

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
 Data File : BM041204.D
 Acq On : 01 Aug 2023 01:28
 Operator : MA/JU
 Sample : 03741-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-P5A

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041204.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	364	371	387	rBV	2082474	2954165	55.85%	8.181%
2	6.975	637	644	661	rBV	1901705	3039296	57.46%	8.417%
3	7.798	777	784	792	rBV	580072	899319	17.00%	2.490%
4	8.975	976	984	999	rBV	1151928	1926355	36.42%	5.335%
5	10.604	1247	1261	1271	rBV	739442	1219008	23.04%	3.376%
6	13.080	1675	1682	1695	rBV	2882718	4006177	75.74%	11.094%
7	13.927	1817	1826	1839	rVB	211764	303933	5.75%	0.842%
8	14.463	1910	1917	1924	rBV	1072534	1471517	27.82%	4.075%
9	15.963	2163	2172	2181	rBV	2356772	3196964	60.44%	8.853%
10	16.168	2203	2207	2216	rBV	46729	92497	1.75%	0.256%
11	16.968	2339	2343	2347	rBV	70439	85516	1.62%	0.237%
12	17.133	2365	2371	2375	rBV5	27051	60396	1.14%	0.167%
13	17.221	2380	2386	2391	rBV	1248731	1709226	32.31%	4.733%
14	17.709	2465	2469	2474	rVB	69309	78421	1.48%	0.217%
15	18.062	2525	2529	2534	rBV	75929	113576	2.15%	0.315%
16	18.121	2534	2539	2550	rVV	530472	807348	15.26%	2.236%
17	18.409	2584	2588	2595	rBV	45239	75130	1.42%	0.208%
18	19.286	2734	2737	2743	rBV	90329	116892	2.21%	0.324%
19	19.403	2753	2757	2769	rBV	160345	282444	5.34%	0.782%
20	19.651	2796	2799	2809	rVB2	104395	165629	3.13%	0.459%
21	19.856	2829	2834	2840	rBV	4619112	5289701	100.00%	14.648%
22	21.133	3047	3051	3059	rVB	337742	501555	9.48%	1.389%
23	21.421	3095	3100	3105	rBV	1539049	1945201	36.77%	5.387%
24	21.833	3167	3170	3178	rVB2	174928	290988	5.50%	0.806%
25	22.015	3196	3201	3205	rBV	2513858	2897388	54.77%	8.024%
26	23.050	3374	3377	3383	rVB2	208285	287671	5.44%	0.797%
27	23.791	3497	3503	3509	rVB	991960	1841515	34.81%	5.100%
28	24.362	3597	3600	3608	rVB3	263757	453110	8.57%	1.255%

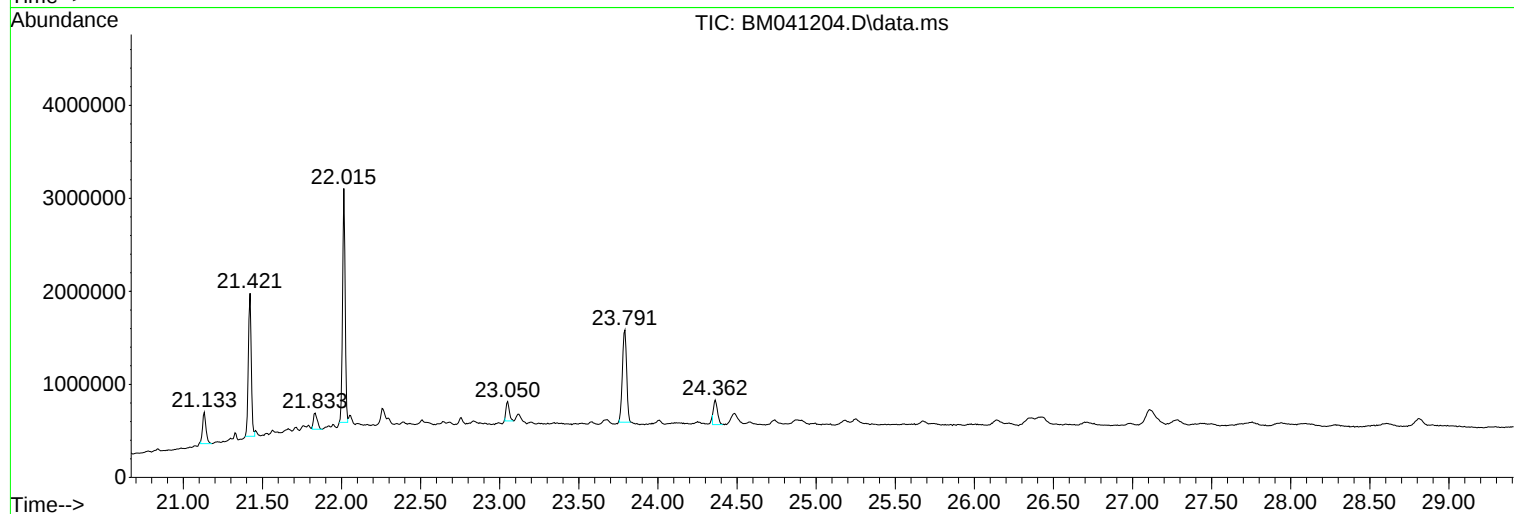
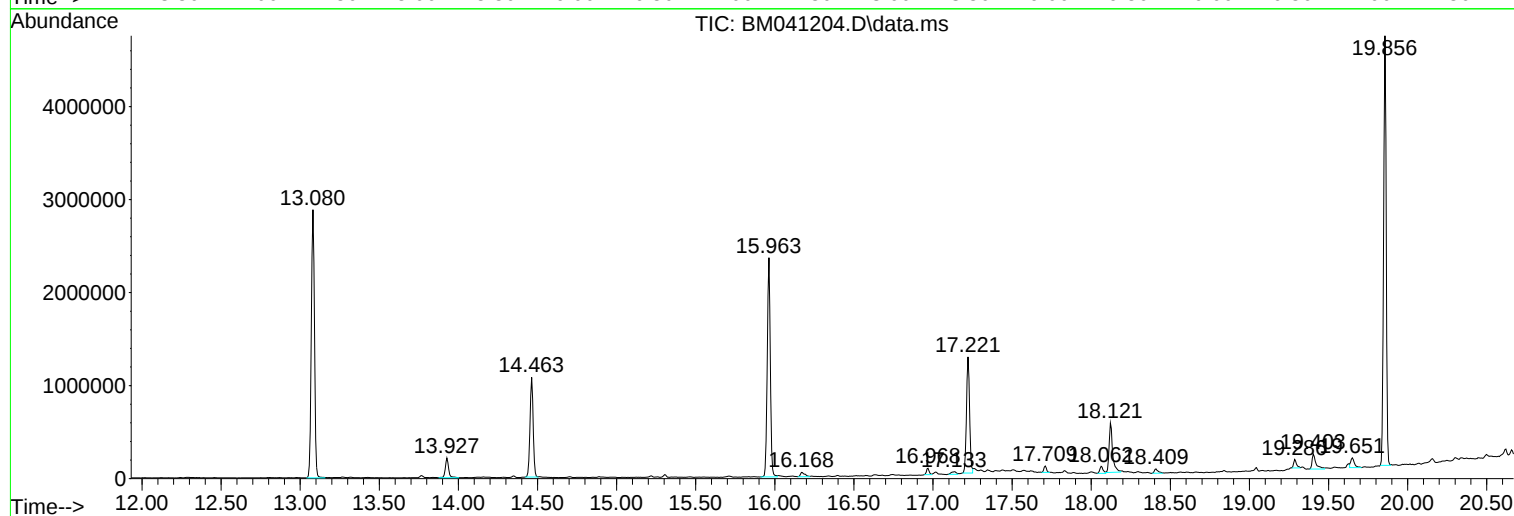
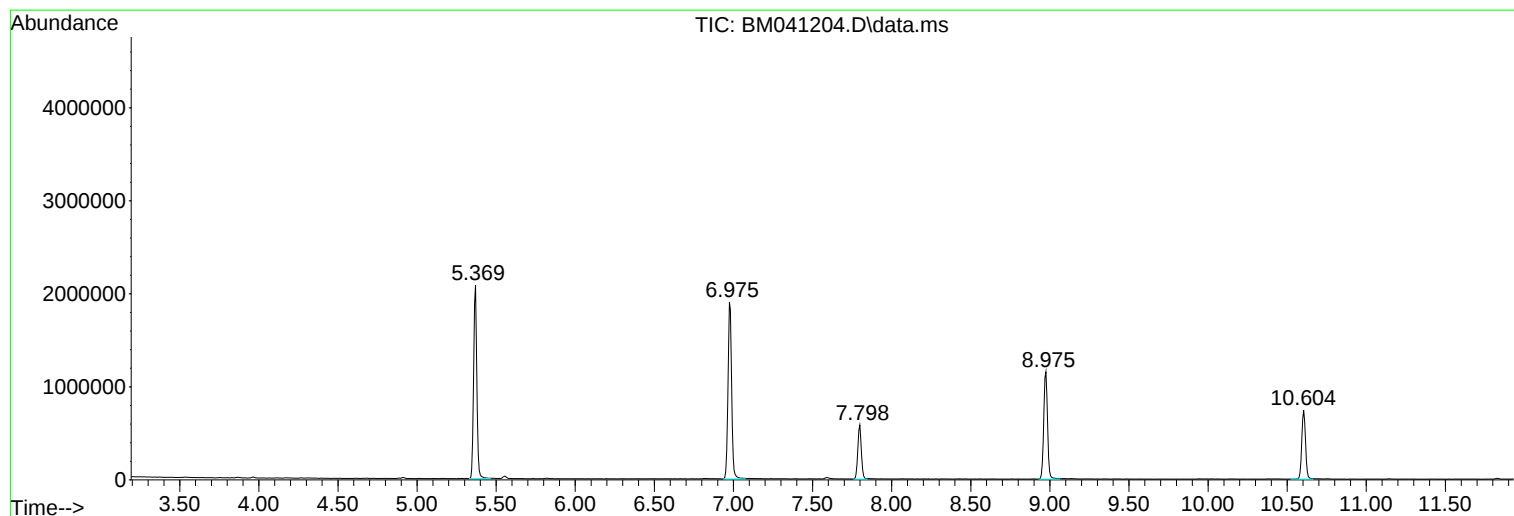
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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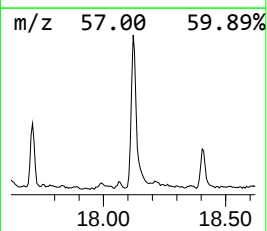
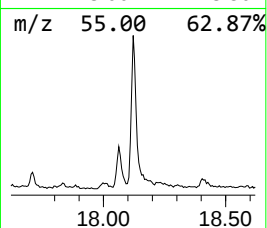
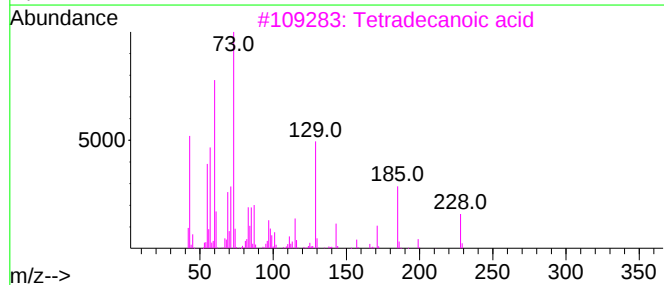
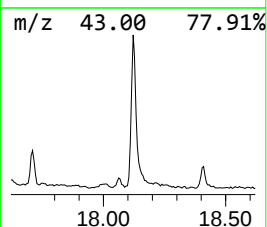
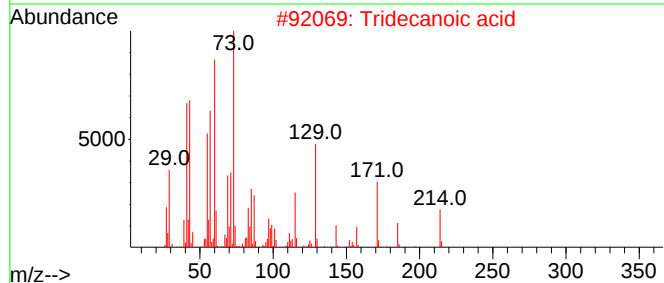
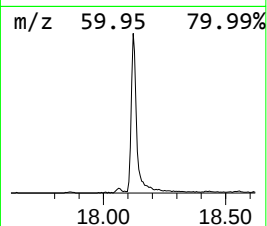
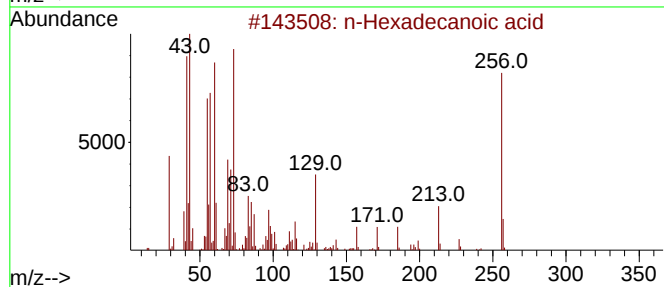
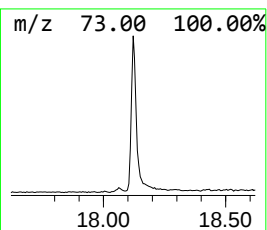
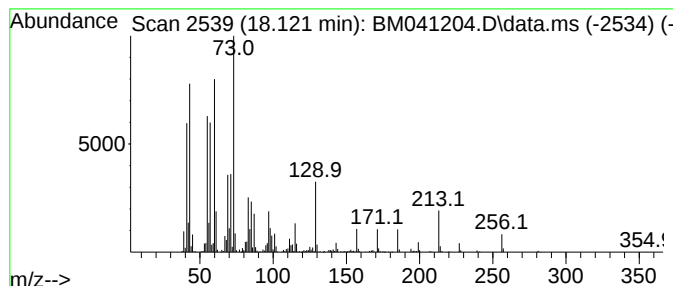
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	9.45 ng	807348	Phenanthrene-d10	17.221

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	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



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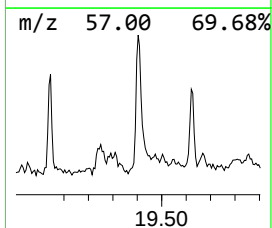
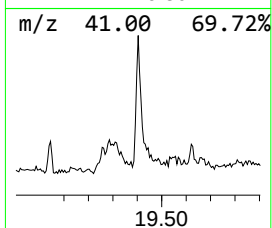
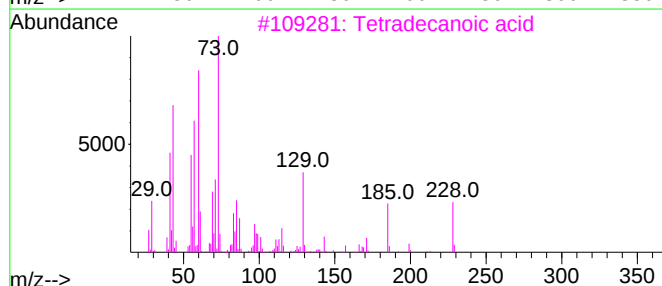
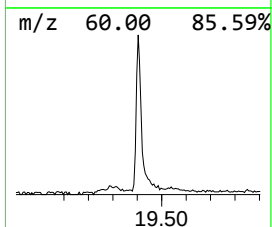
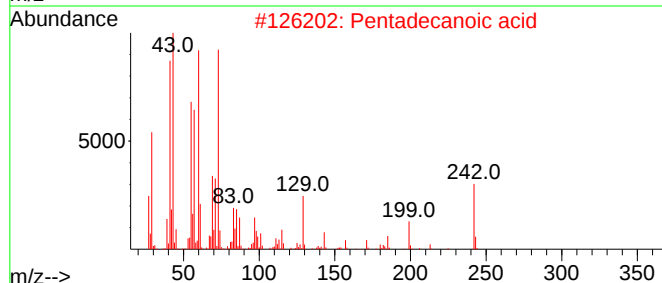
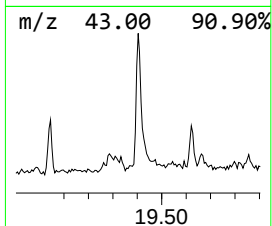
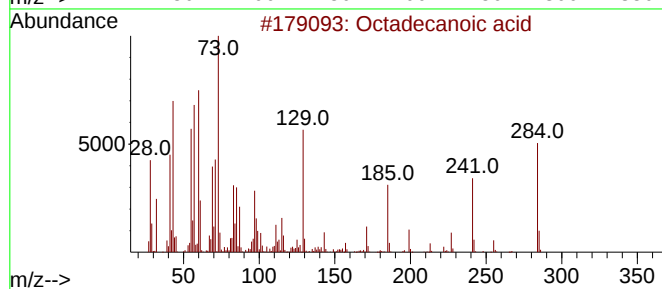
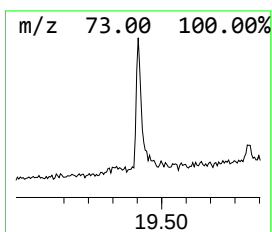
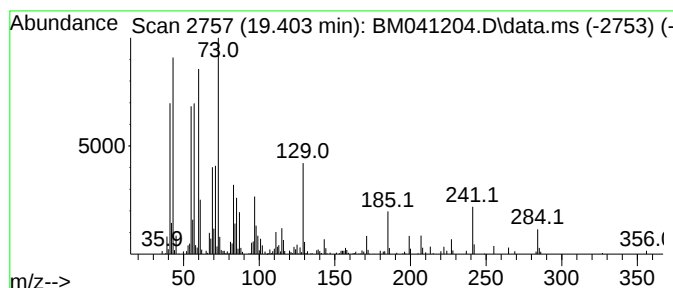
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Peak Number 2 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	2.90 ng	282444	Chrysene-d12	21.421

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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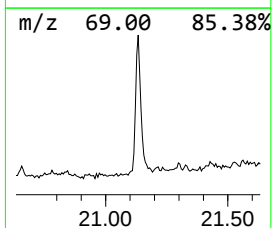
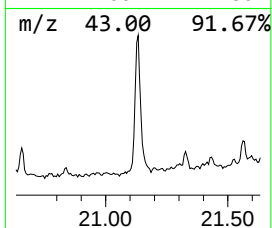
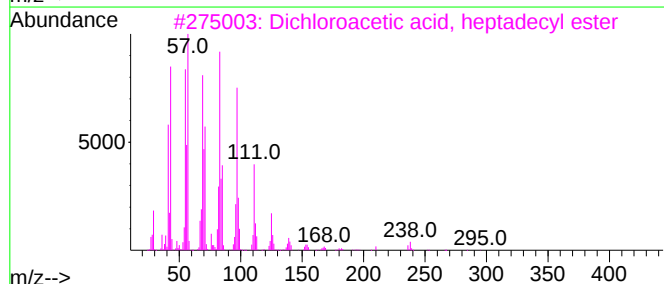
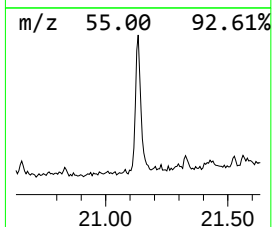
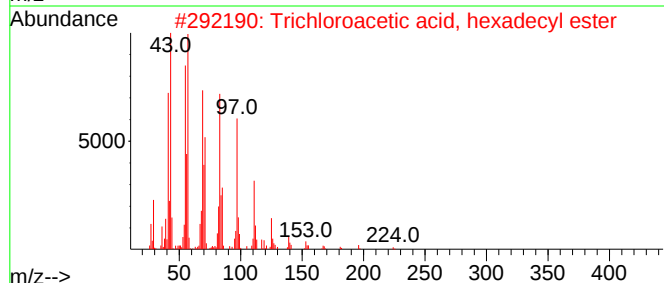
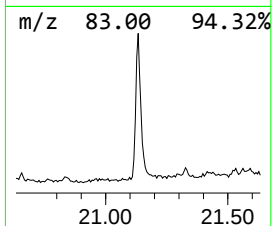
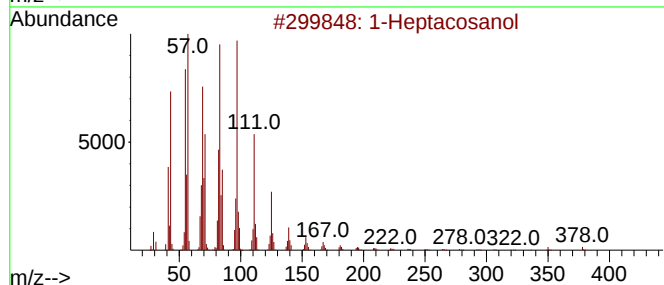
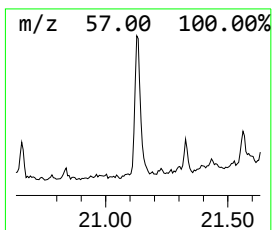
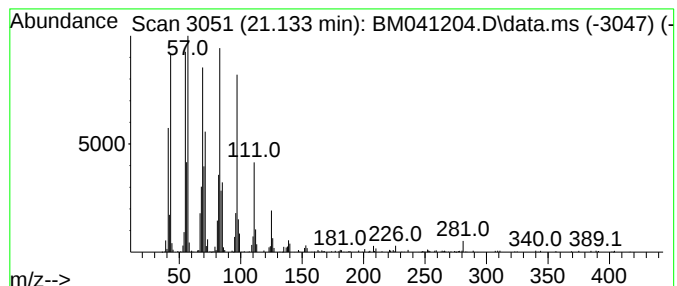
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	5.16 ng	501555	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Pentacos-1-ene	350	C25H50	016980-85-1	94



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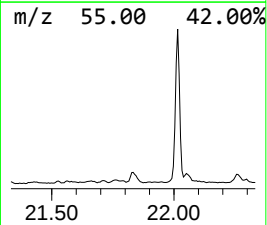
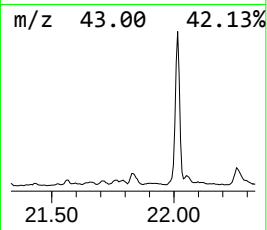
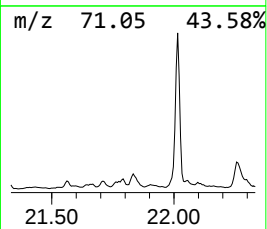
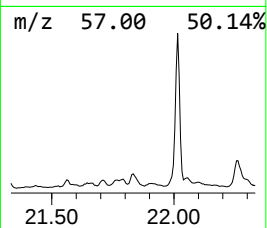
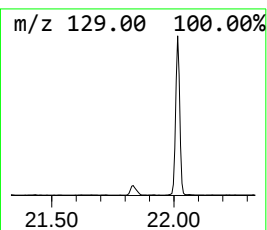
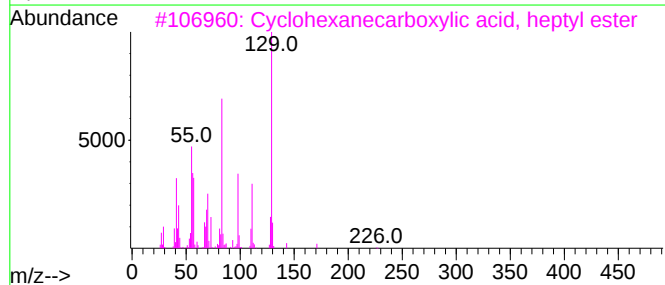
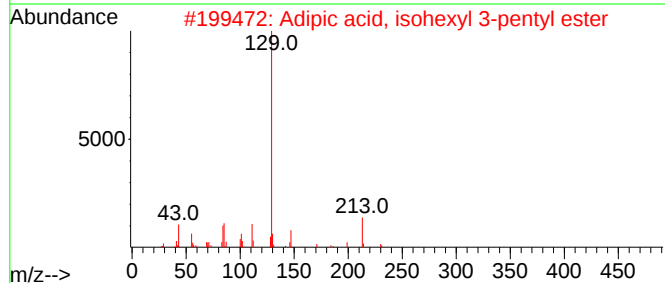
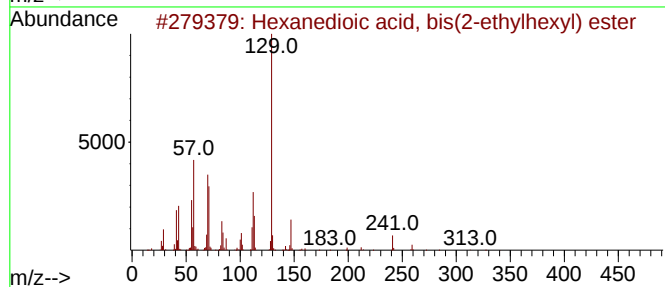
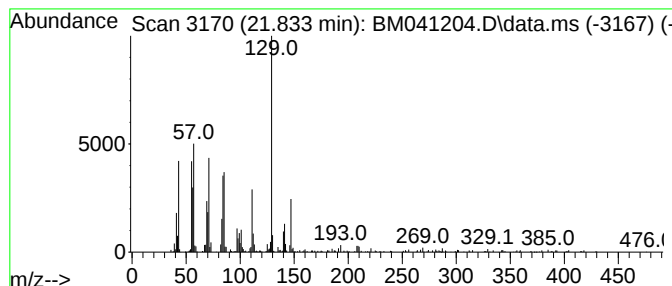
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Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.833	2.99 ng	290988	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	50
2			Adipic acid, isohexyl 3-pentyl e...	300	C17H32O4	1000324-60-7	35
3			Cyclohexanecarboxylic acid, hept...	226	C14H26O2	092319-47-6	30
4			Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	30
5			Carbonic acid, decyl heptadecyl ...	440	C28H56O3	1000383-16-6	27



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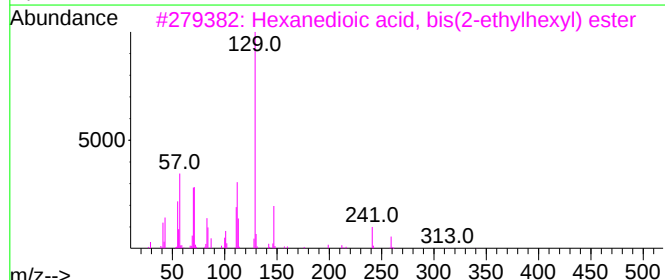
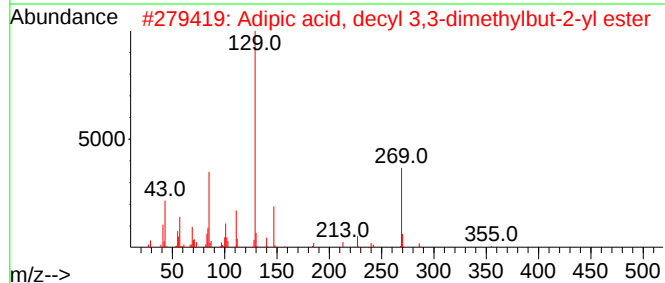
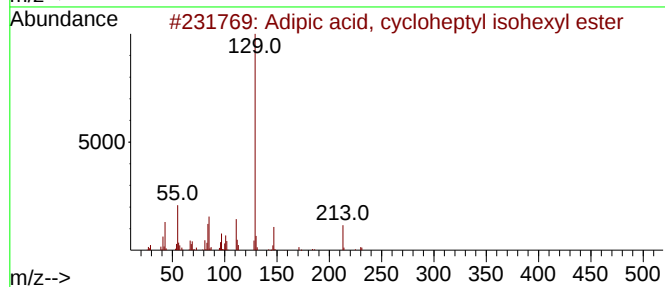
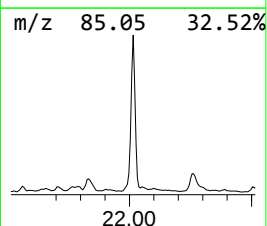
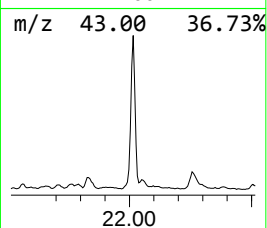
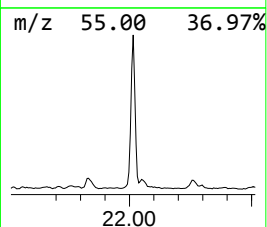
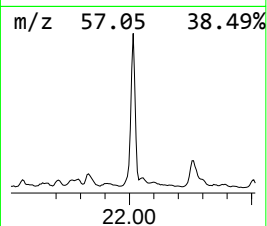
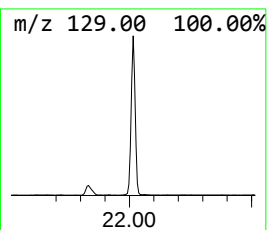
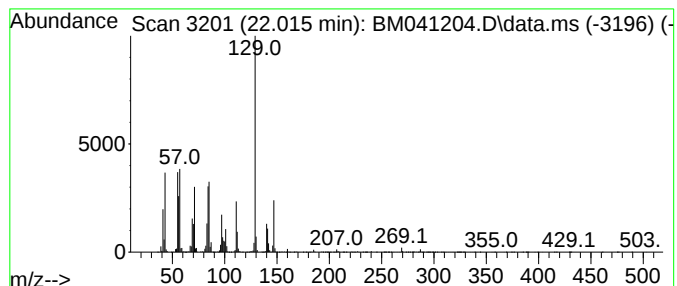
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Peak Number 5 Adipic acid, cycloheptyl is... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.015	29.79 ng	2897390	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, cycloheptyl isohexy...	326	C19H34O4	1000324-71-8	64
2			Adipic acid, decyl 3,3-dimethylb...	370	C22H42O4	1000353-67-5	59
3			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	52
4			Adipic acid, decyl 2,4-dimethylp...	384	C23H44O4	1000353-52-7	43
5			Adipic acid, isohexyl 2-octyl ester	342	C20H38O4	1000324-44-8	43



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B-P5A

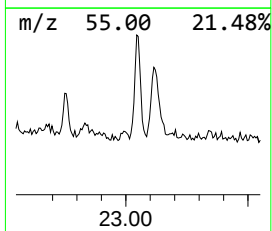
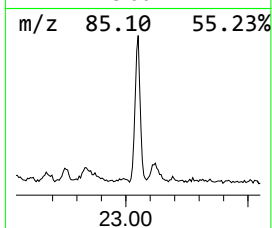
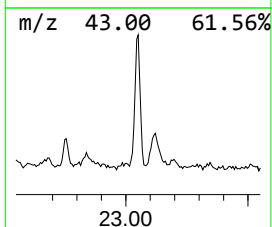
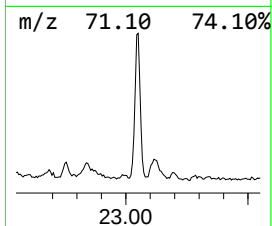
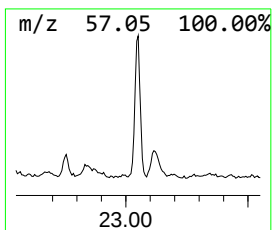
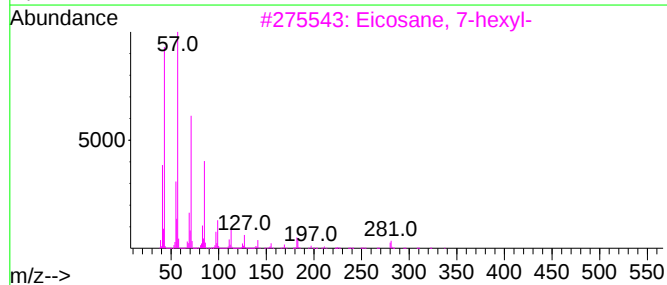
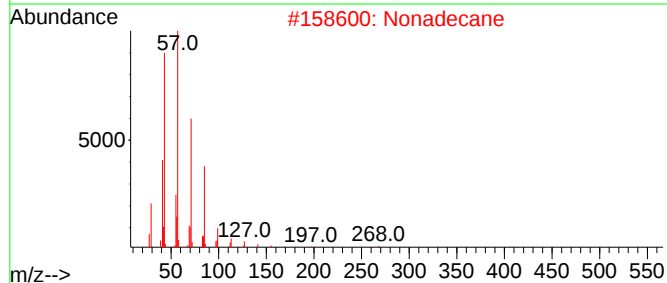
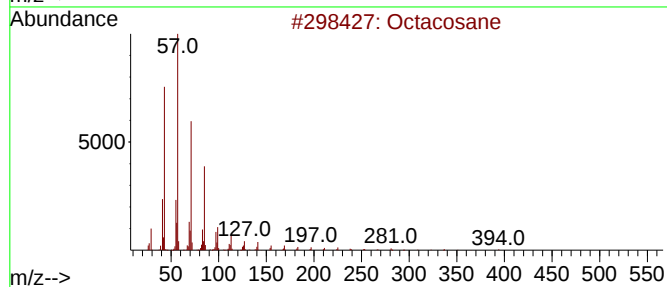
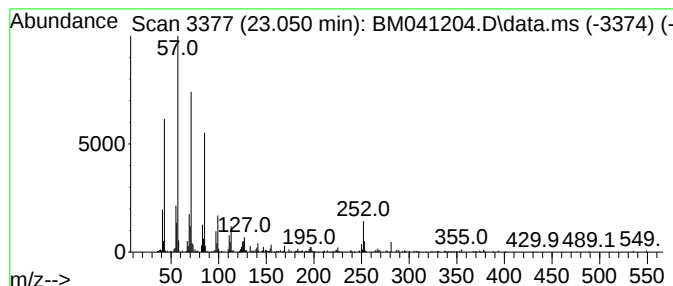
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.050	3.12 ng	287671	Perylene-d12	23.791

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	95
2		Nonadecane	268	C19H40	000629-92-5	90
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	83
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	81
5		Heptadecane, 8-methyl-	254	C18H38	013287-23-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041204.D
Acq On : 01 Aug 2023 01:28
Operator : MA/JU
Sample : 03741-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P5A

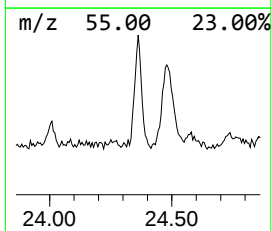
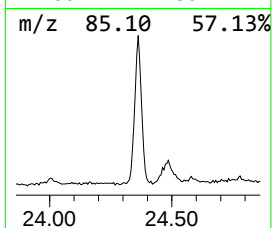
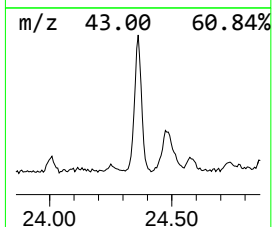
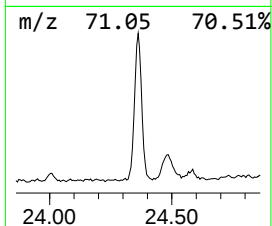
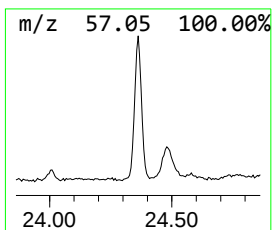
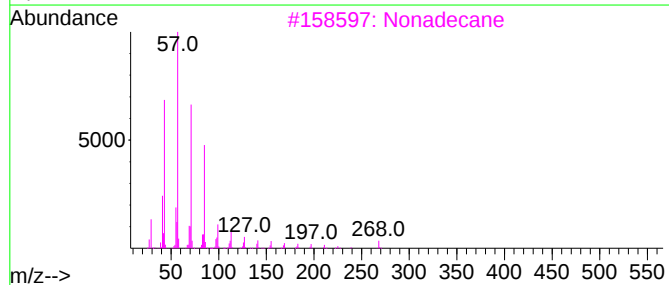
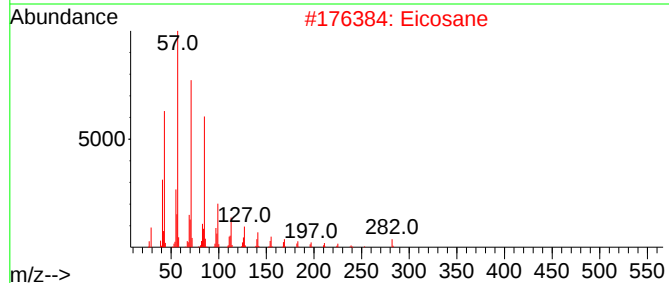
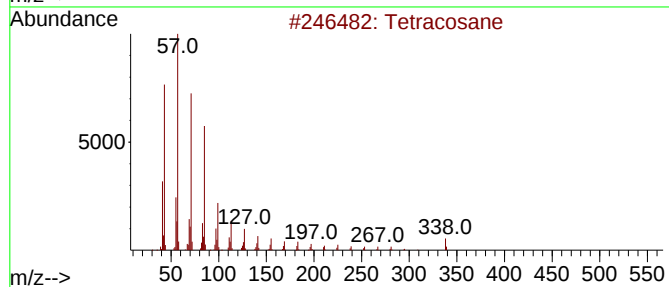
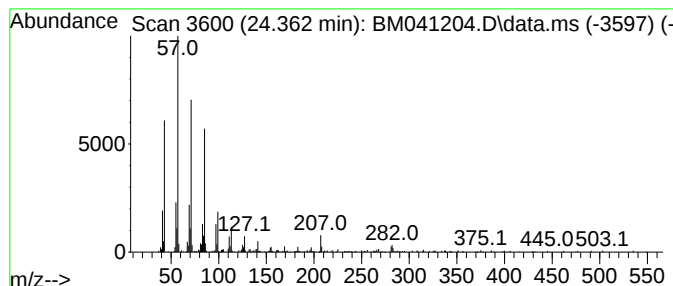
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.362	4.92 ng	453110	Perylene-d12	23.791

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Eicosane	282	C20H42	000112-95-8	90
3			Nonadecane	268	C19H40	000629-92-5	90
4			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	87
5			Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041204.D
Acq On : 01 Aug 2023 01:28
Operator : MA/JU
Sample : 03741-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P5A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.121	9.4	ng	807348	4	17.221	1709230	20.0
Octadecanoic acid	19.404	2.9	ng	282444	5	21.421	1945200	20.0
1-Heptacosanol	21.133	5.2	ng	501555	5	21.421	1945200	20.0
Hexanedioic aci...	21.833	3.0	ng	290988	5	21.421	1945200	20.0
Adipic acid, cy...	22.015	29.8	ng	2897390	5	21.421	1945200	20.0
Octacosane	23.050	3.1	ng	287671	6	23.791	1841520	20.0
Tetracosane	24.362	4.9	ng	453110	6	23.791	1841520	20.0