

Electronic Supplementary Information

Amido Rare-Earth Complexes Supported by Ansa Bis(amidinate) Ligand with Rigid 1,8-Naphthalene Linker: Synthesis, Structures and Catalytic Activity in *rac*-Lactide Polymerization and Hydrophosphonylation of Carbonyl Compounds

Marina V. Yakovenko,^a Natalia Yu. Udilova,^a Tatyana A. Glukhova,^a

Anton V. Cherkasov,^a Georgy K. Fukin,^{a,b} and Alexander A. Trifonov^{a,b,c,*}

[a] G. A. Razuvaev Institute of Organometallic Chemistry of Russian Academy of Sciences,
Tropinina str. 49, 603950 Nizhny Novgorod, GSP-445, Russia, Fax: +007-831-4627497, E-
mail: trif@iomc.ras.ru

[b] Nizhny Novgorod State University, Gagarina av. 23, 603950, Nizhny Novgorod, Russia

[c] Institute of Organoelement compounds of Russian Academy of Sciences, Vavilova str. 28,
119334, Moscow, Russia

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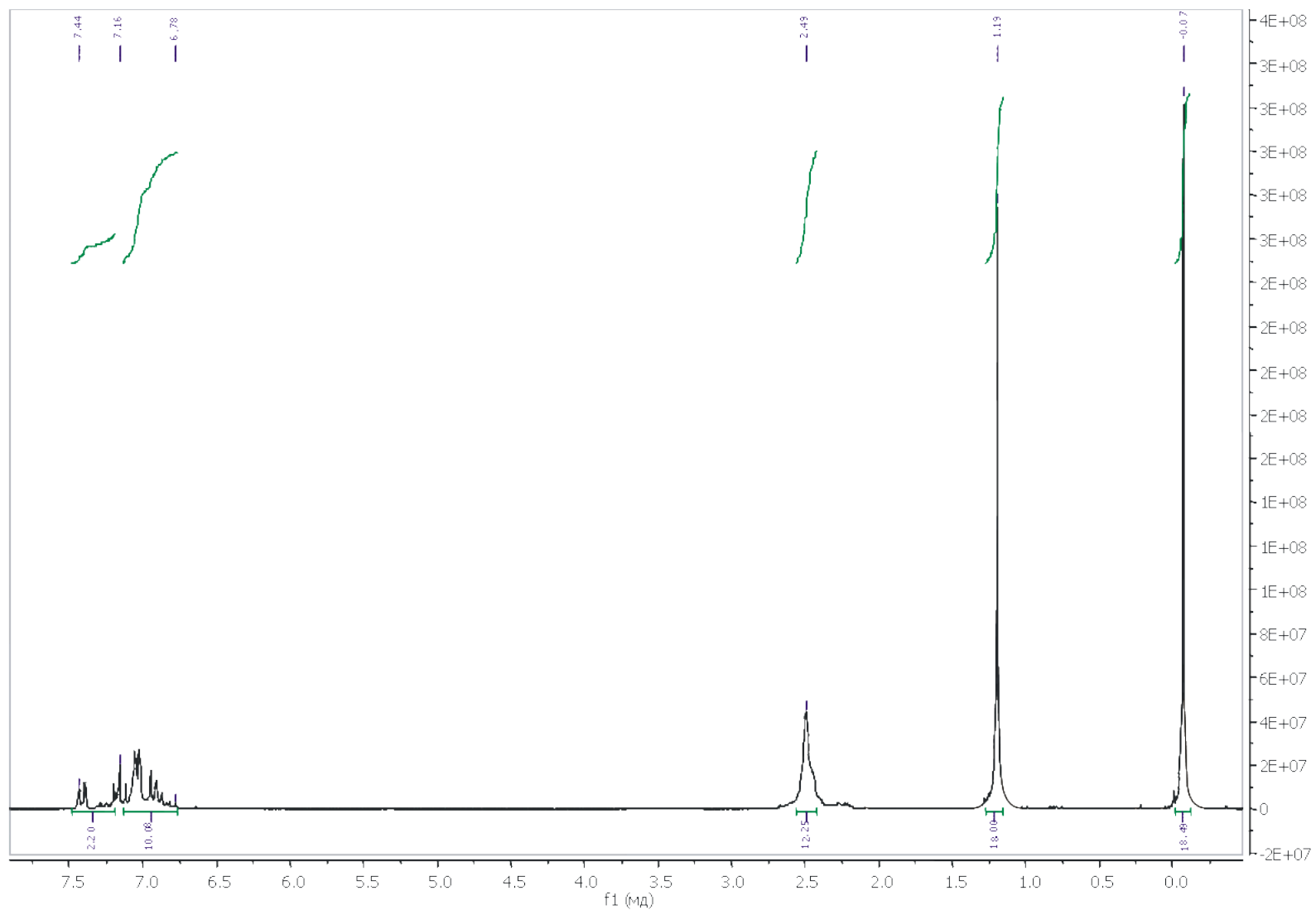


Fig. S1. ^1H NMR spectra of complex $[1,8\text{-C}_{10}\text{H}_6\{\text{NC}(t\text{Bu})\text{N-2,6-Me}_2\text{-C}_6\text{H}_3\}_2]\text{YN}(\text{SiMe}_3)_2$ (**2**), C_6D_6 , 20°C .

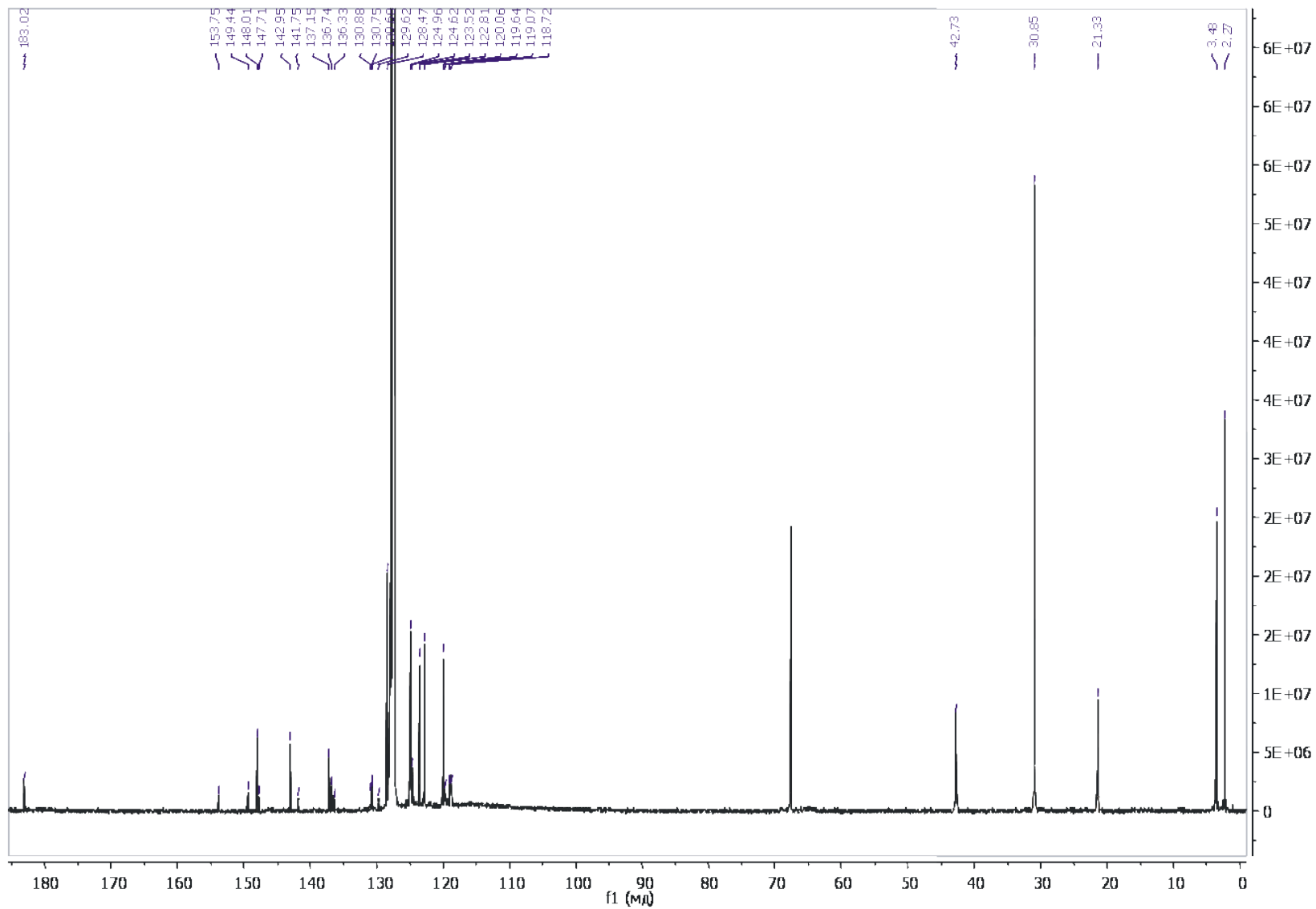


Fig. S2 ^{13}C NMR spectra of complex $[1,8\text{-C}_{10}\text{H}_6\{\text{NC}(t\text{Bu})\text{N-2,6-Me}_2\text{-C}_6\text{H}_3\}_2]\text{YN}(\text{SiMe}_3)_2$ (**2**), C_6D_6 , 20°C .

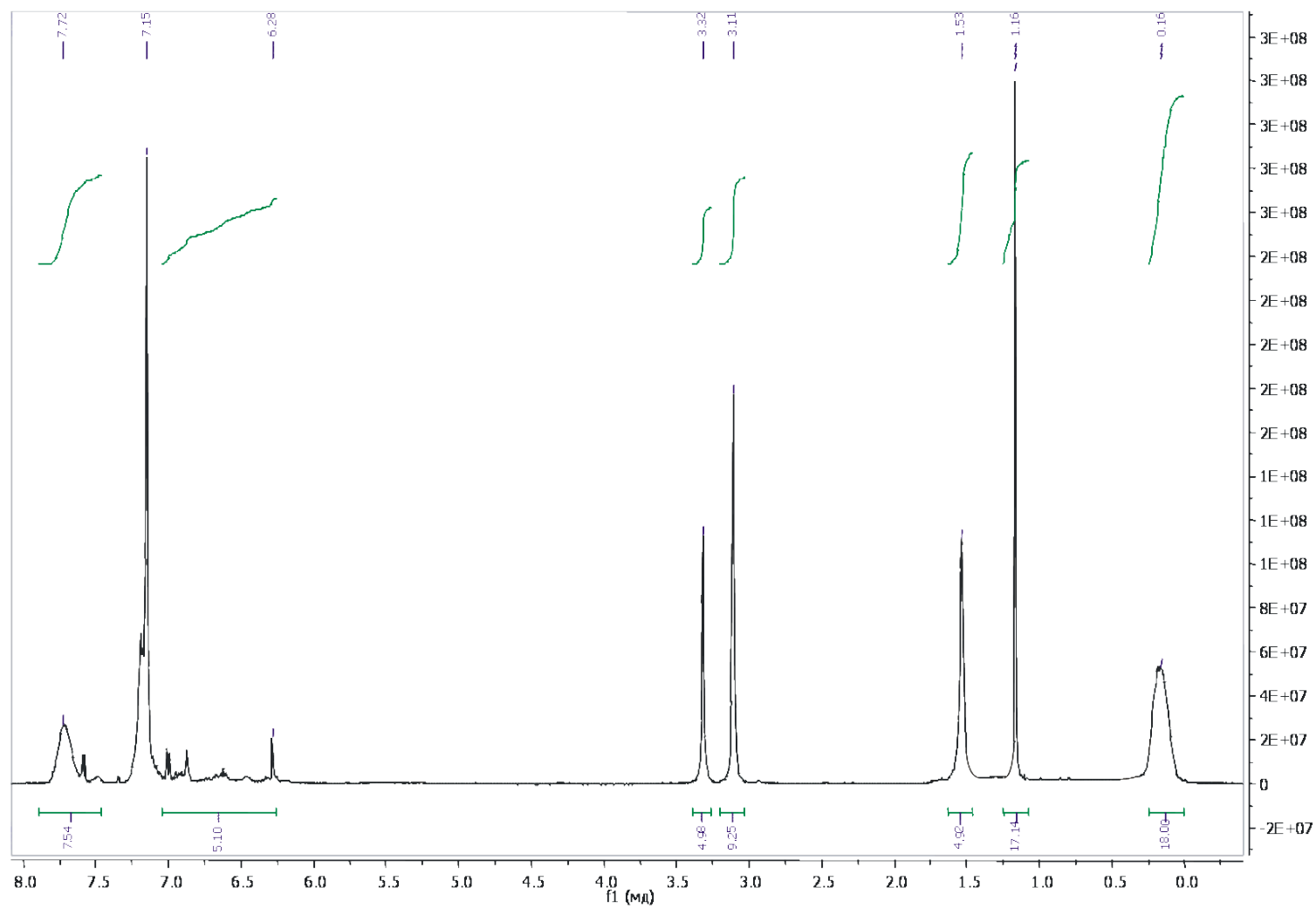


Fig. S3. ^1H NMR spectra of complex $[1,8\text{-C}_{10}\text{H}_6\{\text{NC}(t\text{Bu})\text{N-}2,6\text{-Me}_2\text{-C}_6\text{H}_3\}_2]\text{SmN}(\text{SiMe}_3)_2(\text{THF})$ (**3**), C_6D_6 , 20°C .

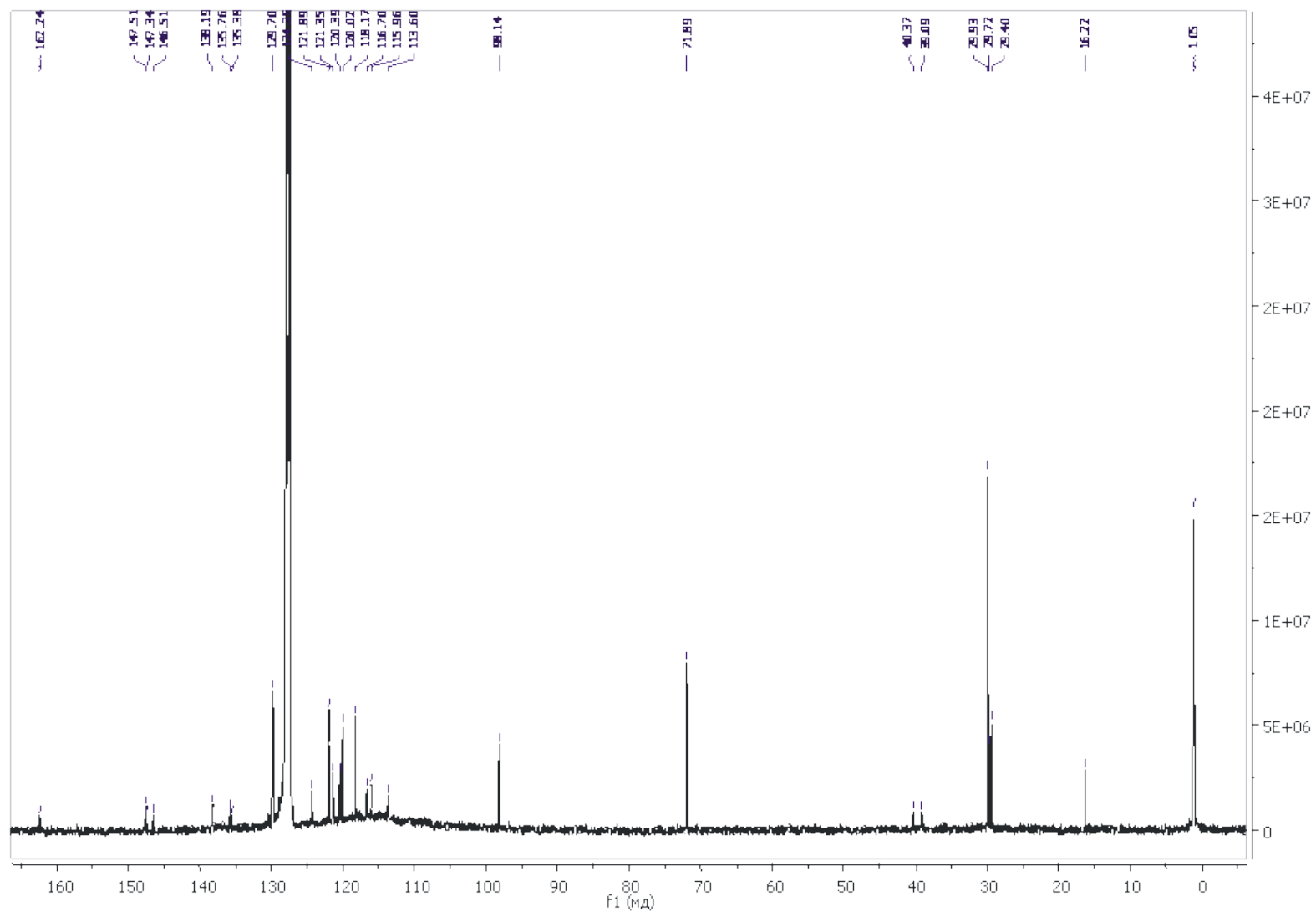


Fig. S4 ^{13}C NMR spectra of complex $[1,8\text{-C}_{10}\text{H}_6\{\text{NC}(t\text{Bu})\text{N-2,6-Me}_2\text{-C}_6\text{H}_3\}_2]\text{SmN}(\text{SiMe}_3)_2(\text{THF})$ (**3**), C_6D_6 , 20°C .

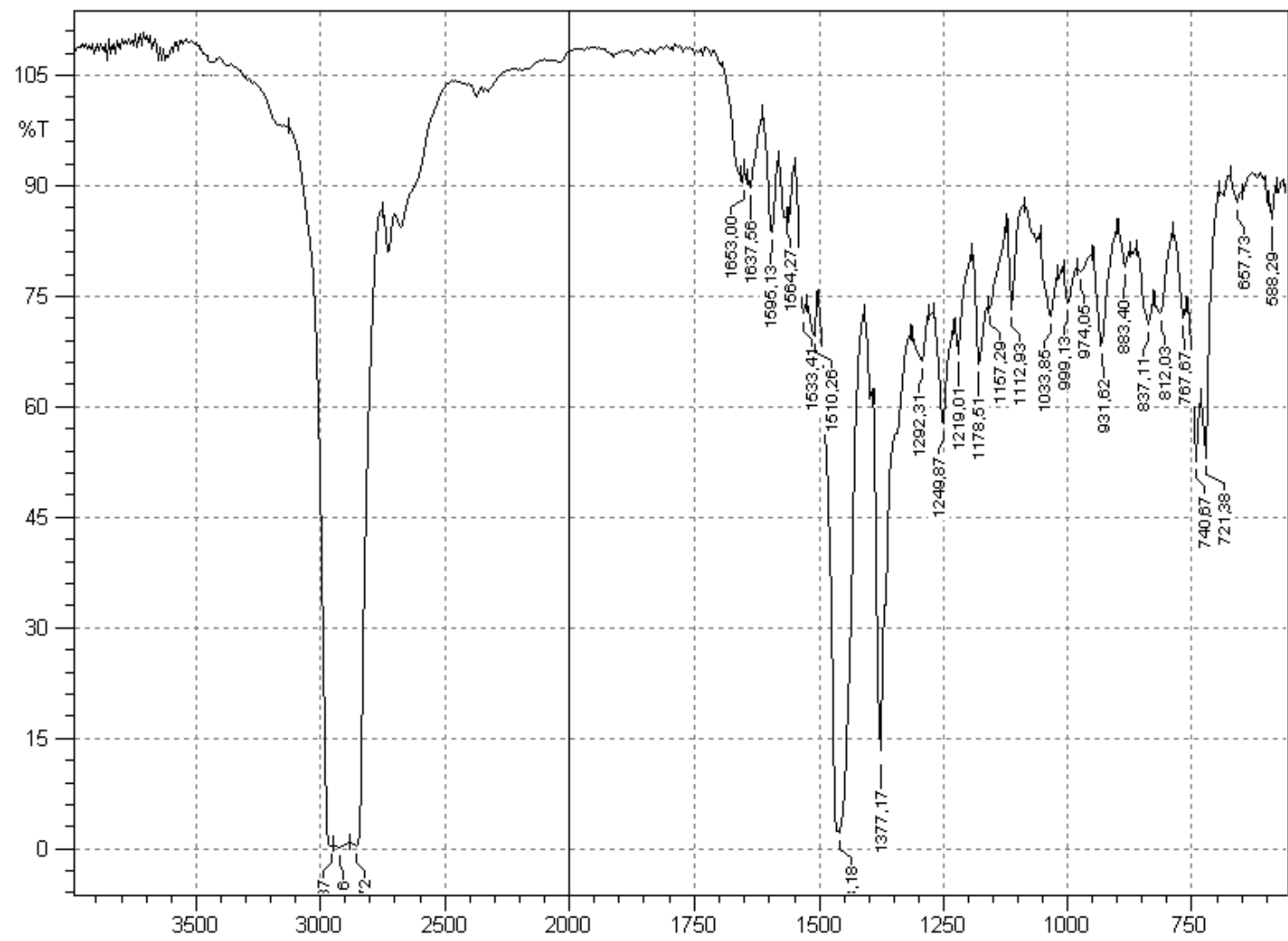


Fig. S5 IR spectra of $[1,8\text{-C}_{10}\text{H}_6\{\text{NC}(t\text{Bu})\text{N-2,6-Me}_2\text{-C}_6\text{H}_3\}_2]\text{Nd}[1,8\text{-C}_{10}\text{H}_6\{\text{NC}(t\text{Bu})\text{N-2,6-Me}_2\text{-C}_6\text{H}_3\}\{\text{NC}(t\text{Bu})\text{NLi(DME)-2,6-Me}_2\text{-C}_6\text{H}_3\}]\cdot\text{Et}_2\text{O}$ (**1**), Nujol, KBr.

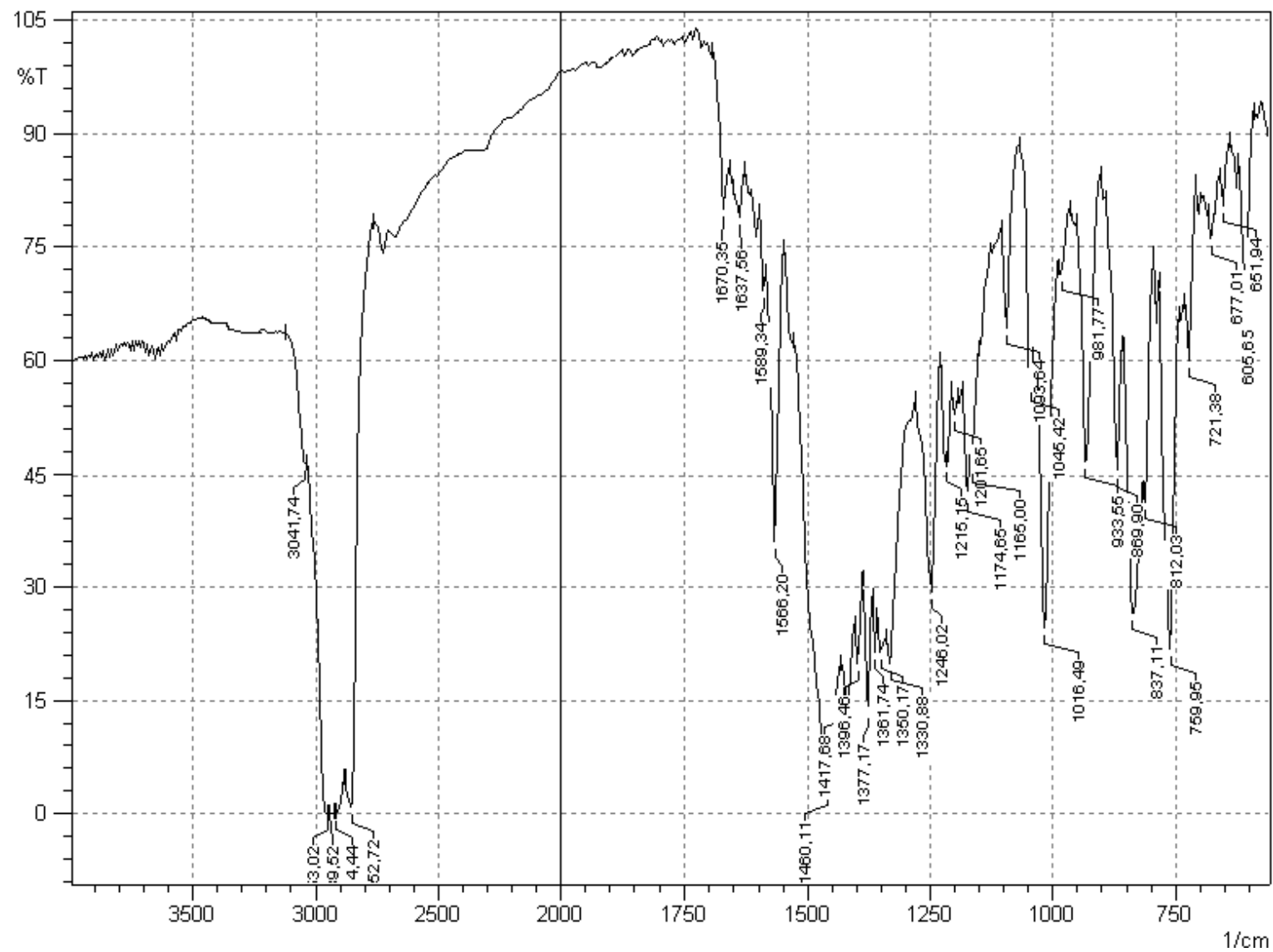


Fig. S6 IR spectra of [1,8- C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]YN(SiMe₃)₂ (**2**), Nujol, KBr.

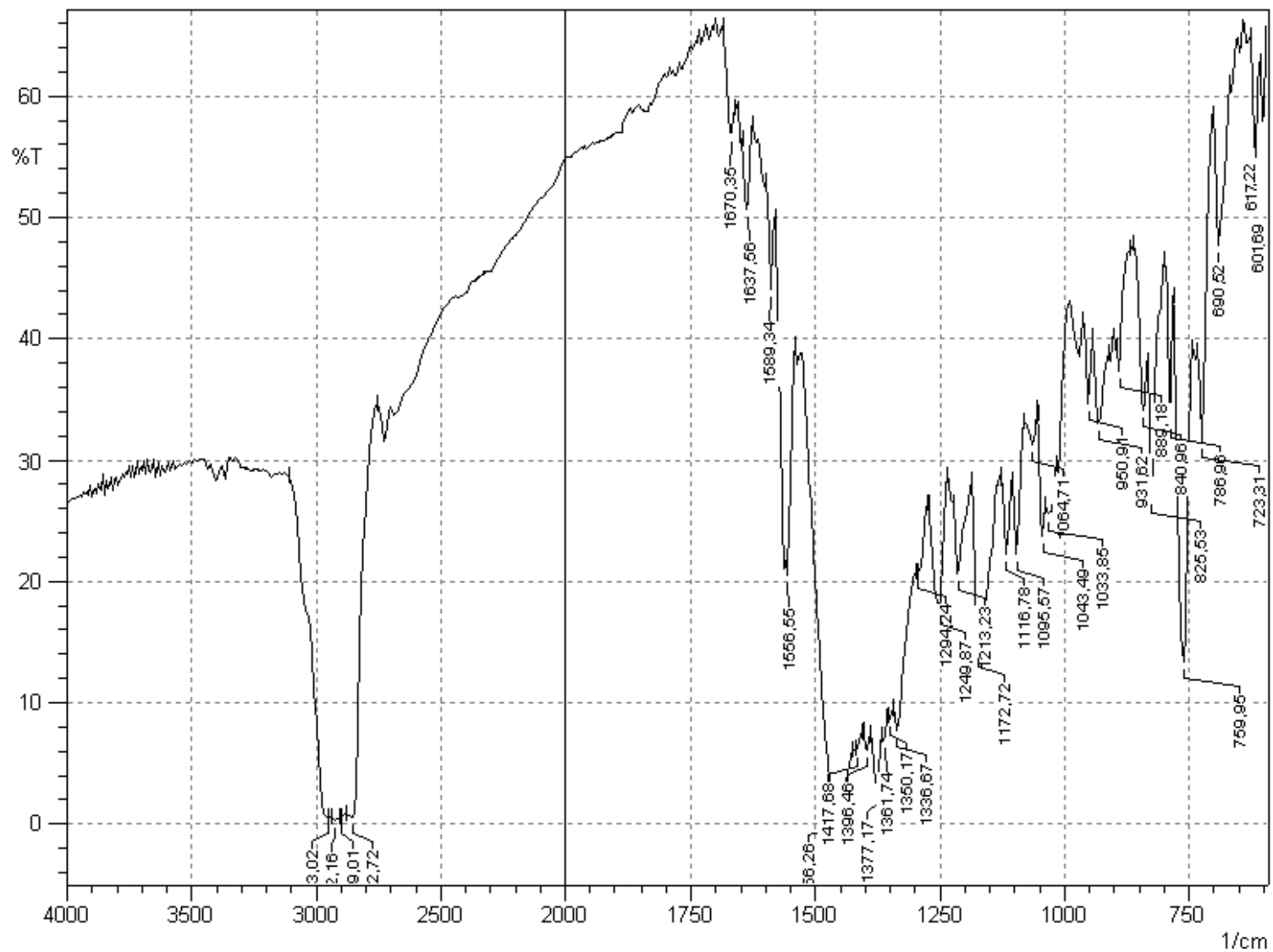


Fig. S7 IR spectra of [1,8- C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]SmN(SiMe₃)₂THF (**3**), Nujol, KBr.

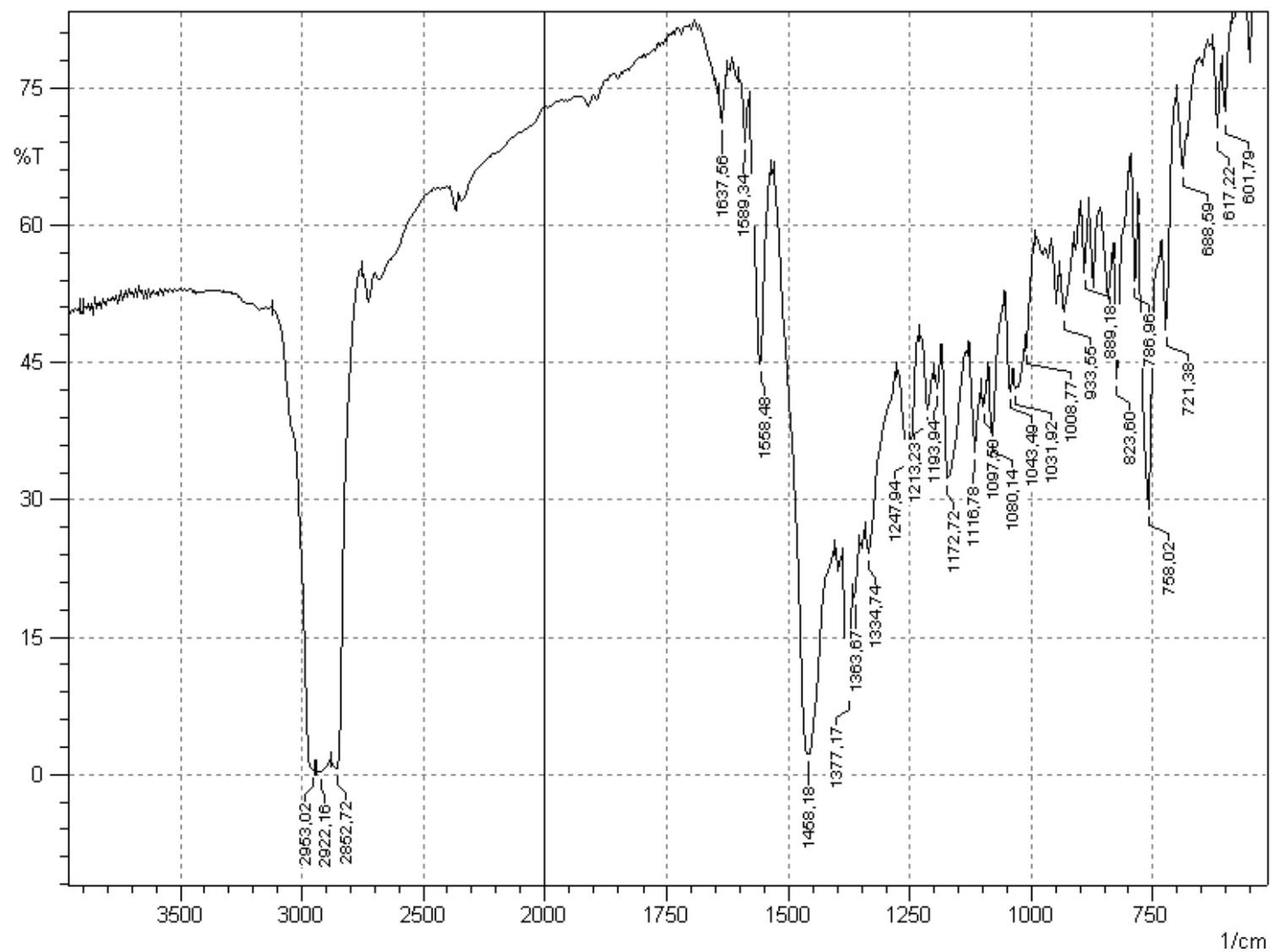


Fig. S8 IR spectra of [1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]NdN(SiMe₃)₂THF (**4**), Nujol, KBr.

Crystallographic data for 1 and 4.

Table S1. Crystal data and structure refinement for [1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]Nd[μ-1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂][Li(DME)] (1)

Empirical formula	C ₈₀ H ₁₀₄ Li N ₈ Nd O ₃
Formula weight	1376.89
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.6452(6) Å alpha = 101.6620(10) deg. b = 15.0817(7) Å beta = 97.1300(10) deg. c = 20.7038(9) Å gamma = 106.0300(10) deg.
Volume	3648.0(3) Å ³
Z, Calculated density	2, 1.253 Mg/m ³
Absorption coefficient	0.764 mm ⁻¹
F(000)	1454
Crystal size	0.26 x 0.24 x 0.13 mm
Theta range for data collection	1.97 to 27.00 deg.
Limiting indices	-16 ≤ h ≤ 15, -13 ≤ k ≤ 19, -26 ≤ l ≤ 25
Reflections collected / unique	23814 / 15794 [R(int) = 0.0201]
Completeness to theta = 27.00	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9072 and 0.8260
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15794 / 34 / 860
Goodness-of-fit on F ²	1.057
Final R indices [I > 2σ(I)]	R1 = 0.0405, wR2 = 0.1023
R indices (all data)	R1 = 0.0507, wR2 = 0.1071
Largest diff. peak and hole	2.097 and -0.597 e.Å ⁻³

Table S2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for ([1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]Nd[μ-1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂][Li(DME)] (1).

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Nd(1)	-1978(1)	-3765(1)	-2545(1)	21(1)
Li(1)	-1160(3)	218(3)	-2227(2)	37(1)
O(1)	-129(2)	1551(1)	-2014(1)	50(1)
O(2)	-2214(1)	890(1)	-1886(1)	45(1)
N(1)	-467(1)	-3935(1)	-3167(1)	30(1)
N(2)	-57(1)	-3205(1)	-1839(1)	28(1)
N(3)	-1950(1)	-5220(1)	-3479(1)	25(1)
N(4)	-1386(1)	-4037(1)	-1393(1)	26(1)
N(5)	-3186(1)	-2889(1)	-2060(1)	28(1)
N(6)	-1608(1)	-2080(1)	-2746(1)	24(1)
N(7)	-4166(1)	-4359(1)	-2636(1)	26(1)
N(8)	-1501(1)	-708(1)	-3124(1)	29(1)
C(1)	524(2)	-3261(1)	-3183(1)	27(1)
C(2)	1184(2)	-2574(1)	-2573(1)	26(1)
C(3)	946(2)	-2591(1)	-1917(1)	27(1)
C(4)	1626(2)	-1889(2)	-1370(1)	34(1)
C(5)	2560(2)	-1181(2)	-1433(1)	39(1)
C(6)	2814(2)	-1145(2)	-2049(1)	36(1)
C(7)	2129(2)	-1828(1)	-2635(1)	29(1)
C(8)	2385(2)	-1776(2)	-3276(1)	35(1)
C(9)	1732(2)	-2430(2)	-3842(1)	36(1)
C(10)	808(2)	-3160(2)	-3794(1)	32(1)
C(11)	-841(2)	-4865(1)	-3441(1)	22(1)
C(12)	-58(2)	-5504(1)	-3577(1)	26(1)
C(13)	-374(2)	-6293(2)	-3206(1)	36(1)
C(14)	-159(2)	-5967(2)	-4324(1)	34(1)
C(15)	1191(2)	-4954(2)	-3297(1)	32(1)
C(16)	-2640(2)	-6108(1)	-3903(1)	25(1)
C(17)	-2852(2)	-6253(1)	-4607(1)	28(1)
C(18)	-3594(2)	-7114(2)	-5002(1)	33(1)
C(19)	-4165(2)	-7816(2)	-4723(1)	37(1)
C(20)	-4003(2)	-7655(2)	-4034(1)	35(1)
C(21)	-3253(2)	-6807(1)	-3619(1)	29(1)
C(22)	-2364(2)	-5492(2)	-4952(1)	33(1)
C(23)	-3146(2)	-6634(2)	-2873(1)	40(1)
C(24)	-272(2)	-3697(1)	-1385(1)	24(1)
C(25)	606(2)	-4026(1)	-968(1)	28(1)
C(26)	53(2)	-5070(2)	-965(1)	35(1)
C(27)	999(2)	-3443(2)	-231(1)	35(1)
C(28)	1645(2)	-4002(2)	-1285(1)	38(1)
C(29)	-1823(2)	-4099(1)	-800(1)	27(1)
C(30)	-2562(2)	-4957(2)	-736(1)	32(1)
C(31)	-3020(2)	-4962(2)	-156(1)	41(1)
C(32)	-2773(2)	-4152(2)	357(1)	49(1)
C(33)	-2081(2)	-3315(2)	286(1)	46(1)
C(34)	-1607(2)	-3270(2)	-285(1)	35(1)
C(35)	-2882(2)	-5852(2)	-1280(1)	44(1)
C(36)	-914(2)	-2315(2)	-344(1)	42(1)
C(37)	-2870(2)	-2016(1)	-1598(1)	29(1)

C(38)	-1803(2)	-1335(1)	-1586(1)	27(1)
C(39)	-1148(2)	-1429(1)	-2100(1)	25(1)
C(40)	-46(2)	-854(1)	-1973(1)	29(1)
C(41)	413(2)	-126(2)	-1382(1)	36(1)
C(42)	-224(2)	43(2)	-920(1)	38(1)
C(43)	-1343(2)	-551(2)	-1004(1)	34(1)
C(44)	-1977(2)	-400(2)	-494(1)	41(1)
C(45)	-2991(2)	-1035(2)	-536(1)	44(1)
C(46)	-3420(2)	-1857(2)	-1070(1)	38(1)
C(47)	-4189(2)	-3471(1)	-2389(1)	25(1)
C(48)	-5210(2)	-3116(2)	-2576(1)	29(1)
C(49)	-5792(2)	-3601(2)	-3310(1)	33(1)
C(50)	-4816(2)	-2040(2)	-2529(1)	34(1)
C(51)	-6095(2)	-3318(2)	-2135(1)	34(1)
C(52)	-5118(2)	-5172(1)	-2802(1)	27(1)
C(53)	-5638(2)	-5463(2)	-2282(1)	33(1)
C(54)	-6570(2)	-6274(2)	-2441(1)	45(1)
C(55)	-6970(2)	-6820(2)	-3094(2)	49(1)
C(56)	-6424(2)	-6564(2)	-3596(1)	41(1)
C(57)	-5504(2)	-5745(2)	-3464(1)	32(1)
C(58)	-5188(2)	-4943(2)	-1554(1)	42(1)
C(59)	-4967(2)	-5485(2)	-4038(1)	35(1)
C(60)	-1740(2)	-1652(1)	-3249(1)	25(1)
C(61)	-2267(2)	-2317(1)	-3957(1)	27(1)
C(62)	-1442(2)	-2273(2)	-4444(1)	34(1)
C(63)	-3284(2)	-2064(2)	-4261(1)	35(1)
C(64)	-2691(2)	-3352(1)	-3921(1)	33(1)
C(65)	-1336(2)	-142(1)	-3597(1)	32(1)
C(66)	-2116(2)	333(2)	-3755(1)	41(1)
C(67)	-1851(3)	979(2)	-4157(1)	56(1)
C(68)	-875(3)	1166(2)	-4396(2)	61(1)
C(69)	-96(3)	724(2)	-4224(1)	53(1)
C(70)	-307(2)	80(2)	-3818(1)	40(1)
C(71)	-3208(2)	160(2)	-3513(1)	48(1)
C(72)	613(2)	-321(2)	-3609(1)	48(1)
C(73)	806(3)	1873(2)	-2308(2)	67(1)
C(74)	-753(3)	2192(2)	-1928(2)	81(1)
C(75)	-1652(3)	1843(2)	-1570(2)	70(1)
C(76)	-3255(2)	532(2)	-1683(2)	64(1)
O(1S)	-5245(3)	1672(3)	-1399(2)	178(2)
C(1S)	-6127(4)	1667(5)	-1888(2)	211(3)
C(2S)	-5893(5)	1269(4)	-2578(2)	145(2)
C(3S)	-5253(4)	2070(4)	-708(2)	166(2)
C(4S)	-4543(5)	1678(5)	-256(3)	246(4)

Table S3. Bond lengths [Å] and angles [deg] for [1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]Nd[μ-1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂][Li(DME)] (1)

Nd(1)-N(5)	2.4596(18)
Nd(1)-N(1)	2.4733(18)
Nd(1)-N(2)	2.4974(16)
Nd(1)-N(4)	2.5563(17)
Nd(1)-N(6)	2.5823(16)
Nd(1)-N(3)	2.6260(16)
Nd(1)-N(7)	2.6320(16)
Nd(1)-C(24)	2.9869(19)
Nd(1)-C(47)	2.995(2)
Nd(1)-C(11)	2.9985(19)
Li(1)-O(1)	1.996(4)
Li(1)-O(2)	1.997(5)
Li(1)-N(8)	2.002(4)
Li(1)-C(40)	2.510(5)
Li(1)-C(39)	2.555(4)
Li(1)-C(41)	2.712(5)
Li(1)-C(65)	2.747(5)
O(1)-C(74)	1.406(4)
O(1)-C(73)	1.410(4)
O(2)-C(75)	1.393(3)
O(2)-C(76)	1.427(4)
N(1)-C(11)	1.327(2)
N(1)-C(1)	1.388(2)
N(2)-C(24)	1.320(3)
N(2)-C(3)	1.398(3)
N(3)-C(11)	1.342(2)
N(3)-C(16)	1.419(2)
N(4)-C(24)	1.356(2)
N(4)-C(29)	1.418(3)
N(5)-C(47)	1.332(2)
N(5)-C(37)	1.382(2)
N(6)-C(60)	1.348(3)
N(6)-C(39)	1.433(2)
N(7)-C(47)	1.344(3)
N(7)-C(52)	1.408(2)
N(8)-C(60)	1.335(3)
N(8)-C(65)	1.422(3)
C(1)-C(10)	1.384(3)
C(1)-C(2)	1.447(3)
C(2)-C(3)	1.432(3)
C(2)-C(7)	1.436(3)
C(3)-C(4)	1.383(3)
C(4)-C(5)	1.397(3)
C(5)-C(6)	1.361(4)

C(6)-C(7)	1.423(3)
C(7)-C(8)	1.418(3)
C(8)-C(9)	1.367(3)
C(9)-C(10)	1.395(3)
C(11)-C(12)	1.573(3)
C(12)-C(13)	1.532(3)
C(12)-C(14)	1.537(3)
C(12)-C(15)	1.541(3)
C(16)-C(21)	1.405(3)
C(16)-C(17)	1.408(3)
C(17)-C(18)	1.394(3)
C(17)-C(22)	1.505(3)
C(18)-C(19)	1.380(3)
C(19)-C(20)	1.377(3)
C(20)-C(21)	1.398(3)
C(21)-C(23)	1.495(3)
C(24)-C(25)	1.569(3)
C(25)-C(28)	1.534(3)
C(25)-C(26)	1.538(3)
C(25)-C(27)	1.543(3)
C(29)-C(34)	1.405(3)
C(29)-C(30)	1.413(3)
C(30)-C(31)	1.398(3)
C(30)-C(35)	1.491(3)
C(31)-C(32)	1.378(3)
C(32)-C(33)	1.369(4)
C(33)-C(34)	1.396(3)
C(34)-C(36)	1.503(3)
C(37)-C(46)	1.384(3)
C(37)-C(38)	1.447(3)
C(38)-C(39)	1.435(3)
C(38)-C(43)	1.436(3)
C(39)-C(40)	1.383(3)
C(40)-C(41)	1.403(3)
C(41)-C(42)	1.354(4)
C(42)-C(43)	1.418(3)
C(43)-C(44)	1.421(3)
C(44)-C(45)	1.352(3)
C(45)-C(46)	1.406(3)
C(47)-C(48)	1.565(3)
C(48)-C(51)	1.535(3)
C(48)-C(49)	1.537(3)
C(48)-C(50)	1.539(3)
C(52)-C(57)	1.409(3)
C(52)-C(53)	1.411(3)
C(53)-C(54)	1.392(3)
C(53)-C(58)	1.509(3)
C(54)-C(55)	1.382(4)
C(55)-C(56)	1.380(4)
C(56)-C(57)	1.394(3)
C(57)-C(59)	1.507(3)
C(60)-C(61)	1.546(3)

C(61)-C(64)	1.525(3)
C(61)-C(62)	1.536(3)
C(61)-C(63)	1.537(3)
C(65)-C(70)	1.409(4)
C(65)-C(66)	1.412(3)
C(66)-C(67)	1.404(4)
C(66)-C(71)	1.501(4)
C(67)-C(68)	1.365(5)
C(68)-C(69)	1.383(5)
C(69)-C(70)	1.400(4)
C(70)-C(72)	1.509(4)
C(74)-C(75)	1.469(5)
O(1S)-C(1S)	1.407(4)
O(1S)-C(3S)	1.438(4)
C(1S)-C(2S)	1.532(4)
C(3S)-C(4S)	1.530(5)
N(5)-Nd(1)-N(1)	153.43(6)
N(5)-Nd(1)-N(2)	111.40(5)
N(1)-Nd(1)-N(2)	65.07(6)
N(5)-Nd(1)-N(4)	89.33(6)
N(1)-Nd(1)-N(4)	105.57(6)
N(2)-Nd(1)-N(4)	52.16(5)
N(5)-Nd(1)-N(6)	65.99(6)
N(1)-Nd(1)-N(6)	87.44(6)
N(2)-Nd(1)-N(6)	88.03(5)
N(4)-Nd(1)-N(6)	122.17(5)
N(5)-Nd(1)-N(3)	144.26(5)
N(1)-Nd(1)-N(3)	51.21(5)
N(2)-Nd(1)-N(3)	103.92(5)
N(4)-Nd(1)-N(3)	108.79(5)
N(6)-Nd(1)-N(3)	121.78(5)
N(5)-Nd(1)-N(7)	51.54(5)
N(1)-Nd(1)-N(7)	142.66(5)
N(2)-Nd(1)-N(7)	149.29(6)
N(4)-Nd(1)-N(7)	98.79(5)
N(6)-Nd(1)-N(7)	103.13(5)
N(3)-Nd(1)-N(7)	94.40(5)
N(5)-Nd(1)-C(24)	105.50(6)
N(1)-Nd(1)-C(24)	82.03(6)
N(2)-Nd(1)-C(24)	25.93(5)
N(4)-Nd(1)-C(24)	26.91(5)
N(6)-Nd(1)-C(24)	108.99(5)
N(3)-Nd(1)-C(24)	103.85(5)
N(7)-Nd(1)-C(24)	125.69(5)
N(5)-Nd(1)-C(47)	25.96(5)
N(1)-Nd(1)-C(47)	154.60(6)
N(2)-Nd(1)-C(47)	135.84(5)
N(4)-Nd(1)-C(47)	99.78(5)
N(6)-Nd(1)-C(47)	80.33(5)
N(3)-Nd(1)-C(47)	118.46(5)
N(7)-Nd(1)-C(47)	26.64(5)
C(24)-Nd(1)-C(47)	122.97(5)

N(5)-Nd(1)-C(11)	166.62(5)
N(1)-Nd(1)-C(11)	25.85(5)
N(2)-Nd(1)-C(11)	80.31(5)
N(4)-Nd(1)-C(11)	103.34(5)
N(6)-Nd(1)-C(11)	109.40(5)
N(3)-Nd(1)-C(11)	26.56(5)
N(7)-Nd(1)-C(11)	120.91(5)
C(24)-Nd(1)-C(11)	87.86(5)
C(47)-Nd(1)-C(11)	143.69(5)
O(1)-Li(1)-O(2)	81.83(16)
O(1)-Li(1)-N(8)	124.1(2)
O(2)-Li(1)-N(8)	124.0(2)
O(1)-Li(1)-C(40)	108.77(18)
O(2)-Li(1)-C(40)	143.9(2)
N(8)-Li(1)-C(40)	79.39(15)
O(1)-Li(1)-C(39)	139.8(2)
O(2)-Li(1)-C(39)	125.1(2)
N(8)-Li(1)-C(39)	68.84(13)
C(40)-Li(1)-C(39)	31.67(8)
O(1)-Li(1)-C(41)	86.29(15)
O(2)-Li(1)-C(41)	121.89(19)
N(8)-Li(1)-C(41)	109.59(18)
C(40)-Li(1)-C(41)	30.86(8)
C(39)-Li(1)-C(41)	54.89(10)
O(1)-Li(1)-C(65)	96.72(17)
O(2)-Li(1)-C(65)	113.42(19)
N(8)-Li(1)-C(65)	29.94(9)
C(40)-Li(1)-C(65)	99.78(15)
C(39)-Li(1)-C(65)	97.64(13)
C(41)-Li(1)-C(65)	124.41(17)
C(74)-O(1)-C(73)	112.7(2)
C(74)-O(1)-Li(1)	109.6(2)
C(73)-O(1)-Li(1)	126.1(2)
C(75)-O(2)-C(76)	113.4(2)
C(75)-O(2)-Li(1)	111.3(2)
C(76)-O(2)-Li(1)	130.4(2)
C(11)-N(1)-C(1)	130.21(18)
C(11)-N(1)-Nd(1)	99.77(12)
C(1)-N(1)-Nd(1)	129.87(13)
C(24)-N(2)-C(3)	130.88(17)
C(24)-N(2)-Nd(1)	98.22(11)
C(3)-N(2)-Nd(1)	130.85(13)
C(11)-N(3)-C(16)	124.69(17)
C(11)-N(3)-Nd(1)	92.40(11)
C(16)-N(3)-Nd(1)	142.85(13)
C(24)-N(4)-C(29)	122.44(16)
C(24)-N(4)-Nd(1)	94.53(12)
C(29)-N(4)-Nd(1)	138.33(13)
C(47)-N(5)-C(37)	131.52(18)
C(47)-N(5)-Nd(1)	100.07(12)
C(37)-N(5)-Nd(1)	128.34(13)
C(60)-N(6)-C(39)	113.82(15)

C(60)-N(6)-Nd(1)	140.08(12)
C(39)-N(6)-Nd(1)	106.07(12)
C(47)-N(7)-C(52)	123.78(17)
C(47)-N(7)-Nd(1)	91.92(11)
C(52)-N(7)-Nd(1)	144.21(13)
C(60)-N(8)-C(65)	126.93(17)
C(60)-N(8)-Li(1)	127.44(19)
C(65)-N(8)-Li(1)	105.42(17)
C(10)-C(1)-N(1)	119.75(17)
C(10)-C(1)-C(2)	119.24(18)
N(1)-C(1)-C(2)	120.45(19)
C(3)-C(2)-C(7)	118.33(17)
C(3)-C(2)-C(1)	124.00(17)
C(7)-C(2)-C(1)	117.67(19)
C(4)-C(3)-N(2)	119.8(2)
C(4)-C(3)-C(2)	118.97(18)
N(2)-C(3)-C(2)	120.40(16)
C(3)-C(4)-C(5)	122.2(2)
C(6)-C(5)-C(4)	120.4(2)
C(5)-C(6)-C(7)	120.3(2)
C(8)-C(7)-C(6)	119.99(19)
C(8)-C(7)-C(2)	120.22(18)
C(6)-C(7)-C(2)	119.8(2)
C(9)-C(8)-C(7)	120.39(19)
C(8)-C(9)-C(10)	120.4(2)
C(1)-C(10)-C(9)	122.07(19)
N(1)-C(11)-N(3)	111.69(17)
N(1)-C(11)-C(12)	123.93(16)
N(3)-C(11)-C(12)	123.44(16)
N(1)-C(11)-Nd(1)	54.38(10)
N(3)-C(11)-Nd(1)	61.05(10)
C(12)-C(11)-Nd(1)	152.97(13)
C(13)-C(12)-C(14)	108.71(17)
C(13)-C(12)-C(15)	106.53(17)
C(14)-C(12)-C(15)	106.92(17)
C(13)-C(12)-C(11)	107.58(17)
C(14)-C(12)-C(11)	114.00(17)
C(15)-C(12)-C(11)	112.80(15)
C(21)-C(16)-C(17)	118.61(17)
C(21)-C(16)-N(3)	119.56(18)
C(17)-C(16)-N(3)	121.18(18)
C(18)-C(17)-C(16)	119.3(2)
C(18)-C(17)-C(22)	118.03(19)
C(16)-C(17)-C(22)	122.57(17)
C(19)-C(18)-C(17)	121.9(2)
C(20)-C(19)-C(18)	118.85(19)
C(19)-C(20)-C(21)	121.1(2)
C(20)-C(21)-C(16)	120.1(2)
C(20)-C(21)-C(23)	119.6(2)
C(16)-C(21)-C(23)	120.27(17)
N(2)-C(24)-N(4)	112.30(17)
N(2)-C(24)-C(25)	125.06(18)

N(4)-C(24)-C(25)	121.76(17)
N(2)-C(24)-Nd(1)	55.84(10)
N(4)-C(24)-Nd(1)	58.56(10)
C(25)-C(24)-Nd(1)	157.83(12)
C(28)-C(25)-C(26)	106.46(18)
C(28)-C(25)-C(27)	108.30(16)
C(26)-C(25)-C(27)	107.58(17)
C(28)-C(25)-C(24)	112.52(17)
C(26)-C(25)-C(24)	108.04(15)
C(27)-C(25)-C(24)	113.58(17)
C(34)-C(29)-C(30)	118.5(2)
C(34)-C(29)-N(4)	119.52(18)
C(30)-C(29)-N(4)	121.70(17)
C(31)-C(30)-C(29)	119.20(19)
C(31)-C(30)-C(35)	119.2(2)
C(29)-C(30)-C(35)	121.6(2)
C(32)-C(31)-C(30)	121.8(2)
C(33)-C(32)-C(31)	119.0(2)
C(32)-C(33)-C(34)	121.5(2)
C(33)-C(34)-C(29)	120.0(2)
C(33)-C(34)-C(36)	118.4(2)
C(29)-C(34)-C(36)	121.6(2)
N(5)-C(37)-C(46)	121.58(19)
N(5)-C(37)-C(38)	118.19(18)
C(46)-C(37)-C(38)	118.84(18)
C(39)-C(38)-C(43)	118.22(18)
C(39)-C(38)-C(37)	123.98(17)
C(43)-C(38)-C(37)	117.68(19)
C(40)-C(39)-N(6)	118.95(19)
C(40)-C(39)-C(38)	118.92(17)
N(6)-C(39)-C(38)	122.11(16)
C(40)-C(39)-Li(1)	72.35(15)
N(6)-C(39)-Li(1)	107.26(15)
C(38)-C(39)-Li(1)	88.40(15)
C(39)-C(40)-C(41)	121.6(2)
C(39)-C(40)-Li(1)	75.98(15)
C(41)-C(40)-Li(1)	82.57(16)
C(42)-C(41)-C(40)	120.5(2)
C(42)-C(41)-Li(1)	84.29(17)
C(40)-C(41)-Li(1)	66.57(14)
C(41)-C(42)-C(43)	120.68(19)
C(42)-C(43)-C(44)	119.98(19)
C(42)-C(43)-C(38)	119.4(2)
C(44)-C(43)-C(38)	120.5(2)
C(45)-C(44)-C(43)	119.8(2)
C(44)-C(45)-C(46)	120.9(2)
C(37)-C(46)-C(45)	121.8(2)
N(5)-C(47)-N(7)	112.09(18)
N(5)-C(47)-C(48)	123.23(17)
N(7)-C(47)-C(48)	123.80(16)
N(5)-C(47)-Nd(1)	53.96(10)
N(7)-C(47)-Nd(1)	61.44(10)

C(48)-C(47)-Nd(1)	154.06(14)
C(51)-C(48)-C(49)	107.66(16)
C(51)-C(48)-C(50)	108.71(18)
C(49)-C(48)-C(50)	106.11(18)
C(51)-C(48)-C(47)	113.39(18)
C(49)-C(48)-C(47)	110.01(17)
C(50)-C(48)-C(47)	110.65(16)
N(7)-C(52)-C(57)	121.60(19)
N(7)-C(52)-C(53)	118.93(18)
C(57)-C(52)-C(53)	119.24(18)
C(54)-C(53)-C(52)	119.3(2)
C(54)-C(53)-C(58)	118.7(2)
C(52)-C(53)-C(58)	121.97(18)
C(55)-C(54)-C(53)	121.4(2)
C(56)-C(55)-C(54)	119.3(2)
C(55)-C(56)-C(57)	121.3(2)
C(56)-C(57)-C(52)	119.3(2)
C(56)-C(57)-C(59)	118.9(2)
C(52)-C(57)-C(59)	121.77(18)
N(8)-C(60)-N(6)	120.79(17)
N(8)-C(60)-C(61)	122.59(18)
N(6)-C(60)-C(61)	116.43(16)
C(64)-C(61)-C(62)	106.71(18)
C(64)-C(61)-C(63)	106.97(17)
C(62)-C(61)-C(63)	108.83(18)
C(64)-C(61)-C(60)	110.79(17)
C(62)-C(61)-C(60)	113.32(16)
C(63)-C(61)-C(60)	109.97(17)
C(70)-C(65)-C(66)	119.3(2)
C(70)-C(65)-N(8)	119.7(2)
C(66)-C(65)-N(8)	120.1(2)
C(70)-C(65)-Li(1)	114.94(17)
C(66)-C(65)-Li(1)	100.02(17)
N(8)-C(65)-Li(1)	44.63(12)
C(67)-C(66)-C(65)	118.2(2)
C(67)-C(66)-C(71)	119.8(2)
C(65)-C(66)-C(71)	122.1(2)
C(68)-C(67)-C(66)	122.6(3)
C(67)-C(68)-C(69)	119.2(3)
C(68)-C(69)-C(70)	120.8(3)
C(69)-C(70)-C(65)	119.8(3)
C(69)-C(70)-C(72)	117.9(3)
C(65)-C(70)-C(72)	122.3(2)
O(1)-C(74)-C(75)	109.2(3)
O(2)-C(75)-C(74)	108.3(3)
C(1S)-O(1S)-C(3S)	117.5(4)
O(1S)-C(1S)-C(2S)	107.5(4)
O(1S)-C(3S)-C(4S)	109.2(4)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for [1,8- $\text{C}_{10}\text{H}_6\{\text{NC}(t\text{Bu})\text{N-2,6-Me}_2\text{-C}_6\text{H}_3\}_2\text{]Nd}[\mu\text{-1,8-}\text{C}_{10}\text{H}_6\{\text{NC}(t\text{Bu})\text{N-2,6-Me}_2\text{-C}_6\text{H}_3\}_2\text{][Li(DME)] (1)$

The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U11 + \dots + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Nd(1)	20(1)	24(1)	21(1)	6(1)	4(1)	9(1)
Li(1)	46(2)	26(2)	38(2)	2(2)	6(2)	14(1)
O(1)	59(1)	32(1)	54(1)	11(1)	14(1)	7(1)
O(2)	54(1)	36(1)	50(1)	9(1)	14(1)	20(1)
N(1)	24(1)	29(1)	36(1)	2(1)	10(1)	10(1)
N(2)	24(1)	33(1)	30(1)	15(1)	3(1)	8(1)
N(3)	23(1)	26(1)	27(1)	7(1)	6(1)	9(1)
N(4)	25(1)	29(1)	24(1)	9(1)	5(1)	10(1)
N(5)	24(1)	27(1)	31(1)	2(1)	5(1)	10(1)
N(6)	28(1)	22(1)	23(1)	7(1)	2(1)	10(1)
N(7)	20(1)	30(1)	28(1)	5(1)	4(1)	8(1)
N(8)	33(1)	26(1)	30(1)	10(1)	5(1)	13(1)
C(1)	22(1)	26(1)	36(1)	8(1)	6(1)	13(1)
C(2)	21(1)	25(1)	36(1)	13(1)	5(1)	11(1)
C(3)	23(1)	29(1)	32(1)	13(1)	2(1)	10(1)
C(4)	33(1)	34(1)	34(1)	9(1)	1(1)	10(1)
C(5)	30(1)	33(1)	43(1)	2(1)	-5(1)	4(1)
C(6)	26(1)	28(1)	54(1)	12(1)	6(1)	6(1)
C(7)	24(1)	28(1)	42(1)	14(1)	8(1)	11(1)
C(8)	29(1)	34(1)	52(1)	21(1)	16(1)	15(1)
C(9)	36(1)	44(1)	42(1)	23(1)	19(1)	23(1)
C(10)	30(1)	37(1)	33(1)	8(1)	7(1)	16(1)
C(11)	25(1)	27(1)	18(1)	7(1)	6(1)	10(1)
C(12)	27(1)	28(1)	26(1)	8(1)	6(1)	12(1)
C(13)	35(1)	38(1)	45(1)	19(1)	11(1)	18(1)
C(14)	36(1)	39(1)	30(1)	4(1)	8(1)	20(1)
C(15)	26(1)	33(1)	39(1)	8(1)	4(1)	13(1)
C(16)	22(1)	28(1)	26(1)	5(1)	3(1)	10(1)
C(17)	25(1)	34(1)	26(1)	5(1)	4(1)	15(1)
C(18)	33(1)	39(1)	25(1)	1(1)	1(1)	17(1)
C(19)	32(1)	32(1)	39(1)	-2(1)	-3(1)	10(1)
C(20)	31(1)	31(1)	42(1)	11(1)	4(1)	7(1)
C(21)	28(1)	31(1)	29(1)	7(1)	3(1)	10(1)
C(22)	34(1)	40(1)	28(1)	10(1)	7(1)	15(1)
C(23)	41(1)	44(1)	34(1)	16(1)	8(1)	8(1)
C(24)	28(1)	23(1)	20(1)	4(1)	2(1)	9(1)
C(25)	29(1)	33(1)	24(1)	10(1)	5(1)	14(1)
C(26)	42(1)	35(1)	36(1)	14(1)	6(1)	21(1)
C(27)	38(1)	43(1)	26(1)	12(1)	0(1)	16(1)
C(28)	35(1)	55(1)	39(1)	24(1)	13(1)	28(1)

C(29)	30(1)	34(1)	23(1)	10(1)	6(1)	16(1)
C(30)	33(1)	40(1)	27(1)	12(1)	8(1)	13(1)
C(31)	40(1)	55(1)	35(1)	20(1)	13(1)	16(1)
C(32)	55(1)	71(2)	30(1)	16(1)	21(1)	29(1)
C(33)	57(1)	55(1)	29(1)	0(1)	11(1)	27(1)
C(34)	38(1)	36(1)	31(1)	5(1)	4(1)	17(1)
C(35)	48(1)	40(1)	37(1)	6(1)	15(1)	4(1)
C(36)	52(1)	32(1)	40(1)	2(1)	4(1)	18(1)
C(37)	30(1)	31(1)	27(1)	6(1)	4(1)	15(1)
C(38)	32(1)	26(1)	26(1)	5(1)	2(1)	14(1)
C(39)	28(1)	23(1)	26(1)	6(1)	0(1)	12(1)
C(40)	29(1)	25(1)	35(1)	10(1)	1(1)	11(1)
C(41)	33(1)	27(1)	43(1)	10(1)	-4(1)	5(1)
C(42)	46(1)	26(1)	34(1)	1(1)	-9(1)	9(1)
C(43)	43(1)	28(1)	29(1)	4(1)	1(1)	16(1)
C(44)	53(1)	37(1)	30(1)	-2(1)	2(1)	20(1)
C(45)	51(1)	52(1)	34(1)	3(1)	15(1)	26(1)
C(46)	34(1)	42(1)	36(1)	4(1)	8(1)	15(1)
C(47)	23(1)	31(1)	24(1)	10(1)	9(1)	10(1)
C(48)	24(1)	34(1)	34(1)	11(1)	7(1)	12(1)
C(49)	26(1)	41(1)	34(1)	11(1)	2(1)	14(1)
C(50)	31(1)	32(1)	44(1)	13(1)	6(1)	14(1)
C(51)	26(1)	42(1)	42(1)	13(1)	11(1)	16(1)
C(52)	21(1)	28(1)	36(1)	10(1)	5(1)	10(1)
C(53)	30(1)	35(1)	37(1)	13(1)	8(1)	12(1)
C(54)	38(1)	46(1)	52(1)	18(1)	15(1)	6(1)
C(55)	31(1)	39(1)	66(2)	11(1)	8(1)	-2(1)
C(56)	32(1)	36(1)	47(1)	4(1)	-1(1)	6(1)
C(57)	26(1)	30(1)	37(1)	3(1)	2(1)	11(1)
C(58)	43(1)	48(1)	39(1)	18(1)	11(1)	15(1)
C(59)	30(1)	39(1)	32(1)	1(1)	5(1)	11(1)
C(60)	22(1)	28(1)	29(1)	9(1)	6(1)	12(1)
C(61)	29(1)	31(1)	24(1)	7(1)	4(1)	13(1)
C(62)	36(1)	41(1)	28(1)	7(1)	11(1)	17(1)
C(63)	32(1)	39(1)	35(1)	9(1)	0(1)	15(1)
C(64)	41(1)	28(1)	24(1)	2(1)	0(1)	9(1)
C(65)	45(1)	25(1)	28(1)	9(1)	4(1)	14(1)
C(66)	59(1)	33(1)	35(1)	8(1)	4(1)	24(1)
C(67)	90(2)	45(1)	46(1)	20(1)	10(1)	38(1)
C(68)	104(2)	41(1)	50(1)	25(1)	22(1)	28(1)
C(69)	74(2)	38(1)	47(1)	16(1)	19(1)	13(1)
C(70)	52(1)	30(1)	38(1)	12(1)	10(1)	10(1)
C(71)	60(1)	54(1)	44(1)	11(1)	6(1)	39(1)
C(72)	37(1)	54(1)	58(2)	20(1)	16(1)	14(1)
C(73)	63(2)	51(2)	75(2)	17(2)	18(2)	-3(1)
C(74)	84(2)	29(1)	136(3)	26(2)	29(2)	20(1)
C(75)	84(2)	35(1)	90(2)	-2(1)	27(2)	26(1)
C(76)	58(2)	62(2)	81(2)	20(2)	27(1)	28(1)
O(1S)	128(3)	133(2)	303(5)	108(3)	53(3)	44(2)
C(1S)	211(6)	183(5)	257(6)	98(5)	12(5)	74(4)
C(2S)	133(4)	132(3)	186(4)	90(3)	21(3)	37(3)
C(3S)	177(4)	145(4)	195(4)	44(3)	137(3)	36(3)

C(4S) 214(4) 319(7) 237(5) 50(5) 166(4) 93(5)

Table S5. Crystal data and structure refinement for [1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]NdN(SiMe₃)₂(THF) (4).

Empirical formula	C ₄₆ H ₆₈ N ₅ Nd O Si ₂
Formula weight	907.47
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 23.9499(16) Å alpha = 90 deg. b = 19.4258(13) Å beta = 116.8780(10) deg. c = 21.8709(14) Å gamma = 90 deg.
Volume	9076.1(10) Å ³
Z, Calculated density	8, 1.328 Mg/m ³
Absorption coefficient	1.236 mm ⁻¹
F(000)	3800
Crystal size	0.35 x 0.26 x 0.23 mm
Theta range for data collection	0.95 to 25.00 deg.
Limiting indices	-28<=h<=28, -23<=k<=23, -26<=l<=26
Reflections collected / unique	69897 / 15735 [R(int) = 0.0415]
Completeness to theta = 25.00	98.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7642 and 0.6716
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15735 / 171 / 1007
Goodness-of-fit on F ²	1.154
Final R indices [I>2sigma(I)]	R1 = 0.0770, wR2 = 0.1598
R indices (all data)	R1 = 0.0858, wR2 = 0.1628
Largest diff. peak and hole	2.409 and -2.191 e.Å ⁻³

Table S6. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for [1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]NdN(SiMe₃)₂(THF) (4).

U(eq) is defined as one third of the trace of the orthogonalized

Uij tensor.

x	y	z	U(eq)
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Nd(1A)	5927(1)	2489(1)	9091(1)	19(1)
Nd(1B)	886(1)	2610(1)	6869(1)	20(1)
Si(1A)	5120(1)	3360(1)	7507(1)	44(1)
Si(2A)	4764(1)	1899(1)	7573(1)	37(1)
Si(1B)	-54(1)	3722(1)	7314(1)	38(1)
Si(2B)	-120(1)	2218(1)	7558(1)	41(1)
N(1A)	6661(2)	1741(2)	8948(2)	22(1)
N(2A)	6891(2)	3081(2)	9338(2)	28(1)
N(3A)	6405(2)	1396(2)	9743(2)	22(1)
N(4A)	6324(2)	3614(2)	9766(2)	24(1)
N(5A)	5169(2)	2625(3)	7960(2)	30(1)
N(1B)	1585(2)	1815(3)	7711(2)	30(1)
N(2B)	1817(2)	3184(2)	7743(2)	28(1)
N(3B)	1331(2)	1472(2)	6648(2)	24(1)
N(4B)	1359(2)	3706(2)	6746(2)	22(1)
N(5B)	113(2)	2877(3)	7217(2)	33(1)
O(1A)	5125(2)	2374(2)	9521(2)	27(1)
O(1B)	22(2)	2348(2)	5680(2)	31(1)
C(1A)	6982(2)	1866(3)	8556(3)	28(1)
C(2A)	6950(3)	1386(3)	8079(3)	32(2)
C(3A)	7269(3)	1482(4)	7684(3)	39(2)
C(4A)	7588(3)	2073(4)	7734(3)	38(2)
C(5A)	7571(2)	2621(3)	8146(3)	31(2)
C(6A)	7853(3)	3265(4)	8142(3)	39(2)
C(7A)	7797(3)	3804(4)	8502(3)	40(2)
C(8A)	7485(3)	3740(3)	8893(3)	35(2)
C(9A)	7231(2)	3120(3)	8957(3)	29(1)
C(10A)	7265(2)	2525(3)	8577(3)	26(1)
C(11A)	6819(2)	1332(3)	9497(2)	21(1)
C(12A)	7433(3)	908(3)	9823(3)	30(1)
C(13A)	7545(3)	545(4)	10482(3)	36(2)
C(14A)	7464(3)	357(4)	9331(3)	49(2)
C(15A)	7979(3)	1426(4)	10007(4)	54(2)
C(16A)	6369(3)	991(3)	10293(3)	24(1)
C(17A)	6021(3)	387(3)	10129(3)	29(2)
C(18A)	5866(4)	81(4)	10607(4)	38(2)
C(19A)	6061(4)	379(5)	11249(4)	42(2)
C(20A)	6409(4)	983(4)	11413(3)	38(2)
C(21A)	6564(3)	1289(3)	10935(3)	24(2)
C(22A)	5851(6)	5(8)	9484(7)	45(1)
C(23A)	7010(6)	1912(7)	11144(7)	38(1)
C(16')	6289(3)	934(3)	10165(3)	24(1)
C(17')	5966(3)	332(3)	9866(3)	29(2)
C(18')	5760(4)	-97(3)	10231(5)	38(2)
C(19')	5877(4)	75(4)	10895(5)	42(2)
C(20')	6199(4)	677(5)	11194(3)	38(2)
C(21')	6405(3)	1106(3)	10829(3)	24(2)
C(22')	5877(6)	73(8)	9160(7)	45(1)
C(23')	6833(6)	1747(7)	11173(7)	38(1)
C(24A)	6886(2)	3538(3)	9805(3)	25(1)
C(25A)	7504(3)	3824(3)	10421(3)	32(2)
C(26A)	7571(3)	4612(3)	10427(4)	43(2)

C(27A)	8097(3)	3502(3)	10449(3)	32(2)
C(28A)	7485(3)	3630(4)	11089(3)	41(2)
C(29A)	6115(1)	4125(2)	10101(2)	29(2)
C(30A)	6042(2)	4797(2)	9857(2)	37(2)
C(31A)	5849(2)	5310(2)	10163(2)	48(2)
C(32A)	5730(2)	5151(2)	10713(3)	50(2)
C(33A)	5803(2)	4479(2)	10956(2)	45(2)
C(34A)	5996(2)	3966(2)	10650(2)	33(2)
C(35A)	6081(3)	4983(3)	9214(4)	44(2)
C(36A)	6023(3)	3244(3)	10908(3)	38(2)
C(37A)	5043(4)	3135(7)	6647(2)	47(1)
C(38A)	4460(2)	3924(4)	7396(6)	49(1)
C(39A)	5880(2)	3820(5)	7872(7)	47(1)
C(37')	4813(6)	3276(8)	6565(2)	47(1)
C(38')	4633(3)	4018(4)	7649(5)	49(1)
C(39')	5880(2)	3799(5)	7766(8)	47(1)
C(40A)	3916(3)	2022(5)	7002(5)	69(3)
C(41A)	5099(3)	1409(4)	7082(4)	49(1)
C(42A)	4756(3)	1299(4)	8239(4)	50(1)
C(43A)	4677(3)	2944(3)	9349(3)	35(2)
C(44A)	4261(3)	2749(4)	9688(3)	42(2)
C(45A)	4296(3)	1972(4)	9722(3)	39(2)
C(46A)	4960(3)	1829(3)	9883(3)	29(2)
C(1B)	2186(2)	3099(3)	8450(3)	23(1)
C(2B)	2495(2)	3660(3)	8850(3)	29(1)
C(3B)	2819(3)	3616(3)	9573(3)	32(2)
C(4B)	2818(3)	3025(3)	9891(3)	27(1)
C(5B)	2491(3)	2432(3)	9519(3)	29(2)
C(6B)	2431(3)	1851(3)	9860(3)	36(2)
C(7B)	2059(3)	1316(3)	9514(3)	44(2)
C(8B)	1765(3)	1314(3)	8795(3)	36(2)
C(9B)	1860(3)	1858(3)	8425(3)	32(2)
C(10B)	2181(2)	2453(3)	8777(3)	25(1)
C(11B)	1733(3)	1400(3)	7322(3)	27(1)
C(12B)	2311(3)	906(3)	7605(3)	31(2)
C(13B)	2583(3)	785(4)	7107(3)	42(2)
C(14B)	2140(3)	198(3)	7795(3)	37(2)
C(15B)	2853(3)	1212(4)	8248(4)	47(2)
C(16B)	1276(1)	1060(2)	6094(1)	27(1)
C(17B)	947(2)	443(2)	5952(2)	34(2)
C(18B)	863(2)	60(2)	5380(2)	43(2)
C(19B)	1107(2)	294(2)	4949(2)	49(2)
C(20B)	1435(2)	911(2)	5091(2)	42(2)
C(21B)	1520(2)	1294(2)	5663(2)	33(2)
C(22B)	610(3)	222(4)	6356(4)	54(2)
C(23B)	1874(3)	1956(4)	5795(3)	42(2)
C(24B)	1907(2)	3598(3)	7318(3)	22(1)
C(25B)	2551(3)	3785(3)	7343(3)	31(2)
C(26B)	3068(3)	3312(4)	7830(3)	44(2)
C(27B)	2770(3)	4536(4)	7556(4)	42(2)
C(28B)	2516(3)	3685(3)	6617(3)	37(2)
C(29B)	1219(1)	4313(2)	6324(2)	32(2)

C(30B)	1260(2)	4966(2)	6601(2)	39(2)
C(31B)	1076(2)	5539(2)	6174(2)	47(2)
C(32B)	851(2)	5459(2)	5471(2)	53(2)
C(33B)	810(2)	4806(2)	5194(2)	47(2)
C(34B)	994(2)	4233(2)	5620(2)	36(2)
C(35B)	1401(3)	5085(4)	7343(3)	42(2)
C(36B)	911(3)	3526(4)	5295(3)	47(2)
C(37B)	-154(3)	4260(4)	6556(4)	48(2)
C(38B)	579(4)	4096(4)	8125(4)	52(2)
C(39B)	-815(3)	3862(4)	7342(4)	58(2)
C(40B)	-978(3)	2194(5)	7310(4)	63(2)
C(41B)	43(4)	1402(4)	7246(5)	65(3)
C(42B)	294(4)	2197(5)	8517(4)	69(3)
C(43B)	-590(3)	2673(4)	5435(2)	65(3)
C(44B)	-819(5)	2650(3)	4653(2)	58(4)
C(45B)	-677(2)	1886(3)	4601(5)	40(3)
C(44')	-1026(2)	2360(5)	4733(3)	58(4)
C(45')	-536(2)	2214(5)	4477(3)	40(3)
C(46B)	16(2)	1937(4)	5131(3)	59(2)

Table S7. Bond lengths [Å] and angles [deg] for [1,8-C₁₀H₆{NC(*t*Bu)N-2,6-Me₂-C₆H₃}₂]NdN(SiMe₃)₂(THF) (4).

Nd(1A)-N(5A)	2.329(4)
Nd(1A)-N(1A)	2.406(5)
Nd(1A)-N(2A)	2.413(5)
Nd(1A)-O(1A)	2.503(4)
Nd(1A)-N(3A)	2.524(4)
Nd(1A)-N(4A)	2.568(5)
Nd(1A)-C(24A)	2.937(5)
Nd(1A)-C(11A)	2.946(5)
Nd(1A)-Si(2A)	3.4259(16)
Nd(1B)-N(5B)	2.357(6)
Nd(1B)-N(1B)	2.405(5)
Nd(1B)-N(2B)	2.452(4)
Nd(1B)-N(4B)	2.484(5)
Nd(1B)-O(1B)	2.539(3)
Nd(1B)-N(3B)	2.592(5)
Nd(1B)-C(24B)	2.907(5)
Nd(1B)-C(11B)	2.966(6)
Nd(1B)-Si(2B)	3.454(2)
Si(1A)-N(5A)	1.711(5)
Si(1A)-C(38A)	1.848(4)
Si(1A)-C(38')	1.850(5)
Si(1A)-C(39')	1.853(4)
Si(1A)-C(37')	1.854(4)
Si(1A)-C(39A)	1.854(4)
Si(1A)-C(37A)	1.856(4)
Si(2A)-N(5A)	1.706(5)
Si(2A)-C(40A)	1.857(7)
Si(2A)-C(41A)	1.867(8)
Si(2A)-C(42A)	1.873(8)

Si(1B)-N(5B)	1.725(6)
Si(1B)-C(39B)	1.872(8)
Si(1B)-C(38B)	1.881(7)
Si(1B)-C(37B)	1.882(8)
Si(2B)-N(5B)	1.697(6)
Si(2B)-C(41B)	1.835(9)
Si(2B)-C(42B)	1.872(8)
Si(2B)-C(40B)	1.875(7)
N(1A)-C(11A)	1.343(7)
N(1A)-C(1A)	1.408(8)
N(2A)-C(24A)	1.358(8)
N(2A)-C(9A)	1.405(8)
N(3A)-C(11A)	1.331(8)
N(3A)-C(16')	1.403(7)
N(3A)-C(16A)	1.471(7)
N(4A)-C(24A)	1.318(7)
N(4A)-C(29A)	1.450(6)
N(1B)-C(11B)	1.330(8)
N(1B)-C(9B)	1.398(7)
N(2B)-C(24B)	1.319(7)
N(2B)-C(1B)	1.401(6)
N(3B)-C(11B)	1.356(7)
N(3B)-C(16B)	1.407(5)
N(4B)-C(24B)	1.358(6)
N(4B)-C(29B)	1.440(5)
O(1A)-C(43A)	1.467(7)
O(1A)-C(46A)	1.478(7)
O(1B)-C(46B)	1.435(8)
O(1B)-C(43B)	1.456(8)
C(1A)-C(2A)	1.376(8)
C(1A)-C(10A)	1.439(8)
C(2A)-C(3A)	1.399(10)
C(3A)-C(4A)	1.356(10)
C(4A)-C(5A)	1.406(9)
C(5A)-C(6A)	1.424(9)
C(5A)-C(10A)	1.446(9)
C(6A)-C(7A)	1.352(10)
C(7A)-C(8A)	1.374(10)
C(8A)-C(9A)	1.384(9)
C(9A)-C(10A)	1.447(8)
C(11A)-C(12A)	1.550(7)
C(12A)-C(13A)	1.515(8)
C(12A)-C(14A)	1.543(9)
C(12A)-C(15A)	1.551(9)
C(16A)-C(17A)	1.3900
C(16A)-C(21A)	1.3900
C(17A)-C(18A)	1.3900
C(17A)-C(22A)	1.479(16)
C(18A)-C(19A)	1.3900
C(19A)-C(20A)	1.3900
C(20A)-C(21A)	1.3900
C(21A)-C(23A)	1.540(14)

C(16')-C(17')	1.3900
C(16')-C(21')	1.3900
C(17')-C(18')	1.3900
C(17')-C(22')	1.544(16)
C(18')-C(19')	1.3900
C(19')-C(20')	1.3900
C(20')-C(21')	1.3900
C(21')-C(23')	1.572(14)
C(24A)-C(25A)	1.584(7)
C(25A)-C(27A)	1.527(9)
C(25A)-C(28A)	1.529(10)
C(25A)-C(26A)	1.539(9)
C(29A)-C(30A)	1.3900
C(29A)-C(34A)	1.3900
C(30A)-C(31A)	1.3900
C(30A)-C(35A)	1.497(9)
C(31A)-C(32A)	1.3900
C(32A)-C(33A)	1.3900
C(33A)-C(34A)	1.3900
C(34A)-C(36A)	1.502(7)
C(43A)-C(44A)	1.534(10)
C(44A)-C(45A)	1.511(10)
C(45A)-C(46A)	1.492(9)
C(1B)-C(2B)	1.383(8)
C(1B)-C(10B)	1.448(8)
C(2B)-C(3B)	1.416(8)
C(3B)-C(4B)	1.344(9)
C(4B)-C(5B)	1.423(8)
C(5B)-C(6B)	1.395(9)
C(5B)-C(10B)	1.449(7)
C(6B)-C(7B)	1.356(9)
C(7B)-C(8B)	1.403(9)
C(8B)-C(9B)	1.410(9)
C(9B)-C(10B)	1.407(8)
C(11B)-C(12B)	1.563(8)
C(12B)-C(13B)	1.521(10)
C(12B)-C(15B)	1.539(8)
C(12B)-C(14B)	1.544(9)
C(16B)-C(17B)	1.3900
C(16B)-C(21B)	1.3900
C(17B)-C(18B)	1.3900
C(17B)-C(22B)	1.504(9)
C(18B)-C(19B)	1.3900
C(19B)-C(20B)	1.3900
C(20B)-C(21B)	1.3900
C(21B)-C(23B)	1.494(7)
C(24B)-C(25B)	1.562(9)
C(25B)-C(26B)	1.524(8)
C(25B)-C(27B)	1.548(9)
C(25B)-C(28B)	1.562(9)
C(29B)-C(30B)	1.3900
C(29B)-C(34B)	1.3900

C(30B)-C(31B)	1.3900
C(30B)-C(35B)	1.520(8)
C(31B)-C(32B)	1.3900
C(32B)-C(33B)	1.3900
C(33B)-C(34B)	1.3900
C(34B)-C(36B)	1.519(8)
C(43B)-C(44')	1.538(4)
C(43B)-C(44B)	1.541(4)
C(44B)-C(45B)	1.538(5)
C(45B)-C(46B)	1.540(4)
C(44')-C(45')	1.536(5)
C(45')-C(46B)	1.540(4)
N(5A)-Nd(1A)-N(1A)	101.27(16)
N(5A)-Nd(1A)-N(2A)	112.99(17)
N(1A)-Nd(1A)-N(2A)	68.62(16)
N(5A)-Nd(1A)-O(1A)	92.69(15)
N(1A)-Nd(1A)-O(1A)	136.51(14)
N(2A)-Nd(1A)-O(1A)	141.11(15)
N(5A)-Nd(1A)-N(3A)	129.24(16)
N(1A)-Nd(1A)-N(3A)	52.77(16)
N(2A)-Nd(1A)-N(3A)	97.54(15)
O(1A)-Nd(1A)-N(3A)	86.68(14)
N(5A)-Nd(1A)-N(4A)	114.94(16)
N(1A)-Nd(1A)-N(4A)	119.07(14)
N(2A)-Nd(1A)-N(4A)	52.93(16)
O(1A)-Nd(1A)-N(4A)	90.41(14)
N(3A)-Nd(1A)-N(4A)	115.82(13)
N(5A)-Nd(1A)-C(24A)	122.16(17)
N(1A)-Nd(1A)-C(24A)	92.64(15)
N(2A)-Nd(1A)-C(24A)	27.22(17)
O(1A)-Nd(1A)-C(24A)	114.25(15)
N(3A)-Nd(1A)-C(24A)	103.72(14)
N(4A)-Nd(1A)-C(24A)	26.64(16)
N(5A)-Nd(1A)-C(11A)	121.18(16)
N(1A)-Nd(1A)-C(11A)	26.70(15)
N(2A)-Nd(1A)-C(11A)	78.83(15)
O(1A)-Nd(1A)-C(11A)	113.23(14)
N(3A)-Nd(1A)-C(11A)	26.76(16)
N(4A)-Nd(1A)-C(11A)	116.51(13)
C(24A)-Nd(1A)-C(11A)	94.75(14)
N(5A)-Nd(1A)-Si(2A)	26.74(13)
N(1A)-Nd(1A)-Si(2A)	89.67(10)
N(2A)-Nd(1A)-Si(2A)	130.78(12)
O(1A)-Nd(1A)-Si(2A)	84.73(9)
N(3A)-Nd(1A)-Si(2A)	103.22(10)
N(4A)-Nd(1A)-Si(2A)	140.31(10)
C(24A)-Nd(1A)-Si(2A)	147.72(12)
C(11A)-Nd(1A)-Si(2A)	101.43(10)
N(5B)-Nd(1B)-N(1B)	105.76(18)
N(5B)-Nd(1B)-N(2B)	102.61(17)
N(1B)-Nd(1B)-N(2B)	67.83(16)
N(5B)-Nd(1B)-N(4B)	108.02(17)

N(1B)-Nd(1B)-N(4B)	116.07(15)
N(2B)-Nd(1B)-N(4B)	52.83(14)
N(5B)-Nd(1B)-O(1B)	88.84(14)
N(1B)-Nd(1B)-O(1B)	128.20(15)
N(2B)-Nd(1B)-O(1B)	157.31(15)
N(4B)-Nd(1B)-O(1B)	105.14(13)
N(5B)-Nd(1B)-N(3B)	134.26(17)
N(1B)-Nd(1B)-N(3B)	52.66(15)
N(2B)-Nd(1B)-N(3B)	103.18(15)
N(4B)-Nd(1B)-N(3B)	117.68(16)
O(1B)-Nd(1B)-N(3B)	81.42(13)
N(5B)-Nd(1B)-C(24B)	114.14(17)
N(1B)-Nd(1B)-C(24B)	88.70(15)
N(2B)-Nd(1B)-C(24B)	26.80(15)
N(4B)-Nd(1B)-C(24B)	27.78(13)
O(1B)-Nd(1B)-C(24B)	130.51(14)
N(3B)-Nd(1B)-C(24B)	105.79(15)
N(5B)-Nd(1B)-C(11B)	125.87(18)
N(1B)-Nd(1B)-C(11B)	26.11(17)
N(2B)-Nd(1B)-C(11B)	81.75(15)
N(4B)-Nd(1B)-C(11B)	116.01(15)
O(1B)-Nd(1B)-C(11B)	107.52(14)
N(3B)-Nd(1B)-C(11B)	27.19(14)
C(24B)-Nd(1B)-C(11B)	93.80(15)
N(5B)-Nd(1B)-Si(2B)	26.24(14)
N(1B)-Nd(1B)-Si(2B)	84.64(14)
N(2B)-Nd(1B)-Si(2B)	109.14(13)
N(4B)-Nd(1B)-Si(2B)	132.72(12)
O(1B)-Nd(1B)-Si(2B)	89.81(11)
N(3B)-Nd(1B)-Si(2B)	108.69(12)
C(24B)-Nd(1B)-Si(2B)	130.09(12)
C(11B)-Nd(1B)-Si(2B)	100.77(13)
N(5A)-Si(1A)-C(38A)	113.7(4)
N(5A)-Si(1A)-C(38')	111.2(4)
C(38A)-Si(1A)-C(38')	17.1(4)
N(5A)-Si(1A)-C(39')	114.0(4)
C(38A)-Si(1A)-C(39')	115.5(4)
C(38')-Si(1A)-C(39')	103.7(4)
N(5A)-Si(1A)-C(37')	117.4(5)
C(38A)-Si(1A)-C(37')	91.2(6)
C(38')-Si(1A)-C(37')	106.5(5)
C(39')-Si(1A)-C(37')	102.8(7)
N(5A)-Si(1A)-C(39A)	110.8(4)
C(38A)-Si(1A)-C(39A)	112.6(4)
C(38')-Si(1A)-C(39A)	99.5(4)
C(39')-Si(1A)-C(39A)	7.3(8)
C(37')-Si(1A)-C(39A)	109.9(7)
N(5A)-Si(1A)-C(37A)	109.9(4)
C(38A)-Si(1A)-C(37A)	108.6(5)
C(38')-Si(1A)-C(37A)	123.5(5)
C(39')-Si(1A)-C(37A)	93.0(6)
C(37')-Si(1A)-C(37A)	17.5(5)

C(39A)-Si(1A)-C(37A)	100.3(6)
N(5A)-Si(2A)-C(40A)	115.6(3)
N(5A)-Si(2A)-C(41A)	114.2(3)
C(40A)-Si(2A)-C(41A)	107.6(4)
N(5A)-Si(2A)-C(42A)	109.4(3)
C(40A)-Si(2A)-C(42A)	102.2(4)
C(41A)-Si(2A)-C(42A)	106.8(4)
N(5A)-Si(2A)-Nd(1A)	37.90(16)
C(40A)-Si(2A)-Nd(1A)	140.5(3)
C(41A)-Si(2A)-Nd(1A)	110.8(2)
C(42A)-Si(2A)-Nd(1A)	75.2(2)
N(5B)-Si(1B)-C(39B)	115.1(3)
N(5B)-Si(1B)-C(38B)	110.5(3)
C(39B)-Si(1B)-C(38B)	107.1(4)
N(5B)-Si(1B)-C(37B)	111.4(3)
C(39B)-Si(1B)-C(37B)	102.2(4)
C(38B)-Si(1B)-C(37B)	110.1(3)
N(5B)-Si(2B)-C(41B)	108.8(4)
N(5B)-Si(2B)-C(42B)	113.3(3)
C(41B)-Si(2B)-C(42B)	107.7(4)
N(5B)-Si(2B)-C(40B)	115.2(3)
C(41B)-Si(2B)-C(40B)	105.1(4)
C(42B)-Si(2B)-C(40B)	106.2(4)
N(5B)-Si(2B)-Nd(1B)	37.9(2)
C(41B)-Si(2B)-Nd(1B)	73.8(3)
C(42B)-Si(2B)-Nd(1B)	111.9(3)
C(40B)-Si(2B)-Nd(1B)	140.3(3)
C(11A)-N(1A)-C(1A)	129.5(5)
C(11A)-N(1A)-Nd(1A)	99.7(3)
C(1A)-N(1A)-Nd(1A)	127.4(3)
C(24A)-N(2A)-C(9A)	128.0(5)
C(24A)-N(2A)-Nd(1A)	98.4(4)
C(9A)-N(2A)-Nd(1A)	130.2(3)
C(11A)-N(3A)-C(16')	127.8(5)
C(11A)-N(3A)-C(16A)	127.6(4)
C(16')-N(3A)-C(16A)	10.9(3)
C(11A)-N(3A)-Nd(1A)	94.6(3)
C(16')-N(3A)-Nd(1A)	137.3(4)
C(16A)-N(3A)-Nd(1A)	137.1(4)
C(24A)-N(4A)-C(29A)	128.3(4)
C(24A)-N(4A)-Nd(1A)	92.5(3)
C(29A)-N(4A)-Nd(1A)	138.6(3)
Si(2A)-N(5A)-Si(1A)	121.8(3)
Si(2A)-N(5A)-Nd(1A)	115.4(3)
Si(1A)-N(5A)-Nd(1A)	121.8(2)
C(11B)-N(1B)-C(9B)	128.6(5)
C(11B)-N(1B)-Nd(1B)	101.2(3)
C(9B)-N(1B)-Nd(1B)	129.1(4)
C(24B)-N(2B)-C(1B)	128.9(5)
C(24B)-N(2B)-Nd(1B)	96.2(3)
C(1B)-N(2B)-Nd(1B)	134.7(4)
C(11B)-N(3B)-C(16B)	128.4(4)

C(11B)-N(3B)-Nd(1B)	92.0(3)
C(16B)-N(3B)-Nd(1B)	139.4(3)
C(24B)-N(4B)-C(29B)	124.5(4)
C(24B)-N(4B)-Nd(1B)	93.7(3)
C(29B)-N(4B)-Nd(1B)	141.8(3)
Si(2B)-N(5B)-Si(1B)	121.7(3)
Si(2B)-N(5B)-Nd(1B)	115.9(3)
Si(1B)-N(5B)-Nd(1B)	120.5(3)
C(43A)-O(1A)-C(46A)	109.7(4)
C(43A)-O(1A)-Nd(1A)	115.7(3)
C(46A)-O(1A)-Nd(1A)	134.5(3)
C(46B)-O(1B)-C(43B)	107.8(3)
C(46B)-O(1B)-Nd(1B)	131.6(3)
C(43B)-O(1B)-Nd(1B)	120.5(3)
C(2A)-C(1A)-N(1A)	119.2(5)
C(2A)-C(1A)-C(10A)	119.4(6)
N(1A)-C(1A)-C(10A)	120.8(5)
C(1A)-C(2A)-C(3A)	121.3(6)
C(4A)-C(3A)-C(2A)	120.6(6)
C(3A)-C(4A)-C(5A)	120.9(6)
C(4A)-C(5A)-C(6A)	120.7(6)
C(4A)-C(5A)-C(10A)	119.3(6)
C(6A)-C(5A)-C(10A)	119.9(6)
C(7A)-C(6A)-C(5A)	120.4(6)
C(6A)-C(7A)-C(8A)	121.2(6)
C(7A)-C(8A)-C(9A)	122.0(6)
C(8A)-C(9A)-N(2A)	120.3(6)
C(8A)-C(9A)-C(10A)	119.7(6)
N(2A)-C(9A)-C(10A)	119.7(5)
C(1A)-C(10A)-C(5A)	117.7(5)
C(1A)-C(10A)-C(9A)	125.5(5)
C(5A)-C(10A)-C(9A)	116.7(5)
N(3A)-C(11A)-N(1A)	110.2(4)
N(3A)-C(11A)-C(12A)	126.1(5)
N(1A)-C(11A)-C(12A)	123.4(5)
N(3A)-C(11A)-Nd(1A)	58.6(3)
N(1A)-C(11A)-Nd(1A)	53.6(3)
C(12A)-C(11A)-Nd(1A)	162.1(3)
C(13A)-C(12A)-C(14A)	107.3(5)
C(13A)-C(12A)-C(11A)	114.1(5)
C(14A)-C(12A)-C(11A)	112.5(4)
C(13A)-C(12A)-C(15A)	106.8(5)
C(14A)-C(12A)-C(15A)	109.3(6)
C(11A)-C(12A)-C(15A)	106.7(5)
C(17A)-C(16A)-C(21A)	120.0
C(17A)-C(16A)-N(3A)	119.4(4)
C(21A)-C(16A)-N(3A)	119.1(4)
C(16A)-C(17A)-C(18A)	120.0
C(16A)-C(17A)-C(22A)	122.9(7)
C(18A)-C(17A)-C(22A)	116.8(7)
C(17A)-C(18A)-C(19A)	120.0
C(20A)-C(19A)-C(18A)	120.0

C(19A)-C(20A)-C(21A)	120.0
C(20A)-C(21A)-C(16A)	120.0
C(20A)-C(21A)-C(23A)	119.8(7)
C(16A)-C(21A)-C(23A)	119.9(7)
C(17')-C(16')-C(21')	120.0
C(17')-C(16')-N(3A)	117.5(4)
C(21')-C(16')-N(3A)	121.8(4)
C(16')-C(17')-C(18')	120.0
C(16')-C(17')-C(22')	122.7(7)
C(18')-C(17')-C(22')	117.0(7)
C(19')-C(18')-C(17')	120.0
C(20')-C(19')-C(18')	120.0
C(21')-C(20')-C(19')	120.0
C(20')-C(21')-C(16')	120.0
C(20')-C(21')-C(23')	121.7(7)
C(16')-C(21')-C(23')	118.0(7)
N(4A)-C(24A)-N(2A)	112.4(4)
N(4A)-C(24A)-C(25A)	123.3(5)
N(2A)-C(24A)-C(25A)	123.1(5)
N(4A)-C(24A)-Nd(1A)	60.9(3)
N(2A)-C(24A)-Nd(1A)	54.3(3)
C(25A)-C(24A)-Nd(1A)	154.3(4)
C(27A)-C(25A)-C(28A)	106.9(5)
C(27A)-C(25A)-C(26A)	108.4(5)
C(28A)-C(25A)-C(26A)	106.5(6)
C(27A)-C(25A)-C(24A)	112.7(5)
C(28A)-C(25A)-C(24A)	107.8(5)
C(26A)-C(25A)-C(24A)	114.2(5)
C(30A)-C(29A)-C(34A)	120.0
C(30A)-C(29A)-N(4A)	117.5(3)
C(34A)-C(29A)-N(4A)	122.5(3)
C(31A)-C(30A)-C(29A)	120.0
C(31A)-C(30A)-C(35A)	117.0(3)
C(29A)-C(30A)-C(35A)	122.5(3)
C(32A)-C(31A)-C(30A)	120.0
C(31A)-C(32A)-C(33A)	120.0
C(34A)-C(33A)-C(32A)	120.0
C(33A)-C(34A)-C(29A)	120.0
C(33A)-C(34A)-C(36A)	117.1(4)
C(29A)-C(34A)-C(36A)	122.7(3)
O(1A)-C(43A)-C(44A)	104.4(5)
C(45A)-C(44A)-C(43A)	103.7(6)
C(46A)-C(45A)-C(44A)	103.1(5)
O(1A)-C(46A)-C(45A)	104.7(5)
C(2B)-C(1B)-N(2B)	119.7(5)
C(2B)-C(1B)-C(10B)	119.5(5)
N(2B)-C(1B)-C(10B)	120.4(5)
C(1B)-C(2B)-C(3B)	121.7(5)
C(4B)-C(3B)-C(2B)	120.1(5)
C(3B)-C(4B)-C(5B)	121.7(5)
C(6B)-C(5B)-C(4B)	120.8(5)
C(6B)-C(5B)-C(10B)	119.8(5)

C(4B)-C(5B)-C(10B)	119.3(5)
C(7B)-C(6B)-C(5B)	121.5(5)
C(6B)-C(7B)-C(8B)	119.8(6)
C(7B)-C(8B)-C(9B)	120.8(6)
N(1B)-C(9B)-C(10B)	121.7(6)
N(1B)-C(9B)-C(8B)	118.7(5)
C(10B)-C(9B)-C(8B)	119.4(5)
C(9B)-C(10B)-C(1B)	124.5(5)
C(9B)-C(10B)-C(5B)	117.8(5)
C(1B)-C(10B)-C(5B)	117.6(5)
N(1B)-C(11B)-N(3B)	111.6(5)
N(1B)-C(11B)-C(12B)	124.2(5)
N(3B)-C(11B)-C(12B)	124.1(5)
N(1B)-C(11B)-Nd(1B)	52.7(3)
N(3B)-C(11B)-Nd(1B)	60.9(3)
C(12B)-C(11B)-Nd(1B)	165.4(4)
C(13B)-C(12B)-C(15B)	104.8(5)
C(13B)-C(12B)-C(14B)	107.9(5)
C(15B)-C(12B)-C(14B)	108.3(5)
C(13B)-C(12B)-C(11B)	113.6(5)
C(15B)-C(12B)-C(11B)	110.8(5)
C(14B)-C(12B)-C(11B)	111.1(5)
C(17B)-C(16B)-C(21B)	120.0
C(17B)-C(16B)-N(3B)	120.4(3)
C(21B)-C(16B)-N(3B)	119.5(3)
C(16B)-C(17B)-C(18B)	120.0
C(16B)-C(17B)-C(22B)	121.0(4)
C(18B)-C(17B)-C(22B)	118.5(3)
C(17B)-C(18B)-C(19B)	120.0
C(20B)-C(19B)-C(18B)	120.0
C(19B)-C(20B)-C(21B)	120.0
C(20B)-C(21B)-C(16B)	120.0
C(20B)-C(21B)-C(23B)	118.2(4)
C(16B)-C(21B)-C(23B)	121.8(4)
N(2B)-C(24B)-N(4B)	110.3(5)
N(2B)-C(24B)-C(25B)	126.3(5)
N(4B)-C(24B)-C(25B)	121.5(5)
N(2B)-C(24B)-Nd(1B)	57.0(3)
N(4B)-C(24B)-Nd(1B)	58.5(3)
C(25B)-C(24B)-Nd(1B)	146.3(4)
C(26B)-C(25B)-C(27B)	107.5(5)
C(26B)-C(25B)-C(28B)	106.8(5)
C(27B)-C(25B)-C(28B)	106.2(5)
C(26B)-C(25B)-C(24B)	111.1(5)
C(27B)-C(25B)-C(24B)	115.1(5)
C(28B)-C(25B)-C(24B)	109.7(4)
C(30B)-C(29B)-C(34B)	120.0
C(30B)-C(29B)-N(4B)	121.1(3)
C(34B)-C(29B)-N(4B)	118.7(3)
C(29B)-C(30B)-C(31B)	120.0
C(29B)-C(30B)-C(35B)	122.9(3)
C(31B)-C(30B)-C(35B)	116.4(3)

C(30B)-C(31B)-C(32B)	120.0
C(33B)-C(32B)-C(31B)	120.0
C(34B)-C(33B)-C(32B)	120.0
C(33B)-C(34B)-C(29B)	120.0
C(33B)-C(34B)-C(36B)	118.4(3)
C(29B)-C(34B)-C(36B)	121.5(3)
O(1B)-C(43B)-C(44')	108.2(5)
O(1B)-C(43B)-C(44B)	101.0(5)
C(44')-C(43B)-C(44B)	30.8(5)
C(45B)-C(44B)-C(43B)	97.5(5)
C(44B)-C(45B)-C(46B)	94.6(5)
C(45')-C(44')-C(43B)	98.6(4)
C(44')-C(45')-C(46B)	101.8(5)
O(1B)-C(46B)-C(45B)	105.4(5)
O(1B)-C(46B)-C(45')	105.2(5)
C(45B)-C(46B)-C(45')	30.9(5)

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for for [1,8- $\text{C}_{10}\text{H}_6\{\text{NC}(\text{tBu})\text{N}-2,6\text{-Me}_2\text{-C}_6\text{H}_3\}_2\text{NdN}(\text{SiMe}_3)_2(\text{THF})$ (4).

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Nd(1A)	20(1)	21(1)	15(1)	-1(1)	8(1)	0(1)
Nd(1B)	21(1)	21(1)	14(1)	-1(1)	5(1)	-2(1)
Si(1A)	43(1)	41(1)	36(1)	11(1)	9(1)	3(1)
Si(2A)	34(1)	41(1)	26(1)	-7(1)	6(1)	-4(1)
Si(1B)	36(1)	41(1)	36(1)	-1(1)	17(1)	5(1)
Si(2B)	43(1)	43(1)	46(1)	3(1)	27(1)	-4(1)
N(1A)	29(2)	20(2)	20(2)	-4(2)	14(2)	1(2)
N(2A)	36(2)	21(2)	32(2)	-2(2)	20(2)	-1(2)
N(3A)	26(2)	23(2)	20(2)	0(2)	13(2)	-4(2)
N(4A)	24(2)	27(2)	20(2)	0(2)	9(2)	2(2)
N(5A)	29(2)	36(3)	25(2)	3(2)	12(2)	4(2)
N(1B)	36(2)	30(3)	21(2)	-1(2)	11(2)	4(2)
N(2B)	32(2)	27(2)	19(2)	1(2)	7(2)	-7(2)
N(3B)	21(2)	29(2)	19(2)	-3(2)	7(2)	4(2)
N(4B)	22(2)	20(2)	18(2)	1(2)	3(2)	-1(2)
N(5B)	34(2)	45(3)	19(2)	-3(2)	11(2)	-11(2)
O(1A)	25(2)	25(2)	33(2)	2(2)	15(1)	2(2)
O(1B)	25(2)	40(2)	18(2)	-4(2)	2(1)	4(2)
C(1A)	34(2)	32(3)	27(2)	8(2)	23(2)	12(2)
C(2A)	36(3)	28(3)	37(3)	11(2)	19(2)	14(2)
C(3A)	50(3)	50(4)	24(3)	9(3)	22(2)	23(3)
C(4A)	37(3)	58(4)	25(3)	16(3)	20(2)	16(3)

C(5A)	22(2)	48(4)	24(2)	14(2)	11(2)	12(2)
C(6A)	25(3)	68(4)	27(3)	21(3)	14(2)	4(3)
C(7A)	28(3)	50(4)	38(3)	17(3)	10(2)	-4(3)
C(8A)	34(3)	30(3)	40(3)	6(3)	16(2)	-2(3)
C(9A)	25(2)	27(3)	38(3)	5(2)	16(2)	1(2)
C(10A)	24(2)	27(3)	29(2)	13(2)	15(2)	8(2)
C(11A)	28(2)	15(2)	18(2)	-10(2)	10(2)	-3(2)
C(12A)	31(3)	32(3)	28(3)	9(2)	16(2)	4(2)
C(13A)	28(3)	49(4)	29(3)	8(3)	12(2)	9(3)
C(14A)	72(4)	39(3)	41(3)	16(3)	30(3)	34(3)
C(15A)	26(3)	61(5)	63(4)	29(4)	9(3)	10(3)
C(16A)	24(2)	23(2)	25(2)	4(2)	10(2)	1(2)
C(17A)	29(2)	25(2)	29(3)	-2(2)	11(2)	2(2)
C(18A)	37(2)	39(3)	38(3)	2(2)	18(2)	-2(2)
C(19A)	39(2)	41(3)	46(3)	8(2)	20(2)	-2(2)
C(20A)	37(2)	40(3)	35(2)	2(2)	17(2)	6(2)
C(21A)	24(2)	25(3)	23(2)	4(2)	9(2)	2(2)
C(22A)	45(1)	45(1)	45(1)	0(1)	20(1)	0(1)
C(23A)	38(1)	38(1)	38(1)	0(1)	17(1)	0(1)
C(16')	24(2)	23(2)	25(2)	4(2)	10(2)	1(2)
C(17')	29(2)	25(2)	29(3)	-2(2)	11(2)	2(2)
C(18')	37(2)	39(3)	38(3)	2(2)	18(2)	-2(2)
C(19')	39(2)	41(3)	46(3)	8(2)	20(2)	-2(2)
C(20')	37(2)	40(3)	35(2)	2(2)	17(2)	6(2)
C(21')	24(2)	25(3)	23(2)	4(2)	9(2)	2(2)
C(22')	45(1)	45(1)	45(1)	0(1)	20(1)	0(1)
C(23')	38(1)	38(1)	38(1)	0(1)	17(1)	0(1)
C(24A)	27(2)	13(2)	37(3)	-4(2)	16(2)	-6(2)
C(25A)	22(3)	32(3)	34(3)	-4(3)	5(2)	2(2)
C(26A)	32(3)	30(3)	51(4)	-3(3)	4(3)	-4(3)
C(27A)	28(3)	30(3)	32(3)	1(2)	9(2)	2(2)
C(28A)	26(3)	52(4)	35(3)	-9(3)	5(3)	-4(3)
C(29A)	25(2)	26(3)	34(3)	-9(2)	10(2)	-4(2)
C(30A)	21(3)	29(3)	43(3)	-5(3)	-1(3)	5(2)
C(31A)	28(3)	32(3)	63(5)	-10(3)	3(3)	0(3)
C(32A)	37(3)	52(4)	54(4)	-19(3)	14(3)	0(3)
C(33A)	38(3)	45(4)	56(4)	-22(3)	24(3)	-6(3)
C(34A)	21(2)	44(3)	31(3)	-16(3)	8(2)	1(2)
C(35A)	40(3)	27(3)	51(4)	8(3)	9(3)	1(3)
C(36A)	44(3)	37(3)	40(3)	-6(3)	24(2)	-5(3)
C(37A)	47(1)	47(1)	46(1)	1(1)	20(1)	-1(1)
C(38A)	48(1)	50(1)	49(1)	0(1)	22(1)	-1(1)
C(39A)	47(1)	47(1)	47(1)	0(1)	21(1)	-1(1)
C(37')	47(1)	47(1)	46(1)	0(1)	22(1)	-1(1)
C(38')	48(1)	50(1)	49(1)	0(1)	22(1)	-1(1)
C(39')	47(1)	47(1)	47(1)	0(1)	21(1)	-1(1)
C(40A)	34(4)	69(5)	80(6)	-17(5)	5(4)	-5(4)
C(41A)	50(1)	50(1)	50(1)	-4(1)	24(1)	2(1)
C(42A)	52(1)	50(1)	49(1)	2(1)	23(1)	-2(1)
C(43A)	35(3)	38(3)	26(3)	10(2)	10(2)	13(3)
C(44A)	33(3)	53(4)	44(3)	11(3)	20(2)	14(3)
C(45A)	34(3)	51(4)	35(3)	2(3)	18(2)	1(3)

C(46A)	35(3)	22(3)	26(3)	7(2)	10(2)	-7(2)
C(1B)	25(2)	21(3)	17(2)	3(2)	4(2)	2(2)
C(2B)	28(2)	26(3)	33(3)	3(2)	14(2)	3(2)
C(3B)	25(3)	34(3)	33(3)	-11(2)	10(2)	0(2)
C(4B)	30(3)	26(3)	17(2)	-4(2)	4(2)	7(2)
C(5B)	32(3)	27(3)	20(2)	-1(2)	6(2)	3(2)
C(6B)	50(3)	30(3)	18(3)	4(2)	8(2)	5(3)
C(7B)	66(4)	25(3)	33(3)	7(3)	17(3)	2(3)
C(8B)	58(4)	21(3)	27(3)	1(2)	17(3)	1(3)
C(9B)	34(3)	34(3)	25(3)	3(2)	9(2)	3(3)
C(10B)	28(2)	25(3)	26(2)	3(2)	15(2)	8(2)
C(11B)	28(3)	19(3)	26(3)	-1(2)	6(2)	-6(2)
C(12B)	26(3)	23(3)	34(3)	2(2)	5(2)	6(2)
C(13B)	29(3)	60(4)	36(3)	1(3)	13(2)	7(3)
C(14B)	50(3)	22(3)	42(3)	2(2)	24(3)	4(3)
C(15B)	32(3)	35(3)	54(4)	-10(3)	1(3)	10(3)
C(16B)	25(2)	33(3)	20(2)	1(2)	8(2)	6(2)
C(17B)	29(3)	38(3)	27(3)	-12(3)	5(2)	-3(3)
C(18B)	29(3)	48(4)	44(3)	-19(3)	8(3)	-7(3)
C(19B)	36(3)	76(5)	27(3)	-22(3)	8(3)	5(3)
C(20B)	35(3)	56(4)	30(3)	-8(3)	11(2)	5(3)
C(21B)	27(3)	48(4)	21(3)	-5(2)	9(2)	9(3)
C(22B)	56(4)	51(4)	44(4)	-9(3)	14(3)	-22(3)
C(23B)	56(3)	43(4)	33(3)	2(3)	25(3)	-7(3)
C(24B)	33(3)	15(2)	14(2)	3(2)	8(2)	2(2)
C(25B)	25(3)	42(3)	22(3)	2(2)	6(2)	1(3)
C(26B)	33(3)	57(4)	42(3)	13(3)	17(3)	5(3)
C(27B)	35(3)	46(4)	50(3)	-4(3)	25(3)	-13(3)
C(28B)	35(3)	36(3)	42(3)	7(3)	21(2)	-1(3)
C(29B)	27(3)	33(3)	34(3)	13(2)	11(2)	-3(2)
C(30B)	36(3)	33(3)	48(3)	14(3)	21(3)	2(3)
C(31B)	46(4)	33(3)	55(4)	10(3)	17(3)	1(3)
C(32B)	37(3)	50(4)	62(4)	33(3)	14(3)	3(3)
C(33B)	29(3)	70(5)	33(3)	26(3)	6(3)	-2(3)
C(34B)	31(3)	48(4)	28(3)	11(3)	12(2)	-3(3)
C(35B)	41(3)	37(4)	46(3)	-5(3)	18(3)	1(3)
C(36B)	43(3)	65(5)	26(3)	-5(3)	9(3)	-9(3)
C(37B)	45(3)	45(4)	50(4)	12(3)	18(3)	11(3)
C(38B)	69(4)	47(4)	39(3)	-9(3)	23(3)	-1(4)
C(39B)	64(4)	50(4)	70(4)	5(4)	39(3)	15(4)
C(40B)	53(3)	63(5)	89(5)	-13(4)	47(3)	-14(4)
C(41B)	56(4)	43(4)	98(6)	20(4)	38(4)	-11(3)
C(42B)	100(5)	74(6)	49(4)	15(4)	47(4)	12(5)
C(43B)	56(4)	107(7)	16(3)	-11(4)	1(3)	25(5)
C(44B)	25(6)	85(9)	43(5)	-32(5)	-3(4)	7(5)
C(45B)	26(4)	72(8)	21(4)	-2(4)	11(3)	-8(4)
C(44')	25(6)	85(9)	43(5)	-32(5)	-3(4)	7(5)
C(45')	26(4)	72(8)	21(4)	-2(4)	11(3)	-8(4)
C(46B)	29(3)	92(6)	39(4)	-23(4)	1(3)	21(4)

GPC of the polylactides.

Table S9.

Entry 1.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 7,445
Processing Stop Time (min) = 10,188
Number of Slices = 165
Weight Average Molecular Weight = 59607
Number Average Molecular Weight = 43665
Z Average Molecular Weight = 78593
Z+1 Average Molecular Weight = 99614
Polydispersity index = 1,365
Peak Molecular Weight = 51768
Z Average / Weight Average = 1,319
Z+1 Average / Weight Average = 1,671

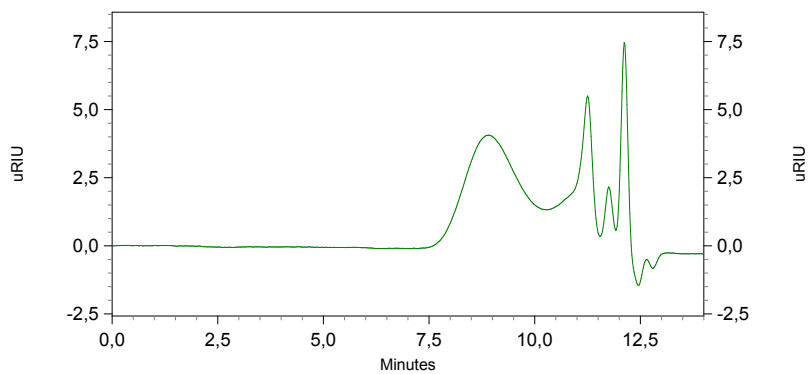
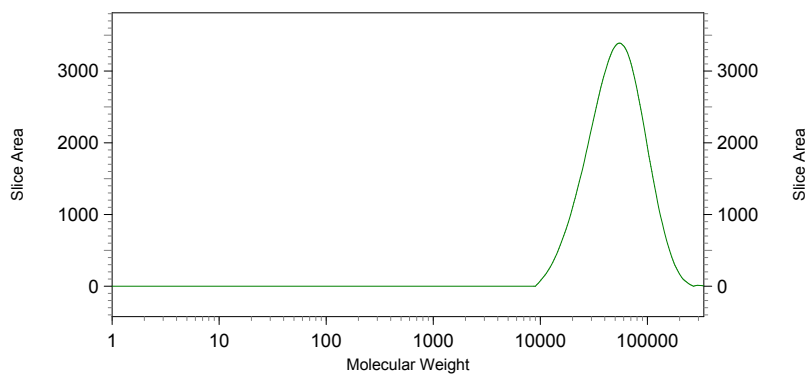


Table S10.
Entry 2.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 6,570
Processing Stop Time (min) = 9,872
Number of Slices = 198
Weight Average Molecular Weight = 251033
Number Average Molecular Weight = 137548
Z Average Molecular Weight = 431639
Z+1 Average Molecular Weight = 663206
Polydispersity index = 1,825
Peak Molecular Weight = 196199
Z Average / Weight Average = 1,719
Z+1 Average / Weight Average = 2,642

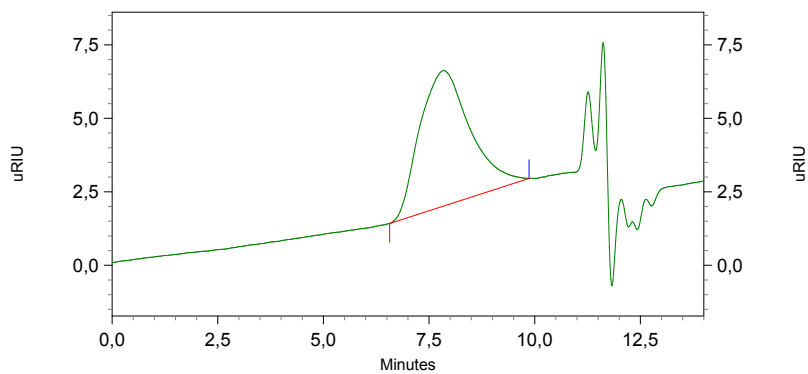
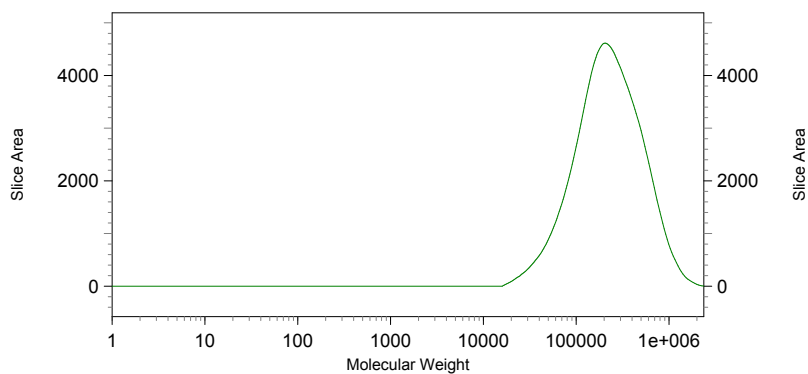


Table S11.
Entry 3.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 9,352
Processing Stop Time (min) = 11,038
Number of Slices = 101
Weight Average Molecular Weight = 6998
Number Average Molecular Weight = 5570
Z Average Molecular Weight = 8562
Z+1 Average Molecular Weight = 10331
Polydispersity index = 1,256
Peak Molecular Weight = 6448
Z Average / Weight Average = 1,223
Z+1 Average / Weight Average = 1,476

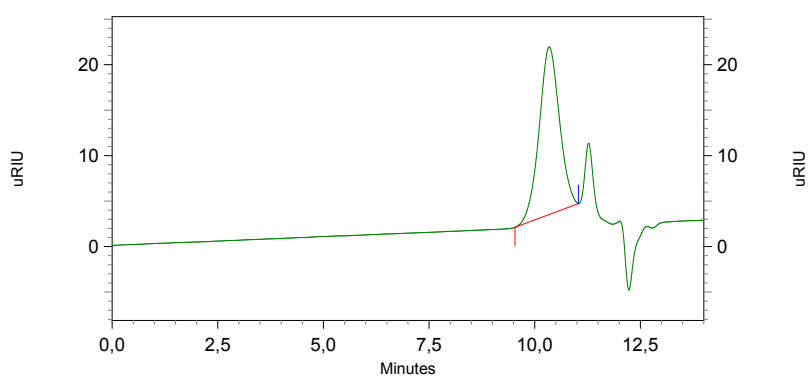
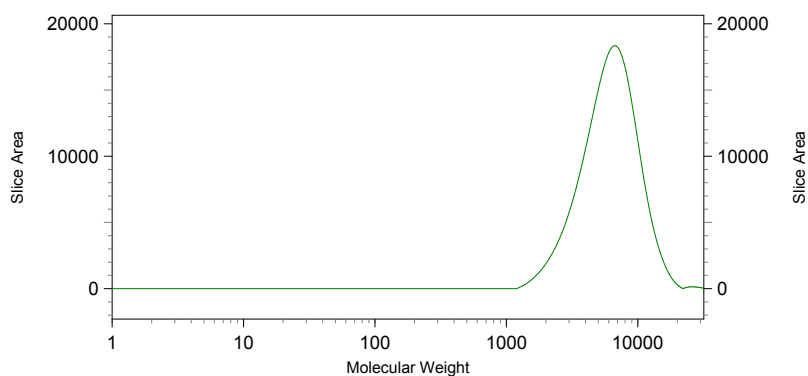


Table S12.
Entry 4.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 7,019
Processing Stop Time (min) = 10,686
Number of Slices = 220
Weight Average Molecular Weight = 91203
Number Average Molecular Weight = 42945
Z Average Molecular Weight = 150547
Z+1 Average Molecular Weight = 220128
Polydispersity index = 2,124
Peak Molecular Weight = 81054
Z Average / Weight Average = 1,651
Z+1 Average / Weight Average = 2,414

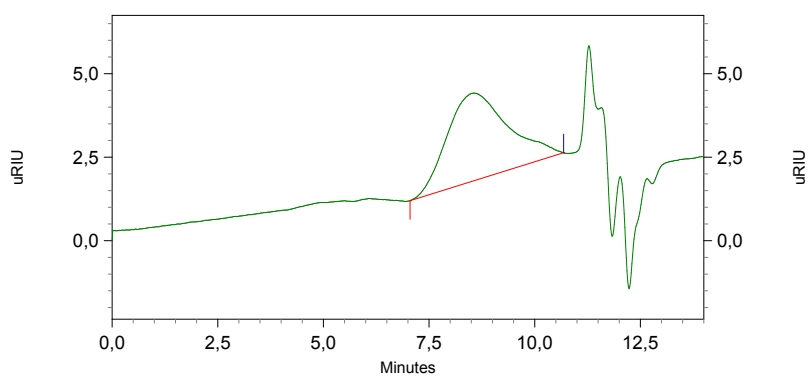
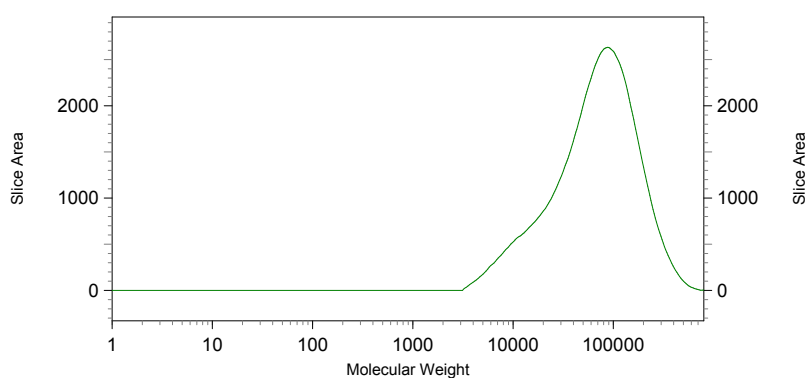


Table S13.
Entry 5.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 7,651
Processing Stop Time (min) = 10,613
Number of Slices = 178
Weight Average Molecular Weight = 48744
Number Average Molecular Weight = 37592
Z Average Molecular Weight = 60256
Z+1 Average Molecular Weight = 73279
Polydispersity index = 1,297
Peak Molecular Weight = 44974
Z Average / Weight Average = 1,236
Z+1 Average / Weight Average = 1,503

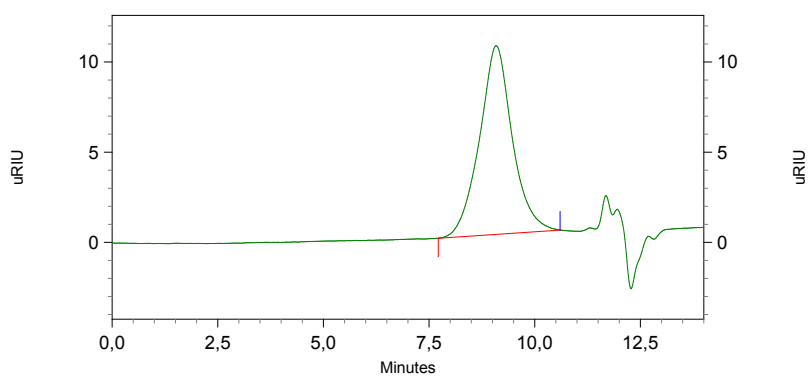
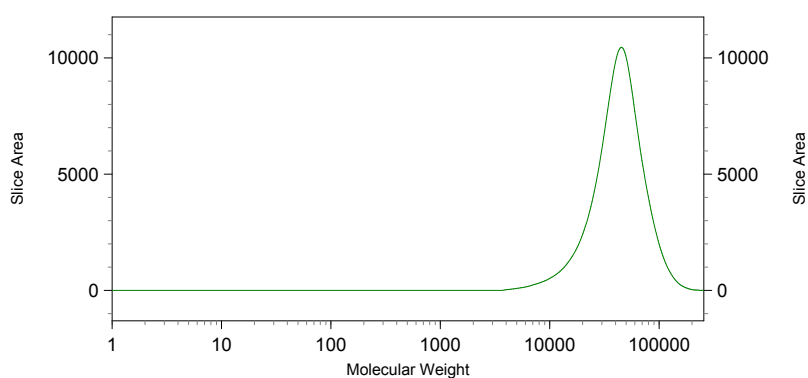


Table S14.
Entry 6.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 7,129
Processing Stop Time (min) = 9,751
Number of Slices = 157
Weight Average Molecular Weight = 100744
Number Average Molecular Weight = 74452
Z Average Molecular Weight = 136004
Z+1 Average Molecular Weight = 179340
Polydispersity index = 1,353
Peak Molecular Weight = 75160
Z Average / Weight Average = 1,350
Z+1 Average / Weight Average = 1,780

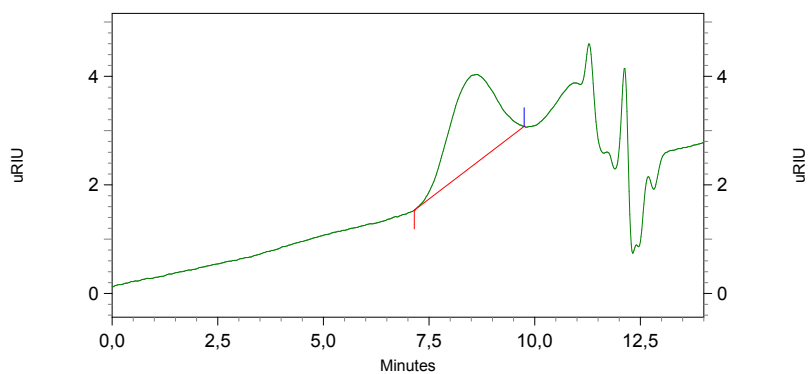
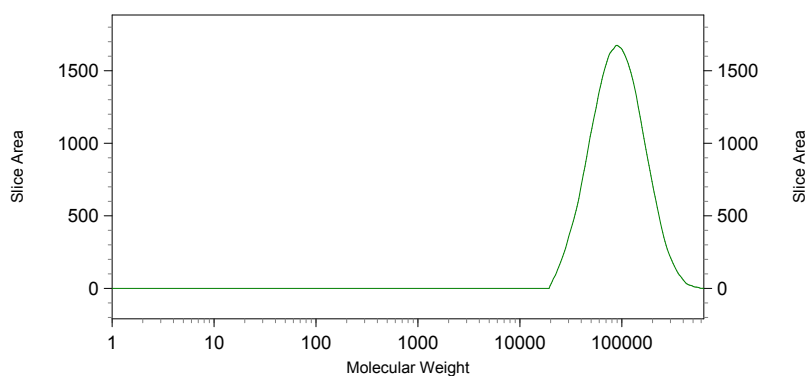


Table S15.
Entry 7.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 6,971
Processing Stop Time (min) = 9,896
Number of Slices = 176
Weight Average Molecular Weight = 136115
Number Average Molecular Weight = 88728
Z Average Molecular Weight = 208255
Z+1 Average Molecular Weight = 302880
Polydispersity index = 1,534
Peak Molecular Weight = 110368
Z Average / Weight Average = 1,530
Z+1 Average / Weight Average = 2,225

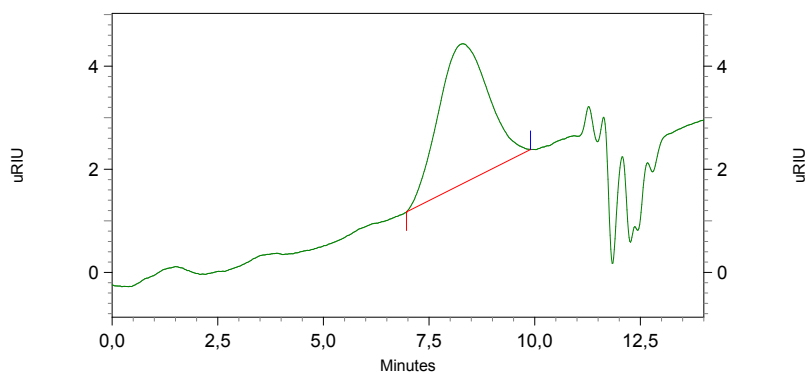
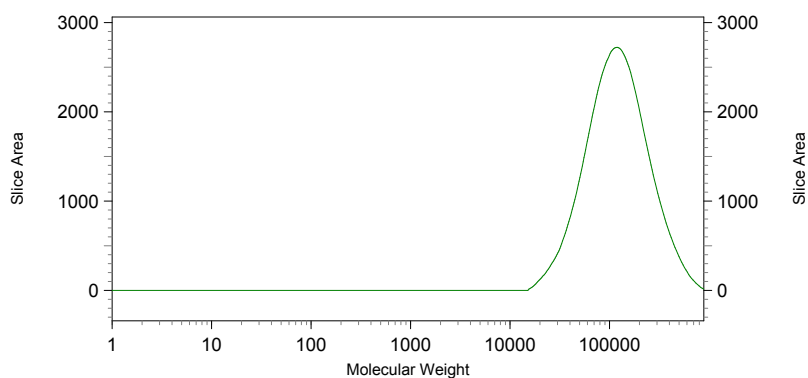


Table S16.
Entry 8.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 6,837
Processing Stop Time (min) = 9,799
Number of Slices = 178
Weight Average Molecular Weight = 154894
Number Average Molecular Weight = 98512
Z Average Molecular Weight = 246164
Z+1 Average Molecular Weight = 371201
Polydispersity index = 1,572
Peak Molecular Weight = 127059
Z Average / Weight Average = 1,589
Z+1 Average / Weight Average = 2,396

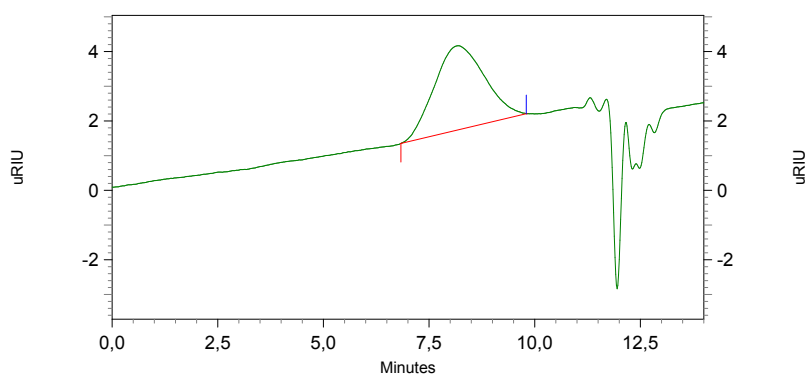
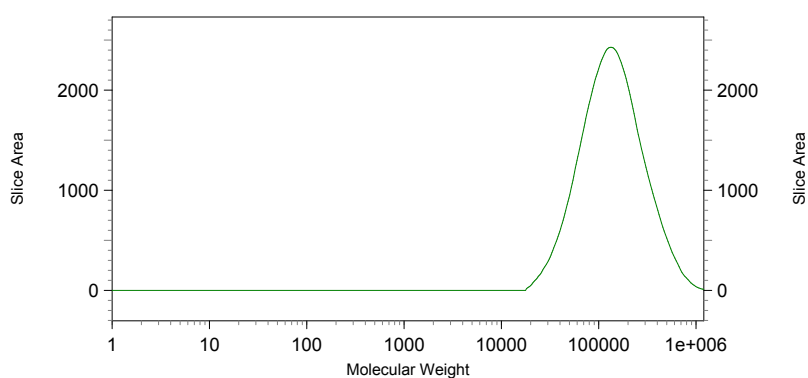


Table S17.
Entry 9.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 6,971
Processing Stop Time (min) = 9,569
Number of Slices = 156
Weight Average Molecular Weight = 139076
Number Average Molecular Weight = 98515
Z Average Molecular Weight = 199543
Z+1 Average Molecular Weight = 277779
Polydispersity index = 1,412
Peak Molecular Weight = 104037
Z Average / Weight Average = 1,435
Z+1 Average / Weight Average = 1,997

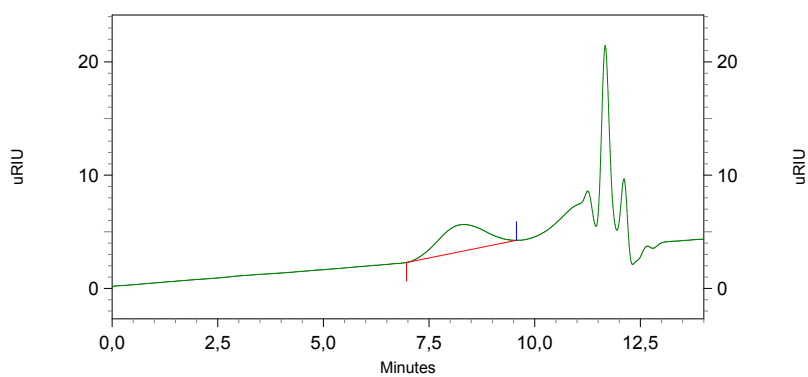
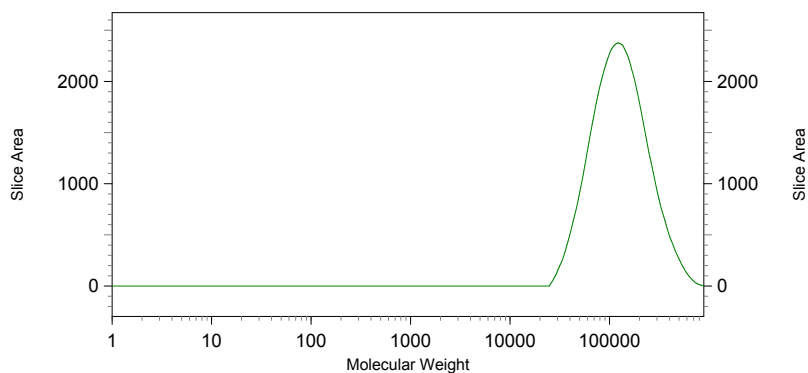


Table S18.
Entry 10.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 6,812
Processing Stop Time (min) = 9,751
Number of Slices = 176
Weight Average Molecular Weight = 157406
Number Average Molecular Weight = 102907
Z Average Molecular Weight = 243118
Z+1 Average Molecular Weight = 356258
Polydispersity index = 1,530
Peak Molecular Weight = 127059
Z Average / Weight Average = 1,545
Z+1 Average / Weight Average = 2,263

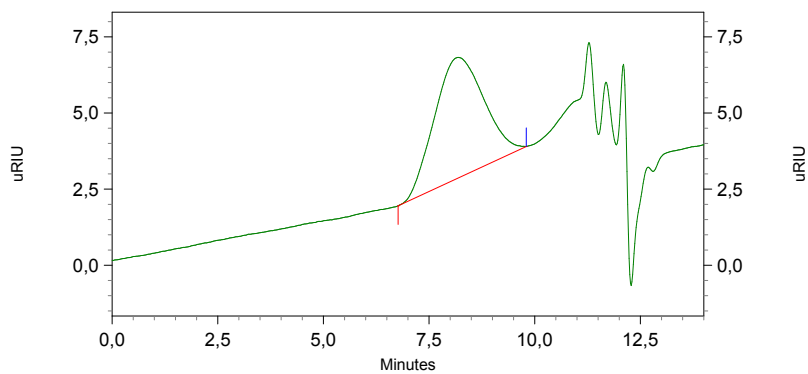
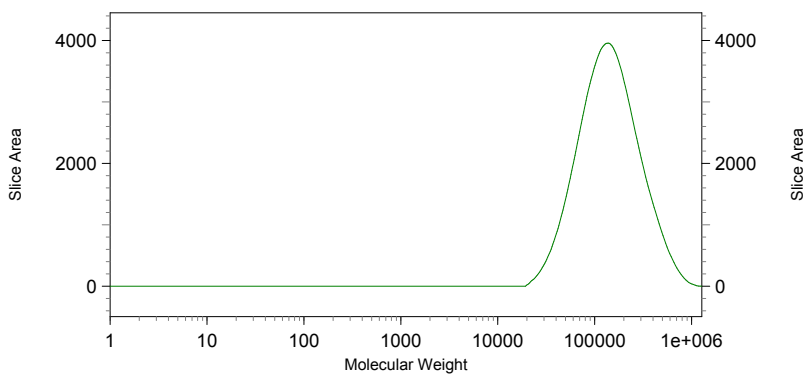


Table S19.
Entry 11.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 6,655
Processing Stop Time (min) = 9,921
Number of Slices = 196
Weight Average Molecular Weight = 230092
Number Average Molecular Weight = 116951
Z Average Molecular Weight = 425425
Z+1 Average Molecular Weight = 666048
Polydispersity index = 1,967
Peak Molecular Weight = 171198
Z Average / Weight Average = 1,849
Z+1 Average / Weight Average = 2,895

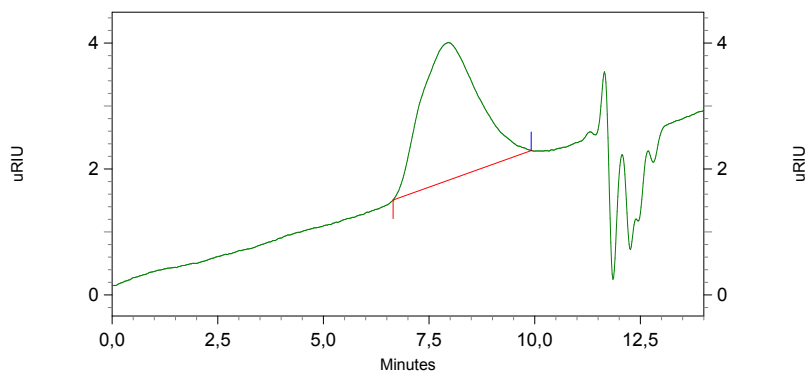
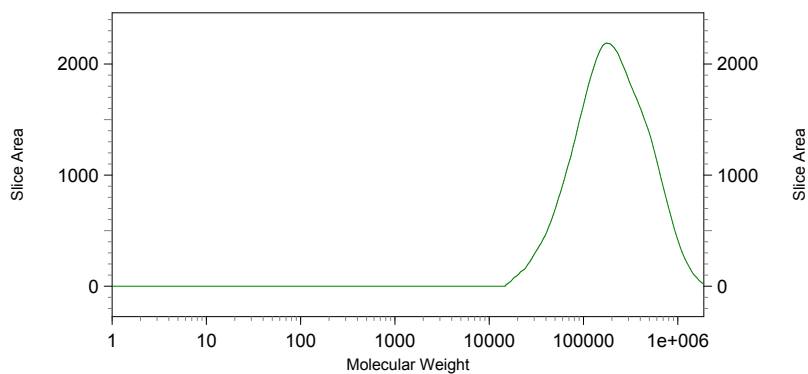


Table S20.
Entry 12.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 9,388
Processing Stop Time (min) = 10,905
Number of Slices = 91
Weight Average Molecular Weight = 10692
Number Average Molecular Weight = 8727
Z Average Molecular Weight = 12571
Z+1 Average Molecular Weight = 14389
Polydispersity index = 1,225
Peak Molecular Weight = 10479
Z Average / Weight Average = 1,176
Z+1 Average / Weight Average = 1,346

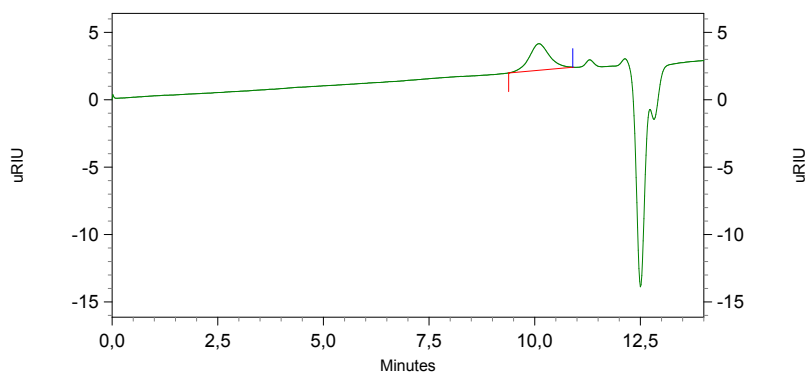
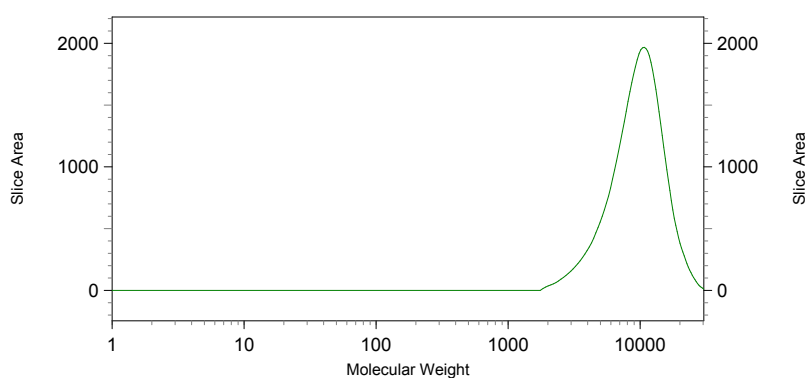


Table S21.
Entry 13.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 9,959
Processing Stop Time (min) = 11,014
Number of Slices = 63
Weight Average Molecular Weight = 5139
Number Average Molecular Weight = 4473
Z Average Molecular Weight = 5783
Z+1 Average Molecular Weight = 6393
Polydispersity index = 1,149
Peak Molecular Weight = 5206
Z Average / Weight Average = 1,125
Z+1 Average / Weight Average = 1,244

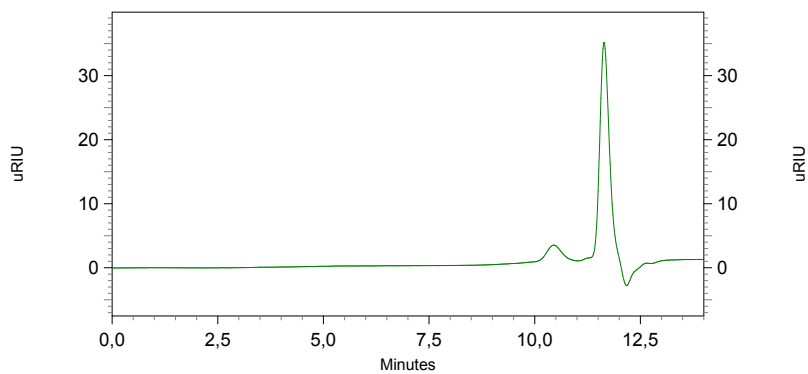
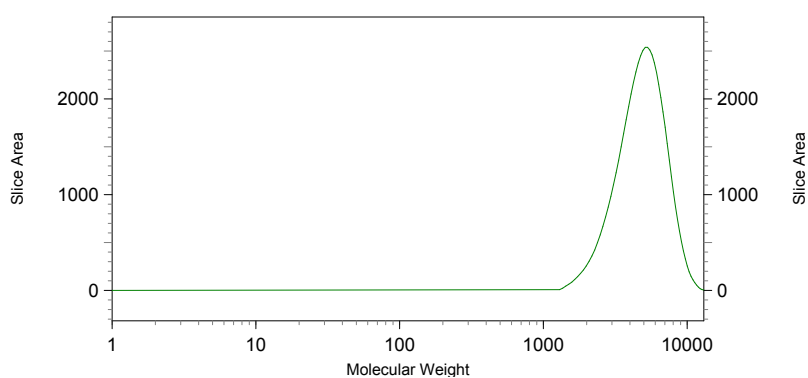


Table S22.
Entry 14.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 8,671
Processing Stop Time (min) = 10,674
Number of Slices = 120
Weight Average Molecular Weight = 18545
Number Average Molecular Weight = 16417
Z Average Molecular Weight = 20759
Z+1 Average Molecular Weight = 23431
Polydispersity index = 1,130
Peak Molecular Weight = 18226
Z Average / Weight Average = 1,119
Z+1 Average / Weight Average = 1,263

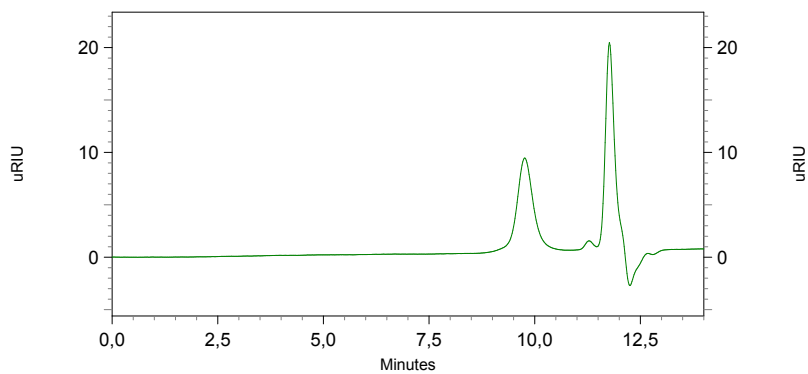
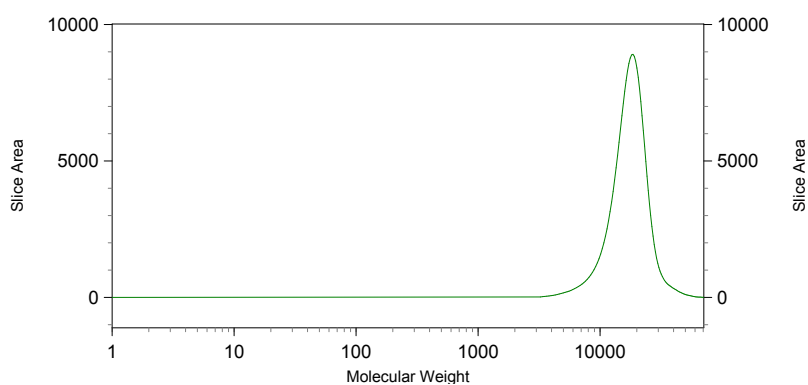


Table S23.
Entry 15.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 8,562
Processing Stop Time (min) = 10,966
Number of Slices = 144
Weight Average Molecular Weight = 27130
Number Average Molecular Weight = 21503
Z Average Molecular Weight = 31532
Z+1 Average Molecular Weight = 35609
Polydispersity index = 1,262
Peak Molecular Weight = 27299
Z Average / Weight Average = 1,162
Z+1 Average / Weight Average = 1,313

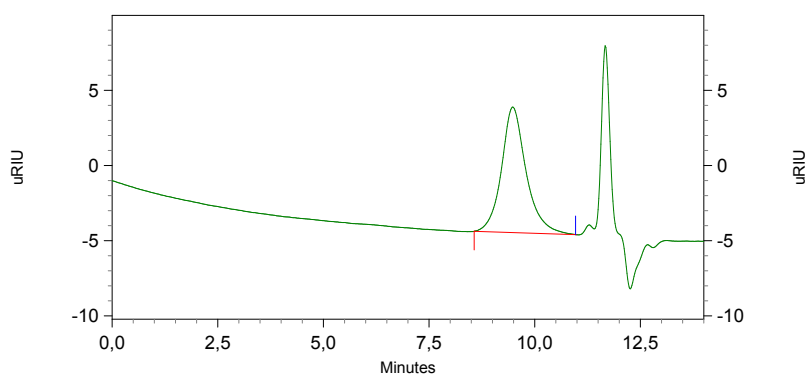
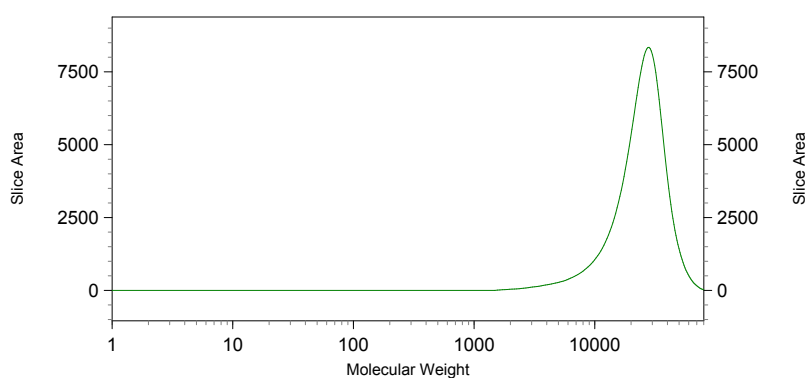


Table S24.
Entry 16.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 8,383
Processing Stop Time (min) = 10,383
Number of Slices = 120
Weight Average Molecular Weight = 30053
Number Average Molecular Weight = 23089
Z Average Molecular Weight = 37510
Z+1 Average Molecular Weight = 44567
Polydispersity index = 1,302
Peak Molecular Weight = 19167
Z Average / Weight Average = 1,248
Z+1 Average / Weight Average = 1,483

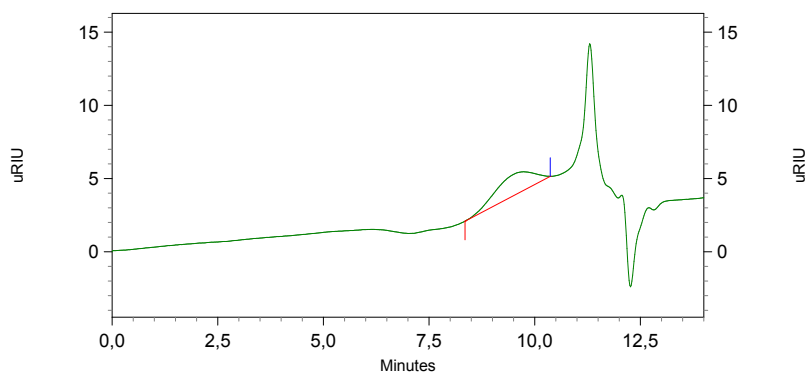
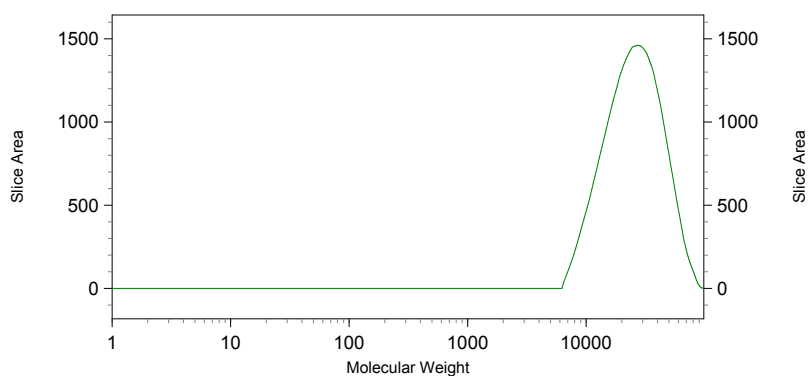


Table S25.
Entry 17.

SEC Summary information

S 2300/S 2400
Processing Start Time(min) = 7,785
Processing Stop Time(min) = 10,383
Number of Slices = 156
Weight Average Molecular Weight = 40889
Number Average Molecular Weight = 29020
Z Average Molecular Weight = 54694
Z+1 Average Molecular Weight = 69081
Polydispersity index = 1,409
Peak Molecular Weight = 27912
Z Average / Weight Average = 1,338
Z+1 Average / Weight Average = 1,689

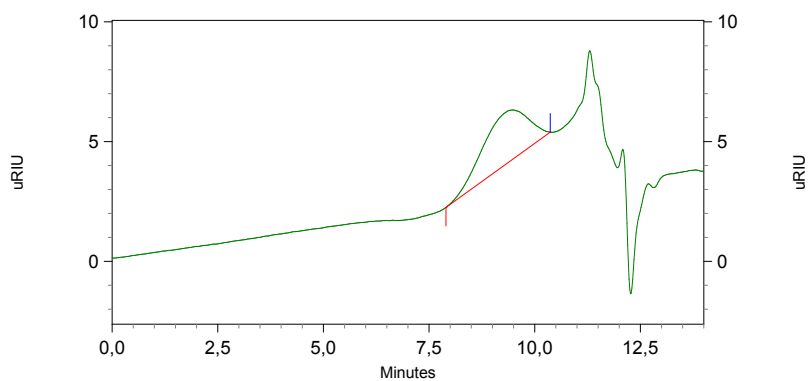
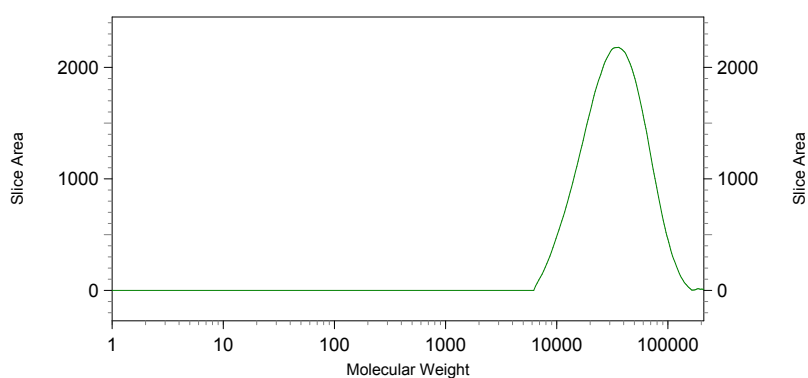


Table S26.
Entry 18.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 7,080
Processing Stop Time (min) = 10,066
Number of Slices = 179
Weight Average Molecular Weight = 108840
Number Average Molecular Weight = 73025
Z Average Molecular Weight = 157564
Z+1 Average Molecular Weight = 218662
Polydispersity index = 1,490
Peak Molecular Weight = 90857
Z Average / Weight Average = 1,448
Z+1 Average / Weight Average = 2,009

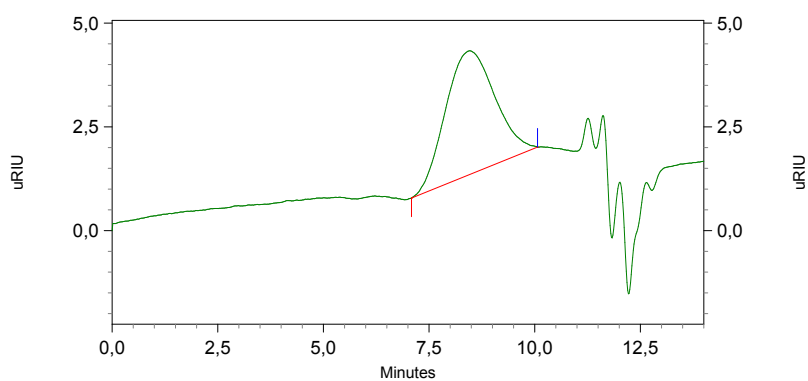
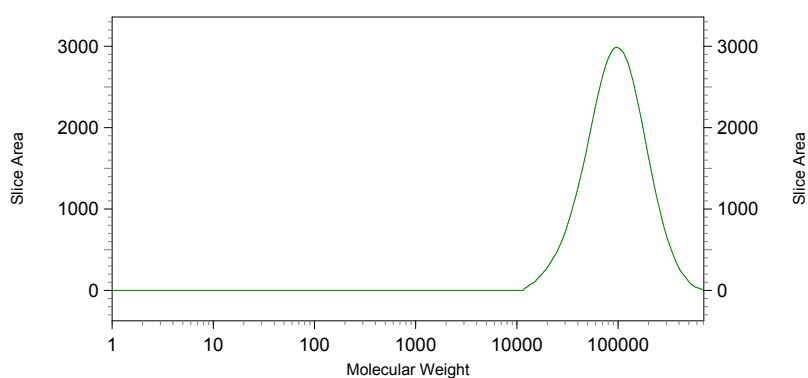
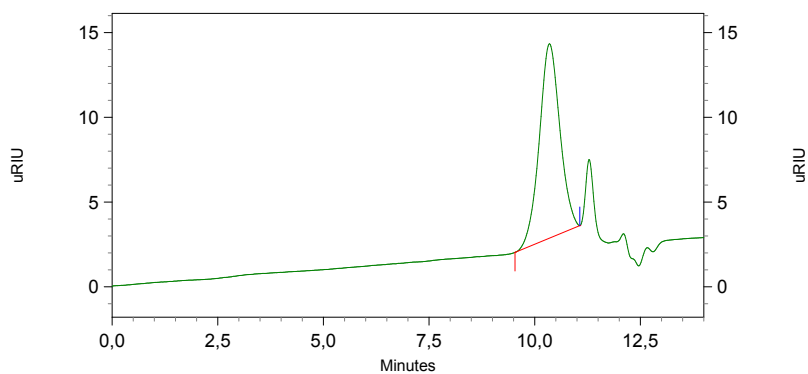
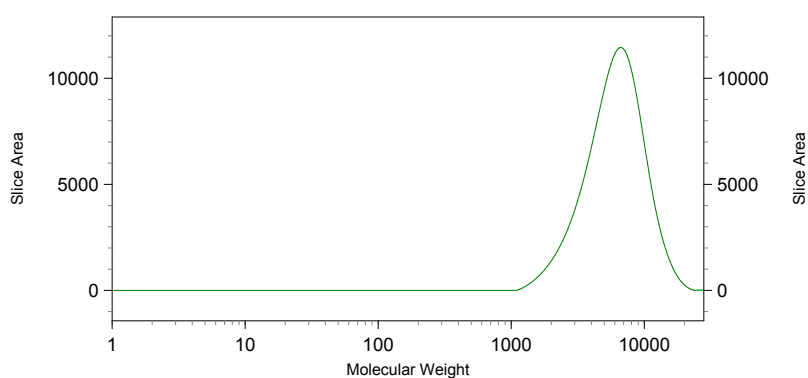


Table S27.
Entry 19.

SEC Summary information

S 2300/S 2400
Processing Start Time (min) = 9,449
Processing Stop Time (min) = 11,063
Number of Slices = 97
Weight Average Molecular Weight = 6921
Number Average Molecular Weight = 5450
Z Average Molecular Weight = 8453
Z+1 Average Molecular Weight = 10009
Polydispersity index = 1,270
Peak Molecular Weight = 6448
Z Average / Weight Average = 1,221
Z+1 Average / Weight Average = 1,446



Example of calculation of Pr PLA (Table 4, Entry 1)

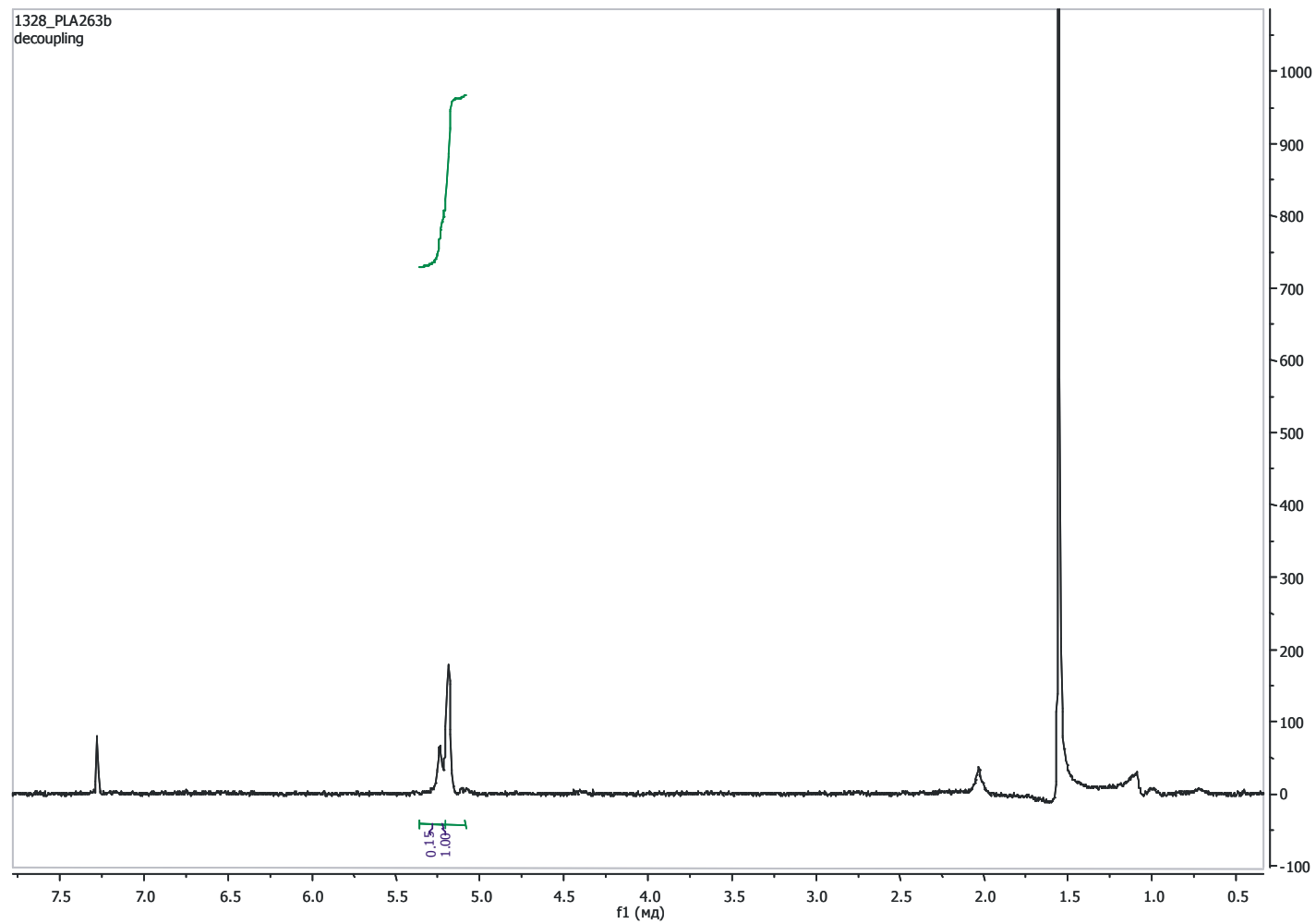


Fig. S9. Proton homo-decoupled ^1H NMR spectra of PLA. $\text{Pr} = ([\text{rnr}] * 2)^{1/2} = (0.15 * 2)^{1/2} = 0.55$

¹H, ¹³C NMR and ³¹P NMR spectra of α-hydroxyphosphonates.

Diethyl hydroxy(3-chlorophenyl)methylphosphonate (7a): NMR (CDCl₃, 20°C, 200 MHz, δ ppm) ¹H: 1.04-1.34 (m, 6H), 3.85-4.22 (m, 4H), 4.99 (d, *J* = 10.9), 7.22-7.36 (m, 2H), 7.37-7.49 (m, 2H). NMR (CDCl₃, 20°C, 50 MHz, δ ppm) ¹³C: 16.35 (d, *J* = 5.5), 63.28 (dd, *J* = 14.2, 7.1 Hz), 70.2 (d, *J* = 159.3 Hz), 128.17-128.61 (m), 133.9 (d, *J* = 3.9 Hz), 135.2 (d, *J* = 2.3 Hz). NMR (CDCl₃, 20°C, 81 MHz, δ ppm) ³¹P: 26.1.

Diethyl hydroxy(4-methylphenyl)methylphosphonate (7b): NMR (CDCl₃, 20°C, 200 MHz, δ ppm) ¹H: 1.18-1.39 (m, 6H), 2.34 (d, 3H), 3.83-4.27 (m, 4H), 4.91 (d, *J* = 10.4), 7.16 (d, *J* = 7.9 Hz, 2H), 7.29-7.45 (m, 2H). NMR (CDCl₃, 20°C, 50 MHz, δ ppm) ¹³C: 16.4 (d, *J* = 5.6), 21.2, 63.1 (m), 70.8 (d, *J* = 159.8 Hz), 127.0 (d, *J* = 5.9 Hz), 129.0 (d, *J* = 2.5 Hz), 133.5 (d, *J* = 2.3 Hz), 137.9 (d, *J* = 3.3 Hz). NMR (CDCl₃, 20°C, 81 MHz, δ ppm) ³¹P: 21.7.

Diethyl hydroxy(4-methoxyphenyl)methylphosphonate (7c): NMR (CDCl₃, 20°C, 200 MHz, δ ppm) ¹H: 1.18-1.28 (m, 6H, CH₃), 3.04 (s, 1H, OH), 3.79 (s, 3H, CH₃), 3.92-4.09 (m, 4H, CH₂), 4.94 (d, 1H, *J* = 10.0 Hz, CH), 6.88 (d, *J* = 8.9 Hz, 2H), 7.40 (dd, *J* = 8.7, 2.0 Hz, 2H). NMR (CDCl₃, 20°C, 50 MHz, δ ppm) ¹³C: 16.4, 63.1 (dd, *J* = 22.6, 7.1), 69.5, 71.2, 113.7, 128.4, 159.6. NMR (CDCl₃, 20°C, 81 MHz, δ ppm) ³¹P: 21.6.

Diethyl hydroxy(phenyl)methylphosphonate (7d): NMR (CDCl₃, 20°C, 200 MHz, δ ppm) ¹H: 1.17-1.30 (m, 6H), 3.71-4.12 (m, 5H, OH, CH₂), 7.26-7.50 (m, 5H). NMR (CDCl₃, 20°C, 50 MHz, δ ppm) ¹³C: 6.51 – 16.19 (m), 63.16 (t, *J* = 7.2 Hz), 69.39, 72.53, 127.05 (d, *J* = 5.8 Hz), 128.14 (d, *J* = 3.1 Hz), 128.30 (d, *J* = 2.5 Hz), 136.47. NMR (CDCl₃, 20°C, 81 MHz, δ ppm) ³¹P: 21.40.

Diethyl 1-hydroxyhexanylphosphonate (7e): NMR (CDCl₃, 20°C, 200 MHz, δ ppm) ¹H: 0.87-0.90 (m, 3H), 1.27-1.83 (m, 14H), 2.78 (s, 1H), 3.78-3.84 (m, 1H), 4.03-4.21 (m, 4H). NMR (CDCl₃, 20°C, 50 MHz, δ ppm) ¹³C: 13.9, 16.5 (d, J = 5.5 Hz), 22.5, 25.9 (d, J = 13.0 Hz), 31.4 (d, J = 7.1 Hz), 62.5 (dd, J = 7.1, 3.9 Hz), 67.9 (d, J = 159.8 Hz). NMR (CDCl₃, 20°C, 81 MHz, δ ppm) ³¹P: 25.6.

Diethyl 1-hydroxypentylphosphonate (7f): NMR (CDCl₃, 20°C, 400 MHz, δ ppm) ¹H: 0.85-0.89 (m, 3H), 1.27-1.36 (m, 8H), 1.43-1.77 (m, 4H), 2.60 (s, 1H), 3.92-3.71 (m, 1H), 4.97-4.26 (m, 4H). NMR (CDCl₃, 20°C, 50 MHz, δ ppm) ¹³C: 13.9, 16.4 (d, J = 5.1 Hz), 22.3, 27.8 (d, J = 13.2 Hz), 31.0, 62.4 (dd, J = 13.7, 7.1 Hz), 67.7 (d, 160.6 Hz). NMR (CDCl₃, 20°C, 162 MHz, δ ppm) ³¹P: 25.6.

Diethyl 1-hydroxy-2-methyl-propylphosphonate (7g): NMR (CDCl₃, 20°C, 400 MHz, δ ppm) ¹H: 1.02 (m, 6H), 1.30 (t, J = 7.1 Hz, 6H), 2.00-2.10 (m, 1H), 2.35 (s, 1H), 3.59-3.62 (m, 1H), 4.17-4.10 (m, 4H) ppm. NMR (CDCl₃, 20°C, 50 MHz, δ ppm) ¹³C: 16.4 (d, J = 5.6 Hz), 17.7 (d, J = 7.7 Hz), 19.8 (d, J = 9.4 Hz), 30.2 (d, J = 2.3 Hz), 62.3 (d, J = 7.2 Hz), 72.9 (d, J = 156.7 Hz). NMR (CDCl₃, 20°C, 162 MHz, δ ppm) ³¹P: 25.2.

Diethyl 1-hydroxybutylphosphonate (7h): NMR (CDCl₃, 20°C, 400 MHz, δ ppm) ¹H: 0.90-0.93 (m, 3H), 1.29-1.45 (m, 6H), 1.57-1.71 (m, 4H), 2.63 (s, 1H), 3.82-3.86 (m, 1H), 4.10-4.15 (m, 4H). NMR (CDCl₃, 20°C, 50 MHz, δ ppm) ¹³C: 13.7 (c.), 16.5 (d, J = 5.3 Hz), 18.9 (d, J = 13.8 Hz), 33.3, 62.5 (dd, J = 12.7, 7.1 Hz), 66.7. NMR (CDCl₃, 20°C, 162 MHz, δ ppm) ³¹P: 25.7.

Diethyl 2-hydroxy-4-phenylbut-3-en-2-ylphosphonate (7i): NMR (CDCl₃, 20°C, 400 MHz, δ ppm) ¹H: 1.26-1.35 (m, 6H), 1.60 (d, *J* = 15.7 Hz, 3H), 3.70 (s, 1H), 4.08-4.19 (m, 4H), 6.35 (dd, *J* = 16.0, 4.2 Hz, 1H), 6.77 (dd, *J* = 16.0, 5.0 Hz, 1H), 7.15-7.65 (m, 5H).