

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040820\
 Data File : BF119881.D
 Acq On : 9 Apr 2020 20:33
 Operator : MA/SJ
 Sample : L2166-12
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-52-46-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-BF040820.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	4.975	483	491	500	rVB	90552	111588	3.11%	0.375%
2	5.381	555	560	563	rBV	3657211	3585079	100.00%	12.059%
3	6.404	728	734	737	rBV	3639909	3529523	98.45%	11.872%
4	6.769	792	796	799	rBV	1400688	1130999	31.55%	3.804%
5	6.928	818	823	826	rBV	3076440	2950559	82.30%	9.925%
6	7.333	886	892	895	rBV	2529373	2302566	64.23%	7.745%
7	8.051	1010	1014	1018	rBV	1486115	1225562	34.19%	4.122%
8	9.133	1193	1198	1201	rBV	4376060	3523295	98.28%	11.851%
9	9.527	1261	1265	1268	rBV	483884	395514	11.03%	1.330%
10	9.810	1309	1313	1316	rBV	1671884	1308595	36.50%	4.402%
11	10.598	1443	1447	1450	rBV	2373893	1973731	55.05%	6.639%
12	11.298	1562	1566	1569	rBV	1241767	1114725	31.09%	3.750%
13	11.827	1652	1656	1664	rBV	307369	302266	8.43%	1.017%
14	12.557	1777	1780	1783	rVB	78960	63548	1.77%	0.214%
15	12.616	1787	1790	1797	rBV	113752	154815	4.32%	0.521%
16	12.710	1803	1806	1808	rBV	62125	49981	1.39%	0.168%
17	12.886	1831	1836	1839	rBV	2767123	2458264	68.57%	8.269%
18	13.274	1899	1902	1908	rVB2	47301	44881	1.25%	0.151%
19	13.368	1914	1918	1922	rVB	250843	208131	5.81%	0.700%
20	13.463	1931	1934	1937	rBV	59266	57716	1.61%	0.194%
21	13.798	1987	1991	2001	rBV	233213	429986	11.99%	1.446%
22	13.933	2010	2014	2018	rBV	1056672	984598	27.46%	3.312%
23	14.110	2041	2044	2050	rVB	96137	96345	2.69%	0.324%
24	14.415	2092	2096	2098	rBV	122338	118043	3.29%	0.397%
25	14.692	2140	2143	2145	rBV	123100	120272	3.35%	0.405%
26	14.715	2145	2147	2150	rVB	119009	101202	2.82%	0.340%
27	15.045	2200	2203	2211	rVB	141738	146357	4.08%	0.492%
28	15.374	2255	2259	2263	rBV	746502	855554	23.86%	2.878%
29	15.415	2263	2266	2271	rVB	129764	173312	4.83%	0.583%
30	15.839	2334	2338	2341	rBV2	76283	105108	2.93%	0.354%
31	16.327	2417	2421	2426	rVB2	60186	106693	2.98%	0.359%

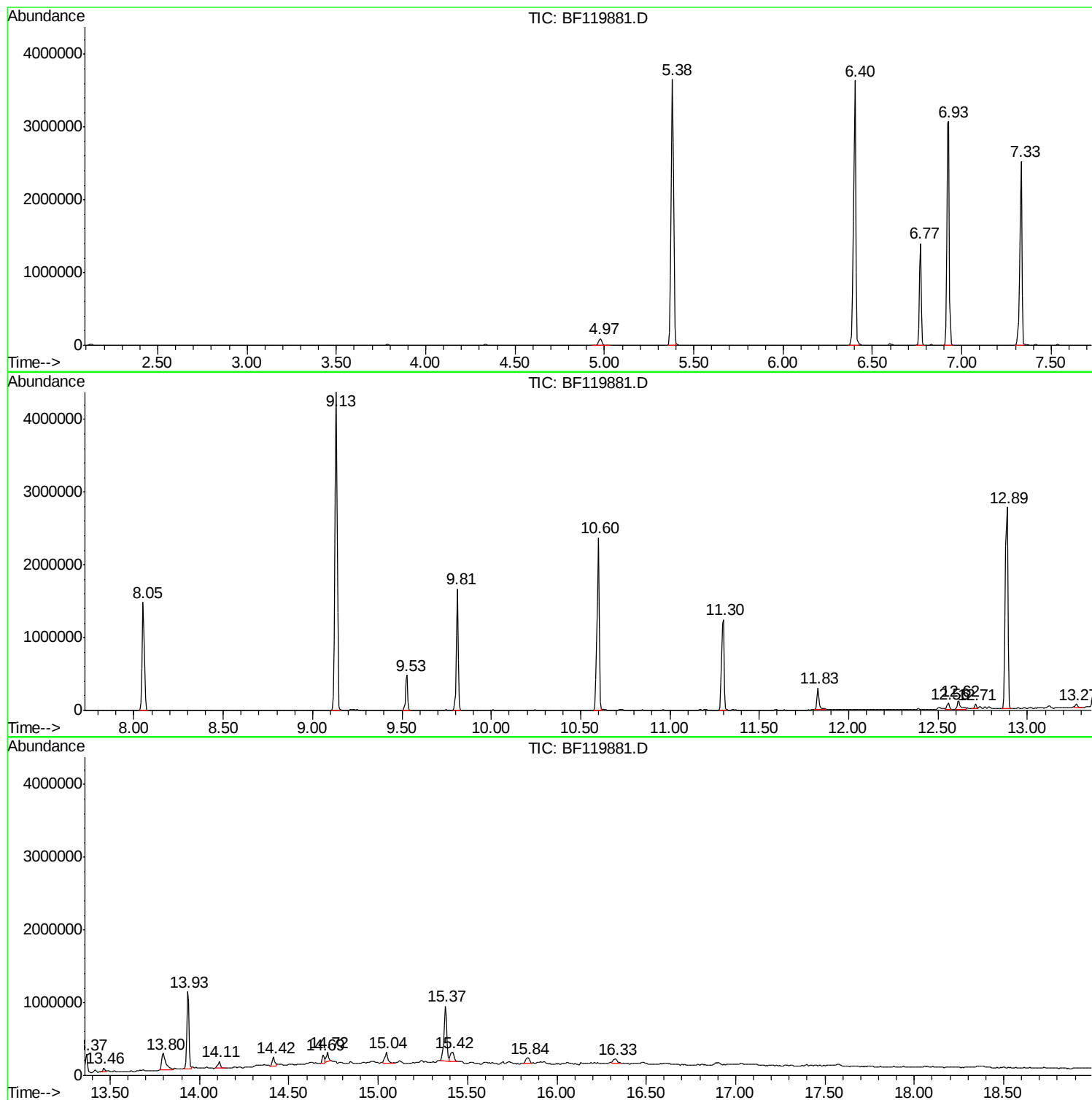
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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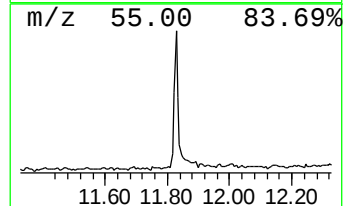
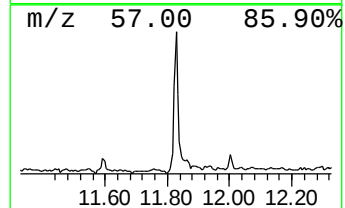
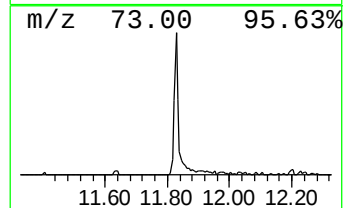
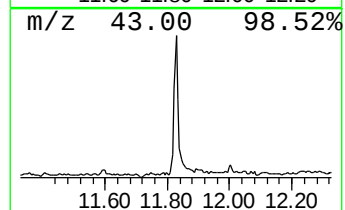
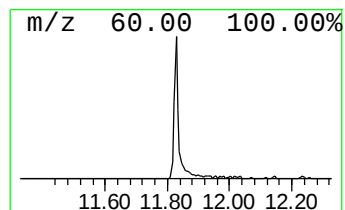
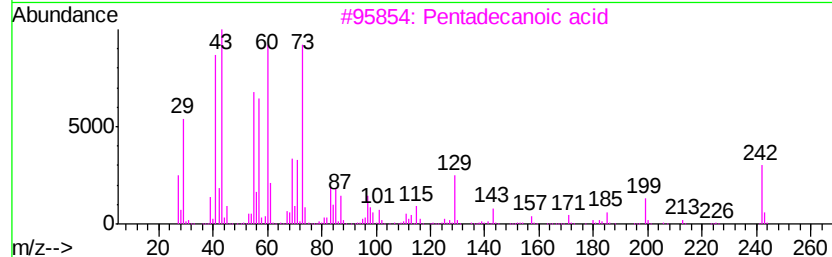
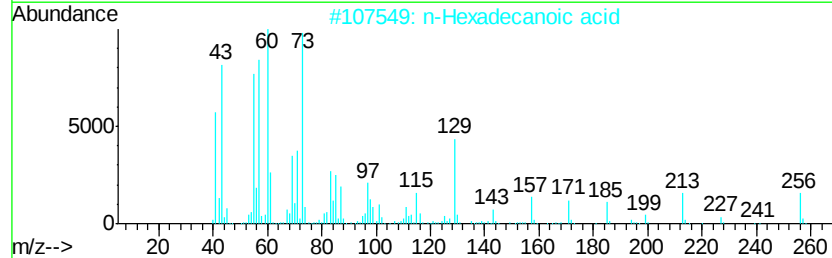
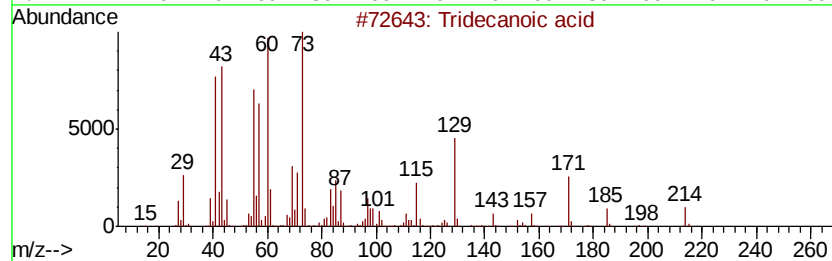
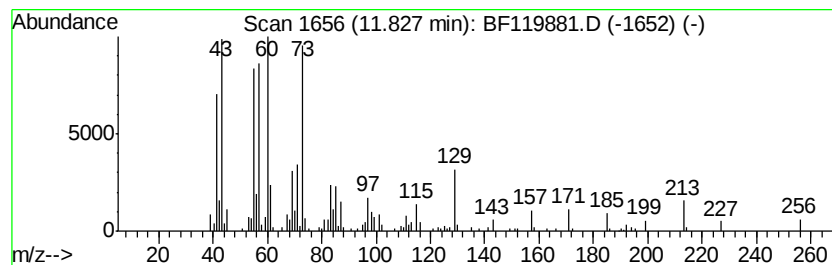
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.83	5.42 ng	302266	Phenanthrene-d10		11.30
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72



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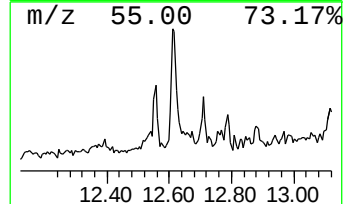
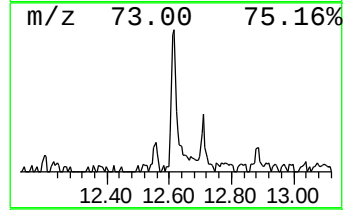
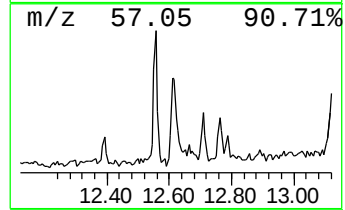
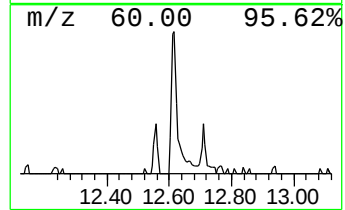
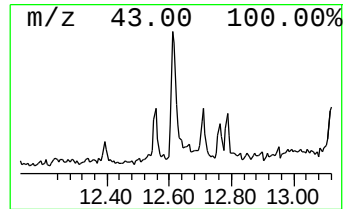
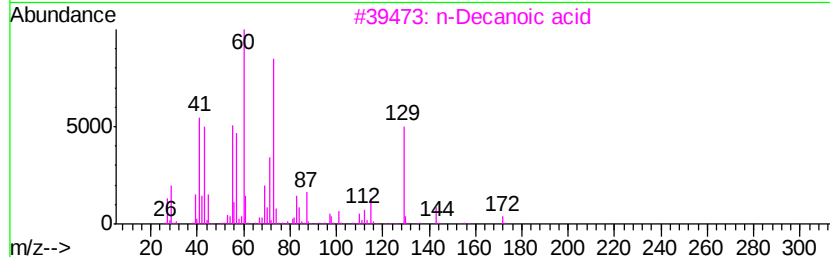
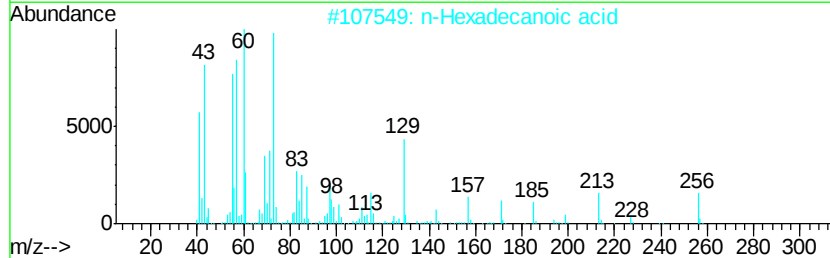
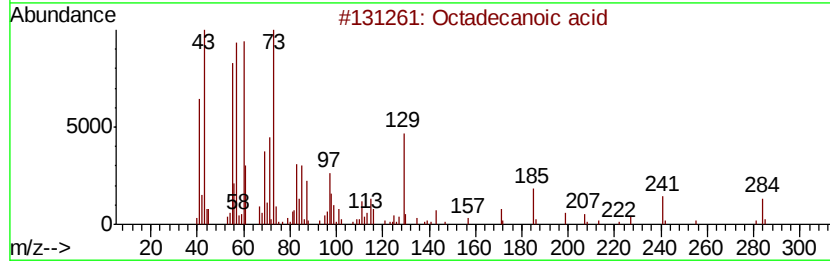
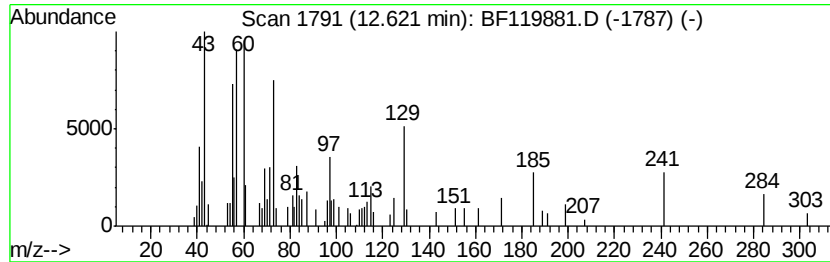
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	3.14 ng	154815	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		n-Decanoic acid	172	C10H20O2	000334-48-5	86
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	46
5		Benzamide, 4-butoxy-N-[2-(2-thie...	303	C17H21N02S	1000319-87-5	46



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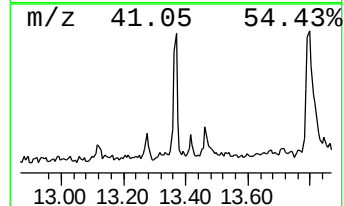
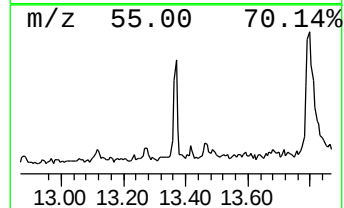
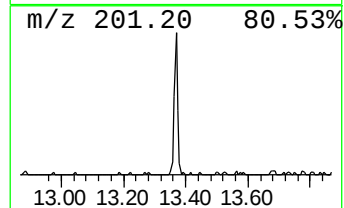
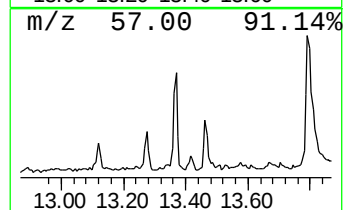
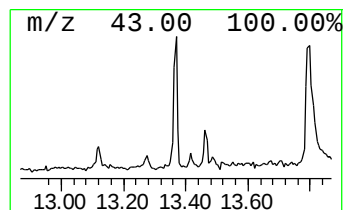
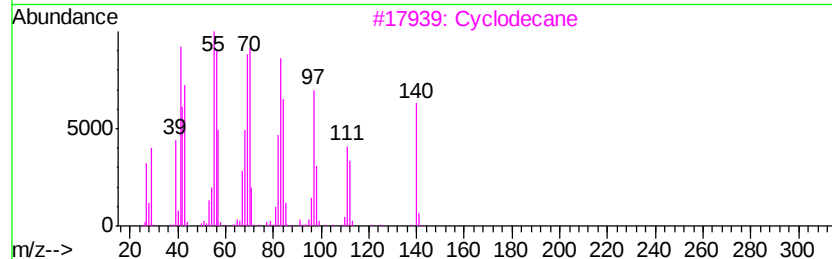
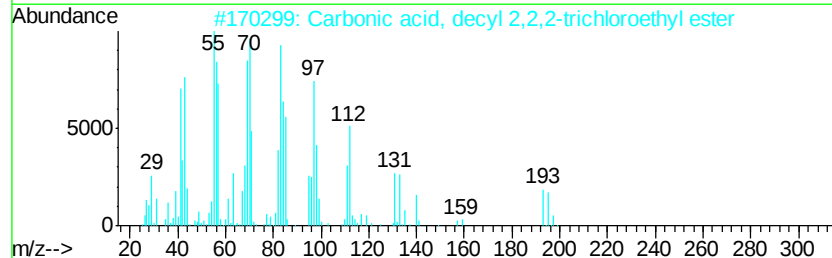
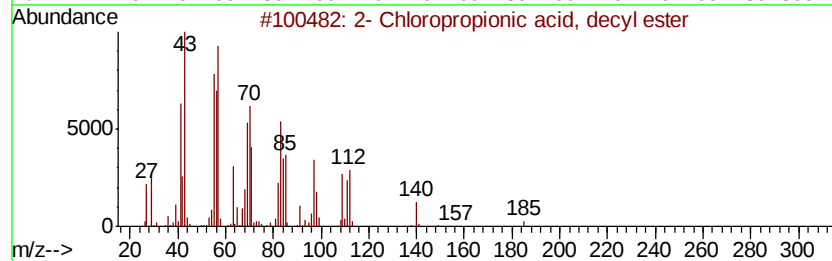
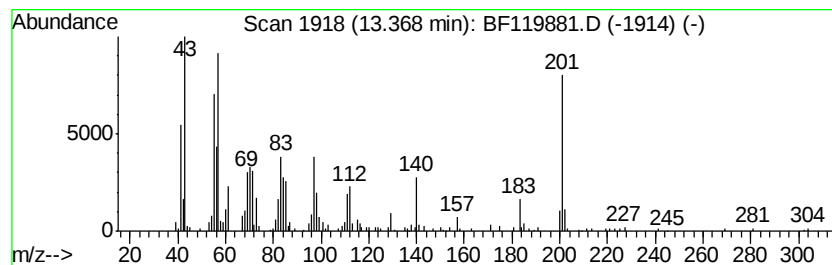
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	4.23 ng	208131	Chrysene-d12	13.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-		Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	46
2			Carbonic acid, decyl 2,2,2-trich...	332	C13H23Cl3O3	1000314-55-6	46
3			Cyclodecane	140	C10H20	000293-96-9	45
4			Cyclooctane	112	C8H16	000292-64-8	42
5			1-Docosene	308	C22H44	001599-67-3	38



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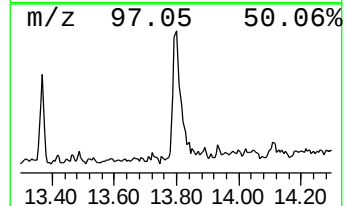
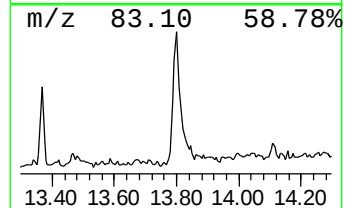
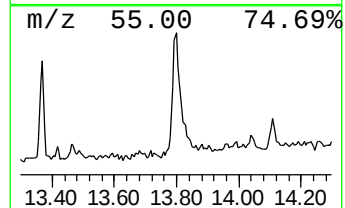
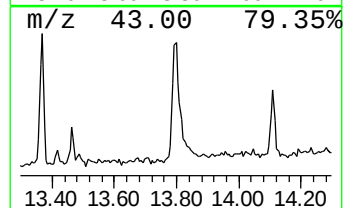
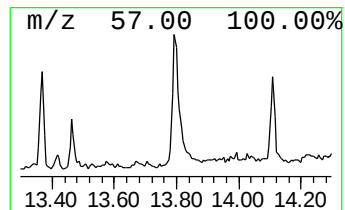
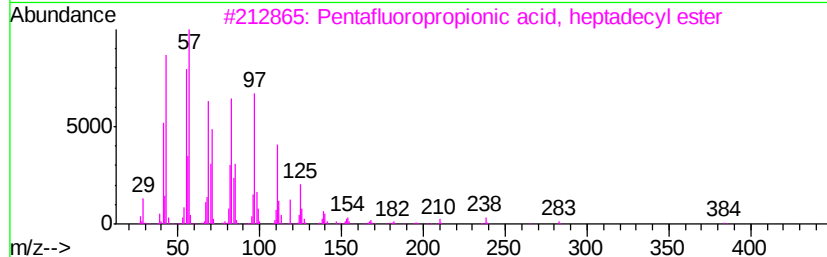
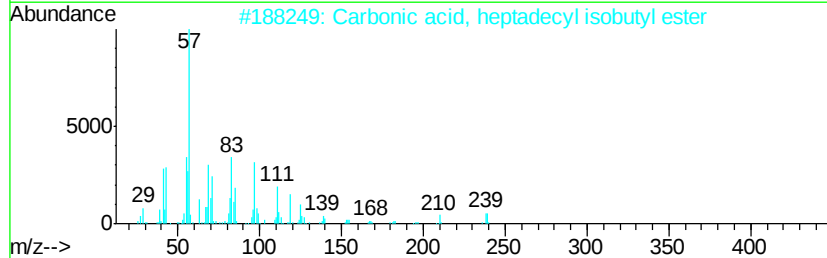
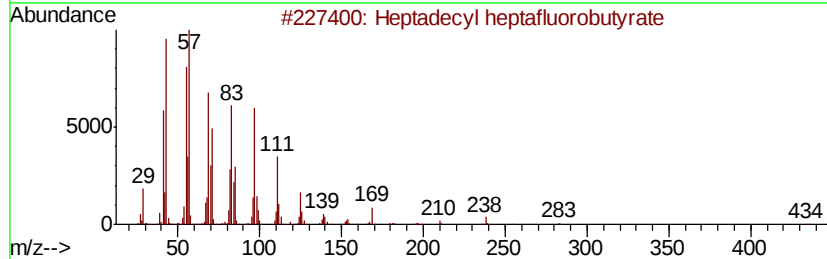
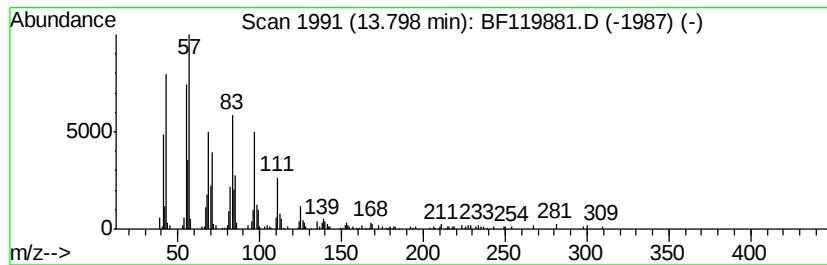
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.80	8.73 ng	429986	Chrysene-d12		13.93	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5		Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91



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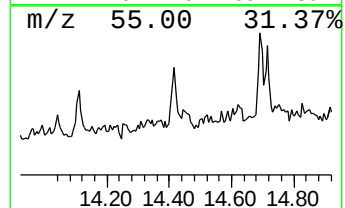
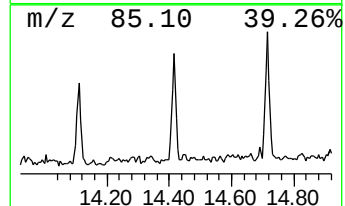
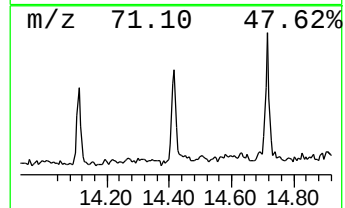
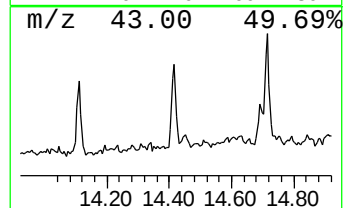
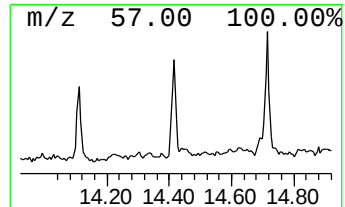
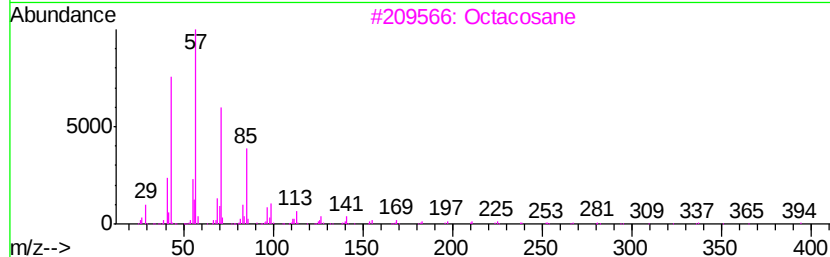
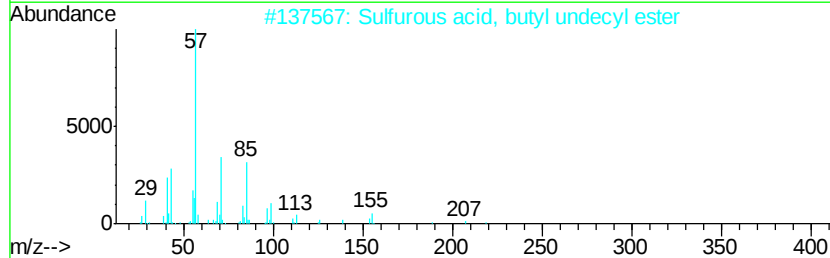
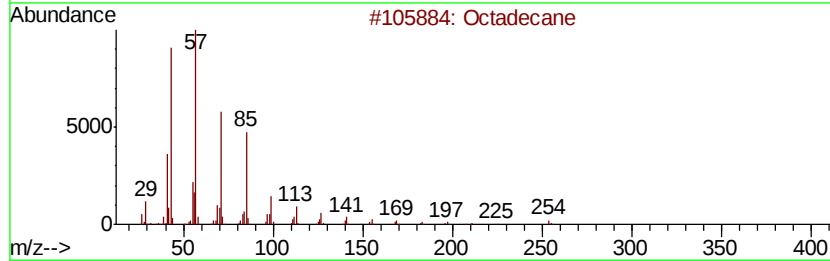
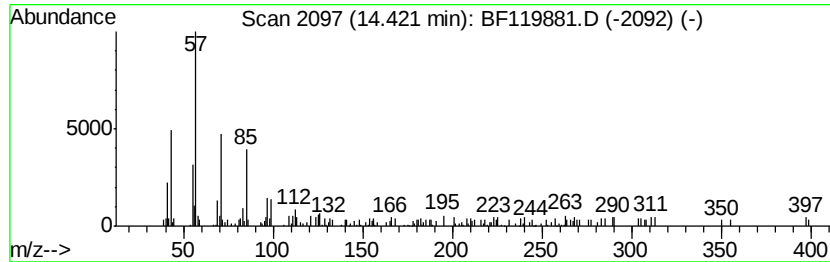
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	2.40 ng	118043	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	89
2		Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	86
3		Octacosane	394	C28H58	000630-02-4	58
4		Heptane, 4-ethyl-	128	C9H20	002216-32-2	46
5		Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	46



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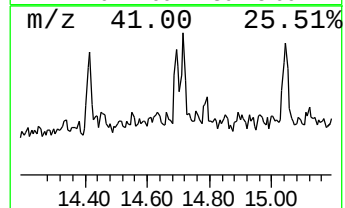
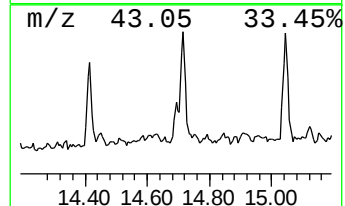
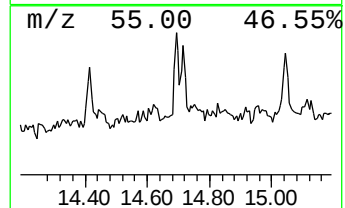
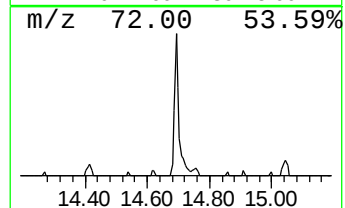
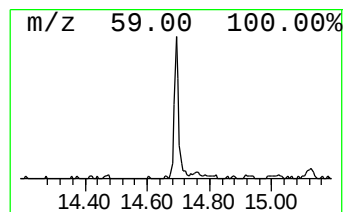
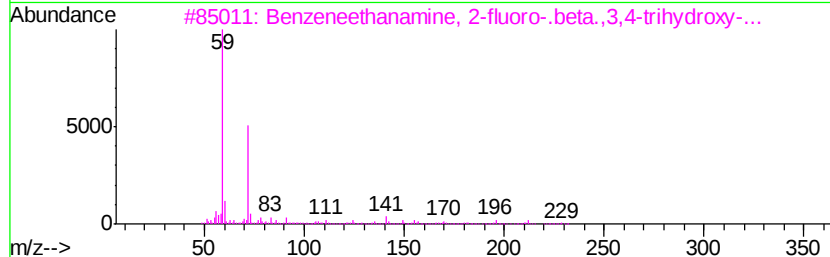
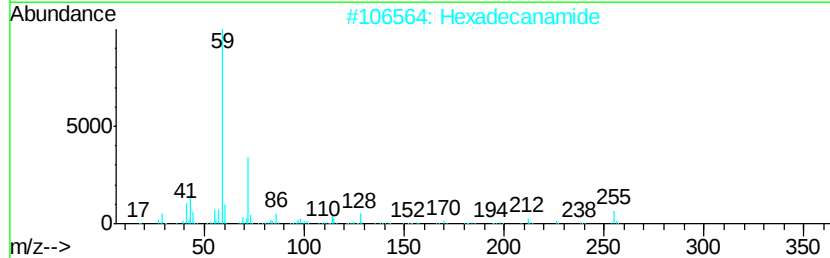
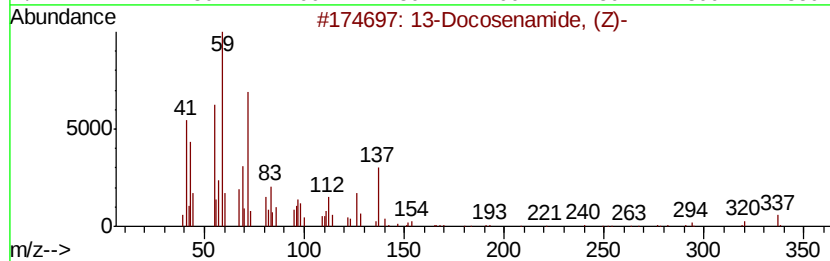
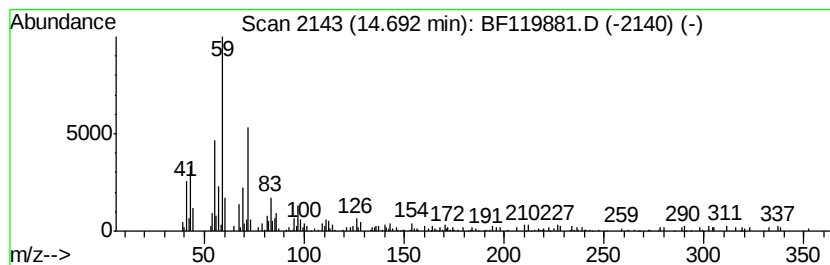
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.81 ng	120272	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2		Hexadecanamide	255	C16H33NO	000629-54-9	59
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
4		Tetradecanamide	227	C14H29NO	000638-58-4	58
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119881.D
Acq On : 9 Apr 2020 20:33
Operator : MA/SJ
Sample : L2166-12
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-52-46-COMP

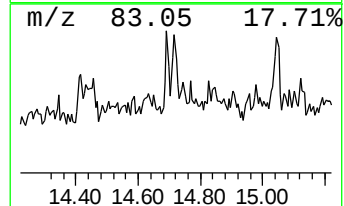
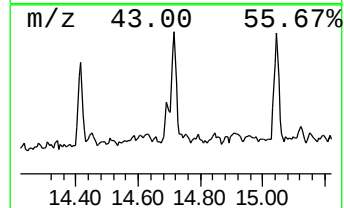
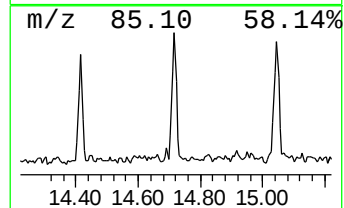
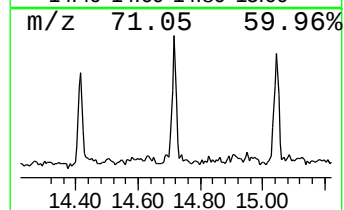
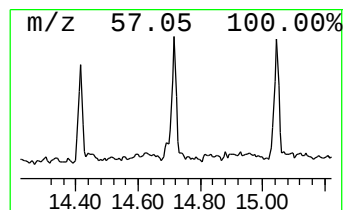
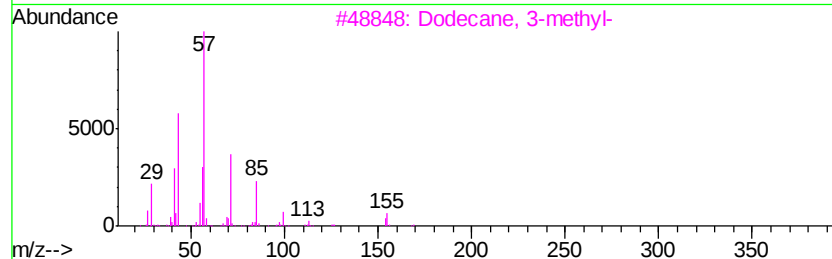
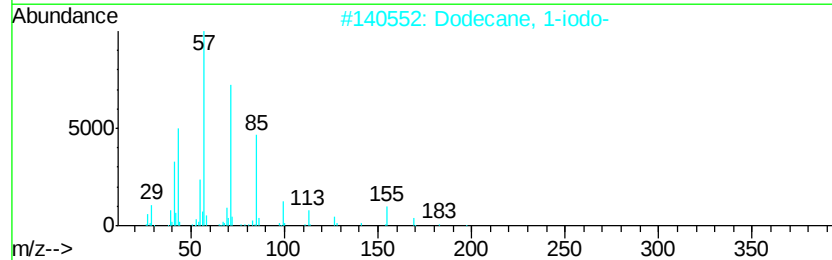
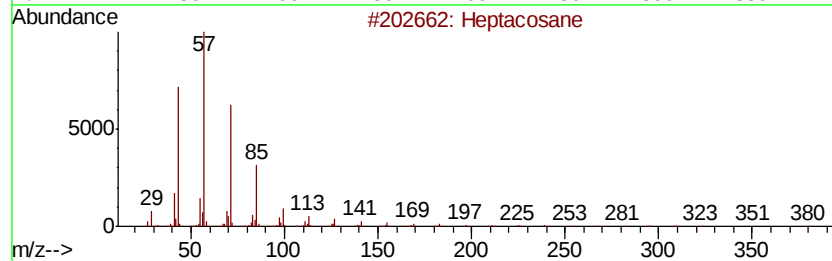
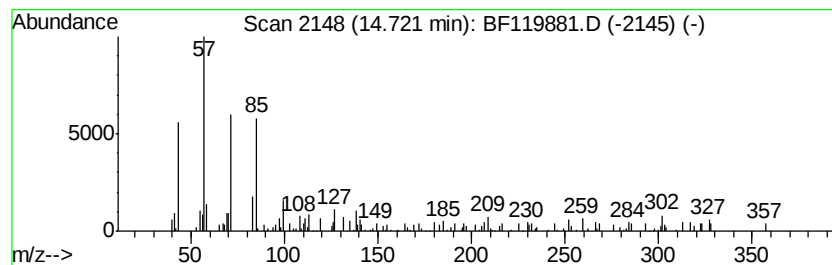
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.37 ng	101202	Perylene-d12	15.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	87
2	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	72
3	Dodecane, 3-methyl-		184	C13H28	017312-57-1	72
4	2-Bromotetradecane		276	C14H29Br	074036-95-6	64
5	Eicosane		282	C20H42	000112-95-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119881.D
Acq On : 9 Apr 2020 20:33
Operator : MA/SJ
Sample : L2166-12
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-52-46-COMP

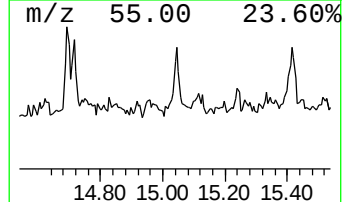
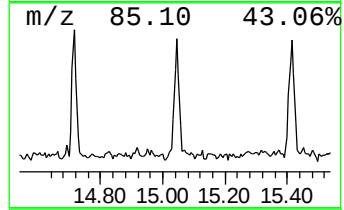
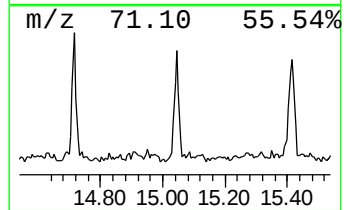
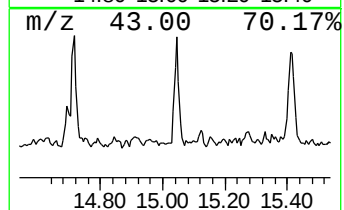
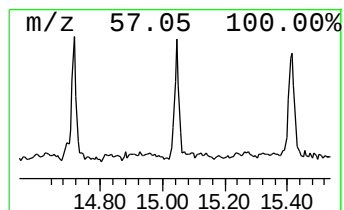
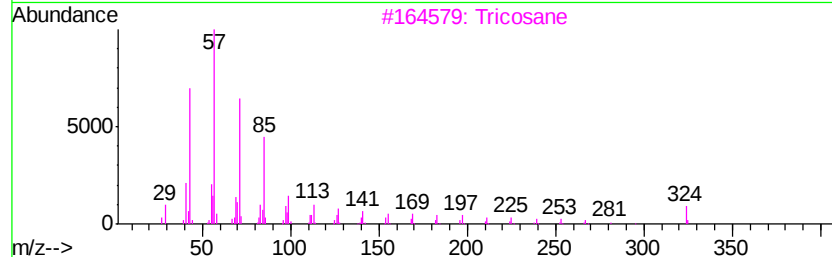
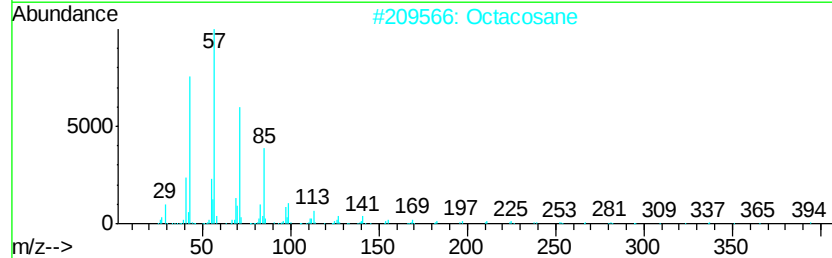
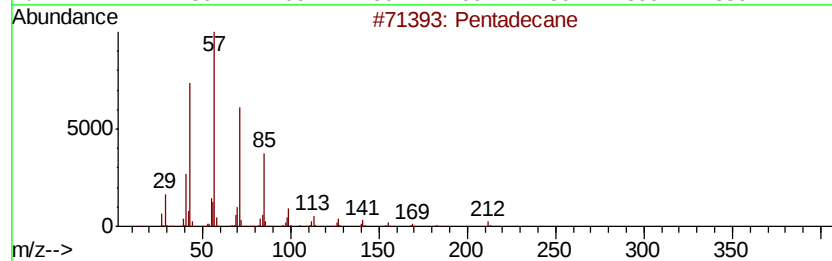
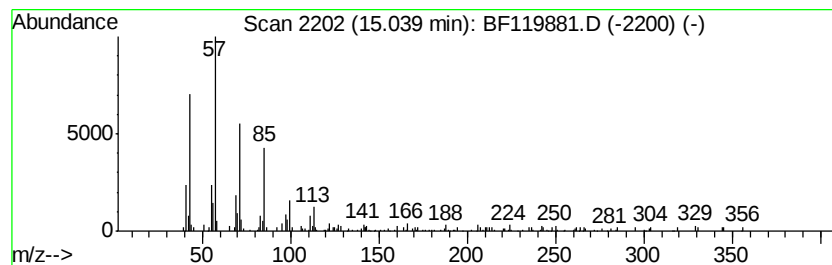
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	3.42 ng	146357	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	91
2		Octacosane	394	C28H58	000630-02-4	87
3		Tricosane	324	C23H48	000638-67-5	87
4		Heneicosane	296	C21H44	000629-94-7	83
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119881.D
Acq On : 9 Apr 2020 20:33
Operator : MA/SJ
Sample : L2166-12
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-52-46-COMP

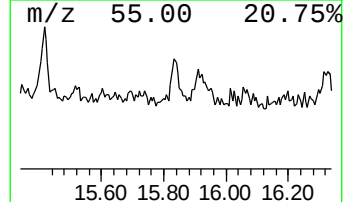
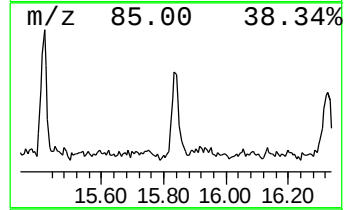
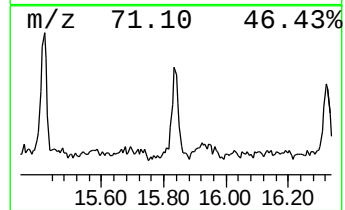
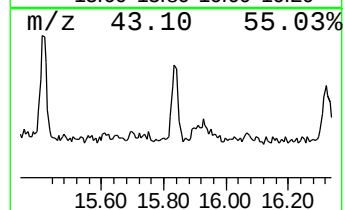
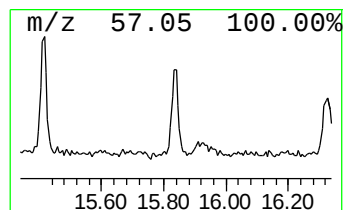
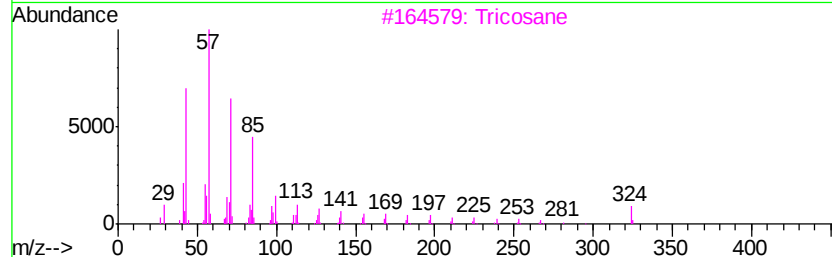
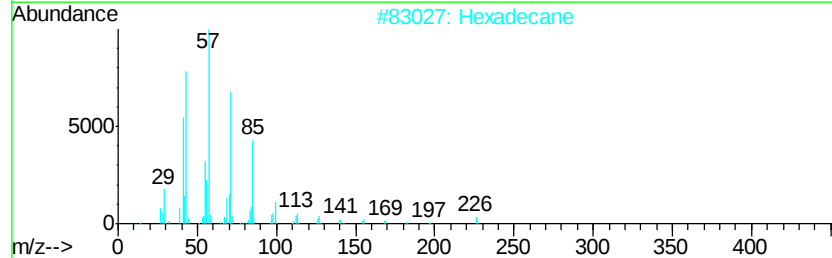
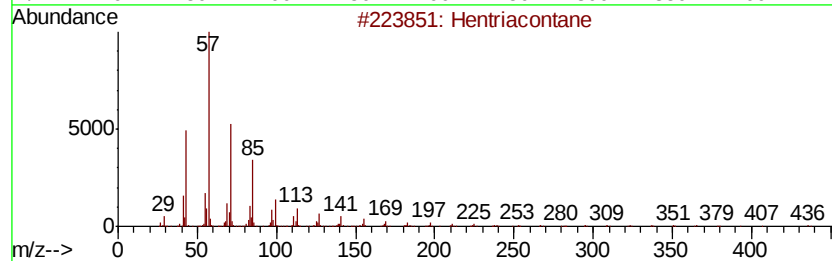
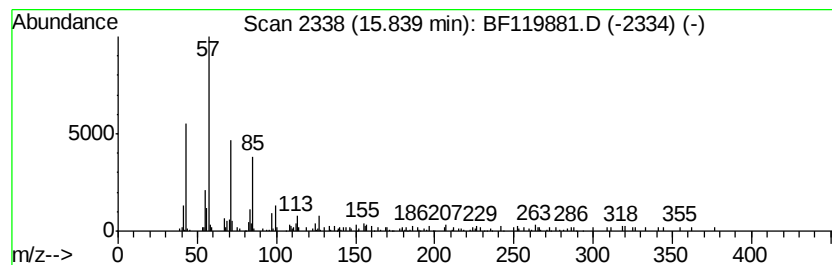
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.46 ng	105108	Perylene-d12	15.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	86
2			Hexadecane	226	C16H34	000544-76-3	80
3			Tricosane	324	C23H48	000638-67-5	78
4			2-methyloctacosane	408	C29H60	1000376-72-8	72
5			Undecane, 5-ethyl-	184	C13H28	017453-94-0	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
 Data File : BF119881.D
 Acq On : 9 Apr 2020 20:33
 Operator : MA/SJ
 Sample : L2166-12
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

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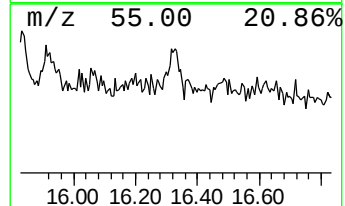
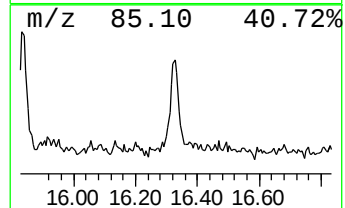
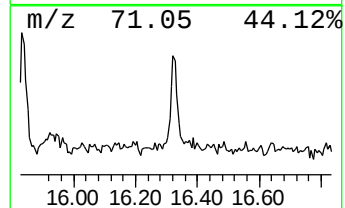
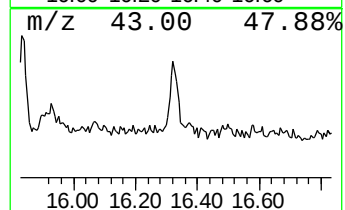
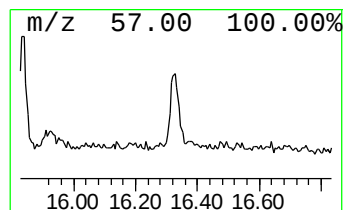
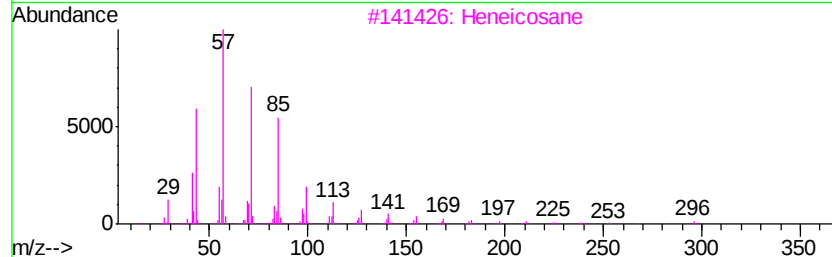
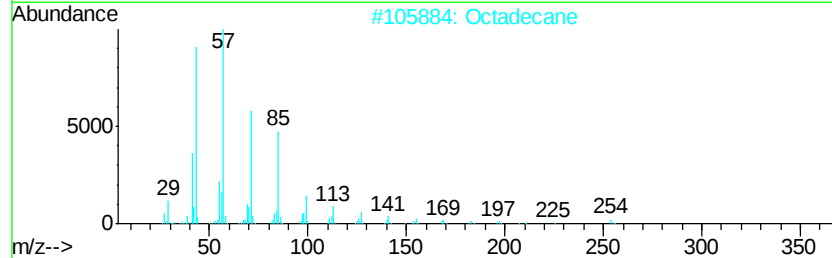
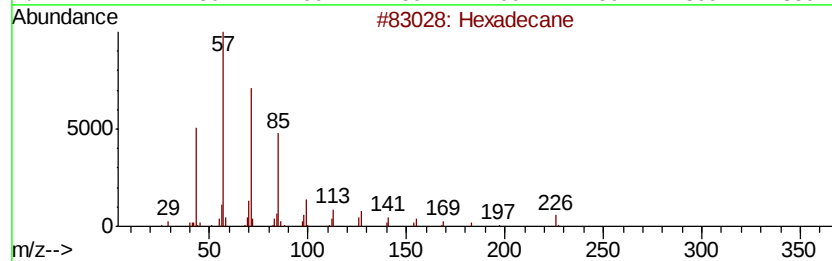
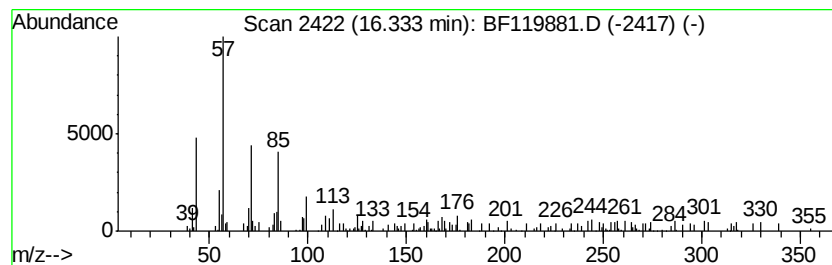
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	2.49 ng	106693	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	78
2		Octadecane	254	C18H38	000593-45-3	78
3		Heneicosane	296	C21H44	000629-94-7	53
4		Tetracosane	338	C24H50	000646-31-1	49
5		Tetratetracontane	619	C44H90	007098-22-8	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040820\
Data File : BF119881.D
Acq On : 9 Apr 2020 20:33
Operator : MA/SJ
Sample : L2166-12
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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
Tridecanoic acid	11.83	5.4 ng		302266	4	11.30	1114730	20.0
Octadecanoic acid	12.62	3.1 ng		154815	5	13.93	984598	20.0
unknown13.37	13.37	4.2 ng		208131	5	13.93	984598	20.0
Heptadecyl heptaf...	13.80	8.7 ng		429986	5	13.93	984598	20.0
Octadecane	14.42	2.4 ng		118043	5	13.93	984598	20.0
13-Docosenamide, ...	14.69	2.8 ng		120272	6	15.37	855554	20.0
Heptacosane	14.72	2.4 ng		101202	6	15.37	855554	20.0
Pentadecane	15.04	3.4 ng		146357	6	15.37	855554	20.0
Hentriacontane	15.84	2.5 ng		105108	6	15.37	855554	20.0
Hexadecane	16.33	2.5 ng		106693	6	15.37	855554	20.0