

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
 Data File : BF135708.D
 Acq On : 11 Oct 2023 12:37
 Operator : CG\JU
 Sample : 04656-13
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-104I

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135708.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	486	489	495	rBV2	23194	43660	2.05%	0.359%
2	5.381	557	560	585	rBV	283704	477922	22.44%	3.925%
3	6.392	730	732	750	rBV	310733	477454	22.42%	3.921%
4	6.739	787	791	800	rVB	614753	537264	25.23%	4.412%
5	7.304	884	887	898	rBV	712945	648971	30.47%	5.330%
6	8.016	1005	1008	1016	rBV	756404	656458	30.82%	5.391%
7	9.092	1187	1191	1201	rBV	1397730	1146718	53.84%	9.418%
8	9.775	1303	1307	1316	rVB	880064	742440	34.86%	6.097%
9	10.192	1373	1378	1386	rVB2	33774	56772	2.67%	0.466%
10	10.575	1439	1443	1453	rBV	218481	256315	12.04%	2.105%
11	11.269	1557	1561	1571	rBV	897442	786818	36.94%	6.462%
12	11.798	1647	1651	1670	rVB	1015366	1508700	70.84%	12.390%
13	12.451	1759	1762	1766	rBV2	46001	58821	2.76%	0.483%
14	12.510	1766	1772	1776	rVV6	90434	244155	11.46%	2.005%
15	12.592	1778	1786	1799	rVB	1344592	2129744	100.00%	17.491%
16	12.863	1828	1832	1836	rBV	1116090	947464	44.49%	7.781%
17	13.427	1924	1928	1937	rBV3	19421	32899	1.54%	0.270%
18	13.592	1948	1956	1965	rBV4	35122	94453	4.43%	0.776%
19	13.933	2010	2014	2025	rBV	478449	472575	22.19%	3.881%
20	14.286	2069	2074	2081	rBV2	42675	71623	3.36%	0.588%
21	14.698	2140	2144	2148	rVB3	22412	25530	1.20%	0.210%
22	14.868	2165	2173	2179	rBV3	37304	86473	4.06%	0.710%
23	15.033	2198	2201	2206	rVB2	28191	36141	1.70%	0.297%
24	15.404	2260	2264	2276	rBV	363912	527556	24.77%	4.333%
25	15.510	2277	2282	2290	rVB4	23637	60042	2.82%	0.493%
26	15.839	2335	2338	2343	rVB3	18061	27678	1.30%	0.227%
27	16.345	2422	2424	2429	rVB5	19413	21640	1.02%	0.178%

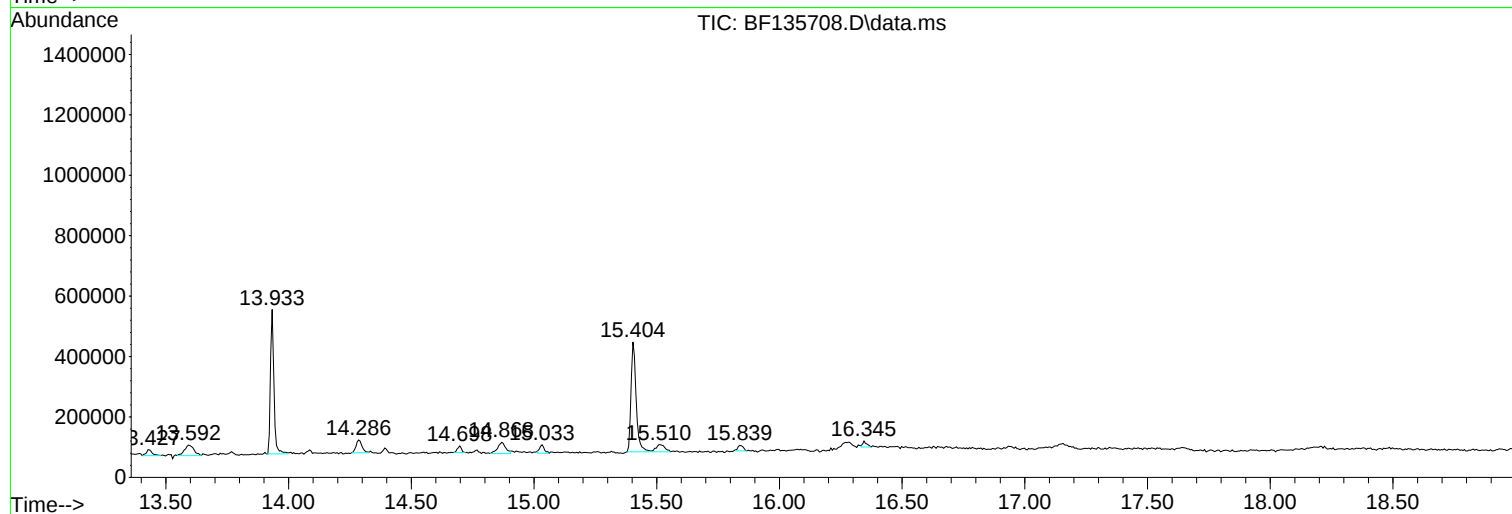
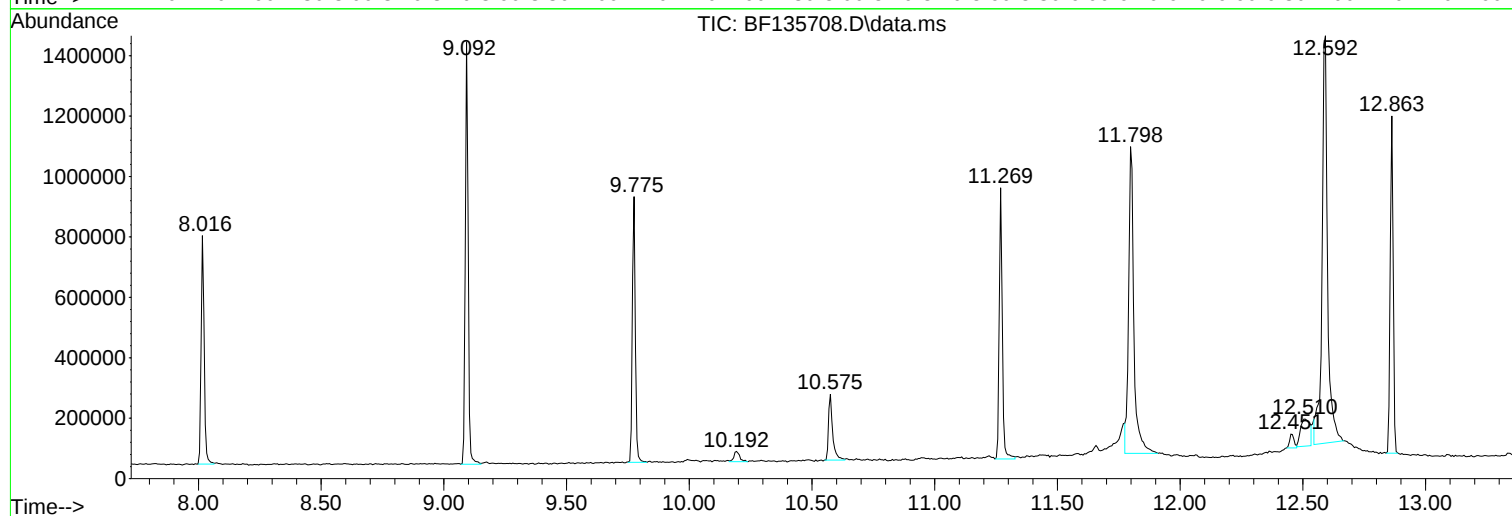
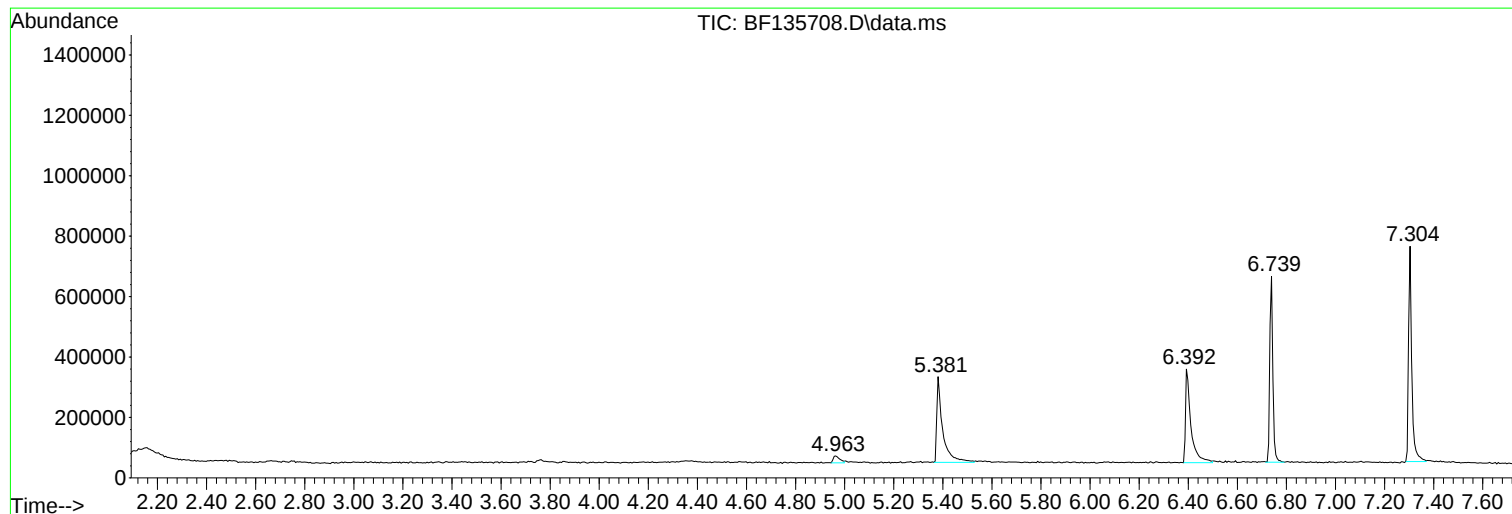
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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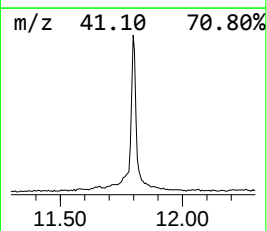
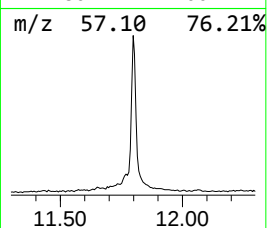
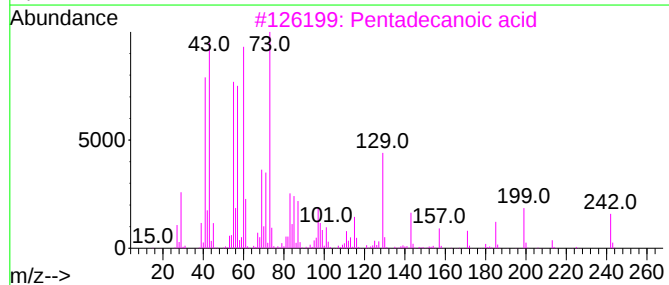
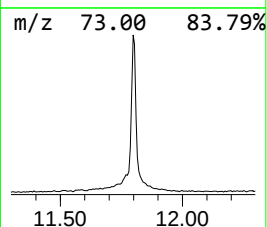
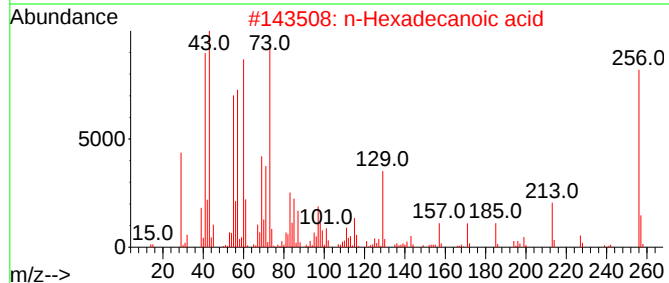
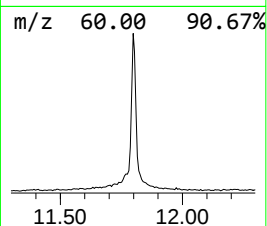
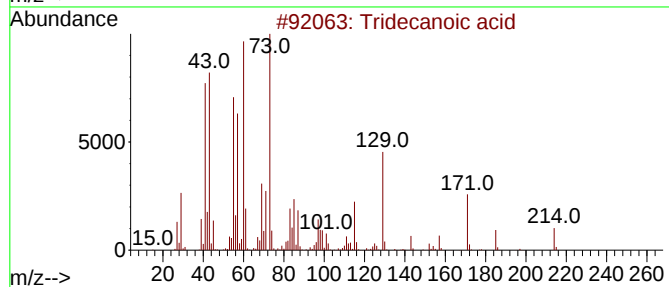
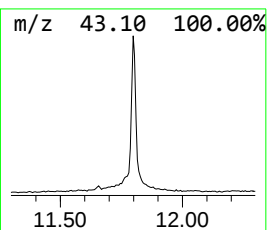
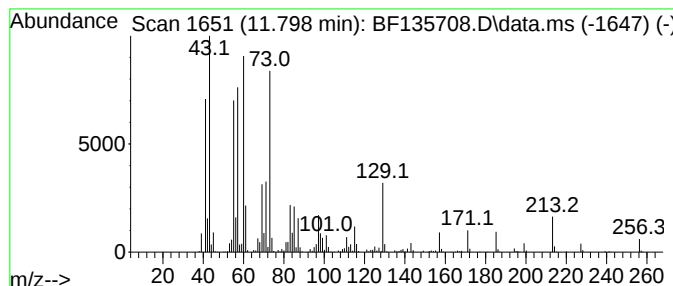
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	38.35 ng	1508700	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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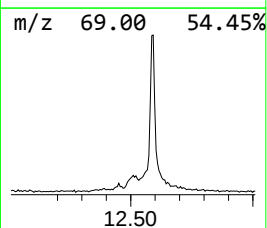
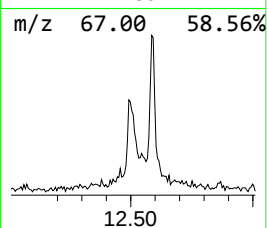
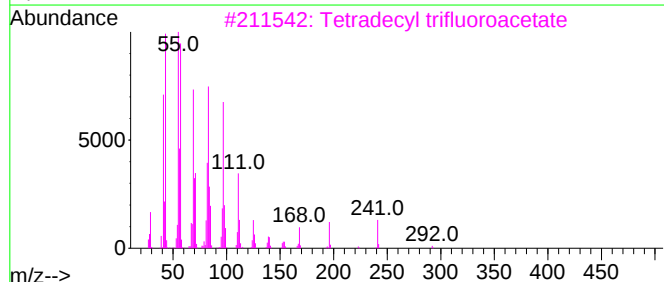
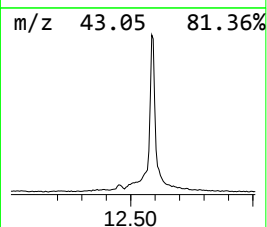
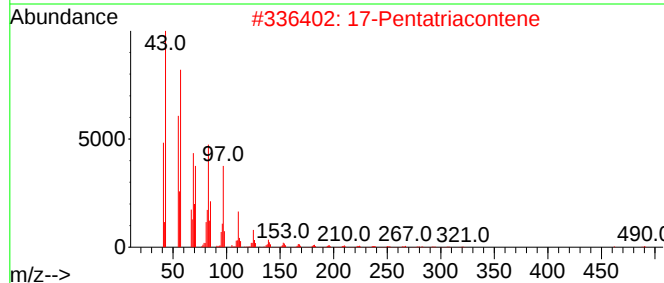
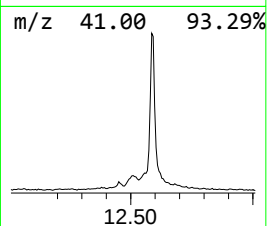
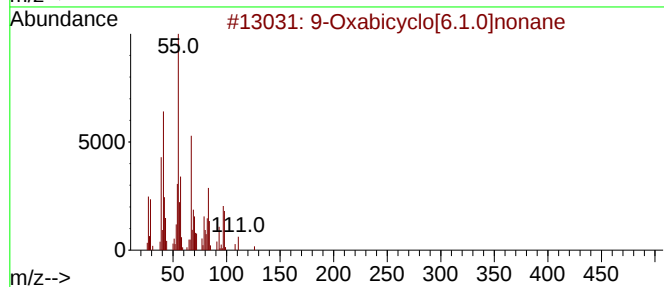
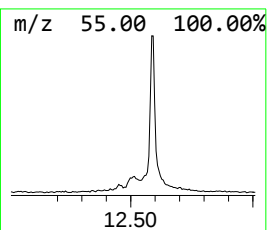
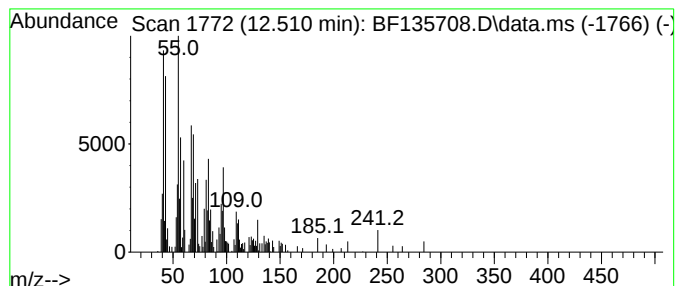
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown12.510 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	6.21 ng	244155	Phenanthrene-d10	11.269

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Oxabicyclo[6.1.0]nonane	126	C8H14O	000286-62-4	38
2		17-Pentatriacontene	491	C35H70	006971-40-0	30
3		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	30
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	30
5		Cyclohexane, isocyanato-	125	C7H11NO	003173-53-3	30



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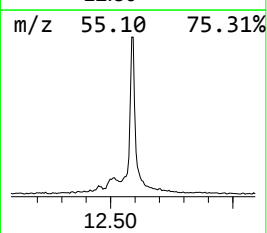
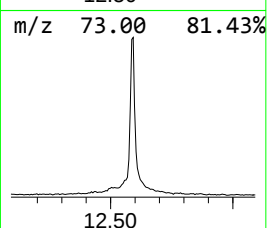
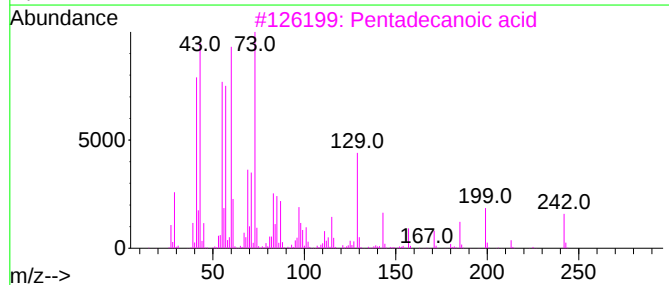
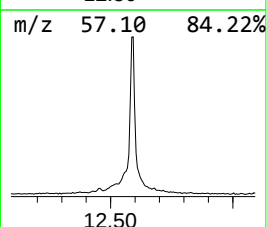
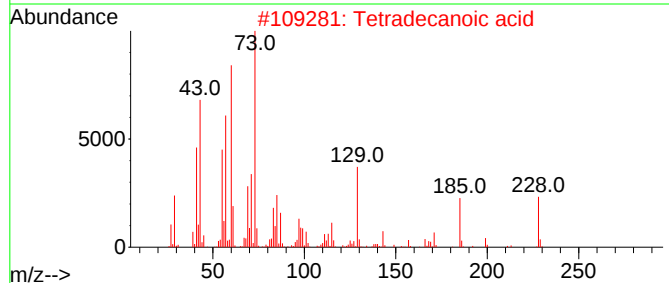
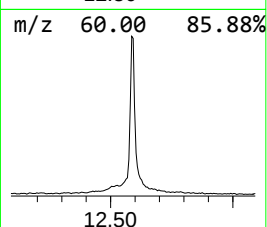
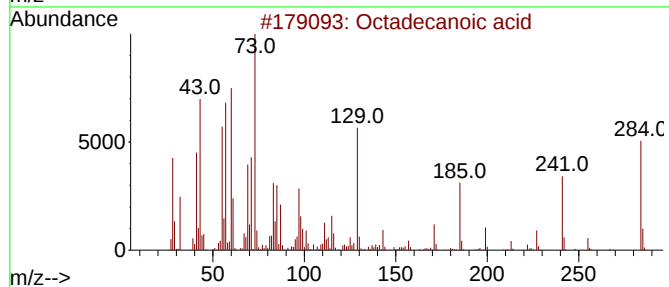
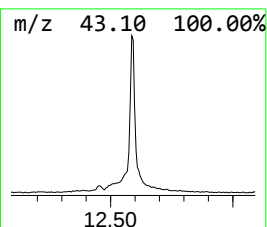
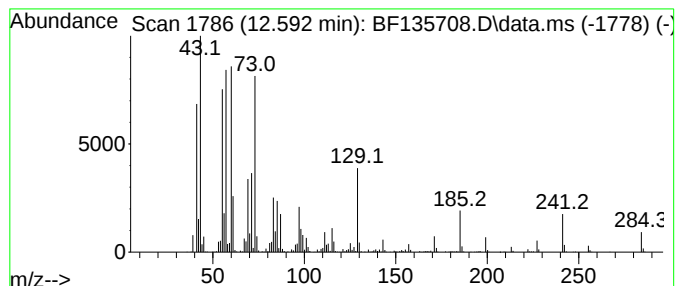
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	54.14 ng	2129740	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4			n-Decanoic acid	172	C10H20O2	000334-48-5	53
5			Undecanoic acid	186	C11H22O2	000112-37-8	49



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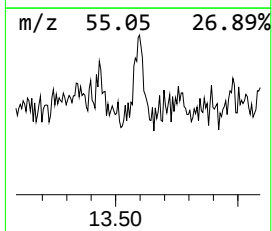
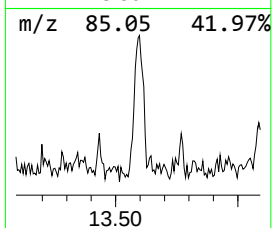
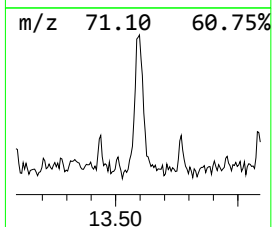
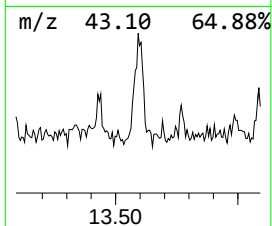
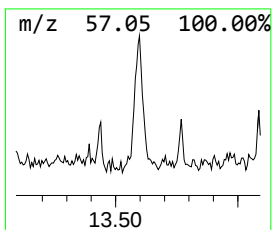
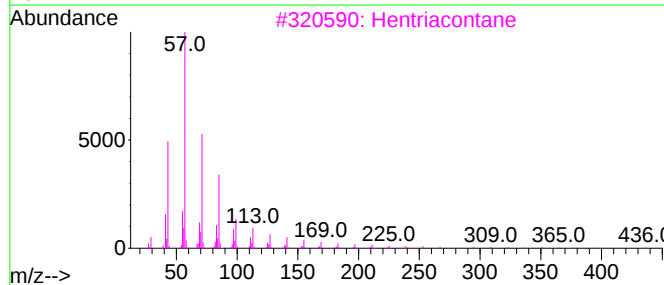
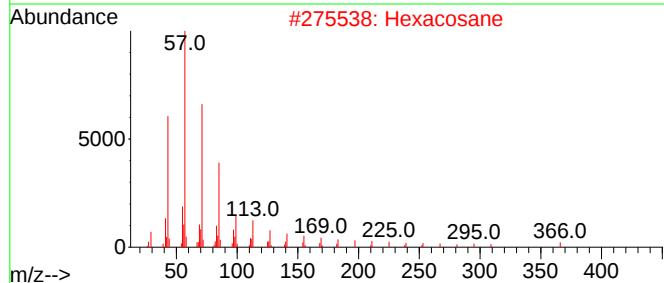
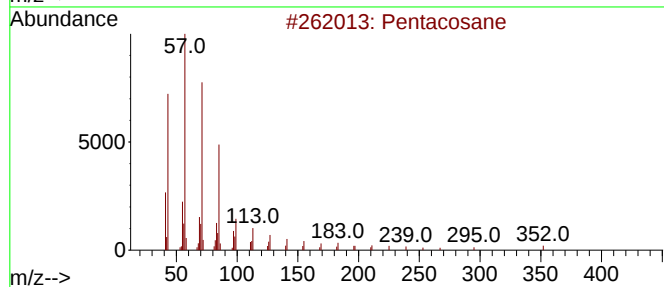
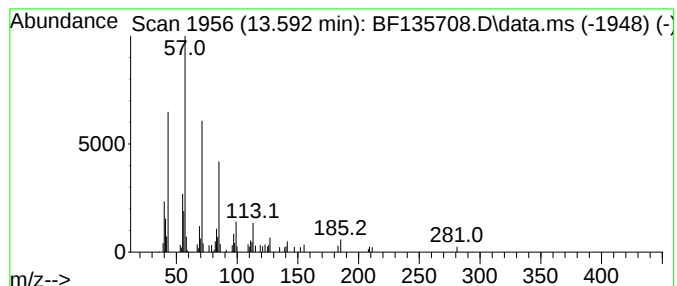
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.592	4.00 ng	94453	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	87
2			Hexacosane	366	C26H54	000630-01-3	87
3			Hentriacontane	437	C31H64	000630-04-6	87
4			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



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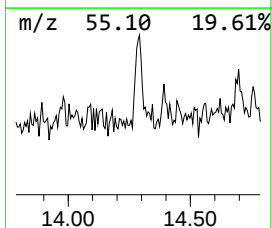
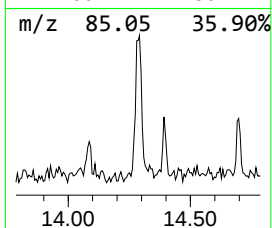
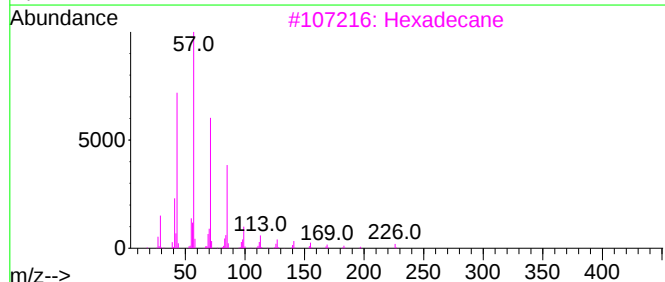
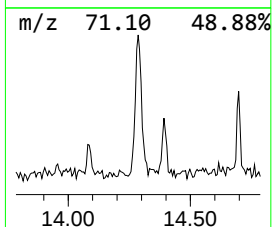
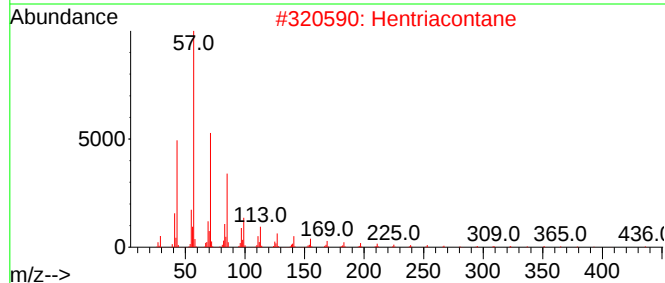
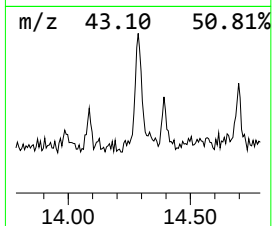
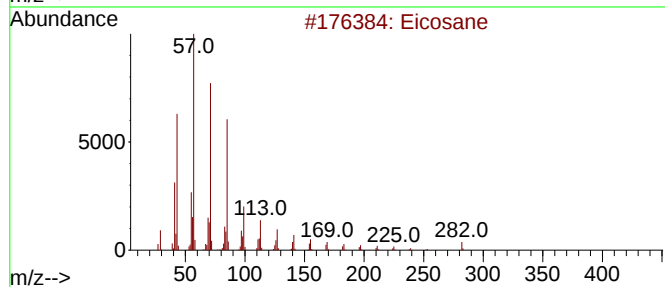
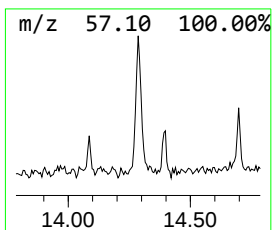
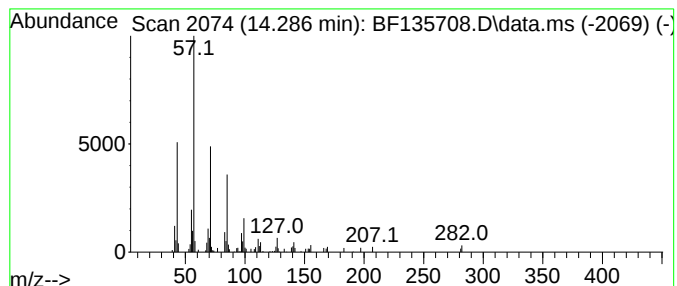
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.286	3.03 ng	71623	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Hexadecane	226	C16H34	000544-76-3	86
4			Octacosane	394	C28H58	000630-02-4	83
5			Hexacosane	366	C26H54	000630-01-3	83



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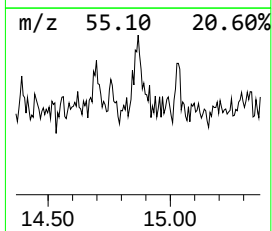
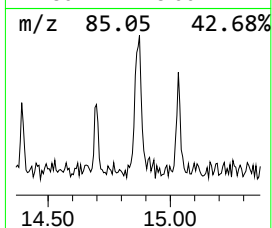
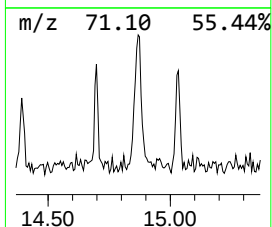
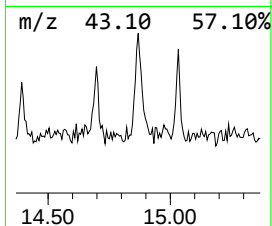
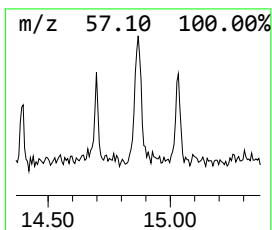
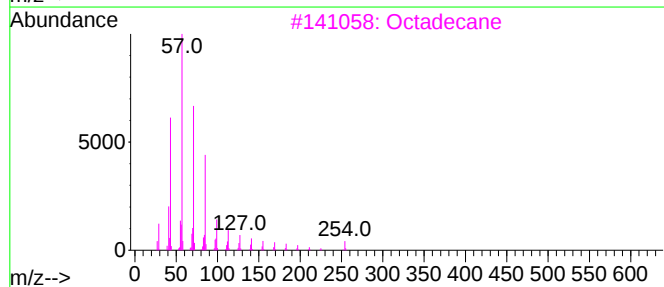
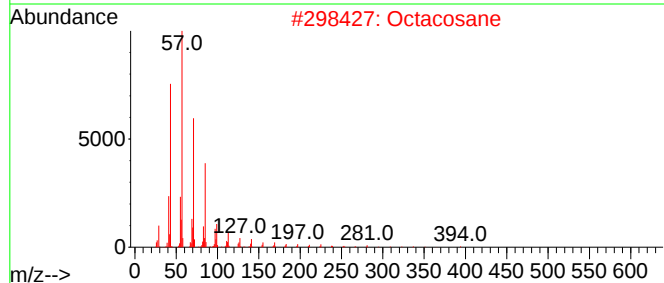
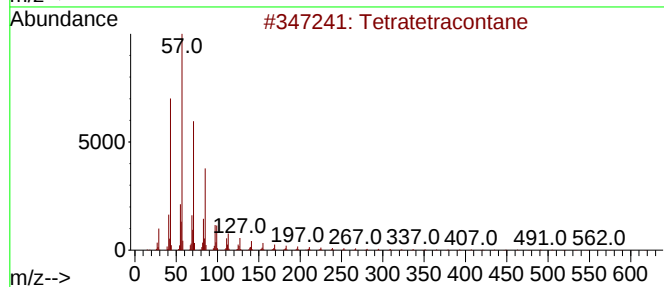
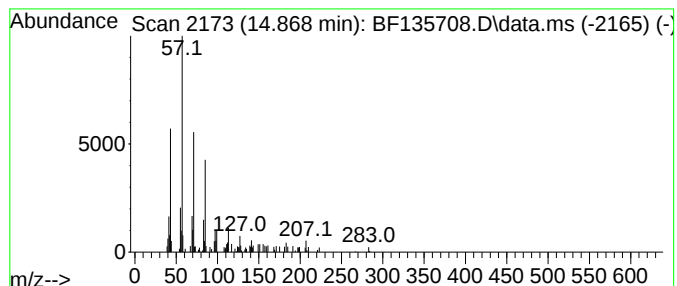
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	3.28 ng	86473	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	87
2			Octacosane	394	C28H58	000630-02-4	86
3			Octadecane	254	C18H38	000593-45-3	83
4			Hexacosane	366	C26H54	000630-01-3	83
5			Docosane	310	C22H46	000629-97-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135708.D
Acq On : 11 Oct 2023 12:37
Operator : CG\JU
Sample : 04656-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

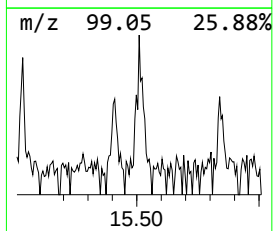
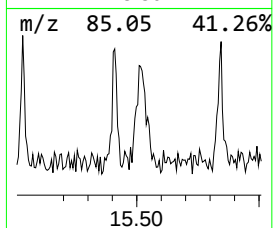
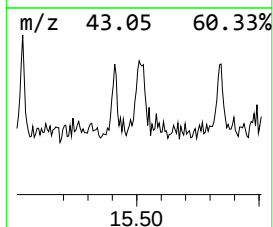
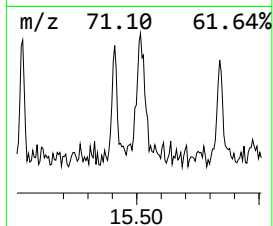
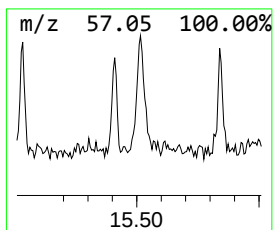
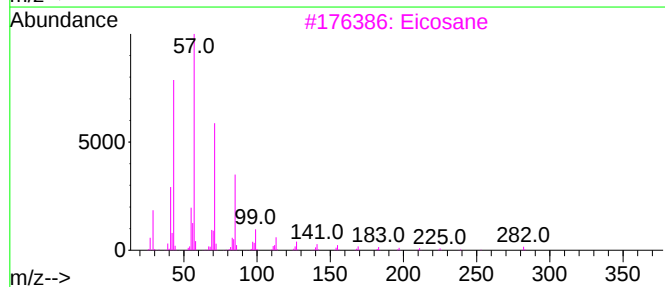
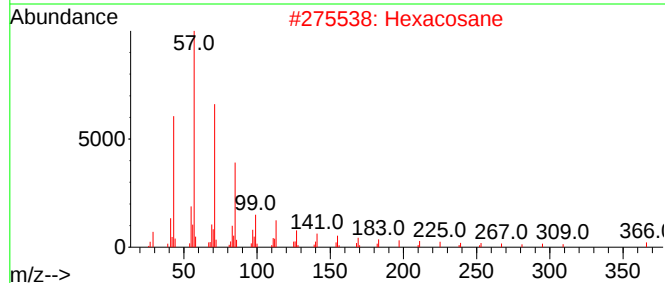
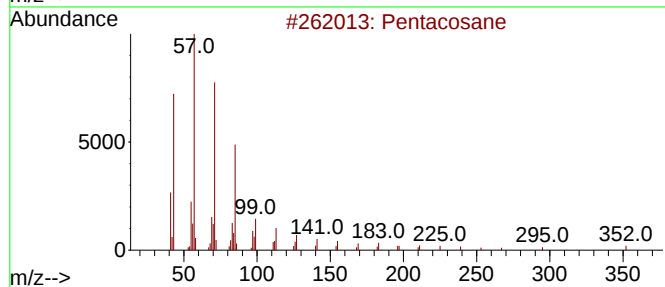
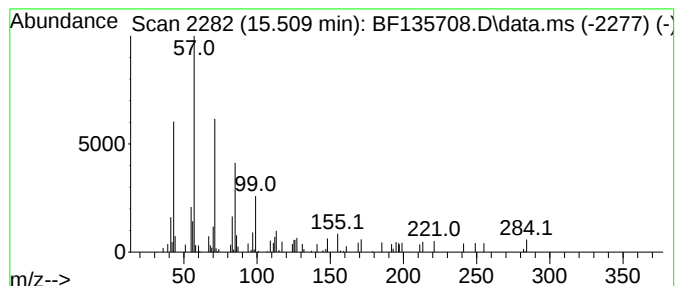
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.509	2.28 ng	60042	Perylene-d12	15.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	72
2	Hexacosane	366	C26H54	000630-01-3	64
3	Eicosane	282	C20H42	000112-95-8	64
4	Tetratetracontane	619	C44H90	007098-22-8	64
5	Hentriacontane	437	C31H64	000630-04-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135708.D
Acq On : 11 Oct 2023 12:37
Operator : CG\JU
Sample : 04656-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-104I

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tridecanoic acid	11.798	38.4	ng	1508700	4	11.269	786818	20.0
unknown12.510	12.510	6.2	ng	244155	4	11.269	786818	20.0
Octadecanoic acid	12.592	54.1	ng	2129740	4	11.269	786818	20.0
Pentacosane	13.592	4.0	ng	94453	5	13.933	472575	20.0
Eicosane	14.286	3.0	ng	71623	5	13.933	472575	20.0
Tetratetracontane	14.868	3.3	ng	86473	6	15.404	527556	20.0
Hexacosane	15.509	2.3	ng	60042	6	15.404	527556	20.0