

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
 Data File : BM044817.D
 Acq On : 29 Mar 2024 15:01
 Operator : MA/JU
 Sample : P1879-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 EB-02(2-4)

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-BM032824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.499	67	70	80	rBV	47352	70435	1.57%	0.244%
2	5.275	366	372	384	rBV	1662673	2389249	53.29%	8.283%
3	6.846	632	639	652	rBV	1572619	2525315	56.33%	8.755%
4	7.663	772	778	786	rBV	414562	657478	14.66%	2.279%
5	8.828	967	976	990	rBV	917246	1563176	34.87%	5.419%
6	10.439	1241	1250	1264	rBV	498416	889285	19.83%	3.083%
7	12.928	1666	1673	1693	rBV	2082203	3052804	68.09%	10.584%
8	14.310	1901	1908	1916	rBV	703491	1058684	23.61%	3.670%
9	14.539	1940	1947	1953	rVB3	23754	54536	1.22%	0.189%
10	15.810	2156	2163	2176	rBV	1638428	2442755	54.48%	8.469%
11	17.068	2370	2377	2381	rBV	880867	1248481	27.85%	4.328%
12	17.110	2381	2384	2391	rVV	262662	367283	8.19%	1.273%
13	17.204	2394	2400	2405	rVB2	48170	76017	1.70%	0.264%
14	17.480	2440	2447	2457	rBV2	29402	72369	1.61%	0.251%
15	17.945	2522	2526	2528	rBV	36871	51710	1.15%	0.179%
16	17.980	2528	2532	2543	rVB2	353654	553305	12.34%	1.918%
17	18.139	2555	2559	2563	rBV2	43125	74016	1.65%	0.257%
18	18.845	2674	2679	2689	rBV2	235874	415927	9.28%	1.442%
19	19.009	2703	2707	2714	rVB2	27774	50619	1.13%	0.175%
20	19.133	2722	2728	2737	rBV	434836	627115	13.99%	2.174%
21	19.268	2747	2751	2759	rBV3	153083	233539	5.21%	0.810%
22	19.498	2781	2790	2799	rBV	385576	600570	13.40%	2.082%
23	19.715	2819	2827	2839	rVB	3493794	4483439	100.00%	15.544%
24	19.827	2841	2846	2853	rVV5	31241	73955	1.65%	0.256%
25	19.962	2865	2869	2872	rBV6	26751	50169	1.12%	0.174%
26	20.004	2872	2876	2879	rVB3	34791	54820	1.22%	0.190%
27	20.156	2898	2902	2907	rVB3	33219	49217	1.10%	0.171%
28	20.751	2999	3003	3009	rBV3	52164	84830	1.89%	0.294%
29	20.998	3040	3045	3050	rBV3	335302	459779	10.26%	1.594%
30	21.268	3084	3091	3095	rBV2	1269029	1812131	40.42%	6.283%
31	21.303	3095	3097	3105	rVB	214843	259973	5.80%	0.901%
32	22.333	3269	3272	3281	rVB3	180189	256144	5.71%	0.888%
33	22.833	3353	3357	3363	rBV	171780	393568	8.78%	1.364%
34	23.403	3450	3454	3462	rVB	148008	281653	6.28%	0.976%
35	23.503	3465	3471	3477	rVV	787306	1509283	33.66%	5.233%

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EB-02(2-4)

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-BM032824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

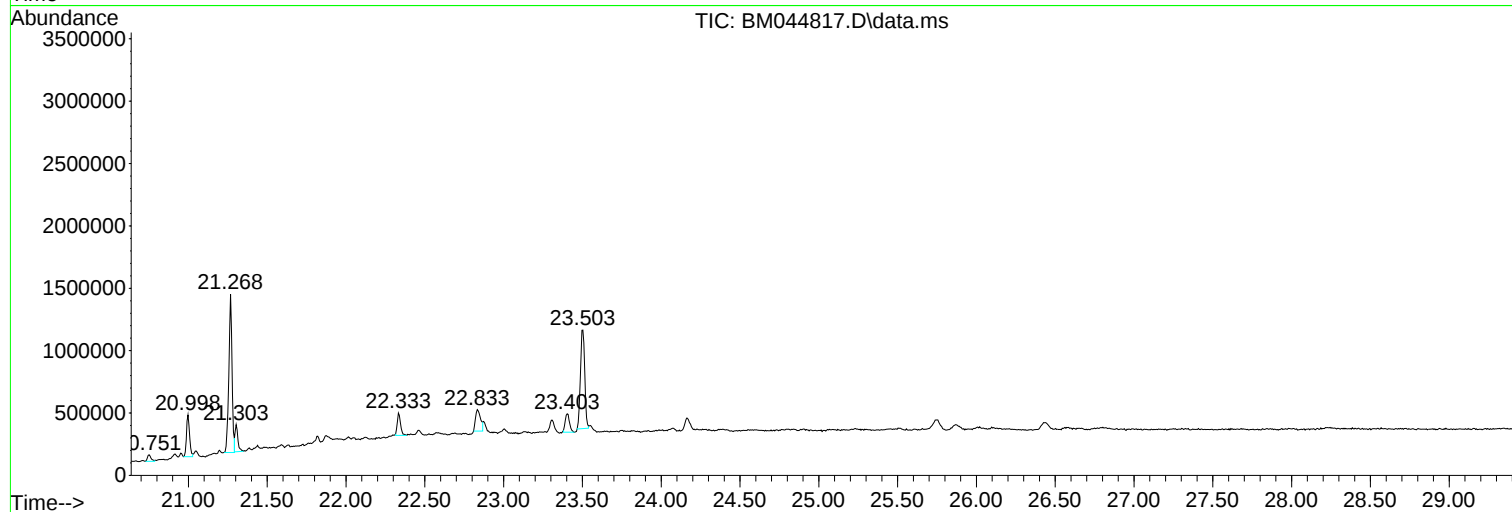
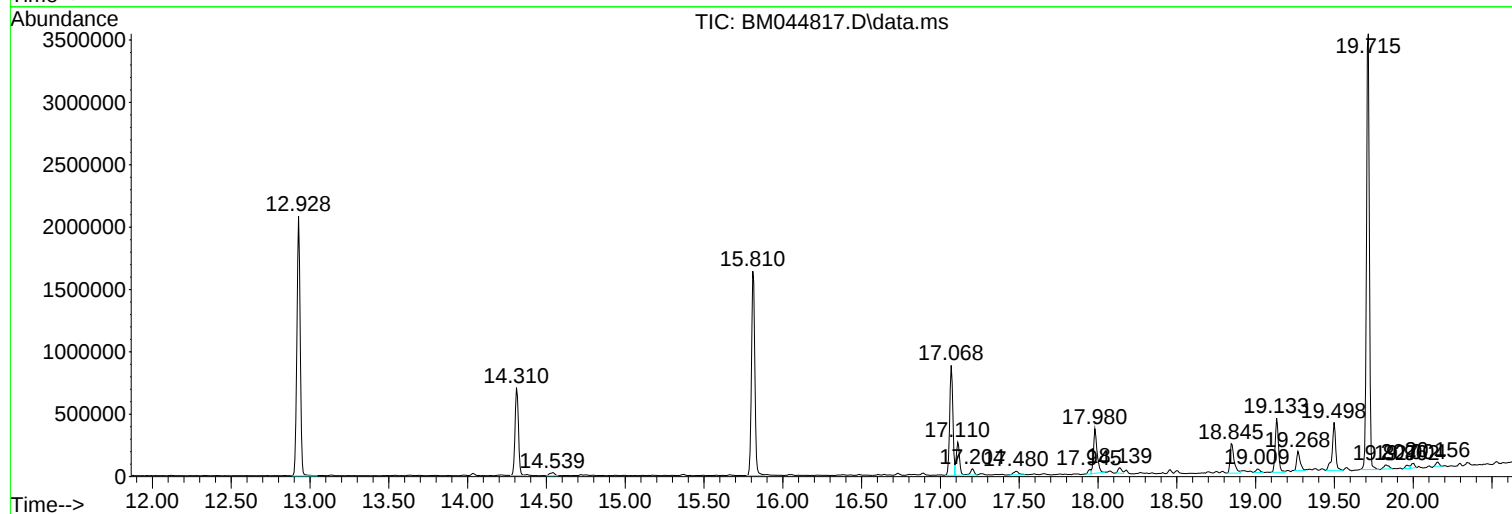
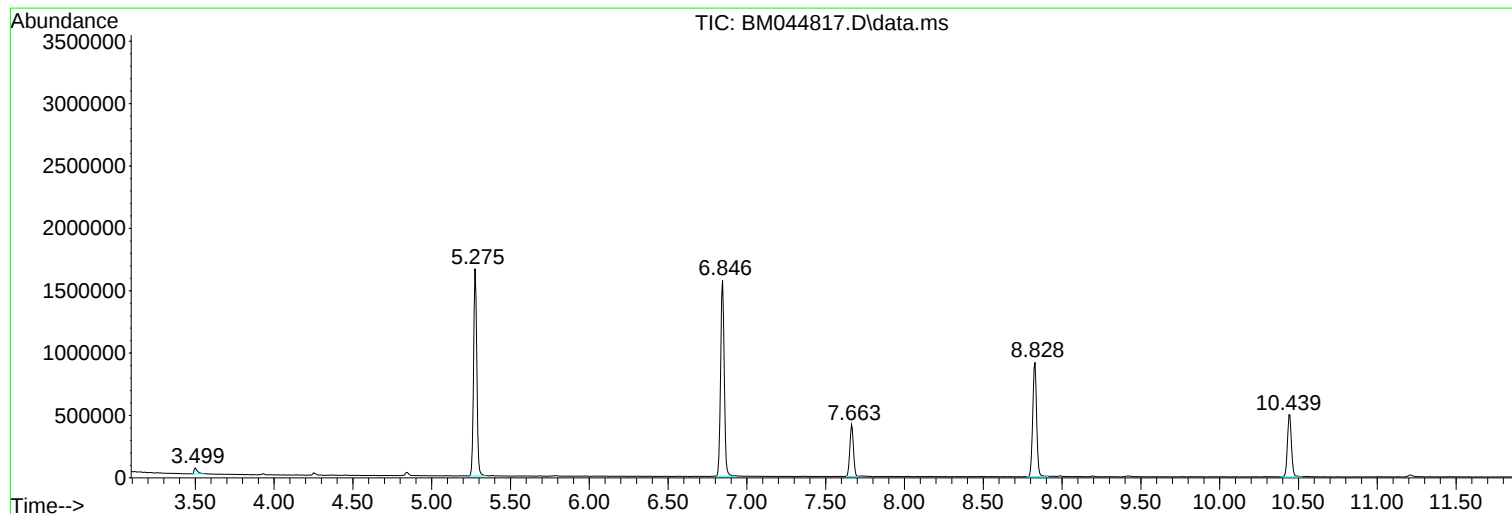
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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EB-02(2-4)

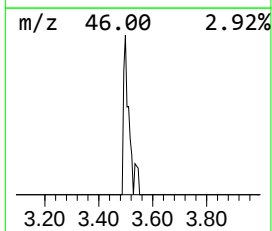
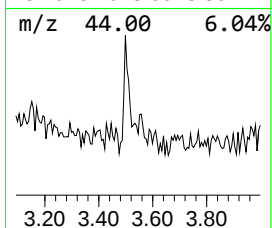
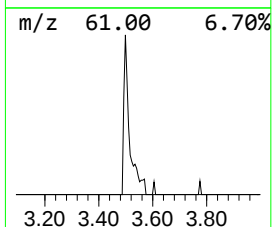
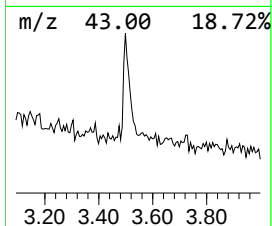
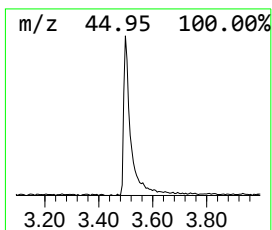
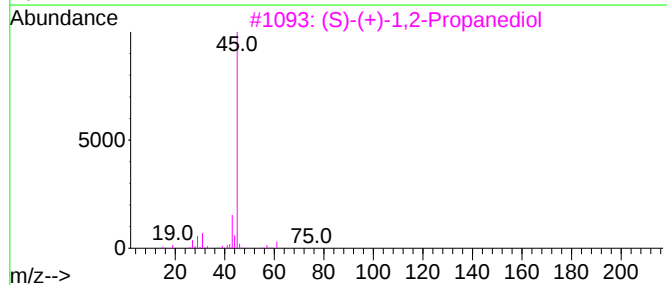
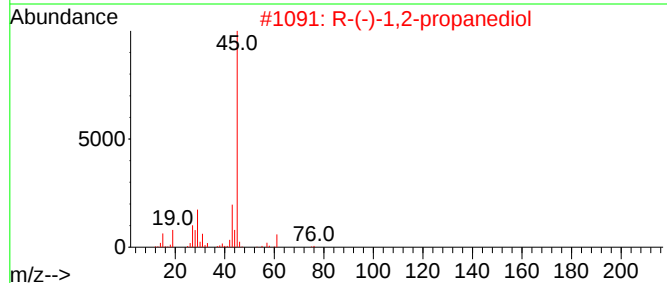
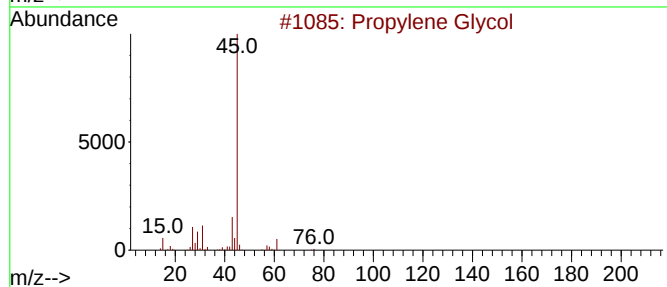
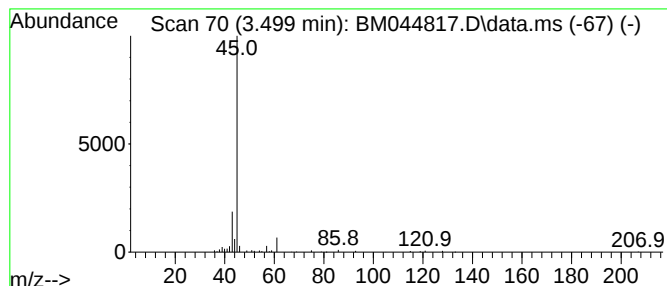
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.499 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.499	2.14 ng	70435	1,4-Dichlorobenzene-d4	7.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	40
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4			2,2-Dichloroethyl methyl ether	128	C3H6Cl2O	034862-07-2	9
5			1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9



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Misc :
ALS Vial : 10 Sample Multiplier: 1

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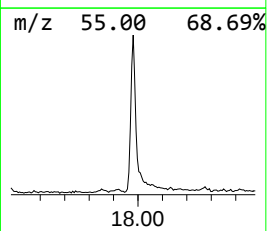
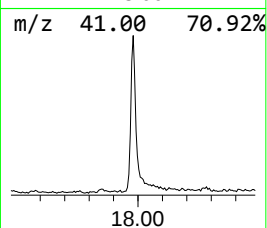
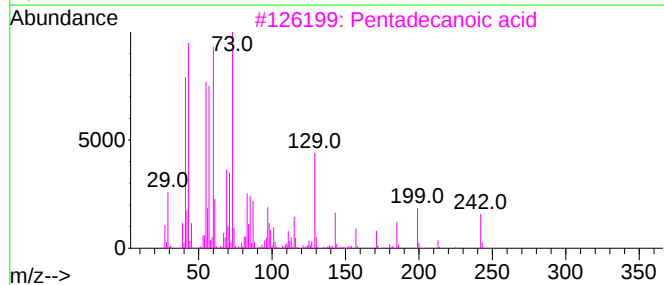
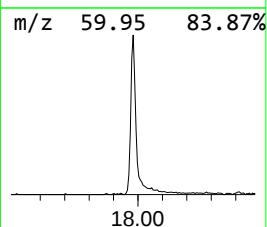
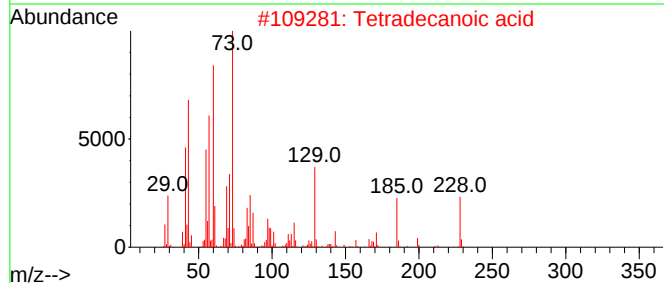
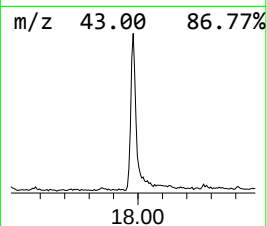
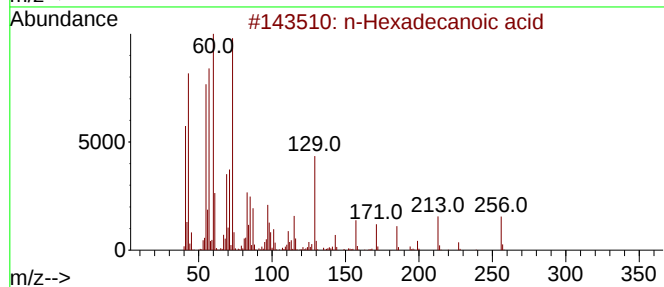
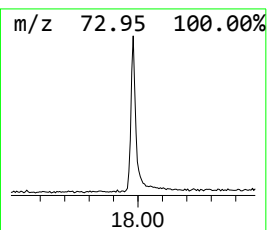
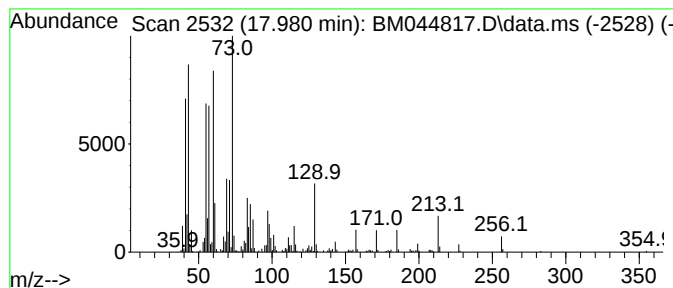
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	8.86 ng	553305	Phenanthrene-d10	17.068

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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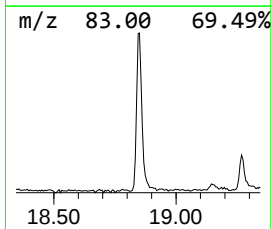
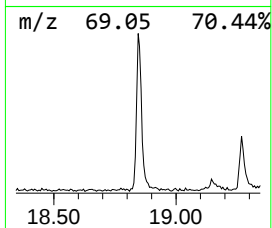
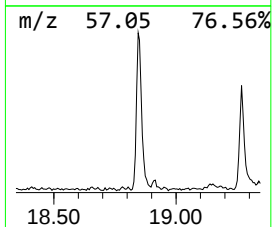
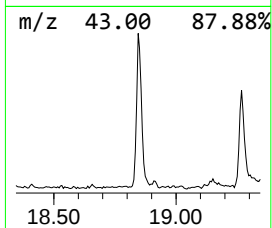
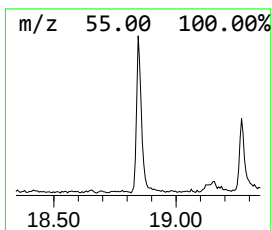
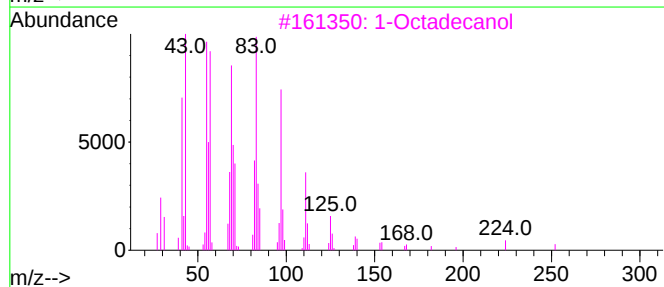
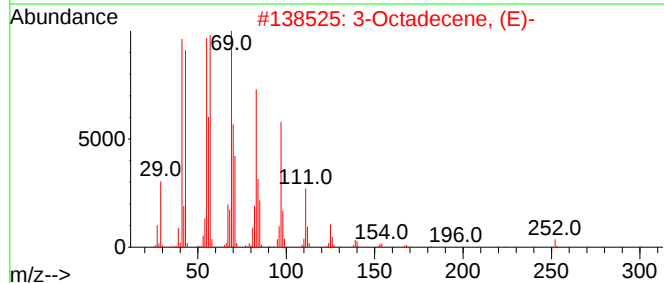
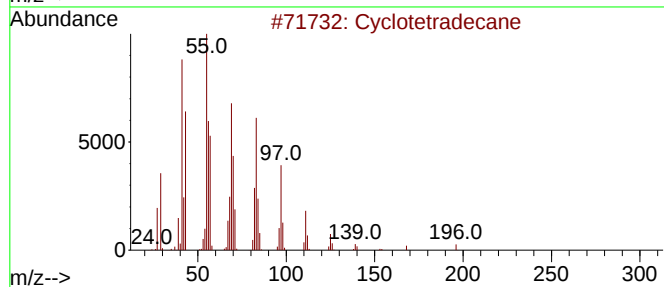
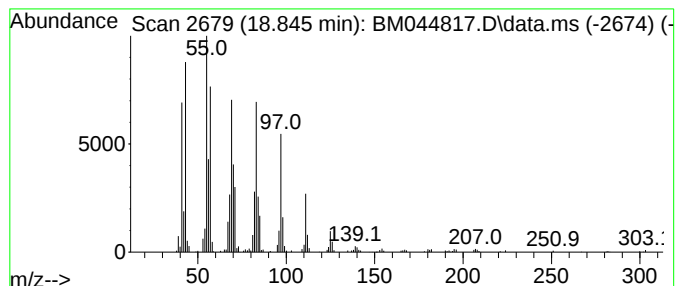
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cyclotetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.845	6.66 ng	415927	Phenanthrene-d10	17.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	94
2			3-Octadecene, (E)-	252	C18H36	007206-19-1	94
3			1-Octadecanol	270	C18H38O	000112-92-5	94
4			1-Hexadecanol	242	C16H34O	036653-82-4	94
5			Bromoacetic acid, tetradecyl ester	334	C16H31BrO2	018992-01-3	91



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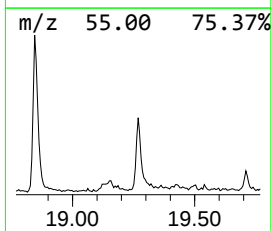
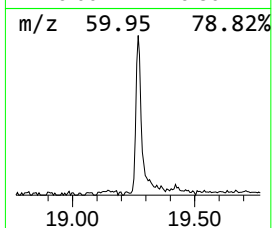
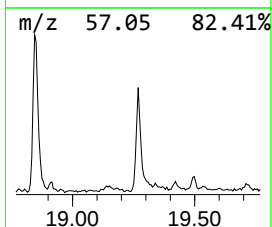
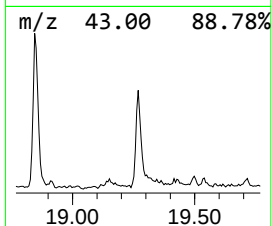
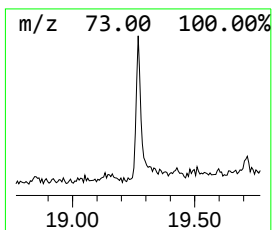
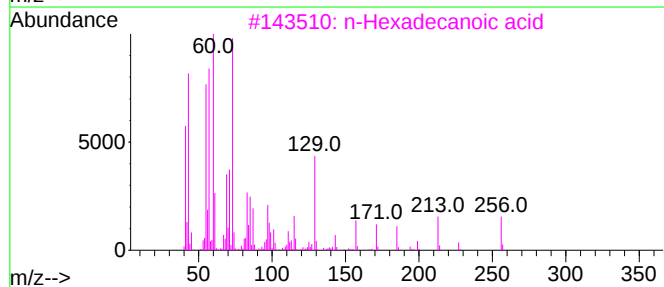
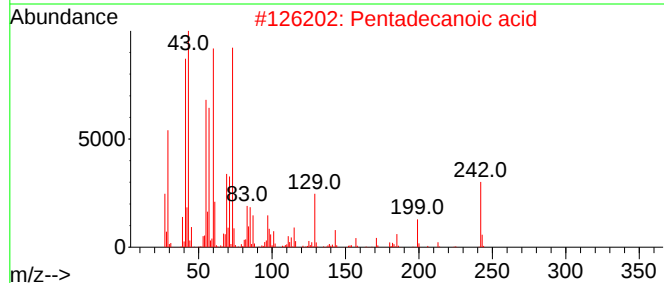
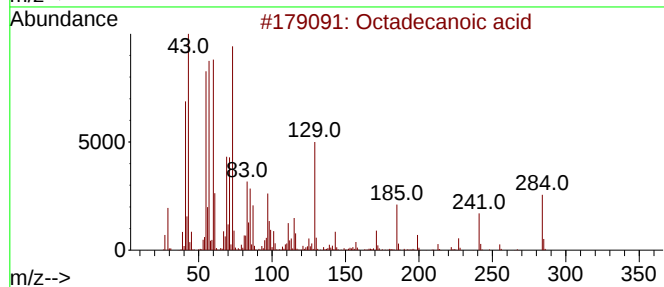
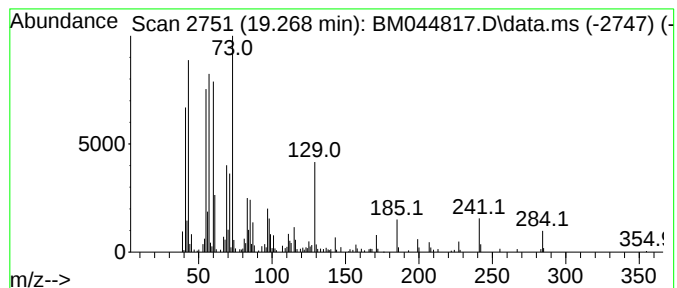
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.268	2.58 ng	233539	Chrysene-d12	21.268	
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	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	43



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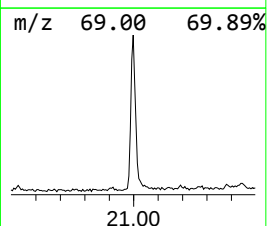
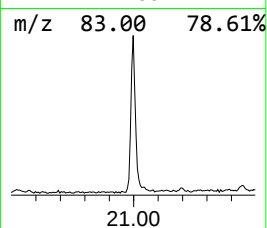
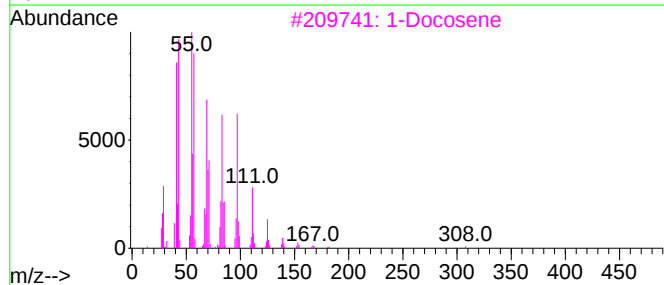
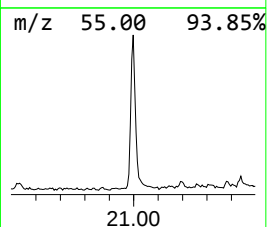
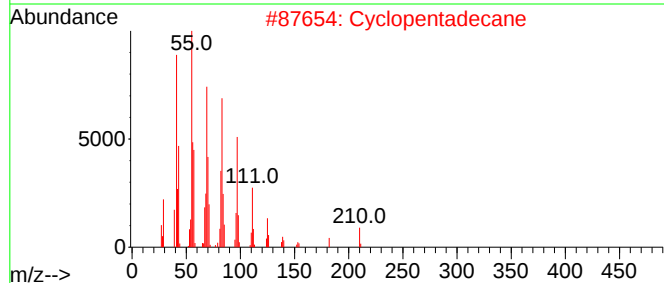
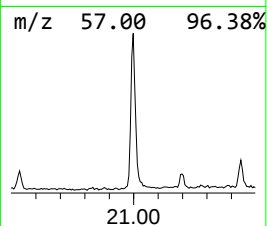
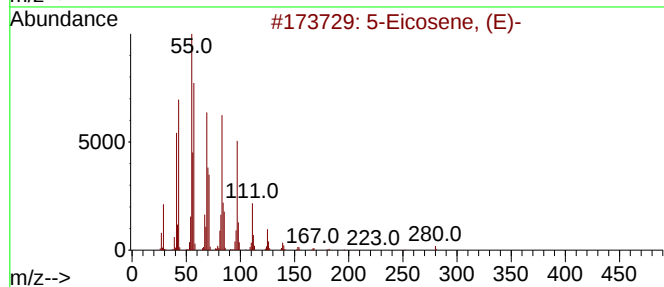
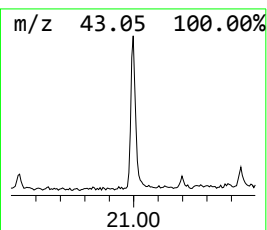
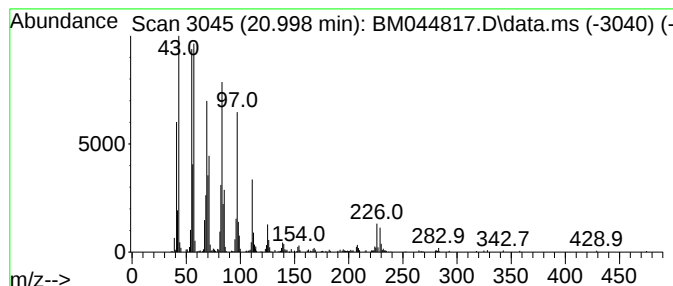
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.998	5.07 ng	459779	Chrysene-d12	21.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2			Cyclopentadecane	210	C15H30	000295-48-7	97
3			1-Docosene	308	C22H44	001599-67-3	93
4			Octacosanol	410	C28H58O	000557-61-9	93
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044817.D
Acq On : 29 Mar 2024 15:01
Operator : MA/JU
Sample : P1879-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-02(2-4)

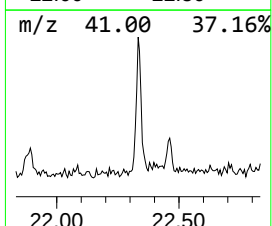
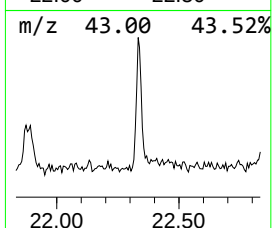
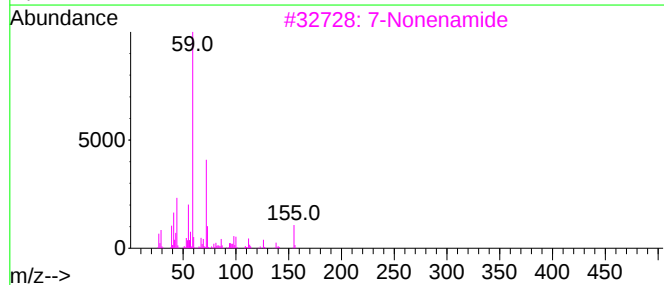
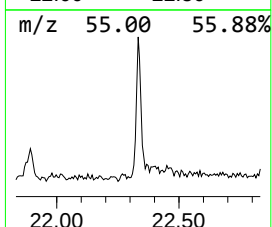
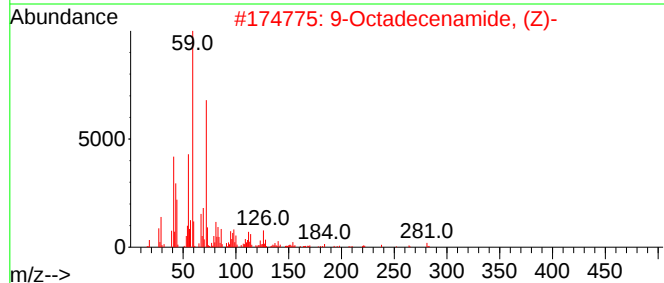
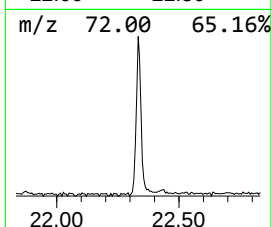
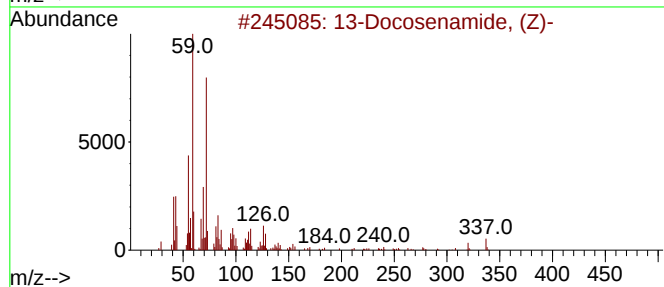
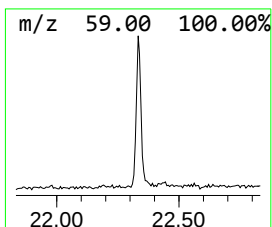
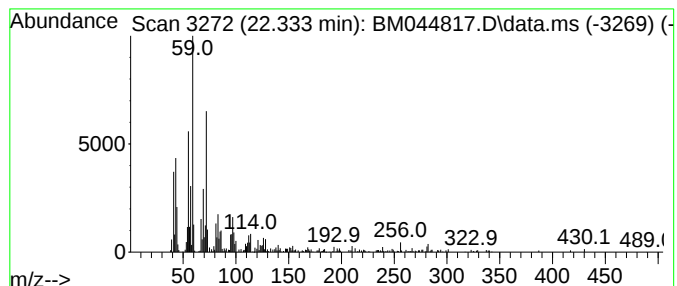
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.333	2.83 ng	256144	Chrysene-d12	21.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
3			7-Nonenamide	155	C9H17NO	090949-53-4	50
4			Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	49
5			Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044817.D
Acq On : 29 Mar 2024 15:01
Operator : MA/JU
Sample : P1879-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-02(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.499	3.499	2.1	ng	70435	1	7.663	657478	20.0
n-Hexadecanoic ...	17.980	8.9	ng	553305	4	17.068	1248480	20.0
Cyclotetradecane	18.845	6.7	ng	415927	4	17.068	1248480	20.0
Octadecanoic acid	19.268	2.6	ng	233539	5	21.268	1812130	20.0
5-Eicosene, (E)-	20.998	5.1	ng	459779	5	21.268	1812130	20.0
13-Docosenamide...	22.333	2.8	ng	256144	5	21.268	1812130	20.0