

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040620\
 Data File : BF119827.D
 Acq On : 7 Apr 2020 17:30
 Operator : MA/SJ
 Sample : L2146-05
 Misc :
 ALS Vial : 60 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-67-66-COMP

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_F\METHODS\8270-BF031820.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	4.993	488	494	503	rVB	34442	46205	1.36%	0.182%
2	5.398	558	563	566	rBV	3376963	3090557	91.07%	12.163%
3	6.422	731	737	740	rBV	3394211	3393422	100.00%	13.355%
4	6.610	766	769	778	rVB	90651	85119	2.51%	0.335%
5	6.787	795	799	802	rBV	1022500	793769	23.39%	3.124%
6	6.945	821	826	829	rBV	2711367	2393542	70.53%	9.420%
7	7.351	890	895	898	rBV	2087281	1828729	53.89%	7.197%
8	8.075	1013	1018	1021	rBV	1074831	950411	28.01%	3.740%
9	9.151	1196	1201	1204	rBV	3792513	3069274	90.45%	12.079%
10	9.269	1219	1221	1225	rVB	64098	49707	1.46%	0.196%
11	9.545	1264	1268	1271	rBV	432449	316082	9.31%	1.244%
12	9.833	1312	1317	1320	rBV	1195356	1108974	32.68%	4.364%
13	10.622	1446	1451	1454	rBV	1945567	1709491	50.38%	6.728%
14	11.316	1566	1569	1573	rBV	994908	920143	27.12%	3.621%
15	11.851	1656	1660	1670	rBV	309873	339807	10.01%	1.337%
16	12.633	1790	1793	1801	rBV2	103576	127102	3.75%	0.500%
17	12.910	1835	1840	1843	rBV	3081863	2639766	77.79%	10.389%
18	13.392	1918	1922	1924	rBV3	35591	39625	1.17%	0.156%
19	13.486	1935	1938	1940	rBV2	40474	37482	1.10%	0.148%
20	13.810	1990	1993	2000	rBV	357987	432227	12.74%	1.701%
21	13.963	2015	2019	2022	rBV	876288	752631	22.18%	2.962%
22	14.063	2034	2036	2039	rBV4	47337	41182	1.21%	0.162%
23	14.133	2045	2048	2054	rVB	60766	60689	1.79%	0.239%
24	14.186	2055	2057	2059	rBV3	39532	45242	1.33%	0.178%
25	14.439	2097	2100	2103	rBV	88331	110009	3.24%	0.433%
26	14.739	2149	2151	2161	rVB2	96508	129715	3.82%	0.510%
27	14.857	2169	2171	2174	rBV4	50029	74991	2.21%	0.295%
28	15.074	2205	2208	2210	rBV	60539	61458	1.81%	0.242%
29	15.410	2261	2265	2269	rBV	460954	527946	15.56%	2.078%
30	15.445	2269	2271	2274	rVV2	55487	56605	1.67%	0.223%
31	15.710	2314	2316	2321	rBV6	49595	83886	2.47%	0.330%
32	16.280	2411	2413	2416	rBV3	59379	93765	2.76%	0.369%

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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_F\METHODS\8270-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

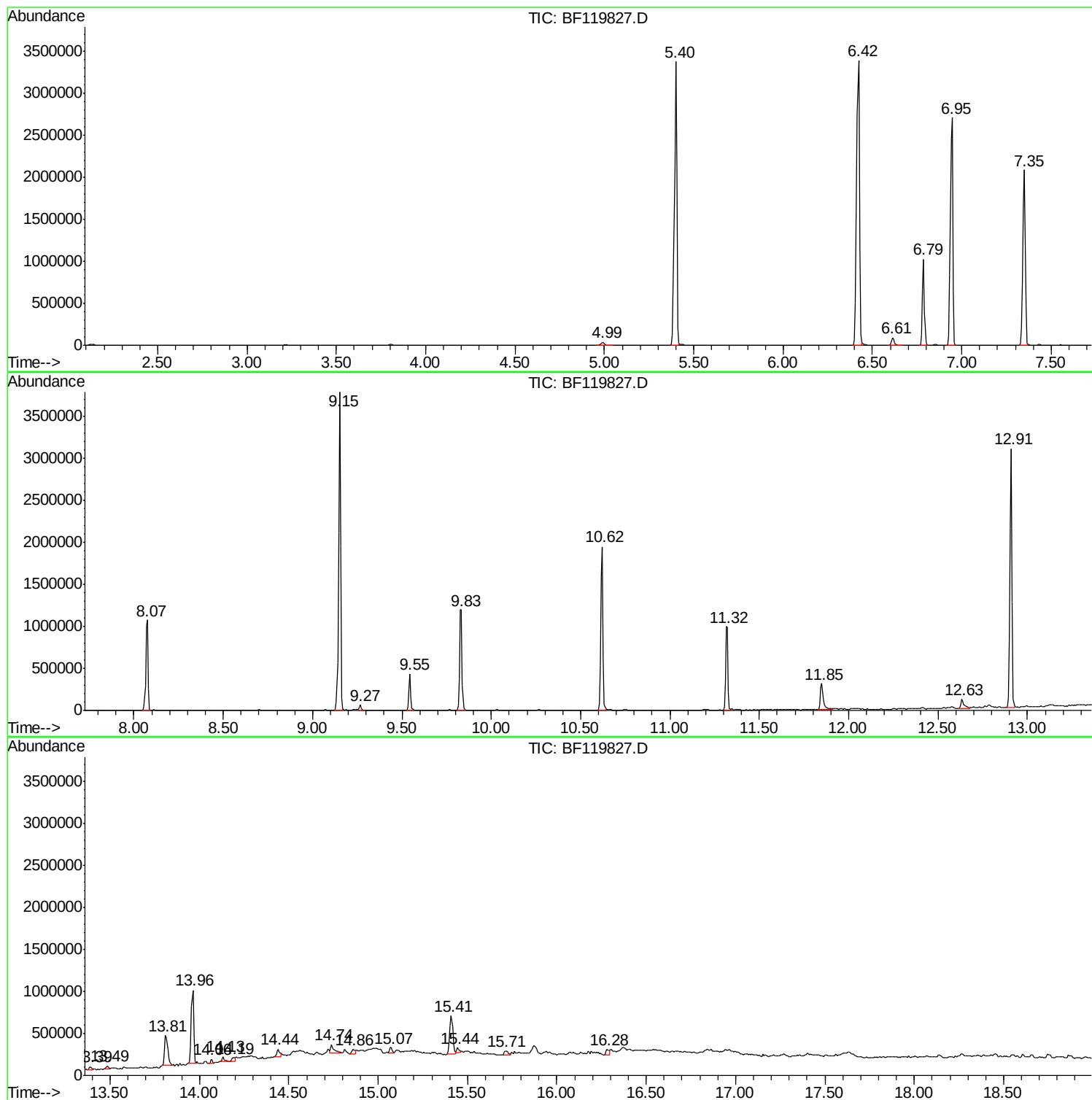
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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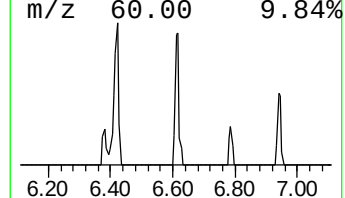
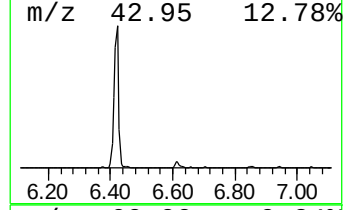
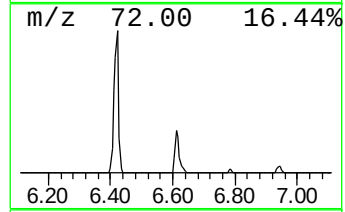
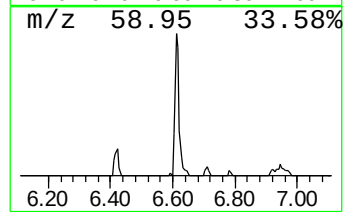
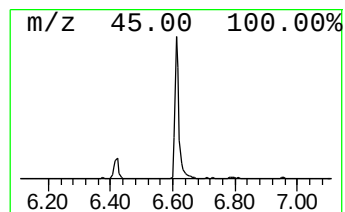
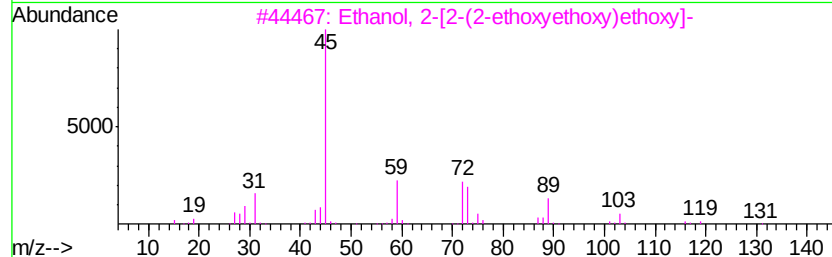
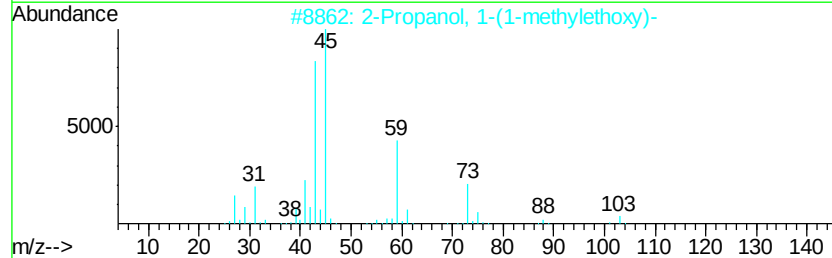
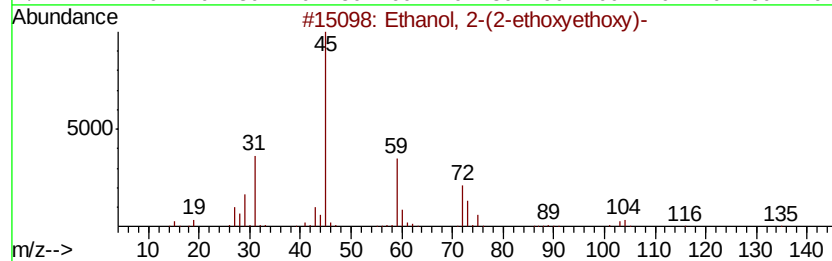
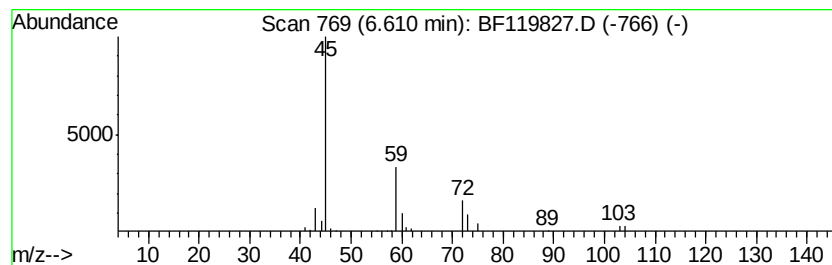
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.61	2.14 ng	85119	1,4-Dichlorobenzene-d4	6.79	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	38
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	25
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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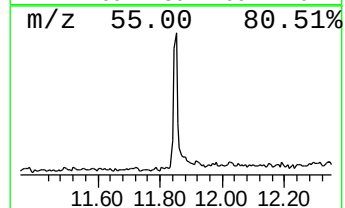
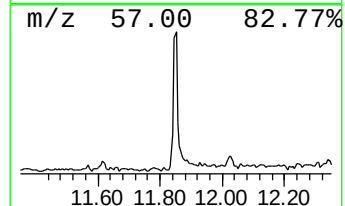
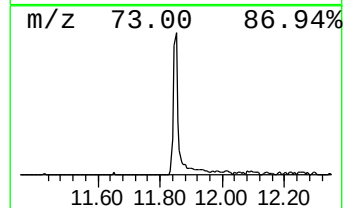
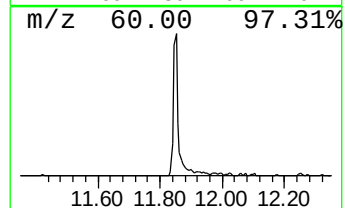
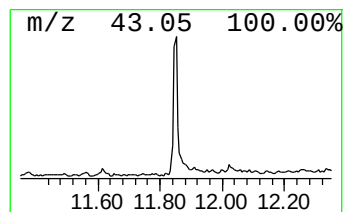
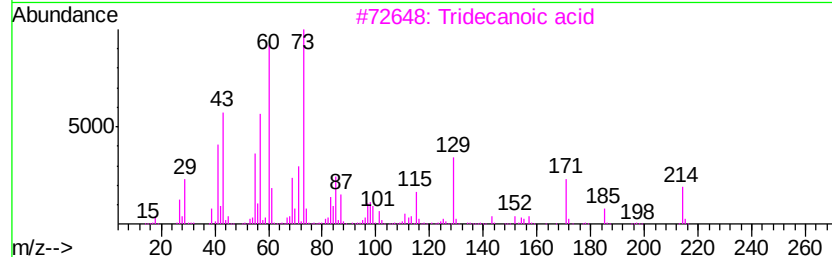
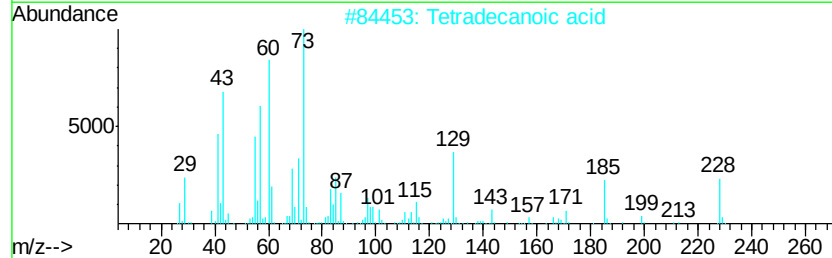
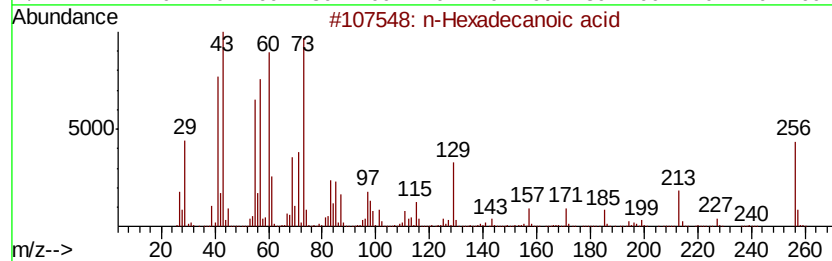
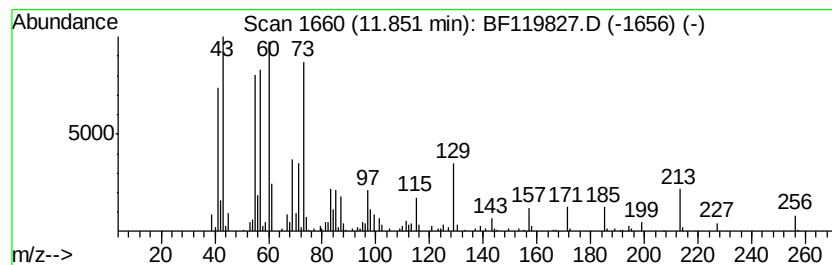
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	7.39 ng	339807	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



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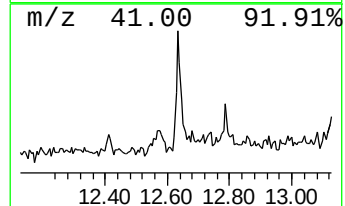
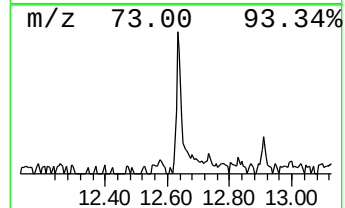
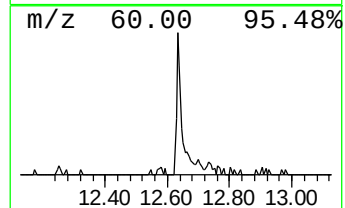
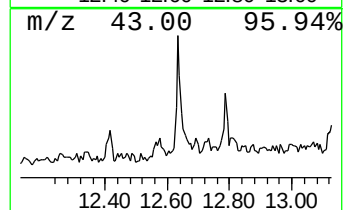
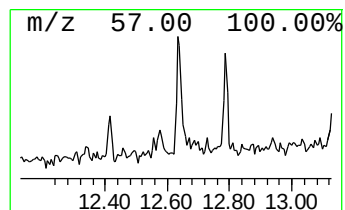
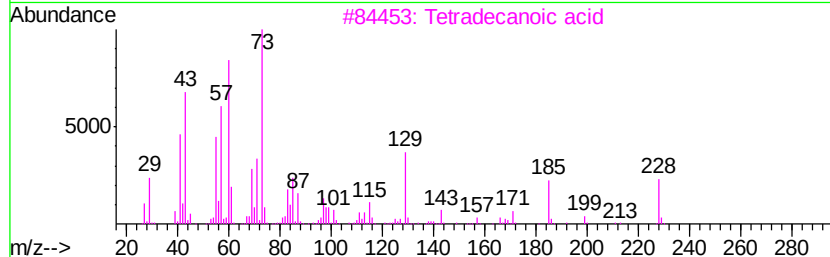
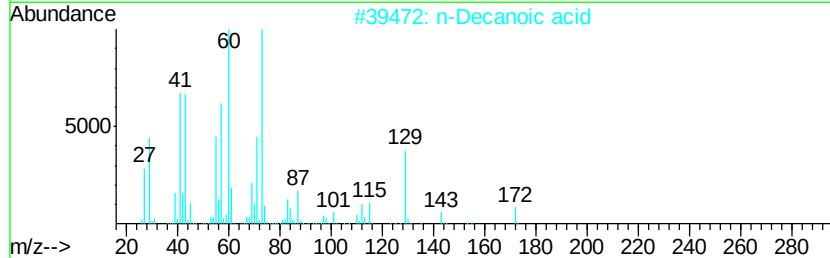
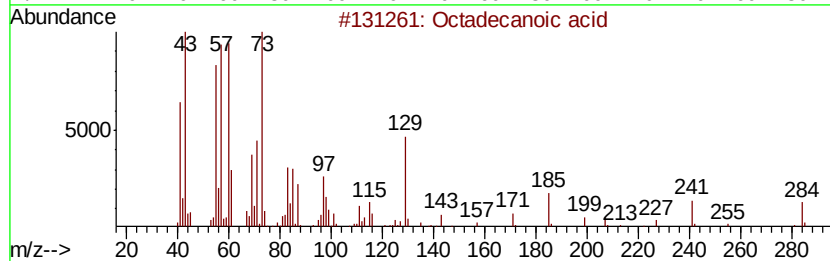
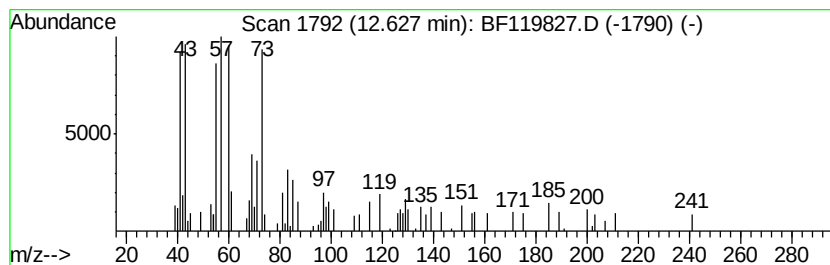
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.63	2.76 ng	127102	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	n-Decanoic acid	172	C10H20O2	000334-48-5	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	20
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	18



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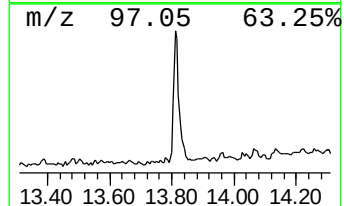
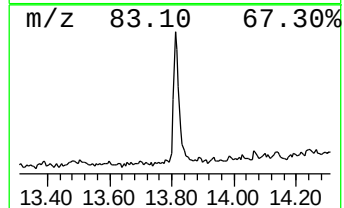
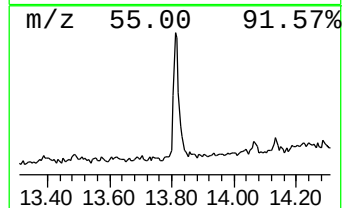
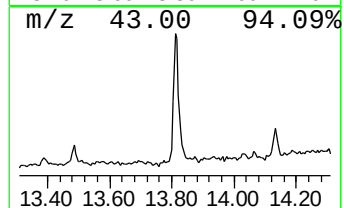
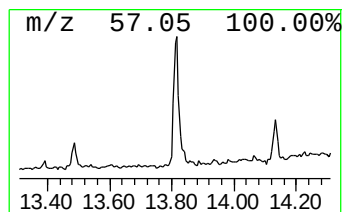
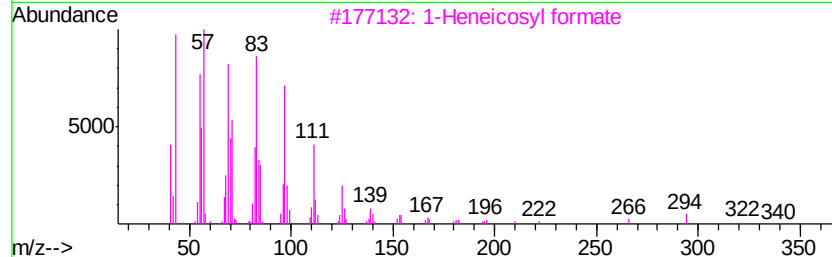
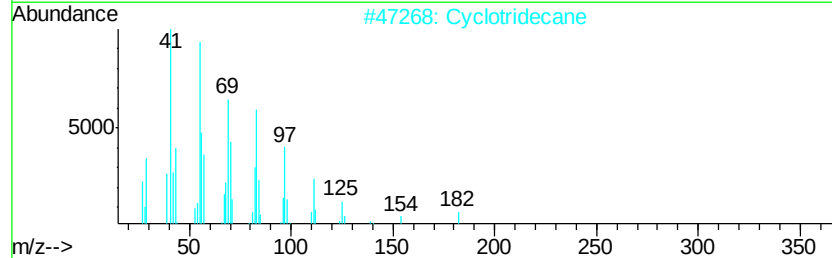
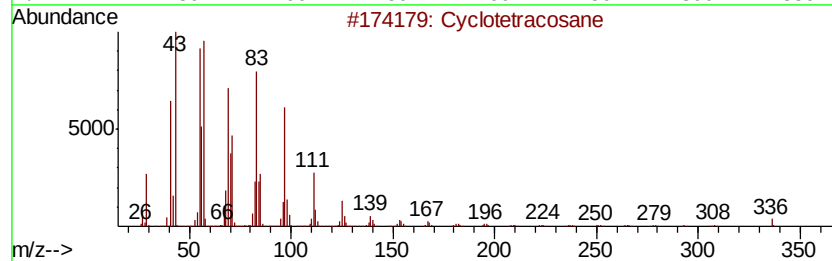
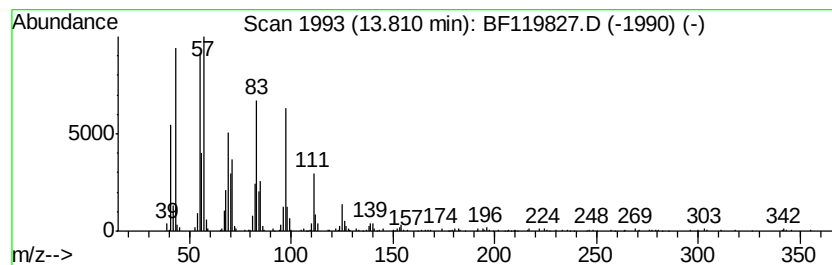
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	11.49 ng	432227	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	95
2		Cyclotridecane	182	C13H26	000295-02-3	95
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94



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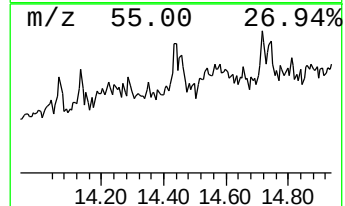
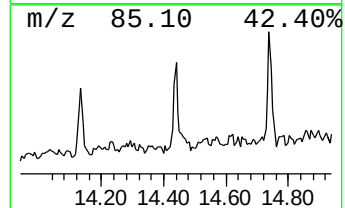
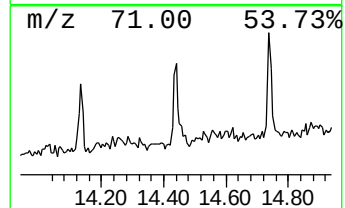
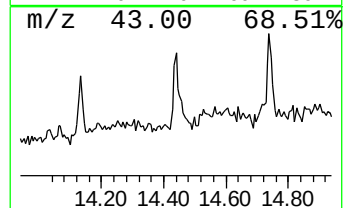
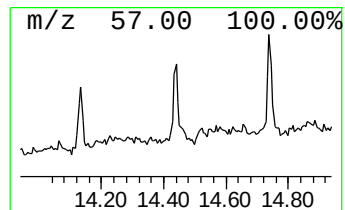
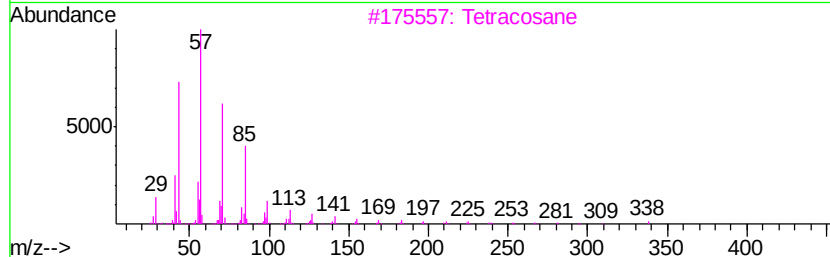
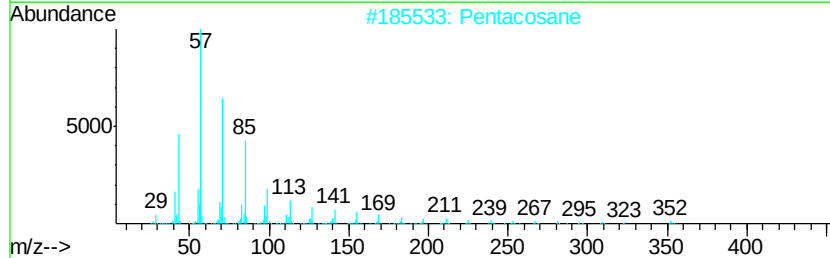
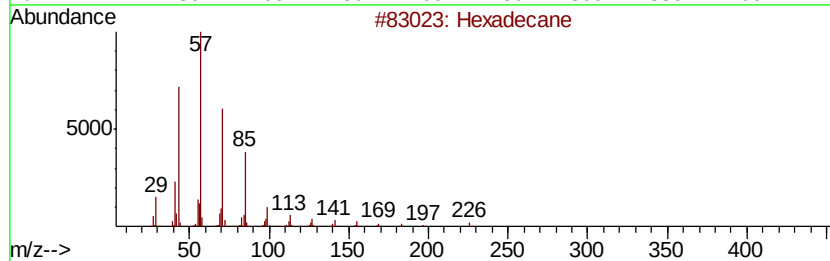
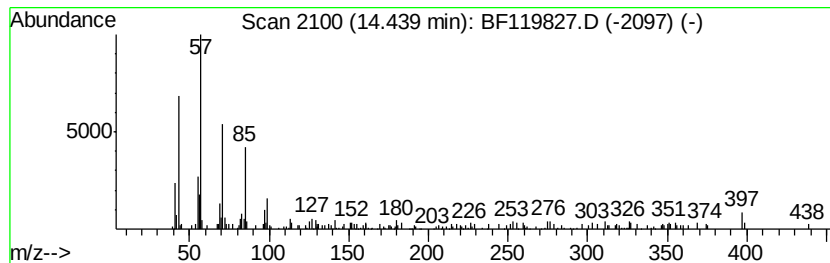
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.92 ng	110009	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Pentacosane		352	C25H52	000629-99-2	64
3	Tetracosane		338	C24H50	000646-31-1	52
4	Sulfurous acid, butyl nonyl ester		264	C13H28O3S	1000309-17-6	52
5	Eicosane		282	C20H42	000112-95-8	52



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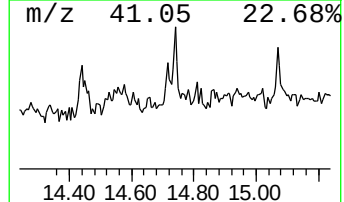
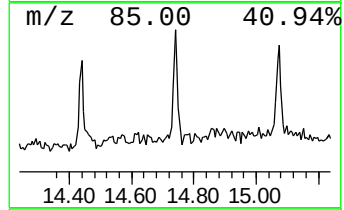
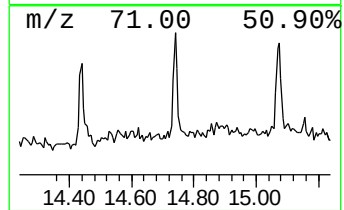
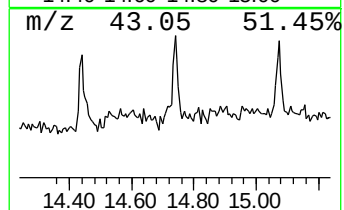
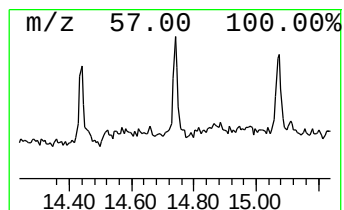
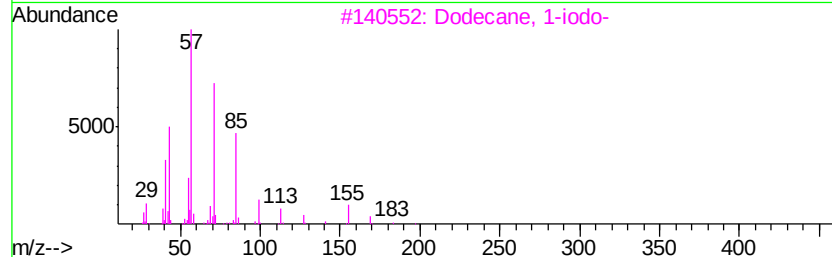
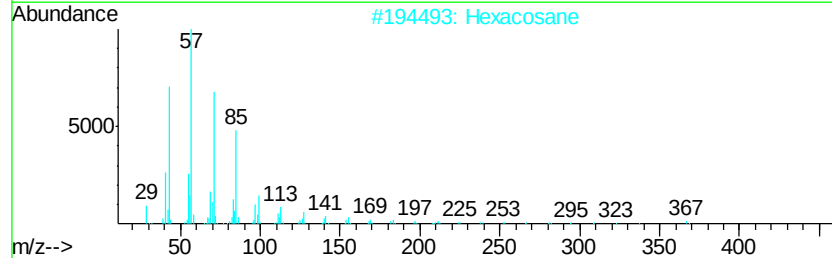
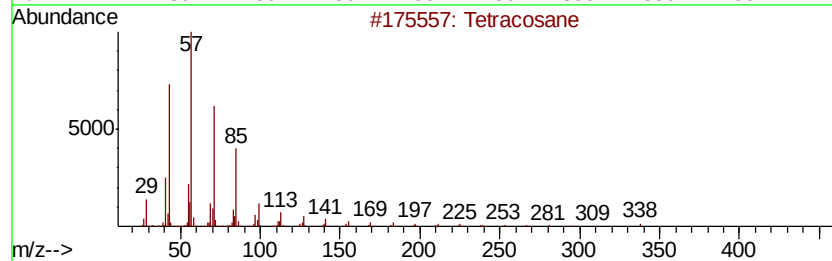
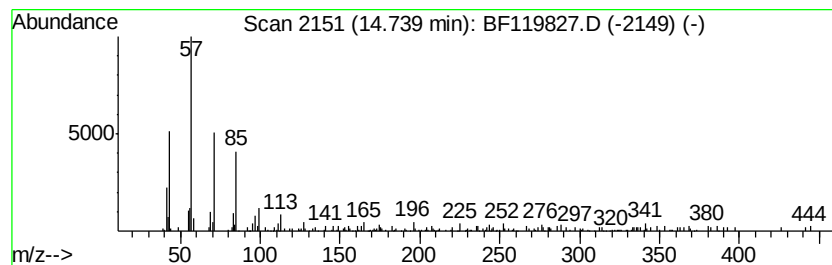
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	4.91 ng	129715	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	93
2		Hexacosane	366	C26H54	000630-01-3	64
3		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
4		Eicosane	282	C20H42	000112-95-8	59
5		Octacosane	394	C28H58	000630-02-4	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
 Data File : BF119827.D
 Acq On : 7 Apr 2020 17:30
 Operator : MA/SJ
 Sample : L2146-05
 Misc :
 ALS Vial : 60 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-67-66-COMP

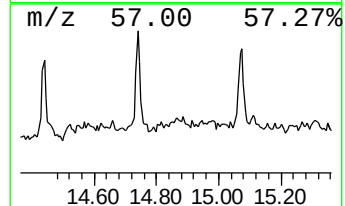
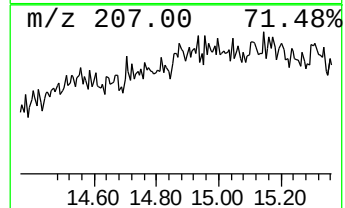
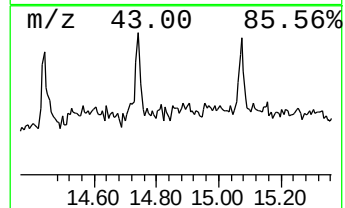
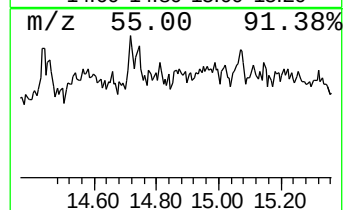
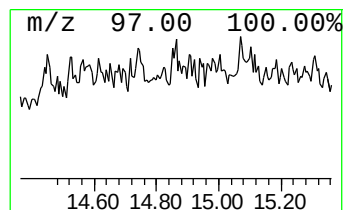
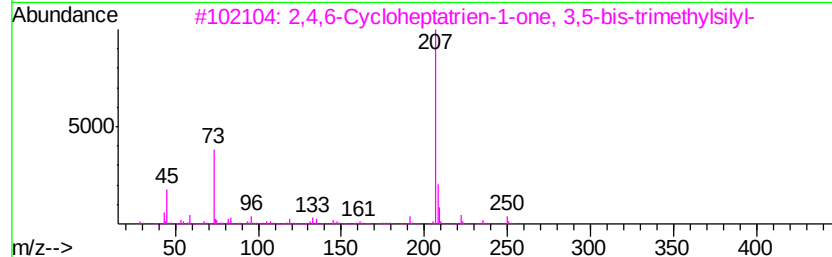
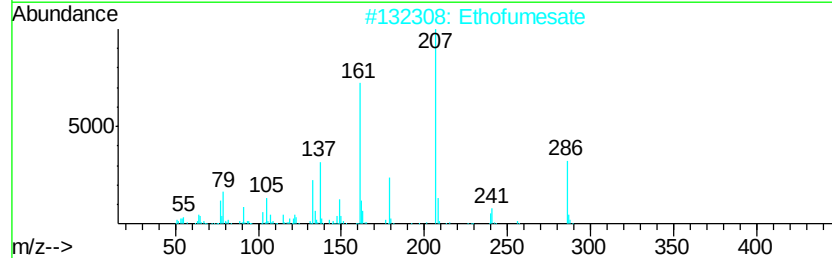
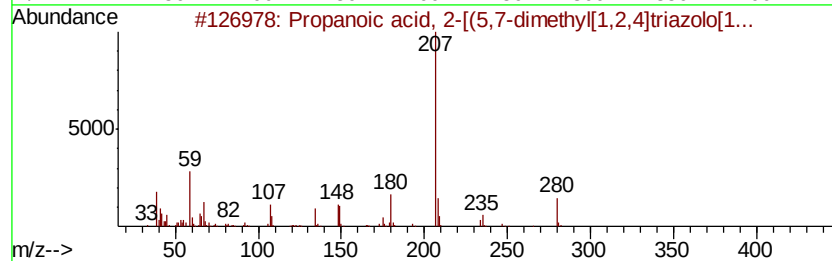
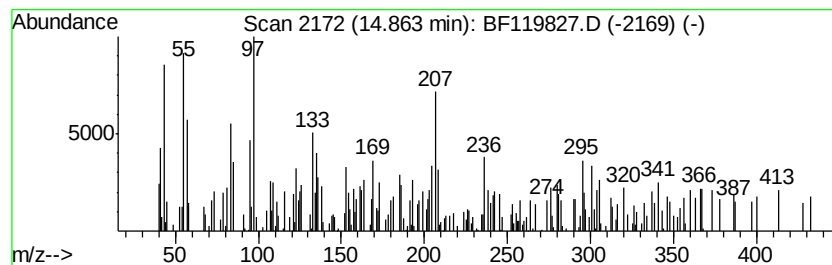
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 unknown14.86 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	2.84 ng	74991	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-[(5,7-dimethyl...	280	C12H16N4O2S	1000319-25-1	15
2		Ethofumesate	286	C13H18O5S	026225-79-6	11
3		2,4,6-Cycloheptatrien-1-one, 3,5...	250	C13H22OSi2	1000161-21-8	11
4		Sulfide, bis(2-cyano-3,4-dihydro...	302	C16H22N4S	1000190-79-0	11
5		tert-Butyl(5-isopropyl-2-methylp...	264	C16H28OSi	1000367-02-3	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119827.D
Acq On : 7 Apr 2020 17:30
Operator : MA/SJ
Sample : L2146-05
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-67-66-COMP

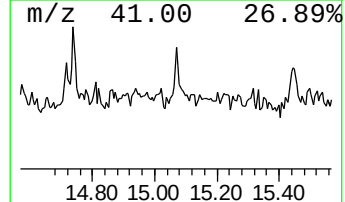
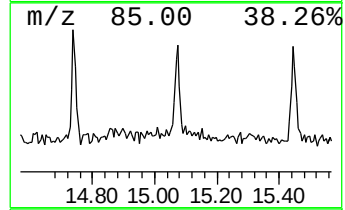
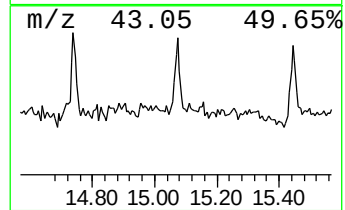
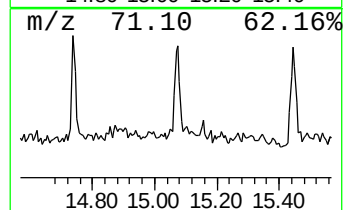
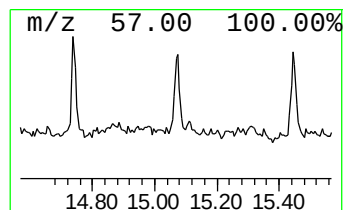
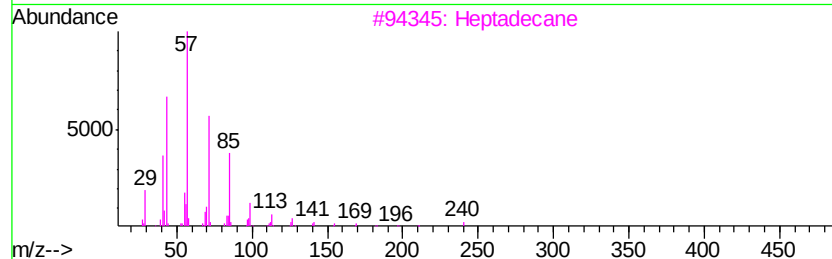
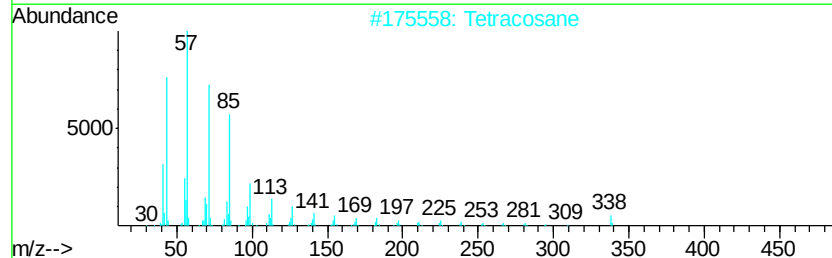
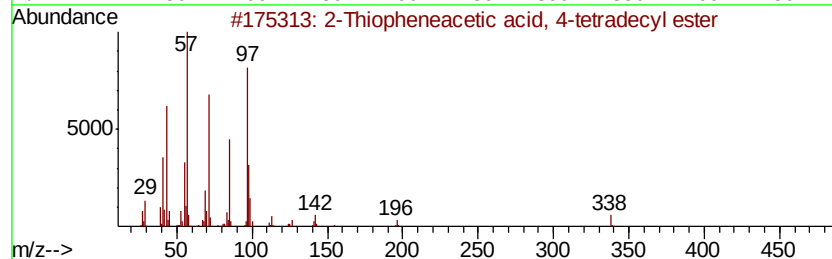
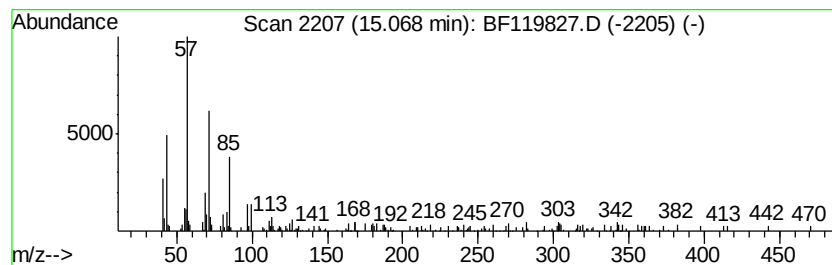
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Thiopheneacetic acid, 4-t... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.33 ng	61458	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	76
2		Tetracosane	338	C24H50	000646-31-1	76
3		Heptadecane	240	C17H36	000629-78-7	70
4		Tridecane	184	C13H28	000629-50-5	70
5		Pentadecane	212	C15H32	000629-62-9	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
 Data File : BF119827.D
 Acq On : 7 Apr 2020 17:30
 Operator : MA/SJ
 Sample : L2146-05
 Misc :
 ALS Vial : 60 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-67-66-COMP

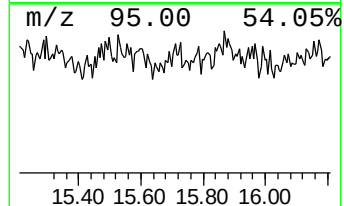
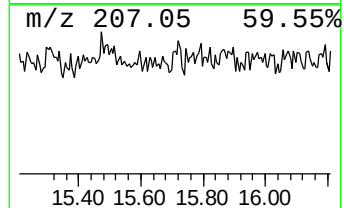
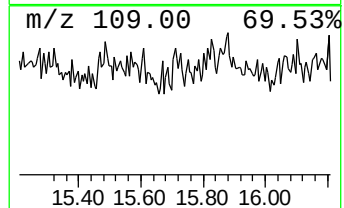
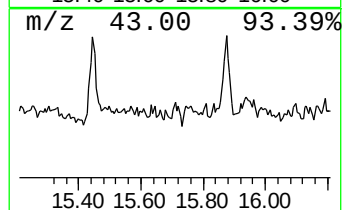
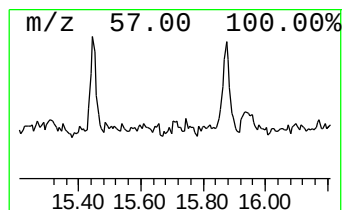
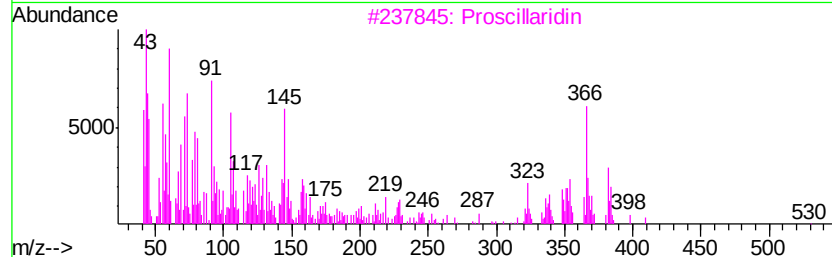
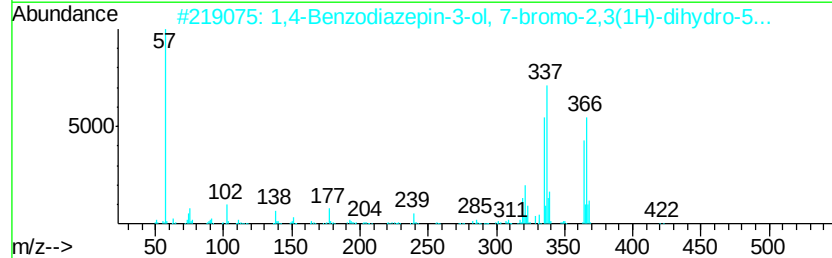
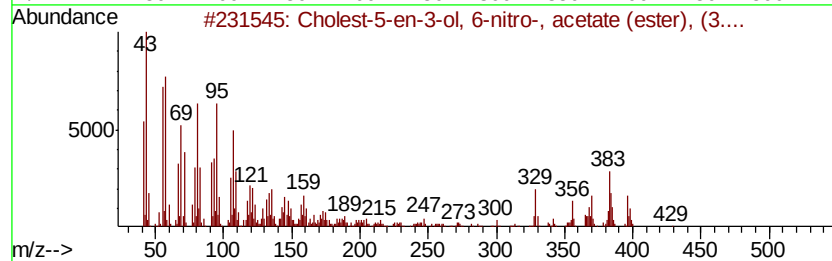
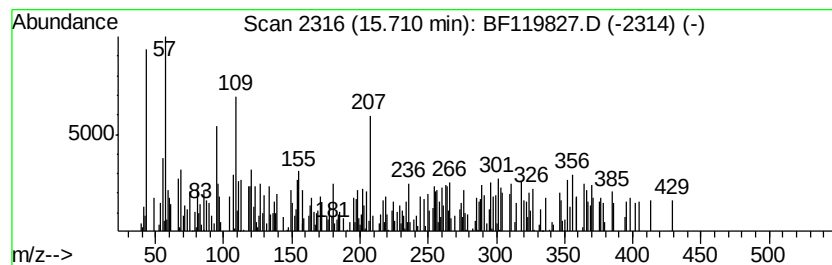
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 unknown15.71 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.18 ng	83886	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholest-5-en-3-ol, 6-nitro-, ace...	473	C29H47NO4	001912-54-5	10
2		1,4-Benzodiazepin-3-ol, 7-bromo-...	420	C18H14BrClN2O3	172986-26-4	9
3		Proscillaridin	530	C30H42O8	000466-06-8	7
4		9,11-Didehydrolumisterol acetate	436	C30H44O2	1000128-09-6	7
5		3.beta.-Acetoxy-5.alpha.-pregnan...	424	C23H37BrO2	071016-66-5	7



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040620\
Data File : BF119827.D
Acq On : 7 Apr 2020 17:30
Operator : MA/SJ
Sample : L2146-05
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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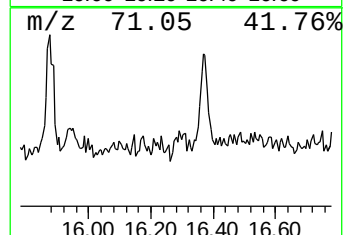
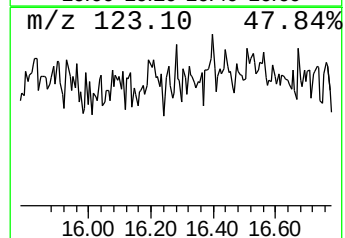
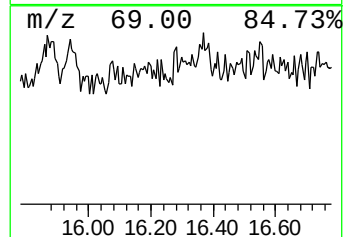
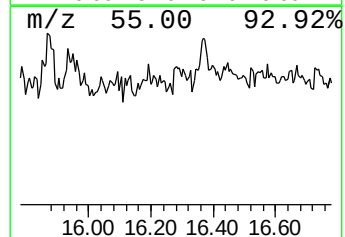
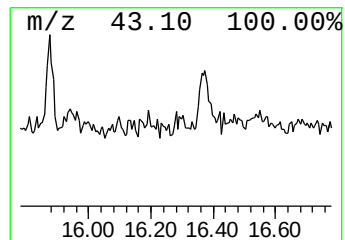
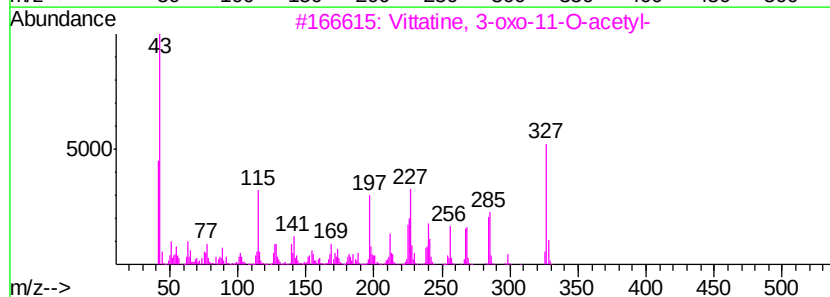
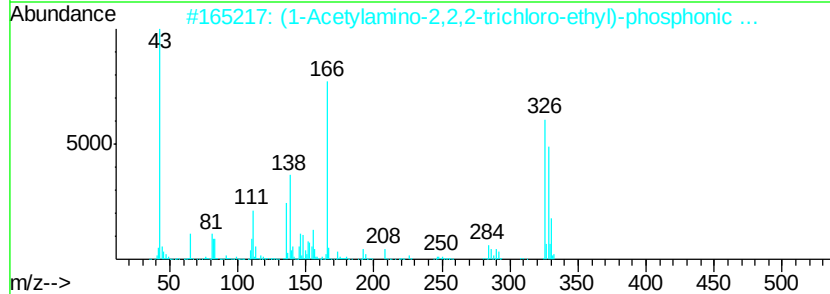
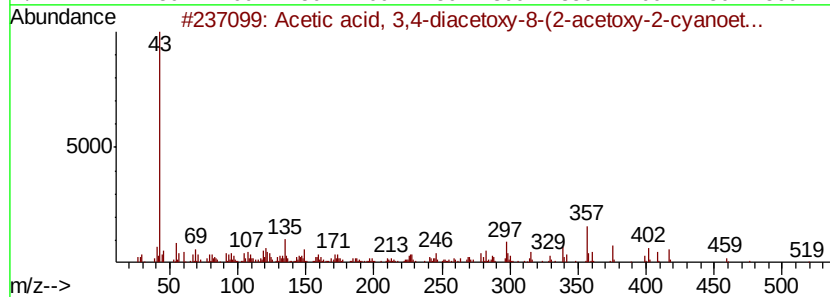
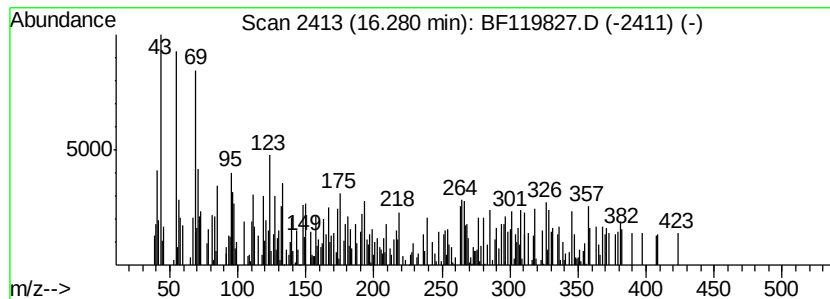
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.28 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.28	3.55 ng	93765	Perylene-d12	15.41

Hit#	of	3	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 3,4-diacetoxv-8-(2-...	519	C27H37N09	1000187-94-6	9
2			(1-Acetylamino-2,2,2-trichloro-e...	325	C8H15Cl3N04P	026404-47-7	9
3			Vittatine, 3-oxo-11-O-acetyl-	327	C18H17N05	1000111-32-8	2



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040620\
Data File : BF119827.D
Acq On : 7 Apr 2020 17:30
Operator : MA/SJ
Sample : L2146-05
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-67-66-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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
Ethanol, 2-(2-eth...	6.61	2.1	ng	85119	1	6.79	793769	20.0
n-Hexadecanoic acid	11.85	7.4	ng	339807	4	11.32	920143	20.0
Octadecanoic acid	12.63	2.8	ng	127102	4	11.32	920143	20.0
Cyclotetracosane	13.81	11.5	ng	432227	5	13.96	752631	20.0
Hexadecane	14.44	2.9	ng	110009	5	13.96	752631	20.0
Tetracosane	14.74	4.9	ng	129715	6	15.41	527946	20.0
unknown14.86	14.86	2.8	ng	74991	6	15.41	527946	20.0
2-Thiopheneacetic...	15.07	2.3	ng	61458	6	15.41	527946	20.0
unknown15.71	15.71	3.2	ng	83886	6	15.41	527946	20.0
unknown16.28	16.28	3.5	ng	93765	6	15.41	527946	20.0