

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011223\
 Data File : BG056266.D
 Acq On : 12 Jan 2023 13:10
 Operator : CG/JU
 Sample : 01093-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TT-214-IDWSO-20230109-1

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056266.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	3	8	18	rVB	122034	183104	6.34%	1.530%
2	5.356	343	352	359	rVB	98791	149895	5.19%	1.253%
3	5.832	427	433	443	rVB	381537	623491	21.59%	5.210%
4	7.447	700	708	719	rBV	385165	678857	23.51%	5.673%
5	8.317	846	856	863	rBB	126511	220377	7.63%	1.842%
6	9.486	1047	1055	1064	rBV	224041	411073	14.24%	3.435%
7	11.149	1330	1338	1346	rBV	172569	303372	10.51%	2.535%
8	13.558	1740	1748	1755	rBV	920938	1416511	49.05%	11.837%
9	14.927	1974	1981	1988	rBV	347750	533107	18.46%	4.455%
10	16.266	2202	2209	2214	rBV	31490	47462	1.64%	0.397%
11	16.402	2226	2232	2241	rBV	741324	1139778	39.47%	9.525%
12	17.665	2440	2447	2457	rVB	518094	785397	27.20%	6.563%
13	18.505	2584	2590	2597	rBV	91414	138957	4.81%	1.161%
14	19.762	2800	2804	2813	rBV9	20362	40365	1.40%	0.337%
15	20.238	2879	2885	2891	rVB	2351061	2887758	100.00%	24.132%
16	21.537	3102	3106	3123	rVB2	126727	262723	9.10%	2.195%
17	21.954	3170	3177	3186	rBV	549208	920226	31.87%	7.690%
18	23.711	3471	3476	3484	rVB3	29543	61716	2.14%	0.516%
19	24.093	3530	3541	3543	rBV10	32113	99570	3.45%	0.832%
20	24.357	3580	3586	3592	rBV10	15585	34464	1.19%	0.288%
21	25.397	3752	3763	3774	rBV2	333613	1028442	35.61%	8.594%

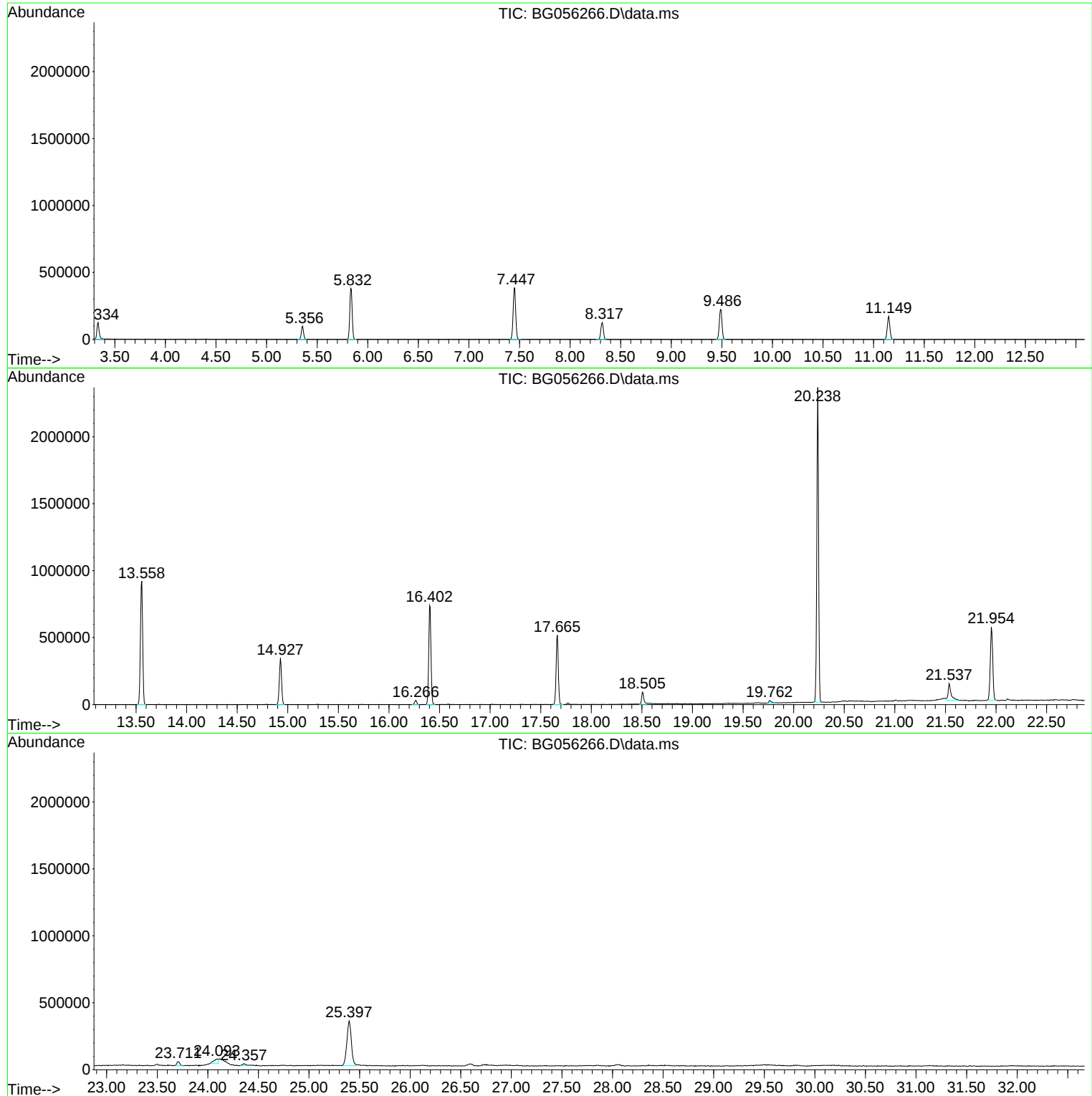
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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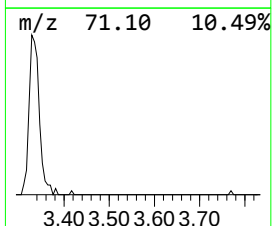
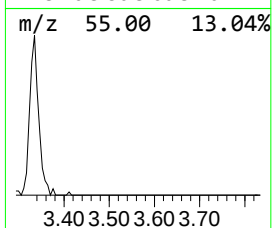
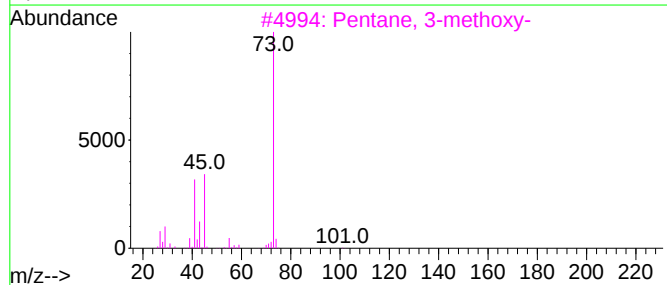
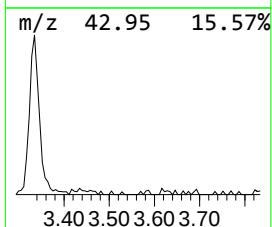
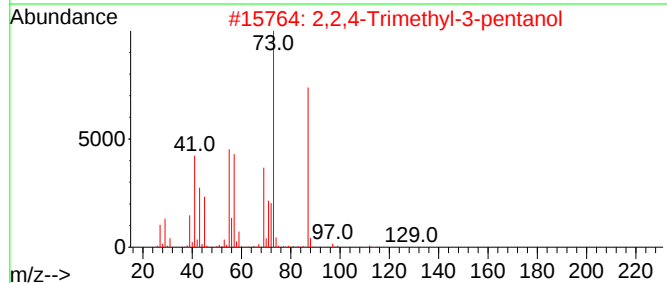
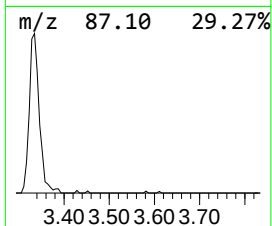
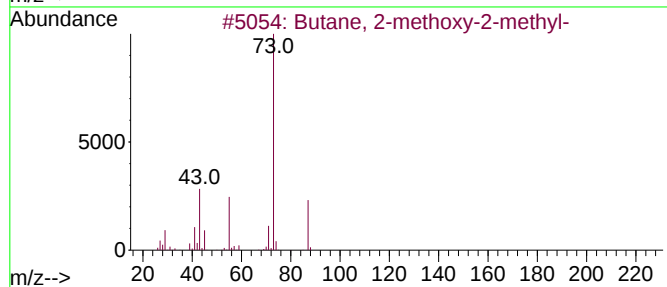
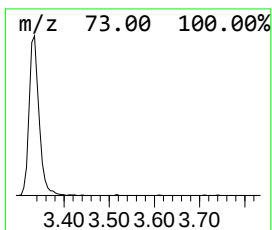
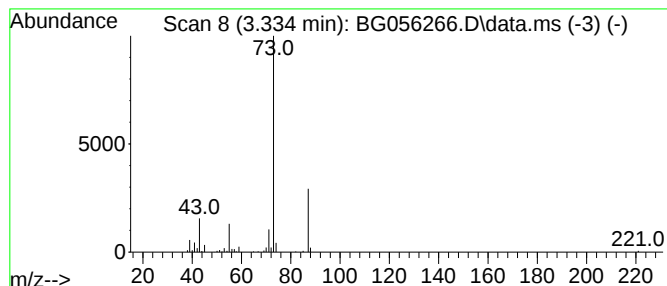
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.334	16.62 ng	183104	1,4-Dichlorobenzene-d4	8.317

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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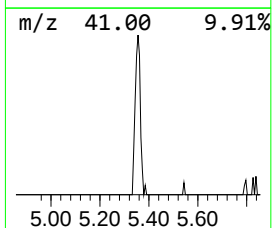
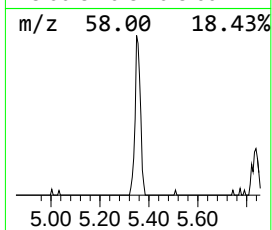
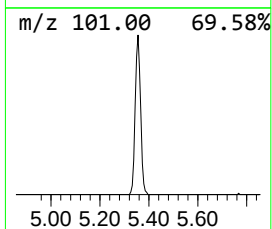
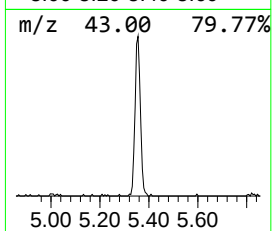
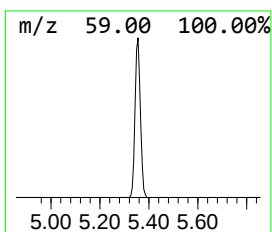
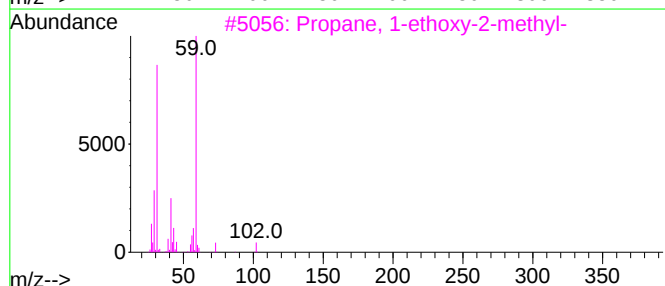
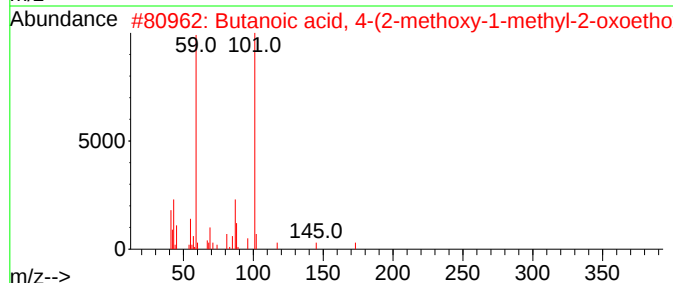
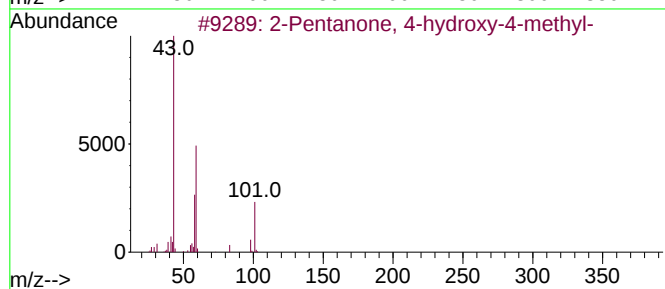
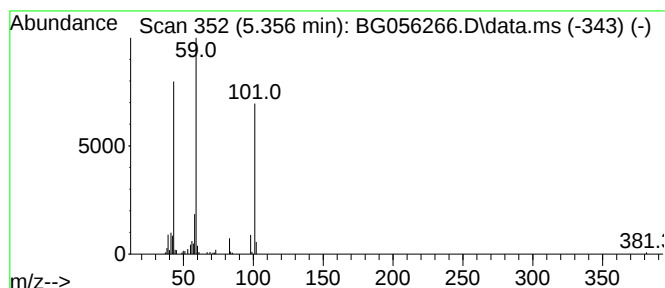
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.356	13.60 ng	149895	1,4-Dichlorobenzene-d4	8.317

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	38
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
4			2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	37
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37



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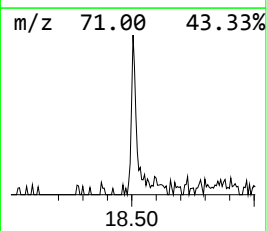
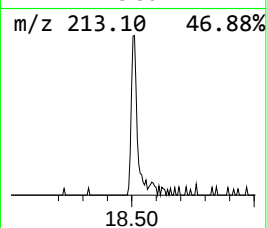
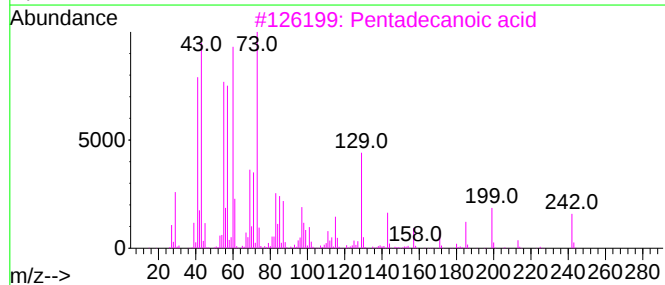
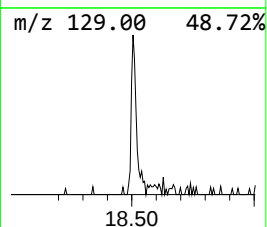
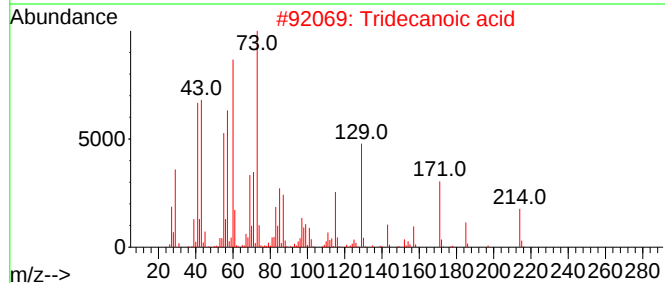
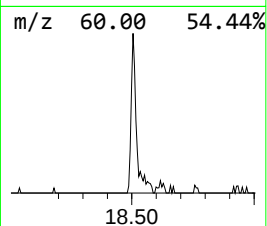
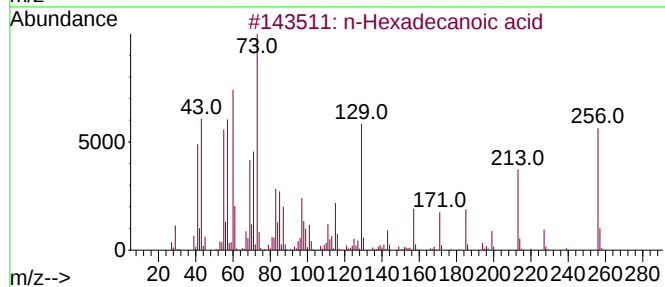
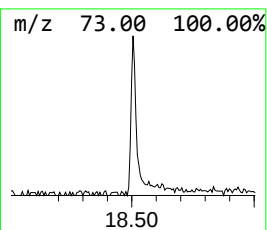
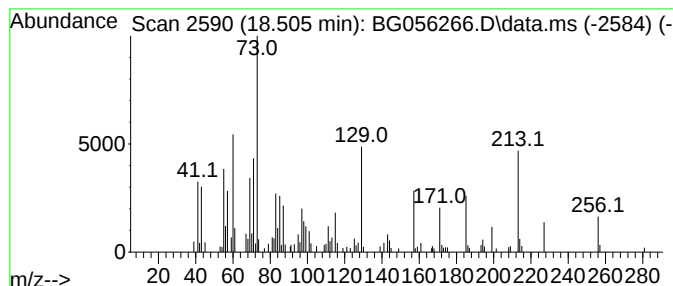
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.505	3.54 ng	138957	Phenanthrene-d10	17.665	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38



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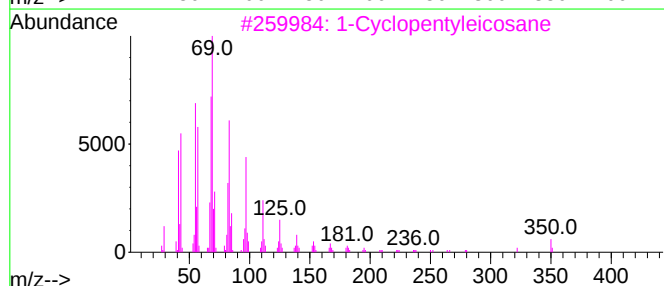
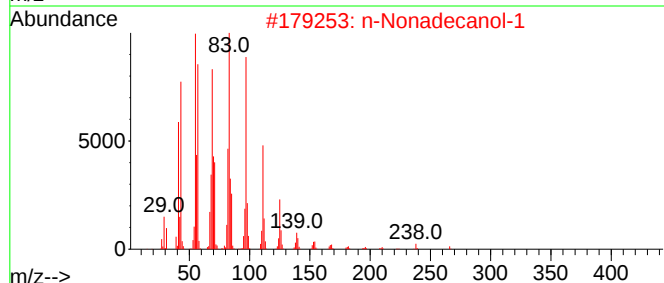
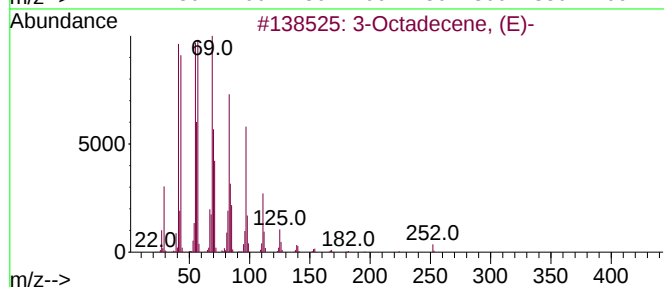
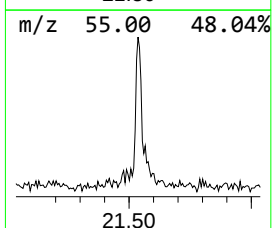
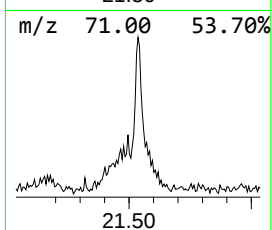
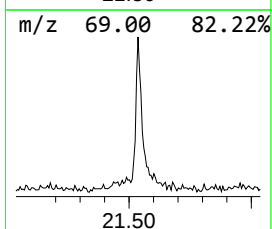
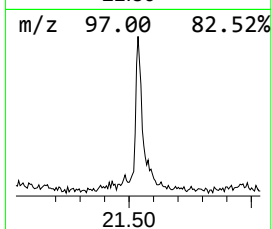
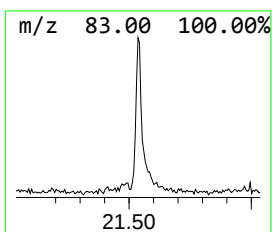
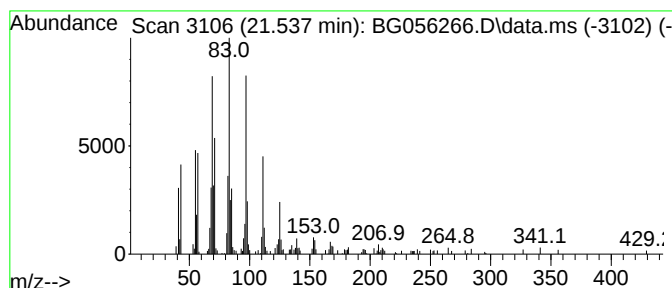
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Peak Number 4 3-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.537	5.71 ng	262723	Chrysene-d12	21.954	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	53
3	1-Cyclopentyleicosane	350	C25H50	1000357-25-6	53
4	11-Methyldodecanol	200	C13H28O	085763-57-1	52
5	1-Hexadecanol	242	C16H34O	036653-82-4	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.334	16.6	ng	183104	1	8.317	220377	20.0
2-Pentanone, 4-...	5.356	13.6	ng	149895	1	8.317	220377	20.0
n-Hexadecanoic ...	18.505	3.5	ng	138957	4	17.665	785397	20.0
3-Octadecene, (E)-	21.537	5.7	ng	262723	5	21.954	920226	20.0