

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
 Data File : BF135144.D
 Acq On : 07 Sep 2023 20:46
 Operator : CG\JU
 Sample : 04256-09
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-8R-4R-9

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rVB	36512	46176	2.13%	0.284%
2	5.004	493	496	506	rVB	38547	47144	2.18%	0.290%
3	5.404	560	564	575	rBV	2294512	2139539	98.90%	13.155%
4	6.416	731	736	755	rVB	2211339	2129459	98.43%	13.093%
5	6.604	765	768	781	rBV	79831	79704	3.68%	0.490%
6	6.769	793	796	800	rBV	771934	612724	28.32%	3.767%
7	7.334	885	892	895	rBV	1541650	1357036	62.73%	8.344%
8	8.051	1010	1014	1017	rBV	970527	802639	37.10%	4.935%
9	9.128	1193	1197	1200	rBV	2558258	2163329	100.00%	13.301%
10	9.245	1213	1217	1220	rBV	31182	29518	1.36%	0.181%
11	9.804	1309	1312	1316	rBV	899845	812472	37.56%	4.995%
12	10.598	1443	1447	1459	rBV	1430863	1267933	58.61%	7.796%
13	10.722	1463	1468	1472	rVV2	33710	44132	2.04%	0.271%
14	11.298	1562	1566	1569	rBV	834390	687286	31.77%	4.226%
15	11.322	1569	1570	1574	rVB	61130	36265	1.68%	0.223%
16	11.839	1654	1658	1663	rBV	349542	344979	15.95%	2.121%
17	12.516	1770	1773	1777	rBV	99869	92398	4.27%	0.568%
18	12.627	1788	1792	1804	rBV	167157	197820	9.14%	1.216%
19	12.745	1807	1812	1815	rVV	88447	80944	3.74%	0.498%
20	12.898	1834	1838	1841	rBV	1692869	1395851	64.52%	8.582%
21	13.327	1909	1911	1916	rBV2	49394	62196	2.88%	0.382%
22	13.368	1916	1918	1923	rVB3	28246	34465	1.59%	0.212%
23	13.445	1928	1931	1934	rVB	47152	36400	1.68%	0.224%
24	13.739	1978	1981	1984	rBV2	64270	66760	3.09%	0.410%
25	13.815	1990	1994	2000	rBV3	89120	129284	5.98%	0.795%
26	13.957	2011	2018	2021	rBV	521970	599165	27.70%	3.684%
27	14.133	2045	2048	2056	rBV4	27012	41545	1.92%	0.255%
28	14.439	2097	2100	2102	rBV2	30113	27293	1.26%	0.168%
29	14.745	2149	2152	2155	rVB2	32627	34640	1.60%	0.213%
30	14.998	2191	2195	2198	rBV	42407	70775	3.27%	0.435%
31	15.080	2206	2209	2215	rBV2	36625	47139	2.18%	0.290%
32	15.357	2254	2256	2261	rVB	31446	41263	1.91%	0.254%
33	15.427	2263	2268	2271	rBV	388834	496735	22.96%	3.054%
34	15.909	2347	2350	2355	rBV2	36550	52347	2.42%	0.322%
35	16.121	2383	2386	2393	rVB7	38544	71731	3.32%	0.441%
36	16.421	2433	2437	2444	rVB3	44114	85160	3.94%	0.524%

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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-BF083023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

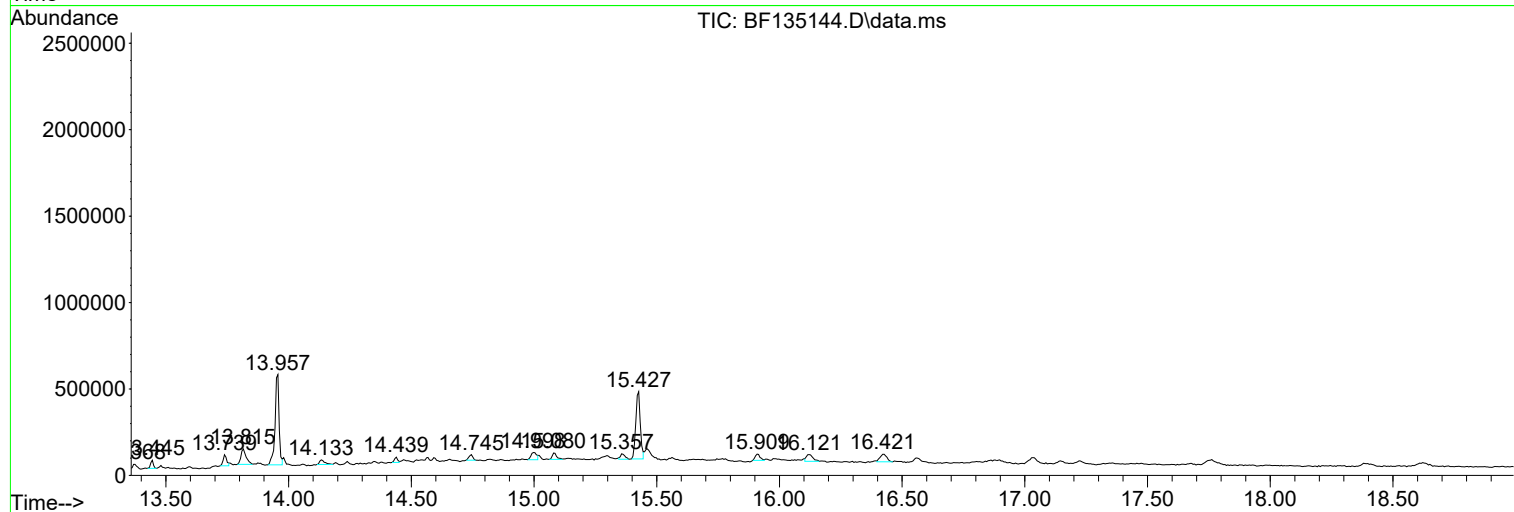
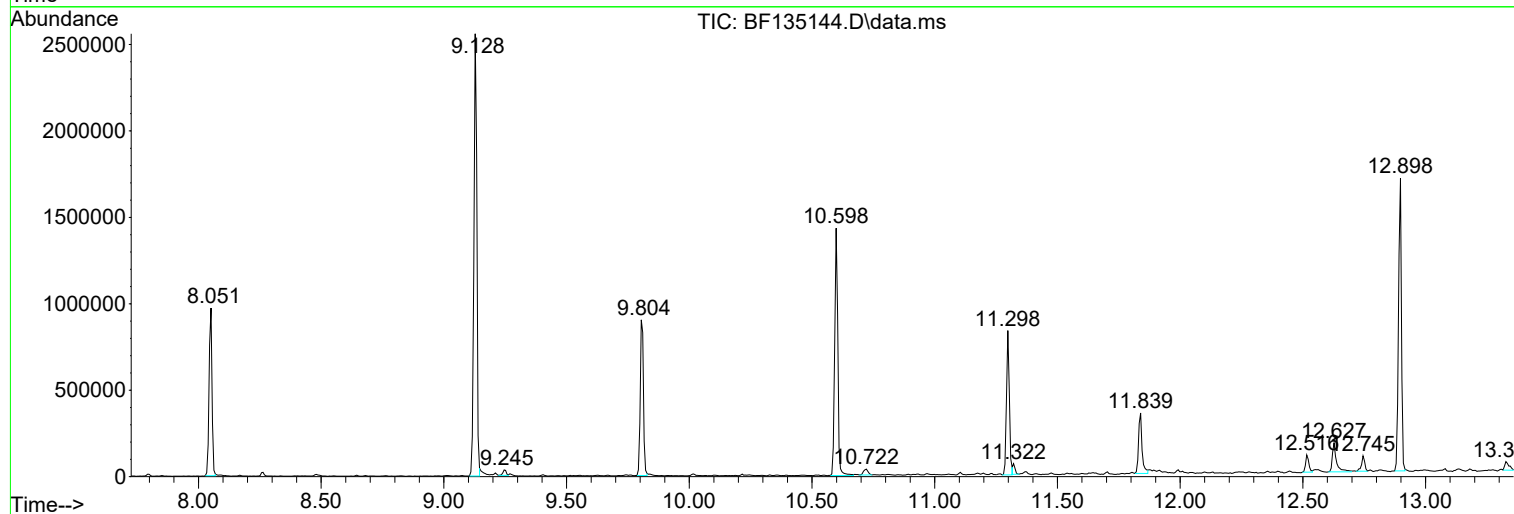
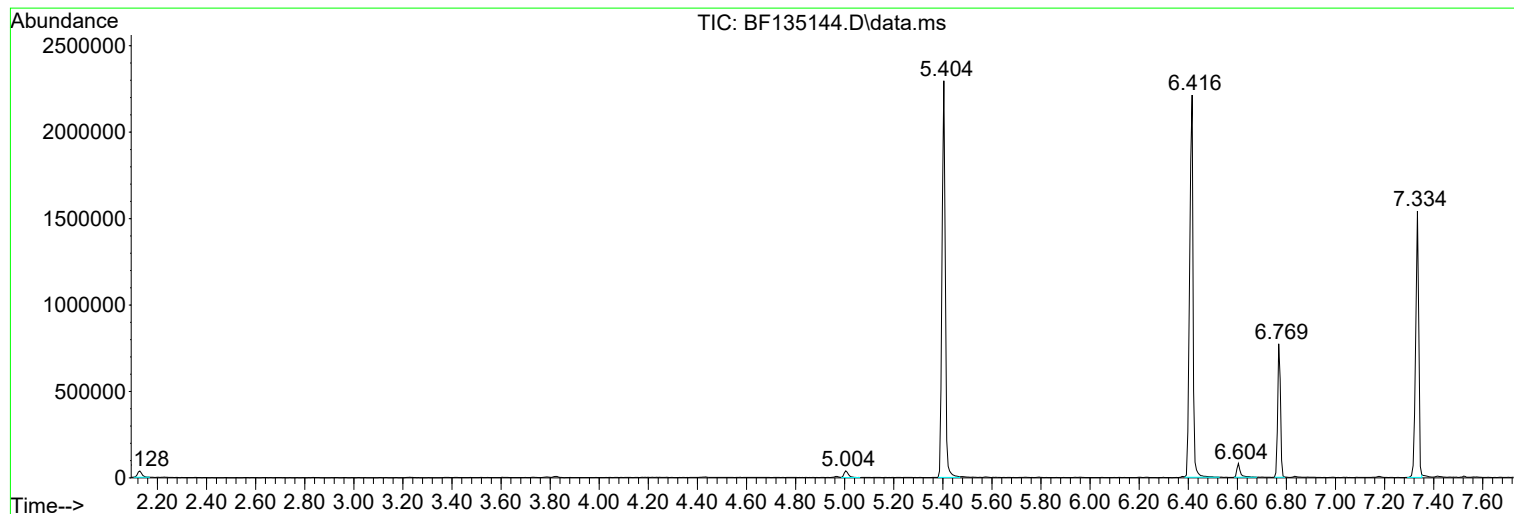
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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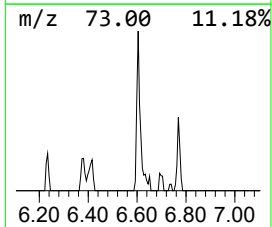
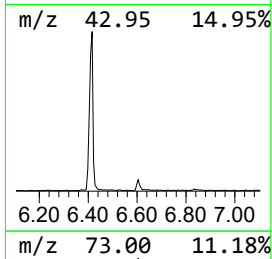
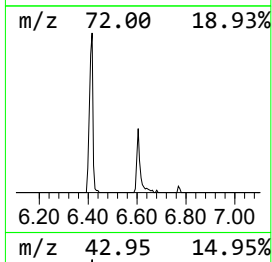
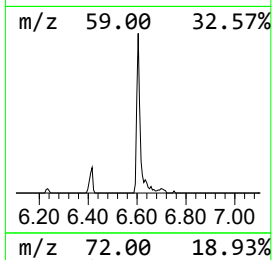
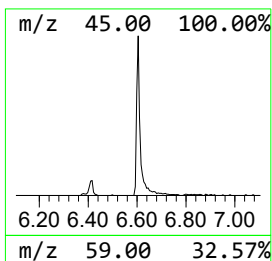
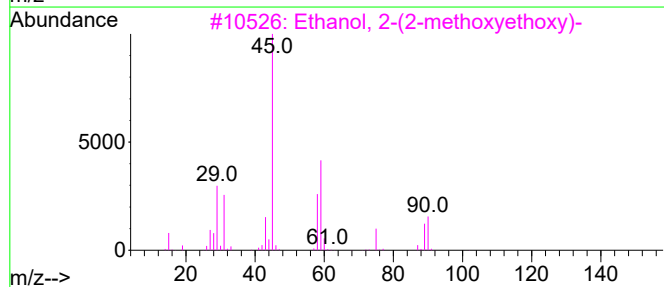
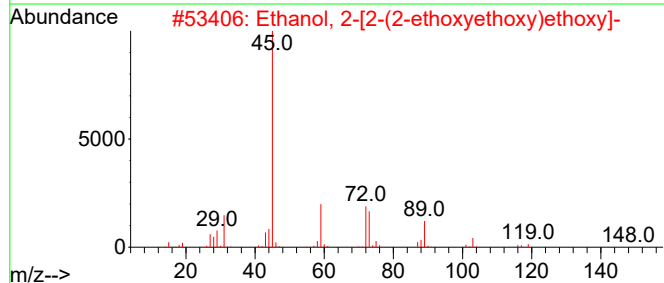
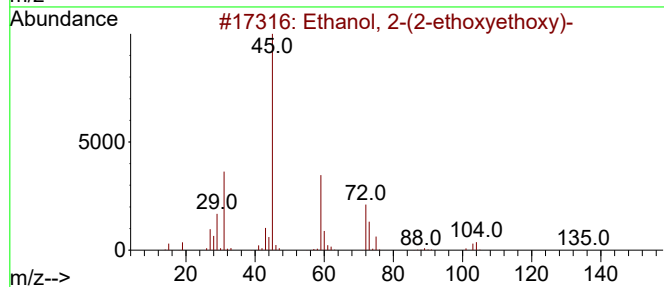
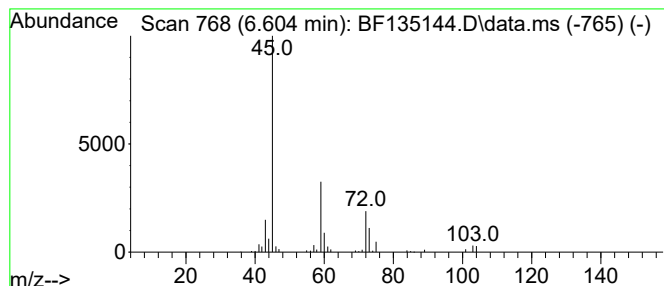
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	2.60 ng	79704	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	72
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4			2-Butanol	74	C4H10O	000078-92-2	45
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39



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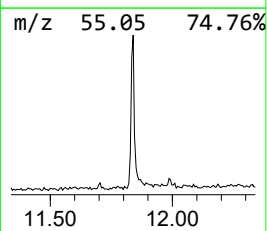
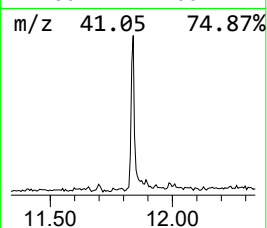
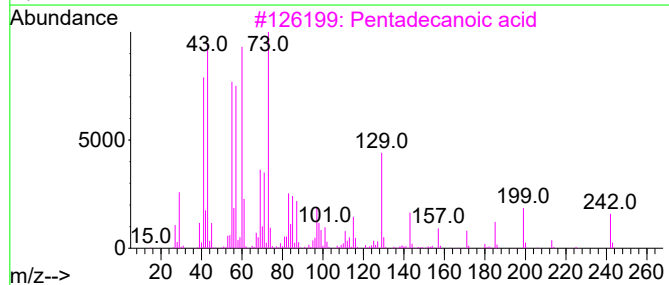
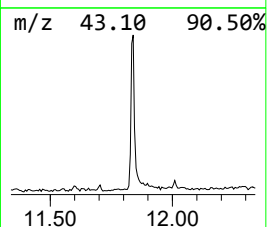
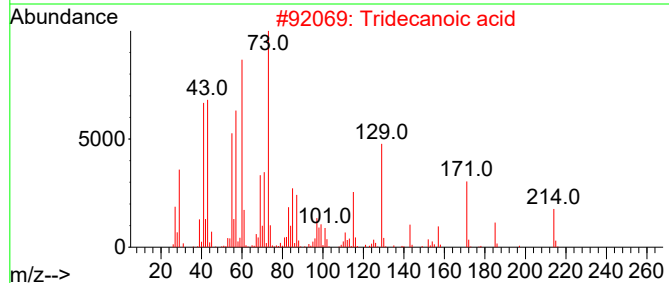
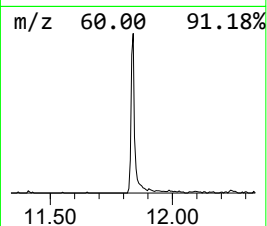
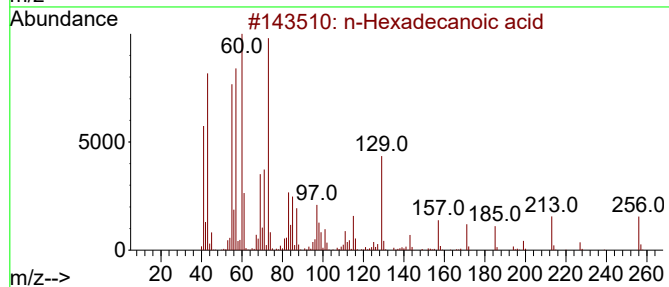
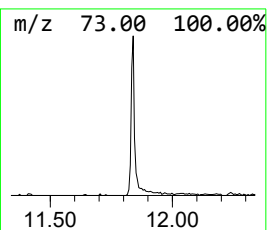
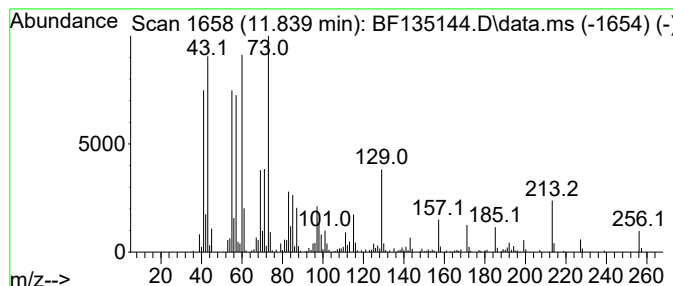
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	10.04 ng	344979	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Undecanoic acid	186	C11H22O2	000112-37-8	91
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	91



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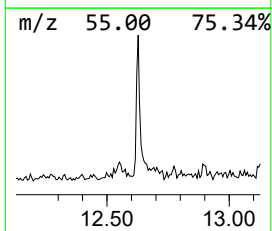
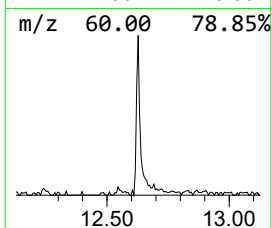
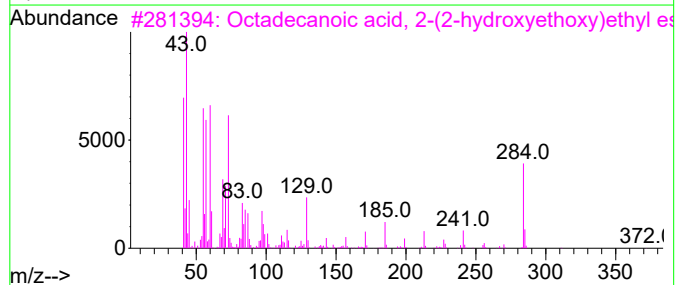
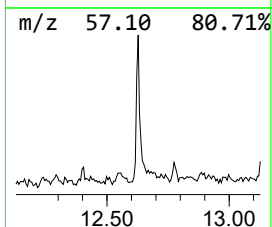
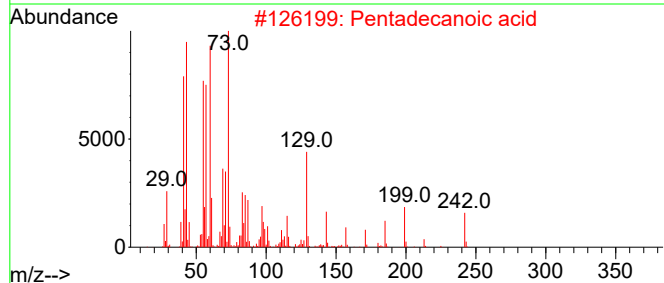
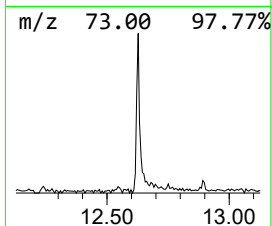
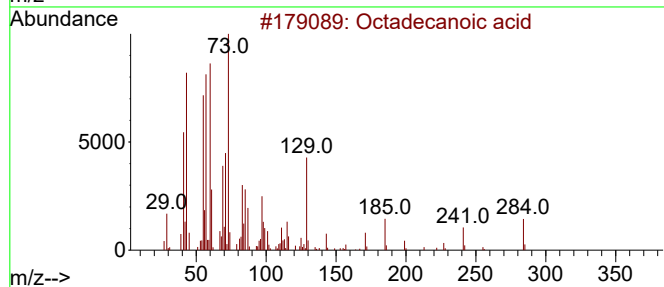
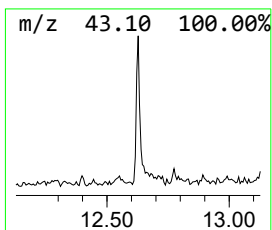
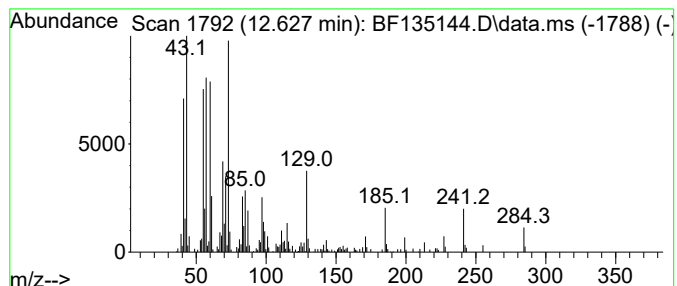
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	6.60 ng	197820	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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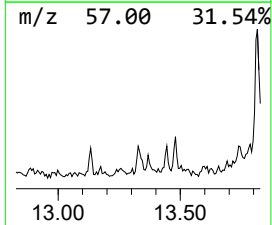
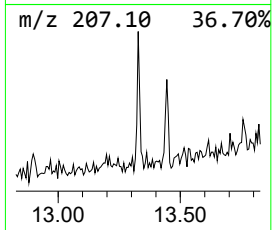
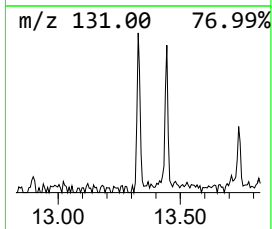
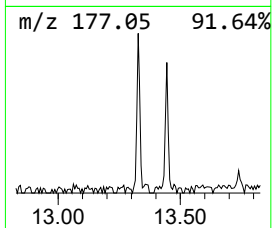
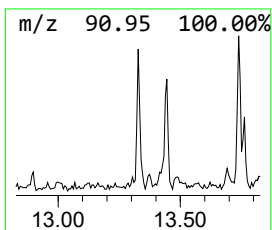
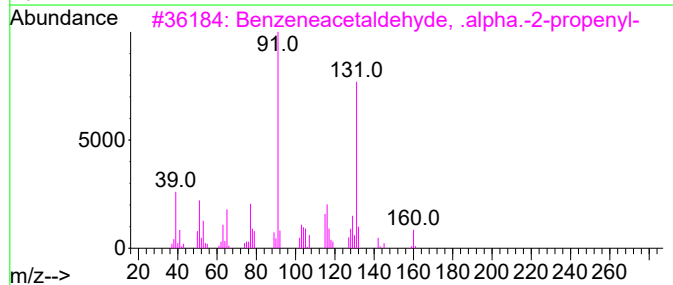
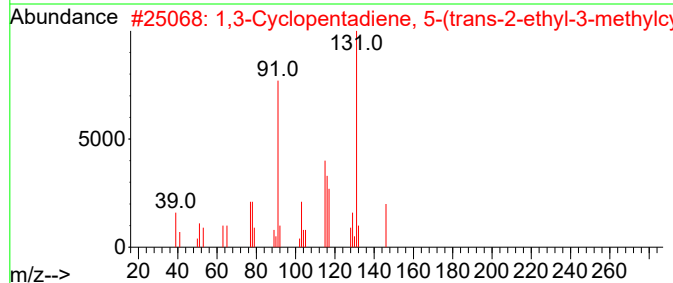
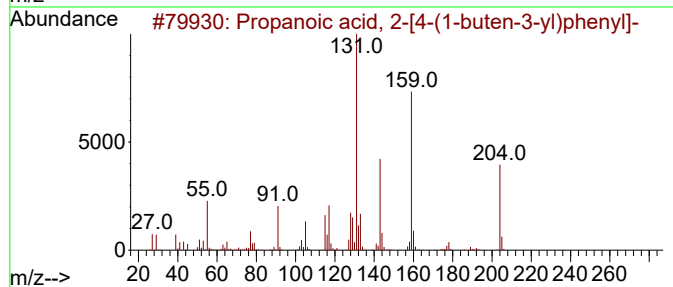
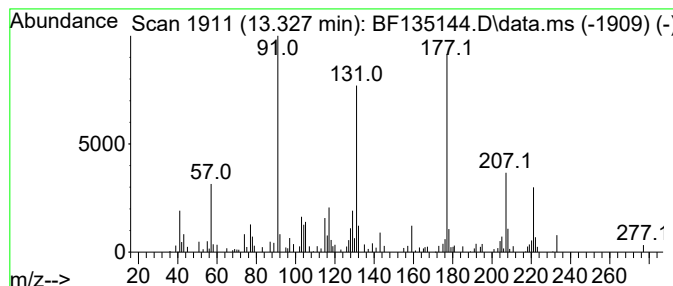
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.327 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.327	2.08 ng	62196	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-[4-(1-buten-3-...	204	C13H16O2	1010162-33-3	30
2			1,3-Cyclopentadiene, 5-(trans-2-...	146	C11H14	079209-36-2	27
3			Benzeneacetaldehyde, .alpha.-2-p...	160	C11H12O	024401-36-3	27
4			3-Chlorotricyclo[5.2.1.0(4,8)]de...	166	C10H11Cl	074876-43-0	25
5			2-Hydroxy-N-(1,2,3,4-tetrahydon...	233	C14H19NO2	1209174-96-8	25



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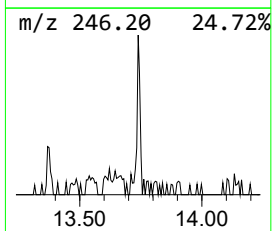
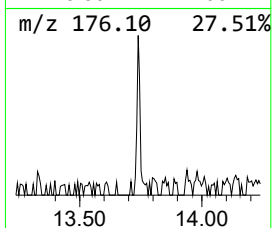
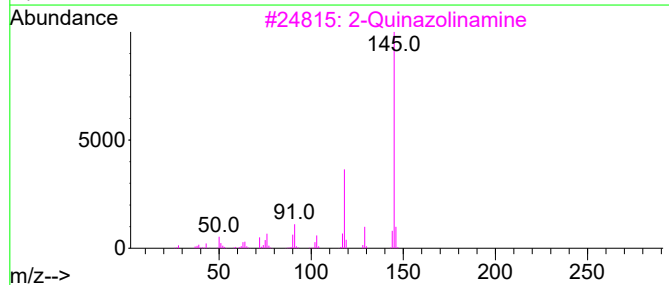
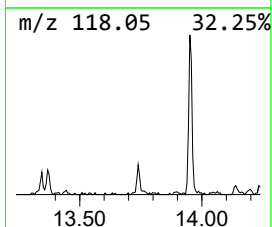
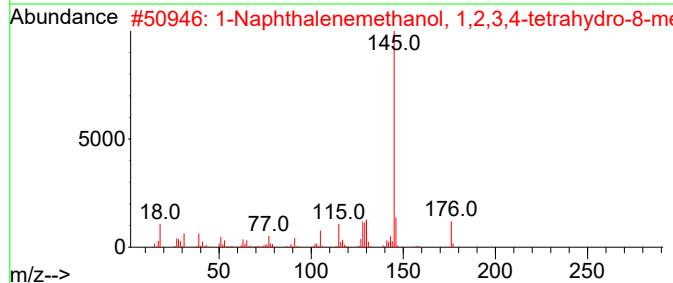
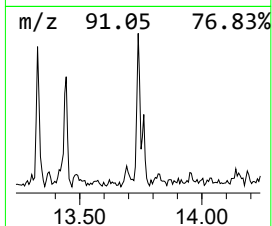
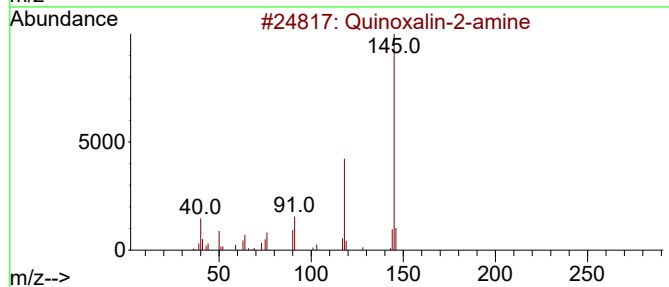
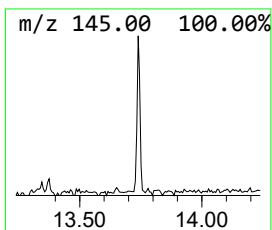
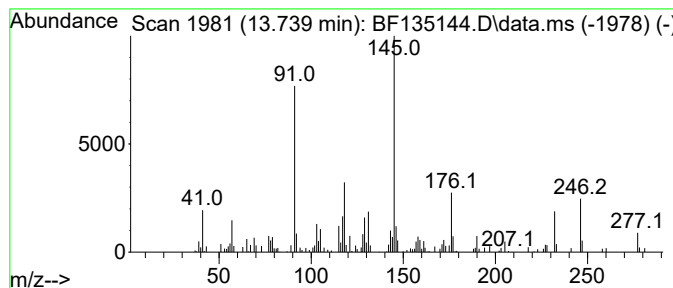
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.739 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	2.23 ng	66760	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Quinoxalin-2-amine	145	C8H7N3	005424-05-5	49
2			1-Naphthalenemethanol, 1,2,3,4-t...	176	C12H16O	036052-28-5	49
3			2-Quinazolinamine	145	C8H7N3	001687-51-0	49
4			Isoquinoline, 2-oxide	145	C9H7NO	001532-72-5	47
5			4-(1H-Imidazol-2-yl)pyridine	145	C8H7N3	021202-42-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
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Acq On : 07 Sep 2023 20:46
Operator : CG\JU
Sample : 04256-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8R-4R-9

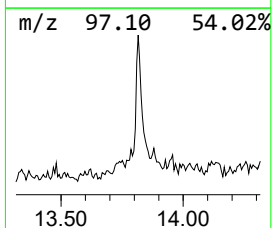
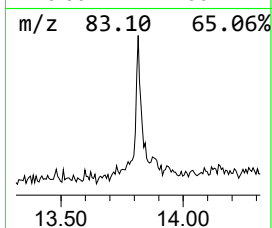
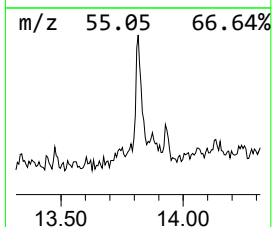
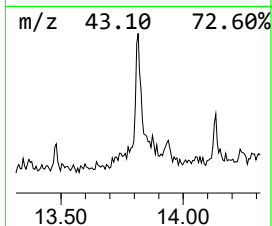
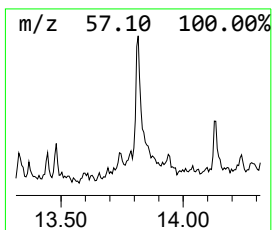
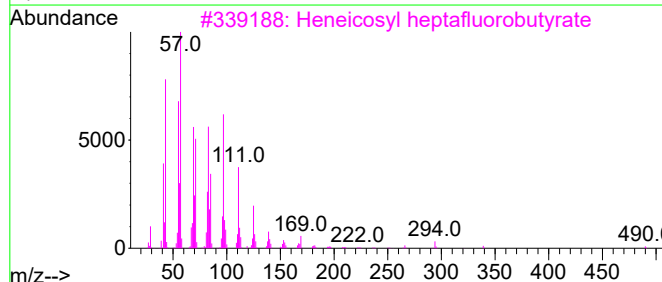
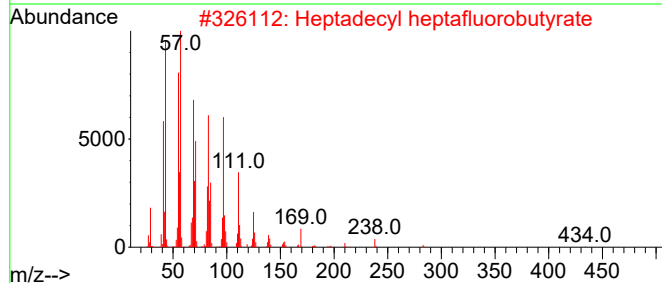
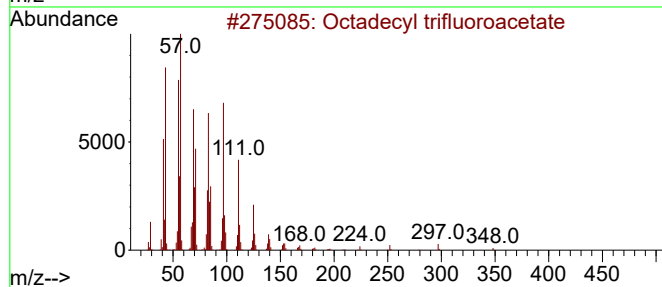
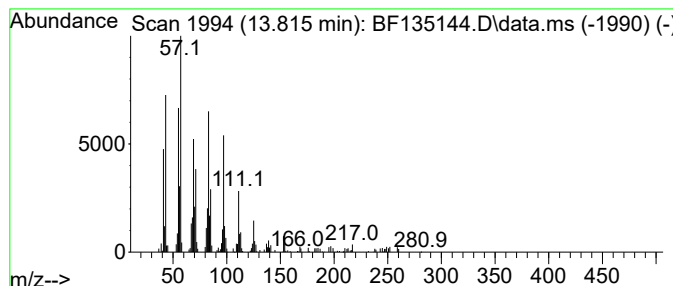
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	4.32 ng	129284	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
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Acq On : 07 Sep 2023 20:46
Operator : CG\JU
Sample : 04256-09
Misc :
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Instrument :
BNA_F
ClientSampleId :
MW-8R-4R-9

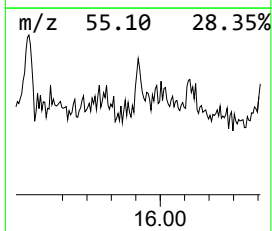
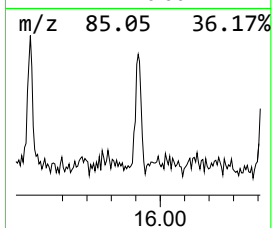
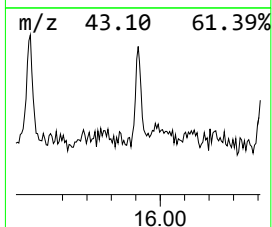
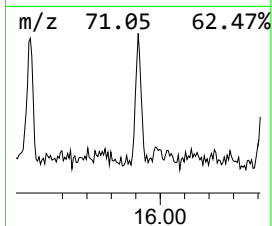
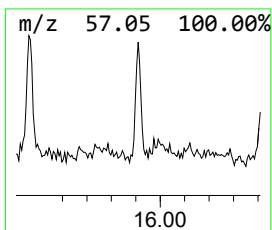
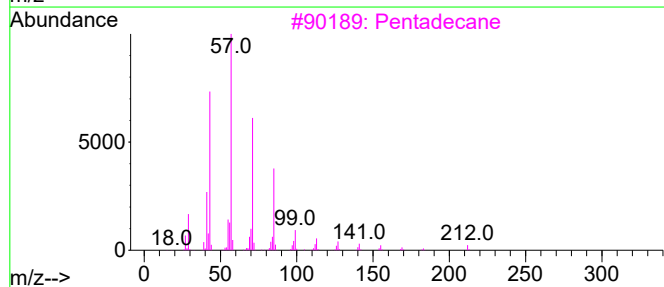
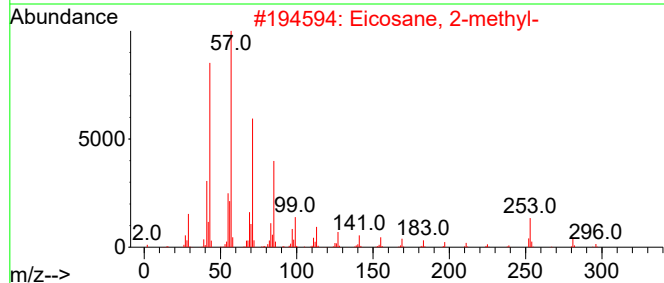
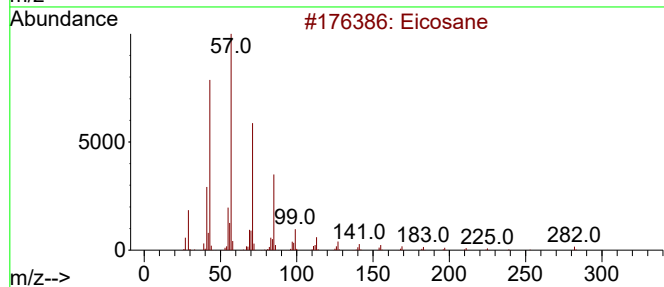
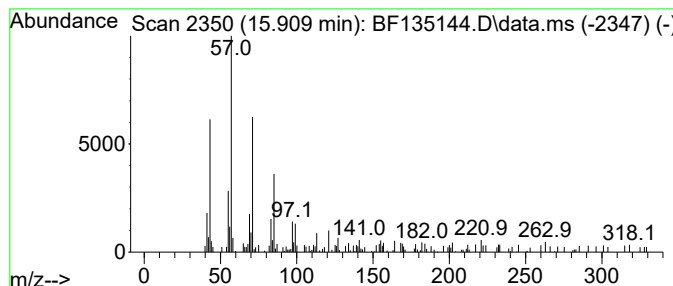
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.910	2.11 ng	52347	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	90
2	Eicosane, 2-methyl-			296	C21H44	001560-84-5	90
3	Pentadecane			212	C15H32	000629-62-9	78
4	Heneicosane			296	C21H44	000629-94-7	78
5	Tridecane			184	C13H28	000629-50-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
Data File : BF135144.D
Acq On : 07 Sep 2023 20:46
Operator : CG\JU
Sample : 04256-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-8R-4R-9

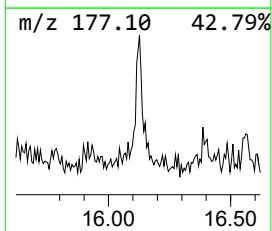
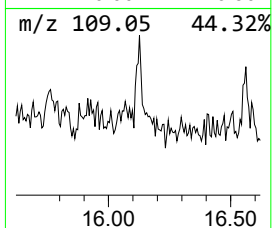
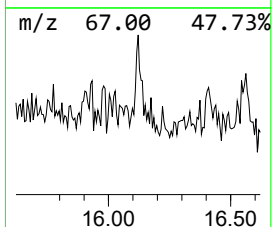
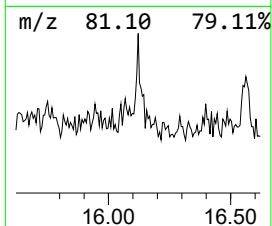
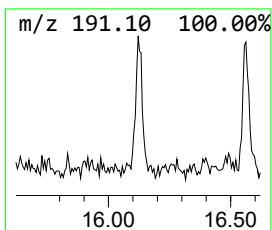
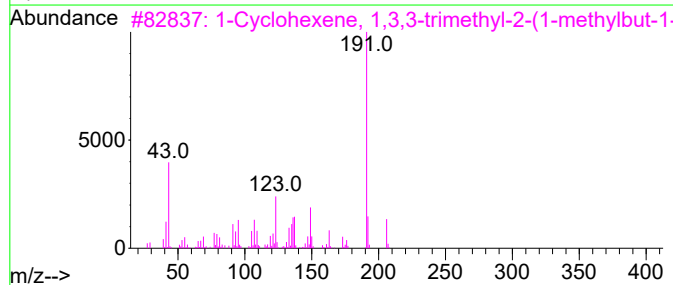
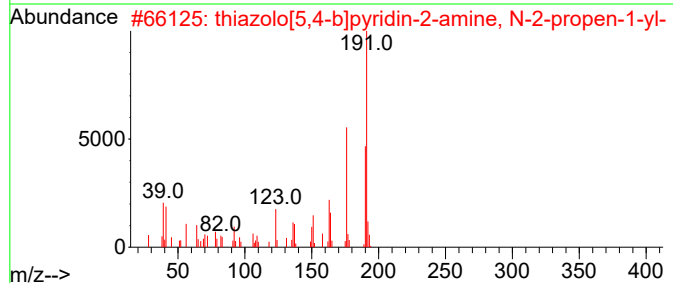
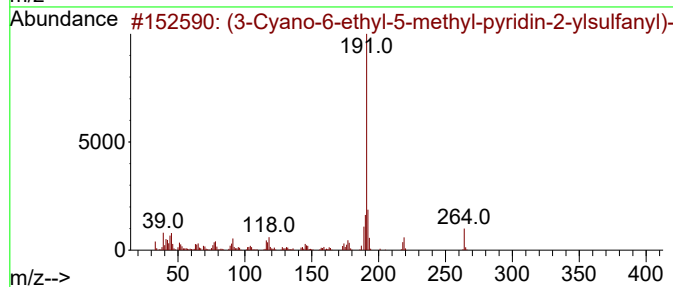
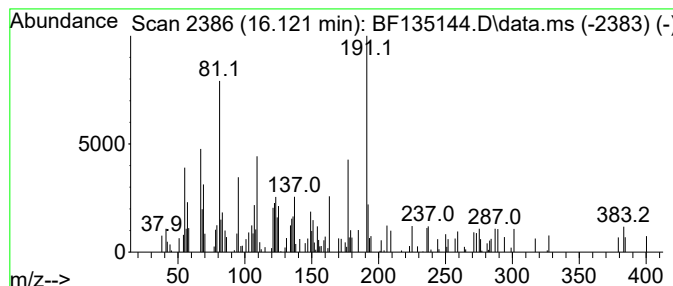
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.121 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	2.89 ng	71731	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(3-Cyano-6-ethyl-5-methyl-pyridi...	264	C13H16N2O2S	1000300-45-4	22
2			thiazolo[5,4-b]pyridin-2-amine, ...	191	C9H9N3S	1000400-23-3	20
3			1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	20
4			3-(5-Fluoro-1,3-dioxo-1,3-dihydr...	237	C11H8FNO4	1000278-27-9	18
5			Anthracene, 9-ethyl-	206	C16H14	000605-83-4	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
Data File : BF135144.D
Acq On : 07 Sep 2023 20:46
Operator : CG\JU
Sample : 04256-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-8R-4R-9

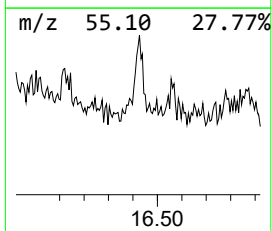
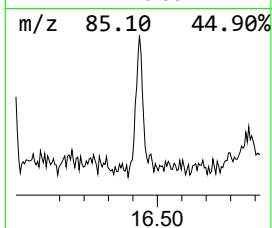
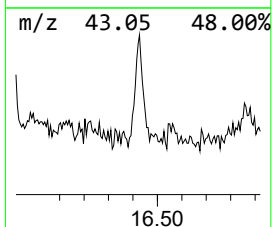
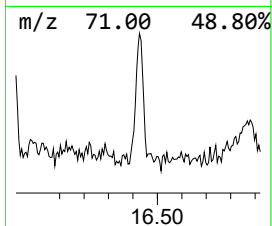
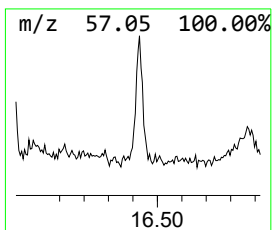
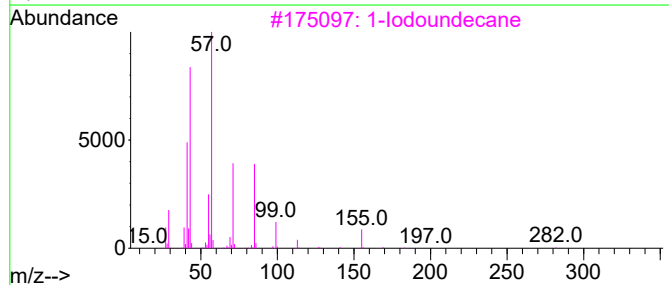
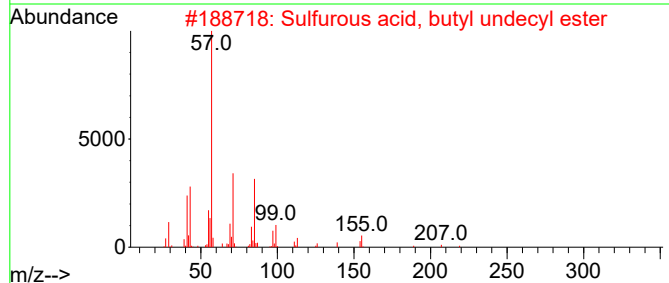
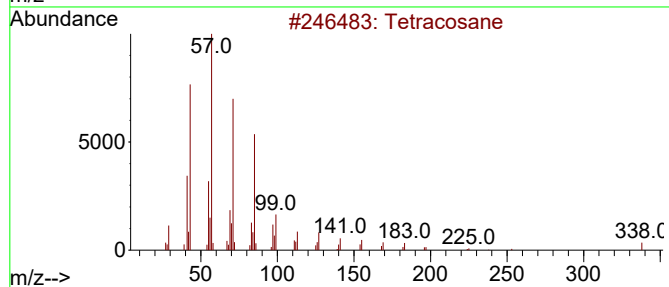
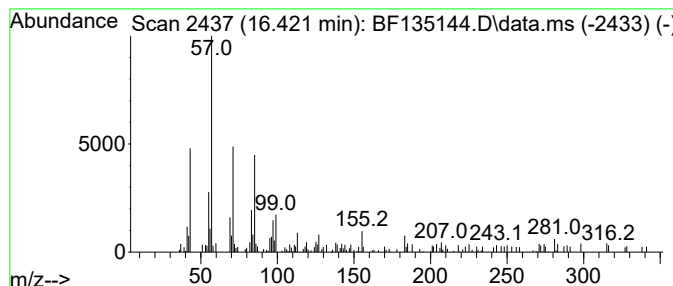
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.421	3.43 ng	85160	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	72
3			1-Iodoundecane	282	C11H23I	004282-44-4	68
4			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	64
5			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
Data File : BF135144.D
Acq On : 07 Sep 2023 20:46
Operator : CG\JU
Sample : 04256-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-e...	6.604	2.6	ng	79704	1	6.769	612724	20.0
n-Hexadecanoic ...	11.839	10.0	ng	344979	4	11.298	687286	20.0
Octadecanoic acid	12.627	6.6	ng	197820	5	13.957	599165	20.0
unknown13.327	13.327	2.1	ng	62196	5	13.957	599165	20.0
unknown13.739	13.739	2.2	ng	66760	5	13.957	599165	20.0
Octadecyl trifl...	13.816	4.3	ng	129284	5	13.957	599165	20.0
Eicosane	15.910	2.1	ng	52347	6	15.427	496735	20.0
unknown16.121	16.121	2.9	ng	71731	6	15.427	496735	20.0
Tetracosane	16.421	3.4	ng	85160	6	15.427	496735	20.0