

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102323\
 Data File : BM042410.D
 Acq On : 23 Oct 2023 19:59
 Operator : MA/JU
 Sample : 04945-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PAT-2-101823

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: BM042410.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	280946	379447	6.97%	1.179%
2	5.522	390	397	405	rBV	2427675	3386154	62.16%	10.522%
3	7.146	664	673	687	rBV	2322751	3535755	64.91%	10.987%
4	7.993	810	817	826	rBV	564634	889676	16.33%	2.764%
5	9.192	1011	1021	1031	rBV	1321374	2131954	39.14%	6.625%
6	10.816	1289	1297	1304	rBV	693531	1147449	21.06%	3.565%
7	13.263	1706	1713	1720	rVB	2582171	3608327	66.24%	11.212%
8	14.639	1941	1947	1955	rVB	903263	1272834	23.37%	3.955%
9	16.127	2194	2200	2211	rVB	1900835	2657817	48.79%	8.259%
10	17.392	2409	2415	2420	rBV	1093477	1515351	27.82%	4.709%
11	17.433	2420	2422	2429	rVB	47463	57667	1.06%	0.179%
12	18.239	2553	2559	2569	rBV	363276	600183	11.02%	1.865%
13	19.445	2759	2764	2771	rVB	155875	209137	3.84%	0.650%
14	19.515	2771	2776	2786	rBV	209029	343287	6.30%	1.067%
15	19.809	2822	2826	2833	rVB	168699	225721	4.14%	0.701%
16	20.004	2854	2859	2867	rBV	4681023	5447290	100.00%	16.926%
17	20.256	2899	2902	2907	rBV3	51040	79806	1.47%	0.248%
18	21.239	3063	3069	3075	rBV4	219765	447107	8.21%	1.389%
19	21.574	3120	3126	3130	rBV	1496276	2001408	36.74%	6.219%
20	21.609	3130	3132	3138	rVB	124296	147490	2.71%	0.458%
21	23.821	3504	3508	3516	rVB2	145291	272541	5.00%	0.847%
22	24.039	3539	3545	3552	rBV	906816	1826073	33.52%	5.674%

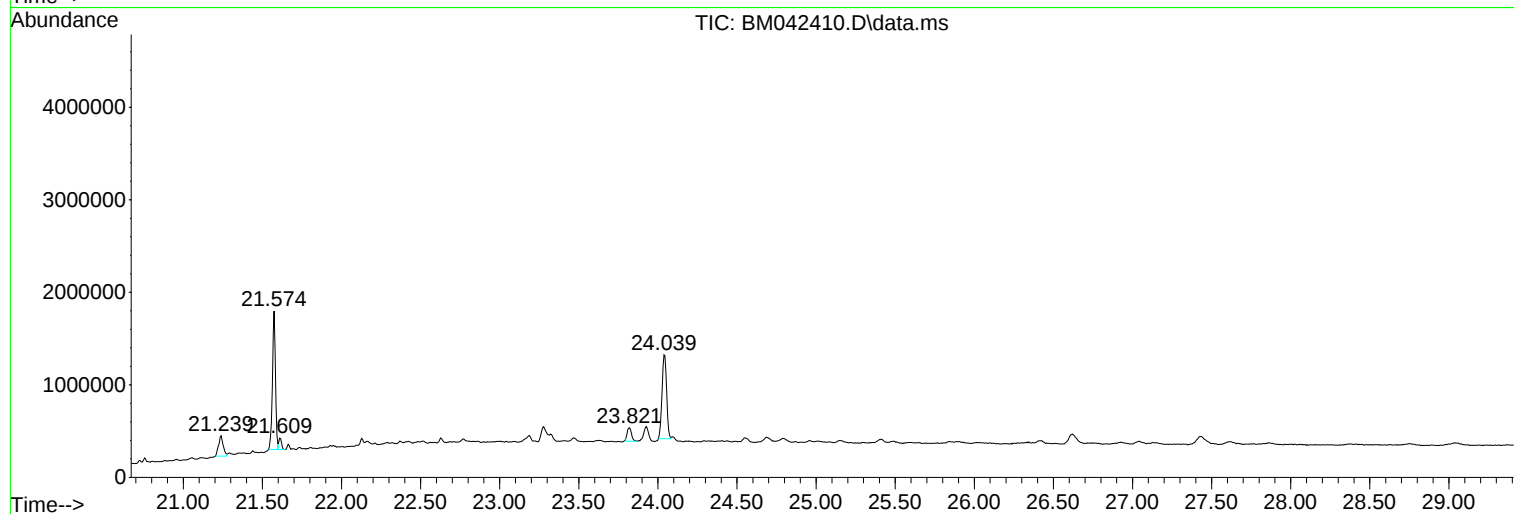
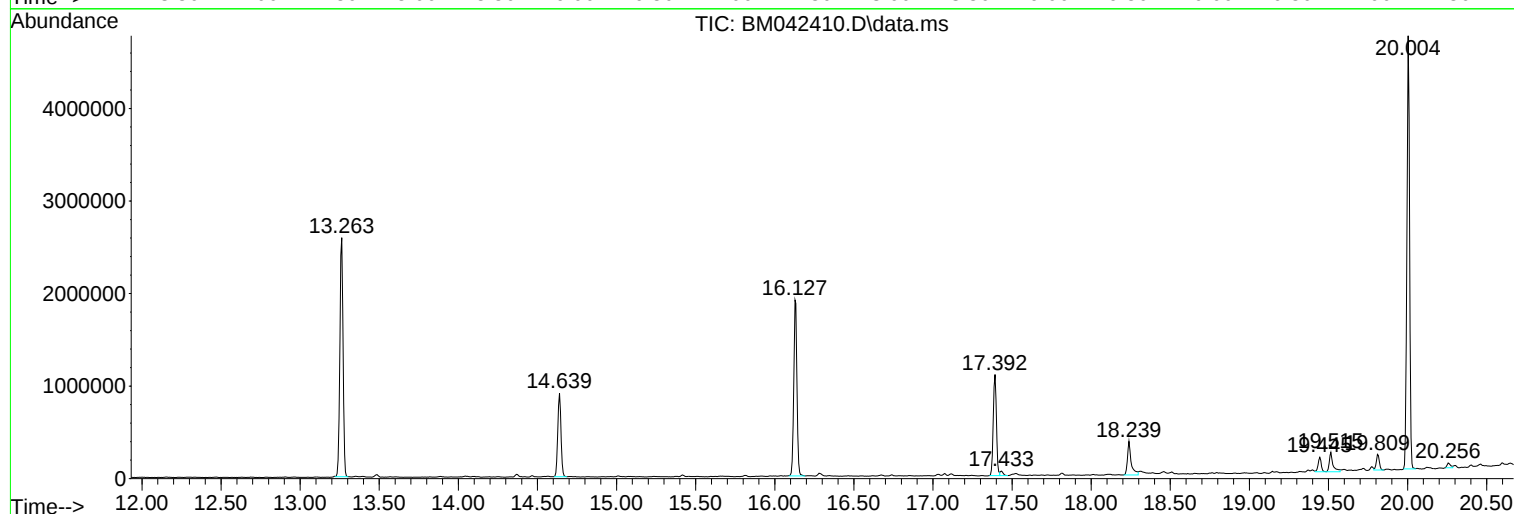
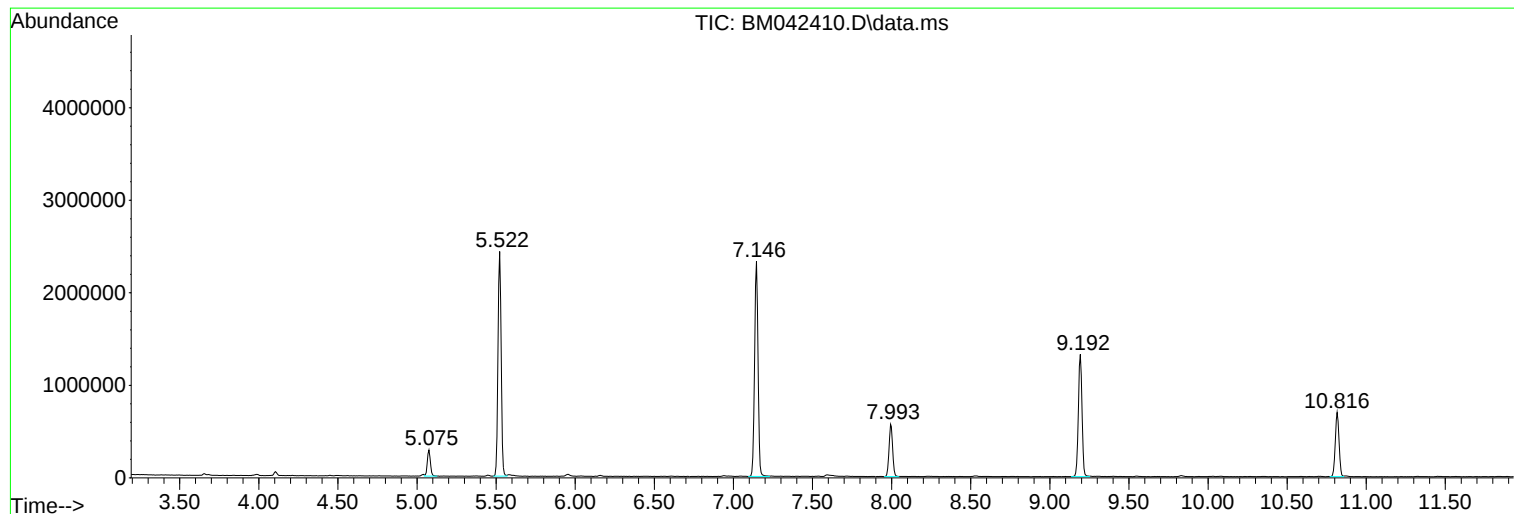
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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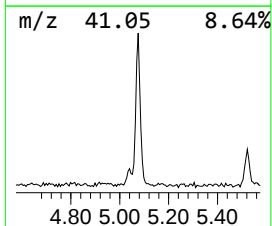
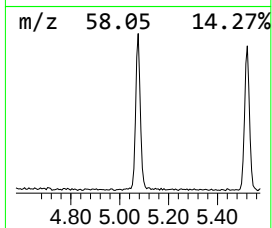
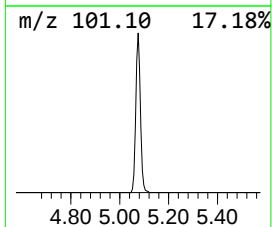
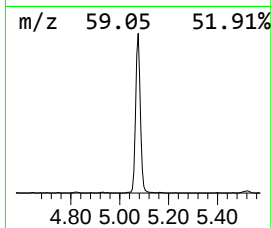
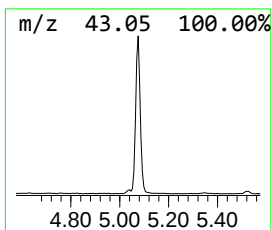
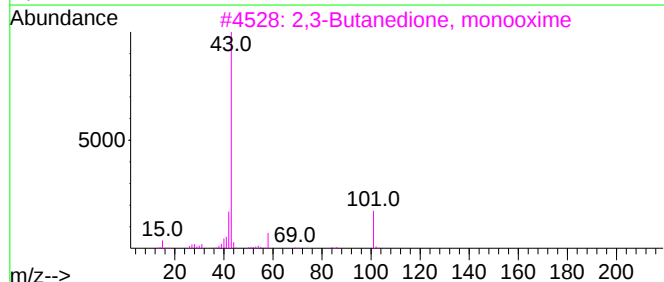
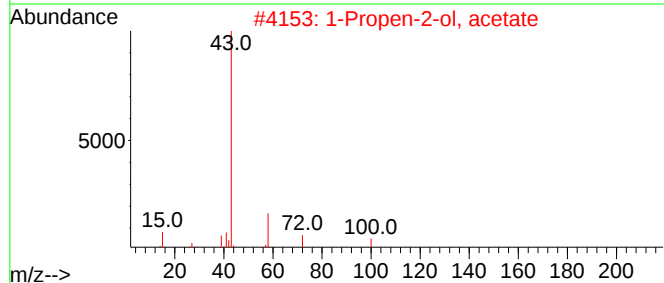
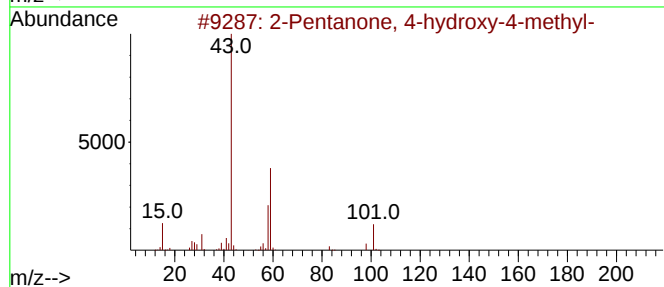
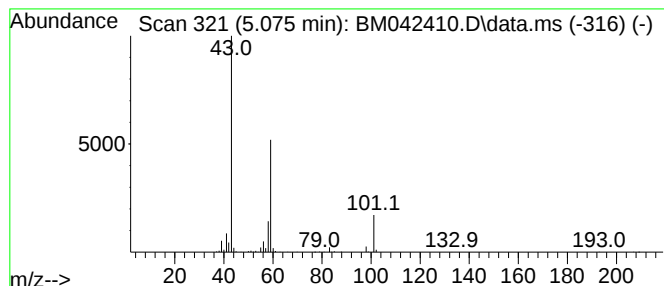
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	8.53 ng	379447	1,4-Dichlorobenzene-d4	7.993

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		



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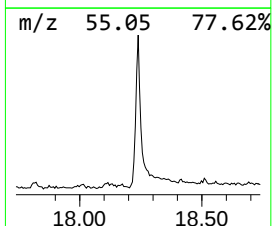
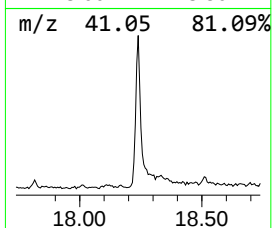
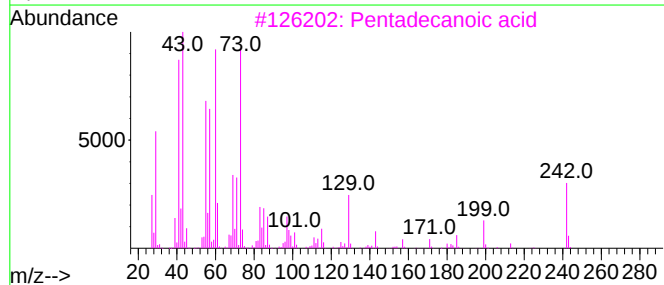
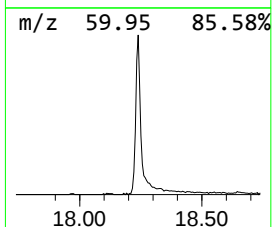
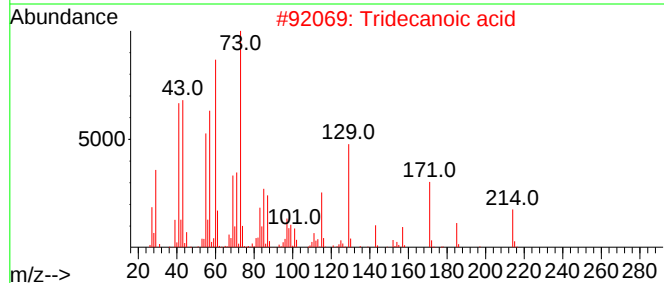
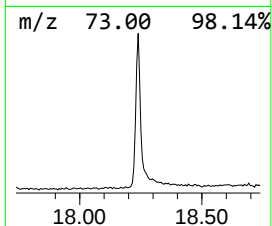
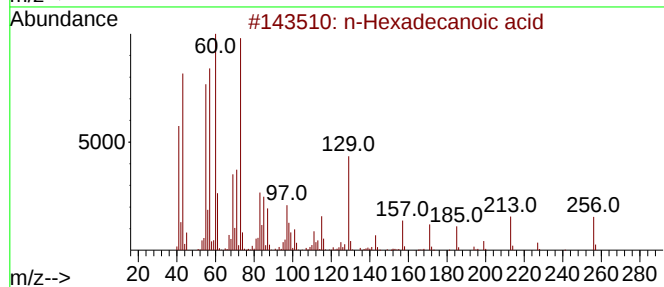
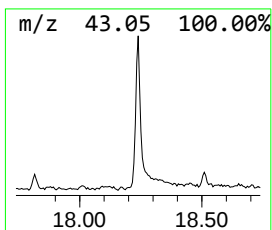
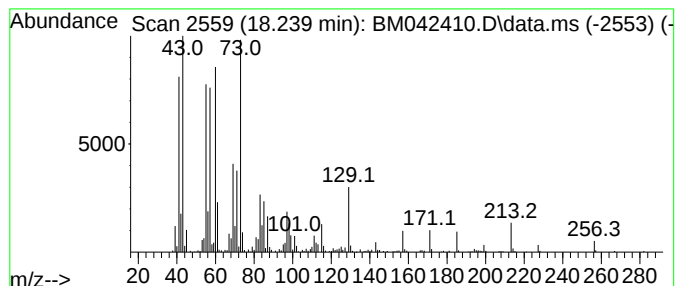
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	7.92 ng	600183	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	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		Isopropyl palmitate	298	C19H38O2	000142-91-6	59



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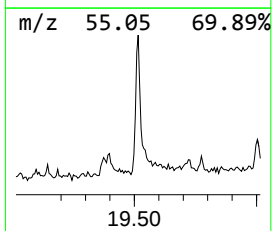
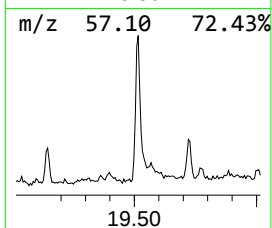
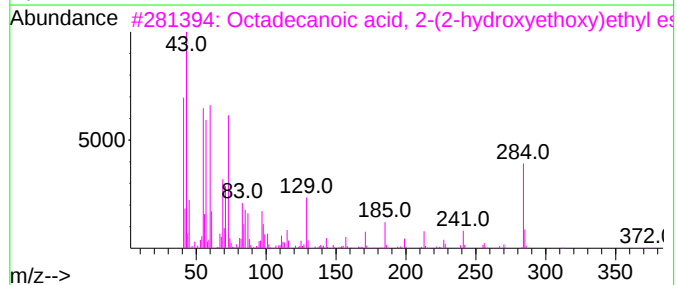
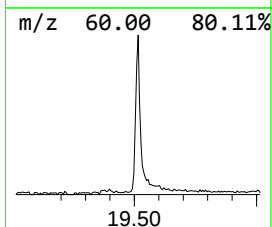
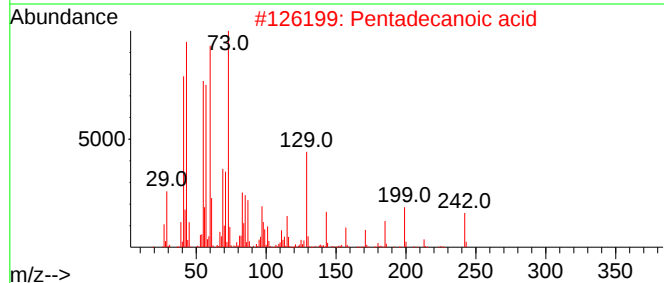
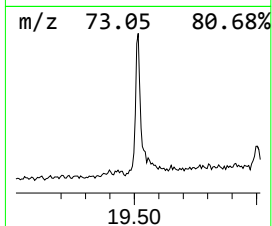
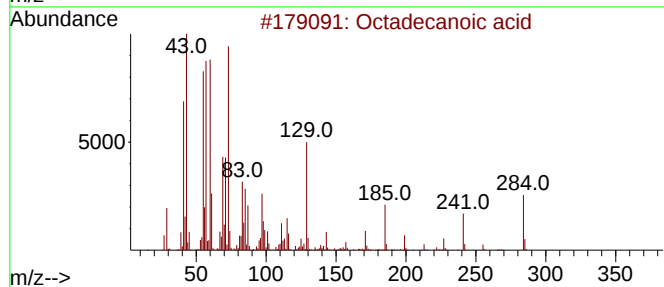
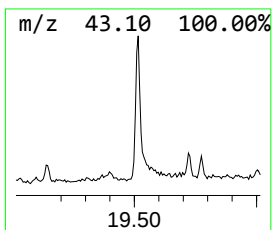
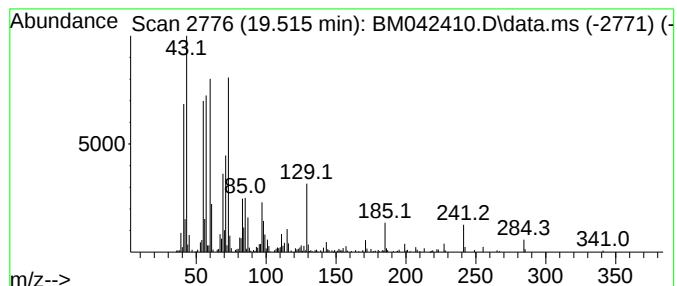
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	3.43 ng	343287	Chrysene-d12	21.574

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	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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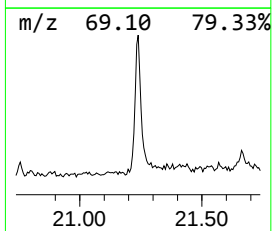
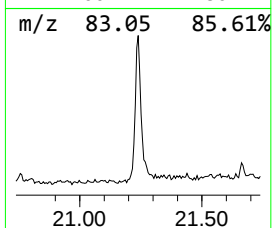
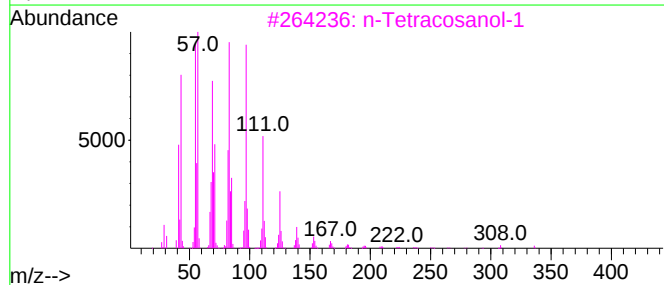
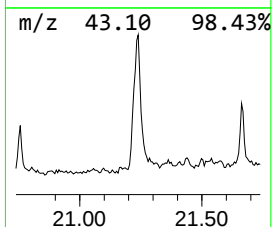
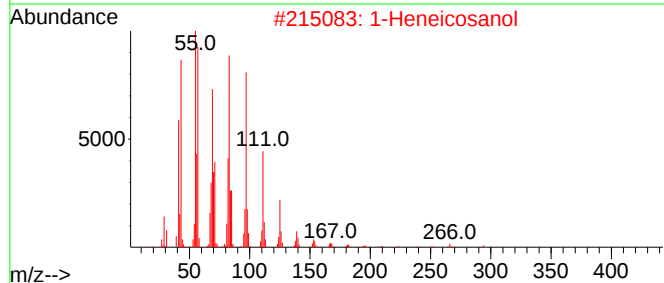
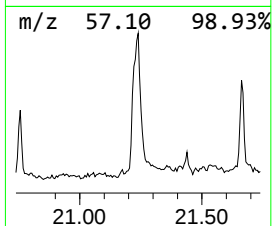
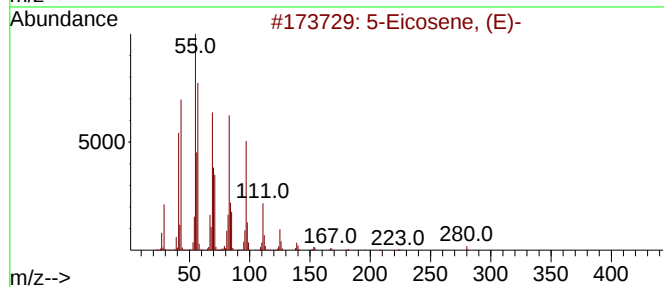
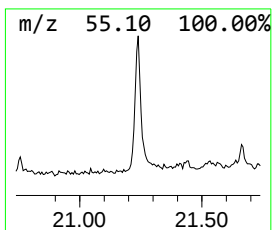
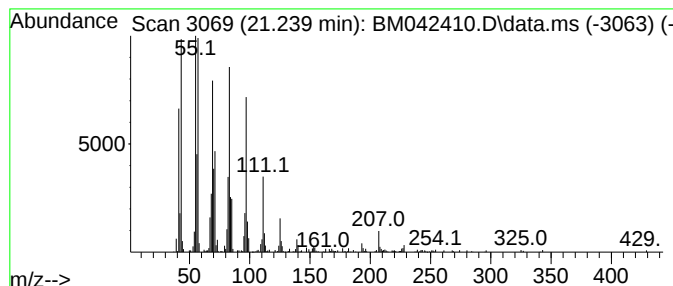
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.239	4.47 ng	447107	Chrysene-d12	21.574

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	1-Heneicosanol		312	C21H44O	015594-90-8	94
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
4	Cyclotetracosane		336	C24H48	000297-03-0	93
5	1-Docosene		308	C22H44	001599-67-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.075	8.5	ng	379447	1	7.993	889676	20.0
n-Hexadecanoic ...	18.239	7.9	ng	600183	4	17.392	1515350	20.0
Octadecanoic acid	19.515	3.4	ng	343287	5	21.574	2001410	20.0
5-Eicosene, (E)-	21.239	4.5	ng	447107	5	21.574	2001410	20.0