

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
 Data File : BF096409.D
 Acq On : 2 Jul 2017 12:02
 Operator : SJ/MA
 Sample : I3950-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B5-8-10.5

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	4.263	366	370	378	rVB2	26146	38463	1.33%	0.139%
2	4.922	477	482	491	rVB	325837	391683	13.53%	1.418%
3	5.345	549	554	557	rBV	2548649	2447488	84.54%	8.859%
4	6.369	722	728	731	rBV	2664808	2854420	98.59%	10.332%
5	6.504	746	751	754	rBV	2546028	2583848	89.24%	9.353%
6	6.734	786	790	793	rBV	1099362	936989	32.36%	3.392%
7	6.887	812	816	820	rBV	1768176	1669152	57.65%	6.042%
8	7.292	879	885	888	rBV	1652582	1567212	54.13%	5.673%
9	7.386	896	901	905	rVB2	26669	31053	1.07%	0.112%
10	8.016	1003	1008	1011	rBV	1526971	1333605	46.06%	4.827%
11	9.092	1185	1191	1194	rBV	3191904	2895233	100.00%	10.480%
12	9.480	1252	1257	1261	rBV	539660	447895	15.47%	1.621%
13	9.710	1292	1296	1299	rBV	51795	45137	1.56%	0.163%
14	9.769	1300	1306	1309	rBV	1288981	1275671	44.06%	4.618%
15	10.210	1378	1381	1384	rVB	89767	70174	2.42%	0.254%
16	10.433	1412	1419	1421	rBV2	24161	34572	1.19%	0.125%
17	10.551	1434	1439	1443	rBV	2088486	2203847	76.12%	7.977%
18	10.680	1458	1461	1469	rBV	92464	90540	3.13%	0.328%
19	11.127	1531	1537	1540	rBV2	59639	53568	1.85%	0.194%
20	11.245	1553	1557	1560	rBV	1438940	1188023	41.03%	4.300%
21	11.780	1643	1648	1651	rBV	106243	99024	3.42%	0.358%
22	12.833	1822	1827	1830	rBV	2815597	2815612	97.25%	10.192%
23	13.310	1902	1908	1912	rBV	139226	132528	4.58%	0.480%
24	13.727	1976	1979	1989	rBV	351293	345870	11.95%	1.252%
25	13.874	1999	2004	2007	rBV	1067771	1083088	37.41%	3.921%
26	14.363	2084	2087	2092	rVB4	36217	44896	1.55%	0.163%
27	14.874	2171	2174	2177	rBV3	33065	44767	1.55%	0.162%
28	14.980	2189	2192	2197	rBV6	25172	38696	1.34%	0.140%
29	15.280	2238	2243	2248	rBV	568481	689036	23.80%	2.494%
30	15.745	2317	2322	2325	rBV4	28697	40887	1.41%	0.148%
31	15.786	2325	2329	2339	rVB8	36163	80019	2.76%	0.290%
32	16.774	2492	2497	2502	rBV6	23765	53212	1.84%	0.193%

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Integration Parameters: rteint.p
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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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

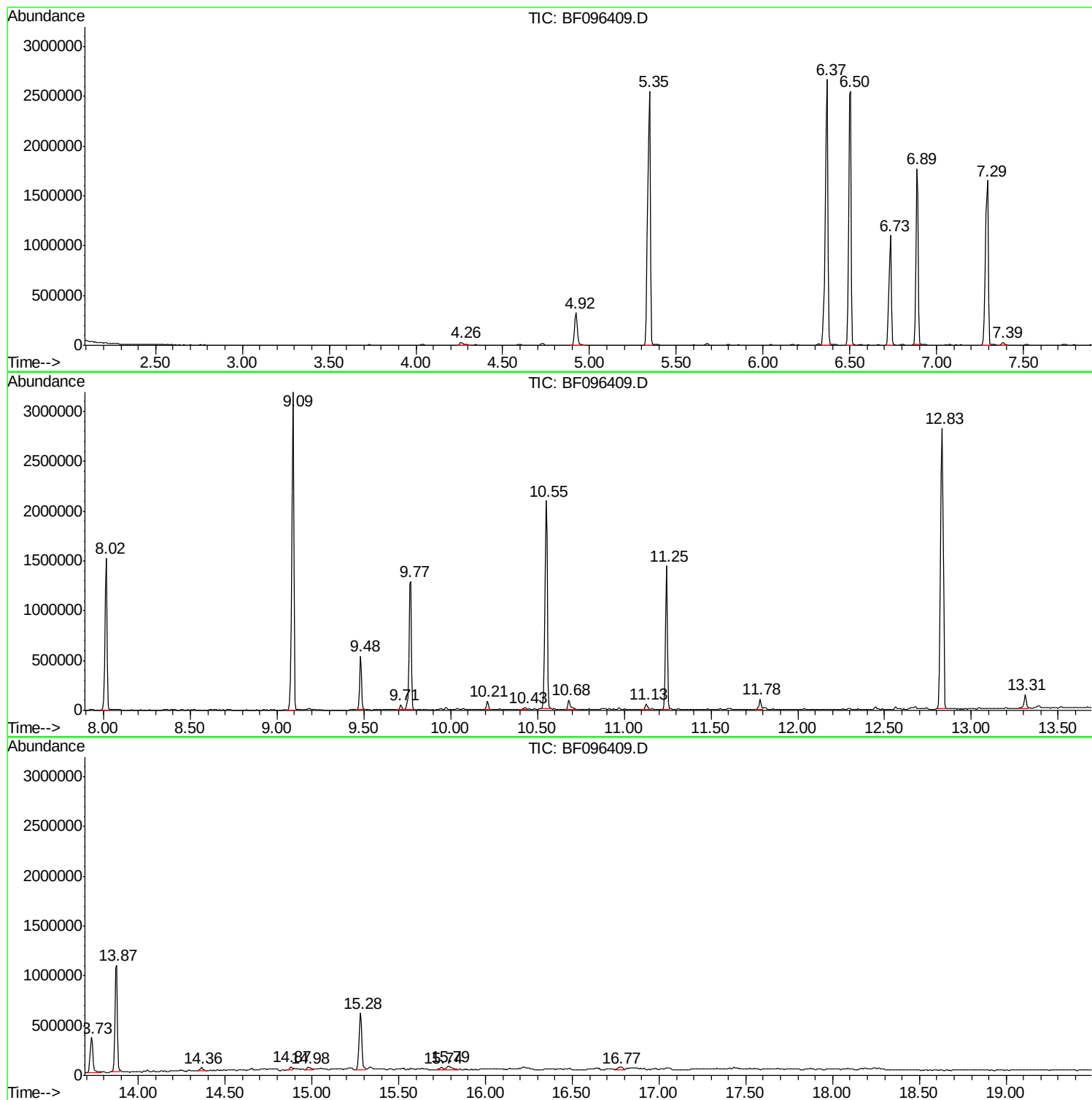
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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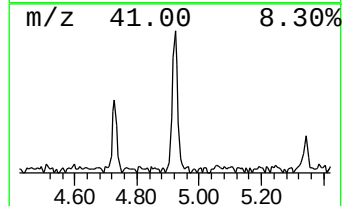
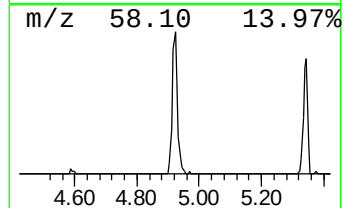
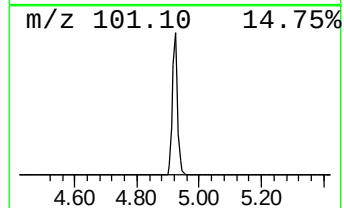
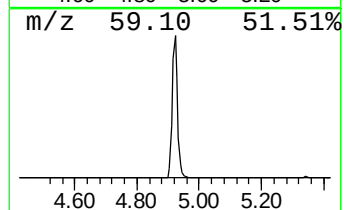
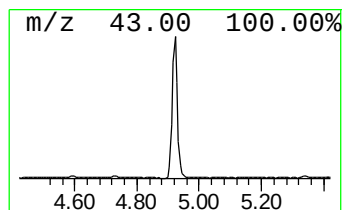
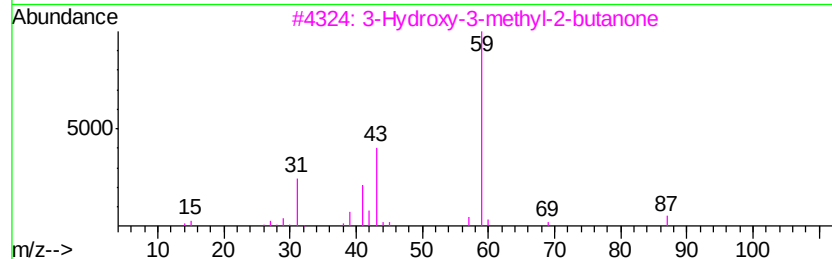
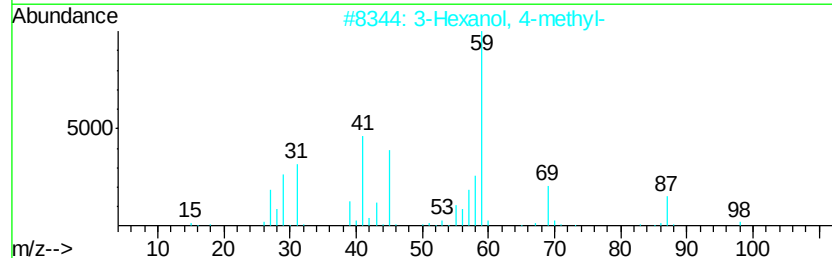
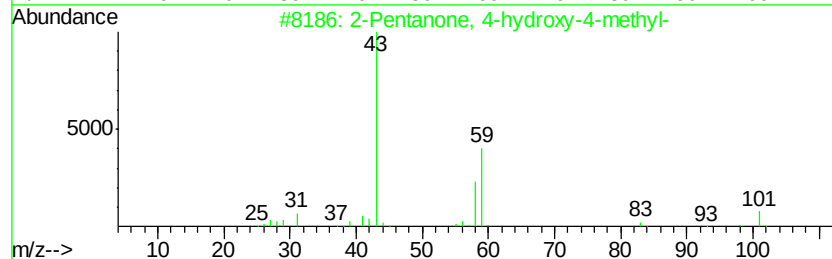
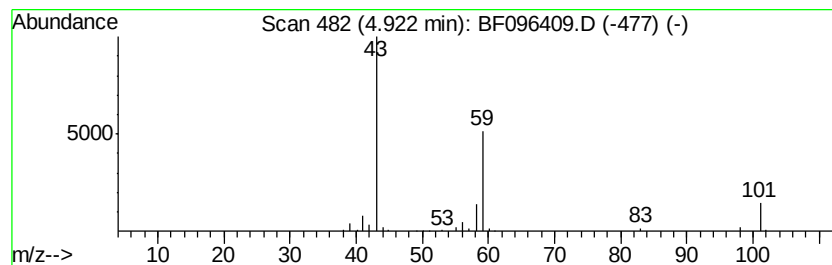
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	8.36 ng	391683	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			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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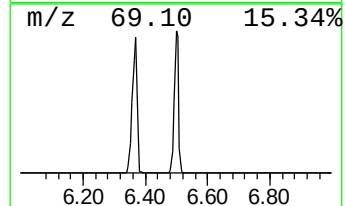
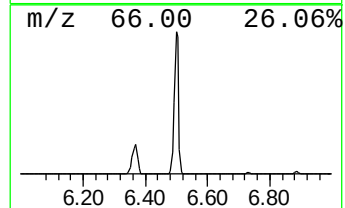
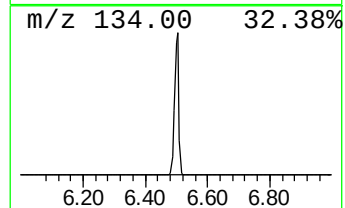
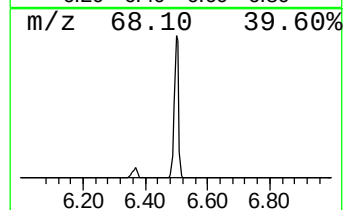
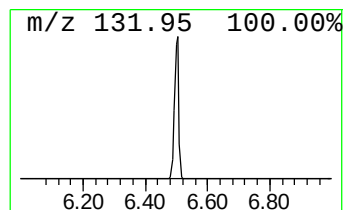
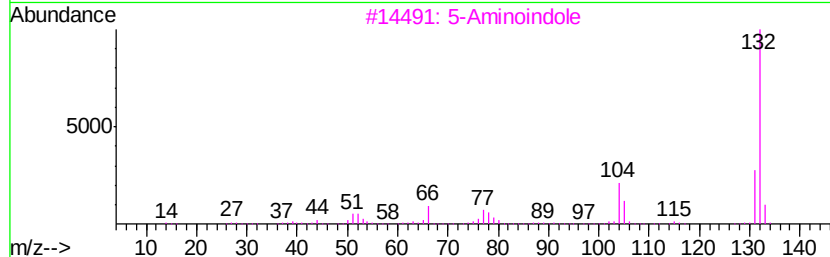
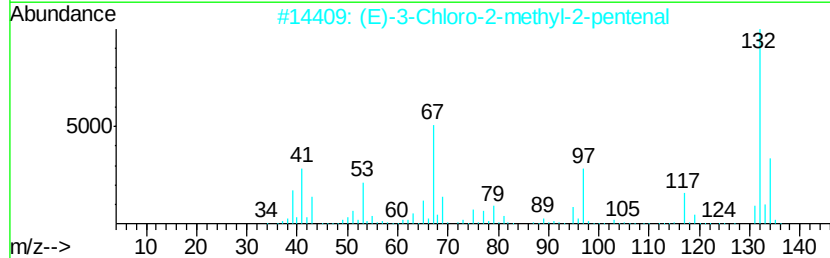
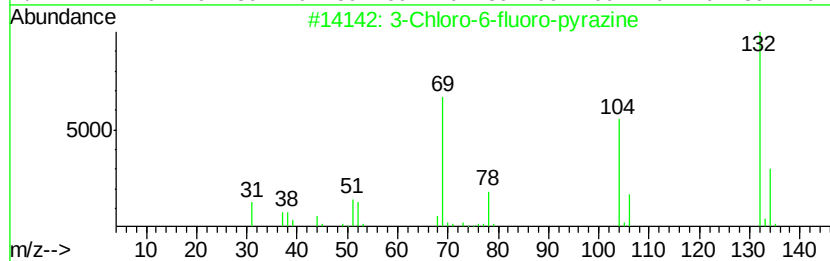
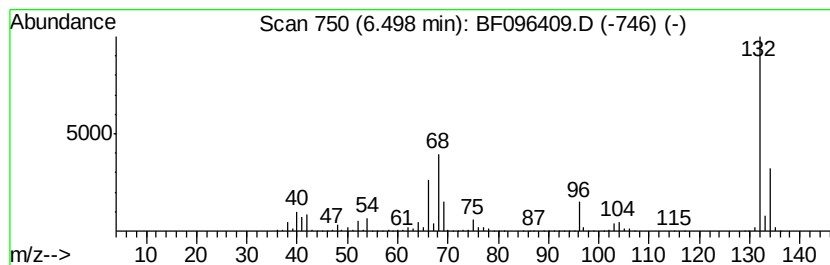
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	55.15 ng	2583850	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	35
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	12
5		Amphetaminil	250	C17H18N2	017590-01-1	12



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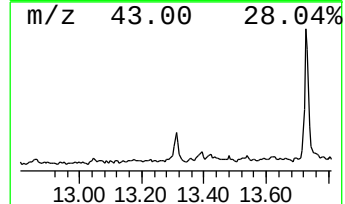
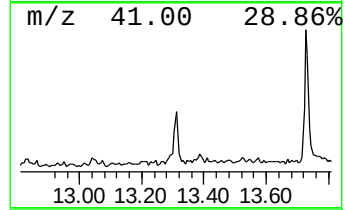
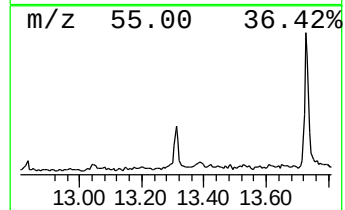
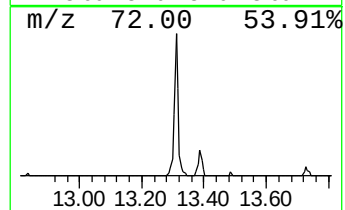
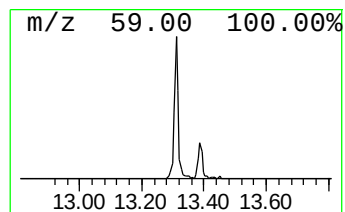
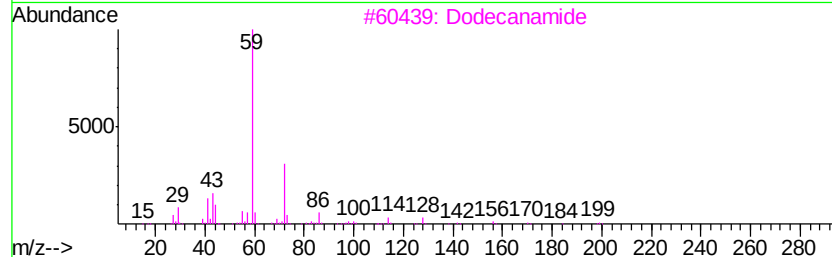
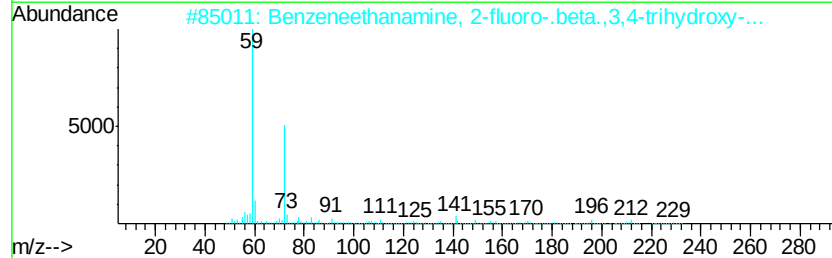
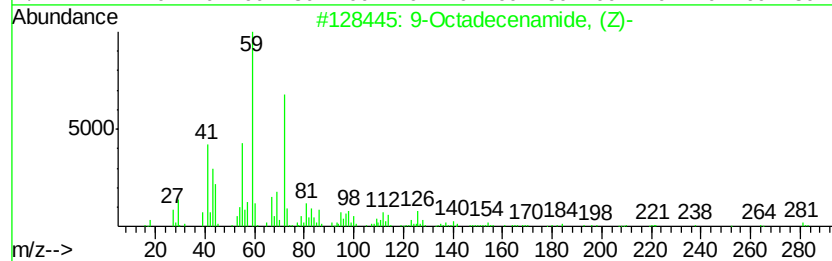
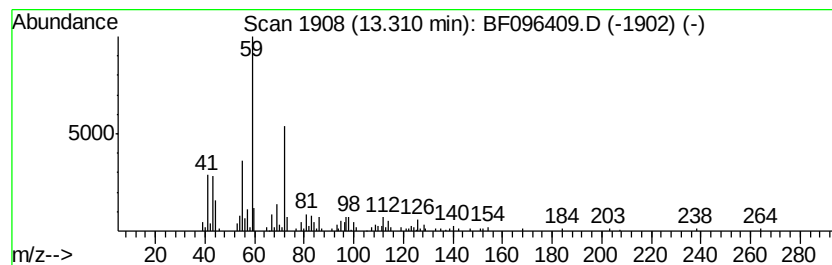
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.31	2.45 ng	132528	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
3	Dodecanamide	199	C12H25NO	001120-16-7	59
4	Hexadecanamide	255	C16H33NO	000629-54-9	59
5	Decanamide-	171	C10H21NO	002319-29-1	56



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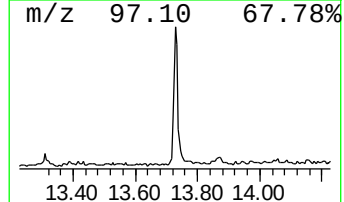
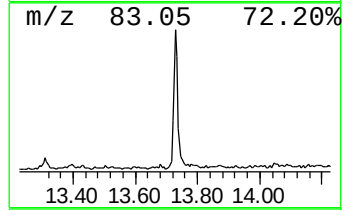
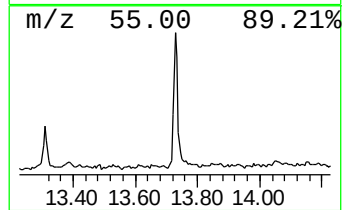
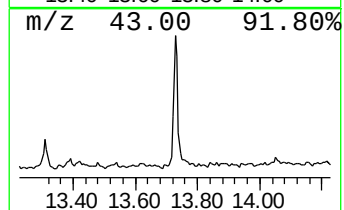
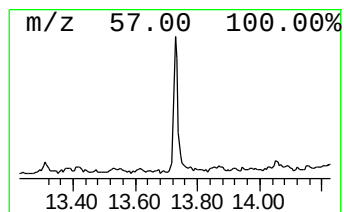
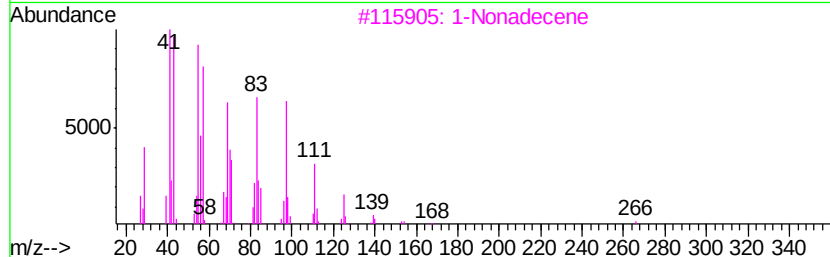
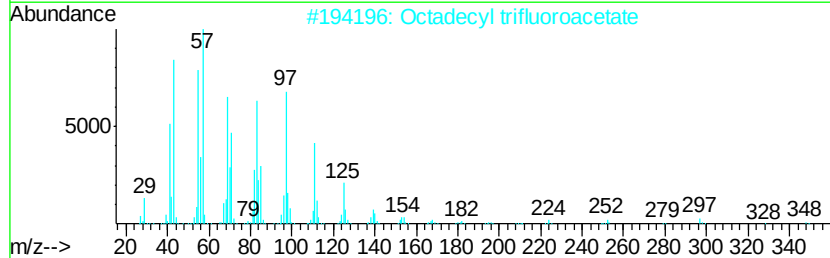
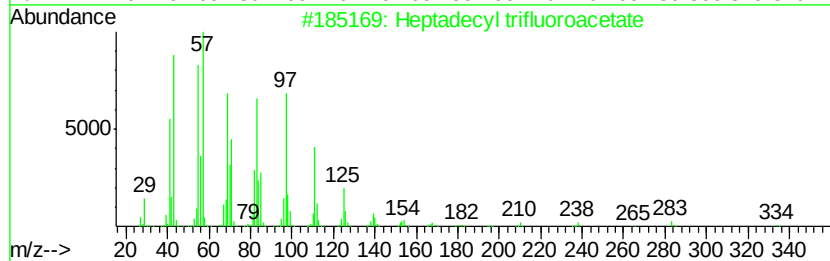
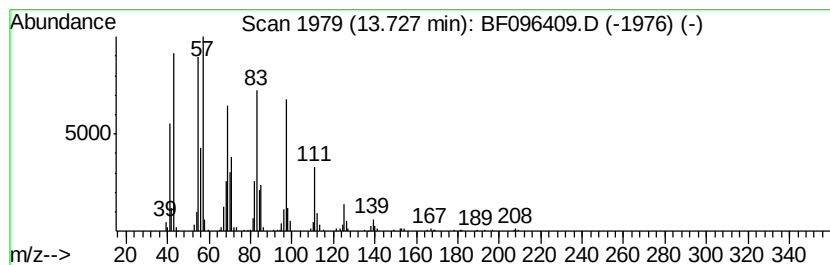
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.39 ng	345870	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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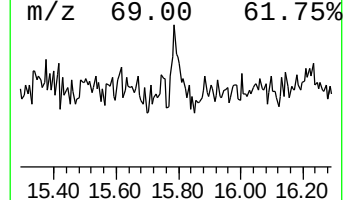
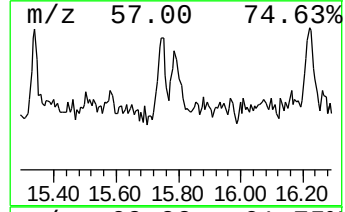
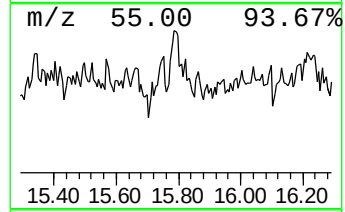
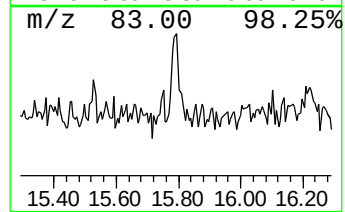
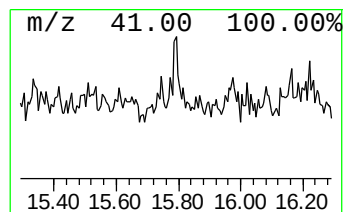
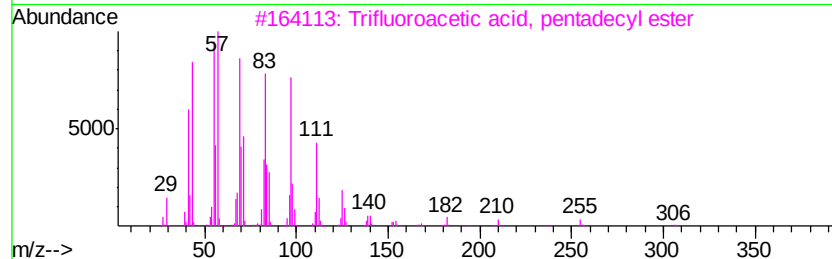
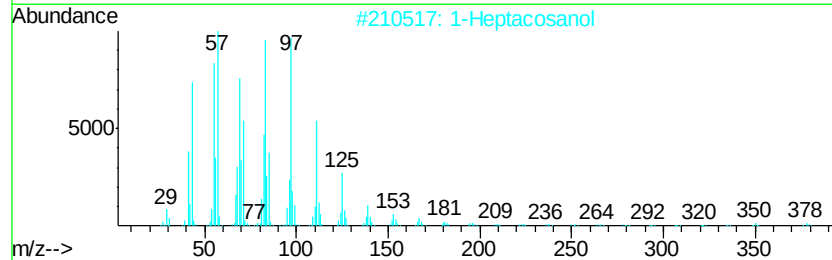
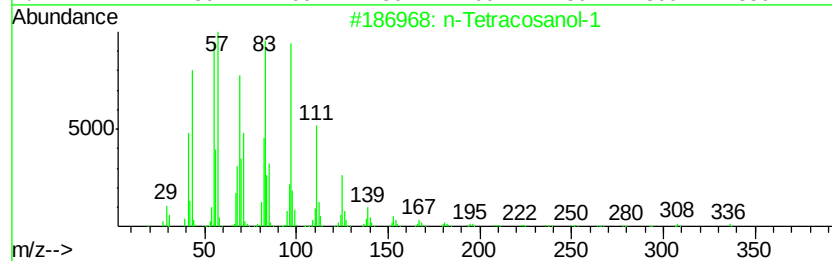
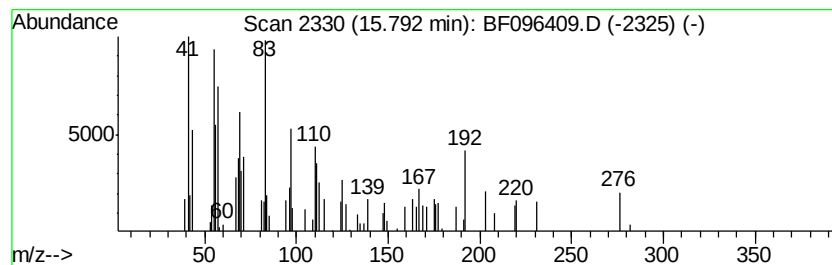
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.32 ng	80019	Perylene-d12	15.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Tetracosanol-1	354 C24H50O	000506-51-4 74
2		1-Heptacosanol	396 C27H56O	002004-39-9 74
3		Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2 59
4		Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5 58
5		Thieno[2,3-d]-1,3-thiaselenol-2-...	238 C5H2S3Se	081803-09-0 53



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	8.4	ng	391683	1	6.73	936989	20.0
unknown6.50	6.50	55.1	ng	2583850	1	6.73	936989	20.0
9-Octadecenamide, ...	13.31	2.5	ng	132528	5	13.87	1083090	20.0
Heptadecyl triflu...	13.73	6.4	ng	345870	5	13.87	1083090	20.0
n-Tetracosanol-1	15.79	2.3	ng	80019	6	15.28	689036	20.0