#	structure	CAS	complexity (15)	coupling analysis	aromaticity	NOE	heteronuclei
1		623-47-2	1	+			
2		620-71-3	1		+	+	
3		2759-55-9	1		+		
4		623-70-1	2	+			
5		140-67-0	2	+	+		
6	ООН	50-78-2	2	+	+		
7	O H	141-32-2	2	+			
8	. "	2591-86-8	2		+	+	

#	structure	CAS	complexity (15)	coupling analysis	aromaticity	NOE	heteronuclei
9	H ₂ N——CF ₃	57946-61-9	2	(+)	+	+	+
10	ОН	14434-41-4	3	+			
11	СООН	86-55-5	3	+	+		
12		91-64-5	3	+	+	+	
13	NH ₂	403-40-7 (1D)	3	+	+	+	+
14	Br NO ₂	517920-70-6	3	+	+	+	+
15	HO////// abs abs abs HO	492-62-6	4	+		+	

#	structure	CAS	complexity (15)	coupling analysis	aromaticity	NOE	heteronuclei
16	HO OH OH	16485-10-2	4	+		+	+
17	abs OH N S	1047626-52-7	5	+		+	
18	abs NH N N N N N N N N N N N N N N N N N N	485-35-8	5	+		+	+
19		No CAS	5	(+)			+
20	81 0H	2216-51-5	5	+		+	