

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
 Data File : BM046712.D
 Acq On : 18 Jul 2024 21:22
 Operator : MA/JU
 Sample : P3246-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-CTW2-BL-02

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-BM071724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046712.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	60	64	70	rBV	54346	67817	1.68%	0.300%
2	4.687	282	289	294	rBV	88486	128064	3.17%	0.567%
3	5.134	358	365	374	rBV	1683451	2321972	57.48%	10.274%
4	6.687	621	629	643	rBV	1628334	2464437	61.01%	10.904%
5	7.487	759	765	773	rVB	356330	558275	13.82%	2.470%
6	8.628	950	959	966	rBV	1057414	1634896	40.47%	7.234%
7	10.245	1227	1234	1241	rBV	417297	660109	16.34%	2.921%
8	10.998	1356	1362	1368	rBV2	26185	44251	1.10%	0.196%
9	12.745	1652	1659	1666	rVB	2532450	3638909	90.09%	16.101%
10	14.133	1887	1895	1901	rVB	581229	833672	20.64%	3.689%
11	15.633	2141	2150	2159	rBV	2006663	2798968	69.29%	12.384%
12	16.886	2357	2363	2368	rBV	652935	877989	21.74%	3.885%
13	17.821	2516	2522	2530	rBV	216460	325660	8.06%	1.441%
14	19.115	2738	2742	2750	rBV3	92708	131285	3.25%	0.581%
15	19.539	2809	2814	2820	rVB	3420677	4039406	100.00%	17.873%
16	20.850	3033	3037	3043	rBV3	157332	207065	5.13%	0.916%
17	21.109	3076	3081	3087	rBV	651698	886793	21.95%	3.924%
18	23.874	3545	3551	3560	rVB	432832	981226	24.29%	4.342%

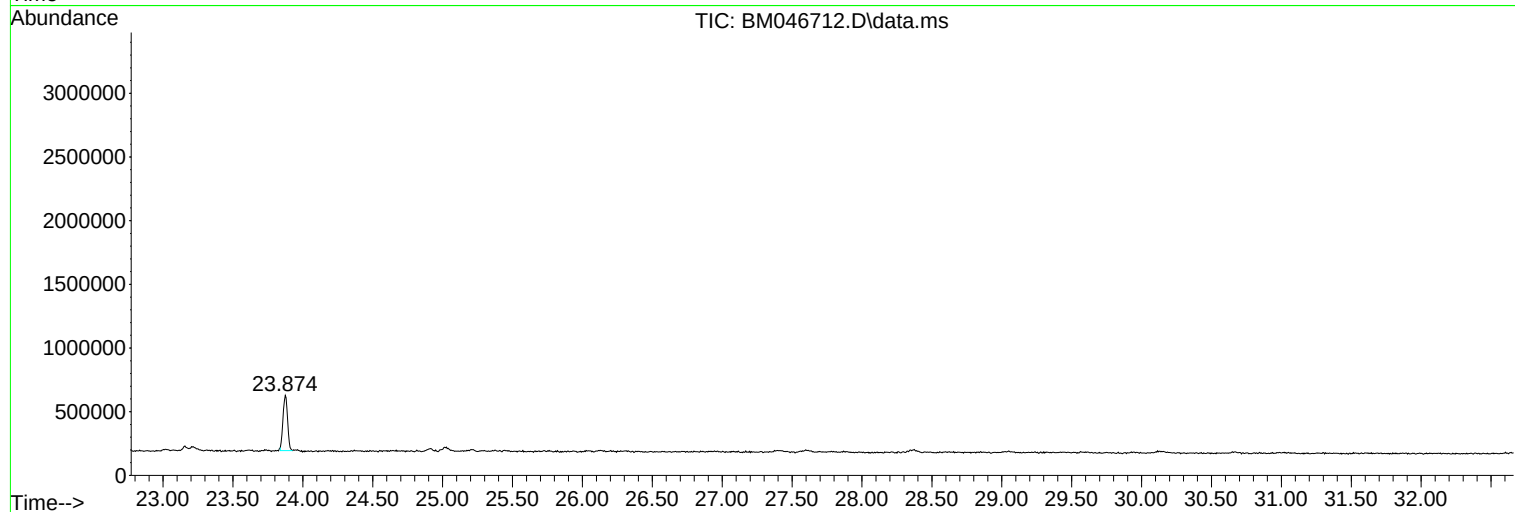
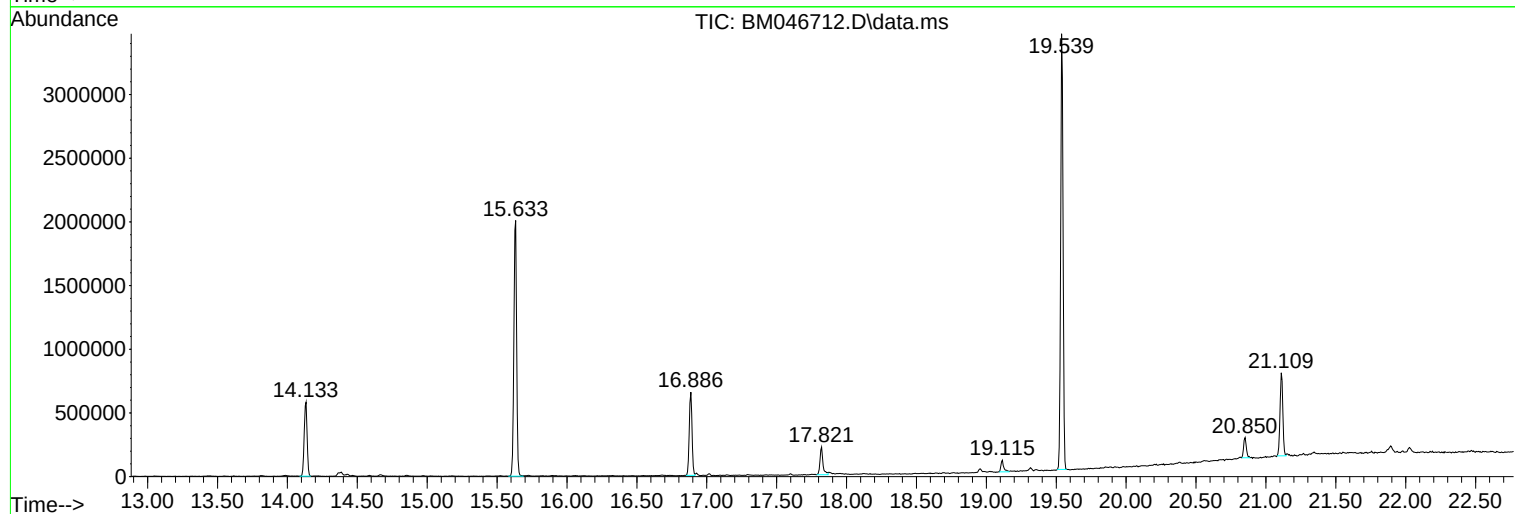
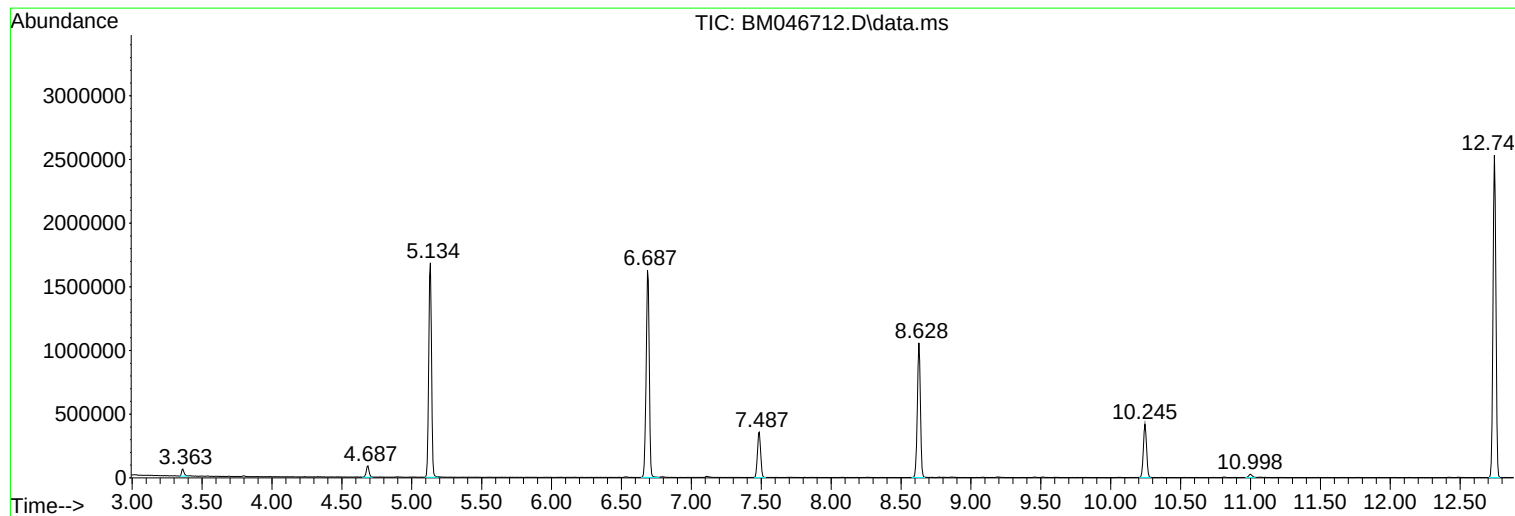
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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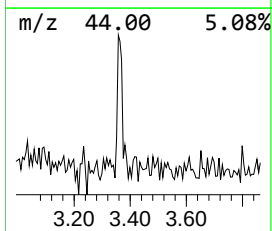
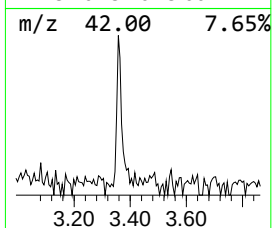
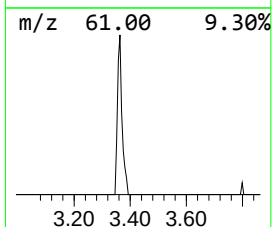
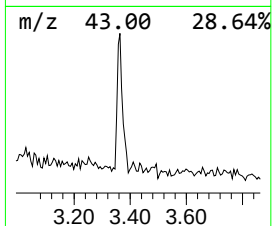
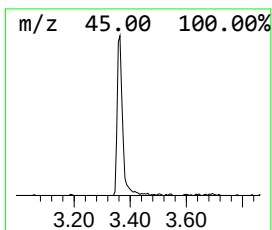
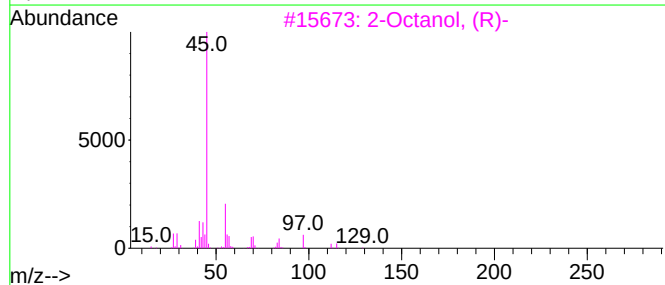
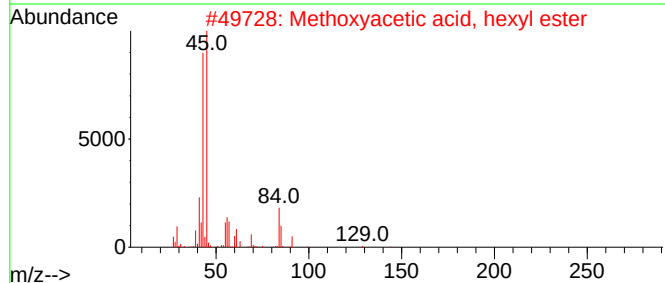
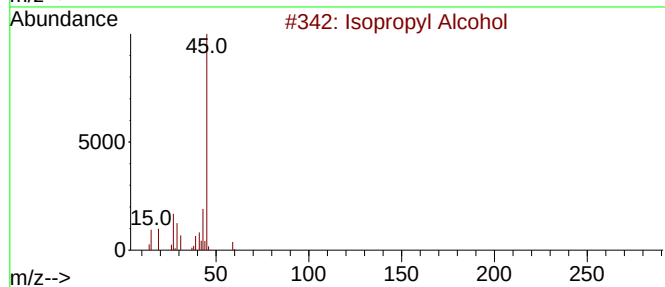
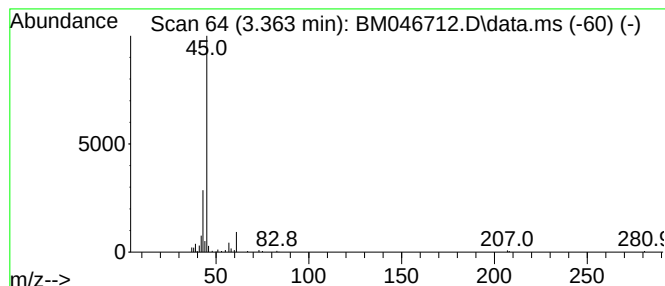
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.363 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	2.43 ng	67817	1,4-Dichlorobenzene-d4	7.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	45
2			Methoxyacetic acid, hexyl ester	174	C9H18O3	145747-16-6	9
3			2-Octanol, (R)-	130	C8H18O	005978-70-1	9
4			Propylene Glycol	76	C3H8O2	000057-55-6	9
5			2-Octanol, (S)-	130	C8H18O	006169-06-8	9



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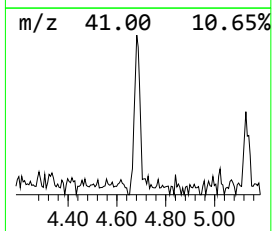
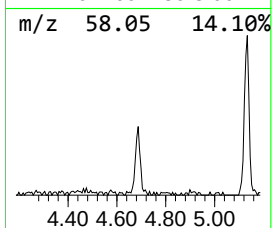
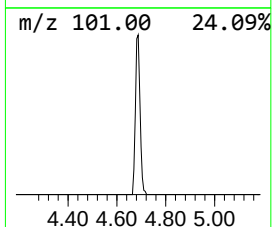
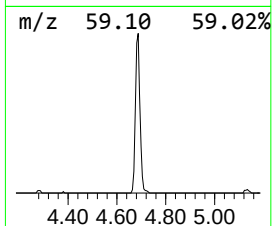
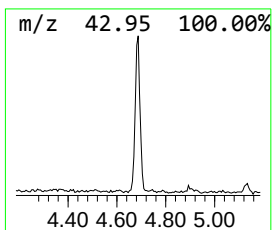
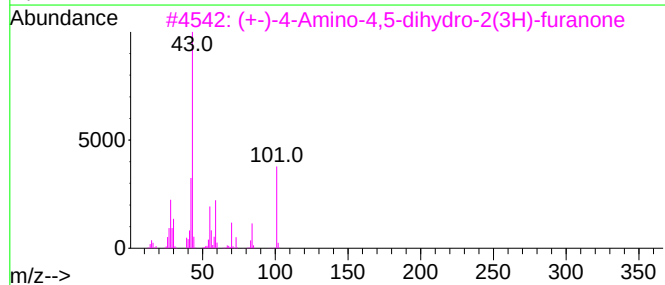
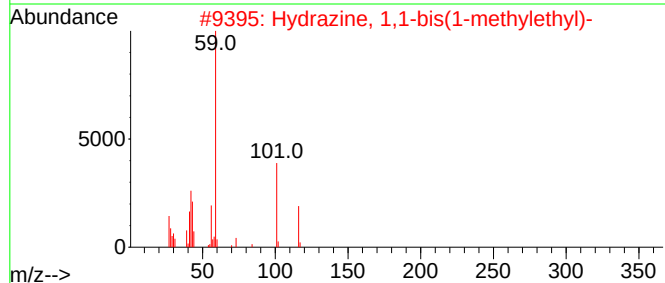
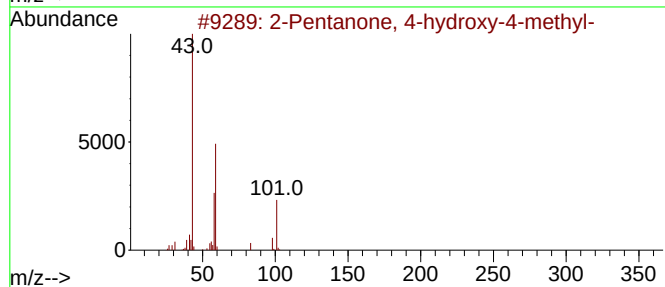
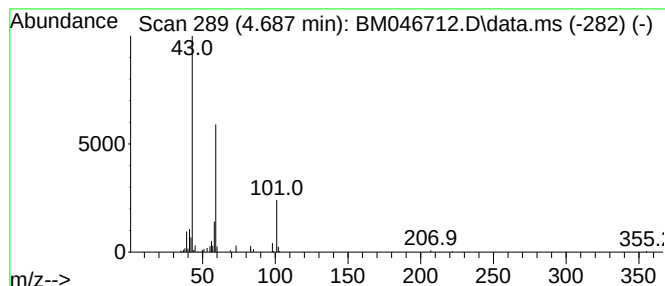
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.687	4.59 ng	128064	1,4-Dichlorobenzene-d4	7.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	47
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	35
4			Tripropylene glycol, propyl ethe...	348	C18H40O4Si	1000367-07-2	28
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27



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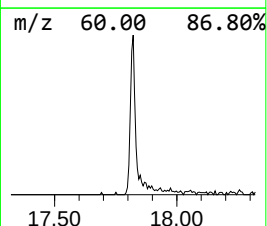
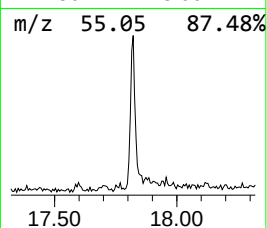
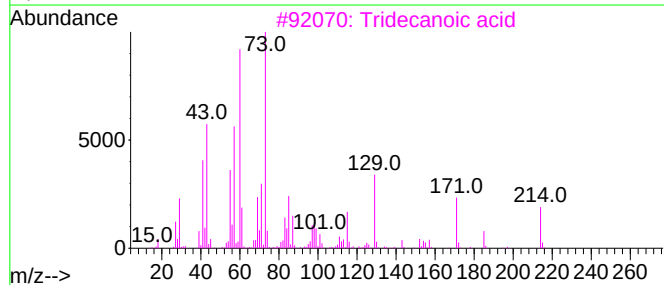
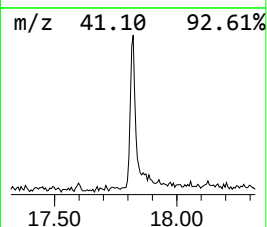
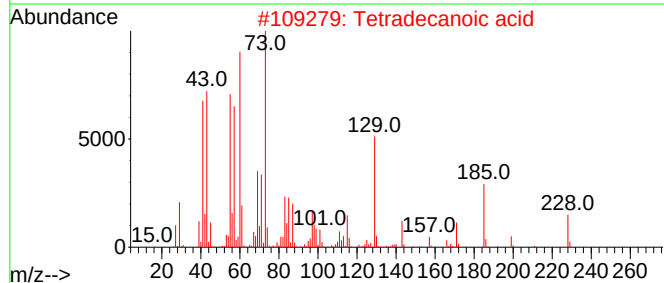
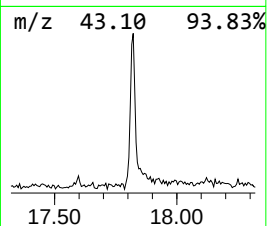
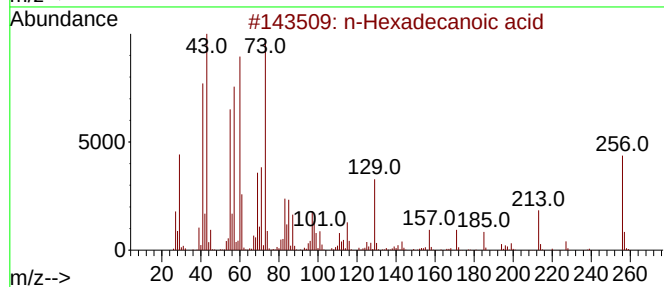
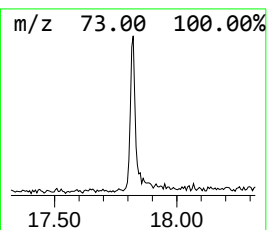
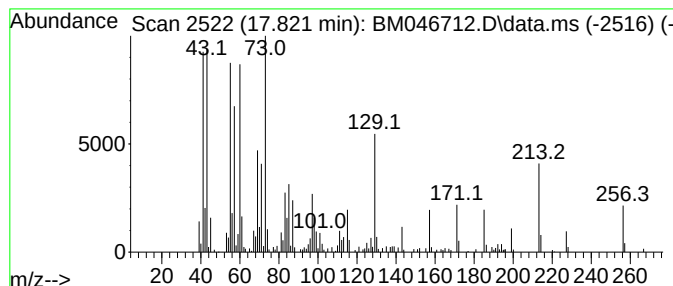
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.821	7.42 ng	325660	Phenanthrene-d10	16.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	92
3			Tridecanoic acid	214	C13H26O2	000638-53-9	78
4			n-Decanoic acid	172	C10H20O2	000334-48-5	66
5			Undecanoic acid	186	C11H22O2	000112-37-8	43



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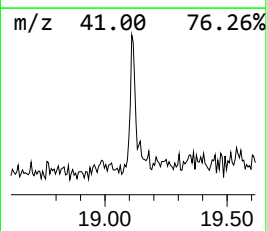
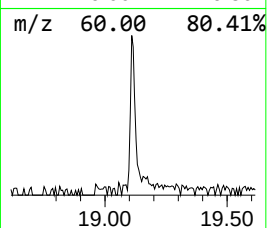
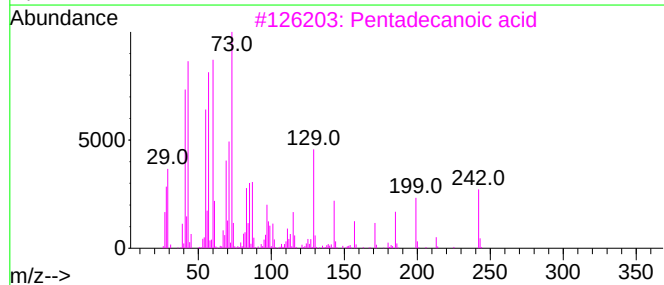
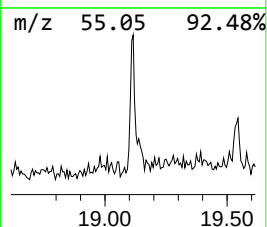
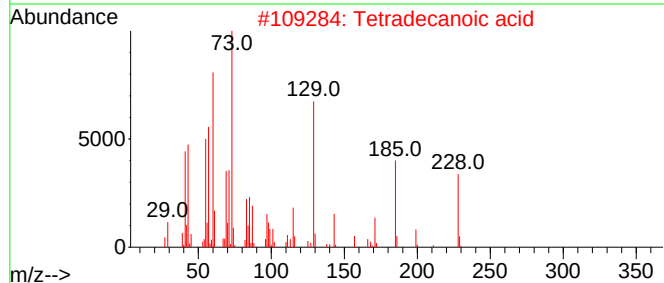
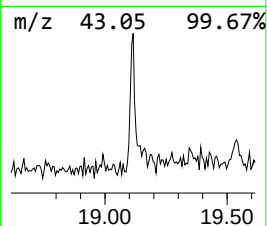
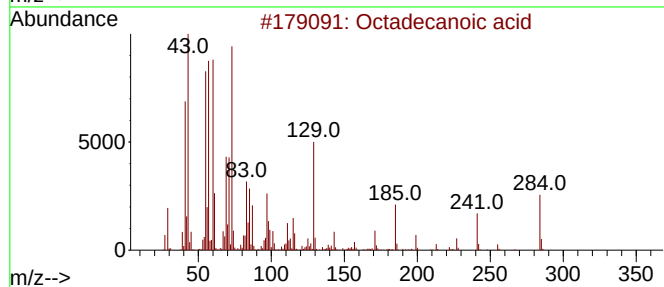
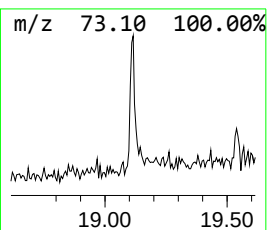
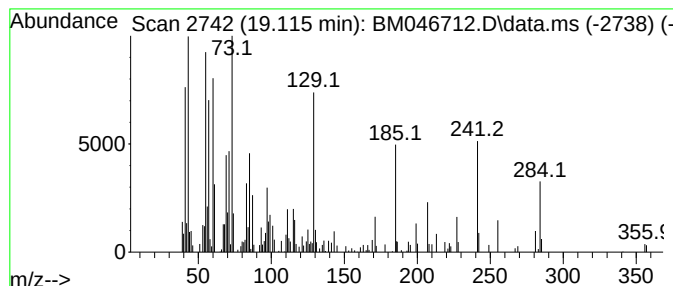
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.115	2.96 ng	131285	Chrysene-d12	21.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4			n-Decanoic acid	172	C10H20O2	000334-48-5	46
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	38



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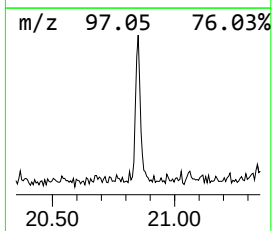
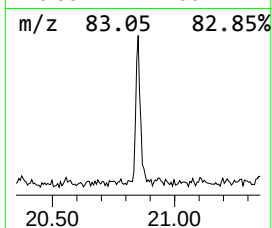
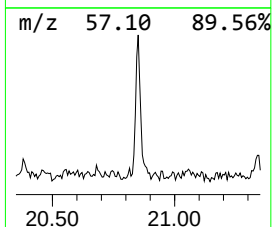
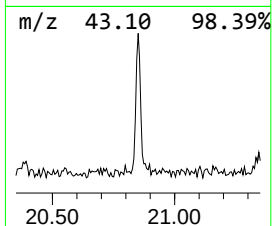
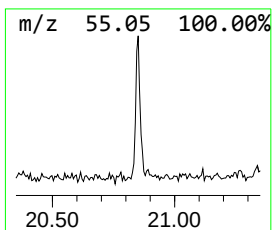
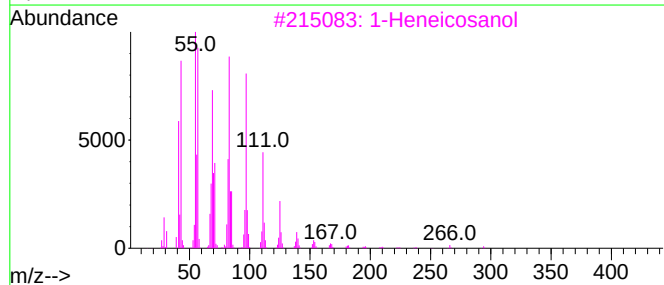
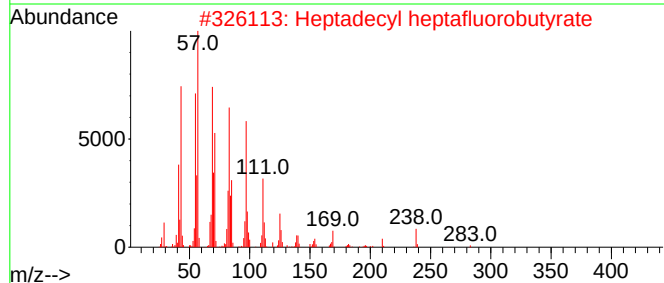
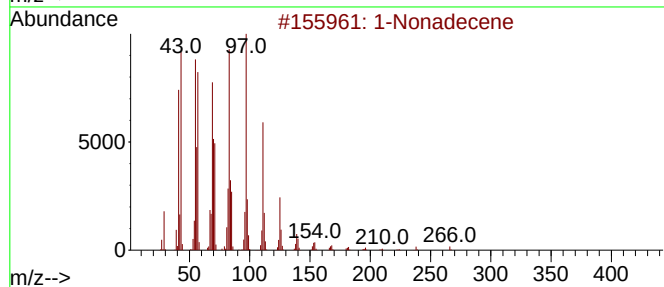
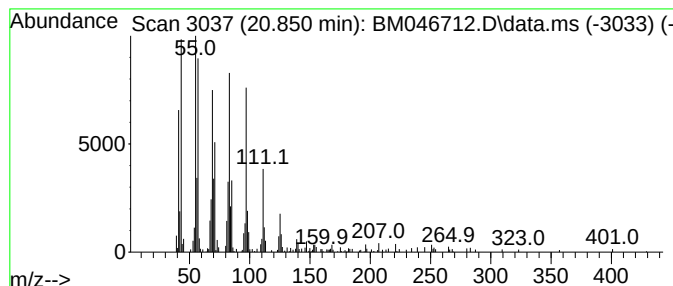
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Peak Number 5 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.850	4.67 ng	207065	Chrysene-d12	21.109	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	98
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	1-Hexacosanol	382	C26H54O	000506-52-5	91



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.363	3.363	2.4	ng	67817	1	7.487	558275	20.0
2-Pentanone, 4-...	4.687	4.6	ng	128064	1	7.487	558275	20.0
n-Hexadecanoic ...	17.821	7.4	ng	325660	4	16.886	877989	20.0
Octadecanoic acid	19.115	3.0	ng	131285	5	21.109	886793	20.0
1-Nonadecene	20.850	4.7	ng	207065	5	21.109	886793	20.0