

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093658.D
 Acq On : 14 Mar 2017 14:59
 Operator : SJ/MA
 Sample : I2224-02
 Misc :
 ALS Vial : 53 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 030917-PRRT-F-D-M

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-BF030717.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	4.847	257	259	266	rBV	417086	686180	13.22%	2.053%
2	4.938	266	267	281	rVB	53077	141437	2.72%	0.423%
3	5.316	298	300	321	rBV	664542	1733191	33.39%	5.185%
4	6.379	391	393	400	rBV	532348	1042632	20.09%	3.119%
5	6.481	400	402	417	rVV	2294685	2924961	56.35%	8.751%
6	6.710	420	422	431	rVV	1009293	1129996	21.77%	3.381%
7	6.859	433	435	449	rVB	3524212	3905946	75.25%	11.686%
8	7.282	470	472	487	rBV	2600812	3444093	66.35%	10.304%
9	7.956	530	531	533	rBV	67505	75818	1.46%	0.227%
10	8.002	533	535	547	rVB	1348332	1383941	26.66%	4.141%
11	9.076	627	629	632	rBV	3701497	5190600	100.00%	15.529%
12	9.762	686	689	691	rBV	1233027	1485003	28.61%	4.443%
13	10.550	756	758	766	rBV	1683115	1881796	36.25%	5.630%
14	10.665	766	768	773	rVB	55318	66909	1.29%	0.200%
15	11.248	817	819	825	rBV	1561018	1519876	29.28%	4.547%
16	12.654	940	942	944	rBV	122288	99240	1.91%	0.297%
17	12.836	955	958	960	rBV	4003010	4361064	84.02%	13.048%
18	13.351	1001	1003	1005	rBV	62066	68399	1.32%	0.205%
19	13.888	1048	1050	1059	rVB	1091249	1214886	23.41%	3.635%
20	14.699	1119	1121	1124	rBV	225187	202872	3.91%	0.607%
21	15.294	1170	1173	1183	rBV	558385	865622	16.68%	2.590%

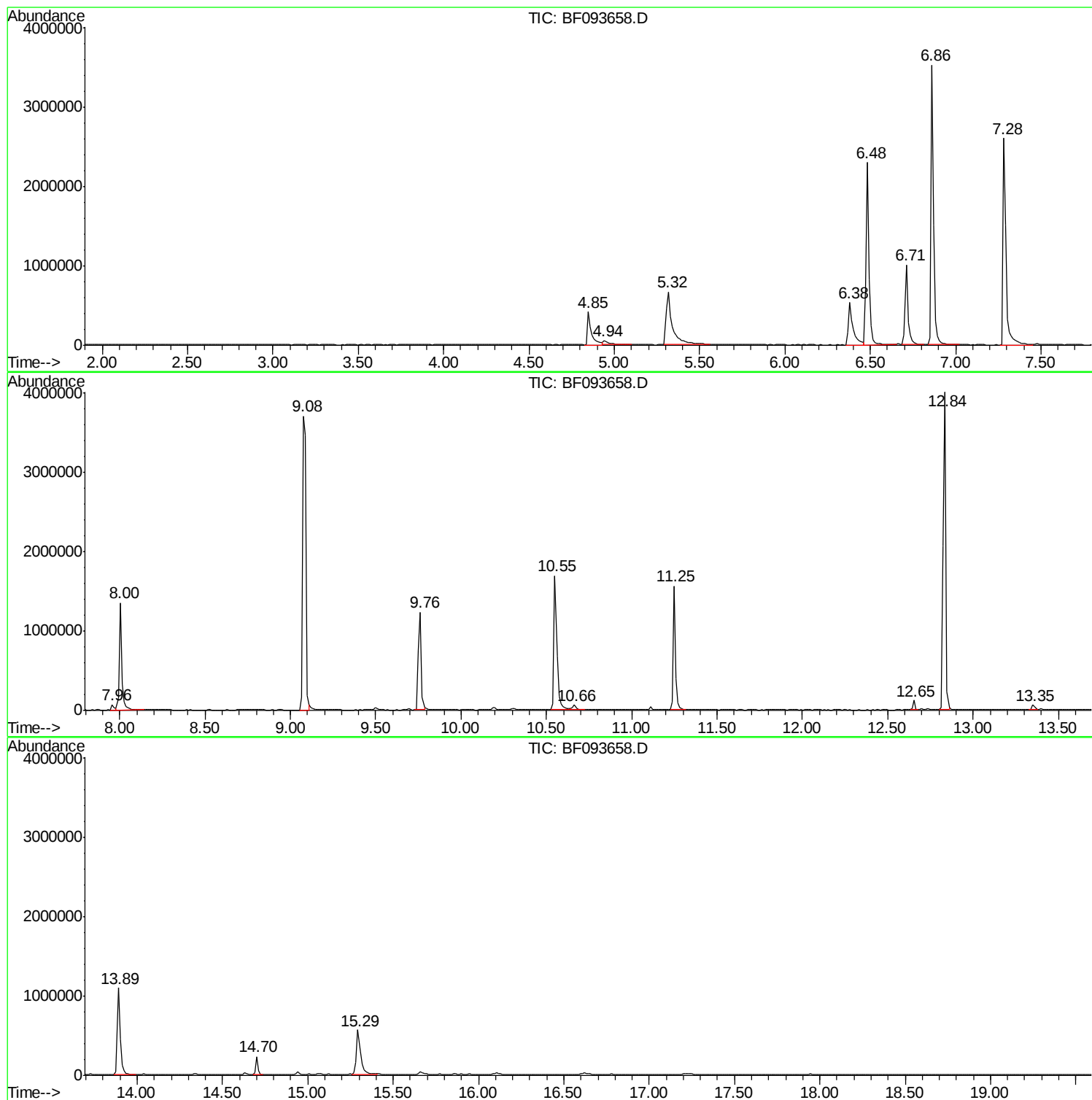
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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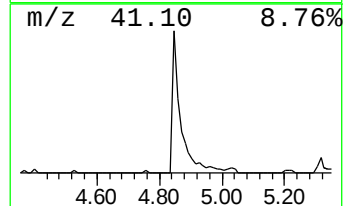
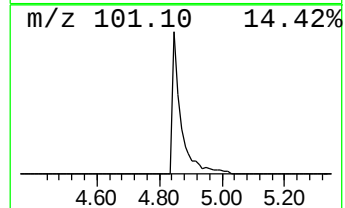
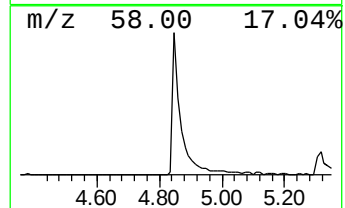
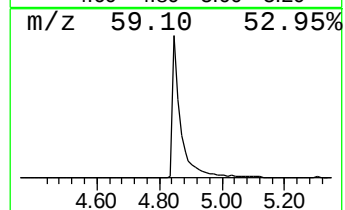
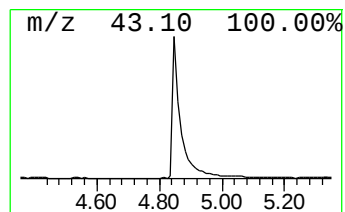
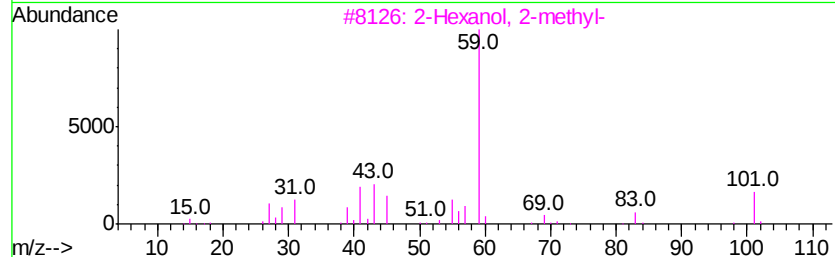
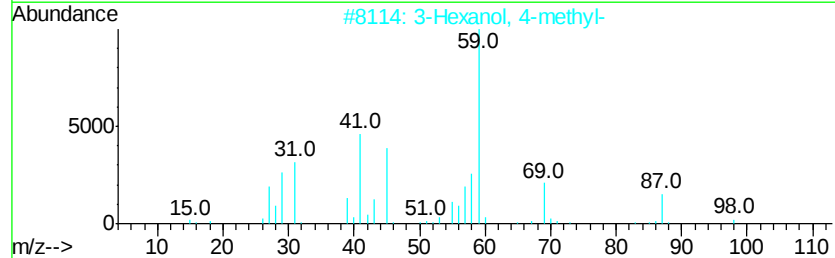
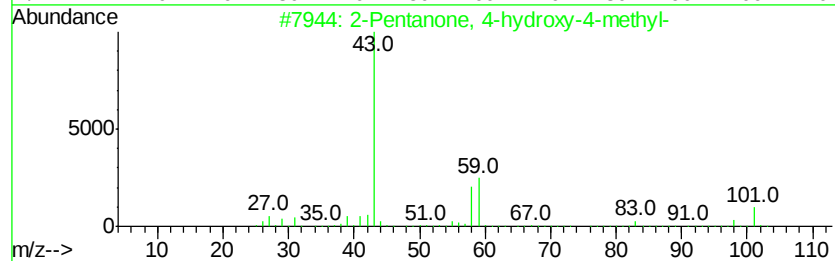
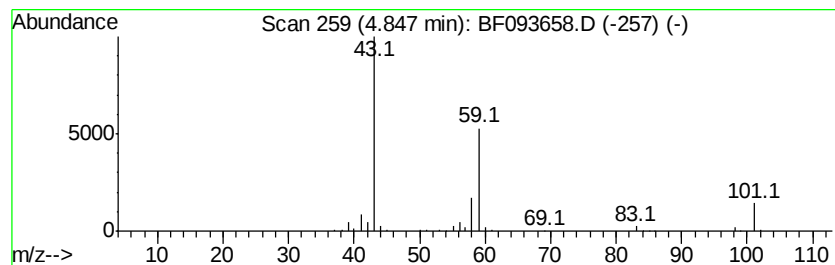
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	12.14 ng	686180	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



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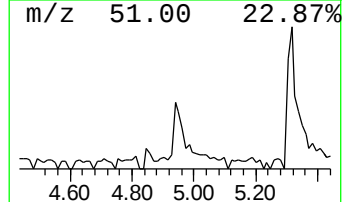
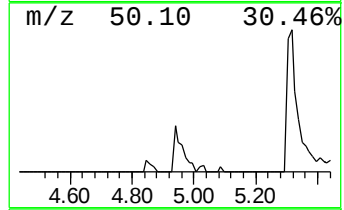
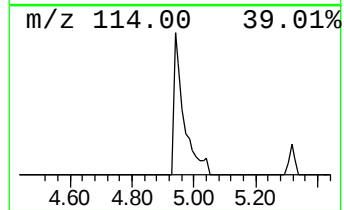
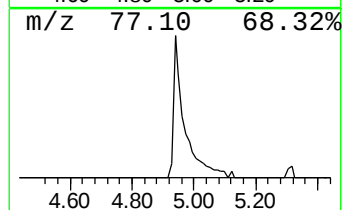
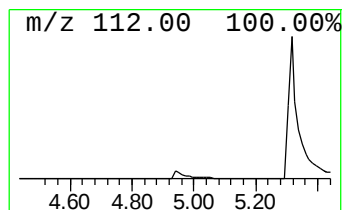
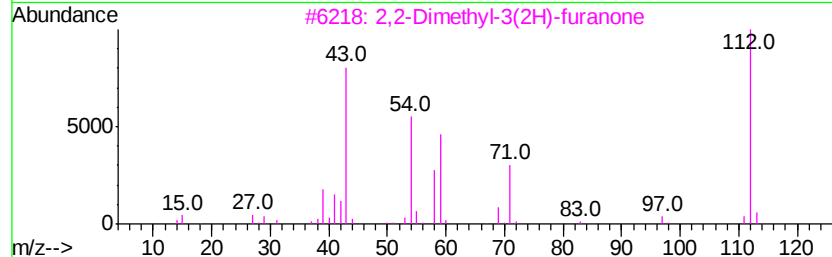
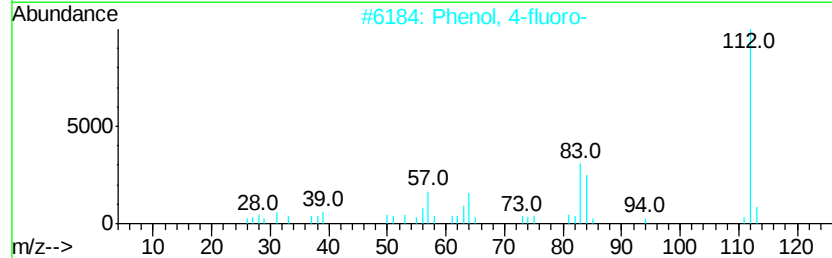
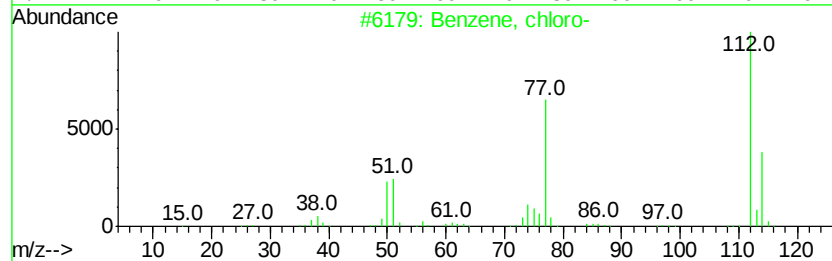
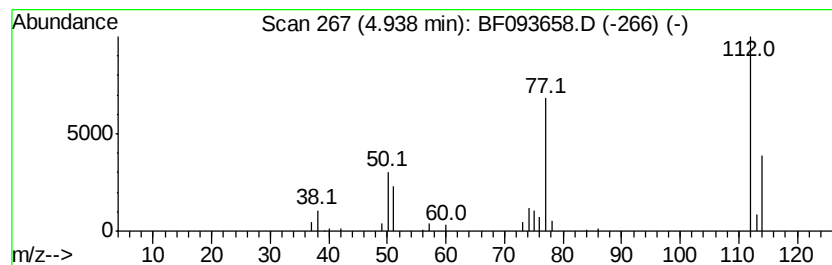
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Peak Number 2 Benzene, chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	2.50 ng	141437	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, chloro-	112	C6H5Cl	000108-90-7	97
2		Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	9
3		2,2-Dimethyl-3(2H)-furanone	112	C6H8O2	035298-48-7	9
4		3-Nitropyrrole	112	C4H4N2O2	005930-94-9	9
5		3-Hydroxypyridazine 1-oxide	112	C4H4N2O2	018259-51-3	9



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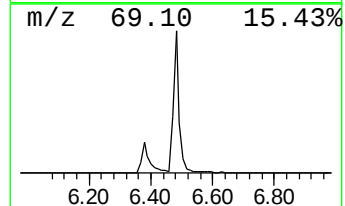
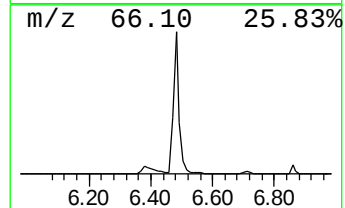
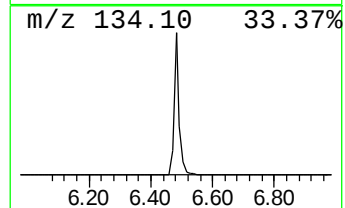
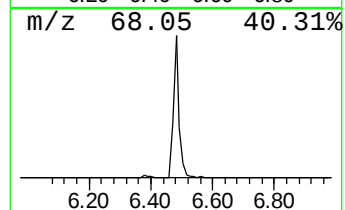
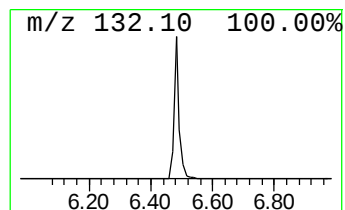
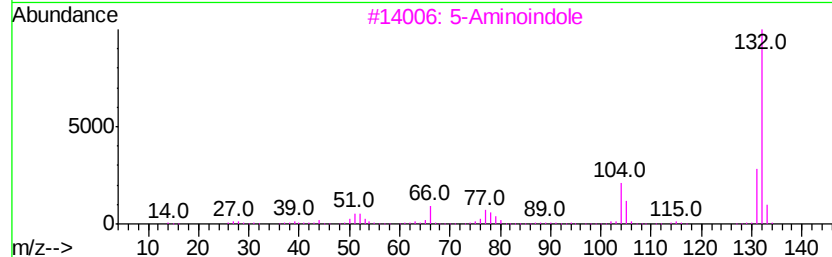
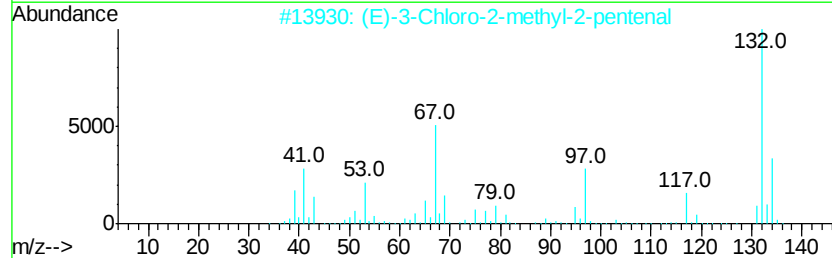
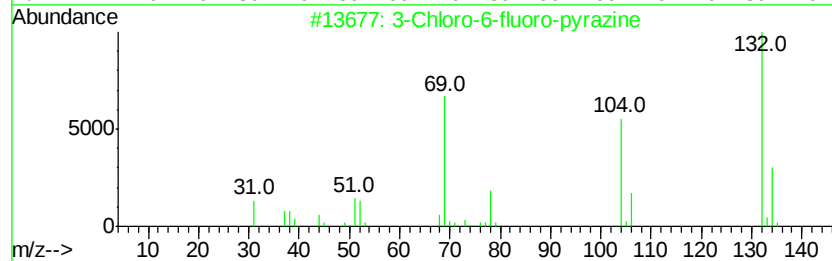
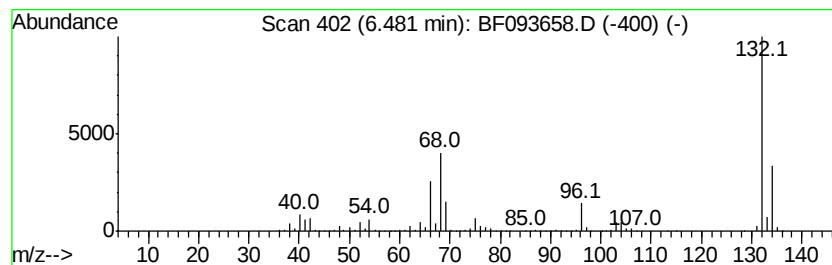
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Peak Number 3 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	51.77 ng	2924960	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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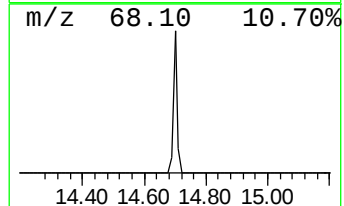
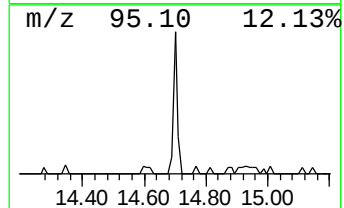
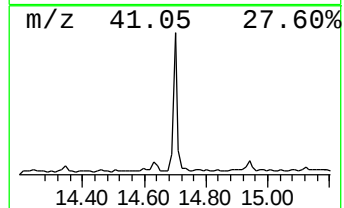
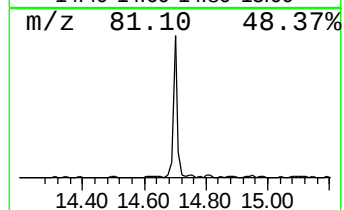
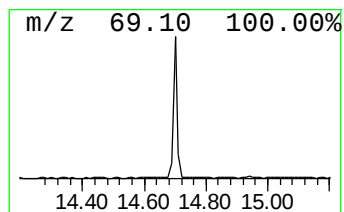
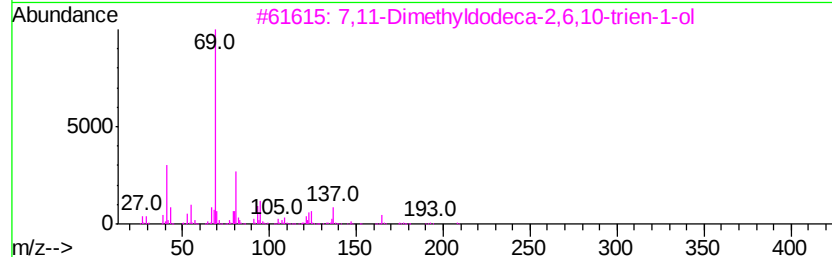
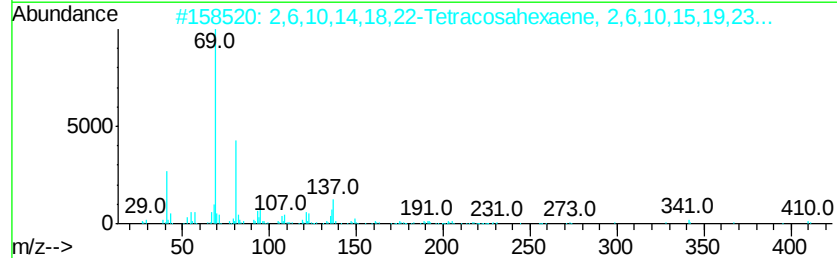
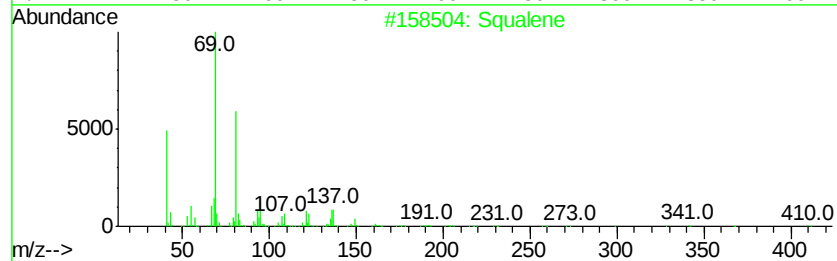
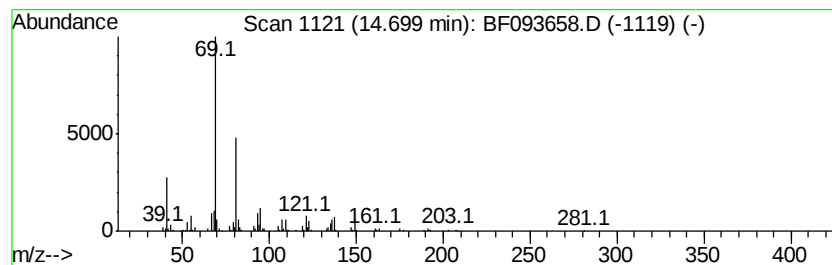
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Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	4.69 ng	202872	Perylene-d12	15.29

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	78
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72
5		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.85	12.1	ng	686180	1	6.71	1130000	20.0
Benzene, chloro-	4.94	2.5	ng	141437	1	6.71	1130000	20.0
unknown6.48	6.48	51.8	ng	2924960	1	6.71	1130000	20.0
Squalene	14.70	4.7	ng	202872	6	15.29	865622	20.0