

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
 Data File : BM029318.D
 Acq On : 02 Apr 2021 13:17
 Operator : CG/JU
 Sample : M1874-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FS-SB18(9-10)

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: BM029318.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	663032	779648	14.75%	2.349%
2	2.987	14	17	29	rVB	146087	181925	3.44%	0.548%
3	5.298	402	410	421	rBV	2227752	3162355	59.82%	9.527%
4	6.875	671	678	693	rBV	2144347	3480025	65.82%	10.484%
5	7.698	811	818	825	rBV	609963	968058	18.31%	2.916%
6	8.851	1007	1014	1025	rBV	1317629	2142586	40.53%	6.455%
7	10.480	1283	1291	1299	rBV	784352	1287768	24.36%	3.879%
8	12.957	1705	1712	1724	rBV	3035311	4425340	83.70%	13.332%
9	13.239	1753	1760	1769	rBV	135767	218810	4.14%	0.659%
10	13.792	1848	1854	1860	rBV	88327	128856	2.44%	0.388%
11	14.333	1940	1946	1958	rVB	1082100	1600069	30.26%	4.820%
12	15.821	2193	2199	2209	rBV	2146309	2908128	55.01%	8.761%
13	17.074	2405	2412	2419	rBV	1208076	1696000	32.08%	5.109%
14	17.974	2560	2565	2572	rBV	114526	171767	3.25%	0.517%
15	19.256	2779	2783	2790	rBV3	40577	66499	1.26%	0.200%
16	19.697	2853	2858	2865	rBV	4193379	5286888	100.00%	15.927%
17	20.397	2970	2977	2990	rBV	551854	727860	13.77%	2.193%
18	20.974	3071	3075	3085	rBV	389006	585030	11.07%	1.762%
19	21.244	3116	3121	3126	rBV	1281505	1605376	30.37%	4.836%
20	22.291	3296	3299	3307	rVB4	124651	173640	3.28%	0.523%
21	23.456	3491	3497	3506	rVB2	841855	1597835	30.22%	4.814%

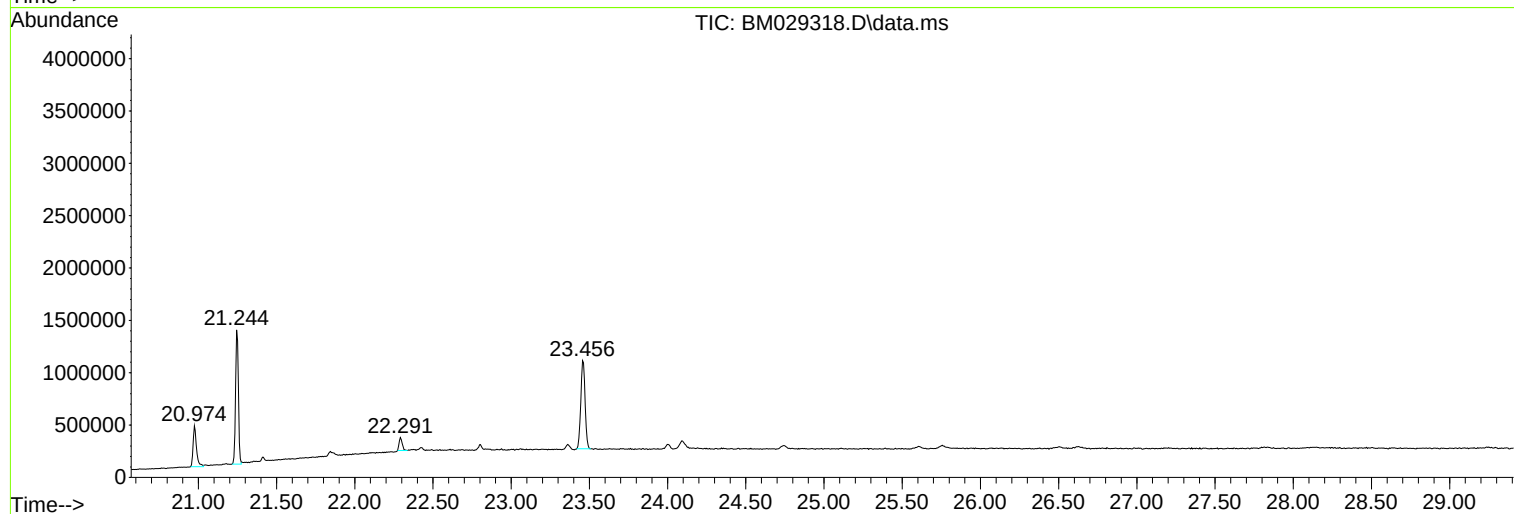
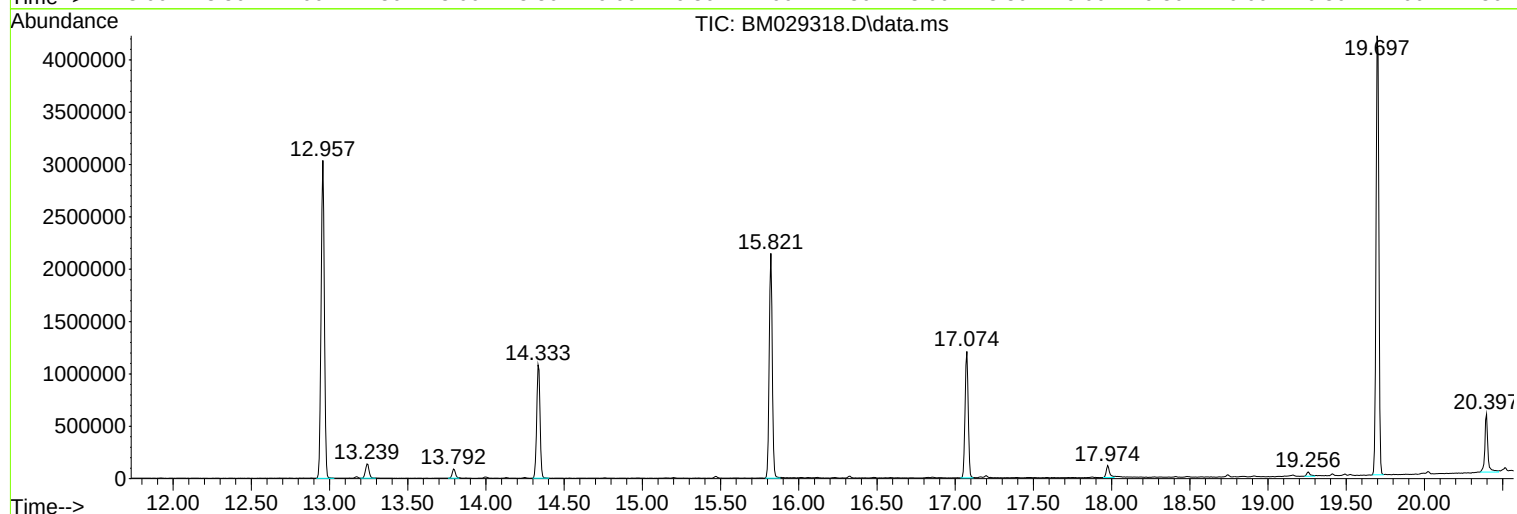
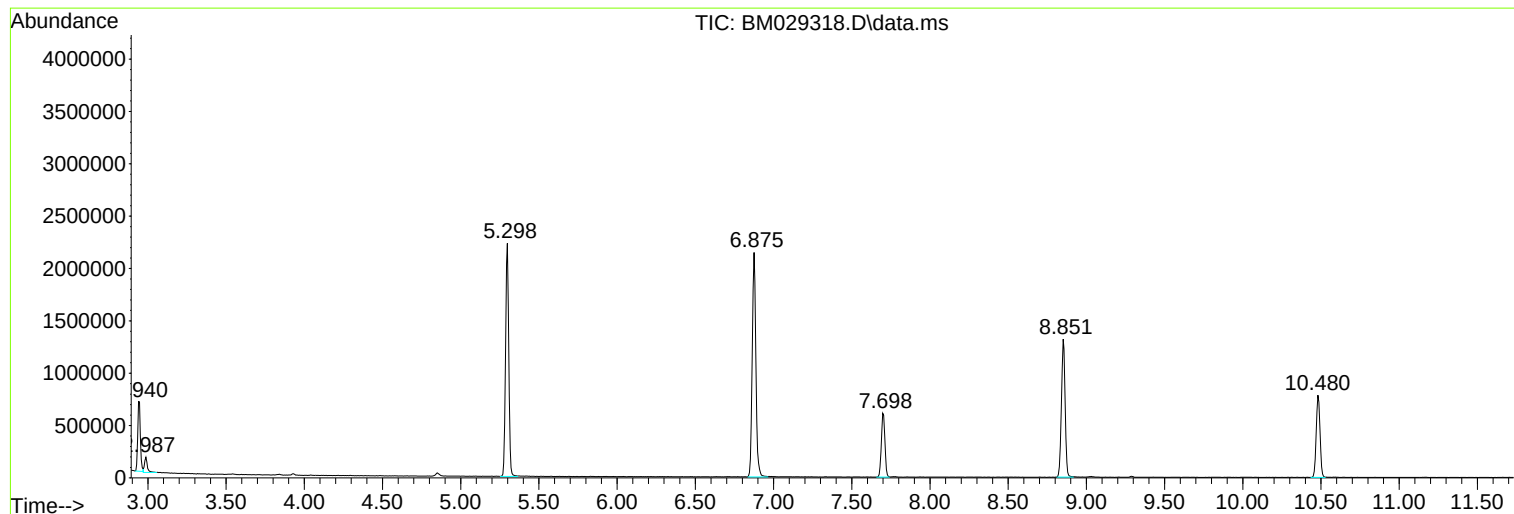
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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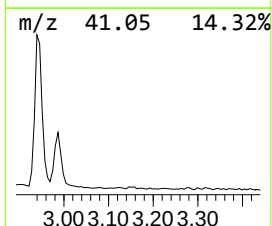
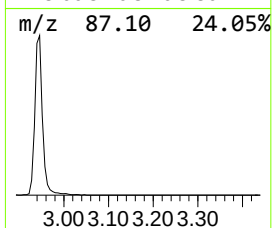
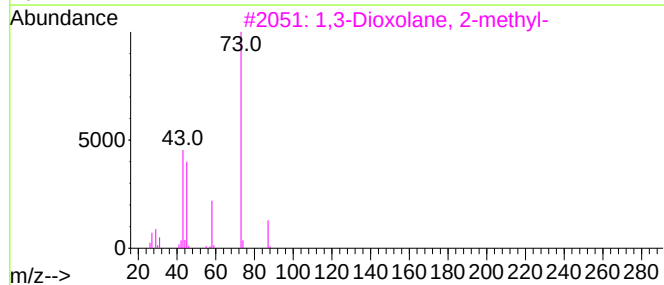
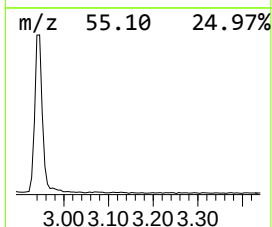
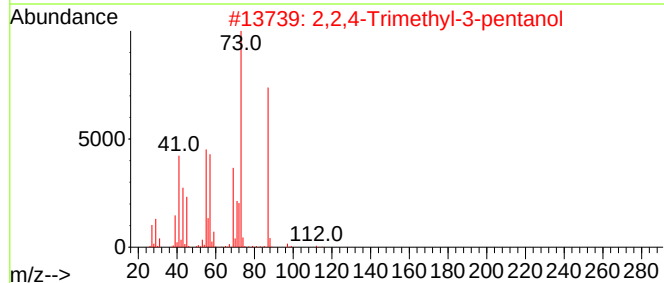
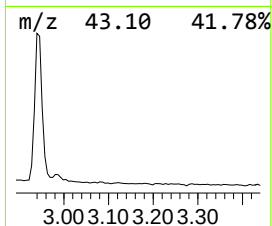
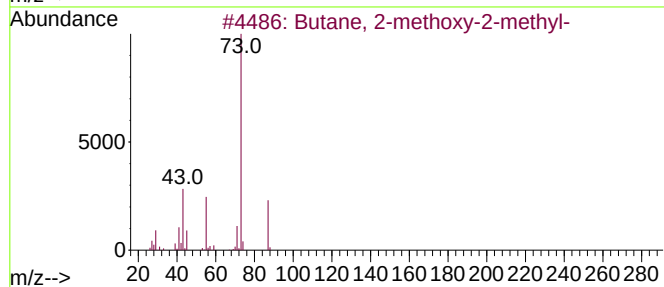
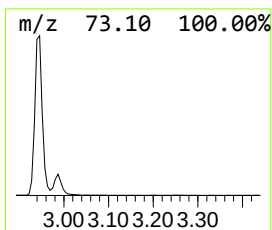
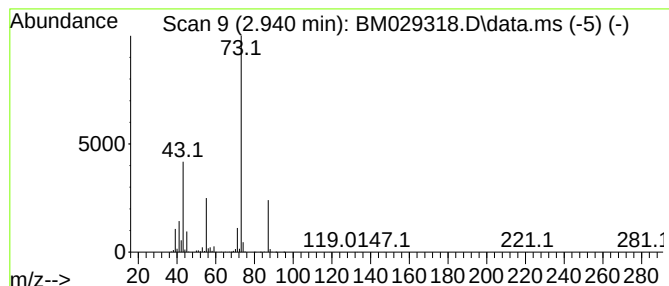
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	16.11 ng	779648	1,4-Dichlorobenzene-d4	7.698

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	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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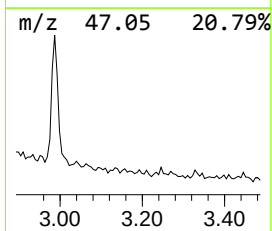
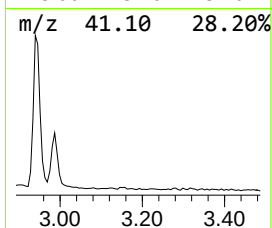
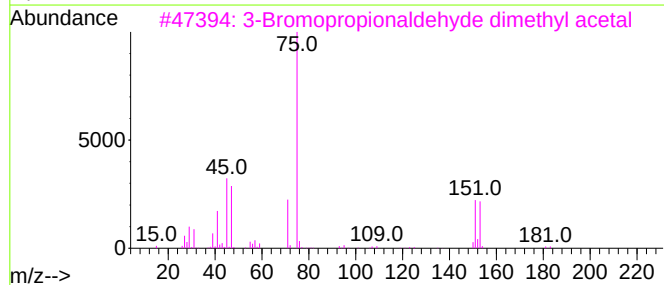
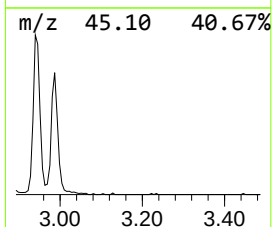
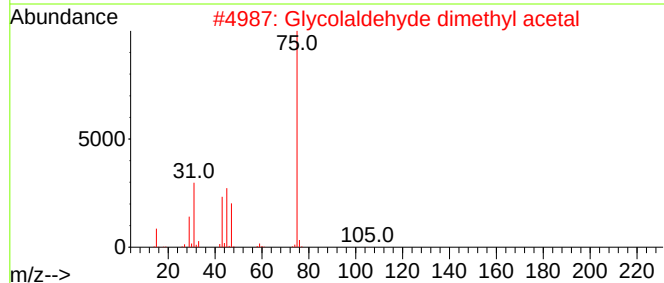
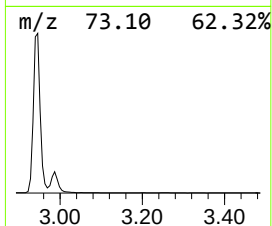
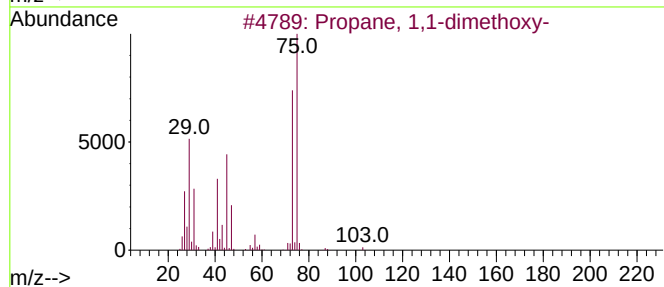
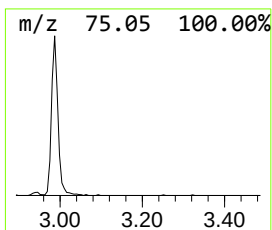
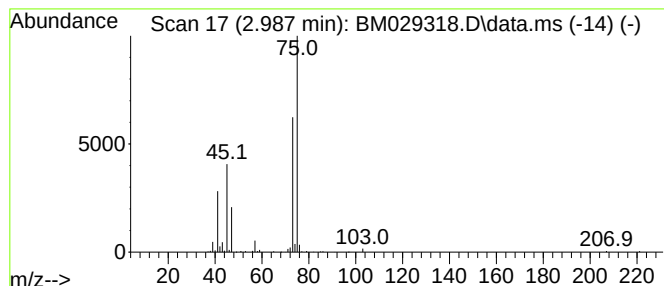
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.987	3.76 ng	181925	1,4-Dichlorobenzene-d4	7.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	56
3			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	38
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
5			5-(1-Ethoxy-ethoxy)-4-methyl-hex...	200	C11H20O3	086845-53-6	10



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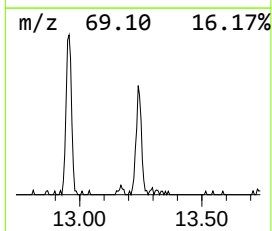
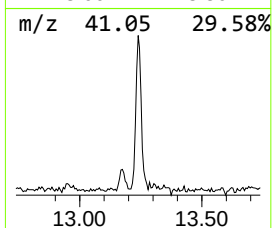
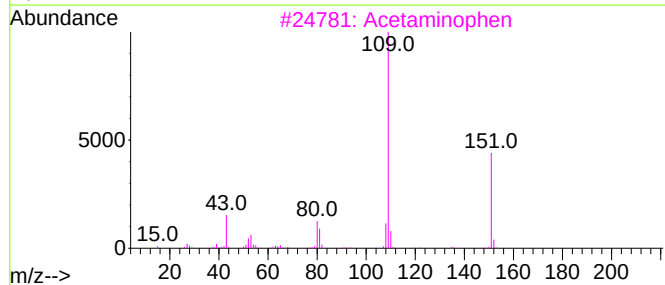
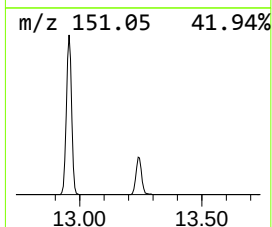
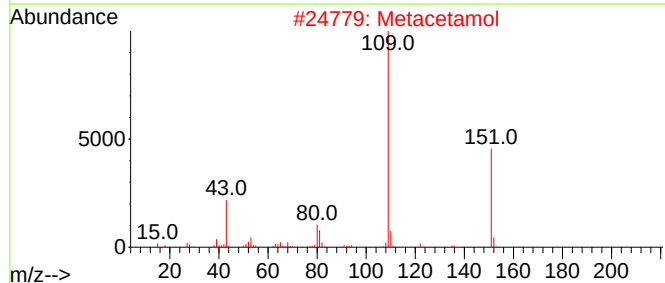
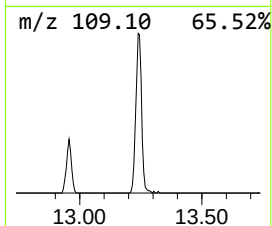
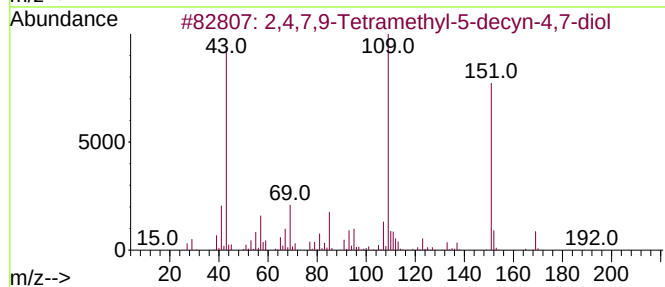
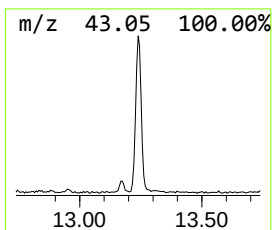
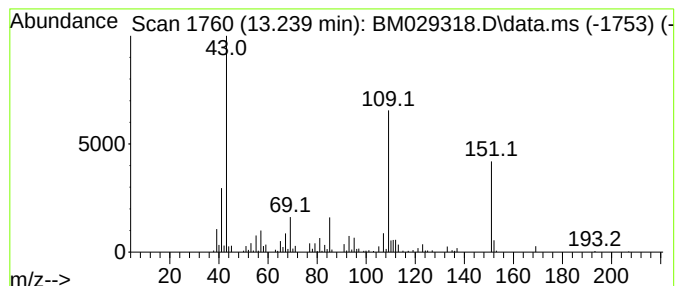
Instrument :
BNA_M
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FS-SB18(9-10)

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

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.239	2.74 ng	218810	Acenaphthene-d10		14.333	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	91
2	Metacetamol		151	C8H9NO2	000621-42-1	58
3	Acetaminophen		151	C8H9NO2	000103-90-2	58
4	p-Isopropoxyaniline		151	C9H13NO	007664-66-6	53
5	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	53



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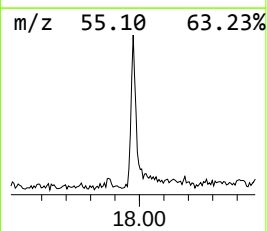
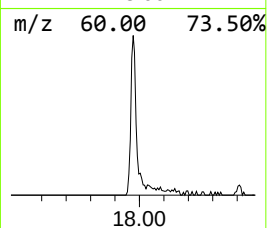
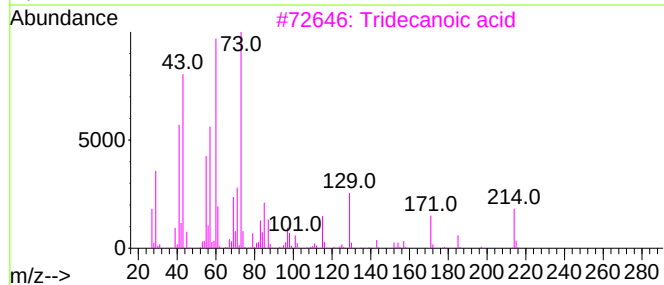
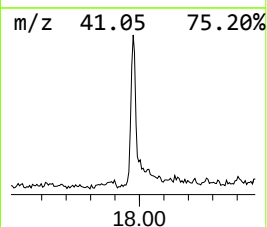
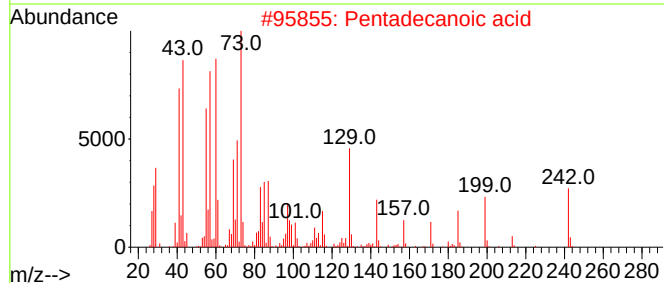
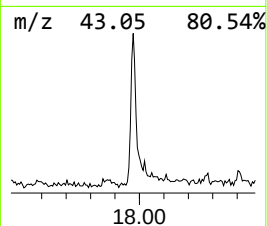
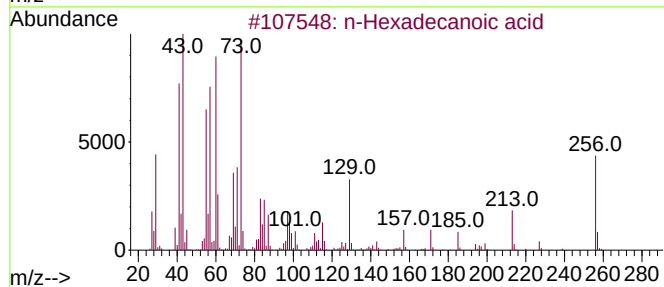
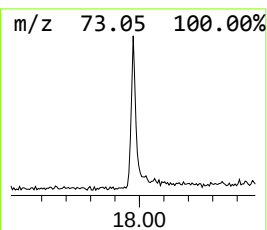
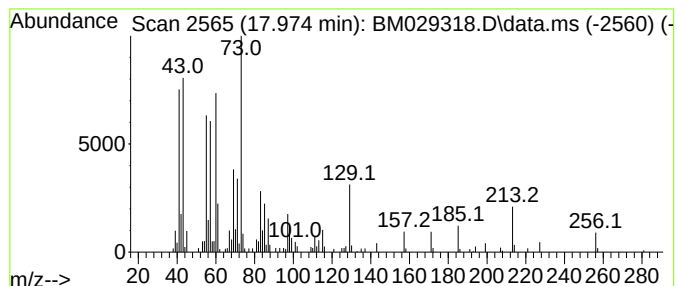
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	2.03 ng	171767	Phenanthrene-d10	17.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3			Tridecanoic acid	214	C13H26O2	000638-53-9	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	47



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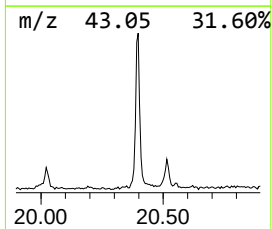
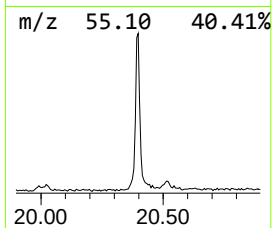
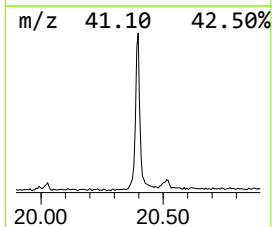
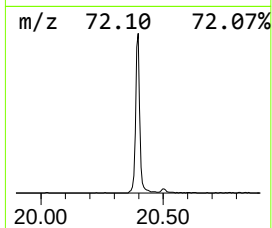
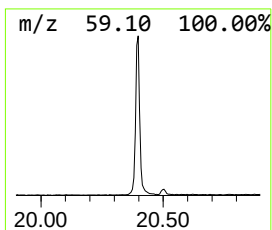
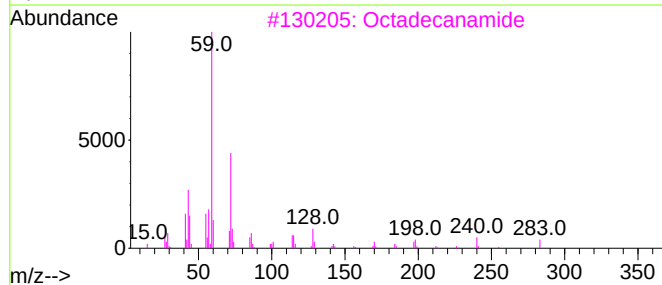
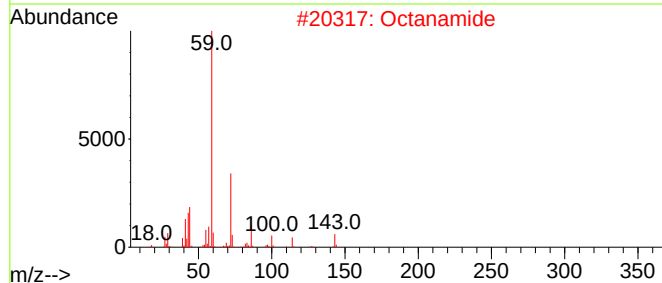
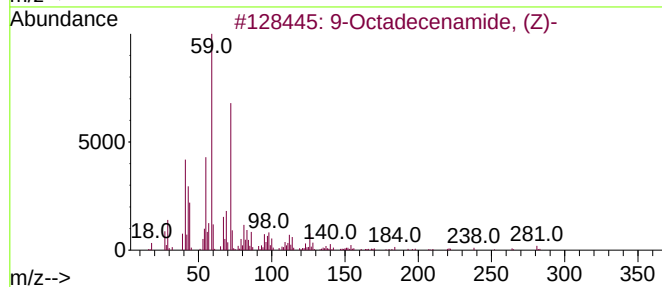
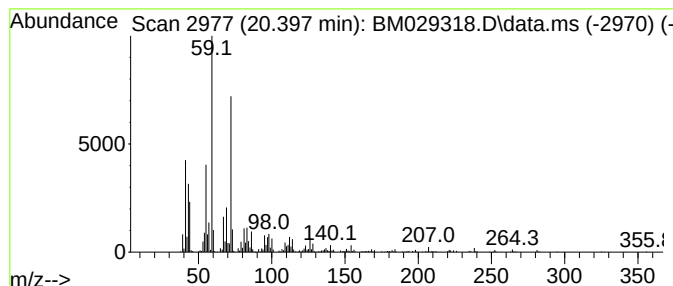
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.397	9.07 ng	727860	Chrysene-d12	21.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2			Octanamide	143	C8H17NO	000629-01-6	72
3			Octadecanamide	283	C18H37NO	000124-26-5	64
4			Tetradecanamide	227	C14H29NO	000638-58-4	64
5			Nonanamide	157	C9H19NO	001120-07-6	64



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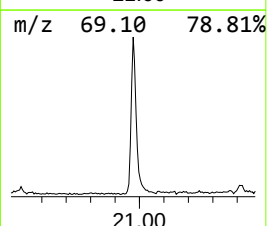
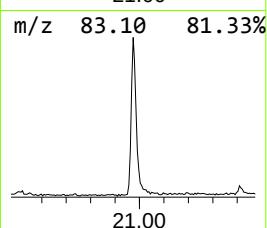
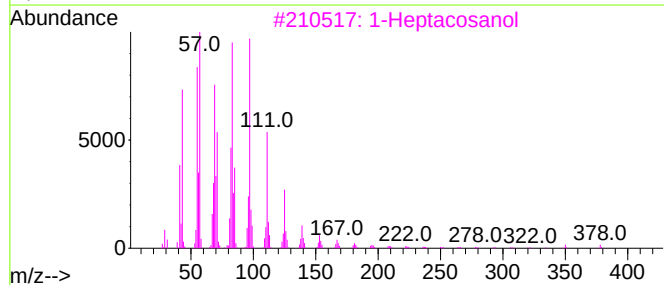
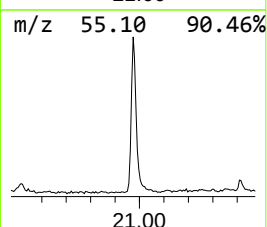
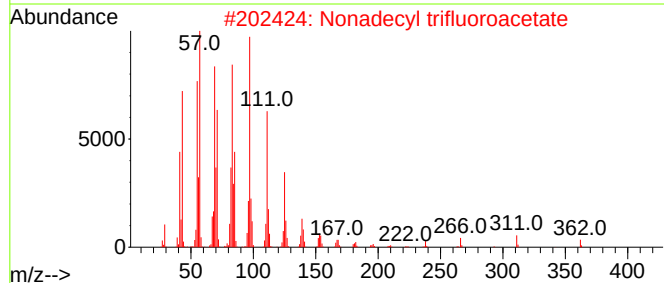
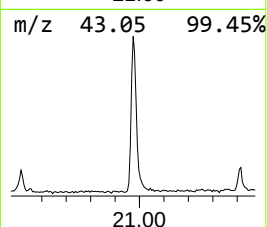
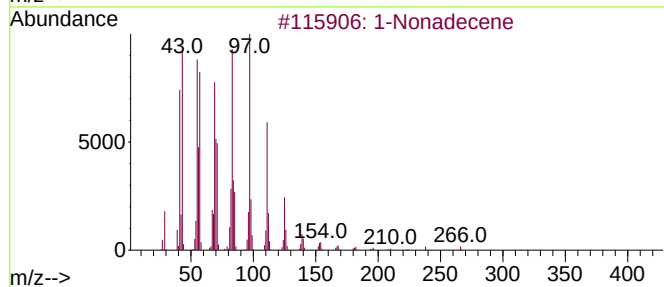
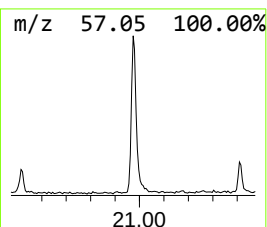
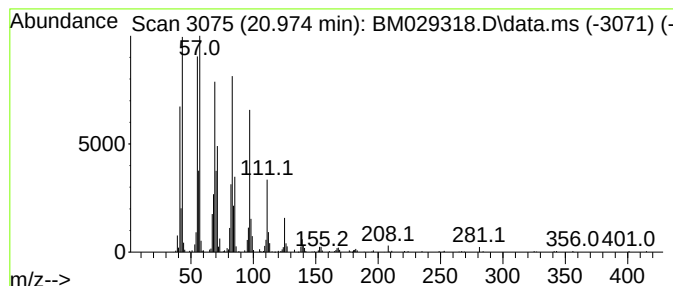
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	7.29 ng	585030	Chrysene-d12	21.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	91
2	Nonadecyl trifluoroacetate			380	C21H39F3O2	1000351-76-3	91
3	1-Heptacosanol			396	C27H56O	002004-39-9	91
4	3-Eicosene, (E)-			280	C20H40	074685-33-9	91
5	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
Data File : BM029318.D
Acq On : 02 Apr 2021 13:17
Operator : CG/JU
Sample : M1874-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

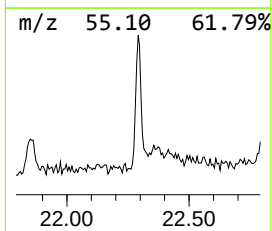
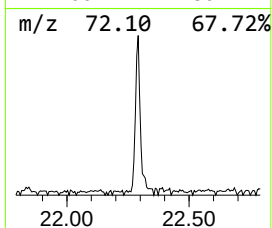
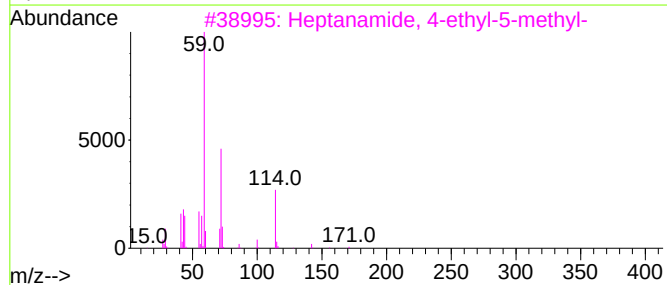
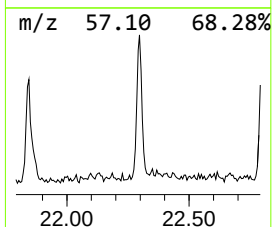
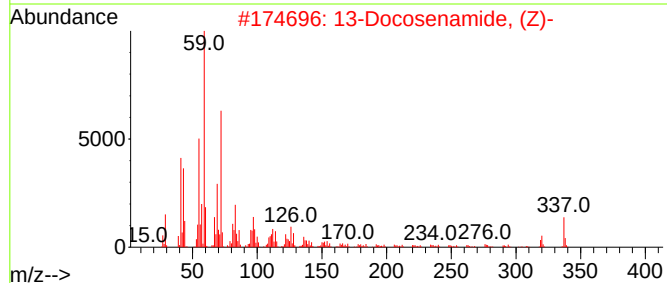
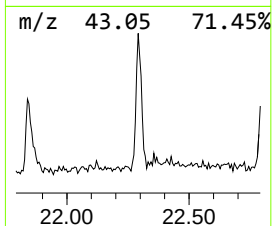
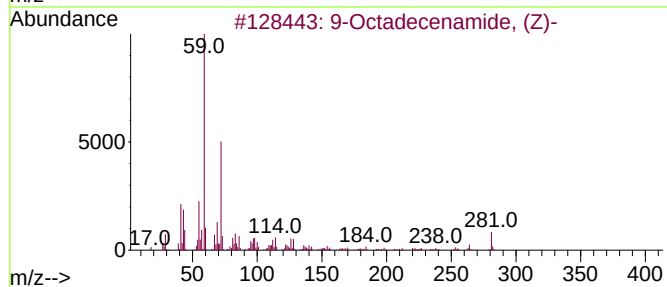
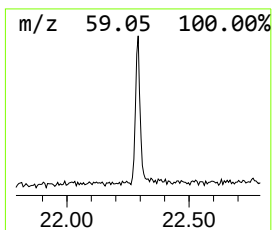
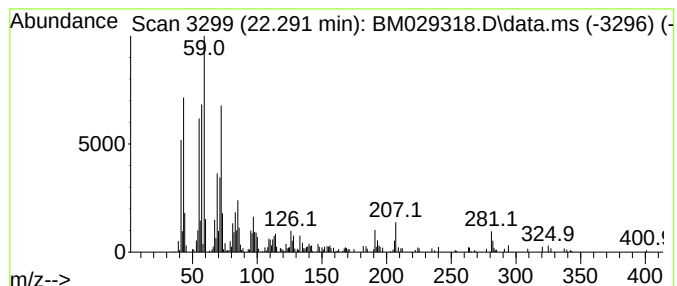
Instrument :
BNA_M
ClientSampleId :
FS-SB18(9-10)

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 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.291	2.16 ng	173640	Chrysene-d12		21.244	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	89
2	13-Docosenamide, (Z)-		337	C22H43NO	000112-84-5	70
3	Heptanamide, 4-ethyl-5-methyl-		171	C10H21NO	054789-40-1	49
4	cis-11-Eicosenamide		309	C20H39NO	010436-08-5	41
5	8-Methyl-6-nonenamide		169	C10H19NO	1000293-20-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
Data File : BM029318.D
Acq On : 02 Apr 2021 13:17
Operator : CG/JU
Sample : M1874-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB18(9-10)

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	16.1	ng	779648	1	7.698	968058	20.0
Propane, 1,1-di...	2.987	3.8	ng	181925	1	7.698	968058	20.0
2,4,7,9-Tetrame...	13.239	2.7	ng	218810	3	14.333	1600070	20.0
n-Hexadecanoic ...	17.974	2.0	ng	171767	4	17.074	1696000	20.0
9-Octadecenamid...	20.397	9.1	ng	727860	5	21.244	1605380	20.0
1-Nonadecene	20.974	7.3	ng	585030	5	21.244	1605380	20.0
13-Docosenamide...	22.291	2.2	ng	173640	5	21.244	1605380	20.0