Table S3. Full list of functional groups for extracting extended reaction centers[7]

Functional group type	No.	Functional groups in SMARTS	Functional group name
C-containing group	1	'*-[C;D3]([C;D1;H3])([C;D1;H3])'	branched C_3 structures
	2	'*-[C;D3]([C;D1;H,H2])([C;D1;H,H2,H3])'	branched C_3 radicals
	3	'[*]@[*]~[*;!r]'	any side chain of cyclic
	4	'*-[C;D3]1-[C;D2]-[C;D2]1'	cyclopropyl
	5	'*-[C;D4]([C;D1])([C;D1])-[C;D1]'	t-butyl
	6	'*-[C;D2]#[C;D1;H]'	acetylenes
O-containing group	7	'*-C(=O)[O;D1]'	carboxylic acids
	8	'*-C(=O)[O;D2]-[C;D1;H3]'	carbonyl methyl ester
	9	'*-C(=O)-[C;D1]'	terminal aldehyde
	10	'*-C(=O)-[C;D1;H3]'	carbonyl methyl
	11	'*-[O;D2]-[C;D2]-[C;D1;H3]'	ethoxy
	12	'*-[O;D2]-[C;D1;H3]'	methoxy
	13	'*-[O;D1]'	side-chain hydroxyls
	14	'*=[O;D1]'	side-chain aldehydes or ketones
N-containing group	15	'*-[N;D2]-[C;D3](=O)-[C;D1;H3]'	methyl amide
	16	'*-C(=O)-[N;D1]'	amide
	17	'*-[N;D2]=[C;D2]=[O;D1]'	isocyanate
	18	'*-[N;D3](=[O;D1])[O;D1]'	nitro
	19	'*-[N;R0]=[O;D1]'	nitroso

	20	'*=[N;R0]-[O;D1]'	oximes
	21	'*=[N;R0]-[C;D1;H3]'	Imines
	22	'*-[N;R0]=[C;D1;H2]'	Imines
	23	'*-[N;D2]=[N;D2]-[C;D1;H3]'	terminal azo
	24	'*-[N;D2]=[N;D1]'	hydrazines
	25	'*-[N;D2]#[N;D1]'	diazo
	26	'*-[C;D2]#[N;D1]'	cyano
	27	'*-[N;D1]'	primary amines
	28	'*=[N;D1]'	
	29	'*#[N;D1]'	nitriles
	30	'*-[N;D2]=[C;D2]=[S;D1]'	isothiocyanate
	31	'*-[S;D4](=[O;D1])(=[O;D1])-[N;D1]'	primary sulfonamide
	32	'*-[N;D2]-[S;D4](=[O;D1])(=[O;D1])-[C;D1;H3]'	methyl sulfonamide
S-containing group	33	'*-[S;D4](=O)(=O)-[O;D1]'	sulfonic acid
	34	'*-[S;D4](=O)(=O)-[O;D2]-[C;D1;H3]'	methyl ester sulfonyl
	35	'*-[S;D4](=O)(=O)-[C;D1;H3]'	methyl sulfonyl
	36	'*-[S;D4](=O)(=O)-[Cl]'	sulfonyl chloride
	37	'*-[S;D3](=O)-[C;D1]'	methyl sulfinyl
	38	'*-[S;D2]-[C;D1;H3]'	methylthio
	39	'*-[S;D1]'	thiols
	40	'*=[S;D1]'	thiocarbonyls

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