

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091818\
 Data File : BF109122.D
 Acq On : 19 Sep 2018 3:48
 Operator : JU/SJ
 Sample : J4930-06
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091318-DBRI-E-D-M

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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	4.901	433	436	442	rBV	145318	148720	4.42%	0.695%
2	5.325	504	508	512	rBV	1191326	1058370	31.46%	4.947%
3	6.348	678	682	694	rBV2	881817	771075	22.92%	3.604%
4	6.490	702	706	709	rBV	2134339	1833266	54.50%	8.570%
5	6.719	742	745	749	rBV	878861	692913	20.60%	3.239%
6	6.878	768	772	775	rBV	2925452	2510696	74.63%	11.737%
7	7.284	835	841	844	rBV	2138037	2022963	60.13%	9.457%
8	8.001	959	963	967	rBV	966625	803623	23.89%	3.757%
9	9.078	1142	1146	1150	rBV	3515511	3364058	100.00%	15.726%
10	9.472	1209	1213	1219	rBV	213516	186245	5.54%	0.871%
11	9.754	1257	1261	1264	rBV	878241	802450	23.85%	3.751%
12	10.536	1390	1394	1406	rBV	1368700	1245205	37.01%	5.821%
13	11.230	1508	1512	1515	rBV	839595	722583	21.48%	3.378%
14	12.813	1776	1781	1784	rBV	3410145	3177053	94.44%	14.852%
15	13.719	1931	1935	1948	rBV2	88711	145293	4.32%	0.679%
16	13.854	1954	1958	1962	rBV	1011009	858271	25.51%	4.012%
17	14.636	2088	2091	2096	rBV	36448	36786	1.09%	0.172%
18	14.707	2100	2103	2107	rVV	75734	71230	2.12%	0.333%
19	14.954	2141	2145	2149	rBV	49562	58418	1.74%	0.273%
20	15.260	2192	2197	2202	rBV	606682	692139	20.57%	3.235%
21	15.313	2202	2206	2211	rVB	55426	76071	2.26%	0.356%
22	15.713	2270	2274	2279	rBV	45971	61920	1.84%	0.289%
23	16.183	2349	2354	2358	rBV2	30412	52779	1.57%	0.247%

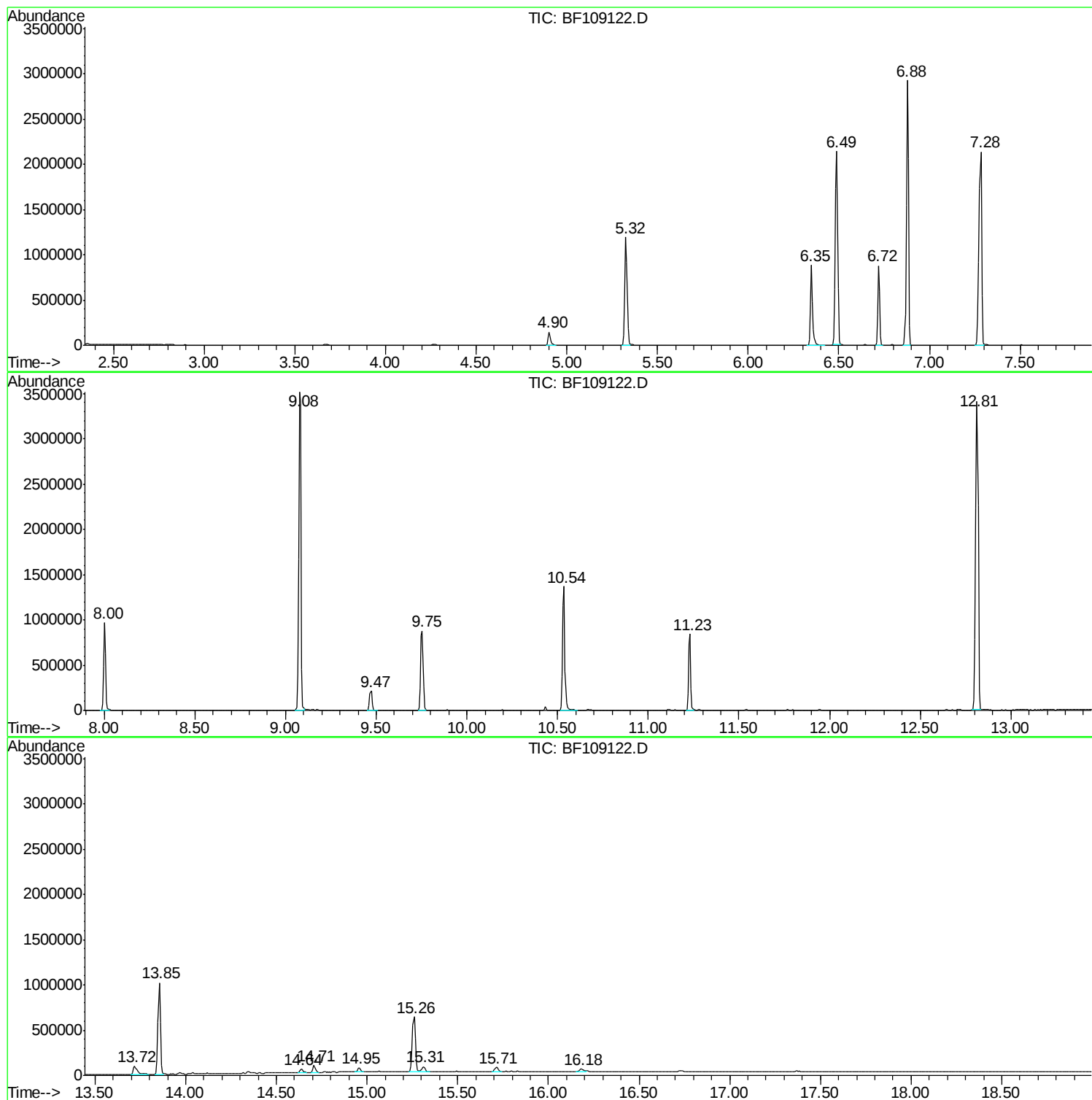
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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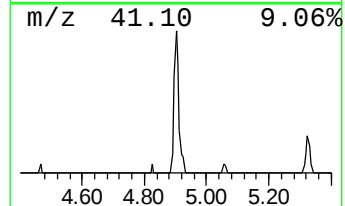
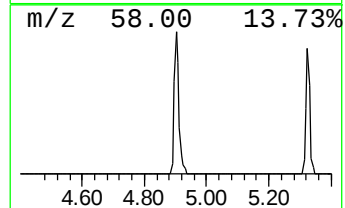
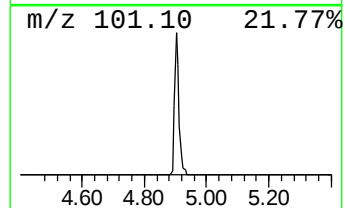
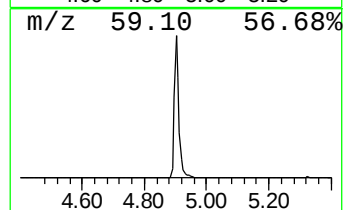
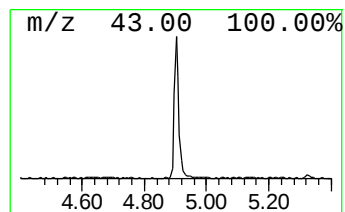
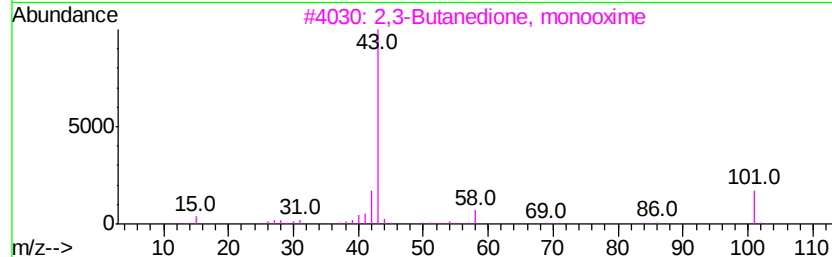
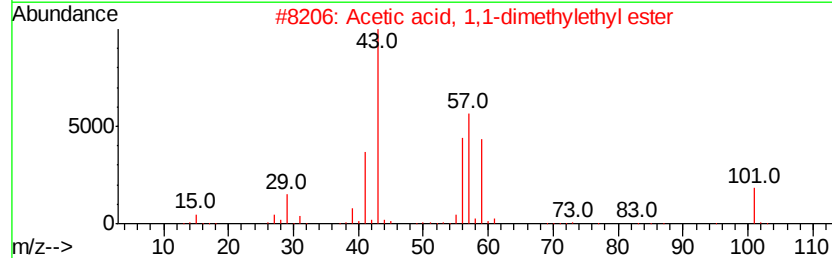
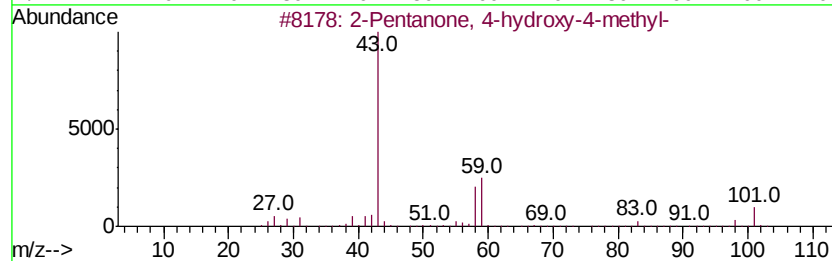
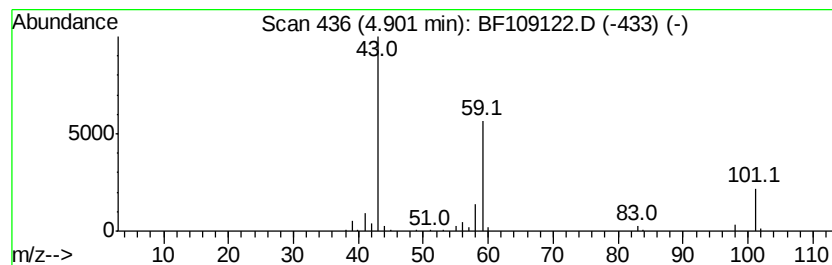
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	4.29 ng	148720	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4		3-Hexanol	102	C6H14O	000623-37-0	28
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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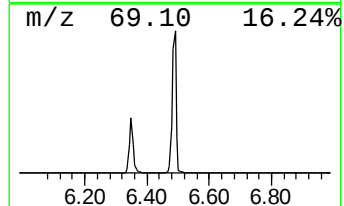
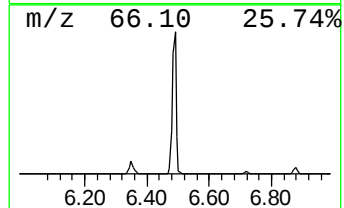
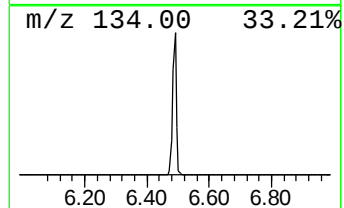
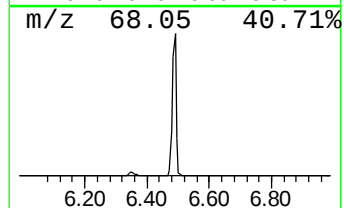
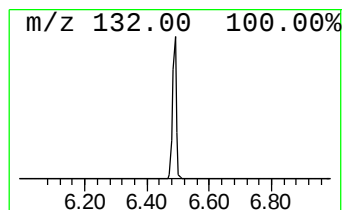
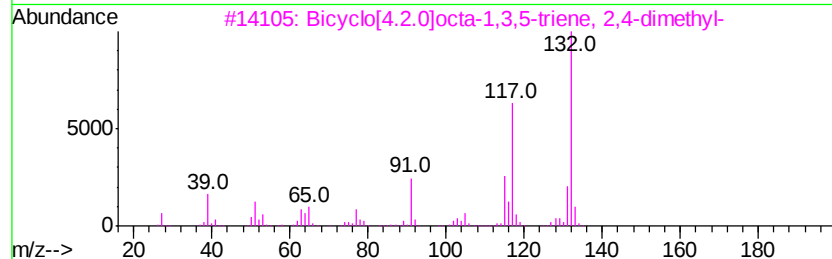
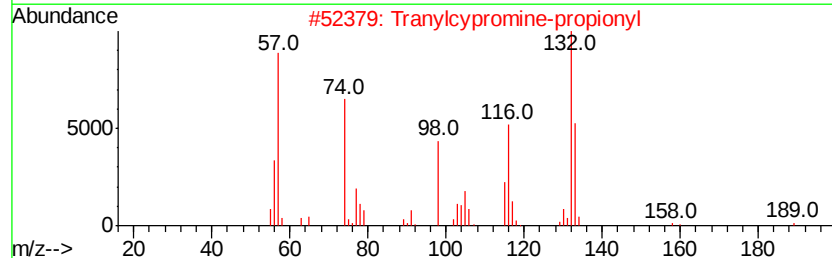
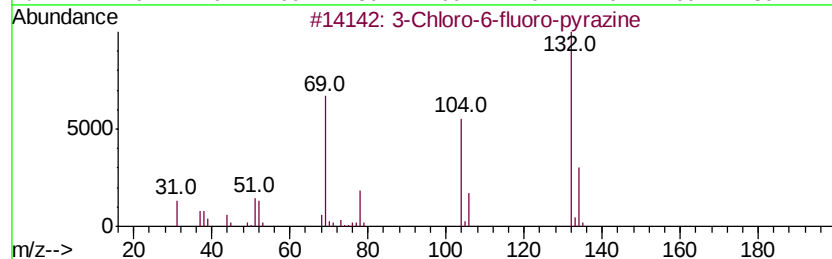
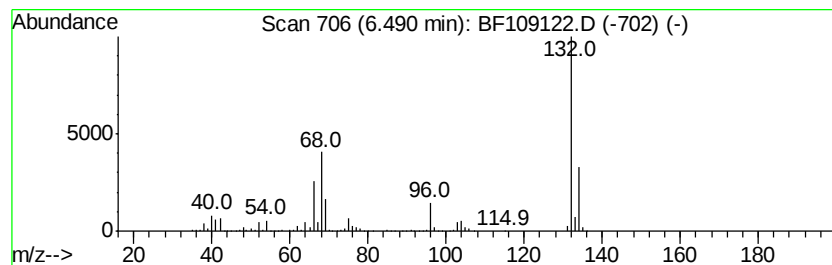
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Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	52.91 ng	1833270	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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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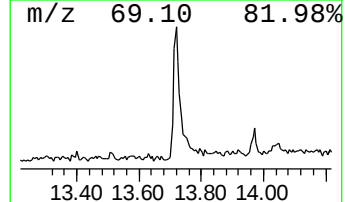
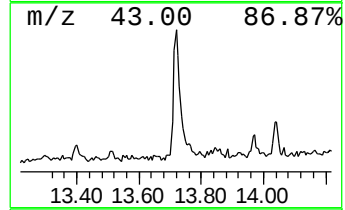
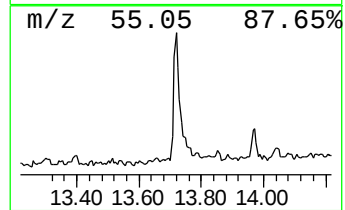
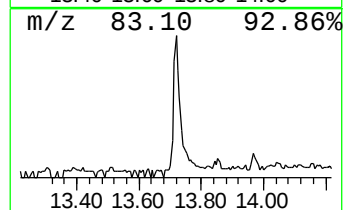
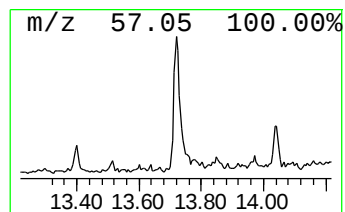
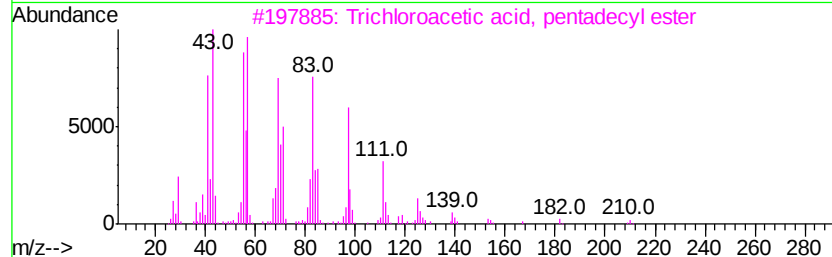
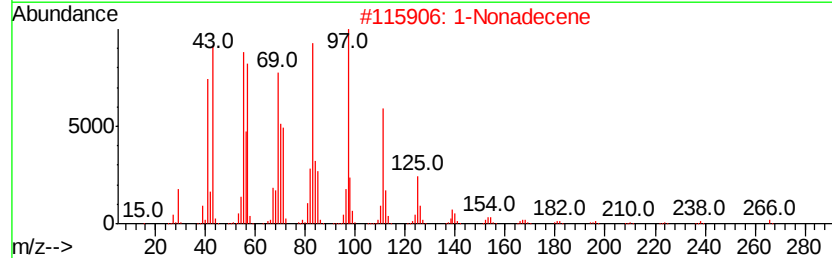
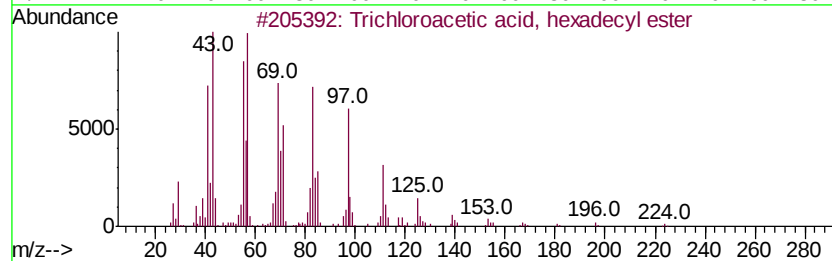
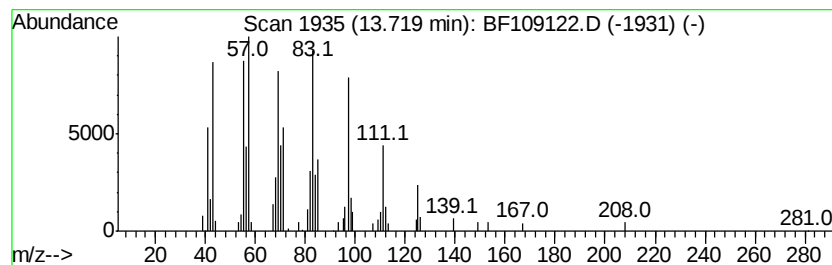
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	3.39 ng	145293	Chrysene-d12	13.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2			1-Nonadecene	266	C19H38	018435-45-5	91
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90



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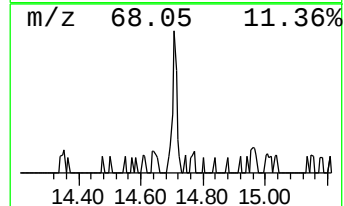
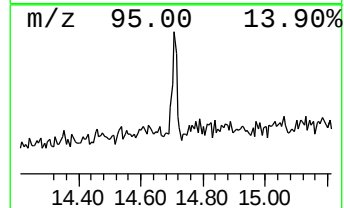
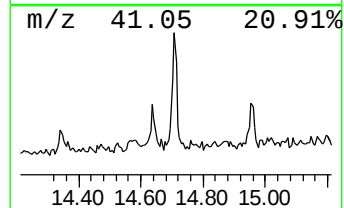
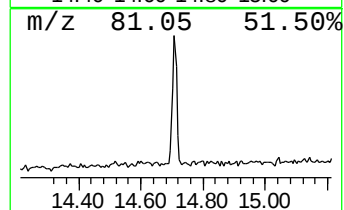
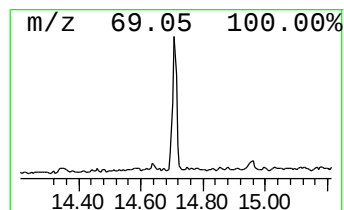
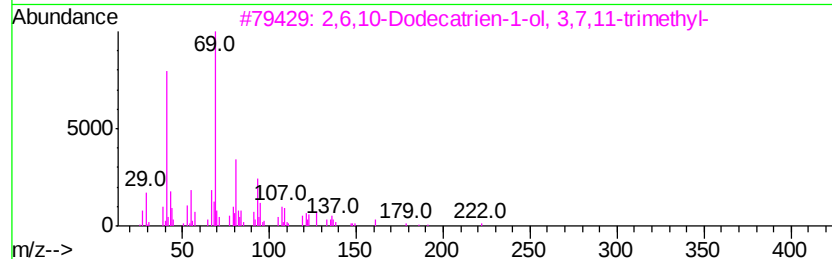
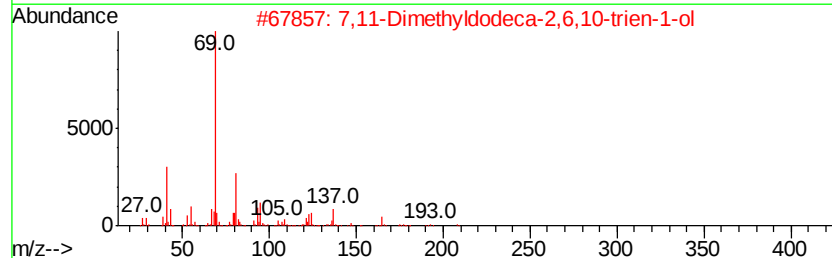
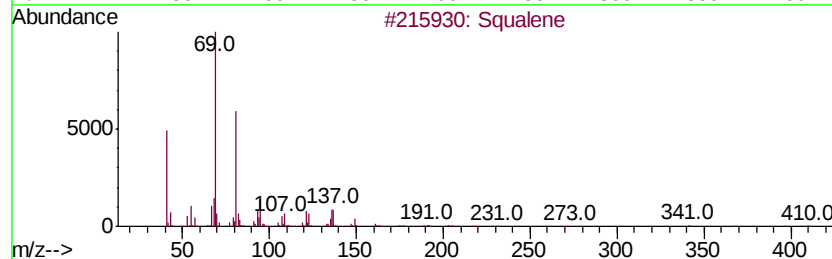
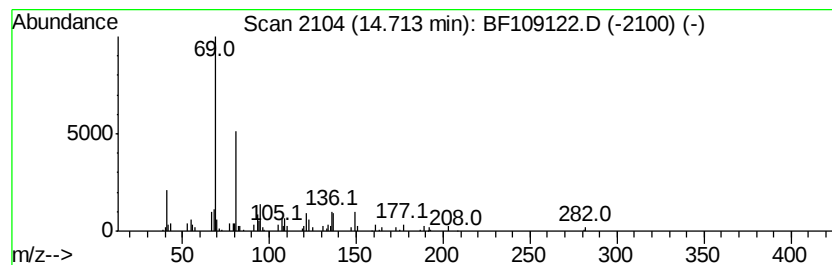
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Peak Number 5 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.06 ng	71230	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	86
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
4		3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	64
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64



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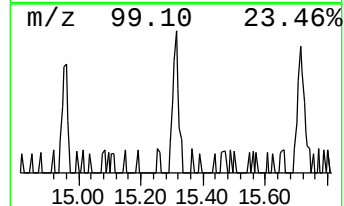
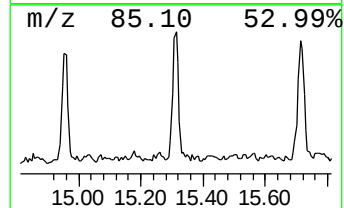
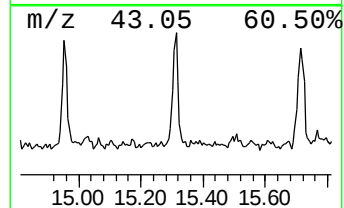
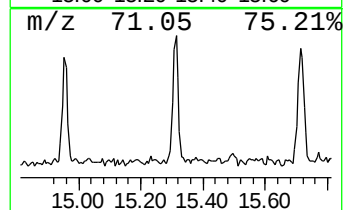
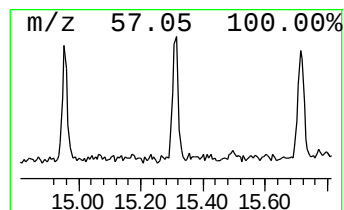
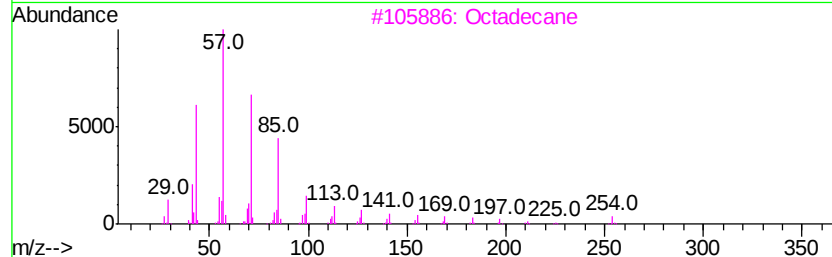
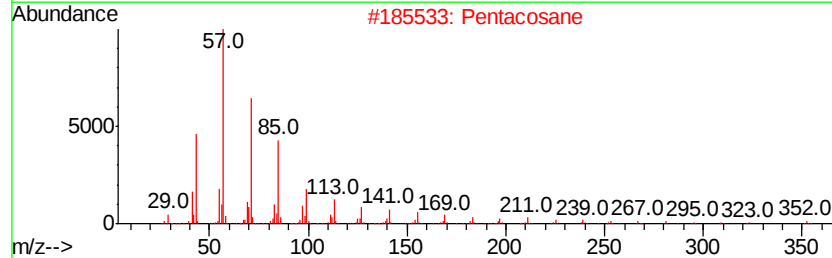
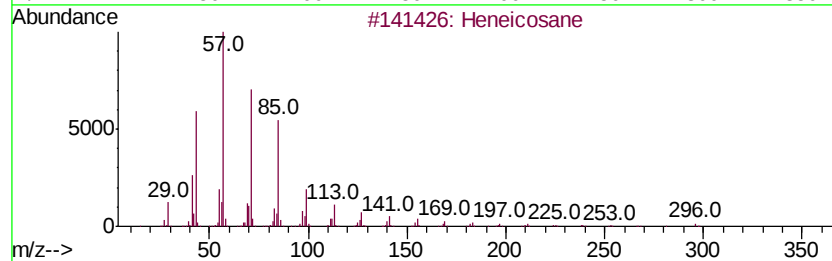
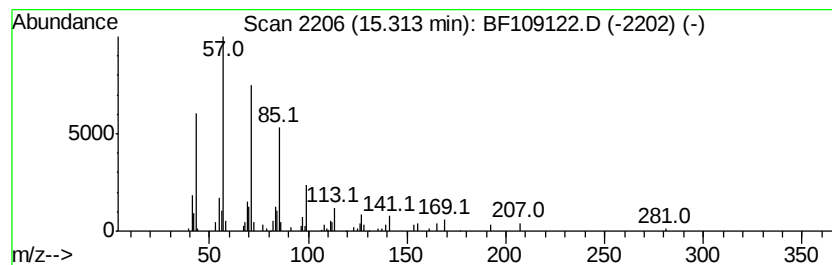
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Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.20 ng	76071	Perylene-d12	15.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Pentacosane		352	C25H52	000629-99-2	90
3	Octadecane		254	C18H38	000593-45-3	86
4	Heptadecane		240	C17H36	000629-78-7	86
5	Hexadecane		226	C16H34	000544-76-3	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	4.3	ng	148720	1	6.72	692913	20.0
unknown6.49	6.49	52.9	ng	1833270	1	6.72	692913	20.0
Trichloroacetic a...	13.72	3.4	ng	145293	5	13.85	858271	20.0
Squalene	14.71	2.1	ng	71230	6	15.26	692139	20.0
Heneicosane	15.31	2.2	ng	76071	6	15.26	692139	20.0