Ions expected for DART analysis of compounds containing various functional groups

Class	Positive	Negative	Notes
Alcohols	$[M+H]^+$ $[2M+H]^+$ $[M+H-H_2O]^+$ derivatize polyols	$[M-H]^-$ for phenols	**Dehydration common, derivatization needed for most alcohols > C_4**
Alkanes	$M^{+\cdot}$ $[M-H]^+$ Alkyl fragments, oxidation from NO^+		**$M^{+\cdot}$ only observed if Vapur not installed and water vapor eliminated**
Alkenes	Usually MH^+ Some fragments		
Amines, Bases	$[M+H]^+$		
Amino acids	MH^+ some fragments		Dimethylaminoethanol derivatives may be useful
Aromatics	**$M^{+\cdot}$ $[M-H]^+$** **May see $[M-H]^+$ for some alkyl aromatics**		
Carbonyls	**$[M+H]^+$** **$[M+NH_4]^+$**		$[M+NH_4]^+$ favored if Vapur used
Carboxylic acids	$[M+H-H_2O]^+$ If ammonium present: $[M+H]^+$, $[M+NH_4]^+$	**$[M-H]^-$**	
Carbohydrates	MH^+ and dehydration fragments for mono-, di- saccharides Derivatize for larger compounds		**In-situ derivatization with TMAH is highly effective: produces trimethylammonium adduct. If N is present in compound, MH^+ observed.**

Esters	**$[M+H]^+$** **$[M+NH_4]^+$**		$[M+NH_4]^+$ favored if Vapur used
Explosives (RDX, HMX, NG, EGDN, PETN, Tetryl)		**$[M+Cl]^-$** **$[M+CH_3CO_2]^-$** **$[M+NO_3]^-$**	Anion dopant such as CH_2Cl_2
Halogenated (e.g. Cl) alkanes		**Cl^- ,Cl_2^-, $[M-Cl]^-$ etc.**	
Metals	$M^{+\cdot}$ and oxides		**Some metals can be detected by forming volatile derivatives (e.g. acetyl acetone). Use a very high cone voltage to produce elemental ions or small oxide or hydroxide fragments.**
Nitroaromatics (including explosives TNT, DNT)	$M^{+\cdot}$, MH^+	**$M^{-\cdot}$** **$[M-H]^-$**	**Negative-ion detection has better detection limits.**
Organometallics	$M^{+\cdot}$ $[M-H]^+$	$M^{-\cdot}$ $[M-H]^-$	**Compound-dependent, may lose a ligand to produce a net positive or negative single charge**
Peptides	$[M+H]^+$, fragments	$[M-H]^-$, fragments	**Not effective except for very small peptides**
Peroxides	**$[M+NH_4]^+$**		
Proteins	Not detected, may see amino acids		**Generally not suitable**
Salts	$Cation^+$	$Anion^-$	**Compound-dependent**

Notes in bold indicate the most likely ions or the preferred handling for a given class.