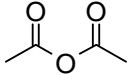
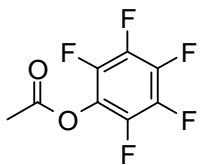
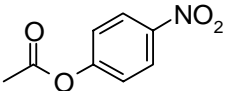
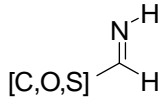
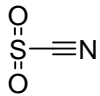
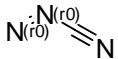
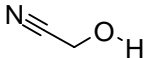
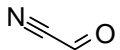
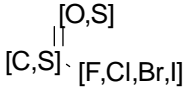



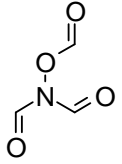
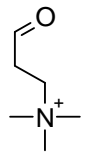
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
1	anhydride		C(=O)OC(=O)	Excluded
2	pentafluorophenyl ester		C(=O)Oc1c(F)c(F)c(F)c(F)c1(F)	Excluded
3	p-nitrophenyl ester		C(=O)Oc1ccc(N(=O)=O)cc1	Excluded

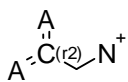

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
4	any carbazide	$\begin{array}{c} \text{N}^- \text{N}^+ \text{N} \\ \text{A}=\text{O} \end{array}$	<chem>O=*N=[N+]=[N-]</chem>	Excluded
5	HOBT ester	$\begin{array}{c} \text{O} \\ \diagdown \\ \text{O} \\ \diagup \\ \text{N}^{(r2)} \\ \diagdown \\ \text{N}^{(r2)} \\ \diagup \\ \text{N}^{(r2)} \end{array}$	<chem>C(=O)Onnn</chem>	Excluded
6	aromatic azide	$\begin{array}{c} \text{A} \\ \diagdown \\ \text{N}=\text{N}^+ \text{N}^- \end{array}$	<chem>cN=[N+]=[N-]</chem>	Excluded

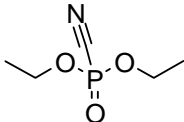

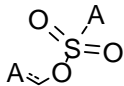
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
7	imine2	 <chem>[C,O,S]C=NH</chem>	<chem>[#6,#8,#16]-[CH1]=[NH1]</chem>	Excluded
8	sulfonyl cyanide	 <chem>O=S(=O)C#N</chem>	<chem>S(=O)(=O)C#N</chem>	Excluded
9	azocyanamide	 <chem>N(r0)=[N(r1)]C#N</chem>	<chem>[N;R0]=[N;R0]C#N</chem>	Excluded

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
10	cyanohydrin		<chem>N#CC[OH]</chem>	Excluded
11	acyl cyanide		<chem>N#CC(=O)</chem>	Excluded
12	acid halide		<chem>[S,C](=[O,S])[F,Br,Cl,I]</chem>	Excluded

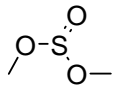
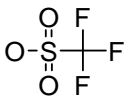
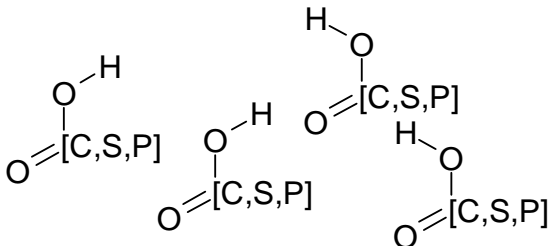
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
13	chloramidine		[Cl]C([C&R0])=N	Excluded
14	P/S halide	[P,S]-[F,Cl,Br,I]	[P,S][F,Cl,Br,I]	Excluded
15	quaternary C, Cl, I, P, S		[C+,Cl+,I+,P+,S+]	Excluded

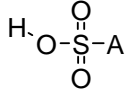

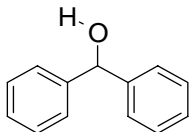
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
16	unacceptable atoms	NOT[H,Li,C,N,O,F,Na,Mg,P,S,Cl,K,Ca,Zn,Br]	[!#6;!#7;!#8;!#16;!#1;!#3;!#9;!#11;!#12;!#15;!#17;!#19;!#20;!#30;!#35]	Excluded
17	triacyloxime		C(=O)N(C(=O))OC(=O)	Excluded
18	b-carbonyl quaternary nitrogen		C(=O)CC[N+,n+]	Excluded

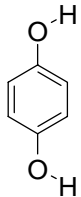
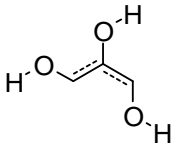
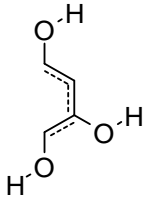
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
19	benzylic quaternary nitrogen	 $\begin{array}{c} A \\   \\ A-C(12)-N^+ \\   \\ A \end{array}$	cC[N+]	Excluded
20	phosphorane	P=	C=P	Excluded
21	Lawesson reagent derivatives	 $\begin{array}{c} S \\    \\ S-P-S \end{array}$	P(=S)(S)S	Excluded



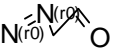
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
22	cyanophosphate		<chem>P(OCC)(OCC)(=O)C#N</chem>	Excluded
23	sulfonate		<chem>COS(=O)(=O)[C,c]</chem>	Excluded
24	Heteroaryl sulfonate		<chem>a-S(=O)(=O)-O- [\$(a[#6]),\$(c[a#!#6]),\$( cc[a#!#6]),\$(ccc[a#!#6]), \$(cccc[a#!#6]),\$(ccccc[a &amp;#!#6])]</chem>	Excluded

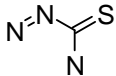



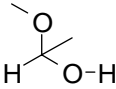
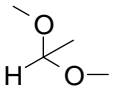

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
25	sulfate ester		<chem>COS(=O)O[C,c]</chem>	Excluded
26	triflate		<chem>OS(=O)(=O)C(F)(F)F</chem>	Excluded
27	polyacidic (4)		<chem>[C,S,P](=O)[OH].[C,S,P](=O)[OH].[C,S,P](=O)[OH].[C,S,P](=O)[OH]</chem>	Allowed


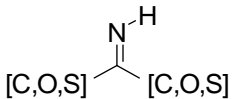

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
28	Sulfonic acid		[OH]-S(=O)(=O)-*	Allowed
29	thiol		[SH]	Allowed
30	benzhydrol		[OH1]-C(-c1ccccc1)-c2ccccc2	Allowed


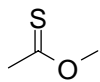
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
31	dihydroxybenzene		<chem>[OH1]c1ccc([OH1])cc1</chem>	Allowed
32	2,3,4-trihydroxyphenyl		<chem>c([OH])c([OH])c([OH])</chem>	Allowed
33	2,4,5-trihydroxyphenyl		<chem>c([OH])c([OH])cc([OH])</chem>	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
34	allene		<chem>*=C=*</chem>	Allowed
35	Azide		<chem>N=N=N</chem>	Allowed
36	azoalkanal		<chem>[N;R0]=[N;R0]CC=O</chem>	Allowed




Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
37	hydrazothiourea		N=NC(=S)N	Allowed
38	Azo	N=N	N=N	Allowed
39	aldehyde		[#6]-[CH1]=O	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
40	hemiacetal		[#6]-O[CH1](-[#6])[OH1]	Allowed
41	acetal		[#6]-O[CH1](-[#6])O-[#6]	Allowed
42	Ketone		[#6]-C(=O)-[#6]	Allowed

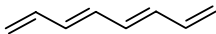
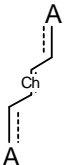
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
43	Ester		<chem>[#6]-C(=O)O-[#6]</chem>	Allowed
44	imine1		<chem>[#6,#8,#16]-C(=[NH1])-[#6,#8,#16]</chem>	Allowed
45	Imine 3		<chem>C=[NH]</chem>	Allowed

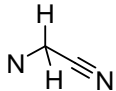
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
46	thioketone		CC(=S)C	Allowed
47	thioester	$S: \begin{matrix} [O,S]^{(r0)} \\ C^{(r0)} C^{(r0)} \end{matrix}$	C[O,S;R0][C;R0](=S)	Allowed
48	thionoester		COC(=S)C	Allowed

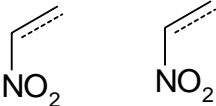
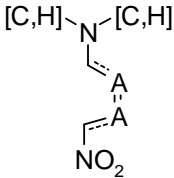
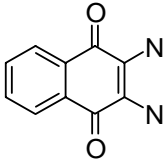


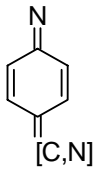
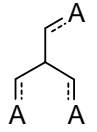
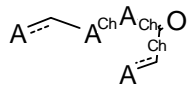
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
49	thioamide		CC(=S)N	Allowed
50	thiourea		NC(=S)N	Allowed
51	nitroso		[N&D2](=O)	Allowed

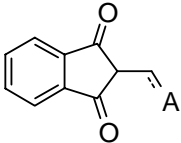
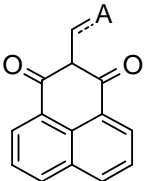
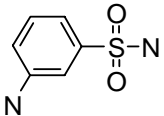



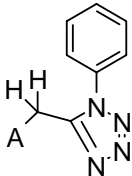
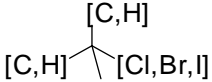
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
55	polyene		<chem>C=CC=CC=CC=C</chem>	Allowed
56	Dye 25		<chem>acC=&amp;!@Cca</chem>	Allowed
57	isonitrile	<chem>C≡N<sup>+</sup></chem>	<chem>[N+]#[C-]</chem>	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
58	thiocyanate	$\text{N}\equiv\text{S}$	SC#N	Allowed
59	cyanamide		N[CH2]C#N	Allowed
60	Dye 16 (1)	$\text{A}\equiv\text{NO}_2$	c([N+](=O)[O-])	Allowed

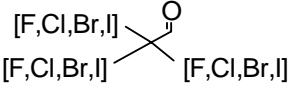
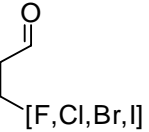
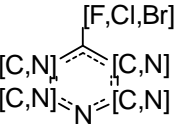
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
61	nitro aromatic 2+		<chem>(a-[N+](=O)[O-].a-[N+](=O)[O-])</chem>	Allowed
62	Dye 29		<chem>O=[N+](-[O-])-caac-[\$(N(-C)C),\$([NH]C),\$([NH2])]</chem>	Allowed
63	Dye 1 (1)		<chem>c1cccc(C(=O)[C,c]([#7])=,:[C,c]([#7])C2(=O))c12</chem>	Allowed

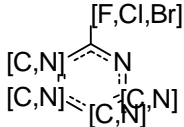

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
64	Dye 7		<chem>N=C1[#6]:,[#6]C(=[C,N])</chem> <chem>[#6]:,[#6]1</chem>	Allowed
65	Dye 11		<chem>*=,[#6]C([#6]=,*)[#6]=,*</chem>	Allowed
66	Dye 9		<chem>ac-*=&amp;!@*-&amp;!@C(=O)-</chem> <chem>&amp;!@ca</chem>	Allowed


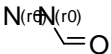
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
67	Dye 32		<chem>c1cccc2C(=O)C(-C:,* )C(=O)c12</chem>	Allowed
68	Dye 6		<chem>c12cccc(C(=O)C(ca)C(=O) )3)c2c3ccc1</chem>	Allowed
69	Dye 22		<chem>NS(=O)(=O)c1cccc([#7])c1</chem>	Allowed

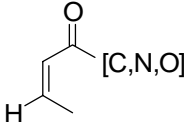
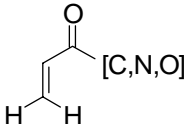
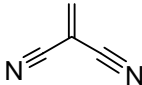
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
70	Dye 2		OCccCO	Allowed
71	Dye 26		c1ccccc1-n2nnnc2[CH2]*	Allowed
72	alkyl halide		[Br,Cl,I][CX4,CH,CH2,CH3]	Allowed

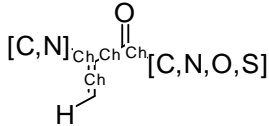
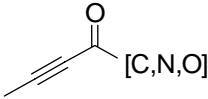
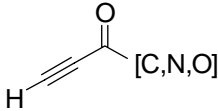


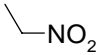
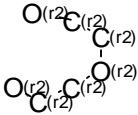
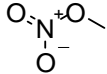
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
73	Perhalo_ketone		O=CC(-[F,Cl,Br,I])(-[F,Cl,Br,I])-[F,Cl,Br,I]	Allowed
74	Beta halo carbonyl		O=CCC[F,Cl,Br,I]	Allowed
75	4-halopyridine		[F,Cl,Br]- [c]1:[c,n]:[c,n]:[n]:[c,n]:[c,n] ]1	Allowed

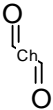
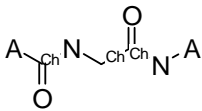

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
76	2-halopyridine		[F,Cl,Br]- [c]1:[c,n]:[c,n]:[c,n]:[c,n]:[n] ]1	Allowed
77	Hetero_hetero		*[N,S,O]-&!@[N,S,O][#6]	Allowed
78	peroxide	O-O	OO	Allowed


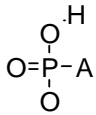
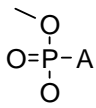
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
79	disulfide	S-S	SS	Allowed
80	hydrazine		[#6]-[NH]-[NH]-[#6]	Allowed
81	acyl hydrazine		[N;R0][N;R0]C(=O)	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
82	vinyl michael acceptor1		<chem>[#6]-[CH1]=C-C(=O)-[#6,#7,#8]</chem>	Allowed
83	vinyl michael acceptor2		<chem>[CH2]=C-C(=O)-[#6,#7,#8]</chem>	Allowed
84	michael acceptor 5		<chem>N#CC(=C)C#N</chem>	Allowed

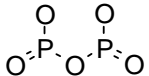
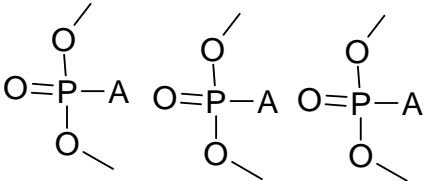

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
85	Michael acceptor 6		<chem>[#6,#7]-&amp;![#6](= &amp;![CH])-&amp;![C(=O)]-&amp;![C,N,O,S]</chem>	Allowed
86	alkynyl michael acceptor1		<chem>[#6]-C#CC(=O)-[#6,#7,#8]</chem>	Allowed
87	alkynyl michael acceptor2		<chem>[CH1]#CC(=O)-[#6,#7,#8]</chem>	Allowed

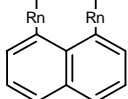
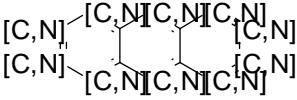
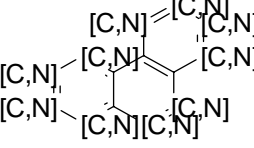
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
88	nitroalkane		<chem>C[N+](=O)[O-]</chem>	Allowed
89	crown ether		<chem>[O;R1][C;R1][C;R1][O;R1][C;R1][C;R1][O;R1]</chem>	Allowed
90	nitrate		<chem>[#6]-O-[N+](=O)[O-]</chem>	Allowed

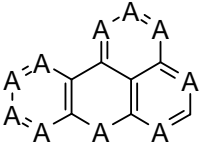
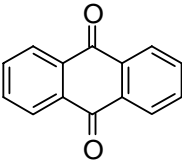
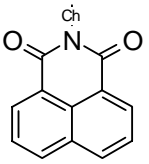
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
91	Oxalyl		<chem>O=C-!@C=O</chem>	Allowed
92	Dipeptide		<chem>*-C(=O)-!@[NH]-C- &amp;!@C(=O)-!@[NH]-*</chem>	Allowed
93	quaternary nitroxy		<chem>C[N+](-[O-])(C)C</chem>	Allowed




Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
94	Triphenylphosphine		a-P(-a)-a	Allowed
95	Phosphoric acid		[OH]-P(=O)(-O)-*	Allowed
96	Phosphoric ester		COP(=O)(-*O	Allowed

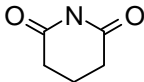
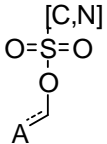
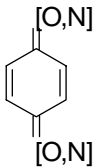


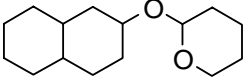
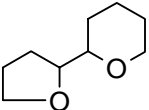
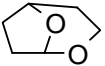
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
97	di/triphosphate		<chem>P(=O)([OH])OP(=O)[OH]</chem>	Allowed
98	tri phosphoric esters		<chem>([#6]OP(=O)(-*)O[#6].[#6]OP(=O)(-*)O[#6].[#6]OP(=O)(-*)O[#6])</chem>	Allowed
99	phosphoramidate		<chem>NP(=O)(N)N</chem>	Allowed

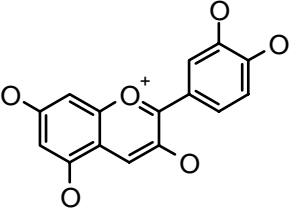
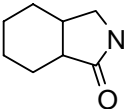
Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
100	Phenalene		<chem>c1(c)c2c(c)cccc2ccc1</chem>	Allowed
101	(poly(azo(anthracene)))		<chem>c12:[c,n]:[c,n]:[c,n]:[c,n]:c1[c,n]c3:[c,n]:[c,n]:[c,n]:[c,n]:[c,n]:c3[c,n]2</chem>	Allowed
102	(poly(azo(phenanthrene)))		<chem>c12:[c,n]:[c,n]:[c,n]:[c,n]:c1:[c,n]:[c,n]:c3:[c,n]:[c,n]:[c,n]:[c,n]:c3[c,n]2</chem>	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
103	Dye 31		a1aaac2ac3acac4aaac(c34)c12	Allowed
104	Dye 4		c12ccccc1C(=O)c3ccccc3C2=O	Allowed
105	Dye 8		c12cccc(C(=O)N(-&!@C)C(=O)3)c2c3ccc1	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
106	epoxide, aziridine, thioepoxide	 [N,O,S]	C1[O,S,N]C1	Allowed
107	propiolactone		C1(=O)OCC1	Allowed
108	b-lactam		N1CCC1=O	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
109	cycloheximide		<chem>O=C1CCCC(N1)=O</chem>	Allowed
110	aromatic Sulfonic ester		<chem>[#6,#7]-S(=O)(=O)Oc</chem>	Allowed
111	quinone		<chem>[\$([o,n]=c1ccc(=[o,n])cc1),\$([O,N]=C1C=CC(=[O,N])C=C1),\$([O,N]=C1[#6]:,[#6]C(=[O,N])[#6]:,[#6]1)]</chem>	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
112	saponin		<chem>O1CCCCC1OC2CCC3CCCC3C2</chem>	Allowed
113	monensin		<chem>O1CCCCC1C2CCCO2</chem>	Allowed
114	squalestatin		<chem>C12OCCC(O1)CC2</chem>	Allowed

Entry	Query Name	ISIS Query	SMARTS	Allowed / Excluded
115	cyanidin		<chem>[OH]c1cc([OH])cc2=[O+]C(=C([OH])Cc21)c3cc([OH])c([OH])cc3</chem>	Allowed
116	cytochalasin		<chem>O=C1NCC2CCCCC21</chem>	Allowed