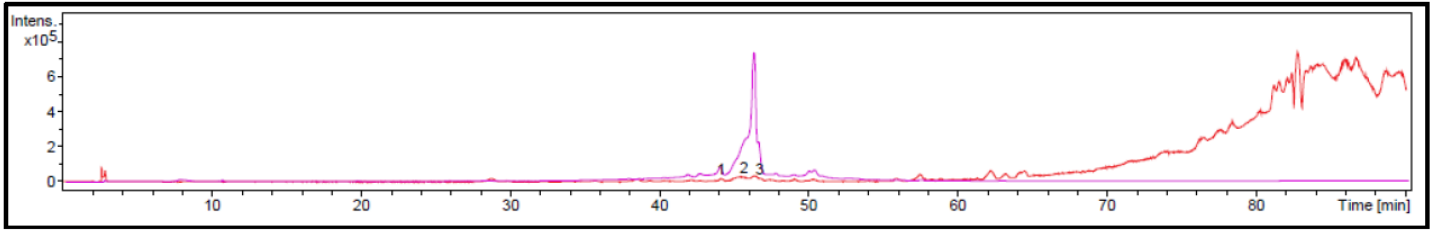
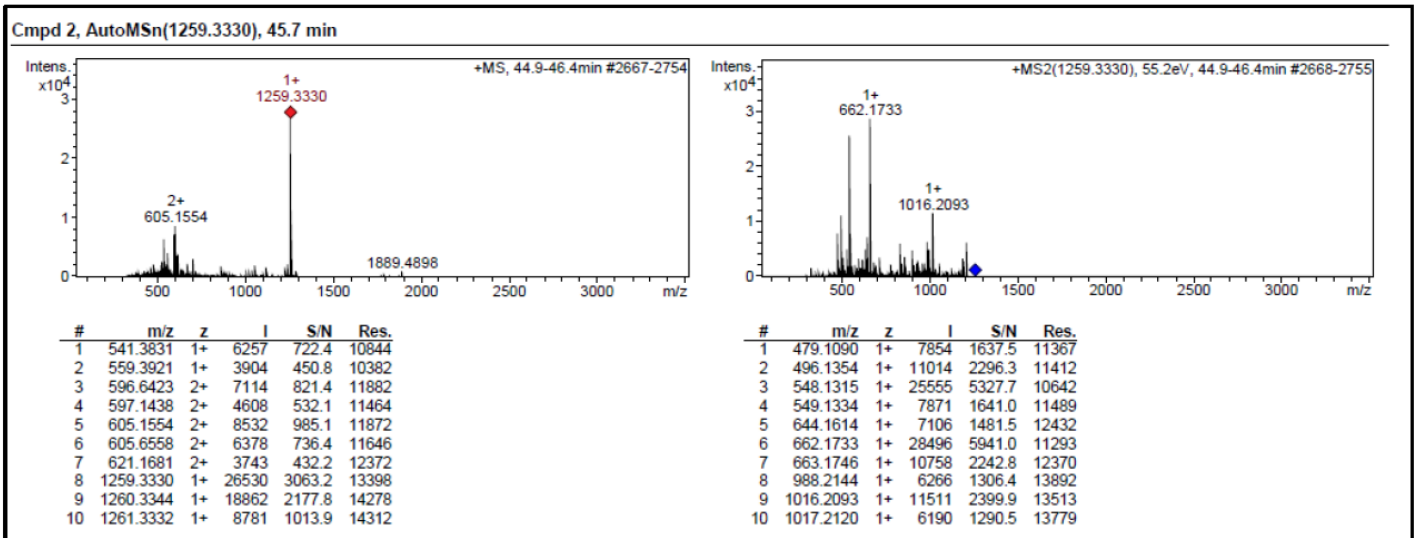


HR-LC/MS-MS data of SKC3 (positive mode)



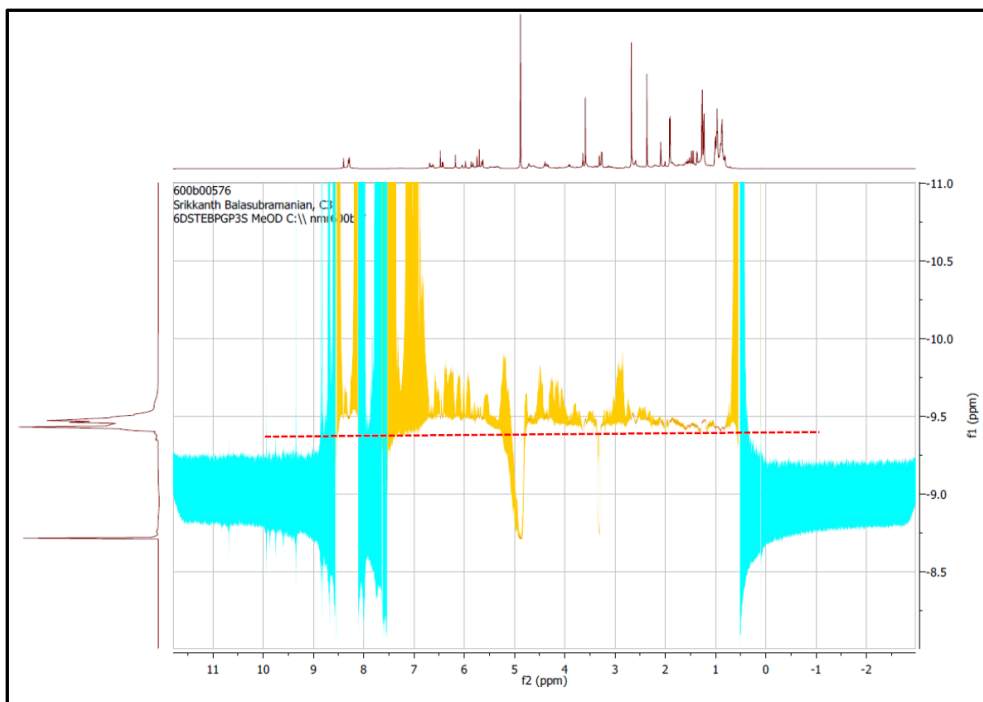
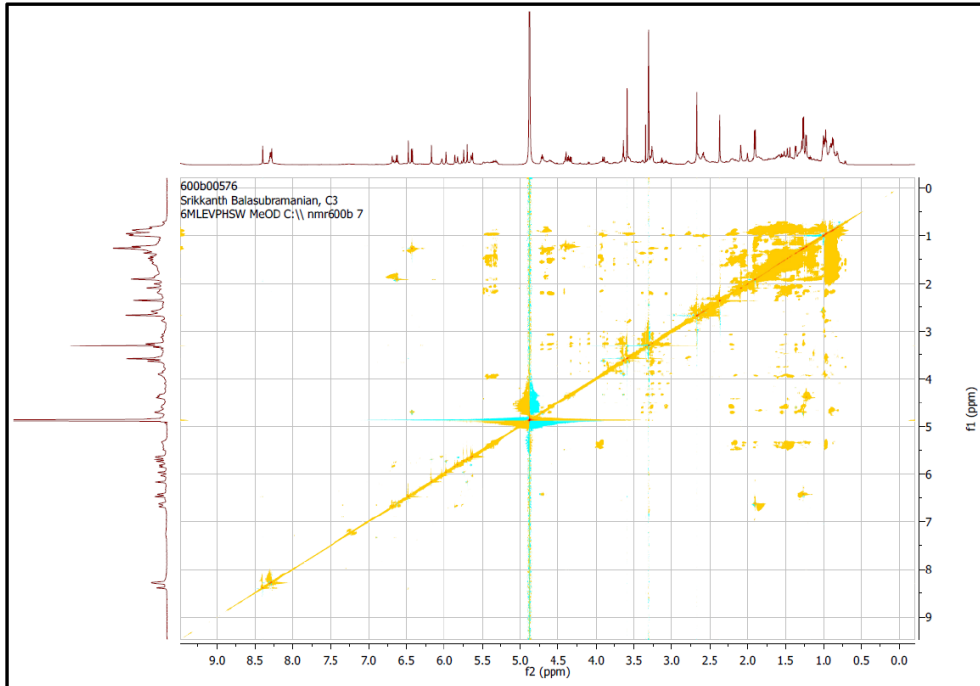
Major mass 1258.3 Da



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
1259.333020	1	C64H55N6O22	11.75	1259.336394	3.4	2.7	21.3	40.5	even		ok	M+H
	2	C63H59N2O26	38.53	1259.335056	2.0	1.6	22.5	35.5	even		ok	M+H
	3	C65H180N3O16	18.99	1259.335813	2.8	2.2	25.5	-22.5	even		ok	M+H
	4	C61H47N16O16	35.84	1259.335046	2.0	1.6	26.1	46.5	even		ok	M+H
	5	C60H51N12O20	81.12	1259.333709	0.7	0.5	27.7	41.5	even		ok	M+H
	6	C62H43N20O12	9.97	1259.336383	3.4	2.7	28.9	51.5	even		ok	M+H
	7	C61H176N9O14	100.00	1259.333128	0.1	0.1	30.2	-21.5	even		ok	M+H
	8	C62H172N13O10	48.90	1259.334465	1.4	1.1	30.4	-16.5	even		ok	M+H
	9	C58H39N26O10	74.20	1259.333698	0.7	0.5	31.6	52.5	even		ok	M+H
	10	C59H55N8O24	72.72	1259.332371	-0.6	-0.5	33.0	36.5	even		ok	M+H
	11	C57H43N22O14	71.68	1259.332361	-0.7	-0.5	33.3	47.5	even		ok	M+H
	12	C59H35N30O6	30.18	1259.335035	2.0	1.6	33.5	57.5	even		ok	M+H
	13	C60H180N5O18	51.52	1259.331790	-1.2	-1.0	33.7	-26.5	even		ok	M+H
	14	C70H55N2O21	5.26	1259.329183	-3.8	-3.0	33.8	44.5	even		ok	M+H
	15	C63H168N17O6	15.48	1259.335803	2.8	2.2	34.3	-11.5	even		ok	M+H
	16	C59H164N23O4	87.08	1259.333117	0.1	0.1	35.8	-10.5	even		ok	M+H
	17	C58H168N19O8	48.16	1259.331780	-1.2	-1.0	36.1	-15.5	even		ok	M+H
	18	C56H47N18O18	27.07	1259.331023	-2.0	-1.6	38.2	42.5	even		ok	M+H
	19	C55H31N36O4	62.15	1259.332350	-0.7	-0.5	38.6	58.5	even		ok	M+H

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule	Adduct
20	C60H31N34O2	7.88	1259.336373	3.4	2.7	38.6	62.5	even	ok	M+H	
21	C60H160N27	39.61	1259.334455	1.4	1.1	38.8	-5.5	even	ok	M+H	
22	C56H27N40	59.99	1259.333687	0.7	0.5	39.9	63.5	even	ok	M+H	
23	C58H59N40O28	25.63	1259.331034	-2.0	-1.6	40.5	31.5	even	ok	M+H	
24	C64H164N21O2	3.11	1259.337140	4.1	3.3	41.0	-6.5	even	ok	M+H	
25	C55H160N29O2	14.91	1259.330432	-2.6	-2.1	42.3	-9.5	even	ok	M+H	
26	C68H43N16O11	3.96	1259.329173	-3.8	-3.1	43.9	55.5	even	ok	M+H	
27	C71H51N6O17	15.29	1259.330521	-2.5	-2.0	44.1	49.5	even	ok	M+H	
28	C55H51N14O22	6.70	1259.329686	-3.3	-2.6	45.2	37.5	even	ok	M+H	
29	C57H63O32	6.00	1259.329696	-3.3	-2.6	49.2	26.5	even	ok	M+H	
30	C69H39N20O7	11.12	1259.330510	-2.5	-2.0	54.3	60.5	even	ok	M+H	
31	C66H31N30O	2.82	1259.329162	-3.9	-3.1	54.7	66.5	even	ok	M+H	
32	C72H47N10O13	29.24	1259.331858	-1.2	-0.9	54.9	54.5	even	ok	M+H	
33	C70H164N17O	5.47	1259.329929	-3.1	-2.5	59.5	-2.5	even	ok	M+H	
34	C70H35N24O3	20.52	1259.331848	-1.2	-0.9	65.2	65.5	even	ok	M+H	
35	C73H43N14O9	33.20	1259.333195	0.2	0.1	66.0	59.5	even	ok	M+H	
36	C72H176N3O11	4.22	1259.329940	-3.1	-2.4	67.3	-13.5	even	ok	M+H	
37	C76H51N4O15	15.04	1259.334543	1.5	1.2	67.6	53.5	even	ok	M+H	
38	C74H168N11O3	25.20	1259.332615	-0.4	-0.3	70.8	-3.5	even	ok	M+H	
39	C73H172N7O7	9.45	1259.331277	-1.7	-1.4	76.0	-8.5	even	ok	M+H	
40	C74H39N18O5	10.45	1259.334533	1.5	1.2	77.4	64.5	even	ok	M+H	
41	C75H55O19	20.64	1259.333206	0.2	0.1	78.5	48.5	even	ok	M+H	
42	C77H47N8O11	3.32	1259.335881	2.9	2.3	79.1	58.5	even	ok	M+H	
43	C75H35N22O	2.22	1259.335870	2.9	2.3	89.0	69.5	even	ok	M+H	
44	C77H176NO9	9.06	1259.333963	0.9	0.7	89.2	-9.5	even	ok	M+H	
45	C78H172N5O5	2.30	1259.335300	2.3	1.8	99.2	-4.5	even	ok	M+H	
46	C79H168N9O	0.38	1259.336637	3.6	2.9	109.7	0.5	even	ok	M+H	
47	C84H43N8O6	0.42	1259.330008	-3.0	-2.4	119.9	67.5	even	ok	M+H	
48	C85H39N12O2	0.64	1259.331345	-1.7	-1.3	132.0	72.5	even	ok	M+H	
49	C85H168N5	0.08	1259.329427	-3.6	-2.9	138.9	4.5	even	ok	M+H	
50	C88H47N2O8	0.39	1259.332693	-0.3	-0.3	152.2	66.5	even	ok	M+H	
51	C90H39N10	0.10	1259.335368	2.3	1.9	152.7	76.5	even	ok	M+H	
52	C89H43N6O4	0.12	1259.334030	1.0	0.8	163.7	71.5	even	ok	M+H	
53	C93H47O6	0.01	1259.336716	3.7	2.9	173.8	70.5	even	ok	M+H	
54	C100H43O	0.01	1259.330842	-2.2	-1.7	186.3	79.5	even	ok	M+H	

DOSY spectra of SKC3

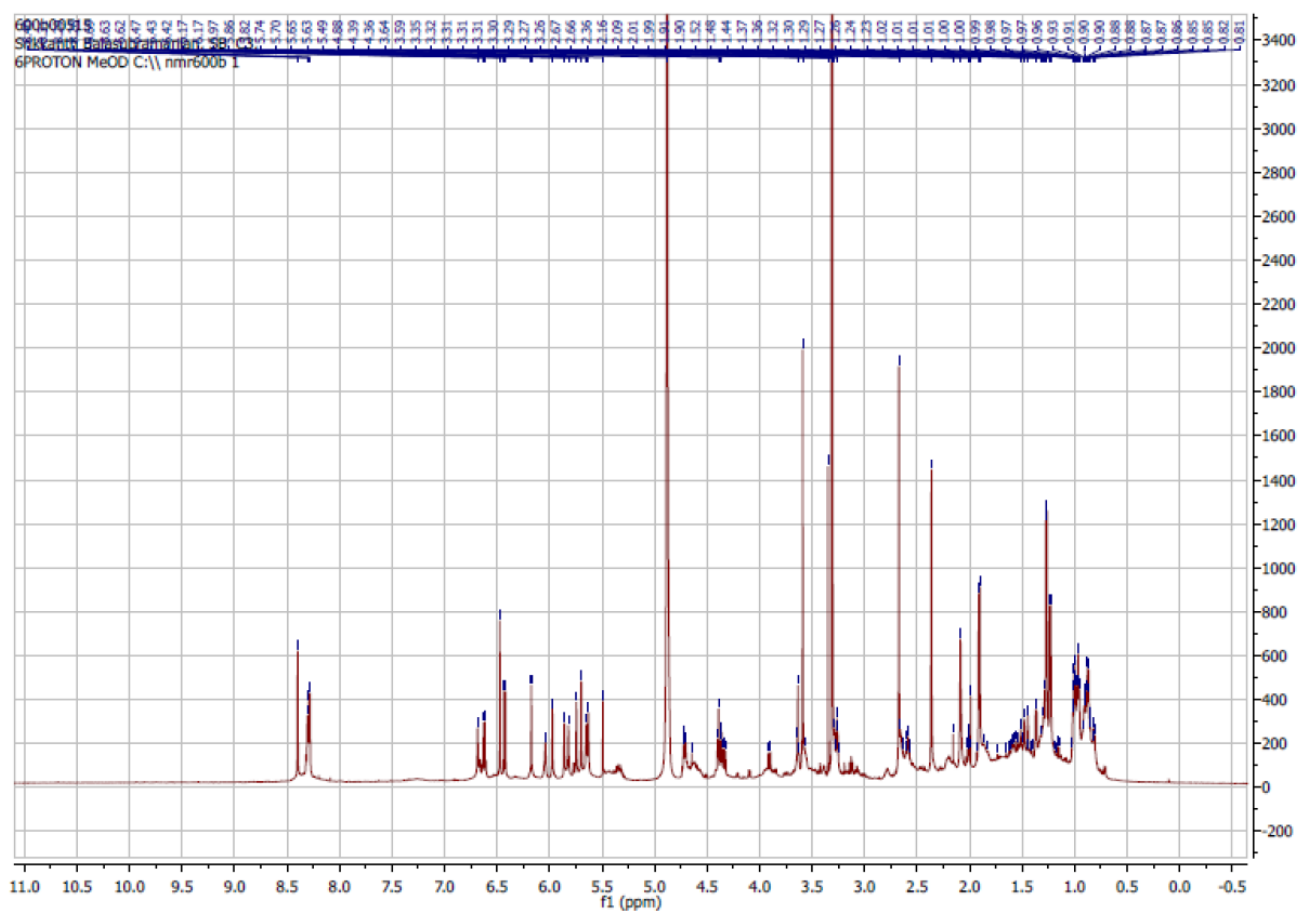


Red dotted line represents the presence of single component in SKC3

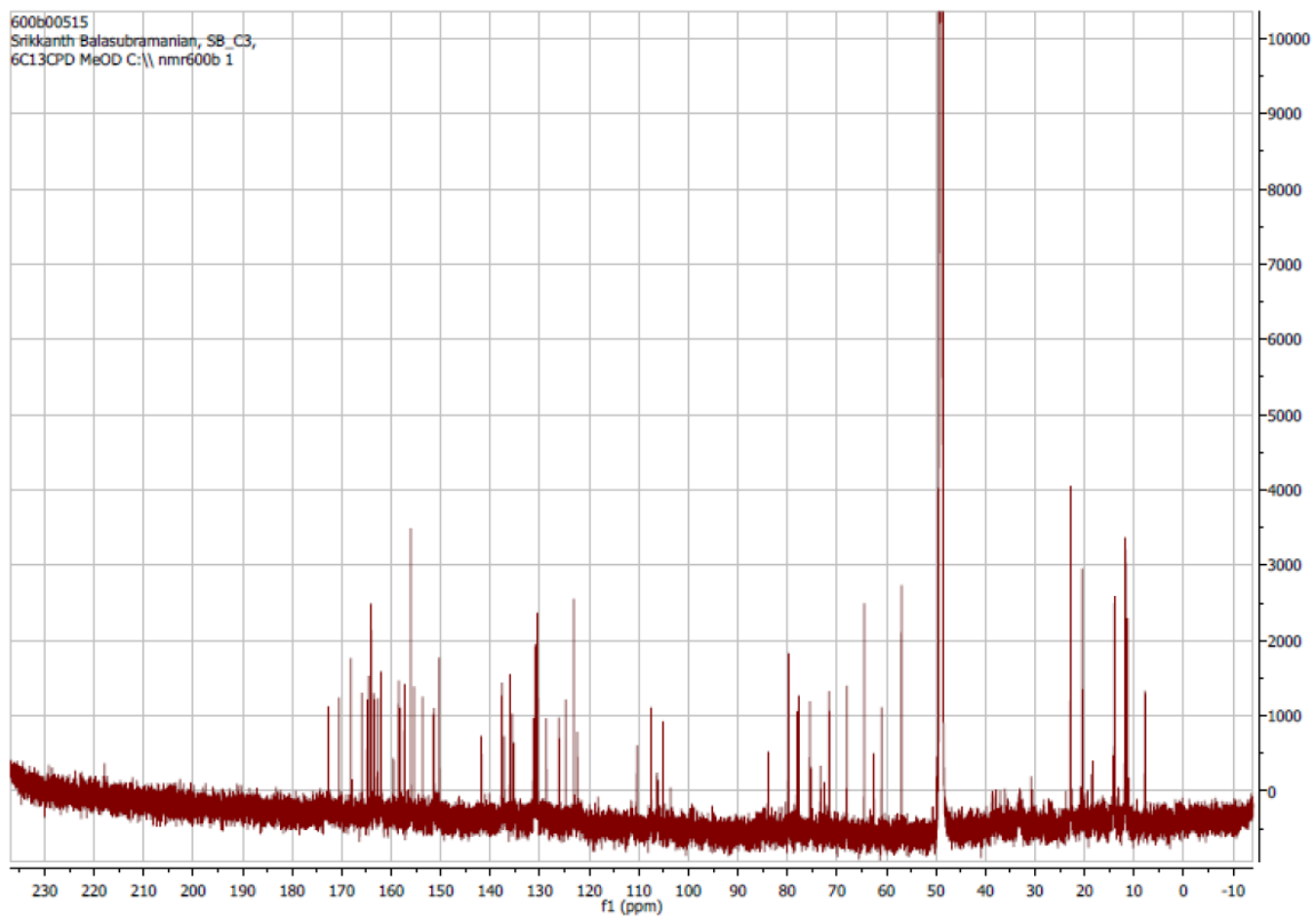
Diffusion coefficient of SKC3: $3.4 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$

Radius of SKC3 particle: 1.055 nm (determined by Stoke's Einstein Equation)

¹H-NMR spectra of SKC3

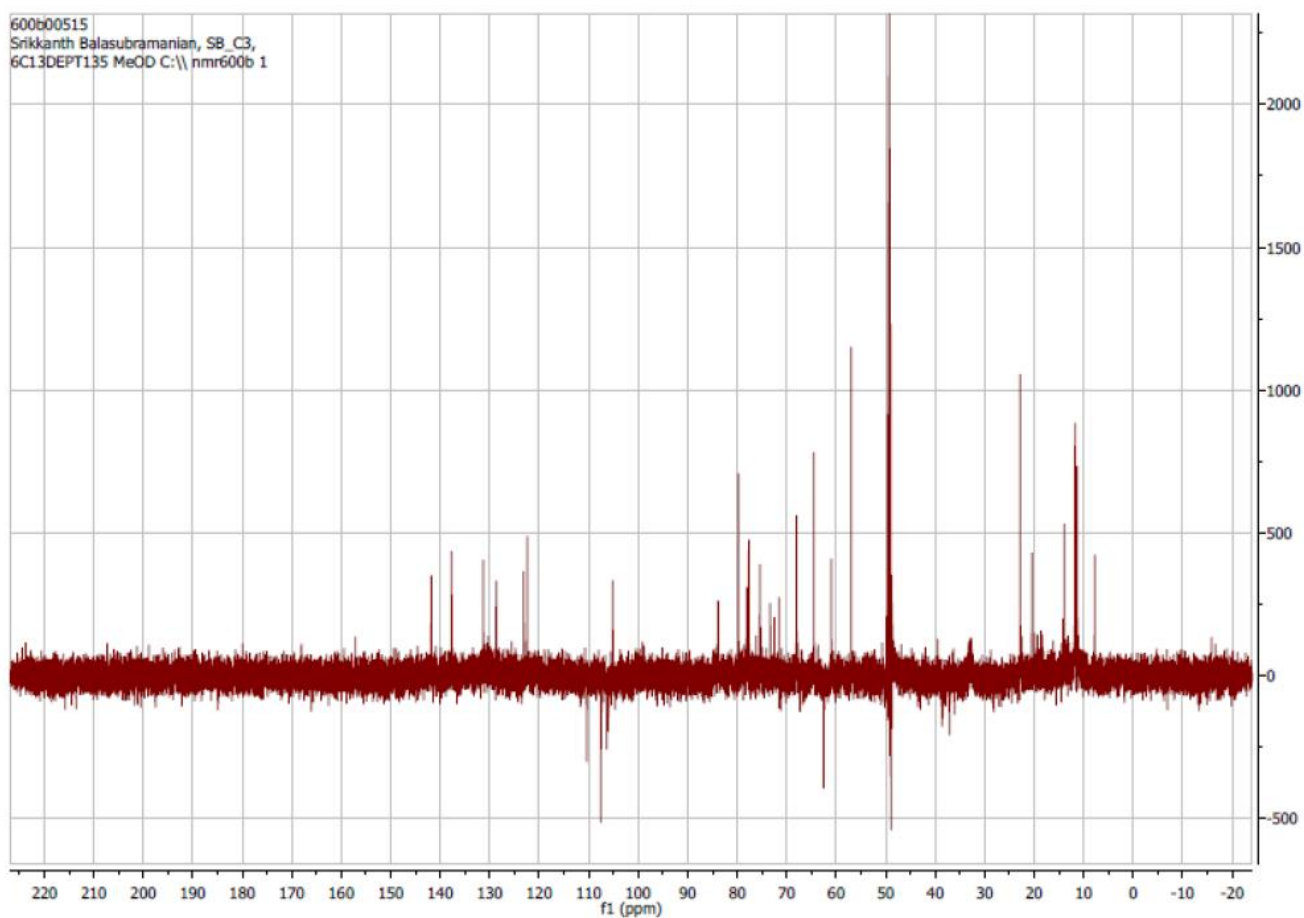


¹³C-NMR spectra of SKC3

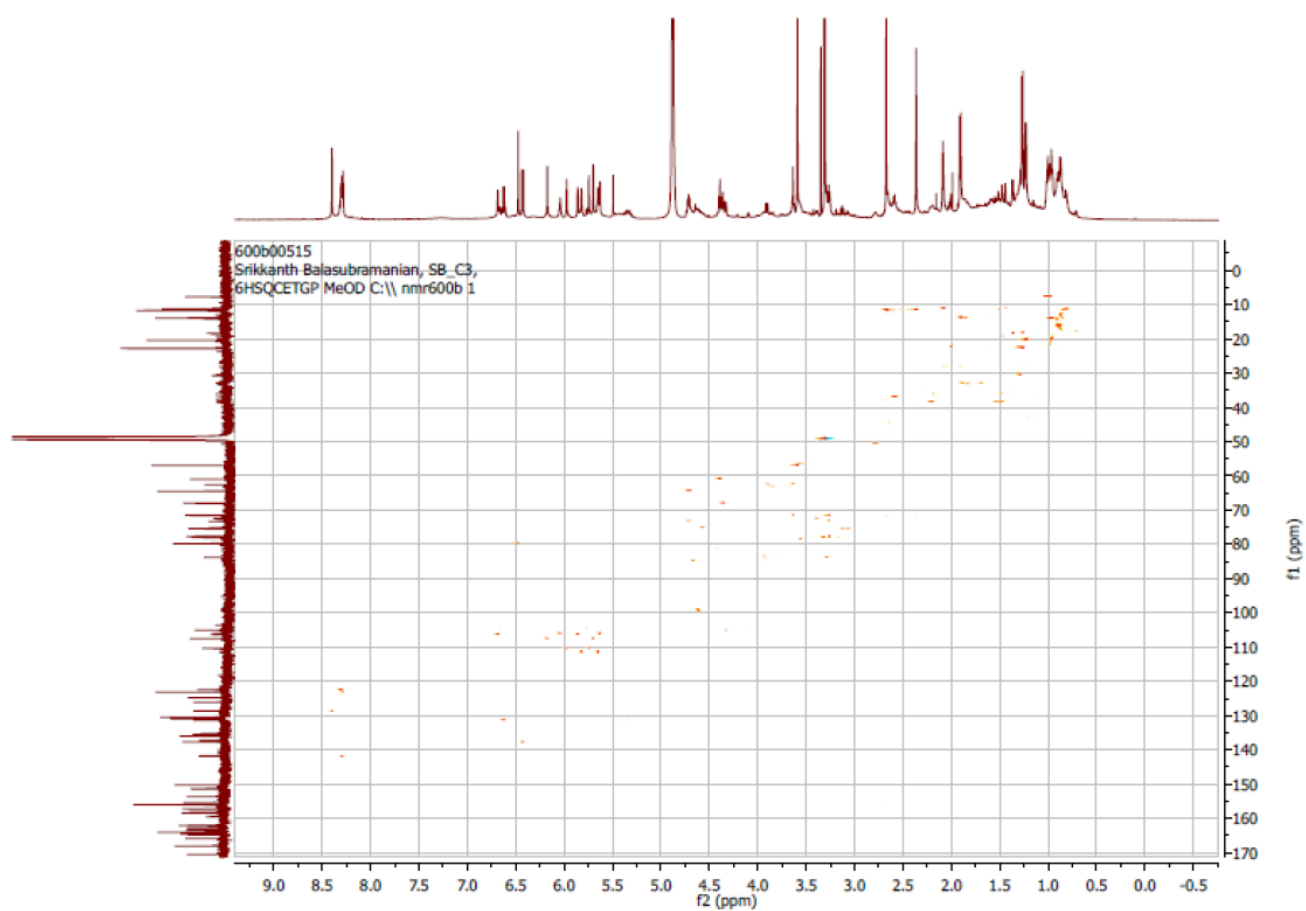


DEPT spectra of SKC3

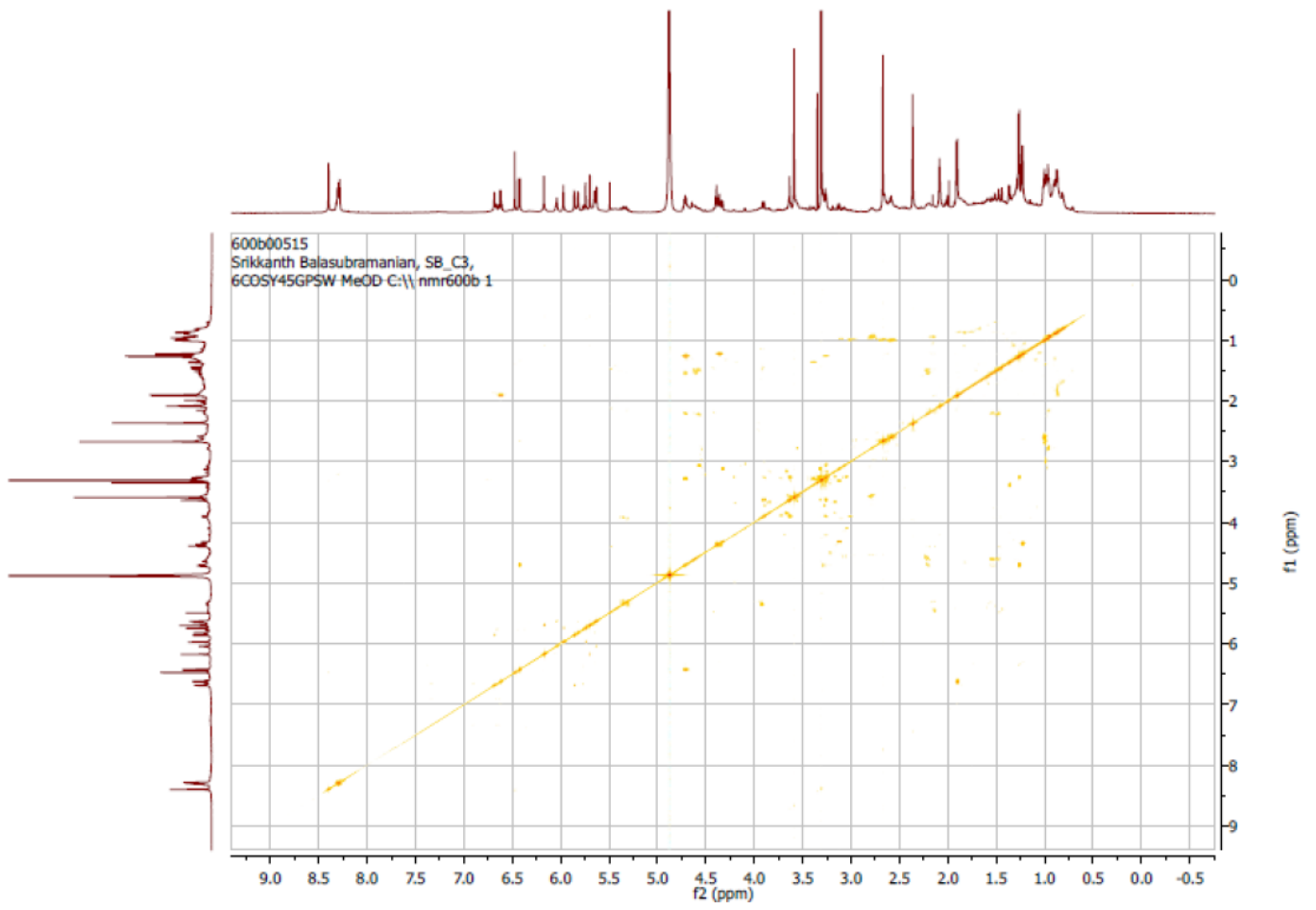
600b00515
Srikanth Balasubramanian, SB_C3,
6C13DEPT135 MeOD C:\nmr600b 1



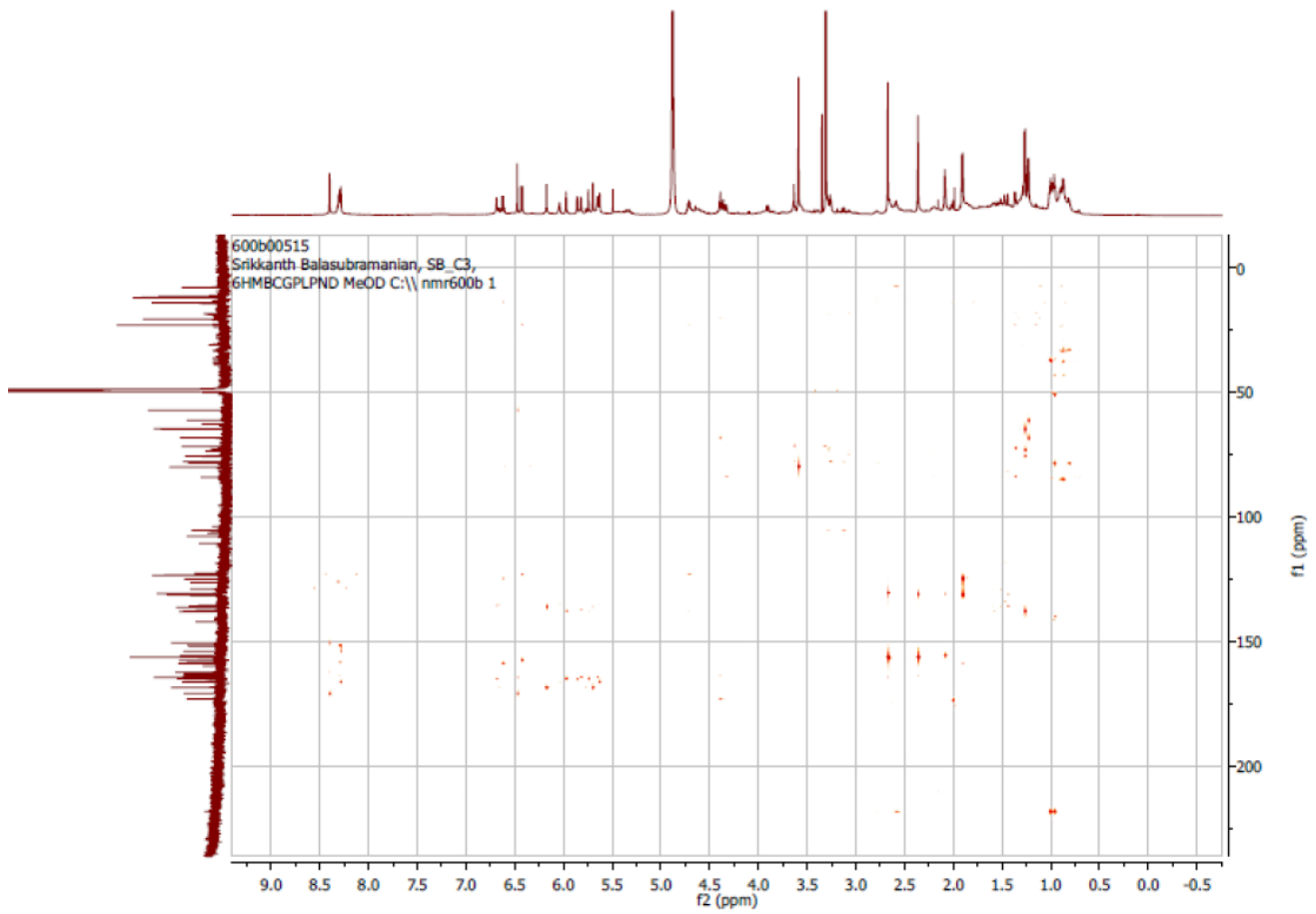
HSQC spectra of SKC3



COSY spectra of SKC3



HMBC spectra of SKC3



ROESY spectra of SKC3

