

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
 Data File : BF096842.D
 Acq On : 18 Jul 2017 12:35
 Operator : SJ/JU
 Sample : I4224-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DEC-02

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-BF071317.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	4.781	470	475	486	rBV	201222	289878	10.46%	1.208%
2	5.216	544	549	552	rBV	2218032	2407127	86.89%	10.031%
3	6.251	720	725	728	rBV	2285506	2474038	89.30%	10.310%
4	6.369	741	745	749	rBV	2449662	2429817	87.71%	10.126%
5	6.598	780	784	787	rBV	771748	652640	23.56%	2.720%
6	6.757	806	811	814	rBV	1837242	1843802	66.55%	7.684%
7	7.163	874	880	883	rBV	1712598	1675930	60.49%	6.984%
8	7.881	997	1002	1005	rBV	1041982	994353	35.89%	4.144%
9	8.957	1180	1185	1188	rBV	2711742	2770384	100.00%	11.545%
10	9.351	1248	1252	1255	rBV	480337	394717	14.25%	1.645%
11	9.628	1294	1299	1303	rBV2	1172475	1045107	37.72%	4.355%
12	10.416	1428	1433	1436	rBV	1654661	1711627	61.78%	7.133%
13	10.545	1452	1455	1463	rBV	56650	63641	2.30%	0.265%
14	10.992	1524	1531	1534	rBV2	49093	47678	1.72%	0.199%
15	11.104	1542	1550	1553	rBV	1106661	967616	34.93%	4.032%
16	12.686	1814	1819	1823	rBV	2271560	2386475	86.14%	9.945%
17	13.174	1895	1902	1908	rBV	185500	192737	6.96%	0.803%
18	13.592	1969	1973	1979	rBV2	122379	142117	5.13%	0.592%
19	13.727	1991	1996	1999	rBV	816283	735969	26.57%	3.067%
20	14.221	2077	2080	2082	rBV2	34981	30800	1.11%	0.128%
21	14.810	2177	2180	2185	rBV2	34159	43149	1.56%	0.180%
22	15.098	2224	2229	2234	rBV	491841	557638	20.13%	2.324%
23	15.145	2234	2237	2241	rVB	37713	42510	1.53%	0.177%
24	15.527	2298	2302	2308	rBV2	32993	44753	1.62%	0.187%
25	15.962	2374	2376	2384	rVB2	30877	51657	1.86%	0.215%

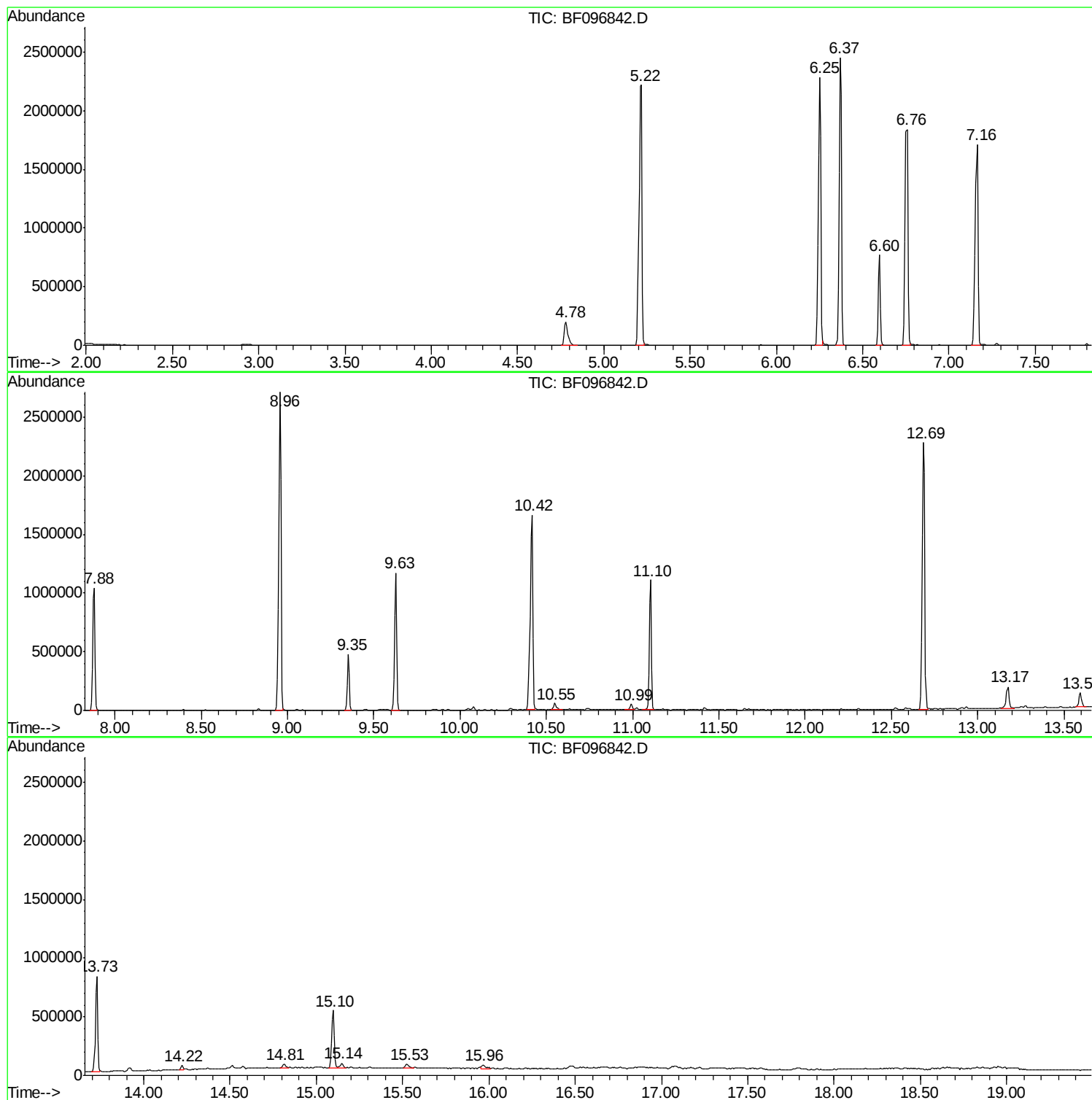
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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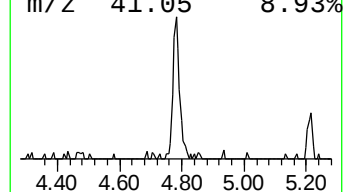
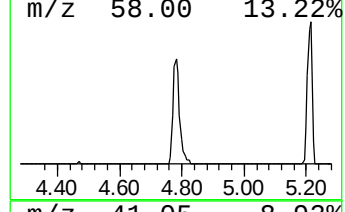
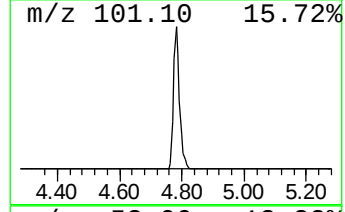
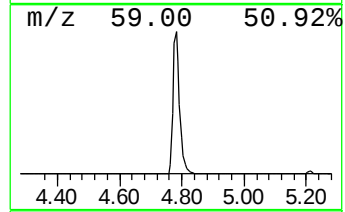
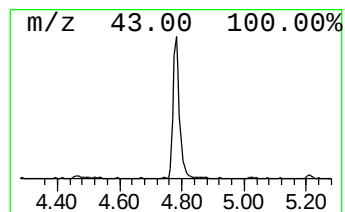
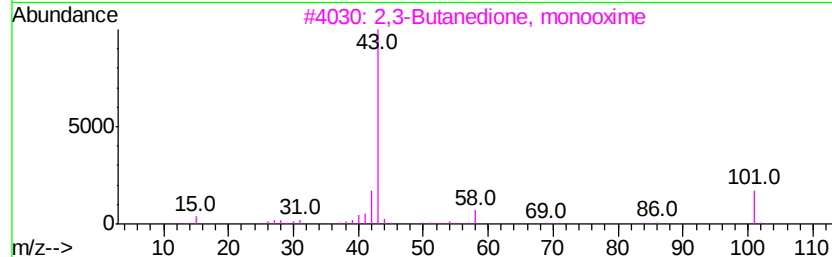
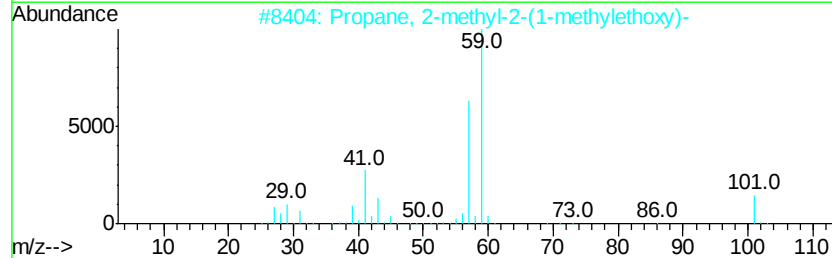
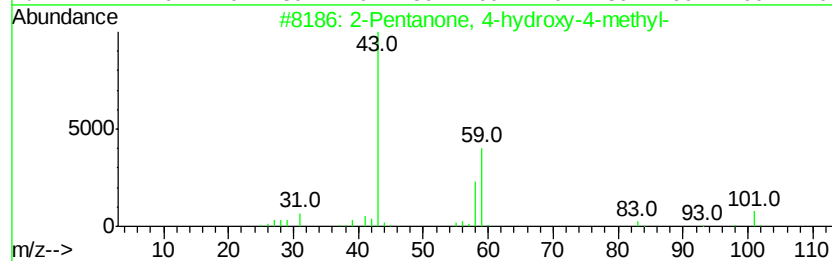
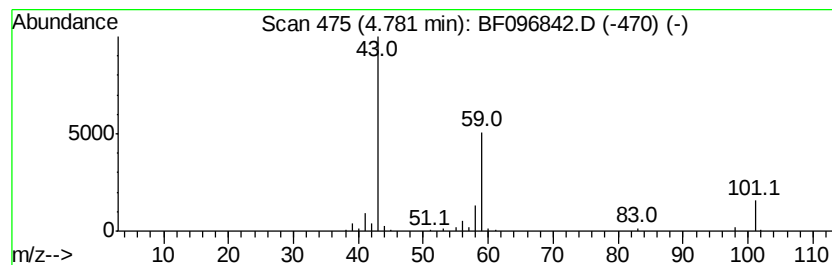
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.78	8.88 ng	289878	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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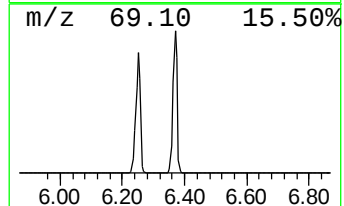
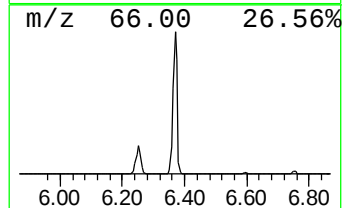
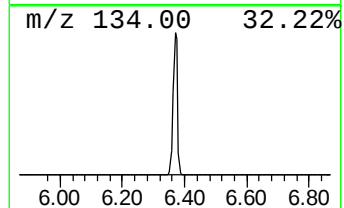
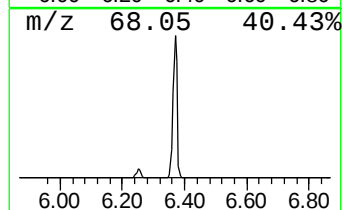
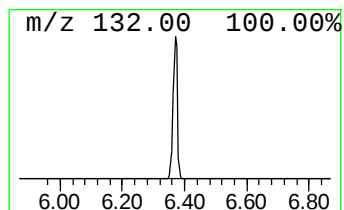
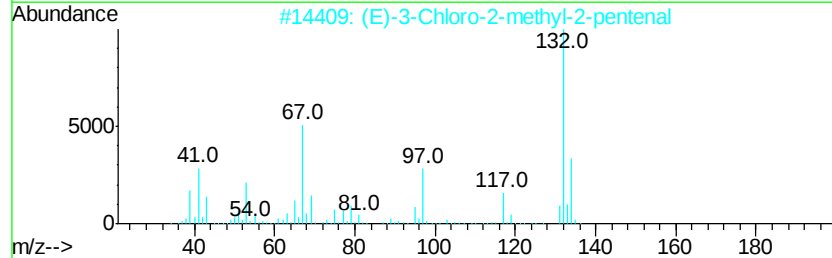
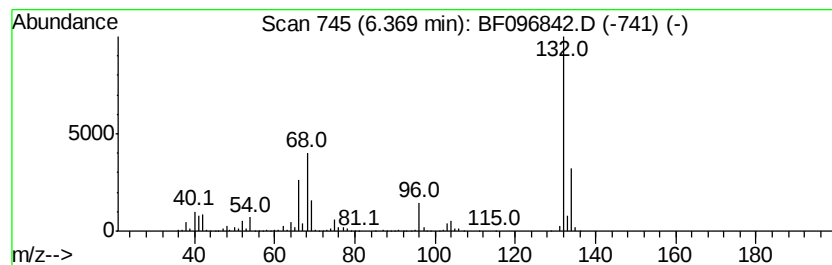
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	74.46 ng	2429820	1,4-Dichlorobenzene-d4	6.60

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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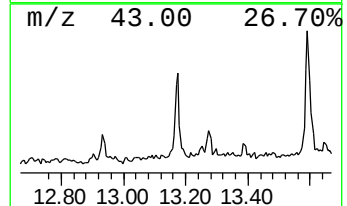
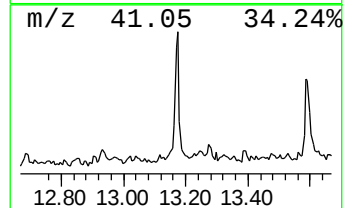
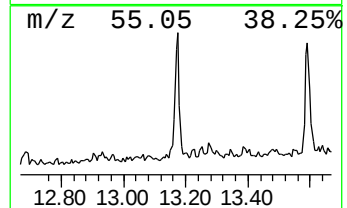
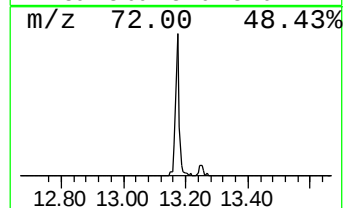
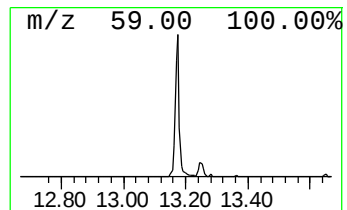
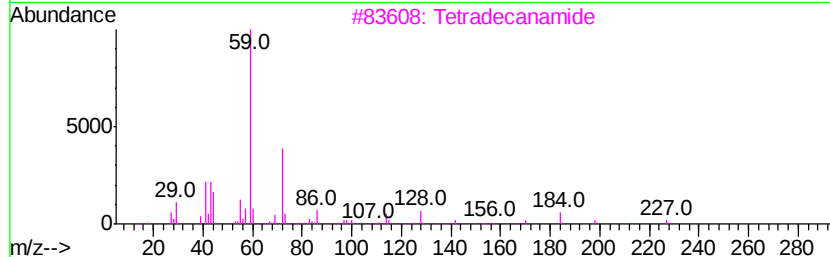
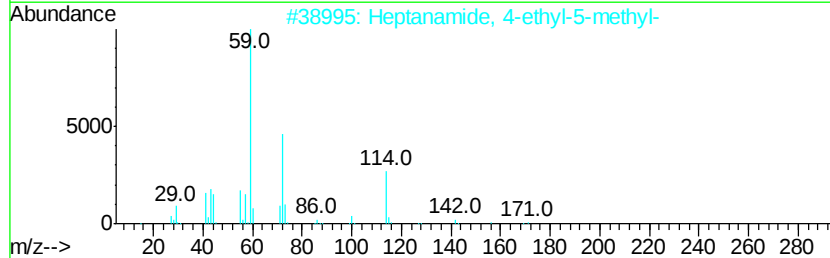
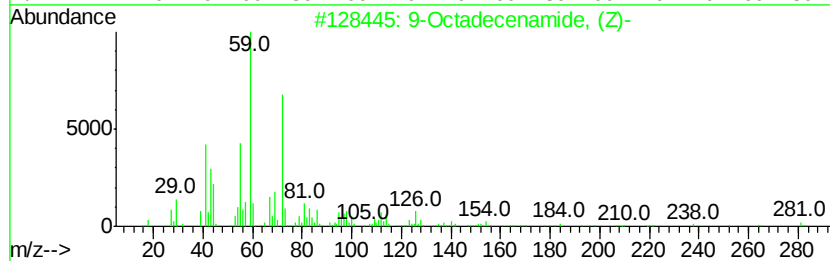
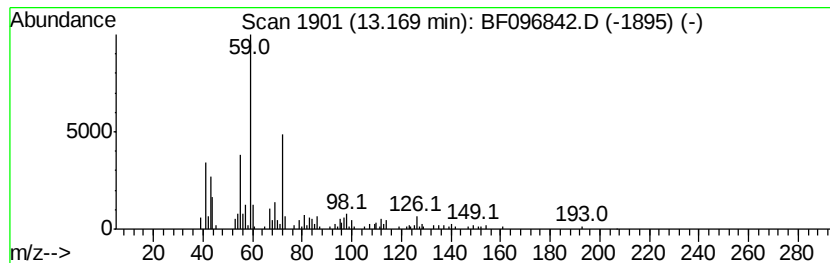
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	5.24 ng	192737	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
3		Tetradecanamide	227	C14H29NO	000638-58-4	72
4		Pentanamide	101	C5H11NO	000626-97-1	64
5		Nonanamide	157	C9H19NO	001120-07-6	59



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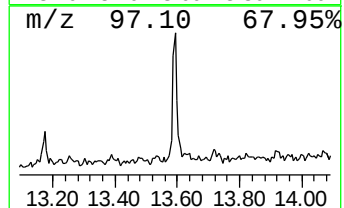
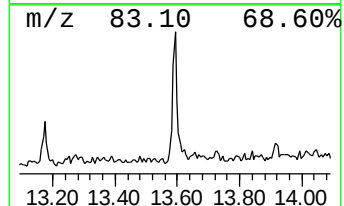
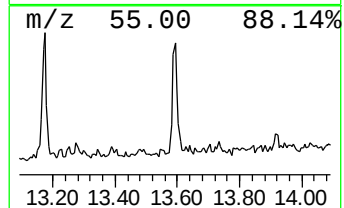
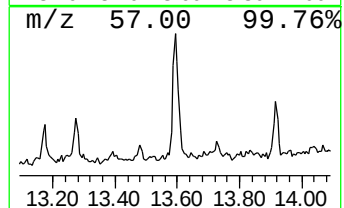
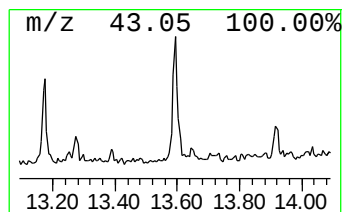
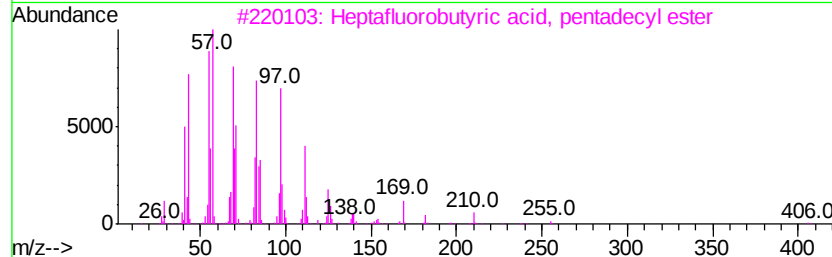
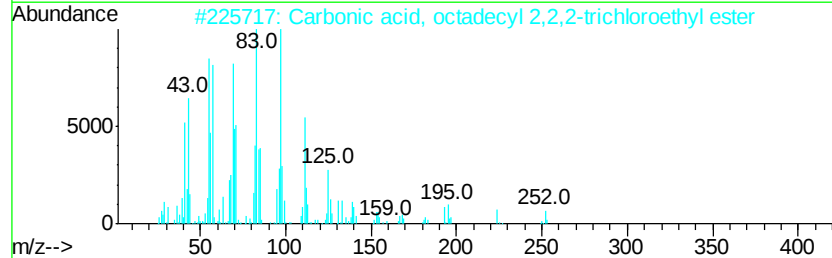
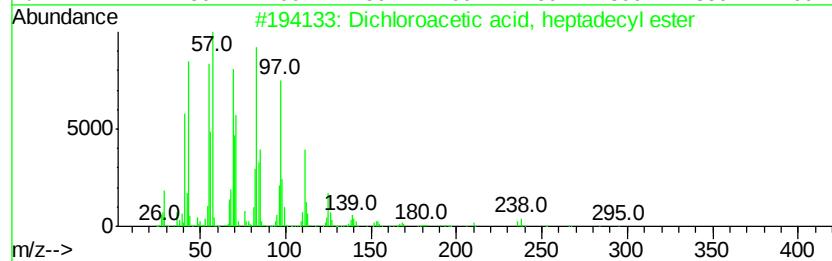
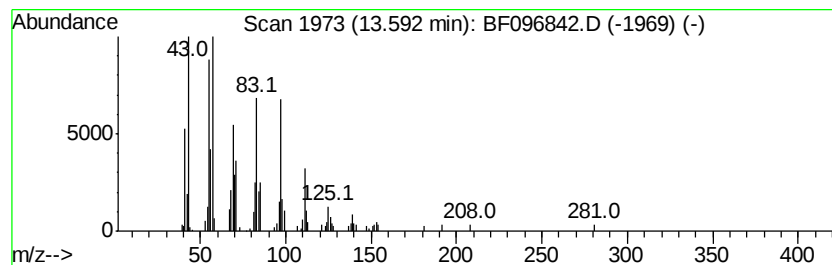
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Dichloroacetic acid, heptadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	3.86 ng	142117	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.78	8.9	ng	289878	1	6.60	652640	20.0
unknown6.37	6.37	74.5	ng	2429820	1	6.60	652640	20.0
9-Octadecenamide, ...	13.17	5.2	ng	192737	5	13.73	735969	20.0
Dichloroacetic ac...	13.59	3.9	ng	142117	5	13.73	735969	20.0