

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080816\
 Data File : BF089666.D
 Acq On : 8 Aug 2016 17:42
 Operator : UM/SJ
 Sample : H4367-13
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C2K1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.627	263	266	284	rVB	126886	316231	19.71%	2.493%
2	5.313	323	326	358	rBV	668847	1230493	76.68%	9.700%
3	6.959	467	470	477	rBV	794248	1232892	76.83%	9.719%
4	7.073	477	480	498	rVB	881660	1453025	90.55%	11.454%
5	7.416	509	510	528	rBV	113570	241132	15.03%	1.901%
6	7.656	528	531	543	rBV	785629	1053494	65.65%	8.304%
7	8.330	587	590	621	rBV	498365	836146	52.11%	6.591%
8	9.450	685	688	716	rBV	202587	345555	21.53%	2.724%
9	11.233	840	844	846	rBV	988923	1604652	100.00%	12.649%
10	11.919	901	904	917	rBB	155987	225444	14.05%	1.777%
11	12.262	932	934	938	rBV	269092	418113	26.06%	3.296%
12	13.131	1007	1010	1012	rBV	19265	25753	1.60%	0.203%
13	13.554	1045	1047	1056	rBV	567165	878271	54.73%	6.923%
14	13.897	1074	1077	1082	rBV	23697	38297	2.39%	0.302%
15	14.662	1142	1144	1153	rVB	287653	419552	26.15%	3.307%
16	17.028	1348	1351	1354	rBV	1130253	1592973	99.27%	12.557%
17	18.286	1459	1461	1465	rBV	45336	87674	5.46%	0.691%
18	18.354	1465	1467	1474	rVB	237256	381999	23.81%	3.011%
19	19.520	1566	1569	1573	rVB	29945	31181	1.94%	0.246%
20	20.023	1611	1613	1622	rBV	189781	273115	17.02%	2.153%

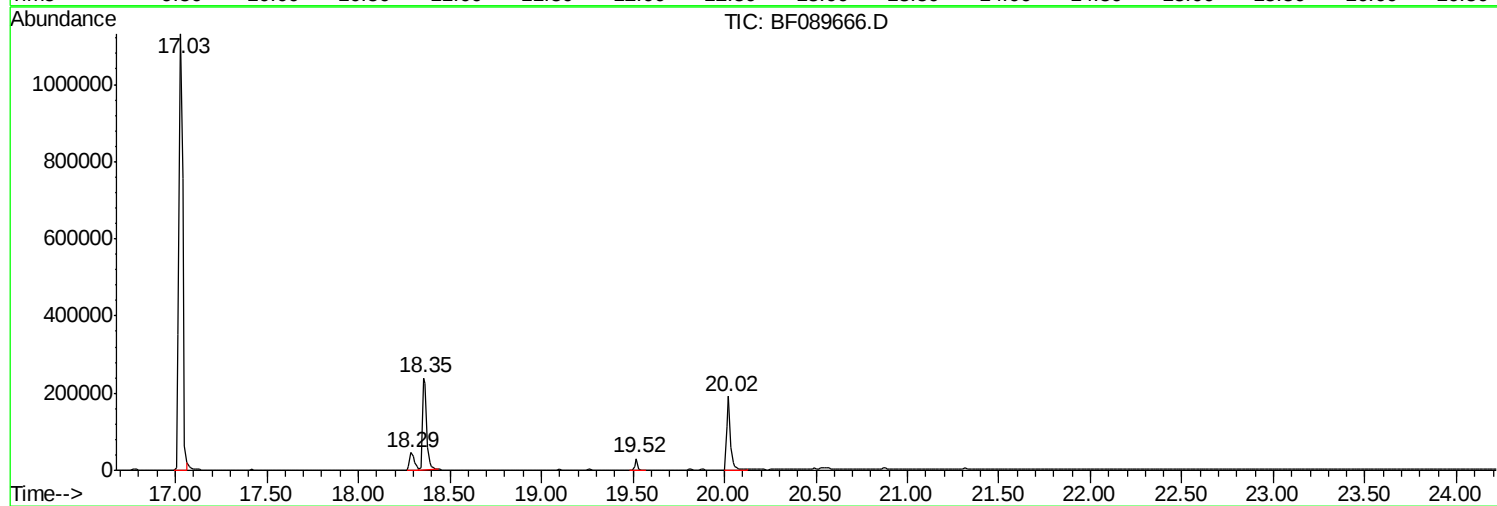
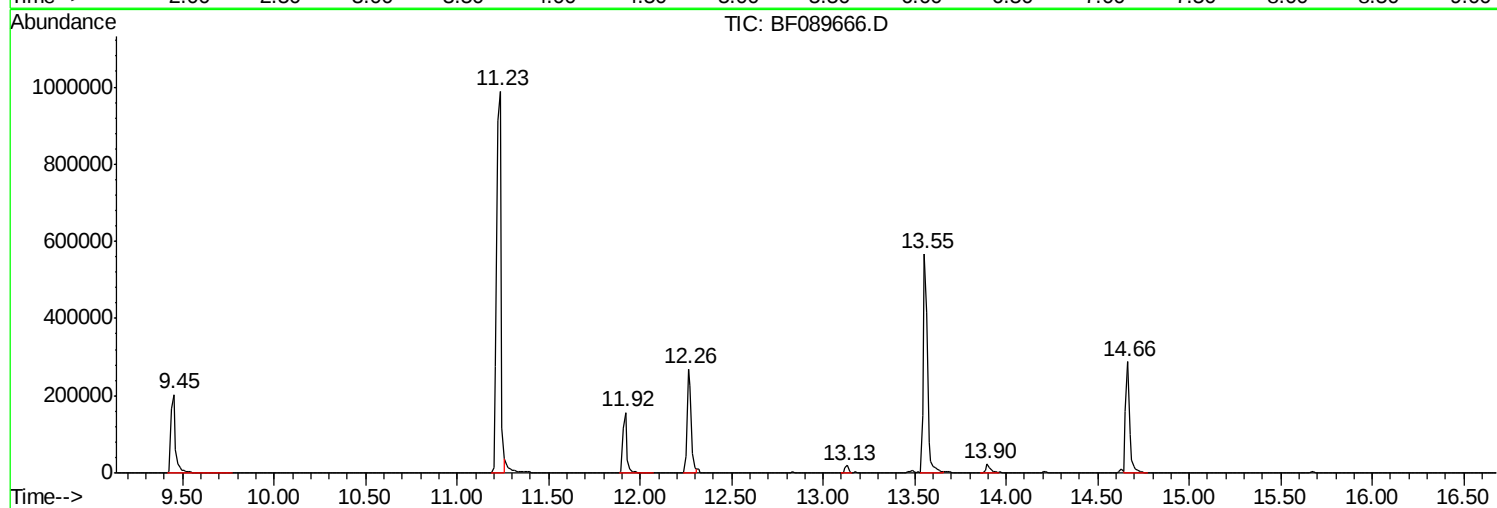
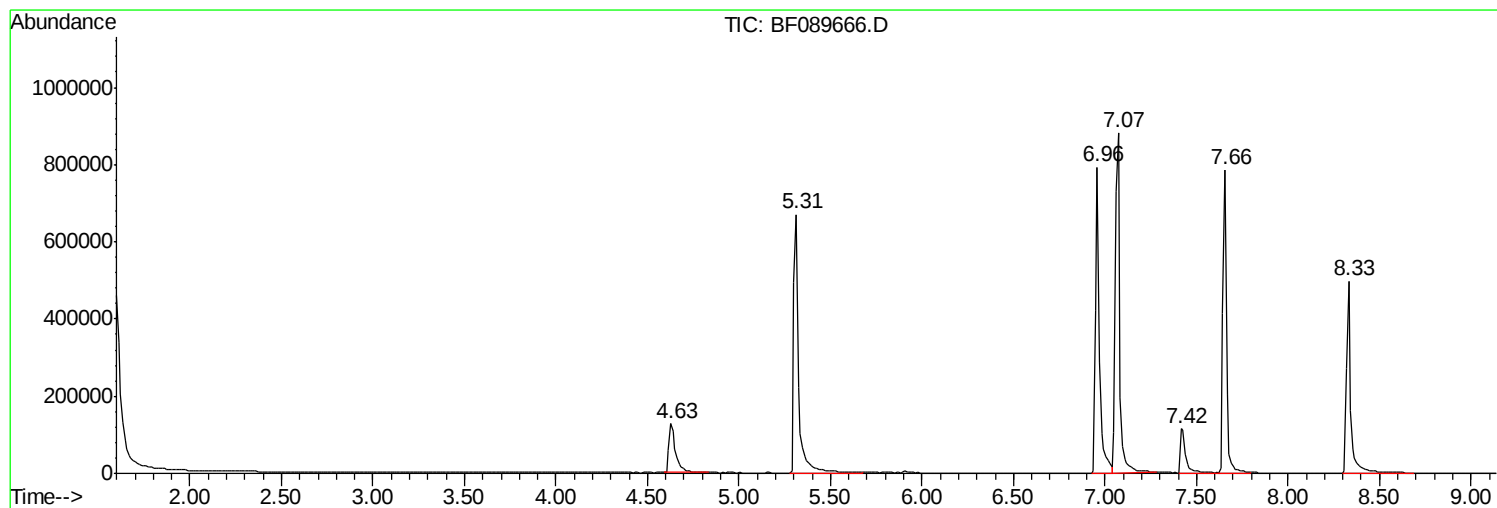
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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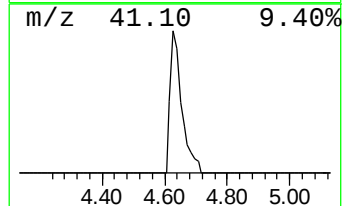
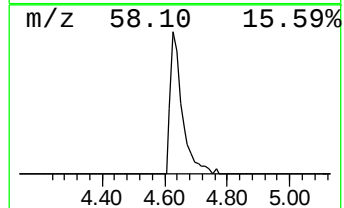
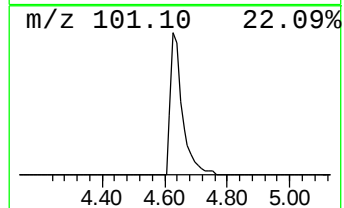
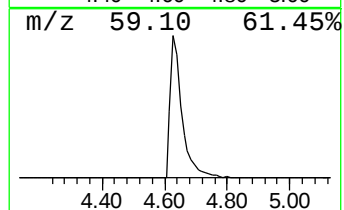
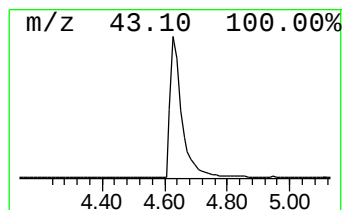
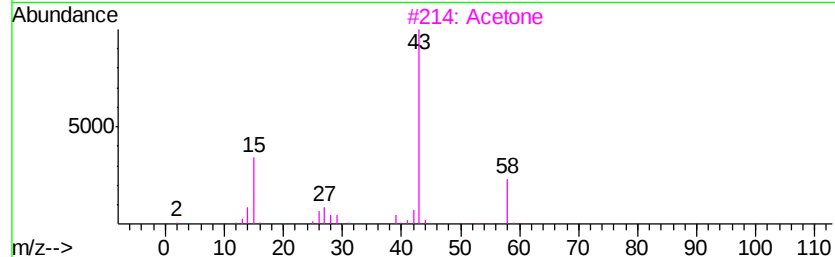
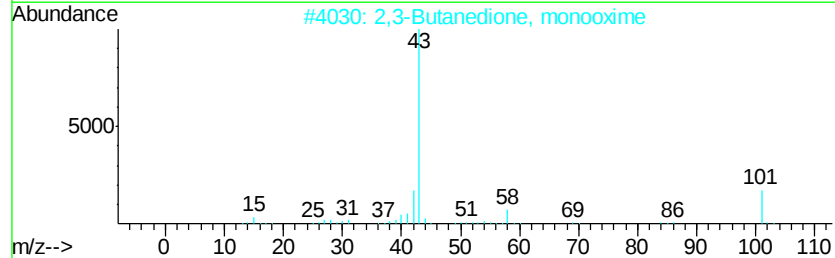
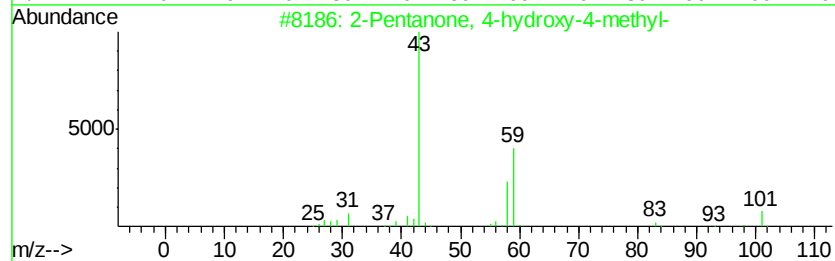
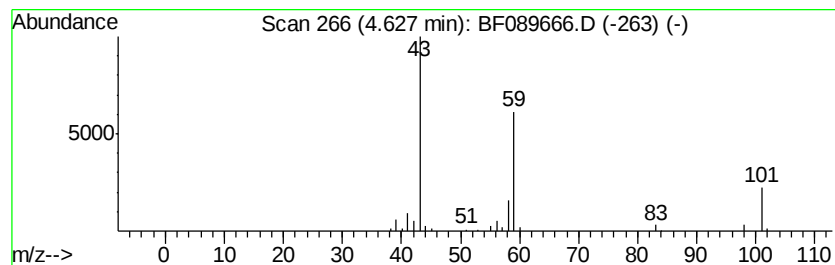
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	26.23 ng	316231	1,4-Dichlorobenzene-d4	7.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetone	58	C3H6O	000067-64-1	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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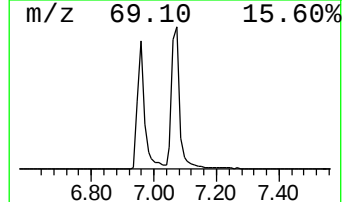
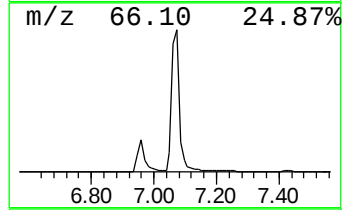
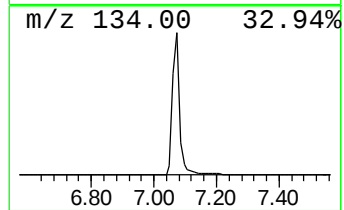
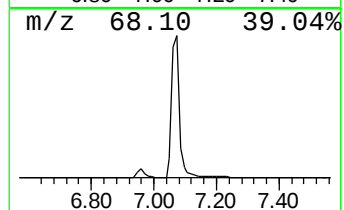
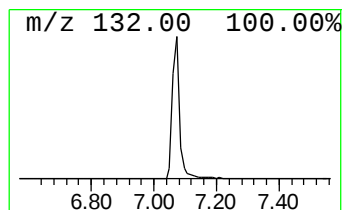
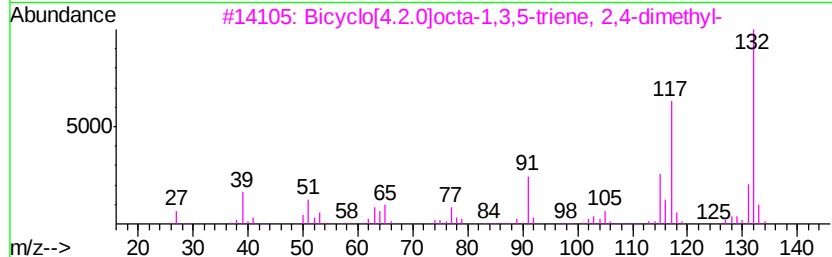
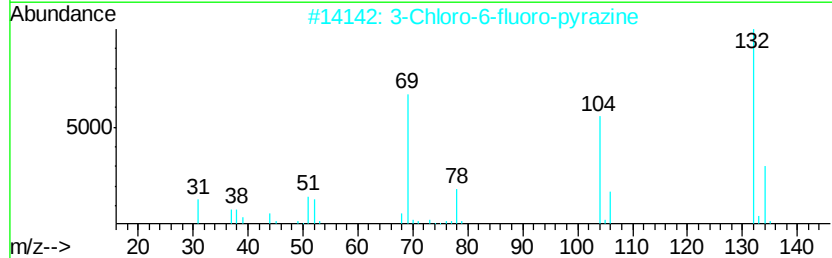
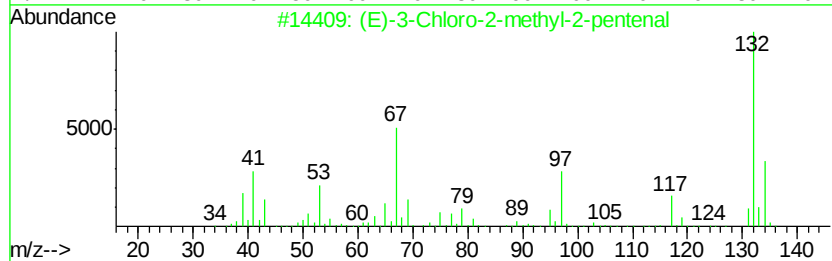
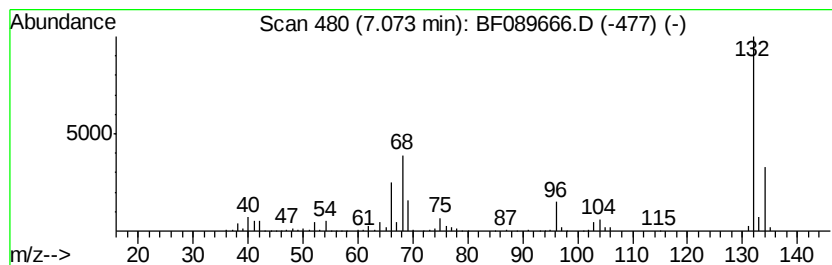
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Peak Number 2 unknown7.07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	120.52 ng	1453030	1,4-Dichlorobenzene-d4	7.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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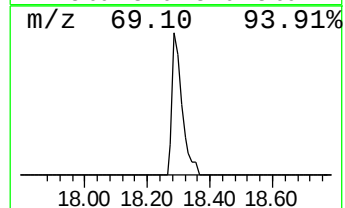
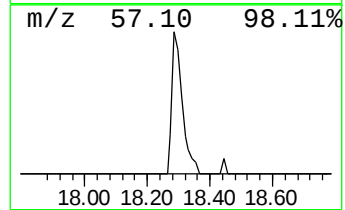
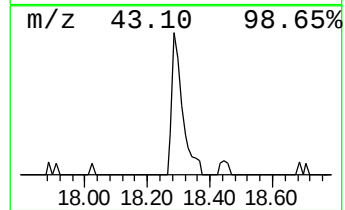
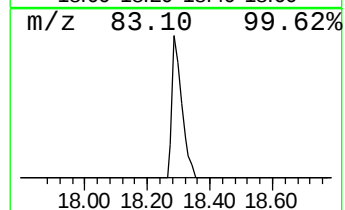
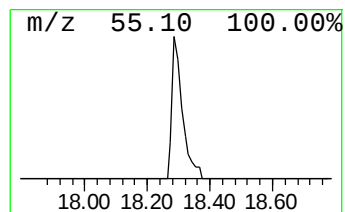
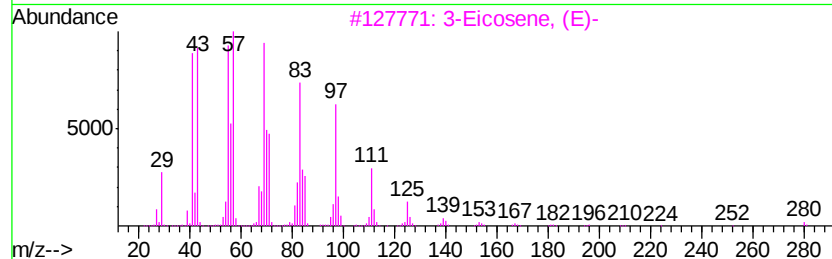
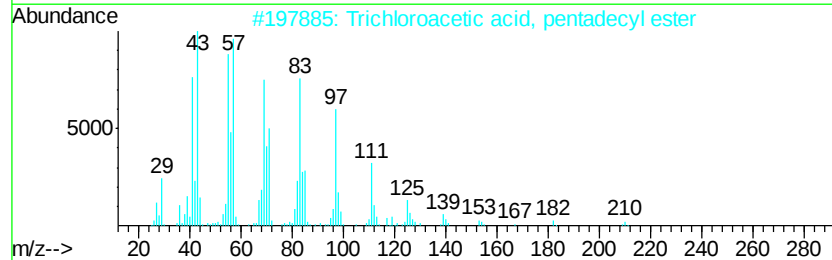
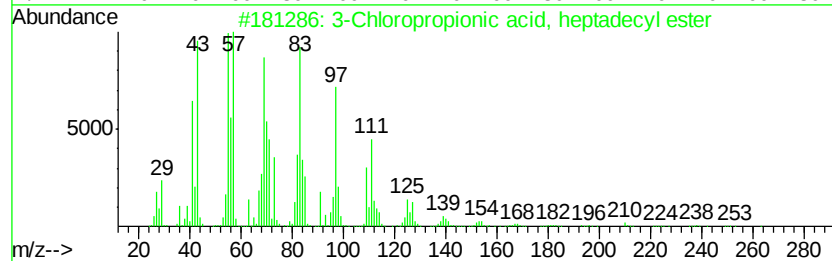
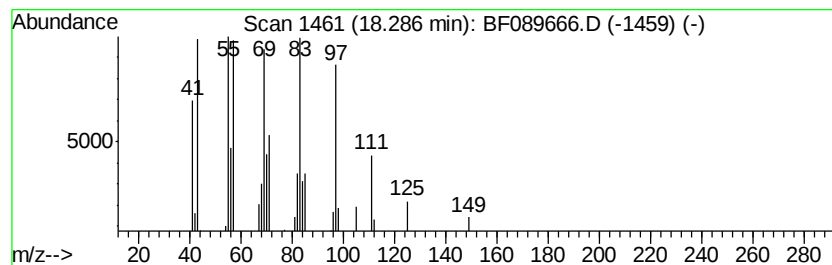
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Peak Number 4 3-Chloropropionic acid, hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	4.59 ng	87674	Chrysene-d12	18.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		11-Tricosene	322	C23H46	052078-56-5	91
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90



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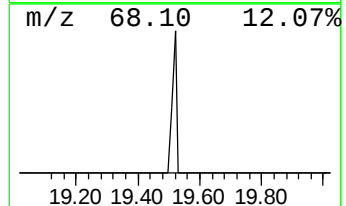
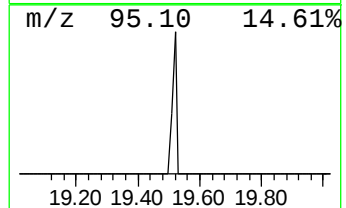
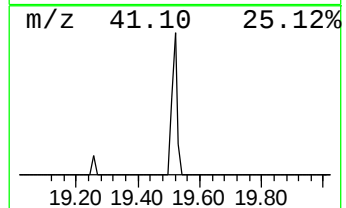
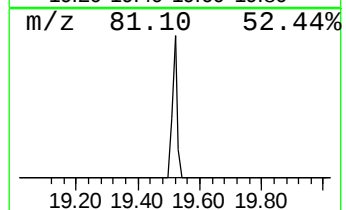
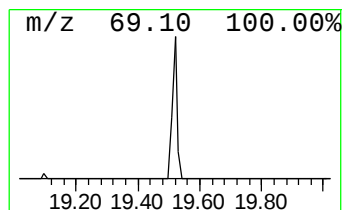
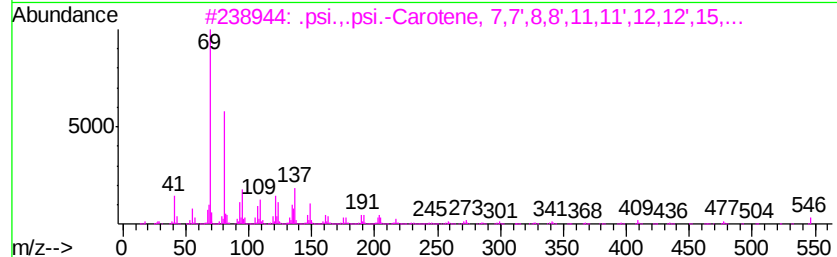
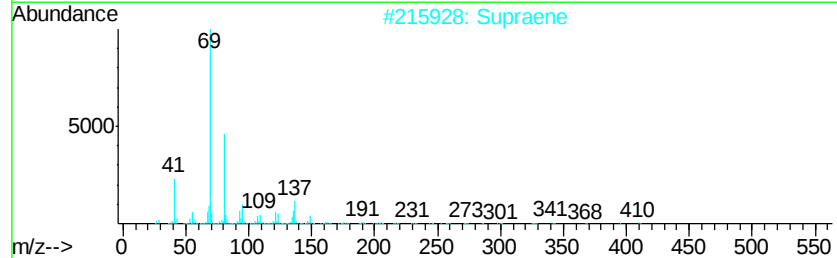
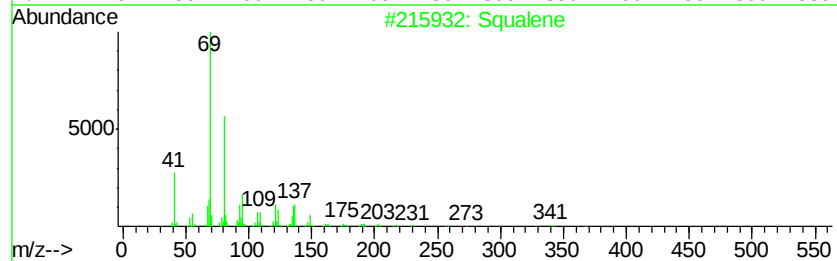
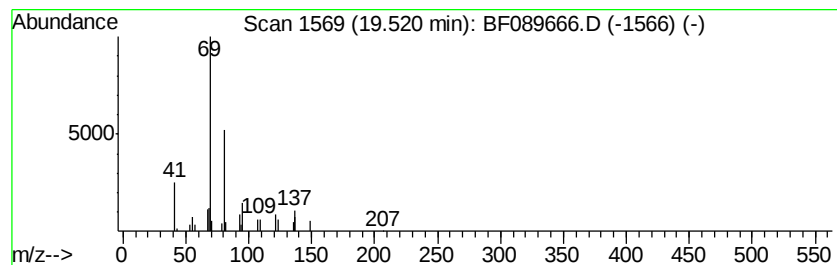
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.52	2.28 ng	31181	Perylene-d12	20.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene		410	C30H50	000111-02-4	91
2	Supraene		410	C30H50	007683-64-9	90
3	.psi.,.psi.-Carotene, 7,7',8,8',...		547	C40H66	000502-62-5	83
4	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	72
5	trans-Farnesol		222	C15H26O	000106-28-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	26.2	ng	316231	1	7.43	241132	20.0
unknown7.07	7.07	120.5	ng	1453030	1	7.43	241132	20.0
3-Chloropropionic...	18.29	4.6	ng	87674	5	18.37	381999	20.0
Squalene	19.52	2.3	ng	31181	6	20.02	273115	20.0