

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
 Data File : BF092369.D
 Acq On : 20 Jan 2017 13:27
 Operator : UM/SJ
 Sample : I1265-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-4WS

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-BF122116.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	4.621	246	248	260	rBV	326923	486708	7.14%	1.076%
2	5.101	288	290	311	rVB	2172693	2416061	35.46%	5.340%
3	6.187	382	385	392	rBV	1434403	2184510	32.06%	4.828%
4	6.290	392	394	397	rVV	5121331	4781169	70.18%	10.568%
5	6.519	412	414	417	rBV	1349810	1237086	18.16%	2.734%
6	6.679	425	428	430	rBV	3950645	4551151	66.80%	10.059%
7	7.102	462	465	467	rBV	3034526	3989676	58.56%	8.818%
8	7.810	524	527	529	rBV	1658474	1696163	24.90%	3.749%
9	8.896	618	622	624	rBV	4584099	6812810	100.00%	15.058%
10	9.296	654	657	659	rBV	152526	153493	2.25%	0.339%
11	9.559	677	680	682	rBV	1566375	1934804	28.40%	4.276%
12	10.005	710	719	721	rBV2	89647	123855	1.82%	0.274%
13	10.348	746	749	751	rBV	3552048	3807285	55.88%	8.415%
14	10.473	758	760	764	rVB	96877	129666	1.90%	0.287%
15	10.919	797	799	801	rBV	86669	94926	1.39%	0.210%
16	11.033	806	809	811	rBV	1886919	1858926	27.29%	4.109%
17	11.593	855	858	865	rBV2	135213	216736	3.18%	0.479%
18	12.371	924	926	932	rBV	134368	182887	2.68%	0.404%
19	12.622	945	948	950	rBV	5258250	5711779	83.84%	12.624%
20	13.571	1029	1031	1037	rBV	60983	143888	2.11%	0.318%
21	13.662	1037	1039	1042	rBV	1416324	1544199	22.67%	3.413%
22	15.011	1154	1157	1165	rVB	875240	1186199	17.41%	2.622%

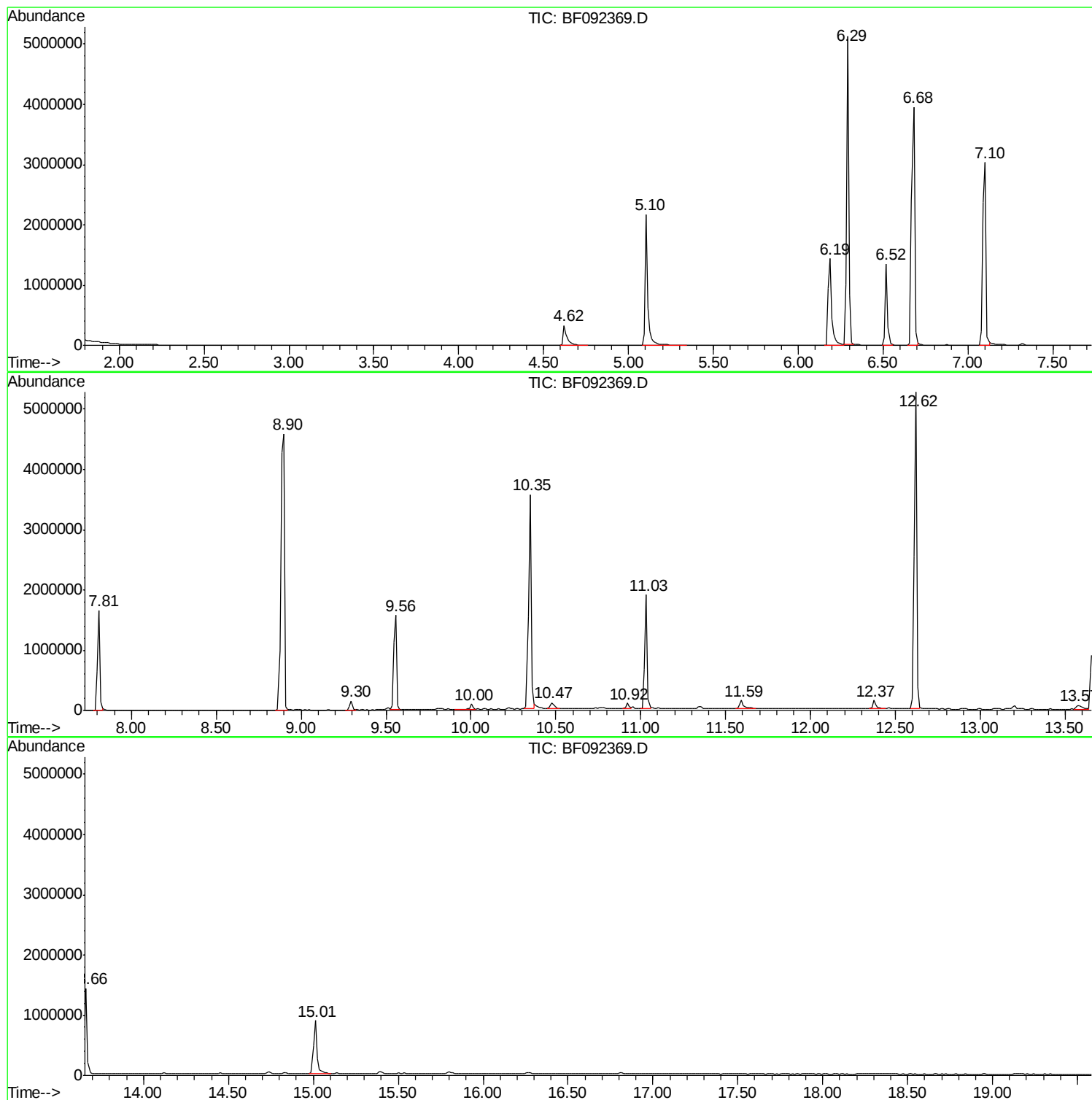
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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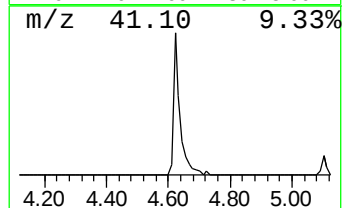
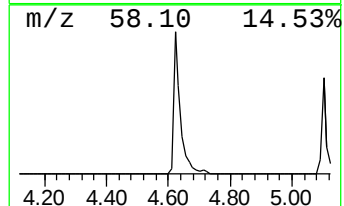
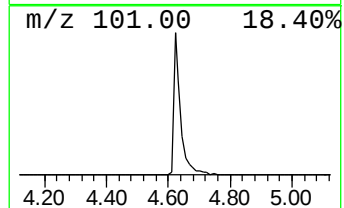
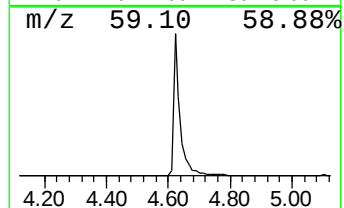
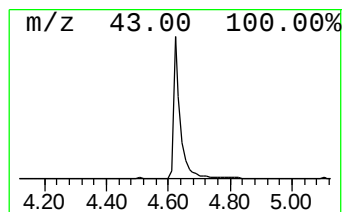
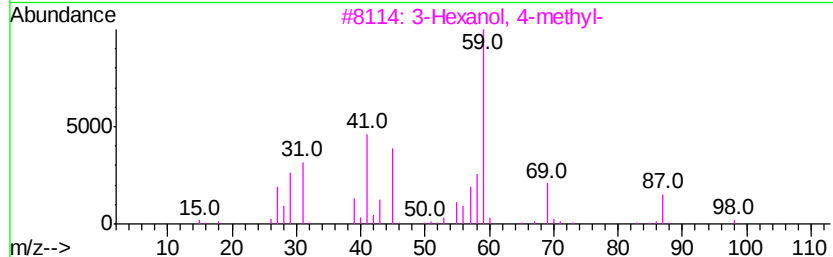
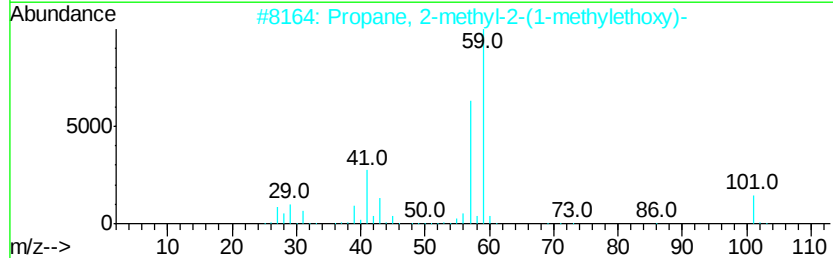
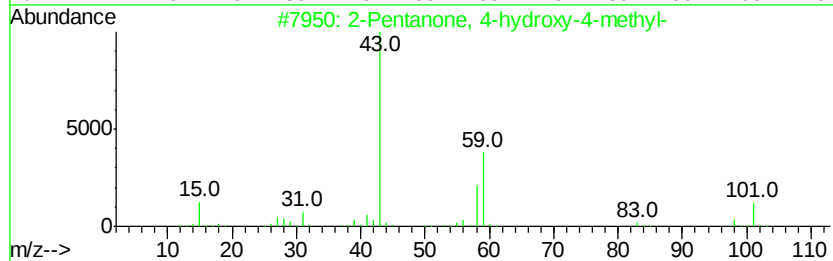
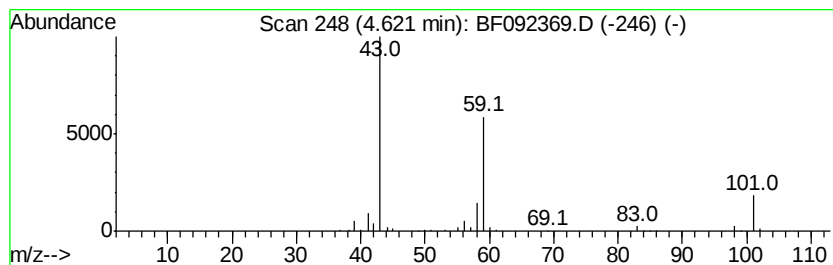
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.62	7.87 ng	486708	1,4-Dichlorobenzene-d4	6.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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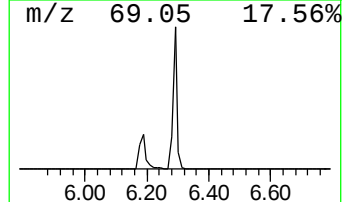
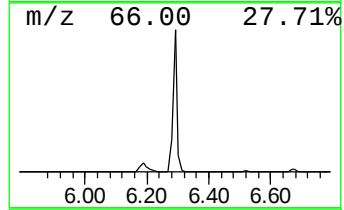
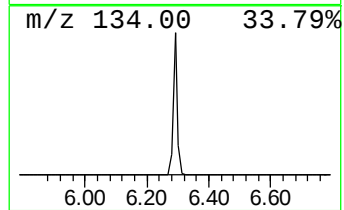
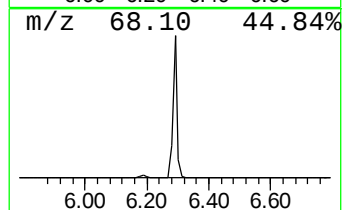
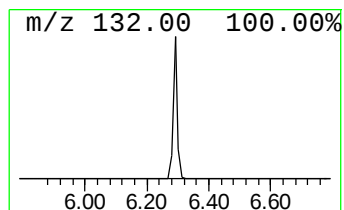
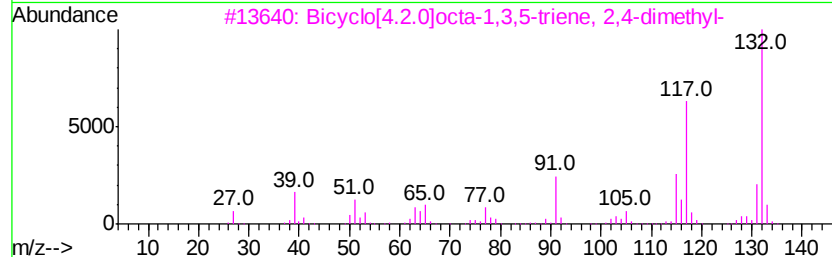
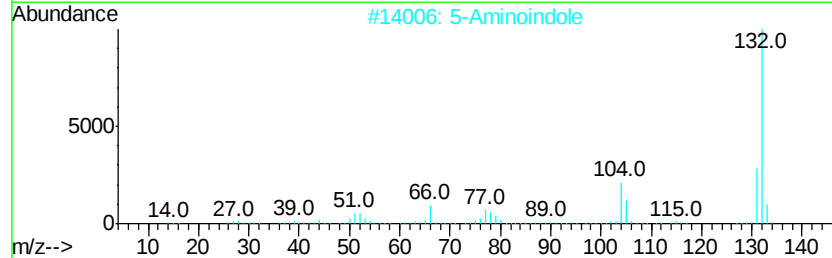
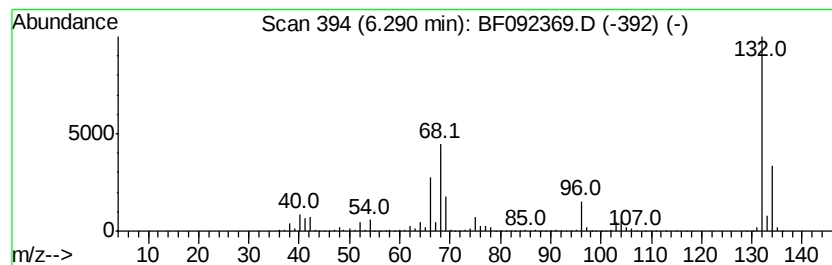
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Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	77.30 ng	4781170	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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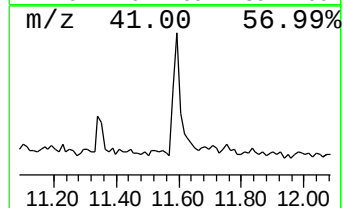
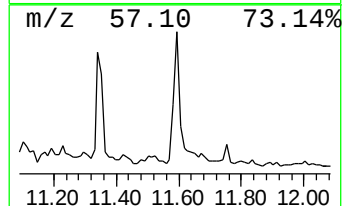
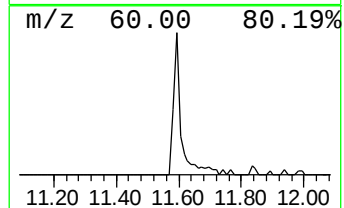
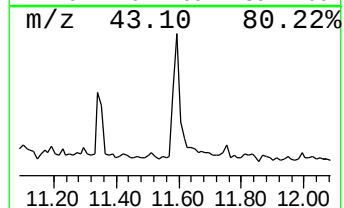
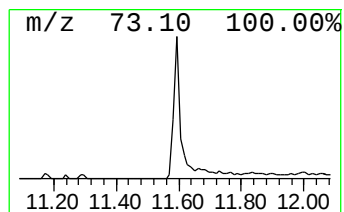
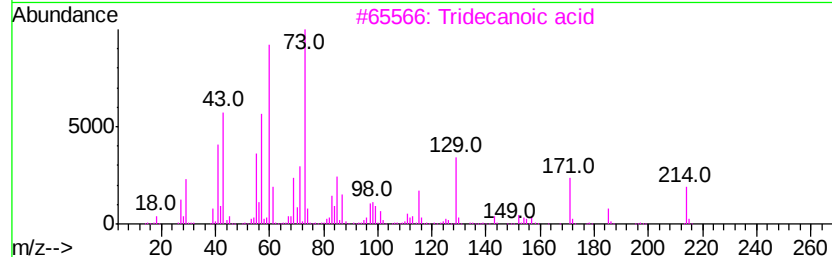
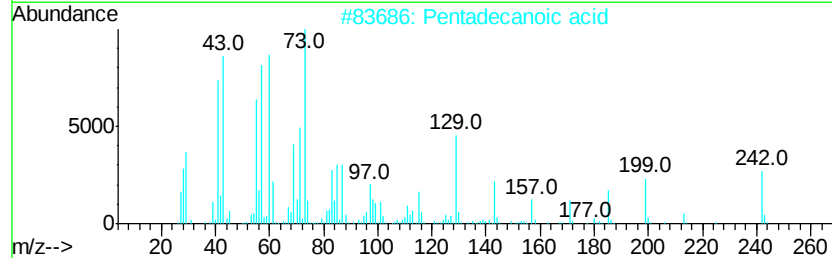
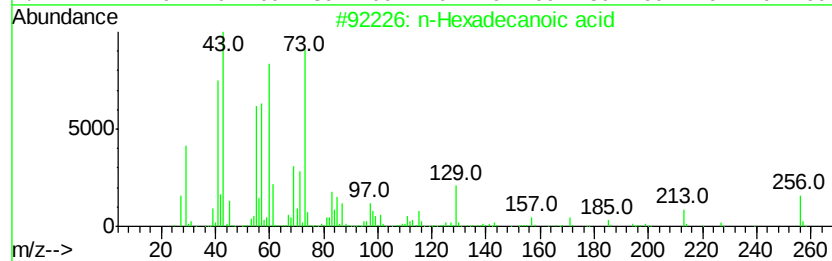
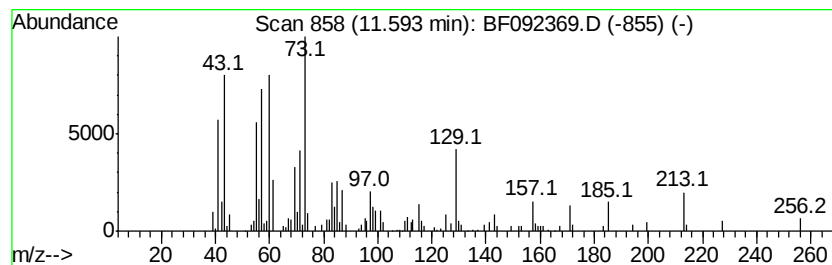
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.33 ng	216736	Phenanthrene-d10	11.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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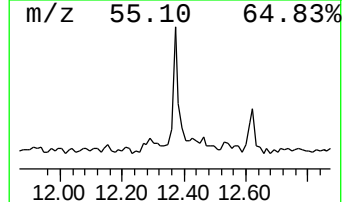
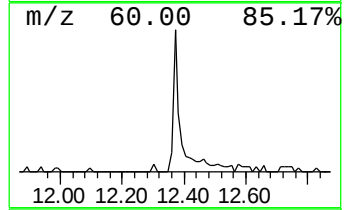
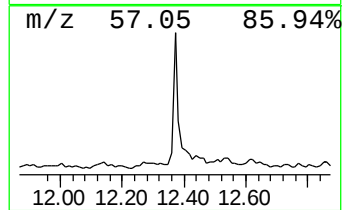
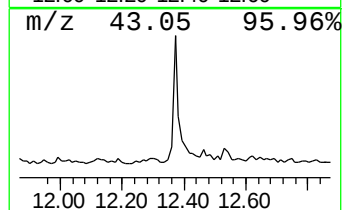
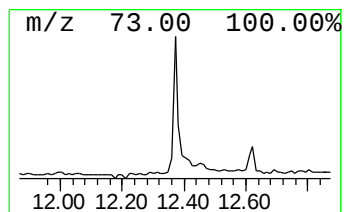
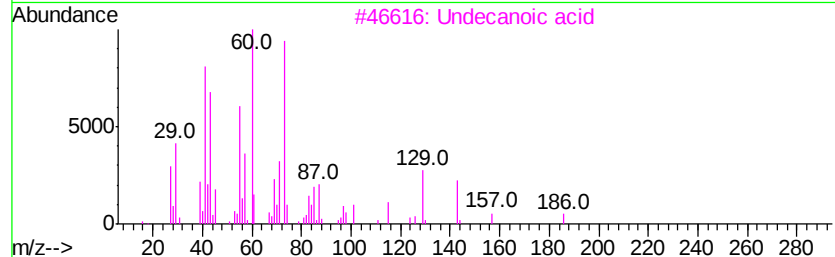
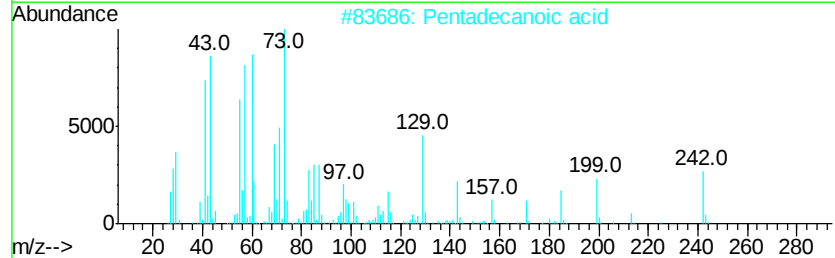
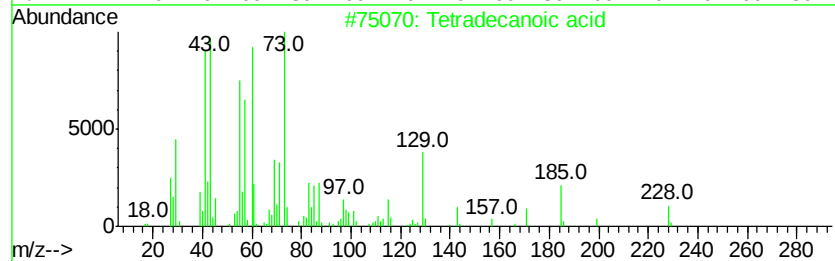
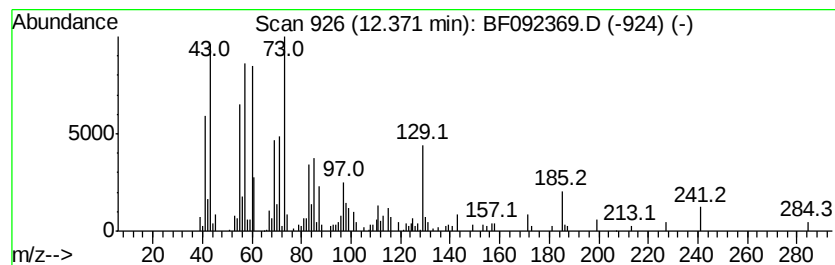
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Peak Number 5 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	2.37 ng	182887	Chrysene-d12	13.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecanoic acid	228 C14H28O2	000544-63-8 83
2		Pentadecanoic acid	242 C15H30O2	001002-84-2 80
3		Undecanoic acid	186 C11H22O2	000112-37-8 46
4		Ethanone, 1-(4,5-dihydro-2-thiaz...	129 C5H7NOS	029926-41-8 38
5		N-Cyclooct-4-enylacetamide	167 C10H17NO	170952-69-9 25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.62	7.9	ng	486708	1	6.52	1237090	20.0
unknown6.29	6.29	77.3	ng	4781170	1	6.52	1237090	20.0
n-Hexadecanoic acid	11.59	2.3	ng	216736	4	11.03	1858930	20.0
Tetradecanoic acid	12.37	2.4	ng	182887	5	13.66	1544200	20.0