

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
 Data File : BF102301.D
 Acq On : 22 Jan 2018 16:03
 Operator : SJ/JU
 Sample : J1228-22
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1

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-BF012218.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	4.910	476	480	493	rBV	159030	223419	7.33%	0.806%
2	5.328	546	551	554	rBV	2598813	2826470	92.74%	10.192%
3	6.357	720	726	743	rBV	2750884	3047690	100.00%	10.990%
4	6.487	743	748	751	rBV	2879559	2993232	98.21%	10.794%
5	6.710	783	786	794	rBV	849640	775073	25.43%	2.795%
6	6.869	809	813	816	rBV	2607296	2237776	73.43%	8.069%
7	7.281	878	883	886	rBV	1962879	1875448	61.54%	6.763%
8	7.463	911	914	919	rVB	47843	42542	1.40%	0.153%
9	7.992	1000	1004	1019	rBV	1083903	1093310	35.87%	3.942%
10	9.075	1182	1188	1191	rBV	3127874	3003600	98.55%	10.831%
11	9.469	1251	1255	1258	rBV	344437	308597	10.13%	1.113%
12	9.680	1287	1291	1295	rVB	40295	33566	1.10%	0.121%
13	9.745	1298	1302	1313	rVB	1210279	1191546	39.10%	4.297%
14	10.180	1372	1376	1379	rVB	41939	41403	1.36%	0.149%
15	10.463	1418	1424	1427	rBV	47119	47227	1.55%	0.170%
16	10.539	1432	1437	1440	rBV	1939568	1905404	62.52%	6.871%
17	10.651	1453	1456	1462	rVB	33524	33705	1.11%	0.122%
18	11.233	1551	1555	1558	rBV	1247194	1139196	37.38%	4.108%
19	12.716	1804	1807	1811	rVB	41733	36325	1.19%	0.131%
20	12.821	1820	1825	1828	rBV	2667763	2664661	87.43%	9.609%
21	13.710	1973	1976	1985	rBV	291971	301208	9.88%	1.086%
22	13.868	1997	2003	2006	rBV	1025482	952824	31.26%	3.436%
23	14.345	2081	2084	2088	rBV5	28773	40016	1.31%	0.144%
24	14.615	2128	2130	2137	rVB4	40722	63843	2.09%	0.230%
25	15.286	2239	2244	2252	rBV	659715	853410	28.00%	3.077%

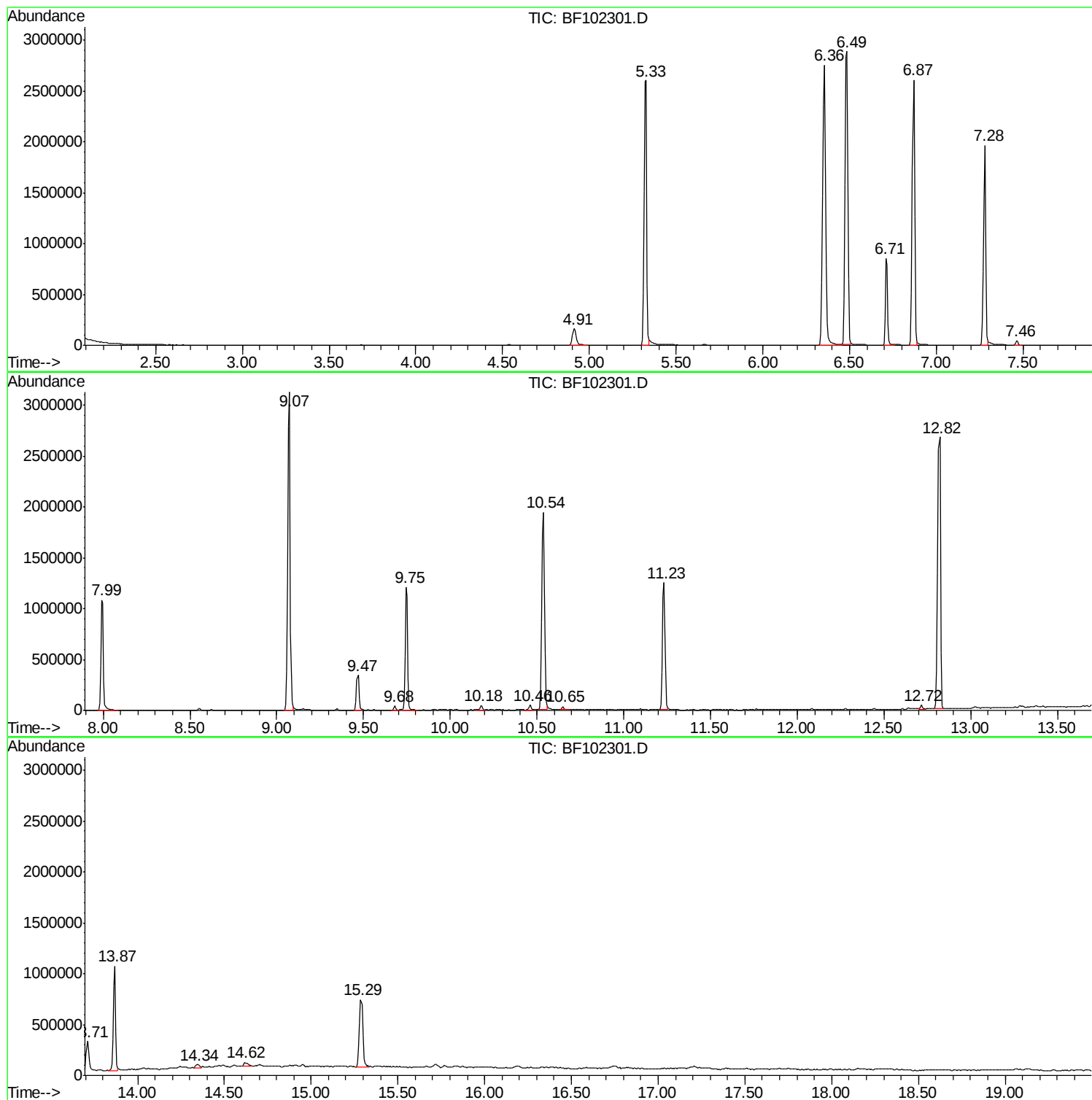
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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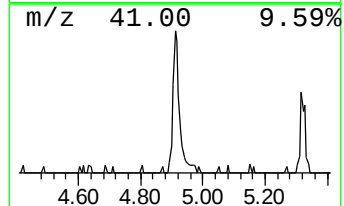
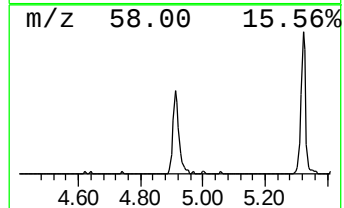
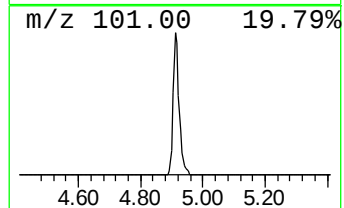
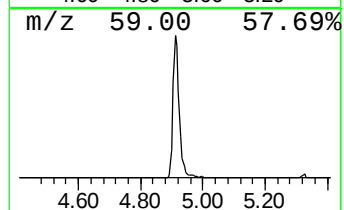
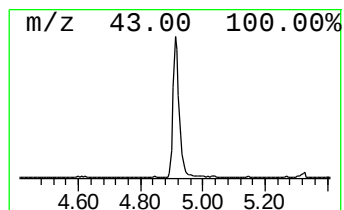
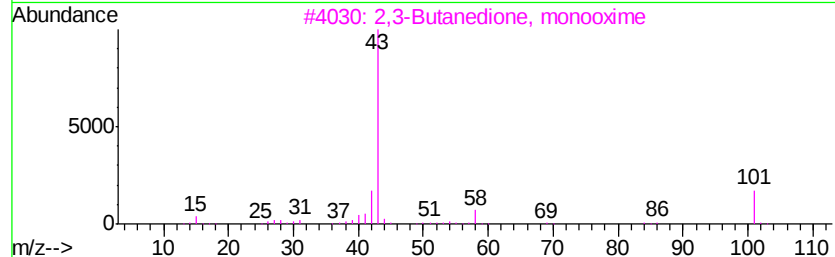
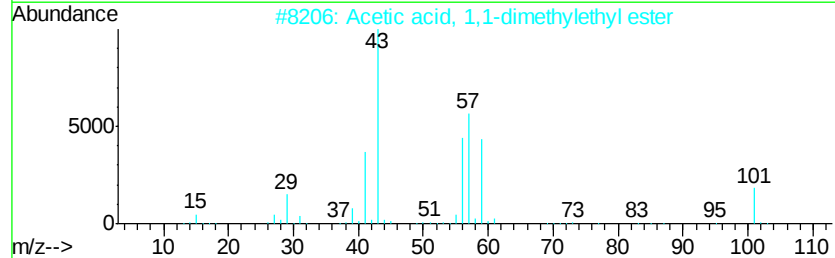
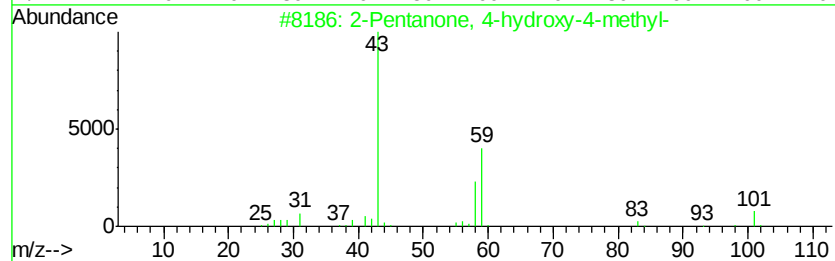
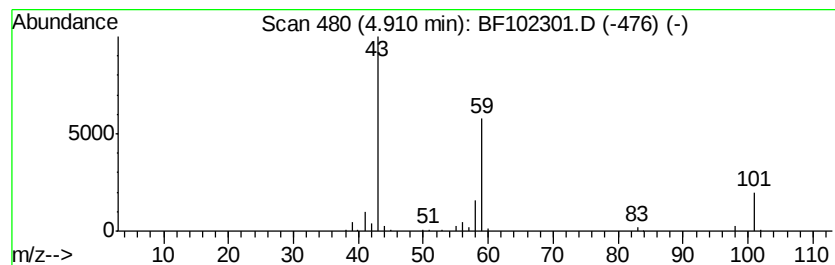
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	5.77 ng	223419	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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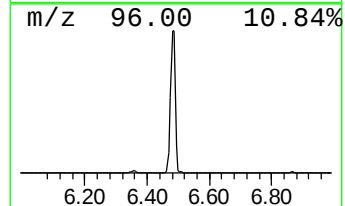
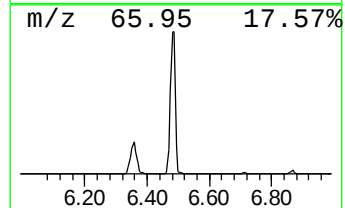
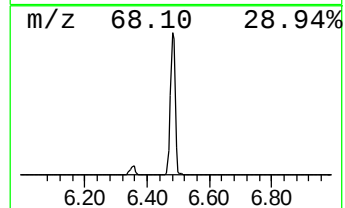
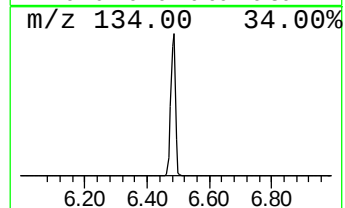
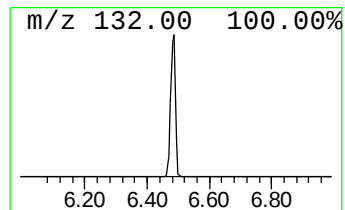
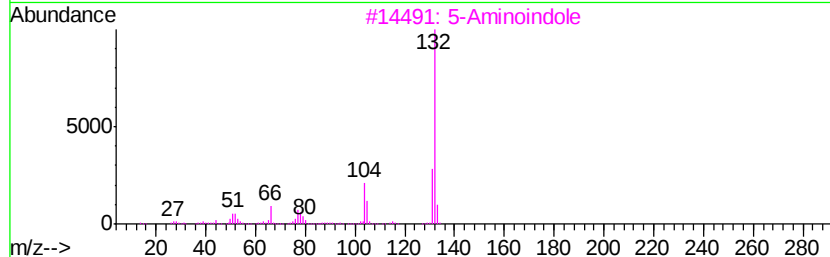
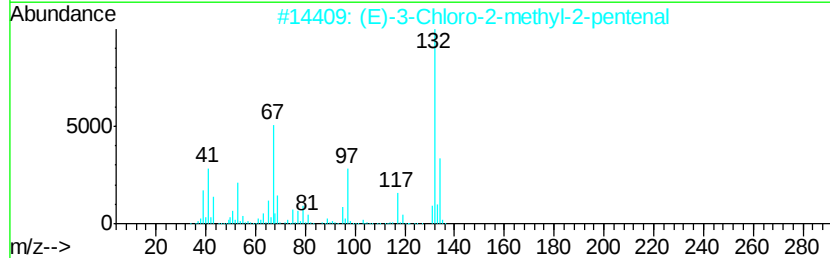
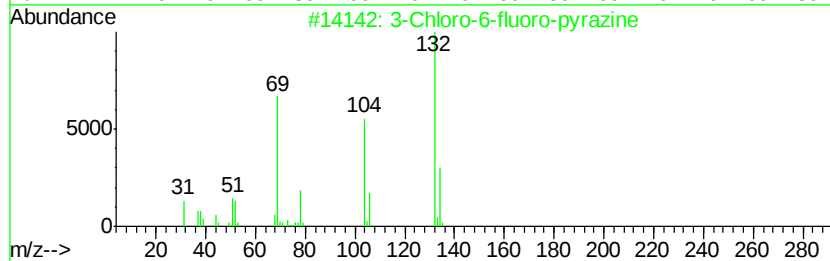
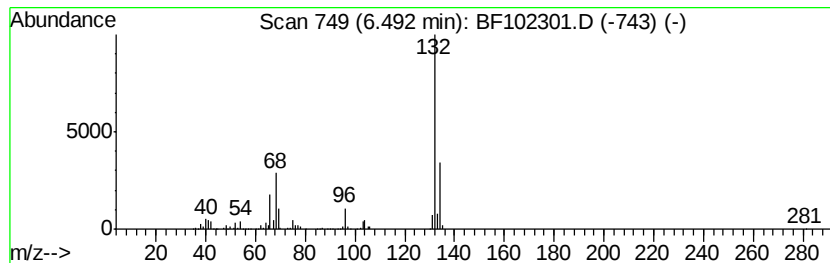
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	77.24 ng	2993230	1,4-Dichlorobenzene-d4	6.71

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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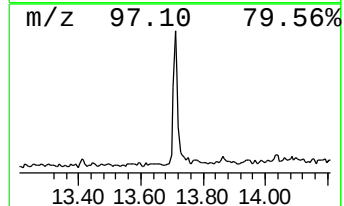
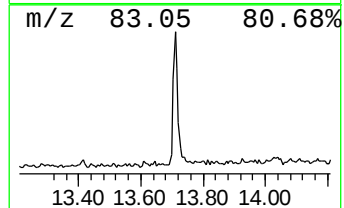
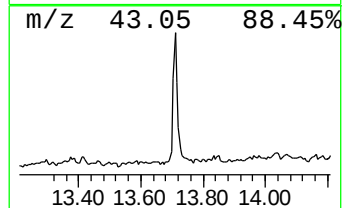
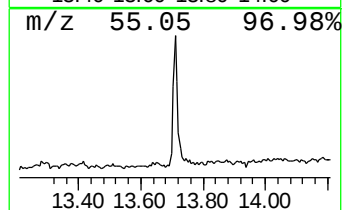
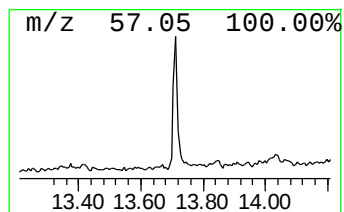
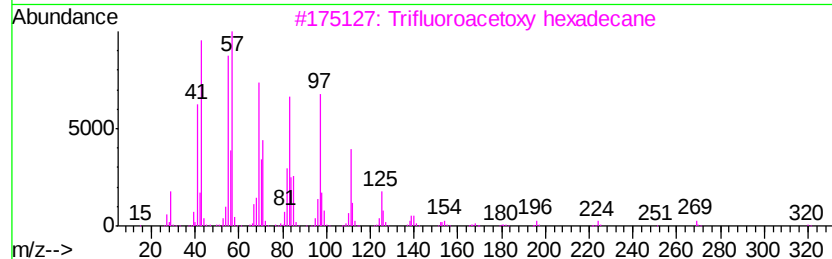
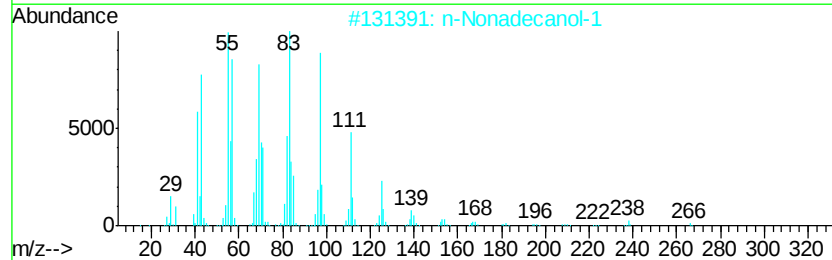
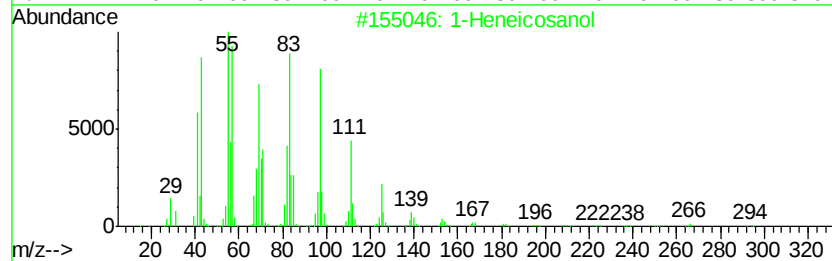
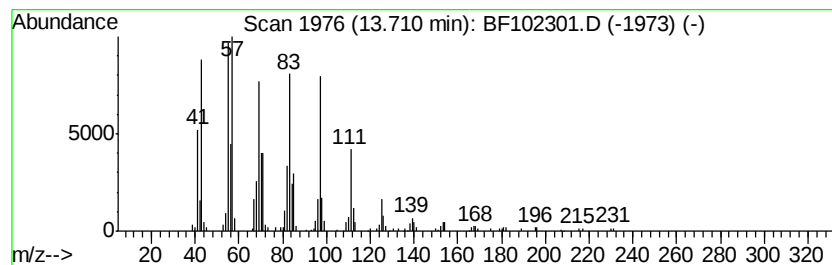
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	6.32 ng	301208	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.91	5.8	ng	223419	1	6.71	775073	20.0
unknown6.49	6.49	77.2	ng	2993230	1	6.71	775073	20.0
1-Heneicosanol	13.71	6.3	ng	301208	5	13.87	952824	20.0