

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
 Data File : BF096646.D
 Acq On : 11 Jul 2017 16:05
 Operator : SJ/JU
 Sample : I4120-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-12-COMP

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	4.875	469	474	486	rVB	391470	551966	18.77%	2.186%
2	5.298	541	546	549	rBV	2529656	2646642	90.00%	10.481%
3	6.328	715	721	730	rBV	2551941	2707117	92.05%	10.721%
4	6.457	738	743	746	rBV	2638238	2626219	89.30%	10.400%
5	6.681	778	781	785	rBV	730303	626403	21.30%	2.481%
6	6.839	804	808	812	rBV	2163866	2023710	68.82%	8.014%
7	7.245	872	877	880	rBV	1746725	1723937	58.62%	6.827%
8	7.963	995	999	1003	rBV	1035709	942158	32.04%	3.731%
9	9.045	1177	1183	1186	rBV	2847186	2940787	100.00%	11.646%
10	9.433	1245	1249	1255	rBV	250238	206818	7.03%	0.819%
11	9.716	1291	1297	1301	rBV	1083269	974871	33.15%	3.861%
12	10.163	1369	1373	1376	rVB	46918	34647	1.18%	0.137%
13	10.504	1425	1431	1434	rBV	1559166	1673013	56.89%	6.625%
14	10.633	1449	1453	1461	rBV	63804	64767	2.20%	0.256%
15	11.192	1544	1548	1552	rBV	1098802	936417	31.84%	3.708%
16	11.733	1637	1640	1643	rBV2	54028	45094	1.53%	0.179%
17	12.780	1813	1818	1821	rBV2	2414113	2425262	82.47%	9.604%
18	13.680	1967	1971	1980	rBV	313130	321934	10.95%	1.275%
19	13.821	1991	1995	1999	rBV	857814	752341	25.58%	2.979%
20	14.315	2075	2079	2084	rBV3	27485	40468	1.38%	0.160%
21	14.580	2120	2124	2133	rBV	274997	293260	9.97%	1.161%
22	14.674	2137	2140	2146	rVB	33534	34513	1.17%	0.137%
23	14.921	2178	2182	2190	rVB4	19266	36224	1.23%	0.143%
24	15.221	2228	2233	2237	rBV	492782	590928	20.09%	2.340%
25	15.709	2313	2316	2321	rVB3	25007	32043	1.09%	0.127%

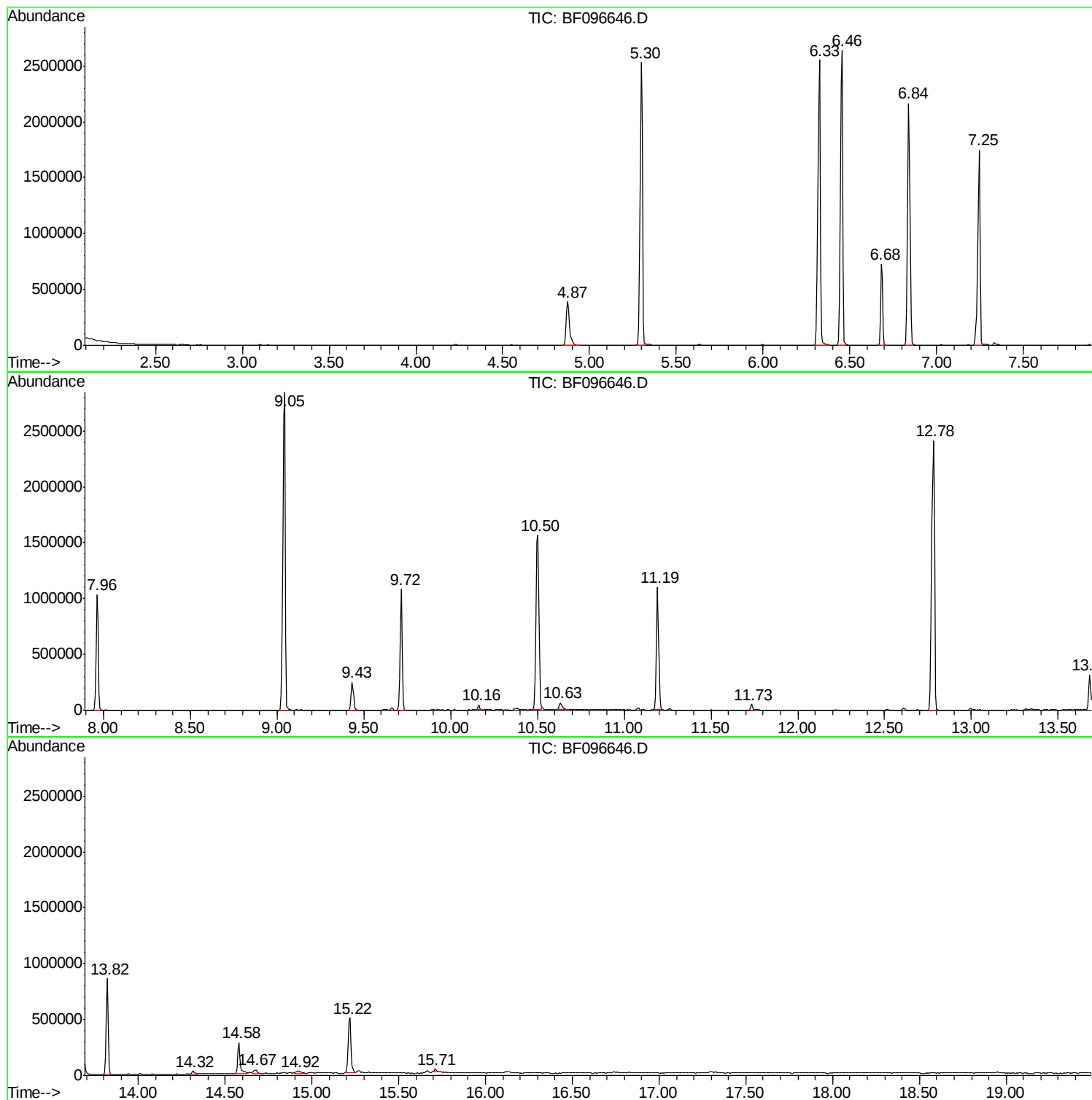
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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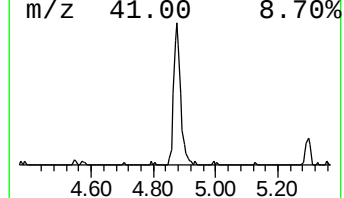
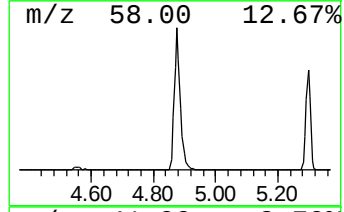
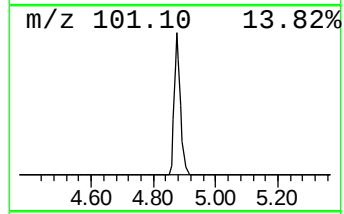
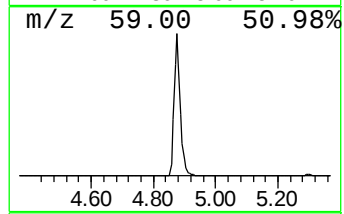
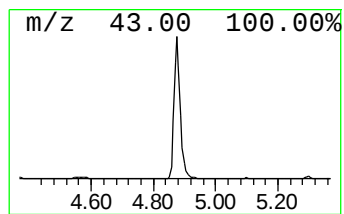
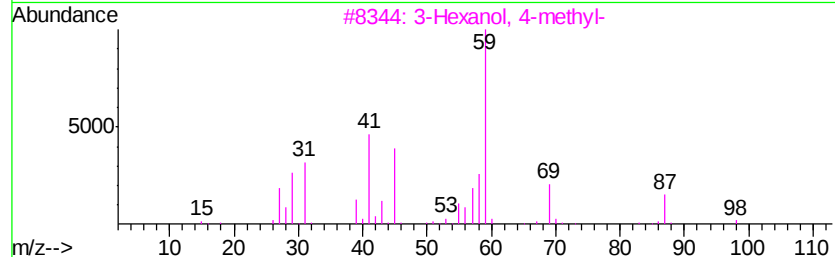
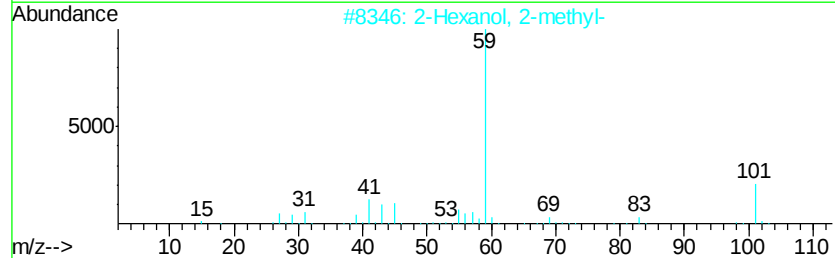
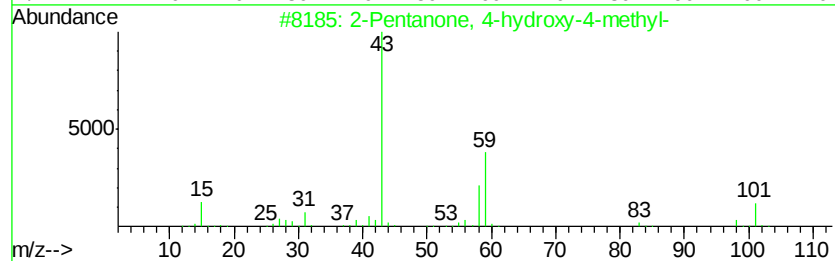
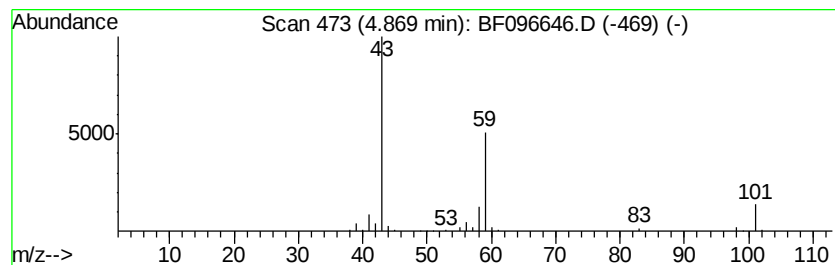
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	17.62 ng	551966	1,4-Dichlorobenzene-d4	6.68

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	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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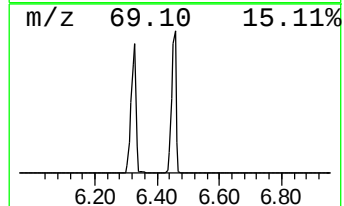
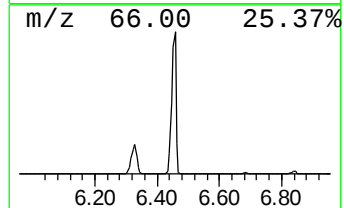
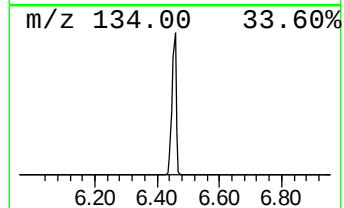
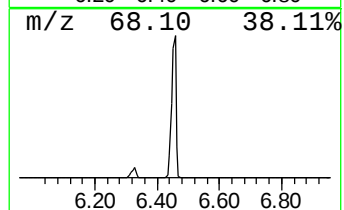
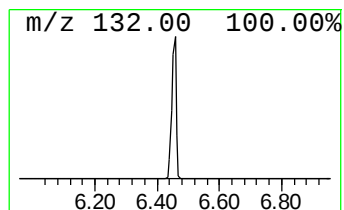
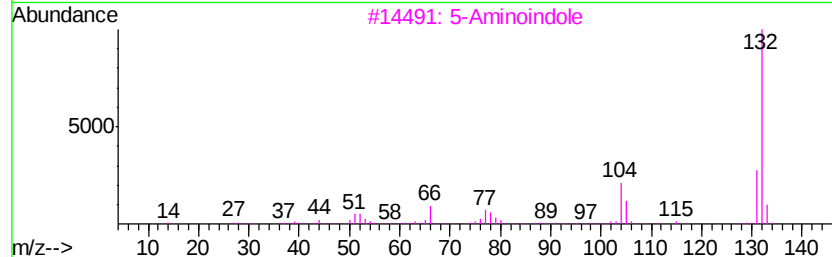
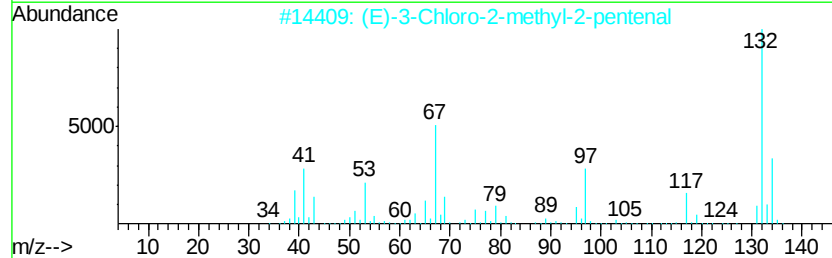
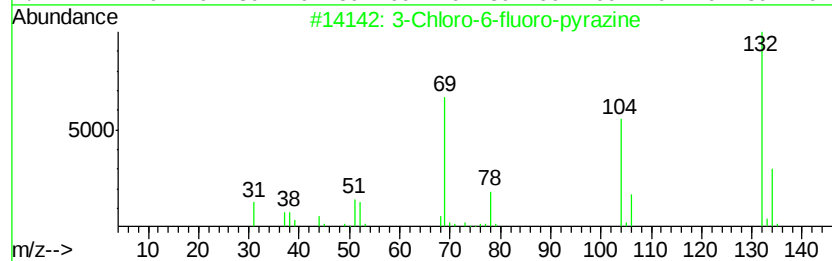
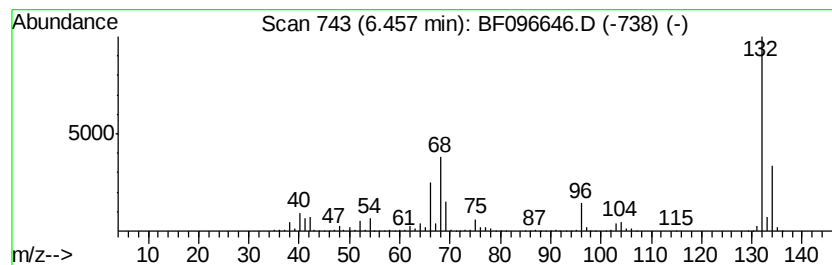
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Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	83.85 ng	2626220	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	2H-Cyclopenta[d]pyridazine, 2-me...			132	C8H8N2	022291-85-6	9



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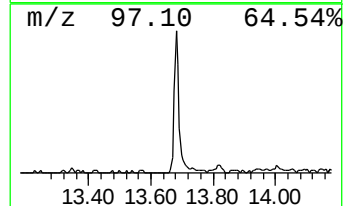
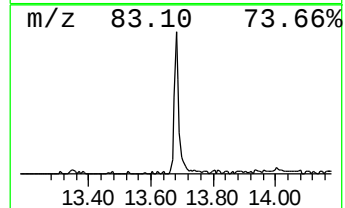
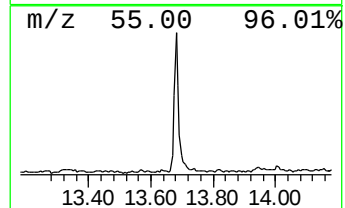
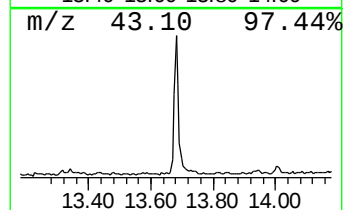
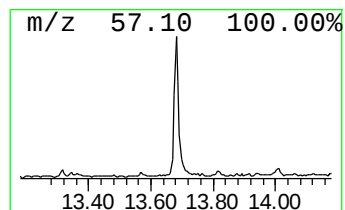
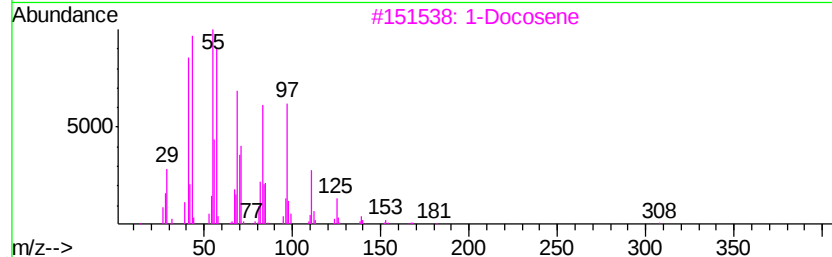
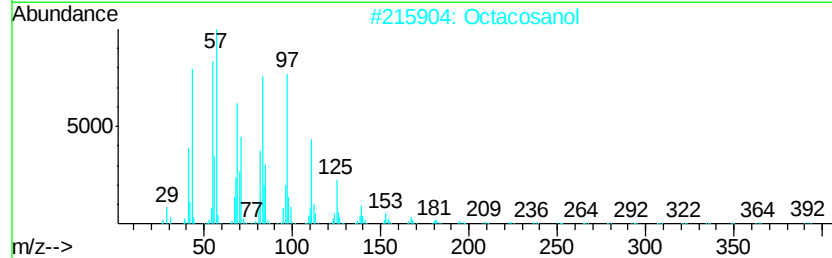
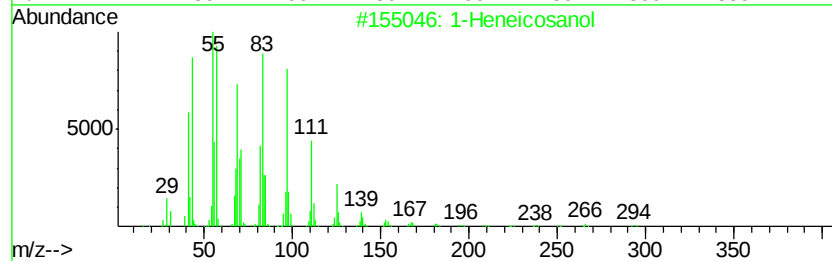
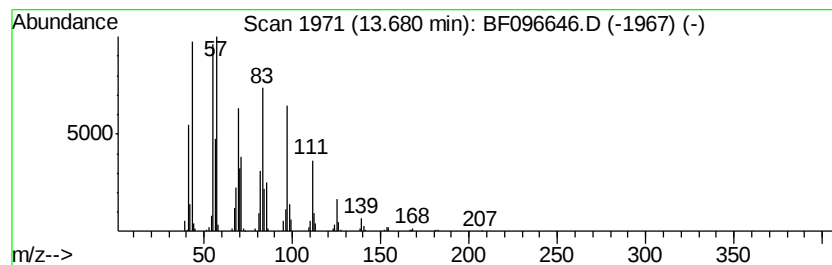
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Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.68	8.56 ng	321934	Chrysene-d12		13.82
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Octacosanol	410	C28H58O	000557-61-9	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91



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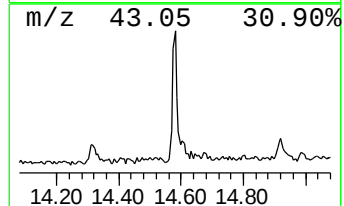
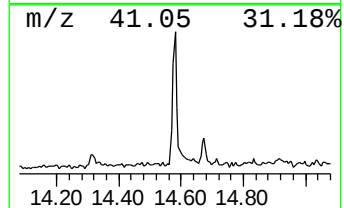
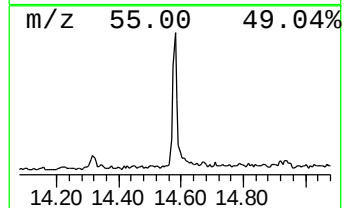
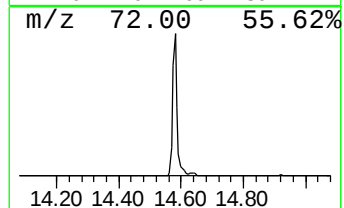
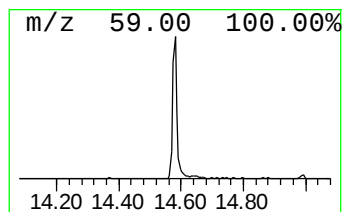
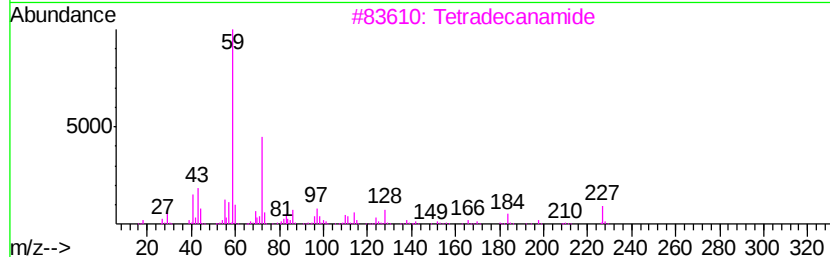
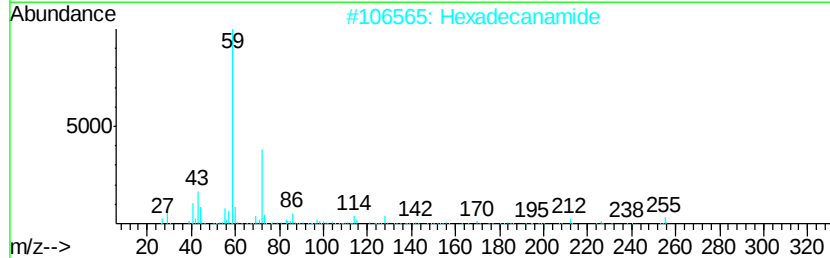
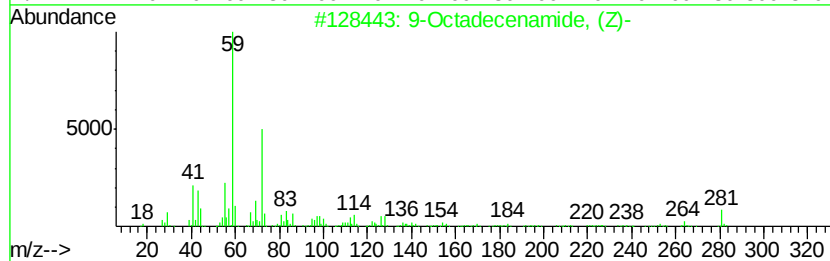
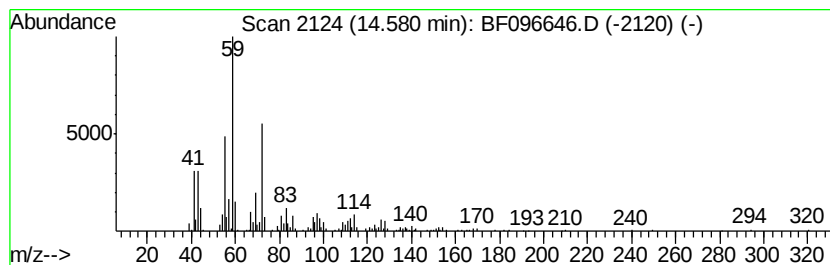
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	9.93 ng	293260	Perylene-d12	15.22

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-			281	C18H35NO	000301-02-0	91
2	Hexadecanamide			255	C16H33NO	000629-54-9	72
3	Tetradecanamide			227	C14H29NO	000638-58-4	64
4	Benzeneethanamine, 2-fluoro-.bet...			229	C11H16FN03	061338-98-5	64
5	Octadecanamide			283	C18H37NO	000124-26-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.87	17.6	ng	551966	1	6.68	626403	20.0
unknown6.46	6.46	83.8	ng	2626220	1	6.68	626403	20.0
1-Heneicosanol	13.68	8.6	ng	321934	5	13.82	752341	20.0
9-Octadecenamide,...	14.58	9.9	ng	293260	6	15.22	590928	20.0