

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG073123\
 Data File : BG058542.D
 Acq On : 31 Jul 2023 14:05
 Operator : MA/JU
 Sample : 03741-17
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-P28B

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_G\Methods\8270-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.388	383	391	402	rBV	660670	1067084	45.34%	7.755%
2	6.986	656	663	678	rBV	643334	1119421	47.57%	8.135%
3	7.814	797	804	812	rBV	180276	304138	12.92%	2.210%
4	8.978	994	1002	1019	rBV	350902	667930	28.38%	4.854%
5	10.617	1273	1281	1295	rBV	245090	444795	18.90%	3.233%
6	13.079	1693	1700	1717	rBV	932923	1521826	64.67%	11.060%
7	13.355	1739	1747	1760	rBV	503557	846759	35.98%	6.154%
8	14.459	1928	1935	1946	rBV	407434	641472	27.26%	4.662%
9	15.952	2183	2189	2215	rBV	820233	1335072	56.73%	9.703%
10	17.209	2396	2403	2414	rBV	517645	810918	34.46%	5.893%
11	18.096	2549	2554	2565	rBV2	67809	149566	6.36%	1.087%
12	19.042	2712	2715	2720	rVB3	23226	26624	1.13%	0.193%
13	19.271	2748	2754	2758	rBV	25582	31833	1.35%	0.231%
14	19.829	2842	2849	2860	rBV	1741154	2353376	100.00%	17.103%
15	20.282	2911	2926	2937	rBV6	93363	459607	19.53%	3.340%
16	20.399	2942	2946	2948	rBV5	28427	44936	1.91%	0.327%
17	20.623	2981	2984	2987	rVB2	20514	24428	1.04%	0.178%
18	21.198	3070	3082	3090	rBV2	20099	99014	4.21%	0.720%
19	21.451	3118	3125	3136	rBV	502525	851784	36.19%	6.190%
20	24.518	3637	3647	3661	rBV	343221	959148	40.76%	6.971%

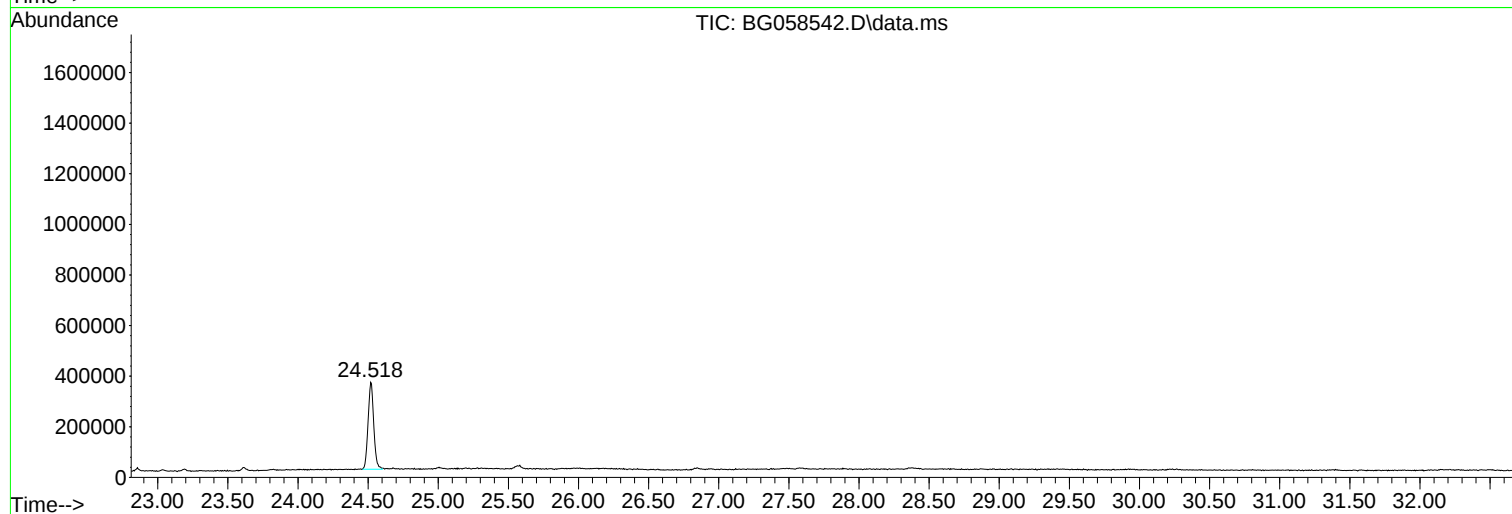
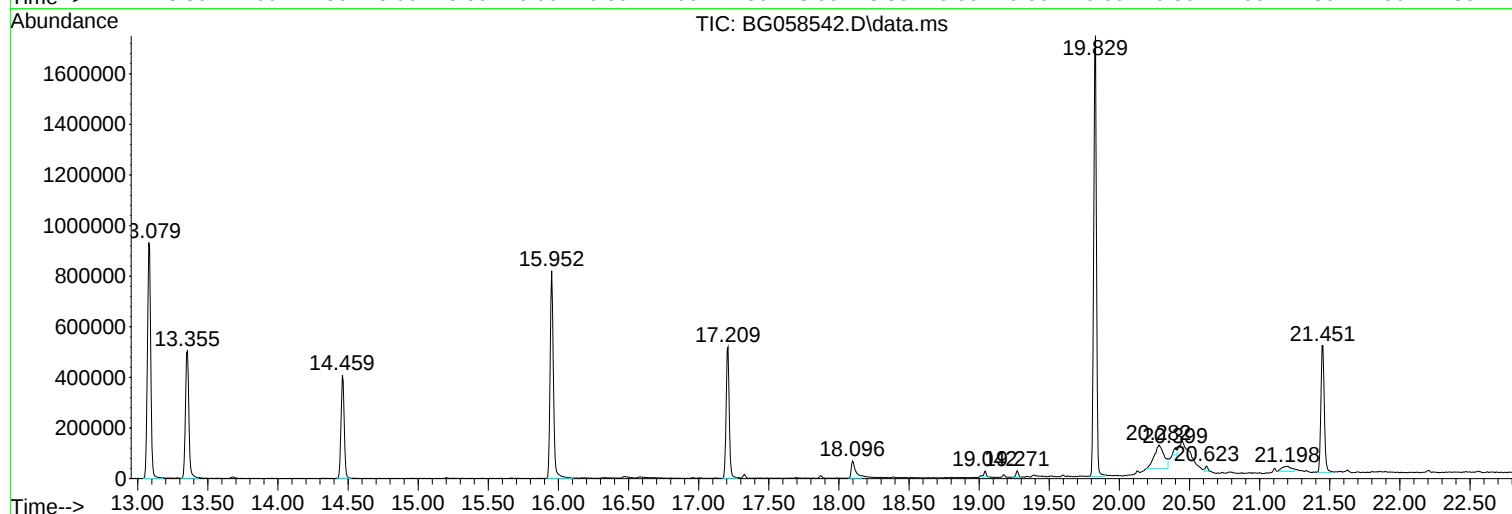
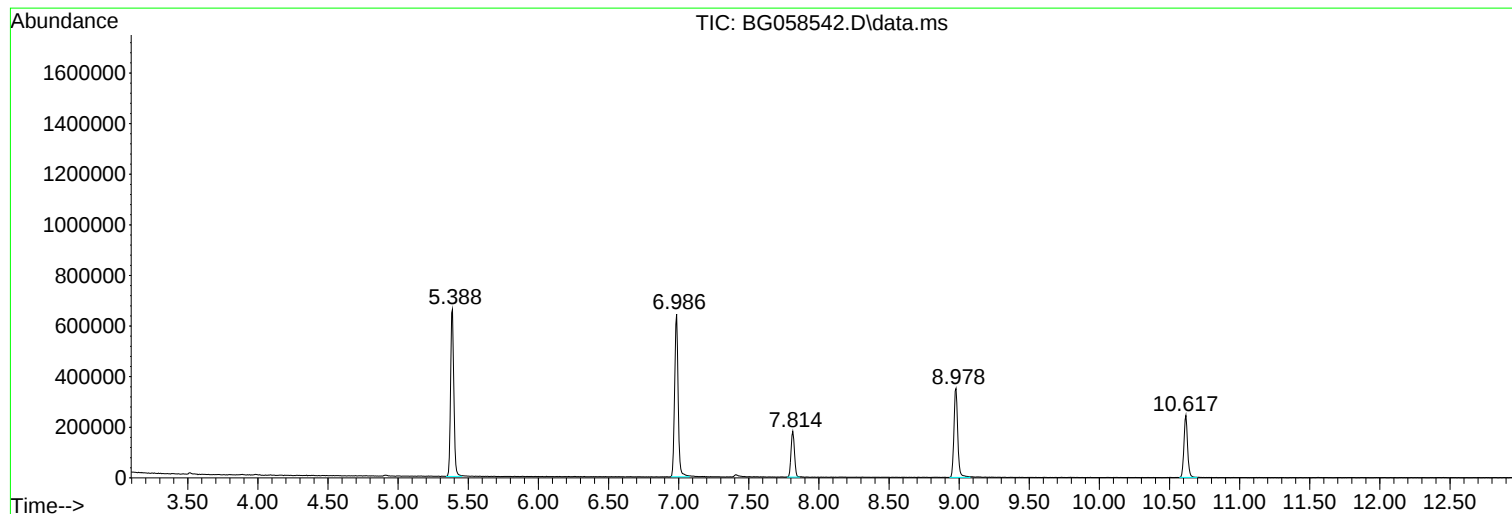
Sum of corrected areas: 13759731

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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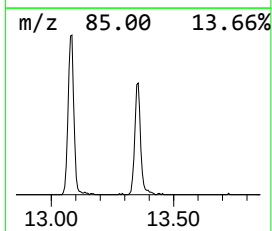
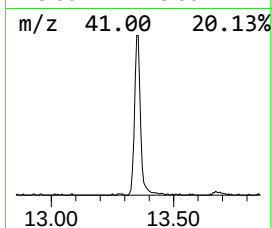
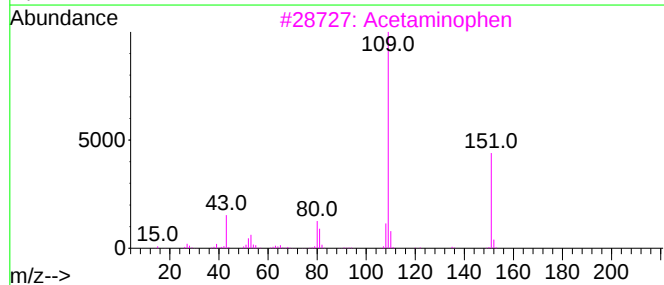
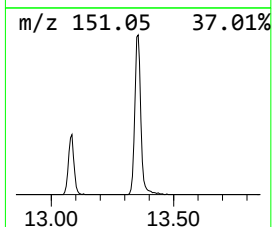
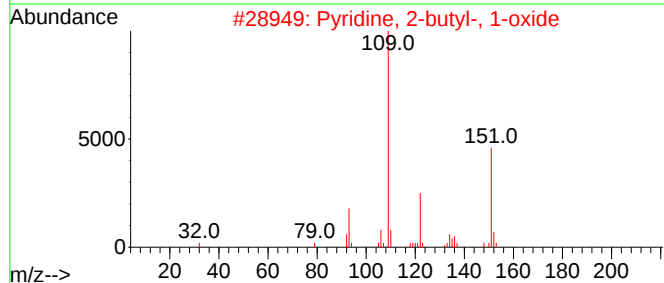
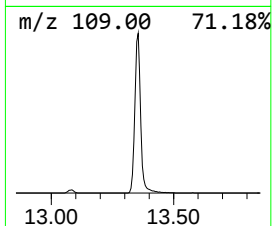
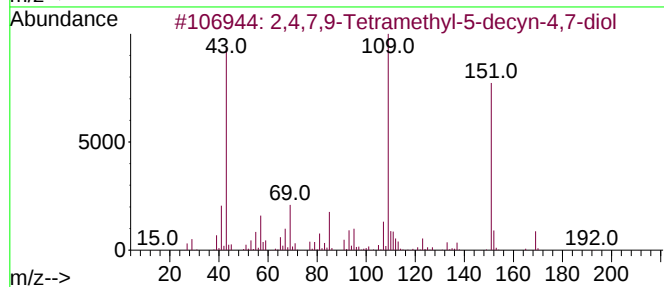
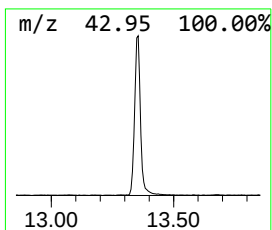
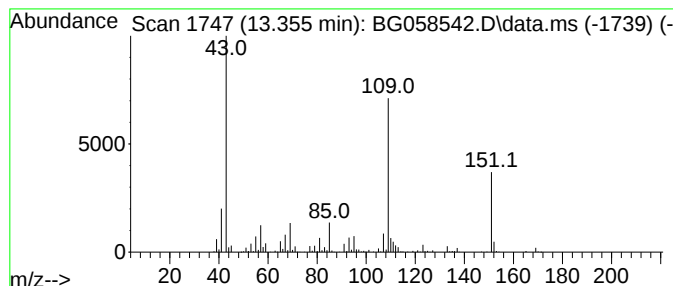
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.355	26.40 ng	846759	Acenaphthene-d10	14.459

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87		
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53		
3	Acetaminophen	151	C8H9NO2	000103-90-2	49		
4	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	47		
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43		



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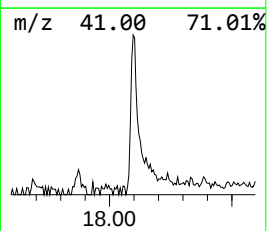
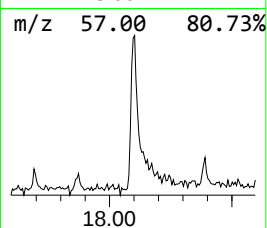
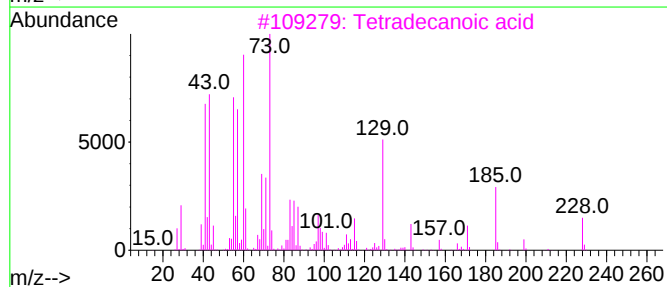
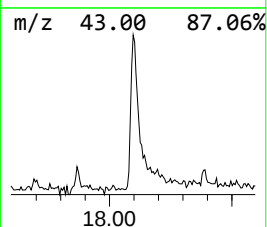
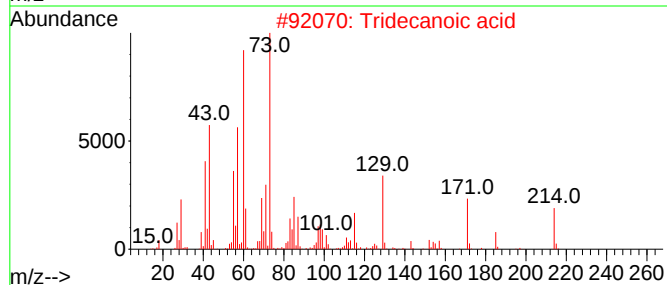
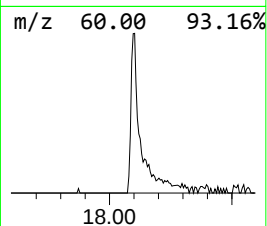
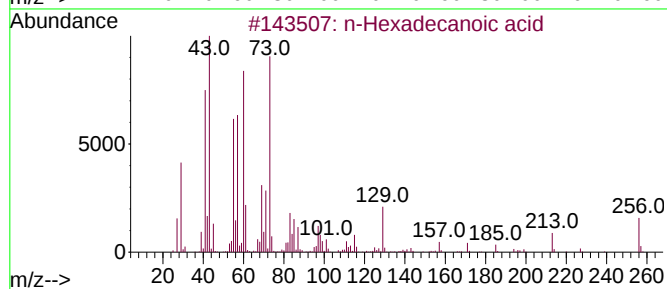
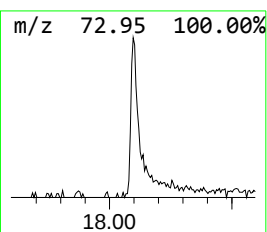
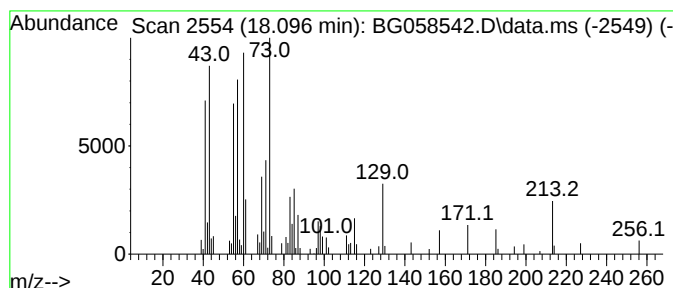
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.096	3.69 ng	149566	Phenanthrene-d10	17.209

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2			Tridecanoic acid	214	C13H26O2	000638-53-9	76
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5			Sulfurous acid, 2-propyl tetra...	320	C17H36O3S	1010309-12-5	18



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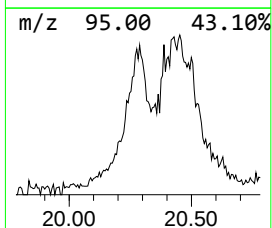
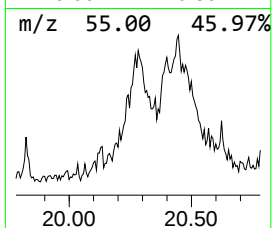
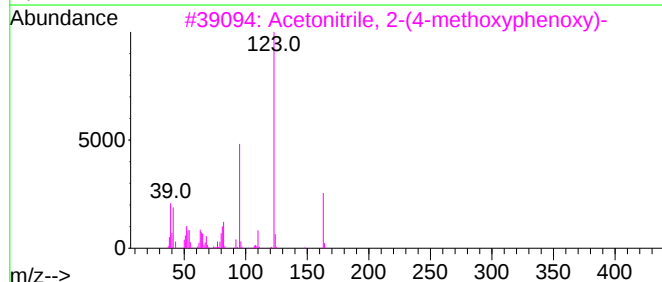
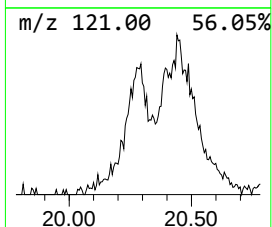
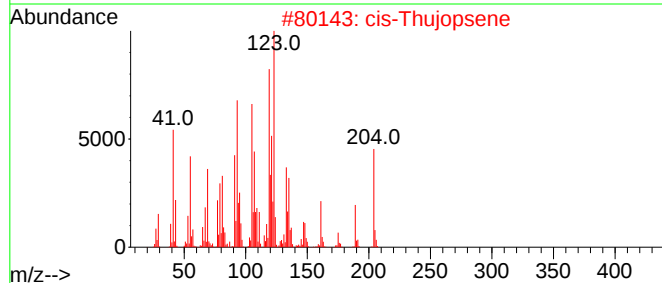
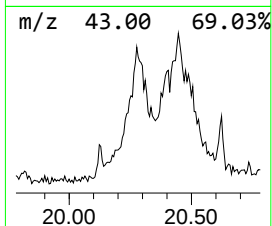
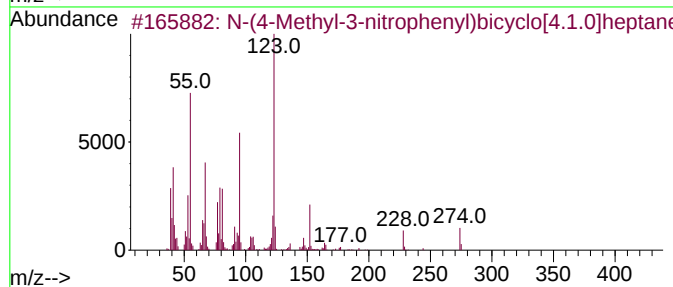
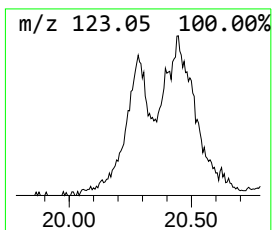
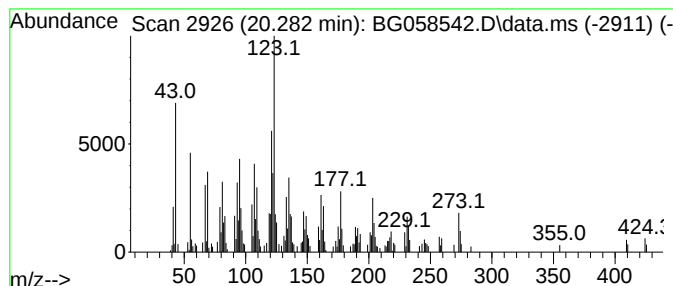
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Peak Number 3 N-(4-Methyl-3-nitrophenyl)b... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.282	10.79 ng	459607	Chrysene-d12	21.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(4-Methyl-3-nitrophenyl)bicycl...	274	C15H18N2O3	301317-78-2	60
2			cis-Thujopsene	204	C15H24	000470-40-6	49
3			Acetonitrile, 2-(4-methoxyphenoxy)-	163	C9H9NO2	022446-12-4	46
4			Bicyclo[4.1.0]heptane-7-carboxam...	257	C16H19NO2	1000278-06-2	46
5			Benzhydrazide, 4-fluoro-N2-[3-(2...	272	C15H13FN2O2	1000264-56-6	43



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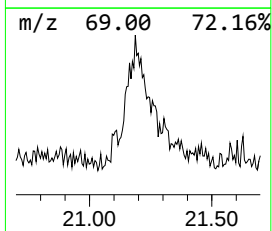
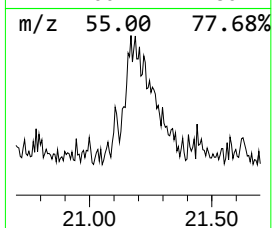
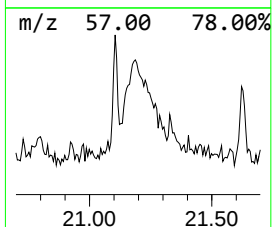
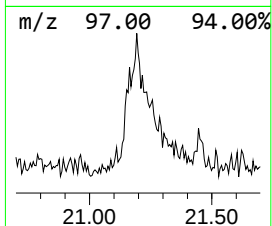
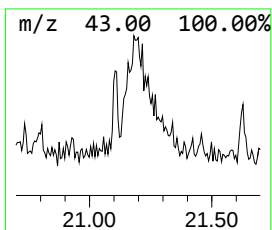
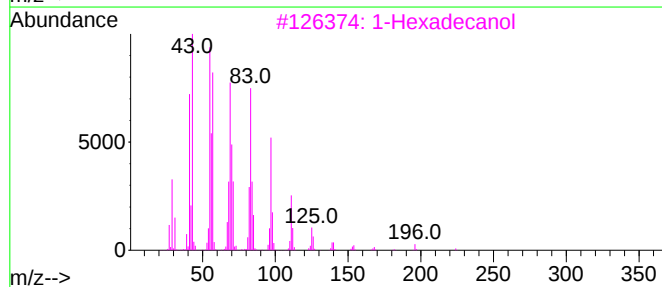
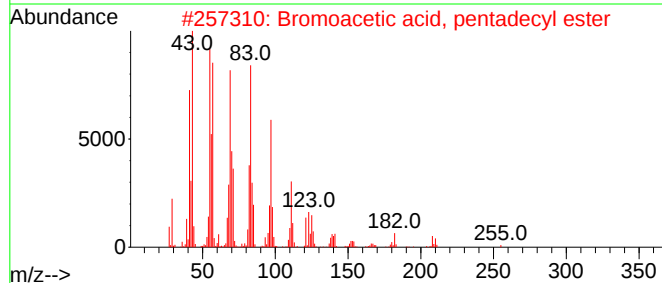
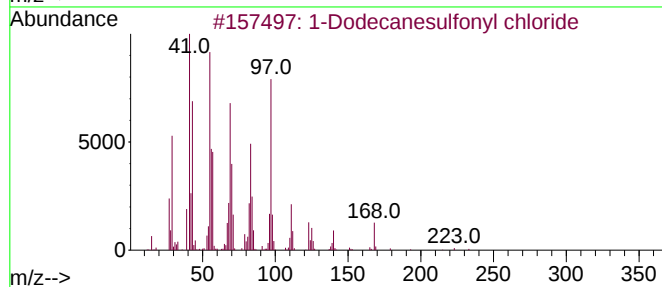
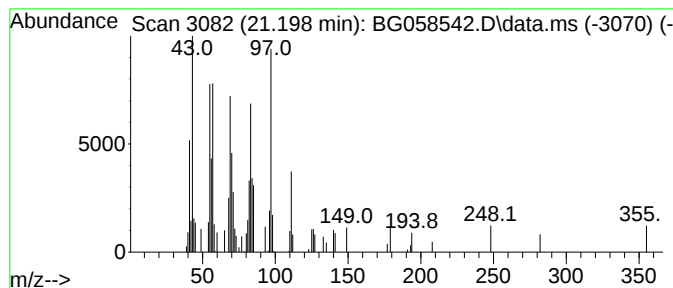
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Peak Number 4 1-Dodecanesulfonyl chloride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.198	2.32 ng	99014	Chrysene-d12	21.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanesulfonyl chloride	268	C12H25ClO2S	010147-40-7	87
2			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	76
3			1-Hexadecanol	242	C16H34O	036653-82-4	70
4			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	70
5			1-Heptacosanol	396	C27H56O	002004-39-9	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	13.355	26.4	ng	846759	3	14.459	641472	20.0
n-Hexadecanoic ...	18.096	3.7	ng	149566	4	17.209	810918	20.0
N-(4-Methyl-3-n...	20.282	10.8	ng	459607	5	21.445	851784	20.0
1-Dodecanesulfo...	21.198	2.3	ng	99014	5	21.445	851784	20.0