

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
 Data File : BF094955.D
 Acq On : 6 May 2017 11:53
 Operator : SJ/MA
 Sample : I2947-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-7.0-7.5

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-BF050217.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	5.037	523	527	546	rBV	229973	450620	18.25%	2.252%
2	5.666	630	634	659	rBV	1211858	1924503	77.95%	9.618%
3	7.260	900	905	921	rBV	1379041	1915745	77.60%	9.575%
4	7.383	921	926	941	rVB	1528391	2177445	88.20%	10.883%
5	7.725	980	984	998	rVB	433823	536791	21.74%	2.683%
6	7.960	1019	1024	1037	rBV	1421880	1645167	66.64%	8.222%
7	8.619	1131	1136	1156	rBV	840295	1174229	47.56%	5.869%
8	9.742	1322	1327	1350	rBV	496351	715847	29.00%	3.578%
9	11.513	1623	1628	1647	rBV	1913549	2468819	100.00%	12.339%
10	12.207	1742	1746	1758	rBV	191355	261836	10.61%	1.309%
11	12.571	1803	1808	1823	rBV2	535492	764705	30.97%	3.822%
12	13.413	1947	1951	1956	rBV	35283	40506	1.64%	0.202%
13	13.865	2023	2028	2043	rBV	849486	1371691	55.56%	6.856%
14	14.189	2078	2083	2086	rBV	33515	40399	1.64%	0.202%
15	14.971	2211	2216	2230	rBV2	486002	729786	29.56%	3.647%
16	15.936	2376	2380	2393	rBV	50876	78986	3.20%	0.395%
17	17.030	2562	2566	2573	rBV2	18648	31357	1.27%	0.157%
18	17.295	2606	2611	2620	rBV	1837863	2178670	88.25%	10.889%
19	18.600	2827	2833	2835	rBV4	14590	26780	1.08%	0.134%
20	18.636	2835	2839	2860	rVB	460898	752430	30.48%	3.761%
21	20.053	3076	3080	3088	rBV	78880	88130	3.57%	0.440%
22	20.306	3119	3123	3135	rBV	340158	495237	20.06%	2.475%
23	20.777	3198	3203	3209	rBV	103295	138918	5.63%	0.694%

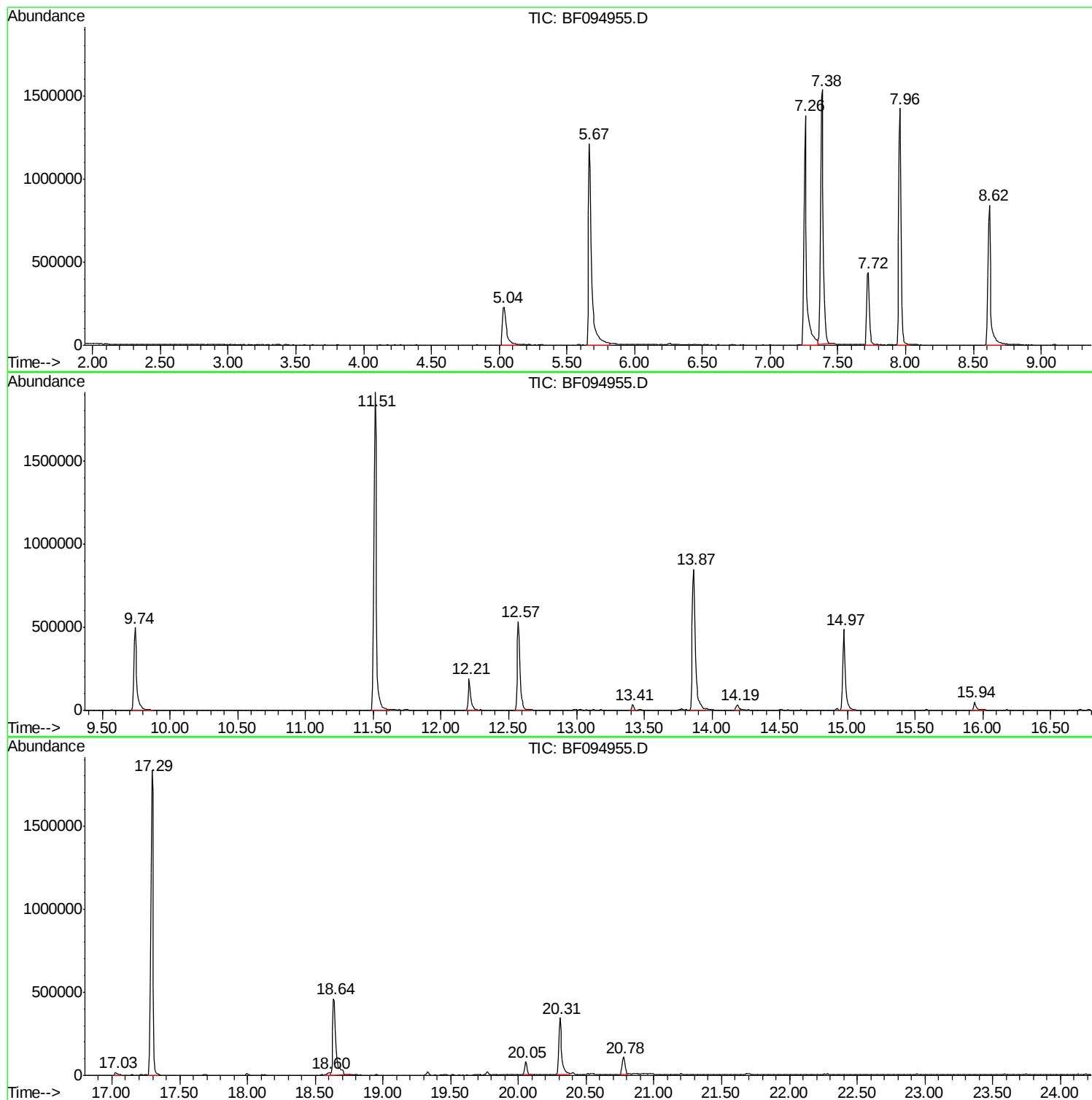
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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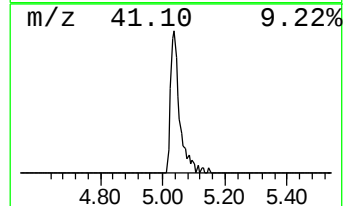
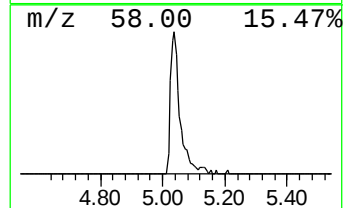
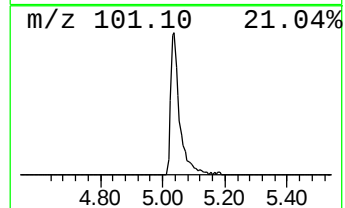
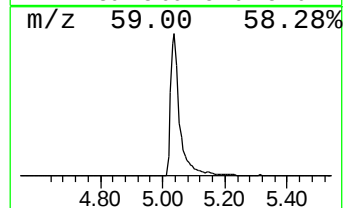
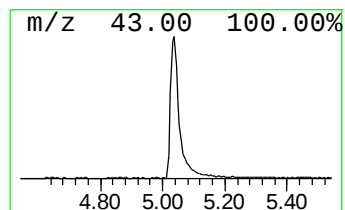
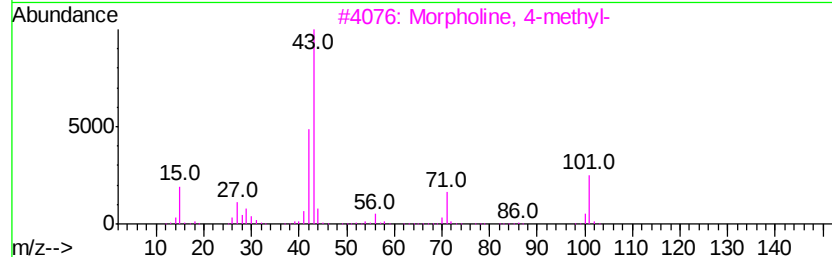
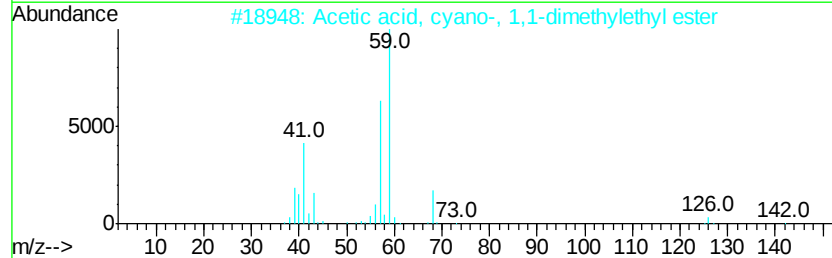
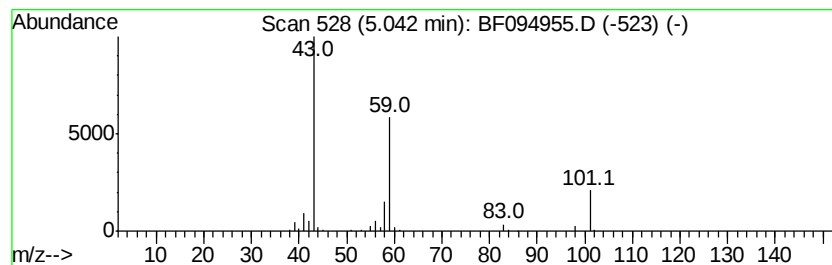
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	16.79 ng	450620	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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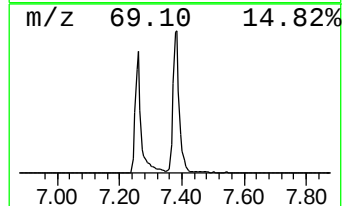
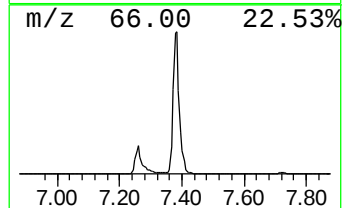
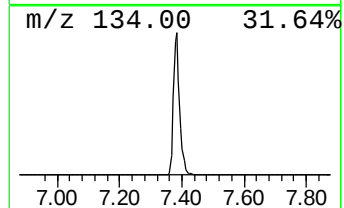
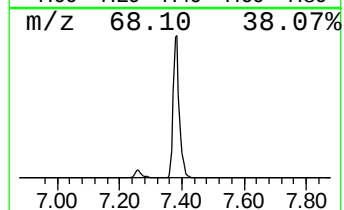
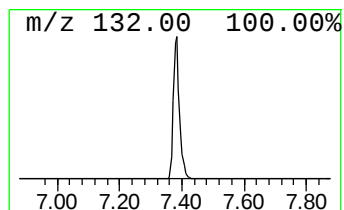
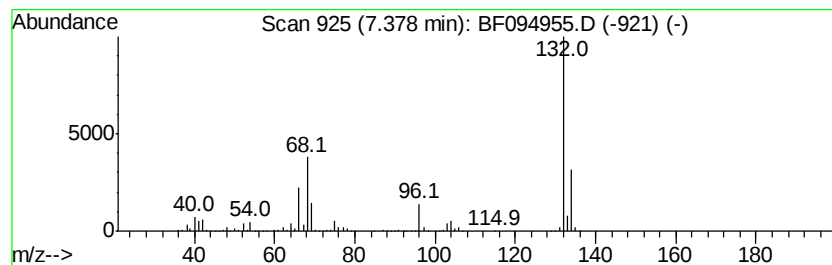
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	81.13 ng	2177450	1,4-Dichlorobenzene-d4	7.72

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		Tranvlcypropane-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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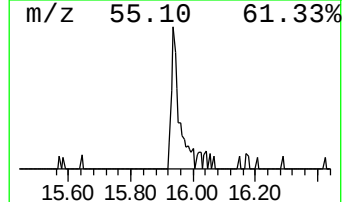
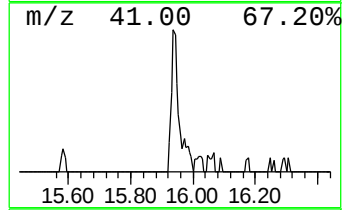
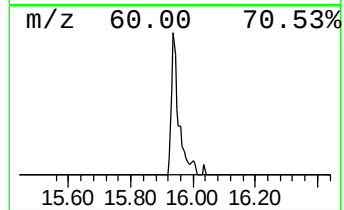
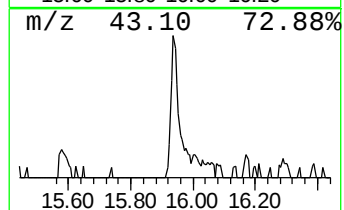
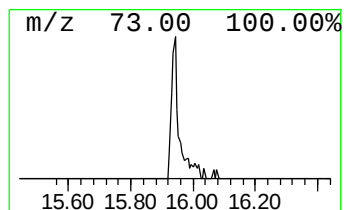
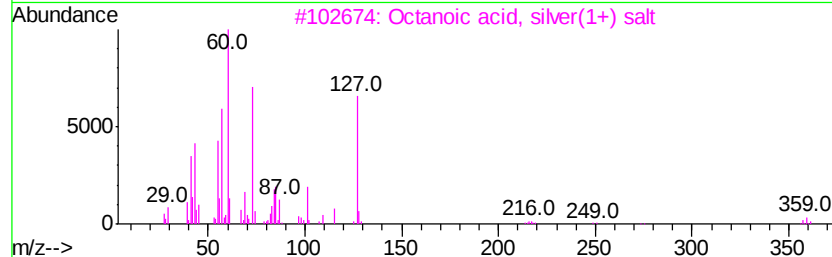
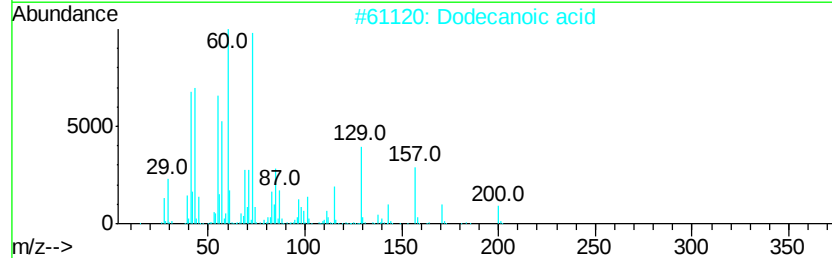
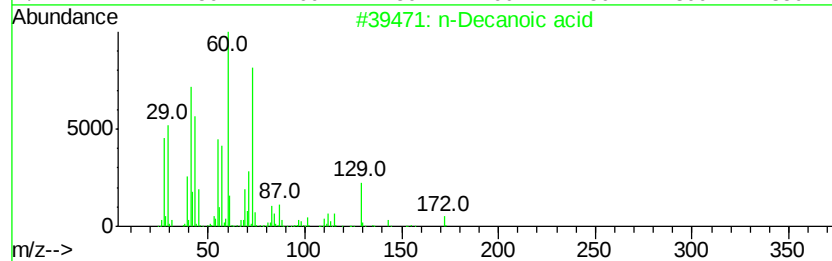
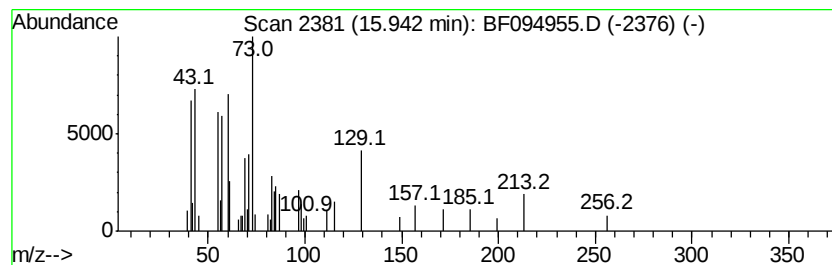
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Peak Number 4 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.16 ng	78986	Phenanthrene-d10	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	53
2		Dodecanoic acid	200	C12H24O2	000143-07-7	50
3		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	35
4		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	11
5		Pentadecane	212	C15H32	000629-62-9	10



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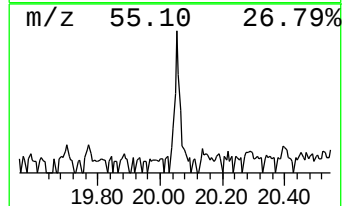
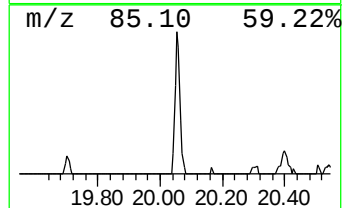
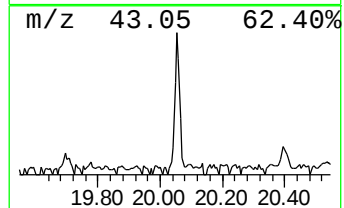
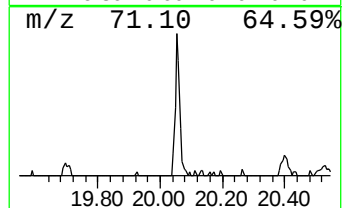
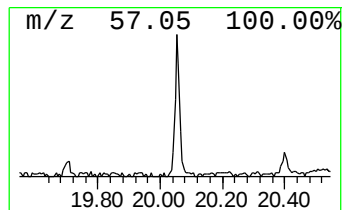
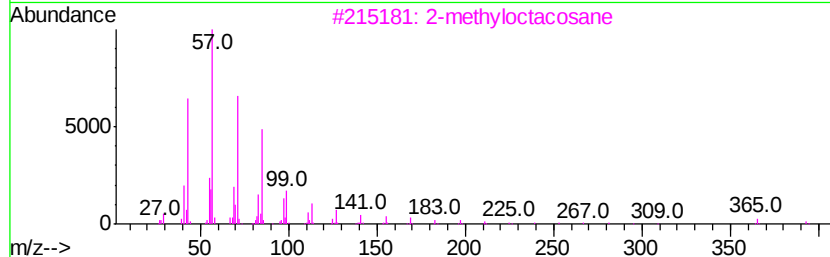
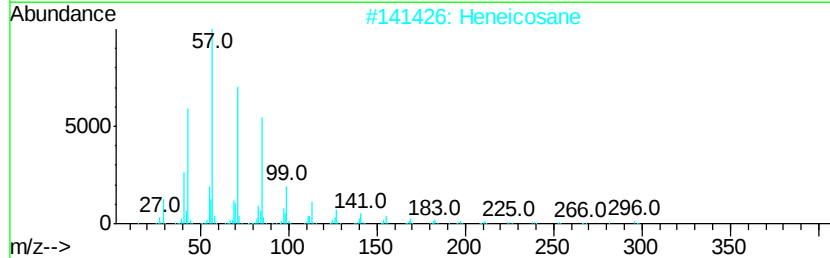
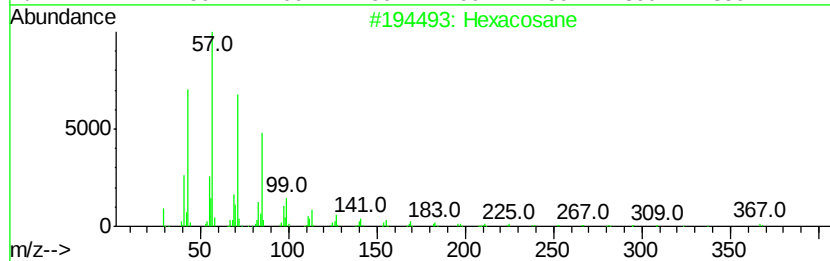
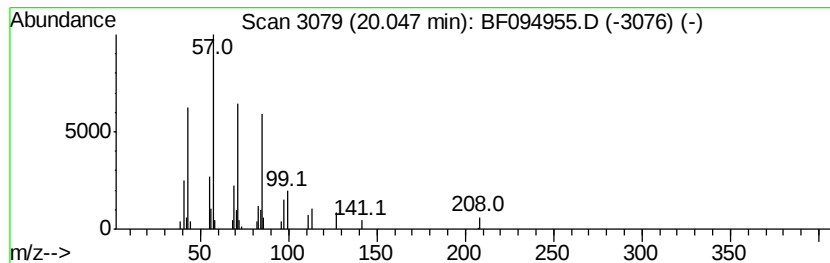
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Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.05	3.56 ng	88130	Perylene-d12	20.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Octadecane		254	C18H38	000593-45-3	91



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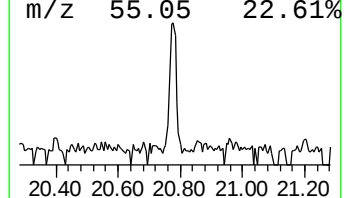
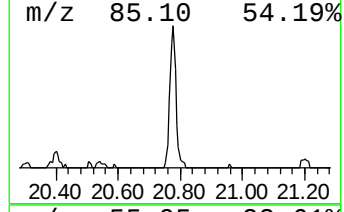
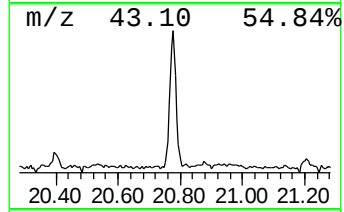
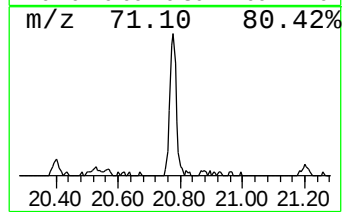
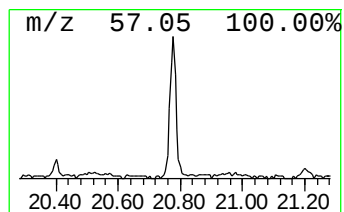
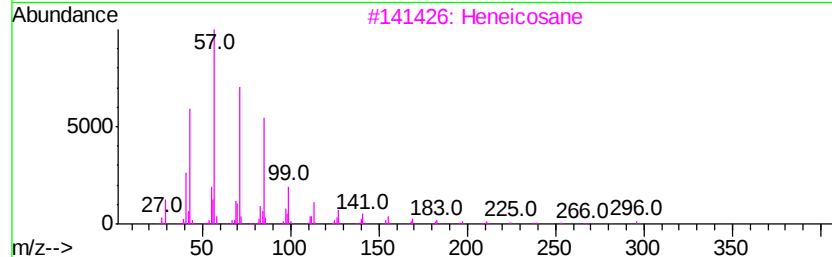
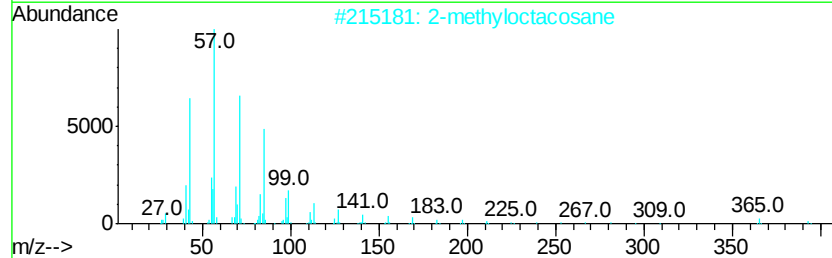
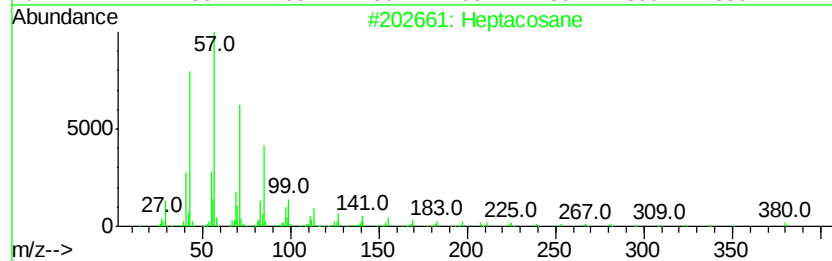
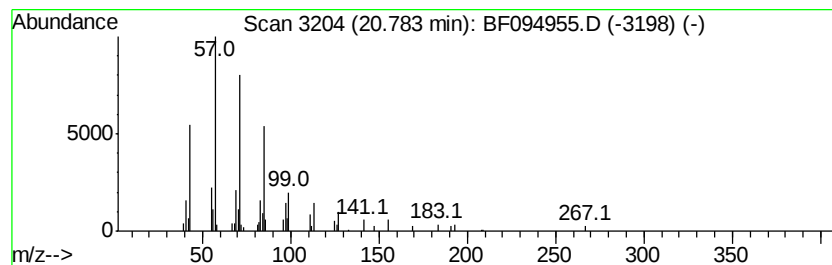
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Peak Number 6 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	5.61 ng	138918	Perylene-d12	20.31

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			triacontane	422	C30H62	000638-68-6	91
5			Hexacosane	366	C26H54	000630-01-3	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	16.8	ng	450620	1	7.72	536791	20.0
unknown7.38	7.38	81.1	ng	2177450	1	7.72	536791	20.0
n-Decanoic acid	15.94	2.2	ng	78986	4	14.97	729786	20.0
Hexacosane	20.05	3.6	ng	88130	6	20.31	495237	20.0
Heptacosane	20.78	5.6	ng	138918	6	20.31	495237	20.0