

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
 Data File : BM042428.D
 Acq On : 24 Oct 2023 20:19
 Operator : MA/JU
 Sample : 04976-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 NB-426-COMP-01

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042428.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	316	321	330	rVB	341233	457669	9.28%	1.433%
2	5.522	390	397	408	rBV	2027617	2848456	57.74%	8.919%
3	7.145	666	673	688	rBV	2016243	3092569	62.69%	9.683%
4	7.587	743	748	759	rBV	30199	53211	1.08%	0.167%
5	7.992	810	817	826	rBV	564452	881986	17.88%	2.762%
6	9.192	1011	1021	1030	rBV	1215677	1983851	40.22%	6.212%
7	10.816	1289	1297	1304	rBV	764248	1249999	25.34%	3.914%
8	13.263	1706	1713	1721	rBV	2508824	3638990	73.77%	11.394%
9	13.480	1743	1750	1760	rBV	154987	245547	4.98%	0.769%
10	14.639	1940	1947	1957	rVB	1086740	1523481	30.88%	4.770%
11	16.127	2192	2200	2214	rBV	1970408	2811256	56.99%	8.802%
12	17.392	2407	2415	2428	rBV	1280751	1817180	36.84%	5.690%
13	18.239	2553	2559	2578	rBV	740894	1195220	24.23%	3.742%
14	19.515	2771	2776	2792	rBV	368445	614348	12.45%	1.924%
15	20.003	2853	2859	2865	rBV	4214998	4932980	100.00%	15.446%
16	20.750	2984	2986	2991	rVB	49418	51575	1.05%	0.161%
17	21.233	3063	3068	3077	rBV	328680	583453	11.83%	1.827%
18	21.439	3100	3103	3106	rVB2	57368	60831	1.23%	0.190%
19	21.574	3121	3126	3134	rBV	1482659	1892353	38.36%	5.925%
20	24.038	3538	3545	3553	rVB	963798	2002372	40.59%	6.270%

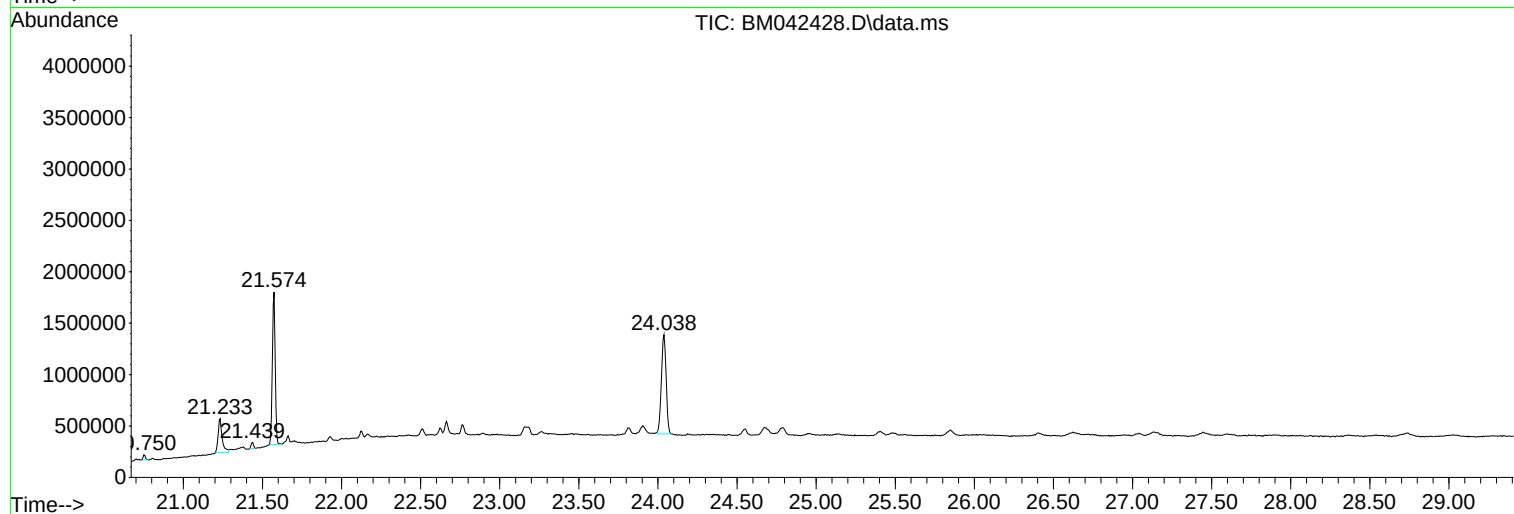
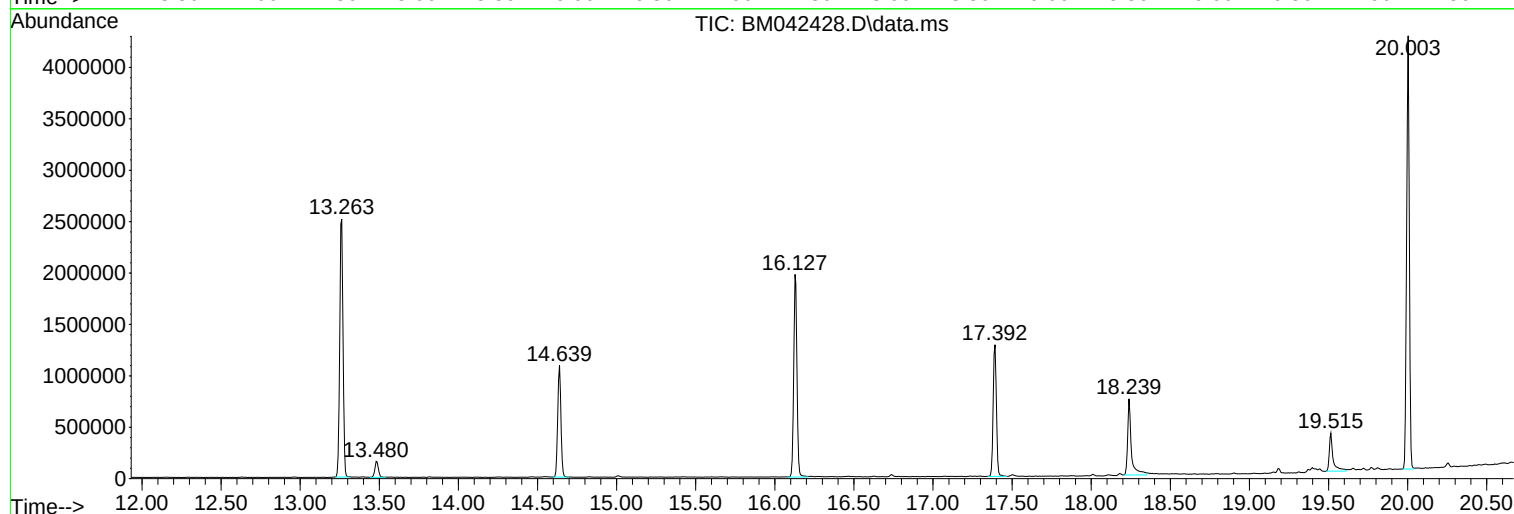
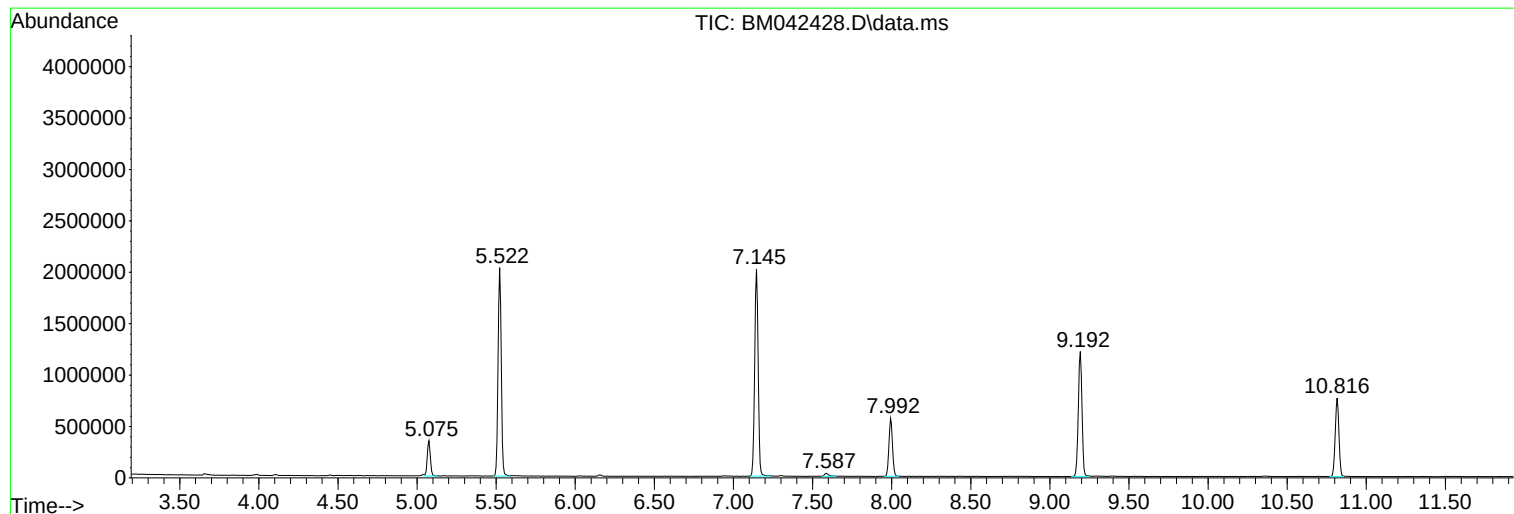
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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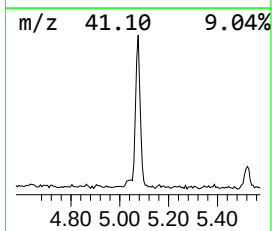
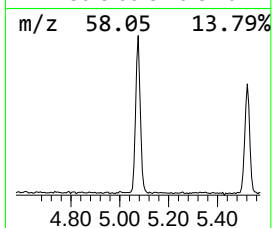
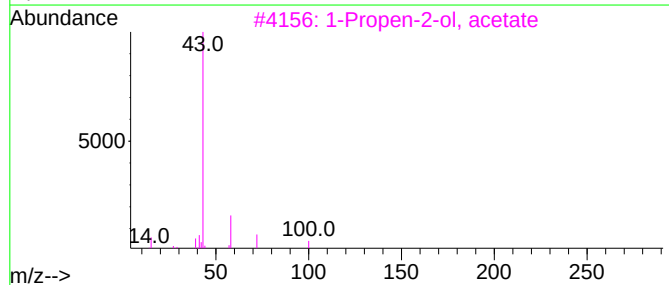
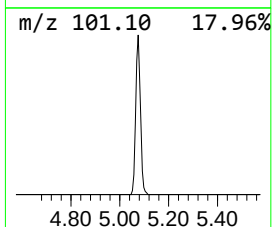
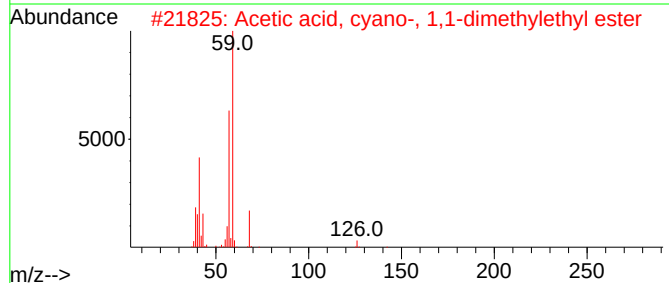
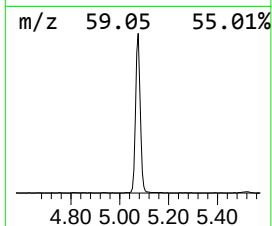
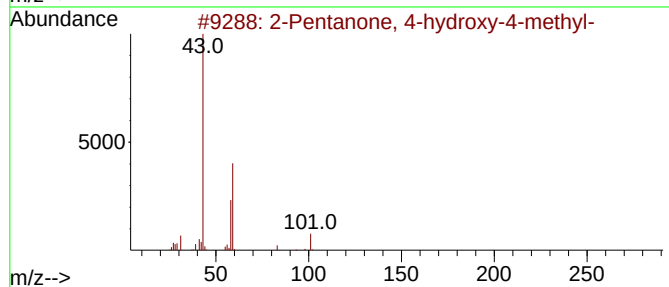
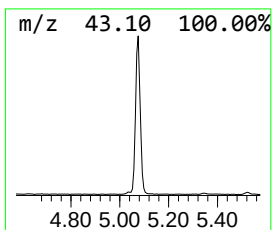
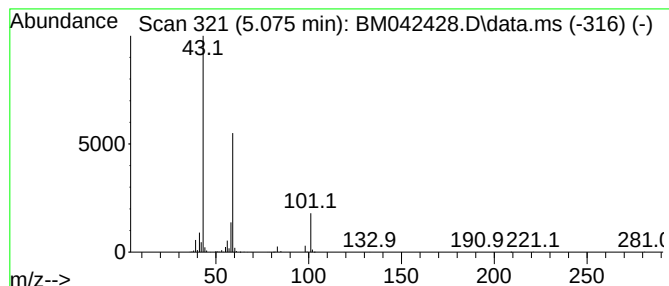
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.075	10.38 ng	457669	1,4-Dichlorobenzene-d4	7.992	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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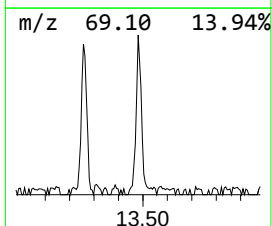
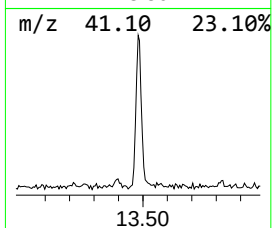
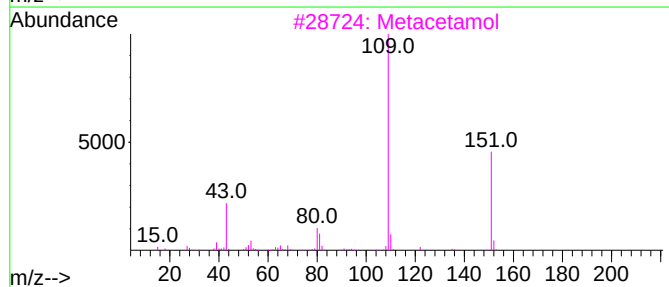
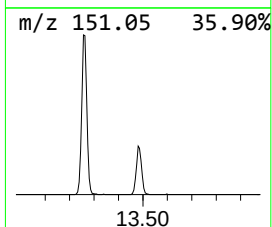
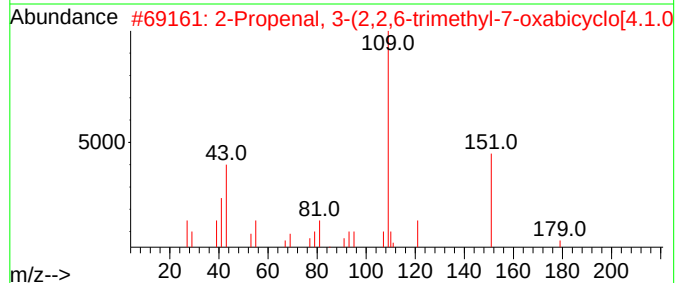
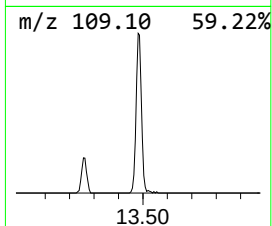
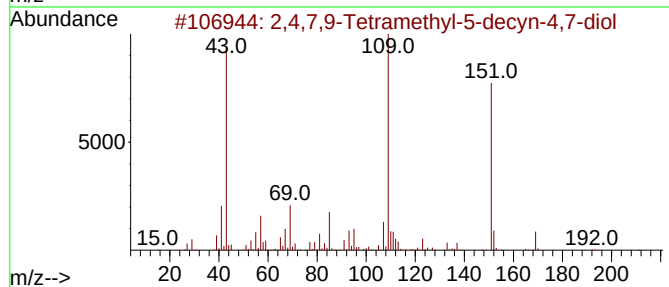
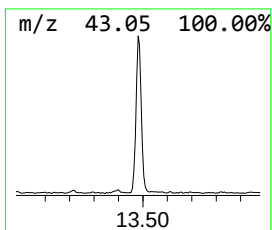
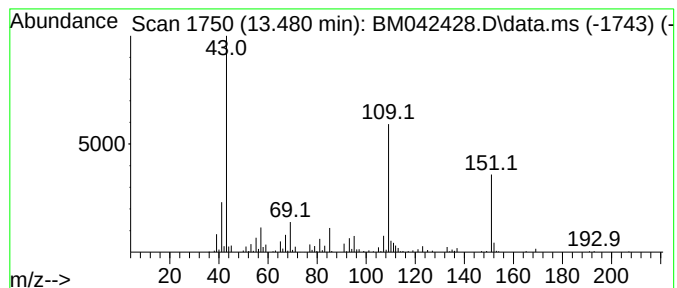
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.480	3.22 ng	245547	Acenaphthene-d10	14.639

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	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59	
3	Metacetamol	151	C8H9NO2	000621-42-1	49	
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	47	
5	Acetaminophen	151	C8H9NO2	000103-90-2	47	



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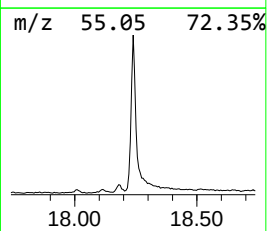
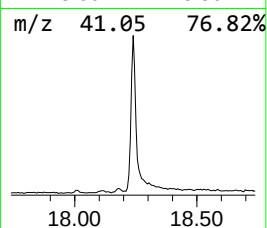
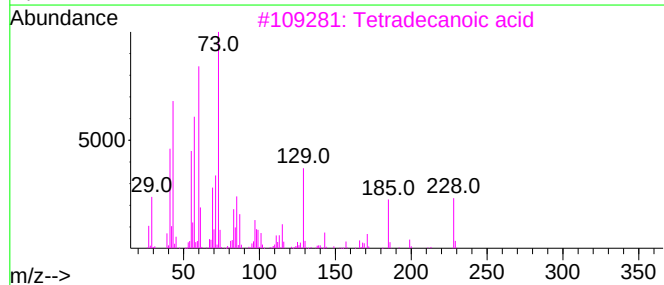
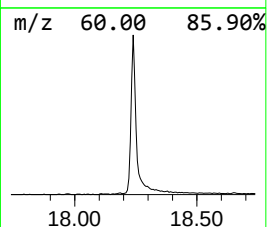
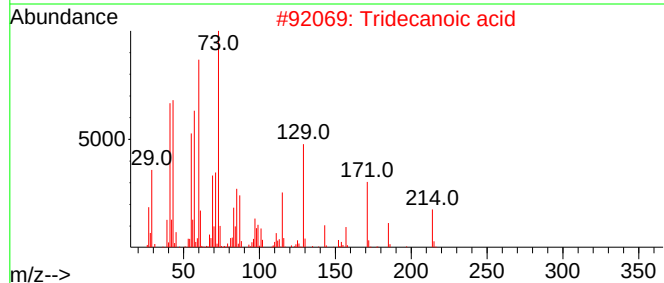
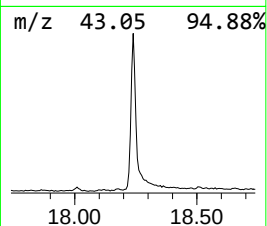
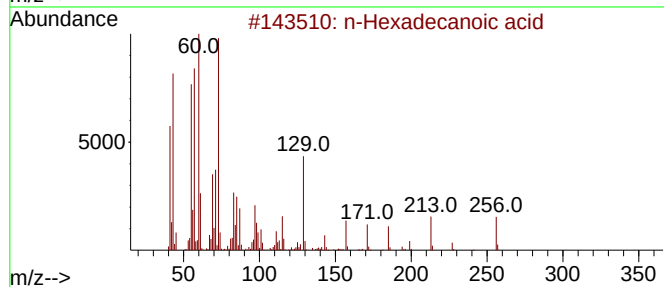
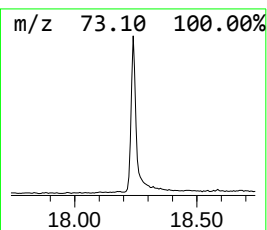
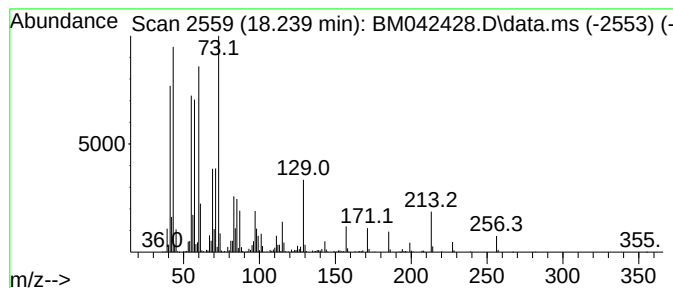
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	13.15 ng	1195220	Phenanthrene-d10	17.392

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	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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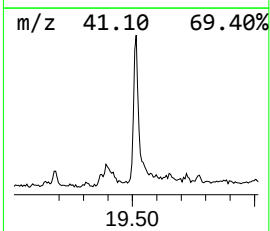
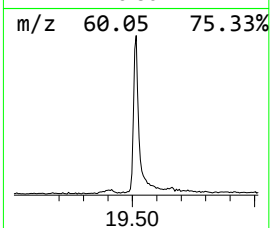
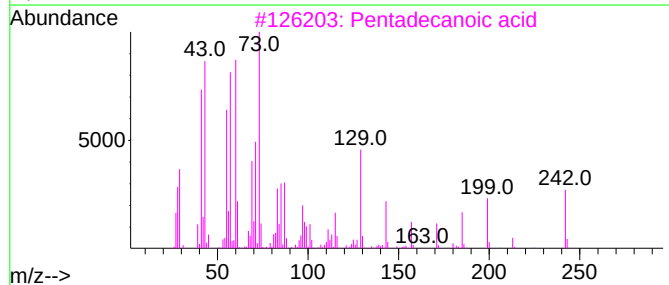
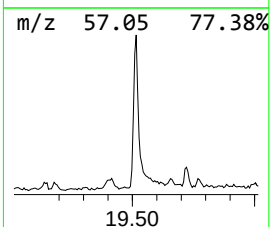
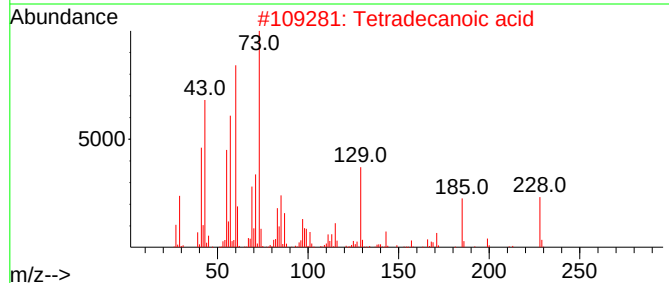
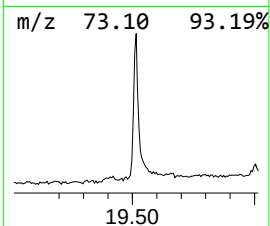
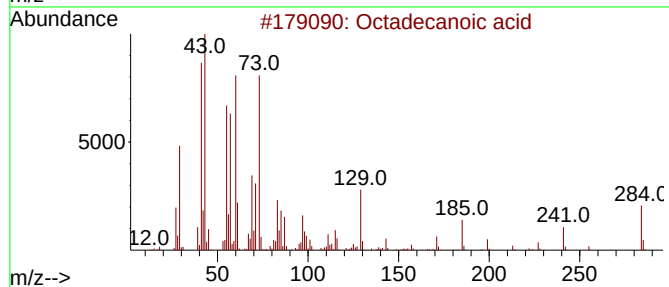
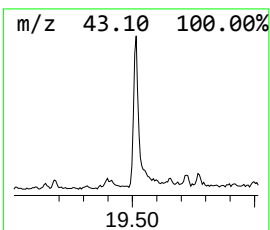
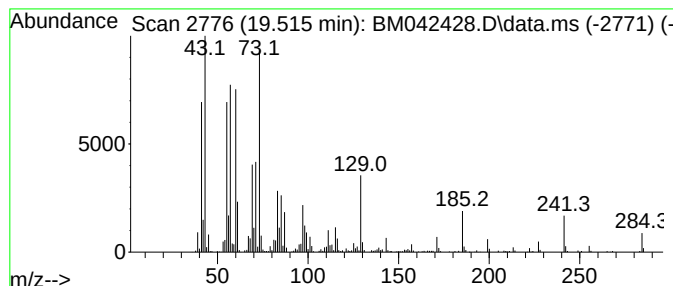
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	6.49 ng	614348	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



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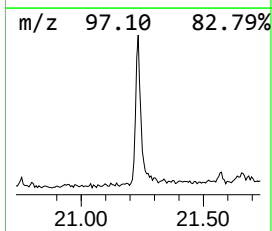
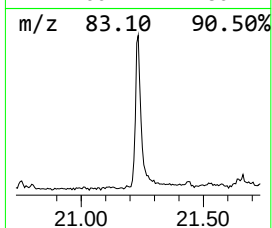
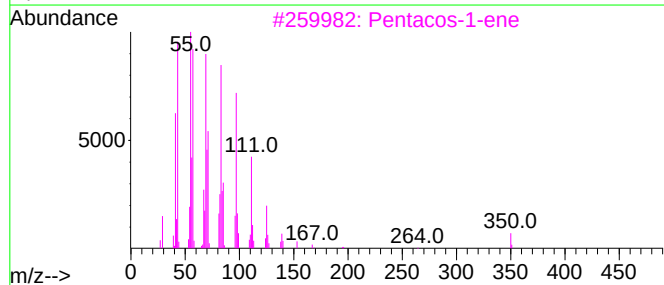
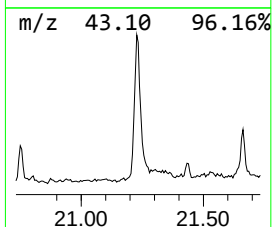
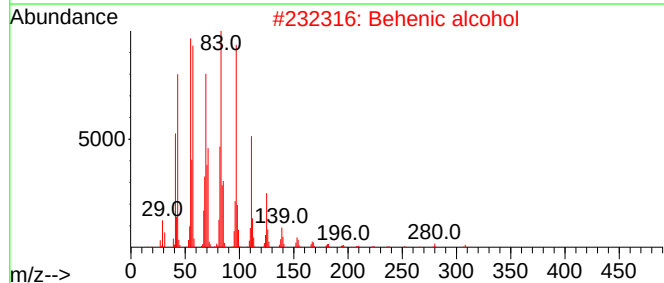
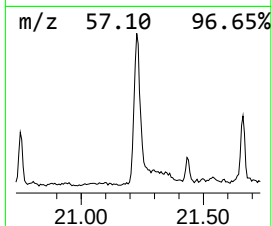
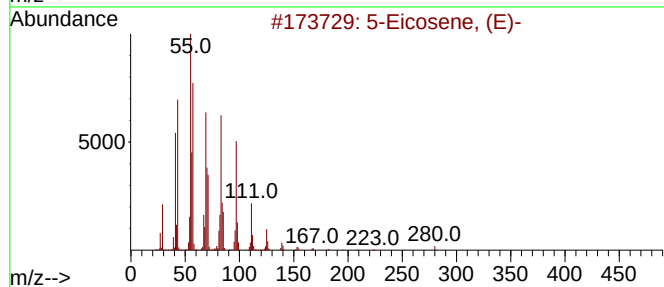
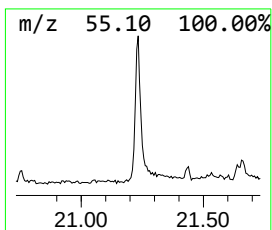
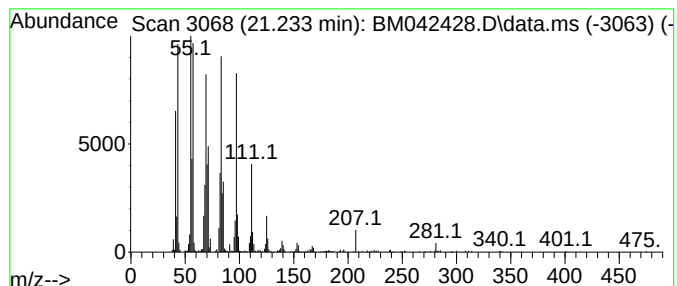
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	6.17 ng	583453	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.075	10.4	ng	457669	1	7.992	881986	20.0
2,4,7,9-Tetrame...	13.480	3.2	ng	245547	3	14.639	1523480	20.0
n-Hexadecanoic ...	18.239	13.2	ng	1195220	4	17.392	1817180	20.0
Octadecanoic acid	19.515	6.5	ng	614348	5	21.574	1892350	20.0
5-Eicosene, (E)-	21.233	6.2	ng	583453	5	21.574	1892350	20.0