

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102323\
 Data File : BM042399.D
 Acq On : 23 Oct 2023 13:18
 Operator : MA/JU
 Sample : 04844-09
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 OR-603-COMP-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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042399.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	317	321	329	rVB	127822	172801	3.13%	0.477%
2	5.522	390	397	411	rBV	2254395	3163210	57.38%	8.731%
3	7.145	664	673	688	rBV	2168413	3340741	60.60%	9.221%
4	7.992	809	817	829	rBV	641587	1023981	18.57%	2.826%
5	9.192	1007	1021	1031	rBV	1222717	1998596	36.25%	5.516%
6	10.704	1272	1278	1283	rBV	42459	61067	1.11%	0.169%
7	10.816	1290	1297	1304	rBV	826976	1367582	24.81%	3.775%
8	12.157	1520	1525	1533	rBV	75828	108073	1.96%	0.298%
9	13.263	1706	1713	1724	rBV	2519792	3623475	65.73%	10.001%
10	13.398	1729	1736	1741	rVV	69376	101146	1.83%	0.279%
11	14.639	1941	1947	1955	rBV	1124445	1589933	28.84%	4.388%
12	16.133	2194	2201	2211	rVB	1912050	2690092	48.80%	7.425%
13	17.392	2409	2415	2419	rBV	1387442	1860163	33.74%	5.134%
14	17.433	2419	2422	2429	rVB	111932	160198	2.91%	0.442%
15	17.521	2429	2437	2442	rBV	32439	77943	1.41%	0.215%
16	18.245	2553	2560	2570	rBV	1274801	2079084	37.71%	5.739%
17	18.692	2632	2636	2643	rBV	54992	82030	1.49%	0.226%
18	19.445	2760	2764	2769	rVB	178016	227764	4.13%	0.629%
19	19.515	2771	2776	2794	rBV	670211	1125764	20.42%	3.107%
20	19.809	2822	2826	2833	rVB	174700	238354	4.32%	0.658%
21	20.003	2853	2859	2867	rBV	4701907	5512697	100.00%	15.216%
22	20.674	2969	2973	2978	rBV	440066	453822	8.23%	1.253%
23	20.721	2978	2981	2984	rVB	141770	138710	2.52%	0.383%
24	21.233	3063	3068	3076	rBV5	290034	532550	9.66%	1.470%
25	21.439	3100	3103	3109	rVB2	71076	78016	1.42%	0.215%
26	21.574	3120	3126	3130	rBV	1674502	2214161	40.16%	6.111%
27	24.038	3538	3545	3560	rVB	1061199	2208052	40.05%	6.095%

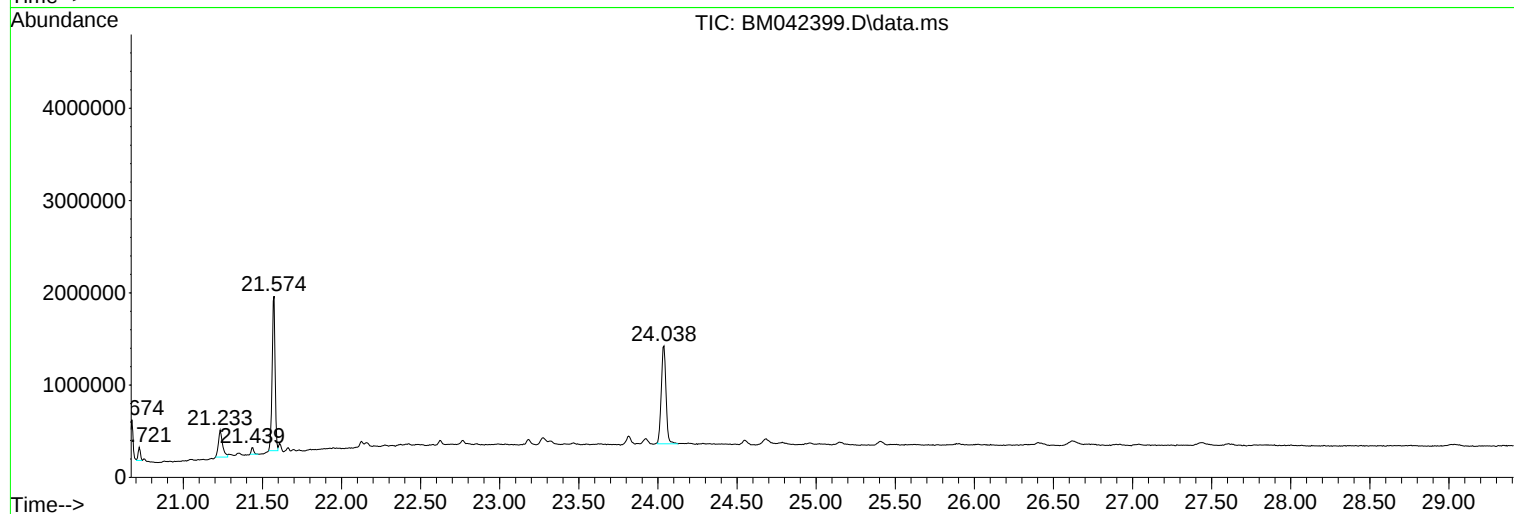
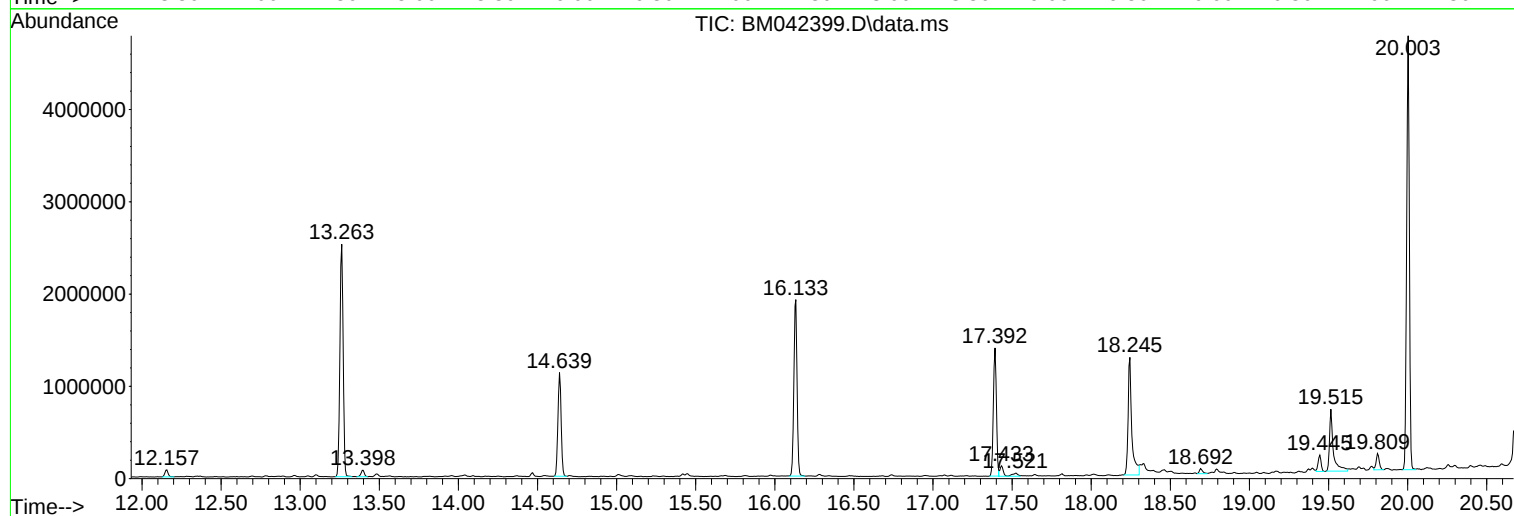
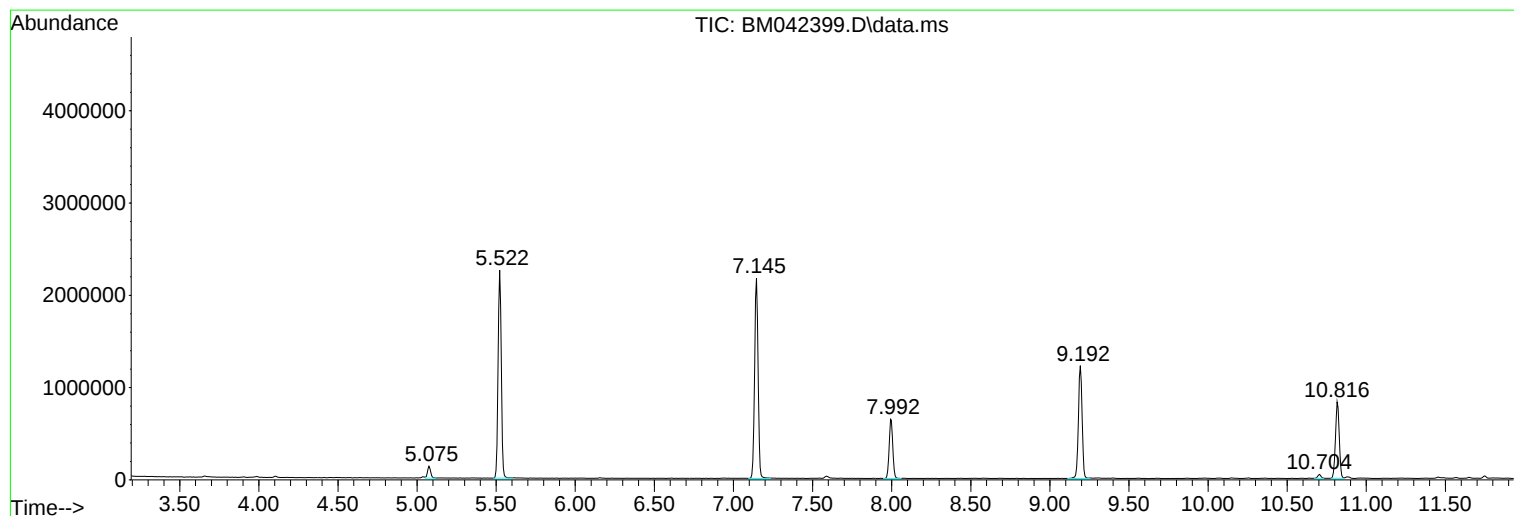
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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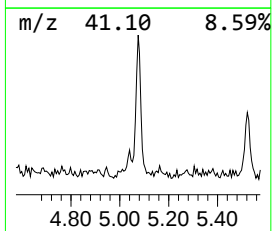
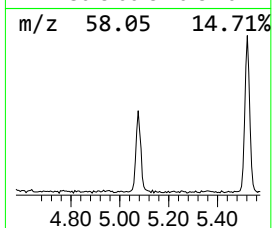
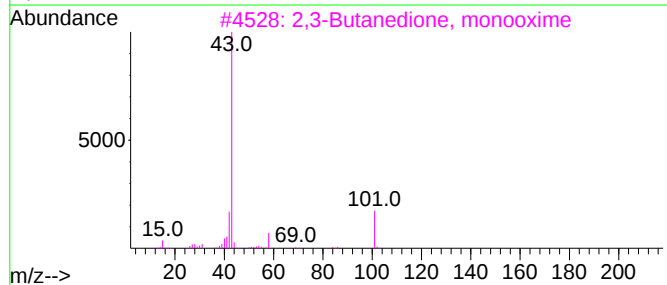
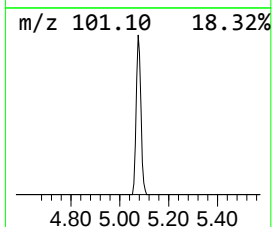
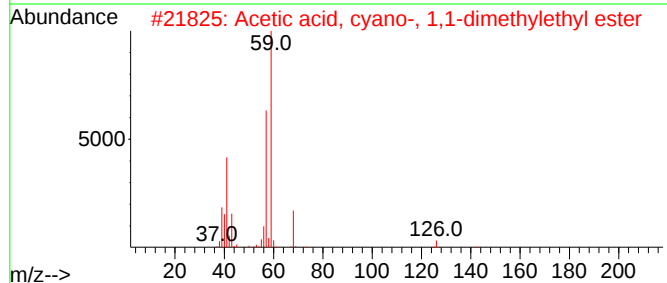
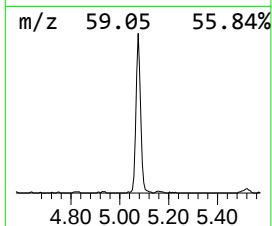
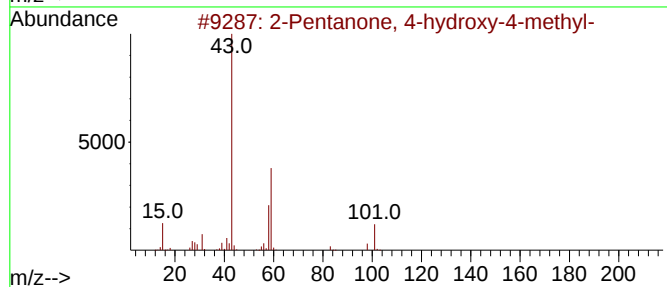
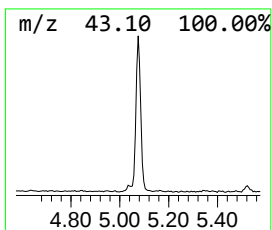
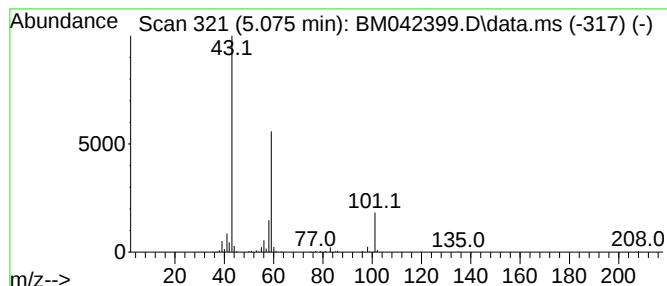
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.38 ng	172801	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	53		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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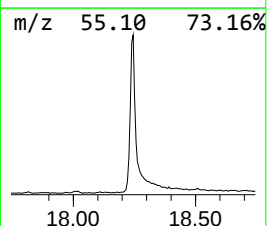
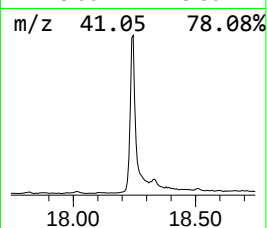
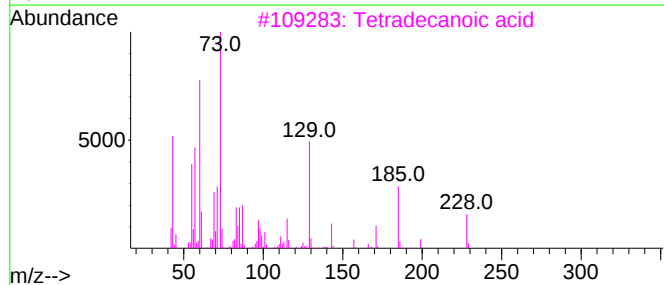
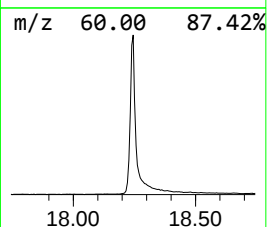
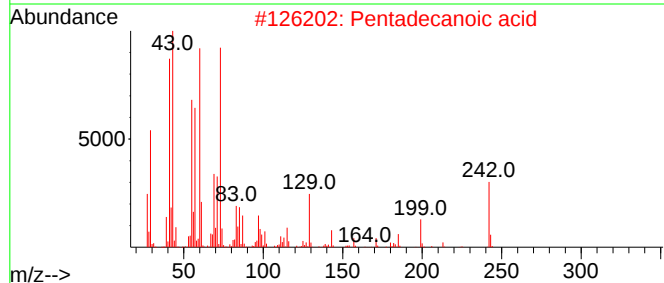
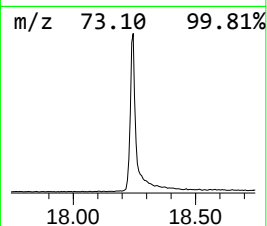
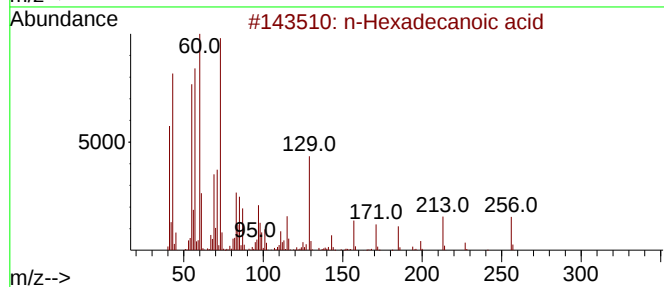
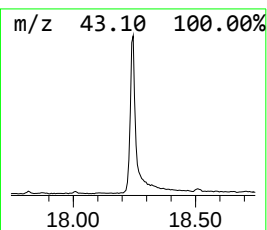
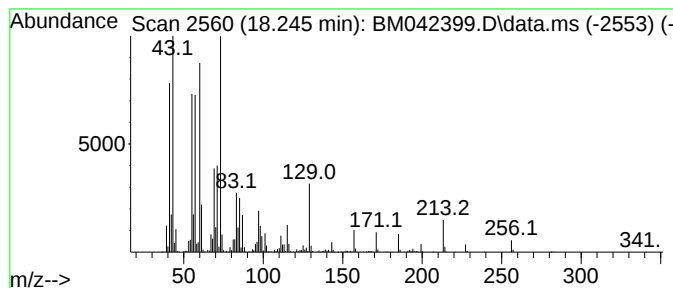
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	22.35 ng	2079080	Phenanthrene-d10	17.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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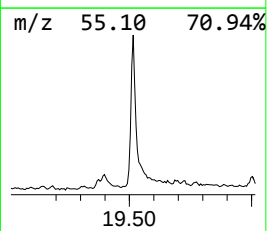
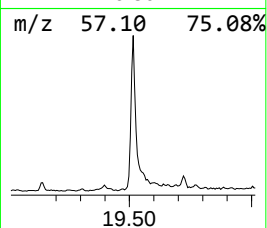
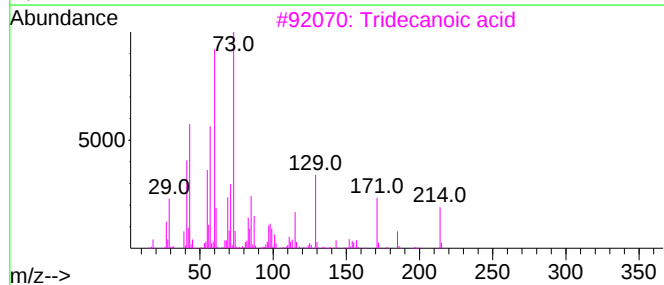
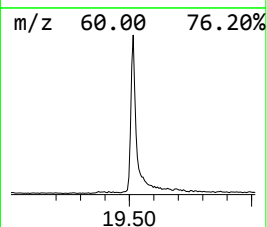
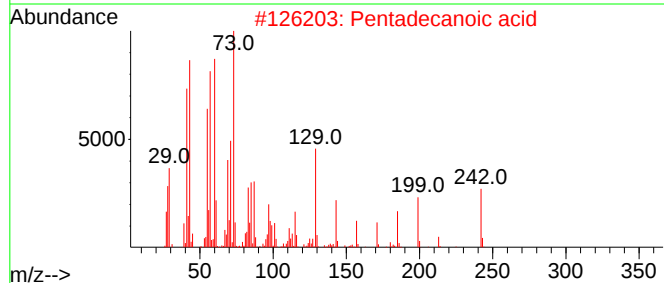
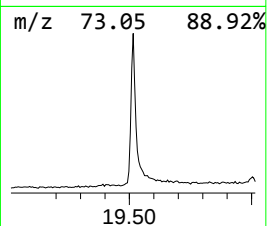
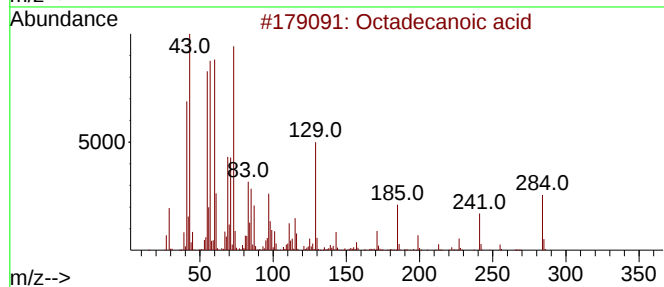
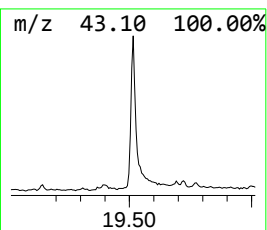
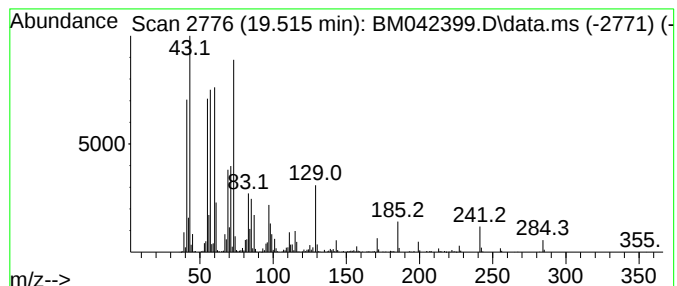
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	10.17 ng	1125760	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			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	35



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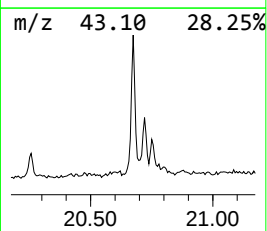
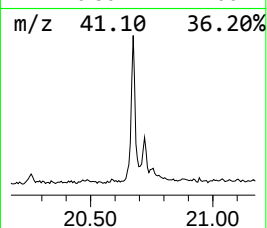
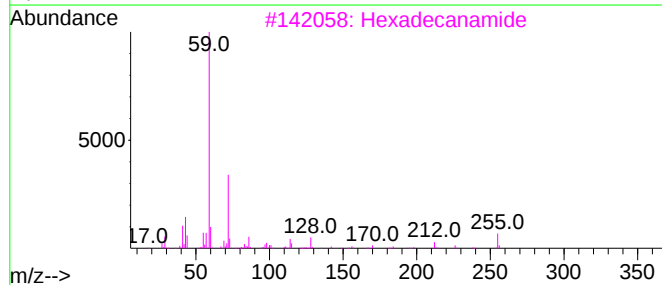
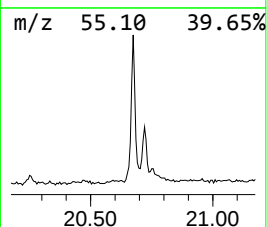
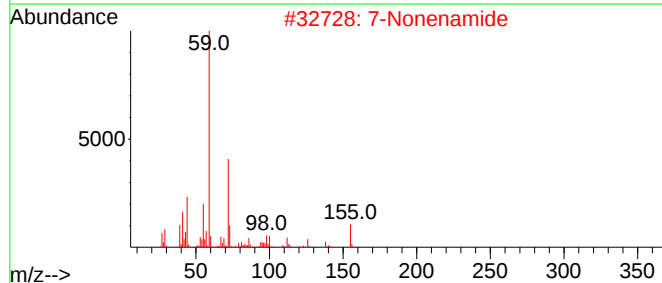
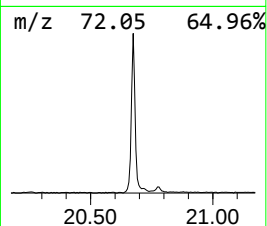
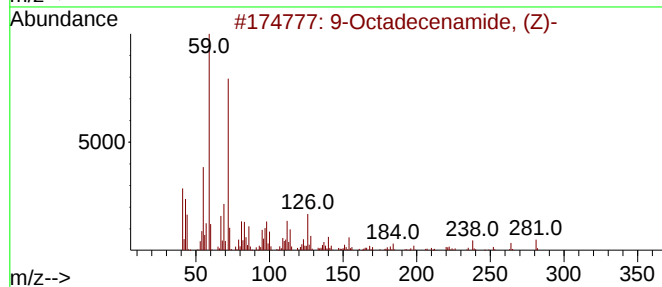
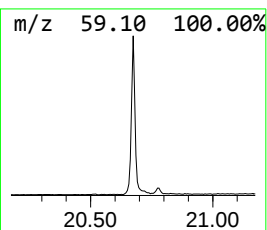
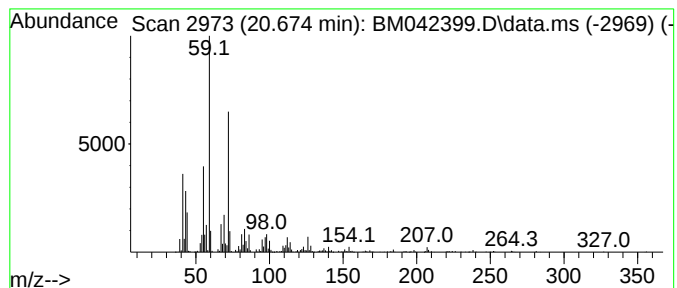
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.674	4.10 ng	453822	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2			7-Nonenamide	155	C9H17NO	090949-53-4	78
3			Hexadecanamide	255	C16H33NO	000629-54-9	72
4			Nonanamide	157	C9H19NO	001120-07-6	59
5			Octanamide	143	C8H17NO	000629-01-6	59



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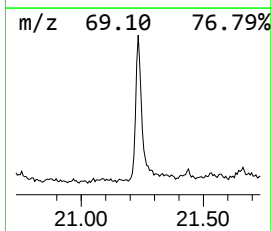
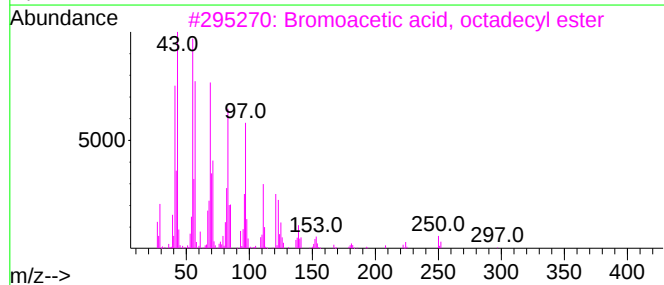
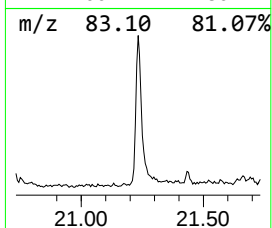
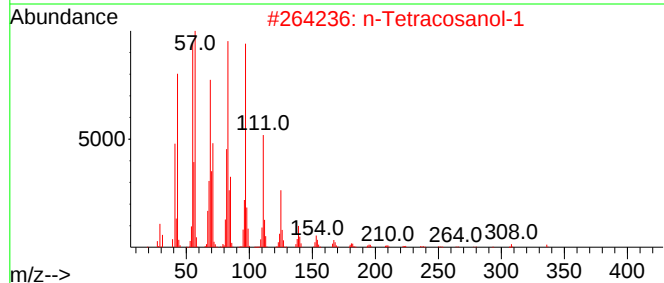
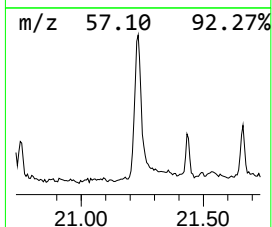
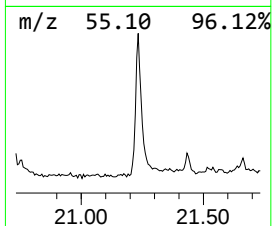
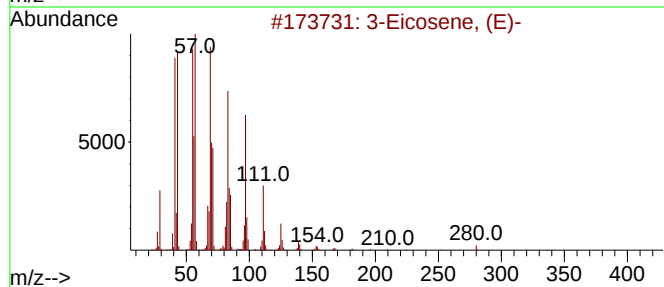
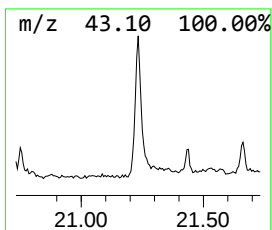
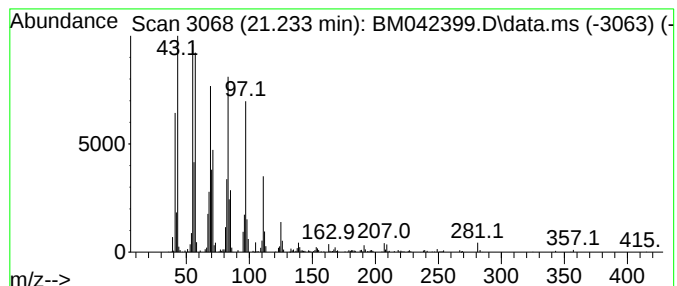
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Peak Number 6 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	4.81 ng	532550	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
4			1-Docosene	308	C22H44	001599-67-3	93
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.075	3.4	ng	172801	1	7.992	1023980	20.0
n-Hexadecanoic ...	18.245	22.4	ng	2079080	4	17.392	1860160	20.0
Octadecanoic acid	19.515	10.2	ng	1125760	5	21.574	2214160	20.0
9-Octadecenamid...	20.674	4.1	ng	453822	5	21.574	2214160	20.0
3-Eicosene, (E)-	21.233	4.8	ng	532550	5	21.574	2214160	20.0