

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040419\
Data File : BF113609.D
Acq On : 5 Apr 2019 3:45
Operator : JU/SJ
Sample : K2240-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-(0-6)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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	3.616	253	260	270	rBV	124463	215520	8.69%	1.051%
2	5.298	542	546	565	rBV	2000384	2207138	88.99%	10.764%
3	6.334	718	722	739	rBV	2102713	2480336	100.00%	12.097%
4	6.457	739	743	759	rVB	2423125	2313002	93.25%	11.280%
5	6.686	778	782	792	rBV	732022	664314	26.78%	3.240%
6	6.839	804	808	823	rVB	1889048	1758262	70.89%	8.575%
7	7.251	874	878	890	rBV	1134616	1166070	47.01%	5.687%
8	7.969	996	1000	1007	rBV	863332	775783	31.28%	3.783%
9	9.039	1178	1182	1192	rBV	2621683	2257092	91.00%	11.008%
10	9.433	1246	1249	1254	rBV	264962	233657	9.42%	1.140%
11	9.716	1293	1297	1312	rVB	919619	793187	31.98%	3.868%
12	10.504	1427	1431	1448	rBV	1334124	1285849	51.84%	6.271%
13	11.198	1545	1549	1552	rBV	865129	767507	30.94%	3.743%
14	11.221	1552	1553	1557	rVB	47960	28018	1.13%	0.137%
15	11.704	1623	1635	1637	rBV7	20896	56823	2.29%	0.277%
16	11.733	1637	1640	1651	rVV2	116864	185429	7.48%	0.904%
17	12.404	1751	1754	1759	rBV	121997	133285	5.37%	0.650%
18	12.515	1771	1773	1777	rBV3	25225	31674	1.28%	0.154%
19	12.633	1790	1793	1796	rVB	104869	80345	3.24%	0.392%
20	12.774	1813	1817	1821	rBV	2096492	1837972	74.10%	8.964%
21	13.827	1992	1996	1999	rBV	600909	571935	23.06%	2.789%
22	14.568	2119	2122	2124	rBV	152157	155915	6.29%	0.760%
23	15.233	2232	2235	2242	rVB	400383	505378	20.38%	2.465%

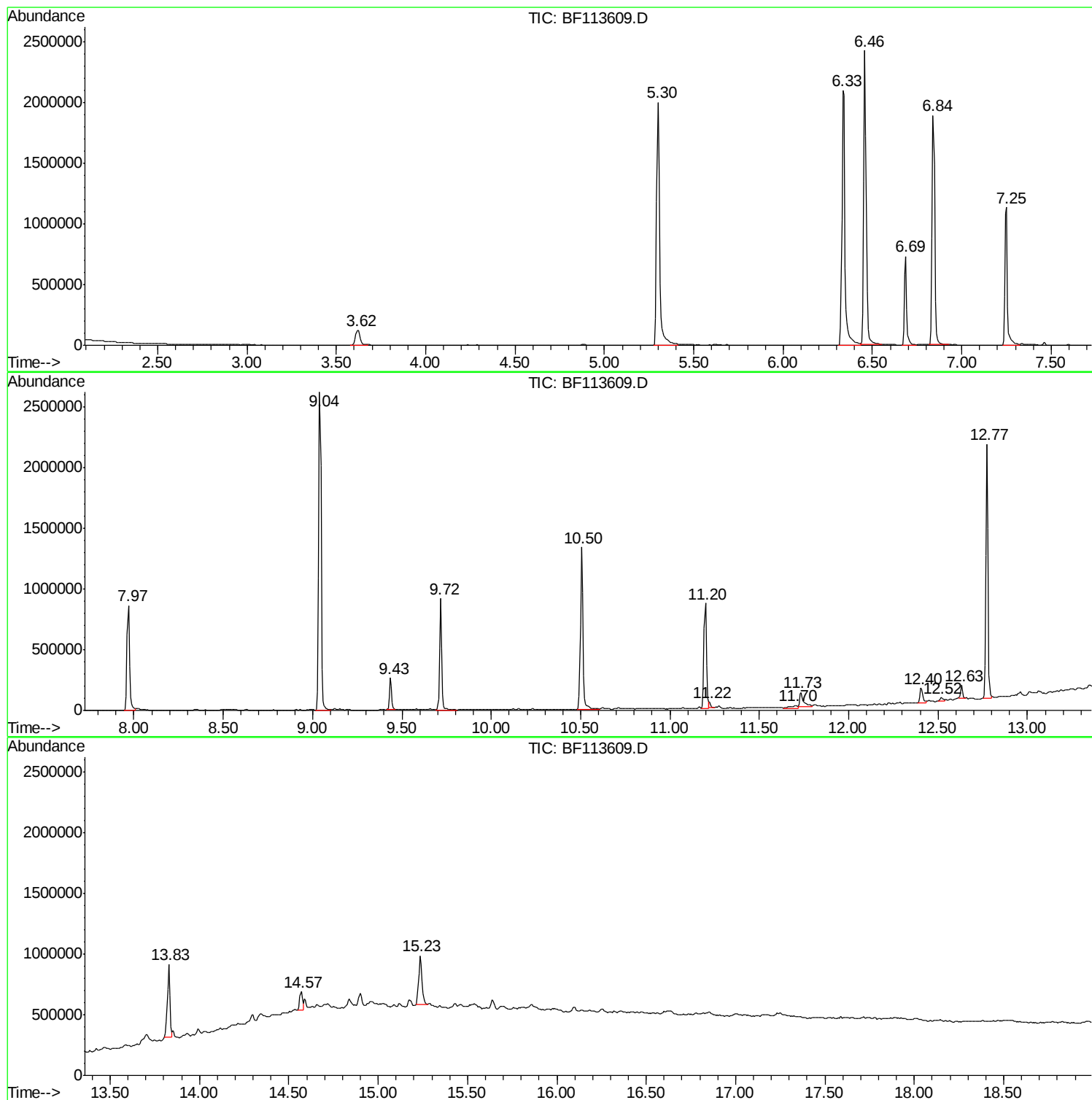
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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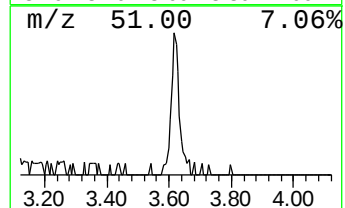
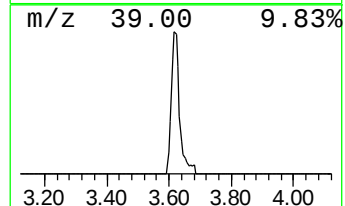
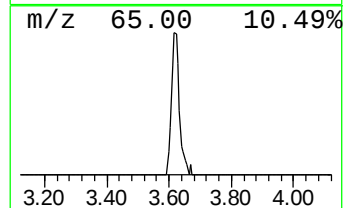
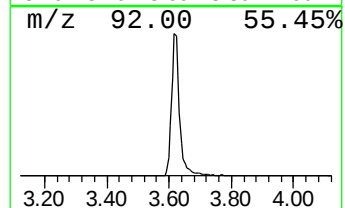
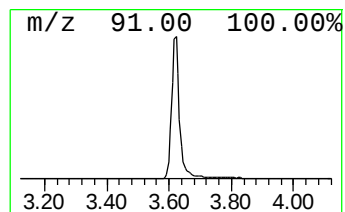
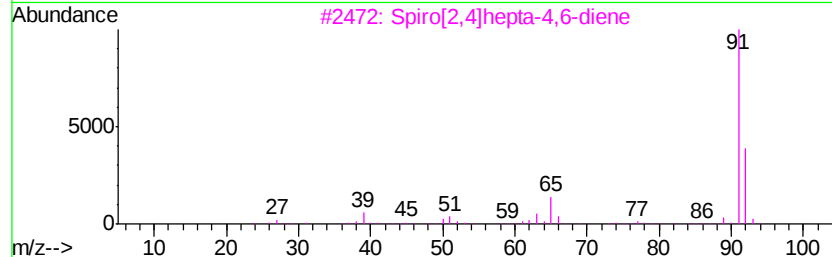
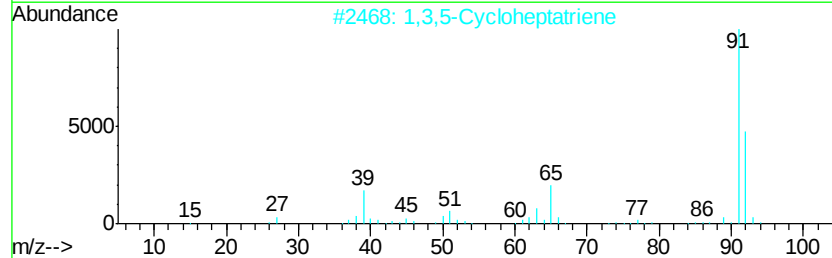
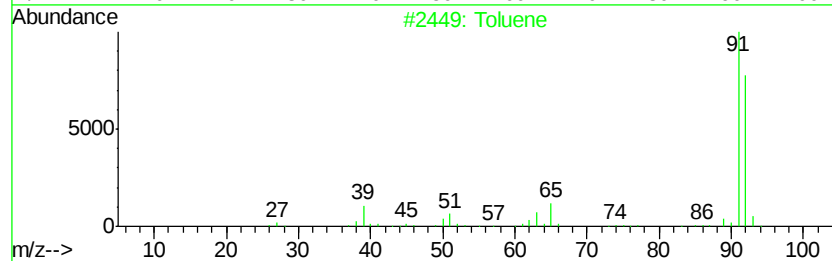
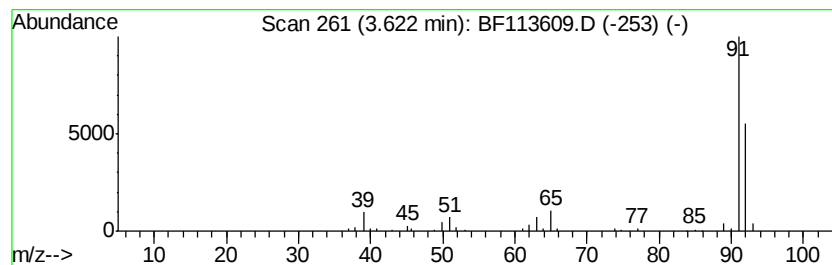
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.62	6.49 ng	215520	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Toluene	92	C7H8	000108-88-3	94
2			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
3			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	81
4			2,5-Norbornadiene	92	C7H8	000121-46-0	72
5			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64



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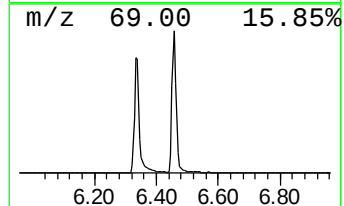
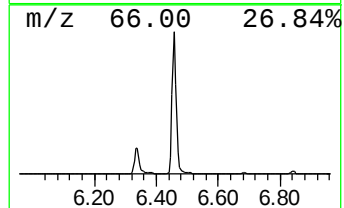
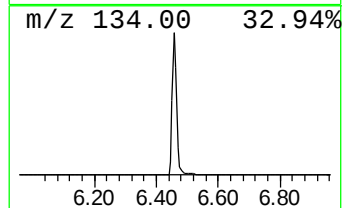
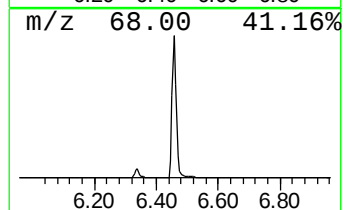
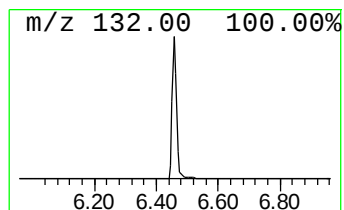
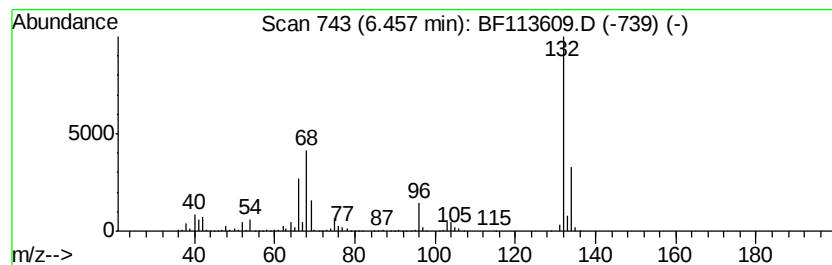
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	69.64 ng	2313000	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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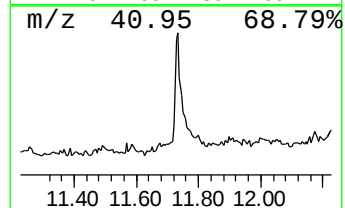
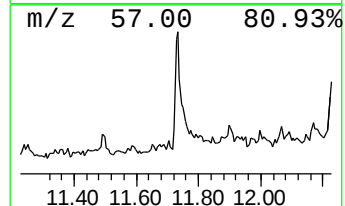
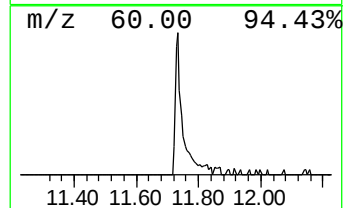
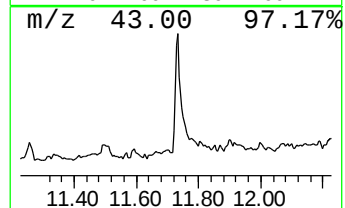
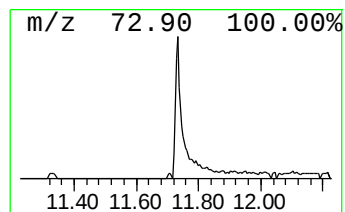
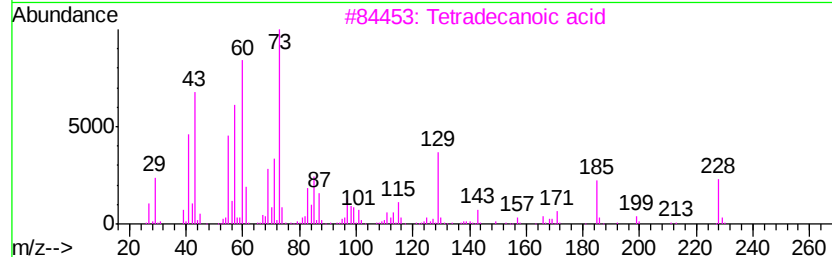
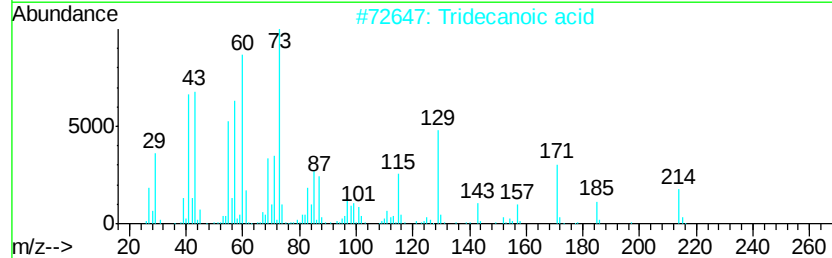
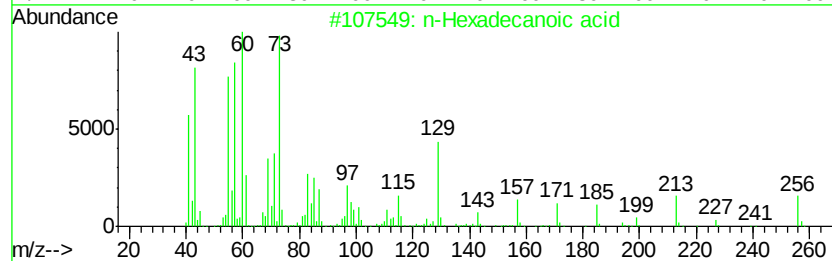
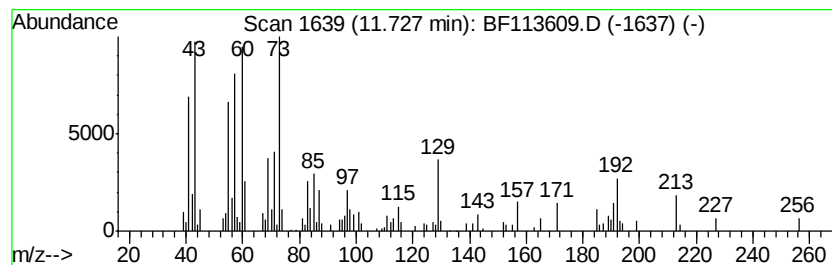
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	4.83 ng	185429	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Dodecanoic acid	200	C12H24O2	000143-07-7	64
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	62



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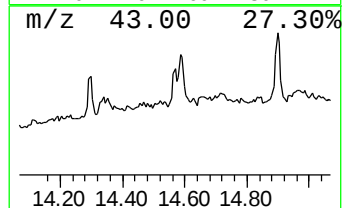
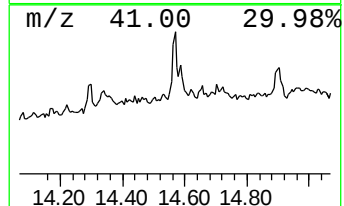
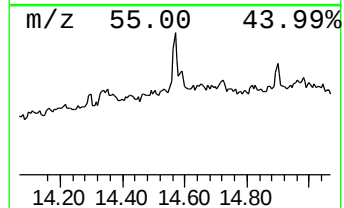
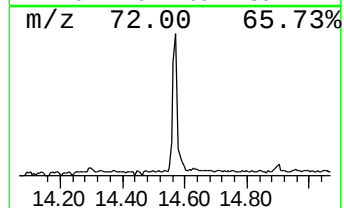
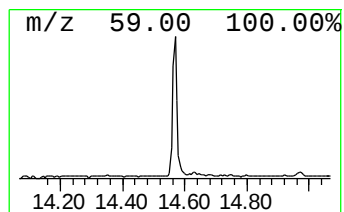
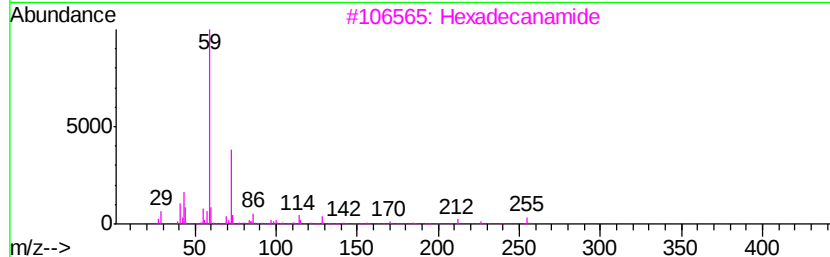
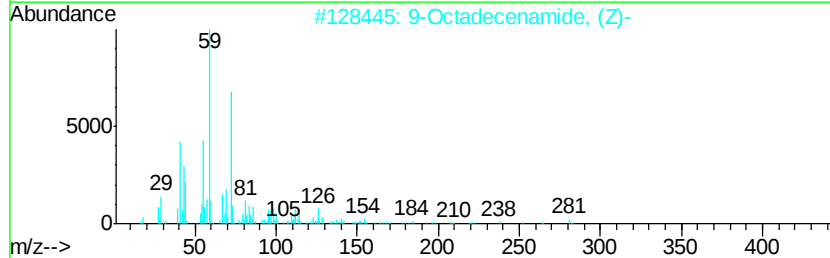
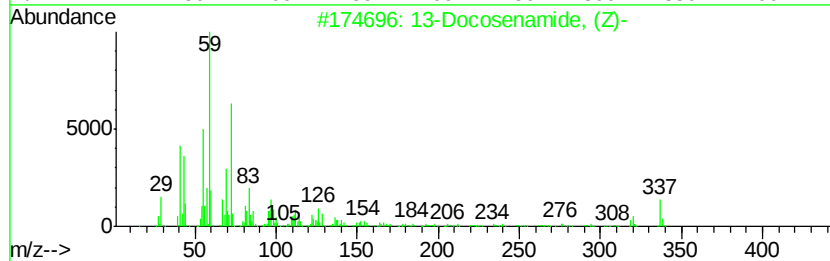
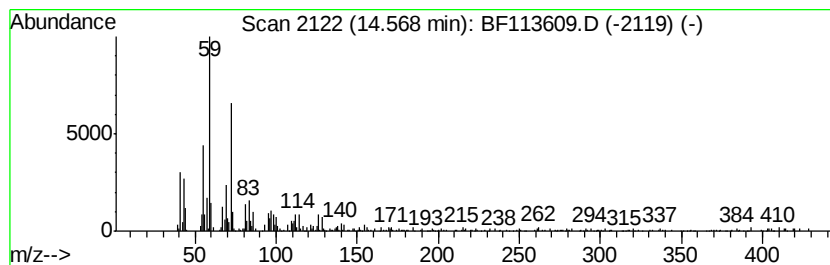
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	6.17 ng	155915	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
3		Hexadecanamide	255	C16H33NO	000629-54-9	72
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	72
5		Dodecanamide	199	C12H25NO	001120-16-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3,5-Cycloheptat...	3.62	6.5	ng	215520	1	6.69	664314	20.0
unknown6.46	6.46	69.6	ng	2313000	1	6.69	664314	20.0
n-Hexadecanoic acid	11.73	4.8	ng	185429	4	11.20	767507	20.0
13-Docosenamide, ...	14.57	6.2	ng	155915	6	15.23	505378	20.0