

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
 Data File : BF096694.D
 Acq On : 12 Jul 2017 16:23
 Operator : SJ/JU
 Sample : I4126-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PP-NW-2

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-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	4.851	465	470	479	rBV	331237	478632	15.80%	2.064%
2	5.281	538	543	546	rBV	2654697	2751201	90.83%	11.864%
3	6.310	712	718	721	rBV	2710851	3029090	100.00%	13.062%
4	6.439	735	740	743	rBV	2606963	2530898	83.55%	10.914%
5	6.669	775	779	782	rBV	757845	698700	23.07%	3.013%
6	6.822	801	805	809	rBV	1996032	1843306	60.85%	7.949%
7	7.228	869	874	877	rBV	1646714	1658820	54.76%	7.153%
8	7.951	992	997	1000	rBV	1223353	1115004	36.81%	4.808%
9	9.027	1175	1180	1183	rBV	2794325	2476138	81.75%	10.678%
10	9.422	1243	1247	1250	rBV	297732	263212	8.69%	1.135%
11	9.698	1290	1294	1298	rBV2	1173431	1033796	34.13%	4.458%
12	10.145	1367	1370	1373	rVB	41343	30651	1.01%	0.132%
13	10.486	1423	1428	1431	rBV	1272827	1215243	40.12%	5.241%
14	10.616	1447	1450	1457	rBV	56050	61525	2.03%	0.265%
15	11.174	1541	1545	1549	rVB	831539	715757	23.63%	3.087%
16	12.762	1810	1815	1818	rBV	1882685	1746916	57.67%	7.533%
17	13.668	1965	1969	1975	rBV2	151581	175432	5.79%	0.757%
18	13.804	1988	1992	2003	rBV	747598	699890	23.11%	3.018%
19	14.392	2086	2092	2094	rBV6	23774	45158	1.49%	0.195%
20	14.562	2118	2121	2124	rBV	80456	86733	2.86%	0.374%
21	15.198	2224	2229	2234	rBV	426801	533145	17.60%	2.299%

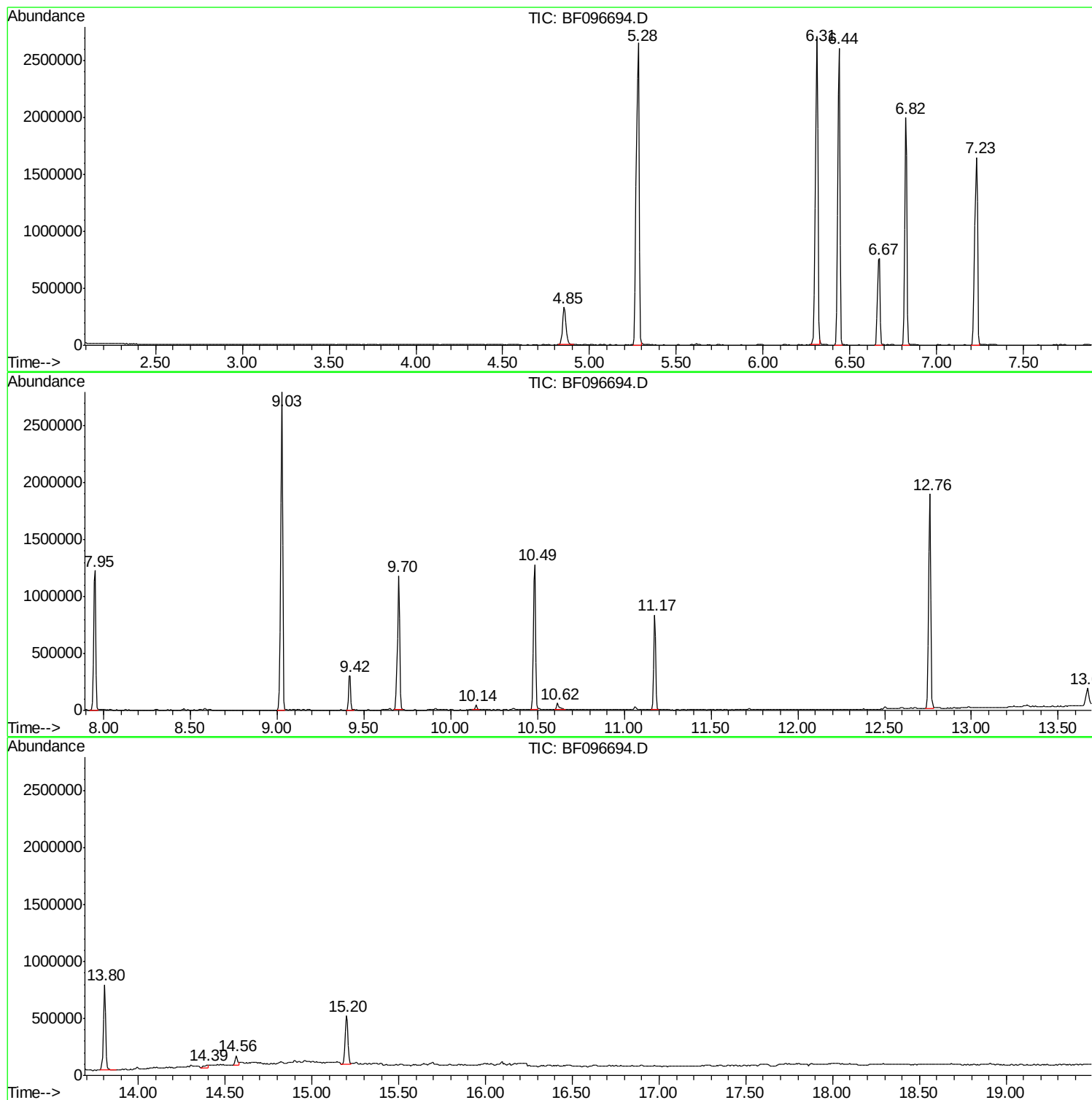
Sum of corrected areas: 23189247

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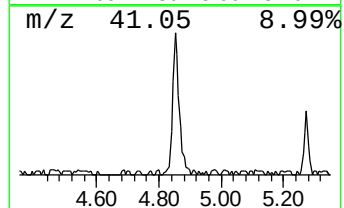
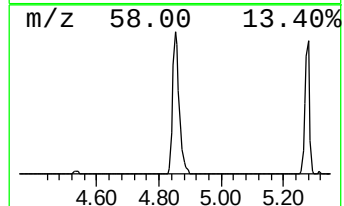
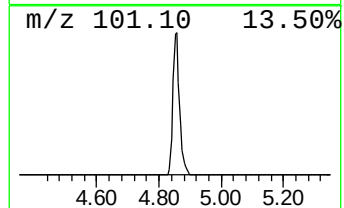
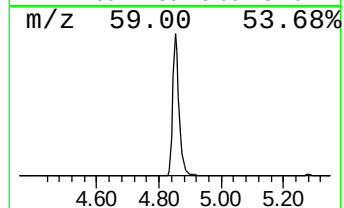
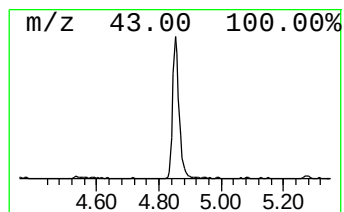
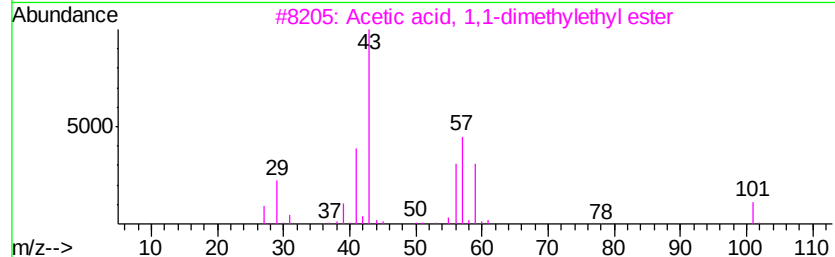
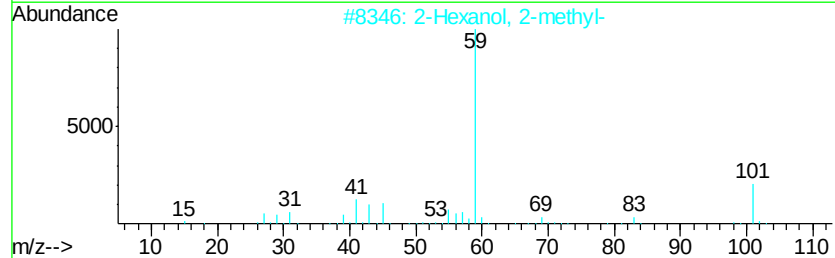
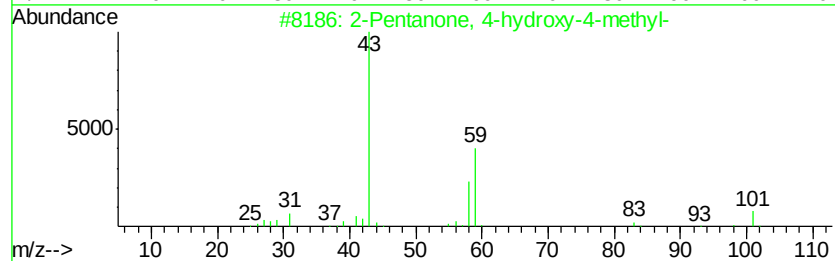
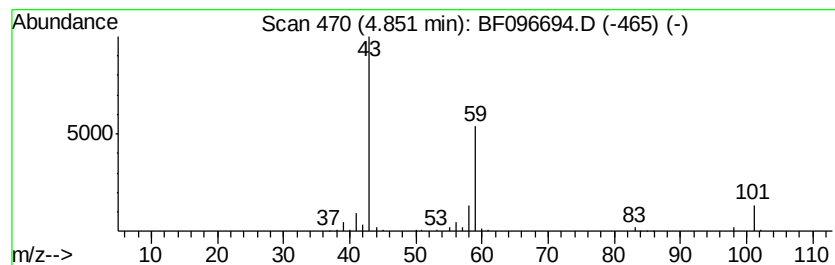
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	13.70 ng	478632	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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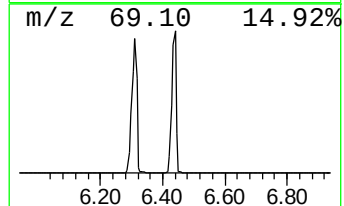
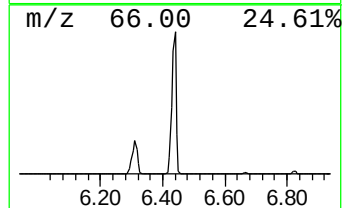
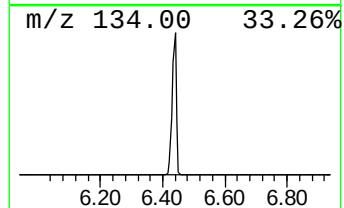
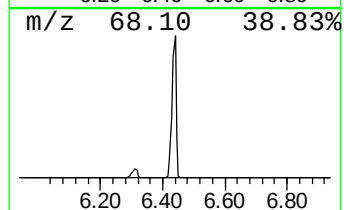
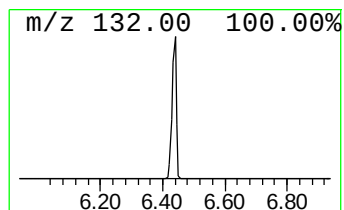
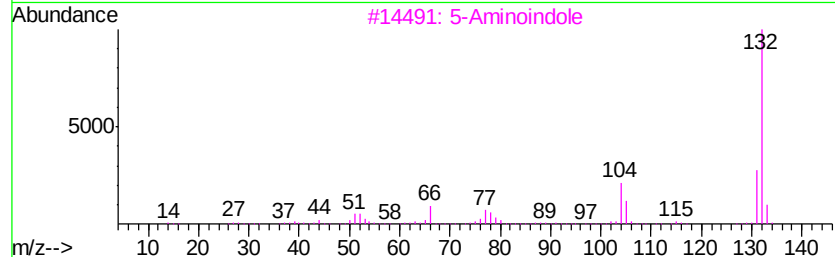
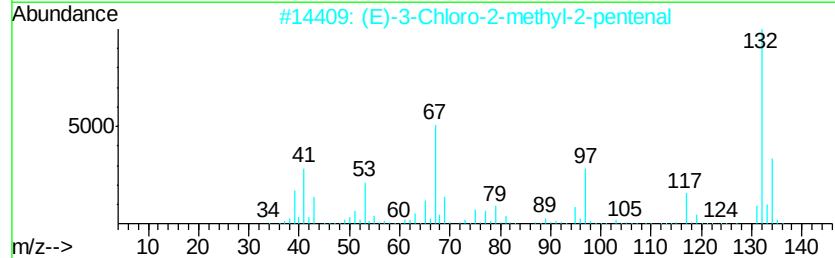
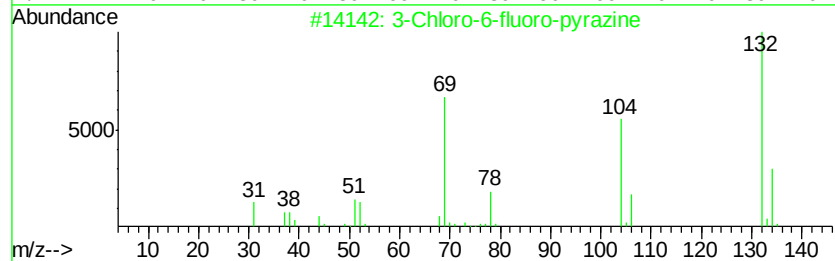
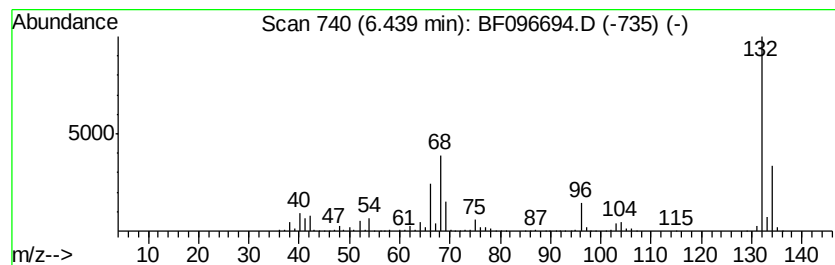
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Peak Number 2 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	72.45 ng	2530900	1,4-Dichlorobenzene-d4	6.67

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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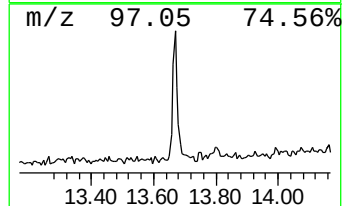
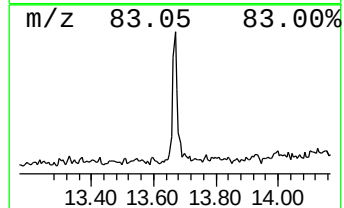
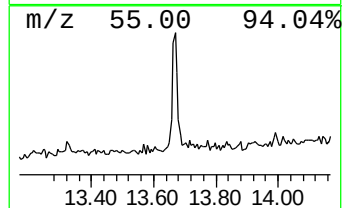
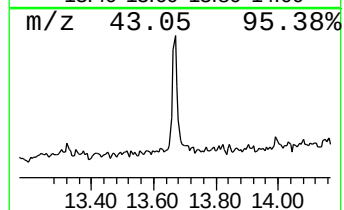
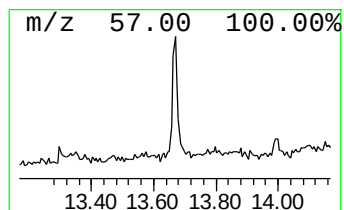
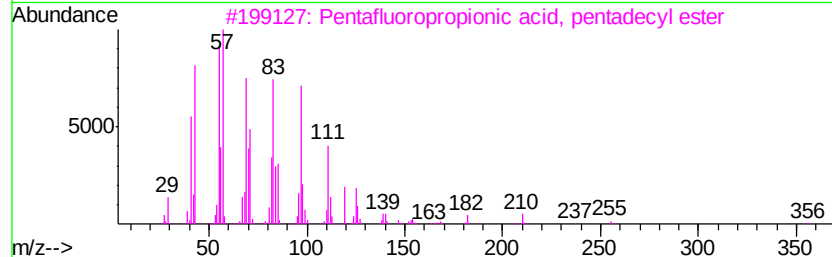
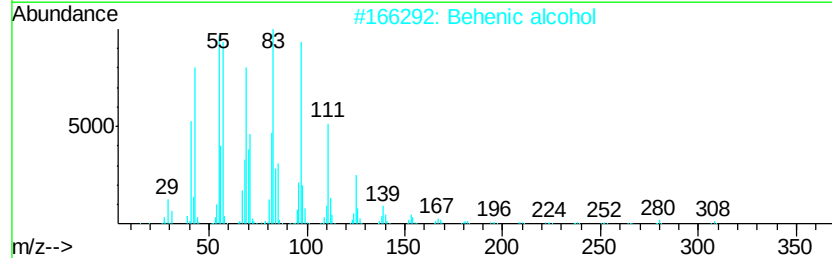
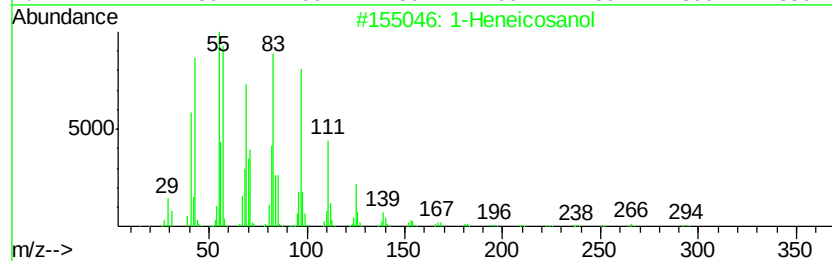
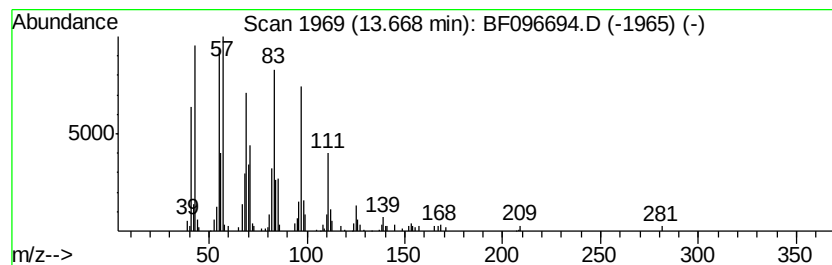
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Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.67	5.01 ng	175432	Chrysene-d12	13.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5	1-Docosene	308	C22H44	001599-67-3	91



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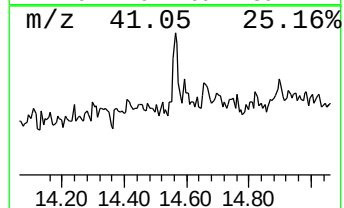
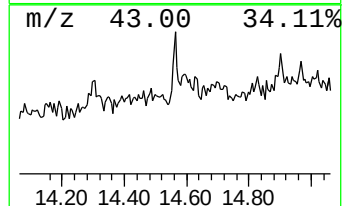
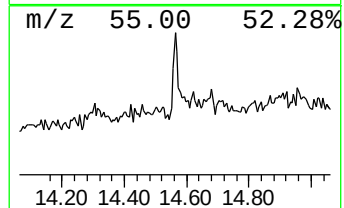
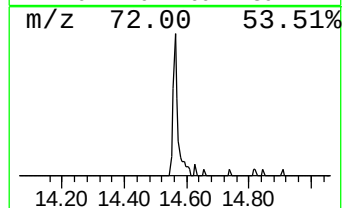
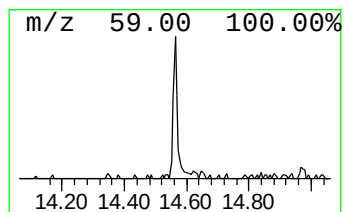
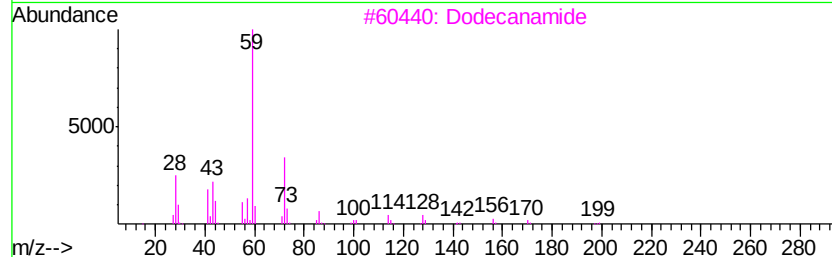
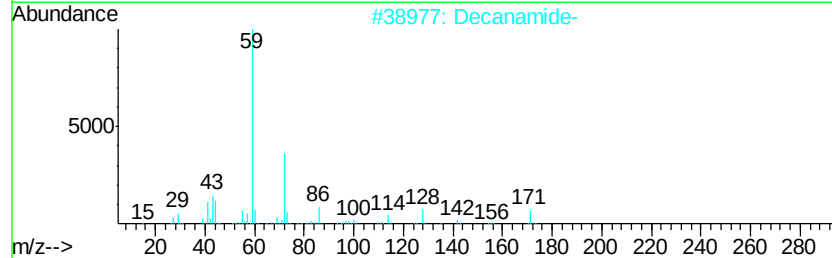
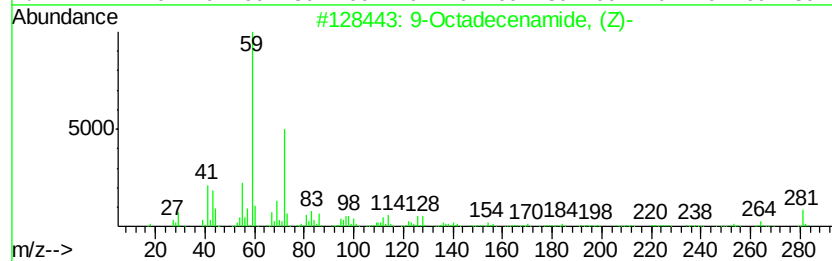
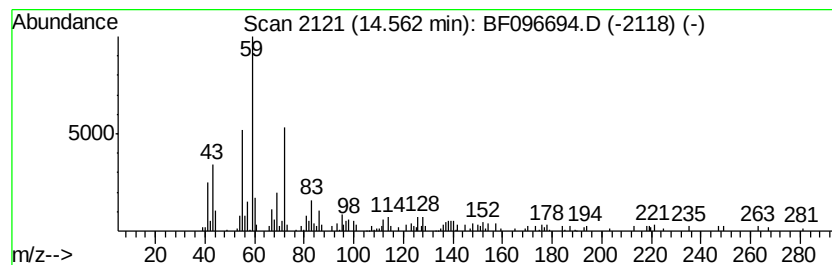
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	3.25 ng	86733	Perylene-d12	15.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		Decanamide-	171	C10H21NO	002319-29-1	72
3		Dodecanamide	199	C12H25NO	001120-16-7	64
4		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64
5		Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.85	13.7	ng	478632	1	6.67	698700	20.0
unknown6.44	6.44	72.5	ng	2530900	1	6.67	698700	20.0
1-Heneicosanol	13.67	5.0	ng	175432	5	13.80	699890	20.0
9-Octadecenamide,...	14.56	3.3	ng	86733	6	15.20	533145	20.0