

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
 Data File : BF136388.D
 Acq On : 04 Dec 2023 18:31
 Operator : CG\JU
 Sample : 05434-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-6

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136388.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.045	498	503	509	rVB	36572	46822	1.55%	0.217%
2	5.440	565	570	573	rBV	2722341	2467972	81.62%	11.444%
3	6.440	735	740	743	rBV	2339056	2425996	80.23%	11.249%
4	6.634	769	773	779	rBV	33377	38222	1.26%	0.177%
5	6.804	798	802	805	rBV	885103	714173	23.62%	3.312%
6	7.363	892	897	900	rBV	1798685	1544523	51.08%	7.162%
7	8.081	1015	1019	1022	rBV	1119519	892634	29.52%	4.139%
8	9.157	1198	1202	1205	rBV	3767158	3023732	100.00%	14.021%
9	9.275	1218	1222	1226	rVB	49111	43899	1.45%	0.204%
10	9.833	1314	1317	1321	rVB	1084451	887714	29.36%	4.116%
11	10.627	1448	1452	1455	rBV	1790926	1458831	48.25%	6.764%
12	11.327	1567	1571	1574	rBV	1013069	822165	27.19%	3.812%
13	11.863	1658	1662	1672	rBV	366176	395885	13.09%	1.836%
14	12.045	1688	1693	1702	rBV3	32623	64053	2.12%	0.297%
15	12.545	1775	1778	1781	rBV	132699	130716	4.32%	0.606%
16	12.592	1781	1786	1791	rVB	161624	171946	5.69%	0.797%
17	12.651	1793	1796	1803	rBV4	93715	108451	3.59%	0.503%
18	12.751	1809	1813	1815	rBV	364403	319535	10.57%	1.482%
19	12.774	1815	1817	1819	rVV	123651	95082	3.14%	0.441%
20	12.821	1823	1825	1830	rVB2	64839	63170	2.09%	0.293%
21	12.927	1838	1843	1846	rBV	3134728	2765704	91.47%	12.824%
22	13.163	1880	1883	1887	rBV2	58506	60925	2.01%	0.283%
23	13.316	1906	1909	1913	rVB	86554	72138	2.39%	0.334%
24	13.463	1930	1934	1937	rBV	233923	215981	7.14%	1.001%
25	13.504	1938	1941	1944	rVV	63473	59077	1.95%	0.274%
26	13.857	1994	2001	2012	rBV3	156743	457450	15.13%	2.121%
27	13.980	2017	2022	2025	rVV	959495	897432	29.68%	4.161%
28	14.004	2025	2026	2030	rVB	79156	51737	1.71%	0.240%
29	14.157	2049	2052	2055	rBV	92456	78584	2.60%	0.364%
30	14.463	2101	2104	2107	rBV	153836	132588	4.38%	0.615%
31	14.774	2154	2157	2160	rBV	88764	87538	2.90%	0.406%
32	14.921	2180	2182	2188	rVB3	64985	77817	2.57%	0.361%
33	15.027	2197	2200	2208	rVB2	75177	144950	4.79%	0.672%
34	15.121	2213	2216	2222	rVB2	126705	169839	5.62%	0.788%
35	15.462	2270	2274	2279	rBV	470380	578740	19.14%	2.684%

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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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

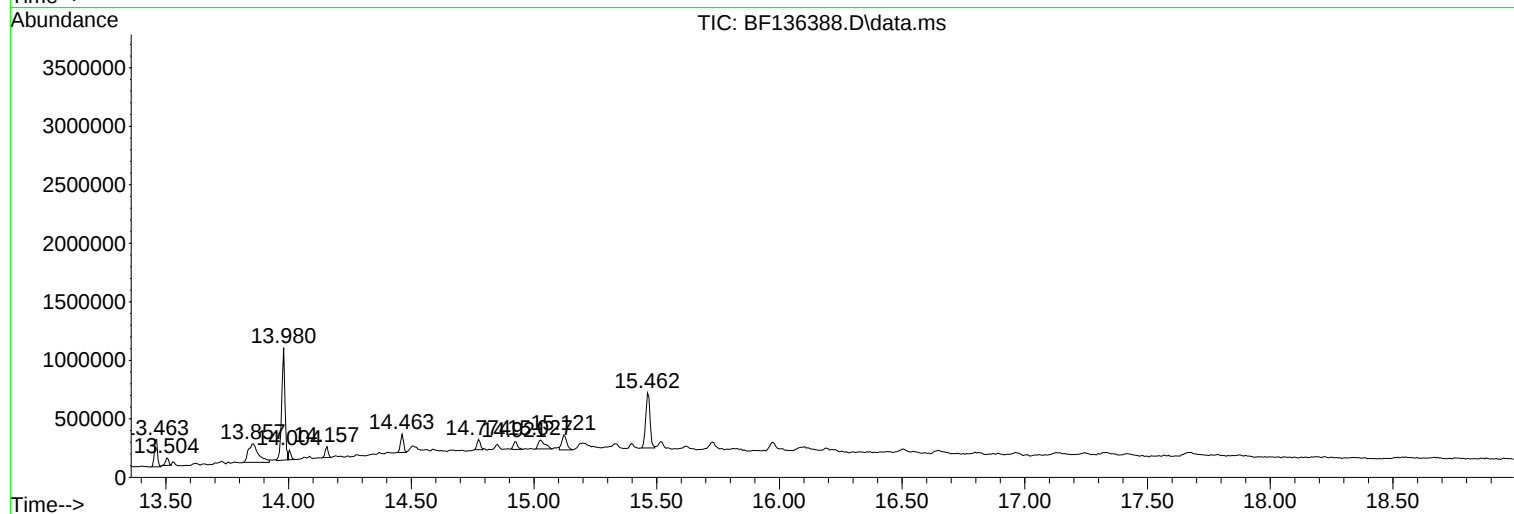
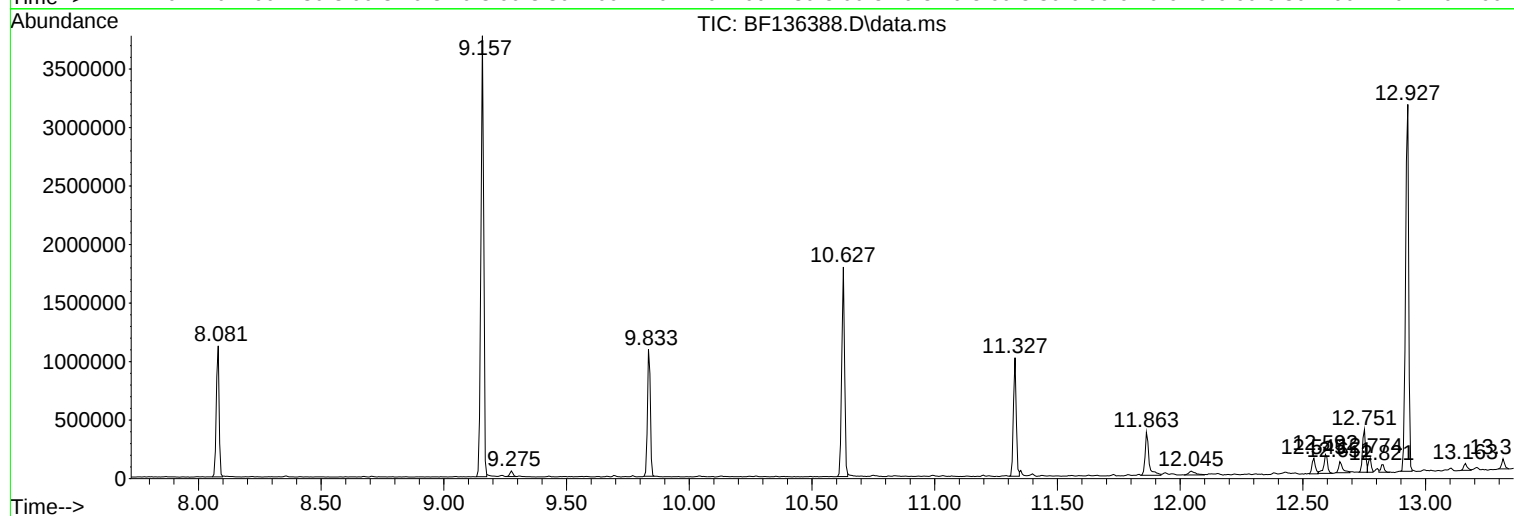
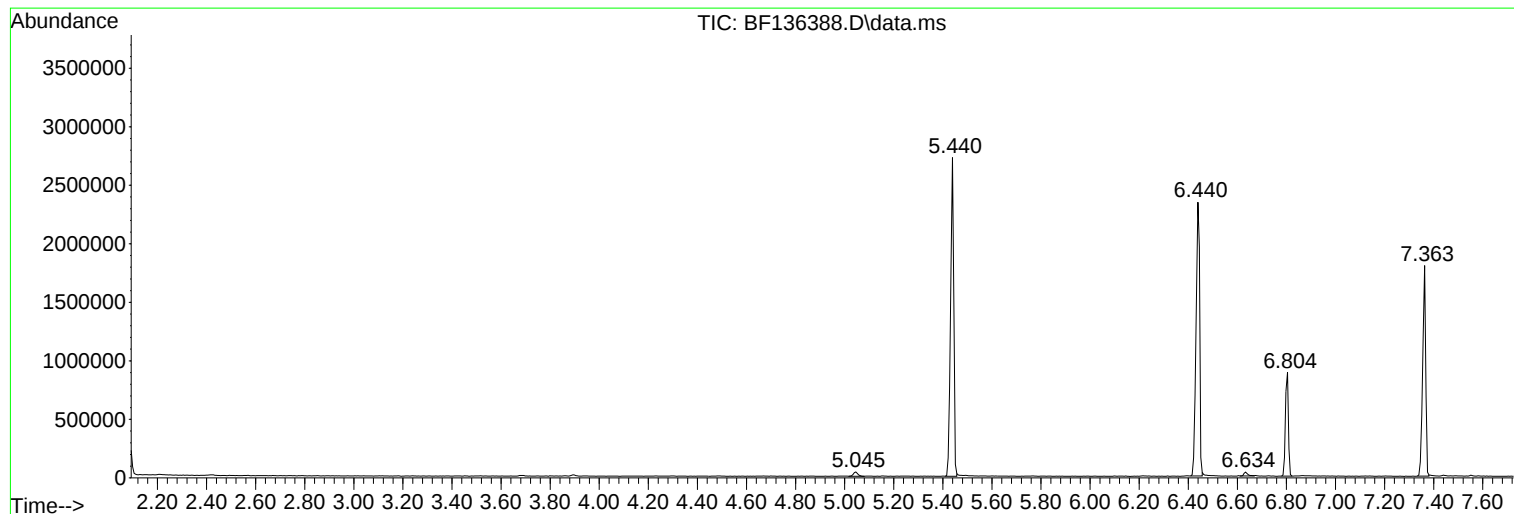
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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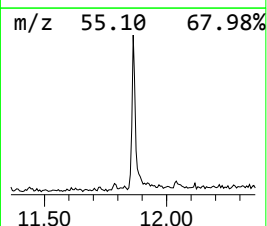
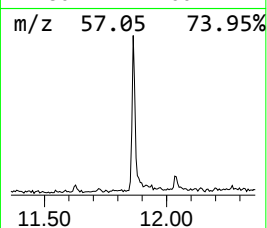
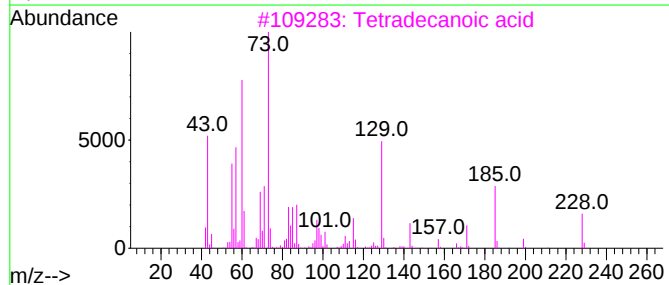
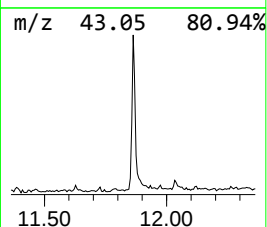
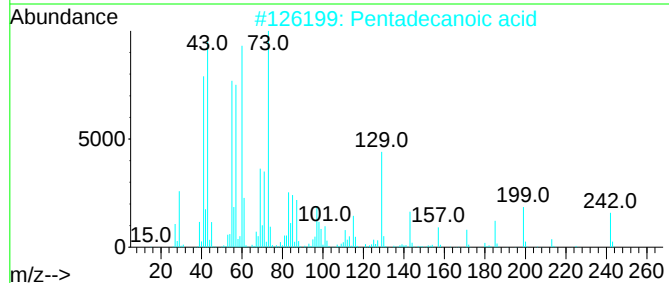
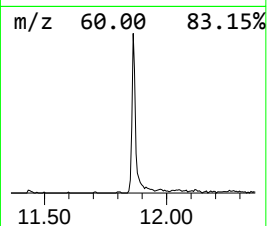
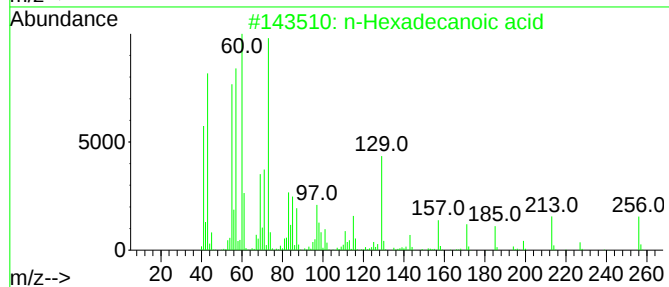
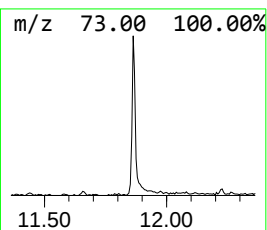
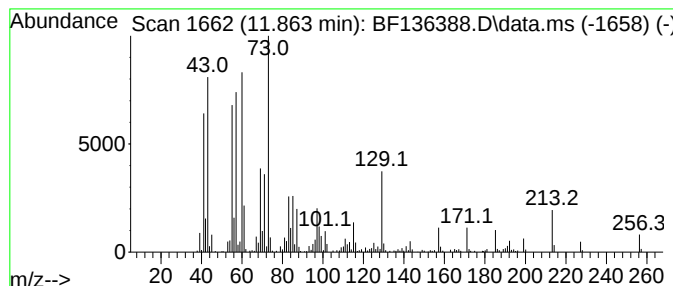
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	9.63 ng	395885	Phenanthrene-d10	11.327

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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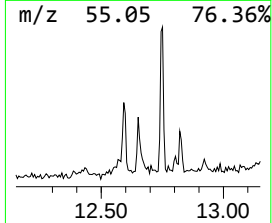
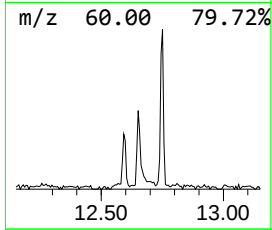
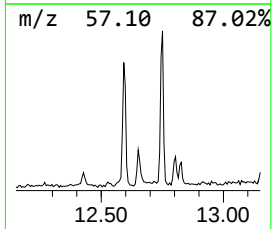
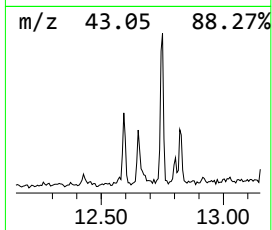
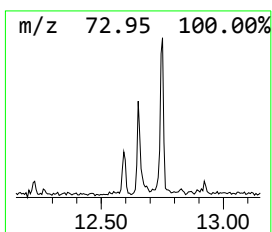
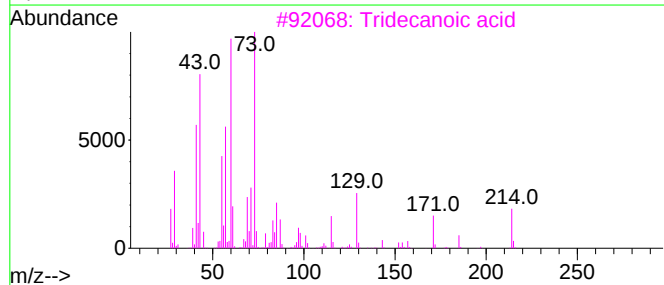
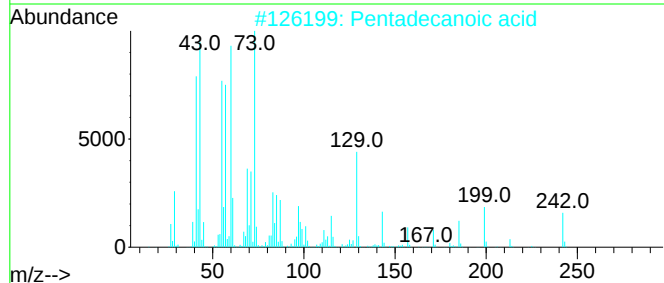
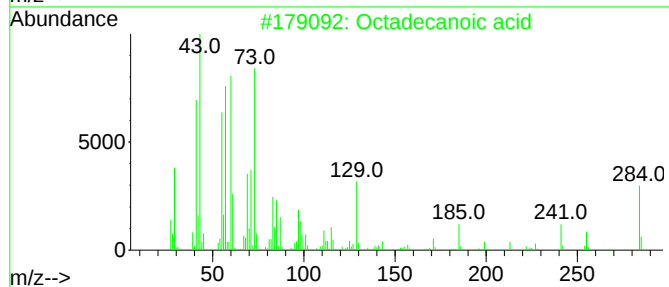
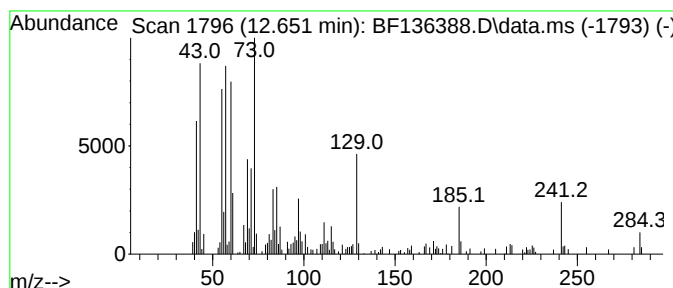
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.64 ng	108451	Phenanthrene-d10	11.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	55
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	30



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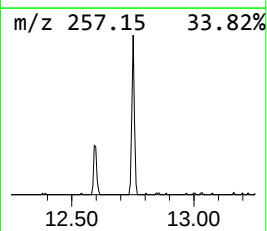
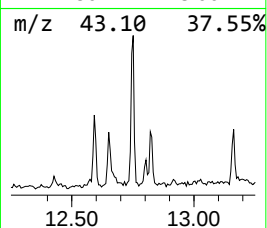
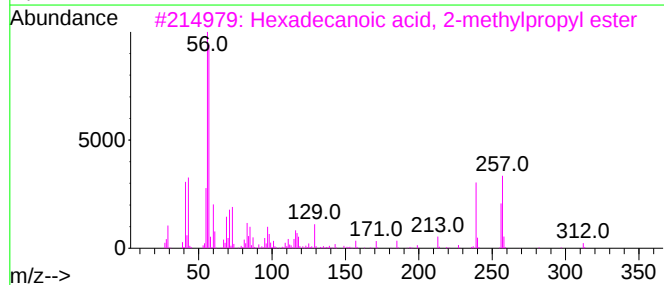
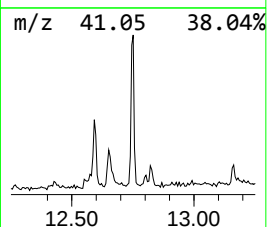
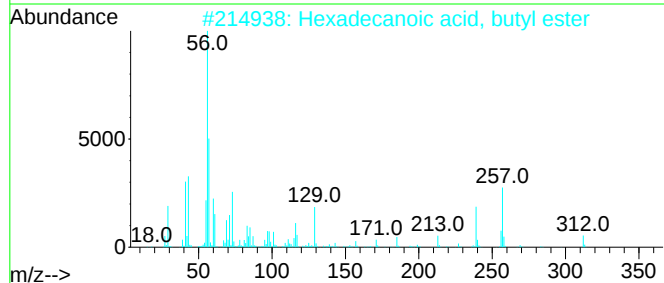
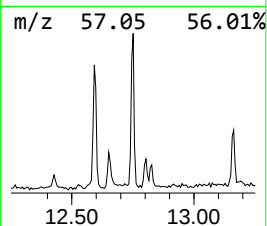
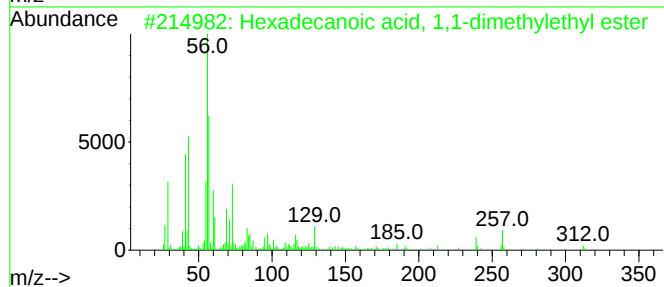
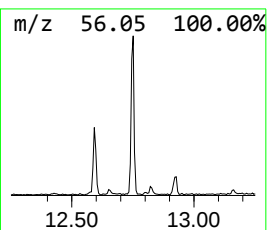
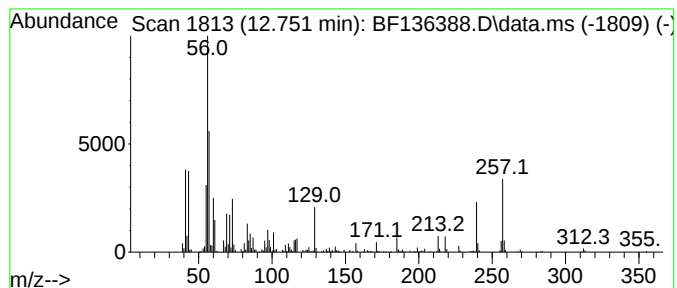
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	7.12 ng	319535	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	78
4			Nipecotic acid	129	C6H11NO2	000498-95-3	47
5			1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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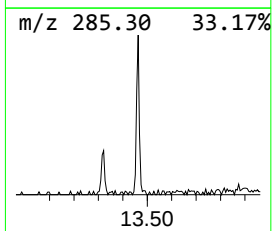
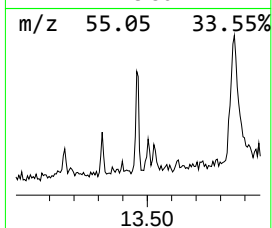
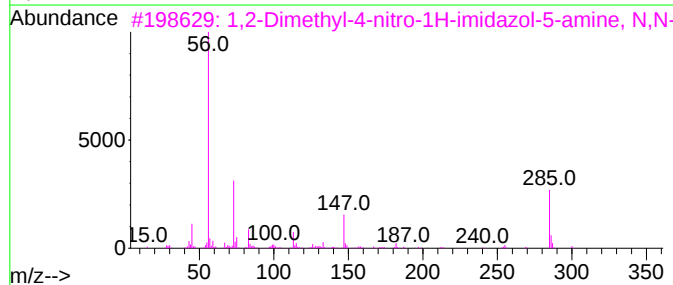
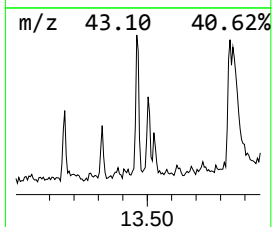
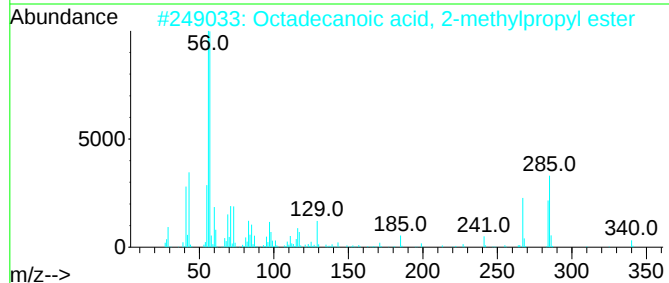
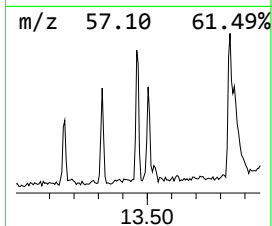
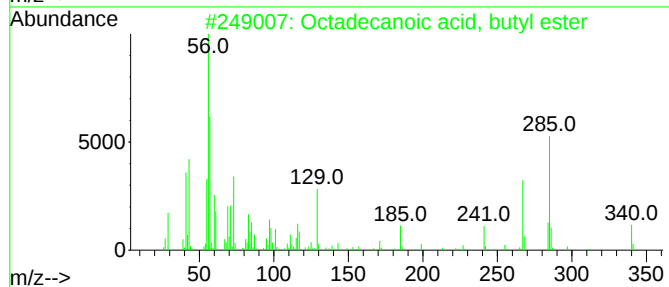
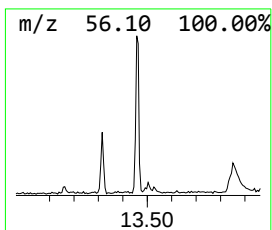
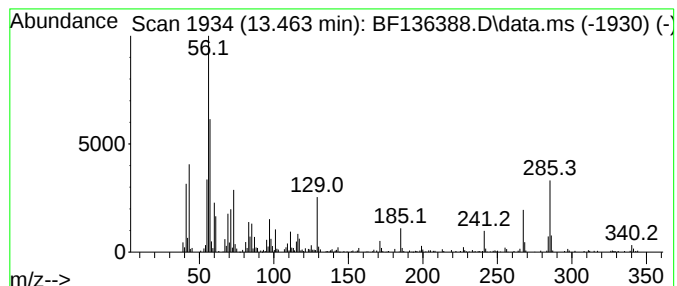
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.463	4.81 ng	215981	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	89
3	1,2-Dimethyl-4-nitro-1H-imidazol...	300	C11H24N4O2Si2	1010471-87-3	47
4	Nipecotic acid	129	C6H11NO2	000498-95-3	43
5	N-(1,5-Dimethyl-3-oxo-2-phenyl-2...	331	C17H25N3O2Si	1000487-90-4	35



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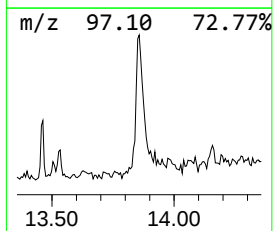
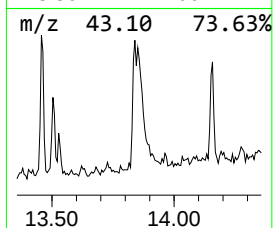
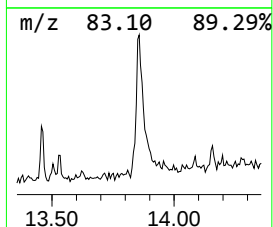
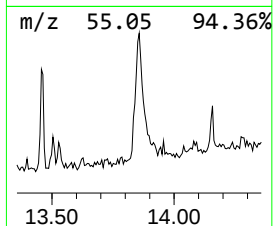
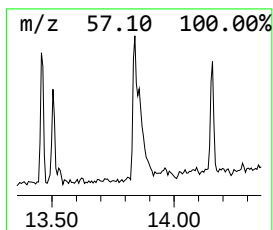
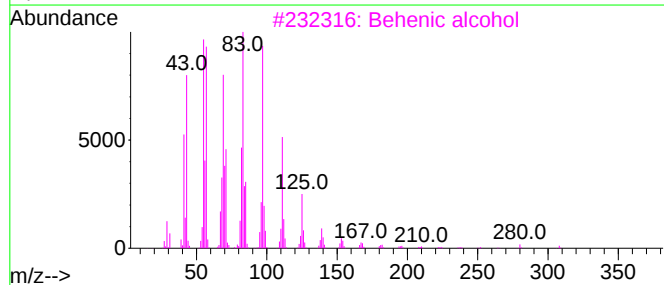
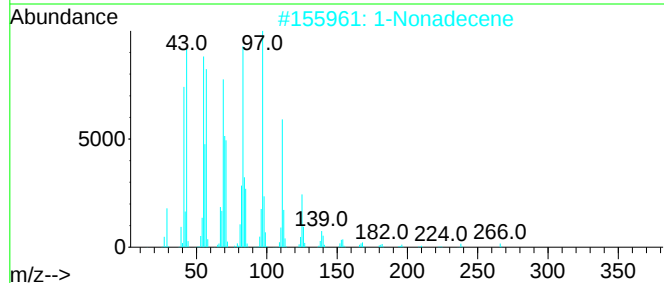
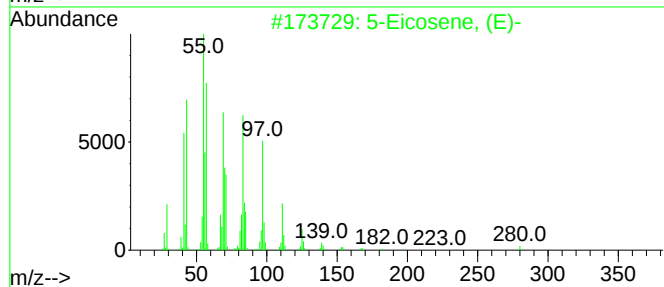
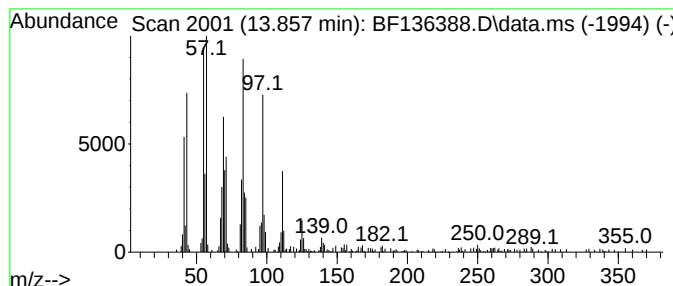
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.857	10.19 ng	457450	Chrysene-d12		13.980	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	1-Nonadecene		266	C19H38	018435-45-5	97
3	Behenic alcohol		326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
5	1-Heptadecene		238	C17H34	006765-39-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136388.D
Acq On : 04 Dec 2023 18:31
Operator : CG\JU
Sample : 05434-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-6

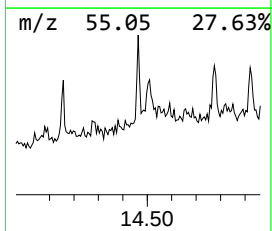
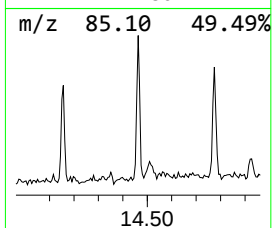
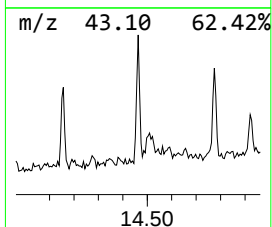
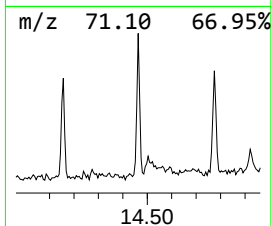
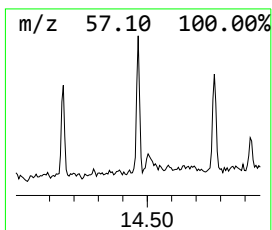
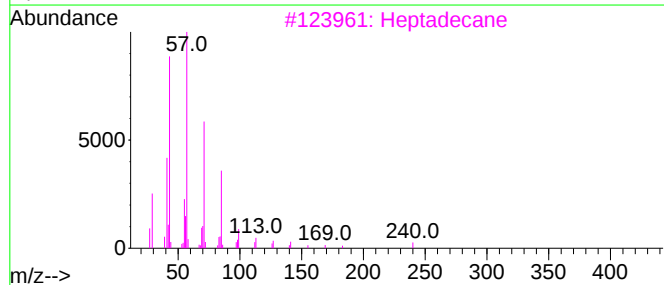
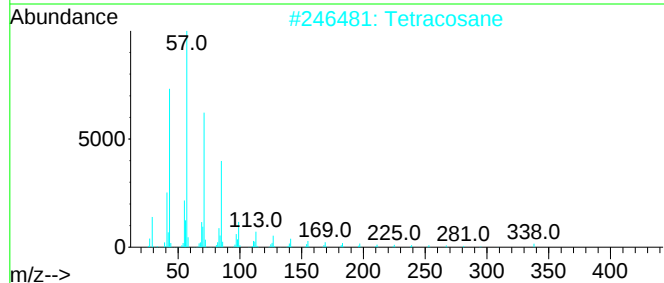
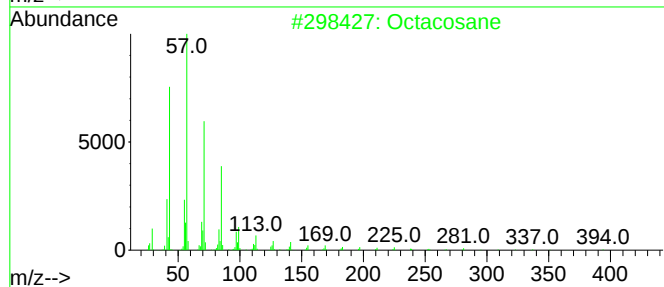
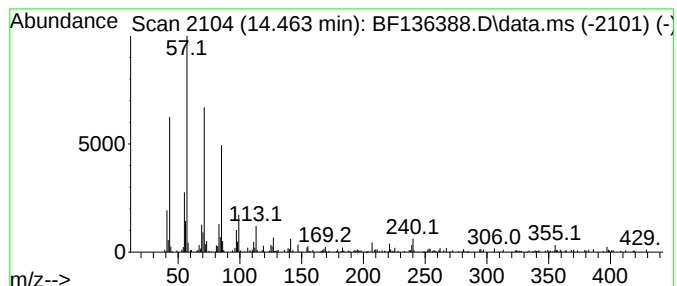
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	2.95 ng	132588	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	99
2			Tetracosane	338	C24H50	000646-31-1	95
3			Heptadecane	240	C17H36	000629-78-7	94
4			Nonacosane	408	C29H60	000630-03-5	93
5			Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136388.D
Acq On : 04 Dec 2023 18:31
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Instrument :
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ClientSampleId :
COMP-6

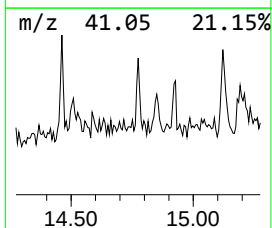
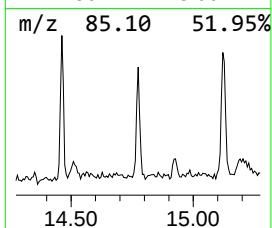
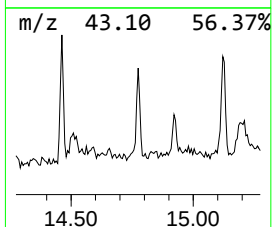
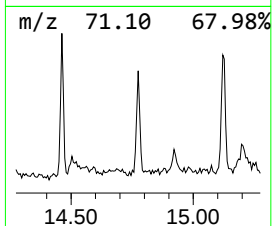
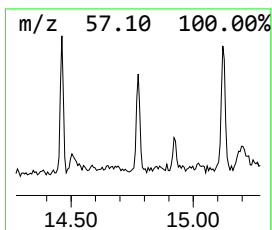
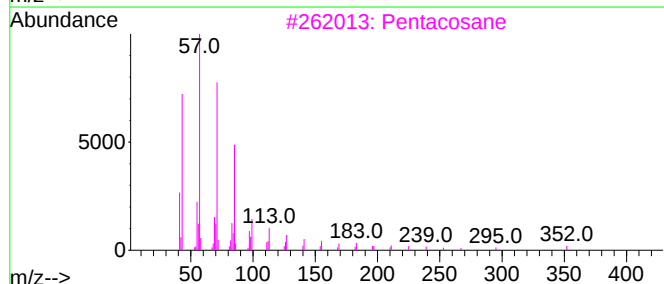
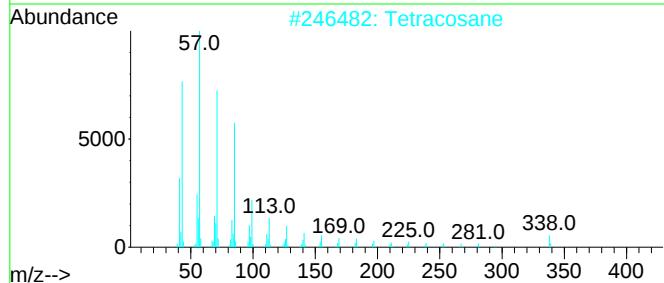
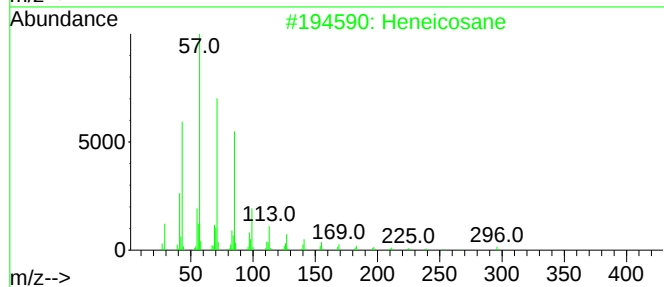
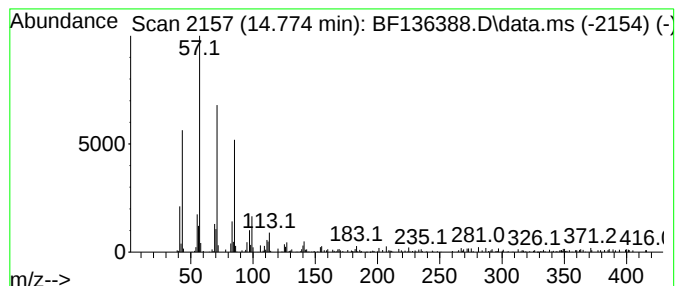
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	3.03 ng	87538	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	97
2		Tetracosane	338	C24H50	000646-31-1	95
3		Pentacosane	352	C25H52	000629-99-2	91
4		Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
5		Tridecane, 7-propyl-	226	C16H34	055045-09-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136388.D
Acq On : 04 Dec 2023 18:31
Operator : CG\JU
Sample : 05434-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-6

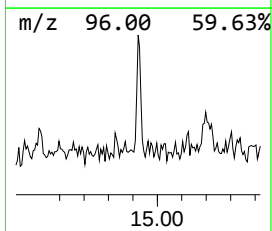
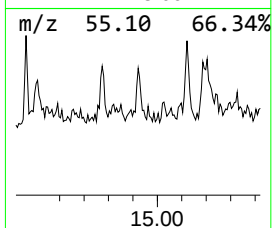
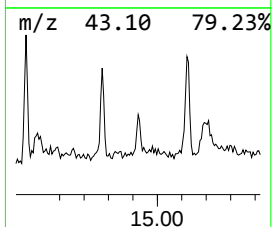
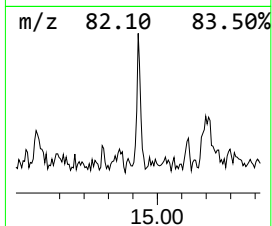
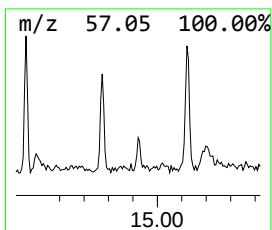
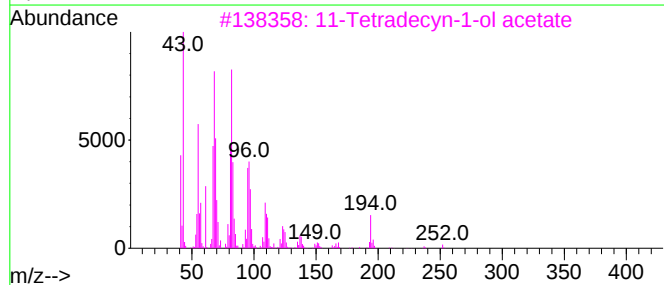
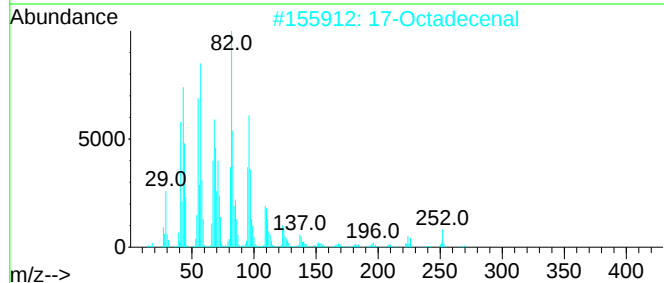
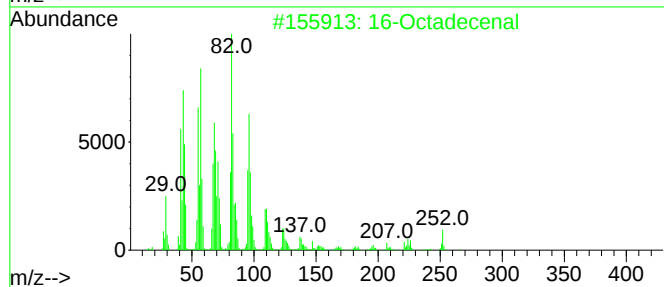
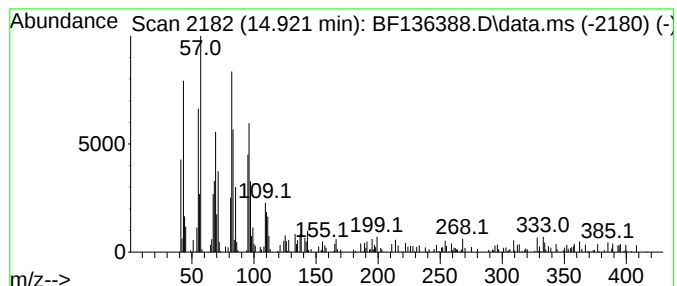
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 16-Octadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	2.69 ng	77817	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			16-Octadecenal	266	C18H34O	056554-87-1	90
2			17-Octadecenal	266	C18H34O	056554-86-0	87
3			11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	87
4			Henicosanal	310	C21H42O	051227-32-8	86
5			Tetracosanal	352	C24H48O	057866-08-7	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136388.D
Acq On : 04 Dec 2023 18:31
Operator : CG\JU
Sample : 05434-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

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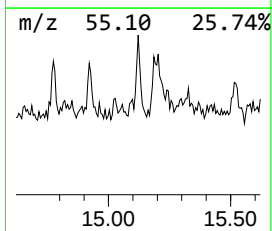
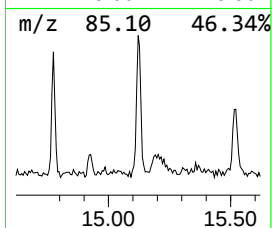
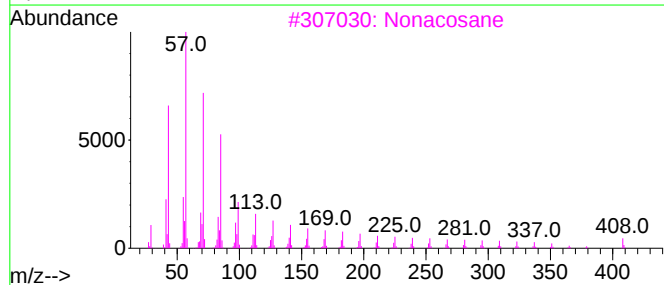
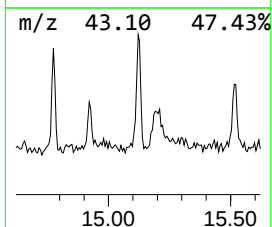
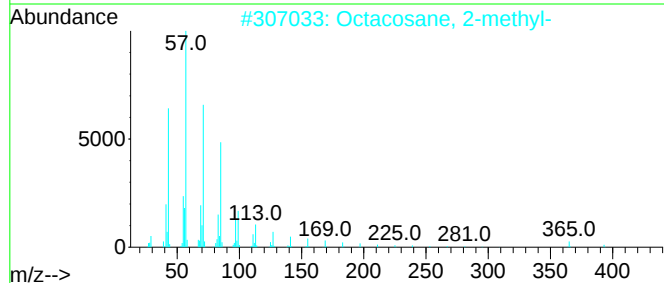
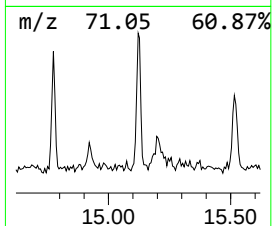
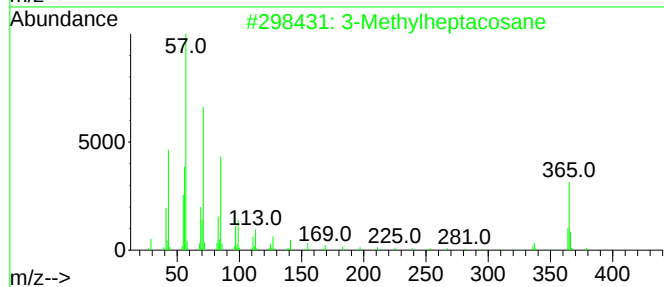
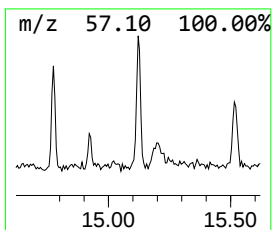
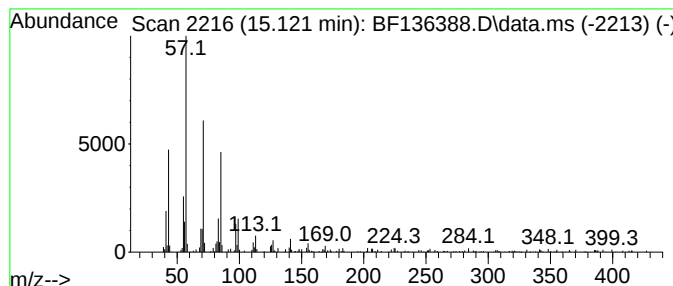
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 3-Methylheptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	5.87 ng	169839	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methylheptacosane	394	C28H58	014167-66-9	93
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3		Nonacosane	408	C29H60	000630-03-5	90
4		Octacosane	394	C28H58	000630-02-4	90
5		2-Methylpentacosane	366	C26H54	000629-87-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136388.D
Acq On : 04 Dec 2023 18:31
Operator : CG\JU
Sample : 05434-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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
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Octadecanoic acid	12.651	2.6	ng	108451	4	11.327	822165	20.0
Hexadecanoic ac...	12.751	7.1	ng	319535	5	13.980	897432	20.0
Octadecanoic ac...	13.463	4.8	ng	215981	5	13.980	897432	20.0
5-Eicosene, (E)-	13.857	10.2	ng	457450	5	13.980	897432	20.0
Octacosane	14.463	3.0	ng	132588	5	13.980	897432	20.0
Heneicosane	14.774	3.0	ng	87538	6	15.463	578740	20.0
16-Octadecenal	14.921	2.7	ng	77817	6	15.463	578740	20.0
3-Methylheptaco...	15.121	5.9	ng	169839	6	15.463	578740	20.0