

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF090117\
 Data File : BF098227.D
 Acq On : 1 Sep 2017 15:29
 Operator : SJ/JU
 Sample : I5025-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-COMP-3-6

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-BF081517.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	4.269	367	371	380	rBV	97220	136928	3.96%	0.489%
2	4.928	478	483	498	rVB	193572	307291	8.88%	1.097%
3	5.339	547	553	556	rBV	2957281	3244705	93.75%	11.579%
4	6.369	722	728	731	rBV	2943708	3460877	100.00%	12.350%
5	6.492	744	749	752	rBV	3065020	3219052	93.01%	11.487%
6	6.722	784	788	791	rBV	771182	711938	20.57%	2.541%
7	6.875	810	814	818	rBV	2523082	2503306	72.33%	8.933%
8	7.286	879	884	887	rBV	1867101	2109182	60.94%	7.527%
9	8.004	1001	1006	1009	rBV	988524	886745	25.62%	3.164%
10	9.080	1184	1189	1192	rBV	3494021	3384527	97.79%	12.078%
11	9.475	1252	1256	1267	rBV	537317	449935	13.00%	1.606%
12	9.751	1299	1303	1313	rVB	939443	875662	25.30%	3.125%
13	10.545	1433	1438	1441	rBV	1580359	1538609	44.46%	5.491%
14	10.657	1454	1457	1466	rVB	41445	46745	1.35%	0.167%
15	11.233	1552	1555	1559	rBV	803219	712978	20.60%	2.544%
16	12.821	1820	1825	1828	rBV	2421803	2214026	63.97%	7.901%
17	13.304	1901	1907	1913	rBV	705048	667345	19.28%	2.381%
18	13.721	1974	1978	1984	rBV2	58598	75862	2.19%	0.271%
19	13.868	1999	2003	2007	rBV	785729	698840	20.19%	2.494%
20	14.621	2127	2131	2138	rVB	185998	200430	5.79%	0.715%
21	15.280	2239	2243	2258	rVB	422282	578043	16.70%	2.063%

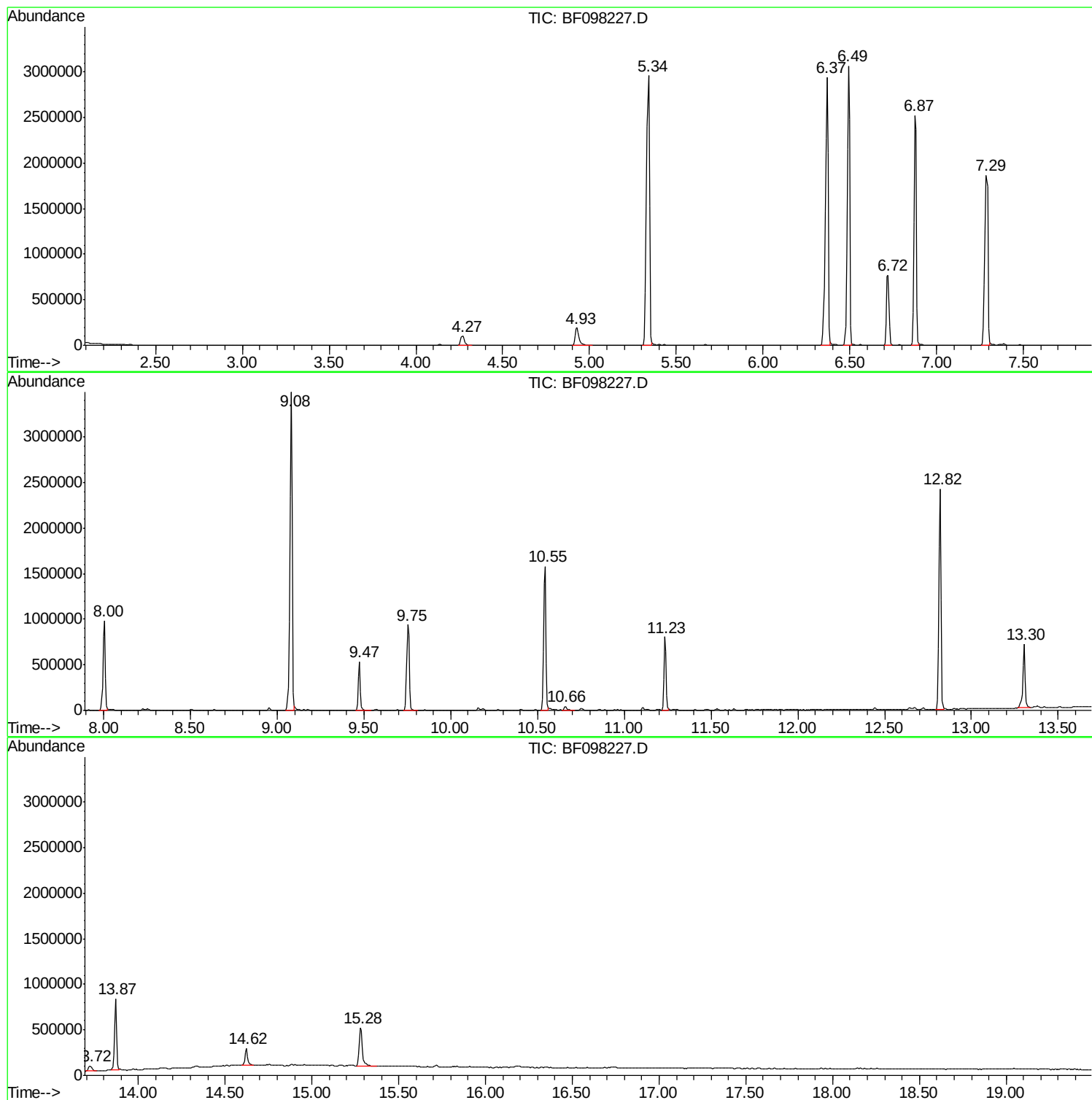
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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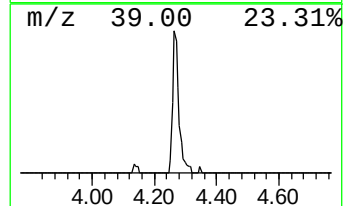
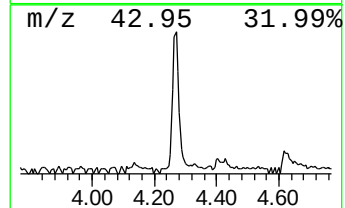
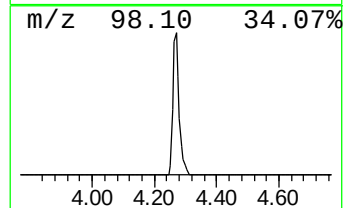
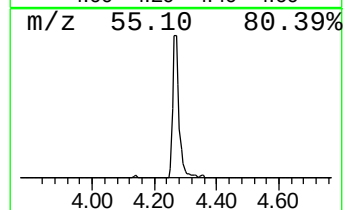
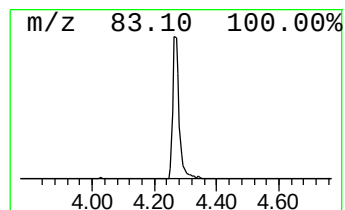
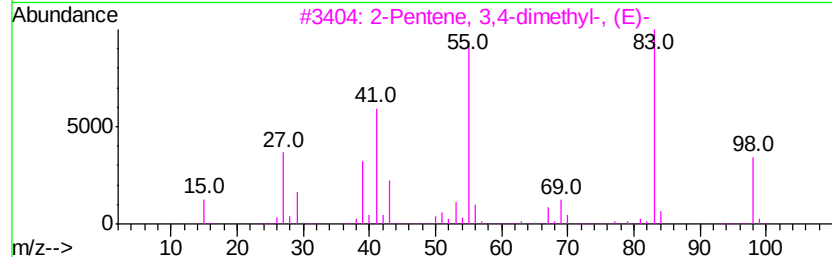
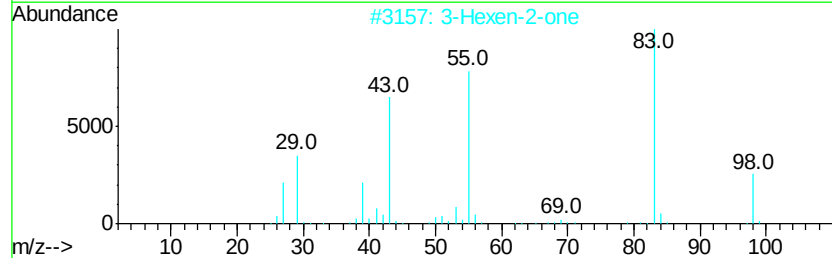
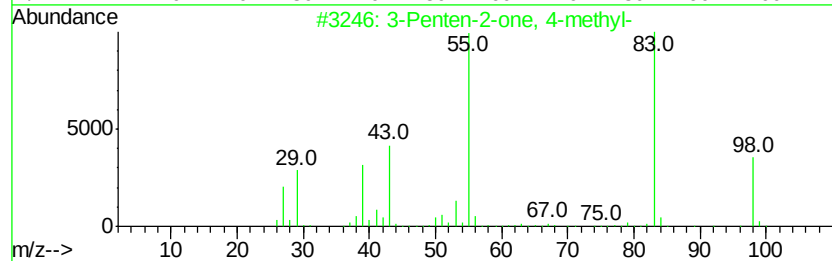
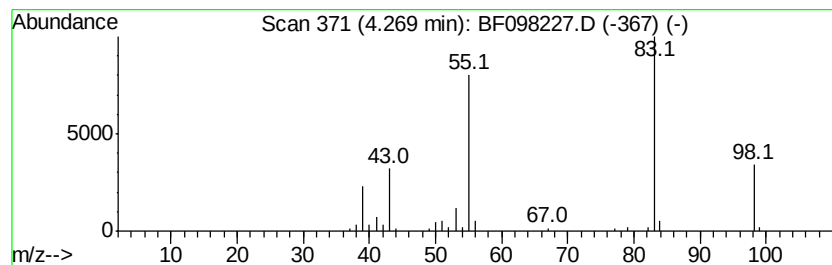
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	3.85 ng	136928	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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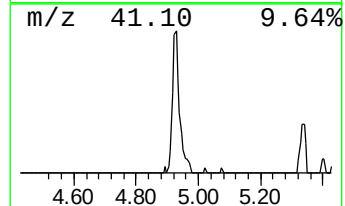
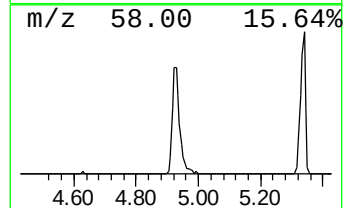
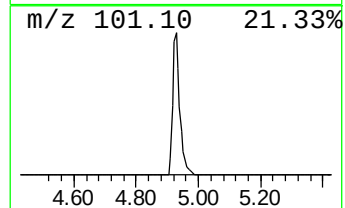
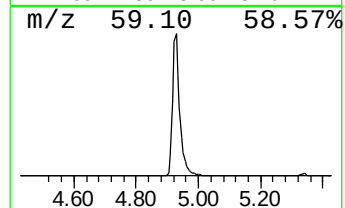
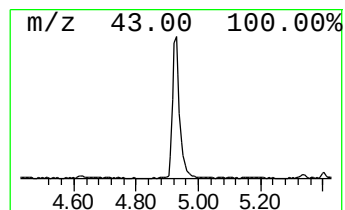
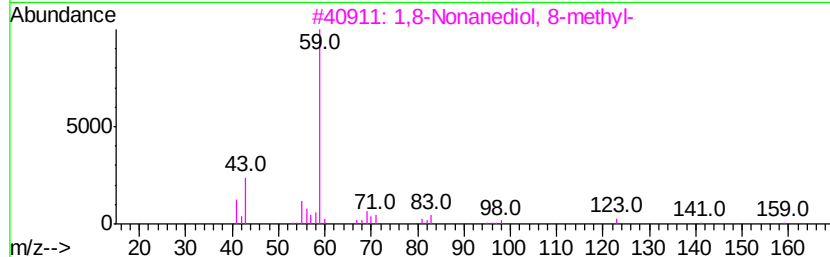
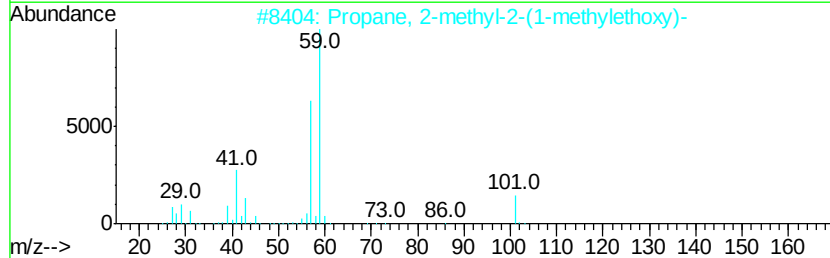
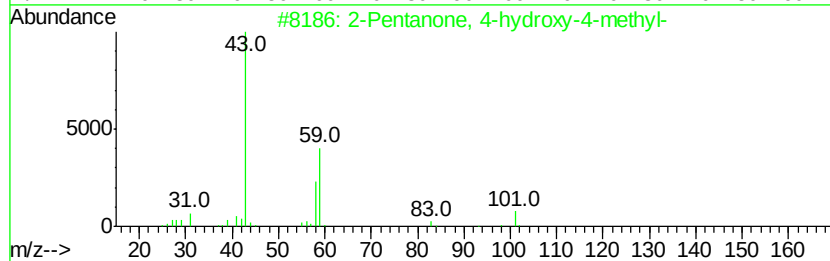
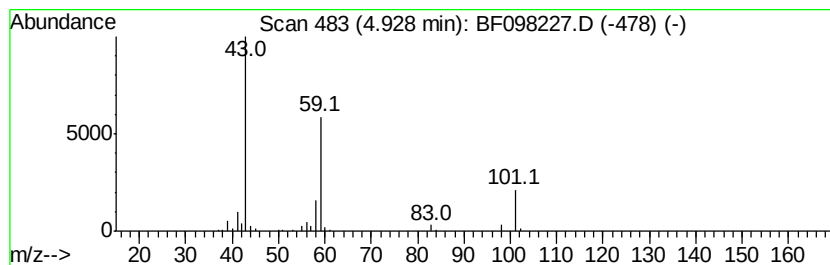
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	8.63 ng	307291	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	56
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	28
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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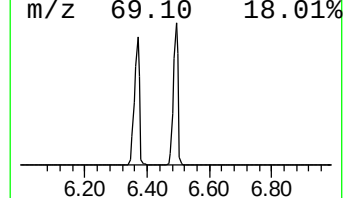
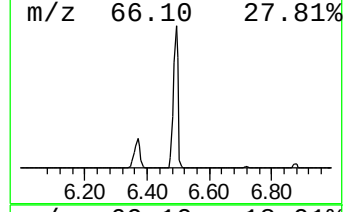
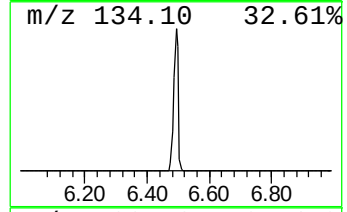
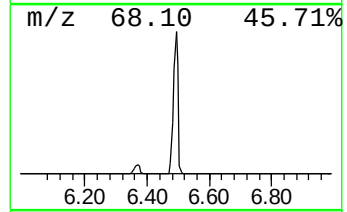
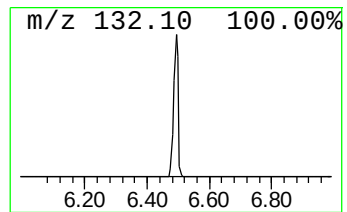
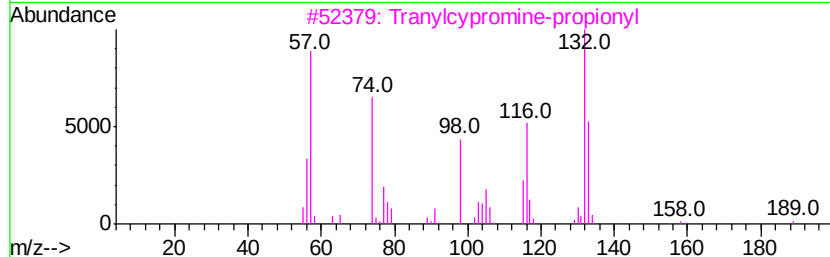
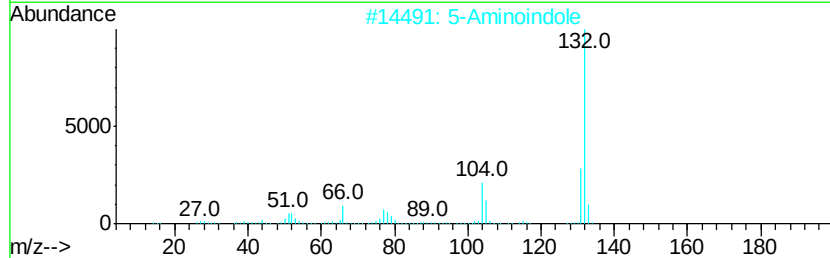
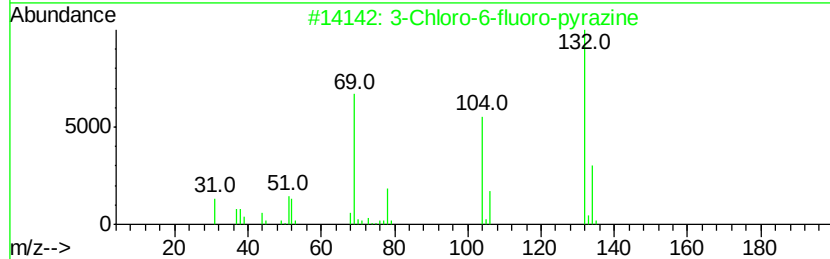
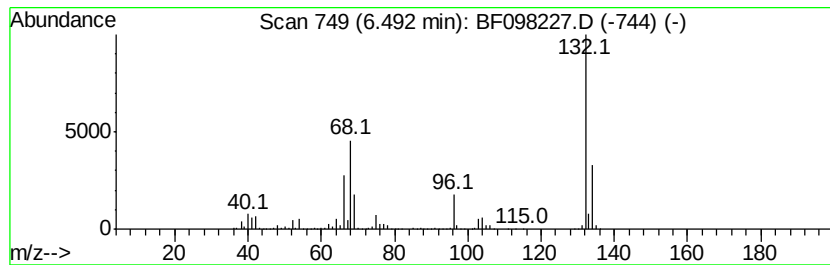
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Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	90.43 ng	3219050	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9



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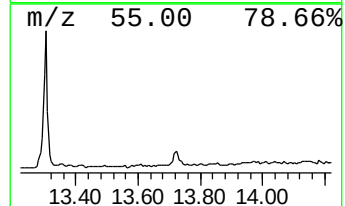
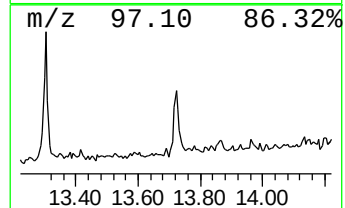
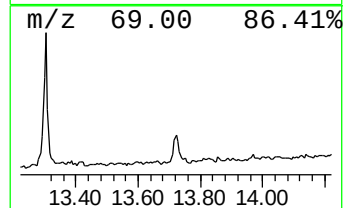
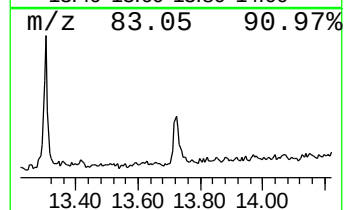
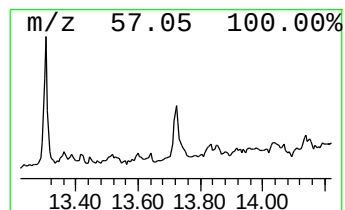
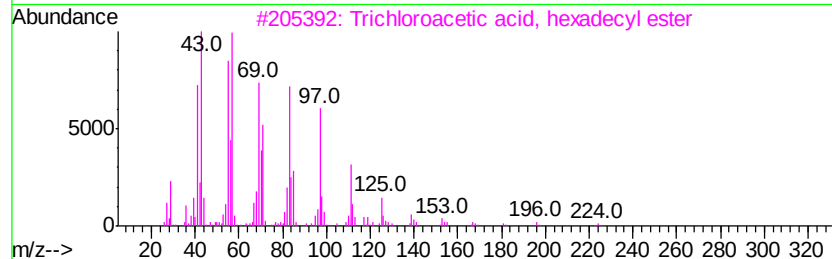
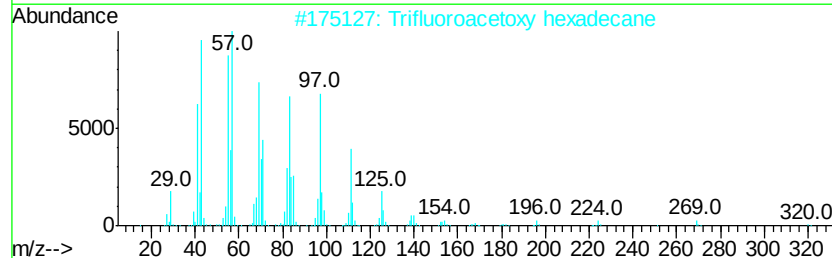
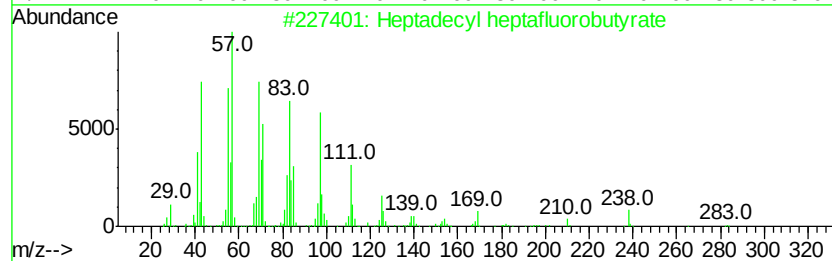
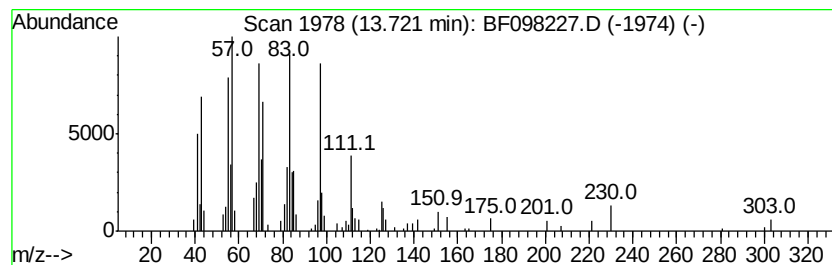
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Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.17 ng	75862	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	76
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	76



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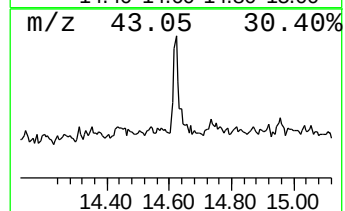
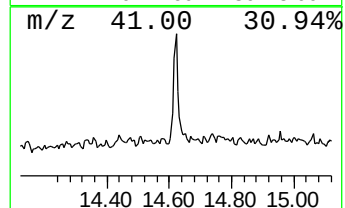
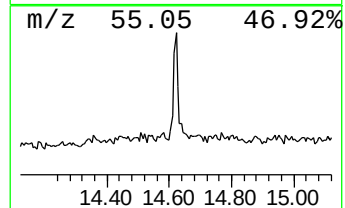
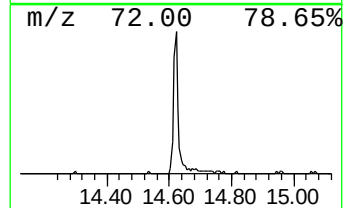
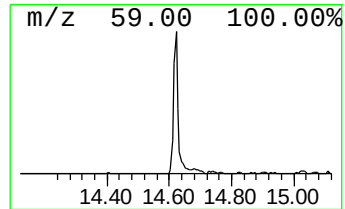
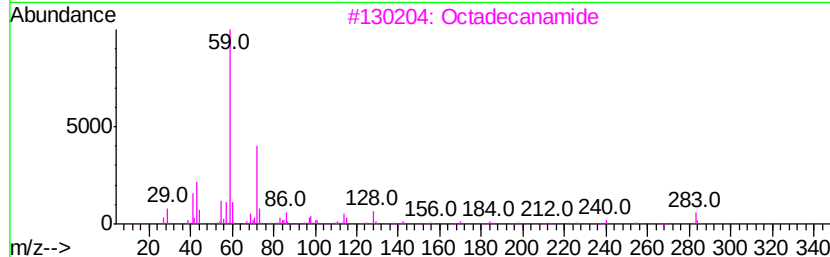
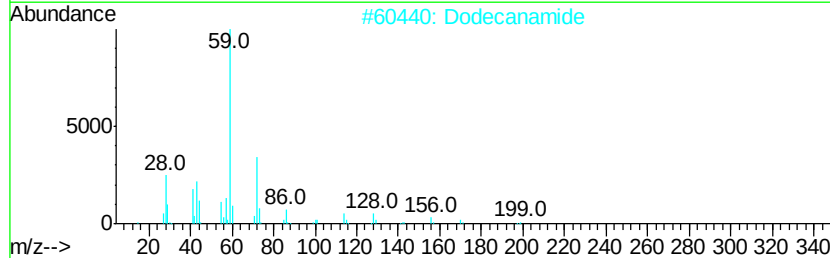
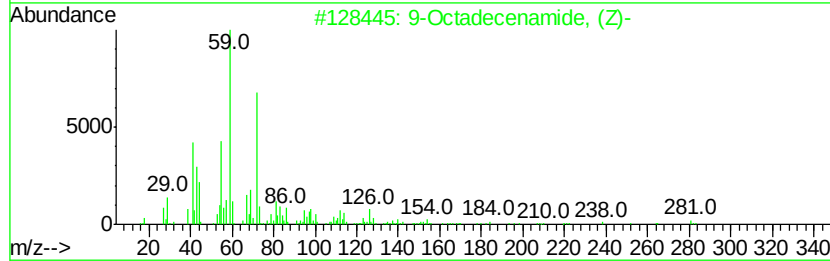
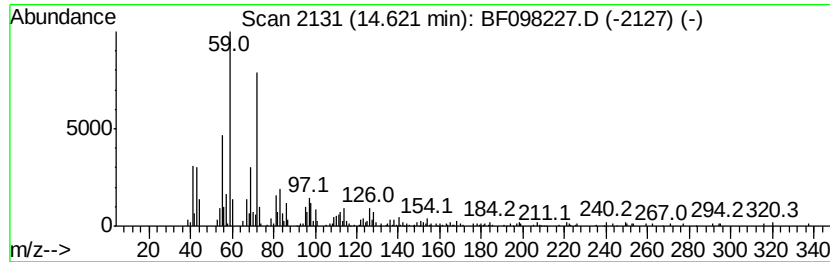
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Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	6.93 ng	200430	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Dodecanamide	199	C12H25NO	001120-16-7	50
3		Octadecanamide	283	C18H37NO	000124-26-5	43
4		Decanamide-	171	C10H21NO	002319-29-1	38
5		6-Chlorohexanoic acid, 2-ethoxye...	222	C10H19ClO3	1000331-04-6	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.27	3.9	ng	136928	1	6.72	711938	20.0
2-Pentanone, 4-hy...	4.93	8.6	ng	307291	1	6.72	711938	20.0
unknown6.49	6.49	90.4	ng	3219050	1	6.72	711938	20.0
Heptadecyl heptaf...	13.72	2.2	ng	75862	5	13.87	698840	20.0
9-Octadecenamide,...	14.62	6.9	ng	200430	6	15.28	578043	20.0