

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
 Data File : BF096385.D
 Acq On : 1 Jul 2017 18:11
 Operator : SJ/MA
 Sample : I3950-12
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B5-10.5-13

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	4.928	478	483	491	rBV	397504	511190	17.18%	2.116%
2	5.351	549	555	558	rBV	2903173	2946076	98.99%	12.194%
3	6.369	722	728	731	rBV	2902466	2976205	100.00%	12.318%
4	6.504	746	751	754	rBV	2996578	2906775	97.67%	12.031%
5	6.733	786	790	793	rBV	823147	698912	23.48%	2.893%
6	6.886	812	816	820	rBV	2089782	2033394	68.32%	8.416%
7	7.292	879	885	888	rBV	1850679	1776130	59.68%	7.351%
8	8.016	1003	1008	1011	rBV	1016243	957377	32.17%	3.963%
9	9.092	1186	1191	1194	rBV	2755970	2554700	85.84%	10.574%
10	9.480	1253	1257	1260	rBV	510365	391159	13.14%	1.619%
11	9.710	1293	1296	1301	rVB	44777	36940	1.24%	0.153%
12	9.763	1301	1305	1309	rBV2	1085840	953123	32.02%	3.945%
13	10.210	1378	1381	1384	rVB	78500	59629	2.00%	0.247%
14	10.551	1434	1439	1442	rBV	1501455	1498741	50.36%	6.203%
15	10.680	1458	1461	1468	rBV	78914	73733	2.48%	0.305%
16	11.239	1553	1556	1560	rBV	813741	761838	25.60%	3.153%
17	11.780	1644	1648	1656	rBV	74811	79983	2.69%	0.331%
18	12.827	1821	1826	1829	rBV	1757669	1539637	51.73%	6.372%
19	13.310	1903	1908	1913	rVB	54667	55499	1.86%	0.230%
20	13.727	1976	1979	1984	rBV2	106244	104641	3.52%	0.433%
21	13.868	1999	2003	2007	rBV	696629	616487	20.71%	2.552%
22	15.280	2238	2243	2249	rVB	541229	628509	21.12%	2.601%

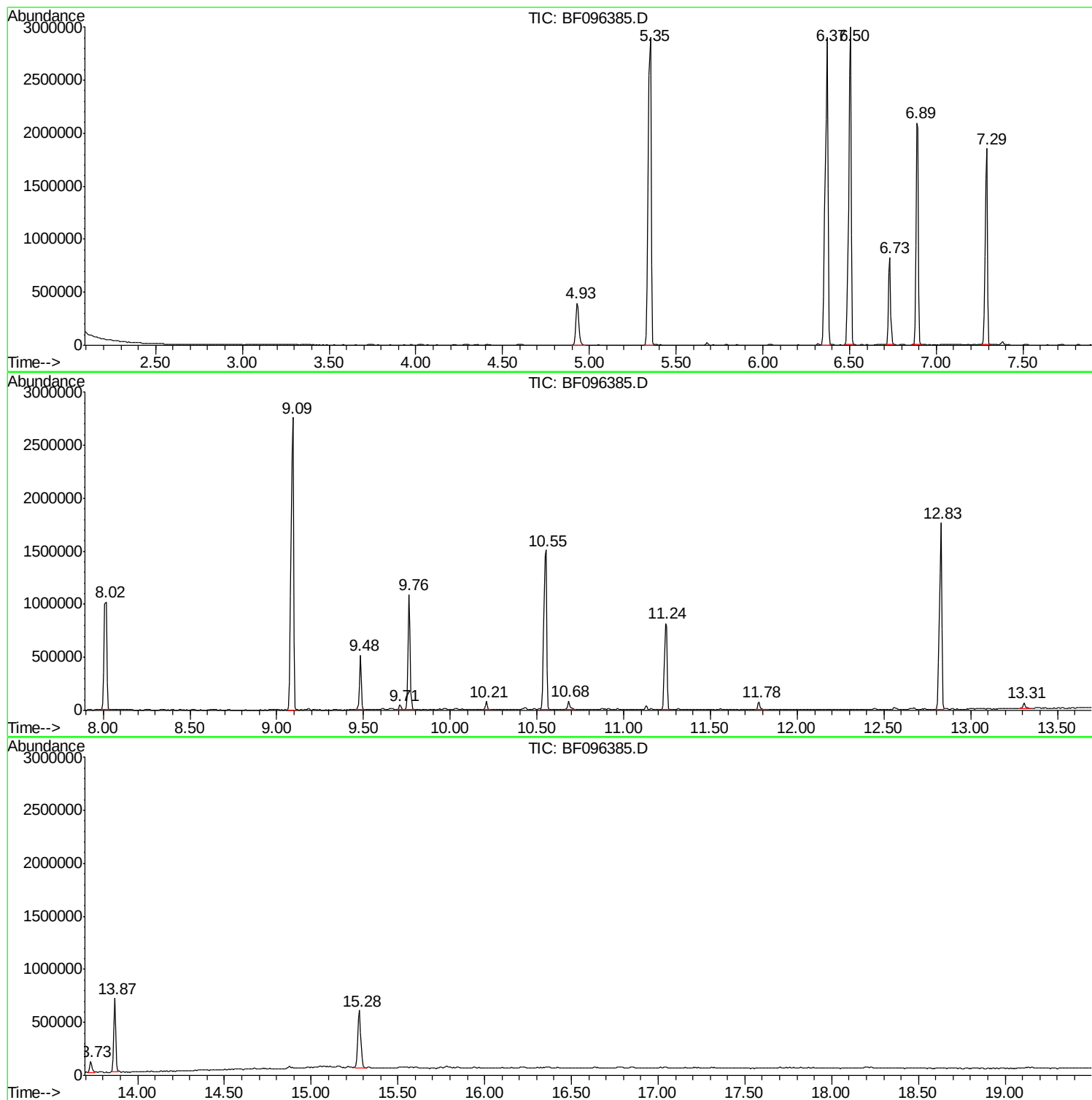
Sum of corrected areas: 24160678

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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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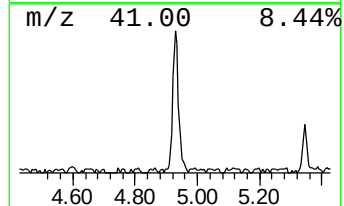
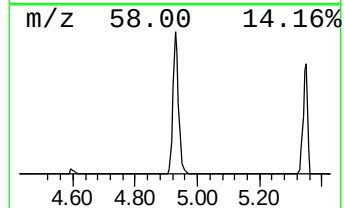
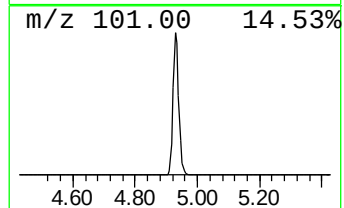
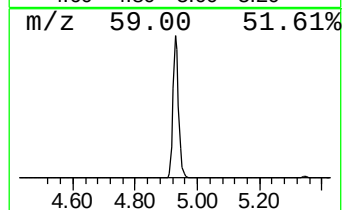
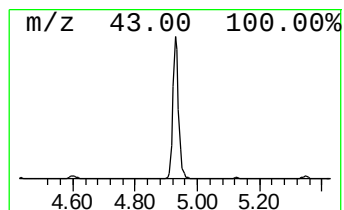
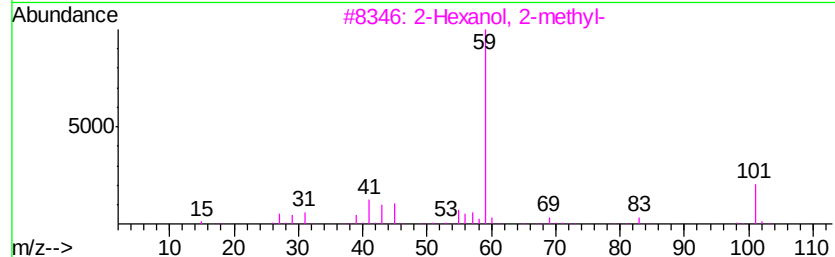
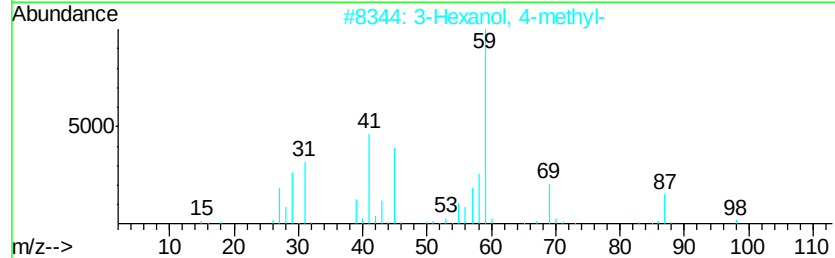
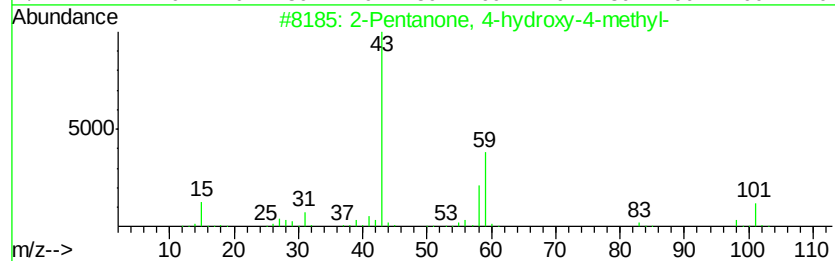
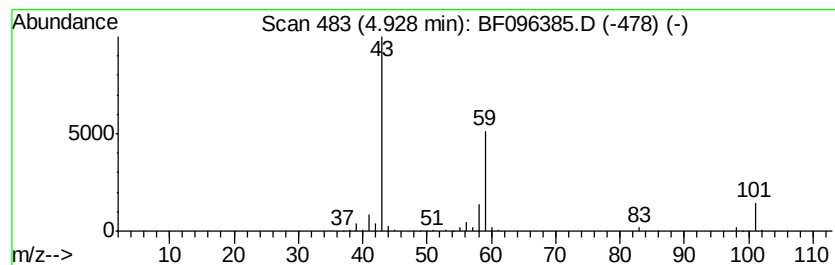
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	14.63 ng	511190	1,4-Dichlorobenzene-d4	6.73

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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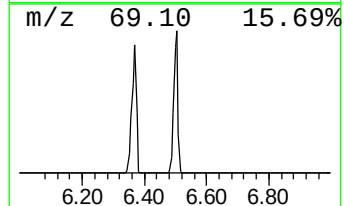
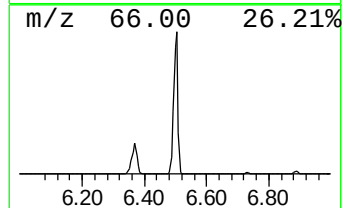
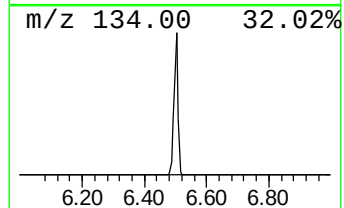
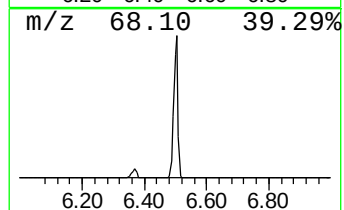
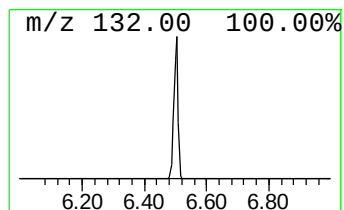
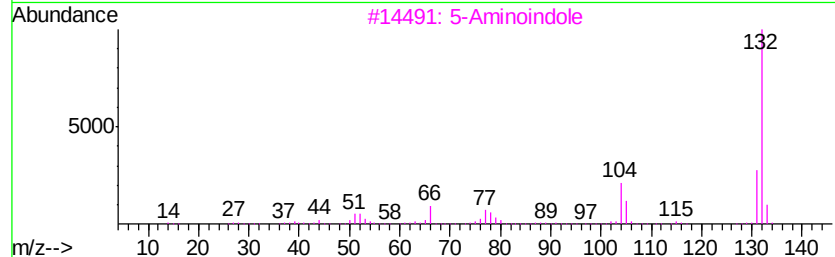
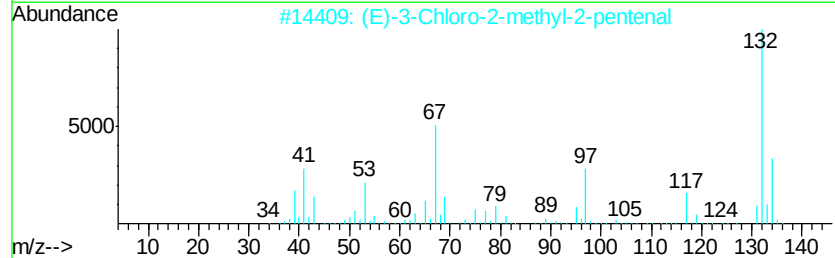
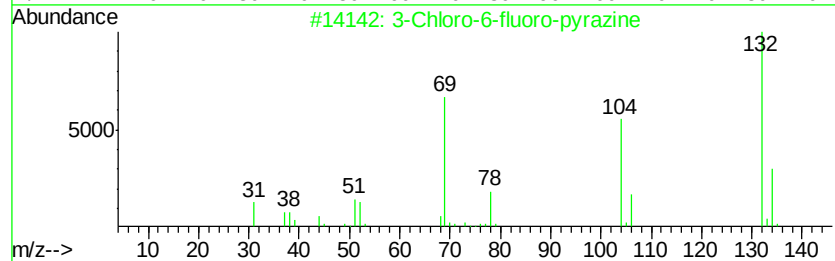
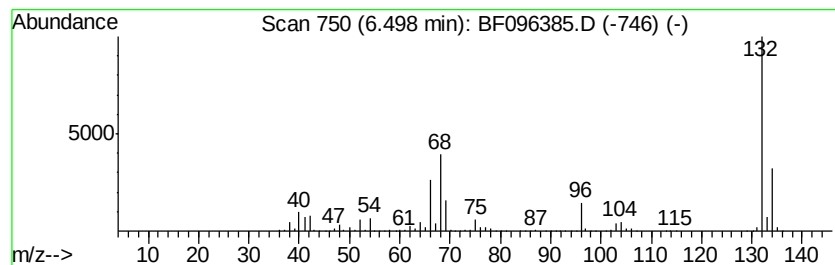
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	83.18 ng	2906780	1,4-Dichlorobenzene-d4	6.73

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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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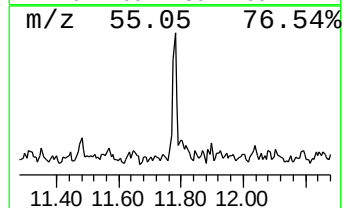
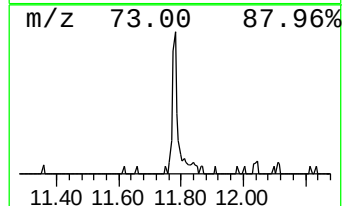
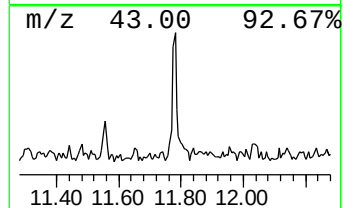
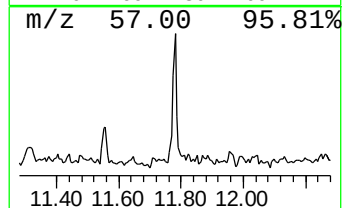
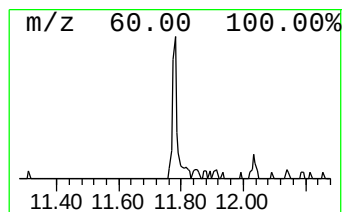
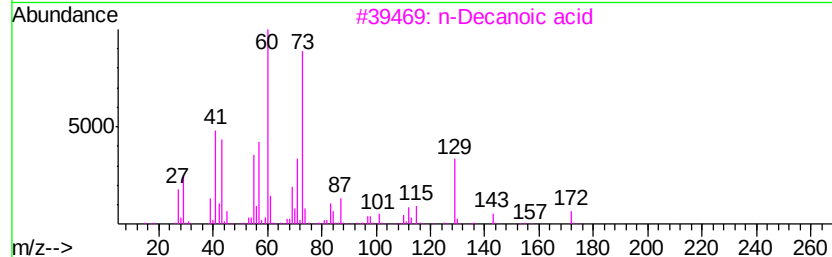
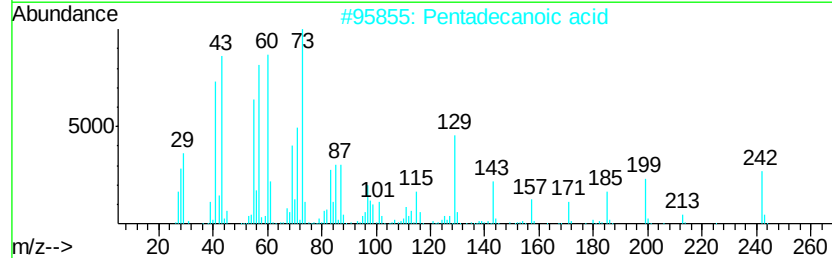
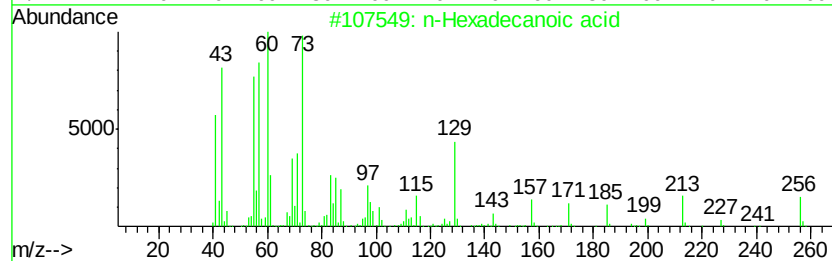
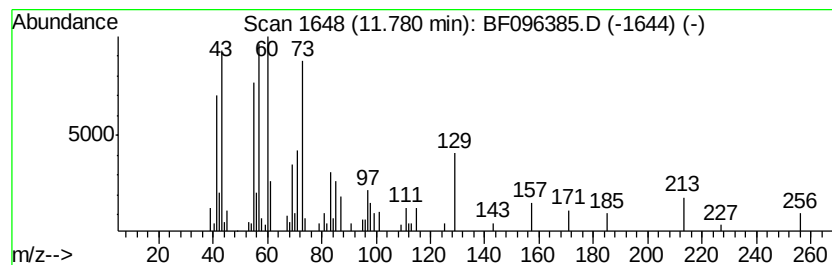
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.78	2.10 ng	79983	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5	Oxalic acid, allyl tridecyl ester	312	C18H32O4	1000309-24-1	18



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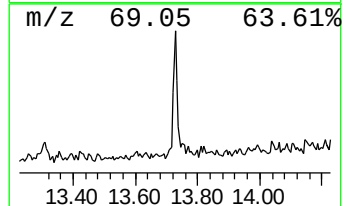
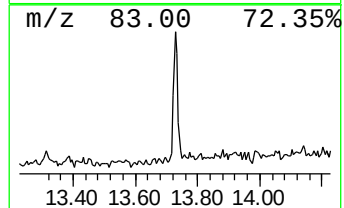
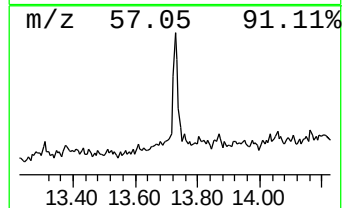
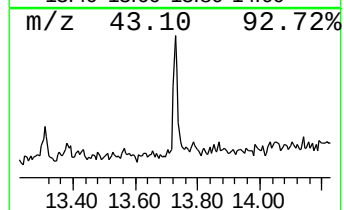
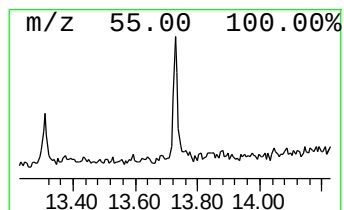
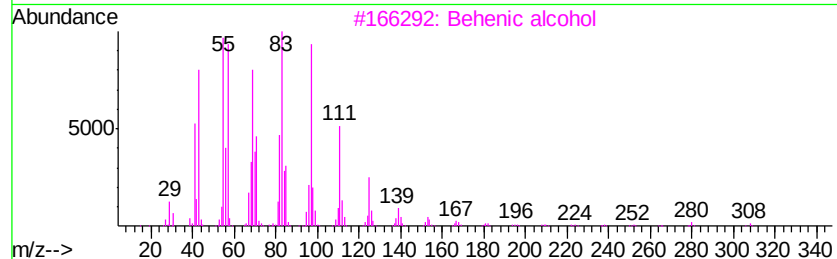
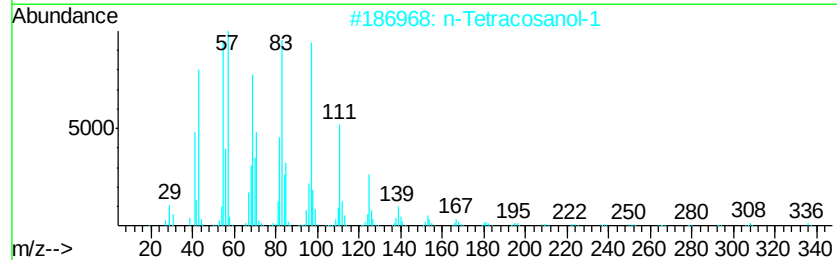
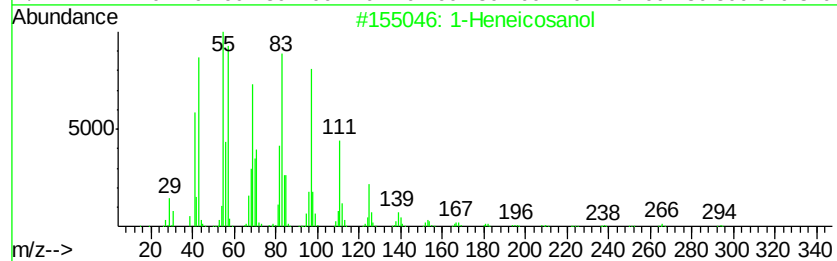
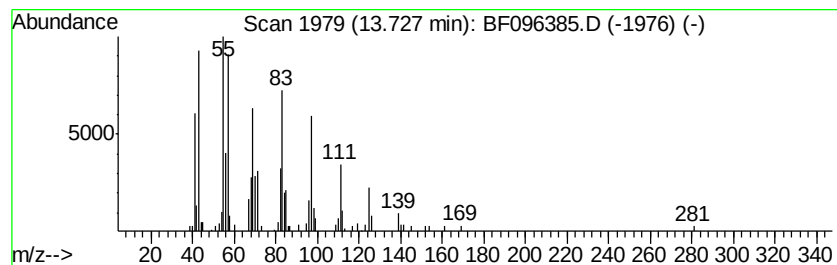
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.39 ng	104641	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5		1-Octadecanol	270	C18H38O	000112-92-5	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	14.6	ng	511190	1	6.73	698912	20.0
unknown6.50	6.50	83.2	ng	2906780	1	6.73	698912	20.0
n-Hexadecanoic acid	11.78	2.1	ng	79983	4	11.24	761838	20.0
1-Heneicosanol	13.73	3.4	ng	104641	5	13.87	616487	20.0