

63 gamma ester glucuronic acid guaiacyl threo
XYZ file generated by Avogadro.

H	0.53130	-0.41410	-2.31260
O	1.41150	-0.83180	-2.35860
C	1.95840	-0.79340	-1.08330
H	1.17080	-0.89860	-0.32300
O	2.61550	0.46990	-0.93120
C	3.23550	0.64830	0.33460
H	3.76710	1.59840	0.28190
C	2.14720	0.78250	1.40050
O	-2.46230	1.54290	3.10440
C	4.24220	-0.47180	0.63580
H	5.07840	-0.33690	-0.05500
O	4.77670	-0.32750	1.93820
H	4.09400	-0.57240	2.57710
C	3.66540	-1.86210	0.39600
H	2.92970	-2.09780	1.17390
O	4.74320	-2.78310	0.45820
H	4.37720	-3.67490	0.42750
C	2.97550	-1.91680	-0.95720
H	3.72060	-1.79210	-1.75320
O	2.33530	-3.17600	-1.05940
C	-0.79900	1.27480	1.36510
C	-1.76490	0.58750	2.32720
H	-1.16090	0.00550	3.02830
C	0.29840	2.07210	2.06660
H	0.07220	3.13580	2.08660
C	-2.67030	-0.35300	1.55190
C	-4.20580	-2.05780	-0.03600
C	-4.03970	-0.16590	1.44760
C	-2.06260	-1.41220	0.86460
C	-2.81790	-2.25090	0.06490
C	-4.80880	-1.02620	0.65720
H	-4.52510	0.64870	1.97140
H	-0.99130	-1.56210	0.94660
H	-5.87950	-0.88760	0.56130
O	1.52130	1.95330	1.30470
O	-4.95900	-2.87820	-0.83430
H	-4.37000	-3.50450	-1.27790
O	-2.31660	-3.27010	-0.69220
C	-0.89810	-3.30670	-0.85660
H	-0.40450	-3.53830	0.08970
H	-0.53930	-2.34760	-1.24220
H	-0.69900	-4.09690	-1.57720
H	-0.32780	0.50700	0.74690
H	0.47040	1.71320	3.08070
O	-1.60470	2.11360	0.52240
C	-0.92900	2.67000	-0.54190
C	0.41980	3.79960	-2.70050
C	-0.62070	4.02460	-0.53570
C	-0.57320	1.87990	-1.63920
C	0.10210	2.44420	-2.71330
C	0.05180	4.58970	-1.61580
H	-0.91060	4.61980	0.32270

H	0.36860	1.80860	-3.55070
H	0.29080	5.64620	-1.60440
H	0.94800	4.23540	-3.53970
O	-0.86780	0.53290	-1.64600
C	-2.19870	0.22990	-2.09900
H	-2.24760	-0.85200	-2.21460
H	-2.37880	0.71440	-3.06130
H	-2.93250	0.56540	-1.36130
H	1.90570	-3.22540	-1.92300
O	1.84490	-0.07950	2.19330
H	-2.90660	2.15660	2.50450

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H	-0.34560	-1.68500	0.06070
O	0.42790	-2.25750	-0.05980
C	1.55590	-1.44770	-0.04440
H	1.32590	-0.48090	0.41650
O	1.94900	-1.25710	-1.40730
C	3.04580	-0.37140	-1.57010
H	3.29600	-0.38850	-2.63150
C	2.58510	1.05110	-1.24070
O	-1.78330	2.39070	-3.09660
C	4.26940	-0.83350	-0.76420
H	4.64170	-1.73880	-1.25310
O	5.31630	0.11510	-0.84090
H	5.04220	0.90580	-0.35580
C	3.91180	-1.19600	0.67560
H	3.67600	-0.28710	1.23780
O	5.00760	-1.79130	1.35250
H	5.26640	-2.59280	0.87730
C	2.69280	-2.11280	0.70880
H	2.93250	-3.06720	0.22030
O	2.25850	-2.32560	2.03920
C	-0.38030	2.15800	-1.22380
C	-1.28400	1.39810	-2.20480
H	-0.67760	0.67050	-2.75550
C	0.91590	2.62580	-1.86880
H	0.72040	3.10910	-2.82400
C	-2.37850	0.65970	-1.46790
C	-4.25090	-0.74140	0.04700
C	-3.24680	1.33950	-0.61960
C	-2.45760	-0.73220	-1.57130
C	-3.39040	-1.43370	-0.81710
C	-4.18290	0.63890	0.13810
H	-3.18660	2.41910	-0.52900
H	-1.77100	-1.25850	-2.22430
H	-4.85700	1.15130	0.81510
O	1.71180	1.46260	-2.15800
O	-5.15460	-1.42720	0.81300
H	-5.04330	-2.37490	0.65240
O	-3.55190	-2.78860	-0.81600
C	-2.63620	-3.55460	-1.59520

H	-2.90890	-4.59580	-1.44000
H	-1.61120	-3.38400	-1.25770
H	-2.72770	-3.30280	-2.65420
H	-0.92690	3.02760	-0.84670
H	1.46930	3.29930	-1.21710
O	-0.06890	1.25930	-0.16040
C	-0.27160	1.67040	1.12950
C	-0.68980	2.34190	3.79370
C	0.09810	2.92270	1.59430
C	-0.85600	0.73380	2.00290
C	-1.05960	1.07590	3.33540
C	-0.11690	3.26370	2.93060
H	0.55230	3.63230	0.91230
H	-1.51120	0.36780	4.01770
H	0.17190	4.24520	3.28560
H	-0.85720	2.59640	4.83340
O	-1.19390	-0.46330	1.45550
C	-1.89750	-1.39410	2.27470
H	-2.12120	-2.24630	1.63320
H	-2.82800	-0.95470	2.64310
H	-1.27640	-1.71810	3.11340
H	3.02540	-2.60180	2.55690
O	2.94820	1.69990	-0.28840
H	-2.25760	1.94380	-3.80750

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H	-4.47020	-1.80420	0.60460
O	-4.99030	-0.98240	0.60880
C	-4.19330	0.04300	0.10240
H	-3.80570	-0.21440	-0.88840
O	-3.10570	0.21000	1.01640
C	-2.22670	1.28950	0.76310
H	-1.56120	1.34000	1.62330
C	-1.36550	1.05930	-0.48280
O	2.89870	-2.21710	-0.48610
C	-2.99270	2.61070	0.64360
H	-3.39030	2.85020	1.63660
O	-2.05900	3.59170	0.23100
H	-2.52590	4.43250	0.14680
C	-4.16610	2.50440	-0.31990
H	-3.79740	2.37980	-1.34320
O	-4.88780	3.72330	-0.21350
H	-5.50940	3.77360	-0.94900
C	-5.03320	1.31190	0.04870
H	-5.46960	1.47400	1.04220
O	-6.04850	1.19940	-0.93280
C	2.02380	0.03060	-0.69350
C	1.82590	-1.45370	-1.01800
H	1.79760	-1.55300	-2.10960
C	0.89370	0.90250	-1.22990
H	1.27170	1.89380	-1.47370
C	0.52260	-1.95150	-0.44140
C	-1.91430	-2.72620	0.63790

C	0.42060	-2.17410	0.93210
C	-0.58300	-2.10540	-1.27320
C	-1.81210	-2.47980	-0.72820
C	-0.80250	-2.56470	1.46600
H	1.28460	-2.03570	1.56880
H	-0.48530	-1.91990	-2.33540
O	-0.07310	1.05200	-0.17230
O	-3.13100	-3.09740	1.14520
H	-3.05790	-3.16540	2.10870
O	-2.96770	-2.63370	-1.43240
C	-2.94280	-2.26580	-2.81000
H	-2.26840	-2.91580	-3.37250
H	-2.63900	-1.22250	-2.92520
H	-3.96090	-2.39540	-3.17020
H	2.10320	0.15710	0.39010
H	0.42020	0.46050	-2.10620
O	3.25150	0.44640	-1.31700
C	4.27220	0.80340	-0.46550
C	6.38000	1.52590	1.17470
C	4.16660	1.94040	0.34190
C	5.43630	0.03210	-0.44690
C	6.50340	0.39540	0.37440
C	5.22600	2.30240	1.17440
H	7.41030	-0.19270	0.39800
H	5.15880	3.17670	1.80720
H	7.20520	1.80890	1.81700
O	5.42260	-1.06220	-1.26100
C	6.55390	-1.93230	-1.21180
H	6.32830	-2.74820	-1.89430
H	7.45340	-1.41010	-1.54370
H	6.69560	-2.32090	-0.20120
H	-6.68590	0.53790	-0.63870
O	-1.80180	0.92140	-1.60080
H	3.72670	-1.89530	-0.87920
O	-1.04760	-2.80960	2.78470
O	2.99320	2.61530	0.23960
C	0.02530	-2.59060	3.69820
H	0.86170	-3.25670	3.47570
H	-0.37240	-2.81520	4.68490
H	0.35500	-1.54980	3.65880
C	2.79910	3.73150	1.10490
H	1.79730	4.09880	0.89280
H	3.53100	4.51530	0.89770
H	2.86660	3.42430	2.15090

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H	-1.15890	-0.86910	-2.56480
O	-2.06240	-1.22530	-2.57760
C	-2.48590	-1.29700	-1.25760
H	-2.03250	-0.49240	-0.66620
O	-2.06720	-2.56350	-0.73220
C	-2.39850	-2.71360	0.63470
H	-2.06220	-3.70920	0.93390

C	-1.61310	-1.72100	1.50030
O	0.46880	-0.76800	-1.43050
C	-3.92120	-2.62530	0.83470
H	-4.35690	-3.46500	0.28760
O	-4.28900	-2.79970	2.18820
H	-3.88480	-2.08310	2.69730
C	-4.47410	-1.33670	0.23550
H	-4.10640	-0.47470	0.80900
O	-5.88830	-1.39620	0.30760
H	-6.23840	-0.55450	-0.00830
C	-4.00110	-1.19590	-1.20450
H	-4.43120	-2.00080	-1.81360
O	-4.42680	0.07260	-1.67030
C	0.61270	0.51560	0.67230
C	1.23190	0.17770	-0.69680
H	1.20360	1.09860	-1.28690
C	0.51490	-0.63440	1.65530
H	1.48500	-1.10320	1.81020
C	2.68120	-0.23830	-0.52380
C	5.33640	-0.93980	-0.07870
C	3.05110	-1.57930	-0.56270
C	3.62720	0.75300	-0.26650
C	4.95680	0.40280	-0.04190
C	4.38280	-1.92290	-0.33910
H	2.31550	-2.34690	-0.76400
H	3.31950	1.79140	-0.24620
O	-0.34350	-1.65650	1.10310
O	6.64880	-1.26140	0.13980
H	6.74000	-2.22310	0.08470
O	5.96130	1.28670	0.21630
C	5.60770	2.66510	0.29320
H	5.20760	3.01670	-0.66060
H	6.52890	3.19580	0.52200
H	4.87760	2.83340	1.08830
H	1.23620	1.28490	1.13690
H	0.11190	-0.28520	2.60450
O	-0.72350	1.00660	0.49990
C	-0.83380	2.33980	0.19810
C	-1.14530	5.03440	-0.38380
C	-0.58880	3.30320	1.17450
C	-1.25560	2.72940	-1.08170
C	-1.41300	4.08500	-1.36860
C	-0.73580	4.65650	0.88780
H	-1.73640	4.40470	-2.34970
H	-0.53640	5.38540	1.66390
H	-1.26600	6.08490	-0.61920
O	-1.47990	1.72120	-1.96040
C	-1.99430	2.07450	-3.24200
H	-2.14020	1.13630	-3.77250
H	-2.94840	2.59800	-3.14280
H	-1.28200	2.69860	-3.78680
H	-4.15350	0.16180	-2.59230
O	-2.07070	-1.10980	2.43520
H	0.22840	-1.51090	-0.85830

O	4.87740	-3.19480	-0.34780
C	3.95130	-4.25610	-0.56910
H	3.18400	-4.26500	0.20850
H	4.53320	-5.17350	-0.52370
H	3.48600	-4.16230	-1.55280
O	-0.17930	2.89520	2.42430
C	-1.25720	2.40820	3.23770
H	-1.77700	1.58780	2.73910
H	-0.81110	2.05380	4.16530
H	-1.95740	3.22040	3.44900