

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
 Data File : BF096843.D
 Acq On : 18 Jul 2017 13:03
 Operator : SJ/JU
 Sample : I4224-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DEC-03

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-BF071317.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	2.887	151	153	172	rBV4	55133	118455	3.60%	0.405%
2	4.787	472	476	491	rVB	215515	357127	10.84%	1.220%
3	5.216	544	549	552	rBV	2850582	3229559	98.02%	11.036%
4	6.257	720	726	729	rBV	2787957	3253581	98.75%	11.119%
5	6.375	741	746	749	rBV	3087736	3126529	94.89%	10.684%
6	6.598	780	784	788	rBV	753863	634918	19.27%	2.170%
7	6.757	806	811	814	rBV	2449091	2336458	70.92%	7.984%
8	7.163	874	880	883	rBV	1849665	2050566	62.24%	7.007%
9	7.287	893	901	909	rVB	49583	60847	1.85%	0.208%
10	7.881	997	1002	1005	rBV	980041	892694	27.09%	3.051%
11	8.957	1180	1185	1189	rBV	2896613	3294728	100.00%	11.259%
12	9.351	1247	1252	1256	rBV	630165	558971	16.97%	1.910%
13	9.628	1294	1299	1303	rBV	1084609	976447	29.64%	3.337%
14	10.416	1427	1433	1436	rBV	1906241	2032617	61.69%	6.946%
15	10.545	1452	1455	1462	rVB	68659	75597	2.29%	0.258%
16	10.992	1527	1531	1534	rBV	61129	51597	1.57%	0.176%
17	11.104	1543	1550	1553	rBV	1069457	951227	28.87%	3.251%
18	11.651	1637	1643	1645	rBV	43263	38946	1.18%	0.133%
19	12.692	1814	1820	1823	rBV	2666116	2874638	87.25%	9.824%
20	13.174	1896	1902	1909	rBV	684099	668240	20.28%	2.284%
21	13.592	1967	1973	1981	rBV	160190	191150	5.80%	0.653%
22	13.727	1991	1996	1999	rBV	812486	804734	24.42%	2.750%
23	14.221	2076	2080	2086	rVB2	44518	62239	1.89%	0.213%
24	15.098	2224	2229	2233	rBV	487187	578008	17.54%	1.975%
25	15.963	2374	2376	2386	rVB6	22725	42784	1.30%	0.146%

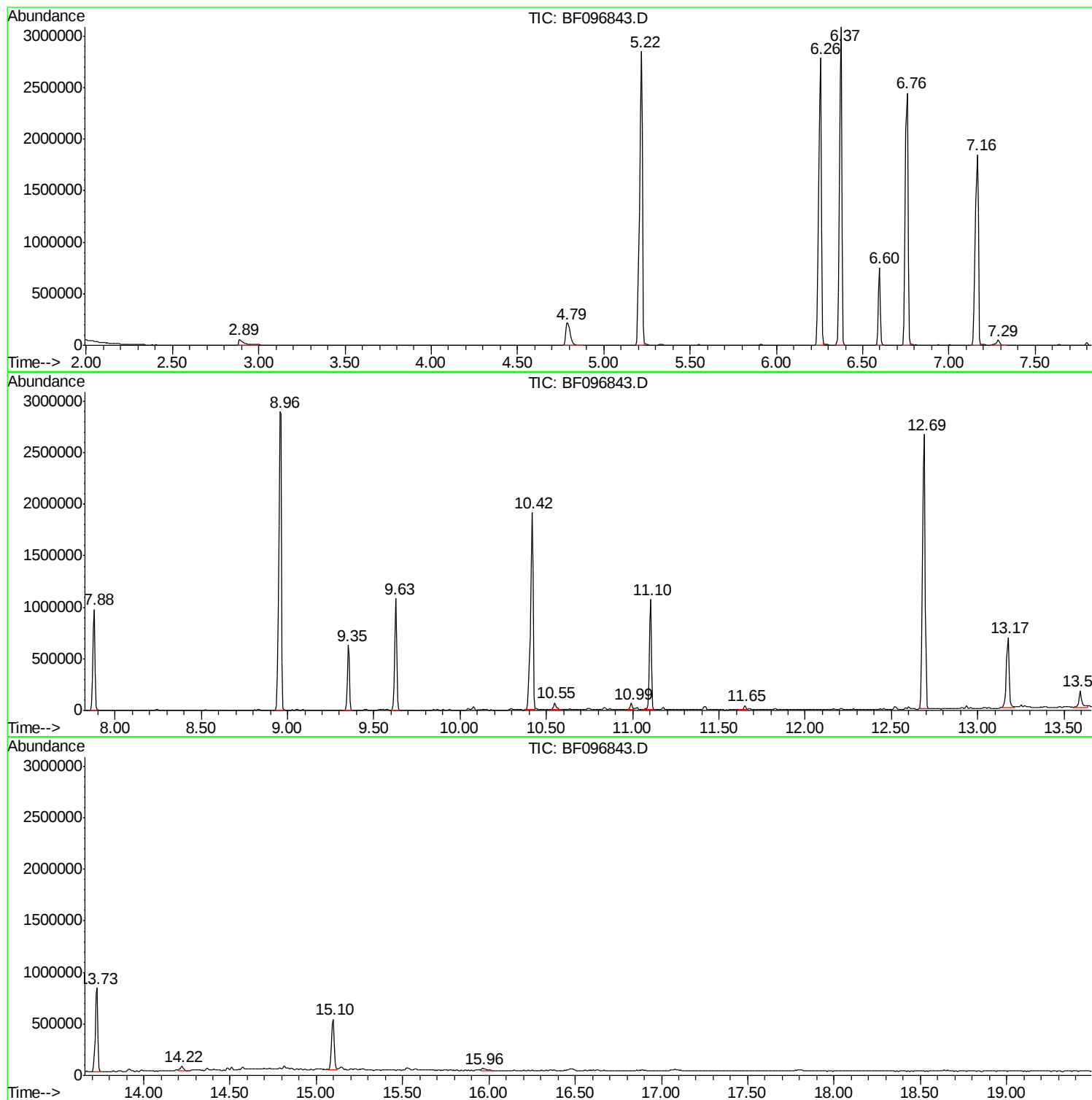
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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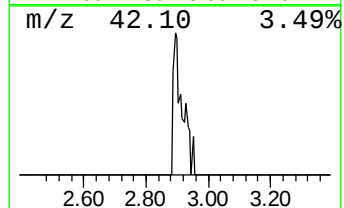
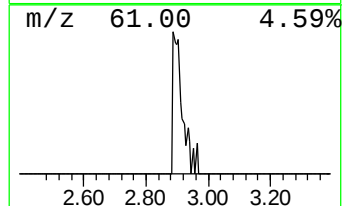
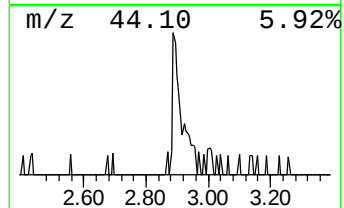
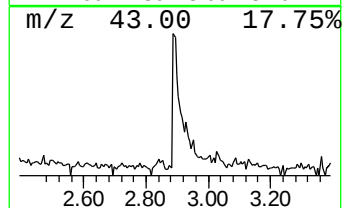
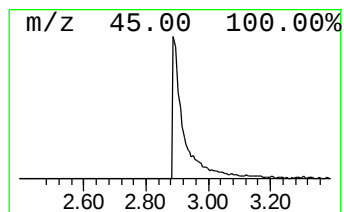
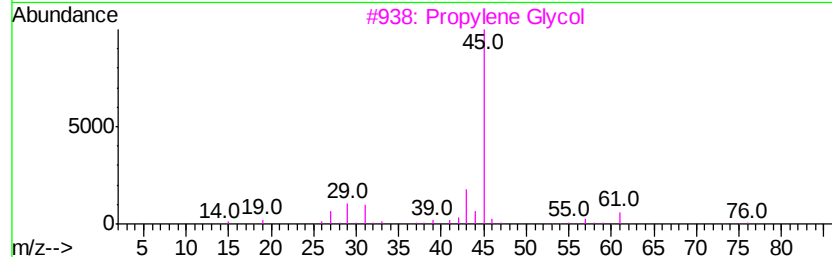
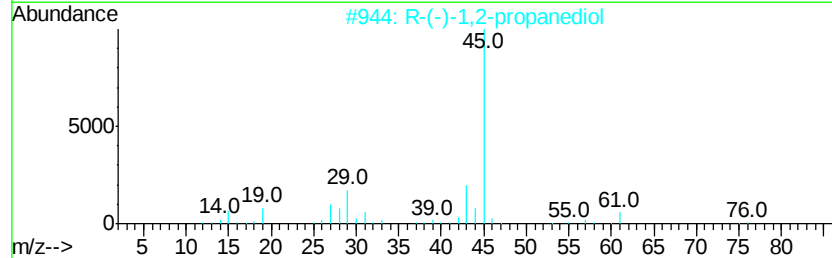
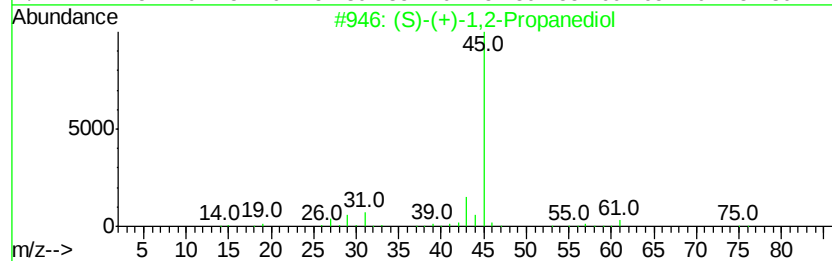
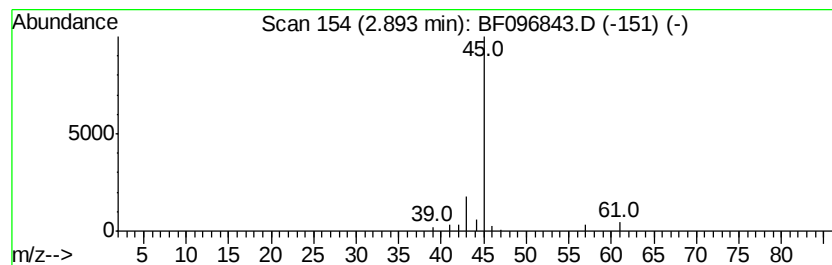
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	3.73 ng	118455	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5		Formamide	45	CH3NO	000075-12-7	7



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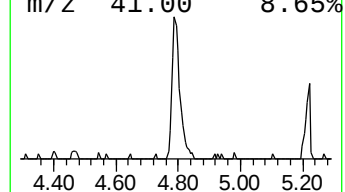
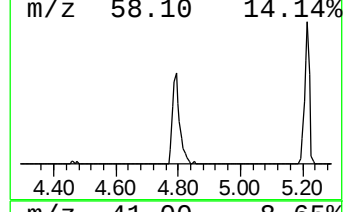
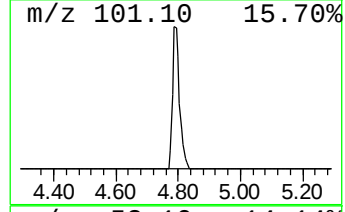
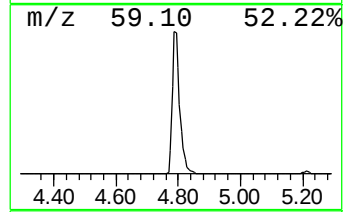
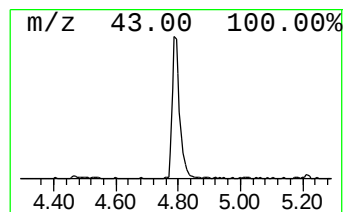
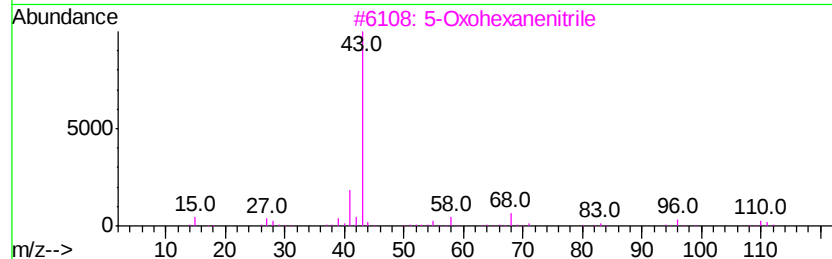
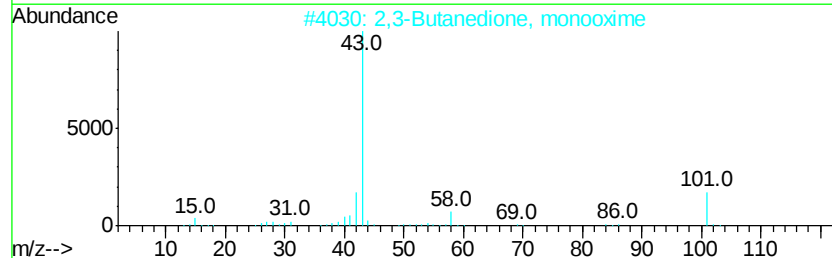
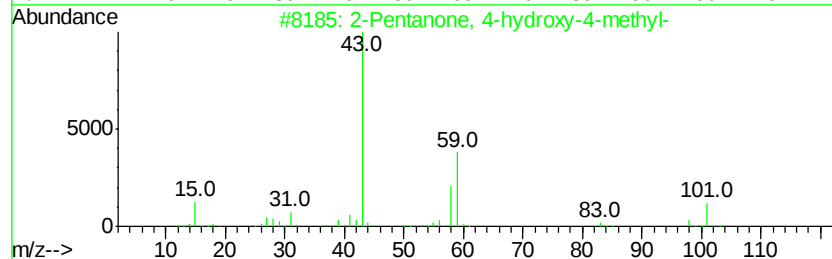
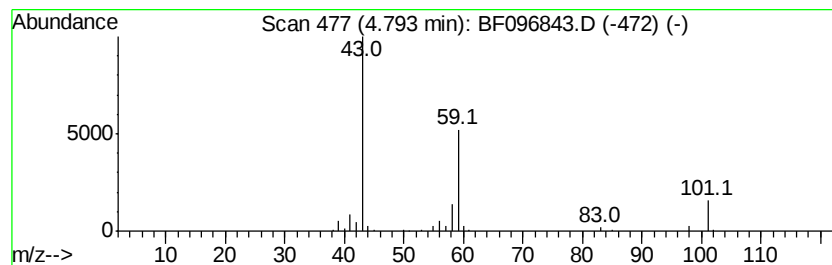
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	11.25 ng	357127	1,4-Dichlorobenzene-d4	6.60

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	16	
3	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9	
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	



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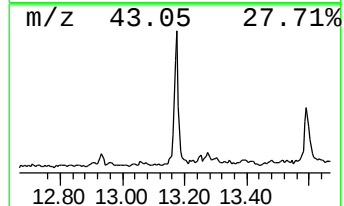
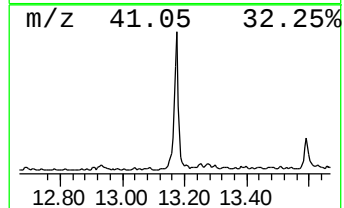
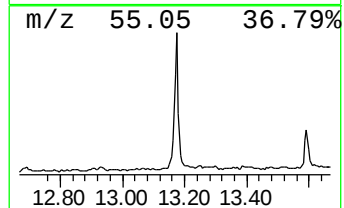
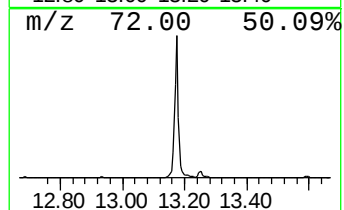
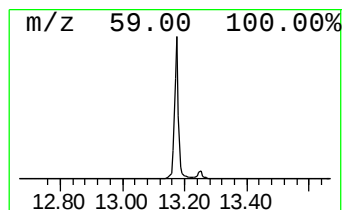
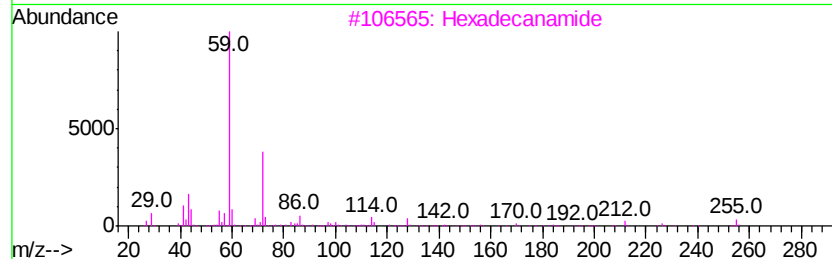
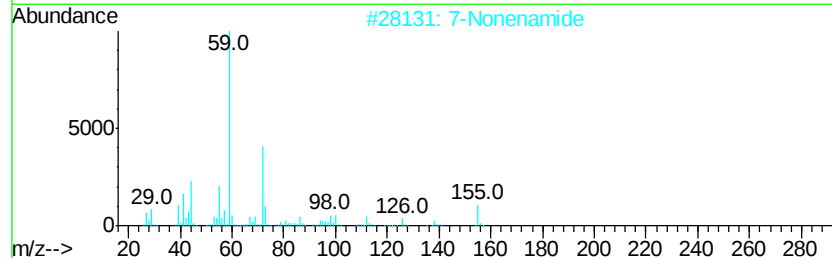
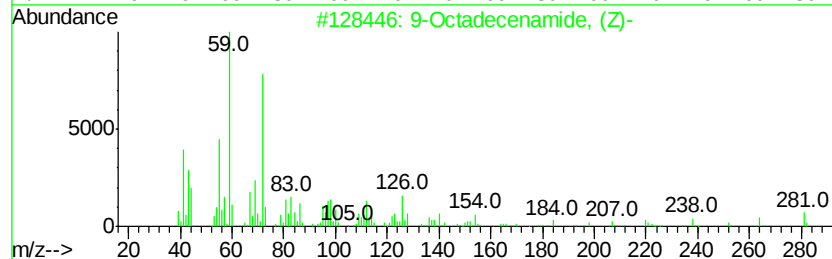
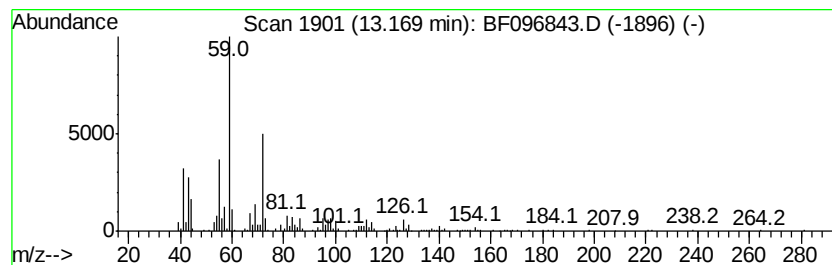
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	16.61 ng	668240	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	92
2		7-Nonenamide	155	C9H17NO	090949-53-4	78
3		Hexadecanamide	255	C16H33NO	000629-54-9	56
4		Dodecanamide	199	C12H25NO	001120-16-7	45
5		Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	43



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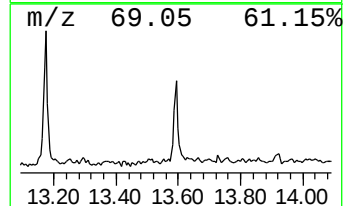
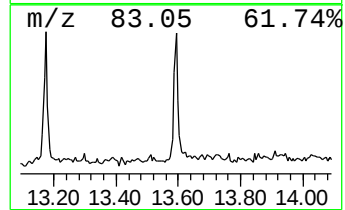
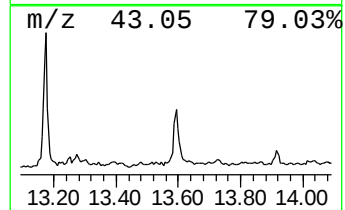
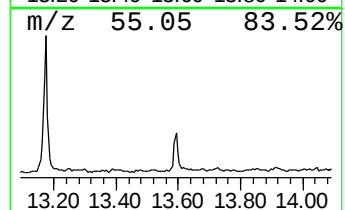
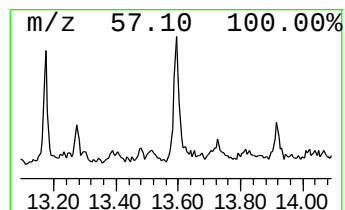
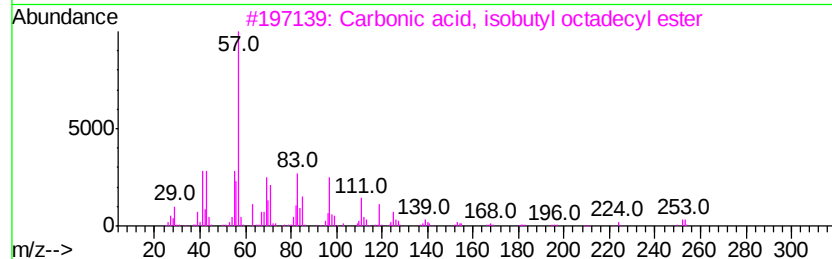
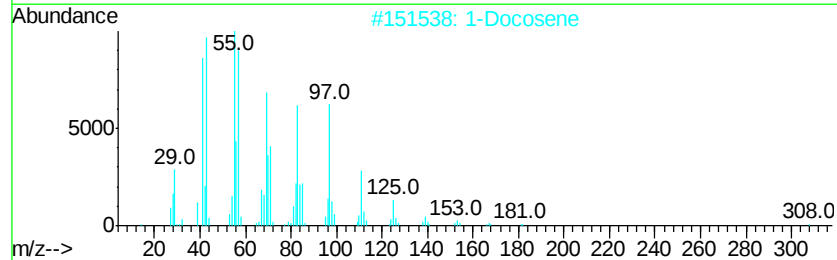
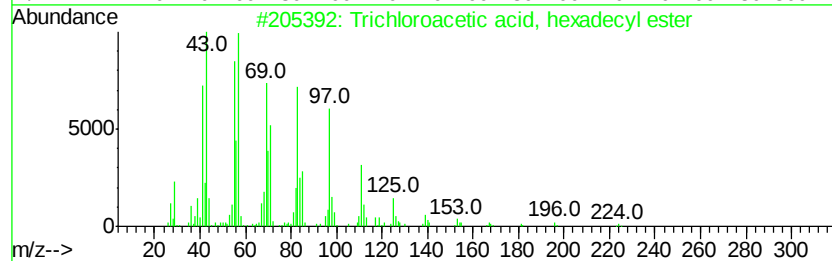
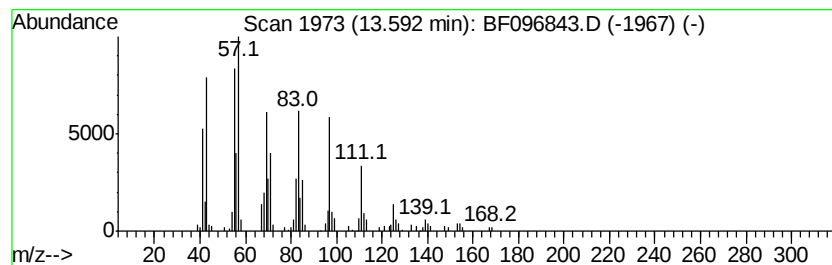
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Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	4.75 ng	191150	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2		1-Docosene	308	C22H44	001599-67-3	91
3		Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	91
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(S)-(+)-1,2-Propa...	2.89	3.7	ng	118455	1	6.60	634918	20.0
2-Pentanone, 4-hy...	4.79	11.3	ng	357127	1	6.60	634918	20.0
9-Octadecenamide, ...	13.17	16.6	ng	668240	5	13.73	804734	20.0
Trichloroacetic a...	13.59	4.8	ng	191150	5	13.73	804734	20.0