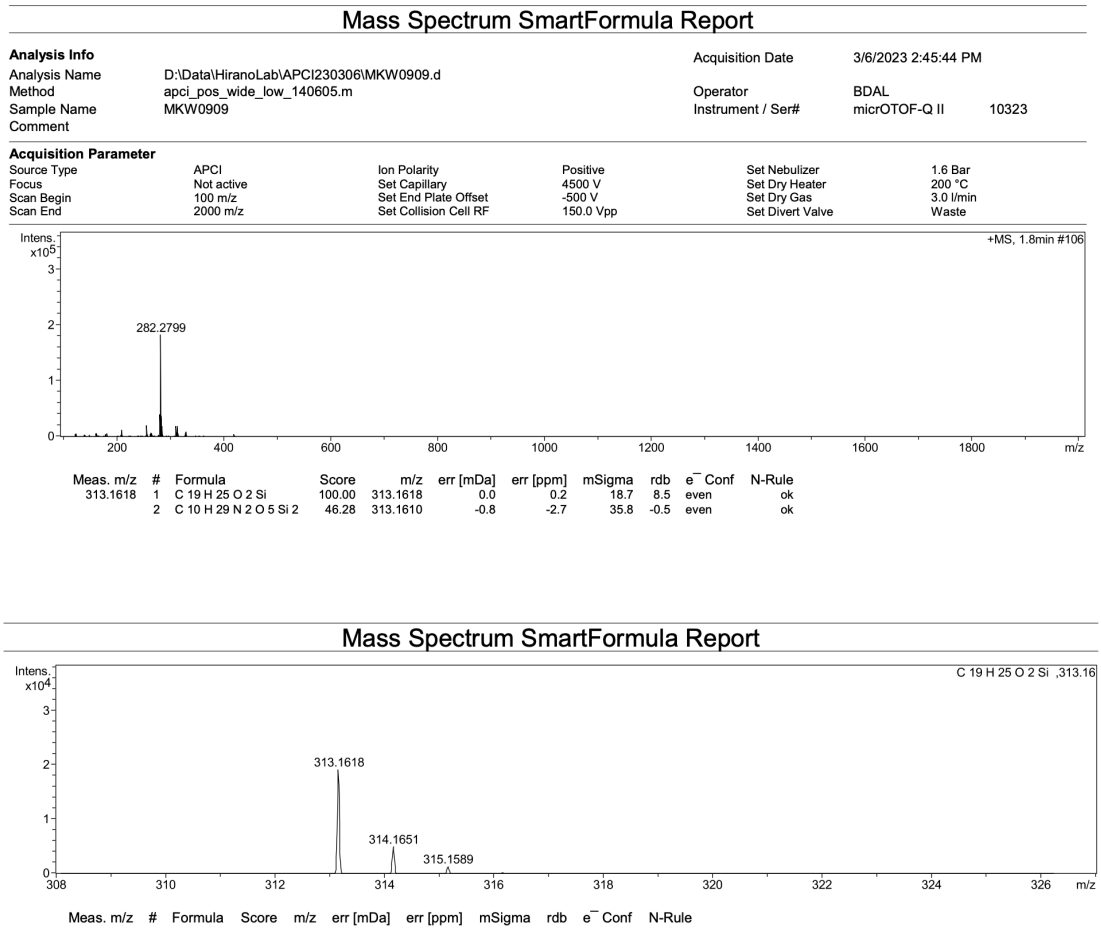


Fig.S23. HRMS Spectra of methyl (2*E*,4*E*,6*E*,8*E*)-9-phenyl-6-(trimethylsilyl)nona-2,4,6,8-tetraenoate (**4ba**) (APCI).

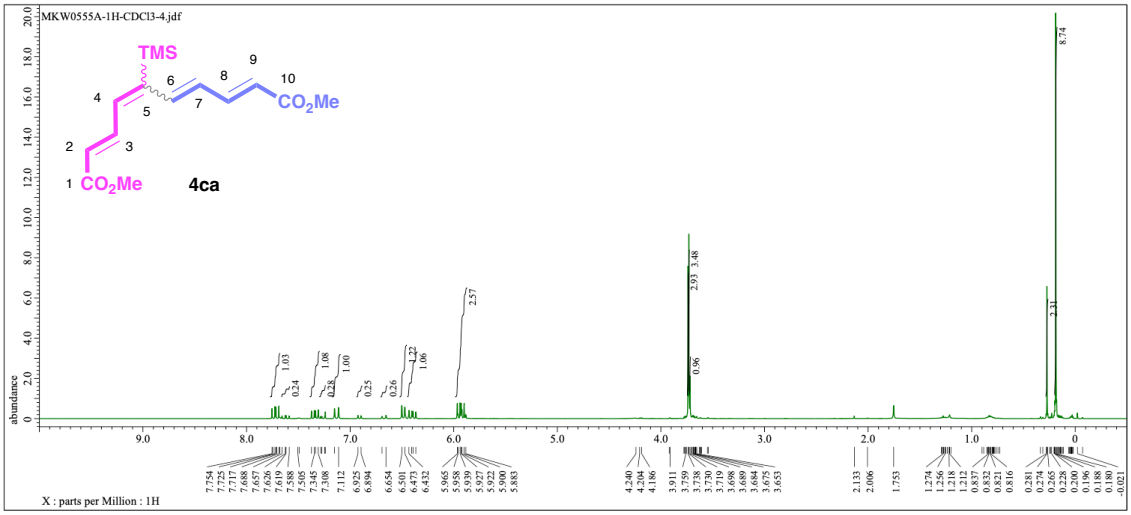


Fig.S24. ^{1}H NMR Spectrum of dimethyl (2*E*,6*E*,8*E*)-5-(trimethylsilyl)deca-2,4,6,8-tetraenedioate (**4ca**) (400 MHz, $CDCl_3$).

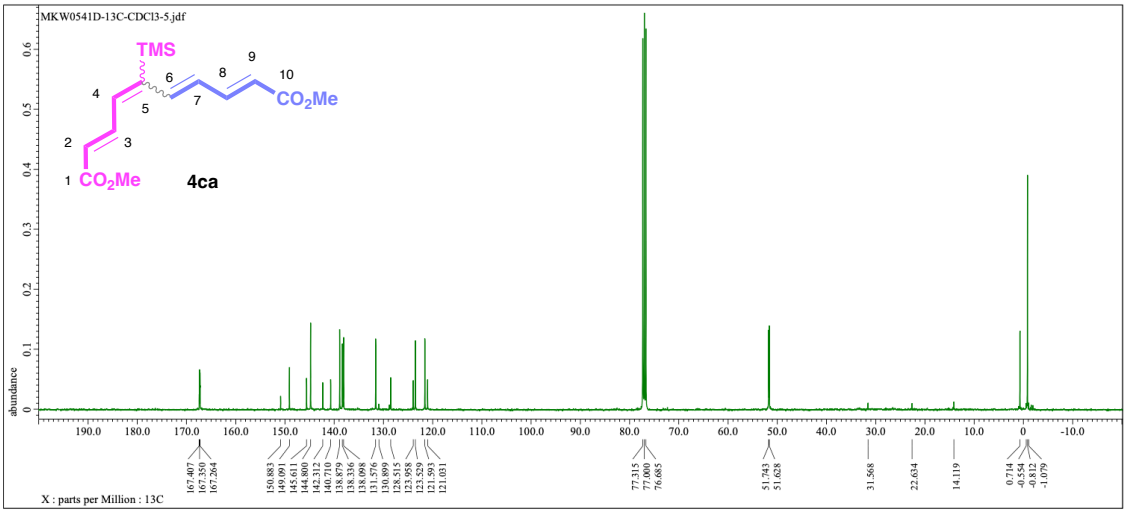


Fig.S25. ^{13}C{^{1}H} NMR Spectrum of dimethyl (2*E*,6*E*,8*E*)-5-(trimethylsilyl)deca-2,4,6,8-tetraenedioate (**4ca**) (100 MHz, $CDCl_3$).

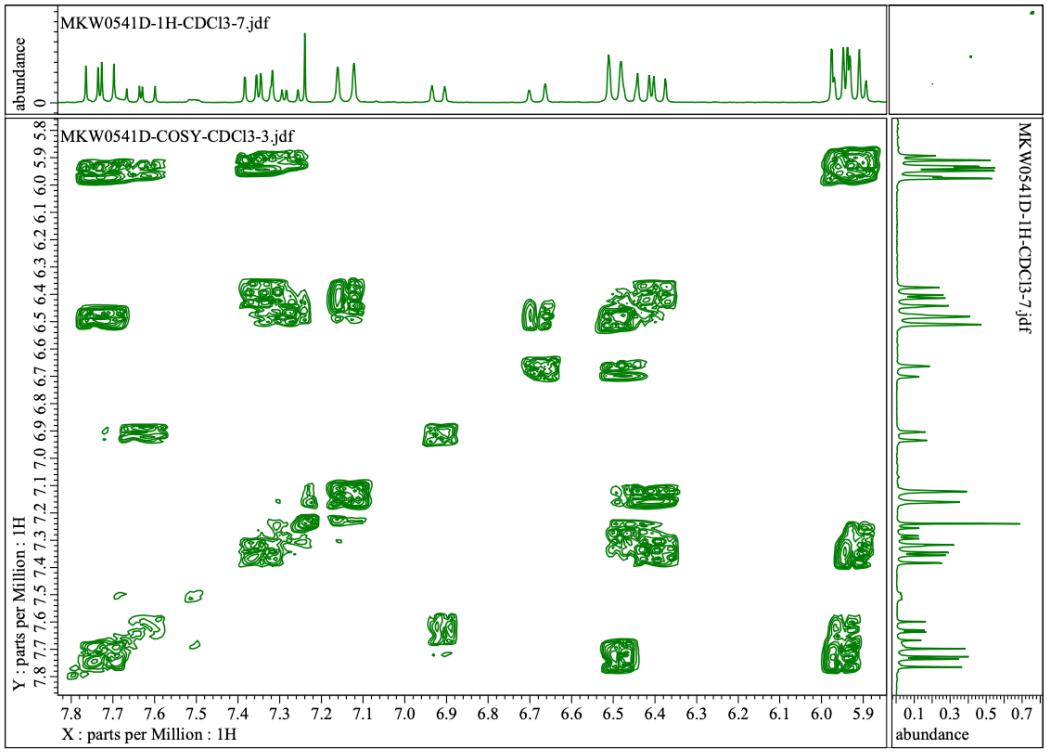


Fig.S26. ^{1}H-^{1}H COSY of dimethyl (2*E*,6*E*,8*E*)-5-(trimethylsilyl)deca-2,4,6,8-tetraenedioate (**4ca**) (400 MHz, $CDCl_3$).

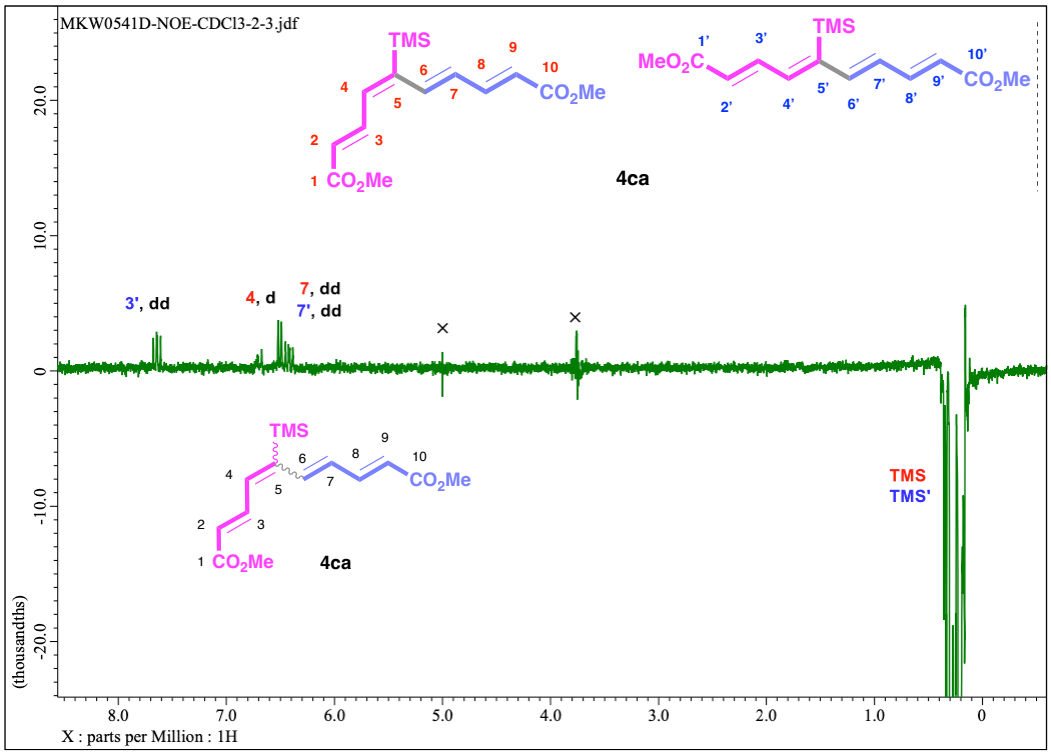


Fig.S27. NOE Spectrum of dimethyl (2*E*,6*E*,8*E*)-5-(trimethylsilyl)deca-2,4,6,8-tetraenedioate (**4ca**) (400 MHz, $CDCl_3$).

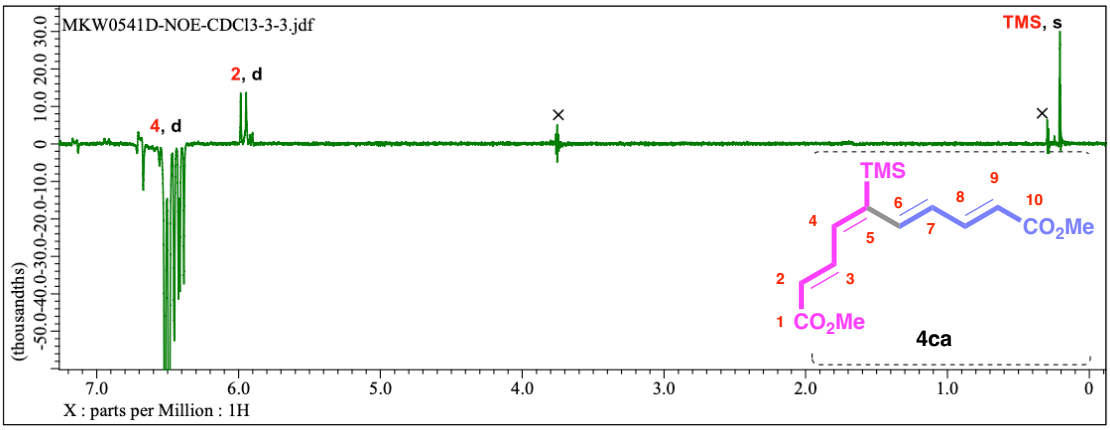


Fig.S28. NOE Spectrum of dimethyl (2*E*,6*E*,8*E*)-5-(trimethylsilyl)deca-2,4,6,8-tetraenedioate (**4ca**) (400 MHz, $CDCl_3$).

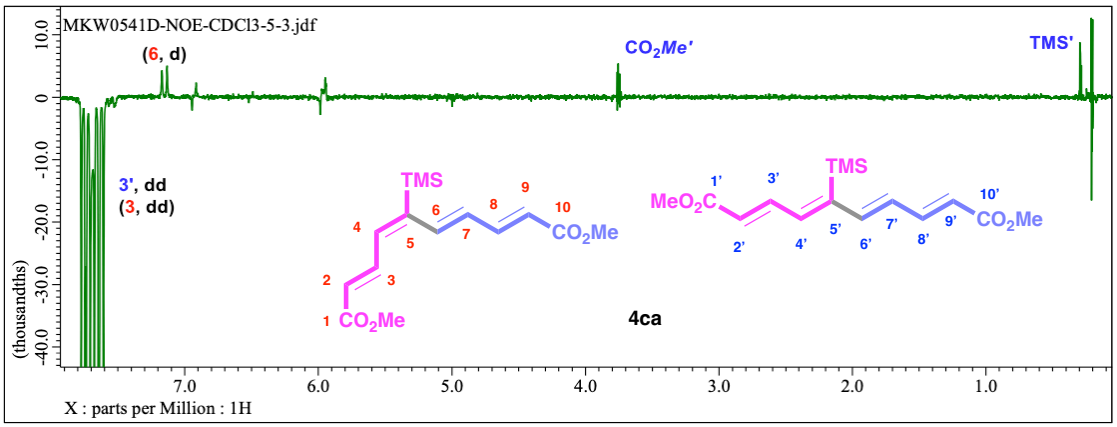


Fig.S29. NOE Spectrum of dimethyl (2*E*,6*E*,8*E*)-5-(trimethylsilyl)deca-2,4,6,8-tetraenedioate (**4ca**) (400 MHz, $CDCl_3$).

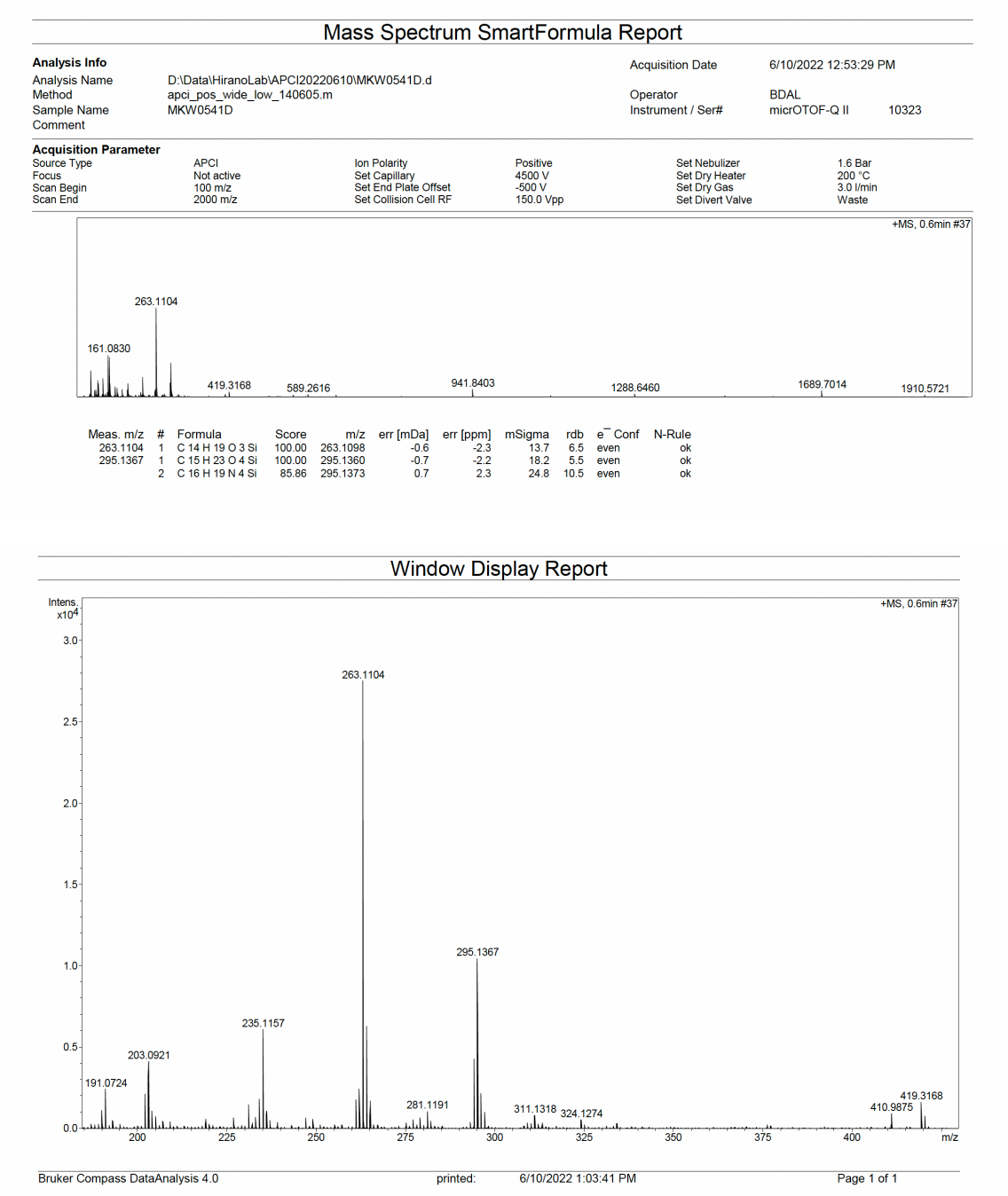


Fig.S30. HRMS Spectra of dimethyl (2*E*,6*E*,8*E*)-5-(trimethylsilyl)deca-2,4,6,8-tetraenedioate (**4ca**) (APCI).

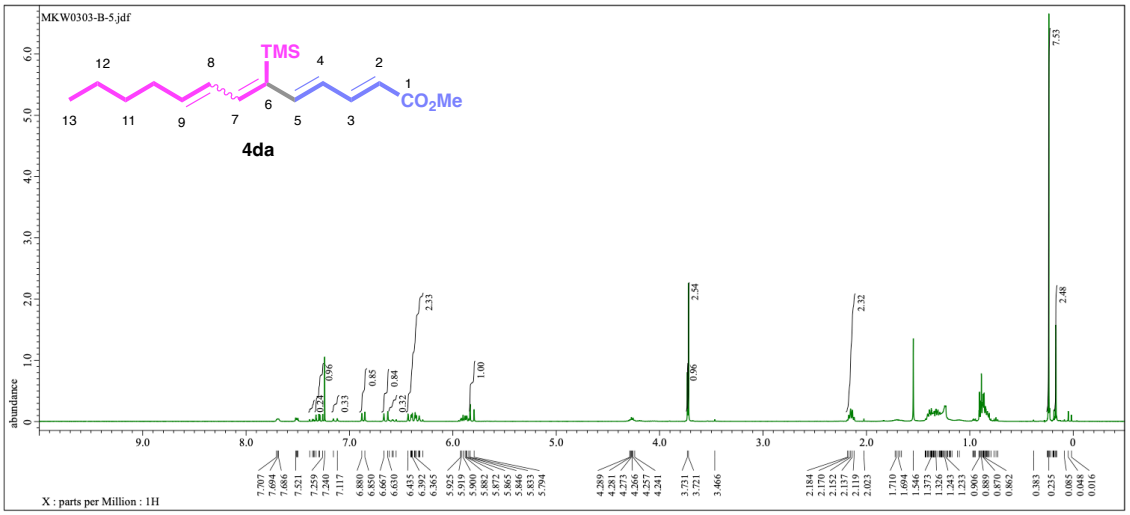


Fig.S31. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)trideca-2,4,6,8-tetraenoate (**4da**) (400 MHz, $CDCl_3$).

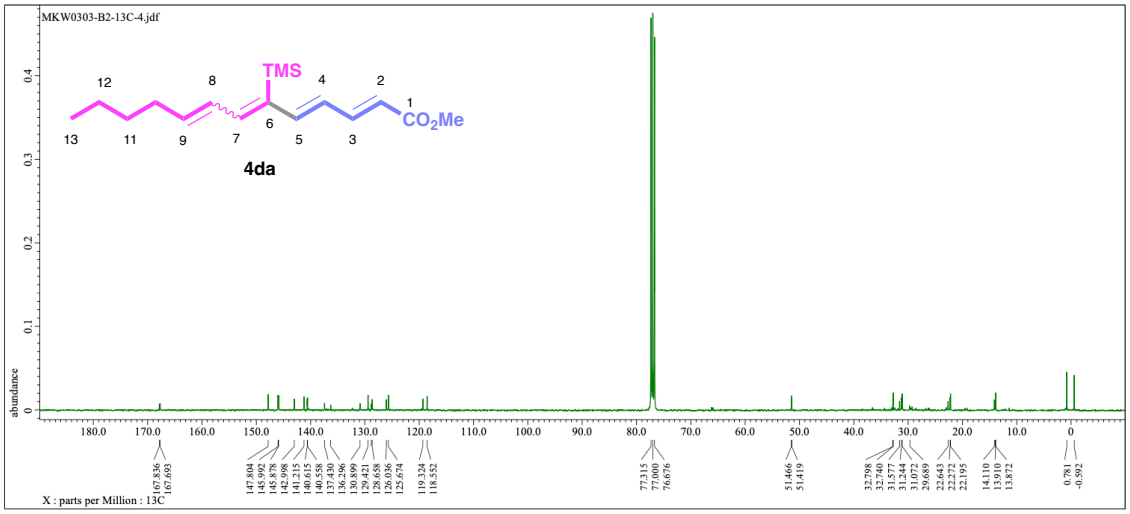


Fig.S32. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)trideca-2,4,6,8-tetraenoate (**4da**) (100 MHz, $CDCl_3$).

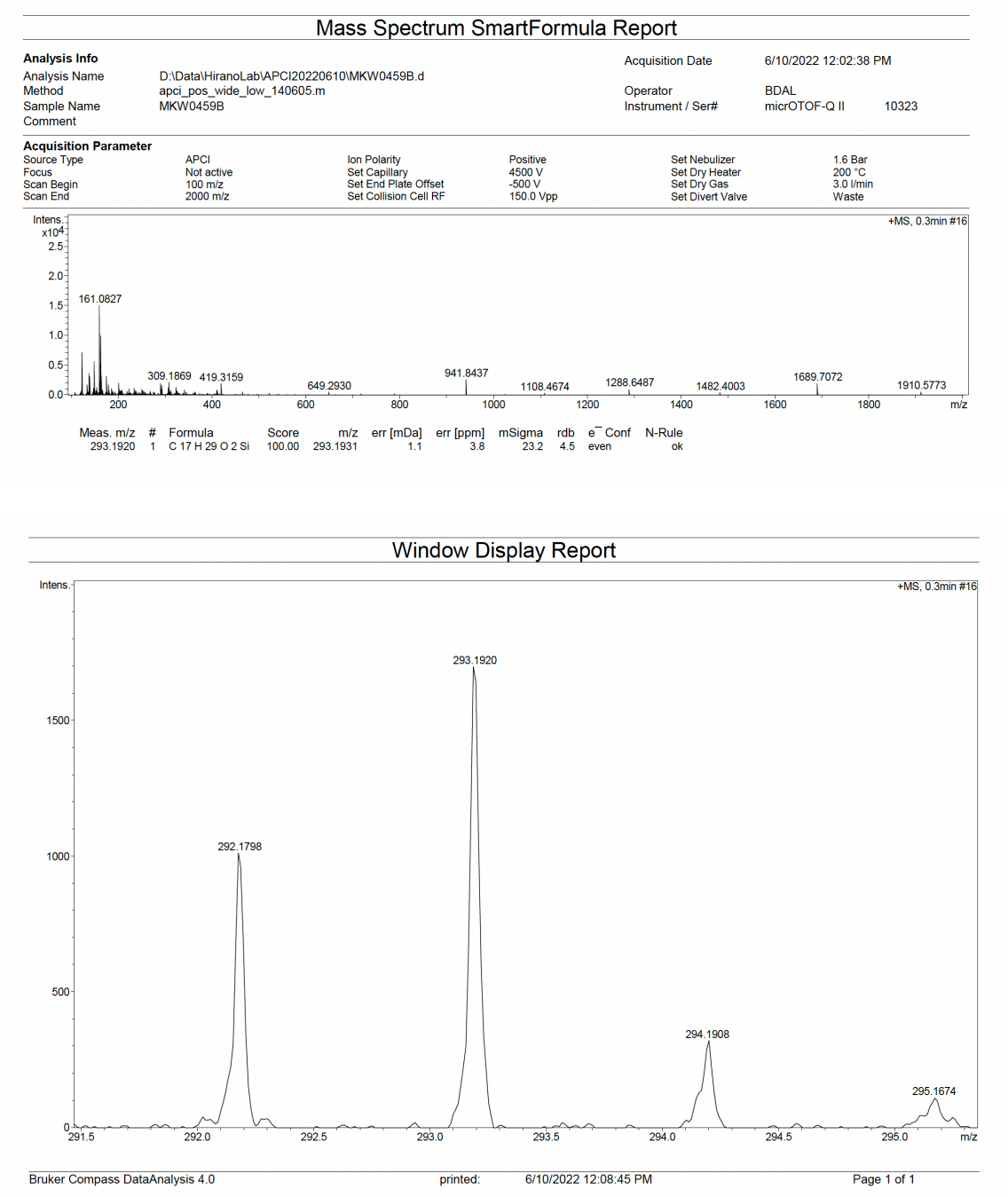


Fig.S33. HRMS Spectra of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)trideca-2,4,6,8-tetraenoate (**4da**) (APCI).

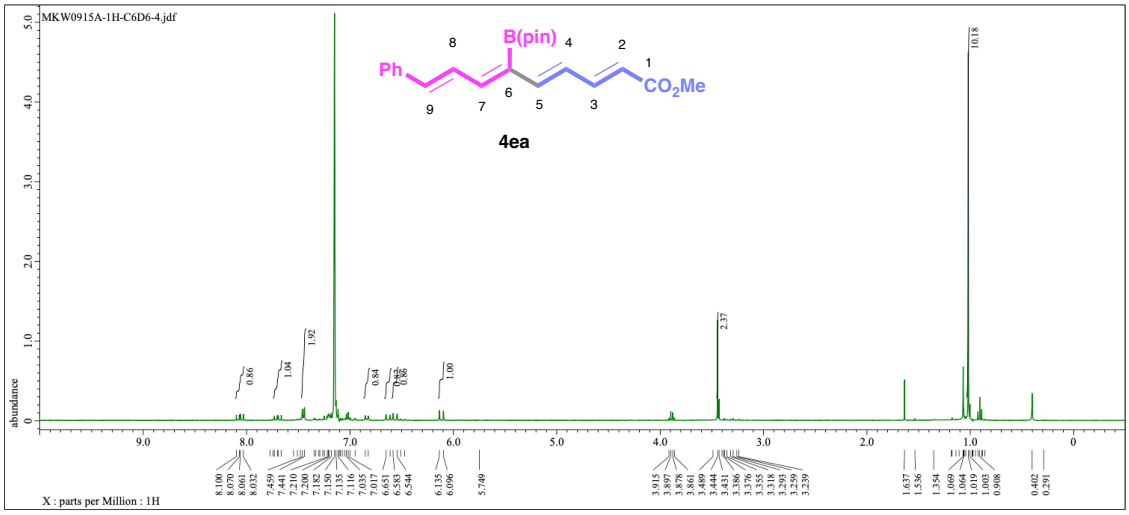


Fig.S34. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)trideca-2,4,6,8-tetraenoate (**4ea**) (400 MHz, $CDCl_3$).

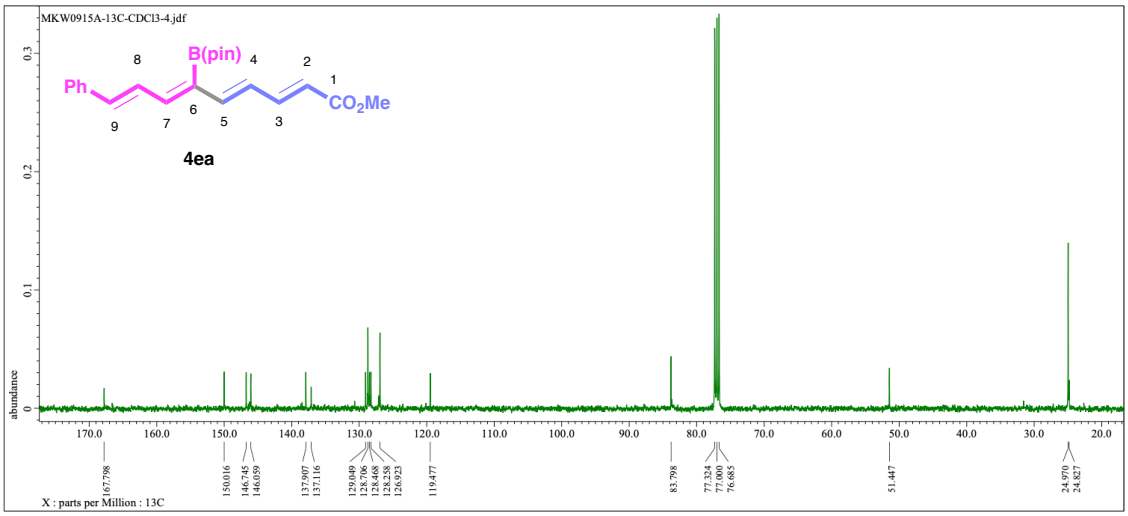


Fig.S35. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)trideca-2,4,6,8-tetraenoate (**4ea**) (100 MHz, $CDCl_3$).

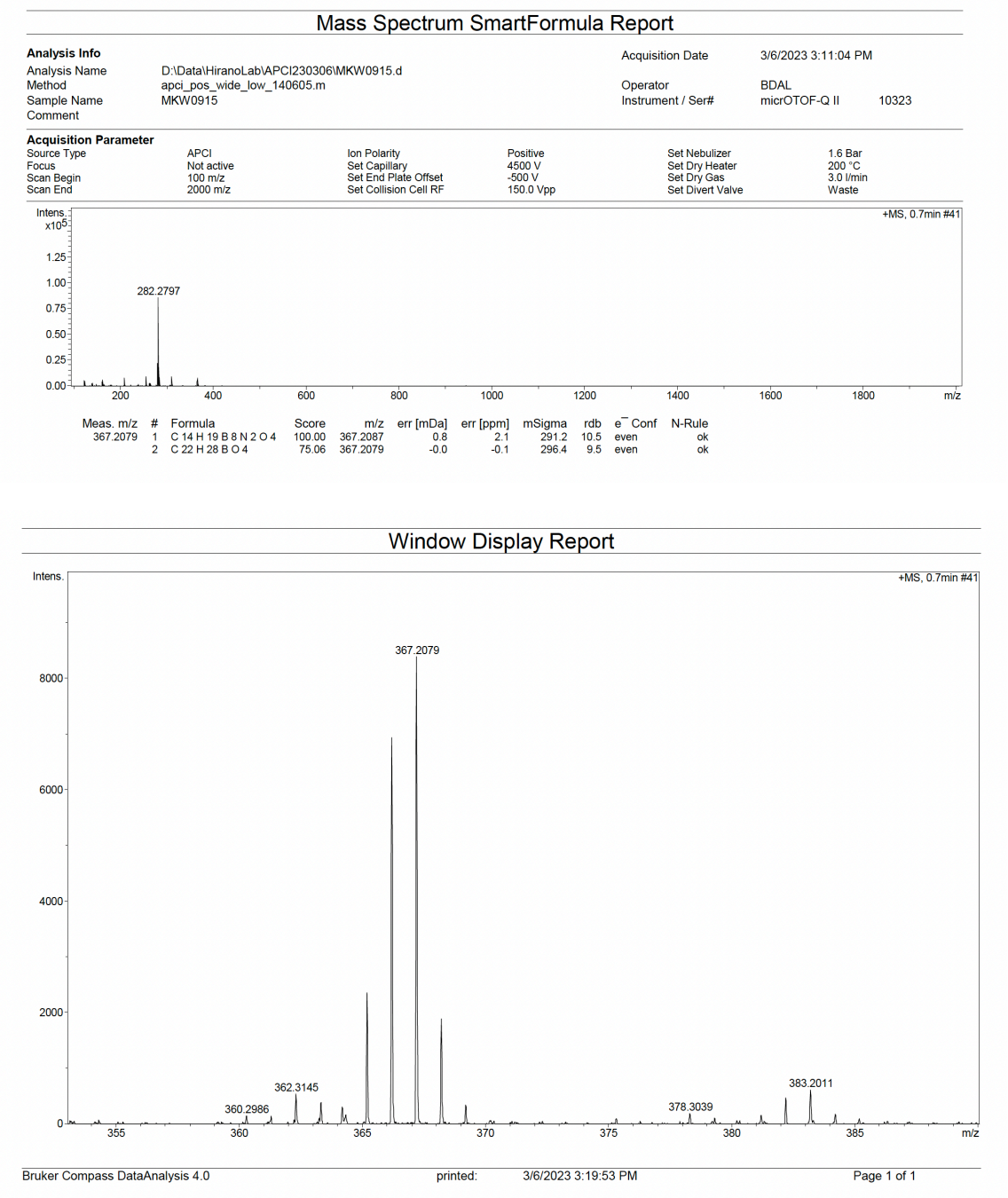


Fig.S36. HRMS Spectra of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)trideca-2,4,6,8-tetraenoate (**4ea**) (APCI).

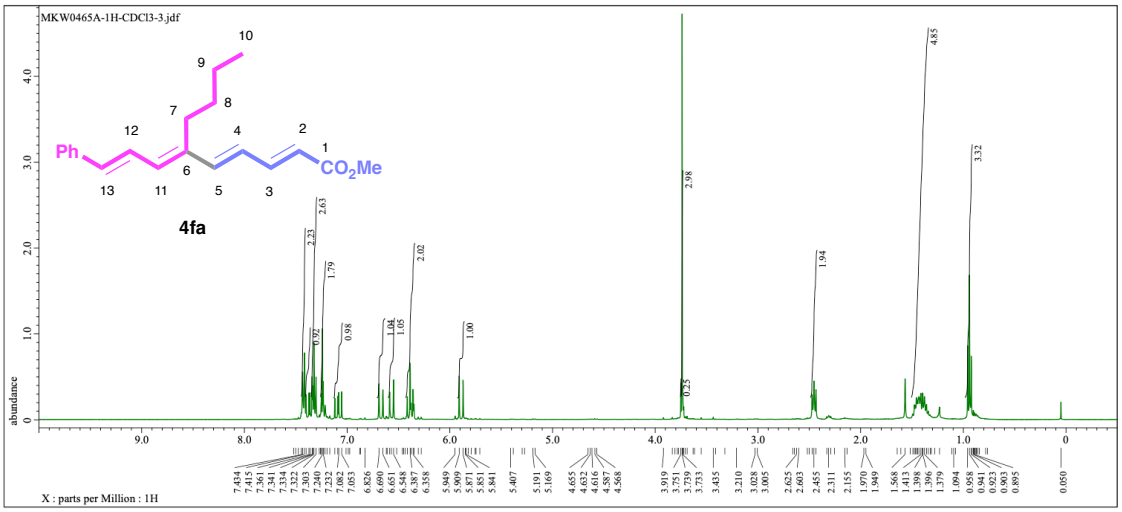


Fig.S37. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,6*E*)-6-((*E*)-3-phenylallylidene)deca-2,4-dienoate (**4fa**) (400 MHz, $CDCl_3$).

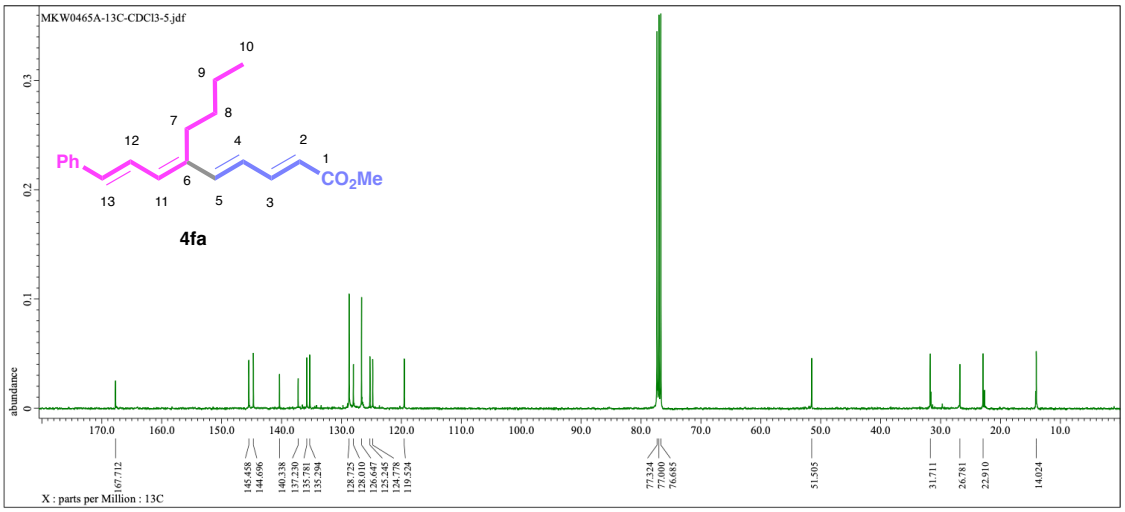


Fig.S38. ^{13}C{^{1}H} NMR Spectrum of methyl (2*E*,4*E*,6*E*)-6-((*E*)-3-phenylallylidene)deca-2,4-dienoate (**4fa**) (100 MHz, $CDCl_3$).

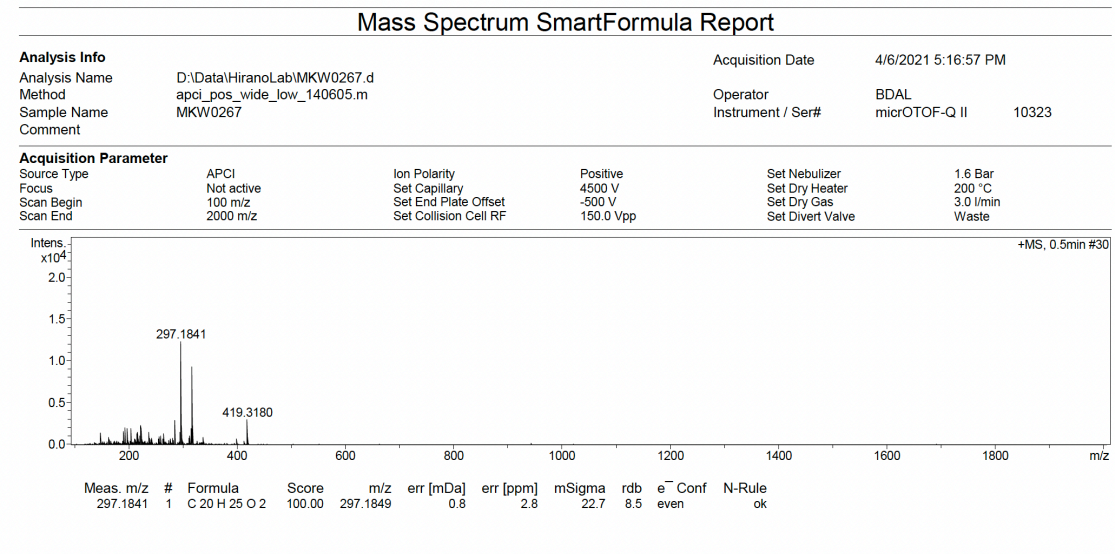


Fig.S39. HRMS Spectrum of methyl (2*E*,4*E*,6*E*)-6-((*E*)-3-phenylallylidene)deca-2,4-dienoate (**4fa**) (APCI).

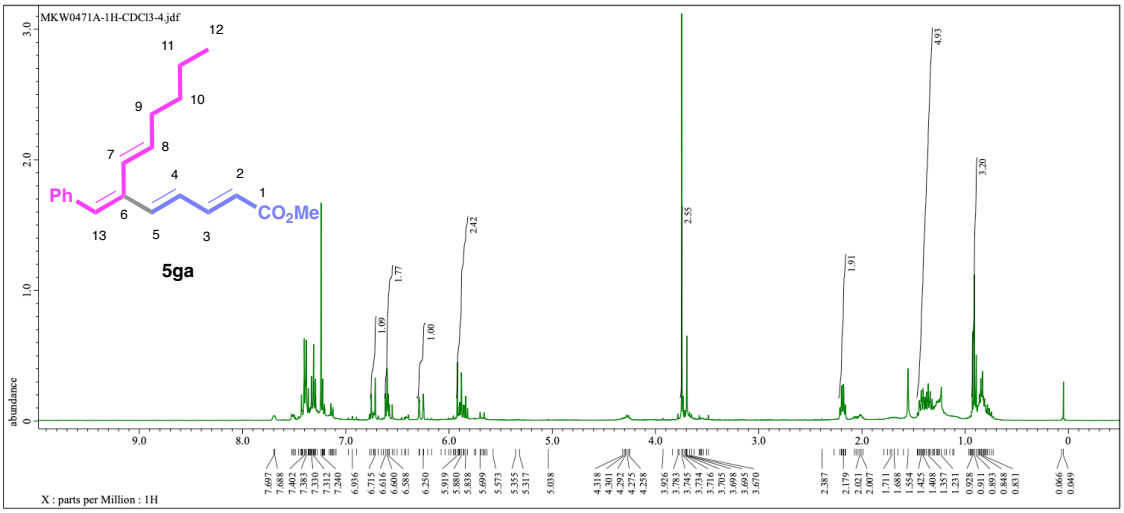


Fig.S40. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,7*E*)-6-((*E*)-3-benzylidene)dodeca-2,4,7-trienoate (**5ga**) (400 MHz, $CDCl_3$).

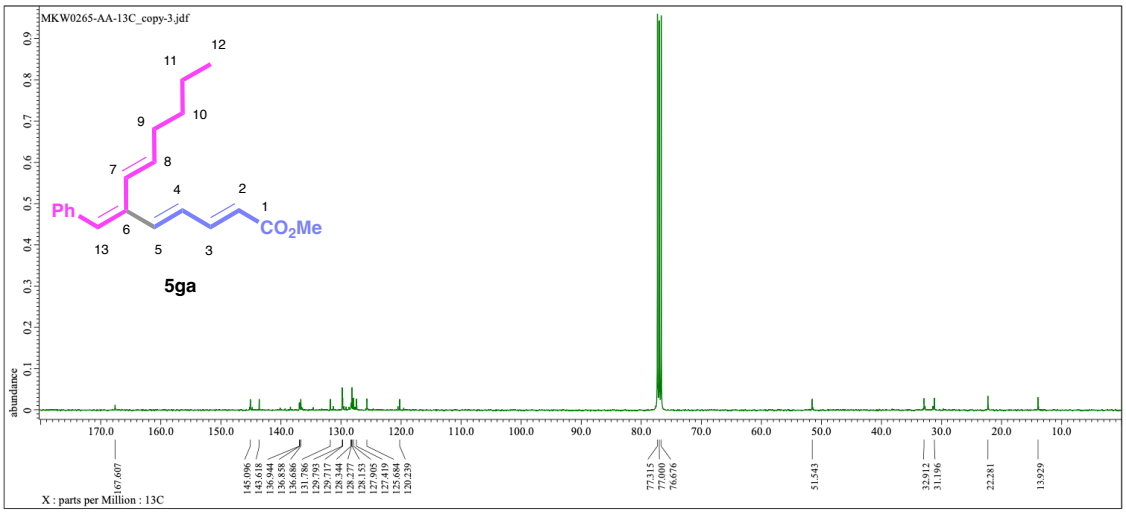


Fig.S41. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl (2*E*,4*E*,7*E*)-6-((*E*)-3-benzylidene)dodeca-2,4,7-trienoate (**5ga**) (100 MHz, $CDCl_3$).

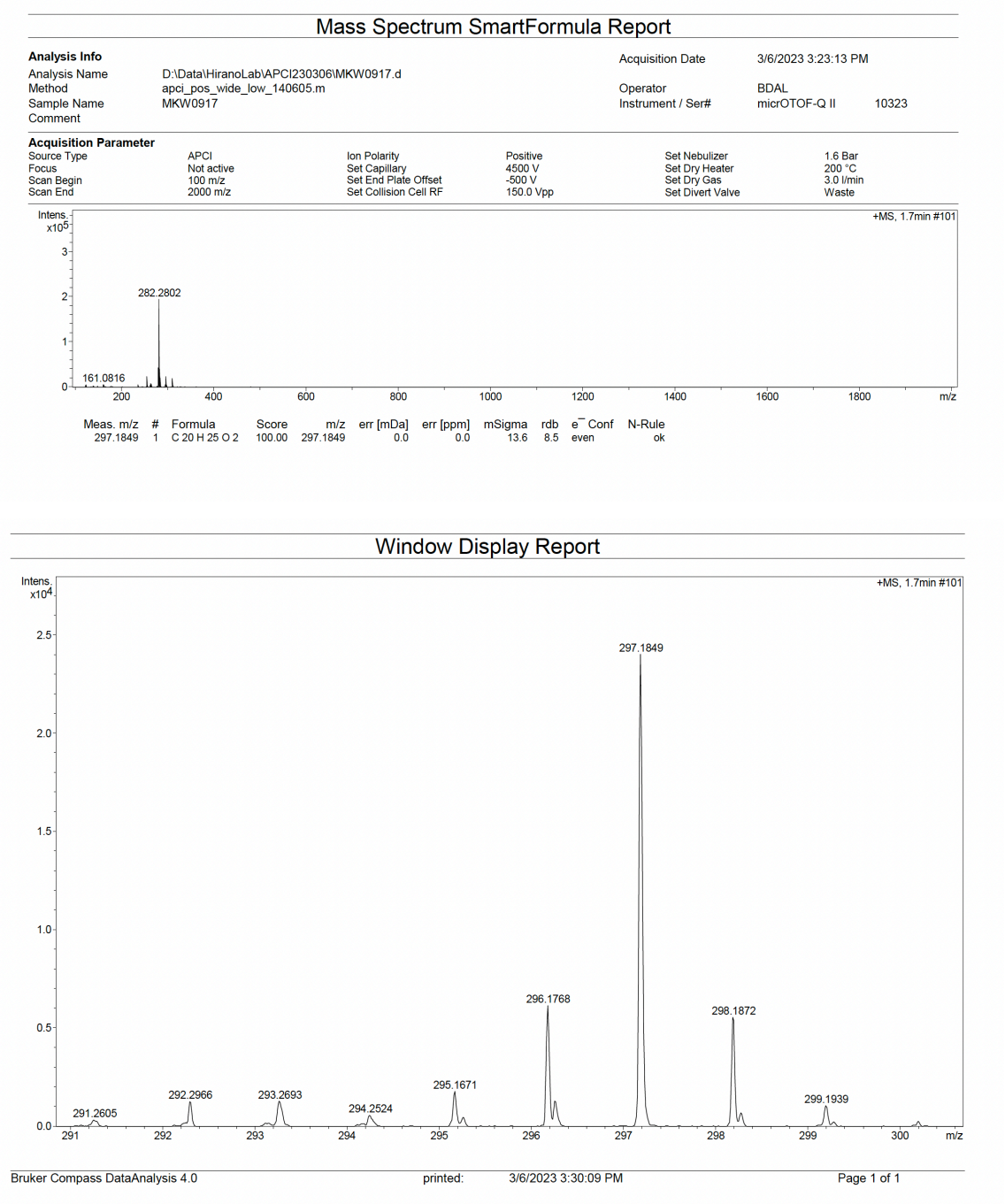


Fig.S42. HRMS Spectra of methyl (2*E*,4*E*,7*E*)-6-((*E*)-3-benzylidene)dodeca-2,4,7-trienoate (**5ga**) (APCI).

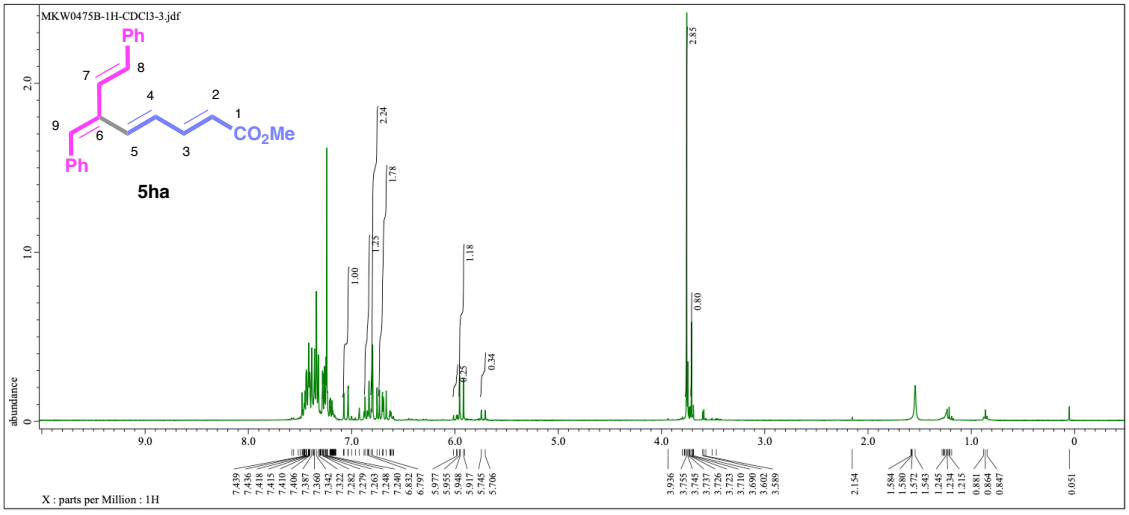


Fig.S43. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,7*E*)-6-((*E*)-benzylidene)-8-phenylocta-2,4,7-trienoate (**5ha**) (400 MHz, $CDCl_3$).

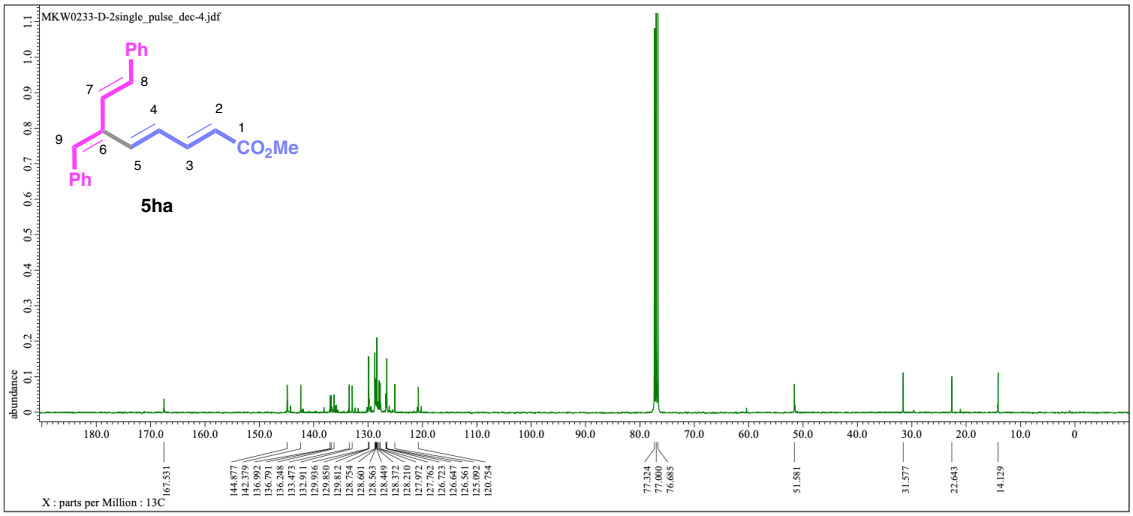


Fig.S44. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl (2*E*,4*E*,7*E*)-6-((*E*)-benzylidene)-8-phenylocta-2,4,7-trienoate (**5ha**) (100 MHz, $CDCl_3$).

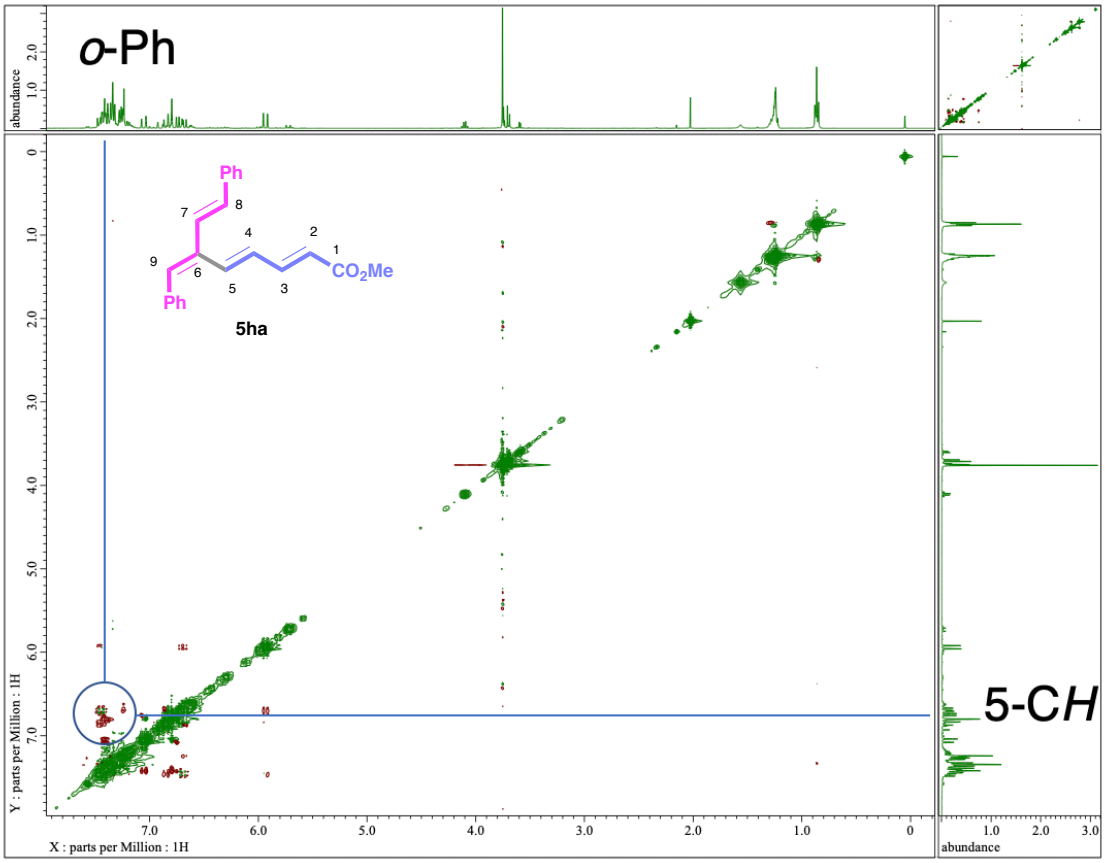


Fig.S45. ^{1}H-^{1}H pNOESY of methyl (2*E*,4*E*,7*E*)-6-((*E*)-benzylidene)-8-phenylocta-2,4,7-trienoate (**5ha**) (400 MHz, $CDCl_3$).

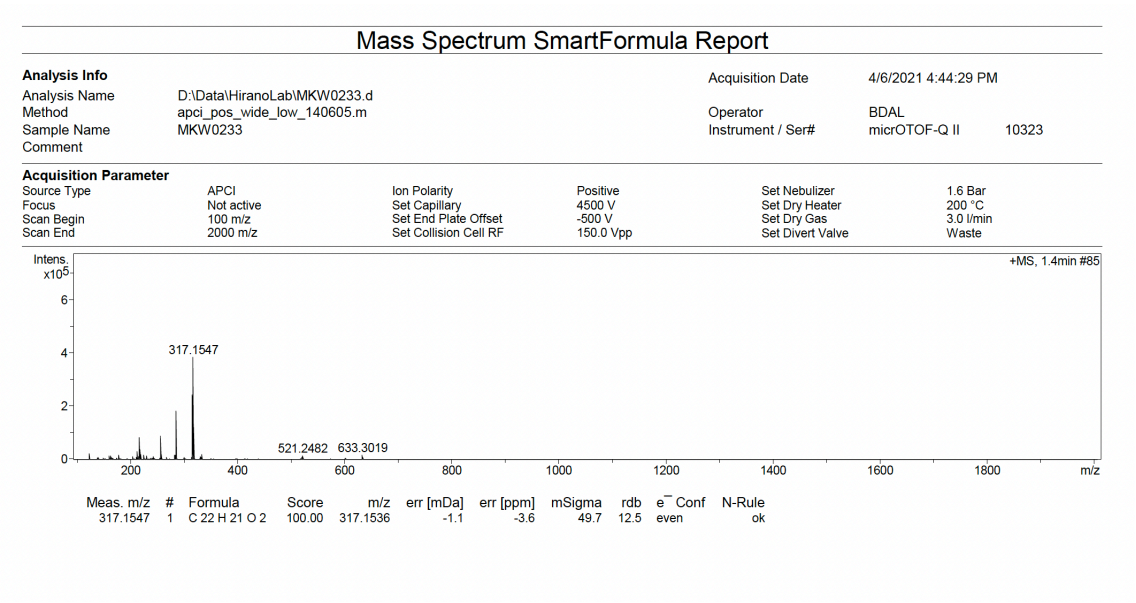


Fig.S46. HRMS Spectrum of methyl (2*E*,4*E*,7*E*)-6-((*E*)-benzylidene)-8-phenylocta-2,4,7-trienoate (**5ha**) (APCI).

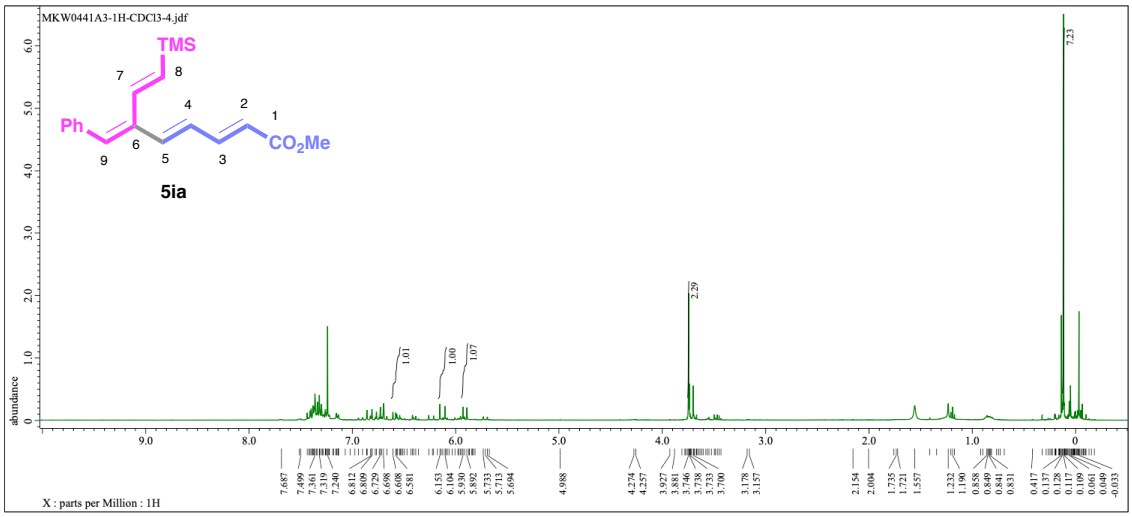


Fig.S47. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,7*E*)-6-((*Z*)-benzylidene)-8-(trimethylsilyl)octa-2,4,7-trienoate (**5ia**) (400 MHz, $CDCl_3$).

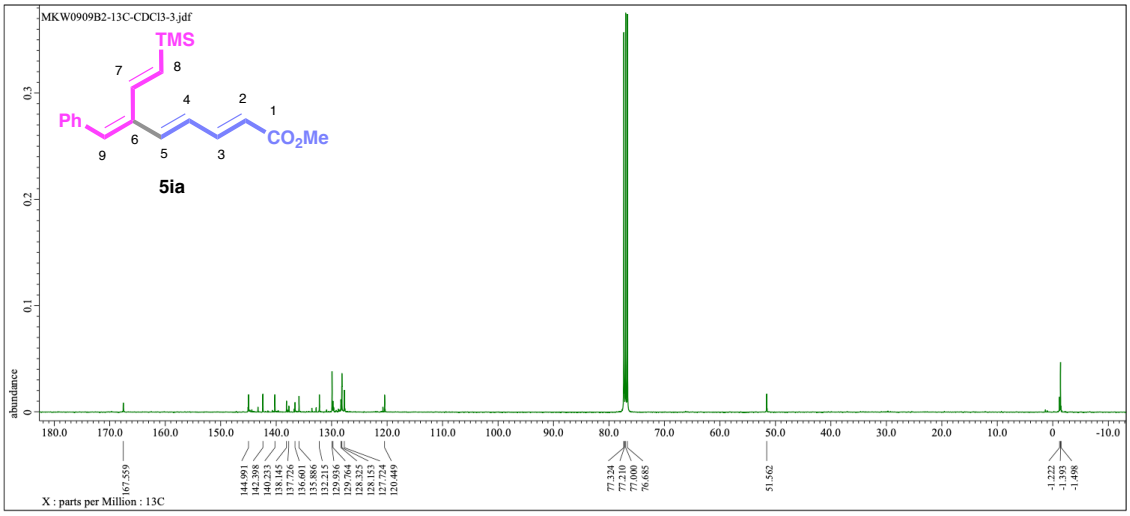


Fig.S48. ^{13}C{^{1}H} NMR Spectrum of methyl (2*E*,4*E*,7*E*)-6-((*Z*)-benzylidene)-8-(trimethylsilyl)octa-2,4,7-trienoate (**5ia**) (100 MHz, $CDCl_3$).

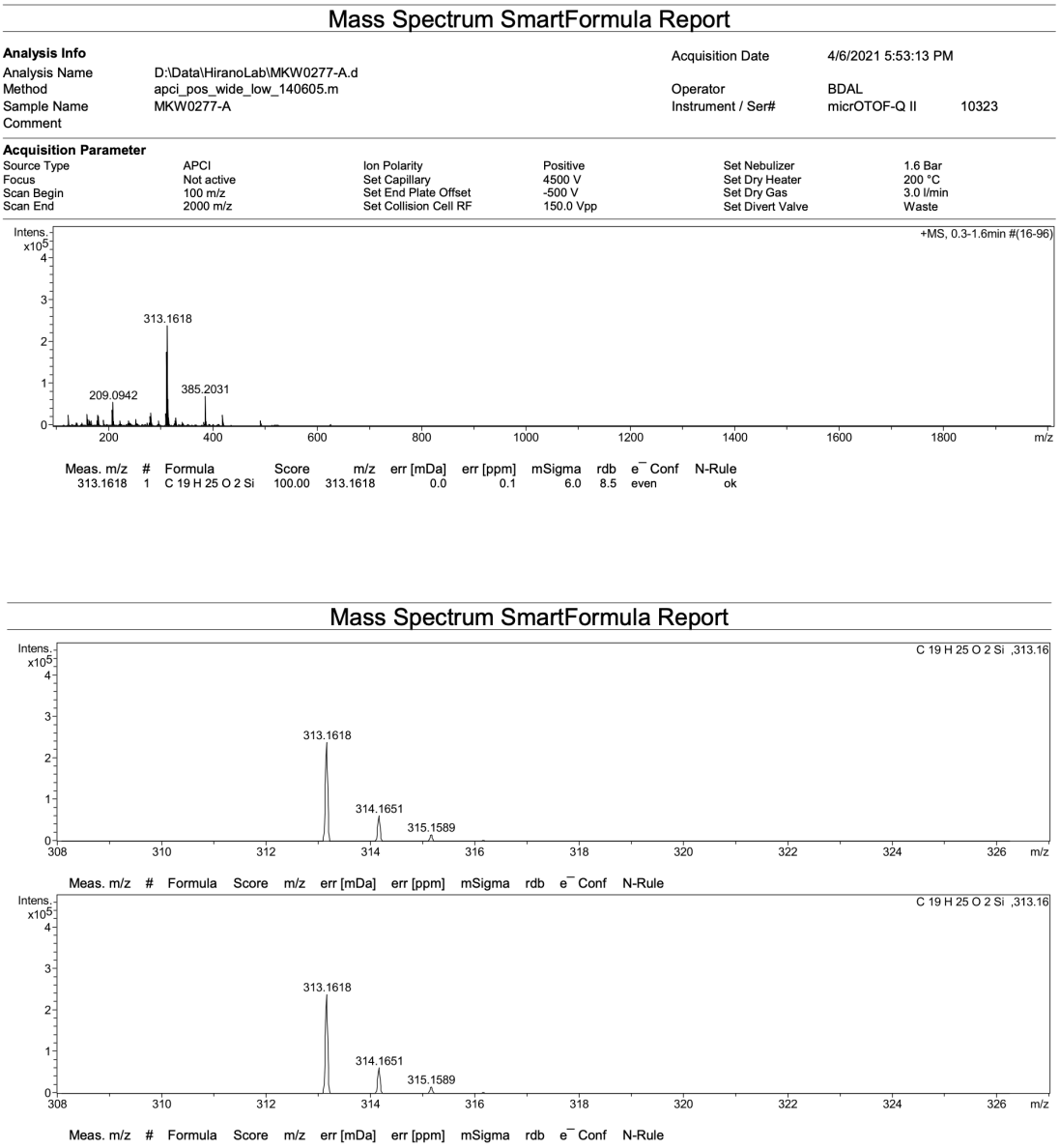


Fig.S49. HRMS Spectra of methyl (2*E*,4*E*,7*E*)-6-((*Z*)-benzylidene)-8-(trimethylsilyl)octa-2,4,7-trienoate (**5ia**) (APCI).

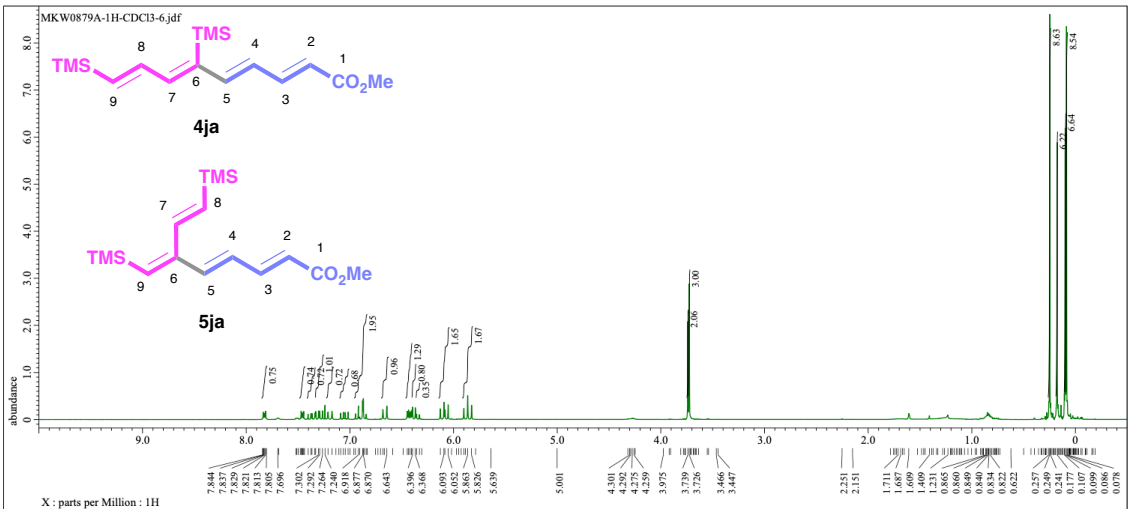


Fig.S50. ^{1}H NMR Spectrum of a mixture of methyl (2*E*,4*E*,6*E*,8*E*)-6,9-bis(trimethylsilyl)nona-2,4,6,8-tetraenoate (**4ja**) and methyl (2*E*,4*E*,6*Z*,7*E*)-8-(trimethylsilyl)-6-((trimethylsilyl)methylene)octa-2,4,7-trienoate (**5ja**) (400 MHz, $CDCl_3$).

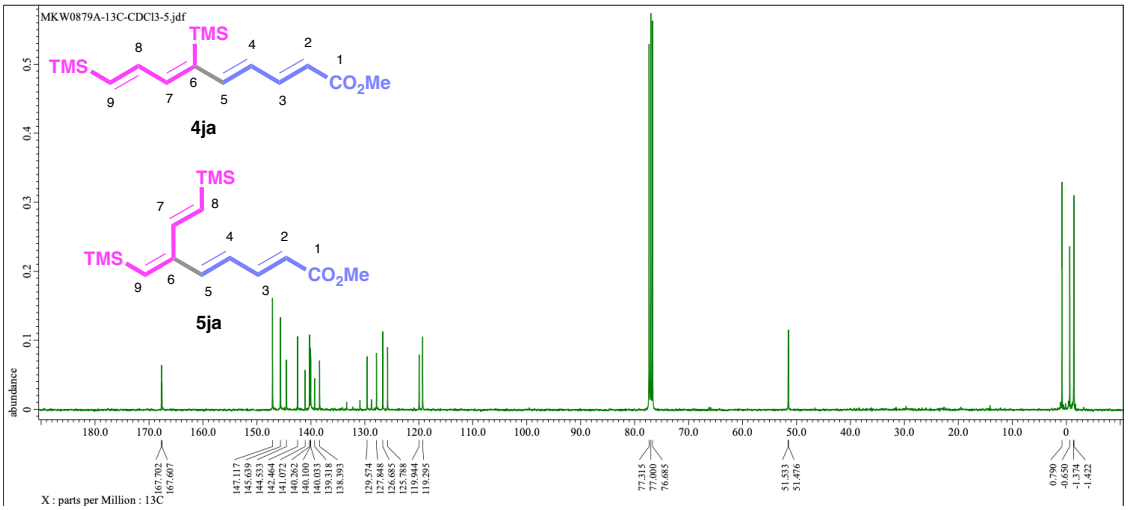


Fig.S51. $^{13}C\{^{1}H\}$ NMR Spectrum of a mixture of methyl (2*E*,4*E*,6*E*,8*E*)-6,9-bis(trimethylsilyl)nona-2,4,6,8-tetraenoate (**4ja**) and methyl (2*E*,4*E*,6*Z*,7*E*)-8-(trimethylsilyl)-6-((trimethylsilyl)methylene)octa-2,4,7-trienoate (**5ja**) (100 MHz, $CDCl_3$).

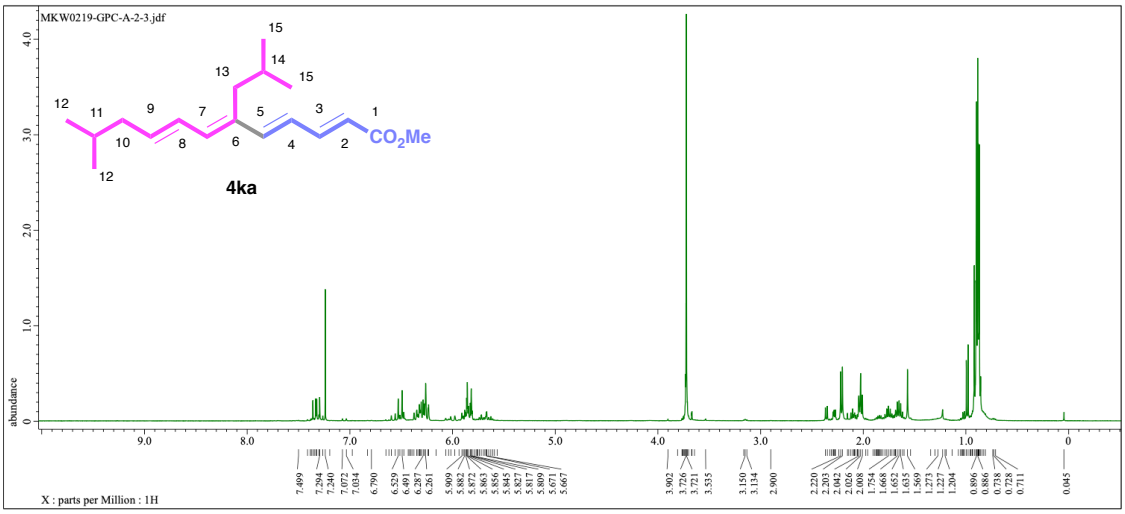


Fig.S52. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,6*E*,8*E*)-6-isobutyl-11-methyldodeca-2,4,6,8-tetraenoate (**4ka**) (400 MHz, $CDCl_3$).

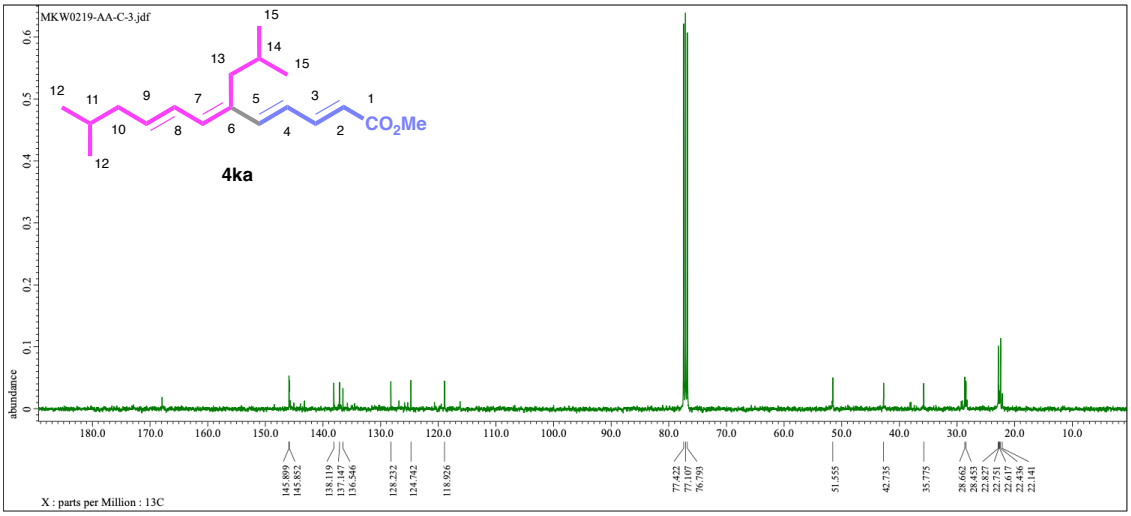


Fig.S53. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl (2*E*,4*E*,6*E*,8*E*)-6-isobutyl-11-methyldodeca-2,4,6,8-tetraenoate (**4ka**) (100 MHz, $CDCl_3$).

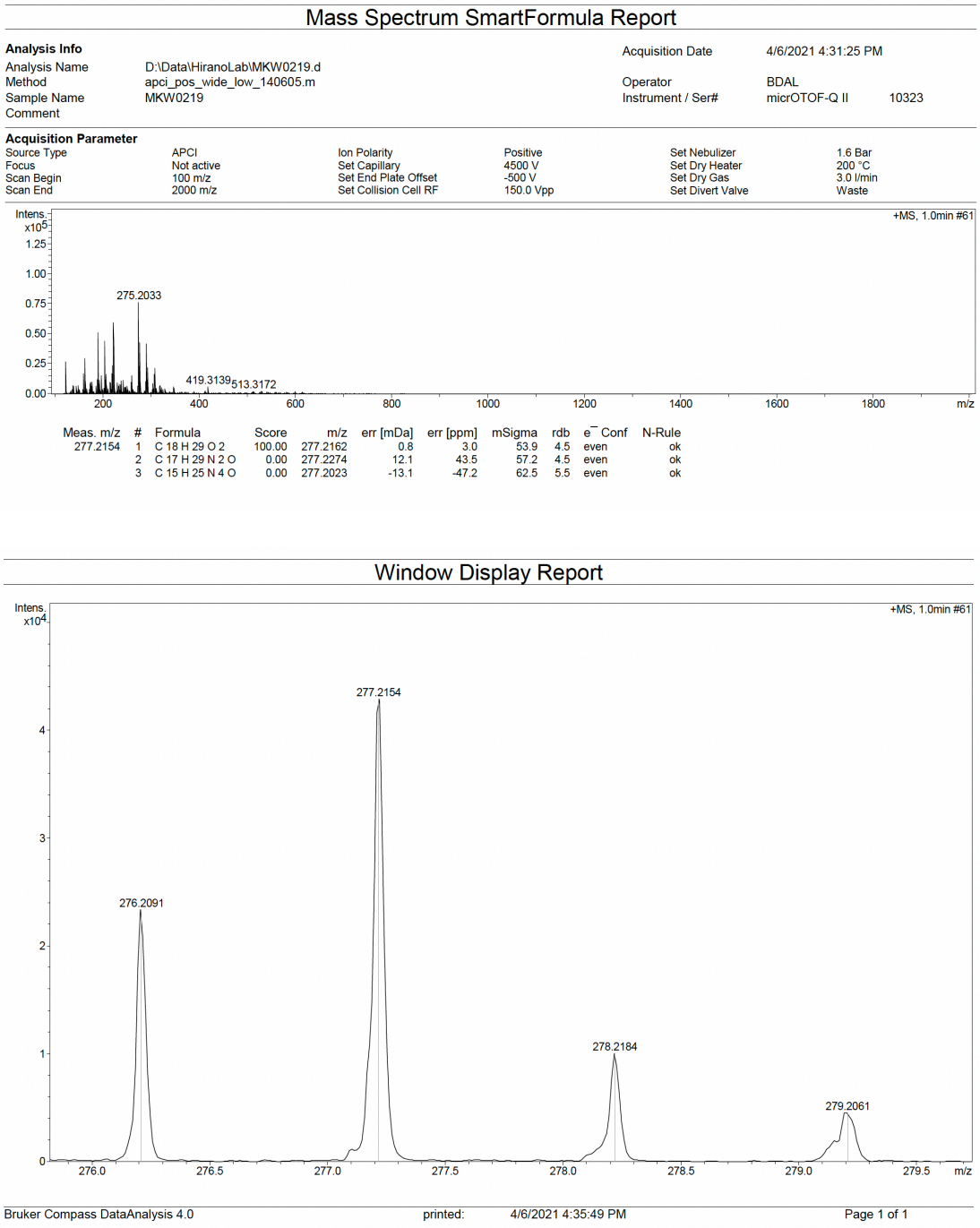


Fig.S54. HRMS Spectra of methyl (2*E*,4*E*,6*E*,8*E*)-6-isobutyl-11-methyldodeca-2,4,6,8-tetraenoate (**4ka**) (APCI).

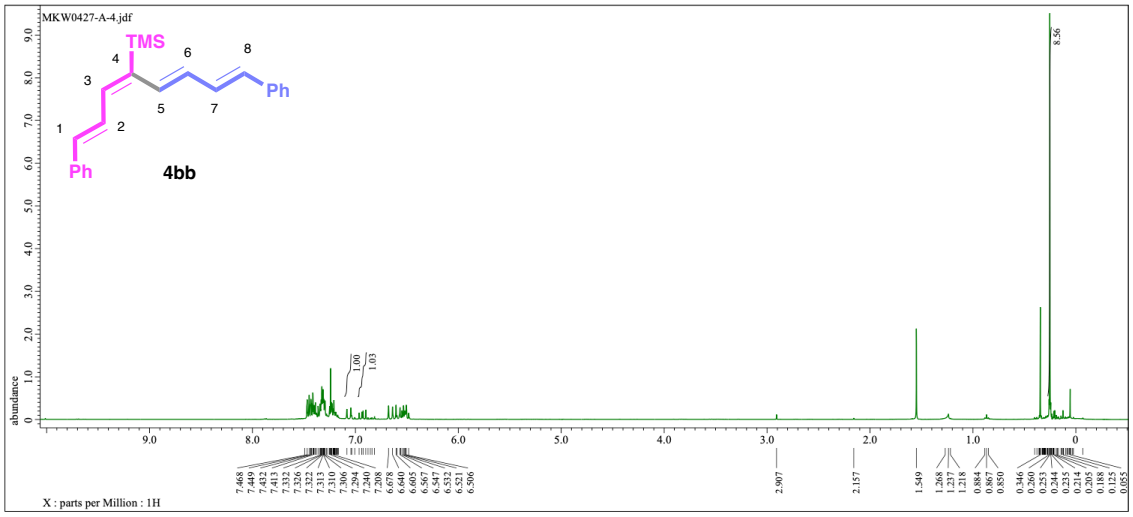


Fig.S55. ^{1}H NMR Spectrum of methyl ((1*E*,3*E*,5*E*,7*E*)-1,8-diphenylocta-1,3,5,7-tetraen-4-yl)trimethylsilane (**4bb**) (400 MHz, $CDCl_3$).

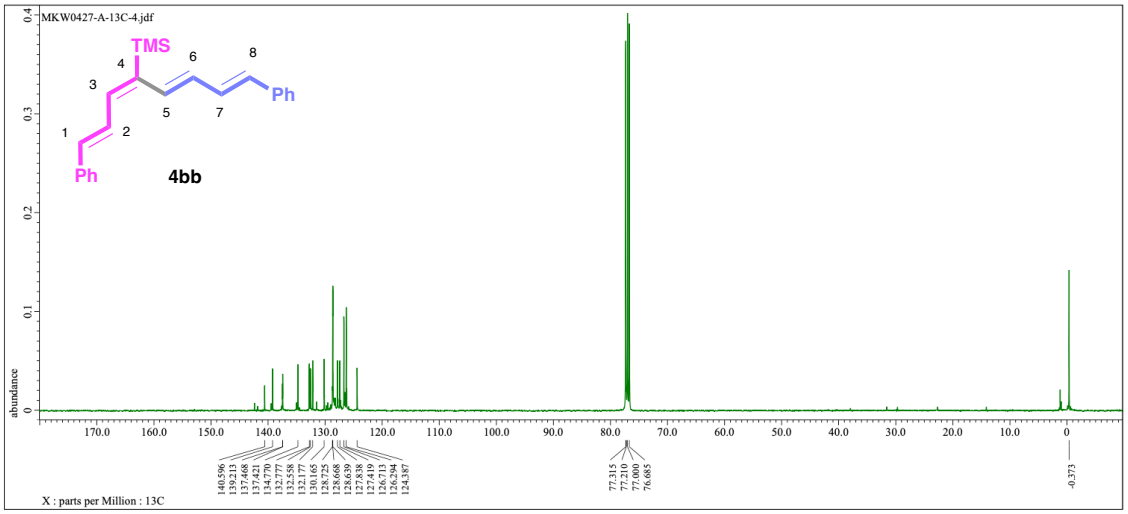


Fig.S56. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl ((1*E*,3*E*,5*E*,7*E*)-1,8-diphenylocta-1,3,5,7-tetraen-4-yl)trimethylsilane (**4bb**) (100 MHz, $CDCl_3$).

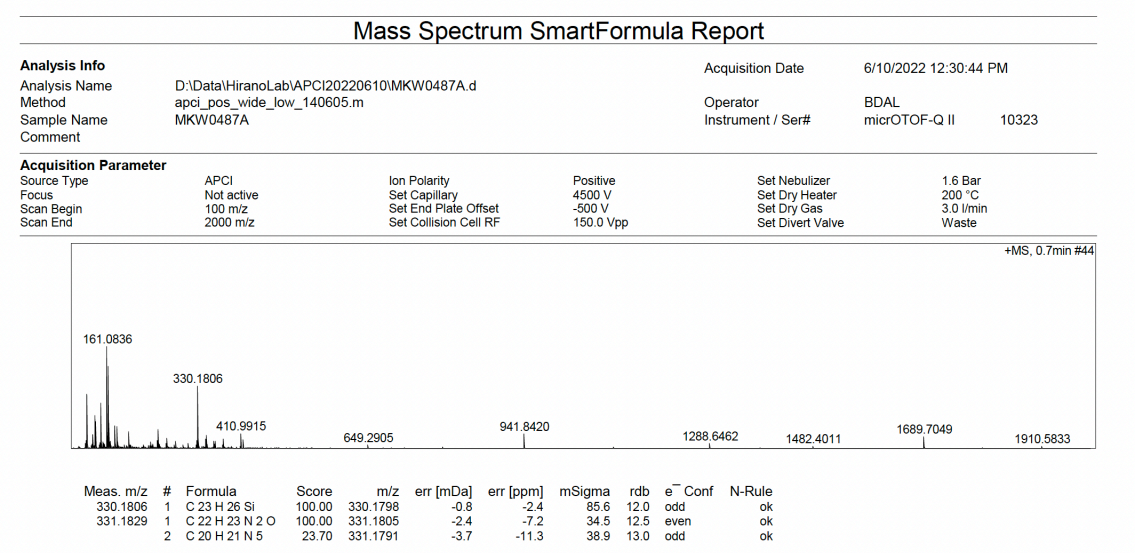


Fig.S57. HRMS Spectrum of methyl ((1*E*,3*E*,5*E*,7*E*)-1,8-diphenylocta-1,3,5,7-tetraen-4-yl)trimethylsilane (**4bb**) (APCI).

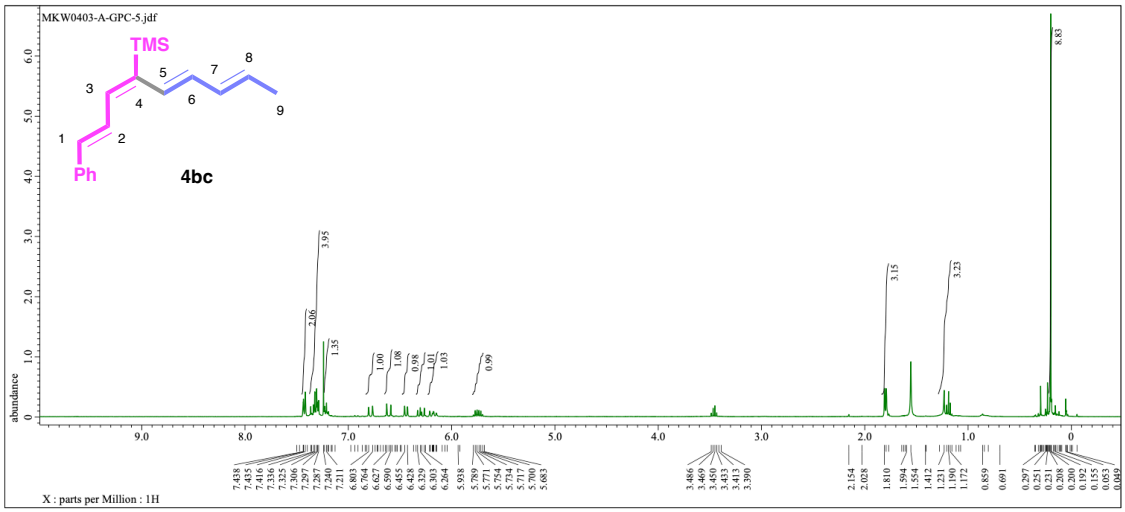


Fig.S58. ^{1}H NMR Spectrum of methyl trimethyl((1*E*,3*E*,5*E*,7*E*)-1-phenylnona-1,3,5,7-tetraen-4-yl)trimethylsilane (**4bc**) (400 MHz, $CDCl_3$).

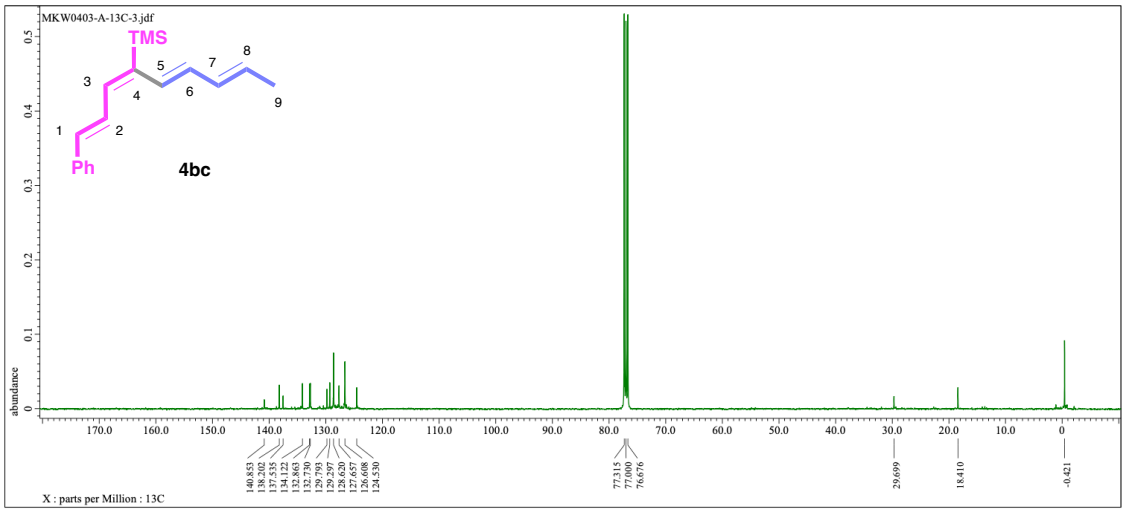


Fig.S59. ^{13}C{^{1}H} NMR Spectra of methyl trimethyl((1*E*,3*E*,5*E*,7*E*)-1-phenylnona-1,3,5,7-tetraen-4-yl)trimethylsilane (**4bc**) (100 MHz, $CDCl_3$).

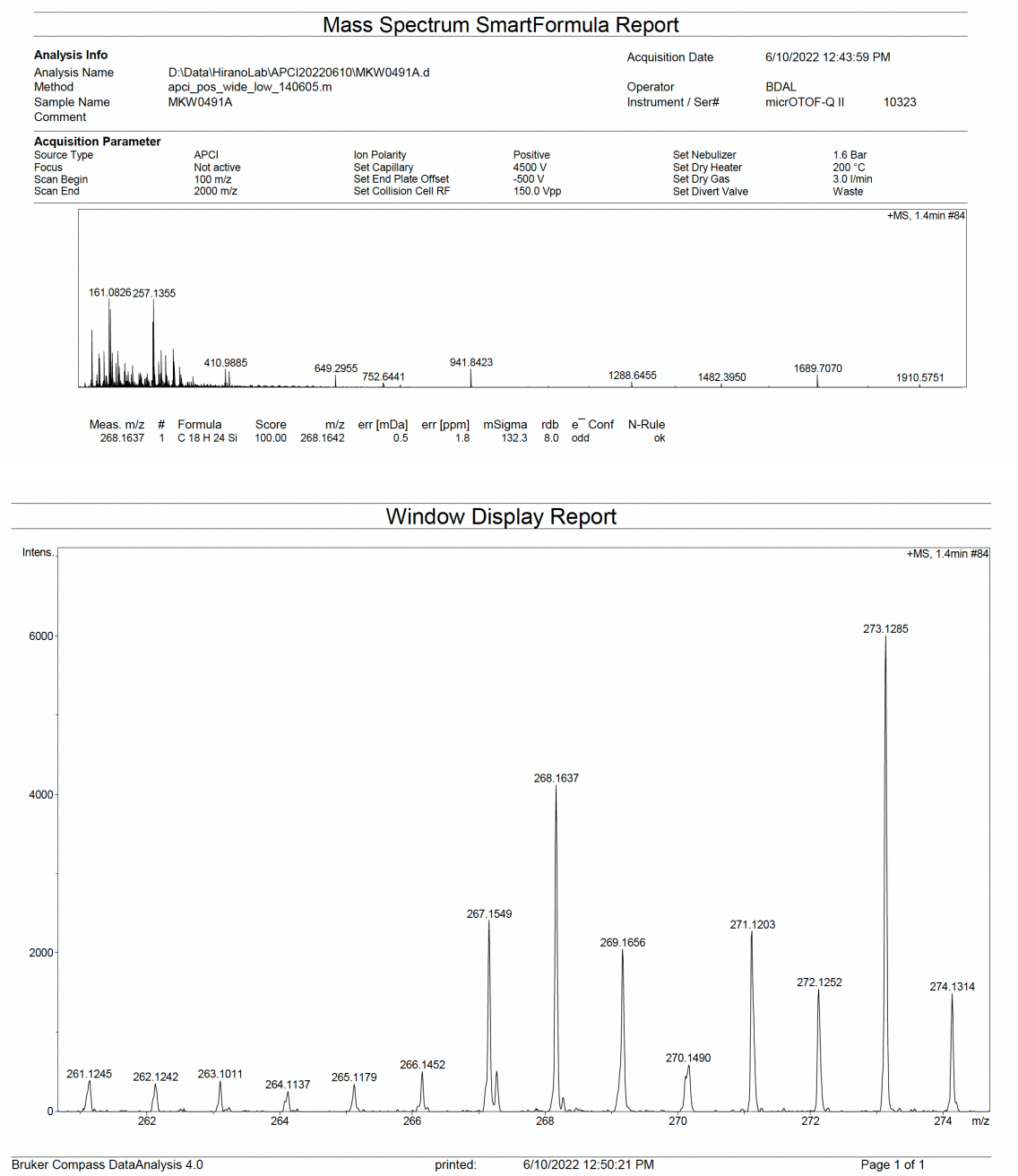


Fig.S60. HRMS Spectra of methyl trimethyl((1*E*,3*E*,5*E*,7*E*)-1-phenylnona-1,3,5,7-tetraen-4-yl)trimethylsilane (**4bc**) (APCI).

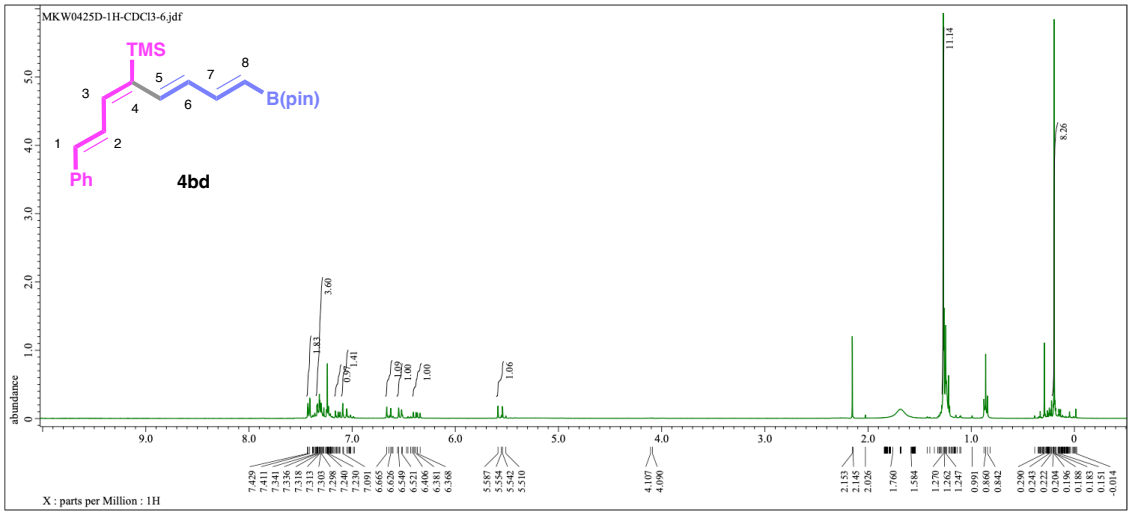


Fig.S61. ^{1}H NMR Spectrum of trimethyl((1*E*,3*E*,5*E*,7*E*)-1-phenyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)octa-1,3,5,7-tetraen-4-yl)silane (**4bd**) (400 MHz, $CDCl_3$).

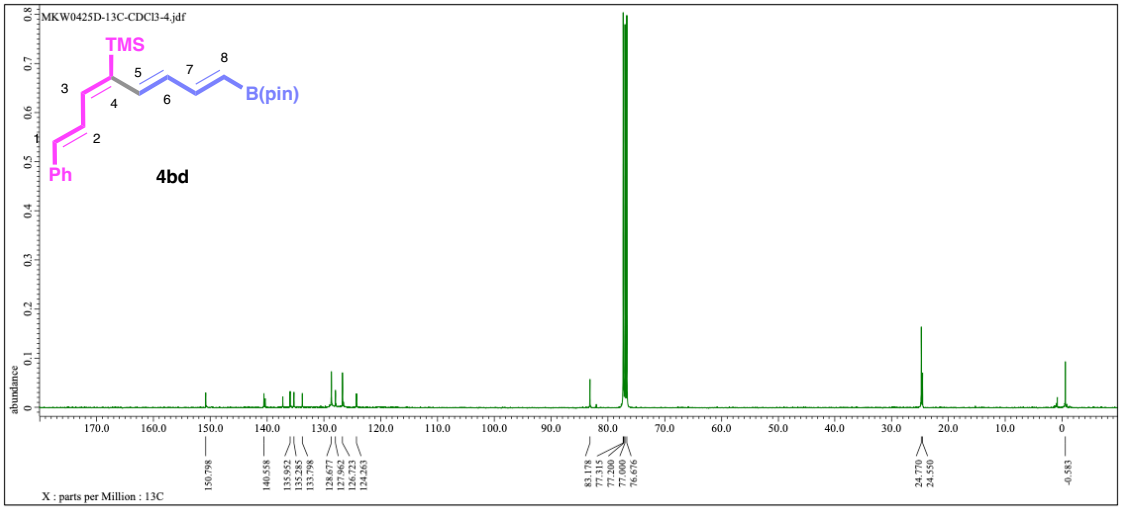


Fig.S62. $^{13}C\{^{1}H\}$ NMR Spectrum of trimethyl((1*E*,3*E*,5*E*,7*E*)-1-phenyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)octa-1,3,5,7-tetraen-4-yl)silane (**4bd**) (100 MHz, $CDCl_3$).

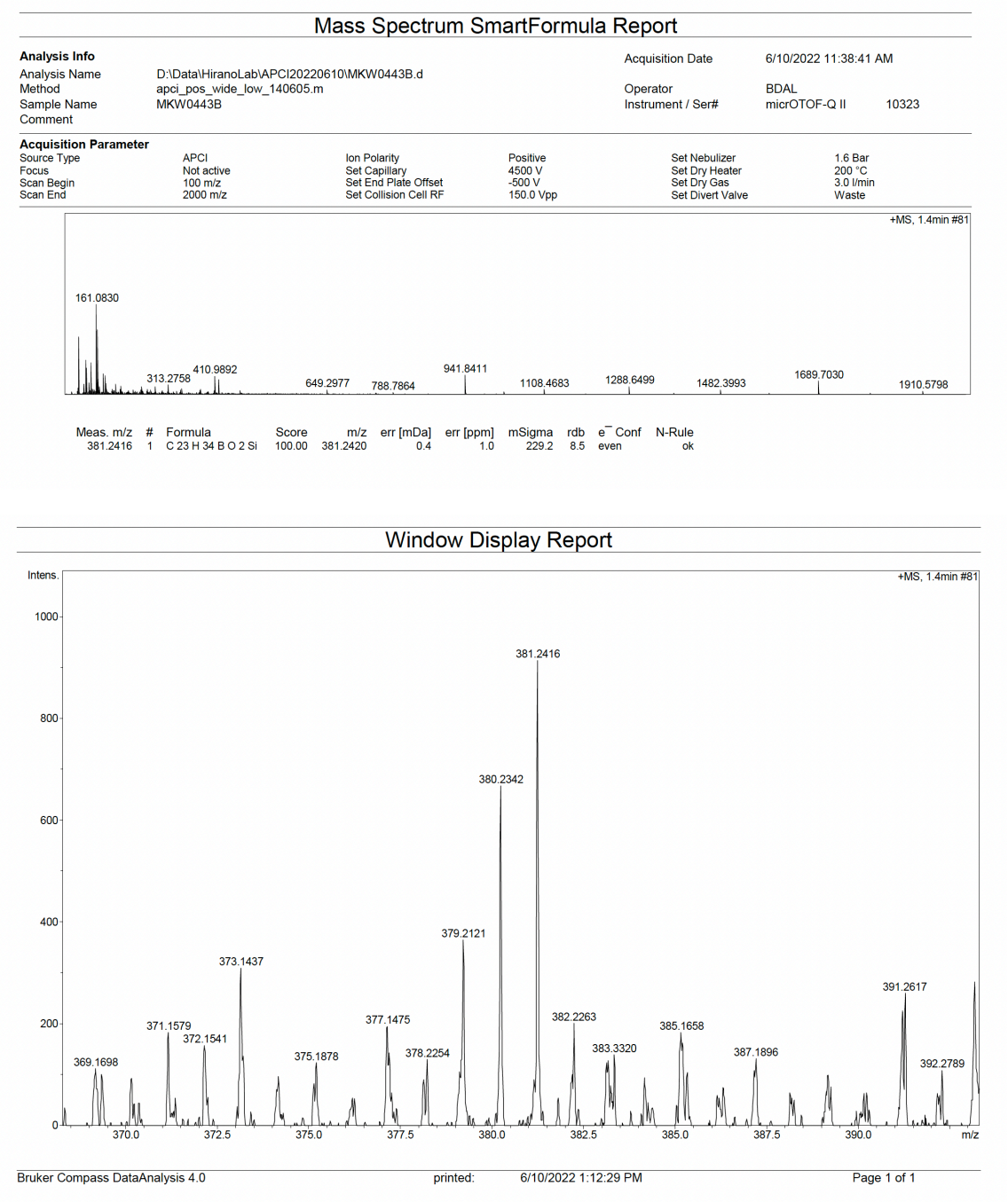


Fig.S63. HRMS Spectra of trimethyl((1*E*,3*E*,5*E*,7*E*)-1-phenyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)octa-1,3,5,7-tetraen-4-yl)silane (**4bd**) (APCI).

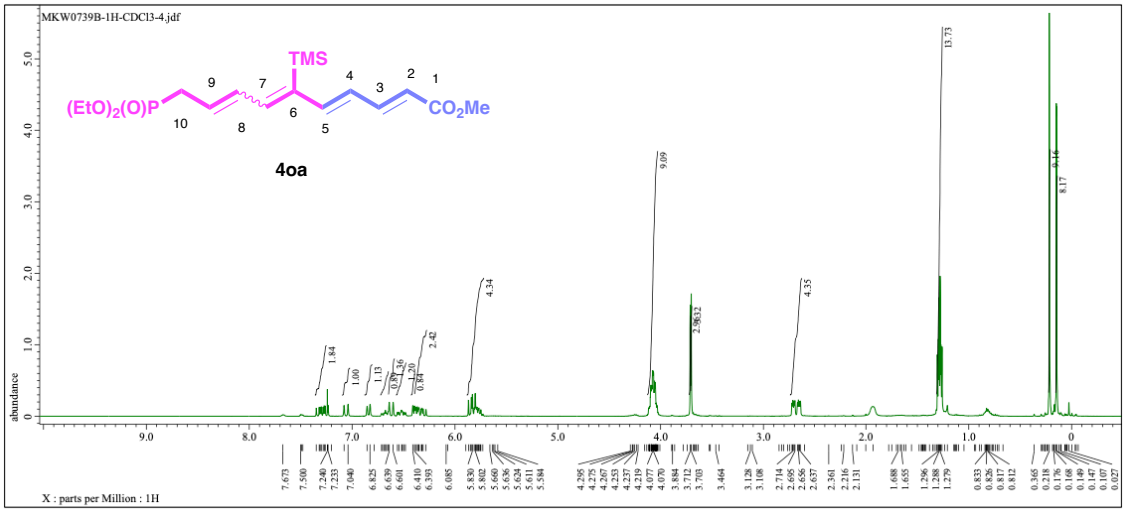


Fig.S64. ^{1}H NMR Spectrum of a mixture of methyl (2*E*,4*E*,6*Z*,8*E*)-10-(diethoxyphosphoryl)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4oa**) and methyl (2*E*,4*E*,6*E*,8*E*)-10-(diethoxyphosphoryl)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4oa**) (400 MHz, $CDCl_3$).

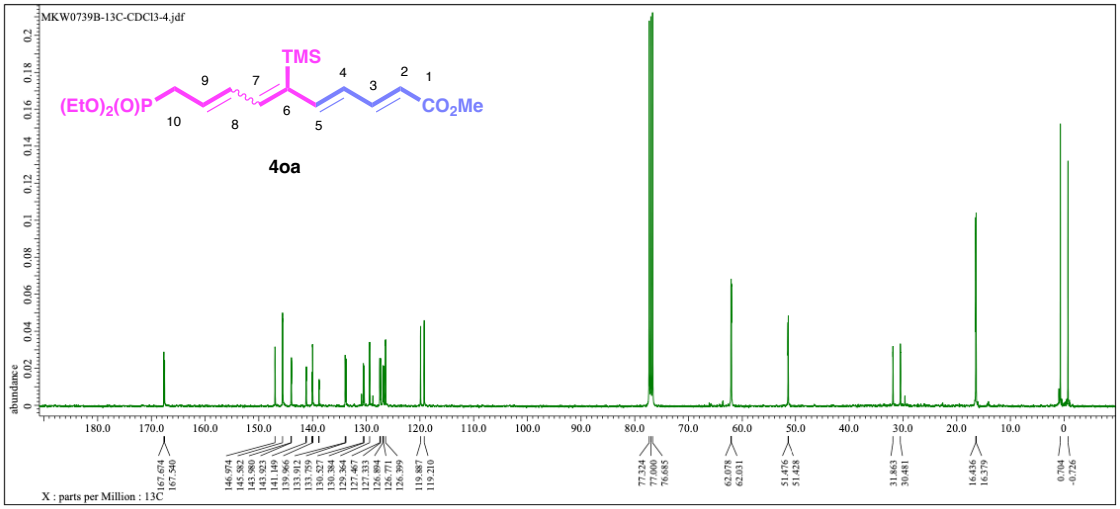


Fig.S65. $^{13}\{^{1}H\}$ NMR Spectrum of a mixture of methyl (2*E*,4*E*,6*Z*,8*E*)-10-(diethoxyphosphoryl)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4oa**) and methyl (2*E*,4*E*,6*E*,8*E*)-10-(diethoxyphosphoryl)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4oa**) (100 MHz, $CDCl_3$).

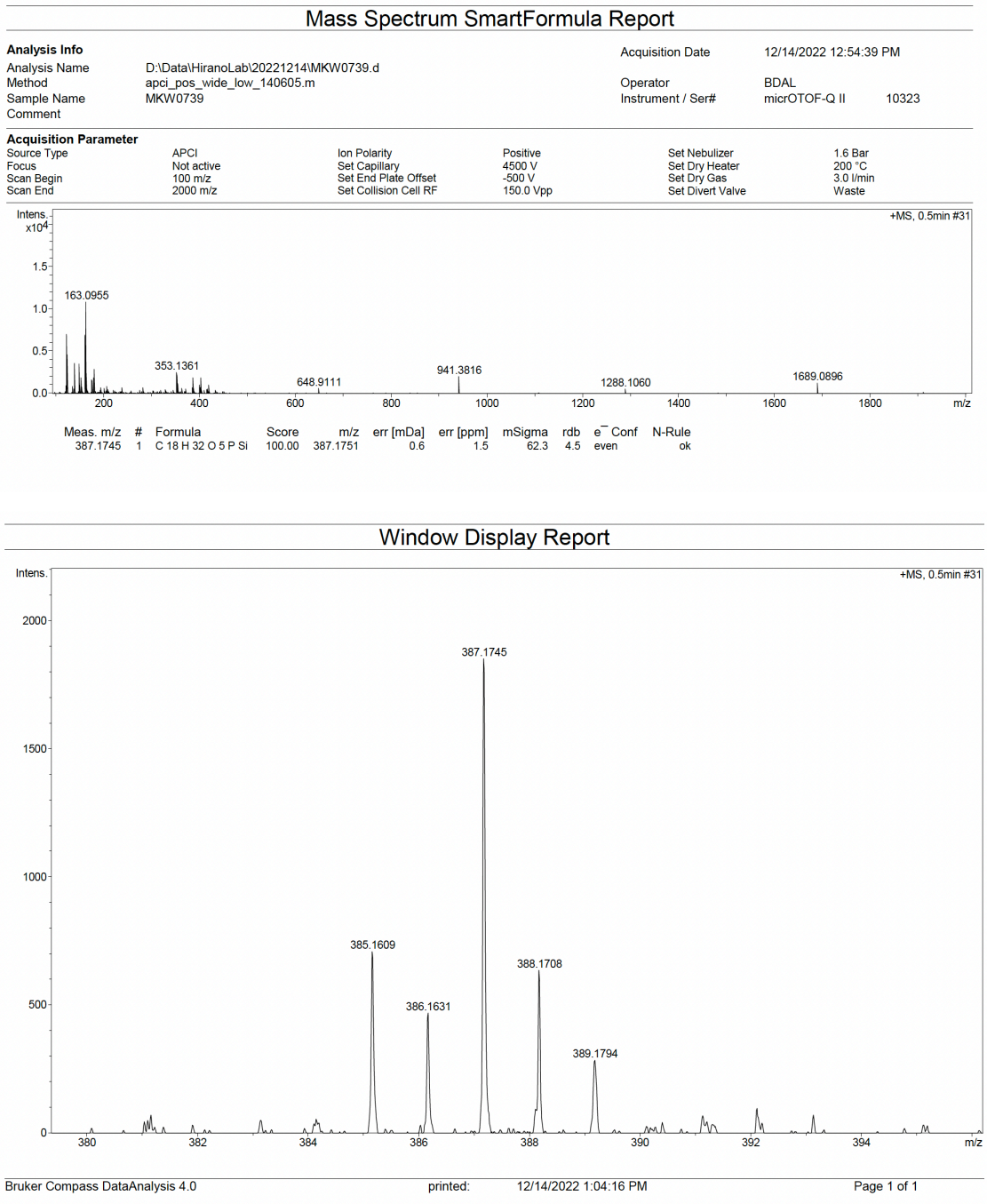


Fig.S66. HRMS Spectra of a mixture of methyl (2*E*,4*E*,6*Z*,8*E*)-10-(diethoxyphosphoryl)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4oa**) and methyl (2*E*,4*E*,6*E*,8*E*)-10-(diethoxyphosphoryl)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4oa**) (APCI).

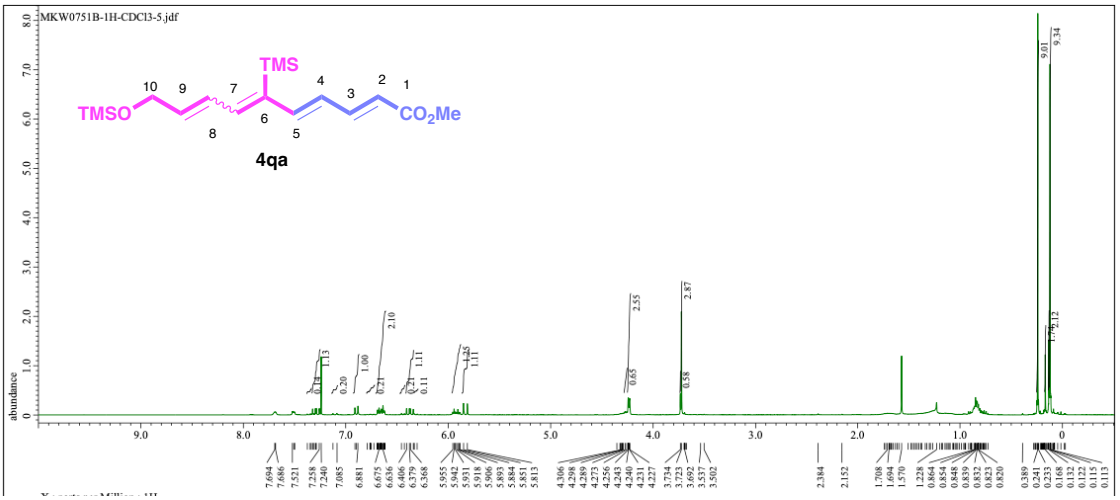


Fig.S67. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)-10-((trimethylsilyl)oxy)deca-2,4,6,8-tetraenoate (**4qa**) (400 MHz, $CDCl_3$).

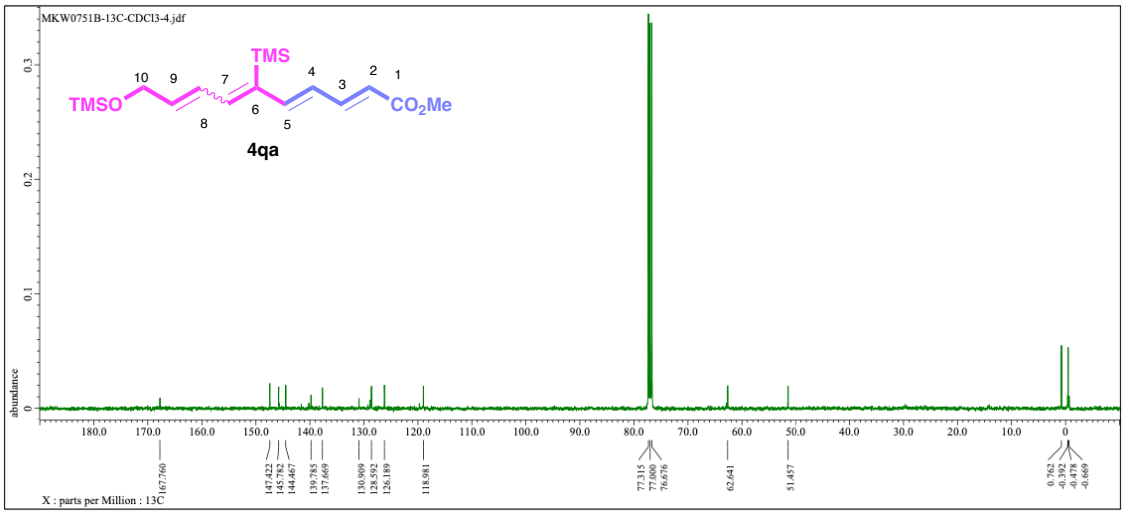


Fig.S68. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)-10-((trimethylsilyl)oxy)deca-2,4,6,8-tetraenoate (**4qa**) (100 MHz, $CDCl_3$).

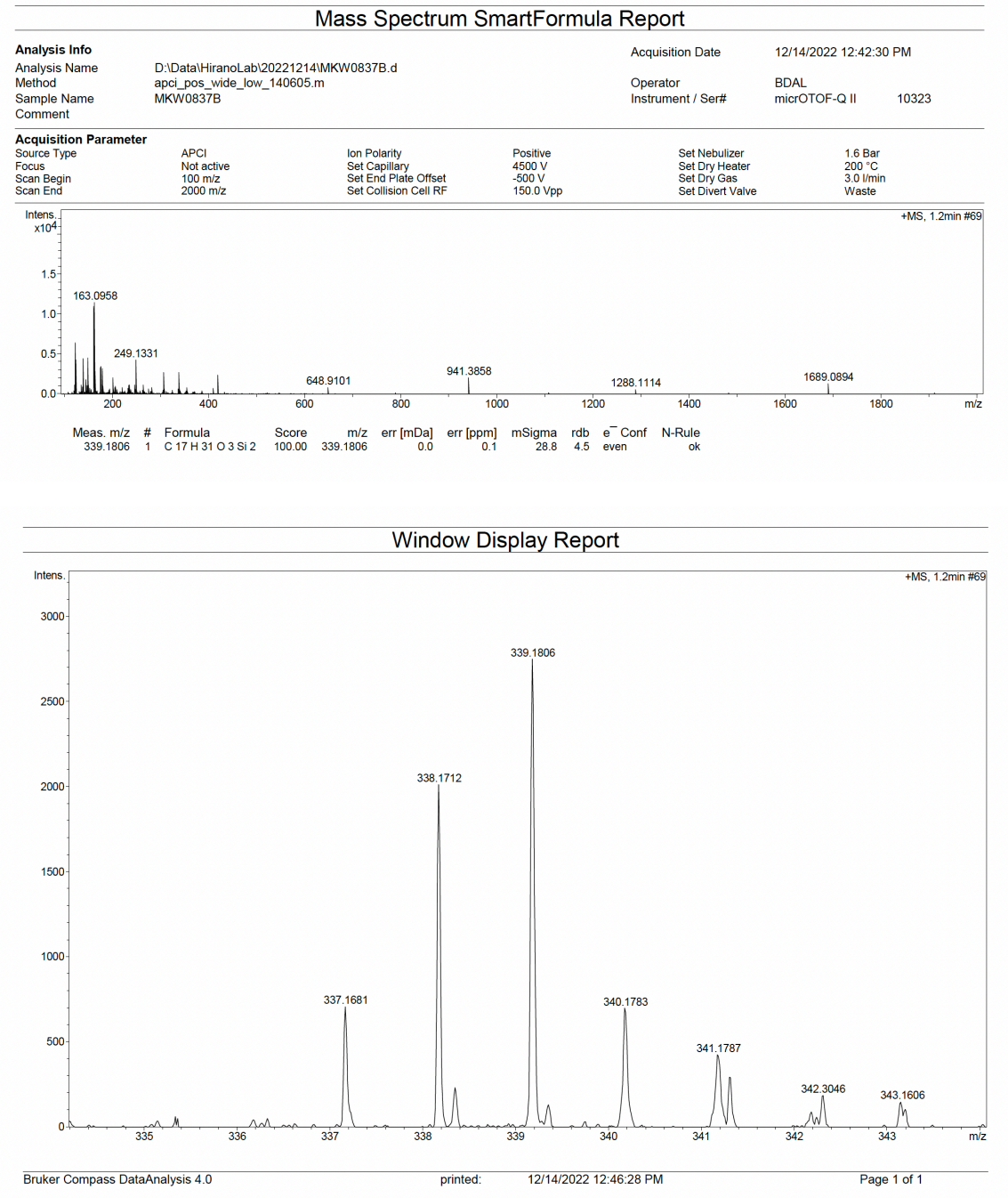


Fig.S69. HRMS Spectra of methyl (2*E*,4*E*,8*E*)-6-(trimethylsilyl)-10-((trimethylsilyl)oxy)deca-2,4,6,8-tetraenoate (**4qa**) (APCI).

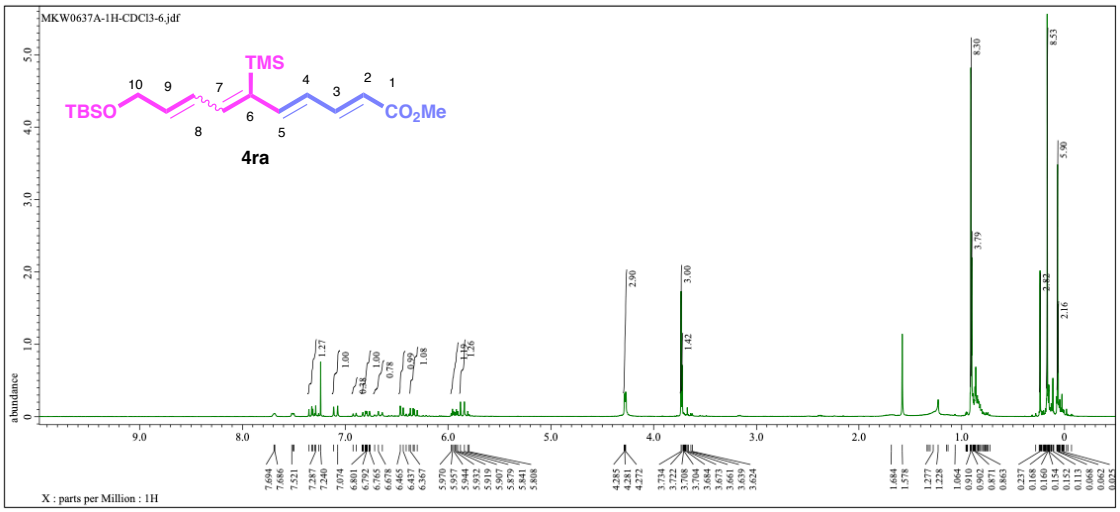


Fig.S70. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,8*E*)-10-((*tert*-butyldimethylsilyl)oxy)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4ra**) (400 MHz, $CDCl_3$).

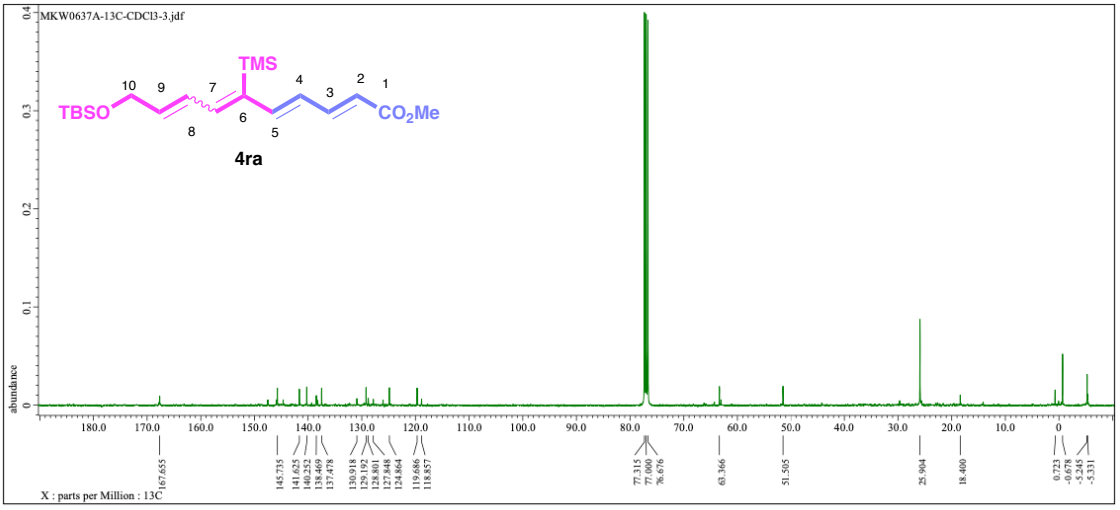


Fig.S71. $^{13}C\{^{1}H\}$ NMR Spectrum of methyl (2*E*,4*E*,8*E*)-10-((*tert*-butyldimethylsilyl)oxy)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4ra**) (100 MHz, $CDCl_3$).

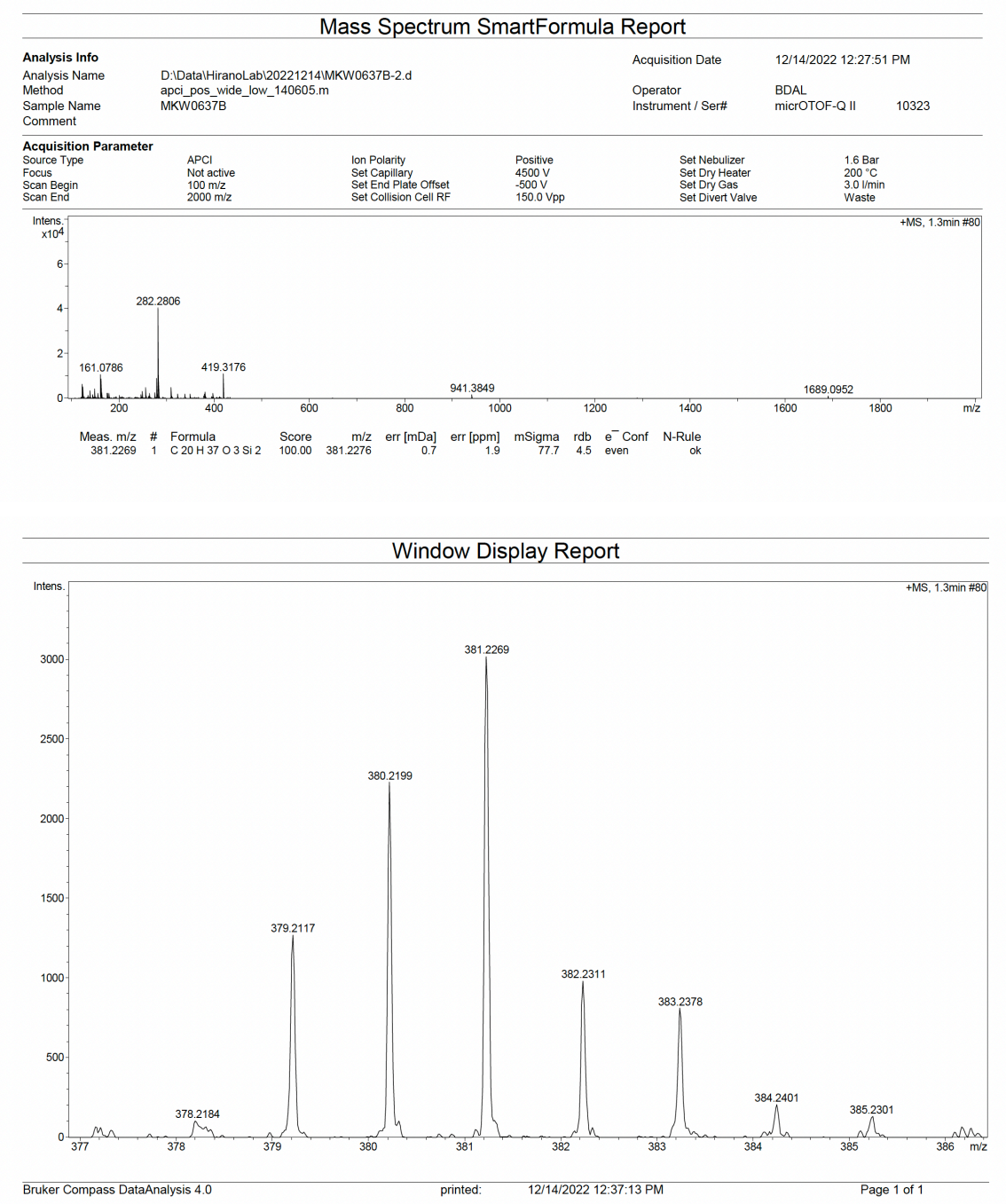


Fig.S72. HRMS Spectra of methyl (2*E*,4*E*,8*E*)-10-((*tert*-butyldimethylsilyl)oxy)-6-(trimethylsilyl)deca-2,4,6,8-tetraenoate (**4ra**) (APCI).

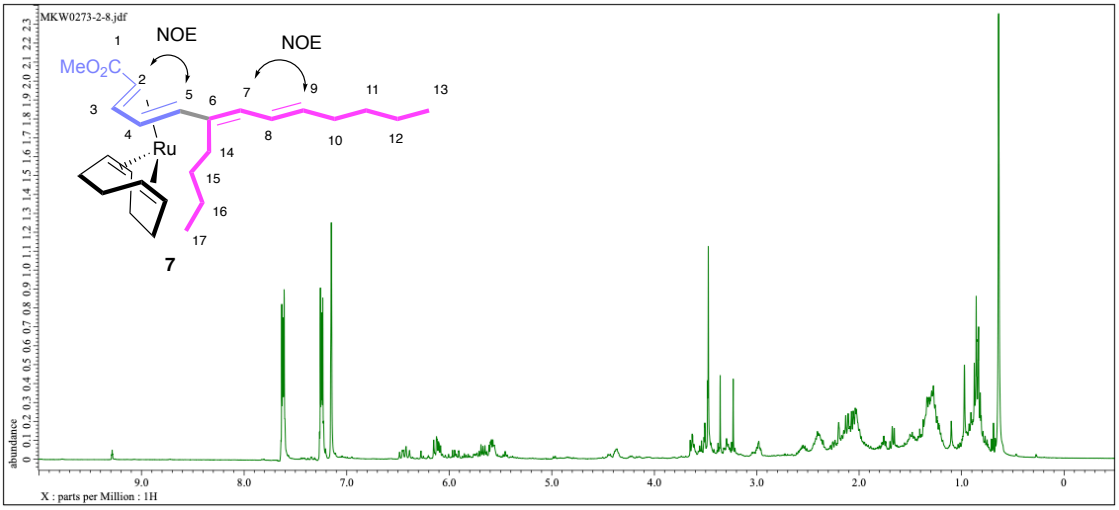


Fig.S73. ^{1}H NMR Spectrum of [Ru(*cisoid*-2-5-η^{4}-methyl (2*E*,4*E*,6*E*,8*E*)-6-butyltrideca-2,4,6,7-tetraenoate)(η^{4}-1,5-cod)] (**7**) (400 MHz, $CDCl_3$).

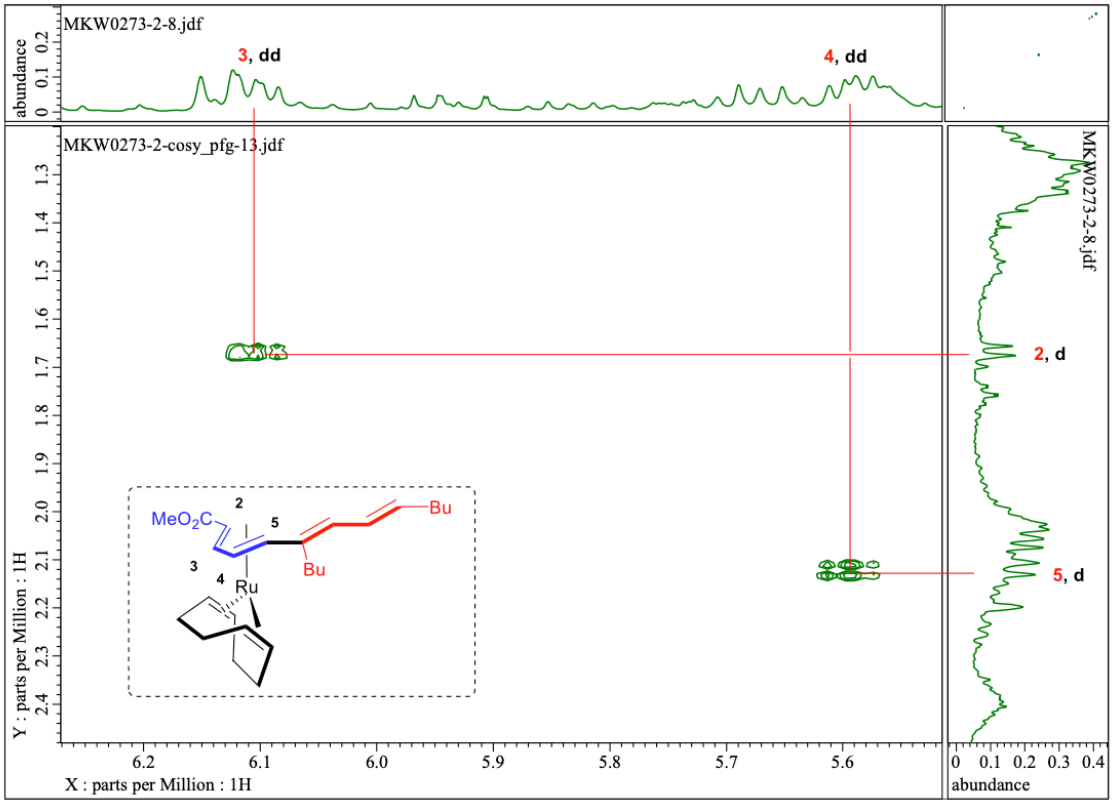


Fig.S74. ^{1}H-^{1}H COSY of [Ru(*cisoid*-2-5-η^{4}-methyl (2*E*,4*E*,6*E*,8*E*)-6-butyltrideca-2,4,6,7-tetraenoate)(η^{4}-1,5-cod)] (**7**) (400 MHz, $CDCl_3$).

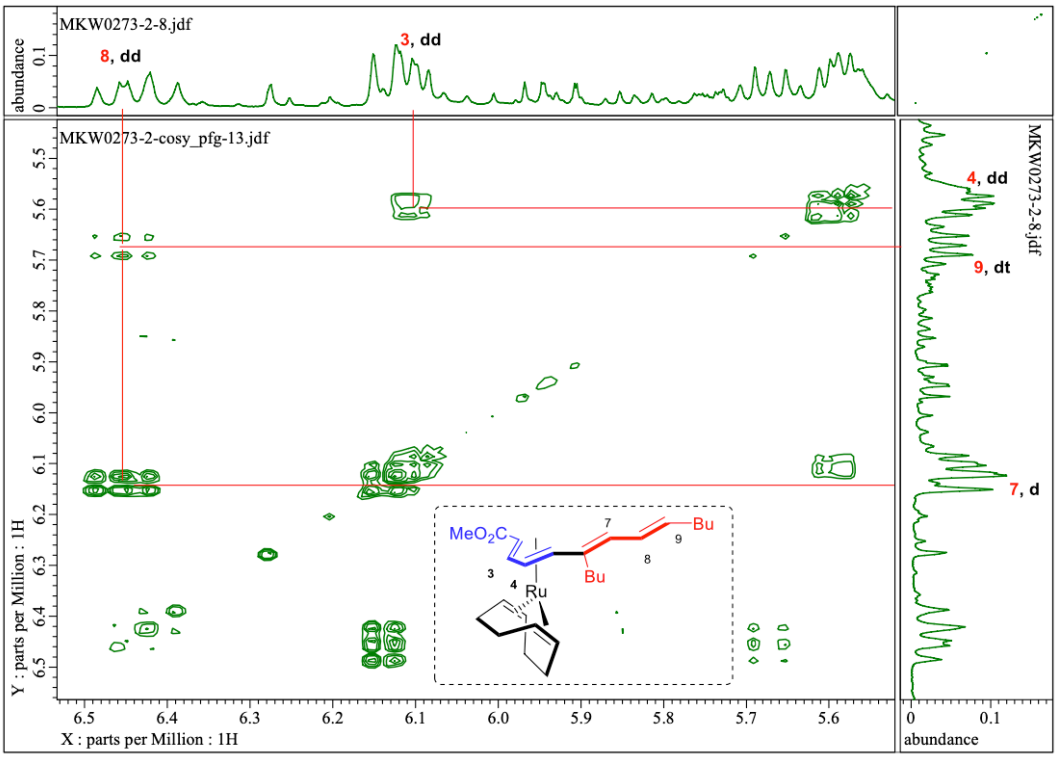


Fig.S75. ^{1}H-^{1}H COSY of [Ru(*cisoid*-2-5-η^{4}-methyl (2*E*,4*E*,6*E*,8*E*)-6-butyltrideca-2,4,6,7-tetraenoate)(η^{4}-1,5-cod)] (**7**) (400 MHz, $CDCl_3$).

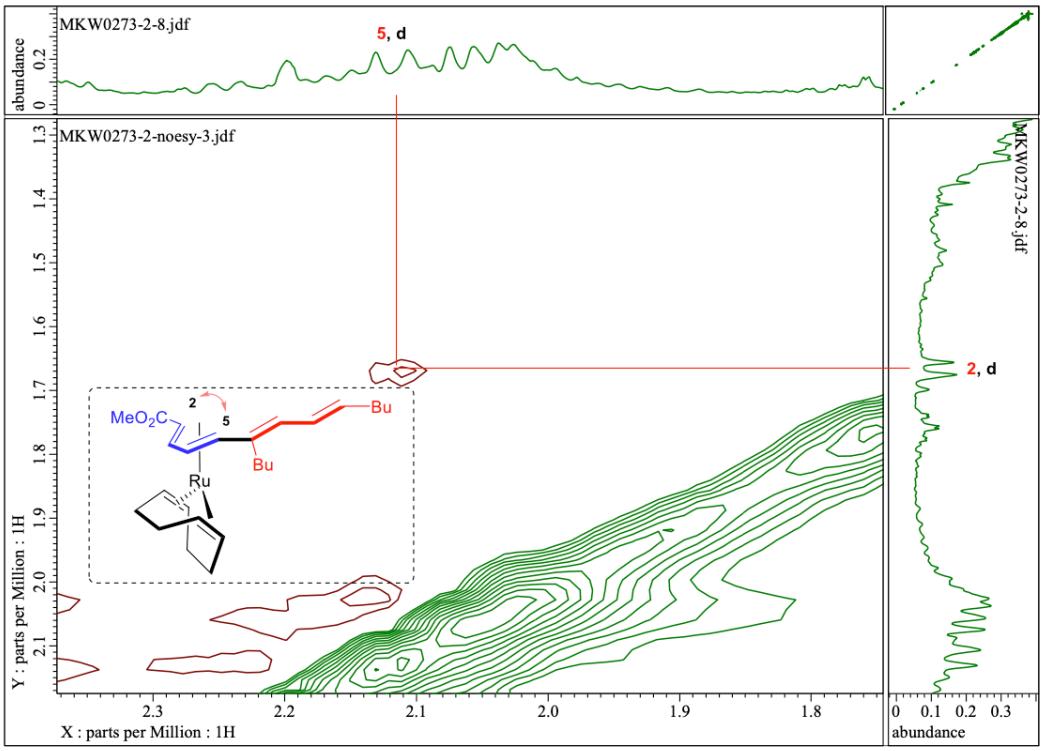


Fig.S76. *p*NOESY of [Ru(*cisoid*-2-5-η^{4}-methyl (2*E*,4*E*,6*E*,8*E*)-6-butyltrideca-2,4,6,7-tetraenoate)(η^{4}-1,5-cod)] (**7**) (400 MHz, $CDCl_3$).

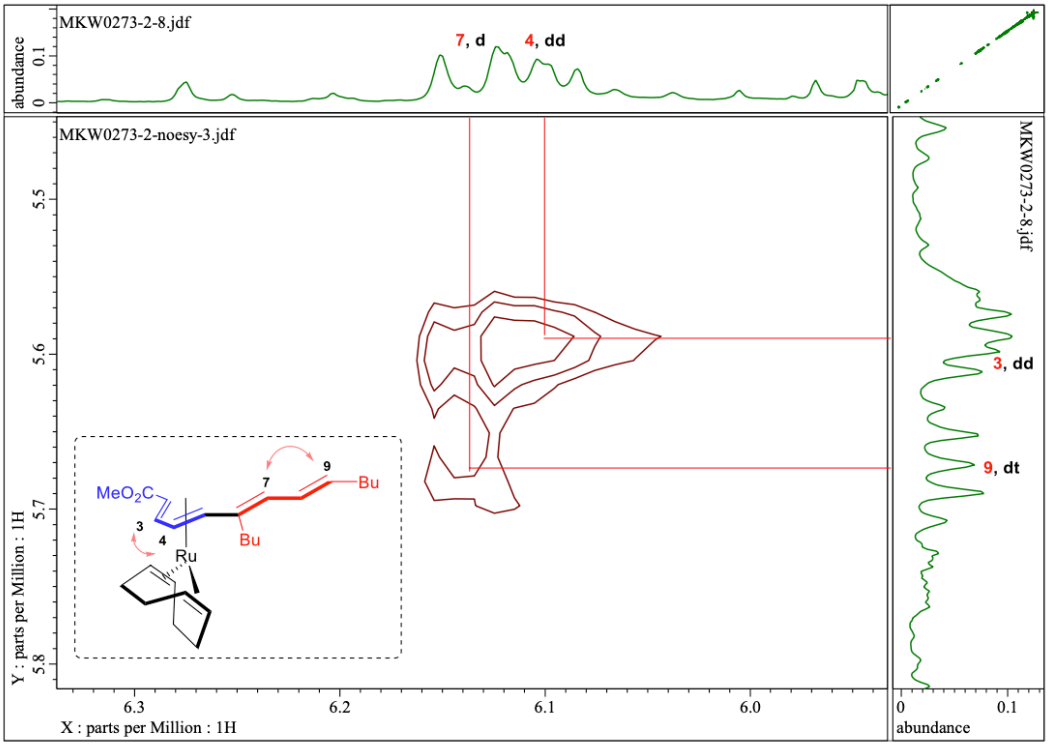


Fig.S77. *p*NOESY of [Ru(*cisoid*-2-5-η^4-methyl (2*E*,4*E*,6*E*,8*E*)-6-butyltrideca-2,4,6,7-tetraenoate)(η^4-1,5-cod)] (**7**) (400 MHz, $CDCl_3$).

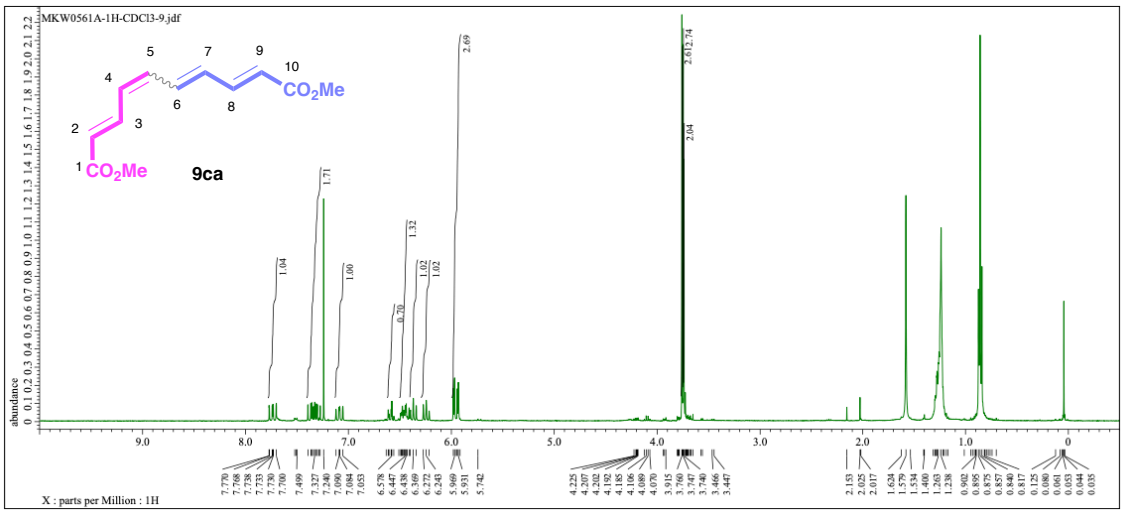


Fig.S78. ^{1}H NMR Spectrum of dimethyl (2*E*,6*E*,8*E*)-deca-2,4,6,8-tetraenedioate (**9ca**) (400 MHz, $CDCl_3$).

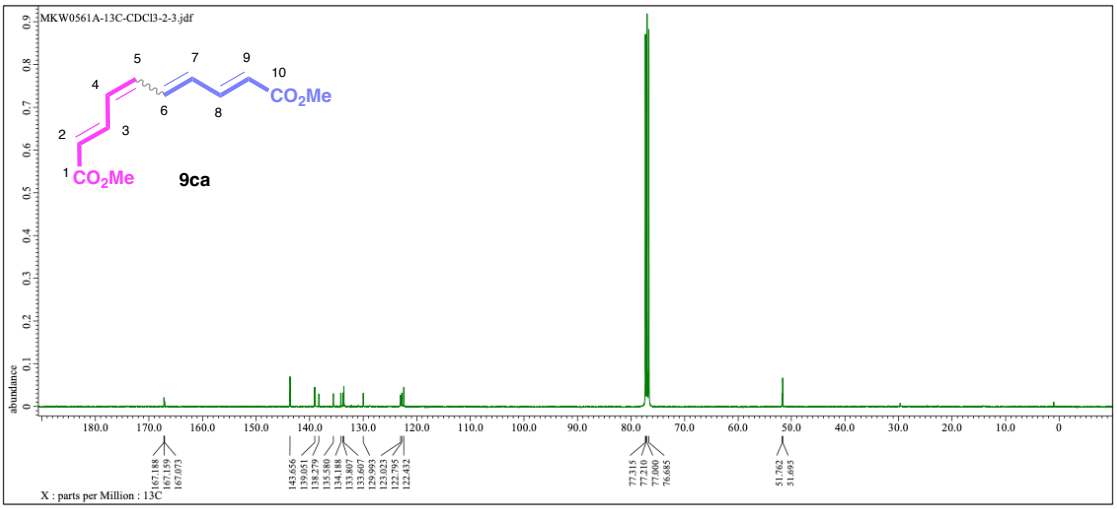


Fig.S79. $^{13}C\{^{1}H\}$ NMR Spectrum of dimethyl (2*E*,6*E*,8*E*)-deca-2,4,6,8-tetraenedioate (**9ca**) (100 MHz, $CDCl_3$).

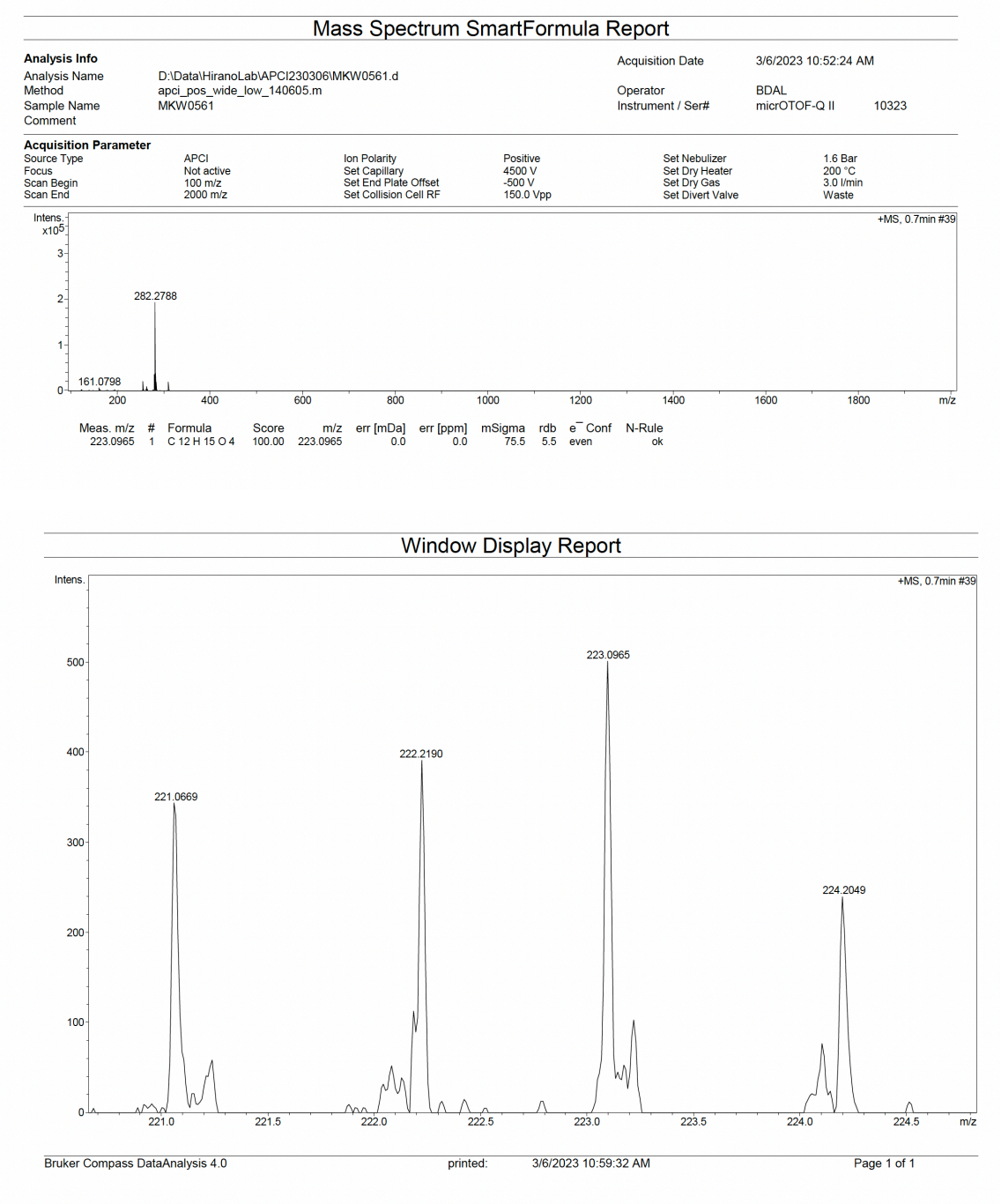


Fig.S80. HRMS Spectra of dimethyl (2*E*,6*E*,8*E*)-deca-2,4,6,8-tetraenedioate (**9ca**) (APCI).

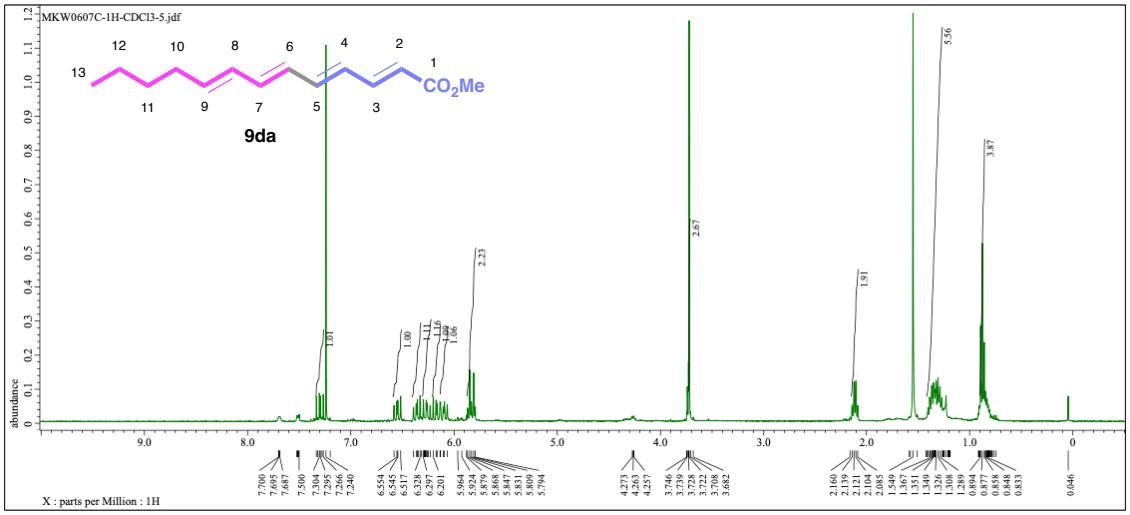


Fig.S81. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,6*E*,8*E*)-trideca-2,4,6,8-tetraenoate (**9da**) (400 MHz, $CDCl_3$).

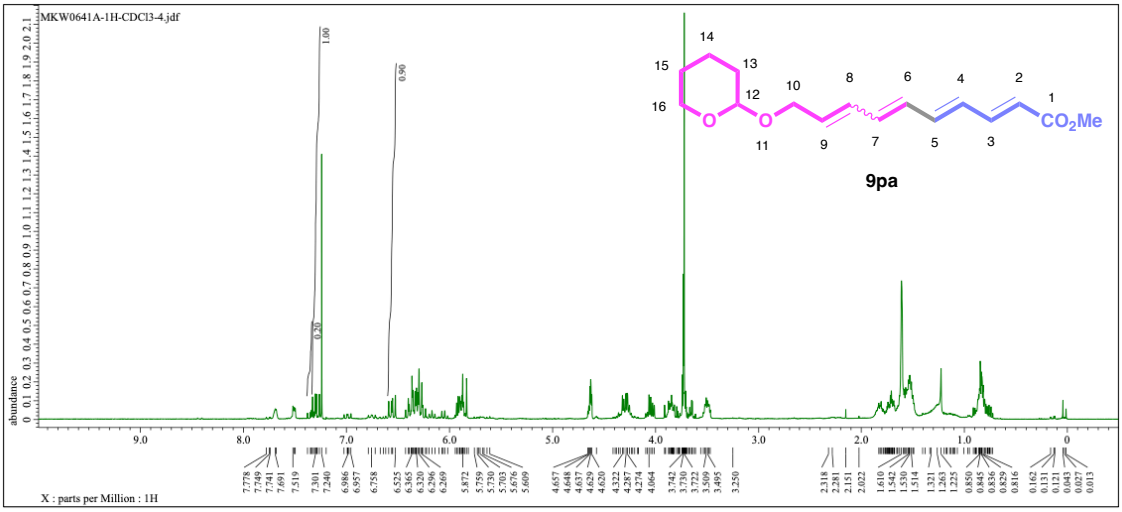
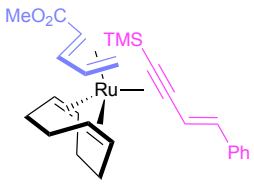


Fig.S82. ^{1}H NMR Spectrum of methyl (2*E*,4*E*,8*E*)-10-((tetrahydro-2*H*-pyran-2-yl)oxy)deca-2,4,6,8-tetraenoate (**9pa**) (400 MHz, $CDCl_3$).

Table S1. Cartesian coordinates of intermediate **4ba**-**A**.



4ba-A

Energy: -994637.0884101

Ru -0.584740 -0.070190 0.776940

C -1.353390 1.913340 1.271090

C -0.022820 2.076680 0.767140

C -1.544370 1.079100 2.391810

C -1.974320 0.120970 -0.971920

C -0.757100 -0.383640 -1.438540

C -1.079910 -2.261040 0.647800

C -2.136940 -1.572710 1.254320

C 1.576480 -0.429270 0.254740

C -0.411790 0.411120 2.930920

C -3.262990 -0.680400 -0.830260

C -0.493120 -1.829460 -1.795030

C -1.086120 -2.809780 -0.774630

C -3.453630 -1.230270 0.586770

C 1.366420 -1.037620 1.336890

C 1.855610 -1.880960 2.391590

Si 2.929650 -0.000350 -0.941200

C 2.336160 0.582400 -2.624580

C 3.922910 -1.586300 -1.168160

C 4.000190 1.316460 -0.134530

H 0.812510 2.185520 1.452950

H -2.113800 1.183530 -1.141920

H -0.115490 0.332400 -1.939350

H -0.420030 -2.801730 1.314990

H -2.199110 -1.652710 2.340430

H -2.554830 0.851650 2.717420

H -2.199460 2.358720 0.759250

C 0.129420 2.842530 -0.478260

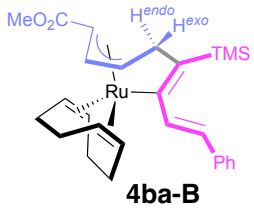
H 0.523990 0.944970 3.076480
H -0.605340 -0.334710 3.695090
H -3.952100 -0.470620 1.199020
H 1.816510 -0.210490 -3.170680
H 0.591860 -1.974010 -1.830700
H 3.309060 -2.372420 -1.619640
H -3.278820 -1.488830 -1.567280
H -2.105960 -3.091700 -1.053940
H -4.106190 -0.030960 -1.084710
H -0.507800 -3.738420 -0.788870
H -0.867320 -2.046150 -2.806030
H -4.116290 -2.107980 0.585550
H 1.666220 1.441610 -2.548340
H 4.291160 -1.958930 -0.206880
H 3.203430 0.885920 -3.221560
H 3.412920 2.221080 0.043560
H 4.787930 -1.416130 -1.818460
H 4.392720 0.962760 0.824080
H 4.849940 1.572400 -0.777140
O 1.382560 3.328890 -0.611020
O -0.734210 3.056190 -1.310860
C 1.621300 4.137770 -1.759990
H 1.055750 5.070570 -1.695160
H 1.336090 3.616840 -2.676520
H 2.691190 4.343020 -1.758810
C 1.128270 -2.469760 3.354220
H 2.932410 -2.040450 2.349620
H 0.057870 -2.284200 3.370270
C 1.629040 -3.351360 4.415620
C 2.945120 -3.835560 4.459580
C 0.749040 -3.732230 5.437800
C 1.167570 -4.556730 6.476470
C 3.364030 -4.659090 5.496410
C 2.478760 -5.022300 6.510660
H -0.276010 -3.371210 5.415850
H 0.468640 -4.835970 7.258620

H 3.647530 -3.577530 3.673210

H 4.386150 -5.024430 5.511630

H 2.809340 -5.667470 7.318360

Table S2. Cartesian coordinates of intermediate **4ba**-**B**.



4ba-B

Energy: -994626.1163129

Ru -0.996870 -0.134950 0.276610

C -1.645020 1.605200 1.524270

C -0.337780 1.875940 1.023490

C -1.868490 0.386380 2.169950

C -2.080860 0.612540 -1.366960

C -0.784610 0.226730 -1.818570

C -1.300180 -2.158240 -0.513480

C -2.470170 -1.726810 0.140680

C 0.920840 -0.741200 0.578910

C -0.697080 -0.454980 2.683490

C -3.354890 -0.175940 -1.676700

C -0.552050 -1.016930 -2.657230

C -1.174900 -2.271880 -2.029080

C -3.700800 -1.190050 -0.572420

C 0.654880 -0.938900 1.880430

C 1.544570 -1.663170 2.789770

Si 2.508540 -0.967710 -0.390750

C 2.677030 0.441000 -1.627750

C 2.512820 -2.659660 -1.221370

C 4.043480 -0.871370 0.717100

H 0.534600 1.641590 1.624910

H -2.233430 1.680830 -1.233130

H -0.088280 1.037340 -2.026530

H -0.656930 -2.831470 0.050100
H -2.670010 -2.144490 1.127750
H -2.857260 0.111330 2.518900
H -2.484630 2.221940 1.215230
C -0.154190 2.977660 0.071910
H -0.221250 0.129560 3.480270
H -1.113730 -1.362050 3.124240
H -4.325900 -0.696140 0.179290
H 2.013690 0.339360 -2.489300
H 0.525900 -1.163760 -2.758900
H 1.652350 -2.808400 -1.878070
H -3.250320 -0.677710 -2.644220
H -2.159960 -2.474380 -2.461360
H -4.185480 0.526470 -1.794450
H -0.565220 -3.149630 -2.266410
H -0.933650 -0.860770 -3.677130
H -4.299580 -2.018470 -0.977540
H 2.445000 1.391170 -1.135900
H 2.493630 -3.448330 -0.461620
H 3.706410 0.486740 -1.999230
H 3.943510 -0.097690 1.485150
H 3.422030 -2.790650 -1.818140
H 4.268080 -1.820440 1.214460
H 4.912400 -0.618080 0.099720
O 1.153280 3.249480 -0.118470
O -1.036470 3.577980 -0.515330
C 1.437970 4.238950 -1.105020
H 0.993280 5.198740 -0.832680
H 1.051690 3.932120 -2.080230
H 2.523720 4.319360 -1.137970
C 1.363510 -1.969980 4.086240
H 2.463240 -1.995380 2.319820
H 0.437690 -1.716180 4.595880
C 2.347720 -2.682220 4.916800
C 3.711840 -2.741360 4.593470
C 1.919410 -3.321860 6.088080

C 2.812630 -4.019380 6.894240
C 4.604560 -3.440160 5.396870
C 4.159900 -4.085750 6.549420
H 0.868580 -3.276860 6.362550
H 2.455420 -4.511390 7.793730
H 4.082930 -2.216760 3.717830
H 5.656210 -3.470880 5.128640
H 4.860080 -4.627030 7.177730

Table S3. Cartesian coordinates of intermediate **4ba-B'**. This compound is an intermediate with a slight rearrangement of **4ba-B**.

Energy: -994617.0353724
Ru -0.128870 0.015040 0.338960
C -0.361130 1.759450 1.687430
C 0.561050 2.702300 0.938850
C -1.162940 -1.391090 1.530070
C 0.220210 -1.709450 1.575660
C 0.551620 -1.471200 -1.159710
C -0.836870 -1.337260 -1.274500
C 1.826580 0.569860 0.471920
C -1.632330 1.425490 1.190450
C 1.672770 1.924240 0.260380
C -1.884650 1.338410 -0.195440
C -2.193290 -2.178690 0.740030
C 0.740890 -2.964200 0.875240
C 1.217740 -2.690540 -0.554460
C -1.813220 -2.382200 -0.741520
C 2.601960 2.689180 -0.576880
Si 3.583300 -0.155350 0.508210
C 3.731780 -1.641980 1.662700
C 4.249360 -0.604860 -1.205320
C 4.748350 1.119220 1.282930
H -0.019600 3.290350 0.215270
H -1.217410 -0.706750 -2.073260

H -1.575120 -0.918980 2.421500
H 1.156390 -0.926760 -1.884460
H 0.755830 -1.424800 2.476950
H -1.342120 1.957560 -0.909270
H -0.214070 1.668280 2.760190
H 1.017570 3.436070 1.616580
H -2.381650 1.005700 1.854730
C -3.174650 0.824240 -0.674540
H -3.131070 -1.620920 0.787030
H 3.504880 -2.597520 1.187110
H 2.296120 -2.525760 -0.555020
H -1.383820 -3.378860 -0.896050
H 3.568890 -1.247210 -1.770950
H -0.057470 -3.714720 0.871950
H -2.722490 -2.349420 -1.349250
H 1.550600 -3.398950 1.466370
H 3.088560 -1.535220 2.541090
H -2.378830 -3.147290 1.226620
H 1.046960 -3.564960 -1.198520
H 4.436380 0.288340 -1.810240
H 4.767400 -1.690400 2.016860
H 4.428940 1.341930 2.307130
H 4.797940 2.066920 0.741420
H 5.202250 -1.135780 -1.100110
H 5.761710 0.705140 1.336830
O -3.240850 0.856820 -2.020490
O -4.080990 0.398090 0.016250
C -4.433020 0.316870 -2.587610
H -4.547450 -0.735050 -2.313560
H -5.310590 0.868820 -2.243780
H -4.319870 0.416770 -3.666020
C 2.554400 4.015490 -0.793070
H 3.362980 2.111550 -1.093530
H 1.764020 4.604930 -0.332950
C 3.487800 4.779870 -1.633350
C 4.718390 4.264750 -2.068630

C 3.148060 6.085990 -2.011340

C 3.993660 6.845850 -2.812420

C 5.563420 5.022460 -2.869480

C 5.204790 6.315520 -3.247910

H 2.203340 6.505620 -1.675390

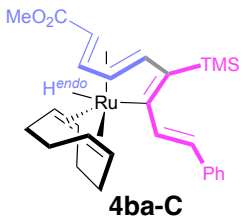
H 3.706380 7.853680 -3.095690

H 5.027590 3.268400 -1.766610

H 6.512010 4.605440 -3.193440

H 5.868670 6.906220 -3.871050

Table S4. Cartesian coordinates of intermediate **4ba**-**C**.



4ba-C

Energy: -994620.7070746

Ru -0.110960 0.103370 -0.306460

C -0.282230 2.129670 0.399500

C 0.583470 2.116390 -0.719130

C -0.920600 -0.505740 1.869660

C 0.375360 -0.951480 1.810260

C 0.139020 -2.041320 -0.814820

C -1.231420 -1.752880 -0.725850

C 2.052870 0.462050 -0.316560

C -1.632560 1.694730 0.187480

C 2.020360 1.803730 -0.524150

C -2.025250 1.210660 -1.065980

C -2.154860 -1.353950 1.661420

C 0.696070 -2.425460 1.652220

C 0.876420 -2.884960 0.199010

C -2.109580 -2.261670 0.417270

C 3.043960 2.834400 -0.628830

Si 3.623480 -0.573470 -0.380820

C 3.956880 -1.542030 1.216870
C 3.569290 -1.699440 -1.898370
C 5.223380 0.414390 -0.643040
H 0.156000 0.170770 -1.858990
H -1.749550 -1.575120 -1.664430
H -1.090620 0.444770 2.367440
H 0.561000 -2.080310 -1.814700
H 1.156980 -0.312360 2.208050
H -1.629070 1.597460 -1.994420
H 0.079130 2.319060 1.405500
H 0.249480 2.485630 -1.686290
H -2.322800 1.604530 1.018810
C -3.334910 0.535500 -1.183880
H -3.006400 -0.678700 1.558700
H 3.579880 -2.567200 1.202390
H 1.935530 -2.871980 -0.053510
H -1.771720 -3.268610 0.689080
H 2.729960 -2.396070 -1.924940
H -0.105650 -2.998270 2.129360
H -3.130930 -2.377230 0.044950
H 1.601470 -2.647760 2.222100
H 3.527160 -1.035670 2.087050
H -2.338120 -1.958220 2.561360
H 0.557380 -3.932160 0.095090
H 3.509300 -1.076110 -2.797320
H 5.039340 -1.598080 1.373610
H 5.471360 1.068740 0.198900
H 5.212230 1.008770 -1.561770
H 4.495030 -2.282610 -1.960390
H 6.037860 -0.314360 -0.735890
O -3.564360 0.155960 -2.451370
O -4.117440 0.321960 -0.278540
C -4.783830 -0.554090 -2.669670
H -4.795700 -1.480220 -2.089800
H -5.642680 0.056340 -2.382930
H -4.810920 -0.773940 -3.735510

C 2.759000 4.133100 -0.825640
H 4.074820 2.526340 -0.513740
H 1.712810 4.432060 -0.893290
C 3.730260 5.229170 -0.938480
C 5.112210 5.016930 -1.064660
C 3.267050 6.552240 -0.922880
C 4.147040 7.625490 -1.014100
C 5.992090 6.087980 -1.154040
C 5.515550 7.398200 -1.127710
H 2.199670 6.737490 -0.832830
H 3.762450 8.640690 -0.996840
H 5.504040 4.004870 -1.104780
H 7.057020 5.899930 -1.251910
H 6.205670 8.232760 -1.200930

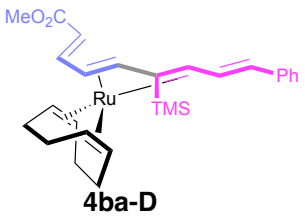
Table S5. Cartesian coordinates of intermediate **4ba-C'**. This compound is an intermediate with a slight rearrangement of **4ba-C**.

Energy: -994609.7211220
Ru -0.610090 0.813550 -0.452620
C 0.039530 -1.216540 -0.053460
C -0.911530 2.397940 1.330910
C -2.165310 1.931290 1.031200
C -1.819230 2.101670 -1.796470
C -0.598500 2.740520 -1.530070
C -2.132460 -0.764070 -0.427030
C 0.415530 -0.374530 1.019730
C 1.313490 0.703940 0.722690
C -1.324710 -1.798720 -0.078320
C 1.720830 0.934890 -0.596350
C -0.324800 3.709060 0.858740
C -3.161980 2.784720 0.271260
C -3.143730 2.581300 -1.249800
C -0.491910 3.984830 -0.648410
C -1.553800 -3.213760 0.178310

Si -3.920270 -0.964380 -0.980790
H -0.341890 0.148260 -1.856310
H 0.172490 2.643940 -2.289750
H -1.895000 1.581130 -2.746690
H 0.778800 -1.570530 -0.768730
H -2.557880 1.102130 1.610750
H -0.406300 1.941600 2.177420
H -0.055300 -0.440140 1.995680
H 0.743010 3.694070 1.084930
H -3.908140 1.856520 -1.525310
H -1.373920 4.610590 -0.828710
H -2.958350 3.833540 0.510430
H 0.367400 4.572890 -0.981610
H 1.575850 1.431400 1.482720
H -4.163260 2.578580 0.657280
H -0.759160 4.533530 1.441910
H -3.423170 3.516890 -1.755630
H 1.877710 0.137840 -1.309540
C 2.432140 2.192900 -0.906830
O 2.768020 2.243380 -2.206000
O 2.684610 3.088090 -0.124170
C 3.417810 3.442950 -2.627400
H 2.764910 4.305600 -2.473280
H 4.345620 3.595050 -2.072020
H 3.625380 3.309690 -3.687710
C -4.056290 -0.542120 -2.818370
C -5.152620 0.022130 0.072650
C -4.590990 -2.738740 -0.902290
H -3.417070 -1.227730 -3.385440
H -3.760560 0.475020 -3.080040
H -5.087260 -0.692520 -3.158120
H -4.667870 -3.128210 0.117970
H -4.009410 -3.441880 -1.506340
H -5.606460 -2.715700 -1.316210
H -5.390200 1.009890 -0.328580
H -4.787180 0.151910 1.096350

H -6.092100 -0.537800 0.130030
C -0.574830 -4.065370 0.528870
H -2.571170 -3.574260 0.102820
H 0.436810 -3.676550 0.647020
C -0.729610 -5.500510 0.801570
C -1.902900 -6.212370 0.505850
C 0.336900 -6.202590 1.380270
C 0.234840 -7.559370 1.669160
C -2.006580 -7.566870 0.795530
C -0.939670 -8.248190 1.380160
H 1.256780 -5.671010 1.610200
H 1.074750 -8.078900 2.120260
H -2.739770 -5.706560 0.033450
H -2.923520 -8.097220 0.556910
H -1.022850 -9.307410 1.602080

Table S6. Cartesian coordinates of intermediate **4ba**-**D**.



4ba-D

Energy: -994645.7699659
Ru -0.307550 1.390150 -0.693100
C -0.277870 -0.712200 -1.488110
C -1.532690 0.789010 1.017130
C -2.343500 1.448370 0.077620
C -0.442980 3.511790 -0.363620
C 0.218860 2.953950 0.748090
C -2.476140 -1.418120 -2.300990
C 0.705880 -0.559110 -0.490090
C 1.653390 0.500230 -0.568170
C -1.488120 -1.561640 -1.386440
C 1.652730 1.375880 -1.690690

C -1.002120 1.378490 2.305570
C -2.850560 2.878340 0.246750
C -1.905790 3.929830 -0.373860
C -0.423740 2.787560 2.117290
C -1.653390 -2.521270 -0.274370
Si -4.142640 -2.279100 -2.355620
H -2.283440 -0.690720 -3.094540
H 1.303470 3.026340 0.753390
H 0.175850 4.030780 -1.097870
H -0.028720 -0.444480 -2.514800
H -2.948630 0.806610 -0.563490
H -1.592010 -0.298490 1.030950
H 0.642250 -1.106380 0.444350
H -0.210570 0.712020 2.665820
H -2.194560 4.090020 -1.418930
H -1.200400 3.545660 2.256270
H -3.012230 3.088680 1.308740
H 0.327060 2.979050 2.889890
H 2.313760 0.691010 0.271910
H -3.834460 2.961280 -0.224890
H -1.784600 1.377050 3.078190
H -2.033600 4.900340 0.127040
H 1.452830 1.008280 -2.695060
C 2.509970 2.568300 -1.646710
O 2.497000 3.224620 -2.825230
O 3.142680 2.968740 -0.685970
C 3.258930 4.429280 -2.863340
H 2.885340 5.146460 -2.128270
H 4.312770 4.228720 -2.656510
H 3.139720 4.824130 -3.871410
C -4.933700 -1.840750 -4.007900
C -5.243950 -1.631690 -0.963680
C -3.976000 -4.151710 -2.218040
H -4.326130 -2.201680 -4.844250
H -5.043830 -0.756500 -4.116730
H -5.928760 -2.288430 -4.098800

H -3.527250 -4.456190 -1.267720
H -3.345200 -4.543880 -3.022210
H -4.958590 -4.629570 -2.297340
H -5.376330 -0.548170 -1.051390
H -4.824090 -1.832450 0.027370
H -6.234960 -2.096680 -1.005420
C -0.699590 -3.323420 0.219020
H -2.664780 -2.610580 0.116290
H 0.297180 -3.283730 -0.217400
C -0.880960 -4.324660 1.281700
C -1.995540 -4.336670 2.133220
C 0.098830 -5.310310 1.457450
C -0.036460 -6.289700 2.435700
C -2.131210 -5.314280 3.110860
C -1.154350 -6.296900 3.265010
H 0.972960 -5.310270 0.811650
H 0.732840 -7.046800 2.550730
H -2.756730 -3.567520 2.043610
H -3.000060 -5.305500 3.761600
H -1.261920 -7.057740 4.031460

Table S7. Cartesian coordinates of transition state **4ba**-**TS1.**

Energy: -994625.5221053
Ru -0.911510 -0.137760 0.393920
C -1.632570 1.663550 1.441230
C -0.286170 1.910360 1.044040
C -1.910430 0.496740 2.179950
C -2.148540 0.536830 -1.234410
C -0.873780 0.178210 -1.739710
C -1.256810 -2.192500 -0.328110
C -2.397270 -1.745820 0.358180
C 1.101860 -0.726280 0.424990
C -0.789740 -0.307030 2.674350
C -3.410050 -0.295520 -1.460830

C -0.643450 -1.087640 -2.543790
C -1.180830 -2.346090 -1.843090
C -3.676580 -1.269250 -0.304950
C 0.889650 -1.006870 1.669040
C 1.634130 -1.668680 2.718420
Si 2.612750 -0.838330 -0.659950
C 2.630820 0.556540 -1.918460
C 2.670880 -2.539750 -1.466700
C 4.153790 -0.645800 0.415970
H 0.539520 1.721940 1.722870
H -2.321210 1.604570 -1.135330
H -0.213000 1.001740 -2.003680
H -0.586370 -2.841400 0.230400
H -2.535530 -2.124900 1.371190
H -2.932610 0.207900 2.397610
H -2.440870 2.267100 1.041230
C -0.032640 2.942980 0.033830
H -0.060130 0.248200 3.260470
H -1.113220 -1.222000 3.159910
H -4.274100 -0.759260 0.458770
H 1.896760 0.422890 -2.716460
H 0.431310 -1.198600 -2.704330
H 1.792260 -2.744250 -2.083820
H -3.330570 -0.834900 -2.410670
H -2.170420 -2.610690 -2.230530
H -4.265290 0.377790 -1.573430
H -0.536030 -3.200090 -2.074280
H -1.088310 -0.983830 -3.544430
H -4.274520 -2.128910 -0.640950
H 2.412310 1.501070 -1.411340
H 2.727020 -3.316110 -0.696520
H 3.621680 0.633800 -2.378760
H 4.068930 0.219610 1.080890
H 3.559130 -2.630350 -2.101350
H 4.347930 -1.531760 1.029130
H 5.032190 -0.494530 -0.221110

O 1.281190 3.245510 -0.044350
O -0.864440 3.472850 -0.681230
C 1.631510 4.192670 -1.051140
H 1.116230 5.141840 -0.888060
H 1.372770 3.813830 -2.043330
H 2.709490 4.326490 -0.969100
C 1.283690 -2.117380 3.935030
H 2.662360 -1.831330 2.401740
H 0.261160 -2.036350 4.286970
C 2.205050 -2.778780 4.872280
C 3.600150 -2.660250 4.783860
C 1.672490 -3.556150 5.909820
C 2.500690 -4.214770 6.812110
C 4.428330 -3.319230 5.684050
C 3.883820 -4.102350 6.700440
H 0.593520 -3.650160 6.001920
H 2.064620 -4.815730 7.604040
H 4.044390 -2.030490 4.018740
H 5.505300 -3.211820 5.599090
H 4.533250 -4.612370 7.404730

Table S8. Cartesian coordinates of transition state **4ba**-**TS2**.

Energy: -994615.5892580
Ru -0.187730 0.153360 -0.113650
C -0.134150 2.128120 0.777940
C 0.508120 2.136910 -0.537510
C -1.151320 -1.223810 1.440200
C 0.190330 -1.551170 1.392340
C 0.316070 -1.543480 -1.443550
C -1.081350 -1.398580 -1.408450
C 1.982150 0.485550 -0.028620
C -1.493420 1.766970 0.842590
C 1.954940 1.770490 -0.476600
C -2.185180 1.348640 -0.315230

C -2.238360 -2.068270 0.804530
C 0.650730 -2.834830 0.721830
C 1.072240 -2.647270 -0.742600
C -2.011950 -2.372830 -0.691200
C 3.011410 2.692900 -0.870090
Si 3.653740 -0.261040 0.433770
C 3.701550 -1.843300 1.465600
C 4.656020 -0.619590 -1.130660
C 4.567380 0.977660 1.540100
H 0.005670 0.908380 -1.505530
H -1.540470 -0.863380 -2.234860
H -1.487780 -0.556300 2.228860
H 0.833650 -1.134890 -2.307960
H 0.858790 -1.101130 2.118590
H -2.005700 1.801300 -1.282540
H 0.440110 2.307910 1.679550
H 0.111700 2.787650 -1.318880
H -1.969610 1.633040 1.809210
C -3.522440 0.761550 -0.150470
H -3.183980 -1.541810 0.931410
H 3.502680 -2.751480 0.892550
H 2.135390 -2.401000 -0.789860
H -1.622200 -3.388980 -0.821320
H 4.149840 -1.370730 -1.747120
H -0.160210 -3.566770 0.783200
H -2.977870 -2.355660 -1.204160
H 1.475960 -3.262490 1.293400
H 3.028540 -1.816740 2.327310
H -2.336460 -3.005830 1.369510
H 0.951330 -3.590640 -1.294150
H 4.793250 0.271190 -1.751110
H 4.722260 -1.927760 1.856720
H 4.044630 1.060930 2.499830
H 4.643860 1.984060 1.122890
H 5.646840 -1.010940 -0.874470
H 5.580560 0.615650 1.749080

O -4.049260 0.404900 -1.337020
O -4.103100 0.588250 0.905480
C -5.321880 -0.235080 -1.274030
H -5.248800 -1.181040 -0.729810
H -6.054820 0.403130 -0.776050
H -5.614120 -0.417130 -2.307120
C 2.818480 3.993770 -1.147880
H 4.008550 2.273910 -0.969930
H 1.811370 4.401470 -1.062890
C 3.843680 4.957980 -1.569400
C 5.217810 4.671760 -1.553950
C 3.442040 6.229300 -2.002460
C 4.371670 7.176600 -2.418350
C 6.147050 5.616550 -1.969870
C 5.730030 6.873510 -2.406220
H 2.382850 6.473290 -2.015520
H 4.033600 8.152930 -2.751840
H 5.568430 3.705710 -1.203510
H 7.204960 5.373200 -1.948100
H 6.459070 7.610090 -2.728610

Table S9. Cartesian coordinates of transition state **4ba**-**TS3**.

Energy: -994607.6784657
Ru -0.553530 0.842370 -0.458130
C 0.134860 -1.221590 -0.320340
C -0.768950 2.022070 1.527090
C -2.032230 1.551460 1.201910
C -1.826260 2.354190 -1.509740
C -0.626930 2.969610 -1.145780
C -2.009340 -0.798960 -0.803480
C 0.677470 -0.473180 0.740130
C 1.477670 0.654660 0.341740
C -1.232840 -1.805070 -0.319260
C 1.670650 0.905870 -1.043600

C -0.263390 3.436660 1.345600
C -3.113680 2.491050 0.693220
C -3.154280 2.620530 -0.835220
C -0.537640 4.021600 -0.045220
C -1.547170 -3.146760 0.127650
Si -3.764050 -1.004860 -1.466110
H -1.136670 0.051340 -1.783340
H 0.116290 3.053980 -1.931690
H -1.905660 2.030690 -2.544020
H 0.724230 -1.413790 -1.212690
H -2.365800 0.629630 1.669630
H -0.206350 1.442820 2.254860
H 0.380210 -0.617390 1.773660
H 0.818700 3.418170 1.497960
H -3.884340 1.915600 -1.234270
H -1.463510 4.608850 -0.045370
H -2.959920 3.474650 1.149830
H 0.267760 4.715120 -0.297450
H 1.875580 1.345700 1.076260
H -4.084180 2.144480 1.059700
H -0.681090 4.084550 2.130170
H -3.512490 3.618950 -1.125000
H 1.824330 0.117530 -1.768670
C 2.303660 2.185890 -1.399650
O 2.548830 2.260530 -2.723190
O 2.569560 3.096610 -0.636340
C 3.124640 3.485680 -3.171100
H 2.466780 4.327790 -2.941820
H 4.093800 3.655550 -2.696370
H 3.243530 3.381350 -4.248620
C -3.896080 -0.128470 -3.131420
C -5.089320 -0.443400 -0.247100
C -4.144960 -2.820630 -1.848140
H -3.132920 -0.524510 -3.810570
H -3.771380 0.954900 -3.087060
H -4.874910 -0.334250 -3.578250

H -4.450090 -3.385660 -0.961740

H -3.295560 -3.335040 -2.307730

H -4.980820 -2.857050 -2.556090

H -5.102900 0.632650 -0.065980

H -4.944940 -0.944250 0.716160

H -6.076270 -0.731350 -0.626030

C -0.621850 -3.996910 0.607600

H -2.590790 -3.440930 0.101530

H 0.412420 -3.656280 0.659880

C -0.864520 -5.358470 1.098340

C -2.072180 -6.041540 0.884910

C 0.149610 -6.017840 1.807010

C -0.037970 -7.303870 2.302200

C -2.260510 -7.325570 1.379750

C -1.246130 -7.962950 2.093220

H 1.095120 -5.508510 1.974460

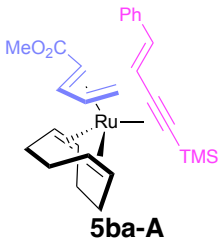
H 0.761490 -7.791850 2.851190

H -2.866880 -5.572190 0.312650

H -3.201820 -7.836370 1.201300

H -1.395450 -8.967460 2.476180

Table S10. Cartesian coordinates of intermediate **5ba**-**A**.



5ba-A

Energy: -994635.4997883

Ru 1.300580 -0.514970 0.160900

C 1.361390 -1.806010 1.925300

C 0.172100 -1.020360 2.021410

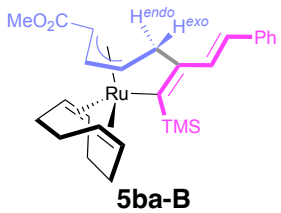
C 2.599000 -1.135320 1.812850

C 0.910730 -2.455980 -0.924290

C 0.019630 -1.515180 -1.436780
C 2.329550 0.086410 -1.722900
C 3.158630 -0.782770 -1.005030
C -0.283560 1.049940 -0.193230
C 2.567670 0.288460 1.764330
C 2.119740 -2.990130 -1.683770
C 0.173560 -0.810880 -2.765860
C 1.595590 -0.284260 -3.007200
C 3.410460 -2.236360 -1.348570
C 0.772910 1.669570 0.098790
C -1.676010 1.151000 -0.544360
Si 1.633490 3.281480 0.392270
C 1.805150 3.619890 2.236060
C 3.332450 3.317860 -0.414600
C 0.530340 4.598020 -0.380010
H 0.161890 -0.117070 2.623570
H 0.484420 -3.130420 -0.188210
H -0.999730 -1.588870 -1.081040
H 2.558840 1.141190 -1.629710
H 3.967050 -0.316770 -0.442060
H 3.503200 -1.707580 1.633150
H 1.308730 -2.887240 1.856350
C -1.117460 -1.721410 1.991370
H 1.947850 0.828270 2.474300
H 3.494770 0.801370 1.518450
H 3.885910 -2.708540 -0.482020
H -0.531050 0.025830 -2.781260
H 1.917500 -2.949600 -2.758830
H 2.189660 -1.018560 -3.561750
H 2.242900 -4.050610 -1.443720
H 1.547390 0.601270 -3.647970
H -0.131360 -1.484570 -3.579630
H 4.134780 -2.309360 -2.172800
H 3.936010 2.452510 -0.123870
H 2.609670 3.032250 2.686760
H 3.262000 3.331380 -1.506710

H	0.876340	3.391760	2.767870
H	0.396710	4.419360	-1.451650
H	-0.459010	4.598990	0.088910
H	3.868480	4.221600	-0.104760
H	2.034500	4.679290	2.395760
H	0.963760	5.596020	-0.253910
O	-2.067770	-1.021220	2.643290
O	-1.349500	-2.794500	1.459020
C	-3.369440	-1.600060	2.662320
H	-3.337540	-2.615720	3.062590
H	-3.800350	-1.626200	1.657930
H	-3.970490	-0.955720	3.302320
C	-2.616340	0.210540	-0.371630
H	-1.953010	2.116000	-0.968640
H	-2.321890	-0.756450	0.021040
C	-4.042820	0.350550	-0.691050
C	-4.680450	1.593860	-0.803870
C	-4.804940	-0.809800	-0.886030
C	-6.156540	-0.732960	-1.203930
C	-6.030900	1.670930	-1.122140
C	-6.773960	0.509120	-1.325730
H	-4.323310	-1.780700	-0.797600
H	-6.727450	-1.643480	-1.356390
H	-4.121520	2.506250	-0.619430
H	-6.509500	2.642100	-1.201340
H	-7.829650	0.572810	-1.569530

Table S11. Cartesian coordinates of intermediate **5ba**-**B**.



5ba-B

Energy: -994639.3868455

Ru	1.691310	0.148620	-0.340040
C	2.561770	1.278180	1.221470
C	1.674920	0.379960	1.880550
C	2.197190	2.248040	0.264770
C	2.137080	-2.052410	-0.659170
C	0.770650	-2.003660	-0.771570
C	1.308710	0.240790	-2.545010
C	2.675860	0.315540	-2.277640
C	-0.166960	0.987910	-0.306450
C	0.938080	3.086690	0.305740
C	3.079730	-2.187080	-1.839780
C	0.090370	-2.054720	-2.119240
C	0.581660	-0.974910	-3.122850
C	3.659280	-0.835410	-2.311330
C	-0.312510	2.278270	0.049120
C	-1.338110	0.142540	-0.575600
Si	-1.979960	3.131510	0.265180
C	-2.707640	2.746480	1.963210
C	-1.682490	4.994480	0.148520
C	-3.237590	2.668900	-1.066270
H	0.671110	0.680100	2.159100
H	2.578010	-2.221370	0.324050
H	0.156290	-2.178330	0.105970
H	0.815800	1.190000	-2.738070
H	3.140170	1.298420	-2.324070
H	3.044270	2.715560	-0.234210
H	3.617780	0.994020	1.252290
C	2.236130	-0.765690	2.598030
H	0.871840	3.598680	1.277600
H	1.021170	3.889680	-0.437770
H	4.508210	-0.565910	-1.670650
H	-0.986120	-1.967280	-1.969370
H	2.568680	-2.686040	-2.667190
H	1.233410	-1.441020	-3.869840
H	3.908090	-2.839360	-1.549210
H	-0.284310	-0.606070	-3.680650

H	0.250390	-3.048950	-2.557350
H	4.070920	-0.949480	-3.323290
H	-0.981250	5.343810	0.913410
H	-1.991220	2.977880	2.758690
H	-1.273520	5.270560	-0.829500
H	-2.966340	1.685810	2.039880
H	-2.787680	2.696300	-2.064510
H	-3.652670	1.669960	-0.906500
H	-2.621940	5.541270	0.283490
H	-3.615990	3.331180	2.146060
H	-4.067730	3.384180	-1.054240
O	1.298200	-1.393740	3.337440
O	3.383880	-1.177410	2.521750
C	1.728770	-2.584410	3.992270
H	2.549310	-2.374170	4.682110
H	2.061400	-3.328930	3.264470
H	0.861140	-2.953030	4.538000
C	-2.015970	-0.521040	0.370530
H	-1.644750	0.065800	-1.618040
H	-1.658350	-0.451510	1.397320
C	-3.189460	-1.380000	0.157150
C	-3.874260	-1.445380	-1.066110
C	-3.652340	-2.173780	1.215330
C	-4.749440	-3.013840	1.057420
C	-4.969660	-2.285440	-1.225300
C	-5.412200	-3.075200	-0.165450
H	-3.138790	-2.129850	2.172350
H	-5.087870	-3.620750	1.891560
H	-3.557620	-0.824430	-1.899080
H	-5.485940	-2.318730	-2.179840
H	-6.270060	-3.728040	-0.291350

Table S12. Cartesian coordinates of intermediate **5ba**-**B'**. This compound is an intermediate with a slight rearrangement of **5ba**-**B**.

Energy: -994623.0796189

Ru -0.401390 0.497380 -0.337490

C 0.151260 -1.275480 -1.549290

C 1.384880 -1.719640 -0.781700

C -1.768370 1.425090 -1.639760

C -0.471110 1.962150 -1.883390

C -0.392040 2.330730 0.874520

C -1.568790 1.623340 1.156280

C 1.646470 0.719850 -0.463070

C -1.173050 -1.440830 -1.122160

C 2.226970 -0.508800 -0.403350

C -1.541120 -1.342430 0.240160

C -2.880890 2.214840 -0.949910

C -0.107600 3.371710 -1.448080

C -0.346990 3.616560 0.053170

C -2.922030 1.984540 0.570870

C 2.449790 1.945050 -0.342330

Si 4.037580 -0.812500 0.094820

C 4.319350 -0.540200 1.941160

C 5.235520 0.255070 -0.895810

C 4.432880 -2.622630 -0.275780

H 1.094430 -2.298900 0.106730

H -1.612060 1.055420 2.084130

H -2.130930 0.700960 -2.366720

H 0.407620 2.230810 1.603210

H 0.041310 1.625560 -2.783320

H -0.855640 -1.657460 1.029250

H 0.293160 -1.163900 -2.622680

H 1.970490 -2.414420 -1.395380

H -1.978440 -1.383540 -1.849580

C -2.961020 -1.316100 0.610790

H -3.840960 1.921820 -1.382550

H 0.452680 4.249840 0.447370

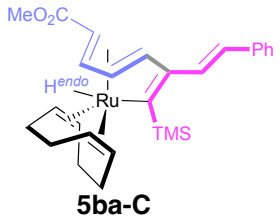
H -3.318650 2.873030 1.082180

H -0.673490 4.093470 -2.054750

H -3.619050 1.171310 0.784480

H	0.944810	3.545910	-1.680070
H	-2.758160	3.279970	-1.174740
H	-1.279020	4.171860	0.206460
H	4.355090	-2.846610	-1.344960
H	3.766020	-3.306390	0.259900
H	5.025420	0.191490	-1.968570
H	5.184840	1.306120	-0.600670
H	3.542830	-1.029270	2.538670
H	4.322140	0.523820	2.192470
H	5.458830	-2.848180	0.035150
H	6.261530	-0.094610	-0.734990
H	5.286670	-0.958290	2.241130
O	-3.116290	-1.336460	1.949740
O	-3.900370	-1.252090	-0.159640
C	-4.463870	-1.273860	2.413240
H	-4.937120	-0.337590	2.106210
H	-5.047340	-2.109900	2.021400
H	-4.405900	-1.327010	3.499360
C	2.866560	2.504420	0.800780
H	2.731860	2.404980	-1.289680
H	2.615610	2.013090	1.739440
C	3.685750	3.720850	0.916900
C	3.764470	4.679130	-0.103720
C	4.414800	3.944240	2.092430
C	5.214550	5.072770	2.237170
C	4.563600	5.807250	0.039690
C	5.294880	6.008350	1.208990
H	4.355700	3.217190	2.898520
H	5.774910	5.222260	3.154950
H	3.182920	4.549450	-1.011860
H	4.608800	6.538520	-0.761560
H	5.915780	6.891600	1.320090

Table S13. Cartesian coordinates of intermediate **5ba**-**C**.



5ba-C

Energy: -994621.9322743

Ru -0.294190 0.384090 0.024040

C 0.323820 -1.350230 -1.094440

C 1.160880 -1.229310 0.050350

C -1.444070 1.183690 -1.875110

C -0.338590 1.988910 -1.713870

C -0.686240 2.282790 1.105800

C -1.899560 1.597610 0.940290

C 1.760090 0.883950 -0.031090

C -1.082140 -1.536720 -0.881400

C 2.353590 -0.330240 -0.026850

C -1.625330 -1.521980 0.408160

C -2.857650 1.516110 -1.454830

C -0.434210 3.410610 -1.179980

C -0.327570 3.542450 0.350170

C -2.978210 2.079840 -0.028160

C 2.459350 2.163980 -0.013270

Si 4.139240 -0.887630 -0.128770

C 4.961770 -0.928200 1.570270

C 5.137560 0.227020 -1.272860

C 4.104100 -2.643250 -0.820800

H 0.072880 0.021610 1.517600

H -2.254790 1.010100 1.782730

H -1.361820 0.391310 -2.614250

H -0.193880 2.196880 2.070310

H 0.540300 1.751760 -2.306000

H -1.094240 -1.896390 1.272080

H 0.697080 -1.163270 -2.096850

H 1.043030 -1.919540 0.884020

H -1.764480 -1.532830 -1.724860

C -3.089210 -1.427090 0.562140

H -3.440040 0.594900 -1.515190
H 0.692310 3.815530 0.625300
H -2.961460 3.175880 -0.047920
H -1.382430 3.835850 -1.526670
H -3.957540 1.802260 0.372800
H 0.349580 4.012340 -1.651490
H -3.299250 2.217980 -2.176820
H -0.967770 4.365020 0.698880
H 3.652240 -2.663060 -1.818250
H 3.518080 -3.309370 -0.178020
H 4.689680 0.263920 -2.271260
H 5.183580 1.249110 -0.886680
H 4.368130 -1.507230 2.285350
H 5.080090 0.082630 1.973480
H 5.113820 -3.059580 -0.899720
H 6.162350 -0.146360 -1.375540
H 5.956470 -1.383850 1.511150
O -3.434660 -1.420990 1.861250
O -3.904570 -1.344730 -0.336700
C -4.829690 -1.274920 2.124590
H -5.197800 -0.326710 1.724850
H -5.396020 -2.093150 1.674630
H -4.929800 -1.293480 3.208560
C 3.298210 2.545540 0.962050
H 2.252100 2.845050 -0.838480
H 3.481030 1.849460 1.779310
C 4.009530 3.830460 1.039270
C 3.648040 4.947950 0.272190
C 5.095880 3.955360 1.915720
C 5.810120 5.144960 2.010310
C 4.360510 6.137300 0.366050
C 5.446820 6.241590 1.233190
H 5.384730 3.102420 2.524600
H 6.651250 5.215670 2.693120
H 2.793130 4.892750 -0.395810
H 4.061940 6.990700 -0.235230

H 6.000040 7.172480 1.306770

Table S14. Cartesian coordinates of intermediate **5ba**-**C'**. This compound is an intermediate with a slight rearrangement of **5ba**-**C**.

Energy: -994610.8517748

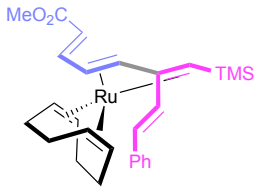
Ru -0.299330 0.390540 0.015180
C 0.327140 -1.347690 -1.092450
C 1.157350 -1.221320 0.056680
C -1.437880 1.180570 -1.894680
C -0.333890 1.987230 -1.730260
C -0.699830 2.293780 1.085670
C -1.911520 1.606750 0.915810
C 1.754670 0.892230 -0.028810
C -1.079910 -1.534750 -0.886900
C 2.349500 -0.321210 -0.016690
C -1.630490 -1.515330 0.399450
C -2.854370 1.513720 -1.484840
C -0.433460 3.411370 -1.203650
C -0.338040 3.550530 0.326620
C -2.984440 2.083750 -0.061530
C 2.452100 2.173220 -0.010730
Si 4.136790 -0.875370 -0.106400
C 4.952790 -0.900940 1.596050
C 5.136550 0.233740 -1.254650
C 4.108800 -2.636060 -0.785760
H 0.058640 0.034930 1.512730
H -2.271490 1.022770 1.758700
H -1.350500 0.384970 -2.629770
H -0.213260 2.212680 2.053510
H 0.548720 1.747860 -2.315930
H -1.103980 -1.885830 1.267830
H 0.706080 -1.164290 -2.093390
H 1.035080 -1.908080 0.892560
H -1.757310 -1.535020 -1.734330

C -3.095310 -1.421320 0.544830
H -3.435580 0.591730 -1.544710
H 0.679250 3.827090 0.607710
H -2.968310 3.179710 -0.086190
H -1.379080 3.834970 -1.559360
H -3.966080 1.807260 0.334480
H 0.353730 4.010920 -1.672250
H -3.291970 2.211940 -2.212780
H -0.982350 4.373430 0.666860
H 3.660180 -2.664350 -1.784470
H 3.522640 -3.299190 -0.140050
H 4.694040 0.260010 -2.255760
H 5.175650 1.259260 -0.876830
H 4.357010 -1.474450 2.313780
H 5.068660 0.113450 1.990940
H 5.119930 -3.050080 -0.858500
H 6.163650 -0.135570 -1.348460
H 5.948140 -1.356080 1.544510
O -3.447980 -1.411350 1.841970
O -3.905710 -1.342670 -0.358820
C -4.844570 -1.265730 2.097150
H -5.211150 -0.318820 1.692980
H -5.407750 -2.085550 1.646120
H -4.950710 -1.281610 3.180590
C 3.281270 2.560500 0.970590
H 2.250850 2.850130 -0.840840
H 3.457030 1.868430 1.792790
C 3.989820 3.846840 1.049350
C 3.639790 4.958150 0.268090
C 5.061880 3.979480 1.942120
C 5.773370 5.170500 2.039290
C 4.349620 6.148860 0.364350
C 5.421790 6.260810 1.248030
H 5.341710 3.131420 2.561940
H 6.603320 5.247230 2.735030
H 2.795930 4.897060 -0.413330

H 4.060110 6.997340 -0.248200

H 5.972970 7.192760 1.323380

Table S15. Cartesian coordinates of intermediate **5ba**-**D**.



5ba-D

Energy: -994609.8707830

Ru -0.073810 0.133810 -0.060880

C 0.016940 -2.014950 -0.439860

C 1.078230 -1.559540 0.435060

C -0.200310 0.444700 -2.249830

C 0.718800 1.383230 -1.761630

C -0.861820 2.128240 0.420460

C -1.865190 1.405630 -0.257660

C 1.918190 0.488420 1.116360

C -1.249800 -1.739300 0.139460

C 2.029850 -0.516240 0.101610

C -1.271370 -1.096030 1.435650

C -1.625520 0.743580 -2.664360

C 0.481480 2.879480 -1.600230

C -0.087380 3.260130 -0.221770

C -2.315470 1.691890 -1.683120

C 2.569260 1.786940 1.052480

Si 3.407200 -0.772690 -1.176160

C 4.508540 -2.054650 -0.345660

C 4.453160 0.755320 -1.520850

C 2.771320 -1.475960 -2.800920

H 1.598660 0.175480 2.111640

H -2.634560 0.948340 0.349620

H 0.221520 -0.428960 -2.740970

H -0.938410 2.188800 1.504970

H 1.759560 1.133660 -1.921450
H -0.610070 -1.411440 2.233280
H 0.125470 -2.380140 -1.453690
H 0.988750 -1.802970 1.490930
H -2.174120 -1.920710 -0.399860
C -2.582300 -0.699300 1.967970
H -2.172960 -0.204900 -2.684780
H 0.733870 3.530720 0.445390
H -2.121140 2.736630 -1.943570
H -0.170520 3.233840 -2.405170
H -3.399860 1.561290 -1.745600
H 1.437380 3.393830 -1.749200
H -1.643170 1.137730 -3.691180
H -0.725710 4.151270 -0.304580
H 2.251450 -0.726280 -3.403660
H 2.099300 -2.325480 -2.647700
H 3.904110 1.569490 -2.003810
H 4.905610 1.145130 -0.604250
H 3.959460 -2.984130 -0.163840
H 4.877990 -1.688290 0.617460
H 3.625050 -1.836210 -3.385480
H 5.267360 0.465740 -2.194900
H 5.374730 -2.288610 -0.973760
O -2.477270 -0.254250 3.237790
O -3.652300 -0.741450 1.384580
C -3.696320 0.172360 3.840420
H -4.136210 1.000850 3.279960
H -4.417020 -0.647880 3.881360
H -3.432930 0.495100 4.846870
C 2.758650 2.588890 2.113330
H 2.867420 2.128340 0.065160
H 2.464540 2.225340 3.097740
C 3.330170 3.940920 2.077260
C 3.513480 4.657370 0.883810
C 3.699440 4.560610 3.279370
C 4.246880 5.838860 3.291710

C 4.061480 5.933830 0.894960
C 4.433350 6.531270 2.098270
H 3.556910 4.026340 4.215090
H 4.527280 6.295470 4.235980
H 3.213410 4.219030 -0.063700
H 4.191820 6.469600 -0.040370
H 4.857820 7.530120 2.104760

Table S16. Cartesian coordinates of transition state **5ba**-**TS1**.

Energy: -994628.0398428
Ru -0.469250 0.368540 -0.393520
C -1.154770 -1.031530 -1.950750
C -0.945820 -1.771100 -0.747190
C -0.099760 -0.228580 -2.424830
C -2.510330 1.041620 -0.317320
C -2.050710 0.808710 1.005340
C 0.103570 2.395520 0.257550
C -0.214300 2.422520 -1.110350
C 0.868740 -0.220380 1.076990
C 1.222650 -0.368910 -1.790840
C -2.742720 2.431410 -0.910490
C -1.699100 1.915620 1.981600
C -0.777630 2.974600 1.358510
C -1.519230 2.944790 -1.682670
C 1.759520 -0.246520 0.127900
C 0.902920 -0.452100 2.507320
Si 3.614240 -0.144120 0.013960
C 4.307490 -1.452220 -1.149040
C 4.091020 1.572530 -0.598500
C 4.307240 -0.410930 1.742220
H -0.006570 -2.281900 -0.557310
H -3.162950 0.269790 -0.715970
H -2.439540 -0.089110 1.484250
H 1.163920 2.359280 0.495790

H 0.625060 2.455710 -1.805930
H -0.241270 0.447440 -3.260560
H -2.147060 -0.953050 -2.382960
C -2.106680 -2.339870 -0.053170
H 1.568580 -1.400010 -1.754890
H 1.967040 0.296170 -2.222180
H -1.585420 2.602200 -2.721310
H -1.190500 1.458470 2.834500
H -3.021750 3.130280 -0.115250
H -1.358840 3.812540 0.960080
H -3.604820 2.389660 -1.583380
H -0.133650 3.401280 2.133790
H -2.615420 2.379920 2.375030
H -1.507870 4.043910 -1.720000
H 3.673570 1.788170 -1.587250
H 4.017810 -1.281570 -2.190200
H 3.729280 2.341890 0.091180
H 3.969040 -2.453020 -0.861930
H 4.017420 0.399510 2.418590
H 3.963110 -1.357130 2.170880
H 5.179960 1.667470 -0.669950
H 5.401940 -1.443410 -1.105490
H 5.401560 -0.436010 1.704010
O -1.723340 -3.120420 0.979130
O -3.278920 -2.129570 -0.309450
C -2.774650 -3.616280 1.802140
H -3.416590 -4.303340 1.245370
H -3.387470 -2.794560 2.183050
H -2.286000 -4.135980 2.625510
C -0.131980 -0.990270 3.169950
H 1.833970 -0.227140 3.024870
H -1.031710 -1.199180 2.598470
C -0.182320 -1.349190 4.591860
C 0.947670 -1.368240 5.422600
C -1.421530 -1.691940 5.149610
C -1.536010 -2.026840 6.494450

C 0.834460 -1.701650 6.766310
C -0.407190 -2.030590 7.309080
H -2.304790 -1.687630 4.515830
H -2.506730 -2.285210 6.906030
H 1.925960 -1.134710 5.013480
H 1.720560 -1.712580 7.393460
H -0.491180 -2.293770 8.358700

Table S17. Cartesian coordinates of transition state **5ba**-**TS2**.

Energy: -994621.5641835
Ru -0.304310 0.364430 -0.035990
C 0.504570 -1.342770 -1.090560
C 1.172850 -1.207010 0.205250
C -1.667340 1.374460 -1.528320
C -0.524770 2.153920 -1.413780
C -0.516890 2.026770 1.422760
C -1.749090 1.367180 1.312560
C 1.753420 0.916930 -0.048970
C -0.890920 -1.553000 -1.121180
C 2.356280 -0.278790 0.158760
C -1.659280 -1.548390 0.060800
C -3.005870 1.720660 -0.908610
C -0.537900 3.489090 -0.679870
C -0.259350 3.397730 0.833970
C -2.942200 2.001640 0.604660
C 2.445690 2.193760 -0.160540
Si 4.136830 -0.861810 0.186670
C 4.848340 -0.861770 1.936240
C 5.242810 0.168250 -0.937540
C 4.106450 -2.644100 -0.436950
H 0.242670 -0.423870 1.267120
H -1.996450 0.627780 2.068770
H -1.725030 0.699030 -2.378090
H 0.111120 1.781110 2.275350

H 0.245780 2.026180 -2.168710
H -1.287110 -1.961450 0.989820
H 1.060430 -1.197670 -2.010340
H 1.126840 -2.039550 0.910630
H -1.411650 -1.533500 -2.074000
C -3.122540 -1.493220 -0.053950
H -3.678860 0.883170 -1.095000
H 0.783010 3.654400 1.026820
H -2.922280 3.082240 0.789600
H -1.511630 3.961450 -0.853280
H -3.859210 1.633900 1.074870
H 0.198480 4.153400 -1.143250
H -3.436000 2.583780 -1.436260
H -0.863730 4.142200 1.370680
H 3.710680 -2.697210 -1.456770
H 3.477490 -3.278840 0.196890
H 4.813120 0.246050 -1.941420
H 5.383100 1.183220 -0.556590
H 4.212660 -1.432450 2.621450
H 4.938490 0.154400 2.333820
H 5.112610 -3.076240 -0.443720
H 6.227990 -0.302790 -1.027110
H 5.845890 -1.314830 1.948550
O -3.706030 -1.476710 1.160040
O -3.760540 -1.445970 -1.089960
C -5.125860 -1.349430 1.153960
H -5.423960 -0.401670 0.696830
H -5.588640 -2.169220 0.600250
H -5.431050 -1.375940 2.198980
C 3.373200 2.619130 0.712010
H 2.158100 2.841020 -0.988430
H 3.635990 1.963690 1.541070
C 4.091540 3.899800 0.651880
C 3.603750 5.007940 -0.055730
C 5.313030 4.029390 1.326580
C 6.037210 5.215650 1.276480

C 4.325720 6.194320 -0.104830
C 5.547310 6.303040 0.557670
H 5.699190 3.182690 1.888660
H 6.984610 5.291610 1.801170
H 2.642340 4.946360 -0.557730
H 3.929350 7.042090 -0.655320
H 6.108120 7.231540 0.520380

Table S18. Cartesian coordinates of transition state **5ba**-**TS3**.

Energy: -994608.7146031
Ru -0.367450 0.384890 0.001390
C 0.268320 -1.495060 -0.865020
C 1.100750 -1.213240 0.239210
C -1.160070 0.916950 -2.055510
C -0.103490 1.785180 -1.772450
C -1.063060 2.363420 0.842310
C -2.187510 1.627200 0.475010
C 1.712630 0.887960 0.340990
C -1.138570 -1.578330 -0.570470
C 2.295260 -0.317620 0.147010
C -1.578060 -1.424190 0.773080
C -2.637460 1.240060 -2.003640
C -0.319740 3.257580 -1.435500
C -0.520720 3.541600 0.063680
C -3.050270 1.983200 -0.730050
C 2.413940 2.176630 0.384930
Si 4.046120 -0.763490 -0.348000
C 5.224000 -0.697700 1.122610
C 4.655170 0.423270 -1.678030
C 3.974190 -2.519420 -1.027700
H 0.590070 0.750320 1.315170
H -2.693070 1.101110 1.277830
H -0.920790 0.070890 -2.697080
H -0.800710 2.364080 1.896840

H 0.860040 1.538640 -2.211240
H -1.038680 -1.832750 1.617700
H 0.624490 -1.460990 -1.890130
H 0.897580 -1.668080 1.205330
H -1.866440 -1.691380 -1.366440
C -3.025580 -1.284650 0.983340
H -3.178460 0.290580 -2.032820
H 0.433120 3.824870 0.515110
H -3.014610 3.068040 -0.881810
H -1.180990 3.621370 -2.006550
H -4.089200 1.738060 -0.496090
H 0.537960 3.832590 -1.799950
H -2.932840 1.804820 -2.900160
H -1.189450 4.402970 0.201700
H 3.308580 -2.579140 -1.895310
H 3.600000 -3.219690 -0.273410
H 3.996940 0.401570 -2.552880
H 4.680620 1.449350 -1.298330
H 4.863330 -1.314160 1.952130
H 5.329260 0.330180 1.484320
H 4.965760 -2.861880 -1.341100
H 5.665860 0.159250 -2.007380
H 6.219110 -1.058520 0.839890
O -3.333760 -1.280170 2.297140
O -3.873850 -1.158540 0.118150
C -4.715730 -1.105820 2.600250
H -5.083050 -0.157870 2.198980
H -5.311100 -1.920090 2.180660
H -4.784040 -1.108150 3.687260
C 3.259750 2.522610 1.364380
H 2.228560 2.854350 -0.446180
H 3.421690 1.811750 2.173870
C 4.023050 3.777830 1.449740
C 3.724350 4.903330 0.668490
C 5.097480 3.858310 2.344790
C 5.862800 5.015570 2.444560

C	4.487400	6.060100	0.767920
C	5.562050	6.121060	1.653930
H	5.336540	2.997930	2.964550
H	6.694040	5.053730	3.141720
H	2.879700	4.881380	-0.014080
H	4.238420	6.921860	0.156330
H	6.155130	7.026730	1.731290