

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102323\
 Data File : BM042401.D
 Acq On : 23 Oct 2023 14:30
 Operator : MA/JU
 Sample : 04844-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 OR-603-COMP-06

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: BM042401.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	331	rVB	151037	203502	3.28%	0.565%
2	5.522	390	397	410	rBV	2598426	3682375	59.36%	10.216%
3	7.146	665	673	687	rBV	2504464	3838539	61.88%	10.649%
4	7.993	810	817	826	rBV	585288	927837	14.96%	2.574%
5	9.192	1011	1021	1031	rBV	1421847	2287235	36.87%	6.345%
6	10.816	1289	1297	1305	rBV	731207	1200080	19.35%	3.329%
7	13.263	1706	1713	1720	rBV	2806041	3995256	64.41%	11.084%
8	14.639	1939	1947	1956	rBV	928791	1326142	21.38%	3.679%
9	16.127	2192	2200	2212	rVB	2100837	2916768	47.02%	8.092%
10	17.392	2404	2415	2420	rBV	1117114	1552380	25.03%	4.307%
11	17.433	2420	2422	2429	rVB	60191	71576	1.15%	0.199%
12	18.239	2551	2559	2569	rBV	672097	1136959	18.33%	3.154%
13	19.445	2761	2764	2768	rVB	56515	65084	1.05%	0.181%
14	19.515	2771	2776	2788	rBV	339345	577229	9.31%	1.601%
15	19.809	2823	2826	2832	rVB	54808	76326	1.23%	0.212%
16	20.004	2853	2859	2868	rBV	5298451	6203137	100.00%	17.209%
17	20.674	2966	2973	2979	rBV	1107322	1390691	22.42%	3.858%
18	20.721	2979	2981	2984	rVB	92204	101148	1.63%	0.281%
19	21.233	3062	3068	3080	rBV2	269964	596451	9.62%	1.655%
20	21.568	3120	3125	3130	rBV	1459722	1894566	30.54%	5.256%
21	24.039	3538	3545	3555	rVB	939580	2002418	32.28%	5.555%

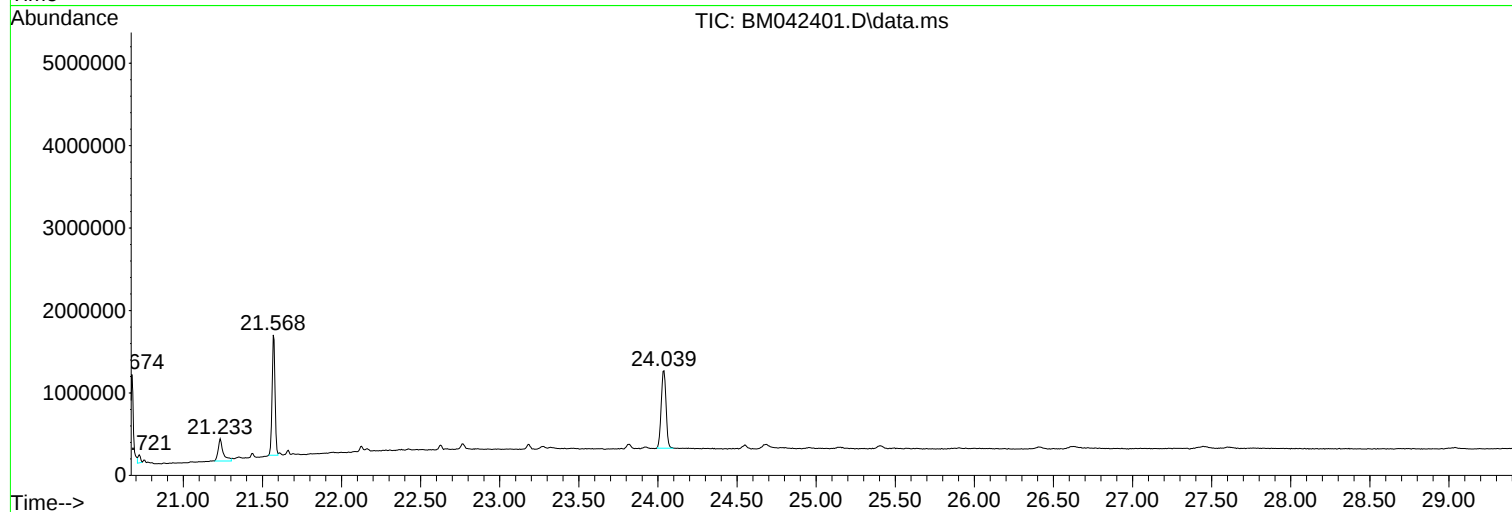
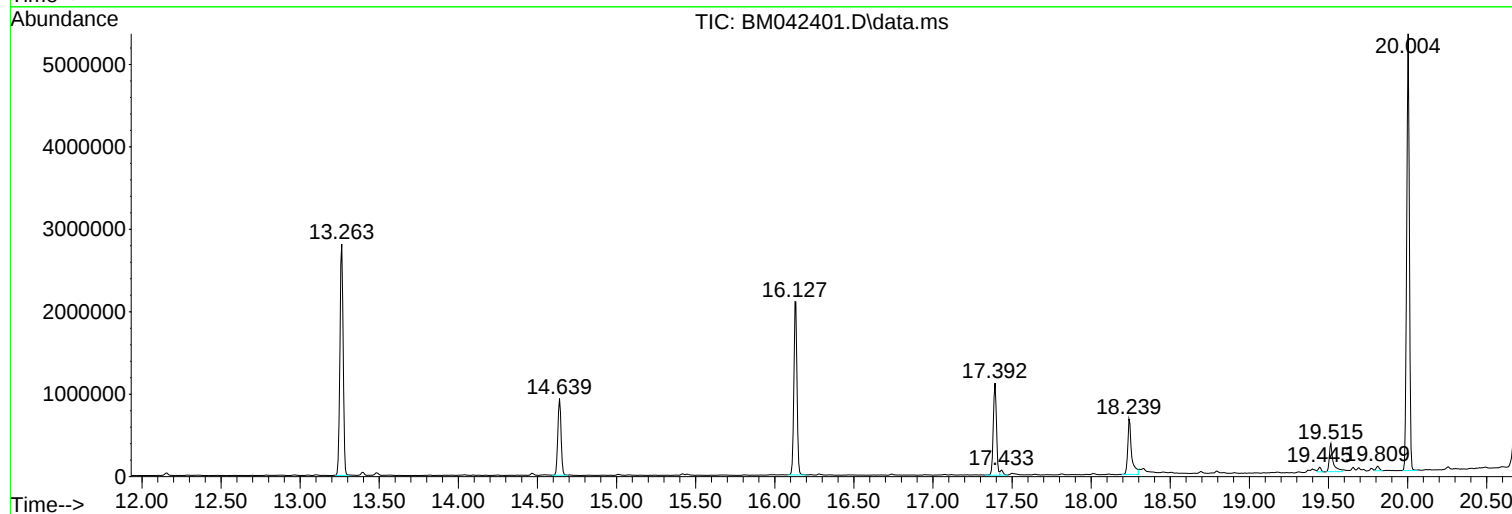
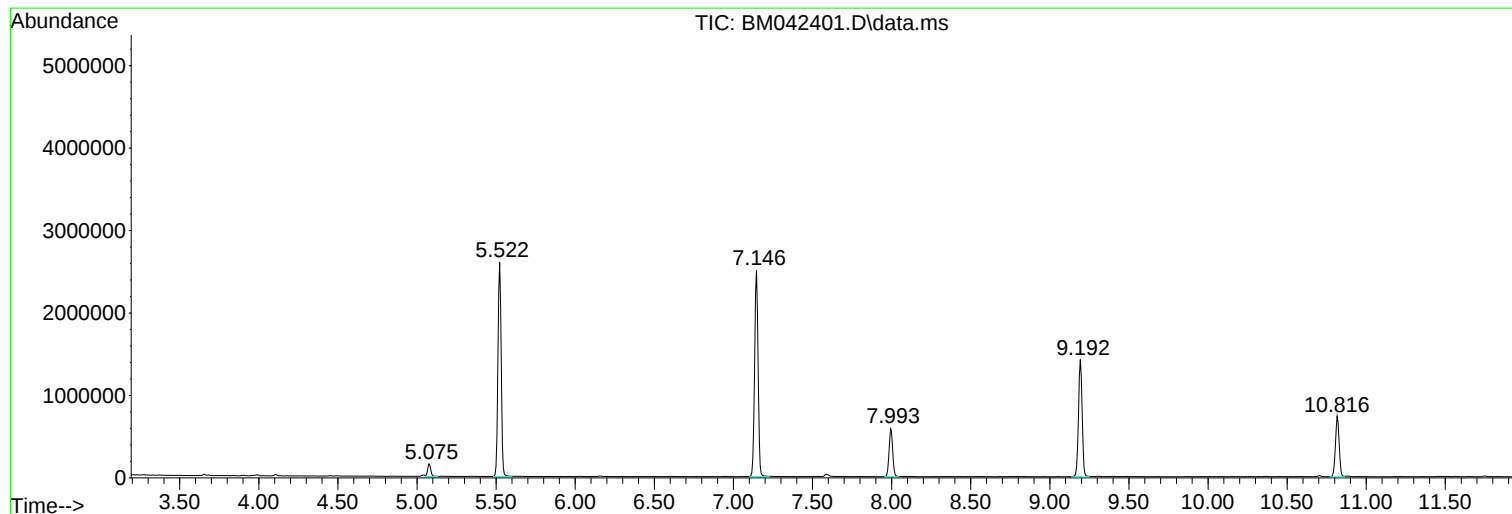
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM042401.D
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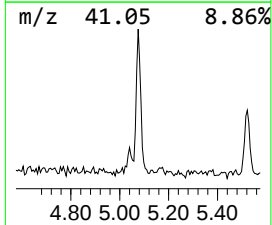
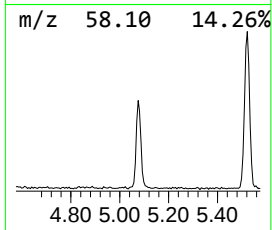
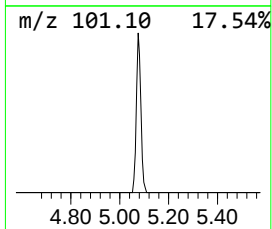
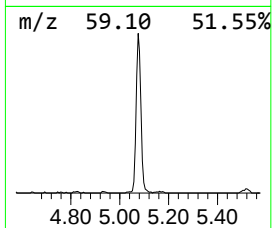
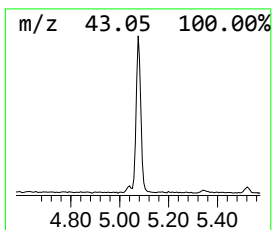
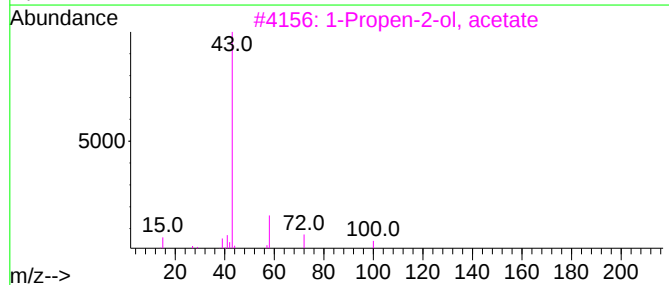
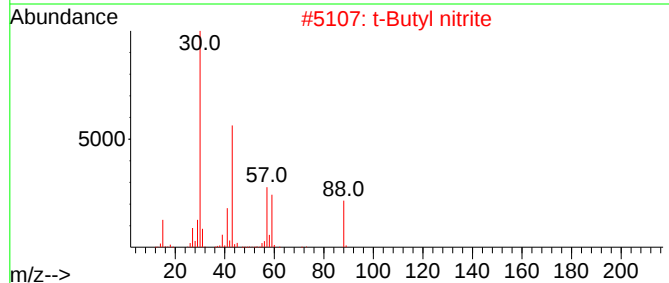
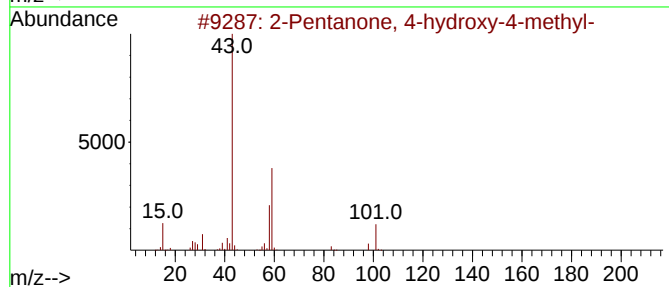
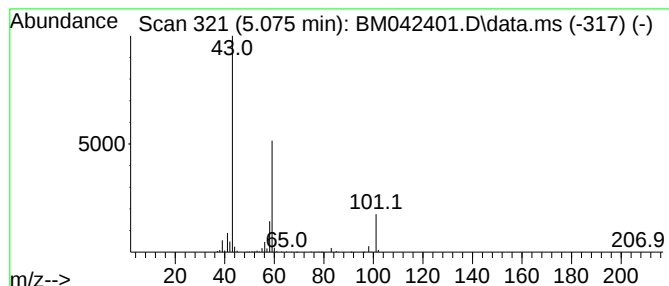
Instrument :
BNA_M
ClientSampleId :
OR-603-COMP-06

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 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.075	4.39 ng	203502	1,4-Dichlorobenzene-d4		7.998	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	t-Butyl nitrite		103	C4H9NO2	000540-80-7	39
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	10
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	9



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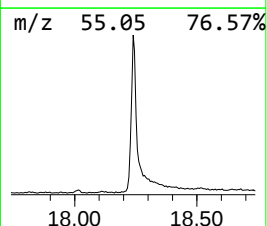
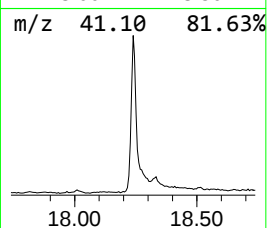
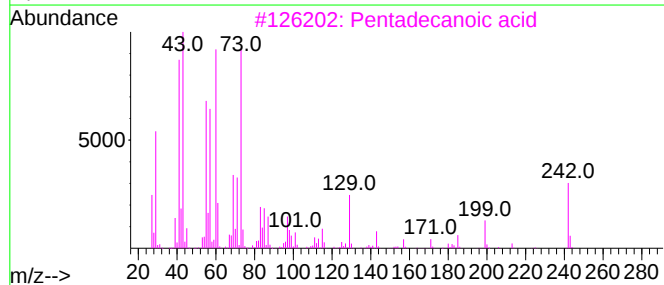
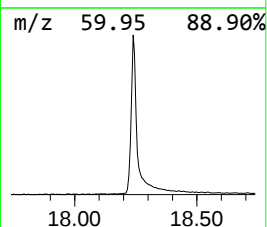
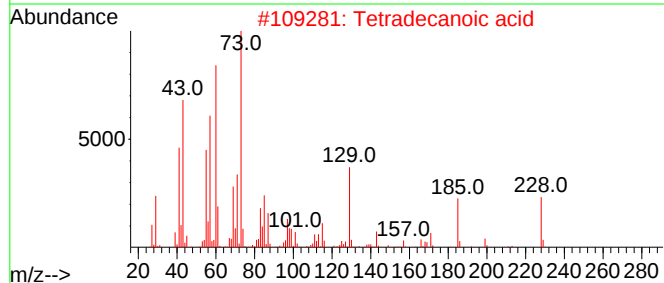
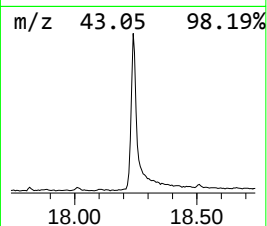
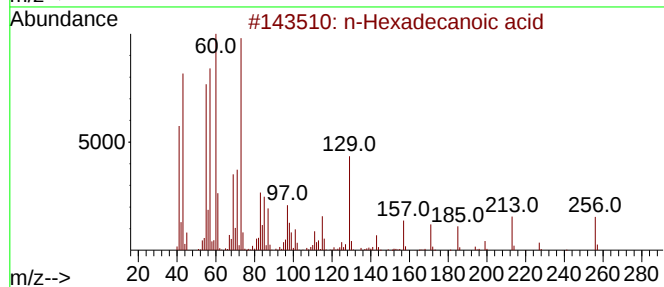
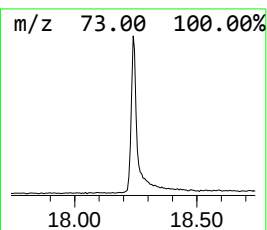
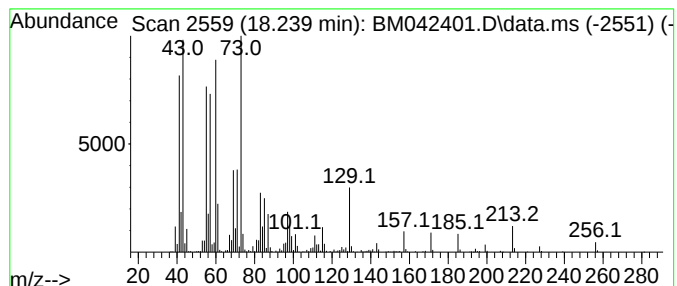
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	14.65 ng	1136960	Phenanthrene-d10	17.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	83
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	72



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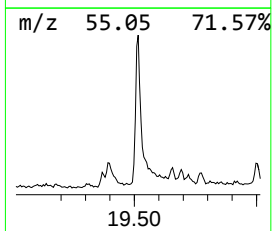
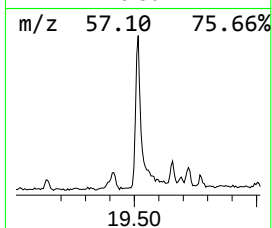
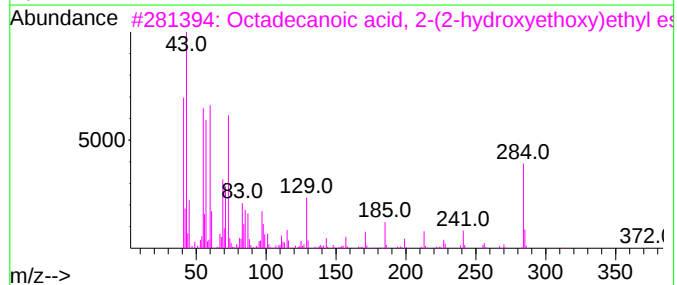
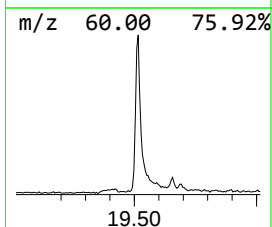
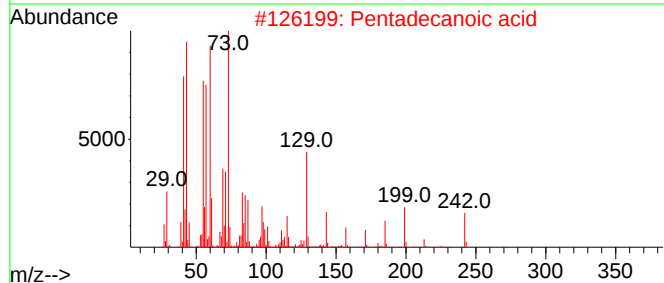
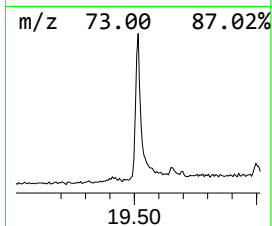
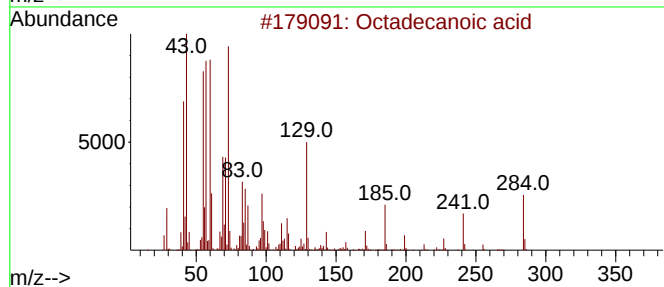
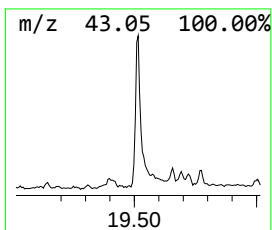
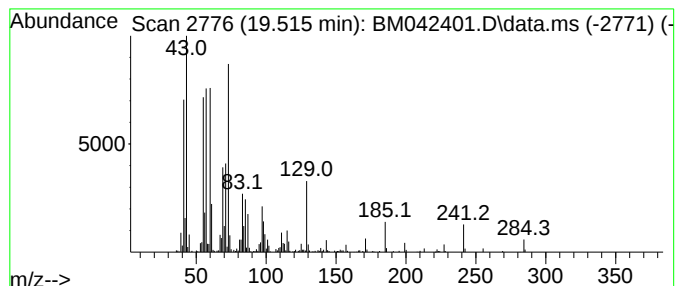
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.515	6.09 ng	577229	Chrysene-d12	21.568	
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	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



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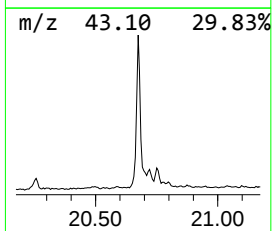
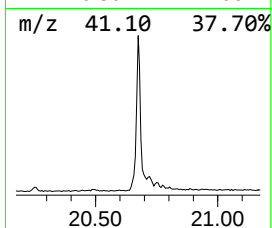
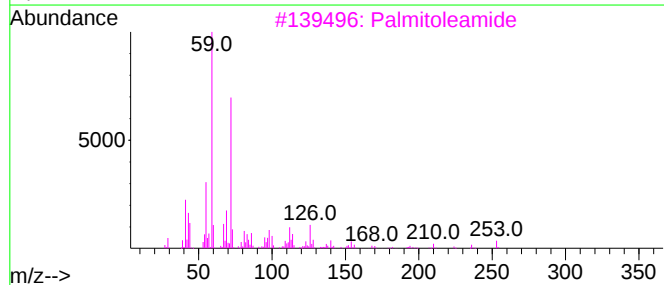
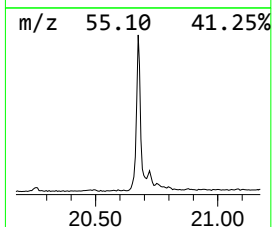
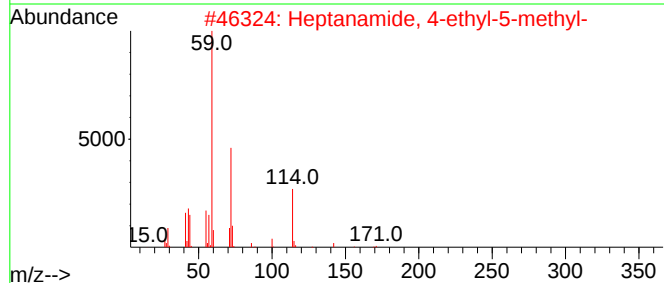
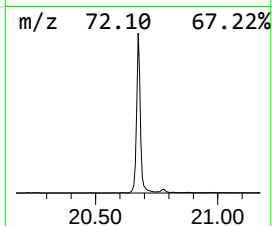
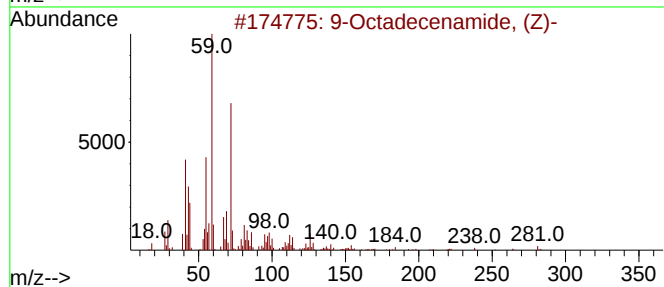
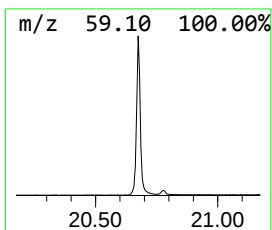
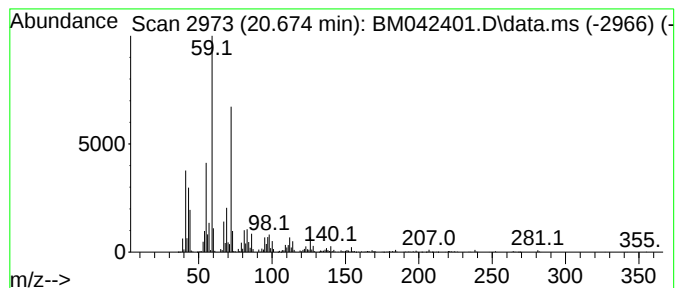
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.674	14.68 ng	1390690	Chrysene-d12		21.568	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	98
2	Heptanamide, 4-ethyl-5-methyl-		171	C10H21NO	054789-40-1	72
3	Palmitoleamide		253	C16H31NO	106010-22-4	64
4	Octanamide		143	C8H17NO	000629-01-6	64
5	Nonanamide		157	C9H19NO	001120-07-6	53



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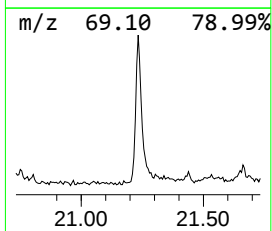
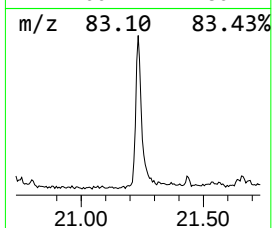
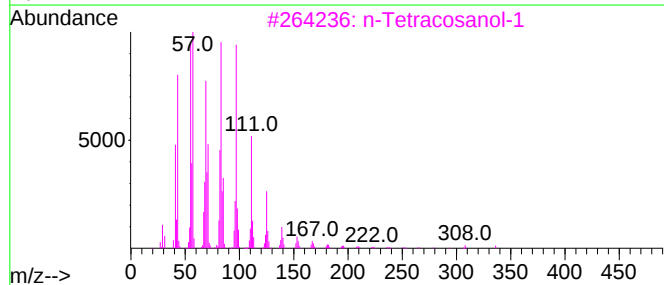
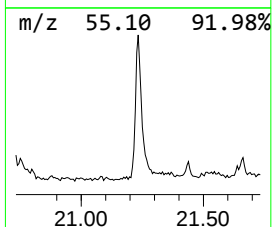
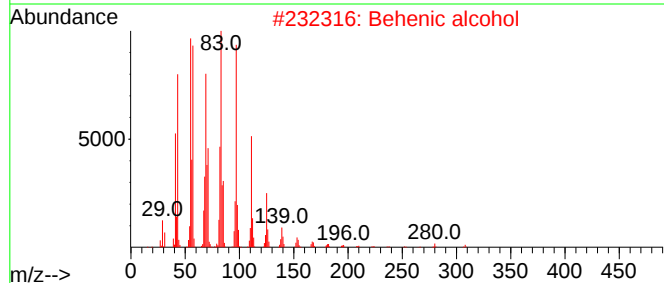
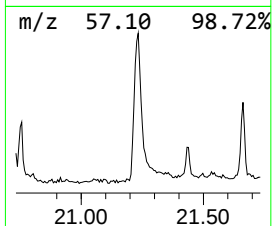
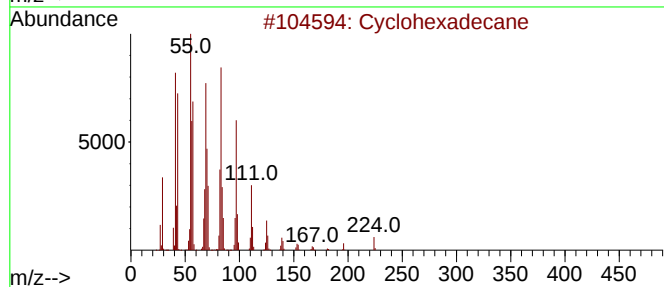
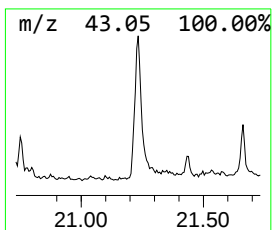
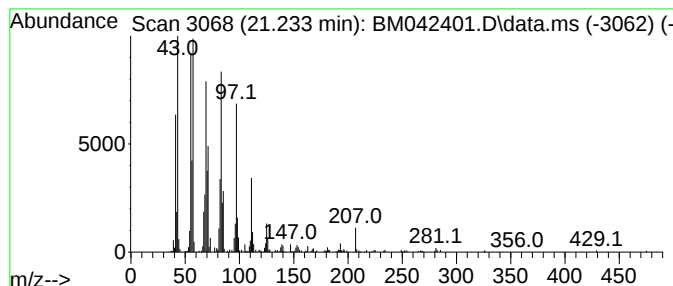
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	6.30 ng	596451	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	97
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.075	4.4	ng	203502	1	7.998	927837	20.0
n-Hexadecanoic ...	18.239	14.7	ng	1136960	4	17.392	1552380	20.0
Octadecanoic acid	19.515	6.1	ng	577229	5	21.568	1894570	20.0
9-Octadecenamid...	20.674	14.7	ng	1390690	5	21.568	1894570	20.0
Cyclohexadecane	21.233	6.3	ng	596451	5	21.568	1894570	20.0