

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020420\
 Data File : BF118805.D
 Acq On : 4 Feb 2020 16:50
 Operator : CG/JU
 Sample : PB126588BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB126588BL

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-BF020320.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	2.905	132	139	148	rVB	85385	149701	1.27%	0.215%
2	5.428	564	568	572	rBV	3018805	2986782	25.37%	4.284%
3	6.434	735	739	747	rBV	2239884	1976570	16.79%	2.835%
4	6.810	799	803	807	rVB	1979278	1647764	13.99%	2.364%
5	6.969	826	830	834	rVB	6090538	5737520	48.73%	8.230%
6	7.375	893	899	902	rBV	4333953	4814793	40.89%	6.906%
7	8.092	1016	1021	1024	rBV	2517356	2238031	19.01%	3.210%
8	8.475	1082	1086	1091	rVB	156736	151614	1.29%	0.217%
9	8.604	1103	1108	1111	rBV	124890	118030	1.00%	0.169%
10	9.169	1198	1204	1208	rBV	8557206	9670166	82.13%	13.871%
11	9.286	1216	1224	1228	rBV	728804	727917	6.18%	1.044%
12	9.557	1266	1270	1274	rBV	585069	482372	4.10%	0.692%
13	9.845	1314	1319	1323	rBV	3209150	2874147	24.41%	4.123%
14	10.633	1447	1453	1456	rBV	5319425	5212510	44.27%	7.477%
15	11.328	1566	1571	1575	rBV	3457426	3116168	26.47%	4.470%
16	11.563	1605	1611	1620	rBV2	69629	131613	1.12%	0.189%
17	11.780	1645	1648	1654	rBV	175105	215151	1.83%	0.309%
18	11.863	1657	1662	1676	rVV	1468275	1786341	15.17%	2.562%
19	12.563	1776	1781	1791	rBV5	144359	284046	2.41%	0.407%
20	12.645	1791	1795	1806	rVV	628523	690351	5.86%	0.990%
21	12.922	1835	1842	1845	rBV	10332079	11774147	100.00%	16.889%
22	13.816	1990	1994	2009	rBV	593453	799876	6.79%	1.147%
23	13.963	2014	2019	2023	rBV	3322478	3036509	25.79%	4.356%
24	14.133	2044	2048	2052	rBV	398461	346098	2.94%	0.496%
25	14.439	2096	2100	2113	rBV	645757	594591	5.05%	0.853%
26	14.739	2147	2151	2159	rVB	803827	770021	6.54%	1.105%
27	14.816	2159	2164	2170	rBV	1582523	1625137	13.80%	2.331%
28	15.068	2202	2207	2218	rBV	751877	886318	7.53%	1.271%
29	15.404	2258	2264	2267	rBV	2021630	2574993	21.87%	3.694%
30	15.439	2267	2270	2282	rVB	656765	888774	7.55%	1.275%
31	15.868	2336	2343	2351	rBV	423873	705885	6.00%	1.013%
32	16.357	2420	2426	2443	rVB	214801	425142	3.61%	0.610%
33	16.604	2462	2468	2478	rBV5	64208	129144	1.10%	0.185%
34	16.933	2517	2524	2531	rBV3	64943	147037	1.25%	0.211%

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ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
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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-BF020320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

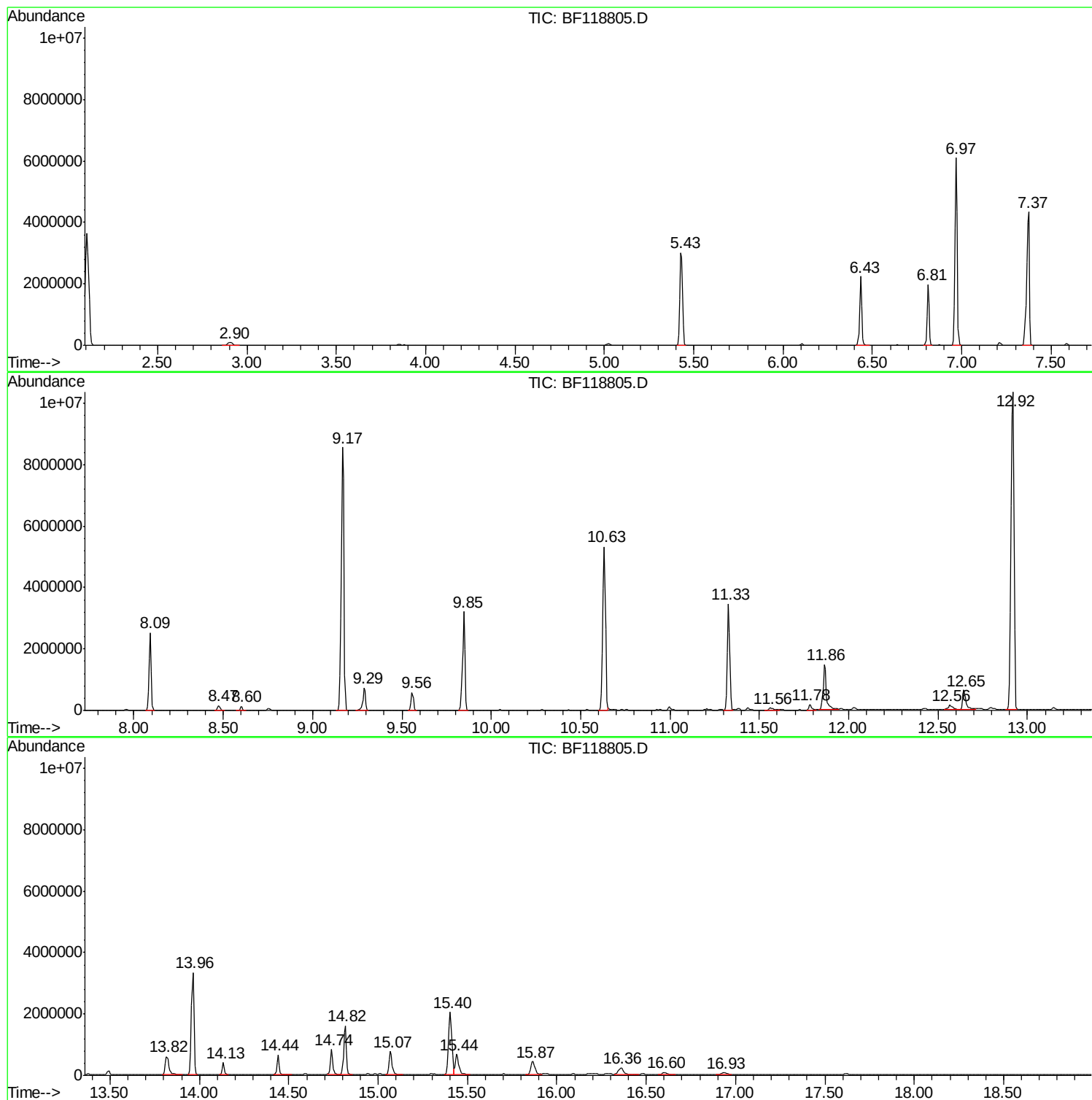
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF020320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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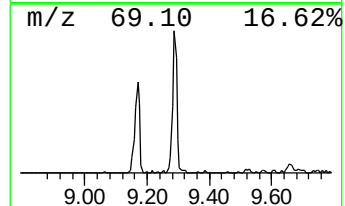
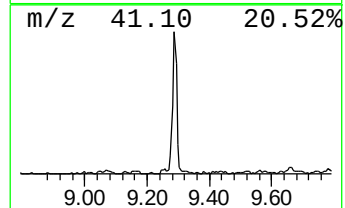
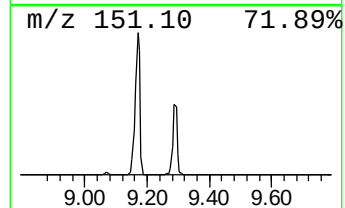
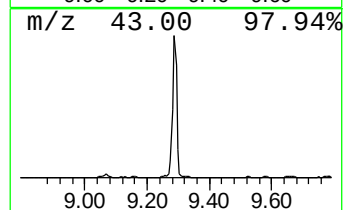
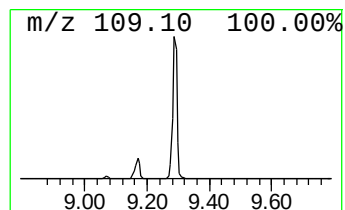
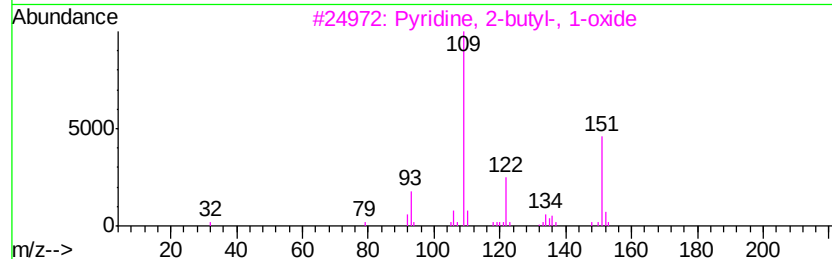
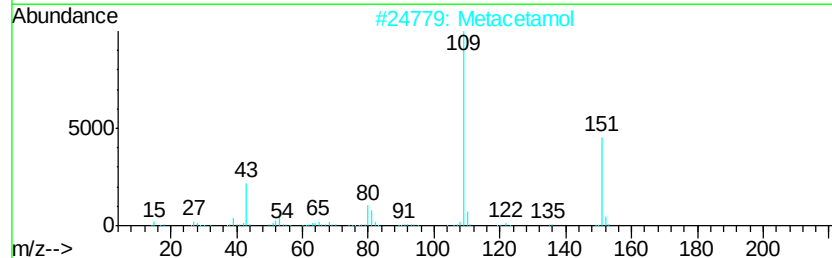
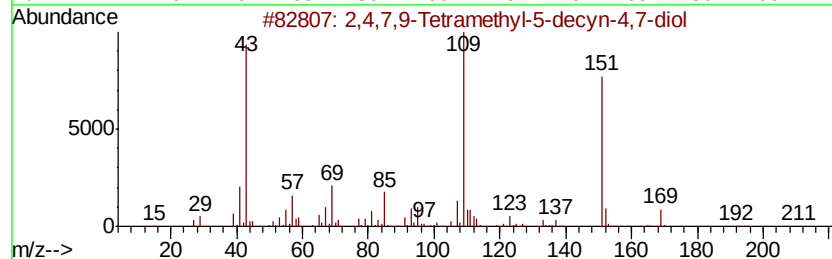
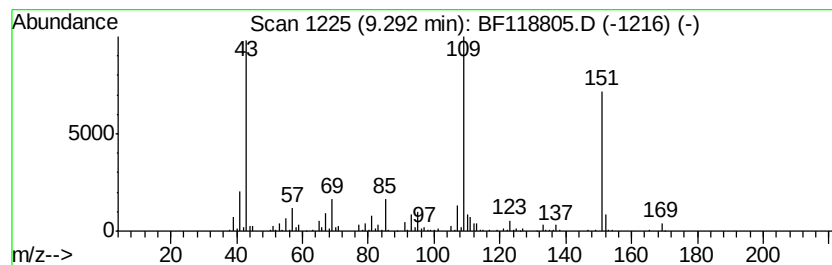
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.29	5.07 ng	727917	Acenaphthene-d10	9.85	
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	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
4	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	43
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	42



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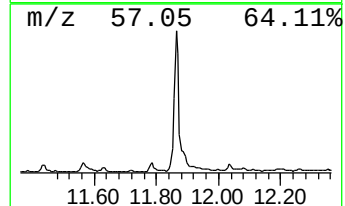
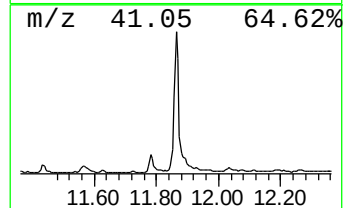
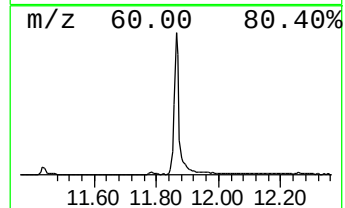
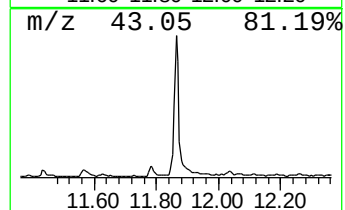
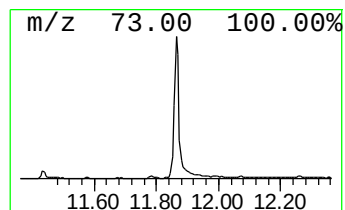
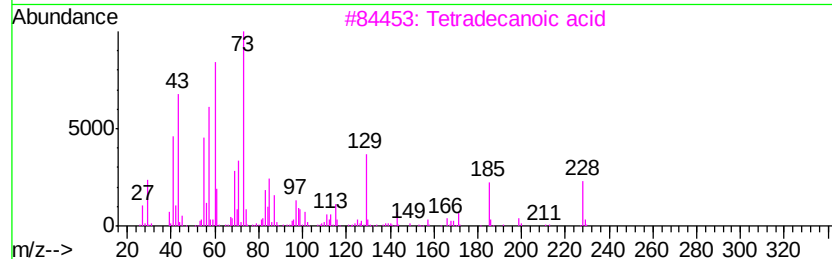
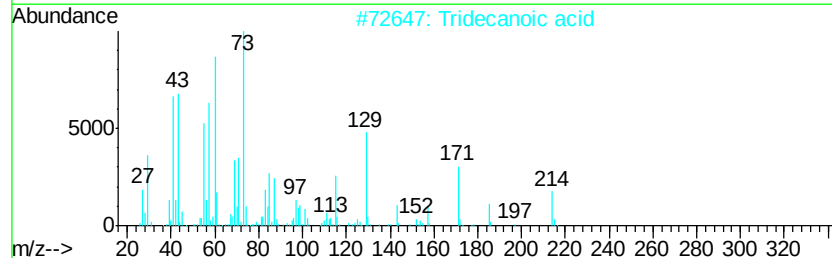
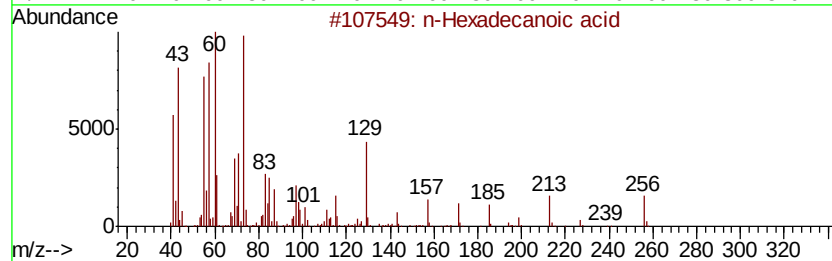
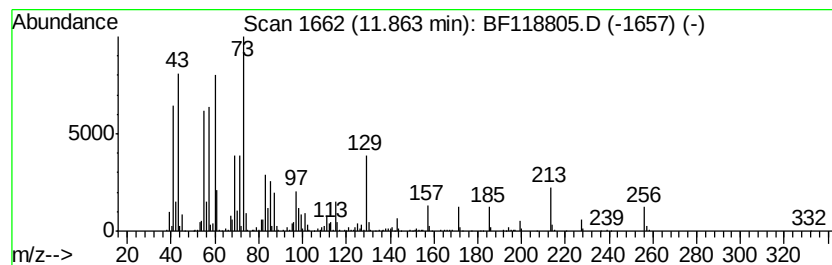
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	11.47 ng	1786340	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90



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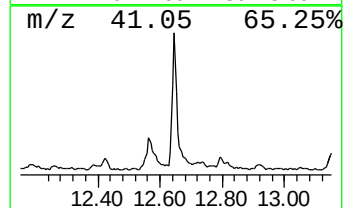
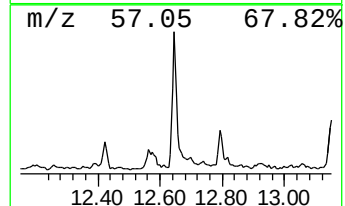
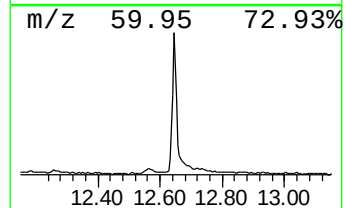
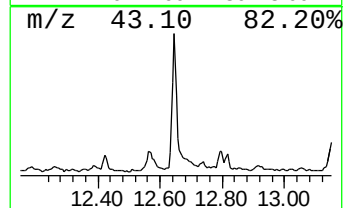
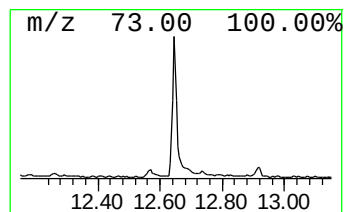
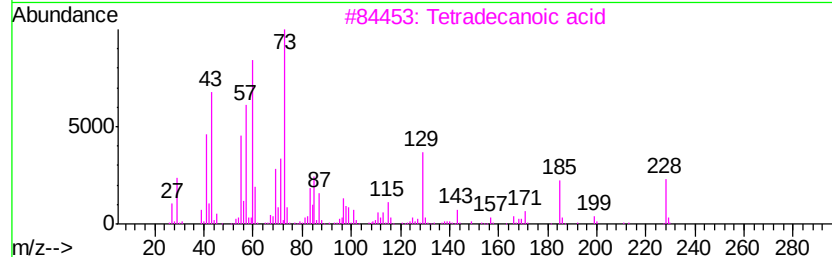
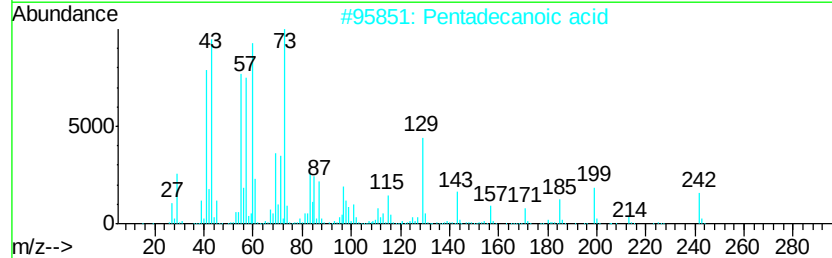
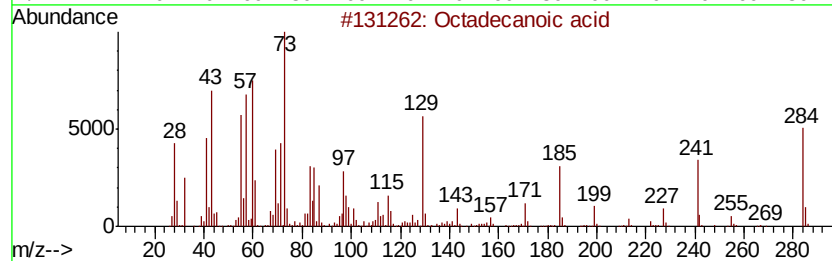
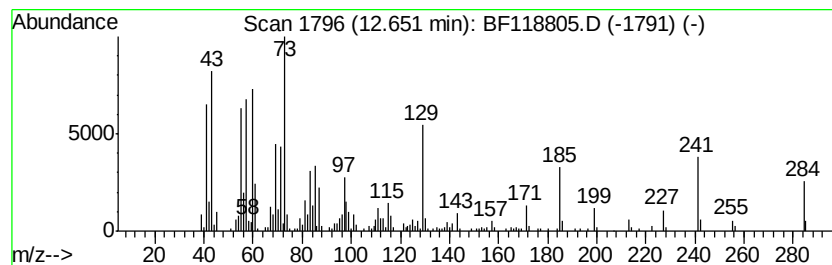
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	4.55 ng	690351	Chrysene-d12	13.96
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 90
3		Tetradecanoic acid	228 C14H28O2	000544-63-8 74
4		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 72
5		n-Decanoic acid	172 C10H20O2	000334-48-5 62



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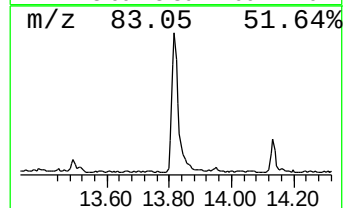
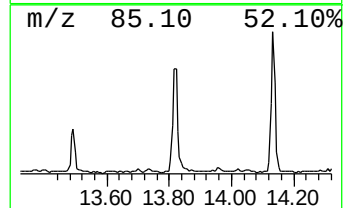
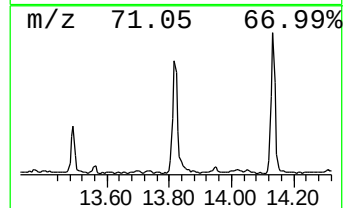
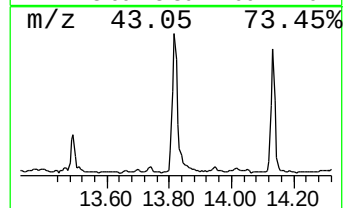
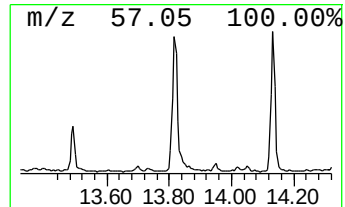
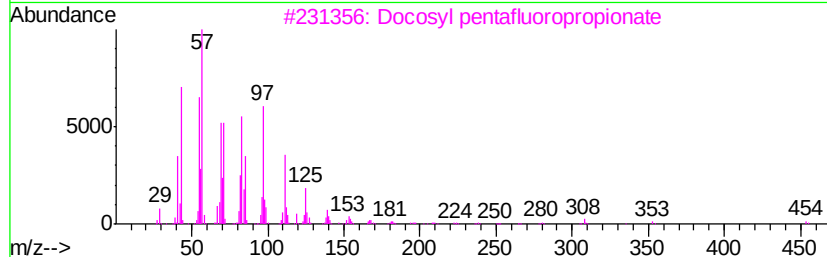
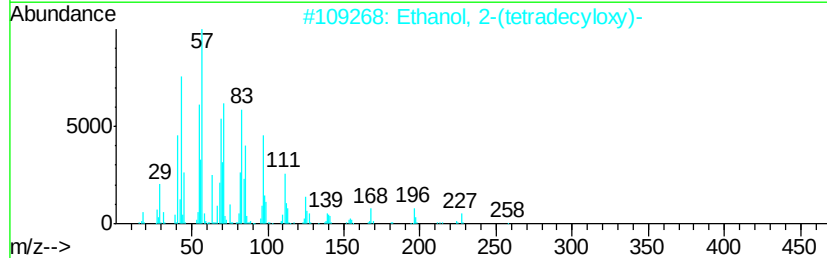
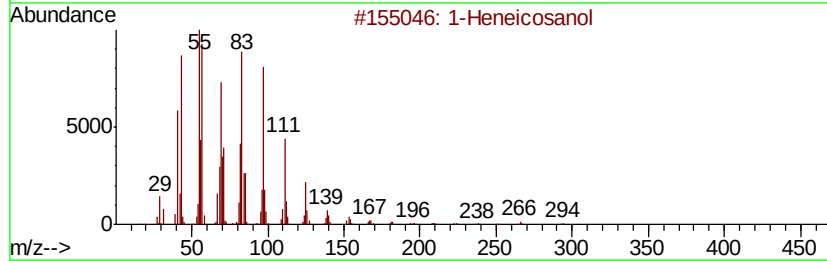
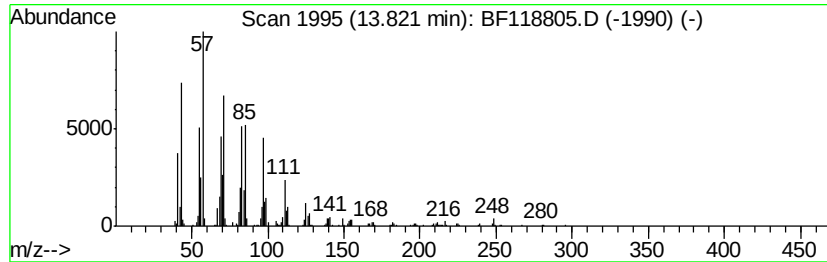
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	5.27 ng	799876	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	92
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
4		1-Eicosene	280	C20H40	003452-07-1	83
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76



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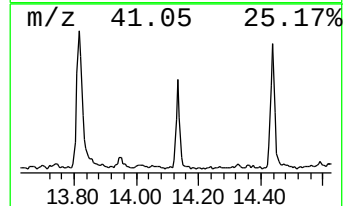
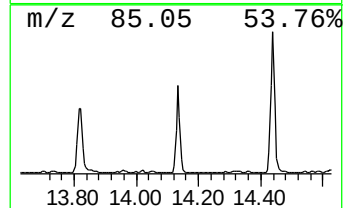
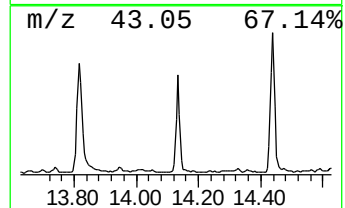
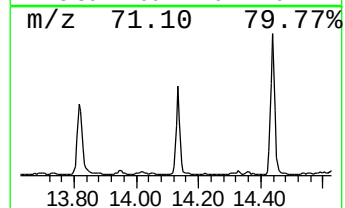
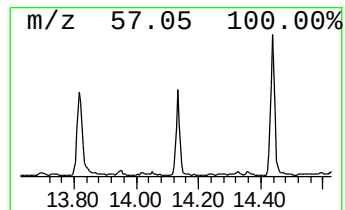
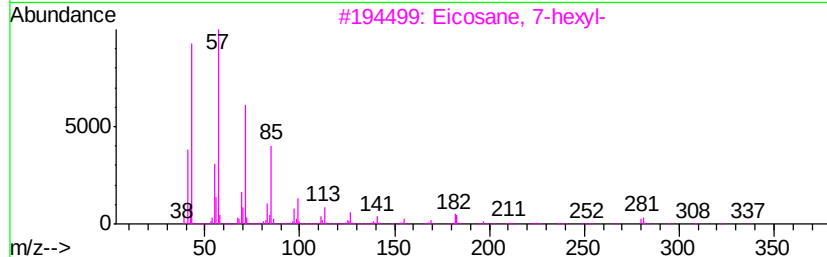
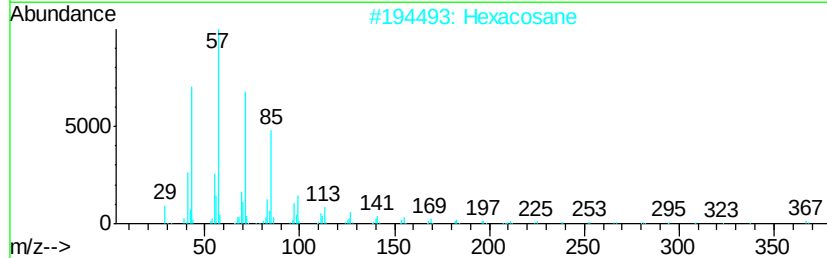
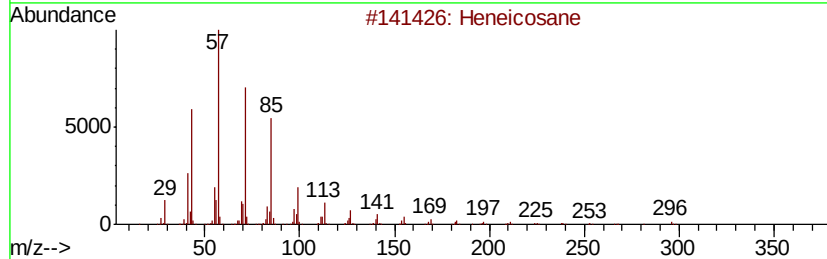
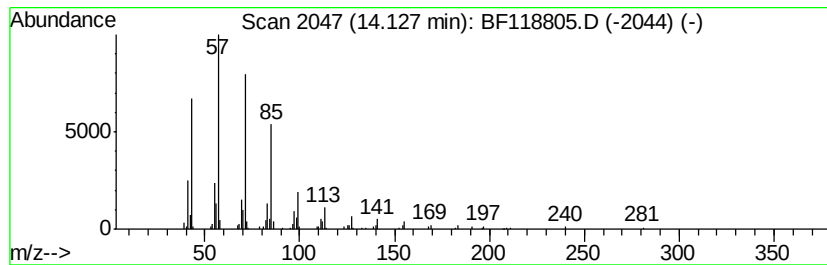
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	2.28 ng	346098	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	90
3	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	90
4	Heptadecane		240	C17H36	000629-78-7	87
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87



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PB126588BL

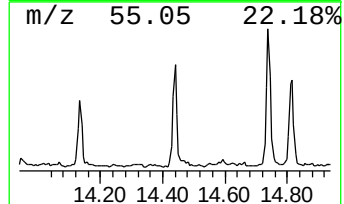
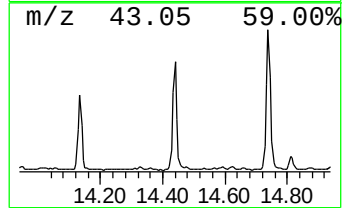
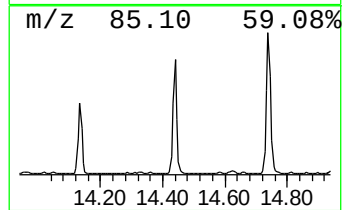
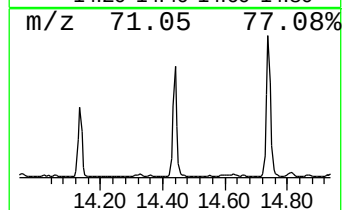
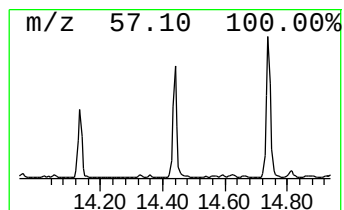
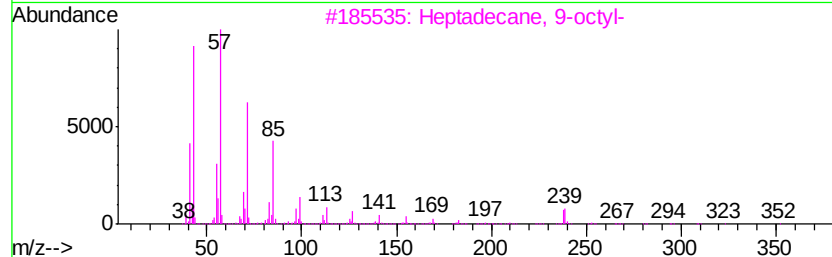
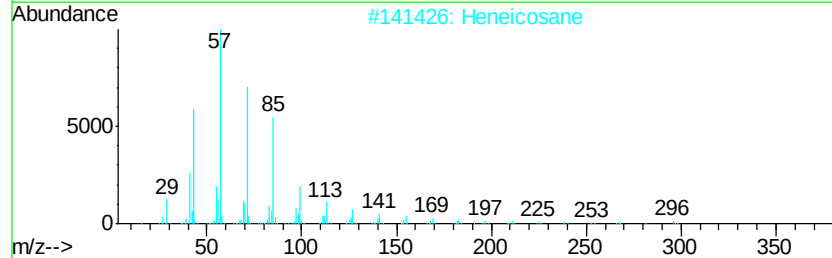
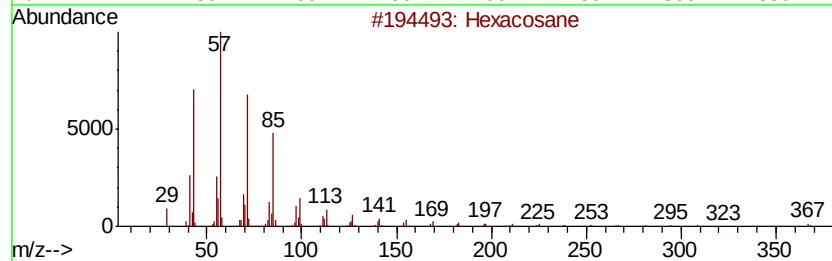
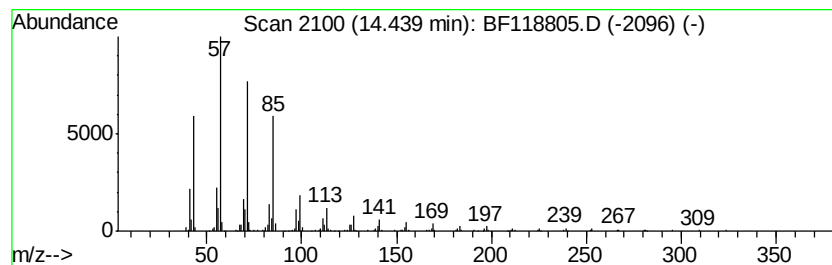
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	3.92 ng	594591	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020420\
Data File : BF118805.D
Acq On : 4 Feb 2020 16:50
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB126588BL

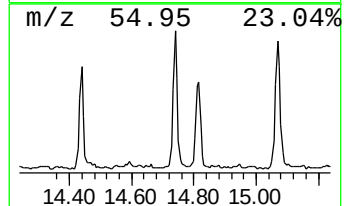
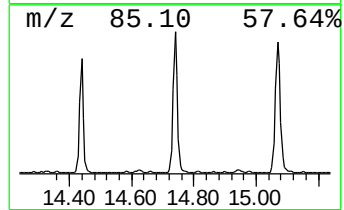
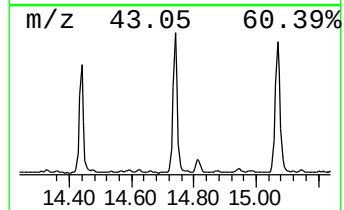
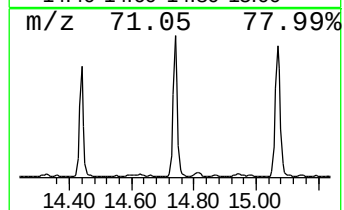
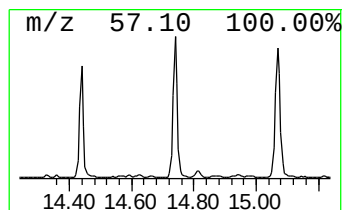
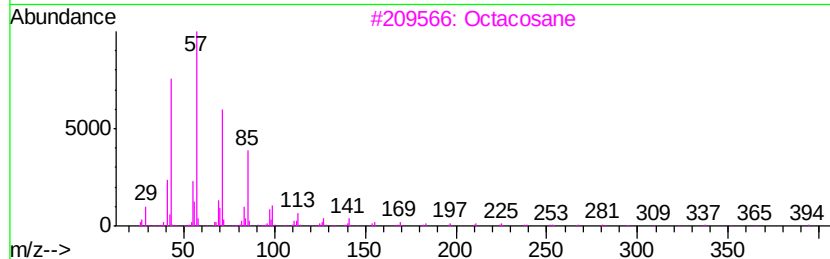
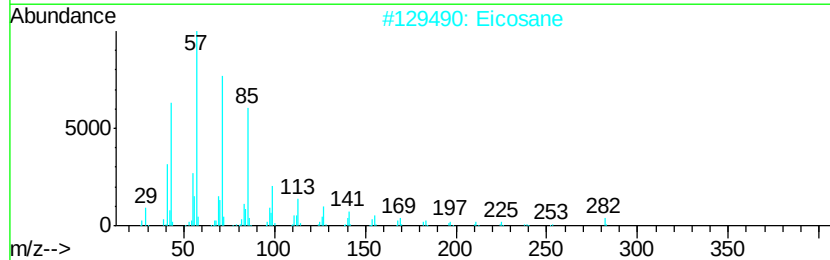
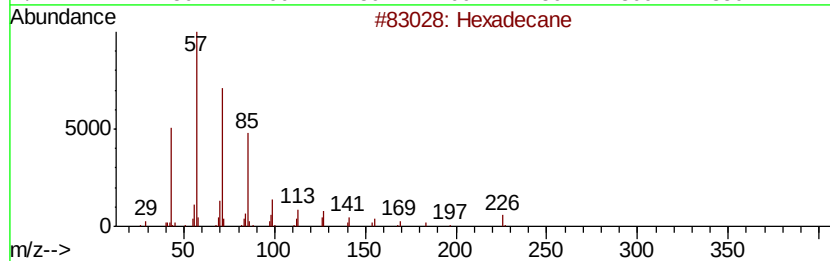
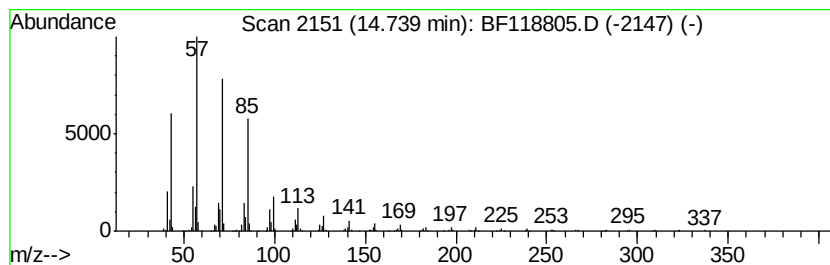
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	5.98 ng	770021	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	94
2		Eicosane	282	C20H42	000112-95-8	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020420\
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Acq On : 4 Feb 2020 16:50
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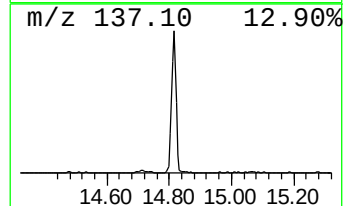
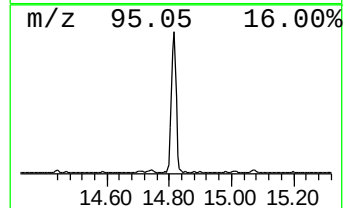
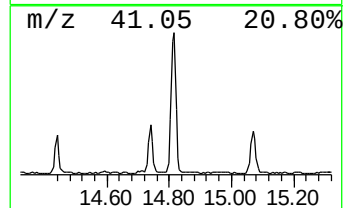
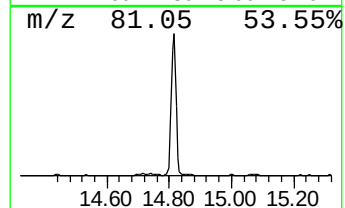
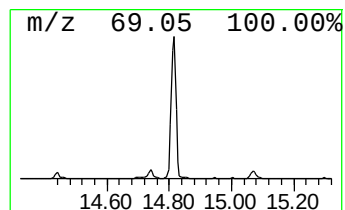
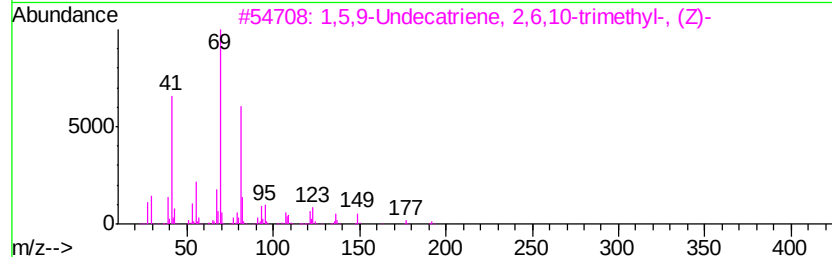
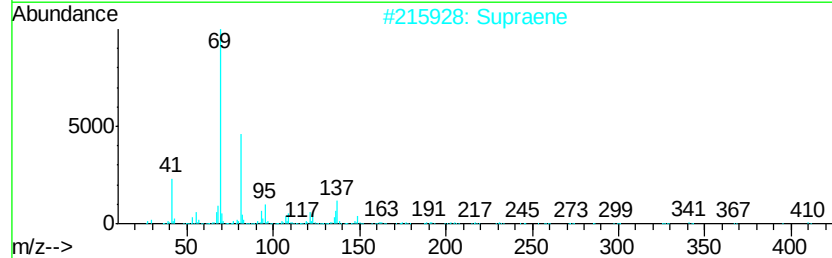
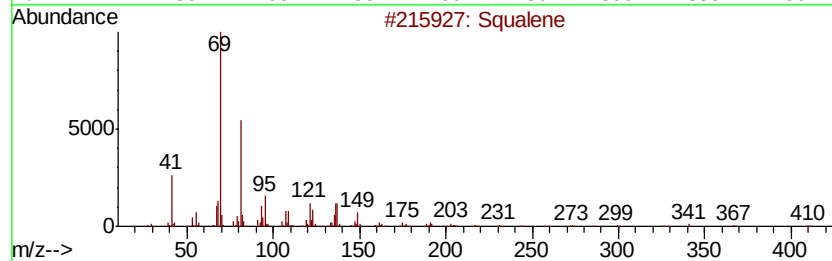
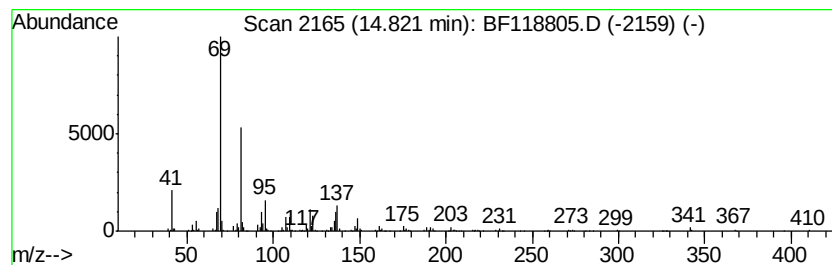
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	12.62 ng	1625140	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	96
2		Supraene	410	C30H50	007683-64-9	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020420\
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Acq On : 4 Feb 2020 16:50
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

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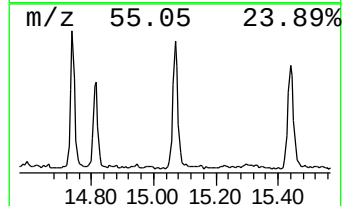
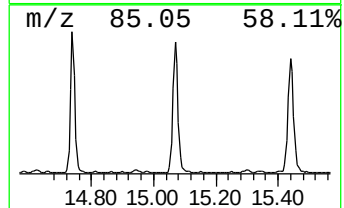
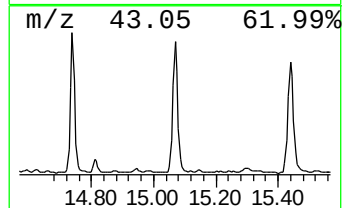
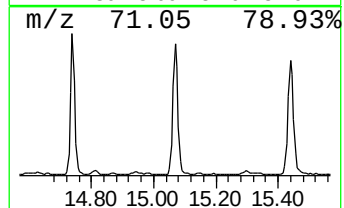
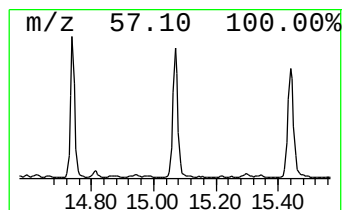
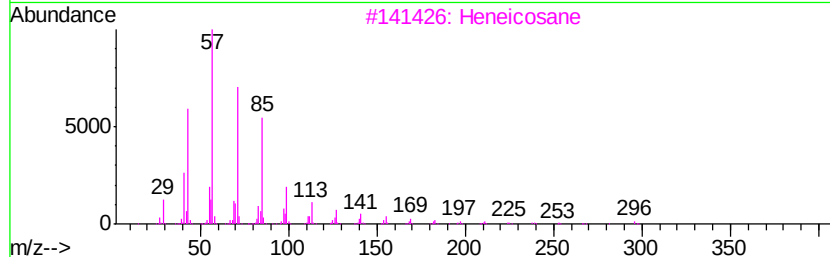
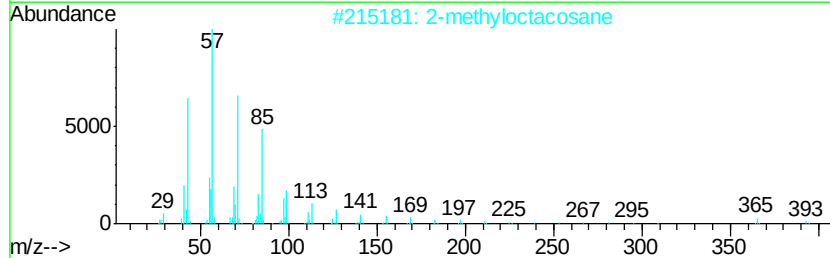
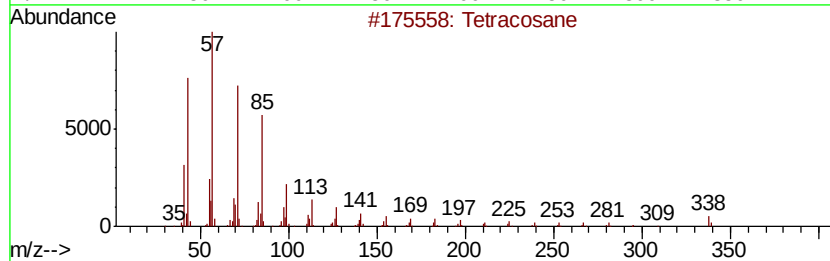
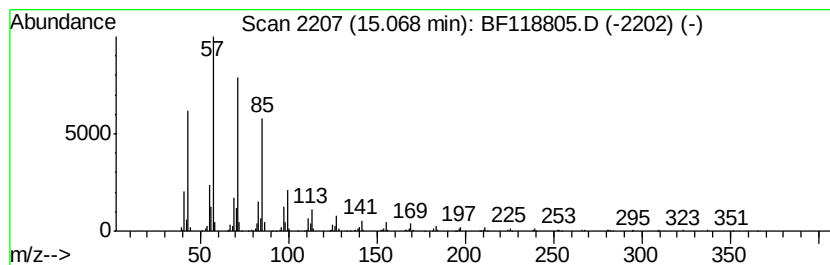
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	6.88 ng	886318	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020420\
Data File : BF118805.D
Acq On : 4 Feb 2020 16:50
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

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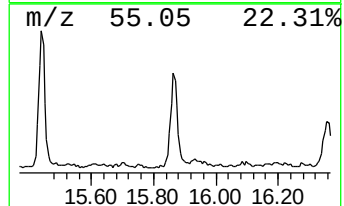
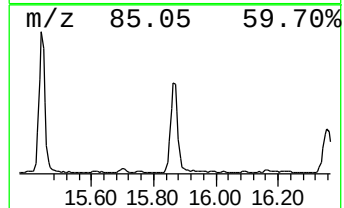
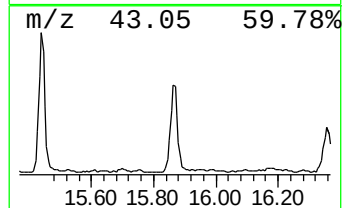
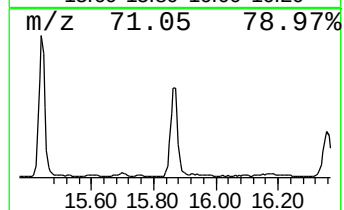
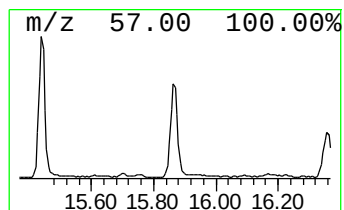
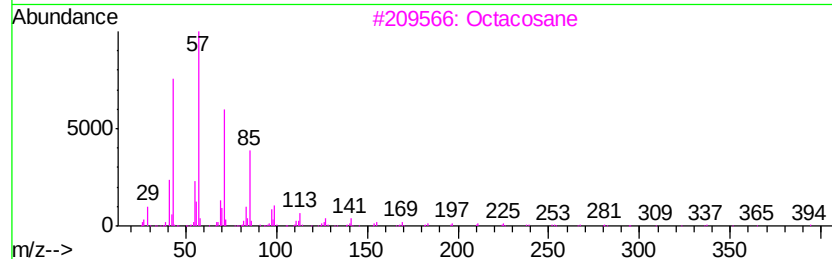
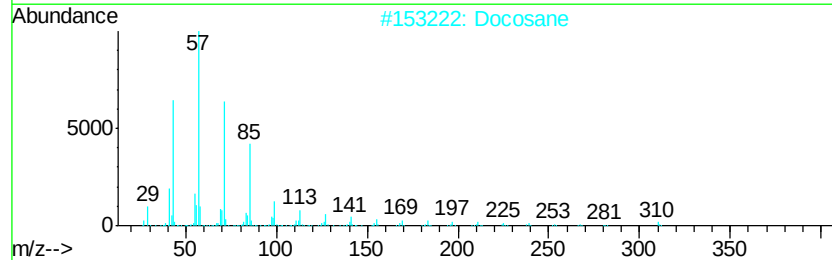
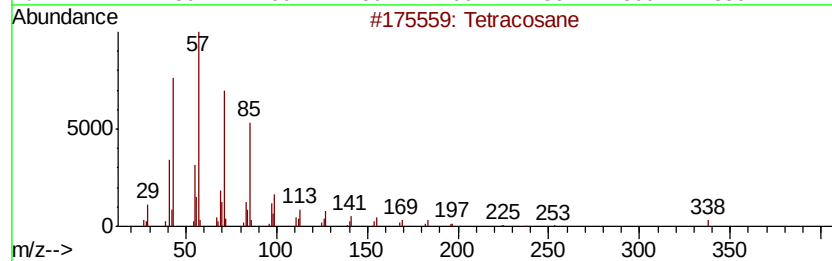
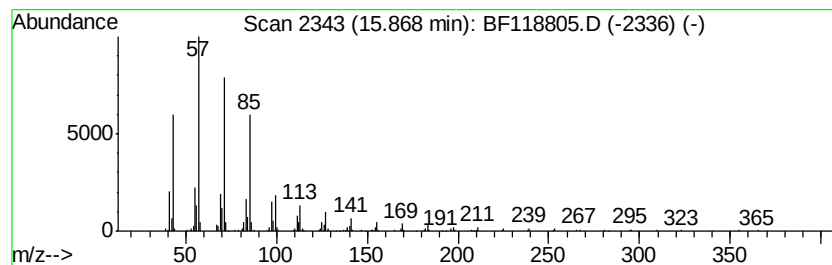
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	5.48 ng	705885	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Docosane	310	C22H46	000629-97-0	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020420\
Data File : BF118805.D
Acq On : 4 Feb 2020 16:50
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

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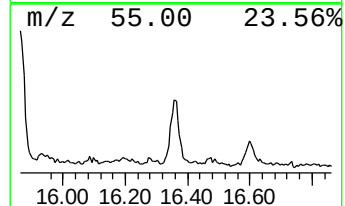
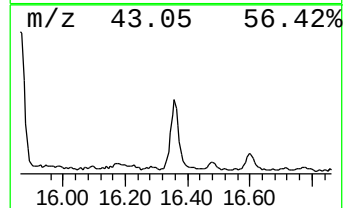
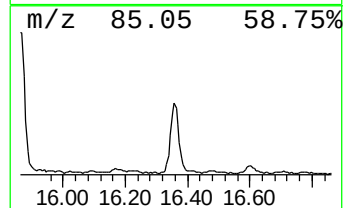
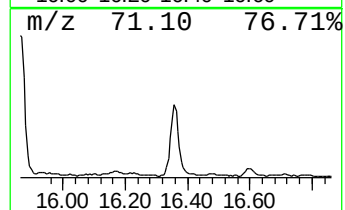
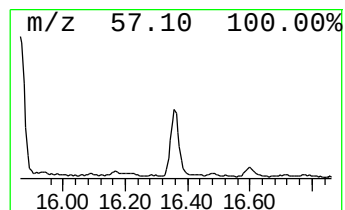
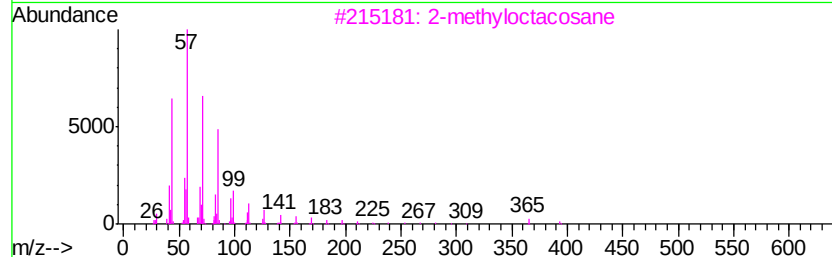
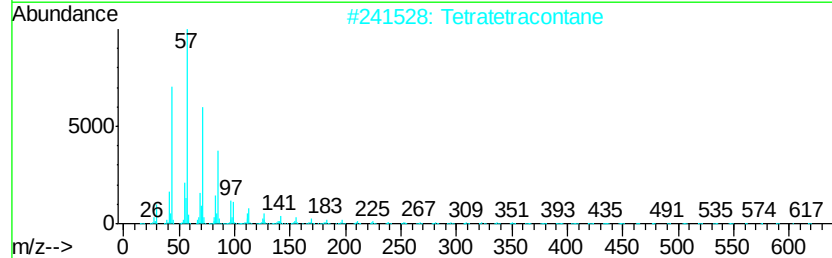
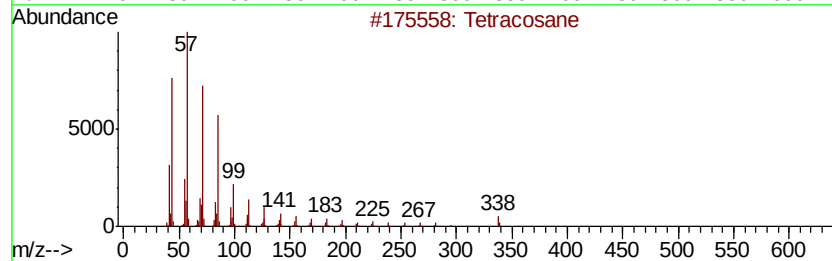
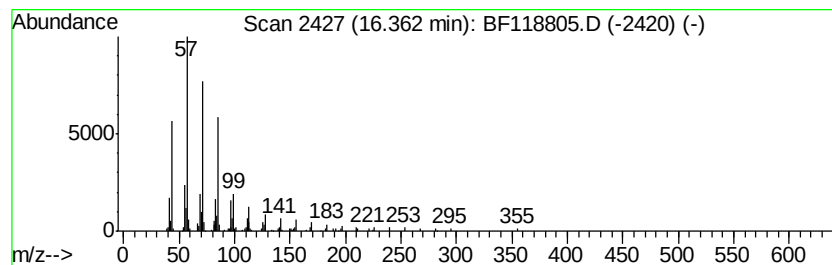
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetratetracontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	3.30 ng	425142	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020420\
Data File : BF118805.D
Acq On : 4 Feb 2020 16:50
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF020320.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
2,4,7,9-Tetrameth...	9.29	5.1 ng		727917	3	9.85	2874150	20.0
n-Hexadecanoic acid	11.86	11.5 ng		1786340	4	11.33	3116170	20.0
Octadecanoic acid	12.65	4.5 ng		690351	5	13.96	3036510	20.0
1-Heneicosanol	13.82	5.3 ng		799876	5	13.96	3036510	20.0
Heneicosane	14.13	2.3 ng		346098	5	13.96	3036510	20.0
Hexacosane	14.44	3.9 ng		594591	5	13.96	3036510	20.0
Hexadecane	14.74	6.0 ng		770021	6	15.40	2574990	20.0
Squalene	14.82	12.6 ng		1625140	6	15.40	2574990	20.0
2-methyloctacosane	15.07	6.9 ng		886318	6	15.40	2574990	20.0
Docosane	15.87	5.5 ng		705885	6	15.40	2574990	20.0
Tetratetracontane	16.36	3.3 ng		425142	6	15.40	2574990	20.0