

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
 Data File : BG048608.D
 Acq On : 6 Apr 2021 17:46
 Operator : CG/JU
 Sample : M1928-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TW-3

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-BG033021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.551	202	206	211	rBV2	16442	26249	1.36%	0.347%
2	5.156	306	309	318	rVB2	19585	27619	1.44%	0.365%
3	5.632	384	390	401	rBV	170454	274166	14.25%	3.626%
4	7.242	652	664	674	rBV2	102929	207538	10.79%	2.745%
5	8.088	800	808	815	rBV	84193	140736	7.32%	1.861%
6	9.263	997	1008	1016	rBV	266039	473661	24.62%	6.264%
7	10.920	1282	1290	1298	rVB	97820	184115	9.57%	2.435%
8	13.364	1699	1706	1718	rBV	684075	1061792	55.20%	14.041%
9	14.181	1841	1845	1854	rBV	25678	44585	2.32%	0.590%
10	14.745	1930	1941	1950	rBV	166275	287682	14.96%	3.804%
11	16.232	2186	2194	2206	rBV	638110	1028061	53.44%	13.595%
12	17.501	2403	2410	2416	rBV	248360	386417	20.09%	5.110%
13	18.382	2553	2560	2569	rBV	259419	379422	19.72%	5.018%
14	19.645	2771	2775	2781	rBV2	105695	144467	7.51%	1.910%
15	20.110	2848	2854	2865	rBV	1467142	1923650	100.00%	25.439%
16	21.414	3072	3076	3088	rBV4	87731	165916	8.63%	2.194%
17	21.796	3134	3141	3150	rBV2	270006	447411	23.26%	5.917%
18	25.139	3701	3710	3722	rBV4	108940	358402	18.63%	4.740%

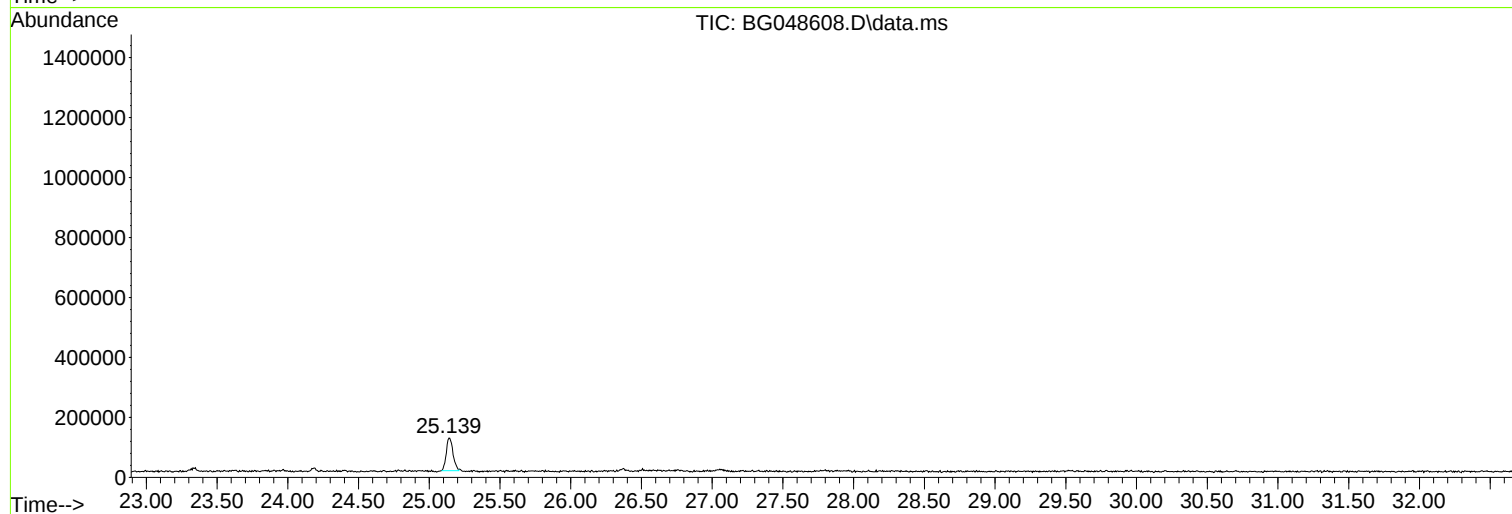
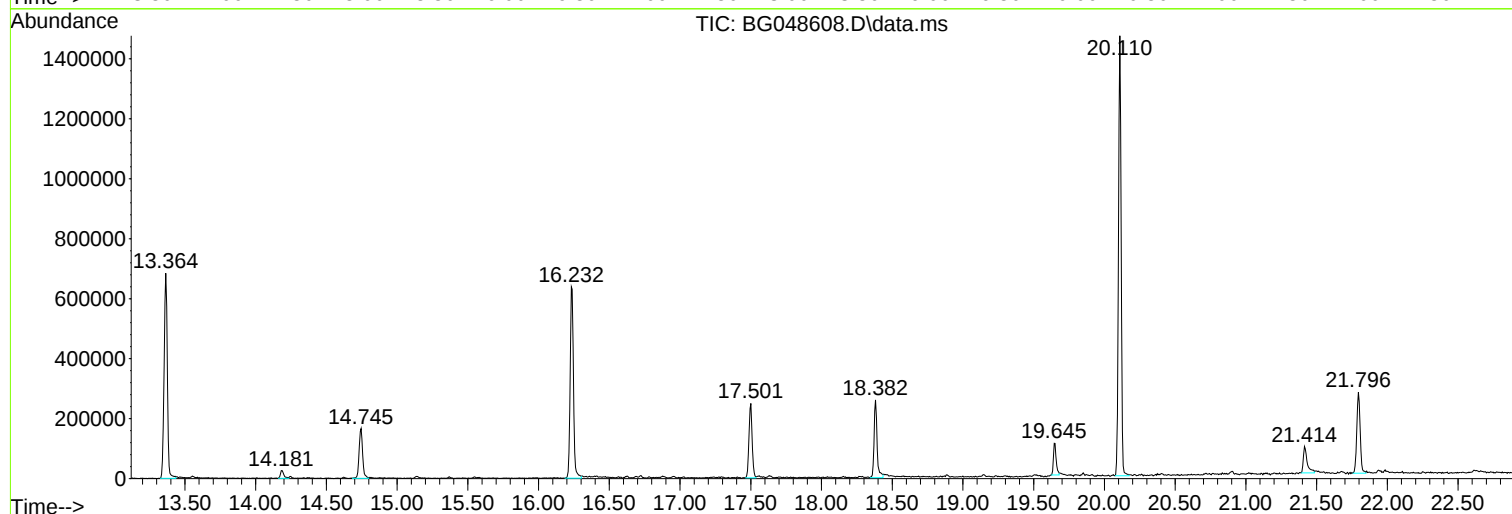
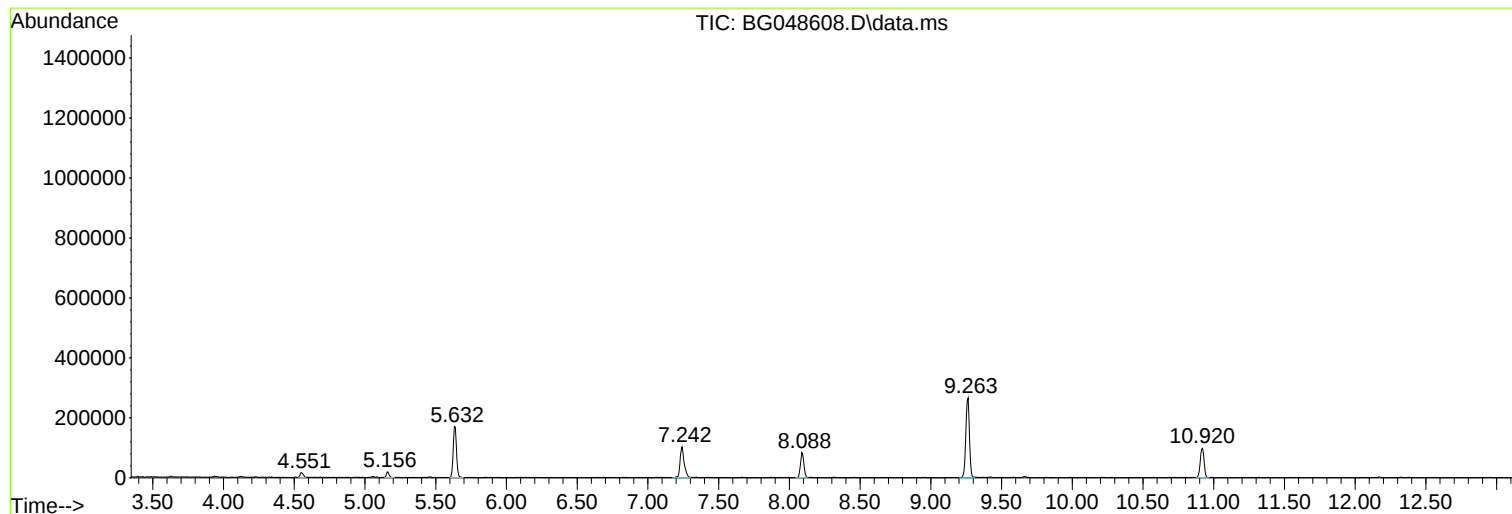
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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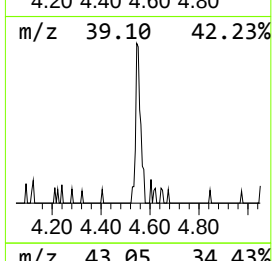
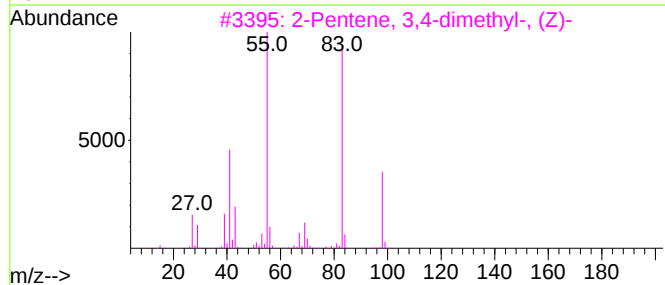
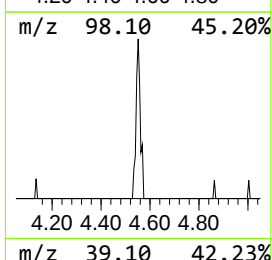
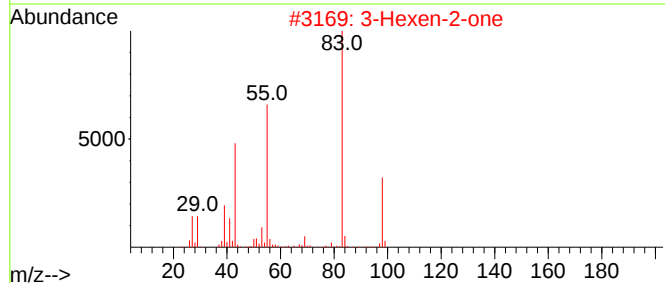
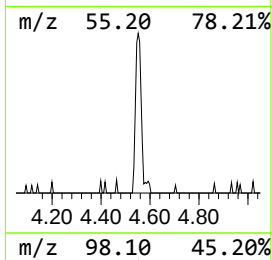
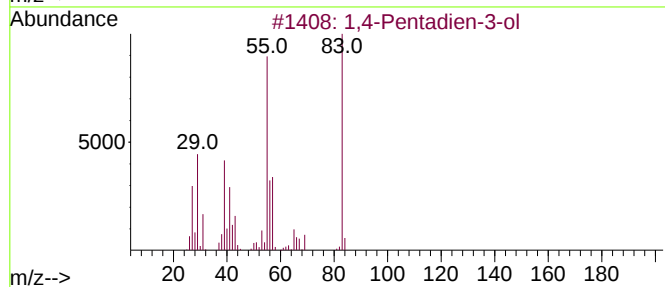
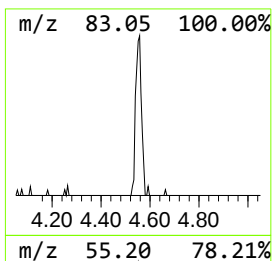
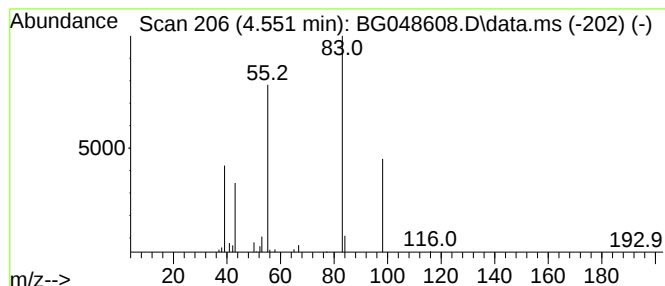
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TIC Integration Parameters: LSCINT.P

Peak Number 1 1,4-Pentadien-3-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.551	3.73 ng	26249	1,4-Dichlorobenzene-d4	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	59
2			3-Hexen-2-one	98	C6H10O	000763-93-9	58
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	58
4			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	58
5			Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	059242-27-2	56



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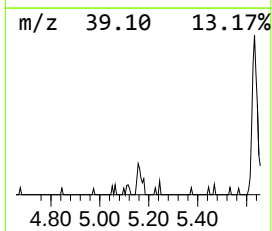
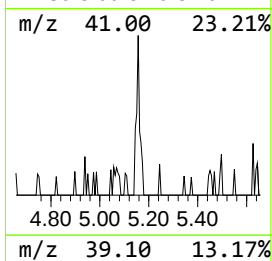
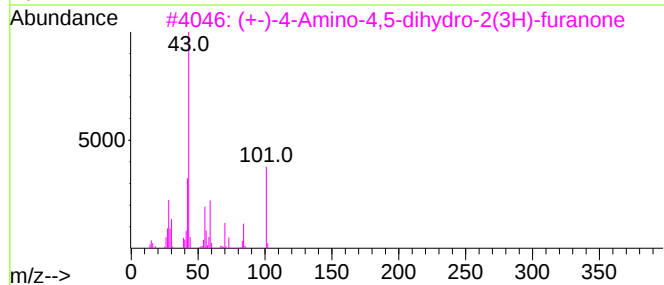
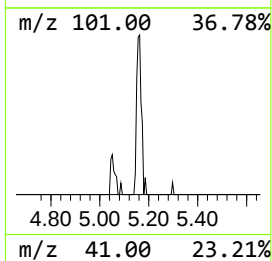
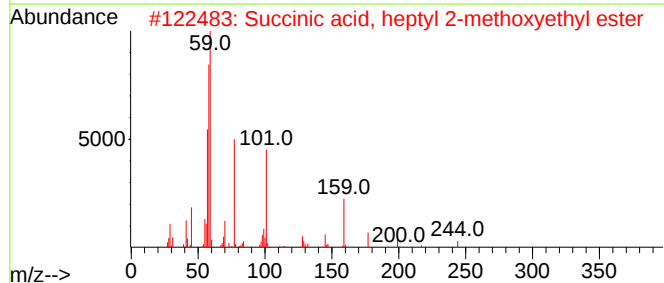
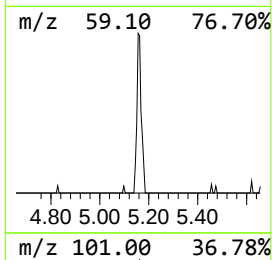
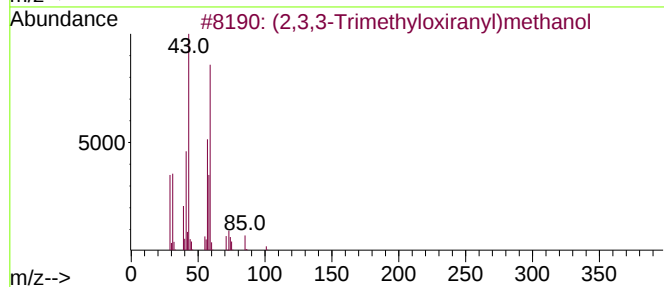
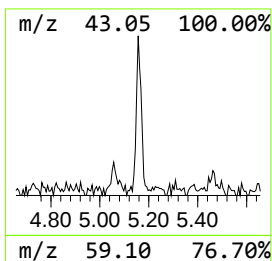
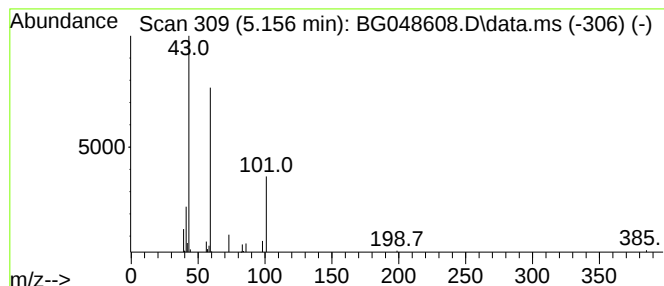
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown5.15 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.156	3.92 ng	27619	1,4-Dichlorobenzene-d4	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	38
2			Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	36
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	35
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	28



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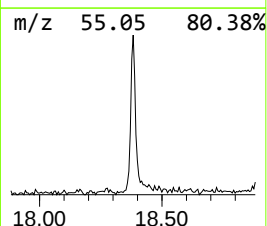
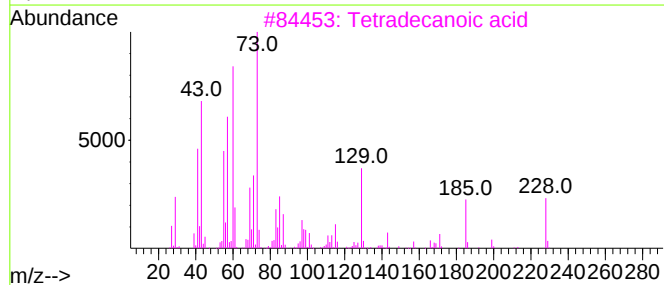
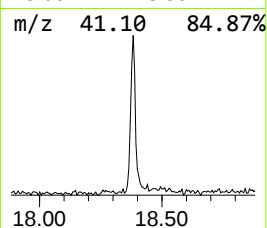
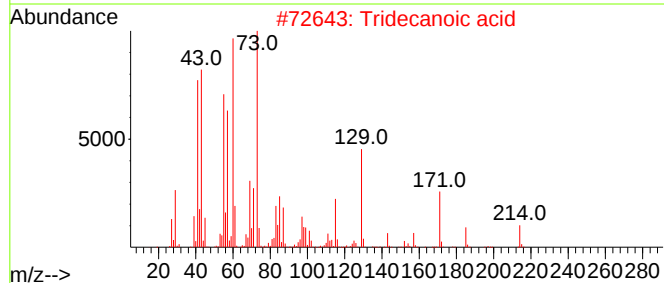
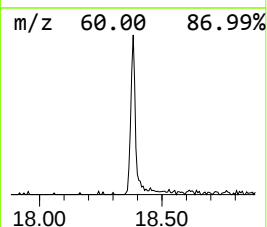
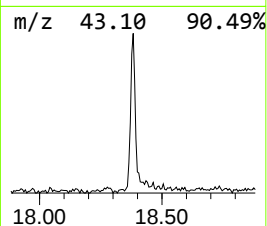
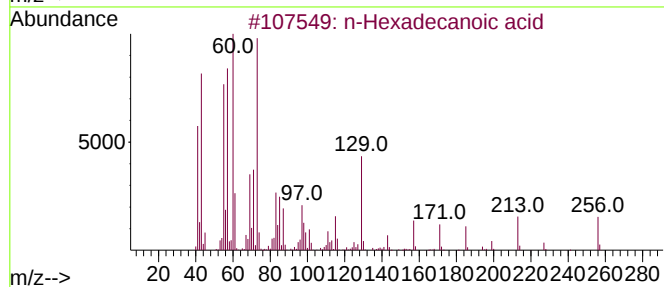
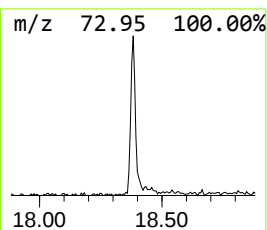
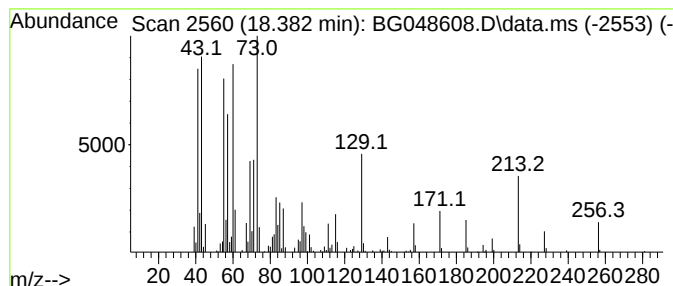
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.382	19.64 ng	379422	Phenanthrene-d10	17.501

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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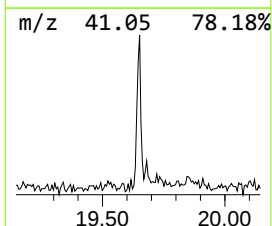
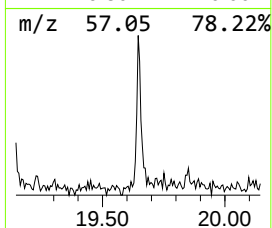
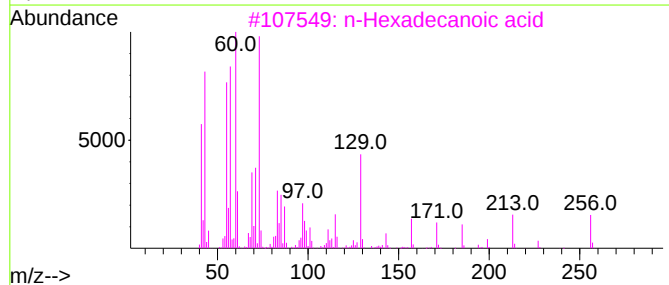
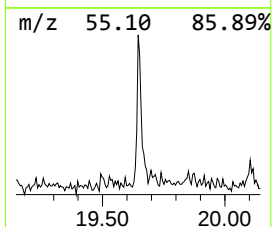
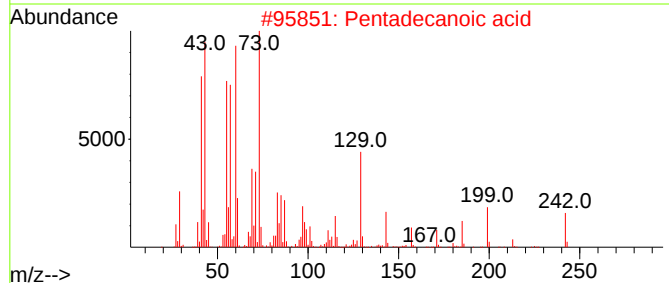
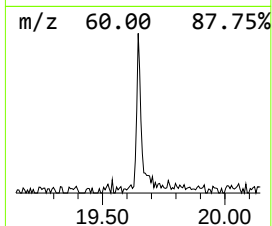
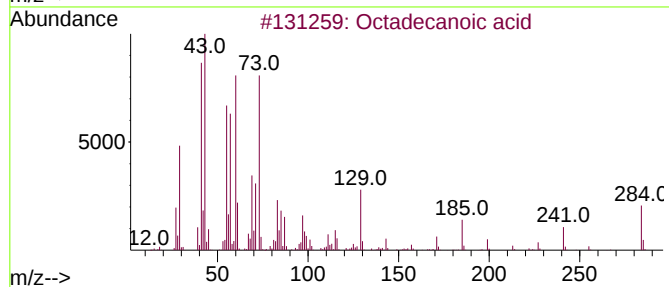
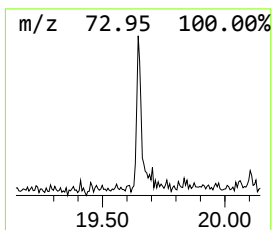
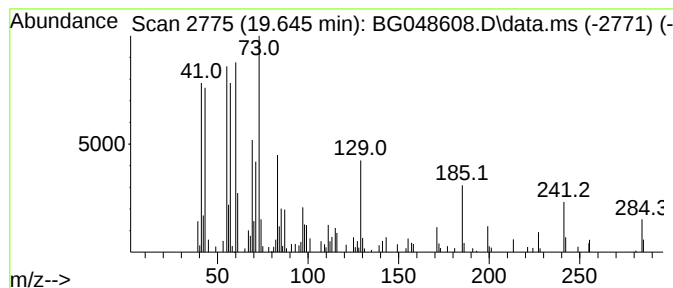
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.645	7.48 ng	144467	Phenanthrene-d10	17.501

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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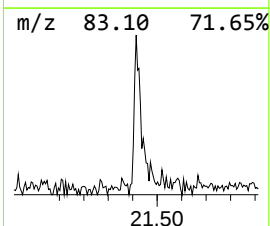
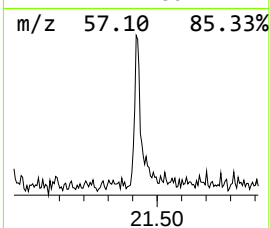
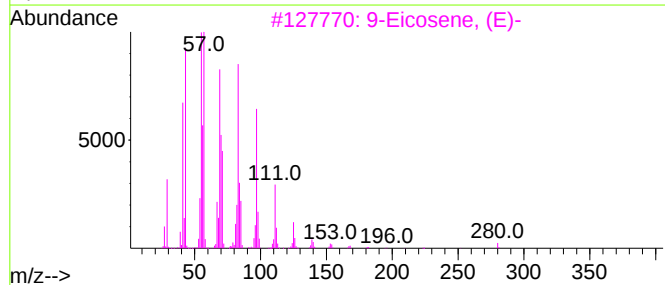
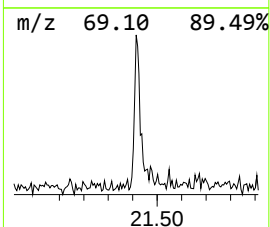
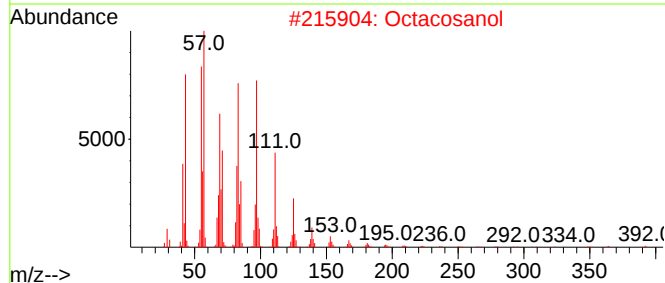
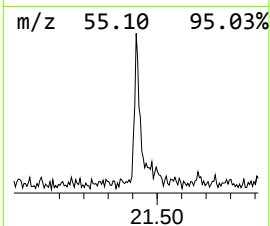
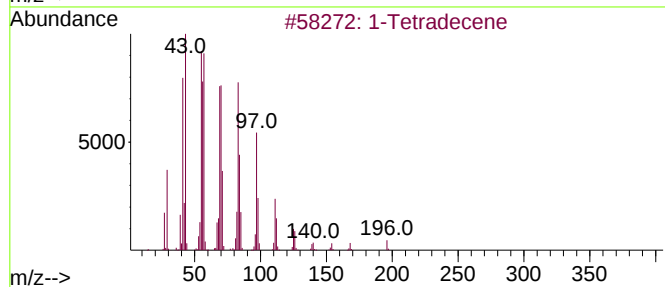
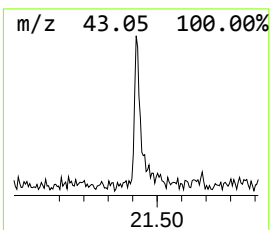
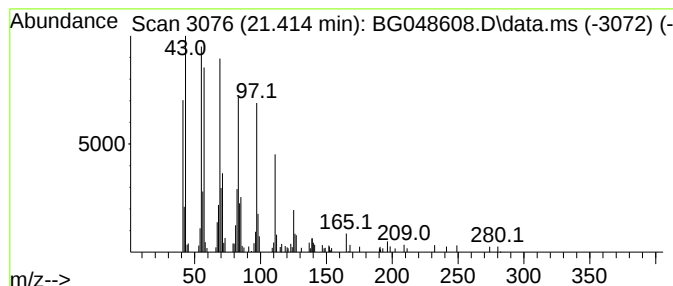
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Peak Number 5 1-Tetradecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.414	7.42 ng	165916	Chrysene-d12	21.796	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecene	196	C14H28	001120-36-1	86
2	Octacosanol	410	C28H58O	000557-61-9	86
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	81
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	70
5	Cycloeicosane	280	C20H40	000296-56-0	70



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,4-Pentadien-3-ol	4.551	3.7	ng	26249	1	8.088	140736	20.0
unknown5.15	5.156	3.9	ng	27619	1	8.088	140736	20.0
n-Hexadecanoic ...	18.382	19.6	ng	379422	4	17.501	386417	20.0
Octadecanoic acid	19.645	7.5	ng	144467	4	17.501	386417	20.0
1-Tetradecene	21.414	7.4	ng	165916	5	21.796	447411	20.0