

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
 Data File : BM034060.D
 Acq On : 23 Feb 2022 19:42
 Operator : CG/JU
 Sample : N1627-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 20220095-BERKELEY-7-ELUTRIATE

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-BM022222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.566	389	396	405	rBV	1769189	2515576	26.17%	4.103%
2	7.166	659	668	680	rVB	1231881	2069608	21.53%	3.376%
3	8.019	805	813	820	rBV	723336	1148198	11.94%	1.873%
4	9.178	1001	1010	1019	rBV	2096402	3402408	35.39%	5.550%
5	10.607	1246	1253	1262	rBV	156372	256612	2.67%	0.419%
6	10.831	1284	1291	1298	rBV	894966	1488670	15.49%	2.428%
7	12.583	1580	1589	1596	rBV	47048	106302	1.11%	0.173%
8	13.283	1701	1708	1715	rBV	5818998	8296772	86.31%	13.533%
9	14.301	1872	1881	1887	rBV3	75514	130279	1.36%	0.212%
10	14.466	1901	1909	1921	rVB	65372	147178	1.53%	0.240%
11	14.648	1930	1940	1947	rBV	1344574	2087542	21.72%	3.405%
12	14.866	1972	1977	1981	rBV	85008	107827	1.12%	0.176%
13	15.460	2072	2078	2083	rBV2	108990	159662	1.66%	0.260%
14	16.130	2186	2192	2199	rBV	4706134	6414912	66.73%	10.463%
15	17.318	2389	2394	2399	rBV	128140	151200	1.57%	0.247%
16	17.389	2400	2406	2412	rBV	1585407	2251336	23.42%	3.672%
17	17.683	2450	2456	2467	rBV	6614943	8228462	85.60%	13.422%
18	18.071	2517	2522	2527	rVB2	177382	238113	2.48%	0.388%
19	18.295	2554	2560	2568	rBV	948686	1478944	15.39%	2.412%
20	18.360	2568	2571	2578	rVB	186923	261517	2.72%	0.427%
21	19.565	2771	2776	2791	rBV	3037404	4400463	45.78%	7.178%
22	20.006	2845	2851	2856	rBV	8078368	9612863	100.00%	15.680%
23	21.277	3063	3067	3077	rBV	496847	688361	7.16%	1.123%
24	21.559	3110	3115	3121	rBV	2146125	2665501	27.73%	4.348%
25	21.995	3186	3189	3195	rVB	121669	144456	1.50%	0.236%
26	24.024	3527	3534	3542	rVB2	1398329	2855119	29.70%	4.657%

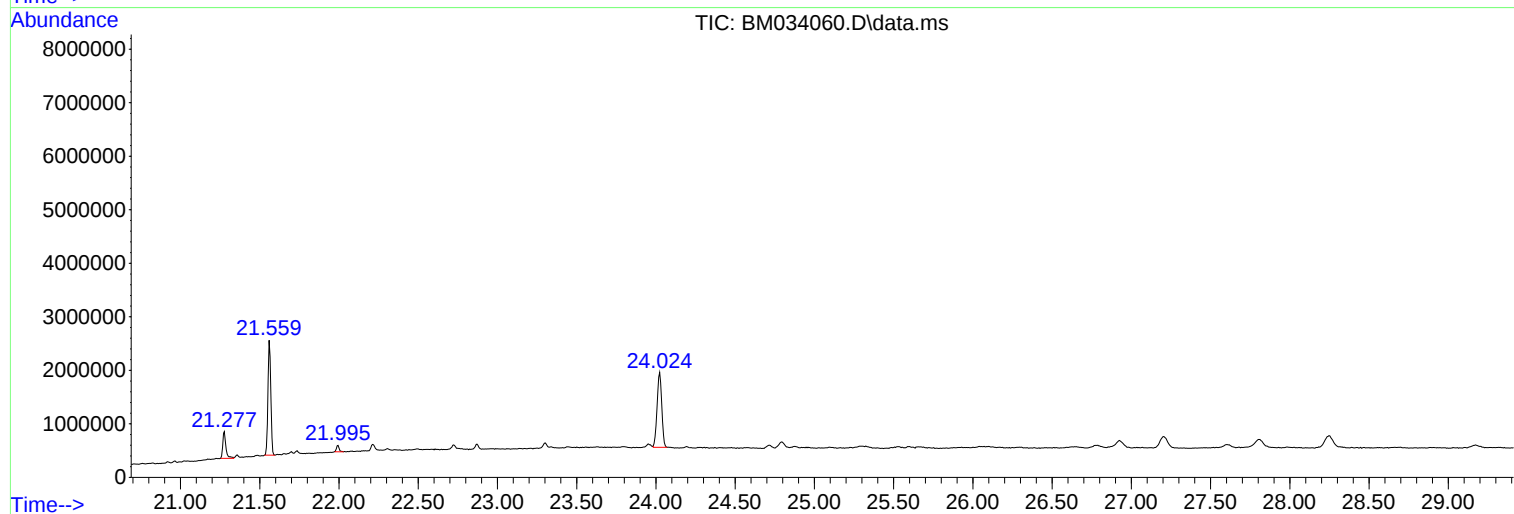
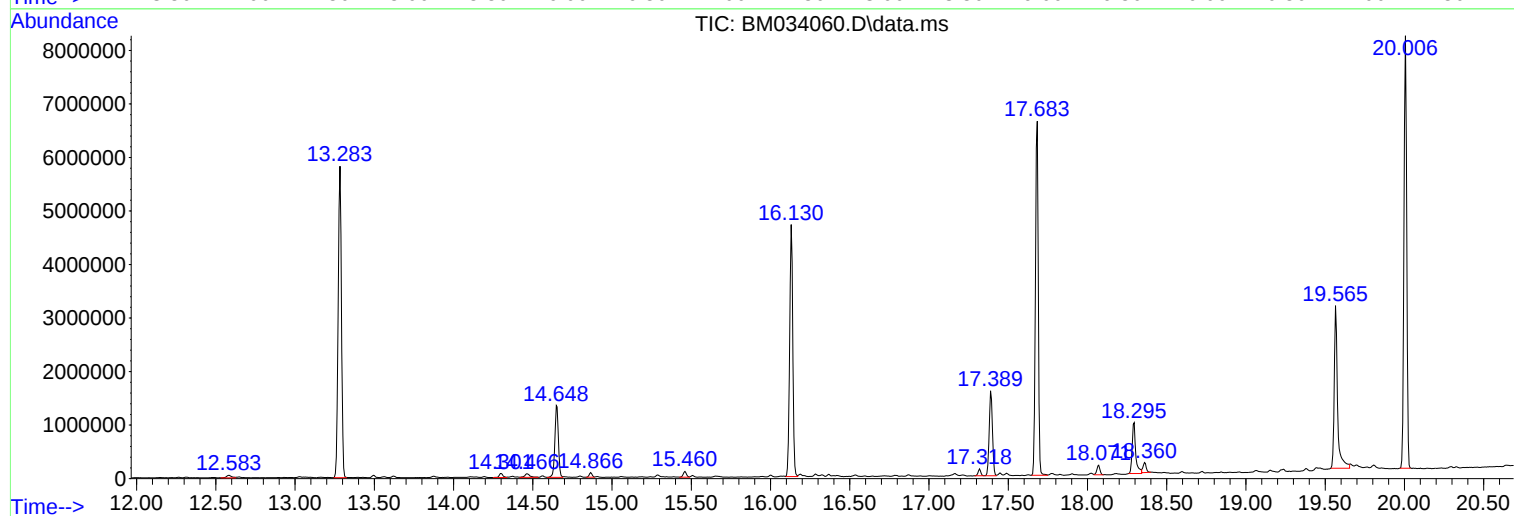
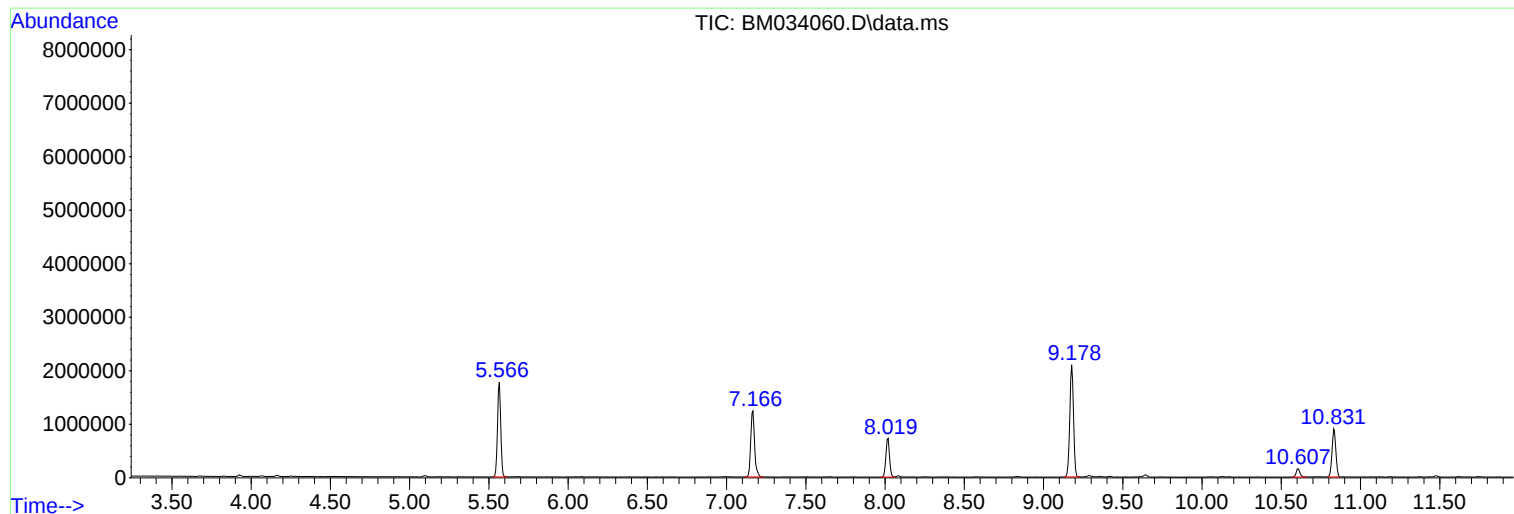
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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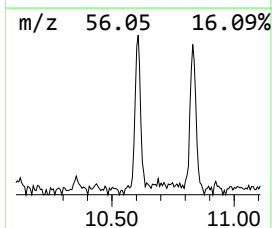
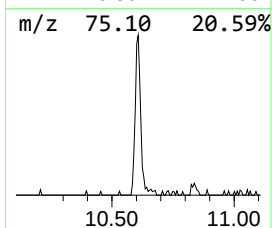
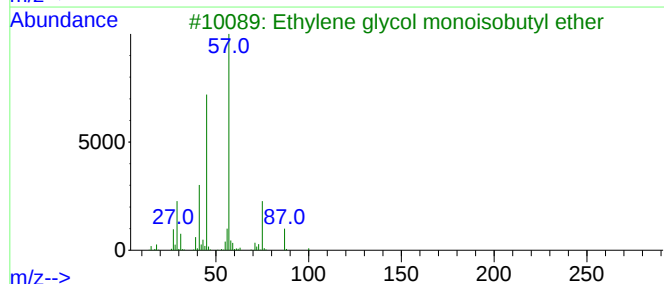
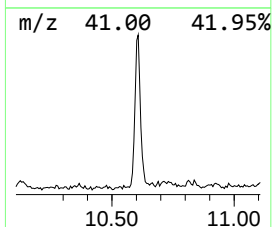
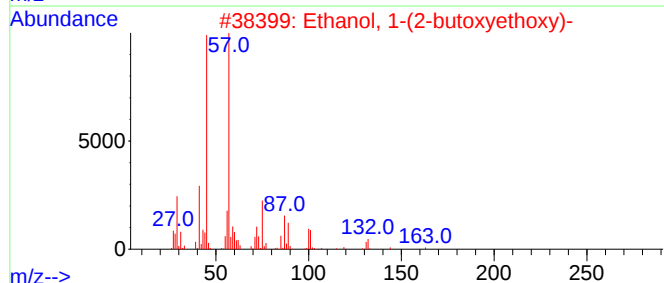
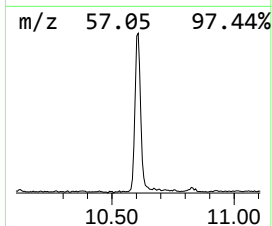
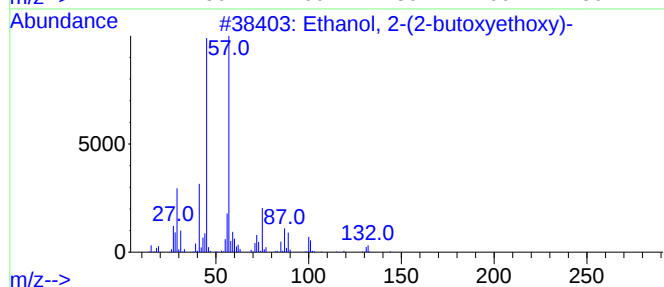
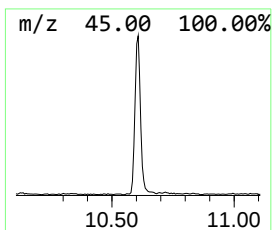
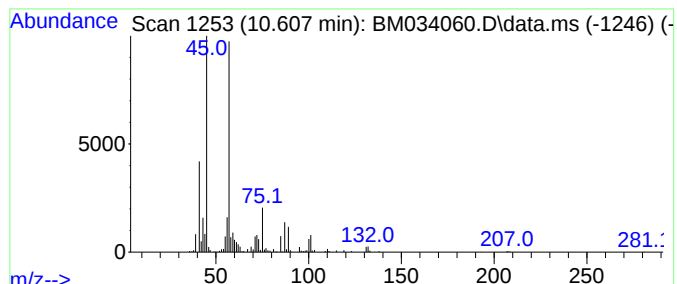
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.607	3.45 ng	256612	Naphthalene-d8	10.831

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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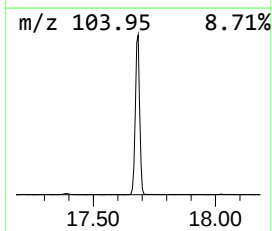
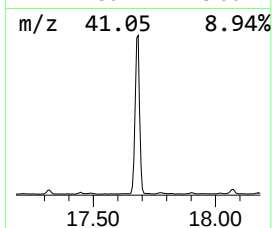
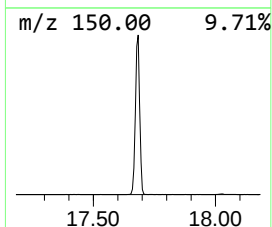
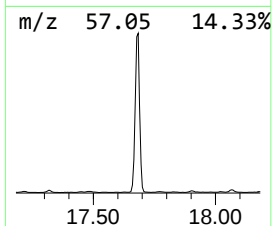
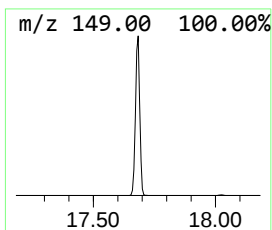
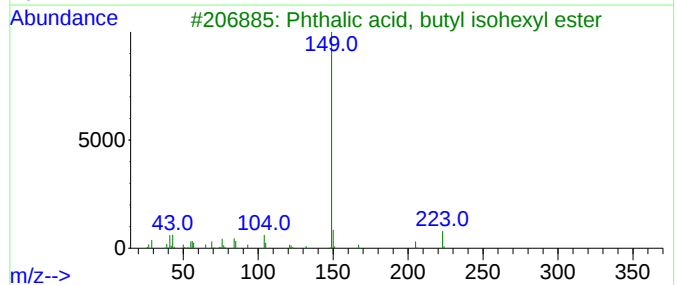
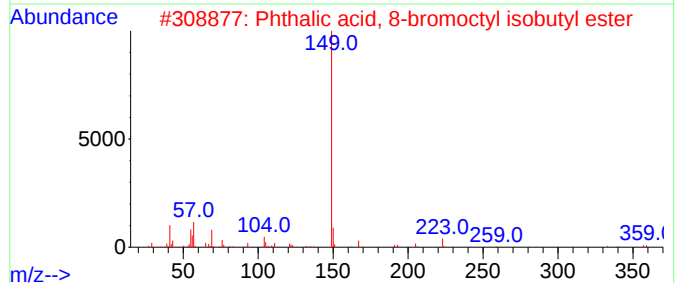
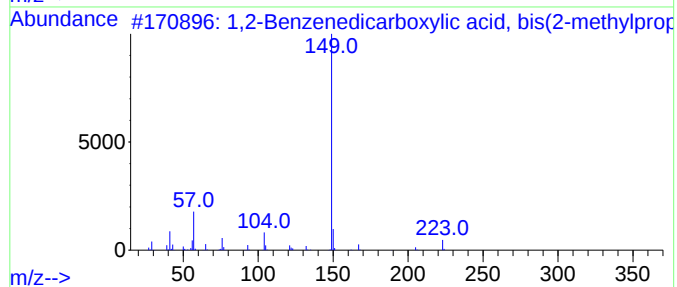
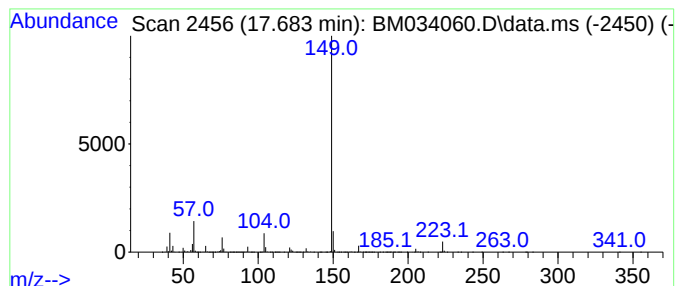
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.683	73.10 ng	8228460	Phenanthrene-d10	17.389	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2	Phthalic acid, 8-bromooctyl isobu...	412	C20H29BrO4	1000382-55-3	83
3	Phthalic acid, butyl isohexyl ester	306	C18H26O4	1000309-03-6	78
4	Phthalic acid, hex-3-yl isobutyl...	306	C18H26O4	1000356-95-4	78
5	Phthalic acid, isobutyl octyl ester	334	C20H30O4	1010309-04-5	78



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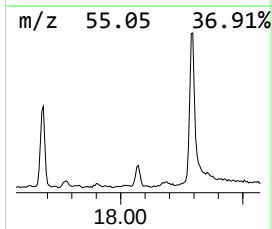
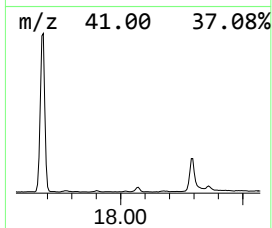
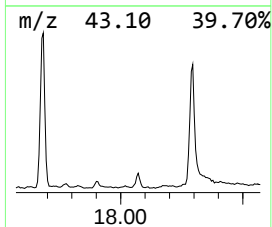
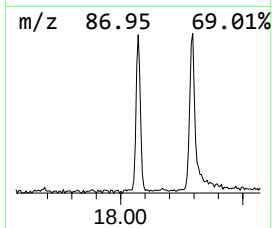
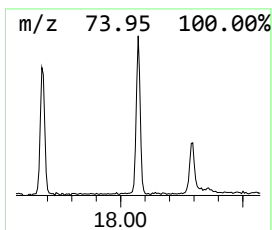
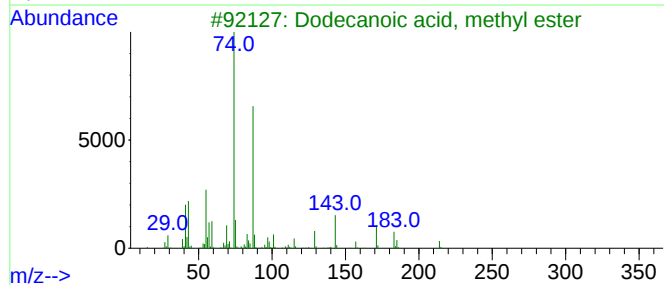
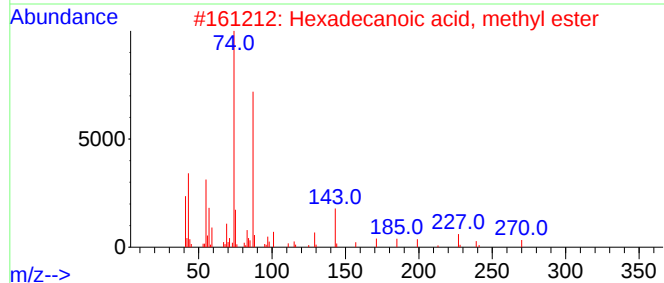
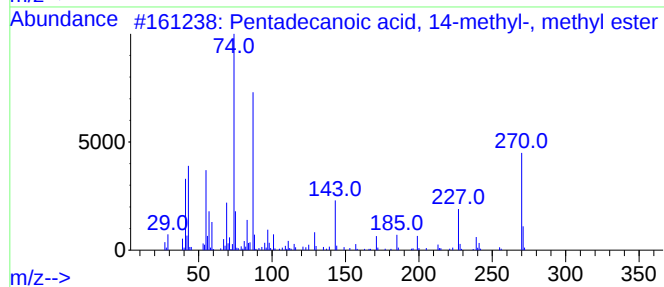
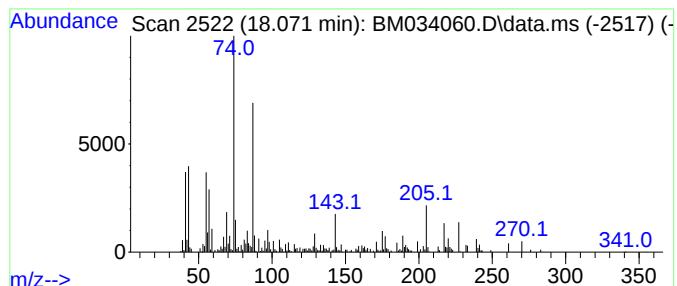
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentadecanoic acid, 14-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.071	2.12 ng	238113	Phenanthrene-d10	17.389

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
3			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	64
4			Cyclopentanetridecanoic acid, me...	296	C19H36O2	024828-61-3	62
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	58



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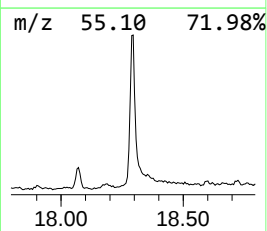
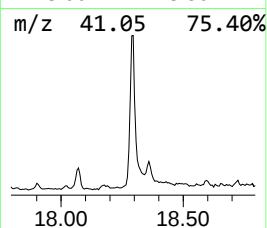
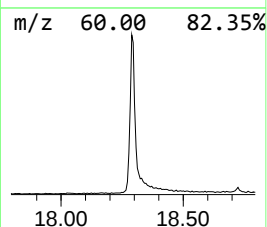
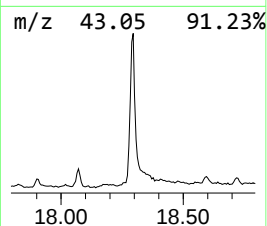
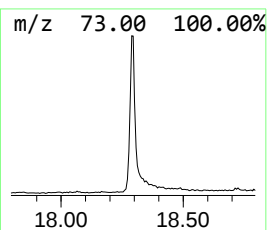
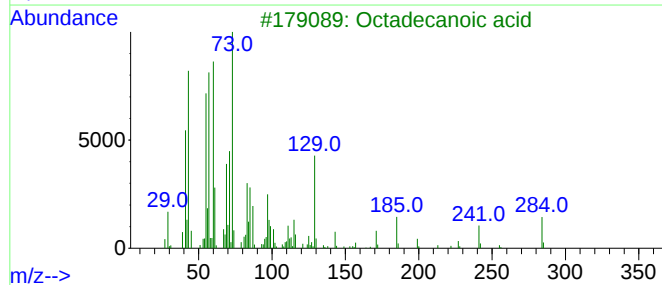
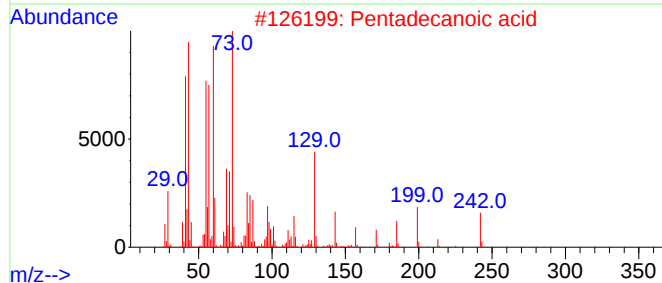
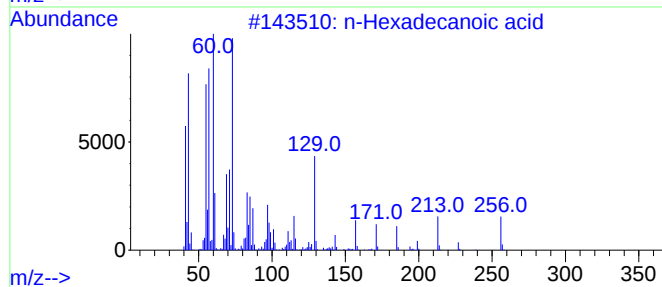
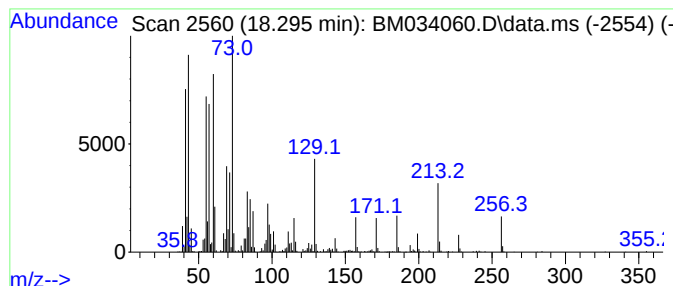
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.295	13.14 ng	1478940	Phenanthrene-d10	17.389

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	87
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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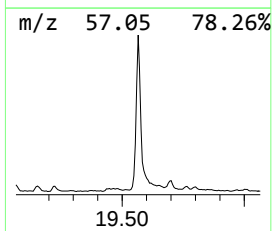
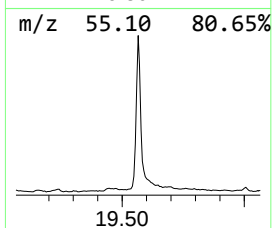
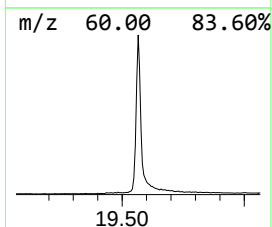
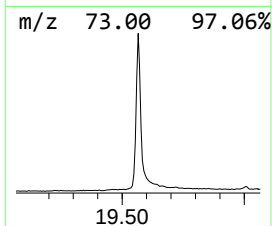
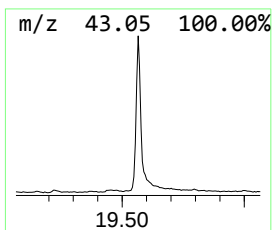
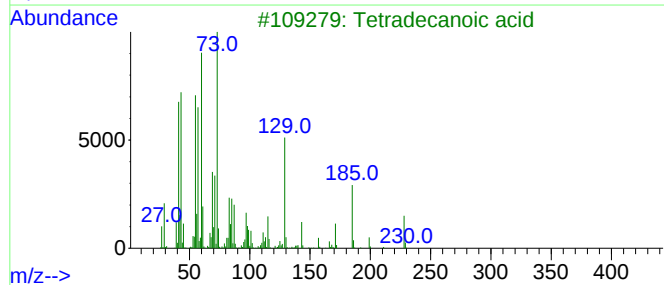
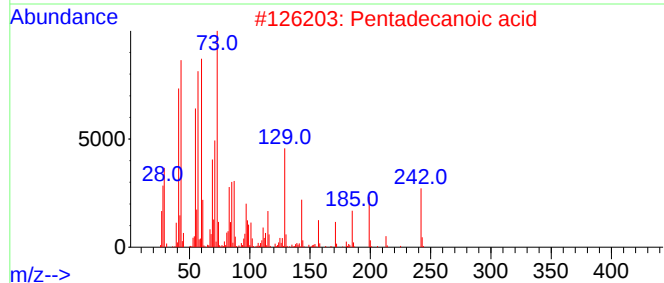
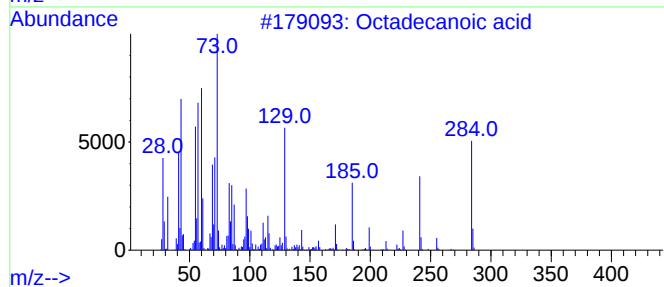
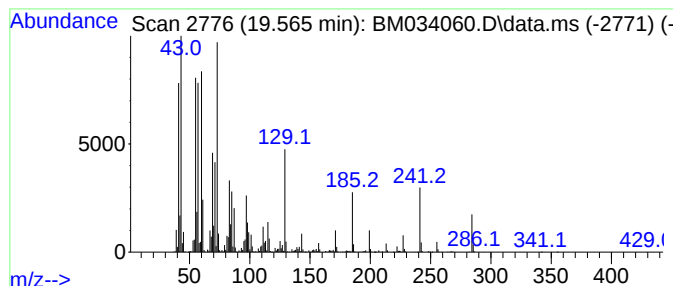
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Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.565	33.02 ng	4400460	Chrysene-d12	21.559

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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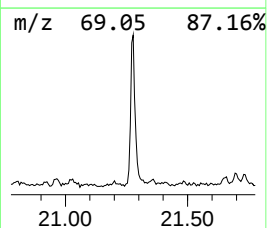
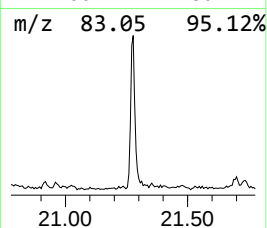
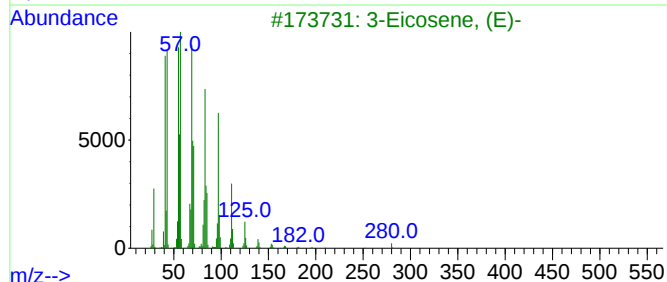
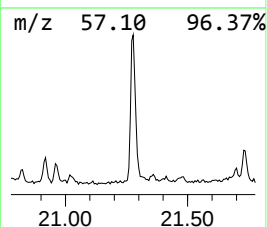
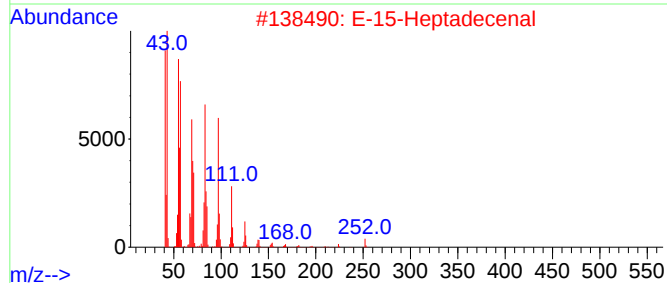
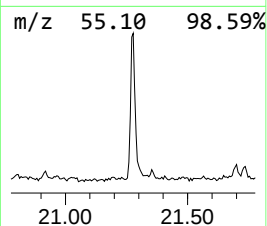
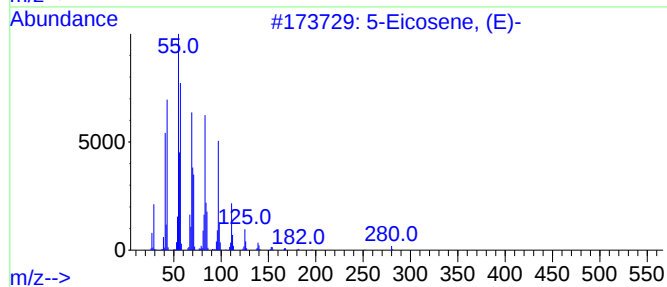
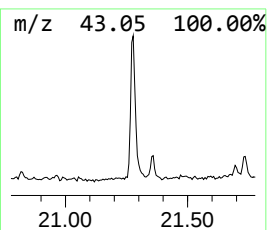
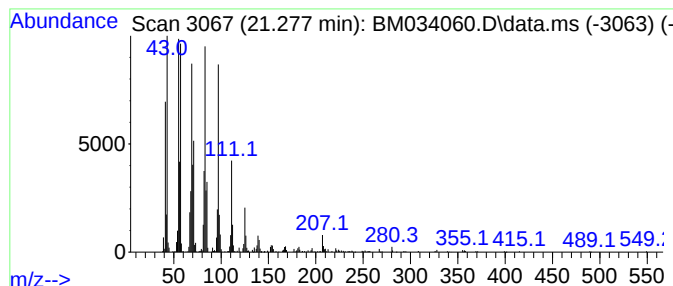
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.277	5.16 ng	688361	Chrysene-d12	21.559

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		E-15-Heptadecenal	252	C17H32O	1000130-97-9	97
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	96
4		1-Heneicosanol	312	C21H44O	015594-90-8	95
5		1-Tricosene	322	C23H46	018835-32-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
Data File : BM034060.D
Acq On : 23 Feb 2022 19:42
Operator : CG/JU
Sample : N1627-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20220095-BERKELEY-7-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.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
Ethanol, 2-(2-b...	10.607	3.5	ng	256612	2	10.831	1488670	20.0
1,2-Benzenedica...	17.683	73.1	ng	8228460	4	17.389	2251340	20.0
Pentadecanoic a...	18.071	2.1	ng	238113	4	17.389	2251340	20.0
n-Hexadecanoic ...	18.295	13.1	ng	1478940	4	17.389	2251340	20.0
Octadecanoic acid	19.565	33.0	ng	4400460	5	21.559	2665500	20.0
5-Eicosene, (E)-	21.277	5.2	ng	688361	5	21.559	2665500	20.0