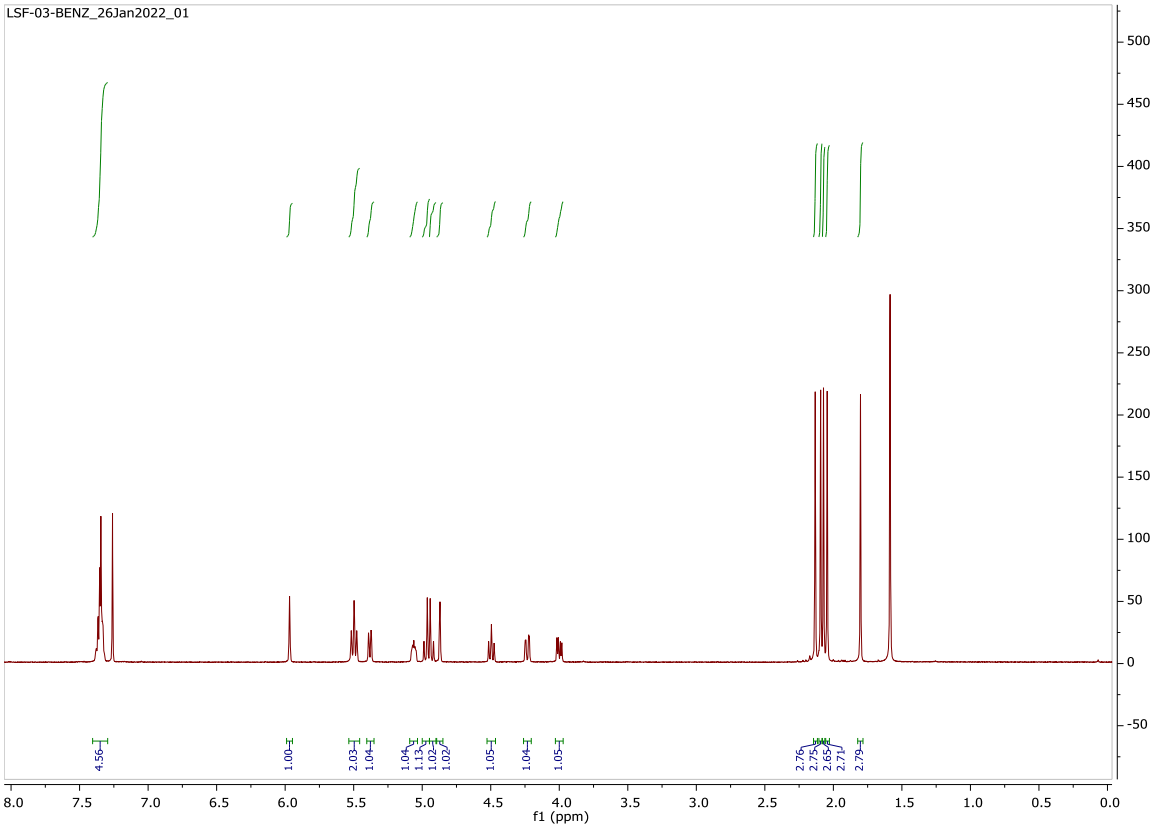
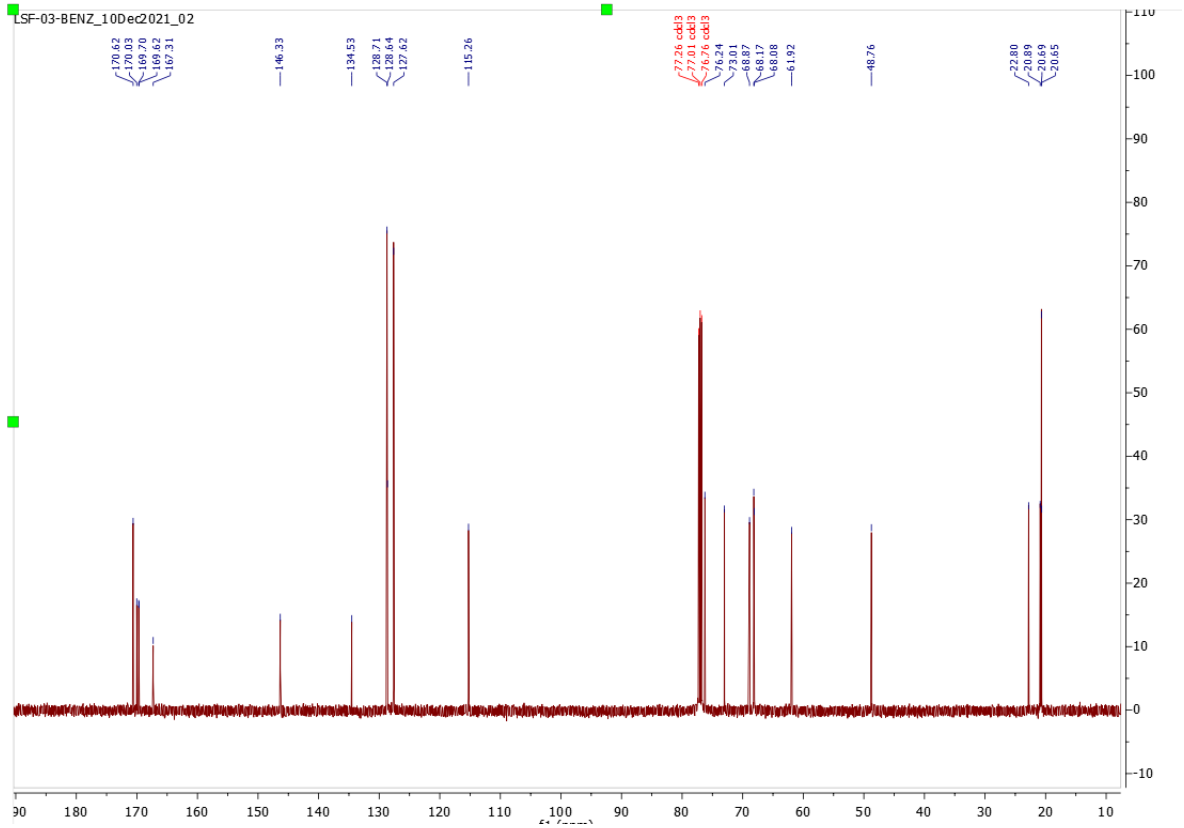
Supporting Information

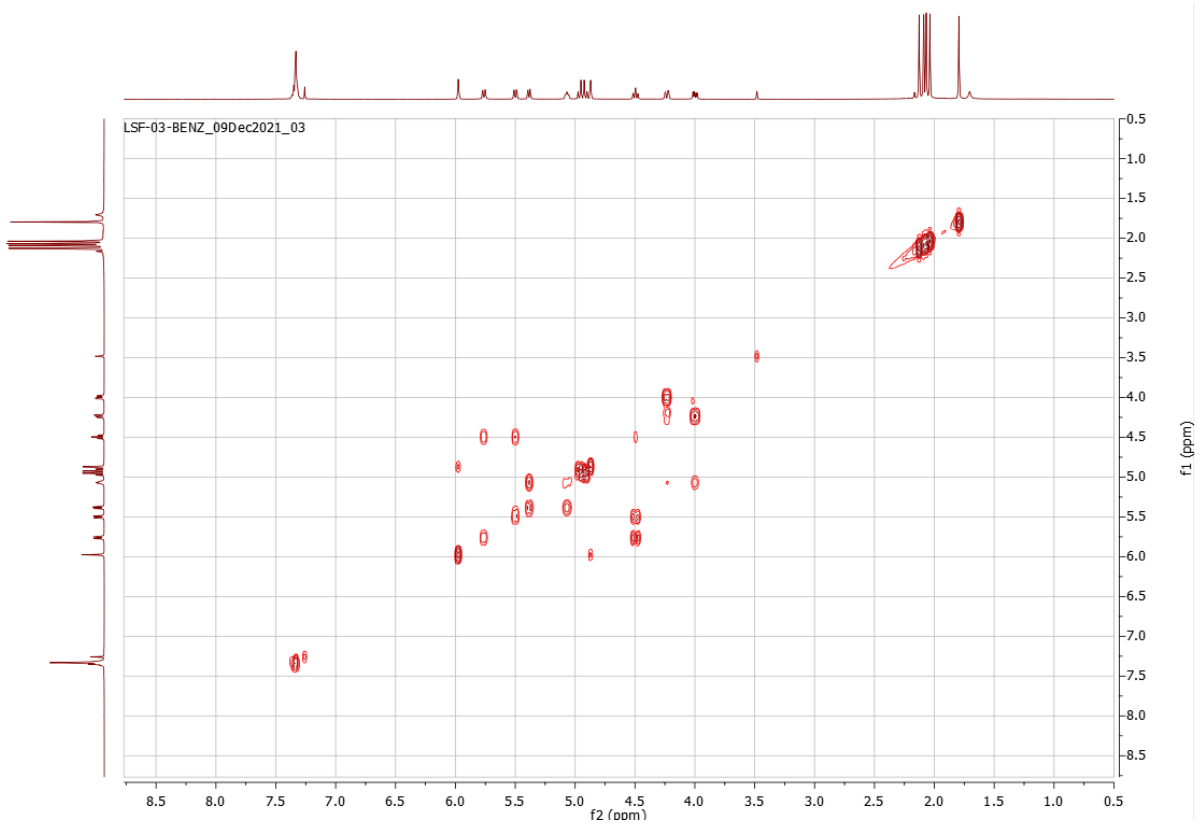
^{1}H NMR spectrum for compound **4**



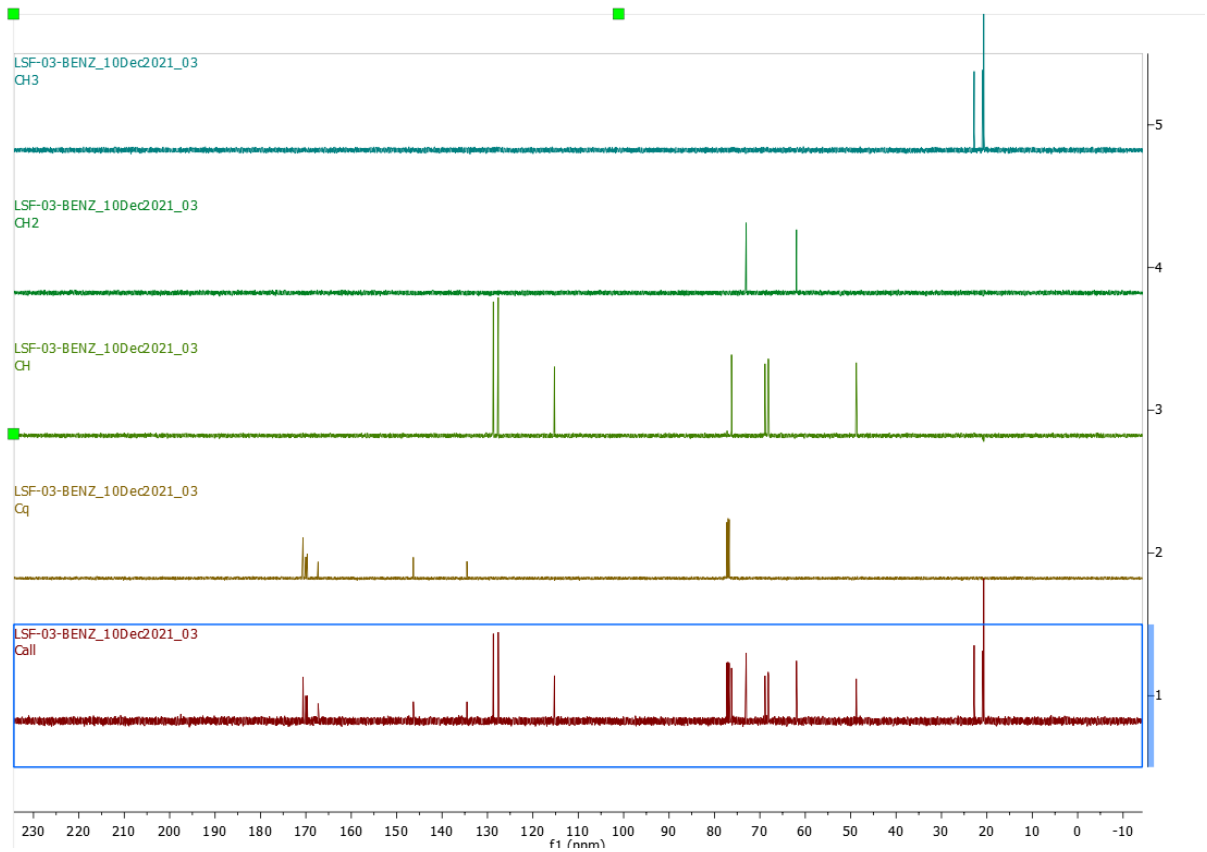
^{13}C NMR spectrum for compound **4**



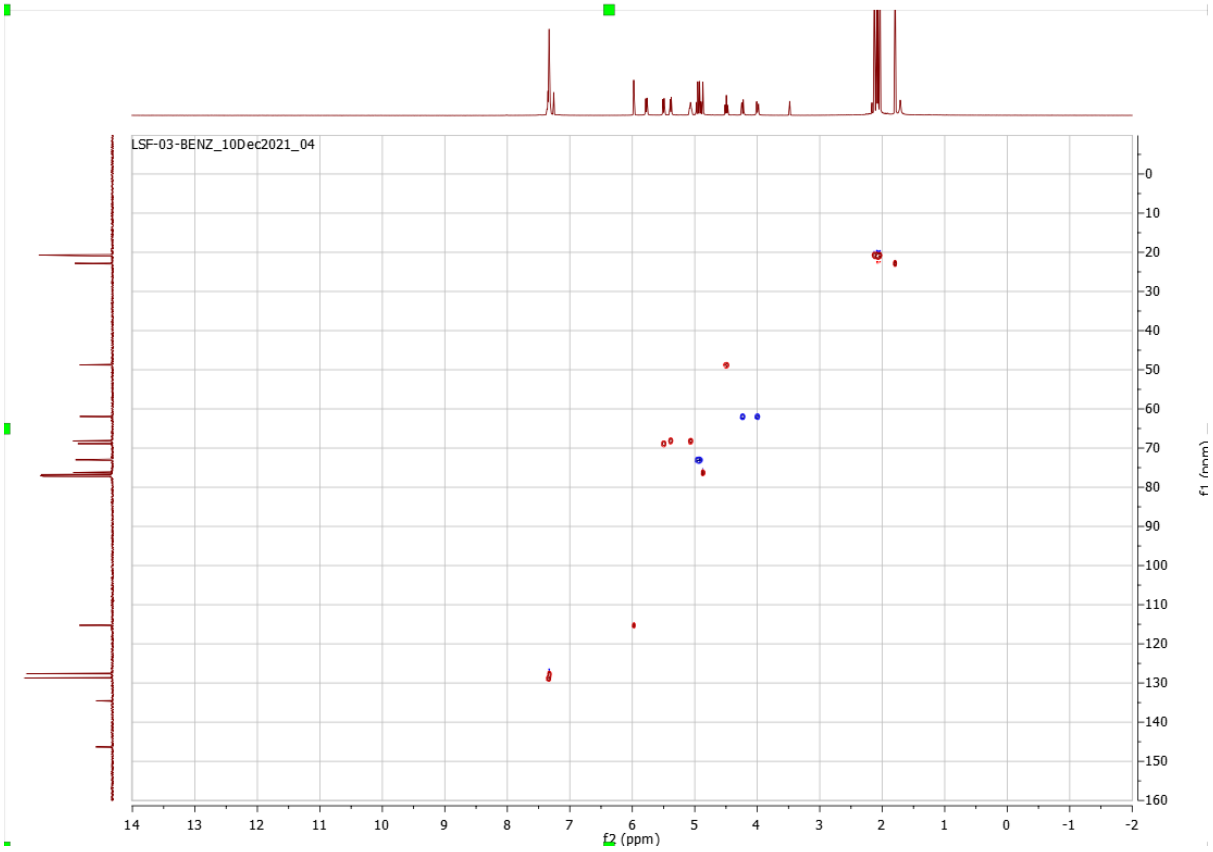
gCOSY spectrum for compound **4**



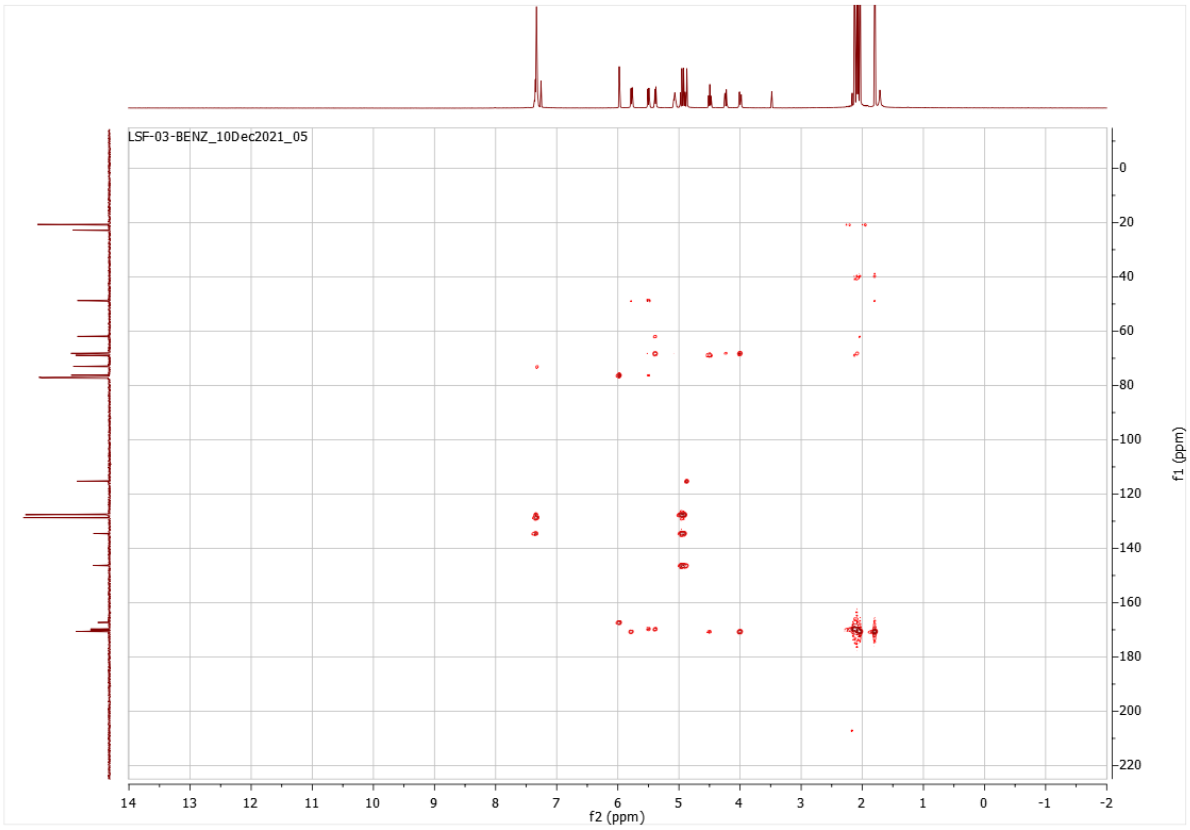
DEPT spectrum for compound **4**



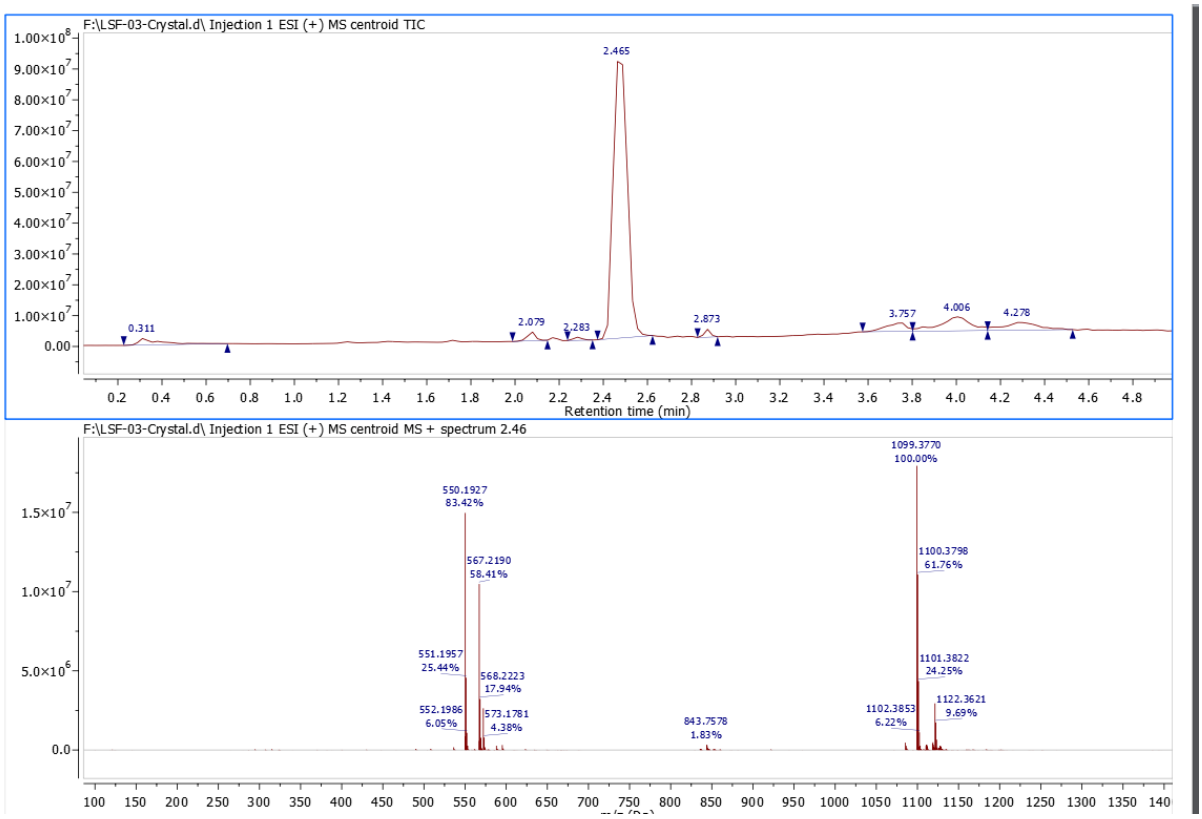
gHSQC spectrum for compound **4**



gHMBC spectrum for compound **4**



LC-MS analysis for compound **4**



Crystallography data for compound **4:**

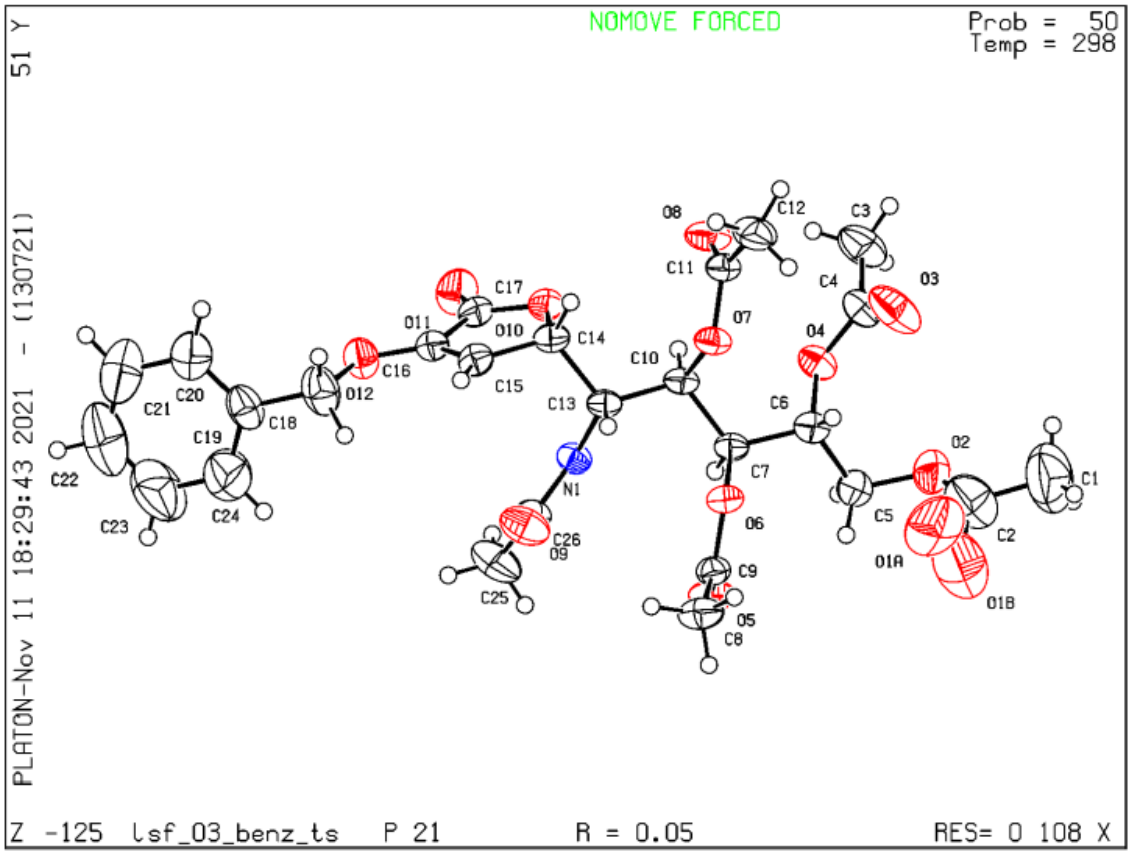


Table S1. Crystal data and structure refinement for lsf_03_benz_ts.

Identification code	lsf_03_benz_ts	
Empirical formula	C26 H31 N O12	
Formula weight	549.52	
Temperature	298.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 10.1989(5) Å	α= 90°.
	b = 8.7455(4) Å	β= 99.068(5)°.
	c = 15.8721(9) Å	γ = 90°.
Volume	1398.01(12) $Å^3$	
Z	2	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	0.104 mm^{-1}	
F(000)	580	
Crystal size	0.40 x 0.30 x 0.10 mm^3	
Theta range for data collection	3.470 to 29.275°.	
Index ranges	-13<=h<=13, -11<=k<=11, -21<=l<=21	
Reflections collected	15990	
Independent reflections	15990 [R(int) = 0.0477]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.78362	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15990 / 292 / 368	
Goodness-of-fit on F^2	0.795	
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.1076	
R indices (all data)	R1 = 0.0959, wR2 = 0.1185	
Absolute structure parameter	-0.1(6)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.201 and -0.216 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for lsf_03_benz_ts. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	2342(3)	5081(3)	5445(2)	34(1)
O(1A)	-578(12)	1903(13)	1712(10)	113(4)
O(1B)	-1460(20)	1498(15)	1648(9)	169(7)
O(2)	-1478(3)	4068(4)	1764(2)	71(1)
O(3)	1122(4)	5963(4)	1347(2)	81(1)
O(4)	337(2)	6345(3)	2568(2)	44(1)
O(5)	-137(2)	2476(3)	4530(2)	51(1)
O(6)	1556(2)	3046(2)	3837(1)	36(1)
O(7)	3195(2)	5443(3)	3298(1)	37(1)
O(8)	3238(3)	7973(3)	3079(2)	55(1)
O(9)	3449(3)	3025(3)	6031(2)	62(1)
O(10)	3642(2)	7888(3)	5172(2)	41(1)
O(11)	3440(3)	9452(3)	6262(2)	61(1)
O(12)	5156(3)	7388(3)	7309(2)	49(1)
C(1)	-1962(8)	2960(10)	416(4)	135(3)
C(2)	-1400(7)	2819(7)	1340(4)	92(2)
C(3)	486(5)	8473(5)	1692(3)	72(1)
C(4)	691(4)	6791(5)	1824(3)	48(1)
C(5)	-925(4)	4074(5)	2650(3)	61(1)
C(6)	459(4)	4739(4)	2782(2)	41(1)
C(7)	1120(3)	4614(4)	3700(2)	32(1)
C(8)	1543(4)	600(4)	4429(3)	52(1)
C(9)	872(3)	2107(4)	4282(2)	37(1)
C(10)	2347(3)	5644(4)	3933(2)	32(1)
C(11)	3590(3)	6717(4)	2912(2)	40(1)
C(12)	4476(4)	6325(5)	2285(3)	59(1)
C(13)	3172(3)	5251(4)	4792(2)	32(1)
C(14)	4276(3)	6426(4)	5076(2)	36(1)
C(15)	5045(3)	6085(4)	5930(2)	37(1)
C(16)	4798(3)	7172(4)	6466(2)	37(1)
C(17)	3902(4)	8311(4)	6005(2)	40(1)
C(18)	6040(5)	6268(5)	7734(3)	65(1)
C(19)	6244(4)	6579(5)	8669(3)	56(1)

C(20)	7181(6)	7582(8)	9031(3)	98(2)
C(21)	7342(8)	7882(11)	9898(5)	130(3)
C(22)	6612(9)	7148(11)	10400(4)	124(3)
C(23)	5650(7)	6179(10)	10045(4)	122(3)
C(24)	5470(6)	5896(7)	9190(4)	94(2)
C(25)	1781(5)	4072(6)	6759(3)	73(2)
C(26)	2595(4)	3993(4)	6049(2)	42(1)

Table S3. Bond lengths [Å] and angles [°] for lsf_03_benz_ts.

N(1)-C(26)	1.346(4)
N(1)-C(13)	1.445(4)
N(1)-H(1)	0.8600
O(1A)-C(2)	1.240(14)
O(1B)-C(2)	1.260(14)
O(2)-C(2)	1.292(6)
O(2)-C(5)	1.431(5)
O(3)-C(4)	1.181(4)
O(4)-C(4)	1.346(4)
O(4)-C(6)	1.446(4)
O(5)-C(9)	1.202(4)
O(6)-C(9)	1.348(4)
O(6)-C(7)	1.448(4)
O(7)-C(11)	1.363(4)
O(7)-C(10)	1.439(4)
O(8)-C(11)	1.199(4)
O(9)-C(26)	1.219(4)
O(10)-C(17)	1.358(4)
O(10)-C(14)	1.452(4)
O(11)-C(17)	1.202(4)
O(12)-C(16)	1.344(4)
O(12)-C(18)	1.427(5)
C(1)-C(2)	1.494(8)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(3)-C(4)	1.496(6)
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(5)-C(6)	1.511(5)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.509(5)
C(6)-H(6)	0.9800
C(7)-C(10)	1.539(5)

C(7)-H(7)	0.9800
C(8)-C(9)	1.486(5)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(10)-C(13)	1.524(5)
C(10)-H(10)	0.9800
C(11)-C(12)	1.486(5)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.539(5)
C(13)-H(13)	0.9800
C(14)-C(15)	1.486(5)
C(14)-H(14)	0.9800
C(15)-C(16)	1.326(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.467(5)
C(18)-C(19)	1.491(6)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-C(20)	1.356(7)
C(19)-C(24)	1.367(7)
C(20)-C(21)	1.386(8)
C(20)-H(20)	0.9300
C(21)-C(22)	1.336(10)
C(21)-H(21)	0.9300
C(22)-C(23)	1.350(11)
C(22)-H(22)	0.9300
C(23)-C(24)	1.363(8)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-C(26)	1.503(5)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600

C(26)-N(1)-C(13)	121.0(3)

C(26)-N(1)-H(1)	119.5
C(13)-N(1)-H(1)	119.5
C(2)-O(2)-C(5)	117.9(4)
C(4)-O(4)-C(6)	117.6(3)
C(9)-O(6)-C(7)	118.9(2)
C(11)-O(7)-C(10)	118.0(3)
C(17)-O(10)-C(14)	108.7(3)
C(16)-O(12)-C(18)	115.3(3)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(1A)-C(2)-O(2)	113.0(8)
O(1B)-C(2)-O(2)	124.2(8)
O(1A)-C(2)-C(1)	130.3(9)
O(1B)-C(2)-C(1)	114.9(9)
O(2)-C(2)-C(1)	113.3(6)
C(4)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
O(3)-C(4)-O(4)	124.3(4)
O(3)-C(4)-C(3)	124.8(4)
O(4)-C(4)-C(3)	110.9(4)
O(2)-C(5)-C(6)	110.7(3)
O(2)-C(5)-H(5A)	109.5
C(6)-C(5)-H(5A)	109.5
O(2)-C(5)-H(5B)	109.5
C(6)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	108.1
O(4)-C(6)-C(7)	107.8(3)
O(4)-C(6)-C(5)	107.3(3)
C(7)-C(6)-C(5)	111.8(3)
O(4)-C(6)-H(6)	109.9

C(7)-C(6)-H(6)	109.9
C(5)-C(6)-H(6)	109.9
O(6)-C(7)-C(6)	107.1(3)
O(6)-C(7)-C(10)	107.4(2)
C(6)-C(7)-C(10)	114.4(3)
O(6)-C(7)-H(7)	109.3
C(6)-C(7)-H(7)	109.3
C(10)-C(7)-H(7)	109.3
C(9)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(9)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(5)-C(9)-O(6)	123.3(3)
O(5)-C(9)-C(8)	125.7(3)
O(6)-C(9)-C(8)	111.0(3)
O(7)-C(10)-C(13)	107.0(2)
O(7)-C(10)-C(7)	108.4(3)
C(13)-C(10)-C(7)	113.4(3)
O(7)-C(10)-H(10)	109.3
C(13)-C(10)-H(10)	109.3
C(7)-C(10)-H(10)	109.3
O(8)-C(11)-O(7)	121.9(3)
O(8)-C(11)-C(12)	126.5(3)
O(7)-C(11)-C(12)	111.5(3)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(1)-C(13)-C(10)	111.2(3)
N(1)-C(13)-C(14)	110.1(3)
C(10)-C(13)-C(14)	112.8(3)
N(1)-C(13)-H(13)	107.5
C(10)-C(13)-H(13)	107.5
C(14)-C(13)-H(13)	107.5

O(10)-C(14)-C(15)	105.1(3)
O(10)-C(14)-C(13)	107.5(2)
C(15)-C(14)-C(13)	112.9(3)
O(10)-C(14)-H(14)	110.4
C(15)-C(14)-H(14)	110.4
C(13)-C(14)-H(14)	110.4
C(16)-C(15)-C(14)	108.4(3)
C(16)-C(15)-H(15)	125.8
C(14)-C(15)-H(15)	125.8
C(15)-C(16)-O(12)	133.6(3)
C(15)-C(16)-C(17)	109.5(3)
O(12)-C(16)-C(17)	116.9(3)
O(11)-C(17)-O(10)	122.0(3)
O(11)-C(17)-C(16)	129.9(4)
O(10)-C(17)-C(16)	108.1(3)
O(12)-C(18)-C(19)	108.9(3)
O(12)-C(18)-H(18A)	109.9
C(19)-C(18)-H(18A)	109.9
O(12)-C(18)-H(18B)	109.9
C(19)-C(18)-H(18B)	109.9
H(18A)-C(18)-H(18B)	108.3
C(20)-C(19)-C(24)	117.5(5)
C(20)-C(19)-C(18)	121.2(4)
C(24)-C(19)-C(18)	121.3(5)
C(19)-C(20)-C(21)	120.5(6)
C(19)-C(20)-H(20)	119.7
C(21)-C(20)-H(20)	119.7
C(22)-C(21)-C(20)	120.7(7)
C(22)-C(21)-H(21)	119.7
C(20)-C(21)-H(21)	119.7
C(21)-C(22)-C(23)	119.3(7)
C(21)-C(22)-H(22)	120.3
C(23)-C(22)-H(22)	120.3
C(22)-C(23)-C(24)	120.3(7)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(23)-C(24)-C(19)	121.5(6)
C(23)-C(24)-H(24)	119.3

C(19)-C(24)-H(24)	119.3
C(26)-C(25)-H(25A)	109.5
C(26)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(26)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(9)-C(26)-N(1)	122.1(3)
O(9)-C(26)-C(25)	122.1(4)
N(1)-C(26)-C(25)	115.8(4)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for lsf_03_benz_ts. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	29(2)	37(2)	37(2)	6(1)	11(1)	3(1)
O(1A)	138(8)	48(6)	146(10)	-23(6)	-2(8)	14(6)
O(1B)	330(20)	61(7)	96(8)	-3(6)	-15(13)	7(10)
O(2)	79(2)	67(2)	58(2)	8(2)	-18(2)	-14(2)
O(3)	127(3)	70(2)	54(2)	16(2)	42(2)	25(2)
O(4)	49(2)	41(2)	43(1)	10(1)	12(1)	8(1)
O(5)	44(2)	43(2)	72(2)	9(1)	29(1)	-3(1)
O(6)	35(1)	30(1)	46(1)	3(1)	12(1)	-4(1)
O(7)	42(1)	32(1)	41(1)	3(1)	18(1)	-4(1)
O(8)	70(2)	34(2)	65(2)	11(1)	22(2)	-7(1)
O(9)	74(2)	44(2)	71(2)	20(2)	22(2)	17(2)
O(10)	48(1)	31(1)	43(2)	4(1)	3(1)	-2(1)
O(11)	76(2)	34(2)	68(2)	-8(1)	-3(2)	14(1)
O(12)	62(2)	39(1)	42(2)	-1(1)	2(1)	10(1)
C(1)	182(7)	144(6)	72(4)	-19(4)	1(4)	1(6)
C(2)	129(5)	72(4)	77(4)	5(3)	26(3)	26(4)
C(3)	93(4)	55(3)	67(3)	25(2)	15(3)	15(2)
C(4)	54(2)	50(2)	41(2)	12(2)	8(2)	9(2)
C(5)	55(3)	71(3)	51(3)	15(2)	-7(2)	-21(2)
C(6)	44(2)	37(2)	43(2)	4(2)	10(2)	-2(2)
C(7)	31(2)	26(2)	40(2)	4(2)	9(2)	1(1)
C(8)	44(2)	38(2)	75(3)	12(2)	12(2)	-2(2)
C(9)	33(2)	36(2)	42(2)	4(2)	7(2)	-6(2)
C(10)	36(2)	24(2)	38(2)	3(2)	14(2)	0(1)
C(11)	39(2)	40(2)	41(2)	8(2)	8(2)	-10(2)
C(12)	66(3)	63(3)	53(3)	8(2)	27(2)	-13(2)
C(13)	32(2)	28(2)	39(2)	2(2)	14(2)	0(1)
C(14)	32(2)	35(2)	44(2)	3(2)	11(2)	-3(2)
C(15)	30(2)	38(2)	44(2)	0(2)	7(2)	1(2)
C(16)	40(2)	33(2)	38(2)	1(2)	7(2)	-4(2)
C(17)	44(2)	31(2)	44(2)	0(2)	5(2)	-6(2)
C(18)	81(3)	58(3)	51(3)	2(2)	-4(2)	24(2)
C(19)	67(3)	56(3)	44(2)	7(2)	3(2)	16(2)

C(20)	106(4)	122(5)	63(3)	1(3)	0(3)	-41(4)
C(21)	144(6)	143(7)	89(5)	-23(5)	-25(4)	-30(5)
C(22)	155(7)	153(7)	60(4)	-12(4)	4(4)	38(6)
C(23)	135(6)	167(8)	73(4)	11(5)	44(4)	2(5)
C(24)	96(4)	114(5)	74(4)	-3(3)	18(3)	-16(4)
C(25)	80(3)	86(4)	60(3)	25(3)	33(3)	8(3)
C(26)	45(2)	39(2)	42(2)	8(2)	9(2)	-5(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for lsf_03_benz_ts.

	x	y	z	U(eq)
H(1)	1677	5684	5448	44
H(1A)	-2912	3034	353	175
H(1B)	-1724	2076	115	175
H(1C)	-1613	3860	186	175
H(3A)	932	9014	2181	93
H(3B)	-447	8698	1617	93
H(3C)	840	8786	1193	93
H(5A)	-894	3036	2869	79
H(5B)	-1485	4673	2964	79
H(6)	1000	4223	2410	53
H(7)	472	4852	4075	42
H(8A)	2271	684	4891	68
H(8B)	1870	288	3921	68
H(8C)	921	-144	4570	68
H(10)	2063	6714	3937	41
H(12A)	4193	5377	2009	77
H(12B)	5372	6222	2575	77
H(12C)	4437	7121	1866	77
H(13)	3600	4263	4731	42
H(14)	4872	6501	4650	47
H(15)	5604	5251	6066	48
H(18A)	6883	6311	7526	84
H(18B)	5668	5254	7621	84
H(20)	7720	8072	8694	128
H(21)	7964	8603	10134	169
H(22)	6766	7302	10987	162
H(23)	5109	5703	10386	159
H(24)	4805	5223	8956	122
H(25A)	1052	3369	6646	95
H(25B)	1445	5091	6797	95
H(25C)	2326	3807	7289	95

Table S6. Hydrogen bonds for lsf_03_benz_ts [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(5)#1	0.86	2.22	3.078(4)	172.9
C(5)-H(5B)...O(11)#2	0.97	2.51	3.327(5)	142.0
C(8)-H(8A)...O(11)#3	0.96	2.55	3.382(5)	145.1
C(12)-H(12B)...O(11)#4	0.96	2.56	3.313(5)	135.1
C(14)-H(14)...O(9)#5	0.98	2.54	3.421(4)	149.5
C(15)-H(15)...O(8)#4	0.93	2.59	3.475(5)	159.7
C(18)-H(18B)...O(8)#4	0.97	2.62	3.288(5)	126.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z+1 #2 -x,y-1/2,-z+1 #3 x,y-1,z

#4 -x+1,y-1/2,-z+1 #5 -x+1,y+1/2,-z+1