

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
 Data File : BF133208.D
 Acq On : 03 May 2023 15:40
 Operator : CG\JU
 Sample : 02583-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CF-22

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-BF042123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133208.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.340	549	553	557	rBV	3518208	3394433	82.32%	11.618%
2	6.369	723	728	731	rBV	3789486	3468732	84.12%	11.872%
3	6.728	786	789	792	rBV	1414301	1061948	25.75%	3.635%
4	7.292	881	885	888	rBV	2785162	2290729	55.55%	7.840%
5	8.010	1004	1007	1011	rBV	1729393	1462065	35.46%	5.004%
6	9.092	1187	1191	1194	rBV	4793216	4123407	100.00%	14.113%
7	9.763	1302	1305	1309	rBV	1963775	1622590	39.35%	5.554%
8	10.475	1423	1426	1430	rBV	360414	270970	6.57%	0.927%
9	10.551	1435	1439	1449	rBV	747548	718350	17.42%	2.459%
10	11.245	1554	1557	1561	rBV	1788342	1502994	36.45%	5.144%
11	11.780	1640	1648	1659	rBV3	180422	382533	9.28%	1.309%
12	12.045	1685	1693	1698	rVB	105226	153604	3.73%	0.526%
13	12.363	1742	1747	1751	rBV	52819	72592	1.76%	0.248%
14	12.433	1755	1759	1765	rVB2	60895	79031	1.92%	0.270%
15	12.563	1776	1781	1793	rBV2	132978	284172	6.89%	0.973%
16	12.833	1823	1827	1830	rBV	3840364	3197617	77.55%	10.944%
17	13.416	1923	1926	1929	rVB	72837	56455	1.37%	0.193%
18	13.745	1979	1982	1984	rBV	72204	61232	1.48%	0.210%
19	13.792	1984	1990	2001	rVV6	72724	273798	6.64%	0.937%
20	13.880	2001	2005	2009	rVB	1133786	936895	22.72%	3.207%
21	14.063	2033	2036	2039	rVB	56845	47312	1.15%	0.162%
22	14.498	2096	2110	2132	rBV7	172371	1295145	31.41%	4.433%
23	14.663	2135	2138	2141	rVB	55704	51534	1.25%	0.176%
24	14.733	2147	2150	2154	rVB	216192	191987	4.66%	0.657%
25	14.804	2158	2162	2166	rVB	308328	326952	7.93%	1.119%
26	14.986	2190	2193	2198	rVB	62246	64008	1.55%	0.219%
27	15.304	2242	2247	2252	rBV	914359	1059003	25.68%	3.625%
28	15.345	2252	2254	2259	rVB2	55109	62886	1.53%	0.215%
29	15.762	2322	2325	2330	rVB2	51575	67352	1.63%	0.231%
30	18.109	2717	2724	2743	rVB3	155608	636523	15.44%	2.179%

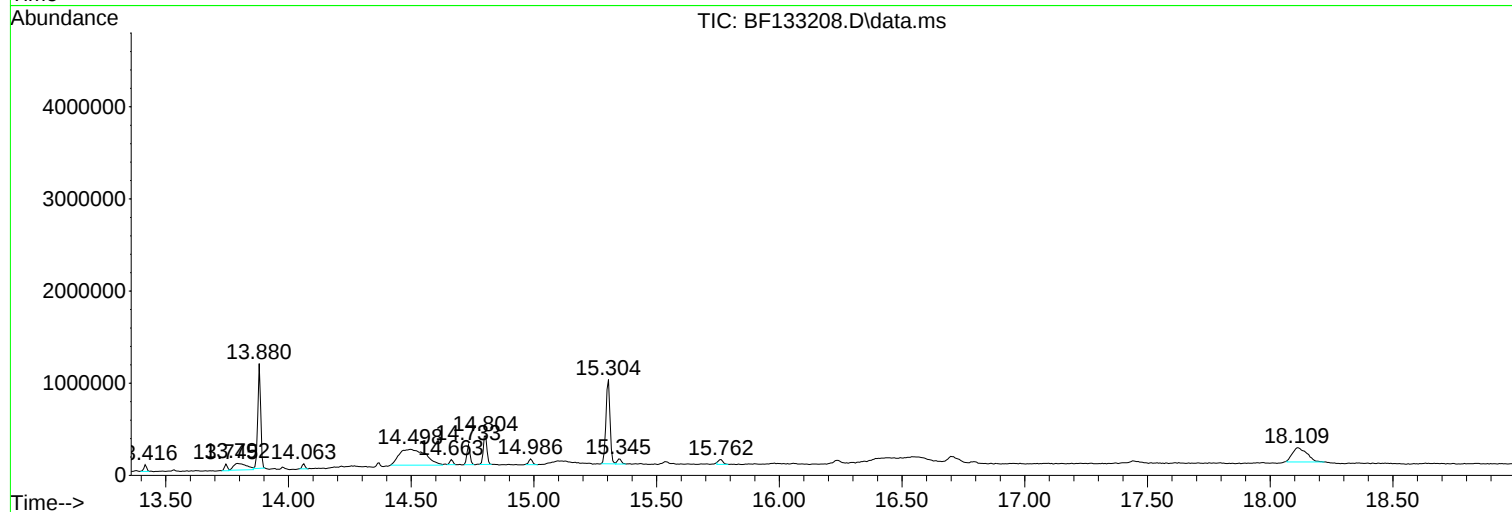
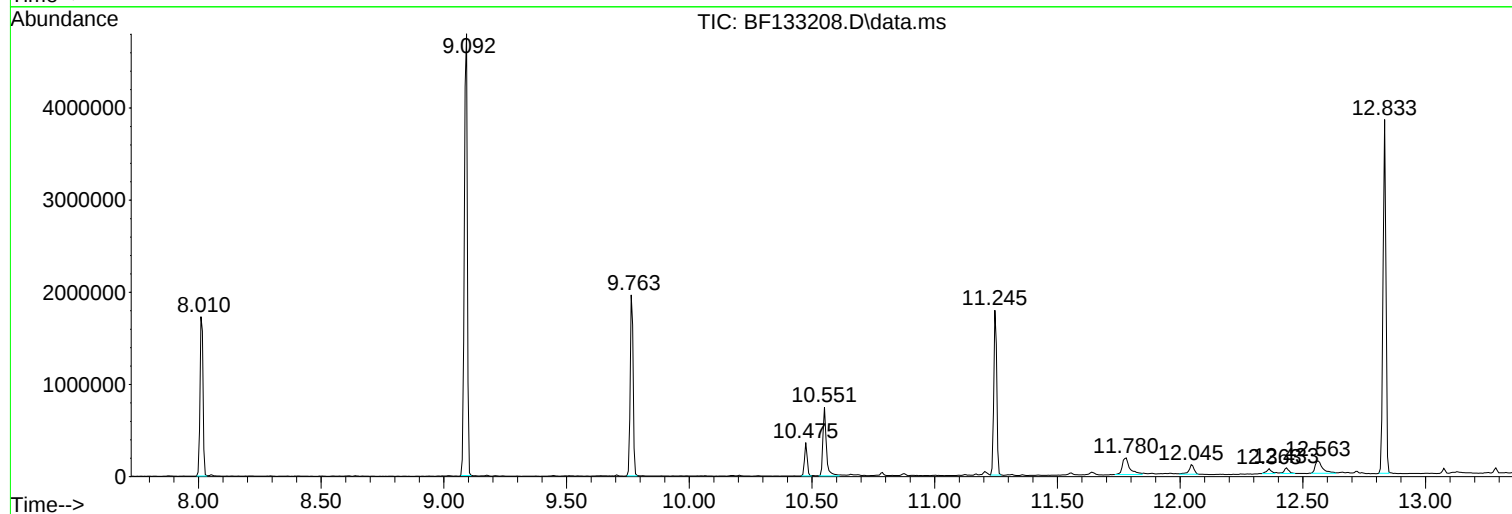
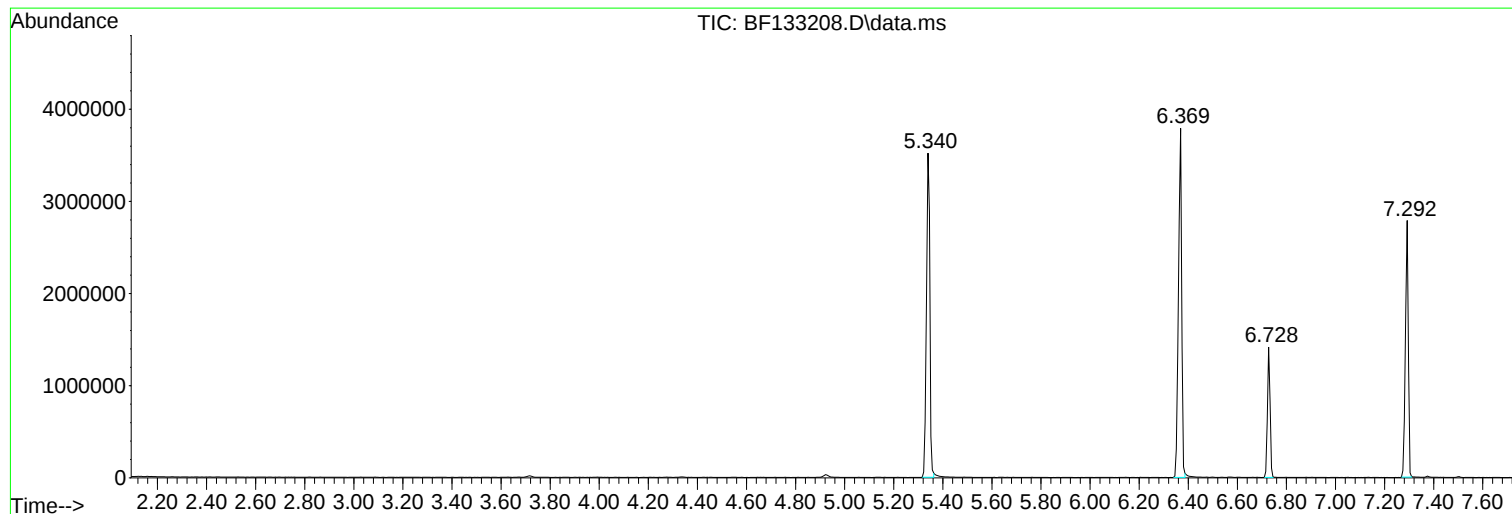
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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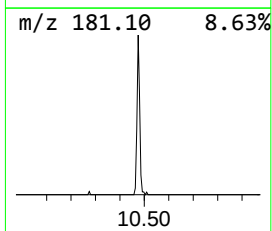
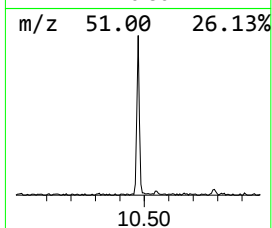
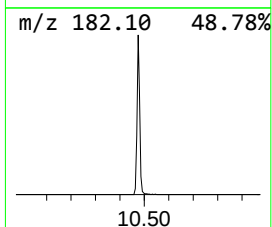
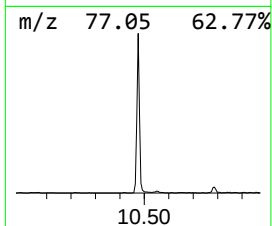
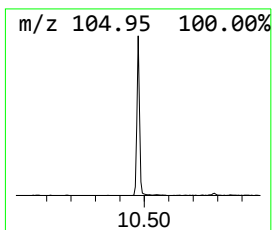
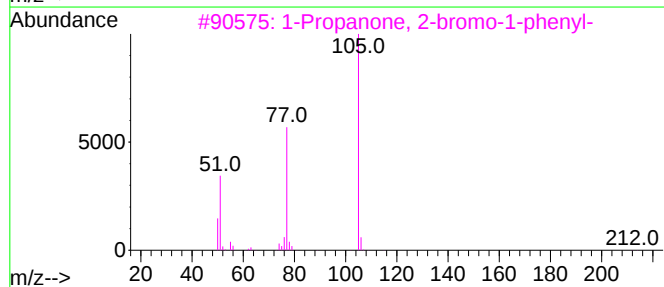
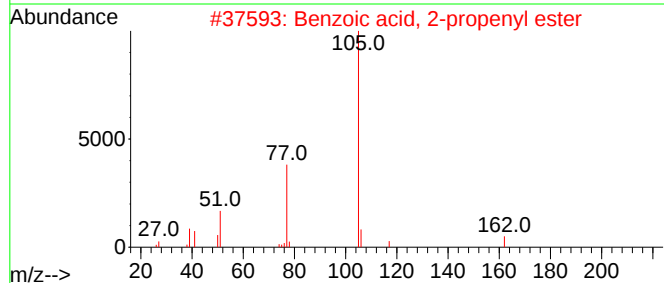
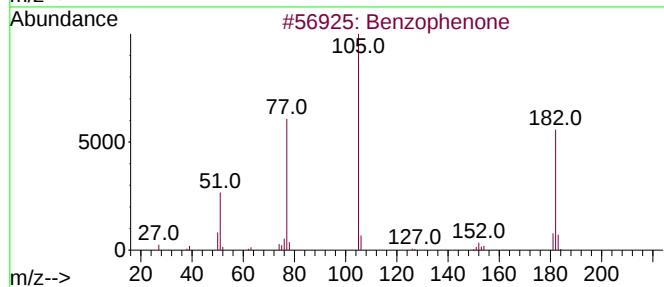
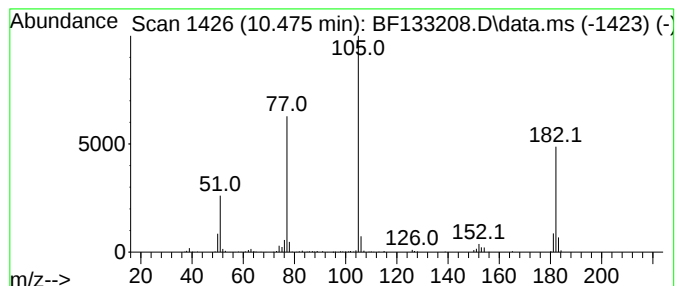
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.34 ng	270970	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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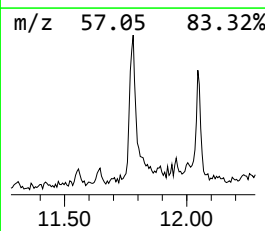
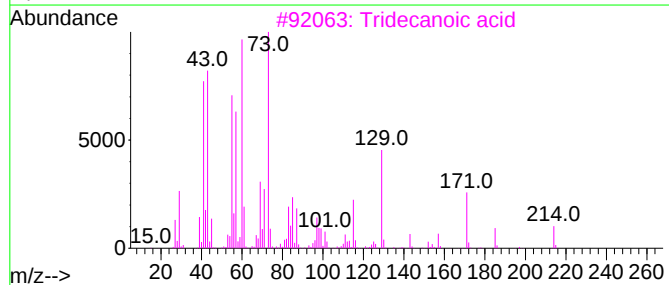
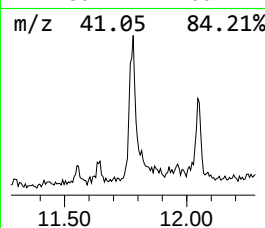
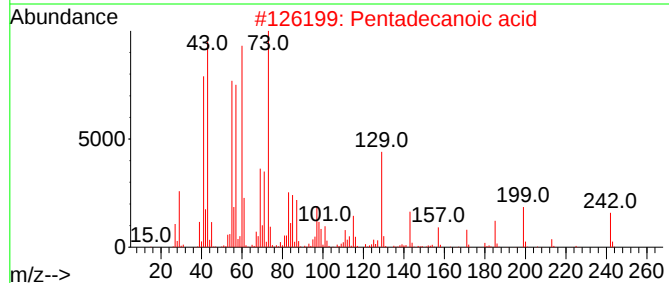
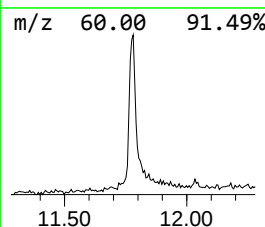
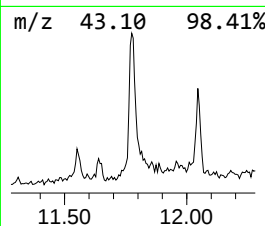
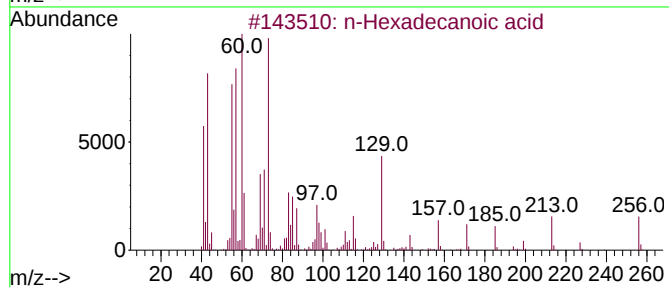
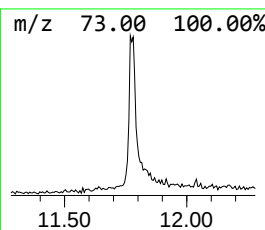
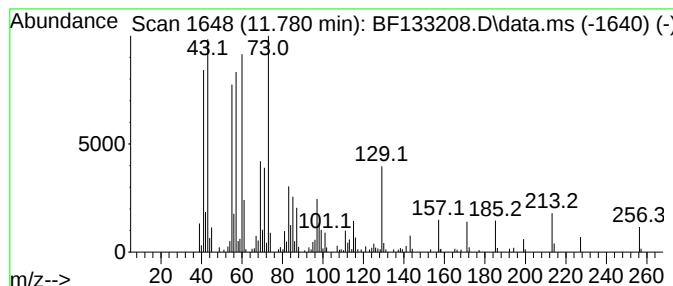
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	5.09 ng	382533	Phenanthrene-d10	11.245

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	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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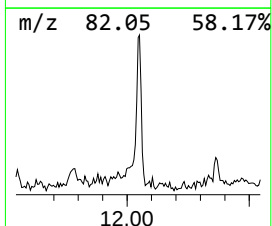
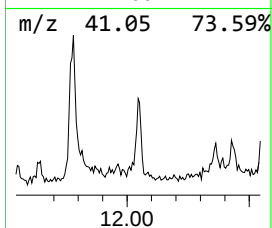
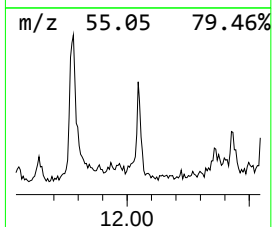
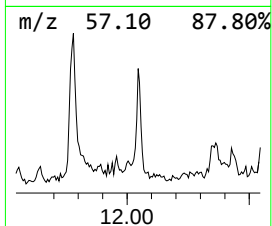
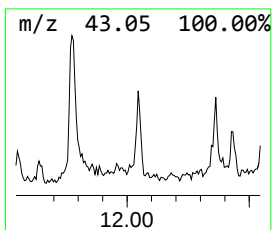
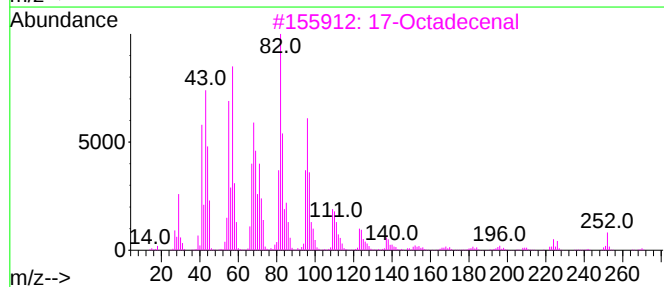
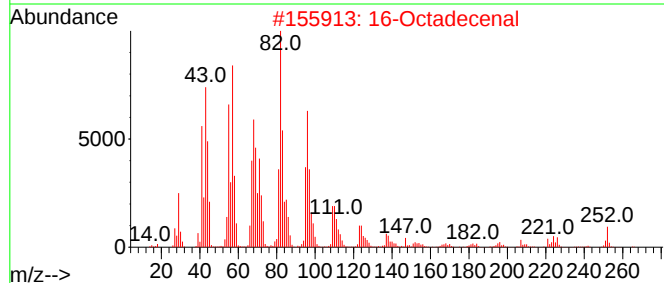
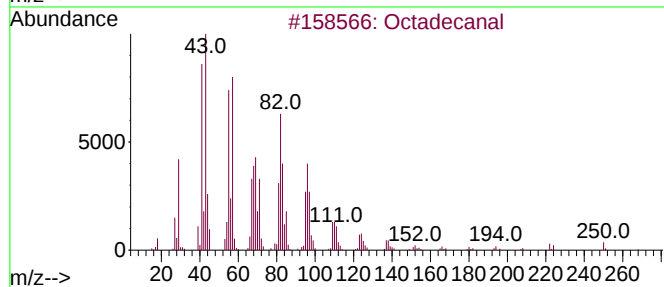
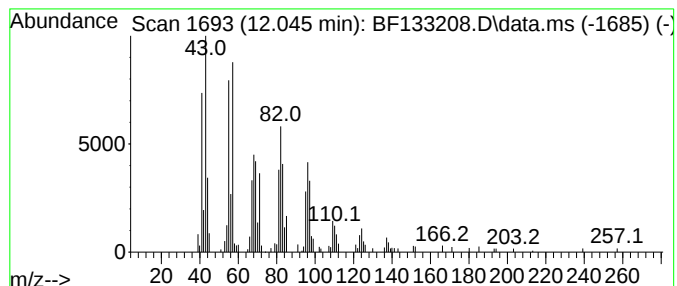
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.045	2.04 ng	153604	Phenanthrene-d10	11.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanal	268	C18H36O	000638-66-4	94
2		16-Octadecenal	266	C18H34O	056554-87-1	91
3		17-Octadecenal	266	C18H34O	056554-86-0	91
4		Hexadecanal	240	C16H32O	000629-80-1	91
5		16-Heptadecenal	252	C17H32O	1010144-57-9	90



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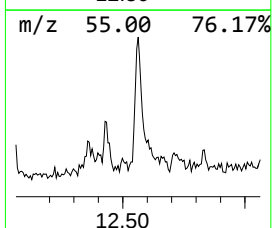
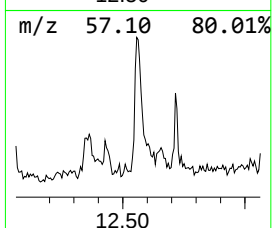
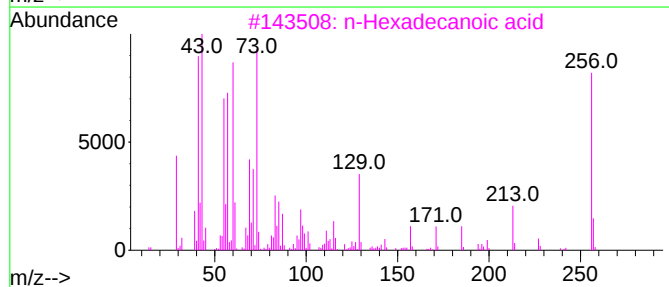
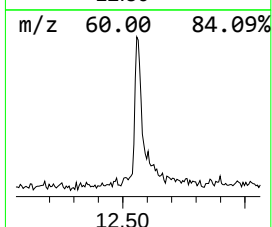
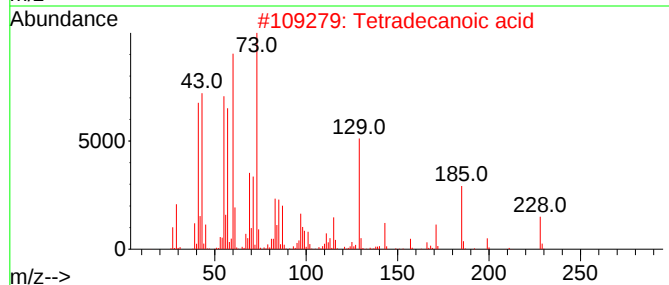
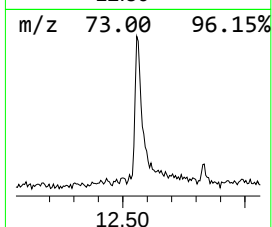
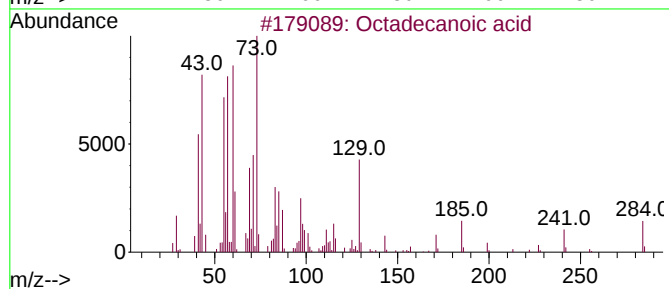
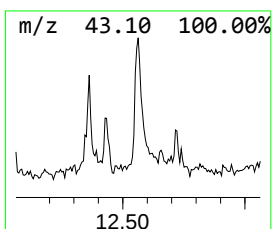
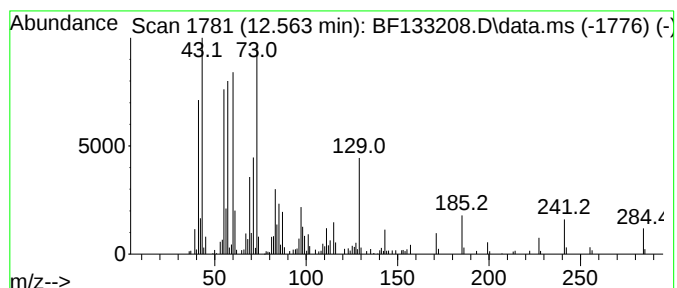
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	6.07 ng	284172	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			n-Decanoic acid	172	C10H20O2	000334-48-5	81



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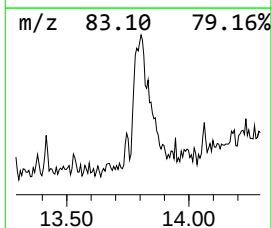
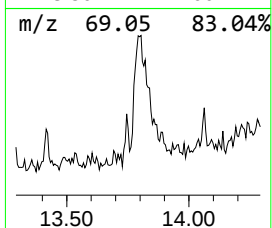
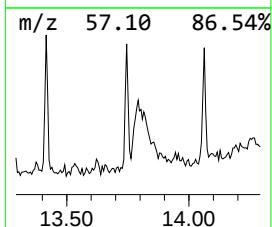
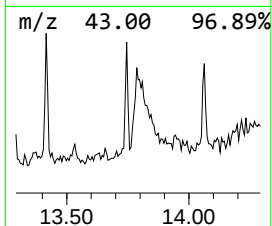
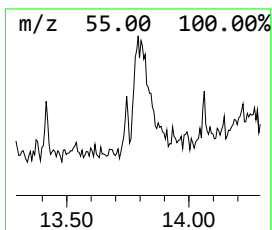
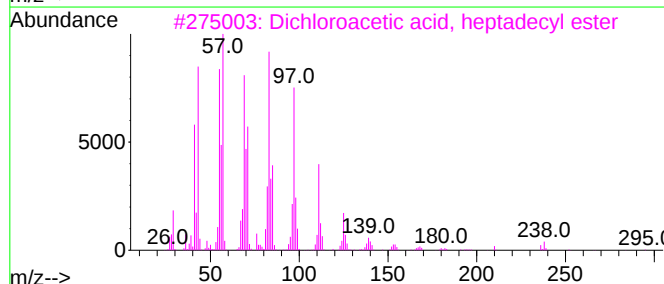
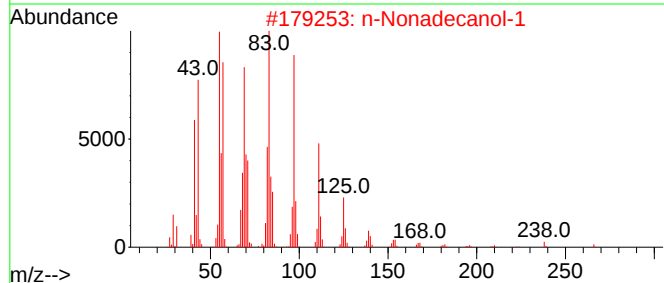
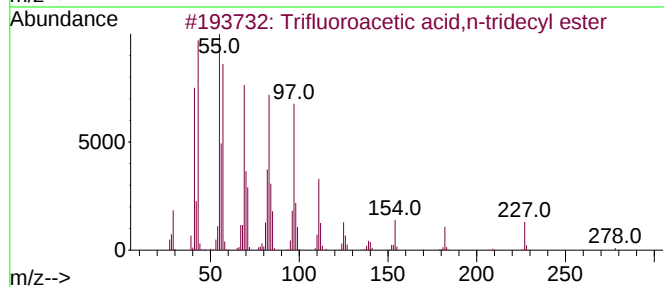
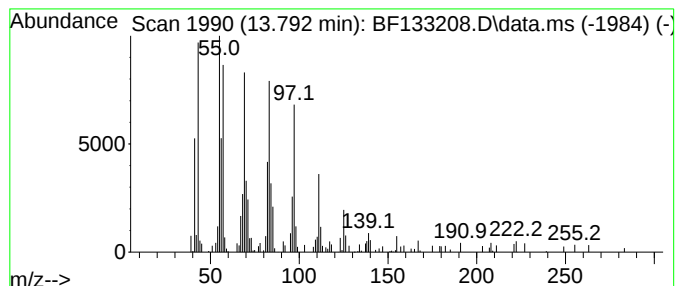
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Trifluoroacetic acid,n-trid... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	5.84 ng	273798	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	91
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
4			Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	87
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87



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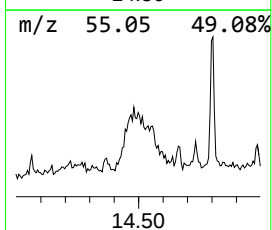
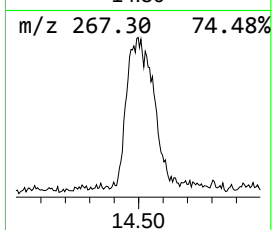
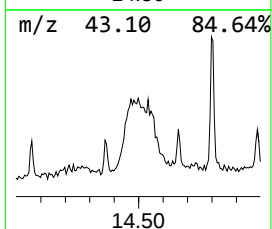
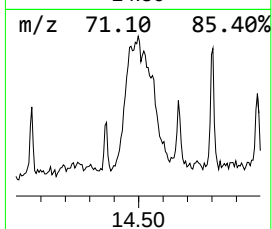
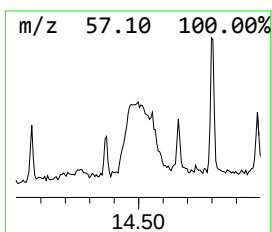
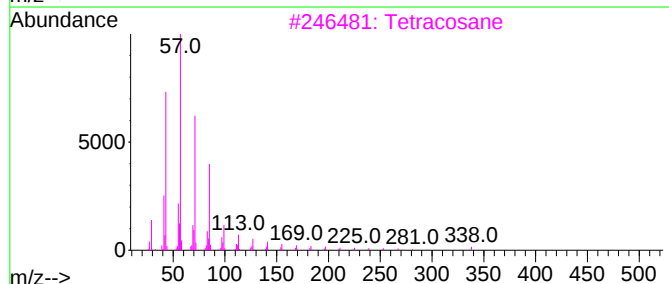
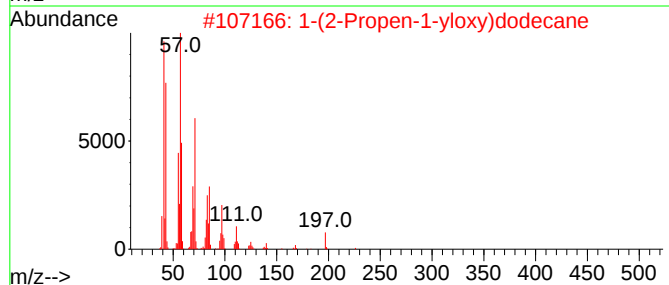
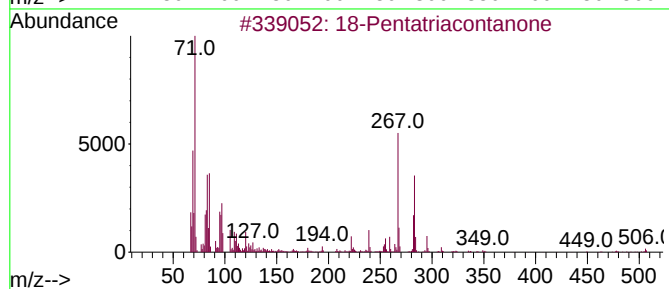
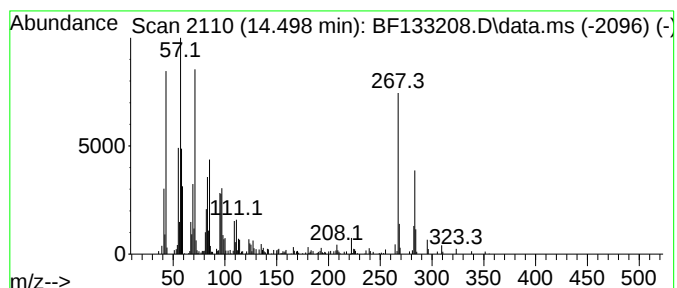
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ClientSampleId :
CF-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 18-Pentatriacontanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.498	27.65 ng	1295150	Chrysene-d12	13.880	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	18-Pentatriacontanone	507	C35H70O	000504-53-0	58
2	1-(2-Propen-1-yloxy)dodecane	226	C15H30O	006145-80-8	38
3	Tetracosane	338	C24H50	000646-31-1	38
4	Heneicosane	296	C21H44	000629-94-7	38
5	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133208.D
Acq On : 03 May 2023 15:40
Operator : CG\JU
Sample : 02583-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-22

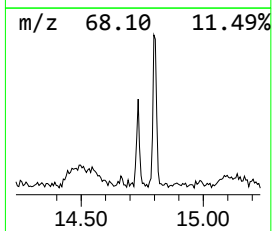
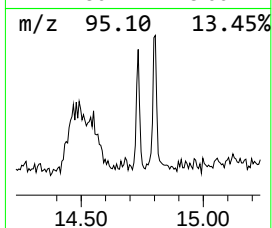
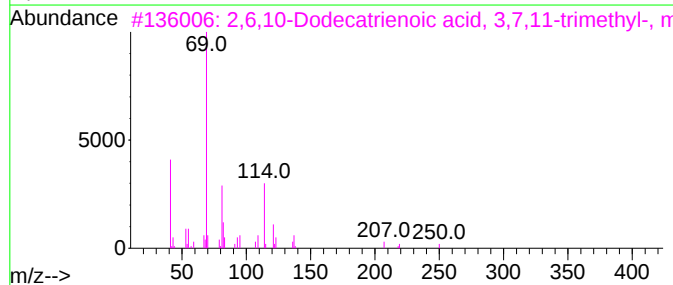
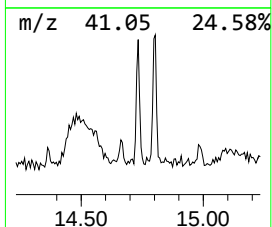
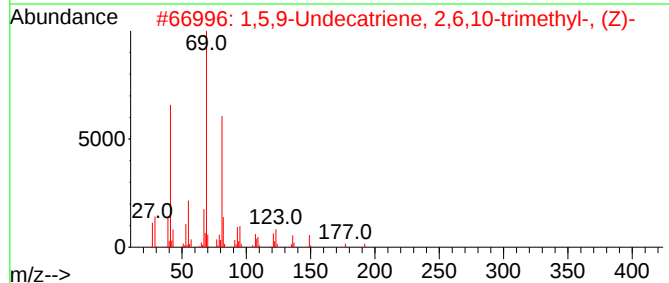
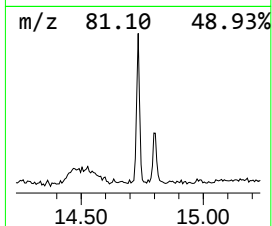
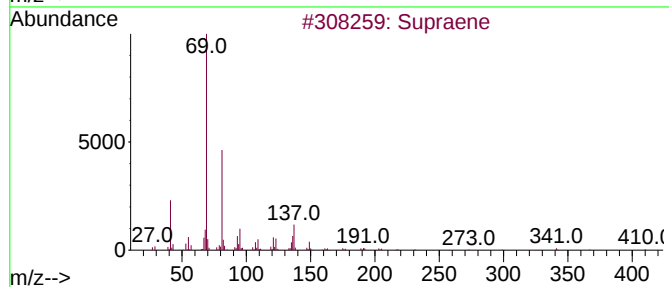
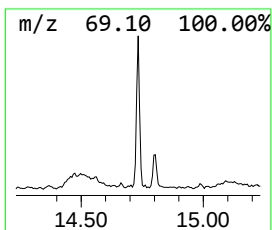
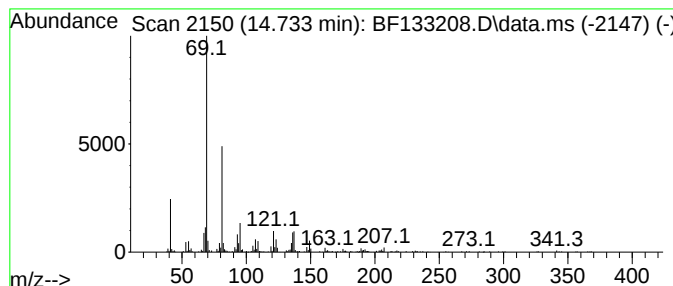
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	3.63 ng	191987	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
3			2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	004176-79-8	59
4			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	53
5			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133208.D
Acq On : 03 May 2023 15:40
Operator : CG\JU
Sample : 02583-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-22

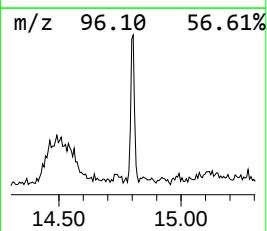
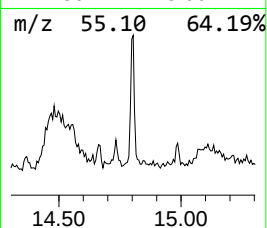
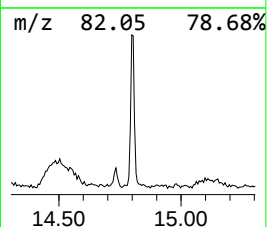
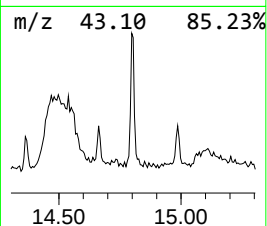
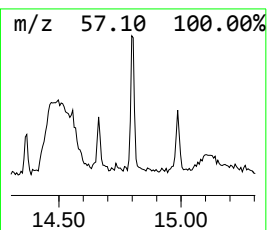
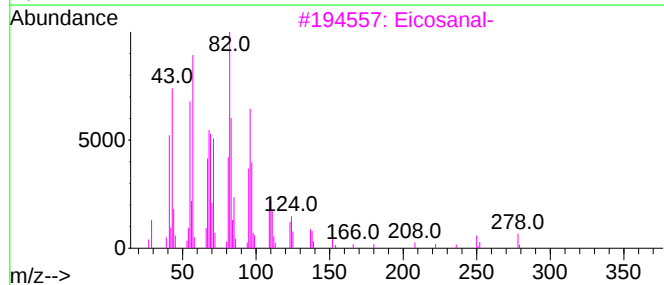
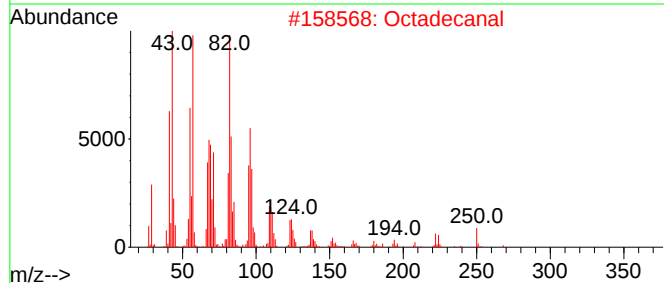
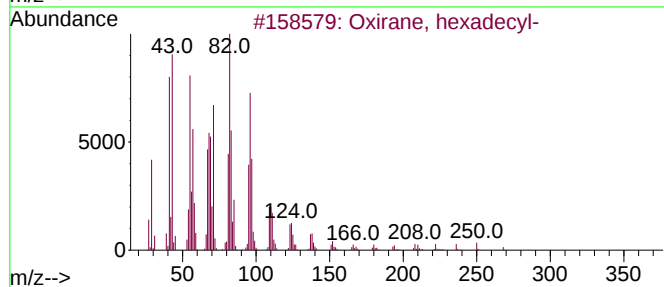
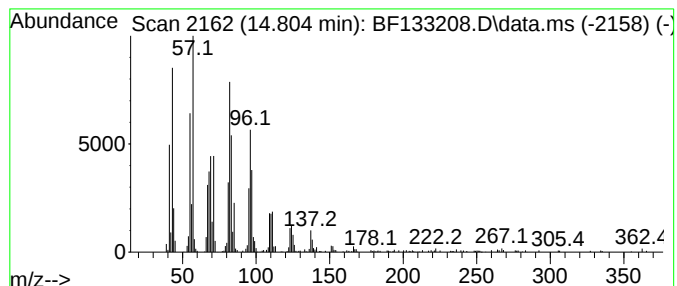
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosanal- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	6.17 ng	326952	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	97
2			Octadecanal	268	C18H36O	000638-66-4	96
3			Eicosanal-	296	C20H40O	002400-66-0	94
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5			Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133208.D
Acq On : 03 May 2023 15:40
Operator : CG\JU
Sample : 02583-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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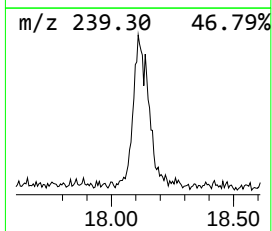
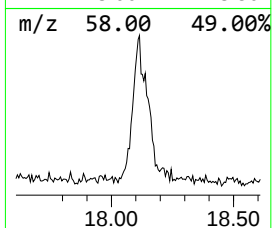
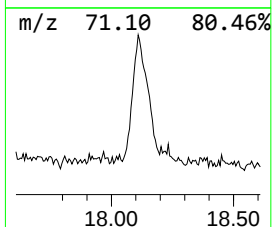
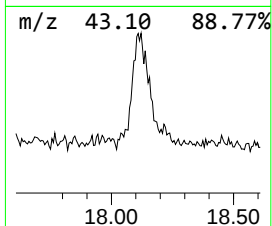
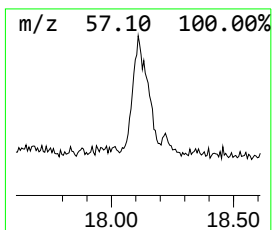
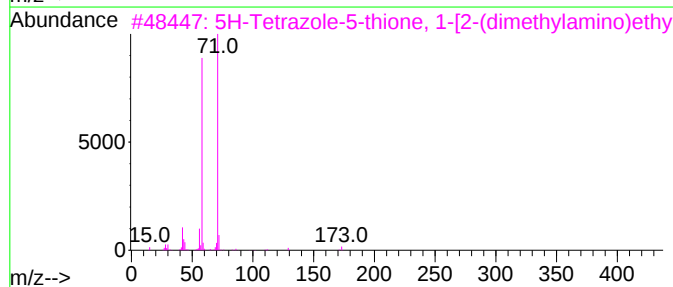
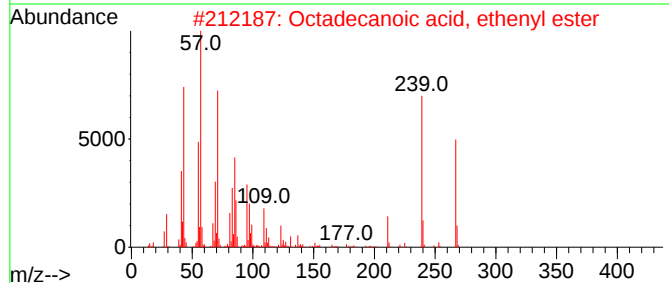
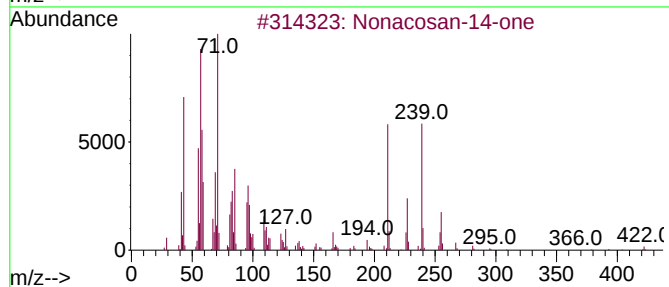
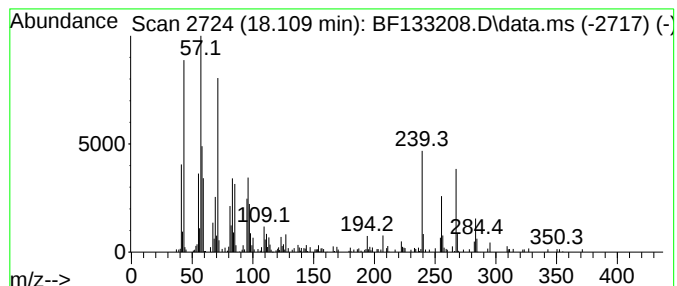
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonacosan-14-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.109	12.02 ng	636523	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonacosan-14-one	422	C29H58O	034394-11-1	52
2		Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	43
3		5H-Tetrazole-5-thione, 1-[2-(dim...	173	C5H11N5S	061607-68-9	22
4		4-Methylheneicosane	310	C22H46	025117-29-7	15
5		2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133208.D
Acq On : 03 May 2023 15:40
Operator : CG\JU
Sample : 02583-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Benzophenone	10.475	3.3	ng	270970	3	9.763	1622590	20.0
n-Hexadecanoic ...	11.780	5.1	ng	382533	4	11.245	1502990	20.0
Octadecanal	12.045	2.0	ng	153604	4	11.245	1502990	20.0
Octadecanoic acid	12.563	6.1	ng	284172	5	13.880	936895	20.0
Trifluoroacetic...	13.792	5.8	ng	273798	5	13.880	936895	20.0
18-Pentatriacon...	14.498	27.6	ng	1295150	5	13.880	936895	20.0
Supraene	14.733	3.6	ng	191987	6	15.304	1059000	20.0
Eicosanal-	14.804	6.2	ng	326952	6	15.304	1059000	20.0
Nonacosan-14-one	18.109	12.0	ng	636523	6	15.304	1059000	20.0