

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
 Data File : BG031740.D
 Acq On : 23 Dec 2017 9:32
 Operator : SJ/JU
 Sample : I7040-06
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PZ-4

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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	3.447	20	27	38	rBV	77610	179410	4.10%	0.982%
2	3.541	38	43	50	rVB	28428	48208	1.10%	0.264%
3	6.238	495	502	511	rBV	294584	514418	11.75%	2.817%
4	7.919	781	788	800	rVB	189961	353459	8.07%	1.935%
5	8.336	849	859	869	rBV	610697	1141162	26.06%	6.248%
6	8.823	935	942	951	rVB	139812	248659	5.68%	1.361%
7	9.164	991	1000	1011	rBV	610449	1154591	26.36%	6.322%
8	10.022	1136	1146	1157	rBV	431027	815365	18.62%	4.464%
9	11.714	1426	1434	1445	rBV	200010	374519	8.55%	2.051%
10	14.088	1830	1838	1850	rBV	1766189	2828009	64.57%	15.484%
11	15.457	2065	2071	2078	rVB2	370648	647949	14.79%	3.548%
12	16.932	2314	2322	2329	rBV	1481552	2333344	53.28%	12.776%
13	18.195	2530	2537	2544	rBV	496727	802773	18.33%	4.395%
14	19.011	2671	2676	2681	rBV2	75785	109144	2.49%	0.598%
15	20.251	2881	2887	2898	rBV2	125612	203466	4.65%	1.114%
16	20.727	2961	2968	2975	rBV	3170371	4379621	100.00%	23.980%
17	21.638	3117	3123	3132	rBV	86967	135761	3.10%	0.743%
18	22.549	3269	3278	3287	rBV2	521576	983547	22.46%	5.385%
19	26.332	3907	3922	3938	rBV2	310452	1010484	23.07%	5.533%

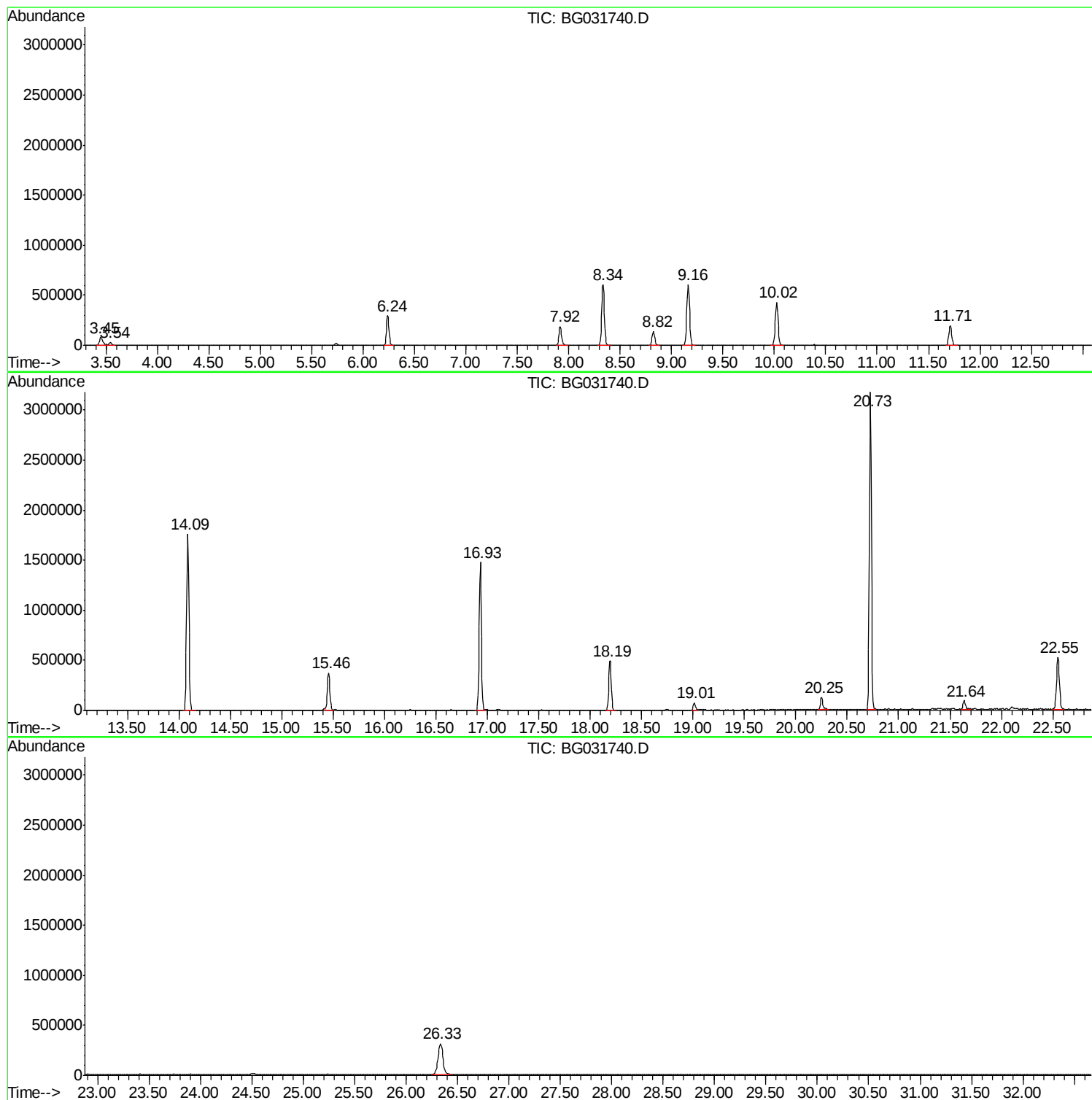
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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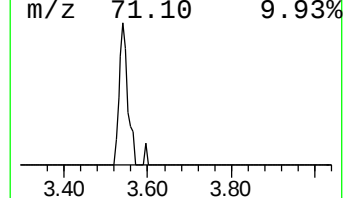
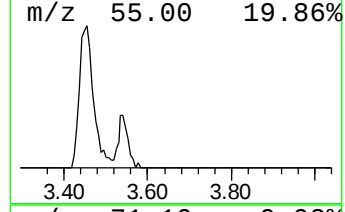
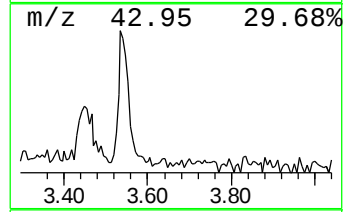
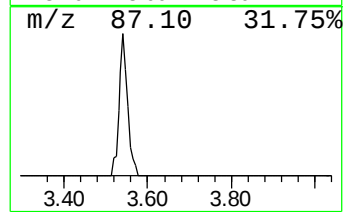
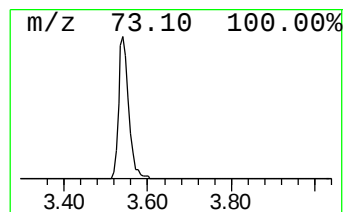
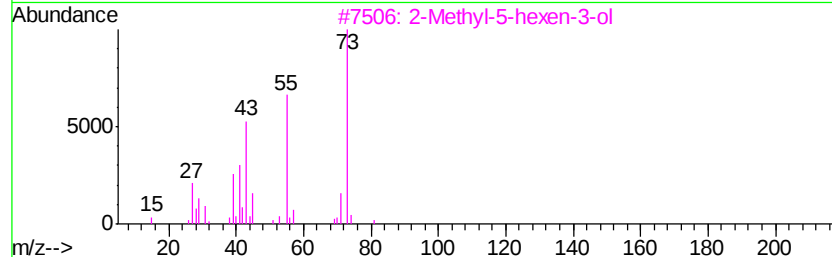
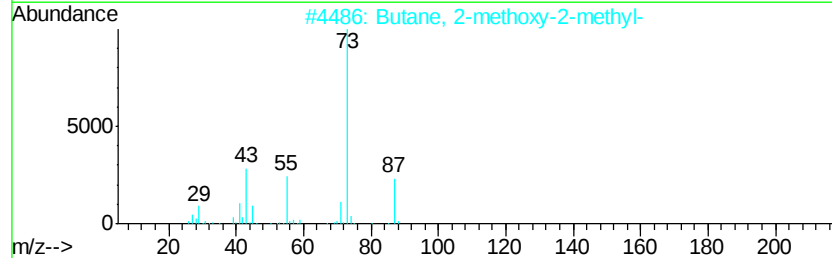
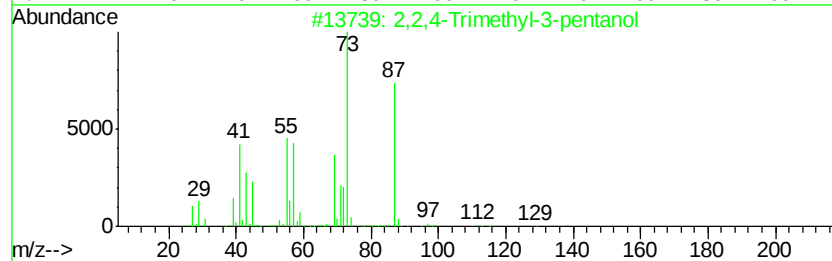
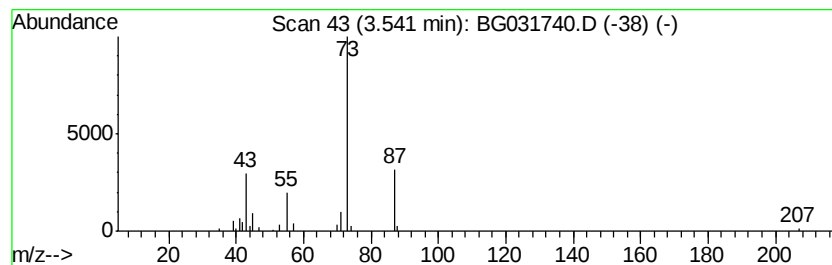
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.54 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	3.88 ng	48208	1,4-Dichlorobenzene-d4	8.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	42		
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	38		
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16		
4	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9		
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9		



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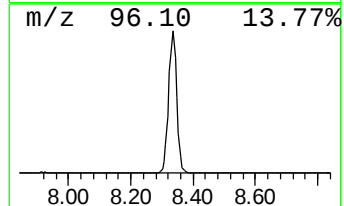
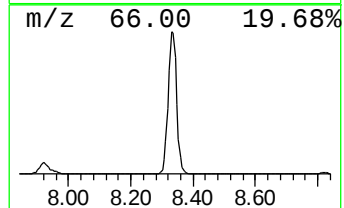
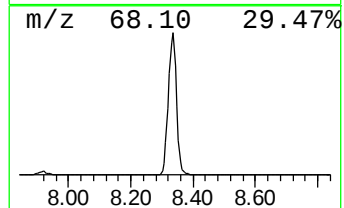
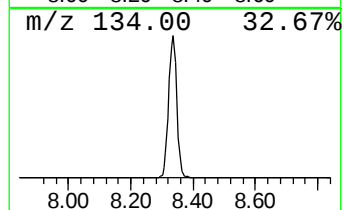
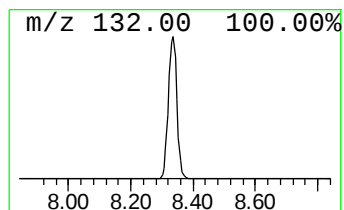
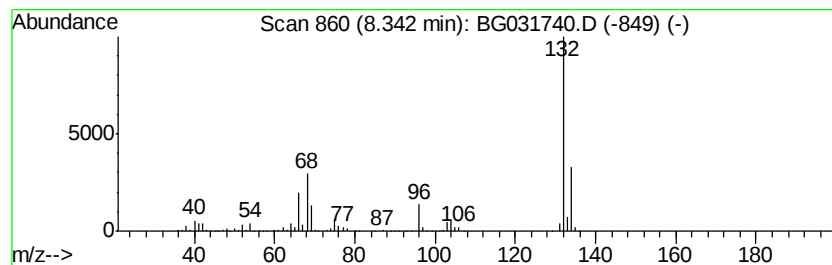
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	91.79 ng	1141160	1,4-Dichlorobenzene-d4	8.82

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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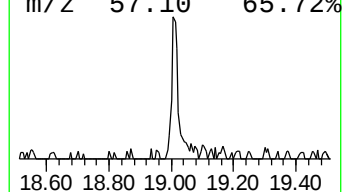
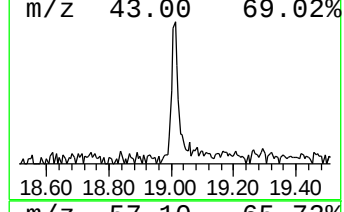
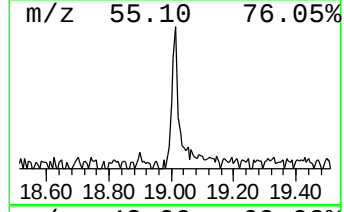
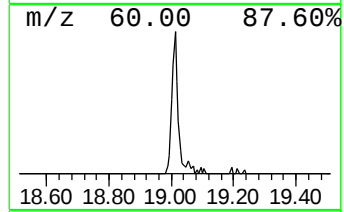
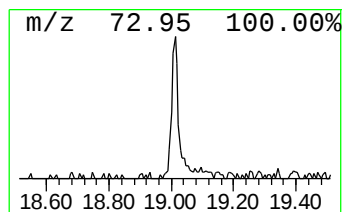
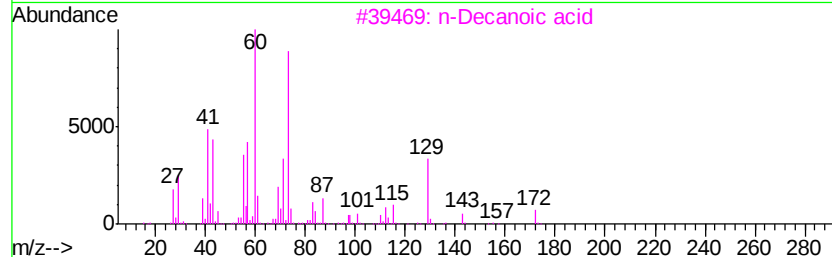
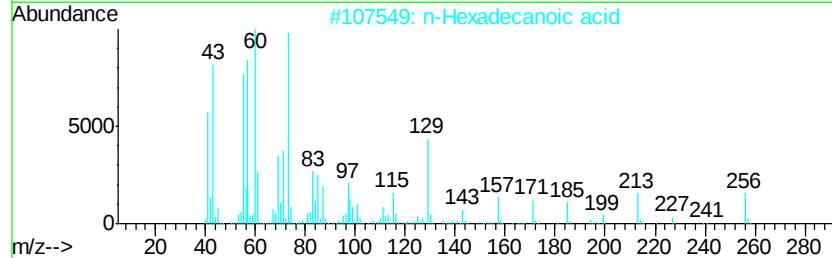
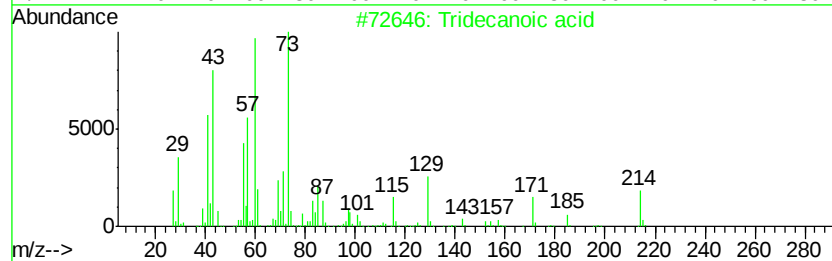
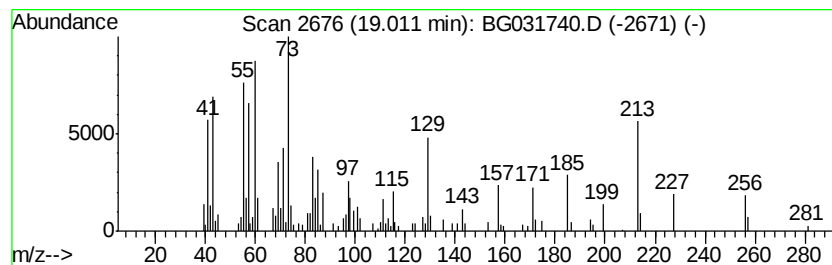
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Peak Number 5 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.01	2.72 ng	109144	Phenanthrene-d10	18.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52



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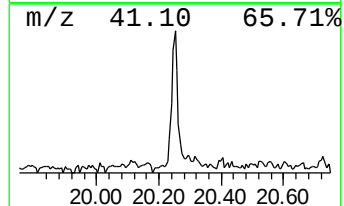
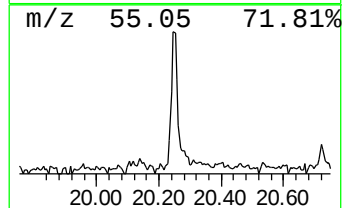
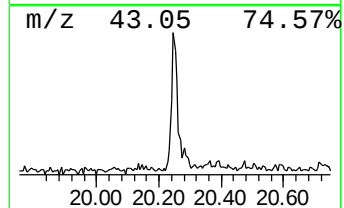
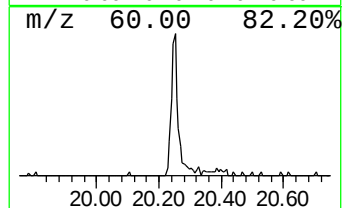
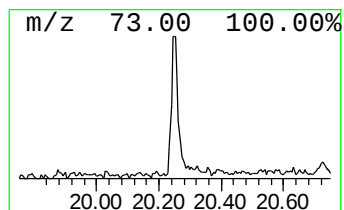
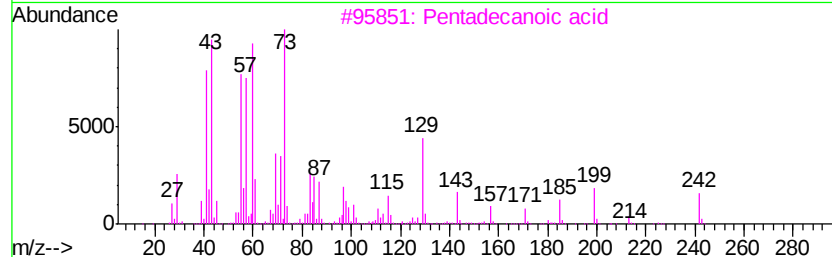
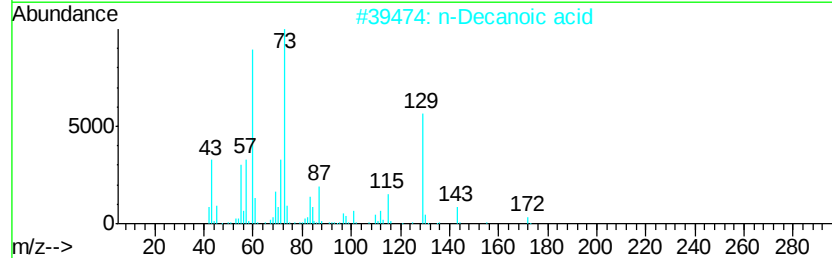
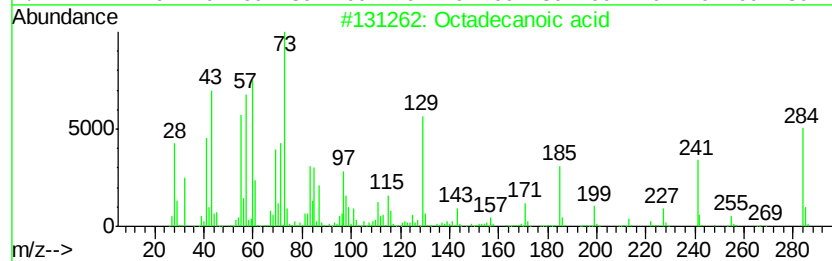
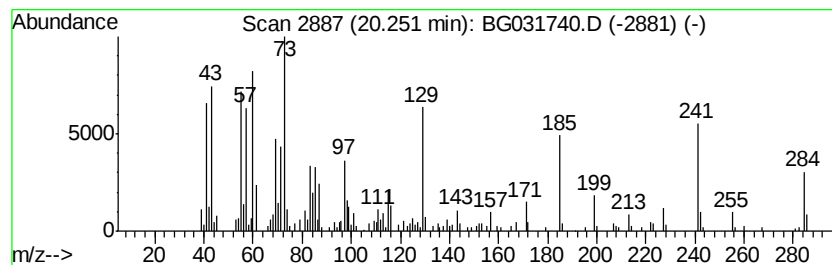
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.25	5.07 ng	203466	Phenanthrene-d10	18.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		n-Decanoic acid	172	C10H20O2	000334-48-5	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	52
5		Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	50



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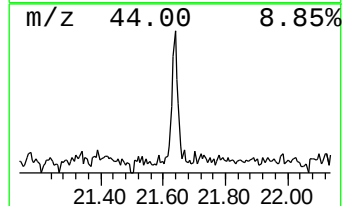
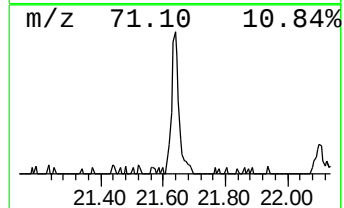
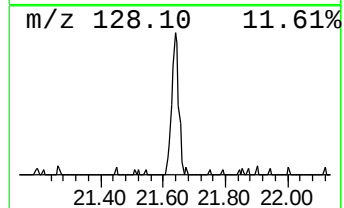
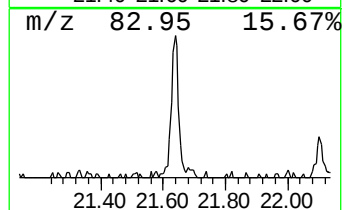
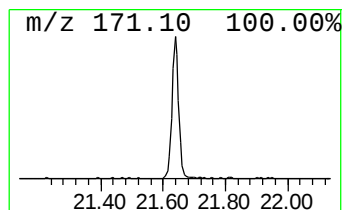
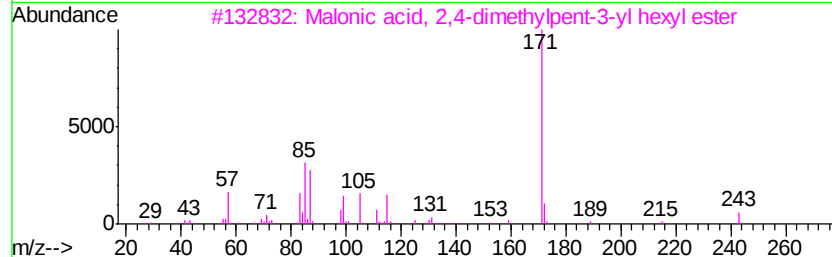
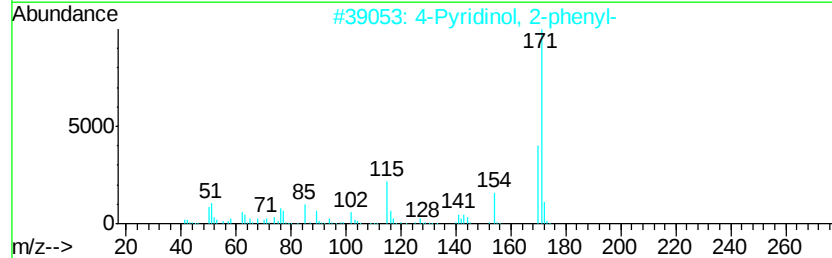
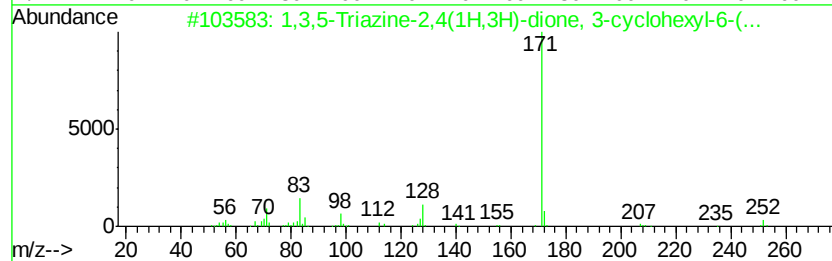
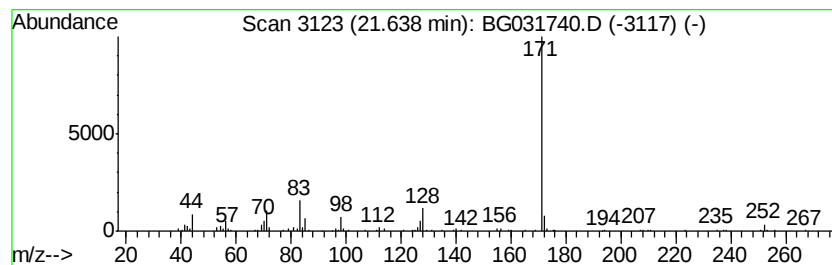
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Peak Number 7 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.64	2.76 ng	135761	Chrysene-d12	22.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazine-2,4(1H,3H)-dione, ...	252	C12H20N4O2	051235-04-2	98
2		4-Pyridinol, 2-phenyl-	171	C11H9NO	1000253-54-5	42
3		Malonic acid, 2,4-dimethylpent-3...	286	C16H30O4	1000349-01-3	38
4		3-Cyanoquinoxaline 1-oxide	171	C9H5N3O	053688-02-1	36
5		1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	171	C6H9N3O3	000827-16-7	36



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.54	3.54	3.9	ng	48208	1	8.82	248659	20.0
unknown8.34	8.34	91.8	ng	1141160	1	8.82	248659	20.0
Tridecanoic acid	19.01	2.7	ng	109144	4	18.19	802773	20.0
Octadecanoic acid	20.25	5.1	ng	203466	4	18.19	802773	20.0
1,3,5-Triazine-2,...	21.64	2.8	ng	135761	5	22.55	983547	20.0