

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
 Data File : BF134901.D
 Acq On : 23 Aug 2023 13:27
 Operator : CG\JU
 Sample : 04080-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ETGI-340

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-BF082223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134901.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	563	568	571	rBV	3532920	3534731	81.50%	11.080%
2	6.434	733	739	742	rBV	3263390	3601421	83.03%	11.289%
3	6.793	796	800	803	rBV	1043705	842753	19.43%	2.642%
4	7.357	890	896	899	rBV	2278863	2397525	55.28%	7.515%
5	8.069	1013	1017	1021	rBV	1352825	1153388	26.59%	3.615%
6	9.151	1196	1201	1204	rBV	4507985	4275519	98.57%	13.402%
7	9.269	1217	1221	1224	rBV	51857	46203	1.07%	0.145%
8	9.828	1311	1316	1320	rBV	1647138	1364643	31.46%	4.277%
9	10.622	1445	1451	1455	rBV	3013727	3140274	72.40%	9.843%
10	11.322	1566	1570	1573	rBV	1800624	1487106	34.29%	4.661%
11	11.345	1573	1574	1578	rVB	100946	55035	1.27%	0.173%
12	11.863	1657	1662	1666	rBV	628409	606398	13.98%	1.901%
13	12.539	1773	1777	1780	rBV	232321	212123	4.89%	0.665%
14	12.651	1792	1796	1806	rBV2	121123	156493	3.61%	0.491%
15	12.769	1810	1816	1819	rVV	211964	226782	5.23%	0.711%
16	12.922	1837	1842	1845	rBV	4308280	4337358	100.00%	13.596%
17	13.504	1932	1941	1943	rBV	38011	50435	1.16%	0.158%
18	13.827	1992	1996	2004	rBV3	361530	489836	11.29%	1.535%
19	13.974	2014	2021	2024	rBV	1140885	1130181	26.06%	3.543%
20	13.998	2024	2025	2031	rVV	105554	88393	2.04%	0.277%
21	14.074	2031	2038	2048	rVV	174246	196229	4.52%	0.615%
22	14.157	2048	2052	2055	rBV	40132	46747	1.08%	0.147%
23	14.463	2098	2104	2111	rBV3	92035	224445	5.17%	0.704%
24	14.580	2119	2124	2128	rVB3	40777	73840	1.70%	0.231%
25	14.621	2128	2131	2136	rBV5	29458	62696	1.45%	0.197%
26	14.663	2136	2138	2145	rVB2	29811	59334	1.37%	0.186%
27	14.916	2178	2181	2185	rVB	107202	109193	2.52%	0.342%
28	15.016	2194	2198	2201	rBV	86102	111640	2.57%	0.350%
29	15.045	2201	2203	2208	rVB2	55243	56600	1.30%	0.177%
30	15.116	2211	2215	2217	rBV	77420	90306	2.08%	0.283%
31	15.145	2217	2220	2226	rVB3	91149	134674	3.10%	0.422%
32	15.321	2246	2250	2254	rBV	44116	51857	1.20%	0.163%
33	15.380	2257	2260	2265	rVB	57118	69811	1.61%	0.219%
34	15.451	2266	2272	2278	rBV	704333	885542	20.42%	2.776%
35	15.710	2312	2316	2321	rVB	39576	55048	1.27%	0.173%
36	15.951	2352	2357	2362	rBV	88447	134606	3.10%	0.422%

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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-BF082223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.010	2362	2367	2375	rVV3	52969	117974	2.72%	0.370%
38	16.774	2492	2497	2505	rVB7	29414	60705	1.40%	0.190%
39	16.933	2519	2524	2535	rBV3	24191	66112	1.52%	0.207%
40	17.092	2546	2551	2556	rBV2	21908	53527	1.23%	0.168%
41	18.604	2804	2808	2818	rVB2	18475	45396	1.05%	0.142%

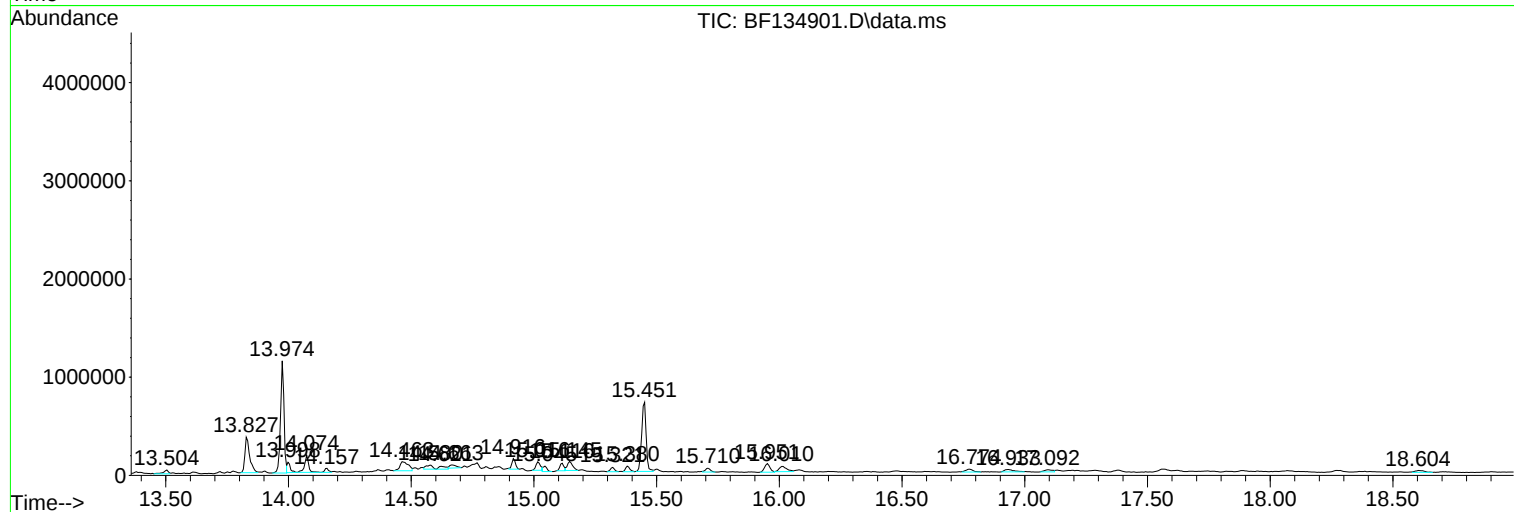
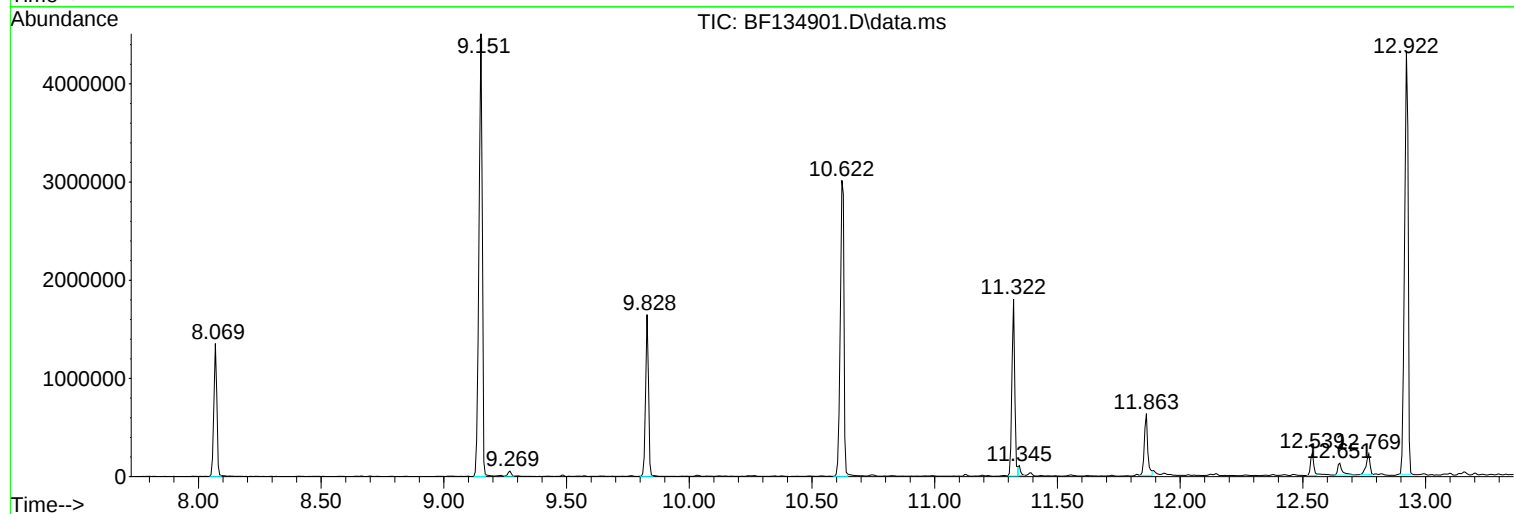
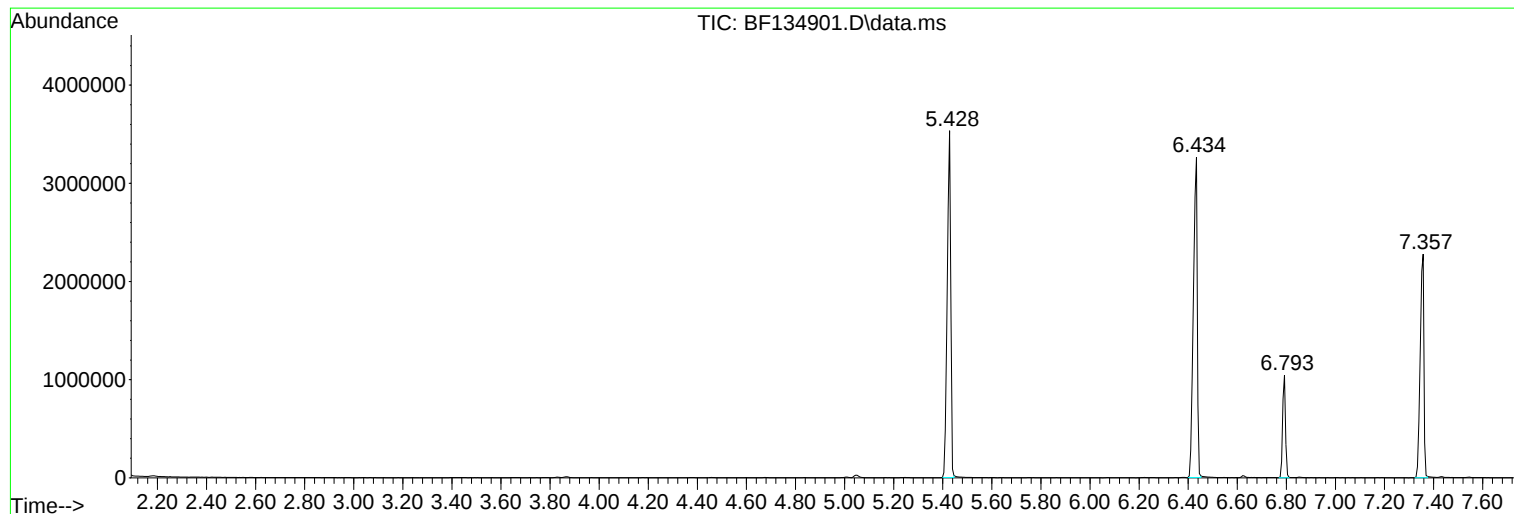
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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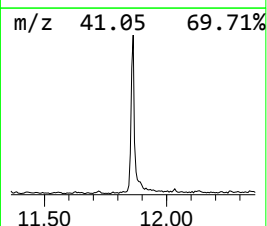
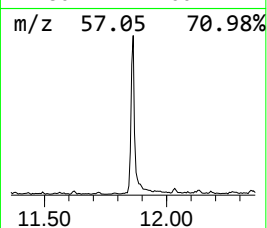
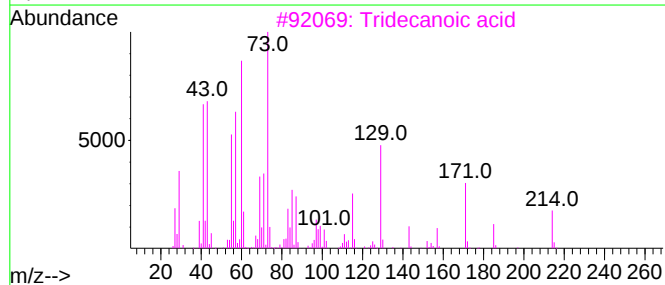
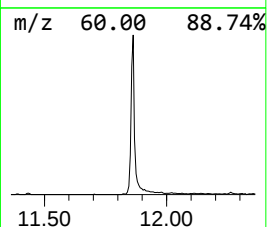
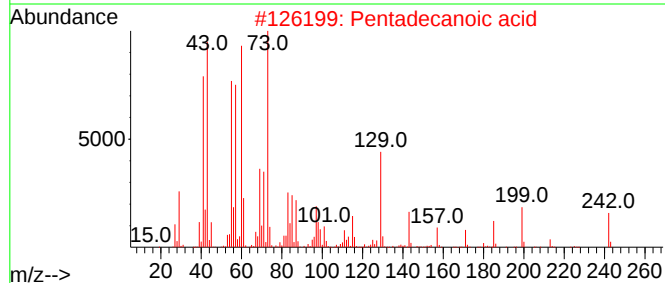
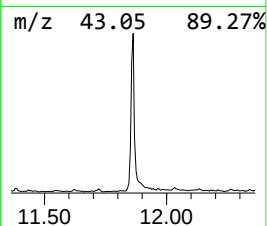
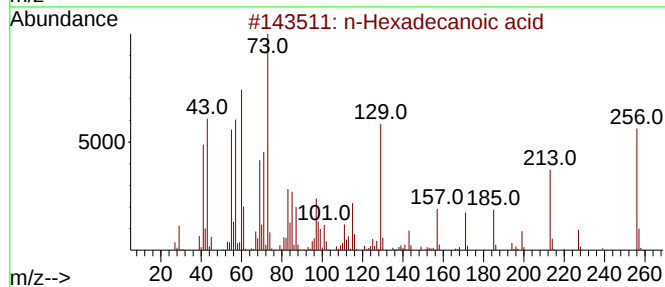
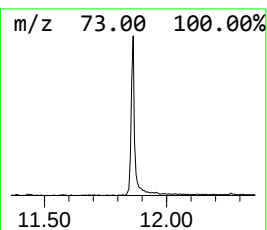
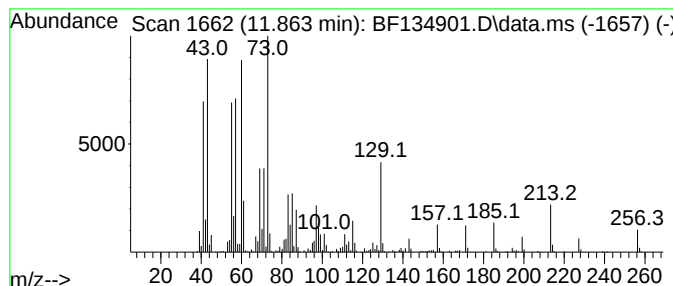
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	8.16 ng	606398	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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Misc :
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Instrument :
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ClientSampleId :
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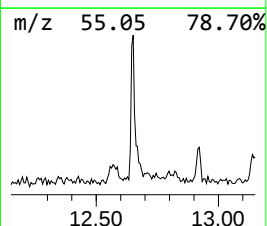
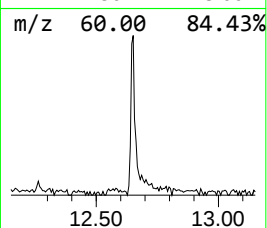
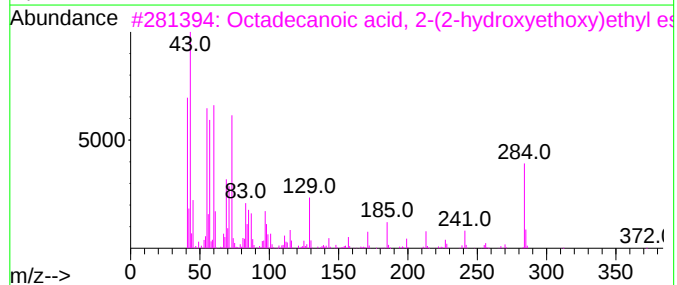
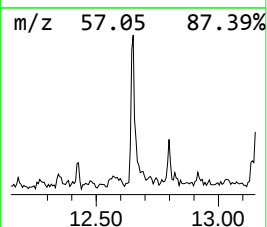
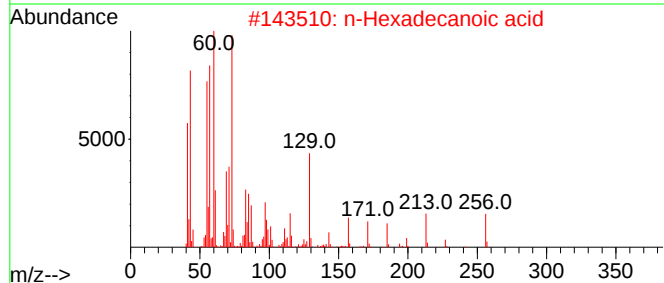
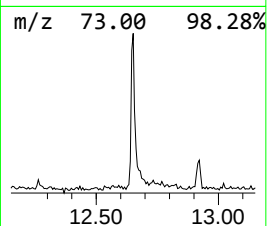
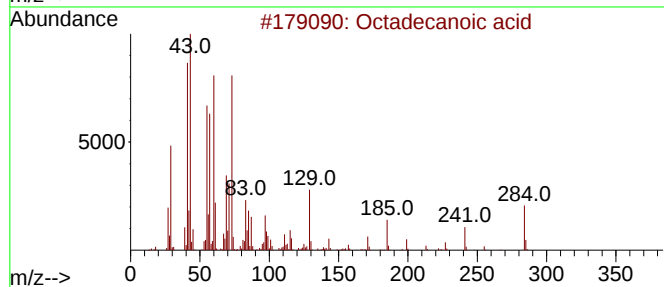
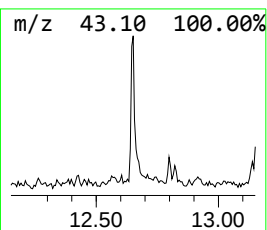
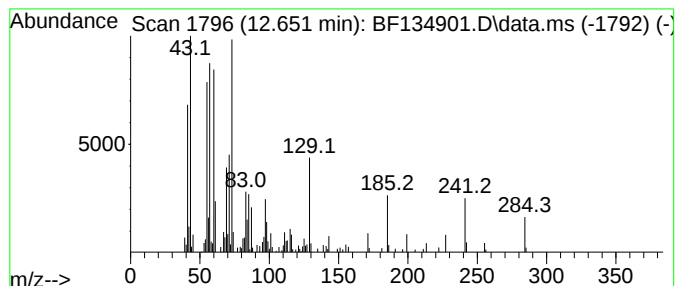
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.77 ng	156493	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	83



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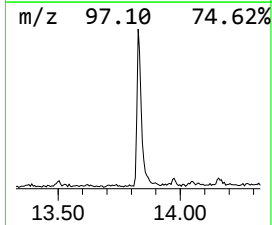
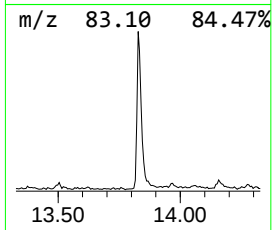
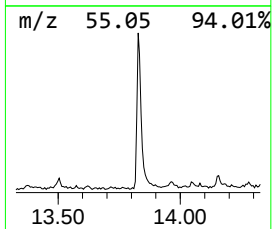
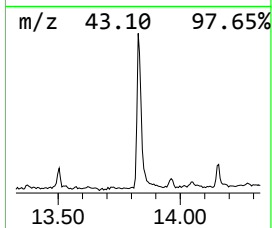
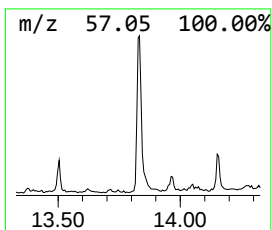
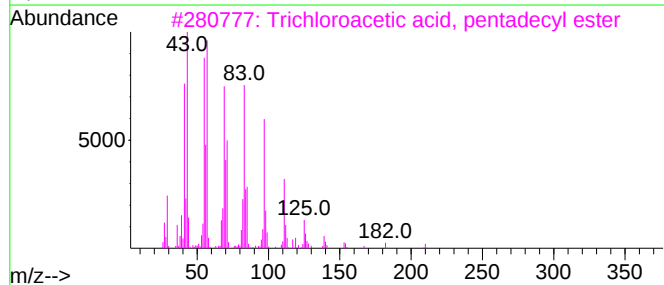
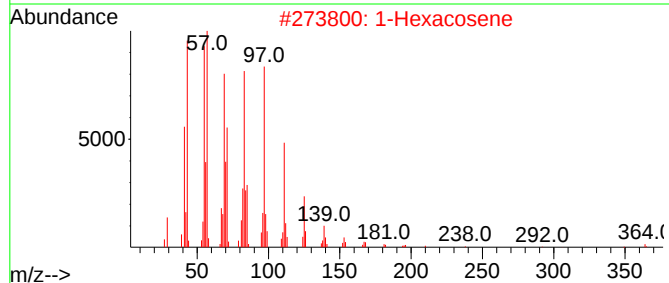
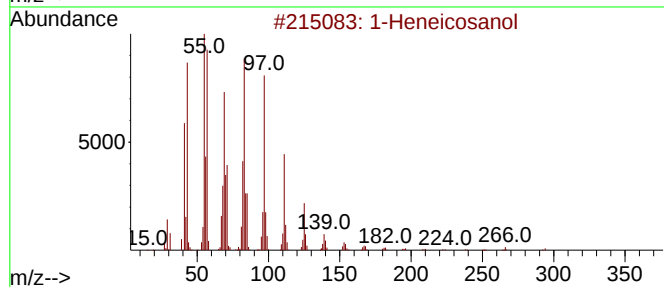
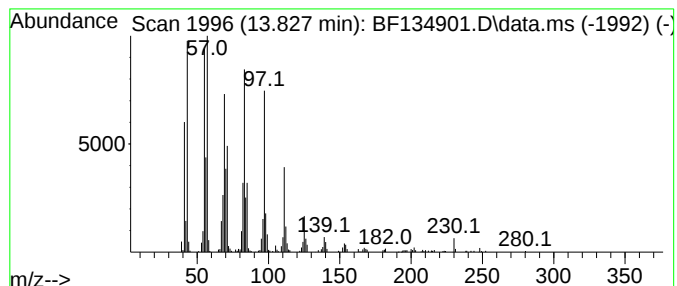
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	8.67 ng	489836	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



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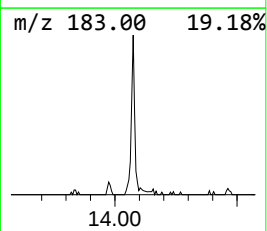
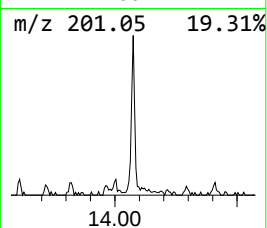
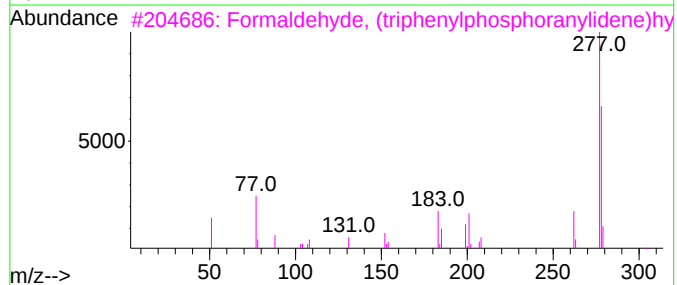
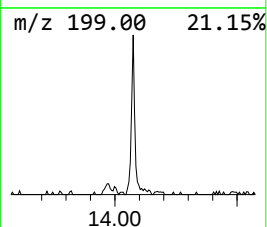
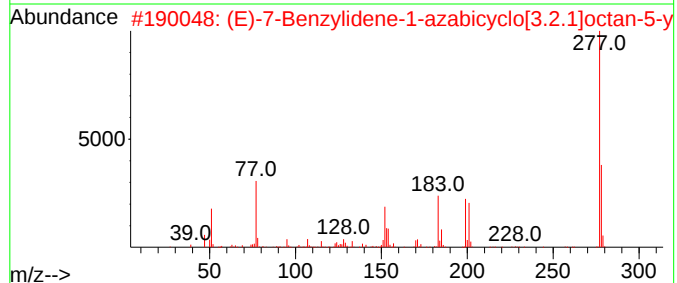
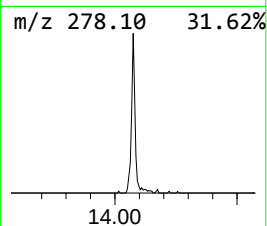
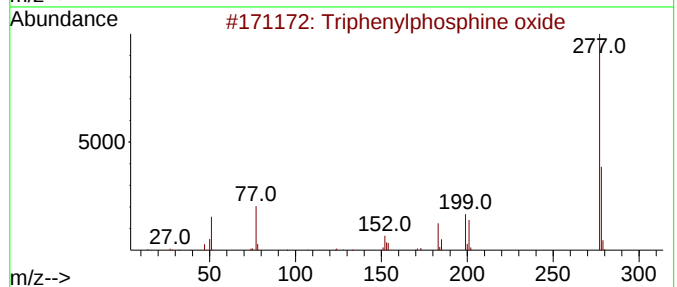
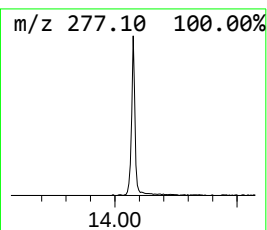
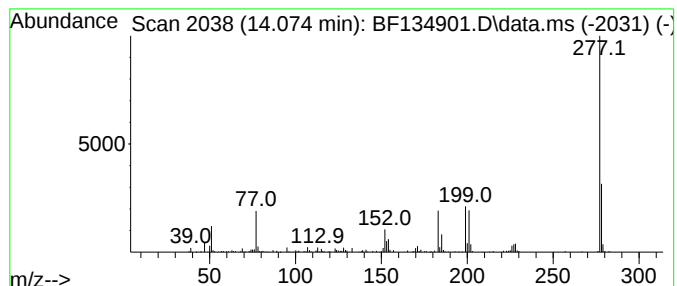
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	3.47 ng	196229	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	53
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37



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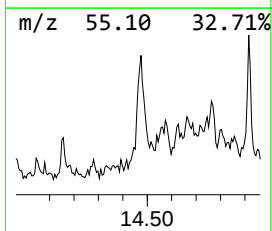
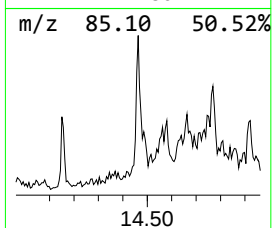
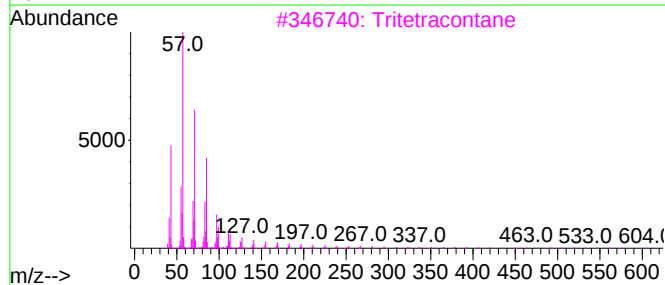
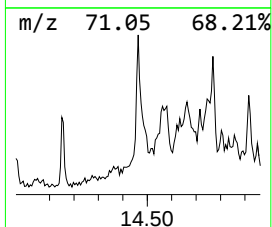
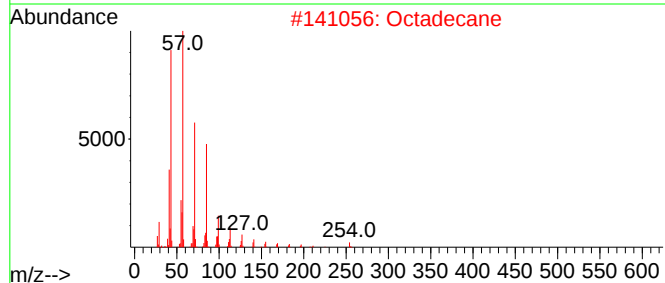
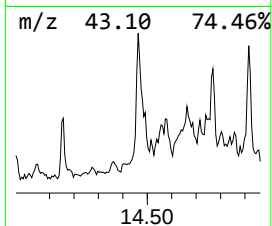
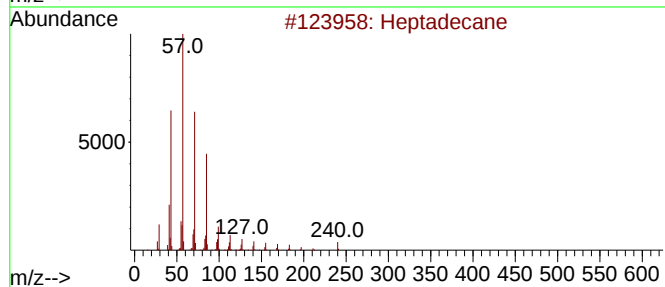
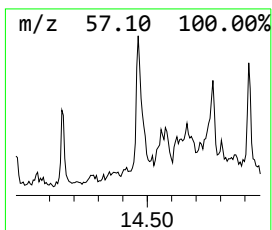
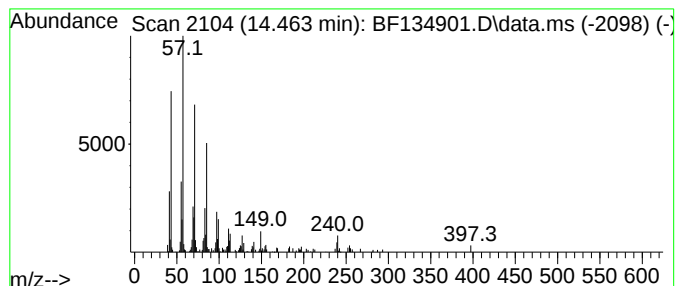
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	3.97 ng	224445	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	96
2			Octadecane	254	C18H38	000593-45-3	96
3			Tritetracontane	605	C43H88	007098-21-7	90
4			Tetratetracontane	619	C44H90	007098-22-8	90
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
Data File : BF134901.D
Acq On : 23 Aug 2023 13:27
Operator : CG\JU
Sample : 04080-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-340

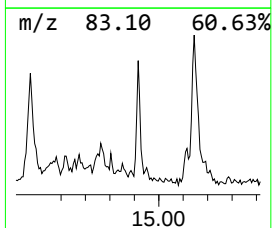
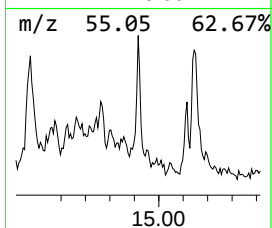
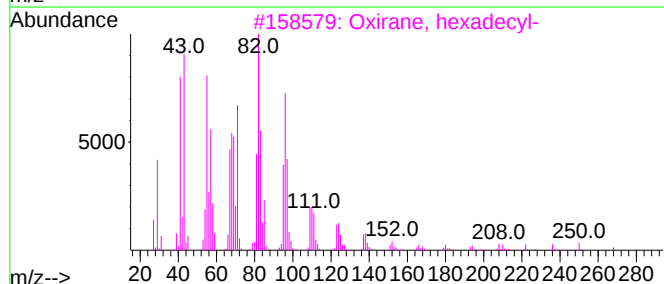
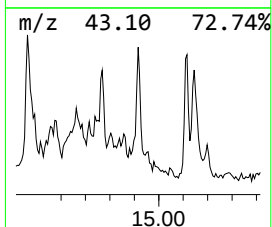
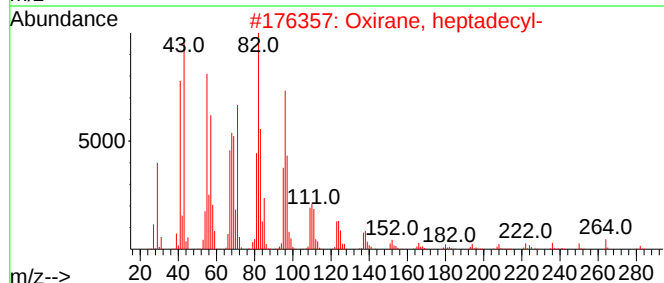
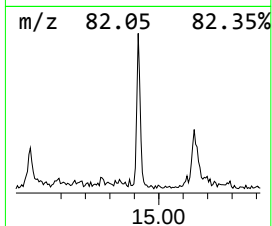
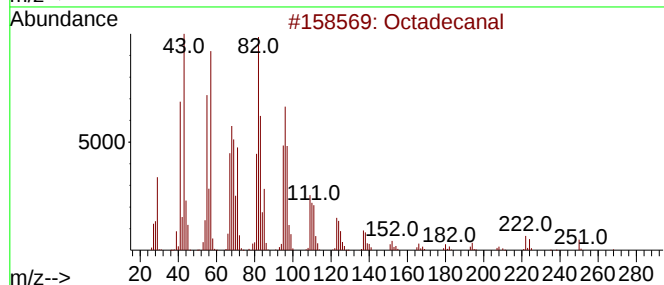
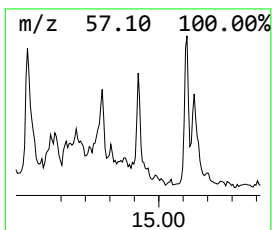
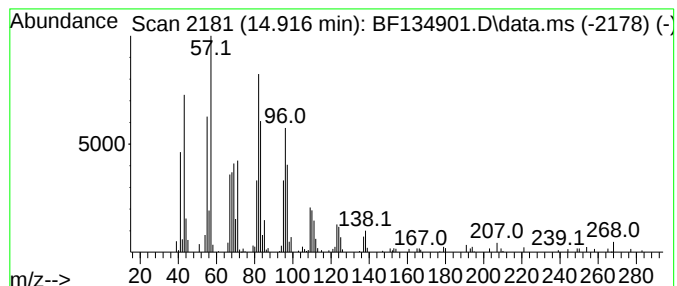
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	2.47 ng	109193	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	91
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	83
5			1,19-Eicosadiene	278	C20H38	014811-95-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
Data File : BF134901.D
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Sample : 04080-01
Misc :
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Instrument :
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ClientSampleId :
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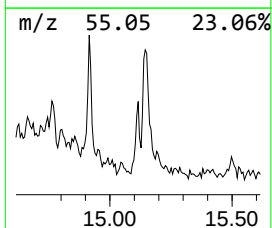
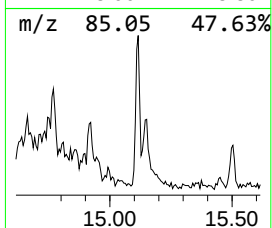
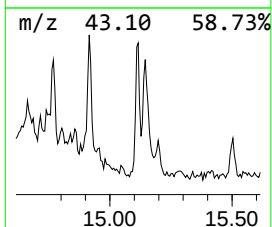
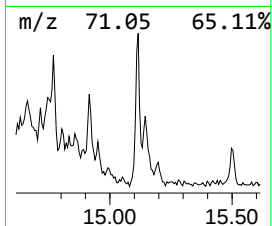
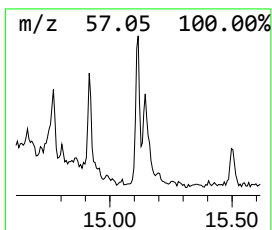
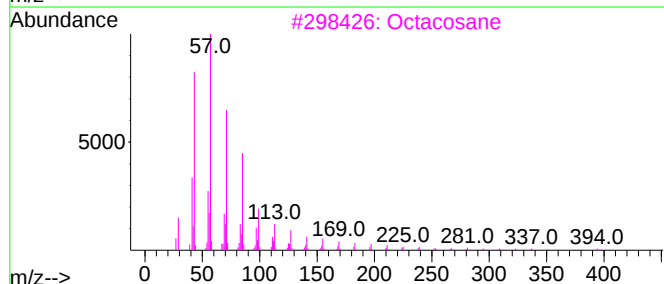
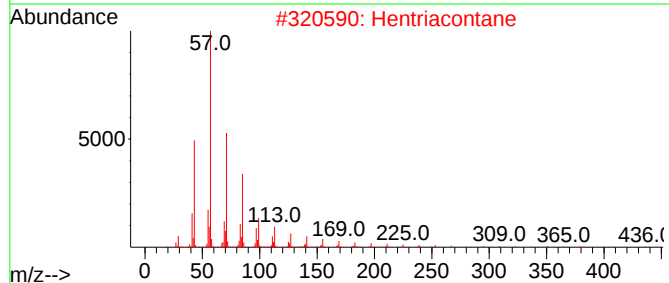
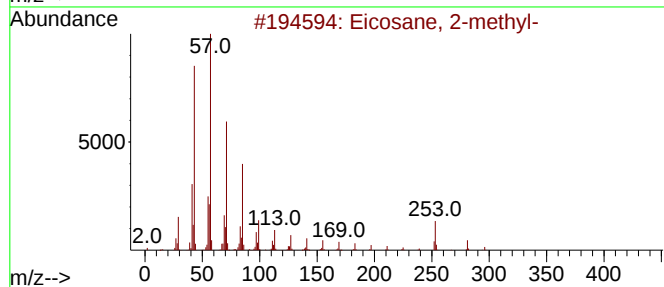
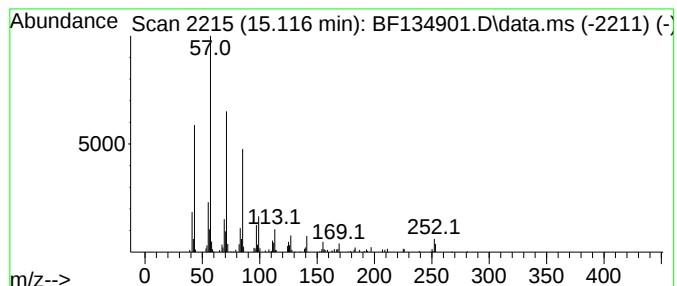
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.116	2.04 ng	90306	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Pentacosane	352	C25H52	000629-99-2	90
5			triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
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Acq On : 23 Aug 2023 13:27
Operator : CG\JU
Sample : 04080-01
Misc :
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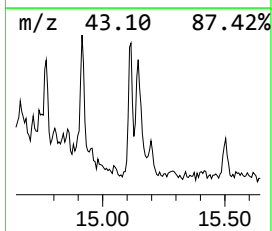
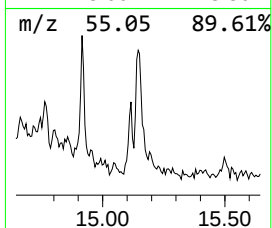
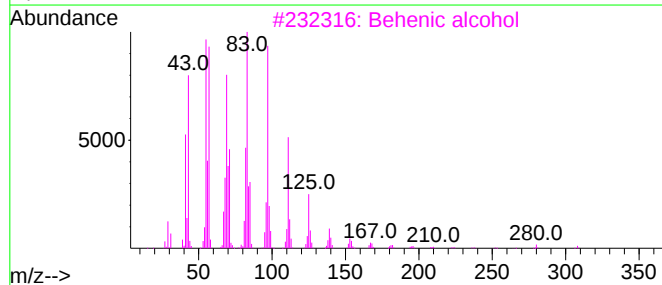
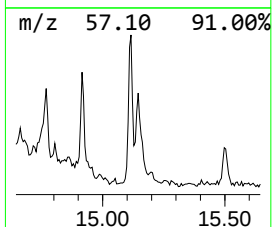
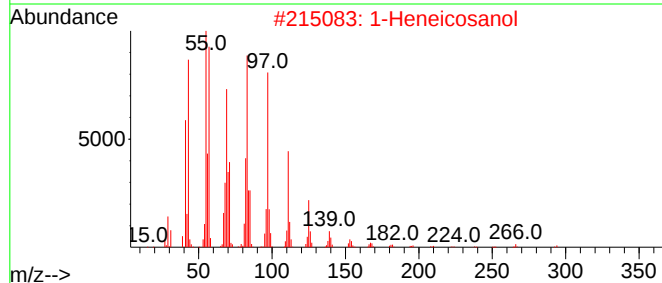
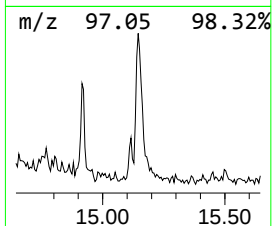
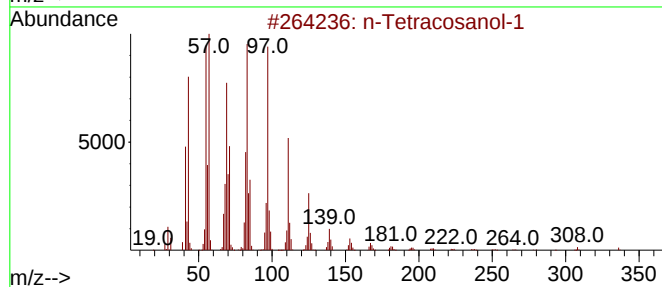
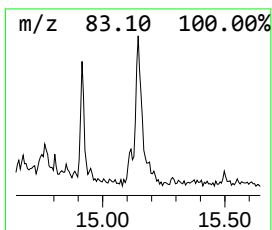
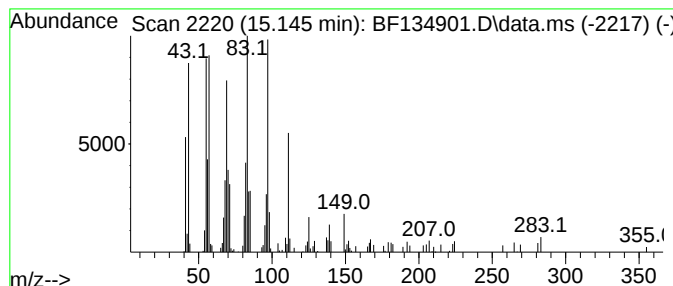
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.145	3.04 ng	134674	Perylene-d12	15.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	1-Hexacosene	364	C26H52	018835-33-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
Data File : BF134901.D
Acq On : 23 Aug 2023 13:27
Operator : CG\JU
Sample : 04080-01
Misc :
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Instrument :
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ClientSampleId :
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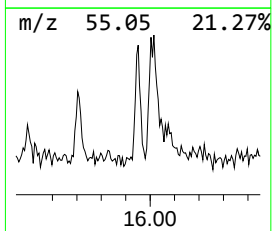
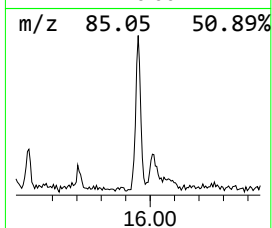
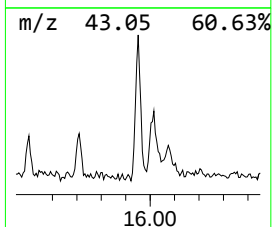
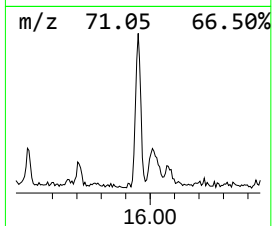
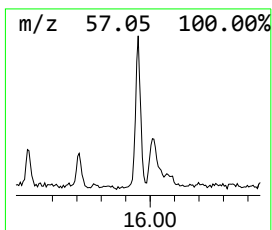
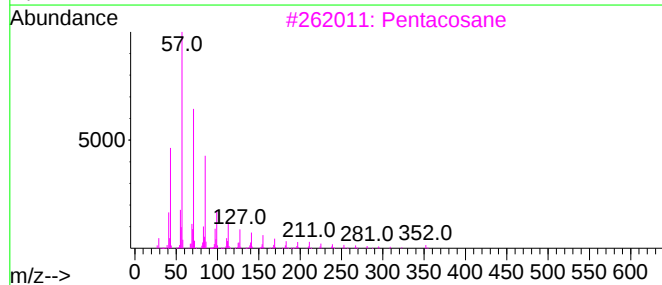
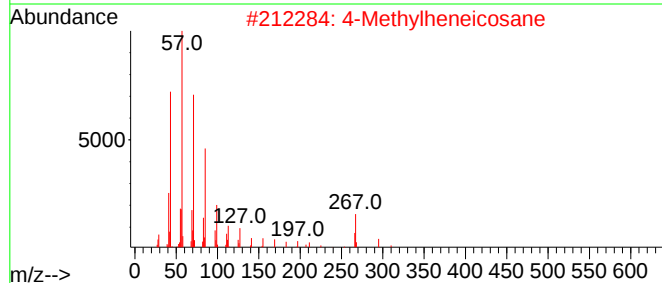
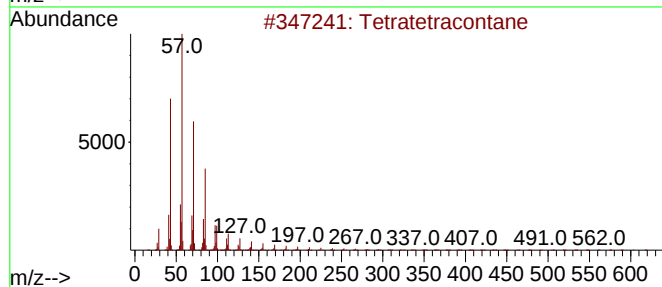
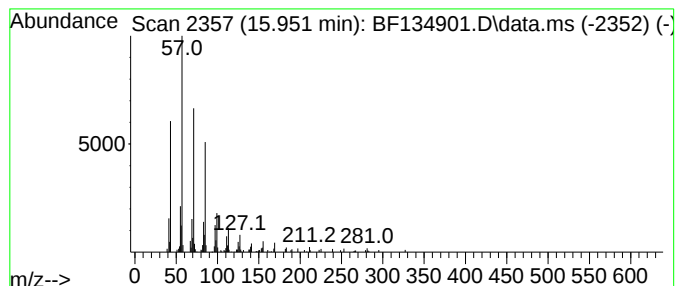
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	3.04 ng	134606	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			4-Methylheneicosane	310	C22H46	025117-29-7	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
Data File : BF134901.D
Acq On : 23 Aug 2023 13:27
Operator : CG\JU
Sample : 04080-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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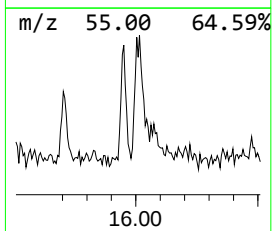
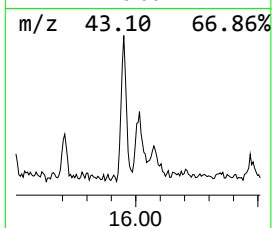
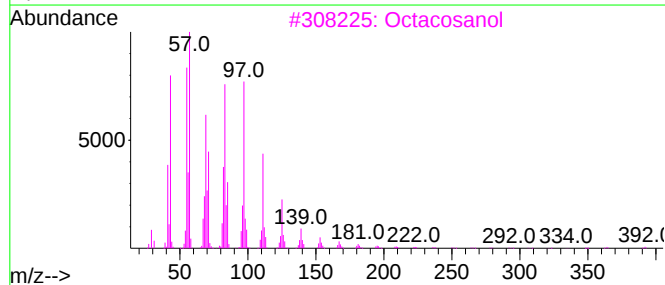
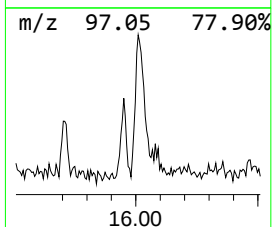
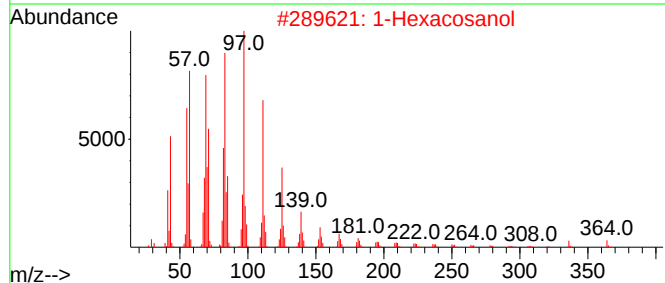
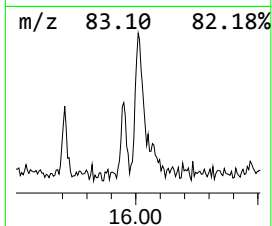
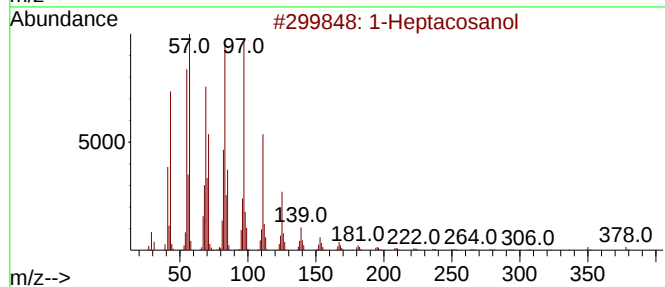
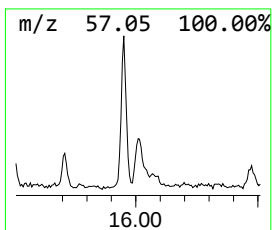
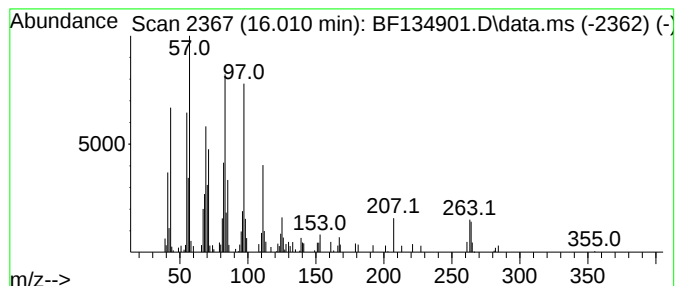
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	2.66 ng	117974	Perylene-d12	15.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	93
2		1-Hexacosanol	382	C26H54O	000506-52-5	90
3		Octacosanol	410	C28H58O	000557-61-9	90
4		Triacontan-15-ol	438	C30H62O	031849-26-0	87
5		Behenic alcohol	326	C22H46O	000661-19-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
Data File : BF134901.D
Acq On : 23 Aug 2023 13:27
Operator : CG\JU
Sample : 04080-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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

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

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					#	RT	Resp	Conc
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Octadecanoic acid	12.651	2.8	ng	156493	5	13.974	1130180	20.0
1-Heneicosanol	13.827	8.7	ng	489836	5	13.974	1130180	20.0
Triphenylphosph...	14.074	3.5	ng	196229	5	13.974	1130180	20.0
Heptadecane	14.463	4.0	ng	224445	5	13.974	1130180	20.0
Octadecanal	14.916	2.5	ng	109193	6	15.451	885542	20.0
Eicosane, 2-met...	15.116	2.0	ng	90306	6	15.451	885542	20.0
n-Tetracosanol-1	15.145	3.0	ng	134674	6	15.451	885542	20.0
Tetratetracontane	15.951	3.0	ng	134606	6	15.451	885542	20.0
1-Heptacosanol	16.010	2.7	ng	117974	6	15.451	885542	20.0