

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082919\
 Data File : BM022421.D
 Acq On : 29 Aug 2019 23:13
 Operator : HP/JU
 Sample : K4573-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S700B-N-1.0-1.5-082719

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BM082919.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.146	361	367	382	rVB	392337	584971	35.49%	6.539%
2	6.722	628	635	648	rBV	381796	636677	38.63%	7.117%
3	7.057	686	692	704	rBV	435258	676677	41.06%	7.564%
4	7.522	765	771	777	rBB	78346	116749	7.08%	1.305%
5	7.828	817	823	833	rVB	329107	523293	31.75%	5.850%
6	8.693	964	970	993	rBV	213860	380062	23.06%	4.249%
7	10.298	1236	1243	1255	rBB	73908	131310	7.97%	1.468%
8	12.787	1660	1666	1684	rBV	582880	832391	50.51%	9.305%
9	13.663	1810	1815	1823	rBB	41576	61565	3.74%	0.688%
10	14.186	1897	1904	1913	rVB	119119	176492	10.71%	1.973%
11	15.698	2155	2161	2172	rBV	609283	861027	52.24%	9.625%
12	16.951	2369	2374	2379	rBV2	159817	218683	13.27%	2.445%
13	17.845	2521	2526	2536	rBV	105278	146687	8.90%	1.640%
14	19.027	2723	2727	2731	rBV	47459	69686	4.23%	0.779%
15	19.063	2731	2733	2737	rVB2	23464	24640	1.50%	0.275%
16	19.139	2741	2746	2758	rBV4	34955	54988	3.34%	0.615%
17	19.392	2786	2789	2795	rVB	27835	34963	2.12%	0.391%
18	19.598	2818	2824	2829	rBV	1478113	1648089	100.00%	18.424%
19	20.298	2936	2943	2951	rBV	124507	151317	9.18%	1.692%
20	20.862	3035	3039	3049	rBV	141926	194757	11.82%	2.177%
21	21.168	3085	3091	3095	rBV	313939	420071	25.49%	4.696%
22	21.480	3141	3144	3148	rBV4	22292	22116	1.34%	0.247%
23	21.745	3186	3189	3198	rVB3	76793	116458	7.07%	1.302%
24	22.704	3349	3352	3362	rVB2	50143	88361	5.36%	0.988%
25	23.351	3457	3462	3469	rBV	214006	397259	24.10%	4.441%
26	23.715	3521	3524	3532	rVB2	48390	85368	5.18%	0.954%
27	23.898	3550	3555	3563	rVB5	60280	124855	7.58%	1.396%
28	24.256	3611	3616	3628	rVB3	67281	165940	10.07%	1.855%

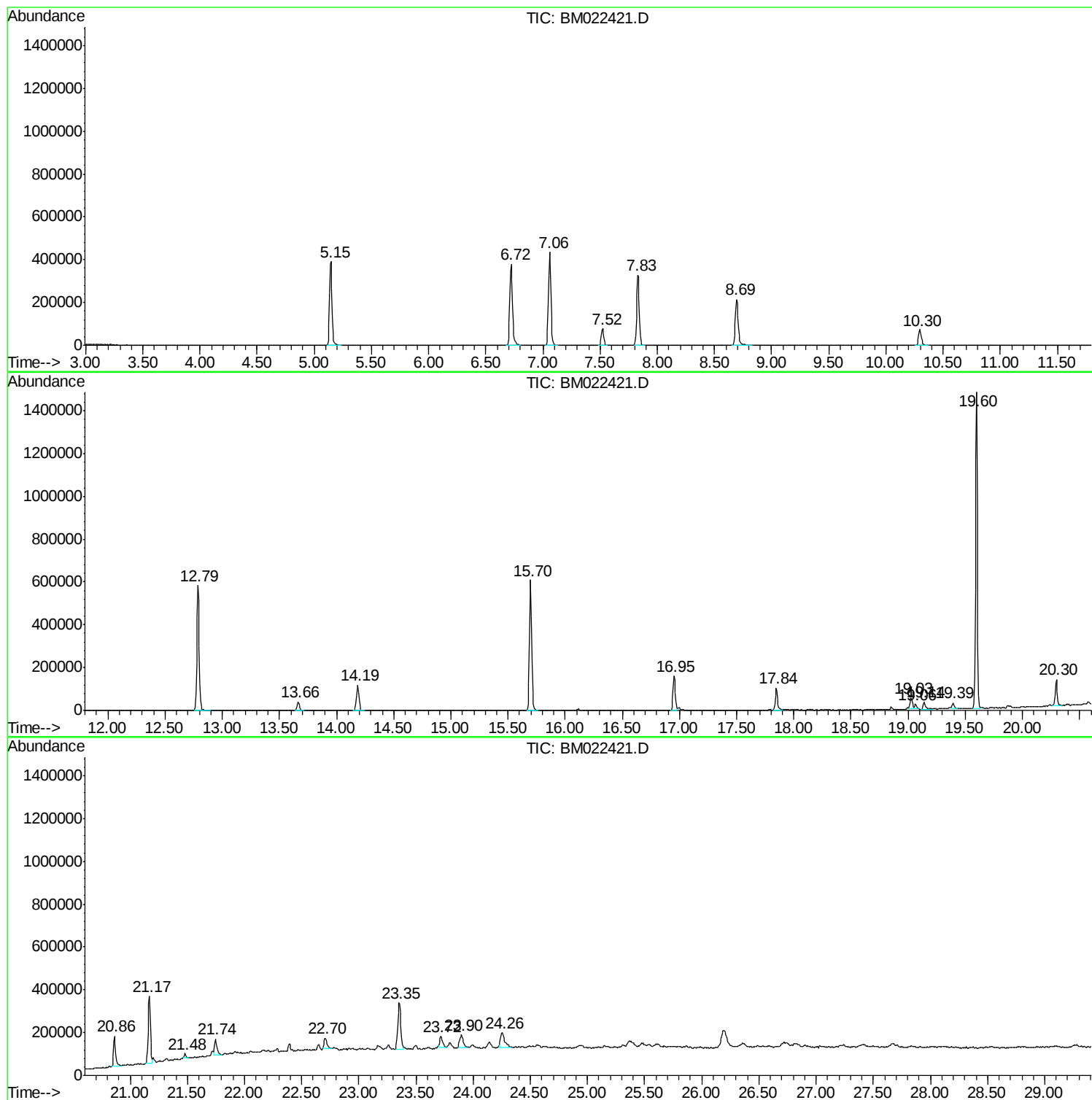
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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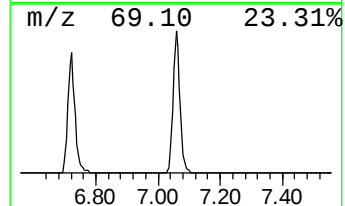
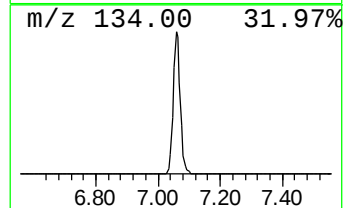
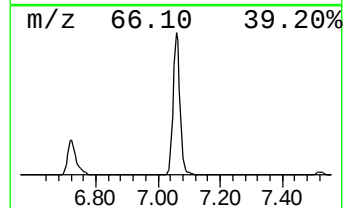
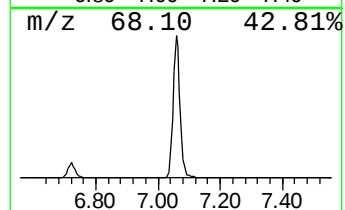
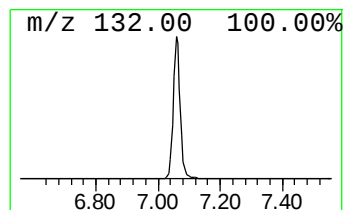
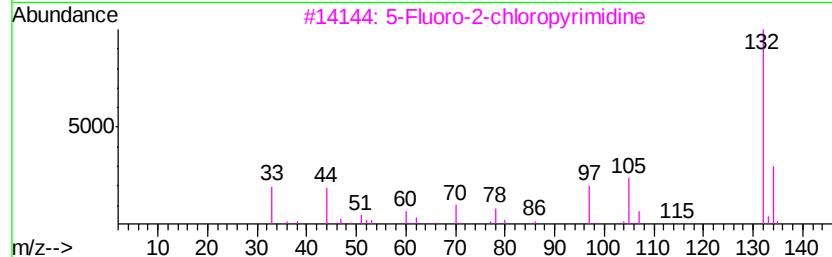
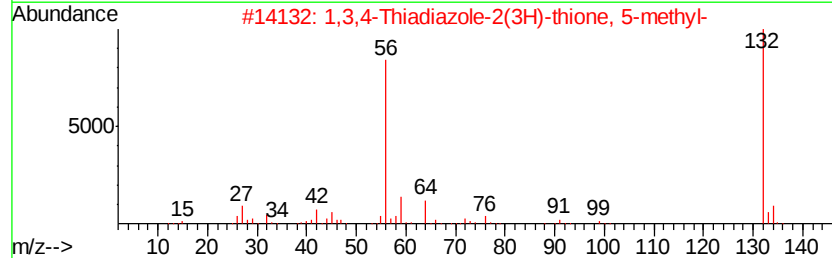
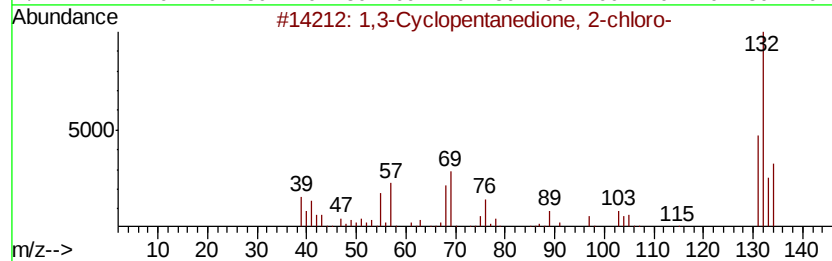
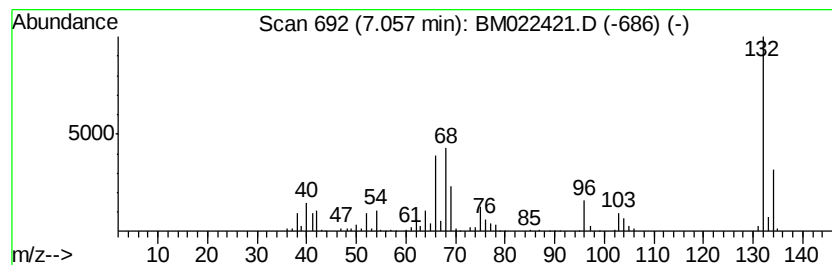
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	115.92 ng	676677	1,4-Dichlorobenzene-d4	7.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	27
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10



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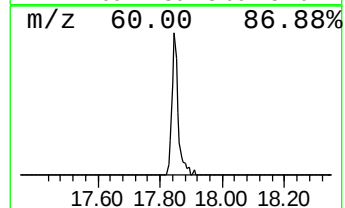
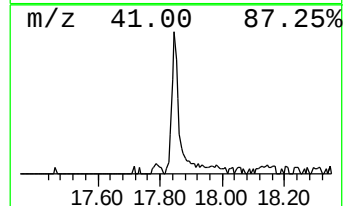
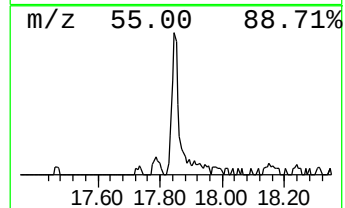
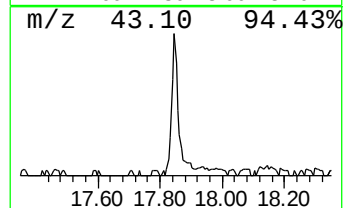
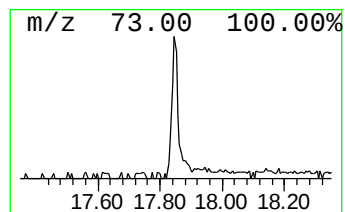
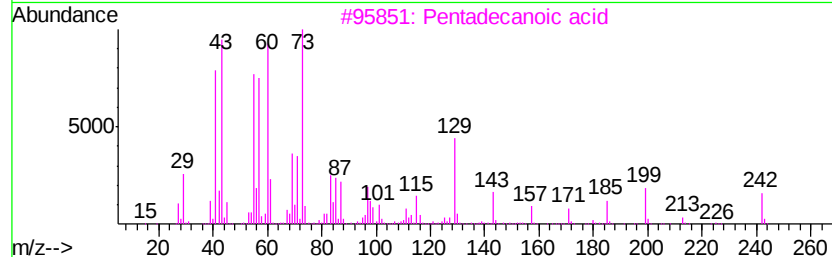
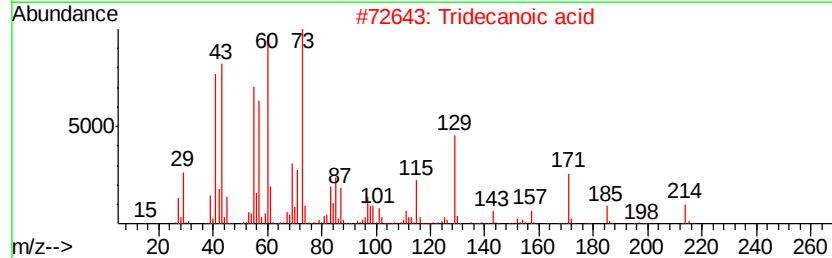
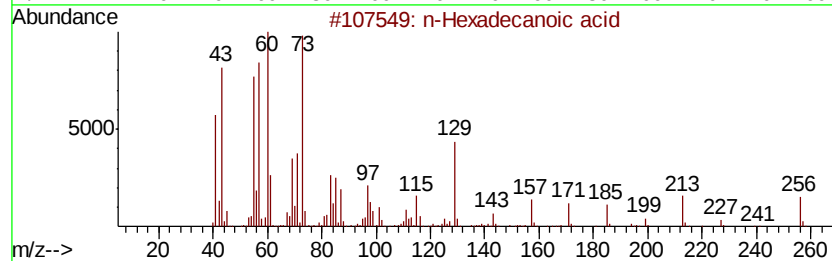
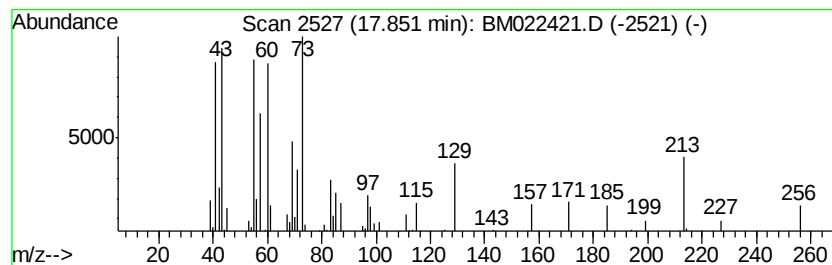
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.85	13.42 ng	146687	Phenanthrene-d10		16.95	
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	76
4	Undecanoic acid		186	C11H22O2	000112-37-8	53
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	52



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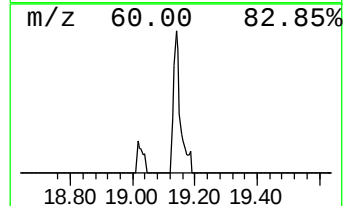
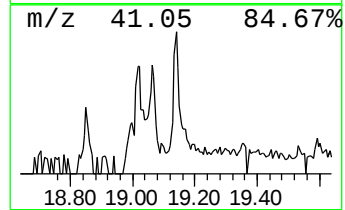
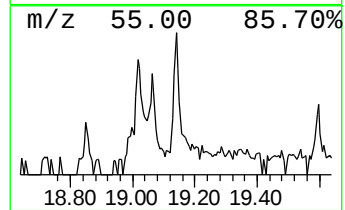
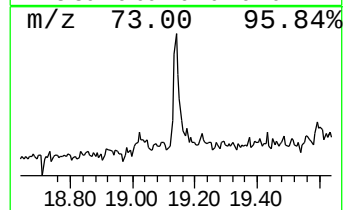
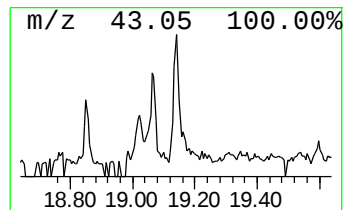
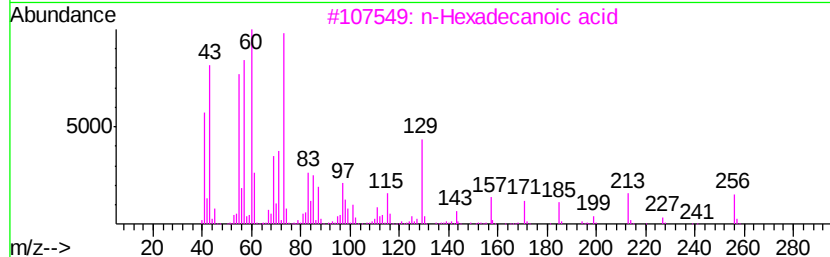
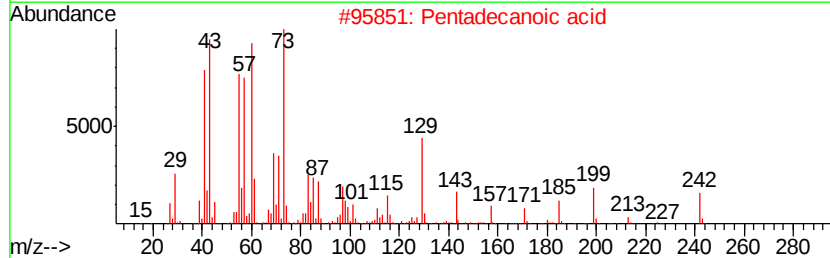
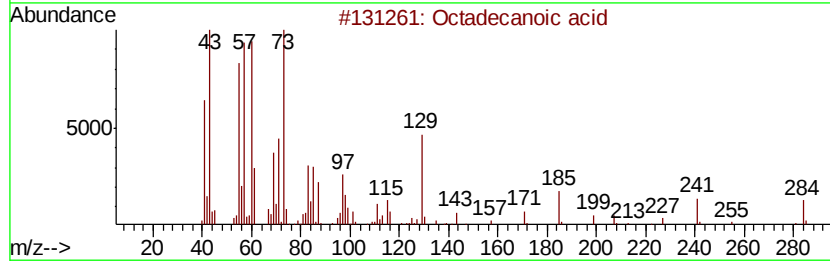
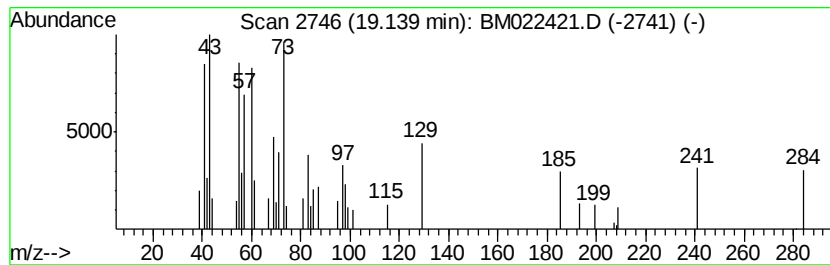
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Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.14	2.62 ng	54988	Chrysene-d12		21.17
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43



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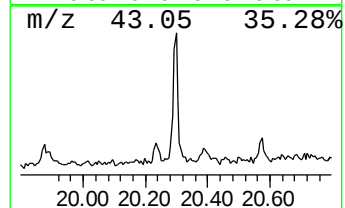
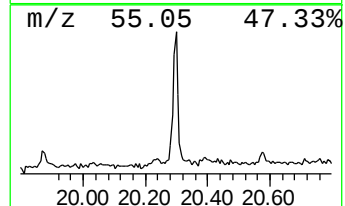
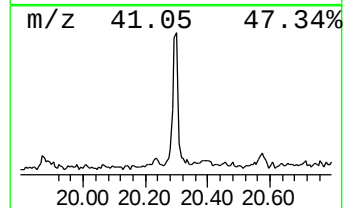
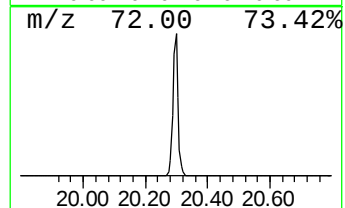
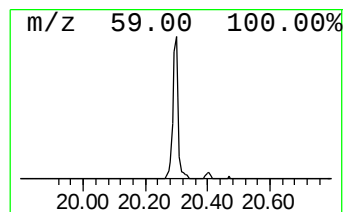
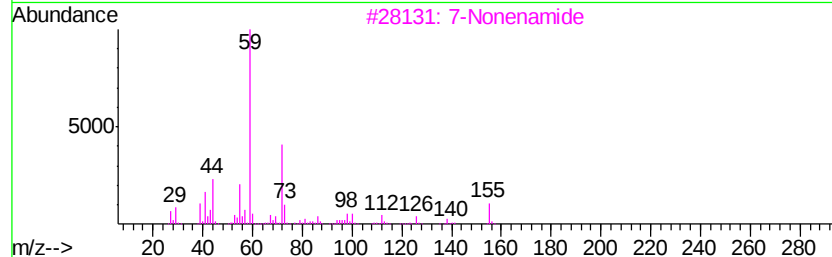
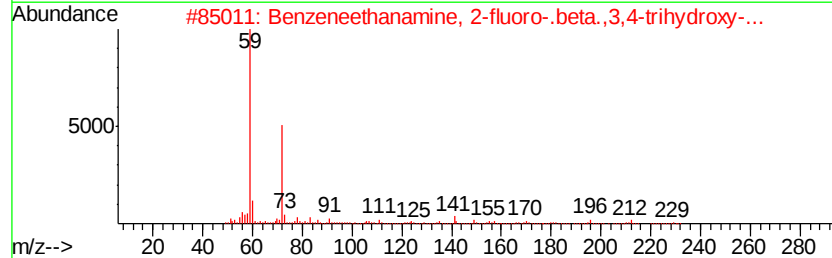
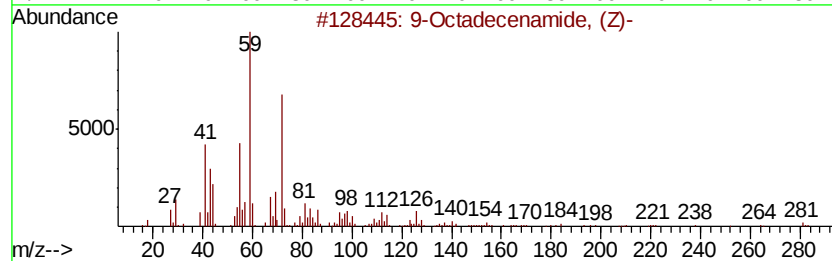
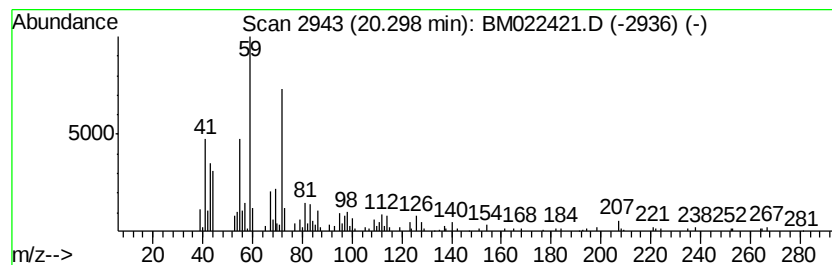
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.30	7.20 ng	151317	Chrysene-d12	21.17
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0	90
2	Benzeneethanamine, 2-fluoro-.bet...	229 C11H16FN03	061338-98-5	59
3	7-Nonenamide	155 C9H17NO	090949-53-4	50
4	Pentadecanamide, 15-bromo-	319 C15H30BrNO	1000163-86-1	43
5	Dodecanamide	199 C12H25NO	001120-16-7	43



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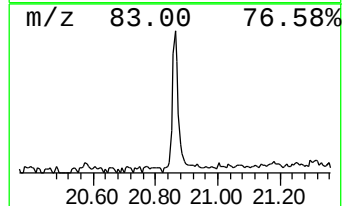
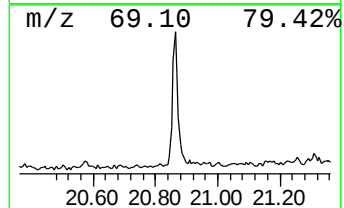
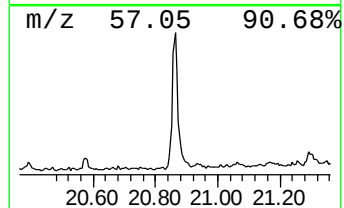
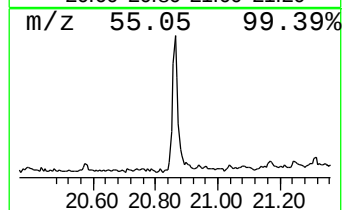
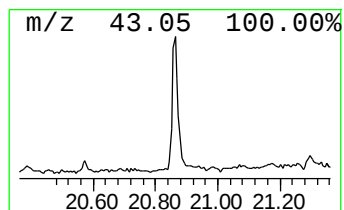
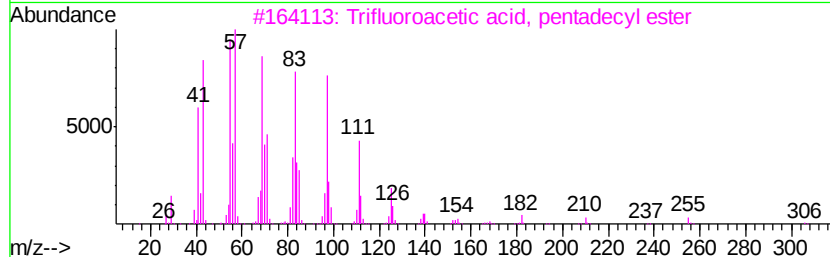
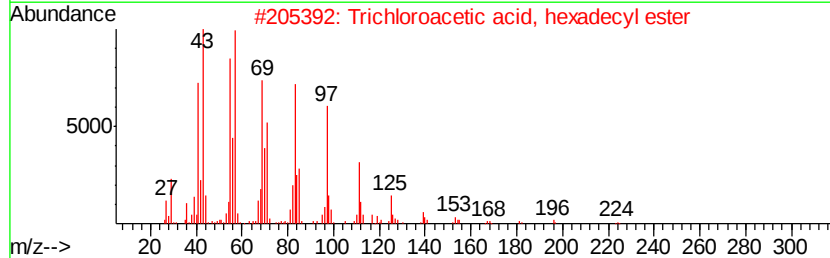
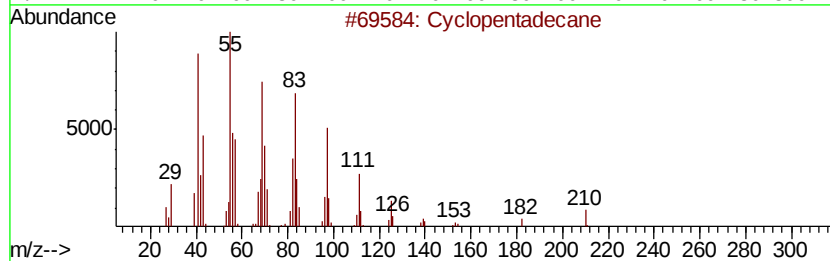
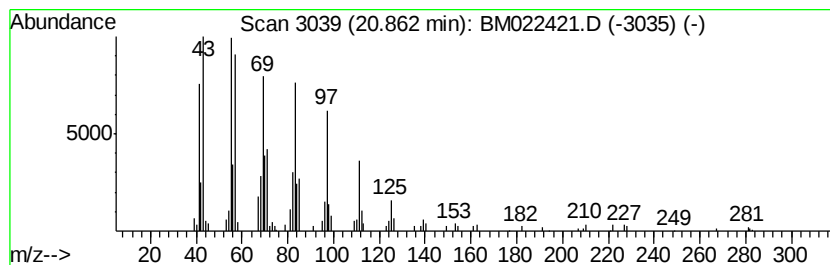
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Peak Number 6 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	9.27 ng	194757	Chrysene-d12	21.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93



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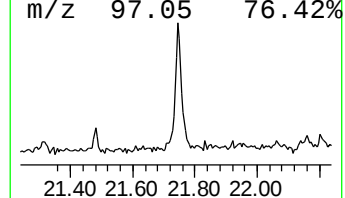
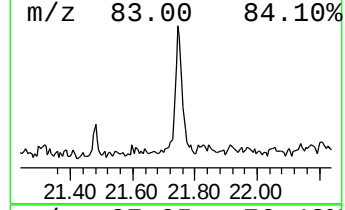
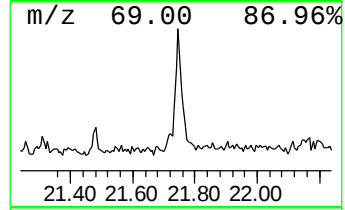
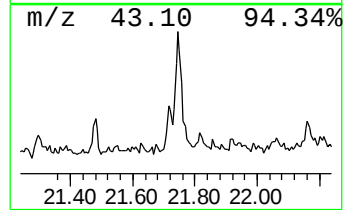
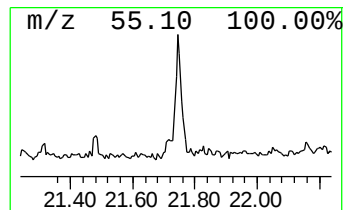
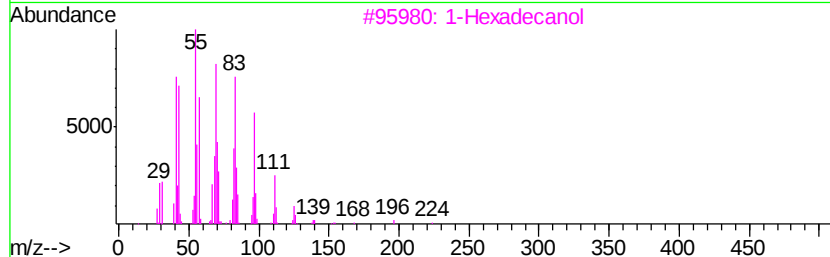
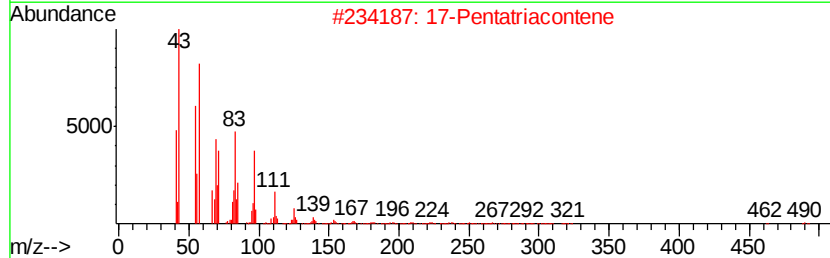
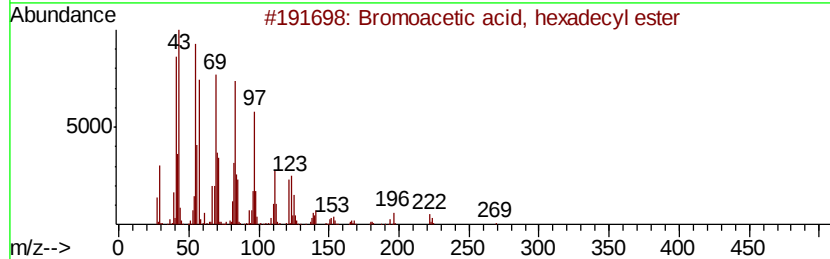
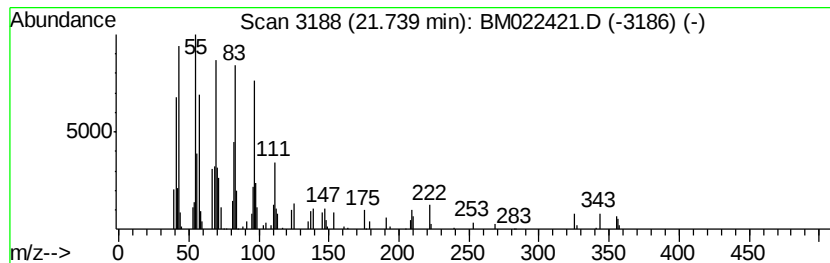
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bromoacetic acid, hexadecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.74	5.54 ng	116458	Chrysene-d12	21.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2			17-Pentatriacontene	491	C35H70	006971-40-0	86
3			1-Hexadecanol	242	C16H34O	036653-82-4	80
4			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	68
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082919\
Data File : BM022421.D
Acq On : 29 Aug 2019 23:13
Operator : HP/JU
Sample : K4573-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S700B-N-1.0-1.5-082719

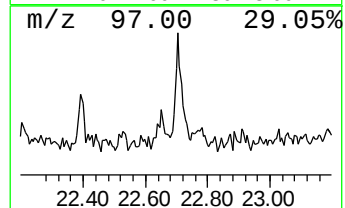
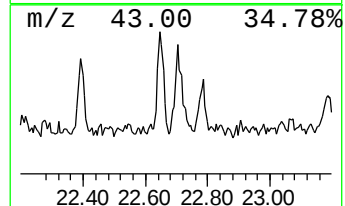
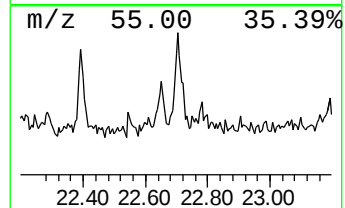
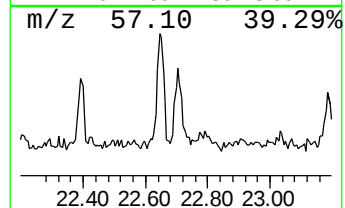
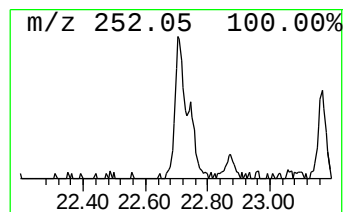
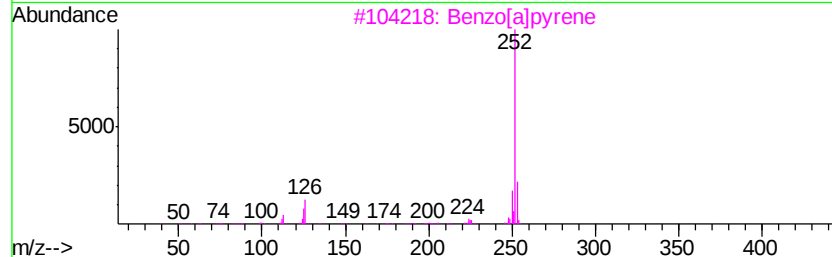
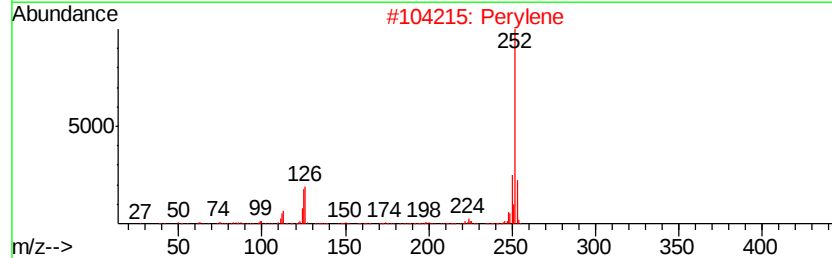
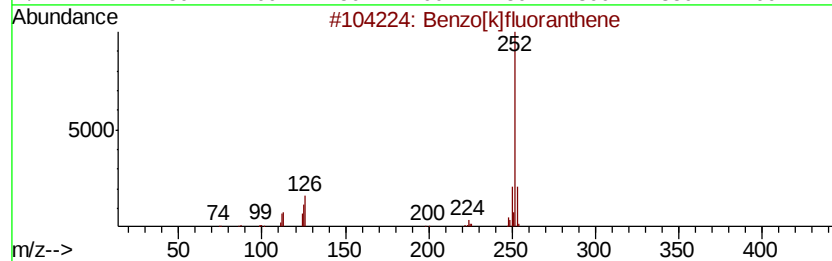
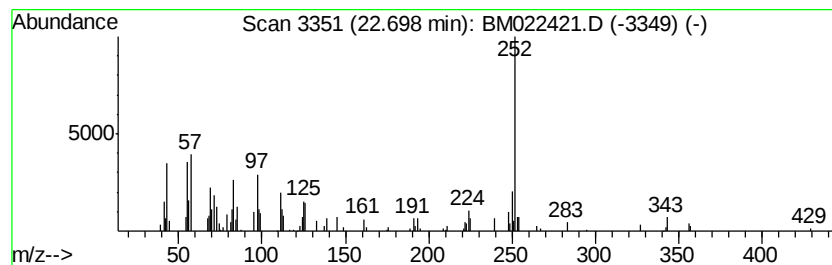
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.70	4.45 ng	88361	Perylene-d12	23.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	60
2		Perylene	252	C20H12	000198-55-0	53
3		Benzo[a]pyrene	252	C20H12	000050-32-8	53
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	53
5		Benzo[e]pyrene	252	C20H12	000192-97-2	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082919\
Data File : BM022421.D
Acq On : 29 Aug 2019 23:13
Operator : HP/JU
Sample : K4573-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S700B-N-1.0-1.5-082719

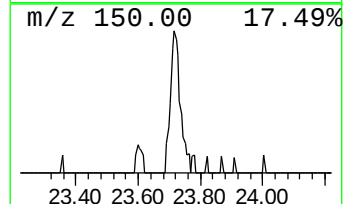
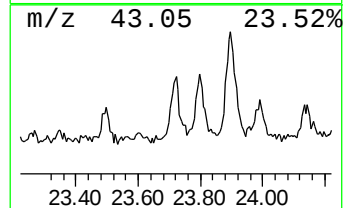
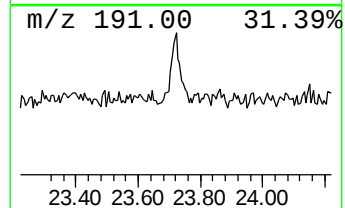
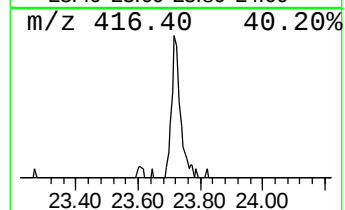
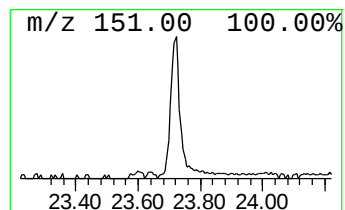
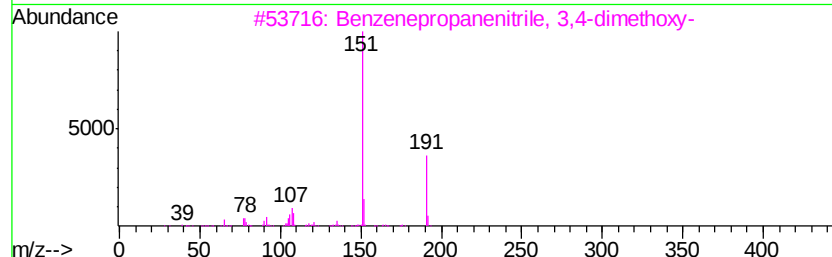
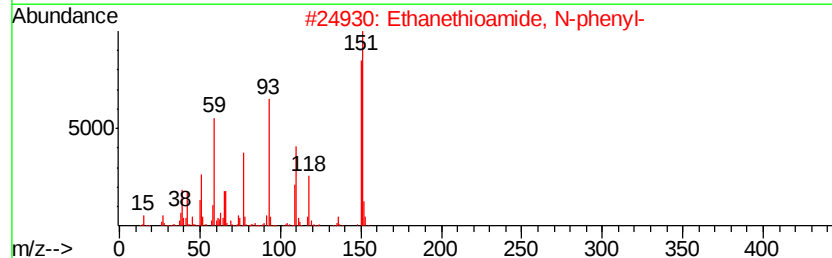
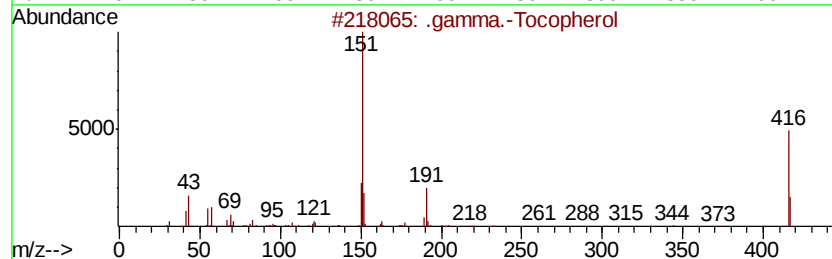
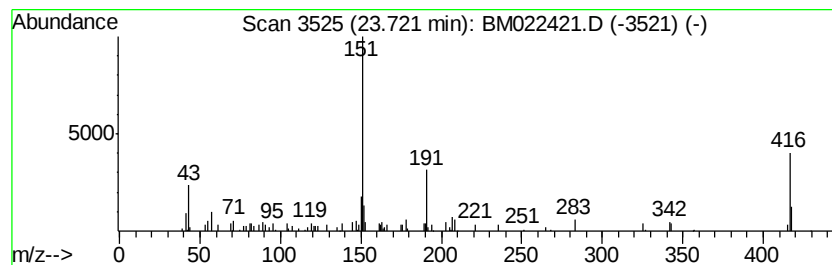
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .gamma.-Tocopherol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.72	4.30 ng	85368	Perylene-d12	23.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	74
2		Ethanethioamide, N-phenyl-	151	C8H9NS	000637-53-6	38
3		Benzenepropanenitrile, 3,4-dimet...	191	C11H13NO2	049621-56-9	38
4		3-Amino-4-methylbenzoic acid	151	C8H9NO2	002458-12-0	35
5		N-(3,5-Bis-trifluoromethyl-pheny...	379	C16H11F6NO5	345991-15-3	32



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082919\
Data File : BM022421.D
Acq On : 29 Aug 2019 23:13
Operator : HP/JU
Sample : K4573-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S700B-N-1.0-1.5-082719

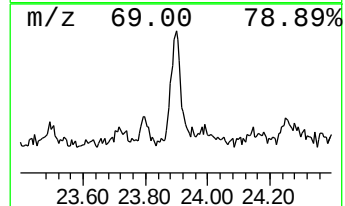
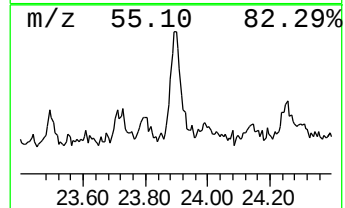
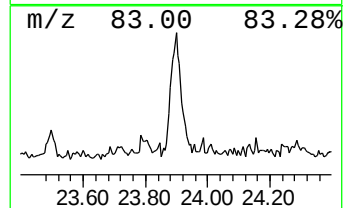
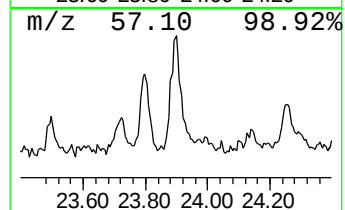
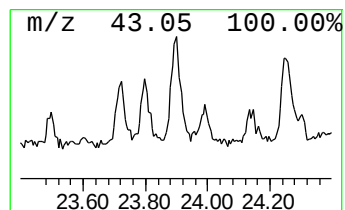
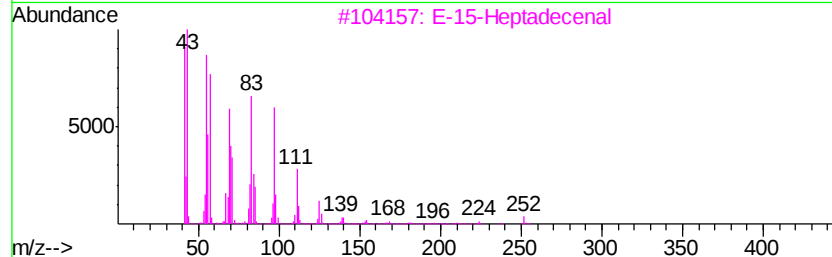
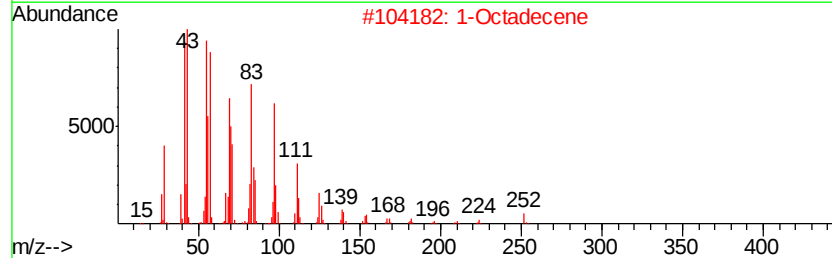
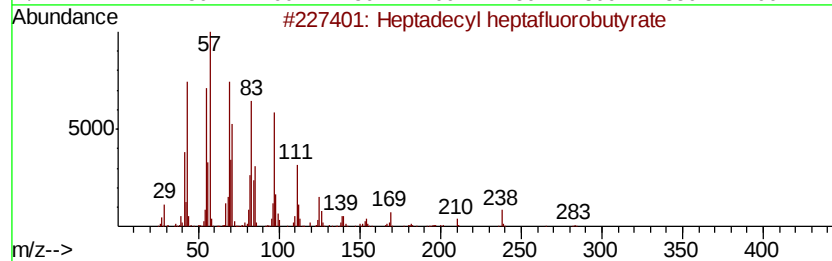
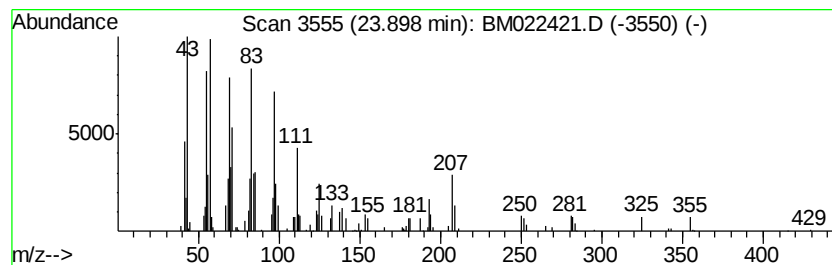
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.90	6.29 ng	124855	Perylene-d12	23.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
2			1-Octadecene	252	C18H36	000112-88-9	86
3			E-15-Heptadecenal	252	C17H32O	1000130-97-9	86
4			1-Heptacosanol	396	C27H56O	002004-39-9	83
5			5-Octadecene, (E)-	252	C18H36	007206-21-5	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082919\
Data File : BM022421.D
Acq On : 29 Aug 2019 23:13
Operator : HP/JU
Sample : K4573-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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S700B-N-1.0-1.5-082719

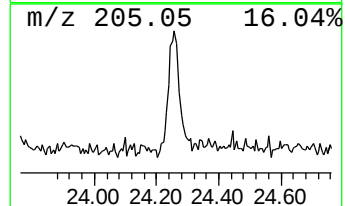
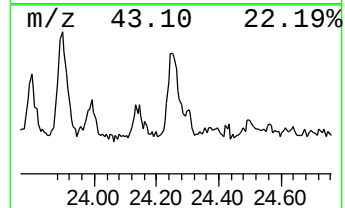
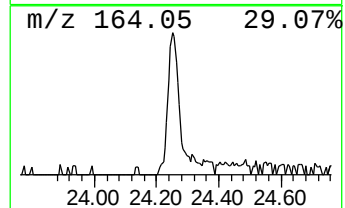
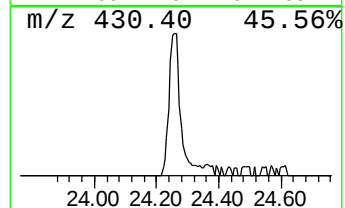
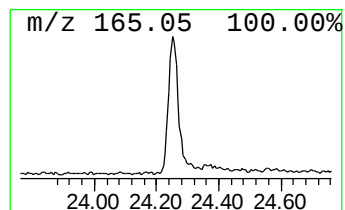
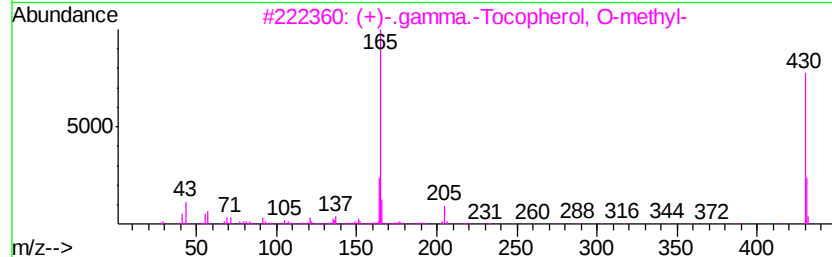
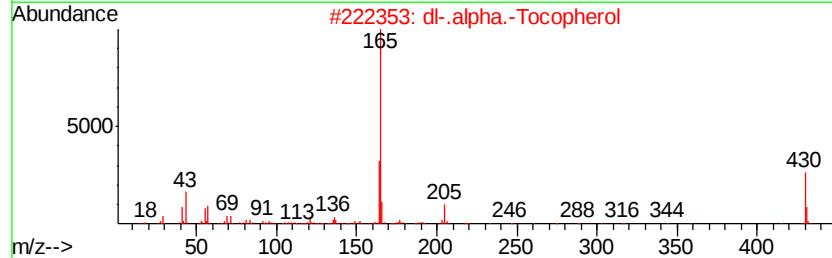
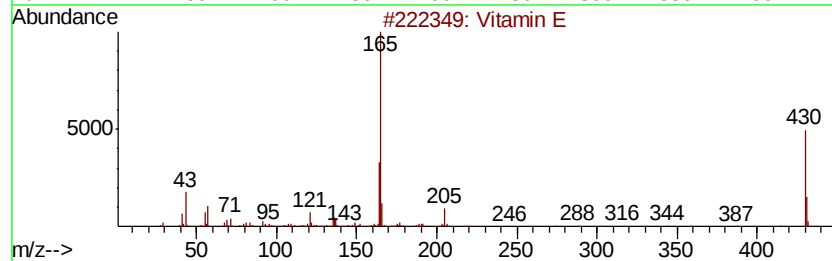
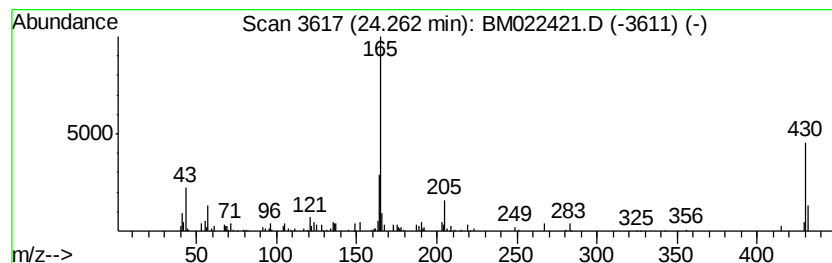
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Vitamin E Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.26	8.35 ng	165940	Perylene-d12	23.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vitamin E	430	C29H50O2	000059-02-9	94
2		dl-.alpha.-Tocopherol	430	C29H50O2	010191-41-0	93
3		(+)-.gamma.-Tocopherol, O-methyl-	430	C29H50O2	1000374-72-2	81
4		.alpha.-Tocopherol-.beta.-D-mann...	592	C35H60O7	1000156-68-2	64
5		3-Fluoro-4-methoxyphenylacetone...	165	C9H8FO	000404-90-0	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM082919\
Data File : BM022421.D
Acq On : 29 Aug 2019 23:13
Operator : HP/JU
Sample : K4573-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S700B-N-1.0-1.5-082719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.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
unknown7.06	7.06	115.9	ng	676677	1	7.52	116749	20.0
n-Hexadecanoic acid	17.85	13.4	ng	146687	4	16.95	218683	20.0
Octadecanoic acid	19.14	2.6	ng	54988	5	21.17	420071	20.0
9-Octadecenamide,...	20.30	7.2	ng	151317	5	21.17	420071	20.0
Cyclopentadecane	20.86	9.3	ng	194757	5	21.17	420071	20.0
Bromoacetic acid,...	21.74	5.5	ng	116458	5	21.17	420071	20.0
Perylene	22.70	4.5	ng	88361	6	23.36	397259	20.0
.gamma.-Tocopherol	23.72	4.3	ng	85368	6	23.36	397259	20.0
Heptadecyl heptaf...	23.90	6.3	ng	124855	6	23.36	397259	20.0
Vitamin E	24.26	8.3	ng	165940	6	23.36	397259	20.0