

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
 Data File : BM029326.D
 Acq On : 02 Apr 2021 18:23
 Operator : CG/JU
 Sample : M1874-08
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FS-SB11(52-53)

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-BM040121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.940	5	9	14	rBV	524042	589112	14.13%	2.260%
2	2.981	14	16	25	rVB	103997	121541	2.92%	0.466%
3	5.293	403	409	421	rBV	1745640	2511954	60.25%	9.635%
4	6.875	668	678	690	rBV	1633002	2676504	64.19%	10.266%
5	7.699	811	818	826	rVB	425400	653631	15.68%	2.507%
6	8.851	1006	1014	1027	rBV	1015840	1667158	39.99%	6.395%
7	10.481	1282	1291	1298	rBV	491876	826892	19.83%	3.172%
8	12.951	1703	1711	1721	rBV	2047270	3037609	72.85%	11.651%
9	13.169	1741	1748	1755	rBV	32613	49756	1.19%	0.191%
10	13.792	1849	1854	1858	rBV	59366	88766	2.13%	0.340%
11	14.169	1913	1918	1928	rVB2	20846	45283	1.09%	0.174%
12	14.333	1939	1946	1953	rBV	665729	984137	23.60%	3.775%
13	15.816	2192	2198	2211	rBV	1616200	2369523	56.83%	9.089%
14	17.069	2405	2411	2417	rBV	758405	1091388	26.18%	4.186%
15	17.974	2559	2565	2581	rBV	320428	512793	12.30%	1.967%
16	19.139	2754	2763	2776	rBV2	273906	685452	16.44%	2.629%
17	19.257	2779	2783	2800	rVB	179298	329984	7.91%	1.266%
18	19.698	2852	2858	2866	rBV	3467578	4169443	100.00%	15.993%
19	20.910	3058	3064	3070	rBV2	130735	220414	5.29%	0.845%
20	20.968	3070	3074	3086	rVV	447000	609318	14.61%	2.337%
21	21.245	3116	3121	3126	rBV	1110739	1362725	32.68%	5.227%
22	23.456	3491	3497	3507	rVB2	771945	1467542	35.20%	5.629%

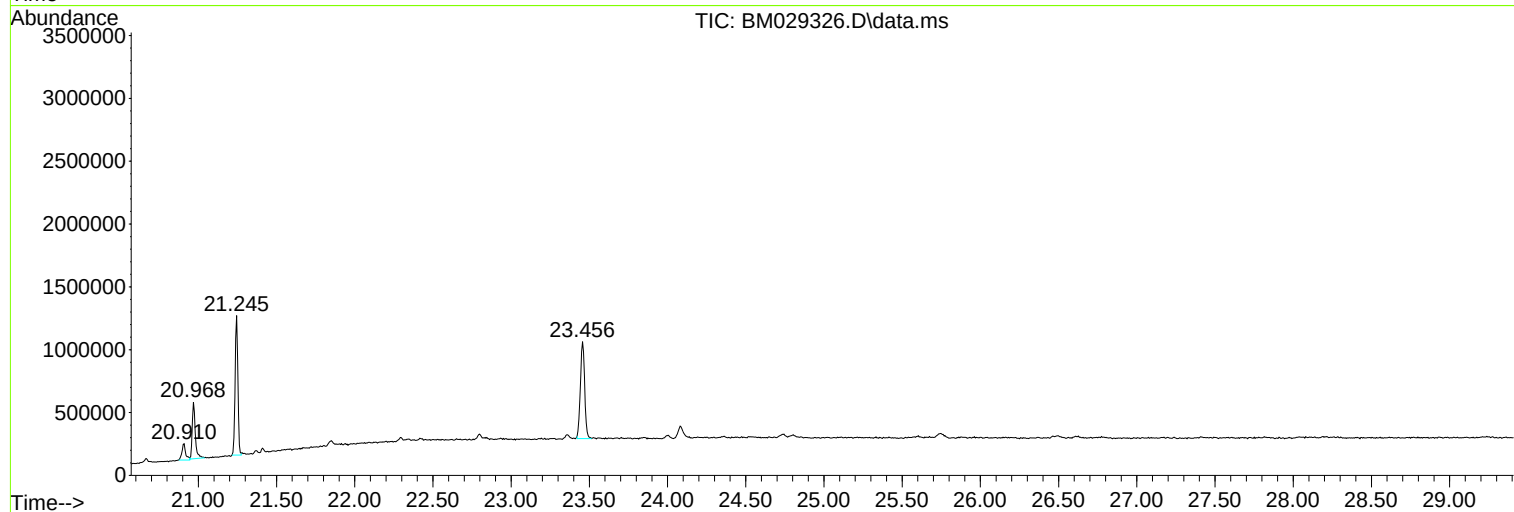
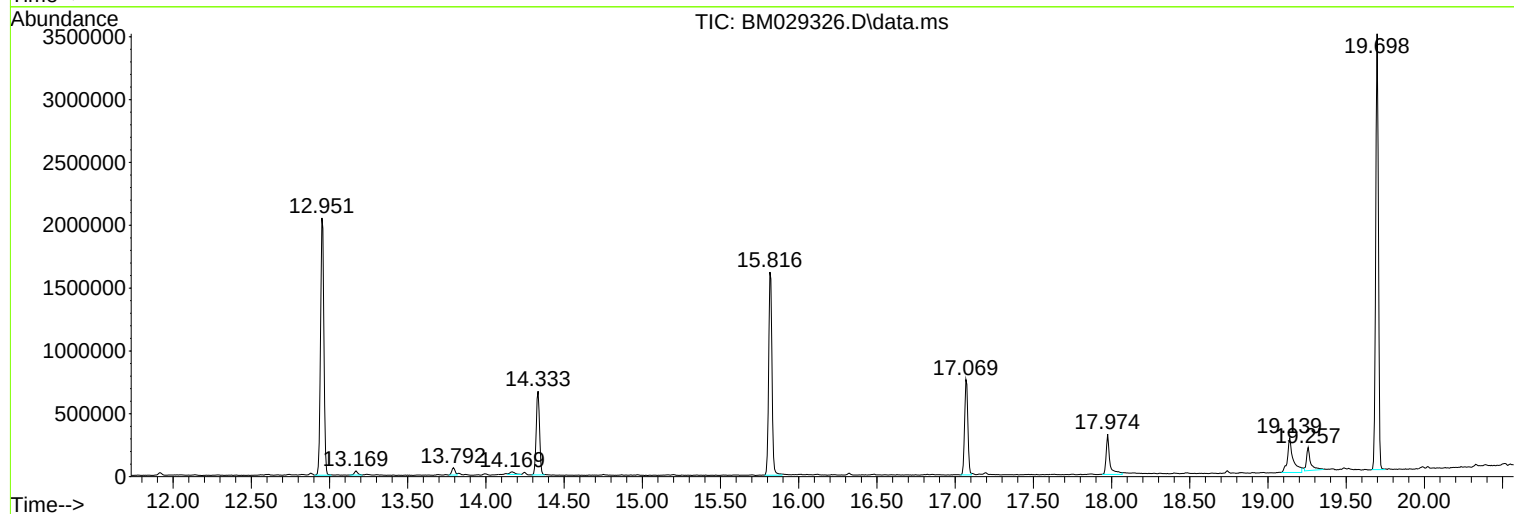
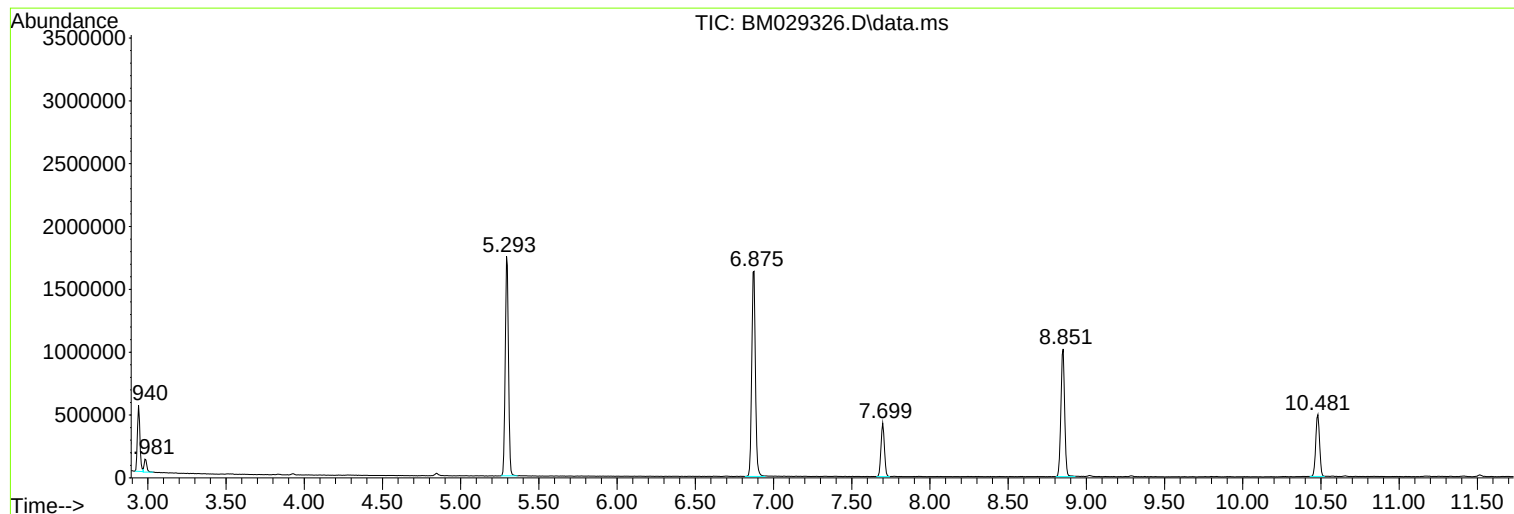
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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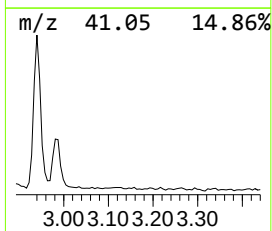
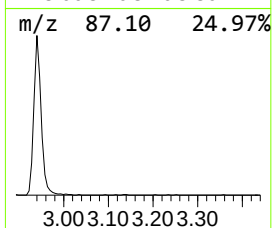
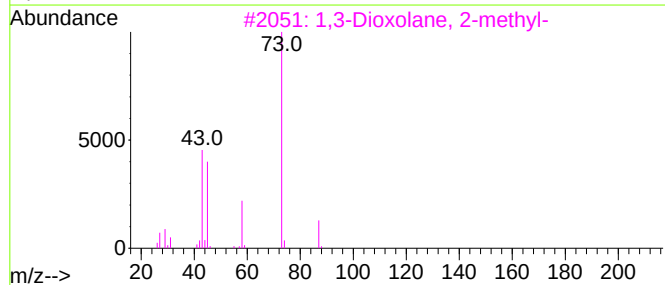
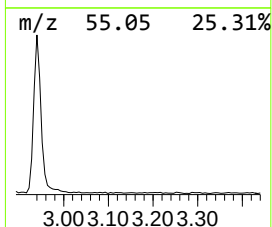
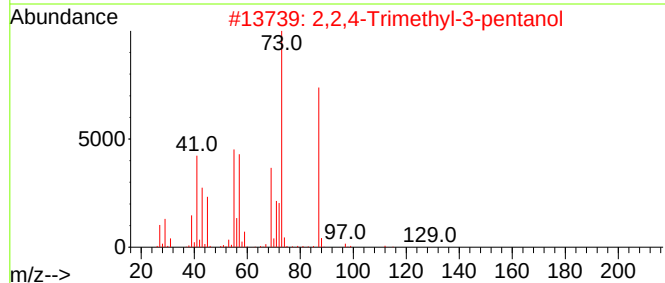
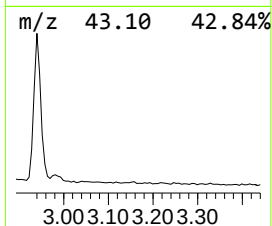
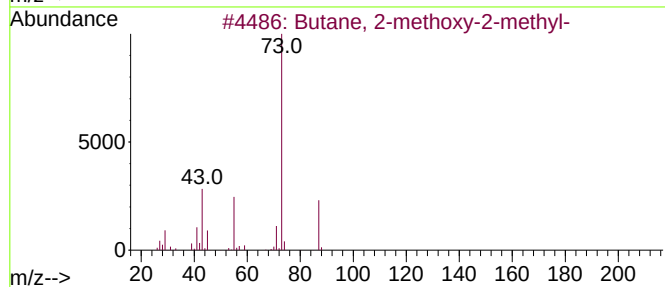
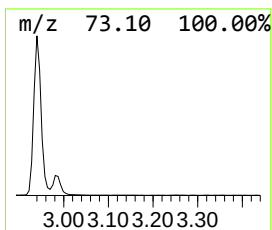
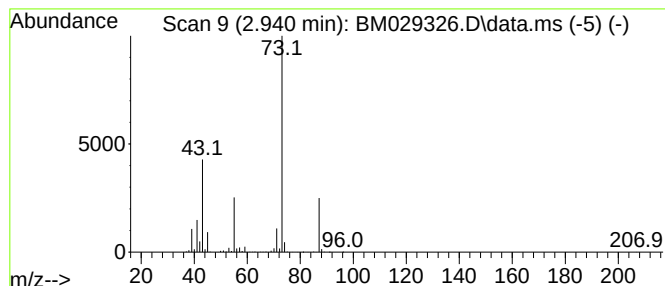
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.940	18.03 ng	589112	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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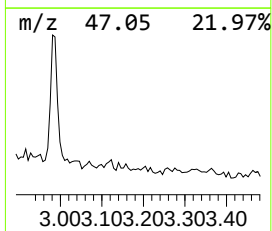
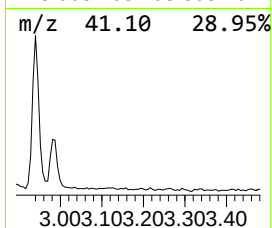
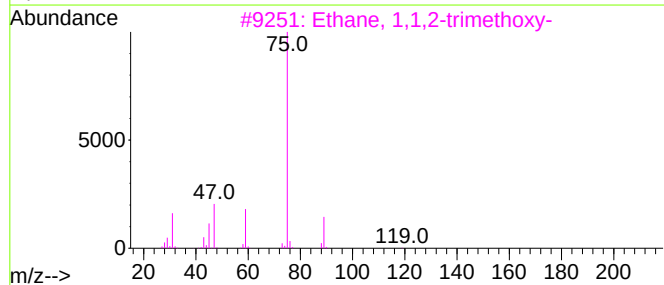
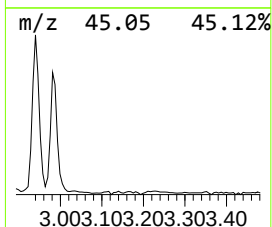
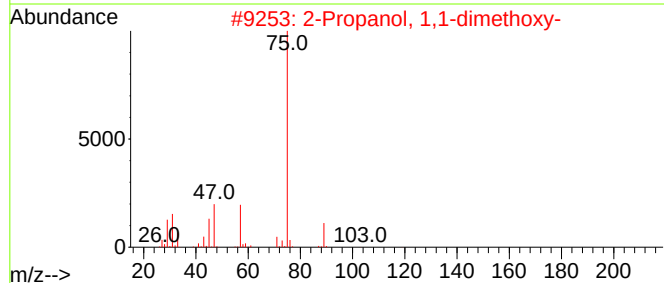
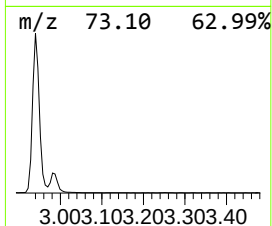
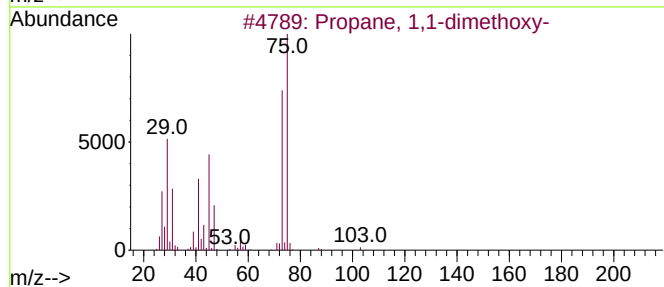
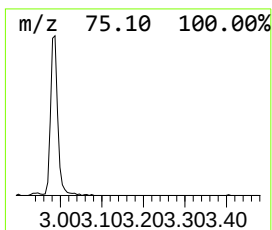
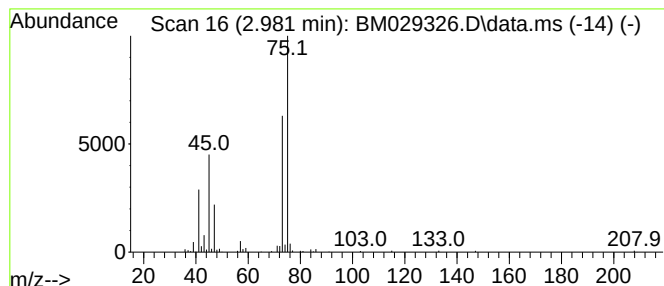
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.981	3.72 ng	121541	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
3			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	33
4			Ethane, 1,1'-[oxybis(methyleneth...	166	C6H14O5S2	054411-14-2	33
5			Benzene, [2-(ethylthio)ethyl]-	166	C10H14S	022914-08-5	33



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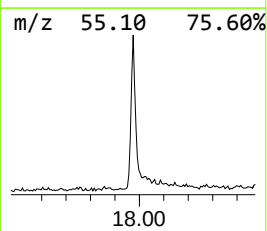
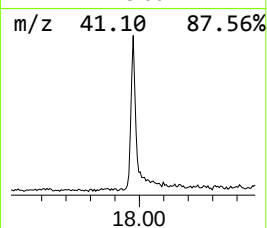
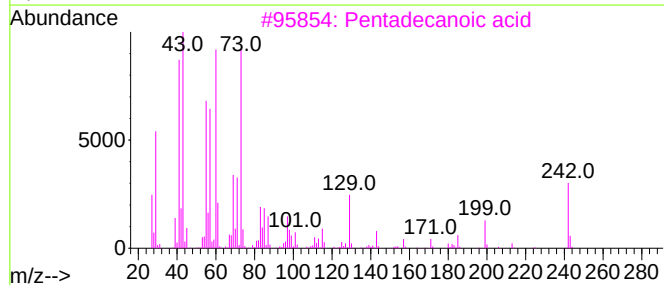
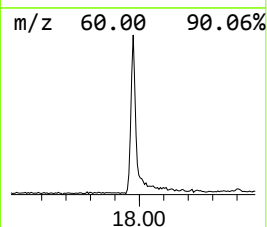
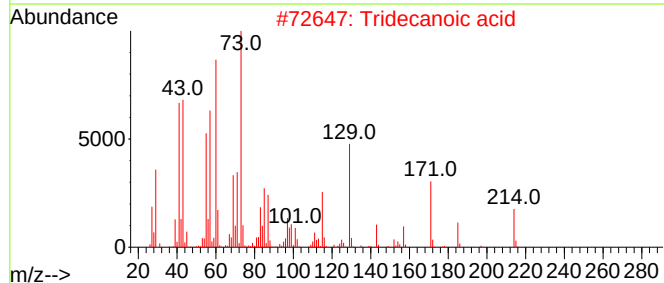
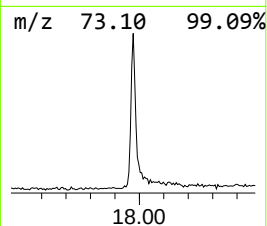
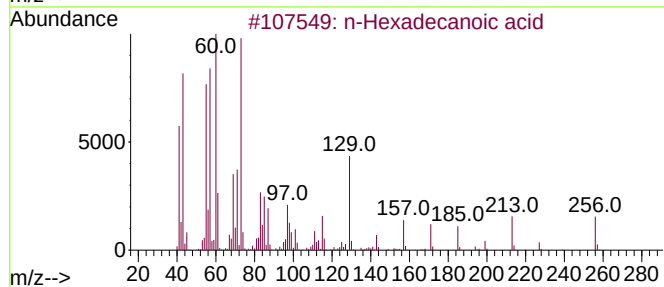
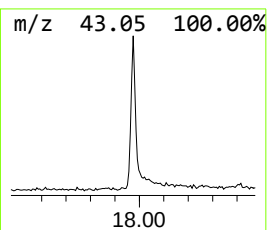
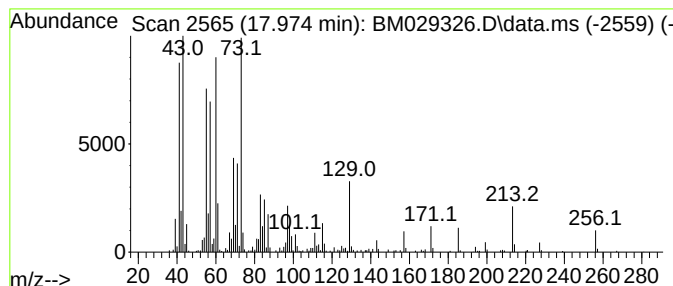
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	9.40 ng	512793	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	68



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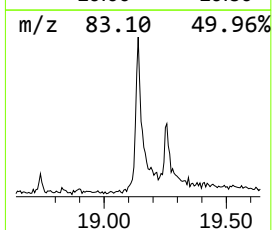
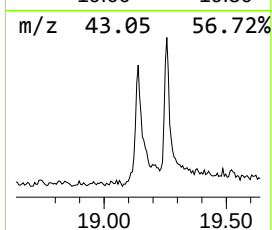
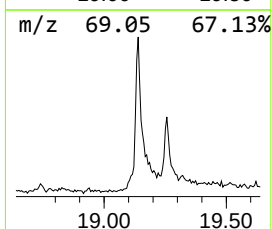
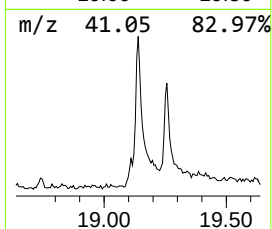
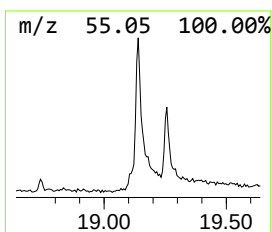
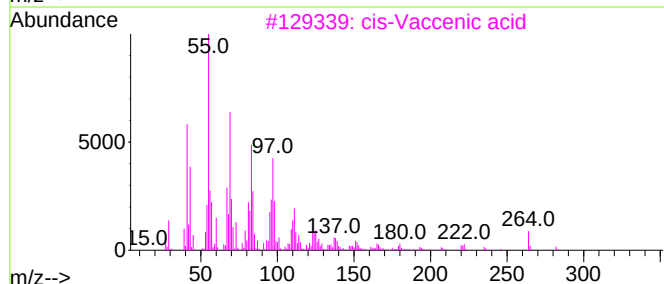
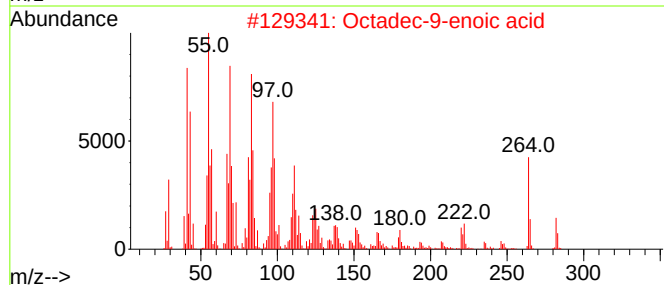
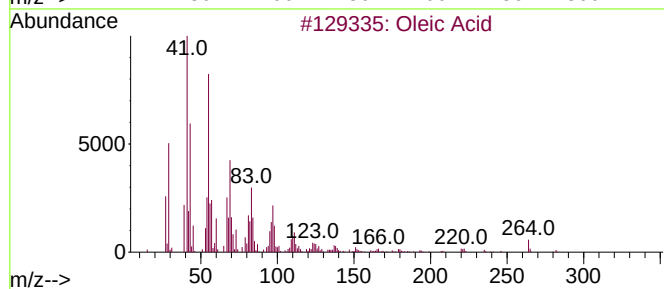
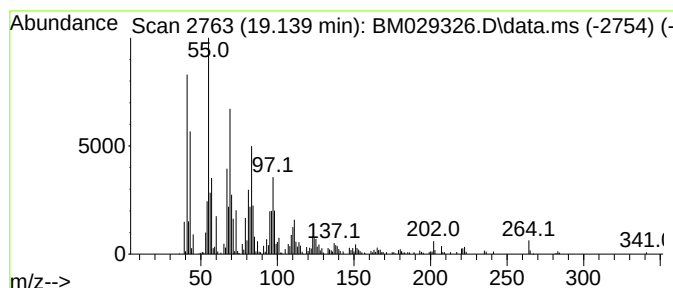
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Oleic Acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.139	12.56 ng	685452	Phenanthrene-d10	17.069	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	90
2	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	87
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
4	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	83
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	76



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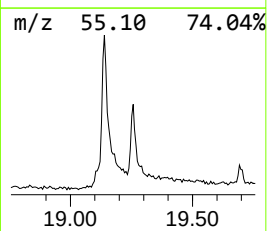
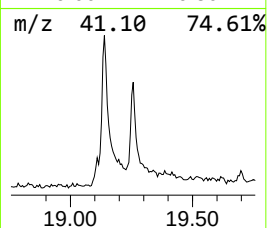
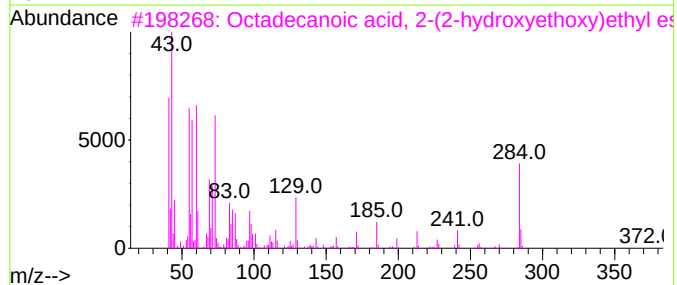
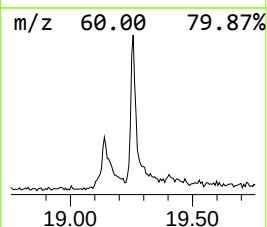
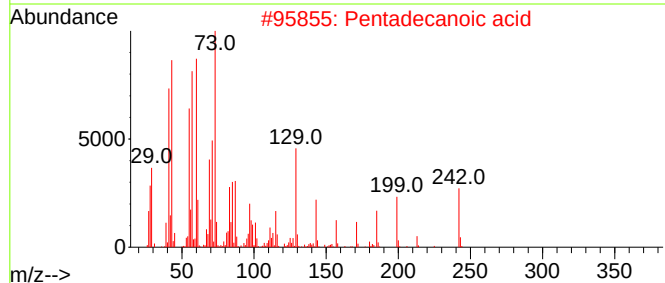
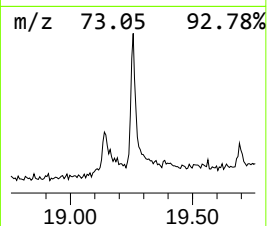
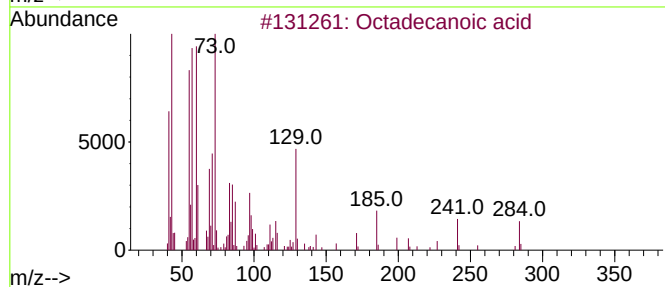
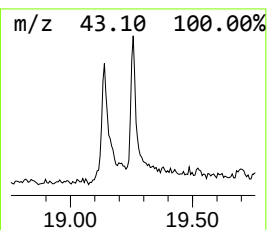
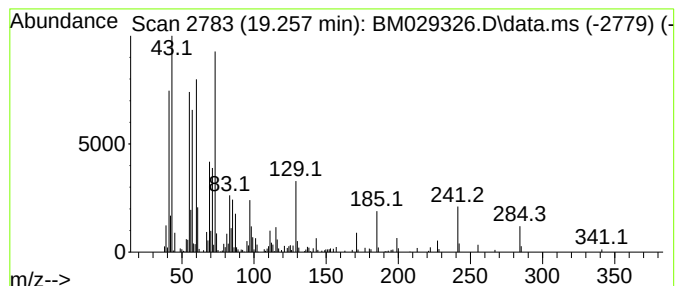
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.257	4.84 ng	329984	Chrysene-d12	21.245

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	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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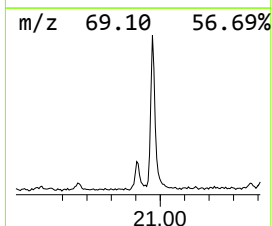
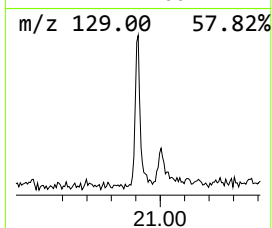
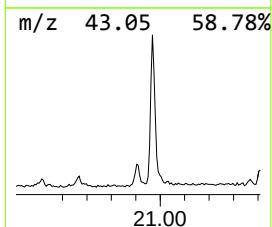
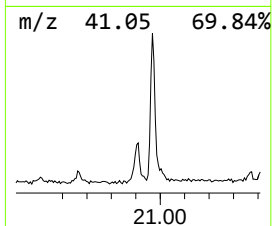
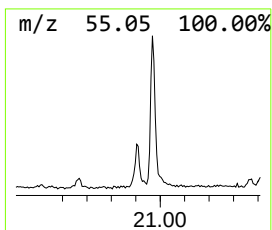
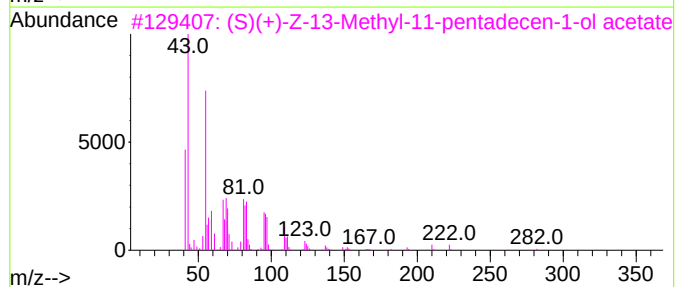
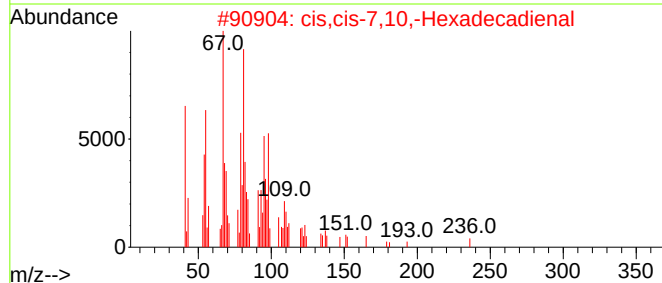
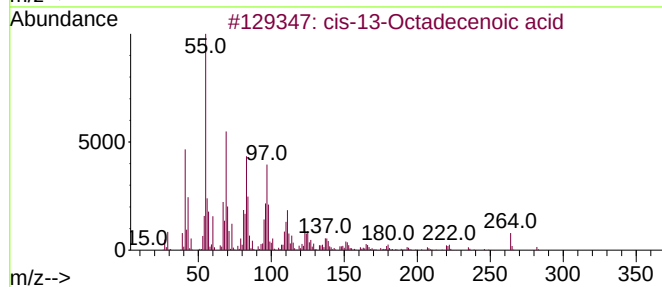
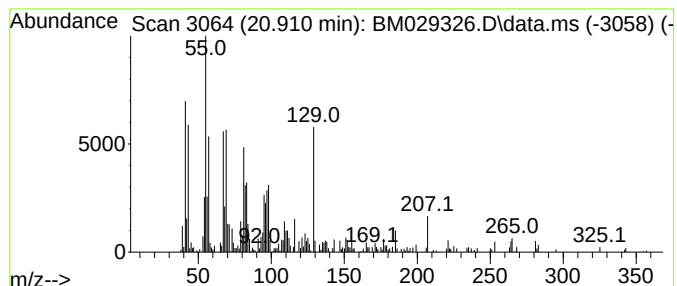
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 cis-13-Octadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.910	3.23 ng	220414	Chrysene-d12	21.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	60
2			cis,cis-7,10,-Hexadecadienal	236	C16H28O	056829-23-3	53
3			(S)(+)-Z-13-Methyl-11-pentadecen...	282	C18H34O2	1000130-84-8	49
4			9-Oxabicyclo[6.1.0]nonane, cis-	126	C8H14O	004925-71-7	47
5			Z,E-2,13-Octadecadien-1-ol	266	C18H34O	1000131-10-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
Data File : BM029326.D
Acq On : 02 Apr 2021 18:23
Operator : CG/JU
Sample : M1874-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

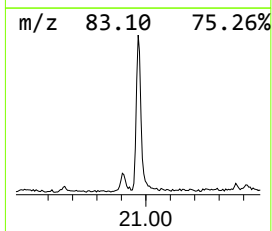
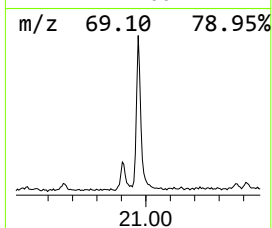
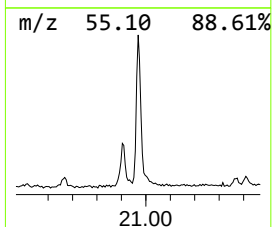
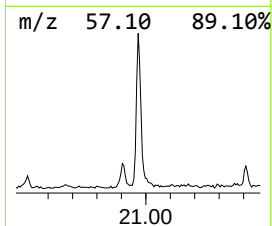
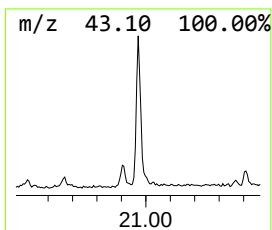
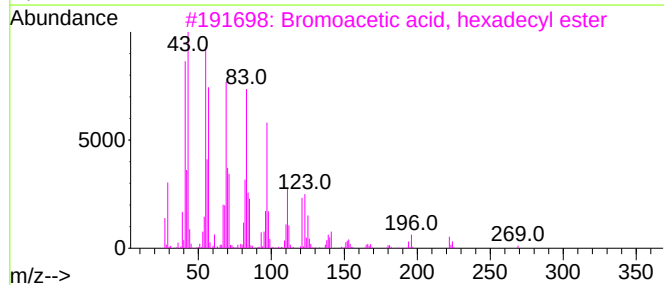
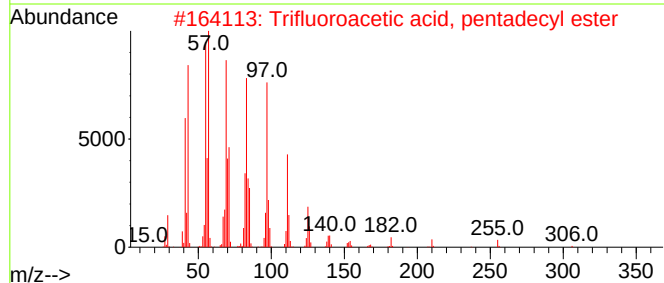
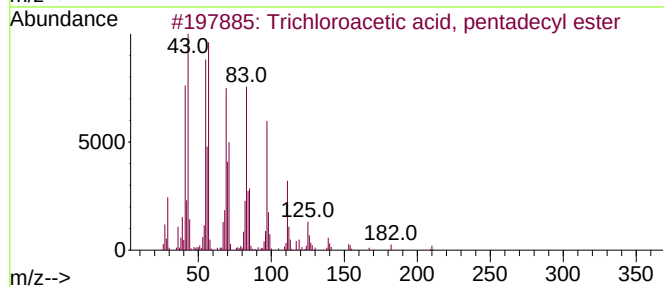
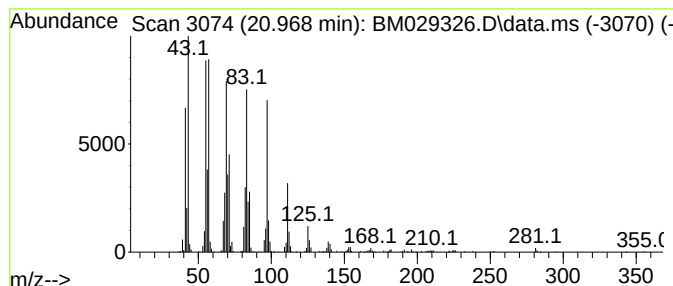
Instrument :
BNA_M
ClientSampleId :
FS-SB11(52-53)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.968	8.94 ng	609318	Chrysene-d12	21.245	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl13O2	074339-53-0	94
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl13O2	074339-52-9	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
Data File : BM029326.D
Acq On : 02 Apr 2021 18:23
Operator : CG/JU
Sample : M1874-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB11(52-53)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.940	18.0	ng	589112	1	7.699	653631	20.0
Propane, 1,1-di...	2.981	3.7	ng	121541	1	7.699	653631	20.0
n-Hexadecanoic ...	17.974	9.4	ng	512793	4	17.069	1091390	20.0
Oleic Acid	19.139	12.6	ng	685452	4	17.069	1091390	20.0
Octadecanoic acid	19.257	4.8	ng	329984	5	21.245	1362730	20.0
cis-13-Octadece...	20.910	3.2	ng	220414	5	21.245	1362730	20.0
Trichloroacetic...	20.968	8.9	ng	609318	5	21.245	1362730	20.0