Electronic Supplementary Material (ESI) for RSC Advances.

Nano-QSAR modeling for predicting biological activity of diverse nanomaterials

Supporting information

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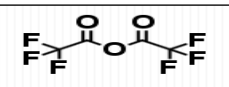
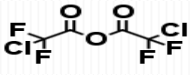
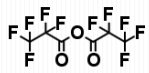
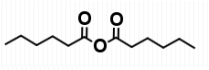
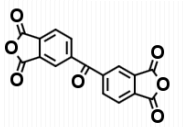
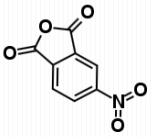
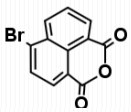
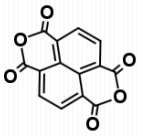
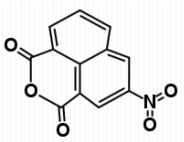
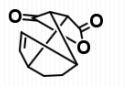
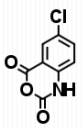
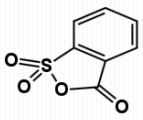
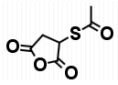
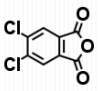
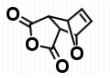
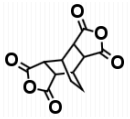
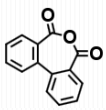
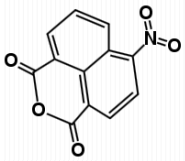
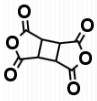
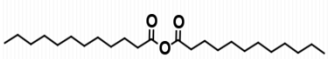
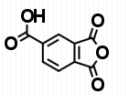
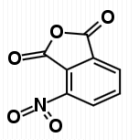
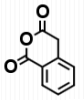
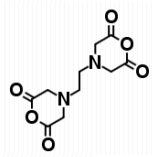
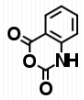
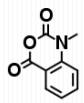
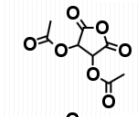
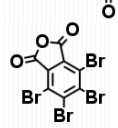
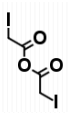
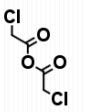
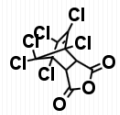
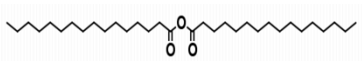
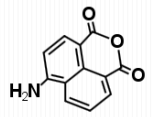
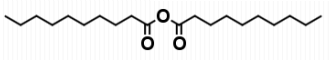
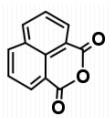
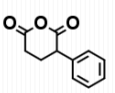
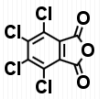
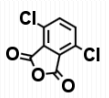
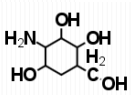
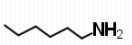
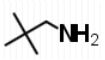
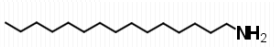
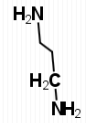
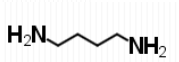
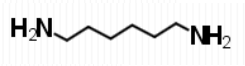
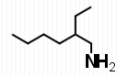
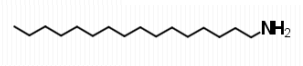
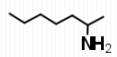
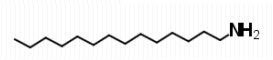
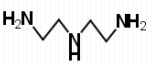
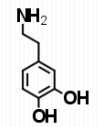
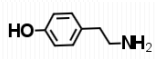
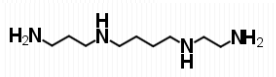
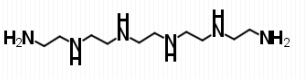
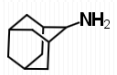
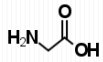
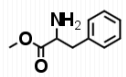
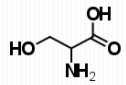
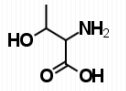
Table SI1. Chemical structure, Coatings name and SMILES of 109 NPs (case study 2).

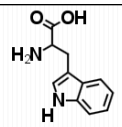
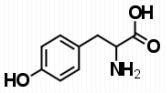
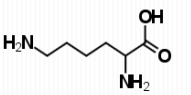
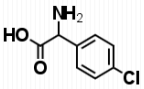
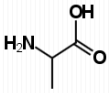
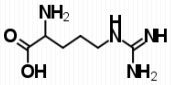
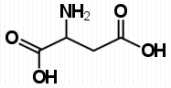
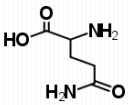
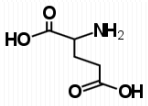
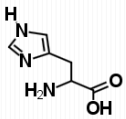
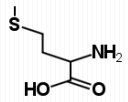
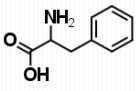
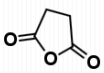
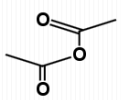
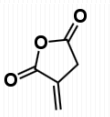
S. No.	Chemical Structure	Coatings name	SMILES notation
1		Trifluoroacetic anhydride	FC(F)(F)C(=O)OC(=O)C(F)(F)F
2		Chlorodifluoroacetic anhydride	FC(F)(Cl)C(=O)OC(=O)C(F)(F)Cl
3		Pentafluoropropanoic anhydride	FC(F)(F)C(F)(F)C(=O)OC(=O)C(F)(F)C(F)(F)F
4		3,3-Dimethyldihydrofuran-2,5-dione	CC1(C)CC(=O)OC1=O
5		Furan-2,5-dione	O=C1OC(=O)C=C1
6		3-Methylfuran-2,5-dione	CC1=CC(=O)OC1=O
7		3,4-Dimethylfuran-2,5-dione	CC1=C(C)C(=O)OC1=O
8		Hexanoic anhydride	CCCCCC(=O)OC(=O)CCCCC
9		3-Methyldihydrofuran-2,5-dione	CC1CC(=O)OC1=O
10		5,5'-Carbonylbis(2-benzofuran-1,3-dione)	O=C1OC(=O)c2cc(ccc12)C(=O)c1ccc2C(=O)OC(=O)c2c1
11		5-Nitro-2-benzofuran-1,3-dione	O=C1OC(=O)c2cc(ccc12)N(=O)=O
12		6-Bromo-1H,3H-benzo[de]isochromene-1,3-dione	Brc1ccc2C(=O)OC(=O)c3cccc1c23
13		1,4,5, 8-Naphthalenetetracarboxylic acid anhydride	O=C1OC(=O)c2ccc3C(=O)OC(=O)c4ccc1c2c34
14		4,5,6,7-Tetrafluoro-2-benzofuran-1,3-dione	Fc1c(F)c(F)c2C(=O)OC(=O)c2c1F
15		5-Nitro-1H,3H-benzo[de]isochromene-1,3-dione	O=C1OC(=O)c2cc(cc3cccc1c23)N(=O)=O
16		4-Hydroxy-2-benzofuran-1,3-dione	Oc1cccc2C(=O)OC(=O)c12

17		4-Oxatricyclo[5.2.2.02,6]undec-8-ene-3,5-dione	O=C1OC(=O)C2C3CCC(C=C3)C12
18		6-Chloro-2H-3,1-benzoxazine-2,4(1H)-dione	Clc1ccc2NC(=O)OC(=O)c2c1
19		3H-2,1-benzoxathiol-3-one 1,1-dioxide	O=C1OS(=O)(=O)c2ccccc12
20		3,4-Dichlorofuran-2,5-dione	ClC1=C(Cl)C(=O)OC1=O
21		S-(2,5-dioxotetrahydrofuran-3-yl) ethanethioate	CC(=O)SC1CC(=O)OC1=O
22		5,6-Dichloro-2-benzofuran-1,3-dione	Clc1cc2C(=O)OC(=O)c2cc1Cl
23		4,10-Dioxatricyclo[5.2.1.02,6]dec-8-ene-3,5-dione	O=C1OC(=O)C2C3OC(C=C3)C12
24		Bicyclo[2.2.2]-7-octene-2,3,5,6-tetracarboxylic Dianhydride	O=C1OC(=O)C2C3C=CC(C12)C1C3C(=O)OC1=O
25		3a,4,7,7a-Tetrahydro-2-benzofuran-1,3-dione	O=C1OC(=O)C2CC=CCC12
26		Dibenz(c,e)oxepin-5,7-dione	O=C1OC(=O)c2ccccc2-c2ccccc12
27		6-Nitro-1H,3H-benzo[de]isochromene-1,3-dione	O=C1OC(=O)c2ccc(c3cccc1c23)N(=O)=O
28		Tetrahydrofuro[3',4':3,4]cyclobuta[1,2-c]furan-1,3,4,6-tetrone	O=C1OC(=O)C2C1C1C2C(=O)OC1=O
29		Lauric anhydride	CCCCCCCCCCCC(=O)OC(=O)CCCCCCCCCCC
30		1,3-Dioxo-1,3-dihydro-2-benzofuran-5-carboxylic acid	OC(=O)c1ccc2C(=O)OC(=O)c2c1
31		5-Methyl-2-benzofuran-1,3-dione	Cc1ccc2C(=O)OC(=O)c2c1

32		4-Nitro-2-benzofuran-1,3-dione	O=C1OC(=O)c2c1cccc2N(=O)=O
33		1H-isochromene-1,3(4H)-dione	O=C1Cc2ccccc2C(=O)O1
34		Dihydro-2H-pyran-2,6(3H)-dione	O=C1CCCC(=O)O1
35		4,4'-Ethane-1,2-diyldimorpholine-2,6-dione	O=C1CN(CCN2CC(=O)OC(=O)C2)CC(=O)O1
36		2H-3,1-benzoxazine-2,4(1H)-dione	O=C1Nc2ccccc2C(=O)O1
37		1-Methyl-2H-3,1-benzoxazine-2,4(1H)-dione	CN1C(=O)OC(=O)c2ccccc12
38		4-Methyldihydro-2H-pyran-2,6(3H)-dione	CC1CC(=O)OC(=O)C1
39		4,5,6,7-Tetrahydro-2-benzofuran-1,3-dione	O=C1OC(=O)C2=C1CCCC2
40		2,5-Dioxotetrahydrofuran-3,4-diyl diacetate	CC(=O)OC1C(OC(C)=O)C(=O)OC1=O
41		4,5,6,7-Tetrabromo-2-benzofuran-1,3-dione	Brc1c(Br)c(Br)c2C(=O)OC(=O)c2c1Br
42		Hexahydro-2-benzofuran-1,3-dione	O=C1OC(=O)C2CCCCC12
43		5,6-Dihydro-1H-cyclopenta[c]furan-1,3(4H)-dione	O=C1OC(=O)C2=C1CCC2
44		Iodoacetic anhydride	ICC(=O)OC(=O)CI
45		Chloroacetic anhydride	ClCC(=O)OC(=O)CCl
46		1,7,8,9,10,10-Hexachloro-4-oxatricyclo[5.2.1.$0^{2,6}$]dec-8-ene-3,5-dione	ClC1=C(Cl)C2(Cl)C3C(C(=O)OC3=O)C1(Cl)C2(Cl)Cl
47		Palmitic anhydride	CCCCCCCCCCCCCCCC(=O)OC(=O)CCCCCCCCCCCCCCC

48		5-amino-1H,3H-benzo[de]isochromene-1,3-dione	Nc1ccc2C(=O)OC(=O)c3cccc1c23
49		Decanoic anhydride	CCCCCCCCCC(=O)OC(=O)CCCCCCCCC
50		8-Oxaspiro[4.5]decane-7,9-dione	O=C1CC2(CCCC2)CC(=O)O1
51		4-Oxatricyclo[5.2.1.$0^{2,6}$]decane-3,5-dione	O=C1OC(=O)C2C3CCC(C3)C12
52		1H,3H-benzo[de]isochromene-1,3-dione	O=C1OC(=O)c2cccc3cccc1c23
53		3-Phenyldihydro-2H-pyran-2,6(3H)-dione	O=C1CCC(C(=O)O1)c1ccccc1
54		4,5,6,7-Tetrachloro-2-benzofuran-1,3-dione	Clc1c(Cl)c(Cl)c2C(=O)OC(=O)c2c1Cl
55		4,7-Dichloro-2-benzofuran-1,3-dione	Clc1ccc(Cl)c2C(=O)OC(=O)c12
56		3,3-Dimethyldihydro-2H-pyran-2,6(3H)-dione	CC1(C)CCC(=O)OC1=O
57		Pentan-1-amine	CCCCCN
58		4-Methylpentan-2-amine	CC(C)CC(C)N
59		3-Amino-6-(hydroxymethyl)cyclohexane-1,2,4-triol	NC1C(O)CC(CO)C(O)C1O
60		Hexan-1-amine	CCCCCCN
61		2-Methylpropan-2-amine	CC(C)(C)N
62		2-Methylpropan-1-amine	CC(C)CN
63		2,2-Dimethylpropan-1-amine	CC(C)(C)CN
64		3-Methylbutan-1-amine	CC(C)CCN
65		Pentan-3-amine	CCC(N)CC
66		2-Methylbutan-2-amine	CCC(C)(C)N
67		Ethane-1,2-diamine	NCCN
68		Pentadecan-1-amine	CCCCCCCCCCCCCCCN

69		Propane-1,3-diamine	NCCCN
70		Butane-1,4-diamine	NCCCCN
71		Hexane-1,6-diamine	NCCCCCCN
72		2-Ethylhexan-1-amine	CCCCC(CC)CN
73		1-Hexadecylamine	CCCCCCCCCCCCCCCCN
74		Heptan-2-amine	CCCCCC(C)N
75		Tetradecan-1-amine	CCCCCCCCCCCCCCN
76		N-(2-Aminoethyl)ethane-1,2-diamine	NCCNCCN
77		Tricyclo[3.3.1.1^{3,7}]decane-1-methanamine	NCC12CC3CC(CC(C3)C1)C2
78		4-(2-Aminoethyl)benzene-1,2-diol	NCCc1ccc(O)c(O)c1
79		4-(2-Aminoethyl)phenol	NCCc1ccc(O)cc1
80		N-(2-Aminoethyl)-N'-(3-aminopropyl)butane-1,4-diamine	NCCCNCCCCNCCN
81		N,N'-Bis(2-aminoethyl)propane-1,3-diamine	NCCNCCCNCCN
82		3,6,9,12-Tetraazatetradecane-1,14-diamine	NCCNCCNCCNCCNCCN
83		Tricyclo[3.3.1.03,7]nonan-3-amine	NC12CC3CC(CC1C3)C2
84		Tricyclo[3.3.1.13,7]decan-2-amine	NC1C2CC3CC(C2)CC1C3
85		Aminoacetic acid	NCC(O)=O
86		Methyl 2-amino-3-phenylpropanoate	COC(=O)C(N)Cc1ccccc1
87		2-Amino-3-hydroxypropanoic acid	NC(CO)C(O)=O
88		2-Amino-3-hydroxybutanoic acid	CC(O)C(N)C(O)=O

89		2-Amino-3-(1H-indol-3-yl)propanoic acid	NC(Cc1c[nH]c2ccccc12)C(O)=O
90		2-ammonio-3-(4-hydroxyphenyl)propanoate	NC(Cc1ccc(O)cc1)C(O)=O
91		2-Amino-3-methylbutanoic acid	CC(C)C(N)C(O)=O
92		2,6-Diaminohexanoic acid	NCCCCC(N)C(O)=O
93		Amino(4-chlorophenyl)acetic acid	NC(C(O)=O)c1ccc(Cl)cc1
94		2-Aminopropanoic acid	CC(N)C(O)=O
95		2-Amino-5-carbamimidamidopentanoic acid	NC(CCCNC(N)=N)C(O)=O
96		2-Aminobutanedioic acid	NC(CC(O)=O)C(O)=O
97		2,5-Diamino-5-oxopentanoic acid	NC(CCC(N)=O)C(O)=O
98		2-Aminopentanedioic acid	NC(CCC(O)=O)C(O)=O
99		2-Amino-3-(1H-imidazol-4-yl)propanoic acid	NC(Cc1c[nH]cn1)C(O)=O
100		2-Amino-4-(methylsulfanyl)butanoic acid	CSCCC(N)C(O)=O
101		2-Amino-3-phenylpropanoic acid	NC(Cc1ccccc1)C(O)=O
102		Dihydrofuran-2,5-dione	O=C1CCC(=O)O1
103		Acetic anhydride	CC(=O)OC(C)=O
104		3-Methylidenedihydrofuran-2,5-dione	C=C1CC(=O)OC1=O
105		1,4-Dioxane-2,6-dione	O=C1COCC(=O)O1

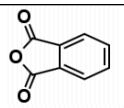
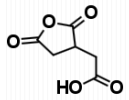
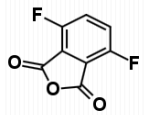
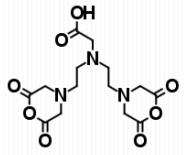
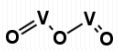
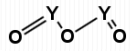
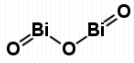
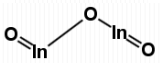
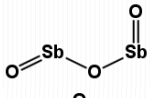
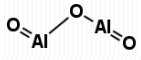
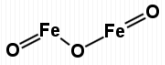
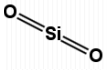
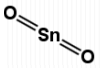
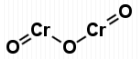
106		2-Benzofuran-1,3-dione	O=C1OC(=O)c2ccccc12
107		(2,5-Dioxotetrahydrofuran-3-yl)acetic acid	OC(=O)CC1CC(=O)OC1=O
108		4,7-Difluoro-2-benzofuran-1,3-dione	Fc1ccc(F)c2C(=O)OC(=O)c12
109		{Bis[2-(2,6-dioxomorpholin-4-yl)ethyl]amino}acetic acid	OC(=O)CN(CCN1CC(=O)OC(=O)C1)CCN1CC(=O)OC(=O)C1

Table SI2: Chemical structure and SMILES of metal oxide NPs (case study 3)

S.No.	Chemical structure	Metal Oxide NPs	SMILES notation
1		ZnO	O = [Zn]
2		CuO	[Cu] = O
3		V_2O_3	O = [V]O[V] = O
4		Y_2O_3	O = [Y]O[Y] = O
5		Bi_2O_3	O = [Bi]O[Bi] = O
6		In_2O_3	O = [In]O[In] = O
7		Sb_2O_3	O = [Sb]O[Sb] = O
8		Al_2O_3	O = [Al]O[Al] = O
9		$Fe2O_3$	O = [Fe]O[Fe] = O
10		SiO_2	O = [Si] = O
11		ZrO_2	O = [Zr] = O
12		SnO_2	O = [Sn] = O
13		TiO_2	O = [Ti] = O
14		CoO	[Co] = O
15		NiO	[Ni] = O
16		Cr_2O_3	O = [Cr]O[Cr] = O

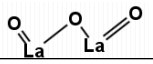
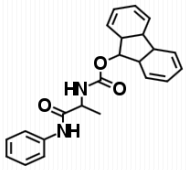
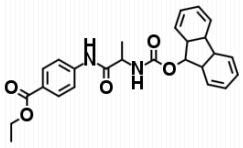
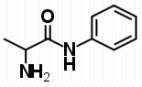
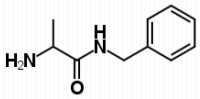
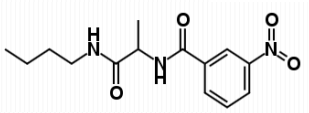
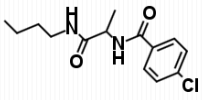
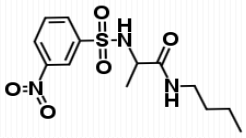
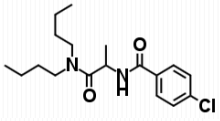
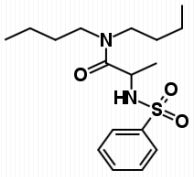
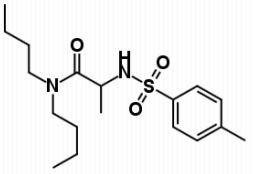
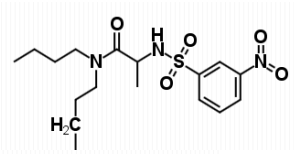
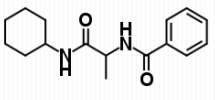
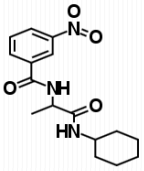
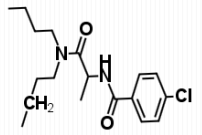
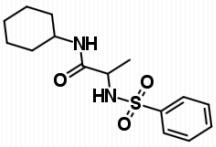
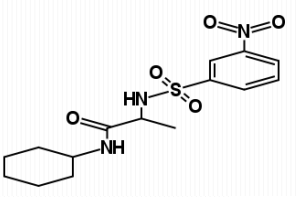
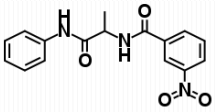
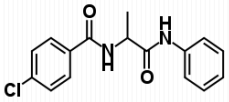
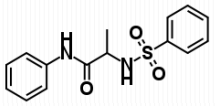
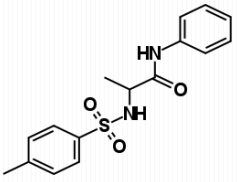
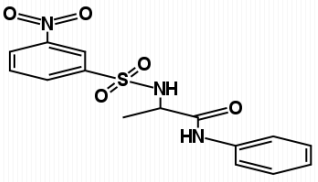
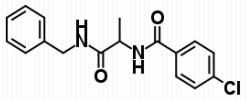
17		La_2O_3	O = [La]O[La] = O

Table SI3: Chemical structure and SMILES of decorator portions of decorated nano tubes (Case study 4)

NT No.	Chemical Structure	[a]SMILES notation
8		CC(NC(=O)OC3C1C=CC=CC1C2C=CC=CC23)C(=O)Nc4ccccc4
11		CCOC(=O)c4ccc(NC(=O)C(C)NC(=O)OC3C1C=CC=CC1C2C=CC=CC23)cc4
16		CC(N)C(=O)Nc1ccccc1
17		CC(N)C(=O)NCc1ccccc1
24		CCCCNC(=O)C(C)NC(=O)c1cccc(N(=O)=O)c1
25		CCCCNC(=O)C(C)NC(=O)c1ccc(Cl)cc1
28		CCCCNC(=O)C(C)NS(=O)(=O)c1cccc(N(=O)=O)c1
33		CCCCN(CCCC)C(=O)C(C)NC(=O)c1ccc(Cl)cc1
34		CCCCN(CCCC)C(=O)C(C)NS(=O)(=O)c1ccccc1
35		CCCCN(CCCC)C(=O)C(C)NS(=O)(=O)c1ccc(C)cc1

36		CCCCN(CCCC)C(=O)C(C)NS(=O)(=O)c1cccc(N(=O)=O)c1
38		CC(NC(=O)c1ccccc1)C(=O)NC2CCCCC2
40		CC(NC(=O)c1cccc(N(=O)=O)c1)C(=O)NC2CCCCC2
41		CCCCN(CCCC)C(=O)C(C)NC(=O)c1ccc(Cl)cc1
42		CC(NS(=O)(=O)c1ccccc1)C(=O)NC2CCCCC2
44		CC(NS(=O)(=O)c1cccc(N(=O)=O)c1)C(=O)NC2CCCCC2
48		CC(NC(=O)c1cccc(N(=O)=O)c1)C(=O)Nc2ccccc2
49		CC(NC(=O)c1ccc(Cl)cc1)C(=O)Nc2ccccc2
50		CC(NS(=O)(=O)c1ccccc1)C(=O)Nc2ccccc2
51		Cc2ccc(S(=O)(=O)NC(C)C(=O)Nc1ccccc1)cc2
52		CC(NS(=O)(=O)c1cccc(N(=O)=O)c1)C(=O)Nc2ccccc2
57		CC(NC(=O)c1ccc(Cl)cc1)C(=O)NCc2ccccc2

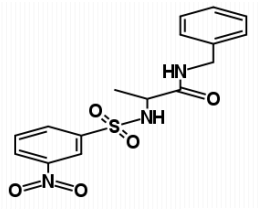
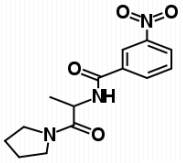
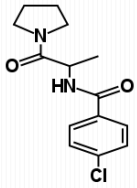
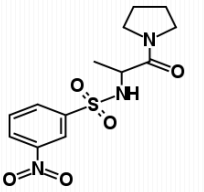
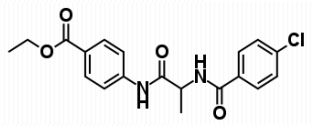
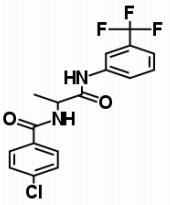
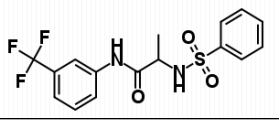
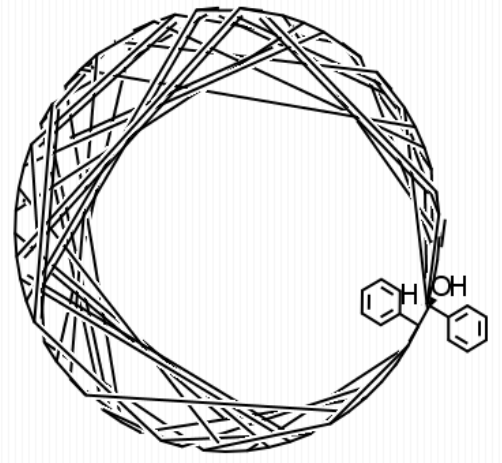
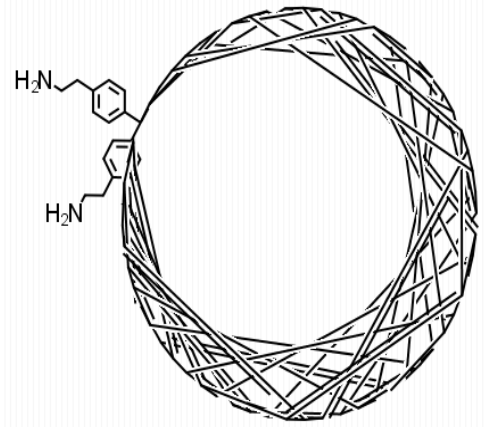
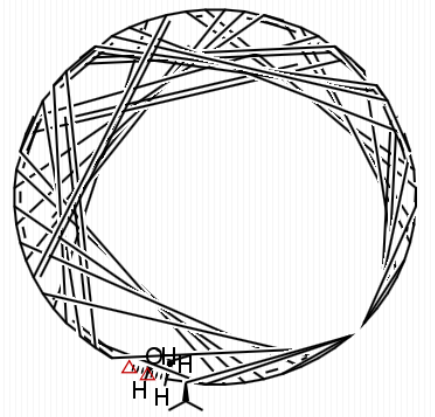
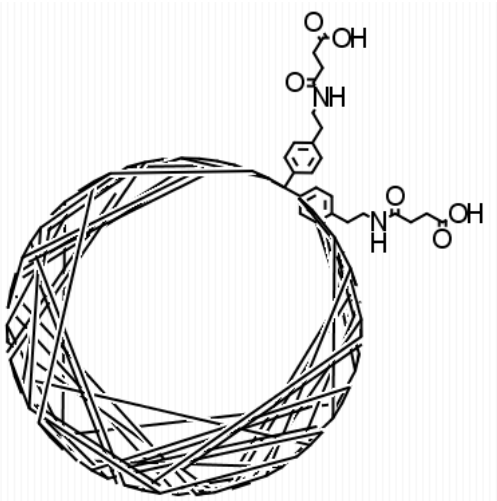
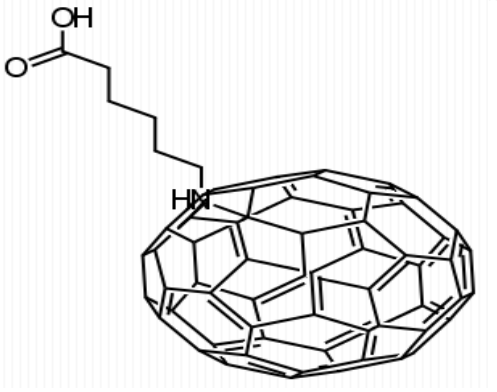
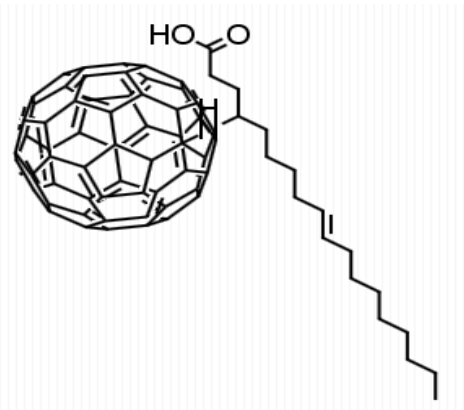
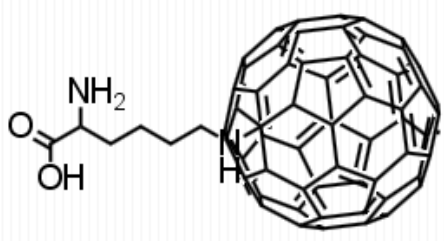
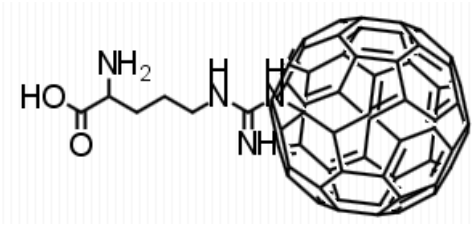
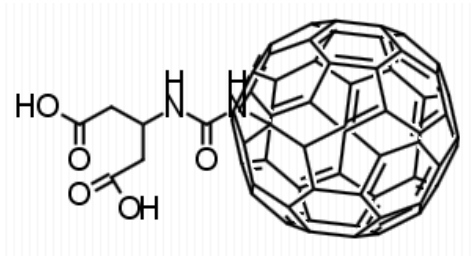
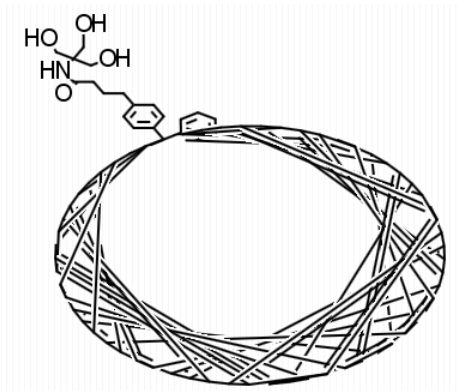
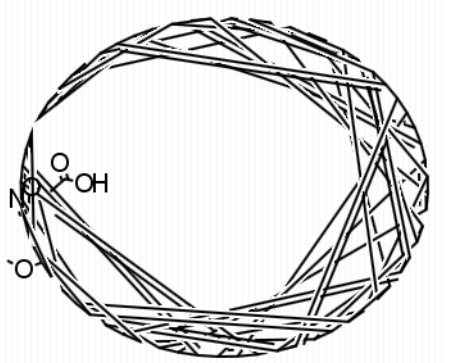
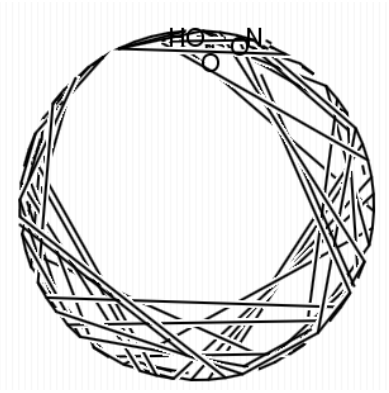
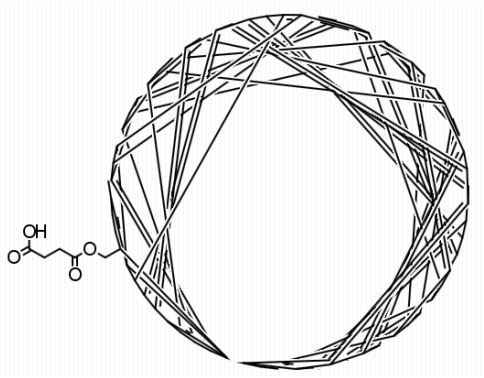
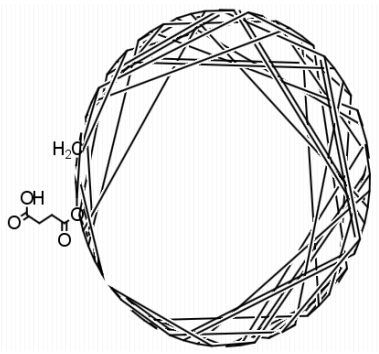
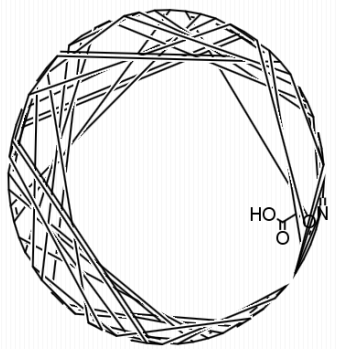
60		CC(NS(=O)(=O)c1cccc(N(=O)=O)c1)C(=O)NCc2ccccc2
64		CC(NC(=O)c1cccc(N(=O)=O)c1)C(=O)N2CCCC2
65		CC(NC(=O)c1ccc(Cl)cc1)C(=O)N2CCCC2
68		CC(NS(=O)(=O)c1cccc(N(=O)=O)c1)C(=O)N2CCCC2
73		CCOC(=O)c2ccc(NC(=O)C(C)NC(=O)c1ccc(Cl)cc1)cc2
81		CC(NC(=O)c1ccc(Cl)cc1)C(=O)Nc2cccc(C(F)(F)F)c2
82		CC(NS(=O)(=O)c1ccccc1)C(=O)Nc2cccc(C(F)(F)F)c2

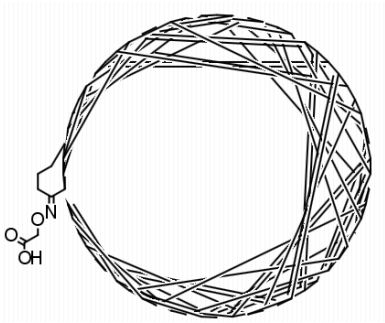
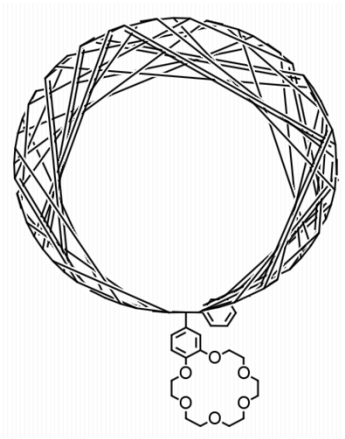
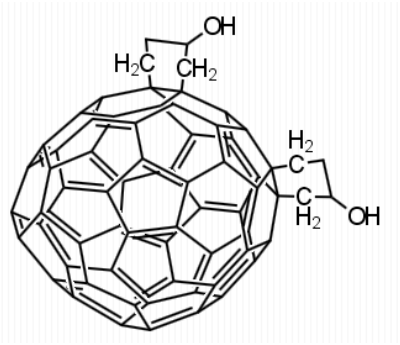
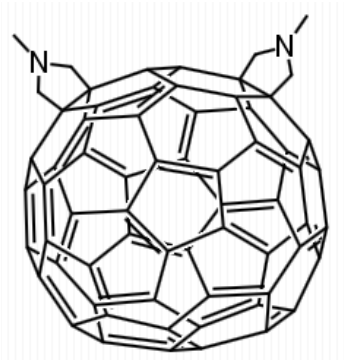
Table SI4: Chemical structure and SMILES of fullerene derivatives (case study 5)

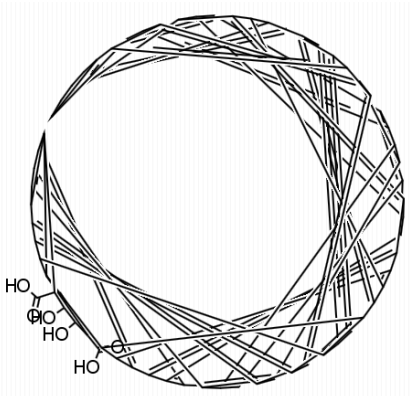
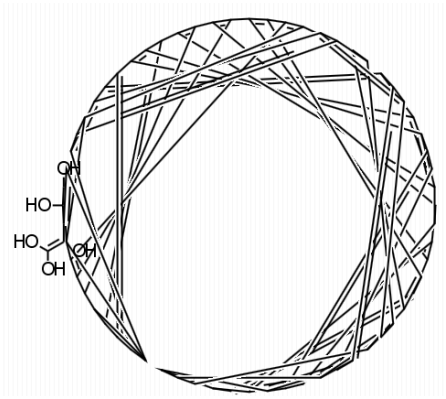
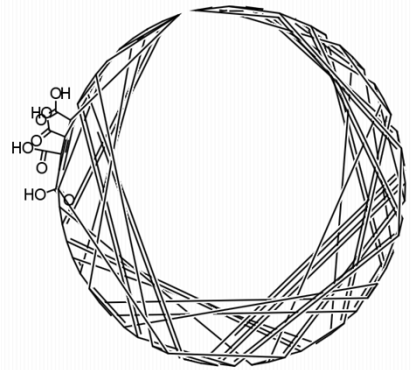
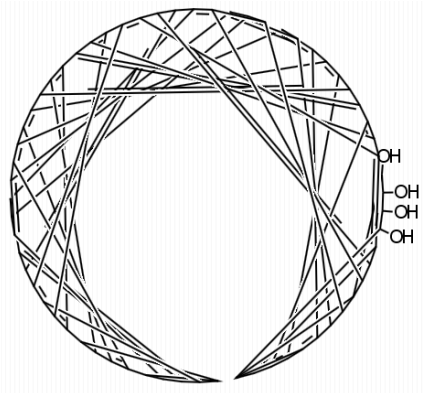
S.No.	Chemical structure	Chemical name	SMILES notation
1		(S)-phenyl({54-phenyldotriaconta cyclo [13.11.27.5^{6,12}.1^{4 ,31}.1 ^{17,21}.1^{19,26}.0^{2, 29}.0^{3,24}.0^{4,31}.0^{5,23}.0^{7,3 2}.0^{8,42}.0^{11,43}.0^{13,45}.0^{14 ,47}.0^{18,53}.0^{20,25}.0^{27,50}.0^ {28,36}.0^{30,34}.0^{33,41}.0^{35,39} .0^{37,49}.0^{38,46}.0^{40,44}.0^{48, 52}.0^{9,61}.0^{10,58}.0^{16,57}.0^{2 2,60}.0^{51,55}.0^{56,59}]henhexaco nta-1(27),2,6 (61),7,9,11,13,15(53), 16 (57),17,19,21(56),22(60),23, 25,28(36),33(41),34,37,39,42,44,46,4 8(52),49,51(55),58-heptacosaen-54-yl})methanol	O[C@@H](c1ccccc1)C%28(c 2ccccc2)C%33%29C%14C% 16=C%32C%19=C%31C=9c %18c3C%34=C7c4c3c%17c %15c%23c4C=%22C=8C6=C %21c%25c5c%13C=%12C%1 1=C5C6=C(C7=8)C%10=C% 34C=9C(=C%10%11)C=%30 C=%12C(C%27c%13c%26C(C=%20C%14=C(C%15=C%1 6c%17c%18%19)C=%24C=% 20C(=C%21C=%22C%23=%2 4)c%25%26)C%27%28%29)C (C=%30%31)=C%32%33
2		2-(4-{54-[4-(2-aminoethyl)phenyl] dotriaconta cyclo[13.11.27.5^{6, 12}.1^{4,31}.1^{17,21}.1^{19,26}.0^{2 ,29}.0^{3,24}.0^{4,31}.0^{5,23}.0^{7,3 2}.0^{8,42}.0^{11,43}.0^{13,45}.0^{14 ,47}.0^{18,53}.0^{20,25}.0^{27,50}.0^ {28,36}.0^{30,34}.0^{33,41}.0^{35,39} .0^{37,49}.0^{38,46}.0^{40,44}.0^{48, 52}.0^{9,61}.0^{10,58}.0^{16,57}.0^{2 2,60}.0^{51,55}.0^{56,59}]henhexaco nta-1(27),2,6(61),7,9,11, 13,15(53), 16(57),17,19,21(56),22(60),23,25,28(36),33(41),34,37,39,42,44,46,48(52), 49,51(55),58-hepta cosaen-54-yl}phenyl)ethan-1-amine	NCCc1ccc(cc1)C%28(c2ccc(CCN)cc2)C%33%29C%14C% 16=C%32C%19=C%31C=9c %18c3C%34=C7c4c3c%17c %15c%23c4C=%22C=8C6=C %21c%25c5c%13C=%12C%1 1=C5C6=C(C7=8)C%10=C% 34C=9C(=C%10%11)C=%30 C=%12C(C%27c%13c%26C(C=%20C%14=C(C%15=C%1 6c%17c%18%19)C=%24C=% 20C(=C%21C=%22C%23=%2 4)c%25%26)C%27%28%29)C (C=%30%31)=C%32%33
3		(18S,20S,21R)-18,21-bis(propan-2-yl)dotriaconta cyclo[8.7.46.1^{4, 7}.0^{1,22}.0^{2,28}.0^{3,16}.0^{5,29} .0^{6,39}.0^{8,12}.0^{9,40}.0^{11,60}. 0^{13,58}.0^{15,57}.0^{17,55}.0^{22, 26}.0^{23,54}.0^{24,47}.0^{25,33}.0^{ 27,31}.0^{30,38}.0^{32,36}.0^{34,46}. 0^{35,43}.0^{37,41}.0^{42,63}.0^{44, 62}.0^{45,49}.0^{48,53}.0^{50,61}.0^{ 51,59}.0^{52,56}.0^{14,64}]tetrahexa conta-2(28),3(16),4,6(39),7 (64),8(12),9,11(60),13,15(57),24,29,3 1,33,35,37,40,42,44,46,48,50(61),51, 53,55,58,62-heptacosaen-20-ol	CC(C)[C@@H]%30C[C@H](O)[C@H](C(C)C)C%23%32C %10C=%14C%29=C%19C=% 28c%13c%26c2c%12C%20= C1C=5C4=C3c(c12)c%27C% 25=C3C%24=C8C4=C7C=5C %21=C%11C=6c%22c9C(C= 67)=C8C(C%23c9c%10c%18 c%22C%15=C%11C(C=%16c %12c%13C%17=C%19C=%1 4C%18=C%15C=%16%17)=C %20%21)C%24=C%31C%25 =C(C=%28c%26%27)C%29C %30%31%32

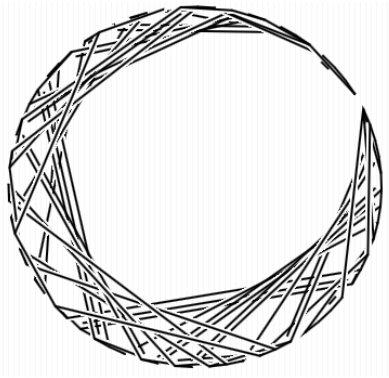
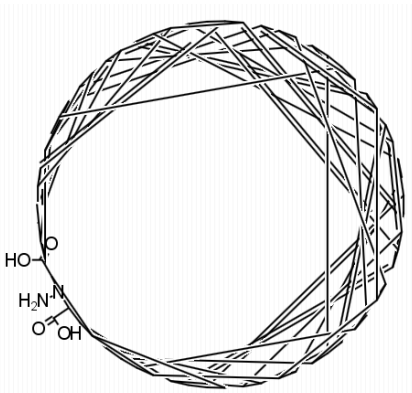
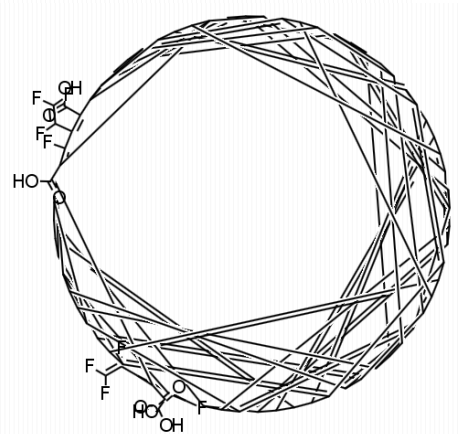
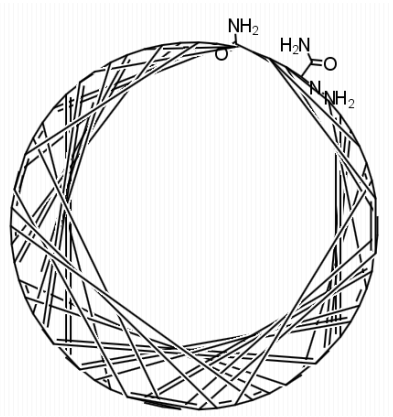
4		3-({2-[4-(54-{4-[2-(3-carboxypropanamido)ethyl] phenyl}dotriacontacyclo[13.11.27.5^{ 6,12}.1^{4,31}.1^{17,21}.1^{19,26}.0^ {2,29}.0^{3,24}.0^{4,31}.0^{5,23}.0^{7 ,32}.0^{8,42}.0^{11,43}.0^{13,45}.0^{ 14,47}.0^{18,53}.0^{20,25}.0^{27,50}. 0^{28,36}.0^{30,34}.0^{33,41}.0^{35, 39}.0^{37,49}.0^{38,46}.0^{40,44}.0^{ 48,52}.0^{9,61}.0^{10,58}.0^{16,57}.0 ^{22,60}.0^{51,55}.0^{56,59}]henhex aconta-1(27),2,6(61),7,9,11, 13,15(53),16(57),17,19,21(56),22(60) ,23,25,28(36),33(41),34,37,39,42,44, 46,48(52),49,51(55),58-heptacosaen-54-yl)phenyl] ethyl}carbamoyl)propanoic acid	O=C(O)CCC(=O)NCCc1ccc(cc1)C%28(c2ccc(CCNC(=O)CCC(=O)O)cc2)C%33%29C%14C%16=C%32C%19=C%31C=9c%18c3C%34=C7c4c3c%17c%15c%23c4C=%22C=8C6=C%21c%25c5c%13C=%12C%11=C5C6=C(C7=8)C%10=C%34C=9C(=C%10%11)C=%30C=%12C(C%27c%13c%26C(C=%20C%14=C(C%15=C%16c%17c%18%19)C=%24C=%20C(=C%21C=%22C%23=%24)c%25%26)C%27%28%29)C(C=%30%31)=C%32%33
5		6-({hentriacontacyclo[14.12.31. 1^{21,34}. 0^{2,10}.0^{3,31}.0^ {4,9} .0^{5,33}.0^{6,35}.0^{7,48}. 0^{8,50}.0^{11,51}.0^{12,28}.0^{13,5 2}.0^{14,58}.0^{15,27}.0^{17,25}.0^{1 8,41}.0^{19,24}.0^{20,39}.0^{22,32}.0 ^{23,30}.0^{26,29}.0^{36,47}.0^{37,4 5}.0^{40,44}.0^{42,59}.0^{43,56}.0^{4 6,55}.0^{49,54}.0^{53,57}.0^{38,60}]h exaconta-1(28), 2(10),3(31),4(9),5 (33),6 (35),7(48),12,14(58),15,17 (25),18,20,22(32),23,26,29,34(60),36 (47),37(45),38,40,42(59),43,46(55),5 2,56-heptacosaen-50-yl}amino) hexanoic acid	O=C(O)CCCCCNC%31%26C%29C5C3=C%25C=%23C%17=C4C=2c%16c1c%15c%14C%12=C1C=%10C=2C=9C(=C34)C5=C8c%30c7c6c%28C%22=C%21C6=C%13C=%11C7=C8C=9C=%10C=%11C%12=C%13C=%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=%27C(=C%19C=%20%21)C%22=C(C=%27C(C=%23%24)C%25%26)C%31c%28c%29%30
6		(9E)-4-({hentriacontacyclo[14.12 .31.1^{21,34} .0^{2,10}.0^{3,31}. 0^{4, 9}.0^{5,33}.0^{6,35}.0^{7, 48}.0^{8,50}.0^{11,51}.0^{12,28}.0^{13,52}.0^{14,58}.0^{15,27}.0^{17,25}.0 ^{18,41}.0^{19,24}.0^{20,39}.0^{22,3 2}.0^{23,30}.0^{26,29}.0^{36,47}.0^{3 7,45}.0^{40,44}.0^{42,59}.0^{43,56}.0 ^{46,55}.0^{49,54}.0^{53,57}.0^{38,6 0}]hexaconta-1(28) ,2(10),3(31),4(9) ,5(33) ,6(35),7(48),12,14(58),15,17 (25),18,20,22(32),23,26,29,34(60),36 (47),37(45),38,40,42(59),43,46(55),5 2,56-heptacosaen-50-yl}amino) octadec-9-enoic acid	O=C(O)CCC(CCCC\C=C\CCCCCCCC)NC%31%26C%29C5C3=C%25C=%23C%17=C4C=2c%16c1c%15c%14C%12=C1C=%10C=2C=9C(=C34)C5=C8c%30c7c6c%28C%22=C%21C6=C%13C=%11C7=C8C=9C=%10C=%11C%12=C%13C=%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=%27C(=C%19C=%20%21)C%22=C(C=%27C(C=%23%24)C%25%26)C%31c%28c%29%30
7		2-amino-6-({hentriacontacyclo [14.12. 31.1^{21,34 }.0^{2,10} .0^{3,31}.0^{ 4,9}.0^{5,33}.0^{6, 35}.0^{7,48}.0^ {8,50}.0^{11,51}.0^{12,28}.0^{13,52}. 0^{14,58}.0^{15,27}.0^{17,25}.0^{18, 41}.0^{19,24}.0^{20,39}.0^{22,32}.0^{ 23,30}.0^{26,29}.0^{36,47}.0^{37,45}. 0^{40,44}.0^{42,59}.0^{43,56}.0^{46, 55}.0^{49,54}.0^{53,57}.0^{38,60}]he xaconta-1(28),2(10),3(31),4 (9),5 (33),6(35),7(48),12,14(58),15,17(25),18,20,22(32),23,26,29,34(60),36(47),37(45),38,40,42(59),43,46(55),52,5 6-heptacosaen-50-yl}amino)hexanoic acid	O=C(O)C(N)CCCCNC%31%26C%29C5C3=C%25C=%23C%17=C4C=2c%16c1c%15c%14C%12=C1C=%10C=2C=9C(=C34)C5=C8c%30c7c6c%28C%22=C%21C6=C%13C=%11C7=C8C=9C=%10C=%11C%12=C%13C=%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=%27C(=C%19C=%20%21)C%22=C(C=%27C(C=%23%24)C%25%26)C%31c%28c%29%30

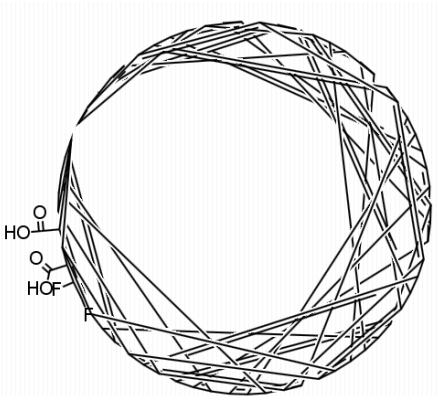
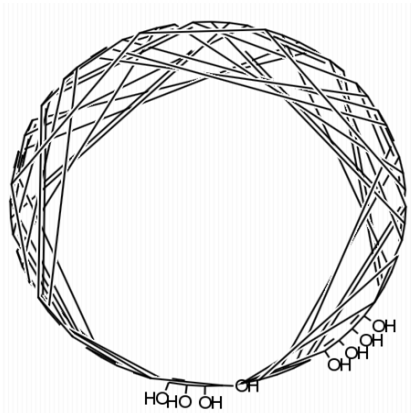
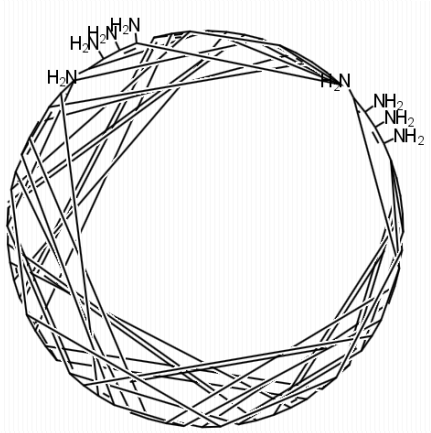
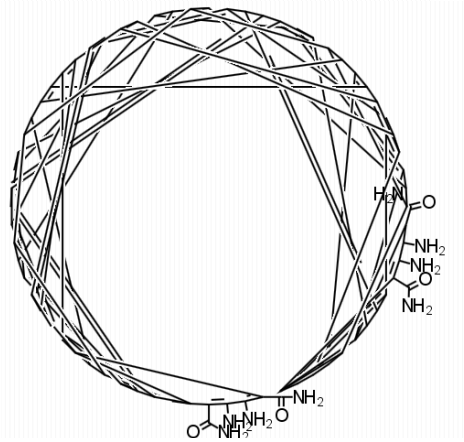
8		2-amino-5-(3-{hentriacontacyclo [14.12.31.1^{21, 34}.0^{2,10}.0^ {3,31}.0^{4,9}.0^{5,33}.0^{6,35}.0^{7,48}.0^{8,50}.0^{11,51}.0^{12,28}.0^{13,52}.0^{14,58}.0^{15,27}.0^{17,25}.0^{18,41}.0^{19,24}.0^{20,39}.0^{22,32}.0^{23,30}.0^{26,29}.0^{36,47}.0^{37,45}.0^{40,44}.0^{42,59}.0^{43,56}.0^{46,55}.0^{49,54}.0^{53,57}.0^{38,60}]hexaconta-1(28) ,2(10),3(31),4(9),5(33),6(35),7(48),12,14(58),15,17(25),18,20,22(32),23,26,29,34(60),36(47),37(45),38,40,42(59),43,46(55),52,56-heptacosaen-50-yl}carbamimidamido)pentanoic acid	O=C(O)C(N)CCCNC(=N)NC%31%26C%29C5C3=C%25C=%23C%17=C4C=2c%16c1c%15c%14C%12=C1C=%10C=2C=9C(=C34)C5=C8c%30c7c6c%28C%22=C%21C6=C%13C=%11C7=C8C=9C=%10C=%11C%12=C%13C=%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=%27C(=C%19C=%20%21)C%22=C(C=%27C(C=%23%24)C%25%26)C%31c%28c%29%30
9		3-[({hentriacontacyclo[14.12.31.1^{21,34}.0^{2,10 }.0^{3,31}.0^{4,9}.0^{5,33}.0^{6,35}.0^{7,48}.0^{8,50}.0^{11,51}.0^{12,28}.0^{13,52}.0^{14,58}.0^{15,27}.0^{17,25}.0^{18,41}.0^{19,24}.0^{20,39}.0^{22,32}.0^{23,30}.0^{26,29}.0^{36,47}.0^{37,45}.0^{40,44}.0^{42,59}.0^{43,56}.0^{46,55}.0^{49,54}.0^{53,57}.0^{38,60}]hexaconta-1(28),2(10),3(31),4(9),5(33),6(35),7(48),12,14(58),15,17(25),18,20,22(32),23,26,29,34(60),36(47),37(45),38,40,42(59),43,46(55),52,56-heptacosaen-50-yl} carbamoyl)amino]pentanedioic acid	O=C(O)CC(CC(=O)O)NC(=O)NC%31%26C%29C5C3=C%25C=%23C%17=C4C=2c%16c1c%15c%14C%12=C1C=%10C=2C=9C(=C34)C5=C8c%30c7c6c%28C%22=C%21C6=C%13C=%11C7=C8C=9C=%10C=%11C%12=C%13C=%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=%27C(=C%19C=%20%21)C%22=C(C=%27C(C=%23%24)C%25%26)C%31c%28c%29%30
10		N-[1,3-dihydroxy-2-(hydroxymethyl)propan-2-yl]-4-(4-{54-phenyldotriacontacyclo [13.11.27.5^{6,12}.1^{4,31}.1^{17,21}.1^{19,26}.0^{2,29}.0^{3,24}.0^{4,31}.0^{5,23}.0^{7,32}.0^{8,42}.0^{11,43}.0^{13,45}.0^{14,47}.0^{18,53}.0^{20,25}.0^{27,50}.0^{28,36}.0^{30,34}.0^{33,41}.0^{35,39}.0^{37,49}.0^{38,46}.0^{40,44}.0^{48,52}.0^{9,61}.0^{10,58}.0^{16,57}.0^{22,60}.0^{51,55}.0^{56,59}]henhexaconta-1(27),2,6(61),7,9,11,13, 15(53),16 (57),17,19,21(56),22(60),23,25,28(36),33(41),34,37,39,42,44,46,48(52),49,51(55),58-heptacosaen-54-yl}phenyl)butanamide	OCC(CO)(CO)NC(=O)CCCc1ccc(cc1)C%28(c2ccccc2)C%33%29C%14C%16=C%32C%19=C%31C=9c%18c3C%34=C7c4c3c%17c%15c%23c4C=%22C=8C6=C%21c%25c5c%13C=%12C%11=C5C6=C(C7=8)C%10=C%34C=9C(=C%10%11)C=%30C=%12C(C%27c%13c%26C(C=%20C%14=C(C%15=C%16c%17c%18%19)C=%24C=%20C(=C%21C=%22C%23=%24)c%25%26)C%27%28%29)C(C=%30%31)=C%32%33
11		2-({[(37Z)-35-methoxydotriacontacyclo[9.8.44.1 ^{2,6}.0^{3,21}.0^{4,53}.0^{5,55}.0^{7,16}.0^{8,56}.0^{9,14}.0^{10,57}.0^{12,45}.0^{13,31}.0^{15,30}.0^{18,29}.0^{19,27}.0^{20,25}.0^{22,52}.0^{23,50}.0^{24,40}.0^{26,39}.0^{28,33}.0^{32,44}.0^{34,39}.0^{34,43}.0^{41,49}.0^{42,47}.0^{46,63}.0^{48,61}.0^{51,60}.0^{54,59}.0^{58,62}.0^{17,64}]tetrahexaconta-1(19),2,4,6,8(56),9,11,13,15,17(64),18(29),20(25),21,23,28(33),30,32(44),41(49),42(47),45,48(61),50,52,54,57,59,62-heptacosaen-37-ylidene]amino}oxy)acetic acid	O=C(O)CO\N=C%30\CC%25%31C%12C=%14C=%15C%29C%17=C%28C%20=C%27C=7c%19c1C%32=C5c2c1c%18c%16c%21c2C=%22C=6C4=C%23c%13c3c%11C=%10C9=C3C4=C(C5=6)C8=C%32C=7C(=C89)C=%26C=%10C(C%25c%11c%12c%13C=%24C=%14C(C=%15C%16=C%17c%18c%19%20)=C%21C=%22C%23=%24)C(C=%26%27)=C%28C%29%31C(OC)C%30

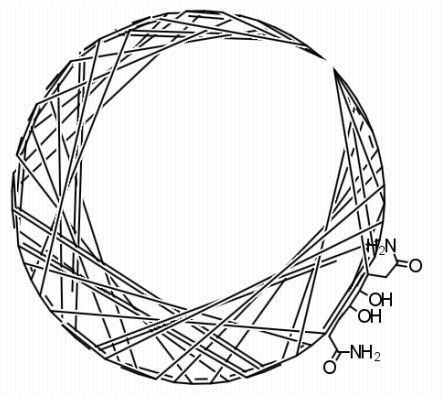
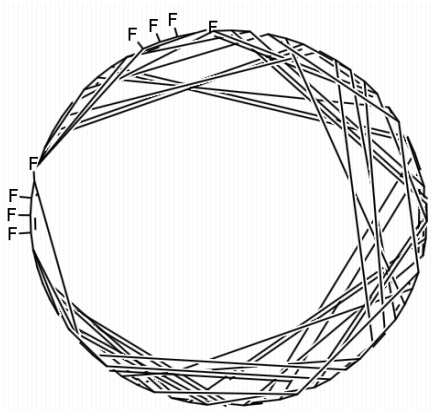
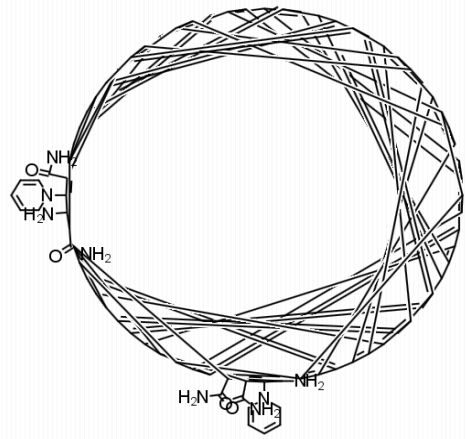
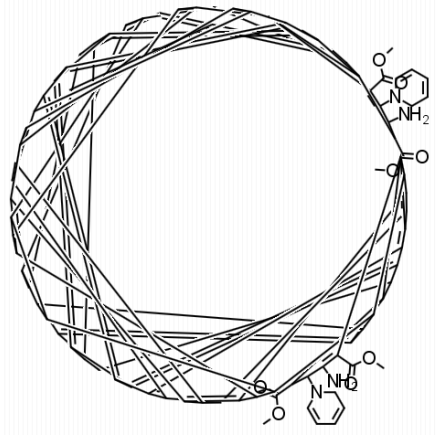
12		2-({[(31E)-dotriacontacyclo[15.12.32.1^{2,6}.1^{4, 19}.1^{22,52}.0^{1,34}.0^{3,28}.0^{5,18}.0^{7,16}.0^{8,13}.0^{10,34}.0^{11,36}.0^{12,56}.0^{14,57}.0^{15,60}.0^{20,24}.0^{21,61}.0^{23,50}.0^{25,48}.0^{27,47}.0^{29,45}.0^{35,44}.0^{37,55}.0^{38,43}.0^{39,54}.0^{40,51}.0^{41,49}.0^{42,46}.0^{53,58}.0^{9,64}.0^{26,63}.0^{59,62}]tetrahexaconta-3,5(18),6(64),7(16),8,11(36),12,14,17(61),19,21,23,25(48),26(63),27,35(44),37,39,41(49),42,46,50,52(62),53(58),54,56,59-heptacosaen-31-ylidene]amino}oxy)acetic acid	O=C(O)CO\N=C%30/CCC%26%32C%18=C5C4C%31c%29c3c2c1c%28C%24=C%23C1=C%13C=%11C2=C9C3=C4C8=C5C=%17C=7c%16c6c%15c%14C%12=C6C=%10C=7C8=C9C=%10C=%11C%12=C%13C=%22c%14c%21c%20c%15c%19c%16C=%17C%18=C%25C%19=C%20C=%27C(=C%21C=%22%23)C%24=C(C=%27C%25%26)C(c%28%29)C%31%32C%30
13		4-({34-methyldotriacontacyclo[16.12.33.1^{29,40 }.0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0^{13,41}.0^{14,59}.0^{15,62}.0^{20,51}.0^{22,50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{30,38}.0^{42,58}.0^{45,57}.0^{47,55}.0^{49,54}.0^{52,63}.0^{53,61}.0^{56,60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16),13(41) ,14,17,20,22(50),24(48),26,28,30(38),32,40(64),42,44,46,49(54),51,53(61),55,57,59,62-octa cosaen-31-yl}methoxy)-4-oxobutanoic acid	O=C(O)CCC(=O)OCC%26C=CC(C)C%32%27C%30C5C3=C%25C=%23C%17=C4C=2c%16c1c%15c%14C%12=C1C=%10C=2C=9C(=C34)C5=C8c%31c7c6c%29C%22=C%21C6=C%13C=%11C7=C8C=9C=%10C=%11C%12=C%13C=%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=%28C(=C%19C=%20%21)C%22=C(C=%28C(C=%23%24)C%25%26%27)C%32c%29c%30%31
14		4-{dotriacontacyclo[18.16.23.3^{2,11}.1^{5,42}.1^{24,49}.0^{3,38}.0^{4,41}.0^{7,51}.0^{9,53}.0^{10,55}.0^{12,35}.0^{13,56}.0^{14,58}.0^{15,34}.0^{16,32}.0^{17,59}.0^{18,30}.0^{19,27}.0^{21,25}.0^{22,57}.0^{23,54}.0^{26,44}.0^{28,43}.0^{29,40}.0^{31,39}.0^{33,37}.0^{44,49}.0^{6,64}.0^{8,63}.0^{36,62}.0^{50,61}.0^{52,60}]tetrahexaconta-1,3 ,5(61),6(64),7,9(53),10(55),11,13,15(34),16(32),17,19,21,23(54),25,27,29(40),30,33(37),35,38,41,51,56,58,62-heptacosaen-47-yloxy}-4-oxobutanoic acid	O=C(O)CCC(=O)OC%29CC%25%31C%10C=%16C=%15C%30C=%28C=%14c%32c%13c2c%12C%22=C1C=5C4=C3c(c12)c%32C%27=C3C%26=C8C4=C7C=5C%23=C%11C=6c%24c9C(C=67)=C8C(C%25c9c%10c%21c%24C%17=C%11C(C=%18c%12c%19c%13C=%14C=%15C=%20C=%16C%21=C%17C=%18C%19=%20)=C%22%23)C%26=C(C%27=%28)C%30%31CC%29
15		2-({[(31Z)-dotriacontacyclo[15.12.32.1^{2,6}.1^ {4,19}.1^{22,52}.0^{1,34}.0^{3,28}.0^{5,18}.0^{7,16}.0^{8,13}.0^{10,34}.0^{11,36}.0^{12,56}.0^{14,57}.0^{15,60}.0^{20,24}.0^{21,61}.0^{23,50}.0^{25,48}.0^{27,47}.0^{29,45}.0^{35,44}.0^{37,55}.0^{38,43}.0^{39,54}.0^{40,51}.0^{41,49}.0^{42,46}.0^{53,58}.0^{9,64}.0^{26,63}.0^{59,62}]tetrahexaconta-3,5(18),6(64),7(16),8,11(36),12,14,17(61),19, 21,23,25(48),26(63),27,32,35(44),37,39,41(49),42,46,50,52(62),53(58),54,56,59-octacosaen-31-ylidene]amino}oxy)acetic acid	O=C(O)CO\N=C%30/C=CC%26%32C%18=C5C4C%31c%29c3c2c1c%28C%24=C%23C1=C%13C=%11C2=C9C3=C4C8=C5C=%17C=7c%16c6c%15c%14C%12=C6C=%10C=7C8=C9C=%10C=%11C%12=C%13C=%22c%14c%21c%20c%15c%19c%16C=%17C%18=C%25C%19=C%20C=%27C(=C%21C=%22%23)C%24=C(C=%27C%25%26)C(c%28%29)C%31%32C%30

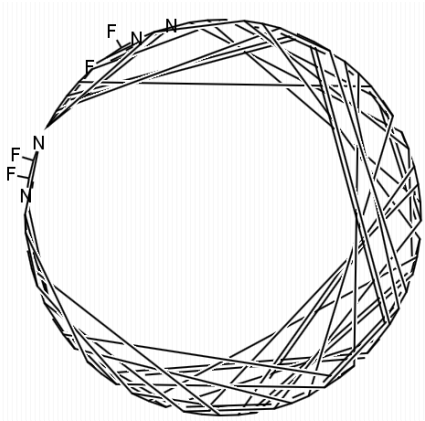
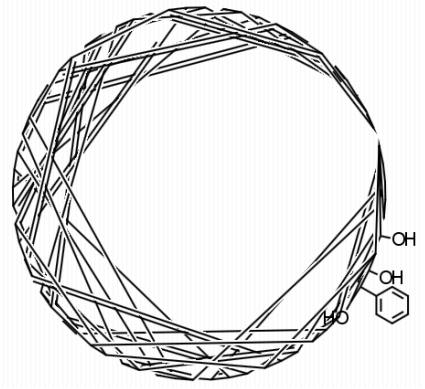
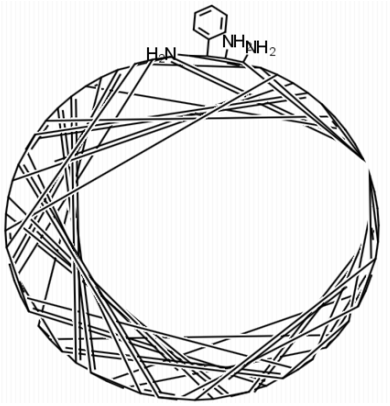
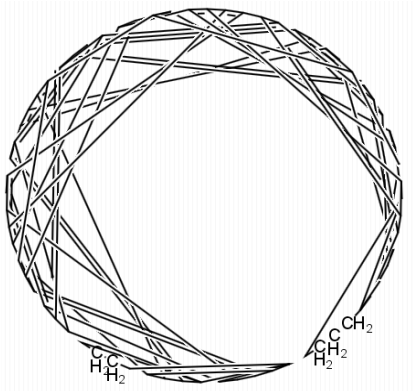
16		2-({[(32E)-28-methyltritriacontacyclo[20.5.35. 1^{2,6}.1^{4,13}.1^{5,8}. 1^{9,19}.0^{1,34}.0^{3,46}.0^{7,24}.0^{10,18}.0^{11,15}.0^{14,49}.0^{16,51}.0^{17,53}.0^{20,54}.0^{21,56}.0^{25,62}.0^{27,60}.0^{28,33}.0^{34,45}.0^{35,59}.0^{36,44}.0^{37,41}.0^{38,58}.0^{39,55}.0^{40,52}.0^{42,50}.0^{43,48}.0^{57,61}.0^{12,65}.0^{23,63}.0^{26,66}.0^{47,64}]hexahexaconta-2,4(64),5,7(24),8,10(18), 11(15),12(65),13,16(51),17(53),19(63),20,22,25(62),26(66),36(44),37(41),38,40(52),42,47,49,54,56,58,60-heptacosaen-32-ylidene]amino}oxy) acetic acid	O=C(O)CO\N=C1/CCCC%29(C)C1C%20%30C%19C%28=C%27C=%33c%18c3c2c%17C=%15C%10=C2C=%31C4=C3C=%33C%26=C6C4=C%32C5=C9c8c7c5c6c%25c%21c7c%22c%13c8C%12=C%11C9=C(C%10=C%11C%16=C%14C%12=C%13C=%24C(=C%14C(C=%15%16)C%20c%17c%18%19)C%29%30C%23C%28=C(C%21=C%22C%23=%24)C%27=C%25%26)C=%31%32
17		18-{28-phenyldotriacontacyclo[11.10.35.1^{2,11}. 1^{3,7}.1^{37,40}.0^{4,24}.0^{5,43}.0^{6,45}.0^{8,47}.0^{9,50}.0^{12,51}.0^{15,23}.0^{16,21}.0^{17,58}.0^{18,56}.0^{19,31}.0^{20,29}.0^{22,26}.0^{25,42}.0^{27,29}.0^{27,41}.0^{30,39}.0^{32,55}.0^{33,38}.0^{34,54}.0^{35,48}.0^{36,46}.0^{49,53}.0^{52,57}.0^{10,61}.0^{14,60}.0^{44,59}]henhexaconta-1(23),2,4(24),5(43),6,8,10(61),11,13(58),14(60),15,17,19(31),20,25(42),32,34,36,38,40(59),44,46,48,50,52,54,56-heptacosaen-28-yl}-2,3,5,6,8,9,11,12,14,15-decahydro-1,4,7,10,13,16-benzohexaoxacyclooctadecine	C1COCCOCCOCCOCCOc2cc(ccc2O1)C%35(c3ccccc3)C%28%34C%19=C%32C=6C=%18C=5c%17c4c%16c%15C%13=C4C=%11C=5C=%10C=6C%31=C9c%30c8c7c%29C%25=C%24C7=C%14C=%12C8=C9C=%10C=%11C=%12C%13=C%14C=%23c%15c%22c%21c%16c%20c%17C=%18C%19=C%27C%20=C%21C=%26C(=C%22C=%23%24)C%25=C(C=%26C%27%28)C%33c%29c%30C(C%31%32)C%33%34%35
18		tritriacontacyclo[15.7.43.1^{3,6}.0^{2,43}.0^{4,45}.0^{5,10}.0^{7,21}.0^{8,19}.0^{9,13}.0^{11,46}.0^{12,53}.0^{14,18}.0^{15,54}.0^{16,57}.0^{20,66}.0^{22,64}.0^{24,63}.0^{25,42}.0^{26,62}.0^{27,36}.0^{28,33}.0^{28,61}.0^{33,58}.0^{34,56}.0^{35,50}.0^{37,42}.0^{37,49}.0^{44,48}.0^{47,52}.0^{51,55}.0^{59,67}.0^{60,65}.0^{23,68}]octahexaconta-1(25),2,4,6(68) ,7,9 ,11(46),12,14,16,18,20,22,24(63),26(62),35(50),44,47(52),48,51(55),53,56,58,64,66-pentacosaene-30,40-diol	OC%16CC%22%18c%30c%21c1c5C=4C%32=C1C%19=C%11C%33=C%10C%31=C3c2c9c8c7c6c2C%23=C3C%24=C(C=4C%25C%27c5c%30C%26C%17C=%15C%29C(C6=C%14c7c%13c%12c8C(=C9%10)C%11=C%20C%12=C(C%13=C(C%14=%15)C%17%18CC%16)C%22C%21=C%19%20)=C%23C(=C%24%25)C%29%28CCC(O)CC%26%27%28)C%31=C%32%33
19		24,32-dimethyl-24,32-diazatritriacontacyclo[13.7. 42.1^{2,17}.1^{10,55}.0^{1,26}.0^{3,49}.0^{4,16}.0^{5,50}.0^{6,14}.0^{7,12}.0^{8,51}.0^{9,53}.0^{11,60}.0^{13,62}.0^{18,64}.0^{19,36}.0^{20,34}.0^{22,29}.0^{26,48}.0^{27,46}.0^{28,43}.0^{30,34}.0^{30,42}.0^{35,40}.0^{37,63}.0^{38,61}.0^{39,58}.0^{41,57}.0^{44,56}.0^{45,54}.0^{47,52}.0^{21,66}.0^{59,65}]hexahexaconta-4(16),5(50),6(14),7,9(53),10(65),11(60),12,15(64),17(66),18,20,28(43),36,38(61),39,41,44,46,48,51,54,56,58,62-pentacosaene	CN%26CC%22%28C%19C%30c6c%27c%25c1c5C=4C%32=C1C%23=C%15C%33=C%14C%31=C3c2c%13c%12c%11c%10c2C9=C3C7=C(C=4C8C(c56)C%30%29CN(C)CC%21%29C(=C78)C9=C%20C%10=C%18c%11c%17c%16c%12C(=C%13%14)C%15=C%24C%16=C(C%17=C%22C%18=C%19C%20%21)C(C%25=C%23%24)C%27%28C%26)C%31=C%32%33

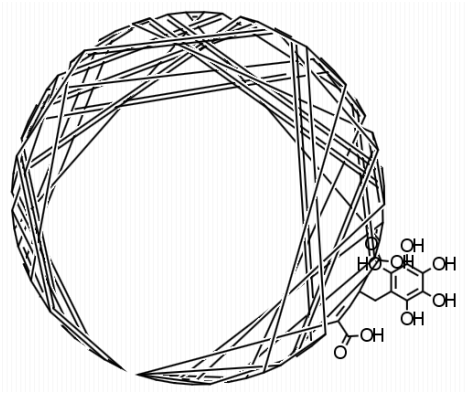
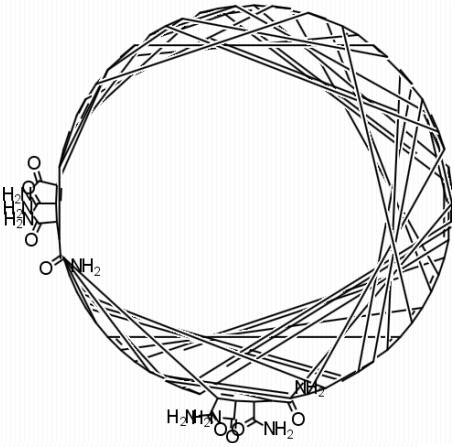
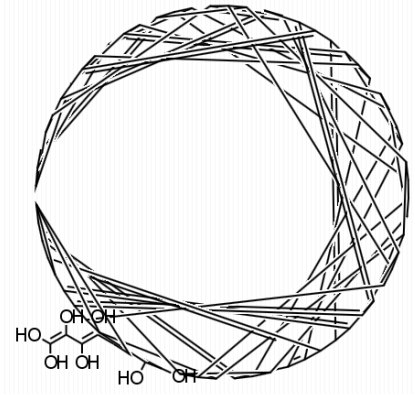
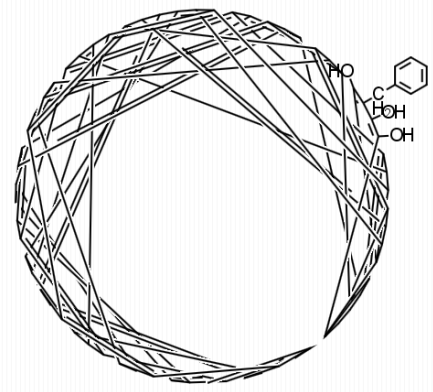
20		32,33-dihydroxydotriacontacyclo [16.12.33.1^{29, 40}.0^{1,35} .0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0 ^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{ 10,37}.0^{11,39}.0^{12,16}.0^{13,41}. 0^{14,59}.0^{15,62}.0^{20,51}.0^{22, 50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{ 30,38}.0^{42,58}.0^{45,57}.0^{47,55}. 0^{49,54}.0^{52,63}.0^{53,61}.0^{56, 60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16), 13(41),14,17,20,22(50),24(48),26,28, 30(38),31,33,40(64),42,44,46,49(54), 51,53(61),55,57,59,62-nona cosaene-31,34-dicarboxylic acid	O=C(O)C%26=C(O)C(O)=C(C (=O)O)C%32%27C%30C5C3 =C%25C=%23C%17=C4C=2 c%16c1c%15c%14C%12=C1 C=%10C=2C=9C(=C34)C5=C 8c%31c7c6c%29C%22=C%2 1C6=C%13C=%11C7=C8C=9 C=%10C=%11C%12=C%13C =%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=% 28C(=C%19C=%20%21)C%2 2=C(C=%28C(C=%23%24)C %25%26%27)C%32c%29c%3 0%31
21		1-{32,33-dihydroxydotriaconta cyclo[15.12.32. 1^{2,6}.1^{4,19 }.1^{22,52}.0^{1,34}.0^{3,28}.0^{5,18} .0^{7,16}.0^{8,13}.0^{10,34}.0^{11,36 }.0^{12,56}.0^{14,57}.0^{15,60}.0^{20 ,24}.0^{21,61}.0^{23,50}.0^{25,48}.0^ {27,47}.0^{29,45}.0^{35,44}.0^{37,55} .0^{38,43}.0^{39,54}.0^{40,51}.0^{41, 49}.0^{42,46}.0^{53,58}.0^{9,64}.0^{2 6,63}.0^{59,62}]tetrahexaconta-3,5(18),6(64),7(16),8,11(36),12,14, 17(61),19,21,23,25(48),26(63),27,30, 32,35(44),37,39,41(49),42,46,50,52(62),53(58),54,56,59-nonacosaen-31-yl}ethene-1,2,2-triol	O/C(O)=C(/O)C=%31C(O)=C(O)C%26%32C%18=C5C4C% 30c%29c3c2c1c%28C%24=C %23C1=C%13C=%11C2=C9 C3=C4C8=C5C=%17C=7c%1 6c6c%15c%14C%12=C6C=% 10C=7C8=C9C=%10C=%11C %12=C%13C=%22c%14c%2 1c%20c%15c%19c%16C=%1 7C%18=C%25C%19=C%20C =%27C(=C%21C=%22%23)C %24=C(C=%27C%25%26)C(c%28%29)C%30%32C=%31
22		dotriacontacyclo[16.12.33.1^{29,40}. 0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0 ^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{ 9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0 ^{13,41}.0^{14,59}.0^{15,62}.0^{20,5 1}.0^{22,50}.0^{24,48}.0^{26,46}.0^{2 7,44}.0^{30,38}.0^{42,58}.0^{45,57}.0 ^{47,55}.0^{49,54}.0^{52,63}.0^{53,6 1}.0^{56,60}.0^{43,64}]tetrahexacont a-3(25), 4(23),6,8(19),9,11(39) ,12(16),13(41),14,17,20,22(50),24(48),26,28,30(38),31,33,40(64),42,44,46 ,49(54),51,53(61),55,57,59,62-nonacosaene-31,32,33,34-tetracarboxylic acid	O=C(O)C%26=C(C(=O)O)C(C (=O)O)=C(C(=O)O)C%32%27 C%30C5C3=C%25C=%23C% 17=C4C=2c%16c1c%15c%14 C%12=C1C=%10C=2C=9C(= C34)C5=C8c%31c7c6c%29C %22=C%21C6=C%13C=%11 C7=C8C=9C=%10C=%11C% 12=C%13C=%20c%14c%19c %18c%15c(c%16%17)C%24= C%18C=%28C(=C%19C=%2 0%21)C%22=C(C=%28C(C= %23%24)C%25%26%27)C% 32c%29c%30%31
23		dotriacontacyclo[16.12.33.1^{29,40}. 0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0 ^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{ 9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0 ^{13,41}.0^{14,59}.0^{15,62}.0^{20,5 1}.0^{22,50}.0^{24,48}.0^{26,46}.0^{2 7,44}.0^{30,38}.0^{42,58}.0^{45,57}.0 ^{47,55}.0^{49,54}.0^{52,63}.0^{53,6 1}.0^{56,60}.0^{43,64}]tetrahexacont a-3(25), 4(23),6,8(19),9,11(39),12 (16),13(41),14,17,20,22(50),24(48),2 6,28,30(38),31,33,40(64),42,44,46,49 (54),51,53(61),55,57,59,62-nonacosaene-31,32,33,34-tetrol	OC%26=C(O)C(O)=C(O)C%3 2%27C%30C5C3=C%25C=% 23C%17=C4C=2c%16c1c%1 5c%14C%12=C1C=%10C=2C =9C(=C34)C5=C8c%31c7c6c %29C%22=C%21C6=C%13C =%11C7=C8C=9C=%10C=% 11C%12=C%13C=%20c%14c %19c%18c%15c(c%16%17)C %24=C%18C=%28C(=C%19 C=%20%21)C%22=C(C=%28 C(C=%23%24)C%25%26%27)C%32c%29c%30%31

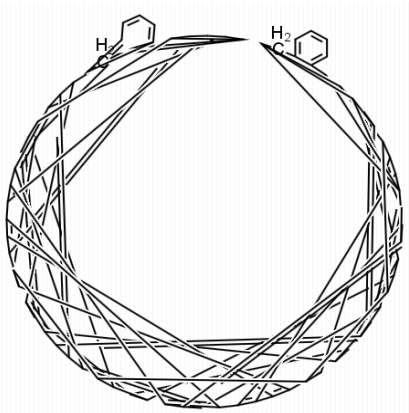
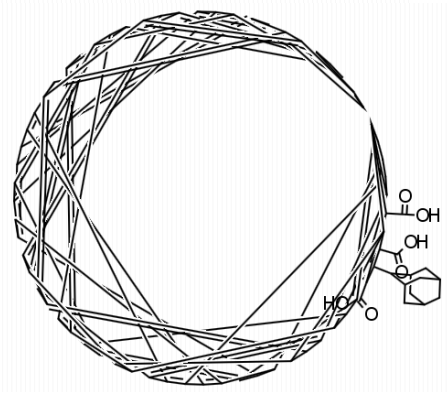
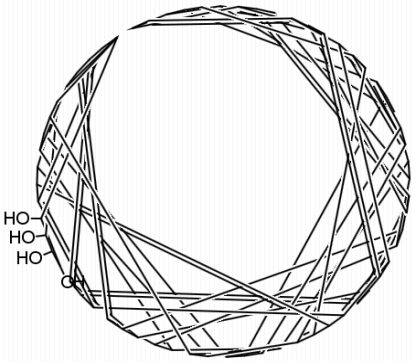
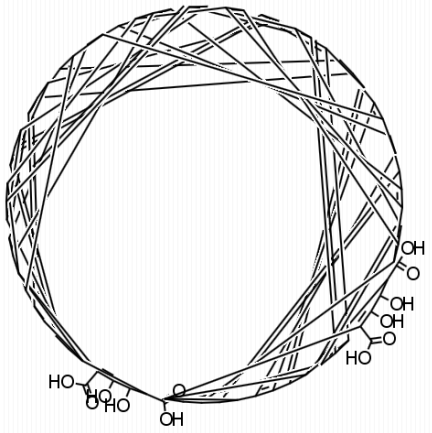
24		tritriacontacyclo[19.11.30.6^{5,8}.0^{2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35}.0^{10,14}.0^{11,37}.0^{12,40}.0^{13,55}.0^{16,56}.0^{18,58}.0^{20,59}.0^{23,32}.0^{24,62}.0^{25,45}.0^{26,31}.0^{27,44}.0^{28,38}.0^{29,36}.0^{30,33}.0^{39,43}.0^{41,54}.0^{42,51}.0^{45,50}.0^{50,61}.0^{52,60}.0^{53,57}.0^{8,67}.0^{15,67}.0^{17,68}]octahexaconta-1(32),2(6),3(22),4(19),5(68),9(35),10(14),11,13(55),16,18(58),20(59),21(62),23,26,28,30,33,36,38,40,42(51),46,48,52(60),53,56,63,65-nonacosaene	C%30=CC=CC%29%33C2=C%28C=1c%27c8C=%22C=1C=%24C2=C%32C%25=C7c6c%31c5c(c%26C=4C%29C%28=C3c%27c9C%10=C3C=4C=%11c%26c%12c5c%13c6C%21=C7C=%23C=%14C(C%15c8c9C%16C%20=C%10C=%11C=%19C%12=C%13C%18=C%21C=%14C%17(C=CC=CC%15%16%17)C%18C=%19%20)C=%22C=%23C=%24%25)C%30%33C%31%32
25		30-amino-30-azadotriacontacyclo[10.10.41.0^{2, 16}.0^{3,25}.0^{4,15}.0^{5,9}.0^{6,26}.0^{7,46}.0^{8,56}.0^{10,14}.0^{11,57}.0^{13,18}.0^{17,21}.0^{19,62}.0^{20,37}.0^{22,35}.0^{23,34}.0^{24,28}.0^{27,45}.0^{28,32}.0^{32,43}.0^{33,41}.0^{36,40}.0^{38,61}.0^{39,51}.0^{42,50}.0^{44,48}.0^{47,55}.0^{49,53}.0^{52,60}.0^{54,58}.0^{59,63}]trihexaconta-1(23),2(16), 3(25),4,6(26),7(46),8,10,14,17,19(62),20(37),21,34,36(40),38,41,43,47,49,51,53,55,57,60-pentacosaene-29,31-dicarboxylic acid	O=C(O)C%30N(N)C(C(=O)O)C%23%31C%16C=%10C=9C%29C=%32C=8c%27c7c2c5c%26C%25=C%20C6=C%19C3=C1C=%18c%17c%15C%11=C1C4C=%12c(c2C(C34)C56)c%13c7C=8C=9C=%14C=%10C(=C%11C=%12C%13=%14)c%15c%16c%22c%17C=%21C=%18C%19=C%20C=%24C=%21C(C%22%23)C=%28C=%24C%25=C(c%26%27)C=%32C=%28C%29%30%31
26		17,42-difluoro-18,43-bis(trifluoroethenyl) tritriacontacyclo [7.6.53.0^{15,26}.0^{14,58}.0^{2,13}.0^{1,20}.0^{25,29}.0^{20,24}.0^{23,31}.0^{4,21}.0^{22,34}.0^{3,7}.0^{5,35}.0^{6,67}.0^{8,12}.0^{10,62}.0^{11,59}.0^{56,60}.0^{27,57}.0^{28,54}.0^{30,52}.0^{32,51}.0^{33,37}.0^{38,50}.0^{40,49}.0^{40,45}.0^{39,65}.0^{45,63}.0^{64,68}.0^{36,66}.0^{46,61}.0^{48,53}.0^{47,55}]octahexaconta-3,5,7,9,11,13,15(26),16,18,21,23(31),25(29),27(57),28(54),30(52),32,34,36(66),37,41,43,47(55),48(53),50,56(60),58,61,63,67-nonacosaene-16,19,41,44-tetracarboxylic acid	F/C(F)=C(/F)C=3C(F)=C(C(=O)O)C%13%14c%15c%16c%12c%17C=%10C=%18C=8C=%19C7C%20c%31c6c%33C=5C=4C2=C1c%33c%30C%21=C1C%23=C(C2C%14(C=3C(=O)O)C=4C=%11C=9C=5C6=C7C=8C=9C=%10C=%11C%12%13)c%15c%22c%24c%16c%25c%17C=%18C=%26C=%19C%29%32C(C(=O)O)=C(C(\F)=C(/F)F)C(F)=C(C(=O)O)C%20%32C(C%28=C%21C(=C%22%23)C=%27C%24=C%25C=%26C%29C=%27%28)c%30%31
27		30-amino-30-azadotriacontacyclo[10.10.41. 0^{2,16}.0^{3,25}.0^{4,15}.0^{5,9}.0^{6,26}.0^{7,46}.0^{8,56}.0^{10,14}.0^{11,57}.0^{13,18}.0^{17,21}.0^{19,62}.0^{20,37}.0^{22,35}.0^{23,34}.0^{24,28}.0^{27,45}.0^{28,32}.0^{32,43}.0^{33,41}.0^{36,40}.0^{38,61}.0^{39,51}.0^{42,50}.0^{44,48}.0^{47,55}.0^{49,53}.0^{52,60}.0^{54,58}.0^{59,63}]trihexaconta-1(23),2(16),3(25),4,6(26),7(46),8,10,14,17,19(62),20(37),21,34,36(40),38,41,43,47,49,51,53,55,57,60-pentacosaene-29,31-dicarboxamide	NC(=O)C%30N(N)C(C(N)=O)C%23%31C%16C=%10C=9C%29C=%32C=8c%27c7c2c5c%26C%25=C%20C6=C%19C3=C1C=%18c%17c%15C%11=C1C4C=%12c(c2C(C34)C56)c%13c7C=8C=9C=%14C=%10C(=C%11C=%12C%13=%14)c%15c%16c%22c%17C=%21C=%18C%19=C%20C=%24C=%21C(C%22%23)C=%28C=%24C%25=C(c%26%27)C=%32C=%28C%29%30%31

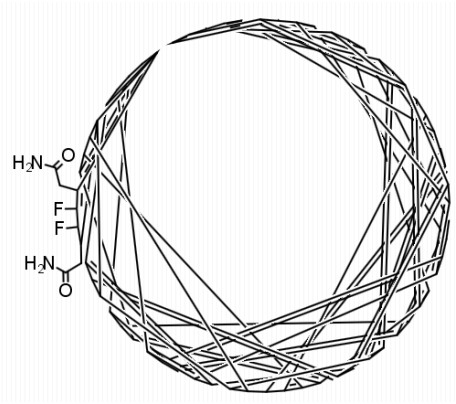
28		32,33-difluorodotriacontacyclo [16.12.33.1^{29, 40}.0^{1,35} .0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0 ^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{ 10,37}.0^{11,39}.0^{12,16}.0^{13,41}. 0^{14,59}.0^{15,62}.0^{20,51}.0^{22, 50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{ 30,38}.0^{42,58}.0^{45,57}.0^{47,55}. 0^{49,54}.0^{52,63}.0^{53,61}.0^{56, 60}.0^{43,64}]tetrahexaconta- 3(25),4(23),6,8(19),9,11(39),12(16),1 3 (41),14,17,20,22(50),24(48),26,28, 30(38),31,33,40(64),42,44,46,49(54), 51,53(61),55,57,59,62-nona cosaene-31,34-dicarboxylic acid	O=C(O)C%26=C(F)C(F)=C(C(=O)O)C%32%27C%30C5C3= C%25C=%23C%17=C4C=2c %16c1c%15c%14C%12=C1C =%10C=2C=9C(=C34)C5=C8 c%31c7c6c%29C%22=C%21 C6=C%13C=%11C7=C8C=9 C=%10C=%11C%12=C%13C =%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=% 28C(=C%19C=%20%21)C%2 2=C(C=%28C(C=%23%24)C %25%26%27)C%32c%29c%3 0%31
29		tritriacontacyclo[19.11.30.6^{5,8}.0^{ 2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,3 5}.0^{10,14}.0^{11,37}.0^{12,40}.0^{1 3,55}.0^{16,56}.0^{18,58}.0^{20,59}.0 ^{23,32}.0^{24,62}.0^{25,45}.0^{26,3 1}.0^{27,44}.0^{28,38}.0^{29,36}.0^{3 0,33}.0^{39,43}.0^{41,54}.0^{42,51}.0 ^{45,50}.0^{50,61}.0^{52,60}.0^{53,5 7}.0^{8,67}.0^{15,67}.0^{17,68}]octah exaconta-1(32),2(6),3(22), 4(19),5(68),9(35),10(14),11,13(55),1 6,18(58),20(59),21(62),23,26,28,30,3 3,36,38,40,42(51),46,48,52(60),53,56 ,63,65-nonacosaen -46,47,48, 49,63,64,65,66-octol	OC%30=C(O)C(O)=C(O)C%2 9%33C2=C%28C=1c%27c8C =%22C=1C=%24C2=C%32C %25=C7c6c%31c5c(c%26C= 4C%29C%28=C3c%27c9C% 10=C3C=4C=%11c%26c%12 c5c%13c6C%21=C7C=%23C =%14C(C%15c8c9C%16C%2 0=C%10C=%11C=%19C%12 =C%13C%18=C%21C=%14C %17(C(O)=C(O)C(O)=C(O)C %15%16%17)C%18C=%19% 20)C=%22C=%23C=%24%25)C%30%33C%31%32
30		tritriacontacyclo[19.11.30.6^{5,8}.0^{ 2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,3 5}.0^{10,14}.0^{11,37}.0^{12,40}.0^{1 3,55}.0^{16,56}.0^{18,58}.0^{20,59}.0 ^{23,32}.0^{24,62}.0^{25,45}.0^{26,3 1}.0^{27,44}.0^{28,38}.0^{29,36}.0^{3 0,33}.0^{39,43}.0^{41,54}.0^{42,51}.0 ^{45,50}.0^{50,61}.0^{52,60}.0^{53,5 7}.0^{8,67}.0^{15,67}.0^{17,68}]octah exaconta-1(32),2(6),3(22) ,4(19),5(68),9(35),10(14),11,13(55),1 6,18(58),20(59),21(62),23,26,28,30,3 3,36,38,40,42(51),46,48,52(60),53,56 ,63,65-nonacosaen-46,47,48 ,49,63,64,65,66-octamine	NC%30=C(N)C(N)=C(N)C%2 9%33C2=C%28C=1c%27c8C =%22C=1C=%24C2=C%32C %25=C7c6c%31c5c(c%26C= 4C%29C%28=C3c%27c9C% 10=C3C=4C=%11c%26c%12 c5c%13c6C%21=C7C=%23C =%14C(C%15c8c9C%16C%2 0=C%10C=%11C=%19C%12 =C%13C%18=C%21C=%14C %17(C(N)=C(N)C(N)=C(N)C %15%16%17)C%18C=%19% 20)C=%22C=%23C=%24%25)C%30%33C%31%32
31		47,48,64,65-tetraaminotritria contacyclo[19.11. 30.6^{5,8}.0^{2 ,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35 }.0^{10,14}.0^{11,37}.0^{12,40}.0^{13 ,55}.0^{16,56}.0^{18,58}.0^{20,59}.0^ {23,32}.0^{24,62}.0^{25,45}.0^{26,31} .0^{27,44}.0^{28,38}.0^{29,36}.0^{30, 33}.0^{39,43}.0^{41,54}.0^{42,51}.0^{ 45,50}.0^{50,61}.0^{52,60}.0^{53,57}. 0^{8,67}.0^{15,67}.0^{17,68}]octahex aconta-1(32),2(6),3(22),4(19), 5(68),9(35),10(14),11,13(55),16,18(5 8),20(59),21(62),23,26,28,30,33,36,3 8,40,42(51),46,48,52(60),53,56,63,65 -nonacosaene-46,49,63,66- tetracarboxamide	NC(=O)C%30=C(N)C(N)=C(C (N)=O)C%29%33C2=C%28C =1c%27c8C=%22C=1C=%24 C2=C%32C%25=C7c6c%31c 5c(c%26C=4C%29C%28=C3 c%27c9C%10=C3C=4C=%11 c%26c%12c5c%13c6C%21= C7C=%23C=%14C(C%15c8c 9C%16C%20=C%10C=%11C =%19C%12=C%13C%18=C% 21C=%14C%17(C(C(N)=O)= C(N)C(N)=C(C(N)=O)C%15% 16%17)C%18C=%19%20)C= %22C=%23C=%24%25)C%3 0%33C%31%32

32		2-[31-(carbamoylmethyl)-32,33-dihydroxydotria contacyclo [16.12.33.1^{29,40}.0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0^{13,41}.0^{14,59}.0^{15,62}.0^{20,51}.0^{22,50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{30,38}.0^{42,58}.0^{45,57}.0^{47,55}.0^{49,54}.0^{52,63}.0^{53,61}.0^{56,60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16),13(41),14,17,20,22(50),24(48),26,28,30(38),31,33,40(64),42,44,46,49(54),51,53(61),55,57,59,62-nonacosaen-34-yl]acetamide	NC(=O)CC%26=C(O)C(O)=C(CC(N)=O)C%32%27C%30C5C3=C%25C=%23C%17=C4C=2c%16c1c%15c%14C%12=C1C=%10C=2C=9C(=C34)C5=C8c%31c7c6c%29C%22=C%21C6=C%13C=%11C7=C8C=9C=%10C=%11C%12=C%13C=%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=%28C(=C%19C=%20%21)C%22=C(C=%28C(C=%23%24)C%25%26%27)C%32c%29c%30%31
33		46,47,48,49,63,64,65,66-octafluorotritriacontacyclo[19.11.30.6^{5,8}.0^{2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35}.0^{10,14}.0^{11,37}.0^{12,40}.0^{13,55}.0^{16,56}.0^{18,58}.0^{20,59}.0^{23,32}.0^{24,62}.0^{25,45}.0^{26,31}.0^{27,44}.0^{28,38}.0^{29,36}.0^{30,33}.0^{39,43}.0^{41,54}.0^{42,51}.0^{45,50}.0^{50,61}.0^{52,60}.0^{53,57}.0^{8,67}.0^{15,67}.0^{17,68}]octahexaconta-1(32),2(6),3(22),4(19),5(68),9(35),10(14),11,13(55),16,18(58),20(59),21(62),23,26,28,30,33,36,38,40,42(51),46,48,52(60),53,56,63,65-nonacosaene	FC%30=C(F)C(F)=C(F)C%29%33C2=C%28C=1c%27c8C=%22C=1C=%24C2=C%32C%25=C7c6c%31c5c(c%26C=4C%29C%28=C3c%27c9C%10=C3C=4C=%11c%26c%12c5c%13c6C%21=C7C=%23C=%14C(C%15c8c9C%16C%20=C%10C=%11C=%19C%12=C%13C%18=C%21C=%14C%17(C(F)=C(F)C(F)=C(F)C%15%16%17)C%18C=%19%20)C=%22C=%23C=%24%25)C%30%33C%31%32
34		47,65-diamino-48,64-bis(1,2-dihydropyridin-1-yl)tritriacontacyclo [19.11.30.6^{5,8}.0^{2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35}.0^{10,14}.0^{11,37}.0^{12,40}.0^{13,55}.0^{16,56}.0^{18,58}.0^{20,59}.0^{23,32}.0^{24,62}.0^{25,45}.0^{26,31}.0^{27,44}.0^{28,38}.0^{29,36}.0^{30,33}.0^{39,43}.0^{41,54}.0^{42,51}.0^{45,50}.0^{50,61}.0^{52,60}.0^{53,57}.0^{8,67}.0^{15,67}.0^{17,68}]octahexaconta-1(32),2(6),3(22),4(19),5(68),9(35),10(14),11,13(55),16,18(58),20(59),21(62),23,26,28,30,33,36,38,40,42(51),46,48,52(60),53,56,63,65-nonacosaene-46,49,63,66-tetracarboxamide	NC(=O)C%32=C(N)C(N1C=CC=CC1)=C(C(N)=O)C%31%35C3=C%30C=2c%29c%10C=9C=2C=%26C3=C%34C%27=C8c7c%33c6c(c%28C=5C%31C%30=C4c%29c%11C%12=C4C=5C=%13c%28c%14c6c%15c7C%16=C8C%17=C(C=9C%18C%20c%10c%11C%19C%24=C%12C=%13C=%23C%14=C%15C%25=C%16C(=C%17%18)C%21(C(C(N)=O)=C(C(N)=C(C(N)=O)C%19%20%21)N%22C=CC=CC%22)C%25C=%23%24)C=%26%27)C%32%35C%33%34
35		46,49,63,66-tetramethyl 47,65-diamino-48,64-bis(1,2-dihydropyridin-1-yl)tritriacontacyclo [19.11.30.6^{5,8}.0^{2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35}.0^{10,14}.0^{11,37}.0^{12,40}.0^{13,55}.0^{16,56}.0^{18,58}.0^{20,59}.0^{23,32}.0^{24,62}.0^{25,45}.0^{26,31}.0^{27,44}.0^{28,38}.0^{29,36}.0^{30,33}.0^{39,43}.0^{41,54}.0^{42,51}.0^{45,50}.0^{50,61}.0^{52,60}.0^{53,57}.0^{8,67}.0^{15,67}.0^{17,68}]octahexaconta-1(32),2(6),3(22),4(19),5(68),9(35),10(14),11,13(55),16,18(58),20(59),21(62),23,26,28,30,33,36,38,40,42(51),46,48,52(60),53,56,63,65-nonacosaene-46,49,63,66-tetracarboxylate	O=C(OC)C%32=C(N)C(N1C=CC=CC1)=C(C(=O)OC)C%31%35C3=C%30C=2c%29c%10C=9C=2C=%26C3=C%34C%27=C8c7c%33c6c(c%28C=5C%31C%30=C4c%29c%11C%12=C4C=5C=%13c%28c%14c6c%15c7C%16=C8C%17=C(C=9C%18C%20c%10c%11C%19C%24=C%12C=%13C=%23C%14=C%15C%25=C%16C(=C%17%18)C%21(C(C(=O)OC)=C(C(N)=C(C(=O)OC)C%19%20%21)N%22C=CC=CC%22)C%25C=%23%24)C=%26%27)C%32%35C%33%34

36		42,43,66,67-tetrafluoro-41,44,65,68-tetraaza tritriacontacyclo[9.9.41.6^{3,16}.1^{10,37}.0^{2,28}.0^{4,29}.0^{5,13}.0^{6,31}.0^{7,12}.0^{8,33}.0^{9,35}.0^{15,61}.0^{17,59}.0^{18,57}.0^{19,22}.0^{21,26}.0^{23,56}.0^{24,54}.0^{25,51}.0^{27,50}.0^{30,49}.0^{32,48}.0^{34,46}.0^{36,40}.0^{38,58}.0^{39,55}.0^{40,45}.0^{45,53}.0^{47,52}.0^{3,64}.0^{14,64}.0^{20,63}.0^{60,62}]octahexaconta-1(20),4,6(31),7,9(35),10,12,15(61),16(63),17,19(22),21(26),23,25(51),27(50),28,30(49),32(48),33,37(62),38(58),41,43,47(52),53,56,59,65,67-nonacosaene	FC%30=NC%33%32C=4C2=C1C%31c5c9C%10=C1C%11=C2C%28=C3c%12c%23C%25=C(C3=4)C%33C=%26c6c(c5c8c7c6C%27=C%29C%24=C%13C%20=C%29C7=C%19c8c9C%18=C%10C%14=C%11C%15=C%28c%12c%16c(C%13C%17%22N=C(F)C(F)=NC%21%22C(=C%14C%15C%16%17)C%18=C%19C%20%21)c%23C%24=C%25C=%26%27)C%31%32N=C%30F
37		33-phenyldotriacontacyclo [16.12.33.1^{29,40} .0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0^{13,41}.0^{14,59}.0^{15,62}.0^{20,51}.0^{22,50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{30,38}.0^{42,58}.0^{45,57}.0^{47,55}.0^{49,54}.0^{52,63}.0^{53,61}.0^{56,60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16),13(41),14,17,20,22(50),24(48),26,28,30(38),31,33,40(64),42,44,46,49(54),51,53(61),55,57,59,62-nonacosaene-31,32,34-triol	OC%27=C(O)C(c1ccccc1)=C(O)C%33%28C%31C6C4=C%26C=%24C%18=C5C=3c%17c2c%16c%15C%13=C2C=%11C=3C=%10C(=C45)C6=C9c%32c8c7c%30C%23=C%22C7=C%14C=%12C8=C9C=%10C=%11C=%12C%13=C%14C=%21c%15c%20c%19c%16c(c%17%18)C%25=C%19C=%29C(=C%20C=%21%22)C%23=C(C=%29C(C=%24%25)C%26%27%28)C%33c%30c%31%32
38		33-phenyldotriacontacyclo[16.12.33.1^{29,40}.0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0^{13,41}.0^{14,59}.0^{15,62}.0^{20,51}.0^{22,50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{30,38}.0^{42,58}.0^{45,57}.0^{47,55}.0^{49,54}.0^{52,63}.0^{53,61}.0^{56,60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16),13(41),14,17,20,22(50),24(48),26,28,30(38),31,33,40(64),42,44,46,49(54),51,53(61),55,57,59,62-nonacosaene-31,32,34-triamine	NC%27=C(N)C(c1ccccc1)=C(N)C%33%28C%31C6C4=C%26C=%24C%18=C5C=3c%17c2c%16c%15C%13=C2C=%11C=3C=%10C(=C45)C6=C9c%32c8c7c%30C%23=C%22C7=C%14C=%12C8=C9C=%10C=%11C=%12C%13=C%14C=%21c%15c%20c%19c%16c(c%17%18)C%25=C%19C=%29C(=C%20C=%21%22)C%23=C(C=%29C(C=%24%25)C%26%27%28)C%33c%30c%31%32
39		tritriacontacyclo[19.11.30.6^{5,8}.0^{2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35}.0^{10,14}.0^{11,37}.0^{12,40}.0^{13,55}.0^{16,56}.0^{18,58}.0^{20,59}.0^{23,32}.0^{24,62}.0^{25,45}.0^{26,31}.0^{27,44}.0^{28,38}.0^{29,36}.0^{30,33}.0^{39,43}.0^{41,54}.0^{42,51}.0^{45,50}.0^{50,61}.0^{52,60}.0^{53,57}.0^{8,67}.0^{15,67}.0^{17,68}]octahexaconta-1(32),2(6),3(22),4(19),5(68),9(35),10(14),11,13(55),16,18(58),20(59),21(62),23,26,28,30,33,36,38,40,42(51),52(60),53,56-pentacosaene	C%30CCCC%29%33C2=C%28C=1c%27c8C=%22C=1C=%24C2=C%32C%25=C7c6c%31c5c(c%26C=4C%29C%28=C3c%27c9C%10=C3C=4C=%11c%26c%12c5c%13c6C%21=C7C=%23C=%14C(C%15c8c9C%16C%20=C%10C=%11C=%19C%12=C%13C%18=C%21C=%14C%17(CCCCC%15%16%17)C%18C=%19%20)C=%22C=%23C=%24%25)C%30%33C%31%32

40		33-[(pentahydroxyphenyl)methyl] dotriacontacyclo [16.12.33.1^{29, 40}.0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0^{13,41}.0^{14,59}.0^{15,62}.0^{20,51}.0^{22,50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{30,38}.0^{42,58}.0^{45,57}.0^{47,55}.0^{49,54}.0^{52,63}.0^{53,61}.0^{56,60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16),13(41),14,17,20,22(50),24(48),26,28,30(38),31,33,40(64),42,44,46,49(54),51,53(61),55,57,59,62-nonacosaene-31,34-dicarboxylic acid	O=C(O)C%27=CC(Cc1c(O)c(O)c(O)c(O)c1O)=C(C(=O)O)C%33%28C%31C6C4=C%26C=%24C%18=C5C=3c%17c2c%16c%15C%13=C2C=%11C=3C=%10C(=C45)C6=C9c%32c8c7c%30C%23=C%22C7=C%14C=%12C8=C9C=%10C=%11C=%12C%13=C%14C=%21c%15c%20c%19c%16c(c%17%18)C%25=C%19C=%29C(=C%20C=%21%22)C%23=C(C=%29C(C=%24%25)C%26%27%28)C%33c%30c%31%32
41		tritriacontacyclo[19.11.30.6^{5,8}.0^{2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35}.0^{10,14}.0^{11,37}.0^{12,40}.0^{13,55}.0^{16,56}.0^{18,58}.0^{20,59}.0^{23,32}.0^{24,62}.0^{25,45}.0^{26,31}.0^{27,44}.0^{28,38}.0^{29,36}.0^{30,33}.0^{39,43}.0^{41,54}.0^{42,51}.0^{45,50}.0^{50,61}.0^{52,60}.0^{53,57}.0^{8,67}.0^{15,67}.0^{17,68}]octahexaconta-1(32),2(6),3(22),4(19),5(68),9(35),10(14),11,13(55),16,18(58),20(59),21(62),23,26,28,30,33,36,38,40,42(51),46,48,52(60),53,56,63,65-nonacosaen -46,47,48,49,63,64,65,66-octacarboxamide	NC(=O)C%30=C(C(N)=O)C(C(N)=O)=C(C(N)=O)C%29%33C2=C%28C=1c%27c8C=%22C=1C=%24C2=C%32C%25=C7c6c%31c5c(c%26C=4C%29C%28=C3c%27c9C%10=C3C=4C=%11c%26c%12c5c%13c6C%21=C7C=%23C=%14C(C%15c8c9C%16C%20=C%10C=%11C=%19C%12=C%13C%18=C%21C=%14C%17(C(C(N)=O)=C(C(N)=O)C(C(N)=O)=C(C(N)=O)C%15%16%17)C%18C=%19%20)C=%22C=%23C=%24%25)C%30%33C%31%32
42		(3E)-4-{32,33-dihydroxydotriacontacyclo [15.12.32.1^{2,6}.1^{4,19}.1^{22,52}.0^{1,34}.0^{3,28}.0^{5,18}.0^{7,16}.0^{8,13}.0^{10,34}.0^{11,36}.0^{12,56}.0^{14,57}.0^{15,60}.0^{20,24}.0^{21,61}.0^{23,50}.0^{25,48}.0^{27,47}.0^{29,45}.0^{35,44}.0^{37,55}.0^{38,43}.0^{39,54}.0^{40,51}.0^{41,49}.0^{42,46}.0^{53,58}.0^{9,64}.0^{26,63}.0^{59,62}]tetrahexaconta-3,5(18),6(64),7(16),8,11(36),12,14,17(61),19,21,23,25(48),26(63),27,30,32,35(44),37,39,41(49),42,46,50,52(62),53(58),54,56,59-nonacosaen-31-yl}buta-1,3-diene-1,1,2,3, 4-pentol	O/C(O)=C(/O)\C(\O)=C(/O)C=%31C(O)=C(O)C%26%32C%18=C5C4C%30c%29c3c2c1c%28C%24=C%23C1=C%13C=%11C2=C9C3=C4C8=C5C=%17C=7c%16c6c%15c%14C%12=C6C=%10C=7C8=C9C=%10C=%11C%12=C%13C=%22c%14c%21c%20c%15c%19c%16C=%17C%18=C%25C%19=C%20C=%27C(=C%21C=%22%23)C%24=C(C=%27C%25%26)C(c%28%29)C%30%32C=%31
43		33-benzyldotriacontacyclo[16.12.33.1^{29,40}.0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0^{13,41}.0^{14,59}.0^{15,62}.0^{20,51}.0^{22,50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{30,38}.0^{42,58}.0^{45,57}.0^{47,55}.0^{49,54}.0^{52,63}.0^{53,61}.0^{56,60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16),13(41),14,17,20,22(50),24(48),26,28,30(38),31,33,40(64),42,44,46,49(54),51,53(61),55,57,59,62-nonacosaene-31,32,34-triol	OC%27=C(O)C(Cc1ccccc1)=C(O)C%33%28C%31C6C4=C%26C=%24C%18=C5C=3c%17c2c%16c%15C%13=C2C=%11C=3C=%10C(=C45)C6=C9c%32c8c7c%30C%23=C%22C7=C%14C=%12C8=C9C=%10C=%11C=%12C%13=C%14C=%21c%15c%20c%19c%16c(c%17%18)C%25=C%19C=%29C(=C%20C=%21%22)C%23=C(C=%29C(C=%24%25)C%26%27%28)C%33c%30c%31%32

44		pentatriacontacyclo[19.11.34.10^{5,8}.0^{2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35}.0^{10,14}.0^{11,37}.0^{12,40}.0^{13,59}.0^{16,60}.0^{18,62}.0^{20,63}.0^{23,32}.0^{24,66}.0^{25,45}.0^{26,31}.0^{27,44}.0^{28,38}.0^{29,36}.0^{30,33}.0^{39,43}.0^{41,58}.0^{42,55}.0^{45,54}.0^{47,52}.0^{54,65}.0^{56,64}.0^{57,61}.0^{8,75}.0^{15,75}.0^{17,76}.0^{68,73}]hexaheptaconta-1(32),2(6),3(22),4(19),5(76),9(35),10(14),11,13(59),16,18(62),20(63),21(66),23,26,28,30,33,36,38,40,42(55),47,49,51,56(64),57,60,68(73),69,71-hentriacontaene	c%31cccc%32CC%30%35C2=C%29C=1c%28c8C=%23C=1C=%25C2=C%34C%26=C7c6c%33c5c(c%27C=4C%30C%29=C3c%28c9C%10=C3C=4C=%11c%27c%12c5c%13c6C%22=C7C=%24C=%14C(C%15c8c9C%16C%21=C%10C=%11C=%20C%12=C%13C%19=C%22C=%14C%17(Cc%18ccccc%18CC%15%16%17)C%19C=%20%21)C=%23C=%24C=%25%26)C%35(Cc%31%32)C%33%34
45		33-(adamantan-2-yl)dotriacontacyclo[16.12.33. 1^{29,40}.0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0^{13,41}.0^{14,59}.0^{15,62}.0^{20,51}.0^{22,50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{30,38}.0^{42,58}.0^{45,57}.0^{47,55}.0^{49,54}.0^{52,63}.0^{53,61}.0^{56,60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16),13(41),14,17,20,22(50),24(48),26,28,30(38),31,33,40(64),42,44,46,49(54),51,53(61),55,57,59,62-nonacosaene-31,32,34-tricarboxylic acid	O=C(O)C%29=C(C(=O)O)C(C3C1CC2CC(C1)CC3C2)=C(C(=O)O)C%35%30C%33C8C6=C%28C=%26C%20=C7C=5c%19c4c%18c%17C%15=C4C=%13C=5C=%12C(=C67)C8=C%11c%34c%10c9c%32C%25=C%24C9=C%16C=%14C%10=C%11C=%12C=%13C=%14C%15=C%16C=%23c%17c%22c%21c%18c(c%19%20)C%27=C%21C=%31C(=C%22C=%23%24)C%25=C(C=%31C(C=%26%27)C%28%29%30)C%35c%32c%33%34
46		dotriacontacyclo[11.10.40.1^{4,16}.0^{1,19}.0^{2,26}.0^{3,7}.0^{5,14}.0^{6,11}.0^{8,27}.0^{9,29}.0^{10,52}.0^{12,53}.0^{15,62}.0^{17,60}.0^{18,42}.0^{24,41}.0^{25,38}.0^{28,37}.0^{30,51}.0^{31,36}.0^{32,50}.0^{33,47}.0^{34,45}.0^{35,39}.0^{40,44}.0^{43,59}.0^{46,58}.0^{48,56}.0^{49,54}.0^{55,63}.0^{57,61}.0^{19,64}]tetrahexaconta-3(7),4,6 (11),8,10(52),12,14,16,18(42),25,27,29,31,33(47),34(45),35,37,39,43,46(58),48,50,53,55,57(61),59,62-heptacosaene-20,21,22,23-tetrol	OC%27C(O)C(O)C(O)C%32%29C%22C%16=C%31C%15=C3C=2c%14c1c%13c%12C%10=C1C=8C=2C=7C%30=C3C(C%26C%30=C6c%25c5c4c%24C%21=C%20C4=C%11C=9C5=C6C=7C=8C=9C%10=C%11C=%19c%12c%18c%17c%13c(c%14%15)C%16=C%17C=%23C(=C%18C=%19%20)C%21=C(C%22=%23)C%28c%24c%25C%26C%27%28%29)=C%31%32
47		47,48,64,65-tetrahydroxytritriacontacyclo[19.11. 30.6^{5,8}.0^{2,6}.0^{3,22}.0^{4,19}.0^{7,34}.0^{9,35}.0^{10,14}.0^{11,37}.0^{12,40}.0^{13,55}.0^{16,56}.0^{18,58}.0^{20,59}.0^{23,32}.0^{24,62}.0^{25,45}.0^{26,31}.0^{27,44}.0^{28,38}.0^{29,36}.0^{30,33}.0^{39,43}.0^{41,54}.0^{42,51}.0^{45,50}.0^{50,61}.0^{52,60}.0^{53,57}.0^{8,67}.0^{15,67}.0^{17,68}]octahexaconta-1(32),2(6),3(22),4(19), 5(68),9(35),10(14),11,13(55),16,18(58),20(59),21(62),23,26,28,30,33,36,38,40,42(51),46,48,52(60),53,56,63,65-nonacosaene-46,49,63,66-tetracarboxylic acid	O=C(O)C%30=C(O)C(O)=C(C(=O)O)C%29%33C2=C%28C=1c%27c8C=%22C=1C=%24C2=C%32C%25=C7c6c%31c5c(c%26C=4C%29C%28=C3c%27c9C%10=C3C=4C=%11c%26c%12c5c%13c6C%21=C7C=%23C=%14C(C%15c8c9C%16C%20=C%10C=%11C=%19C%12=C%13C%18=C%21C=%14C%17(C(C(=O)O)=C(O)C(O)=C(C(=O)O)C%15%16%17)C%18C=%19%20)C=%22C=%23C=%24%25)C%30%33C%31%32

48		2-[31-(carbamoylmethyl)-32,33-difluorodotria contacyclo[16.12.33.1^{29,40}.0^{1,35}.0^{2,28}.0^{3,25}.0^{4,23}.0^{5,35}.0^{6,21}.0^{7,36}.0^{8,19}.0^{9,17}.0^{10,37}.0^{11,39}.0^{12,16}.0^{13,41}.0^{14,59}.0^{15,62}.0^{20,51}.0^{22,50}.0^{24,48}.0^{26,46}.0^{27,44}.0^{30,38}.0^{42,58}.0^{45,57}.0^{47,55}.0^{49,54}.0^{52,63}.0^{53,61}.0^{56,60}.0^{43,64}]tetrahexaconta-3(25),4(23),6,8(19),9,11(39),12(16),13(41),14,17,20,22(50),24(48),26,28,30(38),31,33,40(64),42,44,46,49(54),51,53(61),55,57,59,62-nonacosaen-34-yl]acetamide	NC(=O)CC%26=C(F)C(F)=C(CC(N)=O)C%32%27C%30C5C3=C%25C=%23C%17=C4C=2c%16c1c%15c%14C%12=C1C=%10C=2C=9C(=C34)C5=C8c%31c7c6c%29C%22=C%21C6=C%13C=%11C7=C8C=9C=%10C=%11C%12=C%13C=%20c%14c%19c%18c%15c(c%16%17)C%24=C%18C=%28C(=C%19C=%20%21)C%22=C(C=%28C(C=%23%24)C%25%26%27)C%32c%29c%30%31