

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061323\
 Data File : BM040232.D
 Acq On : 13 Jun 2023 19:27
 Operator : MA/JU
 Sample : 03047-12
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TWP-07

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_M\Methods\8270-BM061323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM040232.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.446	192	197	209	rVB	1885578	2370543	8.69%	1.803%
2	5.063	295	302	316	rBV	6909737	9254329	33.94%	7.040%
3	5.528	375	381	394	rBV	4076966	5662539	20.77%	4.307%
4	6.152	480	487	494	rBV	928846	1279746	4.69%	0.973%
5	7.134	645	654	668	rBV	2292647	3625703	13.30%	2.758%
6	7.975	789	797	806	rBV	2082514	3140206	11.52%	2.389%
7	9.151	988	997	1013	rBV	6951442	11600858	42.55%	8.825%
8	10.793	1268	1276	1287	rBV	2688243	4437567	16.28%	3.376%
9	13.245	1685	1693	1700	rBV	18028074	25913771	95.05%	19.712%
10	14.616	1919	1926	1935	rBV	3968494	5590433	20.51%	4.253%
11	16.104	2172	2179	2195	rBV	9135120	12458362	45.70%	9.477%
12	17.363	2386	2393	2398	rBV	4264499	6213874	22.79%	4.727%
13	18.251	2539	2544	2553	rBV	329457	594369	2.18%	0.452%
14	19.527	2756	2761	2772	rBV	339056	659301	2.42%	0.502%
15	19.980	2832	2838	2843	rBV	23057689	27263401	100.00%	20.739%
16	21.533	3097	3102	3107	rBV	4710009	5872458	21.54%	4.467%
17	23.968	3510	3516	3527	rVB	2807822	5521891	20.25%	4.200%

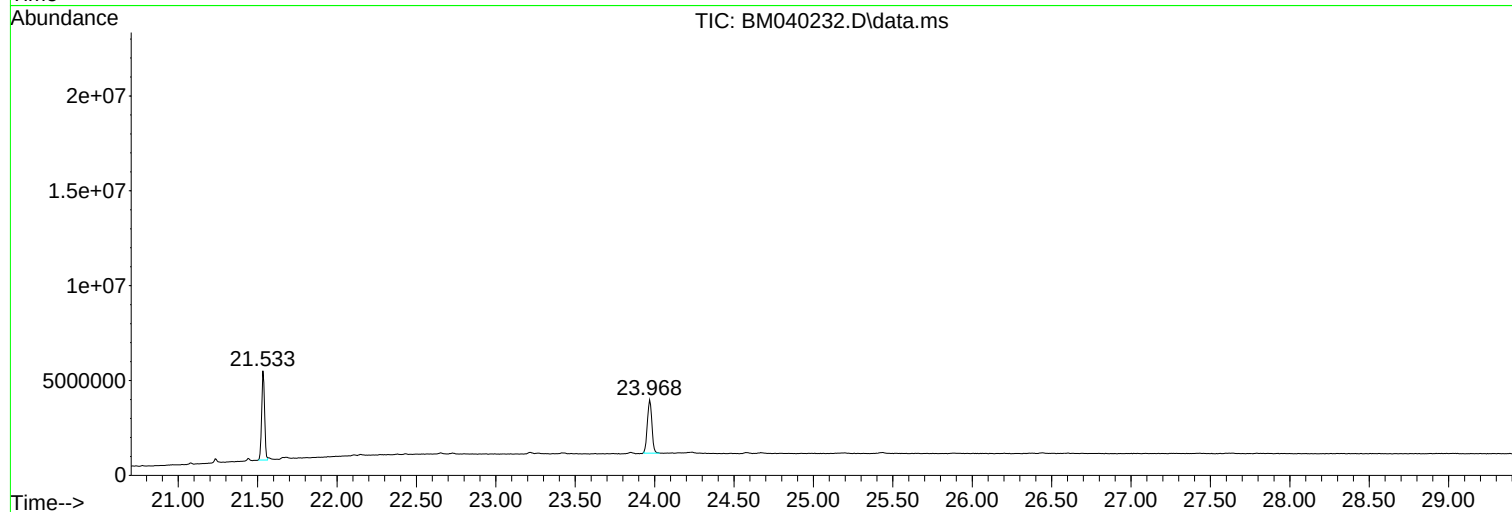
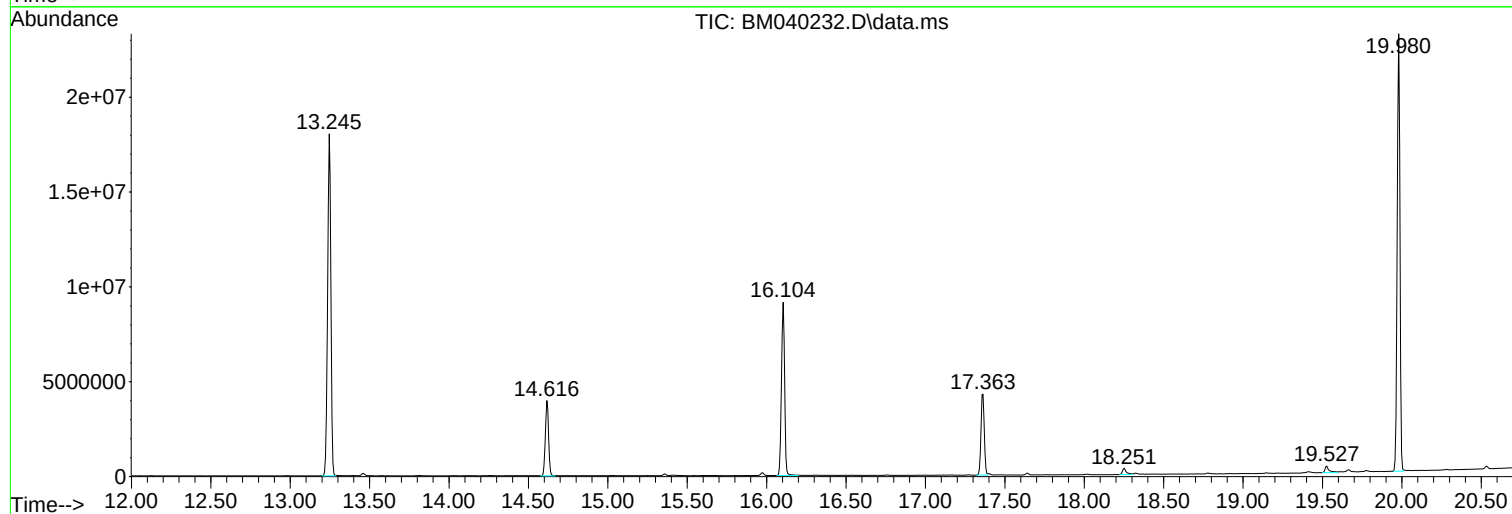
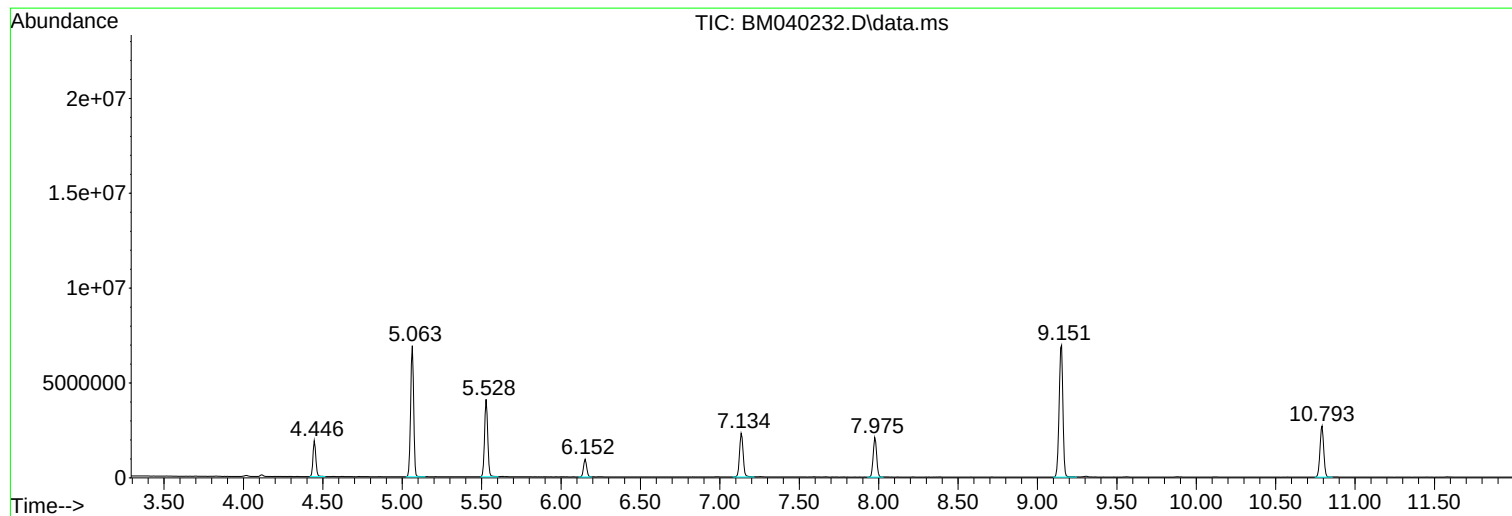
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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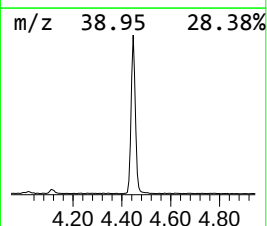
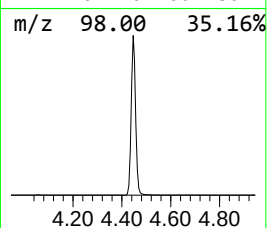
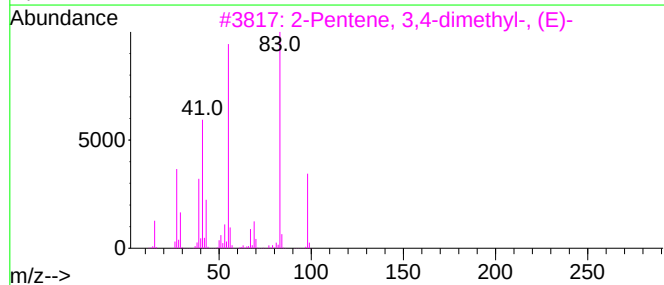
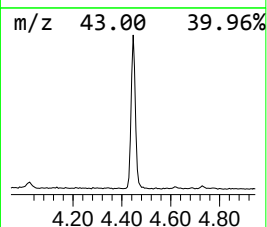
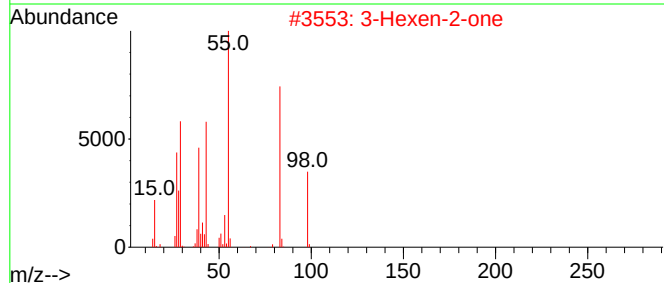
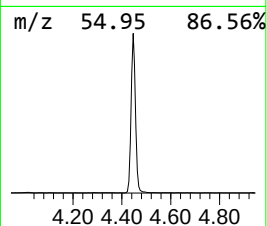
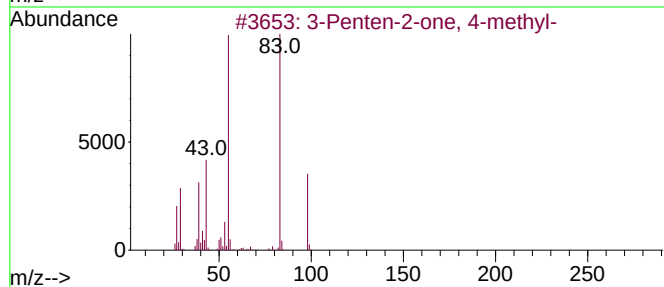
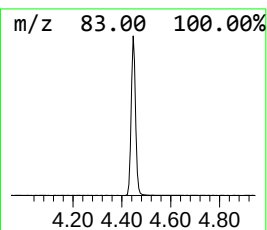
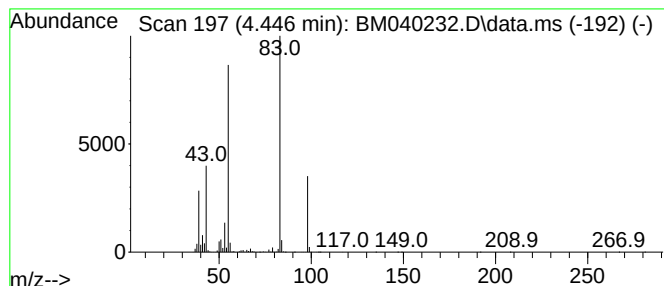
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.446	15.10 ng	2370540	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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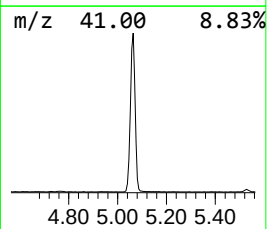
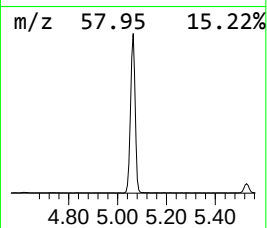
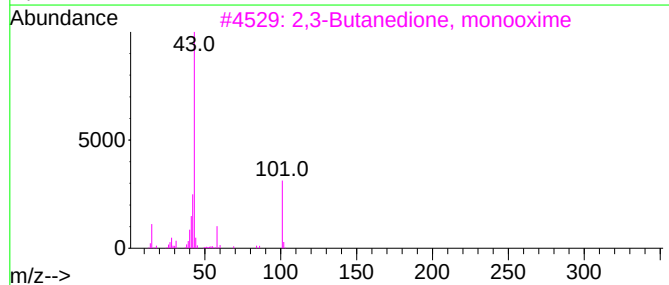
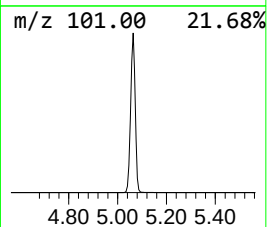
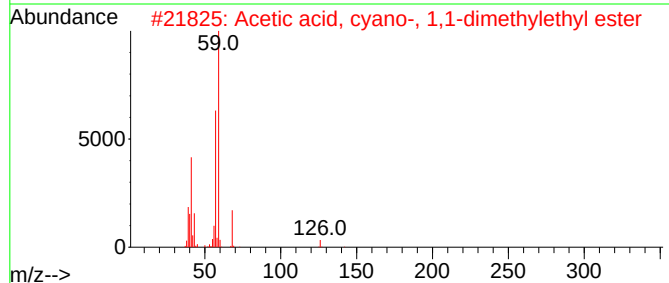
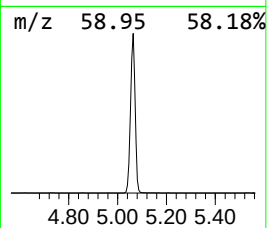
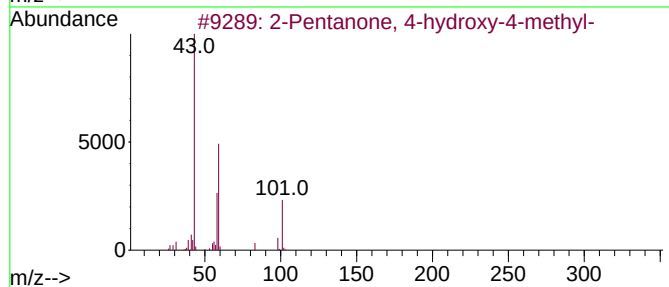
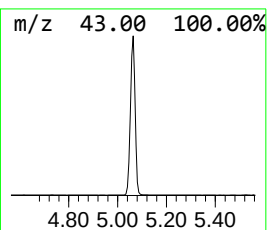
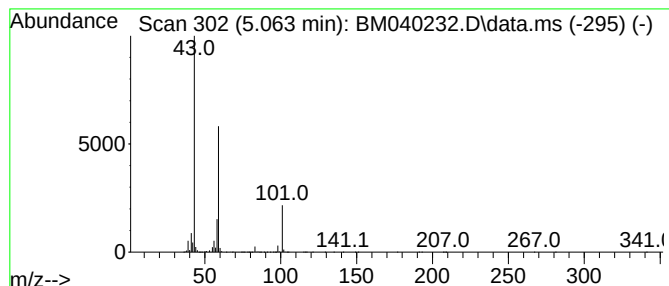
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	58.94 ng	9254330	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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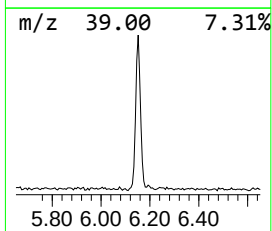
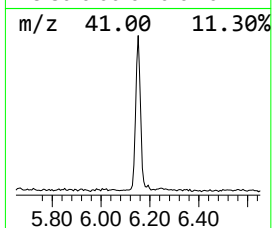
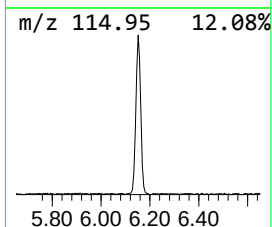
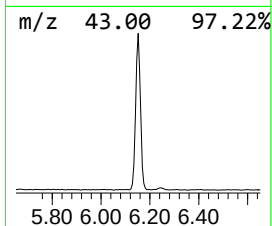
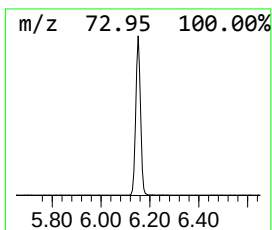
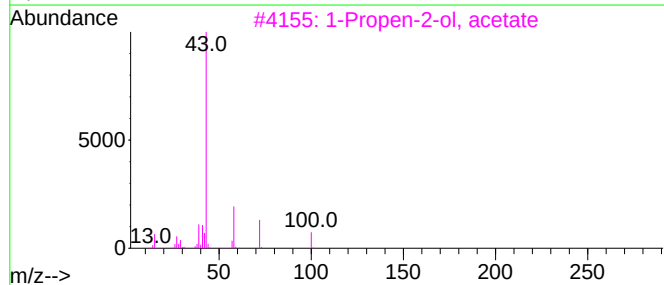
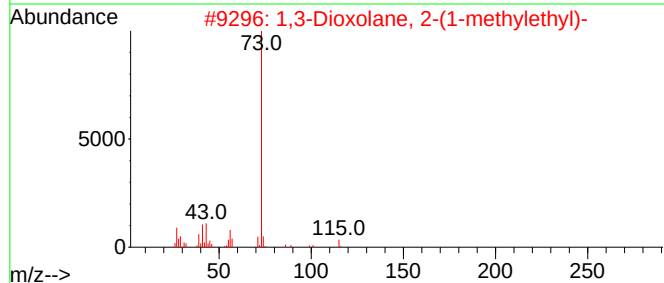
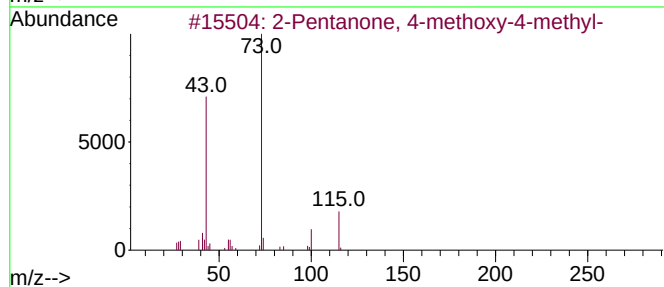
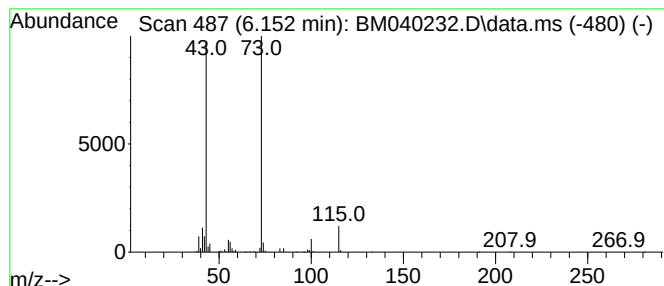
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.152	8.15 ng	1279750	1,4-Dichlorobenzene-d4	7.975

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5		Hexane, 2-methyl-	100	C7H16	000591-76-4	9



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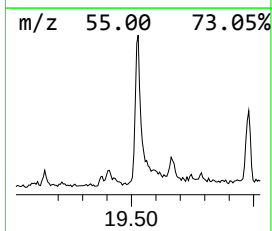
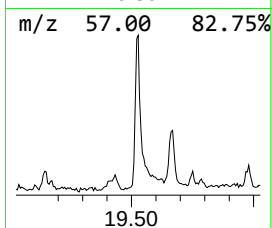
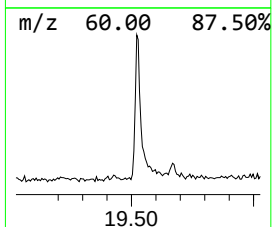
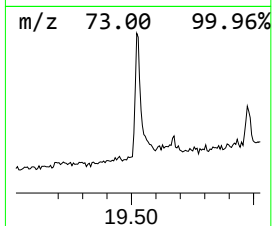
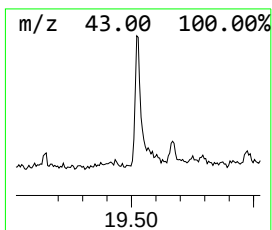
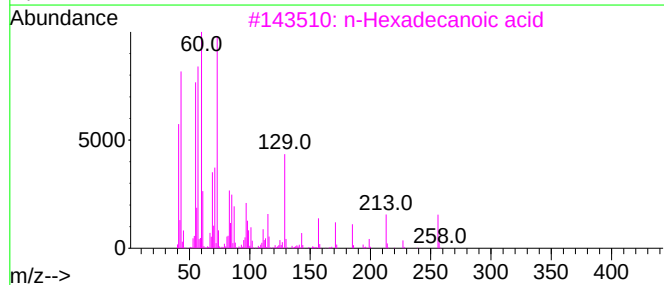
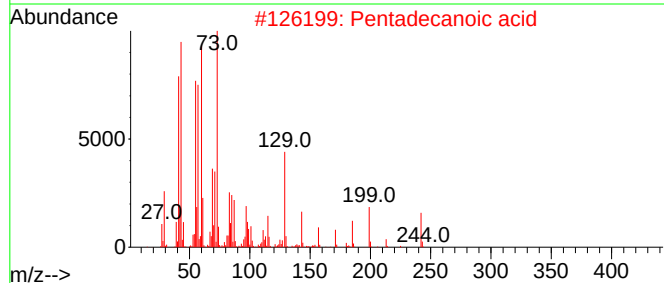
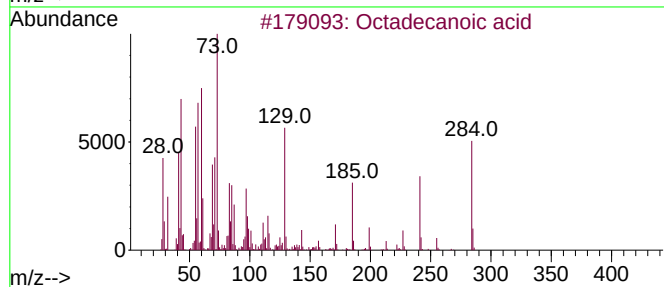
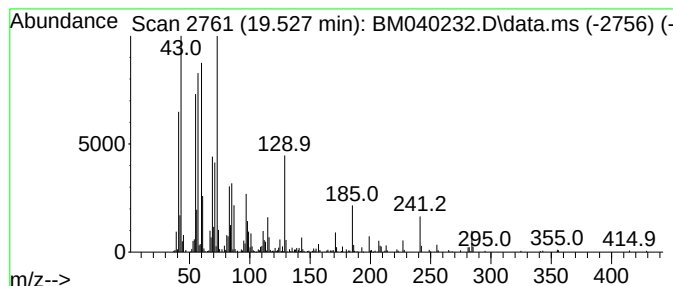
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.527	2.25 ng	659301	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.446	15.1	ng	2370540	1	7.975	3140210	20.0
2-Pentanone, 4-...	5.063	58.9	ng	9254330	1	7.975	3140210	20.0
2-Pentanone, 4-...	6.152	8.2	ng	1279750	1	7.975	3140210	20.0
Octadecanoic acid	19.527	2.3	ng	659301	5	21.533	5872460	20.0