

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
 Data File : BF102306.D
 Acq On : 22 Jan 2018 18:28
 Operator : SJ/JU
 Sample : J1228-25
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-4

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-BF012218.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	4.916	475	481	489	rBV	162611	242841	7.15%	0.813%
2	5.328	546	551	554	rBV	2997355	3083852	90.80%	10.323%
3	6.357	720	726	737	rBV	2909839	3267421	96.21%	10.938%
4	6.487	743	748	751	rBV	3213803	3214065	94.64%	10.759%
5	6.710	783	786	795	rBV	828819	771601	22.72%	2.583%
6	6.869	809	813	816	rBV	2759931	2450594	72.16%	8.204%
7	7.281	878	883	886	rBV	2027203	2003440	58.99%	6.707%
8	7.998	1000	1005	1008	rBV	1072204	1036986	30.53%	3.471%
9	8.557	1096	1100	1104	rBV	40809	39822	1.17%	0.133%
10	9.075	1183	1188	1191	rBV	3688647	3396233	100.00%	11.369%
11	9.469	1251	1255	1258	rBV	307215	261658	7.70%	0.876%
12	9.680	1287	1291	1295	rVB	63726	50376	1.48%	0.169%
13	9.745	1299	1302	1312	rVB	1146008	1139010	33.54%	3.813%
14	10.180	1372	1376	1379	rBV2	52980	48041	1.41%	0.161%
15	10.463	1420	1424	1427	rBV	101368	88029	2.59%	0.295%
16	10.539	1432	1437	1440	rBV	2088850	1965395	57.87%	6.579%
17	10.651	1453	1456	1460	rBV	37365	35744	1.05%	0.120%
18	11.233	1551	1555	1558	rBV	1254620	1082413	31.87%	3.623%
19	12.821	1820	1825	1828	rBV	3228546	2956364	87.05%	9.897%
20	13.710	1973	1976	1986	rBV	357858	365998	10.78%	1.225%
21	13.868	1997	2003	2010	rBV	982067	941467	27.72%	3.152%
22	14.345	2080	2084	2088	rBV5	26241	43287	1.27%	0.145%
23	14.615	2127	2130	2138	rBV2	187992	232053	6.83%	0.777%
24	14.704	2142	2145	2149	rVB	33068	37283	1.10%	0.125%
25	14.957	2184	2188	2190	rBV3	30288	36065	1.06%	0.121%
26	15.292	2239	2245	2254	rBV	672128	877733	25.84%	2.938%
27	15.721	2314	2318	2323	rBV	37344	52759	1.55%	0.177%
28	15.774	2323	2327	2331	rBV3	30412	45026	1.33%	0.151%
29	16.192	2393	2398	2404	rBV3	37004	65137	1.92%	0.218%
30	16.745	2488	2492	2497	rVB7	21474	41738	1.23%	0.140%

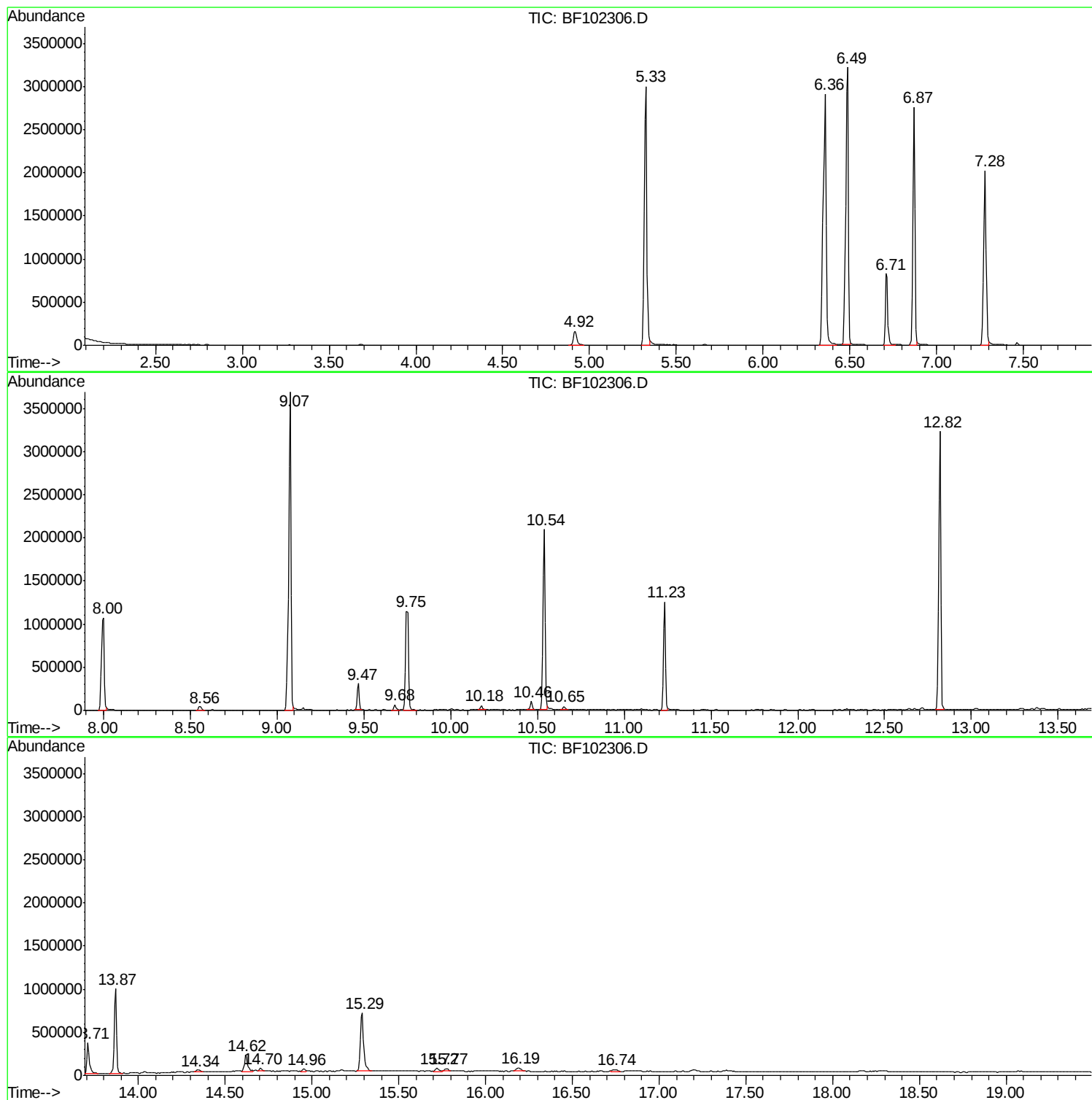
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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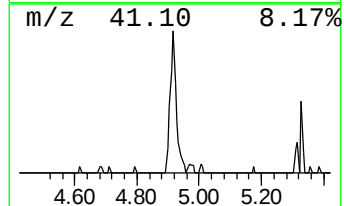
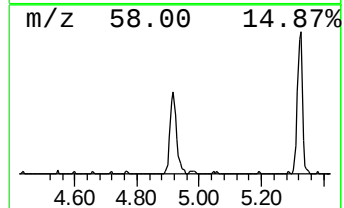
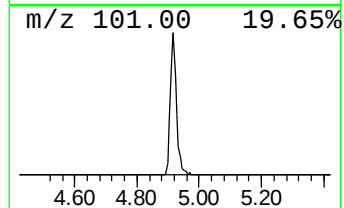
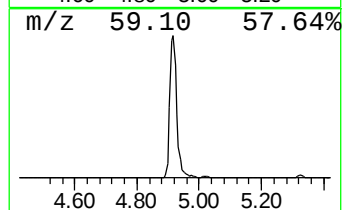
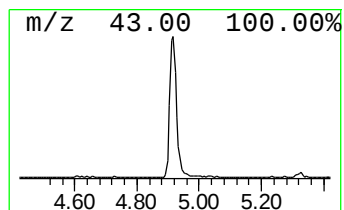
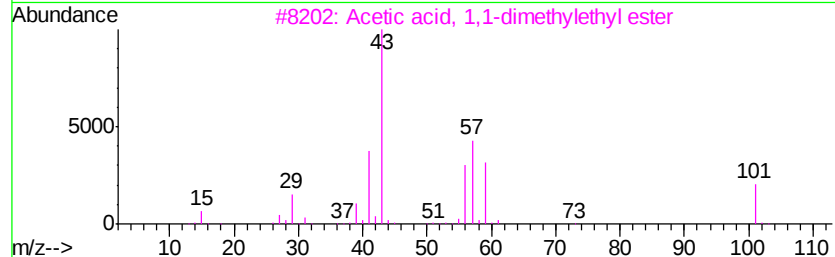
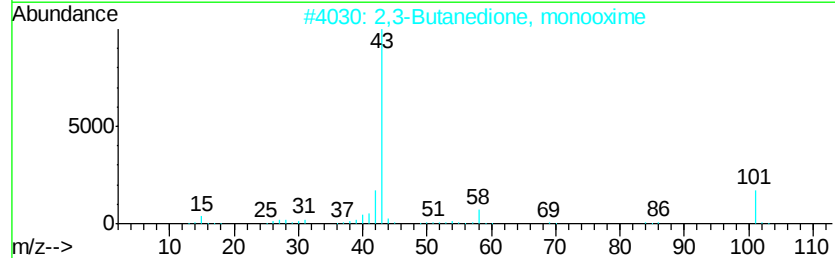
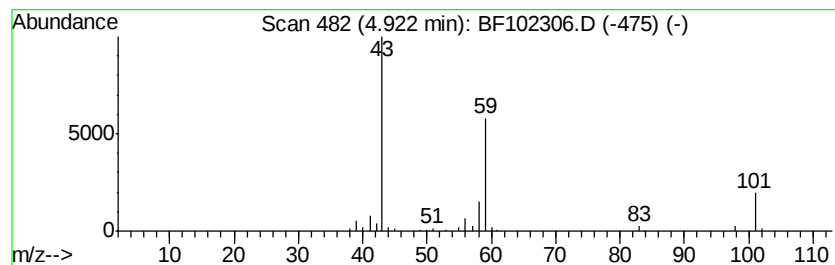
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.29 ng	242841	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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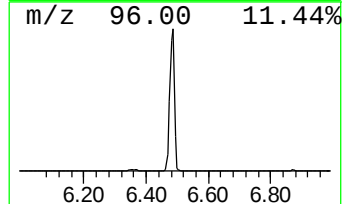
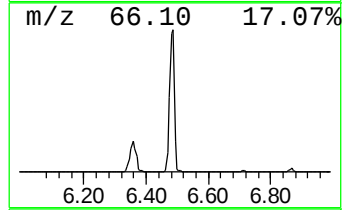
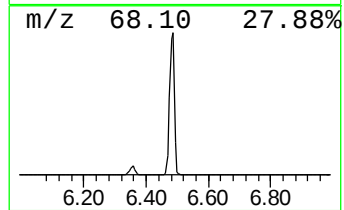
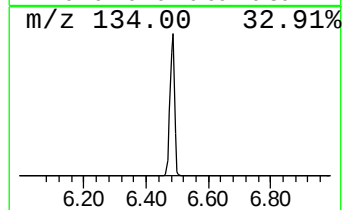
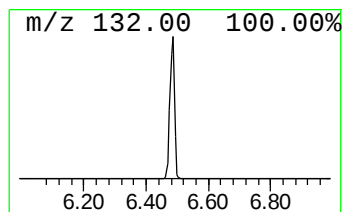
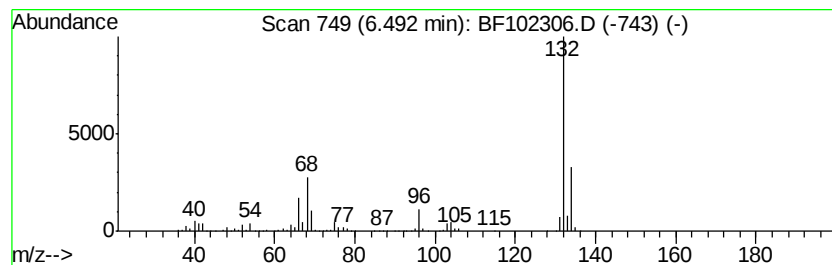
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	83.31 ng	3214070	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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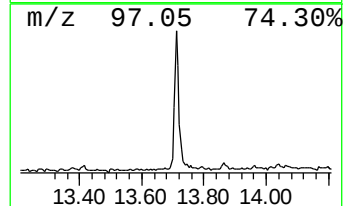
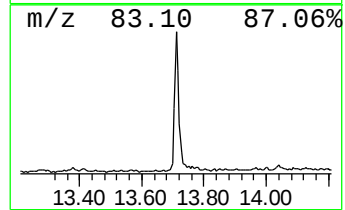
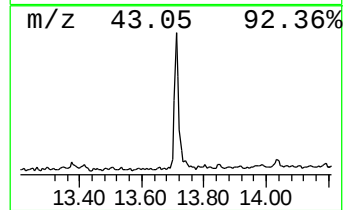
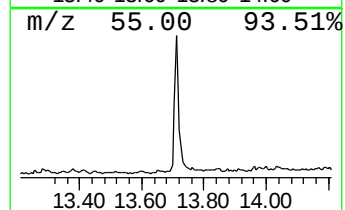
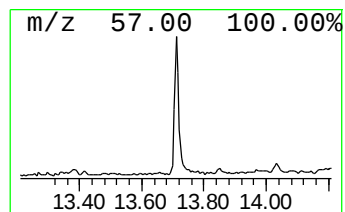
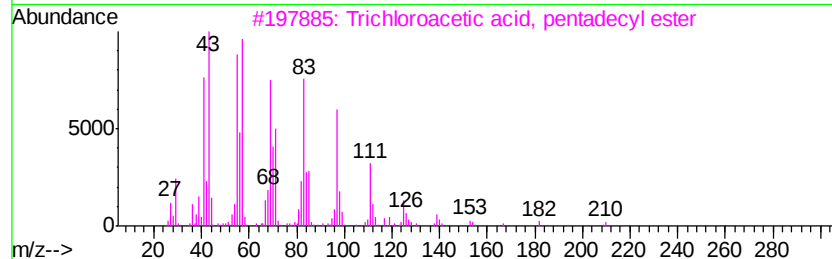
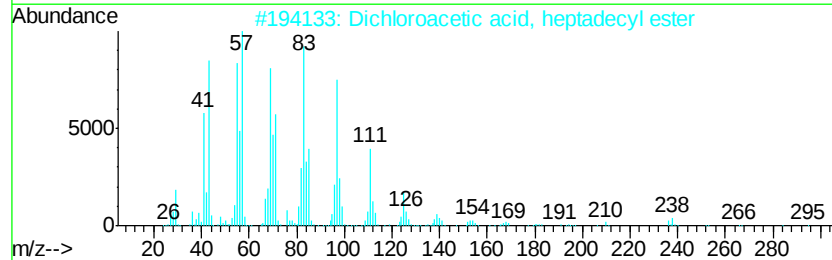
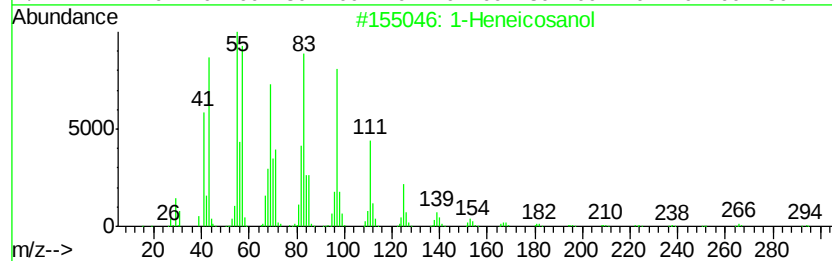
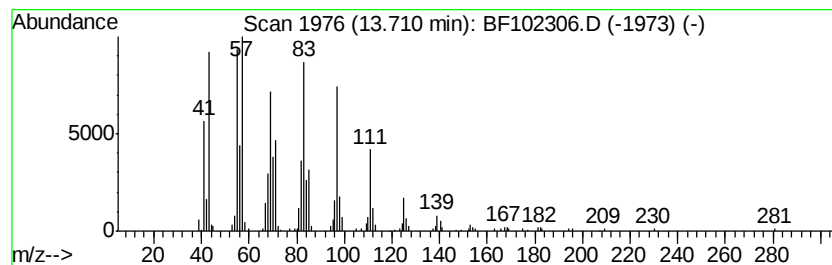
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	7.78 ng	365998	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94



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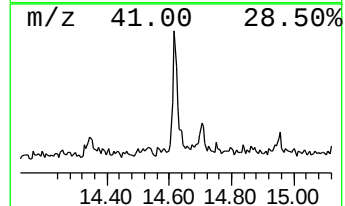
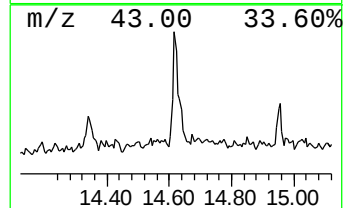
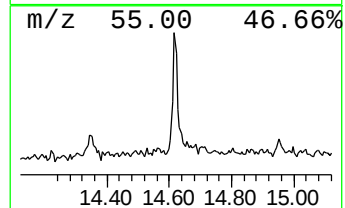
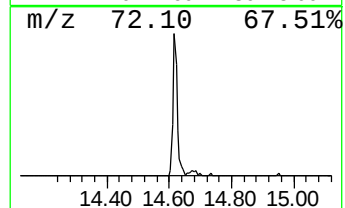
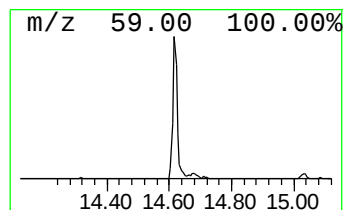
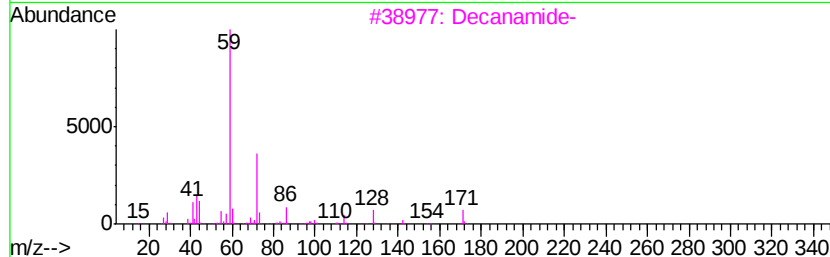
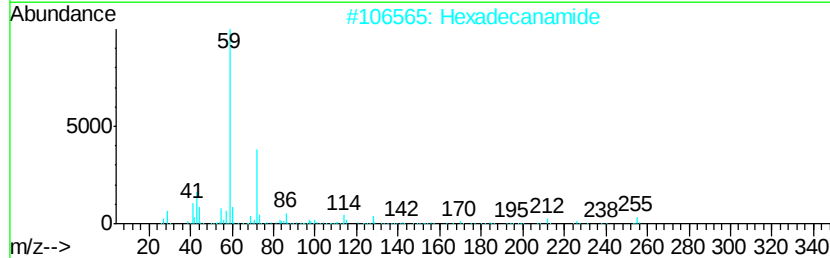
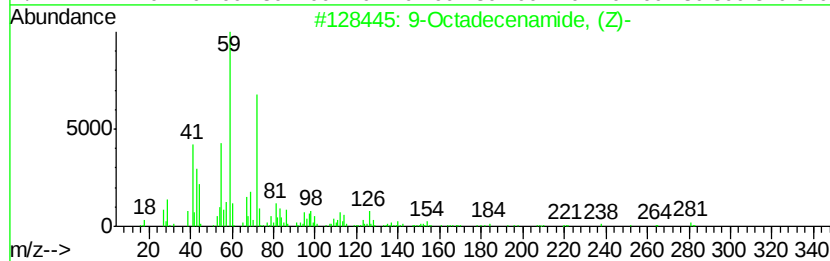
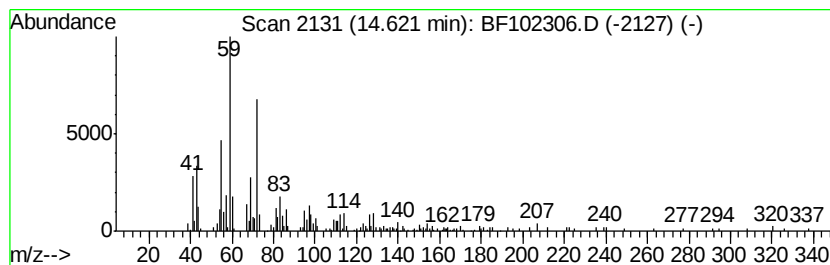
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	5.29 ng	232053	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Hexadecanamide	255	C16H33NO	000629-54-9	72
3		Decanamide-	171	C10H21NO	002319-29-1	64
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
5		Octadecanamide	283	C18H37NO	000124-26-5	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	6.3	ng	242841	1	6.72	771601	20.0
unknown6.49	6.49	83.3	ng	3214070	1	6.72	771601	20.0
1-Heneicosanol	13.71	7.8	ng	365998	5	13.87	941467	20.0
9-Octadecenamide,...	14.62	5.3	ng	232053	6	15.29	877733	20.0