

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136836.D
 Acq On : 29 Dec 2023 18:46
 Operator : CG\JU
 Sample : 05897-10
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-39

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-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	495	499	505	rVB	21608	25800	1.46%	0.210%
2	5.422	563	567	584	rBV	1522730	1386432	78.28%	11.270%
3	6.428	733	738	741	rBV	1533937	1384629	78.18%	11.255%
4	6.781	794	798	801	rBV	535213	409511	23.12%	3.329%
5	7.346	889	894	897	rBV	997175	938208	52.97%	7.626%
6	8.057	1011	1015	1018	rBV	688515	534599	30.18%	4.346%
7	9.134	1193	1198	1202	rBV	1932362	1771180	100.00%	14.397%
8	9.816	1310	1314	1317	rBV	697535	597613	33.74%	4.858%
9	10.610	1445	1449	1452	rBV	1156412	1027067	57.99%	8.349%
10	11.304	1563	1567	1571	rBV	728710	617454	34.86%	5.019%
11	11.804	1649	1652	1655	rBV2	15898	18636	1.05%	0.151%
12	11.839	1655	1658	1672	rVB	221558	252084	14.23%	2.049%
13	12.569	1773	1782	1787	rBV9	13366	35674	2.01%	0.290%
14	12.633	1790	1793	1802	rVV3	26802	44758	2.53%	0.364%
15	12.904	1834	1839	1842	rBV	1758597	1493766	84.34%	12.142%
16	13.433	1924	1929	1932	rBV3	17874	26833	1.51%	0.218%
17	13.480	1932	1937	1946	rVB7	36622	77167	4.36%	0.627%
18	13.810	1989	1993	1997	rVB	34110	29706	1.68%	0.241%
19	13.886	1997	2006	2011	rBV7	17527	60278	3.40%	0.490%
20	13.963	2015	2019	2025	rVB	414748	388950	21.96%	3.162%
21	14.257	2063	2069	2072	rBV2	27328	33666	1.90%	0.274%
22	14.433	2090	2099	2103	rBV2	53942	78658	4.44%	0.639%
23	14.745	2149	2152	2157	rVB	20094	22444	1.27%	0.182%
24	14.892	2173	2177	2182	rVB2	74924	77828	4.39%	0.633%
25	15.086	2206	2210	2217	rVB	68159	79131	4.47%	0.643%
26	15.251	2228	2238	2245	rVB	21825	70395	3.97%	0.572%
27	15.439	2265	2270	2281	rBV	282676	396746	22.40%	3.225%
28	15.680	2307	2311	2316	rBV	69148	88802	5.01%	0.722%
29	15.921	2347	2352	2359	rVB2	63573	97125	5.48%	0.789%
30	16.068	2371	2377	2381	rBV7	14254	27019	1.53%	0.220%
31	16.745	2487	2492	2498	rVB3	47305	87620	4.95%	0.712%
32	17.063	2539	2546	2551	rBV5	14709	36407	2.06%	0.296%
33	18.245	2739	2747	2755	rVB5	30467	86092	4.86%	0.700%

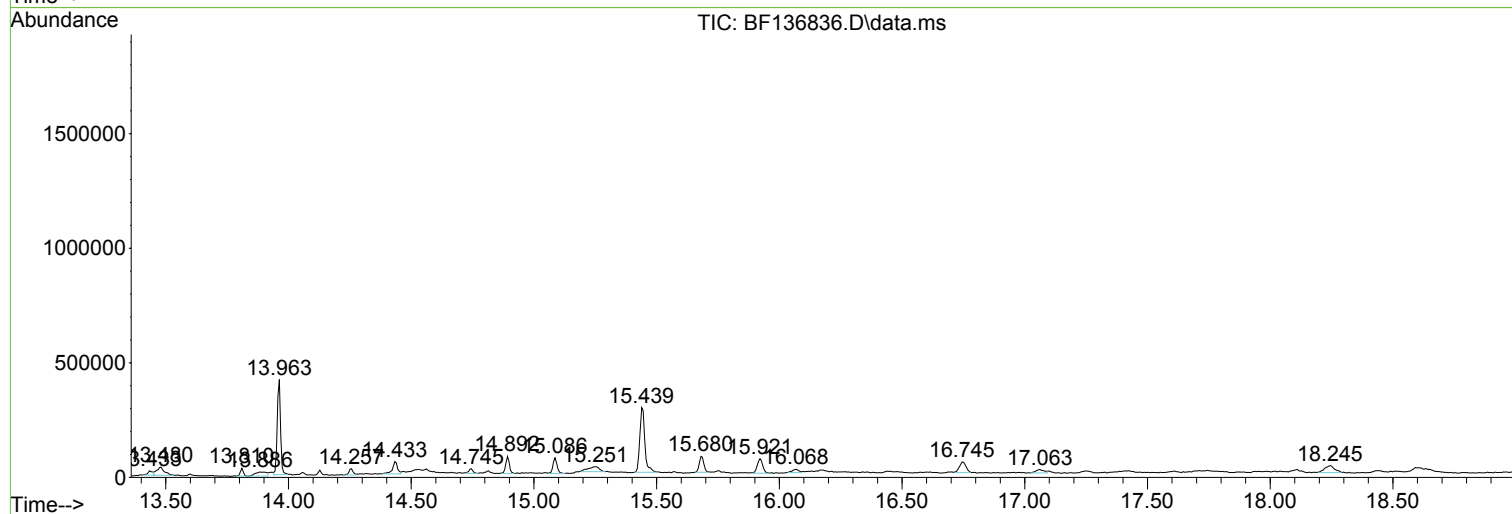
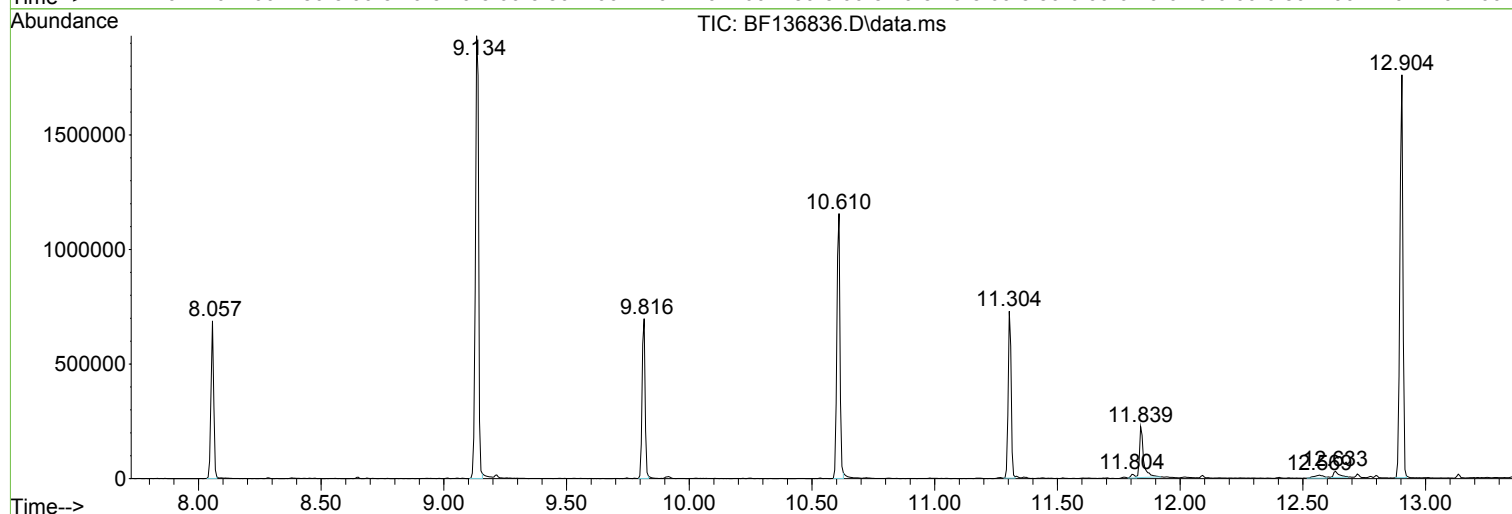
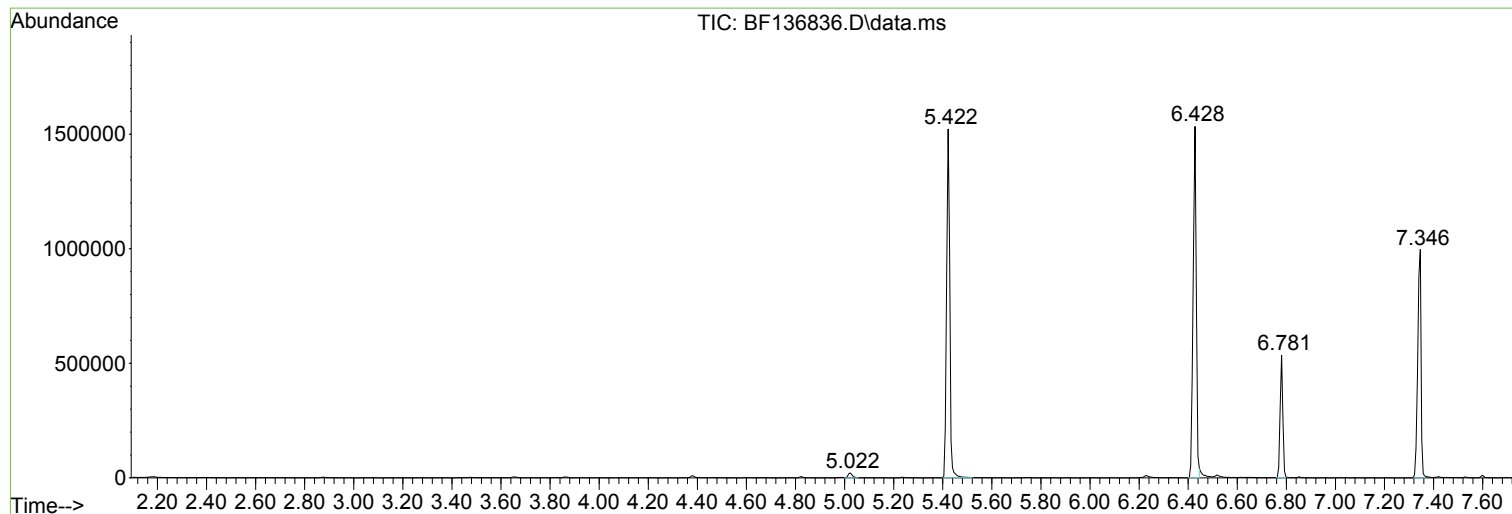
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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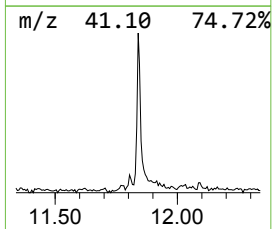
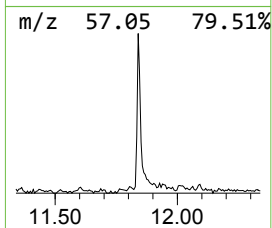
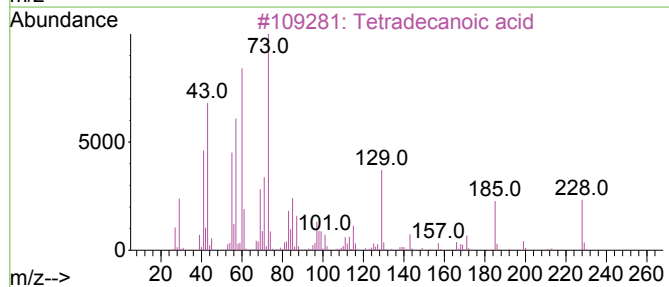
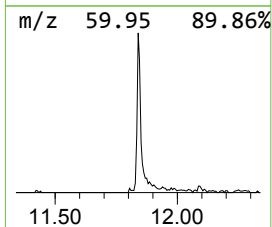
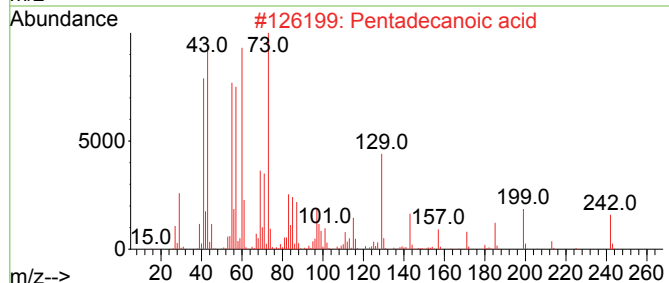
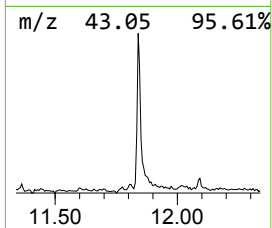
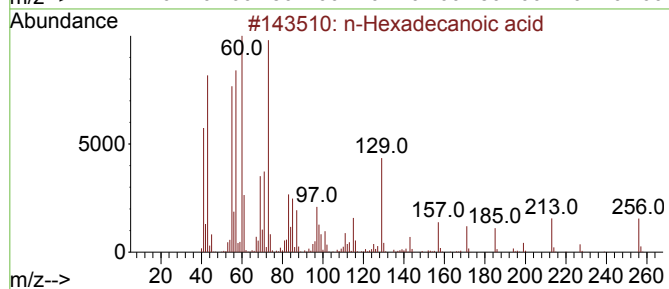
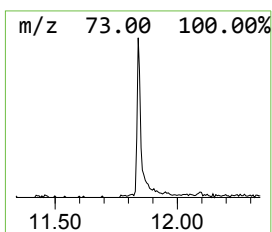
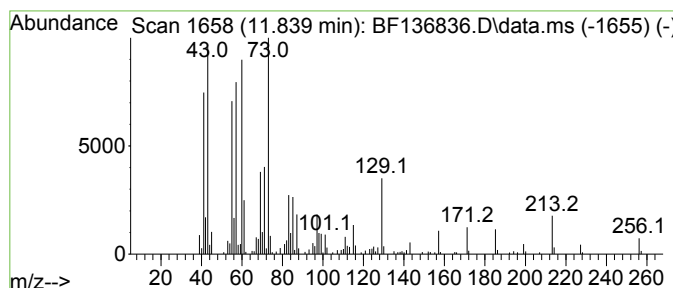
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.839	8.17 ng	252084	Phenanthrene-d10		11.304	
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	90
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
4	Tridecanoic acid		214	C13H26O2	000638-53-9	76
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	46



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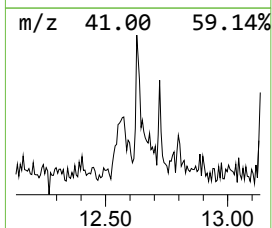
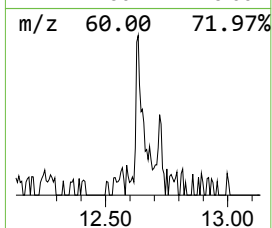
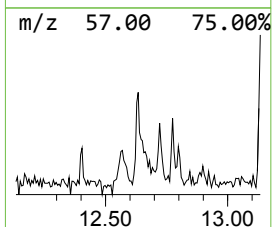
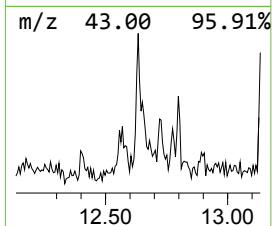
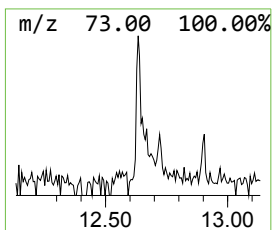
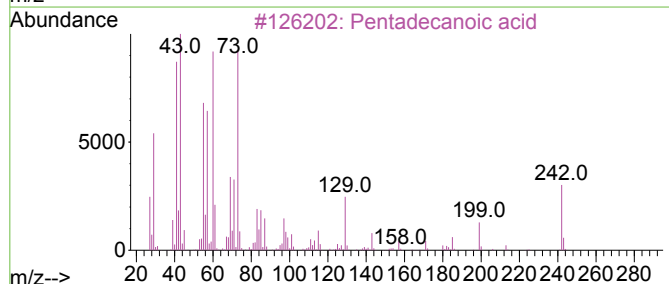
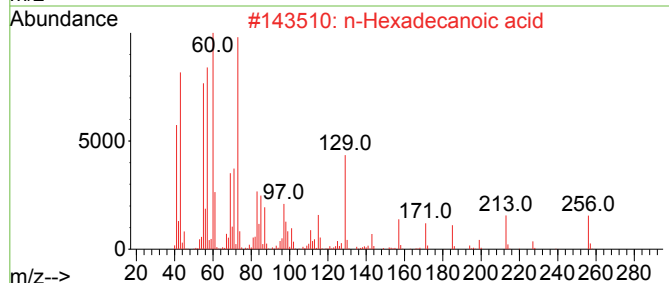
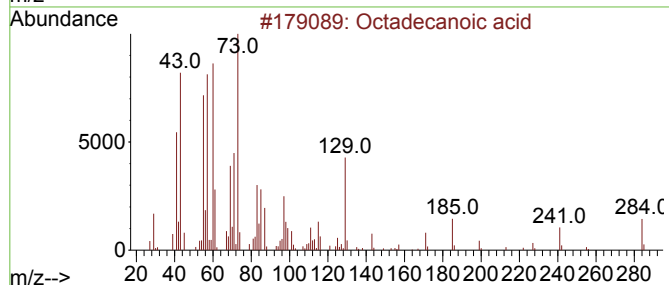
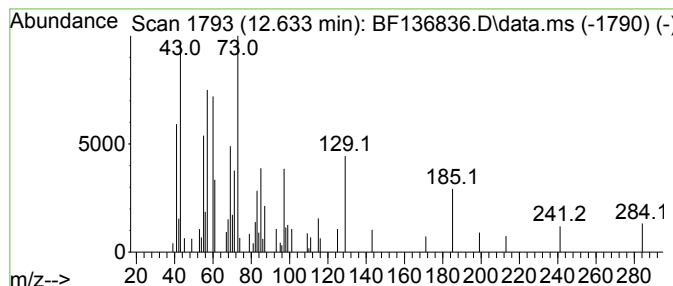
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.30 ng	44758	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	35
4			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	27
5			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	22



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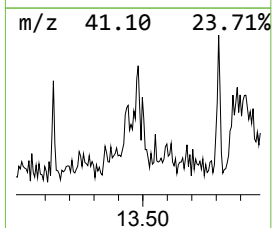
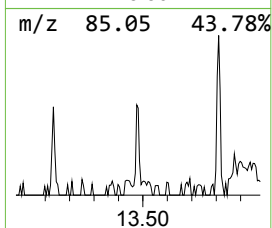
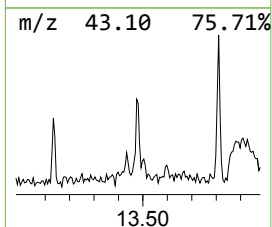
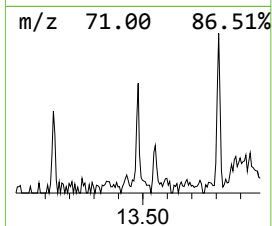
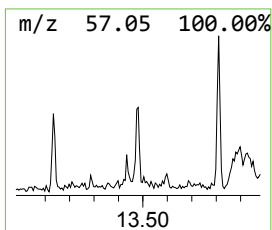
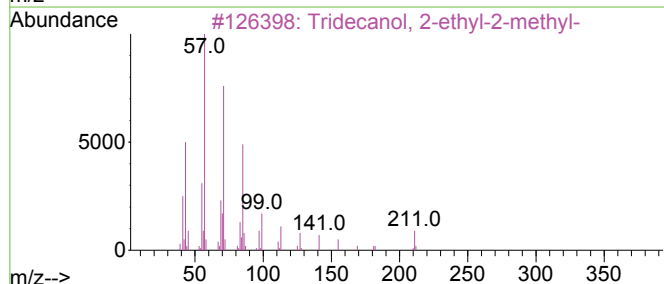
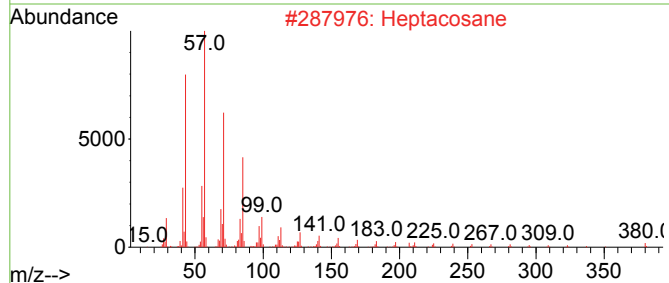
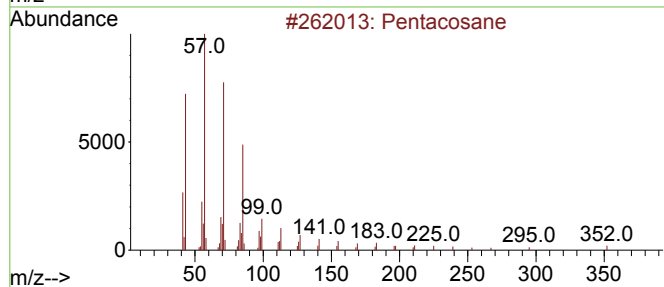
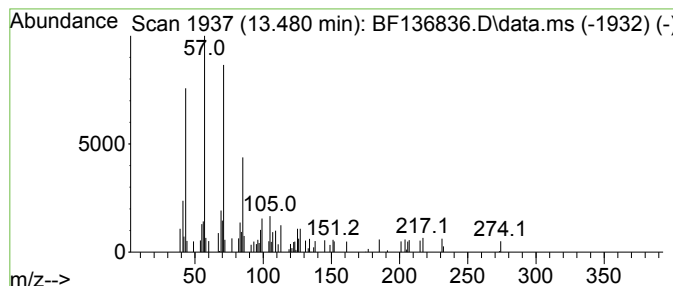
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.480	3.97 ng	77167	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	68
2			Heptacosane	380	C27H56	000593-49-7	64
3			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	64
4			Hexadecane	226	C16H34	000544-76-3	64
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64



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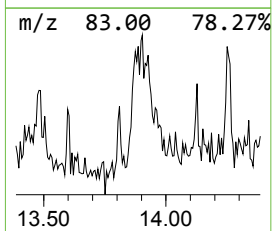
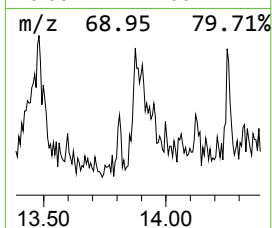
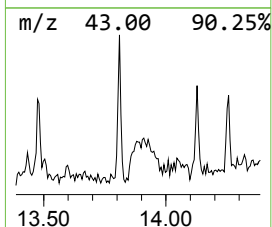
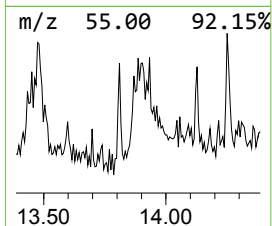
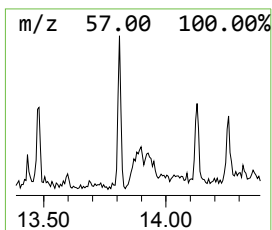
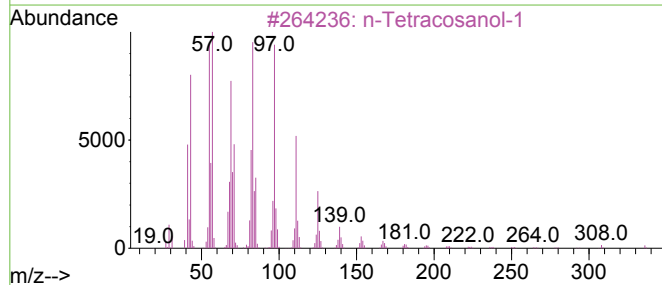
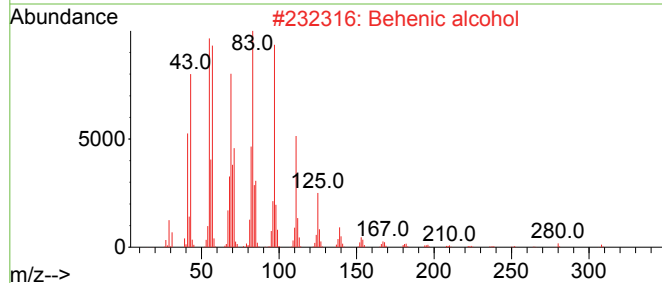
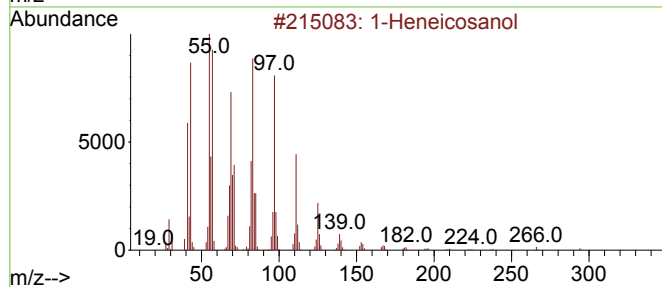
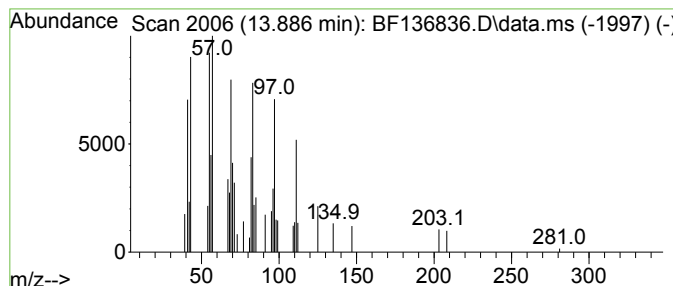
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Heneicosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.886	3.10 ng	60278	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5	1-Octadecanol	270	C18H38O	000112-92-5	87



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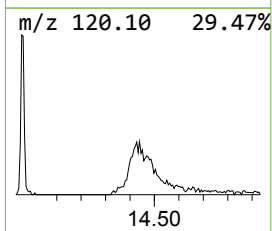
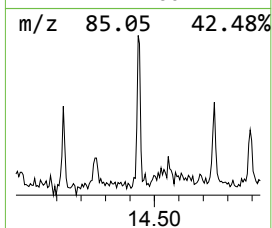
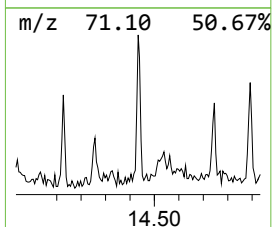
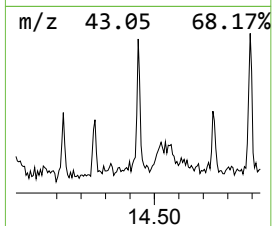
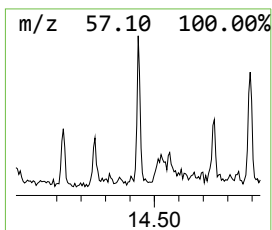
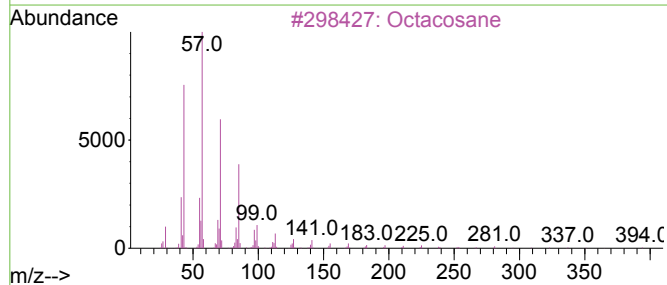
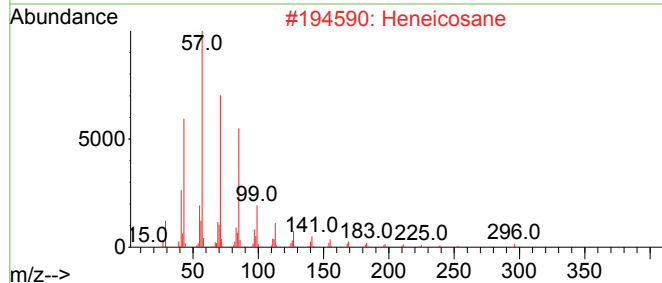
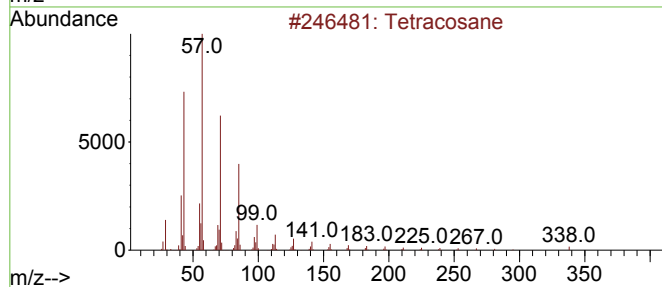
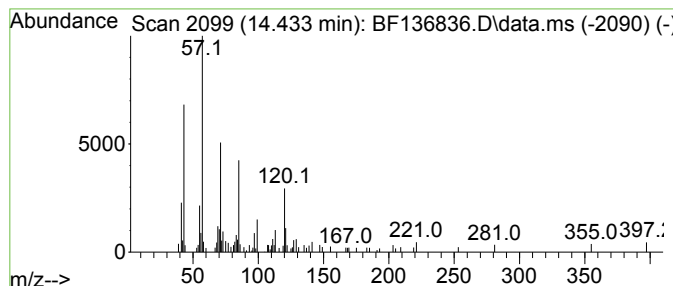
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Peak Number 5 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	4.04 ng	78658	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	62
2			Heneicosane	296	C21H44	000629-94-7	62
3			Octacosane	394	C28H58	000630-02-4	62
4			Nonadecane	268	C19H40	000629-92-5	58
5			Eicosane	282	C20H42	000112-95-8	58



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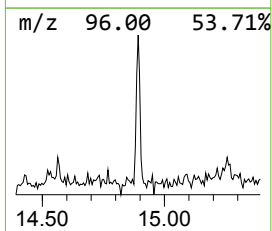
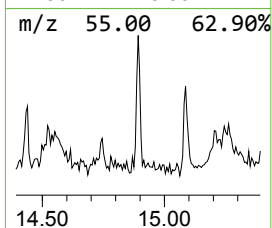
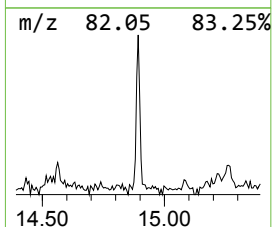
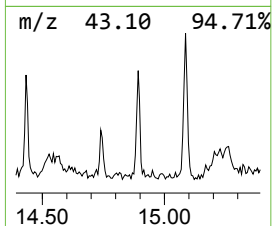
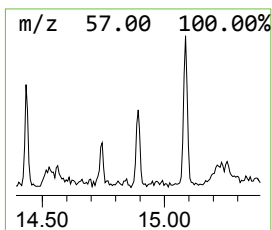
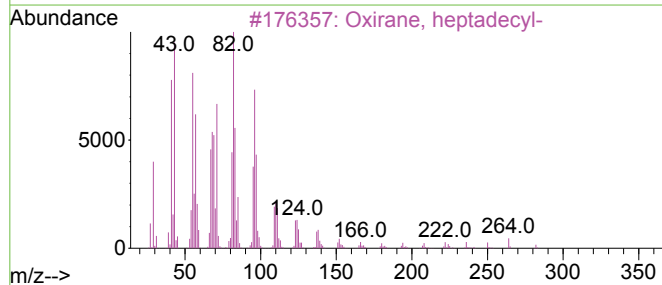
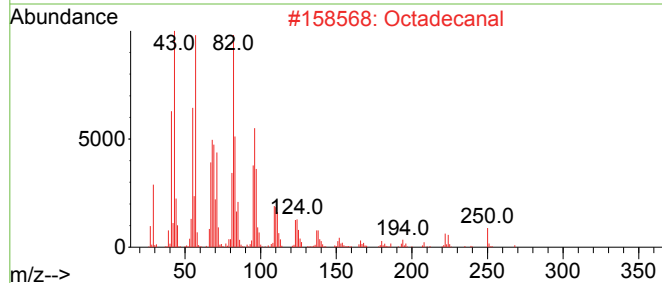
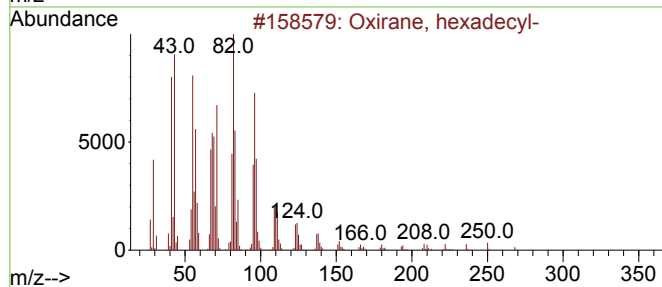
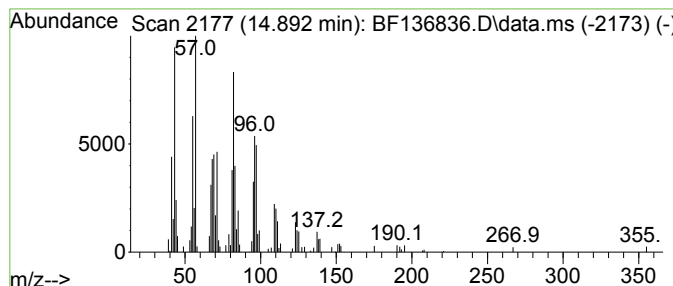
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	3.92 ng	77828	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
2			Octadecanal	268	C18H36O	000638-66-4	90
3			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
4			Eicosanal	296	C20H40O	002400-66-0	90
5			18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136836.D
Acq On : 29 Dec 2023 18:46
Operator : CG\JU
Sample : 05897-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-39

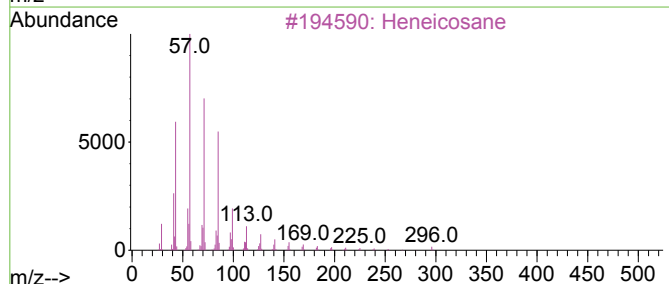
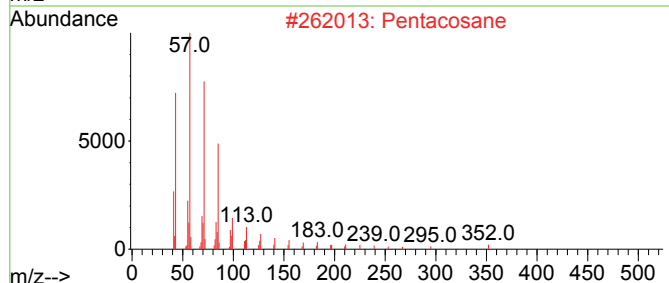
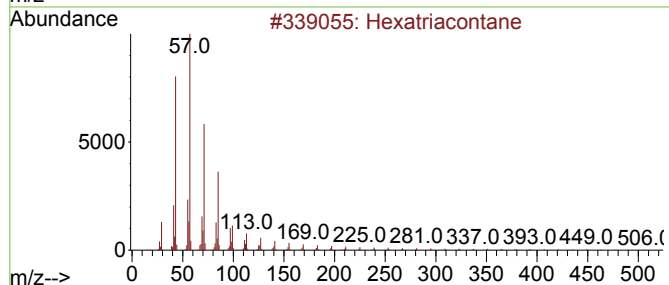
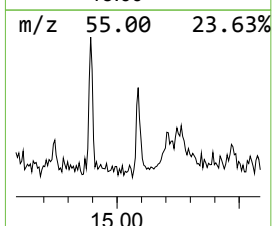
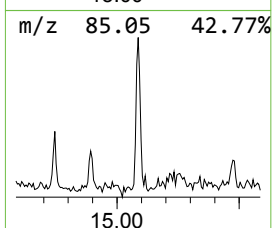
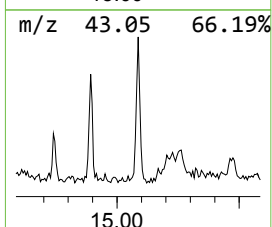
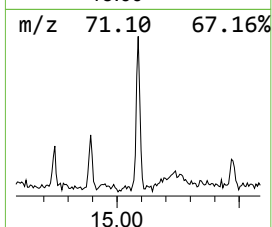
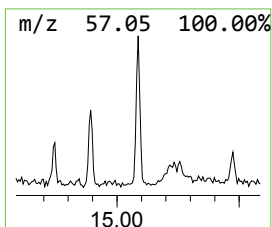
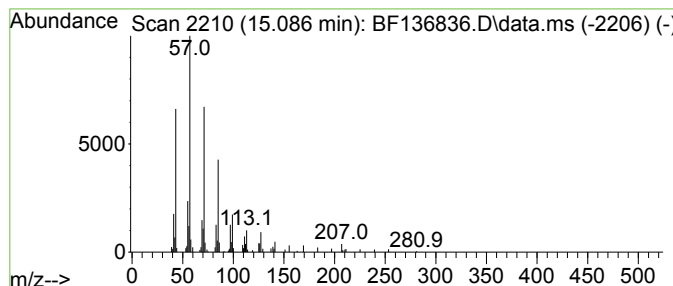
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexatriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	3.99 ng	79131	Perylene-d12	15.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexatriacontane	507	C36H74	000630-06-8	91
2		Pentacosane	352	C25H52	000629-99-2	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136836.D
Acq On : 29 Dec 2023 18:46
Operator : CG\JU
Sample : 05897-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-39

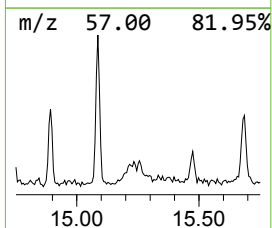
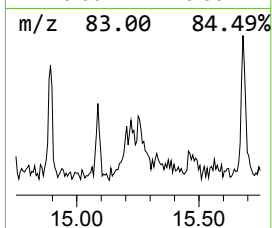
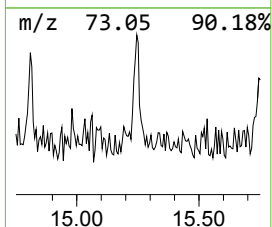
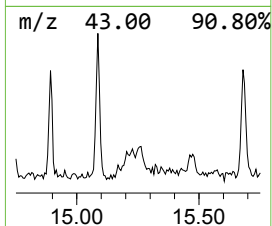
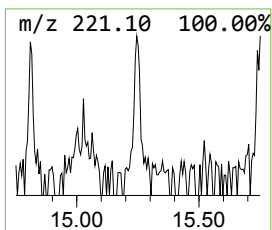
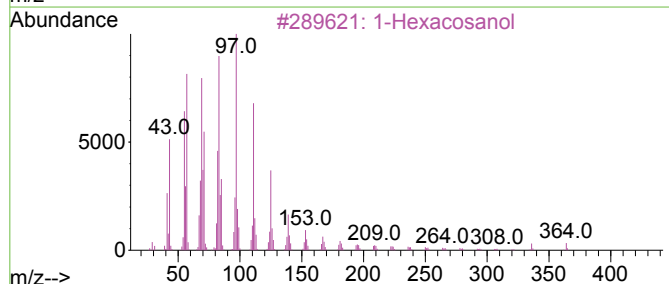
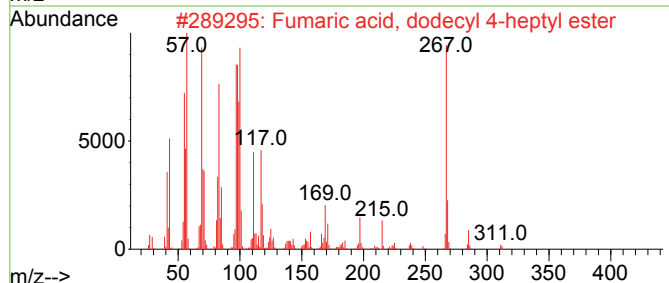
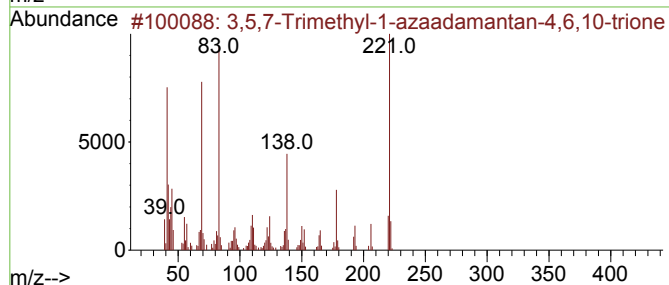
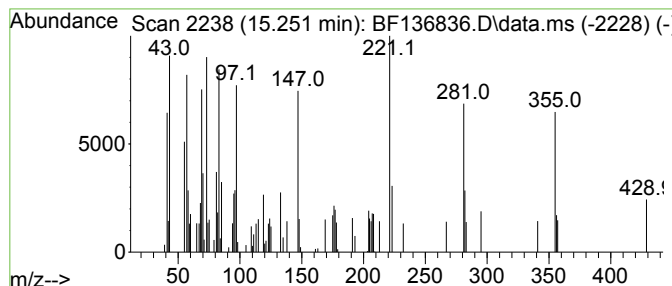
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.251 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.251	3.55 ng	70395	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5,7-Trimethyl-1-azaadamantan-4...	221	C12H15NO3	087510-14-3	35
2			Fumaric acid, dodecyl 4-heptyl e...	382	C23H42O4	1000348-52-2	35
3			1-Hexacosanol	382	C26H54O	000506-52-5	35
4			Silane, [(11-chloroundecyl)oxy]t...	278	C14H31ClOSi	026305-82-8	25
5			Decane, 5,6-bis(2,2-dimethylprop...	278	C20H38	073002-85-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136836.D
Acq On : 29 Dec 2023 18:46
Operator : CG\JU
Sample : 05897-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

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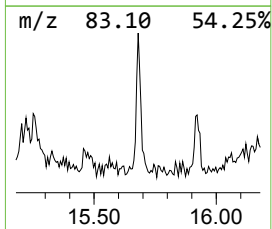
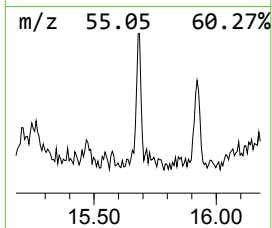
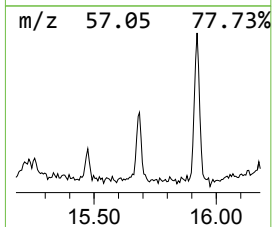
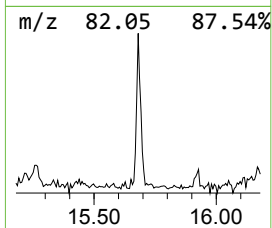
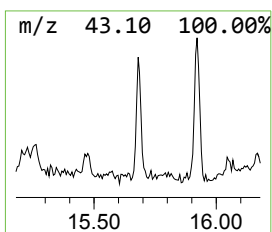
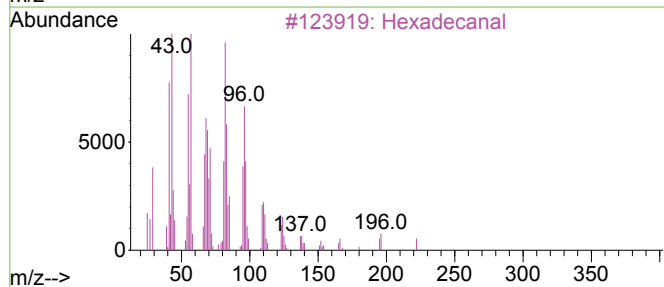
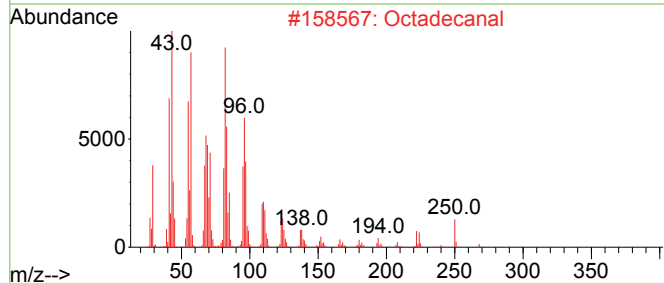
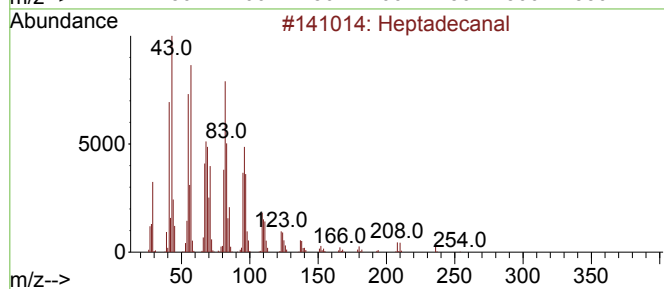
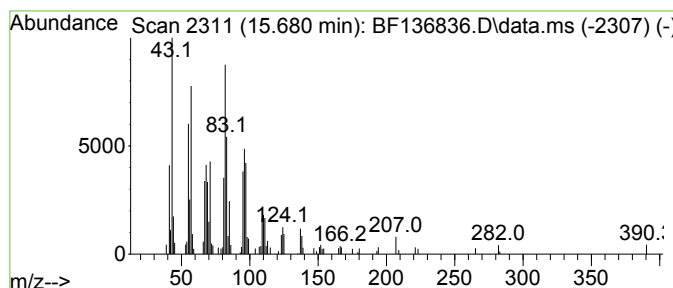
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.680	4.48 ng	88802	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanal	254	C17H34O	1000376-70-0	91
2			Octadecanal	268	C18H36O	000638-66-4	91
3			Hexadecanal	240	C16H32O	000629-80-1	90
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5			Tetracosanal	352	C24H48O	057866-08-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136836.D
Acq On : 29 Dec 2023 18:46
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Sample : 05897-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GHL-SS-39

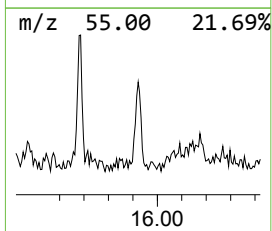
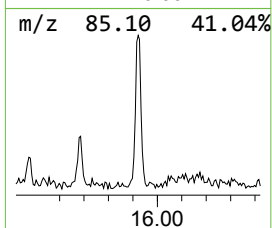
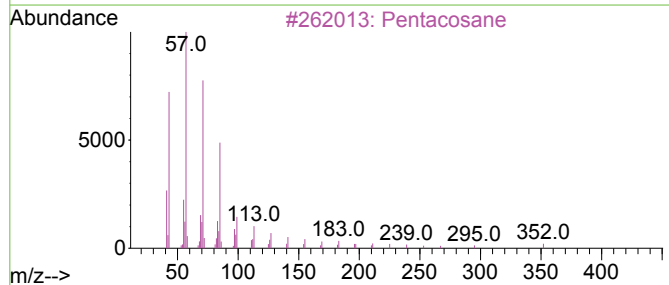
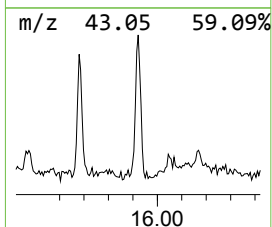
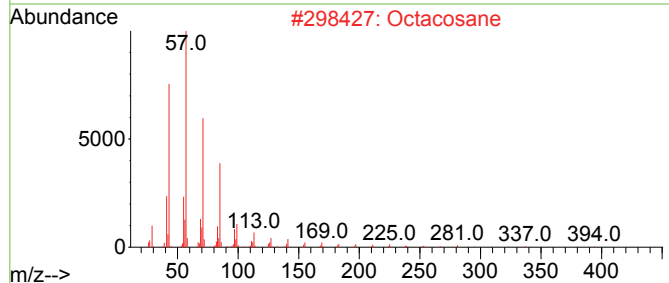
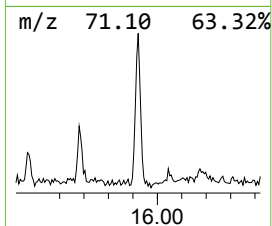
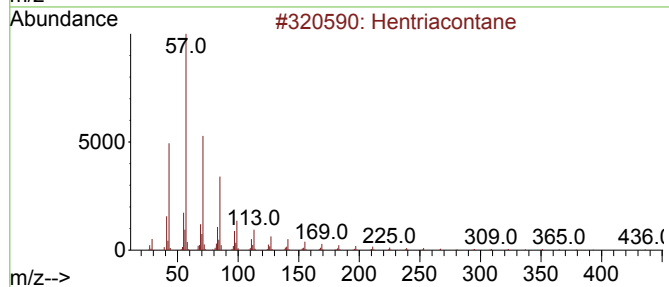
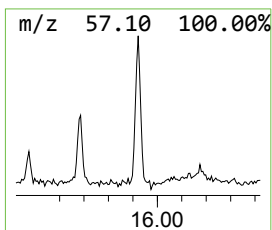
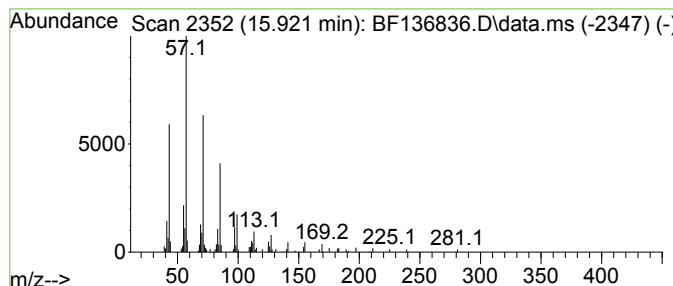
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	4.90 ng	97125	Perylene-d12	15.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136836.D
Acq On : 29 Dec 2023 18:46
Operator : CG\JU
Sample : 05897-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

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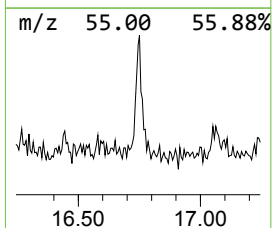
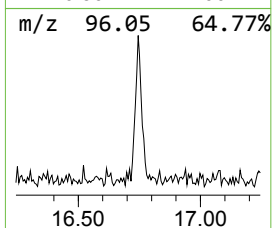
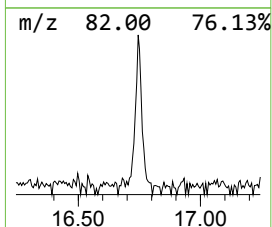
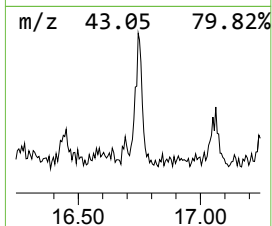
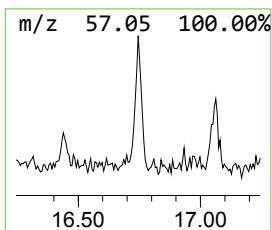
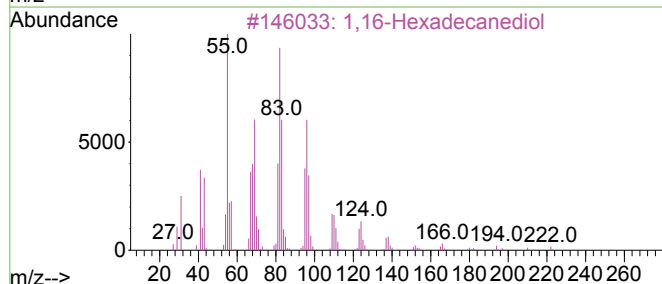
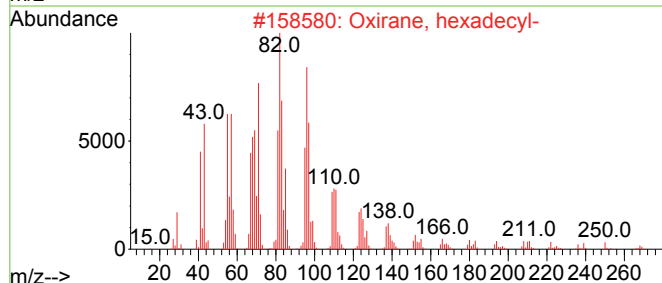
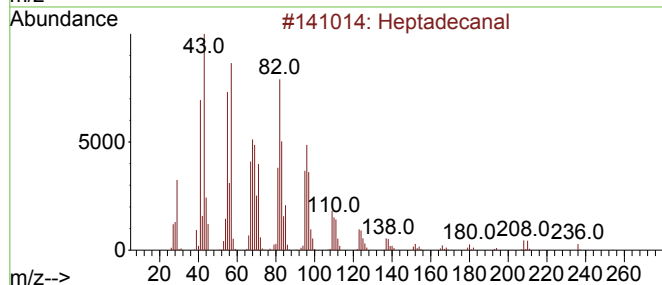
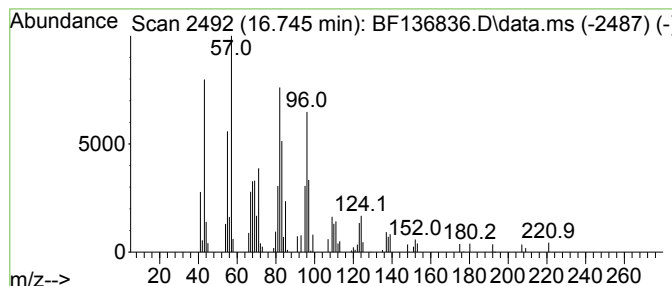
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,16-Hexadecanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	4.42 ng	87620	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanal	254	C17H34O	1000376-70-0	86
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
3			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	58
4			Undecane, 5-cyclohexyl-	238	C17H34	013151-80-9	43
5			Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136836.D
Acq On : 29 Dec 2023 18:46
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Sample : 05897-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

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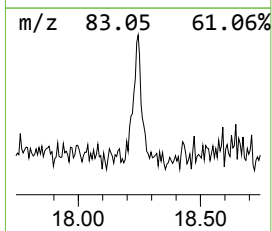
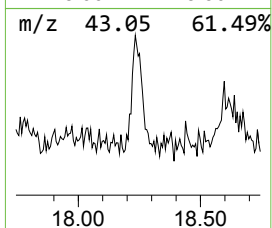
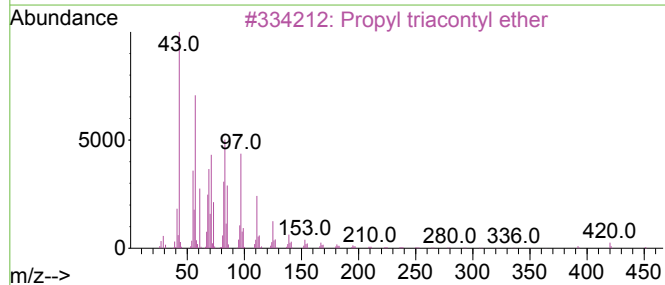
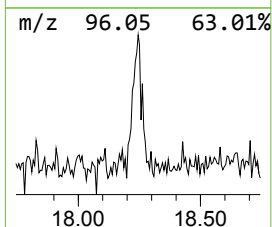
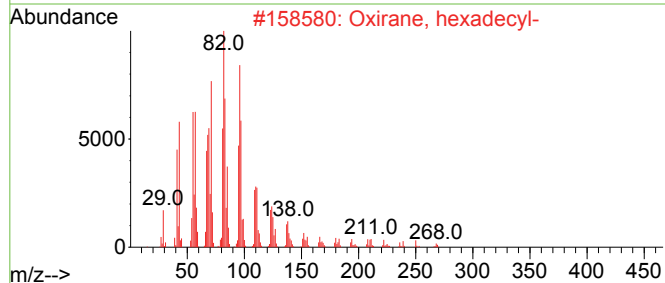
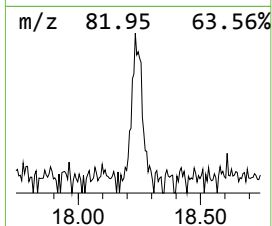
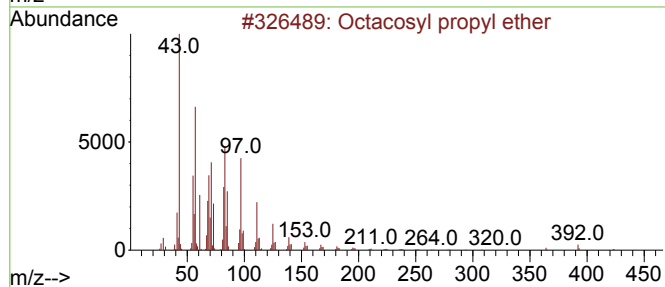
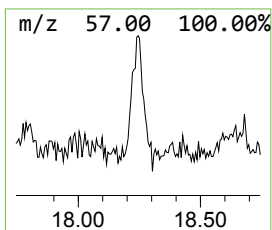
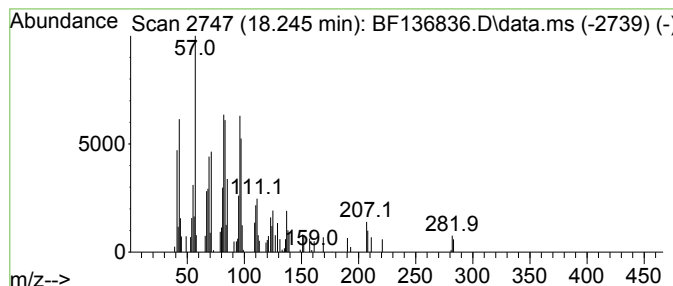
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown18.245 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	4.34 ng	86092	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl propyl ether	452	C31H64O	1000406-28-5	49
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	49
3			Propyl triacontyl ether	481	C33H68O	1000406-28-6	46
4			Methyl tetratriacontyl ether	509	C35H72O	1000406-30-1	46
5			Hexacosyl propyl ether	424	C29H60O	1000406-28-4	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136836.D
Acq On : 29 Dec 2023 18:46
Operator : CG\JU
Sample : 05897-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-39

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
n-Hexadecanoic ...	11.839	8.2	ng	252084	4	11.304	617454	20.0
Octadecanoic acid	12.633	2.3	ng	44758	5	13.963	388950	20.0
Pentacosane	13.480	4.0	ng	77167	5	13.963	388950	20.0
1-Heneicosanol	13.886	3.1	ng	60278	5	13.963	388950	20.0
Tetracosane	14.433	4.0	ng	78658	5	13.963	388950	20.0
Oxirane, hexade...	14.892	3.9	ng	77828	6	15.439	396746	20.0
Hexatriacontane	15.086	4.0	ng	79131	6	15.439	396746	20.0
unknown15.251	15.251	3.5	ng	70395	6	15.439	396746	20.0
Heptadecanal	15.680	4.5	ng	88802	6	15.439	396746	20.0
Hentriacontane	15.921	4.9	ng	97125	6	15.439	396746	20.0
1,16-Hexadecane...	16.745	4.4	ng	87620	6	15.439	396746	20.0
unknown18.245	18.245	4.3	ng	86092	6	15.439	396746	20.0