** Substructure Report Page 1 **

Search Pattern: UnknownID=53|RT=7.151

Structures present:

Number	Probability	Short Name And Description
1	96	CH2/3, primary or secondary saturated carbon
2	96	O, contains oxygen
3	95	-CH2/3-, methylene or methyl group (chain)
4	92	C-O, carbon-oxygen single bond
5	91	-CH2/3-1, exactly one methylene or methyl group (chain)
6	90	>C=O, carbonyl group
7	86	CH3, methyl
8	84	-C=O, non-ring (chain) carbonyl
9	80	CH2, methylene group
10	80	ether, divalent oxygen
11	78	-O-, contains oxygen atom in chain (non-ring)
12	74	Si, contains silicon
13	71	NoAr, no aromatic rings
14	71	C=OO, ester group
15	69	CO-O/OH, carboxyl or ester
16	68	RDB5_PLUS, rings + double bonds count >= 5
17	68	C2H5/CH2CH2, primary or secondary ethyl linkage
18	68	Si(CH3)3, trimethyl silyl
19	67	-CH2-, methylene group (chain)

CCH3, methyl bonded to carbon

Structures absent:

67

20

Number Probability Short Name And Description

1	99	RDB10_PLUS, rings + double bonds count >= 10
2	99	Ar-C, aromatic ring-saturated carbon atom bond (chain)
3	99	Ar-CHx, aromatic-saturated C bond with 1 or more hydrogen atoms
4	99	Ar-O-R, alkyl-aryl ether (chain)
5	99	HC, hydrocarbon (C and H atoms only)
6	99	ArO, aromatic carbon-oxygen bond
7	99	Ar-O, aromatic ring-oxygen atom bond (chain)
8	99	PhCsat, phenyl attached to saturated carbon atom
9	99	Ph-2+sub, phenyl with 2 or more substituents
10	99	PhCO, phenyl carbonyl

MW(Nominal Mass)Information:

Number	MW	Probability
1	1102	8
2	1117	6
3	1145	3
4	1116	2

Clorine and/or Bromine Information:

CI=0, Br=0 Probability=98%

There is a peak (m/z=219 ab=324) above highest possible CIBr cluster