

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096562.D
 Acq On : 7 Jul 2017 16:37
 Operator : SJ/MA
 Sample : I4064-10
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF007-01

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	4.881	471	475	487	rVB	414571	576542	19.96%	2.347%
2	5.310	543	548	551	rBV	2786706	2740166	94.85%	11.153%
3	6.334	717	722	733	rVB	2497444	2888807	100.00%	11.757%
4	6.469	740	745	748	rBV	2556122	2733276	94.62%	11.124%
5	6.692	780	783	787	rBV	779269	687288	23.79%	2.797%
6	6.851	806	810	814	rBV	2273003	2074107	71.80%	8.442%
7	7.257	873	879	882	rBV	1663193	1562052	54.07%	6.358%
8	7.975	997	1001	1005	rBV	954282	843201	29.19%	3.432%
9	9.057	1179	1185	1188	rBV	2863752	2671136	92.47%	10.872%
10	9.445	1247	1251	1254	rBV	209691	167541	5.80%	0.682%
11	9.727	1294	1299	1303	rBV	1034892	909005	31.47%	3.700%
12	10.175	1371	1375	1378	rVB	46424	37276	1.29%	0.152%
13	10.516	1428	1433	1436	rBV	1529915	1536177	53.18%	6.252%
14	10.645	1452	1455	1465	rBV	49869	53266	1.84%	0.217%
15	11.204	1546	1550	1554	rBV	1015790	908867	31.46%	3.699%
16	12.792	1815	1820	1823	rBV2	2461639	2542642	88.02%	10.349%
17	13.692	1969	1973	1981	rBV	228285	235002	8.13%	0.956%
18	13.833	1993	1997	2001	rBV	795321	684918	23.71%	2.788%
19	14.592	2122	2126	2129	rBV	131886	125199	4.33%	0.510%
20	14.686	2139	2142	2146	rVB	37812	37332	1.29%	0.152%
21	15.233	2230	2235	2240	rBV	460710	522855	18.10%	2.128%
22	15.733	2315	2320	2326	rVB6	18135	33313	1.15%	0.136%

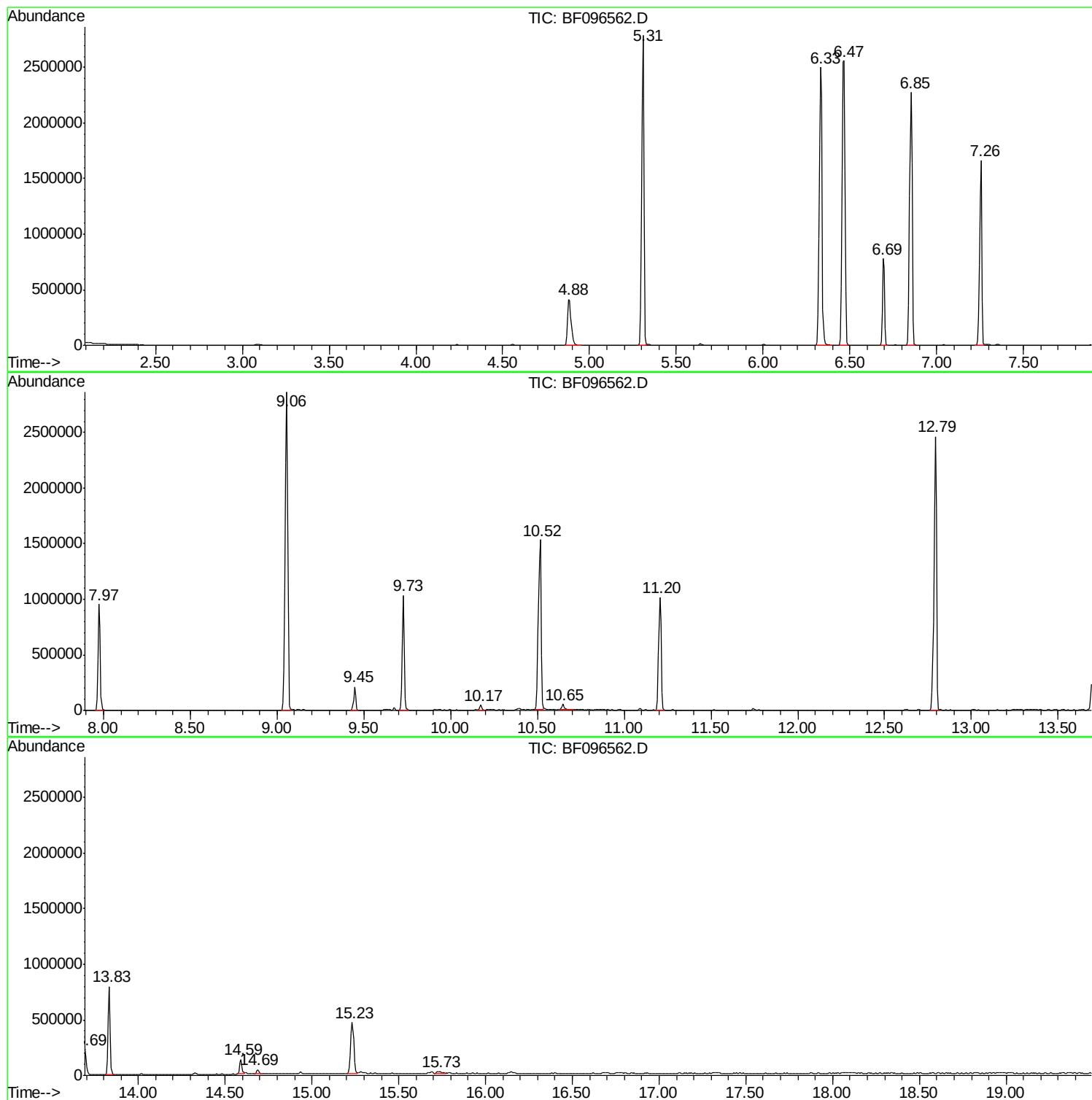
Sum of corrected areas: 24569968

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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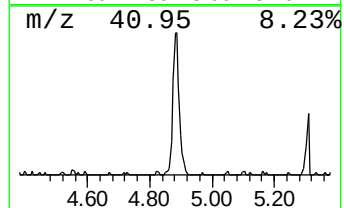
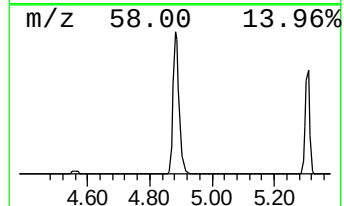
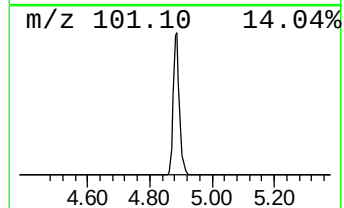
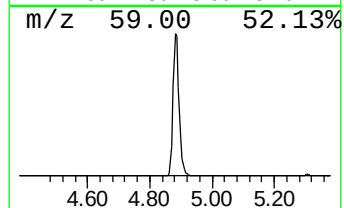
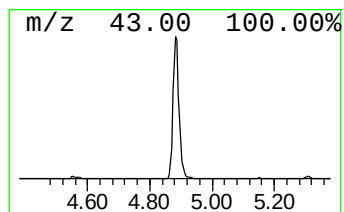
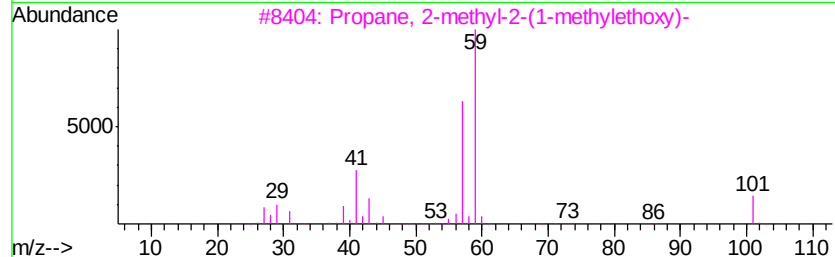
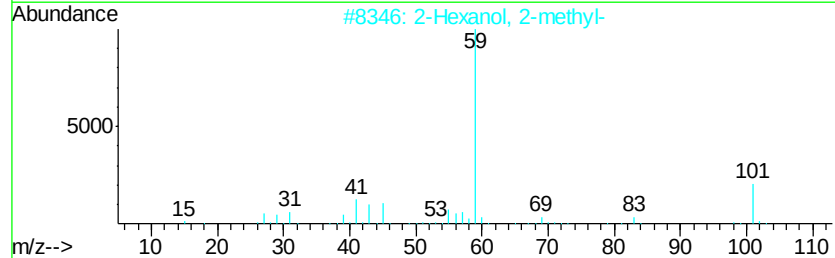
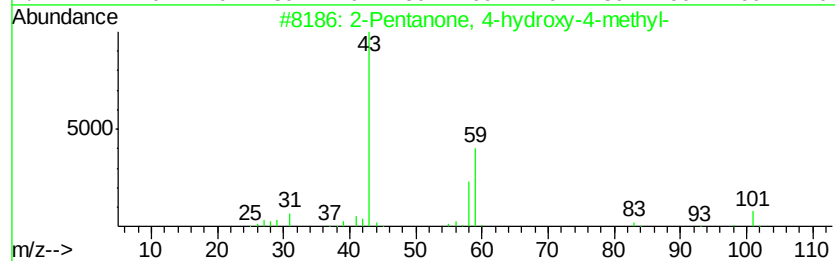
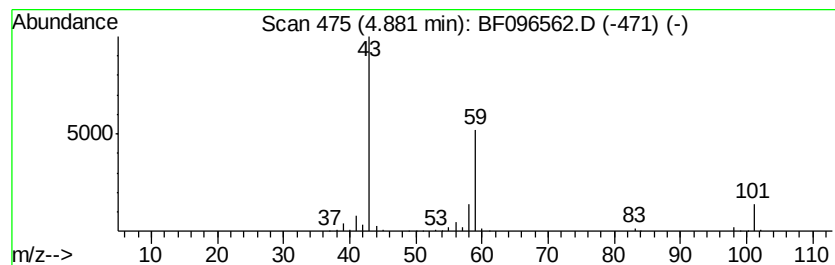
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.88	16.78 ng	576542	1,4-Dichlorobenzene-d4	6.69

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		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28



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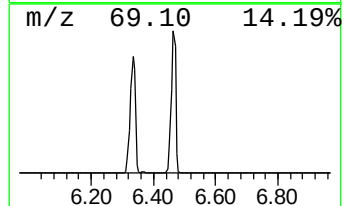
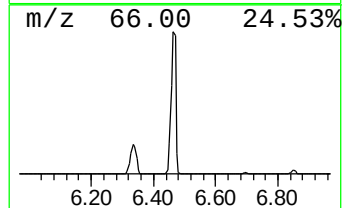
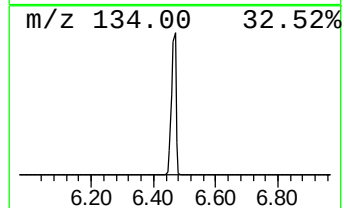
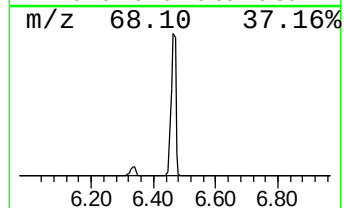
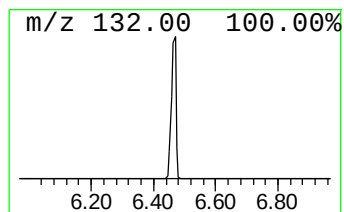
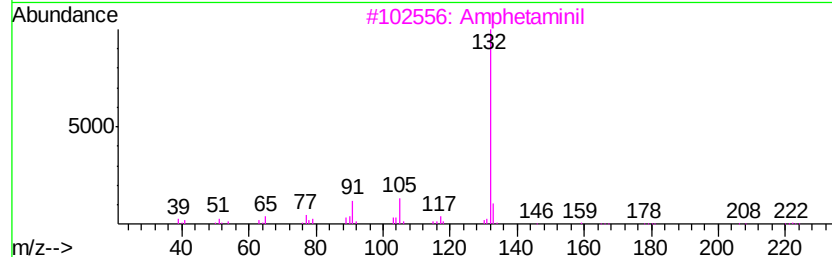
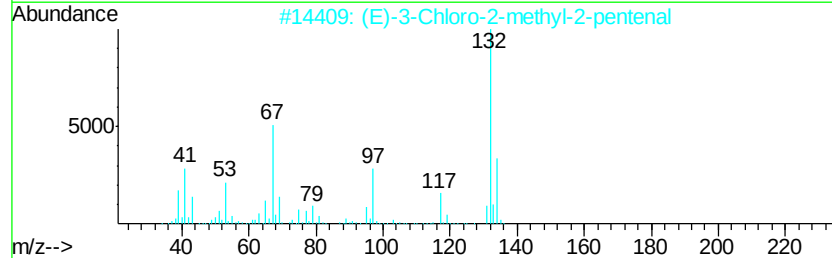
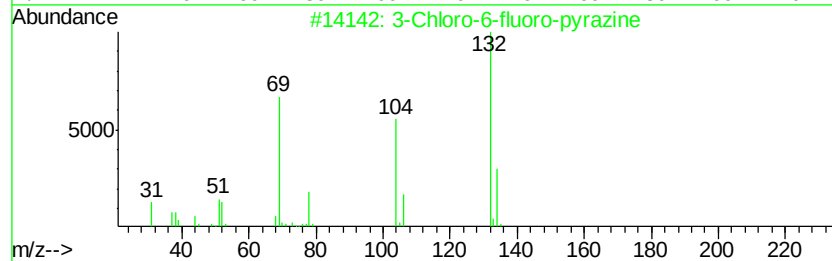
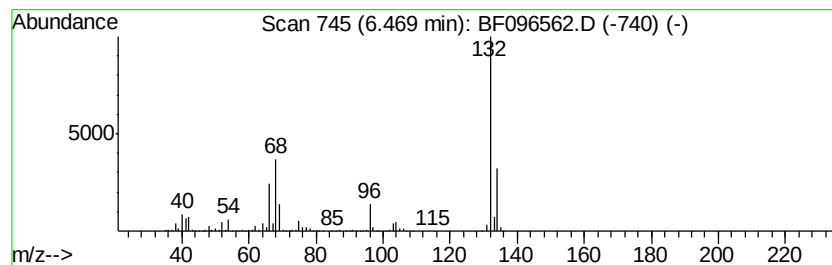
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	79.54 ng	2733280	1,4-Dichlorobenzene-d4	6.69

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		Amphetaminil	250	C17H18N2	017590-01-1	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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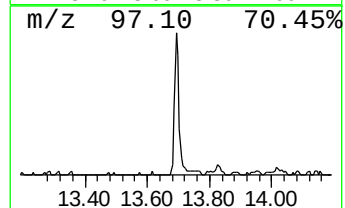
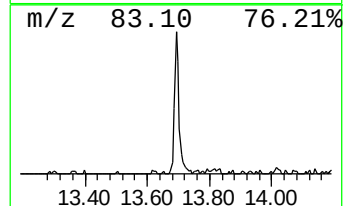
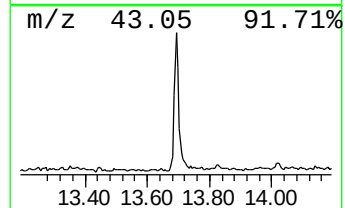
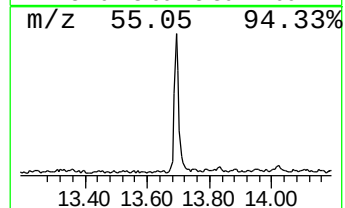
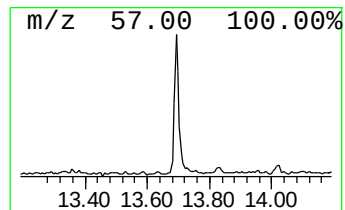
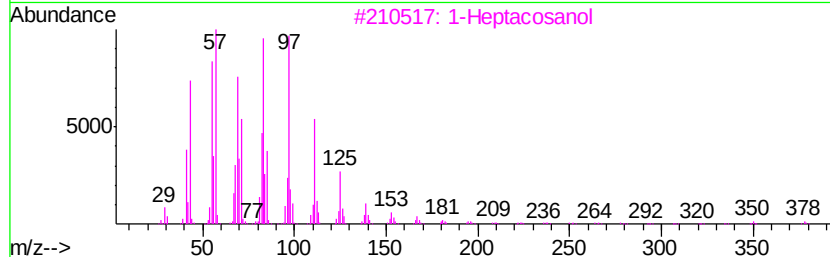
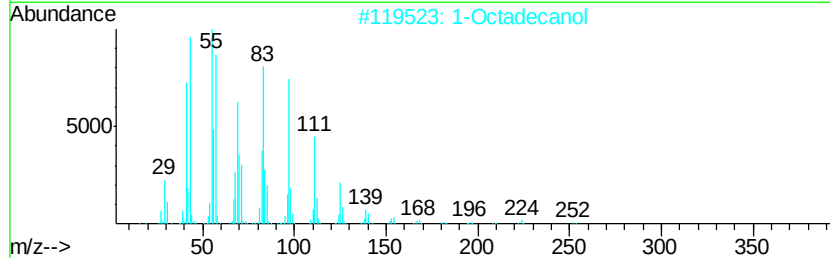
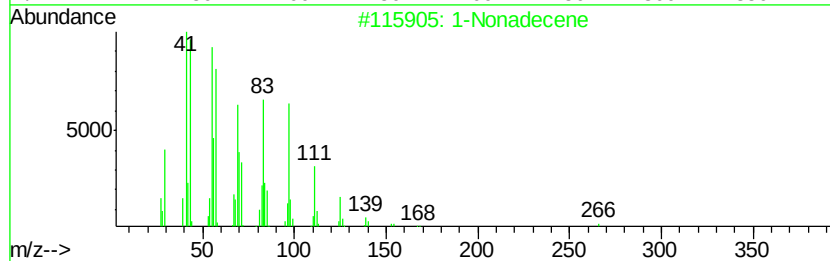
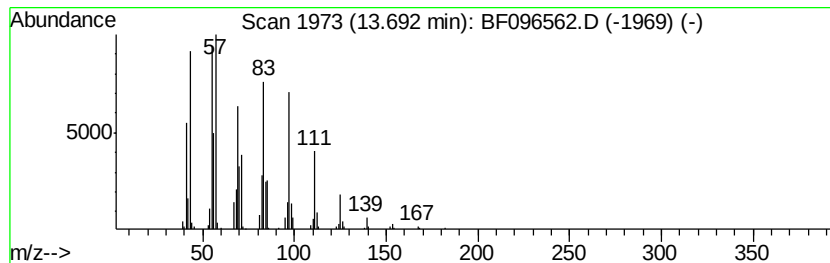
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Peak Number 4 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	6.86 ng	235002	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	1-Octadecanol	270	C18H38O	000112-92-5	90
3	1-Heptacosanol	396	C27H56O	002004-39-9	90
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90



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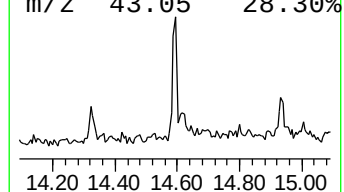
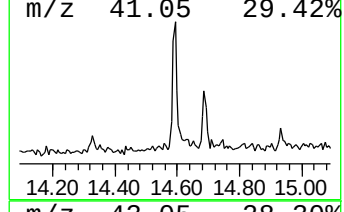
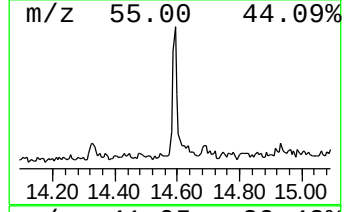
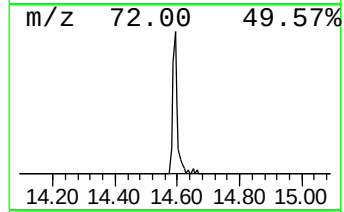
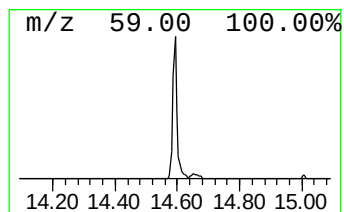
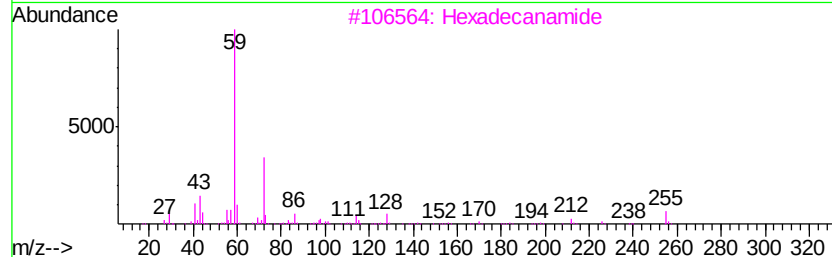
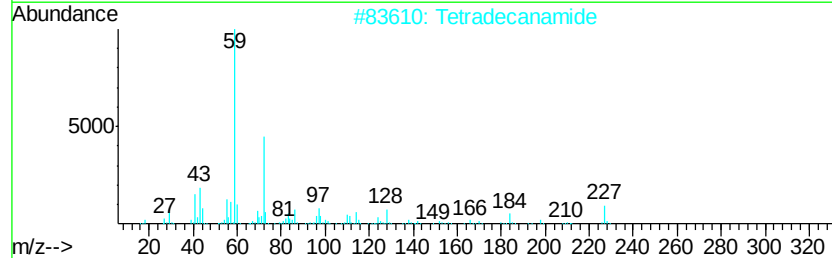
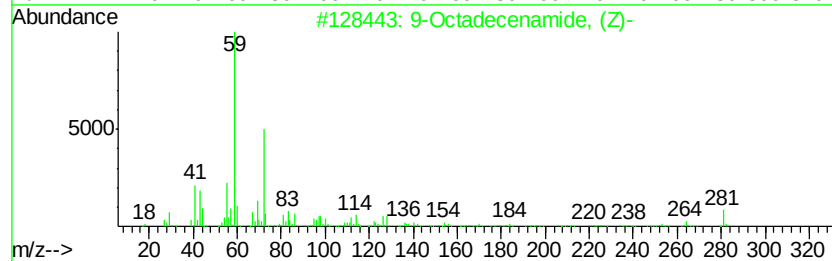
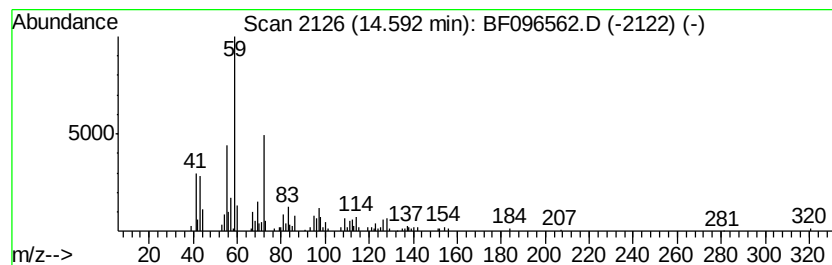
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.59	4.79 ng	125199	Perylene-d12	15.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Tetradecanamide	227	C14H29NO	000638-58-4	78
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	Dodecanamide	199	C12H25NO	001120-16-7	72
5	1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	16.8	ng	576542	1	6.69	687288	20.0
unknown6.47	6.47	79.5	ng	2733280	1	6.69	687288	20.0
1-Nonadecene	13.69	6.9	ng	235002	5	13.83	684918	20.0
9-Octadecenamide,...	14.59	4.8	ng	125199	6	15.23	522855	20.0