

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
 Data File : BF096417.D
 Acq On : 2 Jul 2017 15:44
 Operator : SJ/MA
 Sample : I3950-16
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B6-6-8

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-BF070117.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	2.299	29	36	43	rVB2	34730	65419	2.28%	0.272%
2	3.734	273	280	285	rVB	77029	108512	3.78%	0.452%
3	4.928	478	483	492	rVB	362779	456293	15.88%	1.899%
4	5.345	549	554	557	rBV	2740310	2696833	93.84%	11.222%
5	6.369	723	728	731	rBV	2756466	2873878	100.00%	11.959%
6	6.504	746	751	754	rBV	2998950	2762768	96.13%	11.496%
7	6.734	786	790	793	rBV	1176582	943474	32.83%	3.926%
8	6.892	812	817	820	rBV	2128918	1920820	66.84%	7.993%
9	7.292	880	885	888	rBV	1843461	1632566	56.81%	6.793%
10	7.386	897	901	906	rBV3	35572	41272	1.44%	0.172%
11	8.016	1003	1008	1011	rBV	1573299	1263705	43.97%	5.258%
12	9.092	1186	1191	1194	rBV	2840002	2461149	85.64%	10.241%
13	9.480	1254	1257	1261	rBV	482289	380944	13.26%	1.585%
14	9.710	1293	1296	1301	rBV	47040	40847	1.42%	0.170%
15	9.769	1301	1306	1309	rBV	1144471	1099801	38.27%	4.576%
16	10.210	1378	1381	1384	rVB	62875	47673	1.66%	0.198%
17	10.551	1435	1439	1442	rBV	1377426	1228761	42.76%	5.113%
18	10.680	1458	1461	1468	rBV	75213	77993	2.71%	0.325%
19	11.127	1534	1537	1541	rBV	37255	33213	1.16%	0.138%
20	11.245	1553	1557	1560	rBV	1068505	875204	30.45%	3.642%
21	11.780	1645	1648	1651	rBV3	40799	37745	1.31%	0.157%
22	12.298	1732	1736	1738	rBV2	38738	37320	1.30%	0.155%
23	12.357	1743	1746	1750	rVV4	30419	32133	1.12%	0.134%
24	12.451	1757	1762	1766	rBV2	29934	39535	1.38%	0.165%
25	12.680	1793	1801	1804	rBV3	25169	44226	1.54%	0.184%
26	12.827	1822	1826	1830	rBV	1468004	1309329	45.56%	5.448%
27	13.310	1905	1908	1915	rVB	88613	98686	3.43%	0.411%
28	13.733	1976	1980	1988	rBV	94369	131568	4.58%	0.547%
29	13.874	2000	2004	2007	rBV	789179	726632	25.28%	3.024%
30	15.286	2239	2244	2250	rVB	428317	529838	18.44%	2.205%
31	17.098	2550	2552	2555	rBV3	22406	33553	1.17%	0.140%

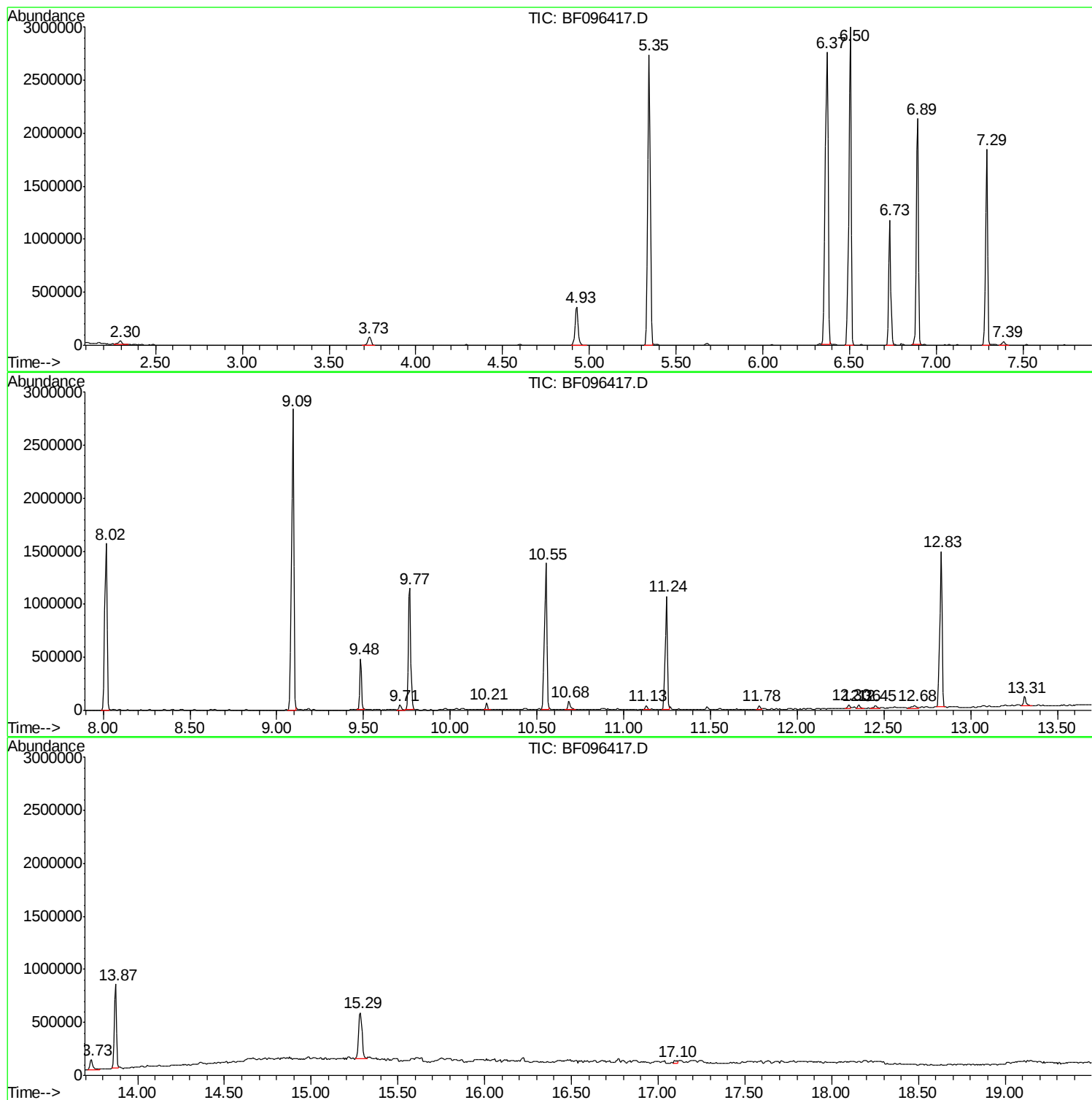
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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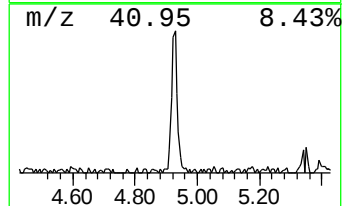
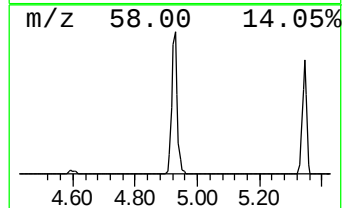
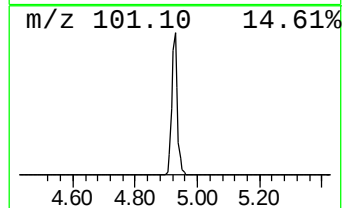
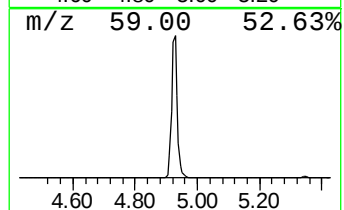
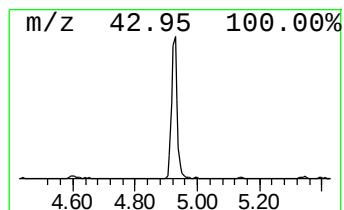
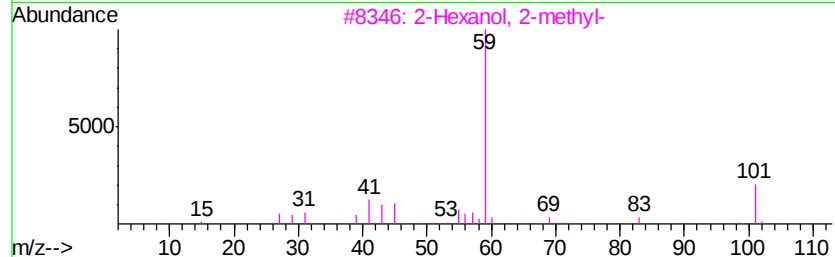
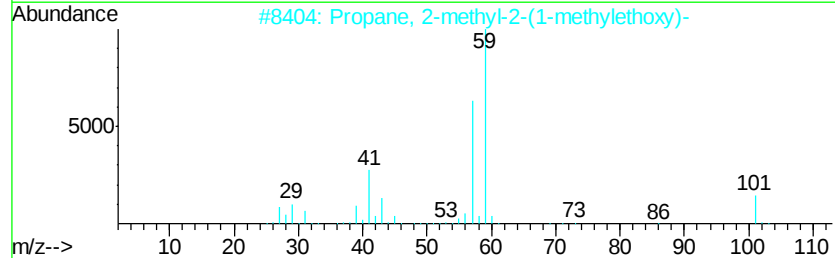
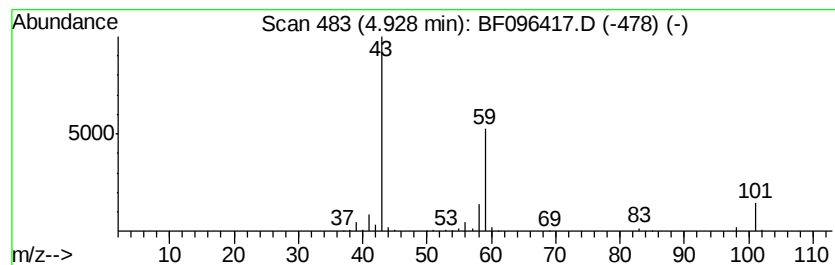
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	9.67 ng	456293	1,4-Dichlorobenzene-d4	6.73

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-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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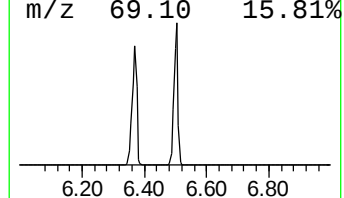
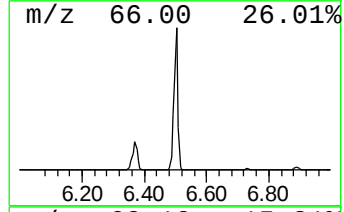
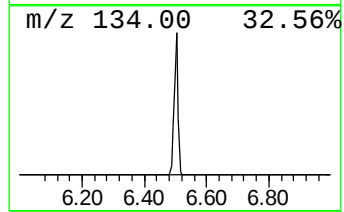
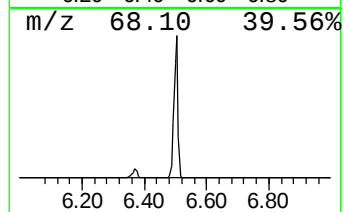
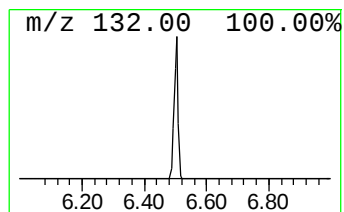
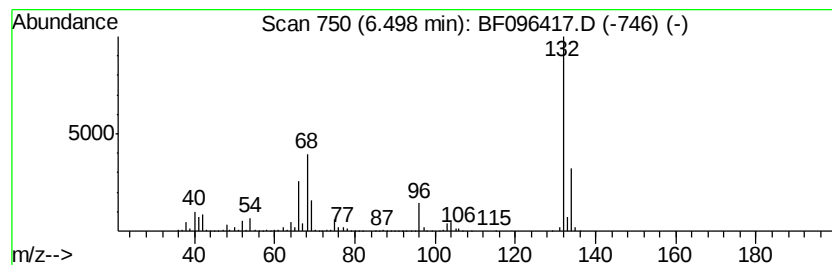
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	58.57 ng	2762770	1,4-Dichlorobenzene-d4	6.73

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	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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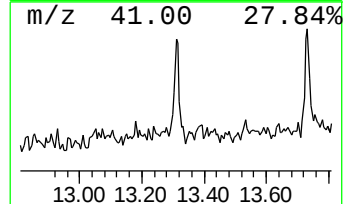
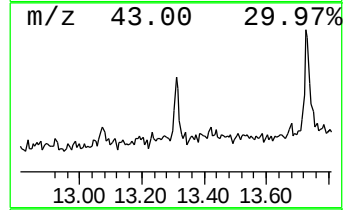
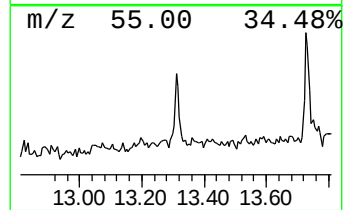
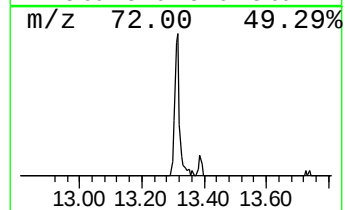
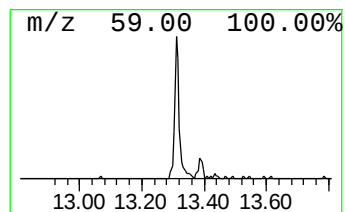
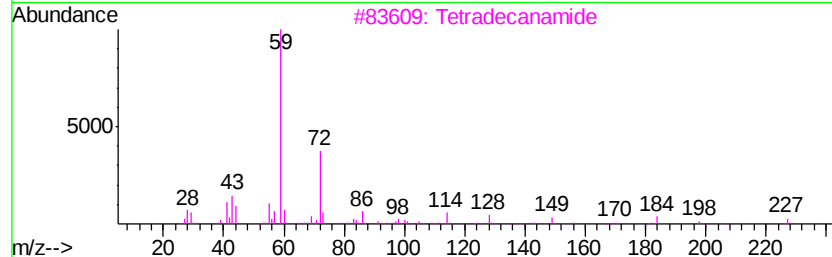
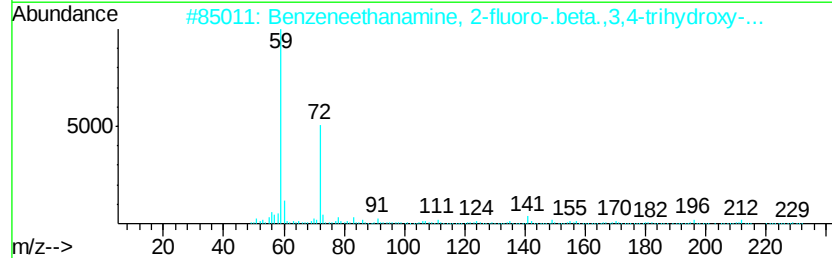
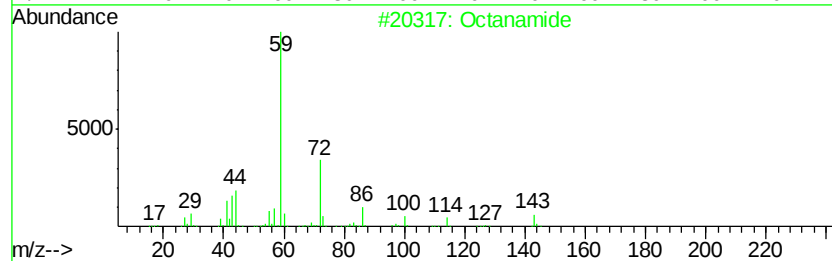
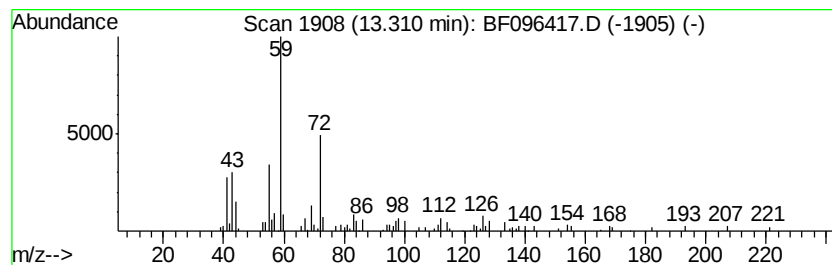
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Peak Number 5 Octanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.31	2.72 ng	98686	Chrysene-d12		13.87
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanamide	143	C8H17NO	000629-01-6	72
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
3	Tetradecanamide	227	C14H29NO	000638-58-4	53
4	Decanamide-	171	C10H21NO	002319-29-1	53
5	Hexadecanamide	255	C16H33NO	000629-54-9	53



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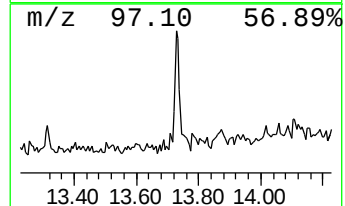
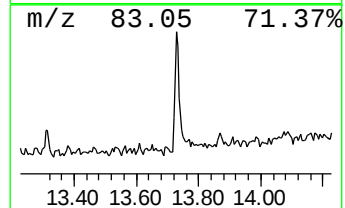
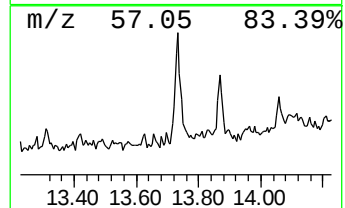
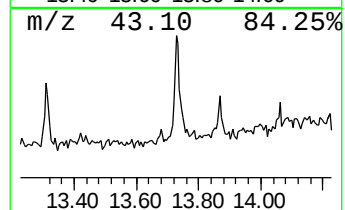
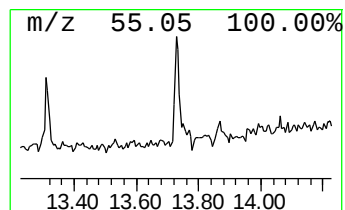
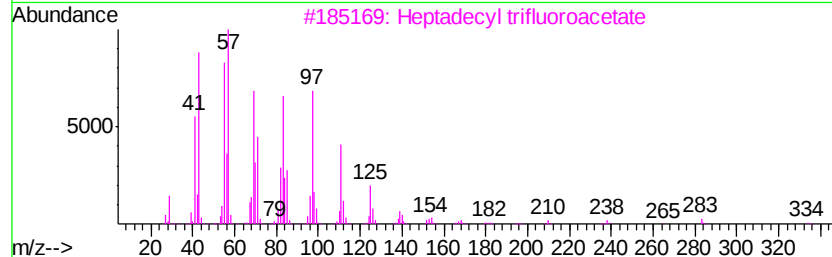
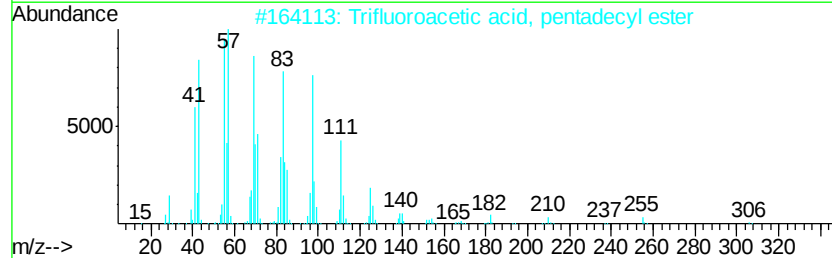
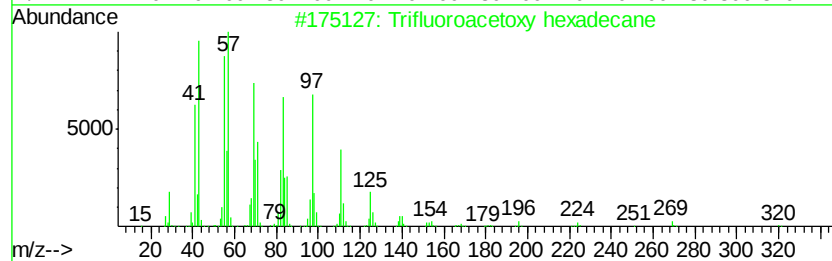
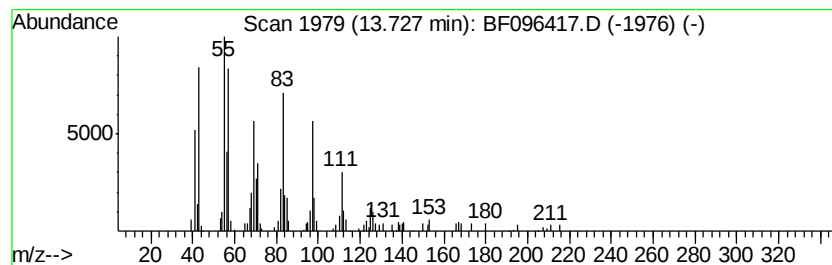
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.62 ng	131568	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4		5-Eicosene, (E)-	280	C20H40	074685-30-6	90
5		1-Octadecanol	270	C18H38O	000112-92-5	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	9.7	ng	456293	1	6.73	943474	20.0
unknown6.50	6.50	58.6	ng	2762770	1	6.73	943474	20.0
Octanamide	13.31	2.7	ng	98686	5	13.87	726632	20.0
Trifluoroacetoxy ...	13.73	3.6	ng	131568	5	13.87	726632	20.0