

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110816\
 Data File : BF091112.D
 Acq On : 9 Nov 2016 6:00
 Operator : UM/SJ
 Sample : H5593-08
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHA-1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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	1.756	4	6	54	rVB	3045378	7600633	100.00%	17.539%
2	4.807	271	273	284	rBV	628854	980300	12.90%	2.262%
3	5.253	309	312	315	rBV	3508303	4061612	53.44%	9.372%
4	6.316	402	405	413	rBV	3714432	4538843	59.72%	10.474%
5	6.430	413	415	418	rBV	4339270	4221007	55.53%	9.740%
6	6.659	433	435	442	rBV	1049268	1021007	13.43%	2.356%
7	6.819	446	449	451	rBV	3333907	3376252	44.42%	7.791%
8	7.230	482	485	494	rBV	2504394	2524936	33.22%	5.826%
9	7.950	545	548	550	rBV	1175950	1257296	16.54%	2.901%
10	9.025	640	642	645	rBV	4603311	4058292	53.39%	9.365%
11	9.425	675	677	679	rBV	477862	411169	5.41%	0.949%
12	9.699	698	701	703	rBV	1292627	1353033	17.80%	3.122%
13	10.488	767	770	772	rBV	1947774	2161386	28.44%	4.988%
14	10.614	779	781	785	rVB	83260	99914	1.31%	0.231%
15	11.174	828	830	834	rBV	1251019	1089668	14.34%	2.514%
16	12.762	966	969	971	rBV	2889373	2848032	37.47%	6.572%
17	13.665	1046	1048	1052	rBV	62922	82840	1.09%	0.191%
18	13.802	1058	1060	1063	rBV	887630	827249	10.88%	1.909%
19	14.648	1131	1134	1137	rBV	78442	81506	1.07%	0.188%
20	15.174	1177	1180	1183	rBV	579867	740488	9.74%	1.709%

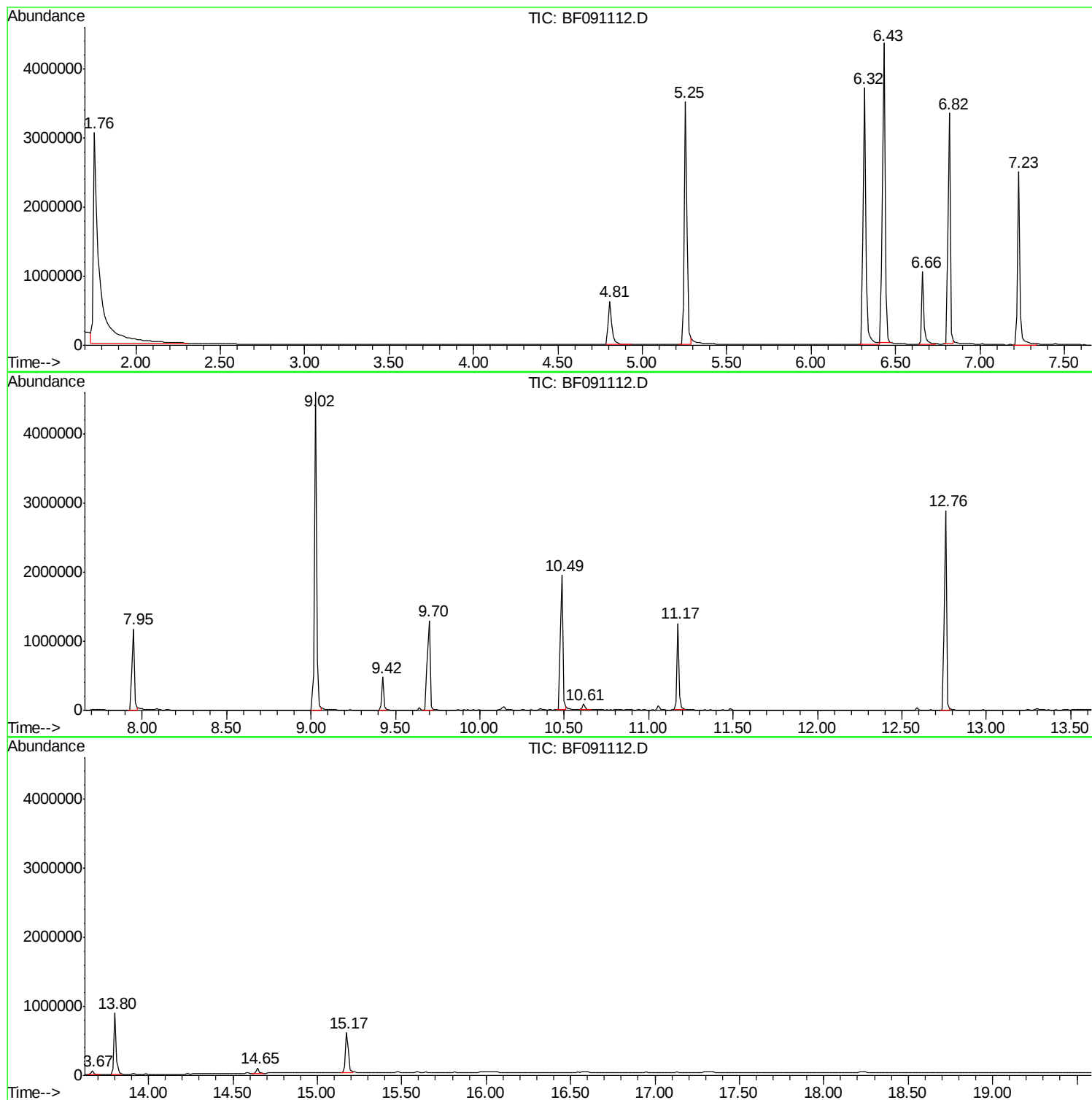
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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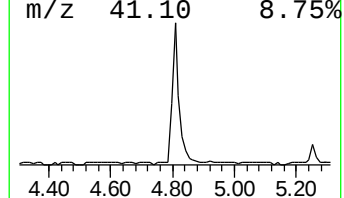
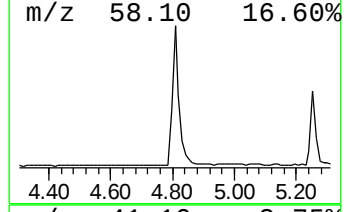
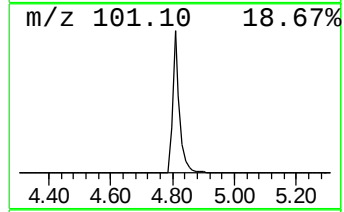
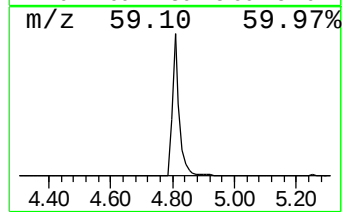
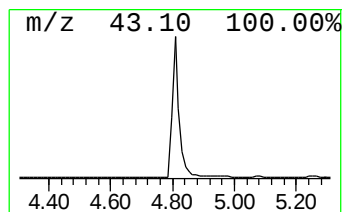
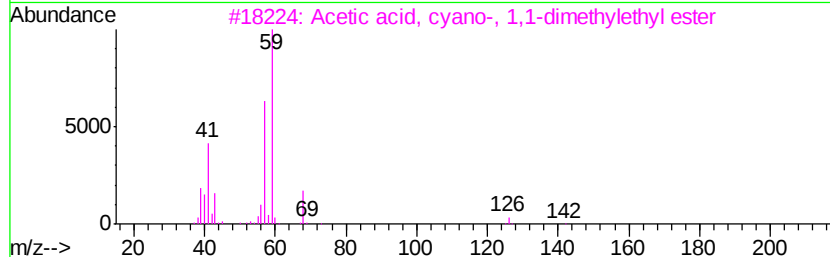
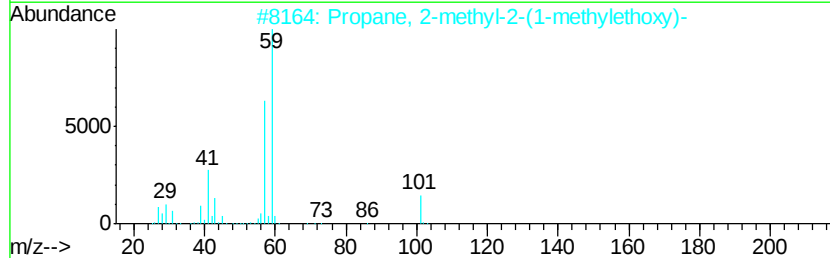
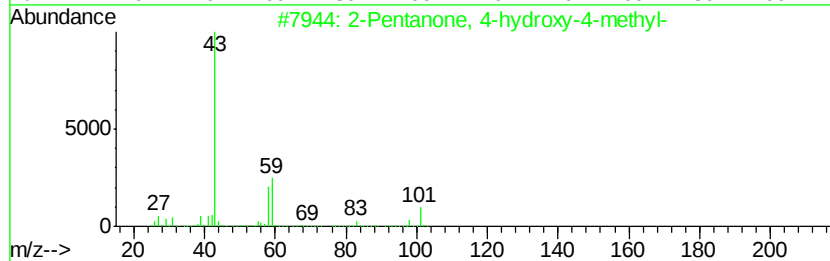
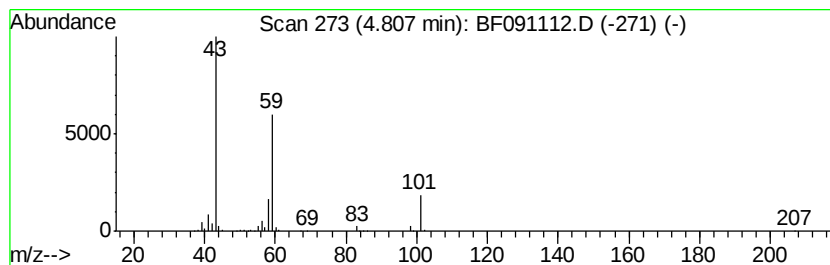
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	19.20 ng	980300	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetone	58	C3H6O	000067-64-1	9



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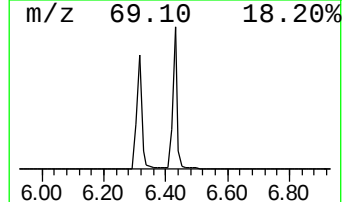
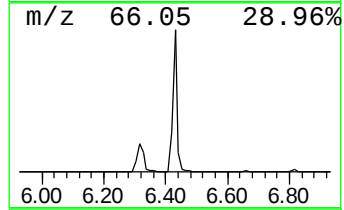
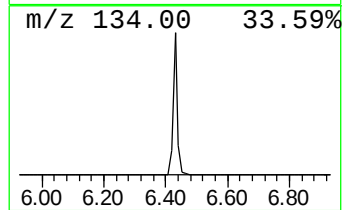
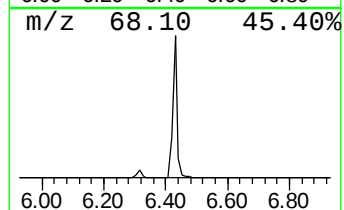
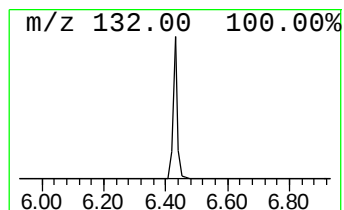
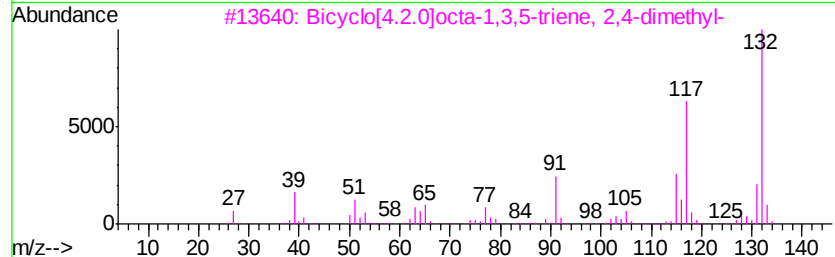
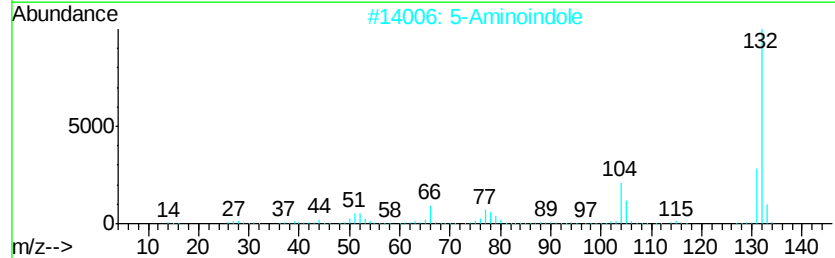
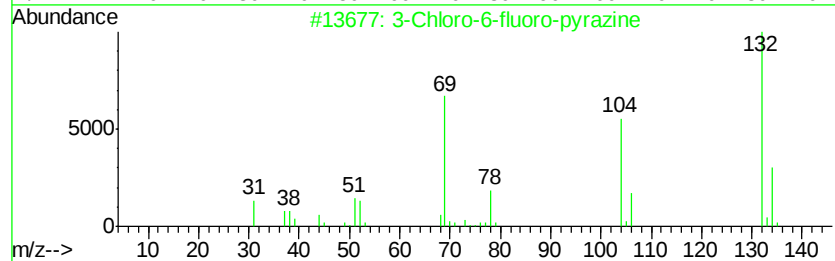
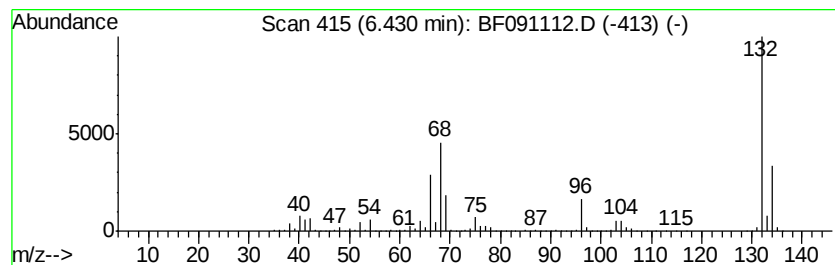
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Peak Number 3 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	82.68 ng	4221010	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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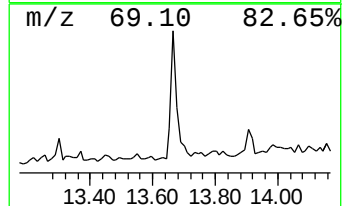
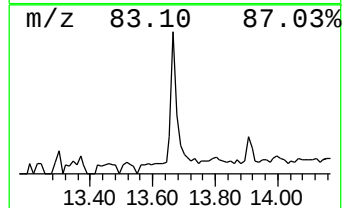
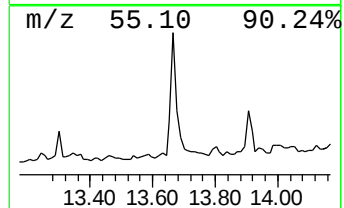
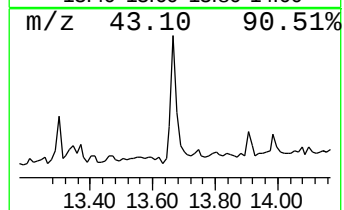
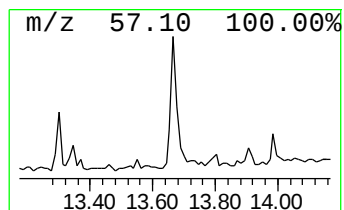
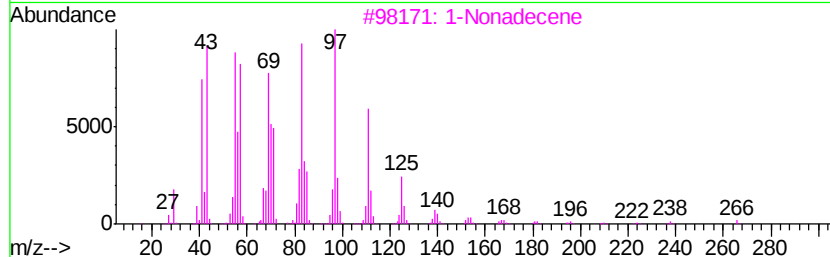
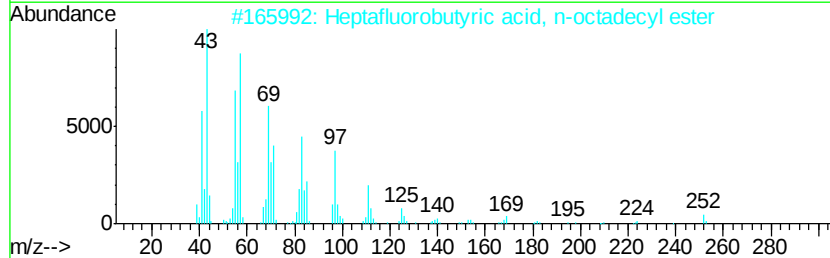
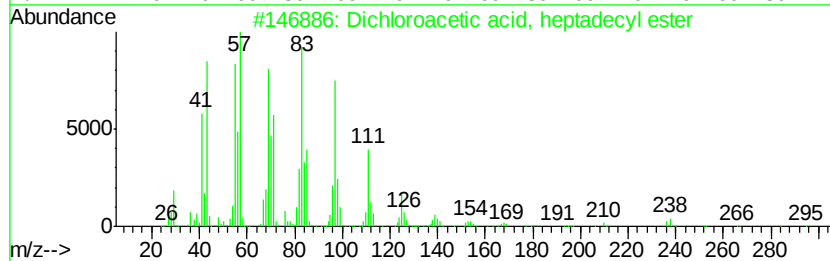
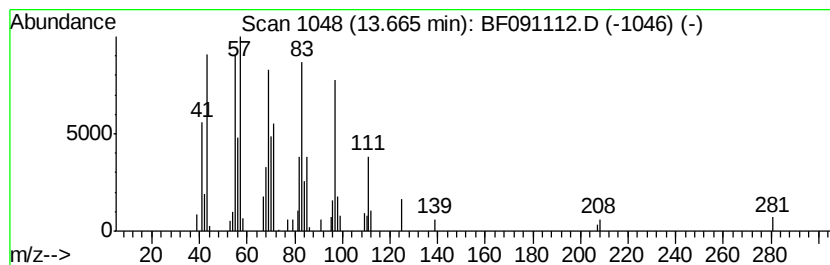
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	2.00 ng	82840	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3		1-Nonadecene	266	C19H38	018435-45-5	90
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90
5		1-Heptadecanol	256	C17H36O	001454-85-9	90



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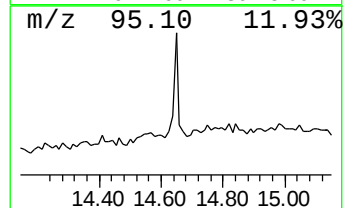
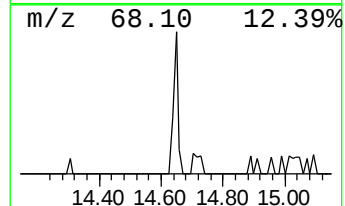
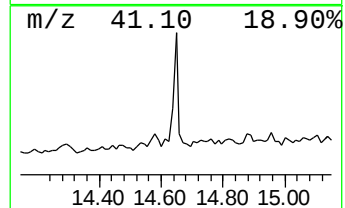
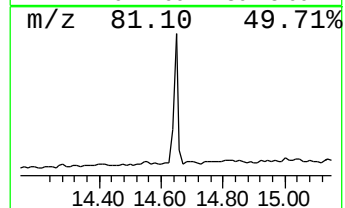
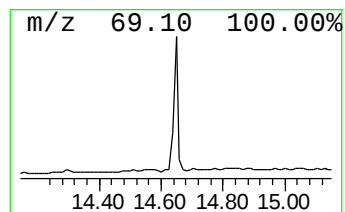
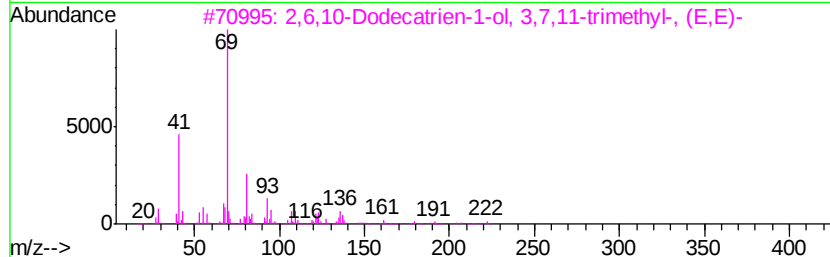
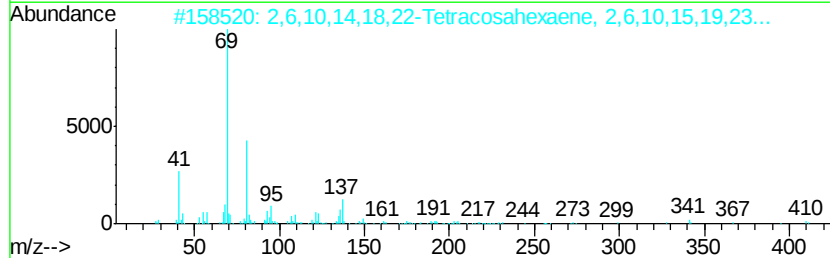
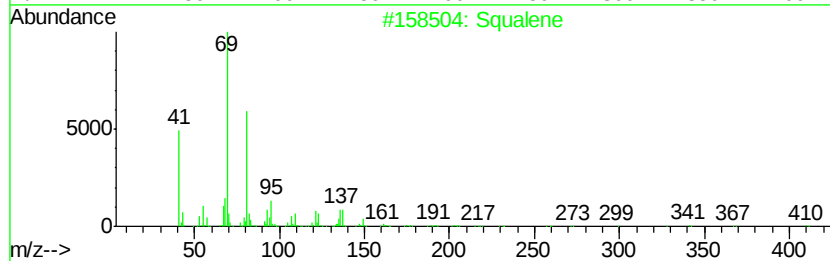
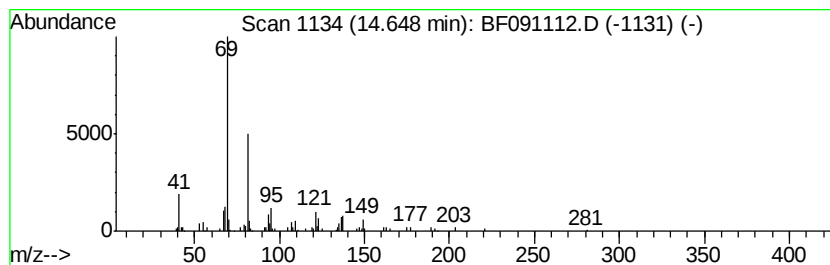
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.20 ng	81506	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	80
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.81	19.2	ng	980300	1	6.66	1021010	20.0
unknown6.43	6.43	82.7	ng	4221010	1	6.66	1021010	20.0
Dichloroacetic ac...	13.67	2.0	ng	82840	5	13.80	827249	20.0
Squalene	14.65	2.2	ng	81506	6	15.17	740488	20.0